

chem-bla-ics

CDK Workshop 2009 #2

Egon Willighagen 

Published April 22, 2009

Citation

Willighagen, E. (n.d.). In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/77t7v-1ed64>

Keywords

Cdk, Jchempaint

Copyright

Copyright © Egon Willighagen 2009. Distributed under the terms of the [Creative Commons Attribution 4.0 International License](#), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

chem-bla-ics

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

- [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
F

MIGUEL

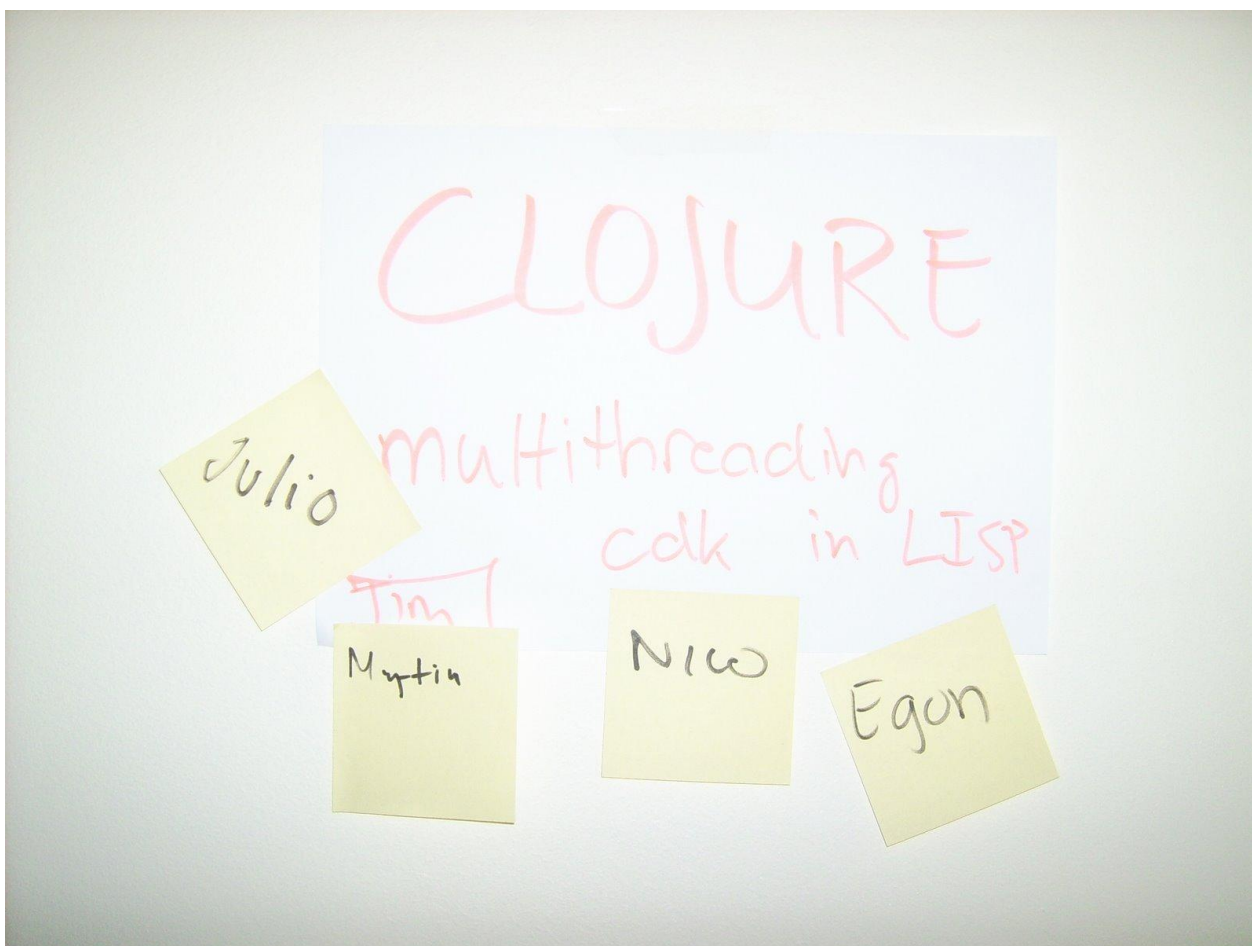
PABLO

J. v. Drie

LUCA
P.

Chris
S.

OLA
S



chem-bla-ics

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](#))