

Molecular Connectivity Tables in Images



Published August 11, 2007

Citation

Willighagen, E. (2007, August 11). Molecular Connectivity Tables in Images. *Chem-bla-ics*. <https://doi.org/10.59350/se3te-3tf95>

Keywords

Publishing, Chemistry, Inchi

Abstract

Rich blogged about to Never Draw the Same Molecule Twice: Viewing Image Metadata in which he shows his molecular editor outputting images of molecular structure where the connectivity table of structure is embedded in the image. His molecular editor can read the image again, and will automatically pick up the embedded connection table. Noel showed that such can not only be done in Java, but in Python too.

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This is important progress, though I would still like to see [InChI](#)s in the documents, and/or the data files as supplementary information. Actually, I would even more like to see that all experimental sections not just list the structure name, but give the InChI. An important spin-off is that when giving spectral information, the atom numbering given by InChI can be used to associate NMR shifts, and IR wavenumbers to atoms and atom groups, removing the ambiguity in those associations as we are used to find in literature.

Chemistry Central is [looking into improving the submission process](#) for molecular data, and hereby request the commenting on, taking into account in ongoing internal discussions, and incorporation of these approaches in the editorial requirements for CC publications:

- including the connection table as metadata in images
- including the InChI in experimental sections for newly synthesized molecules
- use InChI atom numbering to associate NMR shifts with atoms in these experimental sections

I will shortly blog an example experimental section incorporating the InChI.