

Chemical reactions in CML

Egon Willighagen 

Published February 17, 2006

Citation

Willighagen, E. (2006). Chemical reactions in CML. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/zm41a-h0037>

Keywords

Cdk, Cml, Bioinfo

Abstract

Gemma Holiday's article on CMLReact was published in the january issue of the JCIM (doi: 10.1021/ci0502698), which seems to be marked as sample issue right now. She used CMLReact as data format for MACiE (see doi:10.1093/bioinformatics/bti693), a database of 100 enzyme reactions, with fully annotated reaction mechanisms, making this an remarkable and insightfull database.

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

Gemma Holiday's article on CMLReact was published in the january issue of the [JCIM](#) (doi: [10.1021/ci0502698](https://doi.org/10.1021/ci0502698)), which seems to be marked as sample issue right now. She used CMLReact as data format for [MACiE](#) (see doi:[10.1093/bioinformatics/bti693](https://doi.org/10.1093/bioinformatics/bti693)), a database of 100 enzyme reactions, with fully annotated reaction mechanisms, making this an remarkable and insightfull database.

Now, the nice thing is that this CML should be readable and renderable by the [CDK](#), though the webinterface uses SVG and can be used using [FireFox](#) too.