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,

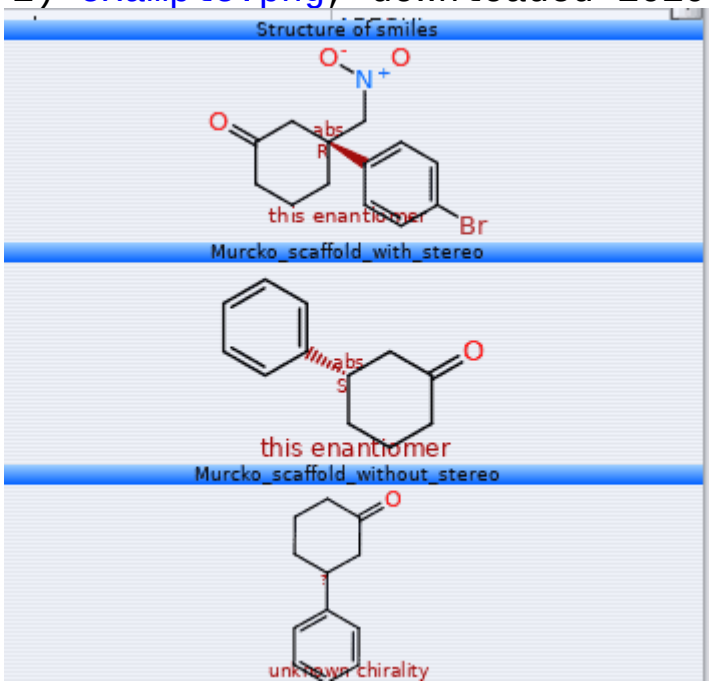
as probed, the «Find and Replace» (under the Edit tab) indeed offers exactly the tool I needed to simplify the SMILES as intended. This change both propagates well in subsequent stages of structure display

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 1610 times



2) example.dwar, downloaded 879 times