

Evaluation of the Anticancer and DNA-binding Characteristics of Dichloro(diimine)zinc(II) Complexes

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Characterization of Zn-1: White powder, IR (solid, ν in cm^{-1}): 1596, 1586, 1509, 1435, 1382, 1367, 1216, 1146, 1106, 973, 957, 873, 834, 784, 749, 685. $^1\text{H-NMR}$ δ : 7.70 (t, 2H, biq), 7.87 (t, 2H, biq), 8.09 (d, 2H, biq), 8.20 (d, 2H, biq), 8.60 (d, 2H, biq), 8.82 (d, 2H, biq). Anal. Calcd for $\text{C}_{18}\text{H}_{12}\text{Cl}_2\text{N}_2\text{Zn}$: C, 55.07; H, 3.01; N, 8.37%; found: C, 54.71; H, 2.65; N, 7.94%.

Characterization of Zn-2: White powder, IR (solid, ν in cm^{-1}): 1671, 1605, 1470, 1446, 1359, 1303, 1286, 1270, 1237, 1190, 1161, 1140, 1080, 1058, 1028, 942, 795, 775, 763, 680, 650, 632, 609. $^1\text{H-NMR}$ δ : 7.66 (t, 2H, py), 7.99 (d, 2H, py), 8.05 (t, 2H, py), 8.69 (d, 2H, py). Anal. Calcd for $\text{C}_{11}\text{H}_8\text{Cl}_2\text{N}_2\text{OZn}$: C, 41.22; H, 2.52; N, 8.74%; found: C, 40.84; H, 2.17; N, 8.31%.

Characterization of Zn-3: Yellow powder, IR (solid, ν in cm^{-1}): 3338, 3060, 1622, 1593, 1556, 1514, 1477, 1460, 1445, 1368, 1288, 1218, 1174, 1128, 1105, 1024, 913, 843, 805, 779, 746, 647. $^1\text{H-NMR}$ δ : 6.80 (br, 2H, $\text{C}_6\text{H}_4\text{-4-OH}$), 7.37 (br, 2H, $\text{C}_6\text{H}_4\text{-4-N=C}$), 7.66 (br, 1H, py), 8.08 (br, 2H, py), 8.69 (s, 1H, azomethine), 8.82 (br, 1H, py), 9.74 (br, 1H, OH). Anal. Calcd for $\text{C}_{12}\text{H}_{10}\text{Cl}_2\text{N}_2\text{OZn}$: C, 43.09; H, 3.01; N, 8.37%; found: C, 42.74; H, 2.63; N, 8.46%.

Characterization of Pt-1: Orange powder, IR (solid, ν in cm^{-1}): 1617, 1595, 1583, 1510, 1431, 1377, 1361, 1286, 1216, 1142, 980, 862, 830, 778, 745, 698. $^1\text{H-NMR}$ δ : 7.71 (t, 2H, biq), 7.88 (t, 2H, biq), 8.10 (d, 2H, biq), 8.21 (d, 2H, biq), 8.61 (d, 2H, biq), 8.82 (d, 2H, biq). Anal. Calcd for $\text{C}_{18}\text{H}_{12}\text{Cl}_2\text{N}_2\text{Pt}$: C, 41.39; H, 2.32; N, 5.36%; found: C, 41.84; H, 2.69; N, 5.44%.

Characterization of Pt-2: Yellow powder, IR (solid, ν in cm^{-1}): 1681, 1596, 1565, 1478, 1445, 1315, 1282, 1247, 1189, 1169, 1105, 1070, 1038, 975, 944, 815, 772, 758, 731, 692, 667, 609. $^1\text{H-NMR}$ δ : 7.88 (dt, 2H, py), 7.18 (dd, 2H, py), 8.39 (dt, 2H, py), 9.13 (d, 2H, py). Anal. Calcd for $\text{C}_{11}\text{H}_8\text{Cl}_2\text{N}_2\text{OPt}$: C, 29.35; H, 1.79; N, 6.22%; found: C, 29.04; H, 1.98; N, 5.89%.

Characterization of Pt-3: Orange powder, IR (solid, ν in cm^{-1}): 3340, 3065, 1616, 1595, 1504, 1476, 1355, 1291, 1260, 1210, 1159, 1103, 982, 934, 837, 776, 740, 645, 596. $^1\text{H-NMR}$ δ : 6.85 (d, $^3J_{\text{HH}} = 7$ Hz, 2H, $\text{C}_6\text{H}_4\text{-4-OH}$), 7.37 (d, $^3J_{\text{HH}} = 7$ Hz, 2H, $\text{C}_6\text{H}_4\text{-4-OH}$), 7.98 (t, $^3J_{\text{HH}} = 7$ Hz, $^3J_{\text{HH}} = 6$ Hz, 1H, py), 8.19 (d, $^3J_{\text{HH}} = 8$ Hz, 1H, py), 8.41 (t, $^3J_{\text{HH}} = 8$ Hz, 1H, py), 9.23 (s, 1H, azomethine), 9.48 (d, $^3J_{\text{HH}} = 6$ Hz, 1H, py), 9.96 (s, 1H, OH). Anal. Calcd for $\text{C}_{12}\text{H}_{10}\text{Cl}_2\text{N}_2\text{OPt}$: C, 31.05; H, 2.17; N, 6.03%; found: C, 30.82; H, 1.91; N, 6.46%.

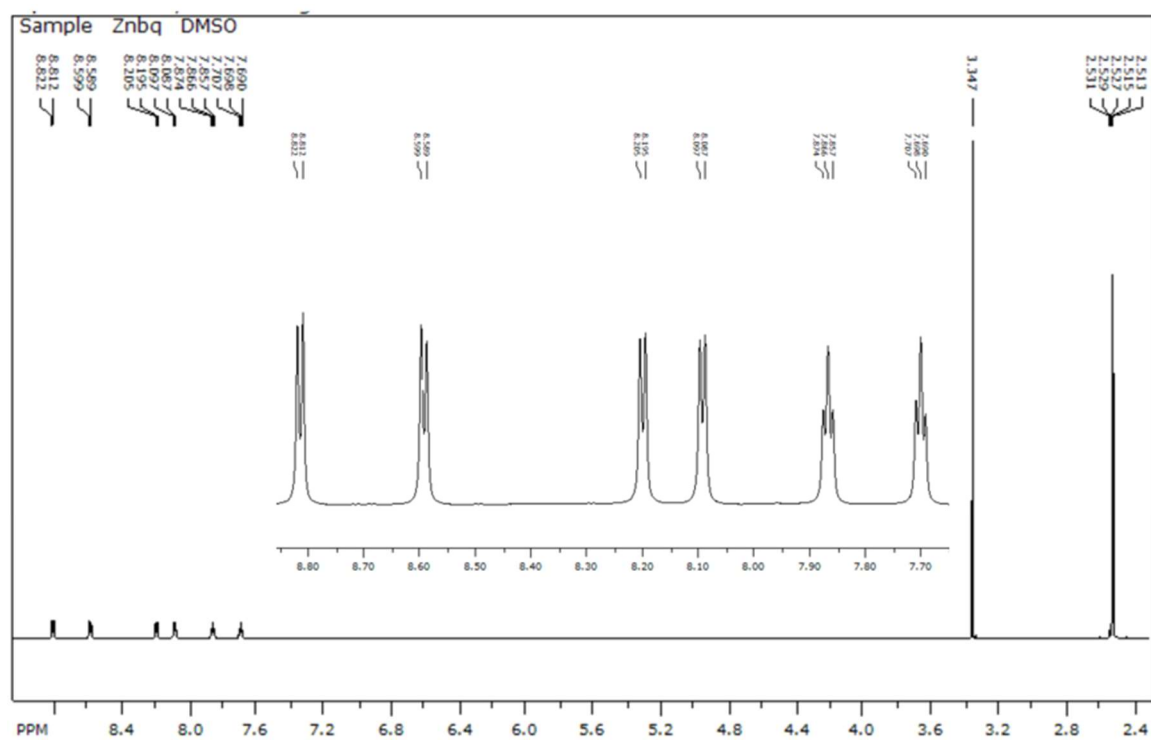


Figure S1. ^1H NMR of complex Zn-1.

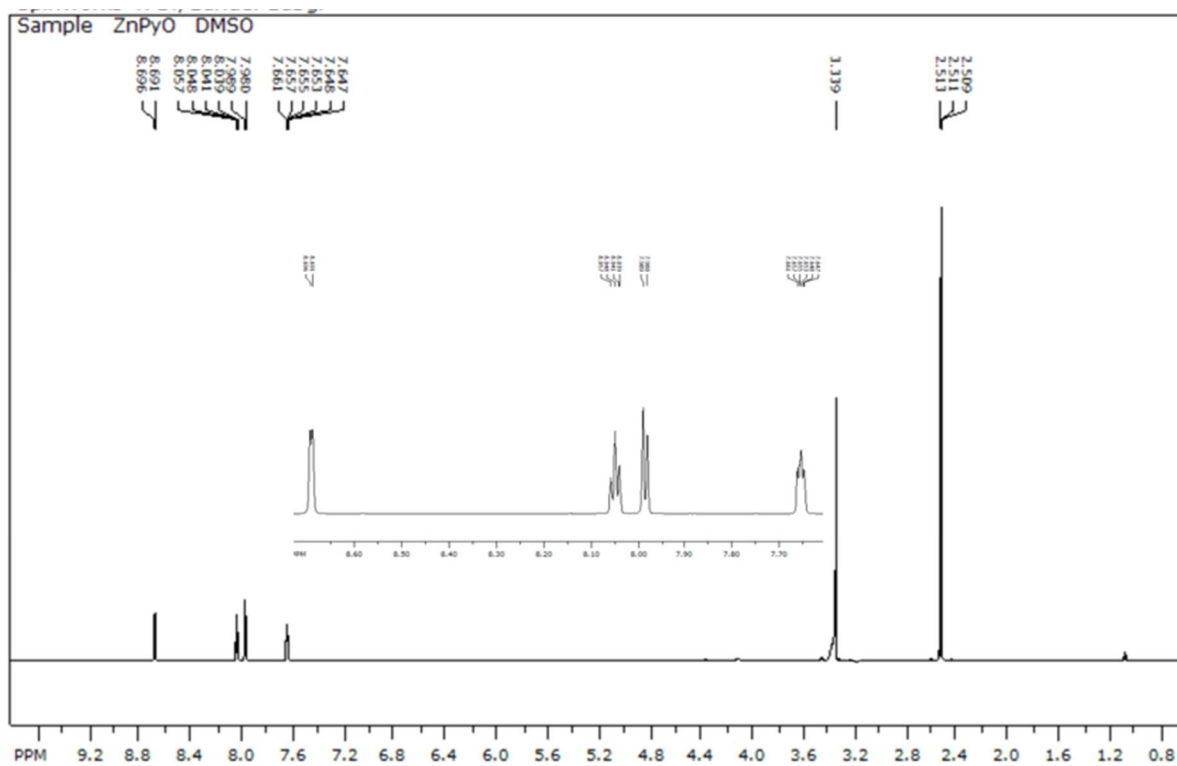


Figure S2. ^1H NMR of complex Zn-2.

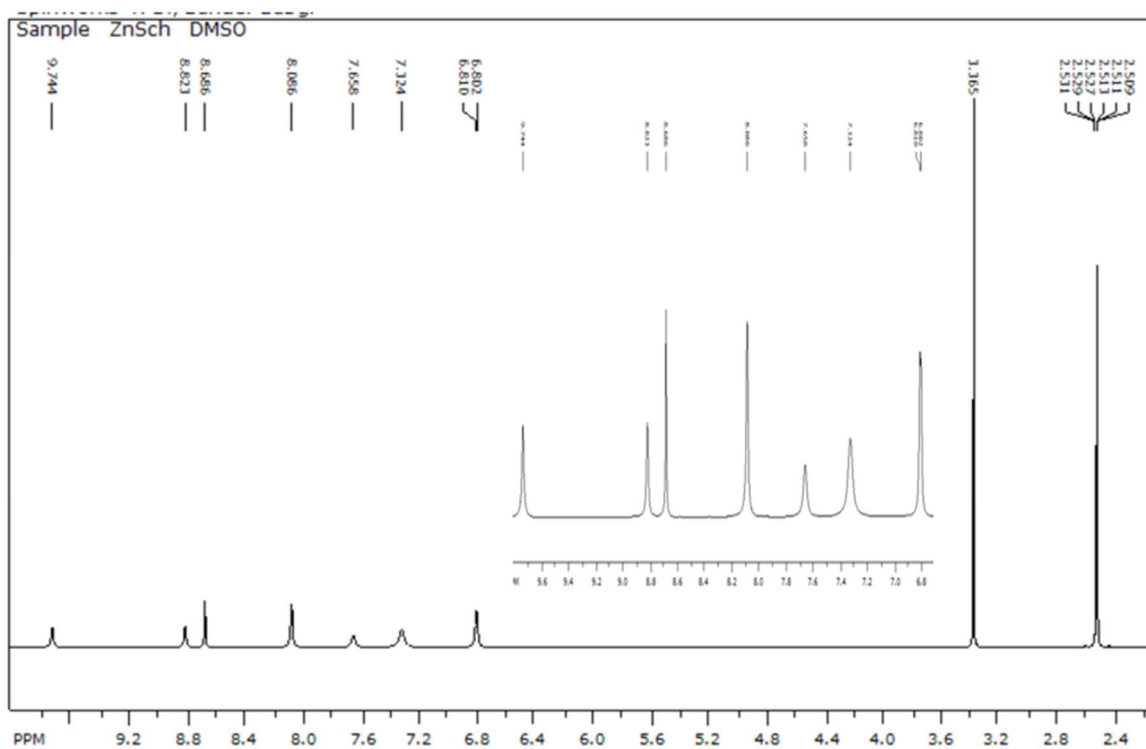


Figure S3. ^1H NMR of complex Zn-3.

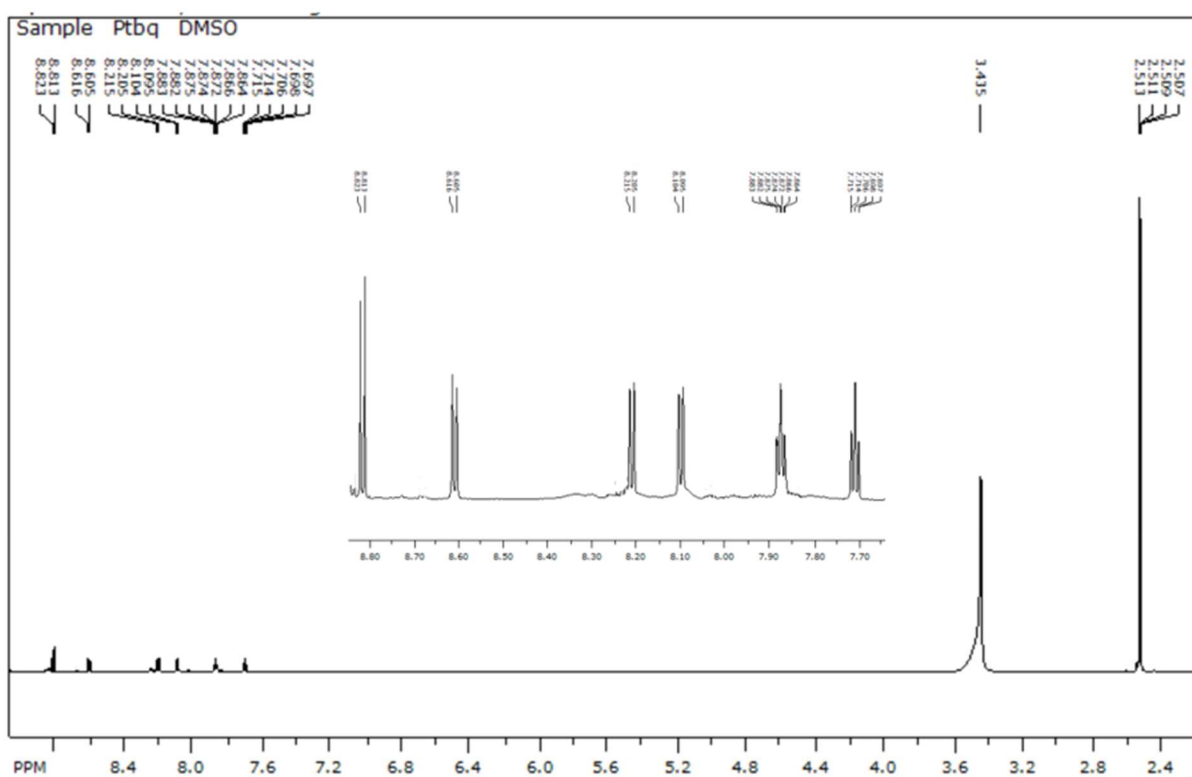


Figure S4. ^1H NMR of complex Pt-1.

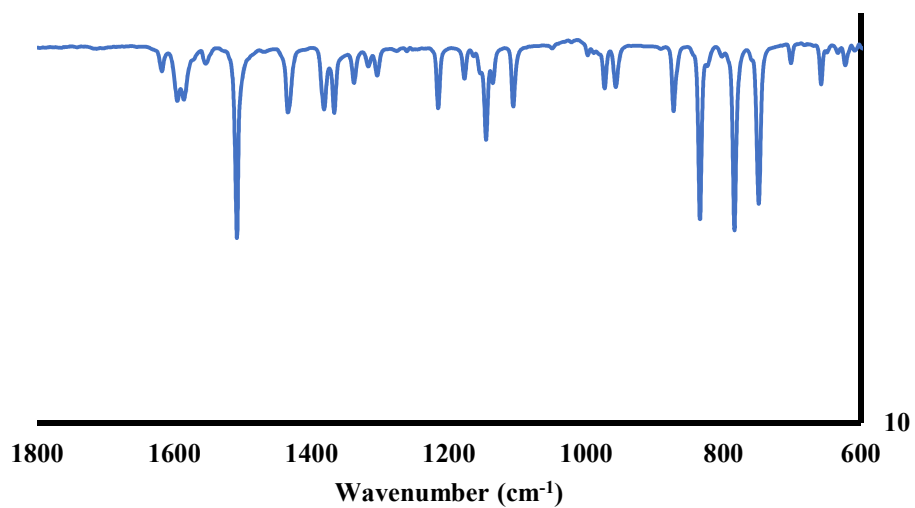


Figure S7. IR spectrum of Zn-1.

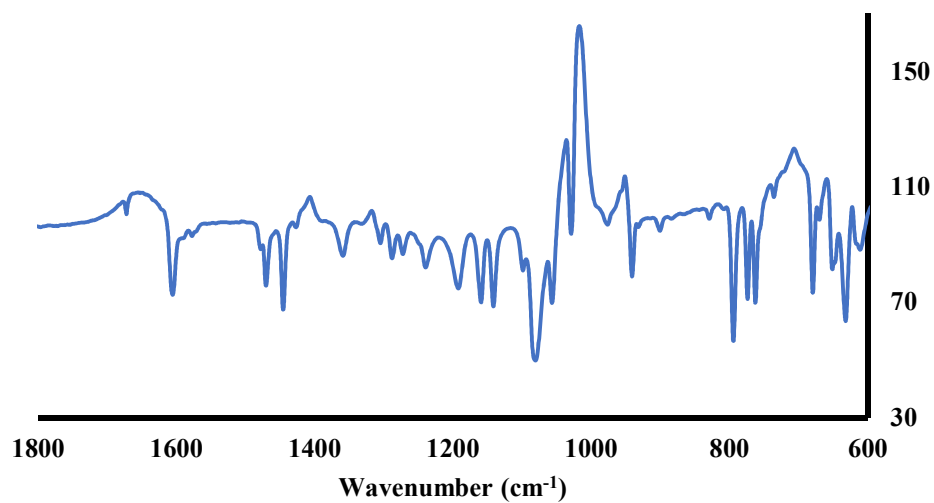


Figure S8. IR spectrum of Zn-2.

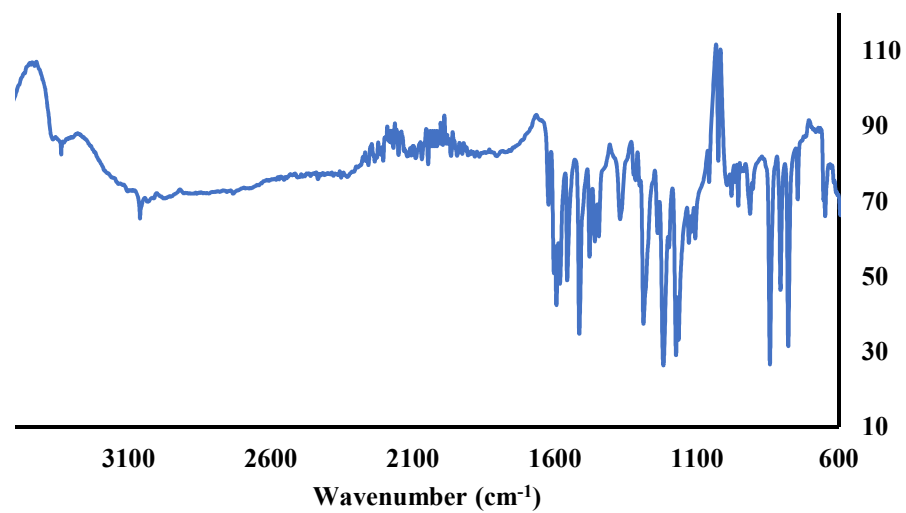


Figure S9. IR spectrum of Zn-3.

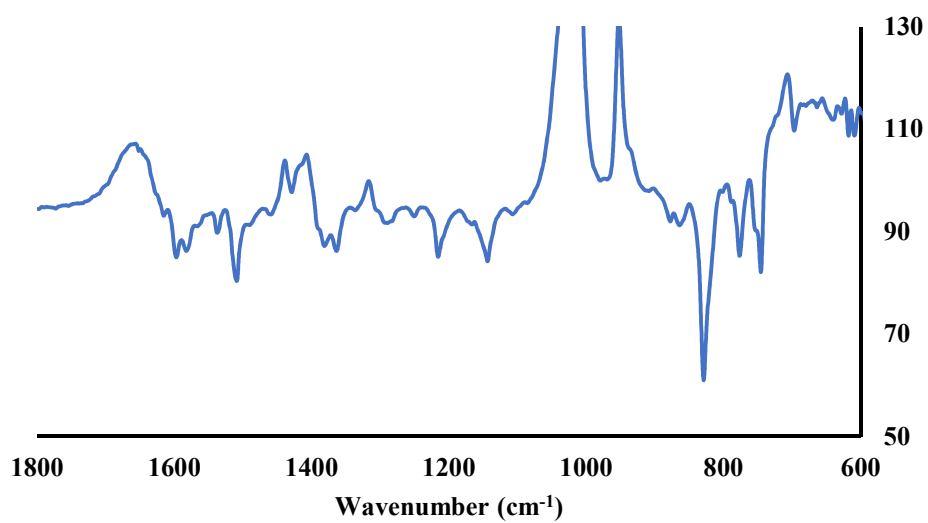


Figure S10. IR spectrum of Pt-1.

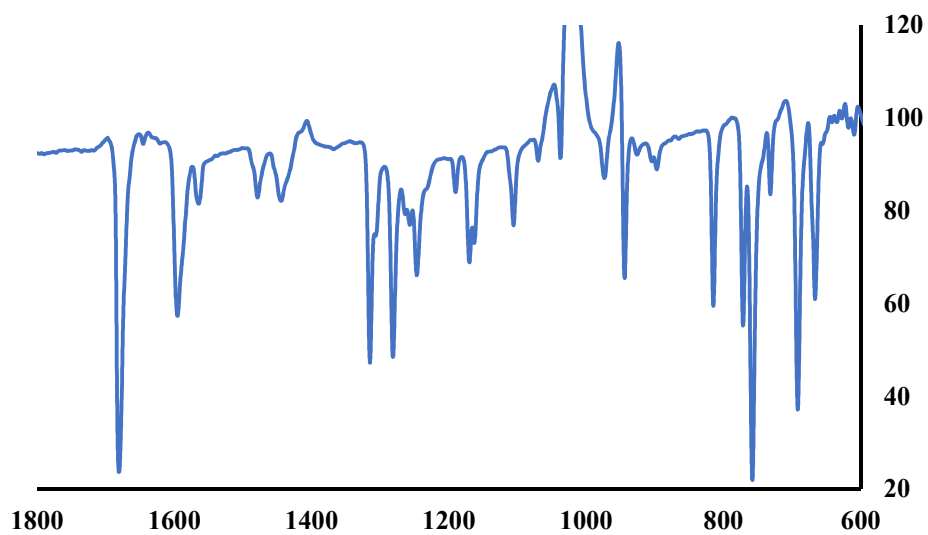


Figure S11. IR spectrum of Pt-2.

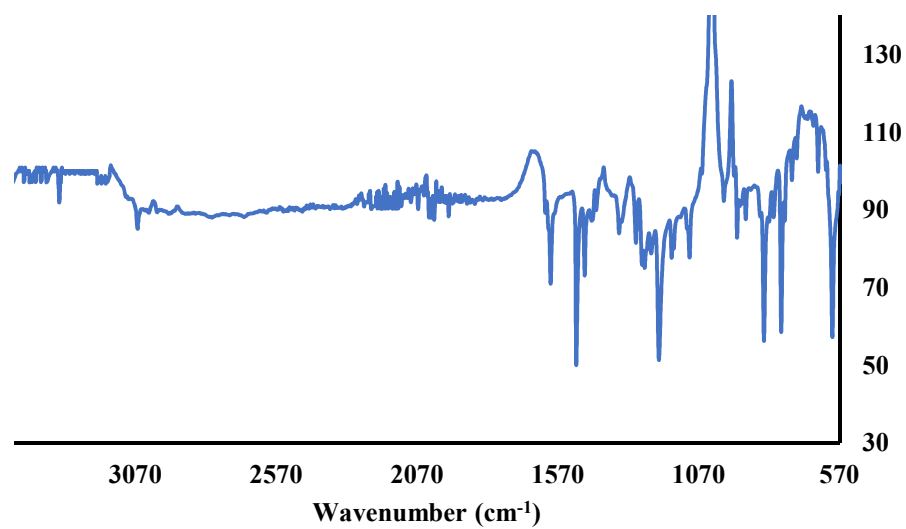


Figure S12. IR spectrum of Pt-3.

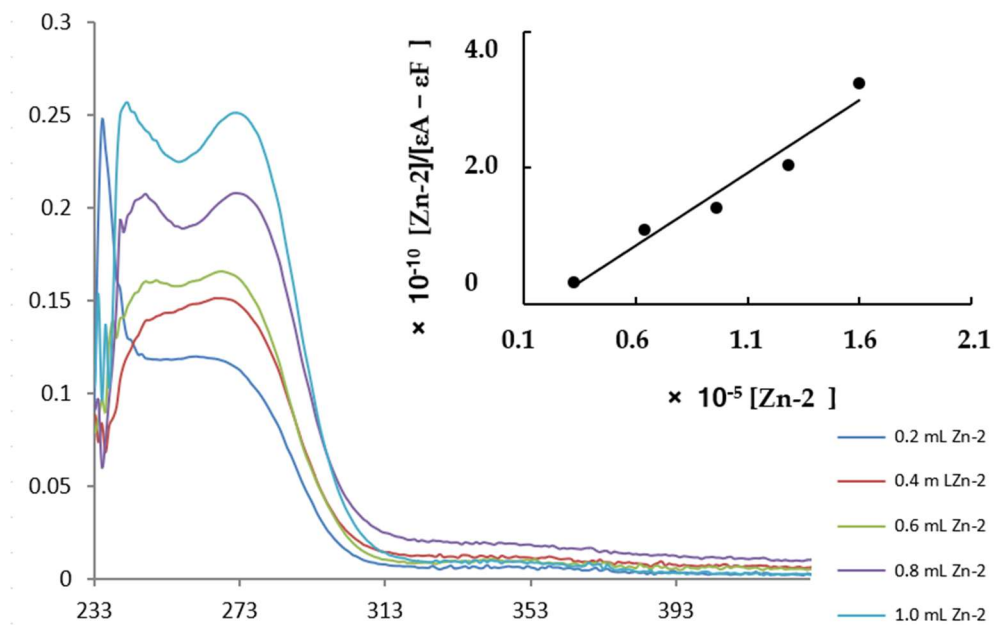


Figure S13. DNA binding studies of Zn-2.

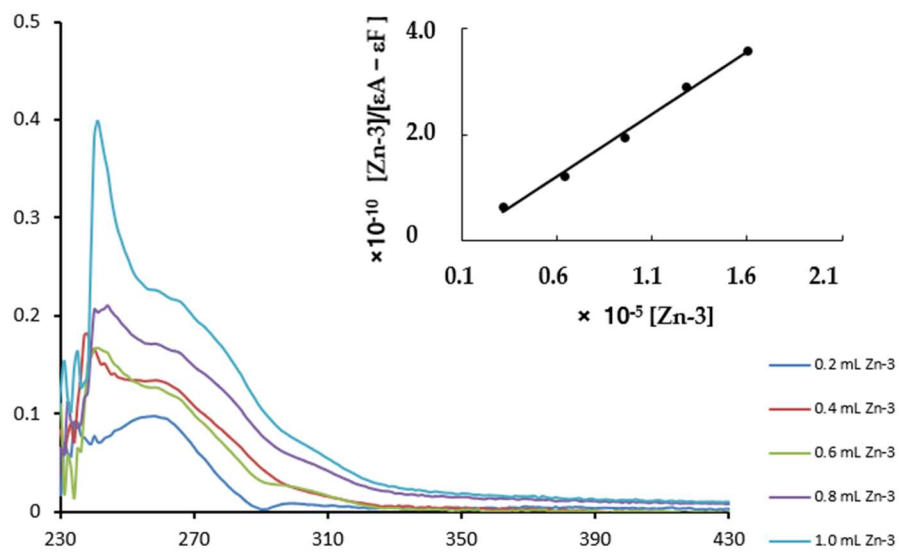


Figure S14. DNA binding studies of Zn-3.

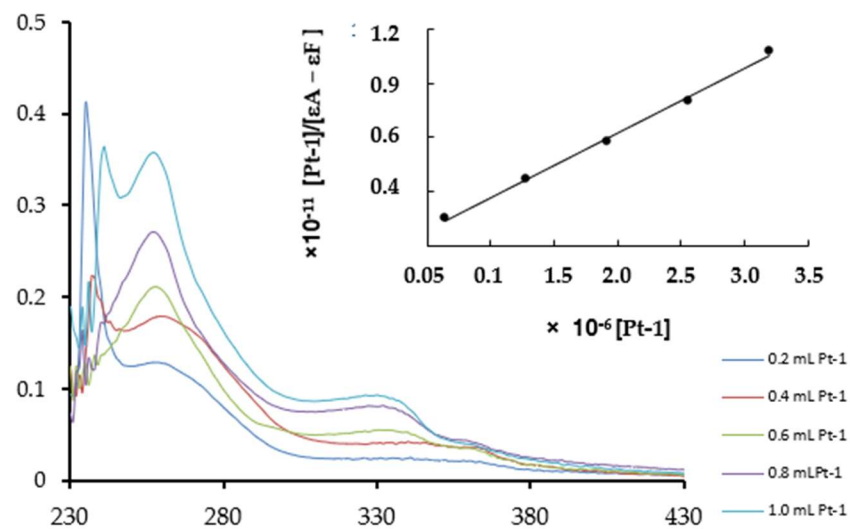


Figure S15. DNA binding studies of Pt-1.

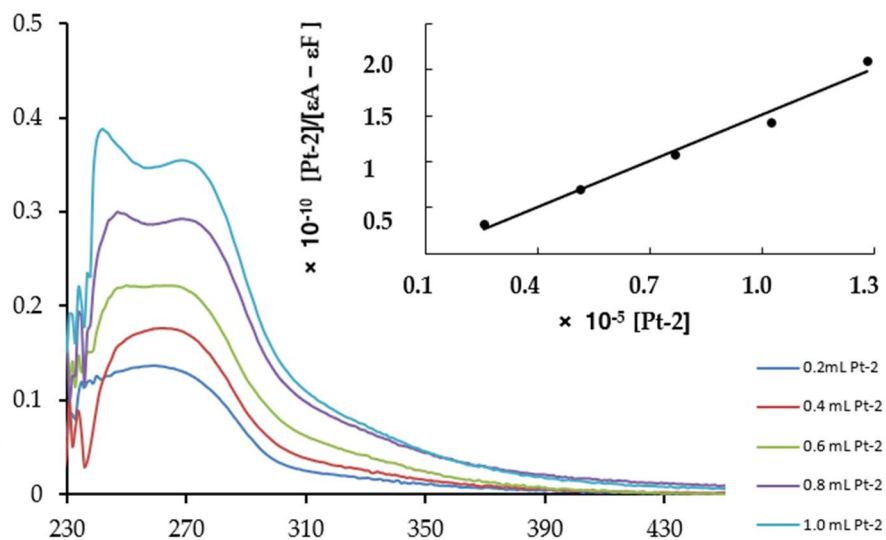


Figure S16. DNA binding studies of Pt-2.

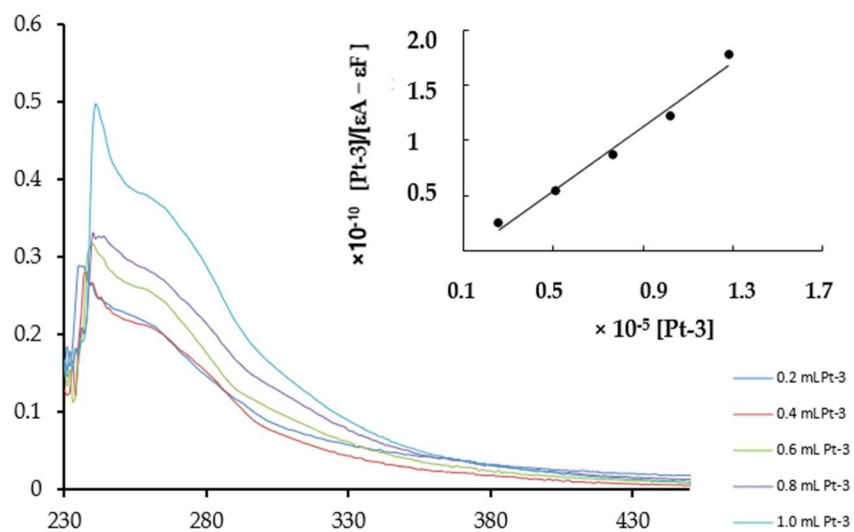


Figure S17. DNA binding studies of Pt-3.

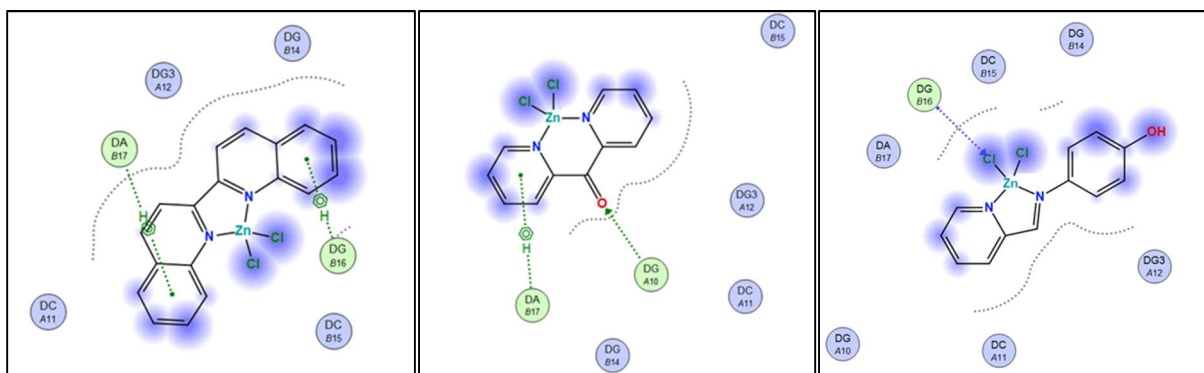


Figure S18. 2D illustration of DNA-zinc complexes adducts as obtained by molecular docking.

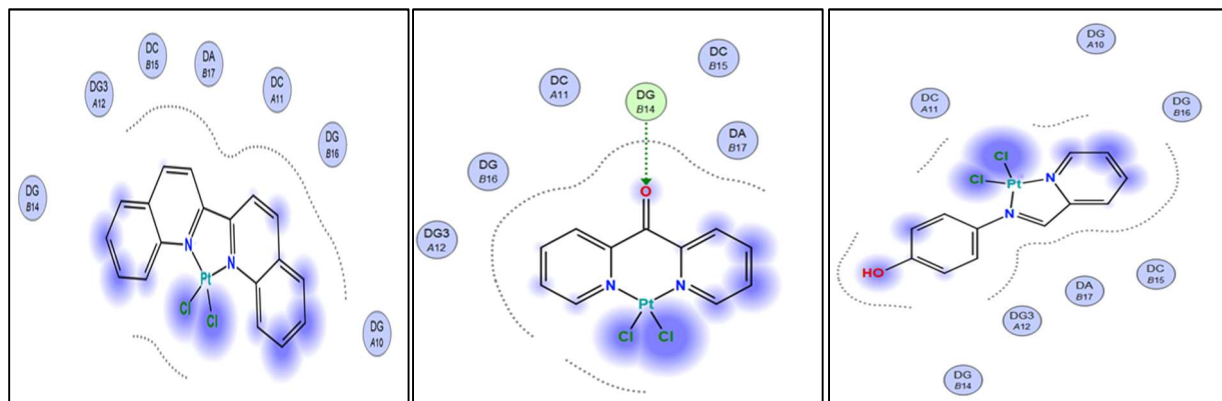


Figure S19. 2D illustration of DNA-zinc complexes adducts as obtained by molecular docking.