Poster Presentation

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Synthesis, molecular docking and DNA binding studies of 4N-substituted hydrazinecarbothioamides

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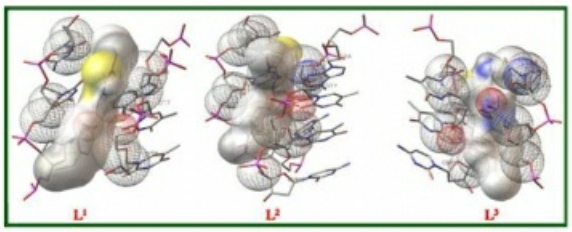
Three 4N-substituted hydrazinecarbothioamides of general formula H5C2(Ph)-CH=N-NH-C(S)-NHR where R=H (L1), CH3 (L2), C2H5 (L3), were resulted by the reaction between 4-ethylbenzaldehyde with 4N-substituted hydrazinecarbothioamides and were characterized by elemental analysis, IR, NMR spectral studies, and X-ray single-crystal diffraction analysis. The formation of ligands evidenced by the IR and NMR spectral data. Single crystal X-ray data indicates that the ligands L1 and L3 crystallized in monoclinic system with space group P21/c. The crystal L2 has a triclinic system with space group P-1. The interactions of the ligands with calf-thymus DNA were then investigated by spectrophotometric method. The experimental results indicated that ligands bound to DNA by intercalation mode. The docking studies of ligands with glucosamine-6-phosphate synthase revealed that the ligands are potent as a drug for target enzyme.



Molecular docked model of ligands with DNA.

Keywords: Hydrazinecarbothioamides, CT-DNA, molecular docking.