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LITERATURE STUDY OF THE BIODEGRADABILITY OF CHEMICALS IN WATER

Volume 2. Permutated Index of Chemicals, Microbial Populations, and Wastewater Treatment Systems with Bibliography

by

Franklin Research Center Philadelphia, Pennsylvania 19103

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Project_Officer

Sidney A. Hannah
Wastewater Research Division
Municipal Environmental Research Laboratory
Cincinnati, Ohio 45268

MUNICIPAL ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U. S. ENVIRONMENTAL PROTECTION AGENCY
CINCINNATI. OHIO 45268

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16. ABSTRACT

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Post-1974 literature on wastewater treatment was retrieved by on-line searching of . eight databases. From 1,000 articles critically examined, 600 were used to generate a three-tiered permutated index keyed to, and presented with the 600 article bibliography in Volume 2; the three levels of the index are name of chemical, name of microbe affecting or affected by said chemical, and treatment process involved. These same 600 articles were used to generate separate biodegradable and nonbiodegradable lists of chemicals, on which a successful feasibility study was carried out to create an algorithm to predict biodegradability using only substructural fragments and molecular weight. The results of this study, in Volume 1, indicated 93% accuracy for biodegradables, but only 70% for nonbiodegradables due to the inadequate selection available. Also in Volume 1 is a report on technological advances in wastewater treatment gleaned from the 1,000 documents. In the same section, in tabular format, are references to commercial literature and some journal articles, supplied with this report to EPA, obtained by canvassing Japanese and West German manufacturers in this field. Rounding out Volume 1 is a condensation of abstracts from the 1913-1974 literature dealing only with adverse effects of chemicals on wastewater treatment, also in tabular format; it is intended to complement references to this topic in the permutated index.

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FOREWORD

The U. S. Environmental Protection Agency was created because of increasing public and government concern about the dangers of pollution to the health and welfare of the American people. Noxious air, foul water, and spoiled land are tragic testimonies to the deterioration of our natural environment. The complexity of that environment and the interplay of its components require a concentrated and integrated attack on the problem.

Research and development is that necessary first step in problem solution; it involves defining the problem, measuring its impact, and searching for solutions. The Municipal Environmental Research Laboratory develops new and improved technology and systems to prevent, treat, and manage wastewater and solid and hazardous waste pollutant discharges from municipal and community sources, to preserve and treat public drinking water supplies, and to minimize the adverse economic, social, health, and aesthetic effects of pollution. This publication is one of the products of that research and provides a most vital communications link between the researcher and the user community.

Franklin Research Center has created a permutated index of the world's literature on wastewater treatment over the period 1974-1979. The three items of information which were extracted from nearly all of 600 articles, and used as the main levels of the index, are name of chemical, name of degrading or affected microorganism, and wastewater treatment process. Each entry is keyed to the bibliographic entry from which it derived.

Francis T. Mayo, Director Municipal Environmental Research Laboratory

ABSTRACT

2 -

This report presents an in-depth hierarchical index and bibliography of 600 post-1974 literature references on aqueous biodegradability of chemicals. The companion report, in Volume 1, presents 1) the results of a successful feasibility study for prediction of biodegradability solely from positive or negative values assigned to standard molecular substructural units - also based on these same 600 articles, 2) brief abstracts of post-1974 advances in wastewater treatment technology plus a guide to current Japanese and West German commercial literature in this field, and 3) a listing from the 1913-1974 literature of chemicals with adverse effects on wastewater treatment processes; the effects and original reference are given.

The index is searchable at three levels, 1) chemical name or chemical class, 2) name of microorganism, or type of microbial population, affecting or being affected by the chemical, 3) wastewater treatment process. The process level is very broad in scope, including such concepts as structure-activity studies, operational parameters, inhibition/toxicity studies, review articles, etc., but many true treatment concepts are exploded to allow easier access to specialized technology via the terminology used in the literature. Certain almost omnipresent concepts are retained as third levels of a particular main entry but are suppressed in the permutating process, even if they are the only entry at the third level, and are not directly searchable.

This report was submitted in fulfillment of Contract No. R806699-01 by Franklin Research Center under the sponsorship of the U. S. Environmental Protection Agency. This report covers the period July 15, 1979 to April 30, 1981, and work was completed as of May 15, 1981.

CONTENTS

Forew	ord		•	•			•	•	•	•	•	٠	•		•	•	•	•	•	•	•	•	•	•	•	•	•		•	iii
Abstr	act		•			•		•		•	•	•		•			•				•		•	•	•		•			iv
Ackno	wled	igme	nt			•	•	•	•	•	•	•		•		•	•	•		•	•	•	•		•	•	•	•		vi
	1.	Int	rod	luc	ti	.or	1			•	•	•	•	•		•	•	•	•	•	•		•	•	•		•		•	1
:	2.	Ind	ex	to	t	:he	e E	3ic	ode	∍g1	cac	lal	oi.l	Lit	-y	٥í	= 0	:he	mi	Lca	als	i	ln	Wa	ate	er	•		•	4
	3.	Bib		gr	aŗ	hy	7 t	:0	tł	ne	B:	io	deç	gra	ada	ids	Lli	ĹtΣ	7 0	í	Cì	er	nic	cal	Ls	iı	ı			92

v

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SECTION 1

INTRODUCTION

This report is made up of an in-depth hierarchical index and compilation of bibliographic citations to the biodegradability of chemical substances in water; full-text copies of papers accompany the index and bibliographic citations.

PURPOSE

The in-depth hierarchical index and accompanying compilation of bibliographic citations were created with the intent of providing the sanitary engineer, the environmental chemist, and the microbiologist with a concise and readily accessible source of information on the biodegradation of chemicals associated with wastewater treatment plants.

The online retrieval of pertinent world literature covers the period from 1974-79 as well as articles published during 1970-73 that did not appear in a previously published EPA study in 1974 (NTIS PB-243-825). Foreign language articles are included to emphasize the worldwide interest of this increasing environmental problem.

THE PERMUTATED INDEX

The creation of a three-tiered, hierarchical permutated index affords the separation of critically analyzed information and the reassembly of this information into concise but convenient and practical units. The various hierarchical levels are described below.

NOMENCLATURE

Chemical Nomenclature (First Tier)

The final choice of chemical names appearing in the index represents a third-generation compromise involving utility to professionals of widely diversified chemical background, industrial importance, an awareness of the relative insensitivity of the biodegradability of closely related homologues to the presence of nontoxic substituents, and, finally, the traditional mechanics of permutated index creation.

To facilitate locating a specific chemical of interest, the following explanatory guidelines are offered:

a. Many of the simpler aliphatic compounds were concentrated under

generic names; the exceptions were properly cross-referenced. For example, oxalic acid is listed under Alkanoic acids and derivatives, polybasic; whereas adipic acid, found as a separate entry, is additionally listed as a "See Also" under Alkanoic acids and derivatives.

b. Significant subclasses within traditional major organic headings were accorded major-heading status as exemplified by:

Alcohols, tertiary aliphatic Amines, poly-, aliphatic Benzenesulfonic acid, non-linear alkyl, long chain

- c. The major benzene derivatives appear as a condensed separate entry under the common or familiar name, such as Aniline and derivatives, Phenol and derivatives, Xylenes and derivatives, and Benzoic acid and derivatives.
- d. Aromatic compounds having more than one common functional group and not sharing a common name are indexed under more than one appropriate entry to facilitate locating them. Where feasible, polyfunctional benzenes have been indexed under the common name indicating the greatest number of substituents.
- e. Specific pesticides are listed as cross-references under the general major heading of Pesticides; herbicides are subclassified by tradename type under the heading of Herbicides.
- f. Surfactants are subclassified and listed as to respective appropriate ionic type and are additionally referred to the specific main chemical class heading.
- g. Acronyms, such as PCB and PVA, are referenced to their respective complete generic name.
- h. Extensive cross-indexing is included to assist the investigator to locate readily the probable source(s) of desired information.

Microbial Population (Second Tier)

The microbial populations responsible for the biodegradation of the chemical substances make up the second level of the permutated index. Major classes of these microbial populations, created to facilitate designation of the system with the major role in the biodegradation process, are as follows:

- a. Activated sludge, either without qualification (where none was indicated in the original text) or with terms to provide an added dimension to describe the specific source and/or some process as it appeared in the original study.
- b. Microbial population, mixed, again either without qualifications or with descriptive terms designating the natural residence of these populations.

- c. Microbial populations as pure cultures, which for purposes of convenience and brevity are identified solely by their respective genera. No further identification by species or strain is indicated in the index, although this information in many instances does appear in the full-text copy of the original paper.
- d. Microbial populations that are significant but used less, such as sewage (either natural or synthetic) and lagoons.

Wastewater Treatment Processes (Third Tier)

The third tier of the permutated index is concerned with the major significant biological wastewater treatment processes. Included are physical and biochemical processes encompassing aerobic and anaerobic biodegradation, metabolic pathways (without identification of the respective metabolites), operational parameters of the processes, as well as kinetics of the biodegradation process. In addition, information pertinent and salient to each respective study may be included to provide accessibility of this specific information to an interdisciplinary group to whom this index is of use and interest. Since this information is specific and self-limiting in its scope to each respective study, it is not permutated against the first and second tiers.

In contrast, headings of major interest and importance to overall interdisciplinary groups (such as structure-activity relationships, review articles, sludge acclimatization processes, inhibitory/toxic effects with or without appropriate parameters as preservatives, pH effect, nutritional effects, etc.) are permutated against both the chemicals (first tier) and microbial populations (second tier).

In conclusion, it is hoped that the permutated index will, indeed, provide a useful source of information presented in a logical, readily accessible form.

SECTION 2

INDEX TO THE BIODEGRADABILITY OF CHEMICALS IN WATER

Abienc acid and derivatives	Achromobacter sp (cont a)	Achromopacter sp (cont a)
Activated sludge	Alkanoic acids and derivatives,	Model ecosystem, terrestrial, natural
Aerobic biodegradation, 289	polybasic, 118	545
Detoxification, 349	Metabolic pathways, 41, 67	Polyethylene glycols, fatty ester
Lagoons, aerated, industrial site	Alkanoic acids, cyclic	Aerobic biodegradation, 431
349	Metabolic pathways, 41	Polyethylene glycols, fatty ether
Structure-activity relationships	Alkenes	Aerobic biodegradation, 431
289	Inhibitory (toxic) effects, 450	Pyrocatechol and derivatives
Lagoons, aerated, industrial site	Structure-activity relationships, 450	
Aerobic biodegradation, 215	Alkenoic acids and derivatives	Metabolic pathways, 41, 67
Detoxification, 215	Metabolic pathways, 41	Model ecosystem, aquatic, simulated 378
Acetobacter sp	Alkyl sulfates, long chain, 442	Sulfanilic acid and derivatives
Alcohols, primary aliphatic	Amides, aliphane, 118	
Identification of microorganisms	•	Identification of microorganisms
164	Inhibitory (toxic) effects, 38	377
Aldehydes		Timber steam processing wastes
Identification of microorganisms	Amines, poly-, aliphatic, 118	Aerobic biodegradation, 408
164		Identification of microorganisms
	Operational parameters, 464	408
Acetophenone and derivatives	Arsenic compounds, organic	Operational parameters, 408
see also Ketones	Operational parameters, 464	Xylenois and derivatives
Arthrobacter sp	Benzene and derivatives	Model ecosystem, terrestrial, natural
Inhibitory (toxic) effects, 84	Metabolic pathways, 67	545
Isolation of enzymes. 84	Benzoic acid and derivatives	4
Metabolic pathways, 84	Metabolic pathways, 41, 67	Acinetobacter sp
Pseudomonas sp	Cirrasols	Alcohols, primary aliphatic
Psychrophilic temperature effect	Aerobic biodegradation, 431	Identification of microorganisms
250	Cresols and derivatives	560
Time-course kinetics, 250	Model ecosystem, terrestrial, natural.	Metabolic pathways, 244
Achromobacter sp	545	Respirometric studies, 560
Adipic acid and derivatives, 118	Crude oil	Alkanes
Metabolic pathways, 41	Mesophilic temperature, effect	Inhibitory (toxic) effects, 450
Alcohols, alicyclic	567	Metabolic pathways, 232
Inhibitory (toxic) effects, 38	Psychrophilic temperature effect	Structure-activity relationships
Metabolic pathways, 41	567	450
Alcohols, primary aliphatic	Cycloaliphatics, substituted	Alkanes, cyclic
Identification of microorganisms	Inhibitory (toxic) effects, 38	Metabolic pathways, 232, 522
164, 303	Metabolic pathways, 41	Structure-activity relationships
Metabolic pathways, 303	Herbicides, chlorpropham type	522
Aldehydes	Phorate inhibitory activity, 257	Alkanes, long chain, branched
Identification of microorganisms	Herbicides, silvex type	Mesophilic temperature, effect
164	Model ecosystem, aquatic, simulated.	567
Alkanes	378	Metabolic pathways, 522
Inhibitory (toxic) effects, 450	Heteroaromatics and derivatives, dicyclic	Psychrophilic temperature effect
Metabolic pathways, 67	Metabolic pathways, 41	567
Structure-activity relationships	Ketones, aliphatic	Structure-activity relationships
450	Inhibitory (toxic) effects, 38	522
Alkanes, long chain, branched	Metabolic pathways, 41	Alkanes, long chain, linear
Mesophilic temperature, effect	Mercury, inorganic, 498	Metabolic pathways, 86, 232
567	Phenol and derivatives	522
Psychrophilic temperature effect	Identification of microorganisms	Structure-activity relationships
567	71	522
Alkanoic acids and derivatives	Metabolic pathways, 67	Alkanoic acids and derivatives
Metabolic pathways, 41, 67	Model ecosystem, aquatic, simulated,	Metabolic pathways, 244

cinetobacter sp (cont'd)	Acinetobacter sp (cont'd)	Activated studge
Alkanoic acids and derivatives, long	Starch and derivatives	Abietic acid and derivatives Aerobic biodegradation, 289
chain	Identification of microorganisms	Detoxification, 349
Metabolic pathways, 86, 522	406	Lagoons, aerated, industrial site
Structure-activity relationships	Sugars and derivatives	349
522	Metabolic pathways, 522	Structure-activity relationships
Alkanoic acids and derivatives,	Structure-activity relationships	289
polybasic	522	
Metabolic pathways, 244	Thiophenois	Alcohol distillery wastes
Alkenes	Metabolic pathways, 542	Anaerobic digestion reactor, 449
Inhibitory (toxic) effects, 450	Toluene and derivatives	Alcohols, alicyclic
Metabolic pathways, 232, 522	Metabolic pathways, 232	Aerobic biodegradation, 386
Structure-activity relationships	Vibrio sp	Identification of microorganisms 38
450, 522	Metabolic pathways, 550	Inhibitory (toxic) effects, 38
Alkenoic acids and derivatives, long	Xylenes and derivatives	Metabolic pathways, 39
chain	Metabolic pathways, 232	Structure-activity relationships
Metabolic pathways, 522	4	386
Structure-activity relationships	Acremonium sp	Alcohols, benzylic
522	Polyethylene	Respirometric studies, 30
Amino acids and derivatives	Isolation of microorganisms, 4	Structure-activity relationships
Metabolic pathways, 522, 542	Achromobacter-alcaligenes sp	153, 473
Structure-activity relationships	Oil refinery wastes, 40	Alcohols, primary aliphatic, 253, 341,
522	Petrochemical wastes, 40	418
Benzene and derivatives		Aerobic biodegradation, 29, 230
Metabolic pathways, 232	Actinomyces sp	386, 447
Biphenyl and derivatives	Alcohols, benzylic	Aerobic digestion reactors compared,
Aerobic biodegradation, 138	Structure-activity relationships	251, 287
Metabolic pathways, 354	153	Assay development, 592
Structure-activity relationships	Alcohols, primary aliphatic	Identification of microorganisms
138	Structure-activity relationships 153	282, 303
Crude oil	Alcohols, secondary aliphatic	Inhibitory (toxic) effects, 144
Mesophilic temperature, effect	Structure-activity relationships	Isolation of microorganisms, 417
567	153	Metabolic pathways, 303, 417
Psychrophilic temperature effect	Aldehydes	471
567	Structure-activity relationships	Michaelis-Menten coefficients
Fellmongery wastes Identification of microorganisms	153	224
406	Alkanoic acids and derivatives	Monad kinetics constants, 224
Fuel oil	Structure-activity relationships	Octanol-water partition coefficients,
Metabolic pathways, 553	153	582
Gasoline	Cellulose and derivatives	Operational parameters, 224, 592
Metabolic pathways, 232	Operational parameters, 285	Petrochemical wastewater treatment
Hexachlorophene	Time-course kinetics, 285	324
Metabolic pathways, 354	Hydroquinone and derivatives	Pseudomonas sp. 417
Hydrocarbons	Structure-activity relationships	Respirometric studies, 30
Metabolic pathways, 232	153	Structure-activity relationships
Petroleum	Propylene glycols	153, 386, 473
Metabolic pathways, 553	Structure-activity relationships	Substrate concentration effect
Phenol and derivatives	153	223, 372
Metabolic pathways, 354	Pyrocatechol and derivatives	Time-course kinetics, 191, 582
Polybutadienes	Structure-activity relationships	Alcohols, primary, long chain Operational parameters, 222
Metabolic pathways, 522	153	Alcohols, secondary aliphatic, 341
Structure-activity relationships	Resorcinol and derivatives	Aerobic biodegradation, 386
522	Structure-activity relationships	Assay development, 592
Polychlorinated biphenyls	153 Rubber, vulcanized, 87	Octanol-water partition coefficients,
Aerobic biodegradation, 138		582
Structure-activity relationships	Activated carbon	Operational parameters, 591
138	Dyes, acid	592
Polychlorobenzenes and derivatives	Biodegradation vs adsorption	Petrochemical wastewater treatment
Metabolic pathways, 354	358	324
Polyethylene glycols Identification of microorganisms	Dyes, direct Biodegradation vs adsorption	Sludge adaptation process, 591
560	358	Structure-activity relationships
Metabolic pathways, 244	Dyes, disperse	153. 386. 473
Respirometric studies, 560	Biodegradation vs adsorption	Time-course kinetics, 191, 582
Propylene glycols	358	Alcohols, tertiary aliphatic
Identification of microorganisms	3.00	Aerobic biodegradation, 386
560		D.O. meter method, 268
Respirometric studies, 560		Octanol-water partition coefficients.

Activated sludge (cont'd)	Activated sludge (cont'd)	Activated sludge (cont'd)
River die-away test. 268	Inhibitory (toxic) effects, 150	274. 393
Structure-activity relationships 386	344	Ammonia and salts
Time-course kinetics 582	Nitrification, 150	Inhibitory (toxic) effects, 231 Innibitory (toxic) effects, cyanide in-
Aldehydes, 253, 418	Petrochemical wastewater treatment 324	hibition, 243
Aerobic biodegradation, 398	Time-course kinetics, 172	Inhibitory (toxic) effects, pnenol in-
Inhibitory (toxic) effects, 453	Alkyl sulfates, long chain	hibition, 243 Inhibitory (toxic) effects, thiocyanat
Respirometric studies, 30	Aerobic biodegradation, 302 Coupled units test, 129	inhibition, 243
Structure-activity relationships	Depuration rate, effect on, 83	Aniline and derivatives, 190
153, 473	Operational parameters, 83	Aerobic biodegradation, 78, 386
Alkanes, 173	Structure-activity relationships	600
Inhibitory (toxic) effects, 144 Alkanes, cyclic, 173, 341	302	Inhibitory (toxic) effects, 66
Alkanes, long chain, linear	Time-course kinetics, 460 Alkyl sulfides	534 Inhibitory (toxic) effects, pH effect,
Time-course kinetics, 191	Anaerobic digestion reactor, 602	225
Alkanoic acids and derivatives, 253, 341,		Inhibitory (toxic) effects, proteolytic
418	Aerobic biodegradation, 128	225
Aerobic digestion reactors compared,	, (,,	Petrochemical wastewater treatment
251, 287 Assay development, 592	Time-course kinetics, 460	324 Respirometric studies, 534
Inhibitory (toxic) effects, 429	Alkyl sulfoxides Identification of microorganisms	Structure-activity relationships
Michaelis-Menten coefficients	295	386
429	Sludge acclimatization process	Substrate concentration effect
Operational parameters, 591, 592	295	66
Sludge adaptation process, 591	Alkylsulfonic acids	Antibiotics, 254, 307
Structure-activity relationships 153, 274, 473	Inhibitory (toxic) effects, 178	Aerobic biodegradation, 386 Aerobic digestion reactors compared
Substrate concentration effect	Aluminum Inhibitory (toxic) effects, 178	251
372	Amides, aliphatic	Inhibitory (toxic) effects, 252
Alkanoic acids and derivatives, long	Aerobic biodegradation, 29	595
chain	Inhibitory (toxic) effects, 28	Structure-activity relationships
Aerobic biodegradation, 302	Isolation of microorganisms, 278	386
Operational parameters, 222	Nutritional parameters, 278	Aromane compounds, aleyetic, 414 Arsenic compounds, inorganic
Sludge adaptation process, 591	Operational parameters, 28 Structure-activity relationships	Inhibitory (toxic) effects, 588
Structure-activity relationships	274	Azo compounds
274, 302	Time-course kinetics, 193	Inhibitory (toxic) effects, 581
Alkanoic acids and derivatives,	Amides, aliphatic, long chain	Structure-activity relationships
polybasic	Structure-activity relationships	530
Aerobic biodegradation, 386 Anaerobic digestion reactor, 543	274	Time-course kinetics, 530
Coupled units test, 129	Amines, alicyclic Identification of microorganisms	Azo dyes Freundlich adsorption isotherms
Petrochemical wastewater treatment	38	101
Structure-activity relationships	Inhibitory (toxic) effects, 38 Metabolic pathways, 39	Inhibitory (toxic) effects, 371 581
386	Amines, aliphatic, 341	Kinetics and equilibrium studies
Alkanoic acids, cyclic	Aerobic biodegradation, 394	101
Coupled units test, 129	Anaerobic biodegradation, 394	Structure-activity relationships
Respirometric studies, 535 Alkenes, 341	Inhibitory (toxic) effects, 504	101, 530
Respirometric studies, 535	Isolation of microorganisms, 278 Nitrification, 504	Time-course kinetics, 530 Benzene and derivatives, 173, 341
Time-course kinetics, 191	Nutritional parameters, 278	Benzenesulfonic acid and non-alkyl
Alkenoic acids and derivatives, 341	River die-away test, 394	substituted derivatives
Aerobic biodegradation, 230	Amines, poly-, aliphatic, 341	Aerobic biodegradation, 175
Coupled units test, 129 Petrochemical wastewater treatment	Aerobic biodegradation, 386	386
324	Assay development, 592 Metabolic pathways, 471	Operational parameters, 591 Petrochemical wastewater treatment
Alkenoic acids and derivatives, long	Operational parameters, 540	324
chain	591, 592	Sludge adaptation process, 591
Aerobic biodegradation, 58	Sludge adaptation process, 540	Structure-activity relationships
Depuration rate, effect on, 83	591	386
Operational parameters, 83 River die-away test, 58	Structure-activity relationships	Benzenesulfonic acid, linear alkyl, long
Structure-activity relationships	386 Amino acids and derivatives	chain Aerobic biodegradation, 58, 302
274	Aerobic biodegradation, 515	Aeropic digestion reactor, 234
Alkyl halides, 341	Polarographic monitoring, 512	235, 482
Anaerobic digestion reactor, 344	Structure-activity relationships	Anaerobic biodegradation, 439

Activated sludge (cont'd)	Activated sludge (cont'd)	Activated sludge (cont'd)
Angerobic digestion reactor, 234	Cellulose and derivatives	Sludge acclimatization process
Inhibitory (toxic) effects, 235	Petrochemical wastewater treatment	141, 142
Inhibitory (toxic) effects of nutrients,	324	Cyanuric acid and derivatives
439	Chloramine and derivatives Inhibitory (toxic) effects, additive,	Structure-activity relationships
River die-away test, 58, 268	178	393
Structure-activity relationships	Chioride	Cycloaliphatics, substituted
302	Inhibitory (toxic) effects, 131	Aerobic biodegradation, 386
Surface water model, 482	Operational parameters, 131	Identification of microorganisms 38
Benzenesulfonic acid, non-linear alkyl,	Chromium	Inhibitory (toxic) effects, 38
long chain Coupled units test, 129	Anaerobic digestion reactor, 344	Metabolic pathways, 39, 471
Benzidine and derivatives	Inhibitory (toxic) effects, 131	Structure-activity relationships
Aerobic digestion reactor, 495	149, 178, 336, 344, 437	386
Operational parameters, 495	546	DDT, Methoxychlor and metabolite
Oxidation product spectrum and ab-	Operational parameters, 131	Aerobic biodegradation, 346
sorbance, 495	Cinnamic acid and derivatives	Dimethyl sulfoxide
Sludge acclimatization process	Anaerobic digestion reactor, 196	Anaerobic digestion reactor, 602
495	Cirrasols Inhibitory (toxic) effects, 430	Dobane JNQ sulfonate
Benzoic acid and derivatives	Cobalt	Anaerobic digestion reactor, 344
Aerobic biodegradation, 175	Inhibitory (toxic) effects, 178	Inhibitory (toxic) effects, 344
386, 398	546	Domestic sewage effluents
Anaerobic digestion reactor, 196 Inhibitory (toxic) effects, 66	Coke oven wastes	Inhibitory (toxic) effects, 336 Dyes
Respirometric studies, 30	- Inhibitory (toxic) effects, 66	Depuration rate, effect on, 83
Structure-activity relationships	231, 480	Inhibitory (toxic) effects, 370
386, 473	Nitrification, 243	371, 534, 581
Substrate concentration effect	Nitrification effect, 480	Langmuir adsorption isotherms
66	Substrate concentration effect	370
Benzothiazole and derivatives	66 Thiosulfate oxidation, 256	Michaelis-Menten coefficients
Aerobic biodegradation, 128	Confectionary wastes	370
Inhibitory (toxic) effects, 128	. Glucose removal and polysaccharide	Nutritional effects, 368
144	accumulation, 501	Operational parameters, 83
Isolation of pure microbial popula- tion, 317	Copper	Respirometric studies, 534 Structure-activity relationships
River die-away test, 317	Anaerobic digestion reactor, 344	530
Biphenyl and derivatives, 296	Inhibitory (toxic) effects, 178	Time-course kinetics, 530
Aerobic biodegradation, 175	336, 344, 437, 546	Dyes, acid
Inhibitory (toxic) effects, 144	Coumarin and derivatives	Inhibitory (toxic) effects, 370
309, 354, 453	Aerobic biodegradation, 175	371, 581
Operational parameters, 315	Cresols and derivatives	Langmuir adsorption isotherms
Time-course kinetics, 316	Aerobic biodegradation, 386	370
Boron	Inhibitory (toxic) effects, 178 309, 480	Michaelis-Menten coefficients
Inhibitory (toxic) effects, 588	Metabolic pathways, 143	370
Brewery wastes	Nitrification effect, 480	Nutritional effects, 368
Glucose removal and polysaccharide accumulation, 501	Structure-activity relationships	Structure-activity relationships 530
Substrate concentration effect	386	Time-course kinetics, 530
372	Cumene and derivatives, 341	Dyes, anthraquinone
Bromate	Aerobic biodegradation, 386	Freundlich adsorption isotherms
Time-course kinetics, 272	Structure-activity relationships	101
Cadmium	386	Kinetics and equilibrium studies
Anaerobic digestion reactor, 344	Cutting fluids (coolants), synthetic and	101
Inhibitory (toxic) effects, 178	semi-synthetic Biodegradation, 1	Structure-activity relationships
344, 546	Inhibitory (toxic) effects with preser-	101
ε-Caprolactam Aerobic biodegradation, 386	vatives, 1	Dyes, basic Inhibitory (toxic) effects, 370
Ammonification, 603	Cyanate	371
Nitrification, 603	Inhibitory (toxic) effects, 231	Langmuir adsorption isotherms
Operational parameters, 591	Cyanide	370
River die-away test, 268	Aerobic digestion reactor, 139	Michaelis-Menten coefficients
Sludge adaptation process, 591	141, 142	370
Structure-activity relationships	Inhibitory (toxic) effects, 139	Dyes, direct
386	141, 231, 429, 546 Kinetics and equilibrium studies	Aerobic biodegradation, 398
Substrate concentration effect	142	Inhibitory (toxic) effects, 371
603 Carbamic acid and derivatives	Michaelis-Menten coefficients	534
Aerobic biodegradation, 268	141, 429	Langmuir adsorption isotherms 370
River die-away test, 268	Respirometric studies, 30	5.0

Activated sludge (cont'd)	Activated sludge (cont'd)	Activated sludge (cont'd)
Michaelis-Menten coefficients	Inhibitory effects, metallic and ionic	Freundlich adsorption isotherms
370 Respirometric studies, 534	species Review, 546	101 Innibitory (toxic) effects, 144
Dyes, disperse	lodate	178, 371, 534
Aerobic biodegradation, 398	Time-course kinetics, 272	Kinenes and equilibrium studies
Inhibitory (toxic) effects, 371	Iron	101
Dyes, pigment Nutritional effects, 368	Anaerobic digestion reactor, 344 Inhibitory (toxic) effects, 178	Operational parameters, 83 Petrochemical wastewater treatment
Dyes, reactive	344	324
Aerobic biodegradation, 398	Isophthalic acid and derivatives	Respirometric studies, 534
Dyes, sulfur	Aerobic digestion reactors compared,	River die-away test, 268
Inhibitory (toxic) effects, 534	287 Kanechlors	Structure-activity relationships 101
Respirometric studies, 534	Aerobic biodegradation, 338	Nickel
Dyes, vat Aerobic biodegradation, 398	Ketones, aliphatic, 253, 341	Inhibitory (toxic) effects, 178
EDTA and salts	Aerobic biodegradation, 386	437. 546
Time-course kinetics, 583	Identification of microorganisms	Nicotinic acid
Epoxides	38	Structure-activity relationships 393
Petrochemical wastewater treatmen	t Inhibitory (toxic) effects, 38 49	Nitriles
Explosives	Metabolic pathways, 39	Aerobic biodegradation, 230
Aerobic biodegradation, 386	Structure-activity relationships	Nitrification, 422
Structure-activity relationships	386, 473	Nitrobenzene and derivatives
386	Kraft pulp wastes	Aerobic bioconversion, 204
Explosives, organic Batch vs continuous-flow system	Aerobic biodegradation, 289 Aerobic digestion reactors compared.	Aerobic biodegradation, 386 Anaerobic bioconversion, 204
564	236	Inhibitory (toxic) effects, 534
Metabolic pathways, 564	Detoxification, 236, 349	Inhibitory (toxic) effects, proteolytic
Fellmongery wastes	Glucose removal and polysaccharide	225
Aerobic digestion, 197 Aerobic digestion reactor, 405	accumulation, 501	Operational parameters, 591
Biomass yield, effect on, 197	Lagoons, aerated, industrial site	Oxidation ditch, 204 Petrochemical wastewater treatment
Operational parameters, 405	Structure-activity relationships	324
Substrate concentration effect	289	Respirometric studies, 534
405	Lead	Sludge adaptation process, 591
Flame retardant, 190	Inhibitory (toxic) effects, 437	Structure-activity relationships
Fluorescent brighteners	Lignin-related compounds	386
Aerobic biodegradation, 146 175	Anaerobic digestion reactor, 196	Nitrosamine, dimethyl- Aerobic biodegradation, 394
Incineration, 146	Lindane and metabolites Aerobic biodegradation, 346	Anaerobic biodegradation, 394
Wet oxidation (Zimpro) reactor	597	River die-away test. 394
146	Sorption, 597	NTA and salts
Food industry wastes	Mercury, inorganic	Aerobic biodegradation, 174
Metabolic pathways, 596 Fruit juice wastes	Adsorption and volatilization	Anaerobic digestion reactor, 263
Glucose removal and polysacchara	357 de Inhibitory (toxic) effects, 429	Heavy metals effect, 174
accumulation, 501	437, 546	Oil refinery wastes
Furan and derivatives	Michaelis-Menten coefficients	Aerobic biodegradation, 108
Aerobic biodegradation, 386	429	Biodegradation, design relationships 108
Inhibitory (toxic) effects, 49 Structure-activity relationships	Operational parameters, 357 Mercury, organo-	. Inhibitory (toxic) effects, 150
386	Aerobic biodegradation, 128	Nitrification, 150
Herbicides, 2.4-D type, 207	Inhibitory (toxic) effects, 128	Respirometric studies, 535
Inhibitory (toxic) effects, 429	Methyl mercaptan	Petrochemical wastes, 341
Michaelis-Menten coefficients 429	Anaerobic digestion reactor, 602	Operational parameters, 540 591
Heteroaromatics and derivatives, dicy	Molybdenum clic Inhibitory (toxic) effects, 20	Sludge adaptation process, 540
Aerobic biodegradation, 78	Municipal wastes, synthetic	591
Structure-activity relationships	Aerobic biodegradation, 89	Phenoi and derivatives
393 Hexachlorophene	Rate constants/retention time	Aerobic biodegradation, 5, 386 Anaerobic digestion reactor, 196
Inhibitory (toxic) effects, 354	89 Substrate concentration effect	Identification of microorganisms
Hydrocarbons	89	295
Aerobic biodegradation, 398	Municipal wastewaters	Inhibitory (toxic) effects, 144
Hydroquinone and derivatives	Aerobic digestion reactor, 484	178, 231, 309, 354, 429
Respirometric studies, 30 Structure-activity relationships	Trickling filters, 484	480 Metabolic pathways, 143
Structure-activity relationships	Naphthalene and derivatives Depuration rate, effect on, 83	Michaelis-Menten coefficients

ctivated studge (cont d)	Activated sludge (cont'd)	Activated sludge (cont'd)
Nitrification effect, 480	Operational parameters, 28	Biocenosis, effect on, 105
Operational parameters, 315	Polychlorinated biphenyls	Sludge acclimatization process
Respirometric studies, 30	Aerobic biodegradation, 337	105
Sludge acclimatization process	Inhibitory (toxic) effects, 144	Structure-activity relationships
295		153, 473
Structure-activity relationships	Substrate concentration effect	
386	271	Proteins
	Polychlorinated terphenyls	Substrate concentration effect
Time-course kinetics, 316	Substrate concentration effect	372
Phenol-formaldehyde resin	271	=
Biodegradation, rates compared	Polychlorobenzenes and derivatives	Pseudomonas sp
248	Aeropic biodegradation, 128	Review, 489
Phenol pitch		Pulp and paper wastes
Inhibitory (toxic) effects, 49	Inhibitory (toxic) effects, 53	Aeration digestion reactors
	128, 144, 354	compared, 520
Phosphonic acid derivatives, alkyl poly-	Polychlorocyclopentadiene dimers	
Aerobic biodegradation, 219	Aerobic biodegradation, 9	Aerobic biodegradation, 128
Inhibitory (toxic) effects, 219	Anaerobic biodegradation, 9	289
Phosphoric acid plasticizers	Polycyclic aromatic hydrocarbons, 121,	Aerobic digestion reactors compared
Octanol-water partition coefficients.		236
434	443	Detoxification, 236, 349
	Polyethylene glycols, 341	
Phosphorodithioic acid and derivatives,	Aerobic biodegradation, 58, 386	Foam process, 594
414	Assay development, 592	Inhibitory (toxic) effects, 128
Phosphorothioic acid and derivatives,	Operational parameters, 591	453
190	592	Lagoons, aerated, industrial site
Phosphorus	•	349
Review, 113, 412	Petrochemical wastewater treatment	Operational parameters, 520
Photographic and municipal wastes, syn-	324	Review, 556
• •	River die-away test, 58	
thetic	Sludge adaptation process, 591	Structure-activity relationships
Aerobic biodegradation, 89	Structure-activity relationships	289
Rate constants/retention time, 89	386	Pyridine and derivatives
Substrate concentration effect	The same of the sa	Aerobic biodegradation, 78
39	Polyethylene glycols, alkylphenoxy-	Inhibitory (toxic) effects, 480
Photoprocess wastes	Coupled units test, 129	Nitrification effect, 480
Aerobic biodegradation, 89°	Polyethylene glycols, fatty ester	Structure-activity relationships
	Depuration rate, effect on, 83	
Rate constants/retention time	Inhibitory (toxic) effects, 430	393
89	Operational parameters, 83	Pyrocatechol and derivatives
Respirometric studies, 30	•	Aerobic biodegradation, 386
Substrate concentration effect	Polyethylene glycols, fatty ether	Anaerobic digestion reactor, 196
89	Aerobic biodegradation, 302	Identification of microorganisms
Phthalic acid and derivatives, 341	Aerobic digestion reactor, 493	282
Aerobic biodegradation, 386	Anaerobic_digestion reactor, 493	
398, 447	Assay development, 592	Inhibitory (toxic) effects, 66
	Coupled units test, 129	Metabolic pathways, 143
Anaerobic biodegradation, 267	Inhibitory (toxic) effects, 430	Structure-activity relationships
Identification of microorganisms		153, 386, 473
266, 267, 281, 282	Operational parameters, 222	Substrate concentration effect
Octanol-water partition coefficients.	592	66
531	Seasonal variations, 493	Pyrrole
Petrochemical wastewater treatment	Structure-activity relationships	
324	302	Structure-activity relationships
	Polymers	393
Rate constants/retention time	Endoacting extracellular enzymes	Quaternary ammonium compounds
531	331	Aerobic digestion reactor, 234
Structure-activity relationships		Aerobic digestion reactor, pilot
386	Exoacting extracellular enzymes	plant, 152
Pimaric acid and derivatives	331	Anaerobic digestion reactor, 234
Aerobic biodegradation, 289	Polystyrenes	332
Detoxification, 349	Biodegradation, rates compared	
	248	Inhibitory (toxic) effects, 304
Lagoons, aerated, industrial site	Polyvinyi alcohol	Resorcinol and derivatives
349	Aerobic biodegradation, 181	Aerobic biodegradation, 386
Structure-activity relationships		Inhibitory (toxic) effects, 178
289	230, 398	Structure-activity relationships
Poly(α-hydroxyacrylic acid)	Batch vs continuous-flow system	153, 386, 473
Coupled units test, 129	181	Salicylic acid and derivatives
Poly(methyl methacrylate)	Operational parameters, 591	Aprobio biodesandesia 200
	Petrochemical wastewater treatment	Aerobic biodegradation, 386
Biodegradation, rates compared	324	Operational parameters, 315
248	Review, 489	Structure-activity relationships
Polyacrylamides		386
Time-course kinetics, 193	Sludge adaptation process, 591	Time-course kinetics, 316
Polyacrylonitrile	Time-course kinetics, 136, 352	Sanucizers
Aerobic biodegradation, 29	355	
Inhibitory (toxic) effects, 28	Propylene glycols	Octanol-water partition coefficients,
aminomony model chiects, 40	liene @rleon	434

Activated sludge (cont'd)	Activated sludge (cont'd)	Activated sludge, acclimated
Settlement tank effluents	Tetralin and derivatives, 341	Alcohois, alicyche
Inhibitory (toxic) effects, 336 Silicon, inorganic	Textile wastes	Aerobic digestion reactor, 381 Oxidation diten, 381
Inhibitory (toxic) effects, 588	Aerobic biodegradation, 29, 181 398	Alcohols, primary aliphatic
Silicones	Batch vs continuous-flow system	Aerobic biodegradation, 291
Petrochemical wastewater treatment	181	Time-course kinetics, 475
324	Inhibitory (toxic) effects, 144	Aldehydes
Silver Review, 22	290, 453	Aerobic biodegradation, 291 Inhibitory (toxic) effects, 21
Sodium	Operational parameters, 529 Review, 489	226
Inhibitory (toxic) effects, 546	Time-course kinerics, 136, 290	Respirometric studies, 21
Soft drink wastes	352, 355	Structure-activity relationships
Glucose removal and polysaccharide	Thiocyanic acid and salts	390
accumulation, 501	Inhibitory (toxic) effects, 66	Time-course kinetics, 390
Solvent wastes Operational parameters, 591	231, 480	Alkanoic acids and derivatives Sludge acclimatization process
Sludge adaptation process, 591	Nitrification effect, 480 Substrate concentration effect, 66	446
Starch and derivatives	Thiosulfate oxidation, 256	Time-course kinetics, 475
Aerobic biodegradation, 507	Tin compounds, organic	Alkenoic acids and derivatives
Substrate concentration effect	Inhibitory (toxic) effects, 483	Identification of microorganisms
372 Standida	589	578
Steroids Substrate concentration effect, 271	Toluene and derivatives, 173, 341	Time-course kinetics, 475 Amiges, aliphatic
Stilbene and derivatives	Aerobic biodegradation, 386 Petrochemical wastewater treatment	Identification of microorganisms
Aerobic biodegradation, 146	324	578
175	Structure-activity relationships	Inhibitory (toxic) effects, 277
Incineration, 146	386	Amines, aliphatic
Wet oxidation (Zimpro) reactor 146	Triclosan	Inhibitory (toxic) effects, 226
Styrene and derivatives, 341	Inhibitory (toxic) effects, 367 Substrate concentration effect	277 Time-course kinetics, 475
Aerobic biodegradation, 146	367	Amino acids and derivatives
230	2,3,5-Triphenyltetrazolium chloride	Inhibitory (toxic) effects, 226
Incineration, 146	Inhibitory (toxic) effects, 53	Aniline and derivatives
Wet oxidation (Zimpro) reactor	Tritox-50	Aerobic biodegradation, 584
146 Sugars and derivatives, 106	Aerobic biodegradation, 346	Inhibitory (toxic) effects, 226 391
Aerobic biodegradation, 386	Urea and derivatives Inhibitory (toxic) effects, 150	Metabolic pathways, 584
Glucose removal and polysaccharide	Nitrification, 150, 413	Structure-activity relationships
accumulation, 501	Structure-activity relationships	391, 392
Inhibitory (toxic) effects, 66	393	Time-course kinetics, 391, 392
Metabolic pathways, 596	Vanadium	Benzene and derivatives
Structure-activity relationships 386	Aerobic biodegradation, 280 Freundlich adsorption isotherms	Time-course kinetics, 475 Benzenesulfonic acid and non-aikyl
Substrate concentration effect	280	substituted derivatives
66, 372	Inhibitory (toxic) effects, 546	Aeropic biodegradation, pilot plant
Sulfate	Operational parameters, 280	57
Inhibitory (toxic) effects, 588	Vanillic acid and derivatives	Benzenesulfonic acid, linear alkyl, long
Sulfide Anaerobic digestion reactor, 344	Anaerobic digestion reactor, 196 Vegetable oils and fats, 106, 341	chain, 436 Aerobic biodegradation, 202
Inhibitory (toxic) effects, 131	Wood preservatives, 296	Benzoic acid and derivatives
231, 344	Xanthate, 190	Aerobic biodegradation, 397
Operational parameters, 131	Xylenes and derivatives, 173	Structure-activity relationships
Sulfite liquor	Xylenols and derivatives	392 Time-course kinetics, 392
Aeration digestion reactors compared, 520	Aerobic biodegradation, 289 386	Benzothiazole and derivatives, 73
Foam process, 594	Anaerobic digestion reactor, 196	Bisphenol A
Operational parameters, 520	Detoxification, 349	Aerobic biodegradation, pilot plant
Surfactants, anionic-cationic complexed	Lagoons, aerated, industrial site	57
Aerobic digestion reactor, 234	349	Calcium
Anaerobic digestion reactor, 234 Tannery wastes	Structure-activity relationships 289, 386	Aerobic biodegradation, 598 ε-Caprolactam
Inhibitory (toxic) effects, 131	Zinc 289, 380	Aerobic digestion reactor, 381
Operational parameters, 131	Anaerobic digestion reactor, 344	Oxidation ditch, 381
Tar plant wastes	Inhibitory (toxic) effects, 178	Cirrasols
Aerobic biodegradation, 78	344, 429, 437, 546	Inhibitory (toxic) effects, 432
Terephthalic acid and derivatives Aerobic digestion reactors compared.	Michaelis-Menten coefficients	Cresols and derivatives
Aerodic digestion reactors compared.	429	Aerobic biodegradation, pilot plant

Activated sludge, acclimated (cont'd) Activated sludge, acclimated (cont'd) Activated sludge, acclimated, continuousflow (cont'd) Structure-activity relationships Phthalic acid and derivatives, 436 Operational parameters, 310 Aerobic biodegradation, 397 389 Sludge acclimatization process Time-course kinetics, 389 Polychlorobenzenes and derivatives Cvanuric acid and derivatives Aerobic biodegradation, 397 Benzenesulfonic acid, linear alkyl, long Time-course kinetics, 475 Polycyclic aromatic hydrocarbons chain DDT, Methoxychlor and metabolites Aerobic biodegradation, 185 River die-away test. 220 Aerobic biogegradation, 584 Polyethylene glycols, fatty ester Metabolic pathways, 584 Inhibitory (toxic) effects, 432 Structure-activity relationships 220 Dves, direct Polyethylene glycols, fatty ether Benzidine and derivatives Aerobic biodegradation, 397 Inhibitory (toxic) effects, 432 Aerobic digestion reactor, 495 Dyes, disperse Polyvinyi alcohol Operational parameters, 495 Aerobic biodegradation, 397 Aerobic biodegradation, 397 Oxidation product spectrum and ab-Dves, reactive Pyrocatechol and derivatives sorbance, 495 Aerobic biodegradation, 397 Structure-activity relationships Sludge acclimatization process 389 Dves, vat 495 Aerobic biodegradation, 397 Time-course kinetics, 389 Cellulose and derivatives Explosives, organic Quaternary ammonium compounds Inhibitory (toxic) effects, 390 Operational parameters, 310 Aerobic digestion reactor, pilot Sludge acclimatization process plant, 125 Resorcinol and derivatives Structure-activity relationships 310 390 Time-course kinetics, 390 Coal carbonization wastes Structure-activity relationships Herbicides, atrazine type Inhibitory (toxic) effects, 364 389 Time-course kinetics, 475 Time-course kinetics, 389 Sludge acclimatization process, 364 Hydrocarbons Dyes Salicylic acid and derivatives Aerobic biodegradation, 397 Operational parameters, 310 Aerobic biodegradation, 397 Hydroquinone and derivatives Sludge acclimatization process Inhibitory (toxic) effects, 390 Structure-activity relationships 310 Structure-activity relationships 389 Fluorescent brighteners 390 Time-course kinetics, 389 Operational parameters, 310 Time-course kinetics, 390 Ketones, aliphatic Sludge acclimatization process Salinity, effect on respiratory activity Aerobic digestion reactor, 381 Review, 227 310 Oxidation ditch. 381 Salinity, effect on volume index Leather, artificial, processing wastes Operational parameters, 310 Review, 227 Inhibitory (toxic) effects, 277 Sludge acclimatization process Santicizers, 436 Naphthalene and derivatives Textile wastes Aerobic biodegradation, 584 Hydrocarbons Aerobic biodegradation, 397 Aerobic biodegradation, pilot plant, Operational parameters, 310 Toluene and derivatives Sludge acclimatization process Structure-activity relationships Inhibitory (toxic) effects, 226 310 390, 392 Metabolic pathways, 584 Iron Time-course kinetics, 390, 392 Model ecosystem, aquatic, simulated, Inhibitory (toxic) effects, 339 Toluic acid and derivatives 584 Mercaptans Aerobic biodegradation, 397 Nitriles Aerobic biodegradation, 112 Xvlenes and derivatives Identification of microorganisms Naphthalene and derivatives Structure-activity relationships 578 Operational parameters, 310 392 Nitrobenzene and derivatives Sludge acclimatization process Time-course kinetics, 392 Structure-activity relationships 310 Xylenois and derivatives Onion processing wastes 390, 391 Structure-activity relationships Time-course kinetics, 390, 391 Aerobic biodegradation, 112 389 NTA and salts Phenol and derivatives Time-course kinetics, 389 Aerobic biodegradation, 463 Aerobic digestion reactor, 60 Zinc Time-course kinetics, 463 Inhibitory (toxic) effects, 122 Inhibitory (toxic) effects, 544 Pesticides 364 Substrate concentration effect Inhibitory (toxic) effects, 226 Sludge acclimatization process 47, 544 Phenol and derivatives 364 Aerobic biodegradation, 5, 185
Aerobic biodegradation, pilot plant.

Activated sludge, acclimated, continuous-Polychlorobenzenes and derivatives Inhibitory (toxic) effects, 122 Alcohols, primary aliphatic Polymers Isolation of microorganisms, 497 Operational parameters, 310 Operational parameters, 310 Structure-activity relationships Sludge acclimatization process Sludge acclimatization process 389 310 Time-course kinetics, 389 Polyvinyl alcohol Alkyl sulfides Phloroglucinol Aerobic biodegradation, 112 Operational parameters, 310 Structure-activity relationships Amines, poly-, aliphatic Operational parameters, 310 Sludge acclimatization process 389 310 Time-course kinetics, 389 Sludge acclimatization process Proteins Photoprocess wastes Operational parameters, 310 Inhibitory (toxic) effects, 21 Benzenesulfonic acid, alkyl, short chain Sludge acclimatization process Respirometric studies, 21 310

Activated sludge, acclimated, continuous-	Activated sludge, acclimated, municipal	Activated sludge, acclimated, municipal
flow (cont'd)	(cont'd)	(cont'd) Aerobic biodegradation, 568
Pulp and paper wastes	Sludge acclimatization process	Operational parameters, 568
Operational parameters, 310 Sludge acclimatization process	491 Alkanoic acids and derivatives, long	Timber steam processing wastes
310	chain	Aerobic biodegradation, 408
Quaternary ammonium compounds	Aerobic biodegradation, 327	Identification of microorganisms 408
Operational parameters, 310	Aikanoic acids, sulfonated, long chain	Operational parameters, 408
Sludge acclimatization process 310	Inhibitory (toxic) effects, 329 Amides, aliphatic, long chain, sulfated	Zinc
Salinity	Aerobic biodegradation, 327	Aerobic biodegradation, 363
Inhibitory (toxic) effects, 517	Amino acids and derivatives	Biomass yield, effect on, 363
Sodium	Aerobic biodegradation, 186	Freundlich adsorption isotherms 363
Inhibitory (toxic) effects, 517 Starch and derivatives	Sludge acclimatization process	Michaelis-Menten coefficients
Operational parameters, 310	Benzenesulfonic acid, linear alkyl, long	363
Sludge acclimatization process, 310	chain	Operational parameters, 363
Styrene and derivatives	Aerobic biodegradation, 327	Activated sludge, acclimated, municipal,
Operational parameters, 310	Benzenesulfonic acid, S-substituted alkyl	continuous-flow Biphenyl and derivatives
Sludge acclimatization process 310	Aerated chamber die-away test 416	Aerobic biodegradation, 496
Sugars and derivatives	River die-away test, 416	Sludge acclimatization process
Operational parameters, 310	Shake flask process, 416	496
Sludge acclimatization process	Structure-activity relationships	Poly(a-hydroxyacrylic acid) Time-course kinetics, 350
310 Thiocyanic acid and salts	416 Biphenyl and derivatives	Time-course kinetics, 350
Inhibitory (toxic) effects, 364	Aerobic biodegradation, 526	Activated sludge, acclimated, sedimentation
Sludge acclimatization process	Cadmium	chamber Alkyl sulfides
364	Aerobic biodegradation, 363	Aerobic biodegradation, 112
Thiols Aerobic biodegradation, 112	Biomass yield, effect on, 363 Freundlich adsorption isotherms	Mercaptans
Activated sludge, acclimated, industrial	63, 363	Aerobic biodegradation, 112
Brewery wastes	Kinetics and equilibrium studies	Onion processing wastes
Identification of microorganisms	63	Aerobic biodegradation, 112 Thiols
502 Coal gasification wastes	Langmuir adsorption isotherms 63	Aeropic biodegradation, 112
Aerobic biodegradation, 433	Michaelis-Menten coefficients	Activated sludge, acclimated, semi-
Batch vs continuous-flow system	363	continuous flow
433	Operational parameters, 363	Mercury, inorganic
Confectionary wastes Identification of microorganisms	Copper Freundlich adsorption isotherms	Volatilization. 356
502	63	Activated sludge and soils, acclimated
Fruit juice wastes	Kinetics and equilibrium studies	Phenol and derivatives Aerobic biodegradation, 60
Identification of microorganisms	63	•
502 Hexachlorophene	Langmuir adsorption isotherms 63	Activated sludge, batch-type, industrial Cellulose and derivatives
Aerobic biodegradation, 469	Fellmongery wastes	Substrate concentration effect
Sorption, 469	Aerobic biodegradation, 186	42
Kraft pulp wastes Identification of microorganisms	Denitrification, 77 Sludge acclimatization process	Activated sludge, boiling-inactivated
502	77. 186	Azo dyes
Phenol and derivatives	Substrate concentration effect	Freundlich adsorption isotherms 101
Aerobic biodegradation, 433	77	Kinetics and equilibrium studies
Batch vs continuous-flow system 433	Mercury, inorganic Aerobic biodegradation, 363	101
Sludge acclimatization process	Biomass yield, effect on, 363	Structure-activity relationships
94	Freundlich adsorption isotherms	101 Dyes, anthraquinone
Soft drink wastes	363 Michaelis-Menten coefficients	Freundlich adsorption isotherms
Identification of microorganisms 502	363	101
Toluene and derivatives	Operational parameters, 363	Kinetics and equilibrium studies
Sludge acclimatization process	Polychlorinated biphenyls	101 Structure-activity relationships
94	Aerobic biodegradation, 526	101
Xylenes and derivatives Sludge acclimatization process	Polyvinyl alcohol Aerobic biodegradation, 568	Naphtnalene and derivatives
94	Operational parameters, 568	Freundlich adsorption isotherms
Activated sludge, acclimated, municipal	Tallow derivatives	101 Kinetics and equilibrium studies
Alcohols, primary aliphatic	Aerobic biodegradation, 327 Textile wastes	101
Oxygen uptake, effect on, 491	textile wastes	

(cont'd) Structure-activity relationships 101 Acrivated studge + cellulose and salts Pheno-loremaldehyde resun Biodegradation, rates compared 248 Polymethyl methacrylate) Acrivated studge, continuous-flow Alkanos acuds and derivatives Acroice biodegradation, 313 Aniline and derivatives Acroice biodegradation, 313 Aniline and derivatives Acroice biodegradation, 313 Aniline and derivatives Co-stantinuous-flow system Acroice biodegradation, 202 Structure-activity relationships 159 Substrate concentration effect 18 Dobasoi 25-9 Model cooxystem, aquatic, natural Model ecosystem, aquatic, natural	Activated studge, boiling-mactivated	Activated studge, continuous-now (contra)	Activated sludge, fresh water (cont'd)
Structure-activity relationships 101 Activated sludge - cellulose and salts Pheno-formaldehyde resun Biodegradation, rates compared 248 Polysymensy Biodegradation, rates compared 248 Polysymens Biodegradation, rates compared 248 Polysymens Biodegradation, rates compared 248 Activated sludge - continuous-flow Alkanoic acids and derivatives, polybasic Activated sludge, continuous-flow Alkanoic acids and derivatives, polybasic Co-substrate concentration effect 159 Rineitory (voice) effects, 159 Structure-activity relationships 159 Substrate concentration effect 159 Benzenesulfonic acid, linear alkyl, long sham Aerobic biodegradation, 202 Structure-activity relationships 261 Benzenesulfonic acid, mon-linear alkyl, model ecosystem, aquatic, natural 316 Chromsim Inhibitory (toxic) effects, 532 Rineitory Model ecosystem, aquatic, natural 316 Explained gradie Co-substrate concentration effect 159 Inhibitory (toxic) effects, 532 Rineitory Model ecosystem, aquatic, natural 316 Explained gradie Co-substrate concentration effect 159 Inhibitory (toxic) effects, 532 Rineitory Model ecosystem, aquatic, natural 316 Explained gradie Co-substrate concentration effect 159 Inhibitory (toxic) effects, 532 Rineitors Inhibitory (toxic) effects, 532 R	(cont'd)	Pulp and paper wastes	Inhibitory (toxic) effects, 203
Subtrate concentration effect 159 Rever die-away test, 159 Structure-activity relationships 159 Benzenesulfonic acid, linear alkyl, long chain Model ecosystem, aquatic, natural Sobsystem, aquatic, natural Substrate concentration effect 159 Benzenesulfonic acid, or see concentration effect 159 Cro-mbstrate concentration effect 159 Lineable or see continuous flow system 101 Substrate concentration effect 159 Lineable or see continuous flow system 101 Substrate concentration effect 159 Lineable or see continuous flow system 101 Substrate concentration effect 159 Lineable or see continuous flow system 101 Substrate concentration effect 159 Lineable or see continuous flow system 101 Substrate concentration effect 159 Lineable or see contentration effect 159 Lineabl	Structure-activity relationships		Activated sludge, high purity oxygen pro-
Activated sludge + cellulose and salts Pheno-formaldehyde resus Biodegradation, rates compared 248 Polystyrenes Biodegradation, rates compared 248 Activated sludge, continuous-flow Ammunition plant wastes Oxidation dich. 204 Antibated sludge, continuous-flow Alkanone acids and derivatives polybasie Co-substrate concentration effect 19 Inhibitory (toxic) effects, 199 River die-away test, 193 Aerobic biodegradation, 202 Structure-activity relationships 261 Benzenesulfonic acid, linear alkyl, long Inhibitory (toxic) effects, 292 Model coopsystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 392 Model coopsystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 199 River die-away test, 199 Model coopsystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 392 Model coopsystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 392 Model coopsystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 392 Model ecosystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 392 Model ecosystem, aquatic, natural 316 Explosives organic Inhibitory (toxic) effects, 392 River die-away test, 199 Inhibitory (toxic) effects, 392 Model ecosystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 392 Model ecosystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 392 Model ecosystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 392 Model ecosystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 392 Model ecosystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 392 Model ecosystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 392 Model ecosystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 392 Model ecosystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 392 Model ecosystem, aquatic, natural 317 Intercourse kinetics, 71 Intercourse kin	The state of the s		
Phenoi-formaldehyda resun Biodegradation, rates compared 248 Polystyrenes Biodegradation, rates compared 248 Polystyrenes Biodegradation, rates compared 248 Polystyrenes Biodegradation, rates compared 248 Activated sludge, continuous-flow Alkanois acids and derivatives, polybasic Aerobic biodegradation, 133 Aniline and derivatives Co-substrate concentration effect 159 River die-away test, 159 Structure-activity relationships 159 Substrate concentration fefect 159 Enzenesulfonic acid, linear alkyl, long Actobic biodegradation, 202 Structure-activity relationships 261 Enzenesulfonic acid, linear alkyl, long chain Model coosystem, aquanc, natural 516 Crowmum Inhibitory (toxic) effects, 48 Substrate concentration effect 159 Dobanol 259 Mode coosystem, aquanc, natural Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and merabolites Co-substrate concentration effect 159 Substrate concentration effect 159 Substrate concentration effect 159 Lindane and metabolites Co-substrate concentration effect 159 Lindane and metabolites Co-substrate concentration effect 159 Lindane and and metabolites Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and menabolites Co-substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 159 Simulation and concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 159 Simulation and concentration effect 159 Lindane and and metabolites Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and menabolites Co-substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and menabolites Inhibitory (toxic) effects, 57 Revolution dich, 204 Antimated sludge, continuous-flow system 71 Substrate concentration effect 169 Lindane and metabolites Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and menabolites Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and menabolites Inhibit			
Phenoi-formaldenyid resinal conceptance of 18 Biodegradation, rates compared 248 Polymentyl methacrylate) Biodegradation, rates compared 248 Polystyrenes Biodegradation, rates compared 36 Activated sludge, continuous-flow Alkanon cacus and derivatives, polybasic Aeroble biodegradation, 1313 Aniline and derivatives Co-ubstrate concentration effect 199 River die-away text, 1313 Aniline and derivatives (Co-ubstrate concentration effect 199 Benzenesulfonic acid, linear alkyl, long chain Model ecosystem, aquatic, natural 316 Enzenesulfonic acid, non-ilinear alkyl, long chain Model ecosystem, aquatic, natural 316 Chromum Inhibitory (toxic) effects, 48 Substrate concentration effect 199 River die-away text, 199 Model ecosystem, aquatic, natural 316 Chromum Inhibitory (toxic) effects, 532 Review, 566 Herbicules, monuron type and metabolites (Ca-ubstrate concentration effect 199 Lindane and metabolites (Ca-ubstrate concentration effect 199 Substrate concentration effect 199 Substrate concentration effect 199 Lindane and metabolites (Ca-ubstrate co			Operational parameters, 518
Activated sludge - continuous-16 Activated sludge - continuous-16 Activated sludge - continuous-16 Activated sludge - continuous-16 Alkanois acids and derivatives polybasic Aerobic biologegadation, 313 River die-away test, 313 Aniline and derivatives Co-substrate concentration effect 19 Inhibitory (toxic) effects, 199 Substrate concentration effect 48 Substrate concentration effect 49 Substrate concentration effect 40 Substrate concentration effect 41 Substrate concentration effect 42 Substrate concentration effect 43 Substrate concentration effect 44 Substrate concentration effect 45 Substrate concentration effect 46 Substrate concentration effect 47 Substrate concentration effect 48 Substrate concentration effect 49 Substrate concentration effec		Biolitass yield, effect on, 301	
Polystyrens Biodegradation, rates compared 248 Polystyrens Biodegradation, rates compared 248 Activated sludge, continuous-flow Alkanon saits and derivatives, polybasic Aerobic biodegradation, 1313 Aniline and derivatives Co-substrate concentration effect 159 Substrate concentration effect 159 Benzenesulfonic acid, linear alkyl, long chain Acobic biodegradation, 235 Benzenesulfonic acid, linear alkyl, long chain Model ecosystem, aquatic, natural 316 Enzenesulfonity (toxic) effects, 48 Substrate concentration effect 18 Dobanol 25-9 Model ecosystem, aquatic, natural 316 Explosives, organic Inhibitory (toxic) effects, 532 Review 5-66 Herbicides, monuron type and menabolites C-substrate concentration effect 159 Substrate concentration effect 24 Explosives, organic Inhibitory (toxic) effects, 532 Review 5-66 Herbicides, monuron type and menabolites C-substrate concentration effect 159 Substrate concentration effect 25 Inhibitory (toxic) effects, 532 Review 5-66 Herbicides, monuron type and menabolites Inhibitory (toxic) effects, 532 Review 5-66 Herbicides, monuron type and menabolites Inhibitory (toxic) effects, 532 Review 5-66 Herbicides, monuron type and menabolites Inhibitory (toxic) effects, 532 Review 5-66 Herbicides, monuron type and menabolites Inhibitory (toxic) effects, 532 Review 6-69 Rev	- · · · · · · · · · · · · · · · · · · ·	Activated studge + cornsteen continuous-	
Biodegradation, rates compared 248 Pobsystems and continuous-flow Alkanors acids and derivatives, polybasic Aeroivated studge, continuous-flow Alkanors acids and derivatives, polybasic Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 Structure-activity relationships 139 Substrate concentration effect 159 Structure-activity relationships 139 Substrate concentration effect 159 Benenesulfonic acid, linear alkyl, long chain Model coosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 148 Dobanol 25-9 Herbicides, monitoring pea and metabolites Inhibitory (toxic) effects, 512 Review de-away test, 159 Structure-activity relationships 150 Substrate concentration effect 17 Itime-course kinetics, 71 Time-course kinetics, 71 Tim	= -		Activated sludge industrial
Activated studge, continuous-flow Alkanone acids and derivatives polybasic — Aerobic biodegradation, 1313 Aniline and derivatives (Co-substrate concentration effect 159 River die-away test, 139 River die-away test, 159 R			
Polystyrems Biodegradation, rates compared 248 Activated sludge, continuous-flow Aca compounds Oxdation dich. 204 Aca continuous-flow system. 71 Substrate concentration effect 71 Time-course kinetics. 71 Resorcined and derivatives Oxdation of microorganisms 163 Ammosia and salts (dentification of microorganisms 163 Ammosia and activatives Oxdation of microorganisms 163 Ammosia and activatives Oxdation of microorganisms 163 Am			
Biodegradation, rates compared 248 Activated studge, continuous-flow Alkanote acids and derivatives, polybasic — Aerobic biodegradation, 313 Aniline and derivatives — Co-substrate concentration effect 159 River die-away test, 313 Arreactivity relationships 159 Substrate concentration effect 159 Benzenesulfonic acid, linear alkyl, long chain — Metabolites — Substrate concentration effect 159 Benzenesulfonic acid, linear alkyl, long chain — Model ecosystem, aquatic, natural 516 Chromium — Model ecosystem, aquatic, natural 516 Chromium — Model ecosystem, aquatic, natural 516 Chromium — Substrate concentration effect 159 Bobanol 35-9 Model ecosystem, aquatic, natural 516 Chromium — Substrate concentration effect 159 River die-away test, 319 Substrate concentration effect 159 River die-away test, 159 River die-away			
Activated sludge, continuous-flow Alkanore acteds and derivatives, polybasic Activated sludge, continuous-flow Alkanore acted and derivatives, polybasic Activated sludge, continuous-flow Malkanore acted and derivatives, polybasic Activated sludge, continuous-flow system Oxidation ditch, 204 Nitrobenzene and derivatives Oxidation ditch, 204 Nitrobenzene and derivatives Oxidation ditch, 204 Nitrobenzene and derivatives Oxidation ditch, 204 Activated sludge, diverse substrates Cocke own wastes Batch vs continuous-flow system Thereourse kinetics, 71 Phenol and derivatives Batch vs continuous-flow system Thereourse kinetics, 71 Phenol and derivatives Batch vs continuous-flow system Thereourse kinetics, 71 Procatechol and derivatives Batch vs continuous-flow system Thereourse kinetics, 71 Procatechol and derivatives Batch vs continuous-flow system Thereourse kinetics, 71 Procatechol and derivatives Batch vs continuous-flow system Thereourse kinetics, 71 Procatechol and derivatives Batch vs continuous-flow system Thereourse kinetics, 71 Procatechol and derivatives Batch vs continuous-flow system Thereourse kinetics, 71 Procatechol and derivatives Batch vs continuous-flow system Thereourse kinetics, 71 Procatechol and derivatives Batch vs continuous-flow system Thereourse kinetics, 71 Procatechol and derivatives Batch vs continuous-flow system Thereourse kinetics, 71 Procatechol and derivatives Batch vs continuous-flow system Thereourse kinetics, 71 Resorting the system of the s			
Activated sludge, continuous-flow Alkanote acids and derivatives, polybasic Aerobic biodegradation, 313 Aniline and derivatives Co-universe concentration effect 159 Inhibitory (toxic) effects, 159 River die-away test, 159 Structure-activity relationships 150 Benzensulfonic acid, linear alkyl, long chain Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 169 Dobanol 25-9 Model coosystem, aquatic, natural 515 Explosives, organic Inhibitory (toxic) effects, 532 Review, 366 Explosives, organic Inhibitory (toxic) effects, 532 Review, 366 Explosives, organic Inhibitory (toxic) effects, 532 Inhibitory (toxic) effects, 532 Inhibitory (toxic) effects, 532 Review, 366 Explosives, organic Inhibitory (toxic) effects, 532 Inhibitory (toxic) e			
Activated sludge, continuous-flow Alkanors actds and derivatives, polybasic Aerobic biodegradation, 313 Alliline and derivatives Co-substrate concentration effect 159 River die-away (est., 159 River die-away (est., 159 River die-away (est., 159 River die-away (est., 159) Substrate concentration effect 159 Substrate concentration effect 159 Benzenesulfonic acid, linear alkyl, long shan Aerobic biodegradation, 202 Structure-activity relationships 261 Benzenesulfonic acid, non-linear alkyl, long shan Model ecosystem, aquatic, natural 516 Chromaum Inhibitory (toxic) effects, 48 Substrate concentration effect 189 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Chromaum Inhibitory (toxic) effects, 532 Reviews 566 Herbicides, monuron type and metabolites Chromaum enabolites Inhibitory (toxic) effects, 532 Reviews 566 Herbicides, monuron type and metabolites Inhibitory (toxic) effects, 532 Riverure-activity relationships 159 Substrate concentration effect 159 Inhibitory (toxic) effects, 532 Reviews 566 Herbicides, monuron type and metabolites Inhibitory (toxic) effects, 532 Review 566 Herbicides, monuron type and metabolites Inhibitory (toxic) effects, 532 Riverure-activity relationships 159 Substrate concentration effect 159 Inhibitory (toxic) effects, 532 Riverure-activity relationships 159 Substrate concentration effect 159 Inhibitory (toxic) effects, 532 Riverure 566 Herbicides, monuron type and metabolites Inhibitory (toxic) effects, 532 Riverure 566 Herbicides and entrabolites Inhibitory (toxic) effects, 532 Riverure 566 Herbicides and entrabolites Inhibitory (toxic) effects, 532 Riverure 569 River die-away test, 179 Substrate concentration effect 159 Substrate conce	248		
Alkanote acids and derivatives. Alkanote acids and derivatives. Aerobic biodegradation, 313 River die-away test, 139 Aniline and derivatives Co-substrate concentration effect 159 Structure-activity relationships 159 Benzenesulfonic acid, linear alkyl, long chain Aerobic biodegradation, 202 Structure-activity relationships 261 Benzenesulfonic acid, non-linear alkyl, long chain Aerobic biodegradation, 202 Structure-activity relationships 261 Benzenesulfonic acid, non-linear alkyl, long chain Amodel ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 366 Explosives, organic Inhibitory (toxic) effects, 532 Review, 366 Inhibitory (toxic) effects, 519 River die-away test, 159 Siructure-activity relationships Siructure-activity relationships 101 Dyes, amhraquinone Freundlich adsorption isotherms 101 Naphthalene and metabolites Inhibitory (toxic) effects, 322 River die-away test, 159 River die-away test, 159 Siructure-activity relationships Inhibitory (toxic) effects, 532 Robertate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Robertate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Robertate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Robertate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Robertate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Robertate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Robertate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Robertate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Robertate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Robertate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Robertate concentration	Activated sludge continuous-flow		
Aerobic biodegradation, 313 River die-away test, 313 Aniline and derivatives Co-substrate concentration effect 159 Benzenesulfonic acid, linear alkyl, long chain Aerobic biodegradation, 202 Siructure-activity relationships 261 Benzenesulfonic acid, linear alkyl, long chain Model ecosystem, aquatic, natural 516 Ciromium Inhibitory (toxic) effects, 48 Substrate concentration effect 48 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Ciromium Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Covered and derivatives Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Covered and derivatives Inhibitory (toxic) effects, 532 River die-away test, 159 Siructure-activity relationships 159 Substrate concentration effect 150 Substrate concentration effe			
Aerobic biodegradation, 313 River die-away test, 313 Aniline and derivatives Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 River die-away test, 159 Structure-activity relationships 159 Substrate concentration effect 159 Substrate concentration effect 159 Substrate concentration effect 159 Substrate concentration effect 159 Senzenesulfonic acid, linear alkyl, long chain Aerobic biodegradation, 202 Structure-activity relationships 261 Benzenesulfonic acid, non-linear alkyl, long chain Model ecosystem, aquatic, natural 316 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 171 Substrate concentration effect 171 Time-course kinetics, 71 Resortion and derivatives Batch vs continuous-flow system 71 Substrate concentration effect 71 Time-course kinetics, 71 Resortion and derivatives Batch vs continuous-flow system 71 Substrate concentration effect 71 Substrate concentration			
Aeroloi Bologegaatation, 313 Aniline and derivatives Cos-ubstrate concentration effect 159 Benzenesulfonic acid, non-linear alkyl, long chain Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 48 Substrate concentration effect 148 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Inhibitory (toxic) effects, 532 River dia-away test, 159 Structure-activity relationships 159 Sinceture-activity relationships 159 Sinceture-activity relationships 159 Sinceture-activity relationships 159 Sinceture-activity relationships 150 Sinceture-activity relationships 151 Sinceture-activity relationships 151 Sinceture-activity relationships 150 Sinceture-activity relationships 151 Sinceture-activity relationships 150 Sinceture-activity relationships 151 Sinceture-activity relationships 151 Sinceture-activity relationships	-		Alkanoic acids and derivatives
Aniline and derivatives Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 Structure-activity relationships 159 Sentensulfonic acid, linear alkyl, long chain Aerobic biodegradation, 202 Structure-activity relationships 261 Sentensulfonic acid, non-linear alkyl, long chain Model ecosystem, aquatic, natural 1516 Substrate concentration effect 159 Substrate concentration effect 159 Sibstrate concentration effect 159 Sibstrate concentration effect 159 Sentensesulfonic acid, linear alkyl, long chain Model ecosystem, aquatic, natural 1516 Substrate concentration effect 159 Substrate concentration effect 171 Time-course kinetics, 71 Pyrocatechol and derivatives Batch vs continuous-flow system 71 Substrate concentration effect 71 Resorcinol and derivatives Batch vs continuous-flow system 71 Substrate concentration effect 71 Resorcinol and derivatives Batch vs continuous-flow system 71 Substrate concentration effect 71 Resorcinol and derivatives Batch vs continuous-flow system 71 Substrate concentration effect 71 Resorcinol and derivatives Batch vs continuous-flow system 71 Substrate concentration effect 71 Resorcinol and derivatives Batch vs continuous-flow system 71 Rime-course kinetics, 71 Resorcinol and derivatives Batch vs continuous-flow system 71 Rime-course kinetics, 71 Resorcinol and derivatives Batch vs continuous-flow system 71 Resorcinol and derivatives Batch vs continuous-flow sy			
Co-substrate concentration effect Substrate concentration effect Substrate concentration effect Time-course kinetics, 71 Phenol and derivatives Batch vs continuous-flow system 163 Amino acids and derivatives Identification of microorganisms 163 Amino acids and derivatives Identification of microorganisms 163 Amino acids and derivatives Identification of microorganisms 163	•		
Inhibitory (toxic) effects, 159 River die-away test, 159 Substrate concentration effect 159 Senzenesulfonic acid, linear alkyl, long chain Aerobic biodegradation, 202 Sruccurre-activity relationships 261 Benzenesulfonic acid, non-linear alkyl, long chain Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 510 Cosubstrate concentration effect 159 River die-away test, 159 Structure-activity relationships 159 Substrate concentration effect 159 River die-away test, 159 Substrate concentration effect 159 Substrate concentration effect 159 Substrate concentration effect 159 River die-away test, 159 Substrate concentration effect 159 Substrate concentration effect 159 Substrate concentration effect 159 River die-away test, 159 Substrate concentration effect 159 Substrate concentration effect 159 Substrate concentration effect 159 Substrate concentration effect 159 River die-away test, 159 Substrate concentration effect 160 Cadmition Inhibitory (toxic) effects, 68 Cellulace and derivatives Aco dyes Freundlich adsorption isotherms 101 Dyes, anthraquinone Freundlich adsorption isotherms 101 Dyes, anthraquinone Freundlich adsorption isotherms 101 Structure-activity relationships 101 Structure-activity relationships 102 Structure-activity relationships 103 Struct			Amines, aliphatic
Inhibitory (toxic) effects, 159 River die-away test, 159 Structure-activity relationships 159 Benzenesulfonic acid, linear alkyl, long chain Aerobic biodegradation, 202 Structure-activity relationships 261 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 159 Bonzenesulfonic acid, non-linear alkyl, long chain Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 159 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 River die-away test, 159 Structure-activity relationships 159 Substrate concentration effect 159 River die-away test, 159 Substrate concentration effect 159 Substrate concentration effect 159 River die-away test, 159 Structure-activity relationships 150 Substrate concentration effect 159 River die-away test, 159 Structure-activity relationships 150 Substrate concentration effect 159 River die-away test, 159 Substrate concentration effect 159 River die-de			Identification of microorganisms
River die-away test. 159 Structure-activity relationships 159 Substrate concentration effect 159 Benzenesulfonic acid. linear alkyl. long chain Aerobic biodegradation, 202 Structure-activity relationships 261 Benzenesulfonic acid. non-linear alkyl. long chain Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 48 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic inhibitory (toxic) effects, 532 Review, 566 Herbeides, monuron type and metabolites Co-substrate concentration effect 159 Substrate concentration effect 159 Structure-activity relationships 101 Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivativ		-	
Structure-activity relationships 159 Substrate concentration effect 159 Benzenesulfonic acid, linear alkyl, long chain Aerobic biodegradation, 202 Siructure-activity relationships 261 Benzenesulfonic acid, non-linear alkyl, long chain Model ecosystem, aquatic, natural 516 Chromum Inhibitory (toxic) effects, 48 Substrate concentration effect 189 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 119 River die-away test, 159 Substrate concentration effect 119 Substrate concentration effect 119 River die-away test, 159 Substrate concentration effect 119 Structure-activity relationships 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Inhibitory (toxic) effects, 532 Polyethylene glycols, fatty ether Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Chloride Activated sludge, fresh water 101 Naphthalene and derivatives Batch vs continuous-flow system 71 Time-course kinetics, 71 Resorcinel and derivatives Batch vs continuous-flow system 71 Time-course kinetics, 71 Resorcinel and derivatives Batch vs continuous-flow system 71 Time-course kinetics, 71 Resorcinel and derivatives Batch vs continuous-flow system 71 Time-course kinetics, 71 Resorcinel and derivatives Batch vs continuous-flow system 71 Time-course kinetics, 71 Resorcinel and derivatives Batch vs continuous-flow system 71 Time-course kinetics, 71 Resorcinel and derivatives Batch vs continuous-flow system 71 Time-course kinetics, 71 Resorcinel and derivatives Batch vs continuous-flow system 71 Time-course kinetics, 71 Resorcinel and derivatives Activated sludge, formaldehyde-inactivated Azo dyes Freundlich adsorption isotherms 101 Dyes, anthraquinone Freundlich adsorption isotherms 101 Structure-activity relationships 101 Naphthalene and derivatives Preundlich adsorption isotherms 101 Naphthalene and derivatives Preundlich adsorption i			Amino acids and derivatives
Structure-activity relationships 159 Substrate concentration effect 159 Benzenesulfonic acid, linear alkyl, long chain Aerobic biodegradation, 202 Structure-activity relationships 261 Benzenesulfonic acid, non-linear alkyl, long chain Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 48 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 Inhibitory (toxic) effects, 532 Nutrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Inhibitory (toxic) eff			
Substrate concentration effect 159 Benzenesulfonic acid, linear alkyl, long chain Aerobic biodegradation, 202 Structure-activity relationships 261 Benzenesulfonic acid, non-linear alkyl, long chain Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 48 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 Substrate concentration effect 159 Substrate concentration effect 48 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 Substrate concentration effect 200 Activated sludge, formaldehyde-inactivated Azo dyes 101 Dyes, anthraquinone Freundlich adsorption isotherms 101 Structure-activity relationships 159 Substrate concentration effect 1601 Caminum Inhibitory (toxic) effects, 35 Chromium Inhibitory (toxic) effects, 35 Overview, 55 Chromium Inhibitory (toxic) effects, 35 Overview, 55 Chro			
Benzenesulfonic acid, linear alkyl, long chain Aerobic biodegradation, 202 Structure-activity relationships 261 Benzenesulfonic acid, non-linear alkyl, long chain Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 Structure-activity relationships 159 Substrate concentration effect 159 Substrate concentration effect 159 Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Inhibitory (toxic) effects, 532 Notrobenzene and derivatives Inhibitory (toxic) effects, 532 Polyethylene glycols, fatty ether Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 68 Cultivated sludge, fresh water Inhibitory (toxic) effects, 68 Cultivated sludge, fresh water Inhibitory (toxic) effects, 55 Inhibitory (toxic) effects, 50 Inhibitory (toxic) effects, 50 Inhibitory (toxic) effects, 68 Chromium Inhibitory (toxic) effects, 52 Inhibitory (toxic) effects, 52 Inhibitory (toxic) effects, 52 Inhibitory (toxic) effects, 52 Inhibitory (tox			Ammonia and salts
Benzenesulfonic acid, linear alkyl, long chain Aerobic biodegradation, 202 Structure-activity relationships 261 Benzenesulfonic acid, non-linear alkyl, long chain Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 48 Dobanol 25-9 Model ecosystem, aquatic, natural inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 Substrate oncentration effect 160 Cadmium Inhibitory (toxic) effects, 53 Copper Inhibitory (toxic) effects, 35 Copper Inhibitory (toxic) effects, 35 Copper Inhibitory (toxic) effects, 35 Cyanide 16ettification of microorganisms 101 Dyes, anthraquinone Freundlich adsorption isotherms 101 Structure-activity relationships 101 St			Identification of microorganisms
Time-course kinetics. 71 Pyrocatechol and derivatives Structure-activity relationships 261 Benzensulfonic acid. non-linear alkyl, long chain Model ecosystem. aquatic. natural 516 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 48 Dobanol 25-9 Model ecosystem, aquatic. natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides. monuron type and mentabolites Co-substrate concentration effect 159 River die-away test, 159 Substrate concentration effect 160 Cadmium Inhibitory (toxic) effects, 53 Copper Inhibitory (toxic) effects, 35 Substrate concentration effect 101 Structure-activity relationships 101 Kinetics and equilibrium studies 101 Naphtalene and derivatives Freundlich adsorption isotherms 101 Naphtalene and derivatives Freundlich adsorption isotherms 101 Naphtalene and derivatives Aerobic biodegradation, 470 Photode			
Aerobic biodegradation, 202 Structure-activity relationships 261 Benzenesulfonic acid, non-linear alkyl, long chain Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 48 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 Sibustrate concentration effect 160 Sibustra	, ,		Brewery wastes
Structure-activity relationships 261 Betzenesulfonic acid. non-linear alkyl, long chain Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 River die-away test, 159 Structure-activity relationships 159 Structure-activity relationships 159 Structure-activity relationships 159 Structure-activity relationships 159 Stubstrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Inhibitory (toxic) effects, 532 Norbenzene and derivatives Innibitory (toxic) effects, 532 Norbenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, fatty ether Aeropic biodegradation, 283 Model ecosystem, aquatic, natural 516 Batch vs continuous-flow system 71 Resorcunel and derivatives Batch vs continuous-flow system 71 Substrate concentration effect, 71 Time-course kinetics, 71 Activated sludge, formaldehyde-inactivated Azo dyes Freundlich adsorption isotherms 101 Dyes, anthraquinone Freundlich adsorption isotherms 101 Structure-activity relationships 101 Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 102 Naphthalene and derivatives Freundl			Operational parameters, 601
Benzenesulfonic acid, non-linear alkyl, long chain Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 48 Substrate concentration effect 48 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 Inhibitory (toxic) effects, 159 Substrate concentration effect 159 Inhibitory (toxic) effects, 159 Inhibitory (toxic) effects, 159 Substrate concentration effect 159 Inhibitory (toxic) effects, 159 Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Inhibitory (toxic) effects, 332 Nitrobenzene and derivatives Inhibitory (toxic) effects, 332 Polyethylene glycols, fatty ether Aerooic biodegradation, 283 Model ecosystem, aquatic, natural 516 Activated sludge, formaldehyde-inactivated Azo dyes Substrate concentration effect 101 Structure-activity relationships 101 Dyes, anthraquinone Freundlich adsorption isotherms 101 Structure-activity relationships 101 Structure-activity relationships 101 Structure-activity relationships 101 Naphthalene and derivatives Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Inhibitory (toxic) effects, 532 Nodel ecosystem, aquatic, natural 516 Activated sludge, formaldehyde-inactivated Azo dyes Inhibitory (toxic) effects, 352 Inhibitory (toxic) effects, 352 Inhibitory (toxic) effects, 352 Inhibitory (toxic) effects, 532 Inhibi			
Benzenesulfonic acid, non-linear alkyl, long chain Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 48 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 River die-away test, 159 Substrate concentration effect 101 Structure-activity relationships 101 Structure-	,		
Time-course kinetics, 71 Cellulose and derivatives Aerobic biodegradation, 55 Coverview, 55 Time-course kinetics, 75 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect		Substrate concentration effect	
Model ecosystem, aquatic, natural 516 Chromium Inhibitory (toxic) effects, 48 Substrate concentration effect 48 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 River die-away test, 159 Substrate concentration effect 159 Substrate concentration effect 159 Substrate concentration effect 169 Lindane and metabolites Inhibitory (toxic) effects, 532 Inhibitory (toxic) effects, 532 Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Inhibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Time-course kinetics, 71 Substrate concentration effect, 71 Time-course kinetics, 71 Substrate concentration effect, 71 Time-course kinetics, 71 Substrate concentration effect, 71 Time-course kinetics, 72 Copper Inhibitory (toxic) effects, 35 Cyanide Identification of microorganisms 163 Penol and derivatives Rerobic biodegradation, 95 Bioreactors compared, 206 Conversion and retention time kinetics, 72 Review, 56 Time-course kinetics, 72 Copper Inhibitory (toxic) effects, 35 Cyanide Identification of microorganisms 163 Penol and derivatives Rerobic biodegradation, 95 Bioreactors compared, 206 Conversion and retention time kinetics, 72 Re			
Since the concentration of fect and the concentration effect are and the concentration effect another and the concentration effect and the concentration effect a		Time-course kinetics, 71	
Inhibitory (toxic) effects, 48 Substrate concentration effect 48 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 River die-away test, 159 Substrate concentration effect 160 Naphthalene and derivatives Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Inhibitory (toxic) effects, 532 Polyethylene glycols, alkyiphenoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Activated sludge, formaldehyde-inactivated Azo dyes Freundlich adsorption isotherms 101 Dyes, anthraquinone Freundlich adsorption isotherms 101 Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and equilibrium studies 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and der		Resorcinol and derivatives	
Substrate concentration effect 48 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 River die-away test, 159 Structure-activity relationships 159 Substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Inhibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Activated sludge, formaldehyde-inactivated Azo dyes Freundlich adsorption isotherms 101 Structure-activity relationships 101 Dyes, anthraquinone Freundlich adsorption isotherms 101 Structure-activity relationships 101 Structure-activity relationships 101 Naphthalene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Explosives, organic 101 Structure-activity relationships 101 Structure-activity relationships 101 Structure-activity relationships 101 Structure-activity relationships 101 Kinetics and equilibrium studies 101 Structure-activity relationships 101 Structure-activity relationships 101 Kinetics and equilibrium studies 101 Structure-activity relationships 101 Structure-activity relationships 101 Kinetics and equilibrium studies 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Kinetics and equilibrium studies 101 Kin	Chromium	Batch vs continuous-flow system	
Substrate concentration effect 48 Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 River die-away test, 159 Substrate concentration effect 159 Substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Inhibitory (toxic) effects, 532 Polyethylene glycols, altyleneoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Substrate concentration effect 101 Naphthalene and derivatives Inhibitory (toxic) effects, 532 Polyethylene glycols, fatty ether Aeropic biodegradation, 283 Model ecosystem, aquatic, natural 516 Inhibitory (toxic) effects, 310 Activated sludge, formaldehyde-inactivated Azo dyes Freundlich adsorption isotherms 101 Structure-activity relationships 101 Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphtha	Inhibitory (toxic) effects, 48	71	
Dobanol 25-9 Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review. 566 Herbicides. monuron type and metabolites Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 Structure-activity relationships 159 Substrate concentration effect 159 Substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Innibitory (toxic) effects, 532 Innibitory (toxic) effects, 532 Innibitory (toxic) effects, 532 Polyethylene glycols, alky ether Aeropic biodegradation, 283 Model ecosystem, aquatic, natural 516 Activated sludge, formaldehyde-inactivated Azo dyes Freundlich adsorption isotherms 101 Dyes, anthraquinone Freundlich adsorption isotherms 101 Structure-activity relationships 101 Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and dequilibrium studies 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and dequilibrium studies 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and dequilibrium studies 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Fr	Substrate concentration effect	Substrate concentration effect, 71	
Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 River die-away test, 159 Substrate concentration effect 159 Substrate concentration effect 159 Substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkyiphenoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Azodyes Freundlich adsorption isotherms 101 Structure-activity relationships 101 Kinetics and equilibrium studies 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Kinetics and equilibrium studies 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Kinetics and equilibrium studies 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Kinetics and equilibrium studies 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Kinetics and equilibrium studies 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Aerobic biodegradation, 470 Polychorobenzenes and derivatives Aerobic biodegradation, 470 Photodegradation, 470 Polyvinyl alcohol Aerobic biodegradation, 55 Overview, 55 Time-course kinetics, 55 Proteins Identification of microorganisms 205 Conversion and retention time kinetics, 206 Identification of microorganisms 205 Conversion and retention time kinetics, 206 Identification of microorganisms 205 Conversion and retention time kinetics, 206 Identification of microorganisms 205 Conversion and retention time kinetics, 206 Identification	48	Time-course kinetics, 71	
Model ecosystem, aquatic, natural 516 Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 River die-away test, 159 Substrate concentration effect 159 Substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy-Aerobic biodegradation, 283 Polyethylene glycols, fatty ether Aeropic biodegradation, 283 Model ecosystem, aquatic, natural 516 Azo dyes Freundlich adsorption isotherms 101 Structure-activity relationships 101 Structure-activity relationships 101 Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Aerobic biodegradation, 4	Dobanol 25-9	Activated sludge, formaldehyde-inactivated	• •
Explosives, organic Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect Inhibitory (toxic) effects, 159 Inhibitory (toxic) effects, 159 Structure-activity relationships I59 Substrate concentration effect I59 Substrate concentration effect I59 Lindane and metabolites Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural Structure-activity relations and equilibrium studies Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural Structure-activity relationships I01 Dyes, anthraquinone Freundlich adsorption isotherms 101 Exincture-activity relationships I01 Structure-activity relationships I01 Naphthalene and derivatives Freundlich adsorption isotherms I01 Structure-activity relationships I01 Naphthalene and derivatives Freundlich adsorption isotherms I01 Naphthalene and derivatives Aerobic biodegradation, 470 Photodegradation, 470 Nitrobenzene and derivatives Aerobic biodegradation, 470 Photodegradation, 470 Nitrobenzene and d	Model ecosystem, aquatic, natural		
Inhibitory (toxic) effects, 532 Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect Inhibitory (toxic) effects, 159 Inhibitory (toxic) effects, 159 River die-away test, 159 Structure-activity relationships 159 Substrate concentration effect 159 Substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkyiphenoxy-Aerobic biodegradation, 283 Polyethylene glycols, fatty ether Aerooic biodegradation, 283 Model ecosystem, aquatic, natural Inhibitory (toxic) effects, 532 Model ecosystem, aquatic, natural Inhibitory (toxic) effects, 532 Review, 566 Inlibitory relationships 101 Dyes, anthraquinone Freundlich adsorption isotherms 101 Kinetics and equilibrium studies 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Kinetics and equilibrium studies 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Kinetics and equilibrium studies 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Aerobic biodegradation, 470 Polychorobenzenes and derivatives Aerobic biodegradation, 470 Polychylene glycols, fatty ether Aerobic biodegradation, 283 Followor	516	Freundlich adsorption isotherms	
Review, 566 Herbicides, monuron type and metabolites Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 River die-away test, 159 Structure-activity relationships 159 Substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Aerobic biodegradation, 283 Polyethylene glycols, alkylphenoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 River die-away test, 159 Structure-activity relationships 159 Lindane and metabolites Innibitory (toxic) effects, 532 Nitrobenzene and derivatives Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Kinetics and equilibrium studies Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Kinetics and equilibrium studies Inhibitory (toxic) effects, 532 Inhibitory (toxic) effects, 203 Nitrate Identification of microorganisms Identification of		101	
Herbicides. monuron type and metabolites Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 River die-away test, 159 Structure-activity relationships 159 Substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Herbicides. monuron type and Structure-activity relationships 101 Dyes, anthraquinone Freundlich adsorption isotherms 101 Structure-activity relationships 101 Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Kinetics and equilibrium studies 101 Kinetics and equilibrium studies 101 Kinetics and equilibrium studies 101 Structure-activity relationships 205, 206 Polychlorobenzenes and derivatives Aerobic biodegradation, 470 Photodegradation, 470 River die-away test, 470 Volatilization, 470 Polyvinyl alcohol Aerobic biodegradation, 55 Overview, 55 Time-course kinetics, 55 Proteins Identification of microorganisms 163 Phenol and derivatives Aerobic biodegradation, 95 Bioreactors compared, 206 Conversion and retention time kinetics, 206 Polychlorobenzenes and derivatives Aerobic biodegradation, 470 Photodegradation, 470 Polyvinyl alcohol Aerobic biodegradation, 55 Overview, 55 Time-course kinetics, 55 Proteins Identification of microorganisms		Kinetics and equilibrium studies	
The bickles. Infolition type and metabolites Co-substrate concentration effect 159 Inhibitory (toxic) effects, 159 River die-away test, 159 Structure-activity relationships 159 Substrate concentration effect 159 Lindane and metabolites 159 Lindane and metabolites 159 Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives 101 Nitrobenzene and derivatives 101 Nitrobenzene and derivatives 101 River die-away test, 159 Substrate concentration effect 159 Lindane and metabolites 101 Naphthalene and derivatives 101 Kinetics and equilibrium studies 101 Naphthalene and derivatives 4eroudlich adsorption isotherms 101 Naphthalene and derivatives 5101 Kinetics and equilibrium studies 101 Kinetics and equilibrium studies 101 Naphthalene and derivatives 4eroudlich adsorption isotherms 101 Kinetics and equilibrium studies		101	
Co-substrate concentration effect 159 Substrate concentration effect 159 Substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkyiphenoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural Medical ecosystem, aquatic, natural Myses, anthraquinone Freundlich adsorption isotherms 101 Kinetics and equilibrium studies Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Aerobic biodegradation, 470 Polychlorobenzenes and derivatives Aerobic biodegradation, 470 Polyvinyl alcohol Aerobic biodegradation, 283 Polyethylene glycols, fatty ether Aeropic biodegradation, 283 Model ecosystem, aquatic, natural Sife Phenol and derivatives Aerobic biodegradation, 95 Bioreactors compared, 206 Conversion and retention time kinetics, 206 Identification of microorganisms 205, 206 Polychlorobenzenes and derivatives Aerobic biodegradation, 470 Polychlorobenzenes Aerobic biodegradation, 470 Polychlorobenzenes Aerobic biodegra			
Dyes, anthraquinone 159 Freundlich adsorption isotherms 101 Conversion and retention time Kinetics and equilibrium studies 159 Structure-activity relationships 101 Structure-activity relationships 101 Structure-activity relationships 101 Structure-activity relationships 101 Structure-activity relationships 205, 206 Identification of microorganisms 20			Phenol and derivatives
Inhibitory (toxic) effects, 159 River die-away test, 159 Structure-activity relationships 159 Substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural Manual assorption isotherms 101 Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 River die-away test, 470 Polyethylene glycols, alkylphenoxy-Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 101 Activated sludge, fresh water Chloride Inhibitory (toxic) effects, 203 Bioreactors compared, 206 Conversion and retention time kinetics, 206 Identification of microorganisms 205, 206 Polychlorobenzenes and derivatives Aerobic biodegradation, 470 Photodegradation, 470 Polyvinyl alcohol Aerobic biodegradation, 55 Overview, 55 Time-course kinetics, 55 Proteins Identification of microorganisms Identification of microorganisms 101 Conversion and retention time kinetics, 206 Identification of microorganisms 205, 206 Polychlorobenzenes and derivatives Aerobic biodegradation, 470 Polyvinyl alcohol Aerobic biodegradation, 55 Overview, 55 Time-course kinetics, 55 Proteins Identification of microorganisms			
River die-away test, 159 Structure-activity relationships 159 Substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy-Aerobic biodegradation, 283 Polyethylene glycols, fatty ether Aerobic biodegradation, 283 Model ecosystem, aquatic, natural Structure-activity relationships 101 Structure-activity relationships 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 River die-away test, 470 Volatilization, 470 Polyvinyl alcohol Aerobic biodegradation, 470 Polyvinyl alcohol Aerobic biodegradation, 55 Overview, 55 Time-course kinetics, 55 Proteins Identification of microorganisms			
Structure-activity relationships 159 Substrate concentration effect 159 Substrate concentration effect 159 Substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy- Aerobic biodegradation, 283 Polyethylene glycols, fatty ether Aerobic biodegradation, 283 Model ecosystem, aquatic, natural Sife Structure-activity relationships 205, 206 Polychlorobenzenes and derivatives Aerobic biodegradation, 470 River die-away test, 470 Volatilization, 470 Polyvinyl alcohol Aerobic biodegradation, 55 Overview, 55 Time-course kinetics, 55 Proteins Identification of microorganisms			Conversion and retention time
Substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkyiphenoxy-Aerobic biodegradation, 283 Polyethylene glycols, fatty ether Aerooic biodegradation, 283 Model ecosystem, aquatic, natural Substrate concentration effect 101 Naphthalene and derivatives Freundlich adsorption isotherms 101 Kinetics and equilibrium studies 101 Kinetics and equilibrium studies 101 Kinetics and equilibrium studies 101 Structure-activity relationships 101 Activated sludge, fresh water Chloride Inhibitory (toxic) effects, 203 Identification of microorganisms 105, 205, 206 Polychlorobenzenes and derivatives Aerobic biodegradation, 470 Photodegradation, 470 River die-away test, 470 Volatilization, 470 Polyvinyl alcohol Aerobic biodegradation, 55 Overview, 55 Time-course kinetics, 55 Proteins Identification of microorganisms			kinetics, 206
Substrate concentration effect 159 Lindane and metabolites Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy- Aerobic biodegradation, 283 Polyethylene glycols, fatty ether Aeropic biodegradation, 283 Model ecosystem, aquatic, natural 516 Naphthalene and derivatives Freundlich adsorption isotherms 101 Kinetics and equilibrium studies 101 Activated sludge, fresh water Chloride Inhibitory (toxic) effects, 203 Identification of microorganisms			
Lindane and metabolites Lindane and metabolites Inhibitory (toxic) effects, 532 Nutrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkyiphenoxy- Aerobic biodegradation, 283 Polyethylene glycols, fatty ether Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Naphthalene and derivatives Freundlich adsorption isotherms 101 Kinetics and equilibrium studies 101 River die-away test, 470 Volatilization, 470 Polyvinyl alcohol Aerobic biodegradation, 55 Overview, 55 Time-course kinetics, 55 Proteins Identification of microorganisms			
Lindane and metabolites Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy- Aerobic biodegradation, 283 Polyethylene glycols, fatty ether Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Freundlich adsorption isotherms Inolatory (toxic) effects, 532 Itol Nitrobenzene and derivatives Kinetics and equilibrium studies Itol River die-away test, 470 Volatilization, 470 Polyvinyl alcohol Aerobic biodegradation, 470 River die-away test, 470 Volatilization, 470 Polyvinyl alcohol Aerobic biodegradation, 470 Proteins Itim-course kinetics, 55 Proteins Identification of microorganisms			
Inhibitory (toxic) effects, 532 Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy- Aerobic biodegradation, 283 Polyethylene glycols, fatty ether Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Ninetics and equilibrium studies Kinetics and equilibrium studies 101 Structure-activity relationships 101 Activated sludge, fresh water Chloride Inhibitory (toxic) effects, 203 Froteins Identification of microorganisms	Lindane and metabolites		
Nitrobenzene and derivatives Innibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy- Aerobic biodegradation, 283 Polyethylene glycols, fatty ether Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Kinetics and equilibrium studies 101 Structure-activity relationships Aerobic biodegradation, 283 101 Activated sludge, fresh water Chloride Inhibitory (toxic) effects, 203 Kiver die-away test, 470 Volatilization, 470 Polyvnyl alcohol Aerobic biodegradation, 55 Overview, 55 Time-course kinetics, 55 Proteins Identification of microorganisms	Inhibitory (toxic) effects, 532		
Innibitory (toxic) effects, 532 Polyethylene glycols, alkylphenoxy- Aerobic biodegradation, 283 Polyethylene glycols, fatty ether Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Notatinzanon, 470 Polyvinyl alcohol Aerobic biodegradation, 55 Overview, 55 Time-course kinetics, 55 Proteins Inhibitory (toxic) effects, 203 Identification of microorganisms	Nitrobenzene and derivatives		· · · · · · · · ·
Aerobic biodegradation, 283 Polyethylene glycols, fatty ether Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Structure-activity relationships Aerobic biodegradation, 55 Overview, 55 Time-course kinetics, 55 Proteins Identification of microorganisms	Innibitory (toxic) effects, 532	•	
Aerobic biodegradation, 283 Polyethylene glycols, fatty ether Aerobic biodegradation, 283 Model ecosystem, aquatic, natural 516 Activated sludge, fresh water Chloride Inhibitory (toxic) effects, 203 Chloride Inhibitory (toxic) effects, 203 Identification of microorganisms		Structure-activity relationships	• •
Activated sludge, fresh water Aeropic biodegradation, 283 Model ecosystem, aquatic, natural 516 Activated sludge, fresh water Chloride Inhibitory (toxic) effects, 203 Identification of microorganisms			
Model ecosystem, aquatic, natural 516 Chloride Inhibitory (toxic) effects, 203 Identification of microorganisms		Activated sludge, fresh water	
Inhibitory (toxic) effects, 203 Identification of microorganisms		Chloride	
	•		
	210	Salinity	

Activated sludge, industrial (cont'd) Sulfate	Activated sludge, industrial, continuous- flow (cont'd)	Activated sludge, municipal (cont'd)
Identification of microorganisms	Ketones, aliphatic	Aldehyaes
163	Metabolic pathways, 569	Identification of microorganisms
Textile wastes	Methanol, phenol, isopropanol, acerone	164
Aerobic biodegradation, 55, 470	mixture	Alkanoic acids and derivatives
Overview, 55	Metabolic pathways, 569	Anaerobic algestion reactor, 15 Fermentation, methanogenic, 15
Photodegradation, 470	Nickel	Alkanoic acids and derivatives, long
River die-away test, 470	Inhibitory (toxic) effects, 167	chain
Time-course kinetics, 55	Phenol and derivatives	Monad kinetics constants, 365
Volatilization, 470	Metabolic pathways, 569	Alkanoic acids and derivatives.
Thiocyanic acid and salts	Zinc	polybasic
Bioreactors compared, 205	Inhibitory (toxic) effects, 167	Aerobic biodegradation, 462
Conversion and retention time	Activated sludge, industrial, porous-pot,	Correlative test evaluations
kinetics, 205	continuous-flow	151
Identification of microorganisms	Carbamic acid and derivatives	Detergent formulation effect
205, 206	Aerobic biodegradation, 167	462 Daniel a distinction 462
Urea and derivatives	Inhibitory (toxic) effects, 167	Diurnal variations, 462
Identification of microorganisms	Copper	Alkanoic acids, cyclic Anaerobic digestion reactor, 15
163 Activated sludge, industrial and municipal	Inhibitory (toxic) effects, 167 Cutting oils	Correlative test evaluations
Alcohols, primary aliphatic	Aerobic biodegradation, 167	151
Aerobic biodegradation, pilot plant,	Inhibitory (toxic) effects, 167	Fermentation, methanogenic, 15
237	Nickel	Alkanoic acids, long chain, esters
Aniline and derivatives	Inhibitory (toxic) effects, 167	Aerobic biodegradation, 457
Inhibitory (toxic) effects, 13	Zinc	Alkenoic acids and derivatives, long
Respirometric studies, 13	Inhibitory (toxic) effects, 167	chain
Structure-activity relationships	Activated sludge, Nocardia-inoculated	Monad kinetics constants, 365
13	Alcohols, primary aliphatic	Alkyl sulfates, long chain
Biphenyi and derivatives	Identification of microorganisms	Aerobic biodegradation, 457
Inhibitory (toxic) effects. 13	282	Correlative test evaluations
Respirometric studies, 13	Phthalic acid and derivatives	151
Structure-activity relationships 13	Identification of microorganisms	Amides, aliphauc
De-icer, aircraft + wastewater, airport	281, 282	Inhibitory (toxic) effects, 348
Aerobic biodegradation, pilot plant,	Pyrocatechol and derivatives	Amines, aliphatic
237	Identification of microorganisms	Correlative test evaluations
Naphthalene and derivatives	282	Amino acids and derivatives
Inhibitory (toxic) effects, 13	Activated sludge, laboratory-pilot plant	Anaerobic digestion reactor, 15
Respirometric studies, 13	Boron	Fermentation, methanogenic, 15
Structure-activity relationships	Inhibitory (toxic) effects, 562	Aniline and derivatives
13	Activated sludge, multi-stage column	Correlative test evaluations
Propylene glycols	Ammonia and salts	151
Aerobic biodegradation, pilot plant,	Substrate concentration effect	Distribution and rate accumulation
237	209	270
Starch and derivatives	Cyanide	Inhibitory (toxic) effects, 369
Structure-activity relationships	Substrate concentration effect 209	Structure-activity relationships
508 Substrate concentration effect	Phenol and derivatives	369
508	Substrate concentration effect	Anthranilic acid
Xylenes and derivatives	209	Correlative test evaluations
Inhibitory (toxic) effects, 13		Azo dyes
Respirometric studies, 13	Activated sludge, municipal	Inhibitory (toxic) effects, 369
Structure-activity relationships	Adipic acid and derivatives	Structure-activity relationships
13	Anaerobic digestion reactor, 15	369
Activoted sludge industrial annuing	Correlative test evaluations	Benzenesultonic acid, alkyl, long chair
Activated sludge, industrial, continuous- flow	151	Aerobic biodegradation, 421
Alcohols, primary aliphatic	Fermentation, methanogenic, 15 Alcohols, alicyclic	Sludge acclimatization process
Metabolic pathways, 569	Anaeropic digestion reactor, 15	421
Alcohols, secondary aliphatic	Fermentation, methanogenic, 15	Benzenesulfonic acid and non-alkyl
Metabolic pathways, 569	Alcohols, primary aliphatic	substituted derivatives
Carbamic acid and derivatives	Correlative test evaluations	Correlative test evaluations
Aerobic biodegradation, 167	151	Inhibitory (toxic) effects, 369
Inhibitory (toxic) effects, 167	Identification of microorganisms	Structure-activity relationships
Copper	164	369
Inhibitory (toxic) effects, 167	Nutritional parameters, 305	Benzenesulfonic acid, linear alkyl, long
Cutting oils	Alcohols, tertiary aliphatic	chain
Aerobic biodegradation, 167	Correlative test evaluations	Aerobic biodegradation, 275
Inhibitory (toxic) effects, 167	151	

Activated sludge, municipal (cont'd)	Activated sludge, municipal (cont'd)	Activated sludge, municipal (cont'd)
Correlative test evaluations	Aerobic biodegradation, 79 Inhibitory (toxic) effects, screening,	Structure-activity relationships 527
Operational parameters, 275	547	Naphthalene and derivatives
Benzenesulfonic acid, non-linear alkyl, long chain	Dyes, basic Aerobic and anaerobic digestion	Aerobic and anaerobic digestion reactors, 547
Correlative test evaluations	reactors, 547	Inhibitory (toxic) effects, 369
151	Aerobic biodegradation, 79	Inhibitory (toxic) effects, screening
Benzenesulfonic acid, S-substituted alkyl	Inhibitory (toxic) effects, screening.	547
Aerated chamber die-away test	547	Structure-activity relationships
416	Dyes, direct	369
River die-away test, 416	Aerobic and anaerobic digestion	Nitrobenzene and derivatives
Shake flask process, 416	reactors, 547	Aerobic biodegradation, 79
Structure-activity relationships	Inhibitory (toxic) effects, screening,	Correlative test evaluations
416	547	151
Benzoic acid and derivatives	Dyes, disperse	Distribution and rate accumulation 270
Anaerobic digestion reactor, 15	Aerobic and anaerobic digestion reactors, 547	
Batch vs continuous-flow system		Inhibitory (toxic) effects, 369 Structure-activity relationships
461	Inhibitory (toxic) effects, screening, 547	369
Biomass yield, effect on, 461	Dyes, mordant	NTA and salts
Correlative test evaluations, 151	Aerobic and anaerobic digestion	Aerobic biodegradation, 411
Fermentation, methanogenic, 15	reactors, 547	462, 563
Operational parameters, 461 Benzothiazole and derivatives	Inhibitory (toxic) effects, screening,	Detergent formulation effect
Aerobic biodegradation, 79	547	462
Biphenyl and derivatives	Dyes, sulfur	Diurnal variations, 462
Aerobic biodegradation, 528	Aerobic and anaerobic digestion	Heavy metals effect, 563
Metabolic pathways, 528	reactors, 547	Phenol and derivatives
Structure-activity relationships	Inhibitory (toxic) effects, screening,	Aerobic biodegradation, 79
528	547	Phloroglucinol
Cadmium	Dyes, vat	Anaerobic digestion reactor, 15
Inhibitory (toxic) effects, 361	Aerobic and anaerobic digestion	Fermentation, methanogenic, 15
Sludge deflocculation, 361	reactors, 547	Poly(ethylene oxide-propylene)
ε-Caprolactam	inhibitory (toxic) effects, screening,	Correlative test evaluations
Nutritional parameters, 305	547	151
Cellulose and derivatives	Ecolytes	Polychlorinated biphenyls
Correlative test evaluations	Biodegradation, rates compared 176, 245	Aerobic biodegradation, 201 528
Chloroalkylenes	EDTA and salts	Distribution and rate accumulation
Aerobic biodegradation, 201	Correlative test evaluations	270
528	151	Metabolic pathways, 528
Metabolic pathways, 528	Explosives, organic	Structure-activity relationships
Structure-activity relationships	Activated sludge, synthetic, 62	201, 528
201, 528	Aerobic biodegradation, 62, 334	Polychlorobenzenes and derivatives
Chromium	Metabolic pathways, 334	Batch vs continuous-flow system
Aerobic biodegradation, 79	Herbicides, atrazine type	461
Inhibitory (toxic) effects, 478	Distribution and rate accumulation	Biomass yield, effect on, 461
Operational parameters, 478	270	Distribution and rate accumulation
Cinnamic acid and derivatives	Herbicides, monuron type and	270
Anaerobic digestion reactor, 15	metabolites	Inhibitory (toxic) effects, 478
Fermentation, methanogenic, 15	Distribution and rate accumulation	Operational parameters, 461
Cresols and derivatives	270	478
Inhibitory (toxic) effects, 369	Hydroquinone and derivatives	Polychlorocyclopentadiene dimers
Structure-activity relationships	Correlative test evaluations	Distribution and rate accumulation
369	151 Variance Malauria	270
Cyanuric acid and derivatives	Ketones, aliphatic	Polyesters
Anaerobic biodegradation, 441 Cycloaliphatics, substituted	Correlative test evaluations, 151 Lignin sulfonates	Isolate, grain processing wastes 554
	Aerobic and anaerobic digestion	Polyethylene
Anaerobic digestion reactor, 15	reactors, 547	Biodegradation, rates compared
Fermentation, methanogenic, 15 Dobanol 45-7	Inhibitory (toxic) effects, screening,	245
Aerobic biodegradation, 75	547	Polyethylene glycols, alkylphenoxy-
Dyes	Mercury, morganic	Aerobic biodegradation, 421
Inhibitory (toxic) effects, 369	Inhibitory (toxic) effects, 361	Sludge acclimatization process
Structure-activity relationships	Sludge deflocculation, 361	421
369	Metals, toxic	Polyethylene glycols, fatty ether
Dyes, acid	Aerobic biodegradation, 375	Aerobic biodegradation, 421
Aerobic and anaerobic digestion	Microbial population, soils	Sludge acclimatization process
reactors, 547	Aerobic biodegradation, 527	421
(Cactors, 547	. icrosic olodesi adation, 527	721

Activated sludge, municipal (cont'd) Polypropylene	Activated sludge, municipal, continuous- flow (cont'd)	Activated sludge, municipal, porous-pot, continuous-flow (cont'd)
Biodegradation, rates compared 245	Chromium Freundlich adsorption isotherms	Inhibitory (toxic) effects, 167
Polystyrenes Biodegradation, rates compared	362 Kinetics and equilibrium studies	Nickel Inhibitory (toxic) effects, 167
176, 245 Polyvinyl alcohol	362 Michaelis-Menten coefficients, 362	Activated sludge, municipal + starch plant wastes
Correlative test evaluations	Operational parameters, 362 Copper	Starch and derivatives Operational parameters, 419
Pyridine and derivatives	Inhibitory (toxic) effects, 167 Cutting oils	Starch plant wastes effect, 419
Correlative test evaluations 151	Aerobic biodegradation, 167 Anaerobic biodegradation, 167	Activated sludge + night soils, municipal Alkanoic acids and derivatives
Pyrocatechol and derivatives Correlative test evaluations	Inhibitory (toxic) effects, 167 Cyanuric acid and derivatives	Aerobic biodegradation, 229 Activated sludge, nitrifying
151 Quaternary ammonium compounds	Aerobic biodegradation, 441	Fertilizer wastes, nitrogenous Aerobic biodegradation, 353
Aerobic digestion reactor, pilot plant, 125	Dyes Inhibitory (toxic) effects, 241	Nitrification, 353 Activated sludge, non-acclimated
Salicylic acid and derivatives Inhibitory (toxic) effects, 369	Nitrification, effects on, 241 Lead	Alcohols, primary aliphatic
Structure-activity relationships 369	Freundlich adsorption isotherms 362	Aerobic biodegradation, 291 Aldehydes
Sugars and derivatives Aerobic biodegradation, 457	Kinetics and equilibrium studies - 362	Aerobic biodegradation, 291 Inhibitory (toxic) effects, 21
Sulfamilic acid and derivatives Correlative test evaluations	Michaelis-Menten coefficients 362	Respirometric studies, 21 Alkanoic acids and derivatives, long
151 Sulfide	Operational parameters, 362 Mercury, inorganic	chain Inhibitory (toxic) effects, 454
Aerobic biodegradation, 79	Freundlich adsorption isotherms 362	Rate and selective adsorption 454
Tannery wastes Aerobic biodegradation, 79	Kinetics and equilibrium studies 362	Benzenesultonic acid, linear alkyl, long chain
Tin compounds, organic Inhibitory (toxic) effects, 478	Michaelis-Menten coefficients 362	Aerobic biodegradation, 202 Biphenyl and derivatives
Operational parameters, 478 Zinc	Operational parameters, 362 Nickel	Inhibitory (toxic) effects, 454 Rate and selective adsorption
Inhibitory (toxic) effects, 361 Sludge deflocculation, 361	Freundlich adsorption isotherms	454 Cadmium
Activated sludge, municipal and synthetic. Antibiotics	362 Inhibitory (toxic) effects, 167	Inhibitory (toxic) effects, 343 Cirrasols
Continuous and intermittent flows compared, 238	Kinetics and equilibrium studies 362	Inhibitory (toxic) effects, 432 Fuel oil
Inhibitory (toxic) effects, 238	Michaelis-Menten coefficients 362	Inhibitory (toxic) effects, 454 Rate and selective adsorption
Activated sludge, municipal, continuous- flow	Operational parameters, 362 Nitrobenzene and derivatives	454
Ammunition plant wastes Aerobic biodegradation, 360	Inhibitory (toxic) effects, 161 Substrate concentration effect	Mercury, inorganic Inhibitory (toxic) effects, 343
Inhibitory (toxic) effects, 360 Aniline and derivatives	TNT 161	Volatilization, 356 Nickel
Inhibitory (toxic) effects, 241 Nitrification, effects on, 241	Aerobic biodegradation, 360 Inhibitory (toxic) effects, 360	Inhibitory (toxic) effects, 343 Photoprocess wastes
Biphenyl and derivatives Aerobic biodegradation, 496	Zinc Freundlich adsorption isotherms	Inhibitory (toxic) effects, 21 Respirometric studies, 21
Sludge acclimatization process 496	362 Inhibitory (toxic) effects, 167	Polyethylene glycols, fatty ester Inhibitory (toxic) effects, 432
Boron Inhibitory (toxic) effects, 562	Kinetics and equilibrium studies 362	Polyethylene glycols, fatty ether Inhibitory (toxic) effects, 432
Cadmium Freundlich adsorption isotherms	Michaelis-Menten coefficients 362	Polyvinyl alcohol Inhibitory (toxic) effects, 454
362 Kinetics and equilibrium studies	Operational parameters, 362 Activated sludge, municipal, porous-pot,	Rate and selective adsorption 454
362 Michaelis-Menten coefficients	continuous-flow Carbamic acid and derivatives	Quaternary ammonium compounds Aerobic digestion reactor, pilot
362	Aerobic biodegradation, 167	plant, 125 Starch and derivatives
Operational parameters, 362 Carbamic acid and derivatives	Inhibitory (toxic) effects, 167 Copper	Inhibitory (toxic) effects, 454 Rate and selective adsorption
Aerobic biodegradation, 167 Anaerobic biodegradation, 167	Inhibitory (toxic) effects, 167 Cutting oils	454 Textile wastes
Inhibitory (toxic) effects, 167	Aerobic biodegradation, 167	

Activated sludge, non-acclimated (cont'd) Activated sludge, non-acclimated, municipal Activated sludge process (cont'd) Review, 221 Inhibitory (toxic) effects, 454 (cont'd) Instrumentation and sampling techni-Rate and selective adsorption, 454 Trickling filters, 18 ques Review, 221 Triton X100 Inhibitory (toxic) effects, 343 Aerobic biodegradation, 18 Kinetic studies and mathematical models Trickling filters, 18 Activated sludge, non-acclimated, municipal Review, 221 Alkanes, long chain, branched Activated sludge, non-acclimated, Microbial analyses activity and ecology municipal, continuous-flow 255 Review, 221 Poly(α -hydroxyacrylic acid) Alkanes, long chain, linear, 255 Pollutants and organics determinations Alkenes, 255 Time-course kinetics, 350 Review, 221 Amines, long chain Activated sludge, OECD-specified Survival of pathogenes Aerobic biodegradation, 18 Adipic acid and derivatives Review, 221 Trickling filters, 18 Interlaboratory comparison, 590 Activated sludge processes Cellulose and derivatives Static vs continuous activation Conceptual model Gravimetric assessment, 420 method, 590 Computational analysis, 147 Hach oxidation, 420 Alcohols, primary aliphatic Operational parameters, 147 Respirometric studies, 420 Interlaboratory comparison, 590 Activated sludge, propanil-enriched Emkapyl 1839 Static vs continuous activation Aniline and derivatives Aerobic biodegradation, 18 method, 590 Mineralization, 585 Trickling filters, 18 Amines, poly-, aliphatic Activated sludge, recycled concentration Enzymes Interlaboratory comparison, 590 Gravimetric assessment, 420 Sugars and derivatives Static vs continuous activation Hach oxidation, 420 Biomass yield, effect on, 319 method, 590 Respirometric studies, 420 Shock loadings effect, 319 ₹-Caprolactam Ethomeens Activated sludge + rice bran Interlaboratory comparison, 590 Aerobic biodegradation, 18 Static vs continuous activation Cyanide Trickling filters, 18 method, 590 Aerobic digestion reactor, 139 Fuel oil, 255 EDTA and salts 140, 142 Hexapon Inhibitory (toxíc) effects, 139 Interlaboratory comparison, 590 Aerobic biodegradation, 18 Kinetics and equilibrium studies Static vs continuous activation Trickling filters, 18 method, 590 142 Lauropal Michaelis-Menten coefficients Naphthalene and derivatives Aerobic biodegradation, 18 Interlaboratory comparison, 590 142 Trickling filters, 18 Operational parameters, 140 Static vs continuous activation Marlipol Sludge acclimatization process method, 590 Aerobic biodegradation, 18 Polycyclic aromatic hydrocarbons 142 Trickling filters, 18 Interlaboratory comparison, 590 Activated sludge, salt water Plurafac RA40 Static vs continuous activation Chloride Aerobic biodegradation, 18 method, 590 Inhibitory (toxic) effects, 203 Trickling filters, 18 Polyethylene glycols, fatty ether Nitrification, effects on, 203 Pluronics Interlaboratory comparison, 590 Aerobic biodegradation, 18 Static vs continuous activation Inhibitory (toxic) effects, 203 Trickling filters, 18 method, 590 Nitrification, effects on, 203 Polyethylene glycois, fatty ester Sugars and derivatives Aerobic biodegradation, 18 Activated sludge, second-stage Interlaboratory comparison, 590 Trickling filters, 18 Ammonia and salts Static vs continuous activation Polyethylene glycols, fatty ether Laboratory-pilot plant studies method, 590 Aerobic biodegradation, 18 145 Activated sludge, oxygen-activated, Operational parameters, 145 Trickling filters, 18 municipal Polymers, bio-Coke oven wastes Polyvinyl alcohol Gravimetric assessment, 420 Laboratory-pilot plant studies Respirometric studies, 64 Hach oxidation, 420 145 Textile wastes Respirometric studies, 420 Operational parameters, 145 Respirometric studies, 64 Proteins Cyanide Activated sludge, phosphate-restricted, Gravimetric assessment, 420 Laboratory-pilot plant studies municipal Hach oxidation, 420 145 Cadmum Respirometric studies, 420 Operational parameters, 145 Aerobic biodegradation, 577 Renex 20 Thiocyanic acid and salts Aerobic biodegradation, 18 Copper Laboratory-pilot plant studies Aerobic biodegradation, 577 Trickling filters, 18 145 Starch and derivatives Activated sludge, primary and secondary Operational parameters, 145 Gravimetric assessment, 420 Aldehydes Activated sludge, semi-continuous flow Hach oxidation, 420 Aerobic biodegradation, 472 Adipic acid and derivatives Respirometric studies, 420 Phenol and derivatives Aerobic biodegradation, 435 Sugars and derivatives Aerobic biodegradation, 472 Alkanoic acids and derivatives. Aerobic biodegradation, 18 Phenol-formaldehyde resin polybasic Gravimetric assessment, 420 Aerobic biodegradation, 472 Aerobic biodegradation, 157 Hach oxidation, 420 Activated sludge process Alkanoic acids, long chain, esters, 286 Respirometric studies, 420

Biochemistry

Activated sludge, semi-continuous flow	Activated sludge + synthetic sewage	Adipic acid and derivatives (cont'd)
(cont'd)	(cont'd)	Activated sludge, municipal
Antibiotics	Amides, aliphane	Anaerobic digestion reactor, 15
Sludge acclimatization process 525	Aerobic biodegradation, 52	Correlative test evaluations
Time-course kinetics, 525	Aniline and derivatives Correlative test evaluations, 233	151
Benzenesulfonic acid, linear alkyl, long	Benzenesulfonic acid, linear alkyl, long	Fermentation, methanogenic, 15
chain, non-terminal, 286	chain	Activated sludge, OECD-specified
Polyethylene glycols, fatty ether, 286	Correlative test evaluations	Interlaboratory comparison, 590 Static vs continuous activation
Quaternary ammonium compounds, 286	233	method, 590
Santicizers	Benzenesulfonic acid, non-linear alkyl,	Activated sludge, semi-continuous flo
Aerobic biodegradation, 435	long chain	Aerobic biodegradation, 435
Activated sludge + sewage, municipal	Aerobic biodegradation, 456	Alternaria sp
Alkanoic acids and derivatives	Correlative test evaluations	Isolation of products, 524
Aerobic biodegradation, 229	233	Bacıllus sp. 118
Activated sludge, sewage plant	Metabolic pathways, 456	Brevibacterium sp., 118
Photoprocess wastes	Structure-activity relationships	Methanobacterium sp
Inhibitory (toxic) effects, 506	456	Anaerobic digestion reactor, 15
Operational parameters, 506	BHT Metabolic pathways, 228	Fermentation, methanogenic, 15
Respirometric studies, 506	Time-course kinetics, 228	Microbial population, soils
Activated sludge, single and two-stage reac-	Carbamic acid and derivatives	Aerobic vs anaerobic conditions
tors	Aerobic biodegradation, 52	119
Fluorescent brighteners	Cresols and derivatives	Structure-activity relationships
Anaerobic biodegradation, 146	Metabolic pathways, 228	UV irradiation effect, 119
Stilbene and derivatives	Time-course kinetics, 228	Protaminobacter sp. 118
Anaerobic biodegradation, 146	Herbicides, atrazine type	Pseudomoras sp
Styrene and derivatives	Correlative test evaluations	Anaerobic biodegradation, 298
Anaerobic biodegradation, 146	233	Metabolic pathways, 298
Activated sludge, soap waste	Mercury, morganic	Aerated stabilization basins
Polyvinyl alcohol, 490	Adsorption and volatilization	Pulp and paper wastes
Starch and derivatives, 490	357	Review, 556
Textile wastes, 490	Operational parameters, 357	Aerobacter sp
Activated sludge + Pseudomonas sp	Phenol and derivatives Correlative test evaluations	Alkyl sulfoxides
Polyvinyl alcohol, 490 Starch and derivatives, 490	233	Identification of microorganisms
Textile wastes, 490	Polychlorinated biphenyls	295
	Aerobic biodegradation, 247	Sludge acclimanization process
Activated sludge, synthetic Alkanoic acids and derivatives	Anaerobic biodegradation, 247	295
Flocculation, nutritional effects, 36	Inhibitory (toxic) effects, 247	Phenol and derivatives
Benzoic acid and derivatives	Polychlorobenzenes and derivatives	Identification of microorganisms
Aerobic biodegradation, 385	Aerobic biodegradation, 52	295
Anaerobic biodegradation, 385	Polyethylene glycols, alkylphenoxy-	Sludge acclimatization process 295
River die-away test, 385	Correlative test evaluations	
Chromium	233	Aeromonas sp Phenol and derivatives
Inhibitory (toxic) effects, 35	Polyethylene glycols, fatty ether Correlative test evaluations	Identification of microorganisms
Copper	233	71
Inhibitory (toxic) effects, 35	Activated sludge, tannery-activated	Quaternary ammonium compounds, 1
Explosives, organic Activated sludge, municipal, 62	Amino acids and derivatives	Aflatoxins
Naphthalene and derivatives	Decomposability, 513	Aspergillus sp
Aerobic biodegradation, 162	Tannery wastes	Mesophilic temperature effect
Inhibitory (toxic) effects, 162	Decomposability, 513	104
Sugars and derivatives	Activated sludge, UNOX pure oxygen	Nutritional effects, 104
Flocculation, nutritional effects	technology	Substrate concentration effect
36	Coal gasification wastes	104
Xylenols and derivatives	Overview, 187	Alcaligenes sp
Flocculation, nutritional effects	Scheme of test facility, 187	Alcohols, primary aliphatic
36	Petrochemical wastes Overview, 187	Idenufication of microorganisms 164
Activated sludge, synthetic, continuous-flow	Scheme of test facility, 187	Aldehydes
Alcohols, primary aliphatic Aerobic biodegradation, 34	Silicones	Identification of microorganisms
Inhibitory (toxic) effects, 34	Overview, 187	164
Activated sludge + synthetic sewage	Scheme of test facility, 187	Metabolic pathways, 37
Activated studge + synthetic sewage Aldehydes	Adipic acid and derivatives	Alkanes, long chain, branched
Aerobic biodegradation, 52	see also Alkanoic acids and derivatives	Mesophilic temperature, effect
Alkyl sulfates, long chain	Achromobacter sp. 118	567
	Metabolic pathways, 41	Psychrophilic temperature effect
233		567

Alleanee	Deluchlarehansanes and derivatives	Alcohols, ancyclic (cont a)
Alkenes	Polychlorobenzenes and derivatives	Gram-positive bacteria
Structure-activity relationships 523	Inhibition of benzoic acid turnover, 410	Inhibitory (toxic) effects, 38
		Lagoons, aerated, industrial site
Alkenoic acids and derivatives	Structure-activity relationships	Aerobic biodegradation, 573
Metabotic pathways, 37	410 Polyesters	Detoxification, 573
Amides, aliphatic Structure-activity relationships	Structure-activity relationships	Methanobacterium sp
120	503	Anaerobic digestion reactor, 15
Amides, aliphatic, long chain	Polyethylene glycols, fatty ester	Fermentation, methanogenic, I
	Aerobic biodegradation, 431	Pseudomonas sp
Structure-activity relationships 120	Polyethylene glycols, fatty ether	Inhibitory (toxic) effects, 38
	Aerobic biodegradation, 431	Sewage, municipal
Aromatic compounds, dicyclic	Pyrocatechol and derivatives	Respirometric studies, 548
Structure-activity relationships	Metabolic pathways, 37	<i>Vibrio</i> sp
523	Stilbene and derivatives	Inhibitory (toxic) effects, 38
Benzene and derivatives	Structure-activity relationships	Alcohols, benzylic
Metabolic pathways, 37	523	Actinomyces sp
Structure-activity relationships	Tetralin and derivatives	Structure-activity relationships
523	Structure-activity relationships	153
Benzenesulfinic acid and derivatives	523	Activated sludge
Metabolic pathways, 37	Toluene and derivatives	Respirometric studies, 30
Benzenesulfonic acid, alkyl, short chain	Metabolic pathways, 37	Structure-activity relationships
Metabolic pathways, 37	Toluic acid and derivatives	153, 473
Benzenesulfonic acid and non-alkyl	Inhibition of benzoic acid turnover,	Bacıllus sp
substituted derivatives	410	Structure-activity relationships
Metabolic pathways, 37	Structure-activity relationships	153, 473
Benzenesulfonic acid, linear alkyl, long	410	Bacterium sp
chain	Xylenes and derivatives	Structure-activity relationships
Metabolic pathways, 37	Inhibition of benzoic acid turnover,	153
Benzoic acid and derivatives	410	Chromobacterium sp
Inhibition of benzoic acid turnover,		Structure-activity relationships
410	Structure-activity relationships 410	153
Metabolic pathways, 37	Alcohol distillery wastes	Micrococcus sp
Structure-activity relationships	Activated sludge	Structure-activity relationships
410	Anaerobic digestion reactor, 449	153
Biphenyl and derivatives	Alcohols	Mycobacterium sp
Aerobic biodegradation, 138	see also Cellulose and derivatives;	Structure-activity relationships
Structure-activity relationships	Polyethylene glycols, etc.;	153
138, 523	Polyvinyl alcohol; Propylene	Pseudomonas sp
Cirrasols	glycols; Starch and derivatives;	Psychrophilic temperature effect
Aerobic biodegradation, 431	Sugars and derivatives; Terpene	250 -
Cresols and derivatives	compounds	Structure-activity relationships
Metabolic pathways, 37	Sewage, municipal	153, 473
Crude oil	Respirometric studies, 548	Time-course kinetics, 250
Mesophilic temperature, effect		Sarcina sp
567	Alcohols, alicyclic	Structure-activity relationships
Psychrophilic temperature effect	see also Terpene compounds	153
567	Achromobacter sp	Sewage, municipal
Naphthalene and derivatives	Inhibitory (toxic) effects, 38	Respirometric studies, 548
Structure-activity relationships	Metabolic pathways, 41	Alcohols, primary aliphatic
523	Activated sludge	Acetobacter sp
Phenol and derivatives	Aerobic biodegradation, 386	Identification of microorganism
Identification of microorganisms	Identification of microorganisms	
71	38	Achromobacter sp
Metabolic pathways, 37	Inhibitory (toxic) effects, 38	Identification of microorganism
Poly(alkyl-β-propiolactones)	Metabolic pathways, 39	164, 303
Structure-activity relationships 503	Structure-activity relationships	Metabolic pathways, 303
	386	Acinetobacter sp
Polyamides	Activated sludge, acclimated	Identification of microorganism.
Structure-activity relationships	Aerobic digestion reactor, 381	560
_	Oxidation ditch, 381	Metabolic pathways, 244
Polycaprolactone Structure actuaty relationships	Activated sludge, municipal	Respirometric studies, 560
Structure-activity relationships	Anaerobic digestion reactor, 15	Actinomyces sp
503 Polyahlamasad hinhanyla	Fermentation, methanogenic, 15	Structure-activity relationships
Polychlorinated biphenyls	Enterobacter sp	153
Aerobic biodegradation, 138	Inhibitory (toxic) effects, 38	Activated sludge, 253, 341, 418
Structure-activity relationships	Flavobacterium sp	Aerobic biodegradation, 29, 230
130	IDDIDUOTY ITAXIC) ATTACTS (¥	306 117

Alcaligenes sp Aerobic digestion reactors compared, Sewage, municipal Identification of microorganisms 251, 287 Identification of microorganisms Assay development, 592 164 560 Arthrobacter sp Identification of microorganisms Respirometric studies, 548, 560 Identification of microorganisms Structure-activity relationships 282, 303 Inhibitory (toxic) effects, 144 164 Review, 500 Bacıllus sp Isolation of microorganisms, 417 Xanthomonas sp Identification of microorganisms Identification of microorganisms Metabolic pathways, 303, 417 282 164 471 Michaelis-Menten coefficients Structure-activity relationships Alcohols, primary, long chain 153, 473 224 Activated sludge Monad kinetics constants, 224 Bacterium sp. 294 Operational parameters, 222 Structure-activity relationships Octanol-water partition coefficients, Pseudomonas sp 153 Operational parameters, 222 Operational parameters, 224 Chromobacterium sp Alcohols, secondary aliphatic 592 Structure-activity relationships Actinomyces sp Petrochemical wastewater treatment 153 Structure-activity relationships Flavobacterium so 324 153 Identification of microorganisms Pseudomonas sp. 417 Activated sludge, 341 Respirometric studies, 30 164, 560 Aerobic biodegradation, 386 Structure-activity relationships Respirometric studies, 560 Assay development, 592 153, 386, 473 Microbial population, acclimated Octanol-water partition coefficients, Substrate concentration effect Metabolic pathways, 318 582 223, 372 Microbial population, isopropanol-Operational parameters, 591 acclimated Time-course kinetics, 191, 582 592 Metabolic pathways, 569 Activated sludge, acclimated Aerobic biodegradation, 291 Petrochemical wastewater treatment Microbial population, raw sewage 324 Time-course kinetics, 475 Aerobic biodegradation, 26 Sludge adaptation process, 591 Microbial population, sewage, municipal Activated sludge, acclimated, Structure-activity relationships continuous-flow Biorefractory index, 199 153, 386, 473 Operational parameters Recommendations, wastewater treat-Time-course kinetics, 191, 582 310 ment, 199 Activated studge, industrial, continuous-Sludge acclimatization process Micrococcus sp. 294 flow 310 Identification of microorganisms Metabolic pathways, 569 Activated sludge, acclimated, municipal Bacıllus sp Oxygen uptake, effect on, 491 Structure-activity relationships, 153 Structure-activity relationships Mycobacterium sp Sludge acclimatization process 153, 473 Identification of microorganisms 491 Bacterium sp., 294 Activated sludge, industrial 164, 303 Structure-activity relationships Identification of microorganisms Metabolic pathways, 303 153 163 Structure-activity relationships Chromobacterium sp Activated sludge, industrial and 153-Structure-activity relationships municipal Nocardia sp 153 Identification of microorganisms Aerobic biodegradation, pilot plant, Microbial population, isopropanol-237 282 acclimated Activated sludge, industrial, continuous-Ozone, stirred-tank reactor, continuous-Metabolic pathways, 569 flow flow Micrococcus sp. 294 Metabolic pathways, 569 Operational parameters, 580 Structure-activity relationships Activated sludge, Nocardia-inoculated Ozonization, 580 153 Pseudomonas sp. 294 Identification of microorganisms Mycobacterium sp Identification of microorganisms 164, 282, 303, 560 282 Structure-activity relationships Activated sludge, municipal 153 Correlative test evaluations Metabolic pathways, 59, 182 Pseudomonas sp. 294 151 297, 303, 539 Metabolic pathways, 297 Identification of microorganisms Respirometric studies, 560 Structure-activity relationships 164 Structure-activity relationships 153, 473 Nutritional parameters, 305 153, 473 Sarcina sp. 294 Activated sludge, non-acclimated Pseudomonas sp pure culture Structure-activity relationships Aerobic biodegradation, 291 Metabolic pathways, 471 153 Activated sludge, OECD-specified Sarcina sp. 294 Sewage, acclimated, municipal Identification of microorganisms Interlaboratory comparison, 590 Petrochemical wastewater treatment Static vs continuous activation 164 51 method, 590 Structure-activity relationships Sewage, municipal Activated sludge, synthetic, continuous-153 Respirometric studies, 548 Sewage, acclimated, municipal flow Aerobic biodegradation, 34 Petrochemical wastewater treatment Alcohols, tertiary aliphatic Activated sludge Inhibitory (toxic) effects. 34

Alcohols, primary aliphatic (cont'd)

Alcohols, primary aliphatic (cont'd)

Alcohols, primary aliphatic (cont'd)

Alcohols, tertiary aliphatic (cont'd)	Aldehydes (cont'd)	Aliphatic compounds (cont'd)
Aerobic biodegradation, 386	Bacıllus sp	Identification of microorganisms
D.O. meter method, 268	Structure-activity relationships	Biodegradability, ultimate, 487
Octanol-water partition coefficients,	153, 473	Review, 487
582	Bacterium sp. 294	Alkanes
River die-away test, 268	Structure-activity relationships	see also Gasoline: Hydrocarbons,
Structure-activity relationships	153	Polypropylene: Terpene com-
386	Chromobacterium sp	pounds
Time-course kinetics, 582	Structure-activity relationships	Achromobacter sp
Activated sludge, municipal	153	Inhibitory (toxic) effects, 450
Correlative test evaluations	Flavobacterium sp	Metabolic pathways, 67
151 Sewage, acclimated, municipal	Identification of microorganisms	Structure-activity relationships
	164	450
Petrochemical wastewater treatment 51	Identification of microorganisms Review, 165	Acinetobacter sp Inhibitory (toxic) effects, 450
Sewage, municipal	Lagoons, aerated, industrial site	Metabolic pathways, 232
Inhibitory (toxic) effects, 548	Aerobic biodegradation, 215	Structure-activity relationships
Respirometric studies, 548	Detoxification, 215	450
•	Microbial population	Activated sludge, 173
Alcohols, tertiary, long chain	Trickling filters, 166	Inhibitory (toxic) effects, 144
Microbial population, river water	Microbial population, acclimated	Activated sludge, industrial
River die-away test, 424	Metabolic pathways, 318	Identification of microorganisms
Aldehydes	Microbial population, loam	163
Acerobacter sp	Structure-activity relationships	Arthrobacter sp
Identification of microorganisms	485	Inhibitory (toxic) effects, 450
164	Micrococcus sp. 294	Structure-activity relationships
Achromobacter sp	Identification of microorganisms	450
Identification of microorganisms	164	Aspergillus sp
164	Structure-activity relationships	Inhibitory (toxic) effects, 450
Actinomyces sp	153	Structure-activity relationships
Structure-activity relationships	Mycobacterium sp	450
153	Identification of microorganisms	Brevibacterium sp
Activated sludge, 253, 418	164	Inhibitory (toxic) effects, 450
Aerobic biodegradation, 398	Structure-activity relationships	Structure-activity relationships
147	153	450
Inhibitory (toxic) effects, 453	Vocardia sp	Candida sp
Respirometric studies, 30	Metabolic pathways, 179	Inhibitory (toxic) effects, 450
Structure-activity relationships	Pseudomonas sp. 294	Structure-activity relationships
153, 473	Identification of microorganisms	450
Activated sludge, acclimated	164	Cladosporium sp
Aerobic biodegradation, 291 Inhibitory (toxic) effects, 21	Structure-activity relationships	Inhibitory (toxic) effects, 450
226	153, 473	Structure-activity relationships 450
Respirometric studies, 21	Sarcina sp. 294 Identification of microorganisms	Corynebacterium sp
Structure-activity relationships	164	Inhibitory (toxic) effects, 450
390	Structure-activity relationships	Structure-activity relationships
Time-course kinetics, 390	153	450
Activated sludge, industrial	Sewage, acclimated, municipal	Cunninghamella sp
Identification of microorganisms	Petrochemical wastewater treatment	Inhibitory (toxic) effects, 450
163	51	Structure-activity relationships
Activated sludge, municipal	Metabolic pathways, 539	450
Identification of microorganisms	Trickling filters	Eupenicillium so
164	Review, 166	Inhibitory (toxic) effects, 450
Activated sludge, non-acclimated	Xanthomonas sp	Structure-activity relationships
Aerobic biodegradation, 291	Identification of microorganisms	450
Inhibitory (toxic) effects, 21	164	Flavobacterium sp
Respirometric studies, 21	Algae species	Inhibitory (toxic) effects, 450
Activated sludge, primary and secondary	Industrial wastewaters Facultative pond, 93	Metabolic pathways, 232
Aerobic biodegradation, 472 Activated sludge + synthetic sewage	Alicyclic compounds	Structure-activity relationships
Aerobic biodegradation, 52	Biodegradability, ultimate	450
Alcaligenes sp	Review. 387	Microbial population
Identification of microorganisms	Identification of microorganisms	Metabolic pathways, 232 Micrococcus sp
164	Biodegradability, ultimate, 487	Metabolic pathways, 232
Metabolic pathways, 37	Review, 487	Mycobacterium sp
Arthrobacter sp	Aliphatic compounds	Inhibitory (toxic) effects, 450
Identification of microorganisms	Biodegradability, ultimate	Structure-activity relationships
164	Dames 207	5 indictate-activity relationships

Aikanes (cont u)	Davis	manes, iong cham, mean (cont a)
Nocurdia sp	Psychrophilic temperature effect	Nocardia sp
Inhibitory (toxic) effects, 450	567	Metabolic pathways, 25, 232
Metabolic pathways, 232, 444	Candida sp	111
Structure-activity relationships	Inhibitory (toxic) effects, 85	Pseudomonas sp
450	Cytophaga sp	Anaerobic biodegradation, 298
	Mesopnilic temperature, effect	Cenetic transfer, 123
Pseudomonas sp		
Genetic transfer, 123	567	Metabolic pathways, 123, 232
Metabolic pathways, 123, 232	Psychrophilic temperature effect	298. 299
299	567	Time-course kinetics, 347
Rhodotorula sp	Flavobacterium sp	Pseudomonas sp acclimated
	Mesophilic temperature, effect	Time-course kinetics, 347
Inhibitory (toxic) effects, 450		
Structure-activity relationships	567	Alkanoic acids and derivatives
450	Psychrophilic temperature effect	see also Adipic acid and derivatives; EI
Sporobolomyces sp	567	TA; NTA and salts;
Inhibitory (toxic) effects, 450	Gram-negative rods	Phenylacetic acid and
		derivatives:
Structure-activity relationships	Mesophilic temperature, effect	
450	567	Poly(α -hydroxyacrylic acid);
Alkanes, cyclic	Psychrophilic temperature effect	Polyacrylie acid:
Acinetobacter sp	567	Sulfophenylaikanoic acids
	Gram-positive cocci	Achromobacter sp
Metabolic pathways, 232, 522		
Structure-activity relationships	Mesophilic temperature, effect	Metabolic pathways, 41, 67
522	567	Acinetobacter sp
Activated sludge, 173, 341	Psychrophilic temperature effect	Metabolic pathways, 244
Cladosporium sp	567	Actinomyces sp
	Microbial population, fresh water,	Structure-activity relationships
Nutritional effects, enrichment	kerosene-cultured	*
552		153
Flavobacterium sp	Metabolic pathways, co-metabolism	Activated sludge, 253, 341, 418
Metabolic pathways, 232, 335	168, 169	Aerobic digestion reactors compared
Microbial population	Pseudomonas sp	251, 287
	Genetic transfer, 123	Assay development, 592
Metabolic pathways, 232		
Microbial population, fresh water,	Mesophilic temperature, effect	Inhibitory (toxic) effects, 429
kerosene-cultured	567	Michaelis-Menten coefficients
Metabolic pathways, co-metabolism	Metabolic pathways, 123	429
168, 169	Psychrophilic temperature effect	Operational parameters, 591
	567	592
Micrococcus sp	Xanthomonas sp	Sludge adaptation process, 591
Metabolic pathways, 232	Mesophilic temperature, effect	
Nocardia sp		Structure-activity relationships
Metabolic pathways, 232, 444	567	153, 274, 473
Pseudomonas sp	Psychrophilic temperature effect	Substrate concentration effect, 372
Metabolic pathways, 232, 335	567	Activated sludge, acclimated
	Alkanes, long chain, linear	Sludge acclimatization process
Sewage, acclimated, municipal		446
Petrochemical wastewater treatment	Acinetobacter sp	
51	Metabolic pathways, 86, 232	Time-course kinetics, 475
Alkanes, long chain, branched	522	Activated sludge, industrial
Achromobacter sp	Structure-activity relationships	Identification of microorganisms
	522	163
Mesophilic temperature, effect		Activated sludge, municipal
567	Activated sludge	
Psychrophilic temperature effect	Time-course kinetics, 191	Anaerobic digestion reactor, 15
567	Activated sludge, non-acclimated,	Fermentation, methanogenic, 15
Acinetobacter sp	municipal, 255	Activated sludge + night soils,
Mesophilic temperature, effect	Candida sp	municipal
	Inhibitory (toxic) effects, 85	Aerobic biodegradation, 229
567		Activated sludge + sewage, municipal
Metabolic pathways, 522	Cladosporium sp	
Psychrophilic temperature effect	Nutritional effects, enrichment	Aerobic biodegradation, 229
567	552	Activated sludge, synthetic
Structure-activity relationships	Flavobacterium sp	Flocculation, nutritional effects
522	Metabolic pathways, 232	36
	Microbial population	Arthrobacter sp
Activated sludge, non-acclimated,		Inhibitory (toxic) effects, 84
municipal, 255	Metabolic pathways, 232	
Alcaligenes sp	Microbial population, fresh water,	Isolation of enzymes, 84
Mesophilic temperature, effect	kerosene-cultured	Metabolic pathways, 84
	Metabolic pathways, co-metabolism	Bacillus sp
567	169	Structure-activity relationships
Psychrophilic temperature effect		153, 473
567	Micrococcus sp	
Arthrobacter sp	Metabolic pathways, 232	Bacterium sp. 294
Mesophilic temperature, effect	Mycobacterium sp	Structure-activity relationships
567	Metabolic pathways, 25	153

Alkanoic acids and derivatives (cont'd)	Alkanoic acids and derivatives, long chain	
Chromobacterium sp	(cont'd)	(cont'd)
Structure-activity relationships	Activated sludge, municipal	Microbial population, sea water
153 Fusarium sp	Monad kinetics constants, 365 Activated sludge, non-acclimated	458 Kiver die-away test, 458
Aerobic biodegradation, 130	Innibitory (toxic) effects, 454	Vicrobial population, septic tank
Hydrogenomonas sp	Rate and selective adsorption	Aerobic percolation, 364, 265
Aerobic biodegradation, 130	454	Anaerobic percolation, 264, 265
Lagoons, aerated, industrial site	Cladosporium sp	Micropial population, soils
Aerobic biodegradation, 215	Nutritional effects, enrichment	Aerobic vs anaerobic conditions
Detoxification, 215	552	119
Methanobacterium sp	, Escherichia sp	Blocking effect, 119
Anaerobic digestion reactor, 15	Metabolic pathways, 273	Moraxella sp
Fermentation, methanogenic, 15	Structure-activity relationships	Metabolic pathways, 192
Microbial population, acclimated	273	Nocardia sp
Metabolic pathways, 318	Lagoons, aerated, industrial site	Metabolic pathways, 444 Penicillium sp
Microbial population, fresh water	Aerobic biodegradation, 215	Metabolic pathways, 192
Sorption, 44	Detoxification, 215	Protaminobacter sp. 118
Substrate concentration effect	Microbial population, fresh water	Pseudomonas sp. 118
14	Microaerophilic biodegradation 327	Metabolic pathways, 539
Microbial population, raw sewage	Microbial population, sea water	Sewage, acclimated, municipal
Aerobic biodegradation, 26		Petrochemical wastewater treatmen
Microbial population, sewage, municipal	River die-away test, 458	51
Biorefractory index, 189, 199	Pseudomonas sp	Sewage, municipal, oxidation pond
Recommendations, wastewater treat- ment, 189, 199	Anaerobic biodegradation, 298	system
Microbial population, soils	Metabolic pathways, 273, 298	Model ecosystem, aquatic, pond
Denitrification, 14	Operational parameters, 222	system, 264, 265
Metabolic pathways, 14	Structure-activity relationships	Sewage, natural
Micrococcus sp. 294	273	Aerobic biodegradation, 157
Structure-activity relationships	Staphylococcus sp	Alkanoic acids, cyclic
153	Metabolic pathways, 273	Achromobacter sp
Mycobacterium sp	Structure-activity relationships	Metabolic pathways, 41
Metabolic pathways, 25	273	Activated sludge
Structure-activity relationships	Alkanoic acids and derivatives, polybasic	Coupled units test, 129
153	Achromobacter sp. 118	Respirometric studies, 535
Nocardia sp	Metabolic pathways, 41, 67	Activated sludge, municipal
Metabolic pathways, 25, 179	Acinetobacier sp	Anaerobic digestion reactor, 15
180, 444	Metabolic pathways, 244	Correlative test evaluations
Pseudomonas sp. 294	Activated sludge	
Anaerobic biodegradation, 298	Aerobic biodegradation, 386	Fermentation, methanogenic, 15 Methanobacterium sp
Metabolic pathways, 288, 297	Anaerobic digestion reactor, 543	Anaerobic digestion reactor, 15
298, 539	Coupled units test, 129	Fermentation, methanogenic, 15
Structure-activity relationships	Petrochemical wastewater treatment	Mycobacterium sp
153, 473	324	Metabolic pathways, 25
Sarcina sp. 294	Structure-activity relationships	Nocardia sp
Structure-activity relationships 153	386	Metabolic pathways, 25
Sewage, acclimated, municipal	Activated sludge, continuous-flow Aerobic biodegradation, 313	Alkanoic acids, long chain, esters
Petrochemical wastewater treatment	River die-away test, 313	Activated sludge, municipal
51	Activated sludge, municipal	Aerobic biodegradation, 457
Structure-activity relationships	Aerobic biodegradation, 462	Activated sludge, semi-continuous flow,
Review, 500	Correlative test evaluations	286
	151	Microbial population, acclimated, 286
Alkanoic acids and derivatives, long chain	Detergent formulation effect	Alkanoic acids, sulfonated
Acinetobacter sp	462	see also Alkyl sulfonates
Metabolic pathways, 86, 522	Diurnal variations, 462	Alkanoic acids, sulfonated, long chain
Structure-activity relationships	Activated sludge, semi-continuous flow	Activated sludge, acclimated, municipal
522	Aerobic biodegradation, 157	Inhibitory (toxic) effects, 329
Activated sludge	Bacillus sp. 118	Escherichia sp
Aerobic biodegradation, 302	Brevibacterium sp. 118	Bacteriocidal/bacteriostatic effects.
Operational parameters, 222 591	Fusarium sp	330
Sludge adaptation process, 591	Aerobic biodegradation, 130	Inhibitory (toxic) effects, 329
Structure-activity relationships	Hydrogenomonas sp	Structure-activity relationships
274, 302	Aerobic biodegradation, 130	330
Activated sludge, acclimated, municipal	Microbial population	Microbial population, sewage
Aerobic biodegradation, 327	Screening tests, 415 Microbial population, fresh water	Structure-activity relationships

Alkanoic acids, sulfonated, long chain	Alkenes (cont'd)	Alkenoic acids and derivatives (cont'd)
(cont'd)	Flavobacterium sp	Time-course kinetics, 475
Pseudomonas sp	Inhibitory (toxic) effects, 450	Alcaligenes sp
Inhibitory (toxic) effects, 329	Metabolic pathways, 232	Metabolic pathways, 37
Salmonella sp Bacteriocidal/bacteriostatic effects.	Structure-activity relationships	Arthrobacter sp
330	450	Identification of microorganisms 579
Inhibitory (toxic) effects, 329	Gram-negative rods	Nitrification, 578
Structure-activity relationships, 330	Structure-activity relationships 523	Fusarium sp
Staphylococcus sp	Lagoons, aerated, industrial site	Aerobic biodegradation, 130
Bacteriocidal/bacteriostatic effects,	Aerobic biodegradation, 215	Hvdrogenomonas sp
330	Detoxification, 215	Aerobic biodegradation, 130
Inhibitory (toxic) effects, 329	Microbial population	Microbial population, 110
Structure-activity relationships	Metabolic pathways, 232	Microbial population, municipal wastes
330	Microbial population, fresh water,	Metabolic pathways, 213
Alkenes	kerosene-cultured	Nutritional effects, enrichment
see also Polybutadienes; Terpene com-	Metabolic pathways, co-metabolism	213
pounds	168, 169	Moraxella sp
Achromobacter sp	Microbial population, raw sewage	Metabolic pathways, 192, 468
Inhibitory (toxic) effects, 450	Aerobic biodegradation, 26 Microbial population, sewage, municipal	Nocardia sp Metabolic pathways, 180, 444
Structure-activity relationships, 450	Biorefractory index, 199	Penicillium sp
Acinetobacter sp	Recommendations, wastewater treat-	Metabolic pathways, 192, 468
Inhibitory (toxic) effects, 450 Metabolic pathways, 232, 522	ment. 199	Pseudomonas sp
Structure-activity relationships	Micrococcus sp	Metabolic pathways, 8
450, 522	Metabolic pathways, 232	Sewage, municipal
Activated sludge, 341	Mycobacterium sp	Respirometric studies, 548
Respirometric studies, 535	Inhibitory (toxic) effects, 450	Alkenoic acids and derivatives, long chain
Time-course kinetics, 191	Structure-activity relationships	Acinetobacter sp
Activated sludge, non-acclimated.	450	Metabolic pathways, 522
municipal, 255	Nocardia sp	Structure-activity relationships
Alcaligenes sp	Inhibitory (toxic) effects, 450	522
Structure-activity relationships	Metabolic pathways, 232	Activated sludge
523	Structure-activity relationships 450	Aerobic biodegradation, 58
Arthrobacter sp	Pseudomonas sp	Depuration rate, effect on, 83
Inhibitory (toxic) effects, 450	Genetic transfer, 123	Operational parameters, 83
Structure-activity relationships 450	Identification of microorganisms	River die-away test. 58
Aspergillus sp	376	Structure-activity relationships 274
Inhibitory (toxic) effects, 450	Metabolic pathways, 59, 123	Activated sludge, municipal
Structure-activity relationships	232	Monad kinetics constants, 365
450	Screening tests, 376	Aspergillus sp
Brevibacterium sp	Rhodotorula sp	Structure-activity relationships
Inhibitory (toxic) effects, 450	Inhibitory (toxic) effects, 450	97
Structure-activity relationships	Structure-activity relationships	Lagoons, aerated, industrial site
450	450	Aerobic biodegradation, 215
Candida sp	Sewage, acclimated, municipal	Detoxification, 215
Inhibitory (toxic) effects, 450	Petrochemical wastewater treatment	Microbial population, soil burial
Structure-activity relationships	Sewage, municipal	Structure-activity relationships
450 Cladosporium sp	Respirometric studies, 548	97 Pseudomonas sp
Inhibitory (toxic) effects, 450	Sporobolomyces sp	Inhibitory (toxic) effects, 572
Nutritional effects, enrichment	Inhibitory (toxic) effects, 450	Alkyl halides
552	Structure-activity relationships	see also Pesticides
Structure-activity relationships	450	Activated sludge, 341
.150	Alkenoic acids	Anaerobic digestion reactor, 344
Corynebacterium sp	see also Chinamic acid and derivatives	Inhibitory (toxic) effects, 150
Inhibitory (toxic) effects, 450	Alkenoic acids and derivatives	344
Structure-activity relationships	Achromobacter sp	Nitrification, 150
450	Metabolic pathways, 41 Activated sludge, 341	Petrochemical wastewater treatment
Cunninghamella sp	Aerobic biodegradation, 230	324
Inhibitory (toxic) effects, 450	Coupled units test, 129	Time-course kinetics, 172 Corynebacterium sp
Structure-activity relationships 450	Petrochemical wastewater treatment	Operational parameters, 374
Eupenicillium sp	324	Trickling filters, 374
Inhibitory (toxic) effects, 450	Activated sludge, acclimated	Lagoons, aerated, industrial site
Structure-activity relationships	Identification of microorganisms	Aerobic biodegradation, 215
450	578	573

likyi naiides (cont.d)	Alkyl sulfides (cont'd)	Alkynes (cont'd)
Detoxification, 215, 573	Aerobic biodegradation, 112	Microbial population, river water
Microbial population, raw sewage	Activated sludge, acclimated, sedimenta-	River die-away test, 424
Aerobic biodegradation, 26	tion chamber	Rhodopseudomonas sp
Inhibitory (toxic) effects, 26	Aerobic biodegradation, 112	Inhibitory (toxic) effects, 323
Microbial population, sewage, municipal	Lagoons, aerated, industrial site	Metabolic pathways, 323
		Sewage, municipal
Biological inhibition value, 199	Aerobic biodegradation, 215	
Biorefractory index, 199	573	Respirometric studies, 548
Inhibitory (toxic) effects, 199	Detoxification, 215, 573	Alternaria sp
Recommendations, wastewater treat-	Microbial population, fresh water sedi-	Adipic acid and derivatives
ment, 199	ment	Isolation of products, 524
Ozone, stirred-tank reactor, continuous-	Biogeochemical cycling, 602	Polyadipate plasticizers
flow		
Operational parameters, 580	Alkyl sulfonates	Isolation of products, 524
	see also Alkanoic acids, sulfonated;	Aluminum
Ozonization, 580	Petroleum sulfonates	Activated sludge
Pseudomonas sp	Alkyl sulfonates and derivatives	Inhibitory (toxic) effects, 178
Time-course kinetics, 347	Activated sludge	Pseudomonas sp
Pseudomonas sp acclimated	Aerobic biodegradation, 128	Inhibitory (toxic) effects, 572
Time-course kinetics, 347	<u> </u>	
Sewage, acclimated, municipal	Inhibitory (toxic) effects, 128	Sewage, municipal
Petrochemical wastewater treatment	Time-course kinetics, 460	Inhibitory (toxic) effects, 345
51	Bacıllus sp	Amides, aliphatic
	Freundlich adsorption isotherms	see also E-Caprolactam;
Alkyl sulfates, long chain	459	
see also Surfactants, anionic	Escherichia sp	Polyacrylamides: Polyamides
Achromobacter sp, 442	Freundlich adsorption isotherms	Achromobacter sp. 118
Activated sludge		Activated sludge
Aerobic biodegradation, 302	459	Aerobic biodegradation, 29
Coupled units test, 129	Microbial population, fresh water	Inhibitory (toxic) effects, 28
Depuration rate, effect on, 83	Microbial population, sea water	Isolation of microorganisms, 278
Operational parameters, 83	458	Nutritional parameters, 278
	River die-away test, 458	Operational parameters, 28
Structure-activity relationships	Pseudomonas sp	Ctrusture activity relations 25
302	Freundlich adsorption isotherms	Structure-activity relationships, 27
Time-course kinetics, 460	459	Time-course kinetics, 193
Activated sludge, municipal		Activated sludge, acclimated
Aerobic biodegradation, 457	Alkyl sulfoxides	Identification of microorganisms
Correlative test evaluations	see also Dimethyl sulfoxide; DMSO	578
151	Activated sludge	Inhibitory (toxic) effects, 277
Activated sludge + synthetic sewage	Identification of microorganisms	Activated sludge, municipal
	295	Inhibitory (toxic) effects, 348
Correlative test evaluations	Sludge acclimatization process	
233		Activated sludge + synthetic sewage
Citrobacter sp. 442	295	Aerobic biodegradation, 52
Enterobacter sp. 442	Aerobacter sp	Alcaligenes sp
Flavobacterium sp. 442	Identification of microorganisms	Structure-activity relationships
Microbial population	295	120
Metabolic pathways, 533	Sludge acclimatization process	Arthrobacter sp
Screening tests, 415	295	Identification of microorganisms
	Arthrobacter sp	578
Microbial population, brackish water		
Aerobic biodegradation, 76	Identification of microorganisms	Nitrification, 578
Microbial population, fresh water	295	Aspergillus sp
Microbial population, sea water	Sludge acclimatization process	Structure-activity relationships
458	295	120
River die-away test, 458	Pseudomonas sp	Bacillus sp. 118
Microbial population, municipal wastes	Identification of microorganisms	Brevibacterium sp. 118
Evolution of bacterial populations	295	Enterobacter sp
16	Sludge acclimatization process	Inhibitory (toxic) effects, 277
	295	
Microbial population, river water		Flavobacterium sp
Evolution of bacterial populations	Sewage, acclimated, municipal	Inhibitory (toxic) effects, 277
16	Petrochemical wastewater treatment	Structure-activity relationships
Pseudomonas sp. 442	51	120
Sewage, municipal	Alkylsulfonic acids	Microbial population, loam
Aerobic biodegradation, 438	Activated sludge	Carbaryl inhibitory and persistance
Anaerobic biodegradation, 438	Inhibitory (toxic) effects, 178	activity, 257
Shigella sp. 442		Microbial population, soils
	Gram-positive organisms	Aerobic vs anaerobic conditions
alkyl sulfides	Inhibitory (toxic) effects, 171	
Activated sludge	Alkynes	119
Anaerobic digestion reactor, 602	Microbial population, loam	Blocking effect, 119
Activated sludge, acclimated,	Carbaryl inhibitory and persistance	Structure-activity relationships
continuous-flow	rotivity 257	119

Amines, aliphatic	A inco make ali-hatia	Amides, aliphatic (cont'd)
Activated sludge, 341	Amines, poly-, aliphatic Achromobacter sp. 118	Protaminobacter sp. 118
Aerobic biodegradation, 394	Activated sludge, 341	Pseudomonas sp
Anaerobic biodegradation, 394	•	Inhibitory (toxic) effects, 277
Inhibitory (toxic) effects, 504	Aerobic biodegradation, 386	Nutritional parameters, 278
Isolation of microorganisms, 278	Assay development, 592	Sewage, acclimated, municipal
	Metabolic pathways, 471	Petrochemical wastewater treatment
Nitrification, 504	Operational parameters, 540	51
Nutritional parameters, 278	591, 592	Vibrio sp
River die-away test, 394	Sludge adaptation process, 540	Inhibitory (toxic) effects, 27?
Activated sludge, acclimated	591	Isolation of microorganisms, 278
Inhibitory (toxic) effects, 226	Structure-activity relationships	Nutritional parameters, 278
277	386	
Time-course kinetics, 475	Activated sludge, acclimated,	Amides, aliphatic, long chain Activated sludge
Activated sludge, industrial	continuous-flow	Structure-activity relationships
Identification of microorganisms	Operational parameters, 310	274
163	Sludge acclimatization process	Alcaligenes sp
Activated sludge, municipal	310	Structure-activity relationships
Correlative test evaluations	Activated sludge, OECD-specified	120
151	Interlaboratory comparison, 590	
Enterobacter sp	Static vs continuous activation	Aspergillus sp Structure-activity relationships
Inhibitory (toxic) effects, 277	method, 590	120
Flavobacterium sp	Bacıllus sp. 118	·
Inhibitory (toxic) effects, 277	Brevibacterium sp. 118	Escherichia sp
Microbial population, 45	Microbial population, municipal wastes	Metabolic pathways, 273
Pseudomonas sp	Inhibitory (toxic) effects, 311	Structure-activity relationships
Inhibitory (toxic) effects, 277	Microbial population, river water	273
Nutritional parameters, 278	Inhibitory (toxic) effects, 427	Flavobacterium sp
Sewage, acclimated, municipal	Structure-activity relationships	Structure-activity relationships
Petrochemical wastewater treatment	427	120
51	Microbial population, soils	Microbial population, river water
Vibrio sp	Aerobic vs anaerobic conditions	River die-away test, 424
Inhibitory (toxic) effects, 277	119	Pseudomonas sp
Isolation of microorganisms, 278	Structure-activity relationships	Metabolic pathways, 273
Nutritional parameters, 278	119	Structure-activity relationships
Amines, aromatic	Protaminobacter sp. 118	273
see Aniline and derivatives; Anthranilic	Pseudomonas sp. 72	Staphylococcus sp
acid; Benzidine and derivatives;	Pseudomonas sp pure culture	Metabolic pathways, 273
Pyridine and derivatives;	Metabolic pathways, 471	Structure-activity relationships
Sulfanilic acid and derivatives	Sewage, synthetic, continuous-flow, 396	273
· ·		Amides, aliphatic, long chain, sulfated
Amines, long chain	Amino acids and derivatives	Activated sludge, acclimated, municipal
see also Quaternary ammonium com-	Acinetobacter sp	Aerobic biodegradation, 327
pounds	Metabolic pathways, 522, 542	Microbial population, fresh water
Activated sludge, non-acclimated,	Structure-activity relationships	Aerobic biodegradation, 327
municipal	522	Amides, aromatic
Aerobic biodegradation, 18	Activated sludge	see Benzoic acid and derivatives;
Trickling filters, 18	Aerobic biodegradation, 515	Phthalic acid and derivatives
Bacteriocidal/bacteriostatic effects	Polarographic monitoring, 512	
Review, 425	Structure-activity relationships	Amines, alicyclic Achromobacter sp
Escherichia sp	274, 393	Inhibitory (toxic) effects, 38
Metabolic pathways, 273	Activated sludge, acclimated	Activated sludge
Structure-activity relationships	Inhibitory (toxic) effects. 226	* 1
273	Activated sludge, acclimated, municipal	38
Microbial population, municipal wastes	Aerobic biodegradation, 186	Inhibitory (toxic) effects, 38
Inhibitory (toxic) effects, 311	Sludge acclimatization process	Metabolic pathways, 39
Microbial population, river water	186	Enterobacter sp
Inhibitory (toxic) effects, 427	Activated sludge, industrial	Inhibitory (toxic) effects, 38
Structure-activity relationships	Identification of microorganisms	Flavobacterium sp
427	163	Inhibitory (toxic) effects, 38
Pseudomonas sp	Activated sludge, municipal	Gram-positive bacteria
Structure-activity relationships	Anaerobic digestion reactor, 15	Inhibitory (toxic) effects, 38
273	Fermentation, merhanogenic, 15	Microbial population, municipal wastes
Staphylococcus sp	Activated sludge, tannery-activated	Inhibitory (toxic) effects, 311
Metabolic pathways, 273	Decomposability, 513	Pseudomonas sp
Structure-activity relationships	Cladosporium sp	Inhibitory (toxic) effects, 38
273	Nutritional effects, enrichment	Vibrio sp
Structure-activity relationships	552	Inhibitory (toxic) effects, 38
Review, 425	Escherichia sp	,

Aniline and derivatives (cont'd)
Activated sludge, industrial and Amino acids and derivatives (cont'd) Metabolic pathways. 273 Ammonia and salts (cont'd) Inhibitory (toxic) effects, evanide inmunicipal Structure-activity relationships hibition, 243 Inhibitory (toxic) effects, 13 Inhibitory (toxic) effects, phenol in-Respirometric studies, 13 Identification of microorganisms hibition, 243 Structure-activity relationships, 13 Biodegradability, ultimate, 487 Inhibitory (toxic) effects, thiocyanate Activated sludge, municipal Review, 487 inhibition, 243 Correlative test evaluations Metabolic pathways Activated sludge, industrial 151 Review, 514 Identification of microorganisms Methanobacterium sp Distribution and rate accumulation 163 270 Anaerobic digestion reactor, 15 Activated sludge, multi-stage column Inhibitory (toxic) effects, 369 Fermentation, methanogenic, 15 Substrate concentration effect Structure-activity relationships Microbial population 209 Metabolic pathways, 514 Activated sludge, second-stage Microbial population, continuous-flow Adaptation of microorganisms Activated sludge, municipal, continuous-Laboratory-pilot plant studies flow 145 Inhibitory (toxic) effects, 241 Operational parameters, 145 Psychrophilic temperature effect Nitrification, effects on, 241 Ammunition plant wastes Activated sludge, propanil-enriched 399 see also Explosives, organic Mineralization, 585 Microbial population, fresh water Activated sludge + cornsteep. Activated sludge + synthetic sewage Microbial population, sea water continuous-flow Correlative test evaluations 458 Oxidation ditch, 204 River die-away test, 458 233 Activated sludge, municipal, continuous-Microbial population, non-acclimated, Bacıllus sp flow Metabolic pathways, 111 soils Aerobic biodegradation, 360 Time-course kinetics, 111 Aerobic biodegradation, 511 Inhibitory (toxic) effects, 360 Metabolic pathways, 511
Microbial population, NTA-acclimated, Microbial population, fresh water + Anilides sewage Metabolic pathways, 111 soils see Herbicides, propanil type and Time-course kinetics, 111 Aerobic biodegradation, 511 metabolites Microbial population, raw sewage Metabolic pathways, 511 Aniline and derivatives Aerobic biodegradation, 26 Microbial population, raw sewage Activated sludge, 190 Microbial population, sewage, municipal Aerobic biodegradation, 26 Aerobic biodegradation, 78, 386 Microbial population, sewage, municipal Biorefractory index, 199 600 Biorefractory index, 189, 199 Recommendations, wastewater treat-Inhibitory (toxic) effects, 66 Recommendations, wastewater treatment, 199 534 Reduced BOD, 61 ment, 189, 199 Inhibitory (toxic) effects, pH effect, Nitrifying bacteria, continuous-culture Microbial population, soils 225 Inhibitory (toxic) effects, 241 Time-course kinetics, 82 Inhibitory (toxic) effects, proteolytic. Nitrification, effects on, 241 Nocardia sp Nitrosomas sp. Metabolic pathways, 179 225 Petrochemical wastewater treatment Inhibitory (toxic) effects, 587 Polyporous sp 324 Time-course kinetics, 82 Pseudomonas sp Respirometric studies, 534 Mineralization, 585 Pseudomonas sp Structure-activity relationships Metabolic pathways, 273, 542 Time-course kinetics, 183 386 Pseudomonas sp acclimated Structure-activity relationships Substrate concentration effect Metabolic pathways, 276 273 Pseudomonas sp TOL-plasmid-bearing 66 Sewage, frozen, acclimated Activated sludge, acclimated Metabolic pathways, 279 Operational parameters, 587 Aerobic biodegradation, 584 Sewage, municipal Substrate concentration effect Inhibitory (toxic) effects, 226 Nutritional effects, 90 587 Temperature effect, 587 Respirometric studies, 548 Metabolic pathways, 584 Sewage, municipal Staphylococcus sp Structure-activity relationships Metabolic pathways, 273 Co-substrate concentration effect 391, 392 Structure-activity relationships 159 Time-course kinetics, 391, 392 River die-away test, 159 Activated sludge, continuous-flow Structure-activity relationships Structure-activity relationships Co-substrate concentration effect 159 Review, 500 159 Thermomonospora sp Substrate concentration effect Inhibitory (toxic) effects, 159 Time-course kinetics. 82 River die-away test, 159 Structure-activity relationships Trichosporon sp Structure-activity relationships Metabolic pathways, 542 Inhibitory (toxic) effects, 159 159 Metabolic pathways, co-metabolism Review, 388 Substrate concentration effect 542 Anthranilic acid 159 Activated sludge, municipal Activated sludge + cornsteep. Ammonia and salts Correlative test evaluations Activated sludge continuous-flow

Oxidation ditch, 204

Inhibitory (toxic) effects, 231

151

Antibiotics Activated sludge, 254, 307	Arsenic compounds, inorganic (cont'd) Nocardia sp	Arthrobacter sp (cont'd) Cresols and derivatives
Aerobic biodegradation, 386 Aerobic digestion reactors compared,	Operational parameters, 464 Pseudomonas sp	Model ecosystem, terrestrial, natural 545
251	Operational parameters, 464	Crude oil
Inhibitory (toxic) effects, 252	Arsenic compounds, organic Achromopacter sp	Mesophilic temperature, effect 567
Structure-activity relationships	Operational parameters, 464	Psychrophilic temperature effect 567
386	Biodegradation, environmental aspects Review, 239	2.4-D
Activated sludge, municipal and syn- thetic	Corynebacterium sp	Batch vs continuous-flow system
Continuous and intermittent flows	Operational parameters, 464	312
compared. 238	Nocardia sp	Furan and derivatives
Inhibitory (toxic) effects, 238	Operational parameters, 464	Aerobic biodegradation, 19
Activated sludge, semi-continuous flow	Pseudomonas sp	Metabolic pathways, 19
Sludge acclimatization process	Operational parameters, 464	Herbicides, 2,4-D type
525	Arthrobacter sp	Batch vs continuous-flow system
Time-course kinetics, 525	Acetophenone and derivatives	312 Votonos alimbatio
Bacillus sp	Inhibitory (toxic) effects, 84	Ketones, aliphatic Aerobic biodegradation, 19
Inhibitory (toxic) effects, 308	Isolation of enzymes, 84	Metabolic pathways, 19
Protozoa, 254	Metabolic pathways, 84 Alcohols, primary aliphatic	Lignin sulfonates
Trickling filters Inhibitory (toxic) effects, 308	Identification of microorganisms	Aerobic biodegradation, 19
,	164	Metabolic pathways, 19
Antifreeze	Aldehydes	Nitriles
Microbial population, raw sewage Aerobic biodegradation, 26	Identification of microorganisms	Identification of microorganisms
_	164	578
Aquatic oil spills Effect on microbial population	Alkanes	Nitrification, 578
Review, 23	Inhibitory (toxic) effects, 450	Phenol and derivatives
Microbial abatement	Structure-activity relationships	Identification of microorganisms
Review, 23	450	295 Inhibitory (toxic) effects, 84
Microbial emulsification and degrada-	Alkanes, long chain, branched Mesophilic temperature, effect	Isolation of enzymes, 84
tion	567	Metabolic pathways, 84
Review, 23	Psychrophilic temperature effect	Model ecosystem, terrestrial, natural
Oil pollutants, sources and behavior	567	545
Review, 23	Alkanoic acids and derivatives	Sludge acclimatization process
Aroclors	Inhibitory (toxic) effects, 34	295
see Polychlorinated biphenyls	Isolation of enzymes, 84	Phenylacetic acid and derivatives
Aromatic compounds	Metabolic pathways, 84	Inhibitory (toxic) effects, 84
Biodegradability, ultimate	Alkenes	Isolation of enzymes, 84
Review, 387	Inhibitory (toxic) effects, 450	Metabolic pathways, 84 Phthalic acid and derivatives
Identification of microorganisms	Structure-activity relationships 450	Metabolic pathways, 117
Biodegradability, ultimate. 487 Review, 487	Alkenoic acids and derivatives	Polyethylene glycols, fatty ester
	Identification of microorganisms	Aerobic biodegradation, 431
Aromatic compounds, dicyclic Activated sludge, 414	578	Polyethylene glycols, fatty ether
Alcaligenes sp	Nitrification, 578	Aerobic biodegradation, 431
Structure-activity relationships	Alkyi sulfoxides	Pyrocatechol and derivatives
523	Identification of microorganisms	Inhibitory (toxic) effects, 84
Flavobacterium sp	295	Isolation of enzymes, 84
Metabolic pathways, 335	Sludge acclimatization process 295	Metabolic pathways, 84, 117 Timber steam processing wastes
Gram-negative rods	Amides, aliphatic	Aerobic biodegradation, 408
Structure-activity relationships 523	Identification of microorganisms	Identification of microorganisms
Pseudomonas sp	578	. 408
Metabolic pathways, 335	Nitrification, 578	Operational parameters, 408
Psychrophilic temperature effect	Benzoic acid and derivatives	Xylenols and derivatives
250	Inhibitory (toxic) effects, 84	Model ecosystem, terrestrial, natural
Time-course kinetics, 250	Isolation of enzymes, 84 Metabolic pathways, 84	545
Arsenic compounds, inorganic	Carbamic acid and derivatives	. Aspergillus sp
Achromobacter sp	Biological membrane filtration	Aflatoxins
Operational parameters, 464	333	Mesophilic temperature effect
Activated sludge	Model ecosystem, aquatic, simulated,	104
Inhibitory (toxic) effects, 588	333	Nutritional effects, 104
Corynebacterium sp	Cirrasols	Substrate concentration effect
Operational parameters, 464	Aerobic biodegradation, 431	104

Aspergillus sp (cont'd)	Aureobasidium sp	Azotobacter sp (cont'd)
Alkanes	Phenol-formaldehyde resin	Model ecosystem, terrestrial, natural,
Inhibitory (toxic) effects, 450	Biodegradation, rates compared	545
Structure-activity relationships	248	Phenol and derivatives
450	Poly(alkyl-β-propiolactones)	Model ecosystem, terrestrial, natural,
Alkenes	Structure-activity relationships	545
Inhibitory (toxic) effects, 450	10	Xylenols and derivatives
Structure-activity relationships	Poly(methyl methacrylate)	Model ecosystem, terrestrial, natural,
450	Biodegradation, rates compared	545
Alkenoic acids and derivatives, long chain	248	Bacillus sp
Structure-activity relationships, 97	Polycaprolactone	Adipic acid and derivatives, 118
Amides, aliphatic	Microbial population, soils, 126	Alcohols, benzylic
Structure-activity relationships	Polyesters	Structure-activity relationships
120	Microbial population, soils, 126	153, 473
Amides, aliphatic, long chain	Polystyrenes Biodegradation, rates compared	Alconols, primary aliphatic
Structure-activity relationships	248	Identification of microorganisms
120		282
Capsaicin and derivatives	Azide inhibitory activity	Structure-activity relationships
Hydroxylation, 293	Herbicides, chlorpropham type	153, 473
Cellulose and derivatives	Microbial population, loam, 257	Alcohols, secondary aliphatic
Operational parameters, 285	Pseudomonas sp. 257	Structure-activity relationships
Time-course kinetics, 285	Azo compounds	153, 473
Herbicides, monuron type and	Activated studge	Aldehydes
metabolites	Inhibitory (toxic) effects, 581	Structure-activity relationships
Metabolic pathways, 216	Structure-activity relationships	153, 473
Herbicides, propanil type and	530	Alkanoic acids and derivatives
metabolites	Time-course kinetics, 530	Structure-activity relationships
Metabolic pathways, 216	Activated sludge + cornsteep,	153, 473 Alkanoic acids and derivatives,
Phenol-formaldehyde resin	continuous-flow Oxidation ditch, 204	polybasic, 118
Biodegradation, rates compared	Pseudomonas sp acclimated	Alkyl sulfonates and derivatives
248	Metabolic pathways, 276	Freundlich adsorption isotherms
Poly(alkyl-β-propiolactones)	Metabolie patitways, 270	459
Structure-activity relationships	Azo dyes	Amides, aliphatic, 118
10	Activated sludge	Amines, poly-, aliphatic, 118
Poly(methyl methacrylate) Biodegradation, rates compared	Freundlich adsorption isotherms	Aniline and derivatives
248	101	Metabolic pathways, 111
Polyamides, 217	Inhibitory (toxic) effects, 371	Time-course kinetics, 111
Structure-activity relationships	581	Antibiotics
12	Kinetics and equilibrium studies	Inhibitory (toxic) effects, 308
Polycaprolactone	Structure-activity relationships	Benzenesulfonic acid, linear alkyl, long
Structure-activity relationships	101, 530	chain
97	Time-course kinetics, 530	Biodegradation, diphasic, 570
Polyesters	Activated sludge, boiling-inactivated	Benzoic acid and derivatives
Structure-activity relationships	Freundlich adsorption isotherms	Structure-activity relationships
97	101	473 Carbamic acid and derivatives
Polyethylene	Kinetics and equilibrium studies	Isolation of microorganisms, 102
Isolation of microorganisms, 4	101	Cresols and derivatives
Structure-activity relationships	Structure-activity relationships	Model ecosystem, terrestrial, natural,
97 Polypropylene	101	545
Structure-activity relationships	Activated sludge, formaldehyde-	Cyanide
97	inactivated	Identification of microorganisms
Polystyrenes	Freundlich adsorption isotherms	206
Biodegradation, rates compared	101	DDT, Methoxychlor and metabolites
248	Kinetics and equilibrium studies	Anaerobic biodegradation, 536
Structure-activity relationships	Structure-activity relationships	Autoclaving effect, 536
97	101	Disinfectants effect, 536
Polyureas, 217	Activated sludge, municipal	Metabolic pathways, 536
Quaternary ammonium compounds	Inhibitory (toxic) effects, 369	Fuel oil
Inhibitory (toxic) effects, 314	Structure-activity relationships	Metabolic pathways, 553
Metabolic pathways, 314	369	Herbicides, carbamate
Starch and derivatives	Pseudomonas sp acclimated	Metabolic pathways, 111
Tensile strength, 96	Metabolic pathways, 276	Time-course kinetics, 111
Vegetable oils and fats	Azotobacter sp	Herbicides, chlorpropham type Metabolic pathways, 474
Structure-activity relationships	Cresols and derivatives	Operational parameters, 160
97	CICSUIS AND DELIVATIVES	Operational parameters, 100

Azotobacter sp (cont'd)

icillus sp (cont'd)	Bacillus sp. (cont a)	Structure-activity relationships
Herbicides, 2,4-D type	Metabolic pathways, 111	133
Operational parameters, 160	Time-course kinetics, 111	Pyridine and derivatives, 294
Herbicides, monuron type and	Xylenois and derivatives	Pyrocatecnol and derivatives
metabolites	Model ecosystem, terrestrial, natural	
Metabolic pathways, 111	545	Structure-activity relationships
Time-course kinetics, 111	Bacillus sp., aerobic	153
Herbiciges, propanil type and	Benzoic acid and derivatives	Resorcinol and derivatives
- metabolites	Inhibitory (toxic) effects, chloram-	Structure-activity relationships
Metabolic pathways, 111	phenicol inhibition, 2	153
	The state of the s	Beijerinckia sp., mutant
Time-course kinetics, 111	Metabolic pathways, 2	Polycyclic aromatic hydrocarbons
Hydroquinone and derivatives	Hydroquinone and derivatives	Metabolic pathways, 154
Structure-activity relationships	Metabolic pathways, 2	• •
153, 473	Phthalic acid and derivatives	Beijerinckia sp, wild type
Ketones, aliphatic	Inhibitory (toxic) effects, chloram-	Polycyclic aromatic hydrocarbons
Structure-activity relationships	phenicol inhibition, 2	Metabolic pathways, 154
473	Metabolic pathways, 2	Benzene and derivatives
Lindane and metabolites	Bacillus sp., anaerobic	Achromobacter sp
Anaerobic biodegradation, 536		·
Petroleum	Benzoic acid and derivatives	Metabolic pathways, 67
Metabolic pathways, 553	Inhibitory (toxic) effects, chloram-	Acinetobacter sp
	phenicol inhibition, 2	Metabolic pathways, 232
Phenol and derivatives	Metabolic pathways, 2	Activated sludge, 173, 341
Batch vs continuous-flow system	Hydroquinone and derivatives	Activated sludge, acclimated
401	Metabolic pathways, 2	Time-course kinetics, 475
Identification of microorganisms	Phthalic acid and derivatives	Alcaligenes sp
205, 206	Inhibitory (toxic) effects, chloram-	Metabolic pathways, 37
Model ecosystem, terrestrial, natural,	phenical inhibition, 2	Structure-activity relationships
545	Metabolic pathways, 2	523
Substrate concentration effect		Cladosporium sp
401	Bacteriocidal/bacteriostatic effects	Numuonal effects, enrichment
Temperature effect, 401	Alkanoic acids, sulfonated, long chain	
Phthalic acid and derivatives	Escherichia sp. 330	552
Identification of microorganisms	Salmonella sp. 330	Flavobacterium sp
282	Staphylococcus sp. 330	Metabolic pathways, 232, 335
	Amines, long chain	Gram-negative rods
Polychlorinated bipnenyls	Review, 425	Structure-activity relationships
Isolation of microorganisms, 366	Quaternary ammonium compounds	523
Polychlorobenzenes and derivatives	Review, 425	Lagoons, aerated, industrial site
Anaerobic biodegradation, 536	Surfactants	Aerobic biodegradation, 215
Polychlorocyclopentadiene dimers	Review. 440	573
Anaerobic biodegradation, 536	1	Detoxification, 215, 573
Propylene glycols	Surfactants, cationic	Metabolic pathways
Structure-activity relationships	Review, 425	Review. 88
153, 473	Bacterium sp	
Pyrocatechol and derivatives	Alcohols, benzylic	Microbial population
Identification of microorganisms	Structure-activity relationships	Metabolic pathways, 232
	153	Microbial population, fresh water,
282	Alcohols, primary aliphatic, 294	kerosene-cultured
Structure-activity relationships	Structure-activity relationships	Metabolic pathways, co-metabolism
153, 473	153	168, 169
Quaternary ammonium compounds, 11	Alcohols, secondary aliphatic, 294	Microbial population, fresh water sedi-
Resorcinol and derivatives		ment
Structure-activity relationships	Structure-activity relationships	Anaerobic biodegradation, 212
153, 473	153	Substrate concentration effect
Sugars and derivatives	Aldehydes, 294	212
Aerobic biodegradation, 403	Structure-activity relationships	Microbial population, hyperentrophic
Stripping and metabolic mechanisms	153	water sediment
403	Alkanoic acids and derivatives, 294	Anaerobic biodegradation, 212
Sulfanilic acid and derivatives	Structure-activity relationships	Microbial population, sewage, municipa
Identification of microorganisms	153	Biorefractory index. 199
377	Hydroquinone and derivatives	
Thiocyanic acid and salts	Structure-activity relationships	Recommendations, wastewater treat-
Identification of microorganisms	153	ment, 199
	Ketones, aliphatic, 294	Microbial population, soils
205, 206	Petroleum	Identification of microorganisms
Timber steam processing wastes	Mesophilic temperature effect	376
Aerobic biodegradation, 408	342	Screening tests, 376
Identification of microorganisms	pH effect, 342	Substrate specificity, 376
408		Micrococcus sp
Operational parameters, 408	Phenol and derivatives, 294	Metabolic pathways, 232
Urea and derivatives	Propylene glycols	• •

chain (cont'd) Activated sludge Vocardia sp chain (cont'd)
Model ecosystem, aquatic, natural, simulated, 135 Metabolic pathways, 232, 444 Pseudomonas sp Aerobic biodegradation, 58, 302 Identification of microorganisms Aerobic digestion reactor, 234 Structure-activity relationships 376 235. 482 135 Metabolic pathways, 232, 335 Anaerobic biodegradation, 439 Microbial population, soils Psychrophilic temperature effect Anaerobic digestion reactor, 234 Aerobic biodegradation, 156 Inhibitory (toxic) effects, 235 250 Screening tests, 156 Screening tests, 376 Inhibitory (toxic) effects of nutrients. Sewage, municipal Time-course kinetics, 250 439 Aerobic biodegradation, 438 Sewage, acclimated, municipal River die-away test, 58, 268 Anaerobic biodegradation, 438 Structure-activity relationships, 302 Surface water model, 482 Petrochemical wastewater treatment Structure-activity relationships 51 Review 492 Benzenesulfonic acid, non-linear alkyl, long Activated sludge, acclimated, 436 Benzenesulfinic acid and derivatives Aerobic biodegradation, 202 chain Alcaligenes sp Activated sludge, acclimated, see also Surfactants, anionic Metabolic pathways, 37 continuous-flow Activated sludge Benzenesulfonic acid, alkyl, long chain River die-away test, 220 Coupled units test, 129 Activated sludge, municipal Activated sludge, continuous-flow Structure-activity relationships Aerobic biodegradation, 421 220 Model ecosystem, aquatic, natural Sludge acclimatization process Activated sludge, acclimated, municipal 516 Aerobic biodegradation, 327 Activated sludge, municipal Gram-positive organisms Activated sludge, continuous-flow Correlative test evaluations Inhibitory (toxic) effects, 171 Aerobic biodegradation, 202 151 Microbial population, municipal wastes Activated sludge + synthetic sewage Structure-activity relationships Evolution of bacterial populations Aerobic biodegradation, 456 261 16 Correlative test evaluations Activated sludge, municipal Microbial population, river water Aerobic biodegradation, 275 Evolution of bacterial populations Operational parameters, 275 Metabolic pathways, 456 16 Activated sludge, non-acclimated Structure-activity relationships Sewage, synthetic 456 Aerobic biodegradation, 202 Phosphate effect, 380 Activated sludge, semi-continuous flow, Microbial population Temperature effect, 380 286 Model ecosystem, aquatic, natural Benzenesulfonic acid, aikyl, short chain 516 Activated sludge + synthetic sewage Benzenesulfonic acid, S-substituted alkyl Activated sludge, acclimated, municipal see also Sulfophenyialkanoic acids Correlative test evaluations, 233 Activated sludge, acclimated. Alcaligenes sp continuous-flow Aerated chamber die-away test Metabolic pathways, 37 Operational parameters, 310 416 Anaerobic biodegradation Sludge acclimatization process Review, 158 River die-away test, 416 310 Shake flask process, 416 Aquatic interactions, microbial Alcaligenes sp Review, 158 Structure-activity relationships Metabolic pathways, 37 416 Bacıllus sp Activated sludge, municipal Benzenesulfonic acid and non-alkyl Biodegradation, diphasic, 570 substituted derivatives Aerated chamber die-away test Correlative test evaluations Activated sludge Activated sludge, municipal, 151 416 Aerobic biodegradation, 175 Identification of microorganisms River die-away test, 416 386 Review, 571 Shake flask process, 416 Operational parameters, 591 Structure-activity relationships Metabolic pathways Petrochemical wastewater treatment 416 Review, 492, 571 Microbial population, river water 324 Microbial population Sludge adaptation process, 591 Aerated chamber die-away test Screening tests, 415 Structure-activity relationships Microbial population, acclimated, 286 416 River die-away test, 416 Microbial population, brackish water Activated sludge, acclimated Shake flask process, 416 Aerobic biodegradation, 76 Aerobic biodegradation, pilot plant, Structure-activity relationships Microbial population, fresh water 416 Metabolic pathways, 109 Activated sludge, municipal Sewage, synthetic Microbial population, sea water Correlative test evaluations Aerated chamber die-away test 458 151 416 Model ecosystem, aquatic, natural Inhibitory (toxic) effects, 369 River die-away test, 416 109 Structure-activity relationships Shake flask process, 416 River die-away test, 458 Microbial population, municipal wastes Structure-activity relationships Alcaligenes sp 416 Aerobic biodegradation, 156 Metabolic pathways, 37 Screening tests, 156 Benzidine and derivatives Benzenesulfonic acid, linear alkyl, long Microbial population, river water, 436 Activated sludge chain Microbial population, river water sedi-Aerobic digestion reactor, 495 see also Surfactants, anionic ment Operational parameters, 495

Benzenesulfonic acid, linear alkyl, long

Benzenesulfonic acid, linear aikyl, long

Benzene and derivatives (cont'd)

enzidine and derivatives (cont'd)	Delice to the man additional (cont. a)	Benzothiazole and derivatives (cont'd) Microbial population, acclimated
Oxidation product spectrum and absorbance, 495	Fusarium sp Metabolic pathways, 188	River die-away test, 317
Sludge acclimatization process	Methanobacterium sp	BHT
495	Anaerobic digestion reactor, 15	Activated sludge + synthetic sewage
Activated sludge, acclimated.	Fermentation, methanogenic, 15	Metabolic pathways, 228
continuous-flow	Microbial population, 45	Time-course kinetics, 228 Biphenyl and derivatives
Aerobic digestion reactor, 495	Microbial population, accimiated,	Acinetobacter sp
Operational parameters, 495	municipal	Aerobic biodegradation, 138
Oxidation product spectrum and ab-	Metabolic pathways, 98	Metabolic pathways, 354
sorbance, 495 Sludge acclimatization process, 495	Nutritional effects, 98 Microbial population, fresh water	Structure-activity relationships
•	Sorption, 44	138
Senzoic acid and derivatives see also Toluic acid and derivatives	Substrate concentration effect	Activated sludge, 296
Achromobacter sp	44	Aerobic biodegradation, 175
Metabolic pathways, 41, 67	Microbial population, municipal wastes	Inhibitory (toxic) effects, 144
Activated sludge	Metabolic pathways, 213	309, 354, 453 Operational parameters, 315
Aerobic biodegradation, 175	Nutritional effects, enrichment	Time-course kinetics, 316
386, 398	213	Activated cludge applicanted municipal
Anaerobic digestion reactor, 196	Microbial population, sewage, municipal	Aerobic biodegradation, 526
Inhibitory (toxic) effects, 66	Reduced BOD, 61	Activated sludge, acclimated, municipal,
Respirometric studies, 30	Microbial population, soils Aerobic biodegradation, 133	continuous-flow
Structure-activity relationships	385	Aerobic biodegradation, 496
386, 473	Anaerobic biodegradation, 385	Sludge acclimatization process
Substrate concentration effect 66	Denitrification, 14	496
Activated sludge, acclimated	. Metabolic pathways, 14	Activated sludge, industrial and
Aerobic biodegradation, 397	River die-away test, 385	municipal
Structure-activity relationships	. Micrococcus sp	Inhibitory (toxic) effects, 13
392	Metabolic pathways, 107	Respirometric studies, 13
Time-course kinetics, 392	Nocardia sp	Structure-activity relationships, 13
Activated sludge, municipal	Metabolic pathways, 179, 444	Activated sludge, municipal Aerobic biodegradation, 528
Anaerobic digestion reactor, 15	Pseudomonas sp	Metabolic pathways, 528
Batch vs continuous-flow system	Inhibition of benzoic acid turnover, 410	Structure-activity relationships
461	Inhibitory (toxic) effects, 183	528
Biomass yield, effect on, 461	Isolation of enzymes, 103	Activated sludge, municipal, continuous-
Correlative test evaluations	Metabolic pathways, 103, 184	flow
151 Fermentation, methanogenic, 15	Operational parameters, 103	Aerobic biodegradation, 496
Operational parameters 161	Structure-activity relationships	Sludge acclimatization process
Activated sludge, synthetic	410, 473	496
Aerobic biodegradation, 385	Time-course kinetics, 183	Activated sludge, non-acclimated
Anaerobic biodegradation, 385	Pseudomonas sp acclimated	Inhibitory (toxic) effects, 454 Rate and selective adsorption
River die-away test, 385	Metabolic pathways, 276	454
Alcaligenes sp	Sewage, acclimated, municipal	Alcaligenes sp
Inhibition of benzoic acid turnover,	Petrochemical wastewater treatment	Aerobic biodegradation, 138
410	Sewage, municipal	Structure-activity relationships
Metabolic pathways, 37		138, 523
Structure-activity relationships 410	Inhibitory (toxic) effects, 183 Sewage, natural, semi-continuous flow	Cunninghamella sp
Arthrobacter sp	Metabolic pathways, 184	Aerobic biodegradation, 528
Inhibitory (toxic) effects, 84	Benzonitrile and derivatives	Metabolic pathways, 528
Isolation of enzymes, 84	Fusarium sp	Structure-activity relationships 528
Metabolic pathways, 84	Metabolic pathways, 188	Flavobacterium sp
Bacıllus sp		Metabolic pathways, 335
Structure-activity relationships	Benzothiazole and derivatives	Gram-negative rods
473	Activated sludge	Structure-activity relationships
Bacillus sp., aerobic Inhibitory (toxic) effects, chloram-	Aerobic biodegradation, 128 Inhibitory (toxic) effects, 128	523
phenical inhibition, 2	144	Microbial population, sewage, municipal
Metabolic pathways, 2	Isolation of pure microbial popula-	Biorefractory index, 199
Bacillus sp., anaerobic	tion, 317	Recommendations, wastewater treat- ment, 199
Inhibitory (toxic) effects, chloram-	River die-away test, 317	Vocardia sp
phenicol inhibition, 2	Activated sludge, acclimated, 73	Metabolic pathways, 354
Metabolic pathways, 2	Activated sludge, municipal	Pseudomonas sp
Cladosporium sp	Aerobic biodegradation, 79	Inhibitory (toxic) effects, 309
Nutritional effects, enrichment	Cunninghamella sp Metabolic pathways 555	Metabolic pathways, 335, 354
552	Metanouc nathways 333	

Biphenyls and derivatives Candida sp (cont'd) Microbial population, liquid cultures Activated sludge DDT. Methoxychlor and metabolites Screening parameters, 494 Time-course kinetics, 272 Anaerobic biodegradation, 536 Microbial population, plate cultures Cadmium Autoclaving effect, 536 Screening parameters, 494 Dismiectants effect, 536 Activated studge Metabolic pathways, 536 Bisphenol A Anaerobic digestion reactor, 344 Lindane and metabolites Activated sludge, acclimated Inhibitory (toxic) effects, 178 Anaerobic biodegradation, 536 Aeropic biodegradation, pilot plant, 344, 546 Polychlorobenzenes and derivatives Activated sludge, acclimated, municipal Anaerobic biodegradation, 536 Aerobic biodegradation, 363 Bjerkandera sp Polychlorocyclopentadiene dimers Phenol-formaldehyde resin Biomass yield, effect on, 363 Anaerobic biodegradation, 536 Freundlich adsorption isotherms Biodegradation, rates compared Pulp and paper wastes 63. 363 Kinetics and equilibrium studies Foam process, 594 Poly(methyl methacrylate) Sulfite liquor Biodegradation, rates compared Foam process, 594 Langmuir adsorption isotherms 248 ε-Caprolactam Polystyrenes 63 Michaelis-Menten coefficients see also Amides, aliphatic Biodegradation, rates compared 363 Activated sludge 248 Operational parameters, 363 Aerobic biodegradation, 386 Activated sludge, industrial Ammonification, 603 Activated sludge Inhibitory (toxic) effects, 68 Nitrification, 603 Inhibitory (toxic) effects, 588 Operational parameters, 591 Activated sludge, municipal Activated sludge, laboratory-pilot plant River die-away test, 268 Inhibitory (toxic) effects, 361 Inhibitory (toxic) effects, 562 Sludge deflocculation, 361 Sludge adaptation process, 591 Activated sludge, municipal, continuous-Activated sludge, municipal, continuous-Structure-activity relationships flow 386 Inhibitory (toxic) effects, 562 Substrate concentration effect Freundlich adsorption isotherms Brevibacterium sp 603 362 Adipic acid and derivatives, 118 Activated sludge, acclimated Kinetics and equilibrium studies Aerobic digestion reactor, 381 362 Inhibitory (toxic) effects, 450 Michaelis-Menten coefficients Oxidation ditch, 381 Structure-activity relationships 362 Activated sludge, municipal 450 Nutritional parameters, 305 Activated sludge, OECD-specified Operational parameters, 362 Alkanoic acids and derivatives, Activated sludge, non-acclimated polybasic, 118 Inhibitory (toxic) effects, 343 Interlaboratory comparison, 590 Alkenes Activated sludge, phosphate-restricted, Static vs continuous activation Inhibitory (toxic) effects, 450 municipal method, 590 Structure-activity relationships Carbamic acid and derivatives Aerobic biodegradation, 268 Aerobic biodegradation, 577 450 Microbial population, sewage, municipal Amides, aliphatic, 118 Inhibitory-(toxic) effects, 199 Coulomb meter method, 268 Amines, poly-, aliphatic, 118 D.O. meter method, 268 Nitrobacter sp Cresols and derivatives Inhibitory (toxic) effects, 124 Capsaicin and derivatives Model ecosystem, terrestrial, natural, Aspergillus sp Nitrosomas sp Hydroxylation, 293 Inhibitory (toxic) effects, 124 Phenol and derivatives Pseudomonas sp Carbamic acid and derivatives Model ecosystem, terrestrial, natural, Sorption, 210, 211 see also Herbicides, chlorpropham type; 545 Sewage, municipal Pesticides Phthalic acid and derivatives Activated sludge Inhibitory (toxic) effects, 345 Metabolic pathways, 117 Aerobic biodegradation, 268 Pyrocatechol and derivatives Calcium River die-away test, 268 Metabolic pathways, 117 Activated sludge, acclimated Activated sludge, industrial, continuous-Xvlenols and derivatives Aerobic biodegradation, 598 flow Model ecosystem, terrestrial, natural, Lagoon pre-treatment Aerobic biodegradation, 167 545 Anaerobic biodegradation, 379 Inhibitory (toxic) effects, 167 Brewery wastes Candida sp Activated sludge, industrial, porous-pot, Activated sludge Alkanes continuous-flow Glucose removal and polysaccharide Inhibitory (toxic) effects, 450 Aerobic biodegradation, 167 accumulation, 501 Structure-activity relationships Inhibitory (toxic) effects, 167 Substrate concentration effect 450 Activated sludge, municipal, continuous-372 Alkanes, long chain, branched flow Activated sludge, acclimated, industrial Aerobic biodegradation, 167 Inhibitory (toxic) effects, 85 Identification of microorganisms Anaerobic biodegradation, 167 Inhibitory (toxic) effects, 167 Activated sludge, municipal, porous-pot, Alkanes, long chain, linear 502 Inhibitory (toxic) effects. 85 Activated sludge, industrial Alkenes Operational parameters, 601 Inhibitory (toxic) effects, 450 continuous-flow Waste treatment facility scheme Structure-activity relationships Aerobic biodegradation, 167 601 Inhibitory (toxic) effects, 167

Bromate

Carbamic acid and derivatives (cont'd)	Cellulomonas sp	Cellulose and derivatives (cont'd)
Activated sludge + synthetic sewage	Toilet paper, dyed	Aerobic biodegradation, 574 Time-course kinetics, 574
Aerobic biodegradation, 52	Inhibitory (toxic) effects, 537	Thermacinomyces sp
Arthrobacter sp	Metabolic pathways, 537	Fermentation, batch system, 292
Biological membrane filtration	Pulp concentration effect, 537	Michaelis-Menten coerficients
333	Cellulose and derivatives	292
Model ecosystem, aquatic, simulated, 333	see also Alcohols	Thermomonospora sp
Bacıllus sp	Actinomyces sp	Time-course kinetics, 82
Isolation of microorganisms, 102	Operational parameters, 185	Chaetomium sp
ε-Caprolactam	Time-course kinenes, 285 Activated sludge	Cellulose and derivatives
Aerobic biodegradation, 268	Petrochemical wastewater treatment	Operational parameters, 285
Coulomb meter method, 268	324	Time-course kinetics, 285
D.O. meter method, 268	Activated sludge, acclimated,	Chloramine and derivatives
Corynebacterium sp	continuous-flow	Activated sludge
Biological membrane filtration 333	Operational parameters, 310	Inhibitory (toxic) effects, additive.
Model ecosystem, aquatic, simulated,	Sludge acclimatization process	178 Trickling filters
333	310	Inhibitory (toxic) effects, 306
Fusarium sp., 258	Activated sludge, batch-type, industrial	Chloride
Biological membrane filtration	Substrate concentration effect 42	Activated sludge
333	Activated sludge, industrial	Inhibitory (toxic) effects, 131
Model ecosystem, aquatic, simulated.	Aerobic biodegradation, 55	Operational parameters, 131
333	Overview, 55	Activated sludge, fresh water
Lumbricillus sp	Time-course kinetics, 55	Inhibitory (toxic) effects, 203
Inhibitory (toxic) effects, 167	Activated sludge, municipal	Activated sludge, salt water
Metabolic pathways	Correlative test evaluations	Inhibitory (toxic) effects, 203
Review, 325 Microbial population, acclimated, soils	151	Nitrification, effects on, 203
Isolation of microorganisms, 102	Activated sludge, non-acclimated,	Pseudomonas sp
Microbial population, raw sewage	municipal Gravimetric assessment, 420	Inhibitory (toxic) effects, 131 Operational parameters, 131
Aerobic biodegradation, 26	Hach oxidation, 420	· · · · · · · · · · · · · · · · · · ·
Microbial population, sewage, municipal	Respirometric studies, 420	Chloroalkylenes
Biorefractory index, 199	Aspergillus sp	Activated sludge, municipal Aerobic biodegradation, 201
Recommendations, wastewater treat-	Operational parameters, 285	528
ment, 199	Time-course kinetics, 285	Metabolic pathways, 528
Mycobacterium sp	Chaetomium sp	Structure-activity relationships
Biological membrane filtration 333	Operational parameters, 285	201, 528
Model ecosystem, aquatic, simulated,	Time-course kinetics, 285	Cunninghamella sp
333	racitification of intercongamisms	Aerobic biodegradation, 528
Nocardia sp	Review, 33 Metabolic pathways	Metabolic pathways, 528
Biological membrane filtration	Review, 33	Structure-activity relationships 528
333	Microbial population	
Model ecosystem, aquatic, simulated,	Metabolic pathways, 27	Chromium
333	Microbial population, cellulolytic	Activated sludge
Penicillium sp	Operational parameters, 285	Anaerobic digestion reactor, 344 Inhibitory (toxic) effects, 131
Biological membrane filtration 333	Time-course kinetics, 285	149, 178, 336, 344, 437, 546
Model ecosystem, aquatic, simulated,	Microbial population, municipal wastes	Operational parameters, 131
333	Identification of microorganisms 406	Activated sludge, continuous-flow
Pseudomonas sp	Microbial population, raw sewage	Inhibitory (toxic) effects, 48
Metabolic pathways, 177	Aerobic biodegradation, 26	Substrate concentration effect
Streptomyces sp	Microbial population, sewage, municipal	48
Biological membrane filtration	Biorefractory index, 199	Activated sludge, industrial Inhibitory (toxic) effects, 35
Model ecosystem, aquatic, simulated,	Recommendations, wastewater treat-	Activated sludge, municipal
333	ment. 177	Aerobic biodegradation, 79
Carbowax	Microbial population, soils Time-course kinetics, 82	Inhibitory (toxic) effects, 478
Microbial population, glycol-	Polyporous sp	Operational parameters, 478
metabolizing	Time-course kinetics, 82	Activated sludge, municipal, continuous
Metabolic pathways, 80	Pseudomonas sp	flow
Review, 80	Identification of microorganisms	Freundlich adsorption isotherms
Casamino acids	406	362 Kinetics and equilibrium studies
Microbial population, continuous-flow	Scierotium sp	362
Adaptation of microorganisms, 399	Operational parameters, 285 Time-course kinetics, 285	Michaelis-Menten coefficients
Psychrophilic temperature effect	Sewage, municipal	362
399		

Chromium (cont'd)	Chromobacterium sp (cont'd)	Citrobacter sp (cont'd)
Operational parameters, 362	Structure-activity relationships	Autoclaving effect, 536
Activated sludge, synthetic	153	Disinfectants effect, 536
Inhibitory (toxic) effects, 35	Resorcinol and derivatives	Metabolic pathways, 536
Colpidium sp	Structure-activity relationships	Lindane and metabolites
Inhibitory (toxic) effects, 486	153	Anaerobic biodegradation, 536
Corynebacterium sp	Ciliata sp	Phenot and derivatives
Operational parameters, 374	Cirrasols	Identification of microorganisms
Trickling filters, 374	Inhibitory (toxic) effects, 432	205、206
Microbial population, sewage, municipal	Polyethylene glycots, fatty ester	Polychlorobenzenes and derivatives
Inhibitory (toxic) and stimulatory ef-	Inhibitory (toxic) effects, 432	Anaerobic biodegradation, 536
fects, 170	Polyethylene glycols, fatty ether	Polychlorocyclopentadiene dimers
Microbial acclimatization, 170	Inhibitory (toxic) effects, 432	Anaerobic biodegradation, 536
Nitrobacter sp	Cinnamic acid and derivatives	Thiocyanic acid and salts
Inhibitory (toxic) effects, 124	see also Alkenoic acids	Identification of microorganisms
Nitrosomas sp	Activated sludge	205, 206
Inhibitory (toxic) effects, 124	Anaerobic digestion reactor, 196	Citrus wastes
Opercularia sp	Activated siudge, municipal	Activated sludge, high purity oxygen
Inhibitory (toxic) effects, 486	Anaerobic digestion reactor, 15	process
Pseudomonas sp	Fermentation, methanogenic, 15	Operational parameters, 518
Inhibitory (toxic) effects, 131 572	Methanobacterium sp	Waste treatment facility scheme
	Anaerobic digestion reactor, 15	518
Operational parameters, 131	Fermentation, methanogenic, 15	-
Sorption, 210, 211 Sewage, municipal	Nocardia sp	Cladosporium sp
Inhibitory (toxic) effects, 345	 Metabolic pathways, 179, 444 	Alkanes
Sewage, synthetic	Pseudomonas sp	Inhibitory (toxic) effects, 450
Inhibitory (toxic) and stimulatory ef-	Metabolic pathways, 137	Structure-activity relationships
fects, 170	Trametes sp	450
Microbial acclimatization, 170	Metabolic pathways, 137	Alkanes, cyclic
Sphaerotilus sp	Cirrasols	Nutritional effects, enrichment
Inhibitory (toxic) effects, 437	Achromobacter sp	552
Vorticeila sp	Aerobic biodegradation, 431	Alkanes, long chain, linear
Inhibitory (toxic) effects, 486	Activated sludge	Nutritional effects, enrichment
Zooglea sp	Inhibitory (toxic) effects, 430	552
Inhibitory (toxic) effects, 437	Activated sludge, acclimated	Alkanoic acids and derivatives, long
Chromobacterium sp	Inhibitory (toxic) effects, 432	chain
Alcohols, benzylic	Activated sludge, non-acclimated	Nutritional effects, enrichment 552
Structure-activity relationships	Inhibitory (toxic) effects, 432	Alkenes
153	Alcaligenes sp	Inhibitory (toxic) effects, 450
Alcohols, primary aliphatic	Aerobic biodegradation, 431	Nutritional effects, enrichment
Structure-activity relationships	Arthrobacter sp	552
153	Aeropic biodegradation, 431	Structure-activity relationships
Alcohols, secondary aliphatic	Ciliata sp	450
Structure-activity relationships	Inhibitory (toxic) effects, 432	Amino acids and derivatives
153	Flavobacterium sp	Nutritional effects, enrichment
Aldehydes	Aerobic biodegradation, 431	552
Structure-activity relationships	Mastigota sp	Benzene and derivatives
153	Inhibitory (toxic) effects, 432 Micrococcus sp	Nutritional effects, enrichment
Alkanoic acids and derivatives	Aerobic biodegradation, 431	552
Structure-activity relationships	Mycobacterium sp	Benzoic acid and derivatives
153	Aerobic biodegradation, 431	Nutritional effects, enrichment
Furan and derivatives	Nocardia sp	552
Aerobic biodegradation, 19	Aerobic biodegradation, 431	Cumene and derivatives
Metabolic pathways, 19	Pseudomonas sp	Nutritional effects, enrichment
Hydroquinone and derivatives	Aerobic biodegradation, 431	552
Structure-activity relationships	Sarcodina sp	Naphthalene and derivatives
153	Inhibitory (toxic) effects, 432	Nutritional effects, enrichment
Ketones, aliphatic	Xanthomonas sp	552
Aerobic biodegradation, 19	Aerobic biodegradation, 431	Phenol and derivatives
Metabolic pathways, 19	City of the city	Nutritional effects, enrichment
Lignin sulfonates Aerobic biodegradation, 19	Citrobacter sp	552
Metabolic pathways, 19	Alkyl sulfates, long chain, 442	Polycyclic aromatic hydrocarbons
Propylene glycols	Cyanide Identification of migropropriams	Nutritional effects, enrichment
Structure-activity relationships	Identification of microorganisms 206	552 Takana and dan and
153	DDT, Methoxychlor and metabolites	Toluene and derivatives
Pyrocatechol and derivatives	Anaerobic biodegradation, 536	Nutritional effects, enrichment

Cladosporium sp (cont'd) Xylenes and derivatives Nutritional effects, enrichment	Coliform bacteria, unidentified Timber steam processing wastes	Copper (cont'd) Opercularia sp
552	Aerobic biodegradation, 408 Identification of microorganisms	Inhibitory (toxic) effects, 486 Pseudomonas sp
Cladosporium sp acclimated	408	Inhibitory (toxic) effects, 572 Sorption, 210, 211
Hydrocarbons Metabolic pathways, 476	Operational parameters, 408	Sewage, municipal
Microbody formation, 476	Colpidium sp Chromium	Inhibitory (toxic) effects, 345
Clostridium sp	Innibitory (toxic) effects, 486	Sphaerotilus sp
Phosphorodithioic acid and derivatives	Copper	Inhibitory (toxic) effects, 437 Trickling filters
Anaerobic biodegradation, 465 Hydrogen sulfide production, 465	Inhibitory (toxic) effects, 486	Inhibitory (toxic) effects, 208
Coal carbonization wastes	Comamonas sp	499
Activated sludge, acclimated,	Quaternary ammonium compounds Aerobic digestion reactor, pilot	Vorticella sp
continuous-flow	plant, 125	Inhibitory (toxic) effects, 486 Zooglea sp
Inhibitory (toxic) effects, 364 Sludge acclimatization process	Conceptual model	Inhibitory (toxic) effects, 437
364	Activated sludge processes	Coriolus sp
-	Computational analysis, 147	Phenol-formaldehyde resin
Coal gasification wastes Activated sludge, acclimated, industrial	Operational parameters, 147	Biodegradation, rates compared
Aerobic biodegradation, 433	Confectionary wastes	248
Batch vs continuous-flow system	see also Sugars and derivatives Activated sludge	Poly(methyl methacrylate)
433	Glucose removal and polysaccharide	Biodegradation, rates compared
Activated sludge, UNOX pure oxygen technology	accumulation, 501	Polystyrenes
Overview, 187	Activated sludge, acclimated, industrial	Biodegradation, rates compared
Scheme of test facility, 187	Identification of microorganisms 502	248
Microbial population + synthetic sewage		Corynebacterium sp
Time-course kinetics, 384	Copper Activated sludge	Alkanes
Cobalt	Anaerobic digestion reactor, 344	Inhibitory (toxic) effects, 450 Structure-activity relationships
Activated sludge	Inhibitory (toxic) effects, 178	-450
Inhibitory (toxic) effects, 178	336, 344, 437, 546	Alkenes
546	Activated sludge, acclimated, municipal Freundlich adsorption isotherms	Inhibitory (toxic) effects, 450
Sewage, municipal Inhibitory (toxic) effects, 345	63	Structure-activity relationships 450
• • •	Kinetics and equilibrium studies	Alkyi halides
Coke oven wastes	63	Operational parameters, 374
Activated sludge Inhibitory (toxic) effects, 66	Langmuir adsorption isotherms	Trickling filters, 374
231. 480	Activated sludge, industrial	Arsenic compounds, inorganic Operational parameters, 464
Nitrification, 243	Inhibitory (toxic) effects, 35	Arsenic compounds, organic
Nitrification effect, 480	Activated sludge, industrial, continuous-	
Substrate concentration effect 66	flow Inhibitory (toxic) effects, 167	Carbamic acid and derivatives
Thiosulfate oxidation, 256	Activated sludge, industrial, porous-pot,	Biological membrane filtration 333
Activated sludge, diverse substrates	continuous-flow	Model ecosystem, aquatic, simulated
Batch vs continuous-flow system 71	Inhibitory (toxic) effects, 167	333
Substrate concentration effect	Activated sludge, municipal, continuous- flow	Chromium Operational parameters, 374
71	Inhibitory (toxic) effects, 167	Trickling filters 374
Time-course kinetics, 71	Activated sludge, municipal, porous-pot,	Phenol and derivatives
Activated sludge, second-stage Laboratory-pilot plant studies	continuous-flow Inhibitory (toxic) effects, 167	Operational parameters, 374
145	Activated sludge, phosphate-restricted,	Trickling filters, 374 Phthalic acid and derivatives
Operational parameters, 145	municipal	Metabolic pathways, 117
Microbial population Lagoons, waste-tip, 479	Aerobic biodegradation, 577 Activated sludge, synthetic	Pyrocatechol and derivatives
Metabolic pathways, 479	Inhibitory (toxic) effects, 35	Metabolic pathways, 117 Timber steam processing wastes
Trickling filters, 479	Colpidium sp	Aerobic biodegradation, 408
Microbial population, lagoons	Inhibitory (toxic) effects, 486	Identification of microorganisms
Isolation of microorganisms, 481 Model ecosystem, aquatic, simulated.	Escherichia sp Inhibitory (toxic) effects, 43	±08
481	Lagoon pre-treatment	Operational parameters, 408
Percolation system, 481	Anaerobic biodegradation, 379	Coryneform bacteria
Thiobacillus sp	Lumbricillus sp	Fuel oil
Thiosulfate oxidation, 256	Inhibitory (toxic) effects, 167	Metabolic pathways, 553

oryneiorm bacteria (cont d)	Cresois and derivatives (cont d)	Crude on (cont d)
Petroleum	Mycobacterium sp	Xanthomonas sp
Metabolic pathways, 553	Model ecosystem, terrestrial, natural.	Mesophilic temperature, effect
Polycaprotactone	545	567
Operational parameters, 32	Paracolobactrum sp	Psychrophilic temperature effect
Vibrio sp	Model ecosystem, terrestrial, natural,	567
Metabolic pathways, 550	545	
	Pseudomonas sp	Cryptococcus sp
Coumarin and derivatives	Inhibitory (toxic) effects, 309	Fuel oil
Activated sludge		Metabolic pathways, 553
Aerobic biodegradation, 175	Model ecosystem, terrestrial, natural.	Petroleum
Cresols and derivatives	545	
Achromobacter sp	pH effect, 74	Metabolic pathways, 553
Model ecosystem, terrestrial, natural,	Substrate concentration effect, 74	Polycaprolactone
	Temperature effect, 74	Operational parameters, 32
545	Sarcina sp	
Activated sludge	Model ecosystem, terrestrial, natural,	Cumene and derivatives
Aerobic biodegradation, 386	545	Activated sludge, 341
Inhibitory (toxic) effects, 178	* '=	Aerobic biodegradation, 386
309, 480	Trickling filters, pilot plant	Structure-activity relationships
Metabolic pathways, 143	Aerobic biodegradation, 74	386
Nitrification effect, 480	Crude oil	
Structure-activity relationships	Achromobacter sp	Cladosporium sp
	Mesophilic temperature, effect	Nutritional effects, enrichment
386	567	552
Activated sludge, acclimated		Microbial population, cumene-
Aerobic biodegradation, pilot plant,	Psychrophilic temperature effect	assimilating
57	567	Identification of microorganisms
Structure-activity relationships	Acinetobacter sp	376
389	Mesophilic temperature, effect	Screening tests, 376
Time-course kinetics, 389	567	
Activated sludge, municipal	Psychrophilic temperature effect	Substrate specificity, 376
	567	Pseudomonas sp
Inhibitory (toxic) effects, 369		Identification of microorganisms
Structure-activity relationships	Alcaligenes sp	376
369	Mesophilic temperature, effect	Psychrophilic temperature effect
Activated sludge + synthetic sewage	567	250
Metabolic pathways, 228	Psychrophilic temperature effect	Screening tests, 376
Time-course kinetics, 228	567	Time-course kinetics, 250
Alcaligenes sp	Arthrobacter sp	Time-course kineties, 250
Metabolic pathways, 37	Mesophilic temperature, effect	Cunninghamella sp
	567	Alkanes
Arthrobacter sp		Inhibitory (toxic) effects, 450
Model ecosystem, terrestrial, natural,		
545	567	Structure-activity relationships
Azotobacter sp	Cytophaga sp	450
Model ecosystem, terrestrial, natural,	Mesophilic temperature, effect	Alkenes
545	567	Inhibitory (toxic) effects, 450
Bacıllus sp	Psychrophilic temperature effect	Structure-activity relationships
Model ecosystem, terrestrial, natural,		450
545	Flavobacterium sp	Benzothiazole and derivatives
Brevibacterium sp	Mesophilic temperature, effect	Metabolic pathways, 555
Model ecosystem, terrestrial, natural,		Biphenyl and derivatives
545	Psychrophilic temperature effect	Aerobic biodegradation, 528
Flavobacterium sp	567	Metabolic pathways, 528
Model ecosystem, terrestrial, natural.	Gram-negative rods	Structure-activity relationships
545	Mesophilic temperature, effect	528
Metabolic pathways	567	Chloroalkylenes
Review, 88	Psychrophilic temperature effect	Aerobic biodegradation, 528
Microbial population, fresh water	567	Metabolic pathways, 528
	Gram-positive cocci	Structure-activity relationships
Aerobic biodegradation, 46		
Anaerobic biodegradation, 46	Mesophilic temperature, effect	528
Microbial population, sewage, municipal		Herbicides, urea
Reduced BOD, 61	Psychrophilic temperature effect	Metabolic pathways, 555
Microbial population, soils	567	Polychlorinated biphenyls
Denitrification, 14	Microbial population, fresh water sedi-	Aerobic biodegradation, 528
Metabolic pathways, 14	ment	Metabolic pathways, 528
Microbial population + synthetic	Time-course kinetics, 551	Structure-activity relationships
sewage	Pseudomonas sp	528
Time-course kinetics, 384		Polycyclic aromatic hydrocarbons
	Mesophilic temperature, effect	
Micrococcus sp	567	Metabolic pathways, 69, 100
Model ecosystem, terrestrial, natural,		Urea and derivatives
545	567	Metabolic pathways, 555

Cunninghamella sp (cont'd)	Cyanide (cont'd)	Cyanuric acid and derivatives (cont'd)
Cutting fluids (coolants), synthetic and	Sludge acclimatization process	Anaerobic biodegradation, 441
semi-synthetic	142	Microbial population, sewage, municipal
Activated sludge	Activated sludge, second-stage	Biological inhibition value, 199
Biodegradation, 1	Laboratory-pilot plant studies	Biorefractory index, 199
Inhibitory (toxic) effects with preser-	145	Inhibitory (toxic) effects, 199
vatives, 1	Operational parameters, 145	Microbial population, soils
Biodegradation	Bacıllus sp	Anaerobic biodegradation, 441
Review, 1	Identification of microorganisms	Cycloaliphatics, substituted
Microbial population, fresh water	206	Achromobacter sp
Biodegradation, I	Citrobacter sp	Inhibitory (toxic) effects, 38
Inhibitory (toxic) effects with preser-	Identification of microorganisms	Metabolic pathways, 41
vatives, 1	206	Activated sludge
Microbial population, fresh water ac- climated	Escherichia sp	Aerobic biodegradation, 386
Biodegradation, 1	Identification of microorganisms	Identification of microorganisms
blodegradation, 1	206	38
Cutting oils	Microbial population, sewage, municipal	Inhibitory (toxic) effects, 38
Activated sludge, industrial, continuous-	Inhibitory (toxic) and stimulatory ef-	Metabolic pathways, 39, 471
flow	fects, 170 Microbial acclimatization, 170	Structure-activity relationships, 386
Aerobic biodegradation, 167	Proteus sp	Activated sludge, municipal
Inhibitory (toxic) effects, 167	Identification of microorganisms	Anaerobic digestion reactor, 15
Activated sludge, industrial, porous-pot,	206	Fermentation, methanogenic, 15 Enterobacter sp
continuous-flow	Pseudomonas sp	Inhibitory (toxic) effects, 38
Aerobic biodegradation, 167	- Identification of microorganisms	Flavobacterium sp
Inhibitory (toxic) effects, 167	206	Inhibitory (toxic) effects, 38
Activated sludge, municipal, continuous-	Rhodopseudomonas sp	Gram-positive bacteria
flow	Inhibitory (toxic) effects, 323	Inhibitory (toxic) effects, 38
Aerobic biodegradation, 167 Anaerobic biodegradation, 167	Metabolic pathways, 323	Methanobacterium sp
Inhibitory (toxic) effects, 167	Sewage, municipal	Anaerobic digestion reactor, 15
Activated sludge, municipal, porous-pot,	Inhibitory (toxic) effects, 345	Fermentation, methanogenic, 15
continuous-flow	Nutritional effects, 90	Microbial biodegradation
Aerobic biodegradation, 167	Sewage, synthetic	Review 521
Inhibitory (toxic) effects, 167	Inhibitory (toxic) and stimulatory ef-	Mycobacterium sp
Lumbricillus sp	fects, 170	Metabolic pathways, 25
Inhibitory (toxic) effects, 167	Microbial acclimatization, 170	Nocardia sp
Cyanate	Staphylococcus sp	Metabolic pathways, 25, 444
Activated sludge	Identification of microorganisms	Pseudomonas sp
Inhibitory (toxic) effects, 231	206	Inhibitory (toxic) effects, 38
	Cyanuric acid and derivatives	Pseudomonas sp pure culture
Cyanide	Activated sludge	Metabolic pathways, 471
Activated sludge Aerobic digestion reactor, 139	Structure-activity relationships, 393	Vibrio sp Inhibitory (toxic) effects, 38
141, 142	Activated sludge, acclimated	Cytophaga sp
Inhibitory (toxic) effects, 139	Time-course kinetics, 475 Activated sludge, municipal	Alkanes, long chain, branched
141. 231, 429, 546	Anaerobic biodegradation, 441	Mesophilic temperature, effect
Kinetics and equilibrium studies	Activated sludge, municipal, continuous-	
142	flow	Psychrophilic temperature effect
Michaelis-Menten coefficients	Aerobic biodegradation, 441	567
141, 429	Fungi, unidentified, acclimated	Crude oil
Respirometric studies, 30	Metabolic pathways, 599	Mesophilic temperature, effect
Sludge acclimatization process	Gram-negative rods	567
141, 142	Microaerophilic mechanisms propos-	Psychrophilic temperature effect
Activated sludge, industrial	ed, 240	567
Identification of microorganisms	Microbial population, acclimated	Timber steam processing wastes
206	Metabolic pathways, 599	Aerobic biodegradation, 408 Identification of microorganisms
Activated sludge, multi-stage column Substrate concentration effect	Microbial population, cyanuric acid-	408
209	degrading Microaerophilic mechanisms propos-	Operational parameters, 408
Activated sludge + rice bran		2,4-D
Aerobic digestion reactor, 139	Microbial population, fresh water sedi-	see Herbicides, 2,4-D type
140, 142	ment	Arthrobacter sp
Inhibitory (toxic) effects, 139	Anaerobic biodegradation, 441	Batch vs continuous-flow system
Kinetics and equilibrium studies	Microbial population, raw sewage	312
142	Aerobic biodegradation, 26	Daedalea sp
Michaelis-Menten coefficients	Inhibitory (toxic) effects, 26	Phenol-formaldehyae resin
142	Microbial population, saline water sedi-	Biodegradation, rates compared
Operational parameters, 140	ment	248

Cunninghamella sp (cont'd)

Daedalea sp (cont'd)	DDT, Methoxychlor and metabolites	Dyes
Poly(methyl methacrylate)	(cont'd)	Activated sludge
Biodegradation, rates compared	Pseudomonas sp	Depuration rate, effect on, 83
248	Anaerobic biodegradation, 536	Inhibitory (toxic) effects, 370
Polystyrenes	Autoclaving effect, 536	371, 534, 581
Biodegradation, rates compared	Disinfectants effect, 536	Langmuir adsorption isotherms
248	Metabolic pathways, 536	370
= '-	Saccnaromyces sp	Michaelis-Menten coefficients
Daphnia sp	Aerobic coprecipitation, 269	370
Explosives, organic	Anaerobic coprecipitation, 269	Nutritional effects, 368
Inhibitory (toxic) effects, 7	Batch vs continuous-flow system	Operational parameters, 83
DDT	269	Respirometric studies, 534
see DDT, Methoxychlor and metabolites	Inhibitory (toxic) effects, 269	Structure-activity relationships.
	De-icer, aircraft + wastewater, airport	530
DDT, Methoxychlor and metabolites	Activated sludge, industrial and	Time-course kinetics, 530
see also Pesticides	municipal	Activated sludge, acclimated,
Activated sludge	Aerobic biodegradation, pilot plant,	continuous-flow
Aerobic biodegradation, 346	237	Operational parameters, 310
Activated sludge, acclimated	Detergent builders	Sludge acclimatization process
Aerobic biodegradation, 304	see Alkanoic acids and derivatives,	310
Metabolic pathways, 584	polybasic; Alkanoic acids,	Activated sludge, municipal
Bacıllus sp	cyclic; Alkenoic acids and	Inhibitory (toxic) effects, 369
Anaerobic biodegradation, 536	derivatives; NTA and salts;	Structure-activity relationships
Autoclaving effect, 536		369
Disinfectants effect, 536	Phosphonic acid derivatives,	Activated sludge, municipal, continuous-
Metabolic pathways, 536	alkyl poly-	flow
Candida sp	Detergent replacements	
Anaerobic biodegradation, 536	see Alkanoic acids and derivatives,	Inhibitory (toxic) effects, 241 Nitrification, effects on, 241
Autoclaving effect, 536	polybasic	
Disinfectants effect, 536	Dichlorophene	Nitrifying bacteria, continuous-culture
Metabolic pathways, 536	see Hexachlorophene	Inhibitory (toxic) effects, 241
Citrobacter sp	Diesel oil	Nitrification, effects on, 241
Anaerobic biodegradation, 536	Microbial population, fresh water	Dyes, acid
Autoclaving effect, 536		Activated carbon
Disinfectants effect, 536	Continuous culture, multistage	Biodegradation vs adsorption
Marshalla matheriana 526	400	358
Escherichia sp	Dimethyl sulfoxide	Activated sludge
Anaerobic biodegradation, 536	see also Alkyl sulfoxides	Inhibitory (toxic) effects, 370
Autoclaving effect, 536	Activated sludge	371, 581
Disinfectants effect, 536	Anaerobic digestion reactor, 602	Langmuir adsorption isotherms
	Microbial population, fresh water sedi-	370
Metabolic pathways, 536	ment	Michaelis-Menten coefficients
Fusarium sp	Anaerobic digestion reactor, 602	370
Aerobic biodegradation, 130	Biogeochemical cycling, 602	Nutritional effects, 368
Hydrogenomonas sp	Time-course kinetics, 602	Structure-activity relationships
Aerobic biodegradation, 130	Escherichia sp	530
Anaerobic biodegradation, 536	Anaerobic digestion reactor, 602	Time-course kinetics, 530
Autoclaving effect, 536	DMF	Activated sludge, municipal
Disinfectants effect, 536	see Amides, aliphatic	Aerobic and anaerobic digestion
Metabolic pathways, 536	DMSO	reactors, 547
Microbial population, fresh water	see Alkyl sulfoxides, Dimethyl sulfoxide	A control of the state of the s
Aerobic biodegradation, 46	The second secon	Inhibitory (toxic) effects, screening,
Anaerobic biodegradation, 46	Dobane JNQ sulfonate	547
Microbial population, loam	Activated sludge	Selenastrum sp
Structure-activity relationships	Anaerobic digestion reactor, 344	Inhibitory (toxic) effects, screening,
485	Inhibitory (toxic) effects, 344	547
Microbial population, raw sewage	Dobanol 25-9	Dyes, anthraquinone
Aerobic biodegradation, 26	Activated sludge, continuous-flow	Activated sludge
Inhibitory (toxic) effects, 26	Model ecosystem, aquatic, natural	Freundlich adsorption isotherms
Microbial population, septic tank	516	101
Inhibitory (toxic) effects, 6	Microbial population	Kinetics and equilibrium studies
Microbial population, sewage, municipal	Model ecosystem, aquatic, natural	101
Biological inhibition value, 199	516	Structure-activity relationships
Biorefractory index, 199	Dobanol 45-7	101
Inhibitory (toxic) effects, 199	Activated sludge, municipal	Activated sludge, boiling-inactivated
Mycoplana sp	Aerobic biodegradation, 75	Freundlich adsorption isotherms
Anaerobic biodegradation, 536	· ·	101
Autoclaving effect, 536	Domestic sewage effluents	Kinetics and equilibrium studies
Disinfectants effect. 536	Activated sludge	101
Metabolic pathways, 536	Inhibitory (toxic) effects, 336	

DDT, Methoxychlor and metabolites

Dyes

Dyes, antinaquinone (cont u)	Dyes, morgant	EDIA and saits (cont'd)
Structure-activity relationships	Activated sludge, municipal	Aerobic biodegradation, 509
101	Aerobic and anaerobic digestion	Microbial population, fresh water
Activated sludge, formaldehyde-	reactors, 547	sediments
inactivated	Inhibitory (toxic) effects, screening,	Aerobic biodegradation, 510
Freundlich adsorption isotherms	547	
101	Selenastrum sp	Metabotic pathways, co-metabolism
		510
Kinetics and equilibrium studies	Inhibitory (toxic) effects, screening,	Seasonal variations, 510
101	547	Microbial population, liquid cultures
Structure-activity relationships	Duras nigment	Aerobic biodegradation, 509
101	Dyes, pigment	Microbial population, soils
Dyes, basic	Activated sludge	Aerobic biodegradation, 509
Activated sludge	Nutritional effects, 368	510
	Dyes, reactive	
Inhibitory (toxic) effects, 370	Activated sludge	Metabolic pathways, co-metabolism
371	Aerobic biodegradation, 398	510
Langmuir adsorption isotherms		Seasonal variations, 510
370 -	Activated sludge, acclimated	Emkapyl 1839
Michaelis-Menten coefficients	Aerobic biodegradation, 397	Activated sludge, non-acclimated,
370	Dyes, sulfur	municipal
Activated sludge, municipal	Activated sludge	
Aerobic and anaerobic digestion	Inhibitory (toxic) effects, 534	Aerobic biodegradation, 18
	Respirometric studies, 534	Trickling filters, 18
reactors, 547		Enterobacter sp
Aerobic biodegradation, 79	Activated sludge, municipal	Alcohols, alicyclic
Inhibitory (toxic) effects, screening.	Aerobic and anaerobic digestion	Inhibitory (toxic) effects, 38
547	reactors, 547	Alkyl sulfates, long chain, 442
Selenastrum sp	Inhibitory (toxic) effects, screening,	
Inhibitory (toxic) effects, screening,	547	Amides, aliphatic
547	Selenastrum sp	Inhibitory (toxic) effects, 277
	Inhibitory (toxic) effects, screening.	Amines, alicyclic
Dyes, direct	547	Inhibitory (toxic) effects, 38
Activated carbon		Amines, aliphauc
Biodegradation vs adsorption	Dyes, vat	Inhibitory (toxic) effects, 277
358	Activated sludge	Cycloaliphatics, substituted
Activated sludge	Aerobic biodegradation, 398	
Aerobic biodegradation, 398	Activated sludge, acclimated	Inhibitory (toxic) effects, 38
	Aerobic biodegradation, 397	Ketones, aliphatic
Inhibitory (toxic) effects, 371		inhibitory (toxic) effects, 38
534	Activated sludge, municipal	Leather, artificial, processing wastes
Langmuir adsorption isotherms	Aerobic and anaerobic digestion	Inhibitory (toxic) effects, 277
370	reactors, 547	Oil refinery wastes, 40
Michaelis-Menten coefficients	Inhibitory (toxic) effects, screening,	Petrochemical wastes, 40
370	547	
Respirometric studies, 534	Selenastrum sp	Enzymes
Activated sludge, acclimated	Inhibitory (toxic) effects, screening,	Activated sludge, non-accilmated.
	547	municipal
Aerobic biodegradation, 397	Ecolytes	Gravimetric assessment, 420
Activated sludge, municipal		Hach oxidation, 420
Aerobic and anaerobic digestion	Activated sludge, municipal	Respirometric studies, 420
reactors, 547	Biodegradation, rates compared	Identification of microorganisms
Inhibitory (toxic) effects, screening,	176. 245	
547	Microbial population, soils	Biodegradability, ultimate, 487
Selenastrum sp	Biodegradation, rates compared	Review, 487
Inhibitory (toxic) effects, screening,	176, 245	Epoxides
	EDTA	Activated sludge
547	see also Alkanoic acids and derivatives	Petrochemical wastewater treatment
Dyes, disperse		324
Activated carbon	EDTA and salts	Sewage, acclimated, municipal
Biodegradation vs adsorption	Activated sludge	Petrochemical wastewater treatment
358	Time-course kinetics, 583	
Activated sludge	Activated sludge, municipal	51
Aerobic biodegradation, 398	Correlative test evaluations	Escherichia sp
Inhibitory (toxic) effects, 371	151	Alkanoic acids and derivatives, long
Activated sludge, acclimated	Activated sludge, OECD-specified	chain
Aerobic biodegradation, 397	Interlaboratory comparison, 590	Metabolic pathways, 273
<u> </u>	Static vs continuous activation	
Activated sludge, municipal		Structure-activity relationships
Aerobic and anaerobic digestion	method, 590	273
reactors, 547	Microbial population, aerated lagoon,	Alkanoic acids, sulfonated, long chain
Inhibitory (toxic) effects, screening,	industrial site	Bacteriocidal/bacteriostatic effects,
547	Model ecosystem, aquatic, industrial.	330
Selenastrum sp	31	Inhibitory (toxic) effects, 329
Inhibitory (toxic) effects, screening,	Microbial population, fresh water sedi-	Structure-activity relationships
547	ment	330
J-71	*******	550

Activated sludge, nitrifying Structure-activity relationships Alkyl sulfonates and derivatives Aerobic biodegradation, 353 386 Freundlich adsorption isotherms Nitrification, 353 Explosives, organic 459 Amides, aliphatic, long chain see also Ammunition plant wastes; Flame retardant Metabolic pathways, 273 Nitrobenzene and derivatives, Activated sludge, 190 Structure-activity relationships TNT Flavobacterium-cytophaga sp 273 Activated sludge Oil refinery wastes, 40 Batch vs continuous-flow system Ammes. long chain Petrochemical wastes, 40 Metabolic pathways, 273 564 Structure-activity relationships Metabolic pathways, 564 Flavobacterium sp Activated sludge, acclimated 273 Alcohols, alicyclic Inhibitory (toxic) effects, 38 Amino acids and derivatives Inhibitory (toxic) effects, 390 Metabolic pathways, 273 Structure-activity relationships Alcohols, primary aliphatic Structure-activity relationships 390 Identification of microorganisms 273 Time-course kinetics, 390 164, 560 Activated sludge, continuous-flow Inhibitory (toxic) effects, 532 Copper Respirometric studies, 560 Inhibitory (toxic) effects, 43 Aldehydes Review, 566 Cyanide Identification of microorganisms Activated sludge + cornsteep, Identification of microorganisms 164 continuous-flow Alkanes DDT. Methoxychlor and metabolites Oxidation ditch, 204 Inhibitory (toxic) effects, 450 Anaerobic biodegradation, 536 Activated sludge, municipal Metabolic pathways, 232 Activated sludge, synthetic, 62 Aerobic biodegradation, 62, 334 Autoclaving effect, 536 Structure-activity relationships Disinfectants effect, 536 450 Metabolic pathways, 536 Metabolic pathways, 334 Alkanes, cyclic Dimethyl sulfoxide Daphnia sp Metabolic pathways, 232, 335 Anaerobic digestion reactor, 602 Inhibitory (toxic) effects. 7 Alkanes, long chain, branched Denitrification Mesophilic temperature, effect Inhibitory (toxic) effects. 43 Review, 566 Lindane and metabolites Gram-negative rods Psychrophilic temperature effect Anaerobic biodegradation, 536 Metabolic pathways, 564 567 Mercury, inorganic Lebistes sp Alkanes, long chain, linear Inhibitory (toxic) effects, 43 Inhibitory (toxic) effects, 7 Metabolic pathways, 232 Milk, water-diluted Microbial population Alkenes Inhibitory (toxic) effects, 43 Metabolic pathways, 565 Inhibitory (toxic) effects, 450 Phenol and derivatives Operational parameters Metabolic pathways, 232 Identification of microorganisms 205, 206 Review, 566 Structure-activity relationships Paramecium sp 450 Polychlorobenzenes and derivatives Inhibitory (toxic) effects, 7 Alkyl sulfates, long chain, 442 Anaerobic biodegradation, 536 Pseudomonas sp Amides, aliphatic Polychiorocyclopentadiene dimers Inhibitory (toxic) effects, 7 Inhibitory (toxic) effects, 277 Time-course kinetics Anaerobic biodegradation, 536 Structure-activity relationships Thiocyanic acid and salts Review, 566 Fellmongery wastes see also Proteins Identification of microorganisms Amides, aliphatic, long chain 205, 206 Structure-activity relationships Acinetobacter sp Ethers 120 Identification of microorganisms Sewage, acclimated, municipal Amines, alicyclic Petrochemical wastewater treatment Inhibitory (toxic) effects, 38 Activated sludge Amines, aliphatic Aerobic digestion, 197 Inhibitory (toxic) effects, 277 Aerobic digestion reactor, 405 Biomass yield, effect on, 197 Ethomeens Activated sludge, non-acclimated, Aromatic compounds, dicyclic Metabolic pathways, 335 municipal Operational parameters, 405 Benzene and derivatives Aerobic biodegradation, 18 Substrate concentration effect Metabolic pathways, 232, 335 Trickling filters, 18 105 Biphenyl and derivatives Activated sludge, acclimated, municipal Aerobic biodegradation, 186 Eupenicillium sp Metabolic pathways, 335 Cirrasols Inhibitory (toxic) effects, 450 Denitrification, 77 Aerobic biodegradation, 431 Structure-activity relationships Sludge acclimatization process Cresols and derivatives 450 77, 186 Model ecosystem, terrestrial, natural, Alkenes Substrate concentration effect, 77 Inhibitory (toxic) effects, 450 Microbial population, municipal wastes Crude oil Structure-activity relationships Identification of microorganisms Mesophilic temperature, effect 450 406 567 Pseudomonas sp Explosives Psychrophilic temperature effect Activated sludge Identification of microorganisms Aerobic biodegradation, 386 406

Explosives (cont'd)

Escherichia sp (cont'd)

Fertilizer wastes, nitrogenous

avooucierium sp (cont a)	Fluorescent originteners (conf. d)	ruran and derivatives (cont'd)
Cycloalipnatics, substituted	Activated sludge, single and two-stage	Structure-activity relationships
Inhibitory (toxic) effects, 38	reactors	386
Gasoline	Anaerobic biodegradation, 146	Arthrobacter sp
		Appoint had a site of a
Metabolic pathways, 232	Biodegradation, environmental aspects	Aerobic biodegradation, 19
Hydrocarbons	Review, 56	Metabolic pathways, 19
Metabolic pathways, 232	Fomes sp	Chromobacterium sp
Ketones, aliphatic	Phenol-formaldehyde resin	Aerobic biodegradation, 19
Inhibitory (toxic) effects, 38	Biodegradation, rates compared	Metabolic pathways, 19
Leather, artificial, processing wastes	248	Microbial biodegradation
Inhibitory (toxic) effects, 277		Review, 521
Naphthalene and derivatives	Poly(methyl methacrylate)	Missobial ====t-i
	Biodegradation, rates compared	Microbial population, acclimated
Metabolic pathways, 335	. 248	Aerobic biodegradation, 19
Phenol and derivatives	Polyethylene	Metabolic pathways, 19
Identification of microorganisms	Isolation of microorganisms, 3	Pseudomonas sp
71		Aerobic biodegradation, 19
Model ecosystem, terrestrial, natural,	Metabolic pathways, 3	Metabolic pathways, 19
545	, , , , , , , , , , , , , , , , , , , ,	Same and the same of the same
	Biodegradation, rates compared	Sewage, municipal
Plycyclic aromatic hydrocarbons	248	Respirometric studies, 548
Metabolic pathways, 335	Food industry waste	Trichosporon sp
Polyamides	Food industry wastes	Aerobic biodegradation, 19
Structure-activity relationships	Activated sludge	Metabolic pathways, 19
12	Metabolic pathways, 596	
·-	Fruit juice wastes	Furfural
Polyethylene glycols	Activated sludge	see Furan and derivatives
Identification of microorganisms		Fusarium sp
560	Glucose removal and polysaccharide	Alkanoic acids and derivatives
Respirometric studies, 560	accumulation, 501	
Polyethylene glycols, fatty ether	 Activated sludge, acclimated, industrial 	Aerobic biodegradation, 130
	Identification of microorganisms	Alkanoic acids and derivatives,
Aerobic biodegradation, 431	502	polybasic
Polymers, bio-		Aerobic biodegradation, 130
pH effect, 593	Fuel oil	Alkenoic acids and derivatives
Substrate concentration effect	Acinetobacter sp	A anabia bandana in a sa
593	Metabolic pathways, 553	Aerobic biodegradation, 130
Surfactant effect, 593	Activated sludge, non-acclimated	Benzoic acid and derivatives
	Inhibitory (toxic) effects, 454	Metabolic pathways, 188
Propylene glycols		Benzonitrile and derivatives
Identification of microorganisms	Rate and selective adsorption	Metabolic pathways, 188
560	454	Carbamic acid and derivatives, 258
Respirometric studies, 560	Activated sludge, non-acclimated,	Distante actu and derivatives, 258
Sulfanilic acid and derivatives	municipal, 255	Biological membrane filtration
	Bacillus sp	333
Identification of microorganisms		Model ecosystem, aquatic, simulated,
377	Metabolic pathways, 553	333
Tetralin and derivatives	Coryneform bacteria	DDT, Methoxychlor and metabolites
Metabolic pathways, 335	Metabolic pathways, 553	Agrapia biodessed the 120
Timber steam processing wastes	Cryptococcus sp	Aerobic biodegradation, 130
Aerobic biodegradation, 408	Metabolic pathways, 553	Herbicides, monuron type and
	Microbial population, fresh water	metabolites
Identification of microorganisms		Metabolic pathways, 134
408	Metabolic pathways, 553	Herbicides, propanil type and
Operational parameters, 408	Pseudomonas sp	metabolites
Toluene and derivatives	Metabolic pathways, 299, 553	Metabolic pathways, 257
Metabolic pathways, 232, 335	Fungi, unidentified, acclimated	Herbicides, urea
Xylenes and derivatives	Cyanuric acid and derivatives	
Metabolic pathways, 232, 335		Metabolic pathways, 257
	Metabolic pathways, 599	Heteroaromatics and derivatives, dicyclic
Xylenols and derivatives	Herbicides, atrazine type	Metabolic pathways, 373
Model ecosystem, terrestrial, natural,	Metabolic pathways, 599	Phenylacetic acid and derivatives
545	Fungus, Pl	Aerobic biodegradation, 130
uorescent brighteners	Poly(alkyl-β-propiolactones)	Polyathylana
see Stilbene and derivatives		Polyethylene
	Structure-activity relationships	Isolation of microorganisms, 3
Activated sludge	503	4
Aerobic biodegradation, 146	Polycaprolactone	Metabolic pathways, 3
175	Structure-activity relationships	Pyrocatechol and derivatives
Incineration, 146	503	Metabolic pathways, 188
Wet oxidation (Zimpro) reactor	Polyesters	
146	Structure-activity relationships	Salicylic acid and derivatives
	• • • • • • • • • • • • • • • • • • • •	Metabolic pathways, 188
Activated sludge, acclimated,	503	Xylenols and derivatives
continuous-flow	Furan and derivatives	Metabolic pathways, 188, 373
Operational parameters, 310	Activated sludge	* ***
Sludge acclimatization process	Aerobic biodegradation, 386	Gas oil
110	Inhibitory (toxic) effects 49	Microbial population, sewage, municipal

Gas on (cont d)	Gram-negative rous (cont'd)	attracted alude type (cont.d)
Inhibitory (toxic) and stimulatory ef-	Cyanuric acid and derivatives	Activated sludge, municipal
fects, 170	Microaerophilic mechanisms propos-	Distribution and rate accumulation
Microbial acclimatization, 170	ed, 240	270
Sewage, synthetic	Explosives, organic	Activated sludge + synthetic sewage
Inhibitory (toxic) and stimulatory ef-	Metabolic pathways, 564	Correlative test evaluations
		233
fects, 170	Naphthalene and derivatives	Fungi, unidentified, acclimated
Microbial acclimatization, 170	Structure-activity relationships	
Gasoline	523	Metabolic pathways, 599
see also Alkanes	NTA and salts	Microbial population, acclimated
Acinetobacter sp	Anaerobic biodegradation, 114	Metabolic pathways, 599
	115	Microbial population, pesticide-
Metabolic pathways, 232	Oil refinery wastes, 40	metabolizing
Flavobacterium sp		Metabolic pathways, 132
Metabolic pathways, 232	Petrochemical wastes, 40	Microbial population, soils
Microbial population	Stilbene and derivatives	
Metabolic pathways, 232	Structure-activity relationships	Metabolic pathways, 132
Microbial population, raw sewage	523	Operational parameters, 132
Aerobic biodegradation, 26	Tetralin and derivatives	Microbial population, soils, organic-
		enriched
Microbial population, sewage, municipal	523	Metabolic pathways, 132
Biorefractory index, 199		Operational parameters, 132
Recommendations, wastewater treat-	Gram-positive bacteria	
ment, 199	Alcohols, alicyclic	Herbicides, carbamate
Micrococcus sp	Inhibitory (toxic) effects, 38	Bacıllus sp .
Metabolic pathways, 232	Amines, alicyclic	Metabolic pathways, 111
		Time-course kinetics, 111
Nocardia sp	Inhibitory (toxic) effects, 38	Microbial population, fresh water +
Metabolic pathways, 232	Cycloaliphatics, substituted	
Pseudomonas sp	Inhibitory (toxic) effects, 38	sewage
Metabolic pathways, 232	Ketones, aliphatic	Metabolic pathways, 111
Geotrichum sp	Inhibitory (toxic) effects, 38	Time-course kinetics, 111
Industrial wastewaters		Marking allowers
Isolation of microorganisms, 586	Gram-positive cocci	Herbicides, chlorpropham type
Polyvinyl acetate	Alkanes, long chain, branched	see also Carbamic acid and derivatives
	Mesophilic temperature, effect	Achromobacter sp
Isolation of microorganisms, 586	567	Phorate inhibitory activity, 257
Polyvinýl alcohol	Psychrophilic temperature effect	Bacillus sp
Isolation of microorganisms, 586	567	Metabolic pathways, 474
Gleophyilum sp	Crude oil	Operational parameters, 160
Phenol-formaldehyde resin		Missabish associated for the state of the st
Biodegradation, rates compared	Mesophilic temperature, effect	Microbial population, fresh water
	567	Sorption, 44
248	Psychrophilic temperature effect	Substrate concentration effect
Poly(methyl methacrylate)	567	44
Biodegradation, rates compared	Oil refinery wastes, 40	Microbial population, loam
248	Petrochemical wastes, 40	Azide inhibitory activity, 257
Polystyrenes		Corporal inhibitory activity, 257
Biodegradation, rates compared	Gram-positive organisms	Carparyl inhibitory and persistance
248	Alkylsulfonic acids	activity, 257
=	Inhibitory (toxic) effects, 171	Diazinon inhibitory and persistance
Gram-negative rods	Benzenesulfonic acid, alkyl, long chain	activity, 257
Alkanes, long chain, branched	Inhibitory (toxic) effects, 171	Microbial population, river water
Mesophilic temperature, effect		Identification of microorganisms
567	Gums	160
Psychrophilic temperature effect	Activated sludge, acclimated,	
567	continuous-flow	Model ecosystem, aquatic, natural
Alkenes	Operational parameters, 310	160
	Sludge acclimatization process	Micrococcus sp
Structure-activity relationships	310	Metabolic pathways, 474
523		Pseudomonas sp
Aromatic compounds, dicyclic	Microbial population	Azide inhibitory activity, 257
Structure-activity relationships	Metabolic pathways, 27	Diazinon inhibitory and persistance
523	Microbial population, soils	
Benzene and derivatives	Operational parameters, 171	activity, 257
	Haliscomenobacter sp	Operational parameters, 160
		Phorate inhibitory activity, 257
523	Sugars and derivatives	77-3-1-1-1 0 4 75 -
Biphenyl and derivatives	Inhibitory (toxic) effects, 409	Herbicides, 2,4-D type
Structure-activity relationships	Halogenated hydrocarbons	Activated sludge, 207
523		Inhibitory (toxic) effects, 429
Crude oil	Microbial biodegradation, mechanisms	Michaelis-Menten coefficients
Mesophilic temperature, effect	Review, 50	429
	Herbicides assazine tum-	Arthrobacter sp
	Herbicides, atrazine type	
Psychrophilic temperature effect	Activated sludge, acclimated	Batch vs continuous-flow system
567	Time-course kinetics, 475	312

	Herbicides, monuron type and metabolites	Herbicides, urea (cont'd) Taloramyces sp
Baeillus sp	(cont'd) simulated, 216	Metabolic pathways, 257
Operational parameters, 160 Microbial population, 45	Microbial population, pesticide-	
Microbial population, fresh water	metabolizing	Heteroaromatics and derivatives, dicyclic Achromovacter sp
Aerobic biodegradation, 46	Metabolic pathways, 132	Metabolic pathways, 41
Anaerobic biodegradation, 46	Microbial population, soils	Activated sludge
Sorption, 44	Metabolic pathways, 132	Aerobic biodegradation, 73
Substrate concentration effect	Operational parameters, 132	Structure-activity relationships
44	Microbial population, soils, organic-	393
Microbial population, pesticide-	enriched	Fusarium sp
metabolizing	Metabolic pathways, 132	Metabolic pathways, 373
Metabolic pathways, 132	Operational parameters, 132	Microbial population, fecal isolates
Microbial population, river water	Penicillium sp	Metabolic pathways, 575
Identification of microorganisms	Metabolic pathways, 216	Microbial population, fresh water
160	Sewage, municipal	Aerobic biodegradation, 46
Model ecosystem, aquatic, natural	Co-substrate concentration effect	Anaerobic biodegradation, 46
160	159	Microbial population, sewage, municipal
Microbial population, river water filtrate	Inhibitory (toxic) effects, 159	Biorefractory index, 199
Anaerobic biodegradation, 561	River die-away test, 159	Recommendations, wastewater treat-
Seasonal variations, 561	Structure-activity relationships	ment, 199
Microbial population, river water sedi-	159	Pseudomonas sp
ment	Substrate concentration effect	Metabolic pathways, 539
Anaerobic biodegradation, 561	159	Sewage, municipal
Seasonal variations, 561	Herbicides, propanil type and metabolites	Nutritional effects, 90
Microbial population, soils	Aspergillus sp	Heterocyclic compounds
Metabolic pathways, 132	Metabolic pathways, 216	Identification of microorganisms
Operational parameters, 132	Bacillus sp	Biodegradability, ultimate, 487
Microbial population, soils, organic-	Metabolic pathways, 111	Review. 487
enriched	Time-course kinetics, 111	Hexachlorophene
Metabolic pathways, 132	Fusarium sp	see also Pesticides
Operational parameters, 132	Metabolic pathways, 257	Acinetobacter sp
Pseudomonas plasmids	Microbial population, fresh water +	Metabolic pathways, 354
Genetic transfer, 383	sewage	Activated sludge
Metabolic pathways, 383	Metabolic pathways, 111	Inhibitory (toxic) effects, 354
Pseudomonas sp	Time-course kinetics, 111	Activated sludge, acclimated, industrial
Aquatic systems, 46	Microbial population, loam	Aerobic biodegradation, 469
Diauxic fermentation, 46	Model ecosystem, terrestrial,	Sorption, 469
Metabolic pathways, 214	simulated, 216	Nocardia sp
Model ecosystem, aquatic, simulated.	1 Emcunary sp	Metabolic pathways, 354
214	Metabolic pathways, 216	Pseudomonas sp
Operational parameters, 160	Taloramyces sp	Metabolic pathways, 354
Herbicides, monuron type and metabolites	Metabolic pathways, 257	Hexapon
Activated sludge, continuous-flow	Herbicides, pyrazon type	Activated sludge, non-acclimated.
Co-substrate concentration effect	Microbial population, pesticide-	municipal
159	metabolizing	Aerobic biodegradation, 18
Inhibitory (toxic) effects, 159	Metabolic pathways, 132	Trickling filters, 18
River die-away test, 159	Microbial population, soils	Humic acid
Structure-activity relationships	Metabolic pathways, 132	Microbial population, sewage, municipal
Substrate concentration effect	Operational parameters, 132	Biorefractory index, 199
159	Microbial population, soils, organic-	Recommendations, wastewater treat-
Activated sludge, municipal	enriched	ment, 199
Distribution and rate accumulation	Metabolic pathways, 132	Humics
270	Operational parameters, 132	Microbial population, raw sewage
Aspergillus sp	Herbicides, silvex type	Aerobic biodegradation, 26
Metabolic pathways, 216	Achromobacter sp	Hyalodendron sp
Bacillus sp	Model ecosystem, aquatic, simulate	Pulp and paper wastes
Metabolic pathways, 111	378	Foam process, 594
Time-course kinetics, 111	Pseudomonas sp	Sulfite liquor
Fusarium sp	Metabolic pathways, 214	Foom process 594
Metabolic pathways, 134	Model ecosystem, aquatic, simulate	su,
Microbial population, fresh water +	214, 378	Hydrocarbons
sewage	Herbicides, urea	see also Alkanes
Metabolic pathways, 111	Cunninghamella sp	Acinetobacter sp
Time-course kinetics, 111	Metabolic pathways, 555	Metabolic pathways, 232
Microbial population, loam	Fusarium sp	Activated sludge
Model ecosystem, terrestrial,	Metabolic pathways, 257	Aerobic biodegradation, 398

Hydrocarbons (cont'd)	Hydroquinone and derivatives (cont'd)	Inhibitory (toxic) effects (cont'd)
Activated sludge, acclimated	Chromobacterium sp	Alcohols, primary alipnatic
Aerobic biodegradation, 397	Structure-activity relationships	Activated sludge, 144
Activated sludge, acclimated.	153	Activated sludge, synthetic,
continuous-flow	Metabolic patnways	continuous-flow, 34
Operational parameters, 310	Review, 88	Alcohols, tertiary aliphatic
Sludge acclimatization process	Microbial population, sewage, municipal	Sewage, municipal, 548
310	Biorefractory index, 199	Aldehydes
Cladosportum sp acclimated	Recommendations, wastewater treat-	Activated sludge, 453
Metabolic pathways, 476	ment, 199	Activated sludge, acclimated
Microbody formation, 476	Micrococcus sp	21. 226
Flavobacterium sp	Structure-activity relationships	Activated sludge, non-acclimated
Metabolic pathways, 232	153	21
Microbial population	Mycobacterium sp	Alkanes
Metabolic pathways, 232	Structure-activity relationships	Achromobacter sp. 450
Micrococcus sp	153	Acinetobacter sp. 450
Metabolic pathways, 232	Nocardia sp	Activated sludge, 144
Nocardia sp	Metabolic pathways, 180, 444	Arthrobacter sp. 450
Metabolic pathways, 232	Pseudomonas sp	Aspergillus sp., 450
Pseudomonas sp	Metabolic pathways, 184, 539	Brevibacterium sp. 450
Metabolic pathways, 232	Structure-activity relationships	Candida sp. 450
Hydrogenomonas sp	153, 473	Cladosporium sp. 450
Alkanoic acids and derivatives	, Sarcina sp	Corynebacterium sp. 450
Aerobic biodegradation, 130	Structure-activity relationships	Cunninghamella sp. 450
Alkanoic acids and derivatives.	- 153	Eupenicillium sp. 450
polybasic	Sewage, natural, semi-continuous flow	Flavobacterium sp. 450
Aerobic biodegradation, 130	Metabolic pathways, 184	Mycobacterium sp. 450
Alkenoic acids and derivatives	·	Nocardia sp. 450
Aerobic biodegradation, 130	Industrial wastewaters	- · · · · · · · · · · · · · · · · · · ·
DDT, Methoxychlor and metabolites	Algae species	Sporobolomyces sp. 450
Aerobic biodegradation, 130	Facultative pond, 93	Alkanes, long chain, branched
Anaerobic biodegradation, 536	Geotrichum sp	Candida sp. 85
Autoclaving effect, 536	Isolation of microorganisms, 586	Alkanes, long chain, linear
Disinfectants effect, 536	Microbial population, soils	Candida sp. 85
Metabolic pathways, 536	Isolation of microorganisms, 586	Alkanoic acids and derivatives
Lindane and metabolites	Pseudomonas sp	Activated sludge, 429
Anaerobic biodegradation, 536	Isolation of microorganisms, 586	Arthrobacter sp. 84
Phenylacetic acid and derivatives	Inhibitory effects, metallic and ionic species:	Alkanoic acids and derivatives, long
Aerobic biodegradation, 130	Activated sludge	chain
Polychlorobenzenes and derivatives	Review, 546	Activated sludge, non-acclimated
Anaerobic biodegradation, 536	Inhibitory (toxic) and stimulatory effects	454
Polychlorocyclopentadiene dimers	Chromium	Alkanoic acids, sulfonated, long chain
Anaerobic biodegradation, 536	Microbial population, sewage,	Activated sludge, acclimated,
lydroquinone and derivatives	municipal, 170	municipal, 329
Actinomyces sp	Sewage, synthetic, 170	Escherichia sp., 329
Structure activity relationships	Cyanide	Pseudomonas sp. 329
153	Microbial population, sewage,	Salmonella sp., 329
Activated sludge	municipal, 170	Staphylococcus sp., 329
Respirometric studies, 30	Sewage, synthetic, 170	Alkenes
Structure-activity relationships	Gas oil	Achromobacter sp., 450
153, 473	Microbial population, sewage,	Acinetobacter sp., 450
Activated sludge, acclimated	municipal, 170	Arthrobacter sp., 450
Structure-activity relationships	Sewage, synthetic, 170	Aspergillus sp., 450
389	Phenol and derivatives	Brevibacterium sp. 450
Time-course kinetics, 389	Microbial population, sewage,	Candida sp. 450
Activated sludge, municipal	municipal, 170	Cladosporium sp, 450
Correlative test evaluations	Sewage, synthetic, 170	Corynebacterium sp. 450
151	Inhibitory (toxic) effects	Cunninghamella sp, 450
Bacıllus sp	Acetophenone and derivatives	Eupenicillium sp. 450
Structure-activity relationships	Arthrobacter sp. 84	Flavobacterium sp. 450
153, 473	Alcohols, alicyclic	Mycobacterium sp, 450
Bacillus sp., aerobic	Achromobacter sp. 38	Nocardia sp, 450
Metabolic pathways, 2	Activated sludge, 38	Rhodotorula sp. 450
Bacillus sp., anaerobic	Enterobacter sp. 38	Sporobolomyces sp. 450
Metabolic pathways, 2	Flavobacterium sp. 38	Alkenoic acids and derivatives, long
Bacterium sp	Gram-positive bacteria, 38	chain
Structure-activity relationships	Pseudomonas sp. 38	Pseudomonas sp. 572
153	Vibrio sp. 38	Alkyl halides

Inhibitory (toxic) effects (cont'd)	Inhibitory (toxic) effects (cont'd)	Inhibitory (toxic) effects (cont'd)
Activated sludge, 150, 344	Activated sludge, industrial and	continuous-flow, 167
Microbial population, raw sewage	municipal, 13	Activated sludge, industrial, porous-
26	Activated sludge, municipal, 369	pot, continuous-flow, 167
Microbial population, sewage,	Activated sludge, municipal,	Activated sludge, municipal,
municipal, 199	continuous-flow, 241	continuous-flow, 167
Alkyl sulfonates and derivatives	Nitrifying bacteria, continuous-	Activated sludge, municipal, porous
Activated sludge, 128	culture, 241	pot. continuous-flow, 167
Alkyisulfonic acids	Nitrosomas sp. 587	Lumbricillus sp., 167
Activated sludge, 178	Structure-activity relationships	Chloramine and derivatives
Gram-positive organisms, 171	159	Trickling filters, 306
Alkynes	Antibiotics	Chloride
Rhodopseudomonas sp. 323	Activated sludge, 252, 595	Activated sludge, 131
Aluminum	Activated sludge, municipal and syn-	Activated sludge, fresh water 203
Activated sludge, 178	thetic, 238	
Pseudomonas sp. 572	Bacillus sp. 308	Activated sludge, salt water 203
Sewage, municipal, 345	Trickling filters, 308	Pseudomonas sp. 131
Amides, aliphatic	Arsenic compounds, morganic	Chromium
Activated sludge, 28	Activated sludge, 588	Activated sludge, 131, 149
Activated sludge, acclimated	Azo compounds	178, 336, 344, 437, 546
277 Activated sludge, municipal, 348	Activated sludge, 581	Activated sludge, continuous-flow
Enterobacter sp. 277	Azo dyes	48
Flavobacterium sp. 277	Activated sludge, 371, 581 Activated sludge, municipal, 369	Activated sludge, industrial
Pseudomonas sp. 277	Benzenesulfonic acid, alkyl, long chain	35
Vibrio sp. 277	Gram-positive organisms, 171	Activated sludge, municipal, 478
Amines, alicyclic	Benzenesulfonic acid and non-alkyl	Activated sludge, synthetic, 35
Achromobacter sp. 38	substituted derivatives	Colpidium sp., 486
Activated sludge, 38	Activated sludge, municipal, 369	Nitrobacter sp. 124
Enterobacter sp. 38	Benzenesulfonic acid, linear alkyl, long	Nitrosomas sp., 124
Flavobacterium sp. 38	chain	Opercularia sp., 486
Gram-positive bacteria, 38	Activated sludge, 235	Pseudomonas sp. 131, 572
Microbial population, municipal	Benzoic acid and derivatives	Sewage, municipal, 345
wastes, 311	Activated sludge, 66	Sphaerotilus sp., 437
Pseudomonas sp. 38	Arthrobacter sp. 84	Vorticella sp. 486
Vibrio sp. 38	Pseudomonas sp. 183	Zoogiea sp. 437
Amines, aliphatic	Sewage, municipal, 183	Cirrasols
Activated sludge, 504	Benzothiazole and derivatives	Activated sludge, 430
Activated sludge, acclimated	Activated sludge, 128, 144	Activated sludge, acclimated
226, 277	Biphenyl and derivatives	432
Enterobacter sp., 277	Activated sludge, 144, 309	Activated sludge; non-acclimated
Flavobacterium sp., 277	354, 4 53	432
Pseudomonas sp. 277	Activated sludge, industrial and	Ciliata sp. 432
Vibrio sp., 277	municipal, 13	Mastigota sp. 432
Amines, long chain	Activated sludge, non-acclimated	Sarcodina sp. 432
Microbial population, municipal	454	Coal carbonization wastes
wastes, 311	Pseudomonas sp. 309	Activated sludge, acclimated,
Microbial population, river water	Boron	continuous-flow, 364
427	Activated sludge, 588	Cobait
Amines, poly-, aliphatic	Activated sludge, laboratory-pilot	Activated sludge, 178, 546
Microbial population, municipal	plant, 562	Sewage, municipal, 345 Coke oven wastes
wastes, 311	Activated sludge, municipal,	Activated sludge, 66, 231, 480
Microbial population, river water	continuous-flow, 562	Copper
427	Cadmium Activated sludge, 178, 344	Activated sludge, 178, 336
Amino acids and derivatives Activated sludge, acclimated		344, 437, 546
226	546 Activated sludge, industrial	Activated sludge, industrial
Ammonia and salts	68	35
Activated sludge, 231	Activated sludge, municipal, 361	Activated sludge, industrial,
Ammunition plant wastes	Activated sludge, non-acclimated	continuous-flow, 167
Activated sludge, municipal,	343	Activated sludge, industrial, porous-
continuous-flow, 360	Microbial population, sewage,	pot, continuous-flow, 167
Aniline and derivatives	municipal, 199	Activated sludge, municipal,
Activated sludge, 66, 534	Nitrobacter sp. 124	continuous-flow, 167
Activated sludge, acclimated	Nitrosomas sp. 124	Activated sludge, municipal, porous-
226, 391	Sewage, municipal, 345	pot, continuous-flow, 167
Activated sludge, continuous-flow	Carbamic acid and derivatives	Activated sludge, synthetic, 35
150	A assume and also does in description	Colpidium sp. 486

Inhibitory (toxic) effects (cont'd)	Inhibitory (toxic) effects (cont'd)	Inhibitory (toxic) effects (cont'd)
Escherichia sp. 43	Activated sludge, 370, 371	Pseudomonas sp. 572
Lumbricillus sp. 167	581	Mercury
Opercularia sp. 486	Dyes, basic	Microbial population, sewage,
Pseudomonas sp. 572	Activated sludge, 370, 371	municipal, 199
Sewage, municipal, 345	Dyes, direct	Mercury, inorganic
Sphaerotilus sp., 437	Activated sludge, 371, 534	Activated sludge, 429, 437
Trickling filters, 208, 499	Dyes, disperse	546
Vorticella sp. 486	Activated sludge, 371	Activated sludge, municipal, 361
Zooglea sp. 437	Dyes, sulfur	Activated sludge, non-accimated
Cresols and derivatives	Activated sludge, 534	343
Activated sludge, 178, 309	Explosives, organic	Escherichia sp. 43
480	Activated sludge, acclimated	Saccharomyces sp, 269
Activated sludge, municipal, 369	390	Sewage, municipal, 345
Pseudomonas sp. 309 Cutting oils	Activated sludge, continuous-flow	Sphaerotilus sp. 437 Vorticella sp. 445
Activated sludge, industrial,	532 Dankria sp. 7	
continuous-flow, 167	Daphnia sp. 7	Zooglea sp. 437 Mercury, organo-
Activated sludge, industrial, porous-	Lebistes sp. 7 Paramecium sp. 7	Activated sludge, 128
pot, continuous-flow, 167	Pseudomonas sp, 7	Milk, water-diluted
Activated sludge, municipal,	Fuel oil	Escherichia sp. 43
continuous-flow, 167	Activated sludge, non-acclimated	Molybdenum
Activated sludge, municipal, porous-	454	Activated sludge, 20
pot, continuous-flow, 167	Furan and derivatives	Naphthalene and derivatives
Lumbricillus sp. 167	Activated sludge, 49	Activated sludge, 144, 178
Cyanate	Herbicides, 2,4-D type	371, 534
Activated sludge, 231	Activated sludge, 429	Activated sludge, acclimated
Cyanide	Herbicides, monuron type and	226
Activated sludge, 139, 141	metabolites	Activated sludge, industrial and
231, 429, 546	Activated sludge, continuous-flow	municipal, 13
Activated sludge + rice bran	159	Activated sludge, municipal, 369
139	Sewage, municipal, 159	Activated sludge, synthetic, 162
Rhodopseudomonas sp. 323	Hexachlorophene	Nickel
Sewage, municipal, 345	Activated sludge, 354	Activated sludge, 178, 437
Cyanuric acid and derivatives	Iron	546
Microbial population, raw sewage	Activated sludge, 178, 344	Activated sludge, industrial,
26	Activated sludge, acclimated,	continuous-flow, 167.
Microbial population, sewage,	continuous-flow, 339	Activated sludge, industrial, porous
municipal, 199 Cycloaliphatics, substituted	Sewage, municipal, 345	pot, continuous-flow, 167
Achromobacter sp, 38	Ketones, aliphatic	Activated sludge, municipal,
Activated sludge, 38	Action to divide 38 to	continuous-flow, 167 Activated sludge, municipal, porous
Enterobacter sp. 38	Activated sludge, 38, 49	pot, continuous-flow, 167
Flavobacterium sp., 38	Enterobacter sp. 38 Flavobacterium sp. 38	Activated sludge, non-acclimated
Gram-positive bacteria, 38	Gram-positive bacteria, 38	343
Pseudomonas sp. 38	Pseudomonas sp. 38	Lumbricillus sp., 167
Vibrio sp. 38	Vibrio sp. 38	Sewage, municipal, 345
DDT, Methoxychlor and metabolites	Lead	Sphaerotilus sp. 437
Microbial population, raw sewage	Activated sludge, 437	Zooglea sp., 437
26	Escherichia sp., 43	Nitriles, long chain
Microbial population, septic tank	Microbial population, sewage,	Microbial population, municipal
6	municipal, 199	wastes, 311
Microbial population, sewage,	Sphaerotilus sp., 437	Nitrobenzene and derivatives
municipal, 199	Vorticella sp. 445	Activated sludge, 534
Saccharomyces sp. 269	Zooglea sp, 437	Activated sludge, continuous-flow
Dobane JNQ sulfonate	Leather, artificial, processing wastes	532
Activated sludge, 344 Domestic sewage effluents	Activated sludge, acclimated	Activated sludge, municipal, 369
Activated sludge, 336	277	Activated sludge, municipal,
Dyes	Enterobacter sp. 277	continuous-flow, 161
Activated sludge, 370, 371	Flavobacterium sp., 277 Pseudomonas sp., 277	<i>Nitrosomas</i> sp. 587 Sewage, municipal, 183
534, 581		Oil refinery wastes
Activated sludge, municipal, 369	Vibrio sp. 277 Lindane and metabolites	Activated sludge, 150
Activated sludge, municipal,	Activated sludge, continuous-flow	Pesticides
continuous-flow, 241	532	Activated sludge, acclimated
Nitrifying bacteria, continuous-	Lysol	226
culture, 241	Trickling filters, 306	Phenol and derivatives
Dyes, acid	Magnesium	Activated sludge, 144, 178

Inhibitory (toxic) effects (cont'd) 231, 309, 354, 429, 480	Inhibitory (toxic) effects (cont'd) Polyvinyl alcohol	Inhibitory (toxic) effects (cont'd) Review, 440
Activated sludge, acclimated,	Activated sludge, non-acclimated	Surfactants, anionic
continuous-flow, 122, 364	454	Review, 321
Arthrobacter sp. 34	Pulp and paper wastes	Surfactants, nonionic
Microbial population, sewage,	Activated sludge, 128, 453	
municipal, 61	Pyridine and derivatives	Review, 321 Tannery wastes
	Activated sludge, 480	
Pseudomonas sp. 309		Activated sludge, 131
Phenol pitch	Microbial population, raw sewage	Pseudomonas sp. 131
Activated sludge, 49	26	Textile wastes
Phenylacetic acid and derivatives Arthrobacter sp, 34	Microbial population, septic tank 6	Activated sludge, 144, 290 453
Phosphonic acid derivatives, alkyl poly-	Microbial population, sewage,	Activated sludge, non-acclimated
Activated sludge, 219	municipal, 199	454
Phosphorothioic acid and derivatives	Nitrosomas sp. 587	Thiocyanic acid and salts
Microbial population, septic tank	Pyrocatechol and derivatives	Activated sludge, 66, 231, 480
6	Activated sludge, 66	Activated sludge, acclimated,
Photoprocess wastes	Arthrobacter sp, 84	continuous-flow, 364
Activated sludge, acclimated	Quaternary ammonium compounds	Thiosuifate
21	Activated sludge, 304	Thiocyanic acid and salts, 256
Activated sludge, non-acclimated	Aspergillus sp. 314	Tin
21	Microbial population, fresh water	Sewage, municipal, 345
Activated sludge, sewage plant	304	Tin compounds, organic
506	Microbial population, river water	Activated sludge, 483, 589
Polyacrylonitrile	+27	Activated sludge, municipal, 478
Activated sludge, 28	Pseudomonad-like sp, 314	TNT
Polycaprolactone	Trickling filters, 306	Activated sludge, municipal,
Microbial population, enrichment	Yeast sp, 314	continuous-flow, 360
cultures. 320	Resorcinol and derivatives	Toilet paper, dyed
Polychlorinated biphenyls	Activated sludge, 178	Cellulomonas sp. 537
Activated sludge, 144	Salicylic acid and derivatives	Myrothecium sp. 537
Activated sludge + synthetic sewage,	Activated sludge, acclimated	Triclosan
247	390	Activated sludge, 367
Polychlorobenzenes and derivatives	Activated sludge, municipal, 369	Pseudomonas sp., 367
Activated sludge, 53, 128, 144	Salinity	2.3,5-Triphenyltetrazolium chloride
354	Activated sludge, acclimated,	Activated sludge, 53
Activated sludge, acclimated,	continuous-flow, 517	Pseudomonas sp. 53
continuous-flow, 122	Activated sludge, fresh water	Urea and derivatives
Activated sludge, municipal, 478	203	Activated sludge, 150
	Activated sludge, salt water	Vanadium
Microbial population, raw sewage	203°	
26		Activated sludge, 546
Microbial population, sewage,	Review, 517	Xylenes and derivatives
municipal, 199	Settlement tank effluents	Activated sludge, industrial and
Pseudomonas sp. 53	Activated sludge, 336	municipal, 13
Polyethylene glycols, alkylphenoxy-	Silicon, inorganic	Zinc
Review, 321, 451, 452	Activated sludge, 588	Activated sludge, 178, 344
Polyethylene glycols, fatty amine	Silver	429, 437, 546
Microbial population, municipal	Review, 22	Activated sludge, acclimated
wastes, 311	Sewage, municipal, 345	544
Polyethylene glycols, fatty ester	Sodium	Activated sludge, industrial,
Activated sludge, 430	Activated sludge, 546	continuous-flow, 167
Activated sludge, acclimated 432	Activated sludge, acclimated, continuous-flow, 517	Activated sludge, industrial, porous- pot, continuous-flow, 167
Activated sludge, non-acclimated	Starch and derivatives	Activated sludge, municipal, 361
432	Activated sludge, non-acclimated	Activated sludge, municipal,
Ciliata sp. 432	454	continuous-flow, 167
Mastigota sp, 432	Sugars and derivatives	Activated sludge, non-acclimated
Sarcodina sp., 432	Activated sludge, 66	343
Polyethylene glycols, fatty ether	Haliscomenobacter sp., 409	Lumbricillus sp., 167
Activated sludge, 430	Sphaerotilus sp., 409	Sewage, municipal, 345
Activated sludge, acclimated	Thiotrix sp. 409	Sphaerotilus sp. 437
432	Sulfate	Stabilization pond, 544
Activated sludge, non-acclimated	Activated sludge, 588	Vorticella sp. 445
432	Sulfide	Zooglea sp. 437
Ciliata sp, 432	Activated sludge, 131, 231	
Mastigota sp. 432	344	Inhibitory (toxic) effects, additive
Review, 321, 451, 452	Pseudomonas sp, 131	Chloramine and derivatives
Sarcodina sp. 432	Surfactants	Activated sludge, 178

Inhibitory (toxic) effects, chloramphenicol	Inhibitory (toxic) wastes	Ketones, aliphatic (cont'd)
inhibition	Photoprocess wastes	Aeropic biodegradation, 19
Benzoic acid and derivatives Bacillus sp. aerobic, 2	Review, 541	Metabolic pathways, 19 Enterobacter sp
Bacillus sp., anaerobic, 2	Iodate	Inhibitory (toxic) effects, 38
Phthalic acid and derivatives	Activated sludge	Flavobacterium sp
Bacıllus sp. aerobic, 2	Time-course kinetics, 272	Inhibitory (toxic) effects, 38
Bacıllus sp., anaerobic, 2	Iron	Gram-positive bacteria
Inhibitory (toxic) effects, cyanide inhibition	Activated sludge	Inhibitory (toxic) effects, 38
Ammonia and salts	Anaerobic digestion reactor, 344 Inhibitory (toxic) effects, 178	Lagoons, aerated, industrial site
Activated sludge, 243	344	Aerobic biodegradation, 573
Inhibitory (toxic) effects, hypersalinety	Activated sludge, acclimated,	Detoxification, 573
Phytane	continuous-flow	Microbial population, acclimated Aerobic biodegradation, 19
Microbial population, soils, 557	Inhibitory (toxic) effects, 339	Metabolic pathways, 19
Inhibitory (toxic) effects of nutrients	Sewage, municipal	Microbial population, isopropanol-
Benzenesulfonic acid, linear alkyl, long	Inhibitory (toxic) effects, 345	acclimated
chain	Isophthalic acid and derivatives	Metabolic pathways, 569
Activated sludge, 439	Activated sludge	Microbial population, loam
Inhibitory (toxic) effects, pH effect	Aerobic digestion reactors compared	Structure-activity relationships
Aniline and derivatives	287	. 485
Activated sludge, 225	Metabolic pathways	Microbial population, raw sewage
Inhibitory (toxic) effects, phenol inhibition	Review, 259	Aerobic biodegradation, 26
Ammonia and salts	Pseudomonas sp	Microbial population, sewage, municipa
Activated sludge, 243	Metabolic pathways, 8	Biorefractory index. 199
Inhibitory (toxic) effects, proteolytic	Kanechlors	Recommendations, wastewater treat- ment, 199
Aniline and derivatives	see Polychlorinated biphenyls Activated sludge	Micrococcus sp. 294
Activated sludge, 225	Activated studge Aerobic biodegradation, 338	Pseudomonas sp. 294
Nitrobenzene and derivatives		Aerobic biodegradation, 19
Activated sludge, 225	Kerosene Microbial population, fresh water,	Inhibitory (toxic) effects, 38
Inhibitory (toxic) effects, screening	kerosene-cultured	Metabolic pathways, 19, 297
Dyes, acid	Metabolic pathways, co-metabolism	Structure-activity relationships
Activated sludge, municipal, 547 Selenastrum sp, 547	. 169	473
Dyes, basic	Ketones	Sarcina sp. 294
		Sewage, acclimated, municipal
Activated sludge, municipal, 547	see Acetophenone and derivatives	7
Activated sludge, municipal, 547 Selenastrum sp, 547	see Acetophenone and derivatives	Petrochemical wastewater treatment
- ·	Ketones, aliphatic	Petrochemical wastewater treatment 51
Selenastrum sp. 547	Ketones, aliphatic see also Terpene compounds	Petrochemical wastewater treatment 51 Trichosporon sp
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547	Ketones, aliphatic see also Terpene compounds Achromobacter sp	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19
Selenastrum sp., 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp., 547 Dyes, disperse	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant Activated sludge, municipal, 547	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp. 547	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, sulfur	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp. 547	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, sulfur Activated sludge, municipal, 547	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp. 547	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp. 547 Selenastrum sp. 547	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp. 547 Lignin sulfonates	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated Aerobic digestion reactor, 381	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501 Lagoons, aerated, industrial site
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp. 547 Lignin sulfonates Activated sludge, municipal, 547	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated Aerobic digestion reactor, 381 Oxidation ditch, 381	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501 Lagoons, aerated, industrial site 349
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp. 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp. 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp. 547	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated Aerobic digestion reactor, 381	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501 Lagoons, aerated, industrial site
Selenastrum sp, 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp, 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp, 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp, 547 Naphthalene and derivatives	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated Aerobic digestion reactor, 381 Oxidation ditch, 381 Activated sludge, industrial, continuous-	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501 Lagoons, aerated, industrial site 349 Structure-activity relationships
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp. 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp. 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp. 547 Naphthalene and derivatives Activated sludge, municipal, 547	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated Aerobic digestion reactor, 381 Oxidation ditch, 381 Activated sludge, industrial, continuous- flow Metabolic pathways, 569 Activated sludge, municipal	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501 Lagoons, aerated, industrial site 349 Structure-activity relationships 289 Activated sludge, acclimated, industrial
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp. 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp. 547 Naphthalene and derivatives Activated sludge, municipal, 547 Selenastrum sp. 547 Naphthalene and derivatives Activated sludge, municipal, 547 Selenastrum sp. 547	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated Aerobic digestion reactor, 381 Oxidation ditch, 381 Activated sludge, industrial, continuous- flow Metabolic pathways, 569 Activated sludge, municipal Correlative test evaluations	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501 Lagoons, aerated, industrial site 349 Structure-activity relationships 289 Activated sludge, acclimated, industrial Identification of microorganisms 502
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp. 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp. 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp. 547 Naphthalene and derivatives Activated sludge, municipal, 547	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated Aerobic digestion reactor, 381 Oxidation ditch, 381 Activated sludge, industrial, continuous- flow Metabolic pathways, 569 Activated sludge, municipal Correlative test evaluations 151	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501 Lagoons, aerated, industrial site 349 Structure-activity relationships 289 Activated sludge, acclimated, industrial Identification of microorganisms 502 Lagoons, aerated, industrial site
Selenastrum sp. 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp. 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp. 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp. 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp. 547 Naphthalene and derivatives Activated sludge, municipal, 547 Selenastrum sp. 547 Inhibitory (toxic) effects, thiocyanate inhibition	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated Aerobic digestion reactor, 381 Oxidation ditch, 381 Activated sludge, industrial, continuous- flow Metabolic pathways, 569 Activated sludge, municipal Correlative test evaluations 151 Arthrobacter sp	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501 Lagoons, aerated, industrial site 349 Structure-activity relationships 289 Activated sludge, acclimated, industrial Identification of microorganisms 502 Lagoons, aerated, industrial site Aerobic biodegradation, 215
Selenastrum sp, 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp, 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp, 547 Naphthalene and derivatives Activated sludge, municipal, 547 Selenastrum sp, 547 Inhibitory (toxic) effects, thiocyanate inhibi-	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated Aerobic digestion reactor, 381 Oxidation ditch, 381 Activated sludge, industrial, continuous- flow Metabolic pathways, 569 Activated sludge, municipal Correlative test evaluations 151 Arthrobacter sp Aerobic biodegradation, 19	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501 Lagoons, aerated, industrial site 349 Structure-activity relationships 289 Activated sludge, acclimated, industrial Identification of microorganisms 502 Lagoons, aerated, industrial site Aerobic biodegradation, 215 573
Selenastrum sp, 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp, 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp, 547 Naphthalene and derivatives Activated sludge, municipal, 547 Selenastrum sp, 547 Inhibitory (toxic) effects, thiocyanate inhibition Ammonia and salts Activated sludge, 243	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated Aerobic digestion reactor, 381 Oxidation ditch, 381 Activated sludge, industrial, continuous- flow Metabolic pathways, 569 Activated sludge, municipal Correlative test evaluations 151 Arthrobacter sp Aerobic biodegradation, 19 Metabolic pathways, 19	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501 Lagoons, aerated, industrial site 349 Structure-activity relationships 289 Activated sludge, acclimated, industrial Identification of microorganisms 502 Lagoons, aerated, industrial site Aerobic biodegradation, 215 573 Detoxification, 215, 573
Selenastrum sp, 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp, 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp, 547 Naphthalene and derivatives Activated sludge, municipal, 547 Selenastrum sp, 547 Inhibitory (toxic) effects, thiocyanate inhibition Ammonia and salts Activated sludge, 243 Inhibitory (toxic) effects with preservatives	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated Aerobic digestion reactor, 381 Oxidation ditch, 381 Activated sludge, industrial, continuous- flow Metabolic pathways, 569 Activated sludge, municipal Correlative test evaluations 151 Arthrobacter sp Aerobic biodegradation, 19 Metabolic pathways, 19 Bacillus sp	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501 Lagoons, aerated, industrial site 349 Structure-activity relationships 289 Activated sludge, acclimated, industrial Identification of microorganisms 502 Lagoons, aerated, industrial site Aerobic biodegradation, 215 573 Detoxification, 215, 573 Lagoon pre-treatment
Selenastrum sp, 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp, 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp, 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp, 547 Naphthalene and derivatives Activated sludge, municipal, 547 Selenastrum sp, 547 Inhibitory (toxic) effects, thiocyanate inhibition Ammonia and salts Activated sludge, 243 Inhibitory (toxic) effects with preservatives Cutting fluds (coolants), synthetic and semi-synthetic	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated Aerobic digestion reactor, 381 Oxidation ditch, 381 Activated sludge, industrial, continuous- flow Metabolic pathways, 569 Activated sludge, municipal Correlative test evaluations 151 Arthrobacter sp Aerobic biodegradation, 19 Metabolic pathways, 19	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501 Lagoons, aerated, industrial site 349 Structure-activity relationships 289 Activated sludge, acclimated, industrial Identification of microorganisms 502 Lagoons, aerated, industrial site Aerobic biodegradation, 215 573 Detoxification, 215, 573 Lagoon pre-treatment Calcium
Selenastrum sp, 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp, 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp, 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp, 547 Naphthalene and derivatives Activated sludge, municipal, 547 Selenastrum sp, 547 Inhibitory (toxic) effects, thiocyanate inhibition Ammonia and salts Activated sludge, 243 Inhibitory (toxic) effects with preservatives Cutting fluids (coolants), synthetic and semi-synthetic Activated sludge, 1	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated Aerobic digestion reactor, 381 Oxidation ditch, 381 Activated sludge, industrial, continuous- flow Metabolic pathways, 569 Activated sludge, municipal Correlative test evaluations 151 Arthrobacter sp Aerobic biodegradation, 19 Metabolic pathways, 19 Bacillus sp Structure-activity relationships	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Wibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501 Lagoons, aerated, industrial site 349 Structure-activity relationships 289 Activated sludge, acclimated, industrial identification of microorganisms 502 Lagoons, aerated, industrial site Aerobic biodegradation, 215 573 Detoxification, 215, 573 Lagoon pre-treatment Calcium Anaerobic biodegradation, 379
Selenastrum sp, 547 Dyes, direct Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, disperse Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, mordant Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, sulfur Activated sludge, municipal, 547 Selenastrum sp, 547 Dyes, vat Activated sludge, municipal, 547 Selenastrum sp, 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp, 547 Lignin sulfonates Activated sludge, municipal, 547 Selenastrum sp, 547 Naphthalene and derivatives Activated sludge, municipal, 547 Selenastrum sp, 547 Inhibitory (toxic) effects, thiocyanate inhibition Ammonia and salts Activated sludge, 243 Inhibitory (toxic) effects with preservatives Cutting fluds (coolants), synthetic and semi-synthetic	Ketones, aliphatic see also Terpene compounds Achromobacter sp Inhibitory (toxic) effects, 38 Metabolic pathways, 41 Activated sludge, 253, 341 Aerobic biodegradation, 386 Identification of microorganisms 38 Inhibitory (toxic) effects, 38 49 Metabolic pathways, 39 Structure-activity relationships 386, 473 Activated sludge, acclimated Aerobic digestion reactor, 381 Oxidation ditch, 381 Activated sludge, industrial, continuous- flow Metabolic pathways, 569 Activated sludge, municipal Correlative test evaluations 151 Arthrobacter sp Aerobic biodegradation, 19 Metabolic pathways, 19 Bacillus sp Structure-activity relationships 473	Petrochemical wastewater treatment 51 Trichosporon sp Aerobic biodegradation, 19 Metabolic pathways, 19 Vibrio sp Inhibitory (toxic) effects, 38 Kraft pulp wastes see also Pulp and paper wastes Activated sludge Aerobic biodegradation, 289 Aerobic digestion reactors compared, 236 Detoxification, 236, 349 Glucose removal and polysaccharide accumulation, 501 Lagoons, aerated, industrial site 349 Structure-activity relationships 289 Activated sludge, acclimated, industrial Identification of microorganisms 502 Lagoons, aerated, industrial site Aerobic biodegradation, 215 573 Detoxification, 215, 573 Lagoon pre-treatment Calcium

.agoon pre-treatment (cont'd)	Lagoons, aerated, industrial site (cont'd)	Leather, artificial, processing wastes
Magnesium	Detoxification, 215, 573	(cont'd)
Anaerobic biodegradation, 379	Pyrocatechol and derivatives	Pseudomonas sp
Manganese	Aerobic biodegradation, 215	Inhibitory (toxic) effects. 277
Anaeropic biodegradation, 379	Detoxification, 215	Vibrio sp
Potassium	Sugars and derivatives	Inhibitory (toxic) effects, 277
Anaerobic biodegradation, 379	Aerobic biodegradation, 215	Lebistes sp
Sodium	Detoxification, 215	Explosives, organic
Anaerobic biodegradation, 379	Terpene compounds	Inhibitory (toxic) effects, 7
Zinc	Aerobic biodegradation, 215	Lignin-related compounds
Anaerobic biodegradation, 379	573	Activated sludge
Lagoons, aerated	Detoxification, 215, 573	Anaerobic digestion reactor, 196
Pulp and paper wastes	Xylenols and derivatives	Pseudomonas sp
Review, 556	Activated sludge, 349	Metabolic pathways, 137
	Aerobic biodegradation, 215	Pseudomonas sp
Lagoons, aerated, industrial site	Detoxification, 215	Metabolic pathways, 539
Abietic acid and derivatives	Lagoons, anaerobic, saline	Trametes sp
Activated sludge, 349	Phosphorodithioic acid and derivatives	Metabolic pathways, 137
Aerobic biodegradation, 215	Anaerobic biodegradation, 465	Lignin sulfonates
Detoxification, 215	Hydrogen sulfide production, 465	•
Alcohols, alicyclic	Isolation of microorganisms, 465	Activated sludge, municipal
Aerobic biodegradation, 573	-	Aerobic and anaerobic digestion
Detoxification, 573	Lagoons, waste-tip	reactors, 547
Aldehydes	Coke oven wastes	Inhibitory (toxic) effects, screening
Aerobic biodegradation, 215	- Microbial population, 479 LAS	547
Detoxification, 215	see Benzenesulfonic acid, linear alkyl,	Arthrobacter sp
Alkanoic acids and derivatives	long chain	Aerobic biodegradation, 19
Aerobic biodegradation, 215	•	Metabolic pathways, 19
Detoxification, 215	Lastanox F	Chromobacterium sp
Alkanoic acids and derivatives, long	see Tin compounds, organic	Aerobic biodegradation, 19
chain	Latex	Metabolic pathways, 19
Aerobic biodegradation, 215	Microbial population, soils	Microbial population, acclimated
Detoxification, 215	Operational parameters, 171	Aerobic biodegradation, 19
Alkenes	Lauropal	Metabolic pathways, 19
Aerobic biodegradation, 215	Activated sludge, non-acclimated,	Pseudomonas sp
Detoxification, 215	municipal	Aerobic biodegradation, 19
Alkenoic acids and derivatives, long	Aerobic biodegradation, 18	Metabolic pathways, 19
chain	Trickling filters, 18	Selenastrum sp
Aerobic biodegradation, 215	Lead	Inhibitory (toxic) effects, screening
Detoxification, 215		547
Alkyl halides	Activated sludge Inhibitory (toxic) effects, 437	Trichosporon sp
Aerobic biodegradation, 215		Aerobic biodegradation, 19
573	Activated sludge, municipal, continuous- flow	Metabolic pathways, 19
Detoxification, 215, 573		Lindane and metabolites
Alkyl sulfides	Freundlich adsorption isotherms 362	see also Pesticides
Aerobic biodegradation, 215	Kinetics and equilibrium studies	Activated sludge
573	362	Aerobic biodegradation, 346, 597
Detoxification, 215, 573	Michaelis-Menten coefficients	Sorption, 597
Benzene and derivatives	362	Activated sludge, continuous-flow
Aerobic biodegradation, 215	Operational parameters, 362	Inhibitory (toxic) effects, 532
573	Escherichia sp	Bacillus sp
Detoxification, 215, 573	Inhibitory (toxic) effects, 43	Anaerobic biodegradation, 536
Ketones, aliphatic	Microbial population, sewage, municipal	Candida sp
Aerobic biodegradation, 573		Anaerobic biodegradation, 536
Detoxification, 573	Inhibitory (toxic) effects, 199 Sphaerotilus sp	Citrobacter sp
Kraft pulp wastes	Inhibitory (toxic) effects, 437	Anaerobic biodegradation, 536
Activated sludge, 349	Vorticella sp	Escherichia sp
Aerobic biodegradation, 215	Inhibitory (toxic) effects, 445	Anaerobic biodegradation, 536
573	Zooglea sp	Hydrogenomonas sp
Detoxification, 215, 573	Inhibitory (toxic) effects, 437	Anaerobic biodegradation, 536
Pimaric acid and derivatives	impitory (toxic) effects, 457	Mycoplana sp
Activated sludge, 349	Leather, artificial, processing wastes	Anaerobic biodegradation, 536
Aerobic biodegradation, 215	Activated sludge, acclimated	Pseudomonas sp
Detoxification, 215	Inhibitory (toxic) effects, 277	Anaerobic biodegradation, 536
Pulp and paper wastes	Enterobacter sp	Rhizobidia sp
Activated sludge, 349	Inhibitory (toxic) effects, 277	Aerobic biodegradation, 246
Aerobic biodegradation, 215	Flavobacterium sp	Lumbricillus sp
573	Inhibitory (toxic) effects, 277	Carbamic acid and derivatives

Lindane and metabolites (cont'd)	Mercury, inorganic (cont'd)	Metabolic pathways
Inhibitory (toxic) effects, 167	Sludge deflocculation, 361	Acetophenone and derivatives
Copper Inhibitory (toxic) effects, 167	Activated sludge, municipal, continuous- flow	Arthrobacter sp. 84
Cutting oils	Freundlich adsorption isotherms	Acinetopacter sp
Inhibitory (toxic) effects, 167	362	Vibrio sp. 550 Adipic acid and derivatives
Nickel	Kinetics and equilibrium studies	Achromobacter sp. 41
Inhibitory (toxic) effects, 167	362	Pseudomonas sp. 298
Zinc	Michaelis-Menten coefficients	Alcohols, alicyclic
Inhibitory (toxic) effects, 167	362	Achromobacter sp. 41
Lysol	Operational parameters, 362	Activated sludge, 39
Trickling filters	Activated sludge, non-acclimated Inhibitory (toxic) effects, 343	Alcohols, primary alipnatic
Inhibitory (toxic) effects, 306	Volatilization, 356	Achromobacter sp. 303
Magnesium	Activated sludge + synthetic sewage	Activated aluder 303 417
Lagoon pre-treatment	Adsorption and volatilization	Activated sludge, 303, 417 471
Anaerobic biodegradation, 379 Pseudomonas sp	357	Activated sludge, industrial,
Inhibitory (toxic) effects, 572	Operational parameters, 357	continuous-flow, 569
	Escherichia sp	Microbial population, acclimated
Manganese Lagoon pre-treatment	Inhibitory (toxic) effects, 43	318
Anaerobic biodegradation, 379	Microbial population, mercury-resistant,	Microbial population, isopropanol
Marlipol	498	acclimated, 569
Activated sludge, non-acclimated,	Pseudomonas sp. 498	Mycobacterium sp, 303
municipal	Sorption, 210, 211 Saccharomyces sp	Pseudomonas sp, 59, 182
Aerobic biodegradation, 18	Aerobic coprecipitation, 269	297, 303
Trickling filters, 18	Anaerobic coprecipitation, 269	Pseudomonas sp pure culture 471
Mastigota sp	Batch vs continuous-flow system	Pseudomonas sp. 539
Cirrasols	269	Alcohols, secondary aliphane
Inhibitory (toxic) effects, 432	Inhibitory (toxic) effects, 269	Activated sludge, industrial,
Polyethylene glycols, fatty ester	Sewage, municipal	continuous-flow, 569
Inhibitory (toxic) effects, 432	Inhibitory (toxic) effects, 345	Microbial population, isopropanol-
Polyethylene glycols, fatty ether	Spnaerotilus sp	acclimated, 569
Inhibitory (toxic) effects, 432	Inhibitory (toxic) effects, 437 Vorticella sp	Pseudomonas sp. 297
Mercaptans	Inhibitory (toxic) effects, 445	Aldehydes
Activated sludge, acclimated, continuous-flow	Zooglea sp	Alcaligenes sp. 37
Aerobic biodegradation, 112	Inhibitory (toxic) effects, 437	Microbial population, acclimated 318
Activated sludge, acclimated, sedimenta-	•	Nocardia sp., 179
tion chamber		Pseudomonas sp. 539
Aeropic biodegradation, 112	Activated sludge Aerobic biodegradation, 128	Alkanes
Mercury	Inhibitory (toxic) effects, 128	Achromobacter sp. 67
Microbial population, sewage, municipal	Biodegradation, environmental aspects	Acinetobacter sp. 232
Inhibitory (toxic) effects, 199	Review, 239	Flavobacterium sp. 232
Mercury, inorganic	Managh His same and a SE-st	Microbial population, 232
Achromobacter sp. 498	Mesophilic temperature, effect Alkanes, long chain, branched	Micrococcus sp. 232 Nocardia sp. 232, 444
Activated sludge	Achromobacter sp. 567	Pseudomonas sp. 123, 232, 299
Adsorption and volatilization	Acinetobacter sp. 567	Alkanes, cyclic
357	Arthrobacter sp. 567	Acinetobacter sp. 232, 522
Inhibitory (toxic) effects, 429 437, 546	Cytophaga sp. 567	Flavobacterium sp. 232, 335
Michaelis-Menten coefficients	Flavobacterium sp. 567	Microbial population, 232
429	Gram-negative rods, 567	Micrococcus sp. 232
Operational parameters, 357	Gram-positive cocci, 567	Nocardia sp. 232, 444
Activated sludge, acclimated, municipal	Pseudomonas sp. 567	Pseudomonas sp. 232, 335
Aerobic biodegradation, 363	Alcaligenes sp. 567 Xanthomonas sp. 567	Alkanes, long chain, branched Acinetobacter sp. 522
Biomass yield, effect on, 363	Crude oil	Pseudomonas sp., 123
Freundlich adsorption isotherms 363	Achromobacter sp. 567	Alkanes, long chain, linear
Michaelis-Menten coefficients	Acinetobacter sp. 567	Acinetobacter sp., 86, 232
363	Arthrobacter sp. 567	522
Operational parameters, 363	Cytophaga sp. 567	Flavobacterium sp., 232
Activated sludge, acclimated, semi-	Flavobacterium sp. 567	Microbial population, 232
continuous flow	Gram-negative rods, 567 Gram-positive cocci, 567	Micrococcus sp. 232
Volatilization, 356	Pseudomonas sp. 567	Mycobacterium sp. 25 Nocardia sp. 25, 232, 444
Activated sludge, municipal	Alcaligenes sp, 567	Pseudomonas sp. 123, 232
Inhibitory (toxic) effects, 361	Xanthomonas sp. 567	298, 299

Metabolic pathways (cont'd)	Metabolic pathways (cont'd)	Metabolic pathways (cont'd)
Alkanoic acids and derivatives	Amino acids and derivatives	municipal, 98
Achromobacter sp. 41. 67	Acinetobacter sp. 522, 542	Microbial population, municipal
Acinetobacter sp. 244	Escherichia sp. 273	wastes, 213
Arthrobacter sp. 84	Microbial population, 514	Microbial population, soils, 14
Microbial population, acclimated	Microbial population, non-	Micrococcus sp., 107
318	acclimated, soils, 511	Nocardia sp. 179, 444
Microbial population, soils, 14	Microbial population, NTA-	Pseudomonas sp. 103, 184
Mycobacterium sp. 25	acclimated, soils, 511	Pseudomonas sp acclimated
Nocardia sp. 25, 179, 180	Nocardia sp. 179	276
144	Pseudomonas sp. 273, 542	Sewage, natural, semi-continuous
Pseudomonas sp. 288, 297	Pseudomonas sp TOL-plasmid-	flow, 184
298	bearing, 279	Pseudomonas sp. 539
Pseudomonas sp. 539	Review, 514	Benzonitrile and derivatives
Alkanoic acids and derivatives, long	Staphylococcus sp. 273	Fusarium sp. 188
chain	Trichosporon sp. 542	Benzothiazole and derivatives
Acinetohacter sp. 86. 522	Aniline and derivatives	Cunninghamella sp. 555
Escherichia sp. 273	Activated sludge, acclimated	BHT
Pseudomonas sp. 273, 298	584	Activated sludge + synthetic sewage.
Staphylococcus sp. 273	Bacillus sp. 111	228
Alkanoic acids and derivatives,	Microbial population, fresh water +	Biphenyl and derivatives
polybasic	sewage, 111	Acinetobacter sp. 354
Achromobacter sp. 41, 67	Pseudomonas sp acclimated	Activated sludge, municipal, 523
Acinetobacter sp. 244	276	Cunninghamella sp. 528
	Aromatic compounds, dicyclic	Flavobacterium sp., 335
Moraxella sp. 192 Nocardia sp. 444	Flavobacterium sp., 335	Nocardia sp. 354
* '	Pseudomonas sp. 335	Pseudomonas sp., 335, 354
Penicillium sp. 192	Azo compounds	Carbamic acid and derivatives
Pseudomonas sp. 539	Pseudomonas sp acclimated	Pseudomonas sp. 177
Alkanoic acids, cyclic	276	Review, 325
Achromobacter sp. 41	Azo dyes	Carbowax
Mycobacterium sp. 25	Pseudomonas sp accismated	Microbial population, glycol-
Nocardia sp., 25	276	metabolizing, 30
Alkenes	Benzene and derivatives	Cellulose and derivatives
Acinetobacter sp. 232, 522	Achromobacter sp., 67	Microbial population, 27
Flavobacterium sp. 232	Acinetobacter sp., 232	Review, 33
Microbial population, 232	Alcaligenes sp. 37	Chloroalkylenes
Micrococcus sp. 232	Flavobacterium sp., 232, 335	Activated sludge, municipal, 528
Nocardia sp. 232	Microbial population, 232	Cunninghamella sp. 528
Pseudomonas sp, 59, 123', 232	Micrococcus sp. 232	Cinnamic acid and derivatives
Alkenoic acids and derivatives	Nocardia sp., 232, 444	Nocardia sp. 179, 144
Achromobacter sp. 41	Pseudomonas sp. 232, 335	Pseudomonas sp. 137
Alcaligenes sp. 37	Review, 88	Trametes sp. 137
Microbial population, municipal	Benzenesulfinic acid and derivatives	Coke oven wastes
wastes, 213	Alcaligenes sp., 37	Microbial population, 479
Moraxella sp. 192, 468	Benzenesulfonic acid, alkyl, short chain	Coryneform bacteria
Nocardia sp. 180, 444	Alcaligenes sp. 37	Vibrio sp. 550
Peniculium sp., 192, 468	• • •	Cresols and derivatives
Pseudomonas sp. 8	Benzenesulfonic acid and non-alkyl substituted derivatives	Activated sludge, 143
Alkenoic acids and derivatives, long		Activated sludge + synthetic sewage
chain	Alcaligenes sp. 37	228
Acinetobacter sp. 522	Benzenesulfonic acid, linear alkyl, long	Alcaligenes sp. 37
Alkyl sulfates, long chain	chain <i>Alcaligenes</i> sp. 37	Microbial population, soils, 14
Microbial population, 533	• •	Review, 88
Alkynes	Microbial population, fresh water 109	Cyanide
Rhodopseudomonas sp. 323	Review, 492, 571	Rhodopseudomonas sp. 323
Amides, aliphatic, long chain	Benzenesulfonic acid, non-linear alkyl,	Cyanuric acid and derivatives
Escherichia sp. 273	long chain	Fungi, unidentified, acclimated
Pseudomonas sp. 273	Activated sludge + synthetic sewage,	599
Staphylococcus sp. 273	456	Microbial population, acclimated
Amines, alicyclic	Benzoic acid and derivatives	599
Activated sludge, 39	Achromobacter sp. 41, 67	Cycloaliphatics, substituted
Amines, long chain	Alcaligenes sp. 37	Achromobacter sp. 41
Escherichia sp. 273	Arthrobacter sp. 84	Activated sludge, 39, 471
Staphylococcus sp. 273	Bacillus sp. aerobic, 2	Mycobacterium sp. 25
Amines, poly-, aliphatic	Bacillus sp., aerobic, 2 Bacillus sp., anaerobic, 2	Nocardia sp. 25, 144
' Activated sludge, 471	Fusarium sp. 188	Pseudomonas sp pure culture
Pseudomonas sp pure culture	Microbial population, acclimated,	471
471	viicrooiai population, accimated,	7/4

Metabolic pathways (cont'd)	Metabolic pathways (cont'd)	Metabolic pathways (cont'd)
DDT. Methoxychlor and metabolites	Aspergillus sp. 216	continuous-flow, 569
Activated sludge, acclimated, 584	Bacillus sp. 111	Arthrobacter sp. 19
Bacillus sp. 536	Fusarium sp. 134	Chromobacterium sp. 19
Candida sp. 536	Microbial population, fresh water +	Microbial population, acclimated
Citrobacter sp. 536	Sewage, 111	19
Escherichia sp. 536	Microbial population, pesticide- metabolizing, 132	Microbial population, isopropanol-
Hydrogenomonas sp. 536 Mycoplana sp. 536	Microbial population, soils, 132	acclimated, 569 Pseudomonas sp. 19, 297
Pseudomonas sp. 536	Microbial population, soils, organic-	Trichosporon sp. 19
Explosives, organic	enriched, 132	Lignin-related compounds
Activated sludge, 564	Penicillium sp, 216	Pseudomonas sp. 137
Activated sludge, municipal, 334	Herbicides, propanil type and	Pseudomonas sp. 539
Gram-negative rods, 564	metabolites	Trametes sp. 137
Microbial population, 565	Aspergillus sp. 216	Lignin sulfonates
Food industry wastes	Bacıllus sp. 111	Arthrobacter sp. 19
Activated sludge, 596	Fusarium sp. 257	Chromobacterium sp, 19
Fuel oil	Microbial population, fresh water +	Microbial population, acclimated
Acinetobacter sp. 553	sewage, 111	19
Bacıllus sp. 553	Penicillium sp. 216	Pseudomonas sp, 19
Coryneform bacteria, 553	Taloramyces sp, 257	Trichosporon sp, 19
Cryptococcus sp, 553	Herbicides, pyrazon type	Metals, toxic
Microbial population, fresh water	Microbial population, pesticide-	Review, 448
553	metabolizing, 132 - Microbial population, soils, 132	Methanol, phenol, isopropanol, acetone mixture
Pseudomonas sp. 299, 553 Furan and derivatives	Microbial population, soils, organic-	
Arthrobacter sp. 19	enriched, 132	Activated sludge, industrial, continuous-flow, 569
Chromobacterium sp. 19	Herbicides, silvex type	Micropial population, isopropanol-
Microbial population, acclimated	Pseudomonas sp. 214	accilmated, 569
19	Herbicides, urea	Naphthalene and derivatives
Pseudomonas sp. 19	Cunninghamella sp. 555	Activated sludge, acclimated
Trichosporon sp. 19	Fusarium sp. 257	584
Gasoline	Tatoramyces sp. 257	Flavobacterium sp. 335
Acinetobacter sp., 232	Heteroaromatics and derivatives, dicyclic	Microbial population, estuarine
Flavobacterium sp. 232	Achromobacter sp, 41	water, 407
Microbial population, 232	Fusarium sp. 373	Oscillatoria sp. 70
Micrococcus sp., 232	Microbial population, fecal isolates,	Pseudomonas sp, 177, 335
Nocardia sp. 232	575	Pseudomonas sp acclimated
Pseudomonas sp. 232	Pseudomonas sp. 539 Hexachiorophene	276 Parisas 226
Gums Migraphal population 27	Acinetobaeter sp. 354	Review, 325
Microbial population, 27 Herbicides, atrazine type	Nocardia sp. 354	Nitrobenzene and derivatives Moraxella sp. 477
Fungi, unidentified, acclimated	Pseudomonas sp. 354	NTA and saits
599	Hydrocarbons	Microbial population, non-
Microbial population, acclimated	Acinetobacter sp., 232	acclimated, soils, 511
599	Cladosporium sp acclimated	Microbial population, NTA-
Microbial population, pesticide-	476	acclimated, soils, 511
metabolizing, 132	Flavobacterium sp. 232	Microbial population, soils, 127
Microbial population, soils, 132	Microbial population, 232	Pseudomonas sp., 127
Microbial population, soils, organic-	Micrococcus sp., 232	Pseudomonas sp mutant, 300
enriched, 132	Nocardia sp. 232	Review, 558
Herbicides, carbamate	Pseudomonas sp. 232	Pesticides
Bacilius sp. 111 Microbial population, fresh water +	Hydroquinone and derivatives	Review, 260, 326
sewage, 111	Bacillus sp. aerobic, 2	Petroleum
Herbicides, chlorpropham type	Bacillus sp. anaerobic, 2 Nocardia sp. 180, 444	Acinetobacter sp. 553 Bacillus sp. 553
Bacillus sp. 474	Pseudomonas sp. 184	Coryneform bacteria, 553
Micrococcus sp. 474	Review, 88	Cryptococcus sp. 553
Herbicides, 2,4-D type	Sewage, natural, semi-continuous	Microbial population, fresh water
Microbial population, pesticide-	flow, 184	553
metabolizing, 132	Pseudomonas sp., 539	Pseudomonas sp., 553
Microbial population, soils, 132	Isophthalic acid and derivatives	Vibrio sp. 550
Microbial population, soils, organic-	Pseudomonas sp, 8	Phenol and derivatives
enriched, 132	Review, 259	Achromobacter sp, 67
Pseudomonas plasmids, 383	Ketones, aliphatic	Acinetobacter sp. 354
Pseudomonas sp. 214 Herbicides, monuron type and	Activated sludge 30	Activated sludge, 143
metabolites	Activated sludge, 39	Activated sludge, industrial,
metabonics	Activated sludge, industrial,	continuous-flow, 569

Metabolic pathways (cont'd)	Metabolic pathways (cont'd)	Metabolic pathways (cont'd)
Alcaligenes sp, 37	Odontia sp. 3	Microbial population, fresh water
Arthrobacter sp. 84	Peniophora sp. 3	109
Microbial population, isopropanol-	Polyethylene glycols	Surfactants
accimated, 569	Acinetobacter sp. 244	Review, 519
Microbial population, soils, 14 Nocardia sp, 354	Microbial population, 27 Microbial population, glycol-	Surfactants, anionic Review, 54, 321, 492
Phenol-degrading bacteria, 155	metabolizing, 80	Surfactants, nonionic
Pseudomonas sp. 354, 576	Pseudomonas sp. 182	Review, 54, 321, 492
<i>37</i> 9	Polyethylene glycois, aikylphenoxy-	Surfactants, tetrapropyiene
Review, 88	Review, 321, 451, 452	Review, 492
Trichosporon sp. 579	Polyethylene glycols, fatty ether	Terephthalic acid and derivatives
Phenylacetic acid and derivatives	Review, 321, 451, 452	Review, 259
Arthrobacter sp. 84 Microbial population, fecal isolates,	Polystyrenes Moraxella sp. 192, 468	Terpene compounds
575	Penicillium sp. 192, 468	Pseudomonas sp. 59 Tetralin and derivatives
Nocardia sp., 179, 444	Polyvinyl alcohol	Flavobacterium sp. 335
Pseudomonas sp. 137	Microbial population, 27	Oscillatoria sp. 70
Trametes sp, 137	Pseudomonas sp	Pseudomonas sp. 335
Phosphonic acid derivatives, alkyl	Vibrio sp. 550	Textile wastes
Pseudomonas sp. 65, 91	Pyrocatechol and derivatives	Microbial population, 27
Phthalic acid and derivatives	Achromobacter sp, 41, 67	Microbial population,
Arthrobacter sp. 117	Activated sludge, 143	liquid-enriched, 322
Bacillus sp. aerobic, 2 Bacillus sp. anaerobic, 2	Alcaligenes sp. 37 - Arthrobacter sp. 84, 117	Microbial population, soil-liquid
Brevibacterium sp. 117	Brevibacterium sp. 117	322 Microbial population, soils, 322
Corynebacterium sp. 117	Corynebacterium sp. 117	Thiophenois
Micrococcus sp. 107	Fusarium sp. 188	Acinetobacter sp. 542
Mycobacterium sp. 117	Microbial population, acclimated,	Pseudomonas sp. 542
Penicillium sp. 116, 117	municipal, 98	Trichosporon sp. 542
Pseudomonas sp. 8, 117	Microbial population, municipal	Toilet paper, dyed
Pseudomonas sp. revertant	wastes, 213	Cellulomonas sp. 537
359	Microbial population, soils, 14	Myrothecium sp. 537
Pseudomonas sp, wild type	Micrococcus sp, 107	Toluene and derivatives
359 Review, 259	Mycobacterium sp. 117	Acinetobacter sp. 232
Plycyclic aromatic hydrocarbons	Nocardia sp. 179, 444 Penicillium sp. 117	Alcaligenes sp. 37
Flavobacterium sp., 335	Pseudomonas sp. 117, 184	Flavobacterium sp. 232, 335 Microbial population, 232
Pseudomonas sp., 335	Sewage, natural, semi-continuous	Micrococcus sp, 232
Polyacrylic acid	flow, 184	Nocardia sp. 232, 444
Microbial population, 27	Quaternary ammonium compounds	Pseudomonas sp. 232, 335
Polybutadienes	Aspergillus sp. 314	Toluic acid and derivatives
Acinetobacter sp. 522	Pseudomonad-like sp, 314	Pseudomonas sp. 8
Polychlorinated biphenyls	Review, 314	Pseudomonas sp. 539
Activated sludge, municipal, 528	Yeast sp. 314	Urea and derivatives
Cunninghamella sp. 528 Polychlorobenzenes and derivatives	Resorcinol and derivatives Pseudomonas sp, 184	Bacillus sp. 111
Acinetobacter sp. 354	Sewage, natural, semi-continuous	Cunninghamella sp. 555 Microbial population, fresh water +
Microbial population, acclimated,	flow, 184	sewage, 111
municipal, 98	Salicylic acid and derivatives	Vanillic acid and derivatives
Microbial population,	Fusarium sp. 188	Moraxella sp., 192, 468
liquid-enriched, 322	Microbial population, acclimated,	Nocardia sp. 179
Microbial population, soil-liquid	municipal, 98	Penicillium sp, 192, 468
322	Nocardia sp. 180, 444	Pseudomonas sp. 539
Microbial population, soils, 322 Nocardia sp, 354	Review, 88 Shale oil wastes	Xylenes and derivatives Acinetobacter sp., 232
Pseudomonas sp. 354	Microbial population, 148	Flavobacterium sp. 232, 335
Polycyclic aromatic hydrocarbons	Silicones	Microbial population, 232
Beijerinckia sp., mutant, 154	Microbial population, soils, 198	Micrococcus sp. 232
Beijerinckia sp., wild type	Starch and derivatives	Nocardia sp. 232
154	Microbial population, 27	Pseudomonas sp. 232, 335
Cunninghamella sp. 69, 100	Stilbene and derivatives	Xylenols and derivatives
Neurospora sp acclimated	Pseudomonas sp. 137	Fusarium sp, 188, 373
249 Polyothylana	Trametes sp. 137 Sugars and derivatives	Nocardia sp. 444
Polyethylene Fomes sp. 3	Acinetobacter sp. 522	Pseudomonas sp, 137 Review, 325
Fusarium sp. 3	Activated sludge, 596	Pseudomonas sp. 539
Microbial population, soils, 3	Sulfophenylaikanoic acids	Trametes sp. 137

Methanol, phenol, isopropanol, acetone Microbial population (cont'd) Metabolic pathways, co-metabolism mixture (cont'd) Metabolic pathways, 569 Alkanes, cyclic Model ecosystem, aquatic, simulated, Microbial population, fresh water. Microbial population, isopropanolkerosene-cultured, 168, 169 Polyethylene glycols acclimated Alkanes, long chain, branched Metabolic pathways, 27 Metabolic pathways, 569 Microbial population, fresh water, Polyethylene glycols, fatty ether kerosene-cultured, 168, 169 Methyl mercaptan Model ecosystem, aquatic, natural Alkanes, long chain, linear Activated sludge 516 Microbial population, fresh water, Anaerobic digestion reactor, 602 Polyvinyl alcohol kerosene-cultured, 169 Microbial population, fresh water sedi-Metabolic pathways. 27 Alkenes ment Quaternary ammonium compounds, 11 Microbial population, fresh water, Anaerobic digestion reactor, 602 Shale oil wastes kerosene-cultured, 168, 169 Biogeochemical eveling, 602 Metabolic pathways, 148 Amino acids and derivatives Time-course kinetics, 602 Starch and derivatives Trichosporon sp. 542 Microbial population Metabolic pathways, 27 Benzene and derivatives Aldehydes Textile wastes Trickling filters, 166 Microbial population, fresh water. Metabolic pathways, 27 kerosene-cultured, 168, 169 Alkanes Toluene and derivatives Metabolic pathways, 232 EDTA and salts Metabolic pathways, 232 Microbial population, fresh water Alkanes, cyclic Xylenes and derivatives Metabolic pathways, 232 sediments, 510 Metabolic pathways, 232 Microbial population, soils, 510 Alkanes, long chain, linear Microbial population, acclimated Metabolic pathways, 232 Kerosene Alcohols, primary aliphatic Microbial population, fresh water, Alkanoic acids and derivatives, Metabolic pathways, 318 kerosene-cultured, 169 polybasic Aldehydes Thiophenols Screening tests, 415 Metabolic pathways, 318 Trichosporon sp. 542 Alkenes Alkanoic acids and derivatives Metals, toxic Metabolic pathways, 232 Metabolic pathways, 318 Activated sludge, municipal Alkenoic acids and derivatives, 110 Aerobic biodegradation, 375 Alkanoic acids, long chain, esters, 286 Alkyl suifates, long chain Benzenesulfonic acid, linear alkyl, long Environmental fate Metabolic pathways, 533 chain, non-terminal, 286 Review, 448 Screening tests, 415 Amines, aliphatic, 45 Benzothiazole and derivatives Metabolic pathways River die-away test, 317 Cyanuric acid and derivatives Review. 448 Amino acids and derivatives Model ecosystem, biotransformation Metabolic pathways, 514 Metabolic pathways, 599 Review, 448 Benzene and derivatives Methanobacterium sp Metabolic pathways, 232 Furan and derivatives Aerobic biodegradation, 19 Adipic acid and derivatives Benzenesulfonic acid, linear alkyl, long Anaerobic digestion reactor, 15 chain Metabolic pathways, 19 Screening tests, 415 Herbicides, atrazine type Fermentation, methanogenic, 15 Alcohols, alicyclic Benzenesulfonic acid, non-linear alkyl, Metabolic pathways, 599 Ketones, aliphanc Anaerobic digestion reactor, 15 long chain Fermentation, methanogenic, 15 Aerobic biodegradation, 19 Model ecosystem, aquatic, natural Metabolic pathways, 19 Alkanoic acids and derivatives 516 Benzoic acid and derivatives, 45 Lignin sulfonates Anaerobic digestion reactor, 15 Fermentation, methanogenic, 15 Cellulose and derivatives Aerobic biodegradation, 19 Metabolic pathways, 19 Alkanoic acids, cyclic Metabolic pathways, 27 NTA and salts Anaerobic digestion reactor, 15 Coke oven wastes Aerobic biodegradation, 549 Fermentation, methanogenic, 15 Lagoons, waste-tip, 479 Amino acids and derivatives Heavy metals effect, 549 Metabolic pathways, 479 Anaerobic digestion reactor, 15 Trickling filters, 479 Water hardness effect, 549 Fermentation, methanogenic, 15 Phenol and derivatives Dobanol 25-9 Anaerobic fermentation. Benzoic acid and derivatives Model ecosystem, aquatic, natural Anaerobic digestion reactor, 15 methanogenic, 195 516 Fermentation, methanogenic, 15 Explosives, organic Phosphoric acid plasticizers Cinnamic acid and derivatives Metabolic pathways, 565 Octanol-water partition coefficients. Anaerobic digestion reactor, 15 Gasoline 434 Phosphorothioic acid and derivatives Fermentation, methanogenic, 15 Metabolic pathways, 232 Aerobic biodegradation, 351 Cycloaliphatics, substituted Gums Anaerobic digestion reactor, 15 Metabolic pathways, 27 Polyethylene glycois. aikylphenoxy-Fermentation, methanogenic, 15 Herbicides, 2,4-D type, 45 Biotower studies, 92 Phloroglucinol Hydrocarbons Isolation of microorganisms, 92 Anaerobic digestion reactor, 15 Polyethylene glycois, fatty ether, 286 Metabolic pathways, 232 Fermentation, methanogenic, 15 Pyrocatechol and derivatives NTA and salts Methanol, phenol, isopropanol, acetone Screening tests, 415 Anaerobic fermentation, mixture Polyacrylic acid methanogenic, 195 Quaternary ammonium compounds, 286 Activated sludge, industrial, continuous-Metabolic pathways, 27 flow Polycyclic aromatic hydrocarbons Santicizers

(cont'd) Microbial population, sea water Octanol-water partition coefficients. 458 Psychrophilic temperature effect 399 Proteins Xylenes and derivatives River die-away test, 458 Aerobic biodegradation, 351 Benzenesultonic acid, linear aikyl, long Adaptation of microorganisms chain Microbial population, acclimated, municipal 399 Metabolic pathways, 109 Benzoic acid and derivatives Psychrophilic temperature effect Microbial population, sea water Metabolic pathways, 98 399 458 Nutritional effects, 98 Urea and derivatives Model ecosystem, aquatic, natural Polychlorobenzenes and derivatives Adaptation of microorganisms 109 Metabolic pathways, 98 Nutritional effects, 98 399 River die-away test, 458 Psychrophilic temperature effect Benzoic acid and derivatives Pyrocatechol and derivatives 399 Sorption, 44 Metabolic pathways, 98 Microbial population, cumene-assimilating Substrate concentration effect Nutritional effects, 98 Cumene and derivatives Salicylic acid and derivatives Cresols and derivatives Identification of microorganisms Metabolic pathways, 98 Aerobic biodegradation, 46 376 Nutritional effects, 98 Anaerobic biodegradation, 46 Screening tests, 376 Microbial population, acclimated, river Cutting fluids (coolants), synthetic and Substrate specificity, 376 water semi-synthetic Microbial population, cyanuric acid-Pluronics Biodegradation, I degrading Aerobic biodegradation, 382 Inhibitory (toxic) effects with preser-Cyanuric acid and derivatives Poly(ethylene glycol-propylene glycol) vatives, 1 Microaerophilic mechanisms propos-Aerobic biodegradation, 382 DDT, Methoxychlor and metabolites ed, 240 Microbial population, acclimated, sewage Aerobic biodegradation, 46 Microbial population, enrichment cultures Anaerobic blodegradation, 46 Sugars and derivatives Polycaprolactone Aerobic biodegradation, 402 Inhibitory (toxic) effects, 320 Continuous culture, multistage Isolation of microorganisms, 320 Operational parameters, 402 400 Nutritional effects, 320 Fuel oil Stripping and metabolic mechanisms Microbial population, estuarine water Metabolic pathways, 553 402, 403 Naphthalene and derivatives Herbicides, chlorpropham type Microbial population, acclimated, soils Isolation of microorganisms, 407 Sorption, 44 Carbamic acid and derivatives Metabolic pathways, 407 Substrate concentration effect Isolation of microorganisms, 102 Microbial population, fecal isolates 44 Polychlorobenzenes and derivatives Herbicides, 2,4-D type Aerobic biodegradation, 46 Heteroaromatics and derivatives, dicyclic Aerobic biodegradation, 262 Metabolic pathways, 575 Microbial population, aerated lagoon, in-Anaerobic biodegradation, 46 Phenylacetic acid and derivatives dustrial site Metabolic pathways, 575 Sorption, 44 EDTA and saits Model ecosystem, aquatic, industrial, Microbial population, fresh water Substrate concentration effect Alkanoic acids and derivatives 14 31 Heteroaromatics and Grivatives, dicyclic Sorption, 44 Microbial population, brackish water Aerobic biodegradation, 46 Substrate concentration effect Alkyl sulfates, long chain Anaerobic biodegradation, 46 44 Aerobic biodegradation, 76 Petroleum Alkanoic acids and derivatives, long Benzenesulfonic acid, linear alkyl. long , Metabolic pathways, 553 chain chain Microaerophilic biodegradation Phenylacetic acid and derivatives Aerobic biodegradation, 76 327 Aerobic biodegradation, 46 "Miracie White" (Miracle White Co.) Anaerobic biodegradation, 46 Microbial population, sea water Aerobic biodegradation, 76 Phosphorothioic acid and derivatives 458 "Surf" (Lever Brothers) Aerobic biodegradation, 46 River die-away test, 458 Aerobic biodegradation. 76 Anaerobic biodegradation. 46 Alkanoic acids and derivatives, "Tide" (Proctor and Gamble) Polychlorinated biphenyls polybasic Aerobic biodegradation, 76 Equilibrium partitioning, 467 Microbial population, sea water Microbial population, cellulolytic Polychlorocyclopentadiene dimers 458 Cellulose and derivatives River die-away test, 458 Anaerobic biodegradation, 46 Polycyclic aromatic hydrocarbons Operational parameters. 285 Alkyl sulfates, long chain Aerobic biodegradation, 46 Time-course kinetics, 285 Microbial population, sea water Anaerobic biodegradation, 46 458 Microbial population, continuous-flow Polyethylene glycols, fatty ether, suifate River die-away test, 458 Amino acids and derivatives Alkyl sulfonates and derivatives Microbial population, sea water Adaptation of microorganisms 458 Microbial population, sea water 399 River die-away test, 458 Psychrophilic temperature effect 458

Microbial population, continuous-flow

Microbial population, fresh water (cont'd)

Quaternary ammonium compounds

Inhibitory (toxic) effects, 304

Operational parameters, 423

Structure-activity relationships, 17

Microbial population, acclimated (cont'd)

399

399

Adaptation of microorganisms

Casamino acids

Amides, aliphatic, long chain, sulfated

Aerobic biodegradation, 327

River die-away test, 458

Amino acids and derivatives

Sulfophenylalkanoic acids (cont'd) Polyvinyl alcohol Percolation system, 481 Thiocyanic acid and salts Metabolic pathways, 109 Isolation of microorganisms, 481 Ozonization effects, 488 Model ecosystem, aquatic, natural Model ecosystem, aquatic, simulated, 109 Microbial population, fresh water sediments 481 EDTA and salts Microbial population, fresh water, ac-Percolation system, 481 Aerobic biodegradation, 510 climated Metabolic pathways, co-metabolism Microbial population, liquid cultures Cutting fluids (coolants), synthetic and Biphenyls and derivatives 510 semi-synthetic Screening parameters, 494 Seasonal variations, 510 Biodegradation, 1 Naphthalene and derivatives EDTA and salts Microbial population, fresh water hydrosoil Time-course kinetics, 200 Aerobic biodegradation, 509 Phthalic acid and derivatives Transformation rates, 200 Microbial population, liquid-enriched Aerobic biodegradation, 242 Polycyclic aromatic hydrocarbons Polychlorobenzenes and derivatives Anaerobic biodegradation, 242 Time-course kinetics, 200 Metabolic pathways, 322 Microbial population, fresh water, Transformation rates, 200 Textile wastes kerosene-cultured Microbial population, fresh water + sewager Metabolic pathways, 322 Alkanes, cyclic Aniline and derivatives Microbial population, loam Metabolic pathways, co-metabolism Metabolic pathways, 111 Aldehydes 168, 169 Time-course kinetics, 111 Structure-activity relationships Alkanes, long chain, branched Herbicides, carbamate Metabolic pathways, co-metabolism 168, 169 485 Metabolic pathways, 111 Alkynes Time-course kinetics, 111 Alkanes, long chain, linear Carbaryl inhibitory and persistance Herbicides, monuron type and activity, 257 Metabolic pathways, co-metabolism metabolites Amides, aliphatic Metabolic pathways, 111 Carbaryl inhibitory and persistance Alkenes Time-course kinetics, 111 activity, 257 Metabolic pathways, co-metabolism Herbicides, propanil type and DDT. Methoxychlor and metabolites 168, 169 metabolites Benzene and derivatives Structure-activity relationships Metabolic pathways, 111 Metabolic pathways, co-metabolism 485 Time-course kinetics, 111 Herbicides, chlorpropham type 168, 169 Urea and derivatives Azide inhibitory activity, 257 Metabolic pathways, 111 Carbaryl inhibitory and persistance Metabolic pathways, co-metabolism Time-course kinetics, 111
Microbial population, glycol-metabolizing activity, 257 169 Diazinon inhibitory and persistance Carbowax Microbial population, fresh water sediment activity, 257 Metabolic pathways, 80 Alkyl sulfides Herbicides, monuron type and Review, 80 Biogeochemical cycling, 602 metabolites Polyethylene glycols Benzene and derivatives Model ecosystem, terrestrial, Metabolic pathways, 80 Review, 80-Anaerobic biodegradation, 212 simulated, 216 Substrate concentration effect Herbicides, propanil type and Microbial population, hyperentrophic water 212 metabolites sediment Crude oil Model ecosystem, terrestrial, Benzene and derivatives Time-course kinetics, 551 simulated, 216 Anaerobic biodegradation, 212 Cyanuric acid and derivatives Ketones, aliphatic Microbial population, isopropanol-Anaerobic biodegradation, 441 Structure-activity relationships acclimated Dimethyl sulfoxide 485 Alcohols, primary aliphatic Anaerobic digestion reactor, 602 Phenylacetic acid and derivatives Metabolic pathways, 569 Biogeochemical cycling, 602 Structure-activity relationships Time-course kinetics, 602 Alcohols, secondary aliphatic 485 Metabolic pathways, 569 EDTA and salts Microbial population, mercury-resistant Ketones, aliphatic Aerobic biodegradation, 509 Mercury, inorganic, 498 Metabolic pathways, 569 Methyl mercaptan Methanol, phenol, isopropanol, acetone Microbial population, municipal wastes Anaerobic digestion reactor, 602 mixture Alkenoic acids and derivatives Biogeochemical cycling, 602 Metabolic pathways, 213 Metabolic pathways, 569 Time-course kinetics, 602 Phenol and derivatives Nutritional effects, enrichment Petroleum Metabolic pathways, 569 Time-course kinetics, 551 Alkyl sulfates, long chain Microbial population, lagoons Poly(vinylpyrrolidone) Coke oven wastes Evolution of bacterial populations Ozonization effects, 488 Isolation of microorganisms, 481 16 Poiyacrylamides Amines, alicyclic Ozonization effects, 488 Model ecosystem, aquatic, simulated, 481 Inhibitory (toxic) effects, 311 Polyacrylic acıd Amines, long chain Percolation system, 481 Ozonization effects, 488 Inhibitory (toxic) effects, 311 Phenol and derivatives Polycaprolactone Amines, poly-, aliphatic Operational parameters, 32 Isolation of microorganisms, 481 Inhibitory (toxic) effects, 311 Polyethylene glycols Model ecosystem, aquatic, simulated, Benzenesulfonic acid, alkyl, long chain 481 Ozonization effects, 488

Microbial population, fresh water (cont'd) Microbial population, fresh water sediment Microbial population, lagoons (cont'd)

Microbial population, municipal wastes	Microbial population, pesticide-	Microbial population, river water (cont'd)
(cont'd)	metabolizing (cont'd)	Inhibitory (toxic) effects, 427
Evolution of bacterial populations	Metabolic pathways, 132	Structure-activity relationships
16	Herbicides, 2.4-D type	427
Benzenesulfonic acid, linear alkyl, long	Metabolic pathways, 132	Amines, poly-, aliphatic
chain	Herbicides, monuron type and	Inhibitory (toxic) effects, 427
Aerobic biodegradation, 156	metabolites	Structure-activity relationships
Screening tests, 156	Metabolic pathways, 132	427
Benzoic acid and derivatives	Herbicides, pyrazon type	Benzenesuifonic acid, alkyl, long chain
Metabolic pathways, 213	Metabotic pathways, 132	Evolution of bacterial populations
Nutritional effects, enrichment, 213	Microbial population, plate cultures	16
Cellulose and derivatives	Biphenyls and derivatives	Benzenesulfonic acid, linear alkyl, long
Identification of microorganisms	Screening parameters, 494	chain, 436
406	Microbial population, raw sewage	Benzenesulfonic acid, S-substituted alkyl
Fellmongery wastes	Alcohols, primary aliphatic	Aerated chamber die-away test
Identification of microorganisms	Aerobic biodegradation, 26	416
. 406	Alkanoic acids and derivatives	River die-away test, 416
Nitriles, long chain	Aerobic biodegradation, 26	Shake flask process, 416
Inhibitory (toxic) effects, 311	Alkenes	Structure-activity relationships
Phthatic acid and derivatives	Aerobic biodegradation, 26	416
Acclimatization, selective mutation, 538	Alkyl halides	Herbicides, chlorpropham type
Pluronics	Aerobic biodegradation, 26	Identification of microorganisms
	Inhibitory (toxic) effects, 26	160
Evolution of bacterial populations 16	Amino acids and derivatives	Model ecosystem, aquatic, natural
Polyethylene glycols	Aerobic biodegradation, 26	160
Biomass yield, effect on, 81	Anıline and derivatives	Herbicides, 2,4-D type
Polyethylene glycols, fatty amine	Aerobic biodegradation, 26	Identification of microorganisms
Inhibitory (toxic) effects, 311	Antifreeze	160
Pyrocatechol and derivatives	Aerobic biodegradation, 26	Model ecosystem, aquatic, natural 160
Metabolic pathways, 213	Carbamic acid and derivatives	Phosphoric acid plasticizers
Nutritional effects, enrichment	Aerobic biodegradation, 26	Octanol-water partition coefficients.
213	Cellulose and derivatives	434
Quaternary ammonium compounds	Aerobic biodegradation, 26	Phthalic acid and derivatives, 194, 436
Structure-activity relationships	Cyanuric acid and derivatives	Pluronics
17	Aerobic biodegradation, 26	Evolution of bacterial populations
Starch and derivatives	Inhibitory (toxic) effects, 26	16
Identification of microorganisms	DDT, Methoxychlor and metabolites	Poly(ethylene glycol-propylene glycol)
406	Aerobic biodegradation, 26	River die-away test, 424
Triton X100	Inhibitory (toxic) effects, 26 Gasoline	Polyethylene glycols, alkylphenoxy-
Evolution of bacterial populations		Operational parameters, 99
16	Aerobic biodegradation, 26 Humics	River die-away test, 284, 424
Microbial population, non-acclimated,	Aerobic biodegradation, 26	Structure-activity relationships
sewage	Ketones, aliphatic	428
Sugars and derivatives	Aerobic biodegradation, 26	Polyethylene glycols, fatty ether
Aerobic biodegradation, 402	Polychlorinated biphenyls	Operational parameters, 99
Operational parameters, 402	Aerobic biodegradation, 26	River die-away test, 284, 424
Stripping and metabolic mechanisms	Polychlorobenzenes and derivatives	426
402	Aerobic biodegradation, 26	Structure-activity relationships
Microbial population, non-acclimated, soils		428
Amino acids and derivatives	Propylene glycols	Quaternary ammonium compounds
Aerobic biodegradation, 511	Aerobic biodegradation, 26	Inhibitory (toxic) effects, 427
Metabolic pathways, 511	Pyridine and derivatives	River die-away test, 424
NTA and saits	Aerobic biodegradation, 26	Structure-activity relationships
Aerobic biodegradation, 511	Inhibitory (toxic) effects, 26	427 Santicizers, 436
Metabolic pathways, 511	Starch and derivatives	Octanol-water partition coefficients,
Microbial population, NTA-acclimated,	Aerobic biodegradation, 26	434
soils	Microbial population, river water	Sugars and derivatives
Amino acids and derivatives	Alcohols, tertiary, long chain	River die-away test, 424
Aerobic biodegradation, 511	River die-away test, 424	Tailow derivatives
Metabolic pathways, 511	Alkyl sulfates, long chain	River die-away test, 424
NTA and salts	Evolution of bacterial populations,	16 Triton X100
Aerobic biodegradation, 511	Alkynes	Evolution of bacterial populations
Metabolic pathways, 511	River die-away test, 424	16
Microbial population, pesticide-	Amides, aliphatic, long chain	
metabolizing	River die-away test, 424	Microbial population, river water filtrate
Herbicides, atrazine type	Amines, long chain	Herbicides, 2,4-D type

(cont'd)
Heteroaromatics and derivatives, dicyclic (cont'd) (cont'd) Anaerobic biodegradation, 561 Recommendations, wastewater treat-Seasonal variations, 561 ment. 189, 199 Biorefractory index, 199 Microbial population, river water sediment Alkenes Recommendations, wastewater treat-Biorefractory index, 199 ment, 199 Benzenesulfonic acid, linear alkyl, long Humic acid Recommendations, wastewater treatchain ment, 199 Biorefractory index, 199 Model ecosystem, aquatic, natural. simulated, 135 Alkyl halides Recommendations, wastewater treat-Biological inhibition value, 199 ment, 199 Structure-activity relationships 135 Biorefractory index, 199 Hydroquinone and derivatives Herbicides, 2,4-D type Inhibitory (toxic) effects, 199 Anaerobic biodegradation, 561 Biorefractory index, 199
Recommendations, wastewater treat-Recommendations, wastewater treat-Seasonal variations, 561 ment. 199 ment. 199 Microbial population, saline water sediment Amino acids and derivatives Ketones, aliphatic Cyanuric acid and derivatives Biorefractory index, 189, 199 Biorefractory index, 199 Anaerobic biodegradation, 441 Recommendations, wastewater treat-Recommendations, wastewater treat-Microbial population, sea water ment, 189, 199 ment. 199 Alkanoic acids and derivatives, long Lead Aniline and derivatives chain Inhibitory (toxic) effects, 199 Biorefractory index, 199 Microbial population, fresh water Mercury Recommendations, wastewater treat-458 Inhibitory (toxic) effects, 199 ment, 199 Alkanoic acids and derivatives. Phenol and derivatives Reduced BOD, 61 polybasic Benzene and derivatives Biorefractory index, 189, 199 Microbial population, fresh water Biorefractory index, 199 Inhibitory (toxic) and stimulatory ef-458 Recommendations, wastewater treatfects, 170 Alkyl sulfates, long chain Inhibitory (toxic) effects, 61 ment, 199 Microbial population, fresh water Microbial acclimatization, 170 Benzoic acid and derivatives 458 Recommendations, wastewater treat-Reduced BOD, 61 Alkyl sulfonates and derivatives Biphenyl and derivatives ment, 189 Microbial population, fresh water Biorefractory index, 199 Reduced BOD, 61 458 Recommendations, wastewater treat-Polychlorinated biphenyls ment, 199 Cadmium Amino acids and derivatives Biorefractory index, 199 Microbial population, fresh water Polychlorobenzenes and derivatives Inhibitory (toxic) effects, 199 458 Biological inhibition value, 199 Carbamic acid and derivatives Benzenesulfonic acid, linear alkyl, long Biorefractory index, 199 Biorefractory index, 199 chain Inhibitory (toxic) effects, 199 Microbial population, fresh water Recommendations, wastewater treat-Reduced BOD, 61 ment, 199 Cellulose and derivatives Propylene glycols Phthalic acid and derivatives, 194 Biorefractory index. 199 Biorefractory index, 199 Polyethylene glycols, fatty ether, sulfate Recommendations, wastewater treat-Recommendations, wastewater treat-Microbial population, fresh water ment. 199 ment, 199 Chromium 458 Pyridine and derivatives Microbial population, septic tank Biological inhibition value, 199 Inhibitory (toxic) and stimulatory ef-Alkanoic acids and derivatives, Biorefractory index. 199 fects, 170 Inhibitory (toxic) effects, 199 polybasic Microbial acclimatization, 170 Recommendations, wastewater treat-Aerobic percolation, 264, 265 Cresols and derivatives Anaerobic percolation, 264, 265 ment. 199 Reduced BOD, 61 DDT, Methoxychlor and metabolites Starch and derivatives Cvanide Biorefractory index, 199 Inhibitory (toxic) effects, 6 Inhibitory (toxic) and stimulatory ef-NTA and salts Recommendations, wastewater treatfects, 170 Aerobic percolation, 263 ment. 199 Microbial acclimatization, 170 Anaerobic digestion reactor, 263 Sugars and derivatives Cyanuric acid and derivatives Phosphorothioic acid and derivatives Biorefractory index, 189, 199 Biological inhibition value, 199 Recommendations, wastewater treat-Inhibitory (toxic) effects. 6 Biorefractory index, 199 ment, 189, 199 Textile wastes Pyridine and derivatives Inhibitory (toxic) effects, 199 Inhibitory (toxic) effects, 6 DDT. Methoxychlor and metabolites Biorefractory index, 199 Microbial population, sewage Biological inhibition value, 199 Recommendations, wastewater treat-Alkanoic acids, sulfonated, long chain Biorefractory index, 199 ment, 199 Structure-activity relationships Inhibitory (toxic) effects, 199 Microbial population, silt loam 328 Phenol-formaldehyde resin Microbial population, sewage, municipal Inhibitory (toxic) and stimulatory ef-Biodegradation, rates compared, 248 Alcohols, primary aliphatic fects, 170 Poly(methyl methacrylate) Biorefractory index, 199 Microbial acclimatization, 170 Biodegradation, rates compared Recommendations, wastewater treat-Gasoline ment. 199 Biorefractory index, 199 Polystyrenes Alkanoic acids and derivatives Recommendations, wastewater treat-Biodegradation, rates compared Biorefractory index, 189, 199 ment, 199 248

Microbial population, sewage, municipal

Microbial population, sewage, municipal

Microbial population, river water filtrate

Missobial population soil burial	Microbial population, soils (cont'd)	Microbial population, soils (cont'd)
Microbial population, soil burial	Aerobic biodegradation, 156	Polyamides
Alkenoic acids and derivatives, long chain	Screening tests, 156	Aerobic vs anaerobic conditions
Structure-activity relationships	Benzoic acid and derivatives	119
97	Aerobic biodegradation, 133	Structure-activity relationships
	385	119
Polycaprolactone Structure-activity relationships	Anaerobic biodegradation, 385	Polycaprolactone
97	Denitrification, 14	Aerobic vs anaerobic conditions
Polyesters	Metabolic pathways, 14	119
Structure-activity relationships	River die-away test, 385	Aureobasidium sp. 126
97	Cellulose and derivatives	Penicillium sp. 126
•	Time-course kinetics, 82	Pseudomonas sp. 126
Polyethylene Structure-activity relationships	Cresols and derivatives	Structure-activity relationships
97	Denitrification, 14	119
	Metabolic pathways, 14	Polychlorinated biphenyls
Polypropylene Structure-activity relationships	Cyanuric acid and derivatives	Aerobic biodegradation, 527
97	Anaeropic biodegradation, 441	Structure-activity relationships
	Ecolytes	527
Polystyrenes	Biodegradation, rates compared	Polychlorobenzenes and derivatives
Structure-activity relationships 97	176, 245	Metabolic pathways, 322
Vegetable oils and fats	EDTA and salts	Polyesters
	Aerobic biodegradation, 509, 510	Aureobasidium sp., 126
Structure-activity relationships	Metabolic pathways, co-metabolism	Penicillium sp., 126
97	510	Pseudomonas sp. 126
Microbial population, soil-liquid	- Seasonal variations, 510	Polyethylene
Polychlorobenzenes and derivatives	Gums	Biodegradation, rates compared
Metabolic pathways, 322	Operational parameters, 171	215
Textile wastes	Herbicides, atrazine type	Isolation of microorganisms, 3
Metabolic pathways, 322	Metabolic pathways, 132	1
Microbial population, soils	Operational parameters, 132	Metabolic pathways, 3
Activated sludge, municipal	Herbicides, 2,4-D type	Polypropylene
Aerobic biodegradation, 527	Metabolic pathways, 132	Biodegradation, rates compared
Structure-activity relationships	Operational parameters, 132	245
527	Herbicides, monuron type and	Polystyrenes
Adipic acid and derivatives	metabolites	Biodegradation, rates compared
Aerobic vs anaerobic conditions	Metabolic pathways, 132	176, 245, 248
119	Operational parameters, 132	Polyvinyi acetate
Structure-activity relationships	Herbicides, pyrazon type	Isolation of microorganisms, 586
119	Metabolic pathways, 132	Polyvinyl alcohol
UV irradiation effect, 119	Operational parameters, 132	Isolation of microorganisms, 586
Alkanoic acids and derivatives	Industrial wastewaters	Proteins
Denitrification, 14	Isolation of microorganisms, 586	Aerobic vs anaerobic conditions
Metabolic pathways, 14	Latex	119
Alkanoic acids and derivatives,	Operational parameters, 171	Structure-activity relationships
polybasic	NTA and saits	119
Aerobic vs anaerobic conditions	Metabolic pathways, 127	Pyrocatechol and derivatives
119	Nylons	Denitrification, 14
Blocking effect, 119	Aerobic vs anaerobic conditions	Metabolic pathways, 14
Amides, aliphatic	119	Silicones
Aerobic vs anaerobic conditions	Structure-activity relationships	Isolation of microorganisms, 198
119	119	Metabolic pathways, 198
Blocking effect, 119	Petroleum sulfonates	Textile wastes
Structure-activity relationships	Operational parameters, 171	Metabolic pathways, 322
119	Phenol and derivatives	Microbial population, soils + cellulose and
Amines, poly-, aliphatic	Denitrification, 14	salts
Aerobic vs anaerobic conditions	Metabolic pathways, 14	Phenol-formaldehyde resin
119	Phenol-formaldehyde resin	Biodegradation, rates compared
Structure-activity relationships	Biodegradation, rates compared	248
119	248	Poly(methyl methacrylate)
Amino acids and derivatives	Phytane	Biodegradation, rates compared
Time-course kinetics, 82	Hypersaline environment, 557	248
Benzene and derivatives	Inhibitory (toxic) effects, hyper-	Polystyrenes
Identification of microorganisms	salinety, 557	Biodegradation, rates compared
376	Poly(methyl methacrylate)	248
Screening tests, 376	Biodegradation, rates compared	Microbial population, soils, organic-
Substrate specificity, 376	248	enriched
Benzenesulfonic acid, linear alkyl, long	Polyacrylamides	Herbicides, atrazine type
chain	Operational parameters, 171	Metabolic pathways, 132

Alkanoic acids and derivatives, 294 Structure-activity relationships 153 Alkenes Mirex see Polychlorocyclopentadiene dimers Molybdenum Activated sludge Mirex See Polychlorocyclopentadiene dimers Aerobic biodegradation, 431 Cresols and derivatives	Microbial population, soils, organic-	Micrococcus sp (cont'd)	Municipal wastes, synthetic (cont'd)
Herbindes, 2.4-D type Metabolic pathways, 132 Operational parameters, 132 Metabolic pathways, 132 Operational parameters, 134 Cresois and derivatives Time-convex kinetics, 184 Aylenols and derivatives Time-convex kinetics, 184 Aylenols and derivatives Time-convex kinetics, 184 Micrococcus gradinal parameters, 108 Structure-activity relationships 153 Alchohsb. pernylic Surcture-activity relationships 153 Alchohsb. pernylic Surcture-activity relationships 153 Alchohsb. pernylic General derivatives Metabolic pathways, 107 Structure-activity relationships 153 Alchohsb. pernylic General derivatives Metabolic pathways, 107 Metabolic pathways, 107 Cirrasols Aeroble biodegradation, 431 Cresols and derivatives, 204 Metabolic pathways, 222 Alkanosi cacids and derivatives Metabolic pathways, 222 Alkanosi cacids and derivatives, 204 Metabolic pathways, 222 Alkanosi cacids and derivatives, 204 Metabolic pathways, 222 Metabolic pathway	,		Substrate concentration effect
Metabolic pathways, 132 Operational parameters 132 Herbicides, monuron type and metabolics and metabolic pathways, 132 Operational parameters, 132 Microbial population - synthetic sewage Coal gasification wastes Time-course kinetics, 384 Cresois and derivatives Time-course kinetics, 384 Microcecus gas Alcohols, primary aliphatic, 294 Afferoncecus gas particular and derivatives and derivatives and derivatives are processed and derivative relationships 153 Alcohols, primary aliphatic, 294 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Structure-activity relationships 164 Structure-activity relationships 164 Structure-activity relationships 164 Mineral oils Identification of microorganisms 164 Metabolic pathways, 222 Alkanes, cyclic Metabolic pathways, 222 Alkanes Metabolic pathways, 222 Alkanes and derivatives Metabolic pathways, 222 Alkanes and derivatives Metabolic pathways, 222 Alkanes and derivatives Metabolic pathways, 222 Herbicides, monuron type and and derivatives, 204 Microbial population in microorganisms 164 Microbial population in microorganisms 164 Microbial population processing wastes Metabolic pathways, 222 Alkanes, cyclic Metabolic pathways, 222 Alkanes, cyclic Metabolic pathways, 222 Alkanes and derivatives Metabolic pathways, 222 Alkanes and derivatives Metabolic pathways, 222 Alkanes and derivatives Metabolic pathways, 222 Herbicides, Month and Metabolic pathways, 222 Herbicides, Month and Metabolic pathways, 222 Herbicides, Mo		Phenol and derivatives. 294	
Departional parameters. 132 Herbiedies, mourton type and metabolites Metabolic pathways, 132 Operational parameters, 132 Herbiedies, parameters, 132 Herbiedies, pyrazon type Metabolic pathways, 132 Operational parameters, 132 Microbia population = synthetic sewage Coal gasification wastes Time-course kinetics, 134 Cresols and derivatives Time-course kinetics, 134 Microbia population = synthetic swage Time-course kinetics, 134 Microbia population = synthetic swage Time-course kinetics, 134 Microbia population = synthetic swage Time-course kinetics, 134 Microbicours applic Simulture-activity relationships 153 Alcohols, primary aliphatic 294 Identification of microorganisms 164 Simulture-activity relationships 153 Alcohols, primary aliphatic 294 Identification of microorganisms 164 Simulture-activity relationships 153 Alcohols, primary aliphatic 294 Identification of microorganisms 164 Simulture-activity relationships 153 Alcohols, primary aliphatic 294 Identification of microorganisms 164 Simulture-activity relationships 153 Alcohols, primary aliphatic 294 Identification of microorganisms 164 Simulture-activity relationships 153 Alcohols, primary aliphatic 294 Identification of microorganisms 164 Simulture-activity relationships 153 Alcohols, primary aliphatic 294 Identification of microorganisms 164 Simulture-activity relationships 153 Alcohols, primary aliphatic 294 Identification of microorganisms 164 Simulture-activity relationships 153 Alcohols, primary aliphatic 294 Identification of microorganisms 164 Simulture-activity relationships 153 Alcohols, primary aliphatic 294 Identification of microorganisms 164 Simulture-activity relationships 153 Alcohols, primary aliphatic 294 Identification of microorganisms 164 Simulture-activity relationships 153 Alcohols, primary aliphatic 294 Identification of microorganisms 164 Simulture-activity relationships 153 Alcohols, primary aliphatic 294 Identification of microorganisms 164 Simulture-activity relationships 153 Alcohols, primary aliphatic 294 Identification of mic			Municipal wastewaters
Herbicides, monuron type and metabolites Metabolic pathways, 132 Operational parameters, 132 Herbicides, pyrazon type Metabolic pathways, 132 Microcourse kinetics, 384 Time-course kinetics, 384 Peneol and derivatives Time-course kinetics, 384 Micrococcus grand derivatives Alcohols, primary aliphatic, 294 Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Structure-activity relationships 164 Structure-activity relationships 165 Metabolic pathways, 232 Alcohols, penylic Accohols primarys, 332 Alcohols, primary aliphatic, 294		= -	
Metabolic pathways, 132 Operational parameters, 152 Herbicides, pyrazon type Metabolic pathways, 132 Operational parameters, 120 Merobal population + synthetic sweep Cast gasification wastes Time-course kinetics, 384 Xylenols and derivatives Time-course kinetics, 384 Xylenols and derivatives Alcohols, benzylic Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Alcohols, primary aliphatic, 294 Alcohols, primary aliphatic, 294 Alcohols, primary aliphatic, 294 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Alcohols, primary aliphatic, 294 Structure-activity relationships 164 Structure-activity relationships 164 Structure-activity relationships 164 Structure-activity relationships 165 Alcohols, primary aliphatic, 294 Structure-activity relationships 164 Structure-activity relationships 165 Alcohols, primary aliphatic, 294 Alcoholic p			Trickling filters, 484
Metabolic pathways, 132 Operational parameters, 132 Herbixedes, pyrazon type Metabolic pathways, 132 Operational parameters, 132 Microbial population + synthettic sewage Coal gasification wastes Time-course kinetics, 384 Cresois and derivatives Time-course kinetics, 384 Phenol and derivatives Time-course kinetics, 384 Phenol and derivatives Microbocars gardinates, 384 Myenols and derivatives Microbocars gardinates, 384 Myenols and derivatives Structure-activity relationships 153 Alcohols, benzylic Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Activated sidemtification of microorganisms 164 Activated sidemtification of microorganisms 164 Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Activated sidemtification, 498 Alcohols, primary ali			_
Metabolic pathways. 122 Operational parameters. 122 Microbial population + synthetic sewage Coal gasification wastes Time-course kinetics. 384 Cresols and derivatives Time-course kinetics. 384 Xylenois and derivatives Alcohols, benaylic Structure-activity relationships 153 Alcohols, primary aliphatic 153 Alcohols, secondary aliphatic. 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydes. 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydes. 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydes. 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydes. 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydes. 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydes. 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydes. 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic. 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydes. 294 Identification of microorganisms Biodegradability, ultimate, 487 Review, 487 Wiretabolic pathways, 232 Alkanoic activity relationships 163 Alcohols, secondary aliphatic Structure-activity relationships 164 Structure-activity relationships 165 Milke water-diluted Expherication of microorganisms B		Aerobic biodegradation, 431	Alcohols, benzylic
Metabolic pathways, 132 Operational parameters, 132 Microbial population + synthetic sewage Coal gastification wastes Time-course kinetics, 384 Phenol and derivatives Time-course kinetics, 384 Phenol and derivatives Time-course kinetics, 384 Phenol and derivatives Time-course kinetics, 384 Micrococcus braylic Structure-activity relationships 135 Alconols, permary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alconols, sprinary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alconols, sprinary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alconols, sprinary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alconols, sprinary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alconols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alconols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alconols, secondary aliphatic, 294 Milk and derivatives Metabolic pathways, 232 Milk and aderivatives Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, company aliphatic, 294 Structure-activity relationships 153 Alkanes Metabolic pathways, 232 Benzole and derivatives, 294 Milk and derivatives Metabolic pathways, 232 Benzole and derivatives Metabolic pathways, 232 Benzole and derivatives Metabolic pathways, 232 Benzole and derivatives Metabolic pathways, 232 Herbicudes, chilorpropham type Metabolic pathways, 474 Hydroquinone and derivatives Metabolic pathways, 474 Hydroquinone and derivatives Metabolic			
Operational parameters. 132 Microbial population + synthetic sewage Coal gasification wastes Time-course kinetics. 384 Cresols and derivatives Time-course kinetics. 384 Phenol and derivatives Time-course kinetics. 384 Xylenols and derivatives Time-course kinetics. 384 Xylenols and derivatives Time-course kinetics. 384 Xylenols and derivatives Structure-activity relationships 153 Alcohols, benzylic Structure-activity relationships 164 Structure-activity relationships 165 Structure-activity relationships 165 Alcohols, secondary aliphatic. 294 Structure-activity relationships 153 Aldehydes, 294 Structure-activity relationships 153 Aldehydes Metabolic pathways, 232 Metabolic pathways,			-
Microbial population + synthetic sewage Coal gasification wastes Time-course kinetics. 184 Time-course kinetics. 184 Phenol and derivatives Time-course kinetics. 184 Phenol and derivatives Time-course kinetics. 184 Phenol and derivatives Time-course kinetics. 184 Micrococcus Phenol and derivatives Time-course kinetics. 184 Micrococcus Phenol and derivatives Structure-activity relationships 153 Alcohols, benzylic Structure-activity relationships 164 Structure-activity relationships 165 Alcohols, secondary aliphatic. 294 Structure-activity relationships 165 Alcohols, secondary aliphatic. 294 Structure-activity relationships 167 Alcohols, secondary aliphatic. 294 Structure-activity relationships 168 Alcohols, secondary aliphatic. 294 Structure-activity relationships 169 Alcohols, secondary aliphatic. 294 Structure-activity relationships 160 Alcohols, secondary aliphatic. 294 Structure-activity relationships 161 Alcohols, secondary aliphatic. 294 Structure-activity relationships 162 Alcohols, secondary aliphatic. 294 Structure-activity relationships 163 Alcohols, secondary aliphatic. 294 Structure-activity relationships 164 Structure-activity relationships 165 Alkanes Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Benzole and derivatives Microbal population, brackish water Aerobic biodegradation, 41 Cresols and derivatives Metabolic pathways, 232 Benzole and derivatives Model ecosystem, terrestrial, natural, 545 Cycloadian mebrane filtration 333 Model ecosystem, terestrial, natural, 545 Cycloadian mebrane filtration 333 Model ecosystem, terestrial, natural, 545 Cycloadian mebrane filtration 333 Model ecosystem, terestrial, natural, 545 Cycloadian mebrane filtration Metabolic pathways, 224 Ben			Alconois, primary aliphatic
Coal gasification wastes Time-course kinetics. 384 Phenol and derivatives Time-course kinetics. 384 Xylenols and derivatives Structure-activity relationships 153 Alcohols. benzylic Structure-activity relationships 164 Structure-activity relationships 165 Structure-activity relationships 167 Alcohols. secondary aliphatic. 294 Structure-activity relationships 168 Structure-activity relationships 169 Alcohols. secondary aliphatic. 294 Structure-activity relationships 169 Alcohols. secondary aliphatic. 294 Structure-activity relationships 160 Structure-activity relationships 161 Aldenydes. 294 Identification of microorganisms 164 Structure-activity relationships 165 Alcohols. secondary aliphatic. 294 Structure-activity relationships 165 Alcohols. secondary aliphatic. 294 Structure-activity relationships 165 Alcohols. secondary aliphatic. 294 Structure-activity relationships 168 Milk. water-diluted Excherchia sp Inhibitory (toxic) effects. 450 Milk. water-diluted Excherchia		•	
Time-course kinetics, 384 Time-course kinetics, 384 Phenol and derivatives Time-course kinetics, 384 Phenol and derivatives Time-course kinetics, 384 Xylenois and derivatives Time-course kinetics, 384 Xylenois and derivatives Time-course kinetics, 384 Time-course kinetics, 384 Alcohols, benzylic Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Structure-activity relationships 153 Alchohols, primary aliphatic, 294 Structure-activity relationships 153 Aldehydes, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alkanes Metabolic pathways, 322 Alkanes, orgicia Metabolic pathways, 232 Alkanes, orgicia Metabolic pathways, 232 Alkanes Metabolic pathways, 232 Herbucides, chlorpropham type Metabolic pathways, 232 Her			
Cresois and derivatives Time-course kinetics, 384 Xylenols and derivatives Time-course kinetics, 384 Xylenols and derivatives Time-course kinetics, 384 Micrococcus sp Alcohols, benzylic Siructure-activity relationships 153 Alcohols, benzylic Siructure-activity relationships 153 Alcohols, benzylic Siructure-activity relationships 164 Siructure-activity relationships 153 Alcohols, secondary aliphatic, 294 Coperational parameters, 408 Toluene and derivatives Metabolic pathways, 232 Xylenols and derivatives Metabolic pathways, 232 Alkanes Metabolic pathways, 232 Alkanes, orgic ham, linear Metabolic pathways, 232 Alkanola acids and derivatives Metabolic pathways, 232 Alkanola caids and derivatives Metabolic pathways, 232 Alkanola			
Phenol and derivatives Time-course kinetics, 384 Xylenols and derivatives Time-course kinetics, 384 Micrococcus sp Alcohols, benzylic Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary alip			153
Time-course kinetics, 384 Xylenols and derivatives Time-course kinetics, 384 Micrococcus sp Alcohols, benzylic Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydes, 294 Structure-activity relationships 153 Alkanes Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, contain and derivatives Metabolic pathways, 232 Benzene and deriva		•	Alcohols, secondary aliphatic
Xylenois and derivatives Time-course kinetics, 384 Micrococcus sp Alcohols, benzylic Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Structure-activity relationships 153 Aldehydes Structure-activity relationships 153 Aldehydes Structure-activity relationships 153 Aldehydes Structure-activity relationships 153 Aldehydes Metabolic pathways, 232 Milkanes Metabolic pathways, 232 Alkanes Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 23			
Time-course kinetics, 384 Micrococcus sp Alcohols, benzylic Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Structure-activity relationships 153 Aldehydes, 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydes, 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydes, 294 Identification of microorganisms 164 Inhibitory (toxic) effects, 450 Mike water-diluted Escherichia sp Inhibitory (toxic) effects, 450 Mikeral oils Metabolic pathways, 232 Alkanes Metabolic pathways, 232 Alkanes, orgic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes, orgic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes, orgic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes, orgic Metabolic pathways, 232 Alkanes orgic pathways, 232 Benzene and derivatives Metabolic pathways, 192 Alkanes Metabolic pathways, 193 Alcohols, benzives Metabolic pathways, 192			
Alcohols, benzylic Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 165 Alkanes Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes long chain, linear Metabolic pathways, 232 Alkanes and derivatives Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 234			
Structure-activity relationships 153 Alcohols, primary aliphatic. 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic. 294 Structure-activity relationships 153 Aldehydes, 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydes, 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydes, 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydes, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alkanes Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes and derivatives Model ecosystem, terrestrial, natural, 545 Surcture-activity relationships 153 Alkanes Metabolic pathways, 232 Alkanes and derivatives Metabolic pathways, 232 Alkanes and derivatives Model ecosystem, terrestrial, natural, 545 Surcture-activity relationships 153 Alkanes and derivatives Metabolic pathways, 234 Alkanes and derivatives Metabolic pathways, 235 Alkanes and derivatives Metabolic pathways, 23 Alkanes and derivatives Metabolic pathways, 23 Alkanes and derivatives Minibitory (toxic) effects, 43 Alkanes and derivatives Metabolic pathways, 23 Alkanes and der			164
Structure-activity relationships 153 Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Structure-activity relationships 153 Alchydse, 294 Identification of microorganisms 164 Structure-activity relationships 153 Aldehydse, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alkanes Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanoic acids and derivatives Metabolic pathways, 234 Alkanoic acids and derivatives Metabolic pathways, 234 Alkanoic acids, cyclic Metabolic pathways, 234 Alkanoic acids and deri			Structure-activity relationships
Alcohols, primary aliphatic, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Structure-activity relationships 153 Aldohydes, 294 Identification of microorganisms 164 Identification of microorganisms 165 Istructure-activity relationships 173 Alkanes Netabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, orgic Metabolic pathways, 232 Alkanes, orgic Metabolic pathways, 232 Alkanes, long chain, detabolic pathways, 232 Alkanes, long chain, altination of microorganisms Biodegradation, 437 Miracle Whiter (Miracle White Co.) Mirobial population, brackish water Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 232 Benzoic acid and derivatives Metabolic pathways, 232 Benzoic acid and derivatives Metabolic pathways, 232 Alkanes long chain, altination and trivatives polybasic Miracle Whiter (Miracle White Co.) Miracle Whiter (Miracle White	·		153
Identification of microorganisms 153 Aldehydes, 294 Identification of mcroorganisms 164 Structure-activity relationships 153 Aldehydes, 294 Identification of mcroorganisms 164 Structure-activity relationships 153 Alkanes Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes long chain, linear Metabolic pathways, 233 Alkanes Metabolic pathways, 232 Benzoic and and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways, 232 Alkanes long land lengthy literated land l			
Structure-activity relationships 153 Alcohols, secondary aliphatic, 294 Structure-activity relationships 153 Aldehydes, 294 Identification of microorganisms 164 Identification of microorganisms 164 Structure-activity relationships 153 Alkanes Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanoic acids and derivatives Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanoic acids, cyclic Metabolic pathways, 232 Alkanoic acids and derivatives Microbial population, brackish water Aerobic blodegradation, 76 Arobic blodegradation, 431 Cresols and derivatives Metabolic pathways, 197 Alkanes Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 197 Crirasols Aerobic blodegradation, 431 Cresols and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives Molopdenum Activated sludge Metabolic pathways, 192 Alkanoic acids and derivatives Mirerobial population, brackish water Aerobic blodegradation, 431 Cresols and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives Molopdenum Activated sludge Metabolic pathways, 192 Alkanoic acids and derivatives Molopdenum Activated sludge Metabolic pathways, 192 Alkanoic acids, cyclic Metabolic pathways, 193 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Cycloaliphatucs, substituted Metabolic pathways, 192 Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways, 192 Alkanoic acids and			
Structure-activity relationships 153 Aldehydes. 294 Identification of microorganisms 164 Structure-activity relationships 153 Alkanes Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 234 Alkanes, long chain, linear Metabolic pathways, 235 Alkanes Metabolic pathways, 235 Alkanes Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 235 Alkanes Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 235 Alkanes Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 235 Alkanes Metabolic pathways, 235 Alkanes Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 235 Alkanoic acids and derivatives Metabolic pathways, 236 Alkanes Metabolic pathways, 237 Alkanes Metabolic pathways, 232 Metabolic pathways, 234 Alkanes Metabolic pathways, 234 Alkanes Metabolic pathways, 235 Alkanes Metabolic pathways, 236 Alkanes Metab		= =	
Alcoholos, secondary aliphatic, 294 Structure-activity relationships 133 Aldehyds, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alkanes Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes and derivatives, 294 Structure-activity relationships 153 Alkenes Metabolic pathways, 232 Alkanes derivatives, 294 Structure-activity relationships 153 Alkenes Metabolic pathways, 232 Alkanoic acids and derivatives Metabolic pathways, 232 Alkanes ong chain, linear Metabolic pathways, 232 Alkanoic acids and derivatives, 294 Structure-activity relationships Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbucides, chlopropham type Metabolic pathways, 232 Herbucides, chlopropham type Metabolic pathways, 234 Herbucides, chlopropham type Metabolic pathways, 234 Hylerocarbons Metabolic pathways, 232 Hylerodizione and derivatives Metabolic pathways, 234 Hylerodizione and derivatives Metabolic pathways, 235 Hylerodizions and derivatives Metabolic pathways, 236 Milk. water-diluted Escherichia sp Inhibitory (toxic) effects, 43 Milkanet, 487 Milkanet, 487 Milex elliuted Scherichia sp Inhibitory (toxic) effects, 43 Milexole Hite Co.) Microbal population, brackish water Aerobic biodegradation, 76 Mirex Metabolic pathways, 232 Model ecosystem, terrestrial, natural, 545 Cycloaliphatics, substituted Metabolic pathways, 246 Metabolic pathways, 25 Hydroquinne and derivatives Metabolic pathways, 246 Metabolic pathways, 246 Metabolic pathways, 246 Metabolic pathways, 246 Me			
Alcohols, secondary aliphatic, 294 Structure-activity relationships 153 Aldehydes, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alkanes Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes long chain, linear Metabolic pathways, 232 Alkanes and derivatives Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Hydroquinone and derivatives Structure-activity relationships Model ecosystem, terrestrial, natural, 545 Milk, water-diluted Escherichia sp Inhibitory (toxic) effects, 43 Mile acid of microorganisms Biodegradability, ultimate, 487 Review, 487 Miracle White: M		Metabolic pathways, 232	
Aldehydes, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alkanes Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes long chain, linear Metabolic pathways, 232 Alkanes Metabolic pathways, 232 Alkanes Metabolic pathways, 232 Benzone and derivatives Metabolic pathways, 232 Benzone and derivatives Metabolic pathways, 197 Cirrasols Alexanes Metabolic pathways, 232 Benzone and derivatives Metabolic pathways, 197 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Hydroquinone and derivatives Structure-activity relationships 153 Structure-activity relationships 164 Structure-activity relationships 164 Structure-activity relationships 164 Structure-activity relationships 164 Milk, water-diluted Escherichia sp Inhibitory (toxic) effects, 43 Alkanois Miracle White (Co.) Microbial population, brackish water Aerobic biodegradation, 76 Mirex See Polychlorocyclopentadiene dimers Molybdenum Activated sludge Inhibitory (toxic) effects, 45 Nitroeb. Co.) Microbial population, brackish water Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives, polybasic Metabolic pathways, 192 Alkanoic acids and derivatives, polybasic Metabolic pathways, 192 Alkanoic acids and derivatives, polybasic Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives, polybasic Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways, 192 Alkanoic acids and derivati			Alkanoic acids and derivatives
Aldehydes, 294 Identification of microorganisms 164 Structure-activity relationships 153 Alkanes Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanoic acids and derivatives, 294 Structure-activity relationships 153 Alkenes Metabolic pathways, 232 Alkanoic acids and derivatives Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzel acid and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Hydroquinone and derivatives Structure-activity relationships Milk, water-diluted Escherichia sp Inhibitory (toxic) effects, 45 Mirracle White Co.) Microbal population, brackish water (Miracle White Co.) Microbal population, brackish water Aerobic biodegradation, 76 Mirex 333 Model ecosystem, aquatic, simulated, 545 Cycloaliphatics, substituted Metabolic pathways, 192 Hydroquinone and derivatives Metabolic pathways, 192, 468 Nitrobarcae Metabolic pathways, 292 Hydroquinone and derivatives Metabolic pathways, 192, 468 Municipal water, 477 Polystyrenes Metabolic pathways, 477 Polystyrenes Metabolic pathways, 474 Hydrocarbons Metaboli	• •		
Identification of microorganisms 164 Structure-activity relationships 153 Alkanes Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes long chain, linear Metabolic pathways, 232 Alkanes and derivatives, 294 Structure-activity relationships 153 Alkenes Microbial population, brackish water Aerobic biodegradation, 76 Mierobial population, brackish water Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives Model ecosystem, terrestrial, natural, 545 Cycloaliphanes, 294 Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 192, 468 Vanilic acid and derivatives M			
Structure-activity relationships 153 Alkanes Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, long chan, linear Metabolic pathways, 232 Alkanes ong chan, linear Metabolic pathways, 232 Alkanes ong chan, linear Metabolic pathways, 232 Alkanoic acids and derivatives, 294 Structure-activity relationships 153 Alkenes Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192 Alkenes Mineral oils Identification of microorganisms Biodegradability, ultimate, 487 Review, 487 (Miracle White Co.) Mirex Aerobic biodegradation, 76 Mirex See Polychlorocyclopentadiene dimers Molybdenum Activated sludge Inhibitory (toxic) effects, 40 Alkenes See Polychlorocyclopentadiene dimers Molybdenum Activated sludge Alkanoic acids and derivatives, polybasic Metabolic pathways, 192 Alkanoic acids and derivatives, polybasic Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways, 192 Alkenes Model ecosystem, terrestrial, natural, 545 Cycloaliphancs, substituted Metabolic pathways, 25 Hydroquinone and derivatives Metabolic pathways, 192 Model ecosystem, terrestrial, natural, 545 Cycloaliphancs, substituted Metabolic pathways, 192 Hydroquinone and derivatives Metabolic pathways, 192 Model ecosystem, terrestrial, natural, 545 Cycloaliphancs, vibrati			
Structure-activity relationships 153 Alkanes Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanoic acids and derivatives, 294 Structure-activity relationships 153 Alkenes Metabolic pathways, 232 Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192 Hydroquinone and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways,			
Alkanes Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanes and derivatives, 294 Structure-activity relationships 153 Alkenes Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzoic acid and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 232 Hydroquinone and derivatives Structure-activity relationships Identification of microorganisms Biodegradatibity, ultimate, 487 Review, 487 (Miracle White* (Miracle White Co.) Microbial population, brackish water Aerobic biodegradation, 76 Mirex Mirex Mole Coosystem, aquatic, simulated, 333 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 192 Alkanes, cyclic Microbial population, brackish water Aerobic biodegradation, 76 Mirex Mole Co.) Mirex Mole Coosystem, aquatic, simulated, 333 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 192 Alkanes (Mirex Metabolic pathways, 192 Alkanes (Mirex Molybdenum Activated sludge Inhibitory (toxic) effects, 20 Moraxella sp Metabolic pathways, 192 Moraxella sp Metabolic pathways, 192 Model ecosys	Structure-activity relationships		
Alkanes Metabolic pathways, 232 Alkanes, cyclic Metabolic pathways, 232 Alkanes, long chain, linear Metabolic pathways, 232 Alkanoic acids and derivatives, 294 Structure-activity relationships Alkenes Metabolic pathways, 232 Alkanoic acids and derivatives Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzole acid and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Hydroquinone and derivatives Structure-activity relationships Model ecosystem, aquatic, simulated, 333 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways, 192, 468 Vanilic acid and derivatives Metabolic pathways, 192, 468 Vanilic acid and derivatives Metabolic pathways, 192 Metabolic pathways,	153		Inhibitory (toxic) effects, 450
Alkanes. cyclic Metabolic pathways, 232 Alkanes. long chain, linear Metabolic pathways, 232 Alkanes. long chain, linear Metabolic pathways, 232 Alkanoic acids and derivatives, 294 Structure-activity relationships 153 Alkenes Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzole acid and derivatives Metabolic pathways, 232 Benzole acid and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides. chlorpropham type Metabolic pathways, 232 Herbicides. chlorpropham type Metabolic pathways, 232 Herbicides. chlorpropham type Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192. 468 Municipal wastes, synthetic Aerobic biodegradation, 89 Rare constants/retention time Review, 487 Miracle White: (Miracle White Co.) Microbial population, brackish water Aerobic biodegradation, 76 Mirex 333 Model ecosystem, aquatic, simulated, 333 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives, polybasic Metabolic pathways, 192 Alkanoic acids and derivatives, polybasic Metabolic pathways, 192 Alkenes Metabolic pathways, 192 Alkenes Metabolic pathways, 192 Alkenes Metabolic pathways, 192 Alkanoic acids and derivatives, polybasic Metabolic pathways, 192 Metabolic pathways, 192 Alkenoic acids and derivatives Metabolic pat			Structure-activity relationships
Metabolic pathways, 232 Alkanes. long chain, linear Metabolic pathways, 232 Alkanoic acids and derivatives, 294 Structure-activity relationships 153 Alkenes Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzoic acid and derivatives Metabolic pathways, 232 Benzoic acid and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, aquatic, simulated, 333 Model ecosystem, aquatic, simulated, 333 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Hydroquinone and derivatives Structure-activity relationships Mircobile poderivatives Metabolic pathways, 192, 468 Mirex Molybdenum Activated sludge Inhibitory (toxic) effects, 20 Moraxella sp Alkanoic acids and derivatives, Metabolic pathways, 192 Alkanoic acids and derivatives, Metabolic pathways, 192, 468 Mitrobale pathways, 192, 468 Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Metabolic pathways, 192 Pholystyrenes Metabolic pathways, 192			
Alkanes. long chain, linear Metabolic pathways, 232 Alkanoic acids and derivatives, 294 Structure-activity relationships 153 Alkenes Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzoic acid and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 232 Hydroquinone and derivatives Structure-activity relationships Microbic biodegradation, 76 Mirex Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 232 Model ecosystem, aquatic, simulated, 333 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways, 192 Alkenoic acids and derivatives Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 477 Polystyrenes Metabolic pathways, 477 Polystyrenes Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 232 Hydroquinone and derivatives Structure-activity relationships Municipal wastes, synthetic Activated sludge Nodel ecosystem, terrestrial, natural, 545 Cycloaliphatics, substituted Metabolic pathways, 25 Hydroquinone and derivatives Metabolic pathways, 192 Hydroquinone and derivatives Metabolic pathways, 192, 468 Vanillic acid and derivatives Metabolic pathways, 192, 468 Vanillic acid and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Alkanoic acids and derivatives Metabolic pathways, 192 Hydroquinone and derivatives Metabolic pathways, 192, 468 Vanillic acid and derivatives Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 192, 468 Nitrobenzene and deriva		"Miracle White" (Miracle White Co.)	
Metabolic pathways, 232 Alkanoic acids and derivatives, 294 Structure-activity relationships 153 Alkenes Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzoic acid and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, aquatic, simulated, 333 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives Metabolic pathways, 192 Alkenoic acids and derivatives Metabolic pathways, 192 Alkenoic acids and derivatives Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 477 Polystyrenes Metabolic pathways, 477 Polystyrenes Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 232 Hydroquinone and derivatives Activated sludge Alkanoic acids and derivatives Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 477 Polystyrenes Metabolic pathways, 477 Polystyrenes Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Model ecosystem, aquatic, simulated, 333 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 192 Metabolic pathways, 192 Hydroquinone and derivatives Metabolic pathways, 192, 468 Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 477 Polystyrenes Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathway		Microbial population, brackish water	
Alkanoic acids and derivatives, 294 Structure-activity relationships 153 Alkenes Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzoic acid and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 192 Alkanoic acids and derivatives, polybasic Metabolic pathways, 192 Alkanoic acids and derivatives, polybasic Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 477 Polystyrenes Metabolic pathways, 477 Model ecosystem, terrestrial, natural, 545 Petroleum Mesophilic temperature effect 342 Phenol and derivatives Model ecosystem, terrestrial, natural, 545 Model ecosystem, terrestrial, natural, 545 Municipal wastes, synthetic Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Activated sludge Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Activated sludge Activated sludge Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Activated sludge Activated sludge Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Activated sludge Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Activated sludge Activatives Metabolic pathways, 192, 468 Mactivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Activatives Metabolic pathways, 192, 468 Mactivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic A		Aerobic biodegradation, 76	
Alkenes Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzoic acid and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 232 Heydroquinone and derivatives Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Acrobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 25 Hydroquinone and derivatives Metabolic pathways, 192, 468 Vanillic acid and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Acrobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 25 Hydroquinone and derivatives Metabolic pathways, 477 Polystyrenes Metabolic pathways, 192, 468 Municipal wastes, synthetic Acrobic biodegradation, 431 Acrobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 25 Hydroquinone and derivatives Metabolic pathways, 477 Polystyrenes Metabolic pathways, 192, 468 Municipal wastes, synthetic Acrobic biodegradation, 431 Acrobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 25 Hydroquinone and derivatives Structure-activity relationships Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 192, 468 Mitrobenzene and derivatives Metabolic pathways, 192, 468 Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 192, 468 Ni			333
Alkenes Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzoic acid and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 197 Girrasols Aerobic biodegradation, 431 Cresols and derivatives Metabolic pathways, 192 Alkenoic acids and derivatives Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 477 Polystyrenes Metabolic pathways, 477 Polystyrenes Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Metabolic pathways, 192, 468 Municipal wastes, synthetic Metabolic pathways, 192, 468 Structure-activity relationships Activated sludge Moraxella sp Model ecosystem, terrestriai, natural, 545 Petroleum Mesophilic temperature effect 342 Phenol and derivatives Model ecosystem, terrestriai, natural, 545 Phhalic acid and derivatives Model ecosystem, terrestriai, natural, 545 Phhalic acid and derivatives Model ecosystem, terrestriai, natural, 545 Petroleum Mesophilic temperature effect 342 Phenol and derivatives Model ecosystem, terrestriai, natural, 545 Phhalic acid and derivatives Model ecosystem, terrestriai, natural, 545 Phhalic acid and derivatives Model ecosystem, terrestriai, natural, 545 Phhalic acid and derivatives Model ecosystem, terrestriai, natural, 545 Phhalic acid and derivatives Model ecosystem, terrestriai, natural, 545 Phhalic acid and derivatives Model ecosystem, terrestriai, natural, 545 Polystyrenes Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 192, 468 Nitrobenzene and		see Polychlorocyclopentadiene dimers	
Metabolic pathways, 232 Benzene and derivatives Metabolic pathways, 232 Benzoic acid and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 474 Hydroquinone and derivatives Metabolic pathways, 474 Hydroquinone and derivatives Metabolic pathways, 474 Hydroquinone and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Metabolic pathways, 192, 468 Municipal wastes, synthetic Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Structure-activity relationships Materiabolic pathways, 192 Activated sludge Aerobic biodegradation, 89 Structure-activity relationships Model ecosystem, terrestrial, natural, 545 Cycloaliphatics, substituted Metabolic pathways, 25 Hydroquinone and derivatives Structure-activity relationships Metabolic pathways, 192, 468 Nitrobenzene and derivatives Metabolic pathways, 192, 468 Vanillic acid and derivatives Metabolic pathways, 192, 468 Vanillic acid and derivatives Model ecosystem, terrestrial, natural, 545 Hydroquinone and derivatives Mesophilic temperature effect 342 Phenol and derivatives Model ecosystem, terrestrial, natural, 545 Hydroquinone and derivatives Mesophilic temperature effect 342 Phenol and derivatives Model ecosystem, terrestrial, natural, 545 Hydroquinone and derivatives Mesophilic temperature effect 342 Phenol and derivatives Model ecosystem, terrestrial, natural, 545 Hydroquinone and derivatives Mesophilic temperature effect 342 Phenol and derivatives Model ecosystem, terrestrial, natural, 545 Hydroquinone and derivatives Mesophilic temperature effect 342 Ph			
Benzene and derivatives Metabolic pathways, 232 Benzoic acid and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192, 468 Vamilic acid and derivatives Metabolic pathways, 192, 468 Vanilic acid and derivatives Metabolic pathways, 192, 468 Vanilic acid and derivatives Metabolic pathways, 192, 468 Vanilic acid and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Aerobic biodegradation, 89 Structure-activity relationships 545 Cycloaliphatics, substituted Metabolic pathways, 25 Hydroquinone and derivatives Structure-activity relationships 153 Petroleum Mesophilic temperature effect 342 Phenol and derivatives Model ecosystem, terrestrial, natural, 545 Phthalic acid and derivatives Metabolic pathways, 192, 468 Metabolic pathways, 192, 468 Vanillic acid and derivatives Metabolic pathways, 192, 468 Metabolic pathways, 192, 468 Vanillic acid and derivatives Metabolic pathways, 192, 468 Metabolic pathways, 192, 468 Metabolic pathways, 192, 468 Mesophilic temperature effect 342 Phenol and derivatives Model ecosystem, terrestrial, natural, 545 Phthalic acid and derivatives Metabolic pathways, 192, 468 Metabolic pathways, 192, 468 Mesophilic temperature effect 342 Phenol and derivatives Metabolic pathways, 192, 468 Metabolic pathways, 192, 468 Mesophilic temperature effect 342 Phenol and derivatives Model ecosystem, terrestrial, natural, 545 Phthalic acid and derivatives Metabolic pathways, 192, 468 Metabolic pathways, 192, 468 Mesophilic temperature effect 342 Phenol and derivatives Model ecosystem, terrestri			
Metabolic pathways, 232 Benzoic acid and derivatives Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192, 468 Vamilic acid and derivatives Metabolic pathways, 192 Phenol and derivatives Model ecosystem, terrestrial, natural, 545 Model ecosystem, terrestrial, natural, 545 Phhtalic acid and derivatives Metabolic pathways, 117 Polyethylene glycols, fatty ester Aerobic biodegradation, 431			
Metabolic pathways, 107 Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Municipal wastes, synthetic Metabolic pathways, 232 Hydroquinone and derivatives Municipal wastes, synthetic Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Aerobic biodegradation, 89 Structure-activity relationships Metabolic pathways, 25 Metabolic pathways, 25 Metabolic pathways, 192, 468 Municipal wastes, synthetic Aerobic biodegradation, 89 Structure-activity relationships Metabolic pathways, 25 Metabolic pathways, 192, 468 Municipal wastes, synthetic Aerobic biodegradation, 89 Structure-activity relationships Metabolic pathways, 25 Metabolic pathways, 192, 468 Municipal wastes, synthetic Aerobic biodegradation, 431 Metabolic pathways, 192, 468 Metabolic pathwa			
Cirrasols Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 192, 468 Metabolic pathways, 477 Polystyrenes Metabolic pathways, 192, 468 Wanillic acid and derivatives Metabolic pathways, 192, 468 Vanillic acid and derivatives Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 192, 468 Vanillic acid and derivatives Metabolic pathways, 192, 468 Vanillic acid and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Aerobic biodegradation, 89 Structure-activity relationships Alkenoic acids and derivatives Mesophilic temperature effect 342 Phenol and derivatives Model ecosystem, terrestrial, natural, 545 Phthalic acid and derivatives Metabolic pathways, 192, 468 Vanillic acid and derivatives Metabolic p			
Aerobic biodegradation, 431 Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 477 Polystyrenes Metabolic pathways, 192, 468 Wanillic acid and derivatives Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 232 Hydroquinone and derivatives Structure-activity relationships Alkelotic acids and derivatives Metabolic pathways, 192, 468 Wanillic acid and derivatives Metabolic pathways, 192, 468 Wanillic acid and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Aerobic biodegradation, 89 Structure-activity relationships Rate constants/retention time 153 Petroleum Mesophilic temperature effect 342 Phenol and derivatives Model ecosystem, terrestrial, natural, 545 Phthalic acid and derivatives Metabolic pathways, 117 Polyethylene glycols, fatty ester Aerobic biodegradation, 431	• •		
Cresols and derivatives Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 477 Polystyrenes Metabolic pathways, 192, 468 Metabolic pathwa		Alkenoic acids and derivatives	
Model ecosystem, terrestrial, natural, 545 Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Metabolic pathways, 474 Hydrocarbons Municipal wastes, synthetic Metabolic pathways, 232 Hydroquinone and derivatives Acrobic biodegradation, 89 Structure-activity relationships Nitrobenzene and derivatives Metabolic pathways, 477 Metabolic pathways, 477 Polystyrenes Metabolic pathways, 192, 468 Vamilic acid and derivatives Model ecosystem, terrestrial, natural, 545 Metabolic pathways, 192, 468 Municipal wastes, synthetic Metabolic pathways, 117 Polyethylene glycols, fatty ester Aerobic biodegradation, 431			Petroleum
Gasoline Metabolic pathways, 232 Herbicides, chlorpropham type Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Structure-activity relationships Polystyrenes Metabolic pathways, 192, 468 Vamilic acid and derivatives Metabolic pathways, 192, 468 Vamilic acid and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Aerobic biodegradation, 89 Structure-activity relationships Rate constants/retention time Polystyrenes Metabolic pathways, 192, 468 Vamilic acid and derivatives Model ecosystem, terrestriai, natural, 545 Model ecosystem, terrestriai, natural, 545 Metabolic pathways, 192, 468 Model ecosystem, terrestriai, natural, 545 Metabolic pathways, 192, 468 Model ecosystem, terrestriai, natural, 545 Metabolic pathways, 192, 468 Model ecosystem, terrestriai, natural, 545 Metabolic pathways, 192, 468 Model ecosystem, terrestriai, natural, 545 Metabolic pathways, 192, 468 Model ecosystem, terrestriai, natural, 545 Metabolic pathways, 192, 468 Model ecosystem, terrestriai, natural, 545 Metabolic pathways, 192, 468 Model ecosystem, terrestriai, natural, 545 Metabolic pathways, 192, 468 Model ecosystem, terrestriai, natural, 545 Metabolic pathways, 192, 468 Model ecosystem, terrestriai, natural, 545 Metabolic pathways, 192, 468 Model ecosystem, terrestriai, natural, 545			
Metabolic pathways. 232 Herbicides, chlorpropham type Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Structure-activity relationships Metabolic pathways, 192, 468 Vamilic acid and derivatives Metabolic pathways, 192, 468 Municipal wastes, synthetic Activated sludge Aerobic biodegradation, 89 Structure-activity relationships Rate constants/retention time Metabolic pathways, 192, 468 Model ecosystem, terrestriai, natural, 545 Phthalic acid and derivatives Metabolic pathways, 117 Polyethylene glycols, fatty ester Aerobic biodegradation, 431		Metabolic pathways, 4//	
Herbicides, chlorpropham type Metabolic pathways, 474 Hydrocarbons Metabolic pathways, 232 Hydroquinone and derivatives Metabolic pathways, 232 Hydroquinone and derivatives Structure-activity relationships Manilic acid and derivatives Municipal wastes, synthetic Activated sludge Aerobic biodegradation, 89 Structure-activity relationships Vanillic acid and derivatives Municipal wastes, synthetic Activated sludge Aerobic biodegradation, 89 Structure-activity relationships Rate constants/retention time Model ecosystem, terrestrial, natural, 545 Phthalic acid and derivatives Metabolic pathways, 117 Polyethylene glycols, fatty ester Aerobic biodegradation, 431			
Metabolic pathways, 474 Hydrocarbons Menabolic pathways, 192, 468 Municipal wastes, synthetic Metabolic pathways, 232 Activated sludge Hydroquinone and derivatives Structure-activity relationships Metabolic pathways, 192, 468 Metabolic pathways, 192, 468 Metabolic pathways, 192, 468 Activated sludge Aerobic biodegradation, 89 Rate constants/retention time Metabolic pathways, 192, 468 Metabolic pathways, 192,	* * * * * =		
Hydrocarbons Municipal wastes, synthetic Metabolic pathways, 232 Activated sludge Metabolic pathways, 117 Hydroquinone and derivatives Aerobic biodegradation, 89 Structure-activity relationships Rate constants/retention time Phthalic acid and derivatives Metabolic pathways, 117 Polyethylene glycols, fatty ester Aerobic biodegradation, 431		Metabolic pathways, 192, 468	
Metabolic pathways, 232 Hydroquinone and derivatives Structure-activity relationships Activated sludge Aerobic biodegradation, 89 Rate constants/retention time Metabolic pathways, 117 Polyethylene glycols, fatty ester Aerobic biodegradation, 431		Municipal wastes, synthetic	Phthalic acid and derivatives
Hydroquinone and derivatives Structure-activity relationships Aerobic biodegradation, 89 Rate constants/retention time Polyethylene glycols, fatty ester Aerobic biodegradation, 431			Metabolic pathways, 117
D-11-1	Hydroquinone and derivatives		
153 89 Polyeinylene glycols, fatty ether	, i		Aerobic biodegradation, 431
	153	89	r oryemylene grycois, fatty ether

Mycobacterium sp (cont'd) Aerobic biodegradation, 431	Naphthalene and derivatives (cont'd) Kinetics and equilibrium studies	Neurospora sp acclimated (cont'd) Metabolic pathways, 249
Propylene glycols	101	Nickel
Structure-activity relationships	Structure-activity relationships	Activated sludge
153	101 Activated sludge, formaldehyde-	Inhibitory (toxic) effects, 178
Pyrocatechol and derivatives Metabolic pathways, 117	inactivated inactivated	437, 546 Activated sludge, industrial, continuous-
Structure-activity relationships	Freundlich adsorption isotherms	flow
153	101	Inhibitory (toxic) effects, 167
Resorcinol and derivatives	Kinetics and equilibrium studies	Activated sludge, industrial, porous-pot.
Structure-activity relationships	101	continuous-flow
153	Structure-activity relationships	Inhibitory (toxic) effects, 167
Sulfanilic acid and derivatives	101	Activated sludge, municipal, continuous-
Identification of microorganisms	Activated sludge, industrial and	flow
377	municipal	Freundlich adsorption isotherms
Xylenols and derivatives	Inhibitory (toxic) effects, 13	362
Model ecosystem, terrestrial, natural,	Respirometric studies, 13	Inhibitory (toxic) effects, 167
545	Structure-activity relationships	Kinetics and equilibrium studies
Mycoplana sp	13	362
DDT, Methoxychlor and metabolites	Activated sludge, municipal	Michaelis-Menten coefficients
Anaerobic biodegradation, 536	Aerobic and anaerobic digestion	362
Autoclaving effect, 536	reactors, 547	Operational parameters, 362
Disinfectants effect, 536	Inhibitory (toxic) effects, 369	Activated sludge, municipal, porous-pot,
Metabolic pathways, 536	Inhibitory (toxic) effects, screening,	continuous-flow
Lindane and metabolites	- 547	Inhibitory (toxic) effects, 167
Anaerobic biodegradation, 536	Structure-activity relationships	Activated sludge, non-acclimated
Polychlorobenzenes and derivatives	369	Inhibitory (toxic) effects, 343
Anaerobic biodegradation, 536	Activated sludge, OECD-specified	Lumbricillus sp
Polychlorocyclopentadiene dimers	Interlaboratory comparison, 590	Inhibitory (toxic) effects, 167
Anaerobic biodegradation, 536	Static vs continuous activation	Sewage, municipal
Myrothecium sp	method, 590	Inhibitory (toxic) effects, 345
Toilet paper, dyed	Activated sludge, synthetic	Sphaerotilus sp
Inhibitory (toxic) effects, 537	Aerobic biodegradation, 162	Inhibitory (toxic) effects, 437
Metabolic pathways, 537	Inhibitory (toxic) effects, 162	Zooglea sp
Pulp concentration effect, 537	Alcaligenes sp	Inhibitory (toxic) effects, 437
	Structure-activity relationships 523	Nicotinic acid
Naphthalene and derivatives	Cladosporium sp	Activated sludge
Activated sludge	Nutritional effects, enrichment	Structure-activity relationships
Depuration rate, effect on, 83	552	393
Freundlich adsorption isotherms	Flavobacterium sp	Nitrate
101	Metabolic pathways, 335	Activated sludge, industrial
Inhibitory (toxic) effects, 144	Gram-negative rods	Identification of microorganisms
178, 371, 534	Structure-activity relationships	163
Kinetics and equilibrium studies 101	523	Nitrification
Operational parameters, 83	Metabolic pathways	Coke oven wastes
Petrochemical wastewater treatment	Review, 325	Activated sludge, 243
324	Microbial population estuarine water	•
Respirometric studies, 534	Isolation of microorganisms, 407	Nitrifying bacteria, continuous-culture Annline and derivatives
River die-away test, 268	Metabolic pathways, 407	Inhibitory (toxic) effects, 241
Structure-activity relationships	Microbial population, fresh water	Nitrification, effects on, 241
101	sediments	Dyes
Activated sludge, acclimated	Time-course kinetics, 200	Inhibitory (toxic) effects, 241
Aerobic biodegradation, 584	Transformation rates, 200	Nitrification, effects on, 241
Aerobic biodegradation, pilot plant,	Oscillatoria sp	
57		Nitriles
Inhibitory (toxic) effects, 226	Pseudomonas sp	Activated sludge
Metabolic pathways, 584	Metabolic pathways, 177, 335	Aerobic biodegradation, 230 Nitrification, 422
Model ecosystem, aquatic, simulated,	Psychrophilic temperature effect	Activated sludge, acclimated
584	250 Time-course kinetics, 250	Identification of microorganisms
Activated sludge, acclimated,	Pseudomonas sp acclimated	578
continuous-flow	Metabolic pathways, 276	Arthrobacter sp
Operational parameters, 310	Selenastrum sp	Identification of microorganisms
Sludge acclimatization process	Inhibitory (toxic) effects, screening,	
310	547	Nitrification, 578
Activated sludge, boiling-inactivated	Neurospora sp acclimated	Nocardia sp
Freundlich adsorption isotherms	Polycyclic aromatic hydrocarbons	Nitrification, 559
101	i dijejene ardmade njarocardons	* ·

Nitriles, long chain	Nitrobenzene and derivatives (cont'd)	Panzaia and and demonitor
Microbial population, municipal wastes	Temperature effect, 587	Benzoic acid and derivatives Metabolic pathways, 179, 444
Inhibitory (toxic) effects, 311	Sewage, municipal	Biphenyl and derivatives
Nitrilotriacetic acid	Innibitory (toxic) effects, 183	Metabolic pathways, 354
see NTA and salts	Sewage, synthetic Chemical oxidation, 161	Carbamic acid and derivatives
Nitrobacter sp		Biological membrane filtration
Cadmium	Structure-activity relationships Review, 388	333
Inhibitory (toxic) effects, 124		Model ecosystem, aquatic, simulate
Chromium	Nitrosamine, dimethyl-	333
Inhibitory (toxic) effects, 124	Activated sludge	Cinnamic acid and derivatives
Polyvinyl alcohol	Aerobic biodegradation, 394	Metabolic pathways, 179, 444
Respirometric studies, 64	Anaerobic biodegradation, 394	Cirrasols
Textile wastes	River die-away test, 394	Aerobic biodegradation, 431
Respirometric studies, 64	Nitrosomas sp	Cycloaliphatics, substituted
	Aniline and derivatives	Metabolic pathways, 25, 444
Nitrobenzene and derivatives	Inhibitory (toxic) effects, 587	Gasoline
see also Explosives, organic	Cadmium	Metabolic pathways, 232
Activated sludge	Inhibitory (toxic) effects, 124	Hexachlorophene
Aerobic bioconversion, 204	Chromium	Metabolic pathways, 354
Aerobic biodegradation, 386	Inhibitory (toxic) effects, 124	Hydrocarbons
Anaerobic bioconversion, 204	Nitrobenzene and derivatives	Metabolic pathways, 232
Inhibitory (toxic) effects, 534	Inhibitory (toxic) effects, 587	
Inhibitory (toxic) effects, proteolytic,		Hydroquinone and derivatives
225	Polyvinyl alcohol	Metabolic pathways, 180, 444
Operational parameters, 591	Respirometric studies, 64	Nitriles
Oxidation ditch, 204	Pyridine and derivatives	Nitrification, 559
Petrochemical wastewater treatment	Inhibitory (toxic) effects, 587	Phenol and derivatives
324	Textile wastes	Metabolic pathways, 354
Respirometric studies, 534	Respirometric studies, 64	Phenylacetic acid and derivatives
Sludge adaptation process, 591	Nocardia sp	Metabolic pathways, 179, 444
Structure-activity relationships	Alcohols, primary aliphatic	Phthalic acid and derivatives
386	Identification of microorganisms	Identification of microorganisms
Activated sludge, acclimated	282	281, 282
Structure-activity relationships	Aldehydes	Polychlorinated biphenyls
390, 391	Metabolic pathways, 179	Aerobic biodegradation, 24
Time-course kinetics, 390, 391		Structure-activity relationships
Activated sludge, continuous-flow	Alkanes	24
Inhibitory (toxic) effects, 532	Inhibitory (toxic) effects, 450	Substrate concentration effect
Activated sludge + cornsteep.	Metabolic pathways, 232, 444	24
continuous-flow	Structure-activity relationships	Polychlorobenzenes and derivatives
Oxidation ditch, 204	450	Metabolic pathways, 354
Activated sludge, municipal	Alkanes, cyclic	Polyethylene glycols, fatty ester
Activated studge, municipal Aerobic biodegradation, 79	Metabolic pathways, 232, 444	Aerobic biodegradation, 431
	Alkanes, long chain, linear	Polyethylene glycols, fatty ether
Correlative test evaluations	Metabolic pathways, 25, 232	Aerobic biodegradation, 431
151	144	Pyrocatechol and derivatives
Distribution and rate accumulation	Alkanoic acids and derivatives	Identification of microorganisms
270	Metabolic pathways, 25, 179	282
Inhibitory (toxic) effects, 369	180, 444	Metabolic pathways, 179, 444
Structure-activity relationships	Alkanoic acids and derivatives,	Rubber, vulcanized, 87
369	polybasic	
Activated sludge, municipal, continuous-	. Metabolic pathways, 444	Salicylic acid and derivatives
flow	Alkanoic acids, cyclic	Metabolic pathways, 180, 444
Inhibitory (toxic) effects, 161	Metabolic pathways, 25	Toluene and derivatives
Substrate concentration effect	Alkenes	Metabolic pathways, 232, 444
161	Inhibitory (toxic) effects, 450	Vanillic acid and derivatives
Moraxella sp	Metabolic pathways, 232	Metabolic pathways, 179
Metabolic pathways, 477	Structure-activity relationships	Xylenes and derivatives
Nitrosomas sp	450	Metabolic pathways, 232
Inhibitory (toxic) effects, 587	Alkenoic acids and derivatives	Xylenols and derivatives
Pseudomonas sp	Metabolic pathways, 180, 444	Metabolic pathways, 444
Time-course kinetics, 183	Amino acids and derivatives	NTA and salts
Sewage, acclimated, municipal	Metabolic pathways, 179	see also Alkanoic acids and derivatives
Petrochemical wastewater treatment	Arsenic compounds, inorganic	Activated sludge
51	Operational parameters, 464	Aerobic biodegradation, 174
	Arsenic compounds, organic	Anaerobic digestion reactor, 263
Sewage, frozen, acclimated Operational parameters, 587	Operational parameters, 464	340
	Benzene and derivatives	Heavy metals effect, 174
Substrate concentration effect	Metabolic pathways 232 1.14	Activated sludge, acclimated
507	Metabolic pathways 232 144	Activated sludge, acclimated

NIA and saits (cont d)	Oil remery wastes (cont d)	PCS
Aerobic biodegradation, 463	Nitrification, 150	see Polychlorinated biphenyls
Time-course kinetics, 463	Respirometric studies, 535	Penicillium sp
Activated sludge, municipal	Enterobacter sp. 40	Polycaprolactone
Aerobic biodegradation, 411	Flavobacterium-cytophaga sp. 40	Microbial population, soils, 126
462. 563	Gram-negative rods, 40	Polyesters
Detergent formulation effect	Gram-positive cocci, 40	Microbial population, soils, 126
462	Pseudomonas sp. 40	Penicillium sp
Diurnal variations, 462	Vibrio sp. 40	
Heavy metals effect, 563	,	Alkanoic acids and derivatives.
Aerobic biodegradation	Onion processing wastes	polybasic
Review, 558	Activated sludge, acclimated.	Metabolic pathways, 192
Anaerobic biodegradation	continuous-flow	Alkenoic acids and derivatives
	Aerobic biodegradation, 112	Metabolic pathways, 192, 468
Review, 558	Activated sludge, accilmated, sedimenta-	Carbamic acid and derivatives
Gram-negative rods	tion champer	Biological membrane filtration
Anaerobic biodegradation, 114	Aerobic biodegradation, 112	333
115	Opercularia sp	Model ecosystem, aquatic, simulated
Metabolic pathways	Chromium	333
Review, 558	Inhibitory (toxic) effects, 486	Herbicides, monuron type and
Microbial population	The state of the s	
Screening tests, 415	Copper	metabolites
Microbial population, acclimated	Inhibitory (toxic) effects, 486	Metabolic pathways, 216
Aerobic biodegradation, 549	Organo-metallic compounds	Herbicides, propanil type and
Heavy metals effect, 549	Biodegradation, environmental aspects	metabolites
Water hardness effect, 549	Review, 239	Metabolic pathways, 216
	Oscillatoria sp	Phenol-formaldehyde resin
Microbial population, non-acclimated,		Biodegradation, rates compared
soils	Naphthalene and derivatives	248
Aerobic biodegradation, 511	Metabolic pathways, 70	Phthalic acid and derivatives
Metabolic pathways, 511	Tetralin and derivatives	Metabolic pathways, 116, 117
Microbial population, NTA-acclimated.	Metabolic pathways, 70	Structure-activity relationships
soils	Ozone, stirred-tank reactor, continuous-	116
Aerobic biodegradation, 511	flow	Poly(alkyl-β-propiolactones)
Metabolic pathways, 511	Alcohols, primary aliphatic	Structure-activity relationships
Microbial population, septic tank	Operational parameters, 580	10
Aerobic percolation, 263	Ozonization, 580	
Anaerobic digestion reactor, 263	Alkyl halides	Poly(methyl methacrylate)
Microbial population, soils	Operational parameters, 580	Biodegradation, rates compared
Metabolic pathways, 127	Ozonization, 580	248
Pseudomonas sp	Styrene and derivatives	Polyamides, 217
Metabolic pathways, 127		Polystyrenes
Pseudomonas sp mutant	Operational parameters, 580	Biodegradation, rates compared
•	Ozonization 580	248
Metabolic pathways, 300	Toluene diisocyanate wastes	Metabolic pathways, 192, 468
Sewage, municipal, oxidation pond	Operational parameters, 580	Polyureas, 217
system	Ozonization, 580	Pyrocatechol and derivatives
Model ecosystem, aquatic, pond	Paecilomyces sp	Metabolic pathways, 117
system, 263	Phenol-formaldehyde resin	Starch and derivatives
Nylons	Biodegradation, rates compared	Tensile strength, 96
Microbial population, soils	248	Vanillic acid and derivatives
Aerobic vs anaerobic conditions	Poly(methyl methacrylate)	Metabolic pathways, 192, 468
119	Biodegradation, rates compared	• • •
Structure-activity relationships	248	Peniophora sp
119		Phenoi-formaldehyde resin
	Polystyrenes	Biodegradation, rates compared
Octopine	Biodegradation, rates compared	248
Pseudomonas sp	248	Poly(methyl methacrylate)
Isolation of enzymes, 395	Paracolobactrum sp	Biodegradation, rates compared
Odontia sp	Cresols and derivatives	248
Polyethylene	Model ecosystem, terrestrial, natural,	Polyethylene
Isolation of microorganisms, 3	545	Isolation of microorganisms, 3
Metabolic pathways, 3	Phenol and derivatives	Metabolic pathways, 3
• •	Model ecosystem, terrestrial, natural,	
Oil refinery wastes	545	Biodegradation, rates compared
see also Petrochemical wastes	Xylenols and derivatives	248
Achromobacter-alcaligenes sp. 40	Ayienois and derivatives	
Activated sludge	Model ecosystem, terrestrial, natural,	
Aerobic biodegradation, 108	545	see also Alkyl halides; Carbamic acid
Biodegradation, design relationship	s., Paramecium sp	and derivatives: DDT, Methox-
108	Explosives, organic	ychlor and metabolites; Hex-
Inhibitory (toxic) effects, 150	Inhibitory (toxic) effects, 7	achlorophene; Lindane and
		• • • •

Pesticides (cont'd)	Petrochemical wastewater treatment	Petrochemical wastewater treatment
metabolites; Phosphorodithioic	(cont'd)	(cont'd)
acid and derivatives;	Amides, aliphatic	Xylenols and derivatives
Phosphorothioic acid and derivatives; Polychlorobenzenes	Sewage, acclimated, municipal, 51 Amines, aliphatic	Sewage, acclimated, municipal
and derivatives;	Sewage, acclimated, municipal	51
Polychlorocyclopentadiene	51	Petrochemicals, industrial
dimers	Aniline and derivatives	Sewage, acclimated, municipal Nitrification-preventive, 51
Activated sludge, acclimated	Activated sludge, 324	Petrochemical wastewater treatment
Inhibitory (toxic) effects, 226	Benzene and derivatives	51
Metabolic pathways	Sewage, acclimated, municipal	Petroleum
Review. 260, 326	51 Benzenesulfonic acid and non-alkyl	Acinetobacter sp
Petrochemical wastes see also Oil refinery wastes	substituted derivatives	Metabolic pathways, 553
Achromobacter-alcaligenes sp. 40	Activated sludge, 324	Bacıllus sp
Activated sludge, 341	Benzoic acid and derivatives	Metabolic pathways, 553
Operational parameters, 540	Sewage, acclimated, municipal	Bacterium sp
591	51	Mesophilic temperature effect 342
Sludge adaptation process, 540	Cellulose and derivatives	pH effect, 342
591	Activated sludge, 324	Coryneform bacteria
Activated sludge, UNOX pure oxygen	Epoxides Activated sludge, 324	Metabolic pathways, 553
technology Overview, 187	Sewage, acclimated, municipal	Cryptococcus sp
Scheme of test facility, 187	51	Metabolic pathways, 553
Enterobacter sp. 40	Ethers	Microbial population, fresh water
Flavobacterium-cytophaga sp. 40	Sewage, acclimated, municipal	Metabolic pathways, 553
Gram-negative rods, 40	51	Microbial population, fresh water sedi- ment
Gram-positive cocci, 40	Ketones, aliphatic	Time-course kinetics, 551
Pseudomonas sp. 40	Sewage, acclimated, municipal	Mycobacterium sp
Vibrio sp., 40	51	Mesophilic temperature effect
Petrochemical wastewater treatment	Naphthalene and derivatives Activated sludge, 324	342
Alcohols, primary aliphatic	Nitrobenzene and derivatives	pH effect, 342
Activated sludge, 324	Activated sludge, 324	Pseudomonas sp
Sewage, acclimated, municipal 51	Sewage, acclimated, municipal	Mesophilic temperature effect
Alcohols, secondary aliphatic	51	342
Activated sludge, 324	Petrochemicals, industrial	Metabolic pathways, 553 pH effect, 342
Sewage, acclimated, municipal	Sewage, acclimated, municipal	Vibrio sp
51	51	Metabolic pathways, 550
Alcohols, tertiary aliphatic	Phenol and derivatives Sewage, acclimated, municipal	Petroleum sulfonates
- Sewage, acclimated, municipal	51	see also Alkyl sulfonates
51 Aldehydes	Phthalic acid and derivatives	Microbial population, soils
Sewage, acclimated, municipal	Activated sludge, 324	Operational parameters, 171
51	Polyethylene glycols	Phellinus sp
Alkanes, cyclic	Activated sludge, 324	Phenol-formaldehyde resin
Sewage, acclimated, municipal	Polyvinyl alcohol	Biodegradation, rates compared 248
51	Activated sludge, 324 Propylene glycols	Poly(methyl methacrylate)
Alkanoic acids and derivatives	Sewage, acclimated, municipal	Biodegradation, rates compared
Sewage, acclimated, municipal 51	51	248
Alkanoic acids and derivatives.	Quaternary ammonium compounds	Polystyrenes
polybasic	Sewage, acclimated, municipal	Biodegradation, rates compared
Activated sludge, 324	51	. 248
Sewage, acclimated, municipal	Silicones	Phenol and derivatives
51	Activated sludge, 324 Styrene and derivatives	Achromobacter sp
Alkenes Sewage, acclimated, municipal	Sewage, acclimated, municipal	Identification of microorganisms 71
51	51	Metabolic pathways, 67
Alkenoic acids and derivatives	Toluene and derivatives	Model ecosystem, aquatic, simulated,
Activated sludge, 324	Activated sludge, 324	378
Alkyl halides	Sewage, acclimated, municipal	Model ecosystem, terrestrial, natural,
Activated sludge, 324	51	545
Sewage, acclimated, municipal	Urea and derivatives Sewage, acclimated, municipal	Acinetopacter sp
51 Alkyl sulfoxides	51	Metabolic pathways, 354
Sewage, acclimated, municipal	Xylenes and derivatives	Activated sludge Aerobic biodegradation, 5, 386
51	Sewage, acclimated, municipal, 51	Anaerobic digestion reactor, 196

identification of missessessions	Sludge applymentations (cont'd)	Phenoi and derivatives (cont'd)
Identification of microorganisms 295	Sludge acclimatization process	Biorefractory index, 189, 199
	Aeromonas sp	Inhibitory (toxic) and stimulatory effects, 170
Inhibitory (toxic) effects, 144	Identification of managers	Inhibitory (taura) -66 (1
178, 231, 309, 354, 429	Identification of microorganisms 71	Inhibitory (toxic) effects, 61
480	Alcaligenes sp	Microbial acclimatization, 170
Metabolic pathways, 143	Alcangenes sp	Recommendations, wastewater treat
Michaelis-Menten coefficients	Identification of microorganisms	ment, 189
429		Reduced BOD, 61
Nitrification effect, 480	Metabolic pathways, 37	Microbial population, soils
Operational parameters, 315	Arthrobacter sp	Denitrification, 14
Respirometric studies, 30	Identification of microorganisms	Metabolic pathways, 14
Sludge acclimatization process	295	Microbial population + synthetic
295	Inhibitory (toxic) effects, 84	sewage
Structure-activity relationships	Isolation of enzymes, 84	Time-course kinetics, 384
386	Metabolic pathways, 84	Micrococcus sp. 294
Time-course kinetics, 316	Model ecosystem, terrestrial, natural,	Model ecosystem, terrestrial, natural
Activated sludge, acclimated	545	545
Aerobic biodegradation, 5, 185	Sludge acclimatization process	Mycobacterium sp
Aerobic biodegradation, pilot plant,	295	Model ecosystem, terrestrial, natural
57	Azotobacter sp	545
Isolation of microorganisms, 497	Model ecosystem, terrestrial, natural,	Nocardia sp
Structure-activity relationships	545	Metabolic pathways, 354
389	Bacillus sp	Paracolobactrum sp
Time-course kinetics, 389	 Batch vs continuous-flow system 	Model ecosystem, terrestrial, natural
Activated sludge, acclimated,	401	545
continuous-flow	Identification of microorganisms	Phenol-degrading bacteria
Aerobic digestion reactor, 60	205, 206	Metabolic pathways, 155
Inhibitory (toxic) effects, 122	Model ecosystem, terrestrial, natural,	Plasmid
364	545	Genetic transfer, 576
Sludge acclimatization process	Substrate concentration effect	Proteus sp
364	401	Identification of microorganisms
Activated sludge, acclimated, industrial	Temperature effect, 401	205, 206
Aerobic biodegradation, 433	Bacterium sp. 294	Pseudomonas sp. 294
Batch vs continuous-flow system	Brevibacterium sp	Batch vs continuous-flow system
433	Model ecosystem, terrestrial, natural,	579
Sludge acclimatization process, 94	545 ,	Identification of microorganisms
Activated sludge and soils, acclimated	Citrobacter sp	71, 205, 206, 295
Aerobic biodegradation, 60	Identification of microorganisms	Inhibitory (toxic) effects, 309
Activated sludge, diverse substrates	205, 206	Metabolic pathways, 354, 576
Batch vs continuous-flow system	Cladosporium sp	579
71	Nutritional effects, enrichment	Model ecosystem, aquatic, simulated
Substrate concentration effect	552	378
71	Corynebacterium sp	Model ecosystem, terrestrial, natural,
Time-course kinetics, 71	Operational parameters, 374	545
Activated sludge, industrial	Trickling filters, 374	pH effect, 74
Aerobic biodegradation, 95	Escherichia sp	Sludge acclimatization process, 295
Bioreactors compared, 206	Identification of microorganisms	Substrate concentration effect
Conversion and retention time	205, 206	_ 74, 579
kinetics, 206	Flavobacterium sp	Temperature effect, 74
Identification of microorganisms	Identification of microorganisms	Time-course kinetics, 183, 579
205. 206	71	Sarcina sp. 294
Activated sludge, industrial, continuous-	Model ecosystem, terrestrial, natural,	Model ecosystem, terrestrial, natural,
flow	545	Samaga and in and it is
Metabolic pathways, 569	Metabolic pathways	Sewage, acclimated, municipal
Activated sludge, multi-stage column	Review, 88	Petrochemical wastewater treatment
Substrate concentration effect	Microbial population, acclimated	Sewage, synthetic
209	Anaerobic fermentation,	Inhibitory (toxic) and stimulatory ef-
Activated sludge, municipal	methanogenic, 195	fects, 170
Aerobic biodegradation, 79	Microbial population, isopropanol-	Microbial acclimatization, 170
Activated sludge, primary and secondary	- · · · C*	Staphylococcus sp
Aerobic biodegradation, 472	Metabolic pathways, 569	Identification of microorganisms
Activated sludge + synthetic sewage	Microbial population, lagoons	205, 206
Correlative test evaluations	Isolation of microorganisms, 481	Structure-activity relationships
233	Model ecosystem, aquatic, simulated,	Review, 388
	481	Trichosporon sp
Aerobacter sp	Percolation system, 481	Batch vs continuous-flow system
Identification of microorganisms	Microbial population, sewage, municipal	570

Phosphoric acid plasticizers (cont'd) Phenol and derivatives (cont'd) Phenol pitch Activated sludge Microbial population, river water Metabolic pathways, 579 Time-course kinetics, 579 Inhibitory (toxic) effects, 49 Octanol-water partition coefficients. Trickling filters, pilot plant 434 Phenylacetic acid and derivatives Aerobic biodegradation, 74 see also Alkanoic acids and derivatives Phosphorodithioic acid and derivatives Vibrio sp see ulso Pesticides Arthrobacter sp Identification of microorganisms, 71 Activated sludge, 414 Inhibitory (toxic) effects, 84 Phenoi-degrading bacteria Clostridium sp Isolation of enzymes, 84 Phenol and derivatives Anaerobic biodegradation, 465 Metaoolic pathways, 84 Metabolic pathways, 155 Hydrogen sulfide production, 465 Fusarium sp Phenol-formaldehyde resin Aerobic biodegradation, 130 Lagoons, anaerobic, saline Anaerobic biodegradation, 465 Activated sludge Hydrogenomonas sp Aerobic biodegradation, 130 Microbial population, fecal isolates Hydrogen sulfide production, 465 Biodegradation, rates compared Isolation of microorganisms, 465 248 Soil systems, flooded and non-flooded Metabolic pathways, 575 Activated sludge + cellulose and salts Model ecosystem, terrestrial, Biodegradation, rates compared Microbial population, fresh water Aerobic biodegradation, 46 simulated, 404 248 Anaerobic biodegradation, 46 Phosphorothioic acid and derivatives Activated sludge, primary and secondary Aerobic biodegradation, 472 Microbial population, loam see also Pesticides Activated sludge, 190 Structure-activity relationships Aspergillus sp Microbial population, acclimated Biodegradation, rates compared 485 Nocardia sp Aerobic biodegradation, 351 248 Microbial population, fresh water Metabolic pathways, 179, 444 Aureobasidium sp Biodegradation, rates compared Pseuaomonas sp Aerobic biodegradation, 46 Anaerobic biodegradation, 46 Metabolic pathways, 137 248 Microbial population, septic tank Trametes sp Bierkandera so Inhibitory (toxic) effects, 6 Biodegradation, rates compared Metabolic pathways, 137 248 Phosphorus Phenylureas Corrolus sp Activated sludge see Herbicides, monuron type and Biodegradation, rates compared Review, 113, 412 metabolites 248 Luxury phosphorus uptake Phenylurethans Daedalea sp Review, 113, 412 see Herbicides, chlorpropham type Biodegradation, rates compared Photographic and municipal wastes, syn-Phialophora sp 248 thetic Pulp and paper wastes Fomes sp Activated sludge Foam process, 594 Biodegradation, rates compared Aerobic biodegradation, 89 Sulfite liquor 248 Rate constants/retention time Foam process, 594 Gleophyllum sp Phloroglucinol Biodegradation, rates compared Substrate concentration effect Activated sludge, acclimated Structure-activity relationships Microbial population, silt loam Photoprocess wastes 389 Biodegradation, rates compared Activated sludge Time-course kinetics, 389 248 Aerobic biodegradation, 89 Activated sludge, municipal Microbial population, soils Rate constants/retention time Anaerobic digestion reactor, 15 Biodegradation, rates compared Fermentation, methanogenic, 15 Respirometric studies, 30 Microbial population, soils + cellulose Methanobacterium sp Substrate concentration effect Anaerobic digestion reactor, 15 Fermentation, methanogenic, 15 and salts Biodegradation, rates compared Activated sludge, acclimated 248 Phorate inhibitory activity Inhibitory (toxic) effects, 21 Paecilomyces sp Herbicides, chlorpropham type Respirometric studies, 21 Biodegradation, rates compared Achromobacter sp. 257 Pseudomonas sp. 257 Activated sludge, non-acclimated 248 Inhibitory (toxic) effects, 21 Penicillium sp Phosphonic acid derivatives, alkyl Respirometric studies, 21 Biodegradation, rates compared Pseudomonas sp Activated sludge, sewage plant 248 Metabolic pathways, 65, 91 Inhibitory (toxic) effects, 506 Operational parameters, 506 Peniophora sp Phosphonic acid derivatives, alkyl poly-Biodegradation, rates compared Respirometric studies, 506 Activated sludge 248 Aerobic biodegradation, 219 Inhibitory (toxic) wastes Phellinus sp Inhibitory (toxic) effects, 219 Review, 541 Biodegradation, rates compared Phthalic acid and derivatives Phosphoric acid plasticizers 248 Activated sludge, 341 Activated sludge Porta sp Aerobic biodegradation, 386 Octanol-water partition coefficients, Biodegradation, rates compared 434 398, 447 248 Anaerobic biodegradation, 267 Microbial population, acclimated Trichoderma sp Identification of microorganisms 266, 267, 281, 282 Octanol-water partition coefficients. Biodegradation, rates compared 248

hthalic acid and derivatives (cont'd)	Pimaric acid and derivatives	Poly(a-nydroxyacrytic acid) (cont'd)
Octanol-water partition coefficients,	Activated sludge	Time-course kinetics, 350
531	Aerobic biodegradation, 289	Sewage, municipal
Petrochemical wastewater treatment	Detoxification, 349	Mineralization, 350
324	Lagoons, aerated, industrial site	Time-course kinetics, 350
Rate constants/retention time	349	Poly(methyl methacrylate)
531	Structure-activity relationships	Activated sludge
Structure-activity relationships	289	Biodegradation, rates compared
386	Lagoons, aerated, industrial site	248
Activated sludge, acclimated, 436	Aerobic biodegradation, 215	Activated sludge + cellulose and salts
Aerobic biodegradation, 397	Detoxification, 215	Biodegradation, rates compared
Activated sludge, Nocardia-inoculated		248
Identification of microorganisms	Plasmid	
	Phenol and derivatives	Aspergillus sp
281, 282	Genetic transfer, 576	Biodegradation, rates compared
Arthrobacter sp	Plurafac RA40	248
Metabolic pathways, 117	Activated sludge, non-acclimated,	Aureobasidium sp
Bacıllus sp	municipal	Biodegradation, rates compared
Identification of microorganisms	Aerobic biodegradation, 18	248
282	Trickling filters, 18	Bjerkandera sp
Bacıllus sp, aerobic	<u>-</u>	Biodegradation, rates compared
Inhibitory (toxic) effects, chloram-	Pluronics	248
phenicol inhibition, 2	Activated sludge, non-acclimated,	Cortolus sp
Metabolic pathways, 2	municipal	Biodegradation, rates compared
Bacillus sp., anaerobic	Aerobic biodegradation, 18	248
Inhibitory (toxic) effects, chloram-	_ Trickling filters, 18	Daedalea sp
phenicol inhibition, 2	Microbial population, acclimated, river	Biodegradation, rates compared
Metabolic pathways, 2	water	248
Brevibacterium sp	Aerobic biodegradation, 382	Fomes sp
Metabolic pathways, 117	Microbial population, municipal wastes	Biodegradation, rates compared
Corvnebacterium sp	Evolution of bacterial populations	248
· y · · · - · · · ·	16	Gleophyllum sp
Metabolic pathways, 117	Microbial population, river water	Biodegradation, rates compared
Metabolic pathways	Evolution of bacterial populations	
Review. 259	16	248
Microbial population, fresh water	Poly(alkyl-β-propiolactones)	Microbial population, silt loam
hydrosoil	Alcaligenes sp	Biodegradation, rates compared
Aerobic biodegradation, 242		248
Anaerobic biodegradation, 242	Structure-activity relationships	Microbial population, soils
Microbial population, municipal wastes	503	Biodegradation, rates compared
Acclimatization, selective mutation,	Aspergillus sp	248
538	Structure-activity relationships	Microbial population, soils + cellulose
Microbial population, river water, 194,	10	and salts
436	Aureobasidium sp	Biodegradation, rates compared
Microbial population, sea water, 194	Structure-activity relationships	248
Micrococcus sp	10	Paecilomyces sp
Metabolic pathways, 107	Fungus, Pl	Biodegradation, rates compared
Mycobacterium sp	Structure-activity relationships	248
Metabolic pathways, 117	503	Penicillium sp
Nocardia sp	Penicillium sp	Biodegradation, rates compared
Identification of microorganisms	Structure-activity relationships	248
281, 282	10	Peniophora sp
Penicillium sp	Poly(ethylene glycol-propylene glycol)	Biodegradation, rates compared
Metabolic pathways, 116, 117	Microbial population, acclimated, river	248
Structure-activity relationships	water	Phellinus sp
116	Aerobic biodegradation, 382	Biodegradation, rates compared
	Microbial population, river water	248
Pseudomonas sp	· · · · · · · · · · · · · · · ·	Porta sp
Identification of microorganisms		Biodegradation, rates compared
282	Poly(ethylene oxide-propylene)	248
Metabolic pathways, 8, 117	Activated sludge, municipal	Trichoderma sp
Pseudomonas sp. revertant	Correlative test evaluations	Biodegradation, rates compared
Metabolic pathways, 359	151	
Pseudomonas sp, wild type	Poly(a-hydroxyacrylic acid)	248
Metabolic pathways, 359	see also Alkanoic acids and derivatives	Poly(vinylpyrrolidone)
	Activated sludge	Microbial population, fresh water sedi
Phytane	Coupled units test, 129	ment
Microbial population, soils	Activated sludge, acclimated, municipal,	Ozonization effects, 488
Hypersaline environment, 557	continuous-flow	
Inhibitory (toxic) effects, hyper-	Time-course kinetics, 350	
salinety, 557	Activated sludge, non-acclimated,	
	Activated studge, non-accimated, municipal, continuous-flow	
	municipal, continuous-now	

Polyacrylamides	Polycaprolactorie (cont d)	Polychiormated ofphenyls (cont d)
see also Amides, aliphatic	Microbial population, fresh water sedi-	Pseudomonas sp
Activated sludge	ment	Aerobic biodegradation, 24
Time-course kinetics, 193	Operational parameters, 32	Structure-activity relationships
Microbial population, fresh water sedi-	Microbial population, soil burial	24
ment	Structure-activity relationships	Substrate concentration effect
Ozonization effects, 488	97	24
Ozonization effects, 400	Microbial population, soils	_ -
Microbial population, soils	Aerobic vs anaerobic conditions	Polychlorinated terphenyls
Operational parameters, 171		Activated studge
Polyacrylic acid	119	Substrate concentration effect
see also Alkanoic acids and derivatives	Structure-activity relationships	271
Microbial population	119	271
Metabolic pathways, 27	Penicillium sp	Polychlorobenzenes and derivatives
Microbial population, fresh water sedi-	Microbial population, soils, 126	see also Pesticides
	Pseudomonas sp	Acinetobacter sp
ment	Microbial population, soils, 126	Metabolic pathways, 354
Ozonization effects, 488	Trichosporon sp	Activated sludge
Polyacrylonitrile		Aerobic biodegradation, 128
Activated sludge	Operational parameters, 32	
Aerobic biodegradation, 29	Polychlorinated biphenyls	Inhibitory (toxic) effects, 53
Inhibitory (toxic) effects, 28	Acinetobacter sp	128, 144, 354
Operational parameters. 28	Aerobic biodegradation, 138	Activated sludge, acclimated
	Structure-activity relationships	Aerobic biodegradation, 397
Polyadipate plasticizers	138	Activated sludge, acclimated,
Alternaria sp	Activated sludge	continuous-flow
Isolation of products, 524	- Aerobic biodegradation, 337	Inhibitory (toxic) effects, 122
Polyamides	Inhibitory (toxic) effects, 144	Activated sludge, industrial
see also Amides, aliphatic, Nylons	Substrate concentration effect	Aerobic biodegradation, 470
	271	2
Alcaligenes sp		Photodegradation, 470
Structure-activity relationships	Activated sludge, acclimated, municipal	River die-away test, 470
12	Aerobic biodegradation, 526	Volatilization, 470
Aspergillus sp., 217	Activated sludge, municipal	Activated sludge, municipal
Structure-activity relationships	Aerobic biodegradation, 201	Batch vs continuous-flow system
12	528	461
Flavobacterium sp	Distribution and rate accumulation	Biomass vield, effect on, 461
Structure-activity relationships	270	Distribution and rate accumulation
12	Metabolic pathways, 528	270
Microbial population, soils	Structure-activity relationships	Inhibitory (toxic) effects. 478
Aerobic vs anaerobic conditions	201. 528	
	=	Operational parameters, 461
119	Activated sludge + synthetic sewage	478
Structure-activity relationships	Aerobic biodegradation, 247	Activated sludge + synthetic sewage
119	Anaerobic biodegradation, 247	Aerobic biodegradation, 52
Penicillium sp., 217	Inhibitory (toxic) effects, 247	Alcaligenes sp
Polybutadienes	Alcaligenes sp	Inhibition of benzoic acid turnover,
see also Alkenes	Aerobic biodegradation, 138	410
Acinetobacter sp	Structure-activity relationships	Structure-activity relationships
Metabolic pathways, 522	138	410
Structure-activity relationships	Bacillus sp	Bacillus sp
522	Isolation of microorganisms, 366	
		Anaerobic biodegradation, 536
Polycaprolactone	Cunninghamella sp	Candida sp
Alcaligenes sp	Aerobic biodegradation, 528	Anaerobic biodegradation, 536
Structure-activity relationships	Metabolic pathways, 528	Citrobacter sp
503	Structure-activity relationships	Anaerobic biodegradation, 536
Aspergiilus sp	528	Escherichia sp
Structure-activity relationships	Microbial population, fresh water	Anaerobic biodegradation, 536
97	Equilibrium partitioning, 467	Hydrogenomonas sp
Aureobasidium sp	Microbial population, raw sewage	Anaerobic biodegradation, 536
Microbial population, soils, 126	Aerobic biodegradation, 26	Microbial population, acclimated,
Coryneform bacteria	Microbial population, sewage, municipal	
Operational parameters, 32	Biorefractory index, 199	Metabolic pathways, 98
Cryptococcus sp	Microbial population, soils	Nutritional effects, 98
Operational parameters, 32		
	Aerobic biodegradation, 527	Microbial population, acclimated, soils
Fungus, Pl	Structure-activity relationships	Aerobic biodegradation, 262
Structure-activity relationships	527	Microbial population, liquid-enriched
503	Vocardia sp	Metabolic pathways, 322
Microbial population, enrichment	Aerobic biodegradation, 24	Microbial population, raw sewage
cultures	Structure-activity relationships	
Inhibitory (toxic) effects, 320	24	Aerobic biodegradation, 26
Isolation of microorganisms, 320	Substrate concentration effect	Inhibitory (toxic) effects, 26
Nutritional effects, 320	24	Microbial population, sewage, municipa

Polychlorobenzenes and derivatives (cont'd)	Polycyclic aromatic hydrocarbons (cont'd)	Polyethylene (cont'd)
Biological inhibition value, 199	Microbial population	Peniophora sp
Biorefractory index, 199	Model ecosystem, aquatic, simulated,	Isolation of microorganisms, 3
Inhibitory (toxic) effects, 199	466	Metabolic pathways, 3 Verticillium sp
Reduced BOD, 61	Microbial population, fresh water	Isolation of microorganisms, 4
Microbial population, soil-liquid Metabolic pathways, 322	Aerobic biodegradation, 46	Polyethylene glycols
Micropial population, sons	Anaerobic biodegradation, 46	Acinetobacter sp
Metabolic pathways, 322	Microbial population, fresh water	Identification of microorganisms
Mycoplana sp	sediments	560
Anaerobic biodegradation, 536	Time-course kinetics, 200 Transformation rates, 200	Metabolic pathways, 244
Nocardia sp	Neurospora sp acclimated	Respirometric studies, 560
Metabolic pathways, 354	Metabolic pathways, 249	Activated sludge, 341
Pseudomonas sp	Pseudomonas sp	Aerobic biodegradation, 58, 386
Anaerobic biodegradation, 536	Metabolic pathways, 335	Assay development, 592
Inhibition of benzoic acid turnover,	Polyesters	Operational parameters, 591 592
Inhibitory (toxic) effects, 53	Activated sludge, municipal	Petrochemical wastewater treatment
Metabolic pathways, 354	Isolate, grain processing wastes	324
Structure-activity relationships	554	River die-away test, 58
410	Alcaligenes sp	Sludge adaptation process, 591
Trickling filters, pilot plant	Structure-activity relationships	Structure-activity relationships
Aerobic biodegradation, 74	503	386
Polychlorocyclopentadiene dimers	Aspergullus sp	Flavobacterium sp
see also Pesticides	- Structure-activity relationships	Identification of microorganisms
Activated sludge	97	560
Aerobic biodegradation, 9	Aureobasidium sp	Respirometric studies, 560
Anaerobic biodegradation, 9	Microbial population, soils, 126 Fungus, Pl	Microbial population
Activated sludge, municipal	Structure-activity relationships	Metabolic pathways, 27
Distribution and rate accumulation	503	Microbial population, fresh water sedi- ment
270 Bacıllus sp	Microbial population, soil burial	Ozonization effects, 488
Anaerobic biodegradation, 536	Structure-activity relationships	Microbial population, glycol-
Candida sp	97	metabolizing
Anaerobic biodegradation, 536	Penicillium sp	Metabolic pathways, 80
Citrobacter sp.	Microbial population, soils, 126	Review, 80
Anaerobic biodegradation, 536	Pseudomonas sp	Microbial population, municipal wastes
Escherichia sp	Microbial population, soils, 126	Biomass yield, effect on, 81
- Anaerobic biodegradation, 536	Polyethylene Acremonium sp	Pseudomonas sp
Hydrogenomonas sp	Isolation of microorganisms, 4	Identification of microorganisms 560
Anaerobic biodegradation, 536	Activated sludge, municipal	Metabolic pathways, 182
Microbial population, fresh water	Biodegradation, rates compared	Respirometric studies, 560
Anaerobic biodegradation, 46 Mycoplana sp	245	Sewage, acclimated, municipal
Anaerobic biodegradation, 536	Aspergillus sp	Biomass yield, effect on, 81
Pseudomonas sp	Isolation of microorganisms, 4	Sewage, municipal
Anaerobic biodegradation, 536	Structure-activity relationships	Identification of microorganisms
Rhizobidia sp	97	560
Aerobic biodegradation, 246	Fomes sp Isolation of microorganisms, 3	Respirometric studies, 560
Polycyclic aromatic hydrocarbons	Metabolic pathways, 3	Polyethylene glycols, alkylphenoxy- see also Surfactants, nonionic
Activated sludge, 121, 443	Fusarium sp	Activated sludge
Activated sludge, acclimated Aerobic biodegradation, 185	Isolation of microorganisms, 3	Coupled units test, 129
Activated sludge, OECD-specified	· 4	Activated sludge, continuous-flow
Interlaboratory comparison, 590	Metabolic pathways, 3	Aerobic biodegradation, 283
Static vs continuous activation	Microbial population, soil burial	Activated sludge, municipal
method, 590	Structure-activity relationships	Aerobic biodegradation, 421
Beijerinckia sp., mutant	97 Microbial population, soils	Sludge acclimatization process
Metabolic pathways, 154	Biodegradation, rates compared	421 Activated sludge + synthetic sewage
Beijerinckia sp., wild type	245	Correlative test evaluations
Metabolic pathways, 154	Isolation of microorganisms, 3	233
Cladosporium sp Nutritional effects, enrichment	4	Inhibitory (toxic) effects
Nutritional effects, enrichment 552	Metabolic pathways, 3	Review, 321, 451, 452
Cunninghamella sp	Odontia sp	Metabolic pathways
Metabolic pathways, 69, 100	Isolation of microorganisms, 3	Review, 321, 451, 452
Flavobacterium sp	Metabolic pathways, 3	Microbial population, acclimated
Merchalia nathways 225		Biotower studies, 92

Isolation of microorganisms, 92	Activated sludge, acclimated	Polyethylene glycols, fatty ether, sulfate
Microbial population, river water	Inhibitory (toxic) effects, 432	(cont'd)
Operational parameters, 99	Activated sludge, continuous-flow	River die-away test, 458
River die-away test, 284, 424	Aerobic biodegradation, 283	Polymers
Structure-activity relationships	Model ecosystem, aquatic, natural	Activated sludge
428	516	Endoacting extracellular enzymes
Structure-activity relationships	Activated sludge, municipal	331
Review, 321, 451	Aerobic biodegradation, 421	Exoacting extracellular enzymes
Polyethylene glycols, etc.	Sludge acclimatization process	331
see also Alcohols	421	Activated sludge, acclimated, continuous-flow
	Activated sludge, non-acclimated	Operational parameters, 310
Polyethylene glycols, fatty amine	Inhibitory (toxic) effects, 432	Sludge acclimatization process
Microbial population, municipal wastes Inhibitory (toxic) effects, 311	Activated sludge, non-acclimated,	310
	municipal	Structure-activity relationships
Polyethylene glycols, fatty ester	Aerobic biodegradation, 18	Review, 218
Achromobacter sp	Trickling filters, 18	Polymers, bio-
Aerobic biodegradation, 431	Activated sludge, OECD-specified	Activated sludge, non-acclimated,
Activated sludge Depuration rate, effect on. 83	Interiaboratory comparison, 590	municipal
Inhibitory (toxic) effects, 430	Static vs continuous activation	Gravimetric assessment, 420
Operational parameters, 83	method, 590	Hach oxidation, 420
Activated sludge, acclimated	Activated sludge, semi-continuous flow,	Respirometric studies, 420
Inhibitory (toxic) effects, 432	286	Flavobacterium sp
Activated sludge, non-acclimated	Activated sludge + synthetic sewage	pH effect, 593
Inhibitory (toxic) effects, 432	- Correlative test evaluations 233	Substrate concentration effect
Activated sludge, non-acclimated,	4/caligenes sp	593
municipal	Aerobic biodegradation, 431	Surfactant effect, 593
Aerobic biodegradation, 18	Arthrobacter sp	Polyporous sp
Trickling filters, 18	Aerobic biodegradation, 431	Amino acids and derivatives
Alcaligenes sp	Ciliata sp	Time-course kinetics, 82
Aerobic biodegradation, 431	Inhibitory (toxic) effects, 432	Cellulose and derivatives
Arthrobacter sp	Flavobacterium sp	Time-course kinetics, 82
Aerobic biodegradation, 431	Aerobic biodegradation, 431	Polypropylene
Ciliata sp	Inhibitory (toxic) effects	see also Alkanes
Inhibitory (toxic) effects, 432	Review, 321, 451, 452	Activated sludge, municipal
Flavobacterium sp	Mastigota sp	Biodegradation, rates compared
Aerobic biodegradation, 431	Inhibitory (toxic) effects, 432	245
Mastigota sp	Metabolic pathways	Aspergillus sp
Inhibitory (toxic) effects, 432	Review, 321, 451, 452	Structure-activity relationships
Micrococcus sp Aerobic biodegradation, 431	Microbial population	97.
Mycobacterium sp	Model ecosystem, aquatic, natural	Microbial population, soil burial
Aerobic biodegradation, 431	516	Structure-activity relationships
Nocardia sp	Microbial population, acclimated, 286	97
Aerobic biodegradation, 431	Microbial population, river water	Microbial population, soils
Pseudomonas sp	Operational parameters, 99	Biodegradation, rates compared
Aerobic biodegradation, 431	River die-away test, 284, 424, 426	245
Sarcodina sp	Structure-activity relationships 428	Polystyrenes
Inhibitory (toxic) effects, 432	Micrococcus sp	Activated sludge
Xanthomonas sp	Aerobic biodegradation, 431	Biodegradation, rates compared
Aerobic biodegradation, 431	Mycobacterium sp	248
Polyethylene glycols, fatty ether	Aerobic biodegradation, 431	Activated sludge + cellulose and salt: Biodegradation, rates compared
see also Surfactants, nonionic	Nocardia sp	248
Achromobacter sp	Aeropic biodegradation, 431	Activated sludge, municipal
Aerobic biodegradation, 431	Pseudomonas sp	Biodegradation, rates compared
Activated sludge	Aerobic biodegradation, 431	176, 245
Aerobic biodegradation, 302	Operational parameters, 222	Aspergillus sp
Aerobic digestion reactor, 493	Sarcodina sp	Biodegradation, rates compared
Anaerobic digestion reactor, 493	Inhibitory (toxic) effects, 432	248
Assay development, 592	Structure-activity relationships	Structure-activity relationships
Coupled units test, 129	Review, 321, 451	97
Inhibitory (toxic) effects, 430	Xanthomonas sp	Aureobasidium sp
Operational parameters, 222 592	Aerobic biodegradation, 431	Biodegradation, rates compared
Seasonal variations, 493	Polyethylene glycols, fatty ether, sulfate	248
Structure-activity relationships	Microbial population, fresh water	Bjerkandera sp
302	Microbial population, sea water	Biodegradation, rates compared

Polystyrenes (cont d)	Polyvinyi alconol (cont'd)	Propylene glycols (cont'd)
Coriolus sp	Review, 489	Identification of microorganisms
Biodegradation, rates compared	Sludge adaptation process, 591	560
248	Time-course kinetics, 136, 352	Respirometric studies, 560
Daedalea sp	355	Actinomyces sp
Biodegradation, rates compared	Activated sludge, accilmated	Structure-activity relationships
248	Aerobic biodegradation, 397	153
Fomes sp	Activated sludge, acclimated,	Activated sludge
Biodegradation, rates compared	continuous-flow	
248	Operational parameters, 310	Biocenosis, effect on, 105
Gleophyllum sp	Sludge acclimatization process	Sludge acclimatization process
	310	105
Biodegradation, rates compared		Structure-activity relationships
248	Activated sludge, acclimated, municipal	153. 473
Microbial population, silt loam	Aerobic biodegradation, 568	Activated sludge, industrial and
Biodegradation, rates compared	Operational parameters, 568	municipal
248	Activated sludge, industrial	Aerobic biodegradation, pilot plant,
Microbial population, soil burial	Aerobic biodegradation, 55	237
Structure-activity relationships	Overview, 55	Bacıllus sp
97	Time-course kinetics, 55	
Microbial population, soils	Activated sludge, municipal	Structure-activity relationships
	Correlative test evaluations	153, 473
Biodegradation, rates compared		Bacterium sp
176, 245, 248	151	Structure-activity relationships
Microbial population, soils + cellulose	Activated sludge, non-acclimated	153
and salts	Inhibitory (toxic) effects, 454	Chromobacterium sp
Biodegradation, rates compared	Rate and selective adsorption	Structure-activity relationships
248	454	153
Moraxella sp	Activated sludge, oxygen-activated,	Flavobacterium sp
Metabolic pathways, 192, 468	municipal	I donnéissais - C
Paecilomyces sp	Respirometric studies, 64	Identification of microorganisms
Biodegradation, rates compared	Activated sludge, soap waste, 490	560
248		Respirometric studies, 560
	Activated sludge + Pseudomonas sp,	Microbial population, raw sewage
Penicillium sp	490	Aerobic biodegradation, 26
Biodegradation, rates compared	Geotrichum sp	Microbial population, sewage, municipal
248	Isolation of microorganisms, 586	Biorefractory index, 199
Metabolic pathways, 192, 468	Microbial population	Recommendations, wastewater treat-
Peniophora sp	Metabolic pathways, 27	ment, 199
Biodegradation, rates compared	Microbial population, fresh water sedi-	Micrococcus sp
248	ment-	•
Phellinus sp	Ozonization effects, 488	Structure-activity relationships
Biodegradation, rates compared	Microbial population, soils	153
		Mycobacterium sp
248	Isolation of microorganisms, 586	Structure-activity relationships
Poria sp	Nitrobacter sp	153
Biodegradation, rates compared	Respirometric studies, 64	Pseudomonas sp
248	Nurosomas sp	Identification of microorganisms
Trichoderma sp	Respirometric studies, 64	560
Biodegradation, rates compared	Pseudomonas sp., 490	Respirometric studies, 560
248	Isolation of microorganisms, 586	Structure-activity relationships
	Sewage, municipal	153, 473
Polyureas 217	Aerobic biodegradation, 574	
Aspergillus sp. 217	Time-course kinetics, 574	Sarcina sp
Penicillium sp. 217	Time-course kinemes, 574	Structure-activity relationships
Polyvinyl acetate	Poria sp	153
Geotrichum sp	Phenol-formaldehyde resin	Sewage, acclimated, municipal
Isolation of microorganisms, 586	Biodegradation, rates compared	Petrochemical wastewater treatment
Microbial population, soils	248	51
		Sewage, municipal
Isolation of microorganisms, 586	Poly(methyl methacrylate)	Identification of microorganisms
Pseudomonas sp	Biodegradation, rates compared	560
Isolation of microorganisms, 586	248	Respirometric studies, 560
Polyvinyl alcohol	Polystyrenes	332,232,332,333
see also Alcohols	Biodegradation, rates compared	Protaminobacter sp
Activated sludge	248	Adipic acid and derivatives, 118
Aerobic biodegradation, 181		Alkanoic acids and derivatives,
	Potassium	polybasic, 118
230, 398	Lagoon pre-treatment	Amides, aliphatic, 118
Batch vs continuous-flow system	Anaerobic biodegradation, 379	Amines, poly-, aliphatic, 118
181	-	ramics, pory-, anymatic, 110
Operational parameters, 591		Proteins
Petrochemical wastewater treatment	see also Alcohols	see also Fellmongery wastes; Tannery
324	Acinetobacter sp	wastes

roteins (cont'd)	Pseudomonas sp (cont'a)	rseudomonas sp (cont u)
Activated sludge	Psychrophilic temperature effect	Metabolic pathways, 59, 123
Substrate concentration effect	250	232
372	Structure-activity relationships	Screening tests, 376
Activated sludge, acclimated.	153, 473	Alkenoic acids and derivatives
continuous-flow	Time-course kinetics, 250	Metabolic pathways, 8
Operational parameters, 310	Alcohols, primary aliphatic, 294	Alkenoic acids and derivatives, long
	Activated sludge, 417	chain
Sludge acclimatization process	Identification of microorganisms	Inhibitory (toxic) effects, 572
310	164, 282, 303, 560	Alkyl halides
Activated sludge, industrial		
Identification of microorganisms	Metabolic pathways, 59, 182	Time-course kinetics, 347
163	297, 303, 539	Alkyl sulfates, long chain, 442
Activated sludge, non-acclimated,	Respirometric studies, 560	Alkyl sulfonates and derivatives
municipal	Structure-activity relationships	Freundlich adsorption isotherms
Gravimetric assessment, 420	153, 473	459
Hach oxidation, 420	Alcohols, primary, long chain	Alkyl sulfoxides
Respirometric studies, 420	Operational parameters, 222	Identification of microorganisms
Identification of microorganisms	Alcohols, secondary aliphatic, 294	295
Biodegradability, ultimate, 487	Metabolic pathways, 297	Sludge acclimatization process
Review, 487	Structure-activity relationships	295
Microbial population, continuous-flow	153, 473	Aluminum
	Aldehydes, 294	Inhibitory (toxic) effects, 572
Adaptation of microorganisms	Identification of microorganisms	Amides, aliphatic
399	164	Inhibitory (toxic) effects, 277
Psychrophilic temperature effect	Metabolic pathways, 539	Nutritional parameters, 278
399	•	•
Microbial population, soils	Structure-activity relationships	Amides, aliphatic, long chain
Aerobic vs anaerobic conditions	153, 473	Metabolic pathways, 273
119	Alkanes	Structure-activity relationships
Structure-activity relationships	Genetic transfer, 123	273
119	Metabolic pathways, 123, 232	Amines, alicyclic
Sewage, municipal	299	Inhibitory (toxic) effects, 38
Nutritional effects, 90	Alkanes, cyclic	Amines, aliphatic
Proteus sp	Metabolic pathways, 232, 335	Inhibitory (toxic) effects, 277
Cyanide	Alkanes, long chain, branched	Nutritional parameters, 278
Identification of microorganisms	Genetic transfer, 123	Amines, long chain
206	Mesophilic temperature, effect	Structure-activity relationships
Phenol and derivatives	567	273
	Metabolic pathways, 123	Amines, poly-, aliphatic, 72
Identification of microorganisms	Psychrophilic temperature effect	Amino acids and derivatives
205, 206	567	Metabolic pathways, 273, 542
Thiocyanic acid and salts	Alkanes, long chain, linear	Structure-activity relationships
Identification of microorganisms	Anaerobic biodegradation, 298	273
205, 206	Genetic transfer, 123	Aniline and derivatives
2		Mineralization, 585
Protozoa	Metabolic pathways, 123, 232	Time-course kinetics, 183
Antibiotics, 254	298, 299	
Decudement dike en	Time-course kinetics, 347	Aromatic compounds, dicyclic
Pseudomonad-like sp	Alkanoic acids and derivatives, 294	Metabolic pathways, 335
Quaternary ammonium compounds	Anaerobic biodegradation, 298	Psychrophilic temperature effect
Inhibitory (toxic) effects, 314	Metabolic pathways, 288, 297	250
Metabolic pathways, 314	298	Time-course kinetics, 250
Daniedaman an mlaumida	Structure-activity relationships	Arsenic compounds, inorganic
Pseudomonas plasmids	153, 473	Operational parameters, 464
Herbicides, 2,4-D type	Alkanoic acids and derivatives, long	Arsenic compounds, organic
Genetic transfer, 383	chain	Operational parameters, 464
Metabolic pathways, 383	Anaerobic biodegradation, 298	Benzene and derivatives
Seudomonas sp	Metabolic pathways, 273, 298, 539	Identification of microorganisms
Acetophenone and derivatives	Operational parameters, 222	376
Psychrophilic temperature effect	Structure-activity relationships	Metabolic pathways, 232, 335
250	273	Psychrophilic temperature effect
Time-course kinetics, 250	Alkanoic acids and derivatives,	250
	polybasic	Screening tests, 376
Activated sludge	Metabolic pathways, 539	Time-course kinetics. 250
Review, 489		Benzoic acid and derivatives
Adipic acid and derivatives	Alkanoic acids, sulfonated, long chain	Inhibition of benzoic acid turnover
Anaerobic biodegradation, 298	Inhibitory (toxic) effects. 329	
Metabolic pathways, 298	Alkenes	410
Alcohols, alicyclic	Genetic transfer, 123	Inhibitory (toxic) effects, 183
Inhibitory (toxic) effects, 38	Identification of microorganisms	Isolation of enzymes, 103
Alcohols, benzylic	376	Metabolic pathways, 103, 184, 539

Pseudomonas sp (cont'd)	Pseudomonas sp (cont'd)	Pseudomonas sp (cont'd)
Operational parameters, 103	Aerobic biodegradation, 19	Petroleum
Structure-activity relationships	Metabolic pathways, 19	Mesophilic temperature effect
410, 473	Gasoline	342
Time-course kinetics, 183	Metabolic pathways, 232	Metabolic pathways, 553
Biphenyl and derivatives	Herbicides, chlorpropham type	pH effect, 342
Inhibitory (toxic) effects, 309	Azide inhibitory activity, 257	Phenol and derivatives, 294
Metabolic pathways, 335, 354	Diazinon inhibitory and persistance	Batch vs continuous-flow system 579
Cadmium Sorption, 210, 211	activity, 257 Operational parameters, 160	
Carbamic acid and derivatives	Phorate inhibitory activity, 257	Identification of microorganisms 71, 205, 206, 295
Metabolic pathways, 177	Herbicides, 2,4-D type	Inhibitory (toxic) effects, 309
Cellulose and derivatives	Aquatic systems, 46	Metabolic pathways, 354, 576
Identification of microorganisms	Diauxic fermentation, 46	579
406	Metabolic pathways, 214	Model ecosystem, aquatic, simulated,
Chloride	Model ecosystem, aquatic, simulated,	
Inhibitory (toxic) effects, 131	214	Model ecosystem, terrestrial, natural,
Operational parameters, 131	Operational parameters, 160	545
Chromium	Herbicides, silvex type	pH effect, 74
Inhibitory (toxic) effects, 131	Metabolic pathways, 214	Sludge acclimatization process
572	Model ecosystem, aquatic, simulated,	
Operational parameters, 131	214, 378	Substrate concentration effect
Sorption, 210, 211	Heteroaromatics and derivatives, dicyclic	
Cinnamic acid and derivatives	Metabolic pathways, 539	Temperature effect, 74
Metabolic pathways, 137	Hexachlorophene	Time-course kinetics, 183, 579 Phenylacetic acid and derivatives
Cirrasols Aerobic biodegradation, 431	Metabolic pathways, 354	Metabolic pathways, 137
Copper	Hydrocarbons	Phosphonic acid derivatives, alkyl
Inhibitory (toxic) effects, 572	Metabolic pathways, 232	Metabolic pathways, 65, 91
Sorption, 210, 211	Hydroquinone and derivatives	Phthalic acid and derivatives
Cresols and derivatives	Metabolic pathways, 184, 539 Structure-activity relationships	Identification of microorganisms
Inhibitory (toxic) effects, 309	153, 473	282
Model ecosystem, terrestrial, natural,	Industrial wastewaters	Metabolic pathways, 8, 117
545	Isolation of microorganisms, 586	Plycyclic aromatic hydrocarbons
pH effect, 74	Isophthalic acid and derivatives	Metabolic pathways, 335
Substrate concentration effect	Metabolic pathways, 8	Polycaprolactone
74	Ketones, aliphatic, 294	Microbial population, soils, 126
Temperature effect, 74	Aerobic biodegradation, 19	Polychlorinated biphenyls
Crude oil	Inhibitory (toxic) effects, 38	Aerobic biodegradation, 24
Mesophilic temperature, effect	Metabolic pathways, 19, 297	Structure-activity relationships 24
567	Structure-activity relationships	Substrate concentration effect
Psychrophilic temperature effect 567	473	24
Cumene and derivatives	Leather, artificial, processing wastes	Polychlorobenzenes and derivatives
Identification of microorganisms	Inhibitory (toxic) effects, 277	Anaerobic biodegradation, 536
376	Lignin-related compounds	Inhibition of benzoic acid turnover,
Psychrophilic temperature effect	Metabolic pathways, 137, 539 Lignin sulfonates	410
250	Aerobic biodegradation, 19	Inhibitory (toxic) effects, 53
Screening tests, 376	Metabolic pathways, 19	Metabolic pathways, 354
Time-course kinetics, 250	Lindane and metabolites	Structure-activity relationships
Cyanide	Anaerobic biodegradation, 536	410
Identification of microorganisms	Magnesium	Polychlorocyclopentadiene dimers
206	Inhibitory (toxic) effects, 572	Anaerobic biodegradation, 536
Cycloaliphatics, substituted	Mercury, inorganic, 498	Polyesters Microbial population, soils, 126
Inhibitory (toxic) effects, 38 DDT, Methoxychlor and metabolites	Sorption, 210, 211	Polyethylene glycols
Anaerobic biodegradation, 536	Naphthalene and derivatives	Identification of microorganisms
Autoclaving effect, 536	Metabolic pathways, 177, 335 Psychrophilic temperature effect	560
Disinfectants effect, 536	250	Metabolic pathways, 182
Metabolic pathways, 536	Time-course kinetics, 250	Respirometric studies, 560
Explosives, organic	Nitrobenzene and derivatives	Polyethylene glycols, fatty ester
Inhibitory (toxic) effects, 7	Time-course kinetics, 183	Aerobic biodegradation, 431
Fellmongery wastes	NTA and salts	Polyethylene glycols, fatty ether
Identification of microorganisms	Metabolic pathways, 127	Aerobic biodegradation, 431
406	Octopine	Operational parameters, 222
Fuel oil	Isolation of enzymes, 395	Polyvinyl acetate
Metabolic pathways, 299, 553	Oil refinery wastes, 40	Isolation of microorganisms, 586
Furan and derivatives	Petrochemical wastes, 40	Polyvinyi alcohol, 490

seudomonas sp (cont'd)	Pseudomonas sp (cont'd)	Pseudomonas sp, revertant
Isolation of microorganisms, 586	376	Phthalic acid and derivatives
Propylene glycols	Metabolic pathways, 232, 335	Metapolic pathways, 359
Identification of microorganisms	Psychrophilic temperature effect	Pseudomonas sp TOL-plasmid-bearing
560	250	Amino acids and derivatives
Respirometric studies, 560	Screening tests, 376	Metabolic pathways, 279
Structure-activity relationships	Time-course kinetics, 250	
153, 473	Toluic acid and derivatives	Pseudomonas sp, wild type
Pyridine and derivatives, 294	Inhibition of benzoic acid turnover,	Phthalic acid and derivatives
Pyrocatechol and derivatives	410	Metabolic pathways, 359
Identification of microorganisms	Metabolic pathways, 8, 539	Pulp and paper wastes
282	Structure-activity relationships	see also Kraft pulp wastes
Metabolic pathways, 117, 184	410	Activated sludge
Model ecosystem, aquatic, simulated		Aeration digestion reactors
378	Inhibitory (toxic) effects, 367	compared, 520
Structure-activity relationships	Substrate concentration effect	Aerobic biodegradation, 128
153, 473	367	289
Quaternary ammonium compounds, 11		Aerobic digestion reactors compared
A -1 4	7 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	236
plant, 125	Vanillic acid and derivatives	Detoxification, 236, 349
Resorcinol and derivatives		Foam process, 594
Metabolic pathways, 184	Metabolic pathways, 539	Inhibitory (toxic) effects, 128
Structure-activity relationships	Vibrio sp	453
	Metabolic pathways, 550	Lagoons, aerated, industrial site
153, 473	Xylenes and derivatives	349
Soil systems, flooded and non-flooded	 Identification of microorganisms 	Operational parameters, 520
Model ecosystem, terrestrial,	376	Review, 556
simulated, 404	Inhibition of benzoic acid turnover,	Structure-activity relationships
Starch and derivatives, 490	410	289
Identification of microorganisms	Metabolic pathways, 232, 335	Activated sludge, acclimated,
406	Psychrophilic temperature effect	continuous-ilow
Stilbene and derivatives	250	Operational parameters, 310
Metabolic pathways, 137	Screening tests, 376	Sludge acclimatization process
Styrene and derivatives	Structure-activity relationships	310
Identification of microorganisms	410	
376	Time-course kinetics, 250, 347	Activated sludge, continuous-flow
Psychrophilic temperature effect	Xylenols and derivatives	Aerobic biodegradation, 301
250	Metabolic pathways, 137, 539	Biomass yield, effect on, 301
Screening tests, 376	Model ecosystem, terrestrial, natural,	Aerated stabilization basins
Time-course kinetics, 250	545	Review. 330
Sulfamilic acid and derivatives		Candida sp
Identification of microorganisms	Pseudomonas sp acclimated	Foam process, 594
377	Alkanes, long chain, linear	Hyatodendron sp
Sulfide	Time-course kinetics, 347	Foam process, 594
Inhibitory (toxic) effects, 131	Alkyl halides	Lagoons, aerated
Operational parameters, 131	Time-course kinetics, 347	Review. 556
Tannery wastes	Aniline and derivatives	Lagoons, aerated, industrial site
Inhibitory (toxic) effects, 131	Metabolic pathways, 276	Aerobic biodegradation, 215
Operational parameters, 131	Azo compounds	573
Terpene compounds	Metabolic pathways, 276	Detoxification, 215, 573
Metabolic pathways, 59	Azo dyes	Phialophora sp
Tetralin and derivatives	Metabolic pathways, 276	Foam process, 594
Metabolic pathways, 335	Benzoic acid and derivatives	Spray irrigation systems
Psychrophilic temperature effect	Metabolic pathways, 276	Review, 556
250	Naphthalene and derivatives	Storage oxidation basins
Time-course kinetics, 250	Metabolic pathways, 276	Review, 556
Textile wastes, 490	Xylenes and derivatives	Trichosporon sp
Thiocyanic acid and salts	Time-course kinetics, 347	Foam process, 594
Identification of microorganisms	Passada	Trickling filters
205, 206	Pseudomonas sp mutant	Review, 556
Thiophenols	NTA and salts	PVA
Metabolic pathways, 542	Metabolic pathways, 300	
Timber steam processing wastes	Pseudomonas sp pure culture	see Polyvinyl alcohol
Aerobic biodegradation, 408	Alcohols, primary aliphatic	Pyridazinones
Identification of microorganisms	Metabolic pathways, 471	see Herbicides, pyrazon type
408	Amines, poly-, aliphatic	Pyridine and derivatives
Operational parameters, 408	Metabolic pathways, 471	see also Quaternary ammonium com-
Toluene and derivatives	Cycloaliphatics, substituted	pounds
Identification of microorganisms	Marchalla and and 191	Activated cludge

vridine and derivatives (cont'd)	Pyrocatechol and derivatives (cont'd)	Pyrrole
Aerobic biodegradation, 78	Alcaligenes sp	Activated sludge
" Inhibitory (toxic) effects, 480	Metabolic pathways, 37	Structure-activity relationships
Nitrification effect, 480	Arthrobacter sp	393
Structure-activity relationships		Quaternary ammonium compounds
393	Isolation of enzymes, 84	see ulso Amines, long chain; Pyridine
Activated sludge, municipal	Metabolic pathways, 84, 117	and derivatives; Surfactants, ca-
Correlative test evaluations	Bacıllus sp	tionic
151	Identification of microorganisms	Activated sludge
Bacterium sp. 294	282	Aerobic digestion reactor, 234
Microbial population, raw sewage	Structure-activity relationships	Aerobic digestion reactor, pilot
Aerobic biodegradation, 26	153, 473	plant, 152
Inhibitory (toxic) effects, 25	Bacterium sp	Anaerobic digestion reactor, 234
Microbial population, septic tank	Structure-activity relationships	332
Inhibitory (toxic) effects, 6	153	Inhibitory (toxic) effects, 304
Microbial population, sewage, municipal	Brevibacterium sp	Activated sludge, acclimated
Biological inhibition value, 199	Metabolic pathways, 117	Aeropic digestion reactor, pilot
Biorefractory index, 199	Chromobacterium sp	plant, 125
Inhibitory (toxic) effects, 199	Structure-activity relationships	Activated sludge, acclimated,
Recommendations, wastewater treat-	153	continuous-flow
ment, 199	Corynebacterium sp	Operational parameters, 310
Micrococcus sp. 294	Metabolic pathways, 117	Sludge acclimatization process
Nitrosomas sp	Fusarium sp	310
Inhibitory (toxic) effects, 587	Metabolic pathways, 188	Activated sludge, municipal
Pseudomonas sp., 294	Lagoons, aerated, industrial site	Aerobic digestion reactor, pilot
Sarcina sp. 294	Aerobic biodegradation, 215	plant, 125
Sewage, frozen, acclimated	Detoxification, 215	Activated sludge, non-acclimated
Operational parameters, 587	Microbial population, acclimated	Aerobic digestion reactor, pilot
Substrate concentration effect	Anaerobic fermentation.	plant, 125
587	methanogenic, 195	Activated sludge, semi-continuous flow,
Temperature effect, 587	Microbial population, acclimated,	286
Sewage, municipal	municipal	Aeromonas sp. 11
Nutritional effects, 90	Metabolic pathways, 98	Aspergillus sp
Respirometric studies, 548	Nutritional effects, 98	Inhibitory (toxic) effects, 314
yrocatechol and derivatives	Microbial population, municipal wastes	
Achromobacter sp	Metabolic pathways, 213	Bacillus sp. 11
Metabolic pathways, 41, 67	Nutritional effects, enrichment	Bacteriocidal/bacteriostatic effects
Model ecosystem, aquatic, simulated		Review, 425
378	Microbial population, soils	Comamonas sp
Actinomyces sp	Denitrification, 14	Aerobic digestion reactor, pilot
Structure-activity relationships	Metabolic pathways, 14	plant, 125
153	Micrococcus sp	Metabolic pathways
Activated sludge	Metabolic pathways, 107	Review, 314
Activated studge Aerobic biodegradation, 386	Structure-activity relationships	Microbial population, 11
Anaerobic digestion reactor, 196	153	Microbial population, acclimated, 286
Identification of microorganisms	Mycobacterium sp	Microbial population, fresh water
282	Metabolic pathways, 117	Inhibitory (toxic) effects, 304
Inhibitory (toxic) effects, 66	Structure-activity relationships	Operational parameters, 423
Metabolic pathways, 143	153	Structure-activity relationships
Structure-activity relationships	Nocardia sp	17
153, 386, 473	Identification of microorganisms	Microbial population, municipal wastes
Substrate concentration effect, 66	282	Structure-activity relationships
Activated sludge, acclimated	Metabolic pathways, 179, 444	17
Structure-activity relationships	Penicillium sp	Microbial population, river water
. 389	Metabolic pathways, 117	Inhibitory (toxic) effects, 427
Time-course kinetics, 389	Pseudomonas sp	River die-away test, 424
Activated sludge, diverse substrates	Identification of microorganisms	Structure-activity relationships
Batch vs continuous-flow system	282	427
71	Metabolic pathways, 117, 184	Pseudomonad-like sp
Substrate concentration effect	Model ecosystem, aquatic, simulated,	
71	378	Metabolic pathways, 314
Time-course kineucs, 71	Structure-activity relationships	Pseudomonas sp. 11
Activated sludge. Nocardia-inoculated	153, 473	Pseudomonas sp. 11
Identification of microorganisms		Aerobic digestion reactor, pilot
	Sarcina sp	plant, 125
282	Structure-activity relationships	Sewage, acclimated, municipal
Activated sludge, municipal	153	Petrochemical wastewater treatment
Correlative test evaluations	Sewage, natural, semi-continuous flow	51

Quaternary ammonium compounds (cont'd)		Review (cont'd)
Staphylococcus sp	Activated sludge process	Metabolic pathways, 492, 571
Structure-activity relationships	Biochemistry, 221	Structure-activity relationships
17	Instrumentation and sampling techni-	
Structure-activity relationships	ques, 221 Kineuc studies and mathematical	Carbamic acid and derivatives
Review, 425 Trickling filters	models, 22!	Metabolic pathways, 325 Carbowax
Inhibitory (toxic) effects, 306	Microbial analyses activity and	Microbial population, glycol-
Yeast sp	ecology, 221	metabolizing, 80
Inhibitory (toxic) effects, 314	Pollutants and organics determina-	Cellulose and derivatives
Metabolic pathways, 314	tions, 221	Identification of microorganisms
Renex 20	Survival of pathogenes, 221	33
Activated sludge, non-acclimated,	Alcohols, primary aliphatic	Metabolic pathways, 33
municipal	Structure-activity relationships	Cresols and derivatives
Aerobic biodegradation, 18	500	Metabolic pathways, 88
Trickling filters, 18	Aldehydes Identification of microorganisms	Cutting fluids (coolants), synthetic and
Resins	165	semi-synthetic Biodegradation, 1
see Textile wastes	Trickling filters, 166	Cycloaliphatics, substituted
Resorcinol and derivatives	Alicyclic compounds	Microbial biodegradation, 521
Actinomyces sp	Biodegradability, ultimate, 387	Enzymes
Structure-activity relationships	Identification of microorganisms	Identification of microorganisms
153	487	487
Activated sludge	Aliphatic compounds	Explosives, organic
Aerobic biodegradation, 386	Biodegradability, ultimate, 387	Activated sludge, continuous-flow
Inhibitory (toxic) effects, 178	Identification of microorganisms	566
Structure-activity relationships 153, 386, 473	487	Denitrification, 566
Activated sludge, acclimated	Alkanoic acids and derivatives Structure-activity relationships	Operational parameters, 566
Structure-activity relationships	500	Time-course kinetics, 566 Fluorescent brighteners
389	Amines, long chain	Biodegradation, environmental
Time-course kinetics, 389	Bacteriocidal/bacteriostatic effects,	aspects, 56
Activated sludge, diverse substrates	425	Furan and derivatives
Batch vs continuous-flow system	Structure-activity relationships	Microbial biodegradanon, 521
71	425	Halogenated hydrocarbons
Substrate concentration effect	Amino acids and derivatives	Microbial biodegradation,
71	Identification of microorganisms	mechanisms. 50
Time-course kinetics, 71 Bacillus sp	487	Heterocyclic compounds
Structure-activity relationships	Metabolic pathways, 514 Structure-activity relationships	Identification of microorganisms 487
153, 473	500	Hydroquinone and derivatives
Bacterium sp	Aniline and derivatives	Metabolic pathways, 88
Structure-activity relationships	Structure-activity relationships	Inhibitory effects, metallic and ionic
153	388	species
Chromobacterium sp	Aquatic oil spills	Activated sludge, 546
Structure-activity relationships	Effect on microbial population	Isophthalic acid and derivatives
153	23	Metabolic pathways, 259
Micrococcus sp Structure-activity relationships	Microbial abatement, 23	Mercury, organo-
153	Microbial emulsification and	Biodegradation, environmental
Mycobacterium sp	degradation, 23	aspects, 239 Metals, toxic
Structure-activity relationships	Oil pollutants, sources and behavior,	Environmental fate, 448
153	Aromatic compounds	Metabolic pathways, 448
Pseudomonas sp	Biodegradability, ultimate, 387	Model ecosystem, biotransformation
Metabolic pathways, 184	Identification of microorganisms	448
Structure-activity relationships	487	Mineral oils
153, 473 Sarcina sp	Arsenic compounds, organic	Identification of microorganisms
Structure-activity relationships	Biodegradation, environmental	487
153	aspects, 239	Naphthalene and derivatives
Sewage, natural, semi-continuous flow	Benzene and derivatives Metabolic pathways, 88	Metabolic pathways, 325
Metabolic pathways, 184	Benzenesulfonic acid, linear alkyl, long	Nitrobenzene and derivatives Structure-activity relationships
Review	chain	388
Activated sludge, acclimated	Anaerobic biodegradation, 158	NTA and salts
Salmity, effect on respiratory	Aquatic interactions, microbial	Aerobic biodegradation, 558
activity, 227	158	Anaerobic biodegradation, 558
Salinity, effect on volume index	Identification of microorganisms	Metabolic pathways, 558
227	571	Organo-metallic compounds

Review (cont'd)	Review (cont'd)	Rhodotorula sp (cont'd)
Biodegradation, environmental aspects, 239	Stilbene and derivatives Biodegradation, environmental	Structure-activity relationships 450
Pesticides Pesticides	aspects, 56	Sulfanilic acid and derivatives
Metabolic pathways, 260, 326		
Phenol and derivatives	Sugars and derivatives Identification of microorganisms	Identification of microorganisms
Metabolic pathways, 88	487	River die-away test
Structure-activity relationships	· - ·	Alcohols, tertiary aliphatic
388	Surfactants Bacteriocidal/bacteriostatic effects.	Activated sludge, 268
Phosphorus		Alcohols, tertiary, long chain
Activated studge, 113, 412	440	Microbial population, river water
Luxury phosphorus uptake, 113	Inhibitory (toxic) effects, 440	424
412	Metabolic pathways, 519	Alkanoic acids and derivatives, long
Photoprocess wastes	Surfactants, anionic	chain
Inhibitory (toxic) wastes, 541	Biodegradability, 455	Microbial population, fresh water
Phthalic acid and derivatives	Inhibitory (toxic) effects, 321	458
Metabolic pathways, 259	Metabolic pathways, 54, 321	Alkanoic acids and derivatives,
Polyethylene glycols	492	polybasic
	Structure-activity relationships	Activated sludge, continuous-flow
Microbial population, glycol- metabolizing, 80	321, 492	313
	Surfactants, cationic	
Polyethylene glycols, alkylphenoxy-	Bacteriocidal/bacteriostatic effects.	Microbial population, fresh water 458
Inhibitory (toxic) effects, 321	425	
451, 452 Matabalia pathwaya 221, 151	Structure-activity relationships	Alkenoic acids and derivatives, long chain
Metabolic pathways, 321, 451 452	425	Activated sludge, 58
	Surfactants, nonionic	Alkyl sulfates, long chain
Structure-activity relationships 321, 451	Biodegradability, 455	Microbial population, fresh water
Polyethylene glycols, fatty ether	Inhibitory (toxic) effects, 321	458
	Metabolic pathways, 54, 321	Alkyl sulfonates and derivatives
Inhibitory (toxic) effects, 321 451, 452	492	Microbial population, fresh water
- ,	Structure-activity relationships	458
Metabolic pathways, 321, 451 452	321, 492	Alkynes
	Surfactants, tetrapropylene	Microbial population, river water
Structure-activity relationships 321, 451	Metabolic pathways, 492	424
Polymers	Structure-activity relationships	Amides, aliphatic, long chain
Structure-activity relationships	492	Microbial population, river water
218	Synthetic organics	424
Polyvinyl alcohol	Microbial biodegradation, 505	Amines, aliphatic
Activated sludge, 489	Tellurium, organo- Biodegradation, environmental	Activated sludge, 394
Proteins		Amino acids and derivatives
Identification of microorganisms	aspects, 239	Microbial population, fresh water
487	Terephthalic acid and derivatives	458
Pseudomonas sp	Metabolic pathways, 259	Aniline and derivatives
Activated sludge, 489	Textile wastes	Activated sludge, continuous-flow
Pulp and paper wastes	Activated sludge, 489	159
Activated sludge, 556	Thiophene Microbial biodegradation, 521	Sewage, municipal, 159
Aerated stabilization basins	Microbial biodegradation, 521 Xylenols and derivatives	Benzenesuifonic acid, linear alkyl, long
556	Metabolic pathways, 325	chain
Lagoons, aerated, 556	•	Activated sludge, 58, 268
Spray irrigation systems, 556	Rhizobidia sp	Activated sludge, acclimated,
Storage oxidation basins, 556	Lindane and metabolites	continuous-flow, 220
Trickling filters, 556	Aerobic biodegradation, 246	Microbial population, fresh water
Quaternary ammonium compounds	Polychlorocyclopentadiene dimers	458
Bacteriocidal/bacteriostatic effects.	Aerobic biodegradation, 246	Benzenesulfonic acid. S-substituted alky
425	Rhodopseudomonas sp	Activated sludge, acclimated.
Metabolic pathways, 314	Alkynes	municipal, 416
Structure-activity relationships	Inhibitory (toxic) effects, 323	Activated sludge, municipal, 416
425	Metabolic pathways, 323	Microbial population, river water
Salicylic acid and derivatives	Cyanide	416
Metabolic pathways, 88	Inhibitory (toxic) effects, 323	Sewage, synthetic, 416
Salinity	Metabolic pathways, 323	Benzoic acid and derivatives
Inhibitory (toxic) effects, 517	Rhodotorula sp	Activated sludge, synthetic, 385
Selenium, organo-	Alkanes	Microbial population, soils, 385
Biodegradation, environmental	Inhibitory (toxic) effects, 450	Benzothiazole and derivatives
aspects, 239	Structure-activity relationships	Activated sludge, 317
Silver	450	Microbial population, acclimated
Activated sludge, 22	Alkenes	317
Inhibitory (toxic) effects, 22	Inhibitory (toxic) effects, 450	ϵ -Caprolactam

Activated sludge, 268 Time-course kinetics, 316 Structure-activity relationships Carbamic acid and derivatives Activated sludge, acclimated Activated sludge, 268 Aerobic biodegradation, 397 Alkanoic acids and derivatives, 294 Herbicides, monuron type and Inhibitory (toxic) effects, 390 Structure-activity relationships metabolites Structure-activity relationships 153 Activated sludge, continuous-flow Cresols and derivatives 390 Model ecosystem, terrestrial, natural. Time-course kinetics, 390 Sewage, municipal, 159 Activated sludge, municipal 545 Naphthalene and derivatives Inhibitory (toxic) effects, 369 Hydroquinone and derivatives Activated sludge, 268 Structure-activity relationships Structure-activity relationships Nitrosamine, dimethyl-153 369 Activated sludge, 394 Ketones, aliphatic, 294 Fusarium sn Poly(ethylene glycol-propylene glycol) Phenol and derivatives, 294 Metabolic pathways, 188 Model ecosystem, terrestrial, natural, Microbial population, river water Metabolic pathways 424 545 Review, 88 Polychlorobenzenes and derivatives Propylene glycois Microbial population, acclimated, Activated sludge, industrial municipal Structure-activity relationships 470 153 Metabolic pathways, 98 Polyethylene glycols Pyridine and derivatives, 294 Nutritional effects, 98 Activated sludge, 58 Pyrocatechol and derivatives Nocardia so Polyethylene glycols, alkylphenoxy-Metabolic pathways, 180, 444 Structure-activity relationships Microbial population, river water 284, 424 153 Salinity Resorcinol and derivatives Activated sludge, acclimated, Polyethylene glycols, fatty ether Structure-activity relationships continuous-flow Microbial population, river water 153 Inhibitory (toxic) effects, 517 284. 424, 426 Xylenols and derivatives Activated sludge, fresh water Polyethylene glycols, fatty ether, sulfate: Model ecosystem, terrestrial, natural, Inhibitory (toxic) effects, 203 Microbial population, fresh water 545 Activated sludge, salt water 458 Sarcodina sp Inhibitory (toxic) effects, 203 Quaternary ammonium compounds Nitrification, effects on, 203 Cirrasols Microbial population, river water Inhibitory (toxic) effects, 432 Inhibitory (toxic) effects 424 Review, 517 Polyethylene glycols, fatty ester Sugars and derivatives Inhibitory (toxic) effects, 432 Salmonella sp Microbial population, river water
424 Polyethylene glycois, tatty ether Inhibitory (toxic) effects, 432 Alkanoic acids, sulfonated, long chain Bacteriocidal/bacteriostatic effects, Tallow derivatives Schizosaccharomyces sp Microbiai population, river water Inhibitory (toxic) effects, 329 Sulfanilic acid and derivatives Identification of microorganisms Structure-activity relationships, 330 Textile wastes 377 Activated sludge, industrial Santicizers Activated sludge Sclerotium sp 170 Octanol-water partition coefficients, Cellulose and derivatives Rubber, vulcanized Operational parameters, 285 434 Actinomyces sp. 87 Activated sludge, acclimated, 436
Activated sludge, semi-continuous flow Selenastrum sp
Aerobic biodegradation, 435
Dyes, acid Time-course kinetics, 285 Nocardia sp. 87 Streptomyces sp. 87 Saccharomyces sp Microbial population, acclimated Inhibitory (toxic) effects, screening, DDT. Methoxychlor and metabolites Octanol-water partition coefficients, Aerobic coprecipitation, 269 Anaerobic coprecipitation, 269 434 Dyes, basic Microbial population, river water, 436 Inhibitory (toxic) effects, screening, Batch vs continuous-flow system Octanol-water partition coefficients, 269 434 Dyes, direct Inhibitory (toxic) effects. 269 Inhibitory (toxic) effects, screening, Sarcina sp Mercury, inorganic Alcohols, benzylic Aerobic coprecipitation, 269 Structure-activity relationships Dyes, disperse Anaerobic coprecipitation, 269 153 Inhibitory (toxic) effects, screening, Batch vs continuous-flow system Alcohols, primary aliphatic, 294 547 269 Dyes, mordant Identification of microorganisms Inhibitory (toxic) effects, 269 164 Inhibitory (toxic) effects, screening, Sulfanilic acid and derivatives Structure-activity relationships Identification of microorganisms Dyes, sulfur 377 Salicylic acid and derivatives Alcohols, secondary aliphatic, 294 Inhibitory (toxic) effects, screening, 547 Activated sludge Structure-activity relationships Dyes, vat 153 Aerobic biodegradation, 386 Aldehyaes, 294 Inhibitory (toxic) effects, screening, Operational parameters, 315 Identification of microorganisms Structure-activity relationships 386 Lignin sulfonates

Salicylic acid and derivatives (cont'd)

River die-away test (cont'd)

Sarcina sp (cont'd)

Selenastrum sp (cont'd)	Sewage, acclimated, municipal (cont'd)	Sewage, municipal (cont'd)
Inhibitory (toxic) effects, screening,	51	Respirometric studies, 548
347	Petrochemicals, industrial	Alkyl sutfates, long chain
Naphthalene and derivatives Inhibitory (toxic) effects, screening,	Nitrification-preventive, 51	Aerobic biodegradation, 438
547	Petrochemical wastewater treatment	Anaerobic biodegradation, 438 Alkynes
Selenium, organo-	Phenol and derivatives	Respirometric studies, 548
Biogegradation, environmental aspects	Petrochemical wastewater treatment	Aluminum
Review, 239	51	Inhibitory (toxic) effects, 345
Settlement tank effluents	Polyethylene glycols	Amino acids and derivatives Nutritional effects, 90
Activated sludge	Biomass yield, effect on, 81 Propylene glycols	Respirometric studies, 548
Inhibitory (toxic) effects, 336	Petrochemical wastewater treatment	Aniline and derivatives
Sewage, acclimated, municipal	51	Co-substrate concentration effect
Alconols, primary aliphatic	Quaternary ammonium compounds	159 Bi
Petrochemical wastewater treatment	Petrochemical wastewater treatment	River die-away test, 159
Alcohols, secondary aliphatic	51 Styrene and derivatives	Structure-activity relationships 159
Petrochemical wastewater treatment	Petrochemical wastewater treatment	Substrate concentration effect
51	51	159
Alcohols, tertiary aliphatic	Toluene and derivatives	Benzenesulfonic acid. linear alkyl, long
Petrochemical wastewater treatment	Petrochemical wastewater treatment	chain Aerobic biodegradation, 438
Aldehydes	51 Urea and derivatives	Anaerobic biodegradation, 438 Anaerobic biodegradation, 438
Petrochemical wastewater treatment	Petrochemical wastewater treatment	Benzoic acid and derivatives
51	51	Inhibitory (toxic) effects, 183
Alkanes, cyclic	Xylenes and derivatives	Cadmium
Petrochemical wastewater treatment	Petrochemical wastewater treatment	Inhibitory (toxic) effects, 345 Cellulose and derivatives
Alkanoic acids and derivatives	51 Xylenols and derivatives	Aerobic biodegradation, 574
Petrochemical wastewater treatment	Petrochemical wastewater treatment	Time-course kinetics, 574
51	51	Chromium
Alkanoic acids and derivatives,	Sewage, frozen, acclimated	Inhibitory (toxic) effects, 345
polybasic	Aniline and derivatives	Cobalt
Petrochemical wastewater treatment	Operational parameters, 587	Inhibitory (toxic) effects, 345 Copper
Alkenes	Substrate concentration effect 587	Inhibitory (toxic) effects, 345
Petrochemical wastewater treatment	Temperature effect, 587	Cyanide
51	Nitrobenzene and derivatives	Inhibitory (toxic) effects, 345
Alkyl halides	Operational parameters, 587	Nutritional effects, 90
Petrochemical wastewater treatment	Substrate concentration effect	Furan and derivatives Respirometric studies, 548
Alkyi sulfoxides	587	Herbicides, monuron type and
Petrochemical wastewater treatment	Temperature effect, 587 Pyridine and derivatives	metabolites
51	Operational parameters, 587	Co-substrate concentration effect
Amides, aliphatic	Substrate concentration affect	159
Petrochemical wastewater treatment 51	301	Inhibitory (toxic) effects, 159 River die-away test, 159
Amines, aliphatic	Temperature effect, 587	Structure-activity relationships
Petrochemical wastewater treatment		159
51	Alcohols	Substrate concentration effect
Benzene and derivatives Petrochemical wastewater treatment	Respirometric studies, 548 Alcohols, alicyclic	159 Heteroaromatics and derivatives, dicyclic
51	Respirometric studies, 548	Nutritional effects, 90
Benzoic acid and derivatives	Alcohols, benzylic	fron
Petrochemical wastewater treatment		Inhibitory (toxic) effects, 345
51	Alcohols, primary aliphatic	Mercury, inorganic
Epoxides Petrochemical wastewater treatment	Identification of microorganisms 560	Inhibitory (toxic) effects, 345 Nickel
51	Respirometric studies, 548, 560	Inhibitory (toxic) effects, 345
Ethers	Alcohols, secondary aliphatic	Nitrobenzene and derivatives
Petrochemical wastewater treatment	Respirometric studies, 548	Inhibitory (toxic) effects, 183
51 Verenes elemente	Alcohois, tertiary aliphatic	Poly(α-hydroxyacrylic acid) Mineralization. 350
Ketones, aliphatic Petrochemical wastewater treatment	Inhibitory (toxic) effects, 548 Respirometric studies, 548	Time-course kinetics, 350
51	Alkenes	Polyethylene glycois
Nitrobenzene and derivatives	Respirometric studies, 548	Identification of microorganisms
Petrochemical wastewater treatment		560

Sewage, municipal (cont'd)	Sewage, synthetic (cont'd)	Sludge acclimatization process (cont'd
Respirometric studies, 560	Microbial acclimatization, 170	continuous-flow, 310
Polyvinyl alcohol	Gas oil	Benzidine and derivatives
Aerobic biodegradation, 574	Inhibitory (toxic) and stimulatory ef-	Activated sludge, 495
Time-course kinetics, 574	fects, 170	Activated sludge, acclimated,
Propylene glycols	Microbial acclimatization, 170	continuous-flow, 495
Identification of microorganisms	Nitrobenzene and derivatives	Biphenyl and derivatives
560	Chemical oxidation, 161	Activated studge, acclimated.
Respirometric studies, 560	Phenol and derivatives	municipal, continuous-flov
Proteins	Inhibitory (toxic) and stimulatory ef-	196
Nutritional effects, 90	fects, 170	Activated studge, municipal.
Pyridine and derivatives	Microbial acclimatization, 170	continuous-flow, 496
Nutritional effects, 90	Sewage, synthetic, continuous-flow	Cellulose and derivatives
Respirometric studies, 548	Amines, poly-, aliphatic, 396	Activated sludge, acclimated,
Silver	Shale oil wastes	continuous-flow, 310
		Coal carbonization wastes
Inhibitory (toxic) effects, 345 Sugars and derivatives	Microbial population	Activated sludge, acclimated,
	Metabolic pathways, 148	continuous-flow, 364
Nutritional effects, 90 Textile wastes	Shigella sp	Cyanide Cyanide
	Alkyl suifates, long chain, 442	
Aerobic biodegradation, 574	Silicon, inorganic	Activated sludge, 141, 142
Time-course kinetics, 574	Activated sludge	Activated sludge + rice bran 142
Tin	Inhibitory (toxic) effects, 588	- · -
Inhibitory (toxic) effects, 345	Silicones	Dyes
Urea and derivatives	_ Activated sludge	Activated sludge, acclimated,
Nutritional effects, 90		continuous-flow, 310
Zinc	Petrochemical wastewater treatment	Fellmongery wastes
Inhibitory (toxic) effects, 345	324	Activated sludge, acclimated,
Nutritional effects, 90	Activated sludge, UNOX pure oxygen	municipal, 77, 186
Sewage, municipal, oxidation pond system	technology	Fluorescent brighteners
Alkanoic acids and derivatives.	Overview, 187	Activated sludge, acclimated,
polybasic	Scheme of test facility, 187	continuous-flow, 310
Model ecosystem, aquatic, pond	Microbial population, soils	Gums
system, 264, 265	Isolation of microorganisms, 198	Activated sludge, acclimated,
NTA and salts	Metabolic pathways, 198	continuous-flow, 310
Model ecosystem, aquatic, pond	Silver	Hydrocarbons
system, 263	Activated sludge	Activated sludge, acclimated,
	Review, 22	continuous-flow, 310
Sewage, natural	Inhibitory (toxic) effects	Naphthalene and derivatives
Alkanoic acids and derivatives,	Review, 22	Activated sludge, acclimated,
polybasic	Sewage, municipal	continuous-flow, 310
Aerobic biodegradation, 157	Inhibitory (toxic) effects, 345	Phenol and derivatives
Sewage, natural, semi-continuous flow	Sludge acclimatization process	Activated sludge, 295
Benzoic acid and derivatives	Alcohols, primary aliphatic	Activated sludge, acclimated,
Metabolic pathways, 184	Activated sludge, acclimated,	continuous-flow, 364
Hydroquinone and derivatives	continuous-flow, 310	Activated sludge, acclimated, in-
Metabolic pathways, 184	Activated sludge, acclimated,	dustrial, 94
Pyrocatechol and derivatives	municipal, 491	
Metabolic pathways, 184	Alkanoic acids and derivatives	Aerobacter sp. 295
Resorcinol and derivatives		Arthrobacter sp. 295
Metabolic pathways, 184	Activated sludge, acclimated 446	Pseudomonas sp. 295
Sewage, synthetic		Polyethylene glycols, alkylphenoxy-
Benzenesulfonic acid, alkyl. long chain	Alkyl sulfoxides	Activated sludge, municipal, 421
Phosphate effect, 380	Activated sludge, 295	Polyethylene glycols, fatty ether
Temperature effect, 380	Aerobacter sp. 295	Activated sludge, municipal, 421
Benzenesuifonic acid, S-substituted alkyl	Arthrobacter sp. 295	Polymers
Aerated chamber die-away test	Pseudomonas sp. 295	Activated sludge, acclimated,
416	Amines, poly-, aliphatic	continuous-rlow, 310
River die-away test, 416	Activated sludge, acclimated,	Polyvinyl alcohol
Shake flask process, 416	continuous-flow, 310	Activated sludge, acclimated,
Structure-activity relationships	Amino acids and derivatives	continuous-flow, 310
416	Activated sludge, acclimated,	Propylene glycols
Chromium	municipal, 186	Activated sludge, 105
	Antibiotics	Proteins
Inhibitory (toxic) and stimulatory ef-	Activated sludge, semi-continuous	Activated sludge, acclimated,
fects, 170	flow, 525	continuous-flow, 310
Microbial acclimatization, 170	Benzenesulfonic acid, alkyl, long chain	Pulp and paper wastes
Cyanide	Activated sludge, municipal, 421	Activated sludge, acclimated,
Inhibitory (toxic) and stimulatory ef-	Benzenesulfonic acid, alkyl, short chain	continuous-flow, 310
fects, 170	Activated sludge, acclimated,	Quaternary ammonium compounds
		Activated sludge, acclimated.

continuous-flow, 310	Activated sludge	Structure-activity relationships
Starch and derivatives	Operational parameters, 591	17
Activated sludge, acclimated,	Sludge adaptation process, 591	Thiocyanic acid and salts
continuous-flow, 310	Sphaerotilus sp	Identification of microorganisms
Styrene and derivatives	Chromium	205, 206
Activated sludge, acclimated,	Inhibitory (toxic) effects, 437	Timber steam processing wastes
continuous-flow, 310	Copper	
Sugars and derivatives	Inhibitory (toxic) effects, 437	Aerobic biodegradation, 408
	Lead	Identification of microorganisms
Activated sludge, acclimated.	Inhibitory (toxic) effects, 437	408
continuous-flow, 310	Mercury, inorganic	Operational parameters, 408
Thiocyanic acid and salts	Inhibitory (toxic) effects, 437	Starch and derivatives
Activated sludge, acclimated.	Nickel	see also Alcohols
continuous-flow, 364	Inhibitory (toxic) effects, 437	Acinetobacter sp
Toluene and derivatives	Sugars and derivatives	Identification of microorganisms
Activated sludge, acclimated, in-		406
dustrial, 94	Inhibitory (toxic) effects, 409	Activated sludge
Xylenes and derivatives	Zinc	
Activated sludge, acclimated, in-	Inhibitory (toxic) effects, 437	Aerobic biodegradation, 507
dustrial, 94	Sporobolomyces sp	Substrate concentration effect
Sludge adaptation process	Alkanes	372
Alcohols, secondary aliphatic	Inhibitory (toxic) effects, 450	Activated sludge, acclimated,
Activated sludge, 591	Structure-activity relationships	continuous-flow
Alkanoic acids and derivatives	450	Operational parameters, 310
Activated sludge, 591	Alkenes	Sludge acclimatization process
Alkanoic acids and derivatives, long	Inhibitory (toxic) effects, 450	310
chain	Structure-activity relationships	Activated sludge, industrial and
Activated sludge, 591	450	municipal
Amines, poly-, aliphatic		Structure-activity relationships
Activated sludge, 540, 591	Spray irrigation systems	508
	Pulp and paper wastes	
Benzenesulfonic acid and non-alkyl	Review, 556	508
substituted derivatives	Stabilization pond	Activated sludge, municipal + starch
Activated sludge, 591	Zinc	plant wastes
ε-Caprolactam	Inhibitory (toxic) effects, 544	Operational parameters, 419
Activated sludge, 591	Substrate concentration effect	
Nitrobenzene and derivatives	544	Starch plant wastes effect, 419
Activated sludge, 591	• • •	Activated sludge, non-acclimated
Petrochemical wastes	Staphylococcus sp	Inhibitory (toxic) effects, 454
Activated sludge, 540, 591	Alkanoic acids and derivatives, long	Rate and selective adsorption
Polyethylene glycols	chain	454
Activated sludge, 591	Metabolic pathways, 273	Activated sludge, non-acclimated.
Polyvinyl alcohol	Structure activity relationships	municipal
Activated sludge, 591	273	Gravimetric assessment, 420
Solvent wastes	Alkanoic acids, sulfonated, long chain	Hach oxidation, 420
Activated sludge, 591	Bacteriocidal/bacteriostatic effects,	Respirometric studies, 420
= ·	330	Activated sludge, soap waste, 490
Sodium	Inhibitory (toxic) effects, 329	Activated sludge + Pseudomonas sp.
Activated sludge	Structure-activity relationships	490
Inhibitory (toxic) effects, 546	330	Aspergillus sp
Activated sludge, acclimated,	Amides, aliphatic, long chain	Tensile strength, 96
continuous-flow	Metabolic pathways, 273	Microbial population
Inhibitory (toxic) effects, 517	Structure-activity relationships	Metabolic pathways, 27
Lagoon pre-treatment	273	Microbial population, municipal wastes
Anaerobic biodegradation, 379	Amines, long chain	Identification of microorganisms
Soft drink wastes	Metabolic pathways, 273	406
Activated sludge	Structure-activity relationships	Microbial population, raw sewage
Glucose removal and polysaccharide	273	Aerobic biodegradation, 26
accumulation, 501		
Activated sludge, acclimated, industrial	Amino acids and derivatives	Microbial population, sewage, municipa
Identification of microorganisms	Metabolic pathways, 273	Biorefractory index, 199
502	Structure-activity relationships	Recommendations, wastewater treat-
	273	ment, 199
Soil systems, flooded and non-flooded	Cyanide	Penicillium sp
Phosphorodithioic acid and derivatives	Identification of microorganisms	Tensile strength, 96
Model ecosystem, terrestrial,	206	Pseudomonas sp., 490
simulated, 404	Phenol and derivatives	Identification of microorganisms
Pseudomonas sp	Identification of microorganisms	406
Model ecosystem, terrestrial,	205, 206	Trichoderma sp
simulated, 404	Quaternary ammonium compounds	Tensile strength, 96
	•	-

Solvent wastes

Staphylococcus sp (cont'd)

Sludge acclimatization process (cont'd)

Steroids	Structure-activity relationships (cont'd)	Structure-activity relationships (cont'd)
Activated sludge	Alcohols, secondary aliphatic	Alkanoic acids and derivatives,
Substrate concentration effect	Actinomyces sp, 153	polybasic
271	Activated sludge, 153, 386	Activated sludge, 386
Stilbene and derivatives	473 2 473	Alkanoic acids, sulfonated, long char
Activated sludge	Bacillus sp., 153, 473	Escherichia sp. 330
Aerobic biodegradation, 146	Bacterium sp. 153	Microbial population, sewage 328
175	Chromobacterium sp. 153 Micrococcus sp. 153	Salmonella sp. 330
Incineration, 146	Mycobacterium sp, 153	Staphylococcus sp. 330
Wet oxidation (Zimpro) reactor	Pseudomonas sp, 153, 473	Alkenes
146	Sarcina sp., 153	Achromobacter sp. 450
Activated sludge, single and two-stage reactors	Alcohols, tertiary aliphatic	Acinetobacter sp. 450, 522
Anaerobic biodegradation, 146	Activated sludge, 386	Alcaligenes sp, 523
Alcaligenes sp	Aldehydes	Arthrobacter sp. 450
Structure-activity relationships	Actinomyces sp. 153	Aspergillus sp, 450
523	Activated sludge, 153, 473	Brevibacterium sp., 450
Biodegradation, environmental aspects	Activated sludge, acclimated	Candida sp. 450
Review, 56	390 B. (6-1-153, 473	Cladosporium sp, 450
Gram-negative rods	Bacillus sp. 153, 473	Corynebacterium sp. 450
Structure-activity relationships	Bacterium sp. 153 Chromobacterium sp. 153	Cunninghameila sp., 450 Eupenicillium sp., 450
523	Microbial population, loam, 485	Flavobacterium sp. 450
Pseudomonas sp	Micrococcus sp, 153	Gram-negative rods, 523
Metabolic pathways, 137	- Mycobacterium sp. 153	Mycobacterium sp. 450
Trametes sp	Pseudomonas sp. 153, 473	Nocardia sp. 450
Metabolic pathways, 137	Sarcina sp., 153	Rhodotorula sp. 450
Storage oxidation basins	Alkanes	Sparobolomyces sp. 450
Pulp and paper wastes	Achromobacter sp. 450	Alkenoic acids and derivatives, long
Review, 556	Acinetobacter sp. 450	chain
Streptomyces sp	Arthrobacter sp., 450	Acinetobacter sp. 522
Carbamic acid and derivatives Biological membrane filtration	Aspergillus sp. 450	Activated sludge, 274
333	Brevibacterium sp. 450	Aspergillus sp. 97
Model ecosystem, aquatic, simulated,	Candida sp. 450 Cladosporium sp. 450	Microbial population, soil burial
333	Corynebacterium sp. 450	Alkyl sulfates, long chain
Rubber, vulcanized, 87	Cunninghamella sp. 450	Activated sludge, 302
Structure-activity relationships	Eupenicillium sp. 450	Amides, aliphatic
Abietic acid and derivatives	Flavobacterium sp. 450	Activated sludge, 274
Activated sludge, 289	Mycobacterium sp. 450	Alcaligenes sp, 120
Activated sludge, municipal	Nocardia-sp, 450	Aspergillus sp., 120
Microbial population, soils, 527	Rhodotorula sp. 450	Flavobacterium sp., 120
Adipic acid and derivatives	Sporobolomyces sp. 450	Microbial population, soils, 119
Microbial population, soils, 119	Alkanes, cyclic	Amides, aliphatic, long chain
Alcohols, alicyctic	Acinetobacter sp. 522	Activated sludge, 274
Activated sludge, 386	Alkanes, long chain, branched	Alcaligenes sp, 120
Alcohols, benzylic	Acinetobacter sp. 522	Aspergillus sp., 120
Actinomyces sp. 153	Alkanes, long chain, linear	Escherichia sp. 273
Activated sludge, 153, 473 Bacullus sp., 153, 473	Acinetobacter sp. 522 Alkanoic acids and derivatives	Flavobacterium sp. 120 Pseudomonas sp. 273
Bacterium sp. 153	Actinomyces sp, 153	Staphylococcus sp. 273
Chromobacterium sp. 153	Activated sludge, 153, 274	Amines, long chain
Micrococcus sp., 153	473	Escherichia sp. 273
Mycobacterium sp. 153	Bacillus sp., 153, 473	Microbial population, river water
Pseudomonas sp. 153, 473	Bacterium sp, 153	427
Sarcina sp. 153	Chromobacterium sp, 153	Pseudomonas sp. 273
Alcohols, primary aliphatic	Micrococcus sp, 153	Review, 425
Actinomyces sp. 153	Mycobacterium sp., 153	Staphylococcus sp. 273
Activated sludge, 153, 386	Pseudomonas sp. 153, 473	Amines, poly-, aliphatic
473 Parallus en 182 172	Review, 500	Activated sludge, 386
Bacıllus sp. 153, 473 Bacterium sp. 153	Sarcina sp. 153	Microbial population, river water 427
Chromobacterium sp. 153	Alkanoic acids and derivatives, long chain	Microbial population, soils, 119
Micrococcus sp. 153	Acinetopacter sp. 522	Amino acids and derivatives
Mycobacterium sp. 153	Activated sludge, 274, 302	Acinetobacter sp. 522
Pseudomonas sp, 153, 473	Escherichia sp. 273	Activated sludge, 274, 393
Review, 500	Pseudomonas sp. 273	Escherichia sp. 273
Sarcina sp. 153	Staphylococcus sp. 273	Pseudomonas sp, 273

ractare-activity relationships (cont a)	Structure-activity relationships (control)	Structure-activity relationships (cont'd)
Review, 500	Activated studge, municipal, 528	Naphthalene and derivatives
Staphylococcus sp. 273	Alcaligenes sp. 138, 523	Activated sludge, 101
Aniline and derivatives	Cunninghamella sp. 528	Activated sludge, boiling-inactivated,
Activated sludge, 386	Gram-negative rods, 523	101
Activated sludge, acclimated	ε-Caprolactam	Activated sludge, formaldehyde-
391, 392	Activated sludge, 386	
	Chloroaikylenes	inactivated, 101
Activated sludge, continuous-flow		Activated sludge, industrial and
159	Activated sludge, municipal, 201	municipal, 13
Activated sludge, industrial and	528	Activated sludge, municipal, 369
municipal, 13	Cunninghamella sp., 528	Alcaligenes sp. 523
Activated sludge, municipal, 369	Cresols and derivatives	Gram-negative rods, 523
Inhibitory (toxic) effects, 159	Activated sludge, 386	Nicotinic acid
Review, 388	Activated sludge, acclimated	Activated sludge, 393
Sewage, municipal, 159	389	Nitrobenzene and derivatives
Antibiotics	Activated sludge, municipal, 369	Activated sludge, 386
Activated sludge, 386	Cumene and derivatives	Activated sludge, acclimated
Aromatic compounds, dicyclic	Activated sludge, 386	390, 391
Alcaligenes sp. 523	Cyanuric acid and derivatives	Activated studge, municipal, 369
Gram-negative rods, 523	Activated sludge, 393	Review, 388
Azo compounds	Cycloaliphatics, substituted	Nylons
Activated sludge, 530	Activated sludge, 386	Microbial population, soils, 119
Azo dyes	DDT, Methoxychlor and metabolites	Phenoi and derivatives
Activated sludge, 101, 530	Microbial population, loam, 485	Activated sludge, 386
Activated sludge, to1, 550 Activated sludge, boiling-inactivated,	-Dyes	
		Activated sludge, acclimated
101	Activated sludge, 530	389
Activated sludge, formaldehyde-	Activated sludge, municipal, 369	Review, 388
inactivated, 101	Dyes, acid	Phenylacetic acid and derivatives
Activated sludge, municipal, 369	Activated sludge, 530	Microbial population, loam, 485
Benzene and derivatives	Dyes, anthraquinone	Phloroglucinol
Alcaligenes sp. 523	Activated sludge, 101	Activated sludge, acclimated
Gram-negative rods, 523	Activated sludge, boiling-inactivated,	389
Benzenesulfonic acid and non-alkyl	101	Phthalic acid and derivatives
substituted derivatives		
	Activated sludge, formaldehyde-	Activated sludge, 386
Activated sludge, 386	inactivated, 101	Penicillium sp., 116
Activated sludge, municipal, 369	Explosives	Pimaric acid and derivatives
Benzenesulfonic acid, linear alkyl, long	Activated sludge, 386	Activated sludge, 289
chain	Explosives, organic	Poly(alkyl-β-propiolactones)
Activated sludge, 302	Activated sludge, acclimated	Alcaligenes sp, 503
Activated sludge, acclimated,	390	Aspergillus sp., 10
continuous-flow, 220	Furan and derivatives	Aureobasidium sp. 10
Activated sludge, continuous-flow	Activated sludge, 386	Fungus, Pl. 503
261	Herbicides, monuron type and	Penicillium sp, 10
Microbial population, river water	metabolites	Polyamides
sediment, 135	Activated sludge, continuous-flow	Alcaligenes sp, 12
Review. 492	159	Aspergillus sp., 12
Benzenesulfonic acid, non-linear alkyl,	Sewage, municipal, 159	Flavobacterium sp., 12
long chain	Heteroaromatics and derivatives, dicyclic	Microbial population, soils, 119
Activated sludge + synthetic sewage,		Polybutadienes
456	Hydroquinone and derivatives	Acinetobacter sp. 522
Benzenesulfonic acid, S-substituted alkyl	Actinomyces sp. 153	Polycaprolactone
Activated sludge, acclimated,	Activated sludge, 153, 473	Alcaligenes sp. 503
municipal, 416		
	Activated sludge, acclimated	Aspergillus sp. 97
Activated sludge, municipal, 416	389	Fungus, Pl. 503
Microbial population, river water	Bacillus sp, 153, 473	Microbial population, soil burial
416	Bacterium sp, 153	97
Sewage, synthetic, 416	Chromobacterium sp. 153	Microbial population, soils, 119
Benzoic acid and derivatives	Micrococcus sp. 153	Polychlorinated biphenyls
Activated sludge, 386, 473	Mycobacterium sp. 153	Acinetobacter sp. 138
Activated sludge, acclimated	Pseudomonas sp. 153, 473	Activated sludge, municipal, 201
392	Sarcina sp. 153	528
Alcaligenes sp. 410	Ketones, aliphatic	Alcaligenes sp. 138
Bacillus sp. 473	• • • • • • • • • • • • • • • • • • • •	Cunninghamella sp. 528
	Activated sludge, 386, 473	
Pseudomonas sp. 410, 473	Bacıllus sp. 473	Microbial population, soils, 527
Biphenyl and derivatives	Microbial population, loam, 485	Nocardia sp. 24
Acinetobacter sp. 138	Pseudomonas sp. 473	Pseudomonas sp. 24
Activated sludge, industrial and	Kraft pulp wastes	Polychlorobenzenes and derivatives
municinal 13	Activated chidae 190	Alcalmanas en 110

tructure-activity relationships (cont a)	Structure-activity relationships (cont.d)	Styrene and derivatives
Pseudomonas sp. 410	wastes, 17	Activated sludge, 341
Polyesters	Microbial population, river water	Aerobic biodegradation, 146
Alcaligenes sp. 503	427	230
Aspergillus sp. 97	Review, 425	Incineration, 146
Fungus, Pl, 503	Staphylococcus sp. 17	Wet oxidation (Zimpro) reactor
Microbial population, soil burial	Resorcinol and derivatives	146
97	Actinomyces sp., 153	Activated sludge, acclimated,
Polyethylene	Activated sludge, 153, 386	continuous-flow
Aspergillus sp. 97	173	Operational parameters, 310
Microbial population, soil burnal	Activated sludge, acclimated	Sludge acclimatization process
97	389	310
Polyethylene glycols	Bacıllus sp. 153, 473	Activated sludge, single and two-stage
Activated sludge, 386	Bacterium sp. 153	reactors
Polyethylene glycols, alkylphenoxy-	Chromobacterium sp, 153	Anaerobic biodegradation, 146
Microbial population, river water	Micrococcus sp., 153	Ozone, stirred-tank reactor, continuous
428	Mycobacterium sp., 153	flow
Review, 321, 451	Pseudomonas sp. 153, 473	Operational parameters, 580
	Sarcina sp., 153, 475	Ozonization, 580
Polyethylene glycols, fatty ether		
Activated sludge, 302	Salicylic acid and derivatives	Pseudomonas sp
Microbial population, river water	Activated sludge, 386	Identification of microorganisms
428	Activated sludge, acclimated	376
Review, 321, 451	390	Psychrophilic temperature effect
Polymers	Activated sludge, municipal, 369	250
Review. 218	Starch and derivatives	Screening tests, 376
Polypropylene	Activated sludge, industrial and	Time-course kinetics, 250
Aspergillus sp. 97	municipal, 508	Sewage, acclimated, municipal
Microbial population, soil burial	Stilbene and derivatives	Petrochemical wastewater treatment
97	Alcaligenes sp. 523	51
Polystyrenes	Gram-negative rods, 523	Sugars and derivatives
Aspergillus sp. 97	Sugars and derivatives	see also Alcohols; Confectionary wastes
Microbial population, soil burial	Acinetobacter sp. 522	
97	Activated sludge, 386	Acinetobacter sp
	G .	Metabolic pathways, 522
Propylene glycols	Surtactants, amonic	Structure-activity relationships
Actinomyces sp. 153	Review, 321, 492	522
Activated sludge, 153, 473	Surfactants, cationic	Activated sludge, 106
Bacillus sp. 153, 473	Review, 425	Aerobic biodegradation
Bacterium sp., 153	Surfactants, nonionic	386
Chromobacterium sp. 153	Review, 321, 492	Glucose removal and polysaccharide
Micrococcus sp., 153	Surfactants, tetrapropylene	accumulation, 501
Mycobacterium sp., 153	Review. 492	Inhibitory (toxic) effects, 66
Pseudomonas sp. 153, 473	Tetralin and derivatives	Metabolic pathways, 596
Sarcina sp. 153	Alcaligenes sp. 523	Structure-activity relationships
Proteins	Gram-negative rods, 523	386
Microbial population, soils, 119	Toluene and derivatives	Substrate concentration effect
		66, 372
Pulp and paper wastes	Activated sludge, 386	Activated sludge, acclimated.
Activated sludge, 289	Activated sludge, acclimated	
Pyridine and derivatives	390, 392	continuous-flow
Activated sludge, 393	Toluic acid and derivatives	Operational parameters, 310
Pyrocatechol and derivatives	Alcaligenes sp, 410	Sludge acclimatization process
Actinomyces sp. 153	Pseudomonas sp. 410	310
Activated sludge, 153, 386	Urea and derivatives	Activated sludge, municipal
473	Activated sludge, 393	Aerobic biodegradation, 457
Activated sludge, acclimated	Vegetable oils and fats	Activated sludge, non-acclimated,
389	Aspergillus sp. 97	municipal
Bacillus sp., 153, 473	Microbial population, soil burial	Aerobic biodegradation, 18
Bacterium sp. 153	97	Gravimetric assessment, 420
Chromobacterium sp., 153	Xylenes and derivatives	Hach oxidation, 420
Micrococcus sp. 153	Activated sludge, acclimated	Respirometric studies, 420
Mycobacterium sp, 153	392	Trickling filters, 18
Pseudomonas sp. 153, 473		Activated sludge, OECD-specified
	Activated sludge, industrial and	Interlaboratory company 500
Sarcina sp. 153	municipal, 13	Interlaboratory comparison, 590
Pyrrole	Alcaligenes sp. 410	Static vs continuous activation
Activated sludge, 393	Pseudomonas sp, 410	method, 590
Quaternary ammonium compounds	Xylenols and derivatives	Activated sludge, recycled concentration
Microbial population, fresh water	Activated sludge, 289, 386	Biomass yield, effect on, 319
17	Activated sludge, acclimated	Shock loadings effect, 319
Microbial population, municipal	389	Activated sludge, syntnetic

Sulfanilic acid and derivatives (cont'd) Surfactants, anionic (cont'd) Sugars and derivatives (cont'd) acids, long chain, esters, Schizosaccharomyces sp Flocculation, nutritional effects Alkanoic acids, sulfonated, long Identification of microorganisms enain: Alkenoic acids and Bacıllus sp 377 derivatives; Alkyl sulfates, long Aerobic biodegradation, 403 Sulfate chain; Alkyl sulfonates and Stripping and metabolic mechanisms Activated sludge derivatives: Amides, aliphatic, Inhibitory (toxic) effects, 588 403 long chain, sulfated; Amino Haliscomenobacter sp Activated sludge, industrial Inhibitory (toxic) effects, 409 acids and derivatives: Identification of microorganisms Identification of microorganisms Benzenesultinic acid and derivatives; Benzenesulfonic Biodegradability, ultimate, 487 Sulfide acid, alkyl, long chain; Review, 487 Activated sludge Benzenesulfonic acid, alkyl. Lagoons, aerated, industrial site Anaerobic digestion reactor, 344 short chain; Benzenesulfonic Aerobic biodegradation, 215 Innibitory (toxic) effects, 131 acid and non-alkyl substituted Detoxification, 215 231, 344 derivatives; Benzenesulfonic Microbial population, acclimated. Operational parameters, 131 sewage acid, linear alkyl, long chain; Activated sludge, municipal Benzenesulfonic acid, non-linear Aerobic biodegradation, 402 Aerobic biodegradation, 79 403 alkyl, long chain; Pseudomonas sp Benzenesulfonic acid. Operational parameters, 402 Inhibitory (toxic) effects, 131 S-substituted alkyl; Dobane JN-Stripping and metabolic mechanisms: Operational parameters, 131 Q sulfonate; "Miracle White" 402, 403 Sulfite liquor (Miracle White Co.); Microbial population, non-acclimated, Activated sludge Phosphonic acid derivatives, sewage Aeration digestion reactors Aerobic biodegradation, 402 alkyl poly-: Polyethylene compared, 520 glycois, alkylphenoxy-; Polyethylene glycols, fatty ether, sulfate; "Surf" (Lever Operational parameters, 402 Foam process, 594 Stripping and metabolic mechanisms i Operational parameters, 520 402 Activated sludge, continuous-flow Brothers); Tallow derivatives: Microbial population, river water Aerobic biodegradation, 301 "Tide" (Proctor and Gamble) River die-away test, 424 Biomass yield, effect on, 301 Microbial population, sewage, municipal Biodegradability Candida sp Biorefractory index, 189, 199 Review, 455 Foam process, 594 Inhibitory (toxic) effects Recommendations, wastewater treat-Hyalodendron sp ment, 189. 199 Review, 321 Foam process, 594 Sewage, municipal Metabolic patnways Phialophora sp Review, 54, 321, 492 Nutritional effects, 90 Foam process, 594 Structure-activity relationships Sphaerotilus sp Trichosporon sp Inhibitory (toxic) effects, 409 Review, 321, 492 Foam process, 594 Tar plant wastes Surfactants, anionic-cationic complexed Biodegradation, accelerative effect, Sulfonated surfactants Activated sludge see Alkanoic acids, sulfonated; Alkyl 78 Thiotrix sp Aerobic digestion reactor, 234 sulfates; Alkyl sulfonates Anaerobic digestion reactor, 234 Inhibitory (toxic) effects, 409 Sulfophenylalkanoic acids Surfactants, cationic Sulfanilic acid and derivatives see also Alkanoic acids and derivatives; see Amines, alicyclic; Amines, long Achromobacter sp Benzenesulfonic acid, alkyl, chain; Amines, poly-, aliphatic; Nitriles, long chain; Quaternary Identification of microorganisms short chain 377 Microbial population, fresh water ammonium compounds Activated sludge, municipal Metabolic pathways, 109 Bacteriocidal/bacteriostatic effects Correlative test evaluations Model ecosystem, aquanc, natural Review, 425 151 109 Structure-activity relationships Bacıllus sp 'Surf'' (Lever Brothers) Review, 425 Identification of microorganisms Microbial population, brackish water Surfactants, nonionic 377 Aerobic biodegradation, 76 see also Alcohols, primary, long chain; Flavobacterium sp Atkanoic acids, long chain, Surfactants Identification of microorganisms esters; Alkyl sulfates, long Bacteriocidal/bacteriostatic effects 377 Review, 440 chain; Amines, long chain; Cir-Mycobacterium sp Inhibitory (toxic) effects rasols: Dobanol 25-9; Dobanol Identification of microorganisms Review, 440 45-7; Emkapyl 1839; 377 Ethomeens: Hexapon: Lauropal; Marlipol: Plurafac Metabolic pathways Pseudomonas sp Review, 519 Identification of microorganisms RA40; Pluronics; Poly(ethylene Surfactants, anionic 377 glycol-propylene glycol); see also Alkyl sulfates, long chain: Rhodotorula sp Alkanes, long chain, linear; Polyethylene glycols. Identification of microorganisms Alkanoic acids and derivatives; aikyiphenoxy-; Polyethylene 377 Alkanoic acids and derivatives, glycols, fatty amine; Saccharomyces sp Polyethylene glycols, fatty ester: long chain; Alkanoic acids and Identification of microorganisms Polyethylene glycols, fatty derivatives, polybasic; Alkanoic, 377

Nitrobacter sp ether; Renex 20; Starch and Detoxification, 215, 573 Respirometric studies, 64 Pseudomonas sp derivatives; Sugars and Vitrosomas sp derivatives; Triton X100; Tween Metabolic pathways, 59 Respirometric studies, 64 80 Tetralin and derivatives Pseudomonas sp. 490 Biodegradability Activated sludge, 341 Sewage, municipal Review, 455 Alcaligenes sp Aerobic biodegradation, 574 Inhibitory (toxic) effects Structure-activity relationships Time-course kinetics, 574 Review, 321 523 Thermactinomyces sp Metabolic pathways Flavobacterium sp Review, 54, 321, 492 Cellulose and derivatives Metabolic pathways, 335 Fermentation, batch system, 292 Structure-activity relationships Gram-negative rods Michaelis-Menten coefficients Review, 321, 492 Structure-activity relationships 292 Surfactants, tetrapropylene Metabolic pathways Thermomonospora sp Oscillatoria sp Review, 492 Amino acids and derivatives Metabolic pathways, 70 Structure-activity relationships Time-course kinetics, 82 Pseudomonas sp Review, 492 Cellulose and derivatives Metabolic pathways, 335 Time-course kinetics, 82 Synthetic organics Psychrophilic temperature effect Thiobacıllus sp Microbial biodegradation 250 Review, 505 Time-course kinetics, 250 Coke oven wastes Thiosulfate oxidation, 256 Tallow derivatives Textile wastes Thiocyanic acid and saits Activated sludge, acclimated, municipal Activated sludge Thiosulfate oxidation, 256 Aerobic biodegradation, 327 Aerobic biodegradation, 29, 181 Microbial population, river water Thiosulfate 398 River die-away test, 424 Thiosulfate oxidation, 256 Batch vs continuous-flow system Thiocyanic acid and salts Taloramyces sp 181 Inhibitory (toxic) effects, 144 Activated sludge Herbicides, propanil type and 290, 453 Inhibitory (toxic) effects, 66 metabolites Metabolic pathways, 257 Operational parameters, 529 231, 480 Review, 489 Nitrification effect, 480 Herbicides, urea Time-course kinetics, 136, 290 Substrate concentration effect Metabolic pathways, 257 352, 355 66 Tannery wastes Activated sludge, acclimated Thiosulfate oxidation, 256 see also Proteins Aerobic biodegradation, 397 Activated sludge, acclimated, Activated sludge Activated sludge, acclimated, municipal continuous-flow Inhibitory (toxic) effects, 131 Aerobic biodegradation, 568 Inhibitory (toxic) effects, 364 Operational parameters, 131 Operational parameters, 568 Sludge acclimatization process Activated sludge, municipal Activated sludge, industrial Aerobic biodegradation, 79 Aerobic biodegradation, 55, 470 Activated sludge, industrial Activated sludge, tannery-activated Overview, 55 Bioreactors compared, 205 Decomposability, 513 Photodegradation, 470 Conversion and retention time Pseudomonas sp River die-away test, 470 kinetics, 205 Inhibitory (toxic) effects, 131 Time-course kinetics, 55 Identification of microorganisms Operational parameters, 131 Volatilization, 470 205, 206 Tar plant wastes Activated sludge, non-acclimated Activated sludge, second-stage Activated sludge Inhibitory (toxic) effects, 454 Laboratory-pilot plant studies Aerobic biodegradation, 78 Rate and selective adsorption 145 Sugars and derivatives 454 Operational parameters, 145 Biodegradation, accelerative effect, Bacıllus sp Activated sludge, oxygen-activated, Identification of microorganisms municipal Tellurium, organo-205, 206 Respirometric studies, 64 Biodegradation, environmental aspects Activated sludge, soap waste, 490 Citrobacter sp Review, 239 Activated sludge + Pseudomonas sp, Identification of microorganisms Terephthalic acid and derivatives 190 205, 206 Activated sludge Microbial population Escherichia sp Aerobic digestion reactors compared, Metabolic pathways, 27 Identification of microorganisms 287 205, 206 Microbial population, liquid-enriched Metabolic pathways Microbial population, lagoons Metabolic pathways, 322 Review, 259 Microbial population, sewage, municipal Isolation of microorganisms, 481 Biorefractory index, 199 Terpene compounds Model ecosystem, aquatic, simulated, see also Alcohols; Alcohols, alicyclic; Recommendations, wastewater treat-Alkanes: Alkenes; Ketones, ment, 199 Percolation system, 481 Microbial population, soil-liquid Proteus sp aliphatic Identification of microorganisms Lagoons, aerated, industrial site Metabolic pathways, 322 Microbial population, soils 205, 206 Aerobic biodegradation, 215 Metabolic pathways, 322 Pseudomonas sp 573

Terpene compounds (cont'd)

Surfactants, nonionic (cont'd)

Textile wastes (cont'd)

Thiocyanic acid and salts (cont'd) Identification of microorganisms 205, 206	Timber steam processing wastes (cont'd) Corynebacterium sp Aerobic biodegradation, 408	Toluene and derivatives (cont'd) Time-course kinetics, 390, 392 Activated sludge, acclimated, industrial
Staphylococcus sp Identification of microorganisms	Identification of microorganisms 408	Sludge acclimatization process 94
205. 206	Operational parameters, 408	Alcaligenes sp
Thiobacillus sp	Cytophaga sp	Metabolic pathways, 37
Thiosulfate oxidation, 256	Aerobic biodegradation, 408 Identification of microorganisms	Cladosporium sp
Thiosuifate	408	Nutritional effects, enrichment 552
Inhibitory (toxic) effects, 256	Operational parameters, 408	Flavobacterium sp
Thiols	Flavobacterium sp	Metabolic pathways, 232, 335
Activated sludge, acclimated,	Aerobic biodegradation, 408	Microbial population
continuous-flow	Identification of microorganisms	Metabolic pathways, 232
Aerobic biodegradation, 112	408	Microcoecus sp
Activated sludge, acclimated, sedimenta- tion chamber	Operational parameters, 408	Metabolic pathways, 232
Aerobic biodegradation, 112	Micrococcus sp	Vocardia sp
	Aerobic biodegradation, 408	Metabolic pathways, 232, 444
Thiophene Microbial biodegradation	Identification of microorganisms	Pseudomonas sp
Review, 521	408	Identification of microorganisms
	Operational parameters, 408 Pseudomonas sp	376
Thiophenois Acinetobacter sp	Aerobic biodegradation, 408	Metabolic pathways, 232, 335 Psychrophilic temperature effect
Metabolic pathways, 542	Identification of microorganisms	250
Pseudomonas sp	408	Screening tests, 376
Metabolic pathways, 542	Operational parameters, 408	Time-course kinetics, 250
Trichosporon sp	Staphylococcus sp	Sewage, acclimated, municipal
Metabolic pathways, 542	Aerobic biodegradation, 408	Petrochemical wastewater treatment
Metabolic pathways, co-metabolism	Identification of microorganisms	51
542	408	Toluene diisocyanate wastes
Thiosulfate	Operational parameters, 408	Ozone, stirred-tank reactor, continuous
Inhibitory (toxic) effects	Tin	flow
Thiocyanic acid and salts, 256	Sewage, municipal Inhibitory (toxic) effects, 345	Operational parameters, 580
Thiobacillus sp		Ozonization, 580
Thiosulfate oxidation, 256	Tin compounds, organic Activated sludge	Toluic acid and derivatives
Thiotrix sp	Inhibitory (toxic) effects, 483	see also Benzoic acid and derivatives
Sugars and derivatives	589	Activated sludge, acclimated
Inhibitory (toxic) effects, 409	Activated sludge, municipal	Aerobic biodegradation, 397 Alcaligenes sp
"Tide" (Proctor and Gamble)	Inhibitory (toxic) effects, 478	Inhibition of benzoic acid turnover.
Microbial population, brackish water Aerobic biodegradation, 76	Operational parameters, 478	410
<u>-</u>	TNT	Structure-activity relationships
Timber steam processing wastes	Activated sludge, municipal, continuous-	
Achromobacter sp Aerobic biodegradation, 408	flow	Pseudomonas sp
Identification of microorganisms	Aerobic biodegradation, 360	Inhibition of benzoic acid turnover,
408	Inhibitory (toxic) effects, 360	410
Operational parameters, 408	Toilet paper, dyed	Metabolic pathways, 8, 539
Activated sludge, acclimated, municipal	Cellulomonas sp	Structure-activity relationships
Aerobic biodegradation, 408	Inhibitory (toxic) effects, 537	410
Identification of microorganisms	Metabolic pathways, 537	Trametes sp
408	Pulp concentration effect, 537 Myrothecium sp	Cinnamic acid and derivatives Metabolic pathways, 137
Operational parameters, 408	Inhibitory (toxic) effects, 537	Lignin-related compounds
Arthrobacter sp	Metabolic pathways, 537	Metabolic pathways, 137
Aerobic biodegradation, 408 Identification of microorganisms	Pulp concentration effect, 537	Phenylacetic acid and derivatives
408	Toluene and derivatives	Metabolic pathways, 137
Operational parameters, 408	Acinetobacter sp	Stilbene and derivatives
Bacillus sp	Metabolic pathways, 232	Metabolic pathways, 137
Aerobic biodegradation, 408	Activated sludge, 173, 341	Xylenols and derivatives
Identification of microorganisms	Aerobic biodegradation, 386	Metabolic pathways, 137
408	Petrochemical wastewater treatment	Triazines
Operational parameters, 408	324	see Heroicides, atrazine type
Coliform bacteria, unidentified	Structure-activity relationships 386	Trichoderma sp
Aerobic biodegradation, 408 Identification of microorganisms	Activated sludge, acclimated	Phenoi-formaldehyde resin
408	Structure-activity relationships	Biodegradation, rates compared
Operational parameters, 408	390, 392	248
Obstational Serminators, 100		

Evolution of bacterial populations Lysol Poly(methyl methacrylate) 16 Inhibitory (toxic) effects, 306 Biodegradation, rates compared Tritox-50 Marlipol 248 Activated sludge, non-acclimated, Activated sludge Polystyrenes municipal, 18 Aerobic biodegradation, 346 Biodegradation, rates compared Municipal wastewaters 248 Unsaturated compounds Activated sludge, 484 Starch and derivatives see Alkenes: Alkynes Phenol and derivatives Tensile strength, 96 Urea and derivatives Corynepacterium sp. 374 Activated sludge Trichosporon sp Plurafac RA40 Amino acids and derivatives Inhibitory (toxic) effects, 150 Activated sludge, non-acclimated, Metabolic pathways, 542 Nitrification, 150, 413 municipal, 18 Metabolic pathways, co-metabolism Structure-activity relationships 393 542 Activated sludge, non-acclimated, Furan and derivatives Activated sludge, industrial municipal, 18 Identification of microorganisms Aerobic biodegradation, 19 Polyethylene glycols, fatty ester Metabolic pathways, 19 163 Activated sludge, non-acclimated. Ketones, aliphatic Bacillus sp municipal, 18 Aerobic biodegradation, 19 Metabolic pathways, 111 Polyethylene glycois, fatty ether Metabolic pathways, 19 Time-course kinetics, 111 Activated sludge, non-acclimated, Lignin sulfonates Cunninghamella sp municipal, 18 Aerobic biodegradation, 19 Metabolic pathways, 555 Pulp and paper wastes Metabolic pathways, 19 Microbial population, continuous-flow Review, 556 Adaptation of microorganisms Phenol and derivatives Quaternary ammonium compounds Batch vs continuous-flow system Inhibitory (toxic) effects, 306 Psychrophilic temperature effect Renex 20 Metabolic pathways, 579 399 Activated sludge, non-acclimated, Microbial population, fresh water + Time-course kinetics, 579 municipal, 18 Polycaprolactone sewage Sugars and derivatives Operational parameters, 32 Metabolic pathways, 111 Activated sludge, non-acclimated, Time-course kinetics, 111 Pulp and paper wastes municipal, 18 Foam process, 594 Sewage, acclimated, municipal Triton X100 Petrochemical wastewater treatment Sulfite liquor Activated sludge, non-acclimated, Foam process, 594 municipal, 18 Thiophenois Sewage, municipal Trickling filters, pilot plant Metabolic pathways, 542 Nutritional effects, 90 Cresols and derivatives Metabolic pathways, co-metabolism Vanadium Aerobic biodegradation, 74 542 Activated sludge Phenol and derivatives Aerobic biodegradation, 280 Trickling filters Aerobic biodegradation, 74 Freundlich adsorption isotherms Alkyl halides Polychlorobenzenes and derivatives Corynebacterium sp. 374 280 Aerobic biodegradation, 74 Inhibitory (toxic) effects, 546 Amines, long chain Xvlenols and derivatives Activated sludge, non-acclimated. Operational parameters, 280 Aerobic biodegradation, 74 municipal, 18 Triclosan Vanillic acid and derivatives Antibiotics Activated sludge Activated sludge Inhibitory (toxic) effects, 308 Inhibitory (toxic) effects, 367 Anaerobic digestion reactor, 196 Chloramine and derivatives Substrate concentration effect Moraxella sp Inhibitory (toxic) effects, 306 367 Metabolic pathways, 192, 468 Pseudomonas sp Nocardia sp Corynebacterium sp. 374 Inhibitory (toxic) effects, 367 Metabolic pathways, 179 Coke oven wastes Substrate concentration effect Penicillium sp Microbial population, 479 367 Metabolic pathways, 192, 468 Copper 2,3,5-Triphenyltetrazolium chloride Pseudomonas sp Inhibitory (toxic) effects, 208 Activated sludge Metabolic pathways, 539 499 Inhibitory (toxic) effects, 53 Vegetable oils and fats Emkapyl 1839 Pseudomonas sp Activated sludge, non-acclimated, Activated sludge, 106, 341 Inhibitory (toxic) effects, 53 municipal, 18 Aspergillus sp Triton X100 Ethomeens Structure-activity relationships Activated sludge, non-acclimated, Activated studge, non-acclimated, municipal, 18 municipal Microbial population, soil burial Aerobic biodegradation, 18 Hexapon Structure-activity relationships Activated sludge, non-acclimated, Trickling filters, 18 97 Microbial population, municipal wastes municipal, 18 Verticillium sp Evolution of bacterial populations Lauropal Polyethylene Activated sludge, non-acclimated, 16 Isolation of microorganisms, 4 municipal, 18 Microbial population, river water

Trickling filters (cont'd)

Trichoderma sp (cont'd)

Triton X100 (cont'd)

Vibrio sp	Xanthomonas sp (cont'd)	Xylenois and derivatives (cont'd)
Acinetobacter sp	Polyethylene glycols, fatty ester	Structure-activity relationships
Metabolic pathways, 550	Aerobic biodegradation, 431	289. 386
Alcohols, alicyclic	Polyethylene glycols, fatty ether	Activated sludge, acclimated
inhibitory (toxic) effects, 38	Aerobic biodegradation, 431	Structure-activity relationships
Amides, aliphatic	Xylenes and derivatives	389
Inhibitory (toxic) effects, 277	Acinetobacter sp	Time-course kinetics, 389
Isolation of microorganisms, 278	Metabolic pathways, 232	Activated sludge, synthetic
Nutritional parameters, 278	Activated sludge, 173	Flocculation, nutritional effects
Amines, alicyclic Inhibitory (toxic) effects, 38	Activated sludge, acclimated	36 Arthrobacter sp
Amines, aliphatic	Structure-activity relationships	Model ecosystem, terrestrial, natural
Inhibitory (toxic) effects, 277	392	545
Isolation of microorganisms, 278	Time-course kinetics, 392	,
Nutritional parameters, 278	Activated sludge, acclimated, industrial Sludge acclimatization process	Model ecosystem, terrestrial, natural
Coryneform bacteria	94	545
Metabolic pathways, 550	Activated sludge, industrial and	Bacıllus sp
Cycloaliphatics, substituted	municipal	Model ecosystem, terrestrial, natural
Inhibitory (toxic) effects, 38	Inhibitory (toxic) effects, 13	545
Ketones, aliphatic	Respirometric studies, 13	Brevibacterium sp
Inhibitory (toxic) effects, 38	Structure-activity relationships, 13	Model ecosystem, terrestrial, natural
Leather, artificial, processing wastes	Alcaligenes sp	545
Inhibitory (toxic) effects, 277	Inhibition of benzoic acid turnover,	Flavobacterium sp
Oil refinery wastes, 40	410	Model ecosystem, terrestrial, natural
Petrochemical wastes, 40	 Structure-activity relationships 	545
Petroleum	410	Fusarium sp
Metabolic pathways, 550 Phenol and derivatives	Cladosporium sp	Metabolic pathways, 188, 373
Identification of microorganisms	Nutritional effects, enrichment	Lagoons, aerated, industrial site Aerobic biodegradation, 215
71	552	Detoxification, 215
Pseudomonas sp	Flavobacterium sp	Metabolic pathways
Metabolic pathways, 550	Metabolic pathways, 232, 335 Microbial population	Review, 325
Vorticella sp	Metabolic pathways, 232	Microbial population + synthetic
Chromium	Microbial population, acclimated	sewage
Inhibitory (toxic) effects, 486	Aerobic biodegradation, 351	Time-course kinetics, 384
Copper	Micrococcus sp	Micrococcus sp
Inhibitory (toxic) effects, 486	Metabolic pathways, 232	Model ecosystem, terrestrial, natural,
Lead	Nocardia sp	545
Inhibitory (toxic) effects, 445	Metabolic pathways, 232	Mycobacterium sp
Mercury, inorganic	Pseudomonas sp	Model ecosystem, terrestrial, natural,
Inhibitory (toxic) effects, 445	Identification of microorganisms	545
Zinc	376	Nocardia sp
Inhibitory (toxic) effects, 445	inhibition of benzoic acid turnover,	Metabolic pathways, 444
Wood preservatives	410	Paracolobactrum sp
Activated sludge, 296	Metabolic pathways, 232, 335	Model ecosystem, terrestrial, natural, 545
-	Psychrophilic temperature effect	Pseudomonas sp
Xanthate	250 Screening tests, 376	Metabolic pathways, 137, 539
Activated sludge, 190	Structure-activity relationships	Model ecosystem, terrestrial, natural,
Xanthomonas sp	410	545
Alcohols, primary aliphatic Identification of microorganisms	Time-course kinetics, 250, 347	Sarcina sp
164	Pseudomonas sp acclimated	Model ecosystem, terrestrial, natural,
Aldehydes	Time-course kinetics, 347	545
Identification of microorganisms	Sewage, acclimated, municipal	Sewage, acclimated, municipal
164	Petrochemical wastewater treatment	Petrochemical wastewater treatment
Alkanes, long chain, branched	51	51
Mesophilic temperature, effect	Xylenols and derivatives	Trametes sp
567	Achromobacter sp	Metabolic pathways, 137 Trickling filters, pilot plant
Psychrophilic temperature effect	Model ecosystem, terrestrial, natural	Aerobic biodegradation, 74
567	545	
Cirrasols	Activated sludge	Yeast sp
Aerobic biodegradation, 431	Aerobic biodegradation, 289	Quaternary ammonium compounds Inhibitory (toxic) effects, 314
Crude oil	386	Metabolic pathways, 314
Mesophilic temperature, effect	Anaerobic digestion reactor, 196	' '
567 Psychrophilia temperature effect	Detoxification, 349	Zinc
Psychrophilic temperature effect 567	Lagoons, aerated, industrial site	Activated sludge
301	349	Anaerobic digestion reactor, 344

```
Zinc (cont'd)
       Inhibitory (toxic) effects, 178
344, 429, 437, 546
       Michaelis-Menten coefficients
            429
    Activated sludge, acclimated
       Inhibitory (toxic) effects, 544
       Substrate concentration effect
            47, 544
    Activated sludge, acclimated, municipal
       Aerobic biodegradation, 363
       Biomass yield, effect on, 363
       Freundlich adsorption isotherms
            363
       Michaelis-Menten coefficients
            363
       Operational parameters, 363
    Activated sludge, industrial, continuous-
            flow
       Inhibitory (toxic) effects, 167
    Activated sludge, industrial, porous-pot,
            continuous-flow
       Inhibitory (toxic) effects, 167
    Activated sludge, municipal
       Inhibitory (toxic) effects, 361
       Sludge deflocculation, 361
    Activated sludge, municipal, continuous-
            flow
       Freundlich adsorption isotherms
            362
       Inhibitory (toxic) effects, 167
       Kinetics and equilibrium studies
       Michaelis-Menten coefficients
           362
       Operational parameters, 362
   Activated sludge, non-acclimated
       Inhibitory (toxic) effects, 343
   Lagoon pre-treatment
       Anaerobic biodegradation, 379
    Lumbricillus sp
       Inhibitory (toxic) effects, 167
   167
Sewage, municipal
       Inhibitory (toxic) effects, 345
       Nutritional effects, 90
   Sphaerotilus sp
       Inhibitory (toxic) effects, 437
   Stabilization pond
       Inhibitory (toxic) effects, 544
      Substrate concentration effect
    Vorticella sp
      Inhibitory (toxic) effects, 445
   Zooglea sp
      Inhibitory (toxic) effects, 437
Zooglea sp
  Chromium
      Inhibitory (toxic) effects, 437
  Copper
      Inhibitory (toxic) effects, 437
  Lead
     Inhibitory (toxic) effects, 437
  Mercury, inorganic
     Inhibitory (toxic) effects, 437
  Nickel
```

Inhibitory (toxic) effects, 437 nc Inhibitory (toxic) effects, 437

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 synthetic and semisynthetic cutting fluids
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