Subject: Re: Lipinski's rule
Posted by nbehrnd on Mon, 29 Jun 2020 07:19:39 GMT
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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")

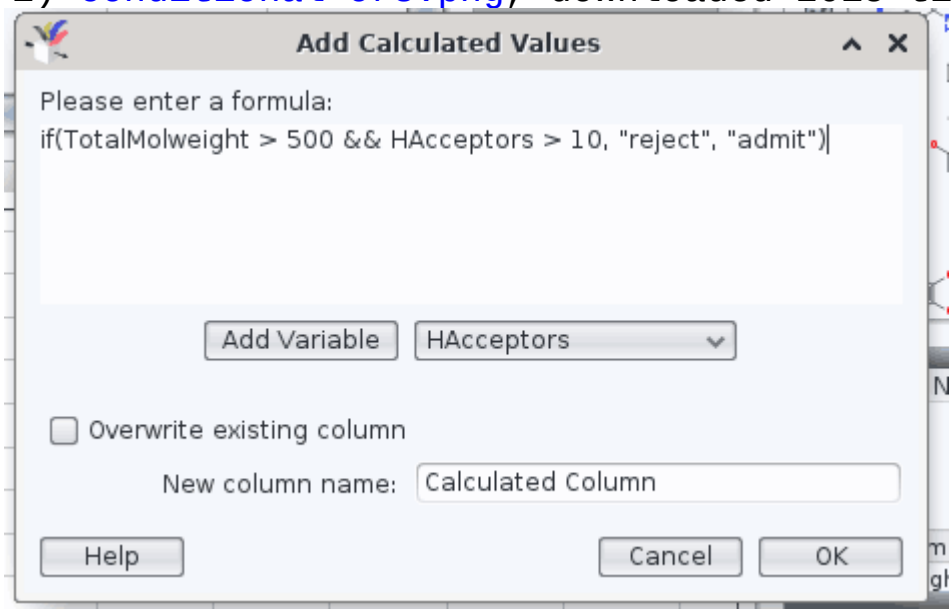
And indeed, there are drugs which do not meet these screening criteria.

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

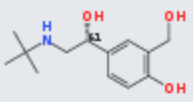
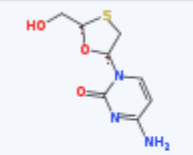
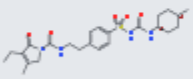
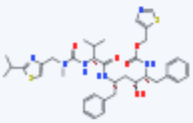
[1] http://openmolecules.org/forum/index.php?t=msg&goto=817& amp; amp;#msg_817
[2] http://www.openmolecules.org/help/jep.html

File Attachments

1) conditional-or8.png, downloaded 2015 times



2) example-or8.png, downloaded 1942 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 929 times