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

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