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")