Subject: Re: Generating derivatives of parent structure
Posted by nbehrnd on Sun, 05 Nov 2023 21:36:35 GMT
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The combinatorial library is generated within a .dwar file and eventually contains an array of the structures of the product, as well as as of the corresponding starting materials.

Departing from here, you can either

- edit this array to selectively copy & paste the column(s) of interest / remove columns not suitable, or
- export the .dwar file as such as a .sdf file which then contains only the structures of the products.

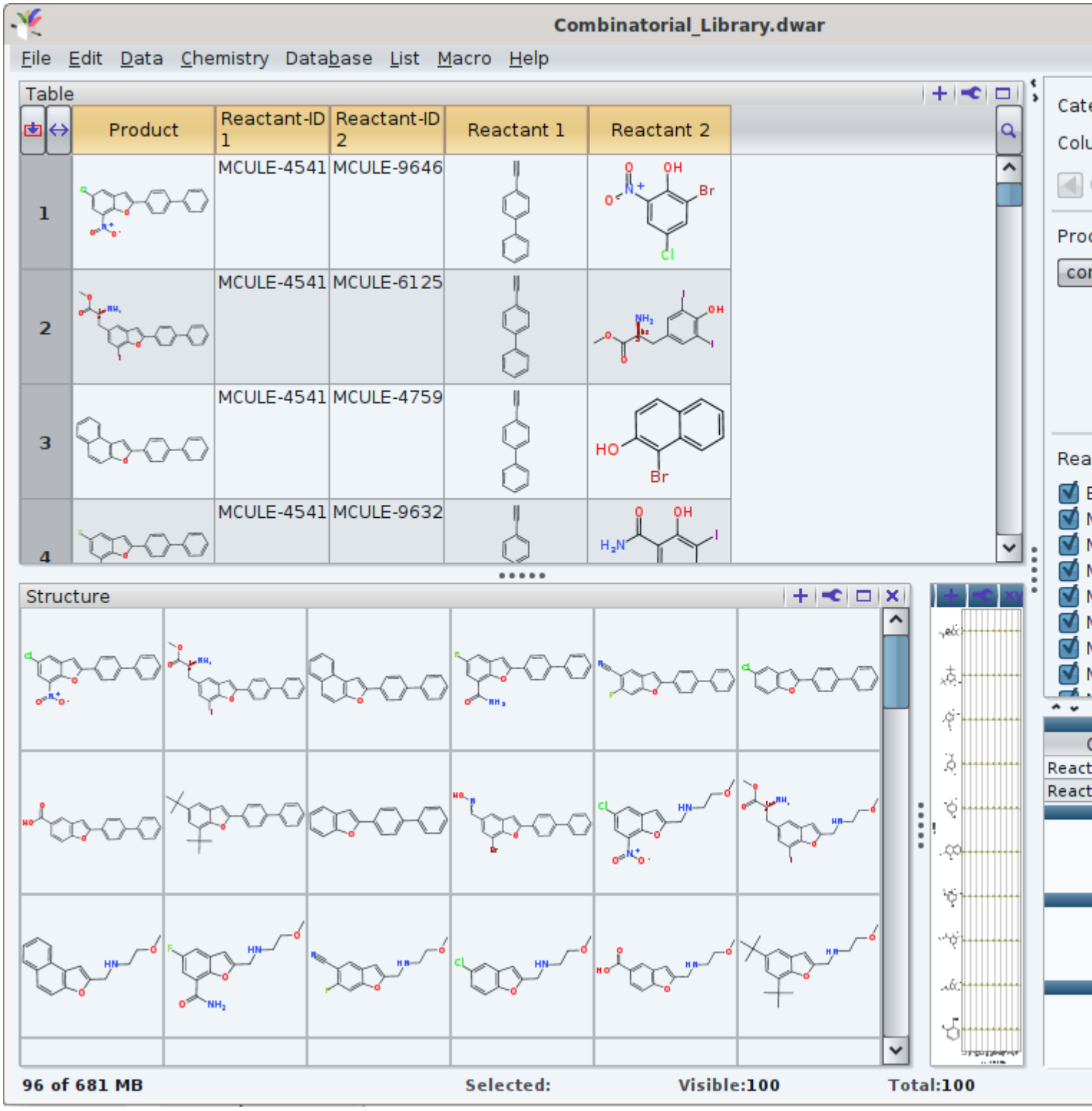
See the .dwar and .png attached for a small 10 by 10 library to yield benzophenones as illustration. This approach DW provides is intuitive, the implementation to recur on compounds only known «in house» or commercially available delivers the results quickly.

Regards,

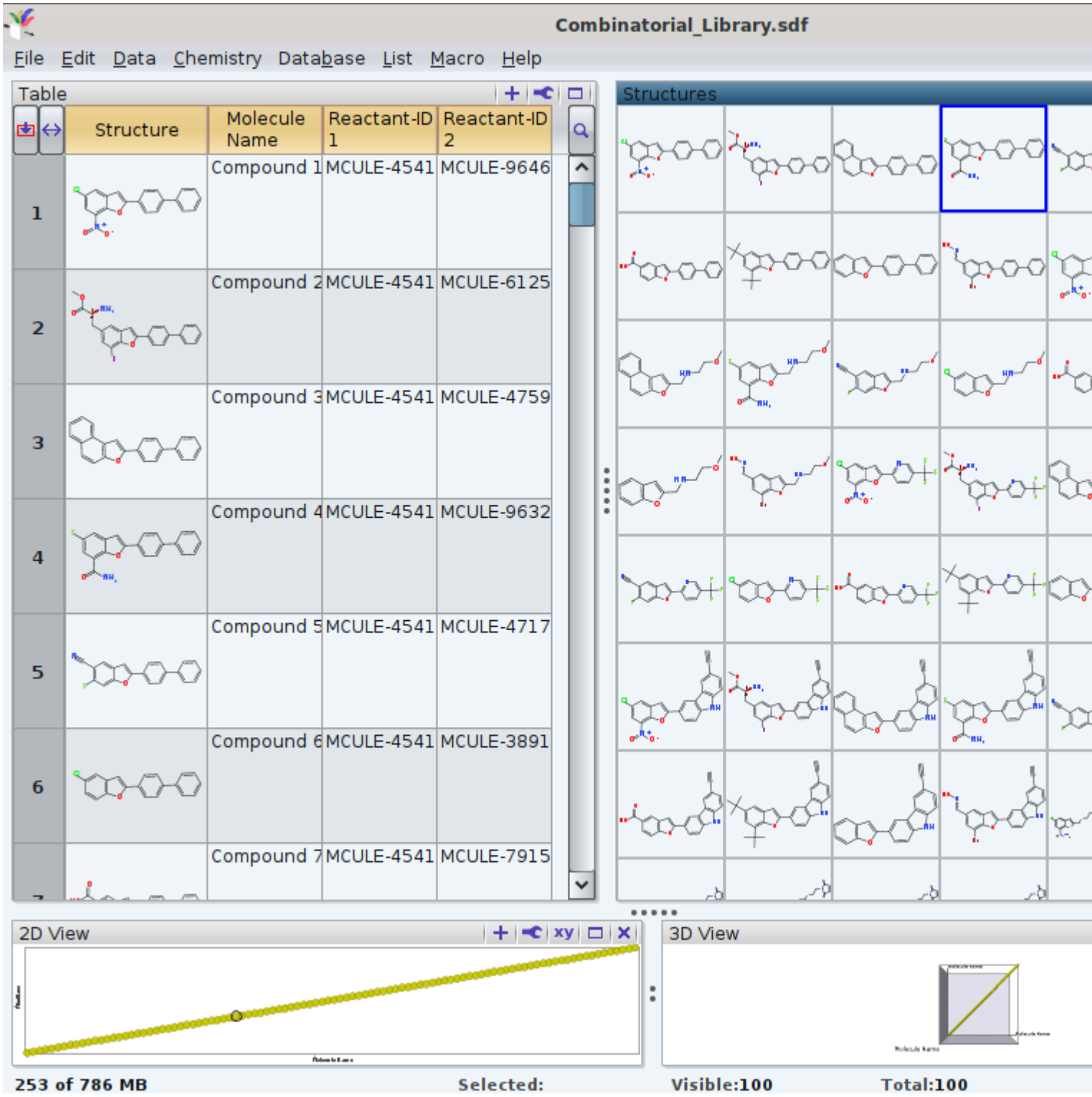
Norwid

File Attachments

1) Combinatorial_Library_dwar_file.png, downloaded 819 times



2) Combinatorial_Library.dwar, downloaded 631 times
3) Combinatorial_Library_exported_sdf_file.png, downloaded 800 times



4) Combinatorial_Library.sdf, downloaded 660 times