Subject: Re: Free Wilson Analysis
Posted by thomas on Sat, 18 Mar 2023 17:25:14 GMT
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Hi Angus,

this cannot be done currently, but it is not the first time to here the request. I may consider...

A way would be (similar to automatic SAR) determining core fragents, e.g. Murcko, and then for all molecules with matching core fragments analyse changing substituents. Then create a result table with these columns:

1 - core fragment with R1,r2,... for every chaging substituent position
2 - substituent position (R1 or R2 or ...)
3 - Structure of substituent at this position
4 - mean contribution of this substituent at this position to activity
5 - count of this substituent found at this position
6 - StdDev of constribution value (this substituent at this position)

Is it this that you have in mind?

Thomas