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