Open Source Components for Chemoinformatics Education

Egon Willighagen and Christoph Steinbeck*

Cologne University Bioinformatics Center (CUBIC), Zulpicher Str. 47, 50674 Koln, Germany

Chemoinformatics has seen the emergence of a number of open software packages and open standards in the last few years, including molecular editors, molecular viewers, toolkits for the conversion of chemical data formats and fully fledged chemoinformatics libraries. These components constitute a chance for chemoinformatics education, allowing the teacher to provide students no only with abstract algorithms or concepts but with concrete implementations, which can be studied in source code and tested with real data. Further, in times of notoriously small education budget, the use of free software packages in courses allows keeping the costs low.

In this talk we give an overview and assess the strengths and limitations of existing open source chemoinformatics software including chemical editors such as JChemPaint, 3D viewers like Jmol, chemoinformatics libraries (CDK and JOELib), conversion packages (OpenBabel) and integrated workbenches like Bioclipse.