Subject: 2D Rubber Band Scaling (RBS)
Posted by dataviz on Sat, 07 Apr 2018 08:25:51 GMT

Hello, do we still have the 2D Rubber Band Scaling (RBS) approach implemented ? I think i did some years ago but I do not find the command on recent version... In the manual I think it is not there..
many thanks

Subject: Re: 2D Rubber Band Scaling (RBS)
Posted by thomas on Mon, 09 Apr 2018 19:59:19 GMT

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