J Proteomics Bioinform 2016, 9:10(Suppl)
http://dx.doi.org/10.4172/0974-276X.C1.089

Temperature effect in polyurethane/graphene/PMMA nanocomposites using Quantum Molecular and Monte Carlo for design of new prosthesis

Norma-Aurea Rangel-Vazquez and **Juan-Ramon Campos-Cruz**
Instituto Tecnologico de Aguascalientes, Mexico

Today, nanotechnology has generated an increase in the design of new nanomaterials which cut across biological barriers for application in the human body. On the other hand, the application of quantum chemistry models allow modeling, predicting and designing new nanomaterials with specific properties and structure for specific applications due to manipulation of nanoscale materials. In this investigation is first model with AM1 cross linking of PU/graphene nanocomposite (NMC), in which graphene was introduced in order to improve the properties of PU and its wide medical application, then the minimum amount is determined for PMMA absorption in the NMC. By applying Monte Carlo method the effect of temperature (273, 308, 310 and 313 °C, respectively) were studied to determine the behavior of NMC/PMMA in the prosthetic design. Calculations were: Molecular geometry where by Gibbs free energy (-22331, -22537, -22560 and -22552), we observed that there are minimal changes of 0.1% to several temperatures (273, 308, 310 and 313K); however, there would be NMC decomposition in the grafting. The partition coefficient (Log P) shows a positive value (24.77) which would be verified that this reaction with polar solutions in the human body. The main signals FTIR about the cross linking of PU/graphene, where were seen that the temperature only causes displacements in the different signals, also observed that the cross linking of the PU/graphene occurs in the carbonyl bonds and CH forming hydrogen bonds and PMMA is added when the absorption is carried out through the CH-graphene. Electrostatic potential maps (MESP) of the NMC at different temperatures were appreciated that nucleophilic zones (CH bonds) identified bonds, while electrophilic zones are located in the carbonyl group. These results verify that the prosthesis has excellent physicochemical properties independently of changes in body temperature.

normarangelvazquez201301@gmail.com

Molecular determination of multi-drug resistant Mycobacterium tuberculosis among HIV infected patients visiting tertiary care hospital, Nepal

Amrit Lama Lo, Alina Maharjan, Ravi Bhakta Sherstha and **Ranjeeta Shah**
Pokhara University, Nepal

Tuberculosis is serious and common opportunistic infection among human immunodeficiency virus (HIV) infected person and emergence of multi-drug resistant tuberculosis (MDR-TB) is growing threat to them due to suppressed immunity. Early detection of disease is an important task. Conventional detection methods are time consuming as compared to molecular detection methods i.e., Polymerase Chain Reaction (PCR). PCR is rapid diagnostic test. The aim of our study is to detect the *Mycobacterium tuberculosis* specific gene *IS6110* and *MPB64*. Furthermore, to detect mutated rpoB gene for MDR-TB confirmation. 40 sputum specimens were collected from HIV infected patients either having symptom of tuberculosis or not enrolled in National Public Health Laboratory, Kathmandu, Nepal. All collected sputum were decontaminated with Modified Petroff's method then subjected to AFB staining and molecular detection method (i.e., Multiplex PCR) for detection of MTB co-infection, furthermore, allele specific PCR was done to detect MDR-TB. Only 7.5% (n=3) found to be smear positive whereas 92.5% (n=37) negative. Both smear positive and negative were further processed for MTB detection with Multiplex PCR and MTB positive further introduced to detect MDR-TB with allele specific PCR. Molecular method showed 12.5% (n=5) were TB co-infection. 60% MDR-TB had been detected among TB positive HIV patients. The prevalence rate of MTB and MDR-TB disease among HIV patients is much higher. The higher rate of MDR-TB is due to limitation in our study. Furthermore, we found that the proportion of HIV/TB co-infection is higher in male than female especially among economically productive age group.

amritlama93@gmail.com