Subject: Re: extension of substructure definition
Posted by nbehrnd on Wed, 30 Aug 2023 16:08:29 GMT
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Dear Thomas,

thanks to your answer, I understand the reasoning to retain entries about an «exact structure» and «variable (query) structure» better.

Tentatively, I attribute my failure to write a dedicated .dwam macro because I didn't identify an entry in DW's macro editor which would provide an additional column about idcoordinates2D. To me (perhaps an erroneous perception), it appears to be a requirement to render all (including future) entries in a DW structure column extendable as (similar as in Markush formulae) a query motif, because a mere look-up of a line <columnName="Structure"> (e.g. by generation of a library of random molecules) followed by the addition of the two lines did not yield the anticipated result.

As a result of testing, a minimal working example .dwar was identified. Only populated with 2,6-lutidine, the .dwar file attached below can serve future users of DW to build their set of reference of (dis)similar motifs for the generation of evolutionary libraries with Markush formula like flexibility in apparently any future row of this very column. The presence of lutidine serves as an example only.

Best regards,

Norwid

File Attachments
1) almost_empty.dwar, downloaded 394 times