

# CompLife'06 - Day 1

Egon Willighagen 

Published September 28, 2006

## Citation

Willighagen, E. (2006). CompLife'06 - Day 1. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/c1cqc-vvg92>

## Keywords

Cdk, Bioclipse, Knime

## Abstract

CompLife'06 started today in Cambridge, UK. About 80 people are attending the meeting, and topics range from systems biology to QSAR. This evening there was a free software session mostly focussing on opensource software.

## Copyright

Copyright © Egon Willighagen 2006. 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

[CompLife'06](#) started today in Cambridge, UK. About 80 people are attending the meeting, and topics range from systems biology to QSAR. This evening there was a free software session mostly focussing on opensource software. Twelve projects were presented, among which the [CDK](#) (by me) and [Bioclipse](#) (by Ola), in five minute presentations, and a two hour demo period during a reception (free speech and free beer :). We had our brand new fliers with us, as well as a large poster for some additional branding.

One research presentation compared a number of fingerprint implementations in a QSAR study, and CDK came out very well, beating a few commercial programs. The free software session was full of CDK, however, with [AMBIT](#), [iBabel](#), [Bioclipse](#) and [KNIME](#) mentioning the CDK.

The latter is really interesting: it's a workflow program just like [Taverna](#) or [PipeLine Pilot](#), which is using the Eclipse RCP as starting point, just like [Bioclipse](#). And like the other two, [KNIME](#) has CDK integration, at least for displaying structures.