BIOTHERMODYNAMIC DATA CAPTURE

Example: Results from Titration Calorimetry (Binding Properties)

Data source: Todorova, N. A.; Schwarz, F. P. *J. Chem. Thermodyn.*, **2007**, *39*, 1038-1048.

General Experiment Description: Drug binding properties for beta-cyclodextrin to NAB (nabumetone) derived from titration calorimetry

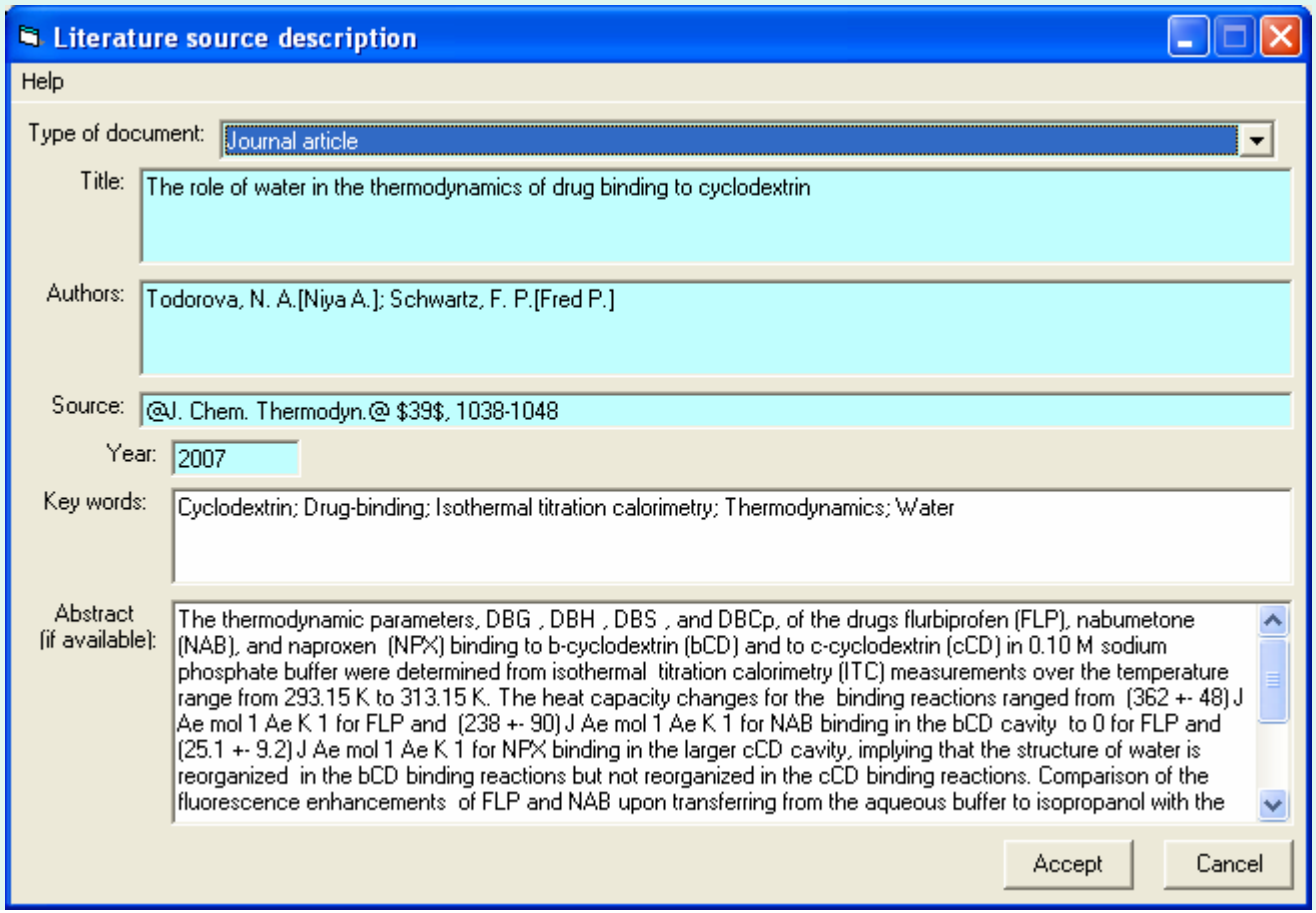
Target Properties for the example: equilibrium constant, Gibbs energy, enthalpy, and entropy for the binding reaction

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.

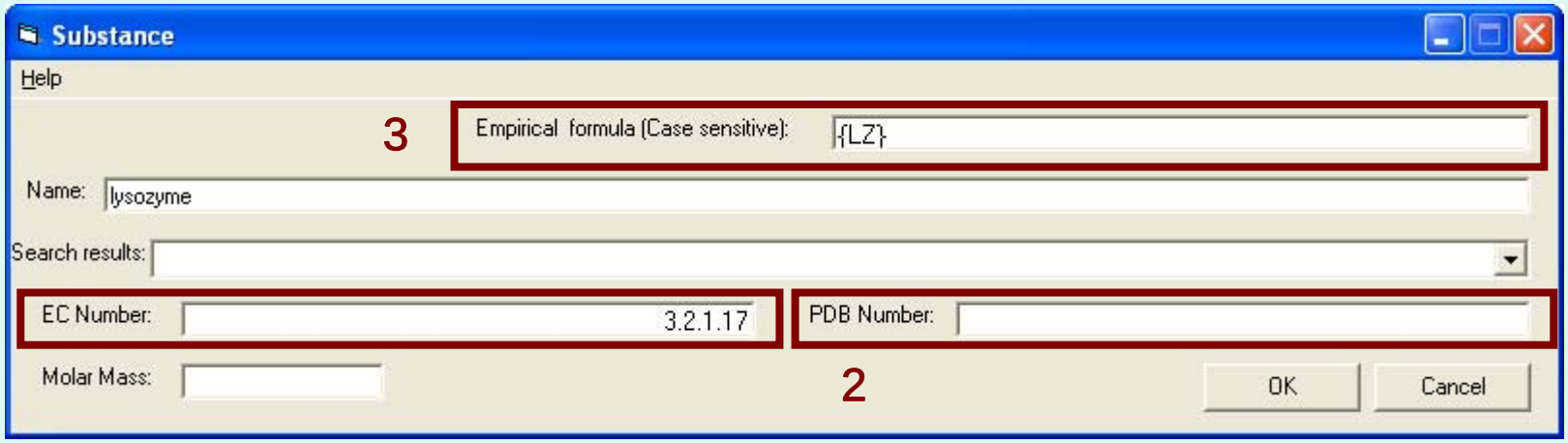
See: http://www.trc.nist.gov/helpdocs/basic/COMPOUNDselection.pdf

and

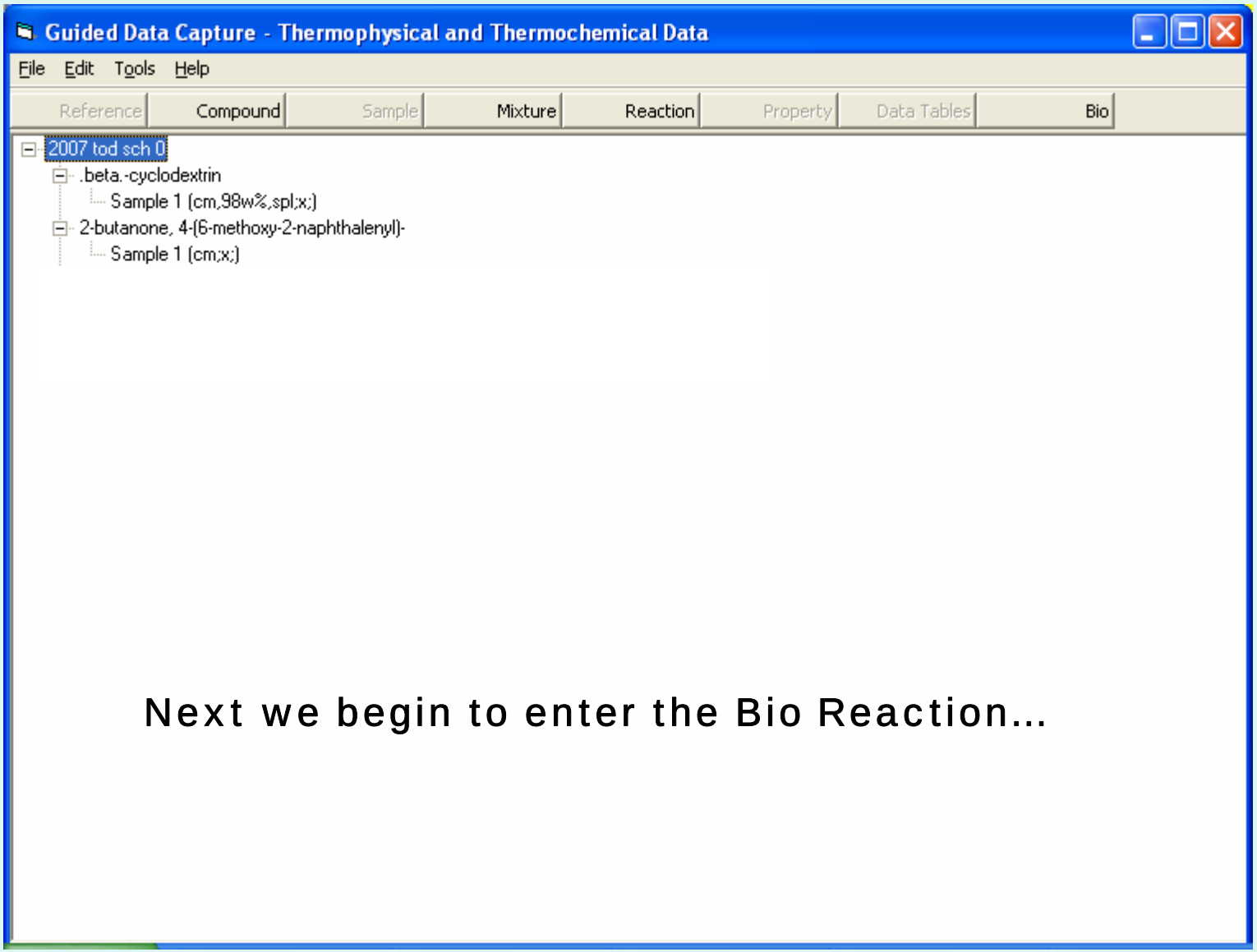
See: http://www.trc.nist.gov/helpdocs/basic/COMPOUNDaddition.pdf

New Features:

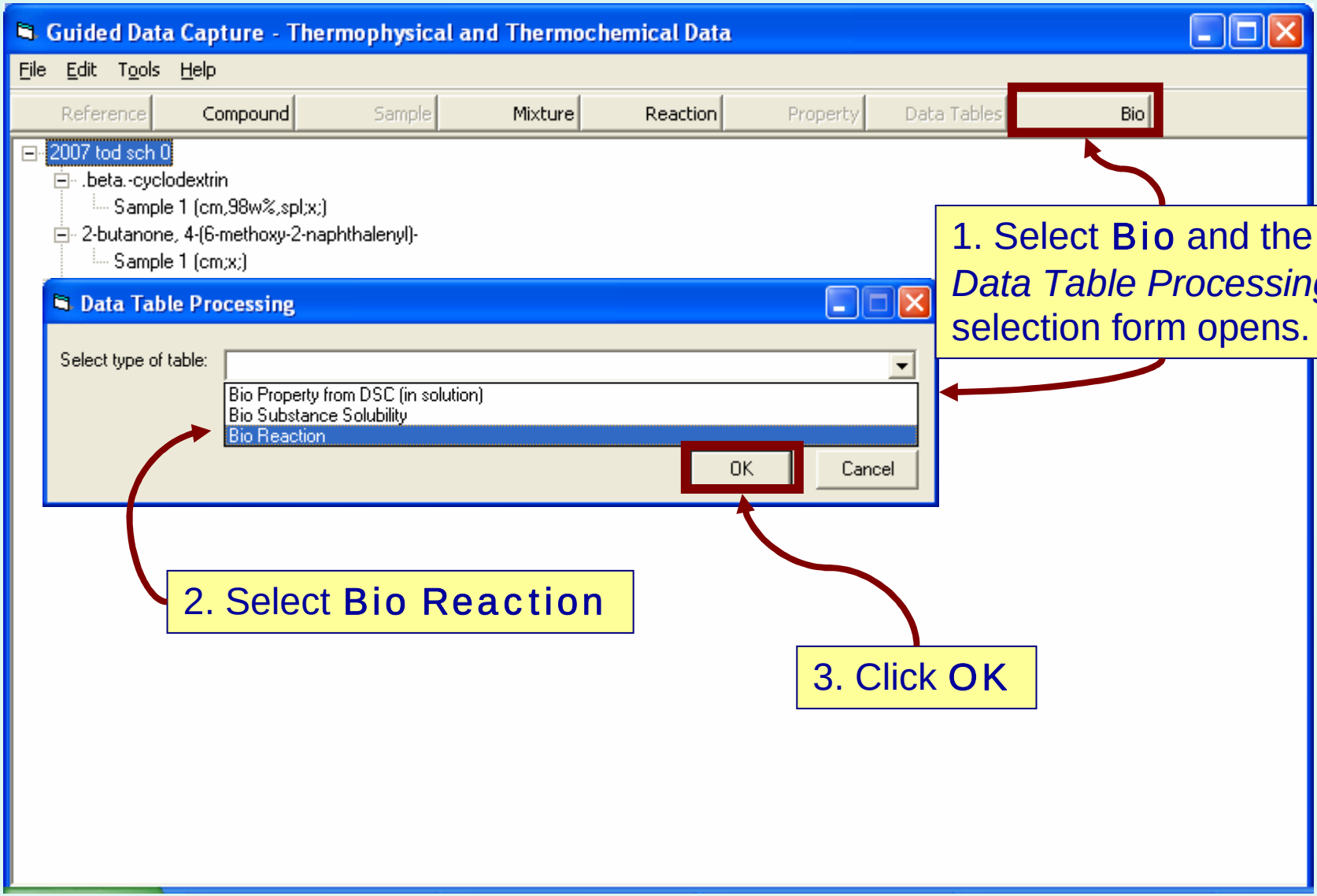
1. **Capture of EC (*Enzyme Commision*) Number is supported**
2. **Capture of PDB (*Protein Data Bank*) Number is supported**
3. **Symbolic formulas are supported (in brackets {*}) to support substances of unspecified empirical formula**



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



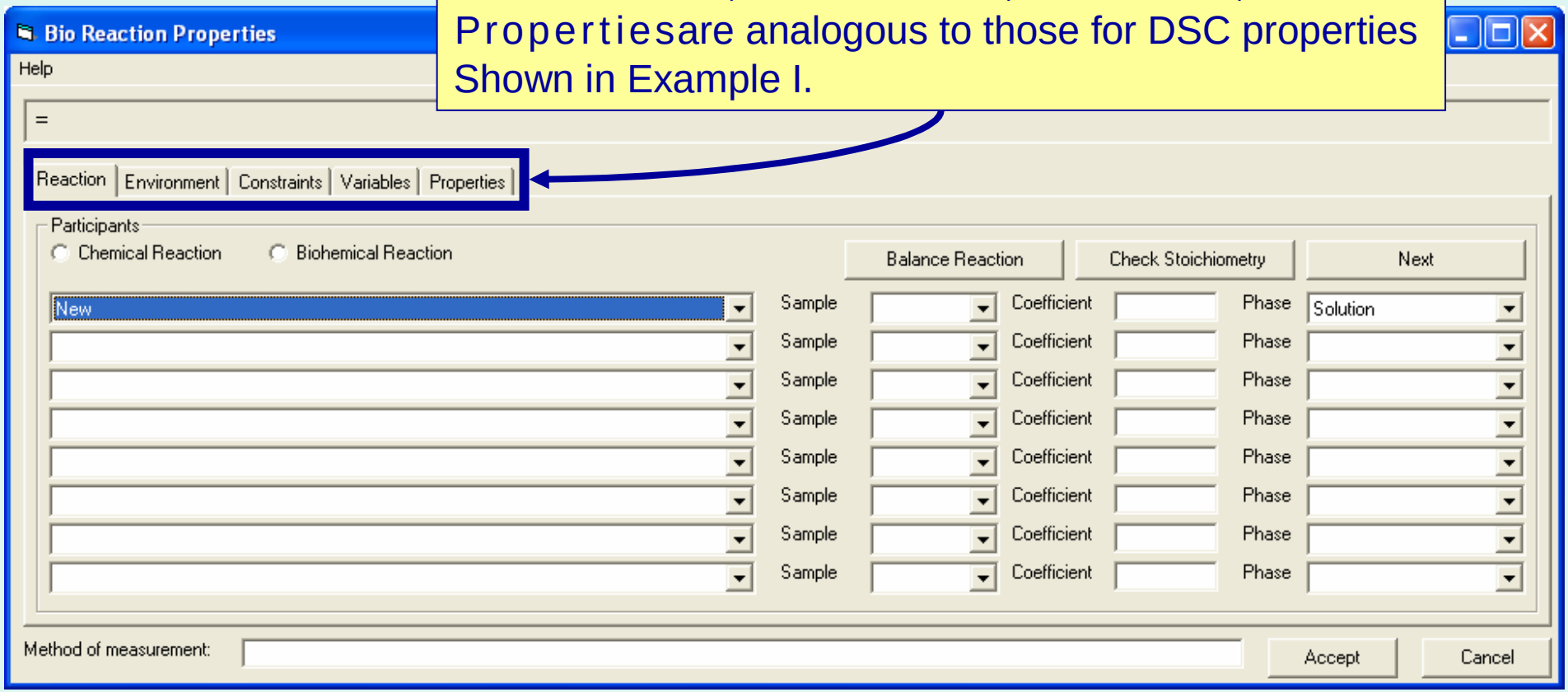
Initiation of Bio Reaction property capture…



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.

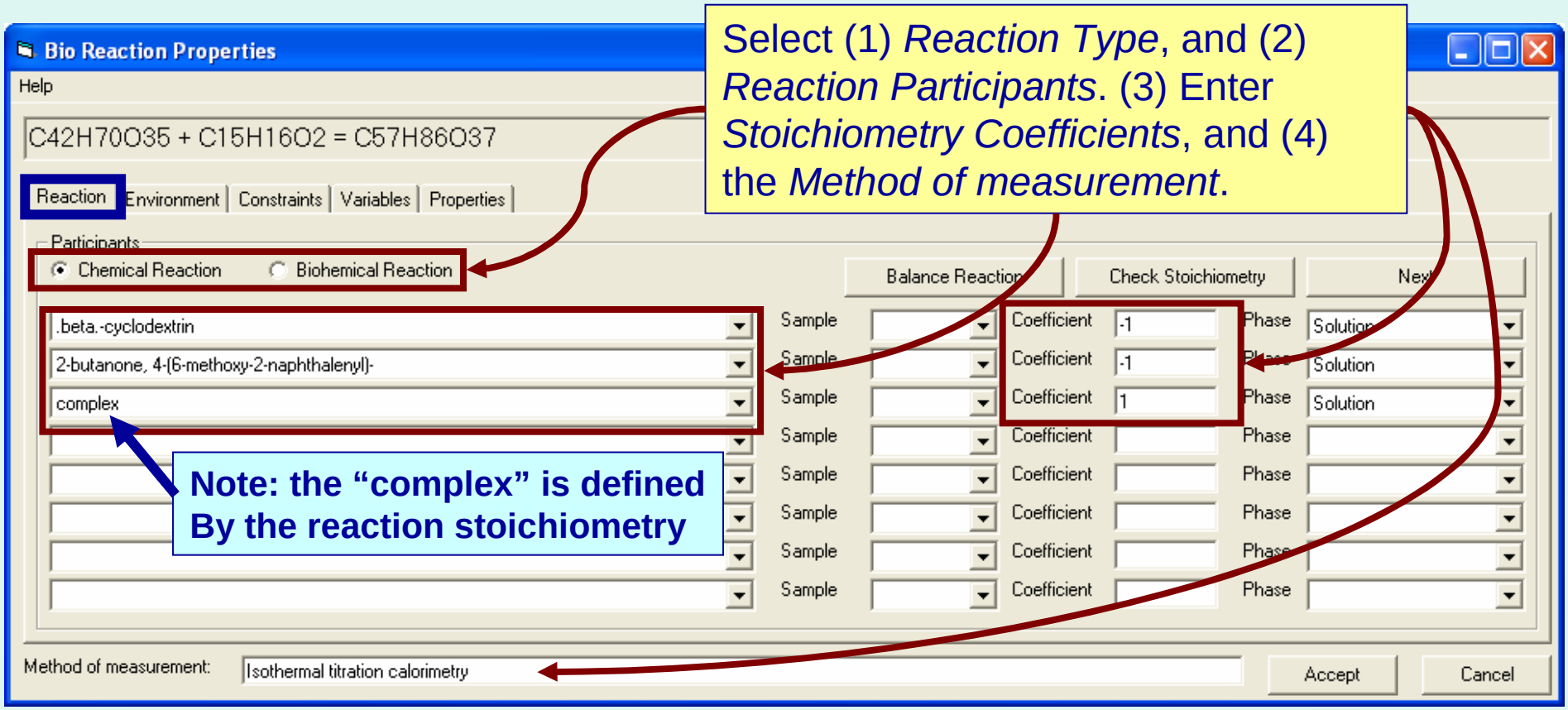


Define the Reaction:

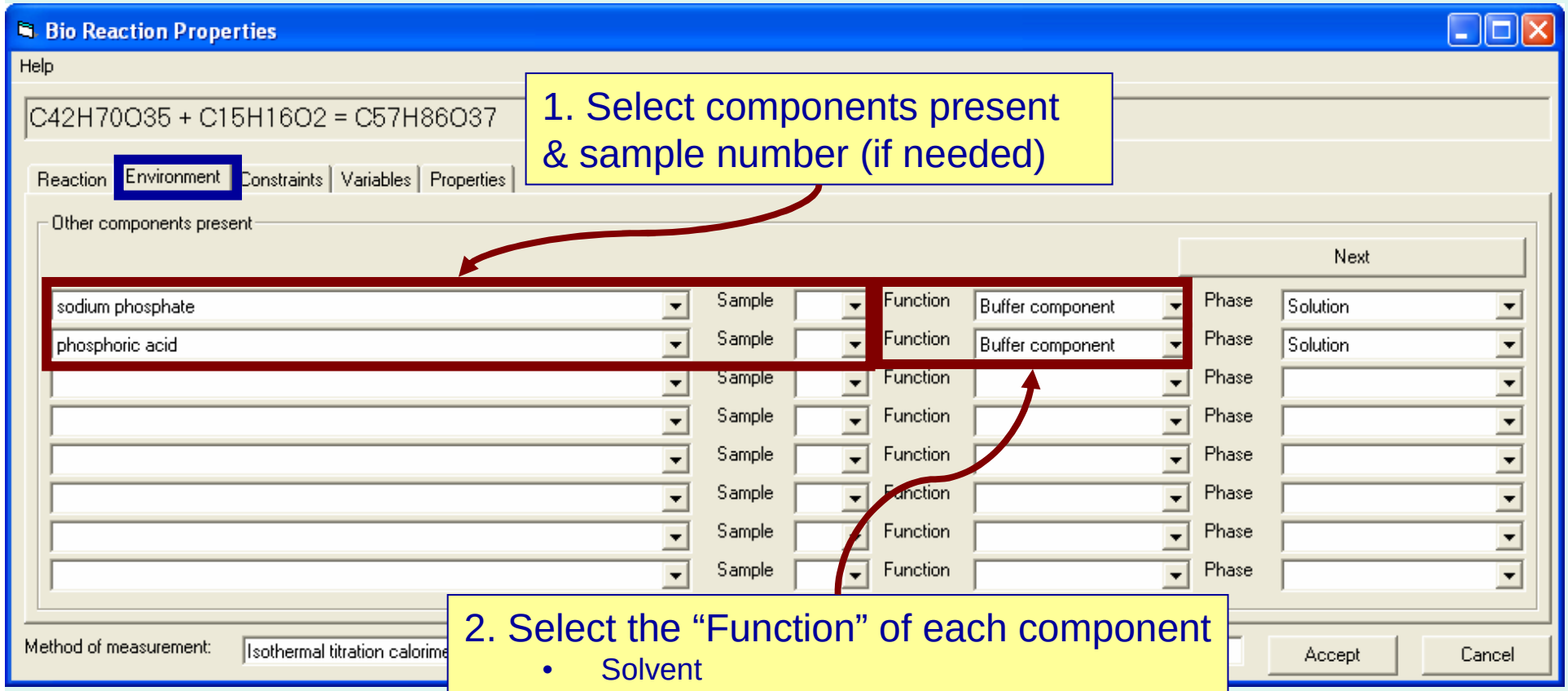
Note: The reaction is defined as equation (1) on the ***2nd*** page of the article**:**

$$\beta CD + NPX \Longleftrightarrow \beta CD \cdot NPX \qquad (1)$$

This is a ***chemical*** reaction, where the components are explicit
(neutral, bound with a counterion, or dissociated)



Define the Environment:

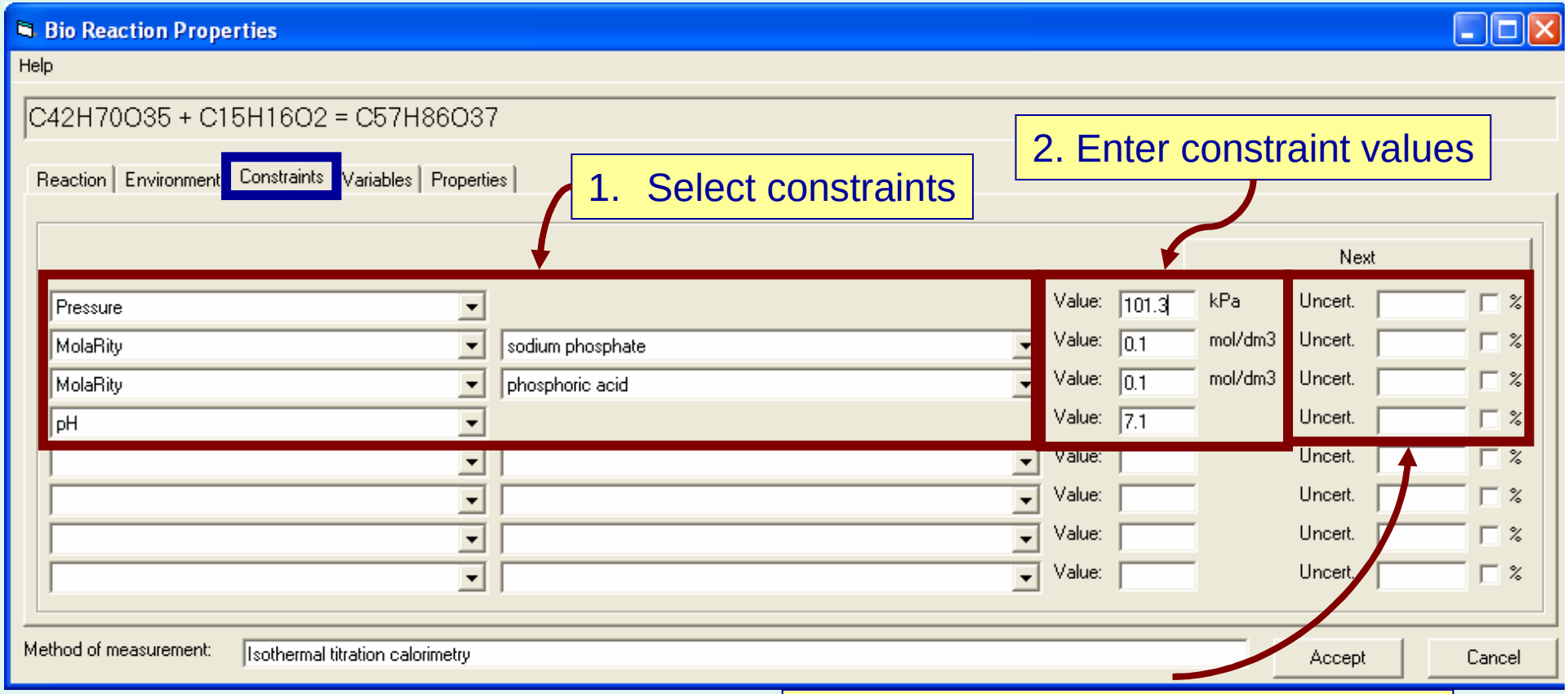


1. Select components present & sample number (if needed)

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

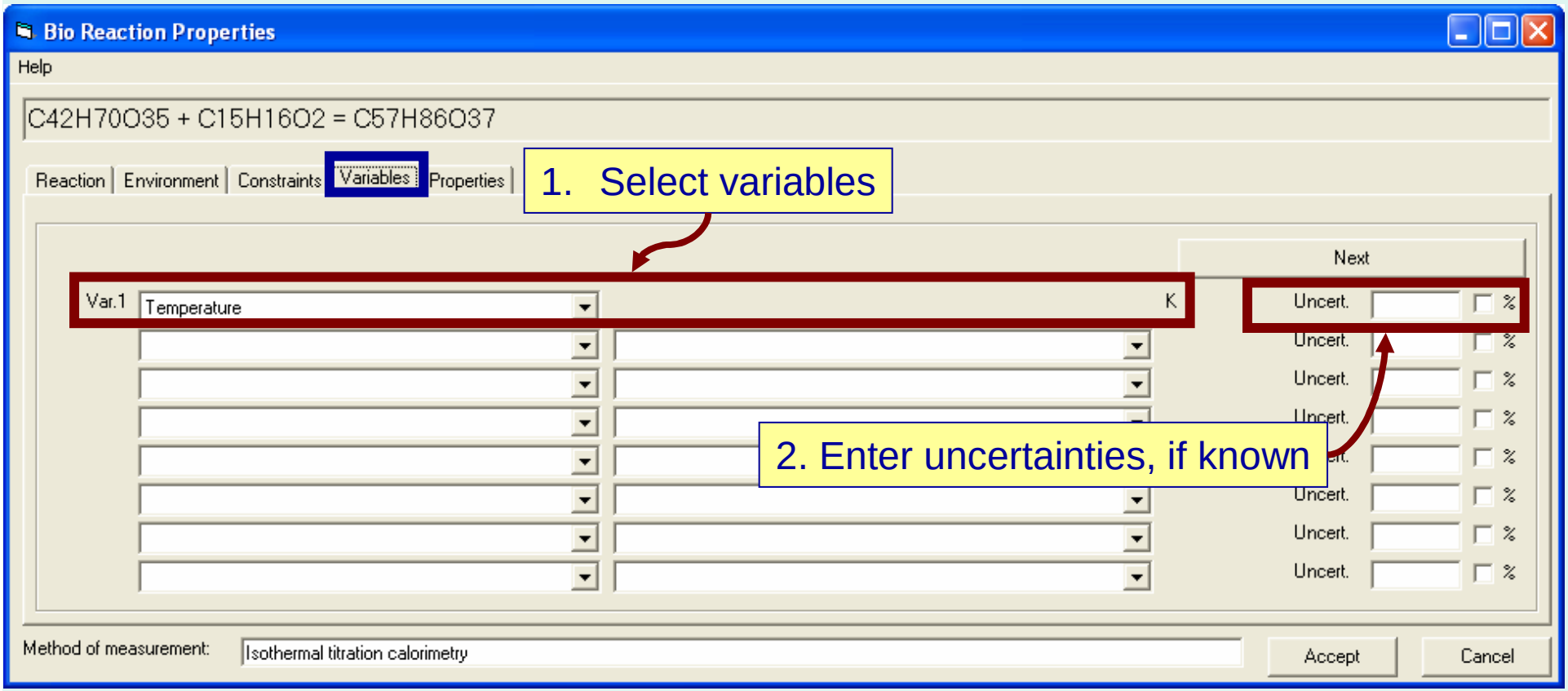
Next...

Define the Constraints:



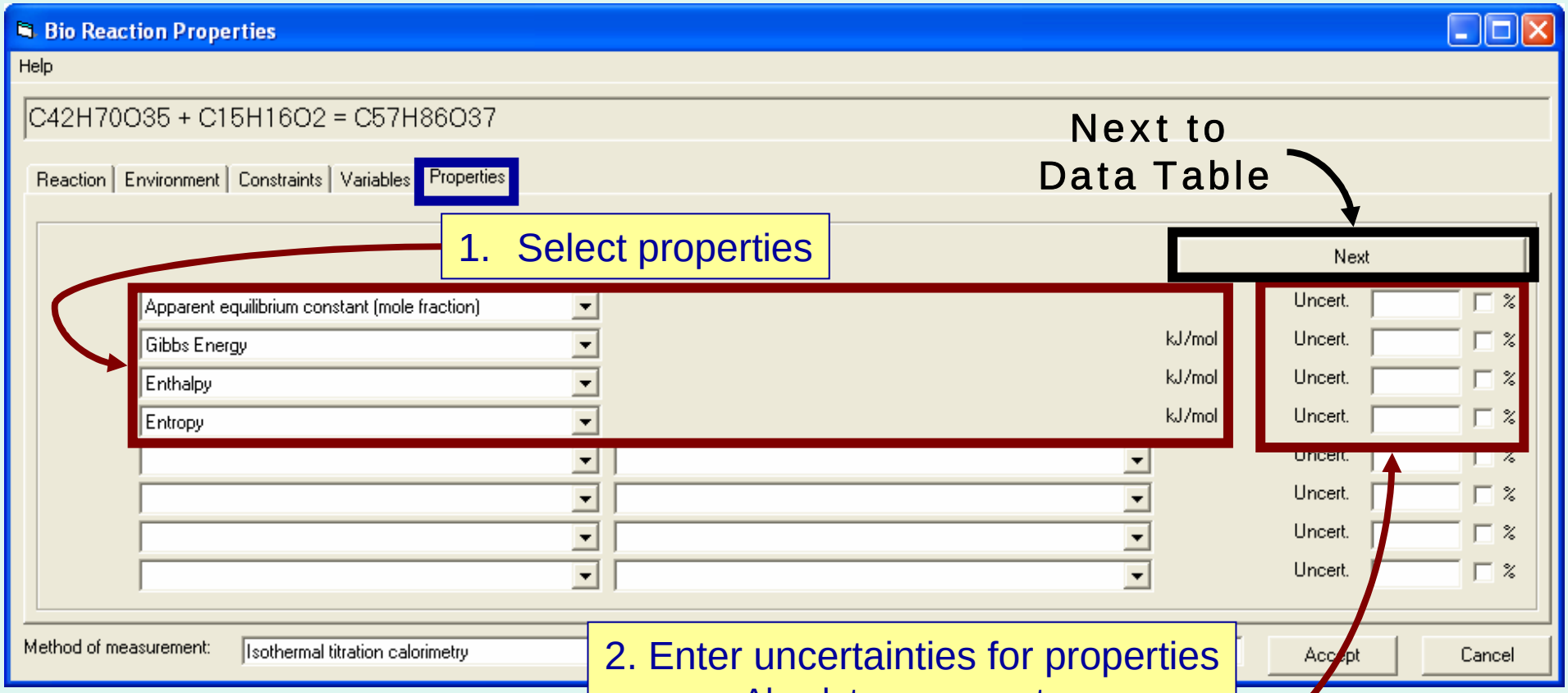
Next tab...

Define the Variables:



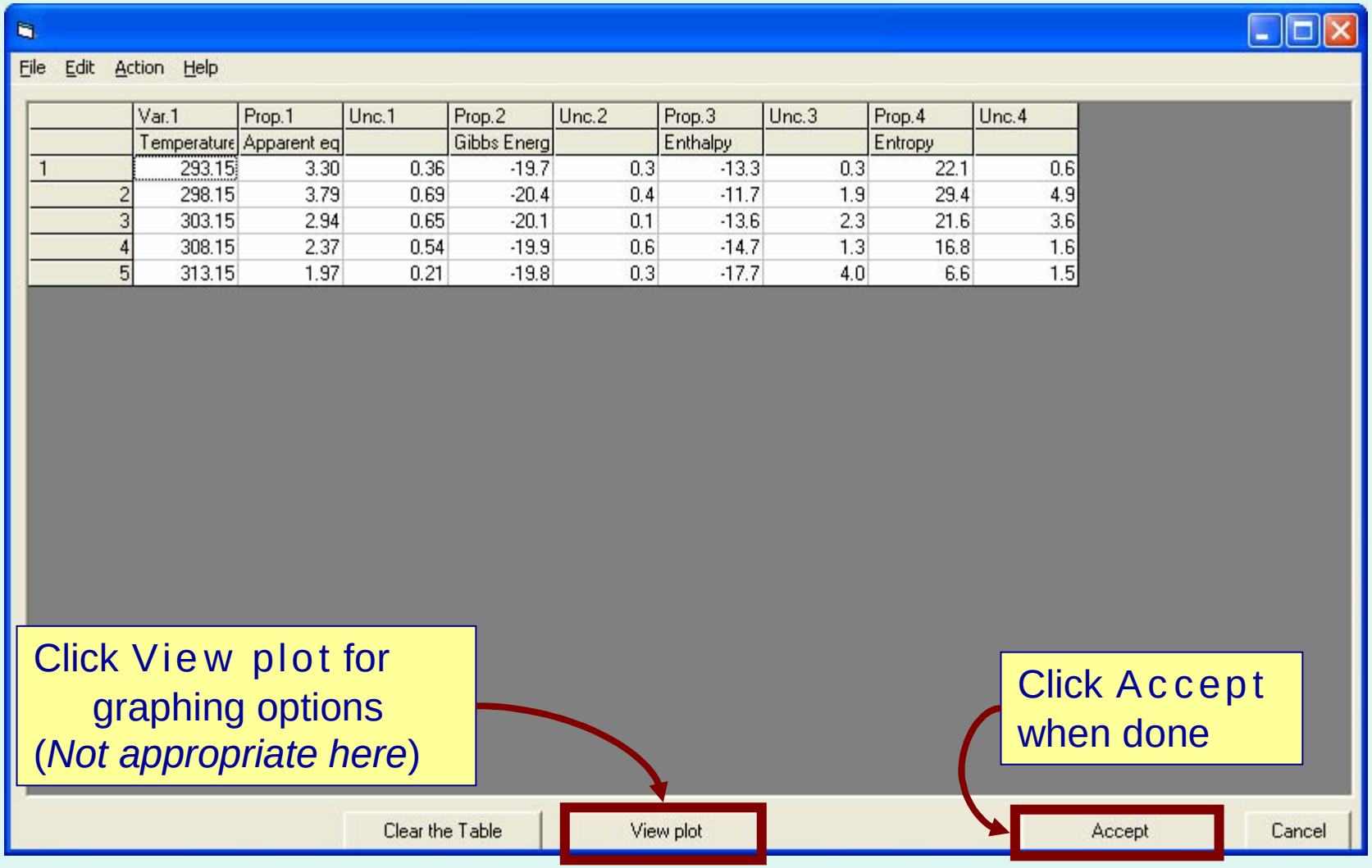
Next tab...

Define the Properties:

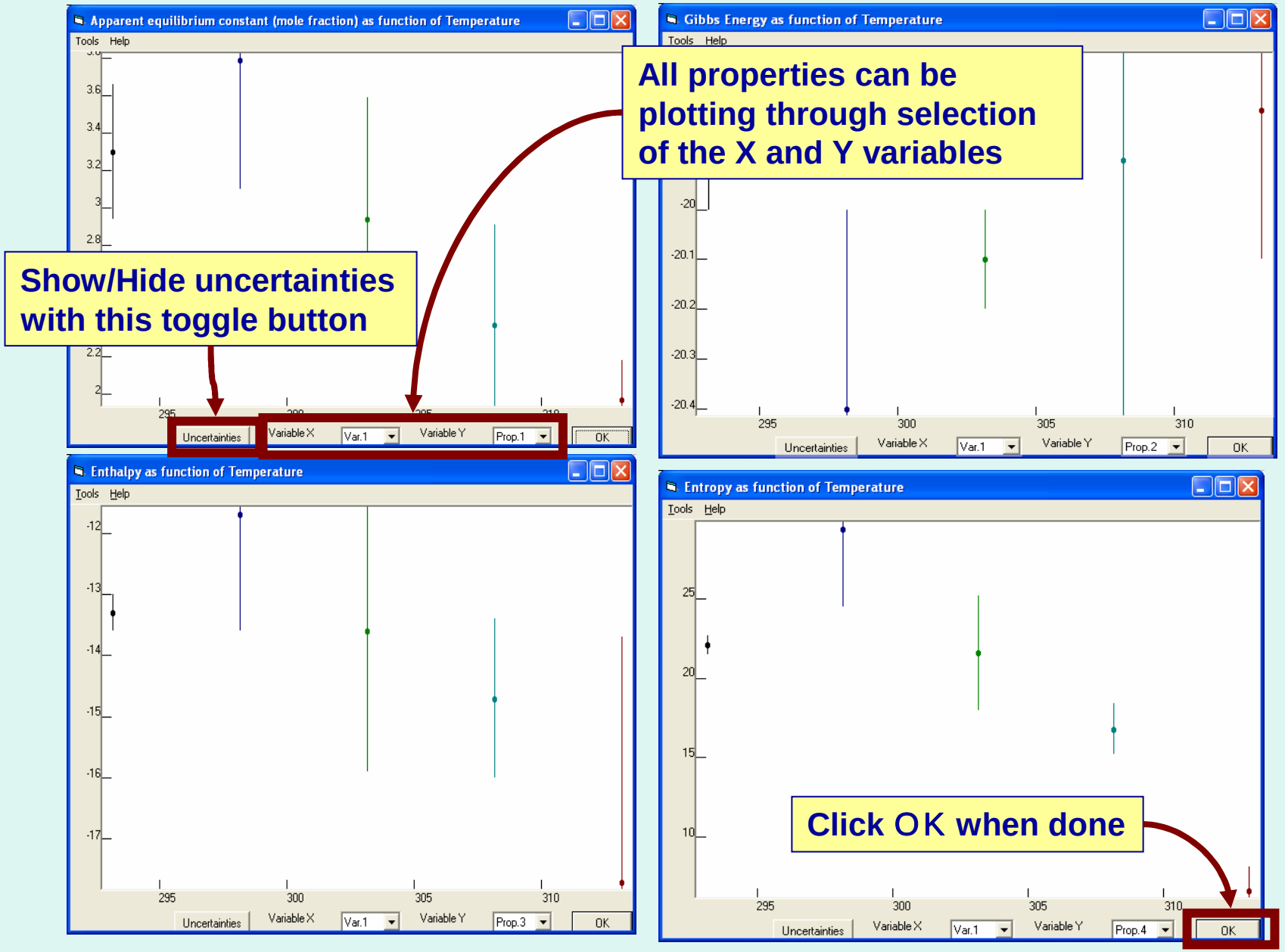


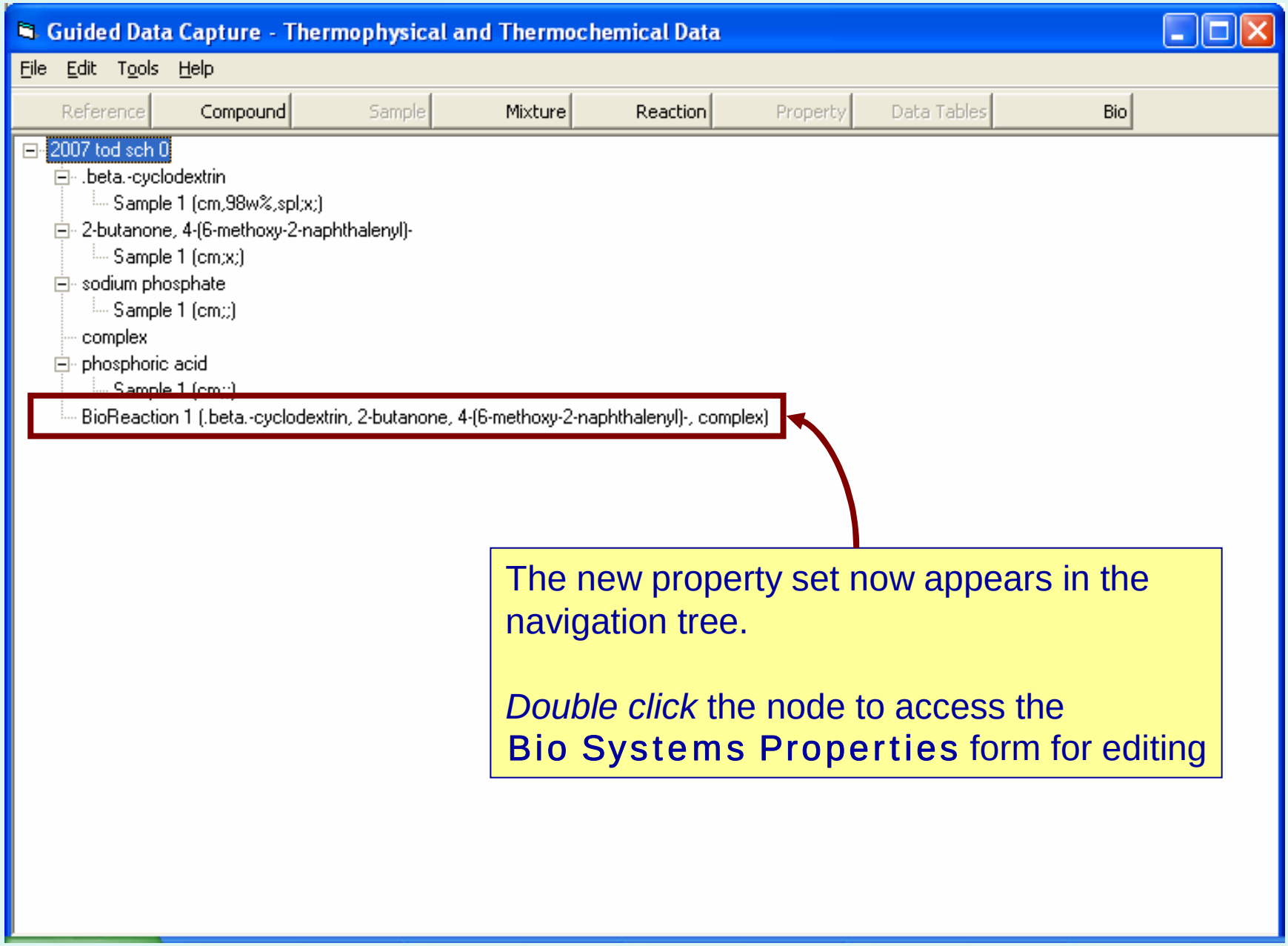
Enter numerical values for *Variables* and *Properties*:

See page 1044 of the example article pdf.



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




Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction Property Data Tables Bio
2007 tod sch 0
.beta.-cyclodextrin
Sample 1 (cm,98w%,spl;x;)
2-butanone, 4-(6-methoxy-2-naphthalenyl)-
Sample 1 (cm;x;)
sodium phosphate
Sample 1 (cm;;)
complex
phosphoric acid
Sample 1 (cm;;)
BioReaction 1 (.beta.-cyclodextrin, 2-butanone, 4-(6-methoxy-2-naphthalenyl)-, complex)
The new property set now appears in the navigation tree.
Double click the node to access the
Bio Systems Properties form for editing