BIOTHERMODYNAMIC DATA CAPTURE

Example: Properties of Enzyme Catalyzed Reactions

Data source: Tewari, Y.B.; Chen, J.; Holden, M.J.; Houk, K.N.; Goldberg, R.N.; *J. Phys. Chem. B*, **1998**, *102*, 8634-8639.

General Experiment Description: Calorimetric determination of reaction enthalpy for the given reaction in the presence of an enzyme catalyst at specified pH and ionic strength

Target Properties for the example: Enthalpy of reaction

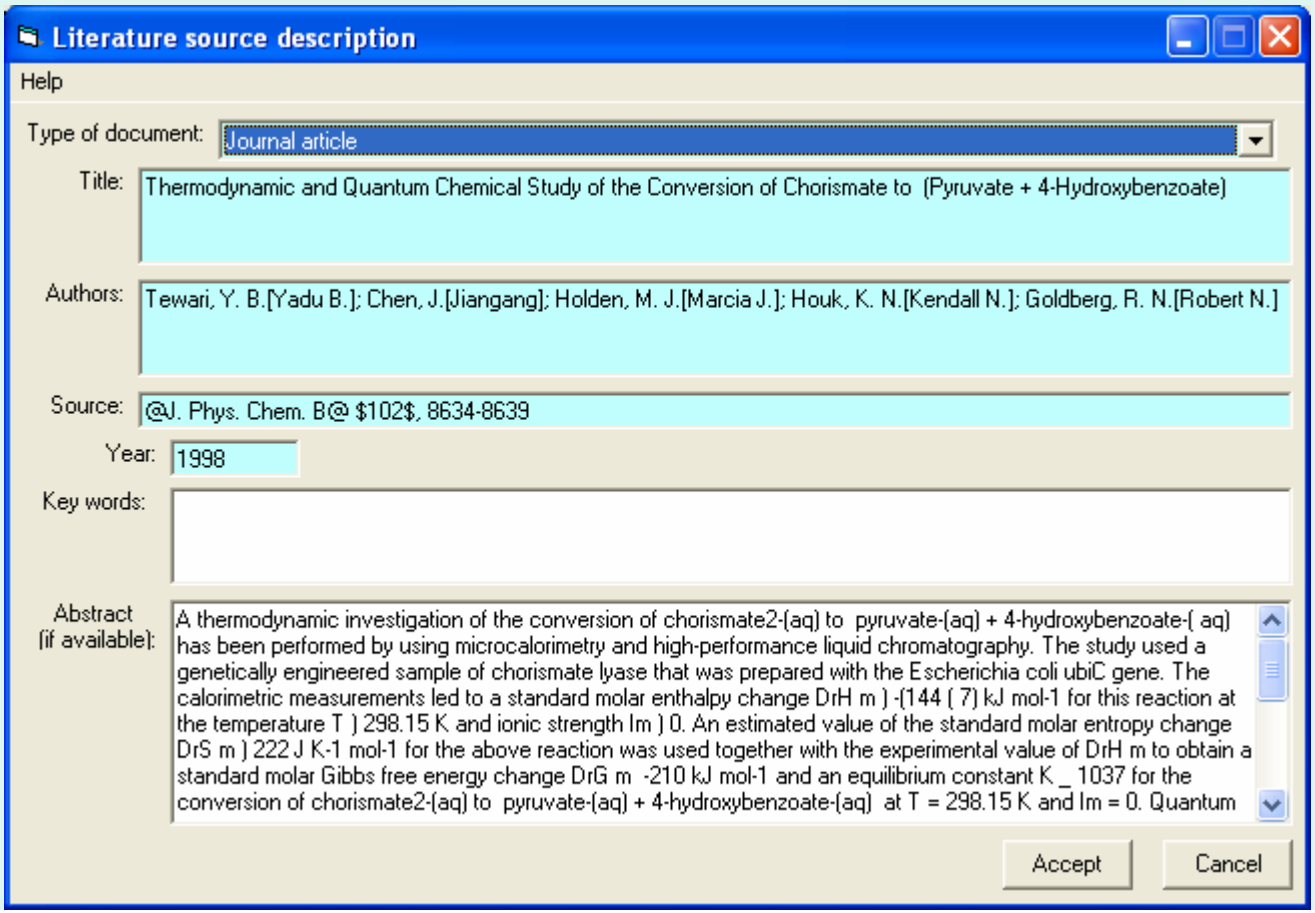
Note: *Multiple properties are reported in the article. In order to keep the example simple, only one property is captured. Capture of other properties is completely analogous.*

Bibliographic information:

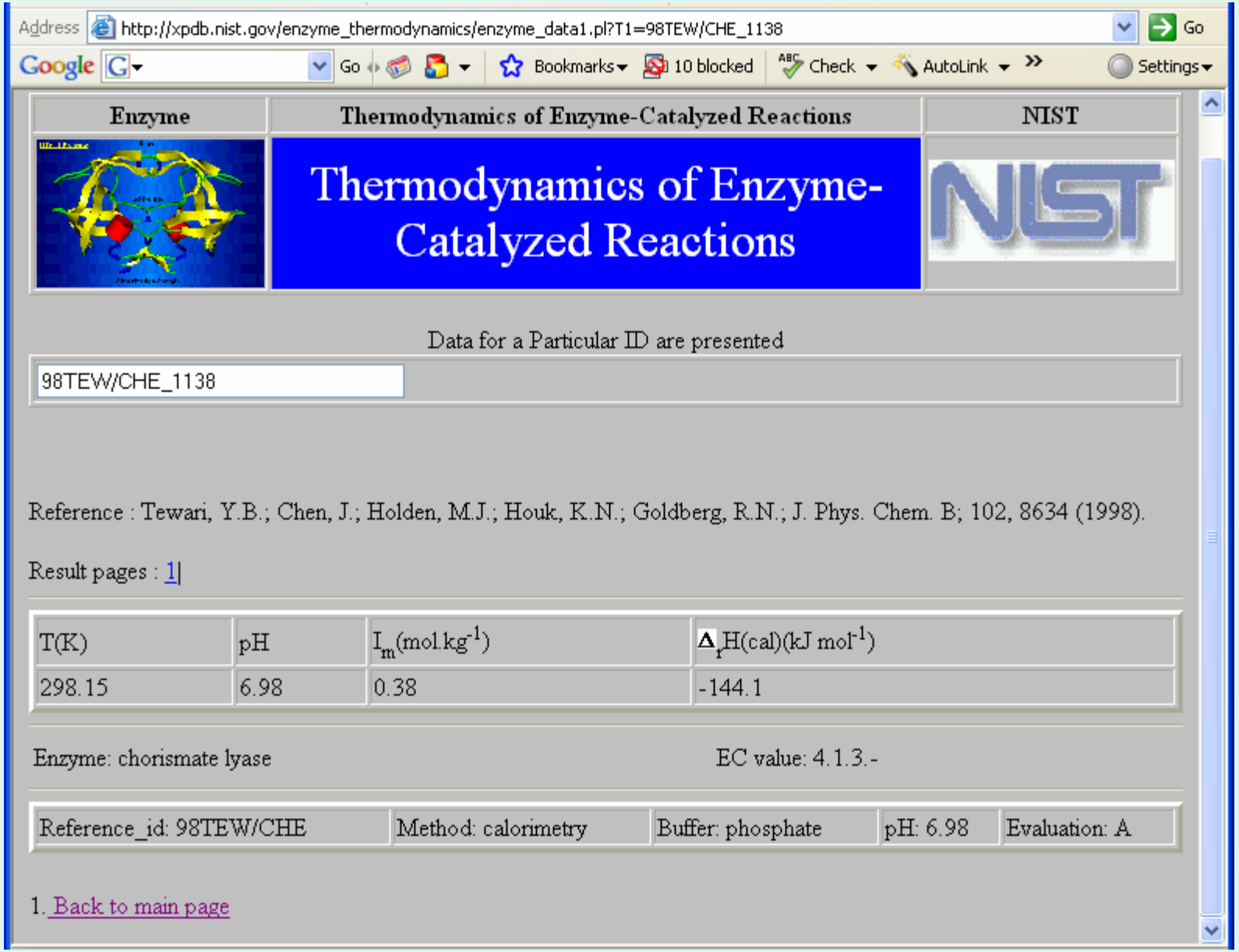
No new additions were made to GDC for biothermodynamic data.

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 captured enthalpy of reaction value and variables were taken from the *NIST Thermodynamics of Enzyme Catalyzed Reactions Database* as shown here…



Address http://xpdb.nist.gov/enzyme_thermodynamics/enzyme_data1.pl?T1=98TEW/CHE_1138 Go

Google Go Bookmarks 10 blocked Check AutoLink Settings

Enzyme	Thermodynamics of Enzyme-Catalyzed Reactions	NIST

Thermodynamics of Enzyme-Catalyzed Reactions

Data for a Particular ID are presented

98TEW/CHE_1138

Reference : Tewari, Y.B.; Chen, J.; Holden, M.J.; Houk, K.N.; Goldberg, R.N.; J. Phys. Chem. B; 102, 8634 (1998).

Result pages : 1

T(K)	pH	I_m(mol.kg^{-1})	Δ_rH(cal)(kJ mol^{-1})
298.15	6.98	0.38	-144.1

Enzyme: chorismate lyase EC value: 4.1.3.-

Reference_id: 98TEW/CHE	Method: calorimetry	Buffer: phosphate	pH: 6.98	Evaluation: A

1. Back to main page

Compound Selection/Addition:

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

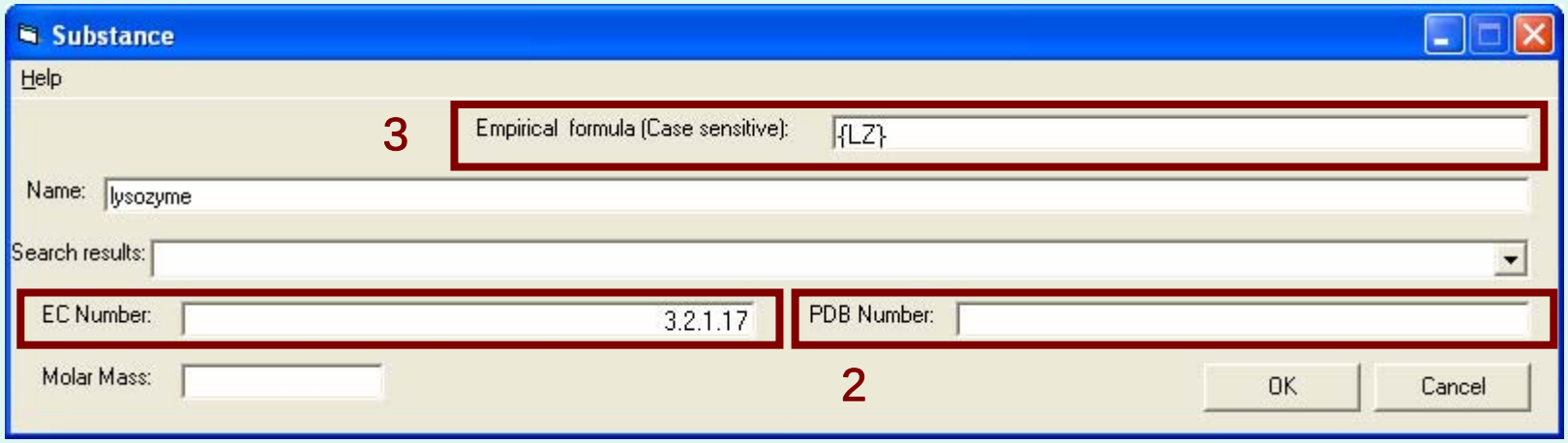
See: http://www.trc.nist.gov/helpdocs/basic/COMPOUNDselection.pdf

and

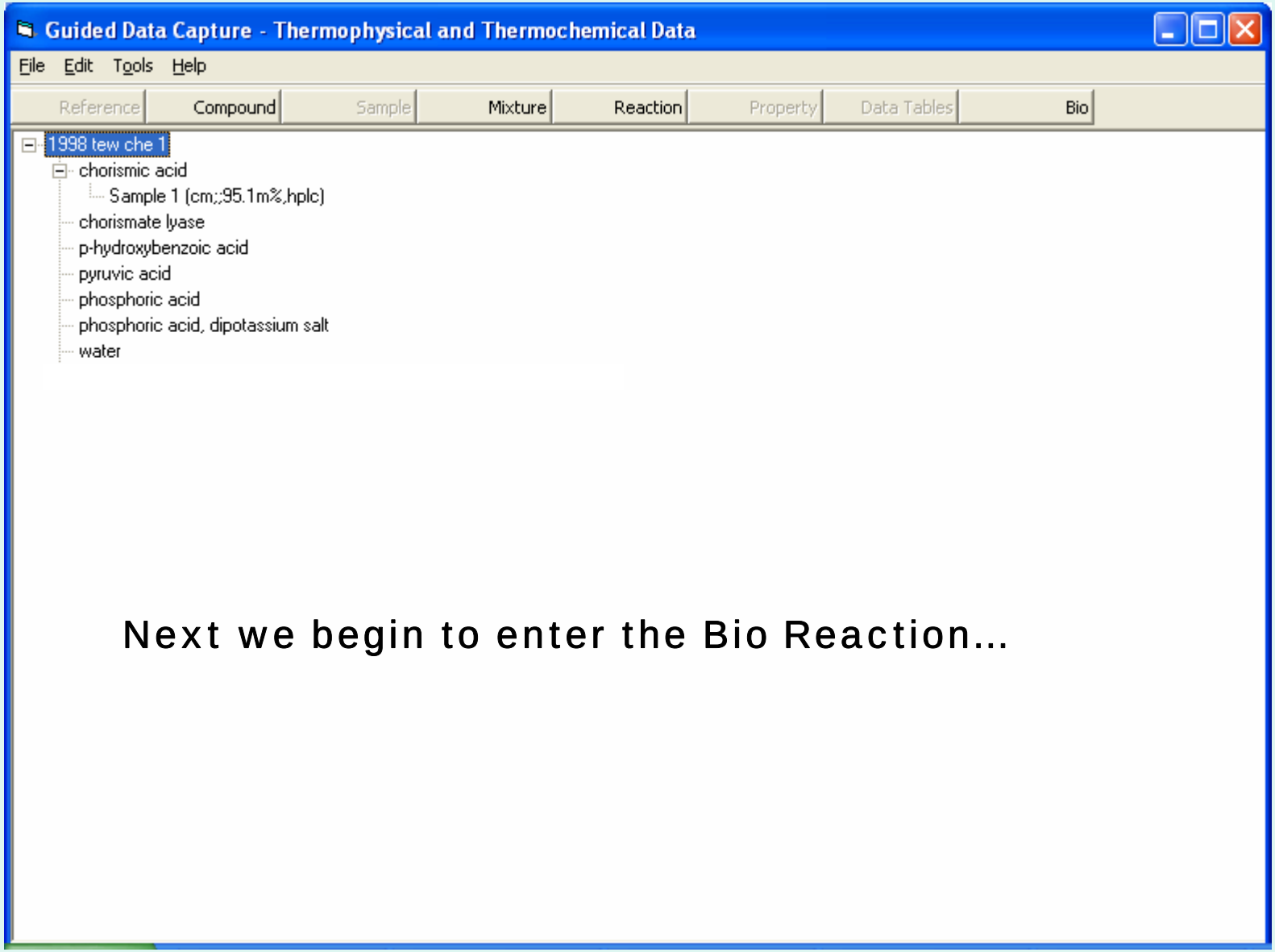
See: http://www.trc.nist.gov/helpdocs/basic/COMPOUNDaddition.pdf

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**

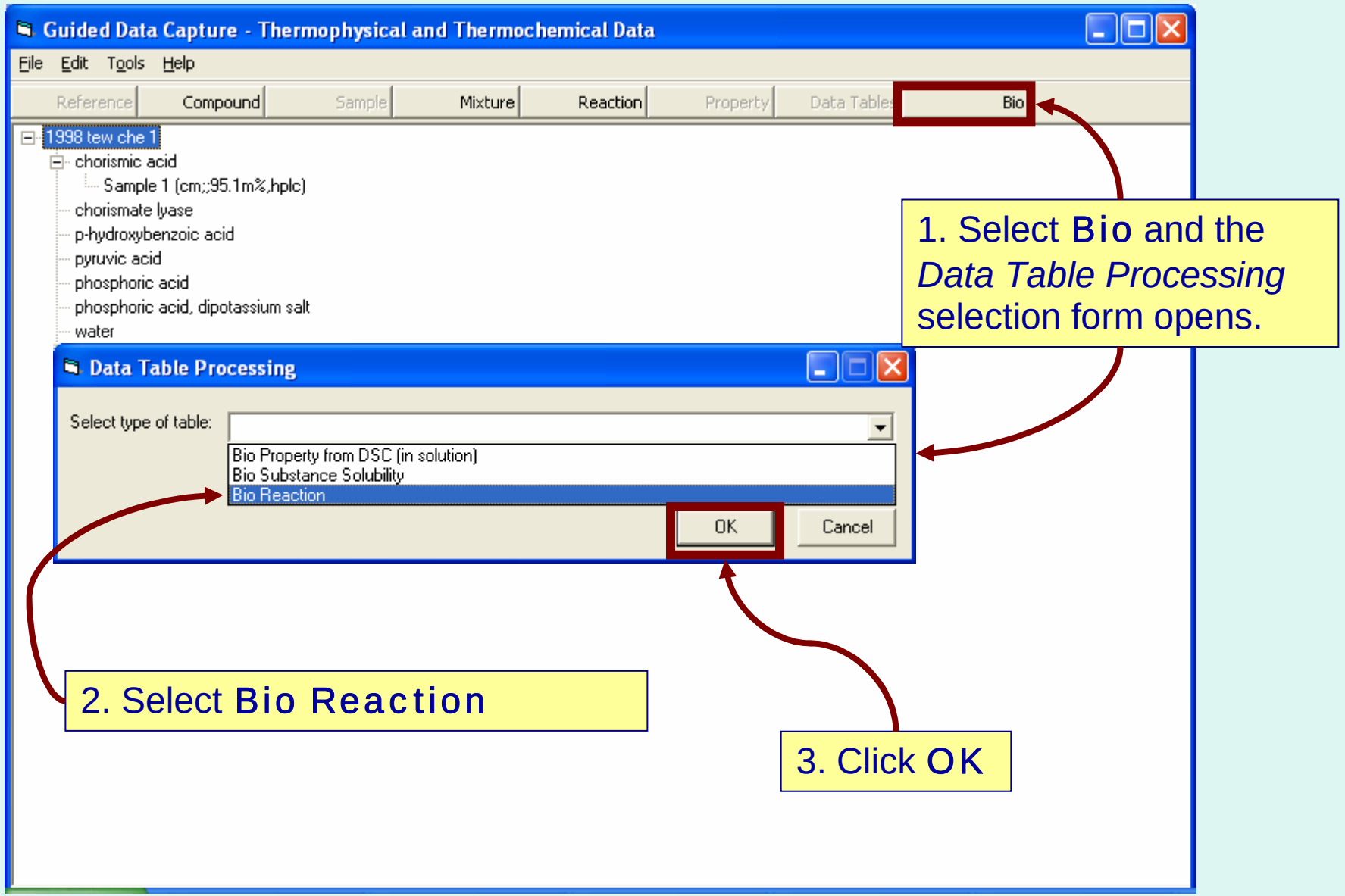


After capture of bibliographic info and specification of the reaction components, the Main GDC form looks like this…



Next we begin to enter the Bio Reaction...

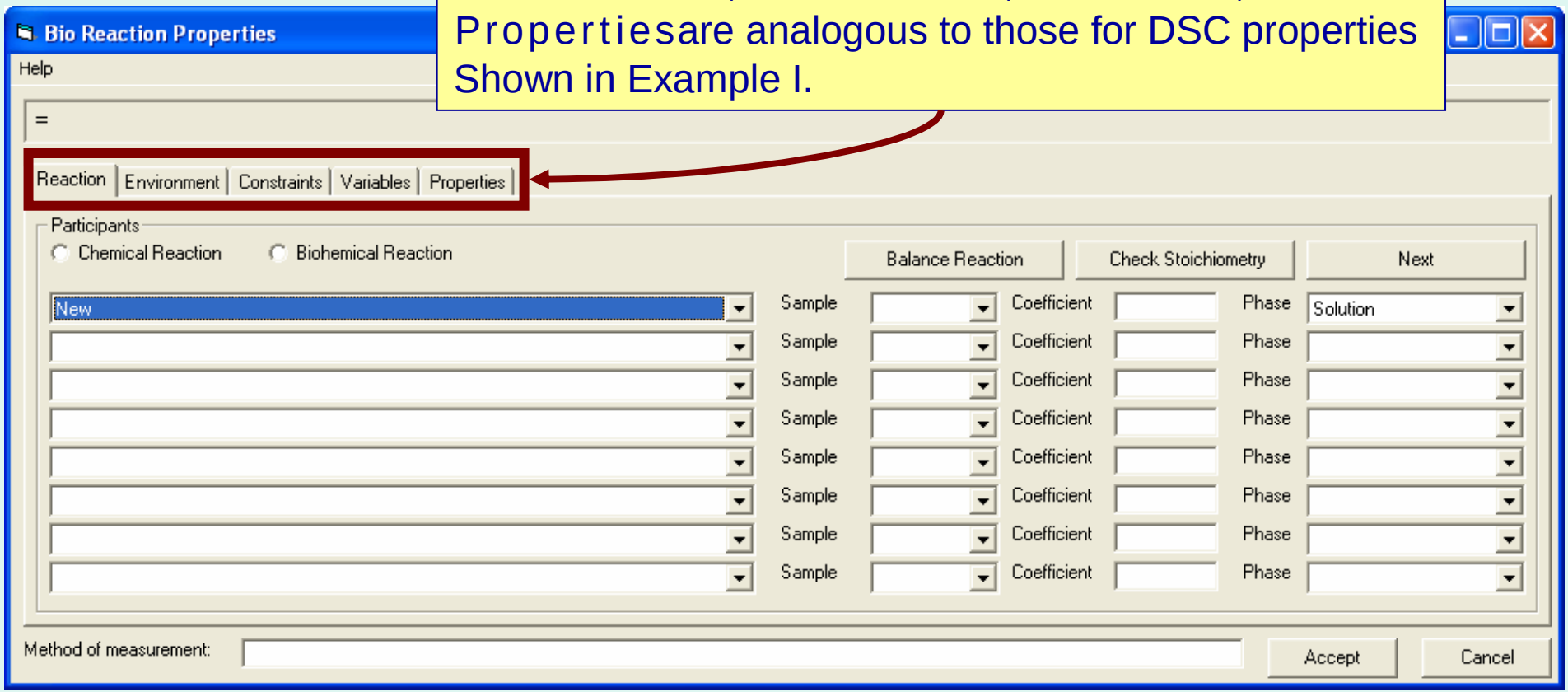
Initiation of Bio Reaction property capture…



Next…

The Bio Reaction Properties form appears...

Tabs to navigate between forms for the **Reaction**, Environment, Constraints, Variables, and Propertiesare analogous to those for DSC properties Shown in Example I.



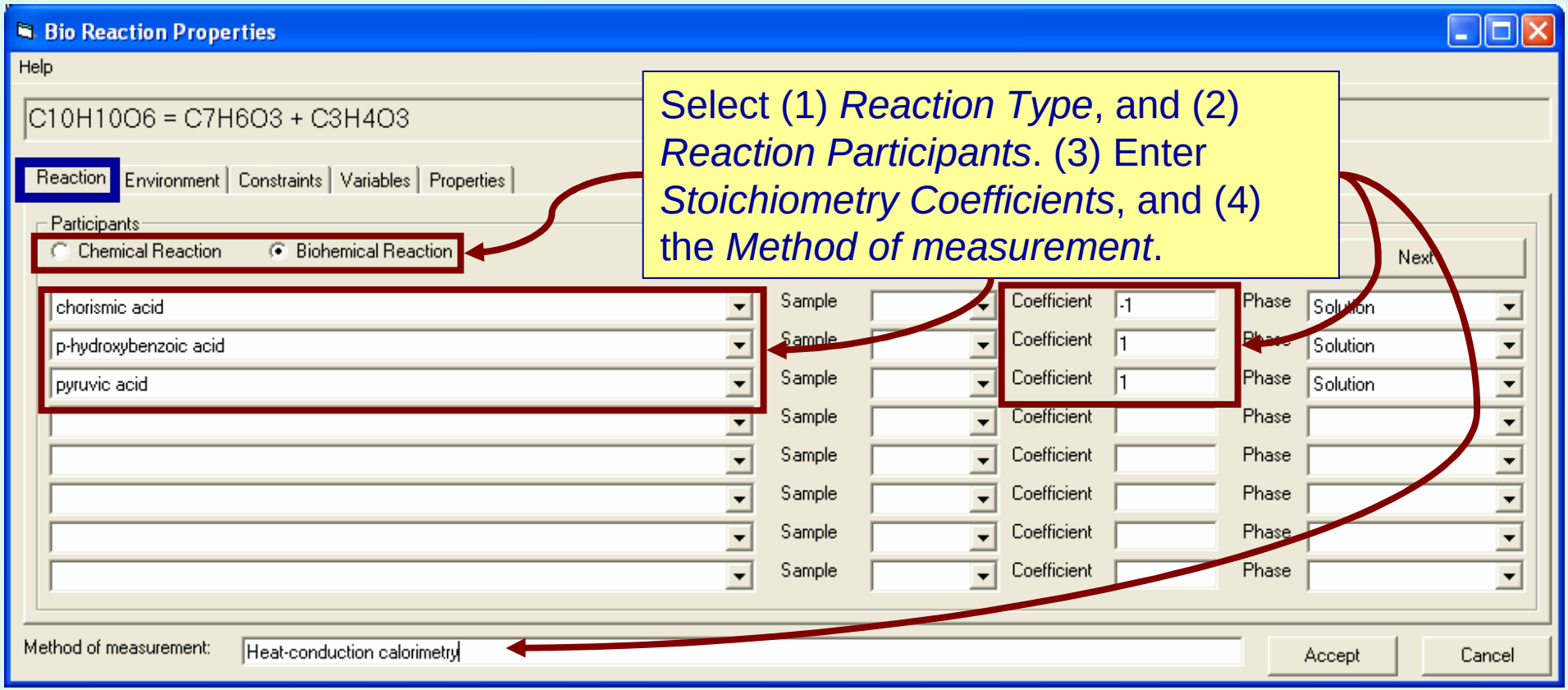
Define the Reaction:

Note: The reaction is defined as equation (1) on the first page of the article:

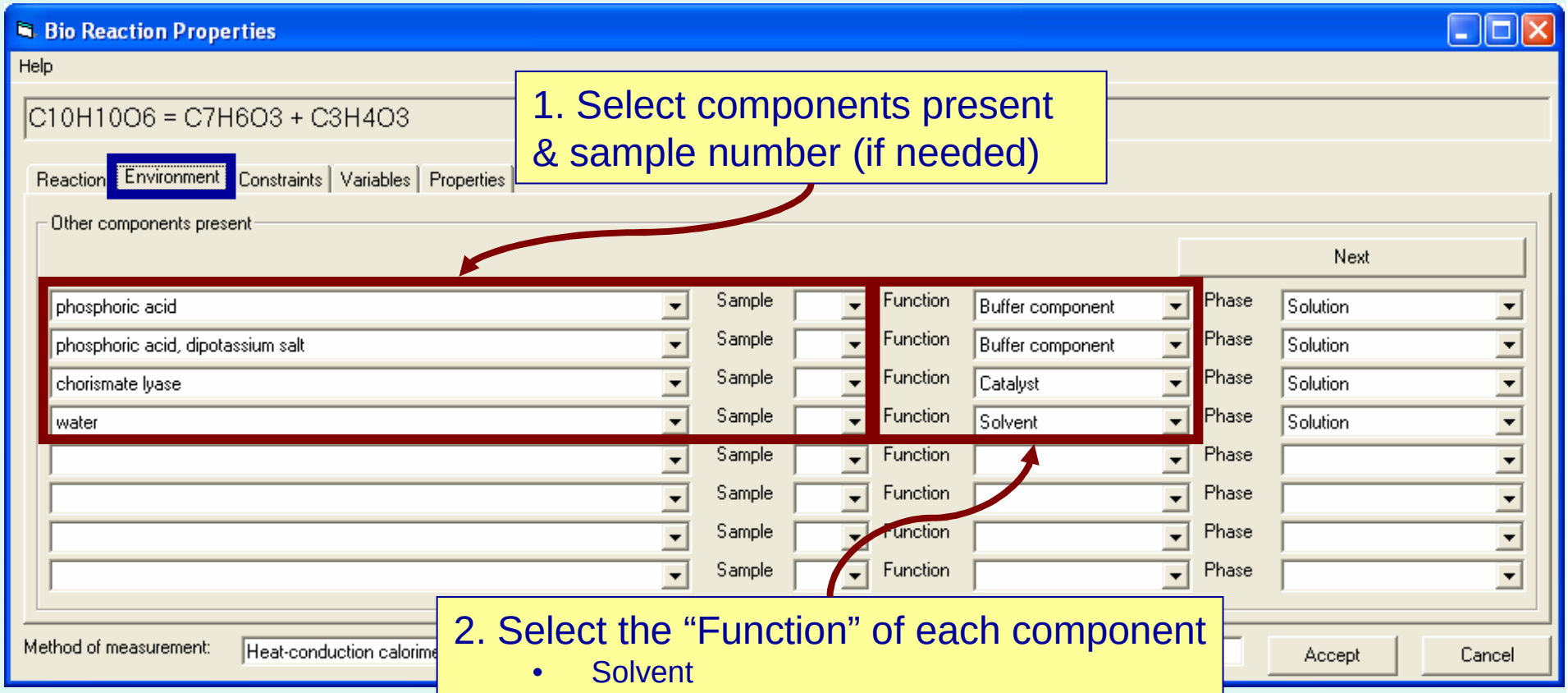
chorismate(aq) = 4-hydroxybenzoate(aq) + pyruvate(aq)

This is a ***biochemical*** reaction, where the components represent all forms (neutral, bound with a counterion, or dissociated)

Ions are not represented in *GDC* at this time, so the participants are shown in their acid forms for balancing of the reaction.



Define the Environment:

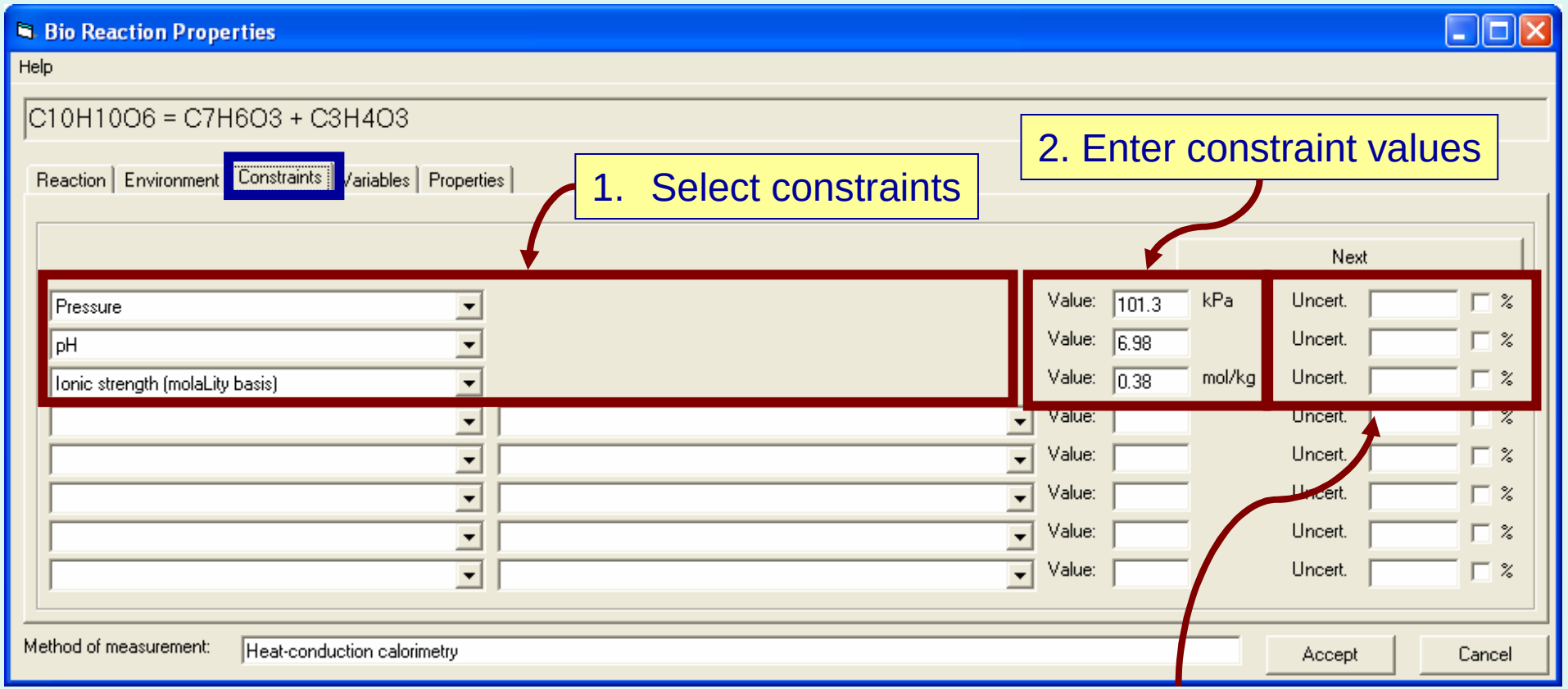


1. Select components present & sample number (if needed)

2. Select the "Function" of each component
   - Solvent
   - Buffer component
   - Catalyst
   - Cofactor
   - Inert

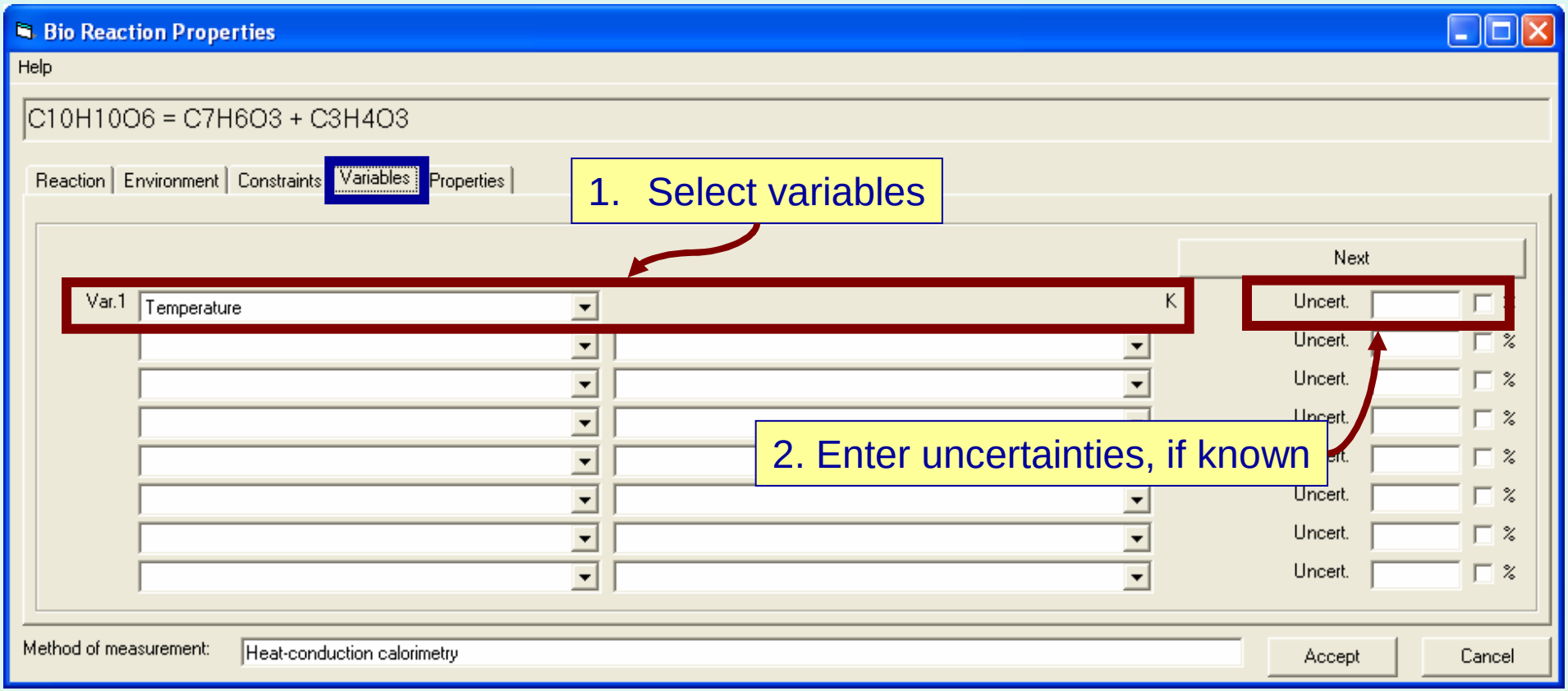
Next...

Define the Constraints:



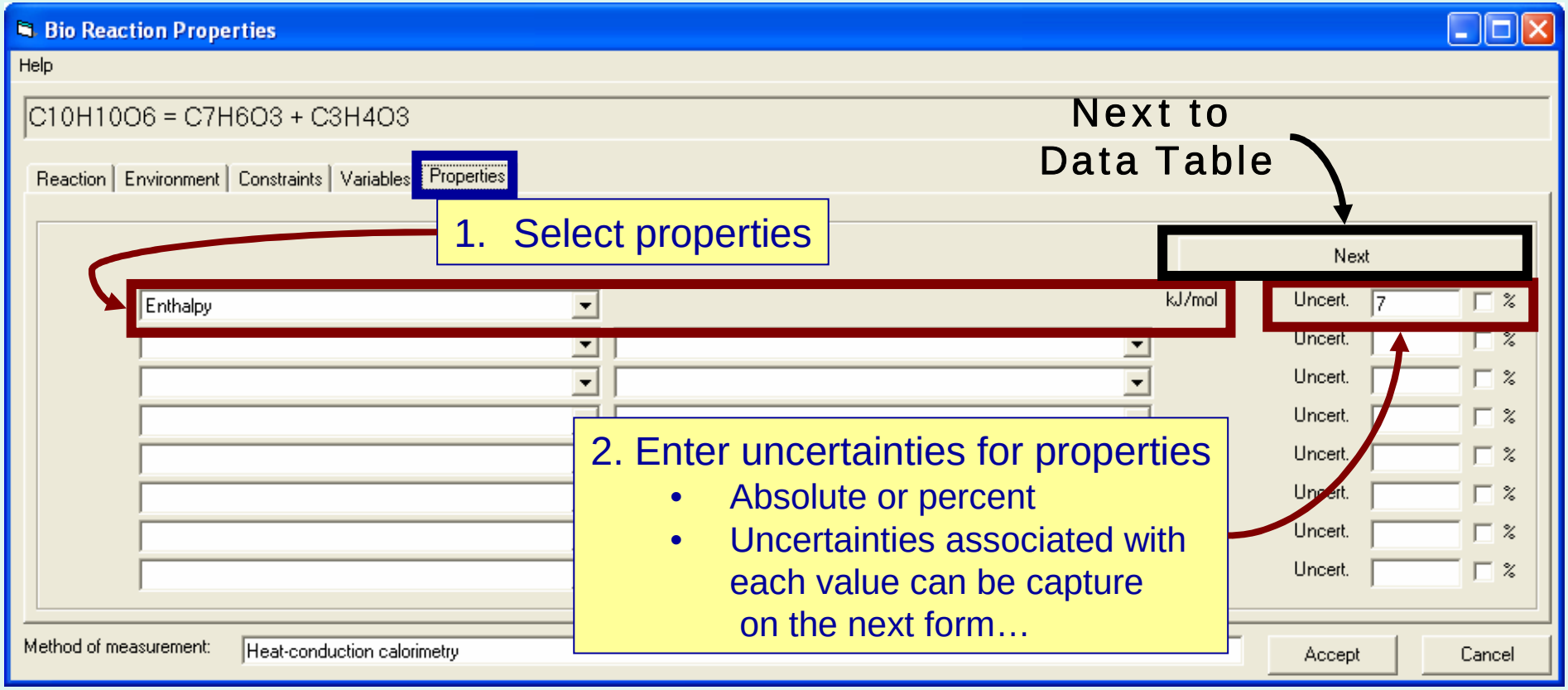
Next tab...

Define the Variables:

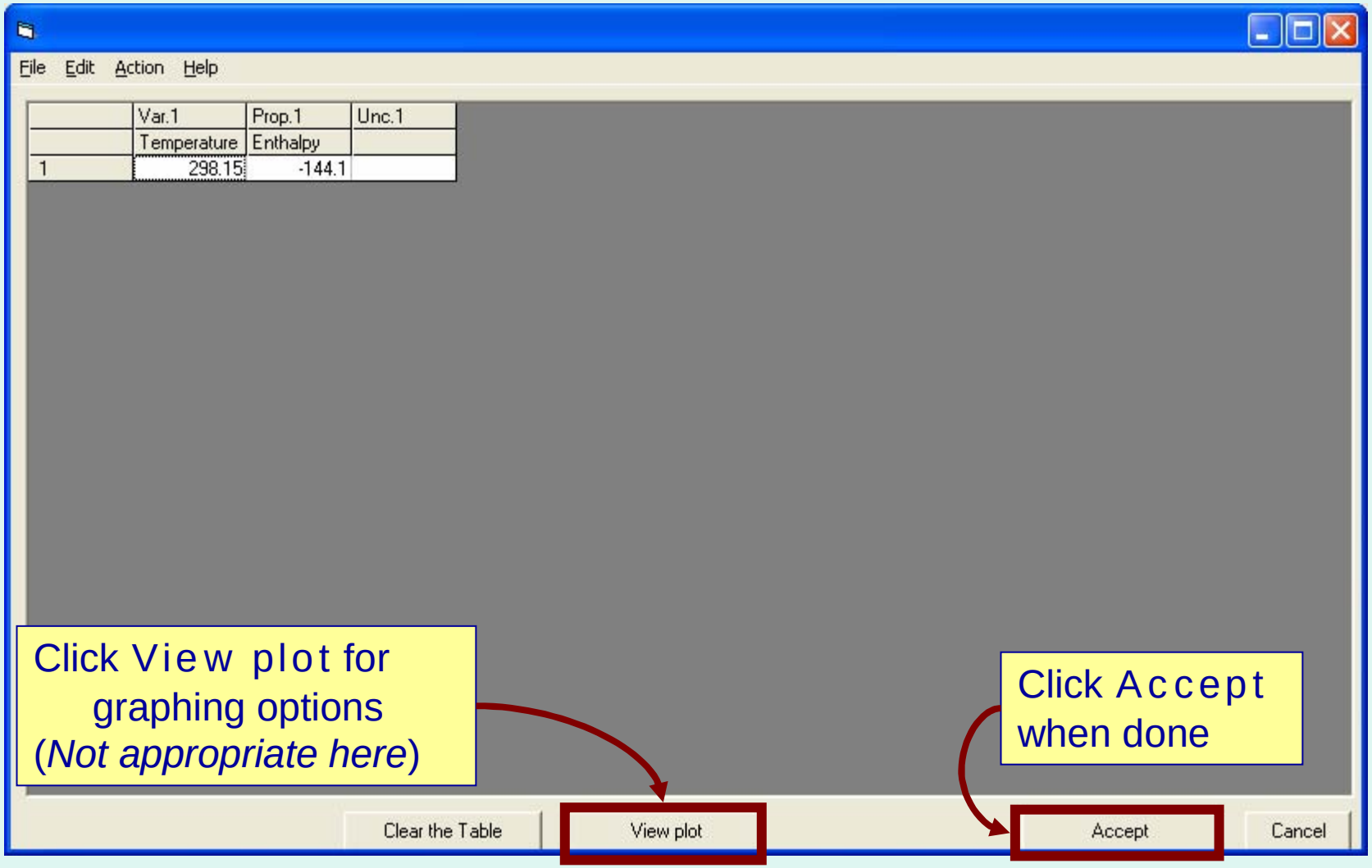


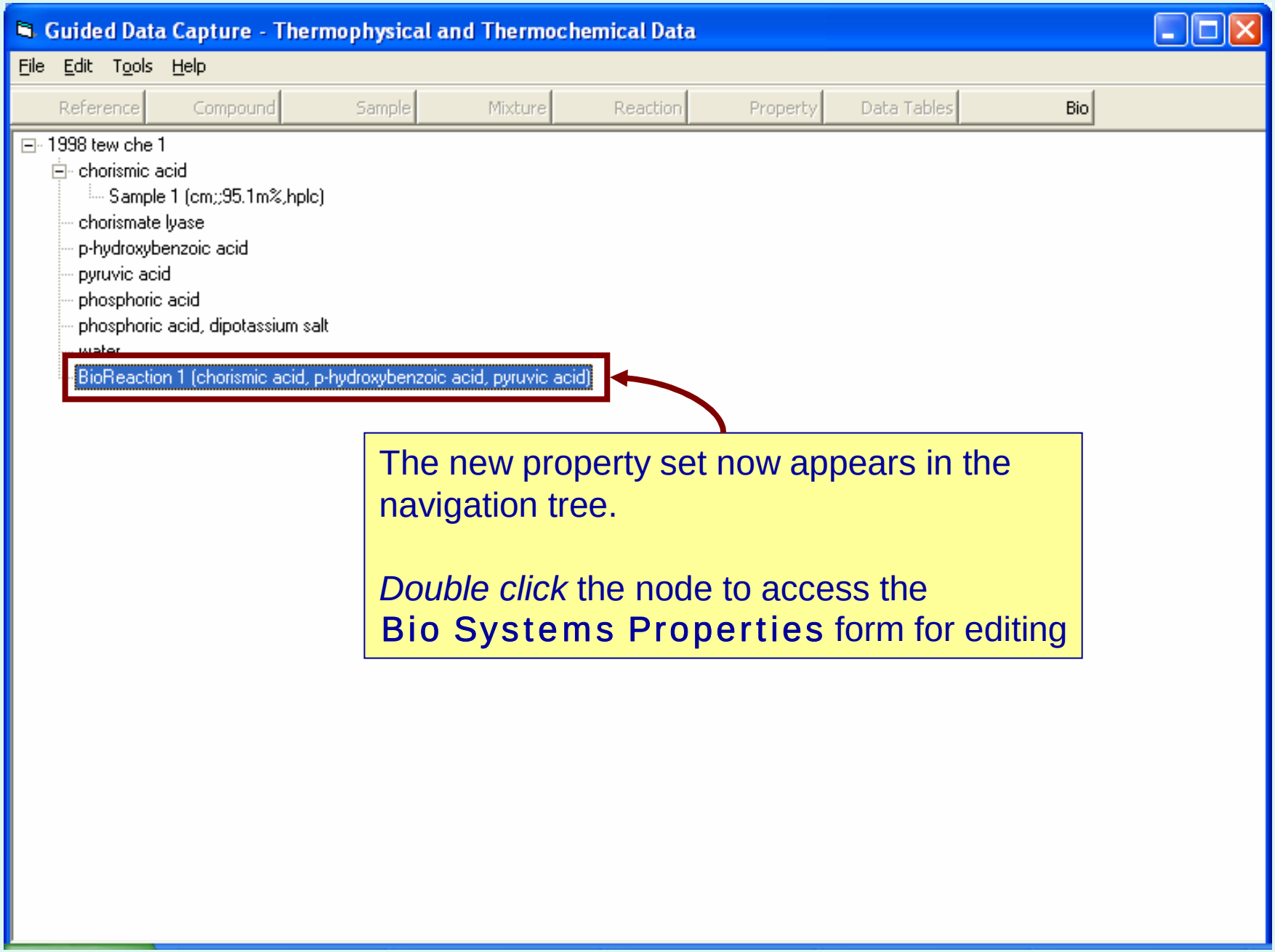
Next tab...

Define the Properties:



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




Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction Property Data Tables Bio
1998 tew che 1
chorismic acid
Sample 1 (cm;;95.1m%,hplc)
chorismate lyase
p-hydroxybenzoic acid
pyruvic acid
phosphoric acid
phosphoric acid, dipotassium salt
water
BioReaction 1 (chorismic acid, p-hydroxybenzoic acid, pyruvic acid)
The new property set now appears in the navigation tree.
Double click the node to access the **Bio Systems Properties** form for editing