Synthetic Receptor Molecules for Selective Fluorescent Detection of 8-oxo-dGTP in aqueous media

Yasufumi Fuchi, Takashi Fukuda and Shigeki Sasaki*

Graduate School of Pharmaceutical Sciences, Kyushu University, 3-1-1 Maidashi, Higashi-ku, Fukuoka 812-8582, Japan.

E-mail: sasaki@phar.kyushu-u.ac.jp

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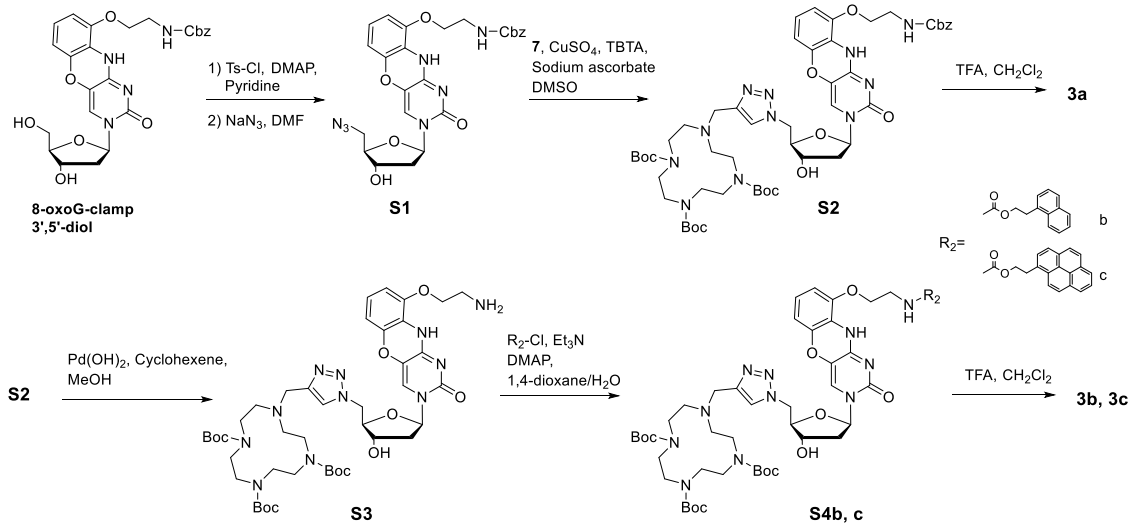
Synthesis of compound **8**

$NaBH(OAc)_3$ (106 mg, 0.5 mmol) was added to a solution of **6** (48 mg, 0.1 mmol) and chloroacetaldehyde in dry THF (1 mL) at room temperature under an argon atmosphere. The reaction mixture was stirred at room temperature for 17 h, and quenched with satd. $NaHCO_3$ aq (20 mL), then extracted with AcOEt. The organic layer was washed with brine, dried over Na_2SO_4 and evaporated *in vacuo*. The resulting residue was purified by flash column chromatography (Hex/AcOEt =64/36) to afford chloroethyl intermediate (54 mg, quant) as a colorless oil. This compound was dissolved in dry DMF, and NaN_3 (13 mg, 0.2 mmol) was added to the mixture under an argon atmosphere. The reaction mixture was stirred at 80 °C for 6 h, distilled by AcOEt (20 mL), and extracted with H_2O (20 mL). The organic layer was washed with brine, dried over Na_2SO_4 and evaporated *in vacuo*. The resulting residue was purified by flash column chromatography (Hex/AcOEt =64/36) to afford compound **8** (48 mg, 89 % in 2 steps) as a colorless oil. ^{1}H-NMR (500 MHz, CD_3OD) δ (ppm): 3.28 (2H, br), 3.57 (2H, br), 3.52 (2H, t, J = 6.0 Hz), 3.41 (4H, br), 3.36 (4H, br), 2.83 (2H, br), 2.16 (4H, br). ^{13}C-NMR (125 MHz, $CDCl_3$) δ (ppm): 157.8, 157.5, 157.3, 81.1, 79.4, 61.5, 56.3, 56.1, 29.1, 28.8, 20.9, 14.5. IR (cm^{-1}): 2343, 2093, 1688, 1164. HR-ESI-MS (m/z): Calcd for $C_{25}H_{47}N7O_6$ $(M+H)^+$ 542.3661. Found 542.3667.



Scheme S1. Synthesis scheme of compounds **3a-c**.

5'-Azido-3'-hydroxy 8-oxoG-clamp (**S1**) A solution of tosyl chloride (95 mg, 0.5 mmol) in pyridine (4 mL) was added dropwise to a solution of 8-oxoG-clamp 3',5'-diol (123 mg, 0.25 mmol) in pyridine (4 mL) over 1 h at room temperature under an argon atmosphere. The reaction mixture was stirred at room temperature for 36 h before quenching with H_2O. The resulting mixture was extracted with AcOEt (20 mL). The organic layer was washed with brine, dried over Na_2SO_4 and evaporated *in vacuo*. The resulting residue was purified by flash column chromatography ($CHCl_3$/MeOH = 97/3) to

afford tosylate intermediate (90 mg) as a yellow amorphous. The tosylate compound was dissolved in DMF (2.2 mL) and stirred with NaN_3 (33 mg, 0.5 mmol) at 70 °C for 19 h. The reaction mixture was distilled with AcOEt (20 mL), and extracted with H_2O (20 mL). The organic layer was washed with brine, dried over Na_2SO_4 and evaporated *in vacuo*. The resulting residue was purified by flash column chromatography ($CHCl_3$/MeOH = 97/3) to afford compound **S1** (59 mg, 44 % in 2 steps) as a yellow amorphous. ^{1}H-NMR (500 MHz, CD_3OD) δ (ppm): 7.35 (1H, s), 7.33-7.25 (5H, br), 6.82 (1H, t, *J* = 8.25 Hz), 6.58 (1H, d, *J* = 8.25 Hz), 6.43 (1H, d, *J* = 8.25 Hz), 6.20 (1H, t, *J* = 8.5 Hz), 5.11 (2H, s), 4.31-4.30 (1H, m), 4.05 (2H, t, *J* = 5.5 Hz), 3.99-3.96 (1H, m), 3.68 (1H, dd, *J* = 13.0, 3.5 Hz), 3.77 (1H, dd, *J* = 13.0, 5 Hz), 3.54 (2H, t, *J* = 5.5 Hz), 2.36-2.31 (1H, m), 2.22-2.16 (1H, m). ^{13}C-NMR (125 MHz, $CDCl_3$) δ (ppm): 159.1, 156.6, 155.6, 148.0, 144.3, 138.4, 129.8, 129.4, 128.9, 128.7, 125.0, 123.2, 109.4, 108.3, 87.4, 86.3, 79.4, 72.4, 69.6, 67.5, 56.1, 53.4, 41.2, 41.0, 32.1, 29.5. IR (cm^{-1}): 2322, 2101, 1680, 1558. HR-ESI-MS (m/z): Calcd for $C_{25}H_{25}N_7O_7$ $(M+H)^+$ 536.1888. Found 536.1895.

Tri-Boc cyclen-5'-triazole 8-oxoG-clamp (**S2**) Compound **S1** (53 mg, 0.10 mmol) and compound **7** (51 mg, 0.10 mmol) were dissolved in DMSO (2.5 mL), and to this solution were added an aqueous solution of $CuSO_4$ (0.015 mmol), sodium ascorbate (0.03 mmol) and a solution of TBTA (0.03 mmol) in DMSO at room temperature. The reaction mixture was stirred at room temperature for 19 h before extracted with AcOEt (25 mL). The organic layer was washed with brine, dried over Na_2SO_4 and evaporated *in vacuo*. The resulting residue was purified by flash column chromatography (AcOEt/MeOH = 92/8) to afford compound **S2** (98 mg, 94 %) as a yellow amorphous. ^{1}H-NMR (500 MHz, CD_3OD) δ (ppm): 7.89 (1H, s), 7.24 (5H, br), 6.89 (1H, s), 6.84 (1H, t, *J* = 8.0 Hz), 6.61 (1H, d, *J* = 8.0 Hz), 6.48 (1H, d, *J* = 8.0 Hz), 6.17 (1H, t, *J* = 6.5 Hz), 5.55 (2H, s), 5.11 (2H, s), 4.79 (1H, dd, *J* = 14.5, 4.0 Hz), 4.73 (1H, dd, *J* = 14.5, 6.0 Hz), 4.36 (1H, br), 4.17-4.14 (1H, m), 4.06 (2H, t, *J* = 5.0 Hz), 4.01-3.93 (2H, m), 3.70 (2H, br), 3.54 (6H, t, *J* = 5.0 Hz), 3.36 (6H, br), 2.62 (4H, br), 2.36-2.31 (1H, m), 2.18-2.13 (1H, m), 1.47 (9H, s), 1.42 (18H, s). ^{13}C-NMR (125 MHz, CD_3OD) δ (ppm): 159.1, 157.4, 156.5, 155.6, 148.1, 144.3, 142.9, 138.4, 136.8, 130.0, 129.6, 129.4, 129.1, 128.7, 127.1, 125.1, 109.4, 108.4, 87.6, 85.4, 80.9, 79.5, 72.1, 69.7, 67.5, 56.1, 55.5, 54.9, 52.2, 41.2, 40.1, 39.5, 29.5, 29.1, 28.8. IR (cm^{-1}): 2975, 1680, 1558, 1474. HR-ESI-MS (m/z): Calcd for $C_{51}H_{71}N_{11}O_{13}$ $(M+H)^+$ 1046.5306. Found 1046.5322.

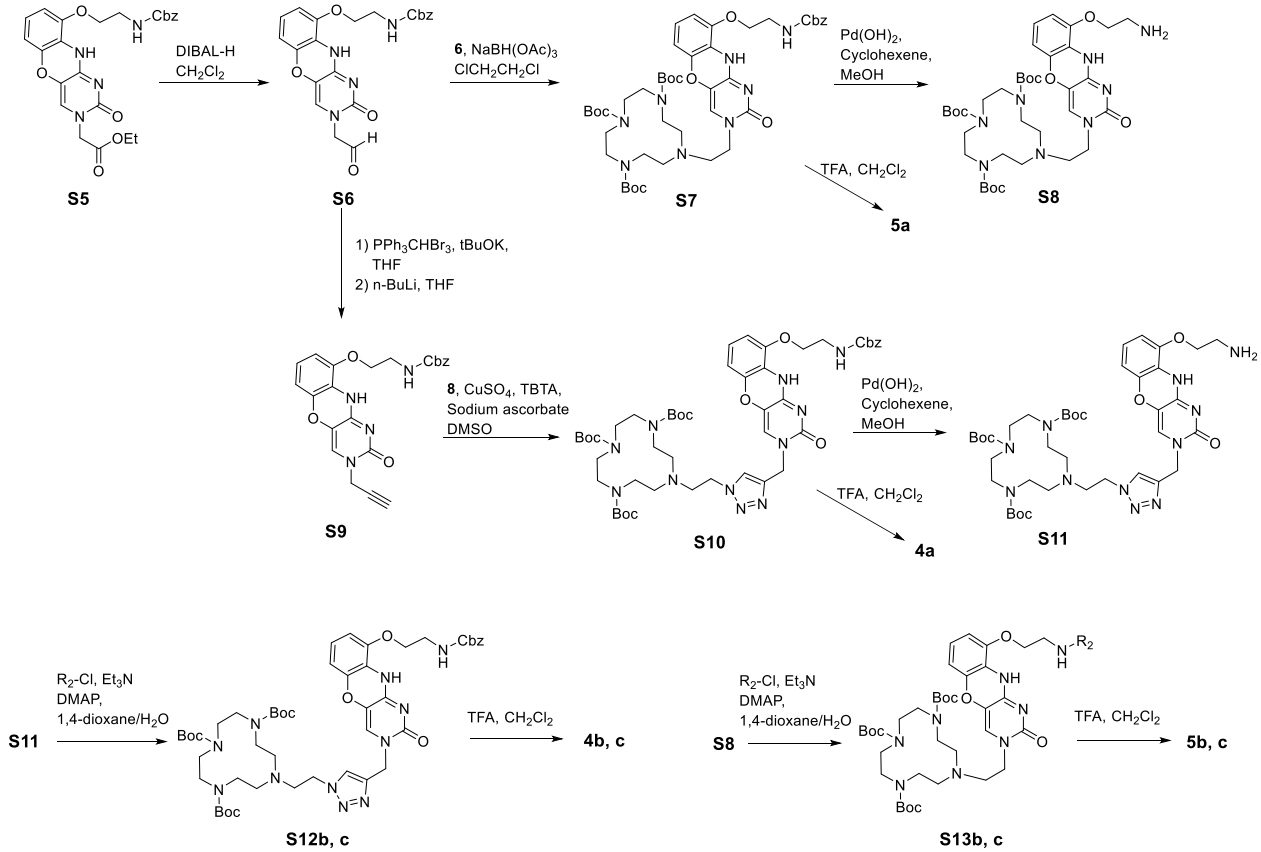
Tri-Boc cyclen-5'-triazole-G-clamp (**S3**) Compound **S2** (52 mg, 0.05 mmol) was dissolved in MeOH/cyclohexene (1:1, 1 mL) solution, and to this solution was added 20 wt% $Pd(OH)_2$/C (35 mg, 0.05 mmol) under argon atmosphere. The reaction mixture was stirred at 70 °C for 2 days. The reaction mixture was filtered through celite, and resulting filtrate was evaporated in vacuo. The residue was purified by flash column chromatography (NH-silica gel, $CHCl_3$/MeOH = 97/3) to afford compound **S3** (22 mg, 48 %) as a pale green amorphous. ^{1}H-NMR (500 MHz, CD_3OD) δ (ppm): 7.93

(1H, s), 6.87 (1H, s), 6.84 (1H, t, *J* = 8.0 Hz), 6.62 (1H, d, *J* = 8.0 Hz), 6.48 (1H, d, *J* = 8.0 Hz), 6.17 (1H, t, *J* = 6.5 Hz), 4.78 (1H, dd, *J* = 14.5, 4.0 Hz), 4.72 (1H, dd, *J* = 14.5, 6.0 Hz), 4.35 (1H, br), 4.16-4.13 (1H, m), 4.06 (2H, t, *J* = 5.0 Hz), 4.01-3.93 (2H, m), 3.54 (4H, br), 3.36 (6H, br), 3.08 (2H, t, *J* = 5.0 Hz), 2.60 (4H, br), 2.35-2.30 (1H, m), 2.17-2.12 (1H, m), 1.46 (9H, s), 1.41 (18H, s). ^{13}C-NMR (125 MHz, CD_3OD) δ (ppm): 157.6, 156.6, 155.8, 148.3, 144.4, 129.8, 127.2, 125.1, 123.2, 117.1, 109.4, 108.4, 87.6, 85.4, 81.0, 79.5, 72.1, 70.8, 70.3, 55.4, 54.9, 52.2, 41.6, 40.1, 30.7, 29.1, 28.8. IR (cm^{-1}): 3416, 2978, 1678, 1474. HR-ESI-MS (m/z): Calcd for $C_{43}H_{65}N_{11}O_{11}$ $(M+H)^+$ 912.4938. Found 912.4958.

Tri-Boc cyclen-5'-triazole-G-clamp naphthylethyl derivative (**S4b**) 1-Naphthalene ethanol (1.72 g, 10 mmol) was dissolved in dry THF and triphosgen (4.45 g, 15 mmol) was added to this mixture at room temperature. The reaction mixture was stirred at room temperature for 2 days before quenched with satd. $NaHCO_3$ aq (100 mL). The resulting mixture was extracted with AcOEt (100 mL). The organic layer was washed with brine, dried over Na_2SO_4 and evaporated *in vacuo*. The resulting residue (2.59g, colorless oil) was used for next step as 2-(1-naphthyl)ethyl chloroformate without further purification. Compound **S3** (20 mg, 0.02 mmol) and 2-(1-naphthyl)ethyl chloroformate (10 mg, 0.04 mmol) were dissolved in 1,4-dioxane/H_2O (9:1, 0.5 mL), and to this mixture were added Et_3N (6 μL, 0.04 mmol) and DMAP (1 piece) at room temperature. The reaction mixture was stirred at room temperature for 20 h, diluted with AcOEt (20 mL) and extracted with satd. $NaHCO_3$ aq (10 mL). The organic layer was washed with brine, dried over Na_2SO_4 and evaporated *in vacuo*. The resulting residue was purified by flash column chromatography ($CHCl_3$/MeOH = 96/4) to afford compound **S4b** (11 mg, 45 %) as a yellow amorphous. ^{1}H-NMR (500 MHz, CD_3OD) δ (ppm): 8.09 (1H, d, *J* = 8.0 Hz), 7.93 (1H, s), 7.79 (1H, d, *J* = 8.0 Hz), 7.66 (1H, d, *J* = 8.0 Hz), 7.45 (1H, t, *J* = 7.0 Hz), 7.39 (1H, t, *J* = 7.5 Hz), 7.36-7.27 (2H, m), 6.89 (1H, s), 6.84 (1H, t, *J* = 8.0 Hz), 6.58 (1H, d, *J* = 8.0 Hz), 6.47 (1H, d, *J* = 8.0 Hz), 6.17 (1H, t, *J* = 6.5 Hz), 4.78 (1H, dd, *J* = 14.5, 4.0 Hz), 4.72 (1H, dd, *J* = 14.5, 6.0 Hz), 4.35 (1H, br), 4.16-4.13 (1H, m), 4.06 (2H, t, *J* = 5.0 Hz), 4.01-3.93 (2H, m), 3.54 (4H, br), 3.36 (6H, br), 3.08 (2H, t, *J* = 5.0 Hz), 2.60 (4H, br), 2.35-2.30 (1H, m), 2.17-2.12 (1H, m), 1.46 (9H, s), 1.41 (18H, s). ^{13}C-NMR (125 MHz, CD_3OD) δ (ppm): 157.6, 156.6, 155.8, 148.3, 144.4, 129.8, 127.2, 125.1, 123.2, 117.1, 109.4, 108.4, 87.6, 85.4, 81.0, 79.5, 72.1, 70.8, 70.3, 55.4, 54.9, 52.2, 41.6, 40.1, 30.7, 29.1, 28.8. IR (cm^{-1}): 3273, 2975, 1679, 1474. HR-ESI-MS (m/z): Calcd for $C_{56}H_{75}N_{11}O_{13}$ $(M+H)^+$ 1110.5619. Found 1110.5617.

Tri-Boc cyclen-5'-triazole-G-clamp pyrenylethyl derivative (**S4c**) 1-Pyrene ethanol[13] was converted to 2-(1-pyrenyl)ethyl chloroformate (dark yellow solid) with triphosgen according to the same procedure of synthesis for compound **S4a**. The resulting chloroformate was used for the synthesis of **S4c** (39 %) by the procedure described above. ^{1}H-NMR (400 MHz, CD_3OD) δ (ppm): 8.31 (1H, d, *J* = 8.8 Hz), 8.09-7.88 (9H, m), 6.82 (1H, t, *J* = 8.4 Hz), 6.76 (1H, s), 6.52 (1H, d, *J* = 8.4 Hz), 6.42 (1H, d,

J = 8.0 Hz), 6.10 (1H, t, *J* = 6.4 Hz), 4.56 (2H, t, *J* = 6.4 Hz), 4.34 (2H, br), 4.17 (2H, br), 3.94 (2H, br), 3.88 (2H, m), 3.65 (2H, br), 3.47 (6H, br), 2.55 (4H, br), 2.32-2.26 (1H, m), 2.14-2.06 (1H, m), 1.44 (9H, s), 1.38 (18H, s). ^{13}C-NMR (125 MHz, CD_3OD) δ (ppm): 156.3, 144.4, 132.7, 132.2, 131.6, 130.6, 129.5, 127.9, 127.1, 126.1, 125.9, 125.8, 125.0, 124.4, 109.4, 108.1, 92.2, 87.8, 85.5, 81.0, 71.4, 69.6, 67.0, 66.5, 64.3, 55.3, 52.4, 41.1, 40.1, 33.9, 29.1, 28.8. IR (cm^{-1}): 2935, 1683, 1557, 1474. HR-ESI-MS (m/z): Calcd for $C_{62}H_{77}N_{11}O_{13}$ $(M+H)^+$ 1184.5775. Found 1184.5782.



Scheme S2. Synthesis scheme of compounds **4a-c**, **5a-c**.

8-oxoG-clamp acetaldehyde (**S6**) Ethyl acetate **S5**[18] (120 mg, 0.25 mmol) was dissolved in dry CH_2Cl_2 (5 mL) and cooled to -78 °C under argon atmosphere. DIBAL-H in hexane (1.0 mmol) was added dropwise to this mixture, and the reaction mixture was stirred at -78 °C for 1 h. The reaction was quenched with MeOH (1 mL) and 1 M HCl aq (1 mL) at -78 °C and warmed to room temperature. AcOEt (40 mL) was added and extracted with H_2O (40 mL). The organic layer was washed with brine, dried over Na_2SO_4 and evaporated *in vacuo*. The resulting residue was purified by flash column chromatography ($CHCl_3$/MeOH = 96/4) to afford compound **S6** (78 mg, 71 %) as a pale yellow amorphous. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 7.31 (5H, m), 7.17 (1H, s), 6.81 (1H, t, *J*

= 8.4 Hz), 6.79 (1H, d, *J* = 8.4 Hz), 6.41 (1H, d, *J* = 8.4 Hz), 5.10 (2H, s), 4.72 (2H, t, *J* = 6.0 Hz), 4.01 (2H, t, *J* = 4.8 Hz), 3.76 (2H, s), 3.53 (2H, t, *J* = 4.8 Hz). ^{13}C-NMR (125 MHz, CD_3OD) δ (ppm): 159.1, 157.8, 156.6, 147.9, 144.3, 138.4, 130.3, 129.5, 129.4, 129.0, 128.8, 128.7, 124.8, 109.4, 108.3, 107.1, 96.1, 94.7, 69.6, 68.4, 67.6, 55.2, 55.1, 41.5, 41.2. IR (cm^{-1}): 3235, 2322, 1675, 1474. HR-ESI-MS (m/z): Calcd for $C_{22}H_{20}N_4O_6$ $(M+H)^+$ 437.1456. Found 437.1472.

Tri-Boc cyclen-ethyl-8-oxoG-clamp (**S7**) $NaBH(OAc)_3$ (71 mg, 0.33 mmol) was added to a solution of **S6** (73 mg, 0.17 mmol) and cyclen compound **6** (79 mg, 0.17 mmol) in dry dichloroethane (1.7 mL) at room temperature under an argon atmosphere. The reaction mixture was stirred at room temperature for 10 h, and quenched with satd. $NaHCO_3$ aq (20 mL), then extracted with AcOEt. The organic layer was washed with brine, dried over Na_2SO_4 and evaporated *in vacuo*. The resulting residue was purified by flash column chromatography ($CHCl_3$/MeOH = 97/3) to afford compound **S7** (140 mg, 94 %) as a yellow amorphous. ^{1}H-NMR (400 MHz, CD_3OD) δ (ppm): 7.88 (1H, s), 7.35-7.25 (5H, m), 6.81 (1H, t, *J* = 8.0 Hz), 6.59 (1H, d, *J* = 8.0 Hz), 6.42 (1H, d, *J* = 8.0 Hz), 5.11 (2H, s), 4.06 (2H, t, *J* = 5.2 Hz), 3.85 (2H, t, *J* = 7.2 Hz), 3.57 (2H, br), 3.53 (4H, t, *J* = 5.2 Hz), 3.40 (8H, br), 2.93 (2H, br), 2.77 (4H, br), 1.45 (27H, s). ^{13}C-NMR (125 MHz, $CDCl_3$) δ (ppm): 156.8, 156.1, 153.8, 143.0, 136.6, 128.6, 128.2, 128.1, 127.7, 123.6, 108.4, 107.1, 80.0, 79.6, 68.5, 67.0, 66.7, 51.1, 50.3, 49.8, 48.3, 47.6, 46.2, 40.6, 32.3, 31.1, 29.8, 29.4, 28.8, 28.7, 28.6. IR (cm^{-1}): 2948, 2359, 1678, 1474. HR-ESI-MS (m/z): Calcd for $C_{45}H_{64}N_8O_{11}$ $(M+H)^+$ 893.4767. Found 893.4722.

Tri-Boc cyclen-ethyl-G-clamp (**S8**) The deprotection of Cbz group was performed by the procedure of synthesis **S3** described above to obtain the compound **S8** (52 %) as a pale green amorphous. ^{1}H-NMR (400 MHz, CD_3OD) δ (ppm): 7.36 (1H, s), 6.82 (1H, t, *J* = 8.4 Hz), 6.61 (1H, d, *J* = 8.4 Hz), 6.42 (1H, d, *J* = 8.4 Hz), 4.05 (2H, t, *J* = 5.2 Hz), 3.86 (2H, br), 3.58 (2H, br), 3.53 (2H, br), 3.40 (8H, br), 3.06 (2H, t, *J* = 4.8 Hz), 2.94 (2H, br), 2.78 (4H, s), 1.46 (27H, s). ^{13}C-NMR (125 MHz, CD_3OD) δ (ppm): 157.5, 156.1, 148.1, 144.3, 129.6, 128.9, 124.8, 117.3, 109.3, 108.4, 81.2, 79.5, 70.9, 41.6, 29.0, 28.9. IR (cm^{-1}): 2976, 1678, 1562, 1474. HR-ESI-MS (m/z): Calcd for $C_{37}H_{58}N_8O_9$ $(M+H)^+$ 759.4400. Found 759.4442.

Propargyl 8-oxoG-clamp (**S9**) t-BuOK (44 mg, 0.4 mmol) was added to a solution of Ph_3PCHBr_3 (208 mg, 0.4 mmol) in dry THF at 0 °C, and the mixture was stirred at 0 °C for 30 min before addition of compound **S6** (88 mg, 0.2 mmol). The reaction mixture was warmed to room temperature and stirred for 24 h. The reaction mixture was quenched with satd. $NaHCO_3$ aq (40 mL) and extracted with $CHCl_3$ (40 mL). The organic layer was washed with brine, dried over Na_2SO_4 and evaporated *in vacuo*. The resulting residue was purified by flash column chromatography ($CHCl_3$/MeOH = 100/0 to 97/3) to afford intermediate dibromoolefine compound. The intermediate compound (50 mg, 0.08

mmol) was dissolved in dry THF and cooled to -78 °C under argon atmosphere. To this mixture was added n-BuLi (0.4 mmol) in hexane dropwise, and the reaction mixture was stirred for 1.5 h at -78 °C. The reaction mixture was quenched with satd. NH_4Cl aq (20 mL) and extracted with $CHCl_3$ (20 mL). The organic layer was washed with brine, dried over Na_2SO_4 and evaporated *in vacuo*. The resulting residue was purified by flash column chromatography ($CHCl_3$/MeOH = 99/1) to afford compound **S9** (21 mg, 58 %) as a yellow amorphous. ^{1}H-NMR (400 MHz, CD_3OD) δ (ppm): 7.36-7.29 (6H, m), 6.83 (1H, t, *J* = 8.0 Hz), 6.60 (1H, d, *J* = 8.0 Hz), 6.44 (1H, d, *J* = 8.0 Hz), 5.11 (2H, s), 4.53 (2H, s), 4.07 (2H, t, *J* = 4.8 Hz), 3.53 (2H, t, *J* = 4.8 Hz), 2.90 (1H, s). ^{13}C-NMR (125 MHz, CD_3OD) δ (ppm): 156.8, 154.7, 146.4, 143.1, 136.7, 128.7, 128.2, 128.0, 127.7, 125.7, 123.8, 123.2, 108.7, 108.1, 106.9, 75.4, 68.7, 67.2, 67.0, 60.5, 41.1, 40.5, 38.8, 38.1, 31.1. IR (cm^{-1}): 3287, 1679, 1559, 1474. HR-ESI-MS (m/z): Calcd for $C_{23}H_{20}N_4O_5$ $(M+H)^+$ 433.1506. Found 433.1519.

Tri-Boc cyclen-ethyl triazole-8-oxoG-clamp (**S10**) The click reaction of alkyne **S9** with azido **8** was performed by the procedure of synthesis **S2** described above to obtain the compound **S10** (88 %) as a pale green amorphous. ^{1}H-NMR (400 MHz, CD_3OD) δ (ppm): 8.09 (1H, s), 7.36-7.24 (6H, m), 6.80 (1H, t, *J* = 8.0 Hz), 6.57 (1H, d, *J* = 8.0 Hz), 6.40 (1H, d, *J* = 8.0 Hz), 5.09 (2H, s), 4.96 (2H, s), 4.55 (2H, d, *J* = 6.4 Hz), 4.04 (2H, t, *J* = 5.2 Hz), 3.52 (2H, t, *J* = 5.2 Hz), 3.47 (2H, br), 3.33 (6H, s), 3.19 (4H, br), 2.73 (4H, br), 1.44 (9H, s), 1.41 (18H, s). ^{13}C-NMR (125 MHz, CD_3OD) δ (ppm): 159.1, 157.2, 156.0, 147.9, 144.2, 138.4, 129.4, 128.9, 128.7, 128.1, 124.9, 117.0, 109.4, 108.4, 81.1, 69.6, 67.5, 56.1, 55.4, 45.5, 41.3, 40.6, 32.1, 30.7, 29.5, 29.0, 28.9. IR (cm^{-1}): 2921, 1681, 1558, 1474. HR-ESI-MS (m/z): Calcd for $C_{48}H_{67}N_{11}O_{11}$ $(M+H)^+$ 974.5094. Found 974.5070.

Tri-Boc cyclen-ethyl triazole-G-clamp (**S11**) The deprotection of Cbz group was performed by the procedure of synthesis **S3** described above to obtain the compound **S11** (40 %) as a pale green amorphous. ^{1}H-NMR (500 MHz, CD_3OD) δ (ppm): 8.09 (1H, s), 7.88 (1H, s), 6.81 (1H, t, *J* = 8.5 Hz), 6.59 (1H, d, *J* = 8.5 Hz), 6.41 (1H, d, *J* = 8.5 Hz), 4.95 (2H, s), 4.56 (2H, br), 4.04 (2H, t, *J* = 5.0 Hz), 3.48 (2H, br), 3.37 (10H, br), 3.19 (2H, br), 3.06 (2H, t, *J* = 5.0 Hz), 2.74 (4H, br). ^{13}C-NMR (125 MHz, CD_3OD) δ (ppm): 158.5, 157.2, 156.2, 148.1, 144.4, 130.4, 129.7, 128.0, 125.6, 124.9, 120.5, 117.1, 116.2, 109.4, 108.4, 81.1, 79.5, 70.8, 45.4, 41.6, 29.0, 28.8. IR (cm^{-1}): 2968, 1675, 1559, 1475. HR-ESI-MS (m/z): Calcd for $C_{40}H_{61}N_{11}O_9$ $(M+H)^+$ 840.4726. Found 840.4714.

Tri-Boc cyclen-ethyl triazole-G-clamp naphthylethyl derivative (**S12b**) The derivatization from **S11** was performed by the procedure of synthesis **S4b** described above to obtain the compound **S12b** (5 %) as a pale yellow amorphous. ^{1}H-NMR (400 MHz, CD_3OD) δ (ppm): 8.08-8.06 (2H, m), 7.76 (1H, d, *J* = 7.2 Hz), 7.63 (1H, d, *J* = 8.0 Hz), 7.41-7.26 (5H, m), 6.79 (1H, t, *J* = 8.0 Hz), 6.54 (1H, d, *J* = 8.0 Hz), 6.39 (1H, d, *J* = 8.0 Hz), 4.94 (2H, s), 4.54 (2H, t, *J* = 6.0 Hz), 4.39 (2H, t, *J* = 7.2 Hz), 3.96 (2H, br),

3.69 (4H, br), 3.46 (2H, br), 3.36 (4H, br), 3.16(2H, br), 2.71 (4H, br), 1.43 (9H, br), 1.40 (18H, br). [1] IR (cm^{-1}): 2972, 1676, 1562, 1474. HR-ESI-MS (m/z): Calcd for $C_{53}H_{71}N_{11}O_{11}$ $(M+Na)^+$ 1060.5227. Found 1060.5219.

Tri-Boc cyclen-ethyl triazole-G-clamp pyrenyllethyl derivative (**S12c**) The derivatization from **S11** was performed by the procedure of synthesis **S4c** described above to obtain the compound **S12c** (14 %) as a pale yellow amorphous. ^{1}H-NMR (500 MHz, CD_3OD) δ (ppm): 8.27 (1H, d, *J* = 9.0 Hz), 8.09 (1H, d, *J* = 7.5 Hz), 8.05 (1H, s), 7.98 (1H, d, *J* = 7.5 Hz), 7.95-7.84 (6H, m), 7.05 (1H, s), 6.72 (1H, t, *J* = 8.0 Hz), 6.40 (1H, d, *J* = 8.0 Hz), 6.28 (1H, d, *J* = 8.0 Hz), 4.55 (2H, t, *J* = 6.0 Hz), 4.50 (2H, br), 3.88-3.86 (2H, m), 3.69 (4H, br), 3.63-3.60 (2H, m), 3.42-3.40 (2H, m), 3.37 (2H, br), 3.24 (4H, br), 3.10 (2H, br), 2.65 (4H, br), 1.40 (9H, s), 1.37 (18H, s). IR (cm^{-1}): 2979, 1679, 1558, 1474. HR-ESI-MS (m/z): Calcd for $C_{59}H_{73}N_{11}O_{11}$ $(M+Na)^+$ 1134.5383. Found 1134.5378.

Tri-Boc cyclen-ethyl G-clamp naphthylethyl derivative (**S13b**) The derivatization from **S8** was performed by the procedure of synthesis **S4b** described above to obtain the compound **S13b** (26 %) as a pale yellow amorphous. ^{1}H-NMR (400 MHz, CD_3OD) δ (ppm): 8.09 (1H, d, *J* = 8.4 Hz), 7.90 (1H, s), 7.79 (1H, d, *J* = 8.4 Hz), 7.67 (1H, d, *J* = 8.4 Hz), 7.47-7.28 (5H, m), 6.82 (1H, t, *J* = 8.0 Hz), 6.58 (1H, d, *J* = 8.0 Hz), 6.42 (1H, d, *J* = 8.0 Hz), 4.39 (2H, t, *J* = 6.4 Hz), 3.99 (2H, br), 3.83 (2H, br), 3.56 (2H, br), 3.49 (4H, br), 3.38 (6H, br), 2.91 (2H, br), 2.76 (4H, br). IR (cm^{-1}): 2979, 1682, 1558, 1475. HR-ESI-MS (m/z): Calcd for $C_{50}H_{68}N_8O_{11}$ $(M+H)^+$ 957.5080. Found 957.5034.

Tri-Boc cyclen-ethyl triazole-G-clamp pyrenyllethyl derivative (**S13c**) The derivatization from **S8** was performed by the procedure of synthesis **S4c** described above to obtain the compound **S13c** (37 %) as a pale yellow amorphous. ^{1}H-NMR (500 MHz, CD_3OD) δ (ppm): 8.27 (1H, d, *J* = 9.0 Hz), 8.10 (1H, d, *J* = 7.5 Hz), 8.02 (1H, d, *J* = 7.5 Hz), 7.96-7.84 (6H, m), 6.98 (1H, s), 6.75 (1H, t, *J* = 8.0 Hz), 6.45 (1H, d, *J* = 8.0 Hz), 6.32 (1H, d, *J* = 8.0 Hz), 4.54 (2H, t, *J* = 6.0 Hz), 3.92 (2H, br), 3.51-3.37 (6H, br), 3.32 (4H, br), 2.76 (2H, br), 2.69 (4H, br), 1.43 (27H, s). IR (cm^{-1}): 2969, 1687, 1555, 1473. HR-ESI-MS (m/z): Calcd for $C_{56}H_{70}N_8O_{11}$ $(M+H)^+$ 1031.5237. Found 1031.5205.

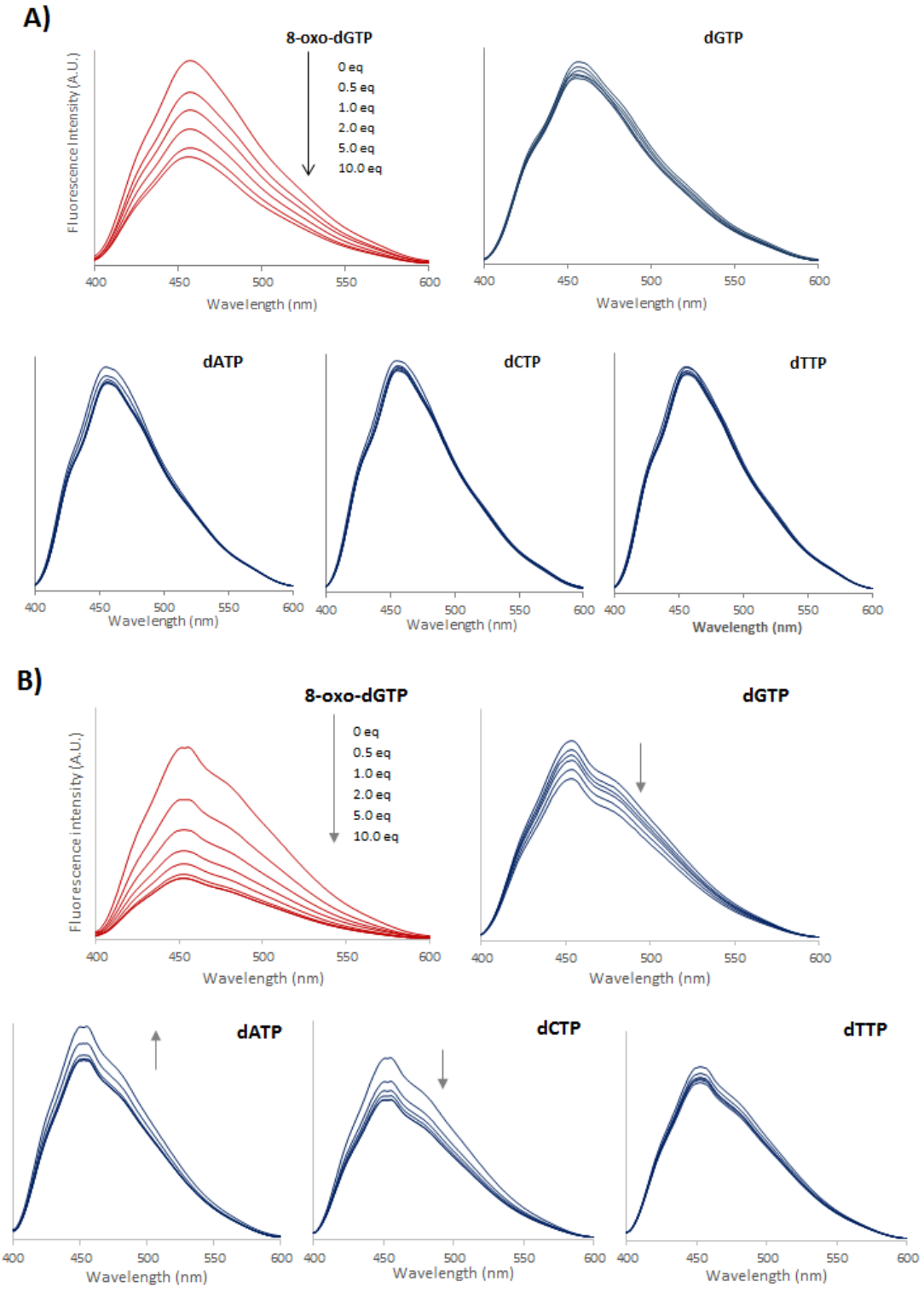
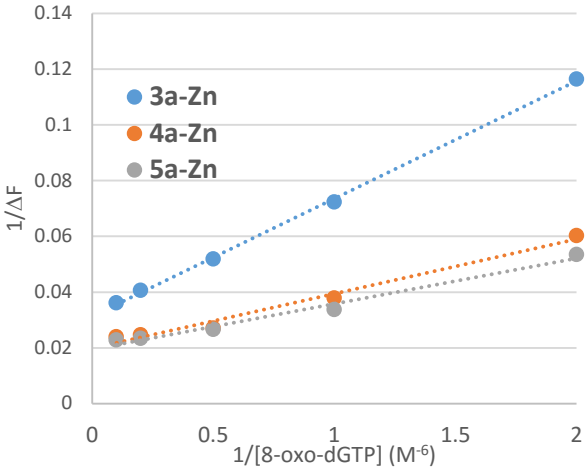


Figure S1. Fluorescence titration experiment with **3a** and **4a-Zn** for nucleoside triphosphates. **A) 3a-Zn**, **B) 4a-Zn.** 0–10 μM Nucleotide was added into a solution of 1 μM **3a** or **4a-Zn** in 10 mM HEPES buffer (pH= 7.4) at 25 °C. Emission spectra were recorded at λ_{ex}= 365 nm.



Benesi-Hildebrand equation;

$$\frac{1}{F - F_0} = \frac{1}{(\varphi_{HG} - \varphi_H)[H]} + \frac{1}{K[H](\varphi_{HG} - \varphi_H)[G]}$$

F; fluorescence intensity,
ϕ; fluorescence quantum yield
[*H*]; Receptor conc.
[G]; 8-oxo-dGTP conc.
K; equilibrium constant

Figure S2. Benesi-Hildebrand plots of **3a**-Zn, **4a**-Zn and **5a**-Zn for 8-oxo-dGTP.

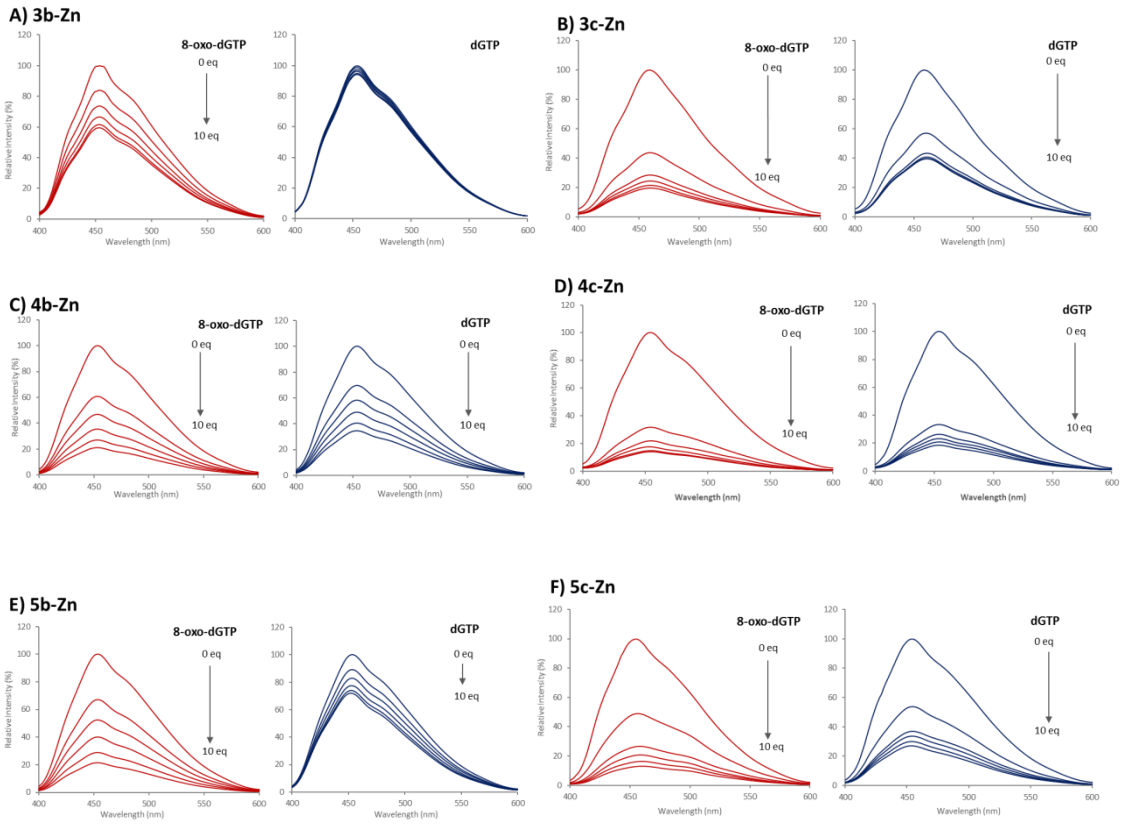


Figure S3. Fluorescence titration spectra of **3b-c** (A, B), **4b-c** (C, D) and **5b-c** (E, F) compounds. 0–10 μM nucleotide was added into a solution of 1 μM 8-oxoGTP Receptor derivatives in 10 mM HEPES buffer (pH= 7.4) at 25 °C. Emission spectra were recorded at λ_{ex}= 365 nm.

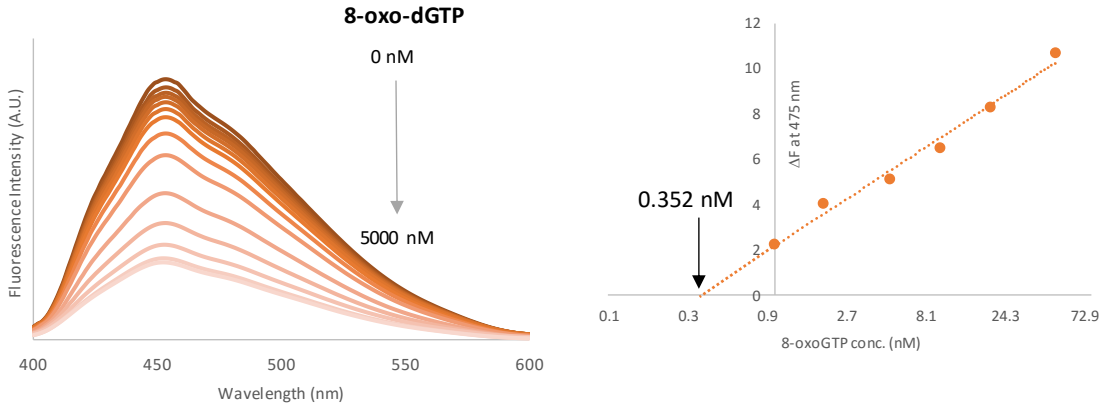


Figure S4. Fluorescence titration of 8-oxo-dGTP from lower concentration (1 nM~) for **5a-Zn**. Left; titration spectrum of 8-oxo-dGTP from 1 nM to 5000 nM in 10 mM HEPES buffer (pH 7.4) using 1 μM of **5a-Zn**. Right; plot of ΔF at 475 nm for 8-oxo-dGTP concentration.

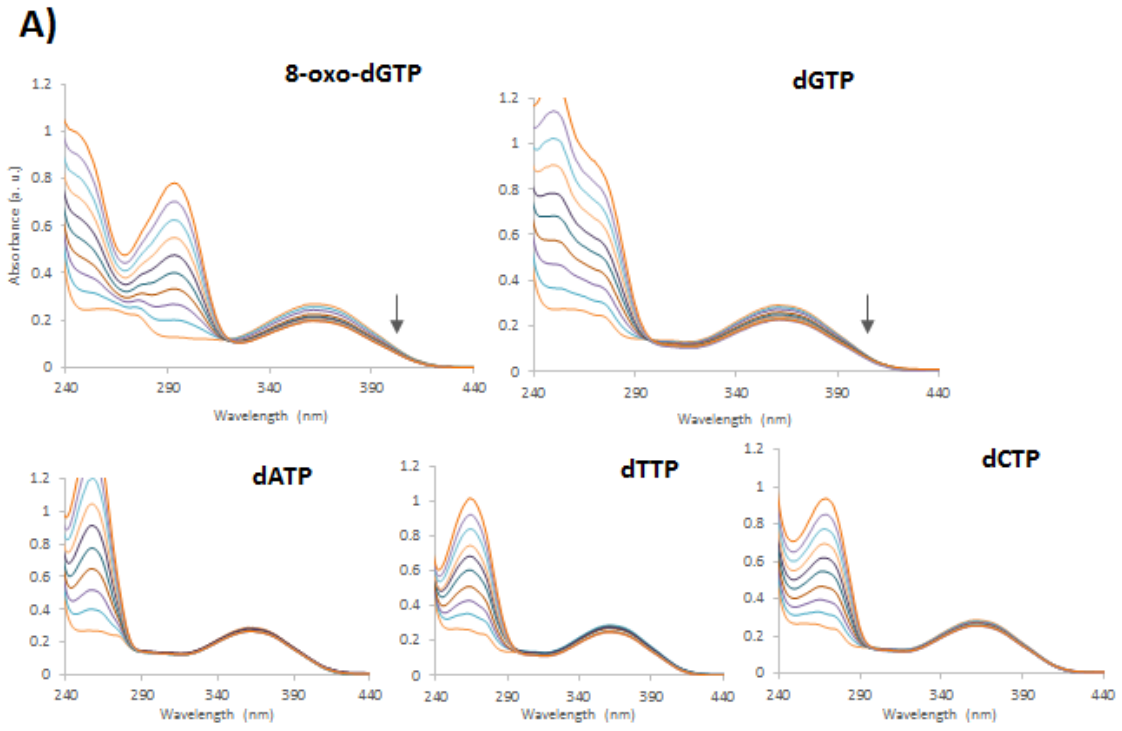


Figure S5 (1). UV-Vis titration experiment with **3a** and **4a-Zn** for nucleoside triphosphates. **A) 3a-Zn**, **B) 4a-Zn**. 0–90 μM nucleotide was added into a solution of 50 μM **3a-Zn** or **4a-Zn** in 10 mM HEPES buffer (pH= 7.4) at 25 °C.

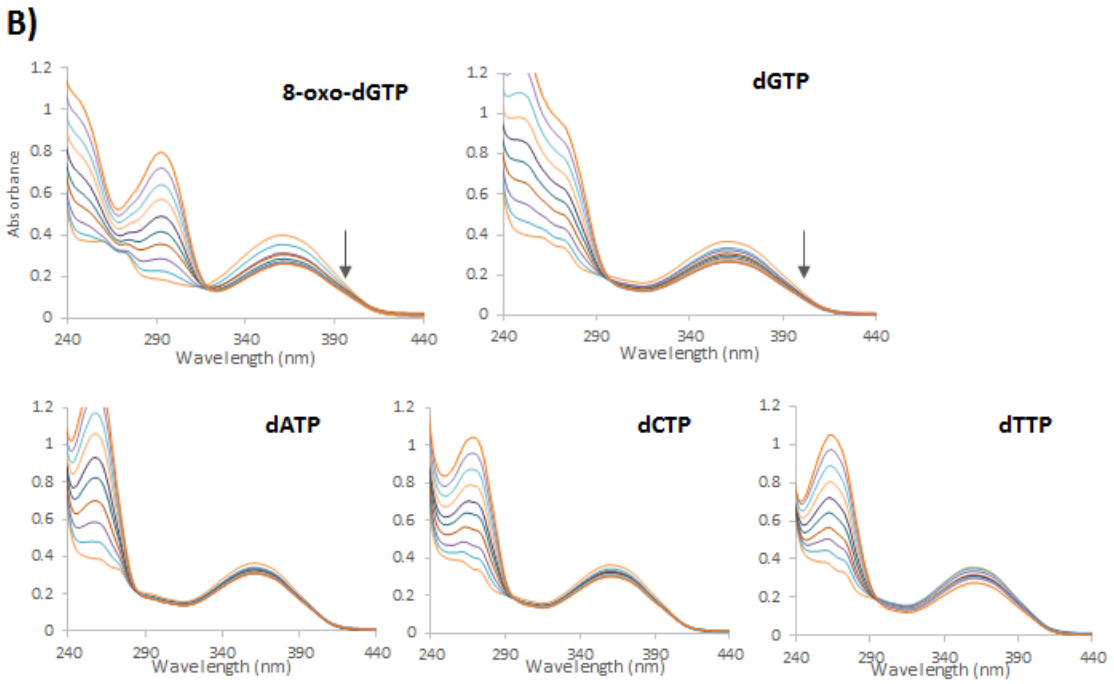


Figure S5 (2). UV-Vis titration experiment with **3a** and **4a-Zn** for nucleoside triphosphates. **A) 3a-Zn**, **B) 4a-Zn**. 0–90 μM nucleotide was added into a solution of 50 μM **3a-Zn** or **4a-Zn** in 10 mM HEPES buffer (pH= 7.4) at 25 °C.

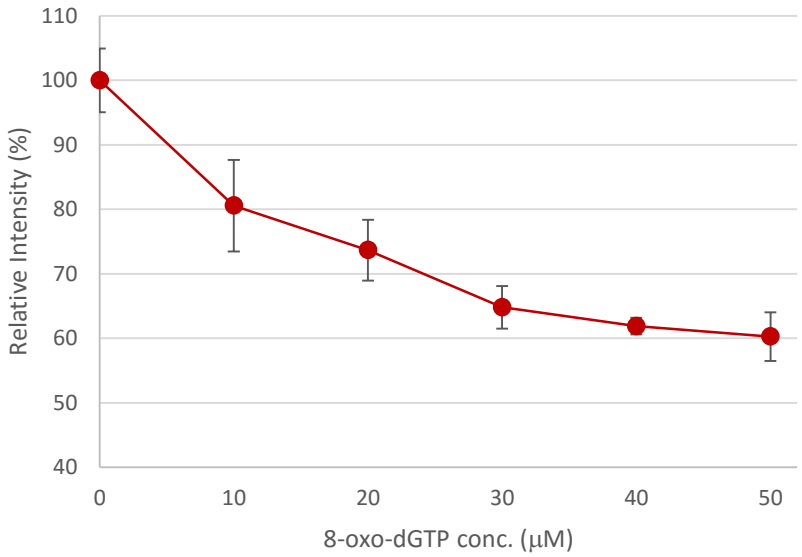
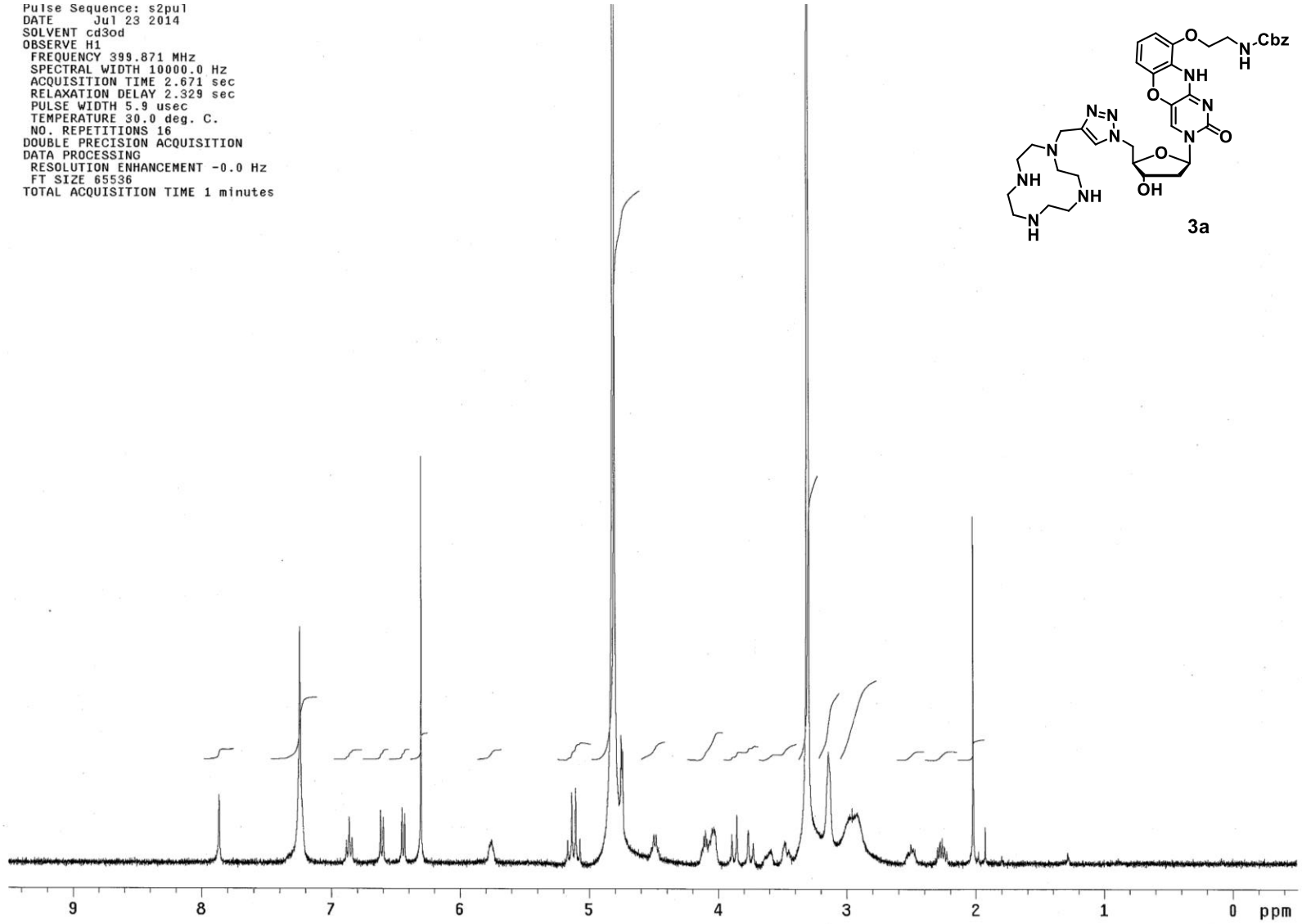


Figure S6. Fluorescence measurement using **5a-Zn** after addition of 8-oxo-dGTP by micro plate reader. The measurements were performed in 10 mM HEPES buffer (pH 7.4) containing HeLa cell lysates with a fluorescence filter for excitation at 355 nm and for emission at 460 nm.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TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 16
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 1 minutes
Cbz
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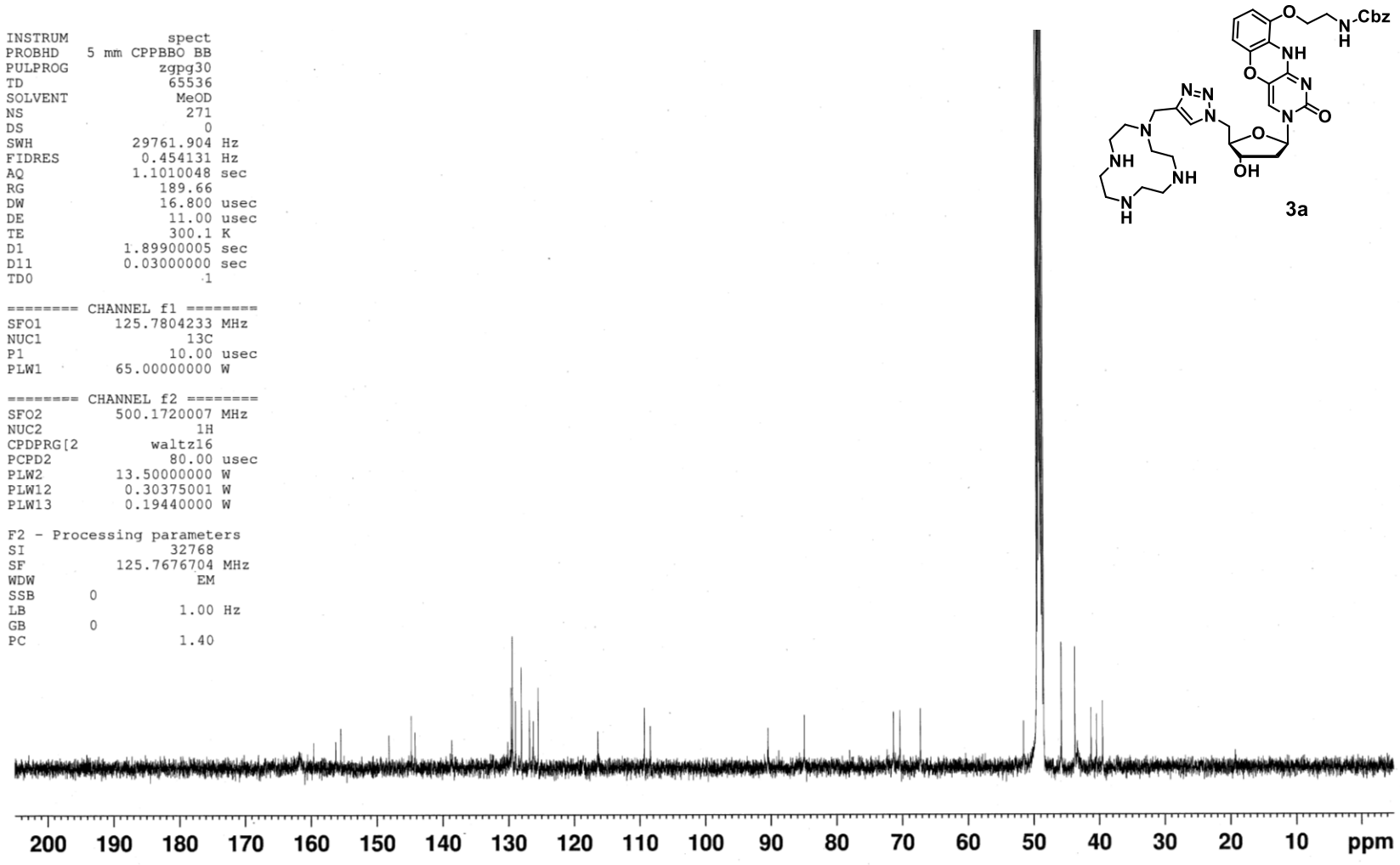
3a
9
8
7
6
5
4
3
2
1
0
ppm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RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
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P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
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NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
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LB 1.00 Hz
GB 0
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Cbz
3a
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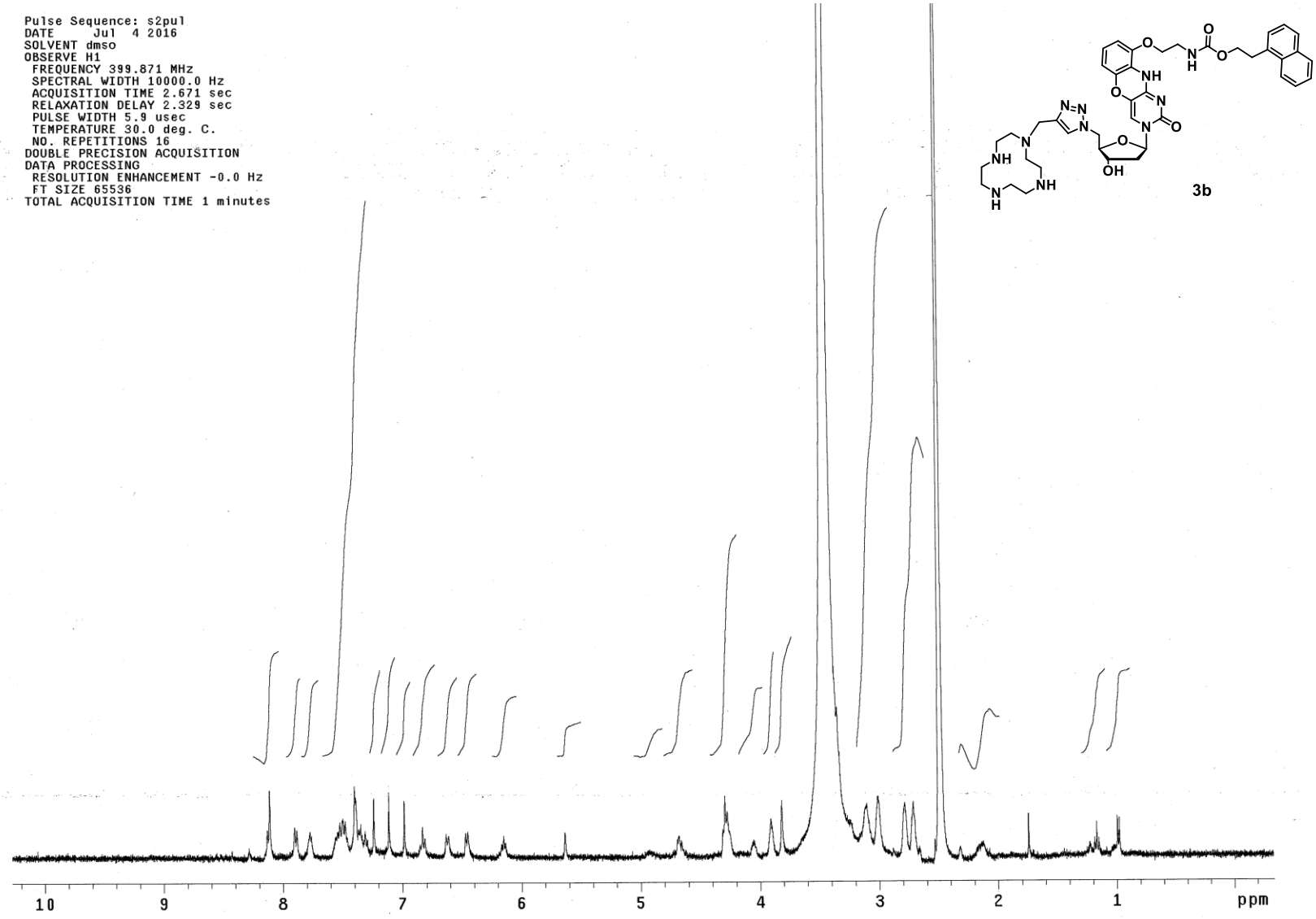
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PULSE WIDTH 5.9 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 16
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 1 minutes
3b
10
9
8
7
6
5
4
3
2
1
ppm

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SOLVENT           MeOD
NS                 675
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FIDRES         0.454131 Hz
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RG              189.66
DW              16.800 usec
DE              11.00 usec
TE              300.1 K
D1           1.89900005 sec
D11          0.03000000 sec
TD0                  1

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PLW1        65.00000000 W

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PCPD2            80.00 usec
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PLW12        0.30375001 W
PLW13        0.19440000 W

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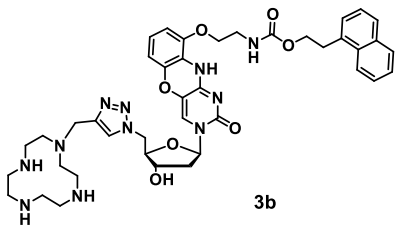

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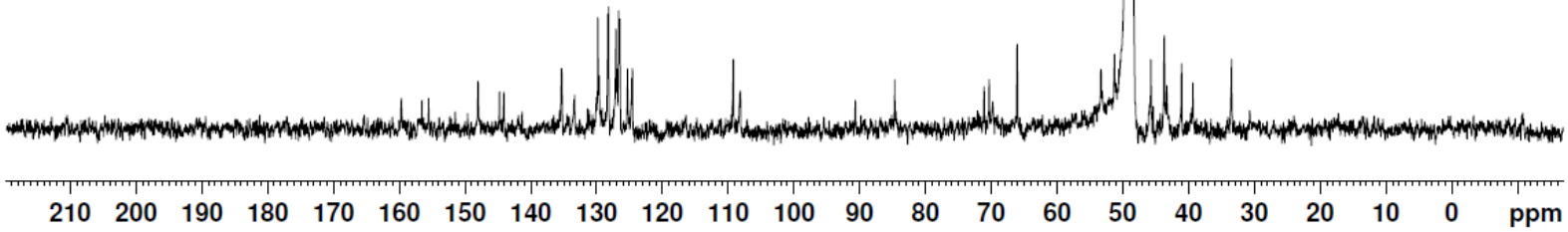

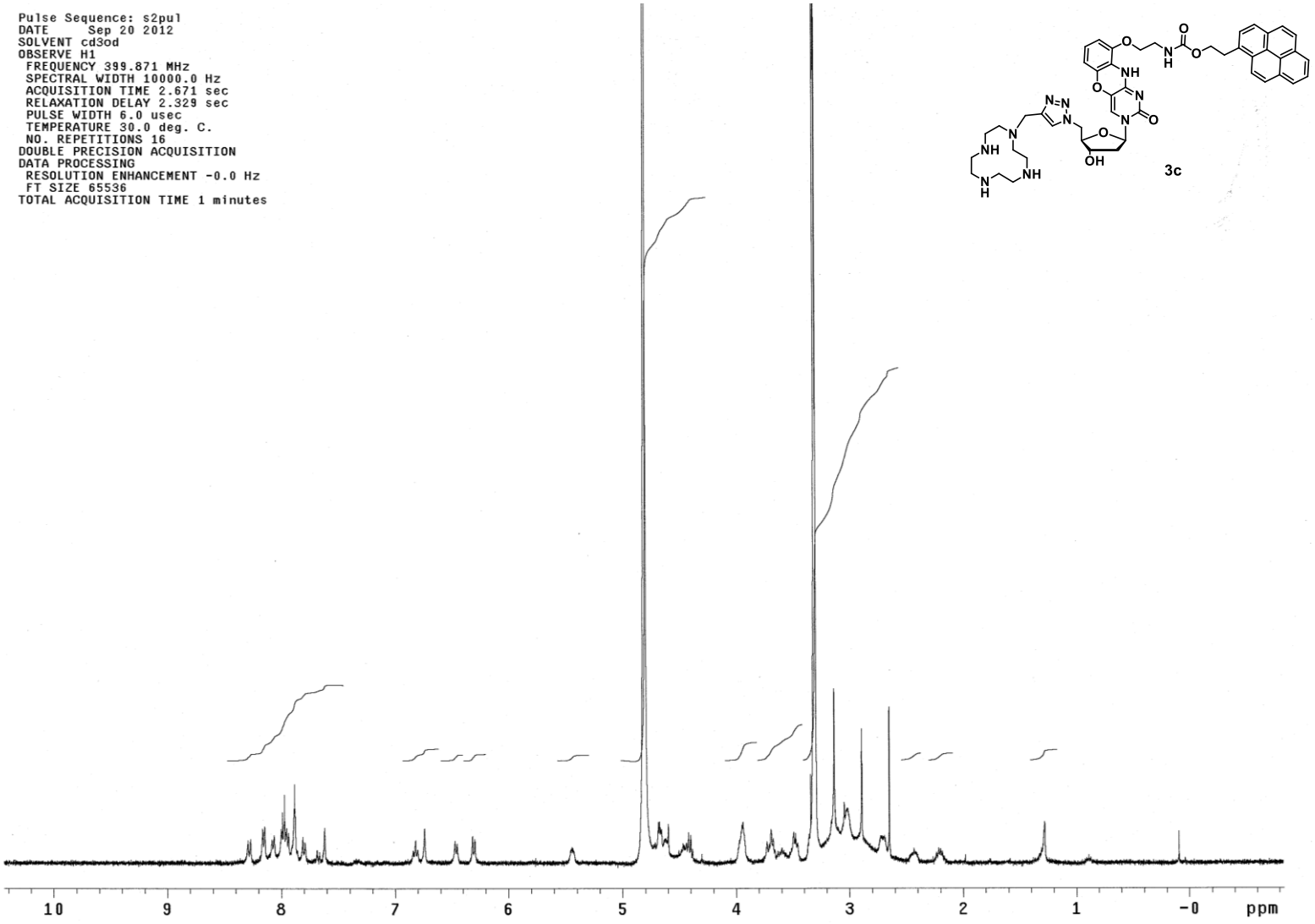
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RELAXATION DELAY 2.329 sec
PULSE WIDTH 6.0 usec
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DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
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1
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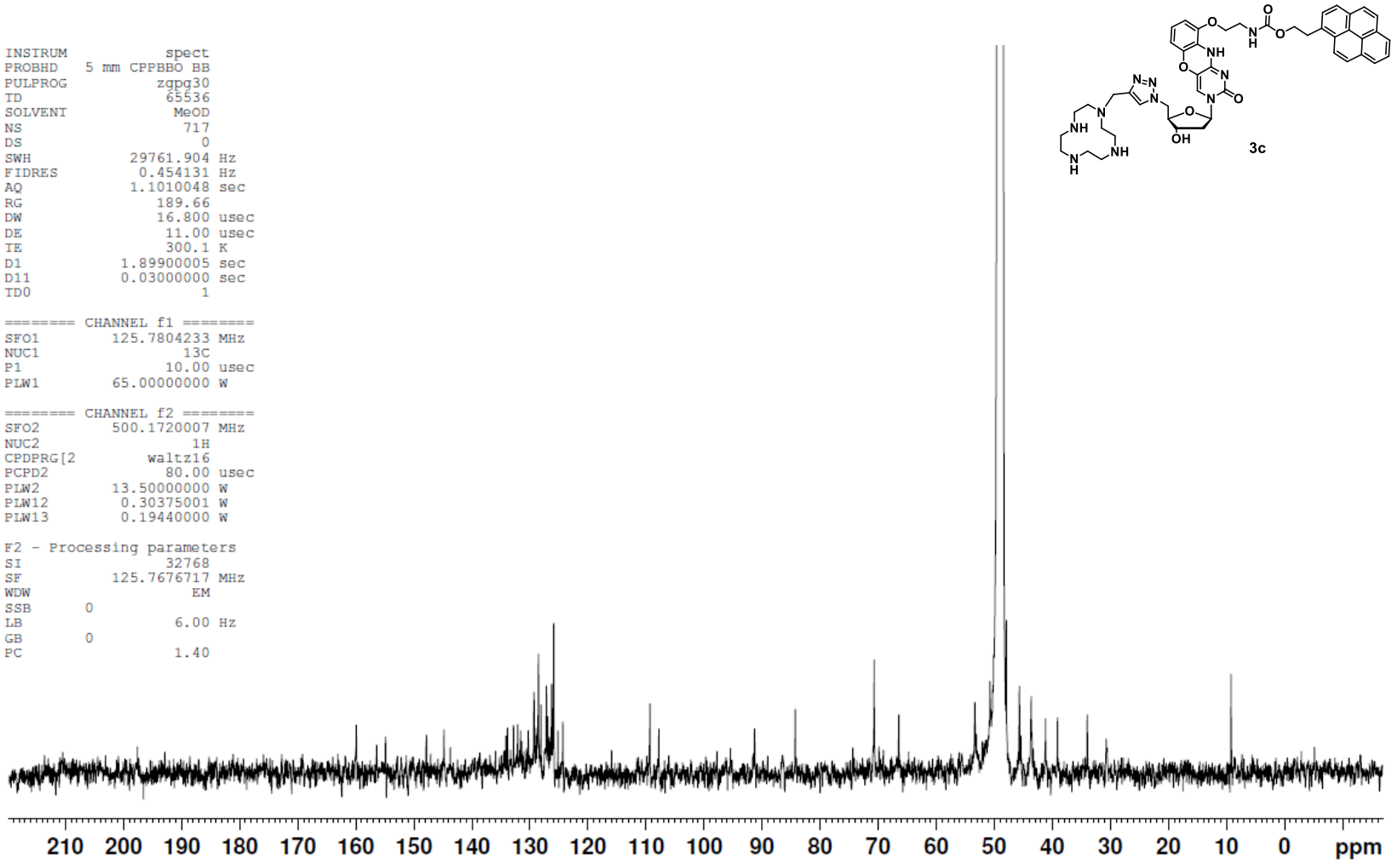
ppm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RG 189.66
DW 16.800 usec
DE 11.00 usec
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D11 0.03000000 sec
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P1 10.00 usec
PLW1 65.00000000 W
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NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
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LB 6.00 Hz
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PC 1.40
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DATE Feb 12 2014
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RELAXATION DELAY 2.329 sec
PULSE WIDTH 5.9 usec
TEMPERATURE 30.0 deg. C.
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DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
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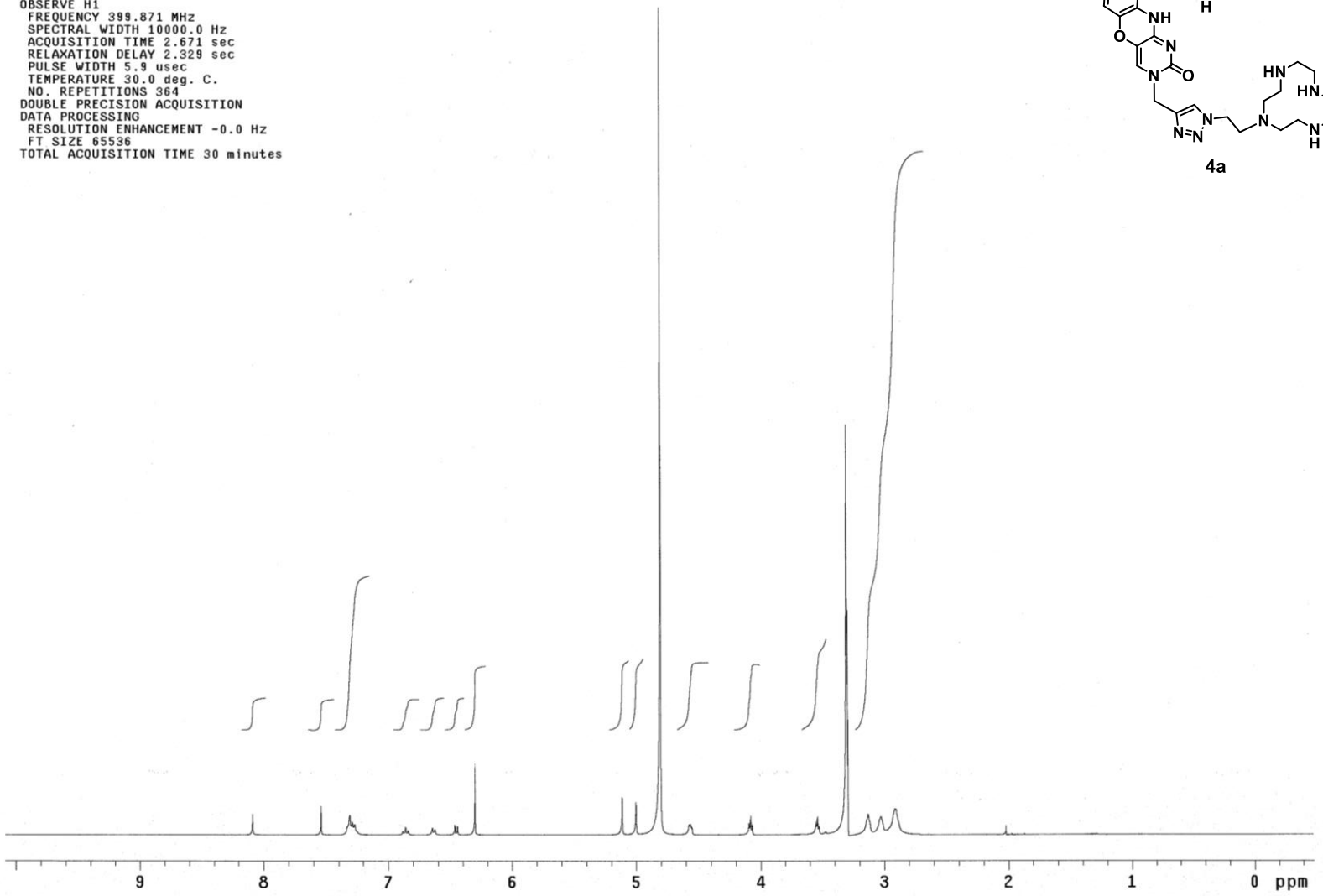

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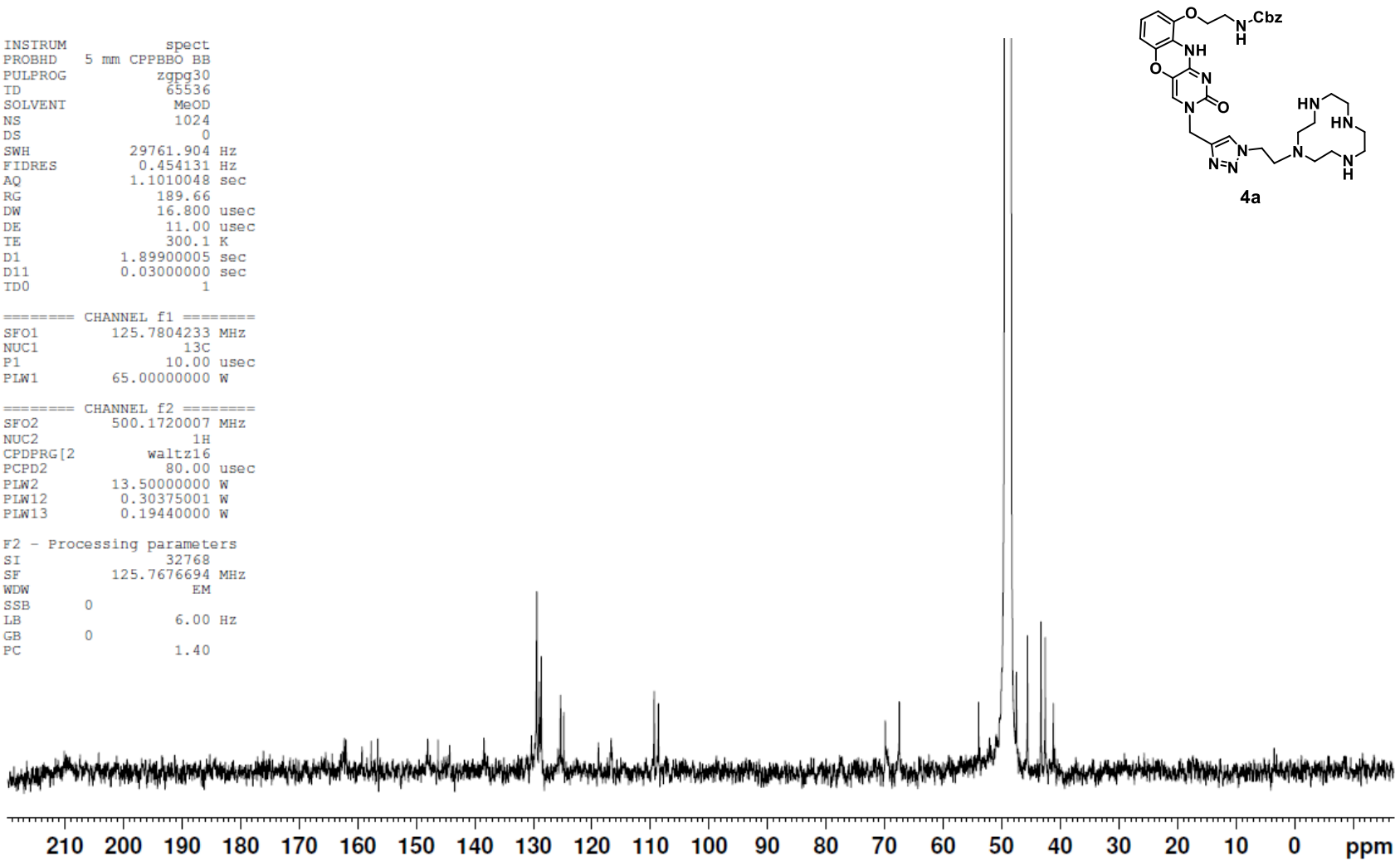
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AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
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NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
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PLW12 0.30375001 W
PLW13 0.19440000 W
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LB 6.00 Hz
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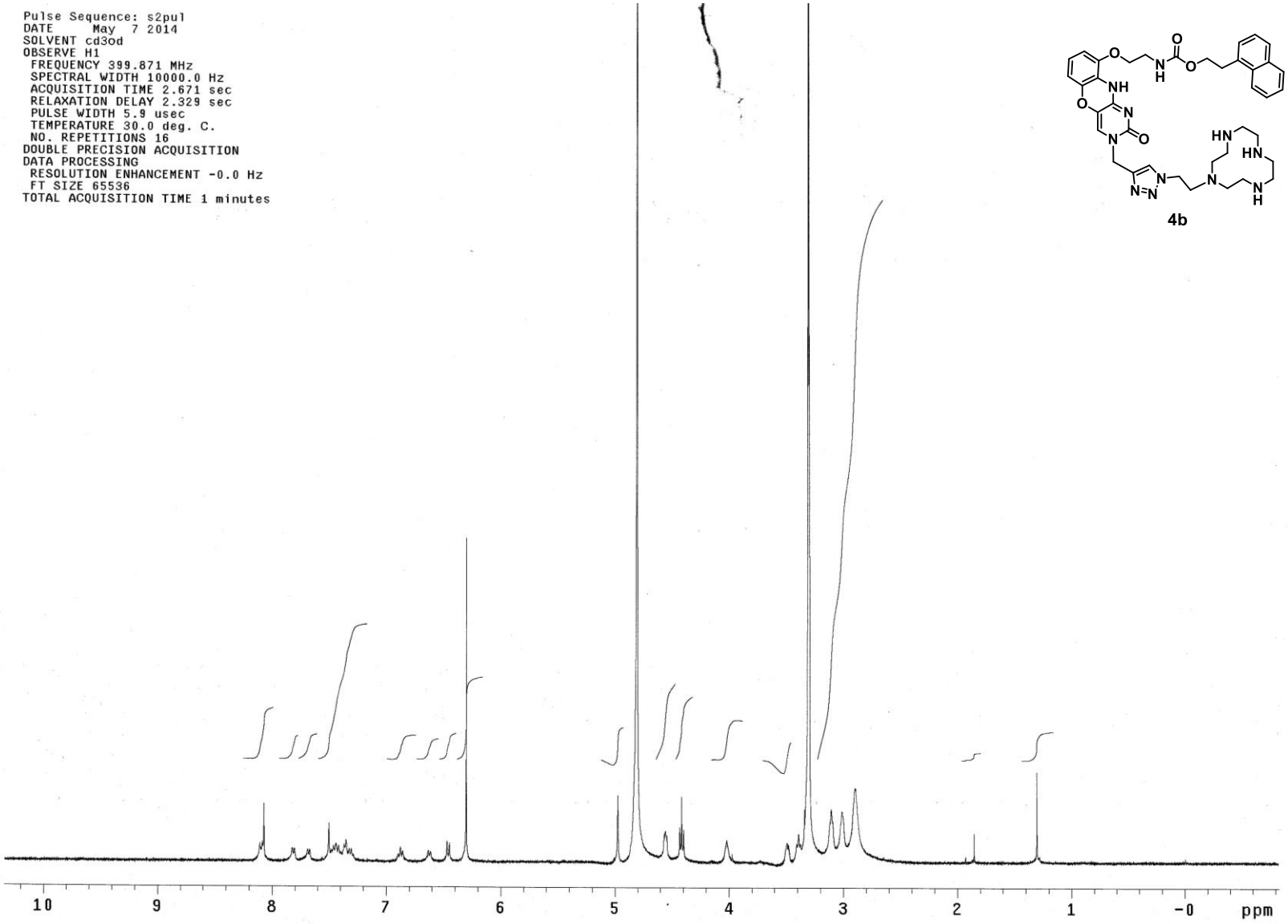
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RELAXATION DELAY 2.329 sec
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DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
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TOTAL ACQUISITION TIME 1 minutes
10
9
8
7
6
5
4
3
2
1
-0
ppm

4b

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SOLVENT            MeOD
NS                   255
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FIDRES          0.454131 Hz
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TE                300.1 K
D1            1.89900005 sec
D11           0.03000000 sec
TD0                    1

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PLW12         0.30375001 W
PLW13         0.19440000 W

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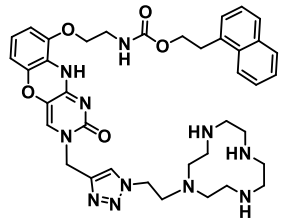

4b

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PULSE WIDTH 5.9 usec
TEMPERATURE 30.0 deg. C.
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DATA PROCESSING
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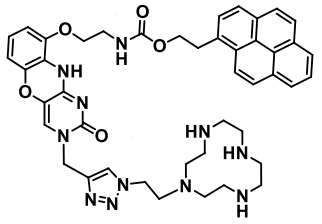

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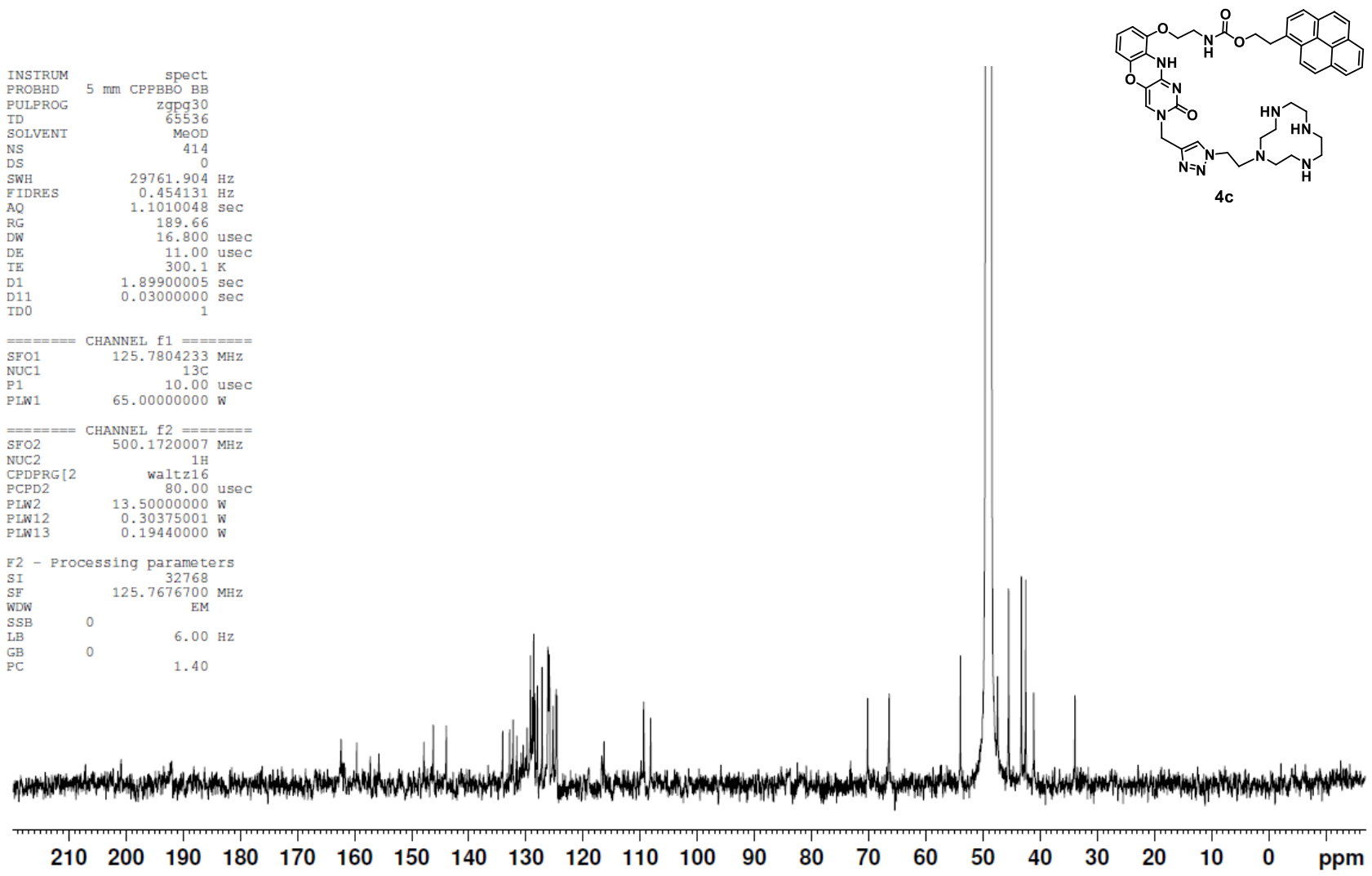
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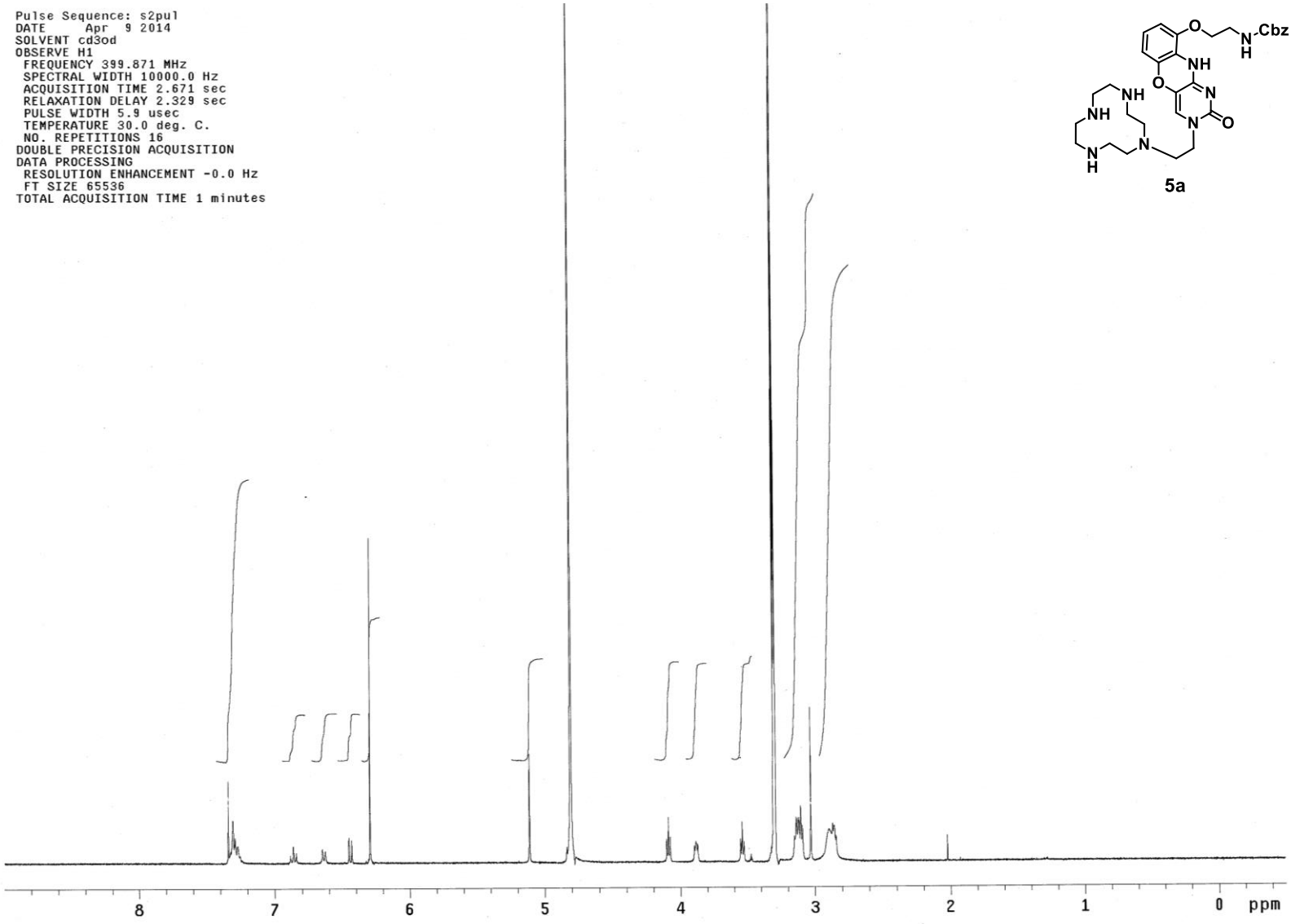
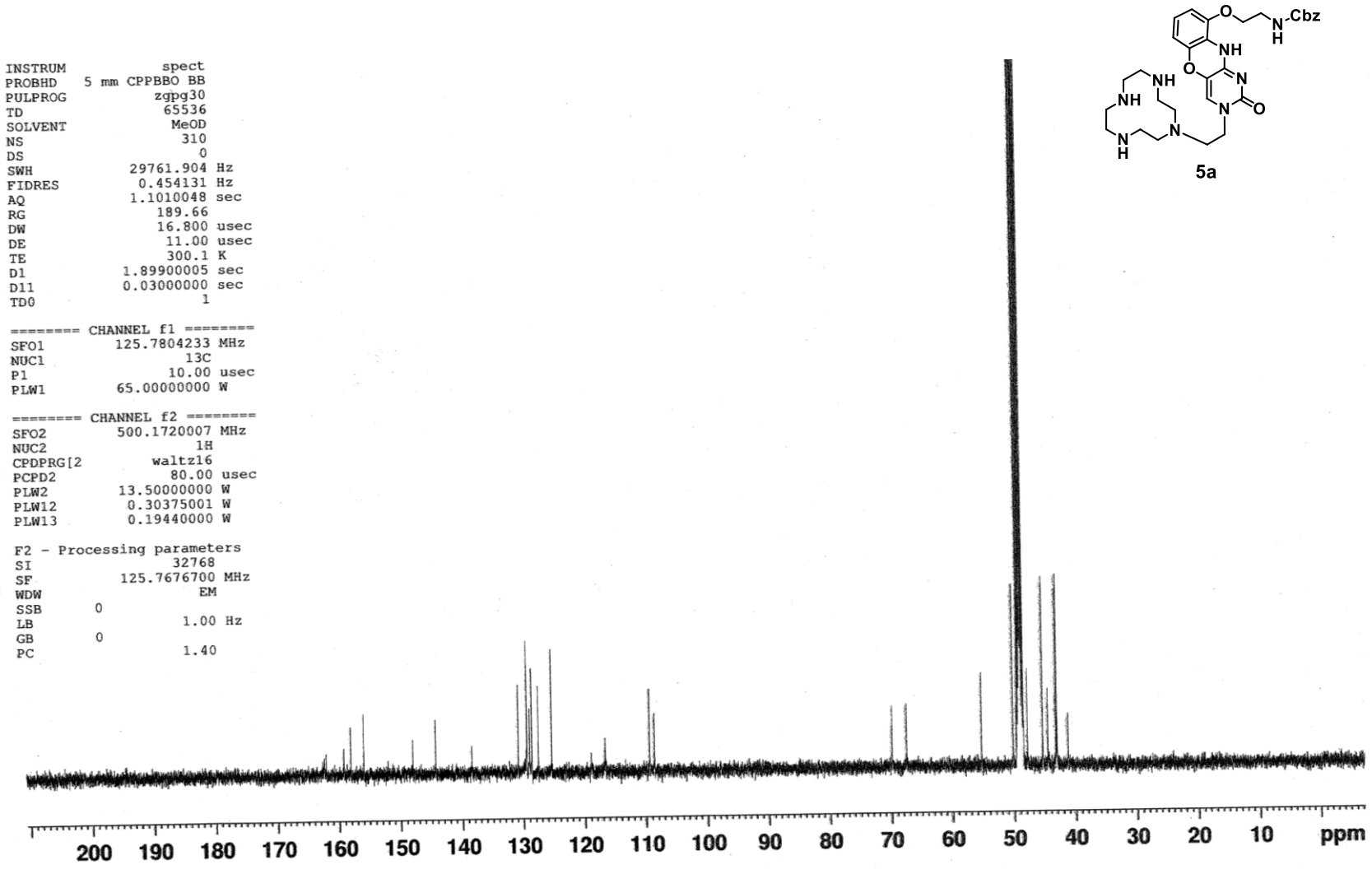
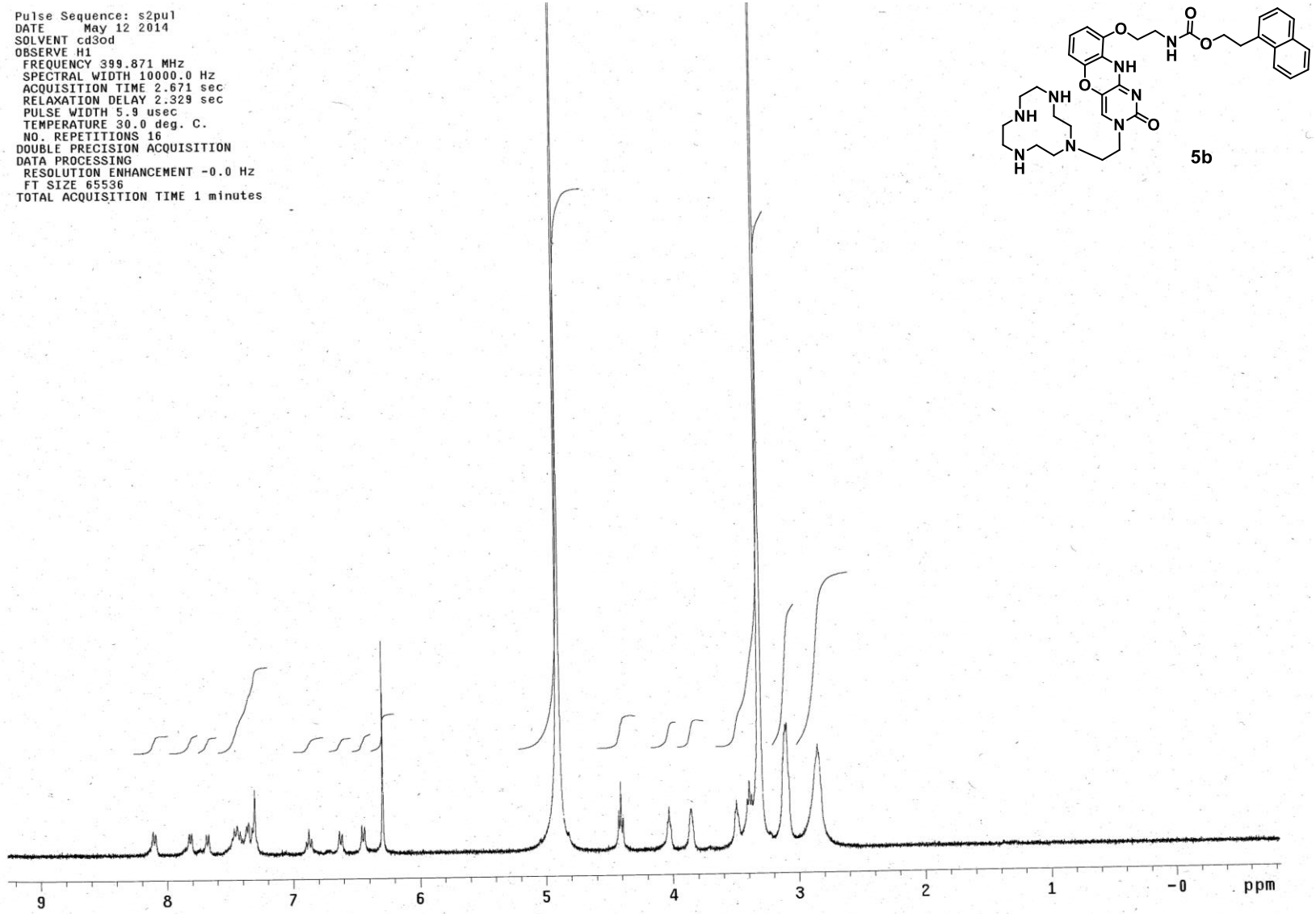
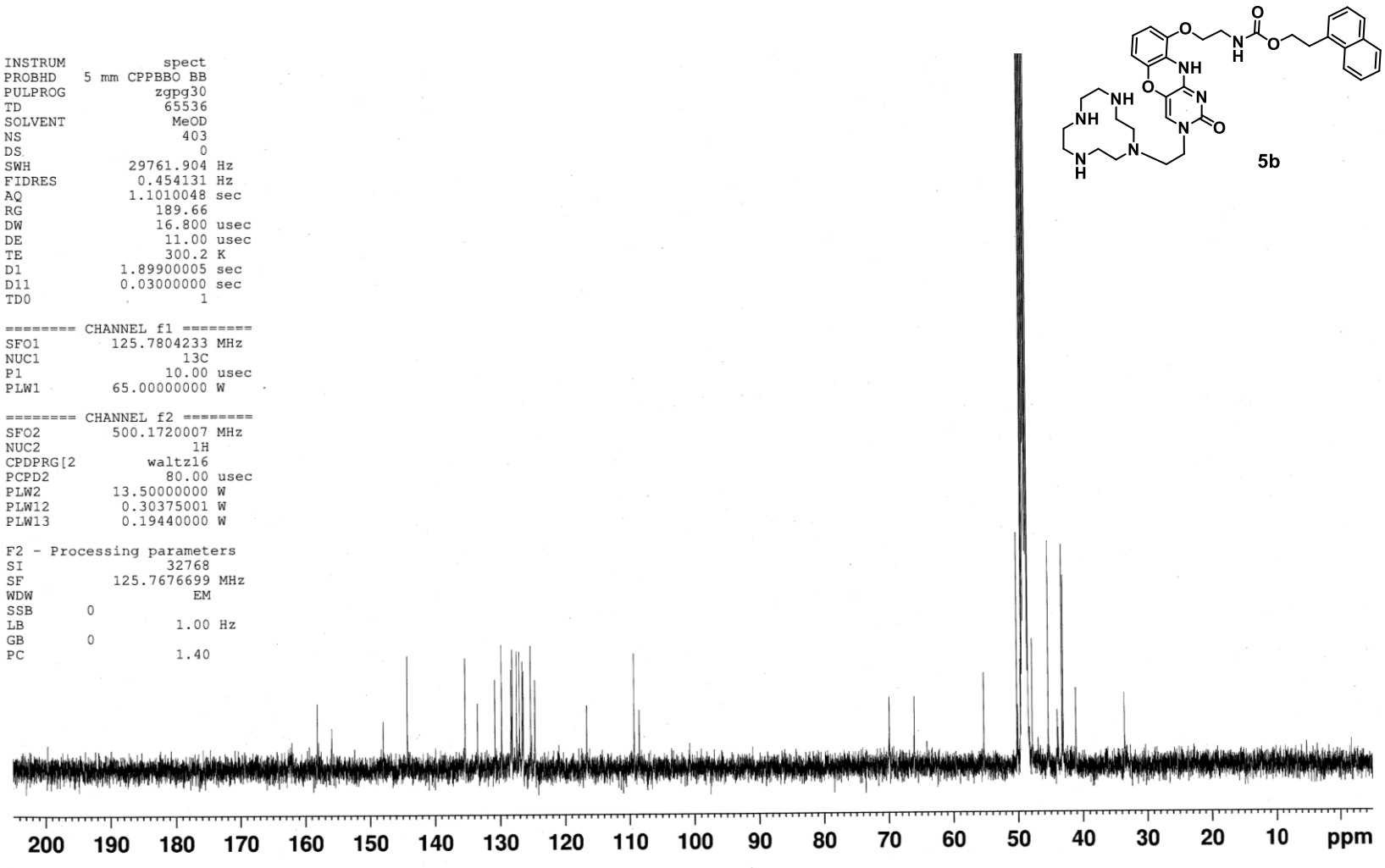
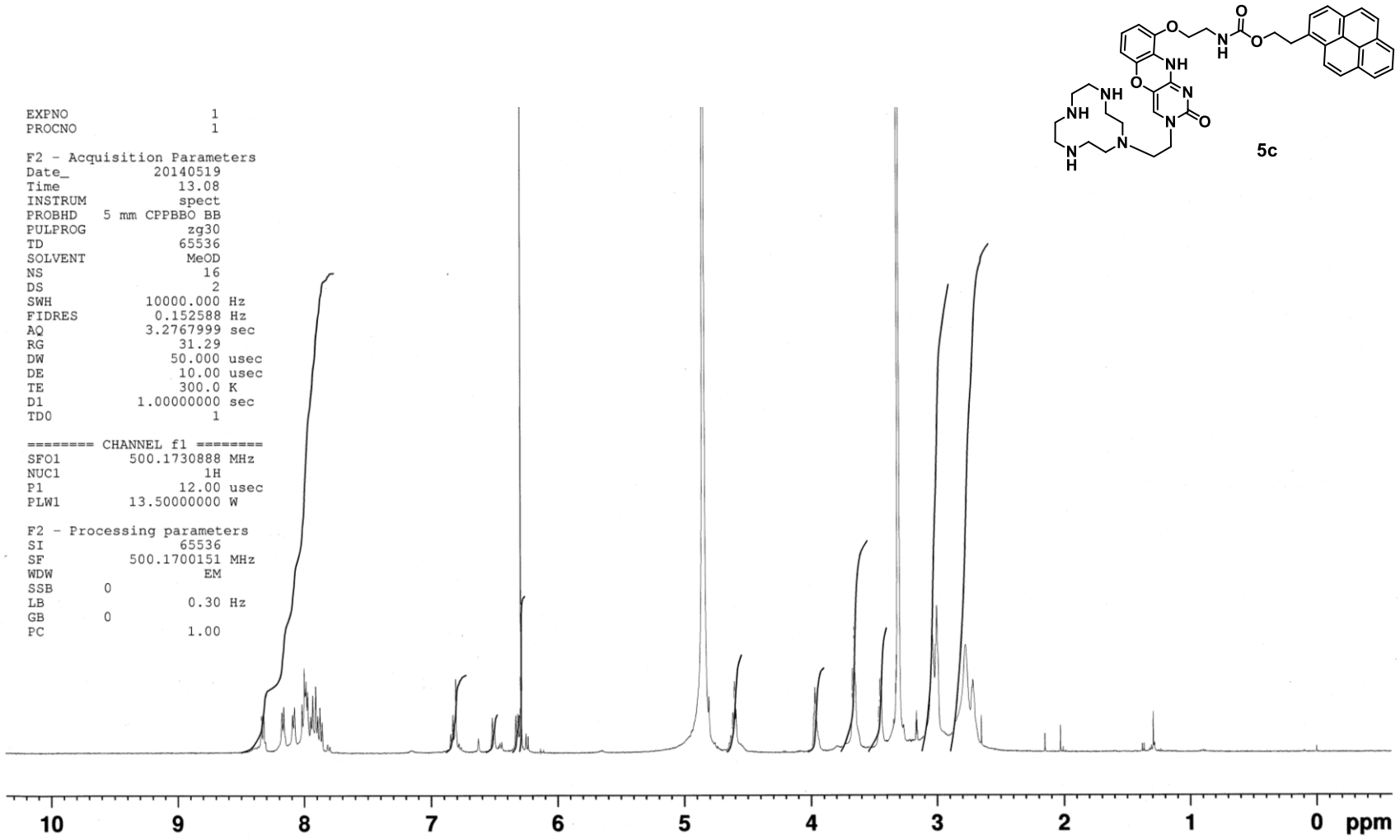
NS 414
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7676700 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 1.40
4c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

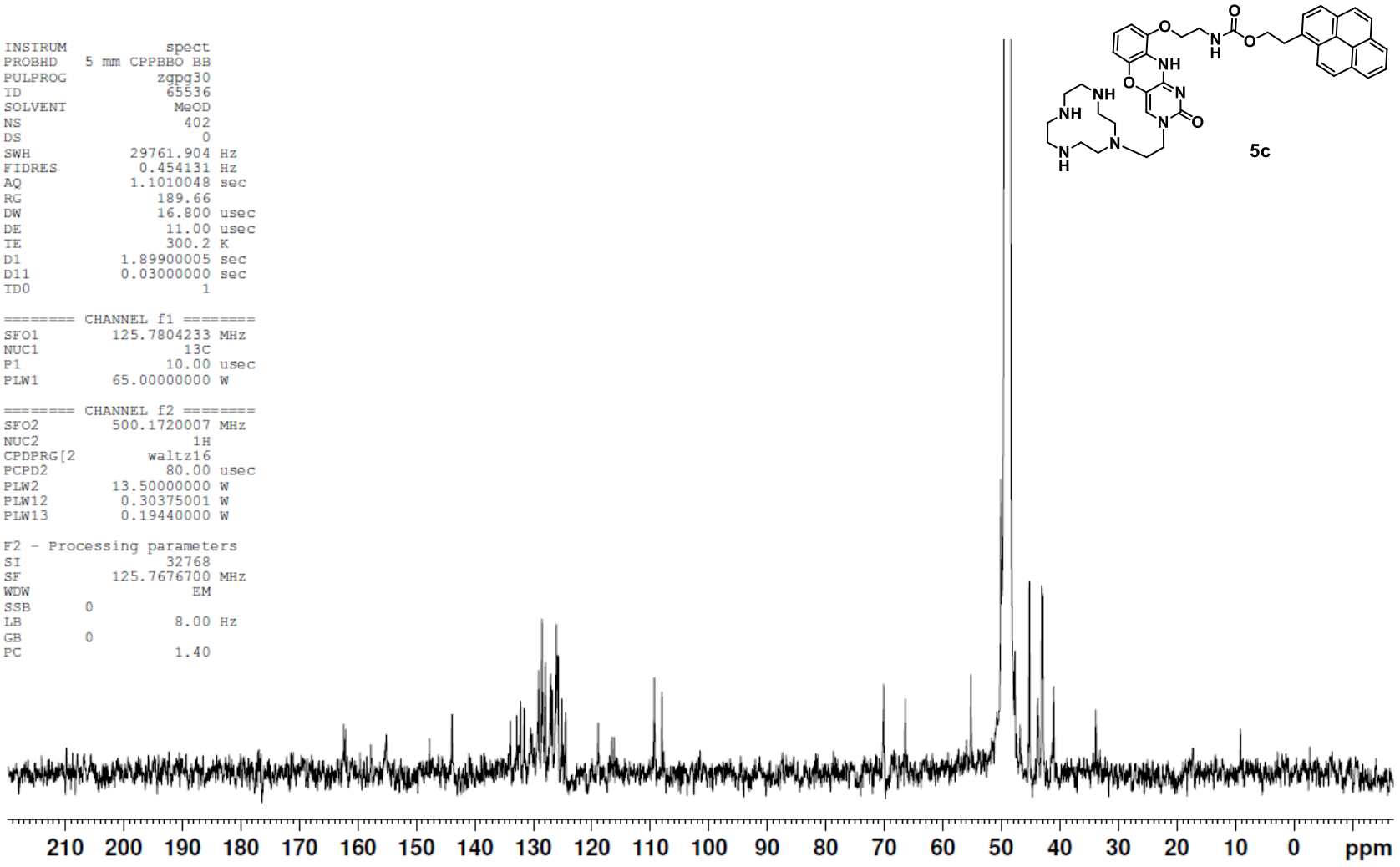

Pulse Sequence: s2pul
DATE Apr 9 2014
SOLVENT cd3od
OBSERVE H1
FREQUENCY 399.871 MHz
SPECTRAL WIDTH 10000.0 Hz
ACQUISITION TIME 2.671 sec
RELAXATION DELAY 2.329 sec
PULSE WIDTH 5.9 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 16
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 1 minutes
O
N-Cbz
H
NH
O
NH
N
NH
N
O
N
N
H
5a
8
7
6
5
4
3
2
1
0
ppm


INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 310
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.1 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7676700 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
N
Cbz
H
NH
O
NH
N
NH
N
O
N
H
5a
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


Pulse Sequence: s2pul
DATE May 12 2014
SOLVENT cd3od
OBSERVE H1
FREQUENCY 399.871 MHz
SPECTRAL WIDTH 10000.0 Hz
ACQUISITION TIME 2.671 sec
RELAXATION DELAY 2.329 sec
PULSE WIDTH 5.9 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 16
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 1 minutes
5b
9
8
7
6
5
4
3
2
1
-0
ppm


INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 403
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7676699 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
5b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140519
Time 13.08
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.29
DW 50.000 usec
DE 10.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1730888 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.50000000 W
F2 - Processing parameters
SI 65536
SF 500.1700151 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
5c


INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 402
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 189.66
DW 16.800 usec
DE 11.00 usec
TE 300.2 K
D1 1.89900005 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7804233 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W
======== CHANNEL f2 ========
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.30375001 W
PLW13 0.19440000 W
F2 - Processing parameters
SI 32768
SF 125.7676700 MHz
WDW EM
SSB 0
LB 8.00 Hz
GB 0
PC 1.40
5c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm