

chem-bla-ics

Free at last!

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Free at last! Well, not quite yet, but close enough anyway: my PhD contract has ended; last friday was my last working day, which my colleagues and I celebrated with a visit to Nijmegen oldest bar, [In de Blauwe Hand](#) . But I still have my manuscript to finish. This formally ends a period of almost 12.5 years at the [Radboud University Nijmegen](#).

Starting last monday I'm at home, trying to get things finished as soon as possible. Mostly working on my laptop, remote logged in into our desktop machine downstairs. A good ADSL (170kB downstream) helps a lot too, and the proxy on my university machine allows me to access the full access journals of my university.

I'm trying to dome some open source chemoinformatics in between writing, and my current QSAR research actually allows me to do some feature enhancement in CDK's QSAR package too. Today, I hope to write and finish a [config file architecture](#) that allow fine tuning which QSAR descriptors should be calculated. I anticipate a default config files to be distributed.

Additionally, I will try to finish running teh CDK JUnit test against [Classpath 0.20](#), which 98% of Java 1.4.2 covered, and the limited support for HTML rendering is most of this last 2%. The Classpath progress has really amazed me over the last few weeks. I have not tested Jmol and JChemPaint against the latest open source java tools, but will try to do that before I go on holiday next week. Results with 0.19 were very promising, as I reported in earlier blog entries.

References