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Master Analytical Scheme for Organic Compounds in Water. Part 2 Appendices to Protocols

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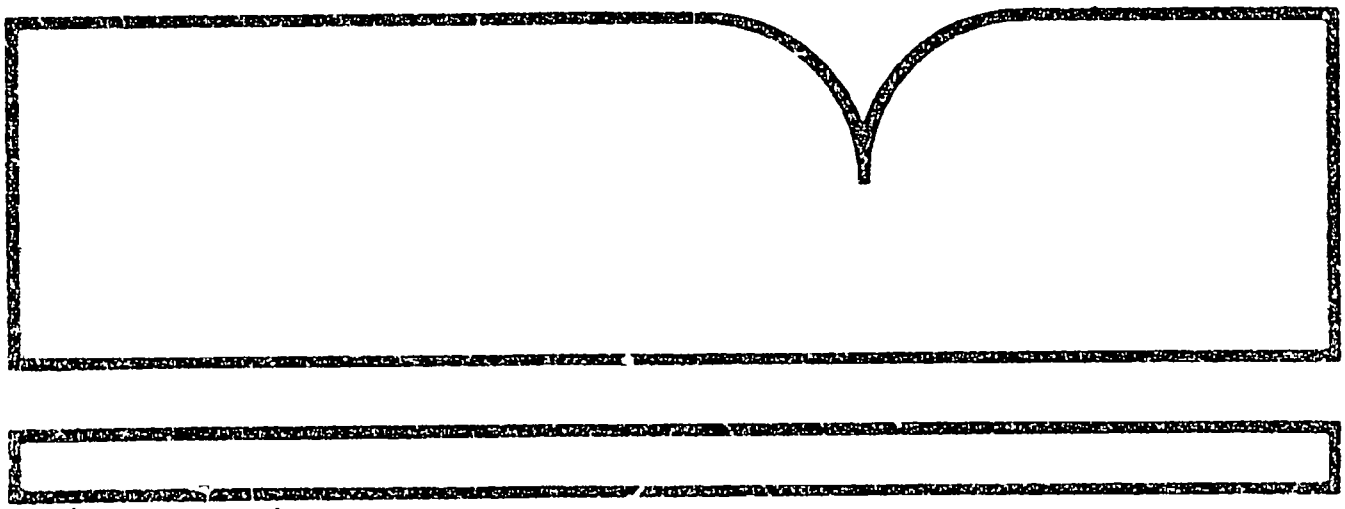

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January 1985

MASTER ANALYTICAL SCHEME FOR ORGANIC COMPOUNDS IN WATER

PART 2. APPENDICES TO PROTOCOLS

by

E. D. Pellizzari, L. S. Sheldon, J. T. Bursey, W. Hargrove,
L. C. Michael and R. A. Zweidinger
Analytical Sciences Division
Chemistry and Life Sciences Group
Research Triangle Institute
P. O. Box 12194
Research Triangle Park, NC 27709

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Project Officer
A. W. Garrison
Analytical Chemistry Branch
Environmental Research Laboratory
U.S. Environmental Protection Agency
Athens, GA 30613

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16 ABSTRACT

A Master Analytical Scheme (MAS) has been developed for the analysis of volatile (gas chromatographable) organic compounds in water. In developing the MAS, it was necessary to evaluate and modify existing analysis procedures and develop new techniques to produce protocols that provide for the comprehensive qualitative-quantitative analysis of almost all volatile organics in many types of water. The MAS provides for analysis of purgeable and extractable, as well as neutral and ionic water soluble, organics in surface and drinking waters and in leachates and various effluents. Nominal lower quantifiable limits range from 0.1 µg/L to 100 µg/L, depending on chemical/physical class of the analyte and complexity of the aqueous matrix. Recoveries are reported for about 280 model compounds of a wide variety of chemical classes and physical properties dosed into representative samples of several major types of water. The appendices include specific instructions on fabrication of the purge and trap apparatus and ancillary devices for purgeable organics, computerized relative molar response and recovery data for standards and analytes, and documentation of the MASQUANT computer program for quantification of MAS data.

17 KEY WORDS AND DOCUMENT ANALYSIS

a DESCRIPTORS	b IDENTIFIERS/OPEN ENDED TERMS	c COSATI Field/Group

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FOREWORD

Nearly every phase of environmental protection depends on a capability to identify and measure specific contaminants in the envrionment. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of envrironmental contaminants, the Analytical Chemistry Branch characterizes chemical constituents of water and soil.

Chemists working in governmental, industrial, and academic laboratories have long recognized a need for a comprehensive analytical methodology for organic compounds in water. To this end, research was begun in 1978 to develop a qualitative-quantitative scheme for the analysis of organics of all volatility classes (amenable to gas cnromatography), of almost all functional groups, in almost any water sample. The result is the Master Analytical Scheme (MAS) for Organic Compounds in Water, a compilation of protocols that employ new techniques and modifications of existing analysis procedures. Users may apply the MAS as a set of protocols for a comprehensive analysis or use individual protocols separately for analysis of organic fractions of particular interest. Among its many applications are epidemiological studies, wasteload allocations, permit application evaluations, trends analyses, watersned management studies, exposure assessments, landfill hazard evaluations, and aqueous source characterizations.

Rosemarie C. Russo, Ph.D.
Director
Environmental Research Laboratory
Athens, Georgia

PREFACE

The Master Analytical Scheme (MAS) represents the first effort to develop a comprehensive qualitative-quantitative scheme for the analysis of organic compounds in water. The MAS is a set of analytical protocols that includes a broad scope of organics with a wide variety of functional groups and physical properties. These protocols provide for the GC/MS/computer analysis of the usual purgeable and extractable compounds, with the addition of various neutral and ionic water soluble compounds; in fact, the MAS is applicable to any compound that can pass unchanged through a gas chromatograph, or can be derivatized to do so. Recoveries have been determined from distilled and drinking water, industrial and municipal effluents, and, in some cases, surface water and energy effluents, so the protocols are expected to be applicable to most water types. One unique feature of the MAS is its comprehensiveness. Another is its qualitative-quantitative aspect: an extensive data base of mass spectrometer detector response and recovery factors allows computer estimation of concentration without recourse to standards for each analyte.

In developing the MAS, existing analytical techniques were evaluated and modified and new techniques were developed to produce the comprehensive protocols. Development was in two stages. An interim set of protocols was developed by October 1980; analysis of environmental samples by these protocols revealed several important deficiencies that were subsequently corrected by additional experimental work. The final result is this first edition of MAS protocols in two parts; this volume, Part 2, contains the Appendices.

Two companion reports resulted from MAS development: Experimental Development of the MAS for Organic Compounds in Water, and Literature Review for Development of the MAS for Organic Compounds in Water. The user can refer to the experimental development report for information on techniques considered for MAS incorporation and experiments dealing with technique optimization and recovery studies. The literature review, which covers

material through June 1982 on techniques for analysis of organics in water, was the starting point for experimental development, and will also be of interest to many users. Neither companion report is essential to MAS use, however; this report (Part 1: Protocols and Part 2: Appendices to Protocols) stands alone as the handbook for implementation. Part 2 includes: Appendix A - specific instructions on fabrication of the purge and trap apparatus and ancillary devices for purgeable organics, Appendix B - hard copy of computerized relative molar response and recovery data for standards and analytes, and Appendix C - documentation of the MASQUANT computer program for quantification of MAS data.

The prospective MAS user should first thoroughly familiarize himself with Chapters 1 and 13 (the Introduction and GC-MS-COMP Analysis Procedures) of Part 1 of this report for an overview and a guide to use of the protocols and these appendices.

ABSTRACT

A Master Analytical Scheme (MAS) has been been developed for the analysis of volatile (gas chromatographable organic compounds in water. In developing the MAS, it was necessary to evaluate and modify existing analysis procedures and develop new techniques to produce protocols that provide for the comprehensive quantitative-qualitative analysis of almost all volatile organics in manytypes of water. The MAS provides for analysis of purgeable and extractable, as well as neutral and ionic water soluble, organics in surface and drinking waters and in leachates and various effluents. Nominal lower quantifiable limits range from 0.1 µg/L to 100 µg/L, depending on chemical/physical class of the analyte and complexity of the aqueous matrix. Recoveries are reported for about 280 model compounds of a wide variety of chemical classes and physical properties dosed into representative samples of several major types of water. The appendices include specific instructions on fabrication of the purge and trap apparatus and ancillary devices for purgeable organics, computerized relative molar response and recovery data for standards and analytes, and documentation of the MASQUANT computer program for quantification of MAS data.

This report was submitted in fulfillment of Contract No. 68-03-2704 by Research Triangle Institute under the sponsorship of the U.S. Environmental Protection Agency. This report covers the period from September 1978 to July 1983, and work was completed as of July 1983.

CONTENTS

Appendices

APPENDIX A

FABRICATION OF PURGE AND TRAP APPARATUS AND ANCILLARY DEVICES

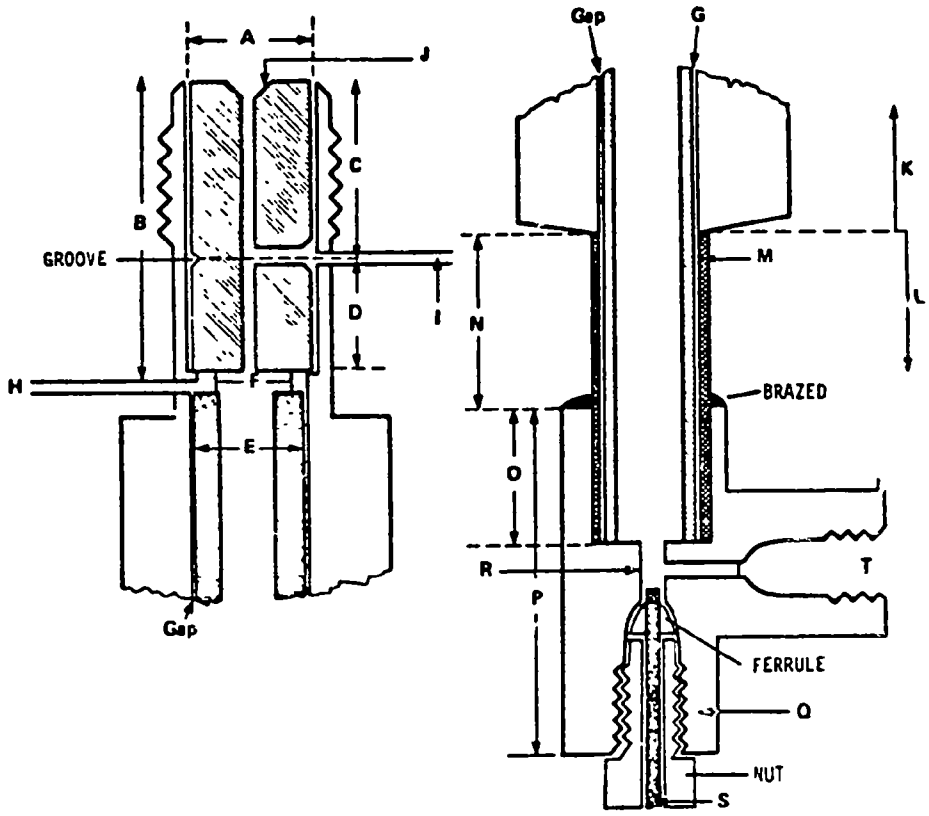
INTRODUCTION

This appendix describes the fabrication of a purge and trap device, an injection port/cryofocussing module, and other ancillary devices for use with the protocols for analysis of volatile organics, VO (Chapter 6), and neutral water soluble low molecular weight compounds, NEWS (Chapter 7). Most of the listed components are commercially available and, where necessary, the fabrication of devices can be easily performed by machine and glass blowing shops. Materials and machine and glass blowing shop labor are estimated to cost approximately $4,000.00.

FABRICATION OF INJECTION PORT

The features of this injection system include the capability for; (1) introduction of VO compounds for the determination of mass spectrometric relative molar response factors; (2) introduction of system performance mixtures; and (3) addition of an external standard (perfluorotoluene) with each water sample analyzed for VO and NEWS compounds and for RMR determinations.

Figure A-1 shows the construction of the injector body. An on-column flash vaporizer packed column injector (Varian Model 1040) is drilled out to 7.5 mm i.d. (A), to a depth of 15 mm. From there, the original 6.4 mm (1/4") i.d. is maintained, forming a lip at a 15 mm depth. Two 1.6 mm (1/16") o.d., 1.0 mm (0.040") i.d. stainless steel tubes are brazed onto the injector body: the carrier gas inlet (H) about 1 mm below the lip (16 mm below the top) on the same side of the injector as the original carrier gas inlet and the septum flush outlet (I) 10 mm below the top just beneath the septum nut threads. The septum flush outlet is attached on the opposite side of the injector body from the carrier inlet. A 1.6 mm (1/16") stainless steel zero dead volume tee (Q, Perkin Elmer No. 0091291) is modified to make the splitter. To minimize dead volume between the glass insert and the splitter outlet, the top of the tee is drilled out (O) to accommodate a piece of 6.4 mm (1/4") i.d. stainless steel tubing (M) 23 mm long (o.d. is not critical), the tee and tubing are brazed together. The bottom of the injector is cut off immediately below the



(A) 7.5 mm i.d.; (B) 16mm; (C) 10 mm; (D) 5 mm; (E) 6.35 mm o.d. glass tube; (F) 2-3 mm; (G) 6.35 mm glass tube; (H) carrier gas inlet (1/16" o.d. SS tubing,; (I) septum purge outlet (1/16" o.d. SS tubing connected to Hoke #1315G2B needle valve); (J) beveled needle guide into stainless steel insert with 1.6 mm i.d. hole; (K) old injector body; (L) new materials; (M) 6.4 mm (1/4") i.d. SS tubing; (N) 13 mm; (O) 10 mm; (P) 24 mm; (Q) zero dead volume SS Tee; (R) 1.2 mm i.d.; (S) Ni capillary tubing; (T) splitter outlet (1.6 mm fitting connected to Hoke #1315G2B needle valve).

Figure A-1. Diagram of injector body.

hexagonal block and the other end of the 6.4 mm i.d. tube connected such that the top of the tee is about 13 mm below the injector body (N). Care must be taken to ensure that these connections, both of which are brazed, are properly aligned. We have found that using a lathe to cut a concentric lip into the bottom of the injector body to accommodate the space tube aids in the alignment process.

The stainless steel insert (J) for the top of the injector has an i.d. of 1.6 mm. The o.d., about 7.1 mm, is matched with 7.5 mm i.d. of the upper part of the injector body (A) such that the fit is close, but not binding. The insert is about 14.5-15 mm long such that the septum will be tightened down snugly over the top. A 1.6 mm (1/16") hole is drilled in one side at about 10 mm from the top (C), even with the septum purge outlet (I). A groove is cut around the insert at the 1.6 mm outlet hole. The top of the insert hole (of J) is beveled to act as a needle guide.

Glass inserts are fabricated from standard 6.35 mm o.d. Pyrex tubing about 7 cm in length such that there is a 2 mm gap between the top of the glass and the bottom of the stainless steel septum purge insert.

The injector is installed in a heating block which also is fabricated to accommodate the six-port high temperature Valco valve. The septum purge outlet (I) is attached to a needle valve (Hoke #1315G2B) and then to vent. The splitter outlet (T) is connected to another needle valve. A shutoff valve (e.g., Whitey SS-0GS2) may also be added for operation in the "splitless" mode, and after the needle valve on the septum purge for shutoff of the purge.

Glass inserts for the injector are easily fabricated from standard 6.35 mm o.d. column tubing of 2-4 mm i.d.; inserts are silanized with dimethylchlorosilane. Replacement in the injector requires approximately 30 sec.

FABRICATION OF HEATING BLOCK AND CRYOTRAP

An aluminum heating sandwich is machined according to the specifications in Figure A-2.

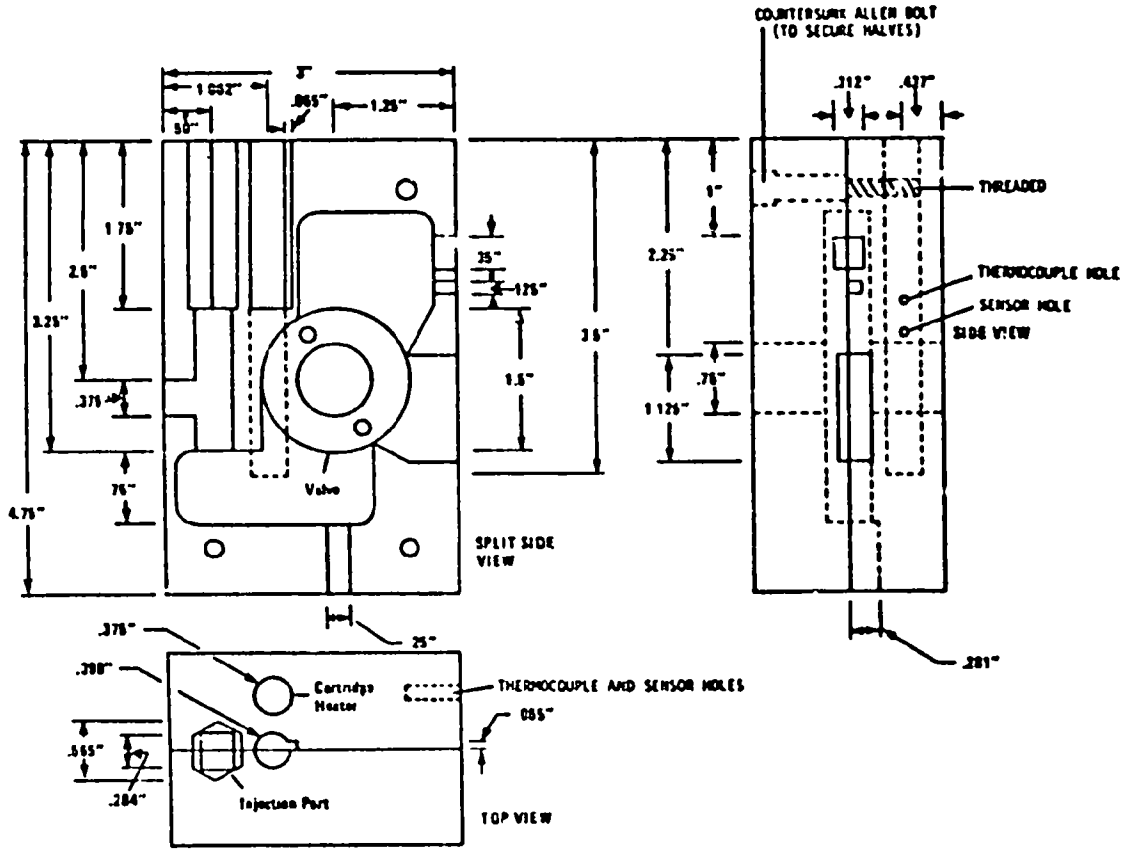


Figure A-2. Specification of heating block (see Fig. A-4).

A cryotrap is fabricated according to the dimensions given in Figure A-3. An aluminum rod (1.9 cm O.D. × 4.0 cm in length) is bored (1.6 cm I.D.) to a depth of 1.5 inches to accept a 150 watt heating cartridge (Table A-1). A helical groove (one-half the diameter of the Ni capillary) is machined around the aluminum cylinder to accept a nickel capillary trap with the dimensions shown in Figure A-3. Also, a groove is made to provide for the return end of the trap (B, Fig. A-3). Two additional grooves are machined (the thicknesses of the thermocouples must be measured for determining width and depth of the grooves; thermocouples should fit snugly) for the controller and sensor thermocouples. An aluminum cup is machined according to the specifications given in Figure A-3 so that it fits snugly over the outside of the capillary trap when it is wrapped on the aluminum cylinder. The aluminum cup is 2 cm deep. The thermocouples are inserted between the capillary trap and the aluminum cylinder at the approximate positions shown in Figure A-3. A 1/16 in Swagelock® union is fastened into the threaded hole of the aluminum cup to provide for filling of the cup with liquid nitrogen during the cryofocussing step.

The injection port system is assembled as shown in Figure A-4. The 1/16 in Ni sample transfer line from the purge and trap system is attached as indicated to the Valco® valve (Fig. A-4, A). All lines are connected so that the flow pattern through the valve and cryotrap are as indicated in Figure A-5 (for valve position A and B). (It is extremely important that the direction of gas flow through the cryotrap is the same for valve position A and B.) Nickel tubing (1/16 in OD, 0.02 in ID) is used for connecting the injector to the Valco® valve (A) and the valve to the 1/16 in zero dead volume Swagelock® union (Fig. A-4, B). The fused silica capillary is passed through the commercial GC injection port and connected flush to the constricted part of B using a graphite ferrule. The injection port system must be secured (bolted) to the commercial GC system to provide stability during usage. The entire assembly (Fig. A-4) is fastened flush with the commercial GC injection port.

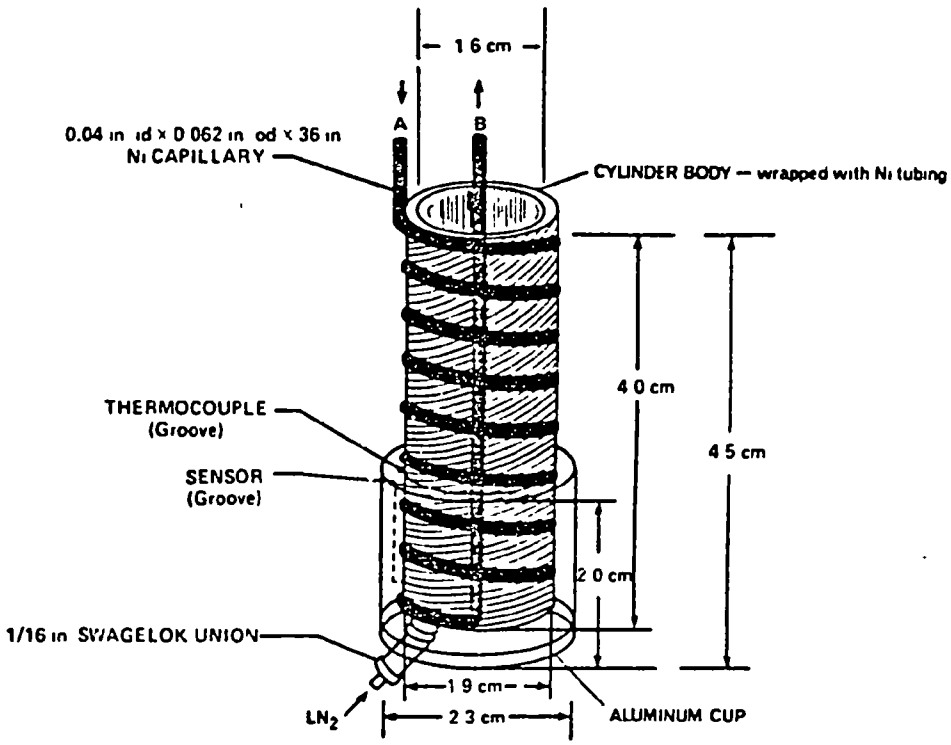


Figure A-3. Diagram of cryofocussing trap.

Table A-1. PARTS LISTING FOR TEMPERATURE CONTROLLERS

Quantity	Manufacturer	Part Number	Description
CONNECTORS			
2	Molex	receptacle 03-09-1091, plug 03-09-2091	9 circuit
2	Molex	receptable 03-09-1061, plug 03-09-2061	6 circuit
2	Molex	receptacle 03-09-1031, plug 03-09-2031	3 circuit
2	Molex	receptacle 03-09-1021, plug 03-09-2021	2 circuit
8	Omega	mated pair NMP-IRCO-MF	miniature thermocouple connectors for type J
MISCELLANEOUS			
	Molex	.093" Pin terminals for above Molex connectors	
40	Molex	02-09-1118 Female	
40	Molex	09-09-2118 Female	
8	Omega	MACL panel adaptor clips	
2	Omega	Model 7035-J-500 meter; 0-260≥C, I/C type J thermocouple	
2	CentraLab	PA-2003 Rotary switch; 6 position non-shorting	
-	Omega	28AWG Thermocouple wire for read out	
2	Littlefuse	3AMP 3AG 312 Fuse	
6	Littlefuse	2AMP 3AG 312 Fuse	
8	Buss	Type HTA fuse holders, panel mount	
8	McGill	Toggle switch SPST No. 90-0003	
CONTROLLERS			
6	Wattlow	Series 100 Temperature controller with type J thermocouples	
HEATERS			
6	Hotwatt	GR16-60	Single rope heater 250 watt, 60" long
1	Hotwatt	HS3715	Cartridge heater 150 watt, 1.5" long
1	Hotwatt	HS3725	Cartridge heater 200 watt, 2.5" long

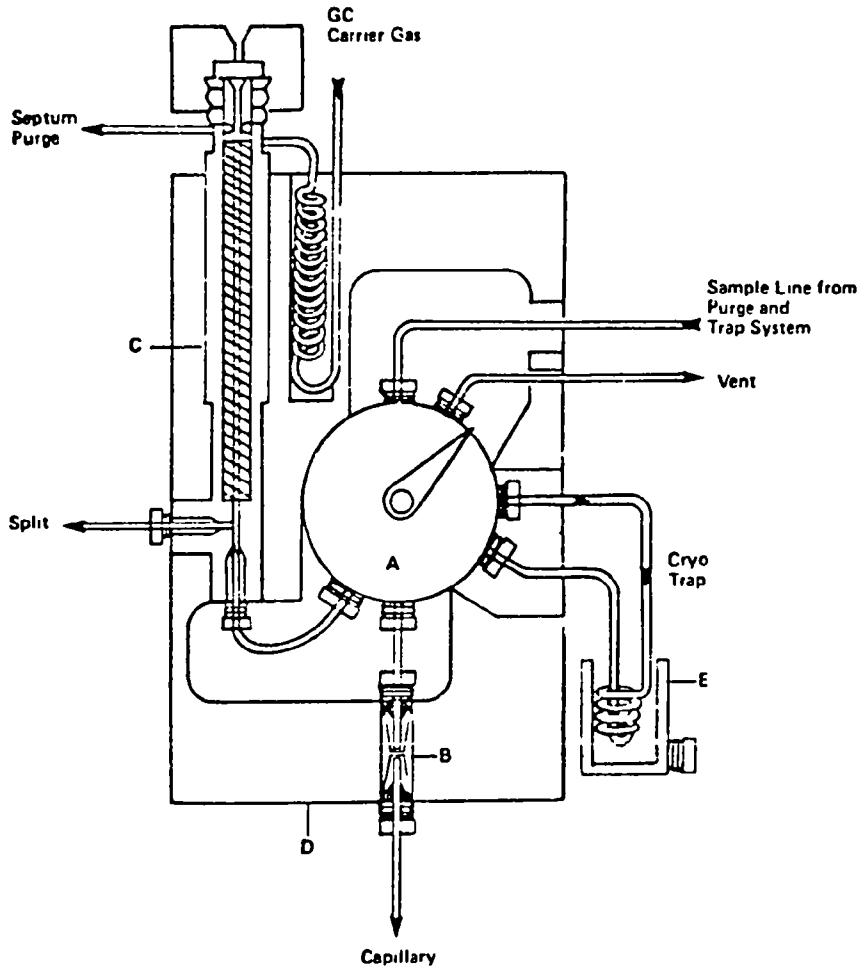


Figure A-4. Diagram of heating block (D) with injector (C), Valco valve (A), and cryofocussing trap (E).

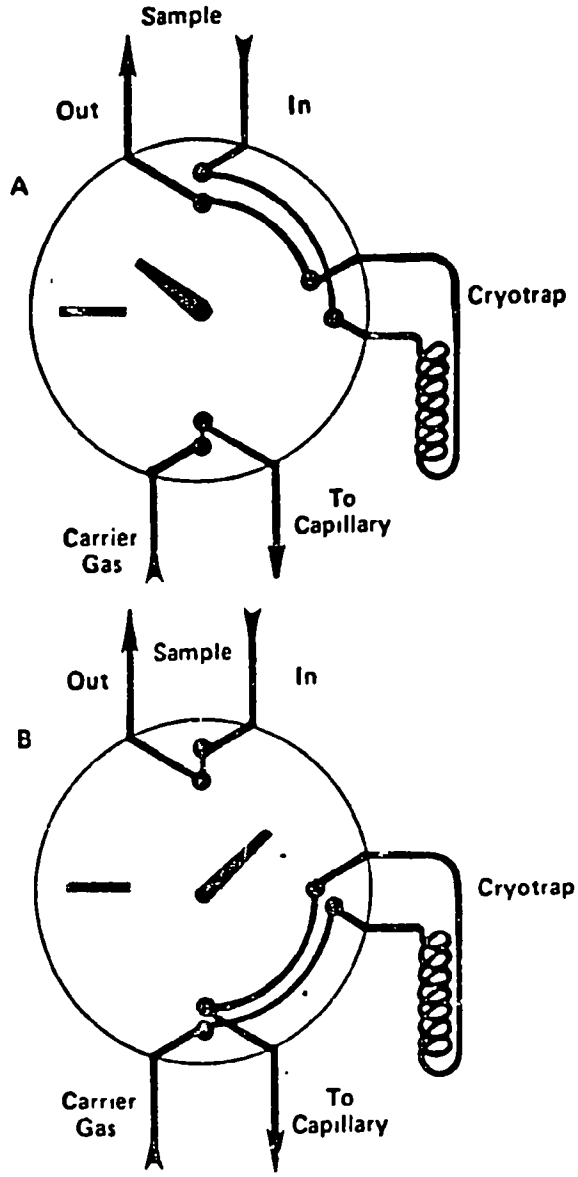


Figure A-5. Valco® valve flow pattern for positions A and B.

ASSEMBLY OF TEMPERATURE CONTROLLER MODULES

Two temperature control modules, each with three controlling channels, are needed, one for the purge and trap system and one for the injection port and cryofocussing devices. Wattlow Series 100 temperature controllers with Type J thermocouples are used for temperature control. Table A-1 provides a parts listing for the two sets of temperature controllers. Each temperature controller set is assembled for inclusion in a bud box. Figure A-6 shows a schematic of the control and readout circuits. Figure A-7 depicts the front panels of the two temperature control modules used for controlling the various heating elements on the purge and trap and injection port systems. As the front panels indicates, there are three channels per temperature control module with individual toggle switches for on/off of each channel as well as overall power. A six-position non-shorting rotary switch is used to monitor the temperatures of the various components. The temperature is read on a pyrometer (Figure A-7).

Temperature control module No. 1 is employed for controlling the Valco valve (8), Tenax trap (4), and sample lines (5,6,20,21 and 22) on the purge and trap system (Figure A-7). Temperature control module No. 2 is used to control the temperatures on the injection port block (1), cryofocussing system (2), and, when executing the NEWS protocol, the heating collar (8) on the purge and trap vessel. The six temperature control channels have separate thermocouples for heat control and temperature readout. In Figure A-6, the thermocouples found in control module No. 1 for the sample lines, Valco valve, and Tenax trap are shown. Control module No. 2 has thermocouples for the injection block, cryofocussing trap, and heating collar for the purge and trap vessel.

The temperature controller and sensor thermocouples and the pyrometers are calibrated against a standard source prior to their use on the purge and trap system.

FABRICATION OF PURGE AND TRAP SYSTEM

Figures A-7 and A-8 depict the front and rear views of the purge and trap system. A parts listing is given in Tables A-2 and A-4. A stand is fabricated that will hold an aluminum plate on a rack system anchored to a wooden

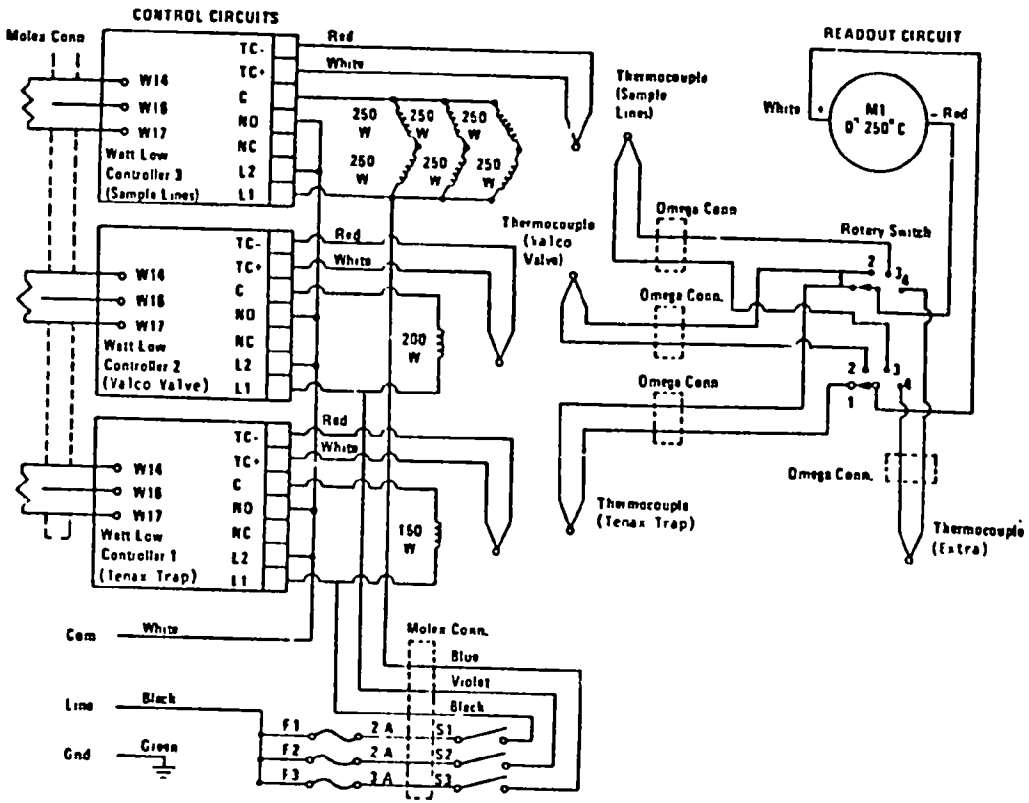


Figure A-6. Schematic of control and readout circuits for temperature control module No. 1.

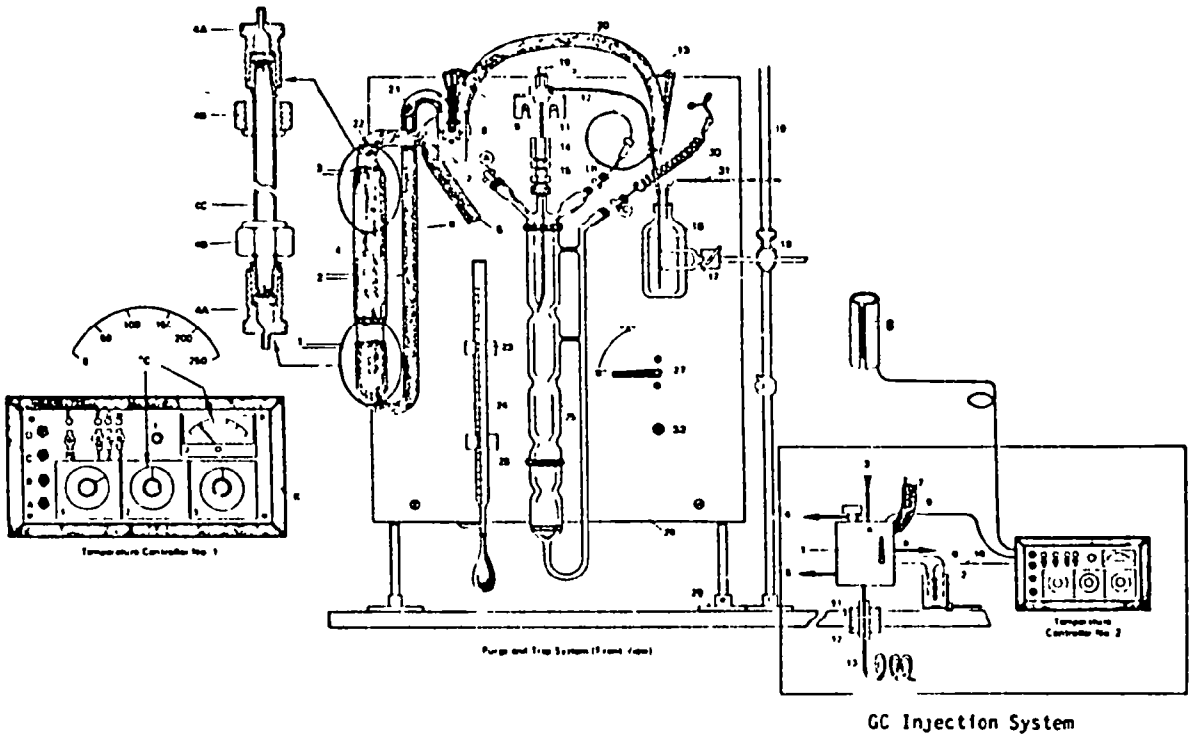


Figure A-7. Purge and trap system with injection system.

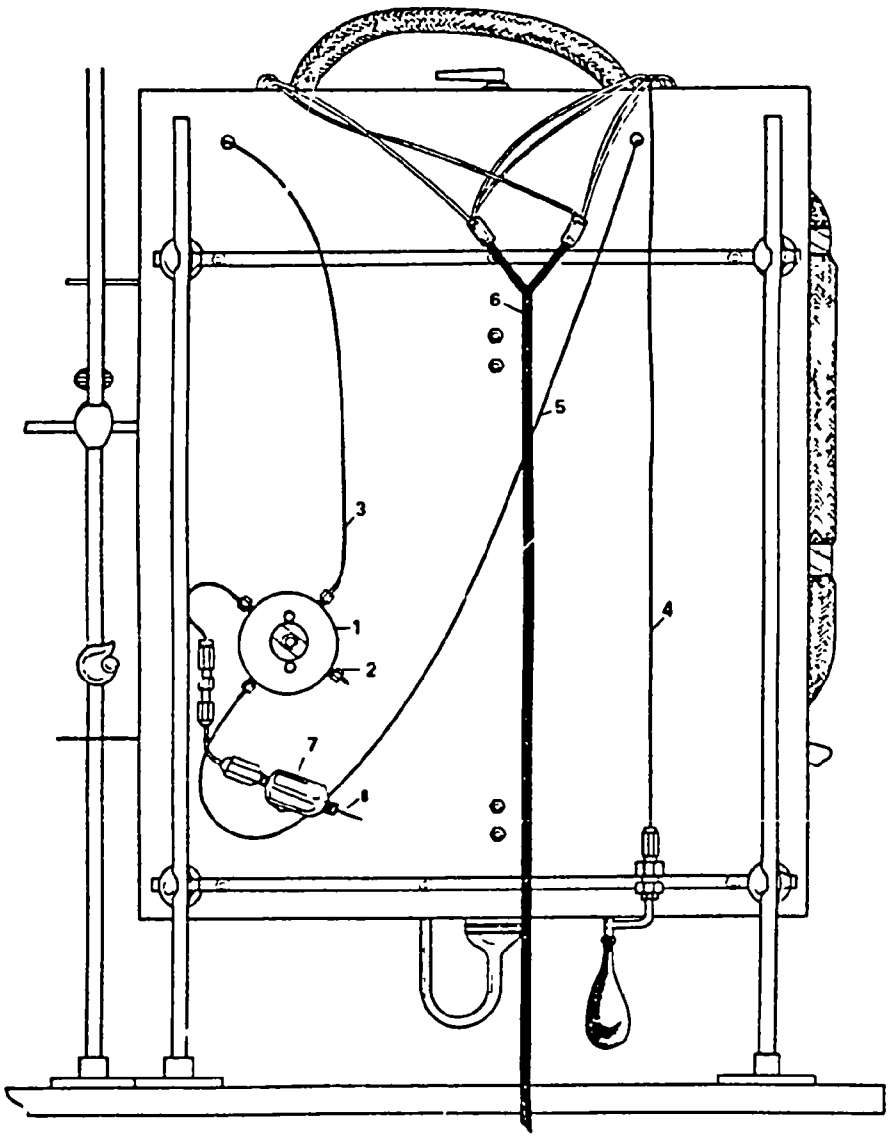


Figure A-8. Purge and trap system (rear view).

Table A-2. COMPONENT IDENTIFICATION - PURGE AND TRAP SYSTEM

Item #	Description
4	Sorbent trap (1.5 g Tenax GC; 35/60 mesh)
4A	3/8 in → 1/16 in stainless steel, fritted (10 μ) reducing union
4B	3/8 in stainless steel nut
4C	10 in × 3/8 in o.d. × 5/16 in i.d. stainless steel tubing
5	Heated/insulated nickel transfer line from 6-port valve to GC injection system (item 7 on right side of Fig. A-7), 1/16 in o.d. × 0.040 in i.d. × 30 in
6	Heated/insulated nickel transfer line from 6-port valve to sorbent trap, 1/16 in o.d. × 0.040 in i.d. × 14 in
7	Support for 6-port valve, Valco
8	Six-port valve, Valco C-6-T, 1/16 in zero dead volume fittings
9	Support bracket for sample valve, Tekmar 1400507000
10	Sample valve, Tekmar 14036
11	Sample introduction needle, Tekmar 14-0033-053
12	Teflon tubing (1/16 in o.d. × ~0.040 in i.d. × ~20 in) with needle (18 gauge × 14 cm)
13	Teflon tubing (1/16 in o.d. × ~0.040 in i.d. × 8 in) with Cheminert® connector (LDC) for connecting to item 20
14 15	Sampler union, Tekmar 14049
16	Sample container, 243 mL, glass, 24 mm septum cap
17	Three-finger clamp, Fisher 05-742
18	Clamp holder, Fisher 05-754
19	Aluminum rod, 1/2 in, Fisher 14-666
20	Heated/insulated nickel transfer line from purge flask connecting line (item 13) to 6-port valve, 1/16 in o.d. × 0.040 in i.d. × 14 in
21	Heated/insulated nickel transfer line from 6-port valve to sorbent trap, 1/16 in o.d. × 0.040 in i.d. × 20 in
22	Heated/insulated nickel transfer line from sorbent trap to 6-port valve, 1/16 in o.d. × 0.040 in i.d. × 5 in
23	Clamp
24	Soap bubble flowmeter

(continued)

Table A-2 (cont'd.)

Item #	Description
25	Purge flask (See Chapter 6, MAS protocols, for details):
	Approximate dimensions - 45 cm × 3.5 cm Purge gas inlet - 1/16 in o.d. Frit porosity - medium Material - borosilicate glass
	A: Microflex® valve, Kontes K-749100-21
	B: Chromaflex® column valve, Kontes K-423600
	C: Chromaflex® column valve, Kontes K-423600
26	Spring, 1-1/2 in
27	Dry purge valve, 4-port, Valco C-4-T, 1/16 in zero dead volume fittings
28	Aluminum panel, 16 in × 26 in × 1/8 in
29	Flexframe foot plate, Fisher 14-666-25
30	Purge gas line, Teflon tubing (1/16 in o.d. × ~0.040 in i.d. × ~20 in) with Cheminert® fitting (LDC)
31	Teflon tubing (1/16 in o.d. × ~0.040 in i.d.) with stainless steel needle (18 gauge × 2.5 cm)
32	Purge gas flow metering valve, Nupro SS-2SG, 1/8 in fittings
	Unspecified Equipment
1	Rope heaters - Hotwatt, Inc., 250 watt, 120V, 60 in
2	Insulation - glass wool sleeve 1/2 in × 1/16 in thick
3	Glass fiber tape - Scotch 27®
4	Nickel tubing (surrounding 1/16 in Ni transfer lines) 1/8 in o.d. × 0.085 in i.d. This sleeve is used to distribute heat more evenly from heating rope to 1/16 in transfer line.
	Vendors
1	Valco Instruments Co., Box 19032, Houston, TX 77024
2	Tekmar Co., P. O. Box 37202, Cincinnati, OH 45222
3	Fisher Scientific Co., various locations
4	Kontes Glass, P. O. Box 739, Vineland, NJ 08360
5	Watlow Winona, Inc., 1265 E. Sanborn St., Winona, MN 55987
6	Hotwatt, Inc., 128 Maple St., Danvers, MA
7	Laboratory Data Control, P. O. Box 10235, Riviera Beach, FL 33404

base. The dimensions of the aluminum are 1/8 in × 16 in × 26 in. It is secured to the aluminum rack stand as indicated in Figure A-8. Holes are drilled through the aluminum plate and on the two crossbars of the aluminum rack and the holes are counter sunk on the plate for bolting the plate in place. All the components then are assembled as indicated in Figure A-7. The relationship of the purge and trap system (Figure A-7) with respect to the injection port system is also indicated. The purge and trap stand should be conveniently located near the injection port system, which is mounted on the gas chromatograph. The N2 transfer line (5, Figure A-7) from the Valco valve (8) of the purge and trap system to the injection port system (right side of Fig. A-7, item 7) is generally 2-1/2 to 3 feet in length; its length is not critical since the sample will be focussed prior to injection onto the GC capillary. Table A-3 identifies the components of the injection system.

The parts listing for the rear view of the purge and trap system is given in Table A-4. For the proper assembly of the six-port and four-port valves, it is important to consult the flow diagrams which are provided with the valves by the manufacturer to insure that the gas flow is properly directed with each rotated position of the valve. Figure A-9 shows the flow pattern during the wet and dry purge steps through the purge and trap system. During purging of a water sample, the purge gas passes through the purge vessel, the six-port Valco® valve, Tenax GC® trap six- port valve and to the bubble meter (Valco valve in position A). During the "dry" purge step, the K-423600 valve (B, Fig. A-7) is closed and the gas is directed to the 1/16 in Swagelock® Tee Union, passing through six-port valve, Tenax GC® trap and to the bubble meter (Valco valve in position A). In either case the GC carrier gas passes through the six-port valve and to the injection port system. During thermal desorption of the Tenax GC® trap, the six-port valve is rotated to position B and the GC carrier gas is directed through the Tenax trap in the reverse direction and then to the injection port system.

Figure A-10 depicts the dimensions of the Tenax trap.

Table A-3. COMPONENT IDENTIFICATION - INJECTION SYSTEM

Item #	Description
1	Heating block, containing 6-port valve (Valco C-6-T)
2	Nickel capillary cryogenic trap
3	Gas chromatograph carrier gas inlet to injector
4	Septum sweep (outlet), closed during operations.
5	Splitter exit (closed)
6	Vent
7	Heater/insulated transfer line from 6-port valve on purge and trap system to injector body, 1/16 in o.d. × 0.040 in i.d. × 30 in (other end of item No. 5, Table A-2)
8	Purge flask heater, 3/4 in diameter × 8 in, Watlow 01808081
9	Electrical connection to injector body heater
10	Electrical connection to cryogenic trap heater
11	Gas chromatograph bulkhead
12	Gas chromatograph injection port
13	Capillary GC column

Table A-4. COMPONENT IDENTIFICATION - PURGE AND TRAP SYSTEM (REAR VIEW)

Item #	Description
1	Dry purge valve, 4-port, Valco C-4-T
2	Capped port
3	Purge gas line to purge flask, 1/16 in o.d. × 0.040 in i.d. × 12 in (connected to line 30, see Fig. A-7)
4	Vent from 6-port valve for monitoring purge gas flow, 1/16 in o.d. × 0.040 in i.d. × 20 in
5	Dry purge line to 6-port valve, 1/16 in o.d. × 0.040 in i.d. × 24 in
6	Heater cable connections to purge and trap temperature controller
7	Purge gas flow metering valve, Nupro SS-2SG
8	Gas line from helium cylinder, 1/8 in copper

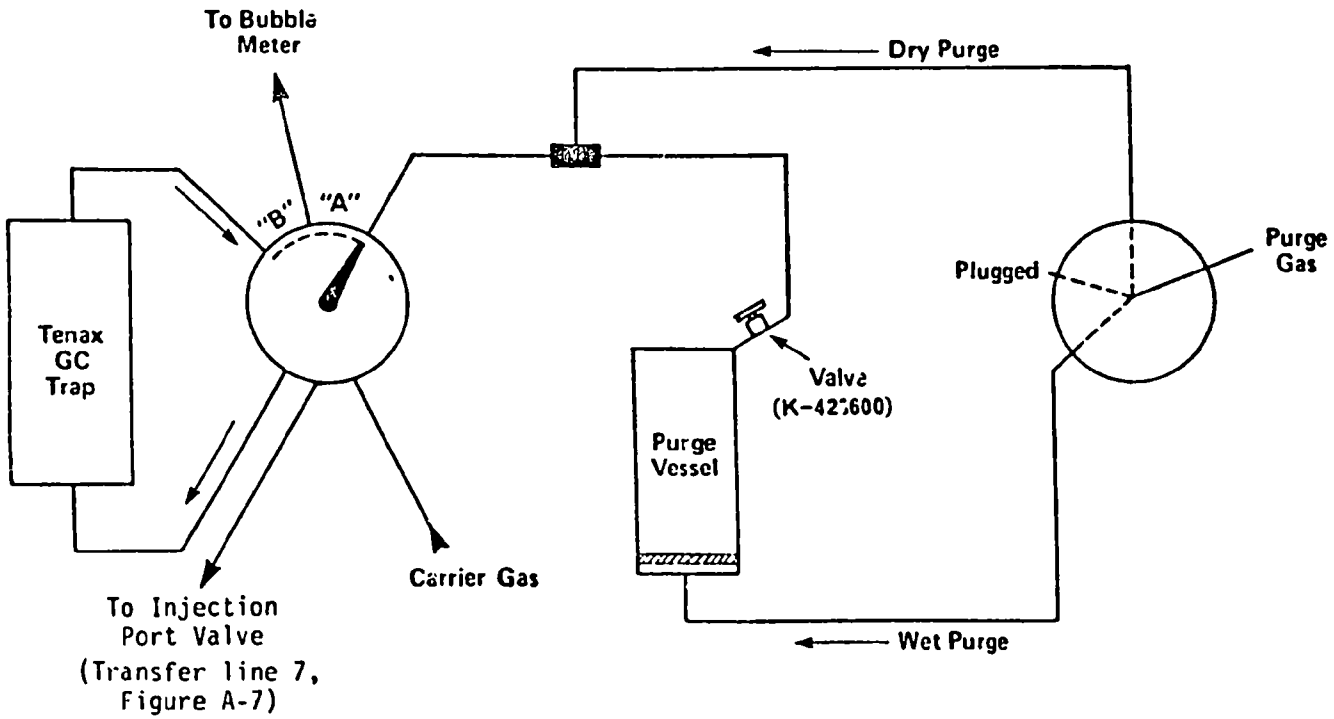


Figure A- 9. Flow diagram of purge and trap system.

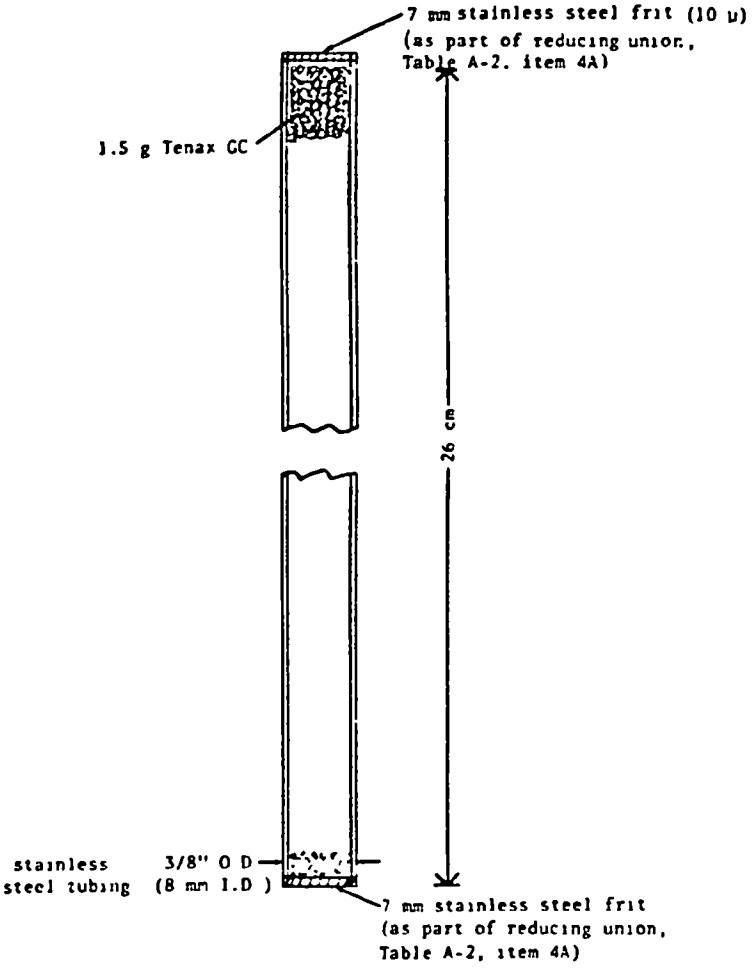


Figure A-10. Tenax trap for purge and trap system (Fig. A-7).

ASSEMBLY OF SAMPLE TRANSFER SYSTEM (VO ANALYSIS PROTOCOL ONLY)

Figure A-11 depicts a schematic of the volatile organic sample transfer system. This is an expansion of a portion of Figure A-7 which shows the relative position of the sample transfer system to the purge and trap vessel. A two-way valve (G) is employed to direct the "on/off" pressurization of the water sample container. Sixteenth inch Teflon tubing is used to connect the two-way valve (G) to a stainless steel needle (F) with its hub removed (18 gauge × 2.5 cm in length). The water sample is delivered into the purge and trap vessel using a stainless steel needle (D, Fig. A-11), also with its hub removed (18 gauge × 14 cm in length), which is attached to a 1/16" Teflon tubing (E) and the three-way sample valve [Fig. A-7 (10)]. The long and short stainless steel needles are inserted respectively through the Teflon faced septum (H) just prior to transfer of the sample.

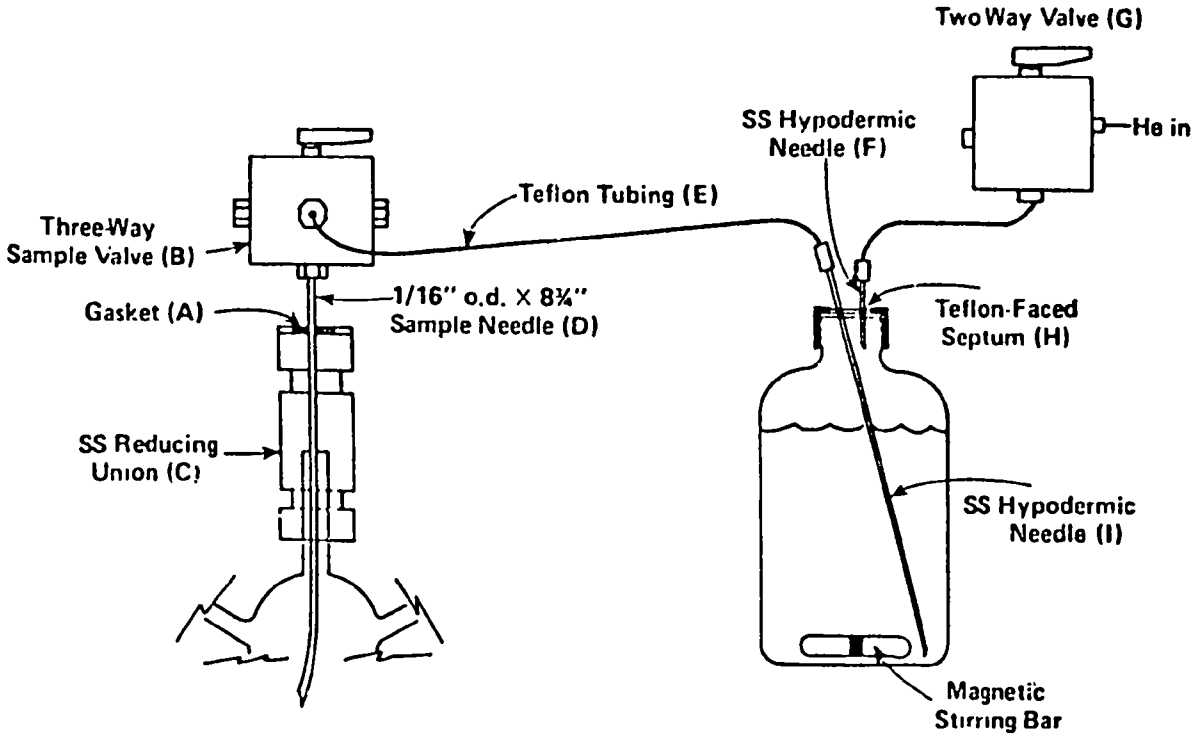


Figure A-11. Schematic of VO sample transfer system.

APPENDIX B

RMR AND RECOVERY DATA FILE FOR INTERNAL AND EXTERNAL STANDARDS AND ANALYTES IN MASQUANT

INTPODUCTION

This Appendix is basically a computer hard copy of recovery and relative molar response (RMR) factors of the Master Analytical Scheme's internal standards and its approximately 200 model compounds. These data are part of the computer files for MASQUANT, a program for calculation of concentrations of analytes detected during implementation of the MAS. The user should refer to Chapter 1 (Section 1.2.7) and Chapter 13 (Section 13.4.2.2) of "Part 1: Protocols" for a discussion of the general approach towards quantitation, whether conducted manually or using MASQUANT.

GENERAL DESCRIPTION OF MASQUANT

MASQUANT has been written to carry out some of the basic calculations used to process data obtained using the Master Analytical Scheme. MASQUANT consists of approximately 2,000 lines of source code written in ANSI subset Fortran 77, which should make it operable on any computer capable of handling this language.

The program consists of a main routine and sixteen subroutines, which will be described in greater detail in Appendix C. The program is written to run interactively, with a continuing dialogue between the user and the computer. After all of the data are processed, a report giving the calculated concentration of each identified component is generated.

In order to use MASQUANT, three files need to be accessed from an external disk or tape. The files are organized in a sequential fashion, and are read or written to in this same manner. These files are 1) a file which contains calculated correction factors for RMRs which can be applied to the library file, if desired; 2) a standard file consisting of internal and external standards, along with associated data including recovery factors and response factors; and 3) a file, written in the identical format as file 2, consisting of data for "unknown" analytes. The compounds and standards are organized into 13 clases, consistent with the MAS Protocols. Detailed formats for the three files are given in Appendix C.

USE OF TABLES

The following table lists the 13 classes of MAS compounds and standards for use with MASQUANT, with page numbers of corresponding data tables. Each table is in three parts: 1) a table of internal and external standards and their identification numbers; 2) a tabulated matrix of standard ion RMRs, which requires more than one page for Classes 3-8; and 3) a table of MASQUANT computer output of recoveries and RMRs of analytes (MAS model compounds), which often requires several pages for each class.

Following are explanations of the MASQUANT computer output hard copy.

For each compound (analyte) listing, data is arranged as follows:

First line: Compound # Recovery Compound name and CAS number

Second and third lines: Analyte ion (m/z) Analyte RMRs vs. standard ions

Standard ions are listed at the top of each page under the standard number. There are usually two ions listed for each standard (and two for each analyte). See the first table in each class for identification of standards by number.

Definitions/Explanations:

Compound #: compound (analyte) number assigned in MASQUANT

Analyte ion: ion (m/z) of analyte for which an RMR has been determined. There are usually two for each compound.

Recovery: recovery determined for the analyte using the prescribed protocol; e.g., 1.00 = 100%, 0.97 = 97%. Compounds whose recovery have not been determined using the prescribed protocol are assigned a numerical value of 0.01.

RMR (relative molar response): space is allocated for two RMR values for each analyte ion measured against each standard. If a standard contains only one ion, a dash (-) is placed at the heading of the second column and no values are listed in that column. A RMR of *** is greater than 9.99; a RMR of 0.00 is less than 0.01. All RMRs were determined using a Finnigan 4021 GC/MS with an Incos Data System.

NOTE: Classes 3-8 use more than 5 standards; there is room for only 5 per page, so there are 2 pages of data for each analyte for these classes.

Table B-1. RMRs AND RECOVERIES FOR VO COMPOUNDS

Class No. 1

Standard ID No.	Standard Name
1	perfluorotoluene (external)
51	d_5-Bromoethane (internal)
52	2,4,6-d_3-Anisole (internal)
53	d_5-Chlorobenzene (internal)
54	d_8-Naphthalene (internal)

MATRIX OF STANDARD ION RMRs

Standard	Ion	Recovery	Standard: Perfluorotoluene m/z 186	Perfluorotoluene m/z 236	2,3,6-d_3-Anisole m/z 81	2,3,6-d_3-Anisole m/z 111	d_5-Chlorobenzene m/z 82	d_5-Chlorobenzene m/z 117	d_{10}-Diethyl ether m/z 50	d_{10}-Diethyl ether m/z 66	d_5-Bromoethane m/z 113	d_5-Bromoethane m/z 115
perfluorotoluene	186	NA	-	.93(3)[a]	1 10(27)	.70(27)	1.13(6)	.55(14)	3 11(270	1.46(28)	1.57(21)	1.61(22)
	236	NA	1.08(3)	-	1.41(25)	.75(25)	1 19(13)	.58(11)	3.30(24)	1.54(25)	1.69(19)	1.73(20)
2,4,6-d_3-anisole	81	0 57	.82(29)	.76(28)	-	.54(1)	.92(17)	.45(18)	2 87(45)	1.32(44)	1.55(34)	1.60(36)
	111	0 57	1.53(30)	1.42(27)	1.87(1)	-	1.71(17)	.84(17)	5.35(45)	2.45(44)	2.88(34)	2.97(35)
d_5-chlorobenzene	82	1 20	.91(19)	.85(16)	1 11(16)	.60(17)	-	.49(2)	3.07(24)	1.43(23)	1.65(18)	1.70(18)
	117	1 20	1.87(17)	1.75(14)	2.25(18)	1.23(17)	2 05(2)	-	6.31(24)	2 92(22)	3 38(18)	3.49(19)
d_{10}-diethyl ether	50	NA	.34(22)	.31(21)	.41(45)	.22(45)	.35(27)	.17(25)	-	.46(2)	.57(21)	.58(22)
	66	NA	.72(24)	.67(22)	.88(44)	.48(44)	.75(26)	.37(25)	2.16(2)	-	1.23(20)	1.27(20)
d_5-bromoethane	113	0 85	.66(21)	.61(19)	.71(30)	.38(31)	.63(16)	.31(17)	1.82(19)	.83(18)	-	1 03(1)
	115	0.85	.64(22)	.59(19)	.69(30)	.37(31)	.61(17)	.30(17)	1.76(20)	.81(19)	.37(1)	-

[a] (CV)

Note: This matrix was generated before final internal standards were selected. The correct standards are listed on the first part of Table B-1 (preceeding page). The matrix as shown here includes d_{10}-diethyl ether, but omits d_8-naphthalene. However, on the RMR and recovery tables on pp. 29-34, values for standards 1, 52, 53, and 54 are given; i.e., naphthalene is included but bromoethane and diethyl ether are not. (There are a few exceptions where bromoethane is used, but naphthalene is not.)

Internal/External Standard File for Cmpd Class # 1

Cmpd#	Recovery Std # 1		Compound Name Std #51		Std #52		Std #53		Std #54
Mass	186	236	113	115	81	111	82	117	136
105	1.25		TOLUENE 108883						
91	2.05	1.89			2.25	1.21	2.13	1.04	0.32
92	1.32	1.21			1.44	0.78	1.37	0.67	0.20
106	0.01		O-XYLENE 95476						
91	2.00	1.87			2.45	1.32	2.29	1.09	0.34
106	1.10	1.03			1.35	0.73	1.25	0.60	0.19
107	0.98		P-XYLENE 106423						
91	1.84	1.62			2.81	1.39	2.39	1.07	0.33
106	1.07	0.95			1.56	0.86	1.48	0.65	0.20
108	0.96		ETHYLBENZENE 100414						
93	3.18	2.12			3.47	1.88	3.30	1.60	0.49
106	1.11	1.02			1.21	0.65	1.15	0.55	0.17
109	0.01		2-METHYLSTYRENE 611154						
117	0.78	0.74			0.93	0.50	0.88	0.42	0.13
116	0.98	0.93			1.18	0.63	1.11	0.53	0.16
110	0.77		1,3,5-TRIMETHYLBENZENE 108678						
105	4.02	3.80			4.80	2.58	4.54	2.16	0.65
120	2.37	2.24			2.83	1.52	2.68	1.27	0.38
111	0.94		1,2,4-TRIMETHYLBENZENE 95636						
105	2.23	1.95			3.20	1.73	2.98	1.32	0.38
120	1.26	1.11			1.85	1.03	1.79	0.78	0.21
112	0.01		ISOPROPYLBENZENE 98828						
105	2.73	2.27			3.11	1.68	2.60	1.23	0.49
120	0.82	0.69			0.95	0.51	0.78	0.37	0.15
113	0.01		O-ETHYLTOLUENE 611143						
105	3.38	3.11			3.70	2.00	3.52	1.71	0.52
120	1.14	1.05			1.24	0.67	1.18	0.58	0.18
114	0.01		P-ETHYLTOLUENE 622968						
105	3.20	2.99			3.92	2.12	3.66	1.75	0.54
120	1.05	0.98			1.28	0.69	1.19	0.57	0.18
115	1.13		SEC-BUTYLBENZENE 135988						
105	3.69	3.09			4.30	2.32	3.54	1.68	0.67
134	0.89	0.75			1.04	0.56	0.86	0.41	0.16
116	0.81		P-DIETHYLBENZENE 105055						
91	0.61	0.56			0.67	0.36	0.63	0.31	0.09
119	2.37	2.18			2.59	1.40	2.47	1.20	0.37
117	1.00		4-METHYLISOPROPYLBENZENE 99876						
119	3.35	3.18			4.00	2.15	3.79	1.80	0.54
134	0.95	0.90			1.14	0.61	1.08	0.51	0.15

Internal/External Standard File for Cmpd Class # 1

Cmpd#	Recovery Std # 1		Compound Name Std #51		Std #52		Std #53		Std #54	
Mass	186	236	113	115	81	111	82	117	136	-
118	0.74		NAPHTHALENE 91203							
128	4.46	3.93			6.67	3.56	5.71	2.73	0.78	
119	0.59		DIPHENYLMETHANE 101815							
167	2.98	2.49			3.45	1.86	2.85	1.35	0.54	
168	3.18	2.62			3.63	1.96	2.99	1.42	0.57	
120	1.13		TERT-BUTYLBENZENE 98066							
119	2.64	2.47			3.24	1.75	3.02	1.44	0.45	
134	0.67	0.63			0.83	0.45	0.77	0.37	0.11	
121	1.16		FLUOROBENZENE 462066							
70	0.30	0.25			0.35	0.19	0.29	0.14	0.05	
96	1.49	1.24			1.73	0.93	1.42	0.68	0.27	
122	0.91		CHLOROBENZENE 108907							
77	0.83	0.73			1.25	0.62	1.03	0.46	0.15	
112	1.65	1.46			2.32	1.33	2.32	0.98	0.29	
123	1.23		BROMOBENZENE 108861							
77	1.90	1.59			2.21	1.19	1.82	0.87	0.35	
156	1.27	1.06			1.53	0.92	1.22	0.58	0.23	
124	0.01		BENZYLCHLORIDE 100447							
91	1.83	1.73	3.31	3.42	2.83	1.52	2.21	1.06		
126	0.46	0.44	0.84	0.86	0.71	0.38	0.56	0.27		
125	1.04		P-BROMOTOLUENE 106387							
91	1.99	1.89			2.39	1.28	2.25	1.07	0.32	
170	1.00	0.95			1.20	0.64	1.13	0.54	0.16	
126	1.06		IODOTOLUENE(P) 624317							
91	2.18	1.82			2.62	1.41	2.15	1.02	0.39	
218	2.82	2.36			3.39	1.83	2.70	1.28	0.51	
127	1.16		1,2-DICHLOROBENZENE 541731							
111	0.85	0.71			0.99	0.53	0.82	0.39	0.15	
146	2.36	1.97			2.74	1.48	2.26	1.07	0.43	
128	1.03		1,3-DICHLOROBENZENE 95501							
111	0.78	0.73			0.93	0.50	0.88	0.42	0.13	
146	2.24	2.11			2.66	1.43	2.52	1.26	0.36	
129	0.83		1,4-DICHLOROBENZENE 106467							
111	0.92	0.84			1.00	0.54	0.95	0.47	0.14	
146	2.73	2.51			2.99	1.61	2.84	1.28	0.42	
130	0.92		2-BROMOCHLOROBENZENE 694804							
196	1.53	1.40			1.67	0.90	1.59	0.78	0.24	
192	2.03	1.86			2.22	1.20	2.11	1.03	0.31	

Internal/External Standard File for Cmpd Class # 1

Cmpd#	Recovery Std # 1		Compound Name Std #51		Std #52		Std #53		Std #54
Mass	186	236	113	115	81	111	82	117	136
131	1.06		4-BROMOCHLOROBENZENE 106398						
190	1.34	1.27			1.60	0.86	1.52	0.72	0.22
192	1.81	1.68			2.12	1.14	2.01	0.96	0.29
132	1.01		1,2,4-TRICHLOROBENZENE 120821						
180	1.83	1.62			2.72	1.46	2.32	1.11	0.33
182	1.80	1.59			2.68	1.44	2.28	1.09	0.32
133	0.70		A,A,A,TRICHLOROTOLUENE 98077						
159	1.63	1.52			1.85	1.03	2.09	1.03	0.27
161	1.10	1.02			1.24	0.69	1.41	0.70	0.18
134	0.01		3-CHLOROBENZONITRILE						
102	1.13	0.97			1.35	0.73	1.11	0.53	0.21
137	4.22	3.63			5.03	1.41	4.15	1.97	0.78
135	0.68		ANISOLE 100663						
78	0.71	0.66			0.87	0.47	0.81	0.39	0.12
108	1.27	1.20			1.57	0.85	1.46	0.70	0.22
36	0.47		BIPHENYL ETHER 101848						
77	1.18	1.08			1.28	0.69	1.22	0.60	0.18
170	3.57	3.28			3.90	2.11	3.70	1.81	0.55
137	0.01		BENZYL ETHER 103504						
91	4.37	4.13			5.20	2.80	1.52	2.35	0.70
92	5.60	5.30			6.67	3.58	2.01	3.01	0.90
138	0.67		PROPYLENE OXIDE 75569						
29	0.52	0.47	0.69	0.70	0.56	0.30	0.49	0.25	
58	0.27	0.24	0.35	0.36	0.28	0.15	0.25	0.12	
139	1.15		DIETHYL ETHER 60297						
31	1.89	1.72	2.50	2.55	2.00	1.07	1.75	0.88	
59	0.62	0.56	0.82	0.83	0.65	0.35	0.57	0.28	
140	0.80		2-METHYLFURAN 534225						
53	0.48	0.45	0.86	0.88	0.74	1.57	0.58	0.28	
82	0.77	0.73	1.39	1.43	1.20	0.22	0.93	0.45	
141	0.98		ALLYL ETHER 557400						
41	1.88	1.77	3.39	3.50	2.92	0.40	2.28	1.09	
69	0.27	0.25	0.48	0.50	0.42	0.64	0.33	0.15	
142	0.70		HEXYL ETHER 112583						
43	4.29	3.97			4.83	2.58	5.42	2.68	0.71
85	3.53	3.26			3.97	2.20	4.47	2.21	0.58
143	1.00		CARBON DISULFIDE 75150						
76	2.26	2.06	3.00	3.06	2.37	1.27	2.07	1.04	

Internal/External Standard File for Cmpd Class # 1

Cmpds	Recovery Std # 1		Compound Name Std #51		Std #52		Std #53		Std #54
Mass	186	236	113	115	81	111	82	117	136
144	1.20		THIOPHENE 110021						
58	0.49	0.47			0.58	0.31	0.55	0.26	0.08
84	0.97	0.92			1.16	0.62	1.10	0.52	0.16
145	1.13		CYCLOPENTANE 287923						
42	1.84	1.68	2.44	2.49	1.91	1.02	1.68	0.84	
70	0.47	0.43	0.63	0.64	0.50	0.27	0.44	0.22	
146	0.85		CYCLOHEXANE 110827						
56	1.34	1.26	2.41	2.49	2.08	1.12	1.62	0.77	
84	0.99	0.93	1.78	1.84	1.54	0.83	1.20	0.57	
147	1.05		HEXANE 110543						
43	0.89	0.83			1.09	0.59	1.02	0.48	0.15
47	0.69	0.65			0.85	0.46	0.79	0.38	0.12
148	1.20		HEPTANE 142825						
57	0.61	0.56			0.67	0.36	0.63	0.31	0.09
71	0.63	0.57			0.68	0.37	0.64	0.31	0.10
149	0.01		1-OCTENE 111660						
41	0.92	0.76			1.06	0.57	0.88	0.42	0.17
55	0.73	0.61			0.85	0.46	0.70	0.33	0.13
150	1.03		OCTANE 111659						
43	1.54	1.36			2.13	1.22	1.78	0.94	0.27
57	0.52	0.46			0.71	0.41	0.60	0.32	0.09
151	0.79		NONANE 111842						
43	2.27	2.13			2.79	1.51	2.60	1.24	0.38
57	1.69	1.58			2.07	1.12	1.93	0.92	0.28
152	0.96		DIPENTENE 5989275						
68	0.61	0.52			0.95	0.47	0.76	0.33	0.11
136	0.14	0.11			0.22	0.12	0.19	0.08	0.02
153	0.89		N-DECANE 629505						
57	2.76	2.56			3.11	1.73	3.50	1.73	0.46
71	1.07	0.98			1.20	0.67	1.35	0.67	0.18
154	0.50		N-UNDECANE 1120214						
43	2.55	2.41			3.04	1.63	2.88	1.37	0.41
57	2.70	2.56			3.22	1.73	3.05	1.45	0.43
155	0.67		N-DODECANE 112403						
43	2.90	2.42			3.36	1.81	2.77	1.32	0.52
57	2.99	2.50			3.46	1.87	2.86	1.36	0.54
156	0.44		N-TRIDECANE 629505						
43	2.98	2.82			3.56	1.91	3.37	1.60	0.48
57	3.56	3.37			4.24	2.28	4.02	1.91	0.57

Internal/External Standard File for Cmpd Class # 1

Cmpd#	Recovery Std # 1		Compound Name Std #51		Std #52		Std #53		Std #54
Mass	186	236	113	115	81	111	82	117	136
157	0.49		N-TETRADECANE 629594						
57	2.19	2.03			2.47	1.37	2.78	1.37	0.36
71	1.28	1.18			1.44	0.80	1.62	0.80	0.21
158	0.01		BROMOMETHANE 74839						
94	1.05	0.99	1.91	1.96	1.53	0.87	1.27	0.61	
96	0.99	0.93	1.79	1.84	1.52	0.82	1.19	0.57	
159	0.01		DICHLOROMETHANE 75092						
49	1.47	1.34	1.95	1.15	1.55	0.83	1.35	0.68	
84	0.85	0.77	1.12	0.73	0.89	0.47	0.78	0.39	
160	0.95		BROMOCHLOROMETHANE 74975						
49	0.95	0.90	1.71	1.76	1.47	0.79	1.15	0.55	
130	0.60	0.56	1.08	1.11	0.93	0.50	0.72	0.35	
161	0.78		CHLOROFORM 67663						
83	1.24	1.17	2.24	2.31	1.93	1.03	1.50	0.72	
85	0.81	0.77	1.47	1.51	1.26	0.68	0.99	0.47	
162	0.01		VINYL CHLORIDE 75014						
62	1.06	0.97	1.41	1.44	1.11	0.59	0.97	0.49	
64	0.33	0.30	0.44	0.45	0.34	0.18	0.30	0.15	
163	0.87		TRANS-1,2-DICHLOROETHYLENE 540590						
61	0.93	0.85	1.23	1.26	0.47	0.52	0.85	0.43	
96	0.65	0.59	0.86	0.88	0.68	0.36	0.59	0.30	
164	1.02		1,2-DICHLOROETHANE 107062						
62	0.52	0.48			0.57	0.31	0.54	0.26	0.08
98	0.12	0.11			0.14	0.07	0.13	0.06	0.02
165	0.77		1,2-DIBROMOETHANE 106934						
107	1.68	1.38			1.91	1.03	1.58	0.75	0.30
109	1.54	1.29			1.79	0.79	1.48	0.70	0.28
166	1.18		TRICHLOROETHYLENE 79016						
95	0.69	0.66			0.83	0.45	0.79	0.38	0.11
130	0.77	0.73			0.92	0.49	0.87	0.42	0.12
167	0.01		1,1,2-TRICHLOROETHANE 79005						
97	0.75	0.69			0.91	0.49	0.87	0.41	0.13
99	0.47	0.44			0.57	0.31	0.54	0.26	0.08
168	0.64		ALLYL CHLORIDE 107051						
39	0.78	0.71	1.03	1.05	0.83	0.44	0.72	0.36	
41	1.23	1.12	1.63	1.66	1.28	0.69	1.12	0.56	
169	0.77		TETRACHLOROETHYLENE 127184						
164	0.83	0.71			1.27	0.72	1.17	0.50	0.15
166	1.08	0.93			1.65	0.94	1.54	0.66	0.19

Internal/External Standard File for Cmpd Class # 1

Cmpd#	Recovery Std # 1		Compound Name Std #51		Std #52		Std #53		Std #54	
Mass	186	236	113	115	81	111	82	117	136	-
170	1.28		1,2-DICHLOROPROPANE 78875							
62	0.50	0.44			0.62	0.33	0.51	0.24	0.10	
63	0.72	0.60			0.85	0.46	0.70	0.33	0.13	
171	0.99		2-BROMO-1-CHLOROPROPANE 3017956							
41	0.40	0.37			0.47	0.26	0.54	0.27	0.07	
77	0.50	0.46			0.58	0.32	0.68	0.33	0.08	
172	0.90		1,2-DIBROMOPROPANE 78751							
121	1.28	1.18			1.40	0.75	1.33	0.64	0.20	
123	1.22	1.12			1.33	0.72	1.27	0.62	0.19	
173	1.17		2-BROMOBUTANE 78762							
41	0.86	0.79			0.97	0.54	1.09	0.54	0.14	
57	1.50	1.40			1.70	0.94	1.92	0.95	0.25	
174	0.01		1,4-DICHLOROBUTANE 110565							
55	1.62	1.35			1.92	1.03	1.57	0.75	0.29	
90	0.32	0.27			0.38	0.20	0.31	0.15	0.06	
175	1.03		1,4-DIBROMOBUTANE 110521							
55	1.57	1.47			1.93	1.04	1.80	0.86	0.27	
135	0.98	0.92			1.21	0.65	1.13	0.54	0.17	
176	0.01		1-BROMO-2-METHYLBUTANE 10422352							
43	1.21	1.14			1.49	0.80	1.39	0.66	0.20	
71	0.56	0.53			0.69	0.37	0.65	0.31	0.09	
177	1.28		1-CHLOROHEXANE 544105							
55	0.69	0.65			0.85	0.46	0.79	0.38	0.12	
91	1.00	0.93			1.22	0.66	1.14	0.54	0.17	
178	1.29		1-BROMOHEXANE 111251							
43	1.66	1.52			1.81	0.98	1.73	0.84	0.26	
135	0.54	0.50			0.59	0.32	0.56	0.27	0.08	
179	0.01		1-BROMODECANE 112298							
135	1.45	1.34			1.63	0.91	1.84	0.91	0.24	
137	1.56	1.44			1.76	0.98	2.06	1.02	0.26	
180	0.76		BENZENE 71432							
78	1.77	1.67	3.18	3.28	2.75	1.47	2.14	1.02	0.21	

Table B-2. RMRs AND RECOVERIES FOR NEWS COMPOUNDS

Class No. 2	
Standard ID No.	Standard Name
1	Perfluorotoluene (external)
55	d_9-t-Butanol (internal)
56	d_5-Nitrobenzene (internal)

MATRIX OF STANDARD ION RMRs

Standard	Ion	Recovery	Standard: Perfluorotoluene m/z 186	Standard: Perfluorotoluene m/z 236	Standard: d_9-t-Butanol m/z 46	Standard: d_9-t-Butanol m/z 65	Standard: d_5-Nitrobenzene m/z 82	Standard: d_5-Nitrobenzene m/z 128
Perfluorotoluene	186	NA	-	1 18 (3)[a]	1.52 (16)	1 07 (21)	0 58 (8)	1 54 ± .14 (9)
	236	NA	0.96 (16)	-	1.73 (16)	1.24 (16)	0 68 (0)	1 77 ± .17 (10)
d_9-t-Butanol	46	0 98	0 61 (11)	0 51 (7)	-	0 64 (18)	0 47 (11)	1 82 ± .27 (15)
	65	0 98	1 01 (19)	0 81 (11)	1 51 (20)	-	0 79 (20)	2 89 ± .51 (17)
d_5-Nitrobenzene	82	0 93	1 30 (6)	1 13 (10)	2 25 (2)	1.32 (19)	-	3.99 ± .04 (1)
	128	0 93	0 59 (6)	0.51 (10)	1 07 (6)	0 59 (20)	0 46 (8)	-

[a]Coefficient of variation for triplicate determinations are given in parenthesis.

Internal/External Standard File for Cmpd Class # 2

Cmpd#	Recovery Std # 1		Compound Name Std #55		Std #56	
Mass	186	236	46	65	82	128
103	1.08		1-PROPANOL 71238			
42	0.14	0.06	0.19	0.07	0.04	0.21
60	0.06	0.02	0.07	0.05	0.03	0.09
104	1.20		1-BUTANOL 71363			
41	0.46	0.20	0.64	0.24	0.17	0.55
56	0.42	0.18	0.57	0.39	0.28	0.49
105	1.13		1-PENTANOL 71410			
42	0.77	0.33	1.30	0.40	0.29	1.00
70	0.24	0.10	0.34	0.23	0.16	0.35
107	1.22		CYCLOHEXANOL 108930			
57	0.07	0.03	0.10	0.01	0.01	0.12
67	0.03	0.01	0.03	0.02	0.01	0.08
108	1.31		1-HEXANOL 111273			
56	1.14	0.48	1.56	0.58	0.43	1.70
84	0.05	0.03	0.08	0.06	0.04	0.09
109	1.06		1-HEPTANOL 111706			
41	1.36	0.58	1.86	0.72	0.52	2.02
70	0.97	0.42	1.33	0.64	0.92	1.45
110	1.00		1-OCTANOL 111875			
41	0.94	0.39	1.16	0.49	0.34	1.40
69	0.39	0.17	0.48	0.43	0.29	0.58
112	0.01		BUTOXYETHANOL 111762			
41	0.45	0.54	0.81	0.47	0.40	0.76
57	0.02	0.02	0.03	0.02	0.02	0.03
114	0.99		PROPIONALDEHYDE 123386			
57	0.09	0.09	0.16	0.09	0.07	0.16
59	0.03	0.03	0.05	0.03	0.02	0.04
115	0.72		BUTYRALDEHYDE(N) 123728			
72	0.15	0.14	0.26	0.15	0.11	0.53
116	0.83		CROTONALDEHYDE 4170303			
41	0.57	0.56	1.03	0.58	0.44	0.97
70	0.32	0.32	0.47	0.28	0.26	0.55
117	0.81		VALERALDEHYDE 110623			
44	0.64	0.63	1.16	0.66	0.50	1.09
58	0.19	0.18	0.33	0.15	0.23	0.31
118	0.45		FURFURAL 98011			
95	0.30	0.32	0.54	0.27	0.23	0.50
96	0.29	0.31	0.53	0.29	0.23	0.49

Internal/External Standard File for Cmpd Class # 2

Cmpd#	Recovery Std # 1		Compound Name Std #55		Std #56	
Mass	186	236	46	65	82	128
119	0.45		METHYL FORMATE 107313			
60	0.17	0.17	0.31	0.17	0.13	0.29
120	0.59		METHYL ACETATE 79209			
43	1.75	1.71	3.16	1.80	1.80	3.00
74	0.24	0.23	0.43	0.29	0.19	0.41
121	0.53		ETHYL ACETATE 141786			
43	2.47	2.41	4.29	2.52	1.90	4.20
61	0.24	0.44	0.44	0.27	0.19	0.42
122	0.65		ALLYL ACETATE 591877			
43	3.10	3.02	5.61	3.17	2.39	5.26
123	0.59		PROPYL ACETATE 109604			
43	3.21	3.12	5.80	3.29	2.47	5.45
61	0.68	0.66	1.22	0.83	0.53	1.14
124	0.45		ETHYL BUTYRATE 105544			
43	1.16	1.13	2.10	0.91	0.77	1.98
71	0.87	0.84	1.57	0.95	0.68	1.47
125	0.53		N-BUTYL ACETATE 123864			
43	2.79	2.70	5.04	2.20	1.97	4.74
56	0.79	0.77	1.42	0.70	0.62	1.34
126	0.79		TETRAHYDROFURAN 109999			
42	1.23	1.25	2.21	1.30	0.98	2.06
72	0.30	0.56	0.56	0.38	0.24	0.53
127	0.36		DIOXANE 123911			
88	0.17	0.18	0.26	0.19	0.14	0.18
58	0.14	0.15	0.31	0.17	0.11	0.22
128	0.01		ACETONE 67641			
43	1.54	1.52	2.79	1.55	1.19	2.62
58	0.56	0.55	1.01	0.66	0.44	0.95
129	0.69		METHYL ETHYL KETONE 78933			
43	2.34	2.28	4.23	2.37	1.80	3.98
72	0.36	0.35	0.64	0.43	0.27	0.60
130	0.52		CYCLOPENTANONE 120923			
55	0.69	0.83	1.25	0.72	0.62	1.13
84	0.24	0.30	0.44	0.26	0.22	0.48
131	0.52		CYCLOHEXANONE 108941			
55	0.68	0.80	1.24	0.72	0.61	1.15
98	0.20	0.28	0.48	0.23	0.20	3.49
133	0.59		ACRYLONITRILE 107131			
53	1.06	1.38	1.15	0.56	0.40	1.33
52	0.89	0.45	1.46	1.11	0.70	1.58

Internal/External Standard File for Cmpd Class # 2

Cmpd#	Recovery Std # 1		Compound Name Std #55		Std #56	
Mass	186	236	46	65	82	128
134	0.95		PROPIONITRILE 107120			
54	1.28	0.51	1.72	0.68	0.45	1.93
55	0.19	0.09	0.27	0.19	0.13	0.30
135	0.57		ISOBUTYRONITRILE 78820			
42	2.64	1.12	3.63	1.39	1.00	3.95
68	1.09	0.46	1.50	1.04	0.72	1.64
136	0.91		BENZONITRILE 100470			
103	4.10	1.74	2.11	1.83	1.54	2.30
76	1.54	0.65	5.63	3.86	2.75	6.14
137	0.96		NITROMETHANE 75525			
61	0.52	0.25	0.64	0.31	0.22	0.69
46	0.46	0.20	0.72	0.56	0.39	0.88
138	0.93		NITROPROPANE 108032 OR 79469			
41	1.87	0.73	2.36	0.91	0.65	2.56
43	1.54	0.65	2.12	1.67	1.02	2.28
139	0.96		NITROBENZENE 98953			
77	2.66	1.13	3.65	1.40	1.00	3.97
123	1.16	0.49	1.59	1.10	0.77	1.73

Table B-3. RMRs AND RECOVERIES FOR WABN COMPOUNDS
(BLLE, pH 8.0/NO FRACTIONATION)

Class No. 3	
Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
54	d_8-Naphthalene (internal)
56	d_5-Nitrobenzene (internal)
57	d_{10}-o-Xylene (internal)
58	d_5-Phenylethanol (internal)
59	d_5-Acetophenone (internal)
60	d_5-Propiophenone (internal)
61	d_{12}-Perylene (internal)
62	d_9-Acridine (internal)
63	d_5-Phenol (internal)

MATRIX OF STANDARD ION RMRs

			Standard							
			d_5-Phenol	d_{10}-o-Xylene		d_8-Naphthalene	d_5-Nitrobenzene		d_5-Phenylethanol	
Compound	Ion	Recovery	m/z 99	m/z 98	m/z 116	m/z 136	m/z 82	m/z 128	m/z 84	m/z 112
d_5-phenol	99	0 85	-	59(9)	99(9)	.17(6)	1 04(5)	1 66(3)	2 44(15)	1 75(15)
d_{10}-o-xylene	99	0 58	1 72(9)[a]	-	1.67(1)	.29(6)	1 79(8)	2.84(8)	4 21(22)	3 02(21)
	116	0 58	1 03(a)	60(0)	-	.18(6)	1 07(8)	1.71(8)	2.53(22)	1 81(21)
d_8-naphthalene	136	0 71	5 97(4)	3.51(7)	5.85(7)	-	6 21(3)	9 98(3)	14 63(15)	10 59(18)
d_5-nitrobenzene	82	0 79	.97(4)	.57(10)	.95(10)	16(3)	-	1 60(1)	2 35(17)	1 70(16)
	128	0 79	.61(2)	35(9)	59(9)	.10(1)	63(1)	-;	1 47(16)	1 07(15)
d_5-phenylethanol	84	0 80	.42(15)	.25(24)	.42(24)	.07/ .71(18)	44(16)	.70(15)	-	.73(2)
	112	0 80	.58(15)	.35(22)	.58(23)	098(18)	61(16)	.95(16)	1.39(2)	-
d_5-propiophenone	82	0 73	1 09(4)	65(13)	1 07(14)	.18(8)	1 13(6)	1.87(6)	2 63(11)	1.90(10)
	110	0 73	2 85(5)	1 67(13)	2 78(14)	48(17)	2 94(6)	4 72(6)	6 84(12)	4 95(11)
d_5-acetophenone	110	0 75	1.52(2)	90(7)	1 50(8)	.25(4)	1 60(5)	2 55(1)	3 71(17)	2.68(16)
	125	0 75	.46(2)	27(8)	45(7)	76(3) .076	48(3)	7n(4)	1 11(18)	.81(17)
d_{12}-perylene	264	0 80	3.56(13)	2 09(7)	3 48(8)	60(9)	3 70(11)	5.90(12)	8 52(25)	6.37(28)
d_9-acridine	188	0 84	1.45(7)	86(15)	1.43(15)	.24(8)	1 51(6)	2.40(6)	3 52(13)	2.55(13)
4-fluoro-2-iodotoluene	109	NA	1.10(4)	65(7)	1 08(8)	.18(3)	1.14(2)	1 82(2)	2 69(18)	1 97(19)
	236	NA	1 43(4)	84(6)	1.39(7)	24(6)	1 48(3)	2.37(3)	3 48(18)	2.52(18)

(Continued)

Compound	Ion	Recovery	Standard: d_5-Propiophenone m/z 82	d_5-Propiophenone m/z 110	d_5-Acetophenone m/z 110	d_5-Acetophenone m/z 125	d_{12}-Perylene m/z 264	d_9-Acridine m/z 188	4-Fluoro-2-Iodotoluene m/z 109	4-Fluoro-2-Iodotoluene m/z 236
d_5-phenol	99	0 85	.92(5)	35(5)	.67(2)	2 21(3)	31(15)	70(7)	.91(5)	.71(4)
d_{10}-o-xylene	98	0 58	1 59(12)	.61(13)	1.13(7)	3 77(7)	53(10)	1.20(13)	1.56(6)	1 21(6)
	116	0 58	.95(13)	.37(12)	67(6)	2 27(7)	32(10)	.72(13)	.94(6)	.73(6)
d_8-naphthalene	136	0 71	5.51(8)	2.13(8)	3.91(4)	13.14(3)	1.76(15)	4 20(8)	5 45(1)	4.20(1)
d_5-nitrobenzene	82	0 79	.89(6)	.34(6)	63(4)	2.12(4)	29(19)	67(6)	.88(2)	.68(3)
	128	0 79	55(6)	.22(6)	39(1)	1 32(3)	18(20)	.42(6)	.55(3)	.42(3)
d_5-phenylethanol	84	0 80	.39(11)	15(10)	28(16)	93(12)	13(28)	.29(11)	38(18)	.30(17)
	112	0 80	.53(10)	21(9)	39(16)	1 28(16)	18(28)	41(13)	.52(19)	42(16)
d_5-propiophenone	82	0 73	-	.39(1)	.71(7)	2 40(6)	33(23)	.76(5)	1.00(7)	.77(7)
	110	0 73	2.60(1)	-	1.85(6)	6 21(6)	87(19)	2 00(5)	2 59(7)	1.99(7)
d_5-acetophenone	110	0 75	1.41(6)	.55(6)	-	5 39(1)	.47(14)	1 10(9)	1 37(4)	1.07(2)
	125	0 75	.42(6)	.16(5)	30(2)	-	.14(18)	32(9)	42(2)	.33(3)
d_{12}-perylene	264	0 80	3 08(14)	1 27(16)	2.37(12)	7 91(12)	-	2.50(16)	3 21(9)	2 51(9)
d_9-acridine	188	0 84	1.33(5)	.52(5)	.95(10)	3.15(11)	39(40)	-	1.32(8)	1 03(8)
4-fluoro-2-iodotoluene	109	NA	1.01(7)	.39(7)	71(2)	2 40(2)	34(12)	.76(8)	-	.77(1)
	236	NA	1 31(7)	51(7)	92(3)	3 11(2)	42(16)	1 00(8)	1 30(1)	-

[a] (CV).

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
110	0.01		P-NITROANILINE 100016							
65	0.44	0.35	0.08		0.52	0.83	0.27	0.46	1.30	0.97
138	0.56	0.45	0.11		0.67	1.07	0.35	0.58	1.68	0.22
111	0.80		2,4-DIMETHYLQUINOLINE 1198374							
156	0.41	0.32	0.08		0.47	0.75	0.26	0.43	0.95	0.68
157	2.01	1.54	0.37		2.31	3.59	1.27	2.11	4.64	3.31
112	0.01		1,8-DIAMINONAPHTHALENE 569415							
114	0.03	0.02	0.00		0.04	0.06	0.02	0.03	0.09	0.06
141	0.05	0.04	0.01		0.06	0.01	0.03	0.05	0.14	0.11
113	0.84		NICOTINE 54115							
84	1.17	0.90	0.22		1.35	2.09	0.74	1.23	2.70	1.92
133	0.28	0.21	0.05		0.32	0.49	0.17	0.29	0.63	0.45
114	0.79		CARBAZOLE 86748							
167	3.73	2.88	0.69		4.30	6.66	2.37	3.92	9.36	6.67
115	0.91		2-AMINOBIPHENYL 90445							
168	6.79	5.11	1.20		7.65	12.18	4.61	6.67	19.13	14.17
169	12.72	9.45	2.22		14.15	22.54	7.42	12.30	35.40	26.19
116	0.76		DIPHENYLAMINE 122394							
168	1.48	1.14	0.27		1.71	2.65	0.94	1.56	3.43	2.45
169	2.79	2.15	0.52		3.22	4.99	1.77	2.93	6.45	4.60
117	0.01		DICYCLOHEXYLAMINE 101837							
56	0.33	0.37	0.06		0.39	0.63	0.21	0.35	1.10	0.78
138	0.96	0.76	0.18		1.12	1.80	0.61	1.02	3.15	2.25
118	0.70		TRIBUTYLAMINE 75649							
100	0.42	0.33	0.08		0.49	0.75	0.27	0.44	0.97	0.69
142	1.53	1.18	0.28		1.77	2.74	0.97	1.61	3.52	2.51
119	0.92		CAFFEINE 58082							
109	0.10	0.08	0.02		0.12	0.17	0.06	0.10	0.23	0.16
194	0.19	0.15	0.04		0.22	0.34	0.12	0.20	0.44	0.32
120	0.62		DIBENZYLAMINE 103491							
91	1.62	1.26	0.30		1.78	2.87	1.16	1.94	3.63	2.67
197	0.13	0.11	0.03		0.15	0.24	0.10	0.16	0.30	0.22
121	0.68		N,N-DIMETHYLDODECYLAMINE 112185							
58	4.72	3.88	0.87		5.47	8.83	3.58	5.99	11.09	8.16
59	0.17	0.13	0.03		0.20	0.30	0.13	0.21	0.40	0.29
122	0.90		ATRAZINE 1912249							
200	2.75	2.20	0.52		3.28	5.23	1.72	2.86	8.17	6.09
215	1.67	1.34	0.31		2.00	3.18	1.05	1.74	4.97	3.71

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
110	0.01		P-NITROANILINE 100016							
65	0.34	1.13	0.49	0.19	0.14		0.04		0.51	
138	0.43	1.84	0.62	0.24	0.19		0.05		0.65	
111	0.80		2,4-DIMETHYLQUINOLINE 1198374							
156	0.29	0.96	0.40	0.15	0.15		0.03		0.43	
157	1.46	4.69	1.93	0.74	0.71		0.15		2.09	
112	0.01		1,8-DIAMINONAPHTHALENE 569415							
114	0.02	0.08	0.03	0.01	0.01		0.00		0.03	
141	0.04	0.12	0.05	0.02	0.01		0.00		0.55	
113	0.84		NICOTINE 54115							
84	0.82	2.74	1.12	0.43	0.41		0.09		1.22	
133	0.19	0.64	0.26	0.10	0.10		0.02		0.29	
114	0.79		CARBAZOLE 86748							
167	2.60	8.72	3.57	1.37	1.28		0.31		4.22	
115	0.91		2-AMINOBIPHENYL 90445							
168	4.75	16.46	7.10	2.75	2.13		0.51		7.45	
169	8.82	30.44	13.14	5.08	3.96		0.95		13.80	
116	0.76		DIPHENYLAMINE 122394							
168	1.03	3.47	1.42	0.55	0.52		0.11		1.55	
169	1.94	6.46	2.68	1.03	0.98		0.22		2.91	
117	0.01		DICYCLOHEXYLAMINE 101837							
56	0.25	0.81	0.33	0.14	0.09		0.03		0.38	
138	0.71	2.34	0.95	0.40	0.26		0.08		1.09	
118	0.70		TRIBUTYLAMINE 75649							
100	0.29	0.99	0.41	0.16	0.15		0.03		0.44	
142	0.99	3.34	1.47	0.57	0.53		0.12		1.59	
119	0.92		CAFFEINE 58082							
109	0.07	0.23	0.09	0.04	0.04		0.01		0.10	
194	0.13	0.45	0.18	0.07	0.07		0.02		0.21	
120	0.62		DIBENZYLAMINE 103491							
91	1.18	3.91	1.52	0.59	0.62		0.11		1.74	
197	0.10	0.32	0.13	0.05	0.05		0.01		0.14	
121	0.68		N,N-DIMETHYLDODECYLAMINE 112185							
58	3.62	12.02	4.66	1.81	1.87		0.34		5.37	
59	0.13	0.43	0.17	0.06	0.07		0.01		0.19	
122	0.90		ATRAZINE 1912249							
200	2.13	7.07	3.05	1.18	0.90		0.22		3.26	
215	1.21	4.30	1.85	0.72	0.55		0.13		1.95	

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std # 2		Compound Name Std #54	Std #56		Std #57		Std #58	
Mass	109	236	136	82	128	98	116	84	112
123	0.01		HEPTANONE 110430						
43	1.21	0.94	0.22	1.33	2.14	0.85	1.14	2.32	2.00
58	0.75	0.58	0.14	0.83	1.33	0.53	0.88	1.69	1.25
124	0.65		BUTOXYETHANOL 111762						
41	0.21	0.17	0.04	0.25	0.40	0.13	0.22	0.49	0.35
57	0.55	0.42	0.10	0.63	1.03	0.35	0.58	1.27	0.91
125	0.70		2-OCTANONE 111137						
43	1.30	1.01	0.24	1.43	2.31	0.91	1.53	2.92	2.15
58	1.02	0.79	0.19	1.11	1.80	0.71	1.19	2.27	1.67
126	0.61		BUTYLPROPIONATE 590012						
57	1.48	1.14	0.27	1.71	2.73	0.90	1.49	4.27	3.15
75	0.44	0.34	0.08	0.51	0.82	0.27	0.45	1.28	0.95
127	0.78		ISOPHORONE 78591						
82	1.77	1.36	0.33	2.04	3.17	1.13	1.86	4.11	2.93
138	0.39	0.30	0.07	0.45	0.72	0.25	0.41	0.90	0.64
128	0.74		FENCHONE 1195759						
69	0.66	0.51	0.12	0.72	1.17	0.47	0.78	1.47	1.08
81	1.44	1.12	0.27	1.58	2.55	1.02	1.71	3.22	2.36
129	0.75		ALPHA-TERPINEOL 98555						
59	0.56	0.43	0.10	0.65	1.00	0.36	0.59	1.31	0.93
136	0.32	0.25	0.06	0.37	0.58	0.21	0.34	0.75	0.53
130	0.95		N-DECANOL 112301						
41	0.40	0.31	0.07	0.46	0.74	0.25	0.42	0.92	0.66
43	0.44	0.34	0.08	0.51	0.79	0.28	0.46	1.02	0.73
131	0.62		DIMETHYLADIPATE 627930						
59	0.56	0.45	0.10	0.64	1.03	0.41	0.69	1.29	0.95
114	0.44	0.35	0.08	0.49	0.79	0.32	0.54	1.00	0.74
132	0.77		METHYL STEARATE 112618						
74	3.42	2.65	0.63	3.89	6.28	2.54	4.25	7.90	5.81
87	2.22	1.72	0.41	2.52	4.07	1.65	2.76	5.13	3.77
133	0.64		N-DECANE 124185						
43	1.47	1.11	0.26	1.67	2.66	0.88	1.46	4.18	3.09
57	1.42	1.08	0.25	1.64	2.61	0.85	1.41	4.05	3.00
134	0.66		N-TRIDECANE 629505						
43	2.18	1.64	0.34	2.48	3.95	1.30	2.16	6.20	4.58
57	2.75	2.09	0.50	3.14	5.01	1.66	2.77	7.93	5.86
135	0.48		N-TETRADECANE 629594						
43	2.52	1.92	0.45	2.88	4.58	1.51	2.51	7.19	5.31
57	3.40	2.55	0.61	3.87	6.16	2.03	3.37	9.67	7.15

Internal/External Standard File for Cmpd Class # 3

Cmpds	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
123	0.01		KEPTANONE 110430							
43	0.88	2.91	1.13	0.44	0.47		0.08		1.30	
58	0.55	1.82	0.71	0.27	0.29		0.05		0.81	
124	0.65		BUTOXYETHANOL 111762							
41	0.15	0.49	0.20	0.09	0.07		0.02		0.22	
57	0.38	1.28	0.52	0.20	0.19		0.04		0.57	
125	0.70		2-OCTANONE 111137							
43	0.95	3.14	1.22	0.47	0.51		0.09		1.40	
58	0.74	2.45	0.95	0.37	0.39		0.07		1.09	
126	0.61		BUTYLPROPIONATE 590012							
57	1.11	3.69	1.59	0.61	0.48		0.12		1.66	
75	0.33	1.11	0.48	0.19	0.15		0.04		0.50	
127	0.78		ISOPHORONE 78591							
82	1.23	4.14	1.70	0.65	0.62		0.14		1.80	
138	0.27	0.91	0.37	0.14	0.14		0.03		0.41	
128	0.74		FENCHONE 1195759							
69	0.48	1.58	0.62	0.24	0.25		0.05		0.71	
81	1.05	3.45	1.35	0.52	0.55		0.10		1.55	
129	0.75		ALPHA-TERPINEOL 98555							
59	0.39	1.31	0.54	0.21	0.20		0.04		0.58	
136	0.23	0.76	0.31	0.12	0.11		0.03		0.34	
130	0.95		N-DECANOL 112301							
41	0.28	0.93	0.38	0.15	0.14		0.03		0.41	
43	0.31	1.63	0.42	0.16	0.15		0.03		0.46	
131	0.62		DIMETHYLADIPATE 627930							
59	0.42	1.40	0.54	0.21	0.22		0.04		0.62	
114	0.33	1.08	0.42	0.16	0.17		0.03		0.48	
132	0.77		METHYLSTEARATE .12618							
74	2.58	8.56	3.32	1.29	1.33		0.24		3.83	
87	1.67	5.55	2.15	0.83	0.87		0.16		2.48	
133	0.64		N-DECANE 124185							
43	1.05	3.59	1.55	0.60	0.47		0.11		1.62	
57	1.01	3.48	1.50	0.58	0.46		0.11		1.58	
134	0.66		N-TRIDECANE 629505							
43	1.56	5.33	2.30	0.89	0.70		0.17		2.41	
57	1.99	6.75	2.94	1.14	0.76		0.21		3.09	
135	0.48		N-TETRADECANE 629594							
43	1.86	6.19	2.67	1.03	0.80		0.19		2.80	
57	2.50	8.33	3.57	1.39	1.08		0.26		3.77	

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std # 2		Compound Name	Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-		82	128	98	116	84	112
136	0.68		N-PENTADECANE 692629								
57	2.78	2.14	0.52			3.22	4.99	1.77	2.94	6.47	4.62
71	1.73	1.33	0.32			2.01	3.11	1.10	1.83	4.03	2.87
137	0.51		N-HEXADECANE 544763								
43	1.90	1.45	0.34			2.16	3.45	1.13	1.89	5.41	3.99
57	2.72	2.08	0.49			3.11	4.96	1.63	2.71	7.78	5.74
138	0.78		N-HEPTADECANE 629787								
57	3.13	2.41	0.58			3.61	5.59	1.99	3.30	7.25	5.17
71	2.07	1.60	0.38			2.39	3.70	1.32	2.18	4.80	3.42
139	0.67		N-OCTADECANE 593453								
57	2.99	2.51	0.59			3.75	5.98	1.88	3.14	8.96	6.63
71	1.98	1.66	0.39			2.48	3.95	1.25	2.08	5.95	4.41
140	0.63		N-NONADECANE 629925								
71	2.12	1.61	0.38			2.42	3.85	1.27	2.11	6.04	4.47
85	1.42	1.08	0.25			1.61	2.57	0.85	1.41	4.03	2.98
141	0.75		N-EICOSANE 112958								
57	4.43	3.41	0.82			5.11	7.92	2.82	4.66	10.26	7.32
71	3.03	2.33	0.56			3.50	5.43	1.93	3.19	7.03	5.01
142	0.66		N-HENEICOSANE 629947								
57	3.93	2.96	0.70			4.43	7.05	2.32	3.86	11.05	8.20
71	2.71	2.05	0.48			3.07	4.88	1.61	2.67	7.65	5.68
143	0.64		N-DOCOSANE 629970								
57	3.73	2.98	0.70			4.46	7.10	2.33	3.88	11.11	8.26
71	2.60	2.08	0.49			3.11	4.96	1.63	2.70	7.76	5.77
144	0.65		N-TRICOSANE 638675								
57	3.99	3.19	0.75			4.77	7.60	2.49	4.14	11.85	8.83
71	2.80	2.24	0.53			3.35	5.34	1.75	2.91	8.33	6.20
145	0.01		PHENYLACETATE 122792								
94	1.84	1.43	0.34			2.01	3.25	1.30	2.18	4.10	3.01
136	0.25	0.20	0.04			0.28	0.45	0.18	0.30	0.57	0.42
146	0.74		BENZYLACETATE 140114								
91	0.52	0.40	0.09			0.57	0.92	0.37	0.62	1.15	0.85
108	1.09	0.85	0.20			1.19	1.92	0.77	1.29	2.43	1.79
147	0.81		METHYLBENZENESULFONATE								
77	1.24	0.94	0.22			1.41	2.25	0.74	1.23	3.54	2.61
172	0.44	0.34	0.08			0.50	0.80	0.26	0.44	1.26	0.93
148	0.67		METHYLTOLUENESULFONATE								
91	1.60	1.21	0.29			1.81	2.89	0.95	1.58	4.53	3.35
155	0.72	0.54	0.13			0.81	1.29	0.42	0.71	2.02	1.50

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
136	0.68		N-PENTADECANE 692629							
57	1.94	6.52	2.68	1.03	0.99		0.22		2.92	
71	1.21	4.06	1.67	0.64	0.62		0.14		1.82	
137	0.51		N-HEXADECANE 544763							
43	1.40	4.66	2.01	0.78	0.61		0.15		2.11	
57	2.01	6.70	2.88	1.12	0.87		0.21		3.03	
138	0.78		N-HEPTADECANE 629787							
57	2.18	7.32	3.01	1.16	1.11		0.24		3.27	
71	1.44	4.85	1.99	0.77	0.73		0.16		2.17	
139	0.67		N-OCTADECANE 593453							
57	2.33	8.10	3.48	1.35	1.01		0.24		3.65	
71	1.55	5.35	2.30	0.89	0.68		0.06		2.41	
140	0.63		N-NONADECANE 629925							
71	1.51	5.27	2.24	0.87	0.68		0.16		2.35	
85	1.01	3.47	1.50	0.58	0.45		0.11		1.57	
141	0.75		N-EICOSANE 1112958							
57	3.08	10.35	4.25	1.63	1.57		0.35		4.63	
71	2.11	7.09	2.91	1.12	1.07		0.23		3.17	
142	0.66		N-HENEICOSANE 629947							
57	2.73	9.53	4.11	1.60	1.07		0.30		4.31	
71	1.89	6.60	2.85	1.10	0.74		0.21		2.99	
143	0.64		N-DOCOSANE 629970							
57	2.89	9.60	4.14	1.60	1.22		0.30		4.35	
71	2.02	6.71	2.89	1.12	0.85		0.21		3.04	
144	0.65		N-TRICOSANE 638675							
57	3.10	10.28	4.42	1.71	1.29		0.32		4.65	
71	2.18	7.22	3.11	1.20	0.90		0.22		3.27	
145	0.01		PHENYLACETATE 122792							
94	1.31	4.43	1.72	0.67	0.70		0.13		1.98	
136	0.18	0.62	0.24	0.09	0.10		0.02		0.28	
146	0.74		BENZYLACETATE 140114							
91	0.38	1.25	0.48	0.19	0.20		0.04		0.56	
108	0.79	2.63	1.02	0.40	0.41		0.07		1.17	
147	0.81		METHYLBENZENESULFONATE							
77	0.91	3.04	1.31	0.51	0.40		0.09		1.38	
172	0.32	1.08	0.47	0.18	0.14		0.03		0.49	
148	0.67		METHYLTOLUENESULFONATE							
91	1.17	3.90	1.68	0.65	0.51		0.12		1.76	
155	0.52	1.74	0.75	0.29	0.23		0.05		0.79	

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
149	1.07		DIMETHYLPHTHALATE 131113							
77	0.81	0.63	0.15		0.94	1.45	0.52	0.85	1.88	1.34
163	5.29	4.07	0.98		6.10	9.46	3.36	5.56	12.22	8.71
150	0.91		ETHYLTOLUENESULFONATE							
91	1.74	1.32	0.31		1.97	3.14	1.03	1.72	4.92	3.65
155	1.18	0.94	0.22		1.40	2.23	0.73	1.21	3.46	2.35
151	1.08		DIETHYLPHTHALATE 84662							
149	3.19	2.43	0.57		3.65	5.79	1.90	3.17	9.08	6.71
177	0.80	0.61	0.14		0.93	1.47	0.48	0.80	2.29	1.69
152	0.96		DIBUTYLPHTHALATE 84742							
57	0.29	0.23	0.05		0.34	0.52	0.19	0.31	0.68	0.48
149	7.17	5.52	1.33		8.27	12.80	4.55	7.54	16.55	11.80
153	0.97		BUTYLBENZYLPHTHALATE							
91	2.09	1.62	0.38		2.28	3.69	1.48	2.48	4.64	3.41
149	3.37	2.62	0.62		3.69	5.95	2.40	4.01	7.49	5.51
154	1.02		DIETHYLHEXYLPHTHALATE 117817							
149	5.22	4.07	0.96		5.71	9.23	3.74	6.26	11.59	8.53
167	1.98	1.54	0.37		2.17	3.51	1.42	2.37	4.40	3.24
155	0.89		BENZALDEHYDE 100527							
77	0.36	0.28	0.07		0.42	0.64	0.23	0.38	0.84	0.66
105	0.40	0.31	0.07		0.46	0.70	0.25	0.42	0.92	0.66
156	0.66		TOLUALDEHYDE 529201							
91	0.54	0.44	0.10		0.65	1.04	0.34	0.57	1.65	1.21
119	0.63	0.51	0.12		0.77	1.23	0.41	0.68	1.95	1.43
157	0.87		ACETOPHENONE 98862							
77	0.38	0.64	0.15		0.96	1.53	0.53	0.87	1.93	1.37
105	1.22	0.94	0.23		1.41	2.25	0.78	1.29	2.85	2.03
158	0.73		SALICYLALDEHYDE 90028							
121	0.56	0.44	0.10		0.61	0.99	0.40	0.67	1.24	0.91
122	0.60	0.47	0.11		0.60	1.07	0.43	0.72	1.34	0.99
159	0.72		ANISALDEHYDE 123115							
135	1.37	1.08	0.25		1.53	2.47	0.91	1.66	3.11	2.29
136	0.96	0.76	0.18		1.07	1.73	0.70	1.16	2.18	1.60
160	0.85		PHENOL 108952							
94	1.07	0.84	0.20		1.18	1.90	0.76	1.27	2.41	1.77
161	0.72		CRESOL 108394							
107	1.21	0.93	0.23		1.40	2.25	0.80	1.29	2.91	2.08
108	1.07	0.82	0.20		1.24	1.99	0.69	1.14	2.58	1.84

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery		Compound Name							
	Std #59		Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
149	1.07		DIMETHYLPHTHALATE 131113							
77	0.57	1.83	0.75	0.29	0.28		0.06		0.85	
163	3.68	11.87	4.88	1.88	1.85		0.41		5.51	
150	0.91		ETHYLTOLUENESULFONATE							
91	1.28	4.25	1.83	0.71	0.55		0.13		1.92	
155	0.91	3.01	1.30	0.50	0.38		0.09		1.36	
151	1.08		DIETHYLPHTHALATE 84662							
149	2.35	7.82	3.34	1.30	1.02		0.24		3.54	
177	0.59	1.97	0.85	0.33	0.26		0.06		0.89	
152	0.96		DIBUTYLPHTHALATE 84742							
57	0.20	0.68	0.28	0.11	0.10		0.02		0.31	
149	4.99	16.75	6.88	2.64	2.52		0.55		7.47	
153	0.97		BUTYLBENZYLPHTHALATE							
91	1.51	5.02	1.95	0.76	0.78		0.14		2.24	
149	2.44	8.10	3.15	1.22	1.26		0.23		3.62	
154	1.02		DIETHYLHEXYLPHTHALATE 117817							
149	4.03	12.58	4.88	1.89	1.90		0.35		5.61	
167	1.53	4.78	1.85	0.72	0.72		0.13		2.13	
155	0.89		BENZALDEHYDE 100527							
77	0.25	0.84	0.35	0.13	0.13		0.03		0.38	
105	0.28	0.93	0.38	0.15	0.14		0.03		0.42	
156	0.66		TOLUALDEHYDE 529204							
91	0.42	1.41	0.61	0.24	0.15		0.05		0.64	
119	0.50	1.66	0.72	0.28	0.22		0.05		0.75	
157	0.87		ACETOPHENONE 98862							
77	0.57	1.95	0.80	0.31	0.29		0.06		0.87	
105	0.85	2.88	1.16	0.45	0.43		0.09		1.28	
158	0.73		SALICYLALDEHYDE 90028							
121	0.41	1.35	0.52	0.20	0.21		0.04		0.60	
122	0.44	1.46	0.56	0.22	0.23		0.04		0.65	
159	0.72		ANISALDEHYDE 123115							
135	1.01	3.36	1.30	0.51	0.53		0.09		1.50	
136	0.71	2.36	0.91	0.35	0.37		0.07		1.05	
160	0.85		PHENOL 108952							
94	0.75	2.60	1.01	0.39	0.41		0.07		1.15	
161	0.72		CRESOL 108394							
107	0.88	2.85	1.17	0.45	0.44		0.10		1.31	
108	0.78	2.52	1.03	0.40	0.39		0.09		1.16	

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std # 2		Compound Name Std #54	Std #56		Std #57		Std #58	
Mass	109	236	136 -	82	128	98	116	84	112
162	0.01		2,3-DIMETHYLPHENOL 526750						
107	0.87	0.67	0.16	1.00	1.61	0.57	0.95	2.08	1.48
122	0.91	0.70	0.17	1.05	1.64	0.58	0.96	2.12	1.51
163	0.74		ISOPROPYLPHENOL(O) 88699						
121	1.79	1.36	0.32	2.04	3.25	1.07	1.78	5.10	3.77
136	0.07	0.56	0.12	0.75	1.19	0.39	0.65	1.87	1.38
164	0.01		O-NITROPHENOL 88755						
65	0.03	0.02	0.00	0.03	0.05	0.02	0.03	0.06	0.05
139	0.13	0.10	0.02	0.14	0.23	0.09	0.15	0.29	0.21
165	0.98		4-CHLORO-3-METHYLPHENOL 59507						
107	0.93	0.71	0.17	1.06	1.68	0.55	0.92	2.64	2.95
142	1.02	0.77	0.18	1.16	1.84	0.61	1.01	2.89	2.14
166	0.01		4-CHLOROCRESOL 59507 OR 1570645						
107	0.83	0.64	0.16	0.97	1.57	0.53	0.88	2.03	1.45
142	0.94	0.72	0.17	1.09	1.77	0.60	0.99	2.29	1.63
167	0.01		1-NAPHTHOL 90153						
115	0.35	0.26	0.06	0.38	0.61	0.20	0.34	0.96	0.72
144	0.61	0.45	0.11	0.67	1.07	0.35	0.29	1.68	1.25
168	0.80		P-TERT-BUTYLPHENOL 98544						
107	0.56	0.43	0.10	0.65	1.03	0.34	0.56	1.60	1.18
135	1.96	1.49	0.35	2.22	3.54	1.17	1.94	5.56	4.11
169	0.76		2-NITROCRESOL 119335						
77	0.26	0.20	0.05	0.30	0.46	0.07	0.27	0.60	0.43
153	0.74	0.57	0.14	0.83	1.33	0.46	0.78	1.72	1.23
170	0.01		2,4-DICHLOROPHENOL 120832						
162	1.13	0.88	0.21	1.24	2.00	0.80	1.34	2.52	1.86
164	0.72	0.53	0.13	0.78	1.27	0.51	0.85	1.60	1.18
171	0.01		2,4,6-TRICHLOROPHENOL 88062						
196	0.81	0.63	0.15	0.89	1.44	0.58	0.97	1.88	1.34
198	0.83	0.64	0.15	0.91	1.46	0.59	0.98	1.90	1.36
172	0.01		DI-TERT-BUTYL-4-METHYLPHENOL 128370						
205	2.53	1.97	0.47	2.78	4.49	1.81	3.03	5.66	4.16
220	0.67	0.52	0.12	0.73	1.18	0.48	0.80	1.49	1.09
173	0.01		PENTACHLOROPHENOL 87865						
264	0.29	0.22	0.05	0.34	0.54	0.19	0.31	0.72	0.52
266	0.47	0.36	0.09	0.55	0.91	0.32	0.54	1.17	0.84
174	0.71		2-METHYLNAPHTHALENE 91576						
141	2.03	1.58	0.38	2.23	3.60	1.44	2.42	4.53	3.34
142	2.51	1.96	0.46	2.76	4.45	1.79	2.99	5.62	4.13

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
162	0.01		2,3-DIMETHYLPHENOL 526750							
107	0.63	2.11	0.84	0.32	0.32		0.07		0.94	
122	0.64	2.14	0.85	0.33	0.32		0.07		0.95	
163	0.74		ISOPROPYLPHENOL(O) 88699							
121	1.28	4.39	1.90	0.73	0.58		0.14		1.99	
136	0.47	1.61	0.69	0.27	0.21		0.05		0.73	
164	0.01		O-NITROPHENOL 88755							
65	0.02	0.07	0.03	0.01	0.01		0.00		0.03	
139	0.09	0.31	0.12	0.05	0.05		0.01		0.14	
165	0.98		4-CHLORO-3-METHYLPHENOL 59507							
107	0.66	2.26	0.98	0.38	0.30		0.07		1.03	
142	0.72	2.49	1.07	0.42	0.32		0.08		1.13	
166	0.01		4-CHLOROCRESOL 59507 OR 1570645							
107	0.58	1.96	0.80	0.31	0.31		0.07		0.91	
142	0.66	2.20	0.85	0.34	0.35		0.08		1.03	
167	0.01		1-NAPHTHOL 90153							
115	0.25	0.83	0.36	0.14	0.11		0.03		0.38	
144	0.44	1.45	0.62	0.24	0.18		0.05		0.66	
168	0.80		P-TERT-BUTYLPHENOL 98544							
107	0.40	1.38	0.66	0.23	0.18		0.04		0.62	
135	1.44	4.79	2.04	0.80	0.63		0.15		2.16	
169	0.76		2-NITROCRESOL 119335							
77	0.18	0.61	0.25	0.10	0.09		0.02		0.27	
153	0.52	1.74	0.71	0.27	0.26		0.06		0.78	
170	0.01		2,4-DICHLOROPHENOL 120832							
162	0.80	2.73	1.05	0.41	0.43		0.08		1.22	
164	0.51	1.70	0.67	0.26	0.27		0.05		0.77	
171	0.01		2,4,6-TRICHLOROPHENOL 88062							
196	0.58	1.97	0.76	0.30	0.91		0.05		0.88	
198	0.58	1.99	0.77	0.30	0.32		0.06		0.89	
172	0.01		DI-TERT-BUTYL-4-METHYLPHENOL 128370							
205	1.85	6.13	2.37	0.92	0.96		0.17		2.73	
220	0.49	1.61	0.62	0.24	0.25		0.05		0.72	
173	0.01		PENTACHLOROPHENOL 87865							
264	0.20	0.68	0.28	0.11	0.11		0.02		0.31	
266	0.36	1.11	0.45	0.07	0.18		0.04		0.50	
174	0.71		2-METHYLNAPHTHALENE 91576							
141	1.48	4.91	1.90	0.74	0.77		0.14		2.19	
142	1.78	6.08	2.36	0.91	0.95		0.17		2.71	

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
175	0.78		ACENAPHTHENE 83329							
153	1.26	0.98	0.23		1.38	2.22	0.89	1.49	2.81	2.06
154	3.40	2.64	0.63		3.73	6.02	2.41	4.04	7.59	5.58
176	0.80		BIPHENYL 92524							
154	2.28	1.78	0.42		2.51	4.04	1.63	2.72	5.10	3.75
177	0.71		1,8-DIMETHYLNAPHTHALENE 569415							
141	1.59	1.24	0.29		1.74	2.82	1.13	1.89	3.55	2.61
156	2.30	1.79	0.42		2.52	4.07	1.63	2.73	5.13	3.77
178	0.85		FLUORENE 86737							
165	2.74	2.13	0.49		3.01	4.85	1.95	3.27	6.12	4.50
166	3.07	2.38	0.57		3.44	5.55	2.23	3.74	6.99	5.14
179	0.74		2,3,5-TRIMETHYLNAPHTHALENE 2245387							
155	1.86	1.44	0.34		2.08	3.36	1.36	2.27	4.24	3.12
170	2.56	1.99	0.47		2.86	4.62	1.86	3.11	5.83	4.29
180	0.01		ANTHRACENE 120127							
178	3.21	2.47	0.60		3.71	5.74	2.04	3.38	7.43	5.30
181	0.80		PYRENE 129000							
202	4.88	3.75	0.95		5.66	8.73	3.27	5.18	11.54	8.23
182	0.45		9,10-DIMETHYLANTHRACENE 781431							
191	1.33	1.03	0.25		1.45	2.35	0.94	1.57	2.96	2.18
206	2.85	2.22	0.53		3.13	5.04	2.01	3.37	6.36	4.68
183	0.78		CHRYSENE 218019							
228	2.21	1.73	0.41		2.42	3.92	1.59	2.66	4.91	3.61
184	0.54		PERYLENE 198550							
252	1.60	1.23	0.30		1.84	2.86	1.02	1.68	3.67	2.62
185	1.35		DICYANOBUTANE 111693							
41	0.66	0.51	0.12		0.72	1.17	0.47	0.79	1.47	1.08
54	0.29	0.23	0.05		0.32	0.52	2.10	0.35	0.66	0.48
186	0.60		BUTYLCARBAMATE 14994775							
41	0.48	0.36	0.08		0.54	0.86	0.28	0.47	1.35	1.00
59	0.24	0.26	0.05		0.29	0.47	0.15	0.25	0.72	0.54
187	0.01		DIBUTYLDISULFIDE 110065							
41	0.73	0.56	0.13		0.84	1.34	0.44	0.73	2.10	1.55
57	3.09	2.36	0.56		3.54	5.64	1.85	3.09	8.84	6.54
188	0.78		BIS(2-CHLOROETHYL)ETHANE 112265							
63	1.71	1.31	0.31		1.97	3.13	1.03	1.71	4.91	3.63
93	0.84	0.65	0.15		0.97	1.54	0.51	0.84	2.42	1.78

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
175	0.78		ACENAPHTHENE 83329							
153	0.92	3.04	1.18	0.46	0.47		0.09		1.35	
154	2.48	8.22	3.19	1.23	1.28		0.23		3.66	
176	0.80		BIPHENYL 92524							
154	1.67	5.52	2.14	0.83	0.87		0.16		2.46	
177	0.71		1,8-DIMETHYLNAPHTHALENE 569415							
141	1.16	3.84	1.49	0.58	0.60		0.11		1.71	
156	1.67	5.55	2.15	0.83	0.87		0.16		2.48	
178	0.85		FLUORENE 86737							
165	2.00	6.62	2.57	0.99	1.04		0.19		2.95	
166	2.28	7.57	2.93	1.14	1.19		0.21		3.38	
179	0.74		2,3,5-TRIMETHYLNAPHTHALENE 2245387							
155	1.38	4.59	1.78	0.69	0.72		0.13		2.05	
170	1.90	6.31	2.44	0.95	0.99		0.18		2.81	
180	0.01		ANTHRACENE 120127							
178	2.24	7.59	3.08	1.19	1.13		0.25		3.35	
181	0.80		PYRENE 129000							
202	3.59	11.47	4.95	1.90	1.80		0.40		5.36	
182	0.45		9,10-DIMETHYLANTHRACENE 781431							
191	0.96	3.19	1.24	0.48	0.50		0.09		1.42	
206	2.06	6.86	2.67	1.03	1.08		0.19		3.06	
183	0.78		CHRYSENE 218019							
228	1.61	5.34	2.07	0.80	0.81		0.15		2.39	
184	0.54		PERYLENE 198550							
252	1.11	3.72	1.53	0.59	0.47		0.12		1.65	
185	1.35		DICYANOBUTANE 111693							
41	0.48	1.59	0.62	0.24	0.25		0.05		0.71	
54	0.22	0.71	0.28	0.11	0.11		0.02		0.32	
186	0.60		BUTYLCARBAMATE 14994775							
41	0.35	1.16	0.50	0.09	0.15		0.04		0.52	
59	0.19	0.63	0.27	0.11	0.08		0.02		0.28	
187	0.01		DIBUTYLDISULFIDE 110065							
41	0.54	1.78	0.78	0.31	0.20		0.06		0.82	
57	2.21	7.62	3.29	1.27	1.00		0.24		3.42	
188	0.78		BIS(2-CHLOROETHYL)ETHAVE 112265							
63	1.27	4.23	1.83	0.71	0.56		0.13		1.91	
93	0.61	2.08	0.90	0.35	0.27		0.06		0.94	

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std # 2		Compound Name Std #54	Std #56		Std #57		Std #58	
Mass	109	236	136	82	128	98	116	84	112
189	0.93		TRIBUTYLPHOSPHATE 126738						
99	4.03	3.10	0.75	4.65	7.20	2.56	4.24	9.28	6.62
155	0.88	0.68	0.16	1.01	1.57	0.56	0.92	2.02	1.44
190	0.01		ALDRIN 309002						
66	1.33	1.03	0.24	1.49	2.40	0.97	1.62	3.03	2.23
263	0.60	0.46	0.11	0.67	1.08	0.44	0.73	1.36	1.00
191	0.67		DIHYDROBENZOFURAN 496162						
91	0.68	0.52	0.13	0.79	1.25	0.43	0.72	1.58	1.13
120	0.97	0.75	0.18	1.12	1.67	0.66	0.78	2.16	1.54
192	0.86		NITROBENZENE 98953						
77	0.86	0.67	0.16	0.94	1.51	0.61	1.02	1.91	1.40
123	0.54	0.42	0.10	0.59	0.95	0.38	0.64	1.20	0.88
193	0.71		BENZOTHIAZOLE 95169						
135	1.56	1.21	0.29	1.71	2.76	1.11	1.86	3.47	2.55
194	0.01		PHENYLCARBAMATE 102090						
94	1.25	0.96	0.23	1.44	2.23	0.79	1.31	2.86	2.06
137	0.02	0.01	0.00	0.02	0.03	0.01	0.02	0.04	0.03
195	0.01		2,4-DINITROTOLUENE 121142						
89	0.35	0.28	0.06	0.40	0.65	0.26	0.44	0.81	0.60
165	0.71	0.53	0.13	0.75	1.21	0.46	0.76	1.53	1.13
196	0.84		BENZYLSULFIDE 538749						
91	3.55	2.68	0.63	4.00	6.38	2.10	3.49	9.99	7.42
123	0.90	0.68	0.16	1.02	1.62	0.53	0.89	2.54	1.88
197	0.86		DIPHENYLSULFONE 127639						
125	3.82	3.44	0.81	5.16	8.21	2.71	4.51	12.95	8.65
218	0.92	0.73	0.17	1.10	1.75	0.58	0.96	2.74	2.03
198	0.93		TRIPHENYLPHOSPHATE 115866						
325	2.59	2.01	0.13	0.79	1.28	0.52	0.87	1.61	1.18
326	0.09	0.07	0.17	1.03	1.67	0.68	1.14	2.09	1.54
199	1.12		DIPHENYLMERCURY 587859						
77	0.72	0.56	0.48	2.85	4.59	1.96	3.28	6.08	4.47
356	0.95	0.74	0.02	0.09	0.15	0.06	0.11	0.20	0.15
200	0.94		TETRAPHENYLTIN						
197	1.40	1.13	0.27	1.70	2.71	0.89	1.47	4.21	3.13
351	1.30	1.05	0.25	1.58	2.51	0.82	1.37	3.91	2.91
201	0.63		BENZYLCHLORIDE 100447						
91	1.55	1.18	0.28	1.77	2.82	0.93	1.54	4.42	3.28
126	0.42	0.32	0.08	0.48	0.76	0.25	0.42	1.20	0.89

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61	Std #62	Std #63
Mass	110	125	82	110	264 -	188 -	99 -
189	0.93		TRIBUTYLPHOSPHATE 126738				
99	2.81	9.43	3.87	1.49	1.41	0.31	4.19
155	0.61	2.05	0.84	0.32	0.31	0.07	0.91
190	0.01		ALDRIN 309002				
66	0.99	3.28	1.27	0.49	0.51	0.09	1.46
263	0.44	1.47	0.57	0.22	0.23	0.04	0.66
191	0.67		DIHYDROBENZOFURAN 496162				
91	0.27	1.59	0.65	0.25	0.24	0.05	0.71
120	0.68	2.27	0.90	0.35	0.33	0.07	0.98
192	0.86		NITROBENZENE 98953				
77	0.61	2.07	0.80	0.31	0.33	0.06	0.94
123	0.38	1.30	0.50	0.20	0.21	0.04	0.59
193	0.71		BENZOTHIAZOLE 95169				
135	1.14	3.76	1.46	0.57	0.59	0.11	1.68
194	0.01		PHENYLCARBAMATE 102090				
94	0.87	2.92	1.20	0.46	0.44	0.10	1.30
137	0.01	0.04	0.01	0.01	0.00	0.00	0.02
195	0.01		2,4-DINITROTOLUENE 121142				
89	0.27	0.88	0.34	0.13	0.14	0.03	0.39
165	0.50	1.66	0.64	0.25	0.26	0.05	0.74
196	0.84		BENZYLSULFIDE 538749				
91	2.47	8.62	3.72	1.44	1.11	0.27	3.90
123	0.63	2.19	0.94	0.37	0.28	0.07	0.99
197	0.86		DIPHENYLSULFONE 127639				
125	3.00	11.09	4.77	1.85	1.22	0.35	5.05
218	0.67	2.36	1.02	0.29	0.30	0.07	1.07
198	0.93		TRIPHENYLPHOSPHATE 115866				
325	1.98	6.58	2.55	0.95	1.03	0.18	0.78
326	0.06	0.22	0.08	0.03	0.03	0.01	1.02
199	1.12		DIPHENYLMERCURY 587859				
77	0.53	1.75	0.68	0.26	0.26	0.05	2.94
356	0.69	2.28	0.88	0.34	0.35	0.06	0.10
200	0.94		TETRAPHENYLTIN				
197	1.10	3.66	1.57	0.61	0.44	0.11	1.56
351	1.03	3.40	1.46	0.57	0.41	0.11	1.54
201	0.63		BENZYLCHLORIDE 100447				
91	1.10	3.81	1.64	0.64	0.50	0.12	1.71
126	0.30	1.03	0.45	0.17	0.12	0.03	0.47

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
202	0.79		4-CHLOROBENZONITRILE 623030							
102	0.55	0.42	0.10		0.63	0.99	0.33	0.55	1.57	1.16
137	2.10	1.57	0.36		2.38	3.79	1.25	2.08	5.95	4.40
203	0.78		3-CHLOROBENZALDEHYDE 587042							
111	0.06	0.05	0.01		0.08	0.12	0.04	0.07	0.20	0.14
139	0.12	0.10	0.02		0.15	0.24	0.08	0.13	0.38	0.28
204	0.78		O-CHLOROANISOLE 766518							
127	0.60	0.46	0.11		0.69	1.09	0.36	0.60	1.71	1.27
142	1.32	1.00	0.24		0.50	2.40	0.79	1.31	3.76	2.78
205	0.01		CHLOROBENZAMIDE 619567							
139	0.70	0.55	0.13		0.77	1.25	0.50	0.84	1.57	1.16
155	0.38	0.30	0.07		0.42	0.68	0.27	0.46	0.85	0.63
206	0.78		3,4-DICHLOROBENZALDEHYDE 6287383							
173	0.48	0.39	0.09		0.58	0.93	0.31	0.57	1.46	1.07
174	0.32	0.26	0.06		0.39	0.62	0.21	0.34	0.98	0.72
207	0.73		1,2,4-TRICHLOROBENZENE 120821							
145	0.34	0.26	0.06		0.40	0.63	0.22	0.36	0.80	0.57
180	1.30	1.00	0.24		1.50	2.40	0.83	1.37	3.03	2.16
208	0.01		2-BROMO-1-CHLOROBENZENE 694804							
190	0.78	0.61	0.14		0.85	1.38	0.55	0.92	1.74	1.28
192	1.04	0.81	0.19		1.14	1.84	0.74	1.24	2.33	1.71
209	0.77		1,2-DICHLORONAPHTHALENE 2050693							
161	0.44	0.34	0.08		0.50	0.78	0.28	0.46	1.01	0.72
196	2.17	1.67	0.40		2.51	3.88	1.38	2.29	5.03	3.58
210	0.69		1,2,4,5-TETRACHLOROBENZENE 95943							
214	1.18	0.90	0.22		1.29	2.09	0.84	1.40	2.63	1.94
216	1.54	1.18	0.28		1.69	2.72	1.09	1.83	3.43	2.52
211	0.80		P-DIBROMOBENZENE 106376							
234	0.68	0.52	0.12		0.77	1.23	0.41	0.67	1.93	1.43
236	1.29	1.00	0.23		1.48	2.36	0.78	1.30	3.77	2.93
212	0.80		4-BROMODIPHENYLETHER							
248	1.08	0.81	0.20		1.19	1.92	0.77	1.29	2.42	1.78
250	1.13	0.88	0.21		1.26	2.04	0.82	1.37	2.57	1.89
213	0.01		HEXACHLOROBENZENE 118741							
284	0.74	0.56	0.13		0.84	1.34	0.44	0.73	2.10	1.55
286	0.60	0.46	0.11		0.68	1.08	0.36	0.59	1.70	1.26
214	0.58		PYRIDINE 110861							
52	0.29	0.22	0.05		0.33	0.51	0.19	0.32	0.67	0.48
79	0.44	0.34	0.08		0.51	0.78	0.30	0.50	1.10	0.78

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
202	0.79		4-CHLOROBENZONITRILE 623030							
102	0.39	1.35	0.58	0.23	0.18		0.04		0.61	
137	1.49	5.12	2.21	0.85	0.67		0.16		2.32	
203	0.78		3-CHLOROBENZALDEHYDE 587042							
111	0.05	0.17	0.07	0.03	0.02		0.00		0.06	
139	0.10	0.32	0.14	0.05	0.04		0.01		0.15	
204	0.78		O-CHLOROANISOLE 766518							
127	0.43	1.48	0.64	0.25	0.17		0.05		0.67	
142	0.94	3.24	1.40	0.54	0.36		0.10		1.46	
205	0.01		CHLORBENZAMIDE 619567							
139	0.51	1.70	0.66	0.26	0.27		0.05		0.76	
155	0.28	0.92	0.36	0.14	0.15		0.03		0.41	
206	0.78		3,4-DICHLOROBENZALDEHYDE 6287383							
173	0.37	1.25	0.54	0.21	0.17		0.04		0.57	
174	0.25	0.84	0.36	0.14	0.11		0.03		0.38	
207	0.73		1,2,4-TRICHLOROBENZENE 120821							
145	0.24	0.80	0.33	0.13	0.12		0.03		0.36	
180	0.89	3.05	1.25	0.48	0.46		0.10		1.36	
208	0.01		2-BROMO-1-CHLOROBENZENE 694804							
190	0.57	1.88	0.73	0.28	0.30		0.05		0.84	
192	0.76	2.52	0.98	0.38	0.40		0.07		1.12	
209	0.77		1,2-DICHLORONAPHTHALENE 2050693							
161	0.31	1.02	0.42	0.16	0.15		0.03		0.46	
196	1.52	5.08	2.08	0.80	0.76		0.17		2.27	
210	0.69		1,2,4,5-TETRACHLOROBENZENE 95943							
214	0.86	2.85	1.11	0.43	0.45		0.08		1.27	
216	1.12	3.72	1.44	0.56	0.58		0.11		1.66	
211	0.80		P-DIBROMOBENZENE 106376							
234	0.49	1.66	0.72	0.28	0.19		0.05		0.75	
236	0.93	3.18	1.38	0.53	0.45		0.10		1.45	
212	0.80		4-BROMODIPHENYLETHER							
248	0.79	2.61	1.01	0.39	0.41		0.07		1.17	
250	0.84	2.78	1.08	0.42	0.44		0.08		1.24	
213	0.01		HEXACHLOROBENZENE 118741							
284	0.53	1.83	0.78	0.30	0.24		0.06		0.82	
286	0.43	1.46	0.63	0.24	0.19		0.05		0.66	
214	0.58		PYRIDINE 110861							
52	0.20	0.68	0.28	0.11	0.10		0.02		0.30	
79	0.33	1.11	0.42	0.16	0.17		0.04		0.50	

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
215	0.66		ALPHA-PICOLINE 109068							
66	0.26	0.20	0.05		0.30	0.46	0.16	0.27	0.59	0.42
93	0.66	0.51	0.12		0.76	1.18	0.40	0.66	1.52	1.09
216	0.84		ANILINE 62533							
66	0.23	0.19	0.04		0.28	0.41	0.15	0.24	0.53	0.38
93	0.76	0.54	0.13		0.81	1.25	0.45	0.74	1.62	1.15
217	0.57		LUTIDINE 108485							
106	0.13	0.10	0.02		0.15	0.25	0.08	0.13	0.39	0.28
107	0.22	0.16	0.04		0.24	0.39	0.13	0.21	0.61	0.45
218	0.01		TOLUIDINE 106490							
106	0.89	0.69	0.16		0.97	1.57	0.64	1.07	1.97	1.45
107	0.71	0.56	0.13		0.78	1.27	0.51	0.86	1.58	1.16
219	0.86		INDOLE 120729							
90	0.72	0.54	0.13		0.82	1.30	0.43	0.71	2.04	1.51
117	1.92	1.45	0.34		2.17	3.46	1.14	1.89	5.43	4.02
220	0.82		2,3,6-TRIMETHYLPYRIDINE 1462846							
120	0.66	0.51	0.12		0.76	1.18	0.42	0.69	1.53	1.09
121	0.90	0.69	0.17		1.03	1.61	0.55	0.91	2.08	1.49
221	0.72		2,6-DIMETHYLANILINE 1300738							
106	0.36	0.27	0.06		0.41	0.65	0.21	0.36	1.02	0.75
121	0.57	0.44	0.10		0.66	1.04	0.34	0.57	1.64	1.21
222	0.88		M-CHLOROANILINE 108429							
127	1.09	0.84	0.20		1.26	1.94	0.69	1.15	2.52	1.79
129	0.34	0.26	0.06		0.29	0.60	0.22	0.36	0.78	0.56
223	0.77		QUINOLINE 91225							
129	1.82	1.41	0.34		1.99	3.22	1.30	2.17	4.06	2.98

Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
215	0.66		ALPHA-PICOLINE 109068							
66	0.18	0.60	0.25	0.09	0.09		0.02		0.27	
93	0.46	1.54	0.63	0.24	0.23		0.05		0.69	
216	0.84		ANILINE 62533							
66	0.17	0.56	0.22	0.09	0.08		0.02		0.24	
93	0.49	1.64	0.67	0.26	0.24		0.05		0.73	
217	0.57		LUTIDINE 108485							
106	0.10	0.33	0.14	0.05	0.04		0.01		0.15	
107	0.16	0.52	0.23	0.09	0.06		0.02		0.24	
218	0.01		TOLUIDINE 106490							
106	0.65	2.15	0.83	0.32	0.32		0.06		0.96	
107	0.52	1.73	0.67	0.26	0.26		0.05		0.77	
219	0.86		INDOLE 120729							
90	0.51	1.75	0.76	0.29	0.23		0.05		0.79	
117	1.40	4.68	2.02	0.78	0.61		0.15		2.12	
220	0.82		2,3,6-TRIMETHYLPYRIDINE 1462846							
120	0.46	1.54	0.63	0.24	0.23		0.05		0.67	
121	0.62	2.10	0.86	0.33	0.32		0.07		0.94	
221	0.72		2,6-DIMETHYLANILINE 1300738							
106	0.26	0.88	0.38	0.15	0.11		0.03		0.40	
121	0.42	1.41	0.61	0.24	0.18		0.04		0.64	
222	0.88		M-CHLORDANILINE 108429							
127	0.76	2.55	1.05	0.40	0.36		0.98		1.14	
129	0.24	0.79	0.33	0.13	0.12		0.03		0.35	
223	0.77		QUINOLINE 91225							
129	1.33	4.40	1.70	0.66	0.69		0.12		1.96	

Table B-4. RMRs AND RECOVERIES FOR WABN COMPOUNDS
(BLLE, pH 8.0/FRACTION NO. 1)

Class No. 4	
Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
54	d_8-Naphthalene (internal)
56	d_5-Nitrobenzene (internal)
57	d_{10}-o-Xylene (internal)
58	d_5-Phenylethanol (internal)
59	d_5-Acetophenone (internal)
60	d_5-Propiophenone (internal)
61	d_{12}-Perylene (internal)
62	d_9-Acridine (internal)
63	d_5-Phenol (internal)

MATRIX OF STANDARD ION RMRs

			Standard							
			d_5-Phenol	d_{10}-o Xylene		d_8-Naphthalene	d_5 Nitrobenzene		d_5-Phenylethanol	
Compound	Ion	Recovery	m/z 99	m/z 98	m/z 116	m/z 136	m/z 82	m/z 128	m/z 84	m/z 112
d_5-phenol	99	NA	-	.59(9)	99(9)	.17(6)	1 04(5)	1 66(3)	2.44(15)	1 75(15)
d_{10}-o-xylene	98	0 46	1.72(9)[a]	-	1.67(1)	.29(6)	1 79(8)	2 84(8)	4 21(22)	3 02(21)
	116	0 46	1 03(a)	60(0)	-	18(6)	1 07(8)	1,71(8)	2 53(22)	1 81(21)
d_8-naphthalene	136	NA	5.97(4)	3.51(7)	5.85(7)	-	6 21(5)	9 98(3)	14 63(15)	10 59(18)
d_5-nitrobenzene	82	NA	97(4)	57(10)	95(10)	.16(3)	-	1 60(1)	2 35(17)	1 70(16)
	128	NA	61(2)	3?(9)	.59(9)	.10(1)	63(1)	-	1 47(16)	1 07(15)
d_5-phenylethanol	84	NA	.42(15)	25(24)	.42(24)	.07/ 27(18)	44(16)	.70(15)	-	.73(2)
	112	NA	58(15)	35(22)	58(23)	.098(18)	.61(16)	95(16)	1 39(2)	-
d_5-propiophenone	82	NA	1 09(4)	65(13)	1 07(14)	.18(8)	1 13(6)	1 82(6)	2 63(11)	1 90(10)
	110	NA	2 85(5)	1 67(13)	2.78(14)	.48(17)	2 94(6)	4 72(6)	6 84(12)	4 95(11)
d_5-acetophenone	110	NA	1 52(2)	90(7)	1.50(8)	25(4)	1 60(5)	2 55(1)	3 71(17)	2.68(16)
	125	NA	46(2)	.27(8)	.45(7)	.06/ .07(3)	48(3)	.76(4)	1 11(18)	81(17)
d_{12}-perylene	264	NA	3 56(13)	2 09(7)	3 48(8)	.60(9)	3 70(11)	5 90(12)	8 52(25)	6.37(28)
d_9-acridine	188	NA	1.45(7)	86(15)	1 43(15)	.24(8)	1 51(6)	2 40(6)	3 52(13)	2.55(13)
4-fluoro-2-iodotoluene	109	NA	1 10(4)	65(7)	1.08(8)	18(3)	1.14(2)	1 82(2)	2 69(18)	1 97(19)
	236	NA	1 43(4)	84(6)	1 39(7)	24(6)	1 48(3)	2 37(3)	3 48(18)	2.52(18)

(continued)

Compound	Ion	Recovery	Standard: d_5-Propiophenone m/z 82	d_5-Propiophenone m/z 110	d_5-Acetophenone m/z 110	d_5-Acetophenone m/z 125	d_{12}-Perylene m/z 264	d_9-Acridine m/z 188	4-Fluoro-2-Iodotoluene m/z 109	4-Fluoro-2-Iodotoluene m/z 236
d_5-phenol	99	NA	.92(5)	95(5)	67(2)	2 21(3)	31(15)	.70(7)	.91(5)	.71(4)
d_{10}-o-xylene	98	0 46	1.59(12)	61(13)	1.13(7)	3.77(7)	53(10)	1 20(13)	1 So(6)	1.21(6)
	116	0 46	95(13)	.37(12)	67(6)	2.27(7)	32(10)	.72(13)	94(6)	.73(6)
d_8-naphthalene	136	NA	5.51(8)	2.13(8)	3 91(4)	13 14(3)	1 76(15)	4.20(8)	5 45(1)	4.20(1)
d_5-nitrobenzene	82	NA	.89(6)	34(6)	63(4)	2 12(4)	29(19)	67(6)	.88(2)	.68(3)
	128	NA	.55(6)	22(6)	.39(1)	1 32(3)	18(20)	42(6	.55(3)	42(3)
d_5-phenylethanol	84	NA	.39(11)	15(10)	28(16)	93(12)	13(28)	.29(11)	.38(18)	.30(17)
	112	NA	.53(10)	21(9)	.39(16)	1.28(16)	18(29)	41(13)	.52(19)	.42(16)
d_5-propiophenone	82	NA	-	.39(1)	.71(7)	2.40(6)	.35(23)	76(5)	1 00(7)	.77(7)
	110	NA	2.60(1)	-	1 85(6)	6 21(6)	87(19)	2 00(5)	2 59(7)	1 99(7)
d_5-acetophenone	110	NA	1 41(6)	.55(6)	-	3.39(1)	47(14)	1 10(9)	1 37(4)	1 07(2)
	125	NA	.42(6)	16(5)	.30(2)	-	14(18)	32(9)	42(2)	.32(3)
d_{12}-perylene	264	NA	3.08(14)	1.27(16)	2.37(12)	7 91(12)	-	2 50(16)	3 21(9)	2.51(9)
d_9-acridine	188	NA	1.33(5)	52(5)	.95(10)	3.15(11)	39(40)	-	1.32(8)	1.03(8)
4-fluoro-2-iodotoluene	109	NA	1.01(7)	.39(7)	.71(2)	2 45(2)	34(12)	.76(8)	-	.77(1)
	236	NA	1.31(7)	51(7)	92(3)	3.11(2)	.42(16)	1 00(8)	1 30(1)	-

[a](CV).

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
100	0.51		N-TRIDECANE 629505							
43	2.18	1.64	0.34		2.48	3.95	1.30	2.16	6.20	4.58
57	2.75	2.09	0.50		3.14	5.01	1.66	2.77	7.93	5.86
101	0.45		N-TETRADECANE 629594							
43	2.52	1.92	0.45		2.88	4.58	1.51	2.51	7.19	5.31
57	3.40	2.55	0.61		3.87	6.16	2.03	3.37	9.67	7.15
102	0.62		N-PENTADECANE 692629							
57	2.78	2.14	0.52		3.22	4.99	1.77	2.94	6.47	4.62
71	1.73	1.33	0.32		2.01	3.11	1.10	1.83	4.03	2.87
103	0.51		N-HEXADECANE 544763							
43	1.90	1.45	0.34		2.16	3.45	1.13	1.89	5.41	3.99
57	2.72	2.08	0.49		3.11	4.96	1.63	2.71	7.78	5.74
104	0.77		N-HEPTADECANE 629787							
57	3.13	2.41	0.58		3.61	5.59	1.99	3.30	7.25	5.17
71	2.07	1.60	0.38		2.39	3.70	1.32	2.18	4.80	3.42
105	0.66		N-OCTADECANE 593453							
57	2.99	2.51	0.59		3.75	5.98	1.88	3.14	8.96	6.63
71	1.98	1.66	0.39		2.48	3.95	1.25	2.08	5.95	4.41
106	0.65		N-NONADECANE 629925							
71	2.12	1.61	0.38		2.42	3.85	1.27	2.11	6.04	4.47
85	1.42	1.08	0.25		1.61	2.57	0.85	1.41	4.03	2.98
107	0.82		N-EICOSANE 112958							
57	4.43	3.41	0.82		5.11	7.92	2.82	4.66	10.26	7.32
71	3.03	2.33	0.56		3.50	5.43	1.93	3.19	7.03	5.01
108	0.65		N-HENEICOSANE 629947							
57	3.93	2.96	0.70		4.43	7.05	2.32	3.86	11.05	8.20
71	2.71	2.05	0.48		3.07	4.88	1.61	2.67	7.65	5.68
109	0.59		N-DOCOSANE 629970							
57	3.73	2.98	0.70		4.46	7.10	2.33	3.88	11.11	8.26
71	2.60	2.08	0.49		3.11	4.96	1.63	2.70	7.76	5.77
110	0.58		N-TRICOSANE 638675							
57	3.99	3.19	0.75		4.77	7.60	2.49	4.14	11.85	8.83
71	2.80	2.24	0.53		3.35	5.34	1.75	2.91	8.33	6.20
111	0.48		2-METHYLNAPHTHALENE 91576							
141	2.03	1.58	0.38		2.23	3.60	1.44	2.42	4.53	3.34
142	2.51	1.96	0.46		2.76	4.45	1.79	2.99	5.62	4.13
112	0.50		ACENAPHTHENE 83329							
153	1.26	0.98	0.23		1.38	2.22	0.89	1.49	2.81	2.06
154	3.40	2.64	0.63		3.73	6.02	2.41	4.04	7.59	5.58

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
100	0.51		N-TRIDECANE 629505							
43	1.56	5.33	2.30	0.89	0.70		0.17		2.41	
57	1.99	6.75	2.94	1.14	0.76		0.21		3.09	
101	0.45		N-TETRADECANE 629594							
43	1.86	6.19	2.67	1.03	0.80		0.19		2.80	
57	2.50	8.33	3.57	1.39	1.08		0.26		3.77	
102	0.62		N-PENTADECANE 692629							
57	1.94	6.52	2.68	1.03	0.99		0.22		2.92	
71	1.21	4.06	1.67	0.64	0.62		0.14		1.82	
103	0.51		N-HEXADECANE 544763							
43	1.40	4.66	2.01	0.78	0.61		0.15		2.11	
57	2.01	6.70	2.88	1.12	0.87		0.21		3.03	
104	0.77		N-HEPTADECANE 629787							
57	2.18	7.32	3.01	1.16	1.11		0.24		3.27	
71	1.44	4.85	1.99	0.77	0.73		0.16		2.17	
105	0.66		N-OCTADECANE 593453							
57	2.33	8.10	3.48	1.35	1.01		0.24		3.65	
71	1.55	5.35	2.30	0.89	0.58		0.06		2.41	
106	0.65		N-NONADECANE 629925							
71	1.51	5.27	2.24	0.87	0.68		0.16		2.35	
85	1.01	3.47	1.50	0.58	0.45		0.11		1.57	
107	0.82		N-EICOSANE 1112958							
57	3.08	10.35	4.25	1.63	1.57		0.35		4.63	
71	2.11	7.09	2.91	1.12	1.07		0.23		3.17	
108	0.65		N-HENEICOSANE 629947							
57	2.73	9.53	4.11	1.60	1.07		0.30		4.31	
71	1.89	6.60	2.85	1.10	0.74		0.21		2.99	
109	0.59		N-DOCOSANE 629970							
57	2.89	9.60	4.14	1.60	1.22		0.30		4.35	
71	2.02	6.71	2.89	1.12	0.85		0.21		3.04	
110	0.58		N-TRICOSANE 638675							
57	3.10	10.28	4.42	1.71	1.29		0.32		4.65	
71	2.18	7.22	3.11	1.20	0.90		0.22		3.27	
111	0.48		2-METHYLNAPHTHALENE 91576							
141	1.48	4.91	1.90	0.74	0.77		0.14		2.19	
142	1.78	6.08	2.36	0.91	0.95		0.17		2.71	
112	0.50		ACENAPHTHENE 83329							
153	0.92	3.04	1.18	0.46	0.47		0.09		1.35	
154	2.48	8.22	3.19	1.23	1.28		0.23		3.66	

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
113	0.01		BIPHENYL 92524							
154	2.28	1.78	0.42		2.51	4.04	1.63	2.72	5.10	3.75
114	0.48		1,8-DIMETHYLNAPHTHALENE 569415							
141	1.59	1.24	0.29		1.74	2.82	1.13	1.89	3.55	2.61
156	2.30	1.79	0.42		2.52	4.07	1.63	2.73	5.13	3.77
115	0.57		DI-T-BUTYLDISULFIDE 110065							
41	0.73	0.56	0.13		0.84	1.34	0.44	0.72	2.10	1.55
57	3.09	2.36	0.56		3.54	5.64	1.85	3.09	8.84	6.54
116	0.96		ALDRIN 309002							
66	1.33	1.03	0.24		1.49	2.40	0.97	1.62	3.03	2.23
263	0.60	0.46	0.11		0.67	1.08	0.44	0.73	1.36	1.00
117	0.01		PYRIDINE 110861							
52	0.29	0.22	0.05		0.33	0.51	0.19	0.32	0.67	0.48
79	0.44	0.34	0.08		0.51	0.78	0.30	0.50	1.10	0.78
118	0.01		ALPHA-PICOLINE 109068							
66	0.26	0.20	0.05		0.30	0.46	0.16	0.27	0.59	0.42
93	0.66	0.51	0.12		0.76	1.18	0.40	0.66	1.52	1.09
119	0.01		ANILINE 62533							
66	0.23	0.19	0.04		0.28	0.41	0.15	0.24	0.53	0.38
93	0.76	0.54	0.13		0.81	1.25	0.45	0.74	1.62	1.15
120	0.01		LUTIDINE 108485							
106	0.13	0.10	0.02		0.15	0.25	0.08	0.13	0.39	0.28
107	0.22	0.16	0.04		0.24	0.39	0.13	0.21	0.61	0.45
121	0.01		TOLUIDINE 106490							
106	0.89	0.69	0.16		0.97	1.57	0.64	1.07	1.97	1.45
107	0.71	0.56	0.13		0.78	1.27	0.51	0.86	1.58	1.16
122	0.01		INDOLE 120729							
90	0.72	0.54	0.13		0.82	1.30	0.43	0.71	2.04	1.51
117	1.92	1.45	0.34		2.17	3.46	1.14	1.89	5.43	4.02
123	0.01		2,3,6-TRIMETHYLPYRIDINE 1462846							
120	0.66	0.51	0.12		0.76	1.18	0.42	0.69	1.53	1.09
121	0.90	0.69	0.17		1.03	1.61	0.55	0.91	2.08	1.49
124	0.01		2,6-DIMETHYLANILINE 1300738							
106	0.36	0.27	0.06		0.41	0.65	0.21	0.36	1.02	0.75
121	0.57	0.44	0.10		0.66	1.04	0.34	0.57	1.64	1.21
125	0.01		4-CHLOROANILINE 108429							
127	1.09	0.84	0.20		1.26	1.94	0.69	1.15	2.52	1.79
129	0.34	0.25	0.06		0.29	0.60	0.22	0.36	0.78	0.56

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
113	0.01		BIPHENYL 92524							
154	1.67	5.52	2.14	0.83	0.87		0.16		2.46	
114	0.48		1,8-DIMETHYLNAPHTHALENE 569415							
141	1.16	3.84	1.49	0.58	0.60		0.11		1.71	
156	1.67	5.55	2.15	0.83	0.87		0.16		2.48	
115	0.57		DI-T-BUTYLDISULFIDE 110065							
41	0.54	1.78	0.78	0.31	0.20		0.06		0.82	
57	2.21	7.62	3.29	1.27	1.00		0.24		3.42	
116	0.96		ALDRIN 309002							
66	0.99	3.28	1.27	0.49	0.51		0.09		1.46	
263	0.44	1.47	0.57	0.22	0.23		0.04		0.66	
117	0.01		PYRIDINE 110861							
52	0.20	0.68	0.28	0.11	0.10		0.02		0.30	
79	0.33	1.11	0.42	0.16	0.17		0.04		0.50	
118	0.01		ALPHA-PICOLINE 109068							
66	0.18	0.60	0.25	0.09	0.09		0.02		0.27	
93	0.46	1.54	0.63	0.24	0.23		0.05		0.69	
119	0.01		ANILINE 62533							
66	0.17	0.56	0.22	0.09	0.08		0.02		0.24	
93	0.49	1.64	0.67	0.26	0.24		0.05		0.73	
120	0.01		LUTIDINE 108485							
106	0.10	0.33	0.14	0.05	0.04		0.01		0.15	
107	0.16	0.52	0.23	0.09	0.06		0.02		0.24	
121	0.01		TOLUIDINE 106490							
106	0.65	2.15	0.83	0.32	0.32		0.06		0.96	
107	0.52	1.73	0.67	0.26	0.26		0.05		0.77	
122	0.01		INDOLE 120729							
90	0.51	1.75	0.76	0.29	0.23		0.05		0.79	
117	1.40	4.68	2.02	0.78	0.61		0.15		2.12	
123	0.01		2,3,6-TRIMETHYLPYRIDINE 1462846							
120	0.46	1.54	0.63	0.24	0.23		0.05		0.67	
121	0.62	2.10	0.86	0.33	0.32		0.07		0.94	
124	0.01		2,6-DIMETHYLANILINE 1300738							
106	0.26	0.88	0.38	0.15	0.11		0.03		0.40	
121	0.42	1.41	0.61	0.24	0.18		0.04		0.64	
125	0.01		M-CHLOROANILINE 108429							
127	0.76	2.55	1.05	0.40	0.38		0.08		1.14	
129	0.24	0.79	0.33	0.13	0.12		0.03		0.35	

Internal/External Standard File for Cmpd Class # 4

Cmpd# / Mass	Recovery Std # 2 109	236	Compound Name / Std #54 136	-	Std #56 82	128	Std #57 98	116	Std #58 84	112
126	0.01		QUINOLINE 91225							
129	1.82	1.41	0.34		1.99	3.22	1.30	2.17	4.06	2.98
127	0.01		P-NITROANILINE 100016							
65	0.44	0.35	0.08		0.52	0.83	0.27	0.46	1.30	0.97
138	0.56	0.45	0.11		0.67	1.07	0.35	0.58	1.68	0.22
128	0.01		2,4-DIMETHYLQUINOLINE 1198374							
156	0.41	0.32	0.08		0.47	0.75	0.26	0.43	0.95	0.68
157	2.01	1.54	0.37		2.31	3.59	1.27	2.11	4.64	3.31
129	0.01		1,8-DIAMINONAPHTHALENE 569415							
114	0.03	0.02	0.00		0.04	0.06	0.02	0.03	0.09	0.06
141	0.05	0.04	0.01		0.06	0.01	0.03	0.05	0.14	0.11
130	0.01		NICOTINE 54115							
84	1.17	0.90	0.22		1.35	2.09	0.74	1.23	2.70	1.92
133	0.28	0.21	0.05		0.32	0.49	0.17	0.29	0.63	0.45
131	0.01		CARBAZOLE 86748							
167	3.73	2.88	0.69		4.30	6.66	2.37	3.92	9.36	6.67
132	0.01		2-AMINOBIPHENYL 90445							
168	6.79	5.11	1.20		7.65	12.18	4.61	6.67	19.13	14.17
169	12.72	9.45	2.22		14.15	22.54	7.42	12.30	35.40	26.19
133	0.01		DIPHENYLAMINE 122394							
168	1.48	1.14	0.27		1.71	2.65	0.94	1.56	3.43	2.45
169	2.79	2.15	0.52		3.22	4.99	1.77	2.93	6.45	4.60
134	0.01		DICYCLOHEXYLAMINE 122394							
56	0.33	0.37	0.06		0.39	0.63	0.21	0.35	1.10	0.78
138	0.96	0.76	0.18		1.12	1.80	0.61	1.02	3.15	2.25
135	0.01		TRIBUTYLAMINE 102829							
100	0.42	0.33	0.08		0.49	0.75	0.27	0.44	0.97	0.69
142	1.53	1.18	0.28		1.77	2.74	0.97	1.61	3.52	2.51
136	0.01		CAFFEINE 58082							
109	0.10	0.08	0.02		0.12	0.17	0.06	0.10	0.23	0.16
194	0.19	0.15	0.04		0.22	0.34	0.12	0.20	0.44	0.32
137	0.01		DIBENZYLAMINE 103491							
91	1.62	1.26	0.30		1.78	2.87	1.16	1.94	3.63	2.67
197	0.13	0.11	0.03		0.15	0.24	0.10	0.16	0.30	0.22
138	0.01		N,N-DIMETHYLDODECYLAMINE 112185							
58	4.72	3.88	0.87		5.47	8.83	3.58	5.99	11.09	8.16
59	0.17	0.13	0.03		0.20	0.30	0.13	0.21	0.40	0.29
139	0.01		ATRAZINE 1912249							
200	2.75	2.20	0.52		3.28	5.23	1.72	2.86	8.17	6.09
215	1.67	1.34	0.31		2.00	3.18	1.05	1.74	4.97	3.71

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61	Std #62	Std #63
Mass	110	125	82	110	264 -	188 -	99 -
126	0.01		QUINOLINE 91225				
129	1.33	4.40	1.70	0.66	0.69	0.12	1.96
127	0.01		P-NITROANILINE 100016				
65	0.34	1.1[illegible]	0.49	0.19	0.14	0.04	0.51
138	0.43	1.84	0.62	0.24	0.19	0.05	0.65
128	0.01		2,4-DIMETHYLQUINOLINE 1198374				
156	0.29	0.96	0.40	0.15	0.15	0.03	0.43
157	1.46	4.69	1.93	0.74	0.71	0.15	2.09
129	0.01		1,8-DIAMINONAPHTHALENE 569415				
114	0.02	0.08	0.03	0.01	0.01	0.00	0.03
141	0.04	0.12	0.05	0.02	0.01	0.00	0.55
130	0.01		NICOTINE 54115				
84	0.82	2.74	1.12	0.43	0.41	0.09	1.22
133	0.19	0.64	0.26	0.10	0.10	0.02	0.29
131	0.01		CARBAZOLE 86748				
167	2.60	8.72	3.57	1.37	1.28	0.31	4.22
132	0.01		2-AMINOBIPHENYL 90445				
168	4.75	16.46	7.10	2.75	2.13	0.51	7.45
169	8.82	30.44	13.14	5.08	3.96	0.95	13.80
133	0.01		DIPHENYLAMINE 122394				
168	1.03	3.47	1.42	0.55	0.52	0.11	1.55
169	1.94	6.46	2.68	1.03	0.98	0.22	2.91
134	0.01		DICYCLOHEXYLAMINE 122394				
56	0.25	0.81	0.33	0.14	0.09	0.03	0.38
138	0.71	2.34	0.95	0.40	0.26	0.08	1.09
135	0.01		TRIBUTYLAMINE 102829				
100	0.29	0.99	0.41	0.16	0.15	0.03	0.44
142	0.99	3.34	1.47	0.57	0.53	0.12	1.59
136	0.01		CAFFEINE 58082				
109	0.07	0.23	0.09	0.04	0.04	0.01	0.10
194	0.13	0.45	0.18	0.07	0.07	0.02	0.21
137	0.01		DIBENZYLAMINE 103491				
91	1.18	3.91	1.52	0.59	0.62	0.11	1.74
197	0.10	0.32	0.13	0.05	0.05	0.01	0.14
138	0.01		N,N-DIMETHYLDODECYLAMINE 112185				
58	3.62	12.02	4.66	1.81	1.87	0.34	5.37
59	0.13	0.43	0.17	0.06	0.07	0.01	0.19
139	0.01		ATRAZINE 1912249				
200	2.13	7.07	3.05	1.18	0.90	0.22	3.26
215	1.21	4.30	1.85	0.72	0.55	0.13	1.95

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std # 2		Compound Name Std #54	Std #56		Std #57		Std #58	
Mass	109	236	136 -	82	128	98	116	84	112
140	0.01		HEPTANONE(2) 110430						
43	1.21	0.94	0.22	1.33	2.14	0.85	1.14	2.32	2.00
58	0.75	0.58	0.14	0.83	1.33	0.53	0.88	1.69	1.25
141	0.01		BUTOXYETHANOL 111762						
41	0.21	0.17	0.04	0.25	0.40	0.13	0.22	0.49	0.35
57	0.55	0.42	0.10	0.63	1.03	0.35	0.58	1.27	0.91
142	0.01		2-OCTANONE 111137						
43	1.30	1.01	0.24	1.43	2.31	0.91	1.53	2.92	2.15
58	1.02	0.79	0.19	1.11	1.80	0.71	1.19	2.27	1.67
143	0.01		BUTYLPROPIONATE 590012						
57	1.48	1.14	0.27	1.71	2.73	0.90	1.49	4.27	3.15
75	0.44	0.34	0.08	0.51	0.82	0.27	0.45	1.28	0.95
144	0.01		ISOPHORONE 78591						
82	1.77	1.36	0.33	2.04	3.17	1.13	1.86	4.11	2.93
138	0.39	0.30	0.07	0.45	0.72	0.25	0.41	0.90	0.64
145	0.01		FENCHONE 1195759						
69	0.66	0.51	0.12	0.72	1.17	0.47	0.78	1.47	1.08
81	1.44	1.12	0.27	1.58	2.55	1.02	1.71	3.22	2.36
146	0.01		ALPHA-TERPINEOL 98555						
59	0.56	0.43	0.10	0.65	1.00	0.36	0.59	1.31	0.93
136	0.32	0.25	0.06	0.37	0.58	0.21	0.34	0.75	0.53
147	0.01		N-DECANOL 112301						
41	0.40	0.31	0.07	0.46	0.74	0.25	0.42	0.92	0.66
43	0.44	0.34	0.08	0.51	0.79	0.28	0.46	1.02	0.73
148	0.01		DIMETHYLADIPATE 627930						
59	0.56	0.45	0.10	0.64	1.03	0.41	0.69	1.29	0.95
114	0.44	0.35	0.08	0.49	0.79	0.32	0.54	1.00	0.74
149	0.01		METHYLSTEARATE 112618						
74	3.42	2.65	0.63	3.89	6.28	2.54	4.25	7.90	5.81
87	2.22	1.72	0.41	2.52	4.07	1.65	2.76	5.13	3.77
150	0.01		N-DECANE						
43	1.47	1.11	0.26	1.67	2.66	0.88	1.46	4.18	3.09
57	1.42	1.08	0.25	1.64	2.61	0.85	1.41	4.05	3.00
151	0.01		PHENYLACETATE 122792						
94	1.84	1.43	0.34	2.01	3.25	1.30	2.18	4.10	3.01
136	0.25	0.20	0.05	0.28	0.45	0.18	0.30	0.57	0.42
152	0.01		BENZYLACETATE 140114						
91	0.52	0.40	0.09	0.57	0.92	0.37	0.62	1.15	0.85
108	1.09	0.85	0.20	1.19	1.92	0.77	1.29	2.43	1.79

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61	Std #62	Std #63
Mass	110	125	82	110	264 -	188 -	99 -
140	0.01		HEPTANONE(2) 110430				
43	0.88	2.91	1.13	0.44	0.47	0.08	1.30
58	0.55	1.82	0.71	0.27	0.29	0.05	0.81
141	0.01		BUTOXYETHANOL 111762				
41	0.15	0.49	0.20	0.09	0.07	0.02	0.22
57	0.38	1.28	0.52	0.20	0.19	0.04	0.57
142	0.01		2-OCTANONE 111137				
43	0.95	3.14	1.22	0.47	0.51	0.09	1.40
58	0.74	2.45	0.95	0.37	0.39	0.07	1.09
143	0.01		BUTYLPROPIONATE 590012				
57	1.11	3.69	1.59	0.61	0.48	0.12	1.66
75	0.33	1.11	0.48	0.19	0.15	0.04	0.50
144	0.01		ISOPHORONE 78591				
82	1.23	4.14	1.70	0.65	0.62	0.14	1.80
138	0.27	0.91	0.37	0.14	0.14	0.03	0.41
145	0.01		FENCHONE 1195759				
69	0.48	1.58	0.62	0.24	0.25	0.05	0.71
81	1.05	3.45	1.35	0.52	0.55	0.10	1.55
146	0.01		ALPHA-TERPINEOL 98555				
59	0.39	1.31	0.54	0.21	0.20	0.04	0.58
136	0.23	0.76	0.31	0.12	0.11	0.03	0.34
147	0.01		N-DECANOL 112301				
41	0.28	0.93	0.38	0.15	0.14	0.03	0.41
43	0.31	1.63	0.42	0.16	0.15	0.03	0.46
148	0.01		DIMETHYLADIPATE 627930				
59	0.42	1.40	0.54	0.21	0.22	0.04	0.62
114	0.33	1.08	0.42	0.16	0.17	0.03	0.48
149	0.01		METHYLSTEARATE 112618				
74	2.58	8.56	3.32	1.29	1.33	0.24	3.83
87	1.67	5.55	2.15	0.83	0.87	0.16	2.48
150	0.01		N-DECANE				
43	1.05	3.59	1.55	0.60	0.47	0.11	1.62
57	1.01	3.48	1.50	0.58	0.46	0.11	1.58
151	0.01		PHENYLACETATE 122792				
94	1.31	4.43	1.72	0.67	0.70	0.13	1.98
136	0.18	0.62	0.24	0.09	0.10	0.02	0.28
152	0.01		BENZYLACETATE 140114				
91	0.38	1.25	0.48	0.19	0.20	0.04	0.56
108	0.79	2.63	1.02	0.40	0.41	0.07	1.17

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std # 2		Compound Name Std #54	Std #56		Std #57		Std #58	
Mass	109	236	136 -	82	128	98	116	84	112
153	0.01		METHYLBENZENESULFONATE						
77	1.24	0.94	0.22	1.41	2.23	0.74	1.23	3.54	2.61
172	0.44	0.34	0.08	0.50	0.80	0.26	0.44	1.26	0.93
154	0.01		METHYLTOLUENESULFONATE(P)						
91	1.60	1.21	0.29	1.81	2.89	0.95	1.58	4.53	3.35
155	0.72	0.54	0.13	0.81	1.29	0.42	0.71	2.02	1.50
155	0.01		DIMETHYLPHTHALATE 131113						
77	0.81	0.63	0.15	0.94	1.45	0.52	0.85	1.88	1.34
163	5.29	4.07	0.98	6.10	9.46	3.36	5.56	12.22	8.71
156	0.01		ETHYLTOLUENESULFONATE(P) 80400						
91	1.74	1.32	0.31	1.97	3.14	1.03	1.72	4.92	3.65
155	1.18	0.94	0.22	1.40	2.23	0.73	1.21	3.46	2.35
157	0.01		DIETHYLPHTHALATE 84662						
149	3.19	2.43	0.57	3.65	5.79	1.90	3.17	9.08	6.71
177	0.80	0.61	0.14	0.93	1.47	0.48	0.80	2.29	1.69
158	0.01		DIBUTYLPHTHALATE 84742						
57	0.29	0.23	0.05	0.34	0.52	0.19	0.31	0.68	0.48
149	7.17	5.52	1.33	8.27	12.80	4.55	7.54	16.55	11.80
159	0.01		BUTYLBENZYLPHTHALATE						
91	2.09	1.62	0.38	2.28	3.69	1.48	2.48	4.64	3.41
149	3.37	2.62	0.62	3.69	5.95	2.40	4.01	7.49	5.51
160	0.01		DIETHYLHEXYLPHTHALATE 117817						
149	5.22	4.07	0.96	5.71	9.23	3.74	6.26	11.59	8.53
167	1.98	1.54	0.37	2.17	3.51	1.42	2.37	4.40	3.24
161	0.01		BENZALDEHYDE 100527						
77	0.36	0.28	0.07	0.42	0.64	0.23	0.38	0.84	0.60
105	0.40	0.31	0.07	0.46	0.70	0.25	0.42	0.92	0.66
162	0.01		TOLUALDEHYDE 529204						
91	0.54	0.44	0.10	0.65	1.04	0.34	0.57	1.65	1.21
119	0.63	0.51	0.12	0.77	1.23	0.41	0.68	1.95	1.43
163	0.01		ACETOPHENONE 96862						
77	0.38	0.64	0.15	0.96	1.53	0.53	0.87	1.93	1.37
105	1.22	0.94	0.23	1.41	2.25	0.78	1.29	2.85	2.03
164	0.01		SALICYLALDEHYDE 90028						
121	0.56	0.44	0.10	0.61	0.99	0.40	0.67	1.24	0.91
122	0.60	0.47	0.11	0.60	1.07	0.43	0.72	1.34	0.99
165	0.01		ANISALDHYDE 123115						
135	1.37	1.08	0.25	1.53	2.47	0.91	1.66	3.11	2.29
136	0.96	0.76	0.18	1.07	1.73	0.70	1.16	2.18	1.60

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
153	0.01		METHYLBENZENESULFONATE							
77	0.91	3.04	1.31	0.51	0.40		0.09		1.38	
172	0.32	1.08	0.47	0.18	0.14		0.03		0.49	
154	0.01		METHYLTOLUENESULFONATE(P)							
91	1.17	3.90	1.68	0.65	0.51		0.12		1.76	
155	0.52	1.74	0.75	0.29	0.23		0.05		0.79	
155	0.01		DIMETHYLPHTHALATE 131113							
77	0.57	1.83	0.75	0.29	0.28		0.06		0.85	
163	3.68	11.87	4.88	1.88	1.85		0.41		5.51	
156	0.01		ETHYLTOLUENESULFONATE(P) 80400							
91	1.28	4.25	1.83	0.71	0.55		0.13		1.92	
155	0.91	3.01	1.30	0.50	0.38		0.09		1.36	
157	0.01		DIETHYLPHTHALATE 84662							
149	2.35	7.82	3.34	1.30	1.02		0.24		3.54	
177	0.59	1.97	0.85	0.33	0.26		0.06		0.89	
158	0.01		DIBUTYLPHTHALATE 84742							
57	0.20	0.68	0.28	0.11	0.10		0.02		0.31	
149	4.99	16.75	6.88	2.64	2.52		0.55		7.47	
159	0.01		BUTYLBENZYLPHTHALATE							
91	1.51	5.02	1.95	0.76	0.78		0.14		2.24	
149	2.44	8.10	3.15	1.22	1.26		0.23		3.62	
160	0.01		DIETHYLHEXYLPHTHALATE 117817							
149	4.03	12.58	4.88	1.89	1.90		0.35		5.61	
167	1.53	4.78	1.85	0.72	0.72		0.13		2.13	
161	0.01		BENZALDEHYDE 100527							
77	0.25	0.84	0.35	0.13	0.13		0.03		0.38	
105	0.28	0.93	0.38	0.15	0.14		0.03		0.42	
162	0.01		TOLUALDEHYDE 529204							
91	0.42	1.41	0.61	0.24	0.15		0.05		0.64	
119	0.50	1.66	0.72	0.28	0.22		0.05		0.75	
163	0.01		ACETOPHENONE 98862							
77	0.57	1.95	0.80	0.31	0.29		0.06		0.87	
105	0.85	2.38	1.18	0.45	0.43		0.09		1.29	
164	0.01		SALICYLALDEHYDE 90028							
121	0.41	1.35	0.52	0.20	0.21		0.04		0.60	
122	0.44	1.46	0.56	0.22	0.23		0.04		0.65	
165	0.01		ANISALDHYDE 123115							
135	1.01	3.36	1.30	0.51	0.53		0.09		1.50	
136	0.71	2.36	0.91	0.35	0.37		0.07		1.05	

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std # 2		Compound Name Std #54	Std #56		Std #57		Std #58	
Mass	109	236	136	82	128	98	116	84	112
166	0.01		PHENOL 108952						
94	1.07	0.84	0.20	1.18	1.90	0.76	1.27	2.41	1.77
167	0.01		CRESOL(P) 106445						
107	1.21	0.93	0.23	1.40	2.25	0.90	1.29	2.91	2.08
108	1.07	0.82	0.20	1.24	1.99	0.69	1.14	2.58	1.84
168	0.01		2,3-DIMETHYLPHENOL 526750						
107	0.87	0.67	0.16	1.00	1.61	0.57	0.95	2.08	1.48
122	0.91	0.70	0.17	1.05	1.64	0.58	0.96	2.12	1.51
169	0.01		ISOPROPYLPHENOL 88699						
121	1.79	1.36	0.32	2.04	3.25	1.07	1.78	5.10	3.77
136	0.07	0.56	0.12	0.75	1.19	0.39	0.65	1.87	1.38
170	0.01		O-NITROPHENOL 88755						
65	0.03	0.02	0.00	0.03	0.05	0.02	0.03	0.06	0.05
139	0.13	0.10	0.02	0.14	0.23	0.09	0.15	0.29	0.21
171	0.01		4-CHLORO-3-METHYLPHENOL 59507						
107	0.93	0.71	0.17	1.06	1.68	0.55	0.92	2.64	2.95
142	1.02	0.77	0.18	1.16	1.84	0.61	1.01	2.89	2.14
172	0.01		4-CHLOROCRESOL						
107	0.83	0.64	0.16	0.97	1.57	0.53	0.88	2.03	1.45
142	0.94	0.72	0.17	1.09	1.77	0.60	0.99	2.29	1.63
173	0.01		1-NAPHTHOL 90153						
115	0.35	0.26	0.06	0.38	0.61	0.20	0.34	0.96	0.72
144	0.61	0.45	0.11	0.67	1.07	0.35	0.29	1.68	1.25
174	0.01		P-TERT-BUTYLPHENOL 98544						
107	0.56	0.43	0.10	0.65	1.03	0.34	0.56	1.60	1.18
135	1.96	1.49	0.35	2.22	3.54	1.17	1.94	5.56	4.11
175	0.01		2-NITROCRESOL 119335						
77	0.26	0.20	0.05	0.30	0.46	0.07	0.27	0.60	0.43
153	0.74	0.57	0.14	0.83	1.33	0.46	0.78	1.72	1.23
176	0.01		2,4-DICHLOROPHENOL 120832						
162	1.13	0.88	0.21	1.24	2.00	0.80	1.34	2.52	1.86
164	0.72	0.53	0.13	0.78	1.27	0.51	0.85	1.60	1.18
177	0.01		2,4,6-TRICHLOROPHENOL 88062						
196	0.81	0.63	0.15	0.89	1.44	0.58	0.97	1.68	1.34
198	0.83	0.64	0.15	0.91	1.46	0.59	0.98	1.90	1.36
178	0.01		DI-TERT-BUTYL-4-METHYLPHENOL 128370						
205	2.53	1.97	0.47	2.78	4.49	1.81	3.03	5.66	4.16
220	0.67	0.52	0.12	0.73	1.18	0.48	0.80	1.49	1.09

Internal/External Standard File for Capd Class # 4

Capd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	168	-	99	-
166	0.01		PHENOL 108952							
94	0.75	2.60	1.01	0.39	0.41		0.07		1.15	
167	0.01		CRESOL(P) 106445							
107	0.88	2.85	1.17	0.45	0.44		0.16		1.31	
108	0.78	2.52	1.03	0.40	0.39		0.09		1.16	
168	0.01		2,3-DIMETHYLPHENOL 526750							
107	0.63	2.11	0.84	0.32	0.32		0.07		0.94	
122	0.64	2.14	0.85	0.33	0.32		0.07		0.95	
169	0.01		ISOPROPYLPHENOL 88699							
121	1.28	4.39	1.90	0.73	0.58		0.14		1.99	
136	0.47	1.61	0.69	0.27	0.21		0.05		0.73	
170	0.01		O-NITROPHENOL 88755							
65	0.02	0.07	0.03	0.01	0.01		0.00		0.03	
139	0.09	0.31	0.12	0.05	0.05		0.01		0.14	
171	0.01		4-CHLORO-3-METHYLPHENOL 59507							
107	0.66	2.27	0.98	0.38	0.30		0.07		1.03	
142	0.72	2.49	1.07	0.42	0.32		0.08		1.13	
172	0.01		4-CHLOROCRESOL							
107	0.58	1.95	0.80	0.31	0.31		0.07		0.91	
142	0.66	2.20	0.85	0.34	0.35		0.08		1.03	
173	0.01		1-NAPHTHOL 90153							
115	0.25	0.83	0.36	0.14	0.11		0.03		0.38	
144	0.44	1.45	0.62	0.24	0.18		0.05		0.66	
174	0.01		P-TERT-BUTYLPHENOL 98544							
107	0.40	1.36	0.66	0.23	0.18		0.04		0.62	
135	1.44	4.79	2.04	0.80	0.63		0.15		2.16	
175	0.01		2-NITROCRESOL 119335							
77	0.18	0.61	0.25	0.10	0.09		0.02		0.27	
153	0.52	1.74	0.71	0.27	0.26		0.06		0.78	
176	0.01		2,4-DICHLOROPHENOL 120832							
162	0.80	2.73	1.05	0.41	0.43		0.08		1.22	
164	0.51	1.70	0.67	0.26	0.27		0.05		0.77	
177	0.01		2,4,6-TRICHLOROPHENOL 88062							
196	0.58	1.97	0.76	0.30	0.91		0.05		0.88	
198	0.58	1.99	0.77	0.30	0.32		0.06		0.89	
178	0.01		DI-TERT-BUTYL-4-METHYLPHENOL 128370							
205	1.85	6.13	2.37	0.92	0.96		0.17		2.73	
220	0.49	1.61	0.62	0.24	0.25		0.05		0.72	

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std # 2		Compound Name / CAS	Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-		82	128	98	116	84	132
179	0.01		PENTACHLOROPHENOL 87865								
264	0.29	0.22	0.05			0.34	0.54	0.19	0.31	0.72	0.52
266	0.47	0.36	0.09			0.55	0.91	0.32	0.54	1.17	0.84
180	0.01		FLUORENE 86737								
165	2.74	2.13	0.49			3.01	4.85	1.95	3.27	6.12	4.50
166	3.07	2.38	0.57			3.44	5.55	2.23	3.74	6.99	5.14
181	0.01		2,3,5-TRIMETHYLNAPHTHALENE 2245387								
155	1.86	1.44	0.34			2.08	3.36	1.36	2.27	4.24	3.12
170	2.56	1.99	0.47			2.86	4.62	1.86	3.11	5.83	4.29
182	0.01		ANTHRACENE 120127								
176	3.21	2.47	0.60			3.71	5.74	2.04	3.38	7.43	5.30
183	0.01		PYRENE 129000								
202	4.88	3.75	0.95			5.66	8.73	3.27	5.18	11.54	8.23
184	0.01		9,10-DIMETHYLANTHRACENE 781431								
191	1.33	1.03	0.25			1.45	2.35	0.94	1.57	2.96	2.18
206	2.85	2.22	0.53			3.13	5.04	2.01	3.37	6.36	4.68
185	0.01		CHRYSENE 218019								
228	2.21	1.73	0.41			2.42	3.92	1.59	2.66	4.91	3.61
186	0.01		PERYLENE 198550								
252	1.60	1.23	0.30			1.84	2.86	1.02	1.68	3.67	2.62
187	0.01		DICYANOBUTANE 111693								
41	0.66	0.51	0.12			0.72	1.17	0.47	0.79	1.47	1.08
54	0.29	0.23	0.05			0.32	0.52	2.10	0.35	0.66	0.48
188	0.01		BUTYLCARBAMATE 14994775								
41	0.48	0.36	0.08			0.54	0.86	0.28	0.47	1.35	1.00
59	0.24	0.26	0.05			0.29	0.47	0.15	0.25	0.72	0.54
189	0.01		BIS(2-CHLOROETHYL)ETHANE 112265								
63	1.71	1.31	0.31			1.97	3.13	1.03	1.71	4.91	3.63
93	0.84	0.65	0.15			0.97	1.54	0.51	0.84	2.42	1.78
190	0.01		TRIBUTYLPHOSPHATE 126738								
99	4.03	3.10	0.75			4.65	7.20	2.56	4.24	9.28	6.62
155	0.88	0.68	0.16			1.01	1.57	0.56	0.92	2.02	1.44
191	0.01		DIHYDROBENZOFURAN(2,3) 496152								
91	0.68	0.52	0.13			0.79	1.25	0.43	0.72	1.58	1.13
120	0.97	0.75	0.18			1.12	1.67	0.66	0.78	2.16	1.54
192	0.01		NITROBENZENE 98953								
77	0.86	0.67	0.16			0.94	1.51	0.61	1.02	1.91	1.40
123	0.54	0.42	0.10			0.59	0.95	0.38	0.64	1.20	0.88

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
179	0.01		PENTACHLOROPHENOL 87865							
264	0.20	0.68	0.28	0.11	0.11		0.02		0.31	
266	0.36	1.11	0.45	0.07	0.18		0.04		0.50	
180	0.01		FLUORENE 86737							
165	2.00	6.62	2.57	0.99	1.04		0.19		2.95	
166	2.28	7.57	2.93	1.14	1.19		0.21		3.36	
181	0.01		2,3,5-TRIMETHYLNAPHTHALENE 2245387							
155	1.38	4.59	1.78	0.69	0.72		0.13		2.05	
170	1.90	6.31	2.44	0.95	0.99		0.18		2.81	
182	0.01		ANTHRACENE 120127							
178	2.24	7.59	3.08	1.19	1.13		0.25		3.35	
183	0.01		PYRENE 129000							
202	3.59	11.47	4.95	1.90	1.80		0.40		5.36	
184	0.01		9,10-DIMETHYLANTHRACENE 781431							
191	0.96	3.19	1.24	0.48	0.50		0.09		1.42	
206	2.06	6.86	2.67	1.03	1.08		0.19		3.06	
185	0.01		CHRYSENE 218019							
228	1.61	5.34	2.07	0.80	0.81		0.15		2.39	
186	0.01		PERYLENE 198550							
252	1.11	3.72	1.53	0.59	0.47		0.12		1.65	
187	0.01		DICYANOBUTANE 111693							
41	0.48	1.59	0.62	0.24	0.25		0.05		0.71	
54	0.22	0.71	0.28	0.11	0.11		0.02		0.32	
188	0.01		BUTYLCARBAMATE 14994775							
41	0.35	1.16	0.50	0.09	0.15		0.04		0.52	
59	0.19	0.63	0.27	0.11	0.08		0.02		0.26	
189	0.01		BIS(2-CHLOROETHYL)ETHANE 112265							
63	1.27	4.23	1.83	0.71	0.56		0.13		1.91	
93	0.61	2.08	0.90	0.35	0.27		0.06		0.94	
190	0.01		TRIBUTYLPHOSPHATE 126738							
99	2.81	9.43	3.87	1.49	1.41		0.31		4.19	
155	0.61	2.05	0.84	0.32	0.31		0.07		0.91	
191	0.01		DIHYDROBENZOFURAN(2,3) 496162							
91	0.27	1.59	0.65	0.25	0.24		0.05		0.71	
120	0.68	2.27	0.90	0.35	0.33		0.07		0.98	
192	0.01		NITROBENZENE 98953							
77	0.61	2.07	0.80	0.31	0.33		0.06		0.94	
123	0.38	1.30	0.50	0.20	0.21		0.04		0.59	

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
193	0.01		BENZOTHIAZOLE 95169							
135	1.56	1.21	0.29		1.71	2.76	1.11	1.86	3.47	2.55
194	0.01		PHENYLCARBAMATE 102090							
94	1.25	0.96	0.23		1.44	2.23	0.79	1.31	2.88	2.06
137	0.02	0.01	0.00		0.02	0.03	0.01	0.02	0.04	0.03
195	0.01		2,4-DINITROTOLUENE 121142							
89	0.35	0.28	0.06		0.40	0.65	0.26	0.44	0.81	0.60
165	0.71	0.53	0.13		0.75	1.21	0.46	0.76	1.53	1.13
196	0.01		BENZYLSULFIDE 538749							
91	3.55	2.68	0.63		4.00	6.38	2.10	3.49	9.99	7.42
123	0.90	0.68	0.16		1.02	1.62	0.53	0.89	2.54	1.88
197	0.01		DIPHENYLSULFONE 127639							
125	3.82	3.44	0.81		5.16	8.21	2.71	4.51	12.95	8.65
218	0.92	0.73	0.17		1.10	1.75	0.58	0.96	2.74	2.03
198	0.01		TRIPHENYLPHOSPHATE 115866							
325	2.59	2.01	0.13		0.79	1.28	0.52	0.87	1.61	1.18
326	0.09	0.07	0.17		1.03	1.67	0.68	1.14	2.09	1.54
199	0.01		DIPHENYLMERCURY 587859							
77	0.72	0.56	0.48		2.85	4.59	1.96	3.28	6.08	4.47
356	0.95	0.74	0.02		0.09	0.15	0.06	0.11	0.20	0.15
200	0.01		TETRAPHENYLTIN							
197	1.40	1.13	0.27		1.70	2.71	0.89	1.47	4.21	3.13
351	1.30	1.05	0.25		1.58	2.51	0.82	1.37	3.91	2.91
201	0.82		BENZYLCHLORIDE 100447							
91	1.55	1.18	0.28		1.77	2.82	0.93	1.54	4.42	3.28
126	0.42	0.32	0.08		0.48	0.76	0.25	0.42	1.20	0.89
202	0.01		4-CHLOROBENZONITRILE 623030							
102	0.55	0.42	0.10		0.63	0.99	0.33	0.55	1.57	1.16
137	2.10	1.57	0.36		2.38	3.79	1.25	2.08	5.95	4.40
203	0.01		3-CHLOROBENZALDEHYDE 587042							
111	0.06	0.05	0.01		0.08	0.12	0.04	0.07	0.20	0.14
139	0.12	0.10	0.02		0.15	0.24	0.08	0.13	0.38	0.28
204	0.01		O-CHLOROANISOLE 766518							
127	0.60	0.46	0.11		0.69	1.09	0.36	0.60	1.71	1.27
142	1.32	1.00	0.24		0.50	2.40	0.79	1.31	3.76	2.78
205	0.01		CHLOROBENZAMIDE 619567							
139	0.70	0.55	0.13		0.77	1.25	0.50	0.84	1.57	1.16
155	0.38	0.30	0.07		0.42	0.68	0.27	0.46	0.85	0.63

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
193	0.01		BENZOTHIAZOLE 95169							
135	1.14	3.76	1.46	0.57	0.59		0.11		1.66	
194	0.01		PHENYLCARBAMATE 102090							
94	0.87	2.92	1.20	0.46	0.44		0.10		1.30	
137	0.01	0.04	0.01	0.01	0.00		0.00		0.02	
195	0.01		2,4-DINITROTOLUENE 121142							
89	0.27	0.88	0.34	0.13	0.14		0.03		0.39	
165	0.50	1.66	0.64	0.25	0.26		0.05		0.74	
196	0.01		BENZYLSULFIDE 538749							
91	2.47	8.62	3.72	1.44	1.11		0.27		3.90	
123	0.63	2.19	0.94	0.37	0.28		0.07		0.99	
197	0.01		DIPHENYLSULFONE 127639							
125	3.00	11.09	4.77	1.85	1.22		0.35		5.05	
218	0.67	2.36	1.02	0.29	0.30		0.07		1.07	
198	0.01		TRIPHENYLPHOSPHATE 115866							
325	1.98	6.58	2.55	0.95	1.03		0.18		0.78	
326	0.06	0.22	0.08	0.03	0.03		0.01		1.02	
199	0.01		DIPHENYLMERCURY 587859							
77	0.53	1.75	0.68	0.26	0.26		0.05		2.94	
356	0.69	2.28	0.88	0.34	0.35		0.06		0.10	
200	0.01		TETRAPHENYLTIN							
197	1.10	3.66	1.57	0.61	0.44		0.11		1.56	
351	1.03	3.40	1.46	0.57	0.41		0.11		1.54	
201	0.82		BENZYLCHLORIDE 100447							
91	1.10	3.81	1.64	0.64	0.50		0.12		1.71	
126	0.10	1.03	0.45	0.17	0.12		0.03		0.47	
202	0.01		4-CHLOROBENZONITRILE 623030							
102	0.39	1.35	0.58	0.23	0.16		0.04		0.61	
137	1.49	5.12	2.21	0.85	0.67		0.16		2.32	
203	0.01		3-CHLOROBENZALDEHYDE 587042							
111	0.05	0.17	0.07	0.03	0.02		0.00		0.08	
139	0.10	0.32	0.14	0.05	0.04		0.01		0.15	
204	0.01		3-CHLOROANISOLE 766518							
127	0.43	1.48	0.64	0.25	0.17		0.05		0.67	
142	0.94	3.24	1.40	0.54	0.36		0.10		1.46	
205	0.01		CHLOROBENZAMIDE 619567							
139	0.51	1.70	0.66	0.26	0.27		0.05		0.76	
155	0.28	0.92	0.36	0.14	0.15		0.03		0.41	

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
206	0.01		3,4-DICHLOROBENZALDEHYDE 6287383							
173	0.48	0.39	0.09		0.58	0.93	0.31	0.57	1.46	1.07
174	0.32	0.26	0.06		0.39	0.62	0.21	0.34	0.98	0.72
207	0.01		1,2,4-TRICHLOROBENZENE 120821							
145	0.34	0.26	0.06		0.40	0.63	0.22	0.36	0.80	0.57
180	1.30	1.00	0.24		1.50	2.40	0.83	1.37	3.03	2.16
208	0.01		2-BROMO-1-CHLOROBENZENE 694804							
190	0.78	0.61	0.14		0.85	1.38	0.55	0.92	1.74	1.28
192	1.04	0.81	0.19		1.14	1.84	0.74	1.24	2.33	1.71
209	0.68		1,2-DICHLORONAPHTHALENE 2050693							
161	0.44	0.34	0.08		0.50	0.78	0.28	0.46	1.01	0.72
196	2.17	1.67	0.40		2.51	3.88	1.38	2.29	5.03	3.58
210	0.53		1,2,4,5-TETRACHLOROBENZENE 95943							
214	1.18	0.90	0.22		1.29	2.09	0.84	1.40	2.63	1.94
216	1.54	1.18	0.28		1.69	2.72	1.09	1.83	3.43	2.52
211	0.43		P-DIBROMOBENZENE 106376							
234	0.68	0.52	0.12		0.77	1.23	0.41	0.67	1.93	1.43
236	1.29	1.00	0.23		1.48	2.36	0.78	1.30	3.77	2.93
212	0.01		4-BROMODIPHENYLETHER 6452493							
248	1.08	0.81	0.20		1.19	1.92	0.77	1.29	2.42	1.78
250	1.13	0.82	0.21		1.26	2.04	0.82	1.37	2.57	1.89
213	0.95		HEXACHLOROBENZENE 118741							
284	0.74	0.56	0.13		0.84	1.34	0.44	0.73	2.10	1.55
286	0.60	0.46	0.11		0.66	1.08	0.36	0.59	1.70	1.26

Internal/External Standard File for Cmpd Class # 4

Cmpd#	Recovery Std #59		Compound Name / Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
206	0.01		3,4-DICHLORBENZALDEHYDE 6287383							
173	0.37	1.25	0.54	0.21	0.17		0.04		0.57	
174	0.25	0.84	0.36	0.14	0.11		0.03		0.38	
207	0.01		1,2,4-TRICHLORBENZENE 120821							
145	0.24	0.80	0.33	0.13	0.12		0.03		0.36	
180	0.89	3.05	1.25	0.48	0.46		0.10		1.36	
208	0.01		2-BROMO-1-CHLORBENZENE 694804							
190	0.57	1.88	0.73	0.28	0.30		0.05		0.84	
192	0.76	2.52	0.98	0.38	0.40		0.07		1.12	
209	0.68		1,2-DICHLORONAPHTHALENE 2050693							
161	0.31	1.02	0.42	0.16	0.15		0.03		0.46	
196	1.52	5.08	2.08	0.80	0.76		0.17		2.27	
210	0.53		1,2,4,5-TETRACHLORBENZENE 95943							
214	0.86	2.85	1.11	0.43	0.45		0.08		1.27	
216	1.12	3.72	1.44	0.56	0.58		0.11		1.66	
211	0.43		P-DIBROMOBENZENE 106376							
234	0.49	1.66	0.72	0.28	0.19		0.05		0.75	
236	0.93	3.18	1.38	0.53	0.45		0.10		1.45	
212	0.01		4-BROMODIPHENYLETHER 6452499							
248	0.79	2.61	1.01	0.39	0.41		0.07		1.17	
250	0.84	2.78	1.08	0.42	0.44		0.08		1.24	
213	0.55		HEXACHLOROBENZENE 118741							
284	0.53	1.83	0.78	0.30	0.24		0.06		0.82	
286	0.43	1.46	0.63	0.24	0.19		0.05		0.66	

Table B-5 RRRs AND RECOVERIES FOR WABN COMPOUNDS
(BLLE, pH 8.0/FRACTION NOS. 2 & 3)

Class No. 5	
Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
54	d_8-Naphthalene (internal)
56	d_5-Nitrobenzene (internal)
57	d_{10}-o-Xylene (internal)
58	d_5-Phenylethanol (internal)
59	d_5-Acetophenone (internal)
60	d_5-Propiophenone (internal)
61	d_{12}-Perylene (internal)
62	d_9-Acridine (internal)
63	d_5-Phenol (internal)

MATRIX OF STANDARD ION RMRs

Compound	Ion	Recovery	Standard: d_5-Phenol m/z 99	d_{10}-o Xylene m/z 98	d_{10}-o Xylene m/z 116	d_8-Naphthalene m/z 136	d_5 Nitrobenzene m/z 82	d_5 Nitrobenzene m/z 128	d_5-Phenylethanol m/z 84	d_5-Phenylethanol m/z 112
d_5-phenol	99	0 66	-	.59(9)	99(9)	.17(6)	1 04(5)	1 66(3)	2.44(15)	1 75(15)
d_{10}-o-xylene	98	NA	1.72(9)[a]	-	1.67(1)	.29(6)	1 79(8)	2 84(8)	4 21(22)	3 02(21)
	116	NA	1 03(a)	60(0)	-	.18(6)	1 07(8)	1.71(8)	2.53(22)	1.81(21)
d_8-naphthalene	136	0 40	5.97(4)	3 51(7)	5.85(7)	-	6.21(3)	9 98(3)	14 63(15)	10.59(18)
d_5-nitrobenzene	82	0 55	.97(4)	57(10)	.95(10)	.16(3)	-	1 60(1)	2 35(17)	1.70(16)
	128	0 55	.61(2)	.35(9)	.59(9)	.10(1)	63(1)	-	1 47(16)	1 07(15)
d_5-phenylethanol	84	0 62	.42(15)	.25(24)	.42(24)	.07/ .99(18)	44(16)	.70(15)	-	.73(2)
	112	0 62	.58(15)	.35(22)	.58(23)	.098(18)	61(16)	.95(16)	1.39(2)	-
d_5-propiophenone	82	0 42	1 09(4)	65(13)	1 07(14)	.18(8)	1 13(6)	1 82(6)	2 63(11)	1 90(10)
	110	0 42	2 85(5)	1 67(13)	2.78(14)	48(17)	2 94(6)	4.72(6)	6 84(12)	4.95(11)
d_5-acetophenone	110	ND	1 52(2)	.90(7)	1 50(8)	.25(4)	1 60(5)	2 55(1)	3.71(17)	2 68(16)
	125	ND	.46(2)	.27(8)	.45(7)	.26(3)	48(3)	.76(4)	1 11(16)	.81(17)
d_{12}-perylene	264	0 78	3 56(13)	2.09(7)	3 48(8)	60(9)	3 70(11)	5.90(12)	8 52(25)	6.37(28)
d_9-acridine	188	0 77	1 45(7)	.86(15)	1.43(15)	.24(8)	1 51(6)	2 40(6)	3.52(13)	2 55(13)
4-fluoro-2-iodotoluene	109	NA	1.10(4)	65(7)	1.08(8)	.18(3)	1.14(2)	1 82(2)	2 69(18)	1 97(19)
	236	NA	1.43(4)	.84(6)	1 39(7)	.24(6)	1 48(3)	2.37(3)	3 48(18)	2 52(18)

(continued)

Compound	Ion	Recovery	Standard: d_5-Propiophenone m/z 82	d_5-Propiophenone m/z 110	d_5-Acetophenone m/z 110	d_5-Acetophenone m/z 125	d_{12} Perylene m/z 264	d_9 Acridine m/z 188	4-Fluoro-2-Iodotoluene m/z 109	4-Fluoro-2-Iodotoluene m/z 236
d_5-phenol	99	0 66	.92(5)	35(5)	67(2)	2 21(3)	31(15)	70(7)	91(5)	.71(4)
d_{10}-o-xylene	98	NA	1 59(12)	61(13)	1 13(7)	3 .7(7)	53(10)	1.20(13)	1.56(6)	1 21(6)
	116	NA	.95(13)	37(12)	67(6)	2.27(7)	32(10)	.72(13)	94(6)	.73(6)
d_8-naphthalene	136	0 40	5 51(8)	2.13(8)	3 91(4)	13 14(3)	1 76(15)	4 20(8)	5.45(1)	4 20(1)
d_5-nitrobenzene	82	0 55	.89(6)	34(6)	63(4)	2 12(4)	29(19)	67(6)	88(2)	68(3)
	128	0 55	55(6)	22(6)	39(1)	1.32(3)	18(20)	42(6)	.55(3)	42(3)
d_5-phenylethenol	84	0 62	.39(11)	15(10)	28(16)	93(12)	13(22)	29(11)	38(18)	.30(17)
	112	0 62	.53(10)	.21(9)	39(16)	1 28(16)	18(28)	.41(13)	.52(19)	.42(16)
d_5-propiophenone	82	0 42	-	39(1)	.71(7)	2 40(6)	33(23)	76(5)	1 00(7)	77(7)
	110	0 42	2 60(1)	-	1 85(6)	6 21(6)	87(19)	2 00(5)	2 59(7)	1 99(7)
d_5-acetophenone	110	ND	1 41(6)	55(6)	-	3 39(1)	47(14)	1 10(9)	1 37(4)	1 07(2)
	125	ND	.42(6)	16(5)	.30(2)	-	14(18)	32(9)	42(7)	.32(3)
d_{12}-perylene	264	0 78	3.08(14)	1.27(16)	2 37(12)	7 91(12)	-	2 50(16)	3 21(9)	2.51(9)
d_9-acridine	188	0 77	1.33(5)	52(5)	.95(10)	3 15(11)	39(40)	-	1.32(8)	1 03(8)
4-fluoro-2-iodotoluene	109	NA	1 01(7)	39(7)	.71(2)	2 40(2)	.34(12)	.76(8)	-	.77(1)
	236	NA	1.31(7)	51(7)	92(3)	3 11(2)	.42(16)	1 00(8)	1.30(1)	-

Internal/External Standard File for Cmpd Class # 5

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
100	0.49		ALPHA-PICOLINE	109068						
66	0.26	0.20	0.05		0.30	0.46	0.16	0.27	0.59	0.42
93	0.66	0.51	0.12		0.76	1.18	0.40	0.66	1.52	1.09
101	0.63		ANILINE	62533						
66	0.23	0.19	0.04		0.28	0.41	0.15	0.24	0.53	0.38
93	0.76	0.54	0.13		0.81	1.25	0.45	0.74	1.62	1.15
102	0.44		INDOLE	120729						
90	0.72	0.54	0.13		0.82	1.30	0.43	0.71	2.04	1.51
117	1.92	1.45	0.34		2.17	3.46	1.14	1.89	5.43	4.02
103	0.60		2,3,6-TRIMETHYLPYRIDINE	1452846						
120	0.66	0.51	0.12		0.76	1.18	0.42	0.69	1.53	1.09
121	0.90	0.69	0.17		1.03	1.61	0.55	0.91	2.08	1.49
104	0.86		2,6-DIMETHYLANILINE	1300738						
106	0.36	0.27	0.06		0.41	0.65	0.21	0.36	1.02	0.75
121	0.57	0.44	0.10		0.66	1.04	0.34	0.57	1.64	1.21
105	0.80		M-CHLOROANILINE	108429						
127	1.09	0.84	0.20		1.26	1.94	0.69	1.15	2.52	1.79
129	0.34	0.26	0.06		0.29	0.60	0.22	0.36	0.78	0.56
106	0.53		QUINOLINE	91225						
129	1.82	1.41	0.34		1.99	3.22	1.30	2.17	4.06	2.98
107	0.55		2,4-DIMETHYLQUINOLINE	1198374						
156	0.41	0.32	0.08		0.47	0.75	0.26	0.43	0.95	0.68
157	2.01	1.54	0.37		2.31	3.59	1.27	2.11	4.64	3.31
108	0.73		CARBAZOLE	87648						
167	3.73	2.88	0.69		4.30	6.66	2.37	3.92	9.36	6.67
109	0.55		2-AMINOBIPHENYL	90415						
168	6.79	5.11	1.20		7.65	12.18	4.61	6.67	19.13	14.17
169	12.72	9.45	2.22		14.15	22.54	7.42	12.30	35.40	26.19
110	0.87		DIPHENYLAMINE	122394						
168	1.48	1.14	0.27		1.71	2.65	0.94	1.56	3.43	2.45
169	2.79	2.15	0.52		3.22	4.99	1.77	2.93	6.45	4.60
111	0.40		TRIBUTYLAMINE	102829						
100	0.42	0.33	0.08		0.49	0.75	0.27	0.44	0.97	0.69
142	1.53	1.18	0.28		1.77	2.74	0.97	1.61	3.52	2.51
112	0.68		CAFFEINE	58082						
109	0.10	0.08	0.02		0.12	0.17	0.06	0.10	0.23	0.16
194	0.19	0.15	0.04		0.22	0.34	0.12	0.20	0.44	0.32
113	0.43		DIBENZYLAMINE	103491						
91	1.62	1.25	0.30		1.78	2.87	1.06	1.94	3.63	2.57
197	0.13	0.11	0.03		0.15	0.24	0.10	0.16	0.30	0.22

Internal/External Standard File for Cmpd Class # 5

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61	Std #62 -	Std #63 -
Mass	110	125	82	110	264	188	99
100	0.49		ALPHA-PICOLINE 109068				
66	0.18	0.60	0.25	0.09	0.09	0.02	0.27
93	0.46	1.54	0.63	0.24	0.23	0.05	0.69
101	0.63		ANILINE 62533				
66	0.17	0.56	0.22	0.09	0.08	0.02	0.24
93	0.49	1.64	0.67	0.26	0.24	0.05	0.73
102	0.44		INDOLE 120729				
90	0.51	1.75	0.76	0.29	0.23	0.05	0.79
117	1.40	4.68	2.02	0.78	0.61	0.15	2.12
103	0.60		2,3,6-TRIMETHYLPYRIDINE 1462846				
120	0.46	1.54	0.63	0.24	0.23	0.05	0.67
121	0.62	2.10	0.86	0.33	0.32	0.07	0.94
104	0.86		2,6-DIMETHYLANILINE 1300738				
106	0.26	0.88	0.38	0.15	0.11	0.03	0.40
121	0.42	1.41	0.61	0.24	0.18	0.04	0.64
105	0.80		4-CHLOROANILINE 106429				
127	0.76	2.55	1.05	0.40	0.38	0.98	1.14
129	0.24	0.79	0.33	0.13	0.12	0.03	0.35
106	0.53		QUINOLINE 91225				
129	1.33	4.40	1.70	0.66	0.69	0.12	1.96
107	0.55		2,4-DIMETHYLQUINOLINE 1198374				
156	0.29	0.96	0.40	0.15	0.15	0.03	0.43
157	1.46	4.69	1.93	0.74	0.71	0.15	2.09
108	0.73		CARBAZOLE 87648				
167	2.60	8.72	3.57	1.37	1.28	0.31	4.22
109	0.55		2-AMINOBIPHENYL 90415				
168	4.75	16.46	7.10	2.75	2.13	0.51	7.45
169	8.82	30.44	13.14	5.08	3.96	0.95	13.80
110	0.87		DIPHENYLAMINE 122394				
168	1.03	3.47	1.42	0.55	0.52	0.11	1.55
169	1.94	6.46	2.68	1.03	0.98	0.22	2.91
111	0.40		TRIBUTYLAMINE 102829				
100	0.29	0.99	0.41	0.16	0.15	0.03	0.44
142	0.99	3.34	1.47	0.57	0.53	0.12	1.59
112	0.68		CAFFEINE 58082				
109	0.07	0.23	0.09	0.04	0.04	0.01	0.10
194	0.13	0.45	0.18	0.07	0.07	0.02	0.21
113	0.43		DIBENZYLAMINE 103491				
91	1.18	3.91	1.52	0.59	0.62	0.11	1.74
197	0.10	0.32	0.13	0.05	0.05	0.01	0.14

Internal/External Standard File for Cmpd Class # 5

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
114	0.74		N,N-DIMETHYLDODECYLAMINE		112185					
58	4.72	3.88	0.87		5.47	8.83	3.58	5.99	11.09	8.16
59	0.17	0.13	0.03		0.20	0.30	0.13	0.21	0.40	0.29
115	0.78		ATRAZINE	1912249						
200	2.75	2.20	0.52		3.28	5.23	1.72	2.86	8.17	6.09
215	1.67	1.34	0.31		2.00	3.18	1.05	1.74	4.97	3.71
116	0.55		HEPTANONE(2)	110430						
43	1.21	0.94	0.22		1.33	2.14	0.85	1.14	2.32	2.00
58	0.75	0.58	0.14		0.83	1.33	0.53	0.88	1.69	1.25
117	0.70		BUTOXYETHANOL	111762						
41	0.21	0.17	0.04		0.25	0.40	0.13	0.22	0.49	0.35
57	0.55	0.42	0.10		0.63	1.03	0.35	0.58	1.27	0.91
118	0.55		2-OCTANONE	111137						
43	1.30	1.01	0.24		1.43	2.31	0.91	1.53	2.92	2.15
58	1.02	0.79	0.19		1.11	1.80	0.71	1.19	2.27	1.67
119	0.31		BUTYLPROPIONATE	590012						
57	1.48	1.14	0.27		1.71	2.73	0.90	1.49	4.27	3.15
75	0.44	0.34	0.08		0.51	0.82	0.27	0.45	1.28	0.95
120	0.71		ISOPHORONE	78591						
82	1.77	1.36	0.33		2.04	3.17	1.13	1.86	4.11	2.93
138	0.39	0.30	0.07		0.45	0.72	0.25	0.41	0.90	0.64
121	0.63		FENCHONE	1195759						
69	0.66	0.51	0.12		0.72	1.17	0.47	0.78	1.47	1.08
81	1.44	1.12	0.27		1.58	2.55	1.02	1.71	3.22	2.36
122	1.11		ALPHA-TERPINEOL	98555						
59	0.56	0.43	0.10		0.65	1.00	0.36	0.59	1.31	0.93
136	0.32	0.25	0.06		0.37	0.58	0.21	0.34	0.75	0.53
123	0.71		N-DECANOL	112301						
41	0.40	0.31	0.07		0.46	0.74	0.25	0.42	0.92	0.66
43	0.44	0.34	0.08		0.51	0.79	0.28	0.46	1.02	0.73
124	0.49		DIMETHYLADIPATE	627930						
59	0.56	0.45	0.10		0.64	1.03	0.41	0.67	1.29	0.95
114	0.44	0.35	0.08		0.49	0.79	0.32	0.54	1.00	0.74
125	0.91		METHYLSTEARATE	112618						
74	3.42	2.65	0.63		3.89	6.28	2.54	4.25	7.90	5.81
87	2.22	1.72	0.41		2.52	4.07	1.65	2.76	5.13	3.77
126	0.32		PHENYLACETATE	122792						
94	1.84	1.43	0.34		2.01	3.25	1.30	2.18	4.10	3.01
136	0.25	0.20	0.05		0.28	0.45	0.18	0.30	0.57	0.42

Internal/External Standard File for Cpds Class 6 5

Cmpds Mass	Recovery Std 059 110	125	Compound Name Std 060 82	110	Std 061 204	-	Std 062 188	-	Std 063 99	-
114	0.74		N,N-DIMETHYLDODECYLAMINE		112185					
58	3.62	12.02	4.00	1.81	1.87		0.36		5.37	
59	0.13	0.43	0.17	0.06	0.07		0.01		0.19	
115	0.76		ATRAZINE 1912249							
200	2.13	7.07	3.05	1.18	0.90		0.22		3.26	
215	1.21	4.33	1.85	0.72	0.55		0.13		1.95	
116	0.55		HEPTANONE(2) 110430							
43	0.88	2.91	1.13	0.44	0.47		0.08		1.30	
58	0.55	1.82	0.71	0.27	0.29		0.05		0.81	
117	0.70		NONYLETHANOL 111762							
41	0.15	0.49	0.20	0.09	0.07		0.02		0.22	
57	0.38	1.24	0.52	0.20	0.19		0.04		0.57	
118	0.55		2-OCTANONE 111137							
43	0.95	3.16	1.22	0.47	0.51		0.09		1.40	
58	0.74	2.45	0.95	0.37	0.39		0.07		1.09	
119	0.81		BUTYLPROPIONATE 590812							
57	1.11	3.69	1.59	0.61	0.48		0.12		1.66	
75	0.33	1.11	0.44	0.19	0.15		0.04		0.50	
120	0.71		ISOPHORONE 78591							
82	1.23	4.14	1.70	0.65	0.62		0.14		1.80	
138	0.27	0.91	0.37	0.14	0.14		0.03		0.41	
121	0.63		FENCHONE 1195759							
69	0.48	1.58	0.62	0.24	0.25		0.05		0.71	
81	1.05	3.45	1.35	0.52	0.55		0.10		1.55	
122	1.11		ALPHA-TERPINEOL 98555							
59	0.39	1.31	0.54	0.21	0.20		0.04		0.58	
136	0.23	0.76	0.31	0.12	0.11		0.03		0.34	
123	0.71		N-DECANOL 112301							
41	0.28	0.93	0.38	0.15	0.14		0.03		0.41	
43	0.31	1.03	0.42	0.16	0.15		0.03		0.46	
124	0.49		DIMETHYLADIPATE 627930							
59	0.42	1.40	0.54	0.21	0.22		0.04		0.62	
114	0.33	1.09	0.42	0.16	0.17		0.03		0.46	
125	0.91		METHYLSTEARATE 112618							
74	2.58	8.56	3.32	1.29	1.33		0.24		3.83	
87	1.67	5.55	2.15	0.83	0.87		0.16		2.46	
126	0.32		PHENYLACETATE 122792							
94	1.31	4.43	1.72	0.67	0.70		0.13		1.98	
136	0.18	0.62	0.24	0.09	0.10		0.02		0.28	

Internal/External Standard File for Code Class # 5

Code#	Recovery Std # 2		Compound Name / Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
127	0.55		BENZYLACETATE 140114							
91	0.52	0.40	0.09		0.57	0.92	0.37	0.62	1.15	0.85
108	1.09	0.85	0.20		1.19	1.92	0.77	1.29	2.43	1.79
128	0.60		DIMETHYLPHTHALATE 131113							
77	0.81	0.63	0.15		0.94	1.65	0.52	0.85	1.88	1.34
163	5.29	4.07	0.98		6.10	9.46	3.36	5.56	12.22	8.71
129	0.70		ETHYLTOLUENESULFONATE(P) H3600							
91	1.74	1.32	0.31		1.77	3.14	1.03	1.72	4.92	3.65
155	1.18	0.94	0.22		1.40	2.23	0.73	1.21	3.46	2.35
130	0.89		DIETHYLPHTHALATE 84662							
149	3.19	2.41	0.57		3.65	5.79	1.90	3.17	9.08	6.71
177	0.80	0.61	0.14		0.93	1.47	0.48	0.80	2.29	1.69
131	1.38		DIBUTYLPHTHALATE 84742							
57	0.29	0.23	0.05		0.34	0.52	0.19	0.31	0.68	0.48
149	7.17	5.52	1.33		8.27	12.80	4.55	7.54	16.55	11.80
132	0.74		BUTYLBENZYLPHTHALATE							
91	2.09	1.62	0.38		2.28	3.69	1.48	2.48	4.64	3.41
149	3.37	2.62	0.62		3.69	5.95	2.40	4.01	7.49	5.51
133	1.04		DIETHYLHEXYLPHTHALATE 117817							
149	5.22	4.07	0.96		5.71	9.23	3.74	6.26	11.59	8.53
167	1.98	1.54	0.37		2.17	3.51	1.42	2.37	4.40	3.24
134	0.43		BENZALDEHYDE 100527							
77	0.36	0.28	0.07		0.42	0.64	0.23	0.38	0.84	0.60
105	0.40	0.31	0.07		0.46	0.70	0.25	0.42	0.92	0.66
135	1.05		TOLUALDEHYDE 529204							
91	0.54	0.44	0.10		0.65	1.04	0.34	0.57	1.65	1.21
119	0.63	0.51	0.12		0.77	1.23	0.41	0.68	1.95	1.43
136	0.01		ACETOPHENONE 98862							
77	0.38	0.64	0.15		0.96	1.53	0.53	0.87	1.93	1.37
105	1.22	0.94	0.23		1.41	2.25	0.78	1.29	2.85	2.03
137	0.67		SALICYLALDEHYDE 90028							
121	0.56	0.44	0.10		0.61	0.95	0.40	0.67	1.24	0.91
122	0.60	0.47	0.11		0.66	1.07	0.43	0.72	1.34	0.99
138	0.72		ANISALDEHYDE 123115							
135	1.37	1.08	0.25		1.53	2.47	0.91	1.66	3.11	2.29
136	0.96	0.76	0.18		1.07	1.73	0.70	1.16	2.18	1.60
139	0.61		PHENOL 108952							
94	1.07	0.84	0.20		1.18	1.90	0.76	1.27	2.41	1.77

Internal/External Standard File for Cmpd Class 8 5

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	148	-	99	-
127	0.55		BENZYLACETATE 140114							
91	0.38	1.25	0.48	0.19	0.20		0.04		0.56	
108	0.79	2.63	1.02	0.40	0.41		0.07		1.17	
128	0.60		DIMETHYLPHTHALATE 131113							
77	0.57	1.83	0.75	0.29	0.28		0.06		0.35	
163	3.68	11.87	4.88	1.88	1.85		0.41		5.51	
129	0.70		ETHYLTOLUENESULFONATE(P) 80400							
91	1.28	4.25	1.63	0.71	0.55		0.13		1.92	
155	0.91	3.01	1.30	0.50	0.38		0.09		1.36	
130	0.89		DIETHYLPHTHALATE 84662							
149	2.35	7.82	3.34	1.30	1.02		0.24		3.54	
177	0.59	1.97	0.85	0.33	0.26		0.06		0.89	
131	1.38		DIBUTYLPHTHALATE 84742							
57	0.20	0.68	0.28	0.11	0.10		0.02		0.31	
149	4.99	16.75	6.88	2.64	2.52		0.55		7.47	
132	0.74		BUTYLBENZYLPHTHALATE							
91	1.51	5.02	1.95	0.76	0.78		0.14		2.24	
149	2.44	8.10	3.15	1.22	1.26		0.23		3.62	
133	1.04		DIETHYLHEXYLPHTHALATE 117817							
149	4.03	12.58	4.88	1.89	1.90		0.35		5.61	
167	1.53	4.78	1.85	0.72	0.72		0.13		2.13	
134	0.43		BENZALDEHYDE 100527							
77	0.25	0.84	0.35	0.13	0.13		0.03		0.38	
105	0.28	0.93	0.38	0.15	0.14		0.03		0.42	
135	1.05		TOLUALDEHYDE 529204							
91	0.42	1.41	0.61	0.24	0.15		0.05		0.64	
119	0.50	1.66	0.72	0.28	0.22		0.05		0.75	
136	0.01		ACETOPHENONE 98862							
77	0.57	1.95	0.80	0.31	0.29		0.06		0.87	
105	0.85	2.88	1.18	0.45	0.43		0.09		1.28	
137	0.67		SALICYLALDEHYDE 90028							
121	0.41	1.35	0.52	0.20	0.21		0.04		0.60	
122	0.44	1.46	0.56	0.22	0.23		0.04		0.65	
138	0.72		ANISALDEHYDE 123115							
135	1.01	3.36	1.30	0.51	0.53		0.09		1.50	
136	0.71	2.36	0.91	0.35	0.37		0.07		1.05	
139	0.61		PHENOL 108952							
94	0.75	2.60	1.01	0.39	0.41		0.07		1.15	

Internal/External Standard File for Cpd Class # 5

Cpd#	Recovery Std # 2		Compound Name	Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-		82	129	98	116	84	112
140	0.62		CRESOL(P)	106445							
107	1.21	0.93	0.23			1.40	2.25	0.80	1.29	2.91	2.08
108	1.07	0.82	0.20			1.24	1.99	0.69	1.14	2.56	1.84
141	0.58		2,3-DIMETHYLPHENOL		526750						
107	0.87	0.67	0.16			1.00	1.61	0.57	0.93	2.08	1.48
122	0.91	0.70	0.17			1.05	1.64	0.58	0.96	2.12	1.51
142	0.57		ISOPROPYLPHENOL		88699						
121	1.79	1.36	0.32			2.04	3.25	1.07	1.78	5.10	3.77
136	0.07	0.55	0.12			0.75	1.19	0.39	0.65	1.87	1.38
143	0.49		O-NITROPHENOL		88755						
65	0.03	0.02	0.00			0.03	0.05	0.02	0.03	0.06	0.05
139	0.13	0.10	0.02			0.14	0.23	0.09	0.15	0.29	0.21
144	1.18		4-CHLORO-3-METHYLPHENOL		59507						
107	0.93	0.71	0.17			1.06	1.68	0.55	0.92	2.64	2.45
142	1.02	0.77	0.18			1.16	1.84	0.61	1.01	2.89	2.14
145	0.89		1-NAPHTHOL	90153							
115	0.35	0.26	0.06			0.38	0.61	0.20	0.34	0.96	0.72
144	0.61	0.45	0.11			0.67	1.07	0.35	0.29	1.68	1.25
146	0.77		P-TERT-BUTYLPHENOL		98544						
107	0.56	0.43	0.10			0.65	1.03	0.34	0.56	1.60	1.18
135	1.96	1.49	0.35			2.22	3.54	1.17	1.94	5.56	4.11
147	0.61		2-NITROCRESOL		119335						
77	0.26	0.20	0.05			0.30	0.45	0.07	0.27	0.60	0.43
153	0.74	0.57	0.14			0.83	1.33	0.46	0.78	1.72	1.23
148	0.81		2,4-DICHLOROPHENOL		120832						
162	1.13	0.88	0.21			1.24	2.00	0.80	1.34	2.52	1.86
164	0.72	0.53	0.13			0.78	1.27	0.51	0.85	1.60	1.18
149	0.30		2,4,6-TRICHLOROPHENOL		88062						
196	0.81	0.63	0.15			0.89	1.44	0.58	0.97	1.88	1.34
198	0.83	0.64	0.15			0.91	1.46	0.59	0.98	1.90	1.36
150	0.69		DI-TERT-BUTYL-4-METHYLPHENOL		128370						
205	2.53	1.97	0.47			2.78	4.49	1.81	3.03	5.86	4.16
220	0.67	0.52	0.12			0.73	1.18	0.48	0.80	1.49	1.09
151	0.48		2-METHYLNAPHTHALENE		91576						
141	2.03	1.58	0.38			2.23	3.60	1.44	2.42	4.53	3.34
142	2.51	1.95	0.46			2.76	4.45	1.79	2.99	5.62	4.13
152	0.50		ACENAPHTHENE		83329						
153	1.26	0.98	0.23			1.38	2.22	0.89	1.49	2.81	2.06
154	3.40	2.64	0.63			3.73	6.02	2.41	4.04	7.59	5.58

Internal/External Standard Ratio for Cmpd Class # 5

Cmpds	Recovery		Compound Name									
	Std #59		Std #60		Std #61		Std #62		Std #63	
Mass	110	125	92	110	204	-	188	-	99	-
140	0.62		CRESOL(P) 106445							
107	0.88	2.85	1.17	0.45	0.44		0.10		1.31	
108	0.78	2.52	1.03	0.40	0.39		0.09		1.16	
141	0.58		2,3-DIMETHYLPHENOL 526750							
107	0.63	2.11	0.44	0.32	0.32		0.07		0.94	
122	0.64	2.14	0.85	0.33	0.32		0.07		0.95	
142	0.57		ISOPROPYLPHENOL 88099							
121	1.24	4.39	1.40	0.73	0.58		0.14		1.99	
136	0.47	1.61	0.69	0.27	0.21		0.05		0.73	
143	0.49		O-NITROPHENOL 88755							
65	0.02	0.07	0.03	0.01	0.01		0.00		0.03	
139	0.09	0.31	0.12	0.05	0.05		0.01		0.14	
144	1.18		4-CHLORO-3-METHYLPHENOL 59507							
107	0.66	2.27	0.98	0.38	0.30		0.07		1.03	
142	0.77	2.69	1.07	0.42	0.32		0.08		1.13	
145	0.89		1-NAPHTHOL 90153							
115	0.25	0.83	0.36	0.14	0.11		0.03		0.38	
144	0.44	1.45	0.62	0.24	0.18		0.05		0.66	
146	0.77		P-TERT-BUTYLPHENOL 98544							
107	0.40	1.38	0.66	0.23	0.18		0.04		0.62	
135	1.44	4.79	2.04	0.80	0.63		0.15		2.16	
147	0.61		2-NITROCRESOL 119339							
77	0.18	0.61	0.25	0.10	0.09		0.02		0.27	
153	0.52	1.74	0.71	0.27	0.26		0.06		0.78	
148	0.91		2,4-DICHLOROPHENOL 120832							
162	0.80	2.73	1.05	0.41	0.43		0.08		1.22	
164	0.51	1.73	0.67	0.26	0.27		0.05		0.77	
149	0.30		2,4,6-TRICHLOROPHENOL 88062							
196	0.58	1.97	0.76	0.30	0.31		0.05		0.86	
198	0.58	1.99	0.77	0.30	0.32		0.06		0.89	
150	0.69		DI-TERT-BUTYL-4-METHYLPHENOL 128370							
205	1.85	6.13	2.37	0.92	0.96		0.17		2.73	
220	0.49	1.61	0.62	0.24	0.25		0.05		0.72	
151	0.48		2-METHYLNAPHTHALENE 91576							
141	1.49	4.91	1.90	0.74	0.77		0.14		2.19	
142	1.78	6.08	2.36	0.91	0.95		0.17		2.71	
152	0.50		ACENAPHTHENE 83329							
153	0.92	3.04	1.18	0.46	0.47		0.09		1.35	
154	2.49	8.22	3.19	1.23	1.28		0.23		3.66	

Internal/External Standard File for Cmpd Class # 5

Cmpd#	Recovery Std # 2		Compound Name / Std #54	Std #56		Std #57		Std #58	
Mass	109	236	136	82	128	98	116	84	112
153	0.84		FLUORENE 86737						
165	2.74	2.13	0.49	3.03	4.85	1.95	3.27	6.12	4.50
166	3.07	2.38	0.57	3.44	5.55	2.23	3.74	6.99	5.14
154	0.48		2,3,5-TRIMETHYLNAPHTHALENE 2245387						
155	1.86	1.44	0.34	2.08	3.35	1.36	2.27	4.24	3.12
170	2.56	1.99	0.47	2.86	4.62	1.86	3.11	5.83	4.29
155	0.66		ANTHRACENE 120127						
178	3.21	2.47	0.60	3.71	5.74	2.04	3.38	7.43	5.30
156	0.78		PYRENE 129000						
202	4.88	3.75	0.95	5.66	8.73	3.27	5.18	11.54	8.23
157	0.63		9,10-DIMETHYLANTHRACENE 781431						
191	1.33	1.03	0.25	1.45	2.35	0.94	1.57	2.96	2.18
206	2.85	2.22	0.53	3.13	5.04	2.01	3.37	6.36	4.69
158	0.95		CHRYSENE 218019						
228	2.23	1.73	0.41	2.42	3.92	1.59	2.66	4.91	3.61
159	1.18		PERYLENE 198550						
252	1.60	1.23	0.30	1.84	2.86	1.02	1.68	3.67	2.62
160	1.04		DICYANOBUTANE 111693						
41	0.66	0.51	0.12	0.72	1.17	0.47	0.79	1.47	1.08
54	0.29	0.23	0.05	0.32	0.52	2.10	0.35	0.66	0.48
161	0.65		BIS(2-CHLOROETHYL)ETHANE 112265						
63	1.71	1.31	0.31	1.97	3.13	1.03	1.71	4.91	3.63
91	0.84	0.65	0.15	0.97	1.54	0.51	0.84	2.42	1.78
162	0.75		TRIBUTYLPHOSPHATE 126738						
99	4.03	3.10	0.75	4.65	7.20	2.56	4.24	9.28	6.62
155	0.88	0.68	0.16	1.01	1.57	0.56	0.92	2.02	1.44
163	0.48		DIHYDROBENZOFURAN(2,3) 496162						
91	0.68	0.52	0.13	0.79	1.25	0.43	0.72	1.58	1.13
120	0.97	0.75	0.18	1.12	1.67	0.66	0.78	2.16	1.54
164	0.58		NITROBENZENE 98953						
77	0.86	0.67	0.16	0.94	1.51	0.61	1.02	1.91	1.40
123	0.54	0.42	0.10	0.59	0.95	0.38	0.64	1.20	0.88
165	0.58		BENZOTHIAZOLE 95169						
135	1.56	1.21	0.29	1.71	2.76	1.11	1.86	3.47	2.55
166	0.48		PHENYLCARBAMATE 102090						
94	1.23	0.96	0.23	1.44	2.23	0.79	1.31	2.48	2.06
137	0.02	0.01	0.00	0.02	0.03	0.01	0.02	0.04	0.03

Internal/External Standard File for Cmpd Class # 5

Cmpd#	Recovery Std #59		Compound Name	Std #60		Std #61		Std #62		Std #63	
Mass	110	125		82	110	264	-	188	-	99	-
153	0.84		FLUORENE 86737								
165	2.00	6.62		2.57	0.99	1.04		0.19		2.95	
166	2.28	7.57		2.93	1.14	1.19		0.21		3.38	
154	0.48		2,3,5-TRIMETHYLNAPHTHALENE 2245387								
155	1.38	4.59		1.78	0.69	0.72		0.13		2.05	
170	1.90	6.31		2.44	0.95	0.99		0.18		2.81	
155	0.66		ANTHRACENE 120127								
178	2.24	7.59		3.08	1.19	1.13		0.25		3.35	
156	0.78		PYRENE 129000								
202	3.59	11.47		4.95	1.90	1.80		0.40		5.36	
157	0.63		9,10-DIMETHYLANTHRACENE 781431								
191	0.96	3.19		1.24	0.48	0.50		0.09		1.42	
206	2.06	6.86		2.67	1.03	1.08		0.19		3.06	
158	0.95		CHRYSENE 218019								
228	1.61	5.34		2.07	0.80	0.81		0.15		2.39	
159	1.18		PERYLENE 198550								
252	1.11	3.72		1.53	0.59	0.47		0.12		1.65	
160	1.04		DICYANOBUTANE 111693								
41	0.48	1.59		0.62	0.24	0.25		0.05		0.71	
54	0.22	0.71		0.28	0.11	0.11		0.02		0.32	
161	0.65		BIS(2-CHLOROETHYL)ETHANE 112265								
63	1.27	4.23		1.63	0.71	0.56		0.13		1.91	
93	0.61	2.08		0.90	0.35	0.27		0.06		0.94	
162	0.75		TRIBUTYLPHOSPHATE 126738								
99	2.81	9.43		3.87	1.49	1.41		0.31		4.19	
155	0.61	2.05		0.84	0.32	0.31		0.07		0.91	
163	0.48		DIHYDROBENZOFURAN(2,3) 496162								
91	0.27	1.59		0.65	0.25	0.24		0.05		0.71	
120	0.68	2.27		0.90	0.35	0.33		0.07		0.98	
164	0.58		NITROBENZENE 98953								
77	0.61	2.07		0.80	0.31	0.33		0.06		0.94	
123	0.38	1.30		0.50	0.20	0.21		0.04		0.59	
165	0.58		BENZOTHIAZOLE 95169								
135	1.14	3.76		1.46	0.57	0.59		0.11		1.68	
166	0.48		PHENYLCARBAMATE 102090								
94	0.87	2.92		1.20	0.46	0.44		0.10		1.30	
137	0.01	0.04		0.01	0.01	0.00		0.00		0.02	

Internal/External Standard File for Cmpd Class # 5

Cmpd# / Mass	Recovery Std # 2		Compound Name / Std #54	Std #56		Std #57		Std #58	
	109	236	136	82	128	98	116	84	112
167	1.05		2,4-DINITROTOLUENE 121142						
89	0.35	0.28	0.06	0.40	0.65	0.26	0.44	0.61	0.60
165	0.71	0.53	0.13	0.75	1.21	0.46	0.76	1.53	1.13
168	0.71		BENZYLSULFIDE 583749						
91	3.55	2.68	0.63	4.00	6.38	2.10	3.49	9.99	7.42
123	0.90	0.68	0.16	1.02	1.62	0.53	0.89	2.54	1.88
169	0.67		DIPHENYLSULFONE 127039						
125	3.82	3.44	0.81	5.16	8.21	2.71	4.51	12.95	8.65
218	0.92	0.73	0.17	1.10	1.75	0.58	0.96	2.74	2.03
170	0.71		TRIPHENYLPHOSPHATE 115866						
325	2.59	2.01	0.13	0.79	1.26	0.52	0.87	1.61	1.18
326	0.09	0.07	0.17	1.03	1.67	0.68	1.14	2.09	1.54
171	0.81		DIPHENYLMERCURY 587859						
77	0.72	0.55	0.48	2.85	4.59	1.96	3.28	6.08	4.47
356	0.95	0.74	0.02	0.09	0.15	0.06	0.11	0.20	0.15
172	0.72		TETRAPHENYLTIN						
197	1.40	1.13	0.27	1.70	2.71	0.89	1.47	4.21	3.13
351	1.30	1.05	0.25	1.58	2.51	0.82	1.37	3.91	2.91
173	0.01		PYRIDINE 110861						
52	0.29	0.22	0.05	0.33	0.51	0.19	0.32	0.67	0.48
79	0.44	0.34	0.08	0.51	0.78	0.30	0.50	1.10	0.78
174	0.01		TOLUIDINE 106490						
106	0.89	0.69	0.16	0.97	1.57	0.64	1.07	1.97	1.45
107	0.71	0.55	0.13	0.78	1.27	0.51	0.86	1.58	1.16
175	0.01		LUTIDINE 108485						
106	0.13	0.10	0.02	0.15	0.25	0.08	0.13	0.39	0.28
107	0.22	0.16	0.04	0.24	0.39	0.13	0.21	0.61	0.45
176	0.01		P-NITROANILINE 100016						
65	0.44	0.35	0.08	0.52	0.83	0.27	0.46	1.30	0.97
138	0.56	0.45	0.11	0.67	1.07	0.35	0.58	1.68	0.22
177	0.01		NICOTINE 54155						
84	1.17	0.90	0.22	1.35	2.09	0.74	1.23	2.70	1.92
133	0.28	0.21	0.05	0.32	0.49	0.17	0.29	0.63	0.45
178	0.01		DICYCLOHEXYLAMINE 101837						
56	0.33	0.37	0.06	0.39	0.63	0.21	0.35	1.10	0.78
138	0.96	0.76	0.18	1.12	1.80	0.61	1.02	3.15	2.25
179	0.01		N-DECANE 124185						
43	1.47	1.11	0.26	1.67	2.66	0.88	1.46	4.18	3.09
57	1.42	1.08	0.25	1.64	2.61	0.85	1.41	4.05	3.00

Internal/External Standard File for Capd Class # 5

Capd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63
Mass	110	125	82	110	264	-	188	-	99	-
167	1.05		2,4-DINITROTOLUENE		121142				
89	0.27	0.88	0.31	0.13	0.14		0.03		0.39
165	0.50	1.66	0.64	0.25	0.26		0.05		0.74
168	0.71		BENZYLSULFIDE		538749				
91	2.37	8.62	3.72	1.44	1.11		0.27		3.90
123	0.53	2.19	0.94	0.37	0.28		0.07		0.99
169	0.67		DIPHENYLSULFONE		127639				
125	3.00	11.09	4.77	1.85	1.22		0.35		5.05
218	0.67	2.36	1.02	0.29	0.30		0.07		1.07
170	0.71		TRIPHENYLPHOSPHATE		115866				
325	1.98	6.58	2.55	0.95	1.03		0.18		0.78
326	0.06	0.22	0.08	0.03	0.03		0.01		1.02
171	0.81		DIPHENYLMERCURY		587859				
77	0.53	1.75	0.68	0.26	0.26		0.05		2.94
356	0.69	2.28	0.88	0.34	0.35		0.06		0.10
172	0.72		TETRAPHENYLTIN						
197	1.10	3.66	1.57	0.61	0.44		0.11		1.56
351	1.03	3.43	1.46	0.57	0.41		0.11		1.54
173	0.01		PYRIDINE		110861				
52	0.20	0.68	0.28	0.11	0.10		0.02		0.30
79	0.33	1.11	0.42	0.16	0.17		0.04		0.50
174	0.01		TOLUIDINE		106490				
106	0.65	2.15	0.83	0.32	0.32		0.06		0.96
107	0.52	1.73	0.67	0.26	0.26		0.05		0.77
175	0.01		LUTIDINE		108485				
106	0.10	0.33	0.14	0.05	0.04		0.01		0.15
107	0.16	0.52	0.23	0.09	0.06		0.02		0.24
176	0.01		P-NITROANILINE		100016				
65	0.34	1.13	0.49	0.19	0.14		0.04		0.51
138	0.43	1.44	0.62	0.24	0.19		0.05		0.65
177	0.01		NICOTINE		54155				
84	0.82	2.74	1.12	0.43	0.41		0.09		1.22
133	0.19	0.64	0.26	0.10	0.10		0.02		0.29
178	0.01		DICYCLOHEXYLAMINE		101837				
56	0.25	0.81	0.33	0.14	0.09		0.03		0.38
138	0.71	2.34	0.95	0.40	0.26		0.08		1.09
179	0.01		N-DECANE		124185				
43	1.05	3.59	1.55	0.60	0.47		0.11		1.62
57	1.01	3.48	1.50	0.58	0.46		0.11		1.58

Internal/External Standard File for Cmpd Class # 5

Cmpd#	Recovery Std # 2		Compound Name Std #54	Std #56		Std #57		Std #58	
Mass	109	236	136	82	128	98	116	84	112
180	0.01		N-TRIDECANE 629505						
43	2.18	1.64	0.34	2.48	3.95	1.30	2.16	6.20	4.58
57	2.75	2.09	0.50	3.14	5.01	1.66	2.77	7.93	5.86
181	0.01		N-TETRADECANE 629594						
43	2.52	1.92	0.45	2.88	4.58	1.51	2.51	7.19	5.31
57	3.40	2.55	0.61	3.87	6.16	2.03	3.37	9.67	7.15
182	0.01		N-PENTADECANE 629629						
57	2.78	2.14	0.52	3.22	4.99	1.77	2.94	6.47	4.62
71	1.73	1.33	0.32	2.01	3.11	1.10	1.83	4.03	2.87
183	0.01		N-HEXADECANE 544763						
43	1.90	1.45	0.34	2.16	3.45	1.13	1.89	5.41	3.99
57	2.72	2.08	0.49	3.11	4.96	1.63	2.71	7.78	5.74
184	0.01		N-HEPTADECANE 629787						
57	3.13	2.41	0.58	3.61	5.59	1.99	3.30	7.25	5.17
71	2.07	1.60	0.38	2.39	3.70	1.32	2.18	4.80	3.42
185	0.01		N-OCTADECANE 593453						
57	2.99	2.51	0.59	3.75	5.98	1.88	3.14	8.96	6.63
71	1.98	1.66	0.39	2.48	3.95	1.25	2.00	5.95	4.41
186	0.01		N-NONADECANE 629952						
71	2.12	1.61	0.38	2.42	3.85	1.27	2.11	6.04	4.47
85	1.42	1.08	0.25	1.61	2.57	0.85	1.41	4.03	2.98
187	0.01		N-EICOSANE 1112958						
57	4.43	3.41	0.82	5.11	7.92	2.82	4.66	10.26	7.32
71	3.03	2.33	0.56	3.50	5.43	1.93	3.19	7.03	5.01
188	0.01		N-HENEICOSANE 629947						
57	3.93	2.96	0.70	4.43	7.05	2.32	3.86	11.05	8.20
71	2.71	2.05	0.48	3.07	4.88	1.61	2.67	7.65	5.68
189	0.01		N-DOCOSANE 629970						
57	3.73	2.98	0.70	4.46	7.10	2.33	3.88	11.11	8.26
71	2.60	2.08	0.49	3.11	4.96	1.63	2.70	7.76	5.77
190	0.01		N-TRICOSANE 638675						
57	3.99	3.19	0.75	4.77	7.60	2.49	4.14	11.85	8.83
71	2.80	2.24	0.53	3.35	5.34	1.75	2.91	8.33	6.20
191	0.01		METHYLBENZENESULFONATE						
77	1.24	0.94	0.22	1.41	2.25	0.74	1.23	3.54	2.61
172	0.44	0.34	0.08	0.50	0.80	0.26	0.44	1.26	0.93
192	0.01		METHYLTOLUENESULFONATE(P)						
91	1.60	1.21	0.29	1.81	2.89	0.95	1.58	4.53	3.35
155	0.72	0.54	0.13	0.81	1.29	0.42	0.71	2.02	1.50

Internal/External Standard File for Cmpd Class # 5

Cmpds	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
180	0.01		N-TRIDECANE 629505							
43	1.56	5.33	2.30	0.89	0.70		0.17		2.41	
57	1.99	6.75	2.94	1.14	0.76		0.21		3.09	
181	0.01		N-TETRADECANE 629594							
43	1.86	6.19	2.67	1.03	0.80		0.19		2.80	
57	2.50	8.33	3.57	1.39	1.08		0.26		3.77	
182	0.01		N-PENTADECANE 629629							
57	1.94	6.52	2.66	1.03	0.99		0.22		2.92	
71	1.21	4.06	1.67	0.64	0.62		0.14		1.82	
183	0.01		N-HEXADECANE 544763							
43	1.40	4.66	2.01	0.78	0.61		0.15		2.11	
57	2.01	6.70	2.88	1.12	0.87		0.21		3.03	
184	0.01		N-HEPTADECANE 629787							
57	2.18	7.32	3.01	1.16	1.11		0.24		3.27	
71	1.44	4.85	1.99	0.77	0.73		0.16		2.17	
185	0.01		N-OCTADECANE 593453							
57	2.33	8.10	3.48	1.35	1.01		0.24		3.65	
71	1.55	5.35	2.30	0.89	0.58		0.06		2.41	
186	0.01		N-NONADECANE 629952							
71	1.51	5.27	2.24	0.87	0.68		0.16		2.35	
85	1.01	3.47	1.50	0.58	0.45		0.11		1.57	
187	0.01		N-EICOSANE 1112958							
57	3.08	10.35	4.25	1.63	1.57		0.35		4.63	
71	2.11	7.09	2.91	1.12	1.07		0.23		3.17	
188	0.01		N-HENEICOSANE 629947							
57	2.73	9.53	4.11	1.60	1.07		0.30		4.31	
71	1.89	6.60	2.85	1.10	0.74		0.21		2.99	
189	0.01		N-DOCOSANE 629970							
57	2.89	9.60	4.14	1.60	1.22		0.30		4.35	
71	2.02	6.71	2.89	1.12	0.85		0.21		3.04	
190	0.01		N-TRICOSANE 638675							
57	3.10	10.28	4.42	1.71	1.29		0.32		4.65	
71	2.18	7.22	3.11	1.20	0.90		0.22		3.27	
191	0.01		METHYLBENZENESULFONATE							
77	0.91	3.04	1.31	0.51	0.40		0.09		1.38	
172	0.32	1.08	0.47	0.18	0.14		0.03		0.49	
192	0.01		METHYLTOLUENESULFONATE(P)							
91	1.17	3.90	1.68	0.65	0.51		0.12		1.76	
155	0.52	1.74	0.75	0.29	0.23		0.05		0.79	

Internal/External Standard File for Cmpd Class # 5

Cmpds	Recovery Std # 2		Compound Name	Std #54		Std #56		Std #57		Std #54	
Mass	109	236	136	-		82	128	98	116	84	112
193	0.01		4-CHLOROCRESOL								
107	0.83	0.64	0.16			0.97	1.57	0.53	0.85	2.03	1.45
142	0.94	0.72	0.17			1.09	1.77	0.60	0.99	2.29	1.63
194	0.01		PENTACHLOROPHENOL		87865						
264	0.29	0.22	0.05			0.34	0.54	0.19	0.31	0.72	0.52
266	0.47	0.36	0.09			0.55	0.91	0.32	0.54	1.17	0.84
195	0.01		BIPHENYL	92524							
154	2.28	1.78	0.42			2.51	4.04	1.63	2.72	5.10	3.75
196	0.01		1,4-DIMETHYLNAPHTHALENE		569415						
141	1.59	1.24	0.29			1.74	2.82	1.13	1.89	3.55	2.61
156	2.30	1.79	0.42			2.52	4.07	1.63	2.73	5.13	3.77
197	0.01		BUTYLCARBAMATE		14994775						
41	0.48	0.36	0.08			0.54	0.86	0.28	0.47	1.35	1.00
59	0.24	0.26	0.05			0.29	0.47	0.15	0.25	0.72	0.54
198	0.01		DI-T-BUTYLDISULFIDE		110065						
41	0.73	0.56	0.13			0.84	1.34	0.44	0.73	2.10	1.55
57	3.09	2.36	0.56			3.54	5.64	1.85	3.09	8.84	6.54
199	0.01		ALDRIN	309002							
66	1.33	1.03	0.24			1.49	2.40	0.97	1.62	3.03	2.23
263	0.60	0.46	0.11			0.67	1.08	0.44	0.73	1.36	1.00
200	0.01		BENZYLCHLORIDE		100447						
91	1.55	1.18	0.28			1.77	2.82	0.93	1.56	4.42	3.28
126	0.42	0.32	0.08			0.48	0.75	0.25	0.42	1.20	0.89
201	0.47		4-CHLOROBENZONITRILE		623033						
102	0.55	0.42	0.10			0.63	0.99	0.33	0.55	1.57	1.16
137	2.10	1.57	0.36			2.38	3.79	1.25	2.08	5.95	4.40
202	0.80		3-CHLOROBENZALDEHYDE		587042						
111	0.06	0.05	0.01			0.08	0.12	0.04	0.07	0.20	0.14
139	0.12	0.10	0.02			0.15	0.24	0.08	0.13	0.38	0.28
203	0.50		3-CHLOROANISOLE		766518						
127	0.60	0.46	0.11			0.69	1.09	0.36	0.60	1.71	1.27
142	1.32	1.00	0.24			0.50	2.40	0.79	1.31	3.76	2.78
204	0.01		CHLOROBENZAMIDE		619567						
139	0.70	0.55	0.13			0.77	1.25	0.50	0.84	1.57	1.16
155	0.38	0.30	0.07			0.42	0.68	0.27	0.46	0.85	0.63
205	0.55		3,4-DICHLOROBENZALDEHYDE		6287383						
173	0.46	0.39	0.09			0.58	0.93	0.31	0.57	1.46	1.07
174	0.32	0.26	0.06			0.39	0.62	0.21	0.34	0.98	0.72

Internal/External Standard File for Cmpd Class # 5

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
193	0.01		4-CHLOROCRESOL							
107	0.58	1.96	0.80	0.31	0.31		0.07		0.91	
142	0.66	2.23	0.85	0.34	0.35		0.08		1.03	
194	0.01		PENTACHLOROPHENOL		87865					
264	0.20	0.68	0.28	0.11	0.11		0.02		0.31	
266	0.36	1.11	0.45	0.07	0.18		0.04		0.50	
195	0.01		BIPHENYL 92524							
154	1.67	5.52	2.14	0.83	0.87		0.16		2.46	
196	0.01		1,8-DIMETHYLNAPHTHALENE		569415					
141	1.16	3.84	1.49	0.58	0.60		0.11		1.71	
156	1.67	5.55	2.15	0.83	0.87		0.16		2.48	
197	0.01		BUTYLCARBAMATE		14994775					
41	0.35	1.16	0.50	0.09	0.15		0.04		0.52	
59	0.19	0.63	0.27	0.11	0.08		0.02		0.28	
198	0.01		DI-T-BUTYLDISULFIDE		110065					
41	0.54	1.78	0.78	0.31	0.20		0.06		0.82	
57	2.21	7.62	3.29	1.27	1.00		0.24		3.42	
199	0.01		ALDRIN 309002							
66	0.99	3.28	1.27	0.49	0.51		0.09		1.46	
263	0.44	1.47	0.57	0.22	0.23		0.04		0.66	
200	0.01		BENZYLCHLORIDE		100447					
91	1.10	3.81	1.64	0.64	0.50		0.12		1.71	
126	0.30	1.03	0.45	0.17	0.12		0.03		0.47	
201	0.47		4-CHLOROBENZONITRILE		623033					
102	0.39	1.35	0.58	0.23	0.18		0.04		0.61	
137	1.49	5.12	2.21	0.85	0.67		0.16		2.32	
202	0.80		3-CHLOROBENZALDEHYDE		587042					
111	0.05	0.17	0.07	0.03	0.02		0.00		0.04	
139	0.10	0.32	0.14	0.05	0.04		0.01		0.15	
203	0.50		O-CHLOROANISOLE		766518					
127	0.43	1.48	0.64	0.25	0.17		0.05		0.67	
142	0.94	3.24	1.40	0.54	0.36		0.10		1.46	
204	0.01		CHLOROBENZAMIDE		619567					
139	0.51	1.70	0.66	0.26	0.27		0.05		0.76	
155	0.28	0.92	0.36	0.14	0.15		0.03		0.41	
205	0.55		3,4-DICHLOROBENZALDEHYDE		6287383					
173	0.37	1.25	0.54	0.21	0.17		0.04		0.57	
174	0.25	0.84	0.36	0.14	0.11		0.03		0.38	

Internal/External Standard File for Cmpd Class # 5

Cmpds	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
206	1.07		1,2,4-TRICHLOROBENZENE		120821					
145	0.34	0.26	0.06		0.40	0.63	0.22	0.36	0.80	0.57
180	1.30	1.00	0.24		1.50	2.40	0.83	1.37	3.03	2.16
207	0.01		2-BROMO-1-CHLOROBENZENE		694804					
190	0.78	0.61	0.14		0.85	1.32	0.55	0.92	1.74	1.28
192	1.04	0.81	0.19		1.14	1.84	0.74	1.24	2.33	1.71
208	0.68		1,2-DICHLORONAPHTHALENE		2050693					
161	0.44	0.34	0.08		0.50	0.78	0.28	0.46	1.01	0.72
196	2.17	1.67	0.40		2.51	3.90	1.38	2.29	5.03	3.58
209	0.53		1,2,4,5-TETRACHLOROBENZENE		95943					
214	1.18	0.90	0.22		1.29	2.00	0.84	1.40	2.63	1.94
216	1.54	1.18	0.28		1.69	2.62	1.09	1.83	3.43	2.52
210	0.43		P-DIBROMOBENZENE		106376					
234	0.68	0.52	0.12		0.77	1.23	0.41	0.67	1.93	1.43
236	1.29	1.00	0.23		1.48	2.36	0.78	1.30	3.77	2.93
711	0.80		4-BROMODIPHENYLETHER		6452499					
246	1.08	0.81	0.20		1.19	1.92	0.77	1.29	2.42	1.78
250	1.13	0.88	0.21		1.26	2.04	0.82	1.37	2.57	1.89
212	0.95		HEXACHLOROBENZENE		118741					
284	0.74	0.56	0.13		0.84	1.34	0.44	0.73	2.10	1.55
286	0.60	0.45	0.11		0.68	1.08	0.36	0.59	1.70	1.26

Internal/External Standard File for Cmpd Class # 5

Cmpds	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
206	1.07		1,2,4-TRICHLOROBENZENE		120821					
145	0.24	0.80	0.33	0.13	0.12		0.03		0.36	
180	0.89	3.05	1.25	0.48	0.46		0.10		1.36	
207	0.01		2-BROMO-1-CHLOROBENZENE			694804				
190	0.57	1.88	0.73	0.28	0.30		0.05		0.84	
192	0.76	2.52	0.98	0.38	0.40		0.07		1.12	
208	0.68		1,2-DICHLORONAPHTHALENE		2050693					
161	0.31	1.02	0.42	0.16	0.15		0.03		0.46	
196	1.52	5.08	2.08	0.80	0.76		0.17		2.27	
209	0.53		1,2,4,5-TETRACHLOROBENZENE			95943				
214	0.86	2.85	1.11	0.43	0.45		0.08		1.27	
216	1.12	3.72	1.44	0.56	0.58		0.11		1.66	
210	0.43		P-DIBROMOBENZENE		106376					
234	0.49	1.66	0.72	0.26	0.19		0.05		0.75	
236	0.93	3.18	1.38	0.53	0.45		0.10		1.45	
211	0.80		4-BROMODIPHENYLETHER			6452499				
248	0.79	2.61	1.01	0.39	0.41		0.07		1.17	
250	0.84	2.78	1.08	0.42	0.44		0.08		1.24	
212	0.95		HEXACHLOROBENZENE		118741					
284	0.53	1.83	0.78	0.30	0.24		0.06		0.82	
286	0.43	1.46	0.63	0.24	0.19		0.05		0.66	

Table B-6. RMRs AND RECOVERIES FOR WABN COMPOUNDS
(BLLE, pH 8.0/FRACTION NO. 3)

Class No. 6	
Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
54	d_8-Naphthalene (internal)
56	d_5-Nitrobenzene (internal)
57	d_{10}-o-Xylene (internal)
58	d_5-Phenylethanol (internal)
59	d_5-Acetophenone (internal)
60	d_5-Propiophenone (internal)
61	d_{12}-Perylene (internal)
62	d_9-Acridine (internal)
63	d_5-Phenol (internal)

MATRIX OF STANDARD ION RATIOS

Compound	Ion	Standard: d_5-Phenol m/z 99	Standard: d_{10}-o-Xylene m/z 98	Standard: d_{10}-o-Xylene m/z 116	Standard: d_8 Naphthalene m/z 136	Standard: d_5 Nitrobenzene m/z 82	Standard: d_5 Nitrobenzene m/z 128	Standard: d_5-Phenylethanol m/z 84	Standard: d_5-Phenylethanol m/z 112
d_5-phenol	99	-	.59(9)	99(9)	17(6)	1 08(5)	1 66(5)	2 46(15)	1 75(15)
d_{10}-o-xylene	98	1 72(9)[a]	-	1 67(1)	23(6)	1 79(8)	2 84(8)	4 21(22)	3 02(23)
	116	1 03(a)	60(0)	-	18(6)	1 07(8)	1 71(8)	2 53(22)	1 81(21)
d_8 naphthalene	136	5 97(4)	3 51(7)	5 85(7)	-	6 21(5)	9 98(5)	14 63(15)	10 59(16)
d_5-nitrobenzene	82	97(4)	57(10)	.95(10)	.16(3)	-	1 60(1)	2 35(17)	1 70(16)
	128	61(2)	35(9)	59(9)	.10(3)	63(1)	-	1 47(16)	1 07(15)
d_5-phenylethanol	84	42(15)	25(24)	42(24)	.071 .71(18)	48(16)	70(15)	-	.93(2)
	112	.58(15)	35(22)	58(23)	098(18)	61(16)	95(16)	1 39(2)	-
d_5-propiophenone	82	1 09(4)	65(13)	1 07(14)	18(8)	1 13(6)	1 82(6)	2 63(13)	1 90(10)
	110	2 85(5)	1 67(13)	2 79(14)	48(17)	2 94(6)	4 72(6)	6 84(12)	4 95(11)
d_5-acetophenone	110	1 52(2)	90(7)	1 50(8)	25(4)	1 60(5)	2 55(1)	3 71(17)	2 68(16)
	125	46(2)	27(8)	45(7)	28(5) .076	48(5)	76(4)	1 11(18)	81(17)
d_{12}-perylene	264	3 56(13)	2 09(7)	3 48(8)	60(9)	3 70(11)	5 90(12)	8 52(25)	6 37(28)
d_5-acridine	188	1 45(7)	84(15)	1 45(15)	24(8)	1 51(6)	2 40(6)	3 52(13)	2 55(13)
4-fluoro 2-iodotoluene	109	1 10(4)	65(7)	1 08(8)	19(3)	1 14(3)	1 82(2)	2 69(18)	1 97(19)
	236	1 45(4)	84(6)	1 33(7)	23(6)	1 46(3)	2 37(3)	3 48(18)	2 52(18)

(continued)

Compound	Ion	Standard: d_5 Propiophenone		d_5 Acetophenone		d_{12} Perylene	d_9 Acridine	4 Fluoro 2 Iodotoluene	
		m/z 82	m/z 110	m/z 110	m/z 125	m/z 264	m/z 189	m/z 109	m/z 236
d_5 phenol	99	92(5)	5.(5)	67(2)	2 28(5)	31(15)	70(*)	91(5)	78(6)
d_{10} p xylene	98	1 59(1.)	6.(13)	1 13(7)	3 7*(7)	55(10)	1 20(13)	1 5(6)	1 28(6)
	106	95(13)	5*(12)	67(6)	2 2*(7)	>.(10)	72(13)	94(4)	75(6)
d_8 naphthalene	136	5 53(8)	2 13(8)	3 91(4)	13 84(3)	1 76(15)	4 20(8)	5 65(8)	4 2*(8)
d_5 nitrobenzene	82	81(6)	56(5)	65(9)	2 12(4)	29(19)	67(6)	88(2)	69(5)
	128	55*6)	22(6)	5.(1)	1 32(5)	19(*0)	62(*)	5.(3)	62(3)
d_5 phenylethanol	84	37(11)	15(10)	28(16)	95(12)	15(28)	29(11)	39(18)	30(17)
	112	9.*10)	21(9)	34(16)	1 28(15)	10(29)	41(15)	5 * 9)	42(16)
d_5 propiophenone	82	-	.3*(1)	21(7)	2 50(6)	33(23)	76(5)	1 00(7)	7*(7)
	110	2 60(1)		1 85(6)	6 21(6)	82(19)	2 09(5)	2 59(7)	1 99(7)
d_5-acetophenone	110	1 41(6)	5.(6)	-	5 39(3)	87(14)	1 10(9)	1 37(6)	1 07(2)
	125	42(6)	16(5)	30(2)	-	18(18)	52(*)	62(2)	.32(3)
d_{12}-perylene	264	5 08.,41	1 27(16)	2 57(12)	7 91(12)	-	2 50(16)	3 21(9)	2 53(9)
d_9-acridine	188	1 33(5)	52(5)	9*(10)	3 15(11)	39(40)	-	1 32(8)	1 03(8)
4 fluoro-2 iodotoluene	109	1 01(7)	39(7)	71(2)	2 40(2)	34(12)	76(8)	-	.7*(1)
	236	1 *.(7)	51(2)	92(5)	3 11(2)	42(16)	1 09(8)	1 30(1)	-

1 (C.V).

Internal/External Standard File for Cmpd Class # 6

Cmpd# / Mass	Recovery Std # 2		Compound Name / Std #54		Std #56		Std #57		Std #58	
	109	236	136	-	82	128	98	116	84	112
100	0.01		PYRIDINE 110861							
52	0.29	0.22	0.05		0.33	0.51	0.19	0.32	0.67	0.48
79	0.44	0.34	0.08		0.51	0.78	0.30	0.50	1.10	0.78
101	0.01		ALPHA-PICOLINE 109068							
66	0.26	0.20	0.05		0.30	0.46	0.16	0.27	0.59	0.42
93	0.66	0.51	0.12		0.76	1.18	0.40	0.66	1.52	1.09
102	0.01		ANILINE 62533							
66	0.23	0.19	0.04		0.28	0.41	0.15	0.24	0.53	0.38
93	0.76	0.54	0.13		0.81	1.25	0.45	0.74	1.62	1.15
103	0.01		LUTIDINE 108485							
106	0.13	0.10	0.02		0.15	0.25	0.08	0.13	0.39	0.28
107	0.22	0.16	0.04		0.24	0.39	0.13	0.21	0.61	0.45
104	0.01		TOLUIDINE(P) 106490							
106	0.85	0.69	0.16		0.97	1.57	0.64	1.07	1.97	1.45
107	0.71	0.56	0.13		0.78	1.27	0.51	0.86	1.58	1.16
105	0.01		INDOLE 120729							
90	0.72	0.54	0.13		0.82	1.30	0.43	0.71	2.04	1.51
117	1.92	1.45	0.34		2.17	3.45	1.14	1.89	5.43	4.02
106	0.01		2,3,6-TRIMETHYLPYRIDINE 1462846							
120	0.66	0.51	0.12		0.76	1.18	0.42	0.69	1.53	1.09
121	0.90	0.69	0.17		1.03	1.61	0.55	0.91	2.08	1.49
107	0.01		2,6-DIMETHYLANILINE 1300738							
106	0.36	0.27	0.06		0.41	0.65	0.21	0.36	1.02	0.75
121	0.57	0.44	0.10		0.66	1.04	0.34	0.57	1.64	1.21
108	0.01		M-CHLOROANILINE 108429							
127	1.09	0.84	0.20		1.26	1.94	0.69	1.15	2.52	1.79
129	0.34	0.26	0.06		0.29	0.60	0.22	0.36	0.78	0.56
109	0.01		QUINOLINE 91225							
129	1.82	1.41	0.34		1.99	3.22	1.30	2.17	4.06	2.98
110	0.01		P-NITROANILINE 100016							
65	0.44	0.35	0.08		0.52	0.83	0.27	0.46	1.30	0.97
138	0.56	0.45	0.11		0.67	1.07	0.35	0.58	1.68	0.22
111	0.01		2,4-DIMETHYLQUINOLINE 1198374							
156	0.41	0.32	0.08		0.47	0.75	0.26	0.43	0.95	0.68
157	2.01	1.54	0.37		2.31	3.59	1.27	2.11	4.64	3.31
113	0.01		NICOTINE 54115							
84	1.17	0.90	0.22		1.35	2.09	0.74	1.23	2.70	1.92
133	0.28	0.21	0.05		0.32	0.49	0.17	0.29	0.63	0.45

Internal/External Standard File for Cmpd Class # 6

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
100	0.01		PYRIDINE 110861							
52	0.20	0.68	0.28	0.11	0.10		0.02		0.30	
79	0.33	1.11	0.42	0.16	0.17		0.04		0.50	
101	0.01		ALPHA-PICOLINE 109068							
66	0.18	0.60	0.25	0.09	0.09		0.02		0.27	
93	0.46	1.54	0.63	0.24	0.23		0.05		0.69	
102	0.01		ANILINE 62533							
66	0.17	0.56	0.22	0.09	0.08		0.02		0.24	
93	0.49	1.64	0.67	0.26	0.24		0.05		0.73	
103	0.01		LUTIDINE 108485							
106	0.10	0.33	0.14	0.05	0.04		0.01		0.15	
107	0.16	0.52	0.23	0.09	0.06		0.02		0.24	
104	0.01		TOLUIDINE(P) 106490							
106	0.65	2.15	0.83	0.32	0.32		0.06		0.96	
107	0.52	1.73	0.67	0.26	0.26		0.05		0.77	
105	0.01		INDOLE 120729							
90	0.51	1.75	0.76	0.29	0.23		0.05		0.79	
117	1.40	4.68	2.02	0.78	0.61		0.15		2.12	
106	0.01		2,3,6-TRIMETHYLPYRIDINE 1462846							
120	0.46	1.54	0.63	0.24	0.23		0.05		0.67	
121	0.62	2.10	0.86	0.33	0.32		0.07		0.94	
107	0.01		2,6-DIMETHYLANILINE 1300738							
106	0.26	0.88	0.38	0.15	0.11		0.03		0.40	
121	0.42	1.41	0.61	0.24	0.18		0.04		0.64	
108	0.01		M-CHLOROANILINE 108429							
127	0.76	2.55	1.05	0.40	0.38		0.08		1.14	
129	0.24	0.79	0.33	0.13	0.12		0.03		0.35	
109	0.01		QUINOLINE 91225							
129	1.33	4.40	1.70	0.66	0.69		0.12		1.96	
110	0.01		P-NITROANILINE 100016							
65	0.34	1.13	0.49	0.19	0.14		0.04		0.51	
138	0.43	1.84	0.62	0.24	0.19		0.05		0.65	
111	0.01		2,4-DIMETHYLQUINOLINE 1198379							
156	0.29	0.96	0.40	0.15	0.15		0.03		0.43	
157	1.46	4.69	1.93	0.74	0.71		0.15		2.09	
113	0.01		NICOTINE 54115							
84	0.82	2.74	1.12	0.43	0.41		0.09		1.22	
133	0.19	0.64	0.26	0.10	0.10		0.02		0.29	

Internal/External Standard File for Cmpd Class # 6

Cmpd#	Recovery Std # 2		Compound Name Std #54	Std #56		Std #57		Std #58	
Mass	109	236	136	82	128	98	116	64	112
114	0.01		CARBAZOLE 86748						
167	3.73	2.88	0.69	4.30	6.66	2.37	3.92	9.36	6.67
115	0.01		2-AMINOBIPHENYL 90415						
168	6.79	5.11	1.20	7.65	12.18	4.61	6.67	19.13	14.17
169	12.72	9.45	2.22	14.15	22.54	7.42	12.30	35.40	26.19
116	0.01		DIPHENYLAMINE 122394						
166	1.48	1.14	0.27	1.71	2.65	0.94	1.56	3.43	2.45
169	2.79	2.15	0.52	3.22	4.99	1.77	2.93	6.45	4.60
117	0.01		DICYCLOHEXYLAMINE 101837						
56	0.33	0.37	0.06	0.39	0.63	0.21	0.35	1.10	0.78
138	0.96	0.76	0.18	1.12	1.80	0.61	1.02	3.15	2.25
118	0.01		TRIBUTYLAMINE 102829						
100	0.42	0.33	0.08	0.49	0.75	0.27	0.44	0.97	0.69
142	1.53	1.18	0.28	1.77	2.74	0.97	1.61	3.52	2.51
119	0.01		CAFFEINE 58082						
109	0.10	0.08	0.02	0.12	0.17	0.06	0.10	0.23	0.16
194	0.19	0.15	0.04	0.22	0.34	0.12	0.20	0.44	0.32
120	0.01		DIBENZYLAMINE 103491						
91	1.62	1.26	0.30	1.78	2.87	1.16	1.94	3.63	2.67
197	0.13	0.11	0.03	0.15	0.24	0.10	0.16	0.30	0.22
121	0.01		N,N-DIMETHYLDODECYLAMINE 112185						
58	4.72	3.68	0.87	5.47	8.83	3.58	5.99	11.09	8.16
59	0.17	0.13	0.03	0.20	0.33	0.13	0.21	0.40	0.29
122	0.01		ATRAZINE 1912249						
200	2.75	2.20	0.52	3.28	5.23	1.72	2.86	8.17	6.09
215	1.67	1.34	0.31	2.00	3.16	1.05	1.74	4.97	3.71
123	0.01		HEPTANONE(2) 110430						
43	1.21	0.94	0.22	1.33	2.14	0.85	1.14	2.32	2.00
58	0.75	0.58	0.14	0.83	1.33	0.53	0.88	1.69	1.25
124	0.01		BUTOXYETHANOL 111762						
41	0.21	0.17	0.04	0.25	0.40	0.13	0.22	0.49	0.35
57	0.55	0.42	0.10	0.63	1.03	0.35	0.58	1.27	0.91
125	0.01		2-OCTANONE 111137						
43	1.30	1.01	0.24	1.43	2.31	0.91	1.53	2.92	2.15
58	1.02	0.79	0.19	1.11	1.80	0.71	1.19	2.27	1.67
126	0.01		BUTYLPROPIONATE 590012						
57	1.48	1.14	0.27	1.71	2.73	0.90	1.49	4.27	3.15
75	0.44	0.34	0.08	0.51	0.82	0.27	0.45	1.28	0.95

Internal/External Standard File for Cmpd Class # 6

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
114	0.01		CARBAZOLE 86748							
167	2.60	8.72	3.57	1.37	1.28		0.31		4.22	
115	0.01		2-AMINOBIPHENYL 90445							
168	4.75	16.46	7.10	2.75	2.13		0.51		7.45	
169	8.82	30.44	13.14	5.08	3.96		0.95		13.60	
116	0.01		DIPHENYLAMINE 122394							
168	1.03	3.47	1.42	0.55	0.52		0.11		1.55	
169	1.94	6.46	2.68	1.03	0.96		0.22		2.91	
117	0.01		DICYCLOHEXYLAMINE 101837							
56	0.25	0.81	0.33	0.14	0.09		0.03		0.38	
138	0.71	2.34	0.95	0.40	0.26		0.08		1.09	
118	0.01		TRIBUTYLAMINE 102829							
100	0.29	0.99	0.41	0.16	0.15		0.03		0.44	
142	0.99	3.34	1.47	0.57	0.53		0.12		1.59	
119	0.01		CAFFEINE 58082							
109	0.07	0.23	0.09	0.04	0.04		0.01		0.10	
194	0.13	0.45	0.18	0.07	0.07		0.02		0.21	
120	0.01		DIBENZYLAMINE 103491							
91	1.18	3.91	1.52	0.59	0.62		0.11		1.74	
197	0.10	0.32	0.13	0.05	0.05		0.01		0.14	
121	0.01		N,N-DIMETHYLDODECYLAMINE 112185							
58	3.62	12.02	4.66	1.81	1.87		0.34		5.37	
59	0.13	0.43	0.17	0.06	0.07		0.01		0.19	
122	0.01		ATRAZINE 1912249							
200	2.13	7.07	3.05	1.18	0.90		0.22		3.26	
215	1.21	4.30	1.85	0.72	0.55		0.13		1.95	
123	0.01		HEPTANONE(2) 110430							
43	0.88	2.91	1.13	0.44	0.47		0.08		1.30	
58	0.55	1.82	0.71	0.27	0.29		0.05		0.81	
124	0.01		BUTOXYETHANOL 111762							
41	0.15	0.49	0.20	0.09	0.07		0.02		0.22	
57	0.38	1.28	0.52	0.20	0.19		0.04		0.57	
125	0.01		2-OCTANONE 111137							
43	0.95	3.14	1.22	0.47	0.51		0.09		1.40	
58	0.74	2.45	0.95	0.37	0.39		0.07		1.09	
126	0.01		BUTYLPROPIONATE 590012							
57	1.11	3.69	1.59	0.61	0.48		0.12		1.66	
75	0.33	1.11	0.48	0.19	0.15		0.04		0.50	

Internal/External Standard File for Cmpd Class # 6

Cmpd#	Recovery Std # 2		Compound Name Std #54	Std #56		Std #57		Std #58	
Mass	109	236	136 -	82	128	98	116	84	112
127	0.01		ISOPHORONE 78591						
82	1.77	1.36	0.33	2.04	3.17	1.13	1.86	4.11	2.93
138	0.39	0.30	0.07	0.45	0.72	0.25	0.41	0.90	0.64
128	0.01		FENCHONE 1195759						
69	0.66	0.51	0.12	0.72	1.17	0.47	0.76	1.47	1.08
81	1.44	1.12	0.27	1.58	2.55	1.02	1.71	3.22	2.36
129	0.01		ALPHA-TERPINEOL 98555						
59	0.56	0.43	0.10	0.65	1.00	0.36	0.59	1.31	0.93
136	0.32	0.25	0.06	0.37	0.58	0.21	0.34	0.75	0.53
130	0.01		N-DECANOL 112301						
41	0.40	0.31	0.07	0.46	0.74	0.25	0.42	0.92	0.66
43	0.44	0.34	0.08	0.51	0.79	0.28	0.46	1.02	0.73
131	0.01		DIMETHYLADIPATE 627930						
59	0.56	0.45	0.10	0.64	1.03	0.41	0.69	1.29	0.95
114	0.41	0.35	0.08	0.49	0.79	0.32	0.54	1.00	0.74
132	0.01		METHYLSTEARATE 112618						
74	3.42	2.65	0.63	3.89	6.28	2.54	4.25	7.90	5.81
87	2.22	1.72	0.41	2.52	4.07	1.65	2.76	5.13	3.77
133	0.01		N-DECANE 124185						
43	1.47	1.11	0.26	1.67	2.65	0.88	1.46	4.18	3.09
57	1.42	1.08	0.25	1.64	2.61	0.85	1.41	4.05	3.00
134	0.01		N-TRIDECANE 629505						
43	2.18	1.64	0.34	2.48	3.95	1.30	2.16	6.20	4.58
57	2.75	2.09	0.50	3.14	5.01	1.66	2.77	7.93	5.86
135	0.01		N-TETRADECANE 629594						
43	2.52	1.92	0.45	2.88	4.58	1.51	2.51	7.19	5.31
57	3.40	2.55	0.61	3.87	6.15	2.03	3.37	9.67	7.15
136	0.01		N-PENTADECANE 692629						
57	2.78	2.14	0.52	3.22	4.99	1.77	2.94	6.47	4.62
71	1.73	1.33	0.32	2.01	3.11	1.10	1.83	4.03	2.87
137	0.01		N-HEXADECANE 544763						
43	1.90	1.45	0.34	2.16	3.45	1.13	1.89	5.41	3.99
57	2.72	2.08	0.49	3.11	4.96	1.63	2.71	7.78	5.74
138	0.01		N-HEPTADECANE 629787						
57	3.13	2.41	0.58	3.61	5.59	1.99	3.30	7.25	5.17
71	2.07	1.60	0.38	2.39	3.70	1.32	2.18	4.80	3.42
139	0.01		N-OCTADECANE 593453						
57	2.99	2.51	0.59	3.75	5.98	1.88	3.14	8.96	6.63
71	1.98	1.66	0.39	2.48	3.95	1.25	2.08	5.95	4.41

Internal/External Standard File for Cmpd Class # 6

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
127	0.01		ISOPHORONE 78591							
82	1.23	4.14	1.70	0.65	0.62		0.14		1.80	
138	0.27	0.91	0.37	0.14	0.14		0.03		0.41	
128	0.01		FENCHONE 1195759							
69	0.48	1.58	0.62	0.24	0.25		0.05		0.71	
81	1.05	3.45	1.35	0.52	0.55		0.10		1.55	
129	0.01		ALPHA-TERPINEOL 98555							
59	0.39	1.31	0.54	0.21	0.20		0.04		0.58	
136	0.23	0.76	0.31	0.12	0.11		0.03		0.34	
130	0.01		N-DECANOL 112301							
41	0.28	0.93	0.38	0.15	0.14		0.03		0.41	
43	0.31	1.63	0.42	0.16	0.15		0.03		0.46	
131	0.01		DIMETHYLADIPATE 627930							
59	0.42	1.40	0.54	0.21	0.22		0.04		0.62	
114	0.33	1.08	0.42	0.16	0.17		0.03		0.48	
132	0.01		METHYLSTEARATE 112618							
74	2.58	8.56	3.32	1.29	1.33		0.24		3.83	
87	1.67	5.55	2.15	0.83	0.87		0.16		2.48	
133	0.01		N-DECANE 124185							
43	1.05	3.59	1.55	0.60	0.47		0.11		1.62	
57	1.01	3.48	1.50	0.58	0.46		0.11		1.56	
134	0.01		N-TRIDECANE 629505							
43	1.56	5.33	2.30	0.89	0.70		0.17		2.41	
57	1.99	6.75	2.94	1.14	0.76		0.21		3.09	
135	0.01		N-TETRADECANE 629594							
43	1.86	6.19	2.67	1.03	0.80		0.19		2.80	
57	2.50	8.33	3.57	1.39	1.08		0.26		3.77	
136	0.01		N-PENTADECANE 692629							
57	1.94	6.52	2.68	1.03	0.99		0.22		2.92	
71	1.21	4.06	1.67	0.64	0.62		0.14		1.82	
137	0.01		N-HEXADECANE 544763							
43	1.40	4.66	2.01	0.78	0.61		0.15		2.11	
57	2.01	6.70	2.88	1.12	0.87		0.21		3.03	
138	0.01		N-HEPTADECANE 629787							
57	2.18	7.32	3.01	1.16	1.11		0.24		3.27	
71	1.44	4.85	1.99	0.77	0.73		0.16		2.17	
139	0.01		N-OCTADECANE 593453							
57	2.33	8.10	3.48	1.35	1.01		0.24		3.65	
71	1.55	5.35	2.30	0.89	0.58		0.06		2.41	

Internal/External Standard File for Cmpd Class # 6

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
140	0.01		N-NONADECANE		629925					
71	2.12	1.61	0.38		2.42	3.85	1.27	2.11	6.04	4.47
85	1.42	1.08	0.25		1.61	2.57	0.85	1.41	4.03	2.98
141	0.01		N-EICOSANE		1112958					
57	4.43	3.41	0.82		5.11	7.92	2.82	4.64	10.26	7.32
71	3.03	2.33	0.56		3.50	5.43	1.93	3.19	7.03	5.01
142	0.01		N-HENEICOSANE		629947					
57	3.93	2.96	0.70		4.43	7.05	2.32	3.86	11.05	8.20
71	2.71	2.05	0.48		3.07	4.88	1.61	2.67	7.65	5.68
143	0.01		N-DOCOSANE		629970					
57	3.73	2.98	0.70		4.46	7.10	2.33	3.88	11.11	8.26
71	2.60	2.08	0.49		3.11	4.96	1.63	2.70	7.76	5.77
144	0.01		N-TRICOSANE		638675					
57	3.99	3.19	0.75		4.77	7.60	2.49	4.14	11.85	8.83
71	2.80	2.24	0.53		3.35	5.34	1.75	2.91	8.33	6.20
145	0.01		PHENYLACETATE		122792					
94	1.84	1.43	0.34		2.01	3.25	1.30	2.18	4.10	3.01
136	0.25	0.20	0.05		0.28	0.45	0.18	0.30	0.57	0.42
146	0.01		BENZYLACETATE		140114					
91	0.52	0.40	0.09		0.57	0.92	0.37	0.62	1.15	0.85
108	1.09	0.85	0.20		1.19	1.92	0.77	1.29	2.43	1.79
147	0.01		METHYLBENZENESULFONATE							
77	1.24	0.94	0.22		1.41	2.25	0.74	1.23	3.54	2.61
172	0.44	0.34	0.08		0.50	0.80	0.26	0.44	1.26	0.93
148	0.01		METHYLTOLUENESULFONATE(P)							
91	1.60	1.21	0.29		1.81	2.89	0.95	1.58	4.53	3.35
155	0.72	0.54	0.13		0.81	1.29	0.42	0.71	2.02	1.50
149	0.01		DIMETHYLPHTHALATE		131113					
77	0.61	0.63	0.15		0.94	1.45	0.52	0.85	1.88	1.34
163	5.29	4.07	0.98		6.10	9.46	3.36	5.56	12.22	8.71
150	0.01		ETHYLTOLUENESULFONATE(P)		80400					
91	1.74	1.32	0.31		1.97	3.14	1.03	1.72	4.92	3.65
155	1.18	0.94	0.22		1.40	2.23	0.73	1.21	3.46	2.35
151	0.01		DIETHYLPHTHALATE		84662					
149	3.19	2.43	0.57		3.65	5.79	1.90	3.17	9.08	6.71
177	0.80	0.61	0.14		0.93	1.47	0.48	0.80	2.29	1.69
152	0.01		DIBUTYLPHTHALATE		84742					
57	0.29	0.23	0.05		0.34	0.52	0.19	0.31	0.68	0.48
149	7.17	5.52	1.33		8.27	12.80	4.55	7.54	16.55	11.80

Internal/External Standard File for Cmpd Class # 6

Cmpds	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
140	0.01		N-NONADECANE 629925							
71	1.51	5.27	2.24	0.87	0.68		0.16		2.35	
85	1.01	3.47	1.50	0.58	0.45		0.11		1.57	
141	0.01		N-EICOSANE 1112958							
57	3.08	10.35	4.25	1.63	1.57		0.35		4.63	
71	2.11	7.09	2.91	1.12	1.07		0.23		3.17	
142	0.01		N-HENEICOSANE 629947							
57	2.73	9.53	4.11	1.60	1.07		0.30		4.31	
71	1.89	6.60	2.85	1.10	0.74		0.21		2.99	
143	0.01		N-DOCOSANE 629970							
57	2.89	9.60	4.14	1.60	1.22		0.30		4.35	
71	2.02	6.71	2.89	1.12	0.85		0.21		3.04	
144	0.01		N-TRICOSANE 638675							
57	3.10	10.28	4.42	1.71	1.29		0.32		4.65	
71	2.18	7.22	3.11	1.20	0.90		0.22		3.27	
145	0.01		PHENYLACETATE 122792							
94	1.31	4.43	1.72	0.67	0.70		0.13		1.98	
136	0.18	0.62	0.24	0.09	0.10		0.02		0.28	
146	0.01		BENZYLACETATE 140114							
91	0.38	1.25	0.48	0.19	0.20		0.04		0.56	
108	0.79	2.63	1.02	0.40	0.41		0.07		1.17	
147	0.01		METHYLBENZENESULFONATE							
77	0.91	3.04	1.31	0.51	0.40		0.09		1.38	
172	0.32	1.09	0.47	0.18	0.14		0.03		0.49	
148	0.01		METHYLTOLUENESULFONATE(P)							
91	1.17	3.90	1.68	0.65	0.51		0.12		1.76	
155	0.52	1.74	0.75	0.29	0.23		0.05		0.79	
149	0.01		DIMETHYLPHTHALATE 131113							
77	0.57	1.83	0.75	0.29	0.28		0.06		0.85	
163	3.68	11.87	4.88	1.88	1.85		0.41		5.51	
150	0.01		ETHYLTOLUENESULFONATE(P) 80400							
91	1.28	4.25	1.83	0.71	0.55		0.13		1.92	
155	0.91	3.01	1.30	0.50	0.38		0.09		1.36	
151	0.01		DIETHYLPHTHALATE 84662							
149	2.35	7.82	3.34	1.30	1.02		0.24		3.54	
177	0.59	1.97	0.85	0.33	0.26		0.06		0.89	
152	0.01		DIBUTYLPHTHALATE 84742							
57	0.20	0.68	0.28	0.11	0.10		0.02		0.31	
149	4.99	16.75	6.88	2.64	2.52		0.55		7.47	

Internal/External Standard File for Cmpd Class # 6

Code	Recovery		Compound Name							
	Std # 2			Std #54		Std #56		Std #57		Std #58
Mass	109	236	136	-	82	128	98	116	84	112
153	0.01		BUTYLBENZYLPHTHALATE							
91	2.09	1.62	0.38		2.28	3.69	1.48	2.48	4.64	3.41
149	3.37	2.62	0.62		3.69	5.95	2.40	4.01	7.49	5.51
154	0.01		DIETHYLHEXYLPHTHALATE 117817							
149	5.22	4.07	0.96		5.71	9.23	3.74	6.26	11.59	8.53
167	1.98	1.54	0.37		2.17	3.51	1.42	2.37	4.40	3.24
155	0.01		BENZALDEHYDE	100527						
77	0.36	0.28	0.07		0.42	0.64	0.23	0.38	0.84	0.60
105	0.40	0.31	0.07		0.46	0.73	0.25	0.42	0.92	0.66
156	0.01		TOLUALDEHYDE(P)	524204						
91	0.51	0.44	0.10		0.62	1.04	0.34	0.57	1.65	1.21
119	0.63	0.51	0.12		0.77	1.21	0.41	0.68	1.95	1.43
157	0.01		ACETOPHENONE	98862						
77	0.38	0.64	0.15		0.96	1.53	0.53	0.87	1.93	1.37
105	1.22	0.94	0.23		1.41	2.25	0.78	1.29	2.85	2.03
158	0.01		SALICYLALDEHYDE	90028						
121	0.56	0.44	0.10		0.61	0.99	0.40	0.67	1.24	0.91
122	0.60	0.47	0.11		0.66	1.07	0.43	0.72	1.34	0.99
159	0.01		ANISALDEHYDE	123113						
135	1.37	1.01	0.25		1.53	2.47	0.91	1.66	3.11	2.29
136	0.96	0.76	0.18		1.07	1.73	0.70	1.16	2.18	1.60
160	0.01		PHENOL 108952							
94	1.07	0.84	0.20		1.18	1.90	0.76	1.27	2.41	1.77
161	0.01		CRESOL(P) 106445							
107	1.21	0.93	0.23		1.40	2.25	0.80	1.29	2.91	2.38
108	1.07	0.82	0.20		1.24	1.99	0.69	1.14	2.58	1.84
162	0.01		2,3-DIMETHYLPHENOL	526750						
107	0.87	0.67	0.16		1.00	1.61	0.57	0.95	2.08	1.48
122	0.91	0.70	0.17		1.05	1.68	0.59	0.96	2.12	1.51
163	0.01		ISOPROPYLPHENOL	88699						
121	1.79	1.36	0.32		2.04	3.25	1.07	1.78	5.10	3.77
136	0.07	0.56	0.12		0.75	1.19	0.39	0.65	1.87	1.38
164	0.01		O-NITROPHENOL	88755						
65	0.03	0.02	0.00		0.03	0.05	0.02	0.03	0.06	0.05
139	0.13	0.10	0.02		0.14	0.23	0.09	0.15	0.29	0.21
165	0.01		4-CHLORO-3-METHYLPHENOL	59507						
107	0.93	0.71	0.17		1.06	1.69	0.55	0.92	2.64	2.05
142	1.02	0.77	0.18		1.16	1.84	0.61	1.01	2.89	2.14

Internal/External Standard File for Cmpd Class # 6

Cmpd#	Recovery Std #59		Compound Name	Std #60		Std #61		Std #62		Std #63	
Mass	110	125		82	110	264	-	188	-	99	-
154	0.01		BUTYLBENZYLPHTHALATE								
91	1.51	5.02		1.95	0.76	0.78		0.14		2.24	
149	2.44	8.13		3.15	1.22	1.26		0.23		3.62	
154	0.01		DIETHYLHEXYLPHTHALATE 117817								
149	4.03	12.56		4.86	1.89	1.90		0.35		5.61	
167	1.53	4.78		1.85	0.72	0.72		0.13		2.13	
155	0.01		BENZALDEHYDE 100527								
77	0.25	0.84		0.35	0.13	0.13		0.03		0.38	
105	0.28	0.93		0.38	0.15	0.14		0.03		0.42	
156	0.01		TOLUALDEHYDE(P) 529204								
91	0.42	1.41		0.61	0.24	0.15		0.05		0.64	
119	0.50	1.66		0.72	0.28	0.22		0.05		0.75	
157	0.01		ACETOPHENONE 98862								
77	0.57	1.95		0.80	0.31	0.29		0.06		0.87	
105	0.85	2.88		1.18	0.45	0.43		0.09		1.28	
158	0.01		SALICYLALDEHYDE 90028								
121	0.41	1.35		0.52	0.20	0.21		0.04		0.60	
122	0.44	1.46		0.56	0.22	0.23		0.04		0.65	
159	0.01		ANISALDEHYDE 123115								
135	1.01	3.36		1.30	0.51	0.53		0.09		1.50	
136	0.71	2.36		0.91	0.35	0.37		0.07		1.05	
160	0.01		PHENOL 108952								
94	0.75	2.60		1.01	0.39	0.41		0.07		1.15	
161	0.01		CRESOL(P) 106445								
107	0.89	2.85		1.17	0.45	0.44		0.10		1.31	
108	0.78	2.52		1.03	0.40	0.39		0.09		1.16	
162	0.01		2,3-DIMETHYLPHENOL 526750								
107	0.63	2.11		0.84	0.32	0.32		0.07		0.94	
122	0.64	2.11		0.85	0.33	0.32		0.07		0.95	
163	0.01		ISOPROPYLPHENOL 88699								
121	1.28	4.39		1.90	0.73	0.58		0.14		1.99	
136	0.47	1.61		0.69	0.27	0.21		0.05		0.73	
164	0.01		O-NITROPHENOL 88755								
65	0.02	0.07		0.03	0.01	0.01		0.00		0.03	
139	0.09	0.31		0.12	0.05	0.05		0.01		0.14	
165	0.01		4-CHLORO-3-METHYLPHENOL 59507								
107	0.66	2.27		0.98	0.38	0.30		0.07		1.03	
142	0.72	2.49		1.07	0.42	0.32		0.08		1.13	

Internal/External Standard File for Cmpd Class # 6

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
166	0.01		4-CHLOROCRESOL							
107	0.83	0.64	0.16		0.97	1.57	0.53	0.88	2.03	1.45
142	0.94	0.72	0.17		1.09	1.77	0.60	0.99	2.29	1.63
167	0.01		1-NAPHTHOL		90153					
115	0.35	0.26	0.06		0.38	0.61	0.20	0.34	0.96	0.72
144	0.61	0.45	0.11		0.67	1.07	0.35	0.29	1.68	1.25
168	0.01		P-TERT-BUTYLPHENOL		98544					
107	0.56	0.43	0.10		0.65	1.03	0.34	0.56	1.60	1.18
135	1.96	1.49	0.35		2.22	3.54	1.17	1.94	5.56	4.11
169	0.01		2-NITROCRESOL		119335					
77	0.26	0.20	0.05		0.30	0.46	0.07	0.27	0.60	0.43
153	0.74	0.57	0.14		0.83	1.33	0.46	0.78	1.72	1.23
170	0.01		2,4-DICHLOROPHENOL		120832					
162	1.13	0.88	0.21		1.24	2.00	0.80	1.34	2.52	1.86
164	0.72	0.53	0.13		0.78	1.27	0.51	0.85	1.60	1.18
171	0.01		2,4,6-TRICHLOROPHENOL		88062					
196	0.81	0.63	0.15		0.89	1.44	0.58	0.97	1.88	1.34
198	0.83	0.64	0.15		0.91	1.45	0.59	0.98	1.90	1.36
172	0.01		DI-TERT-BUTYL-4-METHYLPHENOL				128370			
205	2.53	1.97	0.47		2.78	4.49	1.81	3.03	5.66	4.16
220	0.67	0.52	0.12		0.73	1.18	0.48	0.80	1.49	1.09
173	0.01		PENTACHLOROPHENOL		87865					
264	0.29	0.22	0.05		0.34	0.54	0.19	0.31	0.72	0.52
266	0.47	0.36	0.09		0.55	0.91	0.32	0.54	1.17	0.84
174	0.01		2-METHYLNAPHTHALENE		83329					
141	2.03	1.58	0.38		2.23	3.60	1.44	2.42	4.53	3.34
142	2.51	1.96	0.46		2.76	4.45	1.79	2.99	5.62	4.13
175	0.01		ACENAPHTHENE		83329					
153	1.26	0.98	0.23		1.38	2.22	0.89	1.49	2.81	2.06
154	3.40	2.64	0.63		3.73	6.02	2.41	4.04	7.59	5.58
176	0.01		BIPHENYL	92524						
154	2.28	1.78	0.42		2.51	4.04	1.63	2.72	5.10	3.75
177	0.01		1,8-DIMETHYLNAPHTHALENE			569415				
141	1.59	1.24	0.29		1.74	2.82	1.13	1.89	3.55	2.61
156	2.30	1.79	0.42		2.52	4.07	1.63	2.73	5.13	3.77
178	0.01		FLUORENE	86737						
165	2.74	2.13	0.49		3.01	4.85	1.95	3.27	6.12	4.50
166	3.07	2.38	0.57		3.44	5.55	2.23	3.74	6.99	5.14

Internal/External Standard File for Cmpd Class # 6

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
166	0.01		4-CHLOROCRESOL							
107	0.58	1.96	0.80	0.31	0.31		0.07		0.91	
142	0.66	2.20	0.85	0.34	0.35		0.08		1.03	
167	0.01		1-NAPHTHOL		90153					
115	0.25	0.83	0.36	0.14	0.11		0.03		0.38	
144	0.44	1.45	0.62	0.24	0.18		0.05		0.66	
168	0.01		P-TERT-BUTYLPHENOL		98544					
107	0.40	1.38	0.66	0.23	0.18		0.04		0.62	
135	1.44	4.79	2.04	0.80	0.63		0.15		2.16	
169	0.01		2-NITROCRESOL		119335					
77	0.18	0.61	0.25	0.10	0.09		0.02		0.27	
153	0.52	1.74	0.71	0.27	0.26		0.06		0.78	
170	0.01		2,4-DICHLOROPHENOL		120832					
162	0.80	2.73	1.05	0.41	0.43		0.08		1.22	
164	0.51	1.70	0.67	0.26	0.27		0.05		0.77	
171	0.01		2,4,6-TRICHLOROPHENOL		88062					
196	0.58	1.97	0.76	0.30	0.31		0.05		0.88	
198	0.58	1.99	0.77	0.30	0.32		0.06		0.89	
172	0.01		DI-TERT-BUTYL-4-METHYLPHENOL				128370			
205	1.85	6.13	2.37	0.92	0.96		0.17		2.73	
220	0.49	1.61	0.62	0.24	0.25		0.05		0.72	
173	0.01		PENTACHLOROPHENOL		87865					
264	0.20	0.68	0.28	0.11	0.11		0.02		0.31	
266	0.36	1.11	0.45	0.07	0.18		0.04		0.50	
174	0.01		2-METHYLNAPHTHALENE		83329					
141	1.48	4.91	1.90	0.74	0.77		0.14		2.19	
142	1.78	6.08	2.36	0.91	0.95		0.17		2.71	
175	0.01		ACENAPHTHENE		83329					
153	0.92	3.04	1.18	0.46	0.47		0.09		1.35	
154	2.48	8.22	3.19	1.23	1.28		0.23		3.66	
176	0.01		BIPHENYL		92524					
154	1.67	5.52	2.14	0.83	0.87		0.16		2.46	
177	0.01		1,8-DIMETHYLNAPHTHALENE				569415			
141	1.16	3.84	1.49	0.58	0.60		0.11		1.71	
156	1.67	5.55	2.15	0.83	0.87		0.16		2.48	
178	0.01		FLUORENE		86737					
165	2.00	6.62	2.57	0.99	1.04		0.19		2.95	
166	2.28	7.57	2.93	1.14	1.19		0.21		3.36	

Internal/External Standard File for Cmpd Class # 6

Cmpd#	Recovery Std # 2		Compound Name Std #54	Std #56		Std #57		Std #58	
Mass	109	236	136 -	82	128	98	116	84	112
179	0.01		2,3,5-TRIMETHYLNAPHTHALENE 2245387						
155	1.86	1.44	0.34	2.08	3.36	1.36	2.27	4.24	3.12
170	2.56	1.99	0.47	2.86	4.62	1.86	3.11	5.83	4.29
180	0.01		ANTHRACENE 120127						
178	3.21	2.47	0.60	3.71	5.74	2.04	3.38	7.43	5.30
181	0.01		PYRENE 129000						
202	4.88	3.75	0.95	5.66	8.73	3.27	5.18	11.54	8.23
182	0.01		9,10-DIMETHYLANTHRACENE 781431						
191	1.33	1.03	0.25	1.45	2.35	0.94	1.57	2.96	2.18
206	2.85	2.22	0.53	3.13	5.04	2.01	3.37	6.36	4.68
183	0.01		CHRYSENE 218019						
228	2.21	1.73	0.41	2.42	3.92	1.59	2.66	4.91	3.61
184	0.01		PERYLENE 198550						
252	1.60	1.23	0.30	1.64	2.86	1.02	1.68	3.67	2.62
185	0.01		DICYANOBUTANE 111693						
41	0.66	0.51	0.12	0.72	1.17	0.47	0.79	1.47	1.08
54	0.29	0.23	0.05	0.32	0.52	2.10	0.35	0.66	0.48
186	0.01		BUTYLCARBAMATE 14994775						
41	0.48	0.36	0.08	0.54	0.86	0.28	0.47	1.35	1.00
59	0.24	0.26	0.05	0.29	0.47	0.15	0.25	0.72	0.54
187	0.01		DIBUTYLDISULFIDE 110065						
41	0.73	0.56	0.13	0.84	1.34	0.44	0.73	2.10	1.55
57	3.09	2.36	0.56	3.54	5.64	1.85	3.09	8.84	6.54
188	0.01		BIS(2-CHLOROETHYL)ETHANE 112265						
63	1.71	1.31	0.31	1.97	3.13	1.03	1.71	4.91	3.63
93	0.84	0.65	0.15	0.97	1.54	0.51	0.84	2.42	1.78
189	0.01		TRIBUTYLPHOSPHATE 126738						
99	4.03	3.10	0.75	4.65	7.20	2.56	4.24	9.28	6.62
155	0.88	0.68	0.16	1.01	1.57	0.56	0.92	2.02	1.44
190	0.01		ALDRIN 309002						
66	1.33	1.03	0.24	1.49	2.40	0.97	1.62	3.03	2.23
263	0.60	0.46	0.11	0.67	1.08	0.44	0.73	1.36	1.00
191	0.01		DIHYDROBENZOFURAN 496162						
91	0.68	0.52	0.13	0.79	1.25	0.43	0.72	1.58	1.13
120	0.97	0.75	0.18	1.12	1.67	0.66	0.78	2.16	1.54
192	0.01		NITROBENZENE 98953						
77	0.86	0.67	0.16	0.94	1.51	0.61	1.02	1.91	1.40
123	0.54	0.42	0.10	0.59	0.95	0.38	0.64	1.20	0.88

Internal/External Standard File for Cmpd Class # 6

Cmpd# / Mass	Recovery Std #59		Compound Name / Std #60		Std #61		Std #62		Std #63	
	110	125	82	110	264	-	188	-	99	-
179	0.01		2,3,5-TRIMETHYLNAPHTHALENE		2245387					
155	1.38	4.59	1.78	0.69	0.72		0.13		2.05	
170	1.90	6.31	2.44	0.95	0.99		0.18		2.81	
180	0.01		ANTHRACENE		120127					
178	2.24	7.59	3.08	1.19	1.13		0.25		3.35	
181	0.01		PYRENE		129000					
202	3.59	11.47	4.95	1.90	1.80		0.40		5.36	
182	0.01		9,10-DIMETHYLANTHRACENE		781431					
191	0.96	3.19	1.24	0.48	0.50		0.09		1.42	
206	2.06	6.86	2.67	1.03	1.08		0.19		3.06	
183	0.01		CHRYSENE		218019					
228	1.61	5.34	2.07	0.80	0.81		0.15		2.39	
184	0.01		PERYLENE		198550					
252	1.11	3.72	1.53	0.59	0.47		0.12		1.65	
185	0.01		DICYANOBUTANE		111693					
41	0.48	1.59	0.62	0.24	0.25		0.05		0.71	
54	0.22	0.71	0.29	0.11	0.11		0.02		0.32	
186	0.01		BUTYLCARBAMATE		14994775					
41	0.35	1.16	0.50	0.09	0.15		0.04		0.52	
59	0.19	0.63	0.27	0.11	0.08		0.02		0.28	
187	0.01		DIBUTYLDISULFIDE		110065					
41	0.54	1.78	0.78	0.31	0.20		0.06		0.82	
57	2.21	7.62	3.29	1.27	1.00		0.24		3.42	
188	0.01		BIS(2-CHLOROETHYL)ETHANE		112265					
63	1.27	4.23	1.83	0.71	0.56		0.13		1.91	
93	0.61	2.08	0.90	0.35	0.27		0.06		0.94	
189	0.01		TRIBUTYLPHOSPHATE		126738					
99	2.81	9.43	3.87	1.49	1.41		0.31		4.19	
155	0.61	2.05	0.84	0.32	0.31		0.07		0.91	
190	0.01		ALDRIN		309002					
66	0.99	3.28	1.27	0.49	0.51		0.09		1.46	
263	0.44	1.47	0.57	0.22	0.23		0.04		0.66	
191	0.01		DIHYDROBENZOFURAN		496162					
91	0.27	1.59	0.65	0.25	0.24		0.05		0.71	
120	0.68	2.27	0.90	0.35	0.33		0.07		0.98	
192	0.01		NITROBENZENE		98953					
77	0.61	2.07	0.80	0.31	0.33		0.06		0.94	
123	0.38	1.30	0.50	0.20	0.21		0.04		0.59	

Internal/External Standard File for Cmpd Class # 6

Cmpds	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
193	0.01		BENZOTHIAZOLE		95169					
135	1.56	1.21	0.29		1.71	2.76	1.11	1.86	3.47	2.55
194	0.01		PHENYLCARBAMATE		102090					
94	1.25	0.96	0.23		1.44	2.23	0.79	1.31	2.88	2.06
137	0.02	0.01	0.00		0.02	0.03	0.01	0.02	0.04	0.03
195	0.01		2,4-DINITROTOLUENE		121142					
89	0.35	0.28	0.06		0.40	0.65	0.26	0.44	0.81	0.60
165	0.71	0.53	0.13		0.75	1.21	0.46	0.76	1.53	1.13
196	0.01		BENZYLSULFIDE		538749					
91	3.55	2.68	0.63		4.00	6.38	2.10	3.49	9.99	7.42
123	0.90	0.68	0.16		1.02	1.62	0.53	0.89	2.54	1.88
197	0.01		DIPHENYLSULFONE		127639					
125	3.82	3.44	0.61		5.16	8.21	2.71	4.51	12.95	8.65
218	0.92	0.73	0.17		1.10	1.75	0.58	0.96	2.74	2.03
198	0.01		TRIPHENYLPHOSPHATE		115866					
325	2.59	2.01	0.13		0.79	1.28	0.52	0.87	1.61	1.18
326	0.09	0.07	0.17		1.03	1.67	0.68	1.14	2.09	1.54
199	0.01		DIPHENYLMERCURY		587859					
77	0.72	0.56	0.48		2.85	4.59	1.96	3.28	6.08	4.47
356	0.95	0.74	0.02		0.09	0.15	0.06	0.11	0.20	0.15
200	0.01		TETRAPHENYLTIN							
197	1.40	1.13	0.27		1.70	2.71	0.89	1.47	4.21	3.13
351	1.30	1.05	0.25		1.58	2.51	0.82	1.37	3.91	2.91
201	0.01		BENZYLCHLORIDE		100447					
91	1.55	1.18	0.28		1.77	2.82	0.93	1.54	4.42	3.28
126	0.42	0.32	0.08		0.48	0.76	0.25	0.42	1.20	0.89
202	0.01		4-CHLOROBENZONITRILE		623030					
102	0.55	0.42	0.10		0.63	0.99	0.33	0.55	1.57	1.16
137	2.10	1.57	0.36		2.38	3.79	1.25	2.08	5.95	4.40
203	0.01		3-CHLOROBENZALDEHYDE		587042					
111	0.06	0.05	0.01		0.08	0.12	0.04	0.07	0.20	0.14
139	0.12	0.10	0.02		0.15	0.24	0.08	0.13	0.38	0.28
204	0.01		O-CHLOROANISOLE		766518					
127	0.60	0.46	0.11		0.69	1.09	0.36	0.60	1.71	1.27
142	1.32	1.00	0.24		0.50	2.40	0.79	1.31	3.76	2.78
205	0.01		CHLOROBENZAMIDE		619567					
139	0.70	0.55	0.13		0.77	1.25	0.50	0.84	1.57	1.16
155	0.38	0.30	0.07		0.42	0.68	0.27	0.46	0.85	0.63

Internal/External Standard File for Cmpd Class # 6

Cmpd#	Recovery		Compound Name								
	Std #59		Std #60		Std #61		Std #62		Std #63		
Mass	110	125	82	110	264	-	188	-	99	-	
193	0.01		BENZOTHIAZOLE		95169						
135	1.14	3.76	1.46	0.57	0.59		0.11		1.68		
194	0.01		PHENYLCARBAMATE		102090						
94	0.87	2.92	1.20	0.46	0.44		0.10		1.30		
137	0.01	0.04	0.01	0.01	0.00		0.00		0.02		
195	0.01		2,4-DINITROTOLUENE		121142						
69	0.27	0.88	0.34	0.13	0.14		0.03		0.39		
165	0.50	1.66	0.64	0.25	0.26		0.05		0.74		
196	0.01		BENZYLSULFIDE		538749						
91	2.47	8.62	3.72	1.44	1.11		0.27		3.90		
123	0.63	2.19	0.94	0.37	0.28		0.07		0.99		
197	0.01		DIPHENYLSULFONE		127639						
125	3.00	11.09	4.77	1.85	1.22		0.35		5.05		
218	0.67	2.36	1.02	0.29	0.30		0.07		1.07		
198	0.01		TRIPHENYLPHOSPHATE		115866						
325	1.98	6.58	2.55	0.95	1.03		0.18		0.78		
326	0.06	0.22	0.08	0.03	0.03		0.01		1.02		
199	0.01		DIPHENYLMERCURY		587859						
77	0.53	1.75	0.68	0.26	0.26		0.05		2.94		
356	0.69	2.28	0.88	0.34	0.35		0.06		0.10		
200	0.01		TETRAPHENYLTIN								
197	1.10	3.66	1.57	0.61	0.44		0.11		1.56		
351	1.03	3.40	1.46	0.57	0.41		0.11		1.54		
201	0.01		BENZYLCHLORIDE		100447						
91	1.10	3.81	1.64	0.64	0.50		0.12		1.71		
126	0.30	1.03	0.45	0.17	0.12		0.03		0.47		
202	0.01		4-CHLOROBENZONITRILE		623030						
102	0.39	1.35	0.58	0.23	0.18		0.04		0.61		
137	1.49	5.12	2.21	0.85	0.67		0.16		2.32		
203	0.01		3-CHLOROBENZALDEHYDE		587042						
111	0.05	0.17	0.07	0.03	0.02		0.00		0.06		
139	0.10	0.32	0.14	0.05	0.04		0.01		0.15		
204	0.01		O-CHLOROANISOLE		766518						
127	0.43	1.48	0.64	0.25	0.17		0.05		0.67		
142	0.94	3.24	1.40	0.54	0.36		0.10		1.46		
205	0.01		CHLOROBENZAMIDE		619567						
139	0.51	1.70	0.66	0.26	0.27		0.05		0.76		
155	0.28	0.92	0.36	0.14	0.15		0.03		0.41		

Internal/External Standard File for Cmpd Class # 6

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
206	0.01		3,4-DICHLOROBENZALDEHYDE 6287383							
173	0.48	0.39	0.09		0.58	0.93	0.31	0.57	1.46	1.07
174	0.32	0.26	0.06		0.39	0.62	0.21	0.34	0.98	0.72
207	0.01		1,2,4-TRICHLOROBENZENE 120821							
145	0.34	0.26	0.06		0.40	0.63	0.22	0.36	0.80	0.57
180	1.30	1.00	0.24		1.50	2.40	0.83	1.37	3.03	2.16
208	0.01		2-BROMO-1-CHLOROBENZENE 694804							
190	0.78	0.61	0.14		0.85	1.38	0.55	0.92	1.74	1.26
192	1.04	0.81	0.19		1.14	1.84	0.74	1.24	2.33	1.71
209	0.01		1,2-DICHLORONAPHTHALENE 2050693							
161	0.44	0.34	0.08		0.50	0.78	0.28	0.46	1.01	0.72
196	2.17	1.67	0.40		2.51	3.88	1.38	2.29	5.03	3.58
210	0.01		1,2,4,5-TETRACHLOROBENZENE 95943							
214	1.18	0.90	0.22		1.29	2.09	0.84	1.40	2.63	1.94
216	1.54	1.18	0.28		1.69	2.72	1.09	1.83	3.43	2.52
211	0.01		P-DIBROMOBENZENE 106376							
234	0.68	0.52	0.12		0.77	1.23	0.41	0.67	1.93	1.43
236	1.29	1.00	0.23		1.48	2.36	0.78	1.30	3.77	2.93
212	0.01		4-BROMODIPHENYLETHER							
248	1.06	0.81	0.20		1.19	1.92	0.77	1.29	2.42	1.78
250	1.13	0.88	0.21		1.26	2.04	0.82	1.37	2.57	1.89
213	0.01		HEXACHLOROBENZENE 118741							
284	0.74	0.56	0.13		0.84	1.34	0.44	0.73	2.10	1.55
286	0.60	0.46	0.11		0.68	1.08	0.36	0.59	1.70	1.26

Internal/External Standard File for Cmpd Class # 6

Cmpds	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
206	0.01		3,4-DICHLOROBENZALDEHYDE 6287383							
173	0.37	1.25	0.54	0.21	0.17		0.04		0.57	
174	0.25	0.84	0.36	0.14	0.11		0.03		0.38	
207	0.01		1,2,4-TRICHLOROBENZENE 120821							
145	0.24	0.80	0.33	0.13	0.12		0.03		0.36	
180	0.89	3.05	1.25	0.48	0.46		0.10		1.36	
208	0.01		2-BROMO-1-CHLOROBENZENE 694804							
190	0.57	1.88	0.78	0.28	0.30		0.05		0.84	
192	0.76	2.52	0.98	0.38	0.40		0.07		1.12	
209	0.01		1,2-DICHLORONAPHTHALENE 2050693							
161	0.31	1.02	0.42	0.16	0.15		0.03		0.46	
196	1.57	5.08	2.08	0.80	0.76		0.17		2.27	
210	0.01		1,2,4,5-TETRACHLOROBENZENE 95943							
214	0.86	2.85	1.11	0.43	0.45		0.08		1.27	
216	1.12	3.72	1.44	0.56	0.58		0.11		1.66	
211	0.01		P-DIBROMOBENZENE 106376							
234	0.49	1.66	0.72	0.28	0.19		0.05		0.75	
236	0.93	3.18	1.38	0.53	0.45		0.10		1.45	
212	0.01		4-BROMODIPHENYLETHER							
248	0.79	2.61	1.01	0.39	0.41		0.07		1.17	
250	0.84	2.78	1.08	0.42	0.44		0.08		1.24	
213	0.01		HEXACHLOROBENZENE 118741							
284	0.53	1.83	0.78	0.30	0.24		0.06		0.82	
286	0.43	1.46	0.63	0.24	0.19		0.05		0.66	

Table B-7. RMRs AND RECOVERIES FOR WABN COMPOUNDS
(FU, pH 8.0)

Class No. 7	
Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
54	d_8-Naphthalene (internal)
56	d_5-Nitrobenzene (internal)
57	d_{10}-o-Xylene (internal)
58	d_5-Phenylethanol (internal)
59	d_5-Acetophenone (internal)
60	d_5-Propiophenone (internal)
61	d_{12}-Perylene (internal)
62	d_9-Acridine (internal)
63	d_5-Phenol (internal)

MATRIX OF STANDARD ION RIRs

		Standard							
		d_5-Phenol	d_{10}-o-Xylene		d_8-Naphthalene	d_5-Nitrobenzene		d_5-Phenylethanol	
Compound	Ion	m/z 99	m/z 98	m/z 116	m/z 136	m/z 82	m/z 128	m/z 86	m/z 122
d_5-phenol	99	-	59(9)	93(9)	17(6)	1.08(5)	1.66(3)	2.48(15)	1.75(15)
d_{10}-o-xylene	98	1.72(9)[a]	-	1.67(1)	29(6)	1.79(8)	2.84(8)	4.21(22)	3.02(21)
	116	1.05(2)	60(0)	-	18(6)	1.07(8)	1.73(8)	2.55(22)	1.81(21)
d_8-naphthalene	136	5.97(8)	3.51(7)	5.85(7)	-	6.21(3)	9.28(3)	16.63(15)	10.59(10)
d_5-nitrobenzene	82	.97(6)	57(10)	95(10)	16(3)	-	1.60(3)	2.35(17)	1.70(16)
	128	61(2)	35(3)	59(9)	10(3)	63(3)	-	1.47(16)	1.07(15)
d_5-phenylethanol	86	42(15)	25(20)	42(24)	.97/ 23(10)	44(16)	70(15)	-	.73(2)
	122	.58(15)	35(22)	58(23)	0.9(10)	61(16)	95(16)	1.39(2)	-
d_5-propiophenone	82	1.09(4)	65(13)	1.07(14)	18(8)	1.13(6)	1.82(6)	2.65(11)	1.90(10)
	110	2.85(5)	1.67(13)	2.78(14)	48(17)	2.94(6)	4.72(6)	6.84(12)	4.95(11)
d_5-acetophenone	110	1.52(2)	90(7)	1.50(8)	25(4)	1.60(5)	2.55(3)	3.71(17)	2.68(16)
	125	46(2)	27(8)	45(7)	36(5)	48(3)	74(4)	1.11(18)	81(17)
d_{12}-perylene	264	3.56(13)	2.09(7)	3.48(8)	.97/ 60(9)	3.70(13)	5.90(12)	8.52(25)	6.37(20)
d_9-acridine	188	1.45(7)	84(15)	1.43(15)	28(8)	1.58(6)	2.40(6)	3.52(13)	2.55(13)
4 fluoro 2-iodotoluene	109	1.10(4)	65(7)	1.08(8)	18(3)	1.14(2)	1.82(2)	2.69(10)	1.97(9)
	236	1.43(4)	84(6)	1.39(7)	28(6)	1.48(5)	2.37(3)	3.48(10)	2.52(10)

(continued)

Compound	Ion	Standard: d_5 Propiophenone m/z 82	d_5 Propiophenone m/z 110	d_5 Acetophenone m/z 110	d_5 Acetophenone m/z 125	d_{12} Perylene m/z 264	d_9 Acridine m/z 188	4-Fluoro-2-iodotoluene m/z 109	4-Fluoro-2-iodotoluene m/z 236
d_5 phenol	99	[illegible](5)	35(5)	[illegible](2)	2.28(5)	.31(15)	[illegible](7)	98(5)	71(6)
d_{10} o-xylene	98	1.59(12)	61(83)	1.13(7)	3.37(7)	55(10)	1.20(15)	1.56(6)	1.21(6)
	116	95(33)	57(82)	67(6)	2.27(7)	32(10)	32(15)	94(6)	73(6)
d_8 naphthalene	136	5.51(8)	2.15(8)	3.91(8)	13.16(3)	8.76(15)	4.20(8)	5.45(8)	4.20(1)
d_5-nitrobenzene	82	89(6)	34(6)	65(4)	2.12(8)	29(19)	67(6)	88(2)	.68(3)
	128	55(6)	22(6)	53(1)	1.5(3)	18(20)	42(6)	55(5)	42(3)
d_5 phenylethanol	84	57(88)	35(20)	28(36)	95(82)	134(8)	29(35)	50(18)	30(17)
	112	51(10)	21(3)	51(36)	1.28(36)	140.81	41(35)	57(69)	62(16)
d_5-propiophenone	82	-	39(1)	7(7)	2.80(6)	33(23)	76(5)	1.00(7)	77(7)
	110	2.60(1)		1.85(6)	6.28(6)	87(15)	2.10(5)	2.59(7)	1.99(7)
d_5-acetophenone	110	1.41(6)	55(6)	-	5.55(1)	47(14)	1.10(9)	1.37(6)	1.07(2)
	125	4.(6)	16(5)	30(2)		140(8)	32(9)	42(2)	32(3)
d_{12}-perylene	264	3.08(14)	1.27(16)	2.37(12)	7.91(12)	-	2.50(16)	3.21(9)	2.51(9)
d_9-acridine	188	1.33(5)	52(5)	95(10)	5.85(11)	39(60)	-	1.52(8)	1.03(8)
4-Fluoro-2-iodotoluene	109	1.01(7)	39(7)	71(2)	2.49(2)	54(12)	76(8)	-	77(3)
	236	1.55(7)	51(7)	92(3)	3.19(2)	62(19)	1.09(8)	1.30(3)	-

^{a}(CV).

Internal/External Standard File for Cmpd Class # 7

Cmpd#	Recovery Std # 2		Compound Name Std #54			Std #56		Std #57		Std #59	
Mass	109	236	136	-		82	128	98	116	84	112
100	0.01		PYRIDINE 110861								
52	0.29	0.22	0.05			0.33	0.51	0.19	0.32	0.67	0.48
79	0.44	0.34	0.08			0.51	0.78	0.30	0.50	1.10	0.78
101	0.01		ALPHA-PICOLINE 109068								
66	0.26	0.20	0.05			0.30	0.46	0.16	0.27	0.59	0.42
93	0.66	0.51	0.12			0.76	1.18	0.40	0.66	1.52	1.09
102	0.01		ANILINE 62533								
66	0.23	0.19	0.04			0.28	0.41	0.15	0.24	0.53	0.38
93	0.76	0.54	0.13			0.81	1.25	0.45	0.74	1.62	1.15
103	0.01		LUTIDINE 108485								
106	0.13	0.10	0.02			0.15	0.25	0.08	0.13	0.39	0.28
107	0.22	0.16	0.04			0.24	0.39	0.13	0.21	0.61	0.45
104	0.01		TOLUIDINE 106490								
106	0.89	0.69	0.16			0.97	1.57	0.64	1.07	1.97	1.45
107	0.71	0.56	0.13			0.78	1.27	0.51	0.86	1.58	1.16
105	0.01		INDOLE 120729								
90	0.72	0.54	0.13			0.82	1.30	0.43	0.71	2.04	1.51
117	1.92	1.45	0.34			2.17	3.46	1.14	1.89	5.43	4.02
106	0.01		2,3,6-TRIMETHYLPYRIDINE 1462846								
120	0.66	0.51	0.12			0.76	1.18	0.42	0.69	1.53	1.09
121	0.90	0.69	0.17			1.03	1.61	0.55	0.91	2.08	1.49
107	0.01		2,6-DIMETHYLANILINE 1300739								
106	0.36	0.27	0.06			0.41	0.65	0.21	0.36	1.02	0.75
121	0.57	0.44	0.10			0.66	1.04	0.34	0.57	1.64	1.21
108	0.01		4-CHLOROANILINE 106429								
127	1.09	0.84	0.20			1.26	1.94	0.69	1.15	2.52	1.79
129	0.34	0.26	0.06			0.39	0.60	0.22	0.36	0.78	0.56
109	0.01		QUINOLINE 91225								
129	1.82	1.41	0.34			1.99	3.22	1.30	2.17	4.06	2.98
110	0.01		P-NITROANILINE 100016								
65	0.44	0.35	0.08			0.52	0.83	0.27	0.46	1.30	0.97
138	0.56	0.45	0.11			0.67	1.07	0.35	0.58	1.68	0.22
111	0.01		2,4-DIMETHYLQUINOLINE 1198374								
156	0.41	0.32	0.08			0.47	0.75	0.26	0.43	0.95	0.68
157	2.01	1.54	0.37			2.31	3.59	1.27	2.11	4.64	3.31
112	0.01		1,8-DIAMINONAPHTHALENE								
114	0.03	0.02	0.00			0.04	0.06	0.02	0.03	0.09	0.06
141	0.05	0.04	0.01			0.06	0.01	0.03	0.05	0.14	0.11

Internal/External Standard File for Cmpd Class # 7

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
			PYRIDINE 110861							
100	0.01									
52	0.20	0.68	0.28	0.11	0.10		0.02		0.30	
79	0.33	1.11	0.42	0.16	0.17		0.04		0.50	
			ALPHA-PICOLINE 109068							
101	0.01									
66	0.18	0.60	0.25	0.09	0.09		0.02		0.27	
93	0.46	1.54	0.63	0.24	0.23		0.05		0.69	
			ANILINE 62533							
102	0.01									
66	0.17	0.56	0.22	0.09	0.08		0.02		0.24	
93	0.49	1.64	0.67	0.26	0.24		0.05		0.73	
			LUTIDINE 108685							
103	0.01									
106	0.10	0.33	0.14	0.05	0.04		0.01		0.15	
107	0.16	0.52	0.23	0.09	0.08		0.02		0.24	
			TOLUIDINE 106490							
104	0.01									
106	0.65	2.15	0.83	0.32	0.32		0.06		0.96	
107	0.52	1.73	0.67	0.26	0.26		0.05		0.77	
			INDOLE 120729							
105	0.01									
90	0.51	1.75	0.70	0.29	0.23		0.05		0.79	
117	1.40	4.68	2.02	0.78	0.61		0.15		2.12	
			2,3,6-TRIMETHYLPYRIDINE 1462846							
106	0.01									
120	0.46	1.54	0.63	0.24	0.23		0.05		0.67	
121	0.62	2.10	0.86	0.33	0.32		0.07		0.94	
			2,6-DIMETHYLANILINE 1300738							
107	0.01									
106	0.26	0.88	0.38	0.15	0.11		0.03		0.40	
121	0.42	1.41	0.61	0.24	0.18		0.04		0.64	
			4-CHLOROANILINE 106479							
108	0.01									
127	0.76	2.55	1.05	0.40	0.38		0.08		1.14	
129	0.24	0.79	0.33	0.13	0.12		0.03		0.35	
			QUINOLINE 91225							
109	0.01									
129	1.33	4.40	1.70	0.66	0.59		0.12		1.96	
			P-NITROANILINE 100016							
110	0.01									
65	0.34	1.13	0.49	0.19	0.14		0.04		0.51	
138	0.43	1.84	0.62	0.24	0.19		0.05		0.65	
			2,4-DIMETHYLQUINOLINE 1198374							
111	0.01									
156	0.29	0.96	0.40	0.15	0.15		0.03		0.43	
157	1.46	4.69	1.93	0.74	0.71		0.15		2.09	
			1,8-DIAMINONAPHTHALENE							
112	0.01									
114	0.02	0.08	0.03	0.01	0.01		0.00		0.03	
141	0.04	0.12	0.05	0.02	0.01		0.00		0.55	

Internal/External Standard File for Cmpd Class # 7

Cmpd#	Recovery Std # 2		Compound Name	Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-		82	128	98	116	84	112
113	0.01		NICOTINE	54115							
84	1.17	0.90	0.22			1.35	2.09	0.74	1.23	2.70	1.92
133	0.28	0.21	0.05			0.32	0.49	0.17	0.29	0.63	0.45
114	0.01		CARBAZOLE	86748							
167	3.73	2.88	0.69			4.30	6.66	2.37	3.92	9.36	6.67
115	0.01		2-AMINOBIPHENYL	90415							
168	6.79	5.11	1.20			7.65	12.18	4.61	6.67	14.13	14.17
169	12.72	9.45	2.22			14.15	22.54	7.42	12.30	35.40	26.19
116	0.01		DIPHENYLAMINE	122394							
168	1.48	1.14	0.27			1.71	2.65	0.94	1.56	3.43	2.45
169	2.79	2.15	0.52			3.22	4.99	1.77	2.93	6.45	4.60
117	0.01		DICYCLOHEXYLAMINE	101837							
56	0.33	0.37	0.06			0.39	0.63	0.21	0.35	1.10	0.78
138	0.96	0.76	0.18			1.12	1.80	0.61	1.02	3.15	2.25
118	0.01		TRIBUTYLAMINE	102829							
100	0.42	0.33	0.08			0.49	0.75	0.27	0.44	0.97	0.69
142	1.53	1.18	0.28			1.77	2.74	0.97	1.61	3.52	2.51
119	0.01		CAFFEINE	58082							
109	0.10	0.08	0.02			0.12	0.17	0.06	0.10	0.23	0.16
194	0.19	0.15	0.04			0.22	0.34	0.12	0.20	0.44	0.32
120	0.01		DIBENZYLAMINE	103491							
91	1.62	1.26	0.30			1.76	2.87	1.16	1.94	3.63	2.67
197	0.13	0.11	0.03			0.15	0.24	0.10	0.16	0.30	0.22
121	0.01		N,N-DIMETHYLDODECYLAMINE	112185							
58	4.72	3.88	0.87			5.47	8.83	3.58	5.99	11.09	8.16
59	0.17	0.13	0.03			0.20	0.30	0.13	0.21	0.40	0.29
122	0.01		ATRAZINE	1912249							
200	2.75	2.20	0.52			3.28	5.23	1.72	2.86	8.17	6.09
215	1.67	1.34	0.31			2.00	3.18	1.05	1.74	4.97	3.71
123	0.01		HEPTANONE(2)	110430							
43	1.21	0.94	0.22			1.33	2.14	0.85	1.14	2.32	2.00
58	0.75	0.58	0.14			0.83	1.33	0.53	0.88	1.69	1.25
124	0.01		BUTOXYETHANOL	111762							
41	0.21	0.17	0.04			0.25	0.40	0.13	0.22	0.49	0.35
57	0.55	0.42	0.10			0.63	1.03	0.35	0.58	1.27	0.91
125	0.01		2-OCTANONE	111137							
43	1.30	1.01	0.24			1.43	2.31	0.91	1.53	2.92	2.15
58	1.02	0.79	0.19			1.11	1.80	0.71	1.19	2.27	1.67

Internal/External Standard File for Cmpd Class # 7

Cmpds	Recovery Std #59		Compound Name	Std #60		Std #61		Std #62		Std #63	
Mass	110	125		82	110	264	-	188	-	99	-
113	0.01		NICOTINE		54115						
84	0.82	2.74		1.12	0.43	0.41		0.09		1.22	
133	0.19	0.64		0.26	0.10	0.10		0.02		0.29	
114	0.01		CARBAZOLE		86748						
167	2.60	8.72		3.57	1.37	1.28		0.31		4.22	
115	0.01		2-AMINOBIPHENYL		90445						
168	4.75	16.46		7.10	2.75	2.13		0.51		7.45	
169	8.82	30.44		13.14	5.08	3.96		0.95		13.80	
116	0.01		DIPHENYLAMINE		122394						
168	1.03	3.47		1.42	0.55	0.52		0.11		1.55	
169	1.94	6.46		2.68	1.03	0.98		0.22		2.91	
117	0.01		DICYCLOHEXYLAMINE		101837						
56	0.25	0.81		0.33	0.14	0.09		0.03		0.38	
138	0.71	2.34		0.95	0.40	0.26		0.08		1.09	
118	0.01		TRIBUTYLAMINE		102829						
100	0.29	0.99		0.41	0.16	0.15		0.03		0.44	
142	0.99	3.34		1.47	0.57	0.53		0.12		1.59	
119	0.01		CAFFEINE		58082						
109	0.07	0.23		0.09	0.04	0.04		0.01		0.10	
194	0.13	0.45		0.18	0.07	0.07		0.02		0.21	
120	0.01		DIBENZYLAMINE		103491						
91	1.18	3.91		1.52	0.59	0.62		0.11		1.74	
197	0.10	0.32		0.13	0.05	0.05		0.01		0.14	
121	0.01		N,N-DIMETHYLDODECYLAMINE		112185						
58	3.62	12.02		4.66	1.81	1.87		0.34		5.37	
59	0.13	0.43		0.17	0.06	0.07		0.01		0.19	
122	0.01		ATRAZINE		1912249						
200	2.13	7.07		3.05	1.18	0.90		0.22		3.26	
215	1.21	4.30		1.85	0.72	0.55		0.13		1.95	
123	0.01		HEPTANONE(2)		110430						
43	0.88	2.91		1.13	0.44	0.47		0.08		1.30	
58	0.55	1.82		0.71	0.27	0.29		0.05		0.81	
124	0.01		BUTOXYETHANOL		111762						
41	0.15	0.49		0.20	0.09	0.07		0.02		0.22	
57	0.38	1.28		0.52	0.20	0.19		0.04		0.57	
125	0.01		2-OCTANONE		111137						
43	0.95	3.14		1.22	0.47	0.51		0.09		1.40	
58	0.74	2.45		0.95	0.37	0.39		0.07		1.09	

Internal/External Standard File for Cmpd Class # 7

Cmpd#	Recovery Std # 2		Compound Name Std #54	Std #56		Std #57		Std #58	
Mass	109	236	136 -	82	128	98	116	84	112
126	0.01		BUTYLPROPIONATE 590012						
57	1.48	1.14	0.27	1.71	2.73	0.90	1.49	4.27	3.15
75	0.44	0.34	0.08	0.51	0.82	0.27	0.45	1.28	0.95
127	0.01		ISOPHORONE 78591						
82	1.77	1.36	0.33	2.04	3.17	1.13	1.86	4.11	2.93
138	0.39	0.30	0.07	0.45	0.72	0.25	0.41	0.90	0.64
128	0.01		FENCHONE 1195759						
69	0.66	0.51	0.12	0.72	1.17	0.47	0.78	1.47	1.08
81	1.45	1.12	0.27	1.58	2.55	1.02	1.71	3.22	2.36
129	0.01		ALPHA-TERPINEOL 98555						
59	0.56	0.43	0.10	0.65	1.00	0.36	0.59	1.31	0.93
136	0.32	0.25	0.06	0.37	0.58	0.21	0.34	0.75	0.53
130	0.01		N-DECANOL 112301						
41	0.40	0.31	0.07	0.46	0.74	0.25	0.42	0.92	0.66
43	0.44	0.34	0.08	0.51	0.79	0.28	0.46	1.02	0.73
131	0.01		DIMETHYLADIPATE 627930						
59	0.56	0.45	0.10	0.64	1.03	0.41	0.69	1.29	0.95
114	0.44	0.35	0.08	0.49	0.79	0.32	0.54	1.00	0.74
132	0.01		N-DECANE 124185						
43	1.47	1.11	0.26	1.67	2.66	0.88	1.46	4.18	3.09
57	1.42	1.08	0.25	1.64	2.61	0.85	1.41	4.05	3.00
133	0.01		N-TRIDECANE 629505						
43	2.18	1.64	0.34	2.48	3.95	1.30	2.16	6.20	4.58
57	2.75	2.09	0.50	3.14	5.01	1.66	2.77	7.93	5.86
134	0.01		N-TETRADECANE 629594						
43	2.52	1.92	0.45	2.88	4.58	1.51	2.51	7.19	5.31
57	3.40	2.55	0.61	3.87	6.16	2.03	3.37	9.67	7.15
135	0.01		N-PENTADECANE 692629						
57	2.78	2.14	0.52	3.22	4.99	1.77	2.94	6.47	4.62
71	1.73	1.33	0.32	2.01	3.11	1.10	1.83	4.03	2.87
136	0.01		N-HEXADECANE 544763						
43	1.90	1.45	0.34	2.16	3.45	1.13	1.89	5.41	3.99
57	2.72	2.08	0.49	3.11	4.96	1.63	2.71	7.78	5.74
137	0.01		N-HEPTADECANE 629787						
57	3.13	2.41	0.58	3.61	5.59	1.99	3.30	7.25	5.17
71	2.07	1.60	0.38	2.39	3.70	1.32	2.16	4.80	3.42
138	0.01		N-OCTADECANE 593453						
57	2.99	2.51	0.59	3.75	5.98	1.88	3.14	8.96	5.63
71	1.98	1.66	0.39	2.48	3.95	1.25	2.08	5.95	4.41

Internal/External Standard File for Cmpd Class # 7

Cmpds	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	•	188	•	99	•
126	0.01		BUTYLPROPIONATE 590012							
57	1.11	3.69	1.59	0.61	0.48		0.12		1.66	
75	0.33	1.11	0.48	0.19	0.15		0.04		0.50	
127	0.01		ISOPHORONE 78591							
82	1.23	4.14	1.70	0.65	0.62		0.14		1.80	
138	0.27	0.91	0.37	0.14	0.14		0.03		0.41	
128	0.01		FENCHONE 1195759							
69	0.48	1.58	0.62	0.24	0.25		0.05		0.71	
81	1.05	3.45	1.35	0.52	0.55		0.10		1.55	
129	0.01		ALPHA-TERPINEOL 98555							
59	0.39	1.31	0.54	0.21	0.20		0.04		0.58	
136	0.23	0.76	0.31	0.12	0.11		0.03		0.34	
130	0.01		N-DECANOL 112301							
41	0.28	0.93	0.38	0.15	0.14		0.03		0.41	
43	0.31	1.63	0.42	0.16	0.15		0.03		0.46	
131	0.01		DIMETHYLADIPATE 627930							
59	0.42	1.40	0.54	0.21	0.22		0.04		0.62	
114	0.33	1.08	0.42	0.16	0.17		0.03		0.48	
132	0.01		N-DECANE 124185							
43	1.05	3.59	1.55	0.60	0.47		0.11		1.62	
57	1.01	3.48	1.50	0.58	0.46		0.11		1.58	
133	0.01		N-TRIDECANE 629505							
43	1.56	5.33	2.30	0.89	0.70		0.17		2.41	
57	1.99	6.75	2.94	1.14	0.76		0.21		3.09	
134	0.01		N-TETRADECANE 629594							
43	1.86	6.19	2.67	1.03	0.80		0.19		2.80	
57	2.50	8.33	3.57	1.39	1.08		0.26		3.77	
135	0.01		N-PENTADECANE 692629							
57	1.94	6.52	2.68	1.03	0.99		0.22		2.92	
71	1.21	4.06	1.67	0.64	0.62		0.14		1.82	
136	0.01		N-HEXADECANE 544763							
43	1.40	4.66	2.01	0.78	0.61		0.15		2.11	
57	2.01	6.70	2.88	1.12	0.87		0.21		3.03	
137	0.01		N-HEPTADECANE 629787							
57	2.18	7.32	3.01	1.16	1.11		0.24		3.27	
71	1.44	4.85	1.99	0.77	0.73		0.16		2.17	
138	0.01		N-OCTADECANE 593453							
57	2.33	8.10	3.48	1.35	1.01		0.24		3.65	
71	1.55	5.35	2.30	0.89	0.58		0.06		2.41	

Internal/External Standard File for Cmpd Class # 7

Cmpds	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
139	0.01		N-NONADECANE	629925						
71	2.12	1.61	0.38		2.42	3.85	1.27	2.11	6.04	4.47
85	1.42	1.08	0.25		1.61	2.57	0.85	1.41	4.03	2.98
140	0.01		N-EICOSANE	1112958						
57	4.43	3.41	0.82		5.11	7.92	2.82	4.66	10.26	7.32
71	3.03	2.33	0.56		3.50	5.43	1.93	3.19	7.03	5.01
141	0.01		N-HENEICOSANE	629947						
57	3.93	2.96	0.70		4.43	7.05	2.32	3.86	11.05	8.20
71	2.71	2.05	0.48		3.07	4.88	1.61	2.67	7.65	5.68
142	0.01		N-DOCOSANE	629970						
57	3.73	2.98	0.70		4.46	7.10	2.33	3.88	11.11	8.26
71	2.60	2.08	0.49		3.11	4.96	1.63	2.70	7.76	5.77
143	0.01		N-TRICOSANE	638675						
57	3.99	3.19	0.75		4.77	7.60	2.49	4.14	11.85	8.83
71	2.80	2.24	0.53		3.35	5.34	1.75	2.91	8.33	6.20
144	0.01		PHENYLACETATE	122792						
94	1.84	1.43	0.34		2.01	3.25	1.30	2.18	4.10	3.01
136	0.25	0.20	0.05		0.28	0.45	0.18	0.30	0.57	0.42
145	0.01		BENZYLACETATE	140114						
91	0.52	0.40	0.09		0.57	0.92	0.37	0.62	1.15	0.85
108	1.09	0.85	0.20		1.19	1.92	0.77	1.29	2.43	1.79
146	0.01		METHYLBENZENESULFONATE							
77	1.24	0.94	0.22		1.41	2.25	0.74	1.23	3.54	2.61
172	0.44	0.34	0.08		0.50	0.80	0.26	0.44	1.26	0.93
147	0.01		METHYLTOLUENESULFONATE							
91	1.60	1.21	0.29		1.81	2.89	0.95	1.58	4.53	3.35
155	0.72	0.54	0.13		0.81	1.29	0.42	0.71	2.02	1.50
148	0.01		DIMETHYLPHTHALATE	131113						
77	0.81	0.63	0.15		0.94	1.45	0.52	0.85	1.88	1.34
163	5.29	4.07	0.98		6.10	9.46	3.36	5.56	12.22	8.71
149	0.01		ETHYLTOLUENESULFONATE							
91	1.74	1.32	0.31		1.97	3.14	1.03	1.72	4.92	3.65
155	1.18	0.94	0.22		1.40	2.23	0.73	1.21	3.46	2.35
150	0.01		DIETHYLPHTHALATE	84662						
149	3.19	2.43	0.57		3.65	5.79	1.90	3.17	9.08	6.71
177	0.80	0.61	0.14		0.93	1.47	0.48	0.80	2.29	1.69
151	0.01		DIBUTYLPHTHALATE	84742						
57	0.29	0.23	0.05		0.34	0.52	0.19	0.31	0.68	0.48
149	7.17	5.52	1.33		8.27	12.80	4.55	7.54	16.55	11.80

Internal/External Standard File for Cmpd Class # 7

Cmpd#	Recovery Std #59		Compound Name	Std #60		Std #61		Std #62		Std #63	
Mass	110	125		82	110	264	-	188	-	99	-
139	0.01		N-NONADECANE	629925							
71	1.51	5.27		2.24	0.87	0.68		0.16		2.35	
85	1.01	3.47		1.50	0.58	0.45		0.11		1.57	
140	0.01		N-EICOSANE	1112958							
57	3.08	10.35		4.25	1.63	1.57		0.35		4.63	
71	2.11	7.09		2.91	1.12	1.07		0.23		3.17	
141	0.01		N-HENEICOSANE	629947							
57	2.73	9.53		4.11	1.60	1.07		0.30		4.31	
71	1.69	6.60		2.85	1.10	0.74		0.21		2.99	
142	0.01		N-DOCOSANE	629970							
57	2.89	9.60		4.14	1.60	1.22		0.30		4.35	
71	2.02	6.71		2.89	1.12	0.85		0.21		3.04	
143	0.01		N-TRICOSANE	638675							
57	3.10	10.28		4.42	1.71	1.29		0.32		4.65	
71	2.18	7.22		3.11	1.20	0.90		0.22		3.27	
144	0.01		PHENYLACETATE	122792							
94	1.31	4.43		1.72	0.67	0.70		0.13		1.98	
136	0.18	0.62		0.24	0.09	0.10		0.02		0.28	
145	0.01		BENZYLACETATE	140114							
91	0.38	1.25		0.48	0.19	0.20		0.04		0.56	
108	0.79	2.63		1.02	0.40	0.41		0.07		1.17	
146	0.01		METHYLBENZENESULFONATE								
77	0.91	3.04		1.31	0.51	0.40		0.09		1.38	
172	0.32	1.08		0.47	0.18	0.14		0.03		0.49	
147	0.01		METHYLTOLUENESULFONATE								
91	1.17	3.90		1.68	0.65	0.51		0.12		1.76	
155	0.52	1.74		0.75	0.29	0.23		0.05		0.79	
148	0.01		DIMETHYLPHTHALATE	131113							
77	0.57	1.83		0.75	0.29	0.28		0.06		0.85	
163	3.68	11.87		4.88	1.88	1.85		0.41		5.51	
149	0.01		ETHYLTOLUENESULFONATE								
91	1.28	4.25		1.83	0.71	0.55		0.13		1.92	
155	0.91	3.01		1.30	0.50	0.38		0.09		1.36	
150	0.01		DIETHYLPHTHALATE	84662							
149	2.35	7.82		3.34	1.30	1.02		0.24		3.54	
177	0.59	1.97		0.85	0.33	0.26		0.06		0.89	
151	0.01		DIBUTYLPHTHALATE	84742							
57	0.20	0.63		0.28	0.11	0.10		0.02		0.31	
149	4.99	16.75		6.68	2.64	2.52		0.55		7.47	

Internal/External Standard File for Cmpd Class # 7

Cmpd#	Recovery Std # 2		Compound Name	Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-		82	128	98	116	84	112
152	0.01		BUTYLBENZYLPHTHALATE								
91	2.09	1.62	0.38			2.26	3.69	1.48	2.48	4.6	3.41
149	3.37	2.62	0.62			3.69	5.95	2.40	4.01	7.49	5.51
153	0.01		DIETHYLHEXYLPHTHALATE			117817					
149	5.22	4.07	0.96			5.71	9.23	3.74	6.26	11.59	8.53
167	1.98	1.54	0.37			2.17	3.51	1.42	2.37	4.40	3.24
154	0.01		BENZALDEHYDE		100527						
77	0.36	0.28	0.07			0.42	0.64	0.23	0.38	0.84	0.60
105	0.40	0.31	0.07			0.46	0.70	0.25	0.42	0.92	0.66
155	0.01		TOLUALDEHYDE		529204						
91	0.54	0.44	0.10			0.65	1.04	0.34	0.57	1.65	1.21
119	0.63	0.51	0.12			0.77	1.23	0.41	0.68	1.95	1.43
156	0.01		ACETOPHENONE		98862						
77	0.38	0.64	0.15			0.96	1.53	0.53	0.87	1.93	1.37
105	1.22	0.94	0.23			1.41	2.25	0.78	1.29	2.85	2.03
157	0.01		SALICYLALDEHYDE		90028						
121	0.56	0.44	0.10			0.61	0.99	0.40	0.67	1.24	0.91
122	0.60	0.47	0.11			0.60	1.07	0.43	0.72	1.34	0.99
158	0.01		ANISALDEHYDE		123115						
135	1.37	1.08	0.25			1.53	2.47	0.91	1.66	3.11	2.29
136	0.96	0.76	0.18			1.07	1.73	0.70	1.16	2.18	1.60
159	0.01		PHENOL	108952							
94	1.07	0.84	0.20			1.18	1.90	0.76	1.27	2.41	1.77
160	0.01		CRESOL(P)	106445							
107	1.21	0.93	0.23			1.40	2.25	0.80	1.29	2.91	2.08
108	1.07	0.82	0.20			1.24	1.99	0.69	1.14	2.58	1.84
161	0.01		2,3-DIMETHYLPHENOL		526750						
107	0.87	0.67	0.16			1.00	1.61	0.57	0.95	2.08	1.48
122	0.91	0.70	0.17			1.05	1.64	0.58	0.96	2.12	1.51
162	0.01		ISOPROPYLPHENOL		88699						
121	1.79	1.36	0.32			2.04	3.25	1.07	1.78	5.10	3.77
136	0.07	0.56	0.12			0.75	1.19	0.39	0.65	1.87	1.38
163	0.01		O-NITROPHENOL		88755						
65	0.03	0.02	0.00			0.03	0.05	0.02	0.03	0.06	0.05
139	0.13	0.10	0.02			0.14	0.23	0.09	0.15	0.29	0.21
164	0.01		4-CHLORO-3-METHYLPHENOL			59507					
107	0.93	0.71	0.17			1.06	1.58	0.55	0.92	2.64	2.95
142	1.02	0.77	0.18			1.16	1.84	0.61	1.01	2.89	2.14

Internal/External Standard File for Cmpd Class # 7

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	168	-	99	-
152	0.01		BUTYLBENZYLPHTHALATE							
91	1.51	5.02	1.95	0.76	0.76		0.14		2.24	
149	2.44	8.10	3.15	1.22	1.26		0.23		3.62	
153	0.01		DIETHYLHEXYLPHTHALATE			117817				
149	4.03	12.58	4.88	1.89	1.90		0.35		5.61	
167	1.53	4.78	1.85	0.72	0.72		0.13		2.13	
154	0.01		BENZALDEHYDE		100527					
77	0.25	0.84	0.35	0.13	0.13		0.03		0.38	
105	0.28	0.93	0.38	0.15	0.14		0.03		0.42	
155	0.01		TOLUALDEHYDE		529204					
91	0.42	1.41	0.61	0.24	0.15		0.05		0.64	
119	0.50	1.66	0.72	0.28	0.22		0.05		0.75	
156	0.01		ACETOPHENONE		98862					
77	0.57	1.95	0.80	0.31	0.29		0.06		0.87	
105	0.85	2.88	1.18	0.45	0.43		0.09		1.28	
157	0.01		SALICYLALDEHYDE		90028					
121	0.41	1.35	0.52	0.20	0.21		0.04		0.60	
122	0.44	1.46	0.56	0.22	0.23		0.04		0.65	
158	0.01		ANISALDEHYDE		123115					
135	1.01	3.36	1.30	0.51	0.53		0.09		1.50	
136	0.71	2.36	0.91	0.35	0.37		0.07		1.05	
159	0.01		PHENOL		108952					
94	0.75	2.60	1.01	0.39	0.41		0.07		1.15	
160	0.01		CRESOL(P)		106445					
107	0.88	2.85	1.17	0.45	0.44		0.10		1.31	
108	0.78	2.52	1.03	0.40	0.39		0.09		1.16	
161	0.01		2,3-DIMETHYLPHENOL			526750				
107	0.63	2.11	0.84	0.32	0.32		0.07		0.94	
122	0.64	2.14	0.85	0.33	0.32		0.07		0.95	
162	0.01		ISOPROPYLPHENOL		88699					
121	1.28	4.39	1.90	0.73	0.58		0.14		1.99	
136	0.47	1.61	0.69	0.27	0.21		0.05		0.73	
163	0.01		O-NITROPHENOL		88755					
65	0.02	0.07	0.03	0.01	0.01		0.00		0.03	
139	0.09	0.31	0.12	0.05	0.05		0.01		0.14	
164	0.01		4-CHLORO-3-METHYLPHENOL			59507				
107	0.66	2.27	0.98	0.38	0.30		0.07		1.03	
142	0.72	2.49	1.07	0.42	0.32		0.08		1.13	

Internal/External Standard File for Cmpd Class # 7

Cmpds	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
165	0.01		4-CHLOROCRESOL							
107	0.83	0.64	0.16		0.97	1.57	0.53	0.88	2.03	1.45
142	0.94	0.72	0.17		1.09	1.77	0.60	0.99	2.29	1.63
166	0.01		1-NAPHTHOL	90153						
115	0.35	0.26	0.06		0.38	0.61	0.20	0.34	0.96	0.72
144	0.61	0.45	0.11		0.67	1.07	0.35	0.29	1.68	1.25
167	0.01		P-TERT-BUTYLPHENOL		98544					
107	0.56	0.43	0.10		0.65	1.03	0.34	0.56	1.60	1.18
135	1.96	1.49	0.35		2.22	3.54	1.17	1.94	5.56	4.11
168	0.01		2-NITROCRESOL	119335						
77	0.26	0.20	0.05		0.30	0.46	0.07	0.27	0.60	0.43
153	0.74	0.57	0.14		0.83	1.33	0.46	0.78	1.72	1.23
169	0.01		2,4-DICHLOROPHENOL		120832					
162	1.13	0.88	0.21		1.24	2.00	0.80	1.34	2.52	1.86
164	0.72	0.53	0.13		0.78	1.27	0.51	0.85	1.60	1.18
170	0.01		2,4,6-TRICHLOROPHENOL		88062					
196	0.81	0.63	0.15		0.89	1.44	0.58	0.97	1.88	1.34
198	0.83	0.64	0.15		0.91	1.46	0.59	0.98	1.90	1.36
171	0.01		DI-TERT-BUTYL-4-METHYLPHENOL		128370					
205	2.53	1.97	0.47		2.78	4.49	1.81	3.03	5.66	4.16
220	0.67	0.52	0.12		0.73	1.18	0.48	0.80	1.49	1.09
172	0.01		PENTACHLOROPHENOL		87865					
264	0.29	0.22	0.05		0.34	0.54	0.19	0.31	0.72	0.52
266	0.47	0.36	0.09		0.55	0.91	0.32	0.54	1.17	0.84
173	0.01		2-METHYLNAPHTHALENE		91576					
141	2.03	1.58	0.38		2.23	3.60	1.44	2.42	4.53	3.34
142	2.51	1.96	0.46		2.76	4.45	1.79	2.99	5.62	4.13
174	0.01		ACENAPHTHENE		83329					
153	1.26	0.98	0.23		1.38	2.22	0.89	1.49	2.81	2.06
154	3.40	2.64	0.63		3.73	6.02	2.41	4.04	7.59	5.58
175	0.01		BIPHENYL		92524					
154	2.28	1.78	0.42		2.51	4.04	1.63	2.72	5.10	3.75
176	0.01		1,8-DIMETHYLNAPHTHALENE		569415					
141	1.59	1.24	0.29		1.74	2.82	1.13	1.89	3.55	2.61
156	2.30	1.79	0.42		2.52	4.07	1.63	2.73	5.13	3.77
177	0.01		FLUORENE		86737					
165	2.74	2.13	0.49		3.01	4.85	1.95	3.27	6.12	4.50
166	3.07	2.38	0.57		3.44	5.55	2.23	3.74	6.99	5.14

Internal/External Standard File for Cmpd Class # 7

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
165	0.01		4-CHLOROCRESOL							
107	0.58	1.96	0.60	0.31	0.31		0.07		0.91	
142	0.66	2.20	0.85	0.34	0.35		0.08		1.03	
166	0.01		1-NAPHTHOL 90153							
115	0.25	0.83	0.36	0.14	0.11		0.03		0.38	
144	0.44	1.45	0.62	0.24	0.18		0.05		0.66	
167	0.01		P-TERT-BUTYLPHENOL 98544							
107	0.40	1.38	0.66	0.23	0.16		0.04		0.62	
135	1.44	4.79	2.04	0.80	0.63		0.15		2.16	
168	0.01		2-NITROCRESOL 119335							
77	0.18	0.61	0.25	0.10	0.09		0.02		0.27	
153	0.52	1.74	0.71	0.27	0.26		0.06		0.78	
169	0.01		2,4-DICHLOROPHENOL 120832							
162	0.80	2.73	1.05	0.41	0.43		0.08		1.22	
164	0.51	1.70	0.67	0.26	0.27		0.05		0.77	
170	0.01		2,4,6-TRICHLOROPHENOL 88062							
196	0.58	1.97	0.76	0.30	0.31		0.05		0.88	
198	0.58	1.99	0.77	0.30	0.32		0.06		0.89	
171	0.01		DI-TERT-BUTYL-4-METHYLPHENOL 128370							
205	1.85	6.13	2.37	0.92	0.96		0.17		2.73	
220	0.49	1.61	0.62	0.24	0.25		0.05		0.72	
172	0.01		PENTACHLOROPHENOL 87865							
264	0.20	0.68	0.28	0.11	0.11		0.07		0.31	
266	0.36	1.11	0.45	0.07	0.18		0.04		0.50	
173	0.01		2-METHYLNAPHTHALENE 91576							
141	1.48	4.91	1.90	0.74	0.77		0.14		2.19	
142	1.78	6.08	2.36	0.91	0.95		0.17		2.71	
174	0.01		ACENAPHTHENE 83329							
153	0.92	3.04	1.18	0.46	0.47		0.09		1.35	
154	2.48	8.22	3.19	1.23	1.28		0.23		3.66	
175	0.01		BIPHENYL 92524							
154	1.67	5.52	2.14	0.83	0.87		0.16		2.46	
176	0.01		1,8-DIMETHYLNAPHTHALENE 569415							
141	1.16	3.84	1.49	0.56	0.60		0.11		1.71	
156	1.67	5.55	2.15	0.83	0.87		0.16		2.48	
177	0.01		FLUORENE 86737							
165	2.00	6.62	2.57	0.99	1.04		0.19		2.95	
166	2.28	7.57	2.93	1.14	1.19		0.21		3.38	

Internal/External Standard File for Cmpd Class # 7

Cmpd#	Recovery Std # 2		Compound Name	Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-		82	128	98	116	84	112
178	0.01		2,3,5-TRIMETHYLNAPHTHALENE 2245387								
155	1.86	1.44	0.34			2.08	3.36	1.36	2.27	4.24	3.12
170	2.56	1.99	0.47			2.86	4.62	1.86	3.11	5.83	4.29
179	0.01		ANTHRACENE 120127								
178	3.21	2.47	0.60			3.71	5.74	2.04	3.38	7.43	5.30
180	0.01		PYRENE 129000								
202	4.88	3.75	0.95			5.66	8.73	3.27	5.18	11.54	8.23
181	0.01		9,10-DIMETHYLANTHRACENE 781431								
191	1.33	1.03	0.25			1.45	2.35	0.94	1.57	2.96	2.18
206	2.85	2.22	0.53			3.13	5.04	2.01	3.37	6.36	4.68
182	0.01		CHRYSENE 218019								
228	2.21	1.73	0.41			2.42	3.92	1.59	2.66	4.91	3.61
183	0.01		PERYLENE 198550								
252	1.60	1.23	0.30			1.84	2.96	1.02	1.68	3.67	2.62
184	0.01		DICYANOBUTANE 111693								
41	0.66	0.51	0.12			0.72	1.17	0.47	0.79	1.47	1.08
54	0.29	0.23	0.05			0.32	0.52	2.10	0.35	0.66	0.48
185	0.01		BUTYLCARBAMATE 14994775								
41	0.48	0.36	0.08			0.54	0.86	0.28	0.47	1.35	1.00
59	0.24	0.26	0.05			0.29	0.47	0.15	0.25	0.72	0.54
186	0.01		DIBUTYLDISULFIDE 110065								
41	0.73	0.56	0.13			0.84	1.34	0.44	0.73	2.10	1.55
57	3.09	2.36	0.56			3.54	5.64	1.85	3.09	8.84	6.54
187	0.01		BIS(2-CHLOROETHYL)ETHANE 112265								
63	1.71	1.31	0.31			1.97	3.13	1.03	1.71	4.91	3.63
93	0.84	0.65	0.15			0.97	1.54	0.51	0.84	2.42	1.78
188	0.01		TRIBUTYLPHOSPHATE 126738								
99	4.03	3.10	0.75			4.65	7.20	2.56	4.24	9.28	6.62
155	0.88	0.68	0.16			1.01	1.57	0.56	0.92	2.02	1.44
189	0.01		ALDRIN 309002								
66	1.33	1.03	0.24			1.49	2.40	0.97	1.62	3.03	2.23
263	0.60	0.46	0.11			0.67	1.08	0.44	0.73	1.36	1.00
190	0.01		DIHYDROBENZOFURAN 496162								
91	0.68	0.52	0.13			0.79	1.25	0.43	0.72	1.58	1.13
120	0.97	0.75	0.18			1.12	1.67	0.66	0.78	2.16	1.54
191	0.01		NITROBENZENE 98953								
77	0.86	0.67	0.16			0.94	1.51	0.61	1.02	1.91	1.40
123	0.54	0.42	0.10			0.59	0.95	0.38	0.64	1.20	0.88

Internal/External Standard File for Cmpd Class # 7

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
178	0.01		2,3,5-TRIMETHYLNAPHTHALENE 2245387							
155	1.38	4.59	1.78	0.69	0.72		0.13		2.05	
170	1.90	6.31	2.44	0.95	0.99		0.18		2.81	
179	0.01		ANTHRACENE 120127							
178	2.24	7.59	3.08	1.19	1.13		0.25		3.35	
180	0.01		PYRENE 129000							
202	3.59	11.47	4.95	1.90	1.80		0.40		5.36	
181	0.01		9,10-DIMETHYLANTHRACENE 781431							
191	0.96	3.19	1.24	0.48	0.50		0.09		1.42	
206	2.06	6.86	2.67	1.03	1.08		0.19		3.06	
182	0.01		CHRYSENE 218019							
228	1.61	5.34	2.07	0.80	0.81		0.15		2.39	
183	0.01		PERYLENE 198550							
252	1.11	3.72	1.53	0.59	0.47		0.12		1.65	
184	0.01		DICYANOBUTANE 111693							
41	0.48	1.59	0.62	0.24	0.25		0.05		0.71	
54	0.22	0.71	0.28	0.11	0.11		0.02		0.32	
185	0.01		BUTYLCARBAMATE 14994775							
41	0.35	1.16	0.50	0.09	0.15		0.04		0.52	
59	0.19	0.63	0.27	0.11	0.08		0.02		0.28	
186	0.01		DIBUTYLDISULFIDE 110065							
41	0.54	1.78	0.78	0.31	0.20		0.06		0.82	
57	2.21	7.62	3.29	1.27	1.00		0.24		3.42	
187	0.01		BIS(2-CHLOROETHYL)ETHANE 112265							
63	1.27	4.23	1.83	0.71	0.56		0.13		1.91	
93	0.61	2.08	0.90	0.35	0.27		0.06		0.94	
188	0.01		TRIBUTYLPHOSPHATE 126738							
99	2.81	9.43	3.87	1.49	1.41		0.31		4.19	
155	0.61	2.05	0.84	0.32	0.31		0.07		0.91	
189	0.01		ALDRIN 309002							
66	0.99	3.28	1.27	0.49	0.51		0.09		1.46	
263	0.44	1.47	0.57	0.22	0.23		0.04		0.66	
190	0.01		DIHYDROBENZOFURAN 496162							
91	0.27	1.59	0.65	0.25	0.24		0.05		0.71	
120	0.68	2.27	0.90	0.35	0.33		0.07		0.98	
191	0.01		NITROBENZENE 98953							
77	0.61	2.07	0.80	0.31	0.33		0.06		0.94	
123	0.38	1.30	0.50	0.20	0.21		0.04		0.59	

Internal/External Standard File for Cmpd Class # 7

Cmpd# / Mass	Recovery Std # 2		Compound Name		Std #56		Std #57		Std #58	
	109	236	136	-	82	128	98	116	84	112
192	0.01		BENZOTHIAZOLE	95169						
135	1.56	1.21	0.29		1.71	2.76	1.11	1.86	3.47	2.55
193	0.01		PHENYLCARBAMATE	102090						
94	1.25	0.96	0.23		1.44	2.23	0.79	1.31	2.88	2.06
137	0.02	0.01	0.00		0.02	0.03	0.01	0.02	0.04	0.03
194	0.01		2,4-DINITROTOLUENE	121142						
89	0.35	0.28	0.06		0.40	0.65	0.26	0.44	0.81	0.60
165	0.71	0.53	0.13		0.75	1.21	0.46	0.76	1.53	1.13
195	0.01		BENZYLSULFIDE	538749						
91	3.55	2.68	0.63		4.00	6.38	2.10	3.49	9.99	7.42
123	0.90	0.68	0.16		1.02	1.62	0.53	0.89	2.54	1.88
196	0.01		DIPHENYLSULFONE	127639						
125	3.82	3.44	0.81		5.16	8.21	2.71	4.51	12.95	8.55
218	0.92	0.73	0.17		1.10	1.75	0.58	0.96	2.74	2.03
197	0.01		TRIPHENYLPHOSPHATE	115866						
325	2.59	2.01	0.13		0.79	1.28	0.52	0.87	1.61	1.18
326	0.09	0.07	0.17		1.03	1.67	0.68	1.14	2.09	1.54
198	0.01		DIPHENYLMERCURY	587859						
77	0.72	0.56	0.48		2.85	4.59	1.96	3.28	6.08	4.47
356	0.95	0.74	0.02		0.09	0.15	0.06	0.11	0.20	0.15
199	0.01		TETRAPHENYLTIN							
197	1.40	1.13	0.27		1.70	2.71	0.69	1.47	4.21	3.13
351	1.30	1.05	0.25		1.58	2.51	0.82	1.37	3.91	2.91
200	0.01		BENZYLCHLORIDE	100447						
91	1.55	1.18	0.28		1.77	2.82	0.93	1.54	4.42	3.28
126	0.42	0.32	0.08		0.48	0.76	0.25	0.42	1.20	0.89
201	0.01		4-CHLOROBENZONITRILE	623030						
102	0.55	0.42	0.10		0.63	0.99	0.33	0.55	1.57	1.16
137	2.10	1.57	0.36		2.38	3.79	1.25	2.08	5.95	4.40
202	0.01		3-CHLOROBENZALDEHYDE	587042						
111	0.06	0.05	0.01		0.06	0.12	0.04	0.07	0.20	0.14
139	0.12	0.10	0.02		0.15	0.24	0.08	0.13	0.38	0.28
203	0.01		O-CHLOROANISOLE	766518						
127	0.60	0.46	0.11		0.69	1.09	0.36	0.60	1.71	1.27
142	1.32	1.00	0.24		0.50	2.40	0.79	1.31	3.76	2.79
204	0.01		CHLOROBENZAMIDE	619567						
89	0.70	0.55	0.13		0.77	1.25	0.50	0.84	1.57	1.16
155	0.38	0.30	0.07		0.42	0.68	0.27	0.46	0.85	0.63

Internal/External Standard File for Cmpd Class # 7

Cmpd#	Recovery		Compound Name									
	Std #59		Std #60		Std #61		Std #62		Std #63			
Mass	110	125	82	110	264	-	188	-	99	-		
192	0.01		BENZOTHIAZOLE	95169								
135	1.14	3.76	1.46	0.57	0.59		0.11		1.68			
193	0.01		PHENYLCARBAMATE	102090								
94	0.87	2.92	1.20	0.46	0.44		0.10		1.30			
137	0.01	0.04	0.01	0.01	0.00		0.00		0.02			
194	0.01		2,4-DINITROTOLUENE	121142								
89	0.27	0.88	0.34	0.13	0.14		0.03		0.39			
165	0.50	1.66	0.64	0.25	0.26		0.05		0.74			
195	0.01		BENZYLSULFIDE	538749								
91	2.47	8.62	3.72	1.44	1.11		0.27		3.90			
123	0.63	2.19	0.94	0.37	0.28		0.07		0.99			
196	0.01		DIPHENYLSULFONE	127639								
125	3.00	11.09	4.77	1.85	1.22		0.35		5.05			
218	0.67	2.36	1.02	0.29	0.30		0.07		1.07			
197	0.01		TRIPHENYLPHOSPHATE	115866								
325	1.98	6.58	2.55	0.95	1.03		0.18		0.78			
326	0.06	0.22	0.08	0.03	0.03		0.01		1.02			
198	0.01		DIPHENYLMERCURY	587859								
77	0.53	1.75	0.68	0.26	0.26		0.05		2.94			
356	0.69	2.28	0.88	0.34	0.35		0.06		0.10			
199	0.01		TETRAPHENYLTIN									
197	1.10	3.66	1.57	0.61	0.44		0.11		1.56			
351	1.03	3.40	1.46	0.57	0.41		0.11		1.54			
200	0.01		BENZYLCHLORIDE	100447								
91	1.10	3.81	1.54	0.64	0.50		0.12		1.71			
126	0.30	1.03	0.45	0.17	0.12		0.03		0.47			
201	0.01		4-CHLOROBENZONITRILE	623033								
102	0.39	1.35	0.58	0.23	0.18		0.04		0.61			
137	1.49	5.12	2.21	0.85	0.67		0.16		2.32			
202	0.01		3-CHLOROBENZALDEHYDE	587042								
111	0.05	0.17	0.07	0.03	0.02		0.00		0.08			
139	0.10	0.32	0.14	0.05	0.04		0.01		0.15			
203	0.01		O-CHLOROANISOLE	766518								
127	0.43	1.48	0.64	0.25	0.17		0.05		0.67			
142	0.94	3.24	1.40	0.54	0.36		0.10		1.46			
204	0.01		CHLOROBENZAMIDE	619567								
139	0.51	1.70	0.66	0.26	0.27		0.05		0.76			
155	0.28	0.92	0.36	0.14	0.15		0.03		0.41			

Internal/External Standard File for Cmpd Class # 7

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
205	0.01		3,4-DICHLOROBENZALDEHYDE		6287383					
173	0.48	0.39	0.09		0.58	0.93	0.31	0.57	1.46	1.07
174	0.32	0.26	0.06		0.39	0.62	0.21	0.34	0.98	0.72
206	0.01		1,2,4-TRICHLOROBENZENE		120821					
145	0.34	0.26	0.06		0.40	0.63	0.22	0.36	0.80	0.57
180	1.30	1.00	0.24		1.50	2.40	0.83	1.37	3.03	2.16
207	0.01		2-BROMO-1-CHLOROBENZENE		694804					
190	0.78	0.61	0.14		0.85	1.38	0.55	0.92	1.74	1.28
192	1.04	0.81	0.19		1.14	1.84	0.74	1.24	2.33	1.71
208	0.01		1,2-DICHLORONAPHTHALENE		2050693					
161	0.44	0.34	0.08		0.50	0.78	0.28	0.46	1.01	0.72
196	2.17	1.67	0.40		2.51	3.88	1.38	2.29	5.03	3.58
209	0.01		1,2,4,5-TETRACHLOROBENZENE		95943					
214	1.18	0.90	0.22		1.29	2.09	0.84	1.40	2.63	1.94
216	1.54	1.18	0.28		1.69	2.72	1.09	1.83	3.43	2.52
210	0.01		P-DIBROMOBENZENE		106376					
234	0.68	0.52	0.12		0.77	1.23	0.41	0.67	1.93	1.43
236	1.29	1.00	0.23		1.48	2.36	0.78	1.30	3.77	2.93
211	0.01		4-BROMODIPHENYLETHER		6452499					
248	1.08	0.81	0.20		1.19	1.92	0.77	1.29	2.42	1.78
250	1.13	0.88	0.21		1.26	2.04	0.82	1.37	2.57	1.89
212	0.01		HEXACHLOROBENZENE		118741					
284	0.74	0.56	0.13		0.84	1.34	0.44	0.73	2.10	1.55
286	0.60	0.46	0.11		0.68	1.08	0.36	0.59	1.70	1.26
213	0.01		METHYLSTEARATE		112618					
74	3.42	2.65	0.63		3.89	6.28	2.54	4.25	7.90	5.81
87	2.22	1.72	0.41		2.52	4.07	1.65	2.76	5.13	3.77

Internal/External Standard File for Cmpd Class # 7

Cmpd#	Recovery Std #59		Compound Name Std #60		Std #61		Std #62		Std #63	
Mass	110	125	82	110	264	-	188	-	99	-
205	0.01		3,4-DICHLOROBENZALDEHYDE				6287383			
173	0.37	1.25	0.54	0.21	0.17		0.04		0.57	
174	0.25	0.84	0.36	0.14	0.11		0.03		0.38	
206	0.01		1,2,4-TRICHLOROBENZENE				120821			
145	0.24	0.80	0.33	0.13	0.12		0.03		0.36	
180	0.89	3.05	1.25	0.48	0.46		0.10		1.36	
207	0.01		2-BROMO-1-CHLOROBENZENE				694804			
190	0.57	1.88	0.73	0.28	0.30		0.05		0.84	
192	0.76	2.52	0.98	0.38	0.40		0.07		1.12	
208	0.01		1,2-DICHLORONAPHTHALENE				2050693			
161	0.31	1.02	0.42	0.16	0.15		0.03		0.46	
196	1.52	5.08	2.08	0.80	0.76		0.17		2.27	
209	0.01		1,2,4,5-TETRACHLOROBENZENE				95943			
214	0.86	2.85	1.11	0.43	0.45		0.08		1.27	
216	1.12	3.72	1.44	0.56	0.58		0.11		1.66	
210	0.01		P-DIBROMOBENZENE		106376					
234	0.49	1.66	0.72	0.28	0.19		0.05		0.75	
236	0.93	3.18	1.38	0.53	0.45		0.10		1.45	
211	0.01		4-BROMODIPHENYLETHER				6452499			
248	0.79	2.61	1.01	0.39	0.41		0.07		1.17	
250	0.84	2.78	1.08	0.42	0.44		0.08		1.24	
212	0.01		HEXACHLOROBENZENE		118741					
284	0.53	1.83	0.78	0.30	0.24		0.06		0.82	
286	0.43	1.46	0.63	0.24	0.19		0.05		0.66	
213	0.01		METHYLSTEARATE		112618					
74	2.58	8.56	3.32	1.29	1.33		0.24		3.83	
87	1.67	5.55	2.15	0.83	0.87		0.16		2.48	

Table B-8. RMRs AND RECOVERIES FOR WABN COMPOUNDS
(ACCUMULATOR COLUMN, pH 8.0)

Class No. 8	
Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
54	d_8-Naphthalene (internal)
56	d_5-Nitrobenzene (internal)
57	d_{10}-o-Xylene (internal)
58	d_5-Phenylethanol (internal)
59	d_5-Acetophenone (internal)
60	d_5-Propiophenone (internal)
61	d_{12}-Perylene (internal)
62	d_9-Acridine (internal)
63	d_5-Phenol (internal)

MATRIX OF STANDARD ION RMRs

Compound	Ion	Recovery	Standard: d_5-Phenol m/z 99	d_{10}-o-Xylene m/z 98	d_{10}-o-Xylene m/z 116	d_8-Naphthalene m/z 136	d_5-Nitrobenzene m/z 82	d_5-Nitrobenzene m/z 128	d_5 Phenylethanol m/z 88	d_5 Phenylethanol m/z 112
d_5-phenol	99	0.55	-	.59(2)	.99(9)	17(6)	1.04(5)	1.66(3)	2.44(15)	1.75(15)
d_{10}-o-xylene	98	0.76	1.72(9)[a]	-	1.67(1)	.29(6)	1.79(8)	2.84(8)	4.21(22)	3.02(23)
	116	0.76	1.03(4)	60(0)	-	18(6)	1.07(8)	1.73(8)	2.53(.2)	1.81(23)
d_8-naphthalene	136	0.79	5.97(4)	3.51(7)	5.85(7)	-	6.21(3)	9.98(3)	14.63(15)	10.59(18)
d_5-nitrobenzene	82	0.82	97(4)	57(10)	95(10)	16(3)	-	1.60(1)	2.35(12)	1.70(16)
	128	0.82	61(2)	35(3)	59(3)	10(1)	63(1)	-	1.47(16)	1.07(15)
d_5-phenylethanol	88	0.78	.42(15)	.25(24)	42(24)	.07/ 24(18)	44(16)	70(15)	-	.73(2)
	112	0.78	58(15)	35(22)	.58(23)	098(18)	61(16)	95(16)	1.39(2)	-
d_5-propiophenone	82	0.93	1.09(4)	65(13)	1.07(11)	18(8)	1.13(6)	1.82(6)	2.63(11)	1.90(10)
	110	0.93	2.85(5)	1.67(13)	2.78(14)	48(17)	2.94(6)	4.72(6)	6.84(12)	4.95(11)
d_5-acetophenone	110	0.87	1.52(2)	.90(7)	1.50(8)	25(4)	1.60(5)	2.55(1)	3.71(17)	2.68(16)
	125	0.87	46(2)	27(8)	45(7)	36(3)	48(3)	76(4)	1.13(18)	81(17)
d_{12}-perylene	264	0.62	3.56(13)	2.09(7)	3.48(8)	.0'o .60(9)	3.70(11)	5.90(12)	8.52(.25)	6.37(28)
d_9-acridine	188	0.87	1.45(7)	86(15)	1.43(15)	24(8)	1.51(6)	2.40(6)	3.52(13)	2.55(13)
4-Fluoro-2-iodotoluene	109	NA	1.10(4)	65(7)	1.08(8)	18(3)	1.14(2)	1.82(2)	2.69(18)	1.97(19)
	236	NA	1.43(8)	.64(6)	1.39(7)	24(6)	1.48(3)	2.37(3)	3.48(18)	2.52(18)

(continued)

Compound	Ion	Recovery	Standard: d_5-Propiophenone m/z 82	d_5-Propiophenone m/z 110	d_5-Acetophenone m/z 110	d_5-Acetophenone m/z 125	d_{12}-Perylene m/z 264	d_9-Acridine m/z 188	4-Fluoro-2-iodotoluene m/z 109	4-Fluoro-2-iodotoluene m/z 236
d_5-phenol	99	0.55	92(5)	.35(5)	67(2)	2.21(3)	58(15)	70(7)	91(5)	71(6)
d_{10}-o-xylene	98	0.76	1.59(12)	61(13)	1.83(7)	3.77(7)	53(10)	1.20(23)	1.56(6)	1.21(6)
	116	0.76	95(13)	37(12)	67(6)	2.27(7)	32(10)	72(23)	94(6)	73(6)
d_8-naphthalene	136	0.74	5.51(8)	2.13(8)	5.91(4)	13.14(3)	1.76(15)	4.20(8)	5.45(8)	4.20(8)
d_5 nitrobenzene	82	0.82	89(6)	.34(6)	63(4)	2.32(4)	29(19)	67(6)	88(2)	68(3)
	128	0.82	55(6)	.22(6)	34(1)	1.32(3)	18(20)	42(6)	55(3)	42(3)
d_5-phenylethanol	84	0.78	.39(11)	.35(10)	28(16)	93(12)	33(28)	29(13)	38(18)	.30(17)
	112	0.78	53(10)	.21(9)	19(16)	1.28(16)	18(28)	41(13)	52(19)	42.16)
d_5-propiophenone	82	0.93	-	.39(1)	72(7)	2.40(6)	33(25)	76(5)	1.00(7)	77(7)
	110	0.93	2.60(1)		1.83(5)	6.21(6)	8.(39)	2.00(5)	2.59(7)	1.99(7)
d_5-acetophenone	110	0.87	1.41(6)	55(6)	-	3.39(1)	47(14)	1.10(9)	1.37(4)	1.07(2)
	125	0.87	42(6)	16(5)	50(2)	-	14(18)	32(9)	42(2)	32(3)
d_{12}-perylene	264	0.82	3.08(14)	1.27(16)	2.37(12)	7.91(12)	-	2.50(16)	3.21(9)	2.51(9)
d_9-acridine	188	0.87	1.35(5)	52(5)	95(10)	3.15(11)	37(10)	-	1.32(8)	1.03(6)
4-fluoro-2-iodotoluene	109	NA	1.03(7)	.33(7)	71(2)	2.40(2)	19(12)	76(8)	-	77(1)
	236	NA	1.31(7)	51(7)	92(3)	3.11(2)	42(16)	1.00(4)	1.30(3)	-

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Internal/External Standard File for Cmpd Class # 8

Cmpd#	Recovery Std # 2		Compound Name	Std #54		Std #56		Std #57		Std #61	
Mass	109	236	136	-		82	128	98	116	264	-
100	0.01		PYRIDINE	110861							
52	0.29	0.22		0.05		0.33	0.51	0.19	0.32		
79	0.44	0.34		0.08		0.51	0.78	0.30	0.50		
101	0.36		ALPHA-PICOLINE	109068							
66	0.26	0.20		0.05		0.30	0.46	0.16	0.27		
93	0.66	0.51		0.12		0.76	1.18	0.40	0.66		
102	0.34		ANILINE	62533							
66	0.23	0.19		0.04		0.28	0.41	0.15	0.24		
93	0.76	0.54		0.13		0.81	1.25	0.45	0.74		
103	0.95		LUTIDINE	108685							
106	0.13	0.10		0.02		0.15	0.25	0.08	0.13		
107	0.22	0.16		0.04		0.24	0.39	0.13	0.21		
104	0.01		TOLUIDINE	106490							
106	0.89	0.69		0.16		0.97	1.57	0.64	1.07		
107	0.71	0.56		0.13		0.78	1.27	0.51	0.86		
105	0.95		INDOLE	120729							
90	0.72	0.54		0.13		0.82	1.30	0.43	0.71		
117	1.92	1.45		0.34				1.14	1.89	0.61	
106	0.84		2,3,6-TRIMETHYLPYRIDINE	1462846							
120	0.66	0.51		0.12		0.76	1.18	0.42	0.69		
121	0.90	0.69		0.17		1.03	1.61	0.55	0.91		
107	0.87		2,6-DIMETHYLANILINE	1300738							
106	0.36	0.27		0.06		0.41	0.65	0.21	0.36		
121	0.57	0.44		0.10		0.66	1.04	0.34	0.57		
108	0.95		M-CHLOROANILINE	108429							
127	1.09	0.84		0.20		1.26	1.94	0.69	1.15		
129	0.34	0.26		0.06		0.29	0.60	0.22	0.36		
109	0.91		QUINOLINE	91225							
129	1.82	1.41		0.34		1.99	3.22	1.30	2.17		
110	0.77		P-NITROANILINE	100016							
65	0.44	0.35		0.08		0.52	0.83	0.27	0.46		
138	0.56	0.45		0.11		0.67	1.07	0.35	0.58		
111	0.90		2,4-DIMETHYLQUINOLINE	1198374							
156	0.41	0.32		0.08		0.47	0.75	0.26	0.43		
157	2.01	1.54		0.37		2.31	3.59	1.27	2.11		
112	0.01		1,8-DIAMINONAPHTHALENE								
114	0.03	0.02		0.00		0.04	0.06	0.02	0.03		
141	0.05	0.04		0.01		0.06	0.01	0.03	0.05		

Internal/External Standard File for Cmpd Class # 8

Cmpd# / Mass	Recovery Std #62 188 -	Compound Name Std #63 99 -
100	0.01	PYRIDINE 110861
52	0.02	0.30
79	0.04	0.50
101	0.36	ALPHA-PICOLINE 109068
66	0.02	0.27
93	0.05	0.69
102	0.34	ANILINE 62533
66	0.02	0.24
93	0.05	0.73
103	0.95	LUTIDINE 108485
106	0.01	0.15
107	0.02	0.24
104	0.01	TOLUIDINE 106490
106	0.06	0.96
107	0.05	0.77
105	0.95	INDOLE 120729
90	0.05	0.79
117	0.15	2.12
106	0.84	2,3,6-TRIMETHYLPYRIDINE 1462846
120	0.05	0.67
121	0.07	0.94
107	0.87	2,6-DIMETHYLANILINE 1300738
106	0.03	0.40
121	0.04	0.64
108	0.95	M-CHLORANILINE 108429
127	0.98	1.14
129	0.03	0.35
109	0.91	QUINOLINE 91225
129	0.12	1.96
110	0.77	P-NITRANILINE 100016
65	0.04	0.51
138	0.05	0.65
111	0.90	2,4-DIMETHYLQUINOLINE 1198374
156	0.03	0.43
157	0.15	2.09
112	0.01	1,8-DIAMINONAPHTHALENE
114	0.00	0.03
141	0.00	0.55

Internal/External Standard File for Cmpd Class # 8

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #61	
Mass	109	236	136	-	82	128	98	116	264	-
113	0.62		NICOTINE	54115						
84	1.17	0.90	0.22		1.35	2.09	0.74	1.23		
133	0.28	0.21	0.05		0.32	0.49	0.17	0.29		
114	0.82		CARBAZOLE	86748						
167	3.73	2.88	0.69		4.30	6.66	2.37	3.92		
115	0.82		2-AMINOBIPHENYL	90415						
168	6.79	5.11	1.20		7.65	12.18	4.61	6.67		
169	12.72	9.45	2.22		14.15	22.54	7.42	12.30		
116	0.85		DIPHENYLAMINE	122394						
168	1.48	1.14	0.27		1.71	2.65	0.94	1.56		
169	2.79	2.15	0.52		3.22	4.99	1.77	2.93		
117	0.01		DICYCLOHEXYLAMINE	101837						
56	0.33	0.37	0.06		0.39	0.63	0.21	0.35		
138	0.96	0.76	0.18		1.12	1.80	0.61	1.02		
118	0.82		TRIBUTYLAMINE	102829						
100	0.42	0.33	0.08		0.49	0.75	0.27	0.44		
142	1.53	1.18	0.28		1.77	2.74	0.97	1.61		
119	0.86		CAFFEINE	58082						
109	0.10	0.08	0.02		0.12	0.17	0.06	0.10		
194	0.19	0.15	0.04		0.22	0.34	0.12	0.20		
120	0.50		DIBENZYLAMINE	103491						
91	1.62	1.26	0.30		1.78	2.87	1.16	1.94		
197	0.13	0.11	0.03		0.15	0.24	0.10	0.16		
121	0.69		N,N-DIMETHYLDODECYLAMINE	112185						
58	4.72	3.88	0.87		5.47	8.83	3.58	5.99		
59	0.17	0.13	0.03		0.20	0.30	0.13	0.21		
122	0.71		ATRAZINE	1912249						
200	2.75	2.20	0.52		3.28	5.23	1.72	2.86		
215	1.67	1.34	0.31		2.00	3.18	1.05	1.74		
123	0.66		HEPTANONE(2)	110430						
43	1.21	0.94	0.22		1.33	2.14	0.85	1.14		
58	0.75	0.58	0.14		0.83	1.33	0.53	0.88		
124	0.01		BUTOXYETHANOL	111762						
41	0.21	0.17	0.04		0.25	0.40	0.13	0.22		
57	0.55	0.42	0.10		0.63	1.03	0.35	0.58		
125	0.77		2-OCTANONE	111137						
43	1.30	1.01	0.24		1.43	2.31	0.91	1.53		
58	1.02	0.79	0.19		1.11	1.80	0.71	1.19		

Internal/External Standard File for Cmpd Class # 8

Cmpd# / Mass	Recovery Std #62 188 -	Compound Name Std #63 99 -
113	0.62	NICOTINE 54115
84	0.09	1.22
133	0.02	0.29
114	0.82	CARBAZOLE 86748
167	0.31	4.22
115	0.82	2-AMINOBIPHENYL 90415
168	0.51	7.45
169	0.95	13.80
116	0.85	DIPHENYLAMINE 122394
168	0.11	1.55
169	0.22	2.91
117	0.01	DICYCLOHEXYLAMINE 101837
56	0.03	0.38
138	0.08	1.09
118	0.82	TRIBUTYLAMINE 102829
100	0.03	0.44
142	0.12	1.59
119	0.86	CAFFEINE 58082
109	0.01	0.10
194	0.02	0.21
120	0.50	DIBENZYLAMINE 103491
91	0.11	1.74
197	0.01	0.14
121	0.69	N,N-DIMETHYLDODECYLAMINE 112185
58	0.34	5.37
59	0.01	0.19
122	0.71	ATRAZINE 1912249
200	0.22	3.26
215	0.13	1.95
123	0.66	HEPTANONE(2) 110430
43	0.08	1.30
58	0.05	0.81
124	0.01	BUTOXYETHANOL 111762
41	0.02	0.22
57	0.04	0.57
125	0.77	2-OCTANONE 111137
43	0.09	1.40
58	0.07	1.09

Internal/External Standard File for Cmpd Class # 8

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #61	
Mass	109	236	136	-	82	128	98	116	264	-
126	0.52		BUTYLPROPIONATE		590012					
57	1.48	1.14	0.27		1.71	2.73	0.90	1.49		
75	0.44	0.34	0.08		0.51	0.82	0.27	0.45		
127	0.85		ISOPHORONE		78591					
82	1.77	1.36	0.33		2.04	3.17	1.13	1.86		
138	0.39	0.30	0.07		0.45	0.72	0.25	0.41		
128	0.64		FENCHONE		1195759					
69	0.66	0.51	0.12		0.72	1.17	0.47	0.78		
81	1.44	1.12	0.27		1.58	2.55	1.02	1.71		
129	0.92		ALPHA-TERPINEOL		98555					
59	0.56	0.43	0.10		0.65	1.00	0.36	0.59		
136	0.32	0.25	0.06		0.37	0.58	0.21	0.34		
130	0.94		N-DECANOL	112301						
41	0.40	0.31	0.07		0.46	0.74	0.25	0.42		
43	0.44	0.34	0.08		0.51	0.79	0.28	0.46		
131	0.91		DIMETHYLADIPATE		627930					
59	0.56	0.45	0.10		0.64	1.03	0.41	0.69		
114	0.44	0.35	0.08		0.49	0.79	0.32	0.54		
132	0.45		METHYLSTEARATE		112618					
74	3.42	2.65	0.63		3.89	6.28	2.54	4.25		
87	2.22	1.72	0.41		2.52	4.07	1.65	2.76		
133	0.01		N-DECANE	124185						
43	1.47	1.11	0.26		1.67	2.66	0.88	1.46		
57	1.42	1.08	0.25		1.64	2.61	0.85	1.41		
134	0.44		N-TRIDECANE	629505						
43	2.18	1.64	0.34		2.48	3.95	1.30	2.16		
57	2.75	2.09	0.50		3.14	5.01	1.66	2.77		
135	0.42		N-TETRADECANE		629594					
43	2.52	1.92	0.45		2.88	4.58	1.51	2.51		
57	3.40	2.55	0.61		3.87	6.16	2.03	3.37		
136	0.01		N-PENTADECANE		692692					
57	2.78	2.14	0.52		3.22	4.99	1.77	2.94		
71	1.73	1.33	0.32		2.01	3.11	1.10	1.83		
137	0.45		N-HEXADECANE		544763					
43	1.90	1.45	0.34		2.16	3.45	1.13	1.89		
57	2.72	2.08	0.49		3.11	4.96	1.63	2.71		
138	0.01		N-HEPTADECANE		629787					
57	3.13	2.41	0.58		3.61	5.59	1.99	3.30		
71	2.07	1.60	0.38		2.39	3.70	1.32	2.18		

Internal/External Standard File for Cmpd Class # 8

Cmpd# / Mass	Recovery Std #62 188 -	Compound Name Std #63 99 -	
126	0.52	BUTYLPROPIONATE	590012
57	0.12	1.66	
75	0.04	0.50	
127	0.85	ISOPHORONE	78591
82	0.14	1.80	
138	0.03	0.41	
128	0.64	FENCHONE	1195759
69	0.05	0.71	
81	0.10	1.55	
129	0.92	ALPHA-TERPINEOL	98555
59	0.04	0.58	
136	0.03	0.34	
130	0.94	N-DECANOL	112301
41	0.03	0.41	
43	0.03	0.46	
131	0.91	DIMETHYLADIPATE	627930
59	0.04	0.62	
114	0.03	0.48	
132	0.45	METHYLSTEARATE	112618
74	0.24	3.83	
87	0.16	2.48	
133	0.01	N-DECANE	124185
43	0.11	1.62	
57	0.11	1.58	
134	0.44	N-TRIDECANE	629505
43	0.17	2.41	
57	0.21	3.09	
135	0.42	N-TETRADECANE	629594
43	0.19	2.80	
57	0.26	3.77	
136	0.01	N-PENTADECANE	692692
57	0.22	2.92	
71	0.14	1.82	
137	0.45	N-HEXADECANE	544763
43	0.15	2.11	
57	0.21	3.03	
138	0.01	N-HEPTADECANE	629787
57	0.24	3.27	
71	0.16	2.17	

Internal/External Standard File for Cmpd Class # 8

Cmpds	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #61
Mass	109	236	136	-	82	128	98	116	264	-
139	0.01		N-OCTADECANE		593453				
57	2.99	2.51	0.59		3.75	5.98	1.88	3.14		
71	1.98	1.66	0.39		2.48	3.95	1.25	2.08		
140	0.47		N-NONADECANE		629925					
71	2.12	1.61	0.38		2.42	3.85	1.27	2.11		
85	1.42	1.08	0.25		1.61	2.57	0.85	1.41		
141	0.08		N-EICOSANE		1112958					
57	4.43	3.41	0.82		5.11	7.92	2.82	4.66		
71	3.03	2.33	0.56		3.50	5.43	1.93	3.19		
142	0.63		N-HENEICOSANE		629947					
57	3.93	2.96	0.70		4.43	7.05	2.32	3.86		
71	2.71	2.05	0.48		3.07	4.88	1.61	2.67		
143	0.66		N-DOCOSANE		629970					
57	3.73	2.98	0.70		4.46	7.10	2.33	3.88		
71	2.60	2.08	0.49		3.11	4.95	1.63	2.70		
144	0.66		N-TRICOSANE		638675					
57	3.99	3.19	0.75		4.77	7.60	2.49	4.14		
71	2.80	2.24	0.53		3.35	5.34	1.75	2.91		
145	0.74		PHENYLACETATE		122792					
94	1.84	1.43	0.34		2.01	3.25	1.30	2.18		
136	0.25	0.20	0.05		0.28	0.45	0.18	0.30		
146	0.79		BENZYLACETATE		140114					
91	0.52	0.40	0.09		0.57	0.92	0.37	0.62		
108	1.09	0.85	0.20		1.19	1.92	0.77	1.29		
147	0.36		METHYLBENZENESULFONATE							
77	1.24	0.94	0.22		1.41	2.25	0.74	1.23		
172	0.44	0.34	0.08		0.50	0.80	0.26	0.44		
148	0.46		METHYLTOLUENESULFONATE							
91	1.60	1.21	0.29		1.81	2.89	0.95	1.58		
155	0.72	0.54	0.13		0.81	1.29	0.42	0.71		
149	0.74		DIMETHYLPHTHALATE		131113					
77	0.81	0.63	0.15		0.94	1.45	0.52	0.85		
163	5.29	4.07	0.98		6.10	9.46	3.36	5.56		
150	0.53		ETHYLTOLUENESULFONATE							
91	1.74	1.32	0.31		1.97	3.14	1.03	1.72		
155	1.18	0.94	0.22		1.40	2.23	0.73	1.21		
151	0.87		DIETHYLPHTHALATE		84662					
149	3.19	2.43	0.57		3.65	5.79	1.90	3.17		
177	0.80	0.61	0.14		0.93	1.47	0.48	0.80		

Internal/External Standard File for Cmpd Class # 8

Cmpd# / Mass	Recovery Std #62 188 -	Compound Name Std #63 99 -	
139	0.01	N-OCTADECANE	591453
57	0.24	3.65	
71	0.06	2.41	
140	0.47	N-NONADECANE	629925
71	0.16	2.35	
85	0.11	1.57	
141	0.08	N-EICOSANE	1112958
57	0.35	4.63	
71	0.23	3.17	
142	0.63	N-HENEICOSANE	629947
57	0.30	4.31	
71	0.21	2.99	
143	0.66	N-DOCOSANE	629970
57	0.30	4.35	
71	0.21	3.04	
144	0.66	N-TRICOSANE	638675
57	0.32	4.65	
71	0.22	3.27	
145	0.74	PHENYLACETATE	122792
94	0.13	1.98	
136	0.02	0.28	
146	0.79	BENZYLACETATE	140114
91	0.04	0.56	
108	0.07	1.17	
147	0.36	METHYLBENZENESULFONATE	
77	0.09	1.38	
172	0.03	0.49	
148	0.46	METHYLTOLUENESULFONATE	
91	0.12	1.76	
155	0.05	0.79	
149	0.74	DIMETHYLPHTHALATE	131113
77	0.06	0.85	
163	0.41	5.51	
150	0.53	ETHYLTOLUENESULFONATE	
91	0.13	1.92	
155	0.09	1.36	
151	0.87	DIETHYLPHTHALATE	84662
9	0.24	3.54	
177	0.06	0.89	

Internal/External Standard File for Cmpd Class # 8

Cmpds	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #61	
Mass	109	236	136	-	82	128	98	116	264	-
152	0.01		DIBUTYLPHTHALATE		84742					
57	0.29	0.23	0.05		0.34	0.52	0.19	0.31		
149	7.17	5.52	1.33		8.27	12.80	4.55	7.54		
153	0.64		BUTYLBENZYLPHTHALATE							
91	2.09	1.62	0.38		2.28	3.69	1.48	2.48		
149	3.37	2.62	0.62		3.69	5.95	2.40	4.01		
154	0.74		DIETHYLHEXYLPHTHALATE				117817			
149	5.22	4.07	0.96		5.71	9.23	3.74	6.26		
167	1.98	1.54	0.37		2.17	3.51	1.42	2.37		
155	0.01		BENZALDEHYDE		100527					
77	0.36	0.28	0.07		0.42	0.64	0.23	0.38		
105	0.47	0.31	0.07		0.46	0.70	0.25	0.42		
156	0.88		TOLUALDEHYDE		529204					
91	0.54	0.44	0.10		0.65	1.04	0.34	0.57		
119	0.63	0.51	0.12		0.77	1.23	0.41	0.68		
157	0.92		ACETOPHENONE			98862				
77	0.38	0.64	0.15		0.96	1.53	0.53	0.87		
105	1.22	0.94	0.23		1.41	2.25	0.78	1.29		
158	0.01		SALICYLALDEHYDE			90028				
121	0.56	0.44	0.10		0.61	0.99	0.40	0.67		
122	0.50	0.47	0.11		0.60	1.07	0.43	0.72		
159	0.96		ANISALDEHYDE		123115					
135	1.37	1.08	0.25		1.53	2.47	0.91	1.66		
136	0.60	0.47	0.18		1.07	1.73	0.70	1.16		
160	0.55		PHENOL	108952						
94	1.07	0.84	0.20		1.18	1.90	0.76	1.27		
161	0.63		CRESOL(P)		106445					
107	1.21	0.93	0.23		1.40	2.25	0.80	1.29		
108	1.07	0.82	0.20		1.24	1.99	0.69	1.14		
162	0.95		2,3-DIMETHYLPHENOL		526750					
107	0.87	0.67	0.16		1.00	1.61	0.57	0.95		
122	0.91	0.70	0.17		1.05	1.64	0.58	0.96		
163	0.88		ISOPROPYLPHENOL(O)			88699				
121	1.79	1.36	0.32		2.04	3.25	1.07	1.78		
136	0.07	0.56	0.12		0.75	1.19	0.39	0.65		
164	0.01		O-NITROPHENOL		88755					
65	0.03	0.02	0.00		0.03	0.05	0.02	0.03		
139	0.13	0.10	0.02		0.14	0.23	0.09	0.15		

Internal/External Standard File for Cmpd Class # 8

Cmpd# / Mass	Recovery Std #62 / 188	Compound Name / Std #63 / 99	
152	0.01	DIBUTYLPHTHALATE	84742
57	0.02	0.31	
149	0.55	7.47	
153	0.64	BUTYLBENZYLPHTHALATE	
91	0.14	2.24	
149	0.23	3.62	
154	0.74	DIETHYLHEXYLPHTHALATE	117817
149	0.35	5.61	
167	0.13	2.13	
155	0.01	BENZALDEHYDE	100527
77	0.03	0.38	
105	0.03	0.42	
156	0.88	TOLUALDEHYDE	529204
91	0.05	0.64	
119	0.05	0.75	
157	0.92	ACETOPHENONE	98862
77	0.06	0.87	
105	0.09	1.28	
158	0.01	SALICYLALDEHYDE	90028
121	0.04	0.60	
122	0.04	0.65	
159	0.96	ANISALDEHYDE	123115
135	0.09	1.50	
136	0.04	1.05	
160	0.55	PHENOL	108952
94	0.07	1.15	
161	0.63	CRESOL(P)	106445
107	0.10	1.31	
108	0.09	1.16	
162	0.95	2,3-DIMETHYLPHENOL	526750
107	0.07	0.94	
122	0.07	0.95	
163	0.88	ISOPROPYLPHENOL(O)	88699
121	0.14	1.99	
136	0.05	0.73	
164	0.01	O-NITROPHENOL	88755
65	0.00	0.03	
139	0.01	0.14	

Internal/External Standard File for Cmpd Class # 8

Cmpds	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #61
Mass	109	236	136	-	82	128	98	116	264	-
165	0.90		4-CHLORO-3-METHYLPHENOL 59507						
107	0.93	0.71	0.17		1.06	1.68	0.55	0.92	
142	1.02	0.77	0.18		1.16	1.84	0.61	1.01	
166	0.01		4-CHLOROCRESOL						
107	0.83	0.64	0.16		0.97	1.57	0.53	0.88	
142	0.94	0.72	0.17		1.09	1.77	0.60	0.99	
167	0.01		1-NAPHTHOL 90153						
115	0.35	0.26	0.06		0.38	0.61	0.20	0.34	
144	0.61	0.45	0.11		0.67	1.07	0.35	0.29	
168	0.86		P-TERT-BUTYLPHENOL 98544						
107	0.56	0.43	0.10		0.65	1.03	0.34	0.56	
135	1.96	1.49	0.35		2.22	3.54	1.17	1.94	
169	0.32		2-NITROCRESOL 119335						
77	0.26	0.20	0.05		0.30	0.46	0.07	0.27	
153	0.74	0.57	0.14		0.83	1.33	0.46	0.78	
170	0.78		2,4-DICHLOROPHENOL 120832						
162	1.13	0.88	0.21		1.24	2.00	0.80	1.34	
164	0.72	0.53	0.13		0.78	1.27	0.51	0.85	
171	0.66		2,4,6-TRICHLOROPHENOL 88062						
196	0.81	0.63	0.15		0.89	1.44	0.58	0.97	
198	0.83	0.64	0.15		0.91	1.46	0.59	0.98	
172	0.73		DI-TERT-BUTYL-4-METHYLPHENOL 128370						
205	2.53	1.97	0.47		2.78	4.49	1.81	3.03	
220	0.67	0.52	0.12		0.73	1.18	0.48	0.80	
173	0.00		PENTACHLOROPHENOL 87865						
264	0.29	0.22	0.05		0.34	0.54	0.19	0.31	
266	0.47	0.36	0.09		0.55	0.91	0.32	0.54	
174	0.65		2-METHYLNAPHTHALENE 91576						
141	2.03	1.58	0.38		2.23	3.60	1.44	2.42	
142	2.51	1.96	0.46		2.76	4.45	1.79	2.99	
175	0.76		ACENAPHTHENE 83329						
153	1.26	0.98	0.23		1.38	2.22	0.89	1.49	
154	3.40	2.64	0.63		3.73	6.02	2.41	4.04	
176	0.78		BIPHENYL 92524						
154	2.28	1.78	0.42		2.51	4.04	1.63	2.72	
177	0.78		1,8-DIMETHYLNAPHTHALENE 569415						
141	1.59	1.24	0.29		1.74	2.82	1.13	1.89	
156	2.30	1.79	0.42		2.52	.07	1.63	2.73	

Internal/External Standard File for Cmpd Class # 8

Cmpd#	Recovery Std #62	Compound Name Std #63	
Mass	188 -	99 -	
165	0.90	4-CHLORO-3-METHYLPHENOL	59507
107	0.07	1.03	
142	0.08	1.13	
166	0.01	4-CHLOROCRESOL	
107	0.07	0.91	
142	0.08	1.03	
167	0.01	1-NAPHTHOL	90153
115	0.03	0.38	
144	0.05	0.66	
168	0.86	P-TERT-BUTYLPHENOL	98544
107	0.04	0.62	
135	0.15	2.16	
169	0.32	2-NITROCRESOL	119335
77	0.02	0.27	
153	0.06	0.78	
170	0.78	2,4-DICHLOROPHENOL	120832
162	0.08	1.22	
164	0.05	0.77	
171	0.66	2,4,6-TRICHLOROPHENOL	88062
196	0.05	0.88	
198	0.06	0.89	
172	0.73	DI-TERT-BUTYL-4-METHYLPHENOL	128370
205	0.17	2.73	
220	0.05	0.72	
173	0.00	PENTACHLOROPHENOL	87865
264	0.02	0.31	
266	0.04	0.50	
174	0.65	2-METHYLNAPHTHALENE	91576
141	0.14	2.19	
142	0.17	2.71	
175	0.76	ACENAPHTHENE	83329
153	0.09	1.35	
154	0.23	3.66	
176	0.78	BIPHENYL	92524
154	0.16	2.46	
177	0.78	1,8-DIMETHYLNAPHTHALENE	569415
141	0.11	1.71	
156	0.16	2.48	

Internal/External Standard File for Cmpd Class # 8

Cmpds	Recovery Std # 2		Compound Name	Std #54		Std #56		Std #57		Std #61
Mass	109	236	136	-		82	128	98	116	264	-
178	0.88		FLUORENE	86737						
165	2.74	2.13	0.49			3.01	4.85	1.95	3.27		
166	3.07	2.38	0.57			3.44	5.55	2.23	3.74		
179	0.84		2,3,5-TRIMETHYLNAPHTHALENE	2245387						
155	1.86	1.44	0.34			2.08	3.36	1.36	2.27		
170	2.56	1.99	0.47			2.86	4.62	1.86	3.11		
180	0.78		ANTHRACENE	120127						
178	3.21	2.47	0.60			3.71	5.74	2.04	3.39		
181	0.73		PYRENE	129000						
202	4.89	3.75	0.95			5.66	8.73	3.27	5.18		
182	0.60		9,10-DIMETHYLANTHRACENE	781431						
191	1.33	1.03	0.25			1.45	2.35	0.94	1.57		
206	2.85	2.22	0.53			3.13	5.04	2.01	3.37		
183	0.43		CHRYSENE	218019						
228	2.21	1.73	0.41			2.42	3.92	1.59	2.66		
184	0.62		PERYLENE	198550						
252	1.60	1.23	0.30			1.84	2.86	1.02	1.68		
185	0.71		DICYANOBUTANE	111693						
41	0.66	0.51	0.12			0.72	1.17	0.47	0.79		
54	0.29	0.23	0.05			0.32	0.52	2.10	0.35		
186	0.40		BUTYLCARBAMATE	14994775						
41	0.48	0.36	0.08			0.54	0.86	0.28	0.47		
59	0.24	0.26	0.05			0.29	0.47	0.15	0.25		
187	0.58		DIBUTYLDISULFIDE	110065						
41	0.73	0.56	0.13			0.84	1.34	0.44	0.73		
57	3.09	2.36	0.56			3.54	5.64	1.85	3.09		
188	0.92		BIS(2-CHLOROETHYL)ETHANE	112265						
63	1.71	1.31	0.31			1.97	3.13	1.03	1.71		
93	0.84	0.65	0.15			0.97	1.54	0.51	0.84		
189	0.86		TRIBUTYLPHOSPHATE	126738						
99	4.03	3.10	0.75			4.65	7.20	2.56	4.24		
155	0.88	0.68	0.16			1.01	1.57	0.56	0.92		
190	0.83		ALDRIN	309002						
66	1.33	1.03	0.24			1.49	2.40	0.97	1.62		
263	0.60	0.46	0.11			0.67	1.08	0.44	0.73		
191	0.01		DIHYDROBENZOFURAN	496162						
91	0.68	0.52	0.13			0.79	1.25	0.43	0.72		
120	0.97	0.75	0.18			1.12	1.67	0.66	0.78		

Internal/External Standard File for Cmpd Class # 8

Cmpds	Recovery Std #62	Compound Name Std #63	
Mass	188 -	99 -	
178	0.88	FLUORENE	86737
165	0.19	2.95	
166	0.21	3.38	
179	0.84	2,3,5-TRIMETHYLNAPHTHALENE	2245387
155	0.13	2.05	
170	0.18	2.81	
180	0.78	ANTHRACENE	120127
178	0.25	3.35	
181	0.73	PYRENE	129000
202	0.40	5.36	
182	0.60	9,10-DIMETHYLANTHRACENE	781431
191	0.09	1.42	
206	0.19	3.06	
183	0.43	CHRYSENE	218019
228	0.15	2.39	
184	0.62	PERYLENE	198550
252	0.12	1.65	
185	0.71	DICYANOBUTANE	111693
41	0.05	0.71	
54	0.02	0.32	
186	0.40	BUTYLCARBAMATE	1a994775
41	0.04	0.52	
59	0.02	0.28	
187	0.58	DIBUTYLDISULFIDE	110065
41	0.06	0.82	
57	0.24	3.42	
188	0.92	BIS(2-CHLOROETHYL)ETHANE	112265
63	0.13	1.91	
93	0.06	0.94	
189	0.86	TRIBUTYLPHOSPHATE	126738
99	0.31	4.19	
155	0.07	0.91	
190	0.83	ALDRIN	309002
66	0.09	1.46	
263	0.04	0.66	
191	0.01	DIHYDROBENZOFURAN	496162
91	0.05	0.71	
120	0.07	0.98	

Internal/External Standard File for Cmpd Class # 8

Cmpd#	Recovery Std # 2		Compound Name Std #54		Std #56		Std #57		Std #61	
Mass	109	236	136	-	82	128	98	116	264	-
192	0.70		NITROBENZENE 98953							
77	0.86	0.67	0.16		0.94	1.51	0.61	1.02		
123	0.54	0.42	0.10		0.59	0.95	0.38	0.64		
193	0.85		BENZOTHIAZOLE 95169							
135	1.56	1.21	0.29		1.71	2.76	1.11	1.86		
194	0.01		PHENYLCARBAMATE 102090							
94	1.25	0.96	0.23		1.44	2.23	0.79	1.31		
137	0.02	0.01	0.00		0.02	0.03	0.01	0.02		
195	0.89		2,4-DINITROTOLUENE 121142							
89	0.35	0.28	0.06		0.40	0.65	0.26	0.44		
165	0.71	0.53	0.13		0.75	1.21	0.46	0.76		
196	0.67		BENZYLSULFIDE 538749							
91	3.55	2.68	0.63		4.00	6.38	2.10	3.49		
123	0.90	0.68	0.16		1.02	1.62	0.53	0.89		
197	0.69		DIPHENYLSULFONE 127639							
125	3.82	3.44	0.81		5.16	8.21	2.71	4.51		
218	0.92	0.73	0.17		1.10	1.75	0.58	0.96		
198	0.81		TRIPHENYLPHOSPHATE 115866							
325	2.59	2.01	0.13		0.79	1.28	0.52	0.87		
326	0.09	0.07	0.17		1.03	1.67	0.68	1.14		
199	0.01		DIPHENYLMERCURY 587859							
77	0.72	0.56	0.48		2.85	4.59	1.96	3.28		
356	0.95	0.74	0.02		0.09	0.15	0.06	0.11		
200	0.47		TETRAPHENYLTIN							
197	1.40	1.13	0.27		1.70	2.71	0.89	1.47		
351	1.30	1.05	0.25		1.58	2.51	0.82	1.37		
201	0.35		BENZYLCHLORIDE 100447							
91	1.55	1.18	0.28		1.77	2.82	0.93	1.54		
126	0.42	0.32	0.08		0.48	0.75	0.25	0.42		
202	0.80		4-CHLOROBENZONITRILE 623030							
102	0.55	0.42	0.10		0.63	0.99	0.33	0.55		
137	2.10	1.57	0.36		2.38	3.79	1.25	2.08		
203	0.01		3-CHLOROBENZALDEHYDE 587042							
111	0.06	0.05	0.01		0.08	0.12	0.04	0.07		
139	0.12	0.10	0.02		0.15	0.24	0.08	0.13		
204	0.57		O-CHLOROANISOLE 766518							
127	0.60	0.46	0.11		0.69	1.09	0.36	0.60		
142	1.32	1.00	0.24		0.50	2.40	0.79	1.31		

Internal/External Standard File for Cmpd Class # 0

Cmpd# Mass	Recovery Std #62 188 -	Compound Name Std #63 99 -
192	0.70	NITROBENZENE 98953
77	0.06	0.94
123	0.04	0.59
193	0.85	BENZOTHIAZOLE 95169
135	0.01	1.68
194	0.01	PHENYLCARBAMATE 102090
94	0.10	1.30
137	0.00	0.02
195	0.89	2,4-DINITROTOLUENE 121142
89	0.03	0.39
165	0.05	0.74
196	0.67	BENZYLSULFIDE 538749
91	0.27	3.90
123	0.07	0.99
197	0.69	DIPHENYLSULFONE 127639
125	0.35	5.05
218	0.07	1.07
198	0.81	TRIPHENYLPHOSPHATE 115866
325	0.18	0.78
326	0.01	1.02
199	0.01	DIPHENYLMERCURY 587859
77	0.05	2.94
356	0.06	0.10
200	0.47	TETRAPHENYLTIN
197	0.11	1.56
351	0.11	1.54
201	0.35	BENZYLCHLORIDE 100447
91	0.12	1.71
126	0.03	0.47
202	0.80	4-CHLOROBENZONITRILE 623030
102	0.04	0.61
137	0.16	2.32
203	0.01	3-CHLOROBENZALDEHYDE 587042
111	0.00	0.08
139	0.01	0.15
204	0.57	O-CHLOROANISOLE 766518
127	0.05	0.67
142	0.10	1.46

Internal/External Standard File for Cmpd Class # 6

Cmpd#	Recovery Std # 2		Compound Name Std #54	Std #56		Std #57		Std #61
Mass	109	236	136 -	82	128	98	116	204 -
205	0.01		CHLORJBENZAMIDE 619567					
139	0.70	0.55	0.13	0.77	1.25	0.50	0.84	
155	0.38	0.30	0.07	0.42	0.68	0.27	0.46	
206	1.00		3,4-DICHLORJBENZALDEHYDE 6287383					
173	0.48	0.39	0.09	0.58	0.93	0.31	0.57	
174	0.32	0.26	0.06	0.39	0.62	0.21	0.34	
207	0.71		1,2,4-TRICHLORJBENZENE 120821					
145	0.34	0.26	0.06	0.40	0.63	0.22	0.36	
180	1.30	1.00	0.24	1.50	2.40	0.83	1.37	
208	0.56		2-BROMO-1-CHLORJBENZENE 694804					
190	0.78	0.61	0.14	0.85	1.38	0.55	0.92	
192	1.04	0.81	0.19	1.14	1.84	0.74	1.24	
209	0.87		1,2-DICHLORJNAPHTHALENE 2050693					
161	0.44	0.34	0.08	0.50	0.78	0.28	0.46	
196	2.17	1.67	0.40	2.51	3.88	1.38	2.29	
210	0.77		1,2,4,5-TETRACHLORJBENZENE 95943					
214	1.18	0.90	0.22	1.29	2.09	0.84	1.40	
216	1.54	1.18	0.29	1.69	2.72	1.09	1.83	
211	0.65		P-DIBRJMOBENZENE 106376					
234	0.68	0.52	0.12	0.77	1.23	0.41	0.67	
236	1.29	1.00	0.23	1.48	2.36	0.78	1.30	
212	0.93		4-BROMODIPHENYLETHER 6452499					
248	1.08	0.81	0.20	1.19	1.92	0.77	1.29	
250	1.13	0.88	0.21	1.26	2.04	0.82	1.37	
213	0.64		HEXACHLORJBENZENE 118741					
284	0.74	0.56	0.13	0.84	1.34	0.44	0.73	
286	0.60	0.46	0.11	0.68	1.08	0.36	0.59	

Internal/External Standard File for Cmpd Class # 8

Cmpds Mass	Recovery Std #62 188 -	Compound Name Std #63 99 -	
205	0.01	CHLOROBENZAMIDE	619557
139	0.05	0.76	
155	0.03	0.41	
206	1.00	3,4-DICHLOROBENZALDEHYDE	6287383
173	0.04	0.57	
174	0.03	0.38	
207	0.71	1,2,4-TRICHLOROBENZENE	120821
145	0.03	0.36	
180	0.10	1.36	
208	0.56	2-BROMO-1-CHLOROBENZENE	694804
190	0.05	0.84	
192	0.07	1.12	
209	0.87	1,2-DICHLORONAPHTHALENE	2050693
161	0.03	0.46	
196	0.17	2.27	
210	0.77	1,2,4,5-TETRACHLOROBENZENE	95943
214	0.08	1.27	
216	0.11	1.66	
211	0.65	P-DIBROMOBENZENE	106376
234	0.05	0.75	
236	0.10	1.45	
212	0.93	4-BROMODIPHENYLETHER	6452499
248	0.07	1.17	
250	0.08	1.24	
213	0.64	HEXACHLOROBENZENE	118741
284	0.06	0.82	
286	0.05	0.66	

Table B-9. RMRs AND RECOVERIES FOR ESSA COMPOUNDS

Class No. 9	
Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
3	2-Fluorobiphenyl (external)
64	d_{13}-Heptanoic acid (internal)
65	d_5-Benzoic acid (internal)

MATRIX OF STANDARD ION RMRs

Standard	Ion	Recovery	Standard: 4-Fluoro-2-iodotoluene m/z 109	4-Fluoro-2-iodotoluene m/z 236	2-Fluorobiphenyl m/z 172	d_{13}-Heptanoic acid methyl ester m/z 77	d_{13}-Heptanoic acid methyl ester m/z 91	d_5-Benzoic acid methyl ester m/z 82	d_5-Benzoic acid methyl ester m/z 110
4-fluoro-2-iodotoluene	109	NA	-	.78	.29	.99	3.47	1.73	.87
	236	NA	1.28	-	.37	1.27	4.46	2.21	1.12
2-fluorobiphenyl	172	NA	3.44	2.68	-	3.42	11.96	5.94	3.00
d_{13}-heptanoic acid methyl ester	77	0.65	1.01	.79	.30	-	3.47	1.74	.88
	91	0.65	.29	.23	.084	.29	-	.50	.25
d_5-benzoic acid methyl ester	82	0.92	.58	.45	.17	.58	2.00	-	.51
	110	0.92	1.15	.90	.34	1.14	3.97	1.98	-

Internal/External Standard File for Cmpd Class # 9

Cmpd#	Recovery Std # 2		Compound Name Std # 3		Std #64		Std #65	
Mass	109	236	172	-	77	91	82	110
101	0.79		CHLORDACETIC 79118					
59	0.58	0.46	0.17		0.58	1.86	1.01	0.51
77	0.24	0.19	0.07		0.24	0.76	0.41	0.21
102	0.82		VALERIC 109524					
74	0.58	0.45	0.17		0.58	1.84	1.00	0.51
87	0.18	0.14	0.06		0.18	0.59	0.32	0.16
103	0.01		MERCAPTOPROPIONIC					
61	0.24	0.18	0.07		0.23	0.81	0.41	0.21
120	0.14	0.11	0.04		0.14	0.49	0.25	0.13
104	0.01		MALONIC 141822					
59	0.63	0.49	0.18		0.63	2.03	1.10	0.55
101	0.47	0.37	0.14		0.47	1.51	0.82	0.41
105	0.01		SUCCINIC 110156					
55	0.42	0.33	0.12		0.41	1.44	0.72	0.36
115	0.84	0.65	0.24		0.83	2.88	1.44	0.73
106	0.92		BENZOIC 65850					
77	0.74	0.58	0.22		0.74	2.58	1.28	0.65
105	1.43	1.11	0.42		1.41	4.94	2.45	1.24
107	0.73		DICHLORDACETIC 79436					
59	0.82	0.64	0.24		0.82	0.39	1.42	0.72
83	0.32	0.25	0.09		0.32	0.23	0.55	0.28
108	0.91		P-TOLUIC 99945					
119	1.84	1.43	0.53		1.82	6.35	3.17	1.60
150	0.66	0.51	0.19		0.66	2.28	1.14	0.58
109	0.85		BROMOACETIC 79083					
59	0.12	0.09	0.24		0.12	0.39	0.21	0.10
93	0.07	0.05	0.09		0.07	0.23	0.12	0.06
110	0.82		N-OCTANOIC 124072					
74	1.61	1.26	0.47		1.60	5.56	2.78	1.40
87	0.61	0.48	0.18		0.61	2.12	1.06	0.53
111	0.90		O-METHOXYBENZOIC 579759					
77	0.47	0.36	0.14		0.46	1.61	0.80	0.41
135	1.06	0.81	0.31		1.05	3.65	1.82	0.92
112	0.88		2-NITRO-P-CRESOL 119335					
91	0.40	0.31	0.12		0.40	1.38	0.69	0.35
167	0.42	0.33	0.12		0.41	1.44	0.72	0.36
113	0.91		O-CHLOROBENZOIC 118912					
139	1.43	1.11	0.41		1.41	4.94	2.46	1.24
170	0.42	0.33	0.12		0.41	1.45	0.72	0.36

Internal/External Standard File for Cmpd Class # 9

Cmpd#	Recovery Std # 2		Compound Name Std # 3	-	Std #64		Std #65	
Mass	109	236	172		77	91	82	110
114	0.85		N-NONANOIC	112050				
74	1.73	1.35	0.50		1.72	5.98	2.99	1.51
87	0.75	0.58	0.22		0.74	2.58	1.29	0.65
115	0.88		2,4-DICHLOROPHENOL	120832				
161	0.77	0.60	0.22		0.77	2.67	1.33	0.67
176	0.90	0.70	0.26		0.89	3.10	1.54	0.78
116	0.80		TRICHLOROACETIC	76039				
117	0.12	0.09	0.03		0.12	0.39	0.21	0.11
117	0.88		NITROBENZOIC-(P)	62237				
150	0.00	0.00	0.00		0.00	0.02	0.01	0.0[illegible]
181	0.12	0.09	0.03		0.12	0.39	0.20	0.10
118	0.94		NAPHTHOIC-2	93094				
127	0.78	0.61	0.23		0.78	2.70	1.35	0.68
155	1.05	0.82	0.31		1.05	3.64	1.81	0.92
119	0.87		N-DECANOIC	334485				
74	1.92	1.50	0.56		1.91	6.72	3.32	1.68
87	0.91	0.71	0.26		0.90	3.16	1.56	0.79
120	0.01		2,4-DINITROPHENOL	51285				
168	0.09	0.07	0.03		0.09	0.31	0.16	0.08
198	0.13	0.10	0.04		0.13	0.41	0.22	0.11
121	0.01		3,4-DICHLOROBENZOIC	51445				
173	0.15	0.11	0.04		0.15	0.51	0.25	0.13
204	0.04	0.03	0.01		0.04	0.14	0.07	0.04
122	0.93		2,3,6-TRICHLOROPHENOL	933755				
169	0.42	0.32	0.12		0.41	1.46	0.72	0.36
212	0.68	0.53	0.20		0.68	2.39	1.17	0.59
123	1.06		LAURIC	143007				
74	2.23	1.69	0.65		2.23	7.74	3.87	1.95
87	1.21	0.92	0.35		1.20	4.17	2.08	1.05
124	1.10		2,4-DICHLOROPHENOXYACETIC	94757				
175	0.47	0.36	0.14		0.46	1.61	0.80	0.41
199	0.67	0.52	0.20		0.67	2.33	1.16	0.59
125	0.90		MYRISTIC	544638				
74	3.12	2.43	0.91		3.10	10.80	5.38	2.72
87	1.86	1.45	0.54		1.85	6.45	3.21	1.62
126	0.99		2,4,5-TRICHLOROPHENOXYACETIC	93765				
233	0.53	0.42	0.16		0.53	1.85	0.92	0.46
70	0.23	0.18	0.07		0.23	0.79	0.39	0.20

Internal/External Standard File for Cmpd Class # 9

Cmpds	Recovery Std # 2		Compound Name Std # 3		Std #64		Std #65	
Mass	109	236	172	-	77	91	82	110
127	0.89		PALMITIC 57103					
74	2.86	2.23	0.83		2.85	9.85	4.93	2.49
87	1.78	1.39	0.52		1.77	6.12	3.07	1.55
128	1.00		PENTACHLOROPHENOL 87865					
265	0.50	0.39	0.14		0.49	1.71	0.85	0.43
280	0.47	0.37	0.14		0.47	1.68	0.81	0.41
129	0.63		OLEIC 112801					
55	0.45	0.35	0.14		0.47	1.52	0.81	0.41
69	0.31	0.24	0.09		0.32	1.04	0.56	0.28

Table B-10. RMRs AND RECOVERIES FOR VOSA COMPOUNDS

Class No. 10	
Standard ID No.	Standard Name
3	2-Fluorobiphenyl (external)
67	d_7-Butyric acid (internal)

MATRIX OF STANDARD ION RMRs

Compound	Ion	Recovery	Standard: 2-Fluorobiphenyl m/z 172	Standard: d_7-Butyric Acid Benzyl Ester m/z 50	Standard: d_7-Butyric Acid Benzyl Ester m/z 109
2-Fluorobiphenyl	172	NA	-	8.10	2.63
d_7-Butyric Acid Benzyl Ester	50	1.00	.13	-	.33
	109	1.00	.39	3.06	-

Internal/External Standard File for Cmpd Class #10

Cmpd#	Recovery Std # 3		Compound Name Std #67	
Mass	172	-	50	109
100	0.74		2-METHYLCYCLOPROPANE CARBOXYLIC ACID	
83	0.38		2.94	0.95
190	0.07		0.56	0.18
101	0.78		2-METHYLBUTENOIC ACID	
83	0.28		2.18	0.71
190	0.03		0.21	0.07
102	0.72		DIMETHYLACRYLIC ACID 541479	
83	0.54		4.14	1.34
190	0.04		0.28	0.09
103	0.74		2-METHYLBUTYRIC ACID 623427	
108	0.17		1.28	0.42
192	0.11		0.84	0.27
104	0.88		ISOVALERIC ACID 503742	
108	0.28		2.18	0.71
192	0.07		0.50	0.16
105	0.61		2-HEXENOIC ACID	
97	0.36		2.80	0.91
204	0.02		0.14	0.05
106	0.61		3-HEXENOIC ACID	
144	0.08		0.64	0.21
204	0.01		0.06	0.02
107	0.47		CYCLOPENTYLACETIC ACID	
108	0.29		2.26	0.73
218	0.02		0.20	0.07
108	0.01		ACETIC ACID 64197	
108	0.28		2.24	0.73
150	0.08		0.67	0.22
109	0.90		ACRYLIC ACID 79107	
55	0.08		0.66	0.21
102	0.04		0.28	0.09
110	0.01		PROPIONIC ACID 79094	
108	0.30		2.36	0.77
104	0.09		0.73	0.24
111	0.57		METHACRYLIC ACID 79414	
91	0.28		2.25	0.73
131	0.17		1.33	0.44
112	0.77		CROTONIC ACID 3724650	
69	0.36		2.87	0.93
91	0.24		1.89	0.61

Internal/External Standard File for Cmpd Class #10

Cmpd#	Recovery Std # 3	Compound Name Std #67	
Mass	172 -	50	109
113	0.57	N-BUTYRIC ACID	107926
108	0.37	2.93	0.96
178	0.09	0.70	0.23
114	0.42	ISOBUTYRIC ACID	79312
91	0.44	3.49	1.13
178	0.10	0.80	0.26
115	0.75	N-PENTANOIC ACID	109524
57	0.11	0.84	0.27
91	0.39	3.09	1.01
116	0.60	N-HEXANOIC ACID	142621
43	0.12	0.96	0.31
91	0.48	3.79	1.23
117	0.57	2-ETHYLBUTRIC ACID	88095
71	0.15	1.19	0.39
91	0.33	2.65	0.86
118	0.48	N-HEPTANOIC ACID	111148
43	0.15	1.21	0.39
91	0.51	4.02	1.31
119	0.46	N-OCTANOIC ACID	124072
91	0.66	5.22	1.70
105	0.36	2.83	0.92
120	0.01	N-NONANOIC ACID	112050
91	0.46	3.64	1.19
92	0.14	1.09	0.36
121	0.32	CYCLOHEXANE CARBOXYLIC ACID	98895
55	0.20	1.62	0.53
91	0.46	3.67	1.19
122	0.37	CYCLOHEXYL ACETIC ACID	5292217
81	0.40	3.17	1.03
91	0.69	5.50	1.79

Table B-11. RMRs AND RECOVERIES FOR NOVA COMPOUNDS

Class No. 11	
Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
3	2-Fluorobiphenyl (external)
66	d_7-Naphthalene sulfonic acid (internal)

MATRIX OF STANDARD ION RMRs

Compound	Ion	Recovery	d7-Naphthalene-sulfonic acid methyl ester		2-Fluorobiphenyl	4-Fluoro-2-iodo-toluene		d25 dodecylphosphonic acid diethyl ester
			m/z 134	m/z 229	m/z 172	m/z 109	m/z 236	m/z 129
d7-naphthalenesulfonic acid methyl ester	134	1.10	-	1.71	.23	.81	.63	.63
	229	1.10	.59	-	.14	.67	.37	.14
2-fluorobiphenyl	172	NA	6.46	7.62	-	5.43	8.67	.99
4-fluoro-2-iodotoluene	109	NA	1.31	2.24	.29	-	.78	.29
	236	NA	1.69	2.88	.38	1.29	-	.37

Internal/External Standard File for Cmpd Class #11

Cmpd#	Recovery		Compound Name			
	Std # 2		Std # 3		Std #66	
Mass	109	236	172	-	134	229
100	0.01		THIOGLYCOLIC		68111	
91	0.08	0.06	0.02		0.11	0.20
105	0.39	0.30	0.12		0.53	0.91
101	0.28		SUCCINIC		110156	
55	0.21	0.17	0.06		0.29	0.49
115	0.42	0.32	0.12		0.56	0.96
102	1.10		BENZENESULFONIC		98113	
77	0.98	0.76	0.29		1.25	2.13
172	0.34	0.27	0.10		0.44	0.78
103	0.68		4-NITROBENZOIC		121926	
104	0.07	0.05	0.02		0.09	0.16
150	0.25	0.20	0.07		0.34	0.58
104	1.40		BENZENEPHOSPHONIC		1779482	
91	0.46	0.36	0.13		0.59	1.01
185	0.45	0.35	0.13		0.57	0.98
105	0.72		P-TOLUENESULFONIC		104154	
91	1.16	0.91	0.34		1.48	2.52
186	0.48	0.37	0.14		0.60	1.03
106	0.55		TEREPHTHALIC		100210	
163	1.85	1.44	0.54		2.37	4.04
194	0.44	0.34	0.13		0.56	0.96
107	0.42		3,4-DICHLOROBENZOIC		51445	
173	0.69	0.54	0.20		0.92	1.56
204	0.20	0.16	0.06		0.26	0.45
108	0.92		P-CHLOROBENZENESULFONIC		98668	
111	0.59	0.46	0.17		0.75	1.28
206	0.24	0.19	0.07		0.31	0.52
109	1.10		2-NAPHTHALENESULFONIC		120183	
127	0.87	0.68	0.25		1.08	1.82
222	0.52	0.40	0.15		0.64	1.08
110	0.61		2,4,5-TRICHLOROPHENOXYACETIC		93765	
233	0.46	0.36	0.13		0.58	1.00
270	0.20	0.15	0.06		0.25	0.43
111	0.62		PENTACHLOROPHENOL		87865	
265	0.50	0.39	0.14		0.01	0.01
280	0.47	0.37	0.14		0.01	0.01
112	0.01		OLEIC	112801		
55	0.35	0.27	0.10		0.45	0.76
69	0.24	0.19	0.07		0.31	0.54

Table B-12. RMRs AND RECOVERIES FOR SAM-PT COMPOUNDS

Class No. 12	
Standard ID No.	Standard Name
2	4-Flunro-2-iodotoluene (external)
3	2-Fluorobiphenyl (external)
68	d_9-Butylamine (internal)

MATRIX OF STANDARD ION RATIOS

Compound	Ion	Recovery	Standard: 4-Fluoro-2-iodotoluene 109	Standard: 4-Fluoro-2-iodotoluene 236	Standard: 2-Fluorobiphenyl 172	Standard: d_9-Butylamine 210	Standard: d_9-Butylamine 212
4-fluoro-2-iodotoluene	109	NA	-	.78	.10	4.16	10.68
	236	NA	1.28	-	.39	5.32	13.68
2-fluorobiphenyl	172	NA	3.31	2.58	-	13.74	35.3
d_9-Butylamine	210	0.75	.24	.19	.073	-	2.58
	212	0.75	.094	.073	028	.39	-

Internal/External Standard File for Cmpd Class #12

Cmpd#	Recovery Std # 2		Compound Name Std # 3		Std #68	
Mass	109	236	172	-	210	212
100	0.75		ALLYL AMINE	107119		
41	0.09	0.07	0.03		0.37	0.95
207	0.04	0.03	0.01		0.15	0.39
101	0.75		N-BUTYLAMINE	109739		
190	0.08	0.06	0.03		0.83	2.15
208	0.20	0.16	0.06		0.84	4.11
102	0.76		ISOBUTYLAMINE	78819		
208	0.38	0.30	0.12		1.60	4.11
209	0.11	0.09	0.03		0.47	1.21
103	0.77		SEC-BUTYLAMINE	13952846		
222	0.28	0.22	0.09		1.16	2.99
236	0.05	0.04	0.01		0.20	0.52
104	0.75		T-BUTYLAMINE	75649		
57	0.48	0.38	0.15		2.01	5.18
236	0.30	0.23	0.09		1.25	3.22
105	0.74		N-HEXYLAMINE	111262		
208	0.19	0.15	0.06		0.80	2.07
250	0.22	0.17	0.07		0.92	2.36
106	0.74		CYCLOHEXYLAMINE	108918		
55	0.17	0.13	0.05		0.69	1.78
194	0.10	0.08	0.03		0.44	1.12
107	0.75		2-ETHYLHEXYLAMINE	104756		
208	0.23	0.18	0.07		0.97	2.49
278	0.20	0.15	0.06		0.82	2.11
108	0.75		BENZYLAMINE	100469		
91	0.33	0.26	0.10		1.36	3.49
92	0.08	0.06	0.02		0.32	0.82
109	0.73		ETHYLENE DIAMINE	107153		
208	0.05	0.04	0.02		0.22	0.57
223	0.04	0.04	0.01		0.19	0.48
110	0.75		TRIBUTYLAMINE	102892		
100	0.48	0.38	0.15		2.02	5.18
142	1.71	1.31	0.52		6.98	17.91

Table B-13. RMRs AND RECOVERIES FOR SAM-S COMPOUNDS

Class No. 13	
Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene
3	2-Fluorobiphenyl
70	N-Ethyl-2-fluorobenzylamine

MATRIX OF STANDARD ION RMRs

Compound	Ion	Recovery	Standard: 4-Fluoro-2-Iodotoluene m/z 109	4-Fluoro-2-Iodotoluene m/z 236	2-Fluorobiphenyl m/z 172	N-Ethyl-2-Fluorobenzylamine m/z 109	N-Ethyl-2-Fluorobenzylamine m/z 318
4-Fluoro-2-Iodotoluene	109	NA	-	0 77 (8)[a]	1 28 (1)	0 27 (6)	1 13 (26)
	236	NA	1 34 (1)	-	0 24 (2)	0 17 (6)	1 52 (27)
2-Fluorobiphenyl	172	NA	1 23 (9)	2.43 (8)	-	0 83 (8)	3 57 (26)
N-Ethyl-2-Fluorobenzylamine	109	1.00	4 00 (1)	3.11 (7)	0 32 (0)	-	4 53 (27)
	318	1 00	0 77 (1)	0 60 (6)	0 42 (2)	0 20 (10)	-

[a]Coefficient of variation for triplicate determinations are given in parenthesis.

Internal/External Standard File for Cmpd Class #13

Cmpd#	Recovery Std # 2		Compound Name Std # 3		Std #70	
Mass	109	236	172	-	109	318
100	0.82		DIALLYLAMINE 124027			
181	1.73	1.83	0.75		0.60	2.70
250	0.68	0.57	0.24		0.19	0.80
101	0.64		DIPROPYLAMINE 142847			
181	2.02	1.57	0.56		0.57	2.44
252	1.80	1.47	0.60		0.48	2.09
102	0.45		PIPERIDINE 110894			
181	1.66	1.32	0.55		0.44	1.93
264	1.13	0.91	0.37		0.30	1.31
103	0.15		MORPHOLINE 110918			
181	2.45	1.94	0.79		0.65	2.82
267	0.42	0.34	0.14		0.11	0.49
104	0.45		METHYLPIPERIDINE(2) 626675			
181	2.68	2.13	0.88		0.71	3.09
264	2.88	2.28	0.93		0.76	3.08
105	0.45		DIBUTYLAMINE 111922			
181	0.42	0.31	0.12		0.10	0.98
195	0.15	0.12	0.05		0.04	0.99
106	0.40		DIMETHYLPIPERIDINE(2,6) 671363			
224	0.85	0.66	0.27		0.22	0.97
266	1.76	1.38	0.56		0.46	2.00
107	0.01		DIETHYLAMINE 109897			
181	0.75	1.19	0.48		0.39	1.94
253	0.35	0.06	0.02		0.02	0.11
108	0.01		DIBENZYLAMINE 103491			
91	6.04	4.84	2.00		1.60	6.91
377	0.40	0.32	0.13		0.10	0.53

APPENDIX C

DESCRIPTION OF COMPUTER PROGRAM MASQUANT FOR PROCESSING DATA COLLECTED USING MAS

Description of the Computer Program MASQUANT for Processing and Editing Data Collected Using the Master Analytical Scheme

I. General

A computer program called MASQUANT has been written to carry out some of the basic calculations used to process data obtained using the Master Analytical Scheme. MASQUANT consists of approximately 2,000 lines of source code written in ANSI subset Fortran 77, which should make it operable on any computer capable of handling this language.

The program consists of a main routine and sixteen subroutines, which will be described in greater detail below. The program is written to be run interactively, with a continuing dialogue between the user and the computer. After all of the data are collected, a report giving the calculated concentration of each identified component is generated.

In order to use MASQUANT, three files need to be accessed from an external disk or tape. The files are organized in a sequential fashion, and are read or written to in this same manner. These files are 1) a file which contains calculated correction factors for RMRs, which can be applied to the library file, if desired; 2) a standard file consisting of internal and external standards, along with associated data including recovery factors and response factors; and 3) a file, written in the identical format as file 2, consisting of data for "unknown" analytes. The compounds and standards are organized into 13 classes, consistent with the MAS Protocols. Detailed formats for the three files are given in this Appendix.

II. Description of the Operation of Individual Routines

(1) Main Program

The main program organizes the entire scheme and carries out a number of specific calculations internally. On initialization, it determines in what units the final results are to be reported, the name of the run, the data and the class of unknown being analyzed. It determines if system performance standards (SPS) are to be used in modifying the stored RMR values used in the analysis. It then proceeds to gather information about the external and internal standards to be used in the

analysis After the standards have been entered, the program determines which ion of each internal standard will be used in the calculation for each unknown The protocol is briefly as follows Each internal standard is examined in order For each internal standard, one external standard is chosen for comparison The external standard chosen is that standard whose relative retention time is closest to that of the internal standard The amount of internal standard present is calculated two ways directly from the amount specified by the user corrected for standard recovery (forward calculation) and by calculation using RMRs stored for the particular internal standard/external standard combination (backward calculation) If SPS has been specified, these RMRs are corrected according to the SPS protocol Forward calcuation is carried out once and the reverse calculation is carried out four times for each of the possible combination of ions of internal and external standards (2×2) The internal standard ion chosen is that for which the weight corresponding to the reverse calculation is closest to that of the forward calculation.

A single ion for each internal standard is chosen in this manner, and then the unknowns are processed Data for each individual unknown are collected and the concentration of that component is computed according to the formulas shown in the flow chart, using the internal standard which has been chosen as described previously After all of the unknowns have been processed in this fashion, a report, showing the concentration of each unknown, is generated. At present the program can accommodate 50 unknowns in each pass After each report is generated, the program restarts and the process can be repeated as often as desired

(2) Subroutine BUGTAB

BUGTAB writes out a table of correction factors which are read in using subroutine TABLPW, or which are generated by program SPS The internal standards and external standards are independently listed along with the appropriate correction factor

(3) Subroutine DUPOUT

Subroutine DUPOUT checks the array of standard or unknown numbers for duplicates The arrays must have previously been sorted in ascending

sequence. If a duplicate is found, it is set equal to 10,000 Finally, the array is resorted, and the number of elements in the original array is reduced by the number of duplicate entries found.

(4) Subroutine ENTER

Subroutine ENTER is used to enter a series of numbers which are either internal standards, external standards, or unknowns The subroutine is called four times in the program It is called once by SPS, once for external standard entries, once for internal standard entries, and once for unknown entries The numbers are entered using subroutine INPUT Ten entries are permitted on each line, and the entire list of entries is terminated with a zero entry The program also does range checks for each type of compound. External standard numbers may range from 1 to 49, internal standards from 51 to 99, and unknowns from 101 to 999 After the numbers are acquired, the list is sorted in ascending sequence and duplicates are removed.

(5) Subroutine FILERD

This subroutine reads data from either the standard file or the unknown file Records are read sequentially from the beginning of the file until a match is found for the class number and the standard number If the compound which is sought is not found, an error statement is issued, otherwise all of the file data including the compound name, molecular weight, recovery factor, ion masses, RRFs, etc are returned for each compound sought

(6) Subroutine GETRRF

This subroutine simply returns one chosen RRF from those present in the table Parameters are passed to the subroutine which select the appropriate reference standard and the individual ion of the compound

(7) Subroutine GTDATA

This subroutine queries the user to provide the relative retention time and on-column weight for a given substance The subroutine has three entries one for external standard, one for internal standard, and one for unknowns The data are entered into the system by use of the subroutine INPUT. The program rejects zero values as entries

(8) Subroutine INPUT

INPUT is a modified version of a standard ANSI Fortran subroutine designed to permit field-free input for numeric data The program has been altered for this application. Numbers can be entered into the first fifty columns of each line Only one line of data can be entered by a single subroutine call Numbers can be entered as integers or as floating point numbers containing a single decimal point Delimiters between numbers are either a succession of blanks or a single comma Besides numerals, commas, periods and blanks only the letters "R", "B", and the symbol "?" are allowed as entries "R" returns a code which is used to restart the program, "B" is used to allow the user to back up in the program and repeat the previous section A question mark is used to signal an error, and the entire line can then be re-entered. All other characters, including "+" and "-" are not allowed Further details of this program are found in the source listings

(9) Subroutine ISREP

Subroutine ISREP is a report routine which lists the data stored for internal standards The variables listed are the standard number, its name, molecular weight, relative retention time, mass of ion used for computation, forward and backward calculated weights, and system response

(10) Subroutine REPORT

REPORT writes out the final report for the analysis In addition to reporting pertinent data for each run, each unknown is listed by name and number The calculated concentration of each component is printed either in PPM (mg/l) or in PPB (µg/l)

(11) Subroutine RMRFIX

RMRFIX is a program whereby the RMR values listed for a particular internal standard or unknown are altered by multiplication by the appropriate correction factor which has been previously stored on a disk file The subroutine is called twice once to correct RMRs of internal standards, and once for unknowns Although only a single RMR is used by the main program, for the sake of simplicity all of the RMRs for a given entry are altered

(12) Subroutine SORTUP

Subroutine SORTUP is a very low level sort routine written to order integer numbers in ascending sequence The algorithm used is a simple bubble sort Every number is compared with every other If the numbers are already in sequence, they are left without alteration If they are out of sequence, the numbers are exchanged Although this algorithm is not highly efficient, it is only used for a maximum of fifty entries, and a more sophisticated treatment was not warranted

(13 Subroutine SPS

Subroutine SPS is a major subroutine which determines if system performance standards are to be employed in correcting the RMR values stored If so, then a sequence is entered which calculates correction factors The program is commented very completely in the source listing and by a flow chart. In brief, the program initially determines whether SPS processing is desired, whether a table exists, and whether or not an existing table should be left unaltered, deleted, or updated The system allows storing only a single set of tables for one class of unknowns If more than one class of unknowns are to be process using SPS, then the routine must be executed separately for each class

The program works by obtaining weights, times, and responses for a series of not less than five ions From these data a square matrix of RMRs are calculated, i.e., the RMR of each ion is calculated with respect to every other ion entered Then, the RMRs permanently stored on disk or tape in the file for a single ion are compared with those just calculated, making use of a simple linear regression through the origin The slope of each regression line is the. stored as the correction factor for each ion The correction factors are then written onto disk for permanent storage (until the subroutine SPS is run again)

(14) Subroutine SPSCHK

Subroutine SPSCHK is used to test entries made by the user under SPS protocol to make sure that there is a table entry stored for each ion reported This subroutine is executed twice during the course of the program

(15) Subroutine SYSRES

SYSRES is a data entry subroutine used to have the user enter system responses for a particular compound. The program already knows the ions for which responses are desired, and prompts the user to respond making use of the subroutine INPUT.

(16) Subroutine TABLRK

Subroutine TABLRK is used to communicate between the main program and the SPS table of correction factors It can be used either to read the table or to write new data onto the table In the read mode, the subroutine checks to see whether a table is or is not present for the class requested, and returns either the data or an appropriate return code to indicate that a table is absent

(17) Subroutine YON

Subroutine YON is used to handle alphabetic answers to questions If the first character typed is a "Y" or an "N", the subroutine returns an appropriate code In addition, the subroutine recognizes an "R" character, a "B", and a "?" The R and B are used by the calling program for a system restart or backspace, respectively, and a question mark allows the user to re-enter his answer

FORMAT OF
INTERNAL/EXTERNAL STANDARD FILE AND UNKNOWN
FOR MASTER ANALYTICAL SCHEME

1. Entries (records) in file are ordered by:

   1) class
   2) compound number
   3) ion mass

2. Each entry occupies of 1 or 2 records depending on the number of ions catalogued.

3. DCB=(RECFM=FB,LRECL=440,BLKSIZE=3960), UNIT = 7(IS and XS), 8(Unk)

   A. FIXED PORTION OF RECORD

Description	Format	First Column	Last Column	Byte Length
1) COMPOUND NAME.	36A2	1	72	72
2) BLANK	5X	73	77	5
3) NAME LENGTH	I3	78	80	3
4) MOL. WT.	I4	81	84	4
5) BLANK	2X	85	86	2
6) CPD. NUMBER	I4	87	90	4
7) CPD. CLASS	I2	91	92	2
8) MASS OF ION	I4	93	96	4
9) RECOVERY	F4.2	97	100	4
10) BLANK	1X	101	101	1
11) TYPE FLAG (1-IS; 2-XS; 3-?)	I1	102	102	1
12) NO. OF IONS (1 OR 2)	I1	103	103	1
13) ION NUMBER (1 OR 2)	I1	104	104	1
14) RECORD NUMBER	I4	105	108	4
15) NO. OF STDS. W/RMRs	I2	109	110	2
16) BLANK	10X	111	120	10

B. VARIABLE PORTION

			Standard Number (1)		(2)		(3)		(4)	
Description	Format	Bytes	FB	LB	FB	LB	FB	LB	FB	LB
ST. NO.	I2	2	121	122	141	142	161	162	181	182
ST. FLG. (1-XS; 2-IS)	I1	1	123	123	143	143	163	163	183	183
NO. OF STD. IONS (1 OR 2)	I1	1	124	124	144	144	164	164	184	184
ST. MASS 1	I3	3	125	127	145	147	165	167	185	187
RMR 1	F5.2	5	128	132	148	152	168	172	188	192
ST. MASS 2	I3	3	133	135	153	155	173	175	193	195
RMR 2	F5.2	5	136	140	156	160	176	180	196	200
			(5)		(6)		(7)		(8)	
ST. NO.	I2	2	201	202	221	222	241	242	261	262
ST. FLG. (1-XS; 2-IS)	I1	1	203	203	223	223	243	243	263	263
NO. OF STD. IONS (1 OR 2)	I1	1	204	204	224	224	244	244	264	264
ST. MASS 1	I3	3	205	207	225	227	245	247	265	267
RMR 1	F5.2	5	208	212	228	232	248	252	268	272
ST. MASS 2	I3	3	213	215	233	235	253	255	273	275
RMR 2	F5.2	5	216	220	236	240	256	260	276	280
			(9)		(10)		(11)		(12)	
ST. NO.	I2	2	281	282	301	302	321	322	341	342
ST. FLG. (1-XS; 2-IS)	I1	1	283	283	303	303	323	323	343	343
NO. OF STD. IONS (1 OR 2)	I1	1	284	284	304	304	324	324	344	344
ST. MASS 1	I3	3	285	287	305	307	325	327	345	347
RMR 1	F5.2	5	288	292	308	312	328	332	348	352
ST. MASS 2	I3	3	293	295	313	315	333	335	353	355
RMR 2	F5.2	5	296	300	316	320	336	340	356	360
			(13)		(14)		(15)		(16)	
ST. NO.	I2	2	361	362	381	382	401	402	421	422
ST. FLG. (1-XS; 2-IS)	I1	1	363	363	383	383	403	403	423	423
NO. OF STD. IONS (1 OR 2)	I1	1	364	364	384	384	404	404	424	424
ST. MASS 1	I3	3	365	367	385	387	405	407	425	427
RMR 1	F5.2	5	368	372	388	392	408	412	428	432
ST. MASS 2	I3	3	373	375	393	395	413	415	433	435
RMR 2	F5.2	5	376	380	396	400	416	420	436	440

FORMAT OF CORRECTION FACTOR TABLE FOR
SYSTEM PERFORMANCE STANDARDS
MASTER ANALYTICAL SCHEME

DCB=(RECFM=FB,LRECL=80,BLKSIZE=800), UNIT = 6

FIRST CARD DESCRIPTION

		Format	Bytes	First Column	Last Column
1.	TABLE FLAG. 0-NO TABLE, 1-TABLE	I1	1	1	1
2.	TABLE CLASS	I2	2	2	3
3.	NO. OF STDS. (NTST)	I2	2	4	5
4.	DATE	4A2	8	6	13

SUBSEQENT CARDS (NTST IN NUMBER)

1.	STANDARD NUMBER	I3	3	1	3
2.	INT/EXT FLAG (1 OR 2)	I1	1	4	4
3.	NO. OF FACTORS (1 OR 2)	I1	1	5	5
4.	MASS 1	I3	3	6	8
5.	FACTOR 1	F5.4	5	9	13
6.	MASS 2	I3	3	14	16
7.	FACTOR 2	F5.4	5	17	21

TAPE DOCUMENTATION

The tape RA1375 was written in IBM standard label format in EBCDIC at 1600 B.P.I. The order, names, and contents of the data sets residing on the tape are as follows:

1) EPAQNT.CARD3.STDS

   Card image data for a single test class of standards for primary input file for the program ADD(s).

2) EPAQNT.CLASS3.STDS

   Test data set to be used as standard file input to MASQNT (11). This file can be generated by using ADD(5) with (1) as primary input.

3) EPAQNT.CARD3.ANLS

   Card image data for a single test class of analytes for primary input file for the program ADD(5).

4) EPAQNT.CLASS3.ANLS

   Test data set to be used as analyte file input to MASQNT (11). This file can be generated by using ADD(5) with (3) as primary input.

5) EPAQNT.ADD.SOURCE

   This file comprises the card image source code for the data base creation program ADD. See data base management documentation for input and output file numbers and formats.

6) EPAQNT.REPORT.SOURCE

   This file comprises the card image source code for the listing generation program REPORT. See data base management documentation for input and output file numbers and formats. Can be tested using either (2) or (4) as input.

7) EPAQNT.EDIT.SOURCE

This file comprises the card image source code for the data base modification program EDIT. The sample run can be reproduced by using (8) as control card input and (2) as primary input file. See data base management documentation for input and output file numbers and formats.

8) EPAQNT.EDIT.CNTLCARD

This file comprises card images which are to be used as control cards for EDIT (7) along with (2) in generating a test run.

9) EPAQNT.DELETE.SOURCE

This file comprises the card image source code for the program DELETE. The sample DELETE run can be produced using (10) as control cards and (1) as a primary input file. See data base management documentation for input and output file numbers and formats.

10) EPAQNT.DELETE.CNTLCARD

This file comprises card images which are to be used as control cards for DELETE (9) along with (2) in generating a test run.

11) EPAQNT.MASQNT.SOURCE

This file contains the card image source of the revised MASQNT. Sample analyte, standards, and table files are (4), (2), and (12) respectively.

12) EPAQNT.SPS.TABLES

This is a copy of the System Performance Standards tables used in the sample run of MASQNT.

A copy of a successful run for each of the four data base management programs was included. It should be possible to duplicate the same

output on another machine with the documentation of each program being used and the appropriate combination from the above twelve tape datasets. Perhaps the easiest way to create a new MASQNT data base is to assign standard and analyte IDs according to the ADD documentation, fill out copies of the entry forms provided, and use a combination of the ADD, REPORT, and the editor of the particular machine being used. A sample of blank entry forms for ADD is provided herein.

This second version of MASQNT uses the same fortran unit numbers for input/output as the first;

Unit - User Input
Unit 3 - User Output
Unit 6 - System Performance Standard correction tables
Unit 7 - Standard Database
Unit 8 - Analyte Database

The protocol class names and their corresponding numbers are as follows:

1. Purge and Trap (VO)
2. Elevated Temperature Purge and Trap (NEWS)
3. Batch Liquid-Liquid Partitioning for pH 8 Extractables/ No fractionation (WABN- BLLE)
4. Batch L-L Partitioning for pH 8 Extractables/Fraction No. 1 (WABN)
5. Batch L-L Partitioning for pH 8 Extractables/Fraction No. 2 & 3 (WABN)
6. Batch L-L Partitioning for pH 8 Extractables/Fraction No. 3 (WABN)
7. Flow-Under L-L Partitioning for pH 8 Extractables (WABN-FU)
8. Accumulator Column for pH 8 Extractables (WABN-SC)
9. Batch L-L Partitioning (pH 1) for Acid Extractables (ESSA)
10. Anion Ion-Exchange/Distillation for short chain acids (VOSA)
11. Anion Ion-Exchange for strong acids (NOVA)
12. Cation Ion-Exchange for Primary and Tertiary Amines (SAM-PT)
13. Cation Ion-Exchange for Secondary Amines (SAM-S)

Data Base Management Programs For MASQNT

The data base management system for the master scheme consists of four programs: ADD, DELETE, REPORT, and EDIT. All of the programs are written in ANSI Fortran and are intended to operate in a batch environment. The data base used by MASQNT consists of two files: a standard file which contains the RMR's of standards versus each other and an analyte file which contains RMR's of analytes versus standards. The format of the standard and analyte files are the same and any of the four programs can be used on either file. While the programs should be protable they do not by themselves furnish the capability of modifying the MASQNT data base. The sort utility of the machine being used must be used in preprocessing or postprocessing steps. The control cards to three (DELETE, REPORT, and EDIT) must be sorted in a particular sequence as well as the output files generated by three programs (ADD, REPORT, and EDIT). Also some file handling utilities have to be used in conjunction with the programs which modify the files (ADD, EDIT, and DELETE). These programs use the original data file (standard or analyte) and card images as input and write the updated output to a different file. The renaming, deleting, backup, and changing to the new input file for MASQNT must be done by the user with utility programs on the machine these programs are being run on.

REPORT

The program REPORT produces a formatted listing of the files used by MASQNT from card images specified by the user. REPORT is used to generate listings of the data base, to verify the correctness of new entries made into the data base by ADD.

REPORT reads the MASQNT file from unit 6 and writes a listing output to unit 3. The control cards are read from unit 1 and must be ordered by ascending class number (card columns 15-16) and by ascending compound number (card columns 17-20) within class number. Error messages concerning control cards are written to unit 4. Two types of controls cards are recognized by REPORT: LIST and ALL. The ALL card is used to generate a listing of the entire file. All that is needed to generate a complete file listing specific entries in the file when a complete printout is not desired. A typical use of the LIST option would be to verify the correctness of changes (on a limited number of entries) made by the program EDIT.

```
LIST      26   8    63
LIST    153Ø   9     3
LIST      58   9   761
LIST      61   9   772
```

Format of Control Cards for Report:

	Beginning Column	Ending Column	Field Contents
LIST	1	4	LIST
	11	14	Record # of Compound (right justified)
	15	16	Class # of Compound (right justified)
	17	20	Compound # (right justified)
	21	21	Ion #
ALL	1	3	ALL

The field in column 21 of the LIST card is used for printing out individual ions for a compound entry, i.e., a 1 coded in column 21 will cause the program to list the first ion only and an 2 will cause the program to list the second ion only. Leaving column 21 blank will cause the program to list all ions for the given compound.

The numeric entries in the field columns 11-14, 15-16, and 17-20 must be right justified. The control cards must also appear in order class # and compound # within class #.

Since the LIST card is intended for use with only a few specific entries and since the ALL card can always be used to print the entire file, the number of control cards for REPORT should be limited, thereby making it easy for the user to enter control cards in the proper order. However, in the event ov a large number of LIST cards it should be possible to order the cards in a prior step with the sort program of the particular machine being used.

DELETE

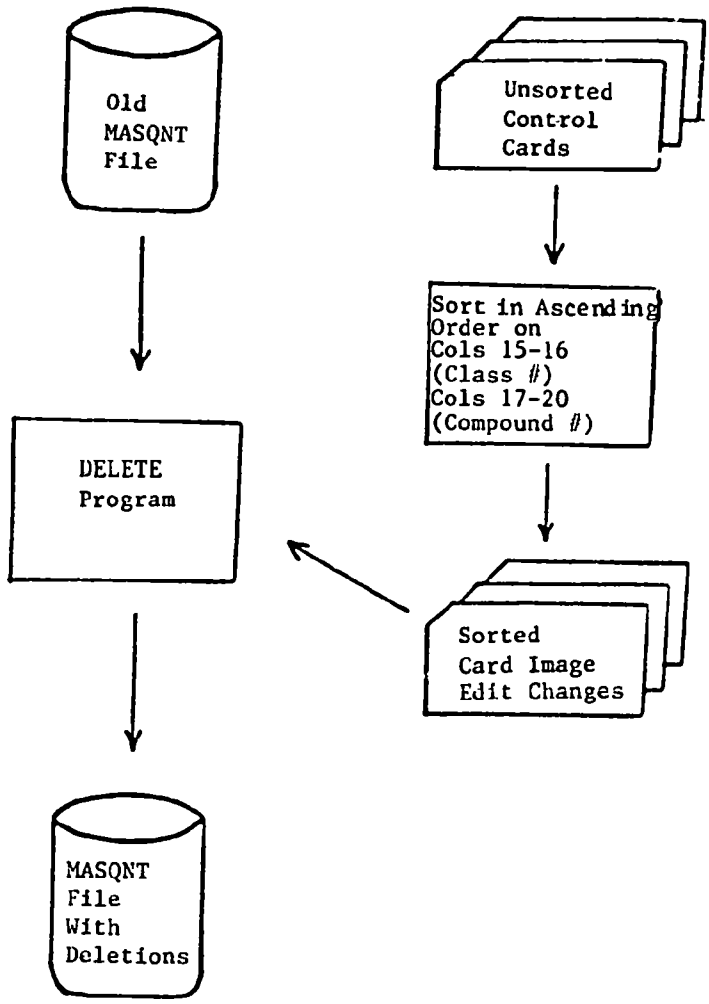
The program DELETE is used to eliminate entries from the data base which are no longer used or which have been found to have been entered incorrectly. DELETE reads control cards specifying which compounds are to be deleted from unit 1, reads the input file from unit 7, and writes the output file to unit 8. Error messages and messages telling which entries were deleted are written to unit 3. Each run of DELETE is in a sense tentative because the original file is left intact. If the user is not satisfied with the error messages returned by the program, he can simply alter the control cards and run DELETE again using the same input and output files. When a DELETE run without error messages is obtained the user can then finalize the deletions by scratching the input file and renaming the output file to the old input file name with the utility programs of his particular machine. ONly one type of control card is recognized by DELETE, the 'DEL' card which is specified by coding DEL in card columns 1-3. The user enters one DEL card for each compound to be deleted from the file. The program expects the cards to be sorted in order of ascending class number and by ascending compound number within class number. Having the cards out of order will cause DELETE to issue an error message. In the event that many entries are to be deleted, it may be advantageous to sort the control cards with a utility program prior to running DELETE.

The format of the DEL cards is as follows:

Beginning Column	Ending Column	Field Contents
1	3	DEL
11	14	Record # of 1st Compound Ion (right justified)
15	16	Class # of Compound (right justified)
17	20	Compound # (right justified)

DEL 1Ø1ØØØ4
DEL 3Ø1ØØ52
DEL 11Ø2ØØ57

As with REPORT the numeric entries in the field columns 11-14, 15-16 and 17-20 are all right justified. Also as with REPORT, the control cards should be entered in order of ascending class # and compound # within class #.



Steps for DELETE Program

EDIT

The program edit is used to modify existing entries in either the standard or analyte files. The control cards are read from unit 1, the old data file is read from unit 7, and the new modified data file is written to unit 8. Messages from EDIT are written to unit 3, like DELETE and ADD, each run with EDIT is tentative because the original file is not modified. The EDIT program can be run as many times as needed until a correct output file is generated. The changes made by EDIT become final only when the input file is scratched. EDIT can be run on the standard file to modify RMR's of standards or on the analyte file to modify RMR's of analytes versus standards. EDIT recognizes three types of control cards: The CRMR card which modifies existing RMR's, the ASTD card which adds RMR's for new standards. The control cards to EDIT must appear in order of ascending class number (card columns 15-16), ascending compound number within class (card columns 17-20), and ascending ion # within compound (card column 21) in order for EDIT to work properly. As with DELETE and REPORT, the sort program of the particular machine may have to be used in the instance of a large number of cards. No sorting of the output file of EDIT is required.

The format of the CRMR is as follows:

Beginning Column	Ending Column	Field Contents
1	3	ADD
6	6	Number of Ions for Compound (1 or 2)
8	9	Number of Standards (1 to 16)
11	12	Class Number (see figure for permissable codes)
14	14	Type (1 to 3) 1 = External Standard 2 = Internal Standard 3 = Analyte
16	19	Mass of 1st compound ion
21	24	Mass of 2nd compound ion
26	29	Compound molecular weight
32	35	Recovery fraction for compound (Real fraction between 0.0 and 1.0)
37	39	Compound ID

The NAME card has only one item: The name of the compound being added which starts in column 6. The STD cards follow the ADD and NAME cards. Each STD card contains the RMR's for a given ion of the compound being added relative to a given standard. The number of ions permitted for a compound is either 1 or 2 and is coded in column 6 of the ADD card. The number of STD cards which are to follow for each ion is coded in columns 8-9 of the ADD card. The STD cards for the second ion - if the compound has two ions - follow the STD cards for the first. The items on a STD card and their respective fields are as follows:

Beginning Column	Ending Column	
1	3	STD
6	6	Ion Number (1 or 2)
8	9	Sequence Number of Standard within Ion (1 to 16)
11	12	Standard ID (Explained Below)
14	14	Standard Type (1 = External, 2 = Internal)
21	23	1st Standard Ion Mass
26	30	1st Standard RMR
32	34	2nd Standard Ion Mass
37	41	2nd Standard RMR

The format of the ASTD card is as follows:

Beginning Column	Ending Column	
1	4	ASTD
11	14	Record # of Compound
15	16	Class # of Compound
17	20	Compound #
21	21	Ion #
26	27	ID # of Standard within Record
29	29	Standard Type (1 = External, 2 = Internal)
31	33	Mass #1
35	39	RMR #1
41	43	Mass #2
45	49	RMR #2

The entries in columns 11-21 are used to locate the correct entry in the data base. The ID number for the standard should be consistent with the instructions to ADD. If there are already sixteen standards for the compound ion the program will print an error message with no change of the standard record.

The DSTD card accomplishes the reverse of the ASTD card - it is used to strike RMR references to standards which are no longer to be used and which have been deleted from the standards file.

The format of the DSTD card is as follow:

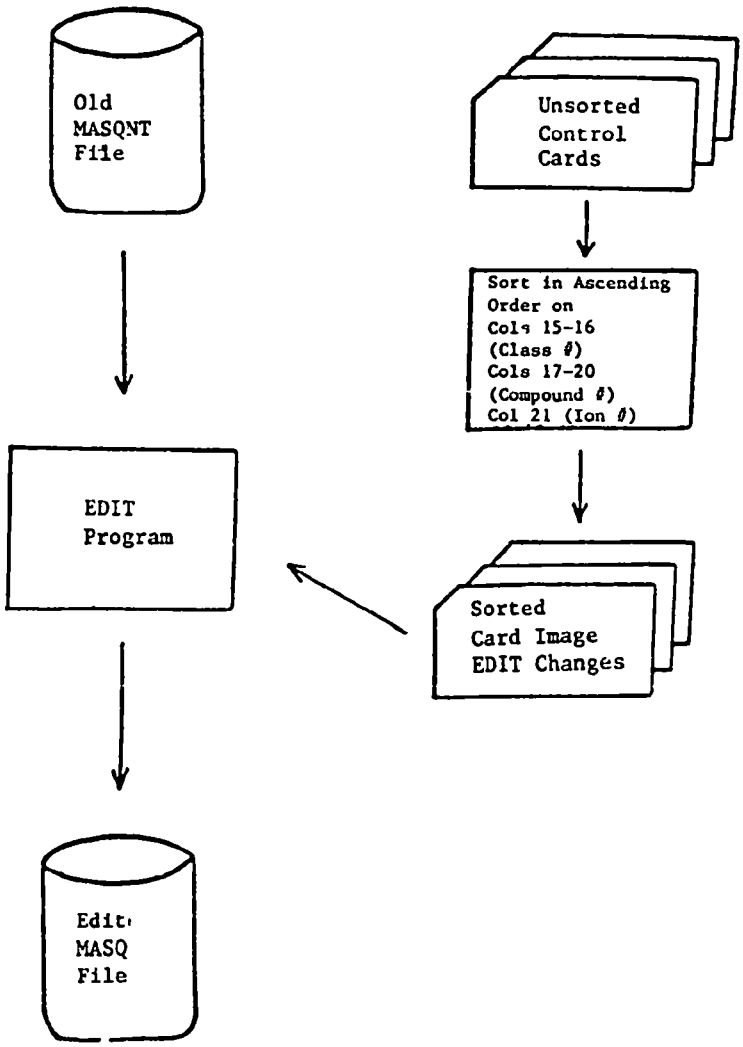
Beginning Column	Ending Column	
1	4	DSTD
11	14	Record # of Compound
15	16	Class # of Compound
17	20	Compound #
21	21	Ion #
23	24	Ordinal # of Standard within Record
26	27	ID # of Standard within Record

The fields in columns 11-21 locate the entry as with the ASTD card. Ordinal number of the standard within the entry (columns 23-24) is used as a check against the standard ID to ensure that the correct standard reference is deleted.

Beginning Column	Ending Column	
1	4	CRMR
11	14	Record # for Compound
15	16	Class # for Compound
17	20	Compound #
21	21	Ion #
23	24	Ordinal # for Standard on Report
26	27	ID # of Standard on Report
31	33	Standard Ion Mass #1
35	39	RMR #1
41	43	Standard Ion Mass #2
45	49	RMR #2

The CRMR control card information is meant to be taken from the output of REPORT. The EDIT program uses the compound #, class #, and ion # to locate the entry in the data base and the record # as a double check. The standard ordinal #, standard ID # and standard ion mass are used to locate the correct standard ion mass on the data base entry matches the mass entered in card columns 31-33, then the data base RMR for that standard is replaced by contents of card columns 35-39. Likewise, if the second standard ion mass on the data base entry matches the mass entered in card columns 41-43 the data base RMR for that standard is replaced by the contents of card columns 45-49. Leaving a standard ion mass field blank will result in no RMR change regardless of the contents of the corresponding RMR field.

The ASTD card is used to add standard references to existing entries in both the analyte and standard files and thereby enter RMR information of existing entries entries versus newly added standards to the data base.



Steps for EDIT Program

ADD

The program ADD is used to add new compounds to the MASQNT data base. ADD reads in the new compounds from card images on unit 1, reads the old MASQNT file from unit 7, and writes the new MASQNT file with added entries to unit 8. Before the new MASQNT file created by ADD can be used by the MASQNT program, it must be sorted in order of ascending class number (columns 91-92) and in order of ascending compound number (columns 87-90) within class #. It is strongly recommended that any new additions to the MASQNT files be proofed by use of the REPORT program before they are used as input data for MASQNT. Like DELETE and EDIT, each run of ADD is tentative until the old file is deleted and the new file is renamed to the old file name.

The ADD program recognizes three kinds of control cards: The ADD card which supplies numeric information on the compound being added, the NAME card which supplies the name of the compound being added, and the STD card which supplies information on the RMR's and ion masses for each entry. The card image input to ADD for each compound consists of first an ADD card, followed by a NAME card, and however many STD cards were specified in the fields for number of ions and number of standard on the ADD card. The program checks for proper sequence of ADD-NAME-STD cards and for the proper number of STD cards following the ADD and NAME cards and issues an appropriate error message if there is a discrepancy.

The items for the ADD card with their respective columns are as follows:

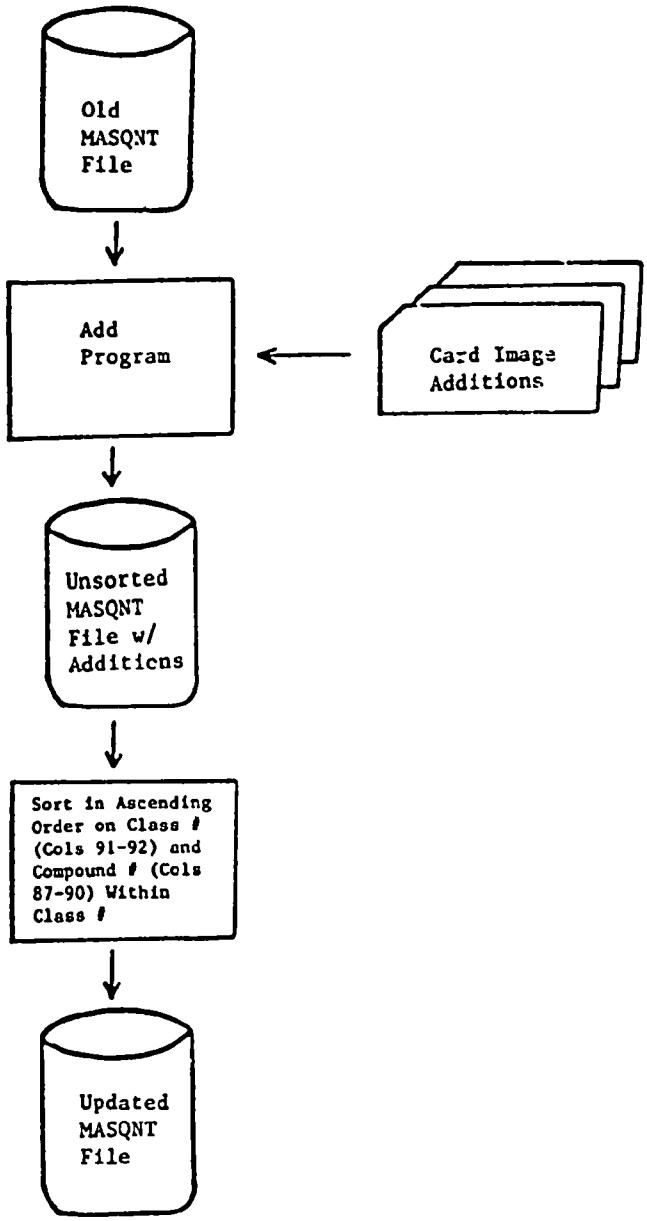
When adding compounds to the data base new compounds ID's have to be assigned. Each new entry must have a compound ID number assigned to it. It is crucial that the compound ID's (columns 11-12 of the STD card) be assigned consistently. The compound numbers must fulfill two requirements: A range requirement and uniqueness within compound class. The compound ID numbers must be within the following ranges:

External Standards	1-49
Internal Standards	51-99
Analytes	100-999

The types for standards must also follow the conditions:

Internal Standards	Type = 2
External Standards	Type = 1
Analytes	Type = 3

Whether making additions to the standard file or to the analyte file, the output file generated by ADD must be sorted in order of increasing class number (columns 91-92) and in order of increasing compound number (columns 87-90) within class number. After being sorted the file should have new entries verified by the REPORT program before the new file is used by MASQNT.



Steps for ADD Program

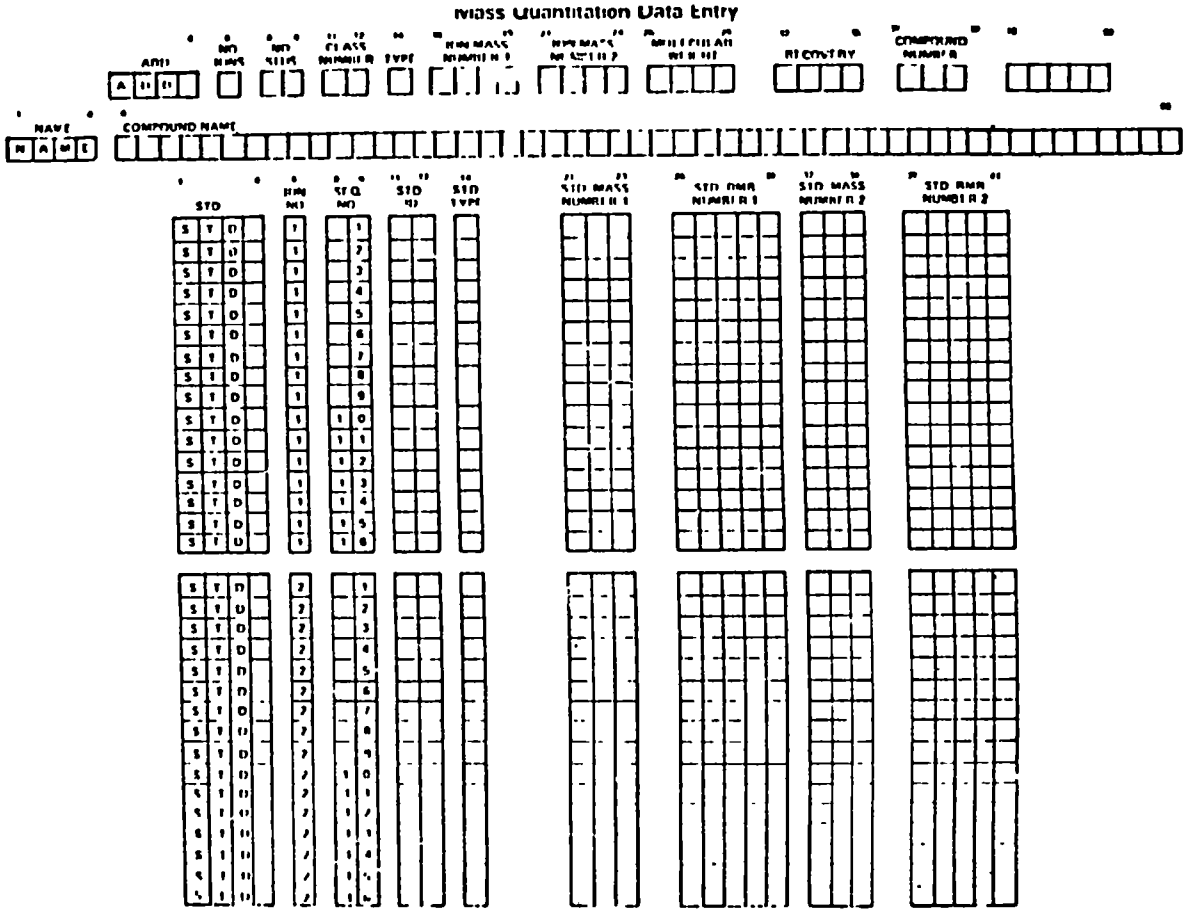

Mass Quantitation Data Entry
NAME
COMPOUND NAME
STD

Figure C-1. Flow Chart of Master Scheme Software

November, 1980

Glossary

PPM = Parts per Million

PPB = Parts per Billion

FACT = Factor

SPS = System Performance Standards

VOL = Volume

IS = Internal Standard

XS = External Standard

RRT = Relative Retention Time

WT = Weight

UNK = Unknown

MW = Molecular Weight

SR = System Response

RMR = Relative Molar Response

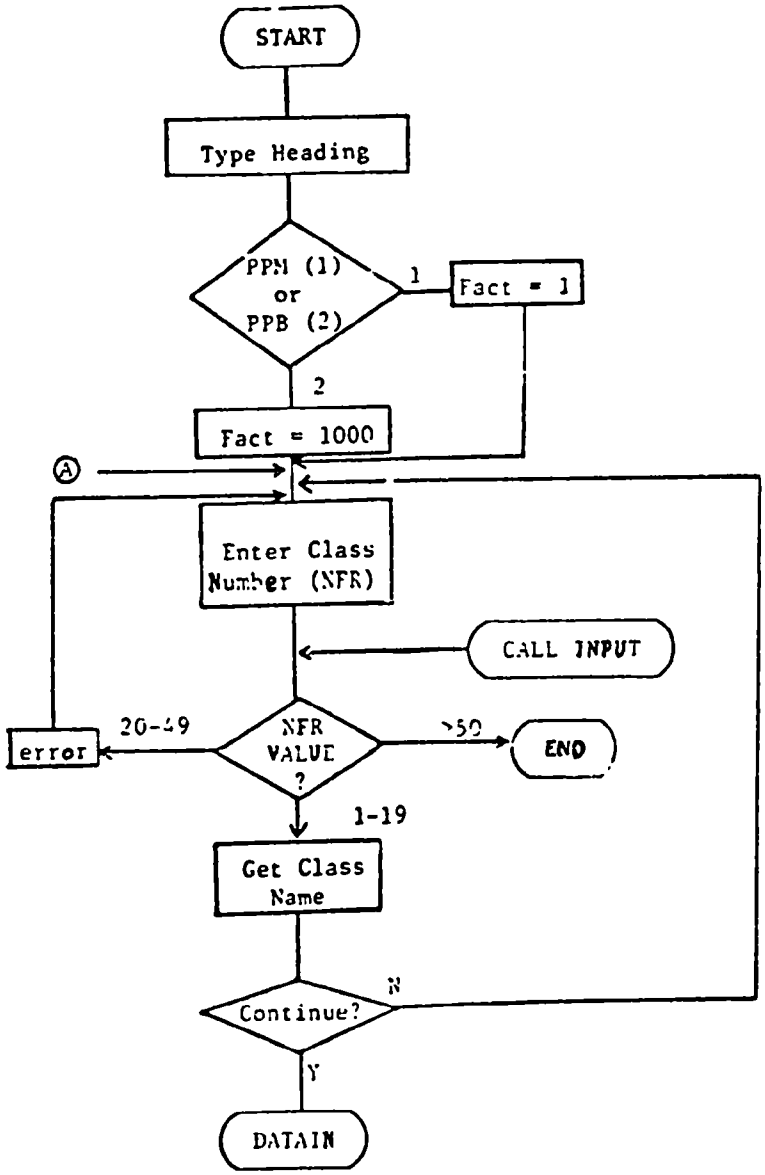
FOR = Forward

BACK = Backward

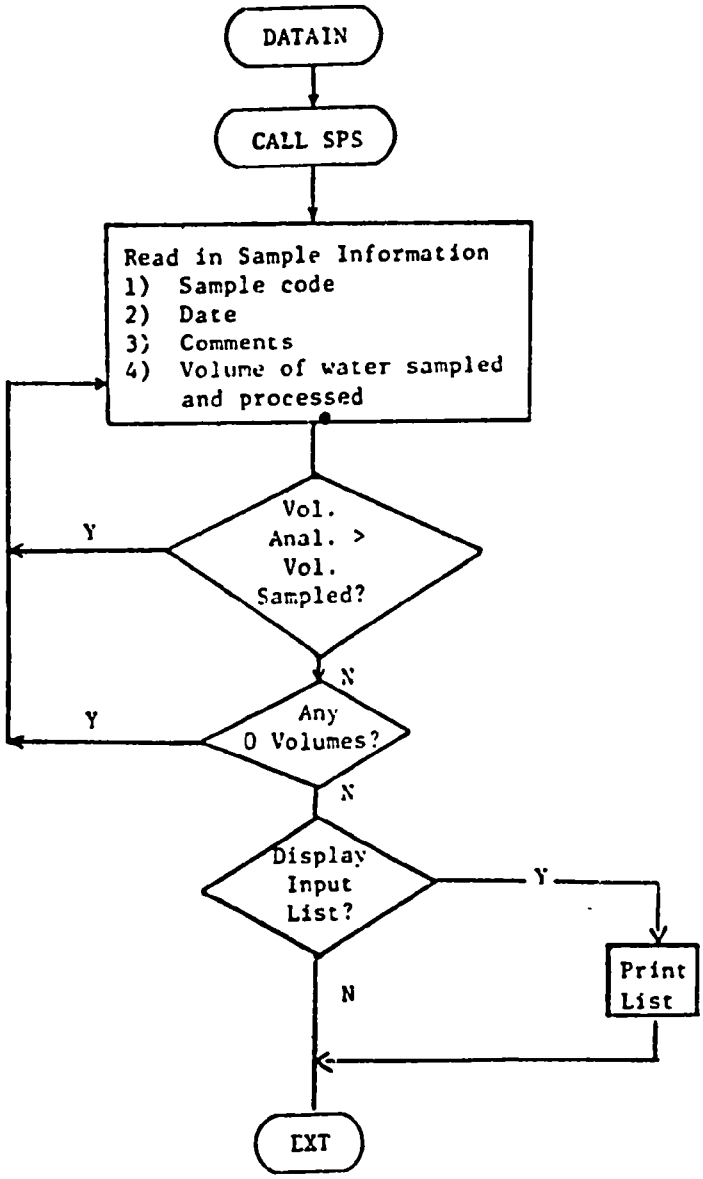
(continued)

Flow Chart of Master Scheme Software

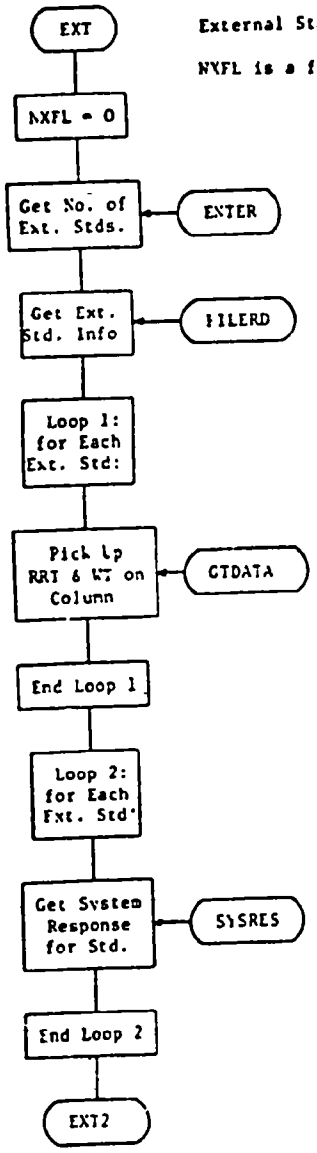
November, 1980



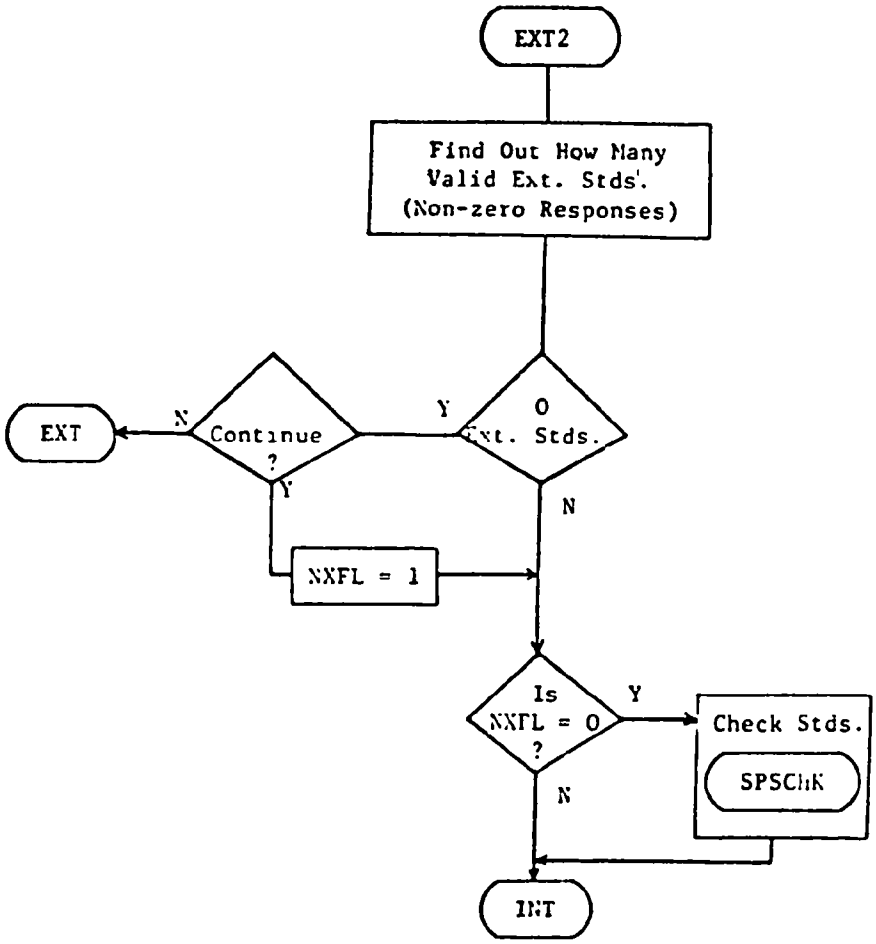
(continued)


DATAIN
CALL SPS
Read in Sample Information
1) Sample code
2) Date
3) Comments
4) Volume of water sampled and processed
Vol. Anal. > Vol. Sampled?
Y
N
Any 0 Volumes?
Y
N
Display Input List?
Y
N
Print List
EXT

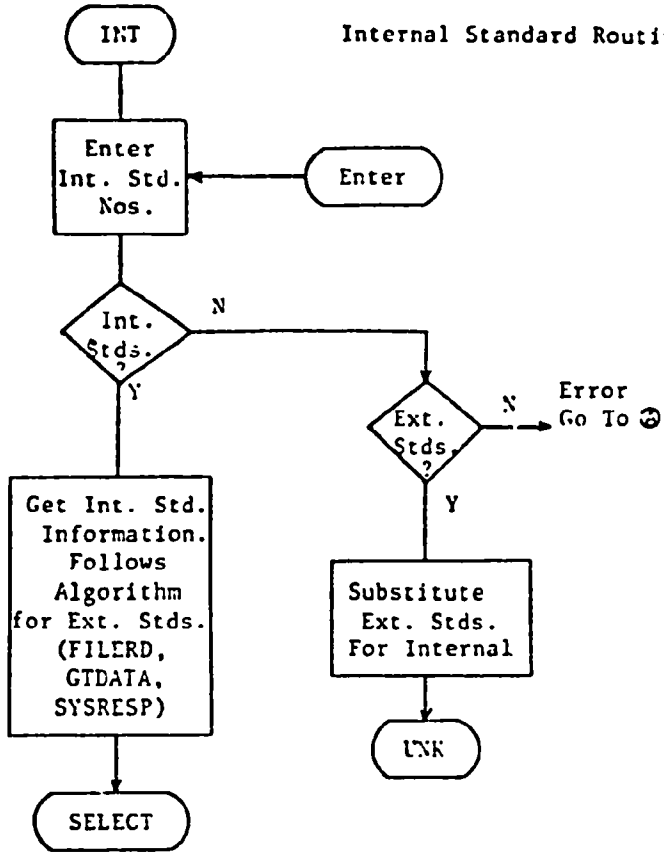
(continued)


EXT
External Standard Information
NXFL is a flag indicating XS.
NXFL = 0
Get No. of Ext. Stds.
ENTER
Get Ext. Std. Info
FILERD
Loop 1: for Each Ext. Std:
Pick up RRT & WT on Column
GTDATA
End Loop 1
Loop 2: for Each Ext. Std
Get System Response for Std.
SYSRES
End Loop 2
EXT2

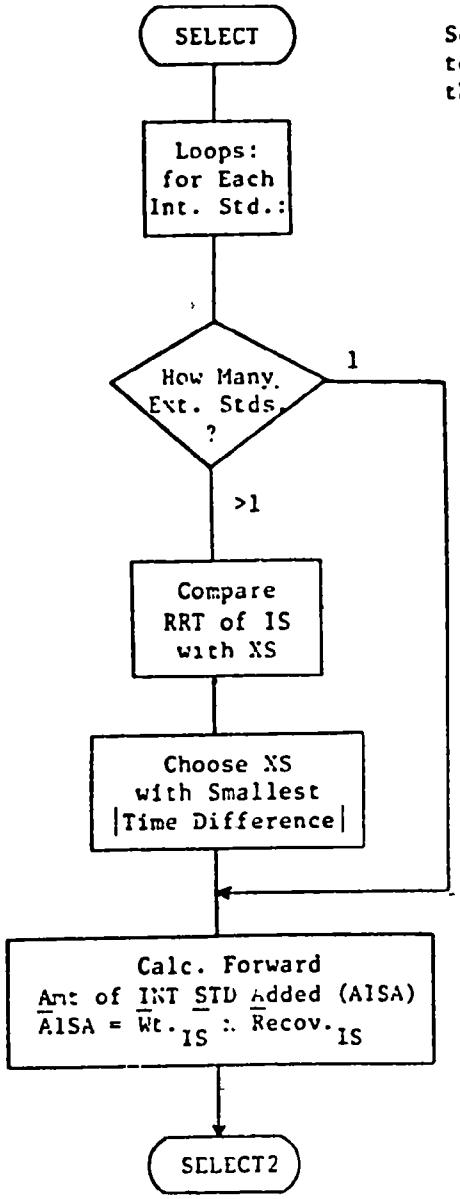
(continued)


EXT2
Find Out How Many Valid Ext. Stds. (Non-zero Responses)
0 Ext. Stds.
Y
Continue ?
N
EXT
Y
NXFL = 1
N
Is NXFL = 0 ?
Y
Check Stds.
SPSChK
N
INT

(continued)

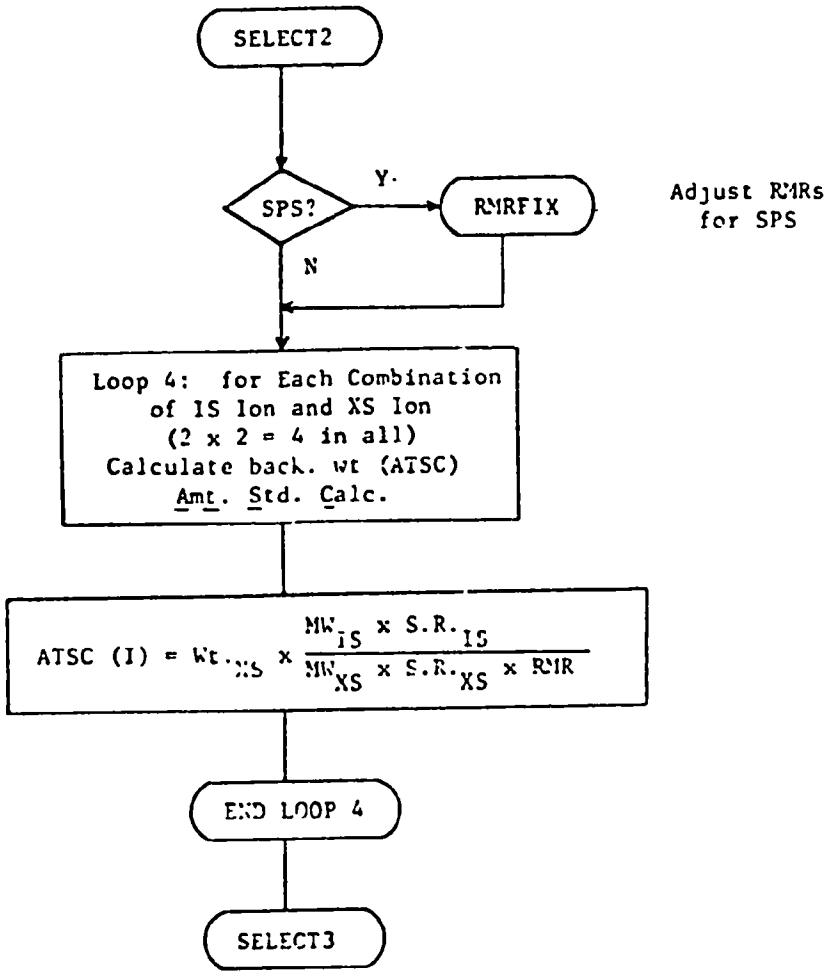

INT
Internal Standard Routine
Enter Int. Std. Nos.
Enter
Int. Stds. ?
N
Y
Ext. Stds. ?
N
Error Go To ②
Y
Get Int. Std. Information. Follows Algorithm for Ext. Stds. (FILERD, GTDATA, SYSRESP)
Substitute Ext. Stds. For Internal
UNK
SELECT

(continued)

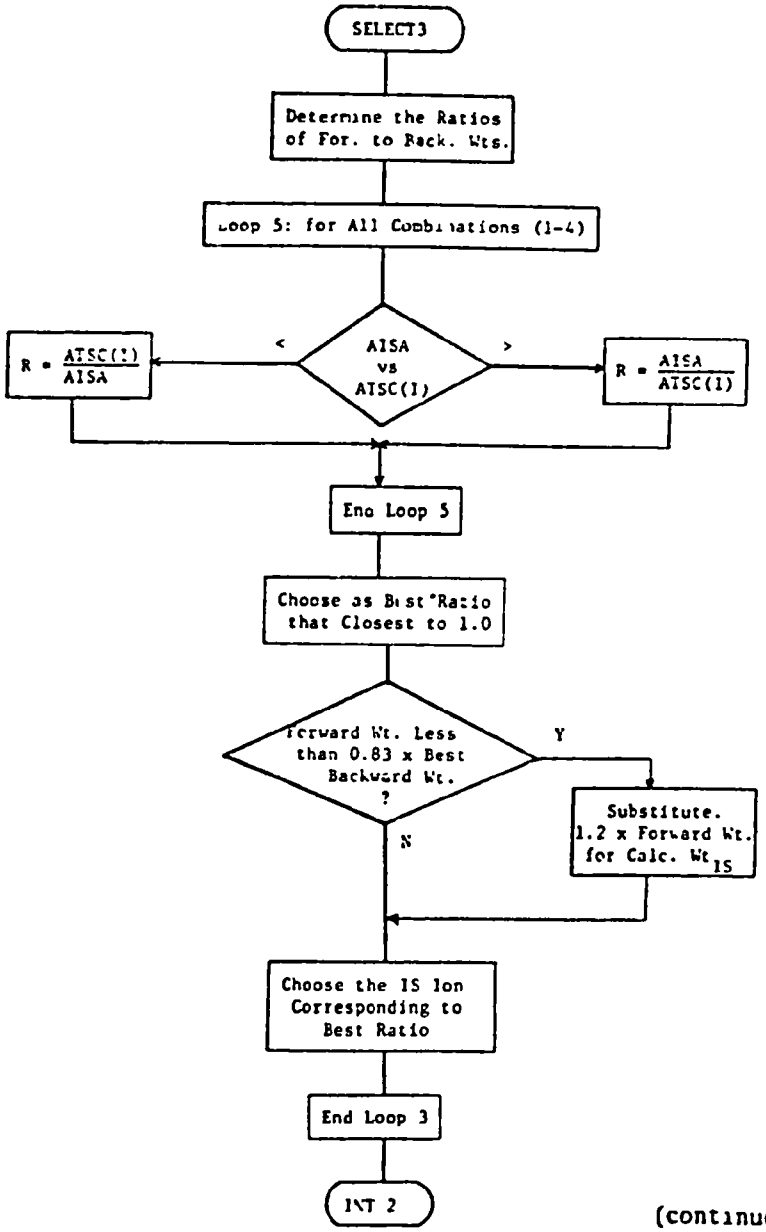


Select which Int. Std. ion to use if data for more than one ion is available.

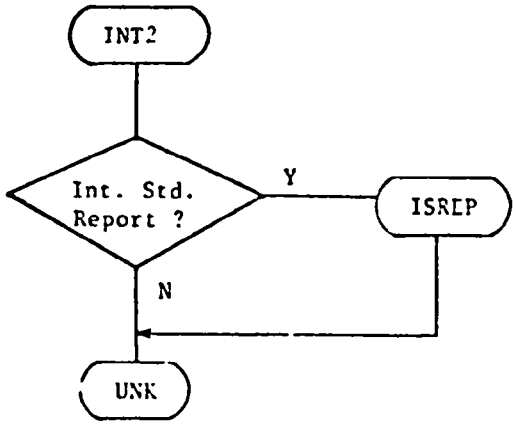
(continued)


SELECT2
SPS?
Y
RMRFIX
Adjust RMRs for SPS
N
Loop 4: for Each Combination of IS Ion and XS Ion (2 x 2 = 4 in all) Calculate back. wt (ATSC) Amt. Std. Calc.
ATSC (I) = Wt.XS x MWIS x S.R.IS / MWXS x S.R.XS x RMR
END LOOP 4
SELECT3

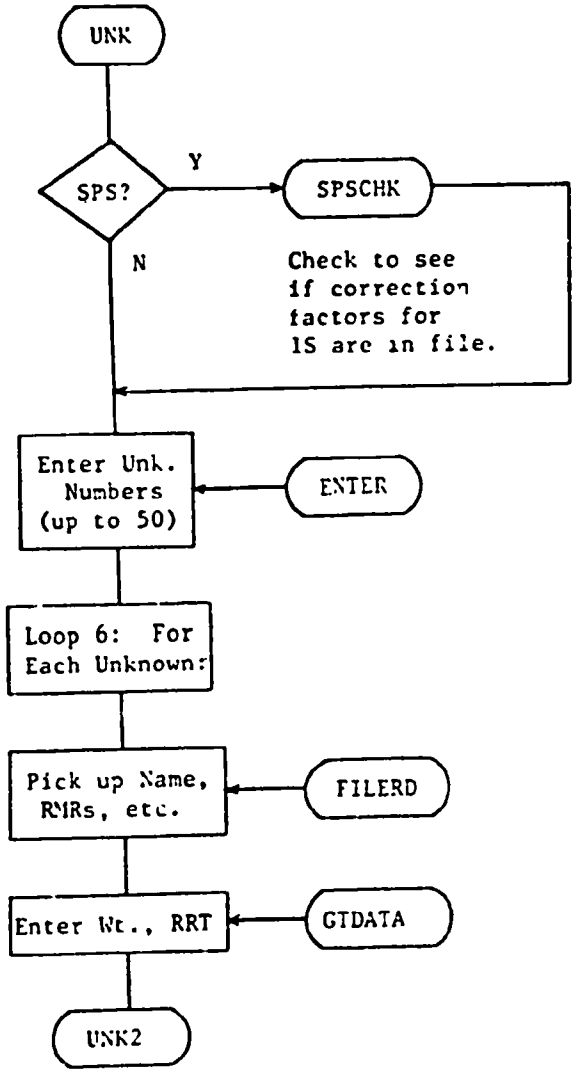
(continued)


SELECT3
Determine the Ratios of For. to Back. Wts.
Loop 5: for All Combinations (1-4)
AISA vs ATSC(I)
<
>
R = ATSC(I) / AISA
R = AISA / ATSC(I)
End Loop 5
Choose as Best Ratio that Closest to 1.0
Forward Wt. Less than 0.83 x Best Backward Wt. ?
Y
N
Substitute. 1.2 x Forward Wt. for Calc. Wt IS
Choose the IS Ion Corresponding to Best Ratio
End Loop 3
INT 2

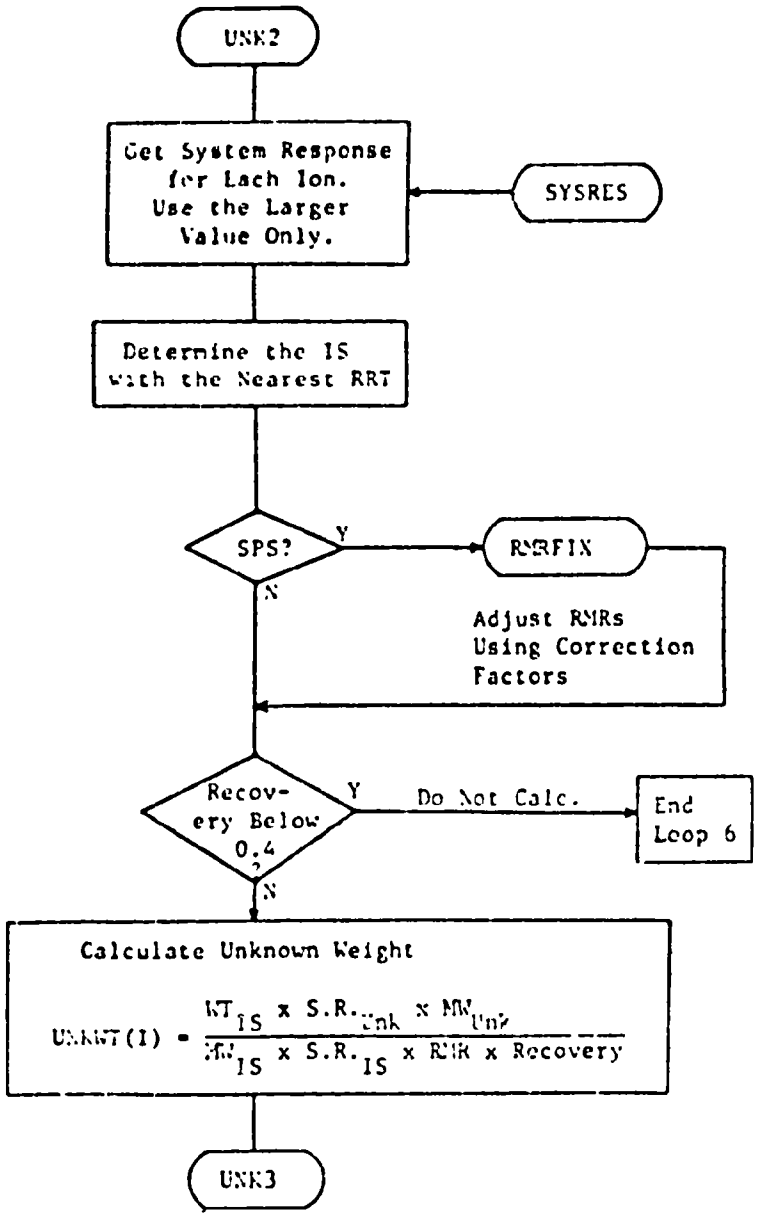
(continued)



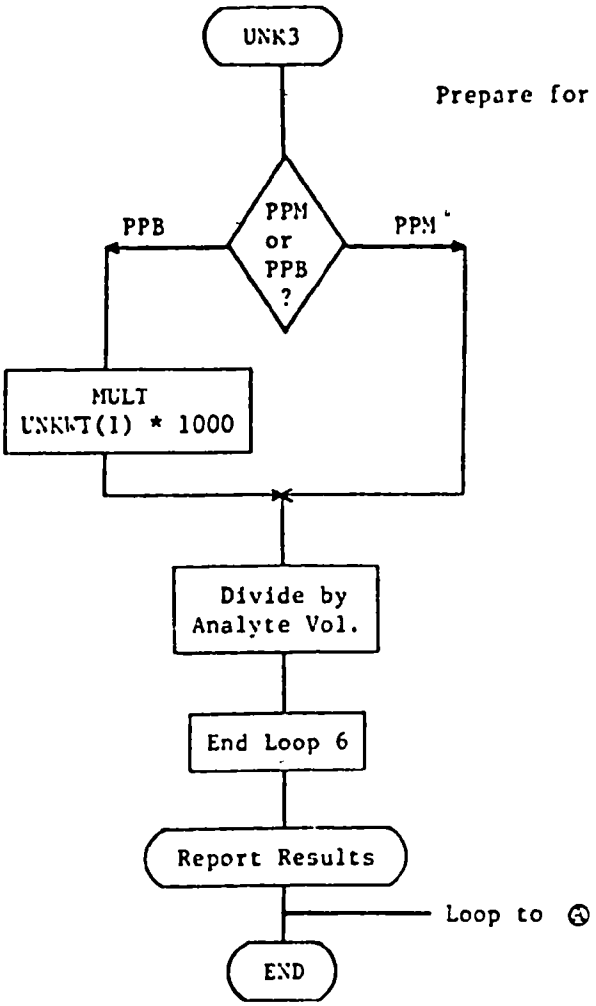
(continued)


UNK
SPS?
Y
SPSCHK
N
Check to see
if correction
factors for
IS are in file.
Enter Unk.
Numbers
(up to 50)
ENTER
Loop 6: For
Each Unknown:
Pick up Name,
RMRs, etc.
FILERD
Enter Wt., RRT
GTDATA
UNK2

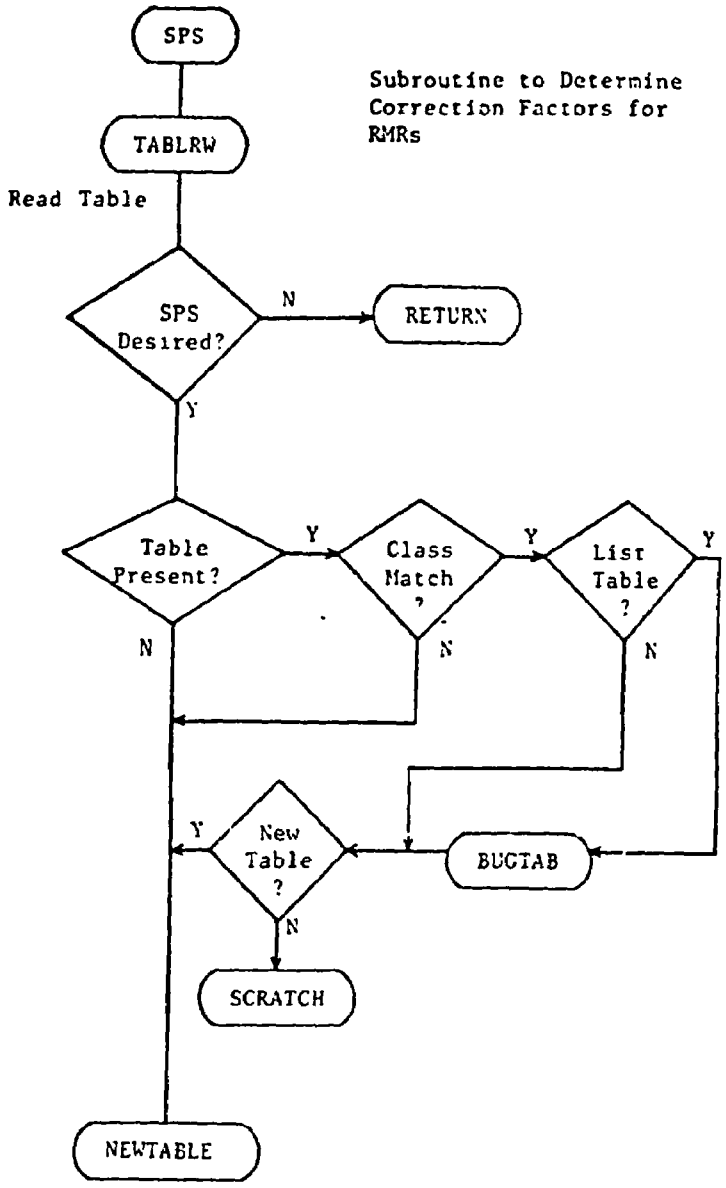
(continued)


UNK2
Get System Response for Each Ion. Use the Larger Value Only.
SYSRES
Determine the IS with the Nearest RRT
SPS?
Y
N
RMRFIX
Adjust RMRs Using Correction Factors
Recov- ery Below 0.4
Y
Do Not Calc.
End Loop 6
N
Calculate Unknown Weight
$UNKWT(I) = \frac{WT_{IS} \times S.R._{Unk} \times MW_{Unk}}{MW_{IS} \times S.R._{IS} \times RMR \times Recovery}$
UNK3

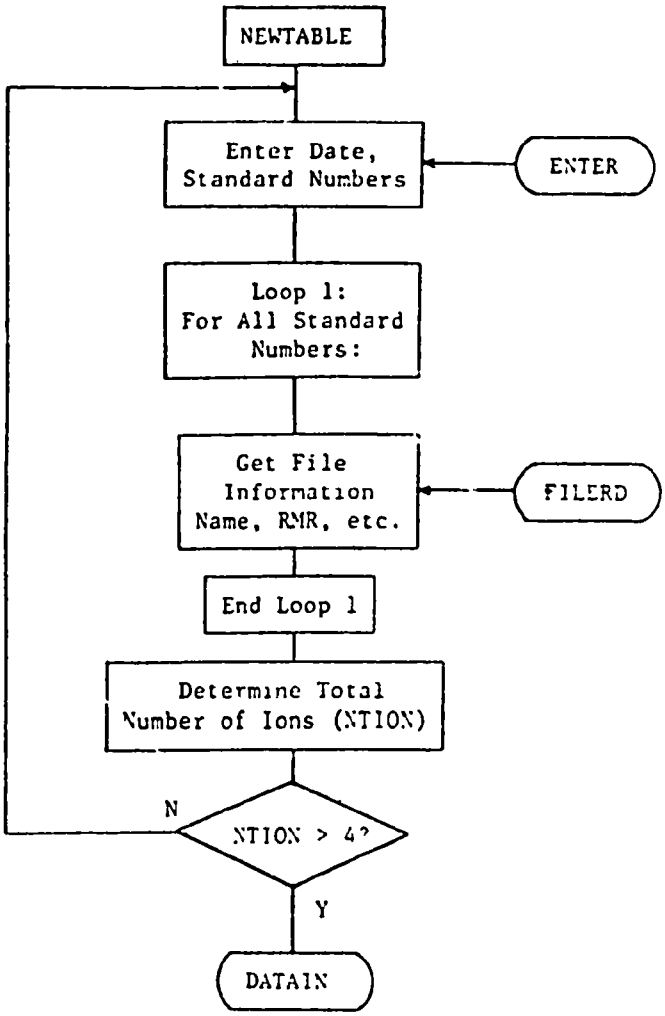
(continued)


UNK3
Prepare for Report
PPM or PPB ?
PPB
PPM
MULT UNKWT(I) * 1000
Divide by Analyte Vol.
End Loop 6
Report Results
Loop to ⊛
END

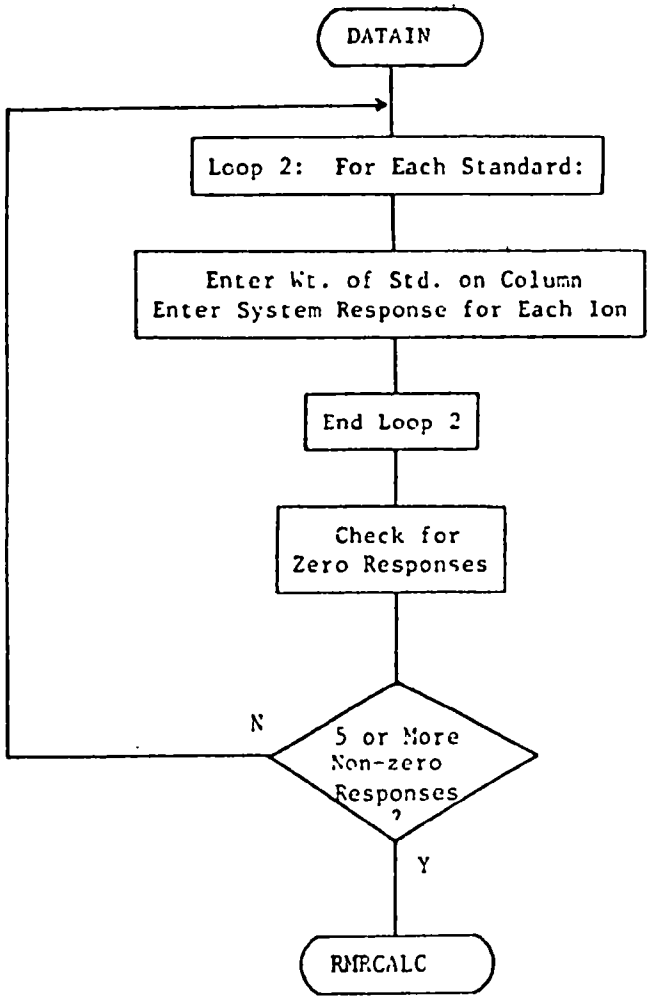
(continued)


SPS
Subroutine to Determine Correction Factors for RMRs
TABLRW
Read Table
SPS Desired?
N
RETURN
Y
Table Present?
Y
Class Match ?
Y
List Table ?
Y
N
N
N
New Table ?
Y
BUGTAB
N
SCRATCH
NEWTABLE

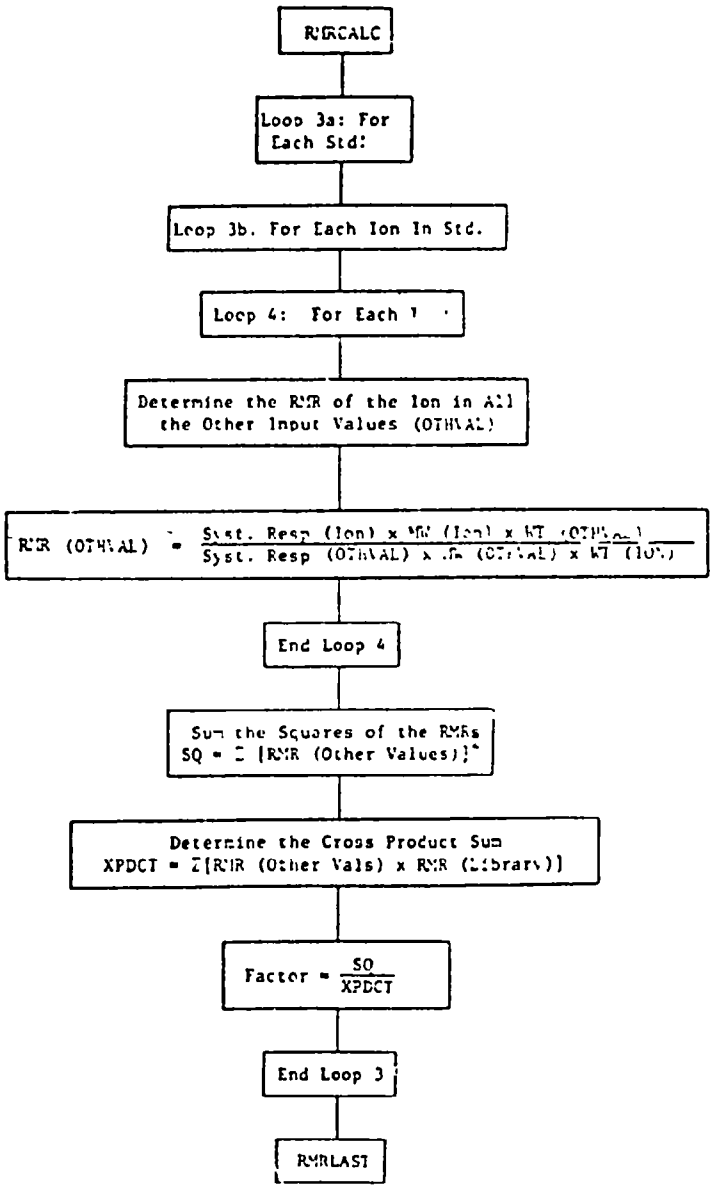
(continued)


NEWTABLE
Enter Date,
Standard Numbers
ENTER
Loop 1:
For All Standard
Numbers:
Get File
Information
Name, RMR, etc.
FILERD
End Loop 1
Determine Total
Number of Ions (NTION)
N
NTION > 4?
Y
DATAIN

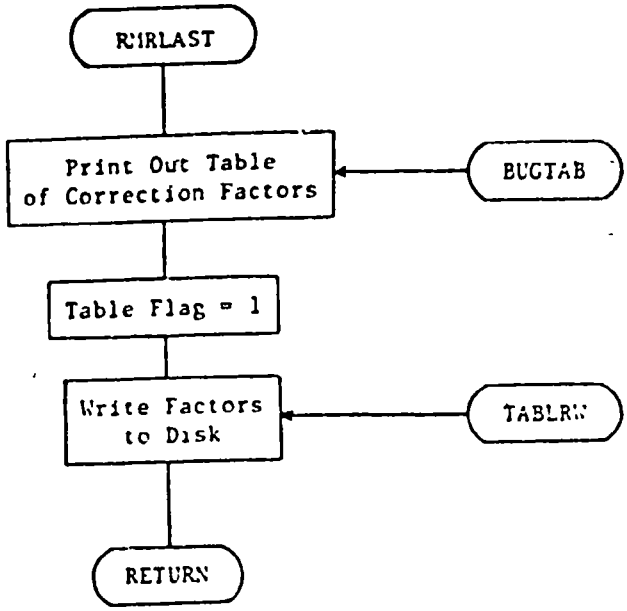
(continued)

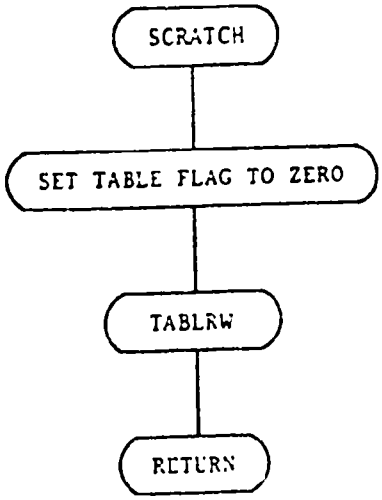

DATAIN
Loop 2: For Each Standard:
Enter Wt. of Std. on Column
Enter System Response for Each Ion
End Loop 2
Check for
Zero Responses
N
5 or More
Non-zero
Responses
?
Y
RMRCALC

(continued)


RMRCALC
Loop 3a: For Each Std:
Loop 3b. For Each Ion In Std.
Loop 4: For Each
Determine the RMR of the Ion in All the Other Input Values (OTHVAL)
End Loop 4
Sum the Squares of the RMRs
Determine the Cross Product Sum
Factor = SQ / XPDCT
End Loop 3
RMRLAST

(continued)


RMRLAST
Print Out Table of Correction Factors
BUGTAB
Table Flag = 1
Write Factors to Disk
TABLRW
RETURN


SCRATCH
SET TABLE FLAG TO ZERO
TABLRW
RETURN