

BIOETHERMODYNAMIC DATA CAPTURE

Example: Solubilities of biomaterials in solution

Data source: Carta, R. *J. Chem. Thermodyn.*, **1998**, 39, 1038-1048.

General Experiment Description: Solubilities of L-cystine, L-tyrosine, L-leucine, and glycine in sodium chloride solutions at various pH values determined gravimetrically.

Target Properties for the example: Molarities of L-cystine in a complex solution.

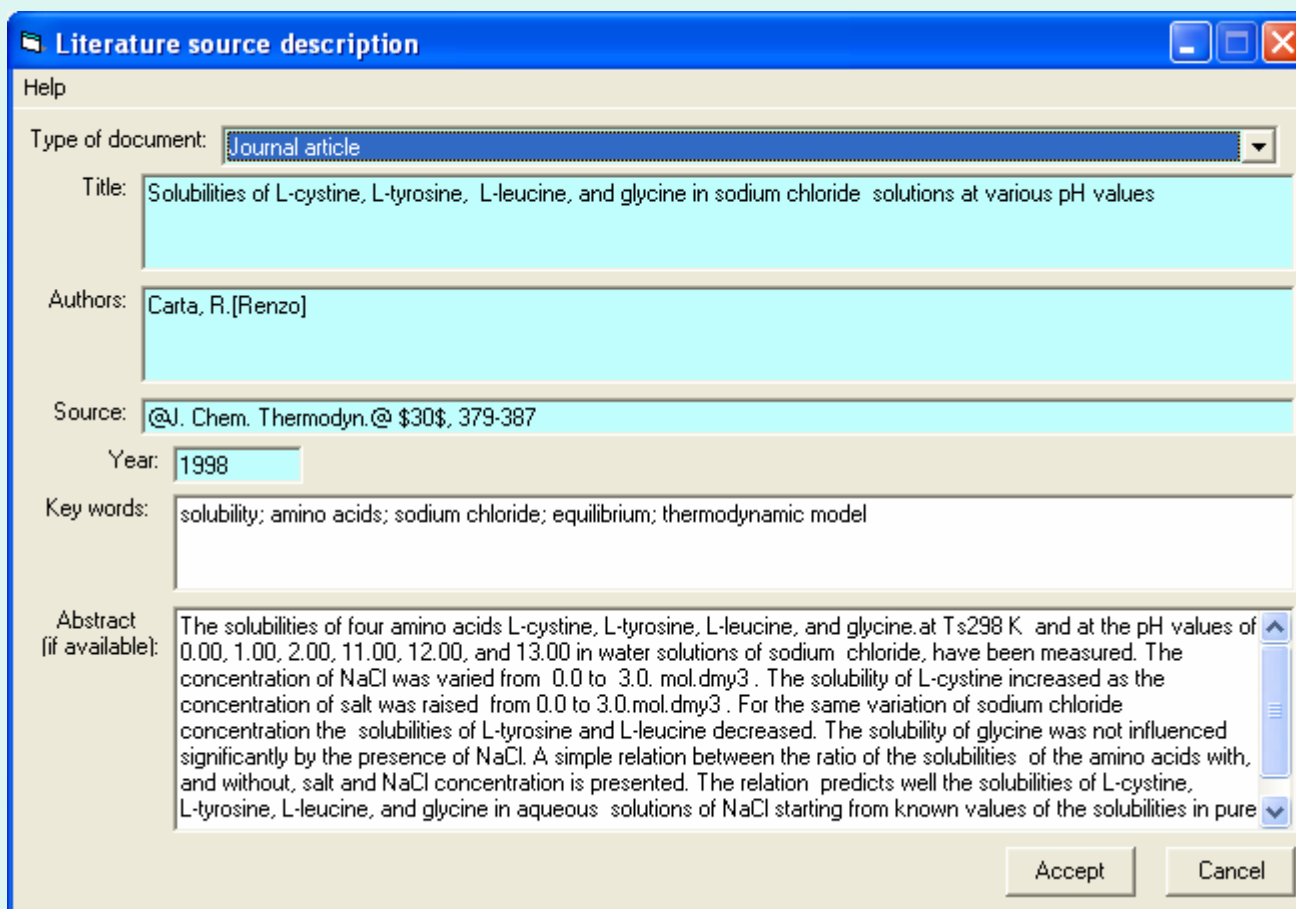
Bibliographic information:

No new additions were made to GDC for biothermodynamic data.

See: <http://www.trc.nist.gov/GDC.html> for general help.

See: <http://www.trc.nist.gov/helpdocs/basic/BIBLIOGRAPHICinfo.pdf>
for specific help on entering bibliographic information.

Here is the captured bibliographic information for the example:

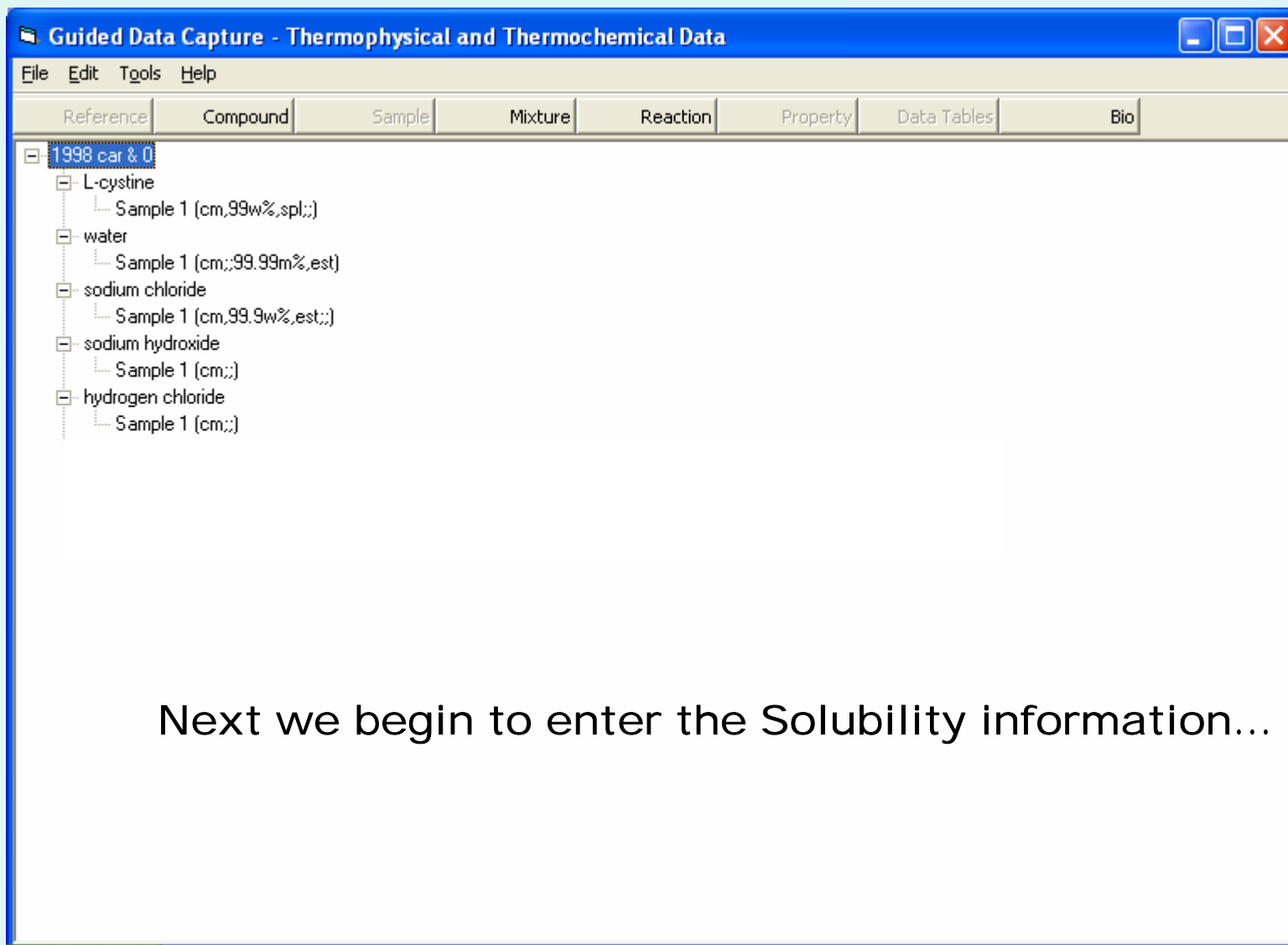


The screenshot shows a dialog box titled "Literature source description" with a "Help" button. The form contains the following fields:

- Type of document: Journal article
- Title: Solubilities of L-cystine, L-tyrosine, L-leucine, and glycine in sodium chloride solutions at various pH values
- Authors: Carta, R. [Renzo]
- Source: @J. Chem. Thermodyn. @ \$30\$, 379-387
- Year: 1998
- Key words: solubility; amino acids; sodium chloride; equilibrium; thermodynamic model
- Abstract (if available): The solubilities of four amino acids L-cystine, L-tyrosine, L-leucine, and glycine at $T=298\text{ K}$ and at the pH values of 0.00, 1.00, 2.00, 11.00, 12.00, and 13.00 in water solutions of sodium chloride, have been measured. The concentration of NaCl was varied from 0.0 to 3.0 mol.dmy³. The solubility of L-cystine increased as the concentration of salt was raised from 0.0 to 3.0 mol.dmy³. For the same variation of sodium chloride concentration the solubilities of L-tyrosine and L-leucine decreased. The solubility of glycine was not influenced significantly by the presence of NaCl. A simple relation between the ratio of the solubilities of the amino acids with, and without, salt and NaCl concentration is presented. The relation predicts well the solubilities of L-cystine, L-tyrosine, L-leucine, and glycine in aqueous solutions of NaCl starting from known values of the solubilities in pure

Buttons: Accept, Cancel

After capture of bibliographic info and specification of the reaction components, the Main GDC form looks like this...



Next we begin to enter the Solubility information...

Initiation of Bio Substance Solubility property capture...

The screenshot shows a software window titled "Guided Data Capture - Thermophysical and Thermochemical Data". The window has a menu bar with "File", "Edit", "Tools", and "Help". Below the menu bar is a tabbed interface with tabs for "Reference", "Compound", "Sample", "Mixture", "Reaction", "Property", "Data Table", and "Bio". The "Bio" tab is selected and highlighted with a red box. The main area of the window displays a tree view of data. The root node is "1998 car & 0", which is expanded to show several sub-nodes: "L-cystine", "water", "sodium chloride", "sodium hydroxide", and "hydrogen chloride". Each sub-node has a "Sample 1" entry with its respective units and conditions. Below the tree view, a "Data Table Processing" dialog box is open. The dialog box has a title bar and a close button. It contains a label "Select type of table:" followed by a list box. The list box contains three items: "Bio Property from DSC (in solution)", "Bio Substance Solubility", and "Bio Reaction". The "Bio Substance Solubility" item is selected and highlighted with a blue background. Below the list box are two buttons: "OK" and "Cancel". The "OK" button is highlighted with a red box. Three yellow callout boxes with red arrows provide instructions: "1. Select Bio and the Data Table Processing selection form opens." points to the "Bio" tab; "2. Select Bio Substance Solubility" points to the selected item in the list box; "3. Click OK" points to the "OK" button.

1. Select Bio and the *Data Table Processing* selection form opens.

2. Select Bio Substance Solubility

3. Click OK

Next...

The Bio System Properties form appears for Solubilities...

These fields are pre-filled in accord with the definition of a solubility

The screenshot shows the 'Bio System Properties' window. At the top, the 'Substance' field is set to 'L-cystine'. Below it, 'Phase 1' is 'Solution' and 'Phase 2' is 'Crystal'. A 'Description' field contains the text 'Select or enter text here'. A set of tabs at the bottom left includes 'Composition', 'Constraints', 'Variables', and 'Properties'. Below the tabs is a section titled 'Other components present' with a table of columns: 'Sample', 'Function', and 'Next'. The 'Method of measurement' field is at the bottom left, and 'Accept' and 'Cancel' buttons are at the bottom right.

Tabs to navigate between forms for the **Composition** (of the solution), **Constraints**, **Variables**, and **Properties** are analogous to those for DSC properties (Example I)

This field supports entry of special crystal descriptors, such as *alpha*, *beta*, *monoclinic*, *amorphous*, etc. At present, these are entered as text strings.

Define the Composition (of the solution):

Substance: L-cystine

Phase 1: Solution

Phase 2: Crystal

Sample #: 1

Composition | Constraints | Variables | Properties

Other components present

Component	Sample	Function
water	1	Solvent
sodium chloride	1	Solvent
sodium hydroxide		Solvent
hydrogen chloride		Solvent

Method of measurement: gravimetric analysis

1. Select components present & sample number (if needed)

2. Select the Function of each component

- Solvent
- Buffer component
- Inert

3. Enter the Method of Measurement

Next...

Define the Constraints:

Substance: L-cystine Sample # 1

Phase 1: Solution

Phase 2: Crystal

Composition | **Constraints** | Variables | Properties

	Value:	Unit	Uncert.	<input type="checkbox"/>	%
Temperature	298	K		<input type="checkbox"/>	%
Pressure	101	kPa		<input type="checkbox"/>	%
				<input type="checkbox"/>	%
				<input type="checkbox"/>	%
				<input type="checkbox"/>	%
				<input type="checkbox"/>	%
				<input type="checkbox"/>	%
				<input type="checkbox"/>	%

Method of measurement: gravimetric analysis

Next

Accept Cancel

1. Select constraints

2. Enter constraint values

3. Enter uncertainties for constraints, if known (absolute or percent)

Next tab...

Define the Variables:

Substance: L-cystine Sample # 1

Phase 1: Solution

Phase 2: Crystal

Composition | Constraints | **Variables** | Properties

Var.	Variable	Unit	Uncert.	%
Var.1	pH		<input type="text"/>	<input type="checkbox"/>
Var.2	Solvent: MolarRity	sodium chloride	<input type="text"/>	<input type="checkbox"/>
			<input type="text"/>	<input type="checkbox"/>
			<input type="text"/>	<input type="checkbox"/>
			<input type="text"/>	<input type="checkbox"/>
			<input type="text"/>	<input type="checkbox"/>
			<input type="text"/>	<input type="checkbox"/>
			<input type="text"/>	<input type="checkbox"/>

Method of measurement: gravimetric analysis Accept Cancel

2. Enter uncertainties, if known

Next tab...

Define the Properties:

Substance: L-cystine Sample # 1

Phase 1: Solution

Phase 2: Crystal Description:

Composition Constraints Variables **Properties**

Next

MolaLity L-cystine mol/kg Uncert. %

1. Select properties (only 1 in the example)

2. Enter uncertainties for properties

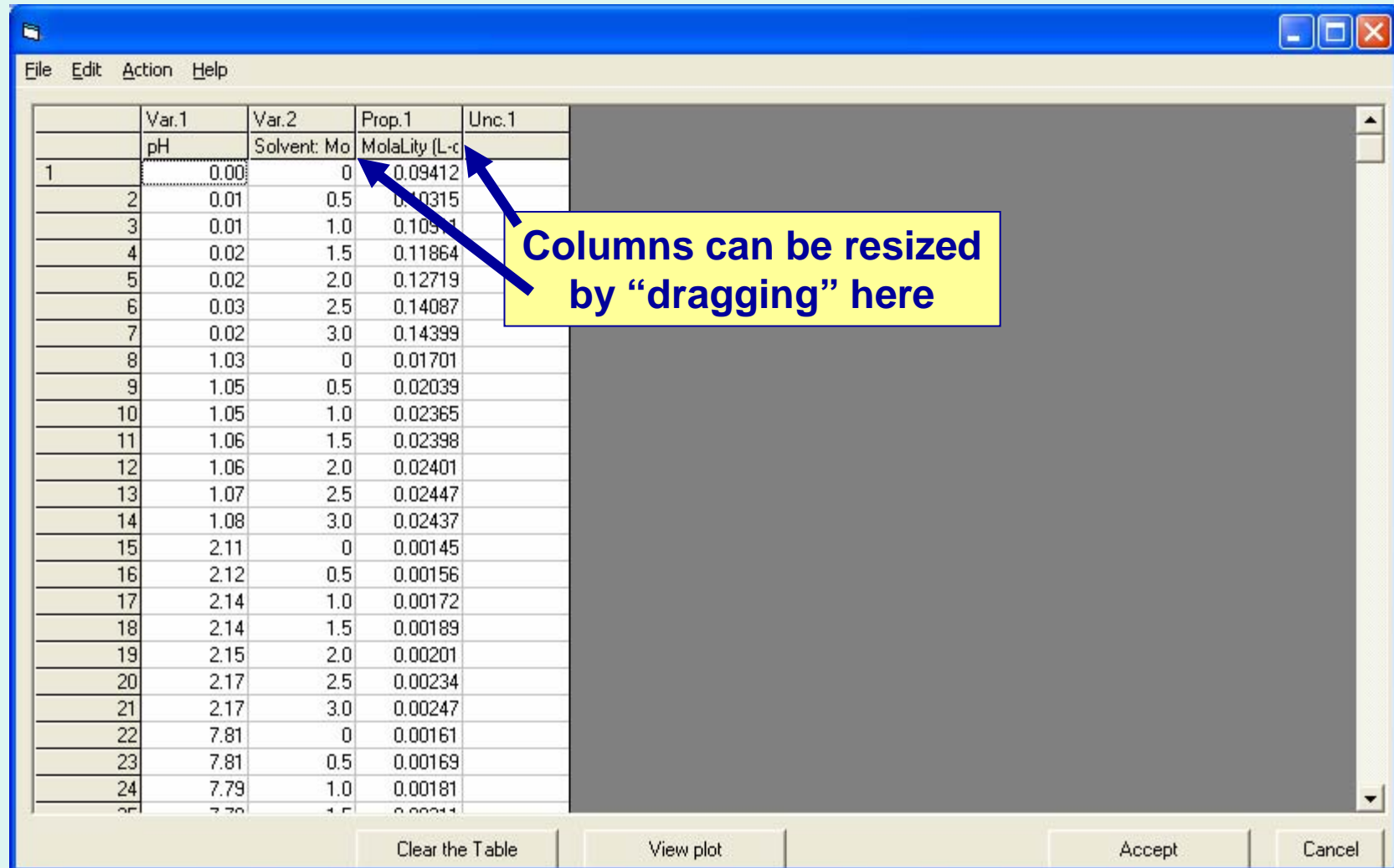
- Absolute or percent
- Uncertainties associated with each value can be capture on the next form...

Method of measurement: gravimetric analysis

Accept Cancel

Enter numerical values for *Variables* and *Properties*:

See page 382 of the example article pdf.



The screenshot shows a software window with a menu bar (File, Edit, Action, Help) and a data table. The table has four columns: Var.1, Var.2, Prop.1, and Unc.1. The first row of data is highlighted. A yellow callout box with blue arrows points to the column headers, stating "Columns can be resized by 'dragging' here".

	Var.1	Var.2	Prop.1	Unc.1
1	pH	Solvent: Mo	MolaLity [L-c	
1	0.00	0	0.09412	
2	0.01	0.5	0.10315	
3	0.01	1.0	0.10971	
4	0.02	1.5	0.11864	
5	0.02	2.0	0.12719	
6	0.03	2.5	0.14087	
7	0.02	3.0	0.14399	
8	1.03	0	0.01701	
9	1.05	0.5	0.02039	
10	1.05	1.0	0.02365	
11	1.06	1.5	0.02398	
12	1.06	2.0	0.02401	
13	1.07	2.5	0.02447	
14	1.08	3.0	0.02437	
15	2.11	0	0.00145	
16	2.12	0.5	0.00156	
17	2.14	1.0	0.00172	
18	2.14	1.5	0.00189	
19	2.15	2.0	0.00201	
20	2.17	2.5	0.00234	
21	2.17	3.0	0.00247	
22	7.81	0	0.00161	
23	7.81	0.5	0.00169	
24	7.79	1.0	0.00181	
25	7.78	1.5	0.00211	

See next page...

Columns are resized to make headings easily readable, if necessary.

File Edit Action Help

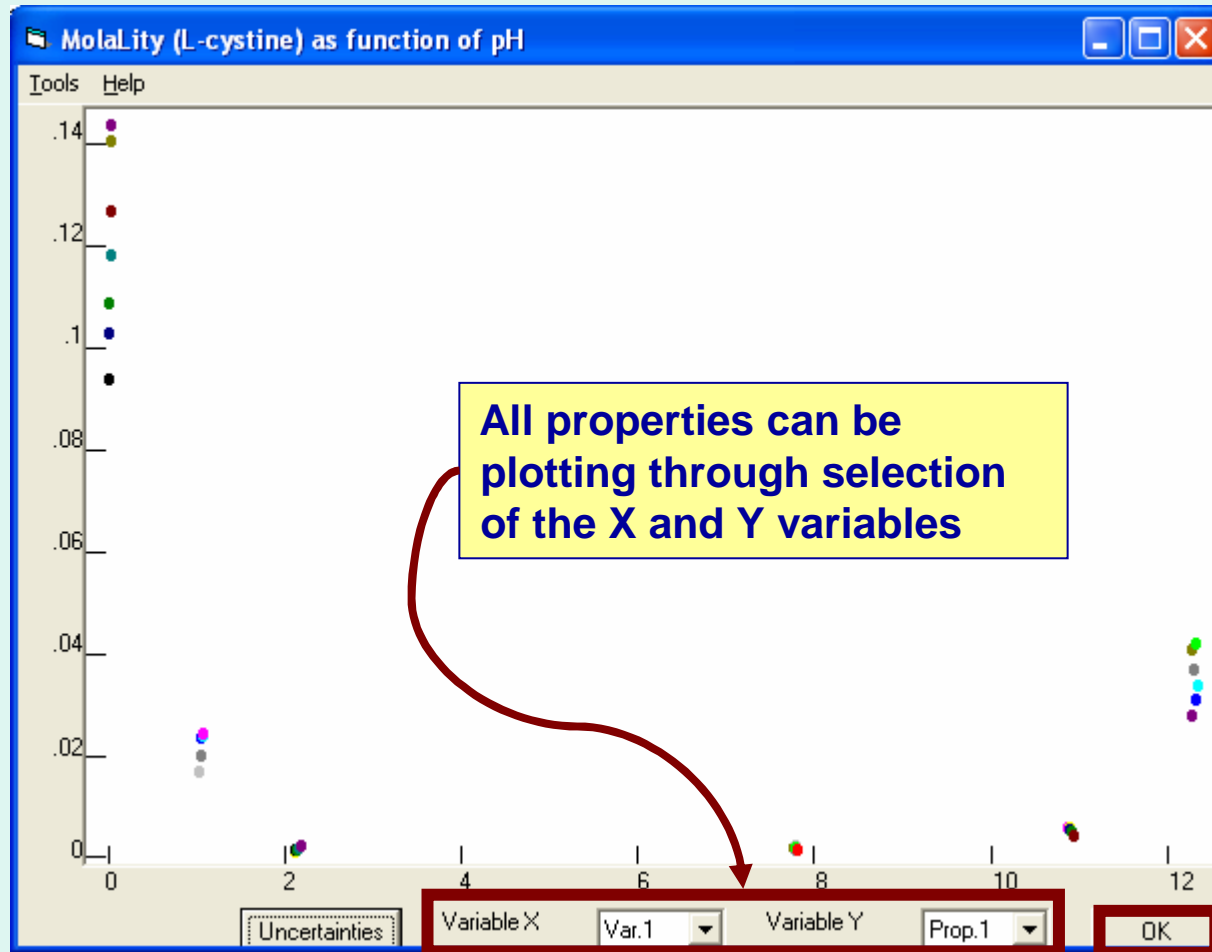
	Var.1	Var.2	Prop.1	Unc.1
	pH	Solvent: MolaRity (sodium chloride)	MolaLity (L-cystine)	
1	0.00		0	0.09412
2	0.01		0.5	0.10315
3	0.01		1.0	0.10911
4	0.02		1.5	0.11864
5	0.02		2.0	0.12719
6	0.03		2.5	0.14087
7	0.02		3.0	0.14399
8	1.03		0	0.01701
9	1.05		0.5	0.02039
10	1.05		1.0	0.02365
11	1.06		1.5	0.02398
12	1.06		2.0	0.02401
13	1.07		2.5	0.02447
14	1.08		3.0	0.02437
15	2.11		0	0.00145
16	2.12		0.5	0.00156
17	2.14		1.0	0.00172
18	2.14		1.5	0.00189
			2.0	0.00201
			2.5	0.00234
			3.0	0.00247
			0	0.00161
23	7.81		0.5	0.00169
24	7.79		1.0	0.00181
25	7.78		1.5	0.00194

Clear the Table View plot Accept Cancel

Click View plot for graphing options

Click Accept when done

Plotting Options: Plot any property against any variable (2-d only)



All properties can be plotting through selection of the X and Y variables

Click OK when done

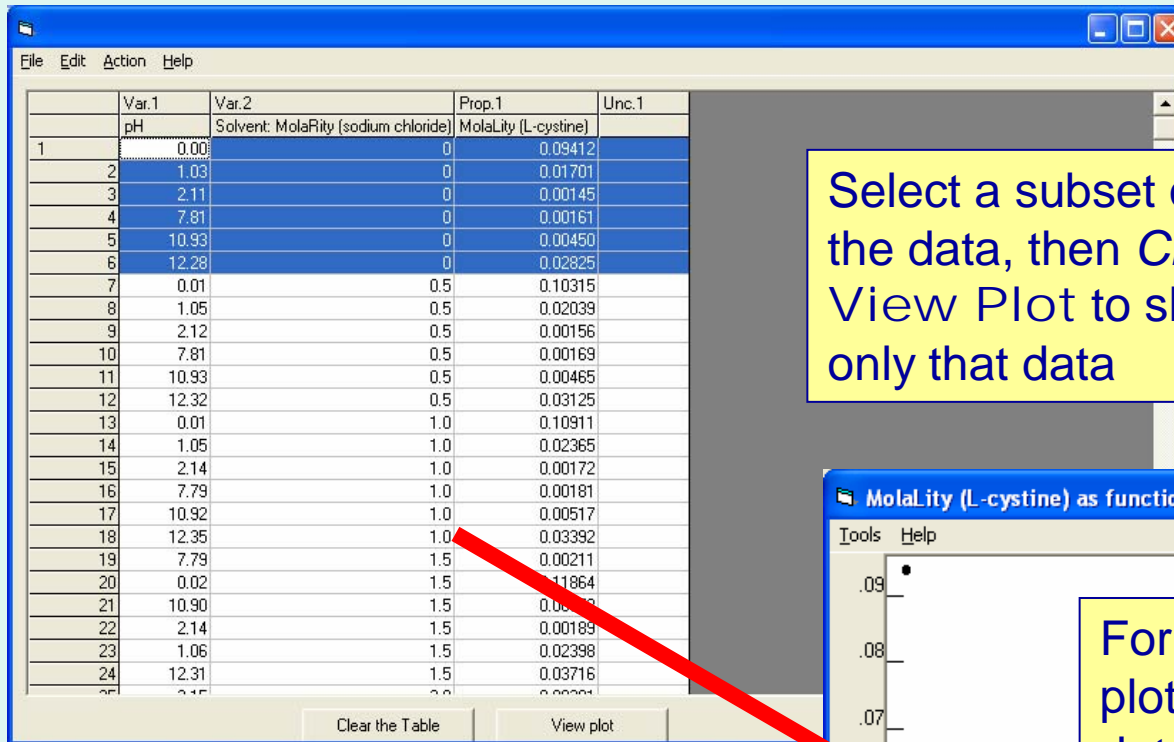
Some additional useful features of GDC plotting

Sort on any column by selecting it and typing Cntl-A

The image shows two overlapping windows from the GDC plotting software. The background window displays a data table with columns: Var.1 (pH), Var.2 (Solvent: MolaRity (sodium chloride)), Prop.1 (MolaLity (L-cystine)), and Unc.1. The foreground window is a sorting dialog box with the same table, but with the 'Prop.1' column selected. A red arrow points from the 'Prop.1' column in the background window to the 'Prop.1' column in the foreground window. The foreground window has buttons for 'Clear the Table', 'View plot', 'Accept', and 'Cancel'.

	Var.1	Var.2	Prop.1	Unc.1
1	0.00	0	0.09412	
2	0.01	0.5	0.10315	
3	0.01	1.0	0.10911	
4	0.02	1.5	0.11864	
5	0.02	2.0	0.12719	
6	0.02	3.0	0.14399	
7	0.03	2.5	0.14087	
8	1.03	0	0.01701	
9	1.05	1.0		
10	1.05	0.5		
11	1.06	1.5		
12	1.06	2.0		
13	1.07	2.5		
14	1.08	3.0		
15	2.11	0		
16	2.12	0.5		
17	2.14	1.5		
18	2.14	1.0		
19	2.15	2.0		
20	2.17	2.5		
21	2.17	3.0		
22	7.76	2.0		
23	7.78	3.0		
24	7.79	2.5		
25	7.79	1.5		

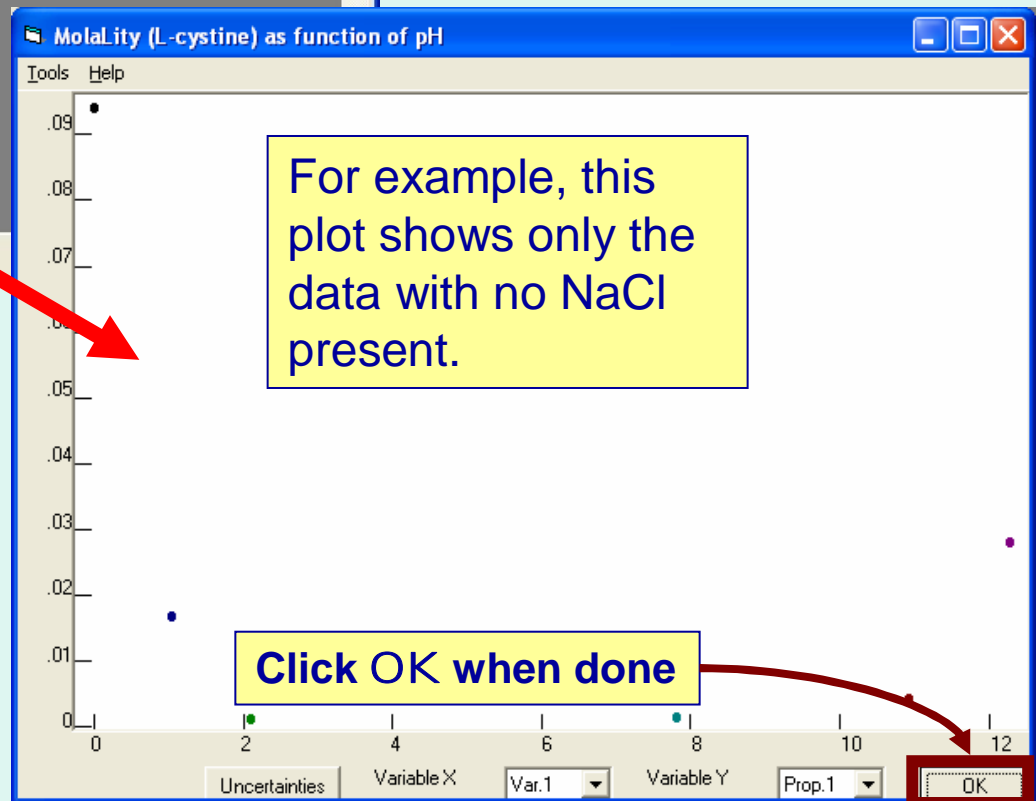
Some additional useful features of GDC plotting



The screenshot shows a data table window with a menu bar (File, Edit, Action, Help) and a table with columns: Var.1 (pH), Var.2 (Solvent: MolarRity (sodium chloride)), Prop.1 (MolarLity (L-cystine)), and Unc.1. Rows 1 through 6 are highlighted in blue. A yellow callout box with a blue border contains the text: "Select a subset of the data, then *Click View Plot* to show only that data". At the bottom of the window are buttons for "Clear the Table" and "View plot".

	Var.1	Var.2	Prop.1	Unc.1
1	0.00		0	0.09412
2	1.03		0	0.01701
3	2.11		0	0.00145
4	7.81		0	0.00161
5	10.93		0	0.00450
6	12.28		0	0.02825
7	0.01		0.5	0.10315
8	1.05		0.5	0.02039
9	2.12		0.5	0.00156
10	7.81		0.5	0.00169
11	10.93		0.5	0.00465
12	12.32		0.5	0.03125
13	0.01		1.0	0.10911
14	1.05		1.0	0.02365
15	2.14		1.0	0.00172
16	7.79		1.0	0.00181
17	10.92		1.0	0.00517
18	12.35		1.0	0.03392
19	7.79		1.5	0.00211
20	0.02		1.5	0.11864
21	10.90		1.5	0.00189
22	2.14		1.5	0.00189
23	1.06		1.5	0.02398
24	12.31		1.5	0.03716

Select a subset of the data, then *Click View Plot* to show only that data



For example, this plot shows only the data with no NaCl present.

Click OK when done

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Reaction Property Data Tables Bio

- 1998 car & 0
 - L-cystine
 - Sample 1 (cm,99w%,spl;:)
 - water
 - Sample 1 (cm;:99.99m%,est)
 - sodium chloride
 - Sample 1 (cm,99.9w%,est;:)
 - sodium hydroxide
 - Sample 1 (cm;:)
 - hydrogen chloride
 - Sample 1 (cm;:)
 - BioProperty Set # 1: Solubility of L-cystine in water + sodium chloride + sodium hydroxide + hydrogen chloride

The new property set now appears in the navigation tree.

Double click the node to access the Bio Systems Properties form for editing