کارگاه‌های آموزشی مرکز اطلاعات علمی

آموزش نرم‌افزار Word برای پژوهشگران

روش تحقیق کمی

آموزش مهارت‌های کاربردی در تدوین و چاپ مقالات ISI

Ligand macromolecule interaction

Mohammad Reza Housaindokht[1*]

Department of Chemistry, Faculty of Sciences, Ferdowsi University of Mashhad

The interaction of ligands to macromolecules is a key element in all biological processes. Ligand interactions are important for molecular recognition, protein engineering, drug design, cellular regulating systems, cell signaling, drug formulation and discovery of novel ligands. Ligands can be small molecules such as metabolites, ions such as Fe (II) or large molecules such as nucleic acid and other protein partners. Some of my recent researches in this subject are as below:

Fundamental research

The interaction between human serum albumin (HSA) and two drugs indicated that amlodipine causes an increase, and that propranolol leads to a decrease in α- helix content of HSA [1]. The presence of quercetin (QUER) increased binding constant of propranolol (PROP) with HSA [2]. The binding sites of SDS on carbonic anhydrase and thiourea (TOU) to cobra cardio toxin A3 (CTX A3) evaluated by MD simulation [3].

Protein engineering

The structures of the native (Amyl-C) and truncated Taka amylase were compared by molecular modeling methods. Using in silico enzyme engineering approach, 50 (Amyl-S1) and 100 (Amyl-S2) amino acids were eliminated from Amyl-C to produce the truncated forms [4].

Recognition research

Based on fluorescence quenching of insulin binding aptamer (IBA) folding, a simple and sensitive insulin aptamer-based biosensor in the range of 2-70 nM was proposed [5]. The aptamer was used as a molecular recognition element. The quenching percentage of fluorescence intensity was proportional to the concentration of K^+ [6].

* Corresponding author. Email: housain@um.ac.ir

Magnetic field effects

The effect of magnetic field (52 mT) on the interaction between two drugs, amlodipine and propranolol, with human serum albumin (HSA) causes the use of spectroscopic methods. The results showed that the binding parameters are different in the absence and presence of the magnetic field [7].

Supercritical CO_2

In supercritical CO_2 there are high structural deviations from native form while in near-critical propane deviations are low and very close to those of in the mild aqueous solution and even are lower than those of in hexane. α-Helix and β-sheet contents of the enzyme remain intact in near-critical propane [8]. Although α-helix and β-sheet content of the enzyme in supercritical CO_2 reduced to some extent, they almost remained unchanged in supercritical CO_2/ionic liquid. At the molecular level, the results of our research reasonably confirmed that the use of ionic liquid molecules is an efficient method for stabilizing enzymes in supercritical CO_2 [9]. We show that natural osmolytes could stabilize protein conformation in supercritical CO2. On the basis of our structural analysis, we introduce a new mechanism for the osmolyte effect in supercritical CO_2, an "inclusion mechanism" [10].

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