

Database Reports

```

SampleID          BITSUI-1
Date              3/26/1998
Ph                8.8
Cond 20°C (µS)   19600
TDS (110 °C, mg/l) 14600

Cations           (mg/l)          (meq/l)
Na+              4.360E+03          1.896E+02
K +              2.100E+01          5.371E-01
Mg++            2.800E+01          2.304E+00
Ca++            5.200E+01          2.595E+00
Mn++            3.910E-01          1.423E-02
Fe++            3.500E-01          1.254E-02
Ba++            4.000E-02          5.825E-04

Anions           (mg/l)          (meq/l)
F-              2.740E+00          1.442E-01
Cl-             1.750E+03          4.936E+01
SO4--          6.200E+03          1.291E+02
HCO3-          9.500E+02          1.557E+01
CO3--          8.600E+01          2.866E+00

Uncharged       (mg/l)
Al tot         .34
H3BO3         12.1
    
```

Reports

Reports in AquaChem are all generated in a separate **Report** window in unformatted ASCII text. These reports can be printed “as is” using the **[Print]** button on the lower left hand corner of the windows or the information can be cut “cut-and-pasted” into a formatted report document

Database Report Types

- Header lists
- Data reports
- Detailed data report
- Tabulation of parameters compared to drinking water standards
- Comparison of database to single parameter
- Statistics for selected parameters
- Other - Periodic Table and Minerals Table

Header List

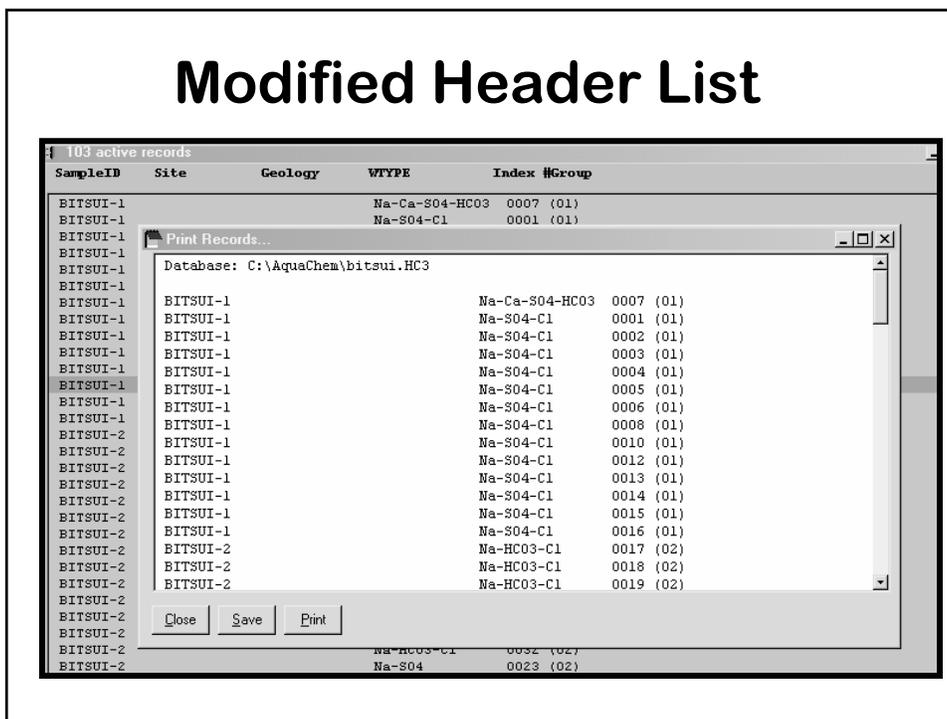
Gives printout of the headers for each record

The screenshot shows the AquaChem software interface. The 'Reports' menu is open, and 'List of headers' is selected. The main window displays a table with the following columns: 'SampleID', 'Site', 'PE', 'Index', and 'HGroup'. The table lists various parameters for samples from sites BITSUI-1 and BITSUI-2.

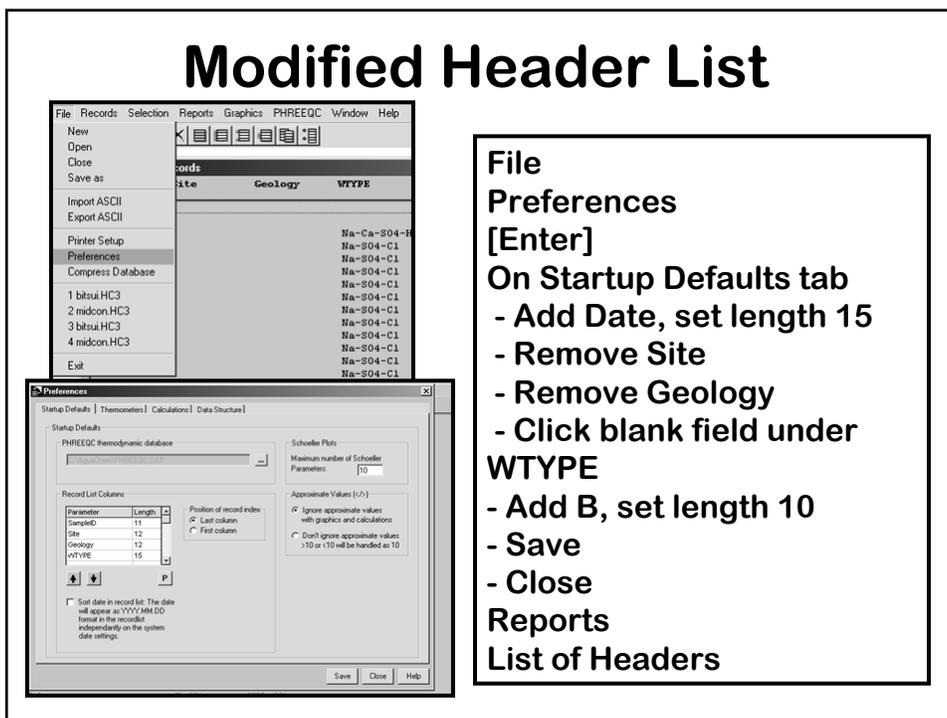
SampleID	Site	PE	Index	HGroup
BITSUI-1			0009	(01)
BITSUI-1			0011	(01)
BITSUI-1		-Ca-S04-HC03	0007	(01)
BITSUI-1		-S04-C1	0001	(01)
BITSUI-1		-S04-C1	0002	(01)
BITSUI-1		-S04-C1	0003	(01)
BITSUI-1		-S04-C1	0004	(01)
BITSUI-1		-S04-C1	0005	(01)
BITSUI-1		-S04-C1	0006	(01)
BITSUI-1		-S04-C1	0008	(01)
BITSUI-1		-S04-C1	0010	(01)
BITSUI-1		Na-S04-C1	0012	(01)
BITSUI-1		Na-S04-C1	0013	(01)
BITSUI-1		Na-S04-C1	0014	(01)
BITSUI-1		Na-S04-C1	0015	(01)
BITSUI-1		Na-S04-C1	0016	(01)
BITSUI-2			0029	(02)
BITSUI-2		Na-HC03-C1	0017	(02)
BITSUI-2		Na-HC03-C1	0018	(02)
BITSUI-2		Na-HC03-C1	0019	(02)
BITSUI-2		Na-HC03-C1	0020	(02)
BITSUI-2		Na-HC03-C1	0021	(02)
BITSUI-2		Na-HC03-C1	0022	(02)
BITSUI-2		Na-HC03-C1	0024	(02)
BITSUI-2		Na-HC03-C1	0025	(02)
BITSUI-2		Na-HC03-C1	0026	(02)
BITSUI-2		Na-HC03-C1	0027	(02)
BITSUI-2		Na-HC03-C1	0028	(02)
BITSUI-2		Na-HC03-C1	0030	(02)
BITSUI-2		Na-HC03-C1	0031	(02)

- Reports
- List of Headers
- [Enter]

Modified Header List



Modified Header List



Modified Header List

103 active records

SampleID	WTYPE	Date	B	Index	#Group
BITSUI-1	Na-Ca-S04-HCO3	6/21/1996		0007	(01)
BITSUI-1				0005	(01)
BITSUI-1				0013	(01)
BITSUI-1				0012	(01)
BITSUI-1				0004	(01)
BITSUI-1				0001	(01)
BITSUI-1				0010	(01)
BITSUI-1				0014	(01)
BITSUI-2				0002	(01)
BITSUI-2				0006	(01)
BITSUI-2				0003	(01)
BITSUI-2				0016	(01)
BITSUI-2				0015	(01)
BITSUI-2				0008	(01)
BITSUI-2				0025	(02)
BITSUI-2				0021	(02)
BITSUI-2					
Na-HCO3-C1		7/11/2000	1	0032	(02)
Na-HCO3-C1		9/27/1996	1.05	0024	(02)

Print Records... Database: C:\AQUACHEM\BITSUIB.HC3

Close Save Print

Data Report

Gives listing of all data for each database record

File Records Selection Reports Graphics PHREEQC Window Help

Compare
Correlation Matrix
Geothermometers
Mix Samples
Statistics
General
Isotopes
Drinking Water Regulations
List of headers
Data
Periodic Table
Minerals

SampleID	Site	WTYPE	Index	#Group
BITSUI-1			0009	(01)
BITSUI-1			0011	(01)
BITSUI-1		Ca-S04-HCO3	0007	(01)
BITSUI-1		S04-C1	0001	(01)
BITSUI-1		S04-C1	0002	(01)
BITSUI-1		S04-C1	0003	(01)
BITSUI-1		S04-C1	0004	(01)
BITSUI-1		S04-C1	0005	(01)
BITSUI-1		S04-C1	0006	(01)
BITSUI-1		S04-C1	0008	(01)
BITSUI-1		S04-C1	0010	(01)
BITSUI-1		Na-S04-C1	0012	(01)
BITSUI-1		Na-S04-C1	0013	(01)
BITSUI-1		Na-S04-C1	0014	(01)
BITSUI-1		Na-S04-C1	0015	(01)
BITSUI-1		Na-S04-C1	0016	(01)
BITSUI-2			0029	(02)

- Reports
- Data
- [Enter]

Data Report

109 Print Records...

SampleID	BITSUI-1	
Date	9/27/1996	
Ph	8.9	
Cond 20°C (µS)	19300	
TDS (110 °C, mg/l)	15300	
Cations (mg/l) (meq/l)		
Na+	5.180E+03	2.253E+02
K +	1.840E+01	4.706E-01
Mg++	3.150E+01	2.592E+00
Ca++	5.110E+01	2.550E+00
Mn++	1.200E-01	4.368E-03
Fe++	2.500E-01	8.954E-03
Ba++	3.000E-02	4.369E-04
Anions (mg/l) (meq/l)		
F-	2.620E+00	1.379E-01
Cl-	2.310E+03	6.516E+01
S04--	7.460E+03	1.553E+02
HCO3-	1.100E+03	1.803E+01
CO3--	1.200E+02	3.999E+00
Uncharged (mg/l)		
Al tot	.29	
H3B03	6.75	

Close Save Print

Detailed Record Report

Includes data and the calculated parameters

File Records Selection Reports Graphics PHREEQC Window Help

109 active records

SampleID	Site	PE	Index #Group
BITSUI-1			0009 (01)
BITSUI-1			0011 (01)
BITSUI-1		Ca-S04-HCO3	0007 (01)
BITSUI-1		S04-Cl	0001 (01)
BITSUI-1		S04-Cl	0002 (01)
BITSUI-1		S04-Cl	0003 (01)
BITSUI-1		S04-Cl	0004 (01)
BITSUI-1		S04-Cl	0005 (01)
BITSUI-1		S04-Cl	0006 (01)
BITSUI-1		S04-Cl	0008 (01)
BITSUI-1		S04-Cl	0010 (01)
BITSUI-1		Na-S04-Cl	0012 (01)
BITSUI-1		Na-S04-Cl	0013 (01)
BITSUI-1		Na-S04-Cl	0014 (01)
BITSUI-1		Na-S04-Cl	0015 (01)
BITSUI-1		Na-S04-Cl	0016 (01)
BITSUI-2			0029 (02)
BITSUI-2		Na-HCO3-Cl	0017 (02)
BITSUI-2		Na-HCO3-Cl	0018 (02)

- Reports
- General
- [Enter]

Detailed Data Report

SampleID	: BITSUI-1			
Location	:			
Site	:			
Sampling Date	: 9/27/1996			
Geology	:			
Watertype	: Na-S04-Cl			
Sum of Anions (meq/l)	: 242.6506			
Sum of Cations (meq/l)	: 230.9411			
Balance:	: -2.47%			
Measured TDS(mg/l)	: 15300.0			
Calculated TDS(mg/l)	: 10557.5			
Hardness	: meq/l	*f	*g	mg/l CaCO3
Total hardness	: 5.14	25.71	14.40	257.1
Permanent hardness	: 0.0	0.00	0.00	0.0
Temporary hardness	: 5.14	25.71	14.40	257.1
Alkalinity	: 22.03	110.15	61.68	1101.5
(1 *f = 10 mg/l CaCO3/l 1 *g = 10 mg/l CaO)				
Major ion composition				
	mg/l	mmol/l	meq/l	meq%
-----	-----	-----	-----	-----
Na+	5180.0	225.315	225.315	47.576
K +	18.4	0.471	0.471	0.099
Ca++	51.1	1.275	2.55	0.538
Mg++	31.5	1.296	2.592	0.547
Cl-	2310.0	65.157	65.157	13.758
S04--	7460.0	77.663	155.326	32.797
HCO3-	1100.0	18.03	18.03	3.807

Drinking Water Regulations

Tabulation Relative to Water Quality Standards

SampleID	Site	Index #Group
BITSUI-1		0009 (01)
BITSUI-1		0011 (01)
BITSUI-1		0007 (01)
BITSUI-1		0001 (01)
BITSUI-1		0002 (01)
BITSUI-1		0003 (01)

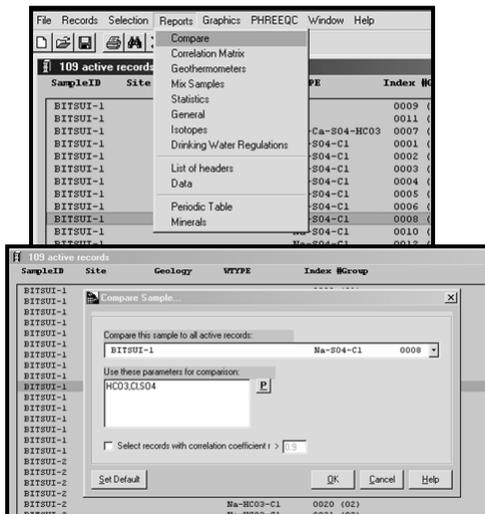
Element	Measured	Recommended	Maximum
pH	8.9	6.5- 8.5	< 9.5
Cond	19300	< 400	< 1250
TDS	15300	< 400	< 1500
Na	5180	< 20	< 200
K	18.4	< 10	< 12
Mg	31.5	< 30	< 30
Mn	0.12	< .02	< .05
Fe	0.25	< .05	< .2
F	2.62	< 1.5	< 1.5
Cl	2310	< 25	< 250
S04	7460	< 25	< 250
Al	0.29	< .05	< .2

Irrigation water:
 Conductivity = 19300 uS (group C4: Very high salinity water)
 Sodium Adsorption Ratio (SAR) : 140.53
 Exchangeable sodium ratio (ESR) : 43.82
 Magnesium hazard (MH) : 50.40

- Reports
- Drinking Water Regulations
- [Enter]
- [>] Advance one record
- [>>] Go to end of list
- [<] Go back one record
- [<<] Go to start of list

Comparison

Compare the complete database with a single record



- Reports
- Compare
- [Enter]
- Pick a sample from dropdown list
- Pick at least three parameters to use for the correlation
- [OK]

Comparison

The screenshot shows a 'Compare sample 8 to active records' dialog box. It displays a table with the following columns: Location, Index, Corr Coeff, Euclidean distance, and Points used for correlation. The data is as follows:

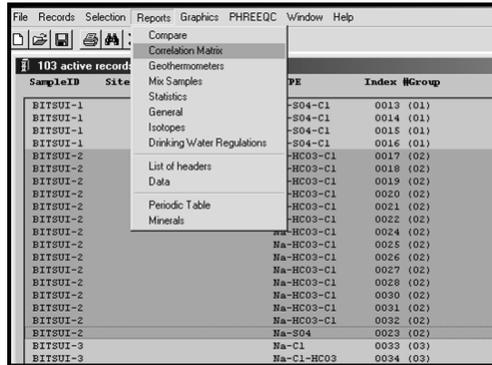
Location	Index	Corr Coeff	Euclidean distance	Points used for correlation
8		1.0	0.0	3
65		1.0	1961.53	2
13		1.0	673.975	3
5		1.0	364.677	3
12		1.0	322.255	3
6		1.0	607.442	3
2		1.0	475.955	3
4		1.0	412.23	3
15		0.999	417.103	3
14		0.999	800.77	3
3		0.999	254.034	3
16		0.999	410.406	3
1		0.999	466.798	3
10		0.998	188.726	3
78		0.975	1159.907	3
56		0.97	1050.349	3
23		0.967	4110.952	3
59		0.966	2512.409	3
80		0.966	2422.946	3
74		0.962	1353.604	3
75		0.96	1748.1	3
76		0.96	1798.592	3
77		0.959	1297.498	3

Correlation coefficient = linear regression of all concentrations of each sample with the designated sample.

Euclidean distance = normalized sum of the differences in absolute concentrations.

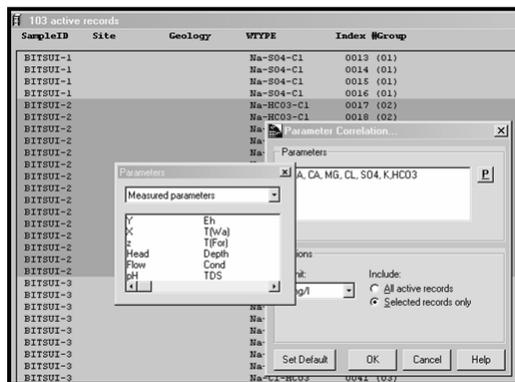
Correlation Matrix

Determines whether groups of samples have parameters that are correlated with one another



- Select all records for Bitsui -2
- Reports
- Correlation matrix

Correlation Matrix



- Choose parameters: NA, CA, MG, SO4, K, HCO3
- Include: Selected records only
- [OK]

Correlation Matrix

Concentrations in mg/l

Correlation coefficient:

	NA	CA	MG	CL	S04	K	HCO3
NA	1.0	-0.94	-0.936	0.968	-0.834	0.252	0.923
CA		1.0	0.997	-0.97	0.905	-0.189	-0.931
MG			1.0	-0.971	0.902	-0.117	-0.922
CL				1.0	-0.88	0.174	0.93
S04					1.0	-4.6E-2	-0.935
K						1.0	7.8E-2
HCO3							1.0

y axis intersection:

	NA	CA	MG	CL	S04	K	HCO3
NA	0.0	78.23	25.71	-54.29	803.39	2.67	-333.16
CA		0.0	0.194	1.3E+3	13.29	7.3	3.6E+3
MG			0.0	1.3E+3	7.87	7.28	3.6E+3
CL				0.0	786.13	4.2	-96.44
S04					0.0	6.97	3.6E+3
K						0.0	3.0E+3
HCO3							0.0

Slope of regression line:

	NA	CA	MG	CL	S04	K	HCO3
NA	1.0	-3.6E-2	-1.2E-2	0.615	-0.362	2.2E-3	1.81
CA		1.0	0.326	-16.12	10.28	-4.3E-2	-47.73
MG			1.0	-49.29	31.29	-0.119	-144.34
CL				1.0	-0.601	2.4E-3	2.87
S04					1.0	0.2E-3	4.8E-3
K						1.0	0.0
HCO3							1.0

- Correlation between Na and K is very low ($r = .253$)
- Correlation between Na and Cl is high ($r = .968$)
- Correlation between Na and HCO3 is high ($r = .923$)

Statistics Reports

Generates set of simple statistics

SampleID	Site	PE	Index	#Group
BITSUI-1		-S04-C1	0013	(01)
BITSUI-1		-S04-C1	0014	(01)
BITSUI-1		-S04-C1	0015	(01)
BITSUI-1		-S04-C1	0016	(01)
BITSUI-2		-HCO3-C1	0017	(02)
BITSUI-2		-HCO3-C1	0018	(02)
BITSUI-2		-HCO3-C1	0019	(02)
BITSUI-2		-HCO3-C1	0020	(02)
BITSUI-2		-HCO3-C1	0021	(02)
BITSUI-2		-HCO3-C1	0022	(02)
BITSUI-2		Na-HCO3-C1	0024	(02)
BITSUI-2		Na-HCO3-C1	0025	(02)
BITSUI-2		Na-HCO3-C1	0026	(02)
BITSUI-2		Na-HCO3-C1	0027	(02)
BITSUI-2		Na-HCO3-C1	0028	(02)
BITSUI-2		Na-HCO3-C1	0030	(02)
BITSUI-2		Na-HCO3-C1	0031	(02)

- Use same set of samples Bitsui – 2
- Reports
- Statistics

Statistics Report



- Choose parameters:
NA, CA, MG, CL, SO4,
HCO3
- Include: Selected
records only
- [OK]

Statistics Report

	Min	Max	Average	St. Dev.	Dev. Coeff	Var%	Sample No
Na	390.0	2220.0	1900.133	438.244	23.064	82.0	15
Ca	3.6	70.3	10.0	16.744	167.436	95.0	15
Mg	1.1	23.2	3.459	5.482	158.505	95.0	15
Cl	130.0	1270.0	1114.267	278.294	24.975	90.0	15
SO4	4.5	744.0	116.1	190.141	163.773	99.0	15
K	1.6	17.0	6.867	3.839	55.901	91.0	15
HCO3	182.0	3610.0	3100.8	858.238	27.678	95.0	15

Dev. Coeff. = σ (data scatter) / Average x 100 ... a normalized measure of variability in the data.

Var% (vairiability) = (Min-Max) / Average x 100 ... a normalized measure of total variability.

Periodic Table

Lists Symbol, Atomic Number and Atomic Mass for all elements

The screenshot shows the AquaChem interface. On the left, a menu is open with 'Periodic Table' selected. The main window displays a table of elements with columns for Name, Symbol, Atomic Number, and Atomic Mass. The table lists elements from Actinium to Cesium.

Name	Symbol	Atomic Number	Atomic Mass
Actinium	Ac	89	227
Aluminium	Al	13	26.98154
Americium	Am	95	243
Antimony	Sb	51	121.757
Argon	Ar	18	39.948
Arsenic	As	33	74.92159
Astatine	At	85	210
Barium	Ba	56	137.327
Berkelium	Bk	97	247
Beryllium	Be	4	9.012182
Bismuth	Bi	83	208.9804
Boron	B	5	10.811
Bromine	Br	35	79.904
Cadmium	Cd	48	112.411
Calcium	Ca	20	40.078
Californium	Cf	98	251
Carbon	C	6	12.011
Cerium	Ce	58	140.115
Cesium	Cs	55	132.9054

- Reports
- Periodic Table

Minerals

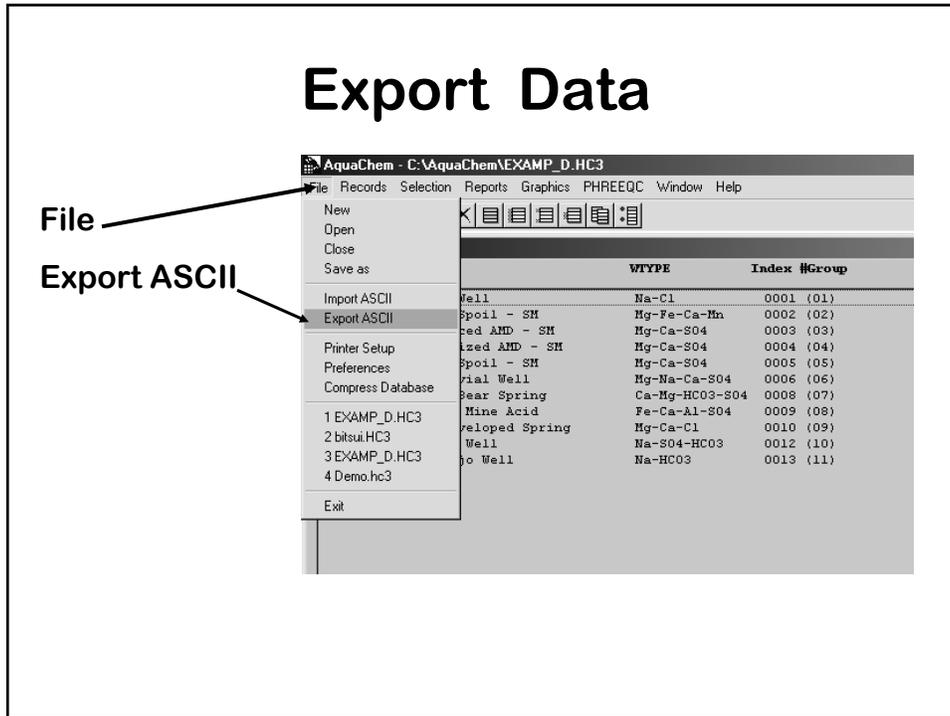
Lists Name, Formula and Formula Weight of most common minerals

The screenshot shows the AquaChem interface. On the left, a menu is open with 'Minerals' selected. The main window displays a table of minerals with columns for Name, Formula, and Formula weight. The table lists minerals such as Calcite, Aragonite, Dolomite, and Quartz.

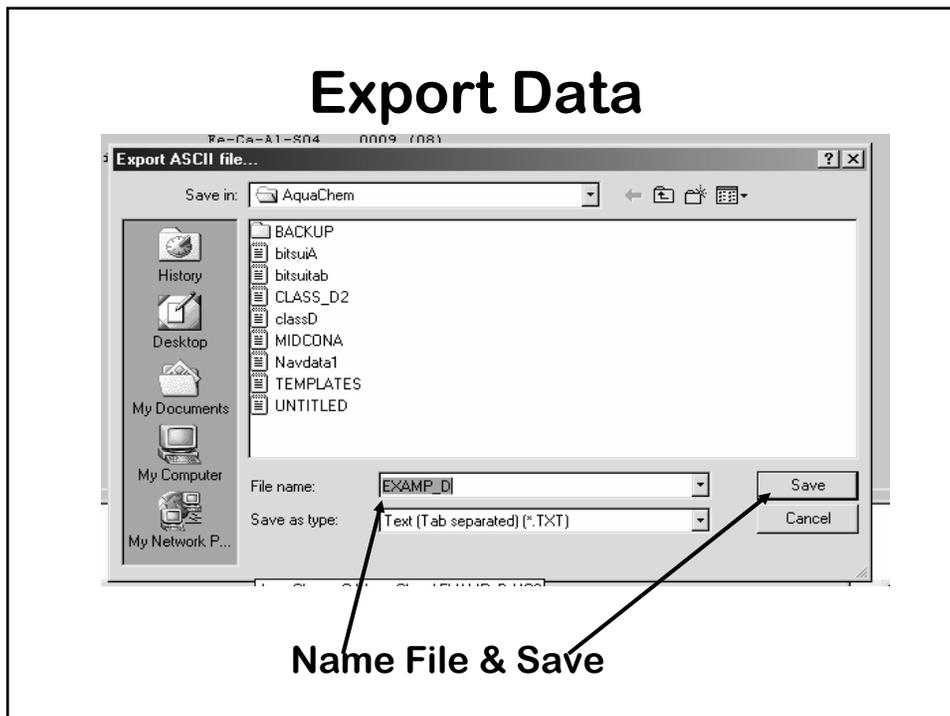
Name	Formula	Formula weight
Calcite	CaCO3	100.0872
Aragonite	CaCO3	100.0872
Dolomite	CaMg(CO3)2	184.4014
Siderite	FeCO3	115.8562
Rhodochrosite	MnCO3	114.9473
Strontianite	SrCO3	147.6292
Witherite	BaCO3	197.3362
Gypsum	CaSO4.2H2O	762.134
Anhydrite	CaSO4	136.1416
Celestine	SiSO4	183.6836
Barite	BaSO4	233.3906
Hydroxyapatite	Ca5(PO4)3OH	502.3114
Fluorite	CaF2	78.0748
SiO2(a)	SiO2	60.0843
Chalcedony	SiO2	60.0843
Quartz	SiO2	60.0843
Gibbsite	Al(OH)3	78.00356
Al(OH)3(a)	Al(OH)3	78.00356
Kaolinite	Al2Si2O5(OH)4	258.1604
Albite	NaAlSi3O8	262.223
Anorthite	CaAl2Si2O8	278.2073

- Reports
- Minerals

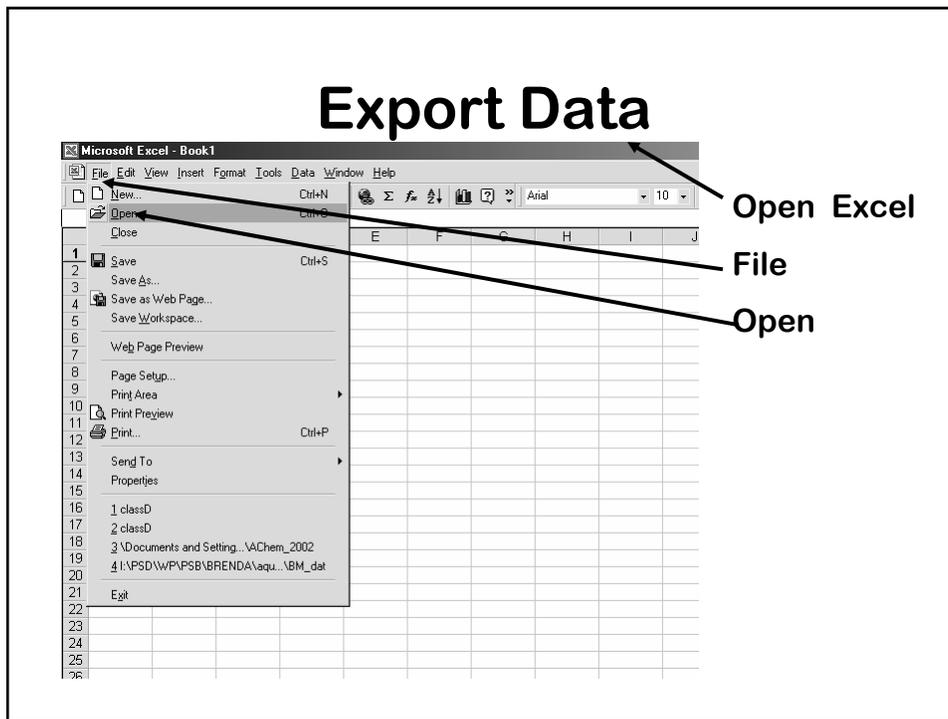
Export Data



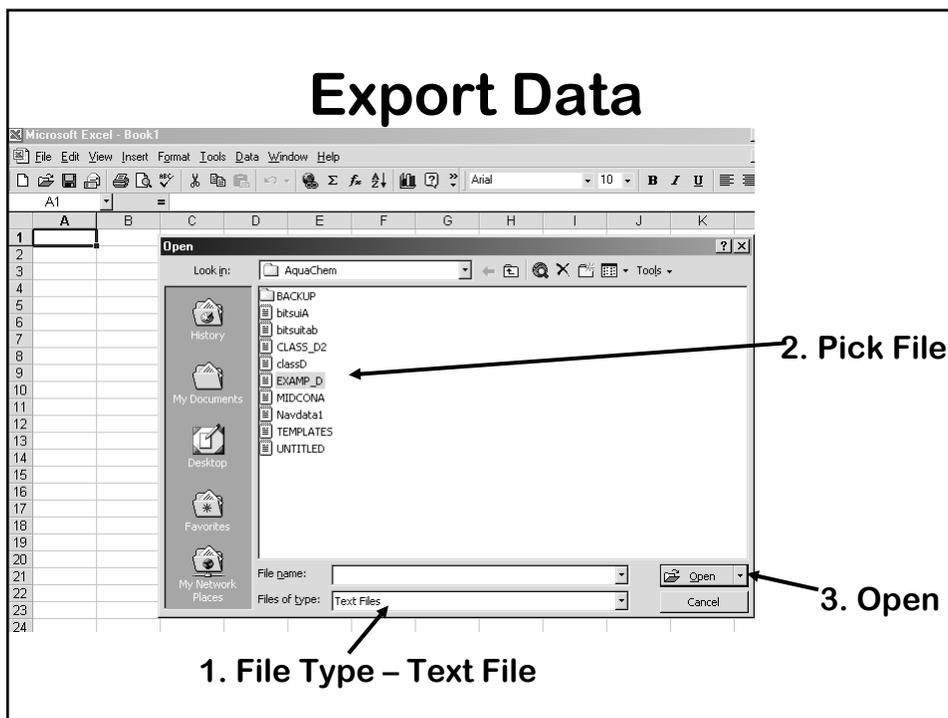
Export Data



Export Data



Export Data



Export Data

The Text Wizard has determined that your data is Delimited. If this is correct, choose Next, or choose the data type that best describes your data.

Original data type

Choose the file type that best describes your data:

- Delimited - Characters such as commas or tabs separate each field.
- Fixed width - Fields are aligned in columns with spaces between each field.

Start import at row: 1 File origin: Windows (ANSI)

Preview of file C:\AquaChem\CLASS_D.TXT.

ID	Sample ID	Site	Location	Date	Op	HD	Ehd	Cond	DT	SD	Acidity	Alk	PA
1	DA		Gas Well										PA
2	DB		Surface Mine Spoil										PA
3	DC		Surface Mine										PA
4	DD		Surface Mine AMD										PA

Start Import at row 1

Next

Export Data

This screen lets you set the delimiters your data contains. You can see how your text is affected in the preview below.

Delimiters

- Tab
- Semicolon
- Comma
- Space
- Other: []

Treat consecutive delimiters as one

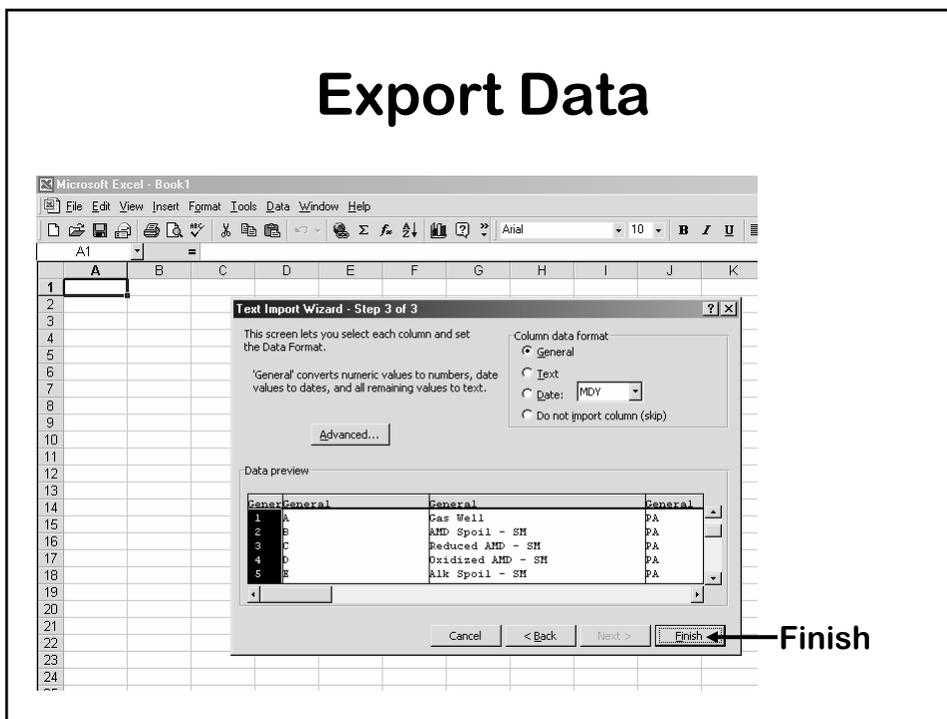
Text qualifier: []

Data preview

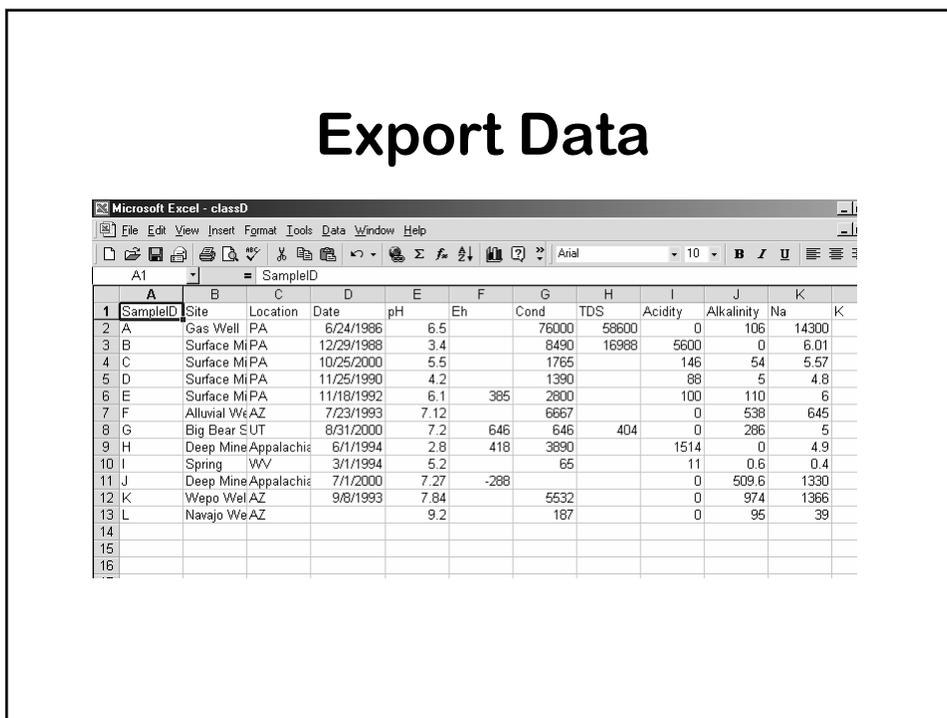
ID	Sample ID	Site	Location	Date	Op	HD	Ehd	Cond	DT	SD	Acidity	Alk	PA
1	A		Gas Well										PA
2	B		AMD Spoil - SM										PA
3	C		Reduced AMD - SM										PA
4	D		Oxidized AMD - SM										PA
5	E		Alk Spoil - SM										PA

Next

Export Data



Export Data



**End of Database
Reports Exercise**