

conclusion of 40 exciting years spent in the biochemistry laboratories of different countries with various cultures.

**Keywords:** Protein Biochemistry, Backbone Conformation, Phosphotransferase System, Phosphotransferase, Proteome Analysis.

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#### **Abstract No.267**

##### **Effect of Butachlor Herbicide on Hemoglobin Structure and Species**

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Butachlor (2-chloro-2', 6'-diethyl-N-(butoxymethyl) acetanilide) is a member of chloroacetanilide class of chemistry and is the herbicidal active ingredient in MACHETER EC. This herbicide is used as a pre-emergence control for the undesirable grasses and broadleaf weeds. The consumption of butachlor in Iran is among the most used pesticides which is mostly applied to rice fields. Extensive use of this herbicide beside other types of pesticides is now a concern for human health, as these chemicals can enter the body through our foods. Although most of these pesticides and their metabolites are excreted from the body, high daily intake cause permanent existence of these pesticides in the body. As a consequence, entrance of this herbicide into the blood stream, brings one of most abundant blood protein, hemoglobin, into contact with butachlor which may manipulate hemoglobin function in the body. In this report, the interaction of hemoglobin with butachlor under physiological condition was assessed and found the changes in protein structure and function which was analyzed by various methods such as UV-Vis, fluorescence as well as biophysical and biochemical investigations. The hemoglobin species upon interaction of butachlor were studied in this report.

**Keywords:** Herbicide, Butachlor, Hemoglobin, Spectroscopy.

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#### **Abstract No.268**

##### **Interaction of Cationic Peptide Drugs with Bacteria and Lipid Bilayers: Short R-, W-Rich Hexapeptides as a Case Study**

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The global emergence of resistance to antimicrobial agents is increasingly limiting the effectiveness of current drugs. The treatment of multidrug-resistant Gram-negative germs represents a particular challenge. Antimicrobial peptides are effective molecules in the innate immune system and might provide a promising alternative towards classical antibiotics. Understanding the structural basis of activity and bacterial selectivity provides one basis for the development of effective peptide-based antimicrobial drugs. Peptides rich in arginine (R) and tryptophan (W) residues are of particular interest as they are found as small antimicrobial motifs in much larger natural compounds. Our recent strategy to induce constraints in RW-rich hexapeptides by cyclization did result in pronounced peptide activity against Gram negative *Escherichia coli*, for instance, cyclo-RRRWWF (c-WFW). The activity of c-WFW against *E. coli* is modulated by lipopolysaccharides (LPS) in the outer bacterial membrane. To elucidate the role of the two tryptophan residues in interactions with *E. coli* membranes, we replaced them by analogues having altered hydrophobicity, dipole and quadrupole moments, hydrogen-bonding ability, amphipathicity, or ring size. The biological activity against *Bacillus subtilis* and erythrocytes increased with increasing peptide hydrophobicity, whereas the effect on *E. coli* revealed a more complex pattern. Isothermal titration calorimetry demonstrated that peptide partitioning into model lipid membranes is driven by both electrostatic and hydrophobic interactions and follows the order: POPC/smooth-LPS >> POPC/rough-LPS > POPC/lipid A = POPC/POPG > POPC. The hydrophobic contributions to binding to POPC and mixed POPC/POPG were comparable. Low hydrophobicity and peptide conformational flexibility reduced binding, showing that peptide-membrane interactions correlate with the biological effect. The highly differentiated activity pattern against *E. coli* was poorly reflected in peptide binding to POPC/lipid A and disappeared in studies with LPS-containing membranes. Stronger partitioning into POPC/smooth-LPS as compared with POPC/r-LPS uncovered a significant role of O-antigen and outer-core oligosaccharides of LPS in anti-*E. coli* activity.

**Keywords:** Cationic Antimicrobial Peptides, Lipid Bilayers, Lipopolysaccharide, Peptide Partitioning, Isothermal Titration Calorimetry.

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