Subject: Re: Saving 2D-structure with labels

Posted by vijaymasand on Mon, 06 Jun 2022 05:37:44 GMT

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Dear Norwid

Thank you for the reply. The solution provided by you is really simple and useful. I also developed images with required labels using your method without any problem. This also solved my third requirement of inclusion of 'white' as an option in 'Look and Feel'.

However, when I tried it for more than 100 molecules, I got error message that it is out of memory. So, it has some limitations. I am using Windows 11 (64 bit), 32 GB RAM, and Datawarrior 05.05.00.

For point number 2, I hope the developers will develop a solution to download data from ChEMBL30.

With regards

Vijay