
Subject: Re: Enumerating Combinatorial Libraries
Posted by [thomas](#) on Wed, 03 Nov 2021 09:11:33 GMT
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Hi Ed,

you could also create a macro with an 'enumerate combichem library' task using one of these methods:

- 1)
 - Launch DataWarrior
 - Macro->Start Recording...
 - Chemistry->Enumerate Combinatorial Library...
 - Macro->Stop Recording
 - Macro->Export Macro...

- 2)
 - Open DataWarrior
 - Press right mouse key and select 'New Macro Editor'
 - In the right panel press the popup button and choose 'New Macro...', give it a name and press OK
 - Open the 'Chemistry' tasks (click '+')
 - Drag the 'Enumerate Combichem Library' task to the new macro's task list
 - Double click the task and configure (define reaction and reactants)
 - Macro->Export Macro...

Afterwards you can:

- Import the macro file into a new DataWarrior window, change it in the macro editor, and export again
- run it from the file menu -> Open Special-Run Macro...
- Import it into any dwar file (then it is saved with the file). Then use Macro->Run Macro...

Hope this helps,

Thomas
