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"Jmol and the CDK add powerful chemical capabilities", says Munos in Nature Reviews Drug Discovery



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Keywords

Drugdiscovery, Jmol, Cdk, Opensource

Abstract

Bernard Munos at Eli Lilly & Co. wrote up a lengthy analysis on open source in drug discovery in Nature Reviews Drug Discovery: Can open-source R&D reinvigorate drug research?

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Bernard Munos at Eli Lilly & Co. wrote up a lengthy analysis on open source in drug discovery in Nature Reviews Drug Discovery: Can open-source R&D reinvigorate drug research? (DOI:10.1038/nrd2131). When scanning the article I saw this quote:

Other tools such as eMolecules, Jmol or the Chemistry Development Kit are adding powerful chemical search and visualization capabilities to the open-source scientist's toolbox.

Unfortunately, the paper does not point to the correct CDK website, but to the CUBIC backend at http://almost.cubic.uni-koeln.de/cdk. Moreover, I don't think the quote does full justice to what the CDK has achieved in the past six years; I'm sure we have achieved more than a fingerprinter and some 2D and 3D rendering!