chem-bla-ics

Open source in drug discovery

Egon Willighagen

Published March 12, 2006

Citation
Willighagen, E. (2006). Open source in drug discovery. In *chem-bla-ics*. chem-bla-ics. https://doi.org/10.59350/29xwa-ehq10

Keywords
Drugdiscovery, Openscience

Abstract
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.

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.