Subject: Comparing Structures from two Datawarrior Files
Posted by ELFritzen on Thu, 29 Jun 2023 14:35:47 GMT
View Forum Message <> Reply to Message

I have two Datawarrior Files that I would like to compare the structures. One file is our corporate database, containing all the compounds we have prepared and registered. This file contains 729 compounds. The other file contains structures that have been enumerated using Datawarrior and contains 690 compounds. The enumerated file contains structures that have already been made and registered and I would like to find these structures and eliminate them from the enumerated file, so as not to target them for synthesis again. I've tried using the "Find Similar Compounds in File...." command, but Datawarrior locks up with the display of many "Uncaught Exception:Null" messages being produced. I end up having to force quit Datawarrior. I've tried using either the "Structure of SMILES{FragFp] or the Structure{Exact] options for the Structure Column[comaparison method]: and get the same result. The comparison starts, and eventually freezes Datawarrior. Is there something I'm missing? Or is there a better way to do this?

Thanks in advance for help.
Edward Fritzen