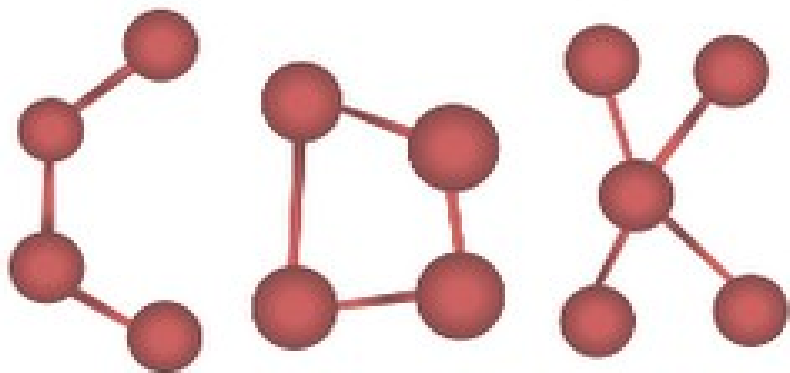# The Chemistry Development Kit

# in the Netherlands

Egon Willighagen & Miguel Rojas-Chertó

BiGCaT - Maastricht University

Div. Anal. Biosciences – Leiden University

*NBIC 2012, Lunteren*

# Open Source Cheminformatics



- Metabolomics
- Drug discovery
- Toxicology

| | | | |
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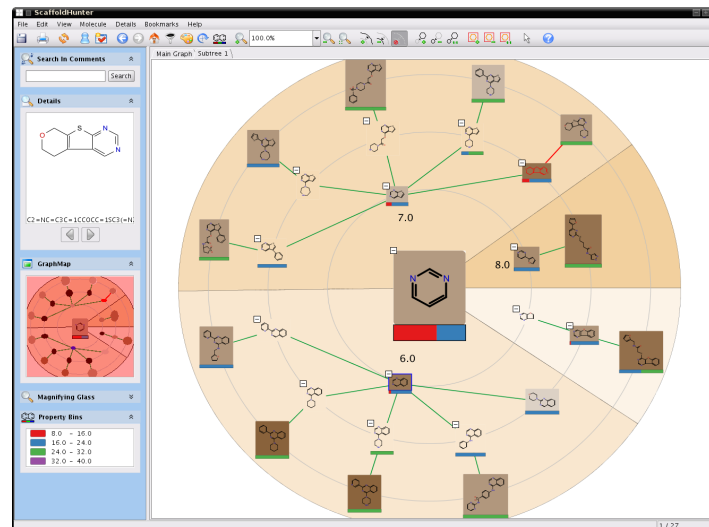


Wetzel et al., Nature Chemical Biology, 2009
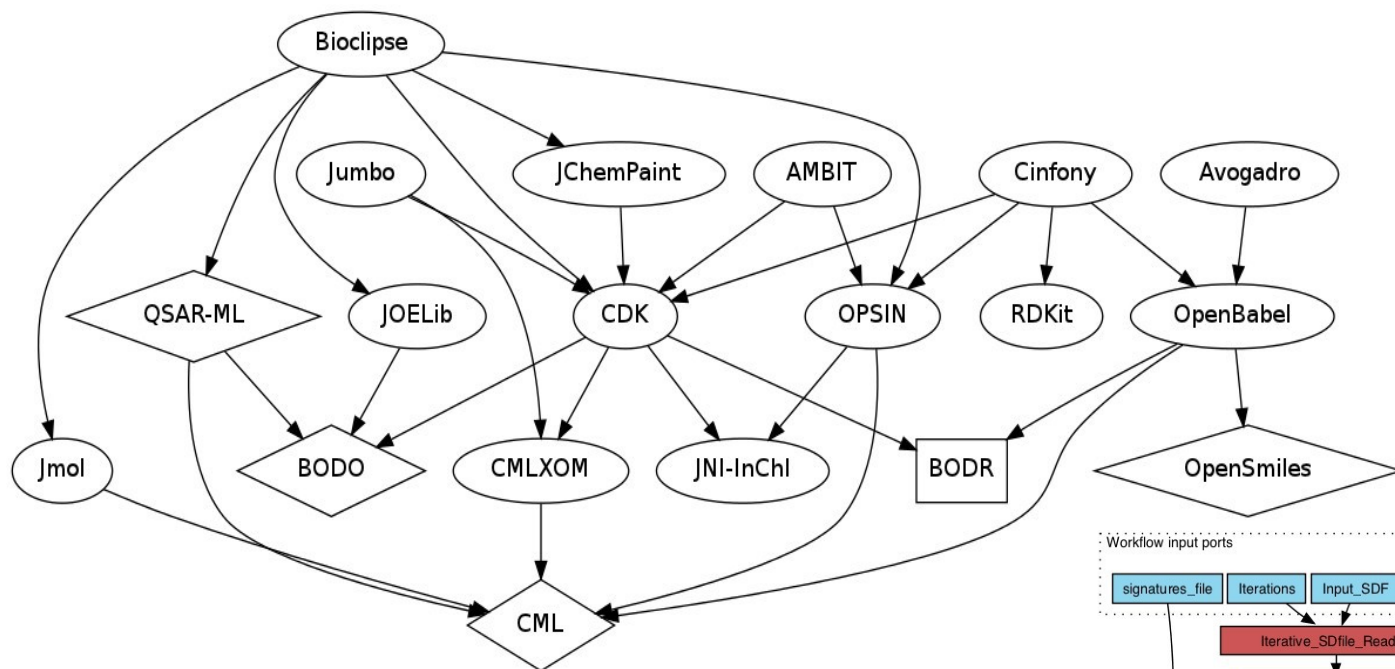
O'Boyle et al., JChemInf, 2011
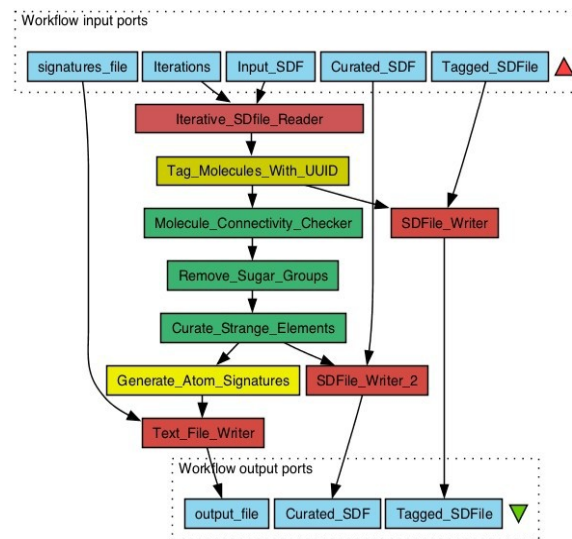
Truszkowski et al., JChemInf, 2011

# History

- Based on Steinbeck's CompChem, 1997
- CML support added in 1999
- Combining JChemPaint and Jmol in 2000
  - meeting @ Notre Dame University
  - funding by Specs & BioSpecs (D. Wife) !
- Now led by Steinbeck (EBI), Guha (NIH), me (BiGCaT)

Date: Tue, 04 May 1999 12:35:10 +0200
From: Christoph Steinbeck
To: Egon Willighagen

> Egon Willighagen wrote:
>
> Dear Christoph Steinbeck,
>
> Yesterday I visited your site on JChemPaint. I like to contribute some
> of my expertise on Java and CML (1).
>
> CML is a markup language that is able to contain chemical information.
> It can contain for example physical properties, for which I use CML in
> my Dictionary on Organic Chemistry (2).
> But is also might contain spectra, bibliographic references etc. And
> of course 2D and 3D structural information.
>
> Therefore I propose to write both CML-input and -output procedures for
> the JChemPaint project.
>
> I hope to hear from you soon.
>
> Yours sincerely,
>
> Egon Willighagen
>
> 1. http://www.xml-cml.org/
> 2. http://www.sci.kun.nl/sigma/Chemisch/Woordenboek/

Dear Egon,

thanks very much for your mail and your offer to write CML-input and
output routines for JChemPaint.
That really sounds great to me and I will give you access to our CVS
tree as soon as we have discussed the details.

Cheers,

Chris

--C. S.
Dr. Christoph Steinbeck (http://www.ice.mpg.de/~stein)

# E. CDK Authors

In acknowledgment to all the work done by the many people who have contributed to the success of the CDK, here is a list of those who wrote smaller or larger parts of the CDK library:

Sam Adams, Jonathan Alvarsson, Rich Apodaca, Saravanaraj N Ayyampalayam, Ulrich Bauer, Stephan Beisken, Arvid Berg, Ed Cannon, Fabian Dortu, Martin Eklund, Matteo Floris, Dan Gezelter, Uli Fechner, Thorsten Flügel, Nimish Gopal, Rajarshi Guha, Yonquan Han, Thierry Hanser, Kai Hartmann, Tobias Helmus, Christian Hoppe, Oliver Horlacher, Miguel Howard, Nina Jeliazkova, Geert Josten, Dmitry Katsubo, Jules Kerssemakers, Anatoli Krassavine, Stefan Kuhn, Uli Köhler, Violeta Labarta, Jonty Lawson, Daniel Leidert, Edgar Luttmann, Todd Martin, John May, Nathanaël Mazuir, Stephan Michels, Scooter Morris, Peter Murray-Rust, Carl Mäsak, Irilenia Nobeli, Peter Odéus, Niels Out, Jerome Pansanel, Julio Peironcely, Chris Pudney, Syed Asad Rahman, Jonathan Rienstra-Kiracofe, Mark Rijnbeek, David Robinson, Miguel Rojas Cherto, Bhupinder Sandhu, Jean-Sebastien Senecal, Onkar Shinde, Sulev Sild, Bradley Smith, Ola Spjuth, Christoph Steinbeck, Aleksey Tarkhov, Stephan Tomkinson, Gilleain Torrance, Andreas Truszkowski, Paul Turner, Jörg Wegner, Yap Chun Wei, Stephane Werner, Egon Willighagen, Lars Willighagen, Yong Zhang, and Daniel Zaharevitz.

**BIOINFORMATICS** **ORIGINAL PAPER**

Vol. 27 no. 17 2011, pages 2376–2383
doi:10.1093/bioinformatics/btr409

Netherlands
Metabolomics Centre

*Structural bioinformatics*

Advance Access publication July 14, 2011

## Elemental composition determination based on MS$^n$

Miguel Rojas-Chertó[1,2,*], Piotr T. Kasper[1,2], Egon L. Willighagen[1,3,4], Rob J. Vreeken[1,2], Thomas Hankemeier[1,2] and Theo H. Reijmers[1,2,*]

[1]Netherlands Metabolomics Centre, [2]Division of Analytical Biosciences, Leiden/Amsterdam Center for Drug Research, Leiden, The Netherlands, [3]Division of Molecular Toxicology, Institute of Environmental Medicine, Karolinska Institutet, Stockholm, Sweden and [4]Plant Research International, Wageningen UR, Wageningen, The Netherlands

Associate Editor: Anna Tramontano
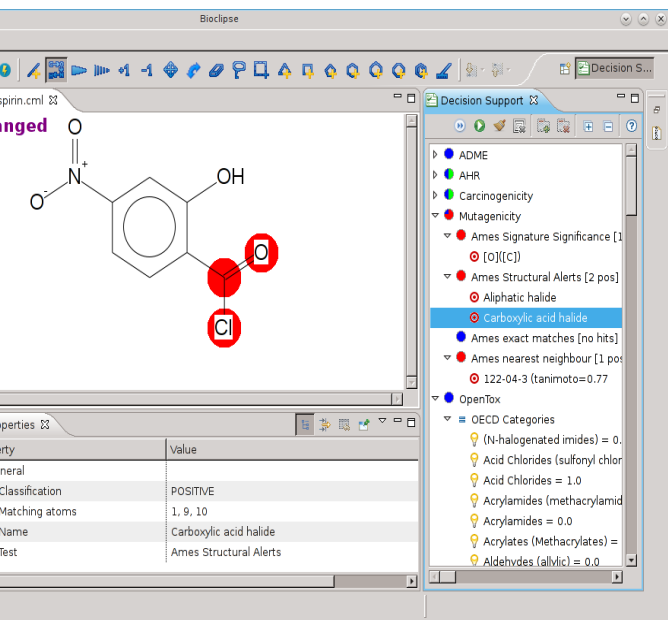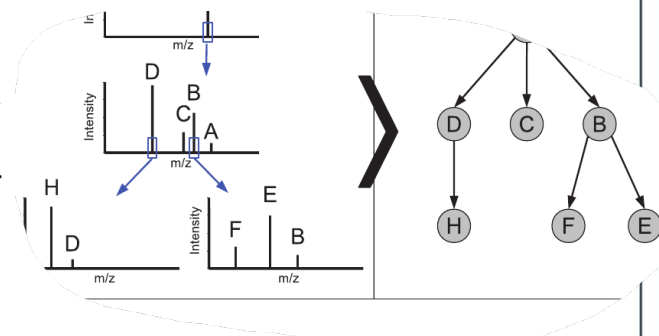
Willighagen *et al.* BMC Research Notes 2011, **4**:487
http://www.biomedcentral.com/1756-0500/4/487

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Research Notes

**SHORT REPORT**                                                    **Open Access**

## Computational toxicology using the OpenTox application programming interface and Bioclipse

Egon L Willighagen[1,2*], Nina Jeliazkova[3], Barry Hardy[4], Roland C Grafström[2,5] and Ola Spjuth[1]

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