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Theoretical investigation on interacting zones of certain flavones

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Quantitative molecular electrostatic potential (MESP) analysis is performed to delineate the reactive sites of the six plant secondary metabolites from the flavone family. Reactive sites are visualized and interpreted through the MESP descriptors (A_+, A_-, σ_+^2, σ^2, υ, $\upsilon\sigma_{Tot}^2$ and MPI) which reveals the accepting and donating propensity of H-bond. In addition, the most negative potential $V_{min}(r)$ is obtained by the presence of delocalized π-electrons or lone pair of electrons in the compounds, as the result of increasing electron density. Also, partial positive charges generated near the H-atoms in the compounds will increase the magnitude of most positive potential $V_{max}(r)$. Density functional theory (DFT) tool is employed to elucidate the MESP for apigenin (**CA**), scutellarein (**CB**), chrysoeriol (**CC**), hispidulin (**CD**), myricetin (**CE**) and mearnsetin (**CF**). Depending on these considerations, active reactive site of the chosen compounds is explored.

Keywords: Molecular polarity index, Electrostatic potential, Electrophilic region, Nucleophilic region, Degree of balance