

Comparative study on synthesis and crystal structures of Ni(II) complexes bearing tetradentate N₂O₂ donor Schiff bases: Biomolecular interactions, cytotoxicities and molecular docking

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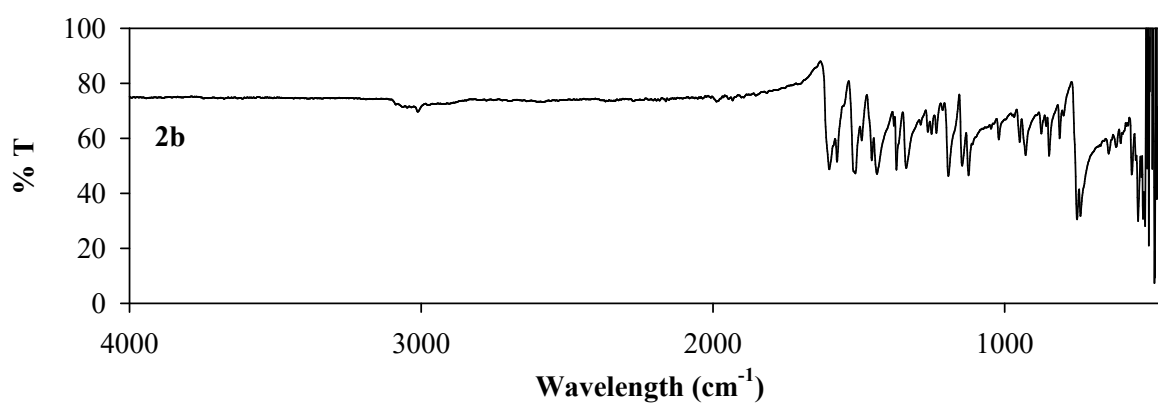
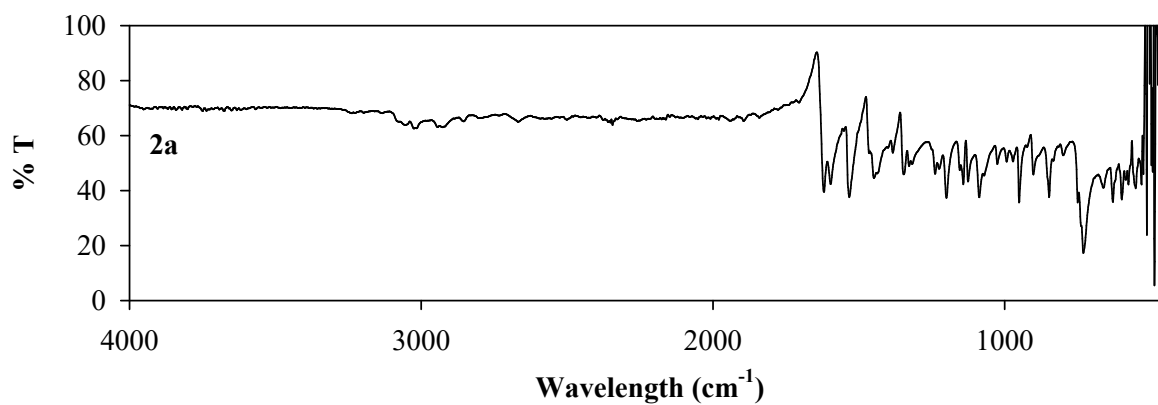
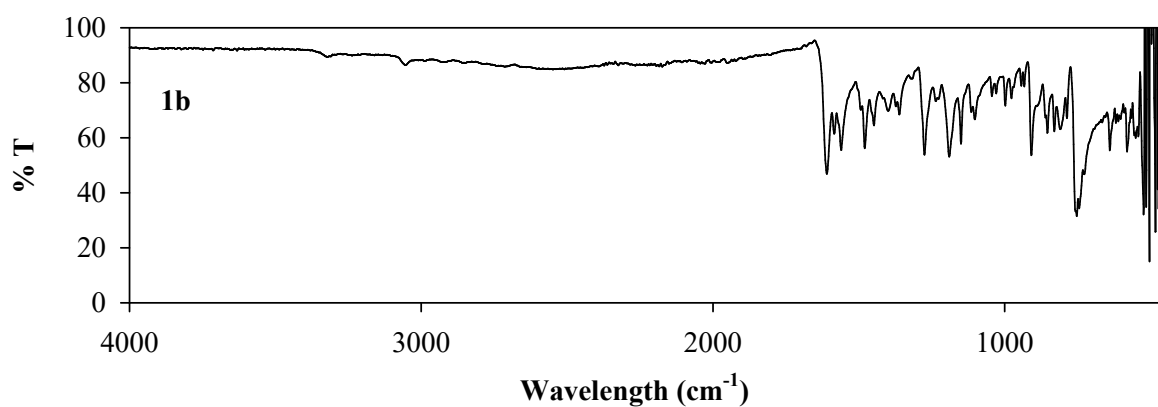
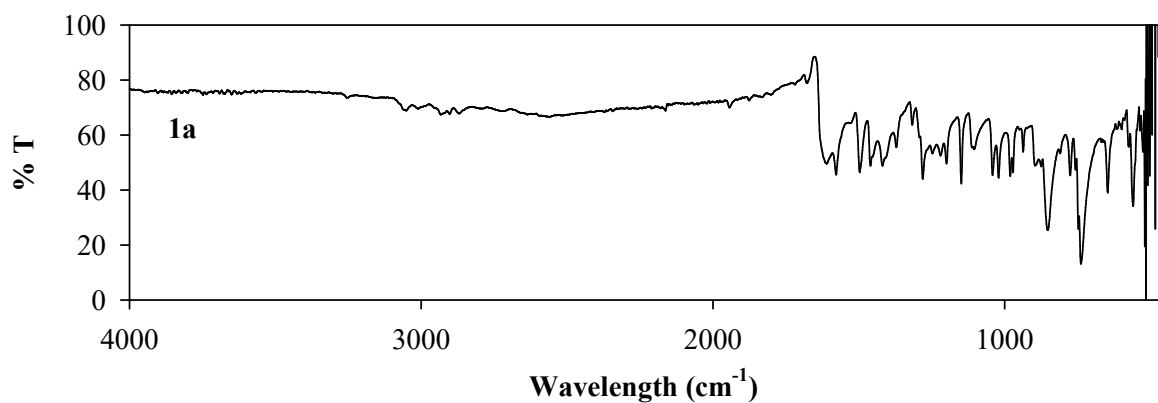


Fig. S1 FTIR spectra of the **1a-b** and **2a-b**

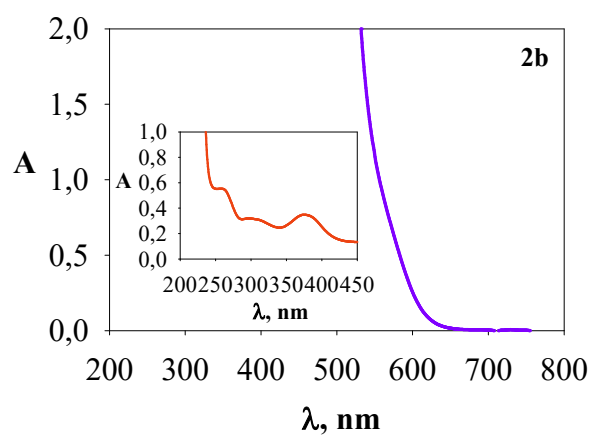
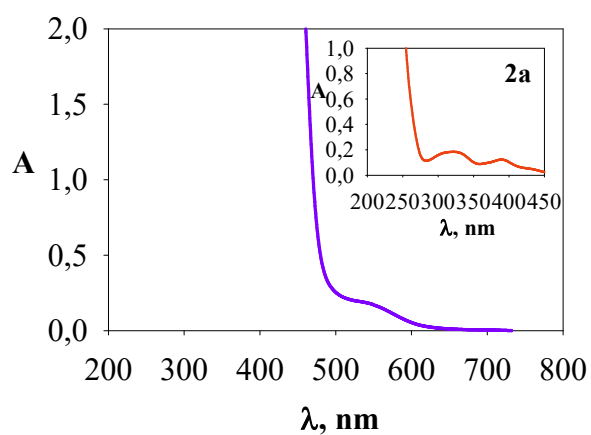
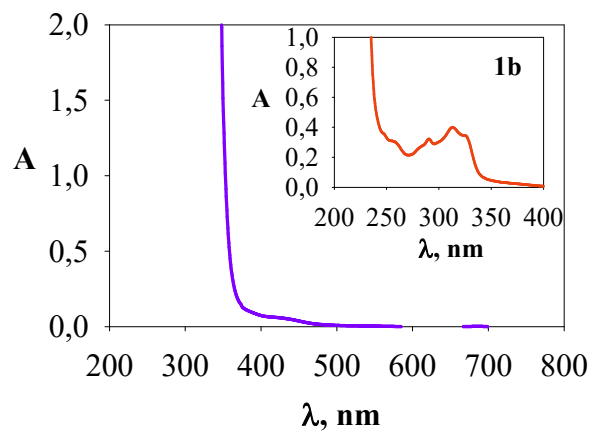
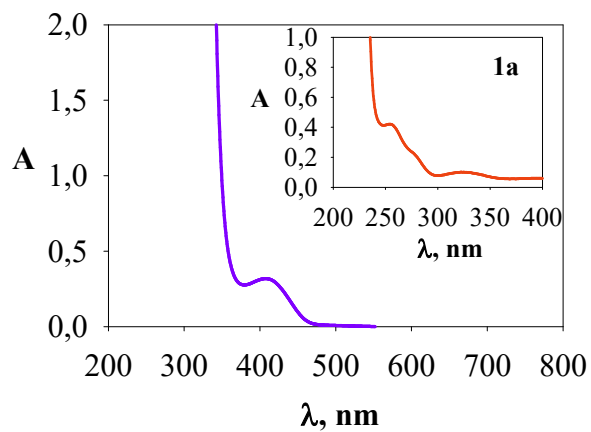


Fig. S2 Electronic absorption spectra of the **1a-b** and **2a-b**

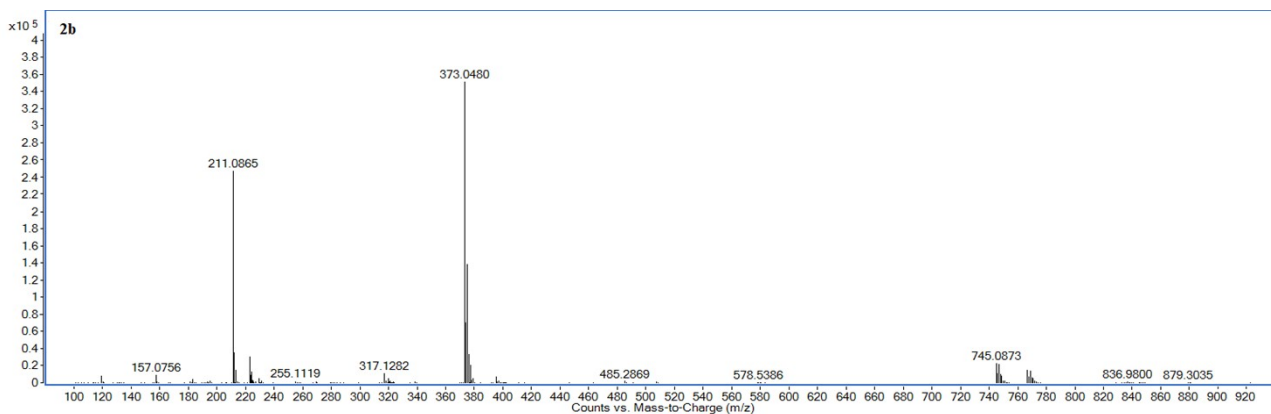
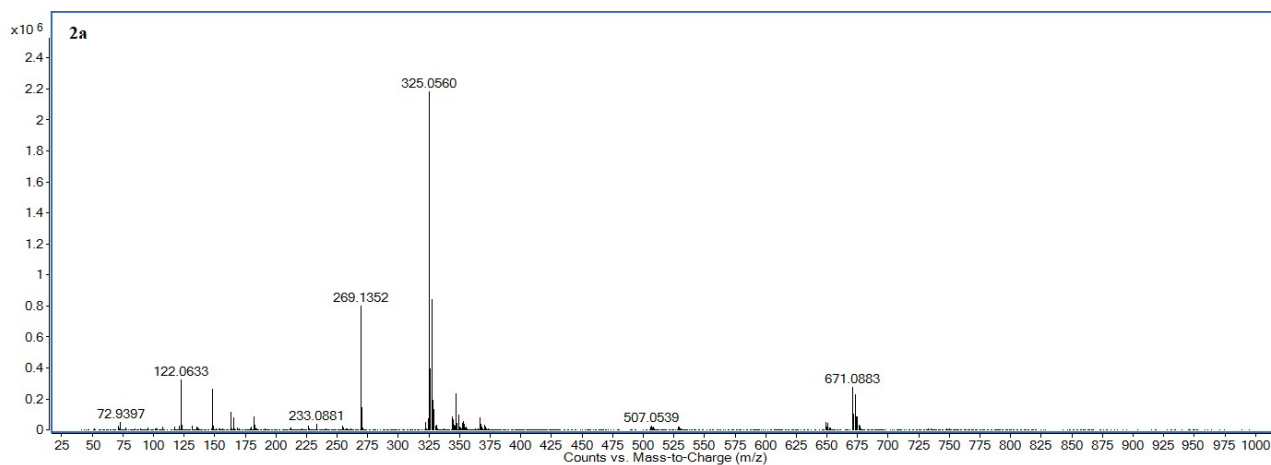
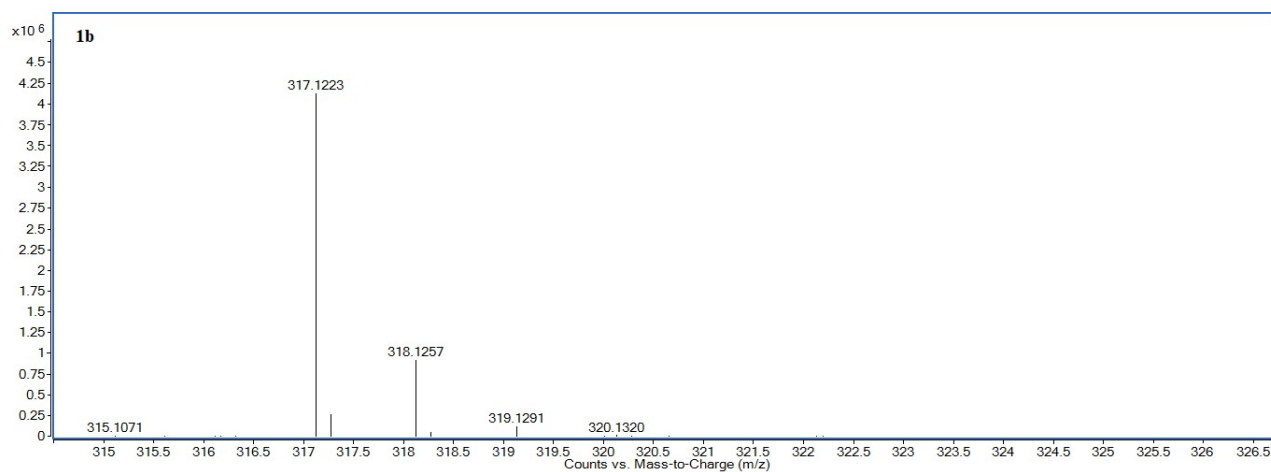
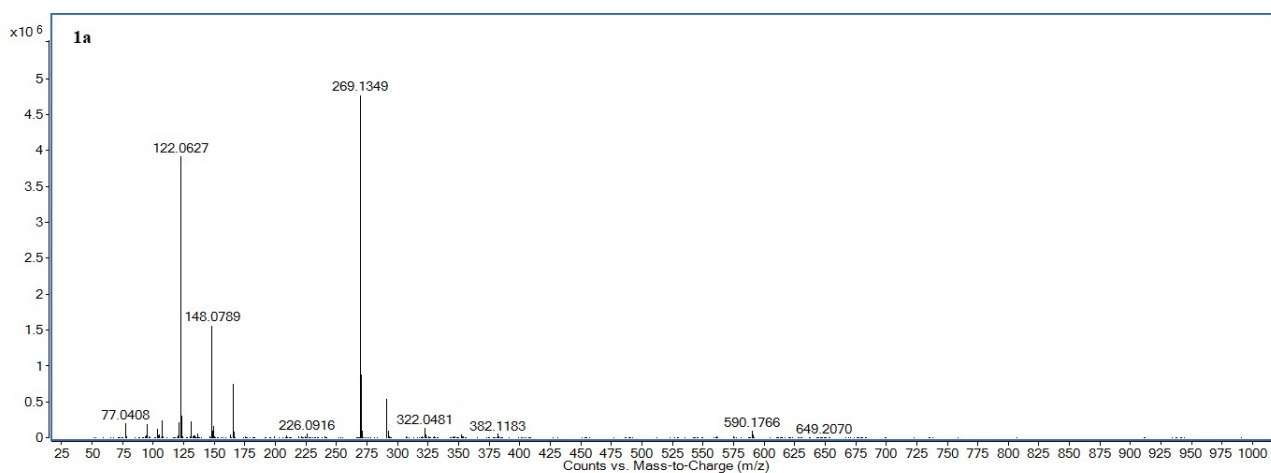


Fig. S3 ESI-MS spectra of the **1a-b** and **2a-b**

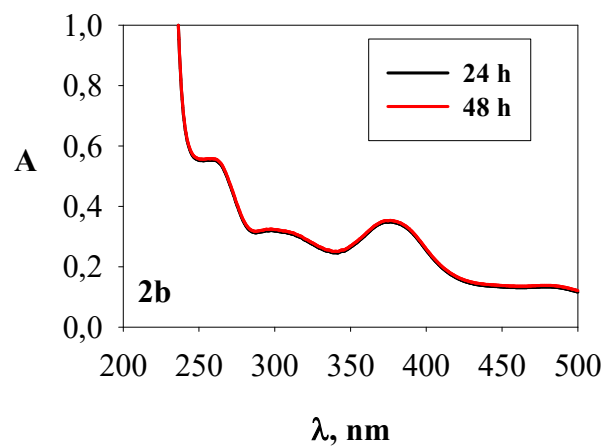
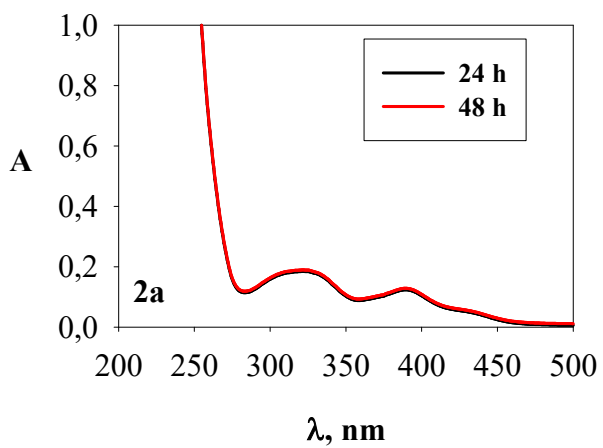
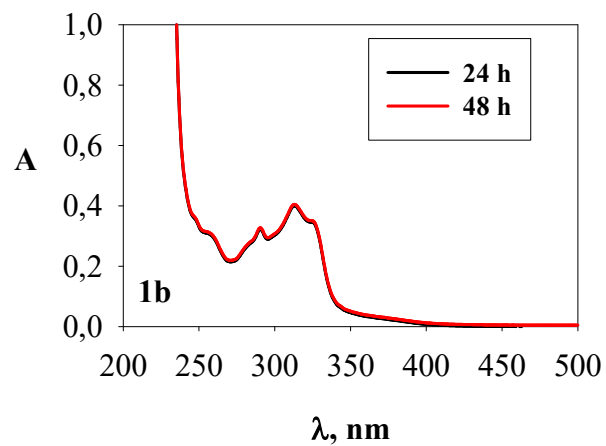
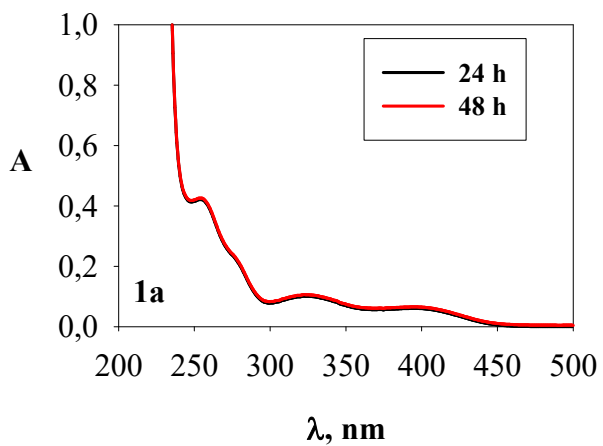


Fig. S4 Electronic absorption spectra of the **1a-b** and **2a-b** in DMSO after standing in different times at ambient temperature.

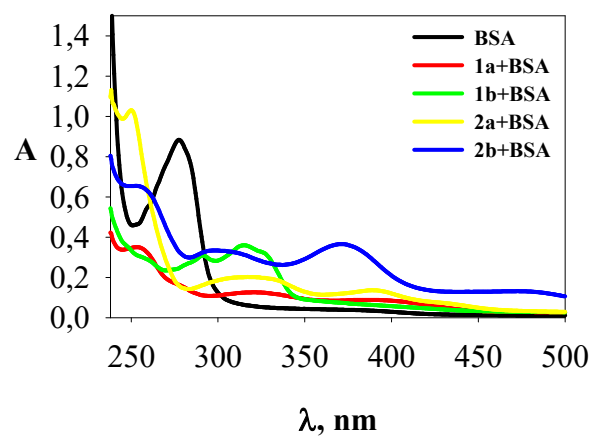


Fig. S5 Electronic absorption spectra of the **1a-b** and **2a-b** upon addition of BSA

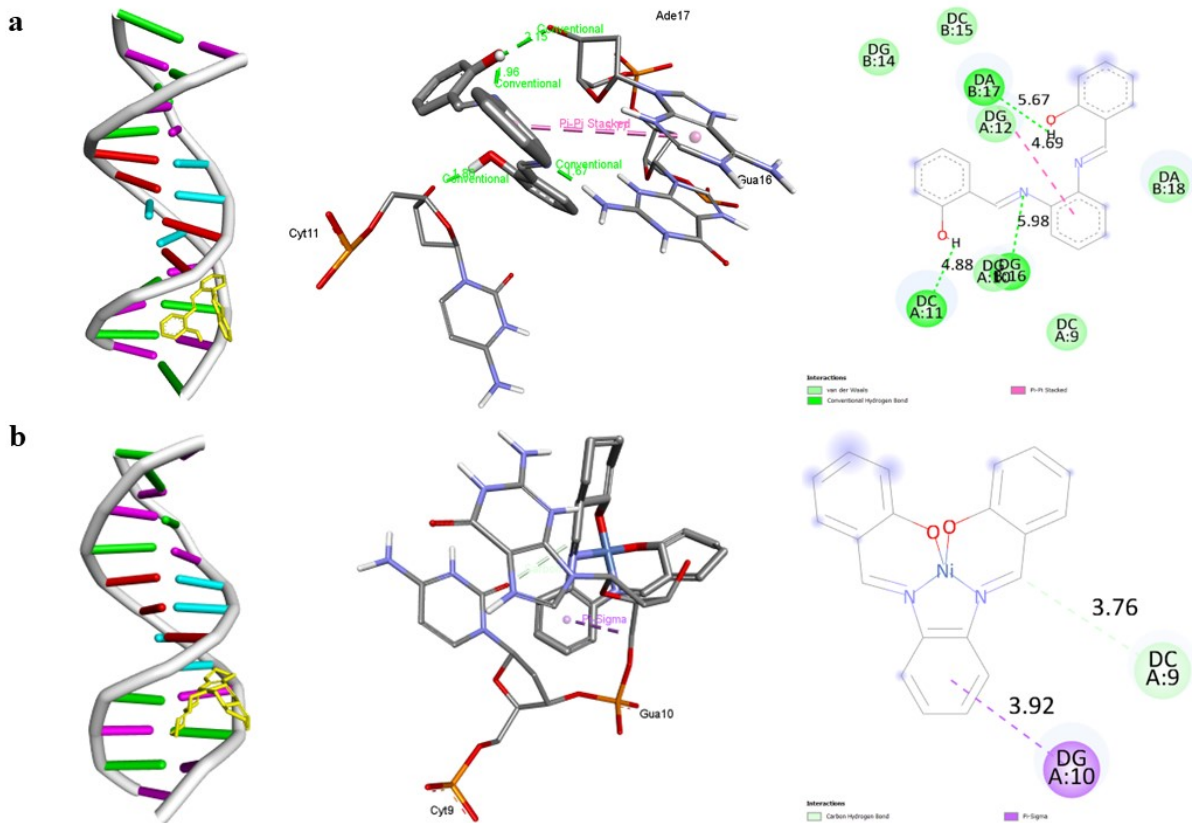


Fig. S6 3D docking structure, 2D and ligand interactions of the **1b** (a) and the **2b** (b) with active sites of B-DNA dodecamer.

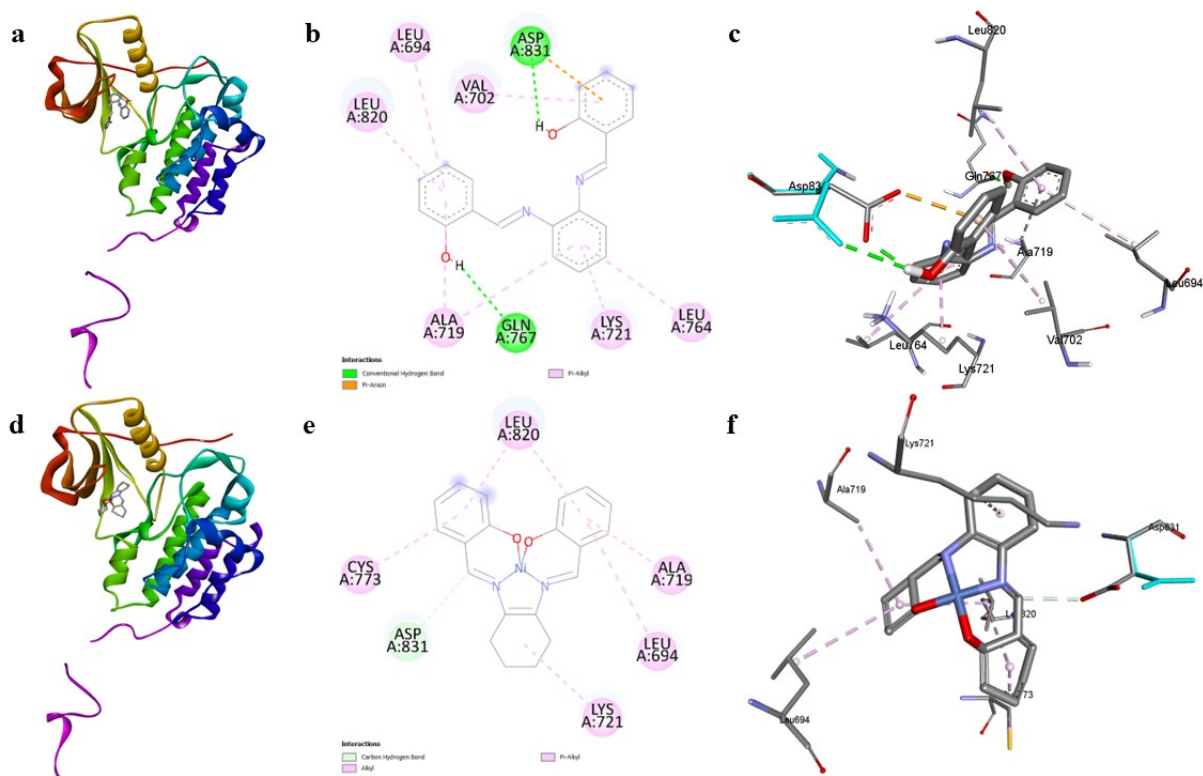


Fig. S7 The **1b** and **2b** superpositions (a and d) and the diagram of intermolecular interactions, 2D (b and e), and 3D structures of the binding sites (c and f) in the complex with tyrosine kinase receptor (PDB ID: 1M17). The Hydrogen-bond interaction is depicted with the green dotted line.