THEORETICAL STUDY ON THE MOLECULAR ELECTRONIC PROPERTIES OF SALICYLIC ACID DERIVATIVES AS ANTI- INFLAMMATORY DRUGS

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A systematic computational study was carried out to determine the structural stability of salicylic acid derivatives as well as the acidic properties of the protonation-deprotonation site and excitation parameters of the considered drugs at different temperatures using quantum chemical calculations. For further structural information, the dipole moment and differences in the energy of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) as Δ(HOMO–LUMO) were compared. A high stability of the salicylic acid derivatives was referred to the large HOMO–LUMO band gap. The result of the current study may give useful information about the drug biochemical functionality based on the physical and chemical nature at different temperatures, and in this way the study on the structural features of analogous molecules of salicylic acid derivatives with higher drug functionality would be possible.

Keywords: salicylamide (SAM), gentisamide (GAM), HOMO–LUMO band gap, excitation energies, *ab initio*.