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Subject: Re: Comparing Structure Files

Posted by [biolive31!!](#) on Mon, 17 Jan 2022 13:39:30 GMT

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Dear Norwid,

Thank you for your help.

I tired to compare the set a and seb . I found 16 similar compounds.

My first conclusion is that DW I installed work well. :)

Now I wondering if my files are, in someway, unanalysable by similarity tool in DW.

These files are sdf files with structures.

I tried an other tool to compare molecule of my files (chemdiff) and it wasn't able to identify similar structure like DW.

Do you know what is the file type required to perform a similarity analysis ?

thank you for your help.

Olivier

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