Subject: fragments
Posted by pc419714@ohio.edu on Thu, 11 Apr 2019 17:34:16 GMT
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Thomas,

How does data warrior define a fragment? Why do you use fragments? My guess would be because of metabolism. Does a fragment correspond with a functional group?

Thanks,

Patrick

Subject: Re: fragments
Posted by thomas on Sun, 14 Apr 2019 20:10:29 GMT
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Hi Patrick,

in DataWarrior the word fragment usually refers to a substructure fragment, which in contrast to a normal molecule is incomplete such open valences are not considered to be filled with hydrogen atoms. Fragments may also contains atom and bond query features.

In some cases, however, 'fragment' also refers to a molecule, e.g. the functionality 'Add largest fragment', which identifies all non-connected parts of a molecule (e.g. in salts) and just copies that one with the highest number of non-hydrogens atoms into a new column. This column then contains 'molecules', where all free atoms valences are implicitly considered to be filled with hydrogen atoms.

Finally it is a matter of the context. I assume this does not fully answer your question. What was the context in your case?

Thomas

Subject: Re: fragments
Posted by pc419714@ohio.edu on Mon, 15 Apr 2019 20:10:53 GMT
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I was just wondering how fragments were defined for purposes of calculating the drug score. Thanks!

Subject: Re: fragments

Posted by thomas on Tue, 16 Apr 2019 14:19:30 GMT
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The drug score does not use fragments. It is a mathematical equation combining other properties. The druglikeness, however, uses >5000 substructures. Everyone has an associated druglikeness contribution value, some positiv, some negativ, which were derived from the frequency these fragments occur in commercial drugs or organic chemicals. I attach a text file, which when opened from DataWarrior shows the chemical structures and the contributions of these fragments.

File Attachments
1) druglikenessFragments.txt, downloaded 1759 times

Subject: Re: fragments
Posted by pc419714@ohio.edu on Tue, 16 Apr 2019 20:56:14 GMT
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This is great! Thanks! One idea my boss had was to modify the code so that it calculated the drug score each generation and picked the best ones. I might try to modify the source code to try this but the way it is set up, if you select compounds with a high drug score to begin with, it generates compounds with high drug scores. We ended up doing 2 evolutions.

This is very helpful knowing more details about the fragments.

Subject: Re: fragments
Posted by Max marine on Sun, 29 Dec 2019 08:21:30 GMT
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I think fragments refer to structure fragments mostly I searched on google and it is saying that fragments sometimes may be referred as molecules I am also looking for a answer .