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