

Using Bioclipse to upload data to an OpenTox server

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Published August 4, 2010

Citation

Willighagen, E. (n.d.). In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/f0s4t-znm21>

Keywords

Bioclipse, Opentox, Cheminf, Myexperiment

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chem-bla-ics

As part of a continuing mashup of [Bioclipse](#) and [OpenTox](#), I sat down with Nina in [Oxford](#) to implement uploading molecules from within Bioclipse with JavaScript to OpenTox servers. This opens the route to calculate QSAR descriptors using the [OpenTox API](#).

As a result, you can (with the code at my laptop) now do (see this [BSL script at MyExperiment](#)):

```
// requires an unspecified Bioclipse development version

ds = opentox.createDataset("http://apps.ideaconsult.net:8080/ambit2/");

opentox.addMolecule(ds, cdk.fromSMILES("CCCCC[N+](C)(C)C"))
opentox.addMolecule(ds, cdk.fromSMILES("ClC(I)Br"))

opentox.deleteDataset(ds);
```

Make sure to check out the other stuff [I have been doing with respect to OpenTox](#).