descriptors is calculated for each amino acid and they are put together to produce a descriptor data matrix for a set of peptides.
Very recently, in our research group we have been involved in the definition of some new amino acid indices (AAI) for use in QSAM study of peptides. We employed the concept of atom in molecule and used the quantum topological molecular similarity (QTMS) descriptors to suggest some new AAIs. In addition, we employed the Moreau and Broto autocorrelation function on the QTMS descriptors of amino acids to extend the QTMS-based AA indices and generate some other novel indices. In another work, to increase the quality of the QSAR models reported for peptides, we proposed here the application of segmented principal component regression (SPCR) method to define more relevant sources of AA indices. Finally, using of multi-way data analysis methods in QSAM study of peptides will be explained. The suggested methods were validated by analysis of some different peptide data sets of relevant biological activities.

Keywords: Amino acid indices, Peptide, Biological activity, Structure-function.

Abstract No.294

A Possible Role of Peroxidase Activity of "heme-ferritin" Complex in Development of Neurodegenerative Diseases

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Ferritin is a ubiquitous protein for the sequestration, storage and release of iron in animal and plant cells. It has been previously shown that each ferritin molecule can bind to 15 - 17 heme moieties. Heme and sometimes heme-protein complexes possess peroxidase activities which cause irreversible damages in cells. In the present study, we reported the peroxidase activity of "heme-ferritin" complex using several oxidizable substrates. First, the ferritin was purified from liver homogenate of sheep by ammonium sulphate precipitation and DEAE ion-exchange chromatography. The peroxidase activity of "heme-ferritin" complex was then measured by using H_2O_2 or t-BHP as oxidant substrates and TMB, L-Dopa or DOPA as a reductant substrates. Results showed that the non-specific peroxidase activity of the "heme-ferritin" system can oxidize the neurotransmitters with high catalytic efficiency. According to the literature, the concentration of ferritin, free heme, and peroxide species increase in neurodegenerative diseases such as AD. There is this possibility that the peroxidase activity of "heme-ferritin" complex play a significant role in development of oxidative damage within involved cells. We will discuss the importance of our observations.

Keywords: AD, Peroxidase Activity, Ferritin, Neurodegenerative Diseases.

Abstract No.295

Interaction of a Novel Photochromic Molecule with Human Serum Albumin Studied by UV-vis Absorption, Fluorescence Spectroscopy, and Docking Calculation

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Photochroism is the phenomena that of reversible transformation between two forms (open and close form) that have different spectra by photo-irradiation. In this work, the interaction of a new photochromic molecule, 2,2-biphenyl-4-yl-2-methyl-6(4-nitrophenyl)-4-phenyl-1,3-diazobicyclo[3.1.0] hex-3-en, with human serum albumin (HSA) has been investigated by UV-vis absorption, fluorescence spectroscopy and docking calculations. 0.1 μM HSA was used in the presence of 0 to 1.47×10^{-5} M photochromic molecule. The interaction of photochromic molecule with HSA causes fluorescence quenching of HSA. The addition of photochrome to a solution of HSA induces quenching of the protein fluorescence and binding constant of interaction was also obtained about 7. 5 μM^{-1}. In other investigation the photochromic molecule absorbance was studied by a UV-Vis spectrophotometer model Perkin Elmer. The photochromic reaction was studied upon variation of time irradiation by UV-vis spectrophotometer. Absorption spectra of photochromic molecule and HSA were obtained as the time of irradiation increase from 0 to 70 s. Absorbance intensity was increased due to the close form of molecule that turn in to the open form. Rate constant of reaction was obtained from absorption spectra about 0.026 s^{-1}. In order to estimate the