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Subject: Export of Chiral compounds

Posted by [andys](#) on Thu, 01 Oct 2020 23:18:41 GMT

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Hello

I have a problem with exporting the results from a Enumerate Combinatorial Library process with racemic centres been described as single chiral forms. The problem is I have a set of chirally pure compounds for reagent set 1 and a set of racemates for reagent set 2, the enumeration process works fine and the products have a chirally resolved atom from reagent set 1 a racemic atom from reagent set 2. Within Datawarrior the bonds are reported correctly as specified chirality and racemic. However, when I export the molecules as an SD file all the chiral centres are classed as resolved and the chirality flags for the racemic atom set in the bond block of the SD file as either 1 or 6 (this seems arbitrary) rather than the correct assignment of 4.

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