The aim of this work was development of models which define the effects of molecular structure on the biological activity of compounds of similar structure. Chelate ligands were prepared by condensation of diamine and the corresponding β-diketone. Copper(II) complexes with chelate ligands containing ethane-1,2-diamine or propane-1,2-diamine as the amine part and pentane-2,4-dione and/or 1-phenylbutane-1,3-dione; pentane-2,4-dione and/or 1,1,1-trifluoropentane-2,4-dione; 1,1,1-trifluoropentane-2,4-dione and/or 1-phenylbutane-1,3-dione as β-diketone part were synthesized (Table 1).

In order to obtain predictive and interpretative models, we were chromatographed of a series of ligand and complexes. Chromatographic separations were carried out by thin layer chromatography on silica gel RP-18 plates, using a Camag horizontal HPTLC development chamber in the tank configuration. The mobile phase used was a mixture of dioxane (as organic modifier) and water. The lipophilicity parameters R_{M}^{\alpha} were determined. All structures were optimized with the HyperChem 7.0 program. Chemical descriptors: volume, surface area, energy of the highest occupied molecular orbital, energy of the lowest unoccupied molecular orbital, dipole moment, refractivity and polarizability were calculated from the structure and related to their lipophilicity parameters by multiple linear regression analysis. The obtained models were useful for interpretation the effects of structure on the lipophilicity i.e. biological activity of compounds of similar structure.