BIOTHERMODYNAMIC 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

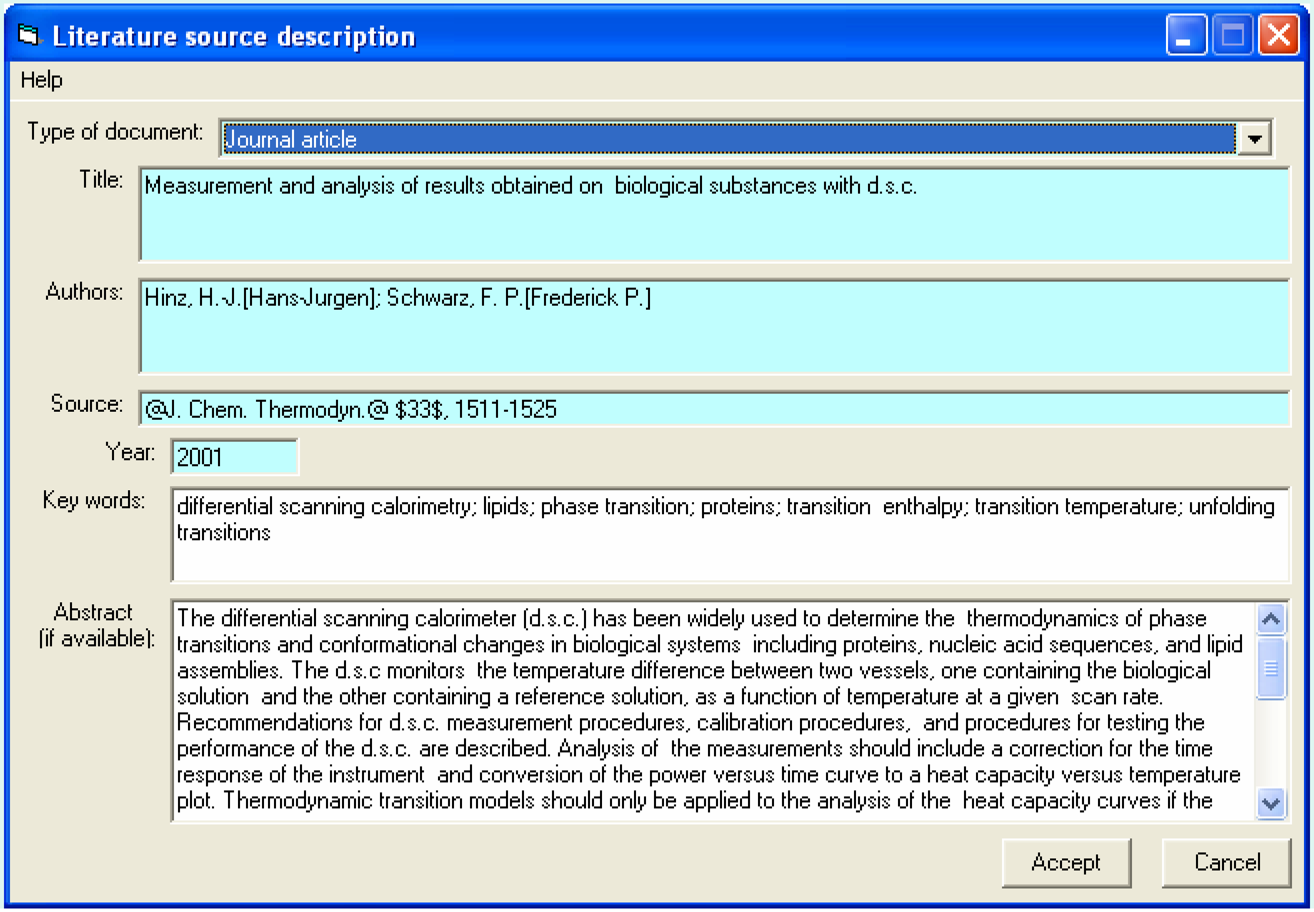
Target Properties: T_G, Enthalpy of transition, van't Hoff enthalpy of transition

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:



Compound Selection/Addition:

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

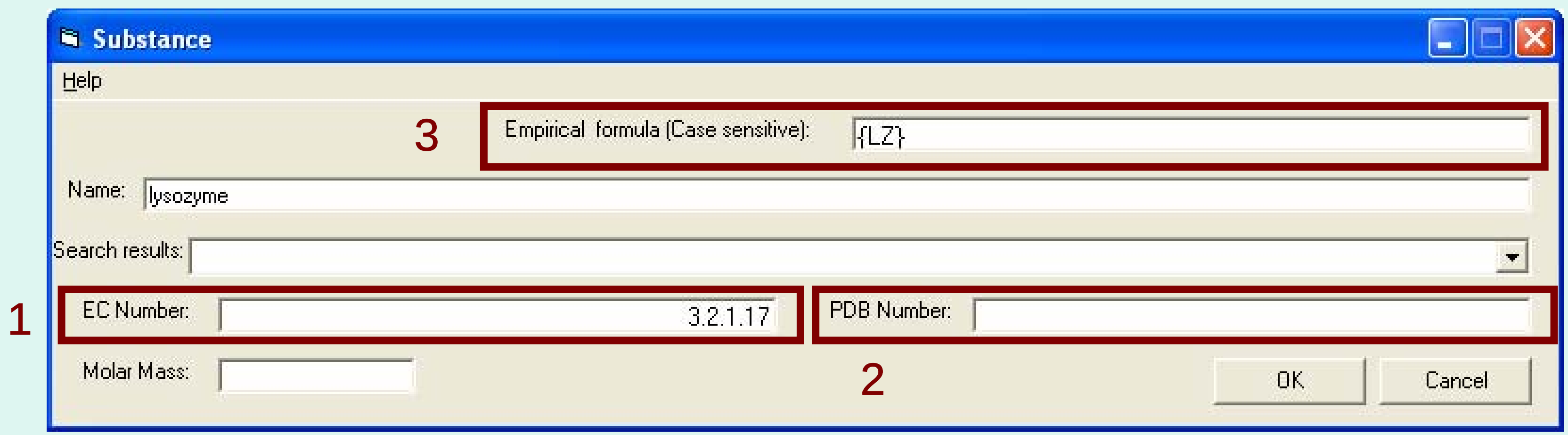
See: http://www.trc.nist.gov/helpdocs/basic/COMPOUNDselection.pdf

and

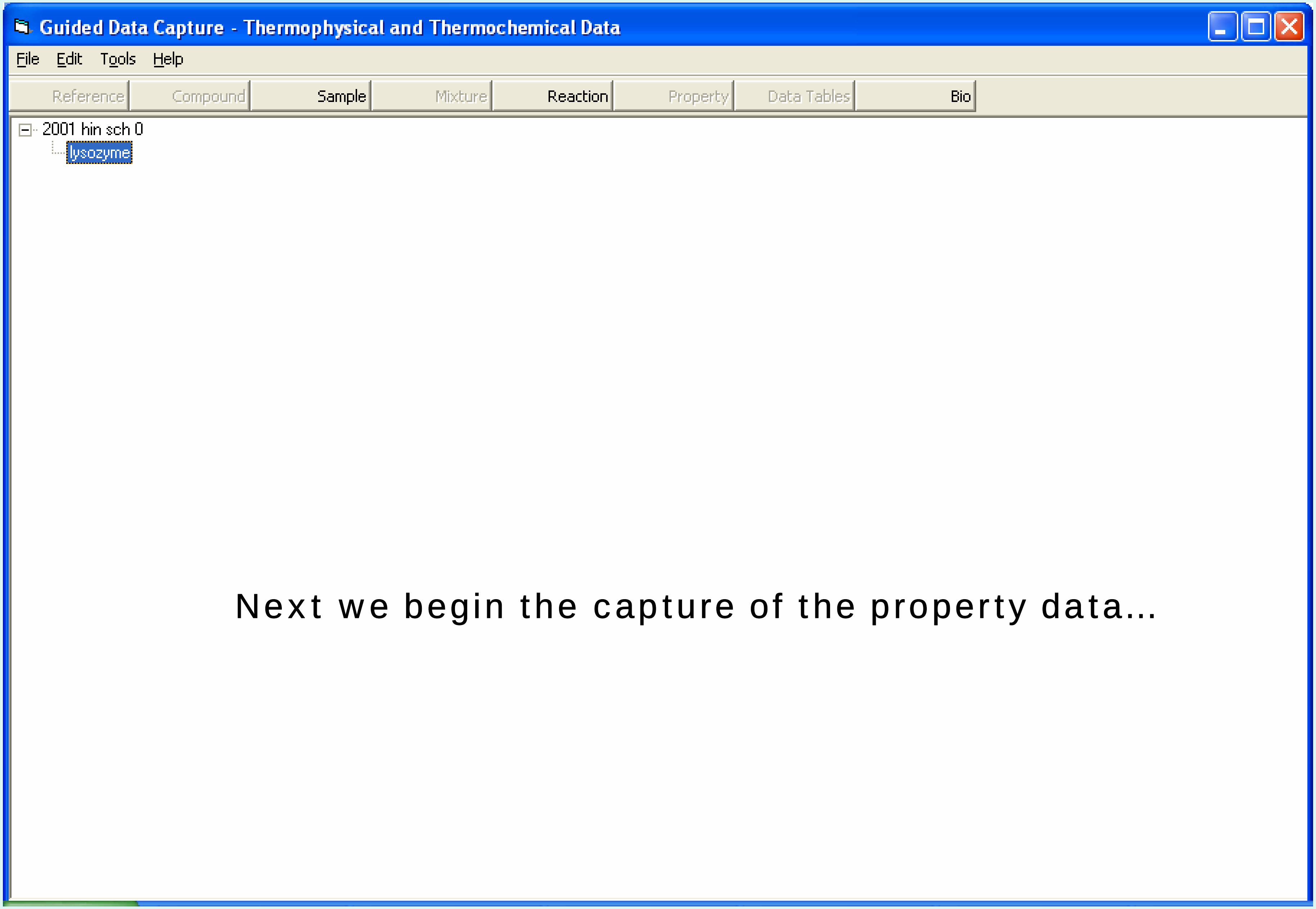
See: http://www.trc.nist.gov/helpdocs/basic/COMPOUNDaddition.pdf

New Features:

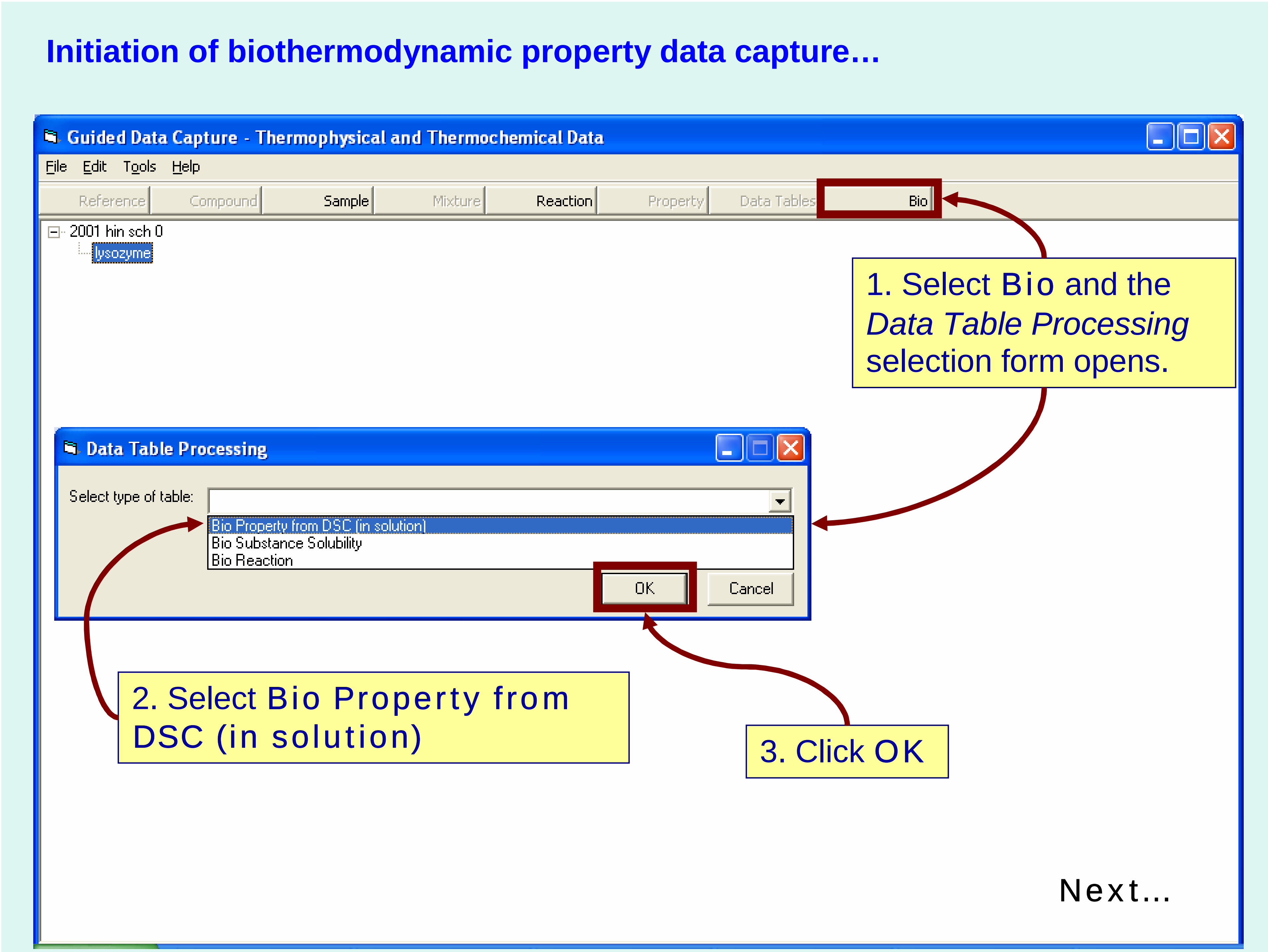
1. **Capture of EC (*Enzyme Commision*) Number is supported**
2. **Capture of PDB (*Protein Data Bank*) Number is supported**
3. **Symbolic formulas are supported (in brackets {*}) to support substances of unspecified empirical formula**



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



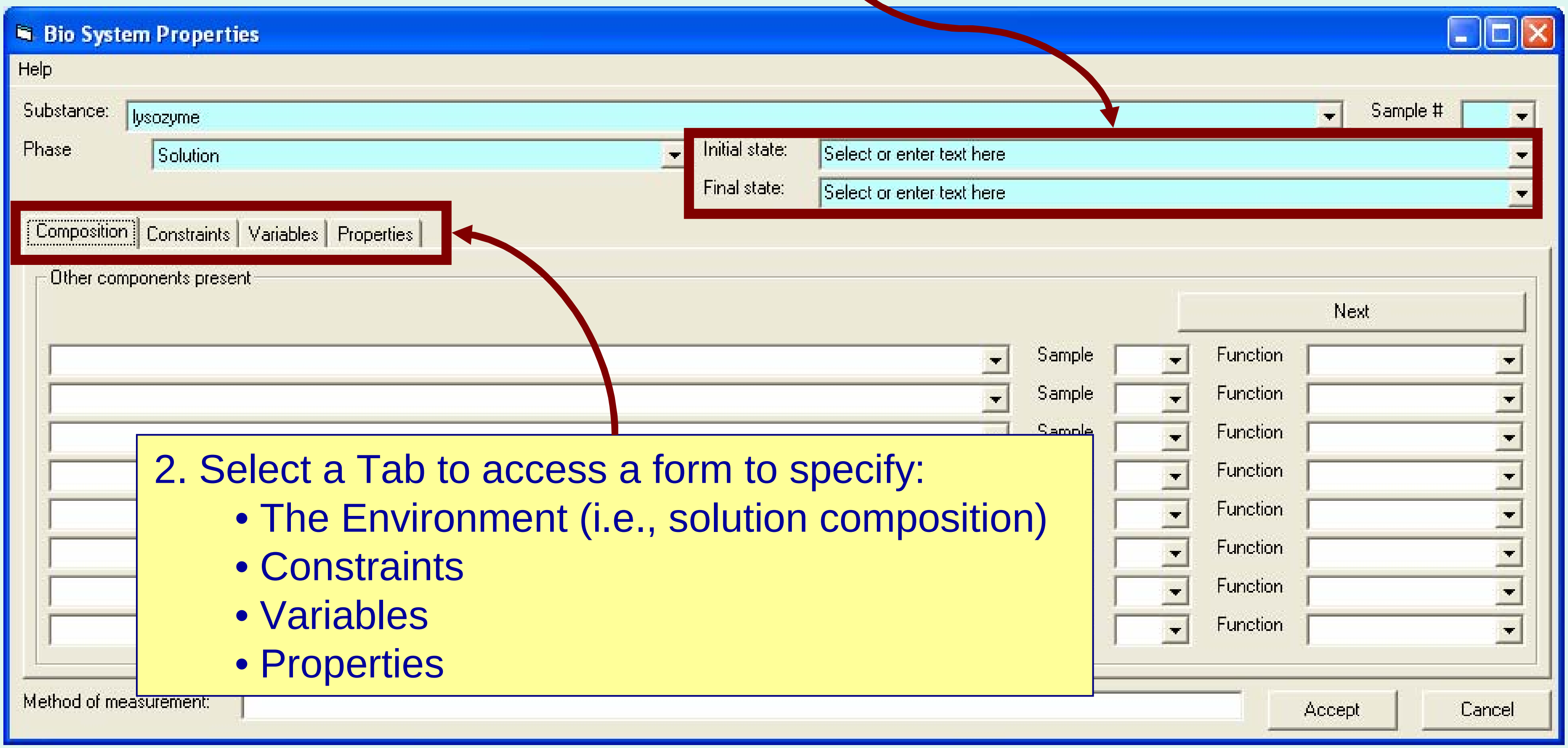
Next we begin the capture of the property data...



Initiation of biothermodynamic property data capture…
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
1. Select Bio and the Data Table Processing selection form opens.
Data Table Processing
Select type of table:
Bio Property from DSC (in solution)
Bio Substance Solubility
Bio Reaction
OK
Cancel
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

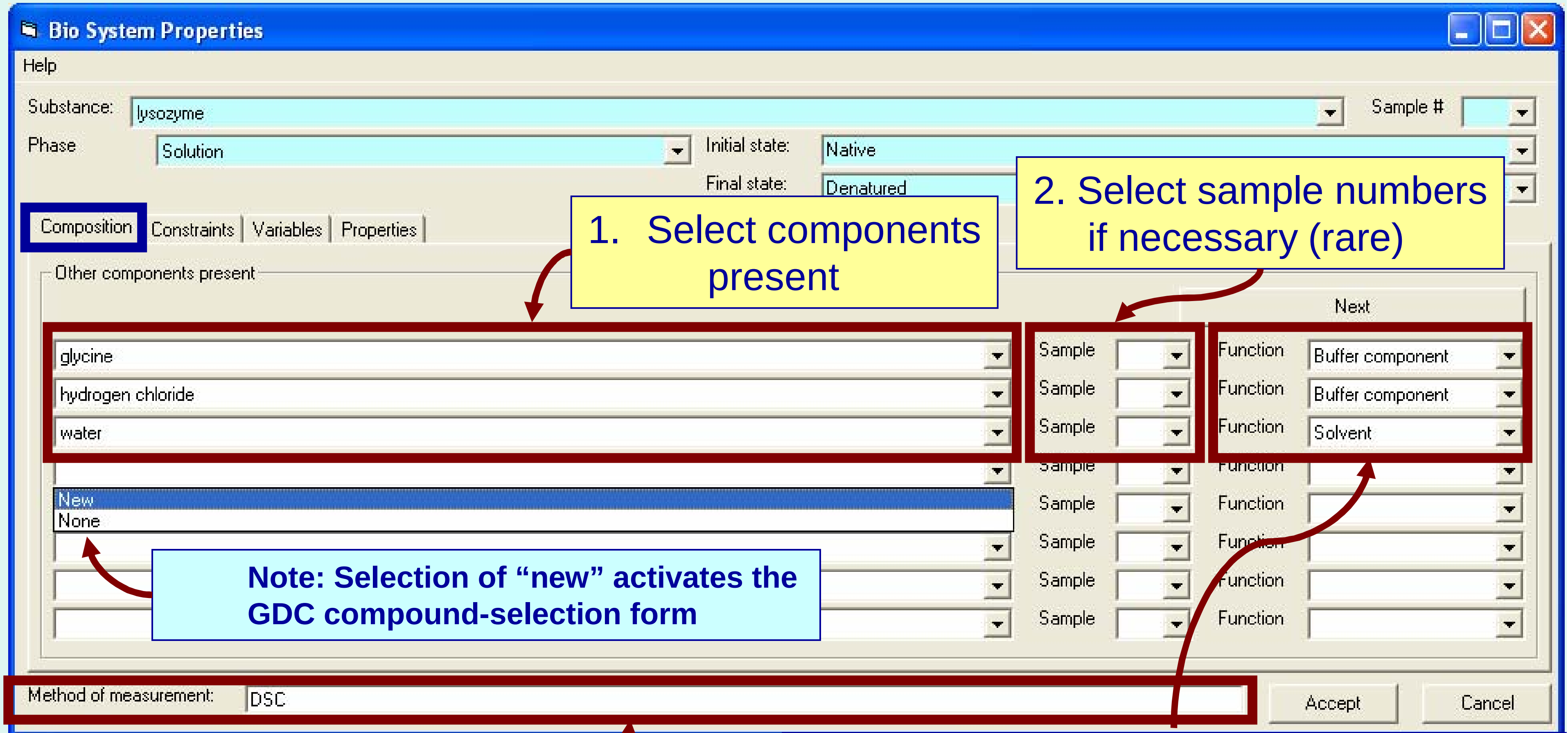


2. Select a Tab to access a form to specify:
    - The Environment (i.e., solution composition)
    - Constraints
    - Variables
    - Properties

Next…

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

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



1. Select components present

2. Select sample numbers if necessary (rare)

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

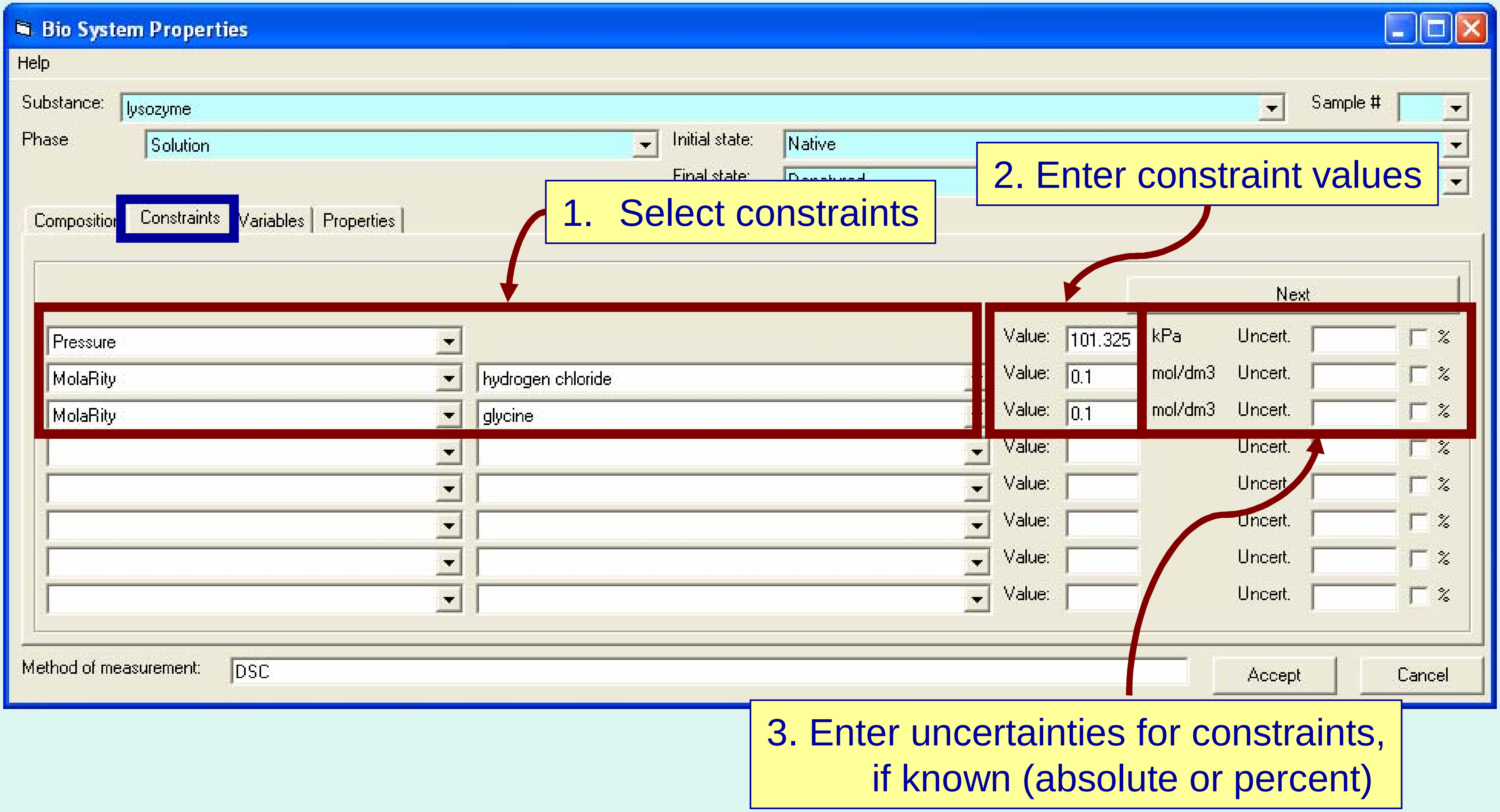
3. Select the “Function” of each component
   - Solvent
   - Buffer
   - Inert

4. Enter the measurement method

Next tab...

Constraints: Specification of fixed quantities

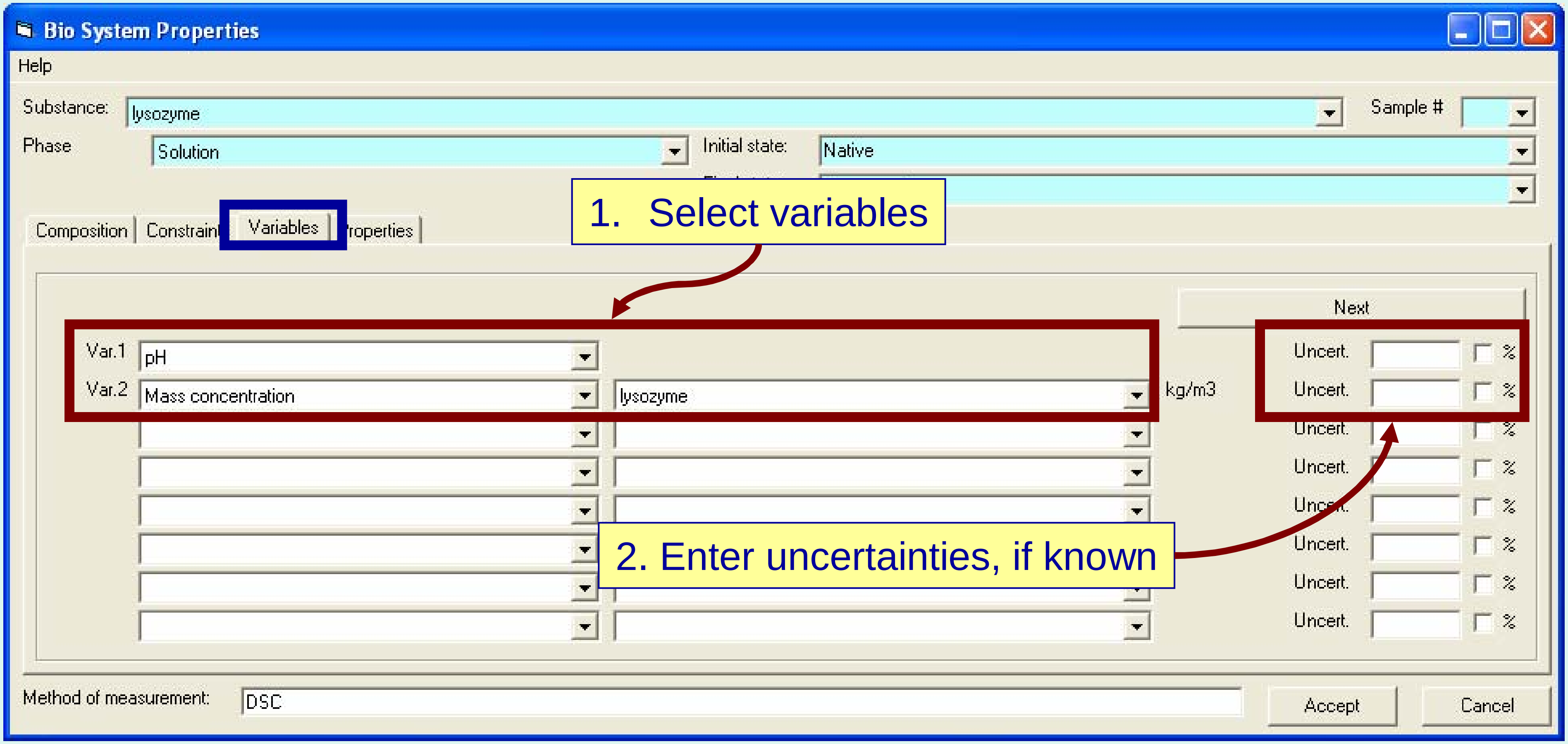
For the example, these are the pressure and buffer composition



Next tab…

Variables: Specification of quantities that are varied

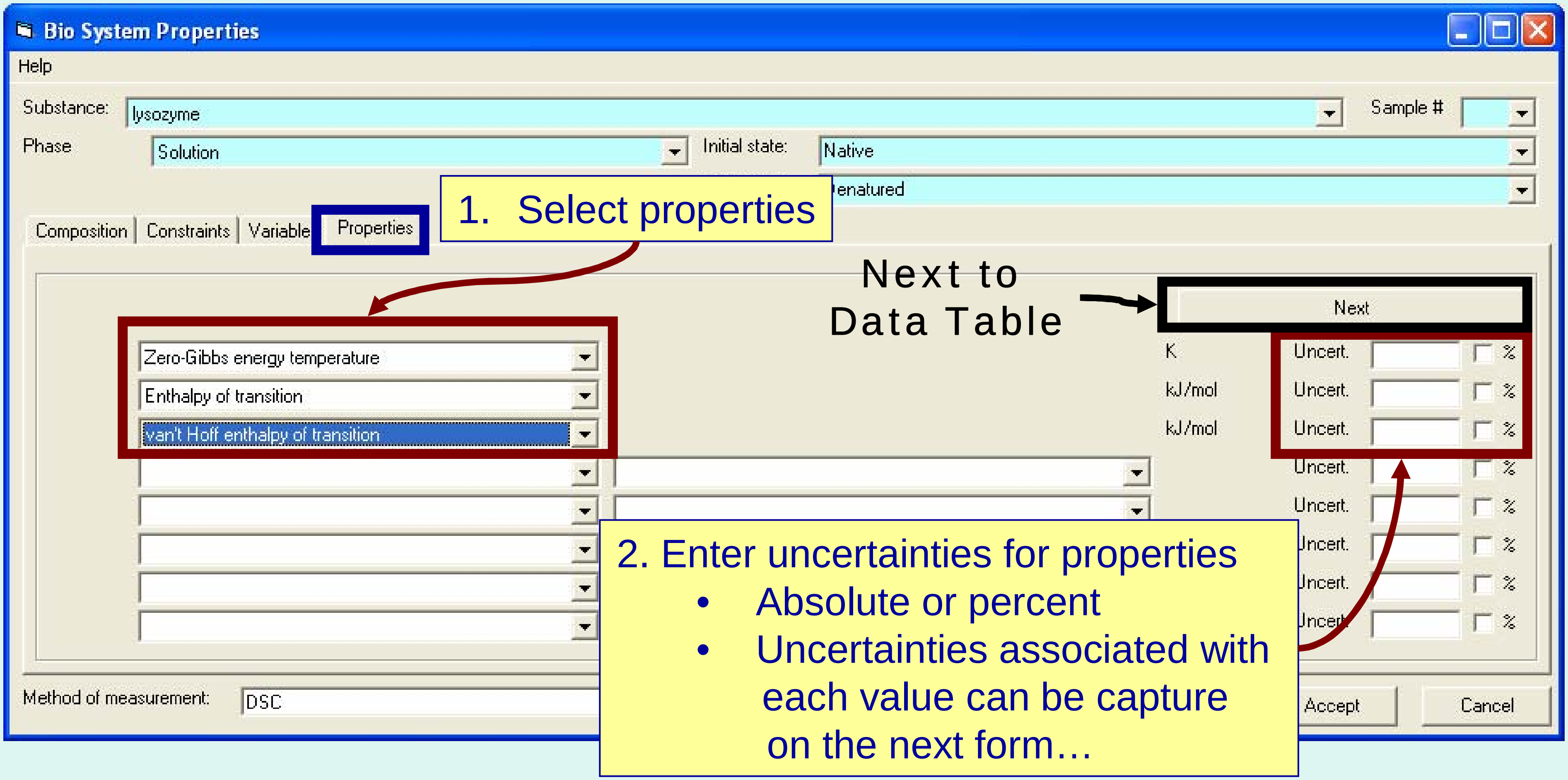
For the example, these are pH and concentration of lysozyme



Next tab...

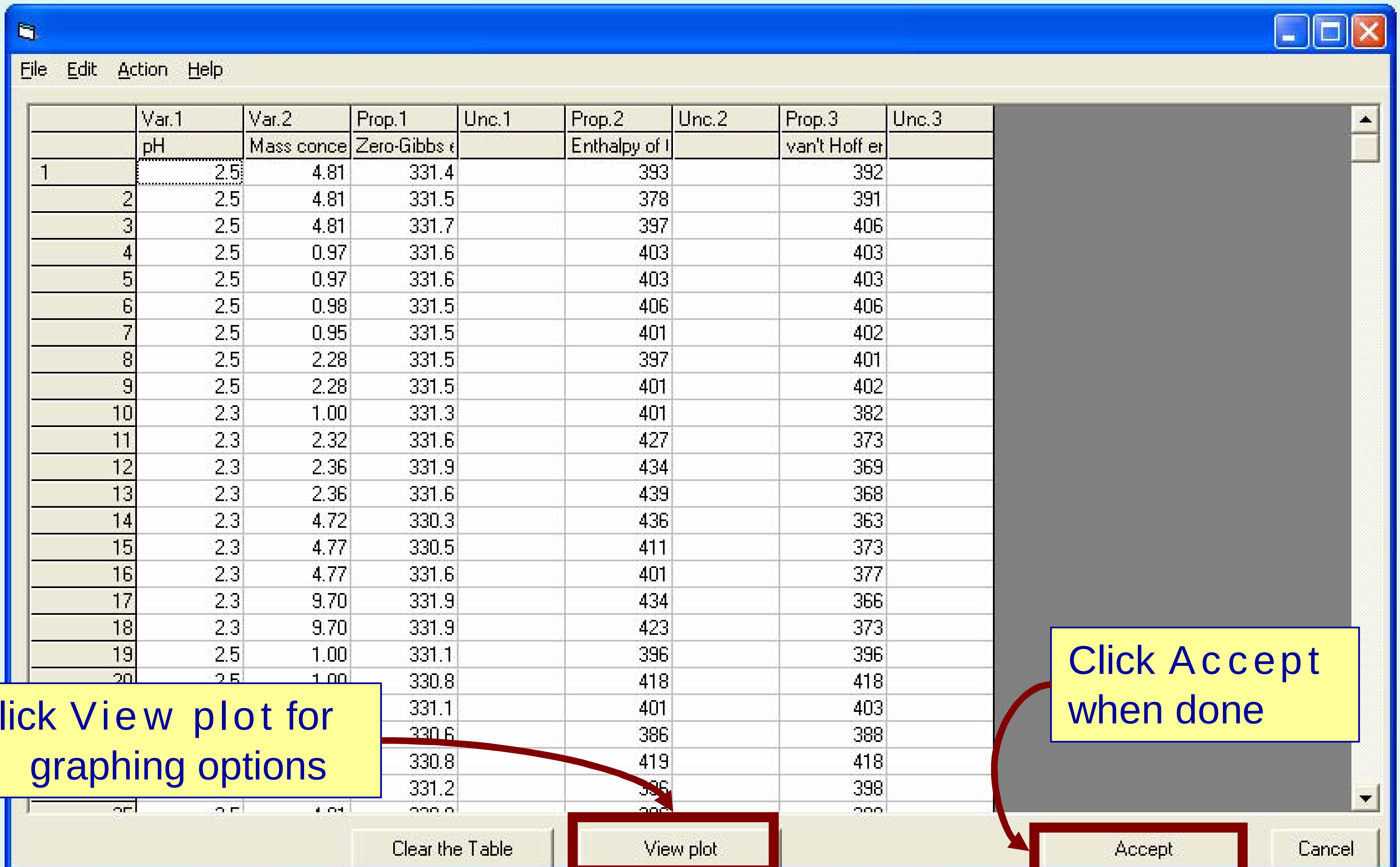
Properties: Specification of properties

For the example, these are pH and concentration of lysozyme



Numerical Data Table: Enter values for variables and properties

For the example:
Variables: pH, conc of lysozyme
Properties: T_G, $\Delta_{trs}H$, $\Delta_{trs}H_{vH}$



	Var.1	Var.2	Prop.1	Unc.1	Prop.2	Unc.2	Prop.3	Unc.3
	pH	Mass conce	Zero-Gibbs e		Enthalpy of t		van't Hoff er	
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	

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

File Edit Action Help

	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 transitio	
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	
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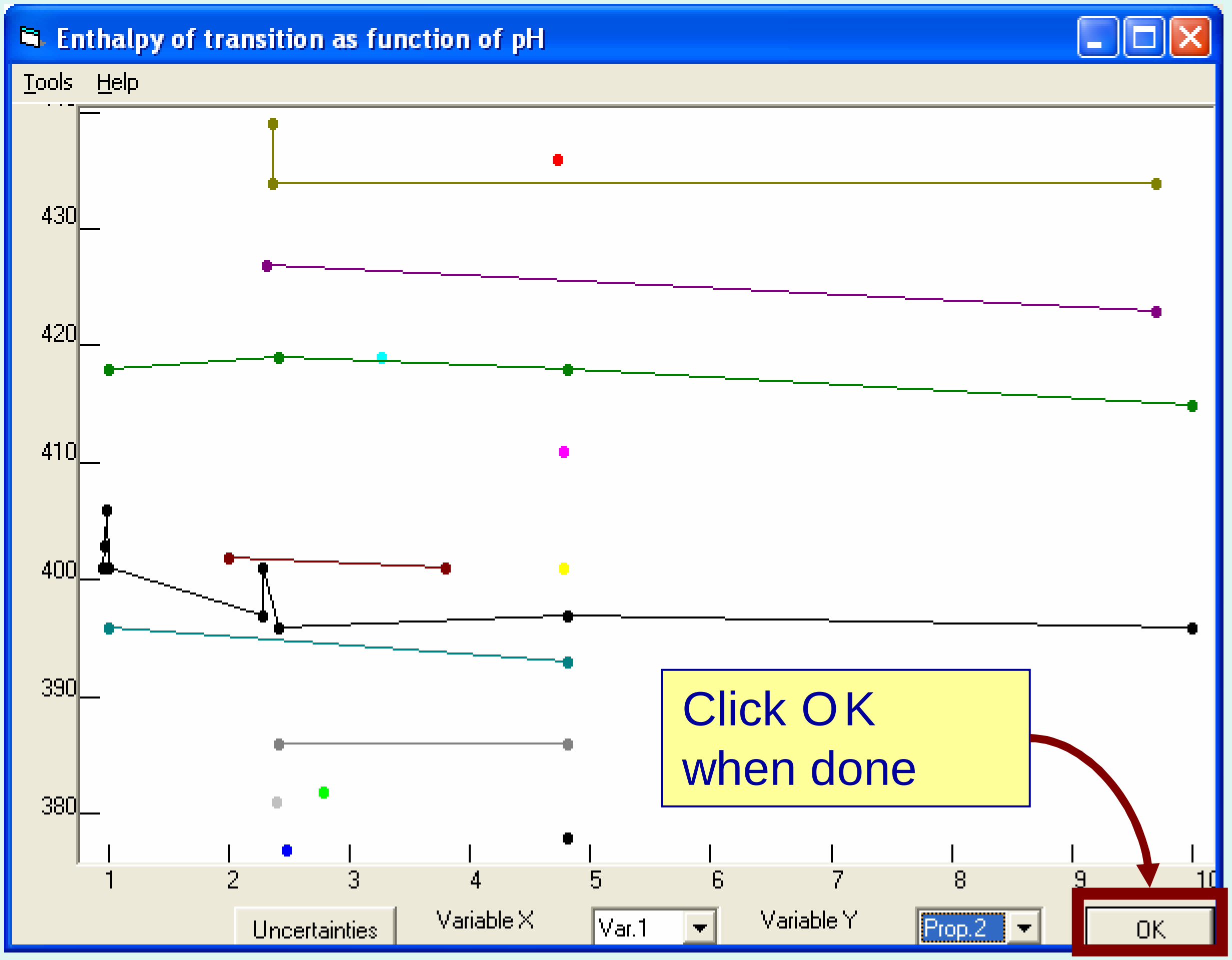
19	2.5	1.00	331.1		396		396	
20	2.5	1.00	330.8		418		418	
21	2.5	1.00	331.1		401		403	
22	2.5	2.41	330.6		386		388	
23	2.5	2.41	330.8		419		418	
24	2.5	2.41	331.2		396		398	

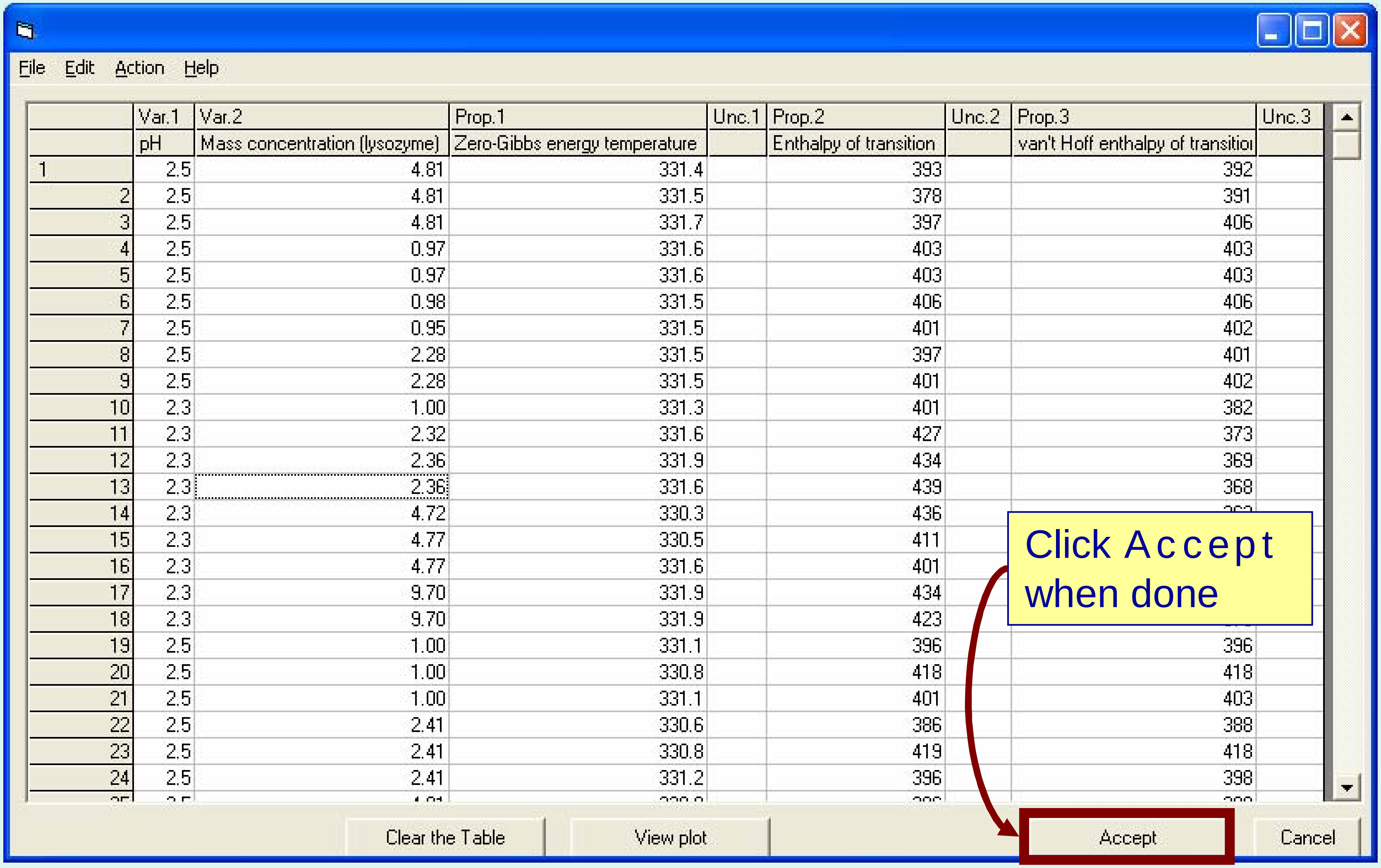
Clear the Table | View plot | Accept | Cancel

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



	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 transitioi	
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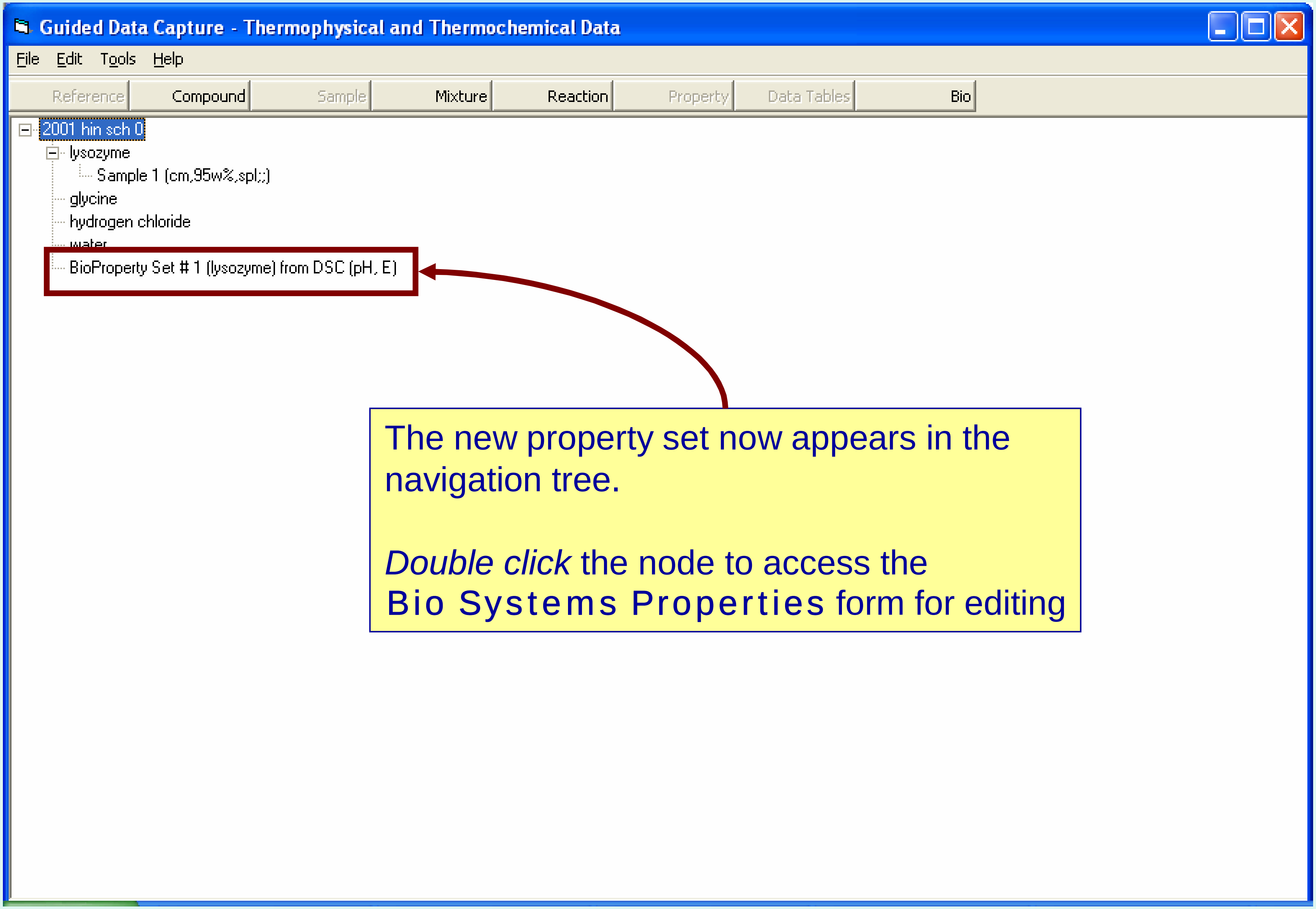
12	2.3	2.36	331.9		434		369	
13	2.3	2.36	331.6		439		368	
14	2.3	4.72	330.3		436		[illegible]	
15	2.3	4.77	330.5		411		[illegible]	
16	2.3	4.77	331.6		401		[illegible]	
17	2.3	9.70	331.9		434		[illegible]	
18	2.3	9.70	331.9		423		[illegible]	
19	2.5	1.00	331.1		396		396	
20	2.5	1.00	330.8		418		418	
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	

Property capture is complete…



The new property set now appears in the navigation tree.

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