chem-bla-ics

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

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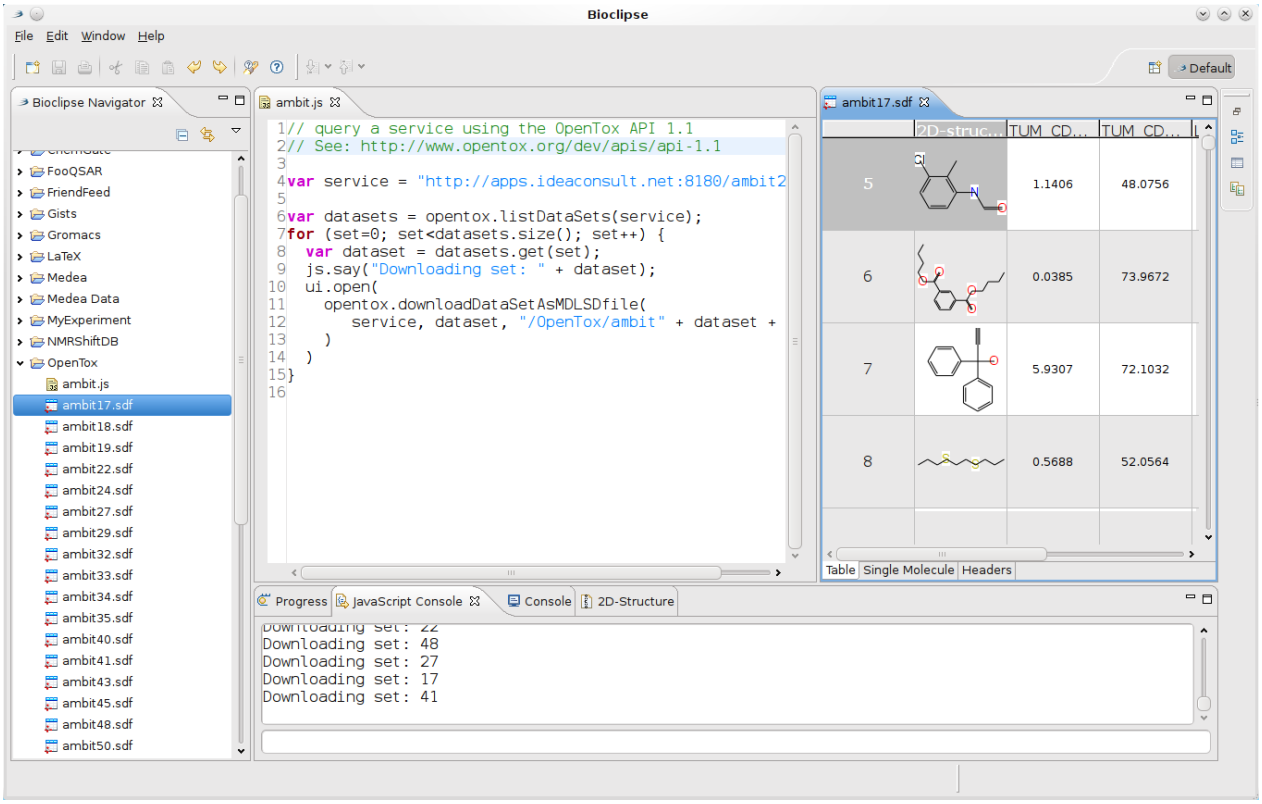
The first week of August I will attend the eCheminfo Predictive ADME & Toxicology Workshop (LinkedIn Event) for which I received a Bursary Award. It will be my first time in Oxford, and I am very much looking forward to it!

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.



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(
```

```
        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.