

chem-bla-ics

Open Source data mining in chemoinformatics

Egon Willighagen 

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On the [7th International Conference on Chemical Structures](#) Jeroen Kazius has a [poster](#) on finding discriminative substructures, that is, molecular fragments which can be discriminate between two activity classes. The software is released as [Gaston](#), is written in C++ and has the GPL license.

Later I encountered [MoSS](#) which has the same goal, but uses a different algorithm. MoSS is written in Java and uses the LGPL license. MoSS reads STN and SMILES as input, which might not be optimal for all users, so a CDK port comes to mind.

References