
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.

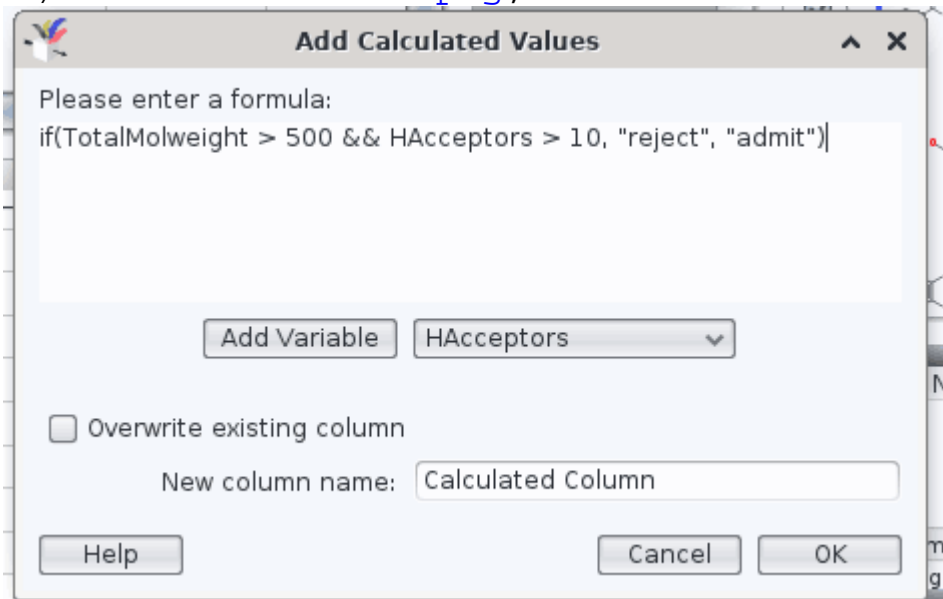
DW's manual describes in detail the syntax to apply here.[2] A minimal example .dwar file is attached below, too.

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

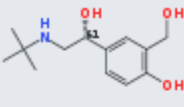
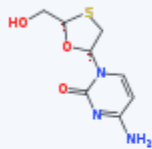
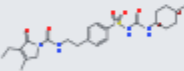
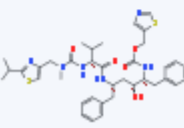
[2] <http://www.openmolecules.org/help/jep.html>

File Attachments

1) [conditional-or8.png](#), downloaded 1639 times



2) [example-or8.png](#), downloaded 1588 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 796 times
