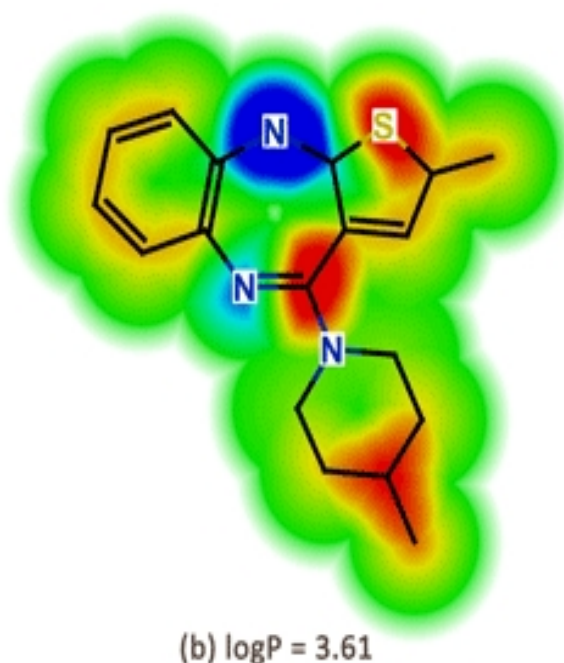
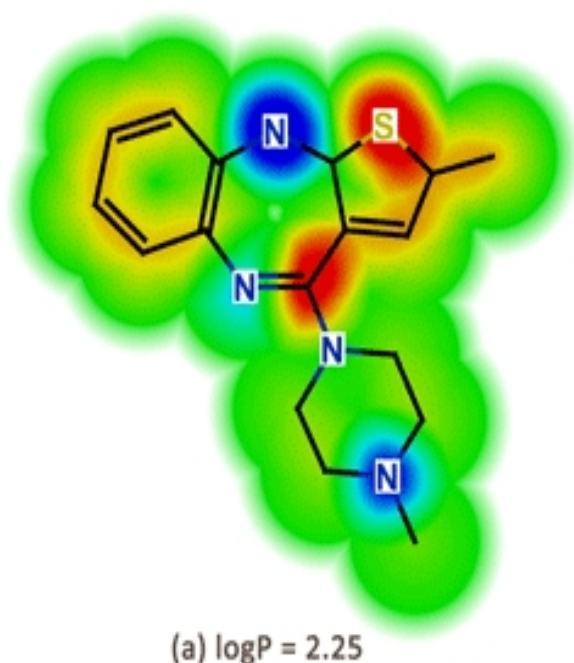


What do the colours mean?

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A red glow behind a region of a molecule indicates that this region is increasing the predicted value. Blue glow indicates regions that are tending to decrease the predicted value. A green glow indicates that a region has no significant overall effect on the property prediction. Another way to look at this is that if a 'blue' functional group is removed from a molecule or substituted with a 'green' or 'red' functionality, we would expect the property value to increase (for example, see the change from molecule (a) - below - to molecule (b) in which the piperazine group has been changed to a piperidine). Alternatively, if a 'red' functional group is removed or replaced with a 'green' or 'blue' functionality, we would expect the property value to decrease (for example, see the change from molecule (a) above to molecule (c) in which the thiophene methyl group has been removed).



It is important to note that the colours indicate changes in predicted property value and not whether this may be good or bad for any given property, as this will depend on the objectives of the drug discovery project.