Subject: Re: Display Full Similarity Matrix
Posted by caius on Mon, 11 Jan 2016 21:01:19 GMT
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I was able to approximate matrix output using macros and the calculated column generation, but the results from chemsim(Flexophore_of_Structure, idcode) don't match the Structure Similarity values available in the similarity chart or the Structure[Structure List, Similarity] filter. For instance, use of chemsim does not yield a self similarity score of 1. Is there any way to get the outputs of "Structure Similarity" or "Structure (is similar to Flexophore)" into the table?