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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 includes a set of fragments, which contain the skeleton 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

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