Subject: Re: AllFragFp
Posted by thomas on Thu, 23 May 2024 20:48:01 GMT
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Hi Christophe,

somewhat: SkelSpheres is like Extended Connectivity FP, but it includes full stereo features and it inlcudes a set of fragments, which contain the sckeleton only (no atom types). This makes it more tolerant to single atom replacements, which don't cause a drastic drop of similarity anymore.

AllFragFp is not just linear paths, it covers all fragments with up to 6 bonds (circular, chains, combinations) that are a substructure of the given molecule.

Thomas