Subject: Toxicity screen
Posted by pc419714@ohio.edu on Sun, 17 Feb 2019 00:02:48 GMT
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I used the calculate properties macro to calculate toxicity for all my molecules. What data sets did you train these algorithms on to make predictions on toxicity? How accurate are the predictions? What sort of algorithms were used?

Also if you could list in the documentation that you could use the calculate properties macro to calculate toxicity it would be helpful. I had to do a lot of experimenting before I figured out how to do this and I couldn't find it in the documentation.

Also since my boss is wondering-- do you have a list of papers published with data warrior? This is really amazing software.

Thank you so so much!

Patrick Chirdon

Subject: Re: Toxicity screen
Posted by thomas on Thu, 07 Mar 2019 16:11:48 GMT
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DataWarrior uses the same algorithm to find toxicity indications as the 18 years old Osiris Property Explorer. We never published details beyond what is explained here: http://www.openmolecules.org/propertyexplorer/toxicity-asses sment.html. It is a fragment based approach based on the RTECS database, which to my knowledge is not available anymore. The fragments that are used as indicators of a potential toxicity risk are available as part of DataWarrior's source code. Many of DataWarrior's algorithms/functionality are not described in any paper just because of lack of time or because they are a kind of known state of the art. Exceptions are a general DataWarrior paper that also describes the "rubberbanding-scaling" for the depiction of chemical space, papers describing the flexophore descriptor, molecular complexity, or the MMFF94 forcefield improvements used in DataWarrior (this is in preparation).

Thomas

Subject: Re: Toxicity screen
Posted by pc419714@ohio.edu on Thu, 14 Mar 2019 21:10:26 GMT
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thanks very much!