A preliminary DFT analysis of phenolic acids in connection with their phytotoxic activity

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We employed a formal QSAR method to find the main interactions regulating the variation of the ability to inhibit the germination of Lactuca sativa seeds by a small group of phenolic acids. The same techique was employed to obtain structure-retention factor relationships. All molecular geometries were fully optimized at the B3LYP/6-31G(d,p) level of theory. From the corrected Mulliken Population Analysis results the numerical values for all electronic local atomic reactivity indices (LARIS) were calculated. Statistically significant results were obtained for both properties. The variation of the numerical values of both properties seems to be associated with interactions with electron rich centers.