

BIOETHERMODYNAMIC 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

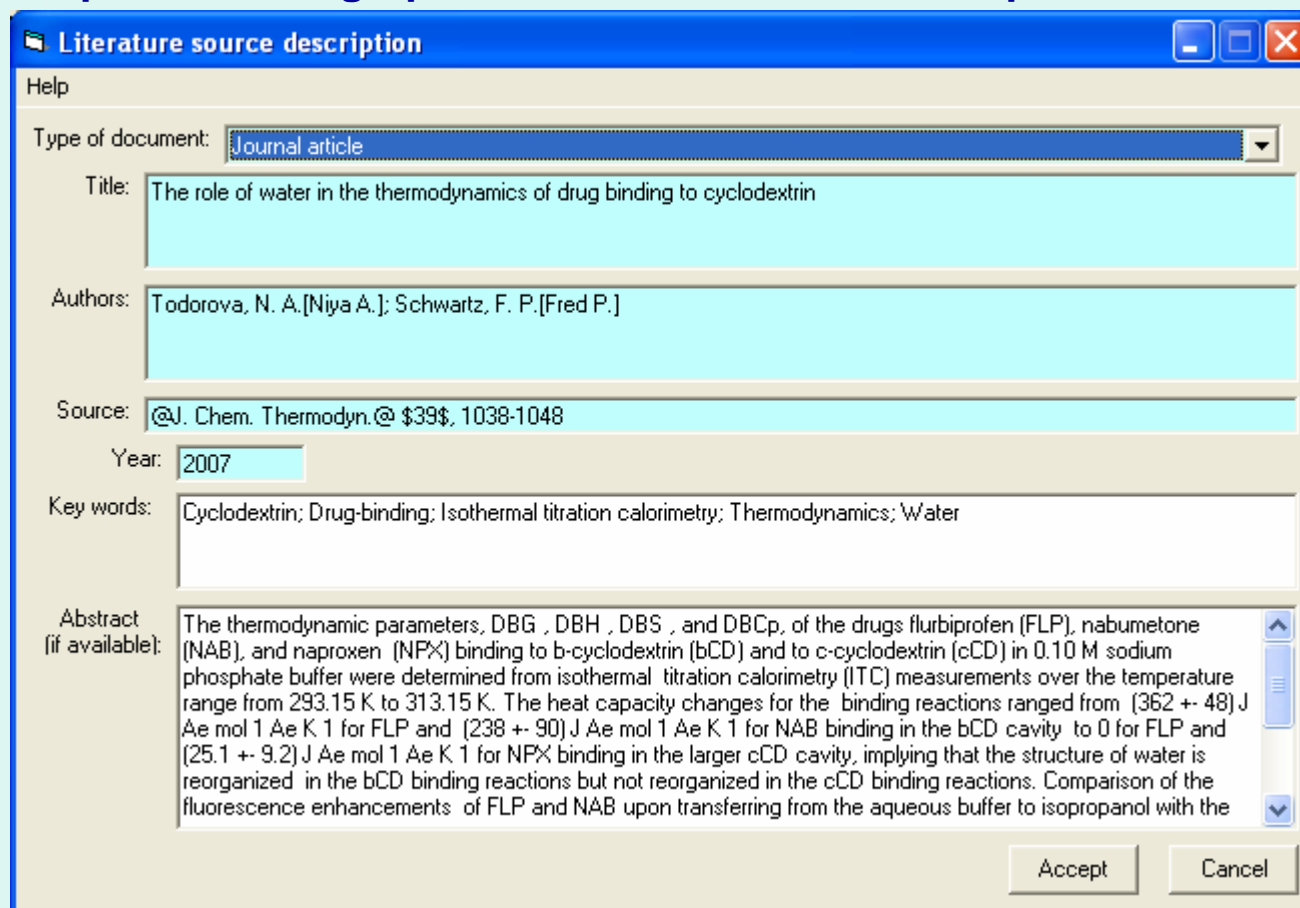
Bibliographic information:

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:



Literature source description

Help

Type of document:

Title:

Authors:

Source:

Year:

Key words:

Abstract (if available):

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

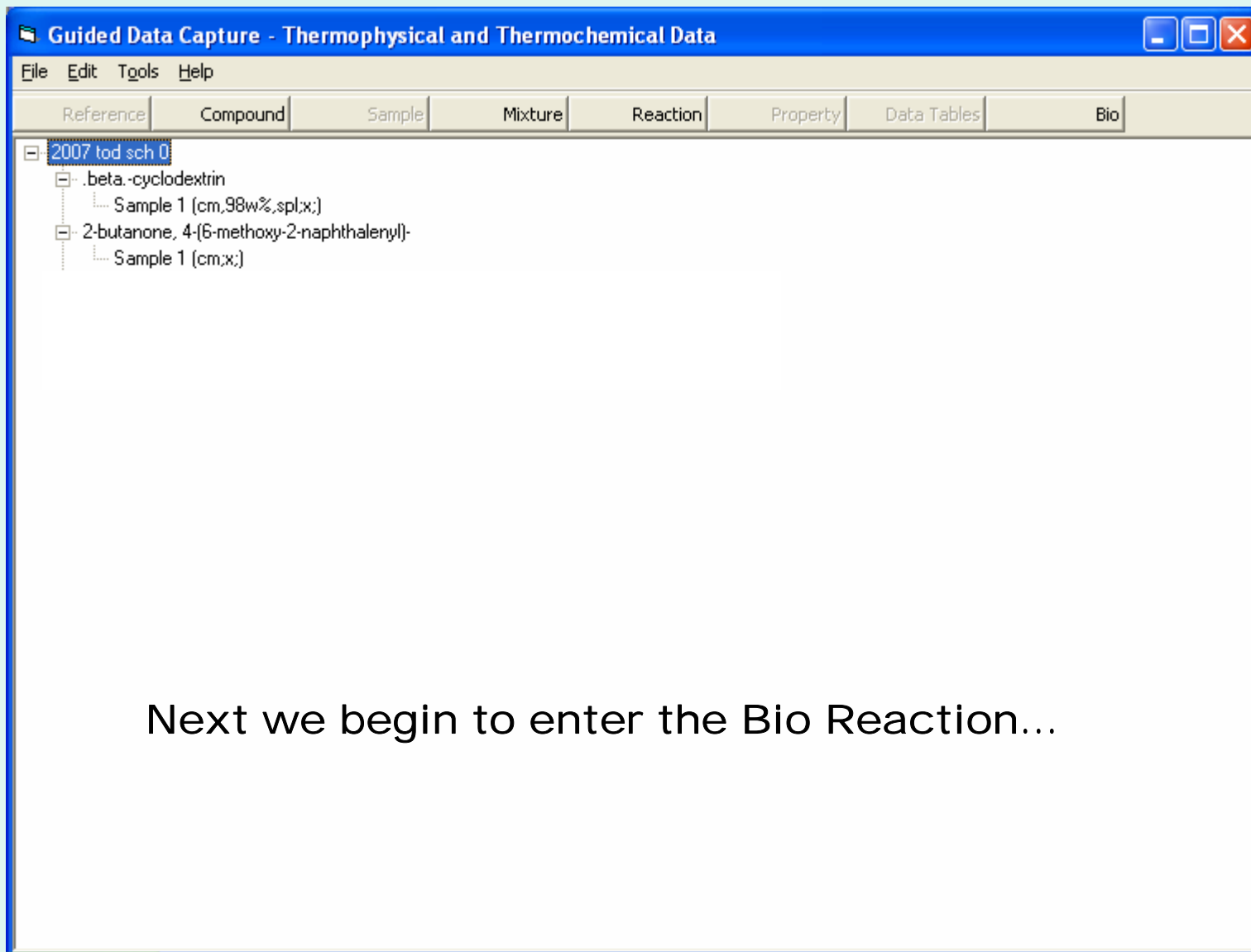
See: <http://www.trc.nist.gov/helpdocs/basic/COMPOUNDaddition.pdf>

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 the reaction components, the Main GDC form looks like this...



Next we begin to enter the Bio Reaction...

Initiation of Bio Reaction property capture...

The screenshot shows the 'Guided Data Capture - Thermophysical and Thermochemical Data' application window. The 'Bio' tab is selected in the top navigation bar. The 'Data Table Processing' dialog box is open, displaying a list of table types: 'Bio Property from DSC (in solution)', 'Bio Substance Solubility', and 'Bio Reaction'. The 'Bio Reaction' option is highlighted. The 'OK' button is also highlighted.

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

2. Select Bio Reaction

3. Click OK

Next...

Define the Reaction:

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



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

The screenshot shows the 'Bio Reaction Properties' dialog box. At the top, the chemical formula C42H70O35 + C15H16O2 = C57H86O37 is displayed. Below it, the 'Reaction' tab is selected. Under 'Participants', the 'Chemical Reaction' radio button is chosen. Three participants are listed: '.beta.-cyclodextrin', '2-butanone, 4-(6-methoxy-2-naphthalenyl)-', and 'complex'. The 'Balance Reaction' table shows coefficients of -1, -1, and 1 for these participants respectively. The 'Method of measurement' is set to 'Isothermal titration calorimetry'. A yellow callout box provides instructions: 'Select (1) Reaction Type, and (2) Reaction Participants. (3) Enter Stoichiometry Coefficients, and (4) the Method of measurement.' Red arrows point from this box to the 'Chemical Reaction' button, the participant list, the coefficient input fields, and the 'Method of measurement' field. A blue callout box notes: 'Note: the "complex" is defined By the reaction stoichiometry', with an arrow pointing to the 'complex' participant.

Help

C42H70O35 + C15H16O2 = C57H86O37

Reaction | Environment | Constraints | Variables | Properties

Participants

Chemical Reaction Biochemical Reaction

Participant	Sample	Coefficient	Phase
.beta.-cyclodextrin	Sample	-1	Solution
2-butanone, 4-(6-methoxy-2-naphthalenyl)-	Sample	-1	Solution
complex	Sample	1	Solution
	Sample		
	Sample		
	Sample		
	Sample		
	Sample		
	Sample		

Method of measurement: Isothermal titration calorimetry

Accept Cancel

Select (1) Reaction Type, and (2) Reaction Participants. (3) Enter Stoichiometry Coefficients, and (4) the Method of measurement.

Note: the "complex" is defined By the reaction stoichiometry

Define the Environment:

Bio Reaction Properties

Help

$C_4H_7O_3S + C_{15}H_{16}O_2 = C_5H_8O_3$

Reaction **Environment** Constraints Variables Properties

Other components present

Component	Sample	Function	Phase
sodium phosphate		Buffer component	Solution
phosphoric acid		Buffer component	Solution

Method of measurement: Isothermal titration calorimetry

Next

Accept Cancel

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:

Bio Reaction Properties

Help

$C_4H_7O_3S + C_{15}H_{16}O_2 = C_5H_8O_3$

Reaction | Environment | **Constraints** | Variables | Properties

1. Select constraints

2. Enter constraint values

		Value:		Uncert.	
Pressure		101.3	kPa		<input type="checkbox"/> %
MolarRity	sodium phosphate	0.1	mol/dm ³		<input type="checkbox"/> %
MolarRity	phosphoric acid	0.1	mol/dm ³		<input type="checkbox"/> %
pH		7.1			<input type="checkbox"/> %
					<input type="checkbox"/> %
					<input type="checkbox"/> %
					<input type="checkbox"/> %
					<input type="checkbox"/> %

Method of measurement: Isothermal titration calorimetry

Next

Accept Cancel

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

Next tab...

Define the Variables:

Help

C42H70O35 + C15H16O2 = C57H86O37

Reaction | Environment | Constraints | **Variables** | Properties

1. Select variables

Var.	Variable	Unit	Uncert.	%
Var.1	Temperature	K		<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>

2. Enter uncertainties, if known

Next

Uncert. %

Uncert. %

Uncert. %

Uncert. %

Uncert. %

Uncert. %

Uncert. %

Uncert. %

Method of measurement:

Accept Cancel

Next tab...

Define the Properties:

Help

C42H70O35 + C15H16O2 = C57H86O37

Reaction | Environment | Constraints | Variables | **Properties**

1. Select properties

Apparent equilibrium constant (mole fraction)			
Gibbs Energy			kJ/mol
Enthalpy			kJ/mol
Entropy			kJ/mol

Next to Data Table

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"/>	%

Method of measurement: Isothermal titration calorimetry

Accept Cancel

2. Enter uncertainties for properties

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

Enter numerical values for *Variables and Properties*:

See page 1044 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 10 columns: Var.1, Prop.1, Unc.1, Prop.2, Unc.2, Prop.3, Unc.3, Prop.4, and Unc.4. The rows represent data points 1 through 5. The 'View plot' button is highlighted with a red box and a red arrow pointing to it from a yellow callout box. The 'Accept' button is also highlighted with a red box and a red arrow pointing to it from another yellow callout box.

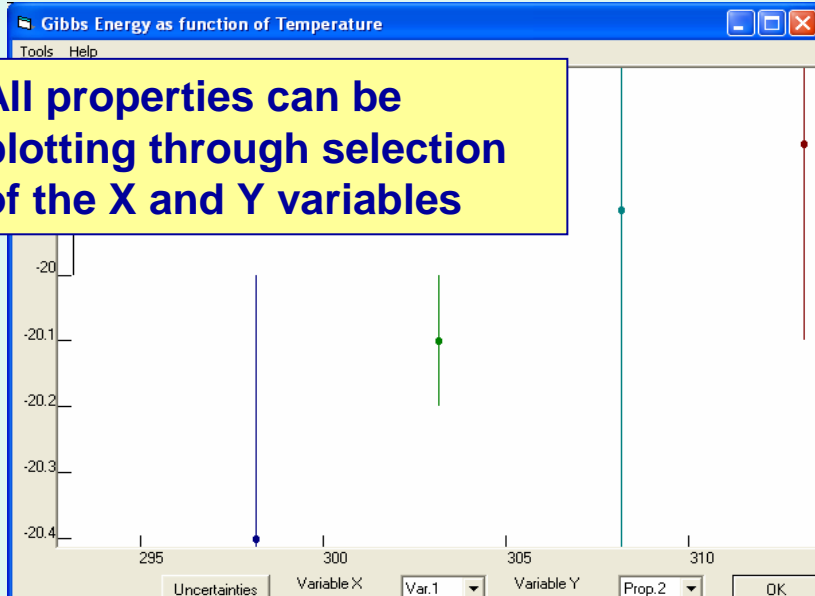
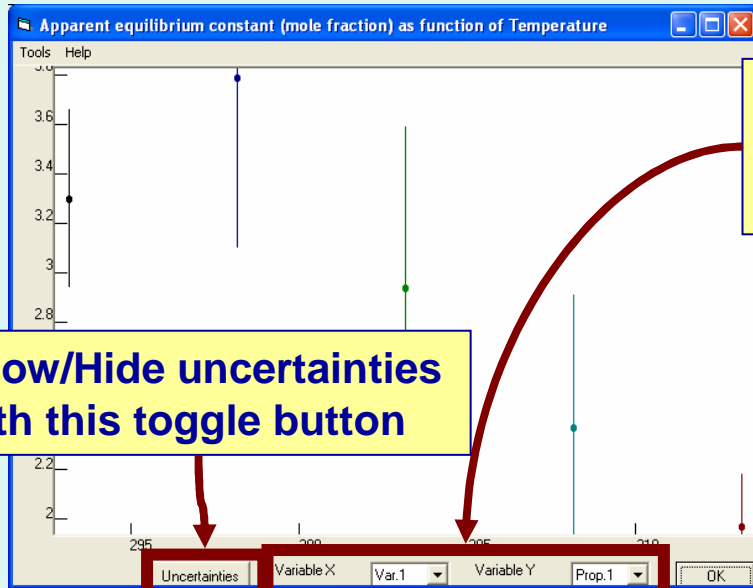
	Var.1	Prop.1	Unc.1	Prop.2	Unc.2	Prop.3	Unc.3	Prop.4	Unc.4
	Temperature	Apparent eq		Gibbs Energ		Enthalpy		Entropy	
1	293.15	3.30	0.36	-19.7	0.3	-13.3	0.3	22.1	0.6
2	298.15	3.79	0.69	-20.4	0.4	-11.7	1.9	29.4	4.9
3	303.15	2.94	0.65	-20.1	0.1	-13.6	2.3	21.6	3.6
4	308.15	2.37	0.54	-19.9	0.6	-14.7	1.3	16.8	1.6
5	313.15	1.97	0.21	-19.8	0.3	-17.7	4.0	6.6	1.5

Click View plot for graphing options
(Not appropriate here)

Click Accept when done

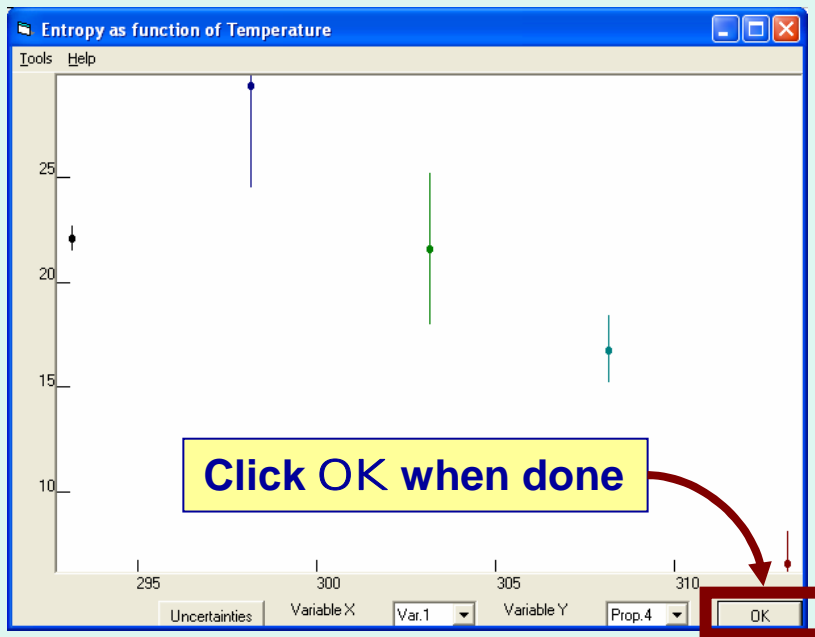
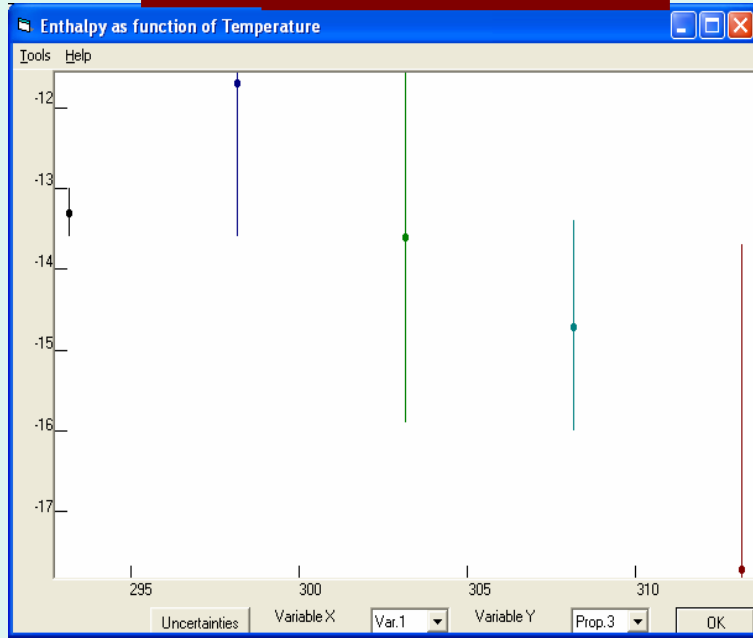
Clear the Table View plot Accept Cancel

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



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

Show/Hide uncertainties with this toggle button



Click OK when done

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