Computational and Theoretical Chemistry

A DFT study of the chemical reactivity properties, spectroscopy and bioactivity scores of bioactive flavonols

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Abstract

Density function theory calculations was used to determine the molecular parameters, electronic and chemical reactivity descriptors, spectroscopy, and non-linear optical properties, electronic dipole moment, polarizability and hyperpolarizability of fifteen (15) flavonol aglycones (no sugar moiety) from plant sources to investigate their possible application as drug candidates. Geometry optimisations was carried out using the hybrid functional and basis set: M06-2X/6-31+G(d,p). Our calculations show that all the flavonols investigated are chemically reactive. Their reactivity is greatest in water hence making them suitable drug candidates since this is the ideal medium for drug delivery. The highest negative charge on the oxygen atom of the hydroxyl and high positive charge on the H atom of C5-OH are vital for antioxidant activity. The most reactive species, from reactivity descriptor calculations, is Gossypetin. All the flavonols are active as enzyme inhibitors and moderately active as G-protein-coupled receptors, ion channel modulators and protease inhibitors. The physicochemical properties show the flavonols have good bioavailability. All the compounds agree with Lipinski's rule of 5, signifying potential use as oral active drugs.