

Open source in drug discovery

Egon Willighagen 

Published March 12, 2006

Citation

Willighagen, E. (2006, March 12). Open source in drug discovery. *Chem-bla-ics*. <https://doi.org/10.59350/29xwa-ehq10>

Keywords

Drugdiscovery, Openscience

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

Geldenhuys et al. published an article in [Drug Discovery Today](#) titled *Optimizing the use of open-source software applications in drug discovery* (DOI:10.1016/S1359-6446(05)03692-5), and approached the review from a bench chemist point of view. Unfortunately, he discusses free, but closed source, program in one go.

He discusses the advantages and problems with opensource, and mentions the often lacking user-friendly GUI (true), and the the lack of literature to validate the program. It was unclear to me wether the last argument applied to the free tools, or to the open source programs; I thought the open-source projects like the [CDK](#), [JOELib](#), [Jmol](#) and [PyMol](#) were quite strong in this area, at least compared to the commercial software I have seen.