Conclusion

New dinuclear transition metal–based {Cu(II), Co(II) and Ni(II)} molecular entities \([\text{C}_{22}\text{H}_{32}\text{N}_4\text{O}_4\text{Cu}_2\text{Cl}_4]\), \([\text{C}_{22}\text{H}_{32}\text{N}_4\text{O}_4\text{Co}_2\text{Cl}_4]\) and \([\text{C}_{22}\text{H}_{32}\text{N}_4\text{O}_4\text{Ni}_2\text{Cl}_4]\)\(\cdot\)\(2\)\(\text{H}_2\text{O}\) derived from amino acid auxiliary ligand L–phenylalanine and bridged by piperazine were designed and synthesized as metallopeptide antitumor potential drug candidates. The structures of the complexes were proposed on the basis of elemental analysis, IR, UV–vis, NMR and EPR spectral studies which revealed pentacoordinate environment of the central metal ion. \textit{In vitro} DNA binding studies of complexes \([\text{C}_{22}\text{H}_{32}\text{N}_4\text{O}_4\text{Cu}_2\text{Cl}_4]\) and \([\text{C}_{22}\text{H}_{32}\text{N}_4\text{O}_4\text{Co}_2\text{Cl}_4]\) were carried out by employing various biophysical techniques \textit{viz.}, electronic absorption and fluorescence spectroscopy and CD spectral studies. The results revealed that complexes interact with DNA through electrostatic binding mode \textit{via} phosphate backbone of DNA helix, in addition to selective binding to the N7 atom of guanine nucleobases. The spectroscopic binding titrations showed that complex \([\text{C}_{22}\text{H}_{32}\text{N}_4\text{O}_4\text{Cu}_2\text{Cl}_4]\) exhibited higher binding propensity as compared to \([\text{C}_{22}\text{H}_{32}\text{N}_4\text{O}_4\text{Co}_2\text{Cl}_4]\). To determine the specific interaction of both complexes towards DNA nucleobases interaction studies with guanosine monophosphate mononucleotide 5'–GMP was also performed by employing UV–vis titration methods which showed that both complexes \([\text{C}_{22}\text{H}_{32}\text{N}_4\text{O}_4\text{Cu}_2\text{Cl}_4]\) and \([\text{C}_{22}\text{H}_{32}\text{N}_4\text{O}_4\text{Co}_2\text{Cl}_4]\) interact electrostatically with phosphate oxygen atoms in addition to the preferential coordinate covalent linkage to guanine nucleobases in agreement with other spectroscopic results. These studies have been validated by computational docking technique with target molecules to examine its mode of DNA binding and the studies revealed the electrostatic interaction, in addition to selective binding towards the minor groove of DNA in G/C rich sequences.