OpenTox

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IDEA consult™

OpenTox

Why integration framework for predictive toxicology?

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

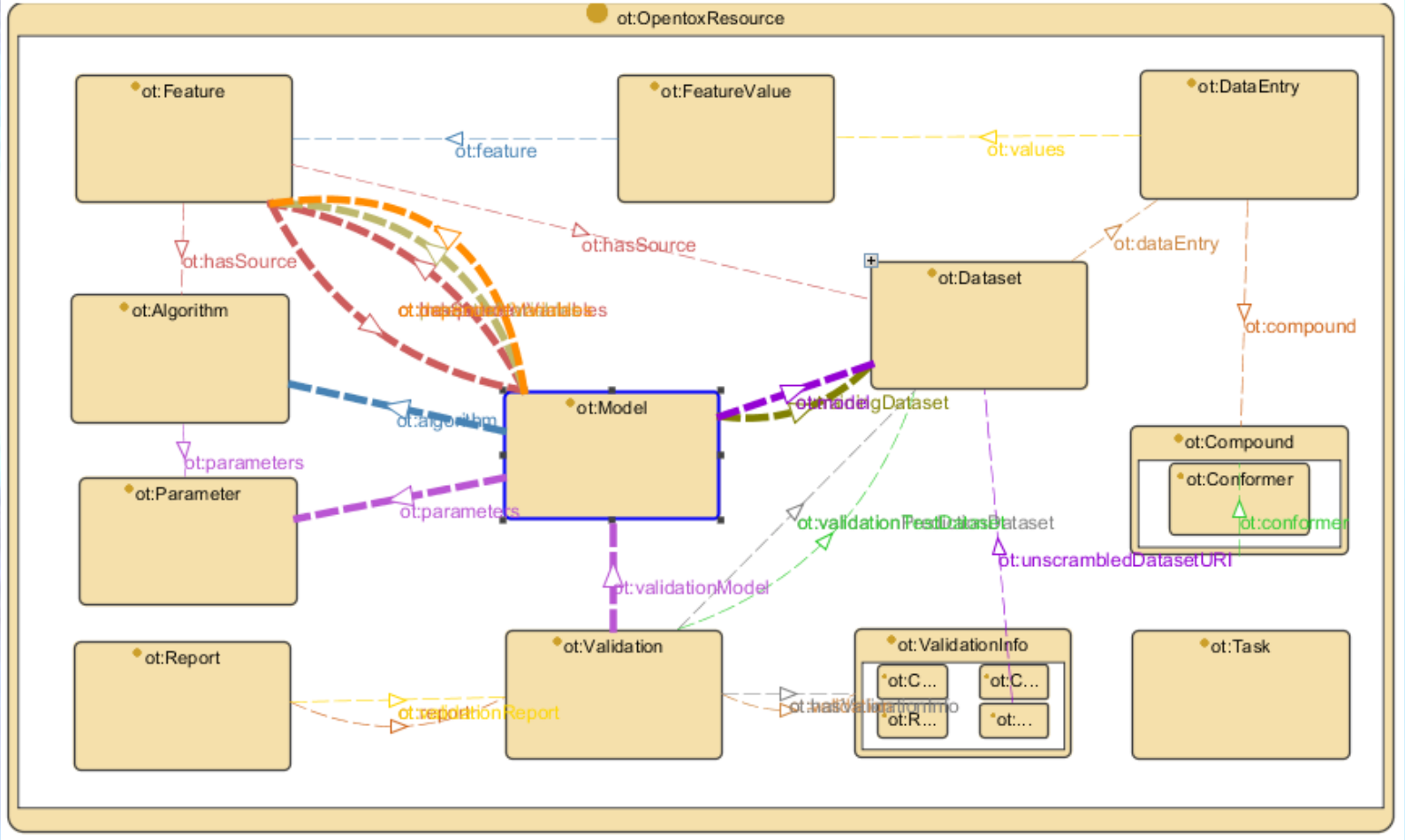
OpenTox Framework approach

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

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)

OpenTox components



OpenTox

Overview of OpenTox API
(Application Programming Interface)

- The way applications talk to each other
- The way developers talk to applications

Report
GET
POST
PUT
DELETE

AppDomain
GET
POST
PUT
DELETE

Dataset
GET
POST
PUT
DELETE

Validation
GET
POST
PUT
DELETE

Model
GET
POST
PUT
DELETE

Feature
GET
POST
PUT
DELETE

Compound
GET
POST
PUT
DELETE

Algorithm
GET
POST
PUT
DELETE

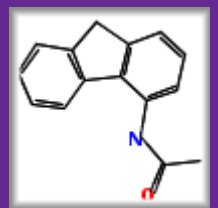
Ontology
GET
POST
PUT
DELETE

OpenTox

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	CN(C1=CC=C(C=C1)N=N/C2=CC=CC=C2)C	3	3.31	225.3	YES	3.123
http://myhost.com/compound/44497	4-acetamidofluorene	O=C(Nc3					
…	…						



http://myhost.com/feature/21573

http://myhost.com/feature/21858

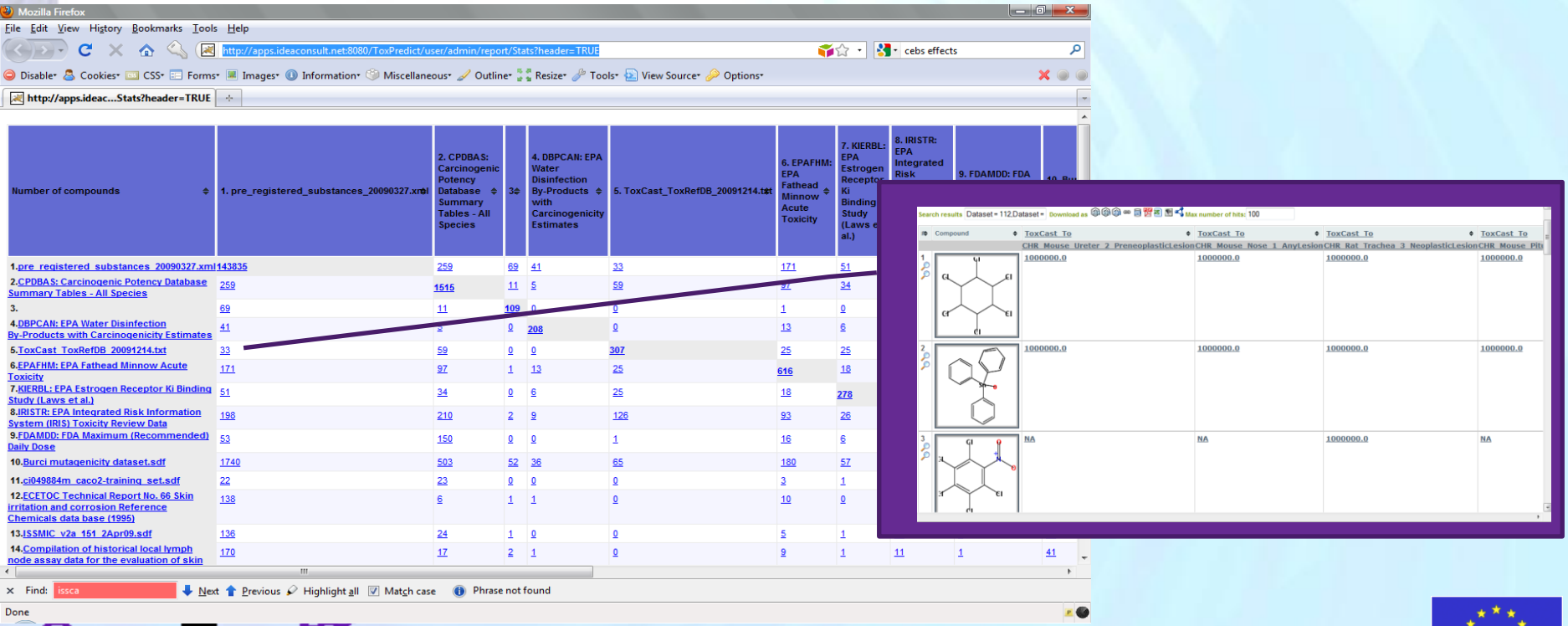
http://myhost.com/feature/22114
a ot:Feature , ot:NumericFeature ;
dc:creator
"http://www.blueobelisk.org/ontologies/chemoinformatics-algorithms/#xlogP" ;
dc:title "XLogP" ;
ot:hasSource
<http://myhost.com/algorithm/org.openscience.cdk.qsar.descriptors.molecular.XLogPDescriptor> ;
= otee:Octanol-water_partition_coefficient_Kow .

Uniform access to the data

- Ontologies are critical to unambiguously describe data
  - Opentox.owl;
  - Blue Obelisk algorithm ontology (cheminformatics algorithms);
  - OpenTox algotihm 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

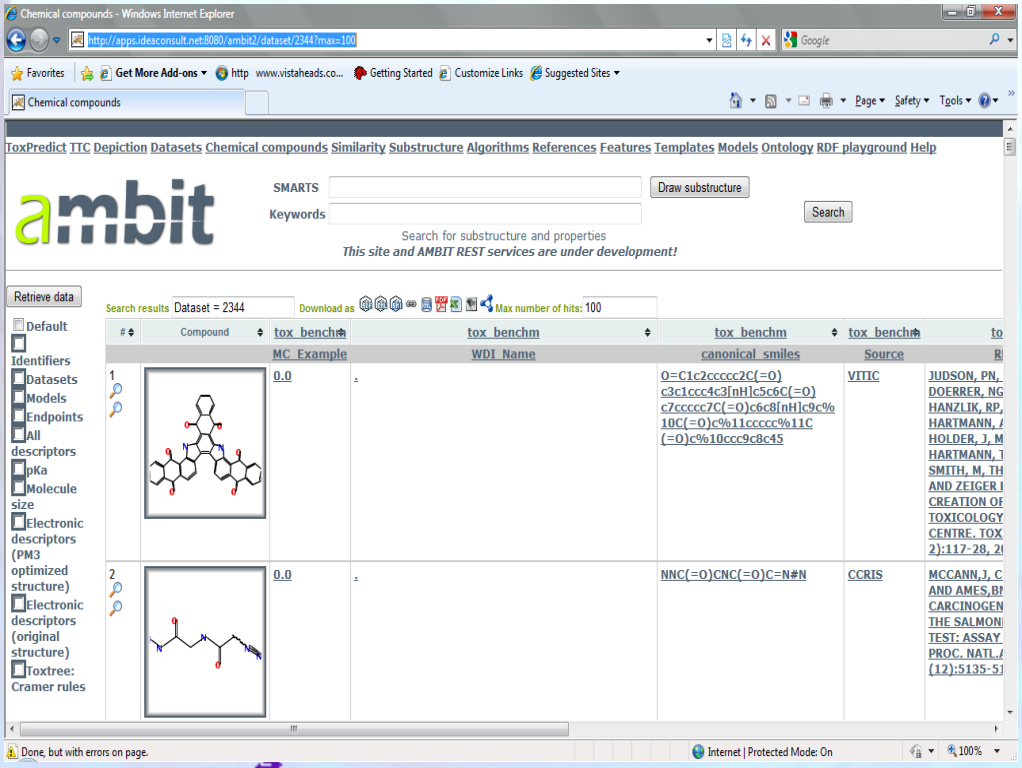
Uniform access to the data

- 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



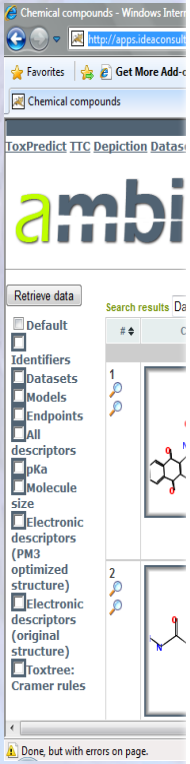
Example: mutagenicity dataset

- http://apps.ideaconsult.net:8080/ambit2/dataset/2344 (the dataset)
- http://apps.ideaconsult.net:8080/ambit2/dataset/2344/metadata (metadata, obviously)



Example: mutagenicity dataset

- Activity




```
@prefix ot:     <http://www.opentox.org/api/1.1#> .
@prefix dc:     <http://purl.org/dc/elements/1.1/> .
@prefix :       <http://apps.ideaconsult.net:8080/ambit2/> .
@prefix ota:    <http://www.opentox.org/algorithmTypes.owl#> .
@prefix otee:   <http://www.opentox.org/echaEndpoints.owl#> .
...
@prefix af:     <http://apps.ideaconsult.net:8080/ambit2/feature/> .

af:28958
    a       ot:Feature , ot:NumericFeature ;
    dc:creator "194.141.0.136" ;
    dc:title "Activity" ;
    ot:hasSource "tox_benchmark_N6512.sdf" ;
    ot:units "" ;
    =       otee:Mutagenicity .

ot:hasSource
    a       owl:ObjectProperty .

ot:units
    a       owl:DatatypeProperty .

ot:Feature
    a       owl:Class .

ot:NumericFeature
    a       owl:Class ;
    rdfs:subClassOf ot:Feature .
```

Query: Is there other mutagenicity data available?

- http://apps.ideaconsult.net:8080/ambit2/feature?sameas=http%3A%2F%2Fwww.opentox.org%2FechaEndpoints.owl%23Mutagenicity

http://apps.ideaconsult.net:8080/ambit2/feature/21590

http://apps.ideaconsult.net:8080/ambit2/feature/21611

http://apps.ideaconsult.net:8080/ambit2/feature/26221

http://apps.ideaconsult.net:8080/ambit2/feature/28958

Disable Cookies Miscellaneous Outline Resize Tools View Source Options

Chemical compounds

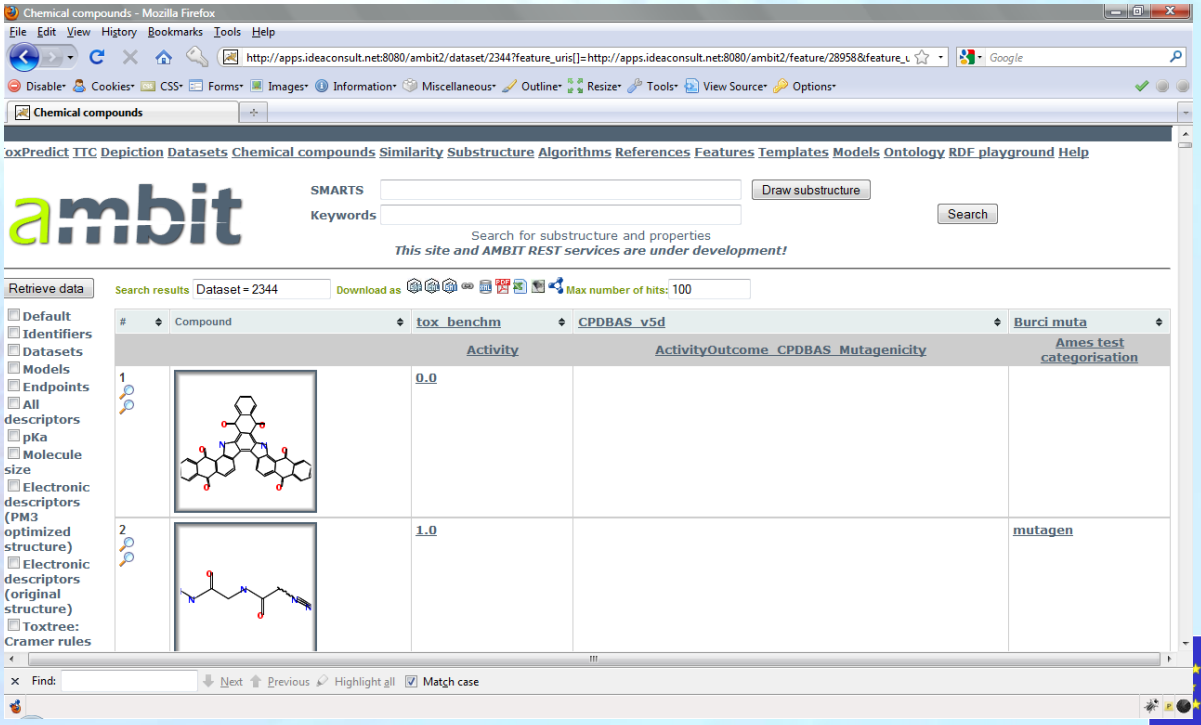
Feature

Find	Name				
	SAL		...endpoints.owl#Mutagenicity	ISSCAN_v3a_1153_19Sept08.1222179139.sdf	NO
	ActivityOutcome_CPDBAS_Mutagenicity		http://www.opentox.org /echaEndpoints.owl#Mutagenicity	CPDBAS_v5d_1547_20Nov2008.sdf	YES
	ActivityOutcome_CPDBAS_Mutagenicity		http://www.opentox.org	ambit2_75288.sdf	NO
	ActivityOutcome_CPDBAS_Mutagenicity				
	ActivityOutcome_CPDBAS_Mutagenicity				
	Mutagenic Activity in TA100 (3=active; 1=inactive)		...opentox.org /echaEndpoints.owl#Mutagenicity	qsar6train.csv	YES
	Ames test categorisation		http://www.opentox.org /echaEndpoints.owl#Mutagenicity	Burci mutagenicity dataset.sdf	YES
	Mutagenic Activity in TA100 (3=active; 1=inactive)		http://www.opentox.org	270.sdf	NO
	Mutagenic Activity in TA100 (3=ac 1=inactive)				
	Prediction feature for http://apps.ideaconsult.net:8080 /ambit2/feature/26701 endpoint prediction			/OpenTox-dev/model/10MOpenToxModel_j48_30	
	Activity		http://www.opentox.org /echaEndpoints.owl#Mutagenicity	tox_benchmark_N6512.sdf	NO

Waiting for apps.ideaconsult.net...

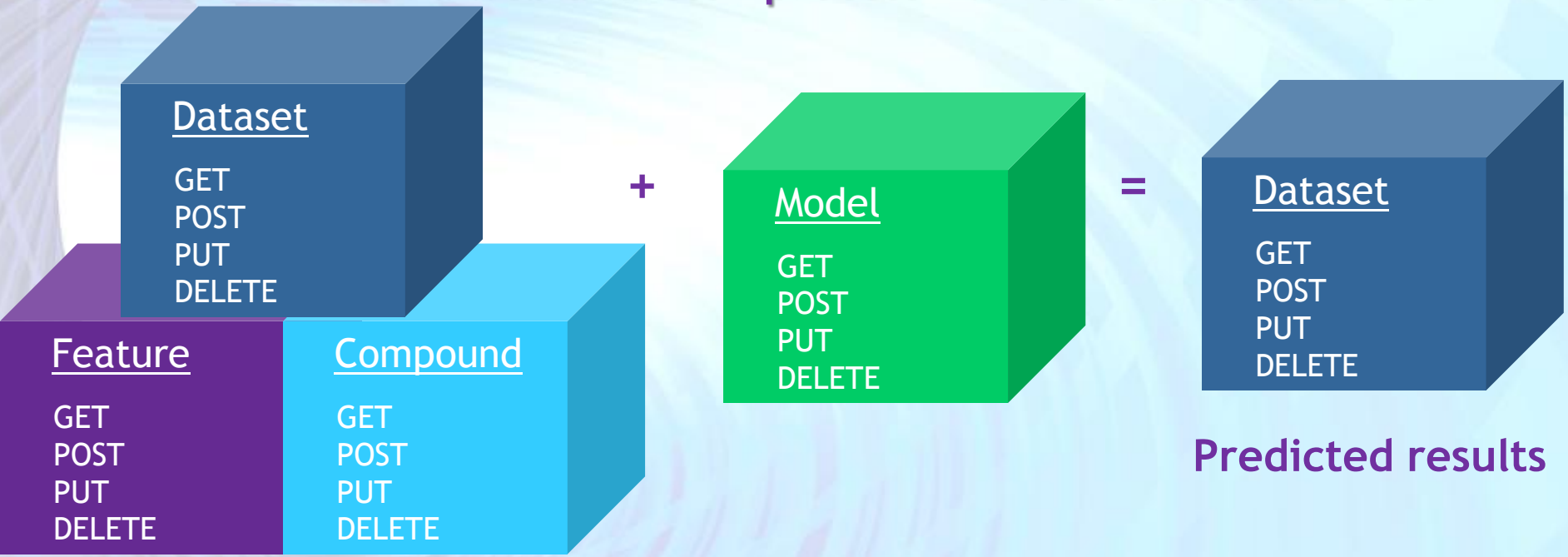
Merge mutagenicity data

- http://apps.ideaconsult.net:8080/ambit2/dataset/2344?feature_uris[]=http://apps.ideaconsult.net:8080/ambit2/feature/28958&feature_uris[]=http://apps.ideaconsult.net:8080/ambit2/feature/21611&feature_uris[]=http://apps.ideaconsult.net:8080/ambit2/feature/26221&feature_uris[]= http://apps.ideaconsult.net:8080/ambit2/feature/21590



Uniform access to calculations

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



Predicted results

ttp://myhost.com/dataset/newcompounds

http://myhost.com/model/predictivemodel1

http://myhost.com/dataset/predictedresults1

List available models

- http://apps.ideaconsult.net:8080/ambit2/model

All models - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://apps.ideaconsult.net:8080/ambit2/model

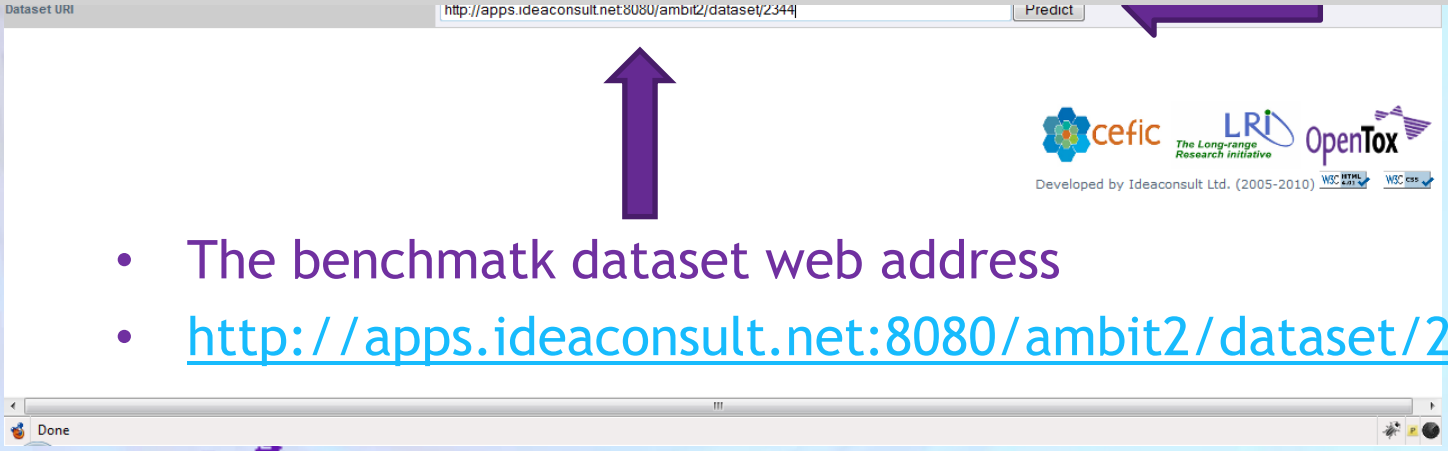
All models

Model name	Algorithm	Dataset	Independ variables
pKa txt	http://apps.ideaconsult.net:8080/ambit2/algorithm/pka		Indepe variabl
ToxTree: Cramer rules txt	http://apps.ideaconsult.net:8080/ambit2/algorithm/toxtreecramer		Indepe variabl
ToxTree: Extended Cramer rules txt	http://apps.ideaconsult.net:8080/ambit2/algorithm/toxtreecramer2		Indepe variabl
ToxTree: Eye irritation txt	http://apps.ideaconsult.net:8080/ambit2/algorithm/toxtreeeye		Indepe variabl
ToxTree: Skin irritation txt	http://apps.ideaconsult.net:8080/ambit2/algorithm/toxtreeskinirritation		Indepe variabl
ToxTree: Structure Alerts for the in vivo micronucleus assay in rodents txt	http://apps.ideaconsult.net:8080/ambit2/algorithm/toxtreemic		Indepe variabl
ToxTree: Michael acceptors txt	http://apps.ideaconsult.net:8080/ambit2/algorithm/toxtreemichaelacceptors		Indepe variabl
ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity txt	http://apps.ideaconsult.net:8080/ambit2/algorithm/toxtreecarc		Indepe variabl
XLogP txt	http://apps.ideaconsult.net:8080/ambit2/algorithm /org.openscience.cdk.qsar.descriptors.molecular.XLogPDescriptor		Indepe variabl
MolecularWeight txt	http://apps.ideaconsult.net:8080/ambit2/algorithm /ambit2.descriptors.MolecularWeight		Indepe

Done

Apply ToxTree module for carcinogenicity and mutagenicity prediction

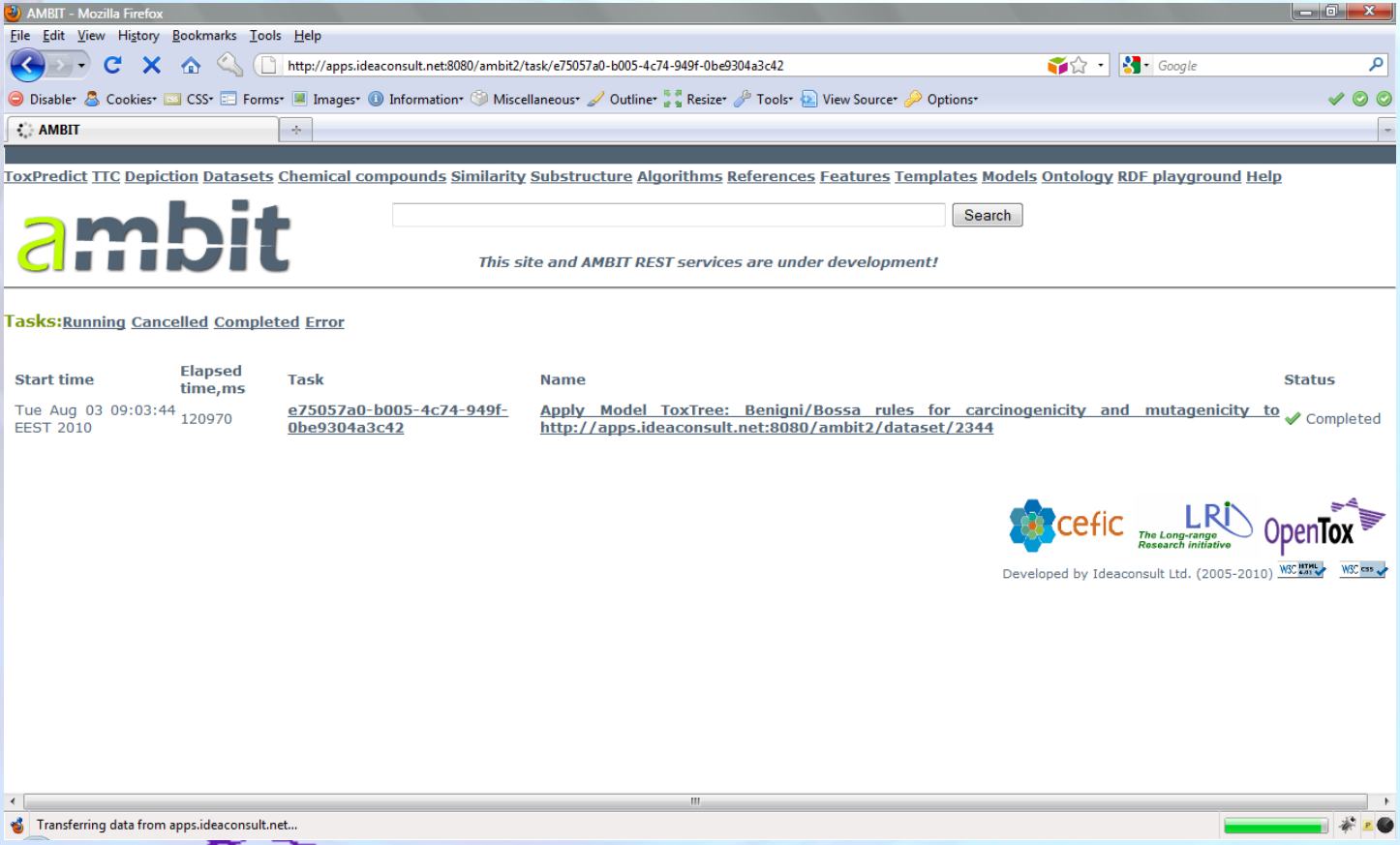
- Clicking 'Predict' button initiates calculations
- It actually sends HTTP POST command to the model URL, with parameter the dataset URL
- curl -X POST -d "dataset_uri=http://apps.ideaconsult.net:8080/ambit2/dataset/2344" http://apps.ideaconsult.net:8080/ambit2/model/8



- The benchmatk dataset web address
- http://apps.ideaconsult.net:8080/ambit2/dataset/2344

Long running calculations - web address again

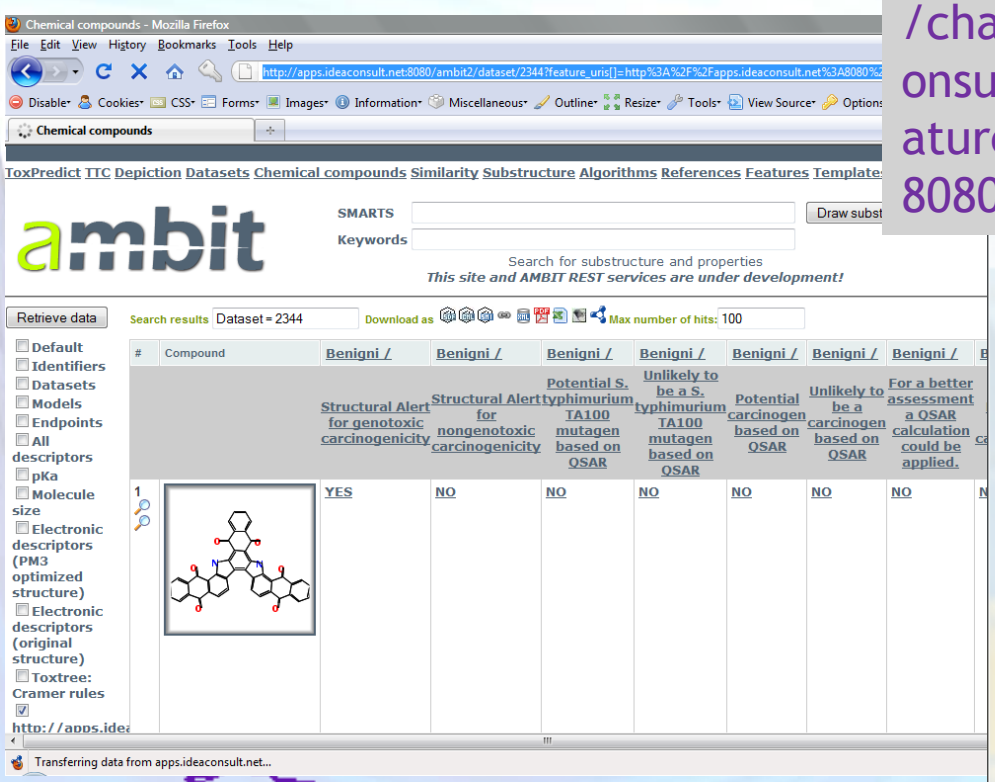
- http://apps.ideaconsult.net:8080/ambit2/task/e75057a0-b005-4c74-949f-0be9304a3c422/model

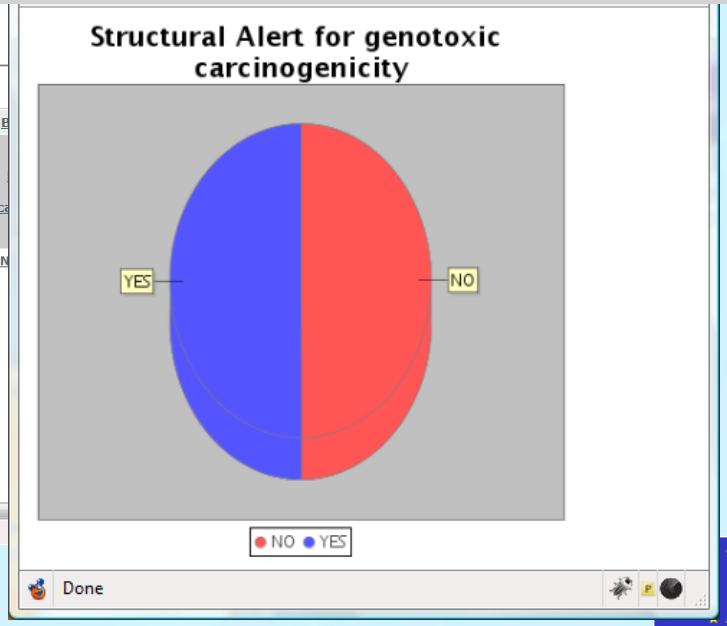


And the results (a dataset web address)

- http://apps.ideaconsult.net:8080/ambit2/dataset/2344?feature_uris[]=http%3A%2F%2Fapps.ideaconsult.net%3A8080%2Fambit2%2Fmodel%2F8%2Fpredicted

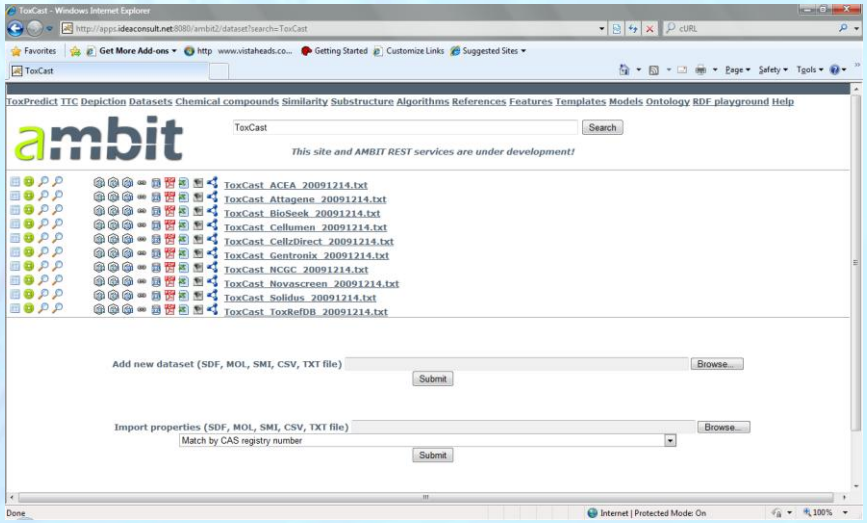
http://apps.ideaconsult.net:8080/ambit2/chart/pie?dataset_uri=http://apps.ideaconsult.net:8080/ambit2/dataset/2344&feature_uris[]=http://apps.ideaconsult.net:8080/ambit2/feature/21858





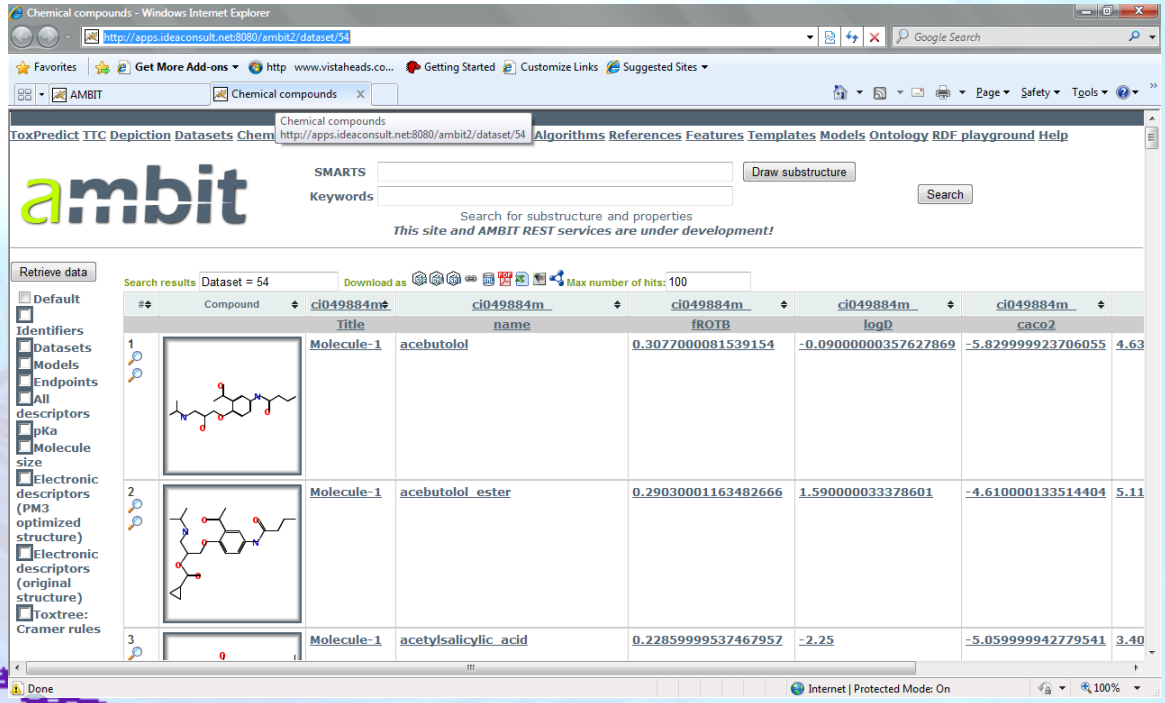
Building blocks for model creation

- A Dataset
  - Datasets can be uploaded (SDF, CSV, SMI, MOL)
    - via HTTP POST to the dataset service
    - Web browser file upload
  - Existing datasets (uploaded by others) can be used
  - Dataset Web address assigned
- Descriptor calculation
- Learning algorithm
- Perform predictions
- Make the model available



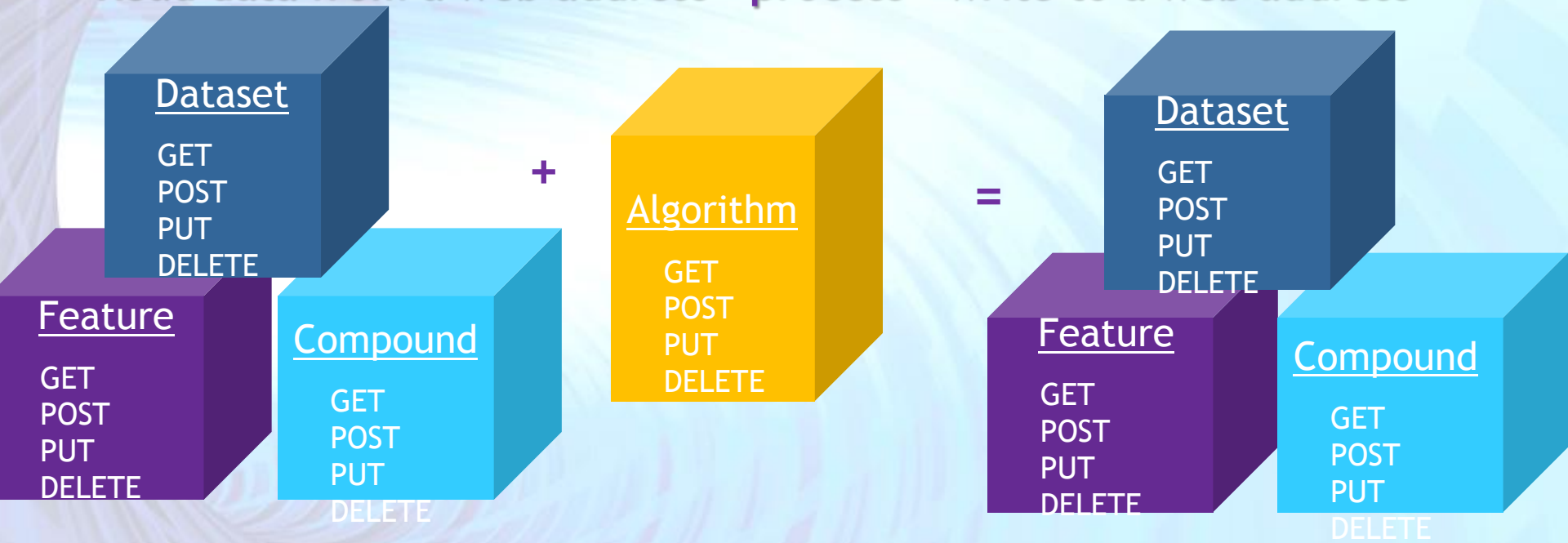
The dataset (Caco-2 dataset from a JCIM publication)

- http://apps.ideaconsult.net:8080/ambit2/dataset/54
- http://apps.ideaconsult.net:8080/ambit2/dataset/54/metadata
- The endpoint (caco2 column) http://apps.ideaconsult.net:8080/ambit2/feature/22200



Uniform approach to data processing (e.g. Descriptors calculation)

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



http://myhost.com/algorithm/neuralnetwork

tp://myhost.com/dataset/trainingset1

http://myhost.com/dataset/results

The algorithms (including descriptors calculation)

- http://apps.ideaconsult.net:8080/ambit2/algorithm

AMBIT - Windows Internet Explorer

http://apps.ideaconsult.net:8080/ambit2/algorithm

ToxPredict TTC Depiction Datasets Chemical compounds Similarity Substructure Algorithms References Features Templates Models Ontology RDF playground Help

ambit

Search

This site and AMBIT REST services are under development!

Name	Description	Type
Clustering: k-means	Generates a model	http://www.opentox.org/algorithmTypes.ow#Clustering
Classification: Decision tree J48	Generates a model	http://www.opentox.org/algorithmTypes.ow#Classification
Regression: Linear regression	Generates a model	http://www.opentox.org/algorithmTypes.ow#Regression
pKa	Generates a model	http://www.opentox.org/algorithmTypes.ow#Rules
ToxTree: Cramer rules	Generates a model	http://www.opentox.org/algorithmTypes.ow#Rules
ToxTree: Extended Cramer rules	Generates a model	http://www.opentox.org/algorithmTypes.ow#Rules
ToxTree: Verhaar scheme for predicting toxicity mode of action	Generates a model	http://www.opentox.org/algorithmTypes.ow#Rules
ToxTree: Eye irritation	Generates a model	http://www.opentox.org/algorithmTypes.ow#Rules
ToxTree: Skin irritation	Generates a model	http://www.opentox.org/algorithmTypes.ow#Rules
ToxTree: Structure Alerts for the in vivo micronucleus assay in rodents	Generates a model	http://www.opentox.org/algorithmTypes.ow#Rules
ToxTree: Skin sensitisation alerts (M. Cronin)	Generates a model	http://www.opentox.org/algorithmTypes.ow#Rules
SmartCYP: Cytochrome P450-Mediated Drug Metabolism	Generates a model	http://www.opentox.org/algorithmTypes.ow#Rules
ToxTree: Michael acceptors	Generates a model	http://www.opentox.org/algorithmTypes.ow#Rules
ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity	Generates a model	http://www.opentox.org/algorithmTypes.ow#Rules
START biodegradation and persistence plug-in	Generates a model	http://www.opentox.org/algorithmTypes.ow#Rules
ToxTree: ILSI/Kroes decision tree for TTC	Generates a model	http://www.opentox.org/algorithmTypes.ow#Rules
XLogP	Processes a dataset	http://www.opentox.org/algorithmTypes.ow#DescriptorCalculation
MolecularWeight	Processes a dataset	http://www.opentox.org/algorithmTypes.ow#DescriptorCalculation

Descriptors calculation

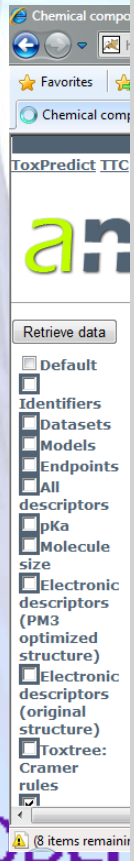
- http://apps.ideaconsult.net:8080/ambit2/algorithm/org.openscience.cdk

  - Clicking 'Predict' button initiates calculations
  - It actually sends HTTP POST command to the algorithm URL, with parameter the dataset URL
  - curl -X POST -d "dataset_uri=http://apps.ideaconsult.net:8080/ambit2/dataset/2344" http://apps.ideaconsult.net:8080/ambit2/algorithm/org.openscience.cdk.qsar.descriptors.molecular.XLogPDescriptor

  - The demo dataset web address
  - http://apps.ideaconsult.net:8080/ambit2/dataset/54

Res
dat

- http:
ttp%
Fpre

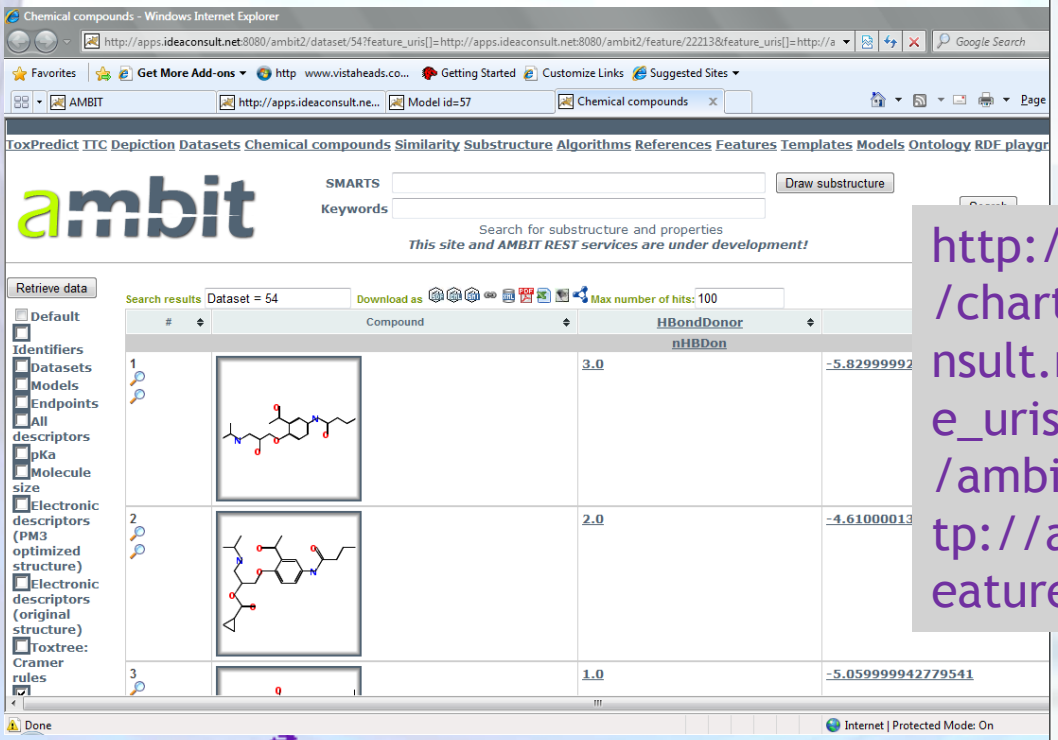


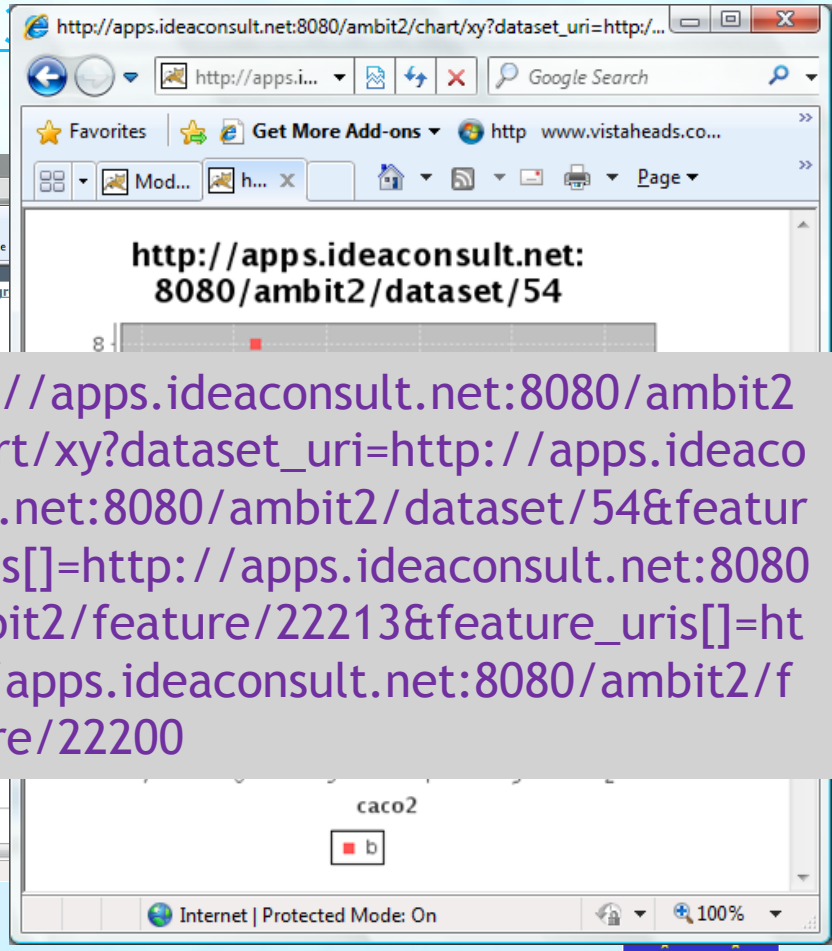
Open
Marc

```
@prefix ot:     <http://www.opentox.org/api/1.1#> .
@prefix dc:     <http://purl.org/dc/elements/1.1/> .
@prefix :       <http://apps.ideaconsult.net:8080/ambit2/> .
@prefix ota:    <http://www.opentox.org/algorithmTypes.owl#> .
@prefix otee:   <http://www.opentox.org/echaEndpoints.owl#> .
@prefix ar:     <http://apps.ideaconsult.net:8080/ambit2/reference/> .
@prefix bx:     <http://purl.org/net/nknouf/ns/bibtex#> .
@prefix rdfs:   <http://www.w3.org/2000/01/rdf-schema#> .
@prefix am:     <http://apps.ideaconsult.net:8080/ambit2/model/> .
@prefix owl:    <http://www.w3.org/2002/07/owl#> .
@prefix xsd:    <http://www.w3.org/2001/XMLSchema#> .
@prefix ac:     <http://apps.ideaconsult.net:8080/ambit2/compound/> .
@prefix ad:     <http://apps.ideaconsult.net:8080/ambit2/dataset/> .
@prefix rdf:    <http://www.w3.org/1999/02/22-rdf-syntax-ns#> .
@prefix ag:     <http://apps.ideaconsult.net:8080/ambit2/algorithm/> .
@prefix af:     <http://apps.ideaconsult.net:8080/ambit2/feature/> .

ot:Algorithm
    a       owl:Class .

ot:hasSource
    a       owl:ObjectProperty .

ot:units
    a       owl:DatatypeProperty .

af:22114
    a       ot:Feature , ot:NumericFeature ;
    dc:creator "http://www.blueobelisk.org/ontologies/chemoinformatics-algorithms/#xlogP" ;
    dc:title "XLogP" ;
    ot:hasSource <http://apps.ideaconsult.net:8080/ambit2/algorithm/org.openscience.cdk.qsar.descriptors.molecular.XLogPDescriptor>
;
    ot:units "" ;
    =       otee:Octanol-water_partition_coefficient_Kow .

ot:Feature
    a       owl:Class .

ot:NumericFeature
    a       owl:Class ;
    rdfs:subClassOf ot:Feature .

<http://apps.ideaconsult.net:8080/ambit2/algorithm/org.openscience.cdk.qsar.descriptors.molecular.XLogPDescriptor>
    a       ot:Algorithm .
```

Merge descriptor with activity - dataset with a web address again

http://apps.ideaconsult.net:8080/ambit2/dataset/54?feature_uris[]=http://apps.ideaconsult.net:8080/ambit2/feature/2221
aconsult.net:8080/ambit2/feature/22200

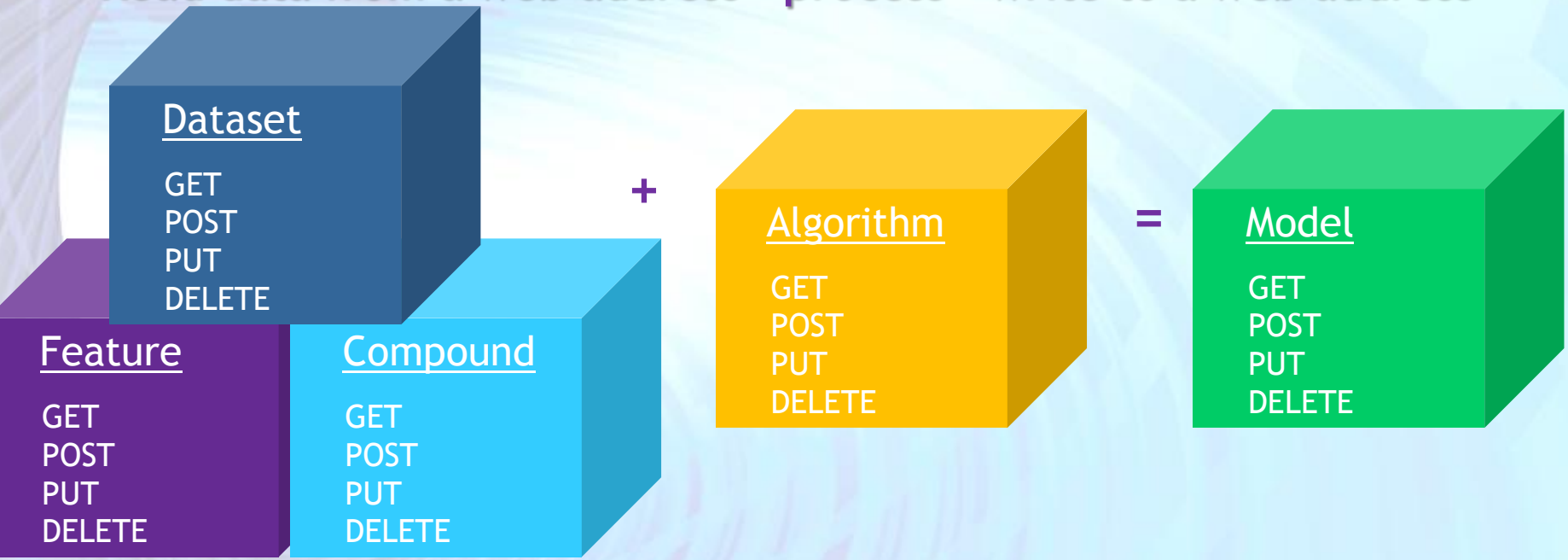




http://apps.ideaconsult.net:8080/ambit2/chart/xy?dataset_uri=http://apps.ideaconsult.net:8080/ambit2/dataset/54&feature_uris[]=http://apps.ideaconsult.net:8080/ambit2/feature/22213&feature_uris[]=http://apps.ideaconsult.net:8080/ambit2/feature/22200

Uniform approach to models creation

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



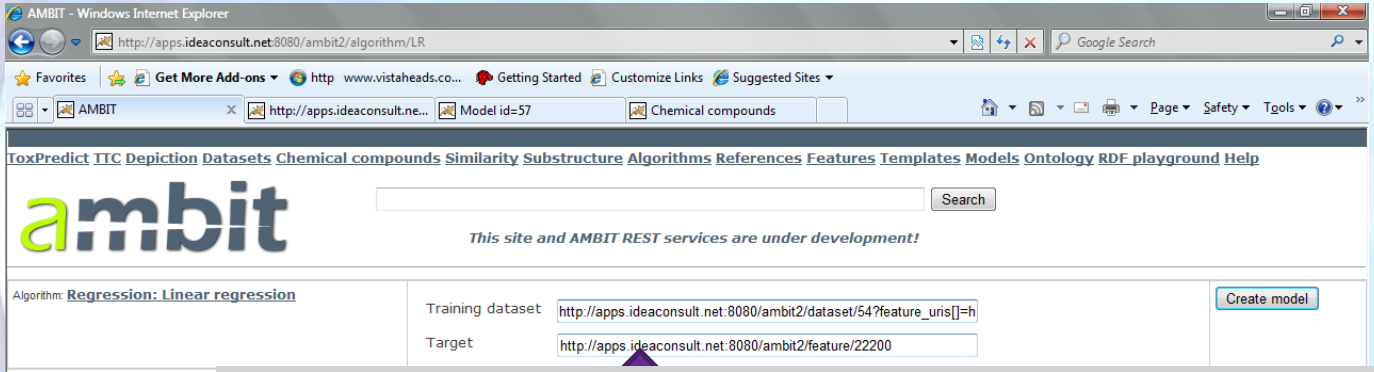
http://myhost.com/algorithm/neuralnetwork

tp://myhost.com/dataset/trainingset1

http://myhost.com/model/predictivemodel1

Build a regression model

- http://apps.ideaconsult.net:8080/ambit2/algorithm/LR



- The de
- http:/

- Clicking 'Predict' button initiates calculations
- It actually sends HTTP POST command to the algorithm URL, with parameter the dataset URL
- curl -X POST -d "dataset_uri=http://apps.ideaconsult.net:8080/ambit2/dataset/54" -d "prediction_feature= http://apps.ideaconsult.net:8080/ambit2/feature/22200 " http://apps.ideaconsult.net:8080/ambit2/algorithm/LR

The model

http://apps.ideaconsult.net:8080/ambit2/model/57

Web add

viahttp://apps.idea

, in t

http://apps.id

http://ap

ed, in

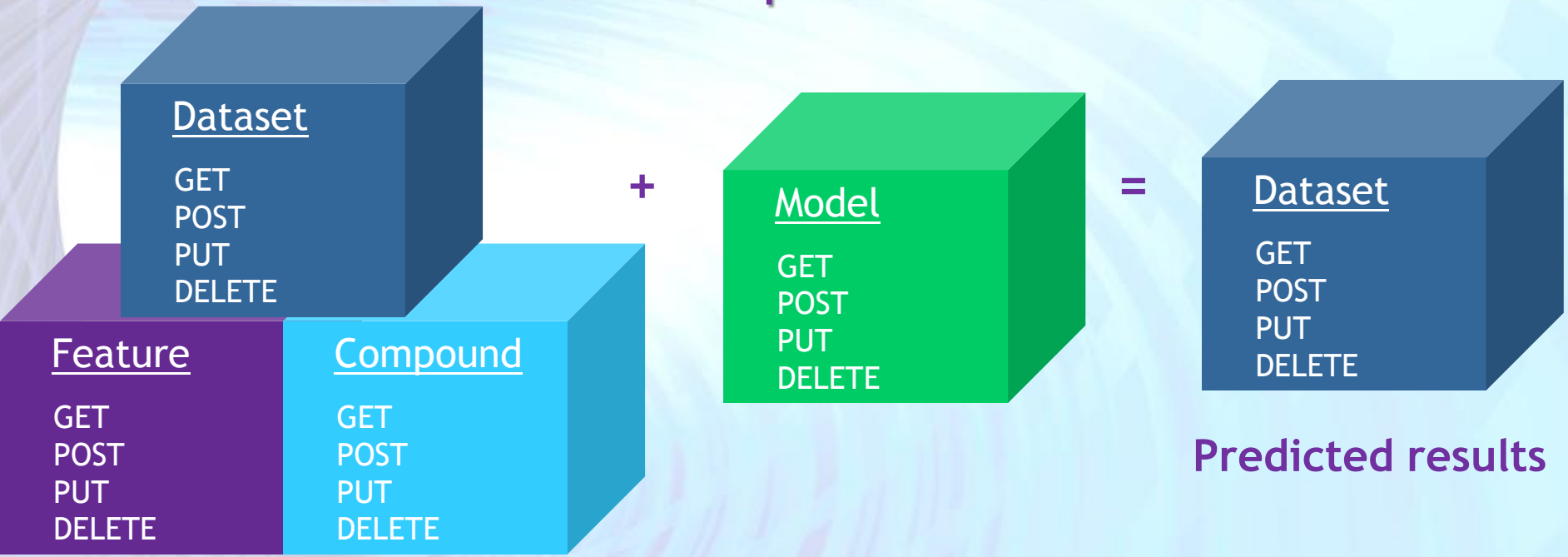
http://apps.ideaconsult.net:8080/ambit2/feature/28963

http://apps.ideaconsult.net:8080/ambit2/model/57?media=text/plain - Windows Internet Explorer

```
-- WEKA Model --
Structures required     NO
-- Data header --
@relation http://apps.ideaconsult.net:8080/ambit2/dataset/54-weka.filters.unsupervised.a

@attribute http://apps.ideaconsult.net:8080/ambit2/feature/22200 numeric
@attribute http://apps.ideaconsult.net:8080/ambit2/feature/22213 numeric

@data

-- Class Index 0--
@attribute http://apps.ideaconsult.net:8080/ambit2/feature/22200 numeric

Linear Regression Model

http://apps.ideaconsult.net:8080/ambit2/feature/22200 =

     -0.2593 * http://apps.ideaconsult.net:8080/ambit2/feature/22213 +
     -4.4086
```

Uniform access to calculations

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



Predicted results

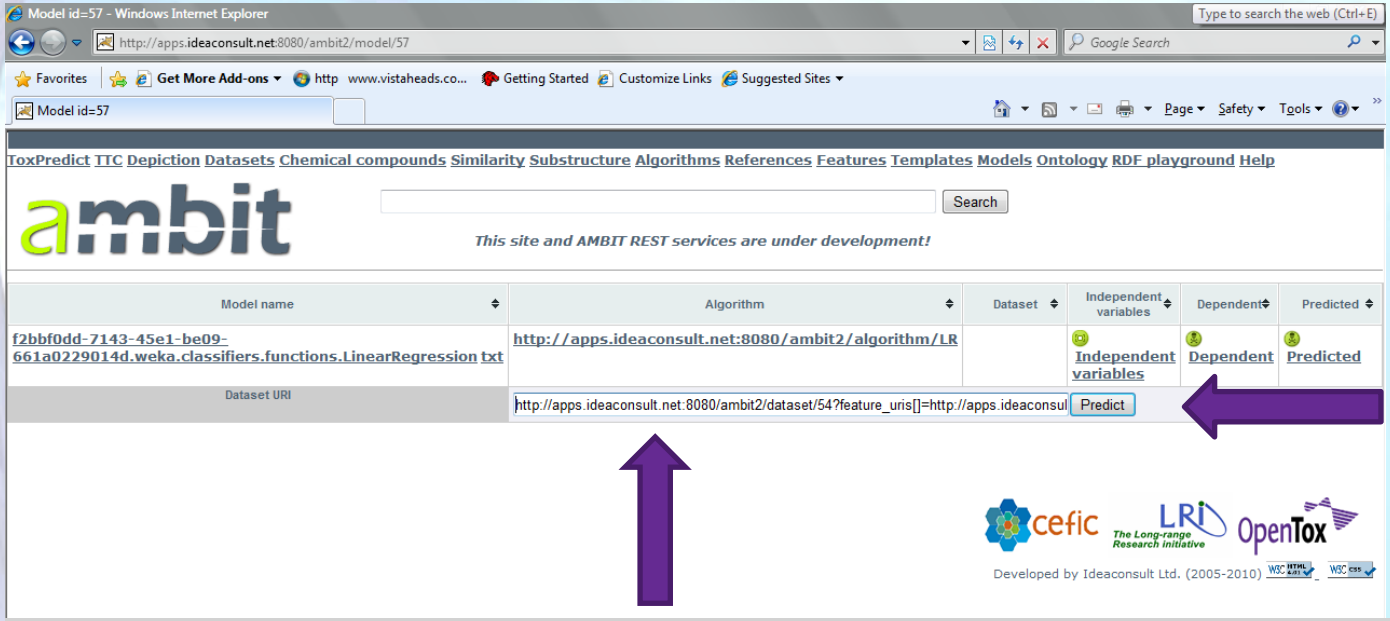
ttp://myhost.com/dataset/newcompounds

http://myhost.com/model/predictivemodel1

http://myhost.com/dataset/predictedresults1

Apply the new regression model

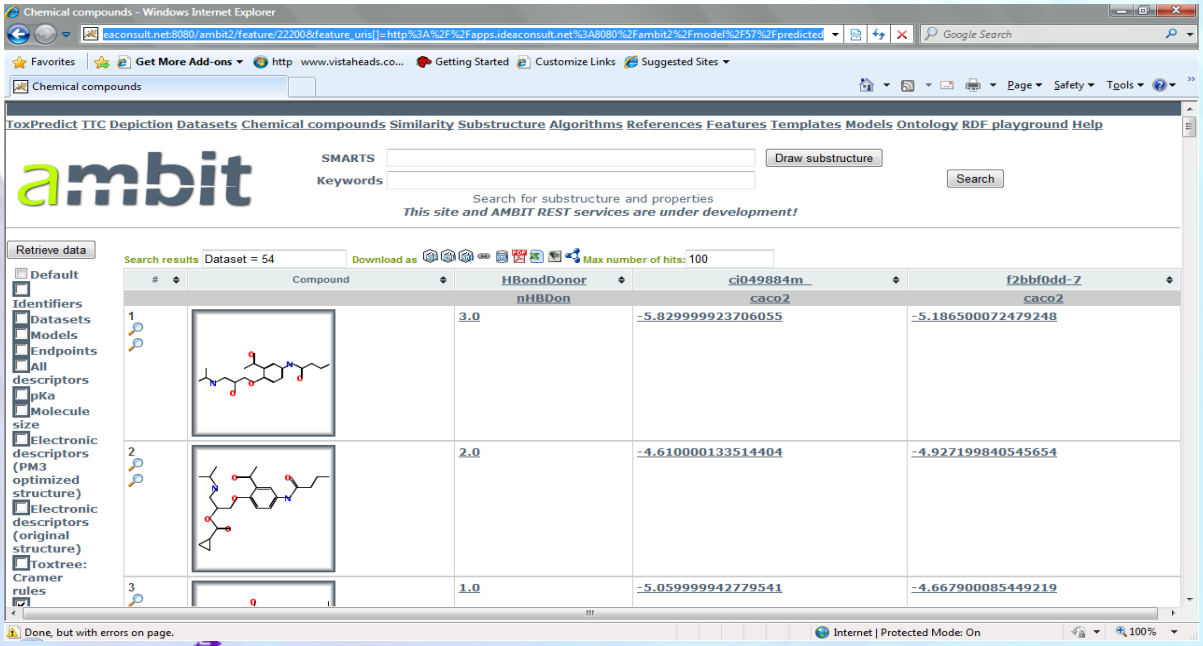
- http://apps.ideaconsult.net:8080/ambit2/model/57 (Model)



- The demo dataset web address http://apps.ideaconsult.net:8080/ambit2/dataset/54?feature_uris[]=http://apps.ideaconsult.net:8080/ambit2/feature/22213&feature_uris[]=http://apps.ideaconsult.net:8080/ambit2/feature/22200

Predictions, finally (at a dataset web address)

- http://apps.ideaconsult.net:8080/ambit2/dataset/54?feature_uris[]=http://apps.ideaconsult.net:8080/ambit2/feature/22213&feature_uris[]=http://apps.ideaconsult.net:8080/ambit2/feature/22200&feature_uris[]=http%3A%2F%2Fapps.ideaconsult.net%3A8080%2Fambit2%2Fmodel%2F57%2Fpredicted



Advanced options (a bit of command line, no web browser)

- http://curl.haxx.se/
- curl is a command line tool for transferring data with URL syntax
- Copy the dataset to a new one:

curl -X POST -d "dataset_uri=http://apps.ideaconsult.net%3A8080%2Fambit2%2Fdataset%2F54%3Ffeature_uris%5B%5D%3Dhttp%3A%2F%2Fapps.ideaconsult.net%3A8080%2Fambit2%2Ffeature%2F22213%26feature_uris%5B%5D%3Dhttp%3A%2F%2Fapps.ideaconsult.net%3A8080%2Fambit2%2Ffeature%2F22200%26feature_uris%5B%5D%3Dhttp%253A%252F%252Fapps.ideaconsult.net%253A8080%252Fambit2%252Fmodel%252F57%252Fpredicted" http://apps.ideaconsult.net:8080/ambit2/dataset

The new URL returned is

http://apps.ideaconsult.net:8080/ambit2/dataset/R3940

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

ttp://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

http://myhost.com/model/predictivemodel1

Ask the Validation service at Freiburg to validate the model

- *curl -d test_dataset_uri=http://apps.ideaconsult.net:8080/ambit2/dataset/R3940 -d prediction_feature=http://apps.ideaconsult.net:8080/ambit2/feature/22200 -d model_uri=http://apps.ideaconsult.net:8080/ambit2/model/57 http://opentox.informatik.uni-freiburg.de/validation*

Task URL returned **http://opentox.informatik.uni-freiburg.de/task/4062**

Query if the task is completed:

- *curl -H "Accept:text/uri-list" http://opentox.informatik.uni-freiburg.de/task/4062*
- *Yes, it is, here is the address of the validation object*

http://opentox.informatik.uni-freiburg.de/validation/18920

The validation resource

```
curl http://opentox.informatik.uni-freiburg.de/validation/18920
---
:regression_statistics:
  :sum_squared_error: 66.4592554978574
  :sample_correlation_coefficient: 0.42022542118295
  :root_mean_squared_error: 0.929035636699631
  :mean_absolute_error: 0.752657632127617
  :r_square: 0.176589404608387
  :target_variance_actual: 1.06200222895221
  :target_variance_predicted: 0.187523074000816
:date: 2010-08-03 09:41:48 +02:00
:test_target_dataset_uri:
:real_runtime: 1
:prediction_dataset_uri:
      http://apps.ideaconsult.net:8080/ambit2/dataset/R3940?feature_uris[]=http%3A%2F%2Fapps.ideaconsult.net%3A8080%2Fambit2%2Fmodel%2F57%2Fpredicted
:algorithm_uri: http://apps.ideaconsult.net:8080/ambit2/algorithm/LR
:percent_without_class: 0.0
:num_without_class: 0
:prediction_feature: http://apps.ideaconsult.net:8080/ambit2/feature/22200
:percent_unpredicted: 0.0
:num_instances: 77
:training_dataset_uri:
:model_uri: http://apps.ideaconsult.net:8080/ambit2/model/57
:num_unpredicted: 0
:test_dataset_uri: http://apps.ideaconsult.net:8080/ambit2/dataset/R3940
```

The validation report

curl -d validation_uris=http://opentox.informatik.uni-freiburg.de/validation/18920 http://opentox.informatik.uni-freiburg.de/validation/report/validation
http://opentox.informatik.uni-freiburg.de/task/4063 ***<---- Task URI***

curl http://opentox.informatik.uni-freiburg.de/task/4063 ←- Ask if completed
---
:description:
:date: 2010-08-03T09:48:31+02:00
:uri: http://opentox.informatik.uni-freiburg.de/task/4063
:hasStatus: Completed
:title:
:percentageCompleted: 0.0
:resultURI:
http://opentox.informatik.uni-freiburg.de/validation/report/validation/160
:due_to_time: 2010-08-03T10:48:31+02:00
:creator:

The validation report (human readable this time)

http://opentox.informatik.uni-freiburg.de/validation/report/validation/160

Validation report - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://opentox.informatik.uni-freiburg.de/validation/report/validation/160

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

Validation report

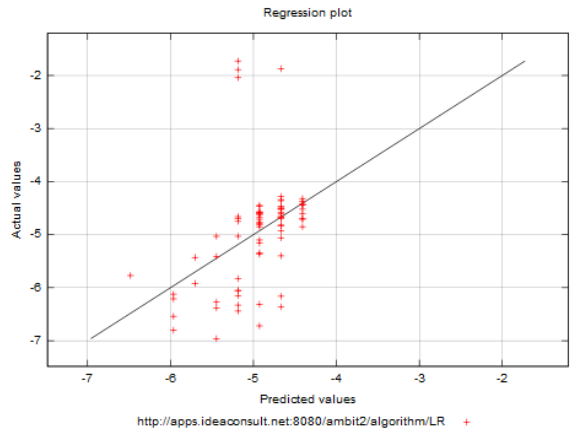
Model uri	http://apps.ideaconsult.net:8080/ambit2/model/57
Test dataset uri	http://apps.ideaconsult.net:8080/ambit2/dataset/R3940
Prediction feature	http://apps.ideaconsult.net:8080/ambit2/feature/22200
Root mean squared error	0.93
Mean absolute error	0.75
R square	0.18

Results

Regression Plot

This section contains the regression plot.

Figure 1. Regression plot



Done

OpenTox web services implementation

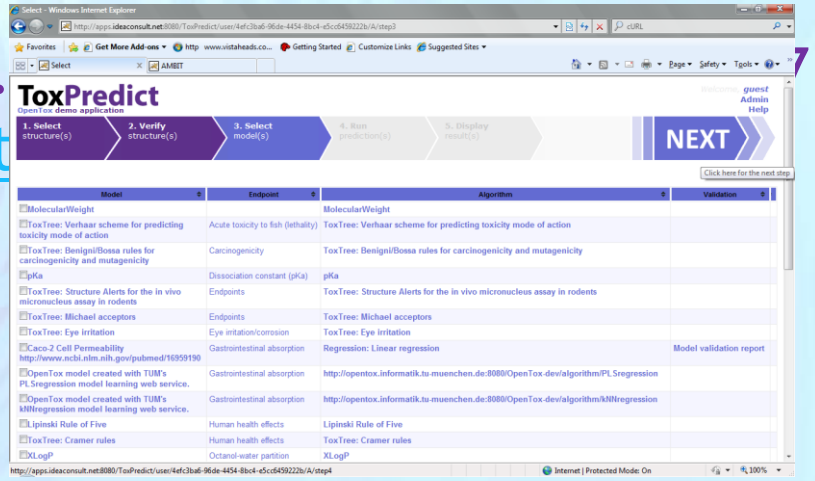
- Could be hosted on a single computer (even a laptop or netbook would do) o
- Could be transparently distributed on multiple servers in various physical locations, in particular for better reliability, resilience and scalability;
- OpenTox webservices could be deployed behind firewalls, in Intranets (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;

Make the model available

Register at OpenTox ontology service

- RDF tripple storage
- Accepts HTTP POST
- SPARQL endpoint

Curl –X POST –d
”uri=http://apps.ideaconsult.
” http://apps.ideaconsult.net



Becomes visible for applications

OpenTox Is A Framework

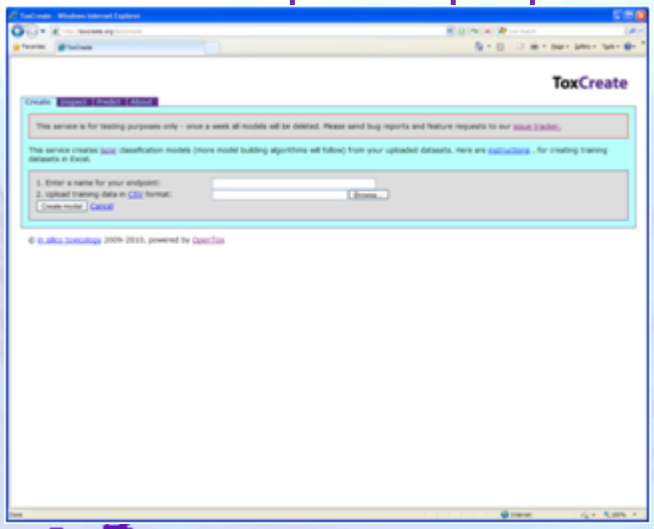
Framework	• Toxicity data • QSAR models • Validation support • Interpretation aids
Unified Access	• Toxicologists • QSAR Modelers • API for new QSAR algorithm development & integration
Open Source	• To optimise impact • To allow inspection / review • To attract external contributors

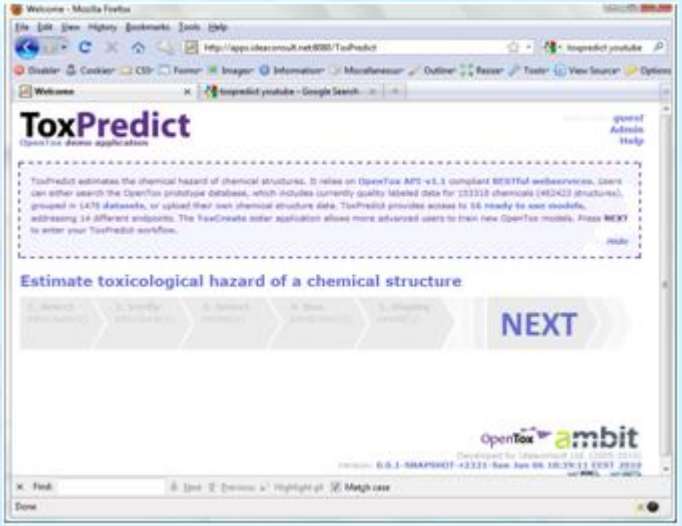
OpenTox services can be used to develop specific applications , or embedded in workflow systems

OpenTox

Demo applications

- Two end user oriented demo applications, making use of OpenTox webservices, have been developed, deployed and are available for testing – **http://toxcreate.org** and **http://toxpredict.org** ;
- ToxCreate creates models from user supplied datasets;
- ToxPredict uses existing OpenTox models to estimate chemicalcompound properties





Exercises (4 options)
http://www.ideaconsult.net/downloads/echeminfo/

- Interested in applying predictive models, but not in OpenTox implementation details
- Interested in building predictive models , but not in OpenTox implementation details
- End users, interested in learning implementation details of OpenTox web services.
-
- Developers

OpenTox

Thank you!