

nanorods were synthesized according to the conventional seed-mediated growth protocol and characterized by UV-Vis spectroscopy, transmission electron microscopy (TEM), and atomic absorption spectroscopy (AAS) for shape, size and yield determination. The typical surface plasmon absorption bands in the visible and near IR region confirmed the rod morphology of the nanostructures. Phosphate, Tris and HEPES buffer solutions were prepared and the pH was adjusted to be 7.4. Concentration of the buffer solutions was 0.05 M in the final working solutions. Prior to use, GNRs were purified by two rounds of centrifugation at 12000 rpm, for 6 minutes. Pellet of the second round with a fixed concentration of gold nanorods were diluted with each buffer solution. UV-Vis spectra of the interacted samples were recorded to monitor the plasmonic bands. Results showed that neither the transverse SPR nor the longitudinal one have changed notably. Although the intensity of LSPR peak has been somewhat affected in buffer medium, the rod morphology is still maintained. Sensitivity of gold nanorods to trace changes in the local environment/ refractive index encourages the possibility of utilizing these nanostructures in development of nanostructures for various biosensing applications.

Keywords: Gold Nanorods, Surface Plasmon Resonance, Nanobiosensor.

Abstract No.249

Investigation of Mechanistic Influence of Mutation D117G in Aequorin from *Aequorea Victoria*: a Molecular Dynamics Simulation Study

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The photoprotein aequorin, isolated from the jellyfish *Aequorea victoria*, is a bioluminescent complex formed with the protein apoaequorin and the prosthetic factor coelenterazine that emits light upon calcium binding. In order to understand the mechanism of the reaction, the study of structure-function relationships was undertaken with respect to modifying certain of its amino acid residues. One of these mutations is the D117G that is located out of substrate binding cavity and Ca²⁺-binding loops. In this study short time molecular dynamics simulations were performed to investigate the influence of this fine change on dynamic properties of substrate binding cavity and Ca²⁺ binding loops that direct emission light properties in this photoprotein. Previous studies showed that this mutation decreases affinity of loops to Ca²⁺ and increase half-life of emission light in the

photoprotein. Our finding revealed that the replacement of ASP with GLY alters dynamics and energetic properties in functional regions of the structure and affects emission light and Ca²⁺-sensitivity properties in photoprotein.

Keywords: Aequorin, Molecular Dynamic Simulation, Ca²⁺-affinity, Life-time.

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Surface Modification of Gold Nanorods with Polyethyleneglycol for Nano Biosensing Applications

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There has been great interest in the domain of nanobiotechnology to design and develop new generation of nanobiosensors. Amongst anisotropic nanoparticles, gold nanostructures of rod morphology (GNRs) have attracted significant attention, for having variety of applications in biomedicine and biosensing. Although many fruitful features of gold nanorods have been introduced so far, the nanostructure itself is believed to show strong cytotoxicity, since it has been synthesized in the presence of hexadecyltrimethylammonium bromide (CTAB). The cationic surfactant is also known to play important role in the stabilization of GNRs, and maintenance of rod morphology. Herein, polyethyleneglycol has been utilized for neutralization of the positively charged GNRs. Gold nanorods were synthesized according to the conventional seed mediated protocol. Formation of the rod morphology, size, monodispersity, concentration and yield of synthesis were characterized by UV-Vis spectroscopy, transmission electron microscopy (TEM) and atomic absorbance spectroscopy (AAS). Excess CTAB was removed by one round of centrifugation at 12000 rpm for 6 minutes. Sample of GNRs with 75 nM concentration was interacted with 400 μ L PEG-4000 (600 mg. mL⁻¹). The mixture was incubated at ambient temperature for 1 hour. Excess PEG was removed by another round of centrifugation. Surface plasmon resonance of bare and pegylated GNRs was monitored via UV-Vis spectrophotometer. Results showed that transverse plasmon resonance (TSPR) and longitudinal plasmon resonance (LSPR) appeared at 528 nm and 708 nm, respectively. Intensity of SPR bands of the pegylated GNRs decreased upon treatment, without any shift in both regions. Although a considerable quantity of the cationic surfactant has been replaced by polyethyleneglycol, stability of GNRs