

Bioclipse-JChemPaint #2

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Keywords

Bioclipse, Jchempaint, Cdk, Chembl

Abstract

Recently, I blogged about Bioclipse-JChemPaint of the imminent Bioclipse 2.0.0 release, a complete rewrite of the Bioclipse application as published in doi:10.1186/1471-2105-8-59. I also blogged about the feature to browse large MDL SF files (Bioclipse 2.1 will have support one or more CML conventions for chemical tables). Ola did some profiling on processing SD files, but also notes that such may be more suitable for the StructureDB

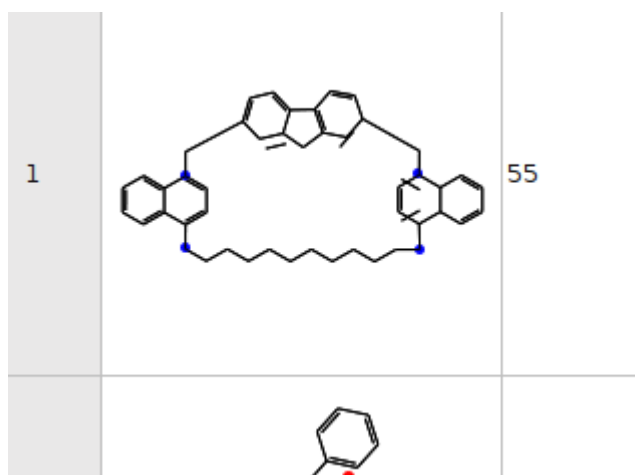
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chem-bla-ics

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Browsing a large set of structures with there properties gives a quick overview of the data set. It also makes bugs shallow, such as the one shown below found when I was browsing the [StarLite](#) database:



The MDL molfile for structure 55 is available from the [bug report I filed against Bioclipse](#).