Subject: Re: Comparing Structures from two Datawarrior Files
Posted by zig on Mon, 03 Jul 2023 18:29:40 GMT
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Dear Edward,

a work around could be to create a unique code for your molecules, with Chemistry>From Chemical Structure > Add Canonical Code..., in both files.

Then you select all these canonical codes in the file containing the molecules of the corporate database, and copy them (Edit> Copy -> they are now in your clipboard)

Switch to the file with enumerated molecules and create a list with the canonical codes copied in your clipboard (List>Create Row List From > Clipboard)

A List Membership filter is created on the right side. You can now hide the molecules that were in the first file.

I hope this helps. :) Another way would be to merge both files using the canonical code as merge key.