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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 387 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		

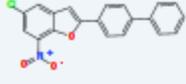
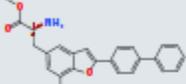
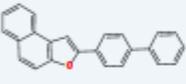
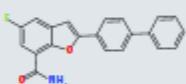
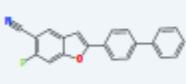
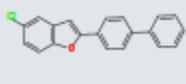
Structure					

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

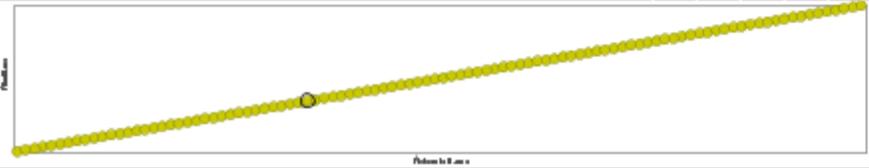
- 2) [Combinatorial\\_Library.dwar](#), downloaded 477 times
- 3) [Combinatorial\\_Library\\_exported\\_sdf\\_file.png](#), downloaded 400 times

**Combinatorial\_Library.sdf**

File Edit Data Chemistry Database List Macro Help

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

2D View



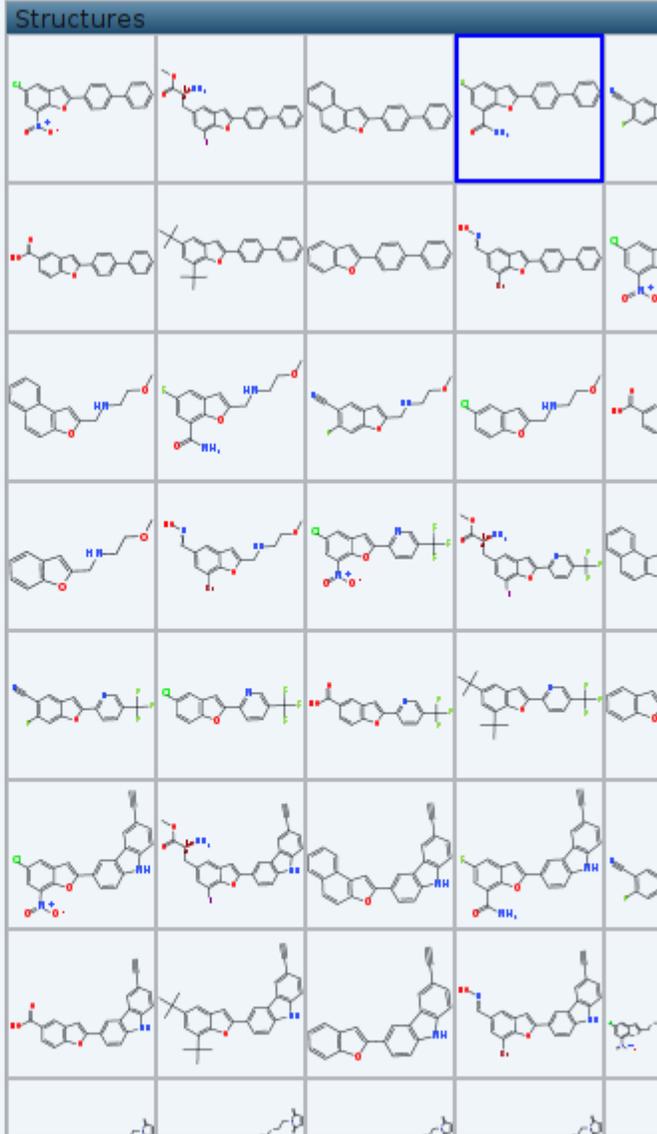
253 of 786 MB Selected:

3D View



Visible:100 Total:100

Structures



4) [Combinatorial\\_Library.sdf](#), downloaded 468 times