Subject: Re: Comparing Structures from two Datawarrior Files Posted by ELFritzen on Thu, 06 Jul 2023 12:51:10 GMT

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Hi zig,

Thanks for your reply and helpful tips. I've found a way to do what I want by merging the two files using structure as the merge key, and by selecting the option to append rows for the compounds not contained in one of the files. I think that works as well.

Ed