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Subject: molecular shape index

Posted by [david.i](#) on Mon, 05 Sep 2016 11:26:26 GMT

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Dear Thomas,

Please, it is possible to have more information about the molecular shape index calculation (any reference or method implemented) ?

best regards

david

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Subject: Re: molecular shape index

Posted by [thomas](#) on Tue, 06 Sep 2016 19:29:18 GMT

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Dear David,

this is a simple algorithm, which first calculates the shortest distance between any two non-hydrogen atoms of the molecule.

The distance between any two atoms is the number of atoms in the chain including both chain ends.

The longest of these shortest connections divided by the number of non-hydrogen atoms of the molecule gives the shape index.

Any unbranched alkane has 1.0, cyclo-pentane has 0.6, adamantane has 0.5 and smaller values than 0.5 are rather rare.

Best wishes, Thomas

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Subject: Re: molecular shape index

Posted by [david.i](#) on Fri, 09 Sep 2016 13:24:09 GMT

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Dear Thomas

Thank you a lot again !

Best regards

David

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