Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

Mononuclear Co(II) polypyridyl complexes: synthesis, molecular structure, DNA binding/cleavage, radical scavenging, docking studies and anticancer activities

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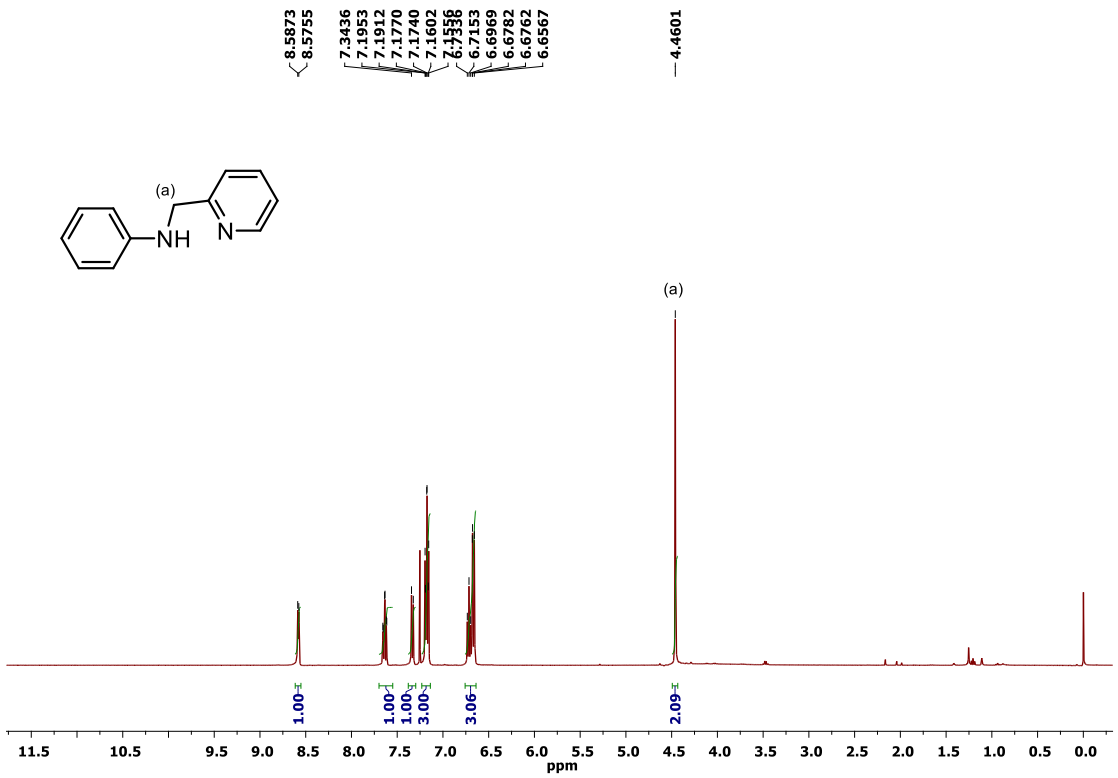


Fig. S1. ^{1}H NMR of N-(pyridin-2-ylmethyl)aniline in $CDCl_3$ at room temperature.

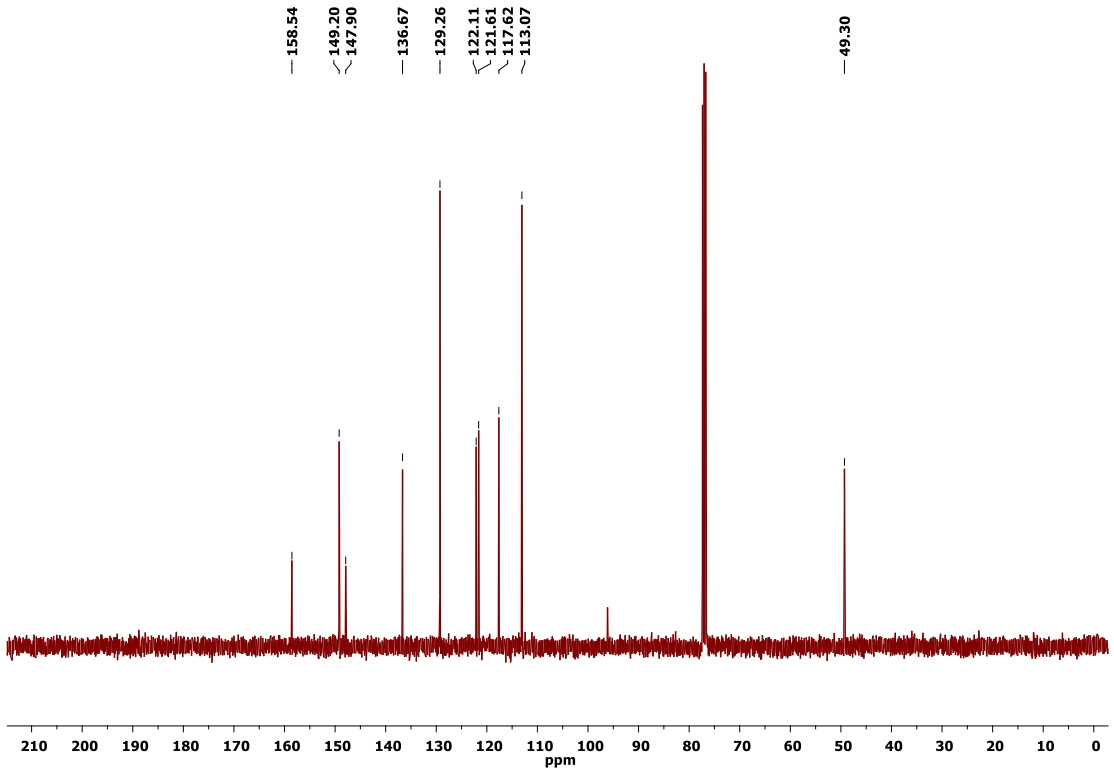


Fig. S2. ^{13}C NMR of N-(pyridin-2-ylmethyl)aniline in $CDCl_3$ at room temperature.

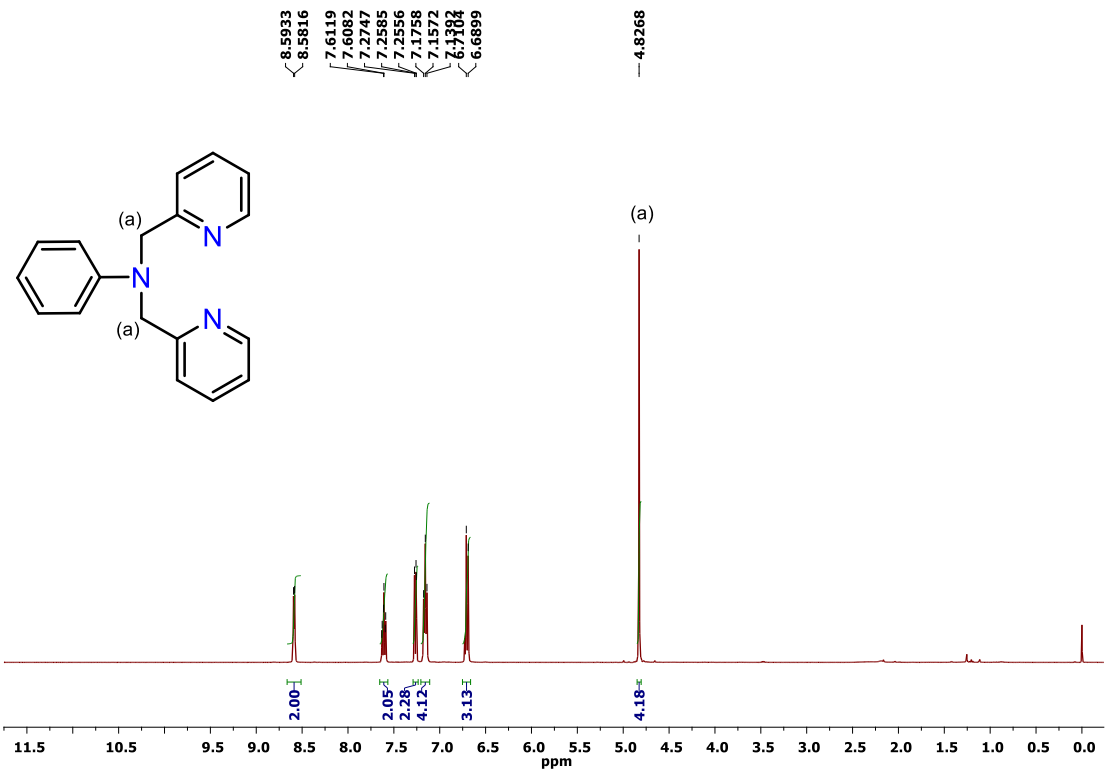


Fig. S3. ^{1}H NMR of **L** in $CDCl_3$ at room temperature.

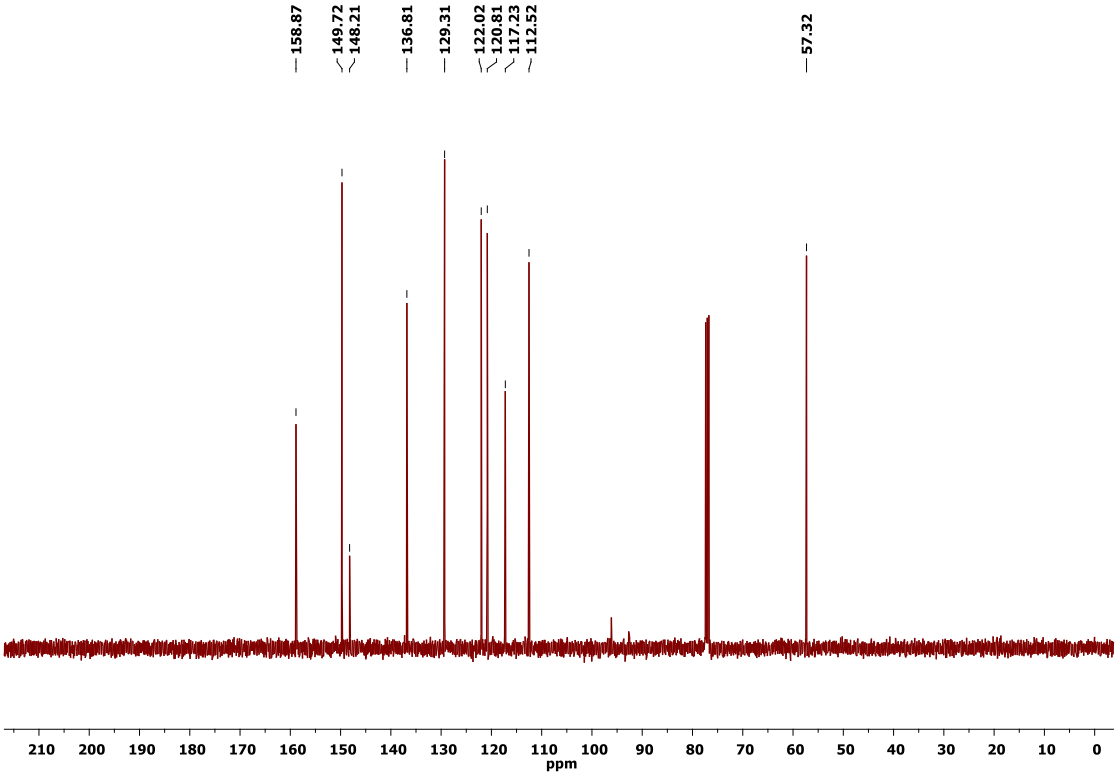


Fig. S4. ^{13}C NMR of **L** in $CDCl_3$ at room temperature.

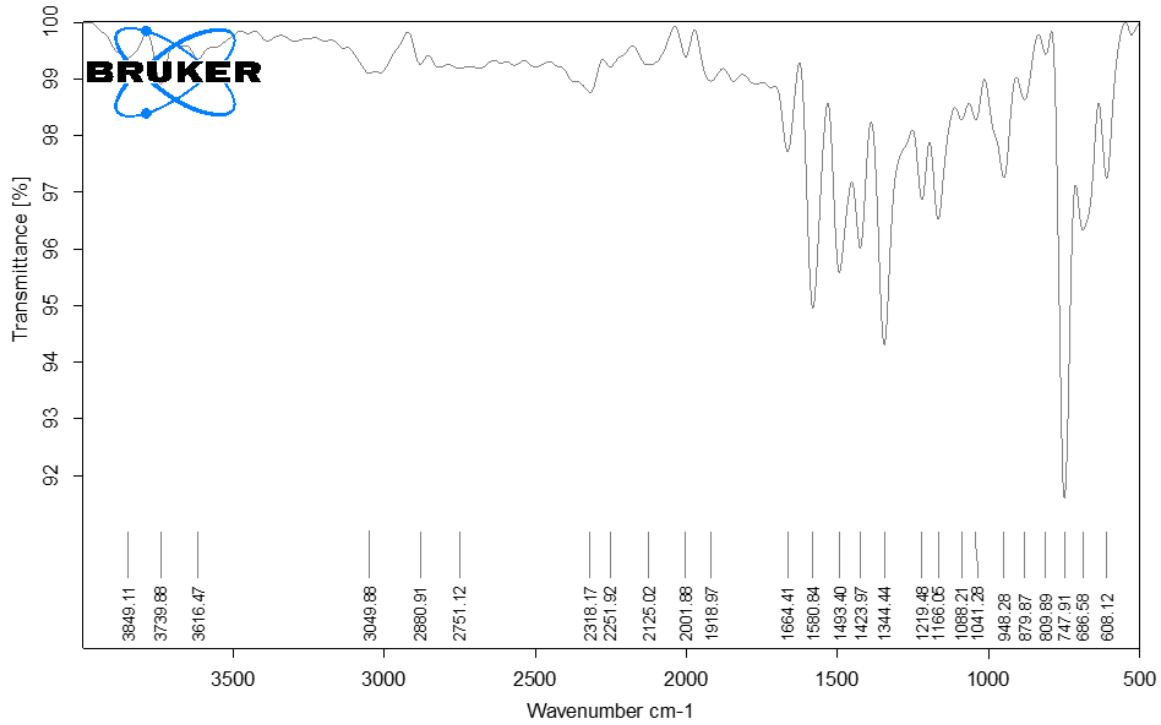


Fig. S5. FT–IR (Solid) spectrum of **L**.

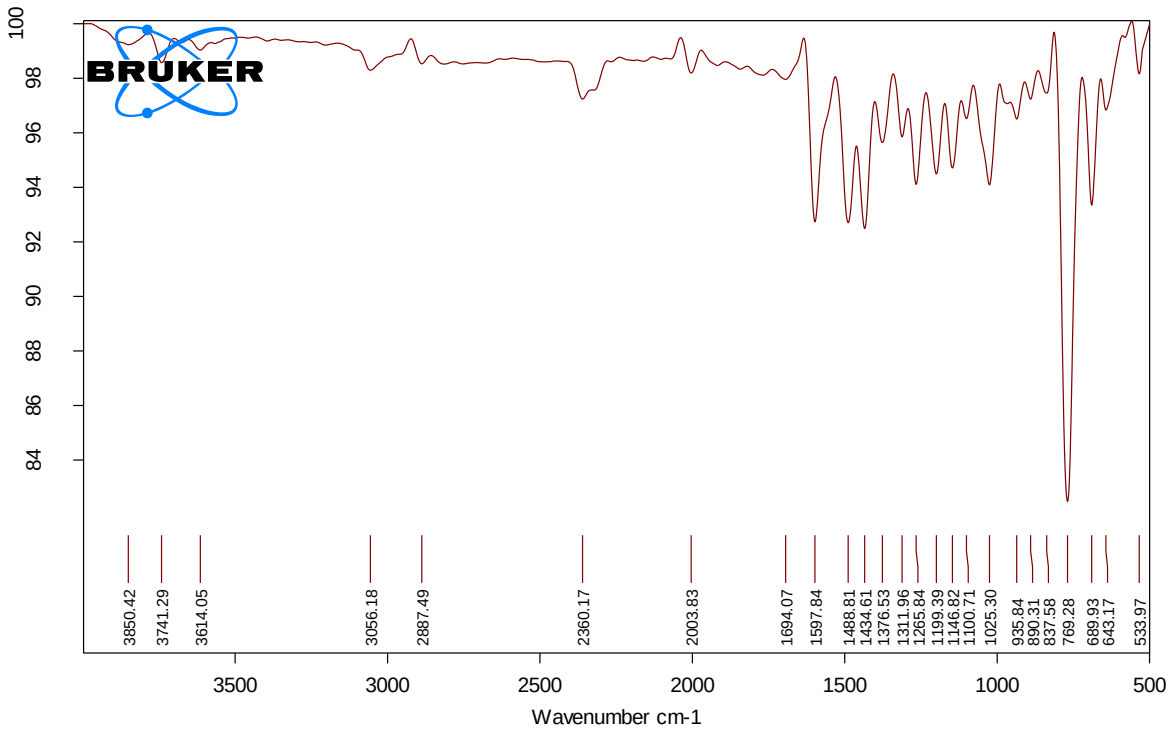


Fig. S6. FT–IR (Solid) spectrum of **1**.

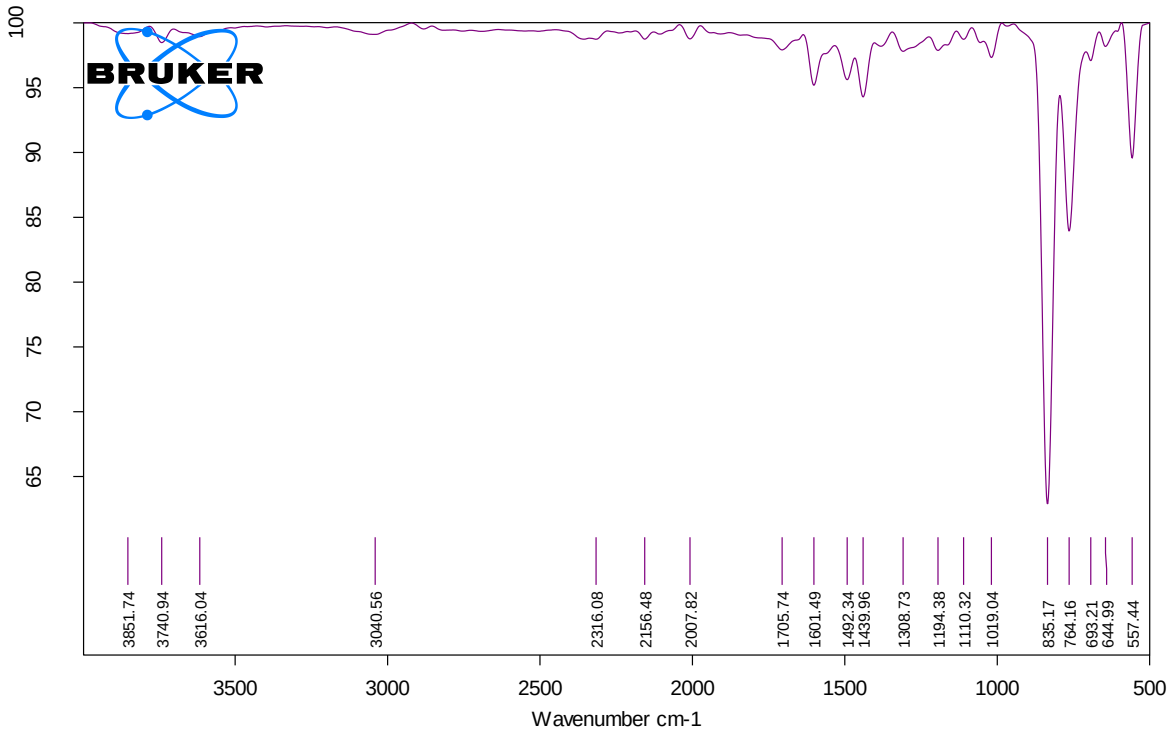


Fig. S7. FT–IR (Solid) spectrum of **2**.

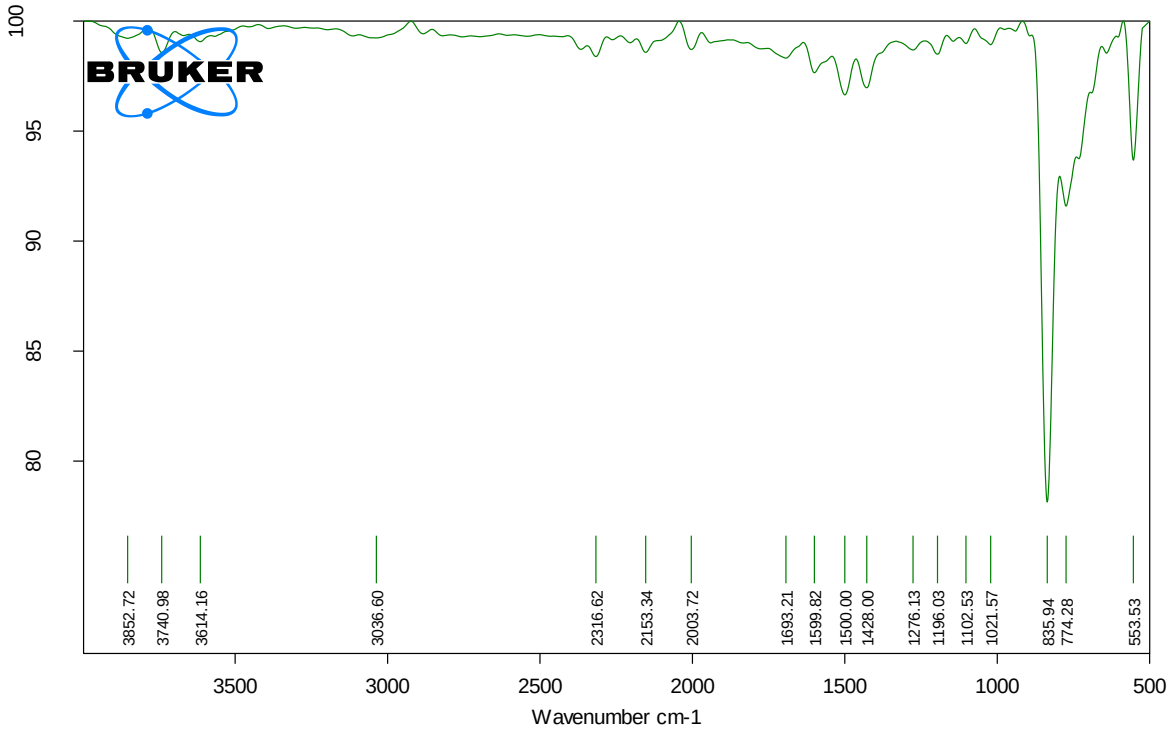


Fig. S8. FT–IR (Solid) spectrum of **3**.

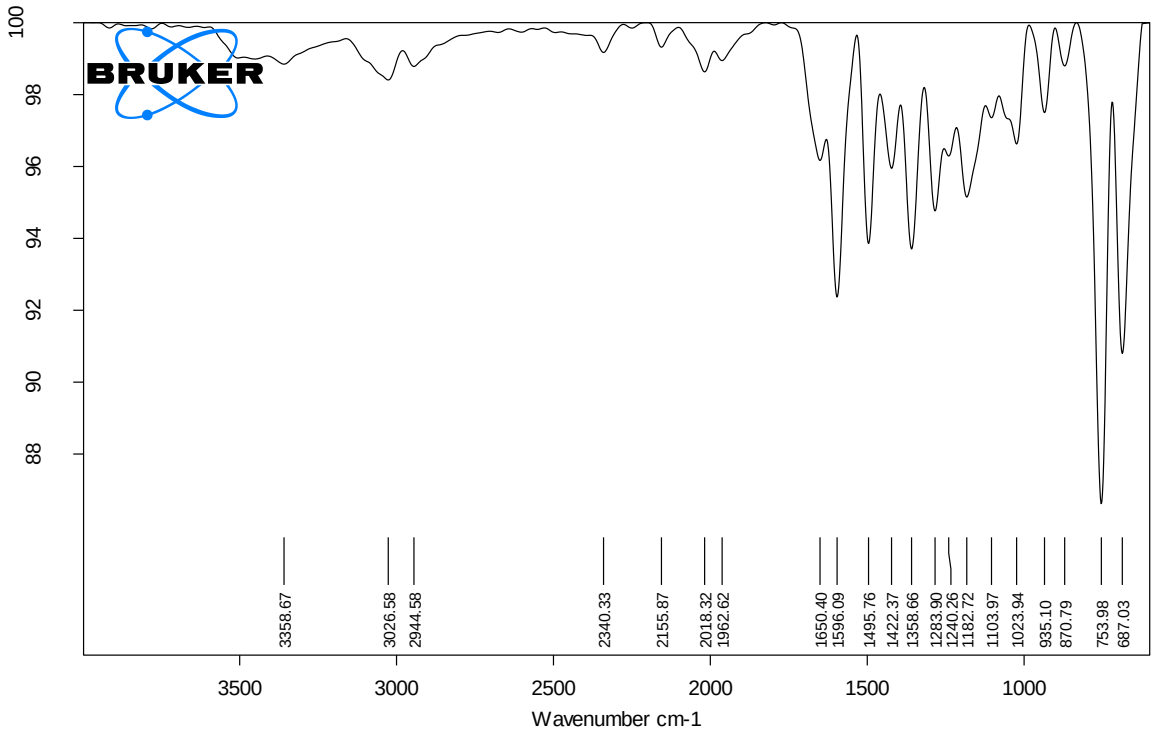
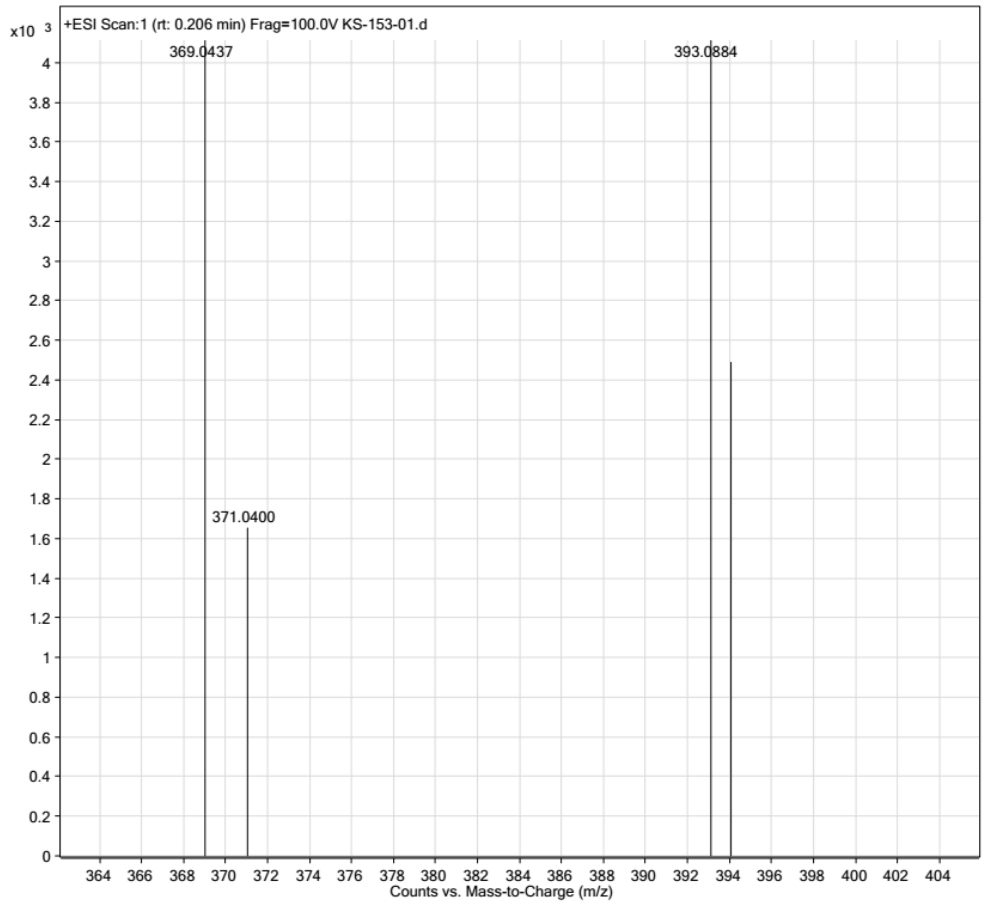


Fig. S9. FT–IR (Solid) spectrum of **4**.



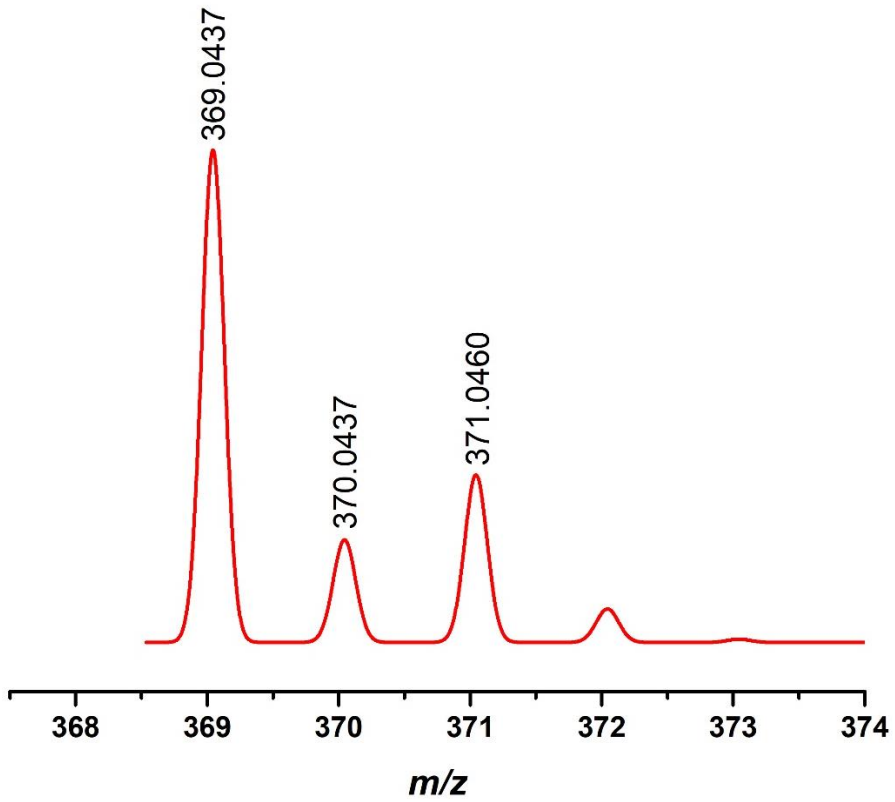


Fig. S10. HRMS spectrum of **1** (top) with their simulated mass spectra (bottom).

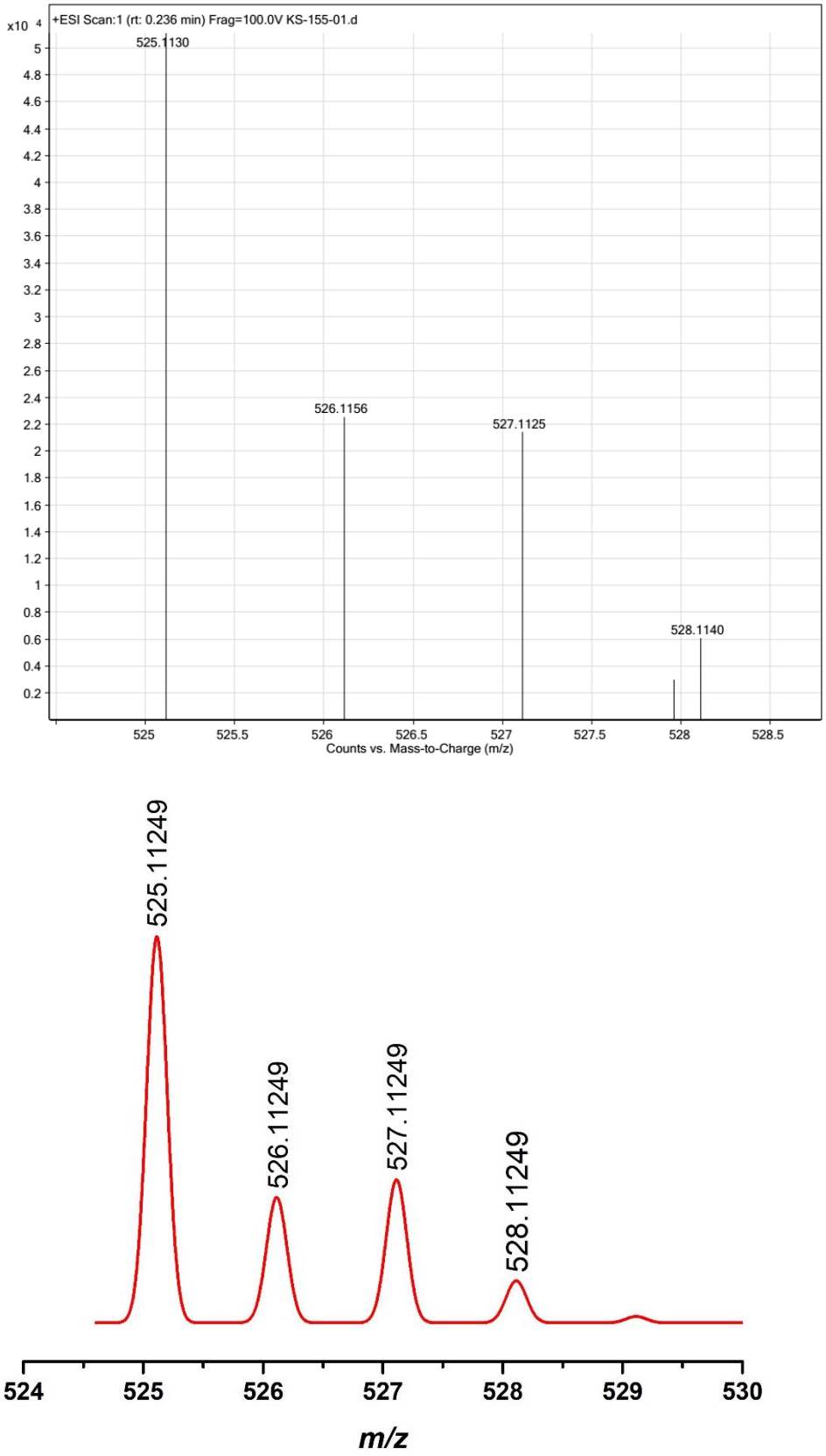
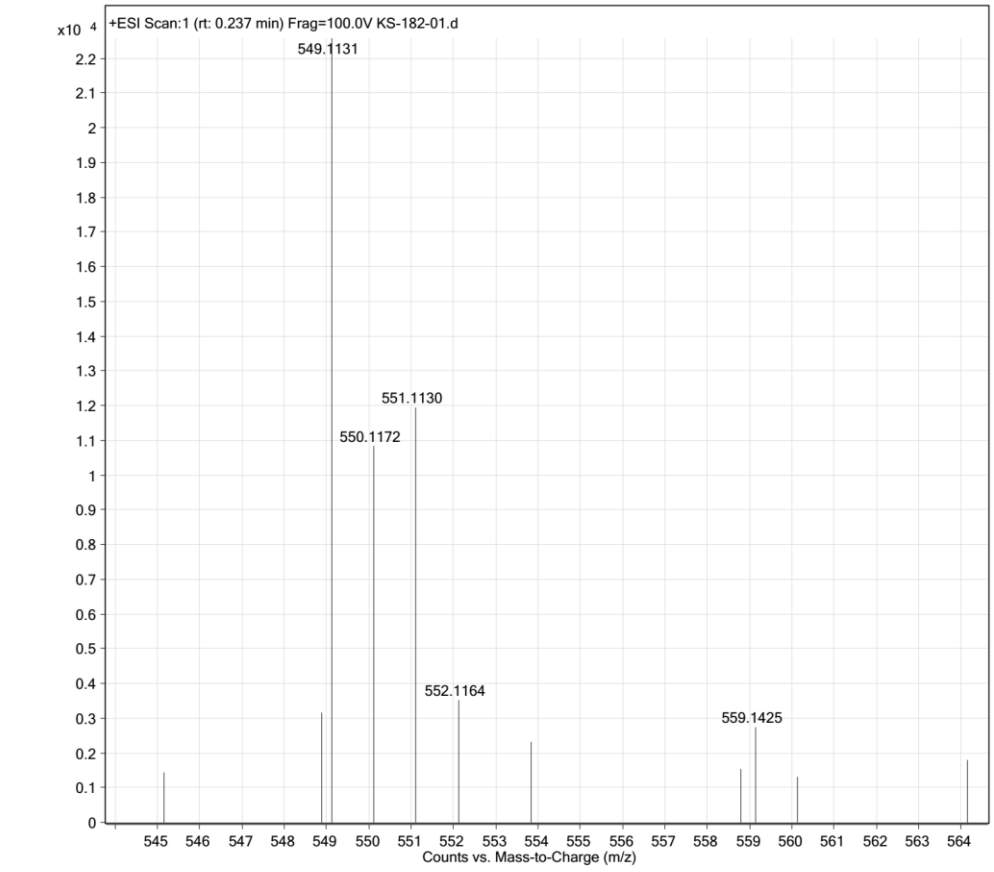


Fig. S11. HRMS spectrum of **2** (top) with their simulated mass spectra (bottom).



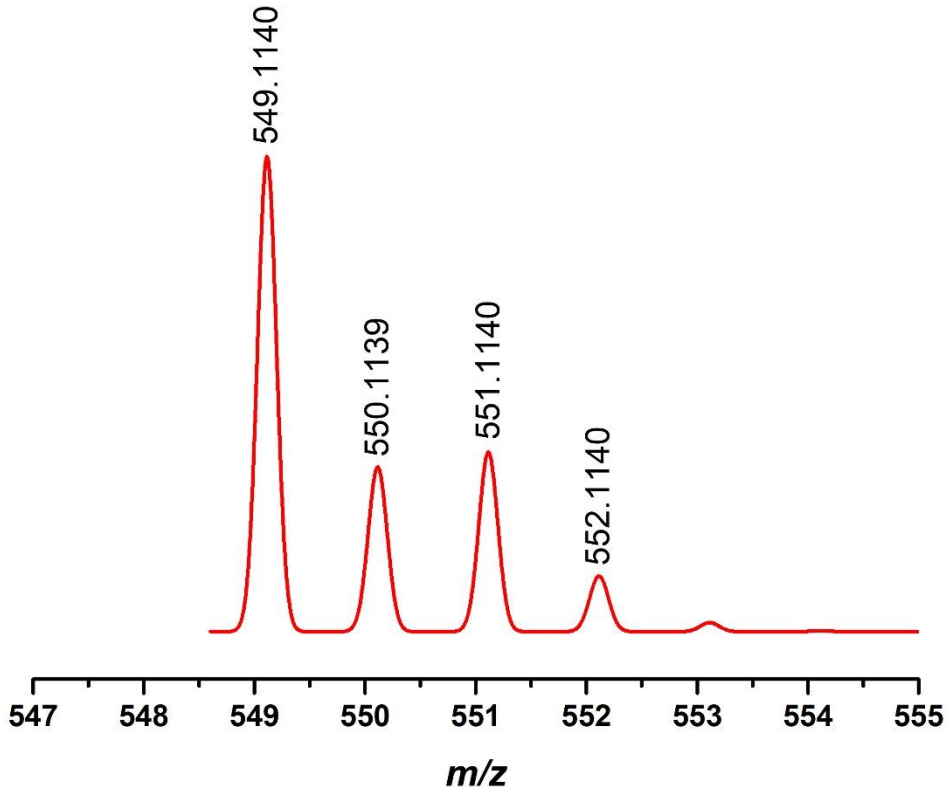


Fig. S12. HRMS spectrum of **3** (top) with their simulated mass spectra (bottom).

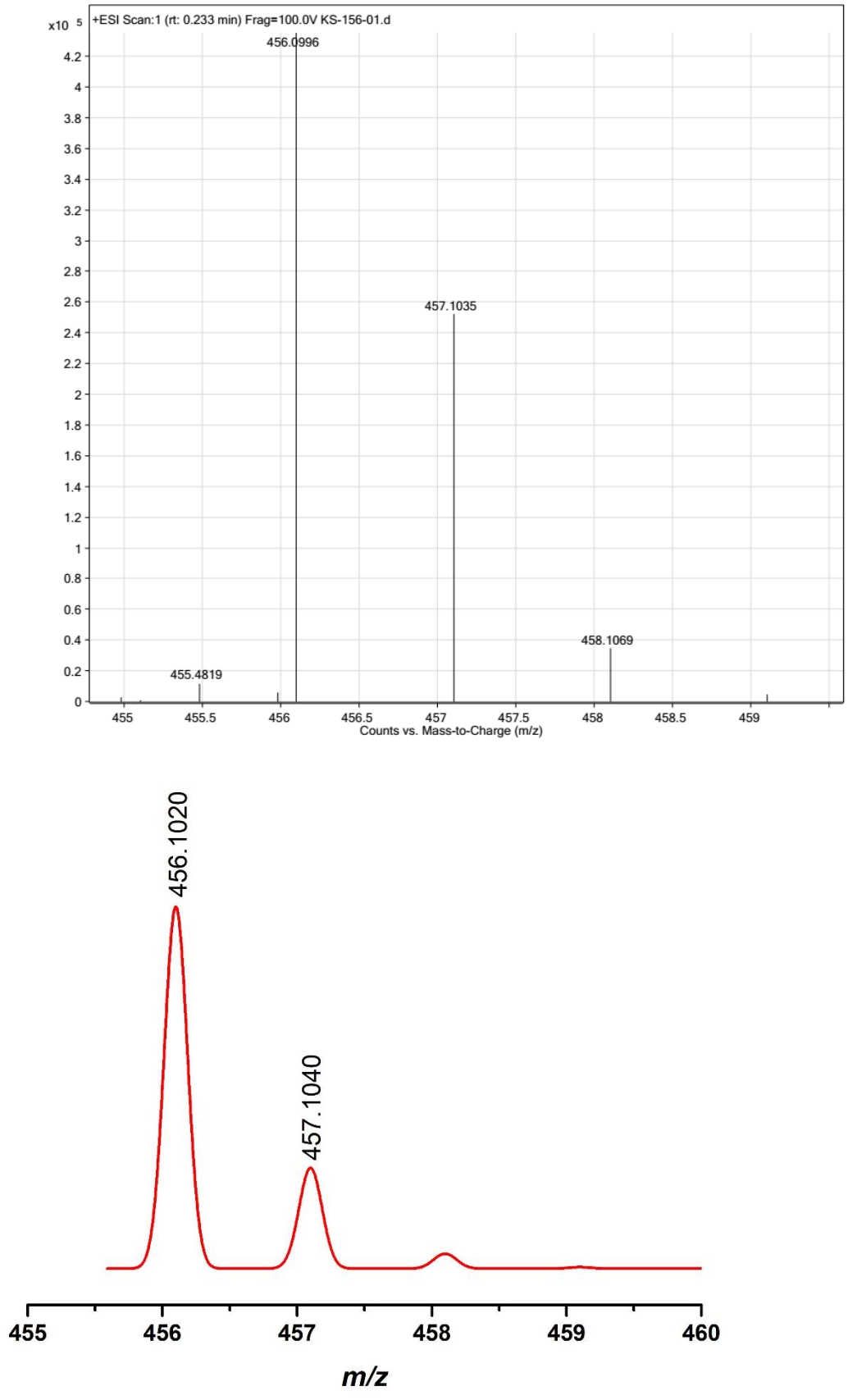


Fig. S13. HRMS spectrum of **4** (top) with their simulated mass spectra (bottom).

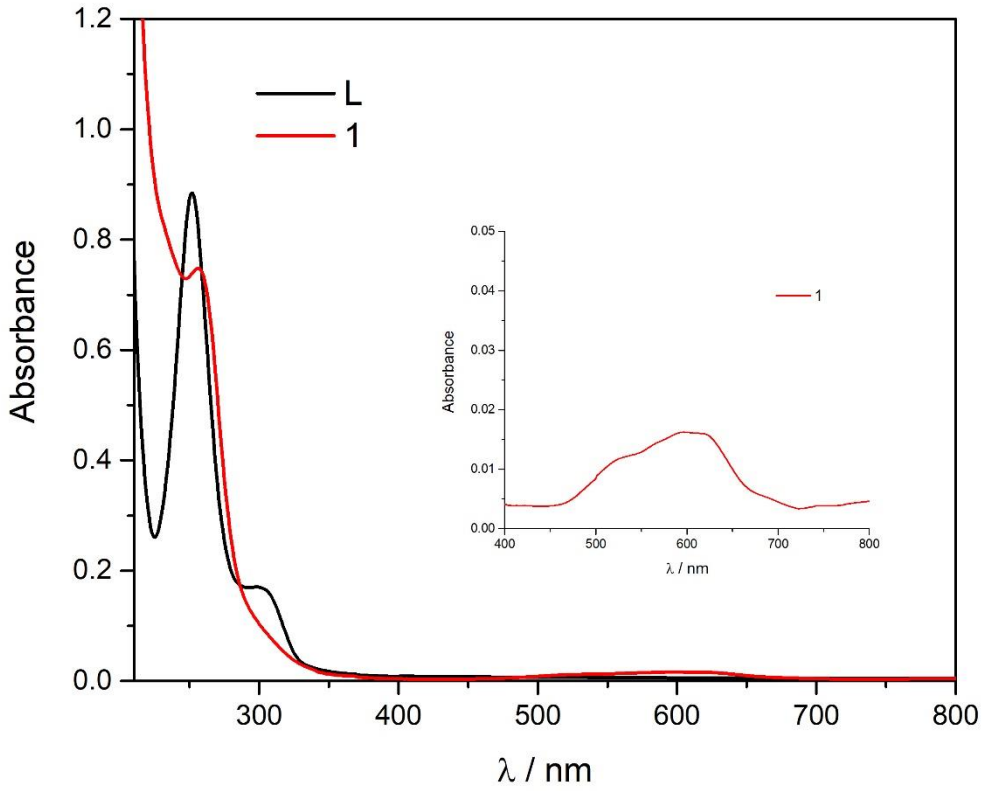


Fig. S14. UV–vis spectrum of **L** and complexes **1** in acetonitrile.

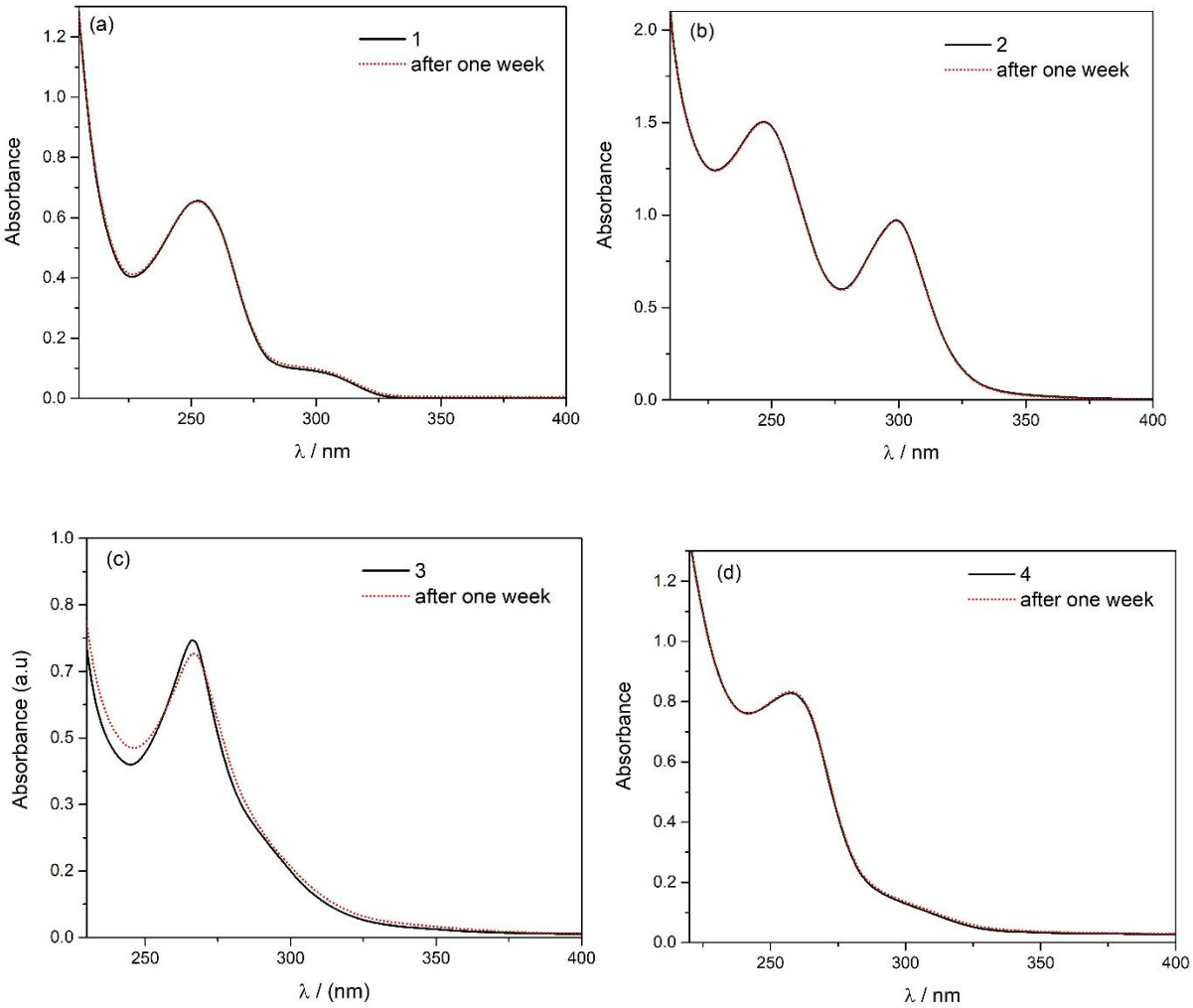


Fig. S15. (a-d) Time dependent UV–vis spectrum of complexes **1-4** in 5 mM Tris-HCl buffer (pH = 7.2) at room temperature.

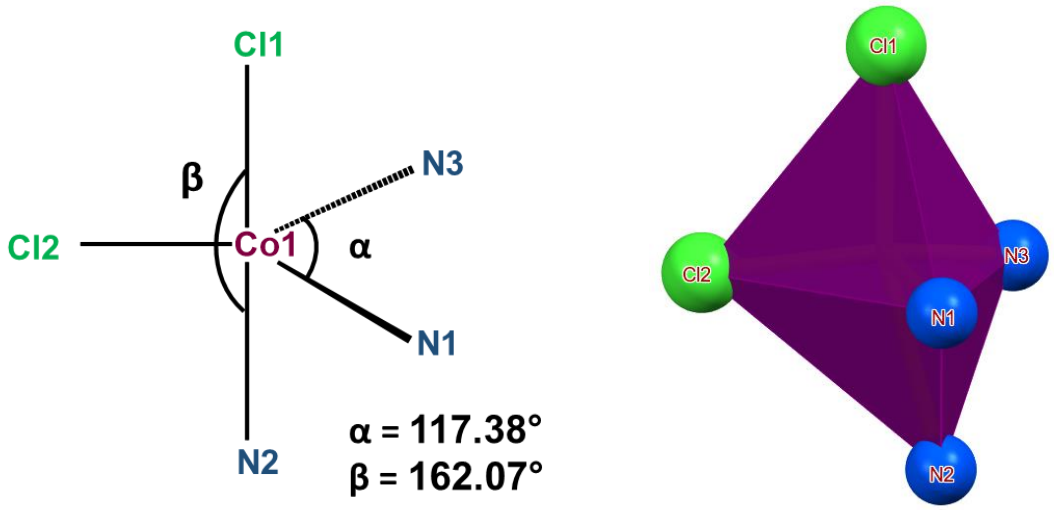
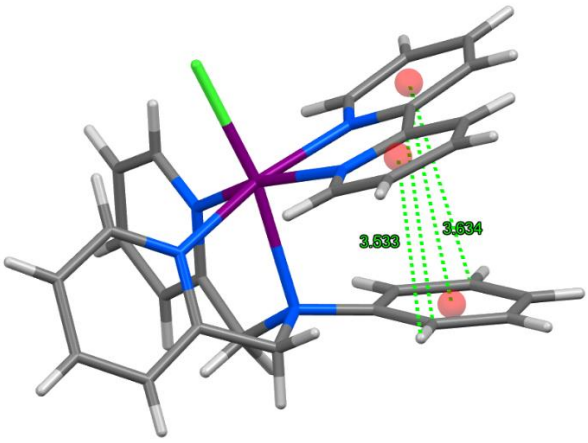
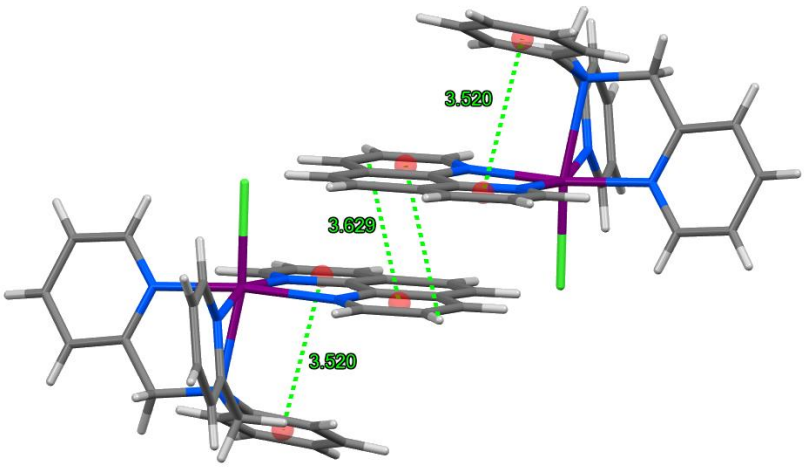


Fig. S16. Schematic drawing of trigonal bipyramidal geometry and polyhedron view of **1**.

a



b



c

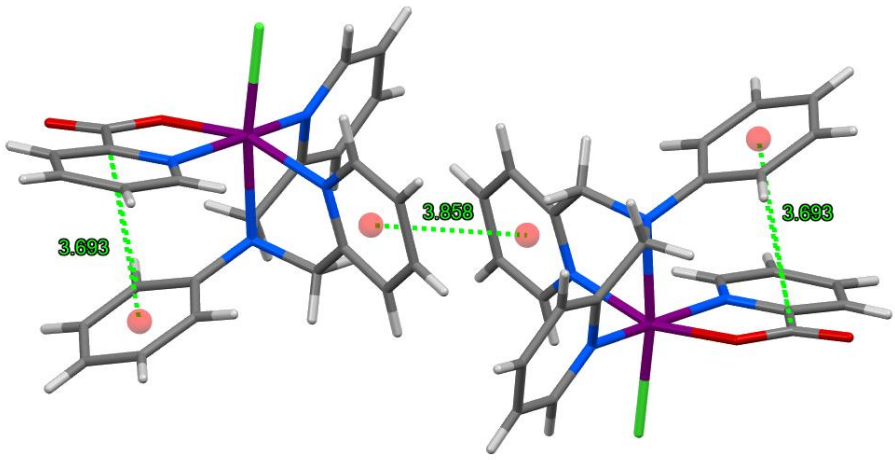


Fig. S17. (a-c) π–π interaction between phenyl group of ligand **L** and bidentate ligands (bpy, phen, pic) in complexes **2**-**4**, respectively.

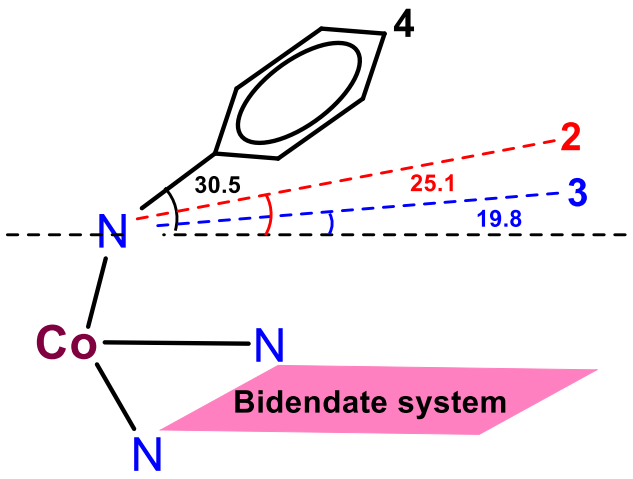


Fig. S18. Schematic drawing of **2–4** with the dihedral angles (°) benzene ring of **L** and the plane of the bidentate ligand system (bpy, phen and pic).

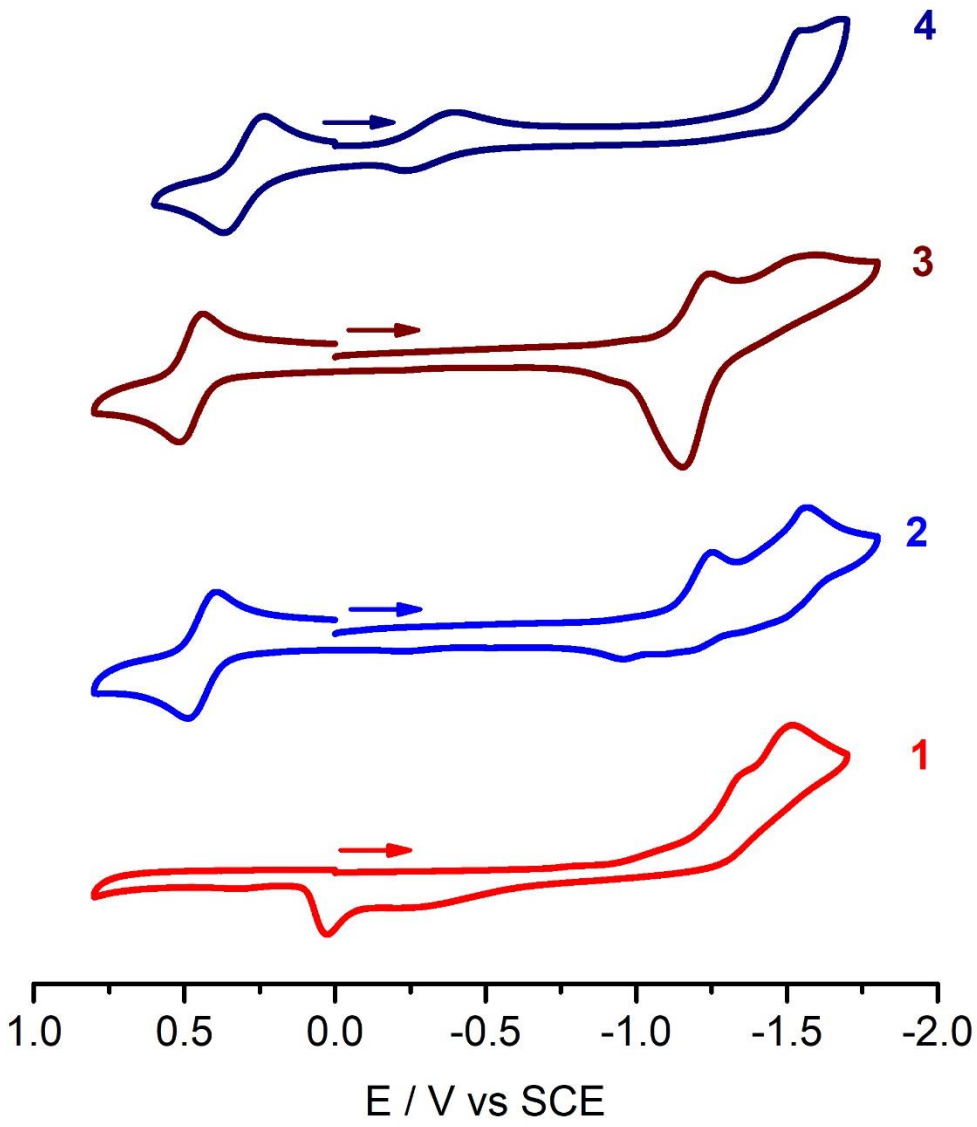


Fig. S19. Cyclic voltammogram of **1–4** (bottom to top) in acetonitrile using 0.1 M TBAP as supporting electrolyte versus SCE, scan rate 100 mV s^{-1}.

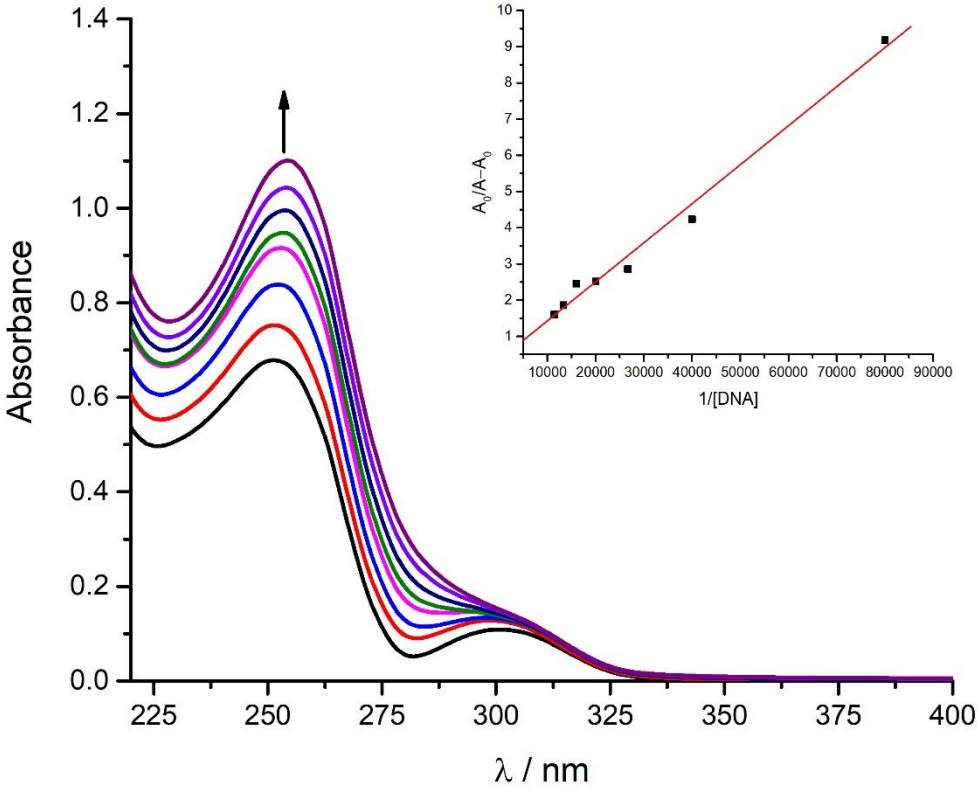


Fig. S20. Absorption spectra of **1** (66.7 μM) in the absence (black) and presence (colour) of ss-DNA (12.5, 25.0, 37.5, 50.0, 62.50, 75.0, 87.5 μM, respectively) in 5 mM Tris-HCl buffer (pH =7.2). The arrow shows the absorbance changes on increasing DNA concentration. Inset: the plot of $A_0/A–A_0$ versus 1/[DNA] for the calculation of binding constant of complex **1**.

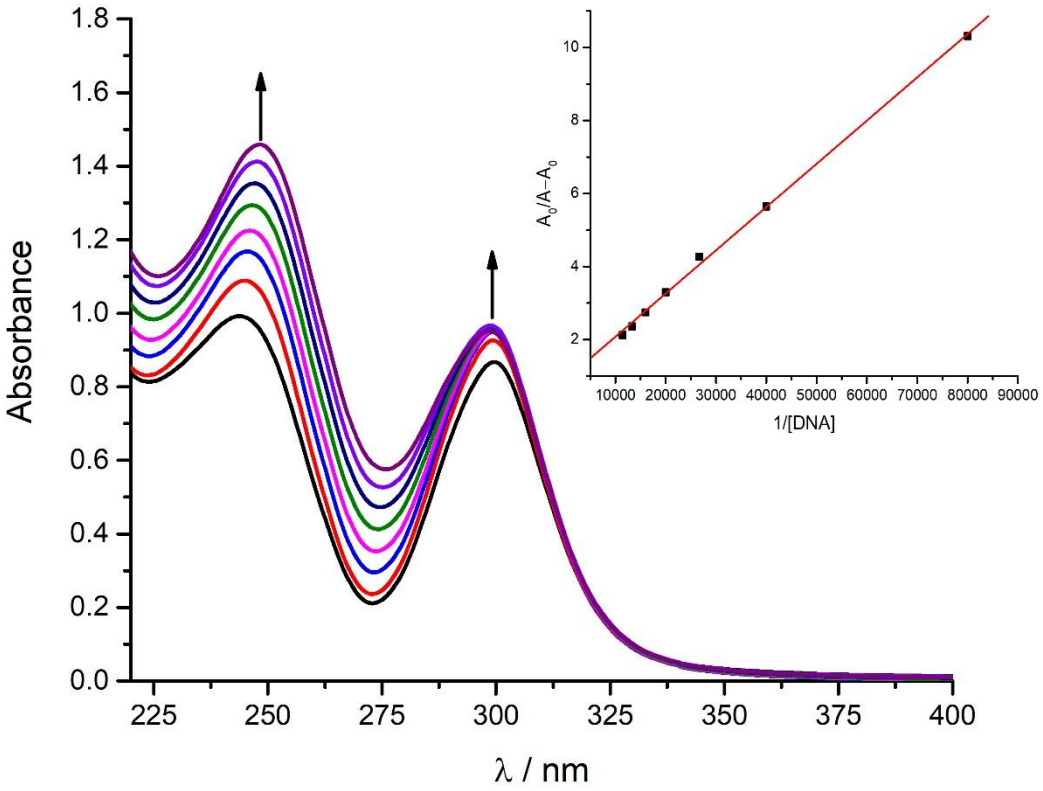


Fig. S21. Absorption spectra of **2** (66.7 μM) in the absence (black) and presence (colour) of ss-DNA (12.5, 25.0, 37.5, 50.0, 62.50, 75.0, 87.5 μM, respectively) in 5 mM Tris-HCl buffer (pH =7.2). The arrow shows the absorbance changes on increasing DNA concentration. Inset: the plot of $A_0/A–A_0$ versus 1/[DNA] for the calculation of binding constant of complex **2**.

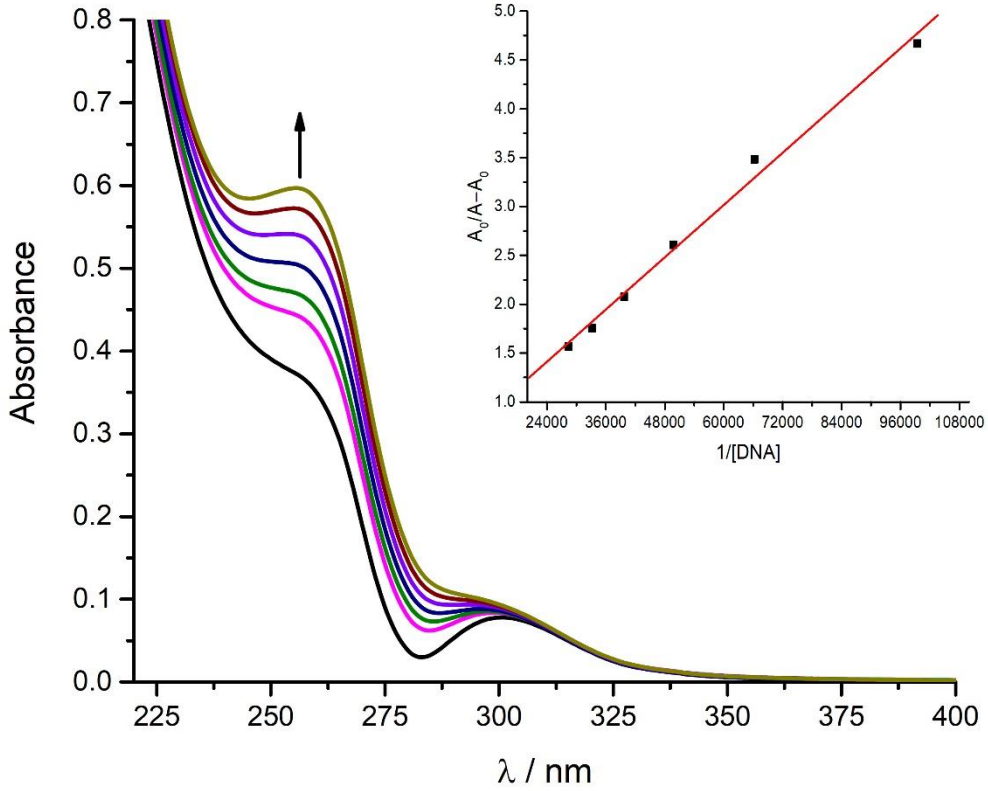


Fig. S22. Absorption spectra of **4** (20 μM) in the absence (black) and presence (colour) of ss-DNA (10.06, 15.09, 20.12, 25.15, 30.18, 35.21 μM, respectively) in 5 mM Tris-HCl buffer (pH =7.2). The arrow shows the absorbance changes on increasing DNA concentration. Inset: the plot of $A_0/A–A_0$ versus 1/[DNA] for the calculation of binding constant of complex **4**.

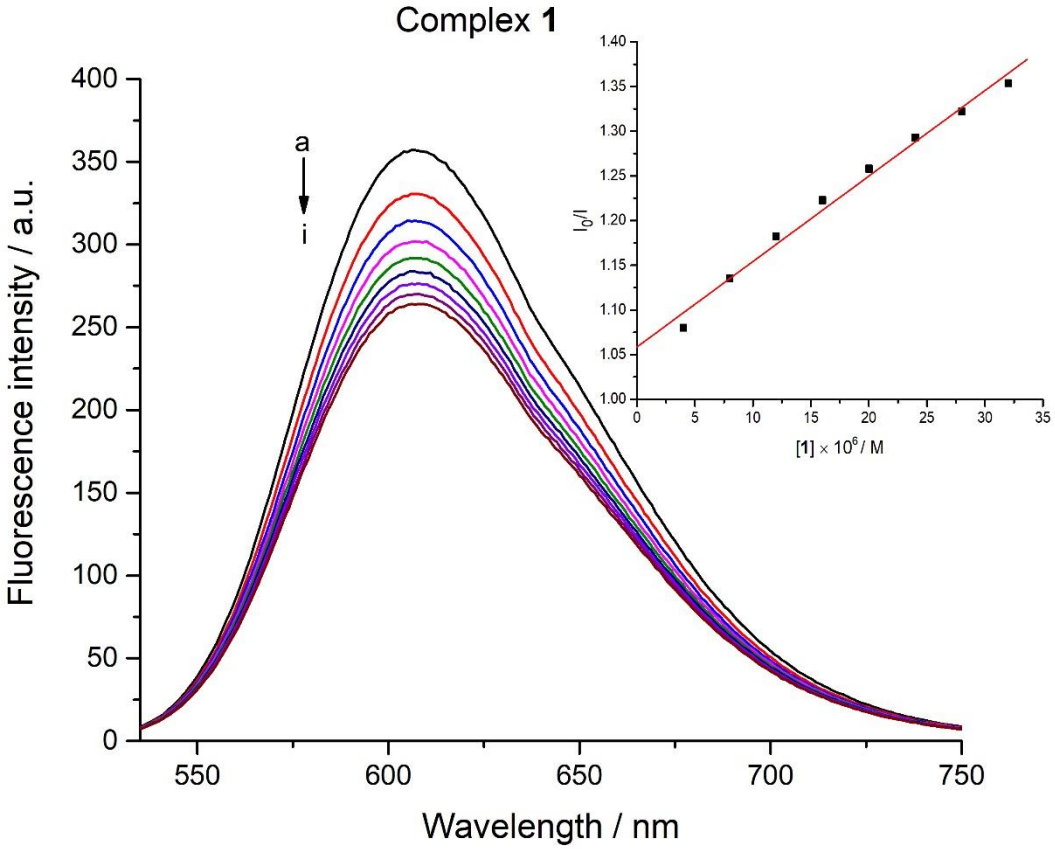


Fig. S23. Emission spectra of EB bound DNA in the presence of **1**. ([DNA] = 1 ×10^{-4} M, [EB] = 1 ×10^{-5} M, [Quencher](μM) for **1**: (a) 0, (b) 4, (c) 8, (d) 12, (e) 16, (f) 20, (g) 24, (h) 28, (i) 32. Inset: the plot of I_0/I versus [Quencher].

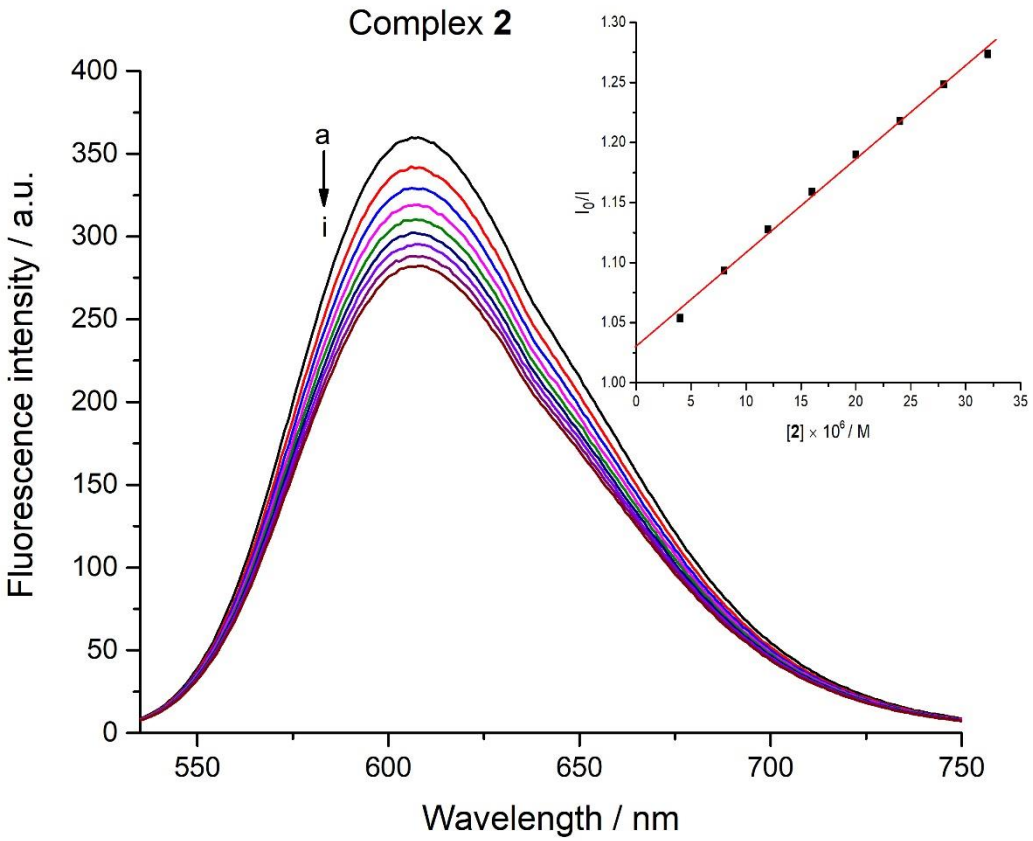


Fig. S24. Emission spectra of EB bound DNA in the presence of **2**. ([DNA] = 1×10^{-4} M, [EB] = 1×10^{-5} M, [Quencher](μM) for **1**: (a) 0, (b) 4, (c) 8, (d) 12, (e) 16, (f) 20, (g) 24, (h) 28, (i) 32. Inset: the plot of I_0/I versus [Quencher].

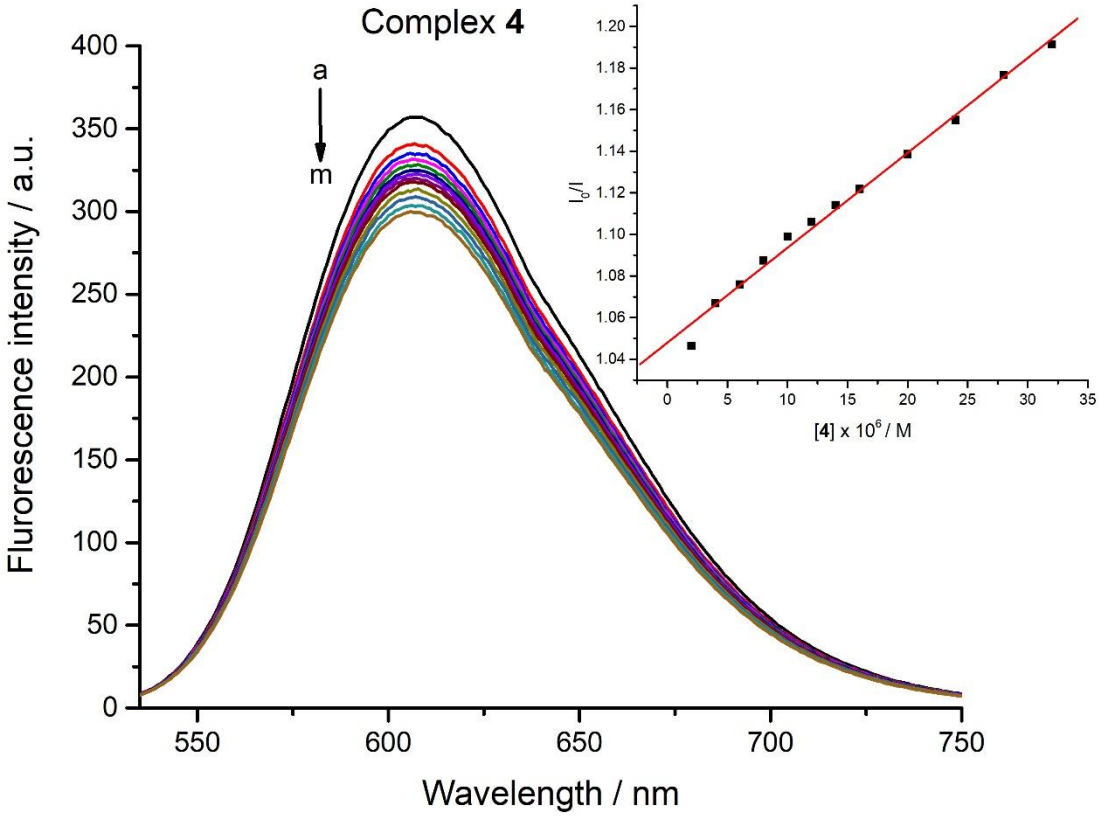


Fig. S25. Emission spectra of EB bound DNA in the presence of **4**. ([DNA] = 1×10^{-4} M, [EB] = 1×10^{-5} M, [Quencher](μM) for **1**: (a) 2, (b) 4, (c) 6, (d) 8, (e) 10, (f) 12, (g) 14, (h) 16, (i) 20, (j) 24, (k) 28, (m) 32. Inset: the plot of I_0/I versus [Quencher].

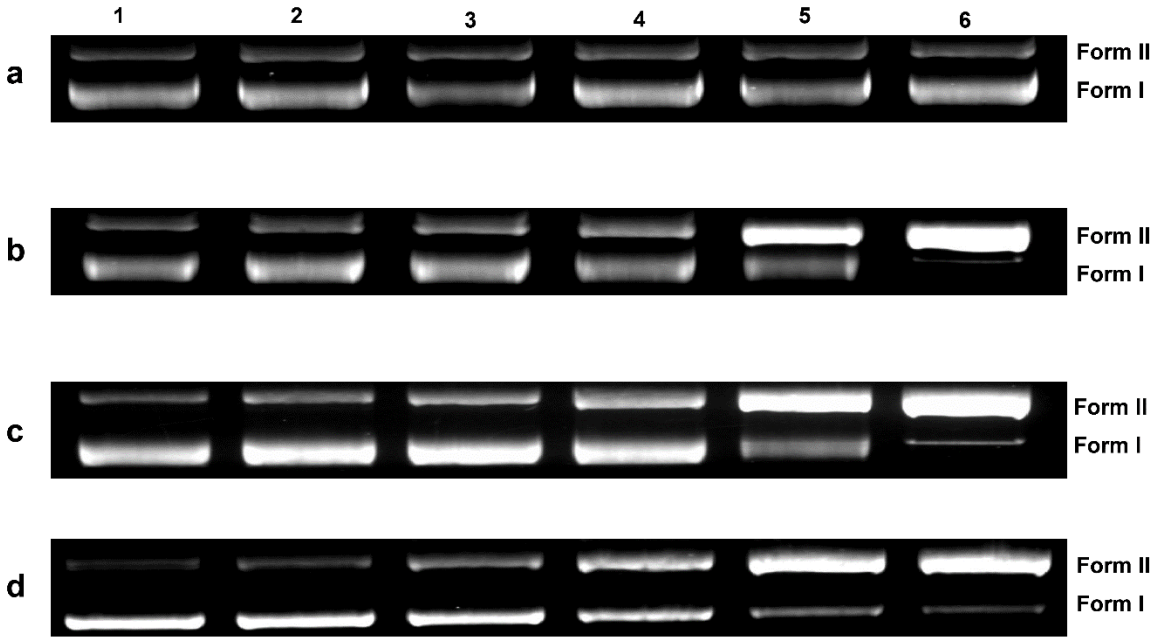
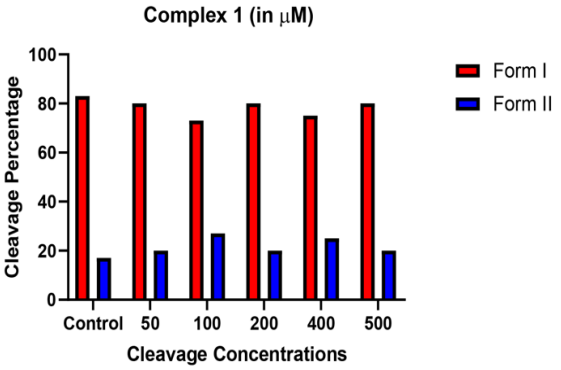


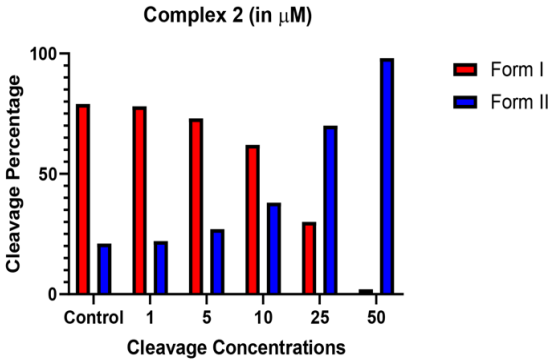
Fig. S26: Agarose gel showing the cleavage of plasmid DNA (pDNA 200 ng/μL) at different concentrations upon incubation at 37 °C for 3 h in 50 mM Tris-HCl buffer (pH 7.2). Lane 1: Control; Lane 2-6: pDNA + Complexes [(a) Complex **1**: 50 μM, 100 μM, 200 μM, 400 μM, 500 μM; (b-c) Complexes **2** and **3**: 1 μM, 5 μM, 10 μM, 25 μM, 50 μM; (d) Complex **4**: 100 μM, 250 μM, 500 μM, 750 μM, 1 mM].

Table S1: Respective Cleavage Concentrations (**1**-**4**) and Percentage of Cleaved Forms of pDNA.

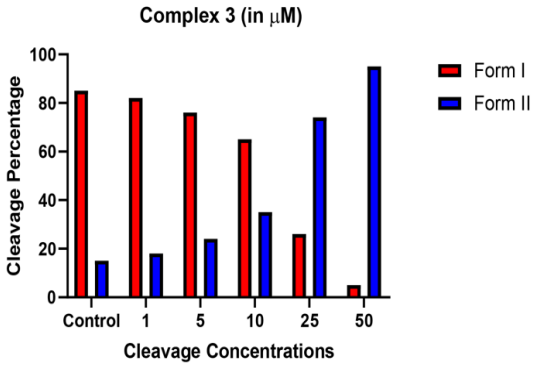
Complex 1			
S.No.	**Concentrations (μM)**	**Form I (%)**	**Form II (%)**
1	Control	83	17
2	50	80	20
3	100	73	27
4	200	80	20
5	400	75	25
6	500	80	20



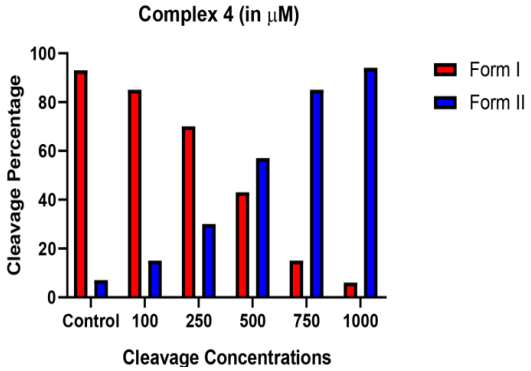
Complex 2			
S.No.	**Concentrations (μM)**	**Form I (%)**	**Form II (%)**
1	Control	79	21
2	1	78	22
3	5	73	27
4	10	62	38
5	25	30	70
6	50	2	98



Complex 3			
S.No.	**Concentrations (μM)**	**Form I (%)**	**Form II (%)**
1	Control	85	15
2	1	82	18
3	5	76	24
4	10	65	35
5	25	26	74
6	50	5	95



Complex 4			
S.No.	**Concentrations (μM)**	**Form I (%)**	**Form II (%)**
1	Control	93	7
2	100	85	15
3	250	70	30
4	500	43	57
5	750	15	85
6	1000	6	94



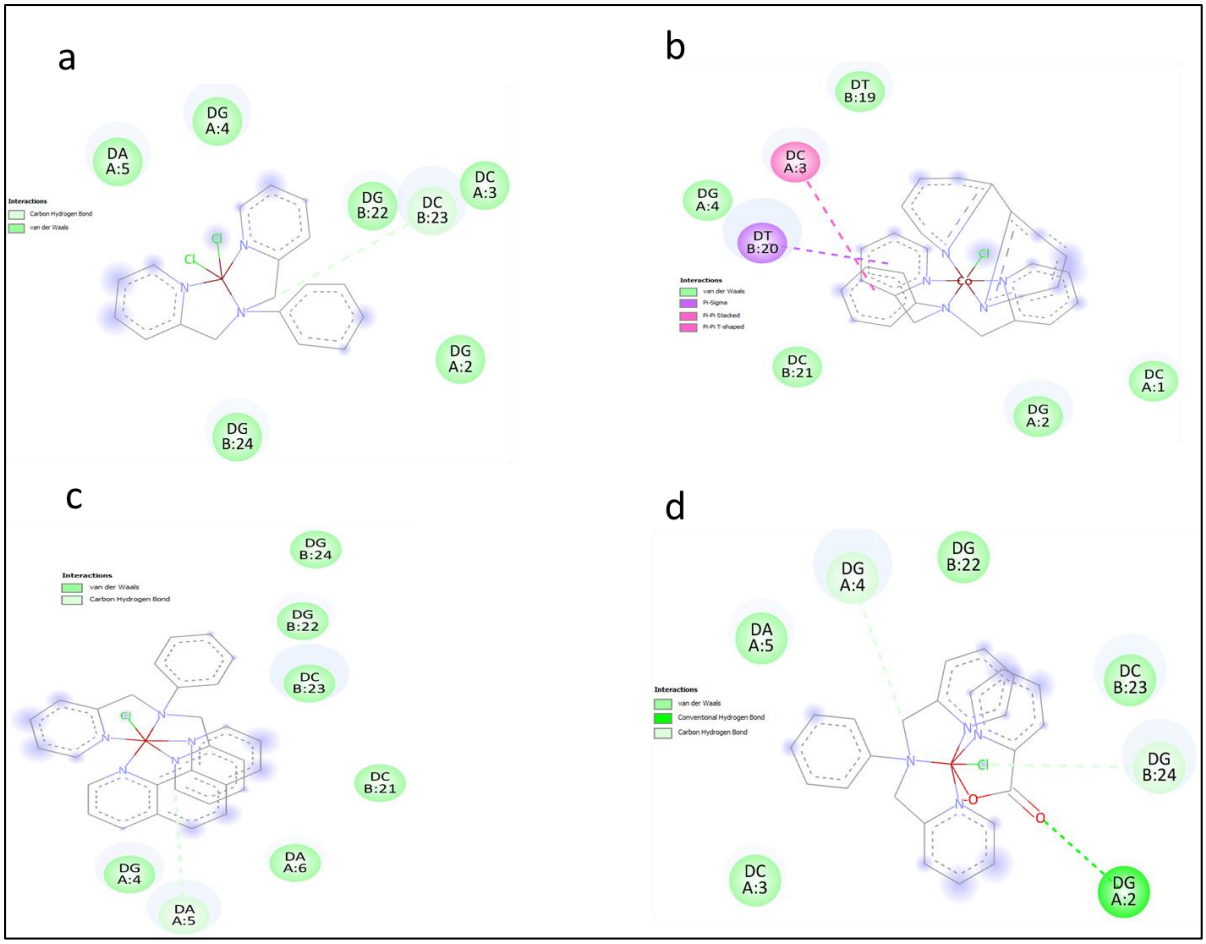


Fig. S27. (a-d) Interactions between complexes (**1**-**4**) and DNA, along with the van der Waals forces are represented in a 2-Dimentional format.

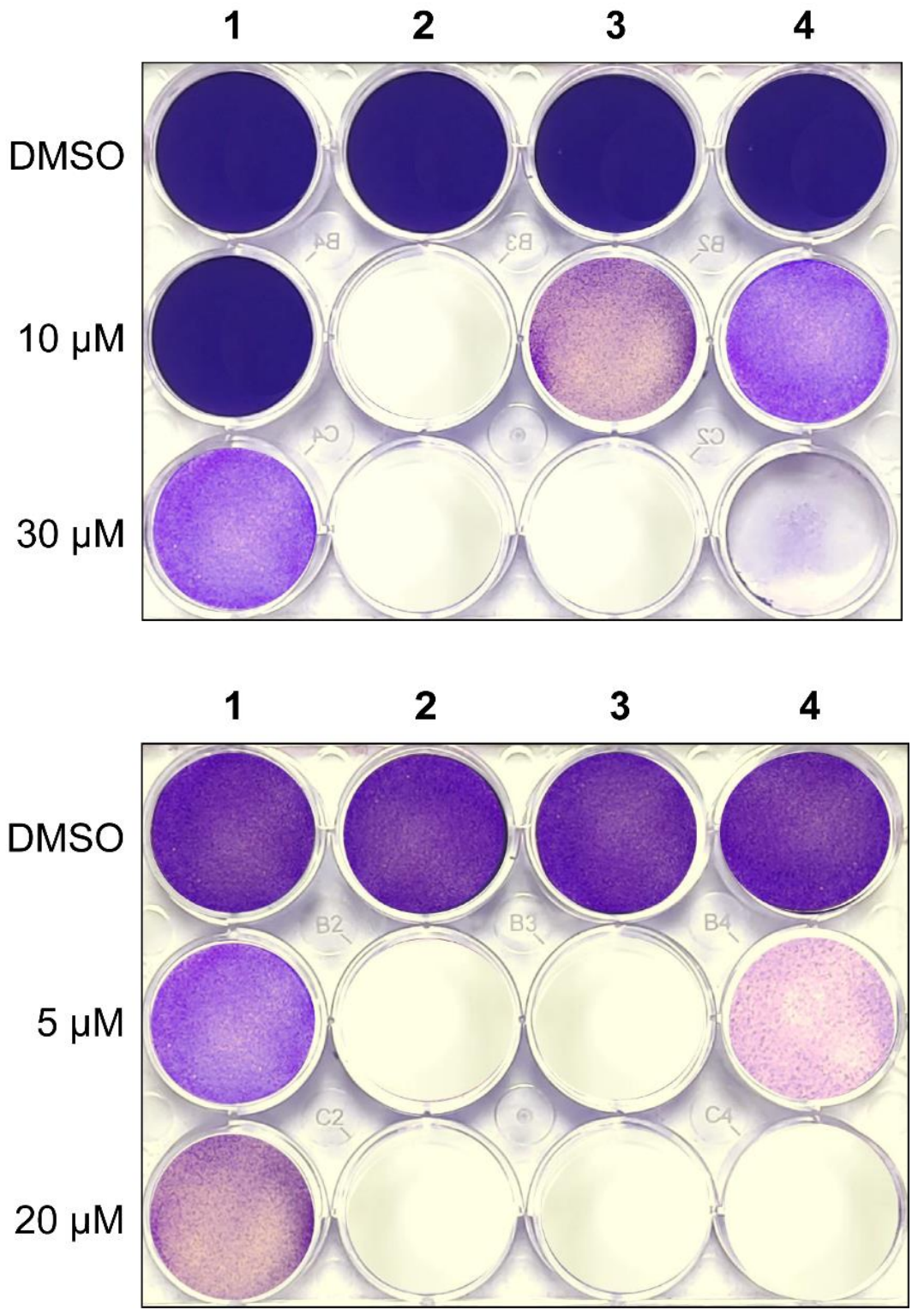


Fig. S28. Crystal violet staining images of A549 cells (top) and MDA-MB-231 cells (bottom) treated with 10 µM and 30 µM of **1-4** for 72 h. The purple colour indicates the number of live cancer cells, whereas its loss signifies the decrease in live cells survival.