

chem-bla-ics

The goal: a live chemblaics CD

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This evening I have been looking at with the [KNOPPIX](#) customization howto, and ran many of the interesting commands. I've setup a environment with Kalzium, OpenBabel, CDK, jython, [PyMOL](#), and for development I included gcj and Eclipse. At some later point I will include kfile_chemical too, but I want to make a deb package first.

Moreover, I also wanted it to include JChemPaint, Jmol and [Taverna](#) (with the CDK extension). However, these depend on Swing, which is not sufficiently provided by open source java virtual machines. I attempted [gij](#) 4.0, [kaffe](#) and [sablevm](#), all without success.

A live CD with all the open source chemo- and bioinformatics tools would be a real killer. We could take a burned live CD with us to conferences and have others run our software on their laptop! But we need to stop use Swing. Fortunately, there seems to be a serious project going on to port JChemPaint and Jmol to a free Java GUI environment, so maybe we can have the live CD up and going before the 2006 conferences start.

References