

What does it mean if a molecule glows completely green?

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Occasionally, a molecule may glow completely green, even if the corresponding property value is high or low. In this case, the glow indicates that the molecule's predicted property value is not strongly influenced by any particular functional groups; the extreme predicted property value is caused by the combined influence of all regions of the molecule. This indicates that small a modification to the molecule is unlikely to significantly affect the predicted property value and a more dramatic change will be necessary to change the prediction.