Subject: Re: Find similars using Flexophore

Posted by sansun on Sat, 16 Jul 2022 11:02:17 GMT

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Thanks Norwid

I have updated the developmental version and I am still having same problem.

I was wondering if absolute stereochemistry needs to be defined for using flexophore? My file has many molecules with undefined stereochemistry.

I'll try other suggestions too.

Thanks SS