Subject: Lipinski's rule
Posted by sansun on Mon, 29 Jun 2020 02:33:47 GMT
View Forum Message <> Reply to Message

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 'calcualated values'

Subject: Re: Lipinski's rule
Posted by nbehrnd on Mon, 29 Jun 2020 07:19:39 GMT
View Forum Message <> Reply to Message

Your are right, this may 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

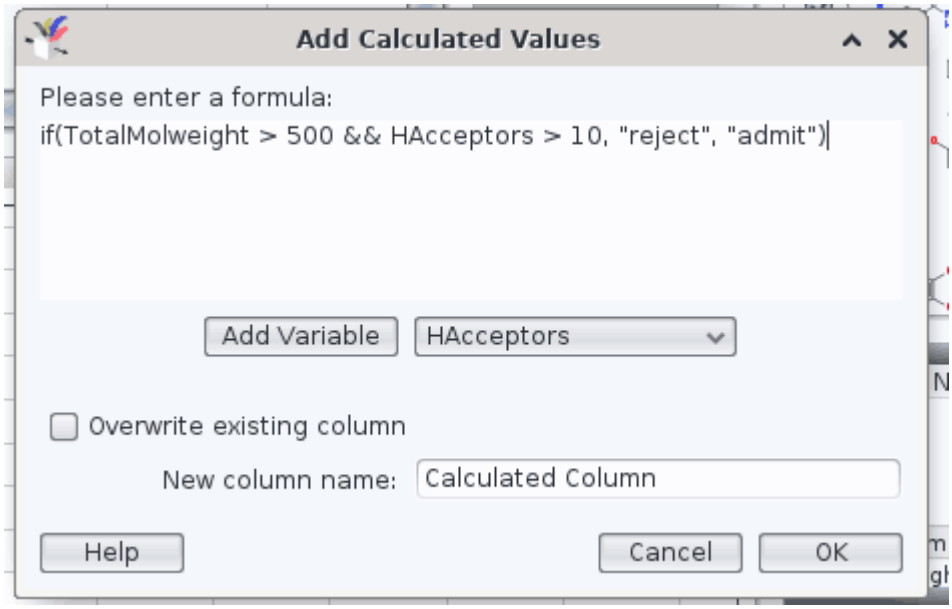
if(TotalMolweight > 500 && HAcceptors > 10, "reject", "admit")

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

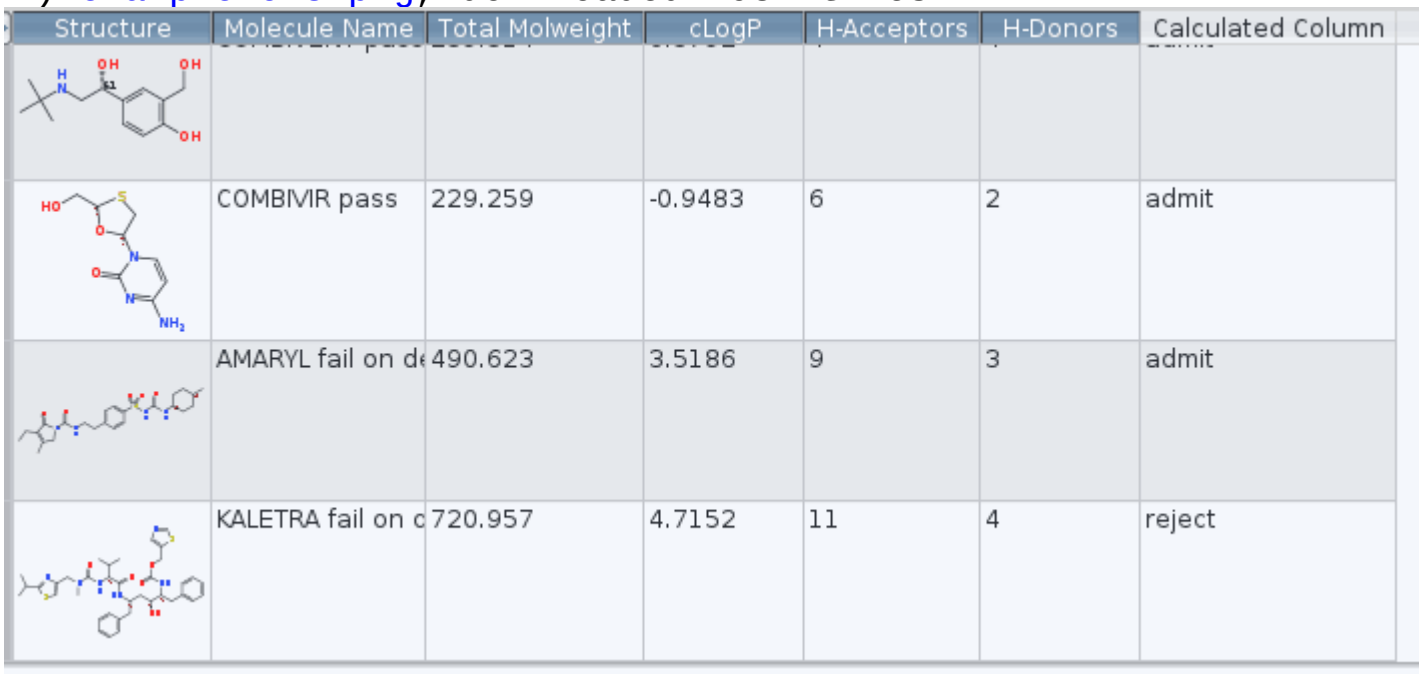
DW's manual describes in detail the syntax to apply here.[2] A minimal example .dwar file is attached below, too.

[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 2053 times



2) example-or8.png, downloaded 1982 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 942 times

Subject: Re: Lipinski's rule
Posted by sansun on Tue, 30 Jun 2020 05:58:51 GMT
View Forum Message <> Reply to Message

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
View Forum Message <> Reply to Message

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
