Application of the MTD Method to Dye-Cellulose Interactions

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The MSD (Minimal Steric Difference) method [1] and later the MTD (Minimal Topologic Difference) method [2] have been developed to model ligand-receptor interactions. The MTD method is based on the analysis effectuated on the hypermolecule, a topological network obtained by molecular superposition.

The MTD method was applied to several classes of textile dyes in order to model the dye binding by the cellulose fibre. Anthraquinone vat, anionic monoazo, disperse azo and heterocyclic monoazo dyes were analyzed by the MTD approach [3, 4]. Valuable dye structure-cellulose affinity information have been obtained. Thus, a similarity between the dye-fiber interactions and receptor-ligand ones was concluded. Attractive dye-cellulose interactions are generally favoured along the molecular axis of the dye molecule and by the length of the molecular conjugated system. Molecular length represents an acceptable approximation for dye-fiber interaction. The repartition of beneficial and detrimental MTD vertices reflect the important electrostatic and steric interactions for dye-cellulose binding interactions. Detrimental interactions are noticed for sulfonic groups in the dye molecules, which seem to contribute to the dye solubilization only. From MTD calculations applied to the disperse dyes, it was concluded that steric interactions are also important for this binding.

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