Subject: Export SMARTS
Posted by zhentg on Fri, 21 Mar 2025 03:30:05 GMT
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DW structure sketcher is powerful for query definition, can the query be export as SMARTS?

Subject: Re: Export SMARTS
Posted by nbehrnd on Sat, 22 Mar 2025 15:40:10 GMT
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Hello zhentg,

as a side note, Noel O'Boyle published a two-part «Smarts for Dummies» blog post including a link to interactively test bench "Smarter SMARTS". Though JavaScript (the eventual/current language of implementation) isn't Java used by DataWarrior, I speculate a similar «preview» were a nice complementary addition to DataWarrior.

Best regards,

Norwid

https://baoilleach.blogspot.com/2018/11/smarts-for-dummies.h tml
https://baoilleach.blogspot.com/2023/02/smarts-for-dummies-p art-ii.html
https://baoilleach.github.io/smartersmarts-js/

Subject: Re: Export SMARTS
Posted by zhentg on Mon, 24 Mar 2025 15:02:28 GMT
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Hi Norwid, thanks for providing the links, they are helpful.

https://smarts.plus/smartsview is a good tool to visualize SMARTS, but it does not provide examples that my SMARTS will match.

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

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Subject: Re: Export SMARTS
Posted by zhentg on Sun, 06 Apr 2025 11:02:46 GMT
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Thanks, Thomas. I did try SMARTSEditor, and it is useful.
Now I acknowledged that the syntax used in DW is not the same as SMARTS, thanks for providing details about this.

Subject: Re: Export SMARTS
Posted by jordenjeck on Fri, 30 May 2025 10:06:12 GMT
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Yes, DW Structure Sketcher supports SMARTS export for defined queries.
