Supporting Information

Dye-functionalized phosphate binding macrocycles: from phosphate to G-quadruplex recognition and "turn-on" fluorescence sensing.

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General

All the solvents were dried according to standard procedures. Reactions were performed in oven-dried round bottom flask. Crude products were purified by column chromatography on silica gel 100-200 mesh. TLC plates were visualized by exposure to ultraviolet light and/or by exposure to acidic ethanolic solution of ninhydrin followed by heating (<1 min) on a heat gun (~250 °C). Organic solutions were concentrated on rotary evaporator at 35–40 °C. **NMR Spectra** were measured on ASCEND 600 FT spectrometer (Bruker Corp., Billerica, MA), 600 MHz for ^{1}H NMR and 150.9 MHz for ^{13}C NMR. The chemical shifts are reported in δ [ppm] relative to external standards (solvent residual peak). The solvent used is reported for each spectrum. **Mass Spectra:** Finnigan MAT TSQ 7000 (ESI). **Melting Point:** Melting Points were determined on Büchi SMP or a Lambda PhotometricsOptiMelt MPA 100. **Absorption spectra** were measured in 1 cm quartz cuvettes with Varian Cary BIO 50 UV/VIS/NIR Spectrometer. **Emission spectra** were recorded with aqueous buffered solution in 1 cm quartz cuvettes (Hellma) on a FluoroMax 4 (Horiba) with a temperature control. **pH-Measurements** were carried out on a Mettler Toledo G20 Titrator equipped with a DG115-SC pH-electrode. The electrode was calibrated with standard calibrating solutions from Mettler Toledo. The reaction vessels were kept at constant temperature 23°C. The starting compounds were purchased from TCI, Sigma-Aldrich and Acros Chemicals.

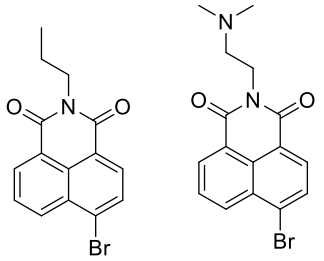
Buffer and dyes stock solutions. Experiments with nucleic acids were performed in 'K-100' buffer, containing 0.1 M KCl and 0.01 M lithium cacodylate ($LiAsO_2Me_2$) in MilliQ water at pH 7.2 (adjusted with HCl). Absorption studies were performed either in the same buffer or in spectroscopic-grade solvents (methanol and DMSO). Macrocycles were dissolved in DMSO to obtain 4 mM stock solutions. Stock solutions of macrocycles were stored at −20 °C. Macrocycles solutions were kept in the dark at all times, to avoid photoinduced degradation.
Oligonucleotides were purchased from Eurogentec (RP- HPLC purification grade) and used without further purification. Stock solutions were prepared at 100 µM in K-100 buffer and stored at 4 °C. Working solutions (c = 5.6 µM) were prepared by dilution of stock solutions in the same buffer.

Table S1. Sequences of DNA oligonucleotides used in the present study.

Abbreviation	Sequence (5'→3')	Structure/origin
dT22	TTTTTTTTTTTTTTTTTTTT	Single-stranded
ds26	CAATCGGATCGAATTCGATCCGATTG	Duplex
myc22	TGAGGGTGGGTAGGGTGGGTAA	Parallel G4
Pu24T	TGAGGGTGGTGAGGGTGGGGAAGG	Parallel G4
KRAS	AGGGCGGTGTGGGAATAGGGAA	Parallel G4
Hras-1	TCGGGTTGCGGGCGCAGGGCACGGGCG	Antiparallel G4
22CTA	AGGGCTAGGGCTAGGG CTAGGG	Antiparallel G4
hTel21T18	GGGTTA GGGTTAGGGTTTGGG	Antiparallel G4
25TAG	TAGGGTTAGGGTTAGGGTTAGGGTT	Hybrid G4
24TTG	TTGGGTTAGGGTTAGGGTTAGGGA	Hybrid G4

Synthesis of compounds

Synthesis of 4



4a **4b**

4-bromo-1,8-naphthalmides bearing either amine **a** or **b** were prepared according to the adapted literature procedures.[4–6] 4-bromo-1,8-naphthalic anhydride (4 mmol) and the corresponding amine (6.0 mmol) were combined in 135 ml of EtOH. The reaction mixture was heated to 85 °C, and refluxed for 4 h. The reaction mixture was allowed to cool to room temperature and the ethanol and the excess of amine were removed under vacuum. The rest was recrystallized from EtOH, filtrated and washed with EtOH to afford the desired product as a white-gray powder.

4a

Product was obtained as a white-gray powder (1.08 g, 85%). ^{1}H NMR ($CDCl_3$, 25 °C, δ, ppm, *J*/Hz): δ= 1.02 (t, *J*=7.5 Hz, 3H), 1.73-1.80 (m, 2H), 4.13-4.15 (m, 2H), 7.85 (dd, *J*=7.4, 8.4 Hz, 1H), 8.05 (d, *J*=7.8 Hz, 1H), 8.43 (d, *J*=7.8 Hz, 1H) 8.58 (d, *J*=8.4 Hz, 1H), 8.67 (d, *J*=7.4 Hz, 1H).

4b

Product was obtained as a white powder (1.1 g, 80%). ^{1}H NMR ($CDCl_3$, 25 °C, δ, ppm, *J*/Hz): δ= 2.37 (br.s, 6H), 2.69 (t, *J*=6.9, 2H), 4.33 (t, *J*=6.9, 2H), 7.85 (dd, *J*=7.2, 8.4 Hz, 1H), 8.05 (d, *J*=7.8 Hz, 1H), 8.42 (d, *J*=7.8 Hz, 1H), 8.58 (d, *J*=8.4 Hz, 1H), 8.66 (d, *J*=7.2 Hz, 1H).

Synthesis of 1

Compound **4a** or **4b** (3.14 mmol) was suspended in TREN (4ml) and the reaction mixture was stirred for 5 days at room temperature. The saturated brine solution (20 ml) was added and the product was extracted by chloroform (5x50 ml). Organic layers were collected and solvent was removed under reduced pressure. Then extraction procedure was repeated to remove traces of the amine. The extracts were dried over anhydrous Na_2CO_3 and concentrated in vacuum to give deep red solid.

1b

Product was obtained as a deep red solid (1.20 g, 93%). Mp: 107-110 °C. ^{1}H NMR ($CDCl_3$, 25 °C, δ, ppm, *J*/Hz): δ= 2.35 (br.s, 6H), 2.62-2.65 (m, 6H), 2.84 (t, *J*=5.9 Hz, 4H), 2.87-2.92 (m, 2H), 3.40 (q, *J*=4.8, 2H), 4.36-4.22 (m, 2H), 6.63 (d, *J*=8.5 Hz, 1H), 7.10 (br.s, 1H, NH), 7.53 (dd, *J*=7.3, 8.4 Hz, 1H), 8.39-8.46 (m, 2H), 8.53 (dd, *J*=1.1, 7.3 Hz, 1H). ^{13}C {^{1}H} NMR ($CDCl_3$, 25 °C, δ, ppm) 37.87, 39.92, 41.31, 45.77, 51.95, 56.65, 57.08, 104.34, 109.70, 120.72, 122.88, 124.39, 127.31, 130.04, 131.10, 134.70, 150.27, 164.21, 164.86. HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{22}H_{32}N_6O_2$, 413.2660; found, 413.2670. Anal. Calcd for $C_{22}H_{32}N_6O_2$: C, 64.05; H, 7.82; N, 20.37. Found: C, 64.21; H, 7.93; N, 20.12.

Synthesis of macrocycles 2a-b

Compound **1** (0.26 mmol) was dissolved in 30 ml MeOH. Then 2,6-Pyridinedicarboxaldehyde (0.29 mmol) in 30 ml MeOH was added dropwise for 10min. Reaction mixture was stirred at room temperature. After 20 h $NaBH_4$ (1.8 mmol) was added by small portions, and reaction mixture was heated to 60°C and stirred for 1 h. Then was cooled to room temperature, solvent was removed by reduced pressure. Water (30 ml) was added, and the product was extracted with $CHCl_3$ (3x30 ml). After removing the solvent the crude product was purified by column

chromatography (silica gel, CH_2Cl_2/MeOH/ $NH_3 \cdot H_2O$ 100: 10: 1). Product was obtained as a yellow solid

2a

Yield 75 mg, 59%. Mp: 117-120 °C. ^{1}H NMR (DMSO-*d6*, 25 °C, δ, ppm, *J*/Hz): δ= 0.88 (t, *J* = 7.4 Hz, 3H), 1.60 (h, *J* = 7.4 Hz, 2H), 2.55 (dq, *J* = 10.7, 5.9 Hz, 8H), 2.77 (t, *J* = 6.5 Hz, 2H), 3.39-3.42 (m, 2H), 3.66 (s, 4H), 3.93 (dd, *J* = 8.6, 6.3 Hz, 2H), 6.68 (d, *J* = 8.6 Hz, 1H), 7.04 (d, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.8 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.55 (t, *J* = 5.3 Hz, 1H), 8.16 (d, *J* = 8.6 Hz, 1H), 8.28 (d, *J* = 7.2 Hz, 1H), 8.44 (d, *J* = 8.4 Hz, 1H). ^{13}C {^{1}H} NMR (DMSO-*d6*, 25 °C, δ, ppm) 11.88, 21.44, 41.19, 41.54, 47.29, 49.07, 53.13, 53.81, 54.47, 104.32, 108.16, 120.32, 120.46, 122.19, 124.49, 128.59, 129.72, 130.89, 134.55, 136.97, 150.84, 163.32, 164.14. HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{56}H_{68}N_{12}O_4$, 973.5565; found, 973.5562. Anal. Calcd for $C_{56}H_{68}N_{12}O_4$: C, 69.11; H, 7.04; N, 17.27. Found: C, 68.91; H, 7.00; N 17.36.

2b

Yield 67 mg, 50%. Mp: 76-79°C. ^{1}H NMR (DMSO-*d6*, 25 °C, δ, ppm, *J*/Hz): δ= 2.18 (s, 6H), 2.45 (t, J = 7.1 Hz, 2H), 2.53-2.58 (m, 8H), 2.77 (t, J = 6.5 Hz, 2H), 3.41 (q, J = 6.4 Hz, 2H), 3.65 (s, 4H), 4.08 (t, J = 7.1 Hz, 2H), 6.68 (d, J = 8.6 Hz, 1H), 7.04 (d, J = 7.6 Hz, 2H), 7.32 (t, J = 7.8 Hz, 1H), 7.44 (t, J = 7.6 Hz, 1H), 7.56 (br.s, 1H, NH), 8.15 (d, J = 8.4 Hz, 1H), 8.27 (d, J = 7.1 Hz, 1H), 8.43 (d, J = 8.4 Hz, 1H). ^{13}C {^{1}H} NMR (DMSO-*d6*, 25 °C, δ, ppm) 37.63, 41.59, 45.89, 47.38, 53.07, 54.01, 54.68, 57.15, 104.33, 108.12, 120.20, 120.44, 122.15, 124.48, 128.63, 129.73, 130.91, 134.58, 136.90, 150.88, 163.26, 164.12. HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{58}H_{74}N_{14}O_4$, 1031.6096; found, 1031.6090. Anal. Calcd for $C_{58}H_{74}N_{14}O_4$: C, 67.55; H, 7.23; N, 19.01. Found: C, 67.25; H, 7.20; N, 18.94.

Synthesis of macrocycles 3a-b

To a solution of a template (10 equiv of tetrabutylammonium chloride) in dry chloroform (40 mL) were added compound **1** (0.26 mmol, 1 equiv) in dry chloroform (30 mL) and the activated pyridine derivative (0.29 mmol, 1.1 equiv) in dry chloroform (30 mL) dropwise from different funnels with stirring. The reaction mixture was stirred at room temperature for 1 day. The solvent was evaporated in a vacuum. The residue was applied to a gradient silica gel column (CH_2Cl_2/MeOH/ $NH_3 \cdot H_2O$ 100: 10: 1), and the appropriate fractions were evaporated to dryness to give products as yellow powders. Fractions with TBACl were purified by recrystallization from MeOH.

3b

Yield 17 mg, 12%. Mp: 235-238°C. ^{1}H NMR (DMSO-*d6*, 25 °C, δ, ppm, *J*/Hz): δ= 2.19 (s, 6H), 2.46 (t, *J* = 7.1 Hz, 2H), 2.89-2.94 (m, 6H), 3.43 (q, *J* = 6.2 Hz, 4H), 3.48 (q, *J* = 6.4 Hz, 2H), 4.09 (t, *J* = 7.1 Hz, 2H), 6.78 (d, *J* = 8.7 Hz, 1H), 7.48 (t, *J* = 5.5 Hz, 1H, NH), 7.52 (dd, *J* = 8.4, 7.3 Hz, 1H), 8.02 – 7.93 (m, 3H), 8.17 (d, *J* = 8.5 Hz, 1H), 8.32 (dd, *J* = 7.3, 1.1 Hz, 1H), 8.52 (dd, *J* = 8.7, 1.1 Hz, 1H), 9.02 (t, *J* = 5.8 Hz, 2H, NH). ^{13}C {^{1}H} NMR ($CDCl_3$, 25 °C, δ, ppm) 37.60, 38.20, 45.85, 51.87, 53.73, 57.10, 104.29, 108.11, 120.44, 122.20, 124.18, 124.58, 128.71, 129.75, 131.02, 134.60, 139.57, 148.97, 150.97, 163.29, 163.60, 164.15. HRMS (ESI-TOF(matrix-dctb)) m/z: $[M+H]^+$ calcd for $C_{58}H_{66}N_{14}O_8$, 1087.5266; found, 1087.5837. Anal. Calcd for $C_{58}H_{66}N_{14}O_8$: C, 64.07; H, 6.12; N, 18.04. Found C, 63.98; H, 6.34; N, 18.02.

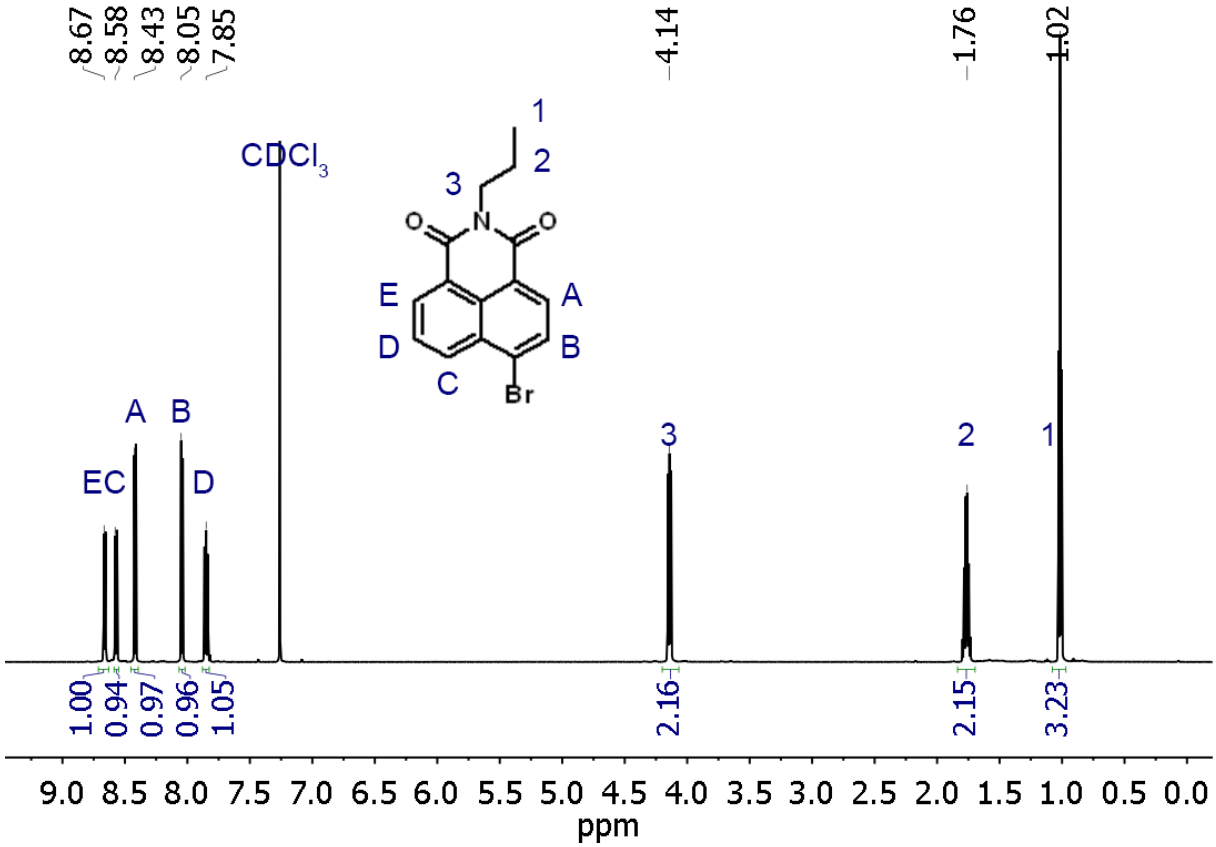


Figure S1. ^{1}H NMR spectrum of **4a** in $CDCl_3$.

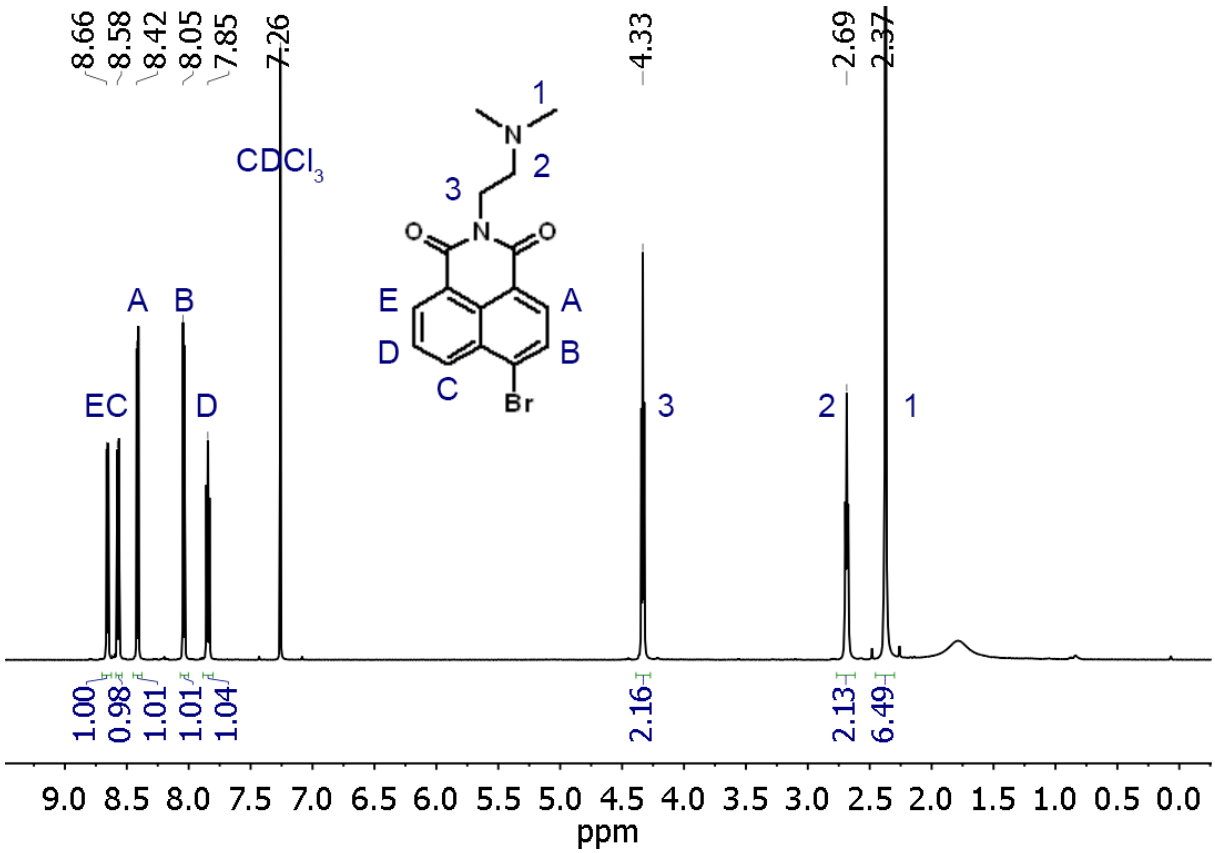


Figure S2. ^{1}H NMR spectrum of **4b** in $CDCl_3$.

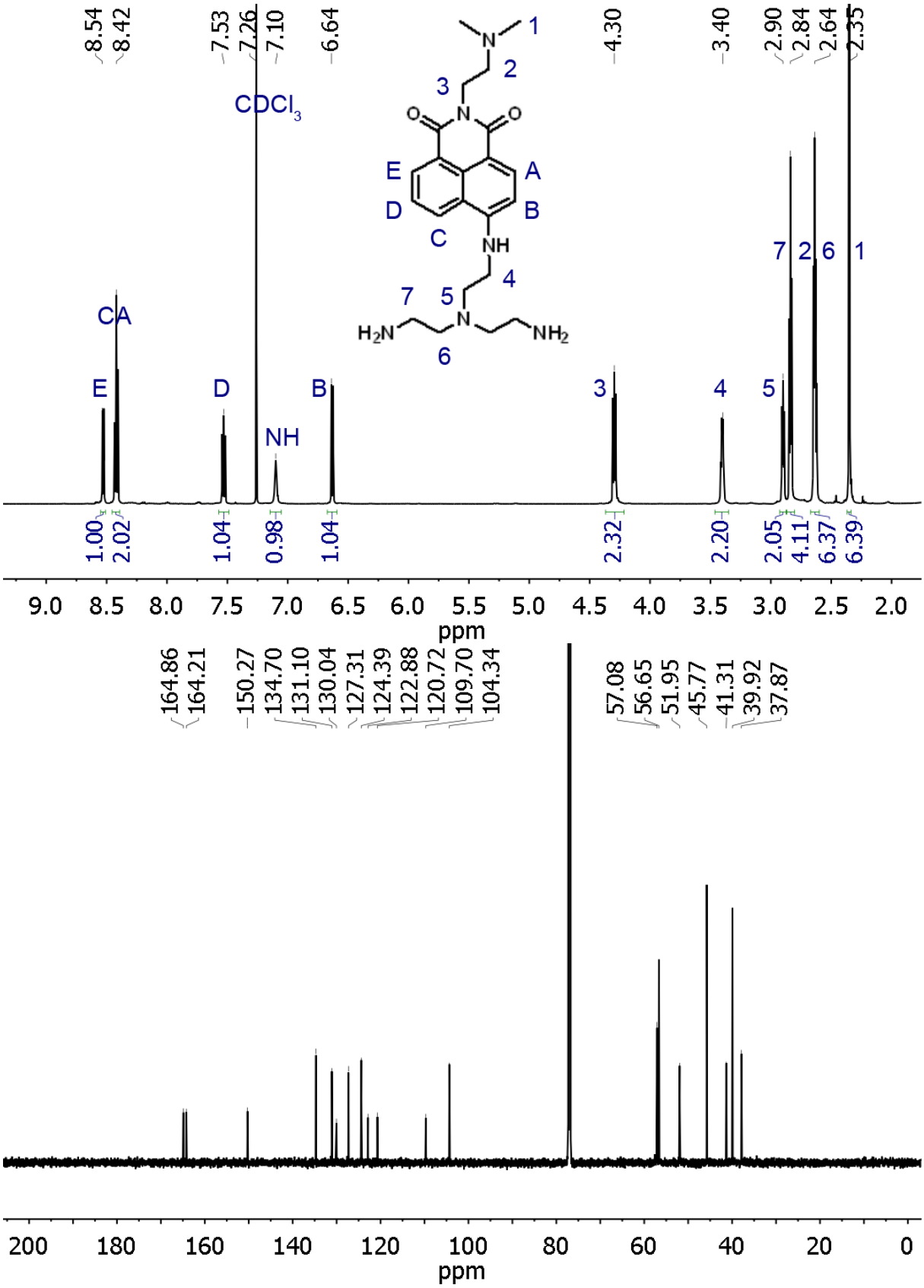


Figure S3. ^{1}H and ^{13}C NMR spectrum of **1b** in $CDCl_3$.

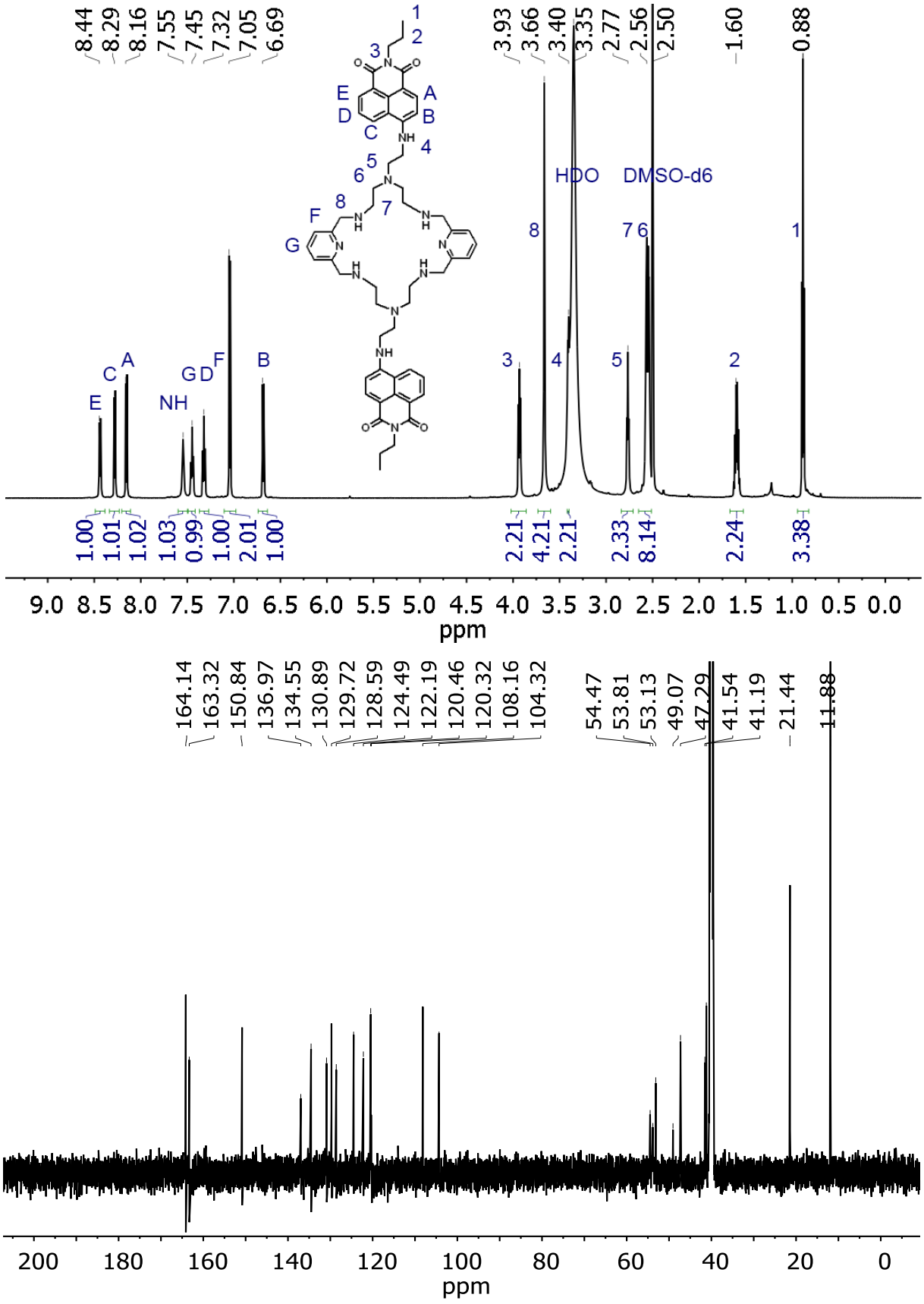


Figure S4. ^{1}H and ^{13}C NMR spectrum of **2a** in DMSO-d6.

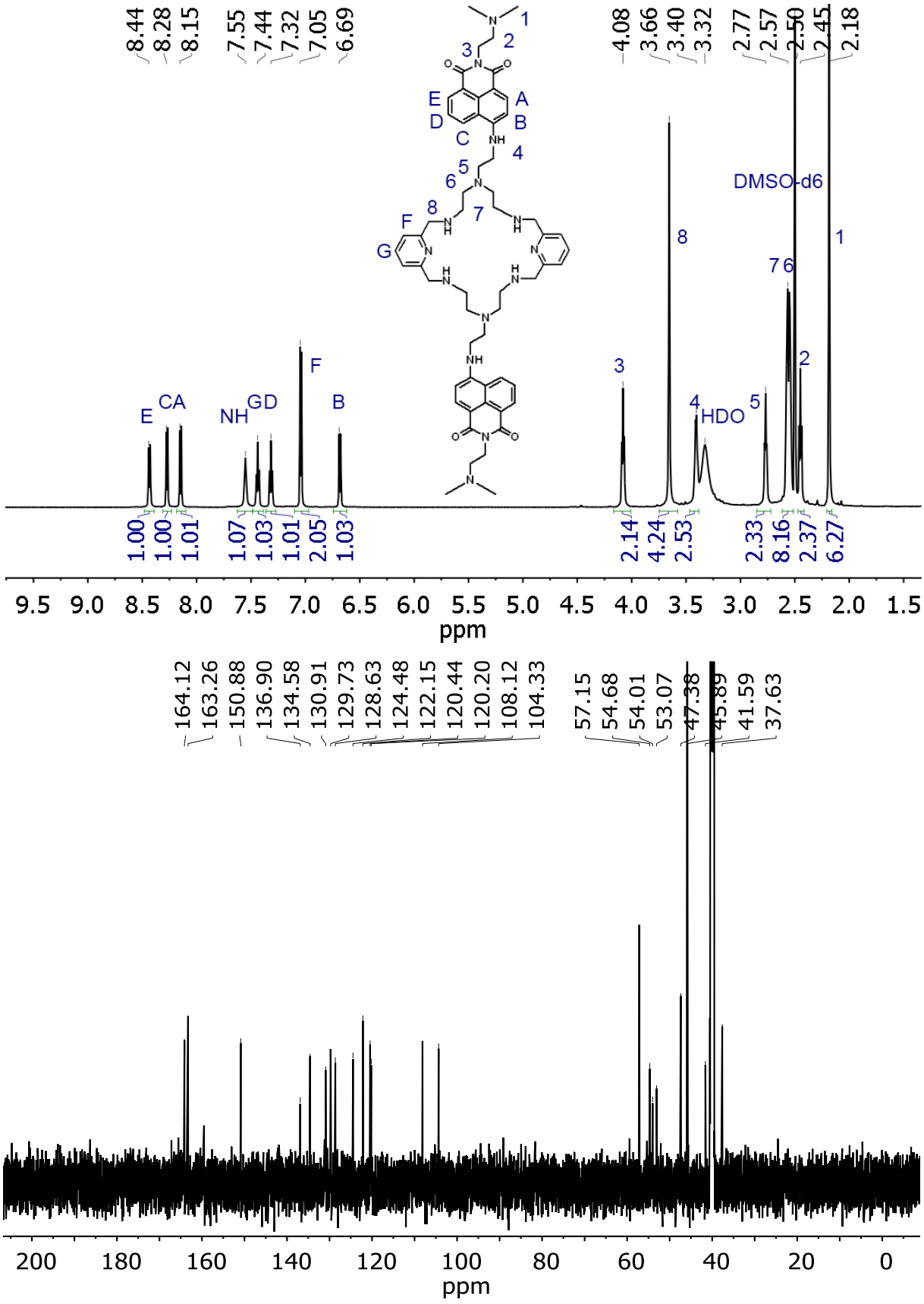


Figure S5. ^{1}H and ^{13}C NMR spectrum of **2b** in DMSO-d6.

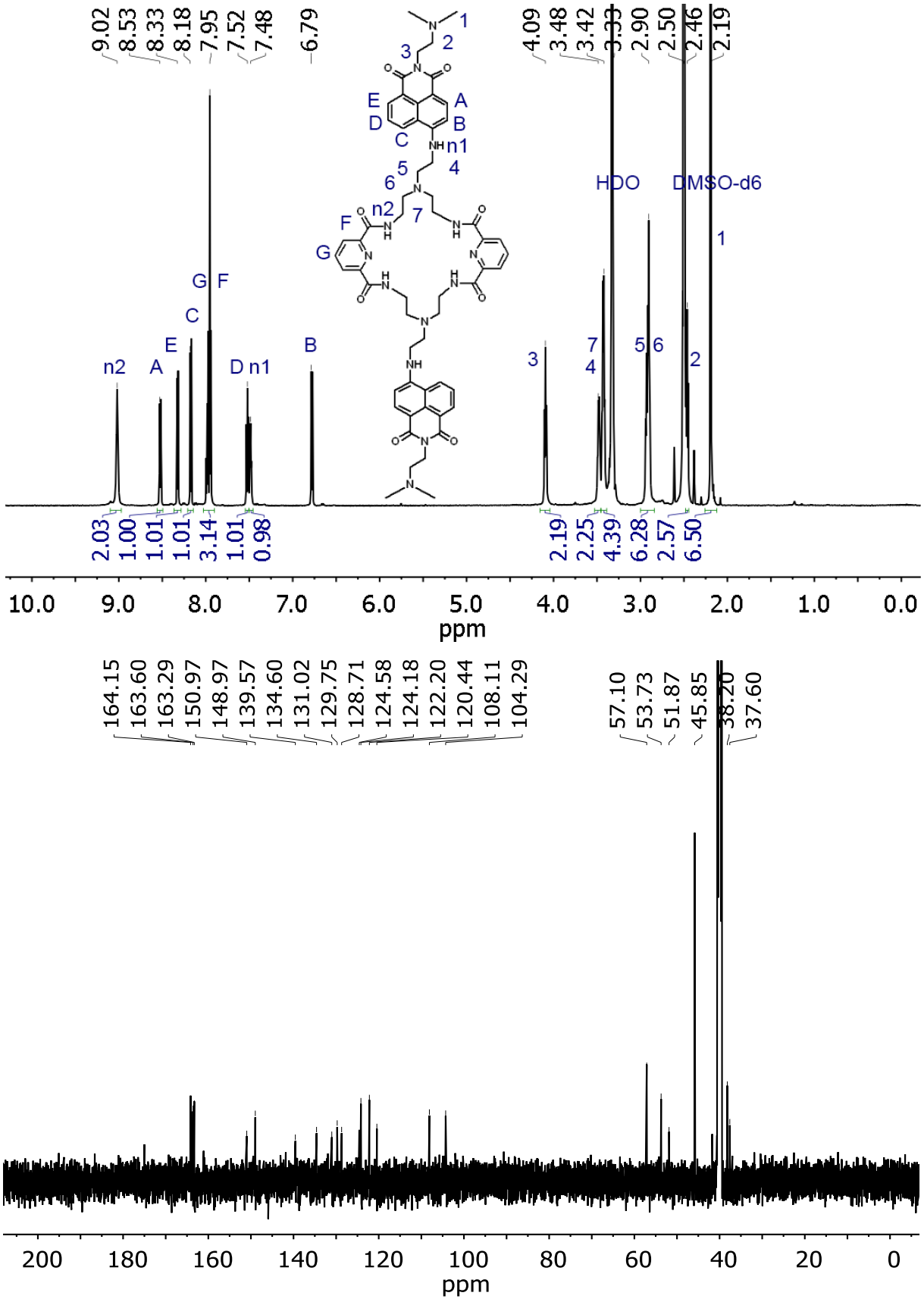


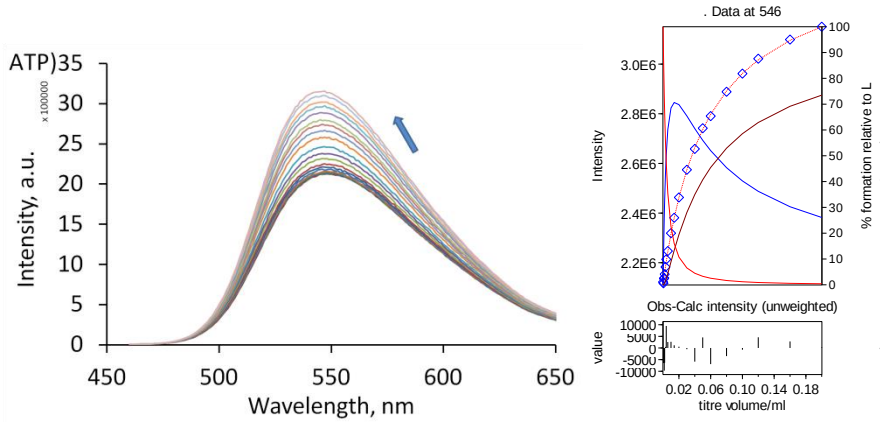
Figure S6. ^{1}H and ^{13}C NMR spectrum of **3b** in DMSO-d6.

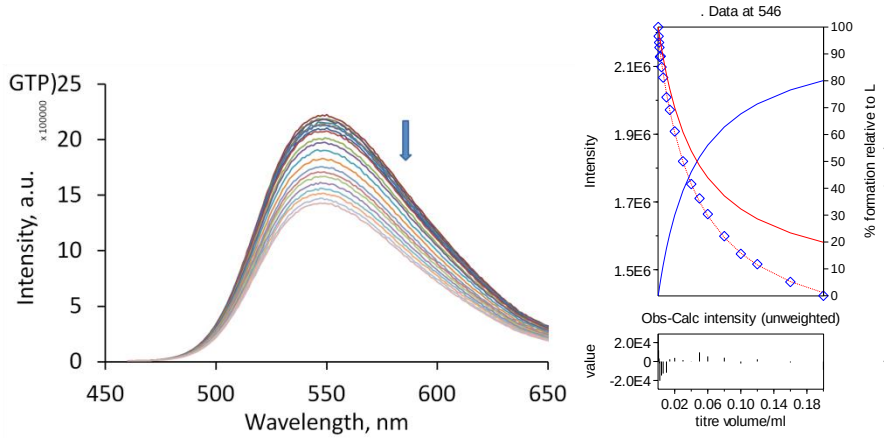
Fluorescence titrations of receptors

Titrations with nucleotides

Stock solutions of receptors with concentrations of 10^{-5} M in a 10 mM $NaAsO_2Me_2*3H_2O$ buffer (5% DMSO), 100 mM KCl, pH 7.2 were prepared for fluorescence binding studies. The titrant (sodium salt, 0.01M) was sequentially added to a 2 mL sample of the host stock solution in the spectrometric cell and the changes in the spectral features were monitored. The total number of data points was 20-40, depending on the stoichiometry of complexation; for a presumed 1:1 complex 20 points were usually measured. The following setup parameters were used for fluorescence titration experiments: ex. 450 nm, slit 2/2, em: 460-650 nm. The resulting data was imported in HypSpec program[7][1][1] and the data was fitted to obtain stability constants with anions. Concentration of receptors was 10^{-5} M.

Below are fluorescence changes observed during the titration and fitting curves exported from HypSpec fitting program.[7] Blue points are the experimental titration data, while red dashed curve is the fitting curve.





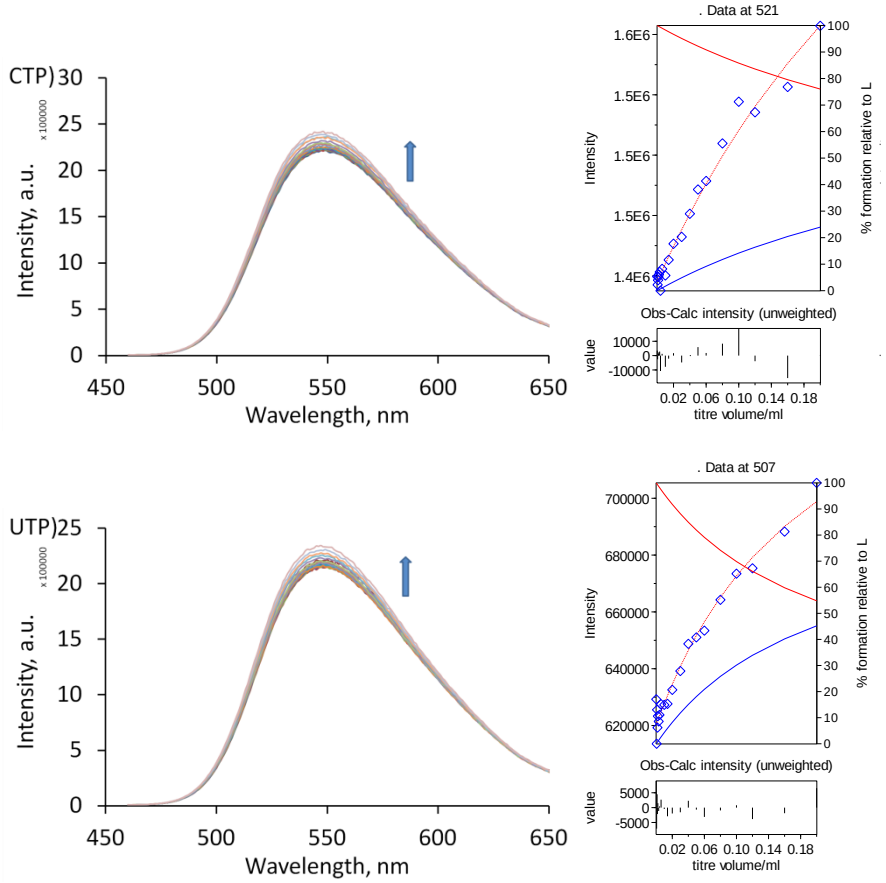
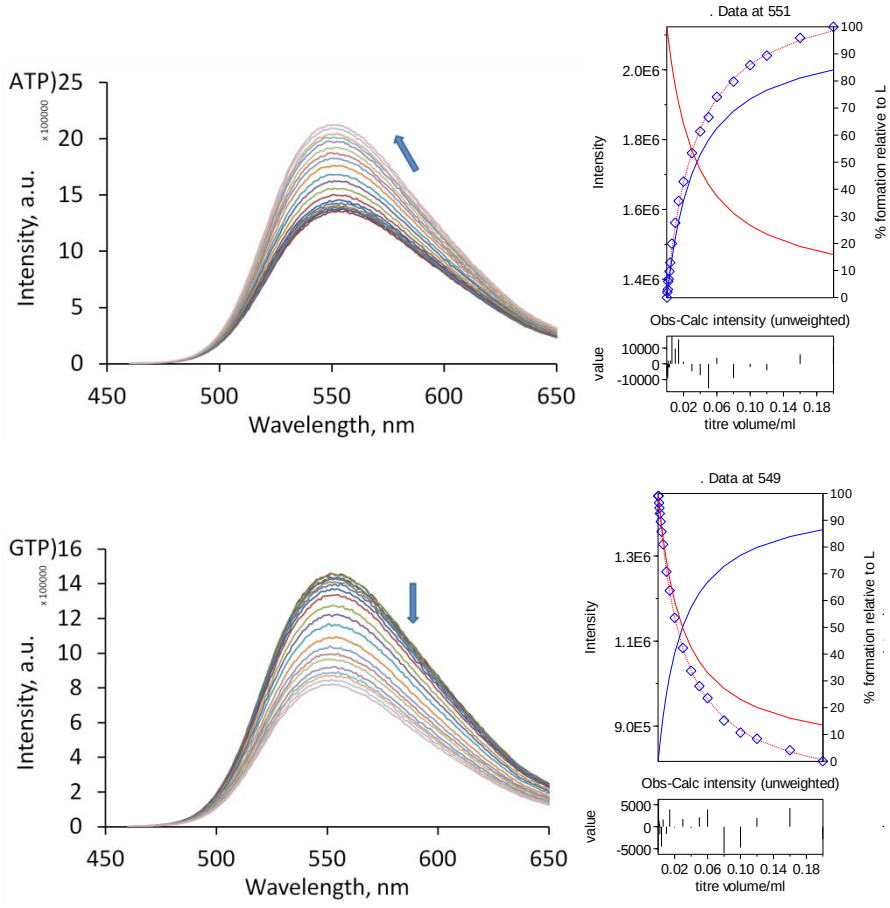


Figure S7. Fluorescence changes for **1a** induced by addition of NTPs (up to 100 equiv).



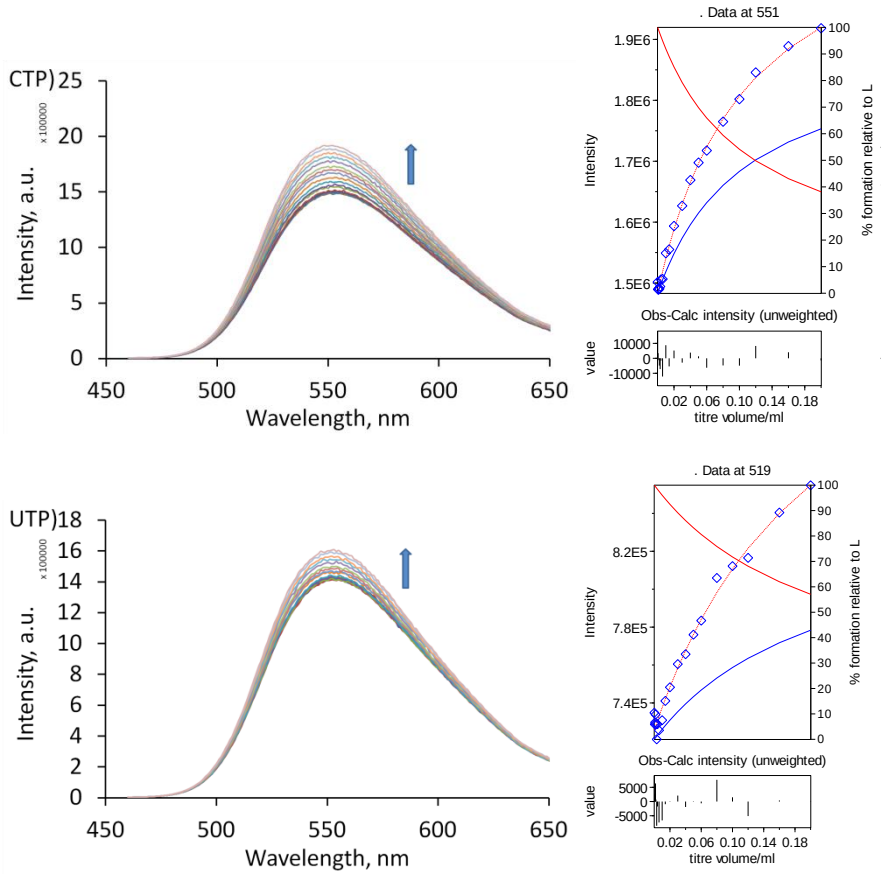
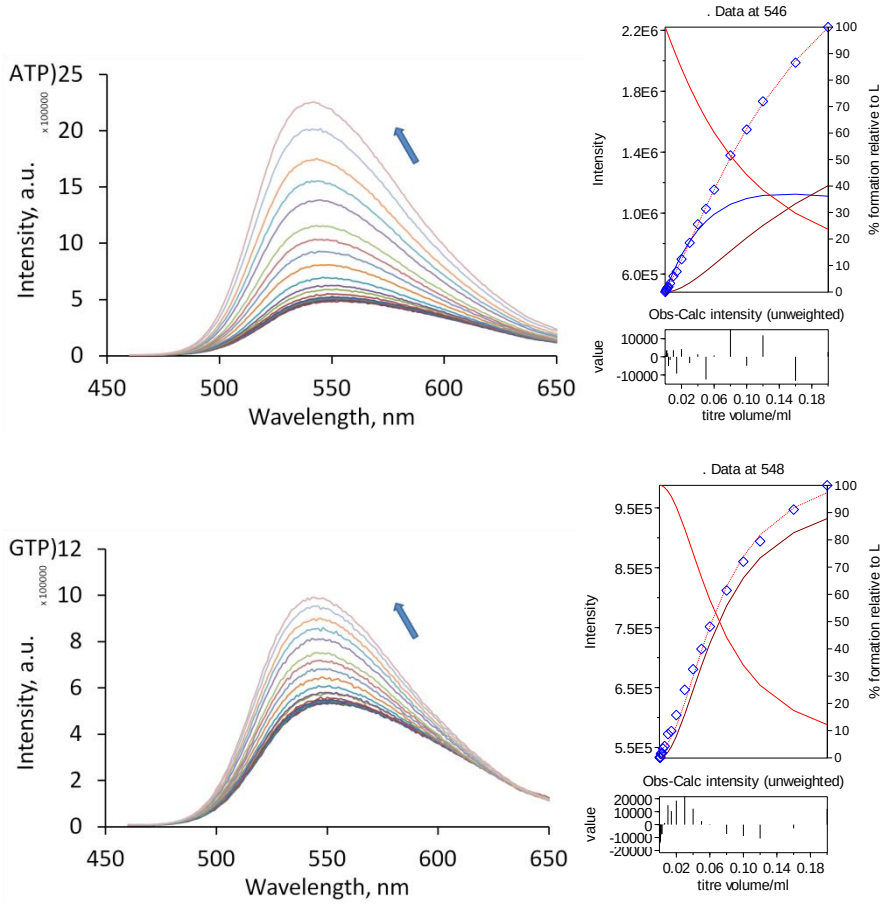


Figure S8. Fluorescence changes for **1b** induced by addition of NTPs (up to 100 equiv).



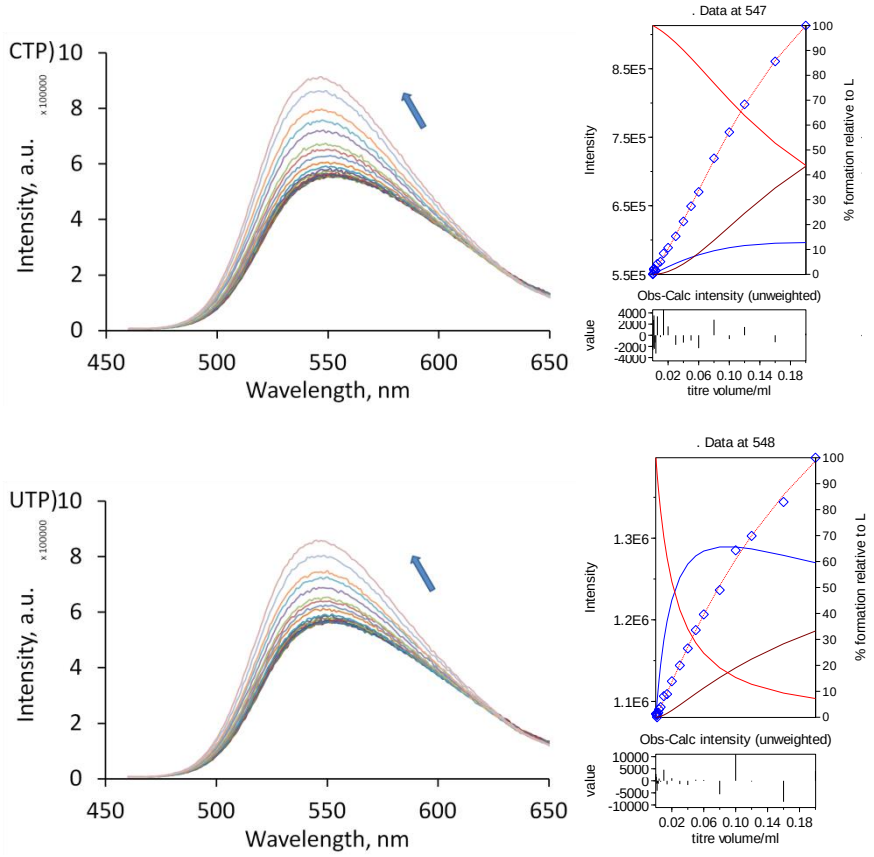
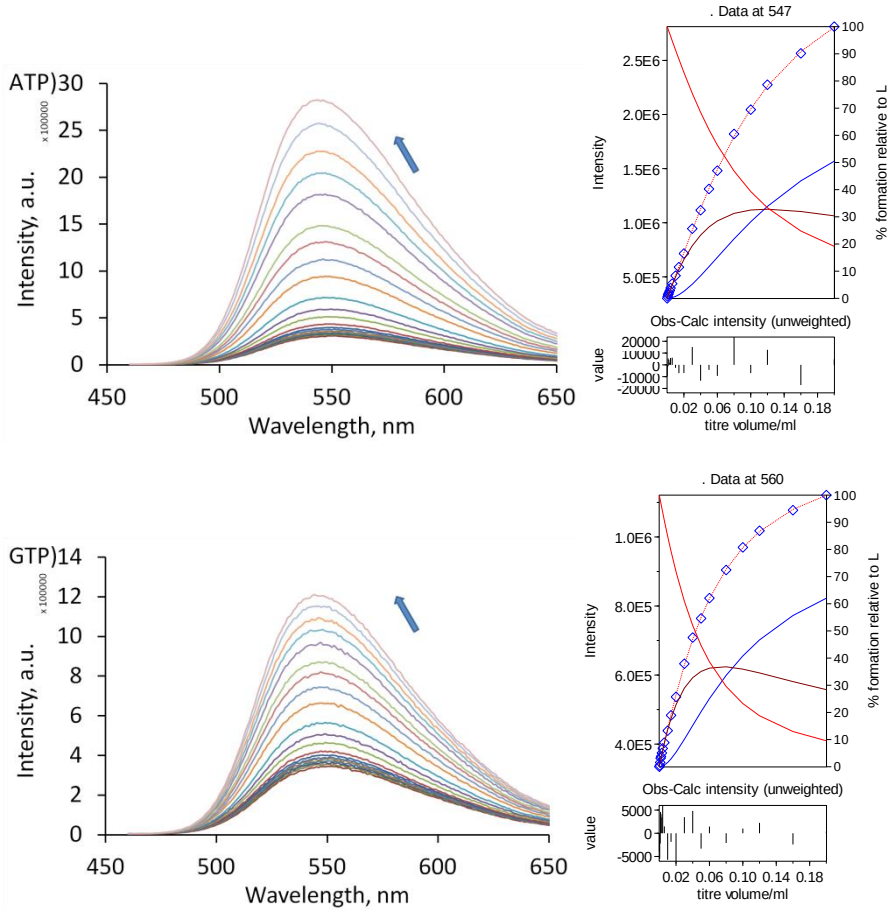


Figure S9. Fluorescence changes for **2a** induced by addition of NTPs (up to 100 equiv).



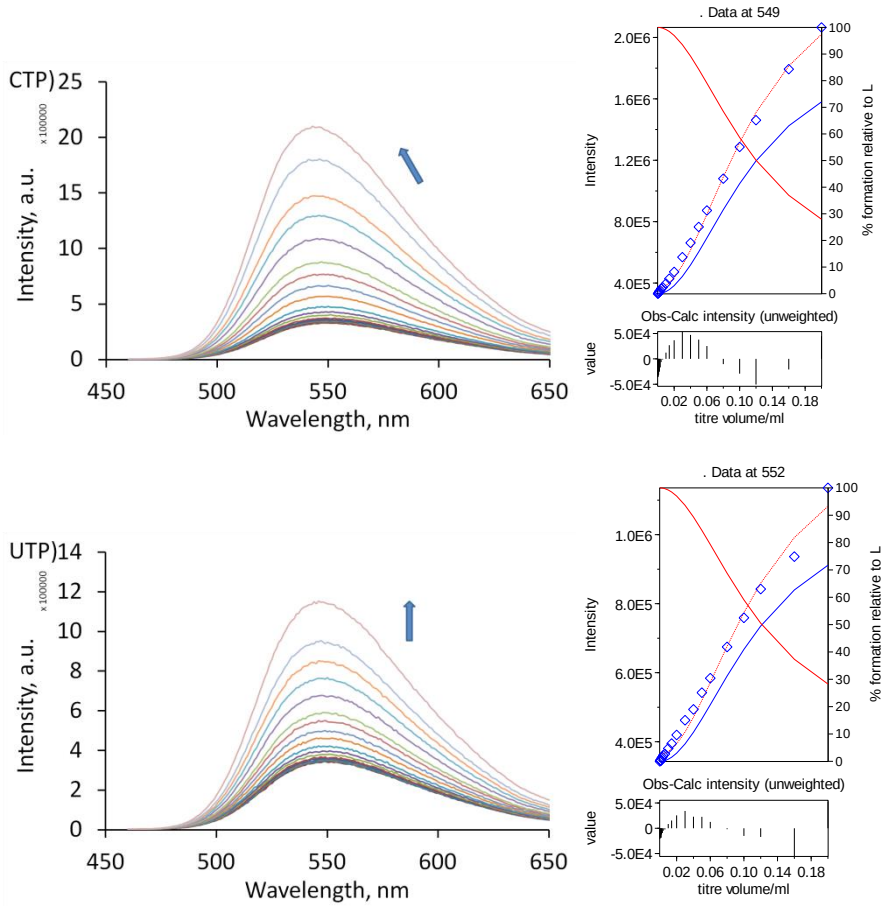
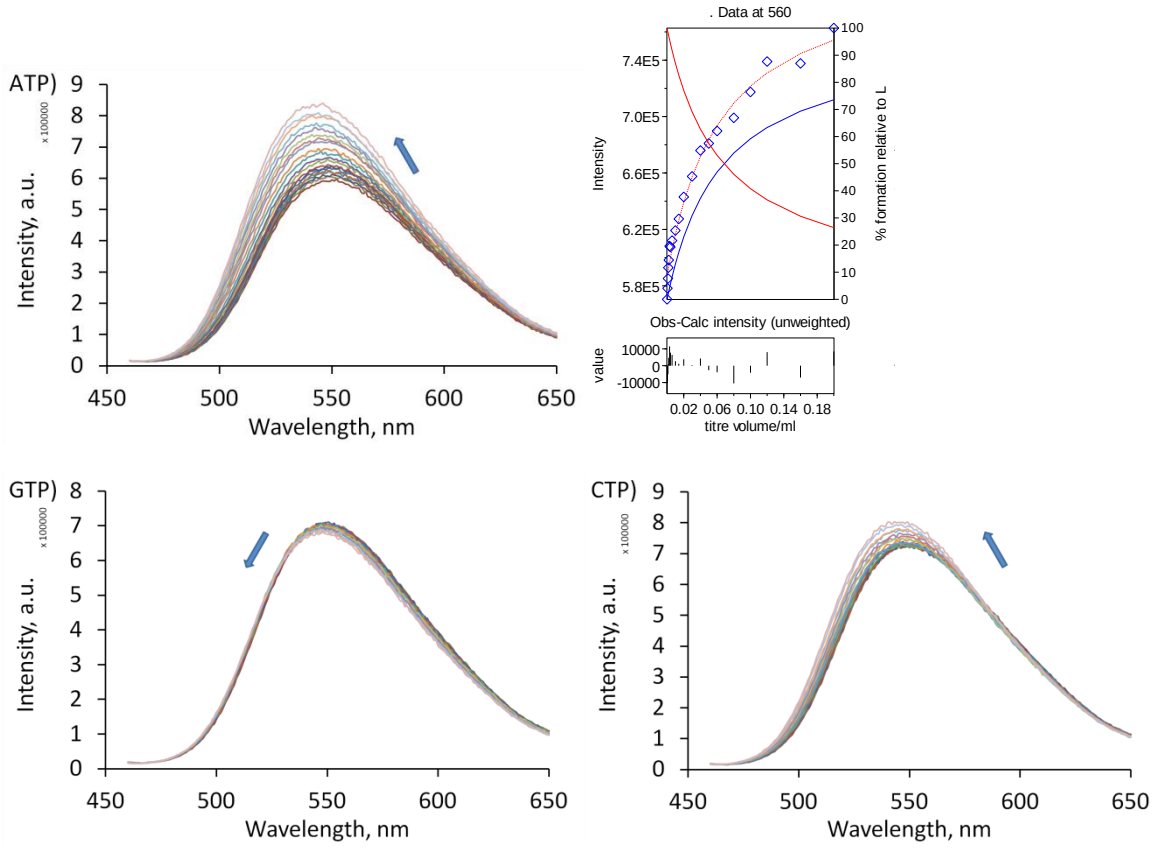


Figure S10. Fluorescence changes for **2b** induced by addition of NTPs (up to 100 equiv).



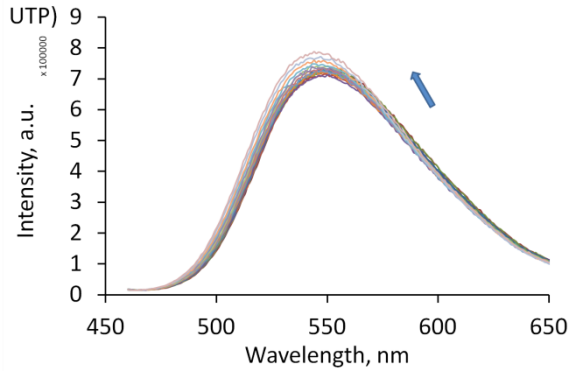
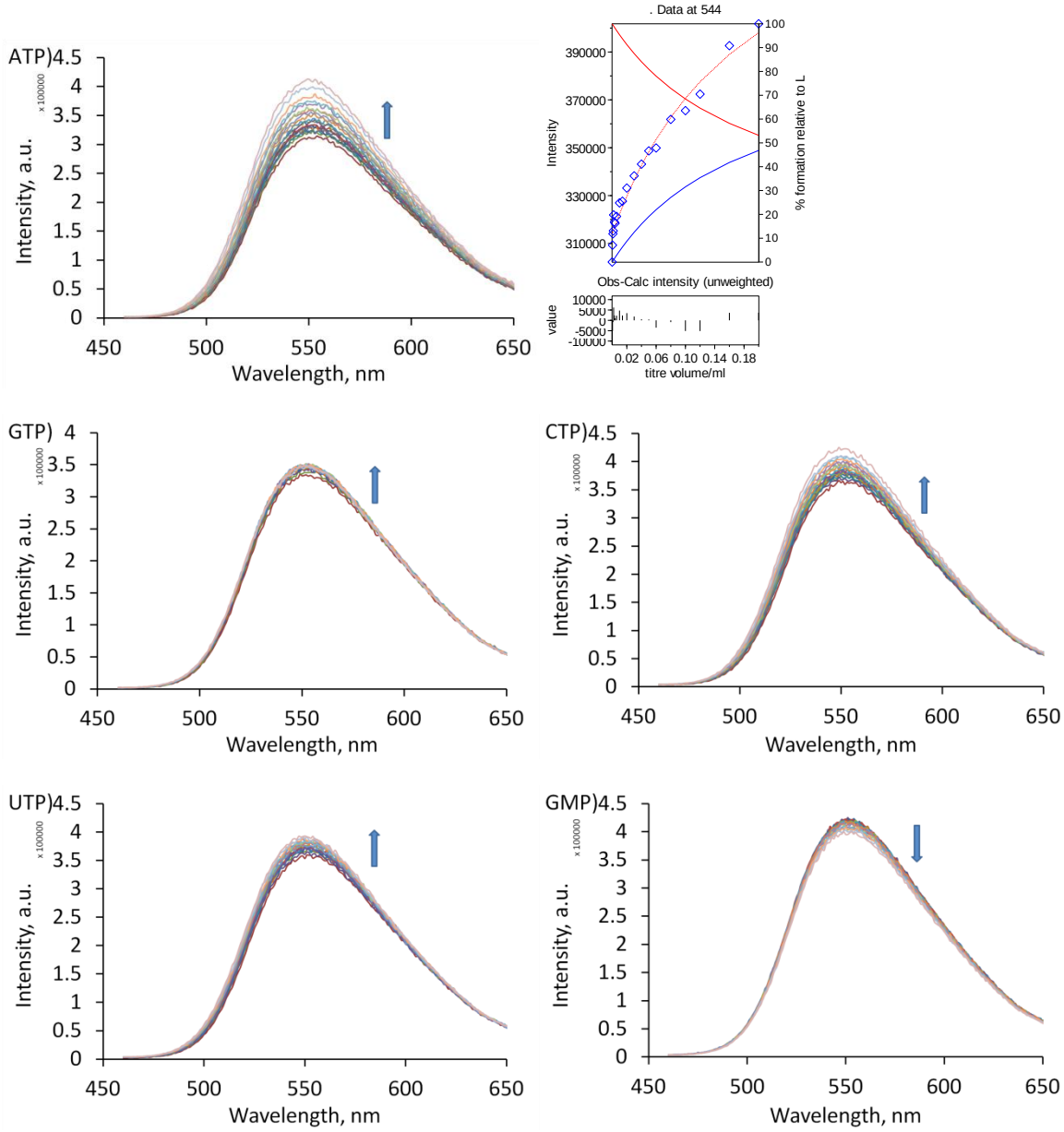


Figure S11. Fluorescence changes for **3a** induced by addition of NTPs (up to 100 equiv).



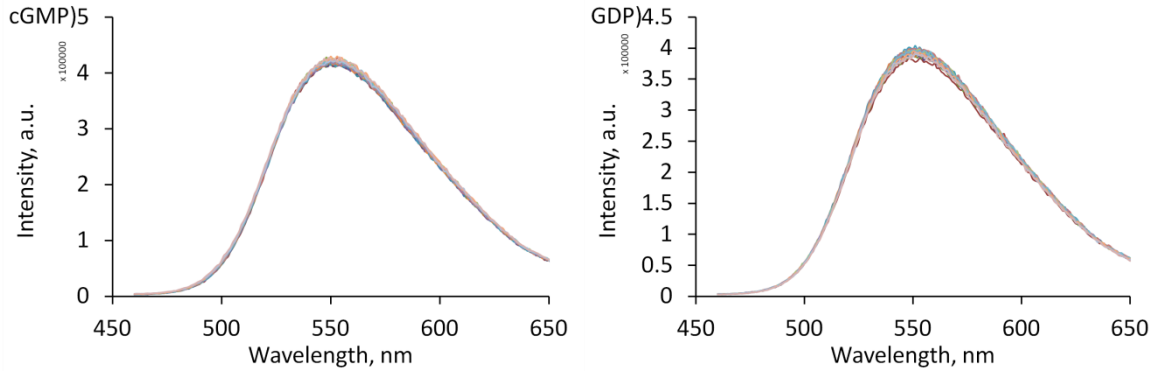


Figure S12. Fluorescence changes for **3b** induced by addition of NTPs (up to 100 equiv) and guanosine mono- and diphosphates.

Titrations with oligonucleotides

For titration with oligonucleotides (3`-NNNN-5`), the same buffer solution was used as for nucleotides. To a receptor solution with $5*10^{-6}$ M concentration, a solution of the receptor ($5*10^{-6}$ M) and a oligonucleotide (0.001 M) was added in portions.

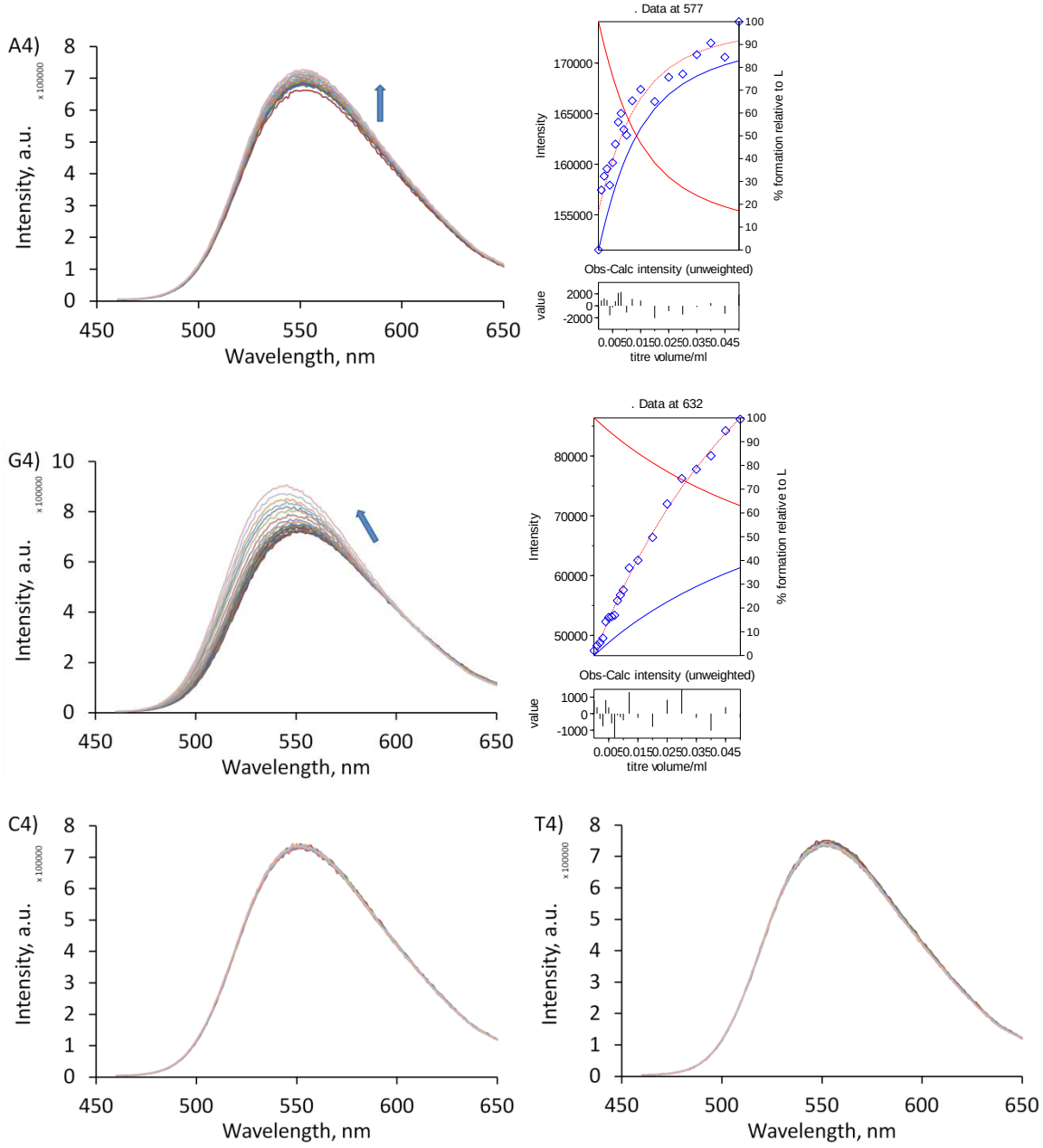


Figure S13. Fluorescence changes for **1b** induced by addition of oligonucleotides (up to 10 equiv).

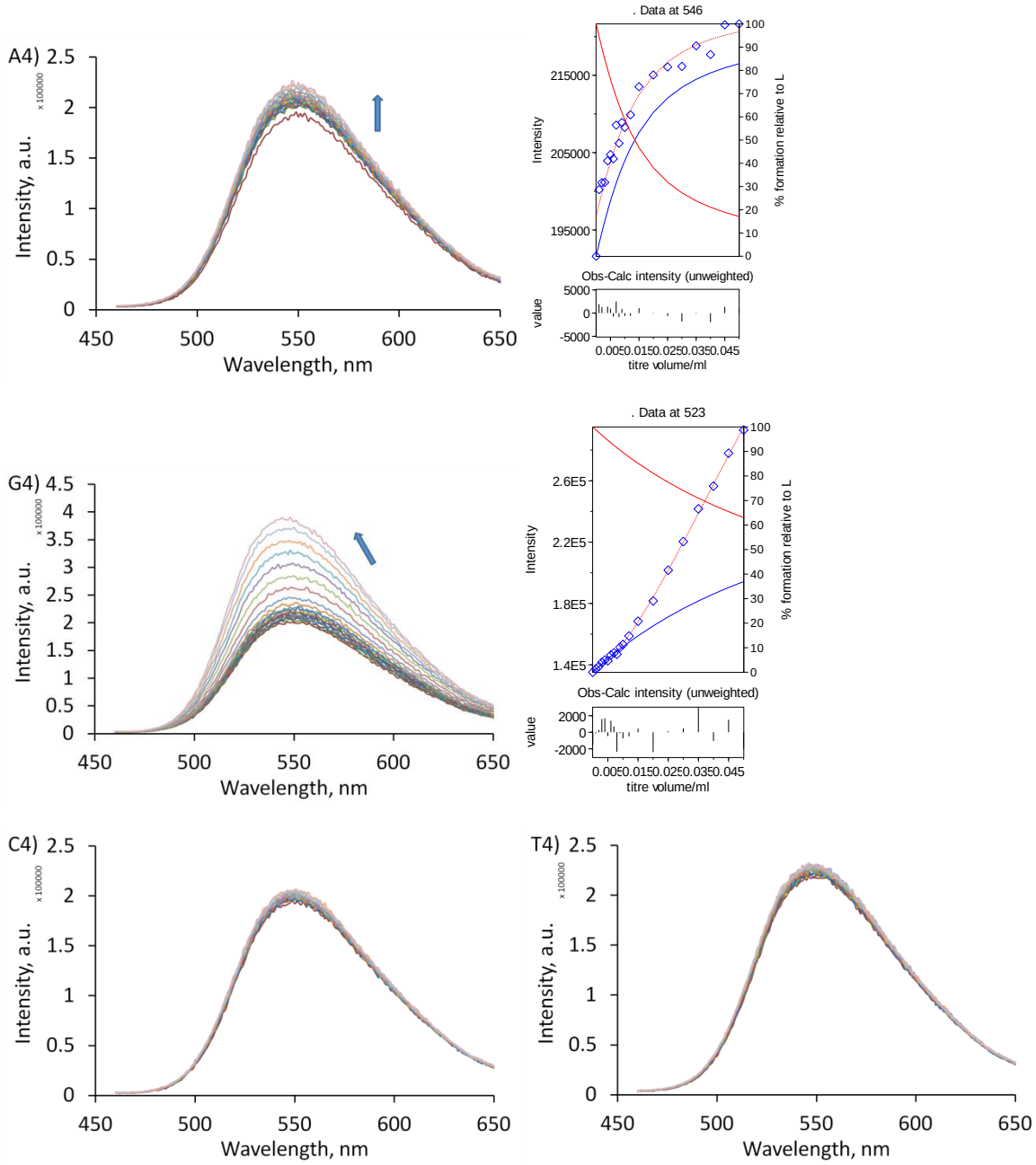
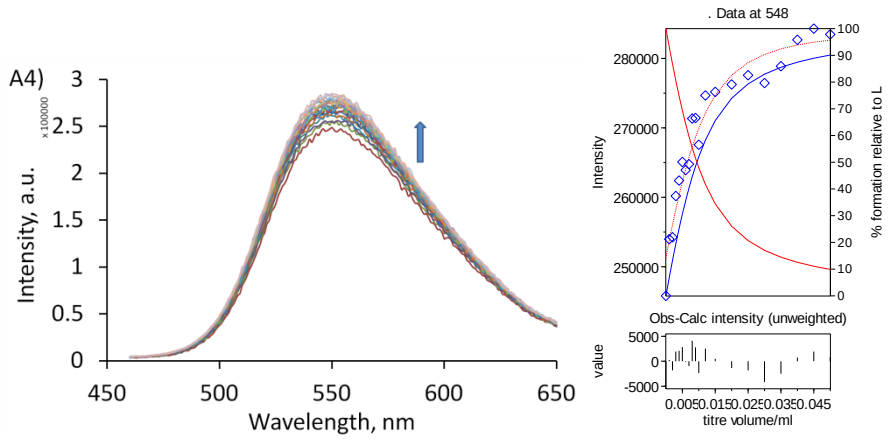


Figure S14. Fluorescence changes for **2b** induced by addition of oligonucleotides (up to 10 equiv).



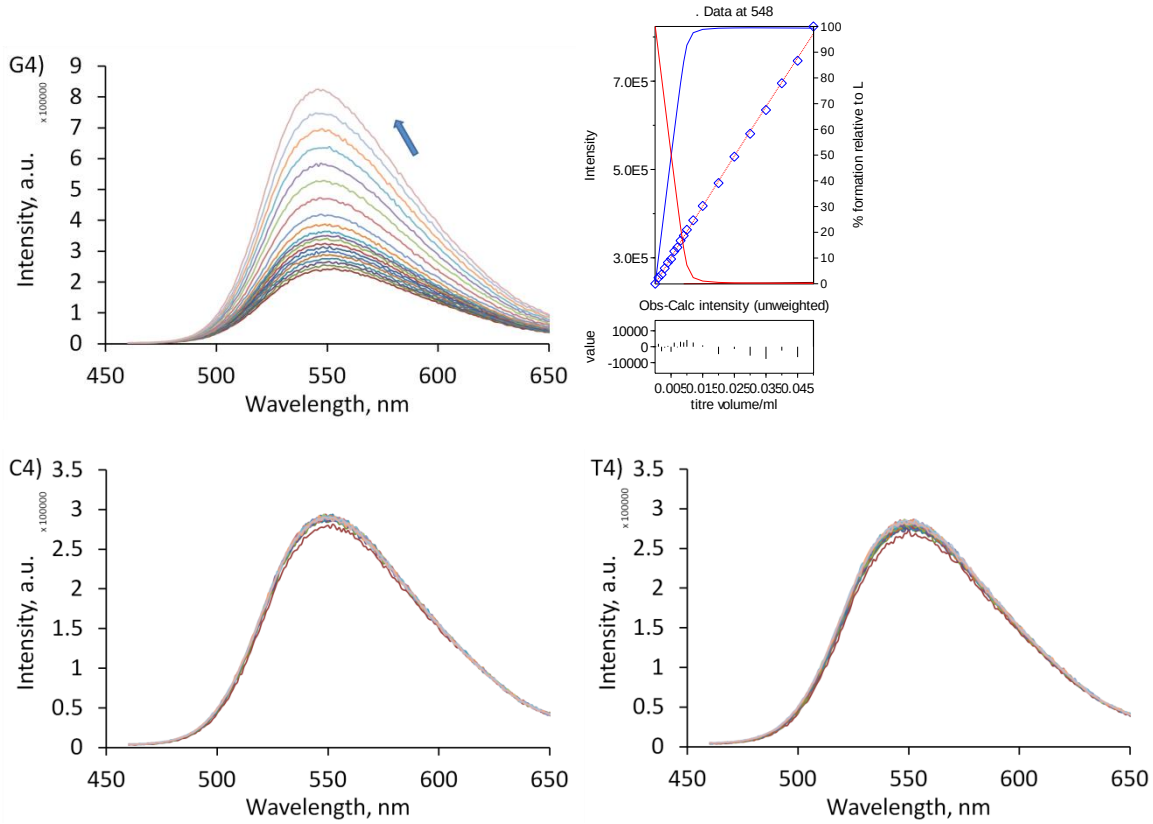


Figure S14. Fluorescence changes for **3b** induced by addition of oligonucleotides (up to 10 equiv).

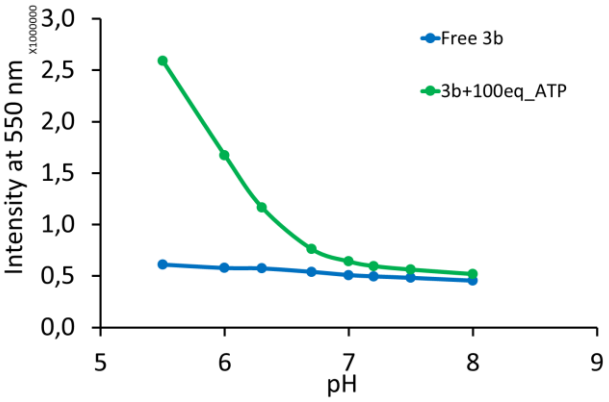


Figure S25. Fluorescence-pH relationship for **3b** in the absence and in the presence of ATP.

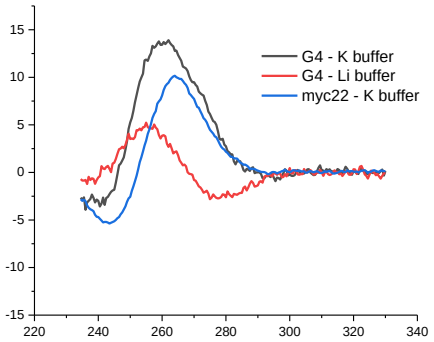


Figure S26. The CD spectra were blank-substracted and converted to molar dichroic adsorption (Δε, cm^{-1}, M^{-1}) based on nucleoside concentration Δε = $\frac{\theta}{32980 \times c \times l}$,where θ is ellipcicity (millidegrees), c is the total nucleoside concentration in sample (M), and l is the path length (cm). Conditions: G4–K buffer: c(G4) = 5 µM, buffer: Na-caco 10 mM, KCl 100 mM, DMSO 5%, pH 7.2; G4–Li buffer: c(G4) = 5 µM, buffer: Li-caco 10 mM, LiCl 100 mM, DMSO 5%, pH 7.2; Myc22-Kbuffer: c(myc22) = 3 µM, buffer: Li-caco 10 mM, KCl 100 mM, pH 7.2.

DFT calculations.

The calculations were performed with the program package Priroda. The structures of G4-quadruplex and the receptor-phosphate complex were first preoptimized. Then the receptor in the 4-fold protonated state without the phosphate anion was attached to G-quadruplex to the most accesable phosphate residues and the overall complex was further optimized. The phosphate residues on the nucleotide were protonated to decrease the overall charge. The charge of the complex was +6: 4 charges on the receptor and 2 charged on potassium cations.

Cartesian coordinates of the final structure:

8	1.06653106	-10.96683502	-6.69514704
6	-0.14365393	-11.31945133	-6.09174252
6	-0.01213847	-11.01007652	-4.62926865
8	0.16494720	-9.64412594	-4.45747519
6	-1.20668447	-11.36024094	-3.78240824
8	-0.81645793	-11.70909405	-2.49635124
6	-1.98079467	-10.08590698	-3.82312608
6	-0.86652082	-9.09505653	-3.75535011
7	-1.18610811	-7.79721975	-4.25029802
6	-2.40101361	-7.30930090	-4.66388130
7	-2.44651341	-6.02149296	-4.73677015
6	-1.17907500	-5.60990429	-4.34147358
6	-0.65692562	-4.32623196	-4.13411474
8	-1.27466440	-3.26035929	-4.27952051
7	0.67170566	-4.32899237	-3.78124499
6	1.40945315	-5.47815895	-3.54411602
7	2.68383098	-5.32708454	-3.19176650
7	0.86600155	-6.68589020	-3.63498306
6	-0.39006713	-6.70772028	-4.04507542
1	-0.37721175	-12.38600540	-6.22442675
1	-0.98018402	-10.75064087	-6.51305723
1	0.86277056	-11.54118061	-4.26250696
1	-1.75819945	-12.22902870	-4.15819502
1	-2.48982906	-10.01421642	-4.77962303
1	-2.69878197	-9.98326492	-3.02327800
1	-0.55725408	-8.93964767	-2.73720527
1	-3.22403097	-7.97286844	-4.88608599
1	1.08021224	-3.40497518	-3.64237523
1	3.09191084	-4.39739561	-3.09739113

1	3.18558979	-6.16083574	-2.92773986
15	-0.24447335	-10.91329479	-1.25942194
8	0.18307146	-11.78757286	-0.14445776
8	-1.30348837	-9.77985096	-0.97891772
8	0.88735676	-9.97713661	-1.84264612
6	2.11889625	-10.44975758	-2.27797294
6	3.19924998	-9.80709267	-1.47884679
8	3.00448895	-8.43930531	-1.52675009
6	3.21010375	-10.10925293	-0.01303437
8	4.48248863	-9.70465755	0.40939778
6	2.19039202	-9.16050625	0.49837029
6	2.55129051	-7.97171354	-0.31514055
7	1.53447938	-7.02422810	-0.53347957
6	0.23504269	-7.21317387	-0.88206106
7	-0.40691975	-6.10984755	-1.07650173
6	0.53008598	-5.12354612	-0.82301491
6	0.44853267	-3.72394133	-0.97968155
8	-0.52066451	-3.11555386	-1.39902604
7	1.64183271	-3.09322500	-0.66963410
6	2.78732586	-3.73447347	-0.26532298
7	3.83360696	-2.97014451	0.08755743
7	2.87542772	-5.04659081	-0.22891092
6	1.73616552	-5.68486786	-0.48432702
1	2.23593020	-10.15250587	-3.31523108
1	2.16985869	-11.53738880	-2.20278716
1	4.16903067	-10.07299614	-1.91519642
1	3.02843714	-11.15377331	0.24823353
1	1.20132828	-9.51298809	0.27496997
1	2.26610327	-8.99326897	1.56373847
1	3.33054471	-7.40812922	0.16670223
1	-0.17351146	-8.19951153	-0.93879622
1	1.60890388	-2.08294606	-0.69450432
1	3.65705085	-1.99258888	0.28145915
1	4.55108356	-3.47440434	0.58183676
15	4.78697586	-9.30263233	1.91121244
8	6.32262230	-9.49749851	2.02527094
8	3.89594603	-9.95279026	2.90283895
8	4.53441525	-7.72445631	1.86795449
6	5.25278568	-6.89279604	1.01323628
6	6.22631788	-6.04848528	1.76149392
8	5.82676601	-4.71380377	1.84537971
6	6.47744751	-6.49586248	3.16113853
8	7.85452747	-6.54270315	3.37828636
6	5.80352736	-5.47247648	4.01838827
6	5.27205944	-4.41290617	3.09845614
7	3.86153507	-4.38248158	2.97001863
6	3.02104092	-5.43809748	2.71670556
7	1.84066331	-5.05965042	2.38145947
6	1.85867298	-3.68266201	2.42667437
6	0.87737477	-2.73222733	2.07450509
8	-0.23220392	-2.94481134	1.58330917
7	1.31494617	-1.43833554	2.27591872
6	2.50423026	-1.11020637	2.86904407
7	2.72930956	0.19427919	3.16364574
7	3.46951795	-1.99495196	3.05742097
6	3.09808183	-3.25495362	2.84738278
1	4.58263302	-6.22142935	0.50043219
1	5.75233889	-7.49264765	0.26502278
1	7.16844797	-6.05273819	1.23821759
1	6.07180309	-7.47521639	3.33326912
1	4.98500729	-5.88786364	4.60167885
1	6.53222418	-5.03827667	4.69350433
1	5.56314611	-3.39260411	3.37124372
1	3.36557531	-6.45011806	2.78448057
1	0.61922443	-0.72296870	2.09434724
1	1.95285368	0.84133083	3.09707022
1	3.36850047	0.31759474	3.93345547
15	8.61069775	-7.92757273	3.60474730
8	7.57100248	-8.96627235	4.02507544
8	9.80449772	-7.75625658	4.49105883
8	9.20378113	-8.32782555	2.17412782
6	8.57210732	-8.26006985	0.94114494

6	9.13638592	-7.11603260	0.17423452
8	10.46872044	-7.36625338	-0.09278059
6	8.50070667	-6.88903904	-1.17538786
8	8.51949883	-5.52788925	-1.44970238
6	9.46402931	-7.53912687	-2.10956287
6	10.75150681	-7.17438364	-1.43468201
7	11.91152191	-7.95040798	-1.75423217
6	13.07068729	-7.51084709	-1.12182760
8	13.15847969	-6.43615294	-0.59579402
7	14.06308460	-8.46008205	-1.06921303
6	13.97322845	-9.80734730	-1.43726814
8	14.76622295	-10.60553074	-1.01956797
6	12.82088470	-10.09749222	-2.30913544
6	12.79382896	-11.42714882	-3.01294446
6	11.86269951	-9.17671967	-2.40166259
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1	8.76701260	-9.18805027	0.40957084
1	9.04542923	-6.21220970	0.77070546
1	7.48038530	-7.26985121	-1.25114191
1	9.31668472	-8.61503410	-2.10065889
1	9.37050056	-7.17697811	-3.13013244
1	10.99851036	-6.12487793	-1.61146009
1	14.91302872	-8.16715240	-0.60746604
1	12.89872646	-12.23740864	-2.29059291
1	11.86346626	-11.55514717	-3.56596947
1	13.62933064	-11.50222206	-3.71085191
1	10.98158741	-9.34530449	-3.00242305
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8	7.81314182	-4.03354263	0.41583359
8	5.97304249	-5.09680176	-1.04895258
8	7.55772829	-3.36243129	-1.98419571
6	8.74357605	-2.63941574	-2.10816813
6	8.45951939	-1.25059283	-1.64883006
8	7.36057472	-0.78701228	-2.35035300
6	8.05981255	-1.13997138	-0.21082613
8	8.35342026	0.17197046	0.14619033
6	6.59765053	-1.36724484	-0.28014034
6	6.24828959	-0.67855138	-1.55217433
7	5.09661865	-1.22267020	-2.19142628
6	4.74772882	-2.52461600	-2.47963738
7	3.55873537	-2.63807750	-2.97409463
6	3.07368803	-1.33261013	-3.02849245
6	1.81612599	-0.82496166	-3.42258763
8	0.84701890	-1.47712302	-3.80740619
7	1.75122607	0.56060982	-3.31799054
6	2.77995229	1.36063516	-2.85893369
7	2.55449390	2.67399979	-2.76856637
7	3.93239236	0.86231804	-2.45031881
6	4.03096247	-0.46124181	-2.55240726
1	9.01935387	-2.62703371	-3.16214275
1	9.54947758	-3.10280895	-1.53949547
1	9.33257866	-0.61454779	-1.83428049
1	8.59033966	-1.82063854	0.45412603
1	6.39145184	-2.41075087	-0.38260844
1	6.06800079	-1.00077748	0.58013266
1	6.00228834	0.37093094	-1.39840639
1	5.41496277	-3.34144402	-2.27488184
1	0.84415585	0.97014761	-3.53781390
1	1.72307575	3.08515406	-3.19243979
1	3.29827762	3.23239303	-2.38283253
15	7.64998579	1.19254196	1.10687554
8	8.54374313	2.17761517	1.76058352
8	6.73734283	0.31596610	2.07355022
8	6.54902792	1.82701933	0.15553248
6	6.81854773	3.08008242	-0.40656251
6	5.95076609	4.10345602	0.24427965
8	4.63347149	3.77638912	-0.01444667
6	6.00447083	4.15271568	1.73715436
8	5.39346600	5.36250830	2.08686113
6	5.08957767	3.05022502	2.12087989
6	4.04542637	3.19581652	1.07710361
7	3.43508244	1.97732604	0.66074228

6	3.84036160	0.66315603	0.67101091
7	2.96418738	-0.14317431	0.16554452
6	1.90190315	0.67171437	-0.19022703
6	0.62818372	0.39088279	-0.76660514
8	0.18647505	-0.68280584	-1.09769320
7	-0.13556090	1.54464793	-0.96373481
6	0.23135839	2.81477141	-0.65132242
7	-0.60678476	3.80888891	-0.80052722
7	1.44861174	3.03482389	-0.14854816
6	2.21825767	1.96499074	0.10046776
1	6.56773186	3.02863193	-1.46523607
1	7.87357998	3.33341575	-0.29575530
1	6.18199968	5.08805323	-0.17629400
1	7.00832605	4.07718086	2.16068101
1	5.56815720	2.09700489	2.04611492
1	4.71255541	3.15473533	3.12740445
1	3.24096012	3.84574866	1.40267837
1	4.78281736	0.38879979	1.10207486
1	-1.07556152	1.36004496	-1.30397046
1	-1.54329669	3.51661468	-1.07549870
1	-0.43397772	4.70778179	-0.32468629
15	4.91541386	5.61792994	3.57780409
8	4.83168077	7.15979481	3.74279141
8	5.59790421	4.79156399	4.60365486
8	3.36151361	5.33029890	3.36781454
6	2.52381849	5.74535608	4.39683485
6	1.61040807	6.76468992	3.82741427
8	1.06059933	6.29874134	2.65458822
6	0.40915945	7.02667332	4.66871643
8	-0.20364939	8.15324974	4.15542269
6	-0.44697943	5.85829782	4.33799076
6	-0.12406339	5.66424847	2.88005042
7	0.00188900	4.28824854	2.52344418
6	1.07422972	3.45730877	2.72967863
7	0.82194990	2.22193503	2.45553493
6	-0.50762057	2.21428990	2.06796336
6	-1.33136642	1.16018450	1.59817290
8	-1.00369513	0.00509893	1.36881399
7	-2.63647604	1.57727742	1.37485099
6	-3.08748364	2.86459875	1.54737186
7	-4.39875889	3.09320021	1.36823785
7	-2.27856088	3.86755013	1.85716259
6	-1.02330518	3.49416280	2.12653685
1	3.08459234	6.15412998	5.23492098
1	1.97633624	4.88702250	4.76844835
1	2.15898776	7.66429138	3.59954214
1	0.61784428	7.14778137	5.73288250
1	-0.17361230	4.98239708	4.91880608
1	-1.50050366	6.05156279	4.51675558
1	-0.89559120	6.05285025	2.22680187
1	2.01546621	3.86641407	3.03473949
1	-3.27109122	0.83060169	1.08951259
1	-5.06482077	2.32425666	1.26673579
1	-4.72448397	3.98909521	1.68898535
15	0.07729585	9.57590675	4.79756355
8	0.07679499	9.33129883	6.34672976
8	-0.87765795	10.57352924	4.25524044
8	1.56970727	9.80664253	4.34778357
6	2.70556927	9.64872169	5.13772869
6	3.68175292	10.56520462	4.51505327
8	3.13852167	11.80907154	4.38042498
6	5.03059578	10.81306934	5.11010551
8	5.89222813	10.92991352	3.99535608
6	4.96367073	12.17427921	5.71882963
6	3.61774850	12.69717407	5.30732584
7	2.61978340	12.79008484	6.34964848
6	2.54448438	11.80121994	7.31112623
8	3.46732116	11.12541103	7.67599058
7	1.26600420	11.57491589	7.77541208
6	0.09150590	12.05729961	7.23661947
8	-0.94331837	11.44614029	7.42454529
6	0.25616178	13.25035381	6.41403913

6	-0.97037411	14.01895046	6.02079868
6	1.49579251	13.53120422	6.01184130
1	3.07813168	8.62915421	5.08895302
1	2.48701286	9.86988735	6.16703320
1	3.83668208	10.14605427	3.54259062
1	5.39076567	10.02717113	5.77502346
1	5.10375118	12.18223381	6.79177570
1	5.74858379	12.77956772	5.27180862
1	3.66845083	13.68886757	4.85020733
1	1.19216251	10.79813385	8.41773510
1	-1.70031691	13.33680820	5.58698034
1	-1.42812002	14.48303127	6.89698458
1	-0.72420692	14.79007530	5.29513884
1	1.69460106	14.36027622	5.35164833
15	6.48253345	9.69951248	3.23155618
8	6.80484724	8.51457119	4.09289122
8	7.65579367	10.26741028	2.35599542
8	5.30925941	9.42905617	2.22311044
6	5.16235638	8.34802914	1.37119222
6	3.70157409	7.98961115	1.41930771
8	3.04766631	8.92832470	2.17998266
6	2.99793434	8.14093590	0.12117633
8	1.68392515	7.76954365	0.33820900
6	2.99904585	9.61964130	0.00600145
6	2.56307840	9.94582081	1.39159465
7	2.92723751	11.22806454	1.82437944
6	4.09793234	11.96277237	1.73115027
7	3.96100712	13.19696712	2.06858277
6	2.60180330	13.33418465	2.34780335
6	1.81574178	14.39567757	2.81022787
7	2.36527419	15.59232044	3.15100479
7	0.50790358	14.16611385	2.99947596
6	0.00206680	12.95774555	2.73782253
7	0.67093956	11.88944817	2.32927942
6	1.96547031	12.12248325	2.18749595
1	5.78203392	7.51493835	1.66555595
1	5.48274660	8.65499401	0.37688938
1	3.54036593	7.00423241	1.82934058
1	3.44287968	7.57960129	-0.70069271
1	3.99080729	10.00903034	-0.18365009
1	2.34513617	10.03759193	-0.74835080
1	1.48831785	9.94842052	1.48943222
1	5.01754761	11.49632072	1.42696249
1	1.73302555	16.37105370	3.25360227
1	3.28699946	15.79003620	2.79055500
1	-1.07079268	12.83998013	2.87921119
15	1.18214047	6.35645390	-0.15015078
8	-0.22017360	6.11884165	0.33186319
8	2.20673728	5.31534719	0.20360537
8	1.11582983	6.54400492	-1.73405826
6	1.03977942	7.78898048	-2.33530855
6	-0.36124519	8.21055603	-2.63498831
8	-0.77339983	7.61914110	-3.81550765
6	-1.34700716	7.80494976	-1.59491158
8	-2.31462884	8.75629616	-1.33500695
6	-1.94006550	6.57283115	-2.14207125
6	-1.67792964	6.63128281	-3.61095428
7	-1.13847494	5.36949825	-4.03319168
6	0.13564742	4.89614010	-3.81643462
7	0.19785865	3.60962343	-3.78369021
6	-1.10725033	3.18047214	-3.96413589
6	-1.66951370	1.88212001	-3.94436717
8	-1.07970667	0.84122473	-3.70067382
7	-3.03139019	1.91362965	-4.23353577
6	-3.79283381	3.06379676	-4.29484081
7	-5.10905361	2.94035625	-4.38553715
7	-3.25306153	4.26783848	-4.23476601
6	-1.93371749	4.26918602	-4.10402727
1	1.58562911	7.74643087	-3.27761102
1	1.51932991	8.53409672	-1.72159207
1	-0.37059194	9.28730011	-2.74344063
1	-0.86280626	7.61406422	-0.65671176

1	-1.43456757	5.72531033	-1.72282577
1	-2.99016309	6.53183556	-1.92971396
1	-2.58181906	6.78690147	-4.19985008
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