Subject: Re: Display Full Similarity Matrix
Posted by thomas on Fri, 15 Jan 2016 21:45:21 GMT
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The Flexophore is the only descriptor that give self-similarity values slightly below 1.0,
because under the hood the Flexophore is generated from a fresh set of representative conformers,
which every time look a little different. Nevertheless, similarity values from two different Flexophore descriptors should usually be above 0.99 if both were generated from the same molecule.
Structure filters, chemsim() function or graphical view axis all use the same flexophore similarity calculation, but have the same issue that there is a slight variation in similarity values, if the flexophore is calculated multiple times.