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pKa Calculation of the Positively Charged Amino Acids in a Protein Chain, An Assessment of Theoretical Procedure

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In this study, the aqueous pKa for two cationic amino acids including lysine and arginine in a peptide chain which composed of eight glycine molecule have been calculated. HF and B3LYP methods using the 6-31+G(d) [1-3] combined with solvation energies that were computed by the SCRF-(CPCM/UFF) continuum models as implemented in Gaussian 09 computational package [4]. pKas were further calculated using two thermodynamic schemes (scheme1 and 2), namely the direct method and the proton exchange method with the inclusion of an explicit solvent water molecule. The results of this research verify that the direct method is not suitable for computing pKa of the amino acids in a peptide chain, while the other scheme in the presence of water molecule significantly improved the pka in comparison to the experimental data. The combination of the proton exchange scheme and CPCM-UFF model performed well with mean absolute deviations (MADs) of ~0.9 pKa unit. Because of the convergence problems, the inclusion of large numbers of water molecule in scheme 2, the computation procedure in the solvated model produces weak results. Comparison between the pKa α, β and random (R) structures of the studied proteins, reveals that the strongest acidic character belongs to β, α and R, respectively at the HF and B3LYP levels of the theory. The reason for this new result returns to this fact that structural differences from the hydrogen bond point of view and natural orbital populations affect the proton affinity of the studied amino acids. Atom in molecule (AIM) and Natural population analysis (NBO) on all structures show that the β structure possess the maximum hydrogen bonds with high electron density relative to other second structures which induces a more positive charge on the acidic hydrogen of the amino acid.

Keywords: pKa, SCRF, Second Structure, Amino acid, Lysine, Arginine.

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Effects of some Flavonoids on the Mushroom

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The inhibitory effects of some flavonoids on the diphenolase activity of mushroom tyrosinase have been investigated with the spectrophotometric technique. The results of kinetic assays showed that the flavonoids induced a reversible inhibition on the enzyme activity. Furthermore, gallic acid and quercetin show non competitive-type of inhibition. The chrysin and naringin induced a competitive manner of inhibiton. The inhibition constants have been determined for these flavonoids and the inhibition strength follows the order of: quercetin < chrysin < naringin < gallic acid. The values of the inhibitor binding constant (K_I) obtained 16.0, 7.9, 3.0, 1.5 mM, respectively. Thus the flavonoids played an important role in the inhibition of the mushroom tyrosinase enzyme.

Keywords: Inhibition, Flavonoids, Kinetic, Mushroom Tyrosinase.

Abstract No.224

Nanobiosensors Designed to Detect Hydrogen Peroxide by Using Catalase Polymer Nafiyn

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The bare surfaces of electrode are not suitable in electrochemical survey of proteins. This, not only leads to decreasing the speed for electron transfer between electrode and protein but also can lead to irreversible absorption of protein on the surface of the electrode, accompanying the conformation changes and loss of protein activity.Hence, it is necessary to provide required groups for the active