Subject: Re: AllFragFp
Posted by nbehrnd on Tue, 16 Apr 2024 20:48:21 GMT
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Hello Christophe,

AllFragFP could be something still very early in implementation into DW and thus not (not yet) documented. If one queries the source code of DataWarrior,[1] and its assisting openchemlib[2] on GitHub, only the later contains this very string only once in file DescriptorConstants.java, lines 88 to 96 as a `DESCRIPTOR_TYPE_MOLECULE`.

Norwid

[1] https://github.com/thsa/datawarrior
[2] https://github.com/Actelion/openchemlib