

Calculating molecular descriptors with OpenTox

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chem-bla-ics

While working during *office hours* on [Oscar](#), I am also trying to finish up some work left from Uppsala. One such thing is the Bioclipse-OpenTox project (see [Using Bioclipse to upload data to an OpenTox server](#) and [Oxford, August 2010: eCheminfo Predictive ADME & Toxicology 2010 Workshop](#)). Today I finished calculating molecular descriptor values with OpenTox servers:

```
// requires an unspecified Bioclipse
// development version
bioclipse.requireVersion("2.6")

service =
  "http://apps.ideaconsult.net:8080/ambit2/";
serviceSPARQL =
  "http://apps.ideaconsult.net:8080/ontology/";

stringMat = opentox.listDescriptors(serviceSPARQL);
stringMat.getColumn("algo");
stringMat.getColumn("desc");

// pick any descriptor
descriptor = stringMat.get(1,1);

opentox.calculateDescriptor(
  service, descriptor,
  cdk.fromSMILES("CCC")
)
```

The first descriptor happens to be a model for predicting the pKa (see [Algorithm or Model: OpenTox API quiz](#)).