Subject: Re: Functionality request: MPO score
Posted by mcmc on Thu, 17 Sep 2020 15:59:39 GMT
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Below is a macro that will calculate the MPO score, based on the six underlying parameters that should already be present in DW.
cLogP, TPSA, HB donor and MW can be calculated within DW. But the most_basic_pKa and cLogD will have to be calculated elsewhere (unless you are one of the happy few to have that unlocked in DW).
The property names need to match exactly of course, so you may need to have to edit the names in the macro before executing it (or change the column aliases to match the macro).

EDIT: update 5 jan 2022. There was a typo in the original post, affecting MPO calculations for compounds with 40 < PSA < 60. Now corrected.

```
<macro name="MPO_score">
<task name="addCalculatedValues">
columnName=MPO_cLogP
isOverwrite=false
formula=min(1,max(0,2.5-0.5*cLogP_DW))
</task>
<task name="addCalculatedValues">
columnName=MPO_TPSA
isOverwrite=false
formula=if(PSA_DW > 40, min(1, max(0, 1 + (1/(120-90))*(90-PSA_DW))), min(1, max(0,
1-0.05*(40-PSA_DW))))
</task>
<task name="addCalculatedValues">
columnName=MPO_cLogD
isOverwrite=false
formula=min(1, max(0, 1 + (1/(4-2))*(2 - cLogD_74)))
</task>
<task name="addCalculatedValues">
columnName=MPO_MW
isOverwrite=false
formula=min(1, max(0, 1 + (1/(500-360))*(360 - MW)))
</task>
<task name="addCalculatedValues">
columnName=MPO_HBD
isOverwrite=false
formula=min(1, max(0, 1 + (1/(3.5-0.5))*(0.5 - HDonors)))
</task>
<task name="addCalculatedValues">
columnName=MPO_pKa
isOverwrite=false
formula=min(1, max(0, 1 + (1/(10-8))*(8 - MostBasicpKa)))
</task>
<task name="addCalculatedValues">
```

columnName=MPO_Score
isOverwrite=false
formula=MPO_HBD+MPO_MW+MPO_TPSA+MPO_cLogD+MPO_cLogP+MPO_pKa
</task>
</macro>