
Subject: Lipinski's rule

Posted by [sansun](#) on Mon, 29 Jun 2020 02:33:47 GMT

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Is there a way to filter/mark compounds that do not comply to 2 or more parameters of the Lipinski's rule of 5 in datawarrior?

Probably it can be done using 'calculated values'

Subject: Re: Lipinski's rule

Posted by [nbehrnd](#) on Mon, 29 Jun 2020 07:19:39 GMT

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You are right, this may be achieved by addition of a new column from the menu Data -> Add Calculated Values. This equally extends the scope of an earlier question by you, too.[1]

Assuming you already have a table with the Lipinski criteria computed, you may then mark the entries where simultaneously the molecular weight exceeds 500 g/mol and a number of HAcceptors is greater than 10 by a test condition of

```
if(TotalMolweight > 500 && HAcceptors > 10, "reject", "admit")
```

And indeed, there are drugs which do not meet these screening criteria.

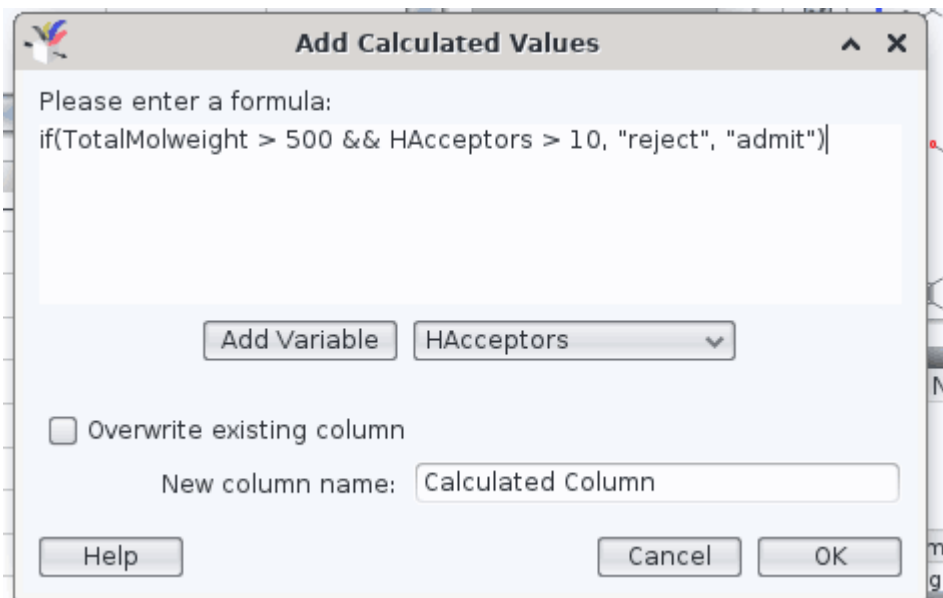
DW's manual describes in detail the syntax to apply here.[2] A minimal example .dwar file is attached below, too.

[1] http://openmolecules.org/forum/index.php?t=msg&goto=817& amp; amp;#msg_817

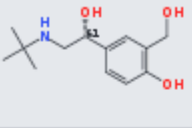
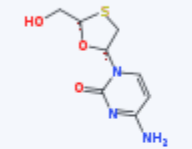
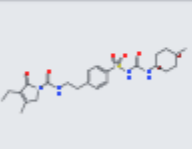
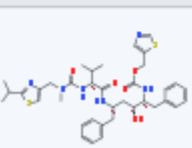
[2] <http://www.openmolecules.org/help/jep.html>

File Attachments

1) [conditional-or8.png](#), downloaded 1647 times



2) [example-or8.png](#), downloaded 1598 times

Structure	Molecule Name	Total Molweight	cLogP	H-Acceptors	H-Donors	Calculated Column
						
	COMBIVIR pass	229.259	-0.9483	6	2	admit
	AMARYL fail on d	490.623	3.5186	9	3	admit
	KALETRA fail on c	720.957	4.7152	11	4	reject

3) [test_list.dwar](#), downloaded 798 times

Subject: Re: Lipinski's rule

Posted by [sansun](#) on Tue, 30 Jun 2020 05:58:51 GMT

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Thanks nbehrnd

However, your equation considers only two parameters at a time while I want to have combination of any 2 parameters at a time (6 possible combinations). Based on your answer I came up with

the following equation that takes care of all possible combinations of 2 parameters and it seems to work:

```
if(TotalMolweight > 500 && HAcceptors > 10 || TotalMolweight > 500 && HDonors > 5 ||  
TotalMolweight > 500 && cLogP > 5 || HAcceptors > 10 && HDonors > 5 || HAcceptors > 10 &&  
cLogP > 5 || cLogP > 5 && HDonors > 5, "reject", "admit")
```

Subject: Re: Lipinski's rule

Posted by [nbehrnd](#) on Wed, 01 Jul 2020 08:11:25 GMT

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Hello Sansun,

you are correct, the answer provided by me only intended to serve a springboard / minimal working example about using two parameters in one .AND. conditional. Thus the indication of the manual page presenting the syntax in greater detail, including an .OR. clause to expand the scope of the test beyond that example. I'm happy for you your derived, more advanced scrutiny works for you, and for any future user who may see this as a as a source of inspiration and reference.

Norwid
