Subject: Enumerating Combinatorial Libraries
Posted by ELFritzen on Sat, 23 Oct 2021 13:21:37 GMT
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I've been enumerating combinatorial libraries in Datawarrior, and it works pretty well. I was wondering if it is possible to save both the generic reaction and the reactant inputs with the enumerated Datawarrior File. As long as the enumerated library file is open, I can return to "enumerate combinatorial library" and make changes to the reactant inputs. I can save the enumerated Datawarrior file, but if I close the file and re-open, I have to re-enter the generic reaction and all the inputs. I know I can save the generic reaction and recall that. It's the reactant inputs that I'd like to save as well so I don't have re-enter them.
Thanks

Ed Fritzen

Subject: Re: Enumerating Combinatorial Libraries
Posted by nbehrnd on Thu, 28 Oct 2021 18:27:48 GMT
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Reformulated as a feature suggest: At present, we define and map a typical reaction (.rdf file) and reagents (.sdf file(s)) accordingly to generate a library saved as .dwar file. For a) a subsequent revision how this library was built, or b) a later correction, or extension of the set of reagents submitted to build the library, one has to retain all of these files.

However, it would be an advantage if the .dwar file were a container of all of these files' content, beyond of storing only the library generated. Then, while reading a .dwar file, Chemistry -> Enumerate Combinational Library would display promptly the generic reaction used earlier (ready to be exported as an .rdf), and offer export of reagent .sdf, too. Conceptually, this were in line with access/subsequent edit of the formulae of Data -> Add Calculated Values already provided.

Norwid

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
