

Searching PubChem from within Bioclipse

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Bioclipse, Pubchem

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chem-bla-ics

For the application note which we are about to submit, I was working on improving the [PubChem Bioclipse](#) API a bit, resulting in new `download` methods:

The search allows using [PubChem Filters](#) which provides many simple means to restrict the search results. For example, we can search molecules and restrict on the molecular weight:

```
lists = pubchem.download(pubchem.search("malaria 300:500[MW]"))
```

Other filters you can use in `pubchem.search` (provided by PubChem itself), includes (with examples):

- **[el]**: `pubchem.search("Au[el]")`
- **[inchi]**: `pubchem.search("\InChI=1S/CH4/h1H4\"[inchi]")`
- **[inchikey]**: `pubchem.search("VNWK TOKETHGBQD-UHFFFAOYSA-N[inchikey]")`
- **[mimass]**: `pubchem.search("375.9785:375.9786[mimass]")`

And many, many more... see the linked [Filters](#) page.

Now, you surely want to look at the hits, for which we use the molecular table editor:

```
list = pubchem.download(pubchem.search("375.9785:375.9786[mimass]"))
cdk.saveSDFFile("/Virtual/hits.sdf", list)
ui.open("/Virtual/hits.sdf")
```

Resulting in:

The screenshot displays the Bioclipse application window. The main area shows a table with columns for '2D-structure', 'IUPAC Name', 'Molecular For...', 'SMILES (Iso...', 'IUPAC Name ...', and 'IUPAC Na...'. The first row contains a chemical structure of 7-amino-N-(2,5-dibromophenyl)heptan-1-amine. The 'Properties' panel on the right shows the following data:

Property	Value
InChI (Standard)	InChI=1S/C13H18Br2N
InChIKey (Standard)	PBNFZRPUTNQL
IUPAC Name (Allowed)	7-amino-N-(2,5-
IUPAC Name (CAS-like Styl)	7-amino-N-(2,5-
IUPAC Name (Preferred)	7-amino-N-(2,5-
IUPAC Name (Systematic)	7-azanyl-N-(2,5-
IUPAC Name (Traditional)	7-amino-N-(2,5-
Molecular Formula	C13H18Br2N2O
Molecular Formula	C13H18Br2N2O
PubChem CID	43714190
SMILES (Canonical)	C1=CC(=C(C=C

The 'Javascript Console' at the bottom shows the execution of the following code:

```
> list = pubchem.download(pubchem.search("375.9785:375.9786[mimass]"))
cdk.saveSDFFile("/Virtual/hits.sdf", list)
ui.open("/Virtual/hits.sdf")
```