
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 537 times

Combinatorial_Library.dwar

File Edit Data Chemistry Database List Macro Help

Table					
	Product	Reactant-ID 1	Reactant-ID 2	Reactant 1	Reactant 2
1		MCULE-4541	MCULE-9646		
2		MCULE-4541	MCULE-6125		
3		MCULE-4541	MCULE-4759		
4		MCULE-4541	MCULE-9632		

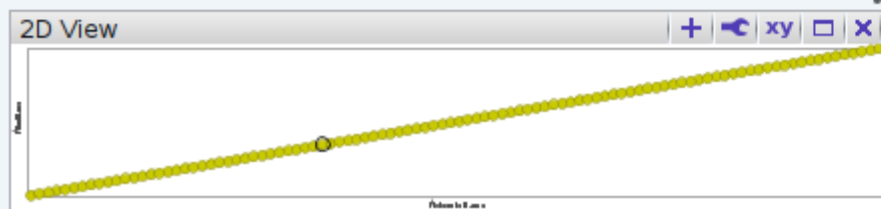
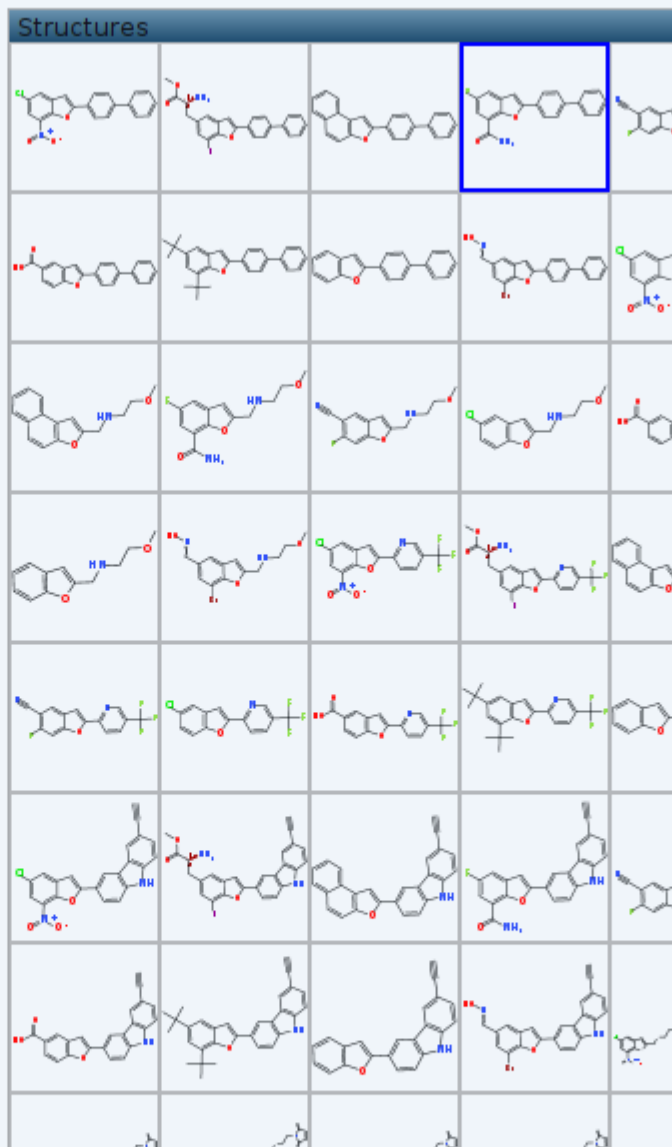
Structure					

96 of 681 MB Selected: Visible:100 Total:100

- 2) [Combinatorial_Library.dwar](#), downloaded 535 times
 3) [Combinatorial_Library_exported_sdf_file.png](#), downloaded 545 times



Table				
	Structure	Molecule Name	Reactant-ID 1	Reactant-ID 2
1		Compound 1	MCULE-4541	MCULE-9646
2		Compound 2	MCULE-4541	MCULE-6125
3		Compound 3	MCULE-4541	MCULE-4759
4		Compound 4	MCULE-4541	MCULE-9632
5		Compound 5	MCULE-4541	MCULE-4717
6		Compound 6	MCULE-4541	MCULE-3891
7		Compound 7	MCULE-4541	MCULE-7915



253 of 786 MB

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Visible:100

Total:100

4) [Combinatorial_Library.sdf](#), downloaded 559 times