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