The goal: a live chemblaics CD

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Abstract
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.

chem-bla-ics

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Moreover, I also wanted it to include JChemPaint, Jmol and Taverna (with the CDK extension). However, these depend on Swing, which is not suffiently 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.