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A new mixed-ligand Cobalt(II) complex with synthesis, characterization and docking study

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A new mixed-ligand complex ([1]) has been synthesized by the reaction of Co(II) ion with 2-(2-(2-Hydroxyethylamino)ethylamino)cyclohexanol (HEAC) in the presence of pyridine-2,6-dicarboxylic acid, (PDCA), and identified by elemental analysis and FT-IR spectroscopy. In the complex, the HEAC coordinates through two N-atoms, and PDC coordinates through one N- and two O- which forms three five-membered chelate rings. As shown in Figure 1, the coordination number of the complex is 5. The τ value is calculated to be 0.10 for the Co atom, indicating a distorted square-pyramidal geometry([2]). The data obtained from molecular docking revealed that the complex has a higher docking score than the doxorubicin in reaction to CatB protein, thus we suggest that the anticancer activity of this compound will be studied (Figure 2).

***Keywords*:** Mixed-ligand complex, Pyridine dicarboxylate, Square-pyramidal geometry, Molecular docking

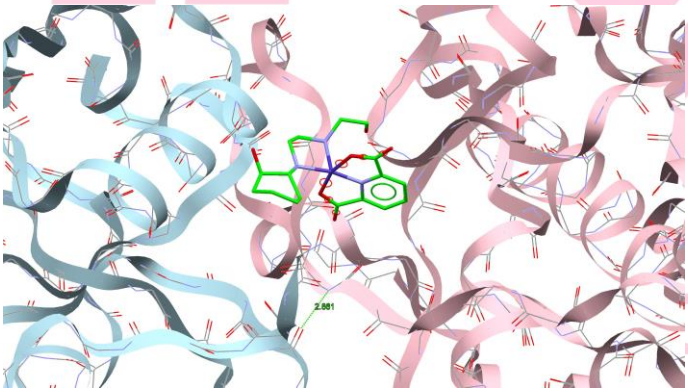


Figure 2. Docking study results, showing the interaction between the complex and CatB protein

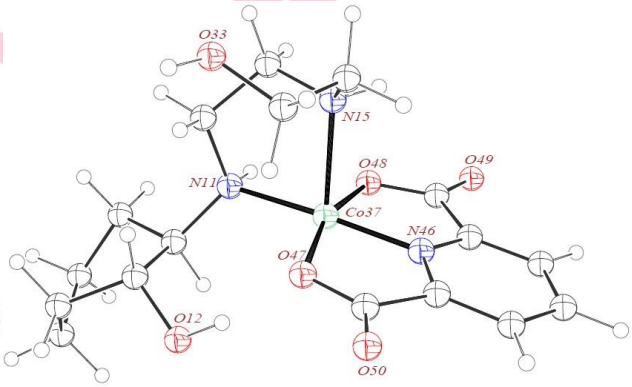


Figure 1.The ortep diagram of complex.

References

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