Subject: translation of the idcodes
Posted by nbehrnd on Thu, 22 Oct 2020 18:05:24 GMT
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When choosing to save (some of) the content a .dwar file into the .txt file, the column about the structures contains the idcode. This condensed string suffices to recreate the molecular structures when this .txt file is read in a pristine session of DataWarrior. Contrasting to, e.g. a SMILES string, it is harder to understand «the grammar» behind this efficient storage of structural information.

Possibly this is less a feature suggest for DW, rather than bridging DW to other programs: Are there plans to to render the idcode format accessible, either as reading input into for, or (/and?) equally as written output by OpenBabel, e.g. for one of the sections 18.1 till and including 18.3 of the current manual about formats in cheminformatics?(1)

Norwid

(1) https://open-babel.readthedocs.io/_/downloads/en/latest/pdf/