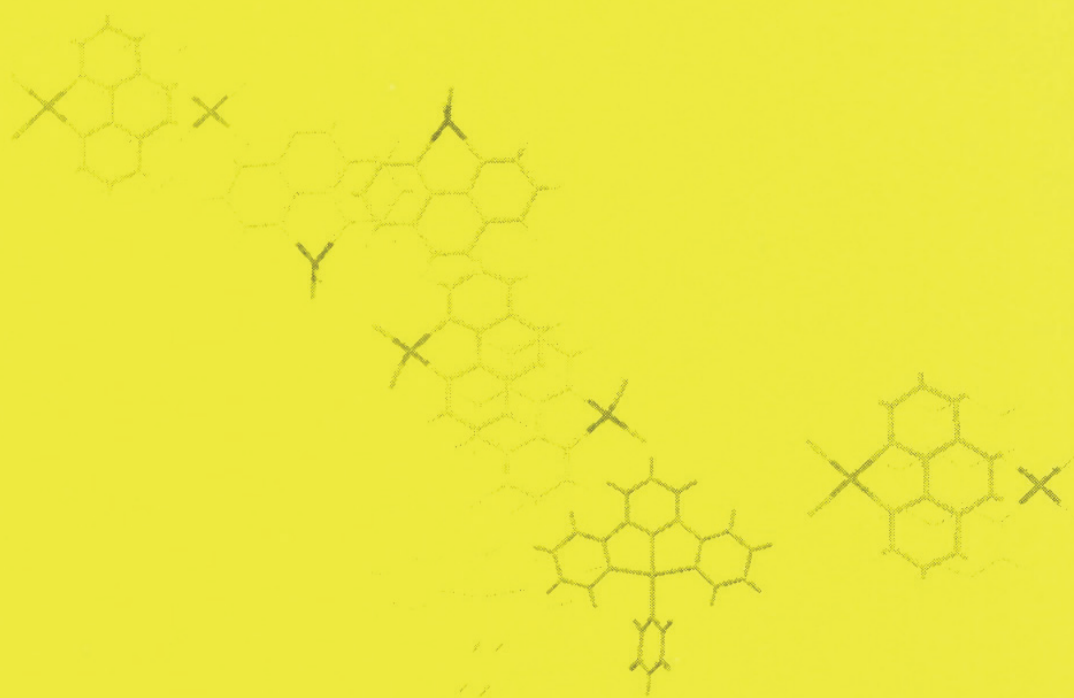


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# HUMBOLDT CONFERENCE ON NONCOVALENT INTERACTIONS

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**BOOK OF ABSTRACT**

## HYDROGEN BONDS AND XH/ $\pi$ INTERACTIONS OF PORPHYRINS IN PROTEINS

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Structures of porphyrin containing proteins from the Protein Data Bank (PDB) Select January 2007, the list of non-redundant protein chains (25% threshold), were searched in order to find out hydrogen bonds and XH/ $\pi$  interactions of porphyrins in proteins. The results revealed that the significant number of conventional hydrogen bonds with acetyl and propionate groups of porphyrins was founded. The most frequently observed donors are charged amino acid residues from porphyrin surrounding. Side-chains hydrogen bonds are more frequent than those with peptide donors; they involve water molecules sometimes that are classified as bridged hydrogen bonds. Besides,  $\pi$ -system of every porphyrin ring is involved in XH/ $\pi$  interactions, most of the porphyrins are making several interactions. We found interactions with C-H and N-H groups as hydrogen atom donors, however the number of CH/ $\pi$  interactions is much larger than number of NH/ $\pi$  interactions. Both five-membered pyrrole rings and six-membered chelate rings are involved in noncovalent interactions; the number of interactions with five-membered is larger than the number of the interactions with six-membered rings.

The conservation scores were calculated for all amino acids in the binding pocket. The average conservation score for the amino acids making noncovalent interactions with the porphyrin is statistically significantly higher than for the amino acids that do not make interactions.

- [1] S. Đ. Stojanović, V. B. Medaković, G. Predović, M. Beljanski, and S. D. Zarić, *J.Biol. Inorg. Chem.*, 12, 1063-1071 (2007).