
Subject: Fuzzy Score

Posted by [vamsi9k](#) on Tue, 23 May 2017 14:18:43 GMT

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Hi Thomas,

Fuzzy score is really an awesome implementation to calculate combined scoring for drug molecules. If possible, please share any publication reference with implementation. I am just curious, is this method same as multi-parameter optimization as mentioned in several places.

Thank you so much for all your effort and your reply help me alot

with regards,
vamsi

Subject: Re: Fuzzy Score

Posted by [thomas](#) on Sat, 27 May 2017 22:21:30 GMT

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Hi Vamsi,

the fuzzy score is meant to combine multiple parameters into one numerical value describing a kind of summary fitness. Therefore it can be used as good basis for a multi-parameter optimization strategy. Fuzzy scores are state-of-the-art. Optibrium, a company that specializes in these matters, uses a similar approach. An alternative approach would be a Pareto-ranking, where you identify those molecules from a larger set, where no other molecule exists that have at least one better property without any property being worse.

Kind regards, Thomas

Subject: Re: Fuzzy Score

Posted by [vamsi9k](#) on Tue, 30 May 2017 09:39:15 GMT

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You are right Thomas

Thank you so much

best regards,
vamsi
