Subject: Re: Export SMARTS
Posted by thomas on Fri, 04 Apr 2025 19:11:47 GMT
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DataWarrior's structure definitions with query features and exclude groups (OpenChemLib functionality) and the query features that can be encoded in SMARTS are partially overlapping and similar, but not really equivalent. And, although, recursive SMARTS and of DataWarrior's exclude groups are used for similar purposes, their concepts are substantially different. Stereochemistry in SMILES and SMARTS is simpler and the aromaticity concept is different. Therefore, direct translation is impossible. DataWarrior does its best to convert back and forth between SMARTS and DataWarrior substructures, but often some features cannot be interpreted one-to-one. Thus, when you are looking for a SMARTS editor I also suggest looking somewhere else, e.g. RD-Kit or at Matthias Rarey's excellent pattern editor:
https://www.zbh.uni-hamburg.de/forschung/amd/software/smarts editor/smartseditor-doku.html