

Why is there a difference between the ways the same functional group glows on two different molecules?

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The Glowing Molecule visualisation shows an analysis of the strongest structural influences on a predicted property value. More specifically, it assesses the sensitivity of the predicted property to the presence of each atom or functional group. For a linear model a functional group would have the same influence, irrespective of the molecule in which it occurred. However, the link between structure and property is rarely linear, as the influence of a functional group will depend on the structural characteristics of the entire molecule. Therefore, the glow for a specific functional group may vary from molecule to molecule depending on the presence of other functionalities.