Subject: Re: 2D Rubber Band Scaling (RBS)

Posted by thomas on Mon, 09 Apr 2018 19:59:19 GMT

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RBS is still part of DataWarrior, but it is called Similarity Analysis there: http://www.openmolecules.org/help/chemistry.html#SimAnalysis

The activity cliff analysis is the same thing, but also visualizes activity differences divided by dissimilarities (SALI values):

http://www.openmolecules.org/help/chemistry.html#SaliAnalysi s

Thomas