

User's Guide for the Chemical Transformation Simulator (CTS) (β -version 1.0)

9/14/15

Chemical Transformation Simulator: A Cheminformatics-based Tool for Predicting Transformation Pathways and Physicochemical Properties

2015 U.S. Environmental Protection Agency

The Chemical Transformation Simulator (CTS) User's Guide is designed to provide the first time user a complete understanding of how to use the CTS tool. The User's Guide may be reviewed from start to finish or by moving directly to a topic of interest through selection of the appropriate topic in the Table of Contents.

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Introduction

The Chemical Transformation Simulator (CTS) provides the calculated physico-chemical properties of a target chemical and its transformation products, which are predicted as a function of the reaction system of interest. This is accomplished through the integration of cheminformatics applications for the encoding of process science underlying transformation pathways, computational chemistry tools for the calculation of physico-chemical properties, and software technologies that provide access to on-line databases for environmental descriptors required for estimating environmental concentrations.

The β-version 1.0 of the CTS consists of 3 modules, the selection and order of execution of which is based on the user's choice of one of three available workflows. The Structure-based Database (SBD) module, the Earth Systems Model (ESM) and Reaction Rate Calculator (RRC), will be functional in the deployable version of the CTS.

β-Version 1.0

- **Chemical Editor (CE):** Provides options for chemical entry, as well as the speciation of the parent chemical
- **Physicochemical Properties Calculator (PPC):** Calculates p-chem properties for the parent chemical and predicted transformation products based on the executions of multiple p-chem calculators
- **Reaction Pathway Simulator (RPS):** Generates potential transformation products based on user-specified reaction conditions

Deployable Version

- Structure-based Database (SBD): Populated with calculated and measured physico-chemical properties of parent and potential transformation products
- Earth Systems Model (ESM): Provides data mining abilities for environmental descriptors such as pH and temperature
- Reaction Rate Calculator (RRC): Calculates transformation products based on the parameterization and execution of QSARs and Algorithms

Background

A key Agency need identified as a high priority in the Chemical Sustainability and Safety (CSS) research program is for high throughput computational systems to simulate environmental fate and transport for organic chemicals for which environmental data are not available. Knowledge of inherent chemical properties (ICP) is essential for the parameterization of environmental fate and transport models. Of the ~85,000 chemicals in the TSCA inventory, it is estimated that high quality measured ICP data are available for less than 2% of these chemicals. Additionally, 20 to 30 new chemicals a month are being assessed through the Office of Pollution Prevention and Toxics (OPPT) Pre-Manufacturing Notification (PMN) process. This ever growing data gap must be addressed through the development of a high throughput computational system for calculating the ICP necessary for the parameterization of environmental fate models used to estimate environmental concentrations of both the parent chemical and predicted transformation products as a function of environmental conditions.

The key components of the CTS are the development of the physico-chemical properties calculator (PPC) and the Reaction Pathway Simulator (RPS). The PPC is based on a consensus approach that would allow the user to compare output generated by a number of calculators that take different approaches to calculating specific physicochemical properties. The calculators we are currently accessing include (1) SPARC (SPARC Performs Automated Reasoning in Chemistry), which uses a mechanistic-based approach, (2) EPI Suite, which uses a fragment-based approach, (3) TEST (Toxicity Estimation Software Tool), which uses QSAR-based approaches, and (4) ChemAxon plug-in calculators, which use an atom-based fragment approach. The output derived from these calculators will enable the user to compare the calculated data with measured data in readily accessible web-based databases.

The output of the RPS is based on the selection and execution of reaction libraries that represent one-step reactions for transformation of reactive functional groups (i.e., reduction and hydrolysis). These one-step reactions represent viable transformation pathways based on the identification and subsequent transformation of reactive functional groups. A reaction library for human metabolism for phase 1 transformations developed by ChemAxon is also available through the CTS. The development of reaction libraries allow us to “encode” the known process science published (current and future) in the peer-reviewed literature. The encoding of process science is accomplished through the use of Chemical Terms Language and Smart Reaction Smile string through cheminformatics applications. The execution of these reaction libraries provides dominant transformation pathways and products for the chemical of interest as a function of environmental conditions.

Using the CTS Software

Accessing the CTS

The CTS can be accessed through <http://134.67.114.1/cts/>. Currently only EPA intranet users have access to the CTS. The home page provides access to the CTS through the selection of one of three CTS workflows and general information concerning the major components of the CTS and the physicochemical calculators. Links to the process science supporting the currently available reaction libraries are also available.

For example:

Selection of one of the examples with reference transformation pathway scheme, and documented supporting the

The CTS is executed by selecting one of three available workflows (see description below) and by entering a single chemical.

Single Chemical Entry

For single chemical entry, the “Go to Users Inputs” is clicked on at the bottom of the Workflow Overview page or the Inputs tab is selected at the top of the workflow frame. The Chemical Editor appears where there is the option to either enter a SMILES String, IUPAC chemical name, or CAS# in the Lookup Chemical box, or to draw a chemical structure using the Chemical Editor (see below). For either case, the appropriate box must be clicked after providing the required information. Details concerning the use of the chemical editor can be found at <https://docs.chemaxon.com/display/marvinsketch/MarvinSketch+User%27s+Guide>.



Generation of .pdf and .html Reports

The .pdf and .html buttons appear on the right of the results page, regardless of the workflow. Clicking on the .pdf button generates a PDF file that is can be viewed in the web browser or using free PDF software. The HTML file can be viewed using a web browser.

Execution of the CTS Workflows

The user executes the CTS through the selection of one of three available workflows:

- Calculate Chemical Speciation
- Calculate p-Chem Properties
- Generate Transformation Products

cts: Chemical Transformation Simulator (alpha version)

Execute CTS Workflow

Calculate Chemical Speciation
Calculate p-Chem Properties
Generate Transformation Products

This web site is under development. It is available for the purposes of receiving feedback and quality assurance from personnel in the EPA.

The Chemical Transformation Simulator (CTS) provides the calculated physico-chemical properties of the parent chemical and transformation products, which are predicted as a function of the reaction system of interest. This is accomplished through the integration of cheminformatics applications for the encoding of process science underlying transformation pathways, computational chemistry tools for the calculation of physico-chemical properties, and software technologies that provide access to on-line databases for environmental descriptors required for estimating environmental concentrations.

The user interacts with the alpha-version of the CTS through the execution of one of three available work flows (green tabs in left column) described below. Each workflow invokes the CTS modules required to provide the data requested by the user. Descriptions of the individual modules are provided by the tabs in the left-hand column.

Calculate Chemical Speciation Workflow: Invokes the Chemical Editor (CE) Module which provides the user options for chemical entry and calculates the speciation (i.e., ionization, tautomer distribution and isomerization) for the chemical of interest.

Calculate Physico-Chemical Properties Workflow: The User inputs chemical information through the CE and then invokes the Physico-Chemical Properties Calculator (PCP) Module. The PCP Module then calls upon four stand-alone widely recognized calculators (EPI Suite, SPARC, ChemAxon, and TEST), all of which calculate p-chem properties by mutually exclusive methods.

Generate Transformation Products Workflow: The User inputs chemical information through the CE and then invokes the Reaction Pathway Simulator (RPS) Module to generate transformation products through the execution of reaction libraries based on user-specified conditions. The User is then given the option to invoke the PCP Module for the calculation of p-chem properties for one or more parent or product chemicals.

Description of CTS Modules

Chemical Editor
P-Chem Properties
Reaction Pathway Simulator

Description of P-Chem Calculators

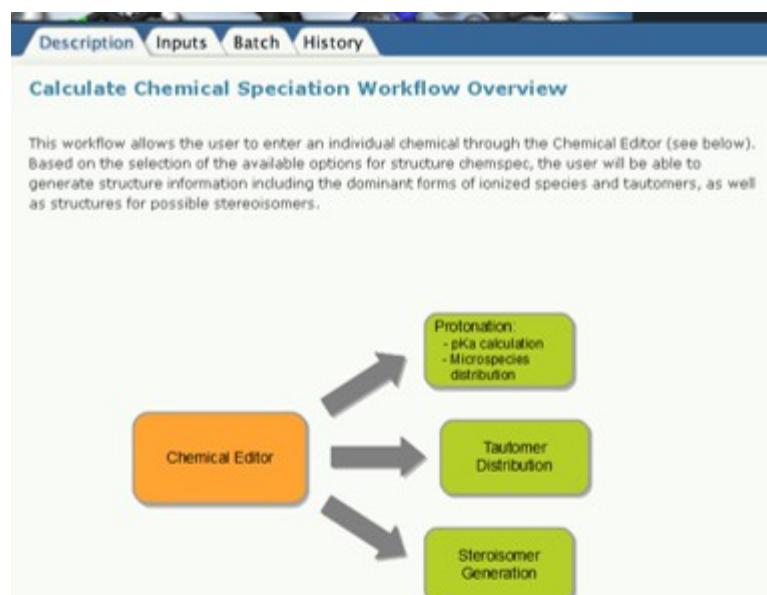
EPI Suite
SPARC
ChemAxon
TEST

Description of Reaction Libraries

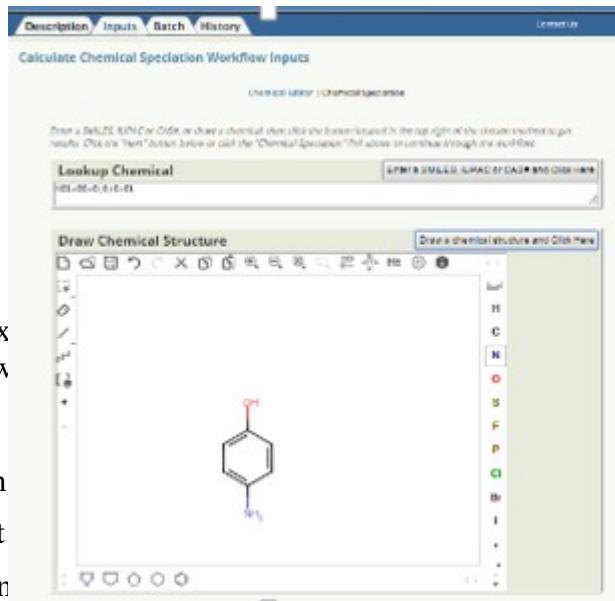
Abiotic Reduction
Abiotic Hydrolysis
Mammalian Metabolism

Calculate Chemical Speciation Workflow

Selection of the Calculate Chemical Speciation Workflow provides this page illustrating the workflow overview. Click on the Go to User Inputs button or the Inputs tab to submit a single chemical for processing, or click on the Batch tab to submit a batch run (currently under construction).



Clicking on the Go to User Inputs button, the user is taken to the chemical editor, the use of which is described on p. 6. For the following example, 4-aminophenol was entered into the Chemical Editor.



After clicking the Next link at the top of the workflow, the user is taken to the “Chemical Speciation” screen for calculating chemical speciation:

- Calculate Ionization
- Calculate Dominant Tautomer Distribution
- Calculate Stereoisomers

Select any combination of the calculators; use the provided default values or to change the default values required by the user. The following parameters can be adjusted:

- Calculate Ionization Constants
 - Number of decimals: Number of decimal places calculated for acidic and basic pK_a values
 - pH Lower limit: Specifies the lower end of the pH range for which the microspecies will be generated
 - pH Upper limit: Specifies the upper end of the pH range for which the microspecies will be generated
 - Generate Major Microspecies at pH: Generates the Major Microspecies at the specified pH.
 - pH step size: Specifies the pH step size for the X-Axis of the plot illustrating the distribution of the microspecies as a function of pH
- Calculate Dominant Tautomer Distribution
 - Maximum Number of Structures: Specifies the maximum number of structures that will be generated.
 - At pH: Specifies the pH at which the dominant tautomer distribution will be calculated
- Calculate Stereoisomers
 - Maximum Number of Structures: Specifies the maximum number of structures that will be generated.

[Description](#) [Inputs](#) [Batch](#) [History](#) [Connect to](#)

Calculate Chemical Speciation Workflow Inputs

Chemical Editor | Chemical Speciation

Select one or more calculation methods to run, then press submit below.

Calculate Ionization Constants (pKa) Parameters

Number of Decimals:	2
pH Lower Limit:	0
pH Upper Limit:	14
pH Step Size:	0.2
Generate Major Microspecies at pH:	7.0
Isoelectric Point (pI)	
pH Step Size for Charge Distribution:	0.5

Calculate Dominant Tautomer Distribution

Maximum Number of Structures:	100
at pH:	7.0

Calculate Stereoisomers

Maximum Number of Structures:	100
-------------------------------	-----

[Defaults](#) [Clear](#) [Back](#) [Submit](#)

Calculate Ionization Constants (pKa) Parameters

Once the calculate button is clicked, click the submit button to view the purpose of this demonstration.

click the submit button for the

[Description](#) [Inputs](#) [Batch](#) [History](#) [Connect to](#)

Calculate Chemical Speciation Workflow Inputs

Chemical Editor | Chemical Speciation

Select one or more calculators of interest, then press submit.

Calculate Ionization Constants (pKa) Parameters

Number of Decimals:	2
pH Lower Limit:	0
pH Upper Limit:	14
pH Step Size:	1.2
Generate Major Microspecies at pH:	7.0
Isoelectric Point (pI)	
pH Step Size for Charge Distribution:	0.5

Calculate Dominant Tautomer Distribution

Maximum Number of Structures:	100
at pH:	7.0

Calculate Stereoisomers

Maximum Number of Structures:	100
-------------------------------	-----

[Defaults](#) [Clear](#) [Back](#) [Submit](#)

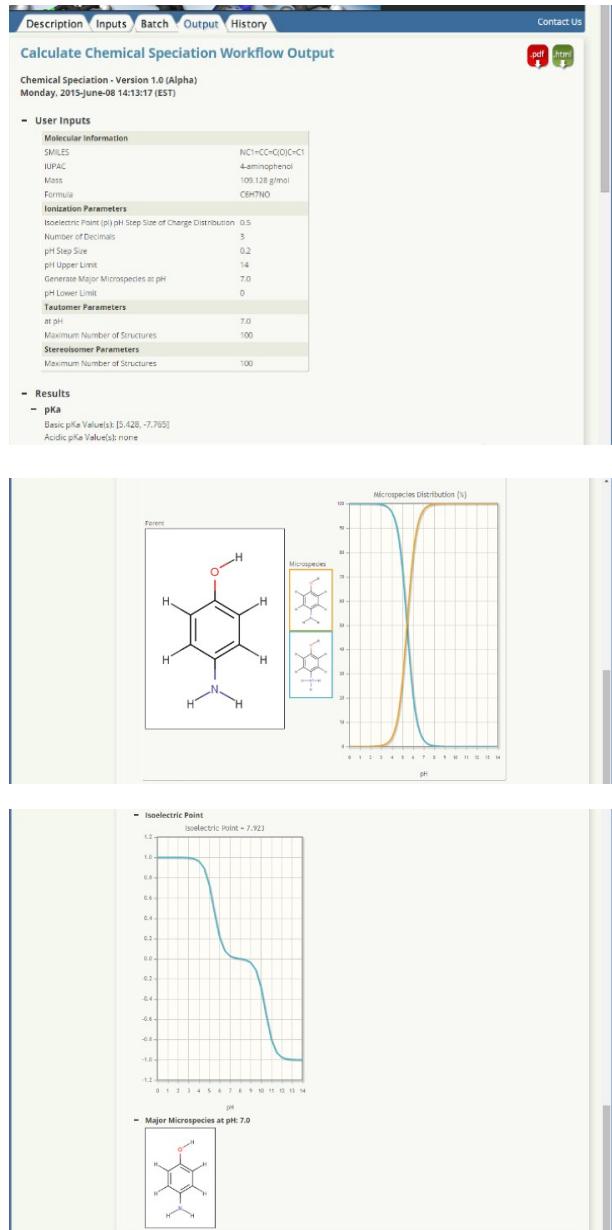
The results of the Inputs: The mole

- **pKa Calc** and the di
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- **Isoelectri** charge on

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nicrospecies, specified.

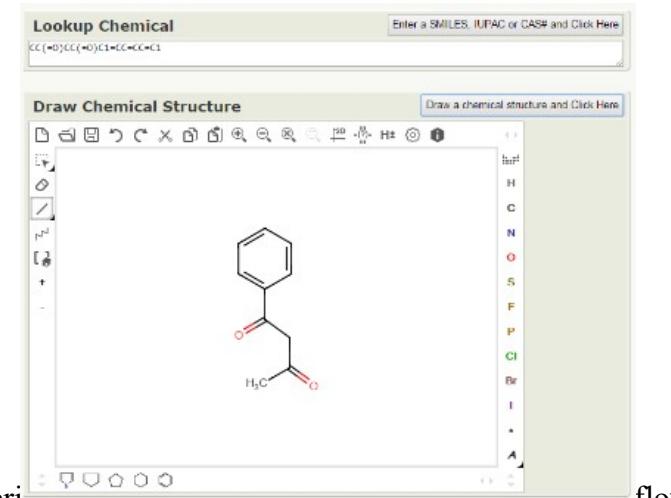
cating the



Major Microspecies: The dominant microspecies formed at the pH selected.

Calculate Dominant Tautomer Distribution

For the purpose of this demonstration, 1-phenylbutane-1,3-dione has been entered into the Chemical Editor.



Clicking the Next button brings up the Calculate Chemical Speciation Workflow page. After selecting the Calculate Dominant Tautomer Distribution option, the number of possible tautomers is displayed. The default values are pH 7.4 and a maximum of 100 structures.

flow Inputs page. a limit for the ill be calculated. The

Results
SMILES: CC(=O)CC(=O)C1=CC=C(C=C1)C2=CC=CC=C2
IUPAC: 1-phenylbutane-1,3-dione
Formula: C10H10O2

Description Inputs Batch History Contact Us

Calculate Chemical Speciation Workflow Inputs

Check one or more calculation methods to run, then hit submit below

Calculate Ionization Constants (pKa) Parameters

Number of Decimals: 2
pH Lower Limit: 0
pH Upper Limit: 14
pH Step Size: 0.2
Generate Major Micropoles at pH: 7.0
Isoelectric Point (pI): 0.5
pH Step Size for Charge Distribution: 0.5

Calculate Dominant Tautomer Distribution

Description Inputs Batch Output History Details

Calculate Chemical Speciation Workflow Output

Chemical Speciation - Version 1.0 (Alpha)
Tuesday, 28-May-05 09:34:11 (EST)

User Inputs

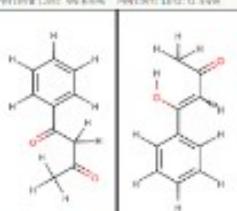
Molecular Information
Name: 1-phenylbutane-1,3-dione
IUPAC: 1-phenylbutane-1,3-dione
Mass: 162.18 g/mol
Formula: C10H10O2

Ionization Parameters
Isoelectric Point (pI): 0.5
pH Step Size of Charge Distribution: 0.5
Number of Decimals: 2
pH Lower Limit: 0
pH Upper Limit: 14
Generate Major Micropoles at pH: 7.0
pH Lower Limit: 0
Tautomer Parameters
at pH: 7.0
Maximum Number of Structures: 100

Tautomer Parameters
Maximum Number of Structures: 100

Results

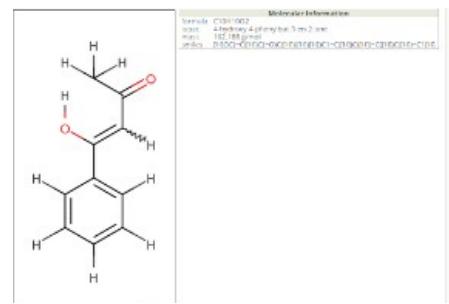
Tautomerization
Percent Dist: 99.45% Percent Dist: 0.55%



The two structures show the resonance between the two possible tautomeric forms of the molecule. In the first structure, the phenyl group is attached to the carbonyl carbon at position 1, and the double bond is at position 3. In the second structure, the phenyl group is attached to the carbonyl carbon at position 3, and the double bond is at position 1.

The Output section displays the results of the calculation. The chemical structure of the molecule is shown, along with its SMILES string, IUPAC name, mass, and formula. The ionization parameters are listed, including the number of decimals, pH lower and upper limits, pH step size, and the generation of major micropoles at a specific pH. The tautomerization parameters are also listed, including the pH at which the calculation was performed, the maximum number of structures, and the maximum number of structures.

or the chemical of
o of the structure.
ILES string is also



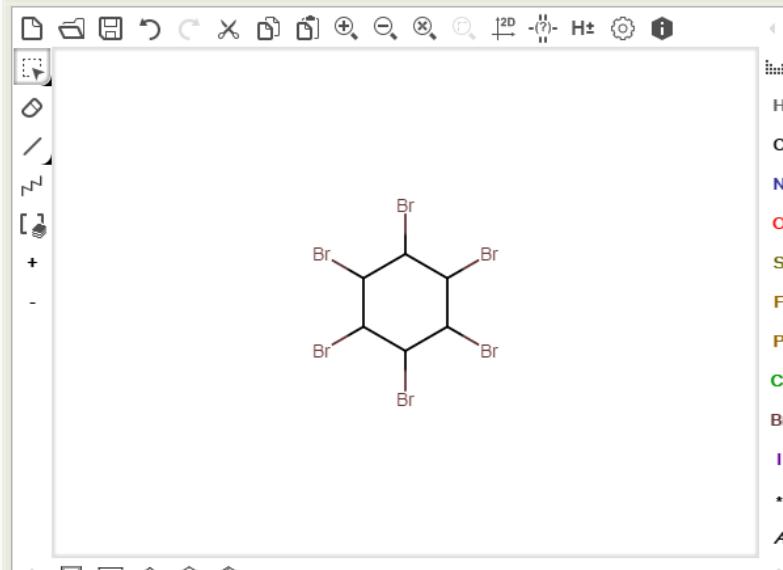
Calculate Stereoisomers

For the purpose of this demonstration, 1,2,3,4,5,6-hexabromocyclohexane has been entered into the Chemical Editor.

Enter a SMILES, IUPAC or CAS#, or draw a chemical, then click the button located in the top right of the chosen method to get results. Click the "next" button below or click the "Chemical Speciation" link above to continue through the workflow.

Lookup Chemical Enter a SMILES, IUPAC or CAS# and Click Here
BrC1C(Br)C(Br)C(Br)C(Br)C1Br

Draw Chemical Structure Draw a chemical structure and Click Here



The chemical editor interface shows a cyclohexane ring with all six carbons substituted with bromine atoms. The structure is drawn in a chair conformation. The editor includes a toolbar with various drawing tools and a periodic table on the right side.

Results

SMILES:	<chem>BrC1C(Br)C(Br)C(Br)C(Br)C1Br</chem>
IUPAC:	1,2,3,4,5,6-hexabromocyclohexane
Formula:	C ₆ H ₆ Br ₆
Weight:	557.538

Clear **Next**

After selecting the Calculate Stereoisomers option, enter a limit for the maximum number of possible stereoisomers. The default value is 100 stereoisomers.

The screenshot shows the 'Calculate Chemical Speciation Workflow Inputs' page. In the 'Calculate Stereoisomers' section, the 'Maximum Number of Structures' is set to 100. Below this, there is a list of calculated stereoisomers for the input molecule.

Clicking on the Next button will take you to the next step in the workflow. Individual structures can be enlarged by placing the cursor over them. The formula, IUPAC name, and CAS number are also displayed.

te that individual structures can be enlarged by placing the cursor over them including the formula, IUPAC name, and CAS number.

The screenshot shows the 'Calculate Chemical Speciation Workflow Output' page. It displays the calculated stereoisomers for the input molecule. The 'Molecular Information' section provides the formula, IUPAC name, mass, and SMILES string for the molecule.

Calculate p-chem properties

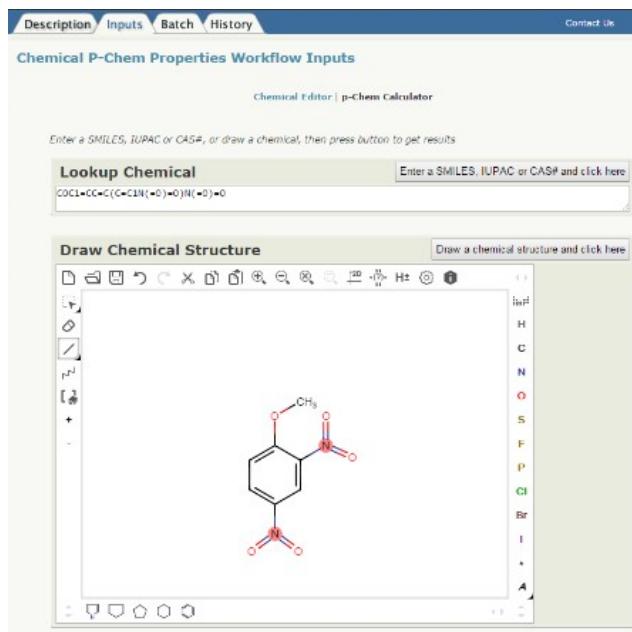
Selection of workflow options for chemical property construction

Provides this page illustrating the selection of workflow options for the Inputs tab to submit a single chemical for a batch run (currently under construction).



For the purpose of this exercise, we will use the chemical editor. Select the 'Inputs' tab.

been entered into the chemical editor. Select the 'Inputs' tab.



Use the Calculate p-Chem Properties Workflow Inputs screen to select p-chem properties and the p-chem calculators of interest. Selection of the All button for the p-chem properties will only provide the available properties for the selected p-chem calculators.

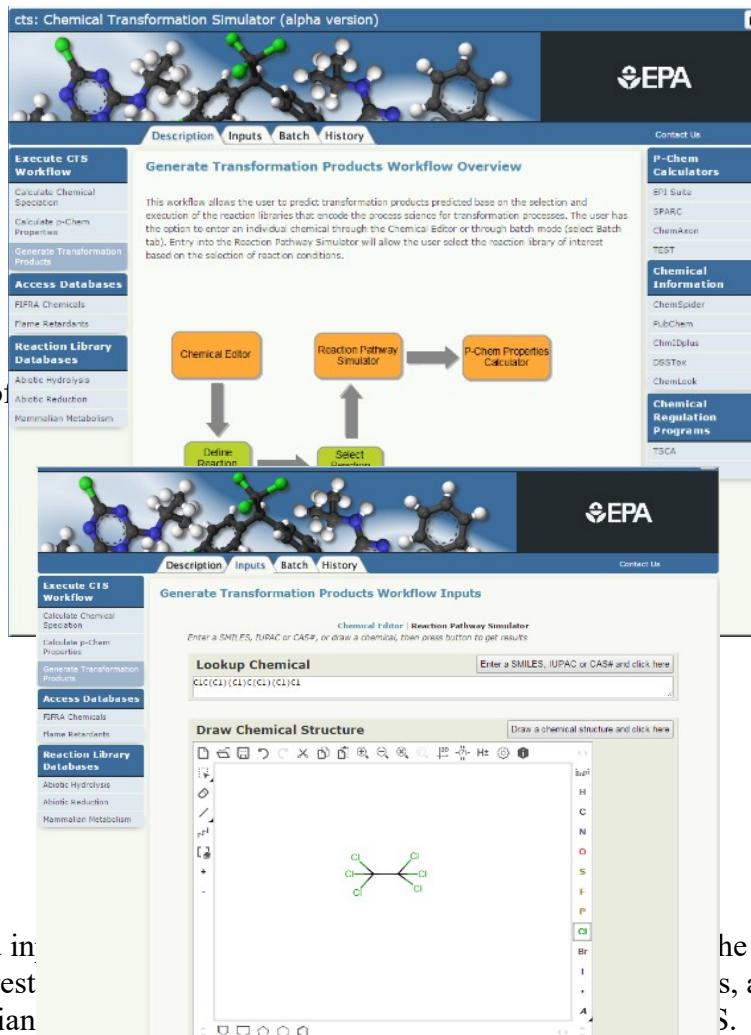
	ChemAxon	EPI Suite	TEST	SPARC	Measured
All	<input checked="" type="checkbox"/>				
Melting Point (°C)	<input type="checkbox"/>				
Boiling Point (°C)	<input type="checkbox"/>				
Water Solubility (mg/L)	<input type="checkbox"/>				
Vapor Pressure (mmHg)	<input type="checkbox"/>				
Molecular Diffusivity (cm ² /s)	<input type="checkbox"/>				
Ionization Constant	<input checked="" type="checkbox"/>				
Henry's Law Constant (atm·m ³ /mol)	<input type="checkbox"/>				
Octanol/Water Partition Coefficient	<input checked="" type="checkbox"/>				
Octanol/Water Partition Coefficient at pH: 7.4	<input checked="" type="checkbox"/>				
Organic Carbon Partition Coefficient	<input type="checkbox"/>				

The Calculate p-Ch selected p-chem pro

f the previously

Generate Transformation Products Workflow

Selection of the Generate Transformation Products Workflow provides this window illustrating the workflow overview. Click on the Go to User Inputs button or the Inputs tab to submit a single chemical for processing, or click on the Batch tab to submit a batch run (currently under construction).



For the purpose of this exercise, we will focus on the chemical editor.

The first required input is the reaction pathways of interest. Phase 1 mammalian metabolism is available for download.

The transformation products are abiotic reduction and photolysis. Three options are

This screenshot shows the 'Generate Transformation Products' form. It features a 'Chemical Editor | Reaction Pathway Simulator' header and a note: 'Choose one of the guidelines to help select the appropriate reaction libraries or choose "User selected (advanced)" to manually select the reaction libraries to use for generating transformation products, then click submit.' Below this is a 'Options for selecting Reaction Libraries' section with three radio buttons: 'Reaction System Guidelines' (selected), 'OCSPP Guidelines', and 'User selected (advanced)'. A 'Reaction Libraries' list includes checkboxes for Abiotic Hydrolysis, Aerobic Biodegradation, Photolysis, Abiotic Reduction, Anaerobic Biodegradation, and Mammalian Metabolism. To the right is a 'Reaction Options' section with dropdowns for 'Number of generations' (set to 1) and 'Likelihood limit' (set to 0.001). At the bottom are 'Clear', 'Back', and 'Submit' buttons.

Selection of the Reaction System Conditions provides 2 options for reaction systems: Environmental or Mammalian.

Selection of the Environmental Reaction System provides the option to select respiration type: Aerobic or Anaerobic.

Selection of anaerobic respiration opens the window with the reactions libraries for the transformation pathways that are currently available and will potentially occur under these reaction conditions, which includes abiotic hydrolysis and abiotic reduction.

Selection of the Reaction System Conditions provides 2 options for reaction systems: Environmental or Mammalian.

Selection of the Environmental Reaction System provides the option to select respiration type: Aerobic or Anaerobic.

Selection of anaerobic respiration opens the window with the reactions libraries for the transformation pathways that are currently available and will potentially occur under these reaction conditions, which includes abiotic hydrolysis and abiotic reduction.

Generate Transformation Products Workflow Inputs

Chemical Editor | Reaction Pathway Simulator

Choose one of the guidelines to help select the appropriate reaction libraries or choose "User selected (advanced)" to manually select the reaction libraries to use for generating transformation products, then click submit.

Options for selecting Reaction Libraries

Reaction System Guidelines OCSPP Guidelines User selected (advanced)

Reaction system

Environmental Mammalian

Select a respiration type

Anaerobic

Reaction Libraries

Abiotic Hydrolysis
 Aerobic Biodegradation
 Photolysis
 Abiotic Reduction
 Anaerobic Biodegradation
 Mammalian Metabolism

Reaction Options

Generation Limit: 1
Population Limit: 0
Likely Limit: 0.001

Defaults Clear Back Submit

Selection of mammalian reaction systems opens the window with the mammalian reactions library selected. This is the only option available for the mammalian reaction system.

P s

Options for selecting Reaction Libraries

Reaction System Guidelines OCSPP Guidelines User selected (advanced)

Reaction system

Environmental Mammalian

Reaction Libraries	
<input type="checkbox"/> Abiotic Hydrolysis	
<input type="checkbox"/> Aerobic Biodegradation	
<input type="checkbox"/> Photolysis	
<input type="checkbox"/> Abiotic Reduction	
<input type="checkbox"/> Anaerobic Biodegradation	
<input checked="" type="checkbox"/> Mammalian Metabolism	

Reaction Options	
Generation Limit:	1 ▼
Population Limit:	0 ▼
Likely Limit:	0.001

Defaults Clear Back Submit

Choose one of the guidelines to help select the appropriate reaction libraries or choose "User selected (advanced)" to manually select the reaction libraries to use for generating transformation products, then click submit.

Options for selecting Reaction Libraries

Reaction System Guidelines OCSPP Guidelines User selected (advanced)

OECD Selection

Fate, Transport, and Transformation (Series 835) Health Effects (Series 870)

Fate, Transport, and Transformation

Laboratory Abiotic Transformation Guidelines ▾

Reaction Libraries	
<input checked="" type="checkbox"/> Abiotic Hydrolysis	
<input type="checkbox"/> Aerobic Biodegradation	
<input type="checkbox"/> Photolysis	
<input checked="" type="checkbox"/> Abiotic Reduction	
<input type="checkbox"/> Anaerobic Biodegradation	
<input type="checkbox"/> Mammalian Metabolism	

Reaction Options	
Generation Limit:	1 ▼
Population Limit:	0 ▼
Likely Limit:	0.001

Defaults Clear Back Submit

Reaction Libraries	
<input type="checkbox"/> Aerobic Biodegradation	
<input type="checkbox"/> Photolysis	
<input type="checkbox"/> Abiotic Reduction	
<input type="checkbox"/> Anaerobic Biodegradation	
<input checked="" type="checkbox"/> Mammalian Metabolism	

Reaction Options	
Generation Limit:	1 ▼
Population Limit:	0 ▼
Likely Limit:	0.001

Defaults Clear Back Submit

Selection of mammalian reaction systems opens the window with the mammalian reactions library selected. This is the only option available for the mammalian reaction system. (i.e., because the abiotic hydrolysis and abiotic reduction are appropriate selections for this option.)

The third option for the selection of reaction libraries is through the selection of the User Selected, which is considered to be an option for the more advanced user. This option provides the ability to select amongst the currently available reaction libraries that are highlighted in bold text.

Choose one of the guidelines to help select the appropriate reaction libraries or choose "User selected (advanced)" to manually select the reaction libraries to use for generating transformation products, then click submit.

Options for selecting Reaction Libraries

Reaction System Guidelines OCSPP Guidelines User selected (advanced)

Reaction Libraries		Reaction Options
<input type="checkbox"/>	Abiotic Hydrolysis	Generation Limit: <input type="text" value="1"/>
<input type="checkbox"/>	Aerobic Biodegradation	Population Limit: <input type="text" value="0"/>
<input type="checkbox"/>	Photolysis	Likely Limit: <input type="text" value="0.001"/>
<input type="checkbox"/>	Abiotic Reduction	
<input type="checkbox"/>	Anaerobic Biodegradation	
<input type="checkbox"/>	Mammalian Metabolism	

After synthesis Reaction

Defaults **Clear**

Back

Submit

- **Generation Limit:** the maximum number of generations of transformation products that will be generated
 - **Population limit:** the maximum number of products that can be formed in one generation (currently not functional)
 - **Likely Limit:** limits the global accumulation of products based on likelihood values (currently not functional)

After selection of the reaction libraries and reaction options have been set, click the "Run" button to generate transformation products. The results screen summarizes the 1st generation of transformation products (the default) and provides the 2nd and 3rd generations. The results screen also lists the abiotic hydrolysis and reduction libraries. Expand the number of generations by clicking the "More" button. Click the drop down at the top left hand corner of the reaction pathway map to change the generation level. The reaction pathway map right below illustrates the reaction pathway map for the formation of the 3rd generation transformation products. Note, that the number of observed generations cannot be increased beyond the number of generations shown on the previous screen. By mousing over a product, a number of reaction pathways leading to that product will be displayed on the reaction pathway map. For this example, **tetrachloroethene** is the third generation from the 2nd product (i.e., **pentachloroethane**) and the second generation from **hexachloroethane**.

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By right-clicking on a product, the molecular and metabolite information for the product is displayed. In the β -version of the CTS, the transmissivity, production and accumulation values have no significance.

Generate Transformation Products Workflow Output

Generate Transformation Pathways Version 1.0 (Alpha)
Monday, 2015-June-08 17:02:32 (EST)

- User Inputs

Molecular Information	
SMILES	<chem>C(Cl)(C(Cl)(C(Cl)(Cl)Cl)Cl)Cl</chem>
IUPAC	hexachloroethane
Mass	236.72 g/mol
Formula	C ₂ C ₆
Reaction Pathway Simulator	
Libraries	hydrolysis, abiotic_reduction
Likely Limit	0.001
Generation Limit	1
Population Limit	none

- Reaction Pathways

Select (right-click) a metabolite to view its properties.

Metabolites can be viewed by generation using the "Display up to" selection below, or view a metabolite's progeny by left-clicking the metabolite of interest.

If some metabolites are hidden, the canvas can be panned by holding down the left-click and moving the mouse.

Display up to: 1st gen ▾

- View Molecular Information

Molecular Information

formula: C₂H₅Cl₆
iupac: 1,1,1,2,2-pentachloroethane
mass: 202.28
smiles: C(Cl)(C(Cl)(C(Cl)(Cl)Cl)Cl)Cl

+ Get p-Chem Data

cts: Chemical Transformation Simulator (alpha version)

The next generation of transformation products that are predicted to form from a selected product are displayed by left-clicking one of the products. For this example, tetrachloroethylene was selected to show the 2nd generation product trichloroethylene.

Expanding below the transformation products table provides a preview for p-

Reaction Pathways

Metabolite Info p-Chem Data

This window is for displaying metabolite data as well as retrieving it. First, right-click a metabolite to view any data it already has. Select the "Get data" tab to get p-chem properties for the metabolite.

CCl2=CCl2

Description Inputs Batch Output History

Generate Transformation Products Workflow Output
Generated: 10/10/2015 10:44:14 AM (EST)
Monday, 10/12/2015 10:44:14 AM (EST)

Show Inputs

Molecular Schematics

- SMILES: CC(Cl)=CC(Cl)
- KEKULÉ:
- Mass: 126.96
- PERIODS: 2.0

Reaction Pathway Simulator

- LODD: 1.00E-10
- Kinetic Limit: 0.001
- Regulation Limit: 1.000
- Population Limit: 10000

Retention Pathways

Metabolite Info p-Chem Data

Select p-chem properties to gather for selected metabolite, then click "Get data" below.

	Overdrive	EPI Suite	TBT	SPIKE	Measured
All	Available	Uncalibrated			
Melting Point (°C)					
Boiling Point (°C)					
Water Solubility (mg/L)					
Vapor Pressure (mmHg)					
Molecular Diffusivity (cm ² /s)					
Ionization Constant					
Hansch's Lipophilicity Coefficient					
Octanol/Water Partition Coefficient at pH 7					
Organic Carbon Partition Coefficient					

Generate Transformation Products Workflow Output

Generated: 10/10/2015 10:44:14 AM (EST)
Monday, 10/12/2015 10:44:14 AM (EST)

Show Inputs

Molecular Schematics

- SMILES: CC(Cl)=CC(Cl)
- KEKULÉ:
- Mass: 126.96
- PERIODS: 2.0

Reaction Pathway Simulator

- LODD: 1.00E-10
- Kinetic Limit: 0.001
- Regulation Limit: 1.000
- Population Limit: 10000

Retention Pathways

Metabolite Info p-Chem Data

Select p-chem properties to gather for selected metabolite, then click "Get data" below.

	Overdrive	EPI Suite	TBT	SPIKE	Measured
All	Available	Uncalibrated			
Melting Point (°C)					
Boiling Point (°C)					
Water Solubility (mg/L)					
Vapor Pressure (mmHg)					
Molecular Diffusivity (cm ² /s)					
Ionization Constant					
Hansch's Lipophilicity Coefficient					
Octanol/Water Partition Coefficient at pH 7					
Organic Carbon Partition Coefficient					

Target

CCl2=CCl2

CC(Cl)=CC(Cl)

CC(Cl)=CC(Cl)Cl

CC(Cl)=CC(Cl)Cl

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To get p-chem data for multiple metabolites, select the option for up to the first, second, or third generation of metabolites, or for all calculated metabolites from the drop-down menu. Then select the properties and calculators to be used, and click the “Get data” button. The results for multiple metabolites will not be presented in the table as they are for a single metabolite. To view the results for multiple metabolites, download and view the PDF report as described on page 11 of this guide.