Subject: Re: Toggle-off absolute configuration while determining Murcko scaffold
Posted by thomas on Fri, 23 Aug 2019 23:09:03 GMT
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Dear Norwid,

to me the current handling is correct: the change from R to S in your sample SMILES is correct, because after the removal of the methylene-nitro group, the stereo-chemistry is correctly retained in the Murcko-scaffold.

If you generate a SMILES from the scaffold, then you may use 'Find and replace' to remove all '@' symbols from them.

Thomas