

chem-bla-ics

CDK Workshop 2009 #2

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Keywords

Cdk, Jchempaint

Abstract

The second CDK Workshop day started off with application presentations, which are well covered by Chris' blog posts:

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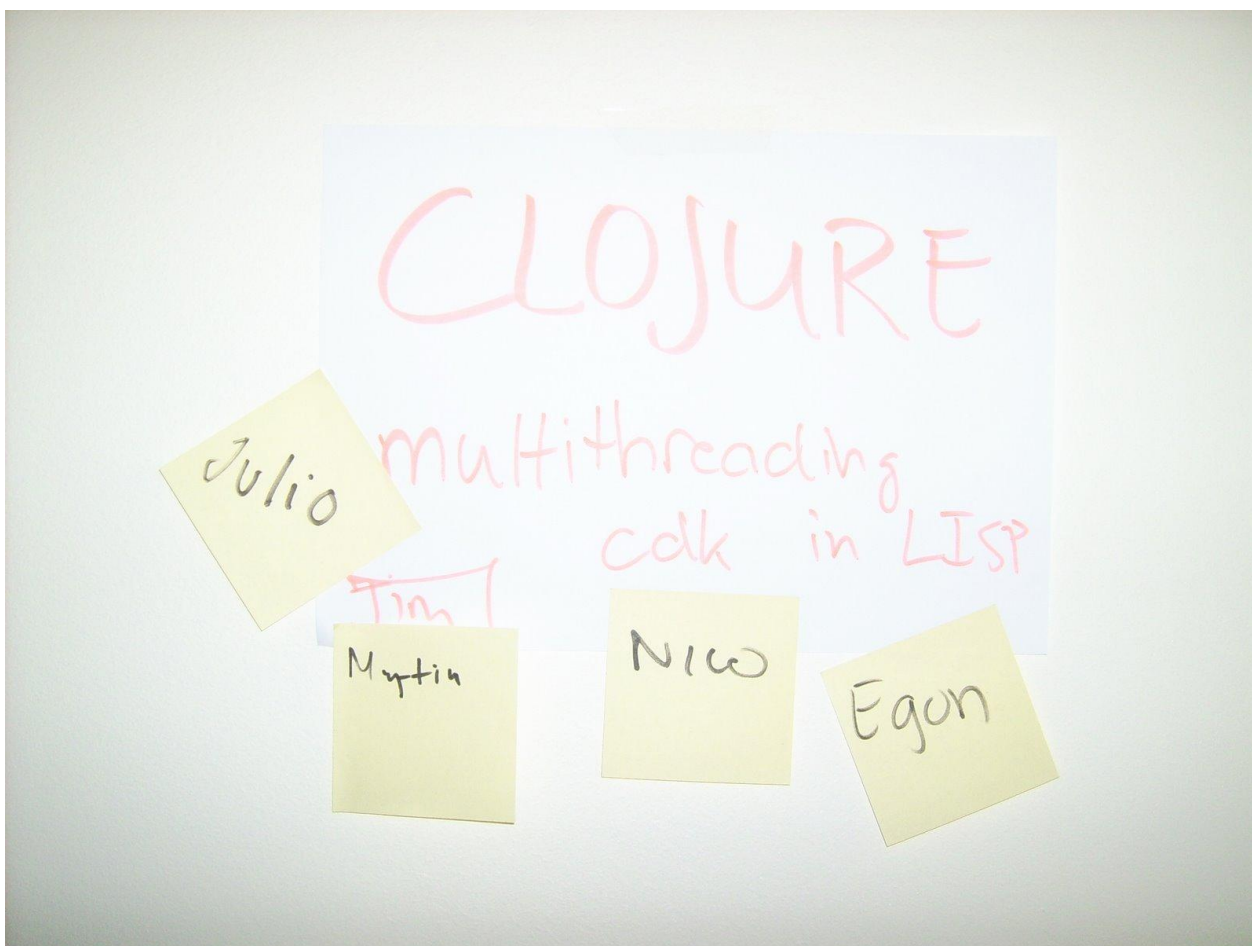
- [John van Drie's talk on CDK in Virtual Drug Discovery](#),
- [Asad Rahman on Small molecules and reaction mechanism - Rewiring the enzyme space](#), and
- [Oliver Karch about Molwind - Using CDK to Visualize Molecule Spaces in a Geospatial Context](#).

You can also find [coverage on Twitter](#) by [Jim](#) and [Nico](#).

The afternoon we had a more development-oriented [unconference](#). It was a bit exciting for me and [Chris](#) as previous such sessions at CDK workshops involved 5 to 10 participants instead some 20+ now, but things nicely self-organized into 5 sessions:

TOP 10
IMPROVE
consultancy!
Colin | NINA

CHEMBL
Pharmacophore
Mining
MARK
PABLO
MIGUEL
J. v. Drie
LUCA P.
Chris S.
OLA S.



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In words, and linking to the coverage in the CDK wiki:

- [JChemPaint/Rendering](#)
- [Mining ChEMBL with CDK pharmacophore stuff](#)
- [Threading group](#)
- [Top 10 improvements \(CDK WS 2009 unconference\)](#)
- [Clojure](#) (see also Jim's blog [2D Molecule Diagrams in Clojure](#))