

Chemical reactions in CML

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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.

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chem-bla-ics

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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.