Subject: exporting R groups of compounds
Posted by jkulpiii on Wed, 06 Mar 2019 15:00:03 GMT
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When I exported as a SDF file, the R groups or fragment data was lost. When I exported as txt file I did get these columns: Scaffold [idcode] R1 [idcode] R2 [idcode]

What file type is the idcode? I do not recognize it. I would like to convert it to smiles.

Thanks for the help

Subject: Re: exporting R groups of compounds
Posted by thomas on Thu, 07 Mar 2019 17:08:58 GMT
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The idcode is a compact canonical representation of the molecule that includes enhanced stereo representation and query features, if the molecules are query fragments. Conceptually, it is similar to the SEMA encoding, which MDL used in REACCS, MACCS and IsisBase. The idcode was never published, but with a few lines of Java code and the Open-Source library 'OpenChemLib' one may parse idcodes, process molecules, generate molfiles or SMILES or make own software compatible with idcodes.
Within DataWarrior you may generate one SMILES column for the Scaffold and every R column before saving as text- or sd-file.

Thomas