INSTRUCTIONS FOR SEARCHING

AQUIRE

AQUATIC INFORMATION RETRIEVAL SYSTEM

EPA

INSTRUCTIONS FOR SEARCHING

AQUIRE

ON CIS

The AQUATIC INFORMATION RETRIEVAL DATA BASE (AQUIRE) is contained within the Environmental Protection Agency's SCIENTIFIC PARAMETERS IN HEALTH AND THE ENVIRONMENT; RETRIEVAL AND ESTIMATION (SPHERE) Environment. AQUIRE is being developed through the collaborative efforts of the EPA Environmental Research Laboratory in Duluth, Minnesota, and the EPA Office of Toxic Substances.

AQUIRE consists of data extracted from papers published worldwide that deal with the toxic effects of chemical substances on aquatic organisms. This version of AQUIRE primarily contains data from papers published in English between 1970 and 1981. Documents to be extracted are identified through literature searches, from review articles and criteria document bibliographies, and from existing aquatic toxicity reprint collections. The data base includes acute and chronic toxicity, bioaccumulation, and sublethal effects data from tests performed on freshwater and salt-water species, except aquatic mammals, birds, and bacteria. The data are formatted into records at the level of the individual tests or observations. Each record contains chemical substance information, test organism details, study protocol, experimental details, and results for one test or

observation within a given reference document. Thus, there can be multiple AQUIRE records for a given chemical from a single paper as well as from several different papers.

The AQUIRE data base contains 38,780 records, or entries, each representing a description of a single test with one chemical substance. These represent aquatic toxicity information for 1,912 unique chemicals. AQUIRE is eventually expected to include data for 4,000 to 5,000 chemicals. Of the 1,912 chemicals in the current version of AQUIRE that have CAS registry numbers, 1,565 were already present in the National Institute for Health (NIH) EPA Chemical Information System's (CIS) Structure and Nomenclature Search System (SANSS). At this time only those 1,565 chemicals from AQUIRE are in SANSS. It is anticipated that the remaining chemicals will be included in SANSS when it is next updated. The AQUIRE data base is expected to be updated two to three times a year.

INSTRUCTIONS FOR SEARCHING AQUIRE

ON CIS

TABLE OF CONTENTS

Page Number

GETTING ON..... 1
NEWS..... 2
LOGGING OFF..... 2

SEARCHING BY: SINGLE **CAS** NUMBERS..... 3
MULTIPLE CAS NUMBERS..... 5
PARAMETER TYPE (**PAR**)..... 6
NAME SEARCHING USING SANSS (**NPROBE**)..... 7
NAME (**NAM**) IN AQUIRE.....10
MOLECULAR WEIGHT IN SANSS (**MW**).....11
MOLECULAR FORMULA IN SANSS (**MF**).....12
CHEMICAL CHARACTERISTICS (**CHC**).....16
STUDY PURPOSE (**PRP**).....17
STUDY RELIABILITY (**REL**).....17
SPECIES NAME (**SPP**).....18
AGE/LIFE STAGE (**AGE**).....18
ROUTE/METHOD (**RTE**).....19
EXPOSURE REGIMEN (**REG**).....19
GENERAL TEST CONDITIONS (**GEN**).....20
TEMPERATURE (**TEMP**).....20
PH (**PHV**).....21
OTHER WATER CHEMISTRY (**OWC**).....21
EFFECT ENDPOINT TYPE (**EFE**).....22
MEASURED/UNMEASURED (**MEA**).....25
REMARKS (**REM**).....25
REFERENCE NUMBER (**RNO**).....27
ACCESSION NUMBER (**ACC**).....27
AUTHOR (**AUT**).....28
YEAR (**YRP**).....28
TITLE (**TLE**) AND JOURNAL/SOURCE (**JRN**).....28

EXISTENCE SEARCHING.....29
USE OF: **SORT** COMAND.....29
STORE COMMAND.....29
STORED FILE.....30
DELETE COMMAND.....30
EXTRACT COMMAND.....30
TYPING OUT TEMPORARY RESULTS FILE..... 3
E CONTROL-O..... 4
EXAMPLE OF **AQUIRE RECORD**..... 4
AQUIRE **FORMATS**..... 5
COMBINING SEARCHES..... 7
SHOWING SANSS RECORDS (**SSHOW**)..... 8
SANSS RECORD FOR METATHION..... 9

Page Number

TYPING AQUIRE DATA FOR CHEMICALS IN SANSS..... 9
USE OF **TRUNCATION (:)**.....10

CHEMICAL TYPE FIELD **(TYP)**.....10
HARDNESS **(HDV)**, ALKALINITY **(ALK)**, AND
DISSOLVED 02 **(DO2)** FIELDS.....20
EFFECT ENDPOINT VALUE FIELD **(EFC)**.....24
CONFIDENCE LIMITS FIELD **(CNF)**.....24
OTHER ENDPOINT DATA FIELD **(OED)**.....24
CITATION **(CIT)**, NUMBER OF DATA LINES **(RDL)**, DATA
COLLECTION IDENTIFIER **(DID)** AND ADD DATE FIELDS **(ADT)**...28

INSTRUCTIONS FOR SEARCHING AQUIRE ON CIS

GETTING ON

Dial **841-1200** (1200, 300 Baud)

Type **<cr> <cr>** (carriage return)

SYSTEM responds with

```
AMS SYSTEM =
```

Type **DECE <cr>**

SYSTEM responds with:

```
ENTER 2 C/R AFTER "GO"
GO
```

Type **<cr> <cr>**

You will then get the message:

```
AMShare Remote Computing Service 2743

    AMShare Monitor 285
@
```

at the @ prompt type your account number, name and password, e.g.

@ **LOG**Δ**XXX.OTS**Δ**PASSWORD <cr>** (no need to use upper case)

The system will then respond with something like the following:

```
Job 46 on TTY 37 Monday, May 21, 1984 10:43:29
STRUCTURE CIS2:  Mounted
STRUCTURE DEV2:  Mounted
```

You will get CIS Banner information and then a "component mnemonic" prompt. Type AQUIRE as follows:

```
Component Mnemonic?  (H for HELP):
```  **AQUIRE <cr>**

After typing AQUIRE **<cr>** you should get a message like:

```
AQUIRE (Version 1.1/2.0 February 1984) ($55/Hr.)
Type News at "Option?" for further detail
```

NEWS

Option? **NEWS <cr>**

will give you the latest AQUIRE news if there is any available online. If there is not, you will receive the message:

```
"NO NEWS ON FILE"
```

LOGGING OFF

When you get ready to stop work do the following:

Option? **LOGOFF <cr>**

You will receive a message like the following:

```
Your approximate total CIS Session cost is $4.26 killed job 23,
User XXX.OTS, Account, TTY 43, at 23-Jan-84          10:03:29,
Used 0:00:04 Resource Units in 0:10:33
  AM Share Remote Computing Service System.  2743, AM Share
    Monitor 283
```

Wait until you see the entire message to turn off your machine and hang up the phone.

SEARCHING BY SINGLE CAS NUMBERS

|Option?| **CAS/12125-02-9 <cr>, or CAS/12125029 <cr>**

The system will respond as follows:

|File: 1 Count: 191|

You have just created a temporary results file (File 1) and there are 191 records in it for CAS Number 12125029.

TYPING OUT A TEMPORARY RESULTS FILE

If you want to see the records in file 1 which you created above, you can do the following:

|Option?| **TYPE Δ 1/2/1-2 <cr>**

file number ↗ ↑ ↖ records

format number

One of the records retrieved from the above follows:

EXAMPLE OF AQUIRE RECORD FOR CAS NUMBER 12125-02-9.

```
                File  1:  Entry      1:  Accession No.        200006
{PAP}  Parameter Type:  FNV:  AQ
{CAS}  CAS Registry Number:  12125-02-9
{NAM}  Chemical Name:  Ammonium chloride
{TYP}  Chemical Type:  TFST
{CHC}  Chemical Characteristics:  NR
{PRP}  Study Purpose:  LC
{REL}  Study Reliability:  1
{SPP}  Species Name:  ORCONECTES NAIS
{AGE}  Age/life Stage:  2.78 CM
{RTE}  Route/Method:  FT
{REG}  Exposure Regimen:  96 H
{GEN}  General Test Conditions:  FW:  LAB
{TEMP} Temperature {Degrees C}:  26 to 27 {C}
{HDV}  Hardness:  96 mg/l CaCO3
{ALK}  Alkalinity:  43 mg/l CaCO3
{DO2}  Dissoluted O2:  {7.8 - 8.2} mg/l
{PHV}  pH:  7.6 to 9.11
{OWC}  Other Water Chemistry:  SFF PAPER
{EEE}  Effect Endpoint Type:  LC50
{EEC}  Effect Endpoint Value:  2590 ug/l {Calc}
{CNF}  Confidence Limits:  1780 - 3790 mg/l {Calc}
{OED}  Other Endpoint Data:  I FTHARGY OBSERVED 6-11 H PRIOR TO
       DEATH.
{MEA}  Measured/Unmeasured:  Measured
{REM}  Remarks:  {CNT} 10% MORTAILITY.
       {SCR} as N.
       N
{RNO}  Reference Number:  210402
{AUT}  Authors:  Evans, J.W.:
{YRP}  Year:  1979
{TLE}  Title:  The Construction and Use of a Continous-Flow
       Bioassay Apparatus to Determine a Preliminary Unionized
       Ammonia 96-Hour LC50 for the Crayfish.  Orconectes nais.
{JRN}  Journal/Source:  M.S. Thesis, University of Kansas,
       Lawrence, KS, 76 P.
{RDD}  Number of Data Lines:  1
{DID}  Data Collection Identifier:  AQUIRE
{ADT}  Add Date:  04-02-83
```

E CONTROL-O

AQUIRE is a very large data base and there will often be several hundred records for a single chemical substance. Later in the instructions there will be more information on how to narrow your search results.

If, by mistake, you ask for the entire file above (or a similar one) to be typed out and it gets too long, type **E control-O** to stop the processing. You may need an additional **<cr>** as well to return to an option? prompt.

SEARCHING BY MULTIPLE CAS NUMBERS

If you have several CAS numbers, you can use the INCAS command as follows:

```
Option? INCAS <cr>
```

You will then see:

```
CAS numbers (cr to end): 7487947 <cr>
CAS numbers (cr to end): 58899 <cr>
CAS numbers (cr to end): 12125-02-0 <cr>
CAS numbers (cr to end): <cr>
```

The final cr gets you out of the INCAS routine. The system will then give you the following:

```
      3 entries accepted.
Entries were not in sequence - being sorted now.
File 3 created, contains 3 CAS Registry Numbers.
```

Now you need to create an AQUIRE file for those CAS numbers as follows:

```
Option? CAS/#3 <cr>
```

3 is the INCAS file number. The system will respond as follows:

```
File:  4      Count:  1221
Option?
```

AQUIRE FORMATS

There are three general format types in AQUIRE:

- ABBREVIATED (Format 1)
- FULL (Format 2)
- USER-SPECIFIED (Format 4)

You have already seen Format 2, or the FULL AQUIRE format. In order to type Format 1 or the ABBREVIATED Format do the following:

```
Option? TYPE △ 4/1/1-4 cr
          File  Abbreviated Format  Records
```

The following is the first record retrieved from the above search:

```
                File  4:  Entry    1:  Accession No.      200003
{ABF} MERCURY CHLORIDE:  7487-94-7 ENV:  AQ 80-210400 {1}
      HETEROPNEOSTES FOLLILUS:  ST:  96H:  LC50:  260 mg/l
      {Calc}:
```

For Format 4, the USER - SPECIFIED Format, you need to set up the format before you type out a file:

Option? **FORMAT**Δ**CAS** Δ**NAM**Δ**EFE**Δ**EFC** <cr>

Above, any field mneumonics in any order can be used.

Option? **TYPE** Δ **4/4/1-5** <cr>

file format records

The system will then give you the five records in Format 4. One of them is shown below:

```
                File  4:  Entry    1:  Accession No.      200003
{CAS} CAS Registry Number:  7487-94-7
{NAM} Chemical Name:  MERCURY CHLORIDE
{EFE} Effect Endpoint Type:  LC50
{EEC} Effect Endpoint Value:  260 mg/l {Calc}
```

If you need a new user specified format you should clear the existing format:

Option? **FORMAT**Δ**CLEAR** <cr>

and then proceed to specify another Format 4.

SEARCHING BY PARAMETER TYPE (PAR)

There are two parameter types in AQUIRE:
AQ for aquatic toxicity or effects data, and
BCF for bioconcentration factor.

Option? **PAR/AQ** <cr> will give you

```
File:  1          Count:  34,043
```

or all the aquatic effects records in AQUIRE.

|Option?| **PAR/BCF <cr>** will give you

|File: 2 Count: 4,737|

or all the bioconcentration factor records in AQUIRE.

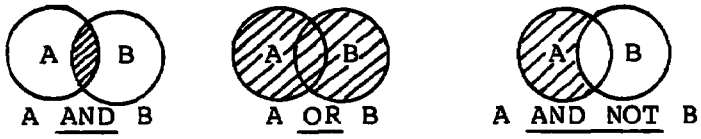
These are large files and if you use these searches you will probably want to use them in combination with other searches, e.g.:

|Option?| **PAR/BCFΔANDΔCAS/58899 <cr>**

|File: 3 Count: 93|

COMBINING SEARCHES

You can use AND, OR, AND NOT - see below:



You can combine file numbers

|Option?| **#1ΔANDΔ#4 <cr>**

You can combine searches:

|Option?| **CAS/50000ΔANDΔNOTΔPAR/AQ <cr>**

Your can combine file numbers and searches

|Option?| **#4ΔANDΔPAR/BCF <cr>**

NAME SEARCHING USING SANSS

If you have a name and not a CAS number you should use SANSS, the CIS synonym (etc.) file. There are long lists of synonyms for SANSS chemicals, whereas SPHERE (AQUIRE) only gives the name used by the author of the article cited. Suppose you have the name metathion.

Do the following:

|Option?| **GOΔSANSS <cr>**

You will get banner information and then another |option?| prompt.

|Option?| **NPROBE <cr>**

The system will respond with:

|Fragment or whole - name search (F/W) (F)?| **W <cr>**

Because METATHION is a whole name, type W.

The system will respond with:

|Specify name (CR to exit):| **METATHION <cr>**

The system will respond:

|File 1, 1 compounds having name: METATHION
|specify name (CR to exit):| **<cr>**

This gets you out of the NPROBE subroutine.

SHOWING SANSS RECORDS (SSHOW)

In order to see the SANSS (not AQUIRE) record for the chemical that you searched on type:

|Option?| **SSHOW**Δ**1 <cr>**

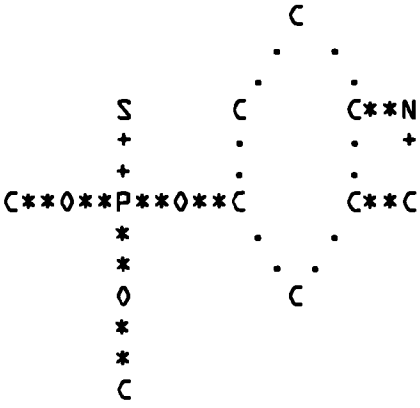
The system will respond as follows:

SANSS RECORD FOR METATHION

```
Entry        1  CAS RN 122-14-5
CTS Sources Of Information

     2 - CTS, EI Mass Spectrometry
     5 - EPA/CIS, OHM/TADS:  A100082
    32 - NIOSH/CIS, RTECS:  TG0350000
   124 - CIS, CI Mass Spectrometry
   130 - CIS, FRSS (Federal Register Search System)

22 Non-CIS References Available
                                                          C9H12NO5PS
```



```
Phosphorothioic acid, O,O-dimethyl O-(3-methyl-4-nitrophenyl)
     ester (9CI)
Phosphorothioic acid, O,O-dimethyl O-(4-nitro-m-toly) ester
     (8CI) ac-47300
m-Cresol, 4-nitro-, O-ester with O,O-dimethyl phosphorothioate
Accothion
  79 more names available
```

TYPING AQUIRE DATA FOR CHEMICAL(S) IN SANSS FILE

You must first return to the AQUIRE data base:

|Option?| **GO△AQUIRE <cr>**

After you receive the AQUIRE banner information you should intersect the SANSS chemical file with the AQUIRE data base as follows:

|Option?| **CAS/$1 <cr>** (the SANSS file for METATHION)

|File: 2 Count: 335|

|Option?| **TYPE△2/1/1-10 <cr>**

Two of the records retrieved follow here:

```
                File   2:  Entry    1:  Accession No.      200015
{ABF}   Fenitrothion:  122-14-5 Env:  AQ 79-210404 {1}
      SALMO GAIRDNERI:  FT:  24H:  LC50:  4300 ug/l:

                File 2:  Entry      2:  Accession No.      204487
{ABF}   BAYER 41831:  122-14-5 ENV:  AQ 64-210646 {164}
      PHYTOPLANKTON ** ST:  4 H:  NA {GRO *}:  1000 mg/l:
```

Note that in both of the preceding records, the CAS number is the same as in our SANSS record based on a search for METATHION, but each record has listed a different name or synonym, i.e., FENITROTHION and BAYER 41831.

SEARCHING BY NAME (NAM) IN AQUIRE

Because we have not yet entered all 1,912 AQUIRE chemicals into SANSS, you should also double check by doing a NAM search in AQUIRE as follows:

Option? **NAM/ANTI-GERM Δ50 <cr>**

No responses for: NAM/ANTI - GERM 50

Option? **NAM/ANTI-GERM:** <cr> See TRUNCATION

File: 3 Count: 8

USE OF TRUNCATION (:)

Truncation of words is accomplished in CIS with the use of a colon (:). Right truncation is the most commonly used form of truncation, but left and imbedded truncation are also possible in CIS.

In the previous NAM/ANTI-GERM: search we weren't sure how the name ended, so we searched for anything with the root word ANTI-GERM, regardless of the suffix in the NAM field.

In the preceding example all names were ANTI-GERM 50 (A-G-50), but that might not have been the case. This chemical (CAS Number 62010280) was in AQUIRE but not in SANSS.

CHEMICAL TYPE FIELD (TYP)

This field contains only one possible data type in AQUIRE, although in other SPHERE Data Bases there are alternatives. In AQUIRE the field always carries the term TEST whereas in other SPHERE Data Bases it can be TEST or ACTIVE INGREDIENT.

An example of the output from this field follows:

(TYP) Chemical Type: TEST

SEARCHING BY MOLECULAR WEIGHT IN SANSS

|Option?| **GO△SANSS <cr>**

|Option?| **MW <cr>**

The system will respond as follows:

|Type MW or range, cr to EXIT|
|User:| **243 <cr>**

you can type a specific molecular weight in as shown here and get the following:

|File = 1, 545 compounds with MW 243|
|Option?| **MW <cr>**

you can type in a range, which is done by typing the lower and upper (in order) ends of the range with a space between the two numbers:

|Type MW or range, cr to EXIT|
|User:| **243△245 <cr>**

you will then get:

|File = 2, 1,892 compounds with MW 243 - 245|
|Option?| **GO△AQUIRE <cr>**

|AQUIRE (Version 1.1/2.0 February 1984) ($55/Hr.)|
|Option?| **CAS/#1 <cr>**

|File: 3 Count: 60|
|Option?| **CAS/#2 <cr>**

|File: 4 Count: 89|

|Option?| **TYPE△4/1/1 <cr>**

This will give you one of the records in the file created by the range search above in the abbreviated format.

```
                File 7:  Entry     1:  Accession No.      201828
{AAF}   2,4-D SODIUM SALT:  2702-9 ENV: AQ 69-210542 {52}
      RASBORA HETEROMORPHA:  NN:  24 H:  LC50?:  1160000 ug/l:
```

SEARCHING BY MOLECULAR FORMULA

This type of search should also be done in SANSS, so if you are not already there you should go there.

|Option?| **GO△SANSS <cr>** or

or

|Component Mnemonic? (H for Help):| **SANSS <cr>**

This search is rather complicated, and you should begin by reading the following information:

The molecular formula search, MF, will search through the data base for all compounds with a specified complete or partial molecular formula. When you command 'MF', the program will type 'CR TO EXIT, COMPLETE (C), PARTIAL (P) or RANGED (R) MF?'. If you respond 'C' to this, then you will first be asked whether the search should be made applicable to "total" or "addend" formulas. An addend formula is any single segment of a dot-disconnected formula, whereas the total formula is the composite of all the segments. If you specify "addend" formula, you will retrieve only those substances having multiple dot-disconnected segments, one of which corresponds to the formula you specify.

If you type C for complete formula you will be asked to enter a complete molecular formula. When you do this, you should specify the complete molecular formula with elements separated from each other by a period or a space, e.g. C17.H27.CL.N3.O Note that the subscript '1' is omitted and there is no '.' at the end of the formula. In the partial molecular formula search, you will be asked how many elements you wish to specify and then you will be queried about each of these, one by one. The ranged molecular formula search is just the same except that you can enter the ranges associated with each element, e.g. C4,8: H10,18 and so on. When any of the MF searches is complete, the program will tell you how many compounds have been retrieved and store them as a file which can subsequently be used by programs such as 'SSHOW'.

The MF command allows the user to retrieve all compounds of a specific, partial or ranged molecular formula.

Option? **MF <cr>**

cr to exit, Complete (C), Partial (P), or Ranged (R) MF?

User: **C <cr>**

Shall the search be done for total formula or the addend formula ?(T/A): **T <cr>**

Type in complete molecular formula.
Use periods or spaces, e.g. C10.H18.0
User: **C6.H7.N1 <cr>**

File = 8, 9 compounds having MF : C6.H7.N1
.....
<cr> to exit, Complete (C), Partial (P), or Ranged (R) MF?
User: **<cr>**

Option? **SETDC $\Delta_0\Delta_1\Delta_0\Delta_1$ <cr>**

(See SANSS training manuals)

Option? **SSHOW Δ_8 <cr>**

How many (E to Exit)? **2 <cr>**

Type E to terminate display
Entry 1 C6H7N
Benzenamine (9Cl)

Entry 2
Pyridine, 4-methyl- (9Cl)
C6H7N

Option? **MF <cr>**

cr to exit, Complete (C), Partial (P), or Ranged (R) MF?
User: **C <cr>**

Shall the search be done for total formula or the addend formula ?(T/A): **A <cr>**

```
Type in complete molecular formula.
Use periods or spaces, e.g. C10.H18.0
User:  C6.H7.N1 <cr>
```

```
File = 9,   84 compounds having MF  :  C6.H7.N1
.............
cr to exit, Complete (C), Partial (P), or Ranged (R)  MF?
User:  <cr>
```

```
Option?  SSHOW 9 <cr>
```

```
How many (E to Exit)?  2 <cr>

Type E to terminate display.
Entry         1                                          C6H7N.ClH
Benzenamine, Hydrochloride (9CI)
---------
Entry         2                                          C6H7N.BrH
Benzenamine, Hydrobromide (9CI)
---------
```

```
Option?  MF <cr>
```

```
cr to exit, Complete (C), Partial (P), or Ranged (R) MF?
User:  P  <cr>
```

```
The number of atom types is :  2 <cr>
Enter atom, and a count for each, e.g. C6
Type 1 is:  C6 <cr>
Type 2 is:  N1 <cr>
File=10, 1730 compounds with partial MF:C6.N1
.............

cr to exit, Complete (C), Partial (P), or Ranged (R) MF?

User:  <cr>
```

```
Option?  SSHOWΔ10 <cr>
```

```
How many (E to Exit)?  2 <cr>

Type E to terminate display.
Entry 1                                                    C6H7NO.ClH
Phenol, 2-amino-, hydrochloride (9CI)
---------
Entry 2                                                    C6H7NO.ClH
Phenol, 4-amino-, hydrochloride (9CI)
```

```
Option?  MF <cr>
```

```
cr to exit, Complete (C), Partial (P), or Ranged (R) MF?
User:  R <cr>
```

```
The number of atom types is:  2 <cr>
```

```
Enter atom, and range for each, e.g.  C6,12
```

```
Type 1 is:  C8,10 <cr>
Type 2 is:  N4,5 <cr>
```

```
File = 11,  1884 compounds having partial MF in range  :
            C8-10.N4-5
.............

cr to exit, Complete (C), Partial (P), or Ranged (R) MF?
User:  <cr>
```

```
Option?  SSHOWΔ11 <cr>
```

```
How many (E to Exit)?  2 <cr>
```

```
Type E to terminate display.
Entry 1                                                    C10H14N4O3
1H-Purine-2,6-dione, 3,7-dihydro-1-(2-hydroxypropyl)-
     3,7-dimethyl - (9CI)
---------
Entry 2                                                    C8H16N4
1,3,6,8-Tetraazatricyclo(4.4.1.13,8) dodecane (8CI9CI)
---------
How many (E to Exit)?  E <cr>
```

SEARCHING ON CHEMICAL CHARACTERISTICS (CHC)

The CHC field contains information about the grade/purity of a chemical. Terms that appear in the field and can be used for searching are listed here:

Grade/Purity Abbreviations

A - Analytical Grade (440)
AAPS - Atomic Absorption Primary Standard (1)
ACS - American Chemical Society Grade (183)
AE - Acid Equivalent (108)
AI - Active Ingredient (341)
An - Analar Grade (17)
AQ - Aqueous Solution (0)
AS - Aqueous Suspension (43)
ASG - Agricultural Supply Grade (48)
B - Biological Grade (42)
C - Commercial Grade (1634)
CO - Concentrate (18)
CP - Chemically Pure (406)
CRP - Chromatographically Pure (7)
CRI - Chromatographically Impure (0)
D - Dust (49)
DC - Detached Crystals (0)
DP - Dispersable Powder (5)
E - Emulsion (203)
EM - Eastman Grand (0)
EC - Emulsifiable Concentrate (1397)
ES - Emulsifiable Solution, Agent (19)
F - Field Grade (447)
FCAAS - Fisher Certified Atomic Absorption Standards (3)
FO - Formulated (6)
FFO - Field Formulated (0)
G - Granule (215)
GAS CR STD - Gas Chromatograph Standards (5)
GS - Gaseous (70)
HG - Heavy Granular (167)
I - Industrial (16)
L - Laboratory Grade (64)
LD - Liquid (58)
ME - Monsanto Electrical Grade (O)
ND - Neutralized, Desensitized (1)
NF - Nonionized Form (0)
ODA - Organic Dispersal Agent (3)
P - Practical Grade (203)
PA - Pro Analysis Quality (24)
PAN - Pestanal Grade (6)
PAR - Particulate (2)
PEL - Pellet (12)
PF - Purified (5)
PH - Pharmaceutical Grade (115)
PO - Powder (0)
PR - Production Grade (0)
PRE - Prepared (5)
PST - Pesticide Grade (34)
PU - Pure (94)
R - Reagent Grade (1597)
RC - Recrystallized (72)
RE - Research Grade (18)
RF - Registered Formulation (0)
RST - Reference Standard (40)
S - Spectrophotometric Grade (35)
SC - Scintillation Grade (0)
SP - Soluble Powder (8)
SPO - Spray Powder (6)
ST - Standard (1)
T - Technical Grade (4330)
TA - Technical Acid Grade (112)
TR - Transformer Grade (1)
UD - Unneutralized, Desensitized (0)
USP - United States Pharmacopeia (22)
WP - Wettable Powder (504)
WS - Water Soluble (6)
WHO - World Health Organization (7)

|Option?| **CHC/A <cr>**

|File: 1 Count: 440|

SEARCHING BY STUDY PURPOSE (PRP)

This field contains information on the purpose of the study. The following controlled terms can be used for searching:

BCF = Bioconcentration factor (4,736)
EC = Effect concentration (2,396)
LC = Lethal concentration (19,454)
OTHER = Other (12,193)

|Option?| **PRP/EC <cr>**

|File: 1 Count: 2,396|

SEARCHES BY STUDY RELIABILITY (REL)

The AQUIRE data base has reliability codes for each of its records. These were established by the EPA Environmental Research Laboratory in Duluth and are based on the following criteria:

1. Meets all criteria

   Methodology section cites accepted procedures and quality assurance

   Control mortality or effect satisfactory (e.g., equal to or less than 10% for acute tests)

   Toxicant concentration was measured

   A solvent control if a solvent is used

   For organic and nonmetallic inorganic chemicals, at least the temperature, pH, and dissolved oxygen should be reported.

   For metals, at least the temperature, pH, dissolved oxygen, and either alkalinity or hardness should be reported (saltwater tests do not need alkalinity or hardness)

2. Meets some criteria

   Procedures generally satisfactory (i.e., followed standard methods), but:

   Control mortality not reported, or high and accounted for statistically

Or, toxicant concentration was unmeasured

Or, water chemistry variables not reported

Or, no solvent control when a solvent is used in the test.

3. Does not meet criteria

Methods section shows weaknesses in experimental procedures, or insufficient methodology description to judge quality of experiments.

Control mortality unsatisfactory (e.g., greater than 10% and not accounted for statistically).

A static test with unmeasured concentrations conducted in the presence of precipitate or some undissolved chemical or in an unacceptable container (i.e., pesticide with plastic liner).

4. Abstract or foreign paper

An example of a search of this field is:

|Option?| **REL/1 <cr>**

This pulls out all AQUIRE records with a study reliability of 1 (meets all criteria).

SEARCHING BY SPECIES NAME (SPP)

Studies can be retrieved based on the Latin name of the species tested. This field is searched based on a genus and species as follows:

|Option?| **SPP/AEDESΔAEGYPTI <cr>**

|File: 1 Count: 189|

Eventually there should probably be a field for common name with some heirarchy included, e.g., FISH, BLUEGILL.

SEARCHING BY AGE/LIFE STAGE (AGE)

There is no complete list of the terms used in this field, but you can search the field using terms you have seen in AQUIRE records.

Examples of some terms found in this field are:

JUVENILE	SUB-ADULT
ADULT	FRY
30-50 MM	SAC FRY
	SWIM UP FRY

SEARCHING BY ROUTE/METHOD (RTE)

In order to search in this field use one of the following codes:

ST = Static (24,683)
FT = Flow through (6,079)
OTHER = Other (4,228)

|Option?| **RTE/ST <cr>**

|File: 1 Count: 24,683|

SEARCHING BY EXPOSURE REGIMEN (REG)

This field can be searched, but the terms are not well controlled. No complete list of terms used is available, but the following terms do occur in the field:

24 H
96 H
48 H
10 D
62 D
12 H
165 D
84 D
373 D
294 D
18 D

|Option?| **REG/96Δ_H <cr>**

|File: 1 Count: 5,866|

SEARCHING BY GENERAL TEST CONDITIONS (GEN)

The terms used in this field are listed here. FW or SW can be combined with LAB or FIELD.

FW = Fresh water (28,281)
SW = Salt water (6,341)
LAB = Laboratory study (36,670)
FIELD = Field study (2,084)

|Option?| **GEN/SW△AND△FIELD <cr>**

|File: 1 Count: 247

|Option?| **GEN/FW <cr>**

|File: 2 Count: 28, 281|

SEARCHING BY TEMPERATURE (DEGREES C) FIELD (TMP)

The temperature of the water is a searchable field. The following table explains how **TMP** can be searched:

Greater than	>	TMP/>45
Greater than or equal to	>=	TMP/>=45
Less than	<	TMP/<.1
Less than or equal to	<=	TMP/<=1
Ranging	TO	TMP/10 TO 11
Equal to		TMP/11

AQUIRE is a large data base and these searches may take greater than a minute.

|Option?| **TMP/10△TO△11 <cr>**

|File: 1 Count: 1,547|

|Option?| **TMP/11 <cr>**

|File: 2 Count: 286 |

HARDNESS (HDV), ALKALINITY (ALK) AND DISSOLVED O_2 (DO2) FIELDS

The above fields are display only fields and cannot be searched.

SEARCHING THE pH (PHV) FIELD

This field can be searched as follows:

Greater than	>	PHV/>9
Greater than or equal to	>=	PHV/>9
Less than	<	PHV/>5
Less than or equal to	<=	PHV/>=5
Ranging	TO	PHV/7 TO 8
Equal to		PHV/7.69

|Option?| **PHV/7.69 <cr>**

|File: 1 Count: 3,506|

|Option?| **PHV/7 Δ TO Δ 8 <cr>**

|File: 2 Count: 17,940|

SEARCHING OTHER WATER CHEMISTRY FIELD (OWC)

This field is the location for water chemistry information that does not fit in other established fields. The field does not have a controlled vocabulary and the output can therefore vary considerably. An example of output is:

(OWC) Other Water Chemistry: 30% SEA Water, CO_2 3.4 PPM
" " : CO_2 9.7 PPM
" " : Dilution H_2O-Hardness, Conductivity
" " : 28 mg/l Suspended Solids

It is free-text searchable but the results of a search with a noncontrolled vocabulary cannot be expected to be comprehensive. Examples of search possibilities that may or may not be of interest are:

|Option?| **OWC/CONDUCTIVITY <cr>**

|File: 1 Count: 1,278|

|Option?| **OWC/CO_2 Δ 9.7 Δ PPM <cr>**

|File: 2 Count: 1|

|Option?| OWC/CO_2<cr>

|File: 3 Count: 336|

You simply did a free-text search for those terms or that term occurring anywhere in the OWC field output.

SEARCHING BY EFFECT ENDPOINT TYPE (EFE)

The effect endpoint type field indicates the specific endpoint measured. Controlled terms used for searching follow:

LC0 - No Mortality Concentration (0)*
LC25 - 25% Lethal Concentration (0)
LC50 - Median Lethal Concentration (18,541)
LC90 - 90% Lethal Concentration (68)
LC100 - Lethal Concentration (596)
LD50 - Median Lethal Concentration When Exposed Through Injections (80)
LD100 - Lethal Concentration Exposed Through Injection (2)
EC20 - 20% Effective Concentration (6)
EC50 - Median Effective Concentration (1191)
LT50 - Lethal Threshold Concentration (731)
LT50* - Mean Survival Time (0)
ET50 - Median Estimated Time (0)
AB - EC50- Abnormalities (22)
AC - EC50- ACHE Activity (25)
AV - EC50- Avoidance (2)
BA - EC50- Byssal Attachment (130
BH - EC50- Behavior (0)
BM - EC50- Biomass (0)
CC - EC50- Color Change (4)
CD - EC50- Cell Division (0)
CF - EC50- Cough Frequency (0)
CH - EC50- Chlorophyll (0)
CL - EC50- Case Leaving (1)
DE - EC50- Detection of Toxicant (10)
OT - EC50- Detachment
DV - EC50- Development (30
EM - EC50- Emergence (0)
EP - EC50- Egg Production (1)
EQ - EC50- Loss of Equilibrium (29)
EZ - EC50- Enzyme Activity (0)
FC - EC50- Food Consumption (0)
FD - EC50- Reduced First Feeding Incidence (10)
FF - EC50- Critical Flicker Rate (0)
FL - EC50- Fluorescence (0)
FP - EC50- Fecal Pellets (0)

*Note that (0) indicates that although the term could have been used by ERL-Duluth, it was not and it is not currently in the data base.

FR - EC50- Filtration Rate (16)
GR - EC50- Growth (174)
HA - EC50- Hatchability (4)
HM - EC50- Hemmorhage (0)
IM - EC50- Immobilization (635)
IN - EC50- Inhibition (4)
IR - EC50- Irritation (17)
MI - EC50- Migration Suppression (0)
OC - EC50- Oxygen Production (110)
PC - EC50- Population Carrying Capacity (0)
PG - EC50- Pigment Change (0)
PH - EC50- Physiological Effect (0)
PP - EC50- Population Size Reduction (3)
PS - EC50- Photosynthesis Effect (4)
PU - EC50- Pupation (0)
RE - EC50- Reproduction (28)
RG - EC50- Regeneration (0)
RR - EC50- Respiratory Rate (0)
SC - EC50- Shell Valve Closure (1)
SW - EC50- Swimming (0)
TE - EC50- Teratogenesis (36)
UP - EC50- Uptake (0)
VD - EC50- Vertebral Damage (0)
ABD - Abundance (591
ABN - Abnormalities (97)
AVO - Avoidance (184)
BCF - Bioconcentration Factor (4,737)
BCFC - Bioconcentration Factor Where Clearance is Recorded in Remarks (0)
BCFD - BCF was calculated using a dry weight tissue concentration
BEH - Behavior (109)
BIO - Biochemical Effect (142)
BMS - Biomass (16)
BSA - Byssal Attachment (5)
CEL - Cellular Effect (44)
CIL - Ciliary Activity (0)
CLN - Rate of Colonization (5)
CLR - Chlorophyll (78)
CYT - Cytogenetic Effect (12)
DRF - Drift (128)
DVP - Development (183)
EMP - Emergence (44)
ENZ - Enzyme Effect (316)
EQU - Equilibrium (220)
FCR - Food Consumption (23)
FLT - Filtration Rate (4)
GRO - Growth (718)
HAT - Hatchability (135)
HEM - Hematological Effect (303)
HIS - Histological Effect (91)
HPS - Hepatosomatic Index (0)
HRM - Hormone Levels Affected (4)
LET - Lethal (858)
LOC - Locomotor Behavior (124)

MOR - Mortality (2,966)
MOT - Motility (36)
NFX - Nitrogen Fixation (11)
OC - Oxygen Consumption (155)
PGR - Population Growth (1,290)
PHY - Physiological Effect (290)
POP - Population (91)
PR - Phototatic Response (0)
PRB - Predatory Behavior (11)
PRV - Predation Vulnerablity (0)
PSE - Photosynthesis Effect (261)
REP - Reproduction (200)
RES - Respiratory Rate (50)
RGN - Regeneration (23)
RSD - Residue (257)
STC - Structural Changes (16)
STR - Stress (606)
TER - Teratogenesis (12)
THL - Thermal Effect (40)
TMR - Tumor Occurrence (5)
VTE - Vertebral Effect (34)
YAB - Yolk Absorption (0)

|Option?| **EFE/LC50 <cr>**

|File: 1 Count: 18,541|

EFFECT ENDPOINT VALUE FIELD (EFC)

This field is **not searchable** at the present time. It is set up, for display only. This information will print out in AQUIRE records, but the records cannot be retrieved by an EFC field search.

An example of data in this field follows:

(EFC) Effect Endpoint Value: 119 mg/l (calc)

CONFIDENCE LIMITS FIELD (CNF)

This field is **not a searchable field.** An example of data in this field follows:

(CNF) Confidence Limits: 91-150 mg/l (calc)

OTHER ENDPOINT DATA (OED) FIELD

This field is not searchable. It is **for display only.**

Examples of data in this field are:

(OED) Other Endpoint Data:	METABOLISM STUDY ALSO DONE.
" " :	LETHARGY OBSERVED 6-10 H PRIOR TO DEATH.
(OED) Other Endpoint Data:	ALGISTATIC AT 2000 AND 5000 UG/L, ALGICIDAL AT > OR EQUAL TO 10000 UG/L.

SEARCHING MEASURED/UNMEASURED (MEA)

This field indicates whether the concentration of the test chemical was measured or unmeasured. This field contains one of the following controlled terms:

Measured (8,702)
Unmeasured (27,835)

|Option?| **MEA/MEASURED <cr>**

|File: 1 Count: 8,702|

SEARCHING REMARKS (REM) FIELD

This is a searchable field, but it is not particulary well set up for searching. The field can contain remarks or comments that the data extractors did not feel belonged in any other AQUIRE field.

Often there will be additional information from another field in the remarks field. This will be indicated in the other field by an asterisk * after the data in that field.

If you wanted to know how many times the term ACT INGRD appeared in the remarks field, you would search as follows:

|Option?| **REM/ACTΔINGRD <cr>**

|File: 1 Count: 484|

Some of the standard codes used in the remarks field follow: (Searching should be done using these codes or any other code found in any AQUIRE remarks field.)

AI	active ingredient
actvy	activity
agric	agricultural
ant	anterior
appl	apply (applied)
applic	application
avg	average
chem	chemical
chg	change
cmpd	compound
co	county
conc	concentration
cont	continue(d)
cult	culture
dec	decrease
descr	described
diam	diameter
dif	difference (different)
dist	distilled
dvp	development
elim	elimination
encl	enclosure
equilib	equilibrium
equiv	equivalent
est	estimate(d)
exp	exposure
expo	exponential
expt	experiment
flt	filter (filtering, filtered)
ft	feet
>	greater than
inc	increase
incub	incubate (incubation)
inhib	inhibit
init	initial
inst	institute
int	interval
<	less than
mad	minimum active dose
mal	malformation
max	maximum
meas	measure(d)
med	medium
mem	membrame
min	minimum
minutes are abbreviated as a	fraction of the hour
mo	month
mod	modified
mort	mortality
mts	mountains

NEF	no effect
N	north
no.	number
NS	not significant
PR	pair
pop	population
post	posterior
precip	precipitate
pu	pupation
r	river
ref	reference
res	research
rptd	reported
sedmt	sediment
sig	significant
solns	solutions
solv	solvent
spec	species
std	standard
syn	synthesis
TDS	total dissolved solids, total solids, dissolved solids
trtmt	treatment
wk	week
wt	weight
yr	year

SEARCHING BY REFERENCE NUMBER (RNO)

To obtain all records from a particular reference, search on a reference number (which you will see on AQUIRE records as you begin using the data base).

|Option?| **RNO/210406 <cr>**

The RNO is also used to obtain the reference from the OTS Library.

SEARCHING BY ACCESSION NUMBER (ACC)

Each AQUIRE record has a unique accession number. This number can be used to retrieve a particular AQUIRE record as follows:

|Option?| **ACC/200006 <cr>**

|File: 1 Count: 1,|

SEARCHING BY AUTHOR (AUT)

Examples are as follows:

|Option?| **AUT/SHEHATA <cr>**

|Option?| **AUT/SHEHATA, S.A. <cr>**

|Option?| **AUT/SHEH: <cr>**

See Truncation

|Option?| **AUT/SHEHATA△AND△NAWAR <cr>**

SEARCHING BY YEAR (YRP)

Examples of the year of publication search:

|Option?| **YRP/1979 <cr>**

|Option?| **YRP/79 <cr>**

|Option?| **YRP/79△TO△80 <cr>**

SEARCHING BY TITLE (TLE) AND JOURNAL/SOURCE (JRN)

Any word or phrase that appears in any AQUIRE record as part of a title or journal/source can be searched:

|Option?| **TLE/MERCURY△AND△FISH <cr>**

One of the titles retrieved from the above search would be:

(TLE) Title: Toxicity of Mercury: A Comparative Study
in Air-Breathing and Non-Air-Breathing Fish

|Option?| **JRN/HYDROBIOLOGIA <cr>**

|File: 1 Count: 443|

CITATION (CIT), NUMBER OF DATA LINES (RDL), DATA COLLECTION IDENTIFIER (DID) AND ADD DATE (ADT) FIELDS

These fields are searchable, but it is highly unlikely that you will want to search on them in AQUIRE. Citation (CIT) is searchable by any part of the data seen in a record; Data Collection Identifier (DID) is always AQUIRE; and ADD DATE (when the record was added to the data base) will probably become more necessary in the future.

EXISTENCE SEARCHING

To create a file with all records that have a particular field in them, do the following:

|Option?| **EXIST/CNF <cr>**

|File: 1 Count: 19,524|

This tells you that 19,524 records in the data base have confidence limits. At the same time, it creates that file of records with confidence limits. You can then choose to search against only that file if you wish.

USE OF SORT COMMAND

The sort command is used to sort a temporary results file on a particular field. Sorting is done either alphabetically or numerically, in descending order, depending on the type of data in a field.
The sort command creates a new temporary results file called sort. Sorting should be done on a small temporary results file (<200 records) because it takes quite a bit of time. Suppose we have a file of 52 records created by the commands EFE/BCF and YRP/81, - File 1.

|Option?| **SORTΔ1/CAS <cr>**

Will sort that file by CAS numbers in descending order.

USE OF STORE COMMAND

The store command is used to save a temporary results file permanently.

In order to STORE a file do the following:

|Option?| **STOREΔ1** (file number) **<cr>**

|File name and extension (default = Z4401.DAT)| **MILES.001 <cr>**

Please name all files and use your last name followed by a period and whatever you like. Do NOT store two files with the same name. The first will be overwritten.

USE OF STORED FILE

When you want to retrieve a stored file, type:

|Option?| **USE Δ MILES.001 <cr>**

```
File MILES.001 containing 30 entries
copied to local file 1
```

USE OF DELETE COMMAND

Please delete all unnecessary files that you have created in the past as follows:

|Option?| **DELETE Δ MILES.PAU <cr>**

|File MILES.001 deleted|

Please keep track of your stored files and delete those not in use.

USE OF EXTRACT COMMAND

This command is for TABLE GENERATION.

Your first step is to create a file. It is recommended that the extract command be done on a short file.

|Option?| **PRP/BCP Δ and Δ YRP/81 <cr>**

will create a file with 52 entries. At the Option? you can then set up the fields that you want in your table as follows:

|Option?| **EXTRACT Δ CAS Δ NAM Δ EFC Δ REL Δ FROM Δ 1 Δ TO Δ MILES.002 <cr>**

Use the first five (5) letters of your name, followed by a period and then three (3) unique letters or numbers for each file that you create.

The next step is to go to the SOS component of CIS, the only place an EXTRACT table can be printed out.

|Option?| **GO Δ SOS <cr>**

The system will then give you a FILE: prompt.
Type in the file that you generated.

|FILE:| **MILES.002 <cr>**

|*| **pef,s**

(print entire file without line numbers) You will get the following table:

7439976	Mercury:	<0.00015 {Calc}	2
143500	Kenone:	10606	2
2385855	Mirex:	12274	2
143500	Kenone:	760	1
2385855	Mirex:	8025	1
3383968	Ahate:	2.3 {Calc}	1
3383968	Ahate:	0.93 {Calc}	1
3383968	Ahate:	0.53 {Calc}	1
3383968	Ahate:	5.5 {Calc}	1
3383968	Ahate:	0.9 {Calc}	1
3383968	Ahate:	0.58 Calc}	1
3383968	Ahate:	5.0 {Calc}	1
3383968	Ahate:	0.61 {Calc}	1
115866	Triphenyl phosphate:	360 {Calc}	2
115866	Triphenyl phosphate:	280 {Calc}	2
115866	Triphenyl phosphate:	300 {Calc}	2
115866	Triphenyl phosphate:	200 {Calc}	2
115866	Triphenyl phosphate:	130 {Calc}	2
115866	Triphenyl phosphate:	340 {Calc}	2
115866	Triphenyl phosphate:	270 {Calc}	2
34364436	CUMYLPHENYL DIPHENYL	2500 {Calc}	2
34364436	CUMYLPHENYL DIPHENYL	3200 {Calc}	2
34364436	CUMYLPHENYL DIPHENYL	2800 {Calc}	2
34364436	CUMYLPHENYL DIPHENYL	4500 {Calc}	2
34364436	CUMYLPHENYL DIPHENYL	3000 {Calc}	2
34364436	CUMYLPHENYL DIPHENYL	2400 {Calc}	2
34364436	CUMYLPHENYL DIPHENYL	1300 {Calc}	2
91203	Naphthalene:	35	2
91203	Naphthalene:	52	2
91203	Naphthalene:	24	2
91203	Naphthalene:	62	2
91203	Naphthalene:	58	2
91203	Naphthalene:	59	2
91203	Naphthalene:	31	2
91203	Naphthalene:	36	2
91203	Naphthalene:	42	2
61949777	TRANS PERMETHRIN:	30	2
ETC.			

At the end of the table, type a carriage return and another asterisk (*) will appear. Type ed (which stands for exit from SOS and delete EXTRACT file). You will then be returned to the OPTION? prompt. If you wish to do additional searching you must return to AQUIRE or some other CIS component.