

BIOETHERMODYNAMIC 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.*

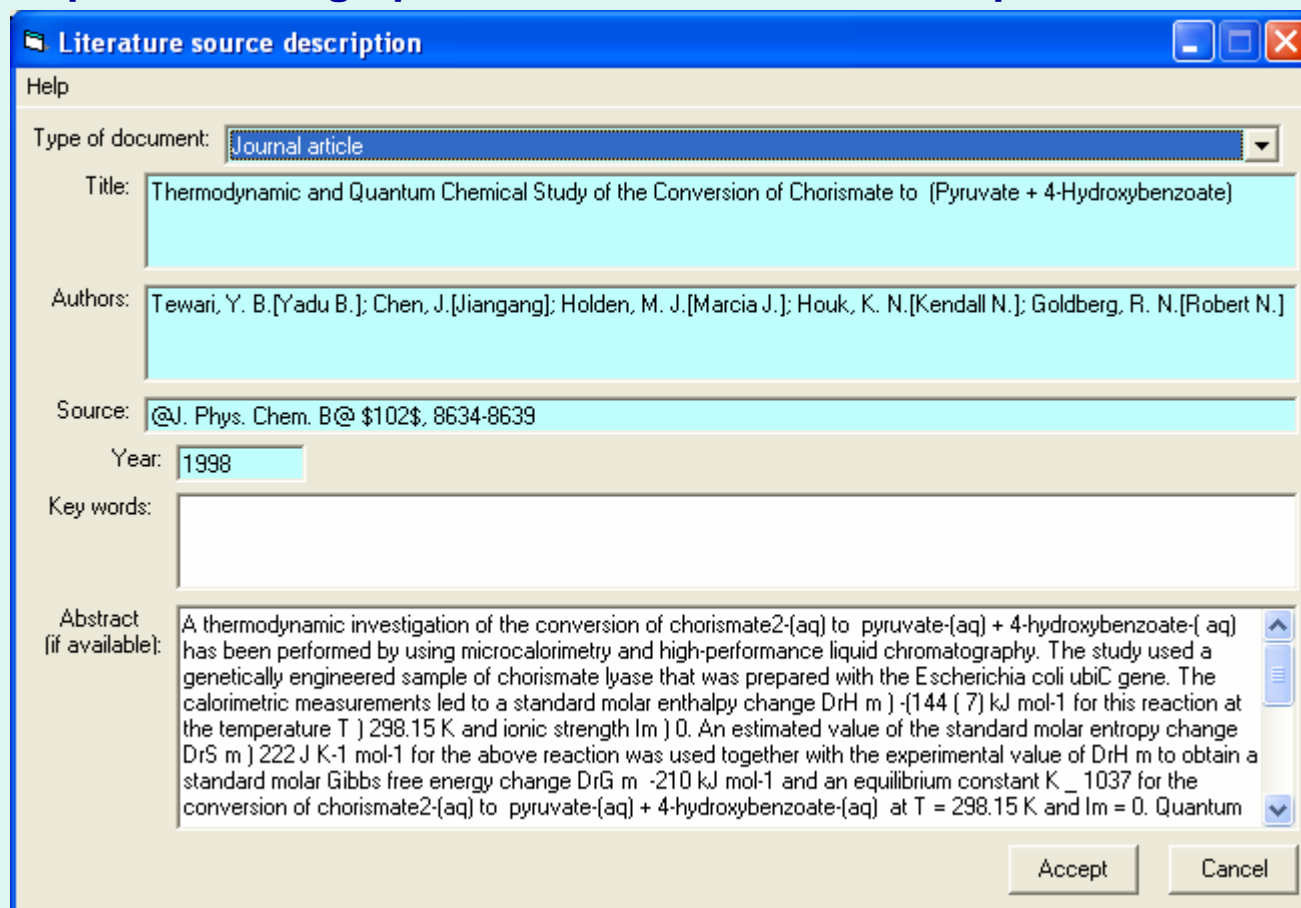
Bibliographic information:

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:



Literature source description

Help

Type of document:

Title: Thermodynamic and Quantum Chemical Study of the Conversion of Chorismate to (Pyruvate + 4-Hydroxybenzoate)

Authors: Tewari, Y. B. [Yadu B.]; Chen, J. [Jiangang]; Holden, M. J. [Marcia J.]; Houk, K. N. [Kendall N.]; Goldberg, R. N. [Robert N.]

Source: @J. Phys. Chem. B@ \$102\$, 8634-8639

Year: 1998

Key words:



Abstract (if available): A thermodynamic investigation of the conversion of chorismate2-(aq) to pyruvate-(aq) + 4-hydroxybenzoate-(aq) has been performed by using microcalorimetry and high-performance liquid chromatography. The study used a genetically engineered sample of chorismate lyase that was prepared with the Escherichia coli ubiC gene. The calorimetric measurements led to a standard molar enthalpy change $\Delta_r H_m^\circ$ (-144 (7) kJ mol⁻¹ for this reaction at the temperature T) 298.15 K and ionic strength I_m) 0. An estimated value of the standard molar entropy change $\Delta_r S_m^\circ$ 222 J K⁻¹ mol⁻¹ for the above reaction was used together with the experimental value of $\Delta_r H_m^\circ$ to obtain a standard molar Gibbs free energy change $\Delta_r G_m^\circ$ -210 kJ mol⁻¹ and an equilibrium constant K_{1037} for the conversion of chorismate2-(aq) to pyruvate-(aq) + 4-hydroxybenzoate-(aq) at T = 298.15 K and I_m = 0. Quantum

Accept Cancel

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

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

Google G Go 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)	$\Delta_r H$ (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
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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

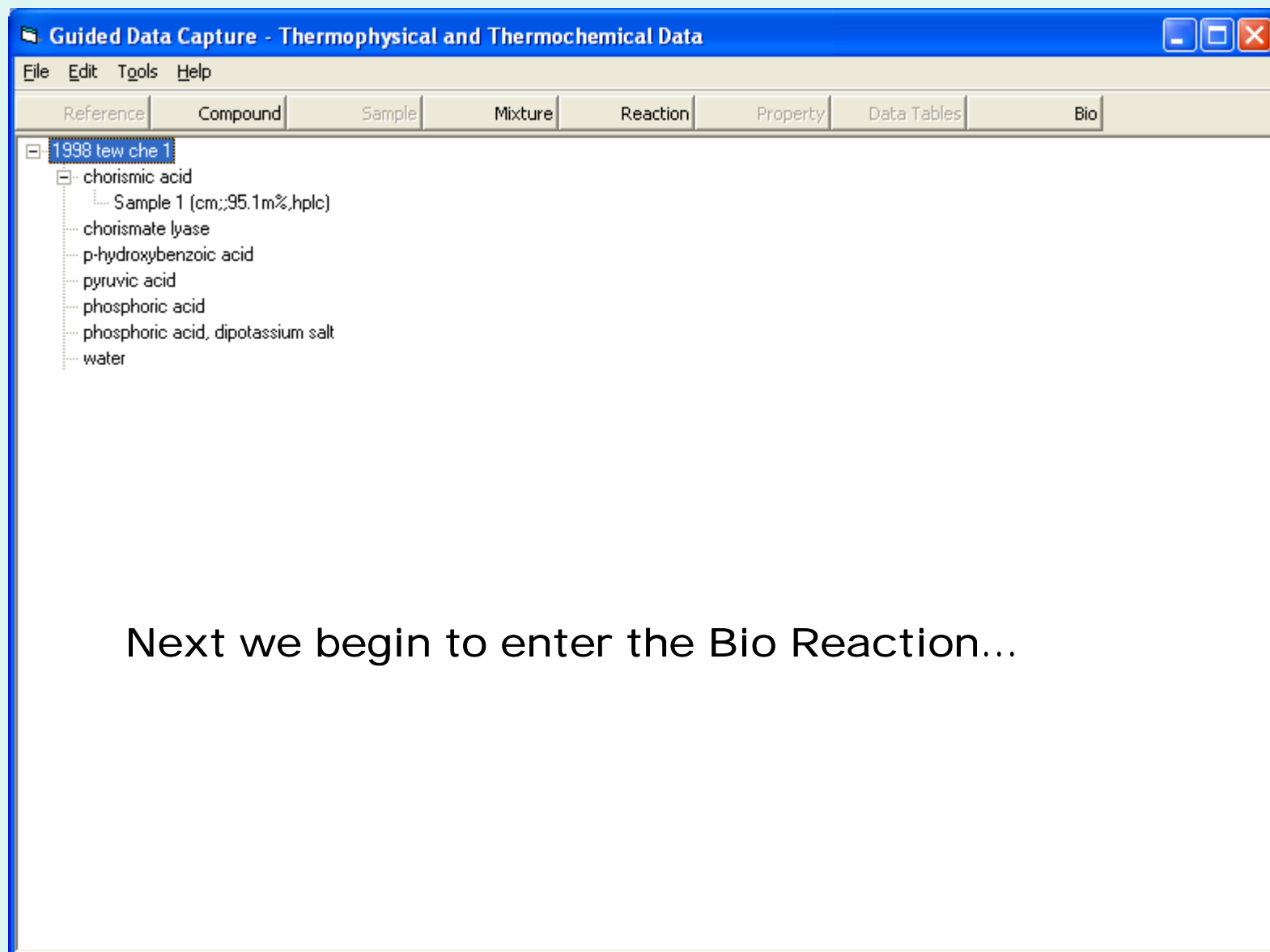
See: <http://www.trc.nist.gov/helpdocs/basic/COMPOUNDaddition.pdf>

New Features:

1. Capture of EC (*Enzyme 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 a software window titled "Guided Data Capture - Thermophysical and Thermochemical Data". The window has a menu bar with "File", "Edit", "Tools", and "Help". Below the menu bar are several tabs: "Reference", "Compound", "Sample", "Mixture", "Reaction", "Property", "Data Table", and "Bio". The "Bio" tab is highlighted with a red box. Below the tabs is a tree view showing a folder "1998 tew che 1" containing several sub-items like "chorismic acid", "Sample 1 (cm;:95.1m%.hplc)", "chorismate lyase", etc. Overlaid on this is a "Data Table Processing" dialog box. It has a label "Select type of table:" followed by a dropdown menu. The dropdown menu is open, showing three options: "Bio Property from DSC (in solution)", "Bio Substance Solubility", and "Bio Reaction". The "Bio Reaction" option is highlighted with a blue background. Below the dropdown are "OK" and "Cancel" buttons. The "OK" button is highlighted with a red box. Three yellow callout boxes with blue text and red arrows provide instructions: "1. Select Bio and the Data Table Processing selection form opens." (pointing to the Bio tab), "2. Select Bio Reaction" (pointing to the Bio Reaction option in the dropdown), and "3. Click OK" (pointing to the OK button).

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

2. Select Bio Reaction

3. Click OK

Next...

The Bio Reaction Properties form appears...

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

Help

=

Reaction | Environment | Constraints | Variables | Properties

Participants

Chemical Reaction Biochemical Reaction

Balance Reaction Check Stoichiometry Next

Sample	Coefficient	Phase
New	Sample	Solution
	Sample	
	Sample	
	Sample	
	Sample	
	Sample	
	Sample	
	Sample	
	Sample	

Method of measurement:

Accept Cancel

Define the Reaction:

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



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.

Help

C10H10O6 = C7H6O3 + C3H4O3

Reaction Environment Constraints Variables Properties

Participants

Chemical Reaction Biochemical Reaction

Participant	Sample	Coefficient	Phase
chorismic acid	Sample	-1	Solution
p-hydroxybenzoic acid	Sample	1	Solution
pyruvic acid	Sample	1	Solution
	Sample		
	Sample		
	Sample		
	Sample		
	Sample		

Method of measurement: Heat-conduction calorimetry

Next

Accept Cancel

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

Define the Environment:

Help

$C_{10}H_{10}O_6 = C_7H_6O_8 + C_3H_4O_3$

Reaction **Environment** Constraints Variables Properties

Other components present

Component	Sample	Function	Phase
phosphoric acid		Buffer component	Solution
phosphoric acid, dipotassium salt		Buffer component	Solution
chorismate lyase		Catalyst	Solution
water		Solvent	Solution

Method of measurement: Heat-conduction 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

$C_{10}H_{10}O_6 = C_7H_6O_3 + C_3H_4O_3$

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

1. Select constraints

2. Enter constraint values

Constraint	Value	Unit	Uncert.	%
Pressure	101.3	kPa		<input type="checkbox"/>
pH	6.98			<input type="checkbox"/>
Ionic strength (molaLity basis)	0.38	mol/kg		<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>
				<input type="checkbox"/>

Method of measurement: Heat-conduction calorimetry

Next

Accept Cancel

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

Next tab...

Define the Variables:

Help

$C_{10}H_{10}O_6 = C_7H_6O_3 + C_3H_4O_3$

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

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

Method of measurement: Heat-conduction calorimetry

Accept Cancel

Next tab...

Define the Properties:

Help

C10H10O6 = C7H6O3 + C3H4O3

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

1. Select properties

Enthalpy kJ/mol

2. Enter uncertainties for properties

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

Next to Data Table

Next

Uncert. 7 %

Uncert. %

Uncert. %

Uncert. %

Uncert. %

Uncert. %

Uncert. %

Uncert. %

Uncert. %

Method of measurement: Heat-conduction calorimetry

Accept Cancel

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

File Edit Action Help

	Var.1	Prop.1	Unc.1
	Temperature	Enthalpy	
1	298.15	-144.1	

Click View plot for graphing options
(*Not appropriate here*)

Click Accept when done

Clear the Table View plot Accept Cancel

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