Subject: Indolizidine stereochemistry
Posted by cmw77 on Fri, 05 Jan 2024 10:31:23 GMT
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Hi,

when drawing molecules containing an indolizidine core, structures are labeled "unknown chirality" and the nitrogen atom displayed in purple even if all stereocenters are defined.

As an example, you may want to use (-)-Swainsonin.

Drawing a wedge or hashed bond sprouting from the nitrogen will change the label to "this enantiomer", however in my opinion this bond type does not make sense at this position.

Best regards,
CMW

Subject: Re: Indolizidine stereochemistry
Posted by thomas on Fri, 05 Jan 2024 12:46:40 GMT
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Hi CMW,

many thanks for the observation. This is indeed a bug, because the nitrogen atom was wrongly considered having a fixed pyramidal geometry due to the bi-cyclic structure. That will be fixed in the next update...

Thomas