Subject: Toxicity Results
Posted by felipe.ferraz on Wed, 11 Mar 2015 15:36:40 GMT
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Hi!

I'm starting to use DataWarrior and I have a doubt about the Toxicity Prediction Results. What does it means a none prediction? I'm asking because on the documentation, there is no mention to a none result, only to low/medium/high risk.

Does it means that there is no risk predicted or that there is no prediction for that category? If it means that there is no prediction, why is that? Cause there is no information on the database to compare with my compound or is it a problem on the compounds structure I'm using?

Thanks!

Subject: Re: Toxicity Results
Posted by thomas on Wed, 11 Mar 2015 21:36:46 GMT
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Hi Felipe,

you are right and I was not really aware of it: While DataWarrior and property explorer use the same mechanism to predict whether there might be a potential toxicity risk of a compound, both tools use different names for the categories. The three property explorer categories high-medium-low are called high-low-none in DataWarrior. The current documentation in DataWarrior is taken from the property explorer and therefore misleading. 'none' is maybe a little more correct, because it means that no substructures are present in the query structure that were identified in the training data to be a potential indication of toxicity in the respective class. I will update the documentaion accordingly.

Thomas

Subject: Re: Toxicity Results
Posted by felipe.ferraz on Thu, 12 Mar 2015 11:29:42 GMT
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Thank you very much for the clarification Thomas!
Regards,
Felipe