

OpenTox Applications

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London, UK



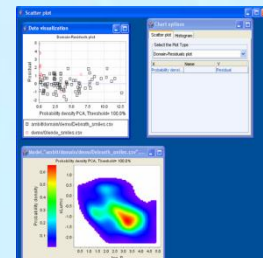
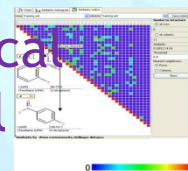
ToxPredict



Introduction

- Develops and maintains several well-known open source software products, in particular
 - Toxtree (used in the application of the threshold of toxicological concern)
 - Toxmatch (for encoding and applying chemical similarity indices)
 - Ambit (a QSAR decision support system, including generic database management, structure conversions and searching, as well as applicability domain assessment).
- These tools have been carefully designed and developed in close co-operation both with academia, regulatory bodies and industry.

- Toxtree 2.1.0 - estimates toxic hazard by applying a decision tree approach
- Toxmatch 1.06 - A chemical similarity evaluation tool
- Ambit Discovery
- Ambit Database Tools
- QMRF repository
- Ambit XT
- Partner in OpenTox FP7 project
- Partner in CADASTER FP7 project



Toxtree 2.1.0

<http://toxtree.sourceforge.net>

Toxtree - Toxic Hazard Estimation by decision tree approach

Toxtree is a full-featured and flexible user-friendly open source application, which is able to estimate toxic hazard by applying a decision tree approach. Toxtree can be applied to datasets from various compatible file types. User-defined molecular structures are also supported - they could be entered by SMILES, or by using the built-in 2D structure diagram editor.

Toxtree Online

Find chemical compounds and apply Toxtree online!

- Threshold of Toxicological Concern (TTC) estimation (Kroes/ILSI decision tree)
- FastTox (Several Toxtree modules)

Multiplatform

The Toxtree application is suitable for a standalone PC and can run on any platform, supported by Java 1.5 or higher.

Modular plugin design

Toxtree has been designed with flexible capabilities for future extensions in mind (e.g. other classification schemes that could be developed at a future date). New decision trees with arbitrary rules can be built with the help of graphical user interface or by developing new plug-ins. Toxtree was

Toxtree (Estimation of Toxic Hazard - A Decision Tree Approach) v2.1.0

Enter SMILES: c1ccccc1N=Cc2ccccc2

Available structure attributes

BSSTM1_1	1.0000
BSSTM1_2	1.0000
BHOMO_1	-8.0269
BHOMO_2	-8.3905
ELLUMO_1	0.4260
ELLUMO_2	0.4398

Error when applying the decs... NO
For a better assessment a Q... NO

Structure diagram

Toxic Hazard

by Benigni / Bossa rulebase (for mutagenicity and carcinogenicity)

Estimate

Structural Alert for genotoxic carcinogenicity

Structural Alert for non-genotoxic carcinogenicity

Potential S. typhimurium TA100 mutagen based on QSAR

Unlikely to be a S. typhimurium TA100 mutagen based on QSAR

Potential carcinogen based on QSAR

☒ Verbose explanation

- QSA18.Polycyclic Aromatic Hydrocarbons **No**
- QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons **No**
- QSA21.Alkyl and aryl N-nitroso groups **No**
- QSA22.Acide and triazene groups **No**
- QSA23.Aliphatic N-nitro **No**
- QSA24.α,β unsaturated alkoxy **No**
- QSA25.Aromatic nitroso group **No**
- QSA26.Aromatic ring N-oxide **No**
- QSA27.Nitro aromatic **No**
- QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) **Yes**
- QSA28bis.Aromatic mono- and dialcylamine **Yes**
- QSA28ter.Aromatic N-acyl amine **No**
- QSA29.Aromatic diazo **Yes**
- QSA30.Coumarins and Furocoumarins **No**

Toxtree was commissioned by [JRC Computational Toxicology](#). Plugins are currently being developed by IdeaConsult and several other organisations.

Toxtree 2.1.0 modules:

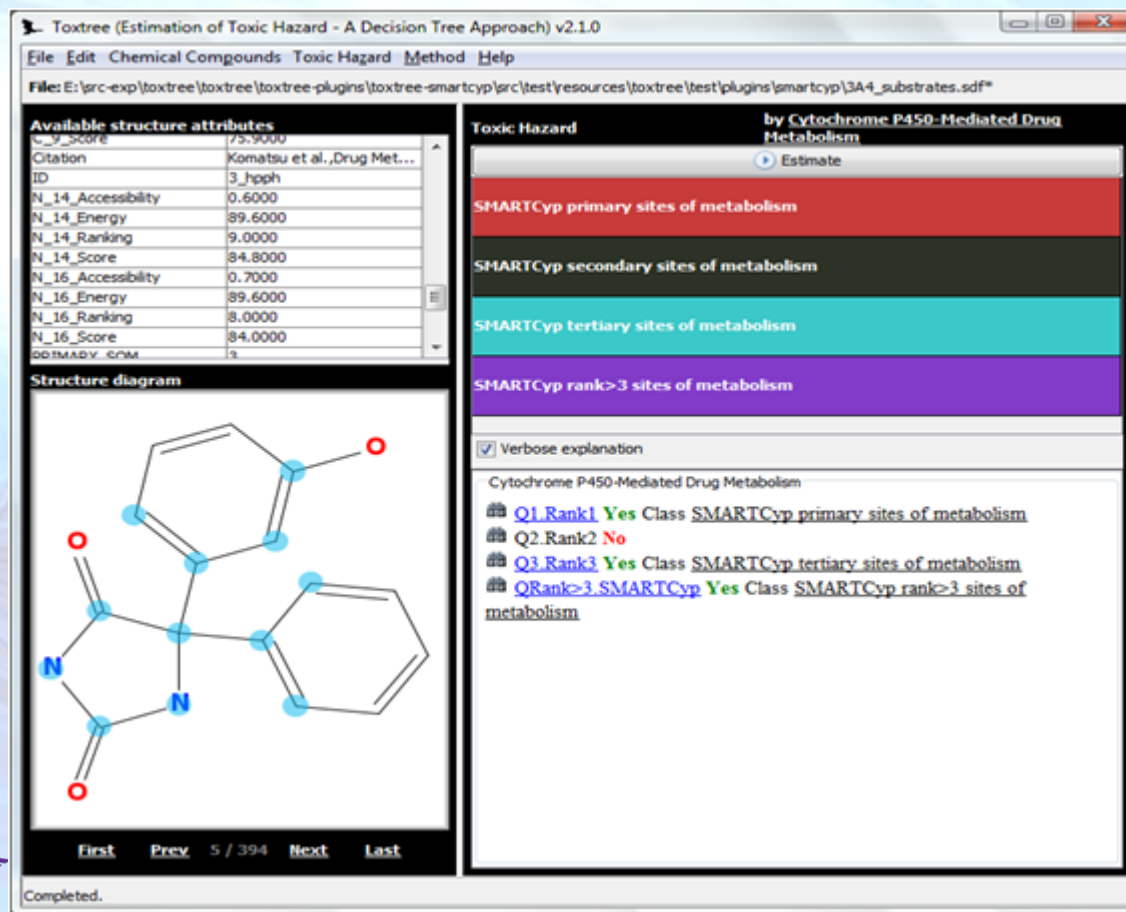
<http://toxtree.sourceforge.net>

1. Cramer rules
2. Verhaar scheme for predicting toxicity mode of actions
3. Skin irritation and corrosion potential estimation
4. Eye irritation and corrosion potential estimation
5. Benigni-Bossa rulebase for carcinogenicity and mutagenicity prediction
6. Cramer rules with extensions
7. Structure Alerts for the in vivo micronucleus assay in rodents
8. START (Structural Alerts for Reactivity in Toxtree) biodegradation and persistence plug-in
9. Michael Acceptors identification
10. Skin sensitisation alerts (new)
11. Kroes TTC decision tree (new)
12. SMARTCyp - Cytochrome P450-Mediated Drug Metabolism (new)

Toxtree 2.1.0 : 3 new modules

SMARTCyp - Cytochrome P450-Mediated Drug Metabolism

Patrik Rydberg, David E. Gloriam, Jed Zaretski, Curt Breneman, Lars Olsen, SMARTCyp: A 2D Method for Prediction of Cytochrome P450-Mediated Drug Metabolism, ACS Med. Chem. Lett., 2010, 1 (3), pp 96-100



Why integration framework for predictive toxicology?

- What if we would like to:
 - Compare multiple models
 - Reproduce a model from the literature
 - Merge data from different sources (files, databases)
 - Find all models available for certain endpoint
 - More ...



Why integration framework for predictive toxicology?

- Challenges:
 - Chemical structures
 - Might be ambiguous
 - Might be error prone or time consuming to reproduce from publications
 - Data
 - **Multiple formats,**
 - **Implicit semantics,** often buried in human readable documentation only
 - Models
 - **Tens of thousands** available, in software or in publications
 - Multiple software solutions, mostly incompatible
 - Predictions **reproducibility** is time consuming and often hard to achieve
 - Automatic **comparison of prediction results** difficult

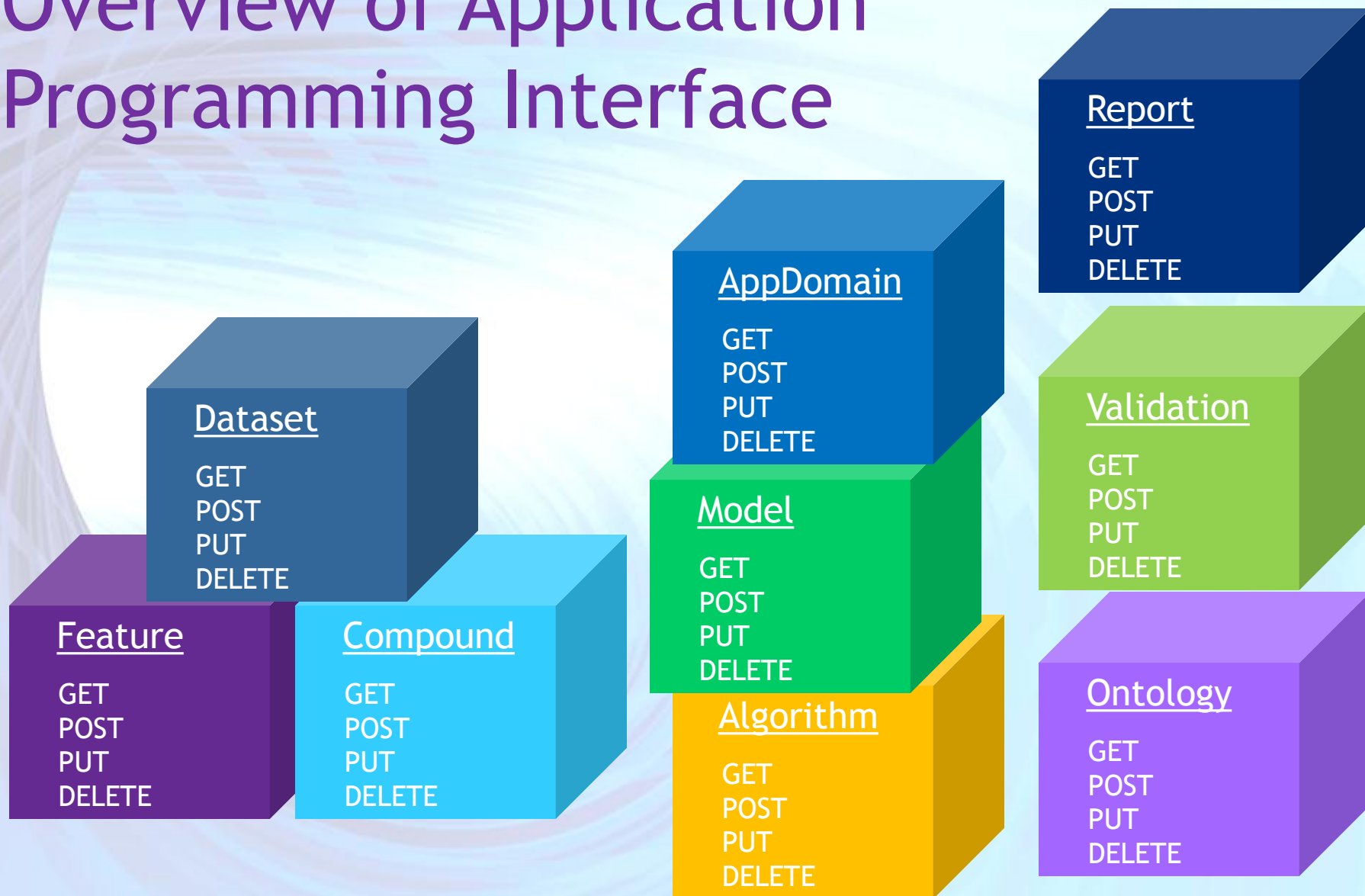
OpenTox Framework approach

User Requirements		Software Requirements
Unambiguous data	⇒	<i>formal way of representing information about data</i>
Unambiguous access	⇒	<i>well-defined interfaces</i>
Transparency of computational tools	⇒	<i>formal way of representing information about methods, well-defined interfaces</i>
Variety of user groups	⇒	<i>simplicity and modularity of design</i>
Need to integrate various resources (e.g., databases, prediction methods, models, ...) to make meaningful predictions	⇒	<i>distributed architecture, interoperability</i>
Need to integrate biological information	⇒	<i>again, modularity of design, extensibility</i>

OpenTox framework

- Distributed Web Services for predictive toxicology
- Several types of Web Services (using REST Web service technology)
- Service types corresponds to following building blocks :
 - Chemical compound;
 - Dataset of chemical compounds and their properties (calculated or measured)
 - Algorithm (descriptor calculation, regression, classification, structural alerts, QC, etc.)
 - Predictive model
 - Report, validation, applicability domain, etc.
- Every object (compound, dataset, algorithm, model, etc.) has an unique web address (e.g. <http://myhost.com/model/bestpredictivemodel>)
- These objects can be created, read, deleted, and updated
- Every object has RDF (W3C Resource Description Framework) representation, defined in OpenTox ontology (opentox.owl)

Overview of Application Programming Interface



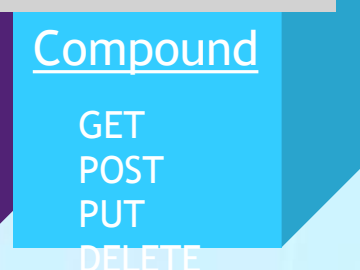
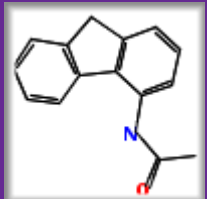
OpenTox datasets: Unified access to data

Everything described by W3C RDF (Resource Description framework)

Compound/ Data	http://myhost.com/feature/21580	http://myhost.com/feature/21589	http://myhost.com/feature/21573	http://myhost.com/feature/21576	http://myhost.com/feature/21588	http://myhost.com/feature/21858	http://myhost.com/feature/22114
http://myhost.com/compound/413	N,N-dimethyl-4-aminoazobenzene	<chem>CN(C1=CC=C(C=C1)N=N/C2=CC=CC=C2)C</chem>	3	3.31	225.3	YES	3.123
http://myhost.com/compound/44497	4-acetamidofluorene	<chem>O=C(Nc3c2c1cccc1Cc2ccc3)C</chem>	1	NP	223.28	YES	2.085
...



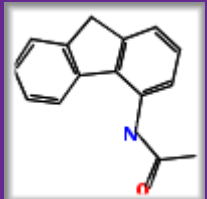
All columns have explicit and machine readable pointers to originating algorithms, models or data



OpenTox datasets: Unified access to data

Everything described by W3C RDF (Resource Description framework)

Compound/ Data	http://myhost.com/feature/21580	http://myhost.com/feature/21589	http://myhost.com/feature/21573	http://myhost.com/feature/21576	http://myhost.com/feature/21588	http://myhost.com/feature/21858	http://myhost.com/feature/22114
http://myhost.com/compound/413	N,N-dimethyl-4-aminoazobenzene	<chem>CN(C1=CC=C(C=C1)N=N/C2=CC=CC=C2)C</chem>	3	3.31	225.3	YES	3.123
http://myhost.com/compound/44497	4-acetamidofluorene	<chem>O=C(Nc1ccc2ccccc2c1)C</chem>					
...					



<http://myhost.com/feature/21573>

af:21573

```

a      ot:Feature , ot:NumericFeature , ot:NominalFeature ;
      dc:creator
      "http://www.epa.gov/NCCT/dssto/sdf_isscan_external.html" ;
      dc:title "Canc" ;
      ot:hasSource "ISSCAN_v3a_1153_19Sept08.1222179139.sdf" ;
      =      otee:Carcinogenicity .
    
```

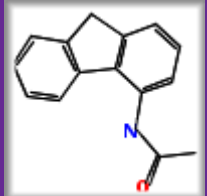
GET
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GET
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DELETE

OpenTox datasets: Unified access to data

Everything described by W3C RDF (Resource Description framework)

Compound/ Data	http://myhost.com/feature/21580	http://myhost.com/feature/21589	http://myhost.com/feature/21573	http://myhost.com/feature/21576	http://myhost.com/feature/21588	http://myhost.com/feature/21858	http://myhost.com/feature/22114
http://myhost.com/compound/413	N,N-dimethyl-4-aminoazobenzene	<chem>CN(C1=CC=C(C=C1)N=N/C2=CC=CC=C2)C</chem>	3	3.31	225.3	YES	3.123
http://myhost.com/compound/44497	4-acetamidofluorene	<chem>CC(=O)Nc1ccc2ccccc2c1</chem>					
...					



<http://myhost.com/feature/21573>

<http://myhost.com/feature/21858>

dc:title "Structural Alert for genotoxic carcinogenicity"
ot:hasSource

<<http://myhost.com/algorithm/Benigni+%2F+Bossa+rulebase+%28for+mutagenicity+and+carcinogenicity%29>> ;

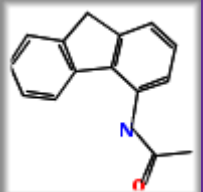
PUT
DELETE

PUT
DELETE

OpenTox datasets: Unified access to data

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Compound/ Data	http://myhost.com/feature/21580	http://myhost.com/feature/21589	http://myhost.com/feature/21573	http://myhost.com/feature/21576	http://myhost.com/feature/21588	http://myhost.com/feature/21858	http://myhost.com/feature/22114
http://myhost.com/compound/413	N,N-dimethyl-4-aminoazobenzene	<chem>CN(C1=CC=C(C=C1)N=N/C2=CC=CC=C2)C</chem>	3	3.31	225.3	YES	3.123
http://myhost.com/compound/44497	4-acetamidofluorene	<chem>CC(=O)Nc1ccc2c(c1)ccc3ccccc23</chem>					
...					



<http://myhost.com/feature/21573>

<http://myhost.com/feature/22114>

```

a      ot:Feature , ot:NumericFeature ;
      dc:creator
      "http://www.blueobelisk.org/ontologies/chemoinformatics-
      algorithms/#xlogP" ;
      dc:title "XLogP" ;
      ot:hasSource
      <http://myhost.com/algorithm/org.openscience.cdk.qsar.descriptors.
      molecular.XLogPDescriptor> ;
      =      otee:Octanol-water_partition_coefficient_Kow .
    
```

Uniform access to the data

- Ontologies are critical to unambiguously describe data
 - Opentox.owl;
 - Blue Obelisk algorithm ontology (cheminformatics algorithms);
 - OpenTox algorithm types ontology;
 - OpenTox endpoints ontology, based on ECHA endpoints classification;
 - Specific endpoints ontologies, developed by OpenTox partners with toxicology expertise;
 - Existing biomedical ontologies.
- Datasets can be easily merged, compared , and calculations reproduced, regardless of their physical place.
- OWL sameAs construct can be used to denote two links point to the same object
- Authentication and authorization to protect sensitive data

Uniform access to the data

- Datasets can be easily merged, compared, and calculations reproduced, regardless of their physical place.
- The dataset service offers property, compound, substructure and similarity searches via uniform OpenTox Application Programming

Mozilla Firefox

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http://apps.ideaconsult.net:8080/ToxPredict/user/admin/report/Stats?header=TRUE

Disable Cookies CSS Forms Images Information Miscellaneous Outline Resize Tools View Source Options

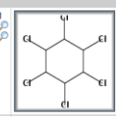
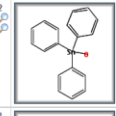
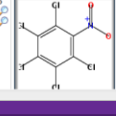
http://apps.ideaconsult.net:8080/ToxPredict/user/admin/report/Stats?header=TRUE

Number of compounds	1. pre-registered substances_20090327.xml	2. CPDBAS: Carcinogenic Potency Database - All Species	3. DBPCAN: EPA Water Disinfection By-Products with Carcinogenicity Estimates	4. ToxCast_ToxRefDB_20091214.txt	5. EPAFHM: EPA Fathead Minnow Acute Toxicity	6. KIERBL: EPA Estrogen Receptor Ki Binding Study (Laws et al.)	7. IRISTR: EPA Integrated Risk System (IRIS) Toxicity Review Data	8. FDAMDD: FDA Maximum (Recommended) Daily Dose	9. Burci mutagenicity dataset.sdf	10. c049884m_caco2-training_set.sdf	11. ECETOX Technical Report No. 66 Skin Irritation and corrosion Reference Chemicals data base (1995)	12. ISSMIC_v2a_151_2Apr09.sdf	13. Compilation of historical local lymph node assay data for the evaluation of skin
1. pre-registered substances_20090327.xml	143835	259	69	41	33	171	51						
2. CPDBAS: Carcinogenic Potency Database Summary Tables - All Species	259	1515	11	5	59	21	24						
3. DBPCAN: EPA Water Disinfection By-Products with Carcinogenicity Estimates	41	11	108	0	9	1	9						
4. ToxCast_ToxRefDB_20091214.txt	33	59	0	0	307	25	25						
5. EPAFHM: EPA Fathead Minnow Acute Toxicity	171	97	1	13	25	616	18						
6. KIERBL: EPA Estrogen Receptor Ki Binding Study (Laws et al.)	51	34	0	6	25	18	278						
7. IRISTR: EPA Integrated Risk System (IRIS) Toxicity Review Data	198	210	2	9	126	93	26						
8. FDAMDD: FDA Maximum (Recommended) Daily Dose	53	150	0	0	1	16	6						
9. Burci mutagenicity dataset.sdf	1740	503	52	36	65	180	57						
10. c049884m_caco2-training_set.sdf	22	23	0	0	0	3	1						
11. ECETOX Technical Report No. 66 Skin Irritation and corrosion Reference Chemicals data base (1995)	138	6	1	1	0	10	0						
12. ISSMIC_v2a_151_2Apr09.sdf	136	24	1	0	0	5	1						
13. Compilation of historical local lymph node assay data for the evaluation of skin	170	17	2	1	0	9	1						

Find: issca Next Previous Highlight all Match case Phrase not found

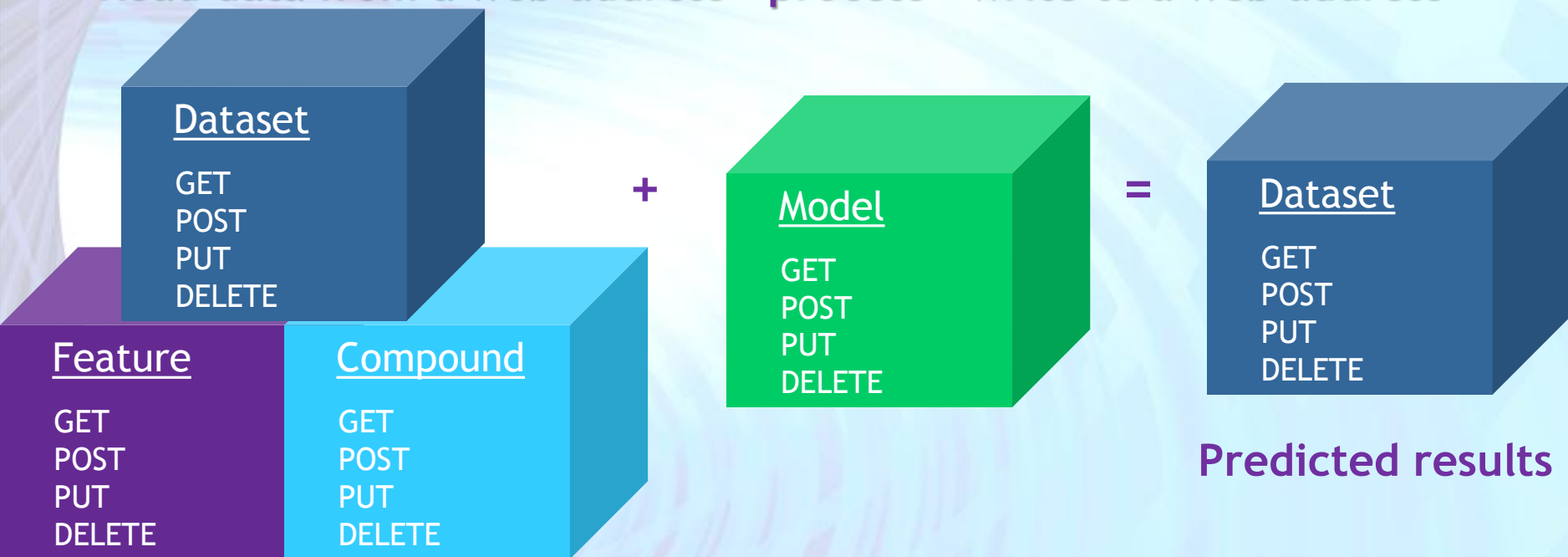
Done

Search results Dataset=112.Dataset= Download as Max number of hits: 100

Compound	ToxCast_To	ToxCast_To	ToxCast_To	ToxCast_To
	CHR_Mouse_Ureter_2_PremneoplasticlesionCHR_Mouse_Nose_1_AnylesionCHR_Rat_Trachea_3_NeoplasticlesionCHR_Mouse_Pit			
1 	1000000.0	1000000.0	1000000.0	1000000.0
2 	1000000.0	1000000.0	1000000.0	1000000.0
3 	NA	NA	1000000.0	NA

Uniform access to calculations

Read data from a web address - process - write to a web address



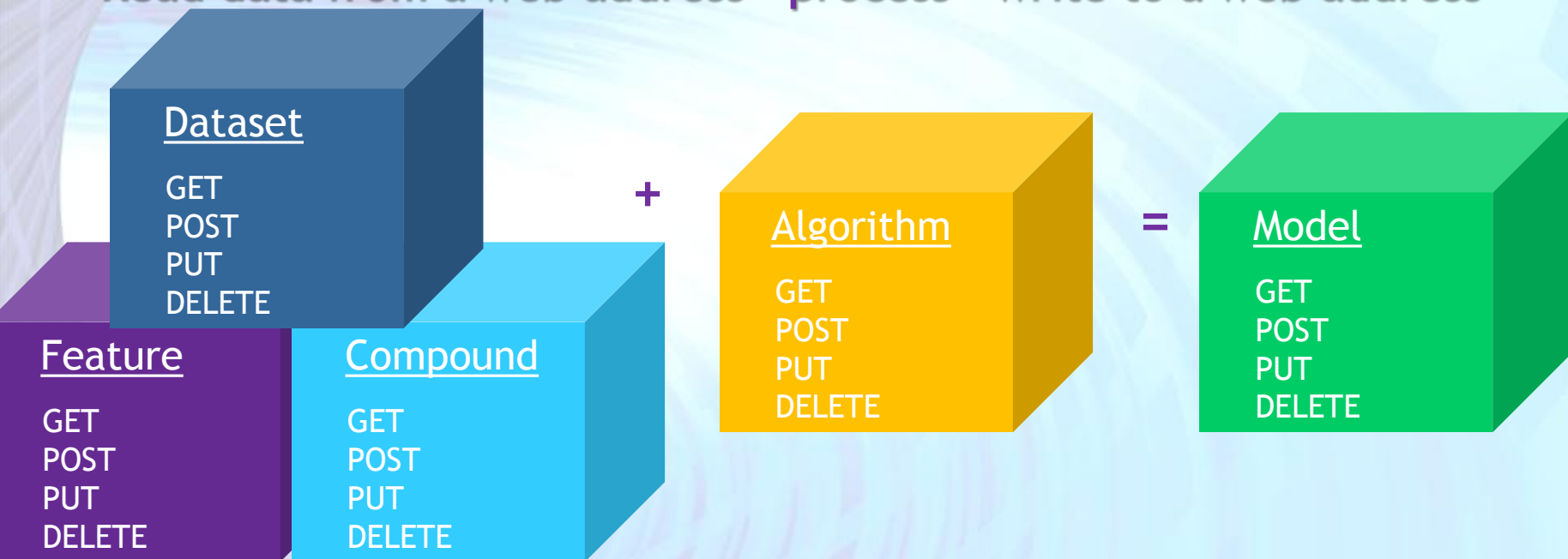
<http://myhost.com/dataset/newcompounds>

<http://myhost.com/model/predictivemodel1>

<http://myhost.com/dataset/predictedresults1>

Uniform approach to models creation

Read data from a web address - process - write to a web address



<http://myhost.com/algorithm/neuralnetwork>

<http://myhost.com/dataset/trainingset1>

<http://myhost.com/model/predictivemodel1>

Uniform approach to models validation and report generation

Read data from a web address - process - write to a web address

<http://myhost.com/dataset/trainingset1>

<http://myhost.com/dataset/predictedresults1>

Validation report

<http://myhost.com/validation>

Validation

GET
POST
PUT
DELETE

+

Dataset

GET
POST
PUT
DELETE

=

Report

GET
POST
PUT
DELETE

Model generating
predictions

Model

GET
POST
PUT
DELETE

<http://myhost.com/report/1>

OpenTox Is A Framework

Framework

- Toxicity data
- In silico models
- Validation support
- Interpretation aids

Unified Access

- Toxicologists
- Modellers
- API for new algorithm development & integration

Open Source

- To optimise impact
- To allow inspection / review
- To attract external contributors

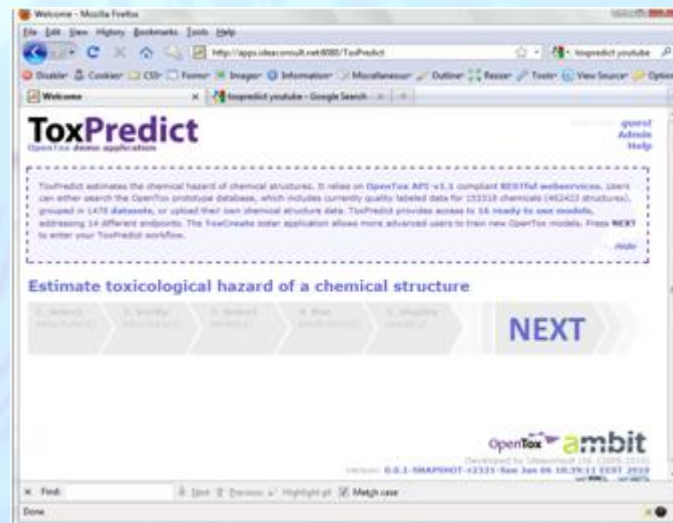
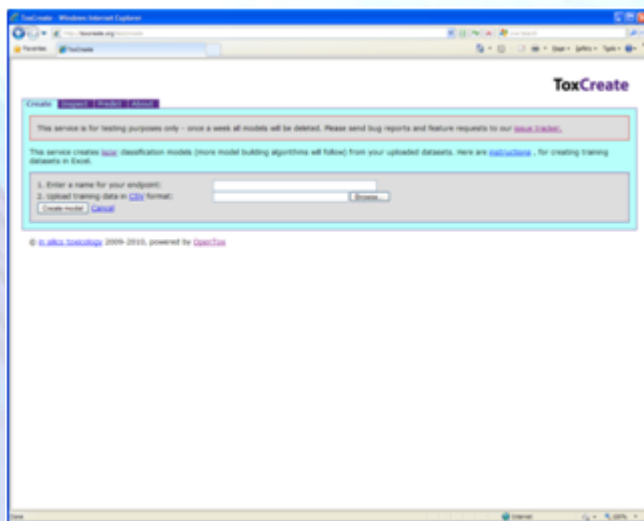
OpenTox services can be used to develop specific applications, or embedded in workflow systems

Implementation: key facts

- OpenTox webservices, regardless of their implementation specifics, could be hosted on a single computer (even a laptop or netbook would do) or could be transparently distributed on multiple servers in various physical locations, in particular for better reliability, resilience and scalability;
- OpenTox webservices could be managed by a single or multiple administrative authorities; a key feature of the OpenTox framework is that it has been **designed in a multi-domain friendly way**, which is essential for data and model sharing, repeatability and validation of prediction results (a must in 21st century!);
- OpenTox webservices could be deployed behind firewalls, in Intranets (or even offline), when very tight security policies would have to be met;
- Third parties, willing to deploy OpenTox webservices could select a relevant subset of services to run, tailored to their specific needs;

Implementation: key facts

- Two end user oriented demo applications, making use of OpenTox webservices, have been developed, deployed and are available for testing - [ToxCreate](#) and [ToxPredict](#);
- ToxCreate creates models from user supplied datasets;
- ToxPredict uses existing OpenTox models to estimate chemicalcompound properties



ToxPredict: demo

Screencast at <http://www.youtube.com/watch?v=H7gkNBz4Lwo>

ToxPredict estimates the chemical hazard of chemical structures. It relies on [OpenTox API-v1.1](#) compliant RESTful webservices. Users can either search the OpenTox prototype database, which includes currently quality labelled data for **~150,000 chemicals**, grouped in more than a dozen datasets, or upload their own chemical structure data. ToxPredict provides access to **16 ready to use models**, addressing **14 different endpoints** (and growing!);

ToxPredict uses the following OpenTox webservices: [Compound](#), [Feature](#), [Dataset](#), [Algorithm](#), [Model](#), [Task](#) and [Ontology](#);

Any model, available via OpenTox API can be easily integrated in ToxPredict by just publishing its Web address



...and now let the show begin!

After having followed this rather technical presentation, please enjoy the live demo and feel free to try how it works at toxpredict.org



We would also appreciate if you could submit any comments, suggestions, bug reports, feature requests and/or other relevant input you might have to our [issue tracker](#) or [mailing list](#).



ToxPredict

Welcome - Mozilla Firefox

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http://apps.ideaconsult.net:8080/ToxPredict

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Welcome

ToxPredict

OpenTox demo application

Welcome, [guest](#)
[Admin](#)
[Help](#)

ToxPredict estimates the chemical hazard of chemical structures. It relies on [OpenTox API-v1.1](#) compliant [RESTful webservices](#). Users can either search the OpenTox prototype database, which includes currently quality labeled data for 153554 chemicals (463141 structures), grouped in 1534 [datasets](#), or upload their own chemical structure data. ToxPredict provides access to **17 ready to use models**, addressing 15 different endpoints. The [ToxCreate](#) sister application allows more advanced users to train new OpenTox models. Press **NEXT** to enter your ToxPredict workflow.

[Hide](#)

Estimate toxicological hazard of a chemical structure

1. Select structure(s)
2. Verify structure(s)
3. Select model(s)
4. Run prediction(s)
5. Display result(s)

NEXT

OpenTox **ambit**

Developed by Ideaconsult Ltd. (2005-2010)

Version: **0.0.2-SNAPSHOT-r2393-Tue Jul 06 09:45:04 EEST 2010**

[WSO API](#) [WSO CSS](#)

Done

ToxPredict

Select - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://apps.ideaconsult.net:8080/ToxPredict/user/beat03e8-e4c6-4007-85f5-cef7d6960625/A/step1/Draw?next=

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Select

ToxPredict

OpenTox demo application

Welcome, *guest*
[Admin](#)
[Help](#)

1. Select structure(s)
2. Verify structure(s)
3. Select model(s)
4. Run prediction(s)
5. Display result(s)

NEXT

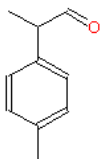
Click here for the next step

Search Draw Upload

Structure diagram

GLR DEL D-R QRY +/- UDO JME

C N O S F Cl Br I P X



Search for
☒ Structure
☐ Substructure
☐ SimilarityTanimoto 0.9

Number of hits 1

1. Select structure(s)
2. Verify structure(s)
3. Select model(s)
4. Run prediction(s)
5. Display result(s)

NEXT

Done

ToxPredict

Verify - Mozilla Firefox
http://apps.ideaconsult.net:8080/ToxPredict/user/beat03e8-e4c6-4007-85f5-cef7d6960625/A/step2

Verify

ToxPredict

OpenTox demo application

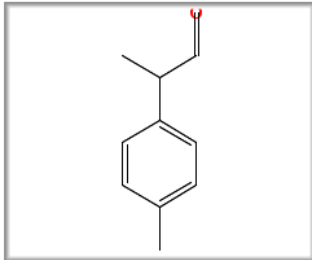
Welcome [guest](#)
[Admin](#)
[Help](#)

1. Select structure(s)
2. Verify structure(s)
3. Select model(s)
4. Run prediction(s)
5. Display result(s)

NEXT

« Page 1 Records per page 1 »

Structure(s) & Experimental Data [SDF](#) [CSV](#) [PDF](#)

1. 

CASRN 99-72-9
Synonym(s) 2-(p-tolyl)propionaldehyde
EINECS 202-782-0
IUPAC name 2-(4-methylphenyl)propanal
InChIKey_std JTZWVKUZNHSSW-SECBINFHSA-N, JTZWVKUZNHSSW-UHFFFAOYSA-N
InChI_std InChI=1S/C10H12O/c1-8-3-5-10(6-4-8)9(2)7-11/h3-7,9H,1-2H3
REACHRegistrationDate 30.11.2010
SMILES CC(C=O)c1ccc(C)cc1

1. Select structure(s)
2. Verify structure(s)
3. Select model(s)
4. Run prediction(s)
5. Display result(s)

NEXT

OpenTox **ambit**
Developed by Ideaconsult Ltd., (2005-2010)
Version: 0.0.2-SNAPSHOT-r2393-Tue Jul 06 09:45:04 EEST 2010

Done

ToxPredict

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http://apps.ideaconsult.net:8080/ToxPredict/user/bead03e8-e4c6-4007-85f5-cef7d6960625/A/step3

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Select

<input checked="" type="checkbox"/> ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity	Carcinogenicity	ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity	
<input checked="" type="checkbox"/> pKa	Dissociation constant (pKa)	pKa	
<input checked="" type="checkbox"/> ToxTree: Structure Alerts for the in vivo micronucleus assay in rodents	Endpoints	ToxTree: Structure Alerts for the in vivo micronucleus assay in rodents	
<input checked="" type="checkbox"/> ToxTree: Michael acceptors	Endpoints	ToxTree: Michael acceptors	
<input checked="" type="checkbox"/> ToxTree: Eye irritation	Eye irritation/corrosion	ToxTree: Eye irritation	
<input checked="" type="checkbox"/> Caco-2 Cell Permeability http://www.ncbi.nlm.nih.gov/pubmed/16959190	Gastrointestinal absorption	Regression: Linear regression	Model validation report
<input checked="" type="checkbox"/> OpenTox model created with TUM's PLRegression model learning web service.	Gastrointestinal absorption	http://opentox.informatik.tu-muenchen.de:8080/OpenTox-dev/algorithm/PLRegression	
<input checked="" type="checkbox"/> OpenTox model created with TUM's kNNregression model learning web service.	Gastrointestinal absorption	http://opentox.informatik.tu-muenchen.de:8080/OpenTox-dev/algorithm/kNNregression	
<input checked="" type="checkbox"/> Lipinski Rule of Five	Human health effects	Lipinski Rule of Five	
<input checked="" type="checkbox"/> ToxTree: Cramer rules	Human health effects	ToxTree: Cramer rules	
<input checked="" type="checkbox"/> XLogP	Octanol-water partition coefficient (Kow)	XLogP	
<input checked="" type="checkbox"/> START biodegradation and persistence plug-in	Persistence: Biodegradation	START biodegradation and persistence plug-in	
<input checked="" type="checkbox"/> SmartCYP: Cytochrome P450-Mediated Drug Metabolism	Protein-binding	SmartCYP: Cytochrome P450-Mediated Drug Metabolism	
<input checked="" type="checkbox"/> ToxTree: Skin irritation	Skin irritation /corrosion	ToxTree: Skin irritation	
<input checked="" type="checkbox"/> ToxTree: Skin sensitisation alerts (M. Cronin)	Skin sensitisation	ToxTree: Skin sensitisation alerts (M. Cronin)	

1. Select structure(s) 2. Verify structure(s) 3. Select model(s) 4. Run prediction(s) 5. Display result(s)

NEXT

Done

ToxPredict

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Run

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1. Select structure(s)
2. Verify structure(s)
3. Select model(s)
4. Run prediction(s)
5. Display result(s)

NEXT

Please wait for the processing of the selected prediction model(s) to be completed and then press **NEXT** to display the results.

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Model	Endpoint	Algorithm	Validation	
<input checked="" type="checkbox"/> Lipinski Rule of Five	Human health effects	Lipinski Rule of Five		Completed ✓
<input checked="" type="checkbox"/> START biodegradation and persistence plug-in	Persistence: Biodegradation	START biodegradation and persistence plug-in		Completed ✓
<input checked="" type="checkbox"/> ToxTree: Cramer rules	Human health effects	ToxTree: Cramer rules		Completed ✓
<input checked="" type="checkbox"/> ToxTree: Skin sensitisation alerts (M. Cronin)	Skin sensitisation	ToxTree: Skin sensitisation alerts (M. Cronin)		Completed ✓
<input checked="" type="checkbox"/> pKa	Dissociation constant (pKa)	pKa		Completed ✓
<input checked="" type="checkbox"/> MolecularWeight		MolecularWeight		Completed ✓
<input checked="" type="checkbox"/> ToxTree: Verhaar scheme for predicting toxicity mode of action	Acute toxicity to fish (lethality)	ToxTree: Verhaar scheme for predicting toxicity mode of action		Completed ✓
<input checked="" type="checkbox"/> Caco-2 Cell Permeability http://www.ncbi.nlm.nih.gov/pubmed/16959190	Gastrointestinal absorption	Regression: Linear regression	Model validation report	Completed ✓

javascript:animatedcollapse.toggle('help_step')

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http://apps.ideaconsult.net:8080/ToxPredict/user/beat03e8-e4c6-4007-85f5-cef7d6960625/A/step5#

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Display

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1. Select structure(s)
2. Verify structure(s)
3. Select model(s)
4. Run prediction(s)
5. Display result(s)

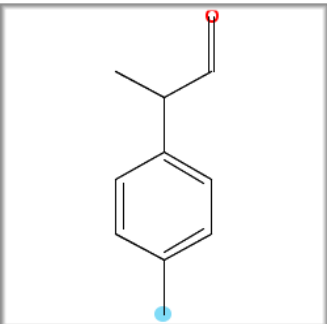
This page lists your ToxPredict workflow results for the structure(s) you have selected and the model prediction(s) you have chosen to run. You could also retrieve the ToxPredict report in various other formats, e.g. [SDF](#), [CML](#), [SMI](#), [PDF](#), [CSV](#), [ARFF](#), [RDF/XML](#) or [RDF/N3](#).

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Structure(s) & Model predictions & Experimental Data [SDF](#) [CSV](#) [PDF](#)

1.



CASRN 99-72-9
Synonym(s) 2-(p-tolyl)propionaldehyde
EINECS 202-782-0
IUPAC name 2-(4-methylphenyl)propanal
InChIKey_std JTZWVKUZNHSSW-SECBINFHSA-N, JTZWVKUZNHSSW-UHFFFAOYSA-N
InChI_std InChI=1S/C10H12O/c1-8-3-5-10(6-4-8)9(2)7-11/h3-7,9H,1-2H3/t9-/m1/s1, InChI=1S/C10H12O/c1-8-3-5-10(6-4-8)9(2)7-11/h3-7,9H,1-2H3
REACHRegistrationDate 30.11.2010
SMILES CC(C=O)c1ccc(C)cc1

OpenTox model created with TUM's PLSregression model learning web service.

Prediction feature for <http://apps.ideaconsult.net:8080/ambit2/feature/22200> endpoint prediction -4.53439998626709

LipinskiFailures [Lipinski Rule of Five](#) 0 0

Done