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Biological affinity of aromatic amino acids in intermolecular π-stacking interaction

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Non-covalent intermolecular interactions are the basis of drug inhibition of a wide range of enzymes that contain amino acid residues phenylalanine and tryptophan with a developed π-conjugated system in their active sites. Previous studies have shown [1-2] that the stability of the complex between the amino acid residue of the enzymes enzymes and the π-conjugated system of the pharmacophore depends on their electron donation and the nature of the frontier molecular orbitals, which determine the type of electronic transitions, and therefore the nature of the intermolecular interaction.

Our spectral fluorescence study by titrating a solution of amino acids with a solution of thiochrome as a natural dye with a π-conjugated system under the same conditions and concentrations showed that the formation of a [π-π]-complex of thiochrome with tryptophan occurs more stably than with phenylalanine (Fig. 1).

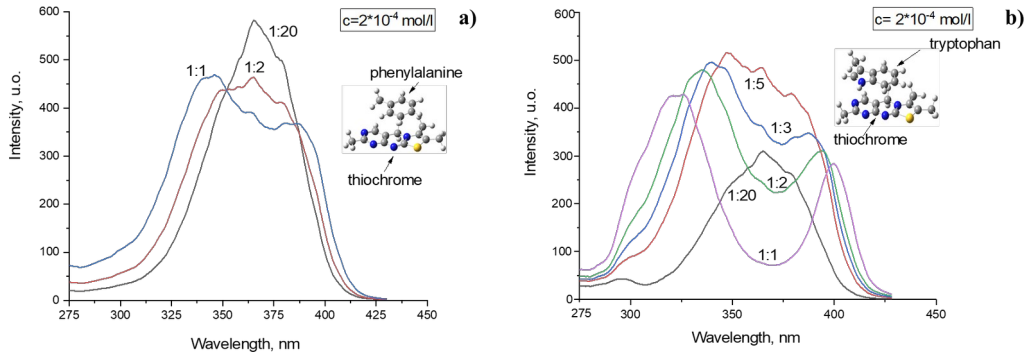

Fig. 1.

Fluorescence titration of a solution of amino acids phenylalanine (a) and tryptophan (b) with thiochrome dye.

Theoretical calculations show that the first electronic transition for both phenylalanine and tryptophan is $\pi \rightarrow \pi^*$, but its intensity is 6 times higher for tryptophan, both amino acid residues enter into π-stack intermolecular interactions, but with different energy (ΔE) complex formation. Biological affinity depends on the donor-acceptor properties of the bio-molecule, and was quantified by the φ_0 parameter: for tryptophan $\varphi_0 = 0.554$, for phenylalanine $\varphi_0 = 0.493$, that is, the tryptophan residue will form more stable intermolecular complexes: ΔE [π-π] complex with tryptophan is -13.6 kcal/mol, and ΔE [π-π] complex with phenylalanine is -9.2 kcal/mol. Such calculations agree well with spectral measurements.

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