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Subject: Free Wilson Analysis

Posted by [amorrison](#) on Fri, 17 Mar 2023 16:44:55 GMT

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Hi Thomas,

I was wondering if you think it would possible to do a Free-Wilson analysis within Datawarrior? Not necessarily a feature you might want to incorporate but if you think it would be achievable and could give me some hints I'd much appreciate it.

I appreciate there are ML models already available in DW, but as a medicinal chemist it's much easier for me to relate to the Free-Wilson models and I've used them successfully in the past. I do have other tools that I can use for this but being able to do it in DW would be marvellous.

Thanks,

Angus

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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

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Subject: Re: Free Wilson Analysis

Posted by [amorrison](#) on Mon, 20 Mar 2023 07:41:39 GMT

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Hi Thomas,

Thanks for the response. Yes that would be perfect, maybe an option to define your own core, similar to the core based SAR analysis and the outputs you suggest would be great.

Many thanks for considering.

Angus

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