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