Subject: Re: AllFragFp
Posted by Christophe on Fri, 26 Apr 2024 07:45:51 GMT
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Hello Thomas,

Thank you for this more detailed reply.
If I've understood correctly, the AllFragFP is more akin to what is more commonly known in chemometrics as a path fingerprints, whereas the SkelSpheres descriptor would be of the Extended Connectivity FP type. Is this correct?

Christophe