

Oxford, August 2010: eCheminfo Predictive ADME & Toxicology 2010 Workshop

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The first week of August I will attend the [eCheminfo Predictive ADME & Toxicology Workshop \(LinkedIn Event\)](#) for which I received a [Bursary Award](#). It will be my first time in Oxford, and I am very much looking forward to it!

The meeting is also bound to be fun. I have not done much in the area of toxicology other than the more general QSAR/QSPR model building with chemometrics. But I have been recently taking to Nina and other of the [OpenTox](#) community, and started to play a bit with the data and computation API they are developing.

The screenshot shows the Bioclipse application window. On the left is the Bioclipse Navigator with a tree view containing folders like 'FooQSAR', 'FriendFeed', 'Gists', 'Gromacs', 'LaTeX', 'Medea', 'Medea Data', 'MyExperiment', 'NMRShiftDB', and 'OpenTox'. Under 'OpenTox', there is a list of files named 'ambit17.sdf' through 'ambit50.sdf'. The central editor displays a JavaScript script in 'ambit.js' that queries the OpenTox API. The script defines a service URL, lists datasets, and iterates through them to download data as MDLSD files. The bottom panel shows the 'JavaScript Console' with log messages: 'Downloading set: 42', 'Downloading set: 48', 'Downloading set: 27', 'Downloading set: 17', and 'Downloading set: 41'. On the right, a table titled 'ambit17.sdf' displays chemical structures and numerical data. The table has columns for '2D-struct...', 'TUM_CD...', and 'TUM_CD...'. The data rows are as follows:

	2D-struct...	TUM_CD...	TUM_CD...
5	<chem>CC1=CC=C(C=C1)N(C)C</chem>	1.1406	48.0756
6	<chem>CCOC(=O)C1=CC=CC=C1C1=CC=CC=C1</chem>	0.0385	73.9672
7	<chem>CC1=CC=C(C=C1)C(=O)C1=CC=CC=C1</chem>	5.9307	72.1032
8	<chem>CCSCSC</chem>	0.5688	52.0564

I started a Bioclipse plugin recently (see screenshot), and placed the source code in [this bioclipse-opentox](#) Git repository on [Gitorious](#) (my [GitHub account](#) is already over the formal limit). The functionality is still quite limited, and the manager currently only provides methods to download data sets ([myexperiment:1192](#)):

```
// query a service using the OpenTox API 1.1
// See: http://www.opentox.org/dev/apis/api-1.1
```

```
var service = "http://apps.ideaconsult.net:8180/ambit2/";
```

```
var datasets = opentox.listDataSets(service);
for (set=0; set<datasets.size(); set++) {
  var dataset = datasets.get(set);
  js.say("Downloading set: " + dataset);
  ui.open(
    opentox.downloadDataSetAsMDLSDfile(
```

chem-bla-ics

```
        service, dataset, "/OpenTox/ambit" + dataset + ".sdf"  
    )  
)  
}
```

Behind this plugin is again the RDF plugin, as OpenTox uses RDF too, a few simple SPARQL queries was all that needed to be defined. And [again](#), the Bioclipse pluigin code base is pretty small.