

Abstract:

Chemotion ELN is a domain-specific electronic lab notebook that was developed for chemists in order to foster the digitalization of their work processes.[1] The Chemotion-ELN offers basic features to manage research data, including tools for structure processing and reaction planning, data requests to external databases and several search functions. It includes also strategies to involve lab devices and to transfer data from different locations to the ELN server. The ELN allows to share or export research data and to generate reports based on the available digital information in an automatic manner. The Chemotion ELN can be connected to a repository for research data which allows the almost effortless transfer of data to an infrastructure offering open access for all scientists. The ELN is part of the strategy of the NFDI4Chem. Therefore, the software will be adapted to serve as suitable instrument to digitalize the research efforts of all sub-disciplines in chemistry in the long run.

[1] Journal of Cheminformatics vol. 9, 2017: 54.

<https://jcheminf.biomedcentral.com/articles/10.1186/s13321-017-0240-0>