

BIOETHERMODYNAMIC DATA CAPTURE

Example: Properties determined with differential scanning calorimetry (DSC methods)

Data source: Hinz, H.J.; Schwarz, F. P. Measurement and analysis of results obtained on biological substances with d.s.c., J. Chem. Thermodyn., **2001**, 33, 1511-1525.

General Experiment Description: Denaturization of lysozyme studied by DSC with pH and lysozyme concentration varied

Target Properties: T_G , Enthalpy of transition, van't Hoff enthalpy of transition

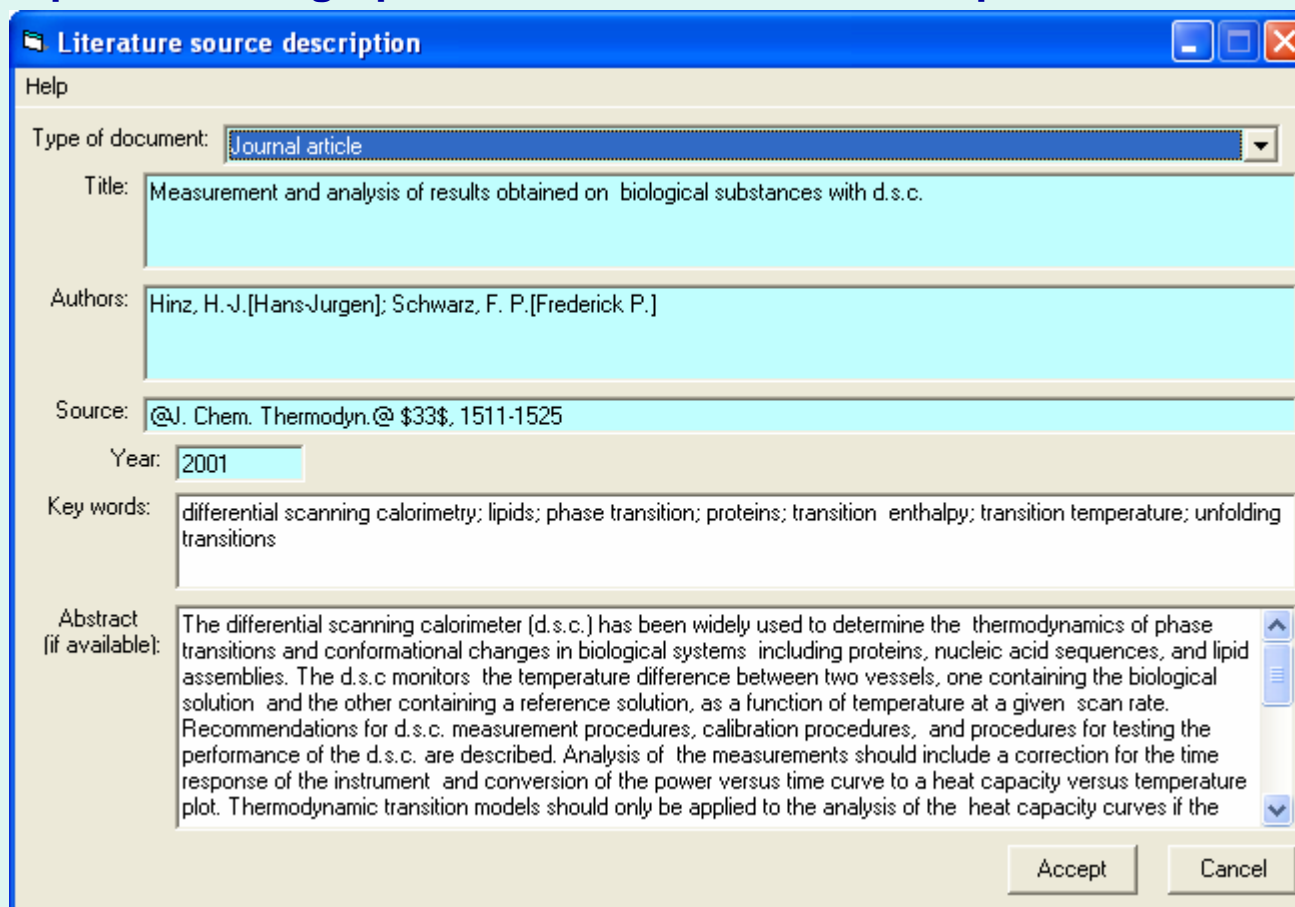
Bibliographic information:

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: Measurement and analysis of results obtained on biological substances with d.s.c.
- Authors: Hinz, H. J.[Hans-Jurgen]; Schwarz, F. P.[Frederick P.]
- Source: @J. Chem. Thermodyn.@ \$33\$, 1511-1525
- Year: 2001
- Key words: differential scanning calorimetry; lipids; phase transition; proteins; transition enthalpy; transition temperature; unfolding transitions
- Abstract (if available): The differential scanning calorimeter (d.s.c.) has been widely used to determine the thermodynamics of phase transitions and conformational changes in biological systems including proteins, nucleic acid sequences, and lipid assemblies. The d.s.c monitors the temperature difference between two vessels, one containing the biological solution and the other containing a reference solution, as a function of temperature at a given scan rate. Recommendations for d.s.c. measurement procedures, calibration procedures, and procedures for testing the performance of the d.s.c. are described. Analysis of the measurements should include a correction for the time response of the instrument and conversion of the power versus time curve to a heat capacity versus temperature plot. Thermodynamic transition models should only be applied to the analysis of the heat capacity curves if the

Buttons: Accept, Cancel

Compound Selection/Addition:

Compound Selection or Addition is very similar to that traditionally used in GDC.

See: <http://www.trc.nist.gov/helpdocs/basic/COMPOUNDselection.pdf>

and

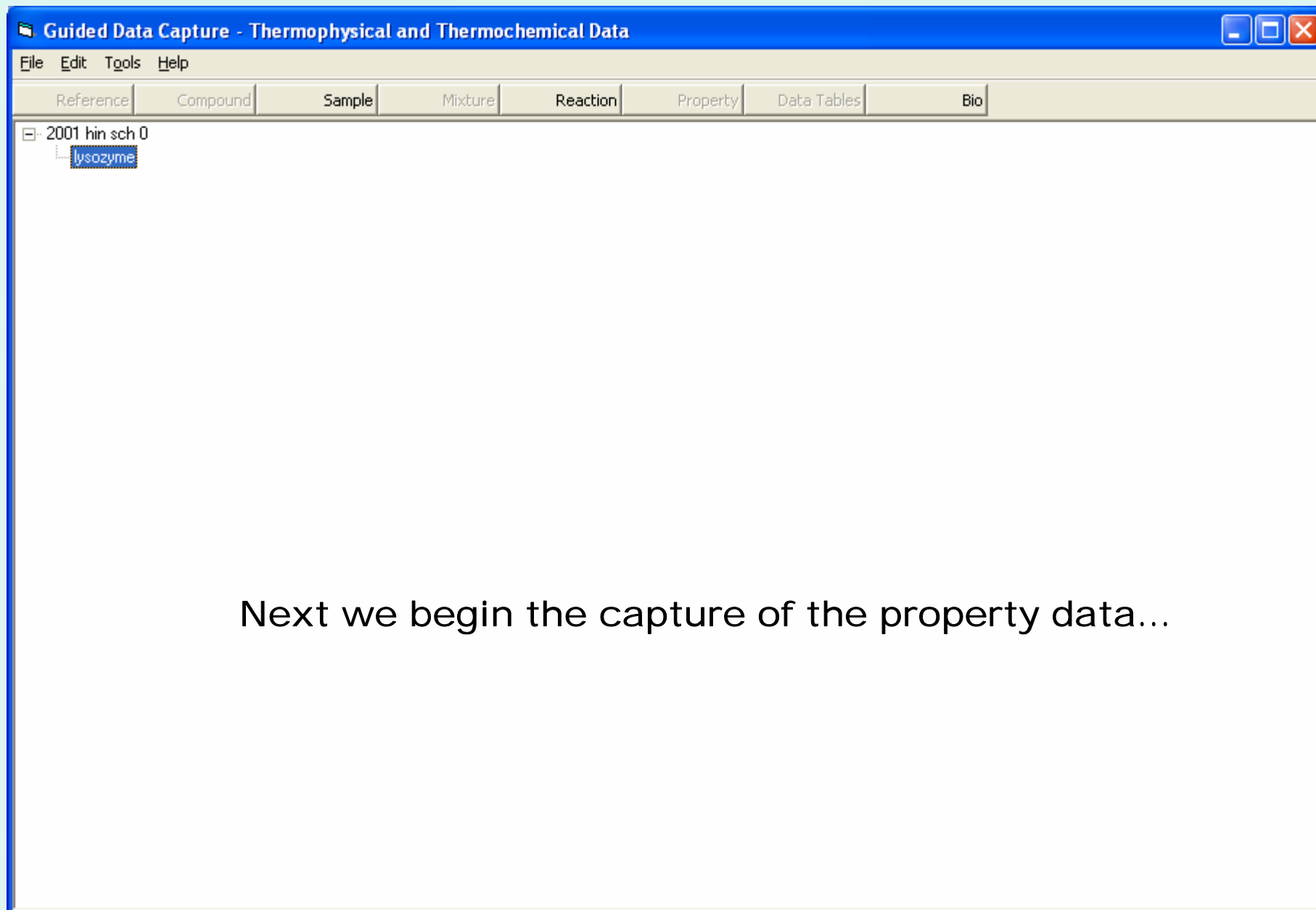
See: <http://www.trc.nist.gov/helpdocs/basic/COMPOUNDaddition.pdf>

New Features:

1. Capture of EC (*Enzyme Commission*) Number is supported
2. Capture of PDB (*Protein Data Bank*) Number is supported
3. Symbolic formulas are supported (in brackets {*}) to support substances of unspecified empirical formula

The screenshot shows a dialog box titled "Substance" with a "Help" button. The "Name" field contains "lysozyme". The "Empirical formula (Case sensitive)" field contains "{LZ}" and is highlighted with a red box and the number 3. The "EC Number" field contains "3.2.1.17" and is highlighted with a red box and the number 1. The "PDB Number" field is empty and highlighted with a red box and the number 2. The "Molar Mass" field is empty. There are "OK" and "Cancel" buttons at the bottom right.

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



Next we begin the capture of the property data...

Initiation of biothermodynamic property data capture...

2001 hin sch 0
lysozyme

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

2. Select Bio Property from DSC (in solution)

3. Click OK

Next...

The Bio System Properties form appears

1. The Initial and Final states of the substance are specified first
 - Select from pull-down menu or
 - Enter text directly

Help

Substance: lysozyme Sample #

Phase: Solution

Initial state: Select or enter text here

Final state: Select or enter text here

Composition | Constraints | Variables | Properties

Other components present

		Next	
	Sample	Function	
	Sample	Function	
	Sample	Function	
	Sample	Function	
	Sample	Function	
	Sample	Function	
	Sample	Function	
	Sample	Function	
	Sample	Function	

Method of measurement:

Accept Cancel

2. Select a Tab to access a form to specify:
 - The Environment (i.e., solution composition)
 - Constraints
 - Variables
 - Properties

Next...

Composition: Specification (compounds other than the “Substance” under study)

For the example, these are the solution components...

Bio System Properties

Substance: lysozyme Sample #

Phase: Solution Initial state: Native Final state: Denatured

Composition Constraints Variables Properties

Other components present:

glycine	Sample	Function
hydrogen chloride	Sample	Function
water	Sample	Function
New	Sample	Function
None	Sample	Function

Method of measurement: DSC Accept Cancel

1. Select components present

2. Select sample numbers if necessary (rare)

Note: Selection of “new” activates the GDC compound-selection form

4. Enter the measurement method

3. Select the “Function” of each component

- Solvent
- Buffer
- Inert

Next tab...

Constraints: Specification of fixed quantities

For the example, these are the pressure and buffer composition

The screenshot shows the 'Bio System Properties' window with the 'Constraints' tab selected. The 'Substance' is 'lysozyme', 'Phase' is 'Solution', 'Initial state' is 'Native', and 'Final state' is 'Denatured'. The 'Constraints' table is as follows:

Name	Value	Units	Uncert.	%
Pressure	101.325	kPa		<input type="checkbox"/>
Molarity	0.1	mol/dm3		<input type="checkbox"/>
Molarity	0.1	mol/dm3		<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>

At the bottom, the 'Method of measurement' is 'DSC'. There are 'Next', 'Accept', and 'Cancel' buttons.

1. Select constraints

2. Enter constraint values

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

Next tab...

Variables: Specification of quantities that are varied

For the example, these are pH and concentration of lysozyme

Bio System Properties

Help

Substance: lysozyme Sample #

Phase: Solution Initial state: Native

Composition | Constraint | **Variables** | Properties

Var.	Variable	Substance	Unit
Var.1	pH		
Var.2	Mass concentration	lysozyme	kg/m3

Next

Uncert.		<input type="checkbox"/>	%
Uncert.		<input type="checkbox"/>	%
Uncert.		<input type="checkbox"/>	%
Uncert.		<input type="checkbox"/>	%
Uncert.		<input type="checkbox"/>	%
Uncert.		<input type="checkbox"/>	%
Uncert.		<input type="checkbox"/>	%
Uncert.		<input type="checkbox"/>	%
Uncert.		<input type="checkbox"/>	%

Method of measurement: DSC

Accept Cancel

1. Select variables

2. Enter uncertainties, if known

Next tab...

Properties: Specification of properties

For the example, these are pH and concentration of lysozyme

1. Select properties

Next to Data Table

2. Enter uncertainties for properties

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

Method of measurement: DSC

Numerical Data Table: Enter values for variables and properties

For the example:

Variables: pH, conc of lysozyme

Properties: T_G , $\Delta_{\text{trs}} H$, $\Delta_{\text{trs}} H_{\text{vH}}$

The screenshot shows a software window with a menu bar (File, Edit, Action, Help) and a data table. The table has columns for variables (Var.1, Var.2) and properties (Prop.1, Prop.2, Prop.3) with corresponding uncertainty columns (Unc.1, Unc.2, Unc.3). The data is organized into 20 rows. The 'View plot' and 'Accept' buttons at the bottom are highlighted with red boxes. A yellow callout box points to the 'View plot' button with the text 'Click View plot for graphing options'. Another yellow callout box points to the 'Accept' button with the text 'Click Accept when done'.

	Var.1	Var.2	Prop.1	Unc.1	Prop.2	Unc.2	Prop.3	Unc.3
	pH	Mass conce	Zero-Gibbs ϵ		Enthalpy of l		van't Hoff ϵ	
1	2.5	4.81	331.4		393		392	
2	2.5	4.81	331.5		378		391	
3	2.5	4.81	331.7		397		406	
4	2.5	0.97	331.6		403		403	
5	2.5	0.97	331.6		403		403	
6	2.5	0.98	331.5		406		406	
7	2.5	0.95	331.5		401		402	
8	2.5	2.28	331.5		397		401	
9	2.5	2.28	331.5		401		402	
10	2.3	1.00	331.3		401		382	
11	2.3	2.32	331.6		427		373	
12	2.3	2.36	331.9		434		369	
13	2.3	2.36	331.6		439		368	
14	2.3	4.72	330.3		436		363	
15	2.3	4.77	330.5		411		373	
16	2.3	4.77	331.6		401		377	
17	2.3	9.70	331.9		434		366	
18	2.3	9.70	331.9		423		373	
19	2.5	1.00	331.1		396		396	
20	2.5	1.00	330.8		418		418	
			331.1		401		403	
			330.6		386		388	
			330.8		419		418	
			331.2		396		398	
			330.8		396		398	

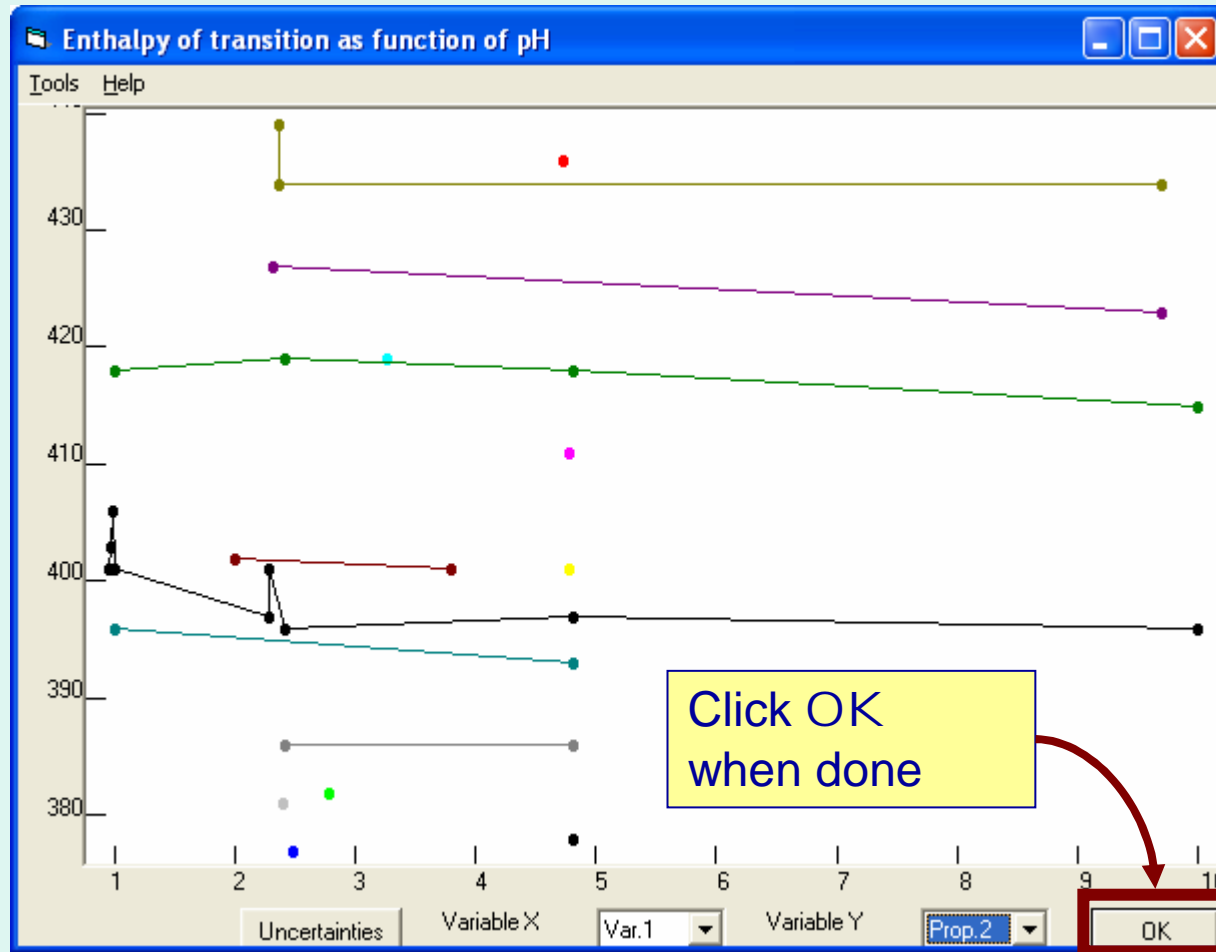
Buttons: Clear the Table, View plot, Accept, Cancel

Note: Columns can be resized (by dragging as in *Excel*) to show full property and variable names, if desired.

The screenshot shows a software window with a menu bar (File, Edit, Action, Help) and a data table. The table has columns for variables (Var.1, Var.2) and properties (Prop.1, Prop.2, Prop.3) with associated uncertainty columns (Unc.1, Unc.2, Unc.3). The data is organized into rows, with the first row highlighted. The table is titled 'Clear the Table', 'View plot', 'Accept', and 'Cancel' buttons are visible at the bottom.

	Var.1	Var.2	Prop.1	Unc.1	Prop.2	Unc.2	Prop.3	Unc.3
	pH	Mass concentration (lysozyme)	Zero-Gibbs energy temperature		Enthalpy of transition		van't Hoff enthalpy of transition	
1	2.5	4.81	331.4		393		392	
2	2.5	4.81	331.5		378		391	
3	2.5	4.81	331.7		397		406	
4	2.5	0.97	331.6		403		403	
5	2.5	0.97	331.6		403		403	
6	2.5	0.98	331.5		406		406	
7	2.5	0.95	331.5		401		402	
8	2.5	2.28	331.5		397		401	
9	2.5	2.28	331.5		401		402	
10	2.3	1.00	331.3		401		382	
11	2.3	2.32	331.6		427		373	
12	2.3	2.36	331.9		434		369	
13	2.3	2.36	331.6		439		368	
14	2.3	4.72	330.3		436		363	
15	2.3	4.77	330.5		411		373	
16	2.3	4.77	331.6		401		377	
17	2.3	9.70	331.9		434		366	
18	2.3	9.70	331.9		423		373	
19	2.5	1.00	331.1		396		396	
20	2.5	1.00	330.8		418		418	
21	2.5	1.00	331.1		401		403	
22	2.5	2.41	330.6		386		388	
23	2.5	2.41	330.8		419		418	
24	2.5	2.41	331.2		396		398	

Graphical Representation: Plot any property against any variable (2-d only)



For the example, this is not very informative...

OK returns to Numerical Data Table

The screenshot shows a software window with a menu bar (File, Edit, Action, Help) and a table of numerical data. The table has columns for variables (Var.1, Var.2) and properties (Prop.1, Prop.2, Prop.3) with associated uncertainty columns (Unc.1, Unc.2, Unc.3). The data is organized into rows, with the first row highlighted. A yellow callout box with the text "Click Accept when done" points to the "Accept" button in the bottom right corner of the window.

	Var.1	Var.2	Prop.1	Unc.1	Prop.2	Unc.2	Prop.3	Unc.3
	pH	Mass concentration (lysozyme)	Zero-Gibbs energy temperature		Enthalpy of transition		van't Hoff enthalpy of transition	
1	2.5	4.81	331.4		393		392	
2	2.5	4.81	331.5		378		391	
3	2.5	4.81	331.7		397		406	
4	2.5	0.97	331.6		403		403	
5	2.5	0.97	331.6		403		403	
6	2.5	0.98	331.5		406		406	
7	2.5	0.95	331.5		401		402	
8	2.5	2.28	331.5		397		401	
9	2.5	2.28	331.5		401		402	
10	2.3	1.00	331.3		401		382	
11	2.3	2.32	331.6		427		373	
12	2.3	2.36	331.9		434		369	
13	2.3	2.36	331.6		439		368	
14	2.3	4.72	330.3		436		363	
15	2.3	4.77	330.5		411		363	
16	2.3	4.77	331.6		401		363	
17	2.3	9.70	331.9		434		363	
18	2.3	9.70	331.9		423		363	
19	2.5	1.00	331.1		396		396	
20	2.5	1.00	330.8		418		418	
21	2.5	1.00	331.1		401		403	
22	2.5	2.41	330.6		386		388	
23	2.5	2.41	330.8		419		418	
24	2.5	2.41	331.2		396		398	
25	2.5	4.81	331.4		393		392	

Property capture is complete...

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Reaction Property Data Tables Bio

2001 hin sch 0

- lysozyme
 - Sample 1 (cm,95w%,spl;)
 - glycine
 - hydrogen chloride
 - water
 - BioProperty Set # 1 (lysozyme) from DSC (pH, E)

The new property set now appears in the navigation tree.

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