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Subject: problems about calculate compound properties

Posted by [zhangyu](#) on Thu, 10 May 2018 02:40:43 GMT

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Dear Thomas,

My version is 4.7.2-64 bits for windows. I would like to calculate compound properties, such as Solubility parameter, Toxicity and drug scores.

The target chemical structure needs to be entered before these work starts, but I have not found

Zhangyu

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Subject: Re: problems about calculate compound properties

Posted by [thomas](#) on Thu, 10 May 2018 10:15:46 GMT

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Dear ZhangYu,

if what you need is to draw a structure (or write/paste a name) and then to predict these druglikeness properties for this one structure, then the easiest solution for you would be to download and use the Osiris Property Explorer from this page:

<http://www.openmolecules.org/propertyexplorer/applet.html>

If you need to predict properties for thousands of structures or need to do any other kind of cheminformatics analysis or data visualization, then DataWarrior would be the better tool, because the Property Explorer just does this one thing.

Of course, you can achieve your task with DataWarrior as well. However, it needs more steps:

->File->New... opens a dialog to create a new file

->Add Column adds a new column for chemical structures

press 'OK' close the dialog

double click the structure field, draw a new structure and press 'OK'

you may close the form view by clicking the 'x' button in its title row

->Chemistry->From Chemical Structure->Calculate Properties...

select the properties and press 'OK'

Best wishes,

Thomas

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