Subject: Re: Generating derivatives of parent structure
Posted by nbehrnd on Sun, 05 Nov 2023 18:14:19 GMT
View Forum Message <> Reply to Message

Hello,

this taps into the generation of a combinatorial library you find below Chemistry -> enumerate combinatorial library. Either you find your reaction among the templates DW ships by default, or you create your own reaction pattern. Tab «reactants» allows you to use molecules already defined in a .dwar, or .sdf; or to let DW select ones which are commercially available (criteria are adjustable).

See chapter «chemical structures», section «combinatorial library» in DW's help or the online web page[1] for additional information. It however is time well invested to follow Isabelle Girault's video tutorial about the topic «RSC CICAG Open Source Tools for Chemistry Workshops:- Advanced DataWarrior»[2] recorded in 2021 around 47:18 min:s on youtube. (There is sequal «DataWarrior workshop by Isabelle Giraud»[3] by her to complement the insight about DW, too.)

Regards,

Norwid

[1] https://openmolecules.org/help/chemistry.html#VirtualLibrari es
[2] https://www.youtube.com/watch?v=mQCf9GakQW0
[3] https://www.youtube.com/watch?v=Is2hLqqSFvM