Subject: SMARTS searching
Posted by amorrison on Mon, 15 Jan 2018 08:16:51 GMT
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Hi,
Is it possible to do a SMARTS search within DataWarrior? The use case here would to use a Macro to search for and annotate problematic structures, e.g. PAINS.
Thanks in advance,
Angus

Subject: Re: SMARTS searching
Posted by thomas on Tue, 16 Jan 2018 22:50:52 GMT
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Hi Angus, reading SMARTS and converting them into DataWarrior format (idcodes) is on the list of things to be done, but not available yet. For a small set of substructures one could always draw them by hand, e.g. within a 'substructure list filter', but for the PAINS collection it would be a pain. An issue for the SMARTS to DataWarrior-idcodes conversion will be that SMARTS's and idcode's query features don't map 1-to-1 and that DataWarrior substructure searches don't allow recursive features. Thus, recursive SMARTS would need to be represented by multiple substructure fragments, which will be difficult to implement and also would have its limits. Thomas

Subject: Re: SMARTS searching
Posted by amorrison on Wed, 17 Jan 2018 17:16:08 GMT
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Hi Thomas,
Thanks for the reply and not a problem.

As an aside I wonder if people would be interested in a 'macro exchange' where people could share Macros they've set up? I find them really useful and would find it very useful (inspiring) to see what other people are setting them up to do. I have a few very rudimentary ones I would be willing to share to get things kicked off.

Angus

Subject: Re: SMARTS searching
Posted by abc123 on Tue, 30 Oct 2018 23:36:14 GMT
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I would like to upvote this feature. Checking for smarts patterns from a file would extend the use of DataWarrior.