

Things to do...

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Abstract

I know I am lagging behind things... been busy and did not have time to reply to everyone yet. Some TOREPLY's go back more then a month. Sorry about that!

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chem-bla-ics

I know I am lagging behind things... been busy and did not have time to reply to everyone yet. Some TOREPLY's go back more than a month. Sorry about that!

Some of the things on my TODO list (in random order): *Bioclipse2 bug fixes, CDK patch reviewing (e.g. vflib), look at the Jmol-CDK bridge and bring it into action in Bioclipse2, RDF for PubChem, convert the Woordenboek Organische Chemie data into in RDF, RDF for NMRShiftDB, align with ChemAxiom, publish about the Bioclipse2 RDF feature, finish the MetWare paper, write a metabolomics feature for Bioclipse2, finish the pKa prediction in the CDK, write 100% coverage CDK 2 CML 2 CDK, implement atom parity stereochemistry from SMILES and/or MDL molfiles, use supervised SOMs in QSAR, user supervised SOMs in proteochemometrics, study variable influence on supervised SOM models, make my thesis Open in the Radboud University library repository (excluding the papers I no longer have copyright on), update the QSAR and algorithm ontologies in OWL, create a web page with life ONS solubility RDF, create an ONS solubility Bioclipse2 feature, study the CDK fingerprint performance compared to the new PubChem fingerprint, make Chemical blogspace aware of the ChemSpider widget, interest people for an unconference in Stockholm or Uppsala, move house, learn to Swedish, get a driver license, implement a memory more-efficient CDK interfaces implementation, promote XMPP services which are better than SOAP, and write more papers, work on CMLSpect for metabolomics, finish the CDK book, finally get a grant application approved, read up with literature and summarize in blog, port the Jmol UFF force field code to the CDK, analyze atom typing in the CDK against PubChem and StarLite, compile strigi-chemistry again KDE 4.2.2, finish egonw.github.com homepage, ... you know the regular list of things to do.*

If you happen to be a masters student interested in doing a internship/practical here in Uppsala (unpaid, but you will learn so much), just email me.