natural product with certain bioactivities that have been isolated from the endophytic fungus *Aspergillus terreus*. Experimental studies have revealed that butyrolactone I inhibits the activities of both CDK1 and CDK2. However, its inhibitory mechanism and the role of Mg^{2+} ion remain uninvestigated. In this study, the effect of butyrolactone I on the CDK1-cyclin B complex in the presence and absence of Mg^{2+} ion in the active site was evaluated by applying a computational methodology. The currently available CDK1 crystal structures do not contain any Mg^{2+} ion, therefore, our first step was to position the Mg^{2+} ion in the CDK1 crystal structure (PDB ID:5HQ0) based on the structural information of CDK2 (PDB ID:1HCK). The stability of the two models (with $Mg^{2+}$and without Mg^{2+}) were investigated by conducting a 200 ns molecular dynamics simulation. The root mean square deviation (RMSD) of the structures with respective to the starting structures were almost stable during the last 100 ns. Subsequently, butyrolactone I was docked into the active site of both models using Autodock Vina, and further molecular dynamic simulation of 200 ns was conducted for the best docking poses of each complex. Stable RMSD values indicated the stability of protein-ligand complex. MM-GBSA binding free energy calculations were conducted to further assess the stability of the complexes. Accordingly, the butyrolactone I CDK1 complex was more favorable in the absence of Mg^{2+} ion (ΔG = -25.50 kcal/mol) than its presence (ΔG = -19.2 kcal/mol).

Keywords: CDK1, Mg^{2+} ion, Butyrolactone I, Computational chemistry

Abstract No: TI 23

A study on complexation, stoichiometry and binding of selected anionic organic pollutants and protonated polyaza macrocycles

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Anionic organic pollutants (AOPs) generated by industrial and laboratory processors are accumulated in the environment while causing health problems for human beings. Therefore, this research project is focused on a fundamental study of the removal of three selected AOPs, namely dianions of hydroquinone, catechol and resorcinol from the environment using a supramolecular approach. Two electron deficient, PPAMs, namely PPAM1 and PPAM2 with different cavity sizes and shapes were synthesized by using a 1:1 molar mixture of diethylenetriamine along with a dialdehyde, terephthalaldehyde and isophthalaldehyde separately as starting materials by carrying out an imine metathesis, a reduction with sodium borohydride followed by a protonation with perchloric acid in order to obtain aqueous medium soluble macrocycle. After characterization of the PPAM1 and PPAM2 using spectroscopic techniques, the complexation is driven by ionic interactions between hexa-cationic PPAMs and dianionic AOPs in an aqueous solution was characterized by UV-visible spectroscopy and fluorescence spectroscopy. Stoichiometry and the binding constant between each PPAM with dianions of hydroquinone, resorcinol and catechol were determined using fluorescence spectroscopy by employing the Job's plot method and dilution method, respectively. The Job's plots of each PPAM and AOP used in this study demonstrated 1:2 stoichiometry between the PPAM and AOP indicating a partial displacement of the counter ion of the macrocycles. Binding constants between PPAMs and AOPs were calculated using the Benesi – Hildebrand equation. Among the three AOPs used in this study, dianions of hydroquinone exhibited the highest binding constants of 2.85×10^6 $mol^{-2}dm^6$ and 2.58×10^6 $mol^{-2}dm^6$ with PPAM1 and with PPAM2, respectively. The dianions of resorcinol exhibited the lowest binding constant of 8.21×10^5 $mol^{-2}dm^6$ and 8.12×10^5 $mol^{-2}dm^6$ for PPAM1 and PPAM2, respectively. In conclusion, fluorescence spectroscopy evidenced the complexation between PPAMs and AOPs. The cavity size and shape of the PPAM as well as the position of the dianions in AOPs

determined the binding constant.

Keywords: Anionic organic pollutants, Protonated polyaza macrocycles, Job's plot, Binding Constant, Benesi – Hildebrand method

Abstract No: TA 13

Removal of Selected Textile Dyes from Effluent Water Using Mineral Adsorbents and Activated Carbon

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Removal ability of the textile dyes, Methylene Blue, Rodamine B and Congo Red from water was investigated in this study. Static experiments were conducted using each dye with selected adsorbents, Kabok, Brick Clay, Granite Chips and activated carbon. In each experiment, 1.00 g of adsorbent was treated with 25.00 cm^3 of 2.6 x 10^{-5} mol dm^{-3} dye solutions. Absorbances of each solution were measured at their respective λ_{max} values at a time duration of 0 - 240 min and their average values are reported. The continuous flow experiments were carried out with best adsorbent for each dye identified by static experiments, using 2.6 x 10^{-5} mol dm^{-3} dye solutions. The flow rate of the column was kept as 10 mL/min. The experiment was conducted for 120 minutes.According to the static experiment results, the natural adsorbents, Kabok and Brick Clay showed the best percentage removal of Methylene Blue with 98.8% and 95.7% which was better compared with activated carbon, 83.3%. In contrast, Rodamine B was best removed by activated carbon with percentage removal of 82.5%. Among the inorganic mineral adsorbents, Brick Clay showed a percent removal of 64.1% for Rodamine B. Congo red was best removed by Brick Clay with 96.6% efficiency compared to 43.4% removal of activated carbon.The breakthrough curves of the continuous flow experiments show the potential of removing congo red and methylene blue using Brick Clay and Kabok respectively.

Keywords: Mineral adsorbents, wastewater, methylene blue, absorption

Abstract No: TA 14

Effect of biochar application on plant uptake of sulfamethoxazole in soil

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The purpose of this study was to assess the effect of cinnamon wood biochar (CWBC) in minimizing the plant uptake of sulfamethoxazole (SUL) from the contaminated soil. For this purpose, *Ipomoea aquatica* was grown in soil and 2.5% w/w CWBC amendment contaminated with 50 mg/kg of SUL for 4 weeks. The results suggest that the root uptake of SUL relatively higher than by shoot. The plant uptake of SUL was significantly reduced by 60% when 2.5% w/w of CWBC was added to the soil. The bioaccumulation factor of SUL in *Ipomoea aquatica* grown in soil was 158.38. This was decreased by 76% with the addition of 2.5% of CWBC to the soil. In contrast to the controlled experiment, the retention of SUL in CWBC amendment was increased by 65%. The present study suggested that the application of CWBC to the agricultural soil effectively decreased the plant uptake while increased SUL retention in soil. Thus, the application of biochar to the soil limits human exposure of SUL *via* food crops.

Keywords: Pharmaceutical and personal care products, biochar, immobilization, plant uptake