Subject: molecular complexity descriptor

Posted by dataviz on Wed, 02 Nov 2016 21:37:44 GMT

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Hello

i just read a recent review in DDT 2016 (O Mendez-Lucio et al) about molecular complexity computed by different tools including datawarrior. I asked the authors and they used version 4.2.2 to compute this descriptor but it seems that this is not present in version 4.4.3? while this parameter seems valuable... maybe of interest to plug it back? many thanks

Bruno