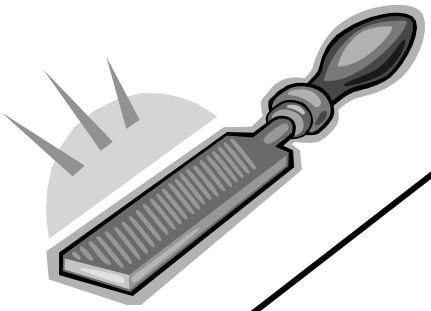
Getting Started Using AquaChem

AquaChem

Basics

Files



Windows

Types of Files

- Essential AquaChem Files:
  - The Database File (.HC3)
  - The Mask File (.MSK)
  - The Database Configuration File (.CFG)
- Files created and used by AquaChem:
  - Spreadsheet Report File (.RPT)
  - Graph Configuration File (.GRF)
  - Print Template File (TEMPLATE.TXT)

Database File - *filename* (.HC3)

Composed of individual records

Table

DBIN	SampleID	Site	Date	pH	Cond	TDS	Na	K	Mg	Ca	Mn	Fe	F	Cl	SO4	HCO3	CO
1	MC-1	Midcontinent	9/10/1993	8.25	185	110	28.9	0	1.9	8.7	0	0			15	86	0
2	MC-2	Midcontinent	9/10/1993	8.26	5700	4960	1600	13.7	29.3	35.8	0	0		90	2200	1390	0
3	MC-3	Midcontinent	9/10/1993	8.64	5600	4890	1610	13.8	30.2	100	0	0		92	2250	1240	10
4	MC-4	Midcontinent	9/10/1993	8.29	1100	775	204	2.4	15.9	41.8	0	0		14	320	274	0
5	MC-5	Midcontinent	9/9/1993	8.51	2100	1630	494	4.5	14.4	26.2	0	0		29	770	470	0
6	MC-6	Midcontinent	9/10/1993	7.22	1250	845	95.3	3.1	48.5	147	.2	0		49	180	580	0

Every record composed of header info. (Location, Date, etc.) and user defined parameters

Database File - *filename* (.HC3)

Database can contain unlimited samples

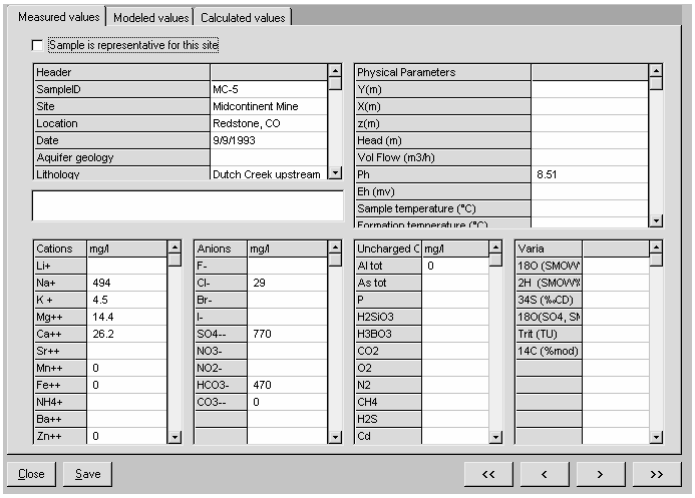
Data can be hand entered or imported from a tab-delimited ASCII text file

Maskfile – *filename*.MSK

Database structure defined in maskfile

Maskfile – *filename*.MSK

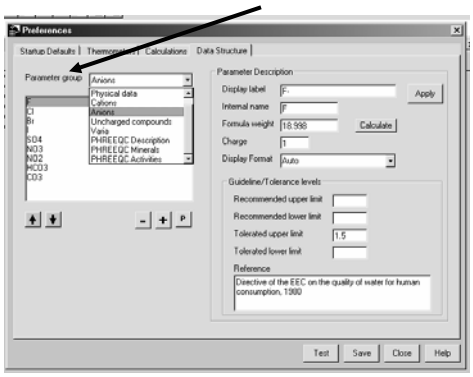
List of all parameters in the database



Maskfile – *filename*.MSK

AquaChem parameters are grouped

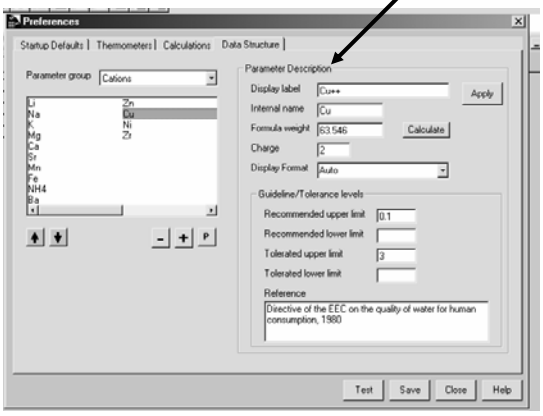
HEADER(site, date); PHYSICAL DATA (pH, temp.)
CATIONS (Na, Mg, K); ANIONS (Cl, SO_4
UNCHARGED COMPOUNDS (Al, SiO_2); VARIA(bacteria, isotopes)
PHREEQC DESCRIPTION, MINERALS and ACTIVITES



Maskfile – *filename*.MSK

Each parameter has related descriptive values

Display label; Internal name; Formula weight; Recommended upper and lower limits; and Tolerated upper and lower limits



Database Configuration File *filename*.CFG

- Contains start-up conditions and coefficients for most calculations
- Calculations are performed in the AquaChem code in a specific order, for example:
  - Default map file
  - Number of Columns in record list
  - Calculations related to PHREEQC

Spreadsheet File (.RPT)

- Contains indexed references to the database parameters
- Default file (DEFAULT.RPT) is set to display every parameter in the database
- Can be customized and saved

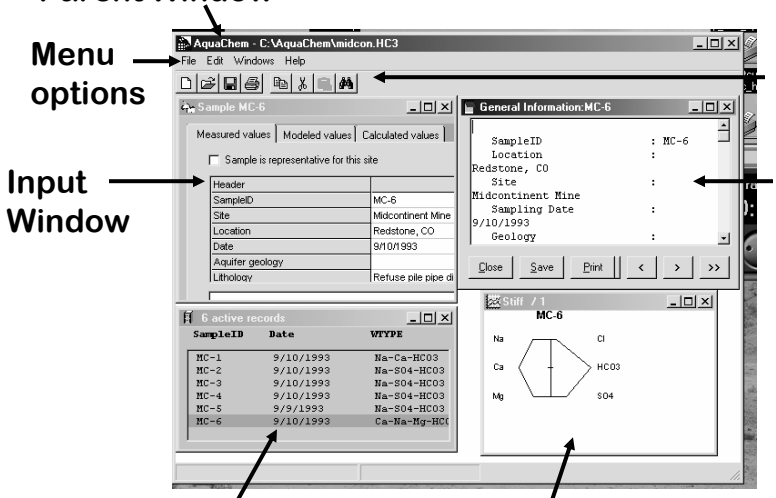
Graph Configuration File .GRF

- Contain the entire configuration of graphs
- Created by choosing **File\Save Configuration** from from the **Graphics Menu**
- Only graph configuration is saved not actual graphics file
- Every change to the data or to a record will be updated next time file is loaded

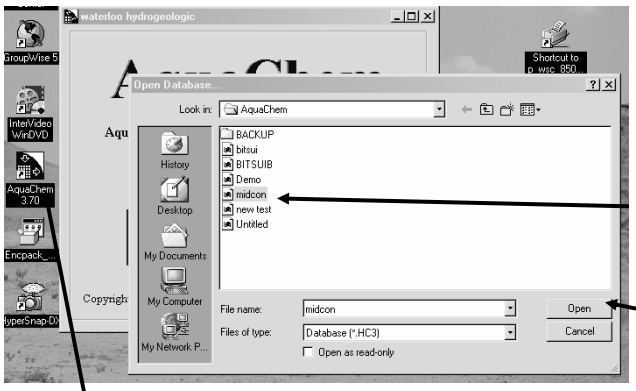
Print Template File (TEMPLATE.TXT)

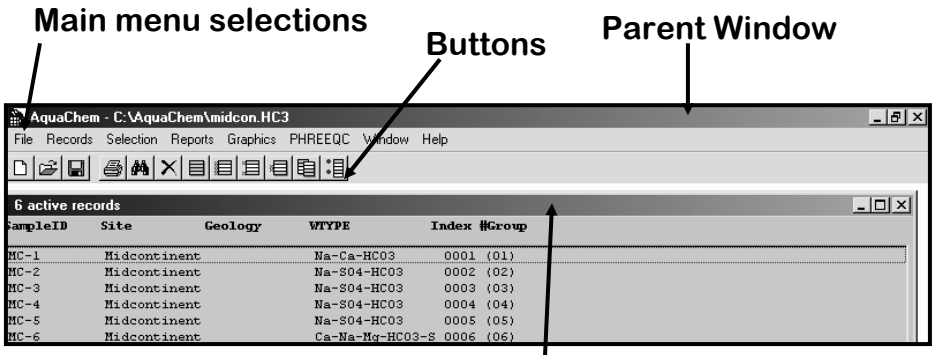
- An ASCII formatted text file containing the settings for various print templates available
- File can be customized using the graphical tools provided in the Print Options or you can edit the TEMPLATE.TXT file (not recommended)

Interface Layout



Let's Get Started !



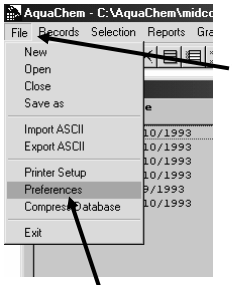


Record List Window will always appear when you open AquaChem and will remain open as long as project database is open.

Record List Window contains summarized information about every record in the database.

Record List Window can be modified

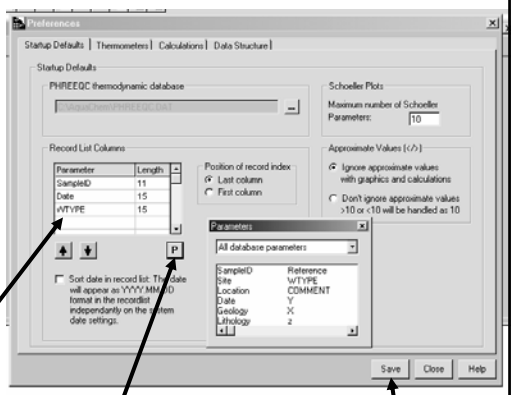
Modify Record List Window



1. Click File

2. Click Preferences

Make sure entire window is visible



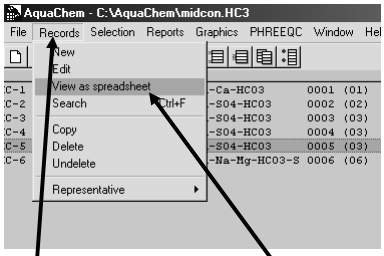
3. Click "P" parameter button

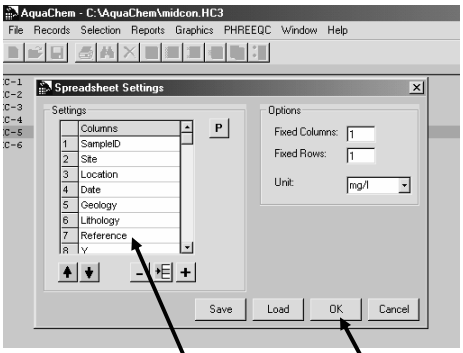
4. Make changes – drag & drop into "Record List Columns"

5. Click Save

View as Spreadsheet

Displays active samples in a spreadsheet format





1. Click Records

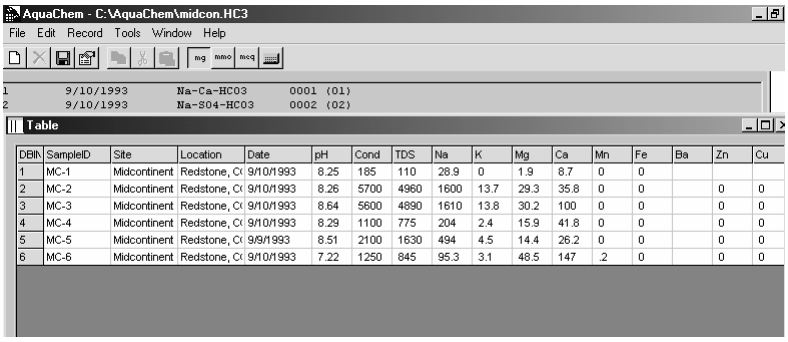
2. Click View as spreadsheet

3. Change "Settings" as needed

4. Click OK

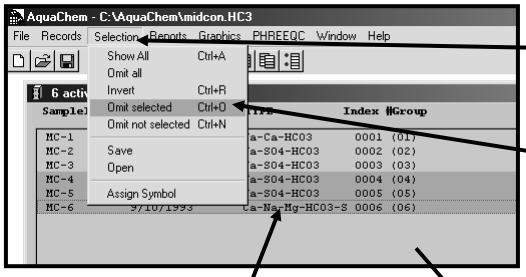
<u>Note</u>: The spreadsheet settings can be saved in a report file. Click "Save" and name file. Click "Load" to load saved view when needed.

Spreadsheet View



DBIN	SampleID	Site	Location	Date	pH	Cond	TDS	Na	K	Mg	Ca	Mn	Fe	Ba	Zn	Cu
1	MC-1	Midcontinent	Redstone, C	9/10/1993	8.25	185	110	28.9	0	1.9	8.7	0	0			
2	MC-2	Midcontinent	Redstone, C	9/10/1993	8.26	5700	4960	1600	13.7	29.3	35.8	0	0		0	0
3	MC-3	Midcontinent	Redstone, C	9/10/1993	8.64	5600	4890	1610	13.8	30.2	100	0	0		0	0
4	MC-4	Midcontinent	Redstone, C	9/10/1993	8.29	1100	775	204	2.4	15.9	41.8	0	0		0	0
5	MC-5	Midcontinent	Redstone, C	9/9/1993	8.51	2100	1630	494	4.5	14.4	26.2	0	0		0	0
6	MC-6	Midcontinent	Redstone, C	9/10/1993	7.22	1250	845	95.3	3.1	48.5	147	.2	0		0	0

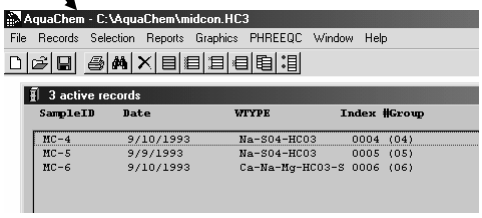
Show Subset of Database



2. Click Selection on menu

3. Click Omit Selected on pull down

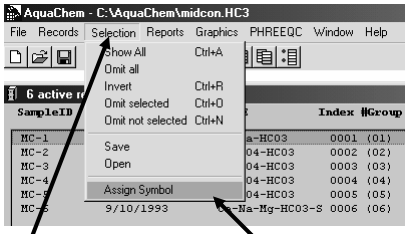
1. Hold Ctrl key and select samples to omit with arrow key

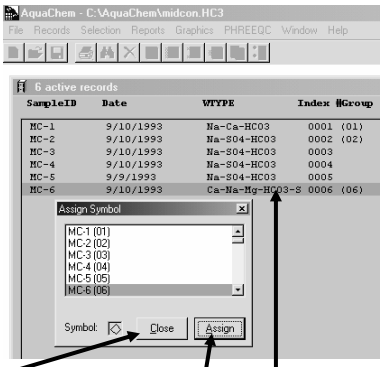


4. Subset

Assign Symbols

Assigns symbol shape to samples for graphing





1. Click Selection

2. Click Assign Symbol or right click on sample record

3. Click Assign for each sample or sample set

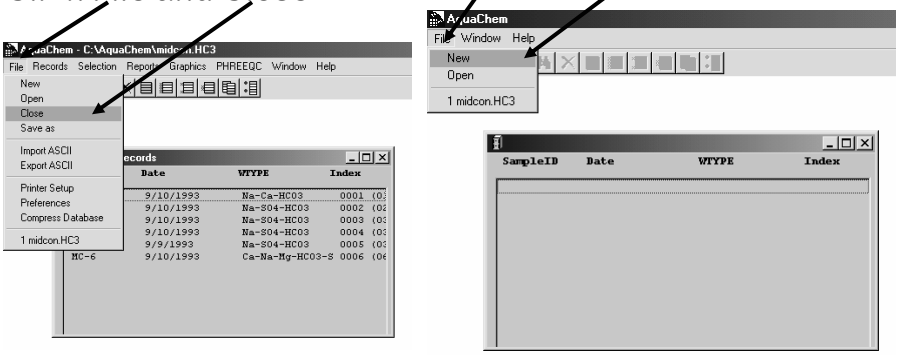
4. Click Close

Creating a New Database

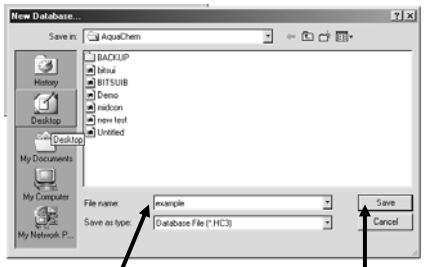
Close Current Database

Click File and Close

Click File and New from main menu



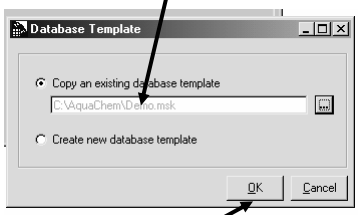
Creating a New Database



Name File

Click Save

Use Demo.msk for database template



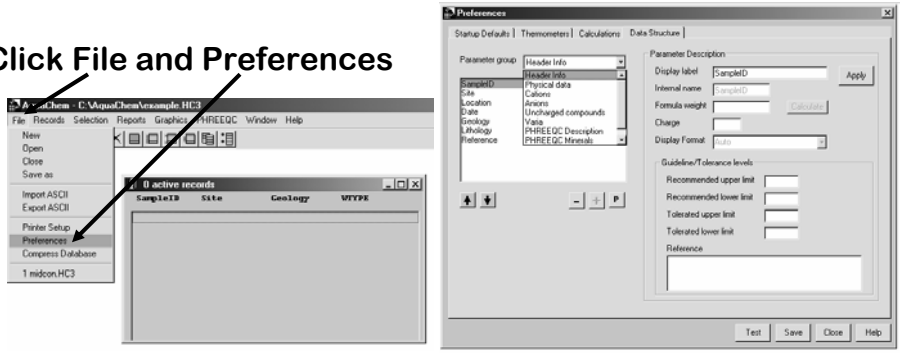
Click OK

Note: It is recommended to use the existing database template provided in demo.msk when first starting to use AquaChem.

Creating a New Database

Can add new parameters to your database by editing the existing mask file

Click File and Preferences



Changes can be made under "Data Structure" tab using pull down "Parameter Group"

Creating a New Database

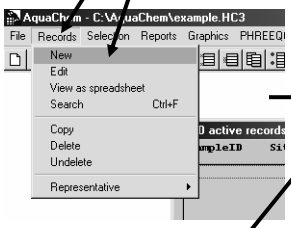
Click Test anytime to check any changes made

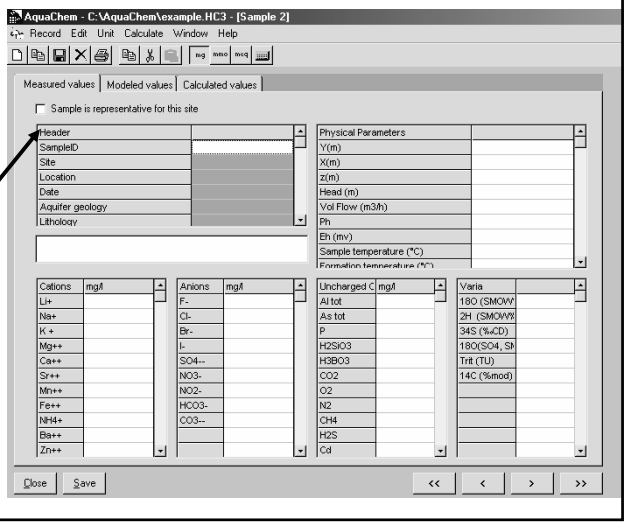
Click Save to save changes

Adding Data to Database

Using "Input" Window

Click Records and New

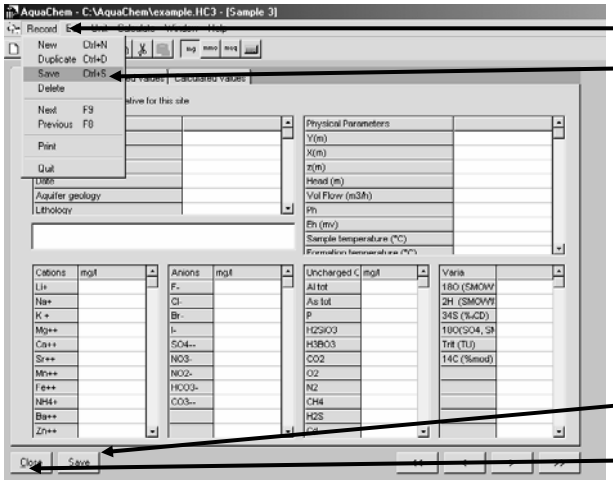




Click "Header" box and enter information

Use <enter> to advance cells

Adding Data to Database



Click Record and Save to save the sample data

Click Record and New to add next record

Click Save and Close when done entering data

<u>Note</u>: Watch units mg and meq. Use "." for all numeric data

Class Exercise

Make an AquaChem database file using class exercise table