Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Stabilization and fluorescence light-up of G-quadruplex nucleic acids using indolyl-quinolinium based probes

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CD titration spectra of *c-MYC* DNA in the absence of added metal ions

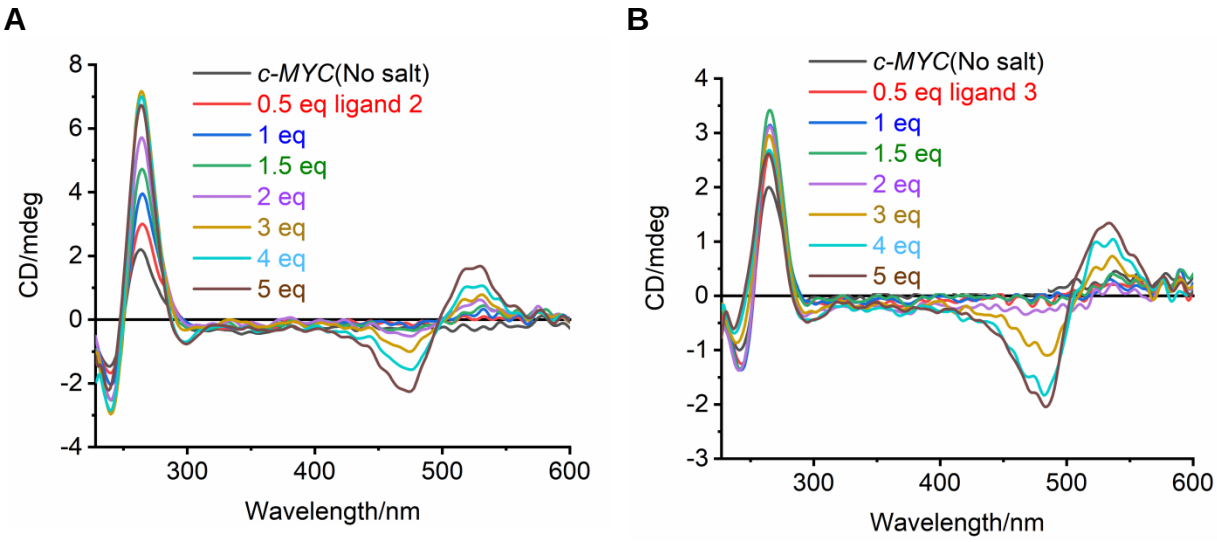


Figure S1. CD titration spectra of *c-MYC* DNA (10 μM in 10 mM lithium cacodylate buffer, pH 7.2) with (A) ligand **2** and (B) ligand **3** in the absence of added metal ions

CD titration spectra of *c-MYC* G4 DNA in the presence of K^+ ions

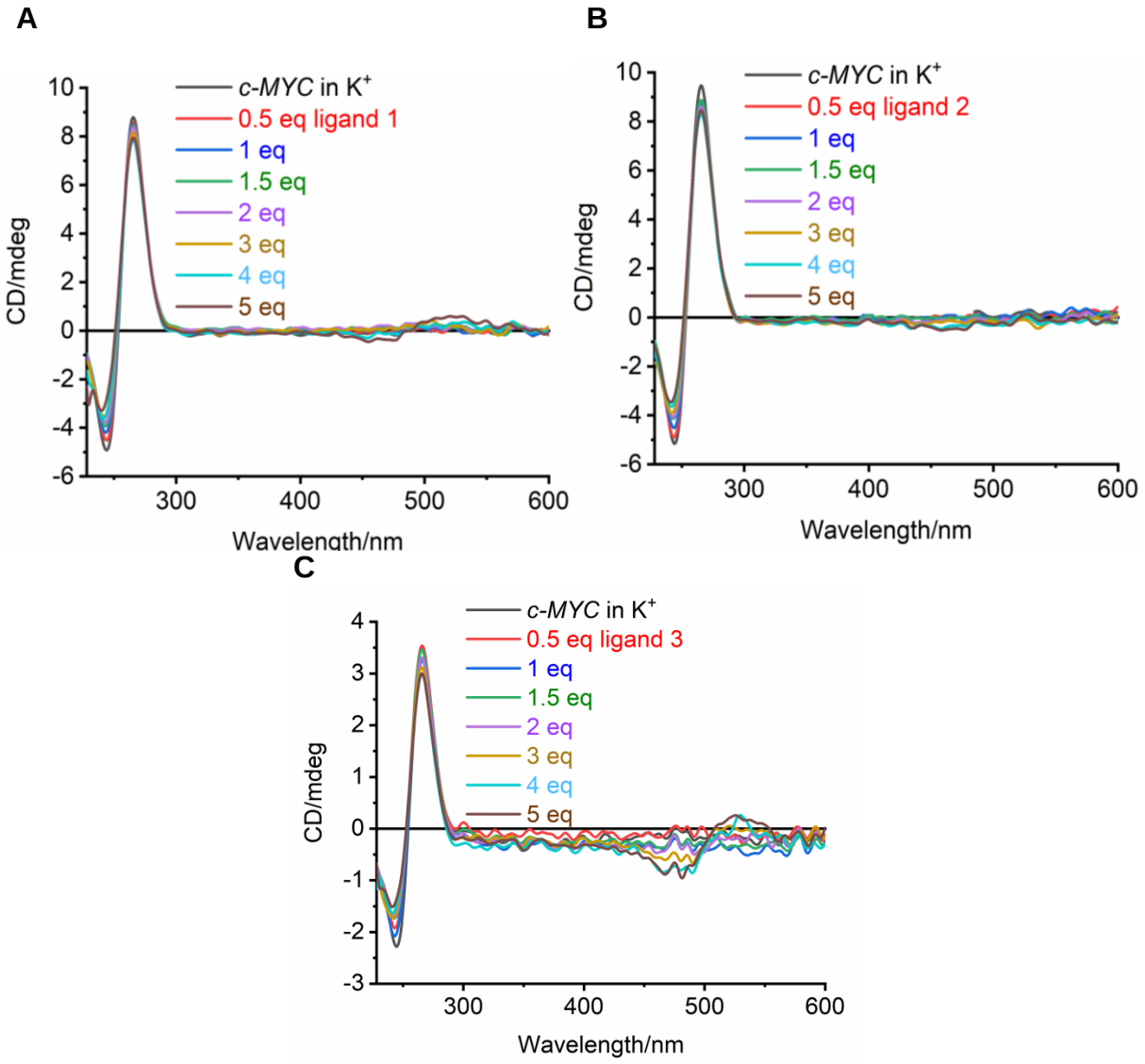


Figure S2. CD titration spectra of *c-MYC* DNA (10 μM in 10 mM lithium cacodylate buffer, pH 7.2) with (A) ligand **1**; (B) ligand **2** and (C) ligand **3** in the presence of 1 mM KCl and 99 mM LiCl.

CD titration spectra of *c-KIT 1* DNA in the absence of added metal ions

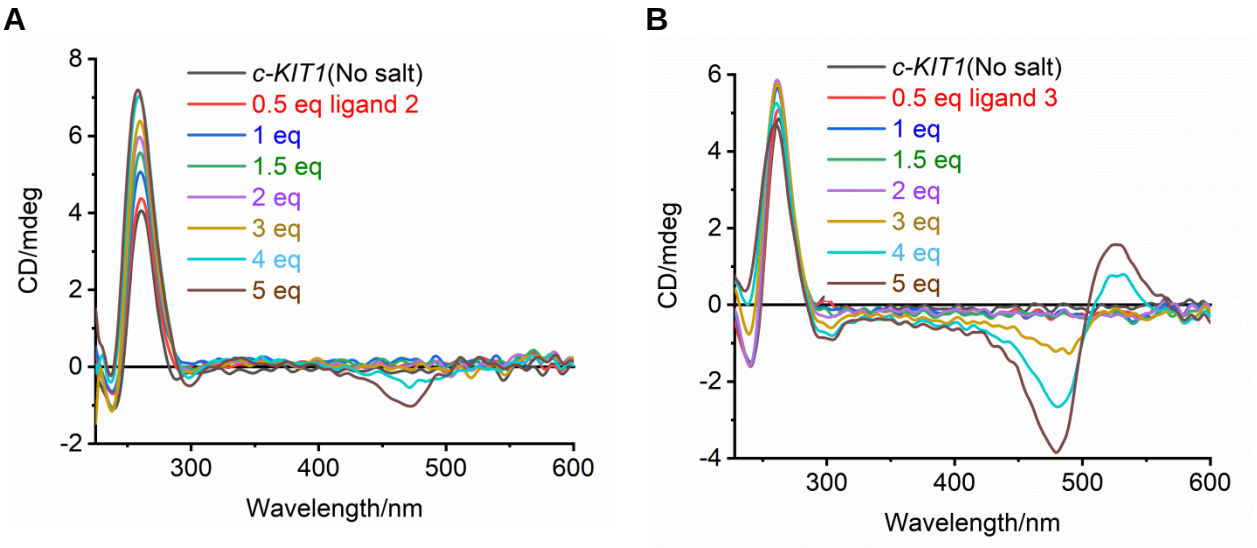


Figure S3. CD titration spectra of *c-KIT 1* DNA (10 μM in 10 mM lithium cacodylate buffer, pH 7.2) with (A) ligand **2** and (B) ligand **3** in the absence of added metal ions.

CD titration spectra of *c-KIT 1* G4 DNA in the presence of K^+ ions

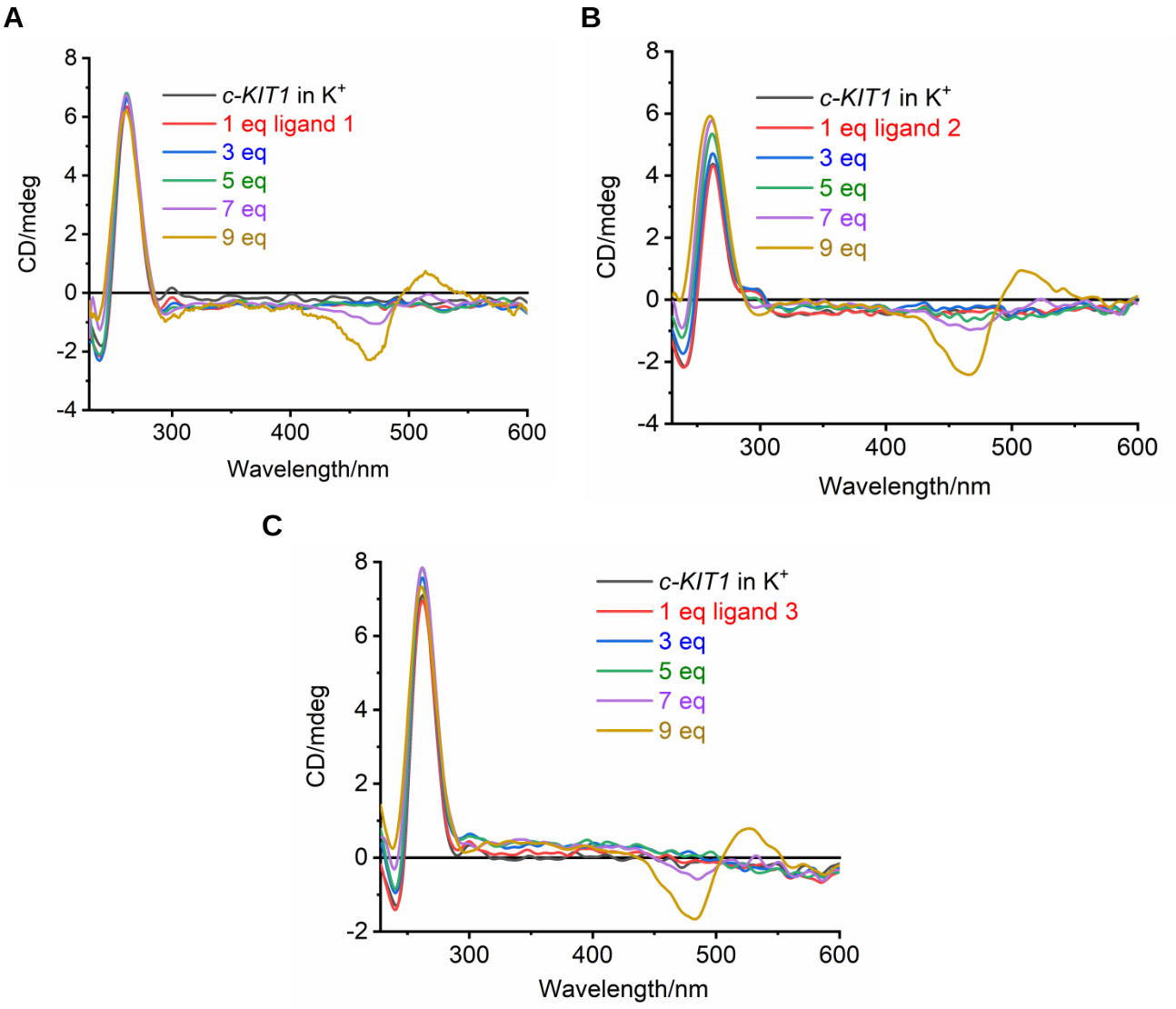


Figure S4. CD titration spectra of *c-KIT 1* DNA (10 μM in 10 mM lithium cacodylate buffer, pH 7.2) with (A) ligand **1**; (B) ligand **2** and (C) ligand **3** in the presence of 10 mM KCl and 90 mM LiCl.

CD titration spectra of telomeric DNA in the absence of added metal ions

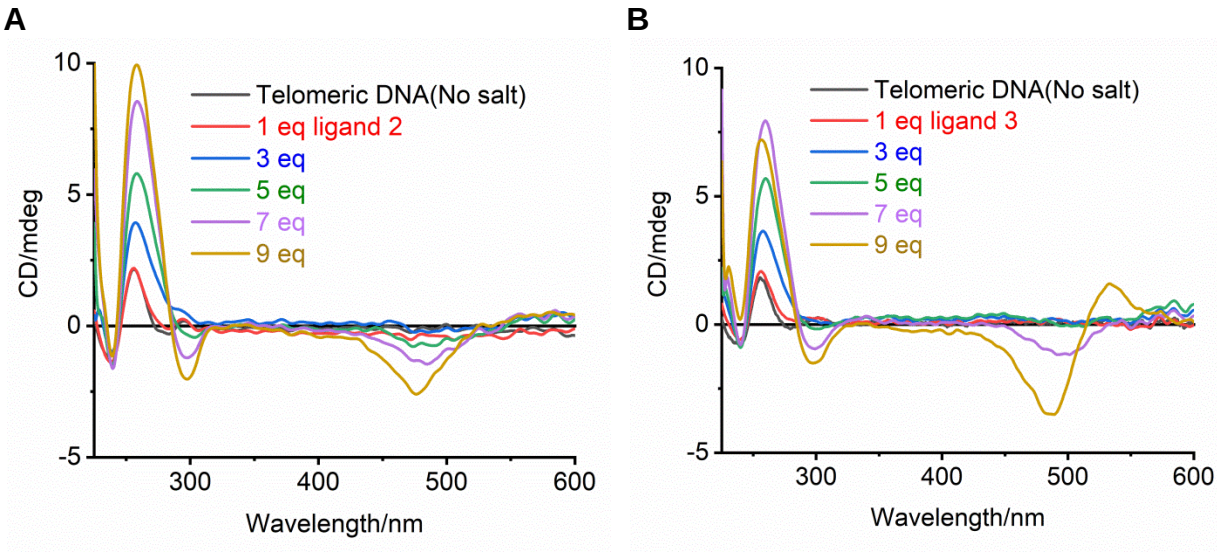


Figure S5. CD titration spectra of telomeric DNA (10 μM in 10 mM lithium cacodylate buffer, pH 7.2) with (A) ligand **2** and (B) ligand **3** in the absence of added metal ions.

CD titration spectra of telomeric G4 DNA in the presence of K^+ ions

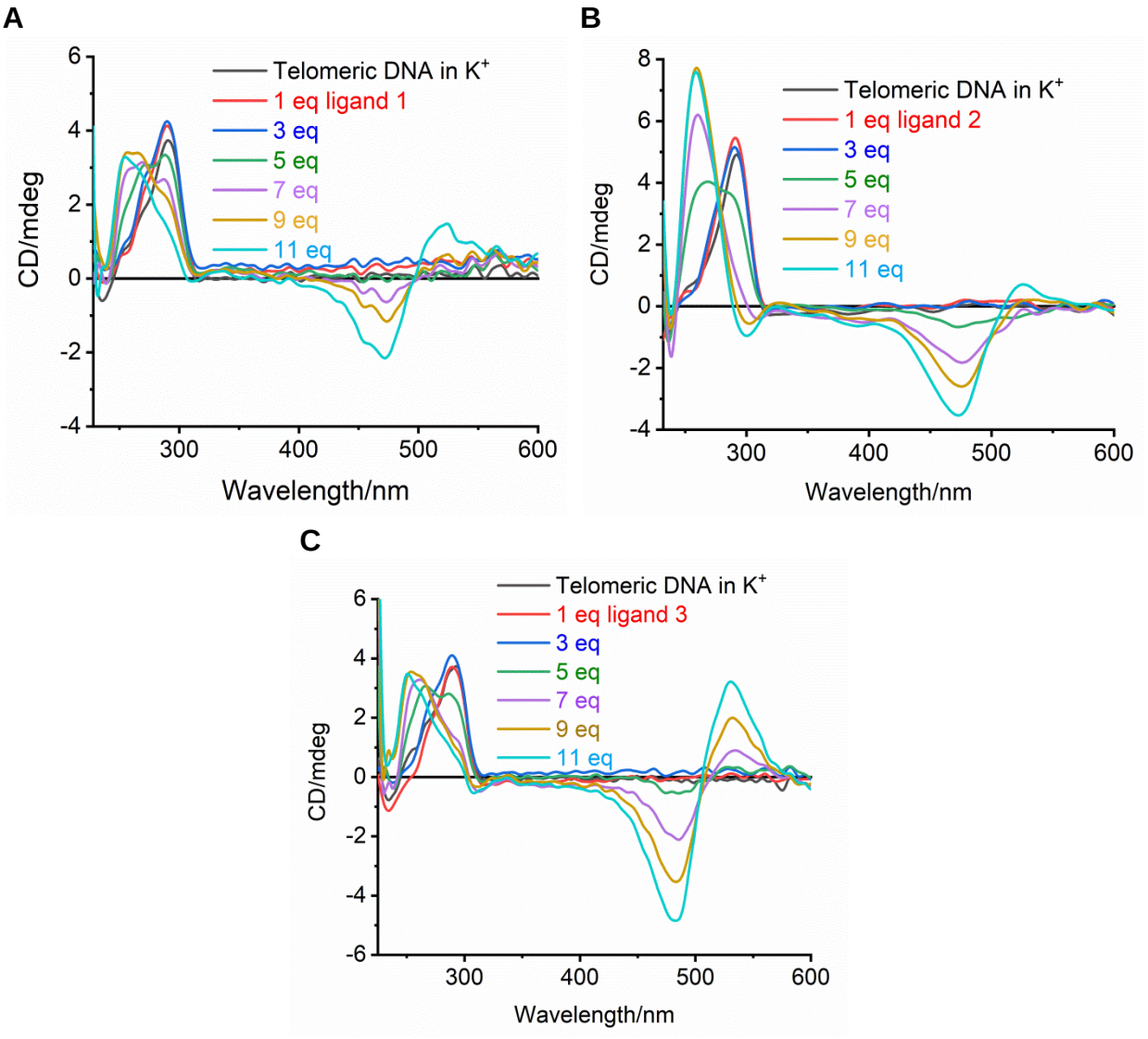


Figure S6. CD titration spectra of telomeric DNA (10 μM in 10 mM lithium cacodylate buffer, pH 7.2) with (A) ligand **1;** (B) ligand **2** and (C) ligand **3** in the presence of 10 mM KCl and 90 mM LiCl.

CD titration spectra of *h-RAS 1* DNA in the absence of added metal ions

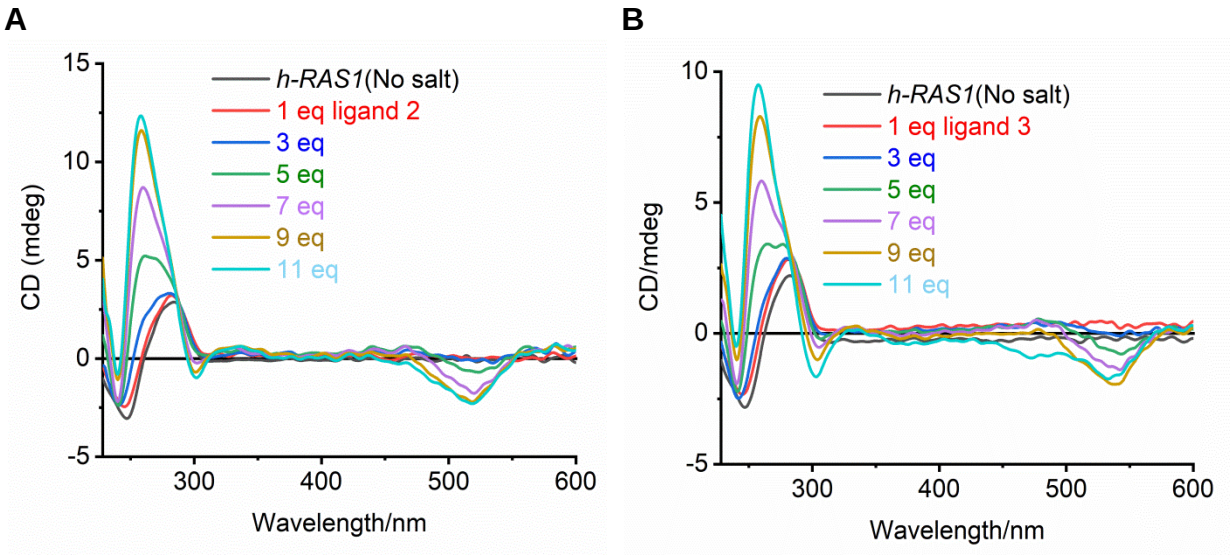


Figure S7. CD titration spectra of *h-RAS 1* DNA (10 μM in 10 mM lithium cacodylate buffer, pH 7.2) with (A) ligand **2** and (B) ligand **3** in the absence of added metal ions.

CD titration spectra of *h-RAS 1* G4 DNA in the presence of K^+ ions

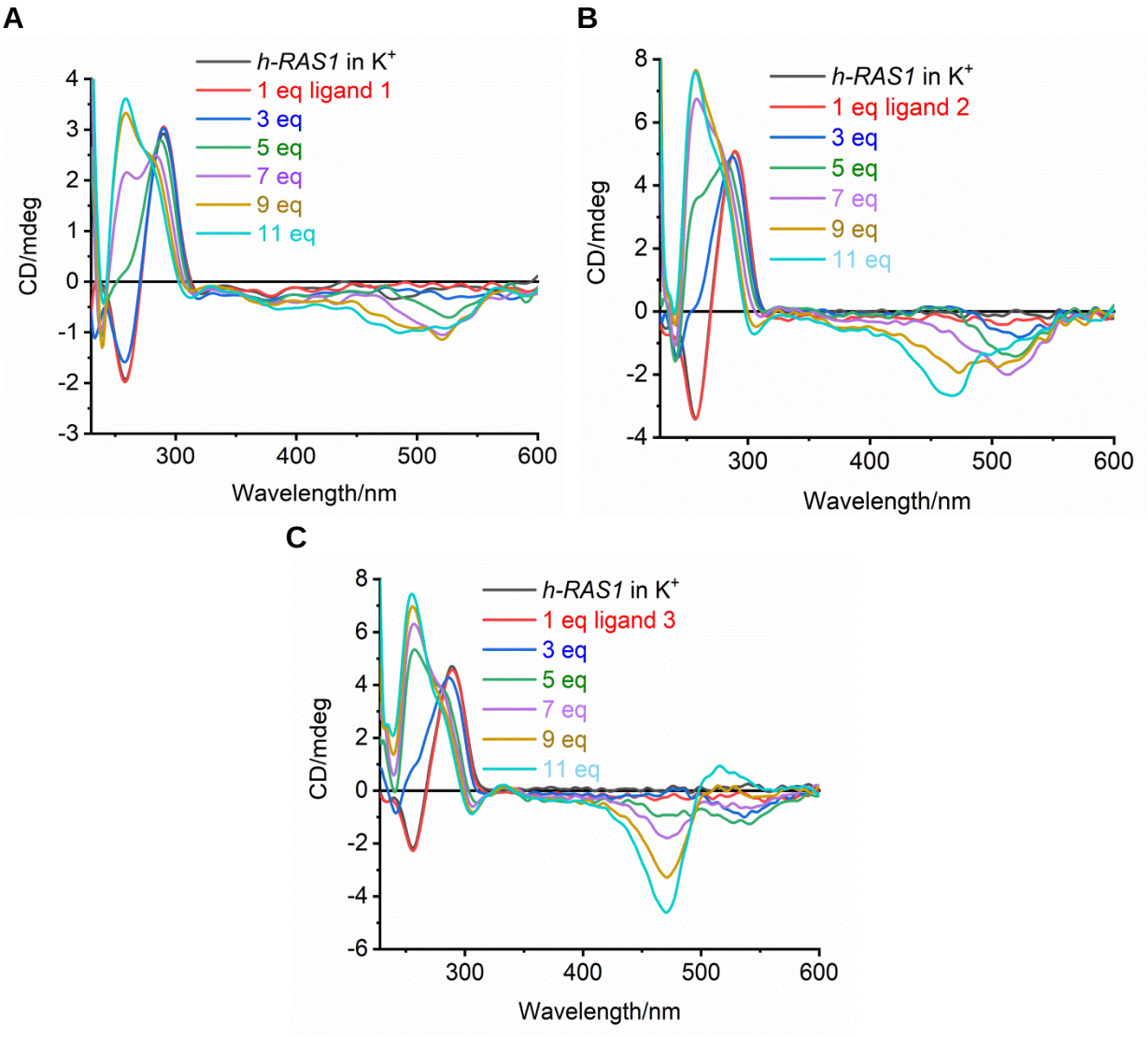


Figure S8. CD titration spectra of *h-RAS 1* DNA (10 μM in 10 mM lithium cacodylate buffer, pH 7.2) with (A) ligand **1;** (B) ligand **2** and (C) ligand **3** in the presence of 50 mM KCl and 50 mM LiCl.

CD melting curves of *c-MYC*, *h-RAS 1* and duplex DNAs with ligands

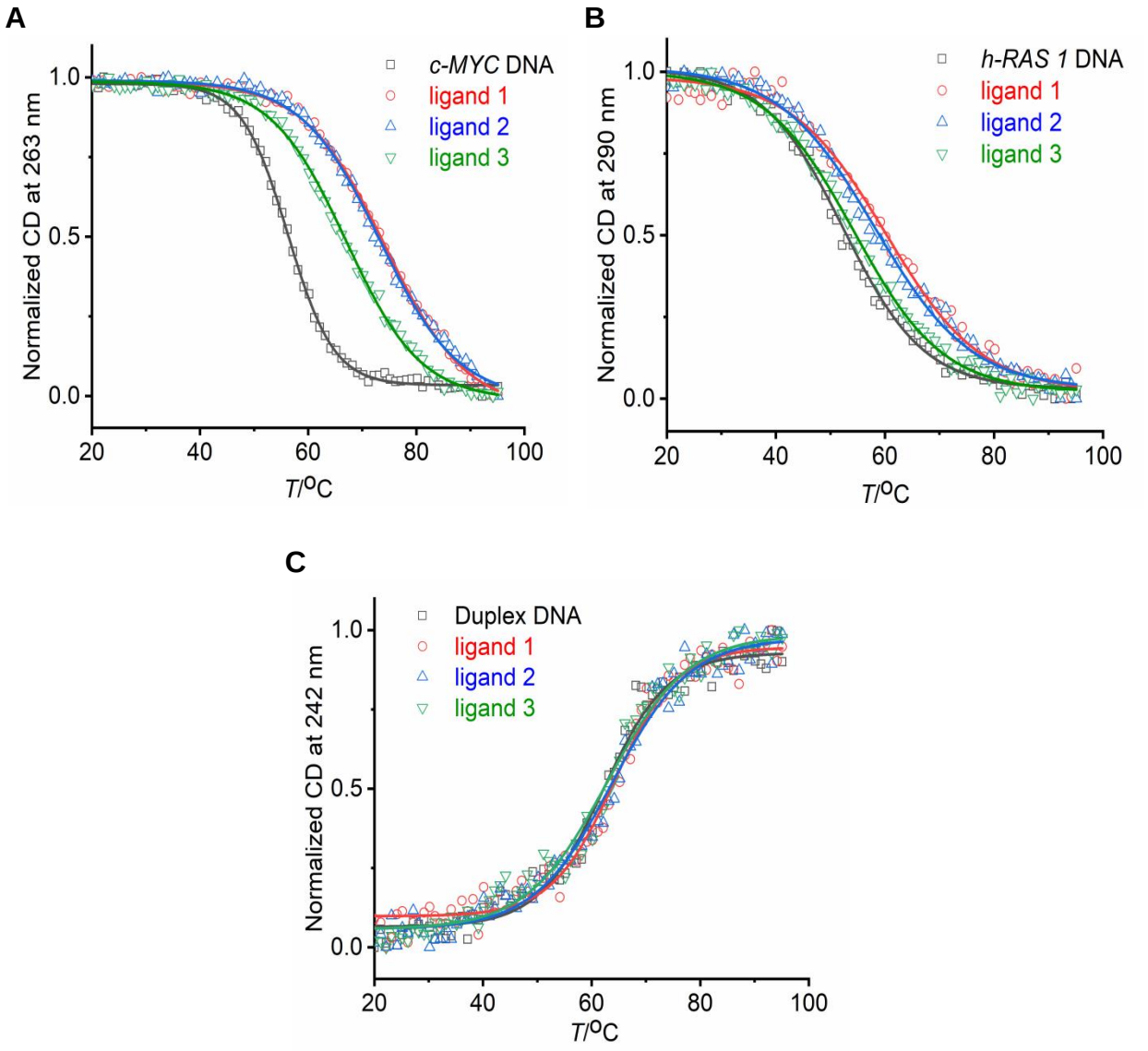


Figure S9. Normalized CD melting curve for 10 μM of (A) *c-MYC* (1 mM KCl and 99 mM LiCl); (B) *h-RAS 1*(10 mM KCl and 90 mM LiCl) and (C) duplex DNA (10 mM KCl and 90 mM LiCl) in 10 mM lithium cacodylate buffer, pH 7.2; in the absence and presence of 3 molar equivalent of ligands.

Absorption and emission spectra of ligand 2 in different solvents

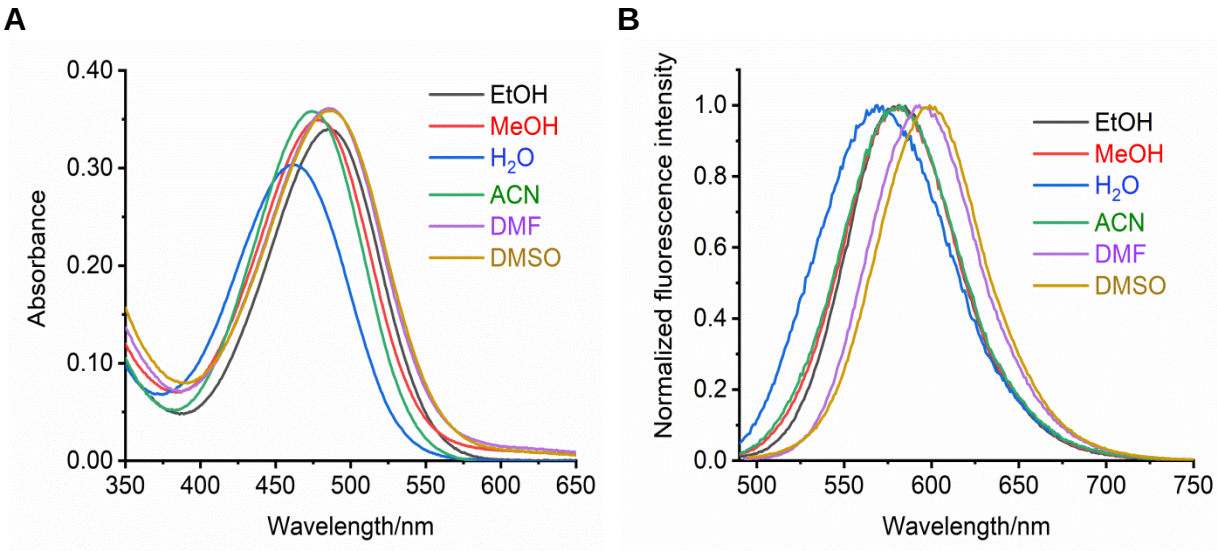


Figure S10. Absorbance and emission spectra of ligand **2**(30 μM) in the presence of various solvents.

Absorption and emission spectra of ligand 3 in different solvents

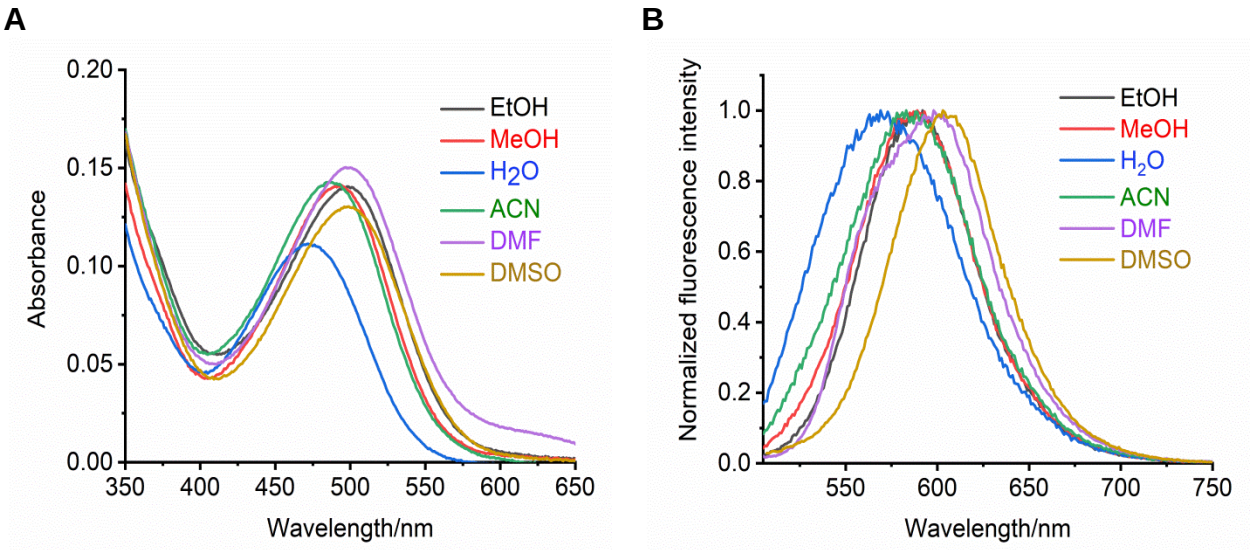


Figure S11. Absorbance and emission spectra of ligand **3** (30 μM) in the presence of various solvents.

Fluorimetric titration curves of ligand 1 with telomeric G4 and duplex DNAs

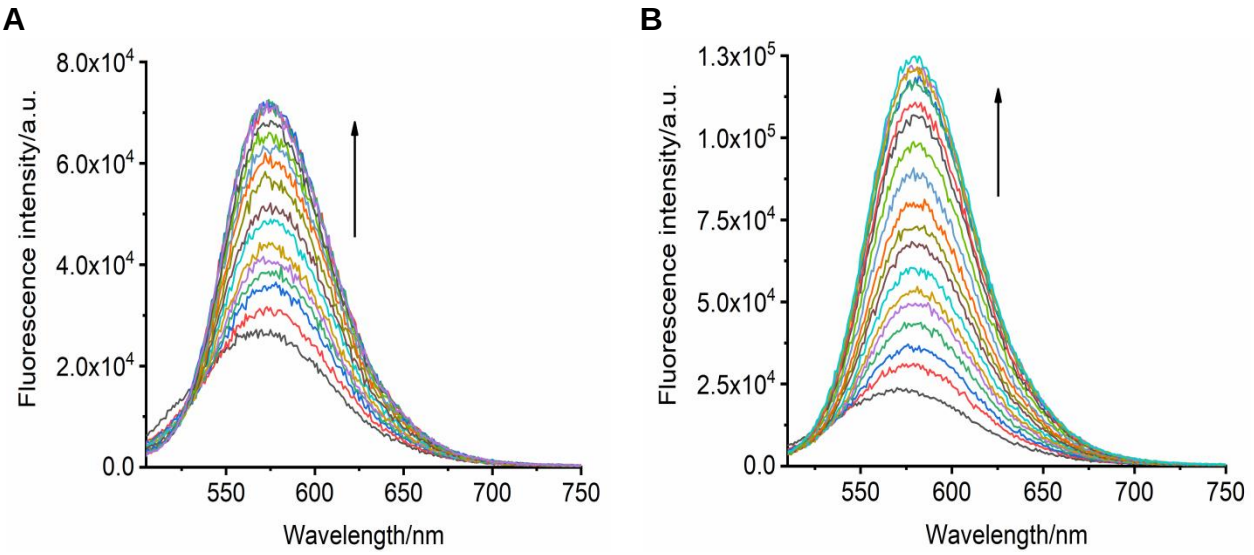


Figure S12. Fluorescence emission spectra of ligand **1** (5 μM in 10 mM lithium cacodylate buffer, pH 7.2) along with (A) telomeric G4 (0-4 μM in 10 mM KCl and 90 mM LiCl) and (B) duplex DNA (0-5 μM in 10 mM KCl and 90 mM LiCl).

Binding curves of ligand 1 with telomeric G4 and duplex DNAs

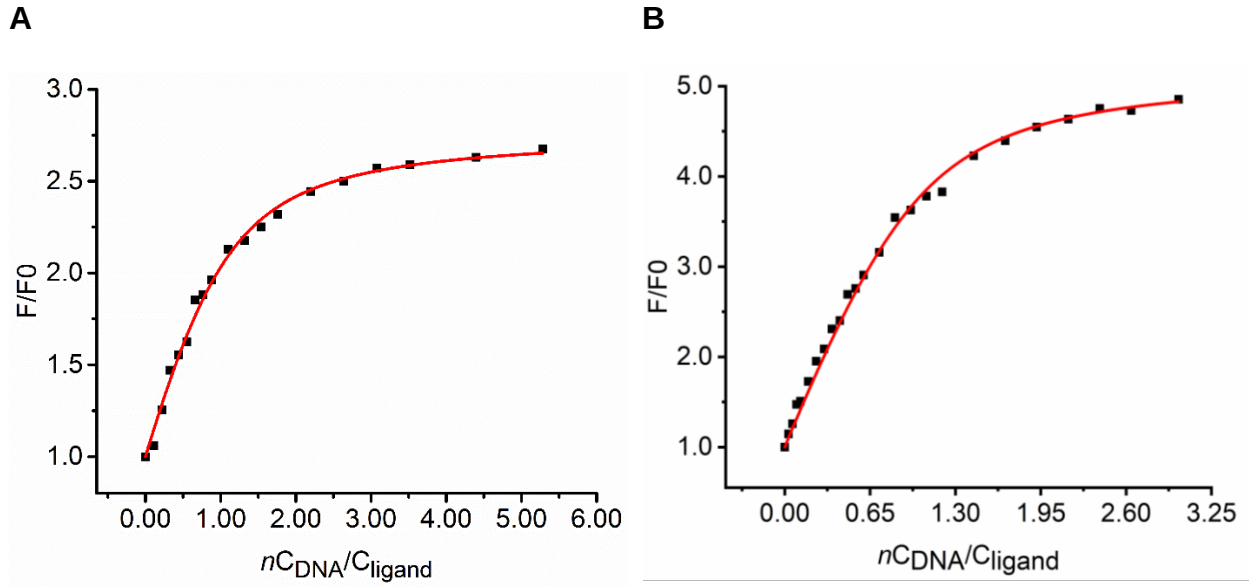


Figure S13. Binding curve (F/F0 Vs nC_{DNA}/C_{ligand}) of ligand **1** (5 μM in 10 mM lithium cacodylate buffer, pH 7.2) along with (A) telomeric G4 (0-4 μM in 10 mM KCl and 90 mM LiCl) and (B) duplex DNA (0-5 μM in 10 mM KCl and 90 mM LiCl).

Fluorimetric titration curves of ligand 2 with different DNAs

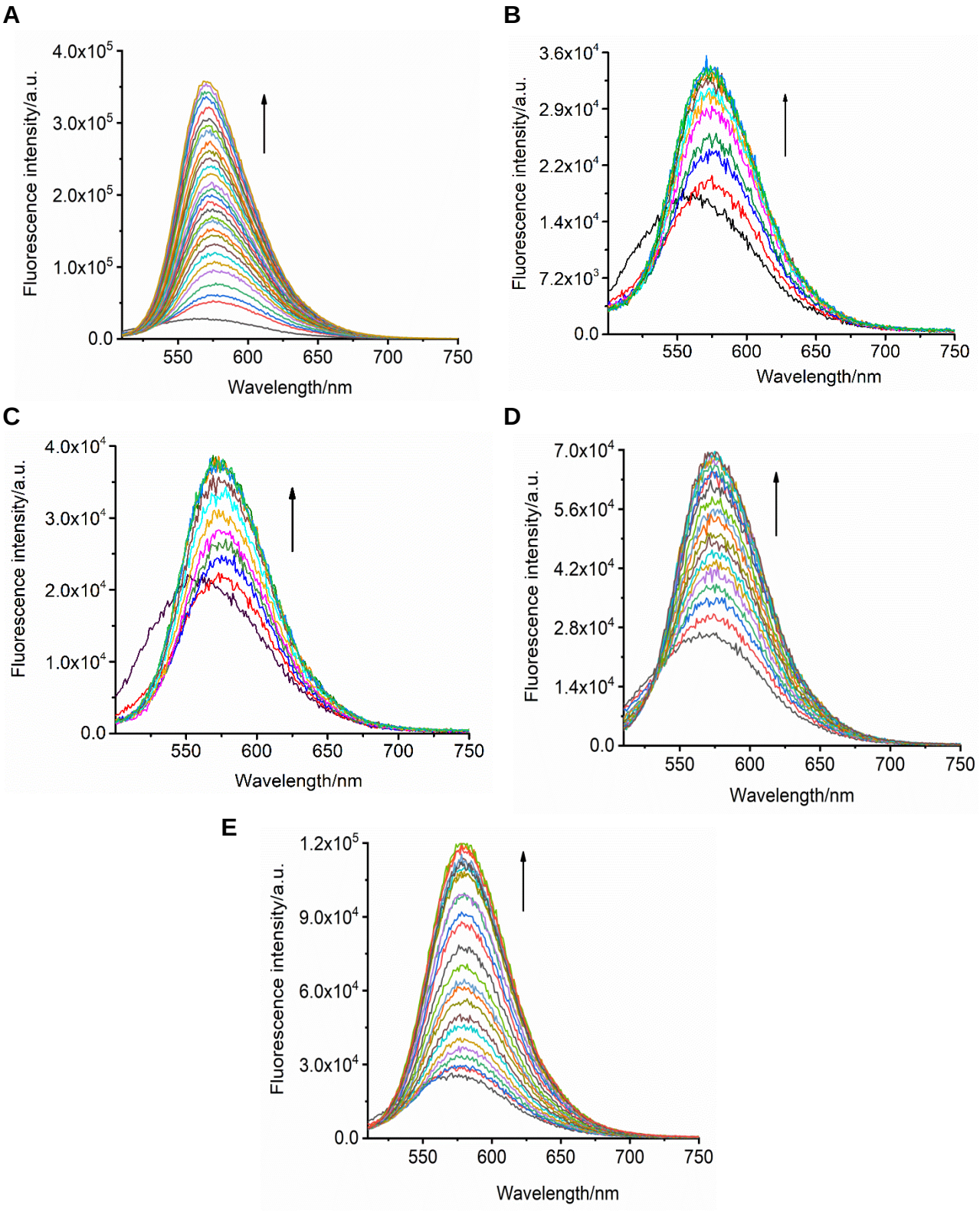
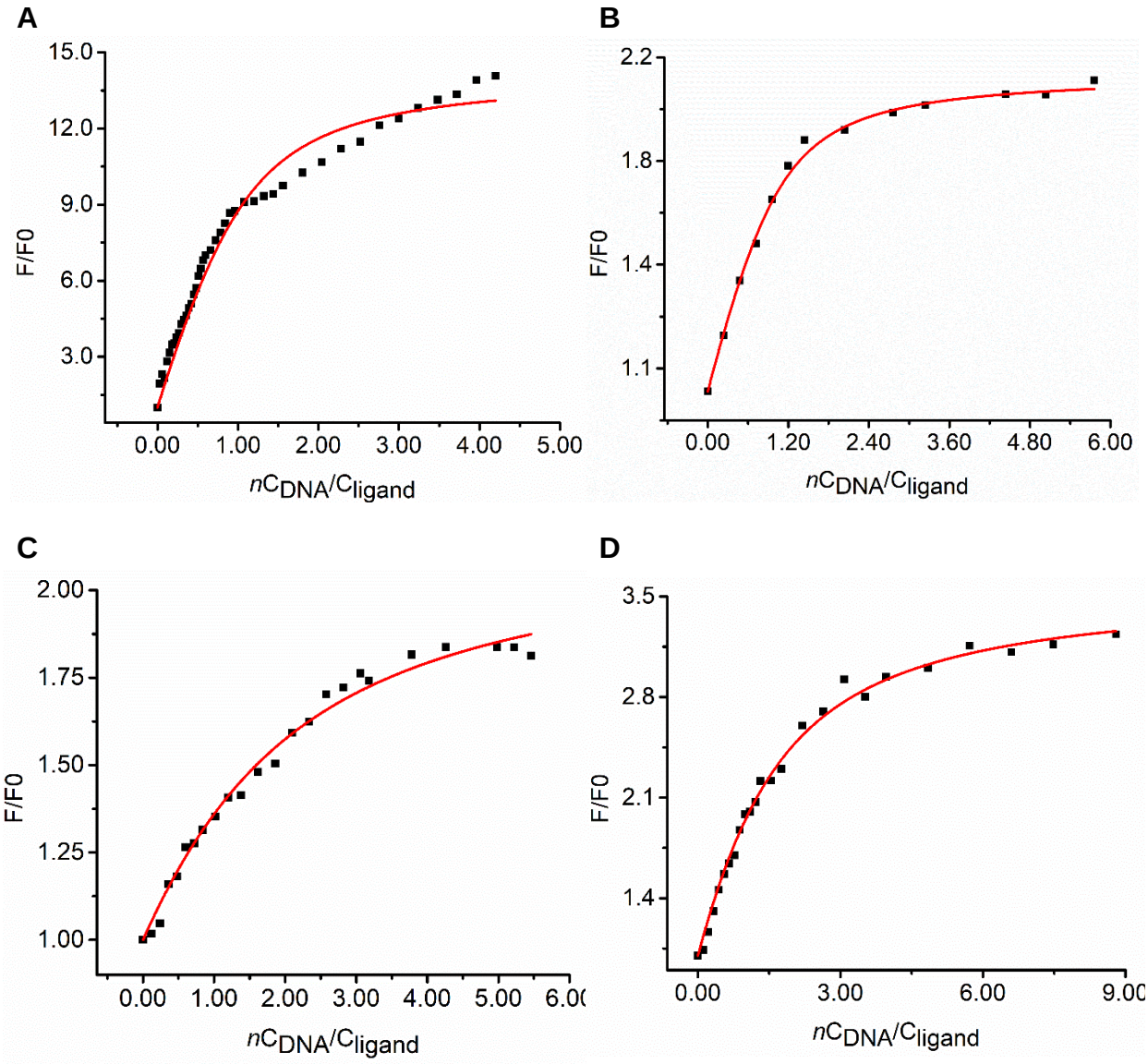


Figure S14. Fluorescence emission spectra of ligand **2** (5 μM in 10 mM lithium cacodylate buffer, pH 7.2) along with (A) *c-MYC* G4 (0-6 μM in 1 mM KCl and 99 mM LiCl); (B) *c-KIT 1* G4 (0-10 μM in 10 mM KCl and 90 mM LiCl); (C) *h-RAS 1* G4 (0-9 μM in 50 mM KCl and 50 mM LiCl); (D) Telomeric

G4 (0-4 μM in 10 mM KCl and 90 mM LiCl) and (E) duplex DNA (0-4 μM in 10 mM KCl and 90 mM LiCl).

Binding curves of ligand 2 with different DNAs



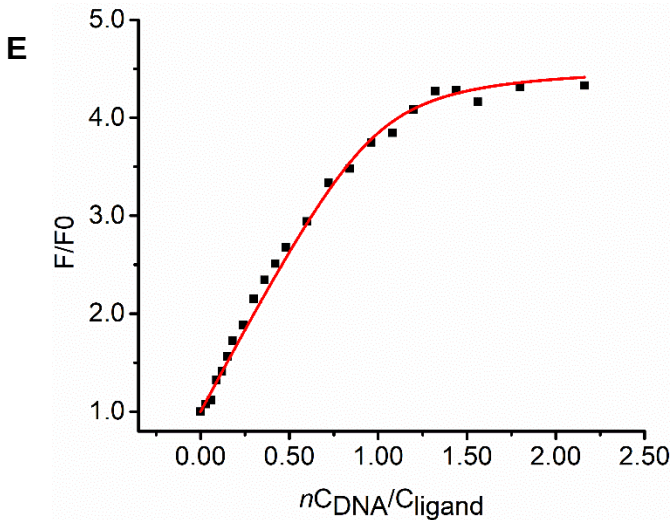
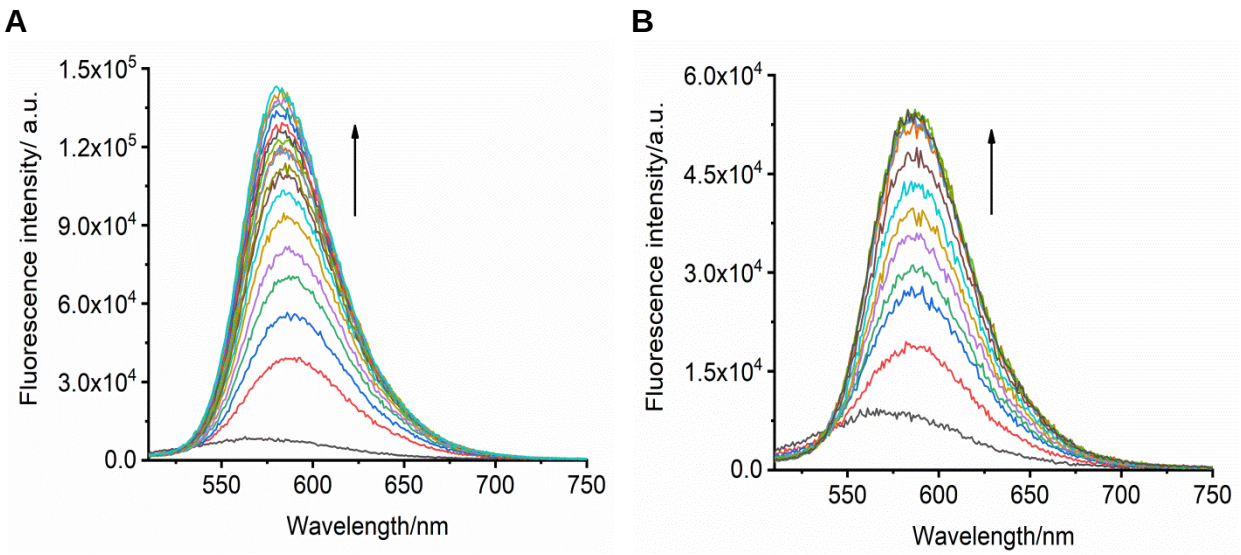


Figure S15. Binding curve (F/F0 Vs nC_{DNA}/C_{ligand}) of ligand **2** (5 μM in 10 mM lithium cacodylate buffer, pH 7.2) along with (A) *c-MYC* G4 (0-6 μM in 1 mM KCl and 99 mM LiCl); (B) *c-KIT 1* G4 (0-10 μM in 10 mM KCl and 90 mM LiCl); (C) *h-RAS 1* G4 (0-9 μM in 50 mM KCl and 50 mM LiCl); (D) Telomeric G4 (0-4 μM in 10 mM KCl and 90 mM LiCl) and (E) duplex DNA (0-4 μM in 10 mM KCl and 90 mM LiCl).

Fluorimetric titration curves of ligand 3 with different DNAs



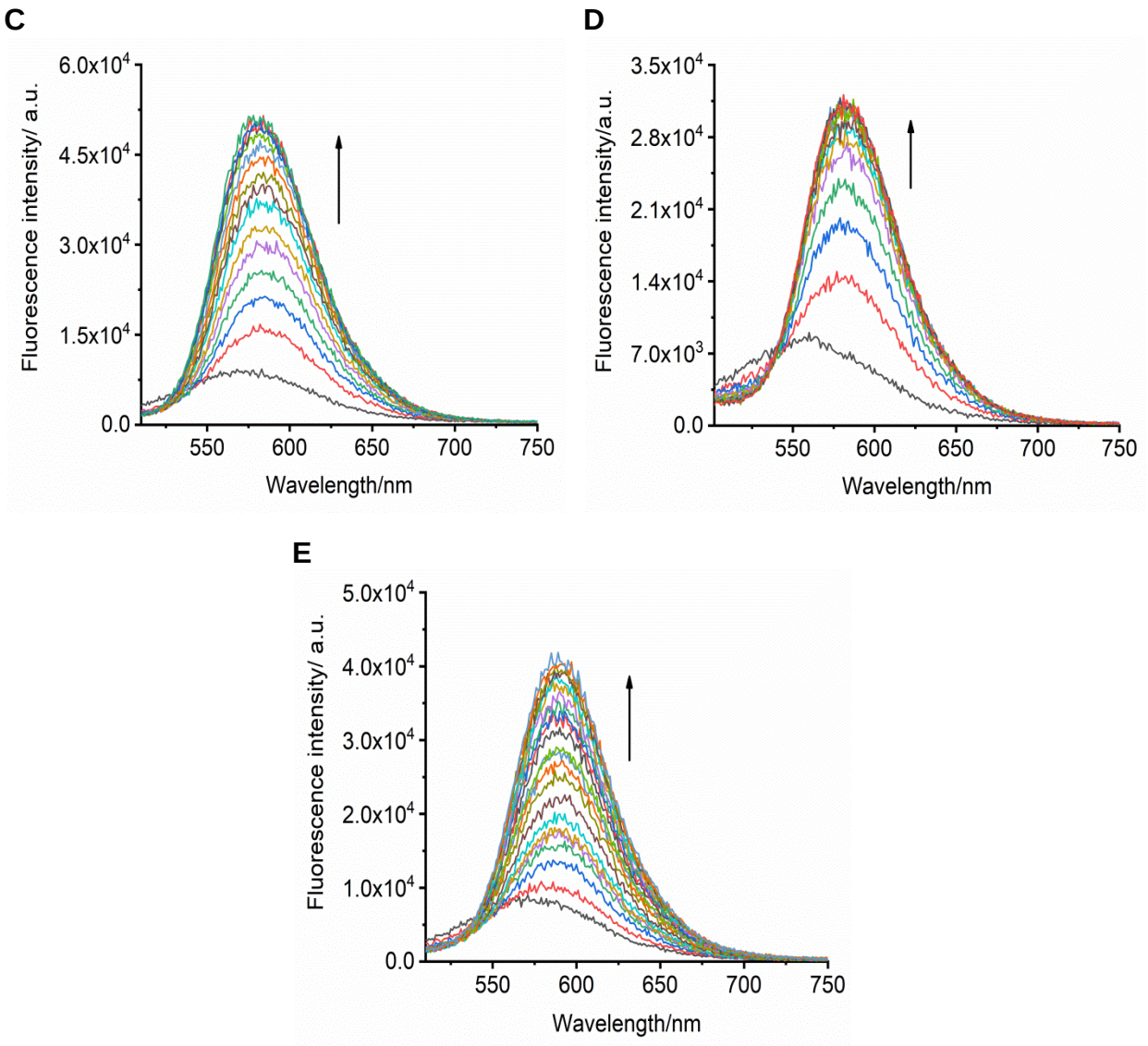


Figure S16. Fluorescence emission spectra of ligand **3** (5 μM in 10 mM lithiumcacodylate buffer, pH 7.2) along with (A) *c-MYC* G4 (0-5 μM in 1 mM KCl and 99 mM LiCl); (B) *c-KIT 1* G4 (0-3 μM in 10 mM KCl and 90 mM LiCl); (C)*h-RAS 1* G4 (0-4 μM in 50 mM KCl and 50 mM LiCl); (D) Telomeric G4 (0-2 μM in 10 mM KCl and 90 mM LiCl) and (E) duplex DNA (0-4 μM in 10 mM KCl and 90 mM LiCl).

TCSPC plots of ligands with different DNAs

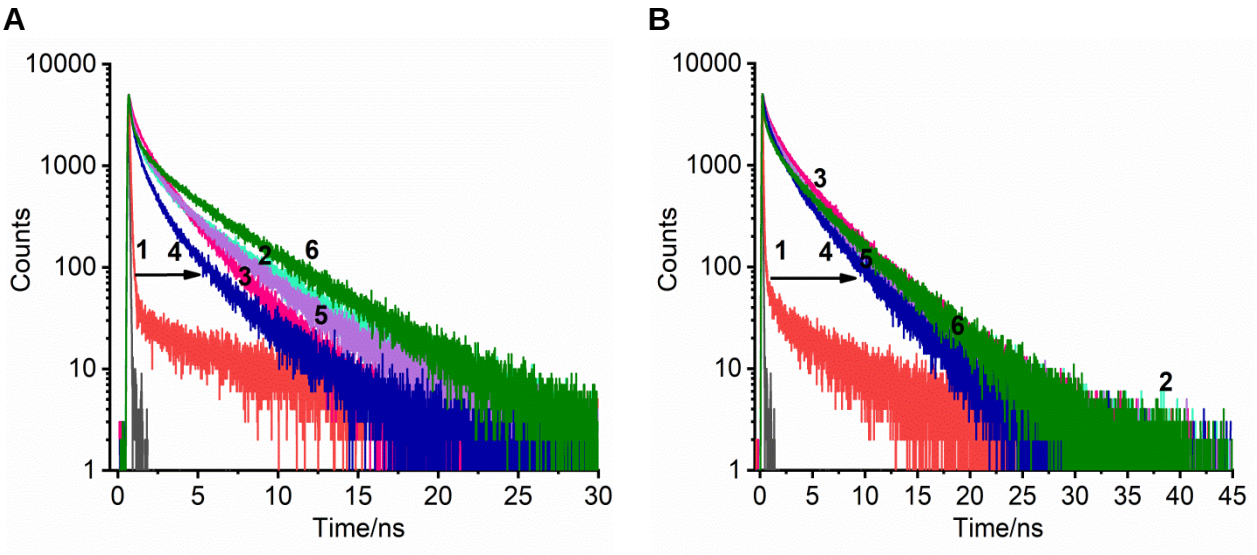
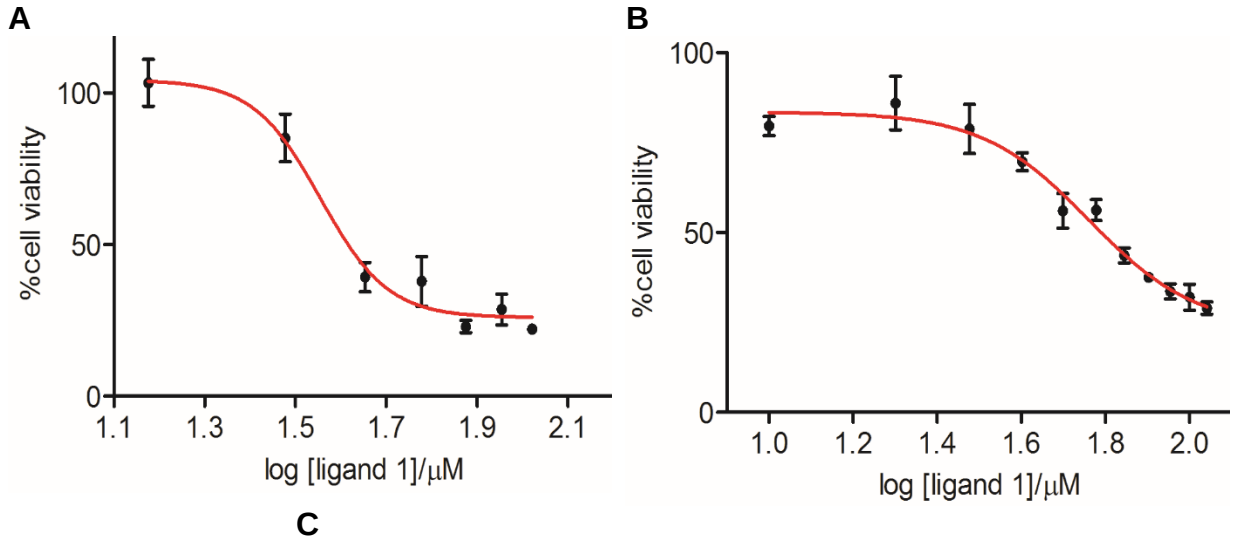


Figure S17. Fluorescence decay traces of (A) ligand **2** and (B) ligand **3** (5 μM in 10 mM lithium cacodylate buffer, pH 7.2) at 575 nm in the absence and presence of G4 DNAs at different solution conditions in (1) 10 mM lithium cacodylate buffer, pH 7.2; ligand **2** and **3** along with (2) *c-MYC* DNA in 1 mM KCl and 99 mM LiCl; (3) *c-KIT1* DNA in 10 mM KCl and 90 mM LiCl; (4) *h-RAS1* in 50 mM KCl and 50 mM LiCl; (5) Telomeric DNA in 10 mM KCl and 90 mM LiCl and (6) duplex DNA in 10 mM KCl and 90 mM LiCl.

Plot of percentage cell viabilities of ligand 1



C

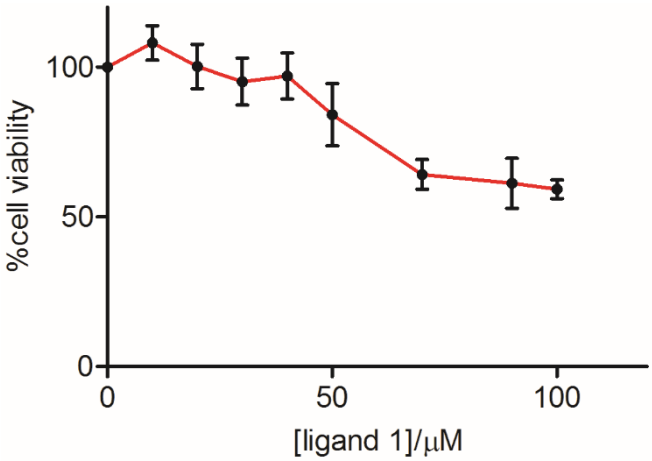


Figure S18. Concentration-dependent percentage cell viabilities determined by MTT assay for; (A) HeLa cells in presence of ligand **1** (15μM –105μM); (B) Lenti-X cells in presence of ligand **1** (10μM –110μM) and; (C) HepG2 cells in presence of ligand **1** (10μM –100μM) for 24 h. The results are the mean value of three replicates. Error bars denote standard deviation (SD) for n = 3.

Fluorescence of ligand 1 in cells treated with DNase and RNase

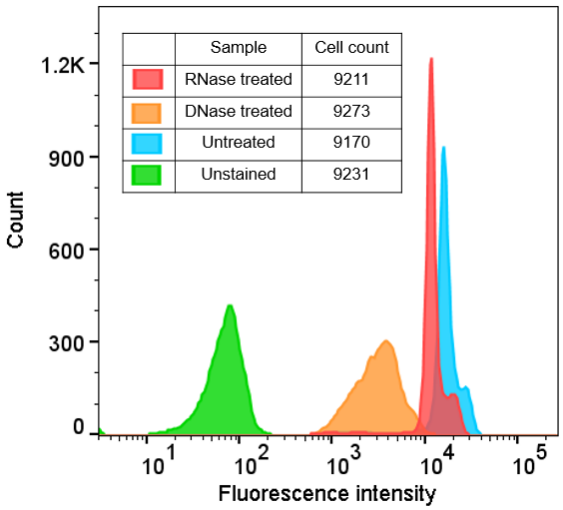
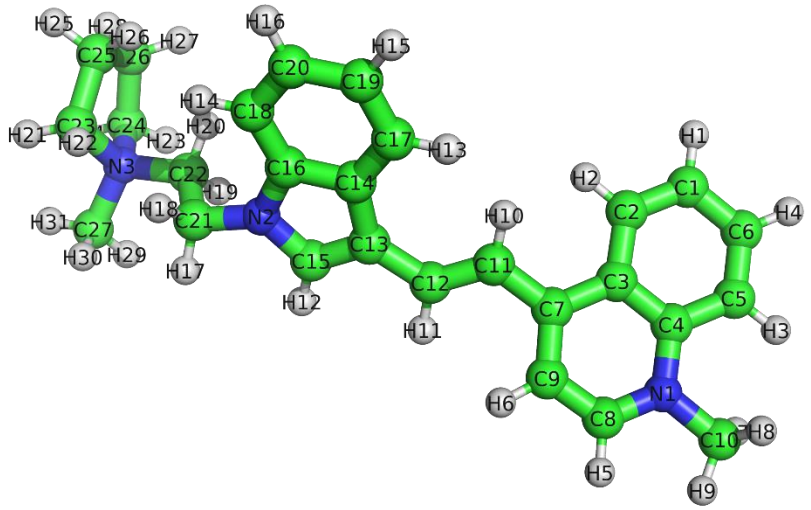


Figure S19. Mean fluorescence intensities of fixed HeLa cells stained with ligand **1** (5 μM, 2 h); with and without DNase (0.1 gm/ml, 30 min) and RNase (0.1gm/ml, 30 min) treatment.

Optimized structure, cartesian coordinates and RESP charges of ligand 1 used for docking



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MOL

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SMALL
Resp
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3	C3	-4.7030	0.1810	0.4660	ca	1	MOL	-0.058621
4	C4	-6.0190	-0.3260	0.4500	ca	1	MOL	0.267613
5	C5	-7.0150	0.2620	1.2540	ca	1	MOL	-0.317736
6	C6	-6.7000	1.3170	2.0590	ca	1	MOL	0.004079
7	H1	-5.1570	2.6460	2.7600	ha	1	MOL	0.171088
8	H2	-3.4200	1.6480	1.3920	ha	1	MOL	0.148530
9	C7	-3.7010	-0.4190	-0.3650	ca	1	MOL	0.314261
10	H3	-8.0190	-0.1080	1.2440	ha	1	MOL	0.195175
11	H4	-7.4650	1.7610	2.6690	ha	1	MOL	0.163783
12	C8	-5.3790	-1.9600	-1.1020	ca	1	MOL	0.079378
13	C9	-4.0800	-1.5020	-1.1380	ca	1	MOL	-0.384766
14	H5	-5.6800	-2.7890	-1.7110	h4	1	MOL	0.194083
15	H6	-3.3980	-1.9720	-1.8170	ha	1	MOL	0.212747
16	C10	-7.6880	-1.9510	-0.4020	c3	1	MOL	-0.214434
17	H7	-7.9760	-2.3000	0.5780	h1	1	MOL	0.136452
18	H8	-8.3720	-1.1910	-0.7460	h1	1	MOL	0.136452
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22	H10	-2.2250	1.1630	-0.2520	ha	1	MOL	0.200649
23	C12	-1.2610	-0.6420	-0.6620	cf	1	MOL	0.004800
24	H11	-1.3920	-1.7070	-0.7550	ha	1	MOL	0.136946

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26	C14	0.6960	1.1270	-0.9310	ca	1	MOL	0.083565
27	C15	1.1650	-1.0650	-0.7550	cc	1	MOL	-0.209961
28	C16	2.0810	0.9530	-0.9940	ca	1	MOL	0.098693
29	C17	0.1770	2.4180	-1.0750	ca	1	MOL	-0.180409
30	H12	1.1470	-2.1330	-0.6690	h4	1	MOL	0.214214
31	C18	2.9620	2.0150	-1.1810	ca	1	MOL	-0.271541
32	C19	1.0390	3.4750	-1.2520	ca	1	MOL	-0.155156
33	H13	-0.8800	2.5990	-1.0710	ha	1	MOL	0.156640
34	C20	2.4240	3.2760	-1.3050	ca	1	MOL	-0.083273
35	H14	4.0250	1.8700	-1.2530	ha	1	MOL	0.174305
36	H15	0.6470	4.4690	-1.3660	ha	1	MOL	0.160749
37	H16	3.0730	4.1180	-1.4560	ha	1	MOL	0.151625
38	N2	2.3530	-0.4030	-0.8720	na	1	MOL	-0.025140
39	C21	3.6570	-1.0110	-0.9100	c3	1	MOL	0.004374
40	H17	3.5350	-2.0460	-1.1940	h1	1	MOL	0.095793
41	H18	4.2450	-0.5320	-1.6810	h1	1	MOL	0.095793
42	C22	4.3190	-0.8940	0.4750	c3	1	MOL	-0.281925
43	H19	3.7750	-1.5070	1.1800	hx	1	MOL	0.165427
44	H20	4.2680	0.1280	0.8140	hx	1	MOL	0.165427
45	C23	6.6910	-0.3490	-0.1300	c3	1	MOL	-0.070540
46	C24	6.2260	-1.2360	1.9960	c3	1	MOL	-0.070540
47	C25	6.8370	0.8270	0.8400	c3	1	MOL	0.013750
48	H21	7.6300	-0.8670	-0.2660	hx	1	MOL	0.115399
49	H22	6.3040	-0.0910	-1.1030	hx	1	MOL	0.115399
50	C26	6.5160	0.2460	2.2380	c3	1	MOL	0.013750
51	H23	5.4760	-1.6690	2.6410	hx	1	MOL	0.115399
52	H24	7.1270	-1.8280	2.0650	hx	1	MOL	0.115399
53	H25	7.8410	1.2250	0.7830	hc	1	MOL	0.046130
54	H26	6.1620	1.6340	0.5870	hc	1	MOL	0.046130
55	H27	5.6680	0.7460	2.6860	hc	1	MOL	0.046130
56	H28	7.3440	0.3500	2.9250	hc	1	MOL	0.046130
57	C27	5.9340	-2.7100	0.0290	c3	1	MOL	-0.319142
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59	H30	5.7430	-2.7230	-1.0330	hx	1	MOL	0.168868
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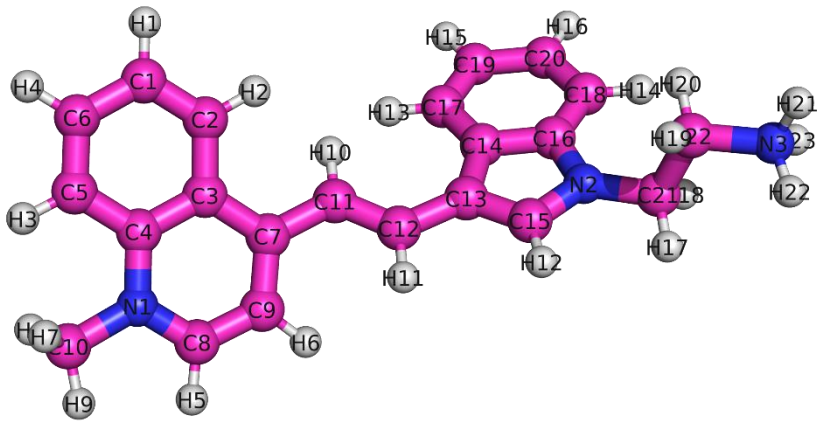
Figure S20. The optimized structure of ligand **1** which was used for docking. The ligand was optimized at HF/6-31G* theory level in Gaussian 16. The ESP charges were then calculated in Gaussian 16. The Cartesian coordinates and RESP charges were then calculated in SYBL Mol2 format using antechamber in AMBER 18. Carbon atoms are represented using green, nitrogen atoms using blue and hydrogen atoms using light grey.

Optimized structure, cartesian coordinates and RESP charges of ligand 2



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3	C3	-3.3430	0.2900	0.3280	ca	1	MOL	-0.115831
4	C4	-4.6840	-0.1340	0.2150	ca	1	MOL	0.321611
5	C5	-5.7080	0.5770	0.8690	ca	1	MOL	-0.343693
6	C6	-5.3990	1.6710	1.6230	ca	1	MOL	0.008923
7	H1	-3.8420	2.9520	2.3770	ha	1	MOL	0.181026

8	H2	-2.0550	1.7420	1.2680	ha	1	MOL	0.141062
9	C7	-2.3110	-0.4360	-0.3510	ca	1	MOL	0.367912
10	H3	-6.7300	0.2700	0.7850	ha	1	MOL	0.201948
11	H4	-6.1860	2.2080	2.1180	ha	1	MOL	0.169680
12	C8	-4.0120	-1.9230	-1.1410	ca	1	MOL	0.093769
13	C9	-2.6860	-1.5510	-1.0780	ca	1	MOL	-0.420022
14	H5	-4.3110	-2.7770	-1.7160	h4	1	MOL	0.194743
15	H6	-1.9760	-2.1140	-1.6480	ha	1	MOL	0.227796
16	C10	-6.3720	-1.7150	-0.6820	c3	1	MOL	-0.258947
17	H7	-6.7760	-1.9650	0.2870	h1	1	MOL	0.151416
18	H8	-6.9640	-0.9420	-1.1470	h1	1	MOL	0.151416
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22	H10	-0.7430	1.0570	-0.2300	ha	1	MOL	0.204577
23	C12	0.1250	-0.8370	-0.3490	cf	1	MOL	0.009083
24	H11	-0.0710	-1.8970	-0.3510	ha	1	MOL	0.138564
25	C13	1.5380	-0.4880	-0.3420	cd	1	MOL	-0.080851
26	C14	2.2150	0.7760	-0.6000	ca	1	MOL	0.103164
27	C15	2.5140	-1.3940	-0.0880	cc	1	MOL	-0.258898
28	C16	3.5840	0.5310	-0.4660	ca	1	MOL	0.047044
29	C17	1.7990	2.0580	-0.9730	ca	1	MOL	-0.184269
30	H12	2.4160	-2.4390	0.1310	h4	1	MOL	0.227034
31	C18	4.5460	1.5150	-0.6730	ca	1	MOL	-0.266520
32	C19	2.7420	3.0400	-1.1750	ca	1	MOL	-0.165137
33	H13	0.7630	2.2860	-1.1260	ha	1	MOL	0.166402
34	C20	4.1070	2.7710	-1.0240	ca	1	MOL	-0.088708
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36	H15	2.4300	4.0260	-1.4640	ha	1	MOL	0.171181
37	H16	4.8220	3.5540	-1.1970	ha	1	MOL	0.163018
38	N2	3.7510	-0.8090	-0.1370	na	1	MOL	0.071603
39	C21	5.0050	-1.4740	0.0490	c3	1	MOL	-0.235183
40	H17	4.8610	-2.5390	-0.0890	h1	1	MOL	0.142602
41	H18	5.7080	-1.1410	-0.7070	h1	1	MOL	0.142602
42	C22	5.5570	-1.1920	1.4530	c3	1	MOL	0.164749
43	H19	4.9340	-1.6210	2.2220	hx	1	MOL	0.078729
44	H20	5.6660	-0.1330	1.6340	hx	1	MOL	0.078729
45	H21	7.3080	-1.6170	2.5440	hn	1	MOL	0.339143
46	H22	6.9260	-2.8060	1.5020	hn	1	MOL	0.339143
47	H23	7.5990	-1.4270	0.9550	hn	1	MOL	0.339143
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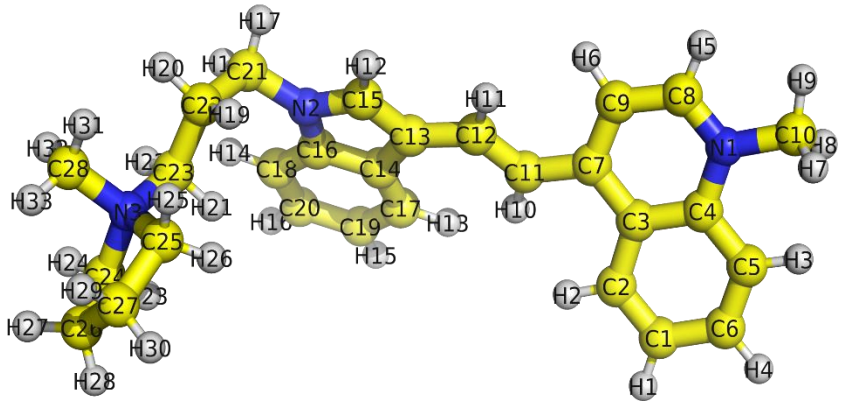
Figure S21. The optimized structure of ligand **2**. The ligand was optimized at HF/6-31+G** theory level in Gaussian 16. The ESP charges were then calculated in Gaussian 16. The Cartesian coordinates and RESP charges were then calculated in SYBL Mol2 format using antechamber in AMBER 18.

Carbon atoms are represented using magenta, nitrogen atoms using blue and hydrogen atoms using light grey.

Optimized structure, cartesian coordinates and RESP charges of ligand 3



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4	C4	-6.0640	-0.7910	0.1180	ca	1	MOL	0.267665
5	C5	-6.9750	-1.2240	1.1010	ca	1	MOL	-0.317433
6	C6	-6.5870	-1.2810	2.4070	ca	1	MOL	0.001964
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11	H4	-7.2890	-1.6120	3.1510	ha	1	MOL	0.163356
12	C8	-5.5760	-0.3450	-2.1290	ca	1	MOL	0.074429
13	C9	-4.2940	0.0560	-1.8340	ca	1	MOL	-0.387021
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18	H8	-8.5230	-0.4900	-1.1390	h1	1	MOL	0.135075
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36	H15	0.4610	3.6590	3.0310	ha	1	MOL	0.162874
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43	H19	3.6440	-0.8360	-1.9990	hc	1	MOL	0.038762
44	H20	4.9840	0.1220	-2.5870	hc	1	MOL	0.038762
45	C23	4.8150	0.0840	-0.4310	c3	1	MOL	-0.211737
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47	H22	5.4210	0.9690	-0.2870	hx	1	MOL	0.107019
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49	C25	4.9740	-2.4030	-0.0780	c3	1	MOL	-0.058084
50	C26	6.6290	-2.3790	1.7260	c3	1	MOL	-0.049737
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55	H26	4.0090	-2.2080	0.3710	hx	1	MOL	0.089768
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57	H28	6.3960	-2.5350	2.7700	hc	1	MOL	0.067819
58	H29	6.4850	-3.9340	0.1980	hc	1	MOL	0.067819
59	H30	5.1890	-3.9980	1.3550	hc	1	MOL	0.067819
60	N3	5.7090	-1.0860	-0.1070	n4	1	MOL	0.298433
61	C28	6.8690	-1.1530	-1.0490	c3	1	MOL	-0.336301
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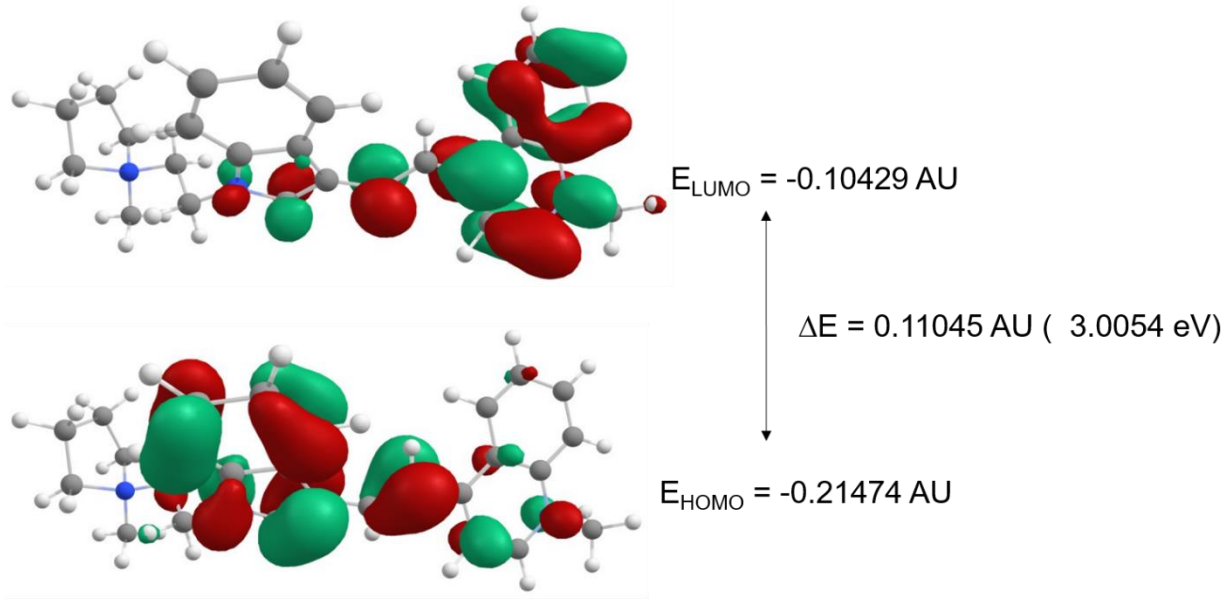
Figure S22. The optimized structure of ligand **3**. The ligand was optimized at HF/6-31G* theory level in Gaussian 16. The ESP charges were then calculated in Gaussian 16. The Cartesian coordinates and RESP charges were then calculated in SYBL Mol2 format using antechamber in AMBER 18. Carbon atoms are represented using yellow, nitrogen atoms using blue and hydrogen atoms using light grey.

Isosurface images of the Frontier Molecular Oribitals of ligands

A



Ligand 1

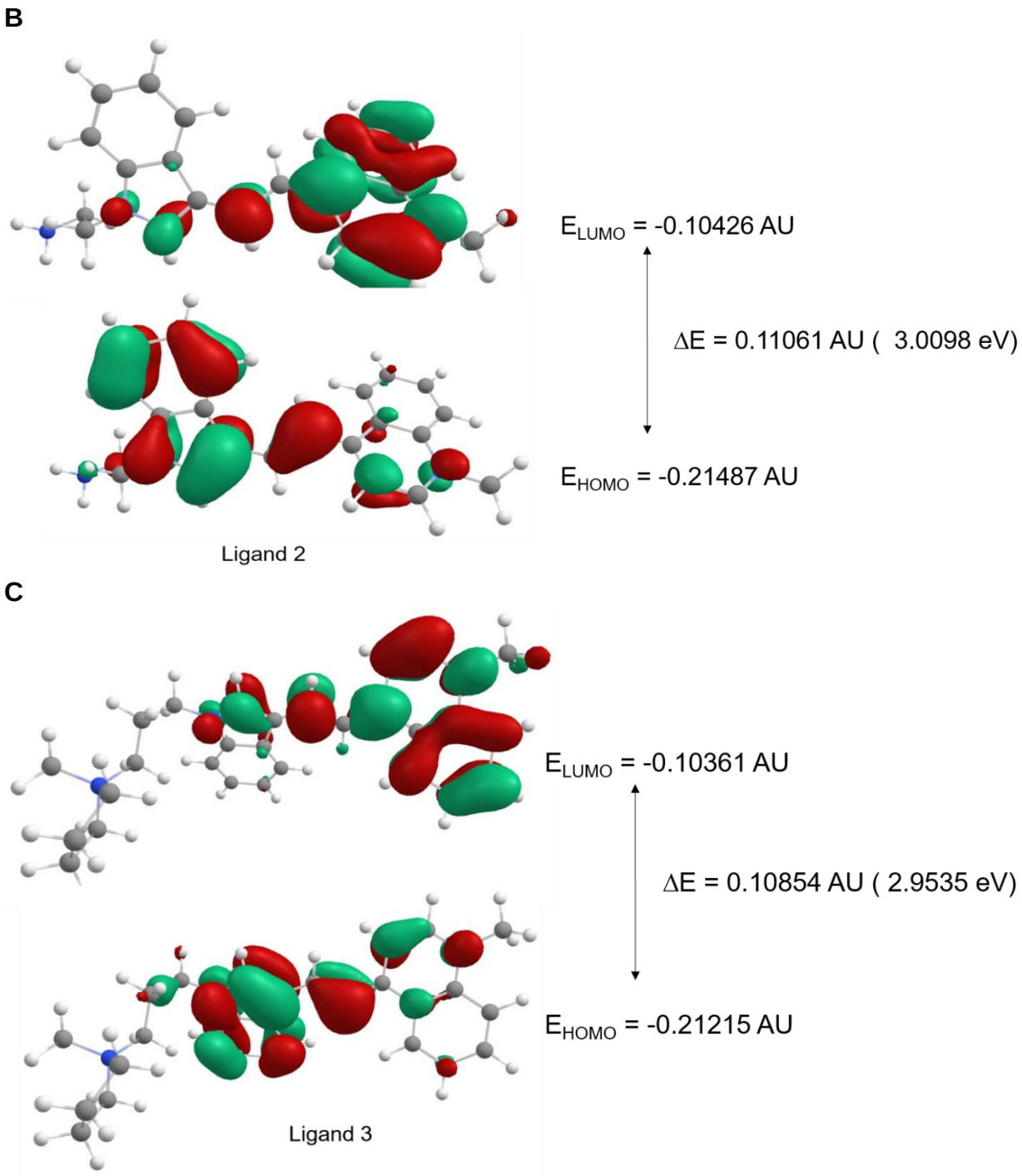


Figure S23. Isosurface plots of Frontier Molecular Orbitals of (A) ligand **1**; (B) ligand **2** and (C) ligand **3**.The energies of the HOMO and LUMO are given.

Docked structures of ligand 1 used for simulation

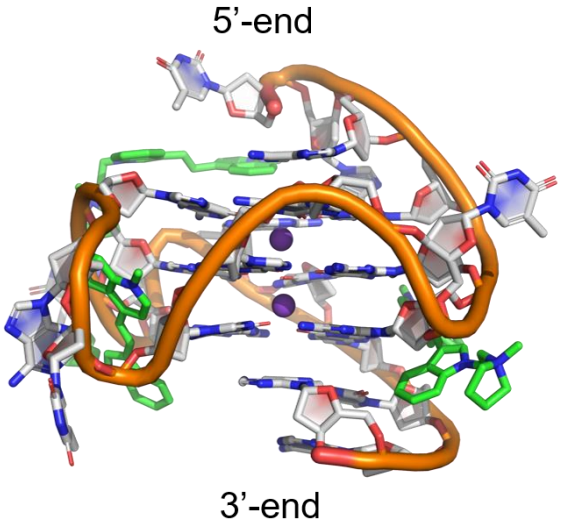


Figure S24. The best conformations with lowest energy of ligand **1** with *c-MYC* G4 DNA (PDB ID: 1XAV) after docking inAutoDock 4.2.6. used for MD simulations. The 3 conformers with different binding modes were chosen from the 250 conformers generated. The ligands are represented in green color.

Per-nucleotide RMSF values of *c-MYC* G4 DNA

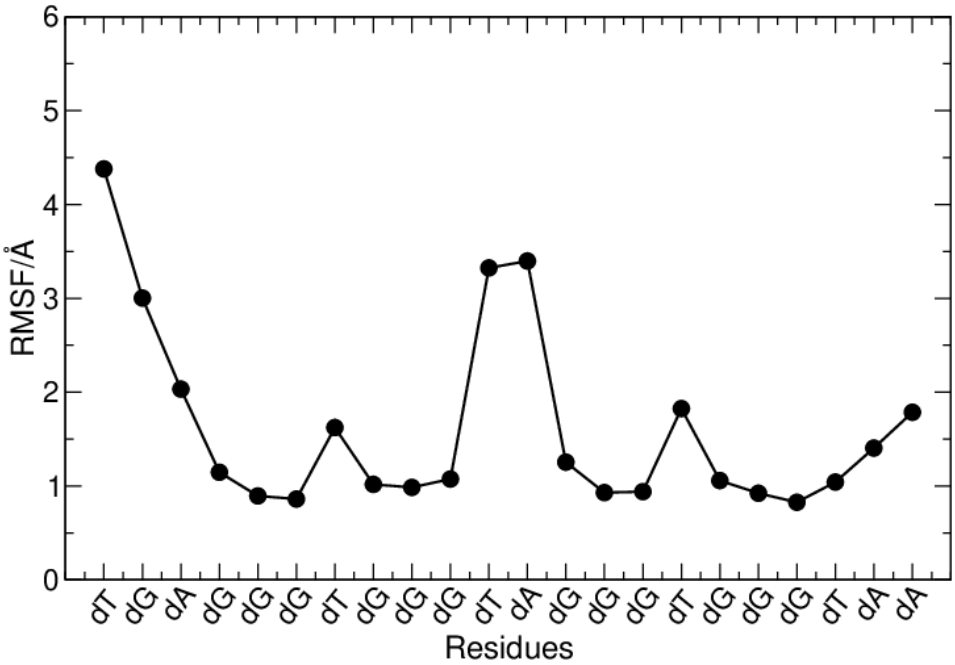


Figure S25. Per-nucleotide-RMSF values of *c-MYC* G4 DNA. The graphs are plotted as fluctuations against the nucleotide number from 5′ to 3′.

Axial view of the pose 1 and pose 2 of the ligand 1

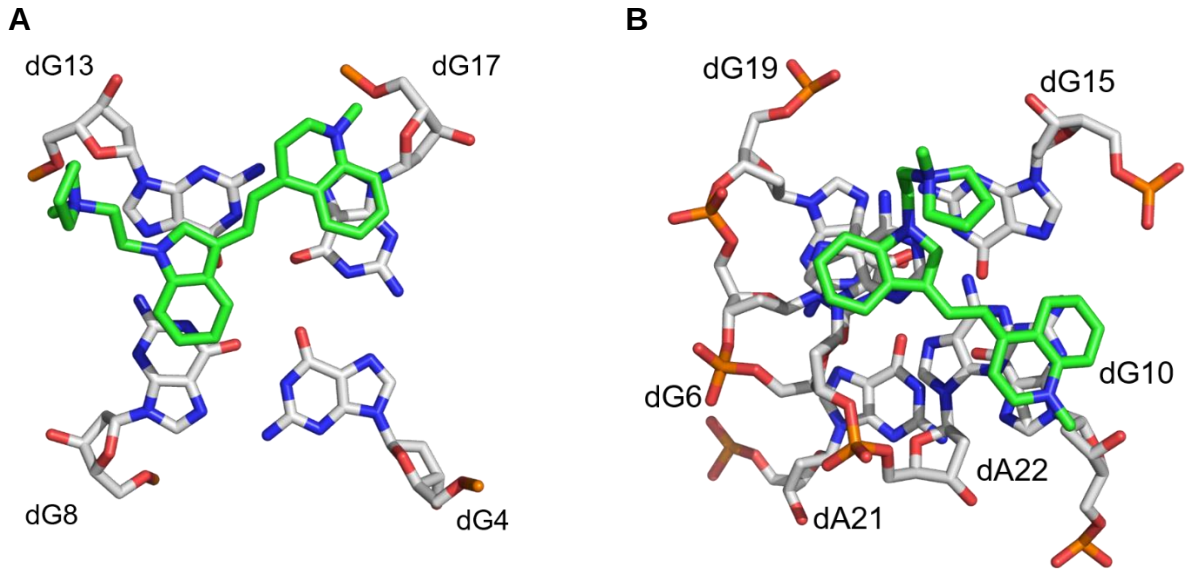


Figure S26. Axial view of ligand (A) pose 1 where the ligand stacked at the 5′- end and (B) Pose 2 where the ligand stacked at the 3′- end on the *c-MYC* G4 quartet. Carbon atoms of DNA are represented using white and carbon atoms of ligand are represented using green, nitrogen atoms using blue, oxygen atoms using red and phosphorus using orange-red

Major non covalent interactions of the ligand 1 poses with the *c-MYC* G4 DNA

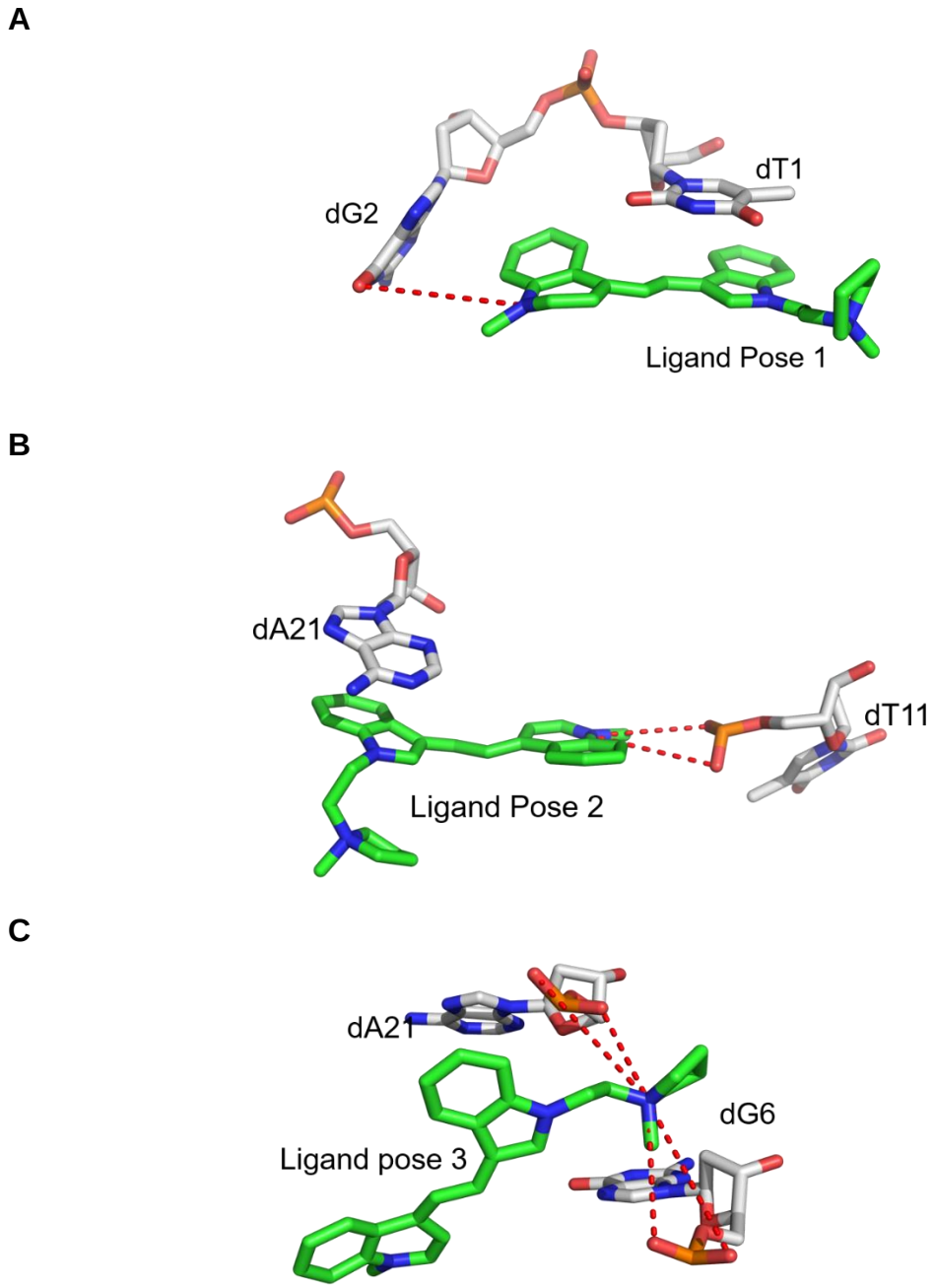


Figure S27. Major interactions of the ligand **1** poses with *c-MYC* G4 DNA is represented. (A) Ligand pose 1 stacking interaction with the flanking nucleotide dT1 and the electrostatic interaction with the dG2; (B) Ligand pose 2 stacking interaction with 3′ flanking nucleotide dA21 and the electrostatic interaction with dT11 and (C) Ligand pose 3 electrostatic interactions with dA21 and dG6. The dashed lines represent the electrostatic interactions. The interactions other than the stacking interactions with the G quartet are represented here.

Orientation of ligand 1 with Telomeric Antiparallel G4 DNA

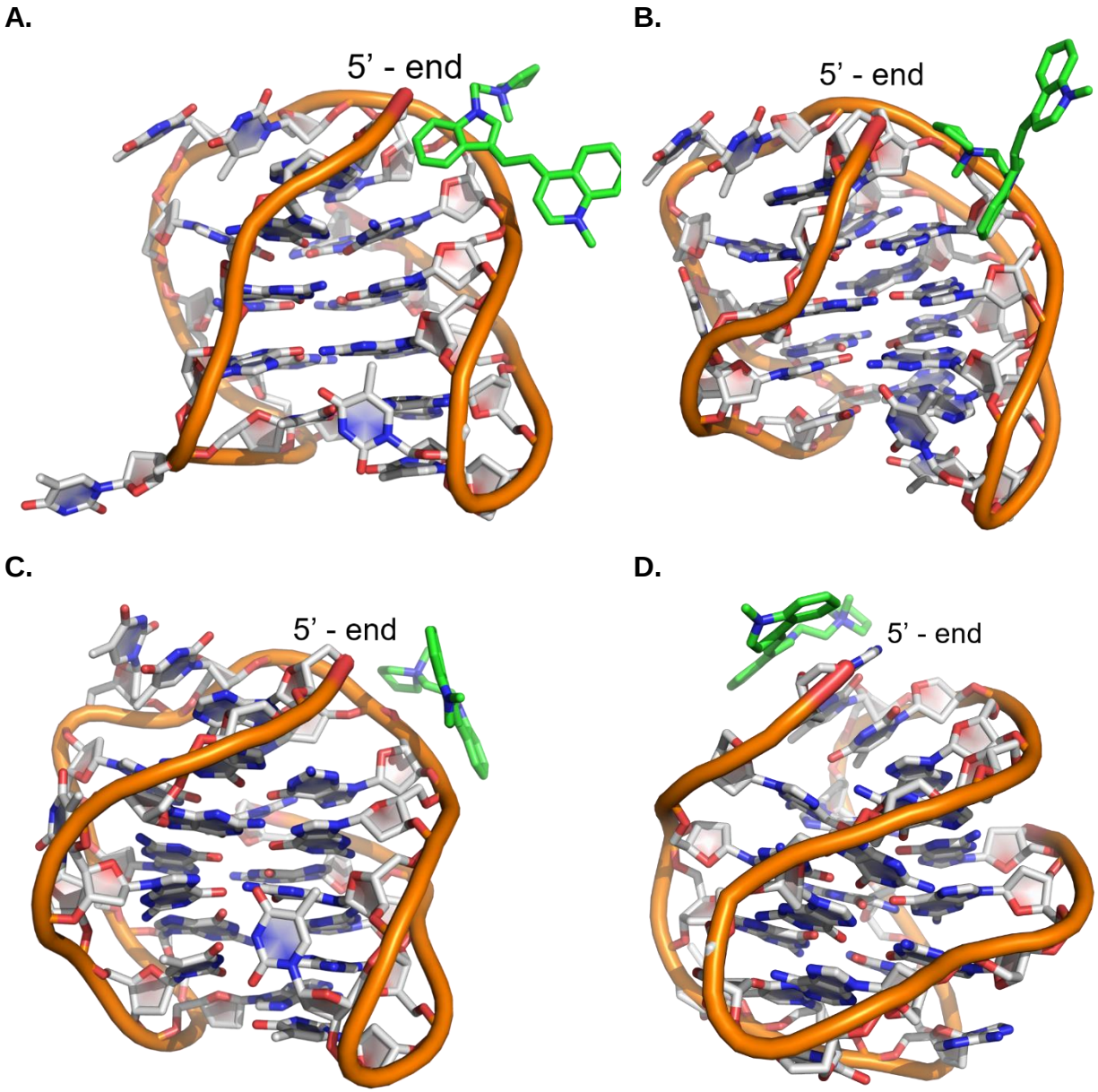


Figure S28. Reorientation of ligand **1** during the course of simulation with Telomeric Antiparallel DNA. Frame at (A) First frame; (B) 5 ns; (C) 10 ns and (D) 500 ns.

Orientation of ligand 1 with Telomeric hybrid 2 G4 DNA

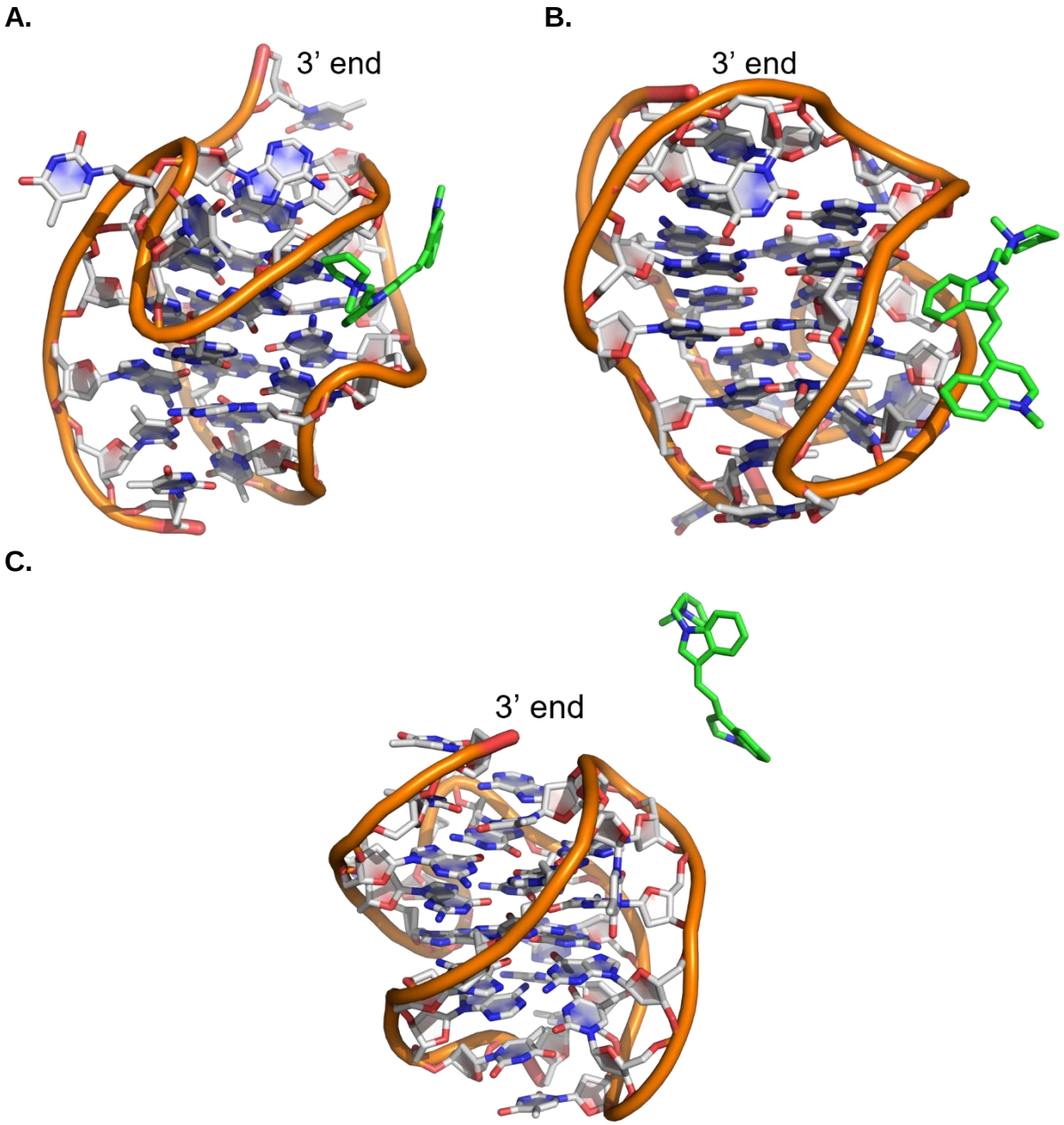


Figure S29. Reorientation of ligand **1** during the course of simulation with Telomeric hybrid 2 DNA. Frame at (A) First frame; (B) 5 ns and (C) 10 ns.

DNA sequences used for various experiments

Table S1. List of oligonucleotides used for the experiments.

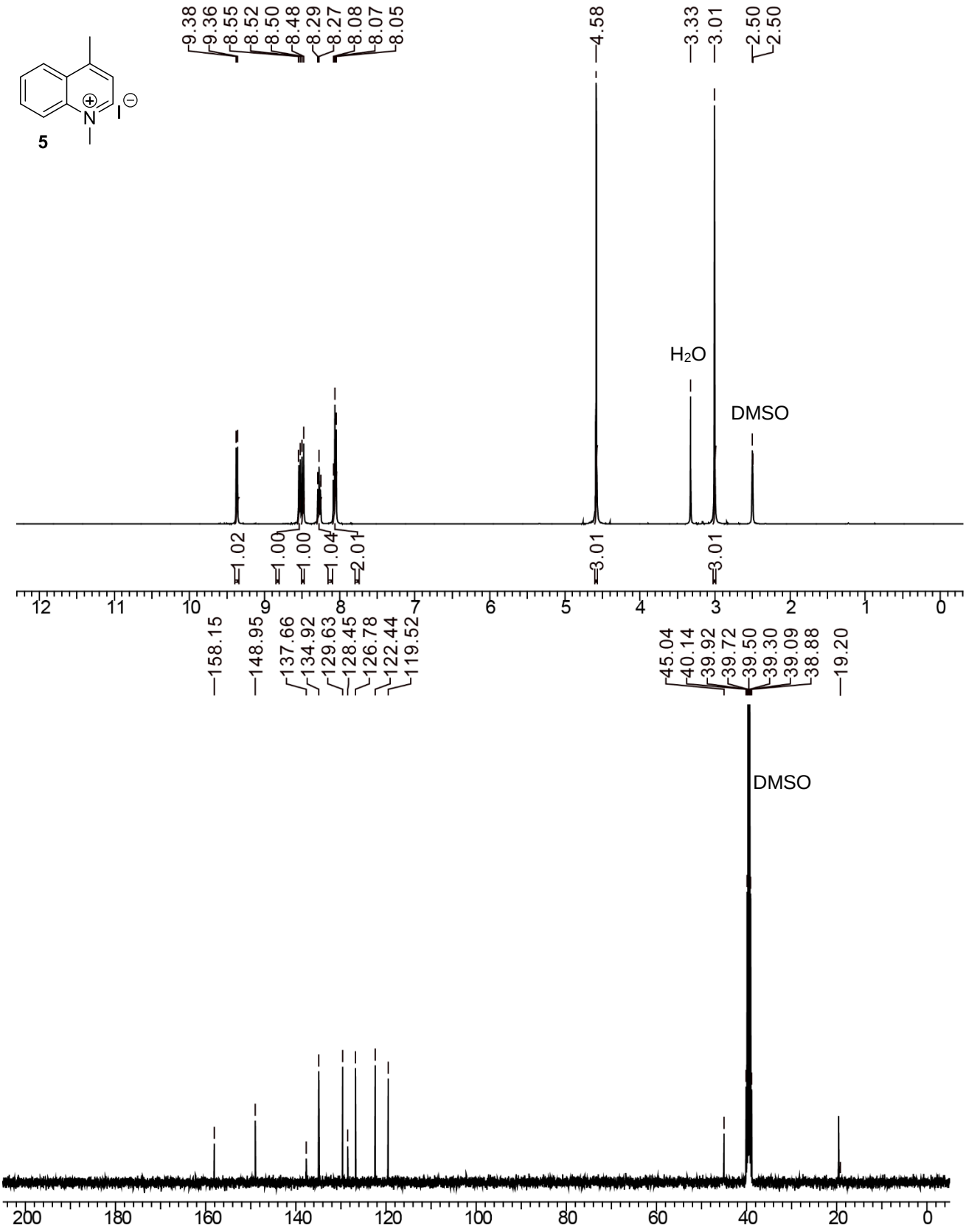
Description	Sequence
Telomeric DNA	5'-AGGGTTAGGGTTAGGGTTAGGG-3'
c-MYC DNA	5'-TGAGGGTGGGTAGGGTGGGTAA-3'
c-KIT1 DNA	5'-GGGAGGGCGCTGGGAGGAGGG-3'
h-RAS 1 DNA	5'-TCGGGTTGCGGGCGCAGGGCACGGGCG -3'
Duplex-17 (DS17)	5'-CCAGTTCGTAGTAACCC-3'
	5'-GGGTTACTA CGAACTGG-3'

Binding energy Parameters of *c-MYC* G4-ligand complexes

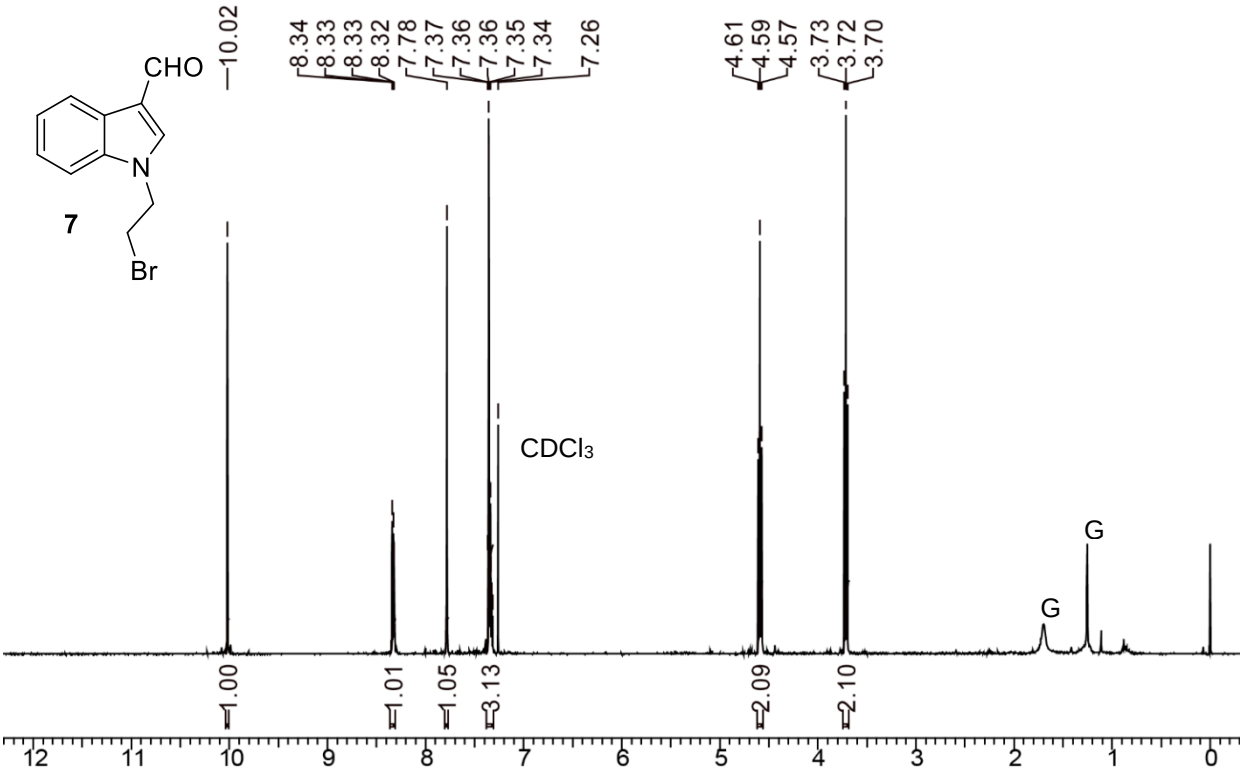
	c-MYC (PDB ID: 1XAV)
ΔE_{ELEC}	-2298.95 ± 87.61
ΔE_{VDW}	-85.15 ± 7.18
$\Delta E_{MM}(\Delta E_{ELEC} + \Delta E_{VDW})$	-2383.61 ± 92.50
ΔPB_{np}	-7.61 ± 0.61
ΔPB_{cal}	2313.40 ± 89.71
$\Delta PB_{solv}(\Delta PB_{np} + \Delta PB_{cal})$	2305.79 ± 89.36
$\boldsymbol{\Delta H_{PB}(\Delta E_{MM} + \Delta PB_{solv})}$	**-77.81 ± 6.08**
$\boldsymbol{T\Delta S}$	**-29.15 ± 9.05**
$\boldsymbol{\Delta G(\Delta H_{PB} - T\Delta S)}$	**-48.66 ± 10.54**

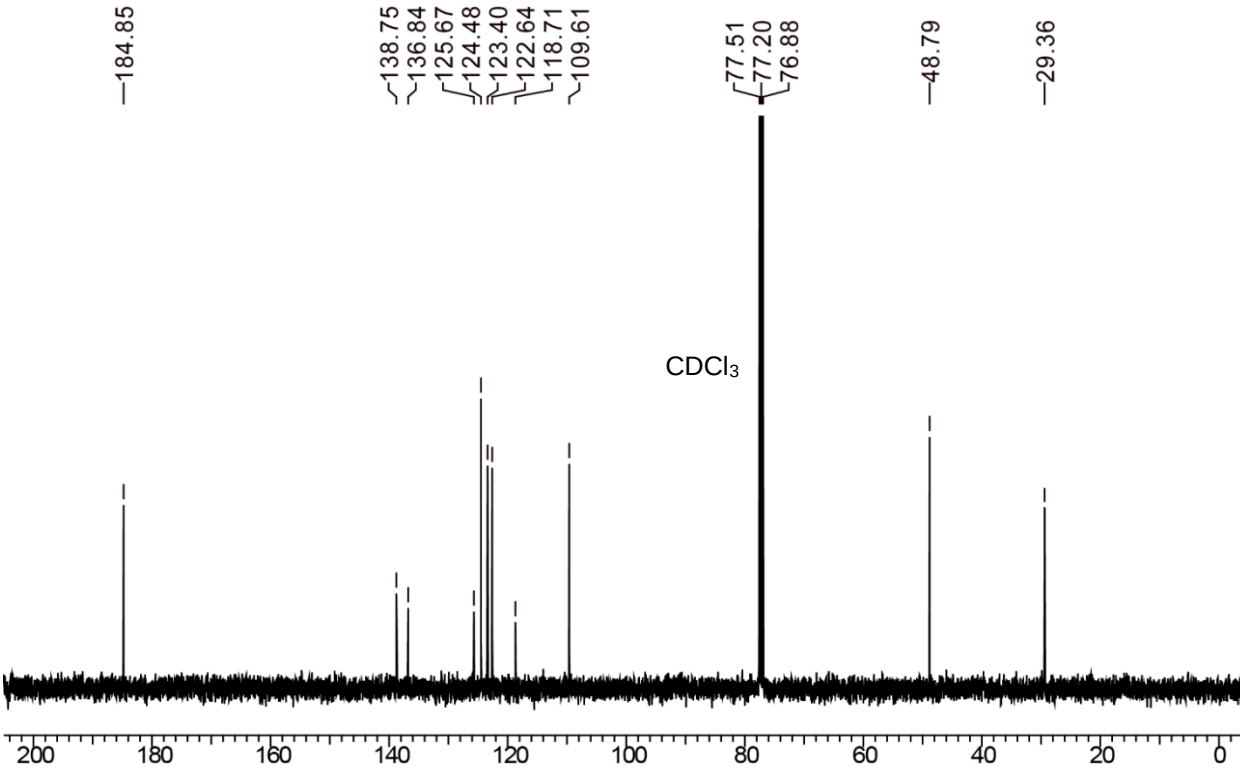
Table S2. Binding free energy components of *c-MYC* G4 DNA and ligand **1** complex has been calculated from the last 20 ns of the 500 ns simulation by considering every 5th frame from a total of 2000 frames. The molecular-mechanical energy calculations were performed using MM/PBSA, and entropy calculations using nmode analysis. ΔE_{ELEC} is the electrostatic contribution. ΔE_{VDW} is the Vander Waals contribution. ΔE_{MM} is the total molecular mechanical energy. $\Delta PB_{np}$is the non-polar contribution to the solvation energy. ΔPB_{cal} is the electrostatic contribution to the solvation energy. ΔPB_{solv} is the total solvation energy. $T\Delta S$ is the solute entropic contribution. $\Delta G(\Delta H - T\Delta S)$ is the estimated binding free energy. All the values are reported in kcal mol^{-1} . For nmode analysis parameters used were: drms = 0.5; dielec(distance dependent dielec) = 4; maxcyc = 10,000 and AMBER prescribed default values were used for PB calculations

^{1}H and ^{13}C NMR spectra of compound 5 (G:Grease)

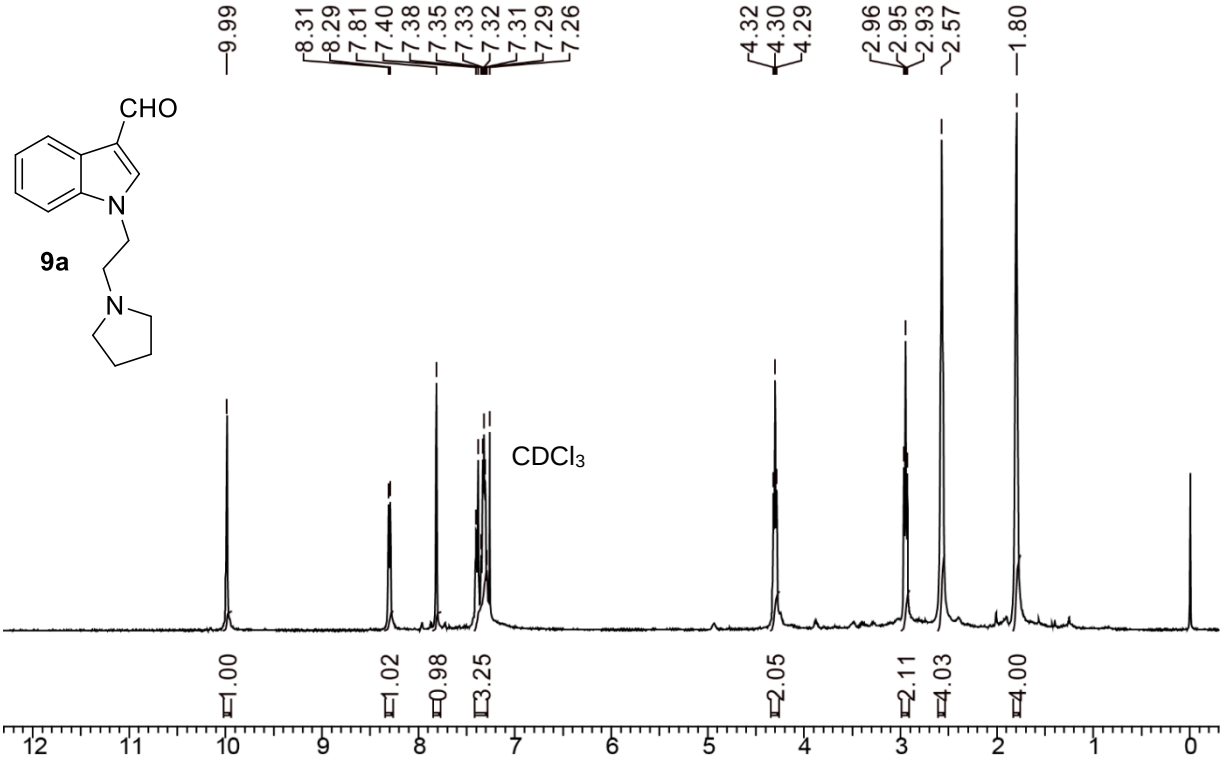


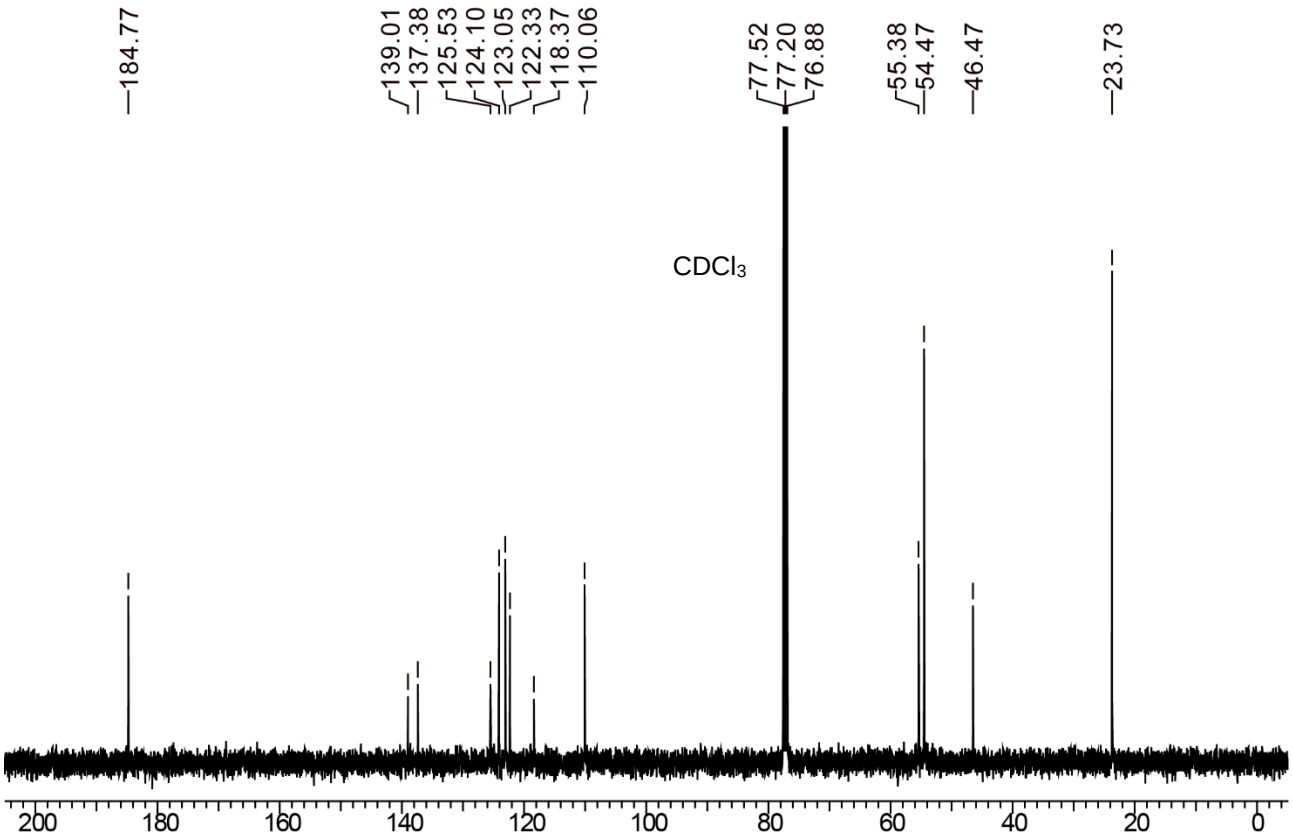
^{1}H and ^{13}C NMR spectra of compound 7



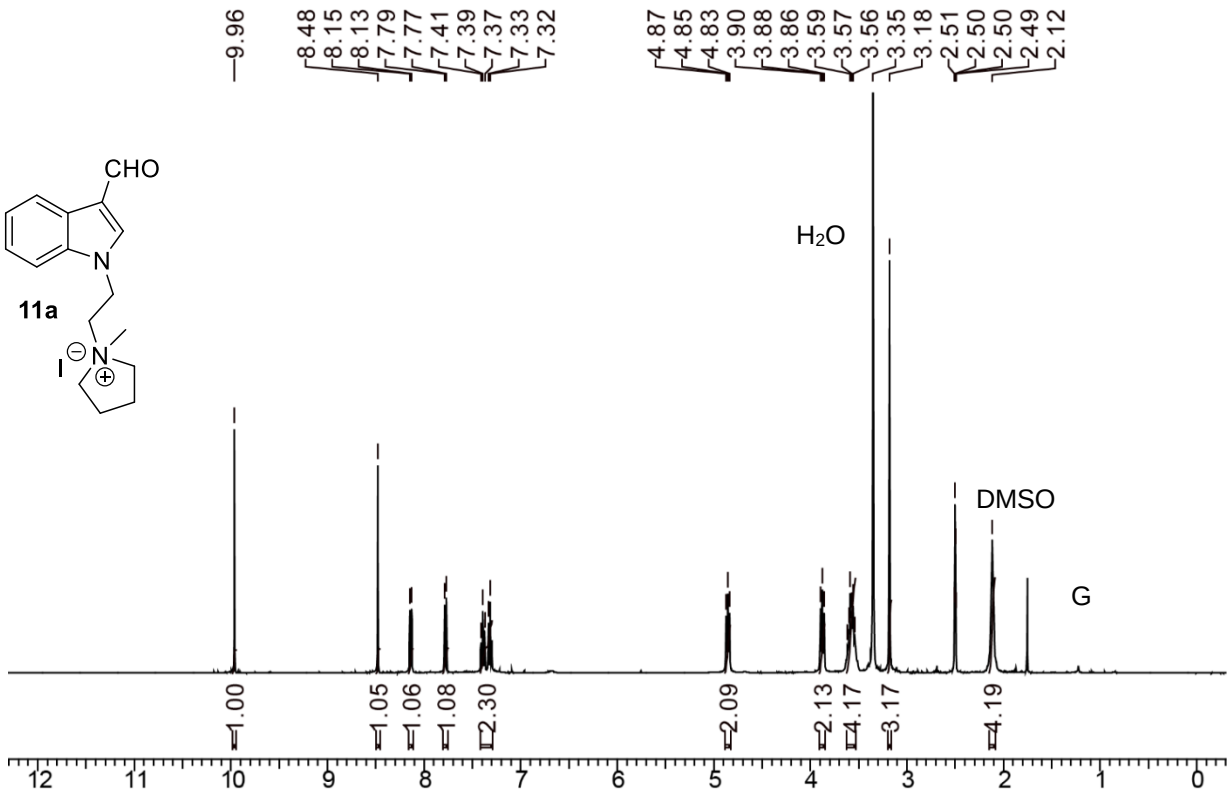


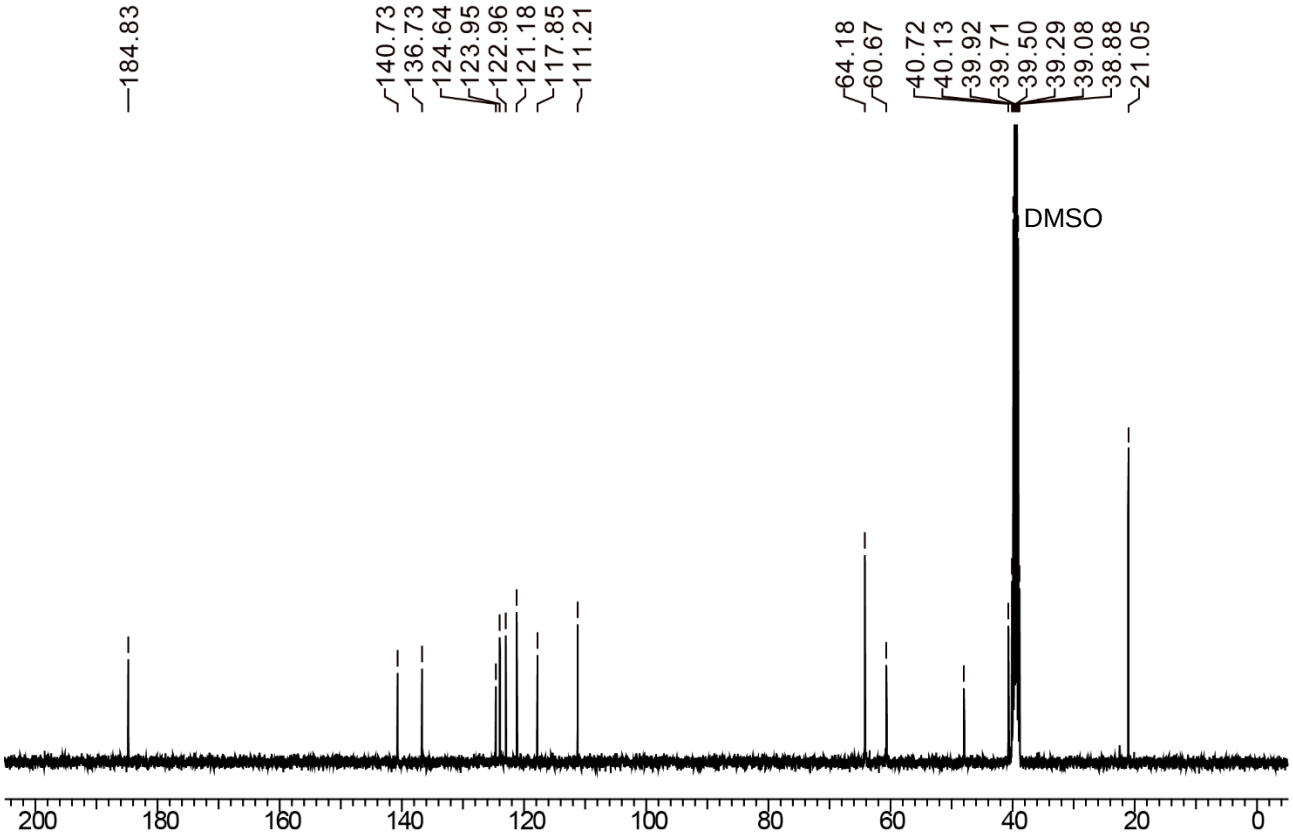
^{1}H and ^{13}C NMR spectra of compound 9a



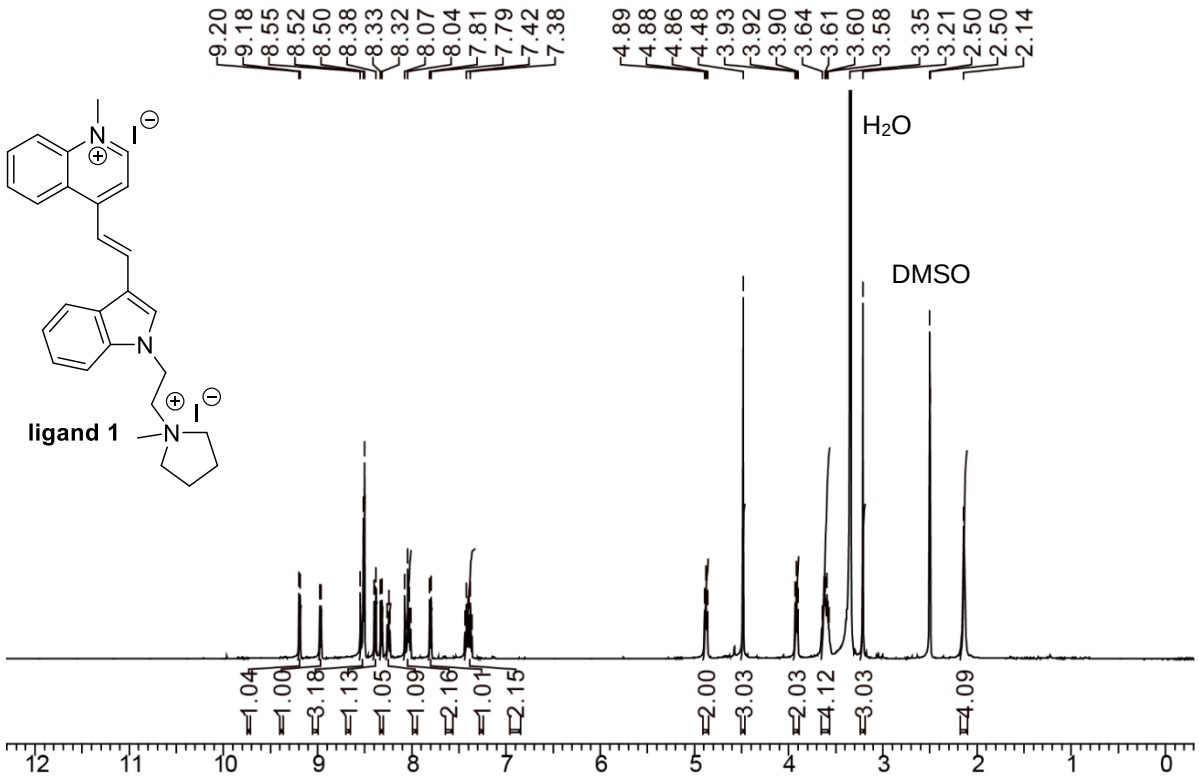


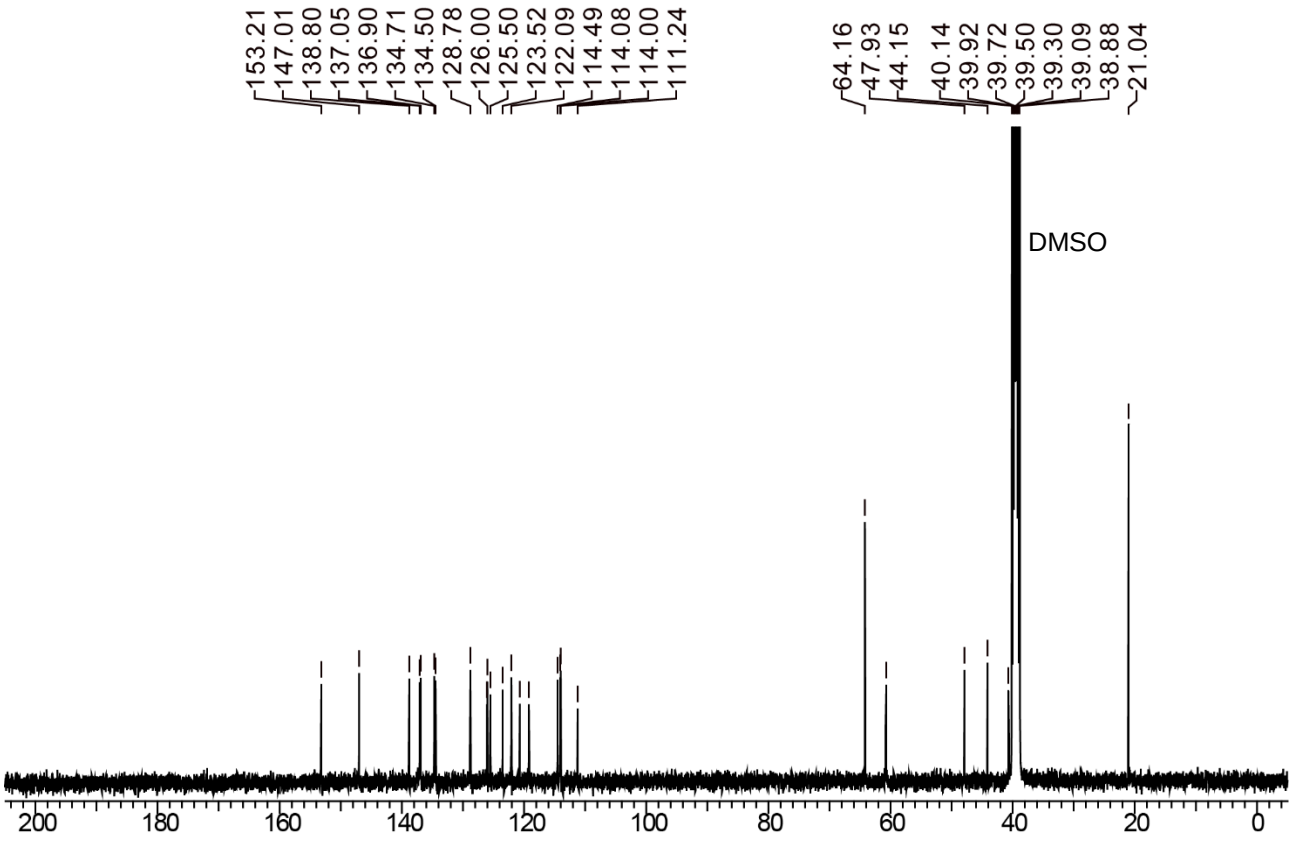
^{1}H and ^{13}C NMR spectra of compound 11a



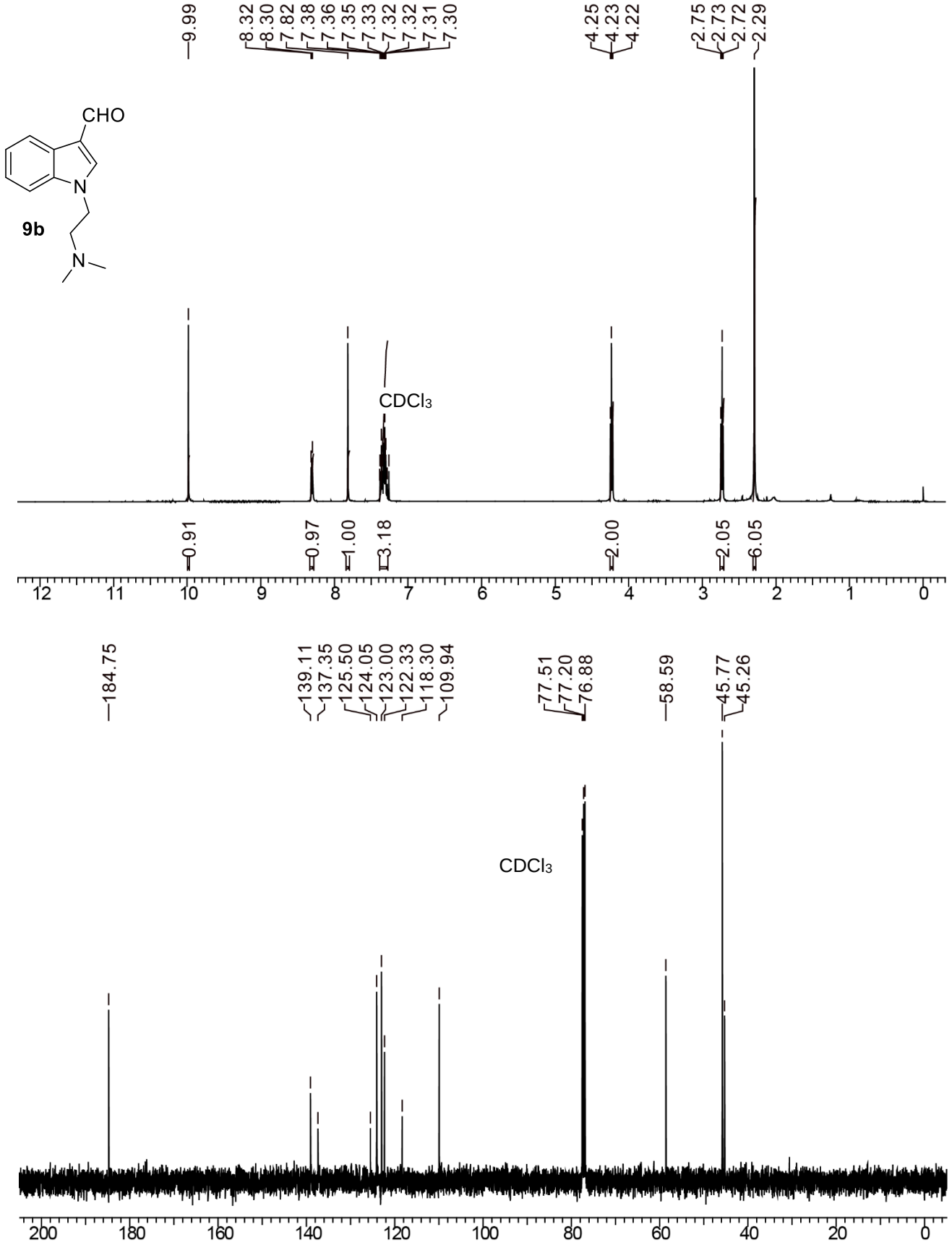

184.83
140.73
136.73
124.64
123.95
122.96
121.18
117.85
111.21
64.18
60.67
40.72
40.13
39.92
39.71
39.50
39.29
39.08
38.88
21.05
DMSO
200
180
160
140
120
100
80
60
40
20
0

^{1}H and ^{13}C NMR spectra of ligand 1

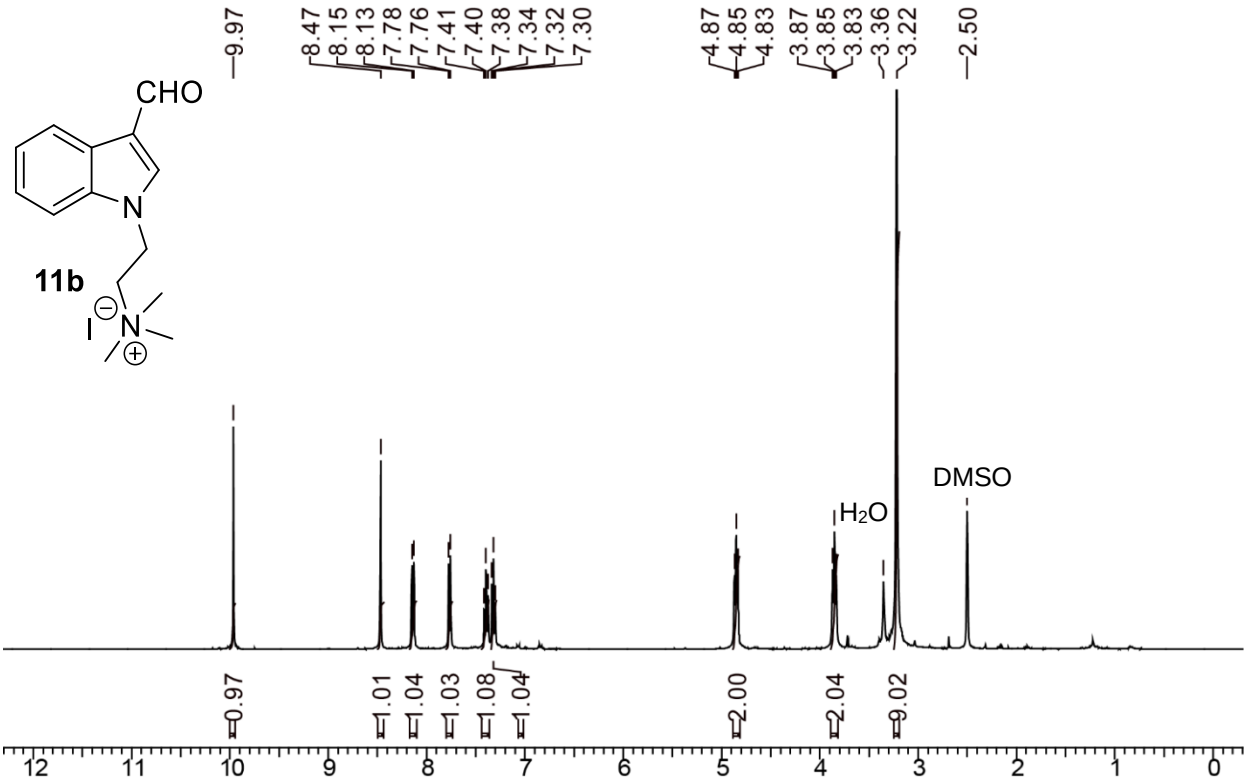


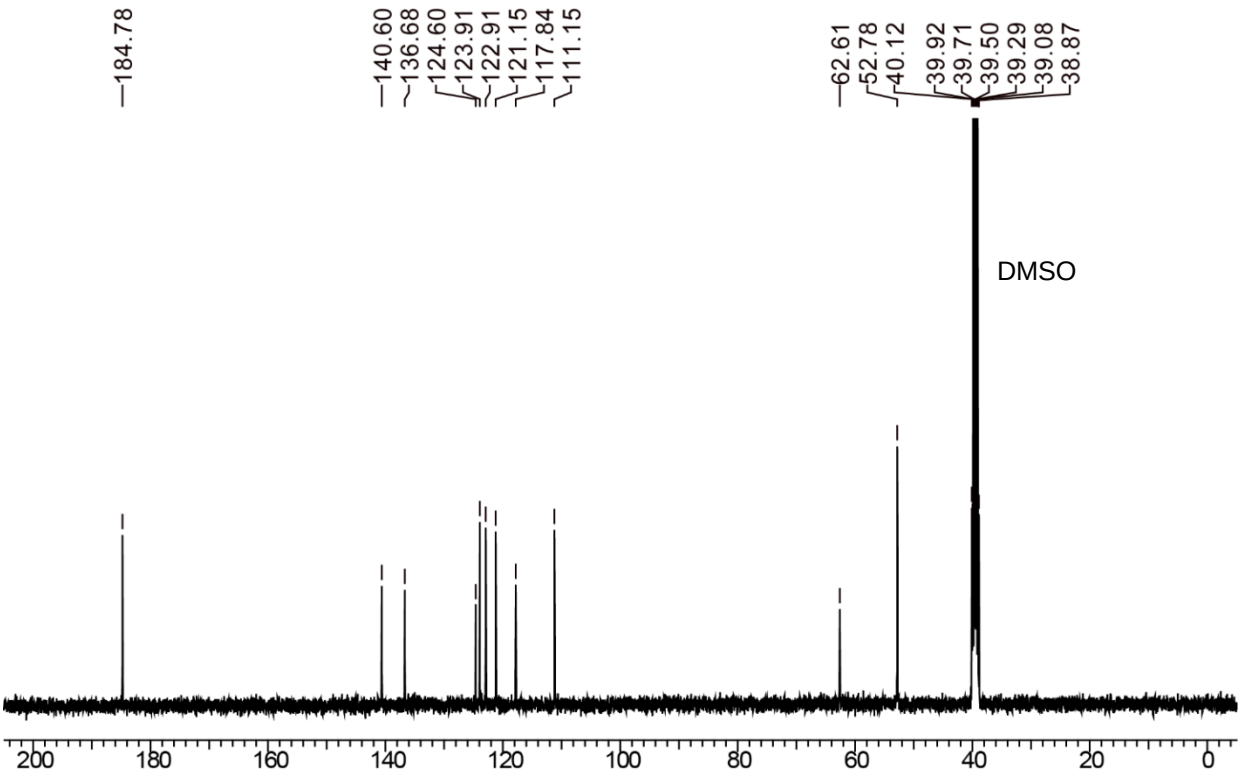


^{1}H and ^{13}C NMR spectra of compound 9b

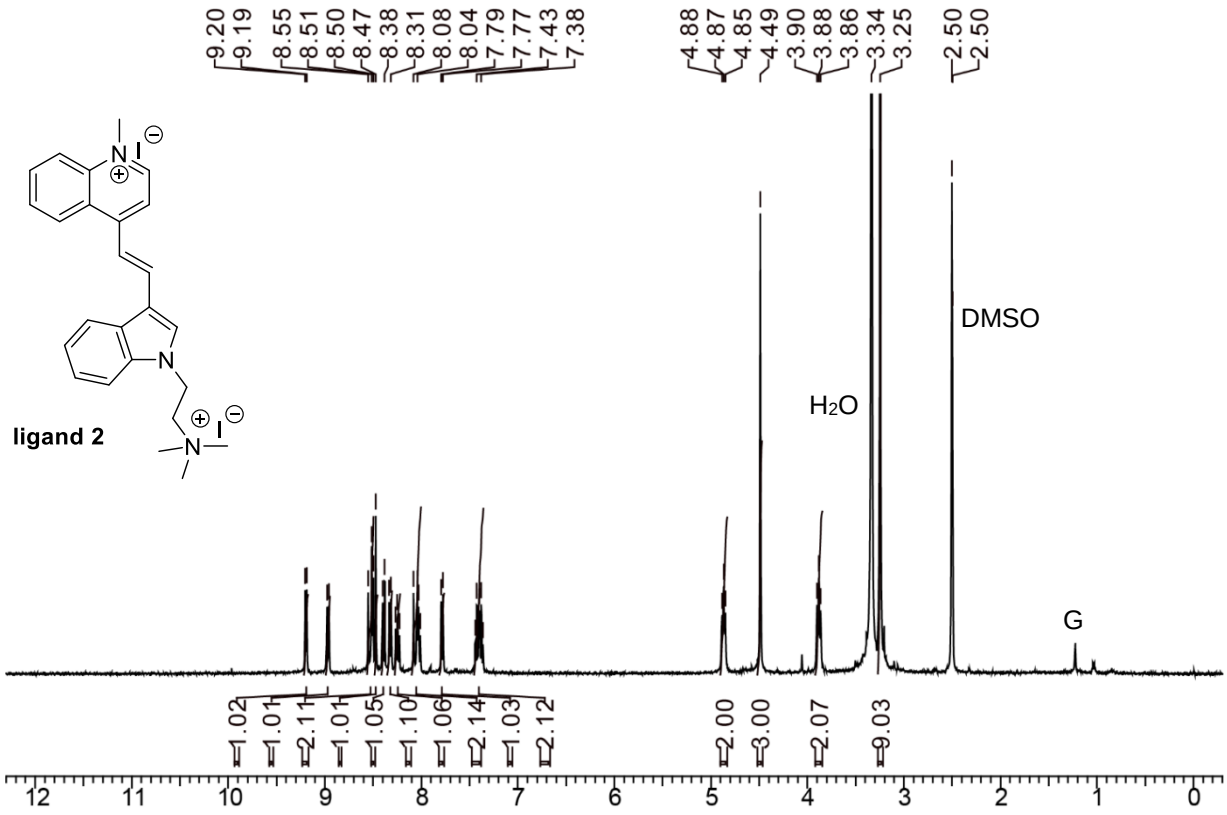


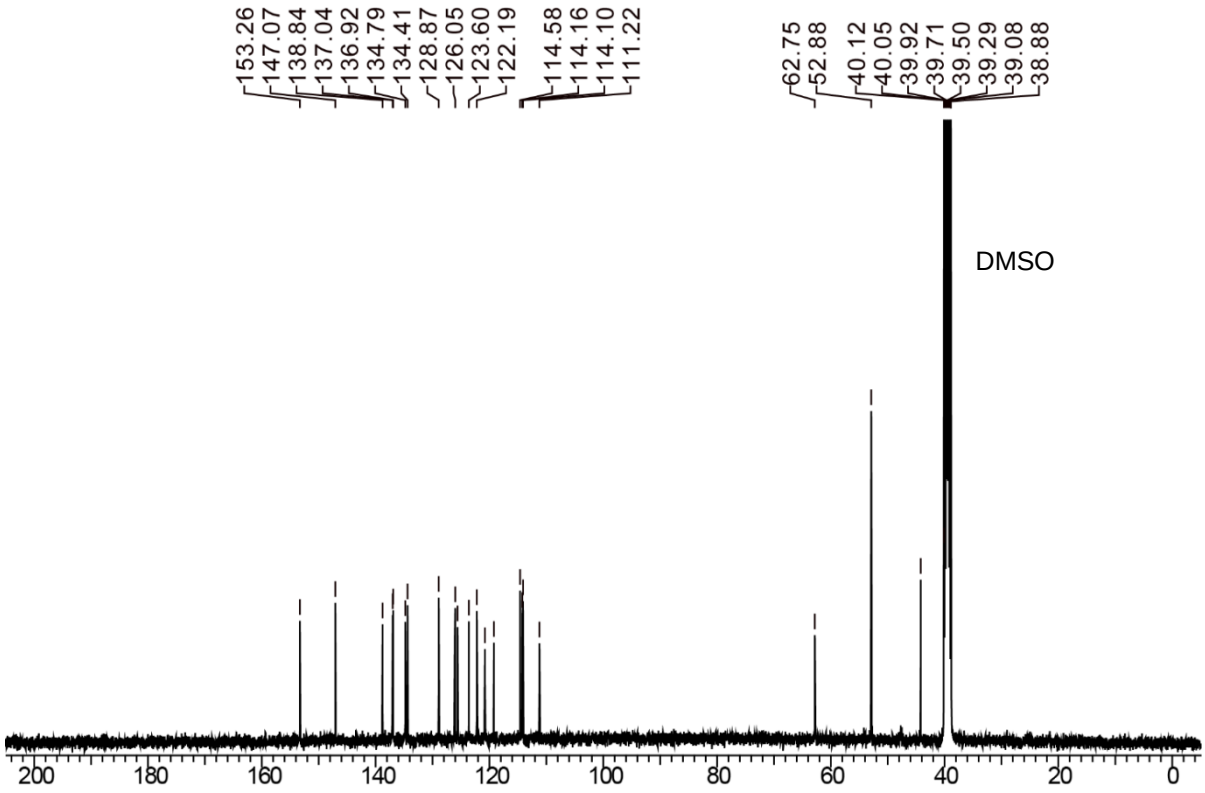
^{1}H and ^{13}C NMR spectra of compound 11b



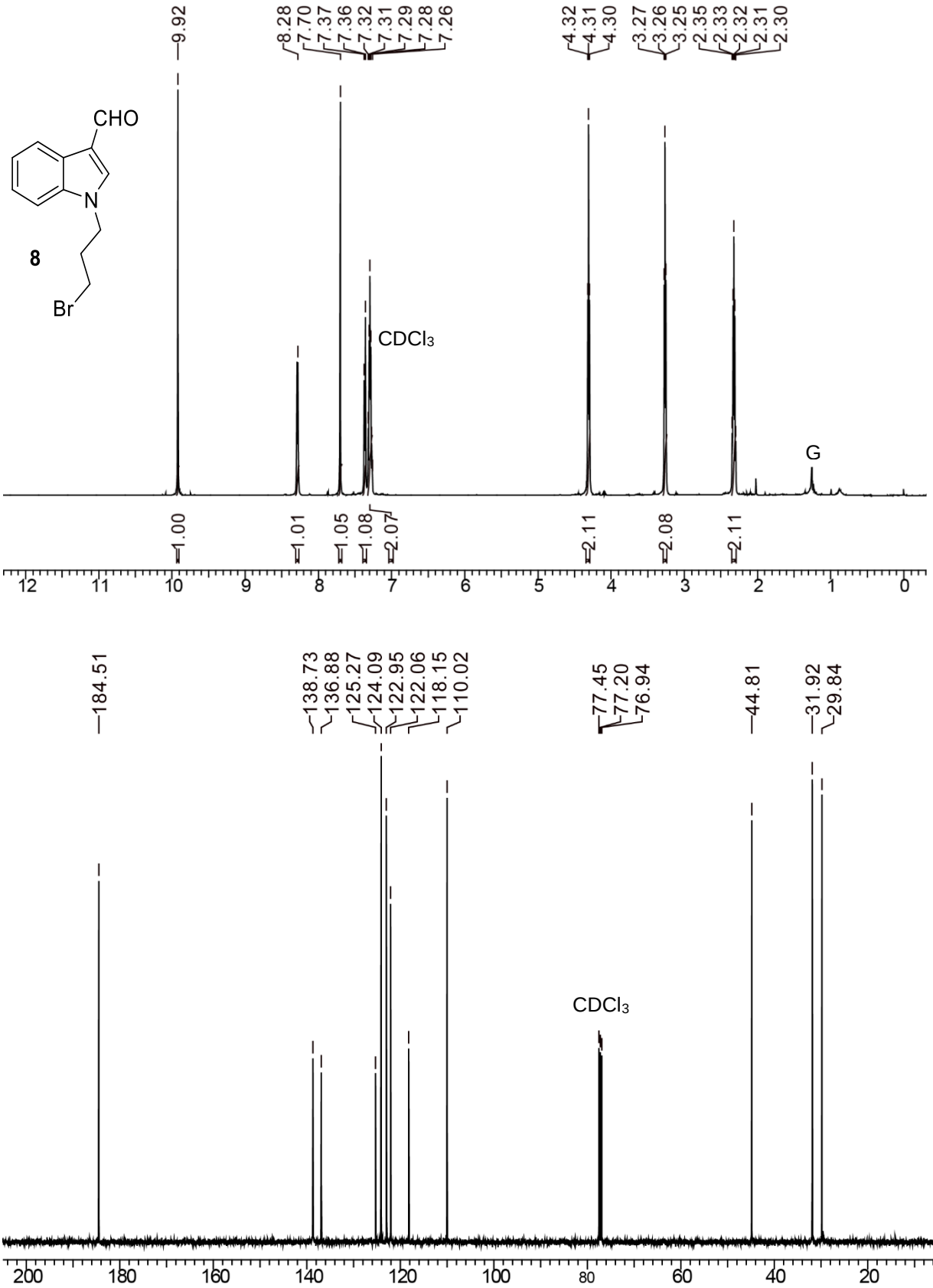


^{1}H and ^{13}C NMR spectra of ligand 2

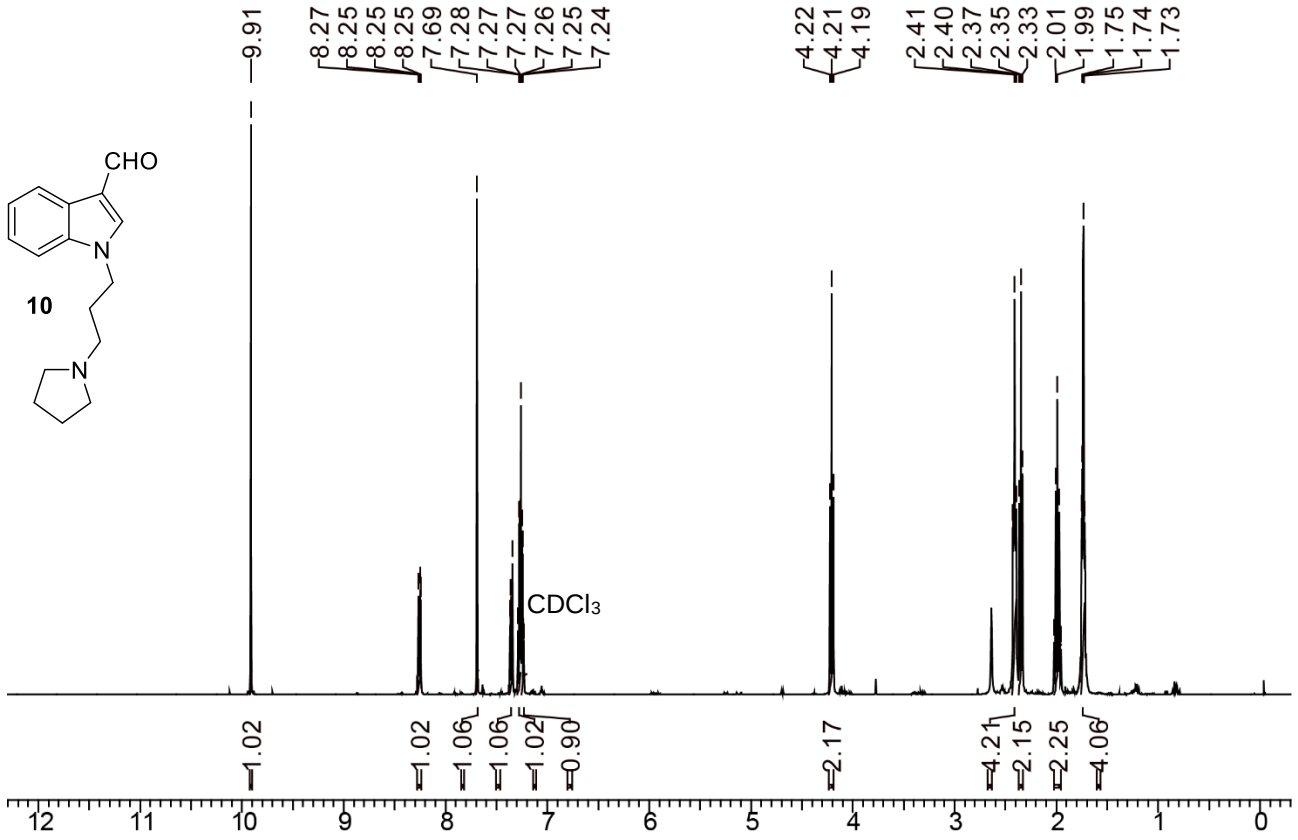


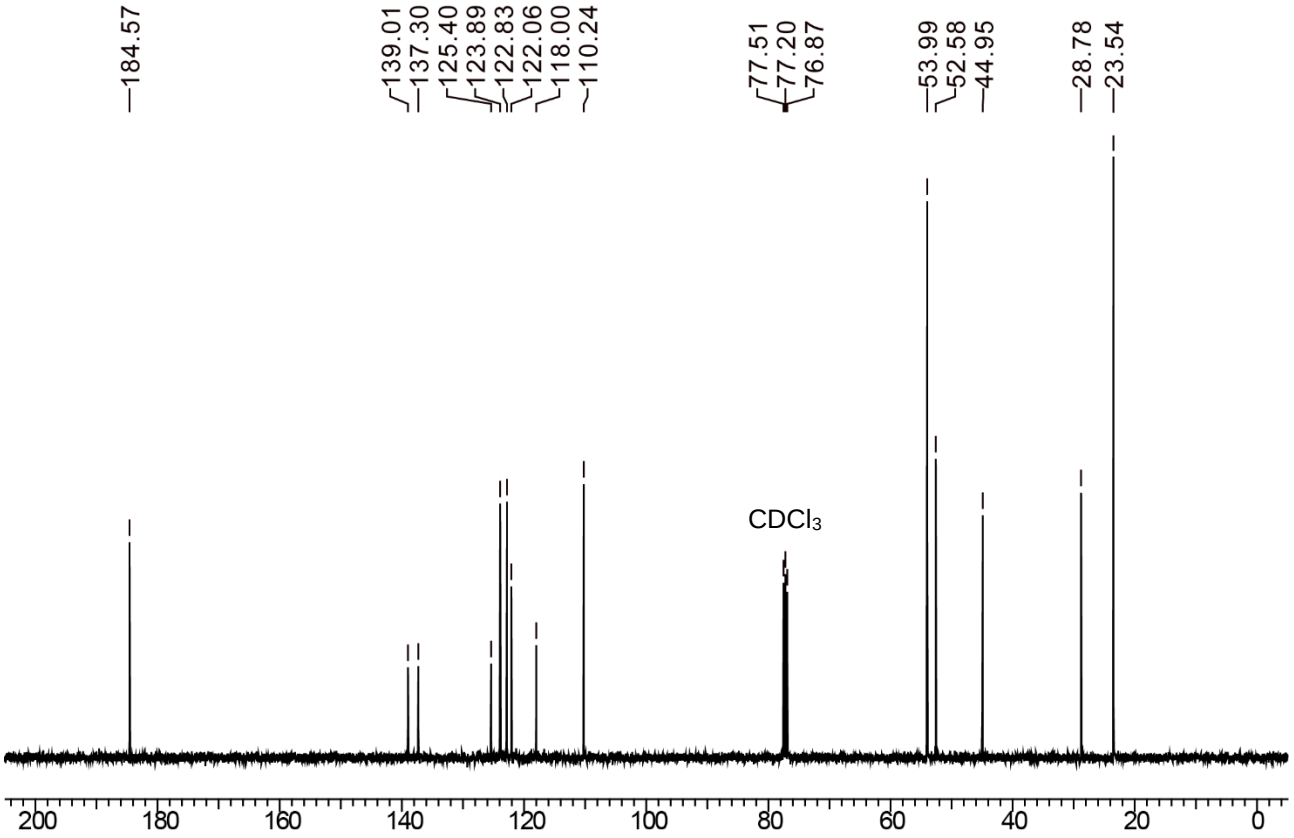


^{1}H and ^{13}C NMR spectra of compound 8

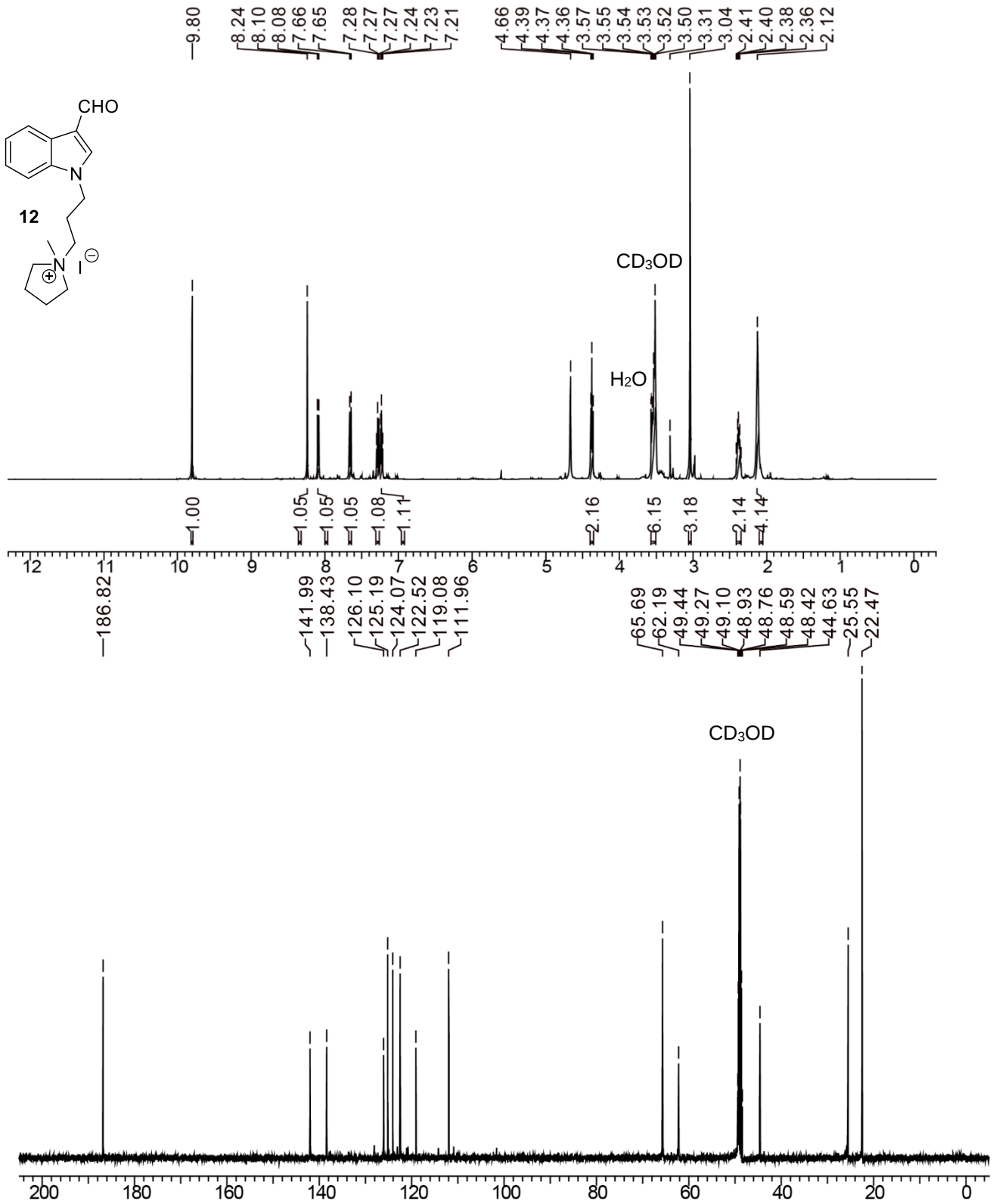


^{1}H and ^{13}C NMR spectra of compound 10





^{1}H and ^{13}C NMR spectra of compound 12



^{1}H and ^{13}C NMR spectra of ligand 3