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The Composite Physical and Chemical Approach to the Solution Spatial Structure of Polypeptide Neurotoxins

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The most fruitful approach to the solution structure of peptides and proteins is a dovetailing of physical (experimental and theoretical) and chemical (selective modification) methods so as to best attain the common purpose of assessing the intra- and intermolecular interactions of the given substance. Of the physical methods the most informative in such study is high resolution NMR spectroscopy.

We have made extensive use of this technique within the framework of the above approach in an analysis of the spatial structures of some polypeptide neurotoxin components of bee and snake venoms.

For signal assignment in the ^{1}H and ^{13}C NMR spectra of the bee venom component apamin (18 amino acid residues, two disulfide bonds) a multifrequency homo- and heteronuclear decoupling procedure was developed, aimed at identification of the spin systems of the particular amino acid residues and determination of the residue position in the amino sequence. The apamin spatial structure has been elucidated by selection of the optimal calculated conformation on the basis of the NMR parameters of the native toxin and its selectively modified analogs.

In a study of snake neurotoxins, mainly neurotoxin II (61 amino acid residues, four disulfide bonds) isolated from the venom of the Central Asian cobra *Naja naja oxiana,* use was made of the dependence of the ^{1}H NMR parameters on the conditions of the aqueous medium, and of selective chemical modification, in particular, insertion of spin labels. Additional information was obtained from comparison of the spectra with those of homologous toxins from other snakes. The contacts revealed between the amino acid side chains provided a general picture of the folding of the backbone and detailed information on the antiparallel β-structure of its central segment. A comparison is made with the known X-ray structure of hydrophidae snake venom erabutoxins, as well as with NMR data for *Naja naja oxiana* cytotoxins I and II.

An EPR study of the binding of selectively spin labeled neurotoxin II derivatives to the *Torpedo marmorata* acetylcholine receptor revealed the role played by lysine residues in this specific interaction.

Synthetic Molecular Membranes and Their Functions

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A variety of dialkyl amphiphiles with alkyl chain lengths of C_{10} to C_{20} and with cationic, anionic, nonionic and zwitterionic head groups form stable bilayer membranes spontaneously when dispersed in water. Further assemblage of the bilayer produces vesicles and lamellae, as examined by electron microscopy. These aqueous membranes undergo the crystal-liquid crystal transition in a way similar to the biolipid membranes.

The bilayer and monolayer membranes are similarly formed from one-headed and two-headed single-chain amphiphiles which contain the rigid segment. Their morphologies are drastically changed by the chemical structure of the rigid segment.

These synthetic molecular membranes provide unique microenvironments for reaction and several examples were found in which the membrane fluidity affected the reaction kinetics.

Intramolecular Hydrophobic and Aromatic-ring Stacking Interactions in Ternary Complexes in Solution

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One possibility of influencing the stability and structure of mixed ligand complexes [1] is through the formation of intramolecular ligand–ligand bonds. *Covalent bond formation* is well-known, *e.g.,* coordinated pyruvate and glycinate form a Schiff base within the coordination sphere of a metal ion [2]. *Ionic bonds* may be formed between oppositely charged side chains: several amino acids are predestinated for such electrostatic interactions [3, 4]. *Hydrogen bond formation* also seems possible [5]