

biocompatibility properties of this material. Hence nanoneuroscience is a recently coined term describing the convergence of the existing but different worlds of nanotechnology, neurobiology that a large body of research is emerging that hints at the potential applications of nanotechnology in neuroscience. In present investigation, applying molecular mechanic(MM) method with OPLS, force field and quantum mechanics(QM) method-using density functional theory(DFT) with B3LYP keyword- we carried out a theoretical study on SWCNTs interaction with sphingomyelin as one of the most important components of the neuron membrane. We study about physical properties of this interaction. Hence, we have investigated places of interaction and electrical properties of this interaction. The result shows that the interaction of sphingomyelin with SWCNT has minimum value of interaction energy and structural stability in solvent. Since physical properties of this system are important for nanoneuroscience practical applications, the present study opens the door to nanoneuroscience.

Keywords: Nanoneuroscience, Sphingomyelin, SWCNT, DFT.

Abstract No.63

Real-Time Differential Scanning Fluorimetry of Quorum Sensing-Mediated Proteolytic Activity in Selected Bacterial Pathogens

*Glenn Oyong*¹, Naser Jafari², Javad Aghamohammadian³,
Mohammad Ehsan Zangeneh⁴, Esperanza Cabrera⁵*

1. Molecular Science Unit, Center for Natural Science and Ecological Research, and Biology Department, De La Salle University Manila, PH
2. Research Department, Ardabil University of Medical Sciences, Ardabil, IR
3. Department of Human Genetics, Mashhad University of Medical Sciences, Mashhad, IR
4. Mehr Clinic, Takhti Street, Iman Square, Hamedan, IR
5. Biology Department, College of Science, De La Salle University, Manila, PH
(E-mail: glenn.oyong@dlsu.edu.ph)

Cellular communication between bacterial pathogens is established through the release of autoinducers upon reaching a certain population density. This mechanism, called quorum sensing (QS), allows synchronization and downstream expression of associated virulence genes leading to an efficient and effective establishment and survival within the host. In bacterial pathogens, several proteases are reportedly secreted during QS and play major roles during

pathogenesis. Aversion of this process is very crucial in order to prevent further damage within the host and can be achieved by anti-quorum sensing (AQS) usually by molecules produced as secondary metabolites from certain plant species. This study developed a real-time proteolytic activity assay by differential scanning fluorimetry using the high-resolution melt (HRM) program of the Rotor-Gene cyclor and the fluorescent dye Flamingo Pink™ based on the principle of substrate protein stability. QS-mediated proteolytic activity from expressed gelE, sspA and apr gene products of *Enterococcus faecalis*, *Staphylococcus aureus* and *Pseudomonas aeruginosa*, respectively, were analyzed with high-precision based on their real-time enzymatic effect on substrate protein stability measured as fluorescence by Flamingo Pink which undergoes dramatic fluorescence enhancement in the presence of denatured protein – a reflection of the thermodynamic state of the protein substrate during enzymatic digestion. A remarkable decrease in fluorescence was observed when bromofenone, an AQS molecule, was added during bacterial culture. The levels of expressed protease gene products were also confirmed by real-time quantitative PCR of the gene transcripts. The developed protocol demonstrates precise detection and measurement of proteolytic activity mediated by the QS signaling pathway. This technique enables rapid screening of AQS molecules such as from plant extracts, and can therefore be applied as a tool for discovery of drugs with potential antimicrobial activity.

Keywords: Fluorescence, Quorum Sensing, Protease, Protein Stability.

Abstract No.64

A Theoretical Investigation on Oxaliplatin Interaction with β -Lactoglobulin

*Behafarid Ghalandari*¹, Adeleh Divsalar², Ali Akbar Saboury³,
Kazem Parivar³, Roya Bazl⁴*

1. Dept. of Biology, Science and Research Branch, Islamic Azad University, Tehran, IR
2. Dept. of Biological Sciences, Tarbiat Moallem University, Tehran, IR
3. Institute of Biochemistry & Biophysics, University of Tehran, IR
4. Center of Excellence in Electrochemistry, University of Tehran, IR
(E-mail: Behafarid.gh@gmail.com)

Bovine β -Lactoglobulin (BLG) as the most important whey protein in milk, is a globular protein belonging to the lipocalin family. According to the crystal structure, BLG comprises predominantly a β -sheet configuration containing nine antiparallel β -strands from A to I. Many investigations have been done about BLG interaction with material for various applications, such as fatty acid, Vitamins and Drugs. But