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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-assessment.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

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