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## Document for adding numbered structures into PeakForest

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# Document for adding numbered structures into PeakForest

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## Instructions for numbering molecules (as far as possible)

- 1) Number the longest hydrocarbon chain, starting with the highest priority of functional groups in the IUPAC nomenclature (COOH > COOR > CONH<sub>2</sub> > CN > CHO > C=O > OH > NH<sub>2</sub> > X > C<sub>x</sub>H<sub>y</sub>), which may pass through heteroatoms (e.g. disulphide bridge of oxidised glutathione).
- 2) Then, number the side chains respecting the priority of functional groups. If there are several possibilities for the numbering of side chains or substituents, choose the one for which the sum of the indices is the lowest.
- 3) Nitrogen and phosphorus atoms should also be numbered. Hydrogen, oxygen and sulphur atoms should not be numbered.
- 4) Avoid special characters such as primes in the numbering. For protons carried by a carbon adjacent to an asymmetric carbon, i.e. magnetically different, they will have the same number on the molecule, and they will be differentiated in the NMR annotation table by using a and b.
- 5) If the compound studied is a mixture of several forms (e.g. pyranose or furanose; alpha or beta), as is the case for sugars, it will not be possible to visualise the numbered molecule in 3D. **In order to visualise a numbered molecule in 3D, a single numbered structure must be uploaded (MDL molfiles format [V3000]).** For compounds presenting only the alpha-pyranose and beta-pyranose (or alpha-furanose and beta-furanose) forms, for example D-glucose, it is sufficient to draw the molecule without indicating the stereochemistry of the anomeric carbon. For the mixture of the four forms mentioned above, its structure will not be viewable in 3D, but in 2D (png format, minimum image resolution: 300 DPI). For this, draw the different forms of the molecule, naming them alpha-pyranose; beta-pyranose; alpha-furanose and beta-furanose and save the files in png format. The numbered molecule will be displayed in 2D.
- 6) Use the freeware ACDLab/ChemSketch package, or among commercial softwares ChemDraw<sup>®</sup> for instance.
- 7) Number the molecule following the instructions detailed above.
- 8) Save the files in png (\*.png), minimum image resolution: 300 DPI and MDL molfile [V3000] (\*.mol) formats.

Note: the svg format does not exist in ACDLab/ChemSketch software!

**Attention: Do not save the file in mol [V2000] format! Only the [V3000] format allows obtaining the 3D numbering.**

- 9) In PeakForest, you must log in to upload the molecule file(s). Click on the name of the chosen compound (or download the excel file of the compound if it does not exist in PeakForest yet, see the document about adding a compound). Choose the wanted NMR spectra and opens its card. On the selected spectral card, select the "Peak List" section, click on the  tab and then on "Browse". Choose the corresponding .png or .mol file or both files. It is possible to upload an image file (.png) and a mol file into PeakForest.