
Subject: Re: Toggle-off absolute configuration while determining Murcko scaffold
Posted by [nbehrnd](#) on Sun, 25 Aug 2019 16:56:16 GMT

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Dear Thomas,

as probed, the «Find and Replace» (under the Edit tab) indeed offers exactly the tool I needed to simplify the SMILES as intended. This change both propagates well in subsequent stages of structure display

as well in the how to retrieve -- either by structure, or by string -- structures sharing a Murcko scaffold in common.

Thank you,
Norwid

File Attachments

- 1) [example.png](#), downloaded 813 times
 - 2) [example.dwar](#), downloaded 516 times
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