TEACHING CHIRALITY WITH JMOL

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Chirality is intrinsically associated to the need of perceiving molecules (or other structures) as three-dimensional entities. Furthermore, it is well known that the ability to visualise in three dimensions varies heavily among individuals. Hence, any tool that provides a representation of molecules as three-dimensional objects may be of good value in understanding chirality.

Among the software available as viewers for 3D models of chemical structures, Jmol [1] stands out because of two major features: the ability to use it embedded in web pages and its open-source licence. The former allows an instructor to prepare tutorials, examples, or exercises that can not only be used in the classroom, but also offered to the students for their study and homework. The second extends its application without any economical or legal limitations.

This presentation will demonstrate some examples of the use of Jmol in illustration of molecular chirality. Among them:

- Interaction and manipulation of the molecular model to help decide about stereochemical assignment and correct nomenclature.
- Illustration of the interdependence and matching between configuration and projection formulas (wedge bonds, Fischer, Haworth, Newman projections).
- Side by side display of two models for comparison and decision on whether they are or not chiral and, eventually, the relationship between them (same molecule, enantiomers or other types of stereoisomers).
- Tutorials on chiral molecules or structures that use molecular models as an integral part of the content.
- Use of molecular models in exercises or quizzes.
- Interface of Jmol with databases, so that a 3D model of the structure can be retrieved from a common, commercial or systematic name, or from a chemical identifier (CAS registry number, SMILES notation, InChI key).
- Drawing of a chemical formula and automatic generation of its 3D structure; analysis of the stereochemical correctness, fine-tuning of the structure to achieve the intended isomer if needed. Storing or sending the resulting model.

References:

1. Jmol: an open-source Java viewer for chemical structures in 3D. http://jmol.org