Supplementary Data for
Central zinc metal-controlled regioselective *meso*-bromination of *zincated* β-silylporphyrins—rapid access to *meso*,β-dual-functionalized porphyrins

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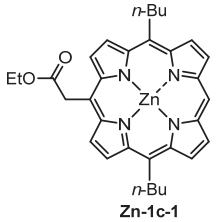
1. General methods

The ^{1}H and ^{13}C NMR spectra were recorded at the room temperature on a JEOL JNM AL-300, a JEOL JNM AL-400, a JEOL JNM ECS-400, a JEOL JNM LA-500, and a JEOL JNM ECZ-500 spectrometer using perdeuterated solvents as internal standards. The chemical shifts of the ^{1}H and ^{13}C{^{1}H} spectra are given in ppm relative to the residual protiated solvent and relative to the solvent $CHCl_3$ (δ = 7.24) ^{1}H NMR and relative to the central resonance of $CDCl_3$ (δ = 77.0) for ^{13}C{^{1}H} NMR. Using benzotrifluoride as an external standard, the ^{19}F NMR spectra were recorded at room temperature on a JEOL JNM ECS-400 spectrometer. The chemical shift values are expressed as δ values (ppm), and coupling constant values (J) are given in hertz (Hz). The following abbreviations were used for signal multiplicities: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; and br, broad. The UV-visible spectra were recorded on a JASCO V-660 dual-beam grating spectrophotometer with a 1-cm quartz cell. The IR spectra were recorded on a JASCO FT/IR-4100 spectrophotometer. The mass spectroscopic data were obtained on JEOL JMS-700, JMS-T100LC spectrometer. The melting point data were not available for the obtained porphyrin derivatives owing to their infusibility below 300 °C. Chromatographic purifications were conducted on silica gel (63–210 μm, spherical, neutral).

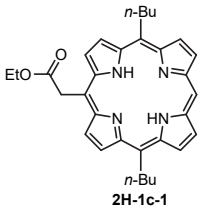
The brominations were conducted in air without establishing anhydrous conditions. Reactions involving moisture sensitive reagents were conducted under an argon atmosphere using standard vacuum line techniques and a glassware that was flame-dried and cooled under argon before use. Dry tetrahydrofuran (THF) and dry dioxane were purchased for the reactions and used without further desiccation. According to the method described in the literature, porphyrin derivatives **2H-1a**, **2H-1b**, **2H-1e**, **Zn-1a**, **2H-2a**, and **2H-2b**[1] were prepared. Other chemicals were purchased from commercial sources and used as received unless stated otherwise.

2. Synthesis of precursors of Zn-1c and 2H-1c



Zn-1c-1

[5,15-Di-*n*-butyl-10-ethoxycarbonylmethylporphyrinato]zinc(II) (Zn-1c-1) Prepared from 10-bromo-5,15-di-*n*-butylporphyrin according to the method described in the literature.[2] Dark purple solid (286 mg, 84%): R_f = 0.52 (silica gel, *n*-hexane/EtOAc = 3:1); ^{1}H-NMR ($CDCl_3$, 300 MHz) δ: 9.86 (1H, s), 9.53 (2H, d, *J* = 4.9 Hz), 9.51 (2H, d, *J* = 4.9 Hz), 9.50 (2H, d, *J* = 4.6 Hz), 9.24 (2H, d, *J* = 4.6 Hz), 5.99 (2H, s), 4.96 (4H, t, *J* = 8.0 Hz), 4.16 (2H, q, *J* = 7.1 Hz), 2.54–2.44 (4H, m), 1.84–1.79 (4H, m), 1.13 (3H, t, *J* = 7.1 Hz), 1.12 (6H, t, *J* = 7.4 Hz); ^{13}C-NMR ($CDCl_3$, THF-d_8, 125 MHz) δ: 173.1, 150.0 (2C), 149.7 (2C), 149.1 (2C), 148.8 (2C), 131.5 (2C), 129.0 (2C), 128.94 (2C), 128.85 (2C), 119.4 (2C), 109.3, 104.4, 60.8, 41.2 (2C), 41.1, 35.2 (2C), 23.6 (2C), 14.14 (2C), 14.07; IR (KBr): 2955, 2856, 1730, 1320, 1174, 1069, 994, 959, 778, cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 414 (5.7), 546 (4.3), 584 (3.6) nm; EI-MS (70 eV) *m/z* (relative intensity): 570 (M^+, 100), 527 (53, M − C_3H_7), 497 (24, M − $CO_2C_2H_5$), 454 (11, M − C_3H_7, $CO_2C_2H_5$), 411 (20, M − $2C_3H_7$, $CO_2C_2H_5$); HRMS (EI) *m/z*: calcd for $C_{32}H_{34}N_4O_2Zn$: 570.1973, found 570.1974; Anal. calcd for $C_{32}H_{34}N_4O_2Zn$: C, 67.19; H, 5.99; N, 9.79, found: C, 67.05; H, 5.91; N, 9.74.



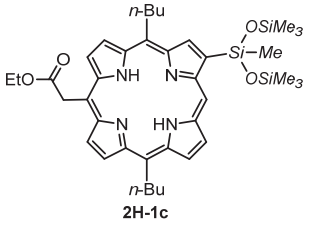
2H-1c-1

5,15-Di-*n*-butyl-10-ethoxycarbonylmethylporphyrin (2H-1c-1)[1] To a solution of **Zn-1c-1** (0.25 mmol) in THF (5 mL) was added a mixed solution of conc. HCl aq. (0.1 mL) and THF (0.9 mL) at room temperature, and the whole was stirred for 20 min at room temperature. The mixture was diluted with THF/Et_2O (2:1, 25 mL), neutralized with aqueous sat. $NaHCO_3$. The combined organic layer was washed successively with water and sat. NaCl, dried over $MgSO_4$, and filtered. The filtrate was concentrated under reduced pressure. The crude product was recrystallized from MeOH/CH_2Cl_2 to give **2H-1c-1** as a dark red-purple solid (121 mg, 97%): R_f = 0.49 (silica gel, *n*-hexane/EtOAc = 3:1); ^{1}H-NMR ($CDCl_3$, 500 MHz) δ: 9.94 (1H, s), 9.58 (2H, d, *J* = 4.9 Hz), 9.51 (2H, d, *J* = 4.9 Hz), 9.46 (2H, d, *J* = 4.6 Hz), 9.26 (2H, d, *J* = 4.6 Hz), 6.01 (2H, s), 4.93 (4H, t, *J* = 8.1 Hz), 4.19 (2H, q, *J* = 7.0 Hz), 2.53–2.46 (4H, m), 1.84–1.79 (4H, m), 1.15 (3H, t, *J* = 7.0 Hz), 1.13 (6H, t, *J* = 7.3 Hz), −2.98 (2H, br s); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ: 172.7, 147.2 (2C, br), 147.0 (2C, br), 145.6 (2C, br), 145.0 (2C, br), 131.7 (2C), 129.1 (2C), 128.4 (2C), 128.3 (2C), 119.2 (2C), 109.2, 104.1, 61.4, 41.5, 40.9 (2C), 34.9 (2C), 23.7 (2C), 14.3 (2C), 14.2; IR (KBr): 3303, 2955, 2859, 1733, 1470, 1243, 1160, 916, 838, 778, 727 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 411 (5.6), 511 (4.2), 544 (3.6), 589 (3.7), 645 (3.5) nm; FAB-MS (dithiothreitol/thioglycerol = 1:1) *m/z* 509 $[M+H]^+$; HRMS-FAB$^+$ ($[M+H]^+$): calcd for $C_{32}H_{37}N_4O_2$: 509.2917, found

509.2918; Anal. calcd for $C_{32}H_{36}N_4O_2$: C, 75.56; H, 7.13; N, 11.01, found: C, 75.45; H, 6.98; N, 10.98.

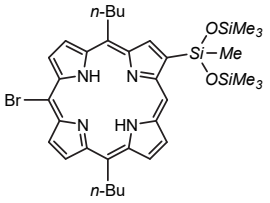
3. General procedure for the preparation of β-silylporphyrins (GP-Si)[1]

An oven-dried 30-mL two-necked flask equipped with a magnetic stirring bar and rubber septum was charged using porphyrin **1** (400 μmol), $[Ir(cod)OMe]_2$ (13.2 mg, 20 μmol, 5 mol%), and 4,4′-di-*tert*-butyl-2,2′-bipyridyl (10.7 mg, 40 μmol, 10 mol%). The reaction vessel was evacuated and flushed using argon (three times), and then dry dioxane (5 mL) and 1,1,1,3,5,5,5-heptamethyltrisiloxane (540 μL, 2 mmol, 5 equiv) were added. The mixture was stirred at 95 °C for 24 h, and the solvent was evaporated to dryness. The crude product was purified using silica gel column chromatography (*n*-hexane/EtOAc = 3:1) and then recrystallized using MeOH/CH_2Cl_2, yielding β-silylporphyrin **1**.



2H-1c

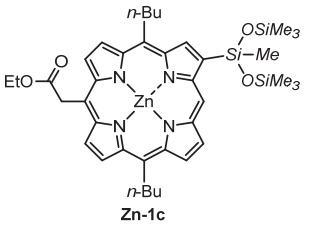
5,15-Di-*n*-butyl-10-ethoxycarbonylmethyl-2-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)porphyrin (2H-1c) The β-silylation of **2H-1c-1** was carried out according to **GP-Si**. Dark red-purple solid (187 mg, 65%): R_f = 0.66 (silica gel, *n*-hexane/EtOAc = 3:1); ^{1}H-NMR ($CDCl_3$, 300 MHz) δ: 10.26 (1H, s), 9.68 (1H, s), 9.60 (1H, d, *J* = 4.9 Hz), 9.59 (1H, d, *J* = 4.9 Hz), 9.54 (1H, d, *J* = 4.9 Hz), 9.53 (1H, d, *J* = 4.9 Hz), 9.49 (1H, d, *J* = 4.8 Hz), 9.27 (1H, d, *J* = 4.8 Hz), 6.02 (2H, s), 5.00–4.94 (4H, m), 4.17 (2H, q, *J* = 7.1 Hz), 2.53–2.48 (4H, m), 1.84–1.79 (4H, m), 1.14 (3H, t, *J* = 7.3 Hz), 1.13 (3H, t, *J* = 7.1 Hz), 1.12 (3H, t, *J* = 7.3 Hz), 0.91 (3H, s), 0.28 (18H, s), −2.86 (2H, br s); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ: 172.9, 148.2 (br), 147.4 (br), 146.2 (br), 145.9 (br), 145.0 (br), 143.2 (br), 141.8 (br), 140.9 (br), 137.2, 132.5, 129.6, 129.0, 128.9, 128.8, 128.7, 128.2, 119.2, 119.0, 109.2, 106.0, 61.5, 41.6, 41.2, 41.0, 35.1, 35.0, 23.94, 23.90, 14.44 (2C), 14.39, 2.8, 2.4 (6C); IR (KBr): 3307, 2956, 1739, 1325, 1254, 1177, 1068, 842, 785, 733 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 414 (5.6), 514 (4.2), 550 (3.6), 592 (3.7), 649 (3.5) nm; FAB-MS (dithiothreitol/thioglycerol = 1:1) *m/z* 729 $[M+H]^+$; HRMS-FAB$^+$ ($[M+H]^+$): calcd for $C_{39}H_{57}N_4O_4Si_3$: 729.3688, found 729.3688; Anal. calcd for $C_{39}H_{56}N_4O_4Si_3$: C, 64.24; H, 7.74; N, 7.68, found: C, 64.25; H, 7.44; N, 7.65.



2H-1d

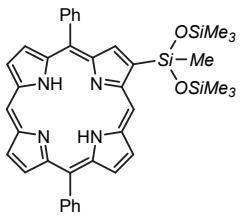
10-Bromo-5,15-di-*n*-butyl-2-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)porphyrin (2H-1d) The β-silylation of 10-bromo-5,15-di-*n*-butylporphyrin[2] was carried out according to **GP-Si**. The crude product was purified by silica gel column chromatography (*n*-hexane/$CHCl_3$ = 2:1). Dark purple solid (164 mg, 91%): R_f = 0.60 ($CHCl_3$/*n*-hexane = 1:2); ^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 10.33 (1H, s), 9.69 (1H, s), 9.68 (1H, d, *J* = 4.9 Hz), 9.65 (1H, d, *J* = 4.9 Hz), 9.40 (1H, d, *J* = 4.9 Hz), 9.38 (1H, d, *J* = 4.9 Hz), 9.30 (1H, d, *J* = 4.9 Hz), 9.28 (1H, d, *J* = 4.9 Hz), 4.90 (2H, t, *J* = 8.0 Hz), 4.74 (2H, t, *J* = 8.0 Hz), 2.54–2.47 (2H, m), 2.46–2.38 (2H, m), 1.85–1.81 (2H, m), 1.78–1.74 (2H, m), 1.17 (3H, t, *J* = 7.3 Hz), 1.11 (3H, t, *J* = 7.3 Hz), 0.98 (3H, s), 0.35 (18H, s), −2.97 (2H, br s); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 148.6 (br), 148.5 (br), 147.8 (br), 146.4 (br), 146.3 (br), 146.0 (br), 145.7 (br), 143.4 (br), 142.1, 137.2, 133.3, 132.7, 132.5, 129.0, 128.7, 128.1, 119.8, 119.6, 106.4, 102.6, 41.0, 40.7, 34.8, 34.6, 23.74, 23.65, 14.3, 14.2, 2.7, 2.3 (6C); IR (KBr): 3306, 2955, 1258, 1062, 979, 842, 780, 754, 733 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 416 (5.8), 517 (4.4), 550

(3.9), 595 (3.8), 651 (3.7) nm; FAB-MS (dithiothreitol/thioglycerol = 1:1) *m/z* 723 [M+2+H], 721 $[M+H]^+$; HRMS-FAB$^+$ ($[M+H]^+$): calcd for $C_{35}H_{50}BrN_4O_2Si_3$: 721.2425, found 721.2432; Anal. calcd for $C_{35}H_{49}BrN_4O_2Si_3$: C, 58.23; H, 6.84; N, 7.76, found: C, 58.40; H, 6.74; N, 7.75.



Zn-1c

[5,15-Di-*n*-butyl-10-ethoxycarbonylmethyl-2-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)porphyrinato]zinc(II) (Zn-1c) The β-silylation of **Zn-1c-1** was conducted according to **GP-Si**. Dark purple solid (271 mg, 98%): R_f = 0.63 (silica gel, *n*-hexane/EtOAc = 3:1); ^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 10.27 (1H, s), 9.75 (1H, s), 9.32 (1H, d, *J* = 4.6 Hz), 9.26 (1H, d, *J* = 4.6 Hz), 8.94 (1H, d, *J* = 4.8 Hz), 8.79 (1H, d, *J* = 4.8 Hz), 8.71 (1H, d, *J* = 4.9 Hz), 8.65 (1H, d, *J* = 4.9 Hz), 5.13 (2H, s), 4.69 (2H, t, *J* = 8.1 Hz), 4.38 (2H, t, *J* = 8.1 Hz), 3.98 (2H, q, *J* = 7.1 Hz), 2.47–2.39 (2H, m), 2.30–2.22 (2H, m), 1.86–1.83 (2H, m), 1.75–1.71 (2H, m), 1.18 (3H, t, *J* = 7.5 Hz), 1.09 (3H, t, *J* = 7.5 Hz), 1.06 (3H, s), 1.05 (3H, t, *J* = 7.1 Hz), 0.40 (18H, s); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ: 172.7, 152.2, 149.6, 149.2, 148.9, 148.8, 148.6, 148.1, 148.0, 141.8, 138.4, 131.8, 128.8, 128.3, 128.2, 128.11, 128.06, 119.1 (2C), 108.6, 106.6, 60.9, 41.1, 40.8, 40.1, 35.1, 34.7, 23.8, 23.7, 14.22, 14.18, 14.06, 2.9, 2.3 (6C); IR (KBr): 2955, 2859, 1733, 1254, 1150, 1059, 845, 774, 754, 733 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 417 (6.0), 549 (4.7), 591 (4.1) nm; FAB-MS (*m*-nitrobenzylalcohol) *m/z* 790 $[M]^+$; HRMS-FAB$^+$ (M^+): calcd for $C_{39}H_{54}N_4O_4Si_3Zn$: 790.2744, found 790.2750; Anal. calcd for $C_{39}H_{54}N_4O_4Si_3Zn$: C, 59.11; H, 6.87; N, 7.07, found: C, 59.25; H, 6.63; N, 7.06.

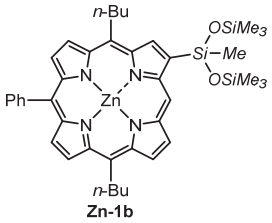


2H-1g

2-(1,1,1,3,5,5,5-Heptamethyltrisiloxan-3-yl)-5,15-diphenylporphyrin (2H-1g) The β-silylation of 5,15-diphenylporphyrin[3] was conducted according to **GP-Si** using 1,1,1,3,5,5,5-heptamethyltrisiloxane (108.1 μL, 0.40 mmol, 1 equiv) at 95 °C for 5 h. The crude product was purified by silica gel column chromatography (*n*-hexane/CH_2Cl_2 = 2:1). Dark red-purple solid (142 mg, 24%): R_f = 0.23 (1/2 CH_2Cl_2/hexane); ^{1}H-NMR ($CDCl_3$, 300 MHz) δ: 10.61 (1H, s), 10.28 (1H, s), 9.38 (2H, d, *J* = 4.6 Hz), 9.36 (1H, d, *J* = 4.6 Hz), 9.24 (1H, s), 9.08 (1H, d, *J* = 4.6 Hz), 9.07 (2H, d, *J* = 4.6 Hz), 8.29–8.26 (4H, m), 7.82–7.79 (6H, m), 0.86 (3H, s), 0.24 (18H, s), −3.07 (2H, br s); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 148.3, 148.1, 147.9, 146.32, 146.26, 146.23, 145.8, 144.4, 141.9, 141.6 (2C), 134.0, 135.0 (2C), 134.9 (2C), 132.3, 132.0, 131.5, 131.4, 131.2, 130.7, 127.79, 127.76, 127.1 (2C), 127.0 (2C), 119.0, 118.9, 107.0, 105.2, 2.6, 2.2 (6C); IR (KBr): 3282, 2957, 1260, 1065, 958, 839, 787, 743, 721 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 409 (5.6), 505 (4.3), 541 (3.7), 578 (3.8) nm; FAB-MS (dithiothreitol/thioglycerol = 1:1) *m/z* 683 $[M+H]^+$; HRMS-FAB$^+$ ($[M+H]^+$): calcd for $C_{39}H_{43}N_4O_2Si_3$: 683.2694, found 683.2689.

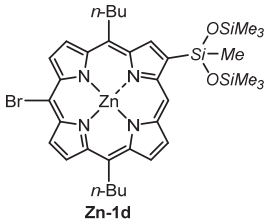
4. General procedure for the preparation of zincated porphyrins (GP-Zn)[4]

A solution of free-base porphyrin **2H-1** (0.1 mmol) and $Zn(OAc)_2 \cdot 2H_2O$ in $CHCl_3$/MeOH (30 mL/10 mL) was stirred for 10 min at room temperature. The mixture was diluted with Et_2O (50 mL) and washed successively using water and brine. The organic layer was dried over $MgSO_4$ and filtered, and the filtrate was concentrated under reduced pressure. The residue was washed successively using *n*-hexane and MeOH, yielding zincated porphyrin **Zn-1**.



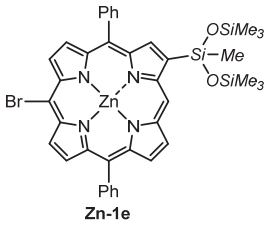
Zn-1b

[5,15-Di-*n*-butyl-2-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)-10-phenylporphyrinato]zinc(II) (Zn-1b) The zincation of **2H-1b** was carried out according to **GP-Zn**. Purple crystal (203 mg, 99%): R_f = 0.54 (silica gel, *n*-hexane/toluene = 1:1); ^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 10.36 (1H, s), 9.89 (1H, s), 9.54 (1H, d, *J* = 4.8 Hz), 9.53 (1H, d, *J* = 4.8 Hz), 9.43 (1H, d, *J* = 4.8 Hz), 9.35 (1H, d, *J* = 4.8 Hz), 8.95 (1H, d, *J* = 4.6 Hz), 8.91 (1H, d, *J* = 4.6 Hz), 8.19–8.17 (2H, m), 7.79–7.73 (3H, m), 5.07 (2H, t, *J* = 8.1 Hz), 4.85 (2H, t, *J* = 8.1 Hz), 2.65–2.57 (2H, m), 2.54–2.46 (2H, m), 1.95–1.87 (2H, m), 1.85–1.78 (2H, m), 1.19 (3H, t, *J* = 7.2 Hz), 1.13 (3H, t, *J* = 7.2 Hz), 0.99 (3H, s), 0.34 (18H, s); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 152.6, 150.28, 150.26, 150.23, 149.9, 149.00, 148.98, 148.95, 143.28, 142.31, 138.7, 134.5 (2C), 132.2, 132.14 (2C), 132.12, 129.2, 128.6, 127.4, 126.5 (2C), 120.10, 120.07, 120.03, 106.7, 41.3, 41.1, 35.5, 35.2, 24.0, 23.9, 14.4, 14.3, 2.9, 2.3 (6C); IR (KBr): 2956, 2850, 1441, 1258, 1062, 1005, 936, 843, 782, 756, 717, 701 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 416 (5.7), 547 (4.3), 580 (3.5) nm; FAB-MS (*m*-nitrobenzylalcohol) *m/z* 780 [M^+]; HRMS-FAB$^+$ (M^+): calcd for $C_{41}H_{52}N_4O_2Si_3Zn$: 780.2690, found 780.2692.



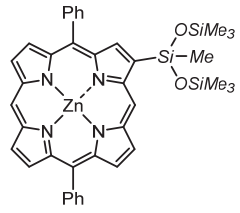
Zn-1d

[10-Bromo-5,15-di-*n*-butyl-2-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)porphyrinato]zinc(II) (Zn-1d) The zincation of **2H-1d** was carried out according to **GP-Zn**. Dark purple crystal (106 mg, 98%): R_f = 0.60 (silica gel, *n*-hexane/toluene = 1:1); ^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 10.19 (1H, s), 9.67 (1H, s), 9.10 (1H, d, *J* = 4.4 Hz), 9.03 (1H, d, *J* = 4.9 Hz), 8.96 (1H, d, *J* = 4.4 Hz), 8.83 (1H, d, *J* = 4.9 Hz), 8.79 (1H, d, *J* = 4.9 Hz), 8.34 (1H, d, *J* = 4.4 Hz), 4.56 (2H, t, *J* = 8.0 Hz), 3.85 (2H, t, *J* = 8.0 Hz), 2.44–2.36 (2H, m), 2.08–2.00 (2H, m), 1.85–1.81 (2H, m), 1.62–1.58 (2H, m), 1.17 (3H, t, *J* = 7.3 Hz), 1.08 (3H, s), 1.01 (3H, t, *J* = 7.3 Hz), 0.40 (18H, s); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 152.6, 149.52, 149.51, 149.08, 149.06, 148.9, 147.3, 147.2, 142.3, 138.7, 132.2, 132.0, 131.8, 128.8, 128.6, 128.1, 119.9, 119.5, 107.2, 103.1, 41.3, 40.7, 35.0, 34.2, 23.9, 23.7, 14.3, 14.2, 3.1, 2.4 (6C); IR (KBr): 2957, 2858, 1257, 1063, 1006, 839, 777, 755, 733 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 419 (5.9), 551 (4.4), 593 (3.7) nm; FAB-MS (*m*-nitrobenzylalcohol) *m/z* 784 [M+2], 782 [M]$^+$; HRMS-FAB$^+$ (M^+): calcd for $C_{35}H_{47}BrN_4O_2Si_3Zn$: 782.1482, found 782.1481.



Zn-1e

[10-Bromo-2-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)-5,15-diphenylporphyrinato]zinc(II) (Zn-1e) The zincation of **2H-1e** was carried out according to **GP-Zn**. Dark red-purple crystal (53.0 mg, 98%): R_f = 0.34 (silica gel, *n*-hexane/toluene = 1:1); ^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 10.51 (1H, s), 9.75 (1H, d, *J* = 4.4 Hz), 9.74 (1H, d, *J* = 4.4 Hz), 9.35 (1H, d, *J* = 4.4 Hz), 9.20 (1H, s), 9.04 (1H, d, *J* = 4.4 Hz), 9.03 (1H, d, *J* = 4.4 Hz), 8.99 (1H, d, *J* = 4.4 Hz), 8.21–8.19 (4H, m), 7.82–7.75 (6H, m), 0.82 (3H, s), 0.23 (18H, s); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 154.0, 150.8, 150.7, 150.6, 150.3, 150.1, 149.44, 149.35, 143.0, 142.43, 142.39, 142.37, 134.7 (2C), 134.6 (2C), 133.17, 133.15, 132.96, 132.95, 132.93, 132.4, 127.72, 127.70, 126.8 (2C), 126.7 (2C), 121.2, 121.0, 108.4, 104.8, 2.7, 2.2 (6C); IR (KBr): 2956, 1259, 1060, 1003, 843, 789, 753, 733, 701 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 418 (5.9), 547 (4.5), 585 (3.5) nm; FAB-MS (*m*-nitrobenzylalcohol) *m/z* 824 [M+2], 822 $[M]^+$; HRMS-FAB$^+$ (M^+): calcd for $C_{39}H_{39}BrN_4O_2Si_3Zn$: 822.0856, found 822.0863.

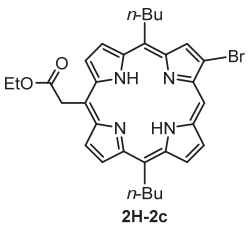


Zn-1g

[2-(1,1,1,3,5,5,5-Heptamethyltrisiloxan-3-yl)-5,15-diphenylporphyrinato]zinc(II) (Zn-1g) The zincation of **2H-1g** was carried out according to **GP-Zn**. Dark red-purple crystal (108 mg, 99%): R_f = 0.43 (silica gel, *n*-hexane/toluene = 1:1); ^{1}H-NMR ($CDCl_3$, 300 MHz) δ: 10.64 (1H, s), 10.15 (1H, s), 9.45 (1H, d, *J* = 4.6 Hz), 9.33 (1H, d, *J* = 4.6 Hz), 9.32 (1H, d, *J* = 4.6 Hz), 9.32 (1H, s), 9.15 (1H, d, *J* = 4.6 Hz), 9.11 (1H, d, *J* = 4.6 Hz), 9.07 (1H, d, *J* = 4.6 Hz), 8.28–8.23 (4H, m), 7.82–7.78 (6H, m), 0.87 (3H, s), 0.26 (18H, s); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 153.1, 150.3, 150.2, 150.1, 149.8, 149.51, 149.49, 149.44, 142.71, 142.67, 142.4, 141.9, 134.8 (2C), 134.7 (2C), 132.51, 132.50, 132.47, 132.0, 131.74, 131.71, 127.56, 127.54, 126.8 (2C), 126.7 (2C), 120.0, 119.9, 108.1, 106.0, 2.8, 2.2 (6C); IR (KBr): 2955, 1252, 1034, 995, 845, 786, 751, 700 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 410 (6.1), 538 (4.7), 575 (3.8) nm; EI-MS (70 eV) *m/z* (relative intensity): 744 (100, M^+), 729 (6, M − CH_3); HRMS (EI) *m/z*: calcd for $C_{39}H_{40}N_4O_2Si_3Zn$: 744.1751, found 744.1752.

5. General procedure for the bromination of free-base porphyrins 2H-1 with NBS (GP-NBS-2H-1)[1] (Table 1)

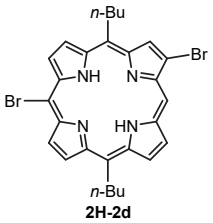
A solution of NBS (19.6 mg, 110 μmol, 1.1 equiv) in $CHCl_3$ (10 mL) was added to a solution of free-base β-silylpophyrin **2H-1** (100 μmol) in $CHCl_3$ (10 mL) over 10 min at 0 °C. The reaction mixture was allowed to warm to room temperature while being stirred for 30 min, solvent was evaporated to dryness, and crude product was purified by silica gel column chromatography (*n*-hexane/toluene = 4:1) and then recrystallized from *n*-hexane/CH_2Cl_2, yielding β-bromoporphyrin **2H-2**.



2H-2c

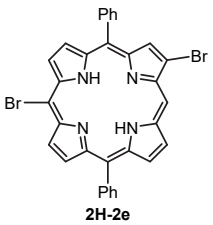
2-Bromo-5,15-di-*n*-butyl-10-ethoxycarbonylmethylporphyrin (2H-2c) The bromination of **2H-1c** was carried out according to **GP-NBS-2H-1**. Purple crystal (33.0 mg, 41%): R_f = 0.58 (silica gel, *n*-hexane/EtOAc = 3:1); ^{1}H-NMR ($CDCl_3$, 500 MHz) δ: 10.04 (1H, s), 9.52 (1H, d, *J* = 4.9 Hz), 9.47 (1H, d, *J* = 4.5 Hz), 9.42 (1H, d, *J* = 4.9 Hz), 9.41 (1H, d, *J* = 4.6 Hz), 9.39 (1H, d, *J* = 4.5 Hz), 9.34 (1H, s), 9.29 (1H, d, *J* = 4.6 Hz), 5.92 (2H, s), 4.83 (2H, t, *J* = 8.1 Hz), 4.72 (2H, t, *J* = 8.1 Hz), 4.18 (2H, q, *J* = 7.0 Hz), 2.48–2.38 (4H, m), 1.82–1.73 (4H, m), 1.15

(3H, t, J = 7.0 Hz), 1.12 (6H, t, J = 7.5 Hz), 1.11 (3H, t, J = 7.5 Hz), −3.18 (1H, br s), −3.25 (1H, br s); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ: 172.5, 154.2 (br), 152.9 (br), 151.8 (br), 147.6 (br), 140.1 (br), 139.3 (br), 138.7 (br), 138.1 (br), 132.0, 131.4, 131.0, 129.0, 126.3, 125.7, 125.6, 123.8, 119.4, 119.0, 109.5, 101.4, 61.3, 41.3, 40.8, 40.6, 34.70, 34.65, 23.6 (2C), 14.2 (2C); IR (KBr): 3130, 2956, 2854, 1737, 1314, 1259, 1153, 1085, 1014, 839, 775, 755, 733 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 424 (5.3), 562 (3.9), 605 (3.7) nm; FAB-MS (dithiothreitol/thioglycerol = 1:1) *m/z* 589 [M+2+H], 587 [M+H]$^+$; HRMS-FAB$^+$ ([M+H]$^+$): calcd for $C_{32}H_{36}BrN_4O_2$: 587.2022, found 587.2027.



2H-2d

2,10-Dibromo-5,15-di-*n*-butylporphyrin (2H-2d) The bromination of **2H-1d** was carried out according to **GP-NBS-2H-1**. Dark purple solid (199 mg, 71%): R_f = 0.53 (silica gel, *n*-hexane/toluene = 1:1); ^{1}H-NMR ($CDCl_3$, 300 MHz) δ: 10.03 (1H, s), 9.70 (1H, d, J = 4.8 Hz), 9.64 (1H, d, J = 4.8 Hz), 9.41 (1H, d, J = 4.8 Hz), 9.38 (1H, d, J = 4.8 Hz), 9.31 (1H, d, J = 4.6 Hz), 9.30 (1H, d, J = 4.6 Hz), 9.30 (1H, s), 4.81 (2H, t, J = 8.0 Hz), 4.70 (2H, t, J = 8.0 Hz), 2.45–2.35 (4H, m), 1.78–1.75 (4H, m), 1.11 (3H, t, J = 7.3 Hz), 1.10 (3H, t, J = 7.3 Hz), −3.28 (2H, br s); ^{13}C-NMR ($CDCl_3$, THF-d_8, 100 MHz) δ: 154.8 (br), 152.2 (br), 152.0 (br), 147.6 (br), 140.2 (br), 139.8 (br), 138.0 (br), 137.0 (br), 135.7, 131.5, 131.0, 130.2, 129.2, 125.7 (2C), 124.1, 120.2, 119.5, 103.0, 101.8, 40.7, 40.5, 34.5, 34.4, 23.5 (2C), 14.0 (2C); IR (KBr): 3302, 2955, 2854, 1469, 1062, 975, 919, 847, 782, 712 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 418 (5.4), 517 (4.1), 552 (3.5), 595 (3.5), 652 (3.5) nm; FAB-MS (dithiothreitol/thioglycerol = 1:1) *m/z* 583 [M+4+H], 581 [M+2+H], 579 [M+H]$^+$; HRMS-FAB$^+$ ([M+H]$^+$): calcd for $C_{28}H_{29}Br_2N_4$: 579.0759, found 579.0756; Anal. calcd for $C_{28}H_{28}Br_2N_4$: C, 57.95; H, 4.86; N, 9.65, found: C, 58.02; H, 5.09; N, 9.48.

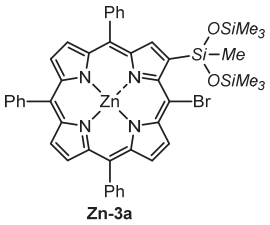


2H-2e

2,10-Dibromo-5,15-diphenylporphyrin (2H-2e) The bromination of **2H-1e** was carried out according to **GP-NBS-2H-1**. Dark purple solid (46.6 mg, 74%): R_f = 0.58 (silica gel, *n*-hexane/toluene = 1:1); ^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 10.31 (1H, s), 9.74 (1H, d, J = 4.9 Hz), 9.64 (1H, d, J = 4.9 Hz), 9.38 (1H, d, J = 4.9 Hz), 9.00 (1H, d, J = 4.9 Hz), 8.99 (1H, d, J = 4.9 Hz), 8.86 (1H, s), 8.82 (1H, d, J = 4.9 Hz), 8.18–8.16 (4H, m), 7.79–7.77 (6H, m), −3.02 (2H, br s); ^{13}C-NMR ($CDCl_3$, THF-d_8, 100 MHz) δ: 154.5 (br), 153.2 (br), 152.0 (br), 149.2 (br), 140.9, 140.6, 140.1 (br), 139.8 (br), 139.1 (br), 137.9 (br), 135.0, 134.9, 134.5, 134.4 (2C), 134.3 (2C), 134.1, 129.8, 129.1 (2C), 129.0, 127.9, 127.8, 126.8 (2C), 126.7 (2C), 120.5, 119.8, 103.8, 102.8; IR (KBr): 3312, 3057, 1595, 1484, 1238, 1174, 1058, 974, 794, 725, 697 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 417 (5.7), 514 (4.5), 547 (3.8), 590 (3.9), 646 (3.6) nm; ESI-MS *m/z* 623 [M+4+H], 621 [M+2+H], 619 [M+H]$^+$; HRMS-ESI$^+$ m/z ([M+H]$^+$): calcd for $C_{32}H_{21}Br_2N_4$: 619.0133, found 619.0131; Anal. calcd for $C_{32}H_{20}Br_2N_4$: C, 61.96; H, 3.25; N, 9.03, found: C, 61.53; H, 3.32; N, 8.89.

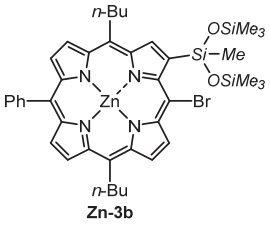
6. General procedure for the bromination of zincated porphyrin Zn-1 with NBS (GP-NBS-Zn-1) (Table 1)

A solution of NBS (19.6 mg, 110 μmol, 1.1 equiv) in $CHCl_3$ (10 mL) was added to a solution of zincated β-silylpophyrin **Zn-1** (100 μmol) in $CHCl_3$ (10 mL) over 1 min at room temperature. The reaction mixture was then stirred at room temperature for 30 min, solvent was evaporated to dryness, and crude product was purified by silica gel column chromatography (cyclohexane/CH_2Cl_2 = 4:1), yielding *meso*-bromoporphyrin **Zn-3**.



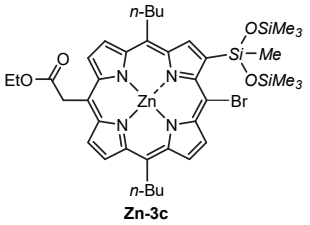
Zn-3a

[20-Bromo-2-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)-5,10,15-triphenylporphyrinato]zinc(II) (Zn-3a) The bromination of **Zn-1a** was carried out according to **GP-NBS-Zn-1**. Dark green solid (42.4 mg, 72%): R_f = 0.44 (silica gel, *n*-hexane/EtOAc = 10:1); ^{1}H-NMR ($CDCl_3$, 300 MHz) δ: 9.83 (1H, d, *J* = 4.8 Hz), 9.45 (1H, s), 8.95 (1H, d, *J* = 4.8 Hz), 8.89 (1H, d, *J* = 4.8 Hz), 8.87 (1H, d, *J* = 4.8 Hz), 8.87 (1H, d, *J* = 4.6 Hz), 8.85 (1H, d, *J* = 4.6 Hz), 8.19–8.15 (6H, m), 7.77–7.72 (9H, m), 0.93 (3H, s), 0.15 (18H, s); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 154.5, 150.9, 150.62, 150.55, 150.52, 150.49, 150.0, 149.7, 147.8, 144.1, 142.7, 142.6, 142.5, 134.5 (2C), 134.42 (2C), 134.39 (2C), 134.1, 132.9, 132.5, 132.4, 132.32, 132.30, 127.75, 127.72, 127.69, 126.75 (2C), 126.71 (2C), 126.69 (2C), 121.9, 121.7, 121.1, 106.6, 4.1, 2.1 (6C); IR (KBr): 2955, 1487, 1440, 1258, 1087, 1054, 844, 795, 752, 702 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 423 (5.8), 554 (4.4), 594 (3.8) nm; FAB-MS (*m*-nitrobenzylalcohol) *m/z* 900 [M+2], 898 [M]$^+$; HRMS-FAB$^+$ (M^+): calcd for $C_{45}H_{43}BrN_4O_2Si_3Zn$: 898.1169, found 898.1170; Anal. calcd for $C_{45}H_{43}BrN_4O_2Si_3Zn$: C, 59.96; H, 4.81; N, 6.22, found: C, 60.35; H, 4.65; N, 6.33.



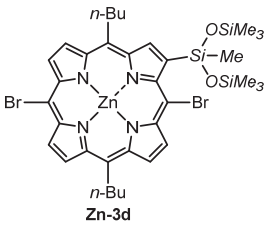
Zn-3b

[20-Bromo-5,15-di-*n*-butyl-2-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)-10-phenylporphyrinato]zinc(II) (Zn-3b) The bromination of **Zn-1b** was carried out according to **GP-NBS-Zn-1**. Dark purple solid (84.0 mg, 70%): R_f = 0.41 (silica gel, *n*-hexane/EtOAc = 10:1); ^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 10.11 (1H, s), 9.53 (1H, d, *J* = 4.9 Hz), 9.35 (1H, d, *J* = 4.9 Hz), 9.01 (1H, d, *J* = 4.4 Hz), 8.97 (1H, d, *J* = 4.9 Hz), 8.79 (1H, d, *J* = 4.9 Hz), 8.65 (1H, d, *J* = 4.4 Hz), 8.08–8.06 (2H, m), 7.77–7.71 (3H, m), 4.92 (2H, t, *J* = 8.0 Hz), 4.27 (2H, t, *J* = 8.0 Hz), 2.60–2.52 (2H, m), 2.27–2.19 (2H, m), 1.92–1.88 (2H, m), 1.70–1.67 (2H, m), 1.18 (3H, t, *J* = 7.4 Hz), 1.08 (3H, s), 1.06 (3H, t, *J* = 7.4 Hz), 0.32 (18H, s); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 153.4, 150.3, 150.0, 149.8, 149.6, 149.52, 149.48, 148.7, 144.2, 143.9, 142.8, 134.4 (2C), 133.9, 132.6, 132.2, 128.9, 128.8, 128.7, 127.5, 126.6 (2C), 121.1, 120.5, 120.3, 105.6, 41.5, 40.8, 35.8, 34.8, 24.0, 23.7, 14.4, 14.2, 4.3, 2.3 (6C); IR (KBr): 2956, 2858, 1258, 1068, 1009, 842, 789, 754 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 425 (5.9), 558 (4.4), 600 (4.0) nm; FAB-MS (*m*-nitrobenzylalcohol) *m/z* 860 [M+2], 858 [M]$^+$; HRMS-FAB$^+$ (M^+): calcd for $C_{41}H_{51}BrN_4O_2Si_3Zn$: 858.1795, found 858.1799.



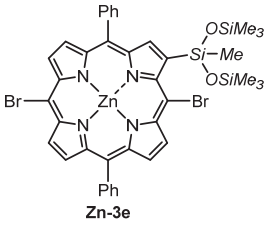
Zn-3c

[20-Bromo-5,15-di-*n*-butyl-10-ethoxycarbonylmethyl-2-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)porphyrinato]zinc(II) (Zn-3c) The bromination of **Zn-1c** was conducted according to **GP-NBS-Zn-1** with pyridine (24.4 μL, 0.30 mmol, 1 equiv). The crude product was purified by silica gel column chromatography (*n*-hexane/EtOAc = 10:1). Dark green solid (123 mg, 47%): R_f = 0.17 (1/10 AcOEt/*n*-hexane); ^{1}H-NMR ($CDCl_3$, 500 MHz) δ: 9.92 (1H, s), 9.64 (1H, d, *J* = 4.6 Hz), 9.05 (1H, d, *J* = 4.6 Hz), 8.81 (1H, d, *J* = 4.6 Hz), 8.74 (1H, d, *J* = 4.6 Hz), 8.62 (1H, d, *J* = 4.6 Hz), 8.59 (1H, d, *J* = 4.6 Hz), 5.15 (2H, s), 4.54 (2H, t, *J* = 8.2 Hz), 4.16 (2H, t, *J* = 8.2 Hz), 3.98 (2H, q, *J* = 7.1 Hz), 2.37–2.31 (2H, m), 2.16–2.10 (2H, m), 1.83–1.80 (2H, m), 1.68–1.65 (2H, m), 1.13 (3H, t, *J* = 7.4 Hz), 1.13 (3H, s), 1.06 (3H, t, *J* = 7.1 Hz), 1.05 (3H, t, *J* = 7.4 Hz), 0.37 (18H, s); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ: 172.4, 153.1, 149.5, 149.1, 149.0, 148.90, 148.88, 148.7, 148.6, 143.9, 143.6, 133.8, 128.9, 128.8, 128.44, 128.394, 128.385, 120.37, 119.6, 109.1, 105.5, 61.0, 41.2, 40.7, 40.2, 35.4, 34.7, 23.9, 23.6, 14.2, 14.10, 14.07, 4.4, 2.3(6C); IR (KBr): 2956, 2856, 1737, 1313, 1260, 1153, 1060, 1015, 865, 838, 775, 755, 733 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 424 (5.9), 559 (4.4), 603 (4.0) nm; FAB-MS (*m*-nitrobenzylalcohol) *m/z* 870 [M+2], 868 [M]$^+$; HRMS-FAB$^+$ (M^+): calcd for $C_{39}H_{53}BrN_4O_4Si_3Zn$: 868.1849, found 868.1852; Anal. Calcd for $C_{39}H_{53}BrN_4O_4Si_3Zn$: C, 53.75; H, 6.13; N, 6.43, found: C, 53.69; H, 5.89; N, 6.48.



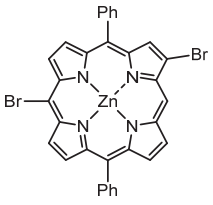
Zn-3d

[10,20-Dibromo-5,15-di(*n*-butyl)-2-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)porphyrinato]zinc(II) (Zn-3d) The bromination of **Zn-1d** was carried out according to **GP-NBS-Zn-1**. Dark purple solid (57.9 mg, 66%): R_f = 0.49 (silica gel, *n*-hexane/EtOAc = 10:1); ^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 9.96 (1H, s), 9.70 (1H, d, *J* = 4.9 Hz), 9.57 (1H, d, *J* = 4.6 Hz), 9.50 (1H, d, *J* = 4.8 Hz), 9.35 (1H, d, *J* = 4.8 Hz), 9.31 (1H, d, *J* = 4.6 Hz), 9.24 (1H, d, *J* = 4.9 Hz), 4.87 (2H, t, *J* = 8.2 Hz), 4.70 (2H, t, *J* = 8.2 Hz), 2.47–2.43 (2H, m), 2.39–2.31 (2H, m), 1.82–1.80 (2H, m), 1.75–1.71 (2H, m), 1.12 (3H, t, *J* = 7.2 Hz), 1.07 (3H, t, *J* = 7.2 Hz), 1.00 (3H, s), 0.24 (18H, s); ^{13}C-NMR ($CDCl_3$, THF-d_8, 100 MHz) δ: 153.7, 150.6, 150.5, 149.6, 149.3, 149.1, 148.8, 144.36, 144.35, 143.9, 134.3, 133.2, 132.9, 129.8, 129.7, 129.5, 121.6, 120.7, 105.9, 103.5, 41.6, 41.2, 35.7, 35.2, 23.9, 23.7, 14.31, 14.25, 4.2, 2.2 (6C); IR (KBr): 2957, 1258, 1058, 1011, 867, 841, 780, 754, 733 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 425 (5.7), 561 (4.1), 607 (4.0) nm; FAB-MS (*m*-nitrobenzylalcohol) *m/z* 864 [M+4], 862 [M+2], 860 [M]$^+$; HRMS-FAB$^+$ (M^+): calcd for $C_{35}H_{46}Br_2N_4O_2Si_3Zn$: 860.0587, found 860.0586; Anal. calcd for $C_{35}H_{46}Br_2N_4O_2Si_3Zn$: C, 48.64; H, 5.37; N, 6.48, found: C, 48.91; H, 5.37; N, 6.40.



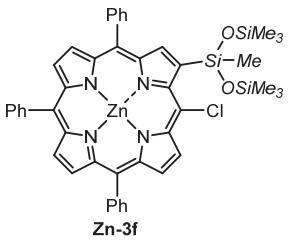
Zn-3e

[10,20-Dibromo-2-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)-5,15-diphenylporphyrinato]zinc(II) (Zn-3e) The bromination of **Zn-1e** was conducted according to **GP-NBS-Zn-1** in the presence of 1 equiv of succinimide. Dark green solid (80.3 mg, 54%): R_f = 0.50 (silica gel, *n*-hexane/EtOAc = 10:1); ^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 9.71 (1H, d, *J* = 4.8 Hz), 9.63 (1H, d, *J* = 4.8 Hz), 9.60 (1H, d, *J* = 4.4 Hz), 9.29 (1H, s), 8.83 (1H, d, *J* = 4.4 Hz), 8.82 (1H, d, *J* = 4.4 Hz), 8.82 (1H, d, *J* = 4.4 Hz), 8.13–8.11 (4H, m), 7.73–7.71 (6H, m), 0.87 (3H, s), 0.09 (18H, s); ^{13}C-NMR ($CDCl_3$, THF-d_8, 100 MHz) δ: 154.8, 150.74, 150.70, 150.6, 150.4, 150.2, 149.9, 149.8, 147.9, 144.0, 142.8, 142.6, 134.6 (2C), 134.5 (2C), 134.1, 133.23, 133.17, 133.0, 132.9, 132.8, 127.6 (2C), 126.5 (2C), 126.5 (2C), 122.0, 121.1, 106.8, 104.5, 4.0, 2.0 (6C); IR (KBr): 2956, 1259, 1080, 1017, 1005, 840, 786, 753, 728, 700 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 424 (5.9), 558 (4.6), 598 (4.1) nm; FAB-MS (*m*-nitrobenzylalcohol) *m/z* 904 [M+4], 902 [M+2], 900 [M]$^+$; HRMS-FAB$^+$ (M^+): calcd for $C_{39}H_{38}Br_2N_4O_2Si_3Zn$: 899.9961, found 899.9978; Anal. calcd for $C_{39}H_{38}Br_2N_4O_2Si_3Zn$: C, 51.81; H, 4.24; N, 6.20, found: C, 51.91; H, 4.36; N, 6.27.



Zn-2e

[2,10-Dibromo-5,15-diphenylporphyrinato]zinc(II) (Zn-2e) The bromination of **Zn-1e** was conducted according to **GP-NBS-Zn-1** in the absence of succinimide. Dark purple solid (44.7 mg, 25%): R_f = 0.26 (silica gel, *n*-hexane/EtOAc = 10:1); ^{1}H-NMR ($CDCl_3$, THF-d_8, 500 MHz) δ: δ: 10.14 (1H, s), 9.61 (2H, d, *J* = 4.6 Hz), 9.21 (1H, d, *J* = 4.6 Hz), 8.85 (1H, s), 8.85 (1H, d, *J* = 4.6 Hz), 8.83 (1H, d, *J* = 4.6 Hz), 8.82 (1H, d, *J* = 4.6 Hz), 8.11–8.05 (4H, m), 7.70–7.63 (6H, m); ^{13}C-NMR ($CDCl_3$, THF-d_8, 125 MHz) δ: 150.7, 150.6, 150.4, 150.1, 149.5, 148.1, 146.2, 142.5, 142.2, 134.4 (2C), 134.3 (2C), 132.9 (2C), 132.7, 132.6, 132.54, 132.51, 132.1, 127.4, 127.3, 126.4 (2C), 126.3 (2C), 121.1, 120.9, 120.3, 104.6, 103.4 (2C); IR (KBr): 2924, 1597, 1489, 1319, 1273, 1072, 1001, 789, 744, 698 cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 420 (5.6), 551 (4.3), 591 (3.4) nm; EI-MS (70 eV) *m/z* (relative intensity): 684 [100, M+4], 682 [98, M+2], 680 [36, M^+], 604 [13, M − C_6H_5]; HRMS (EI) *m/z*: calcd for $C_{32}H_{18}N_4Br_2$: 679.9190, found 679.9190.



Zn-3f

[20-Cloro-2-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)-5,10,15-triphenylporphyrinato]zinc(II) (Zn-3f) A solution of NCS (14.7 mg, 110 μmol, 1.1 equiv) in $CHCl_3$ (10 mL) was added to a solution of zincated β-silylpophyrin **Zn-1a** (100 μmol) in $CHCl_3$ (10 mL) over 1 min at room temperature. The reaction mixture was stirred at room temperature for 3 h, solvent was evaporated to dryness, and crude product was purified by silica gel column chromatography (cyclohexane/CH_2Cl_2 = 10:1). Dark green solid (62.0 mg, 70%): R_f = 0.39 (1/10 AcOEt/*n*-hexane); ^{1}H-NMR ($CDCl_3$, 500 MHz) δ: 9.71 (1H, d, *J* = 4.6 Hz), 9.30 (1H, s), 8.89 (1H, d, *J* = 4.6 Hz), 8.80 (1H, d, *J* = 4.6 Hz), 8.78 (1H, d, *J* = 4.6 Hz), 8.78 (1H, d, *J* = 4.6 Hz), 8.77 (1H, d, *J* = 4.6 Hz), 8.15–8.14 (6H, m), 7.71–7.69 (9H, m), 0.85 (3H, s), 0.11 (18H, s); ^{13}C-NMR ($CDCl_3$, THF-d_8, 125 MHz) δ: 152.7, 150.7, 150.5, 150.3, 150.2, 150.0, 149.4, 148.6, 146.5, 143.15, 143.14, 143.06, 141.6, 134.6 (2C), 134.48 (2C), 134.47 (2C), 132.3, 132.01, 131.98, 131.92, 131.87, 131.86, 130.6, 127.40, 127.36, 126.46 (2C), 126.45 (2C), 126.41 (2C), 121.3, 121.0, 120.6, 114.2, 3.1, 2.0 (6C); IR (KBr): 3047, 2955, 1258, 1089, 1055, 1007, 839, 795, 752, 721, 703

cm^{-1}; UV/vis (CH_2Cl_2) λ_{max} (log ε): 423 (5.9), 554 (4.5), 591 (3.9) nm; FAB-MS (*m*-nitrobenzylalcohol) *m/z* 856 [M+2], 854 $[M]^+$; HRMS-FAB$^+$ (M^+): calcd for $C_{45}H_{43}ClN_4O_2Si_3Zn$: 854.1674, found 854.1675; Anal. calcd for $C_{45}H_{43}ClN_4O_2Si_3Zn$: C, 63.07; H, 5.06; N, 6.54, found: C, 63.24; H, 5.10; N, 6.55.

7. General procedure for the bromination of 2H-1a (Table 2, other than NBS)

A solution of the brominating agent (DBDMH, Br_2, Br_2·1,4-dioxane, BDMS, 110 μmol, 1.1 equiv) in $CHCl_3$ (10 mL) was added to a solution of free-base β-silylpophyrin **2H-1a** (100 μmol) in $CHCl_3$ (10 mL) over 10 min at 0 °C. The reaction mixture was allowed to warm to room temperature while being stirred for 2 h. The reaction was quenched using sat. aqueous $Na_2S_2O_3$. The organic layer was washed successively using water and brine, dried over $MgSO_4$, and filtered. The filtrate was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography (*n*-hexane/toluene = 4:1) and then recrystallized from *n*-hexane/CH_2Cl_2, yielding β-bromoporphyrin **2H-2a**.

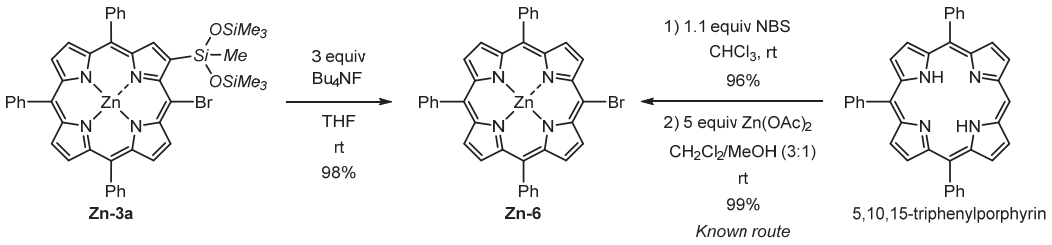
8. General procedure for the bromination of Zn-1a (Table 2, other than NBS, NCS)

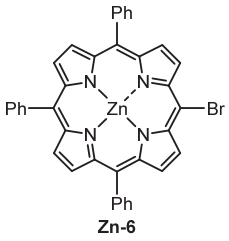
A solution of the brominating agent (DBDMH, Br_2, Br_2·1,4-dioxane, BDMS, 110 μmol, 1.1 equiv) in $CHCl_3$ (10 mL) was added to a solution of free-base β-silylpophyrin **2H-1a** (100 μmol) in $CHCl_3$ (10 mL) over 1 min at 0 °C. The reaction mixture was allowed to warm to room temperature while being stirred for 30–90 min (3 h for NCS). The reaction was quenched with sat. aqueous $Na_2S_2O_3$. The organic layer was washed successively using water and brine, dried over $MgSO_4$, and filtered. The filtrate was concentrated under reduced pressure, and the crude product was purified by silica gel column chromatography (cyclohexane/toluene = 4:1), yielding a mixture of **Zn-2a**, **Zn-3a**, and recovered **Zn-1a**. The yields of **Zn-2a**, **Zn-3a** and recovered **Zn-1a** were determined by the integral ratio of the mixture's ^{1}H-NMR spectra.

9. Determination of the structure of Zn-3a

The structure of **Zn-3a** was determined by comparing the ^{1}H-NMR spectrum of the desilylated product **Zn-6** with those of [5-Bromo-10,15,20-triphenylporphyrinato]zinc (II) (**Zn-6**),[5] which was synthesized from 5,10,15-triphenylporphyrin via a known procedure.[4,6]

Scheme S1





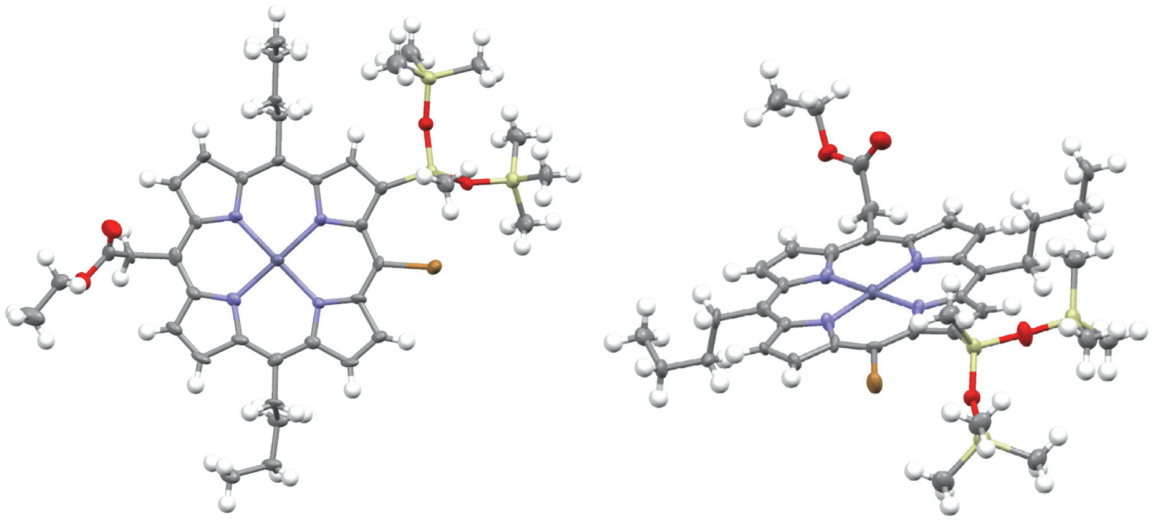
[5-Bromo-10,15,20-triphenylporphyrinato]zinc (II) (Zn-6) A solution of Bu_4NF (1 mol/L in THF, 200 μL, 3.0 equiv) was added to a solution of *meso*-bromo-β-silylpophyrin **Zn-3a** (67 μmol) in THF (15 mL). The solution was stirred at room temperature for 30 min, and the solvent was evaporated to dryness. The crude product was purified by silica gel column chromatography (silica gel, *n*-hexane/EtOAc = 3:1) and then recrystallized from *n*-hexane/ CH_2Cl_2 to give **Zn-6**. Purple solid (44.2 mg, 98%): ^{1}H-NMR ($CDCl_3$, 300 MHz) δ: 9.68 (2H, d, J = 4.6 Hz), 8.89 (2H, d, J = 4.6 Hz), 8.79 (4H, s), 8.15–8.13 (6H, m), 7.73–7.68 (9H, m); ESI-MS *m/z* 680 [M+2], 678 $[M]^+$; HRMS-ESI$^+$ m/z (M^+): calcd for $C_{38}H_{23}BrN_4Zn$: 678.0398, found 678.0390.

10. X-ray crystal structure of Zn-3c

Single crystals of **Zn-3c** were mounted on a MicroMount® polyimide tip using paraffin oil. Using filtered Cu Kα radiation, all measurements were taken using a Rigaku R-AXIS RAPID imaging plate diffractometer. The data were corrected for Lorentz and polarization effects and numerical absorption. The structures were solved by direct methods[7] and expanded by Fourier techniques. The non-hydrogen atoms were refined anisotropically, and the hydrogen atoms were refined using a riding model. All calculations were conducted using the CrystalStructure[8] crystallographic software package, except for refinement, which was conducted using SHELXL 2014.[9]

Table S1. Experimental Data for the X-ray Crystallography of **Zn-3c**

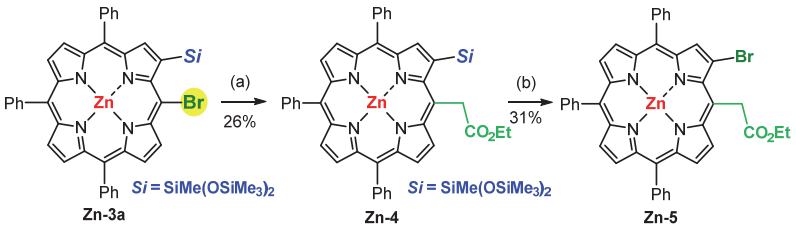
parameter		parameter		parameter	
formula	$C_{39}H_{53}N_4O_4BrSi_3Zn$	β/deg	102.47000	no. of measured reflections	23355
Mw	871.41	γ/deg	91.92000	no. of unique reflections	7189
crystal size/mm	0.181 x 0.017 x 0.005	V/Å^3	2029.22248	R_{int}	0.2528
crystal system	triclinic	space group	P-1 (#2)	goodness of fit	1.046
a/Å	9.34408	Z	2	R_1	0.1381
b/Å	13.50930	g/cm	1.426	wR_2	0.3577
c/Å	16.70250	μ (Cu Kα)/cm^{-1}	31.994	Structure solv	SHELXT
α/deg	98.85800	T/K	93	Refinement	SHELXL 2014/7



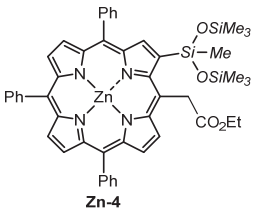
(a) **(b)**

Figure S1. Crystal structure of **Zn-3c**; atomic thermal ellipsoids are drawn at the 30% probability level for non-hydrogen atoms. (a) Top view. (b) Front view. Hydrogen atoms are omitted for clarity. (CCDC, 2035888)

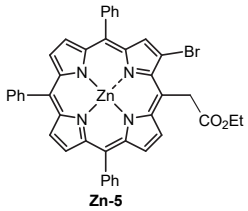
11. Functionalization of Zn-3a



Reaction conditions—(a) $BrZnCH_2CO_2Et$ (50 equiv), $Pd(OAc)_2$ (10 mol%), Cy_3P (20 mol%), THF, 60 °C, and 2 d; (b) NBS (1.5 equiv), $CHCl_3$, room temperature, and 1 h



[7-(1,1,1,3,5,5,5-Heptamethyltrisiloxan-3-yl)-5-(2-ethoxycarbonylethyl)-10,15,20-triphenylporphyrinato]zinc(II) (Zn-4) An oven-dried 50 mL two-necked flask equipped with a magnetic stirring bar and rubber septum was charged using Zn dust (650 mg, 10 mmol) and CuCl (94 mg). The reaction vessel was evacuated and flushed using argon (three times), and dry THF (4 mL) was added. The suspension was heated at 65 °C for 2 h using an oil bath. During this activation period, another oven-dried 5 mL flask was evacuated and flushed using argon (tree times) and then charged using dry THF (1 mL) and ethyl bromoacetate (280 µL, 2.5 mmol). The reaction vessel containing the Zn(Cu) couple was removed from the oil bath. To initiate the reaction, approximately one tenth of the THF–ethyl bromoacetate solution was added using a syringe to the stirred, still-hot Zn(Cu) couple suspension. The rest of the solution was added at such a rate as to maintain a gentle reflux (ac. 10 min). The reaction mixture was stirred and heated at 65 °C for 2 h. A mixture of *meso*-boromoporphyrin **Zn-3a** (45 mg, 0.05 mmol), $Pd(OAc)_2$ (1.1 mg, 10 mol%), and Cy_3P (2.8 mg, 20 mol%) in THF (10 mL) was then added to the resulting ~0.5-M THF solution of the zinc enolate. This reaction mixture was then heated under argon at 65 °C for 2 d and then allowed to reach room temperature. The reaction mixture was filtered using filter paper, diluted using Et_2O, and washed using aqueous NH_4Cl and brine. The organic layer was dried over anhydrous $MgSO_4$ and concentrated in vacuo. Column chromatography on silica gel (CH_2Cl_2), followed by recrystallization from CH_2Cl_2/MeOH, yielded the product **Zn-4**. Purple solid (11.8 mg, 26%): R_f = 0.33 (1/1 CH_2Cl_2/*n*-hexane); ^{1}H-NMR ($CDCl_3$, 500 MHz) δ: 9.48 (1H, d, J = 4.6 Hz), 9.39 (1H, s), 8.98 (1H, d, J = 4.6 Hz), 8.88 (1H, d, J = 5.0 Hz), 8.85 (2H, s), 8.85 (1H, d, J = 5.0 Hz), 8.18–8.16 (6H, m), 7.76–7.69 (9H, m), 6.42 (2H, s), 4.16 (2H, q, J = 7.1 Hz), 1.14 (3H, t, J = 7.1 Hz), 0.69 (3H, s), 0.16 (18H, s); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ: 173.9, 155.1, 151.1, 150.4, 150.3, 150.01, 149.98, 149.4, 149.1, 146.4, 143.0, 142.8, 142.7, 140.6, 134.37 (2C), 134.34 (2C), 134.32 (2C), 132.7, 132.2, 131.9, 131.8, 131.7, 129.2, 127.47, 127.46, 127.43, 126.53 (2C), 126.5 (2C), 126.48 (2C), 121.4, 121.0, 119.8, 112.8, 61.0, 43.0, 14.2, 2.5, 1.9 (6C).; IR (KBr): 3055, 2956, 1743, 1597, 1512, 1487, 1439, 1365, 1340, 1257, 1194, 1161, 1027, 843, 791, 754, 721, 702 cm^{-1}; UV/vis ($CHCl_3$) λ_{max} (log ε): 428 (5.9), 562 (4.5), 600 (3.9) nm; FAB-MS (*m*-nitrobenzylalcohol) *m/z* 906 (M^+); HRMS-FAB$^+$ (M^+): calcd for $C_{49}H_{50}N_4O_4Si_3Zn$: 906.2431, found 906.2425.



Zn-5

[7-Bromo-5-(2-ethoxycarbonylethyl)-10,15,20-triphenylporphyrinato]zinc(II) (Zn-5) A solution of NBS (5.5 mg, 31 μmol, 1.4 equiv) in $CHCl_3$ (2 mL) was added to a solution of zincated β-silylpophyrin **Zn-4** (20 mg, 22 μmol) in $CHCl_3$ (2 mL) over 1 min at room temperature. This reaction mixture was stirred at room temperature for 1 h, and the solvent was evaporated to dryness. The crude product was purified by silica gel column chromatography (CH_2Cl_2 only) and then recrystallized from *n*-hexane/CH_2Cl_2, yielding **Zn-5**. Purple solid (5.3 mg, 31%): R_f = 0.56 (CH_2Cl_2); ^{1}H-NMR ($CDCl_3$, 500 MHz) δ: 9.39 (1H, d, *J* = 5.0 Hz), 9.06 (1H, s), 8.94 (1H, d, *J* = 5.0 Hz), 8.88 (1H, d, *J* = 4.6 Hz), 8.86 (1H, d, *J* = 4.6 Hz), 8.85 (1H, d, *J* = 4.6 Hz), 8.84 (1H, d, *J* = 4.6 Hz), 8.16–8.14 (6H, m), 7.79–7.70 (9H, m), 6.34 (2H, s), 4.31 (2H, q, *J* = 7.1 Hz), 1.30 (3H, t, *J* = 7.1 Hz); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ: 173.1, 151.4, 150.9, 150.7, 150.5, 150.2, 150.0, 147.0, 143.9, 142.49, 142.46, 142.44, 137.3, 134.39 (2C), 134.35 (2C), 134.33 (2C), 133.0, 132.40, 132.37, 132.36, 132.31, 129.1, 127.7, 127.61, 127.59, 126.63 (2C), 126.62 (2C), 126.58 (2C), 121.6, 121.4, 120.1, 117.1, 111.4, 61.3, 39.9, 14.4; IR (KBr): 3101, 3055, 2979, 1718, 1622, 1597, 1487, 1439, 1327, 1194, 1155, 1070, 1031, 999, 964, 906, 792, 750, 732, 704 cm^{-1}; UV/vis ($CHCl_3$) λ_{max} (log ε): 428 (5.5), 562 (4.1), 603 (3.6) nm; FAB-MS (*m*-nitrobenzylalcohol) *m/z* 766 [M+2], 764 $[M]^+$; HRMS-FAB$^+$ (M^+): calcd for $C_{42}H_{29}BrN_4O_2Zn$: 764.0765, found 764.0762.

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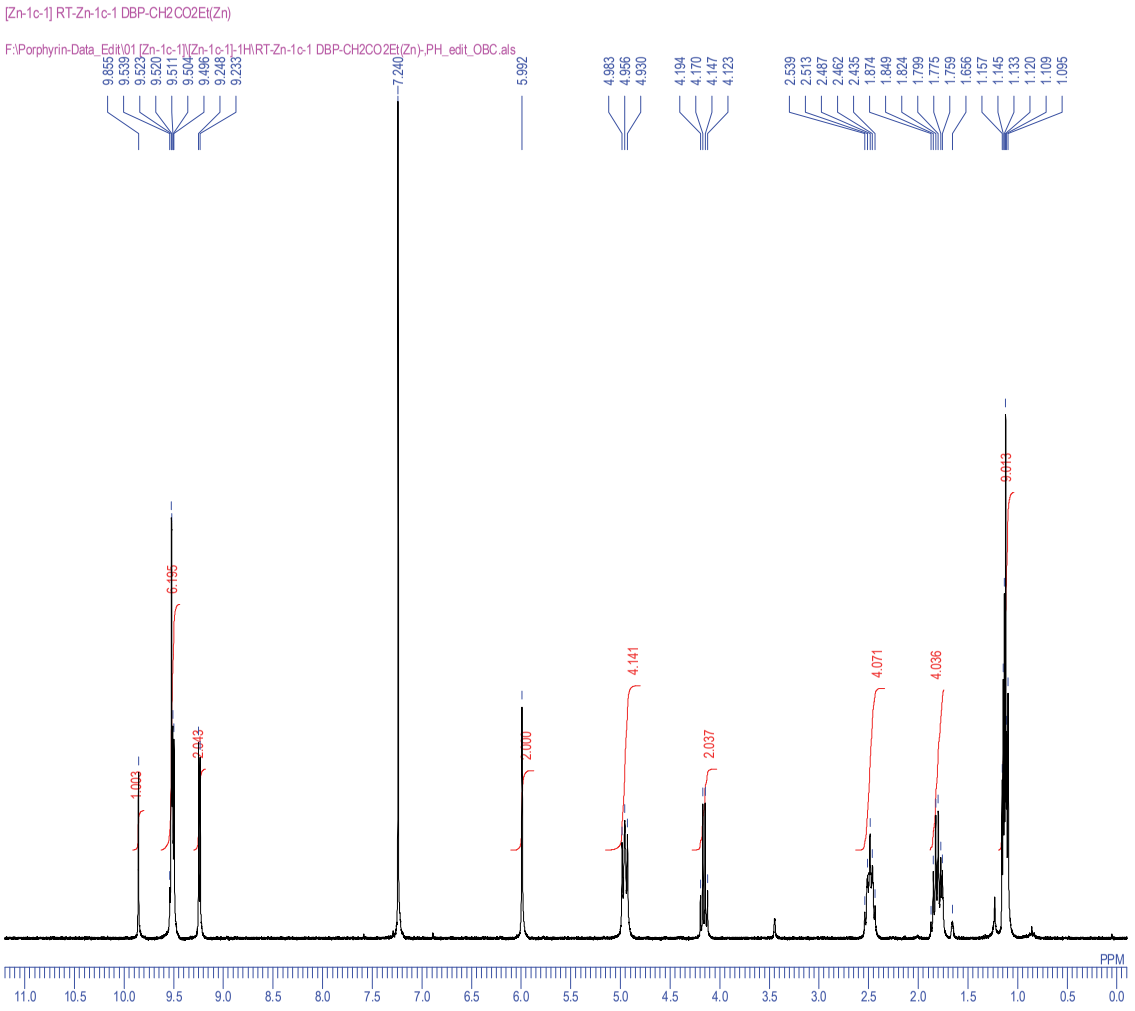
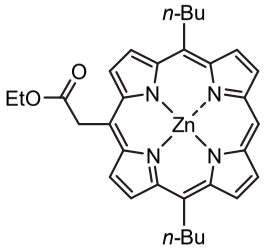
9 SHELXL Version 2014/7: G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112.

13. NMR Spectra

Zn-1c-1

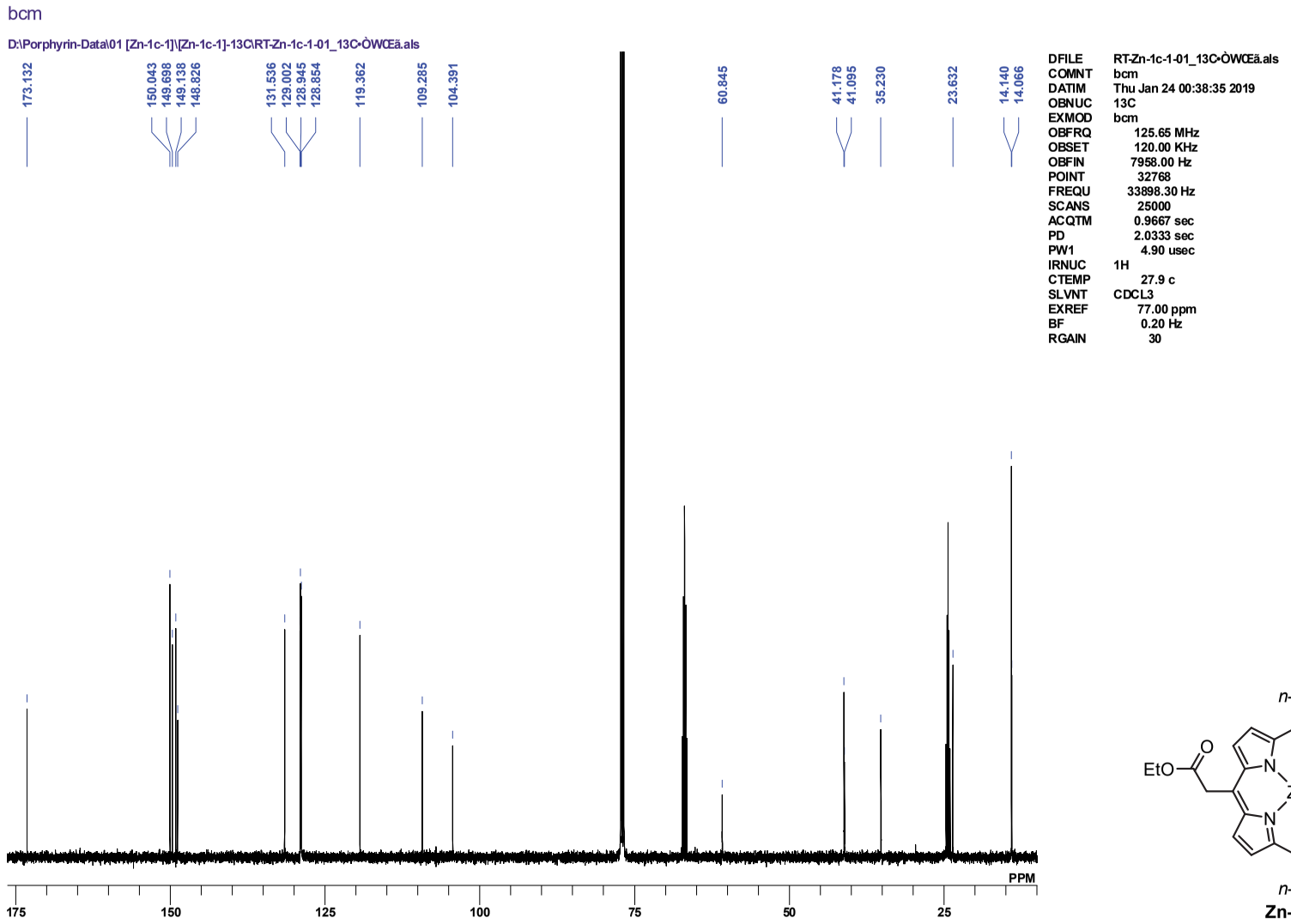



```
DFILE  RT-Zn-1c-1 DBP-CH2CO2Et(Zn)-,PH_edit_OBC.als
COMNT[Zn-1c-1] RT-Zn-1c-1 DBP-CH2CO2Et(Zn)
DATIM Thu Jan 31 16:14:55 2019
OBNUCH
EXMODNON
OBFRQ    300.40 MHz
OBSET    130.00 KHz
OBFIN    1150.00 Hz
POINT     32768
FREQU    6006.01 Hz
SCANS       16
ACQTM    5.4559 sec
PD       1.5440 sec
PW1       5.20 usec
IRNUC 1H
CTEMP    24.8 c
SLVNTCDCL3
EXREF    7.24 ppm
BF       0.20 Hz
RGAIN       19
```

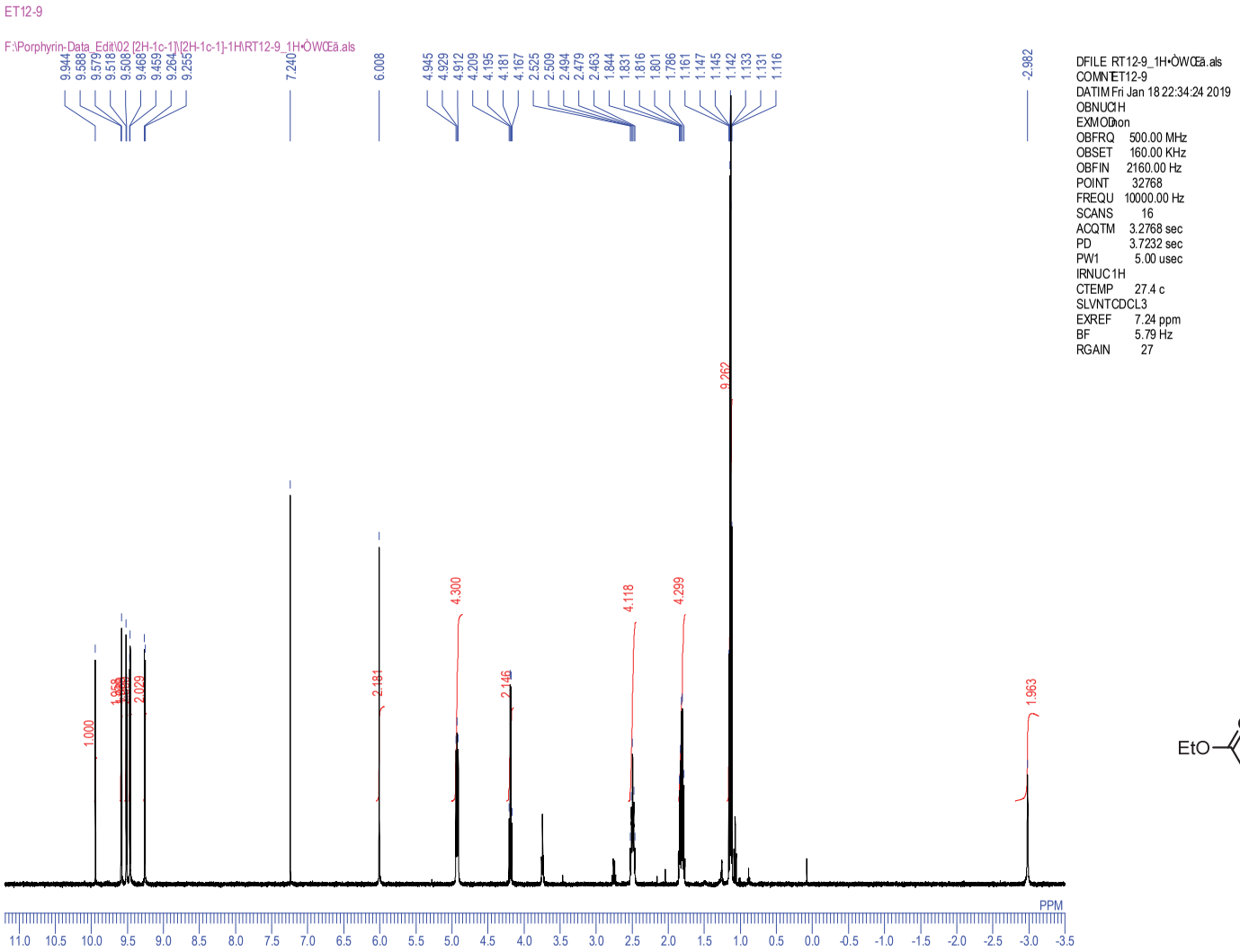


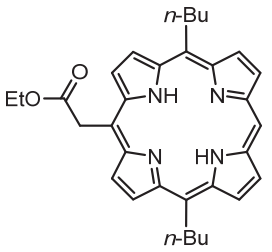
Zn-1c-1

Zn-1c-1


bcm
D:\Porphyrin-Data\01 [Zn-1c-1]\[Zn-1c-1]-13C\RT-Zn-1c-1-01_13C-ÒWŒä.als
173.132
150.043
149.698
149.138
148.826
131.536
129.002
128.945
128.854
119.362
109.285
104.391
60.845
41.178
41.095
35.230
23.632
14.140
14.066
DFILE RT-Zn-1c-1-01_13C-ÒWŒä.als
COMNT bcm
DATIM Thu Jan 24 00:38:35 2019
OBNUC 13C
EXMOD bcm
OBFRQ 125.65 MHz
OBSET 120.00 KHz
OBFIN 7958.00 Hz
POINT 32768
FREQU 33898.30 Hz
SCANS 25000
ACQTM 0.9667 sec
PD 2.0333 sec
PW1 4.90 usec
IRNUC 1H
CTEMP 27.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.20 Hz
RGAIN 30
PPM
175
150
125
100
75
50
25
n-Bu
EtO
O
N
N
Zn
N
N
n-Bu
Zn-1c-1

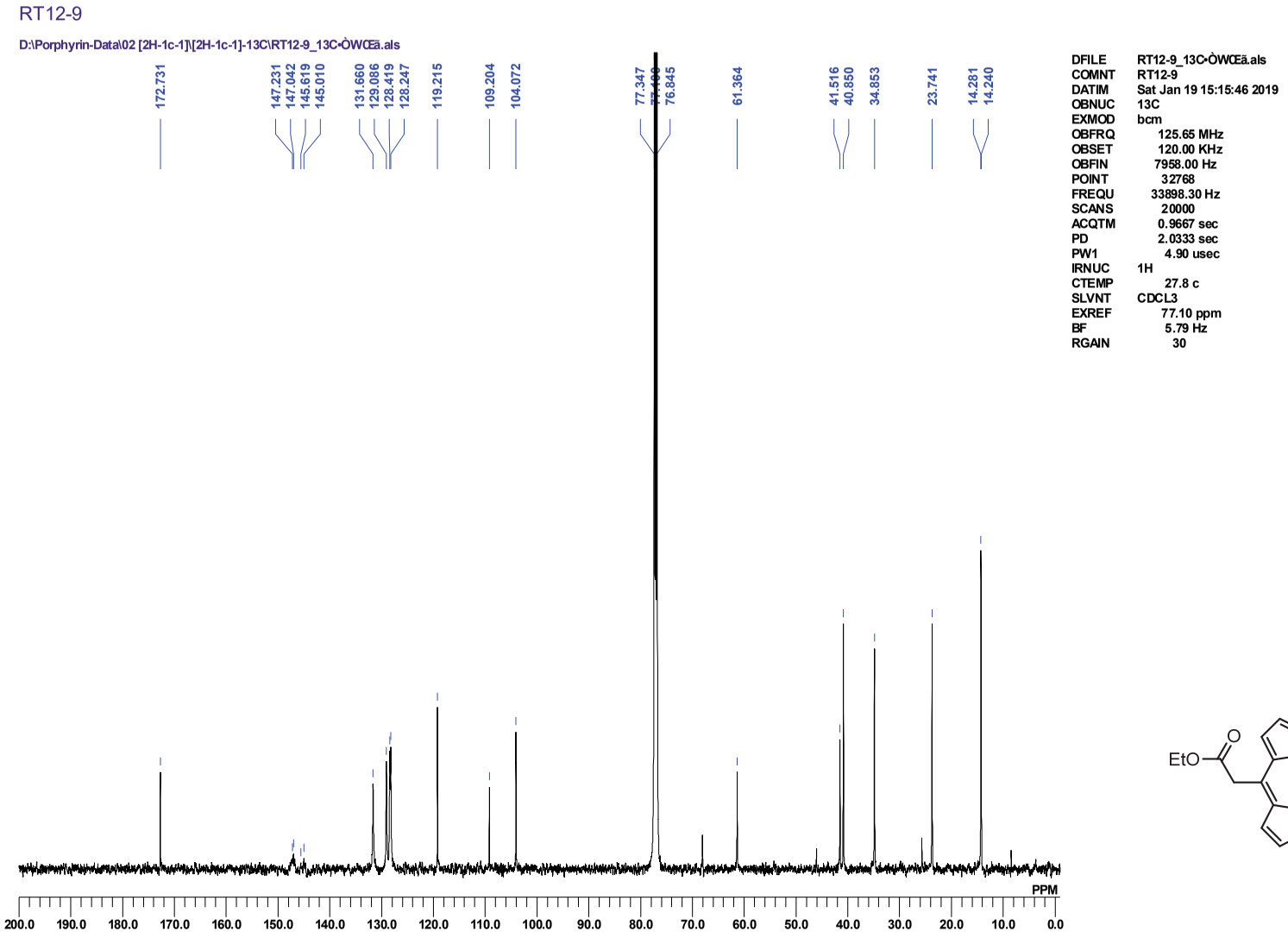
2H-1c-1


ET12-9
F:\Porphyrin-Data_Edit\02 [2H-1c-1]\[2H-1c-1]-1H\RT12-9_1H•ÒWŒä.als
9.944
9.588
9.576
9.513
9.508
9.468
9.459
9.264
9.255
7.240
6.008
4.945
4.929
4.912
4.209
4.195
4.181
4.167
2.525
2.509
2.494
2.479
2.463
1.844
1.831
1.816
1.801
1.786
1.161
1.147
1.145
1.142
1.133
1.131
1.116
-2.982
DFILE RT12-9_1H•ÒWŒä.als
COMNTET12-9
DATIM Fri Jan 18 22:34:24 2019
OBNUC1H
EXMODnon
OBFRQ 500.00 MHz
OBSET 160.00 KHz
OBFIN 2160.00 Hz
POINT 32768
FREQU 10000.00 Hz
SCANS 16
ACQTM 3.2768 sec
PD 3.7232 sec
PW1 5.00 usec
IRNUC1H
CTEMP 27.4 c
SLVNTCDCL3
EXREF 7.24 ppm
BF 5.79 Hz
RGAIN 27
9.262
4.300
4.118
4.299
2.181
2.146
2.029
1.963
1.000
PPM
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5 -3.0 -3.5


n-Bu
O
EtO
NH
N
N
HN
n-Bu

2H-1c-1

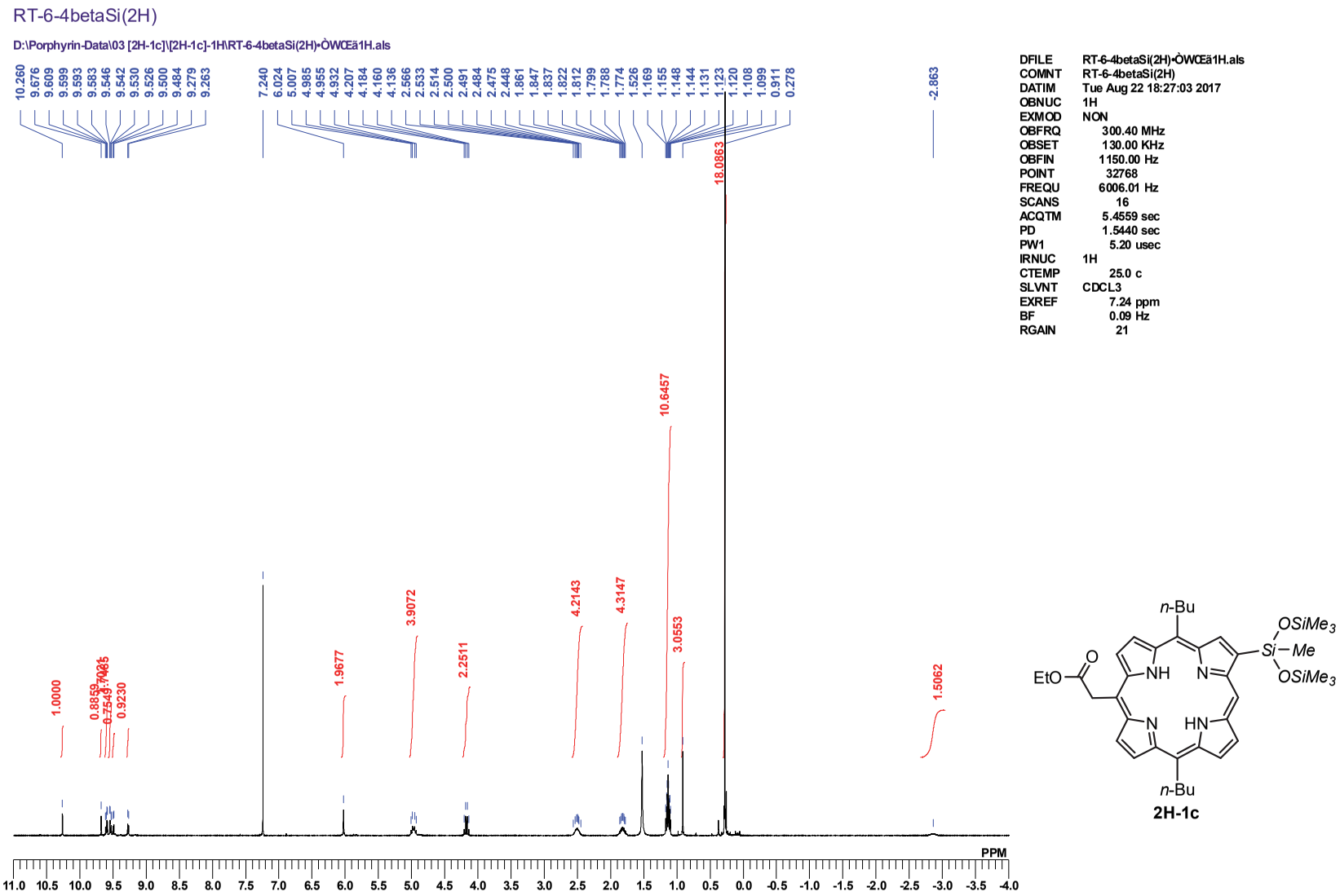
2H-1c-1


RT12-9
D:\Porphyrin-Data\02 [2H-1c-1]\[2H-1c-1]-13C\RT12-9_13C•ÒWŒã.als
172.731
147.231
147.042
145.619
145.010
131.660
129.086
128.419
128.247
119.215
109.204
104.072
77.347
76.845
61.364
41.516
40.850
34.853
23.741
14.281
14.240
DFILE RT12-9_13C•ÒWŒã.als
COMNT RT12-9
DATIM Sat Jan 19 15:15:46 2019
OBNUC 13C
EXMOD bcm
OBFRQ 125.65 MHz
OBSET 120.00 KHz
OBFIN 7958.00 Hz
POINT 32768
FREQU 33898.30 Hz
SCANS 20000
ACQTM 0.9667 sec
PD 2.0333 sec
PW1 4.90 usec
IRNUC 1H
CTEMP 27.8 c
SLVNT CDCL3
EXREF 77.10 ppm
BF 5.79 Hz
RGAIN 30
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0

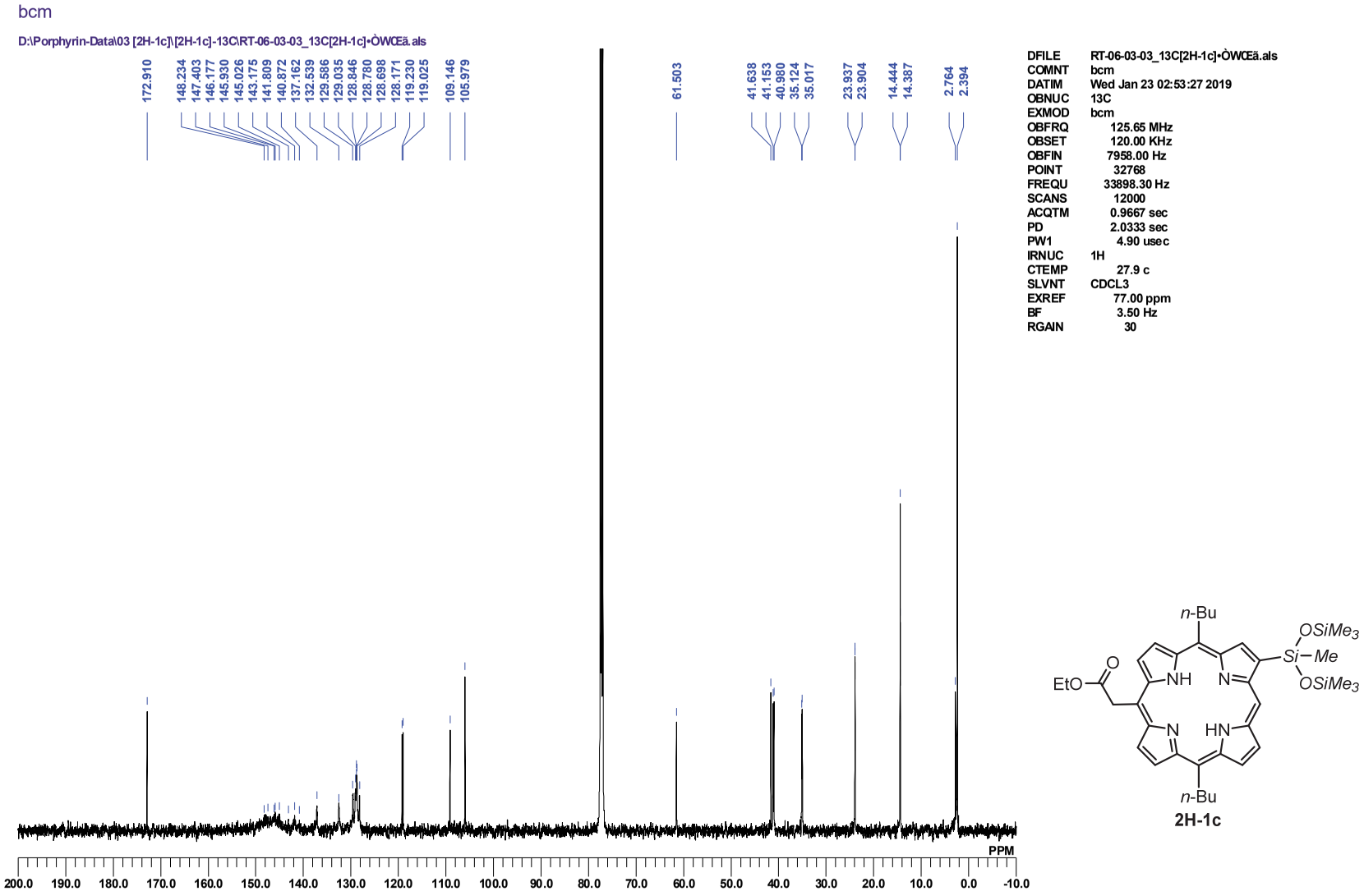
n-Bu
EtO
O
NH
N
N
HN
n-Bu

2H-1c-1

2H-1c


RT-6-4betaSi(2H)
D:\Porphyrin-Data\03 [2H-1c]\[2H-1c]-1H\RT-6-4betaSi(2H)•ÒWŒÈä1H.als
DFILE RT-6-4betaSi(2H)•ÒWŒÈä1H.als
COMNT RT-6-4betaSi(2H)
DATIM Tue Aug 22 18:27:03 2017
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.00 Hz
POINT 32768
FREQU 6006.01 Hz
SCANS 16
ACQTM 5.4559 sec
PD 1.5440 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 25.0 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.09 Hz
RGAIN 21
10.260 9.676 9.609 9.599 9.593 9.583 9.546 9.542 9.530 9.526 9.500 9.484 9.279 9.263
7.240 6.024 5.007 4.985 4.955 4.932 4.207 4.184 4.160 4.136 2.566 2.533 2.514 2.500 2.491 2.484 2.475 2.448 1.861 1.847 1.837 1.822 1.812 1.799 1.788 1.774 1.526 1.169 1.155 1.148 1.144 1.131 1.123 1.120 1.108 1.099 0.911 0.278
-2.863
18.0863
10.6457
4.2143
4.3147
3.9072
3.0553
2.2511
1.9677
1.5062
1.0000
0.8859
0.7549
0.9230
PPM
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5 -3.0 -3.5 -4.0
n-Bu
OSiMe3
Si–Me
OSiMe3
EtO
O
NH
N
N
HN
n-Bu
2H-1c

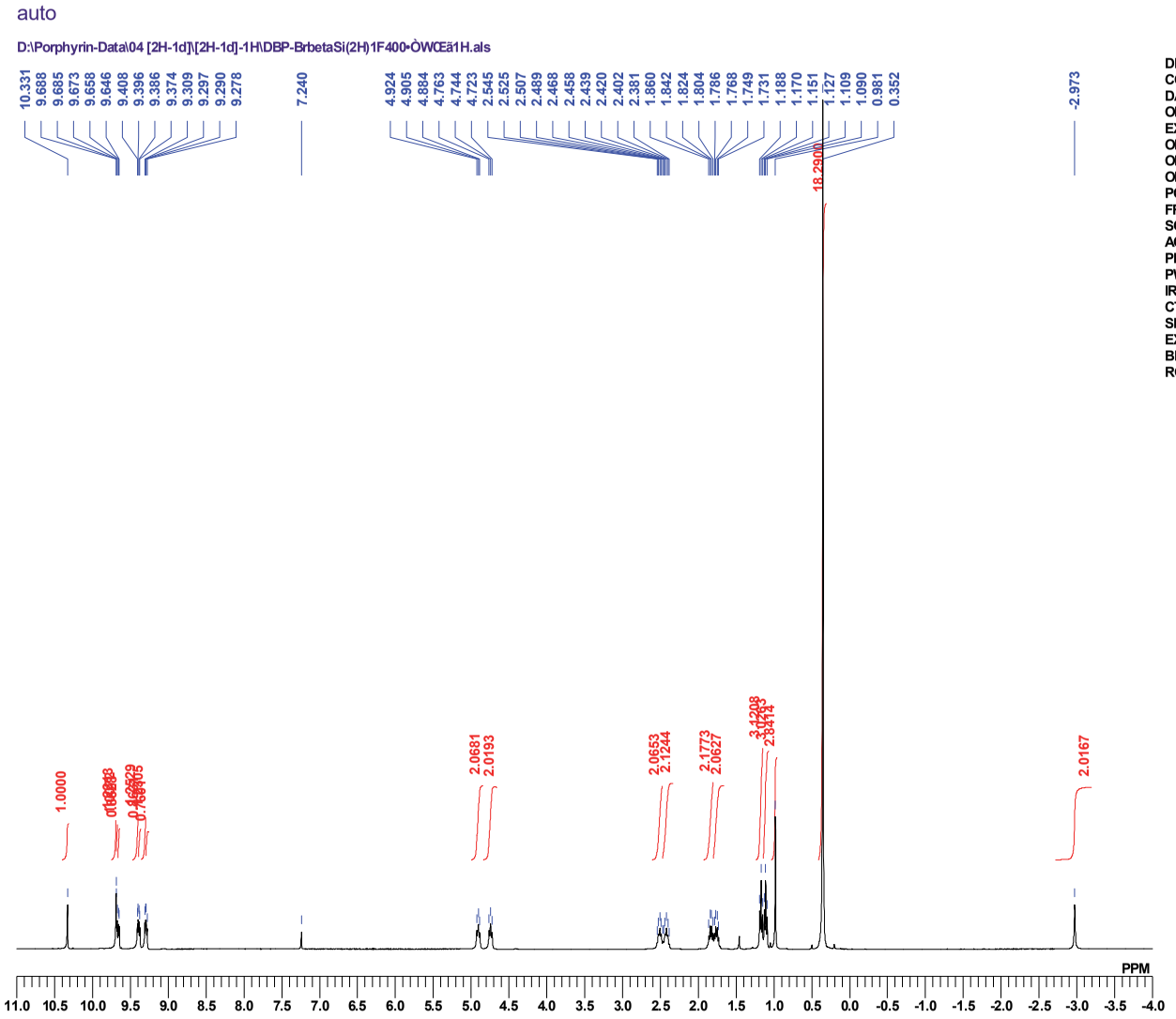
2H-1c

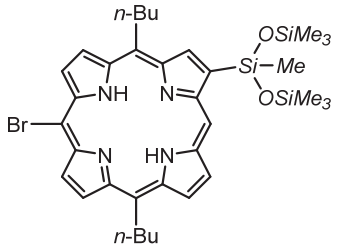

bcm
D:\Porphyrin-Data\03 [2H-1c]\[2H-1c]-13C\RT-06-03-03_13C[2H-1c]•ÒWŒã.als
172.910
148.234
147.403
146.177
145.930
145.026
143.175
141.809
140.872
137.162
132.539
129.586
129.035
128.846
128.780
128.698
128.171
119.230
119.025
109.146
105.979
61.503
41.638
41.153
40.980
35.124
35.017
23.937
23.904
14.444
14.387
2.764
2.394
DFILE RT-06-03-03_13C[2H-1c]•ÒWŒã.als
COMNT bcm
DATIM Wed Jan 23 02:53:27 2019
OBNUC 13C
EXMOD bcm
OBFRQ 125.65 MHz
OBSET 120.00 KHz
OBFIN 7958.00 Hz
POINT 32768
FREQU 33898.30 Hz
SCANS 12000
ACQTM 0.9667 sec
PD 2.0333 sec
PW1 4.90 usec
IRNUC 1H
CTEMP 27.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 3.50 Hz
RGAIN 30
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0

n-Bu
OSiMe3
Si
Me
OSiMe3
O
EtO
NH
N
N
HN
n-Bu

2H-1c

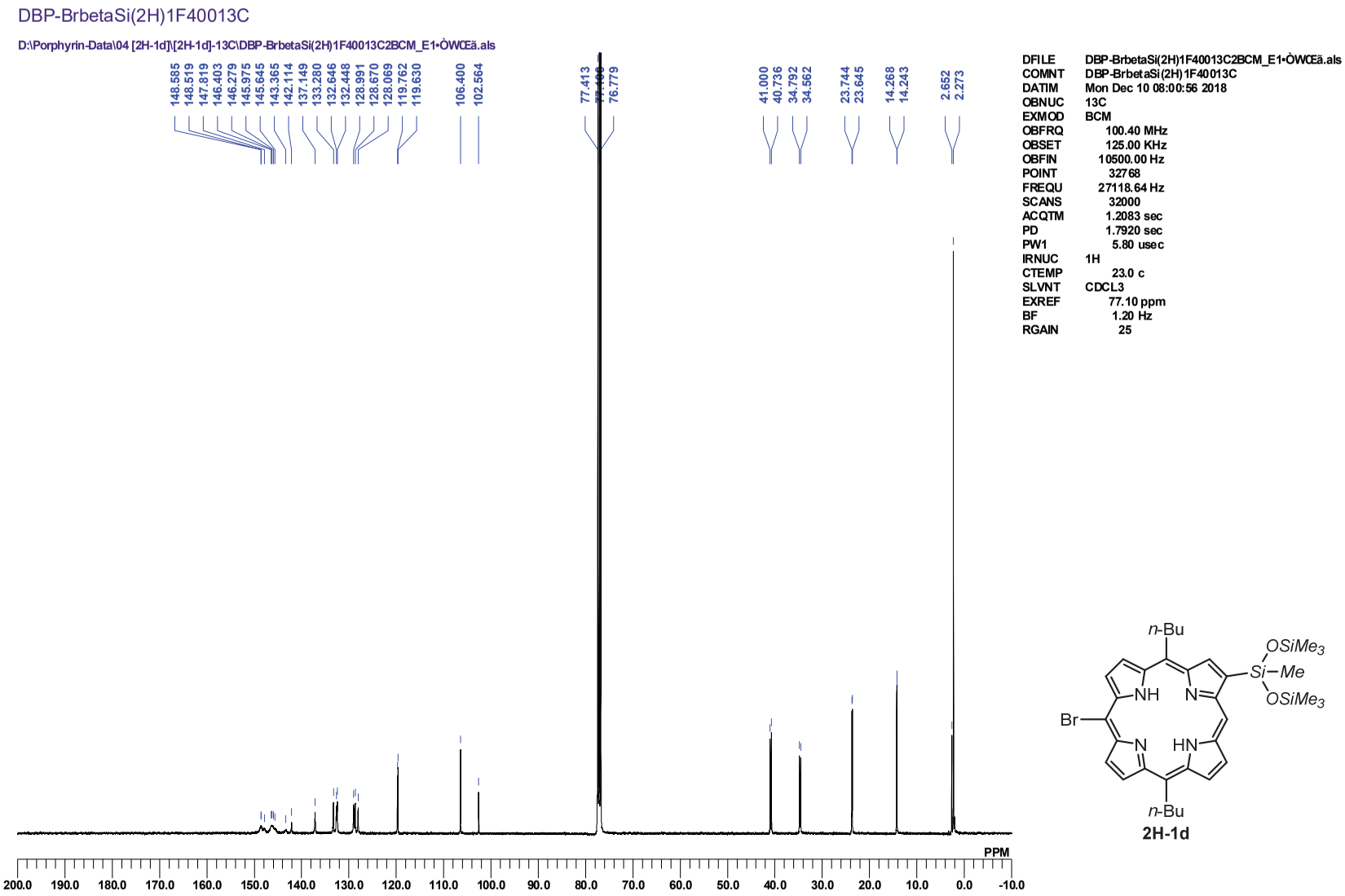
2H-1d


auto
D:\Porphyrin-Data\04 [2H-1d]\[2H-1d]-1H\DBP-BrbetaSi(2H)1F400-ÒWŒã1H.als
10.331
9.688
9.685
9.673
9.658
9.646
9.408
9.396
9.386
9.374
9.309
9.297
9.290
9.278
7.240
4.924
4.905
4.884
4.763
4.744
4.723
2.545
2.525
2.507
2.489
2.468
2.458
2.439
2.420
2.402
2.381
1.860
1.842
1.824
1.804
1.786
1.768
1.749
1.731
1.188
1.170
1.151
1.127
1.109
1.090
0.981
0.352
-2.973
18.2900
DFILE DBP-BrbetaSi(2H)1F400-ÒWŒã1H.als
COMNT auto
DATIM Fri Dec 07 19:23:36 2018
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.80 usec
IRNUC 1H
CTEMP 21.7 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 1.20 Hz
RGAIN 15
1.0000
2.0681
2.0193
2.0653
2.1244
2.1773
2.0627
2.0167
PPM
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5 -3.0 -3.5 -4.0


n-Bu
OSiMe3
Si
Me
OSiMe3
NH
N
Br
N
HN
n-Bu

2H-1d

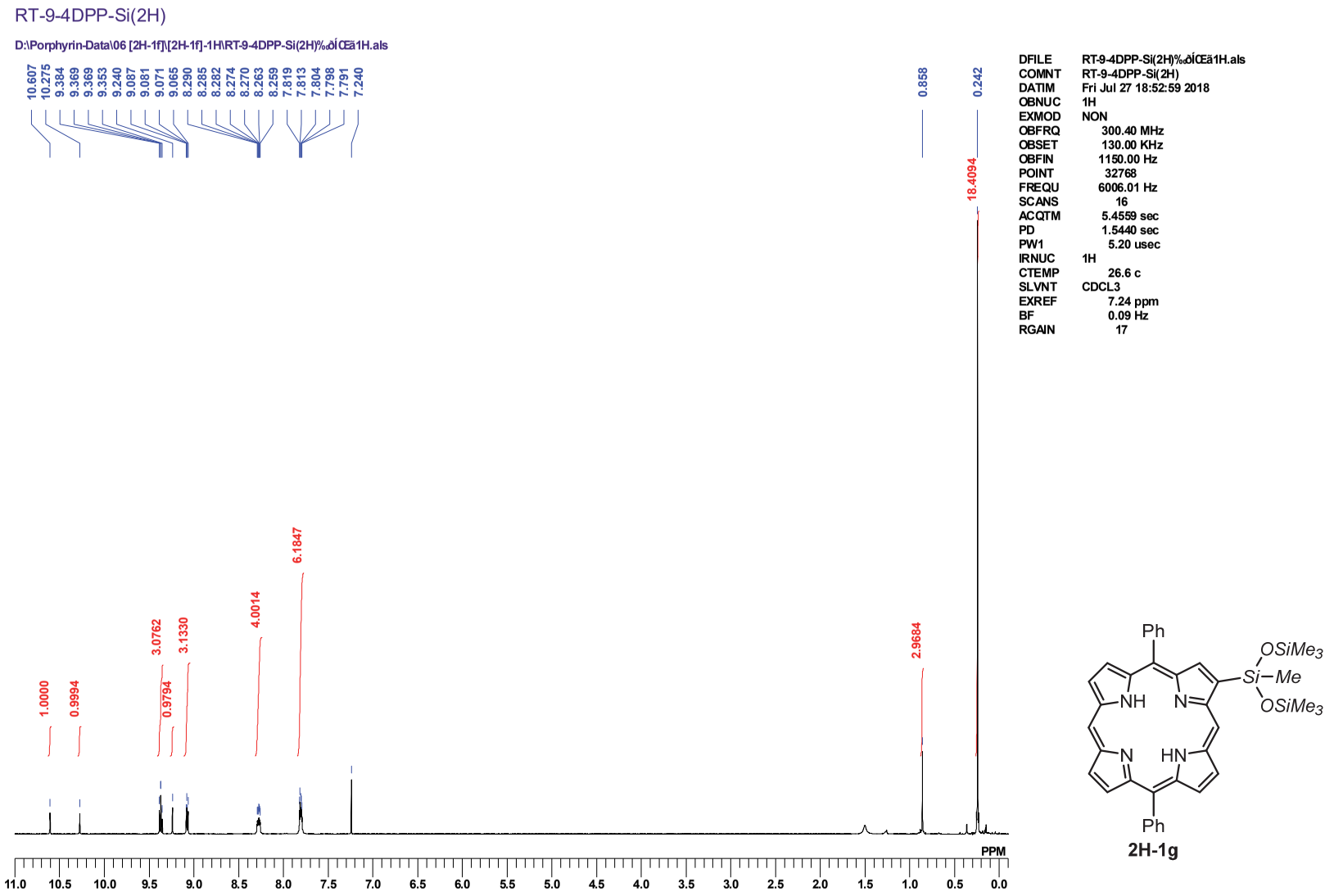
2H-1d


DBP-BrbetaSi(2H)1F40013C
D:\Porphyrin-Data\04 [2H-1d]\[2H-1d]-13C\DBP-BrbetaSi(2H)1F40013C2BCM_E1•ÒWŒã.als
148.585
148.519
147.819
146.403
146.279
145.975
145.645
143.365
142.114
137.149
133.280
132.646
132.448
128.991
128.670
128.069
119.762
119.630
106.400
102.564
77.413
77.100
76.779
41.000
40.736
34.792
34.562
23.744
23.645
14.268
14.243
2.652
2.273
DFILE DBP-BrbetaSi(2H)1F40013C2BCM_E1•ÒWŒã.als
COMNT DBP-BrbetaSi(2H)1F40013C
DATIM Mon Dec 10 08:00:56 2018
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 32000
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRNUC 1H
CTEMP 23.0 c
SLVNT CDCL3
EXREF 77.10 ppm
BF 1.20 Hz
RGAIN 25
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0

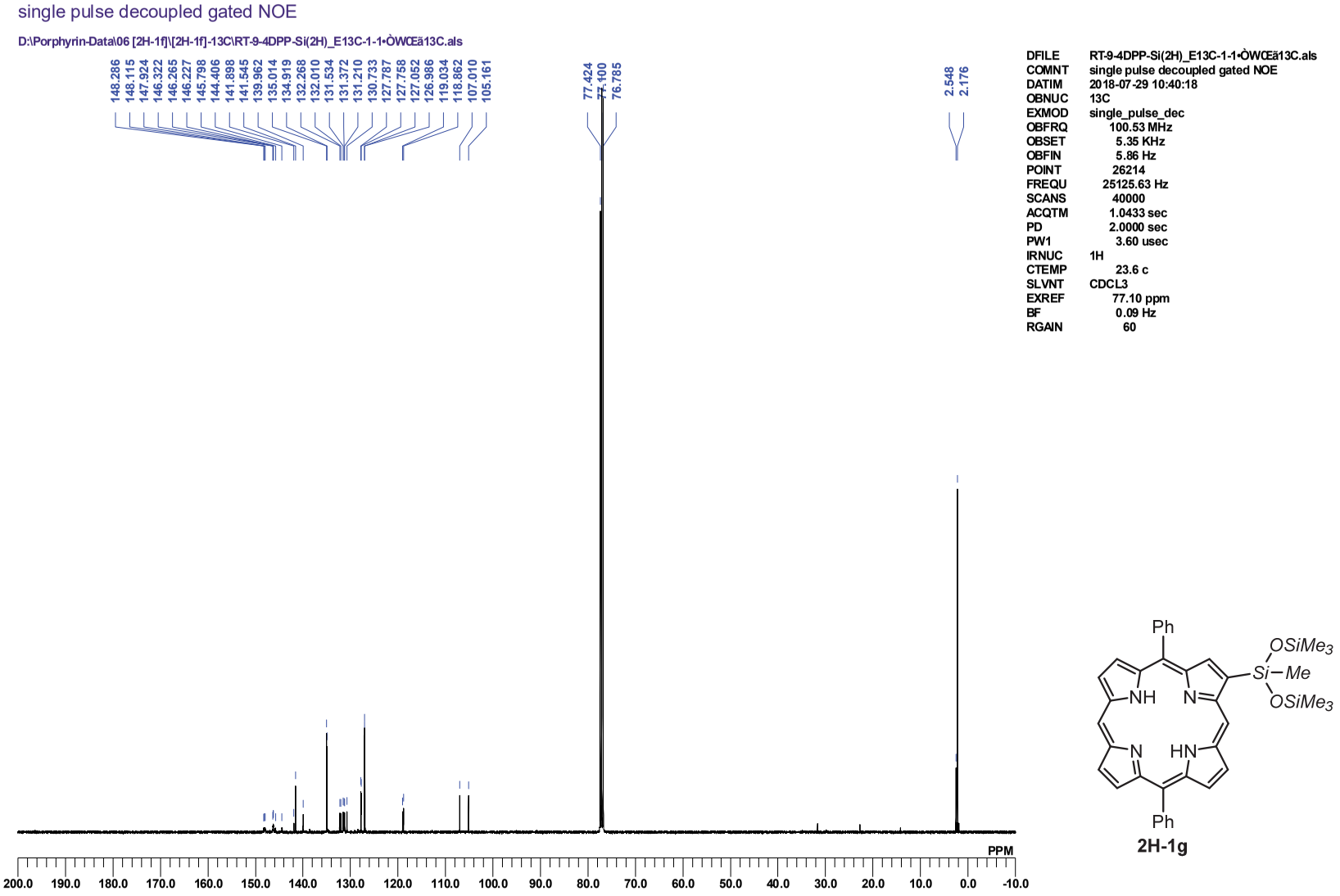
n-Bu
OSiMe3
Si–Me
OSiMe3
NH
N
Br
N
HN
n-Bu

2H-1d

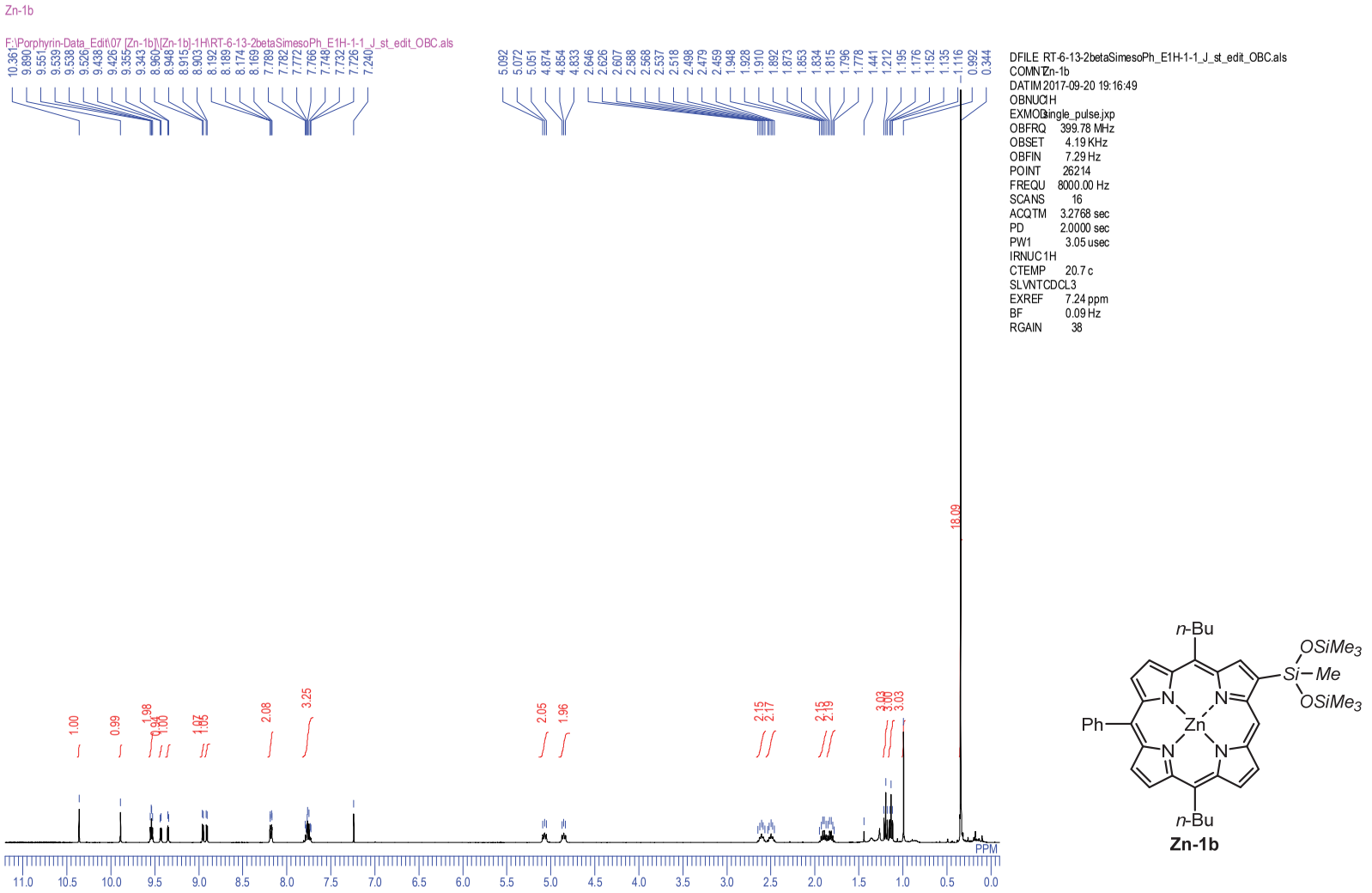
2H-1g


RT-9-4DPP-Si(2H)
D:\Porphyrin-Data\06 [2H-1f]\[2H-1f]-1H\RT-9-4DPP-Si(2H)‰ôÍŒã1H.als
10.607
10.275
9.384
9.369
9.369
9.353
9.240
9.087
9.081
9.071
9.065
8.290
8.285
8.282
8.274
8.270
8.263
8.259
7.819
7.813
7.804
7.798
7.791
7.240
0.858
0.242
18.4094
DFILE RT-9-4DPP-Si(2H)‰ôÍŒã1H.als
COMNT RT-9-4DPP-Si(2H)
DATIM Fri Jul 27 18:52:59 2018
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.00 Hz
POINT 32768
FREQU 6006.01 Hz
SCANS 16
ACQTM 5.4559 sec
PD 1.5440 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 26.6 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.09 Hz
RGAIN 17
1.0000
0.9994
3.0762
0.9794
3.1330
4.0014
6.1847
2.9684
PPM
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Ph
OSiMe3
Si–Me
OSiMe3
NH
N
N
HN
Ph
2H-1g

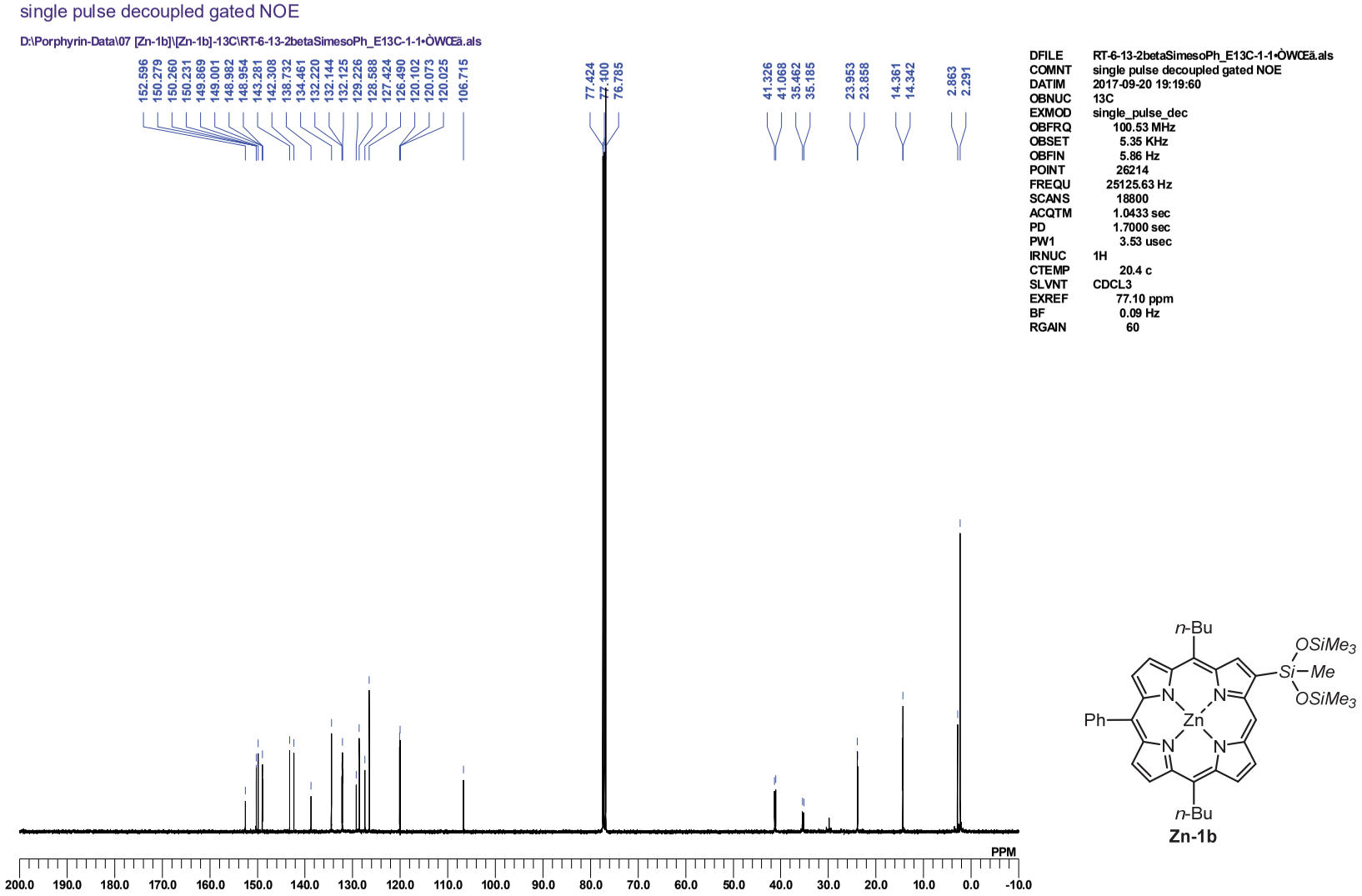
2H-1g


single pulse decoupled gated NOE
D:\Porphyrin-Data\06 [2H-1f]\[2H-1f]-13C\RT-9-4DPP-Si(2H)_E13C-1-1•ÒWŒä13C.als
148.286
148.115
147.924
146.322
146.265
146.227
145.798
144.406
141.898
141.545
139.962
135.014
134.919
132.268
132.010
131.534
131.372
131.210
130.733
127.787
127.758
127.052
126.986
119.034
118.862
107.010
105.161
77.424
77.100
76.785
2.548
2.176
DFILE RT-9-4DPP-Si(2H)_E13C-1-1•ÒWŒä13C.als
COMNT single pulse decoupled gated NOE
DATIM 2018-07-29 10:40:18
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 40000
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.60 usec
IRNUC 1H
CTEMP 23.6 c
SLVNT CDCL3
EXREF 77.10 ppm
BF 0.09 Hz
RGAIN 60
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0
Ph
OSiMe3
Si—Me
OSiMe3
NH
N
N
HN
Ph
2H-1g

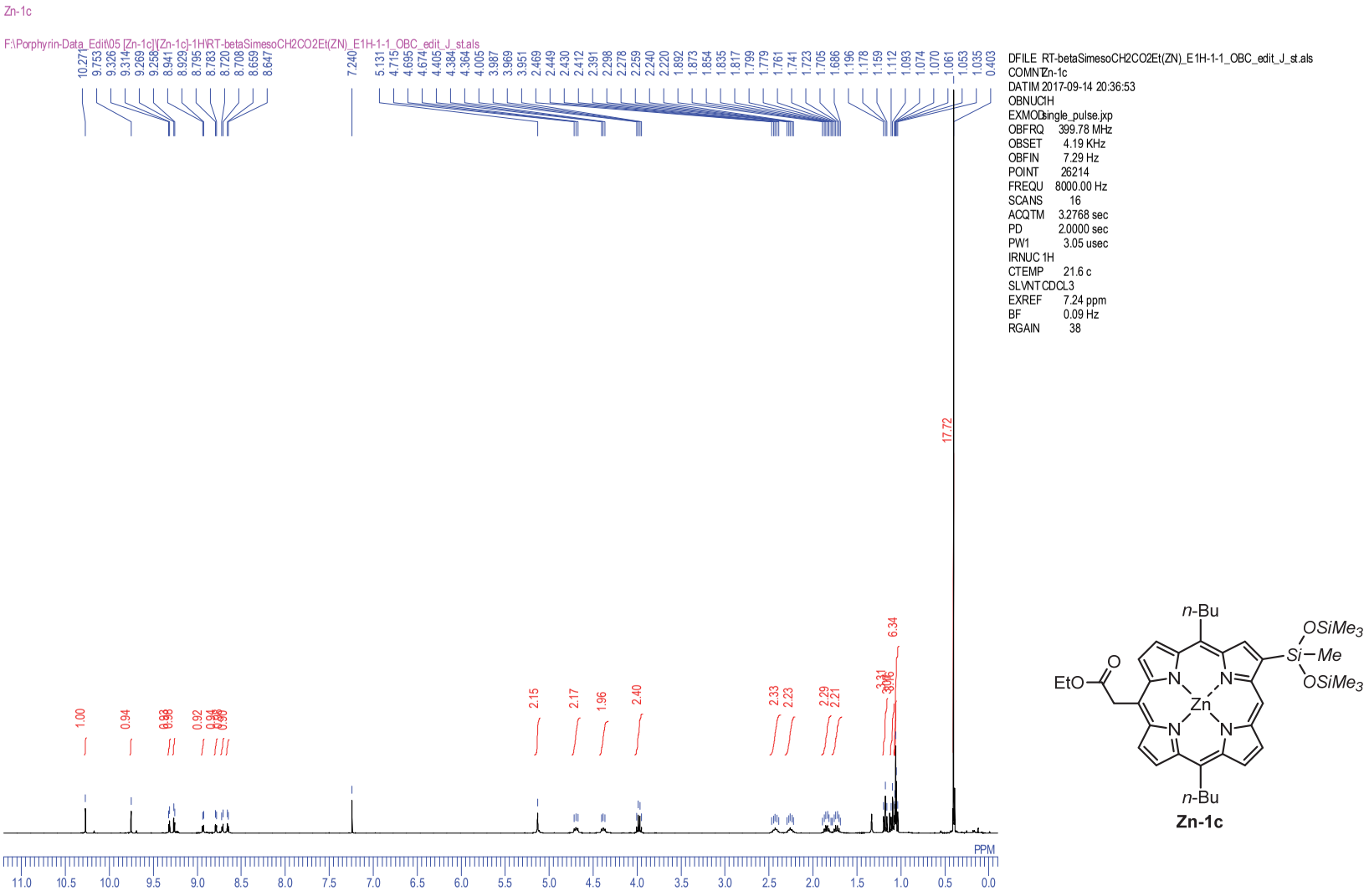
Zn-1b


Zn-1b
F:\Porphyrin-Data_Edit\07 [Zn-1b]\[Zn-1b]-1H\RT-6-13-2betaSimesoPh_E1H-1-1_J_st_edit_OBC.als
DFILE RT-6-13-2betaSimesoPh_E1H-1-1_J_st_edit_OBC.als
COMNTZn-1b
DATIM 2017-09-20 19:16:49
OBNUCH
EXMODsingle_pulse.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 26214
FREQU 8000.00 Hz
SCANS 16
ACQTM 3.2768 sec
PD 2.0000 sec
PW1 3.05 usec
IRNUC1H
CTEMP 20.7 c
SLVNTCDCL3
EXREF 7.24 ppm
BF 0.09 Hz
RGAIN 38
PPM
n-Bu
OSiMe3
Si
Me
OSiMe3
Ph
Zn
N
n-Bu
Zn-1b

Zn-1b


single pulse decoupled gated NOE
D:\Porphyrin-Data\07 [Zn-1b]\[Zn-1b]-13C\RT-6-13-2betaSimesoPh_E13C-1-1•ÒWŒã.als
152.596
150.279
150.260
150.231
149.869
149.001
148.982
148.954
143.281
142.308
138.732
134.461
132.220
132.144
132.125
129.226
128.588
127.424
126.490
120.102
120.073
120.025
106.715
77.424
77.100
76.785
41.326
41.068
35.462
35.185
23.953
23.858
14.361
14.342
2.863
2.291
DFILE RT-6-13-2betaSimesoPh_E13C-1-1•ÒWŒã.als
COMNT single pulse decoupled gated NOE
DATIM 2017-09-20 19:19:60
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 18800
ACQTM 1.0433 sec
PD 1.7000 sec
PW1 3.53 usec
IRNUC 1H
CTEMP 20.4 c
SLVNT CDCL3
EXREF 77.10 ppm
BF 0.09 Hz
RGAIN 60
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0
n-Bu
OSiMe3
Si–Me
OSiMe3
Ph
Zn
N
n-Bu
Zn-1b

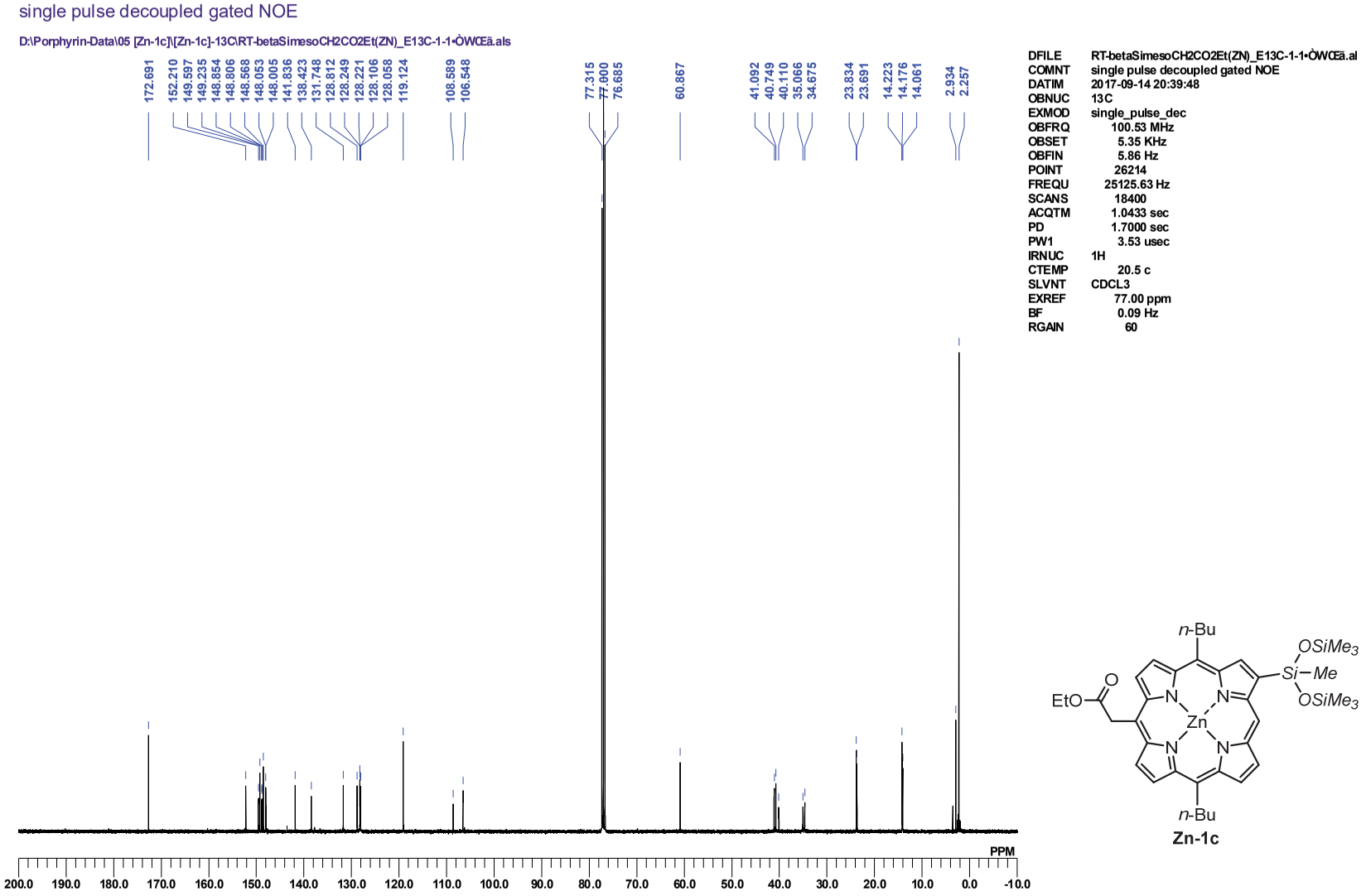
Zn-1c


Zn-1c
F:\Porphyrin-Data_Edit\05 [Zn-1c]\[Zn-1c]-1H\RT-betaSimesoCH2CO2Et(ZN)_E1H-1-1_OBC_edit_J_st.als
DFILE RT-betaSimesoCH2CO2Et(ZN)_E1H-1-1_OBC_edit_J_st.als
COMNTZn-1c
DATIM 2017-09-14 20:36:53
OBNUCH
EXMODsingle_pulse.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 26214
FREQU 8000.00 Hz
SCANS 16
ACQTM 3.2768 sec
PD 2.0000 sec
PW1 3.05 usec
IRNUC 1H
CTEMP 21.6 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.09 Hz
RGAIN 38
PPM

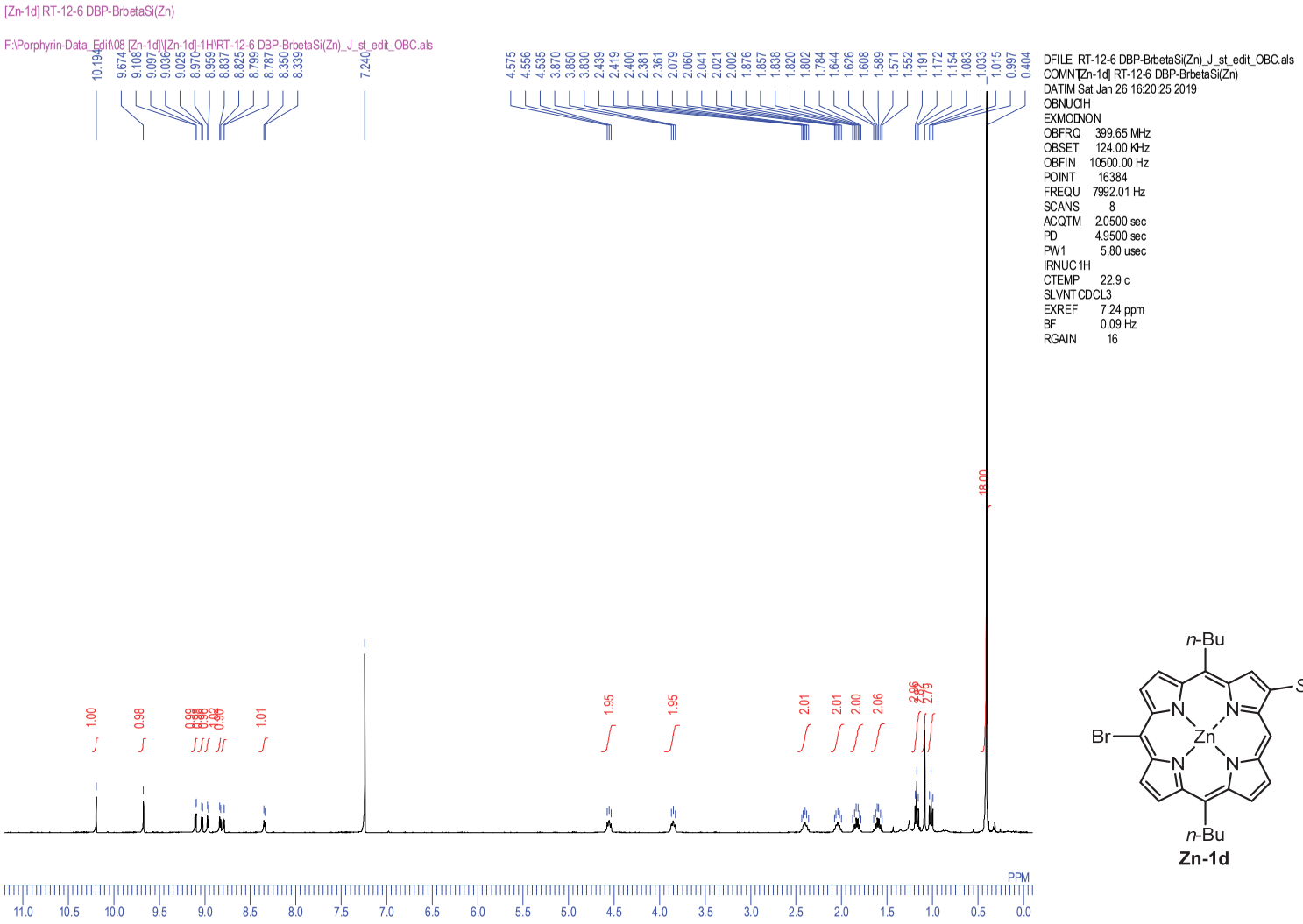
n-Bu
OSiMe3
Si–Me
OSiMe3
EtO
O
N
N
Zn
N
N
n-Bu

Zn-1c

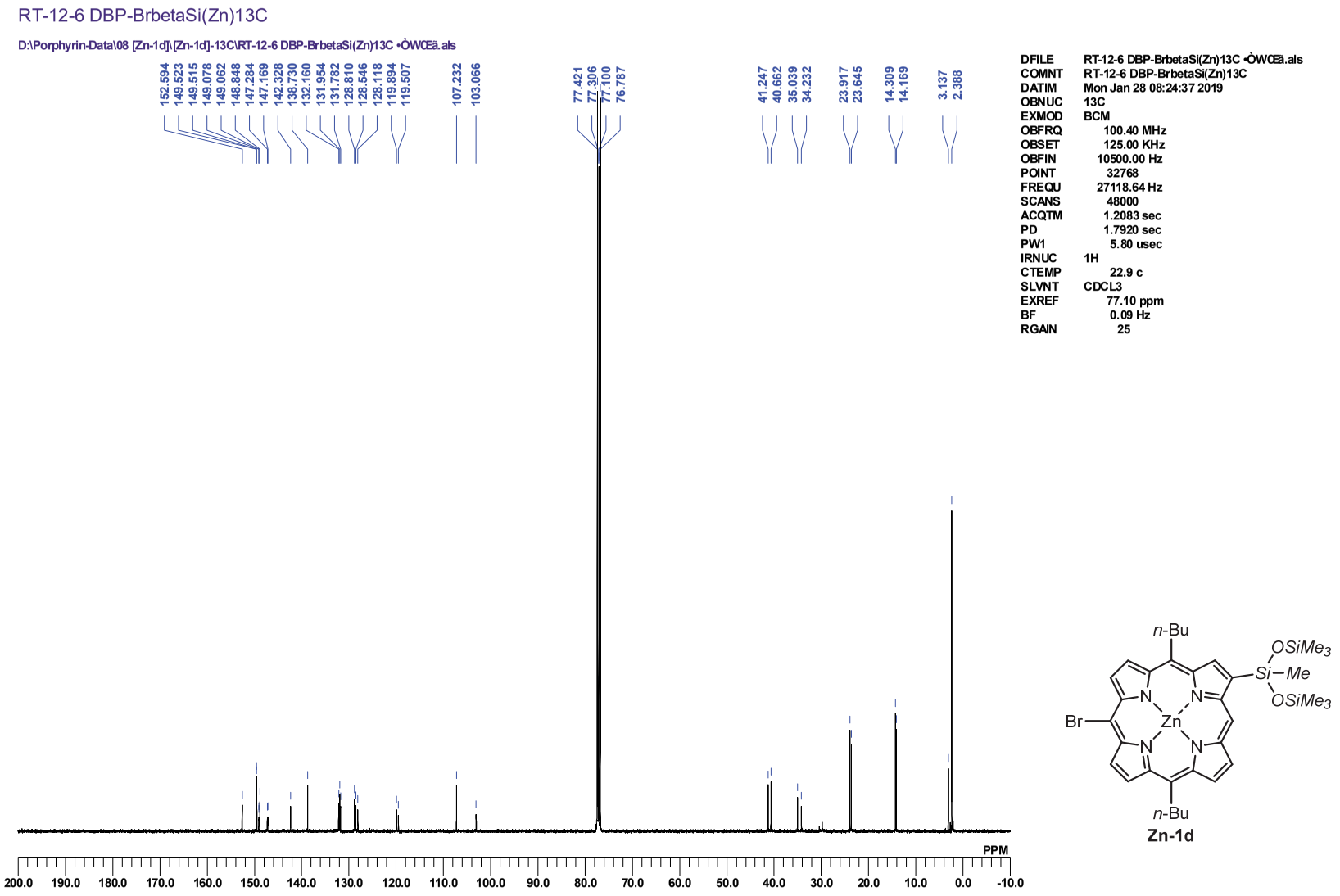
Zn-1c


single pulse decoupled gated NOE
D:\Porphyrin-Data\05 [Zn-1c]\[Zn-1c]-13C\RT-betaSimesoCH2CO2Et(ZN)_E13C-1-1-ÒWŒã.als
172.691
152.210
149.597
149.235
148.854
148.806
148.568
148.053
148.005
141.836
138.423
131.748
128.812
128.249
128.221
128.106
128.058
119.124
108.589
106.548
77.315
77.000
76.685
60.867
41.092
40.749
40.110
35.066
34.675
23.834
23.691
14.223
14.176
14.061
2.934
2.257
DFILE RT-betaSimesoCH2CO2Et(ZN)_E13C-1-1-ÒWŒã.al
COMNT single pulse decoupled gated NOE
DATIM 2017-09-14 20:39:48
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 18400
ACQTM 1.0433 sec
PD 1.7000 sec
PW1 3.53 usec
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.09 Hz
RGAIN 60
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0
n-Bu
OSiMe3
Si–Me
OSiMe3
EtO
O
N
N
Zn
N
N
n-Bu
Zn-1c

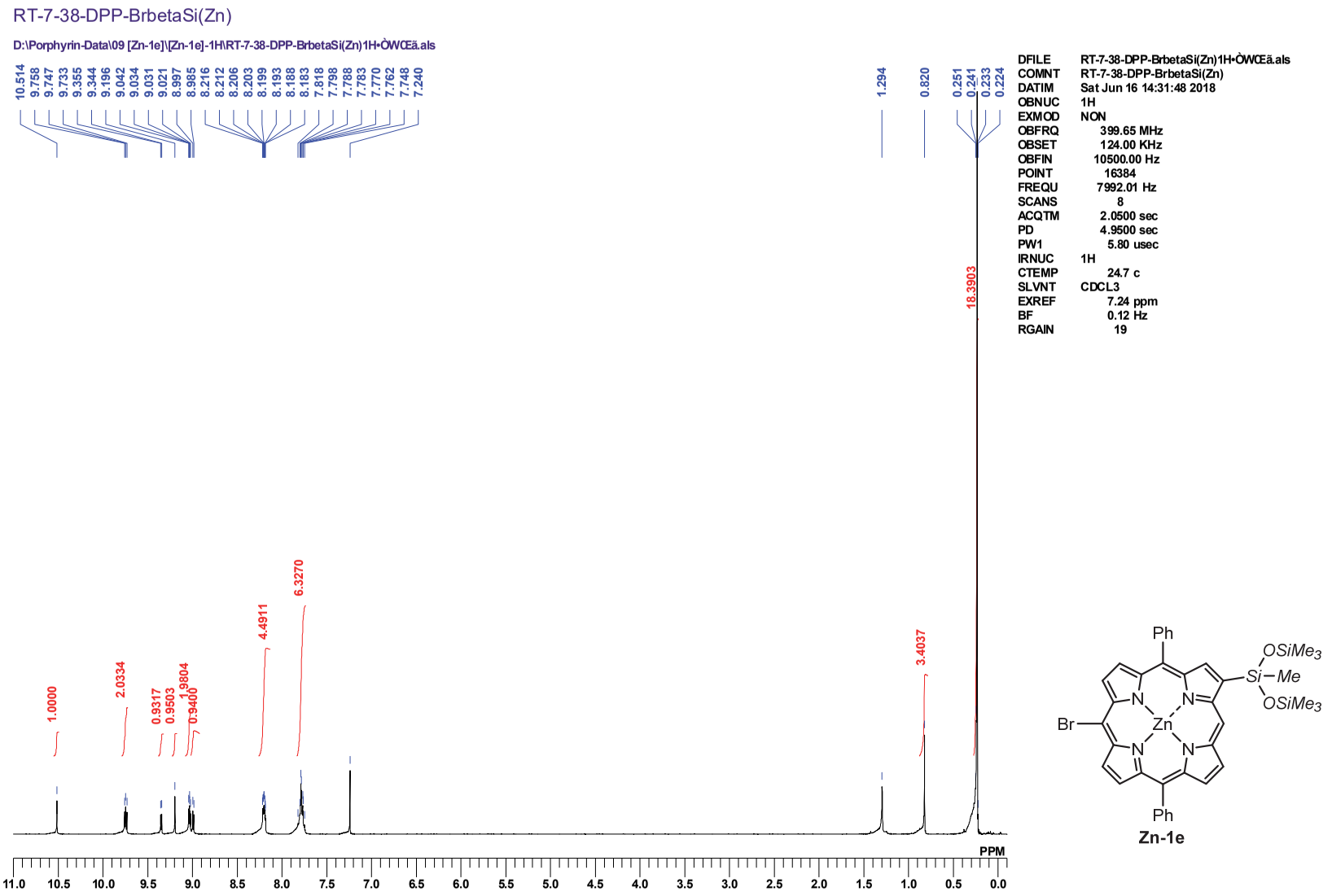
Zn-1d


[Zn-1d] RT-12-6 DBP-BrbetaSi(Zn)
F:\Porphyrin-Data_Edit\08 [Zn-1d]\[Zn-1d]-1H\RT-12-6 DBP-BrbetaSi(Zn)_J_st_edit_OBC.als
DFILE RT-12-6 DBP-BrbetaSi(Zn)_J_st_edit_OBC.als
COMNT [Zn-1d] RT-12-6 DBP-BrbetaSi(Zn)
DATIM Sat Jan 26 16:20:25 2019
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.80 usec
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.09 Hz
RGAIN 16
PPM
n-Bu
OSiMe3
Si
Me
OSiMe3
Br
Zn
N
n-Bu
Zn-1d

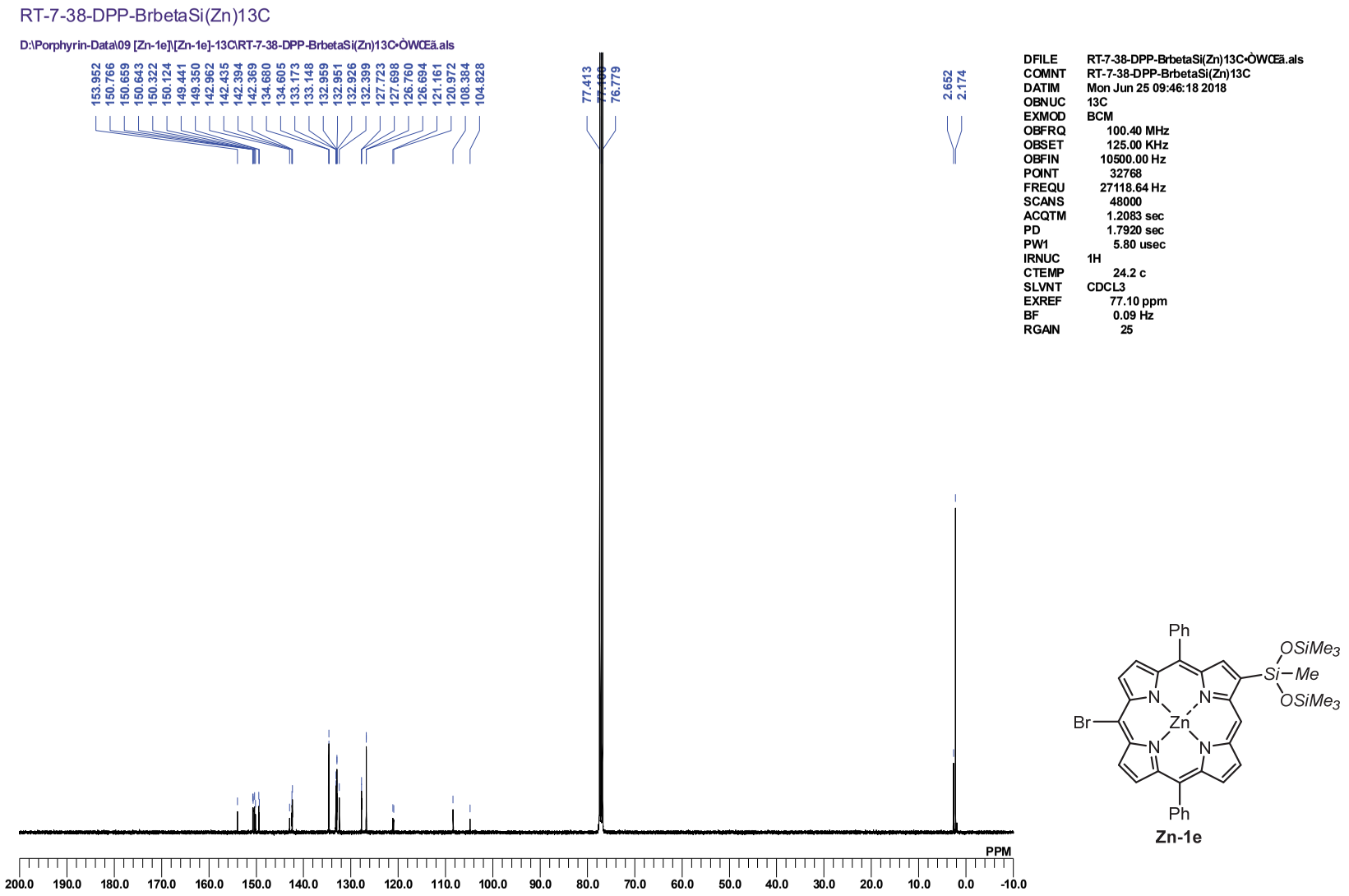
Zn-1d


RT-12-6 DBP-BrbetaSi(Zn)13C
D:\Porphyrin-Data\08 [Zn-1d]\[Zn-1d]-13C\RT-12-6 DBP-BrbetaSi(Zn)13C •ÒWŒEã.als
152.594
149.523
149.515
149.078
149.062
148.848
147.284
147.169
142.328
138.730
132.160
131.954
131.782
128.810
128.546
128.118
119.894
119.507
107.232
103.066
77.421
77.306
77.100
76.787
41.247
40.662
35.039
34.232
23.917
23.645
14.309
14.169
3.137
2.388
DFILE RT-12-6 DBP-BrbetaSi(Zn)13C •ÒWŒEã.als
COMNT RT-12-6 DBP-BrbetaSi(Zn)13C
DATIM Mon Jan 28 08:24:37 2019
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 48000
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 77.10 ppm
BF 0.09 Hz
RGAIN 25
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0
n-Bu
OSiMe3
Si
Me
OSiMe3
Br
N
N
Zn
N
N
n-Bu
Zn-1d

Zn-1e

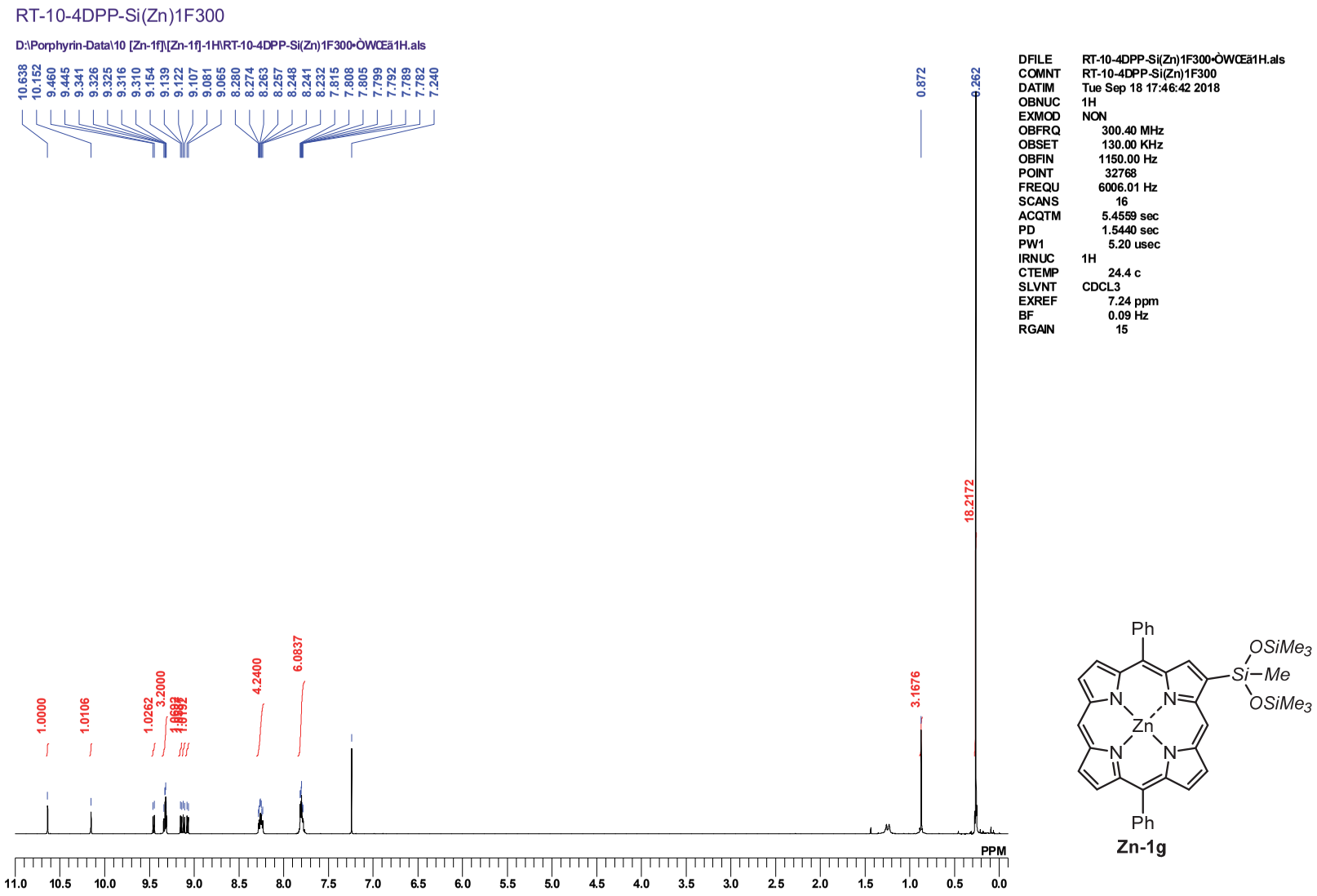

RT-7-38-DPP-BrbetaSi(Zn)
D:\Porphyrin-Data\09 [Zn-1e]\[Zn-1e]-1H\RT-7-38-DPP-BrbetaSi(Zn)1H•ÒWŒÈä.als
10.514 9.758 9.747 9.733 9.355 9.344 9.196 9.042 9.034 9.031 9.021 8.997 8.985 8.216 8.212 8.206 8.203 8.199 8.193 8.188 8.183 7.818 7.798 7.788 7.783 7.770 7.762 7.748 7.240
1.294 0.820 0.251 0.241 0.233 0.224
DFILE RT-7-38-DPP-BrbetaSi(Zn)1H•ÒWŒÈä.als
COMNT RT-7-38-DPP-BrbetaSi(Zn)
DATIM Sat Jun 16 14:31:48 2018
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.80 usec
IRNUC 1H
CTEMP 24.7 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 19
18.3903
6.3270
4.4911
3.4037
2.0334
1.9804
1.0000
0.9317
0.9503
0.9400
PPM
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Ph
OSiMe3
Si
Me
OSiMe3
N
N
Zn
N
N
Br
Ph
Zn-1e

Zn-1e

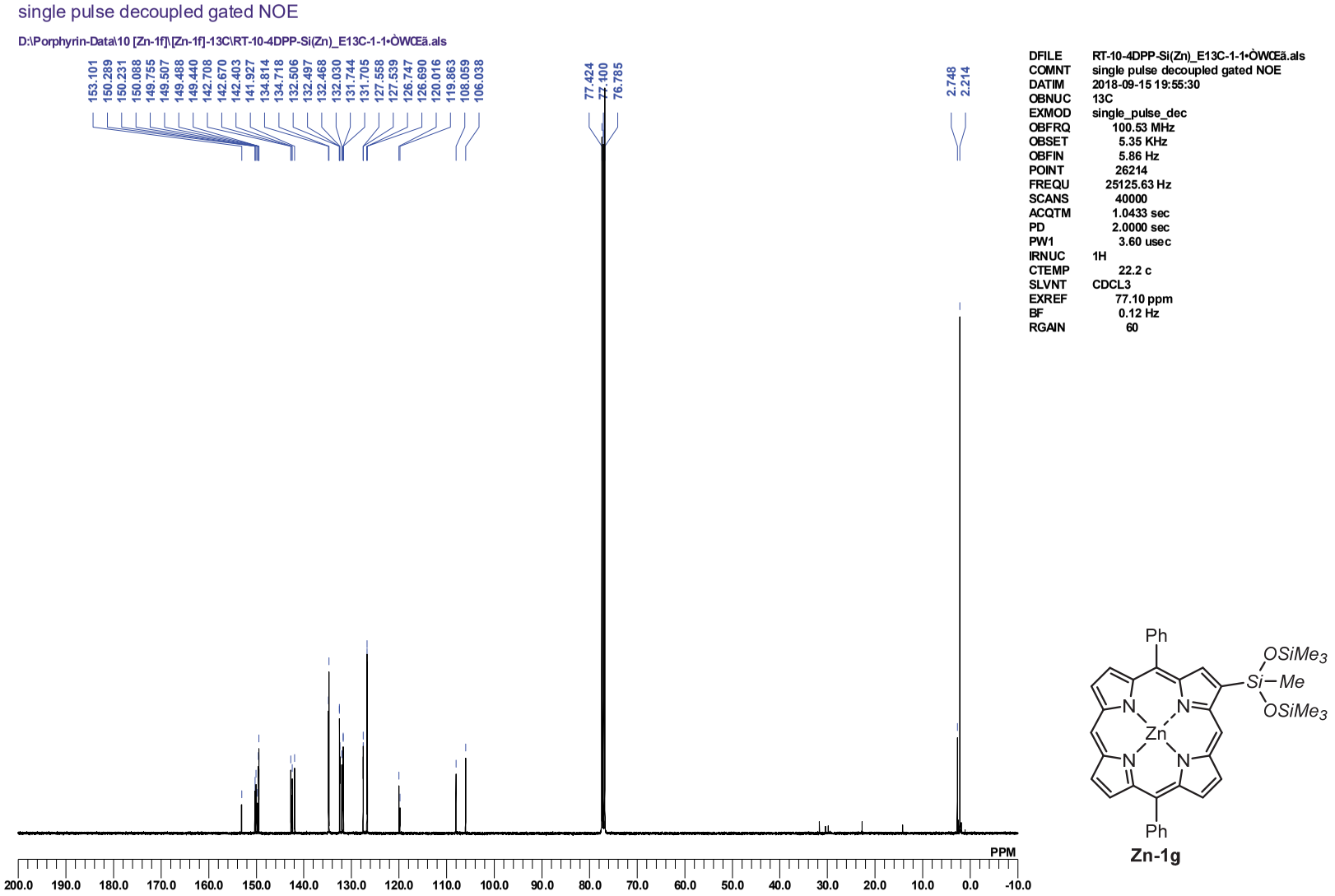

RT-7-38-DPP-BrbetaSi(Zn)13C
D:\Porphyrin-Data\09 [Zn-1e]\[Zn-1e]-13C\RT-7-38-DPP-BrbetaSi(Zn)13C•ÒWŒä.als
153.952
150.766
150.659
150.643
150.322
150.124
149.441
149.350
142.962
142.435
142.394
142.369
134.680
134.605
133.173
133.148
132.959
132.951
132.926
132.399
127.723
127.698
126.760
126.694
121.161
120.972
108.384
104.828
77.413
77.100
76.779
2.652
2.174
DFILE RT-7-38-DPP-BrbetaSi(Zn)13C•ÒWŒä.als
COMNT RT-7-38-DPP-BrbetaSi(Zn)13C
DATIM Mon Jun 25 09:46:18 2018
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 48000
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRNUC 1H
CTEMP 24.2 c
SLVNT CDCL3
EXREF 77.10 ppm
BF 0.09 Hz
RGAIN 25
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0
Ph
OSiMe3
Si–Me
OSiMe3
N
N
Br
Zn
N
N
Ph

Zn-1e

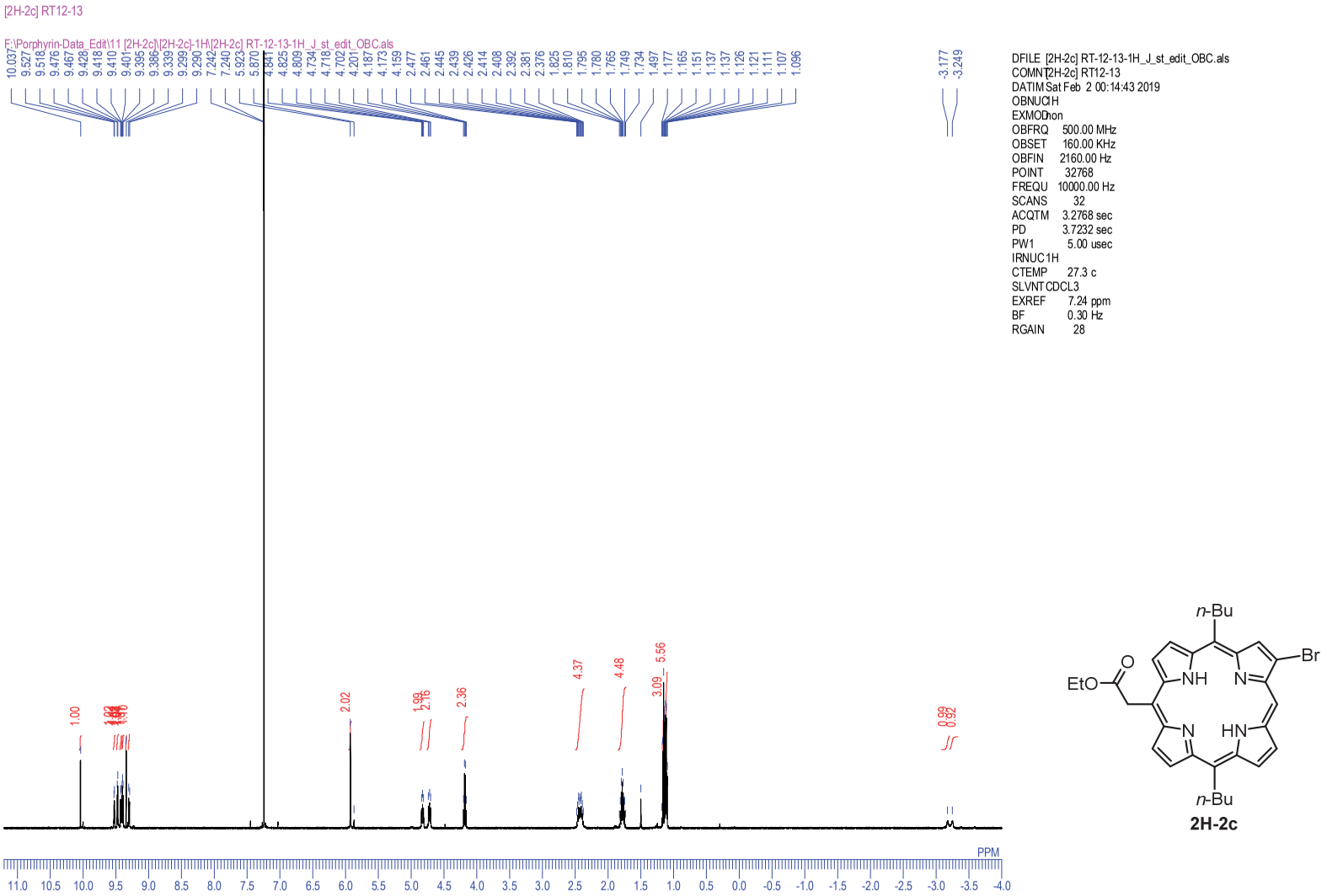
Zn-1g


RT-10-4DPP-Si(Zn)1F300
D:\Porphyrin-Data\10 [Zn-1f]\[Zn-1f]-1H\RT-10-4DPP-Si(Zn)1F300•ÒWŒã1H.als
10.638 10.152 9.460 9.445 9.341 9.326 9.325 9.316 9.310 9.154 9.139 9.122 9.107 9.081 9.065 8.280 8.274 8.263 8.257 8.248 8.241 8.232 7.815 7.808 7.805 7.799 7.792 7.789 7.782 7.240
0.872
9.262
DFILE RT-10-4DPP-Si(Zn)1F300•ÒWŒã1H.als
COMNT RT-10-4DPP-Si(Zn)1F300
DATIM Tue Sep 18 17:46:42 2018
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.00 Hz
POINT 32768
FREQU 6006.01 Hz
SCANS 16
ACQTM 5.4559 sec
PD 1.5440 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 24.4 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.09 Hz
RGAIN 15
18.2172
1.0000
1.0106
1.0262
3.2000
4.2400
6.0837
3.1676
PPM
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Ph
OSiMe3
Si–Me
OSiMe3
N
N
Zn
N
N
Ph
Zn-1g

Zn-1g


single pulse decoupled gated NOE
D:\Porphyrin-Data\10 [Zn-1f]\[Zn-1f]-13C\RT-10-4DPP-Si(Zn)_E13C-1-1•ÒWŒä.als
153.101
150.289
150.231
150.088
149.755
149.507
149.488
149.440
142.708
142.670
142.403
141.927
134.814
134.718
132.506
132.497
132.468
132.030
131.744
131.705
127.558
127.539
126.747
126.690
120.016
119.863
108.059
106.038
77.424
77.100
76.785
2.748
2.214
DFILE RT-10-4DPP-Si(Zn)_E13C-1-1•ÒWŒä.als
COMNT single pulse decoupled gated NOE
DATIM 2018-09-15 19:55:30
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 40000
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.60 usec
IRNUC 1H
CTEMP 22.2 c
SLVNT CDCL3
EXREF 77.10 ppm
BF 0.12 Hz
RGAIN 60
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0
Ph
OSiMe3
Si
Me
OSiMe3
N
N
Zn
N
N
Ph
Zn-1g

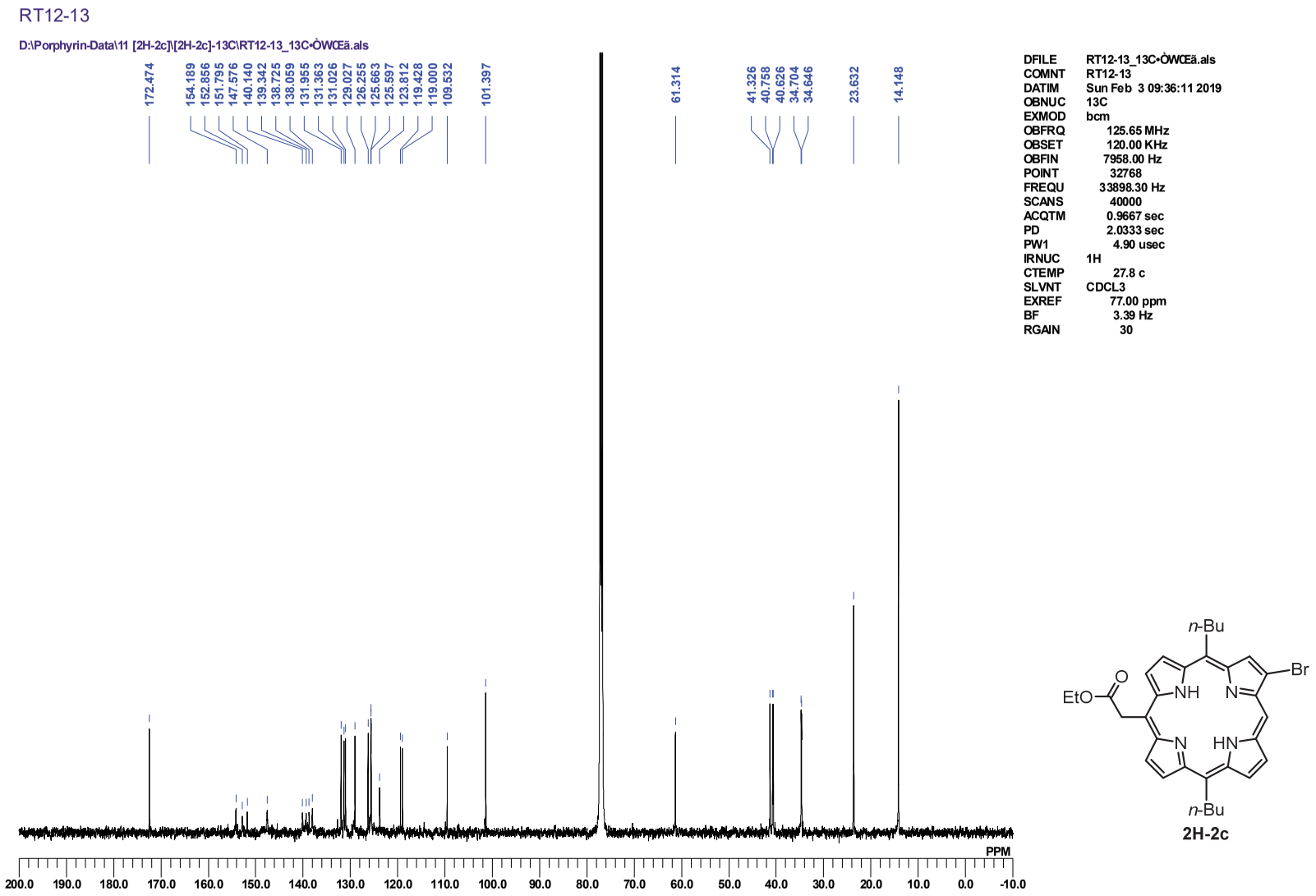
2H-2c


[2H-2c] RT12-13
F:\Porphyrin-Data_Edit\11 [2H-2c]\[2H-2c]-1H\[2H-2c] RT-12-13-1H_J_st_edit_OBC.als
DFILE [2H-2c] RT-12-13-1H_J_st_edit_OBC.als
COMNT [2H-2c] RT12-13
DATIM Sat Feb 2 00:14:43 2019
OBNUC 1H
EXMOD non
OBFRQ 500.00 MHz
OBSET 160.00 KHz
OBFIN 2160.00 Hz
POINT 32768
FREQU 10000.00 Hz
SCANS 32
ACQTM 3.2768 sec
PD 3.7232 sec
PW1 5.00 usec
IRNUC 1H
CTEMP 27.3 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.30 Hz
RGAIN 28
PPM

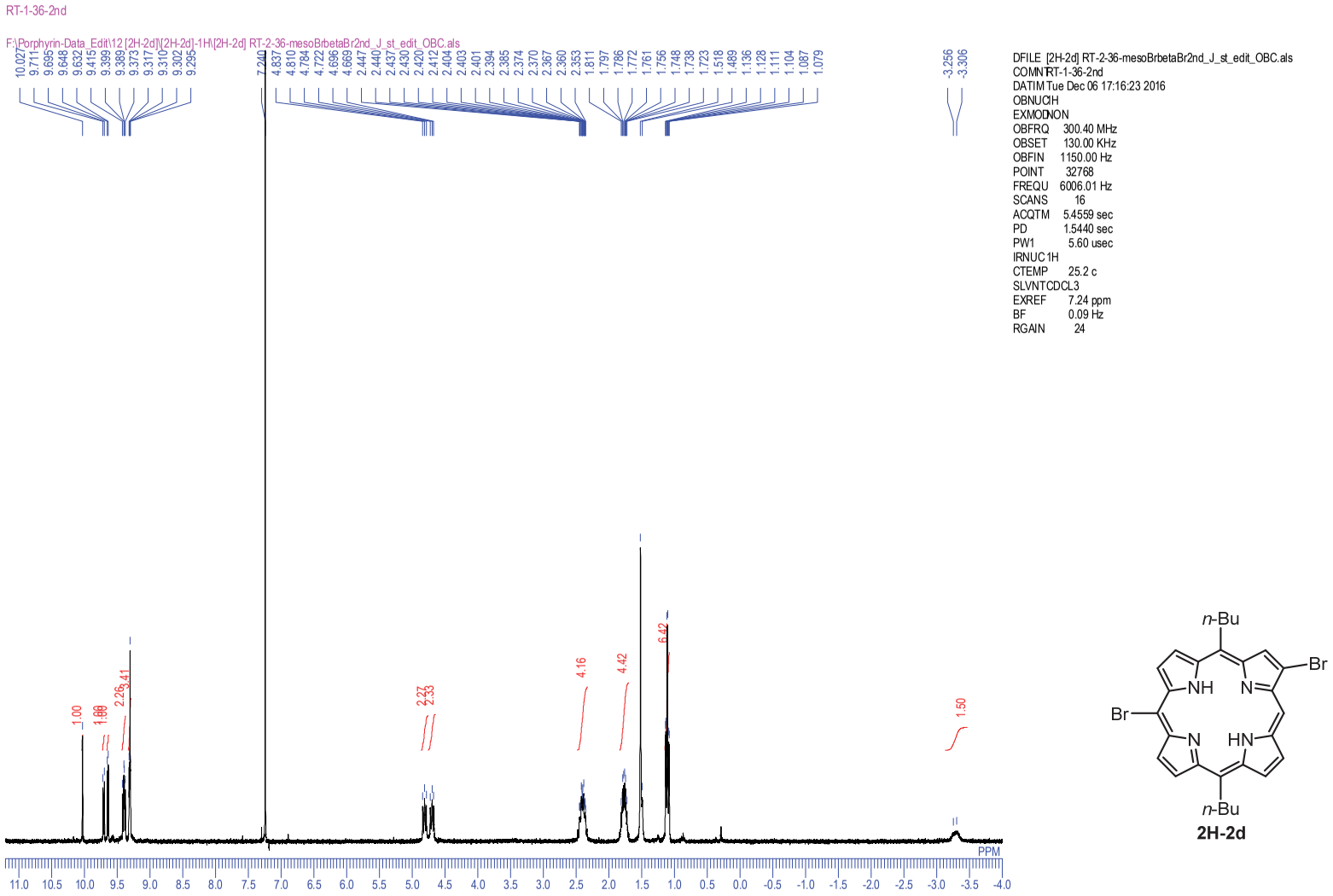
n-Bu
Br
O
EtO
NH
N
N
HN
n-Bu

2H-2c

2H-2c

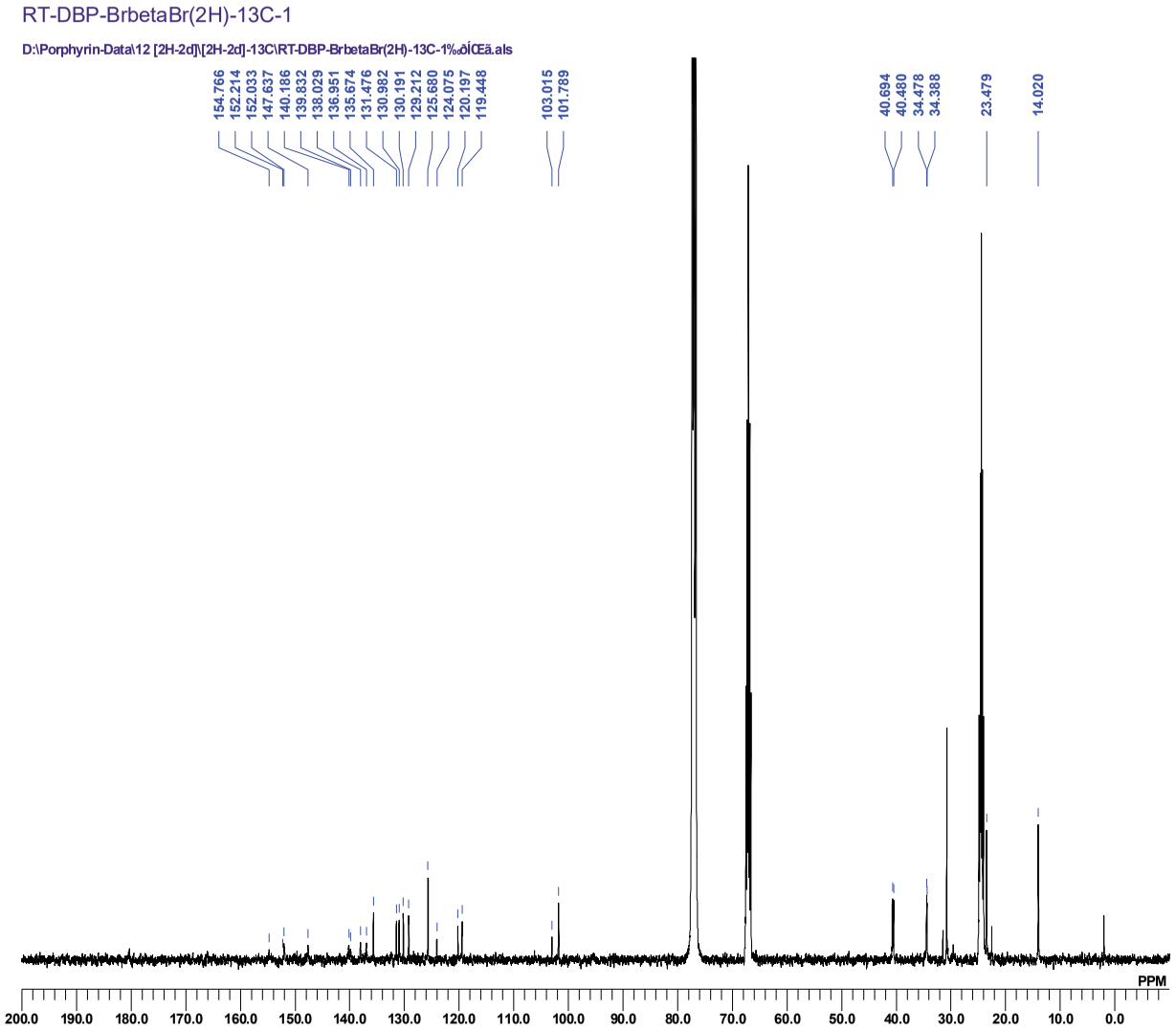

RT12-13
D:\Porphyrin-Data\11 [2H-2c]\[2H-2c]-13C\RT12-13_13C•ÒWŒã.als
172.474
154.189
152.856
151.795
147.576
140.140
139.342
138.725
138.059
131.955
131.363
131.026
129.027
126.255
125.663
125.597
123.812
119.428
119.000
109.532
101.397
61.314
41.326
40.758
40.626
34.704
34.646
23.632
14.148
DFILE RT12-13_13C•ÒWŒã.als
COMNT RT12-13
DATIM Sun Feb 3 09:36:11 2019
OBNUC 13C
EXMOD bcm
OBFRQ 125.65 MHz
OBSET 120.00 KHz
OBFIN 7958.00 Hz
POINT 32768
FREQU 33898.30 Hz
SCANS 40000
ACQTM 0.9667 sec
PD 2.0333 sec
PW1 4.90 usec
IRNUC 1H
CTEMP 27.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 3.39 Hz
RGAIN 30
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0
n-Bu
Br
EtO
O
NH
N
N
HN
n-Bu
2H-2c

2H-2d

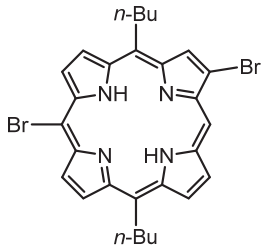

RT-1-36-2nd
F:\Porphyrin-Data_Edit\12 [2H-2d]\[2H-2d]-1H\[2H-2d] RT-2-36-mesoBrbetaBr2nd_J_st_edit_OBC.als
DFILE [2H-2d] RT-2-36-mesoBrbetaBr2nd_J_st_edit_OBC.als
COMNT RT-1-36-2nd
DATIM Tue Dec 06 17:16:23 2016
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.00 Hz
POINT 32768
FREQU 6006.01 Hz
SCANS 16
ACQTM 5.4559 sec
PD 1.5440 sec
PW1 5.60 usec
IRNUC 1H
CTEMP 25.2 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.09 Hz
RGAIN 24
PPM
n-Bu
Br
NH
N
Br
N
HN
n-Bu

2H-2d

2H-2d

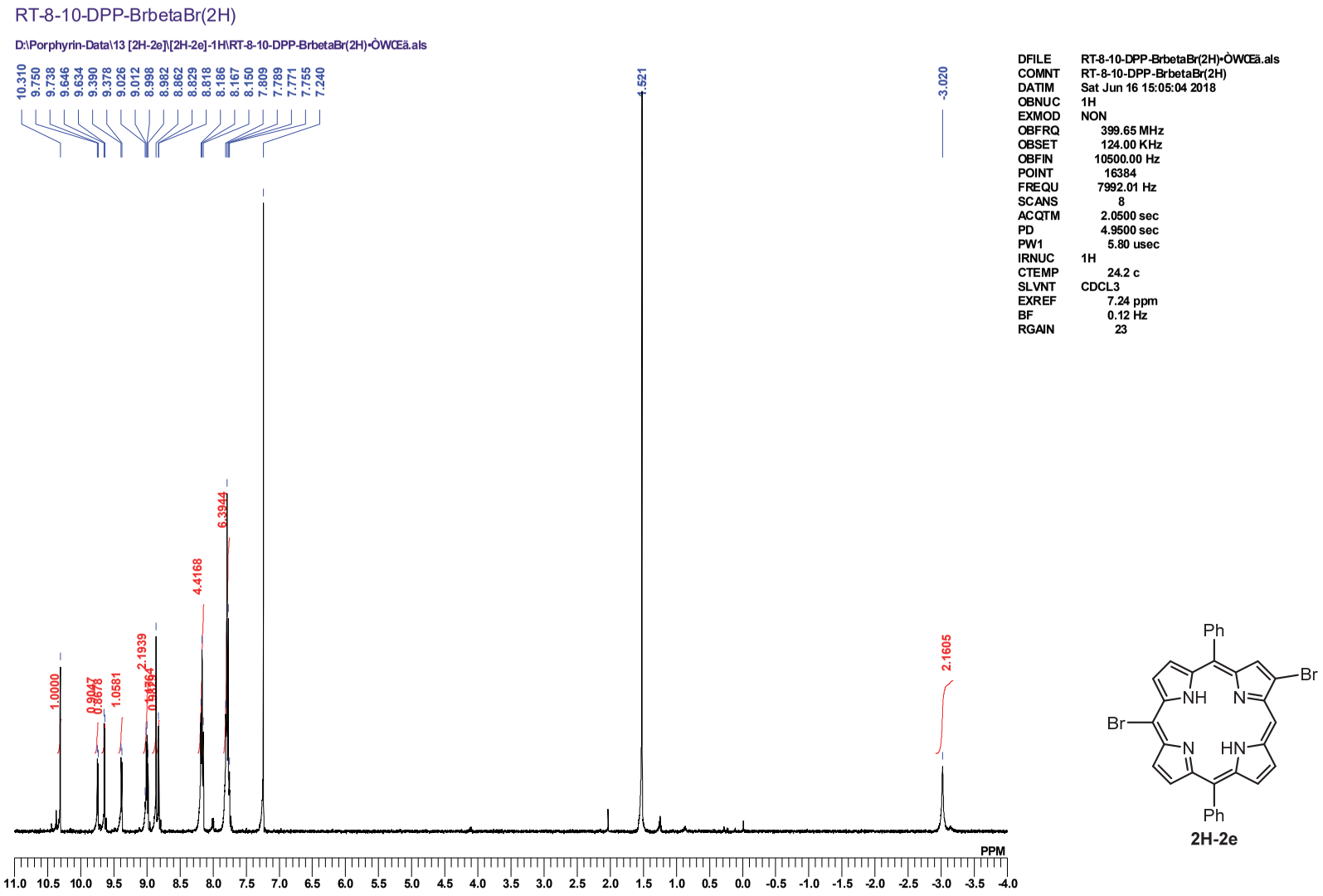


DFILE	RT-DBP-BrbetaBr(2H)-13C-1‰ðÍŒã.als
COMNT	RT-DBP-BrbetaBr(2H)-13C-1
DATIM	Tue Feb 12 09:07:43 2019
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	52000
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.80 usec
IRNUC	1H
CTEMP	23.0 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	3.02 Hz
RGAIN	25



2H-2d

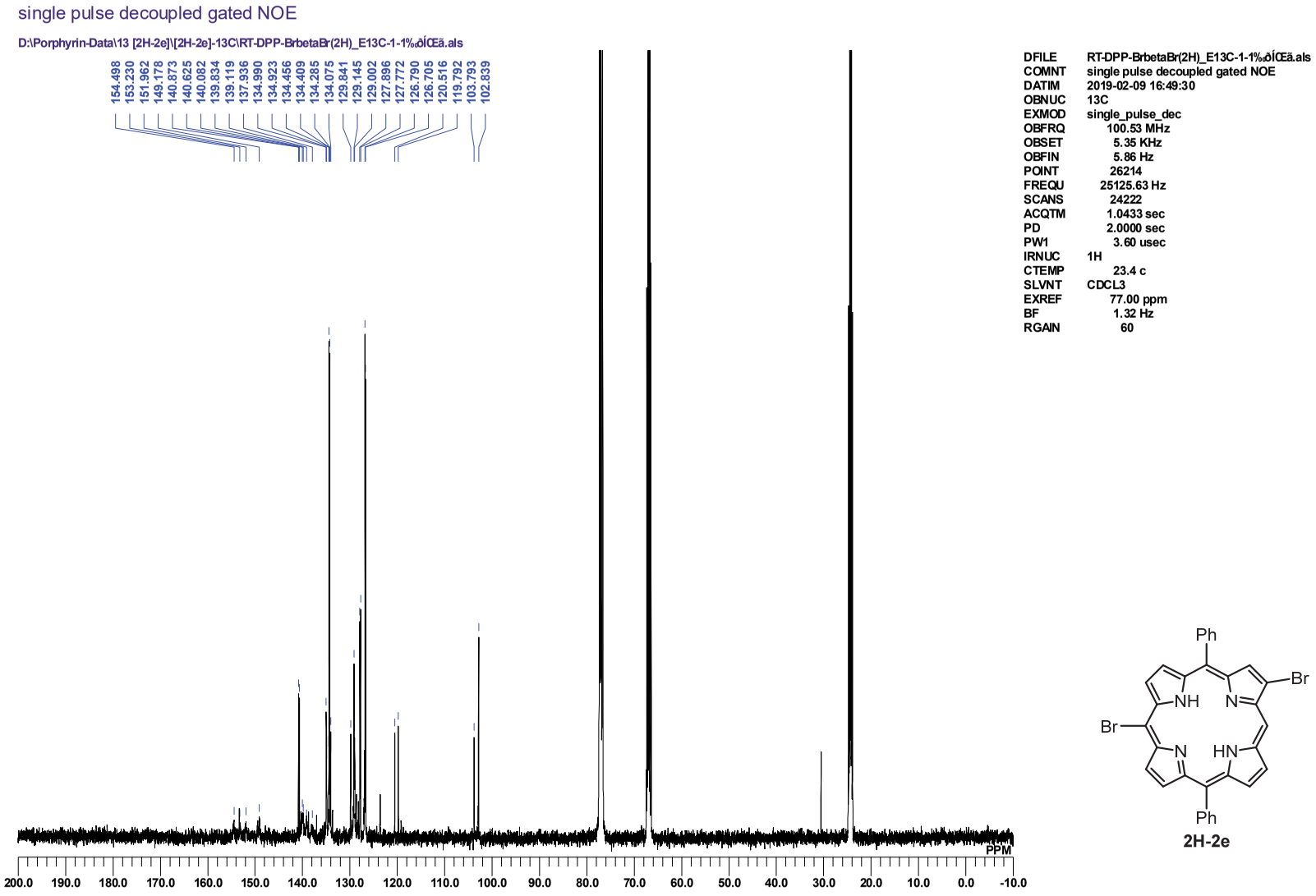
2H-2e


RT-8-10-DPP-BrbetaBr(2H)
D:\Porphyrin-Data\13 [2H-2e]\[2H-2e]-1H\RT-8-10-DPP-BrbetaBr(2H)•ÒWŒEã.als
10.310
9.750
9.738
9.646
9.634
9.390
9.378
9.026
9.012
8.998
8.982
8.862
8.829
8.818
8.186
8.167
8.150
7.809
7.789
7.771
7.755
7.240
4.521
-3.020
DFILE RT-8-10-DPP-BrbetaBr(2H)•ÒWŒEã.als
COMNT RT-8-10-DPP-BrbetaBr(2H)
DATIM Sat Jun 16 15:05:04 2018
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.80 usec
IRNUC 1H
CTEMP 24.2 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 23
6.3944
4.4168
2.1939
2.1605
1.0581
1.0000
0.9047
0.8678
PPM
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5 -3.0 -3.5 -4.0

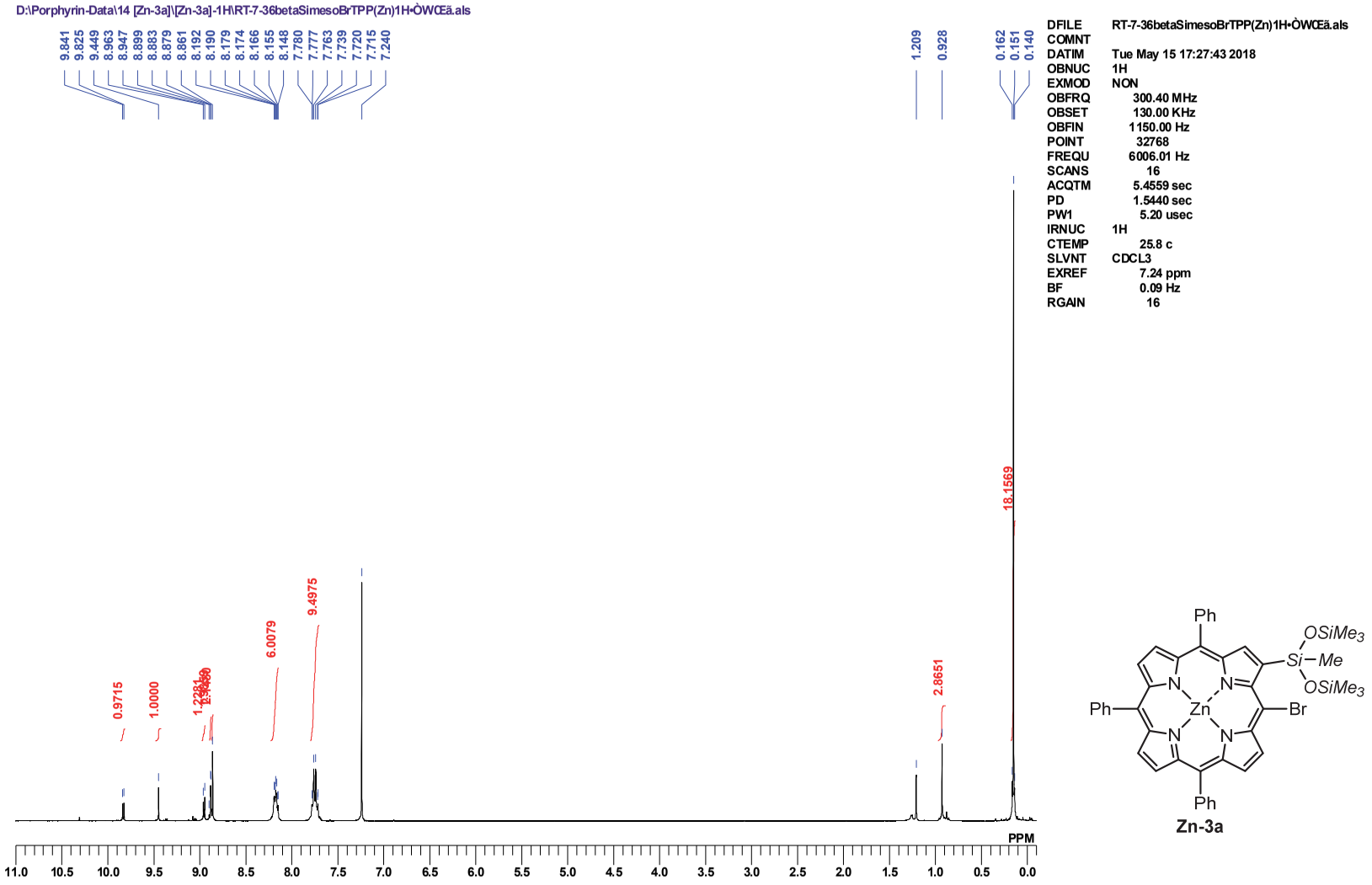
Ph
Br
NH
N
Br
N
HN
Ph

2H-2e

2H-2e

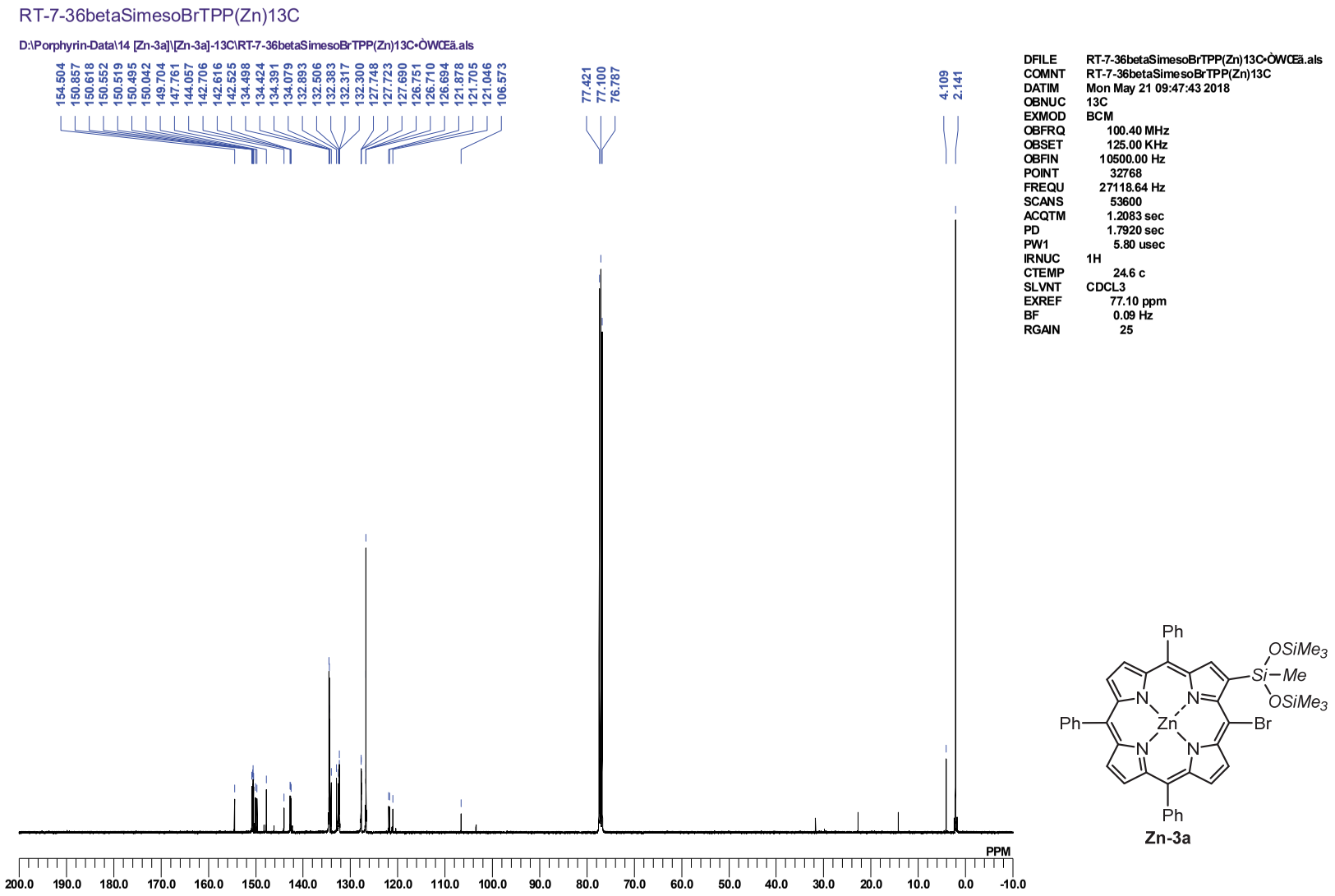

single pulse decoupled gated NOE
D:\Porphyrin-Data\13 [2H-2e]\[2H-2e]-13C\RT-DPP-BrbetaBr(2H)_E13C-1-1‰ÒÍŒä.als
154.498
153.230
151.962
149.178
140.873
140.625
140.082
139.834
139.119
137.936
134.990
134.923
134.456
134.409
134.285
134.075
129.841
129.145
129.002
127.896
127.772
126.790
126.705
120.516
119.792
103.793
102.839
DFILE RT-DPP-BrbetaBr(2H)_E13C-1-1‰ÒÍŒä.als
COMNT single pulse decoupled gated NOE
DATIM 2019-02-09 16:49:30
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 24222
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.60 usec
IRNUC 1H
CTEMP 23.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.32 Hz
RGAIN 60
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0
Ph
Br
NH
N
Br
N
HN
Ph
2H-2e

Zn-3a


D:\Porphyrin-Data\14 [Zn-3a]\[Zn-3a]-1H\RT-7-36betaSimesoBrTPP(Zn)1H•ÒWŒä.als
9.841
9.825
9.449
8.963
8.947
8.899
8.883
8.879
8.861
8.192
8.190
8.179
8.174
8.166
8.155
8.148
7.780
7.777
7.763
7.739
7.720
7.715
7.240
1.209
0.928
0.162
0.151
0.140
DFILE RT-7-36betaSimesoBrTPP(Zn)1H•ÒWŒä.als
COMNT
DATIM Tue May 15 17:27:43 2018
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.00 Hz
POINT 32768
FREQU 6006.01 Hz
SCANS 16
ACQTM 5.4559 sec
PD 1.5440 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 25.8 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.09 Hz
RGAIN 16
18.1569
9.4975
6.0079
2.8651
1.0000
0.9715
PPM
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Ph
OSiMe3
Si–Me
OSiMe3
Ph
N
N
Zn
N
N
Br
Ph

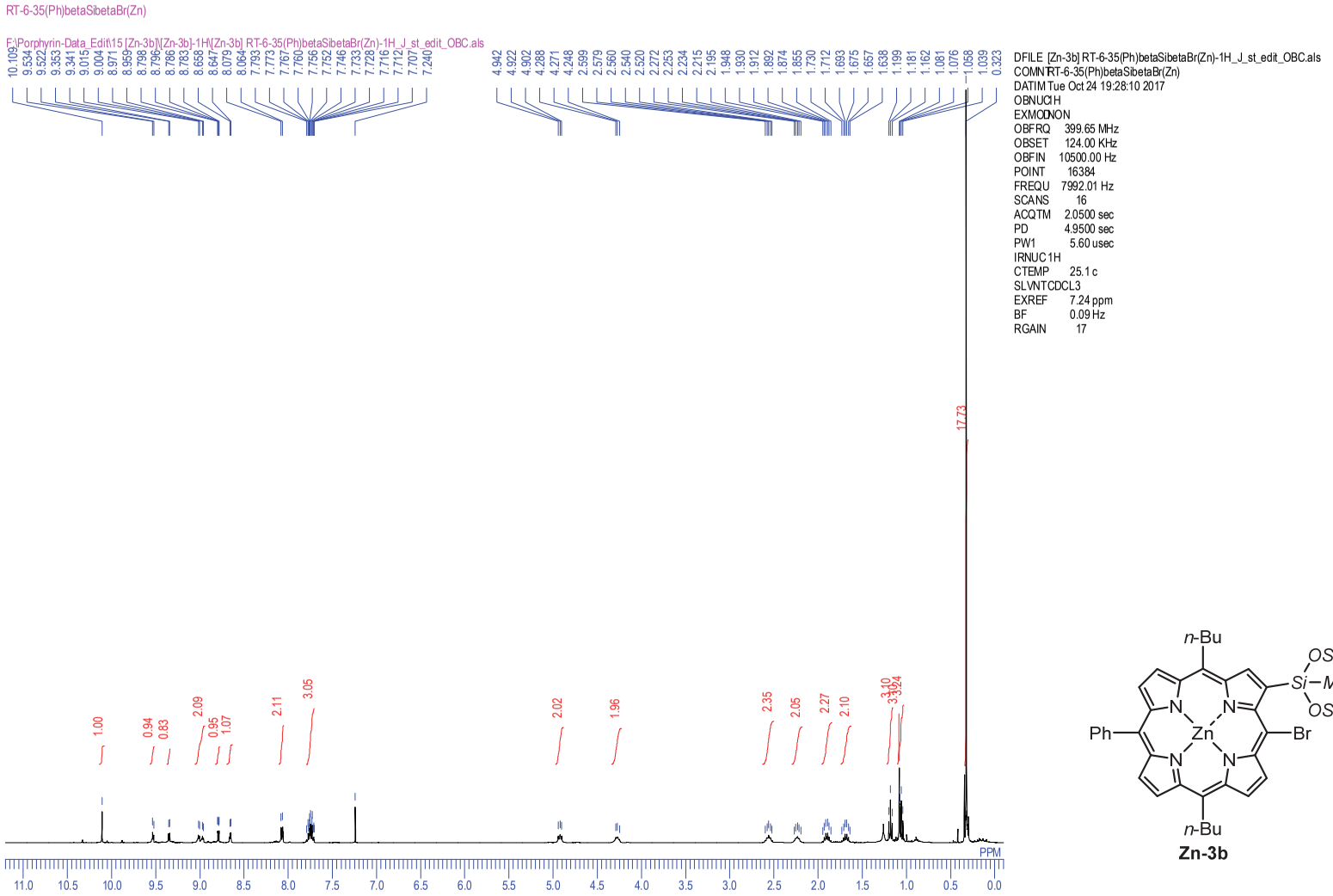
Zn-3a

Zn-3a

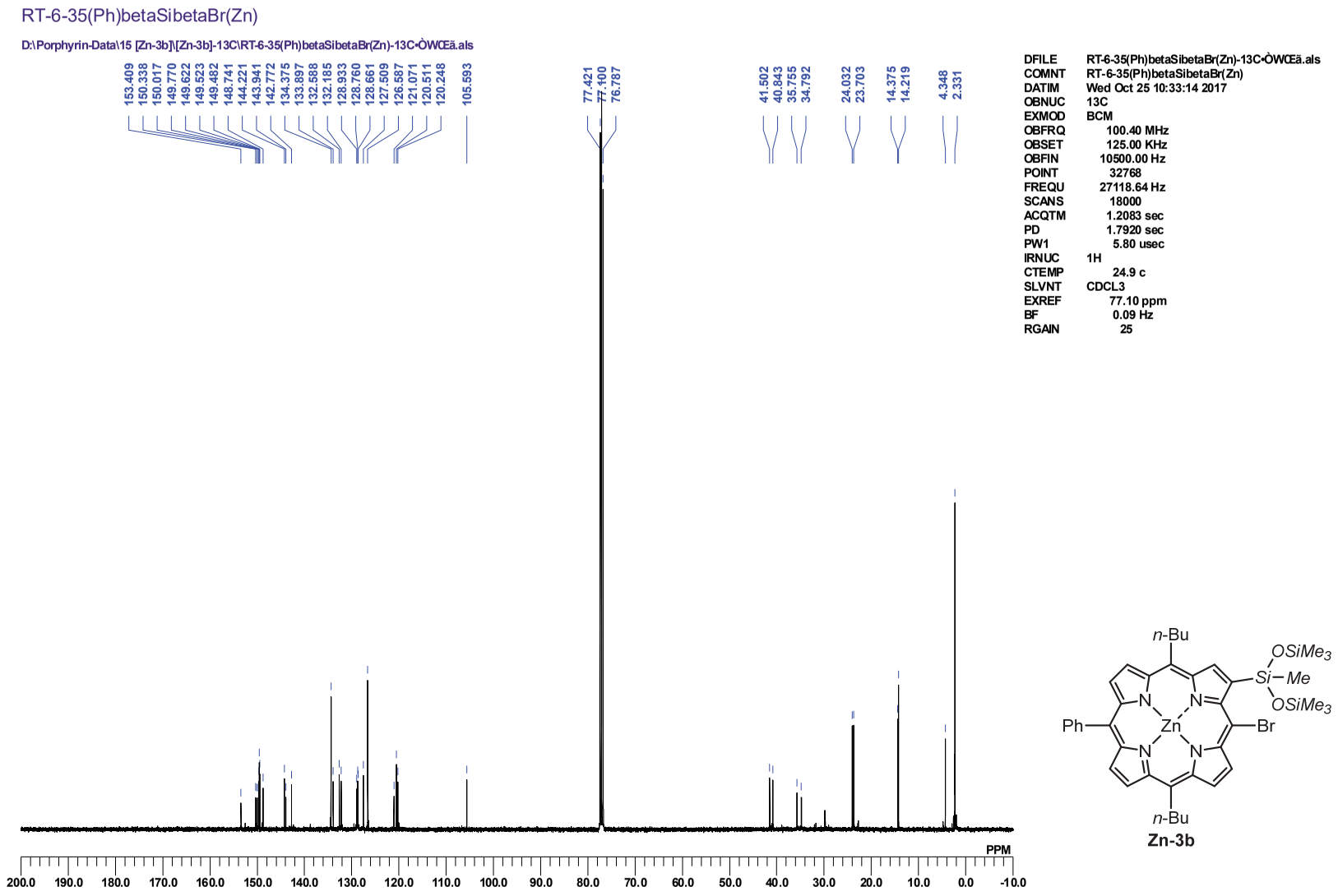

RT-7-36betaSimesoBrTPP(Zn)13C
D:\Porphyrin-Data\14 [Zn-3a]\[Zn-3a]-13C\RT-7-36betaSimesoBrTPP(Zn)13C•ÒWŒÈä.als
154.504
150.857
150.618
150.552
150.519
150.495
150.042
149.704
147.761
144.057
142.706
142.616
142.525
134.498
134.424
134.391
134.079
132.893
132.506
132.383
132.317
132.300
127.748
127.723
127.690
126.751
126.710
126.694
121.878
121.705
121.046
106.573
77.421
77.100
76.787
4.109
2.141
DFILE RT-7-36betaSimesoBrTPP(Zn)13C•ÒWŒÈä.als
COMNT RT-7-36betaSimesoBrTPP(Zn)13C
DATIM Mon May 21 09:47:43 2018
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 53600
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRNUC 1H
CTEMP 24.6 c
SLVNT CDCL3
EXREF 77.10 ppm
BF 0.09 Hz
RGAIN 25
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0
Ph
OSiMe3
Si–Me
OSiMe3
Ph
Zn
Br
Ph
N
N
N
N

Zn-3a

Zn-3b

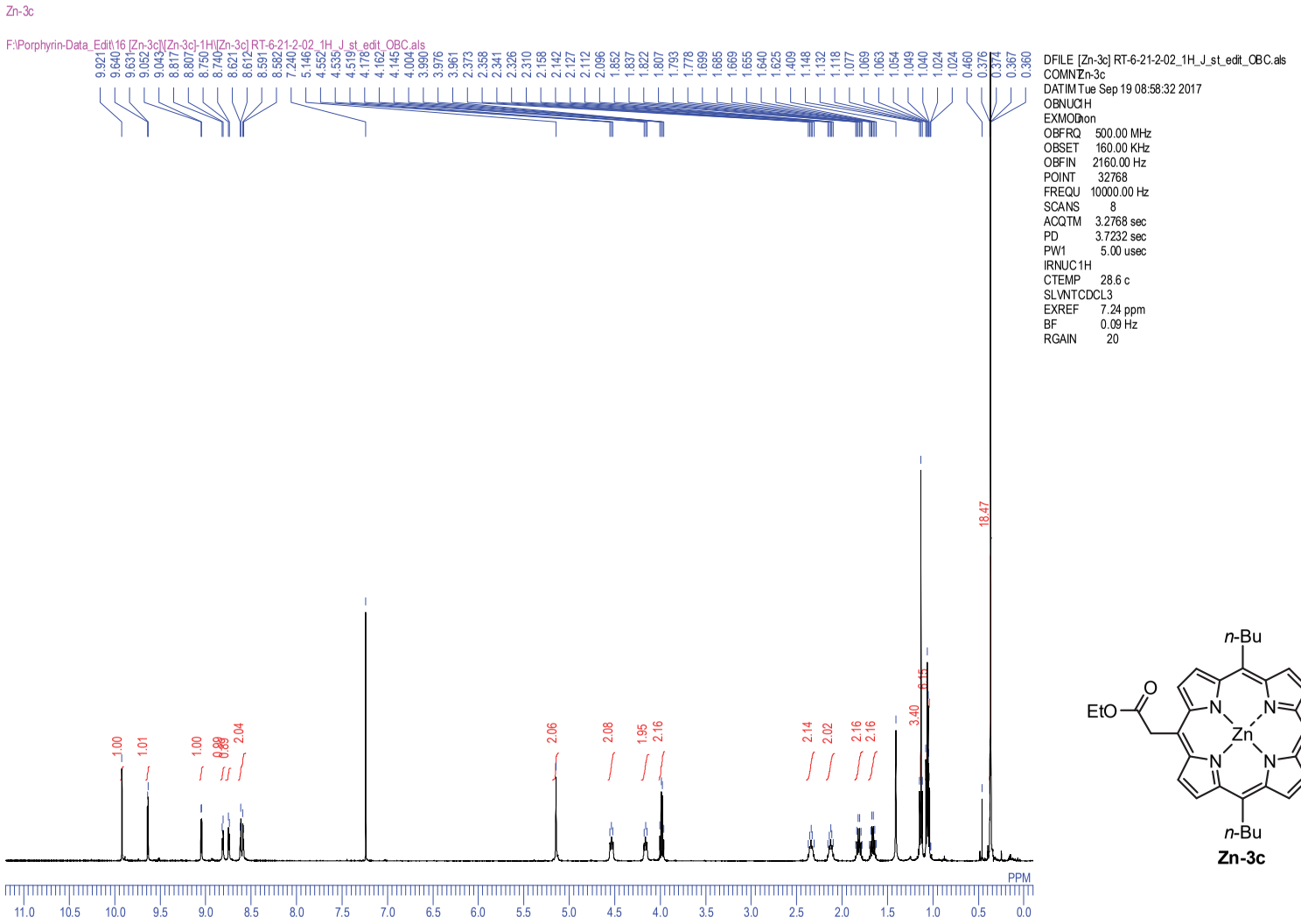

RT-6-35(Ph)betaSibetaBr(Zn)
F:\Porphyrin-Data_Edit\15 [Zn-3b]\[Zn-3b]-1H\[Zn-3b] RT-6-35(Ph)betaSibetaBr(Zn)-1H_J_st_edit_OBC.als
DFILE [Zn-3b] RT-6-35(Ph)betaSibetaBr(Zn)-1H_J_st_edit_OBC.als
COMNT RT-6-35(Ph)betaSibetaBr(Zn)
DATIM Tue Oct 24 19:28:10 2017
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 16
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.60 usec
IRNUC 1H
CTEMP 25.1 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.09 Hz
RGAIN 17
PPM
n-Bu
OSiMe3
Si—Me
OSiMe3
Ph
Br
Zn
N
n-Bu
Zn-3b

Zn-3b


RT-6-35(Ph)betaSibetaBr(Zn)
D:\Porphyrin-Data\15 [Zn-3b]\[Zn-3b]-13C\RT-6-35(Ph)betaSibetaBr(Zn)-13C•ÒWŒã.als
153.409
150.338
150.017
149.770
149.622
149.523
149.482
148.741
144.221
143.941
142.772
134.375
133.897
132.588
132.185
128.933
128.760
128.661
127.509
126.587
121.071
120.511
120.248
105.593
77.421
77.100
76.787
41.502
40.843
35.755
34.792
24.032
23.703
14.375
14.219
4.348
2.331
DFILE RT-6-35(Ph)betaSibetaBr(Zn)-13C•ÒWŒã.als
COMNT RT-6-35(Ph)betaSibetaBr(Zn)
DATIM Wed Oct 25 10:33:14 2017
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 18000
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.80 usec
IRNUC 1H
CTEMP 24.9 c
SLVNT CDCL3
EXREF 77.10 ppm
BF 0.09 Hz
RGAIN 25
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0
n-Bu
OSiMe3
Si
Me
OSiMe3
N
N
Ph
Zn
Br
N
N
n-Bu

Zn-3b

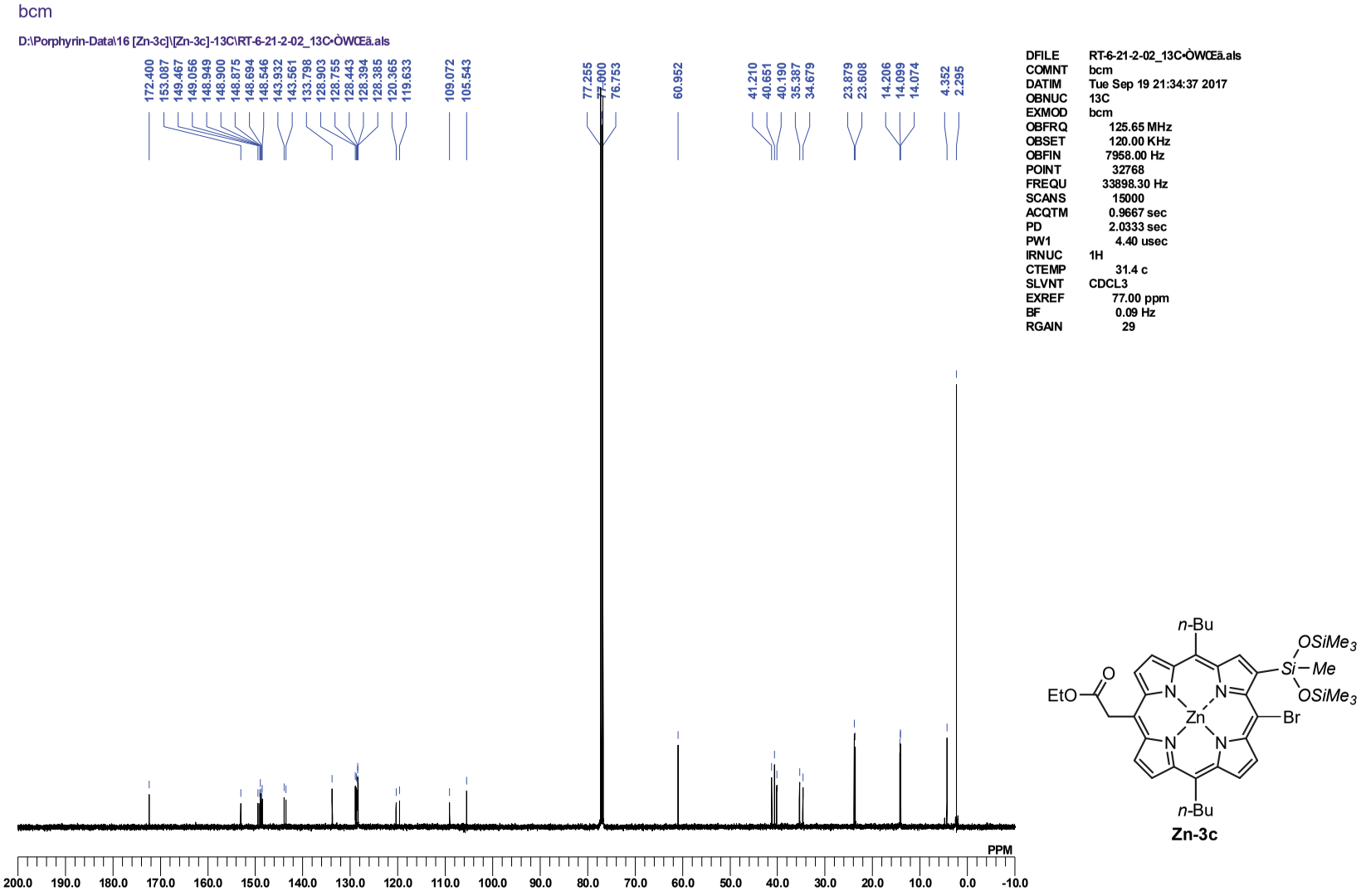
Zn-3c


Zn-3c
F:\Porphyrin-Data_Edit\16 [Zn-3c]\[Zn-3c]-1H\[Zn-3c] RT-6-21-2-02_1H_J_st_edit_OBC.als
DFILE [Zn-3c] RT-6-21-2-02_1H_J_st_edit_OBC.als
COMNT Zn-3c
DATIM Tue Sep 19 08:58:32 2017
OBNUC 1H
EXMOD non
OBFRQ 500.00 MHz
OBSET 160.00 KHz
OBFIN 2160.00 Hz
POINT 32768
FREQU 10000.00 Hz
SCANS 8
ACQTM 3.2768 sec
PD 3.7232 sec
PW1 5.00 usec
IRNUC 1H
CTEMP 28.6 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.09 Hz
RGAIN 20
PPM

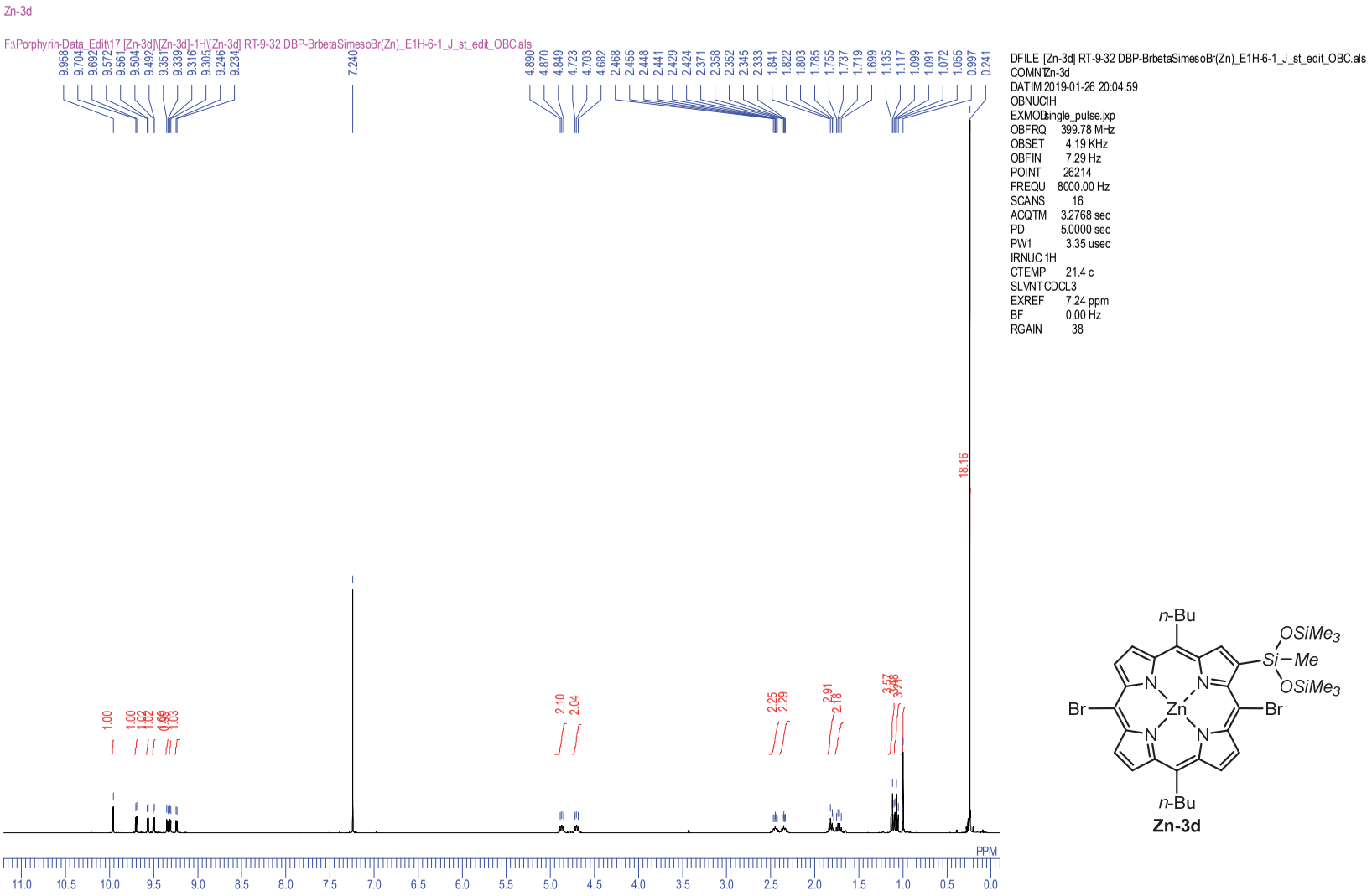
n-Bu
OSiMe3
Si—Me
OSiMe3
EtO
O
N
N
Zn
N
N
Br
n-Bu

Zn-3c

Zn-3c


bcm
D:\Porphyrin-Data\16 [Zn-3c]\[Zn-3c]-13C\RT-6-21-2-02_13C-ÒWŒã.als
172.400
153.087
149.467
149.056
148.949
148.900
148.875
148.694
148.546
143.932
143.561
133.798
128.903
128.755
128.443
128.394
128.385
120.365
119.633
109.072
105.543
77.255
77.000
76.753
60.952
41.210
40.651
40.190
35.387
34.679
23.879
23.608
14.206
14.099
14.074
4.352
2.295
DFILE RT-6-21-2-02_13C-ÒWŒã.als
COMNT bcm
DATIM Tue Sep 19 21:34:37 2017
OBNUC 13C
EXMOD bcm
OBFRQ 125.65 MHz
OBSET 120.00 KHz
OBFIN 7958.00 Hz
POINT 32768
FREQU 33898.30 Hz
SCANS 15000
ACQTM 0.9667 sec
PD 2.0333 sec
PW1 4.40 usec
IRNUC 1H
CTEMP 31.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.09 Hz
RGAIN 29
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0
n-Bu
OSiMe3
Si—Me
OSiMe3
EtO
O
N
N
Zn
N
N
Br
n-Bu
Zn-3c

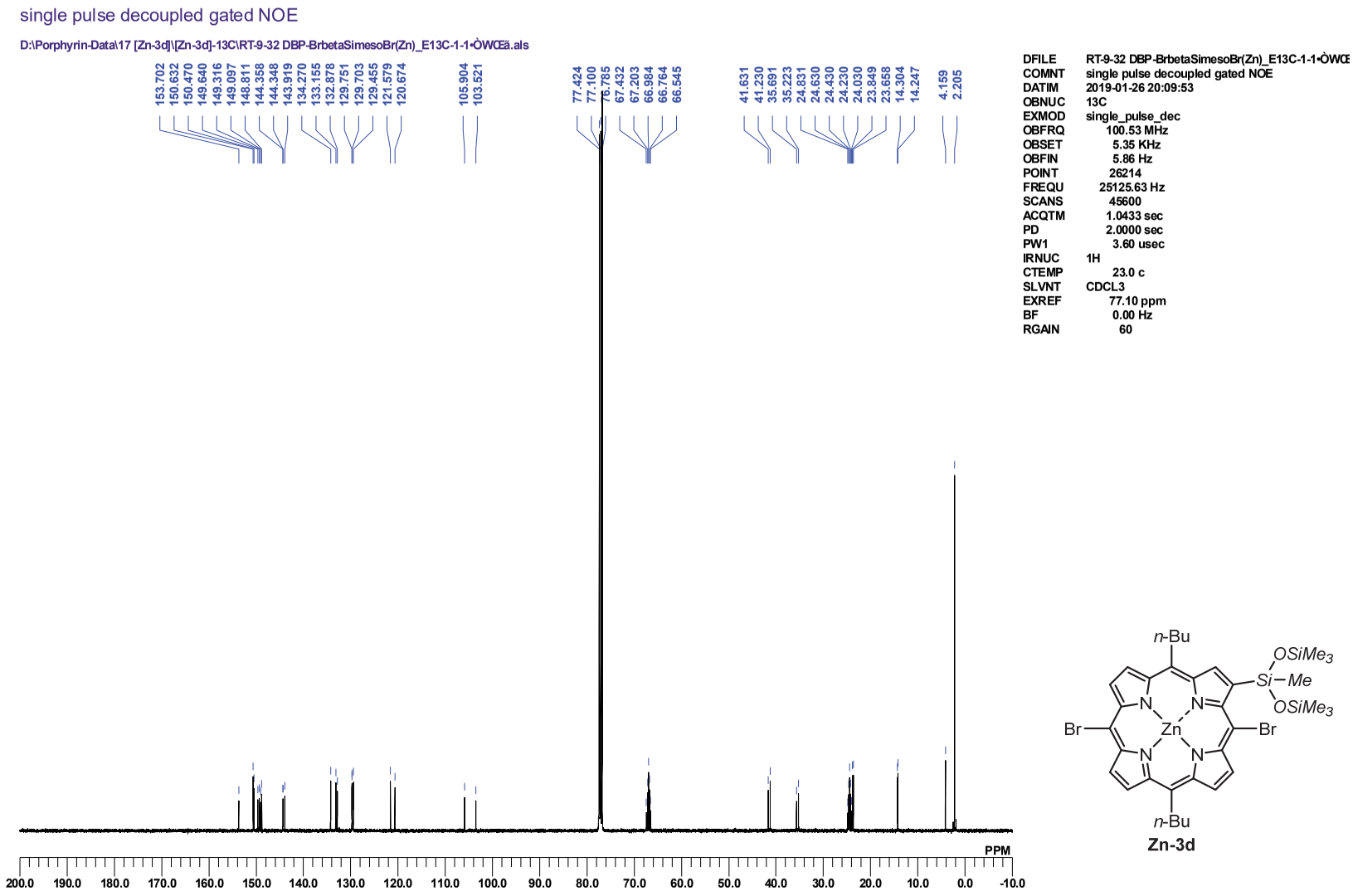
Zn-3d


Zn-3d
F:\Porphyrin-Data_Edit\17 [Zn-3d]\[Zn-3d]-1H\[Zn-3d] RT-9-32 DBP-BrbetaSimesoBr(Zn)_E1H-6-1_J_st_edit_OBC.als
DFILE [Zn-3d] RT-9-32 DBP-BrbetaSimesoBr(Zn)_E1H-6-1_J_st_edit_OBC.als
COMNT Zn-3d
DATIM 2019-01-26 20:04:59
OBNUC 1H
EXMOD single_pulse.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 26214
FREQU 8000.00 Hz
SCANS 16
ACQTM 3.2768 sec
PD 5.0000 sec
PW1 3.35 usec
IRNUC 1H
CTEMP 21.4 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.00 Hz
RGAIN 38
PPM

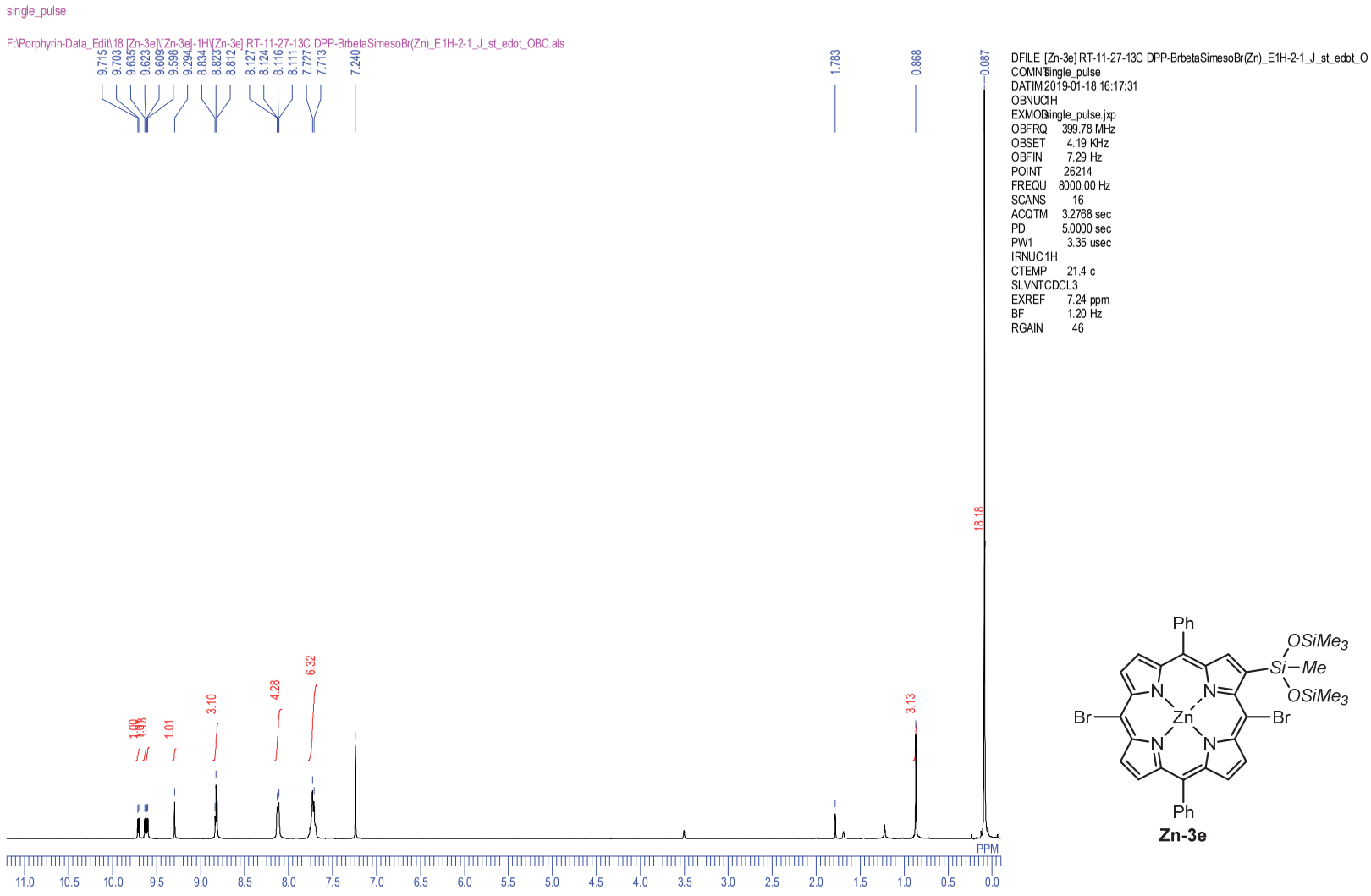
n-Bu
OSiMe3
Si–Me
OSiMe3
Br
Br
Zn
N
N
N
N
n-Bu

Zn-3d

Zn-3d


single pulse decoupled gated NOE
D:\Porphyrin-Data\17 [Zn-3d]\[Zn-3d]-13C\RT-9-32 DBP-BrbetaSimesoBr(Zn)_E13C-1-1•ÒWŒä.als
153.702
150.632
150.470
149.640
149.316
149.097
148.811
144.358
144.348
143.919
134.270
133.155
132.878
129.751
129.703
129.455
121.579
120.674
105.904
103.521
77.424
77.100
76.785
67.432
67.203
66.984
66.764
66.545
41.631
41.230
35.691
35.223
24.831
24.630
24.430
24.230
24.030
23.849
23.658
14.304
14.247
4.159
2.205
DFILE RT-9-32 DBP-BrbetaSimesoBr(Zn)_E13C-1-1•ÒWŒ
COMNT single pulse decoupled gated NOE
DATIM 2019-01-26 20:09:53
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 45600
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.60 usec
IRNUC 1H
CTEMP 23.0 c
SLVNT CDCL3
EXREF 77.10 ppm
BF 0.00 Hz
RGAIN 60
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0
n-Bu
OSiMe3
Si
Me
OSiMe3
N
N
Br
Zn
Br
N
N
n-Bu
Zn-3d

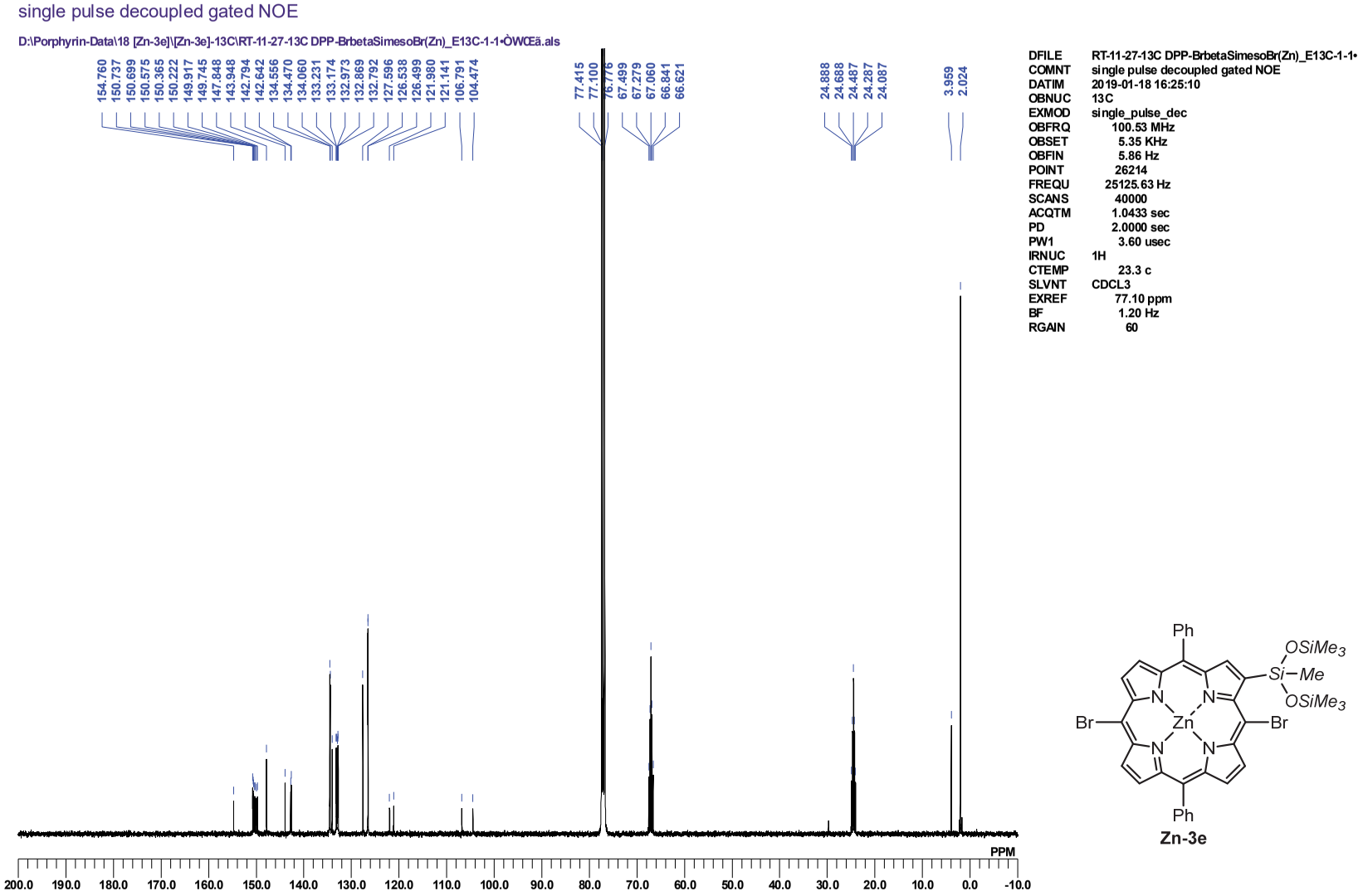
Zn-3e


single_pulse
F:\Porphyrin-Data_Edit\18 [Zn-3e]\[Zn-3e]-1H\[Zn-3e] RT-11-27-13C DPP-BrbetaSimesoBr(Zn)_E1H-2-1_J_st_edot_OBC.als
9.715
9.703
9.635
9.623
9.609
9.598
9.294
8.834
8.823
8.812
8.127
8.124
8.116
8.111
7.727
7.719
7.240
1.783
0.868
0.087
DFILE [Zn-3e] RT-11-27-13C DPP-BrbetaSimesoBr(Zn)_E1H-2-1_J_st_edot_O
COMNT single_pulse
DATIM 2019-01-18 16:17:31
OBNUC 1H
EXMOD single_pulse.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 26214
FREQU 8000.00 Hz
SCANS 16
ACQTM 3.2768 sec
PD 5.0000 sec
PW1 3.35 usec
IRNUC 1H
CTEMP 21.4 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 1.20 Hz
RGAIN 46
18.18
6.32
4.28
3.13
3.10
1.01
PPM
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

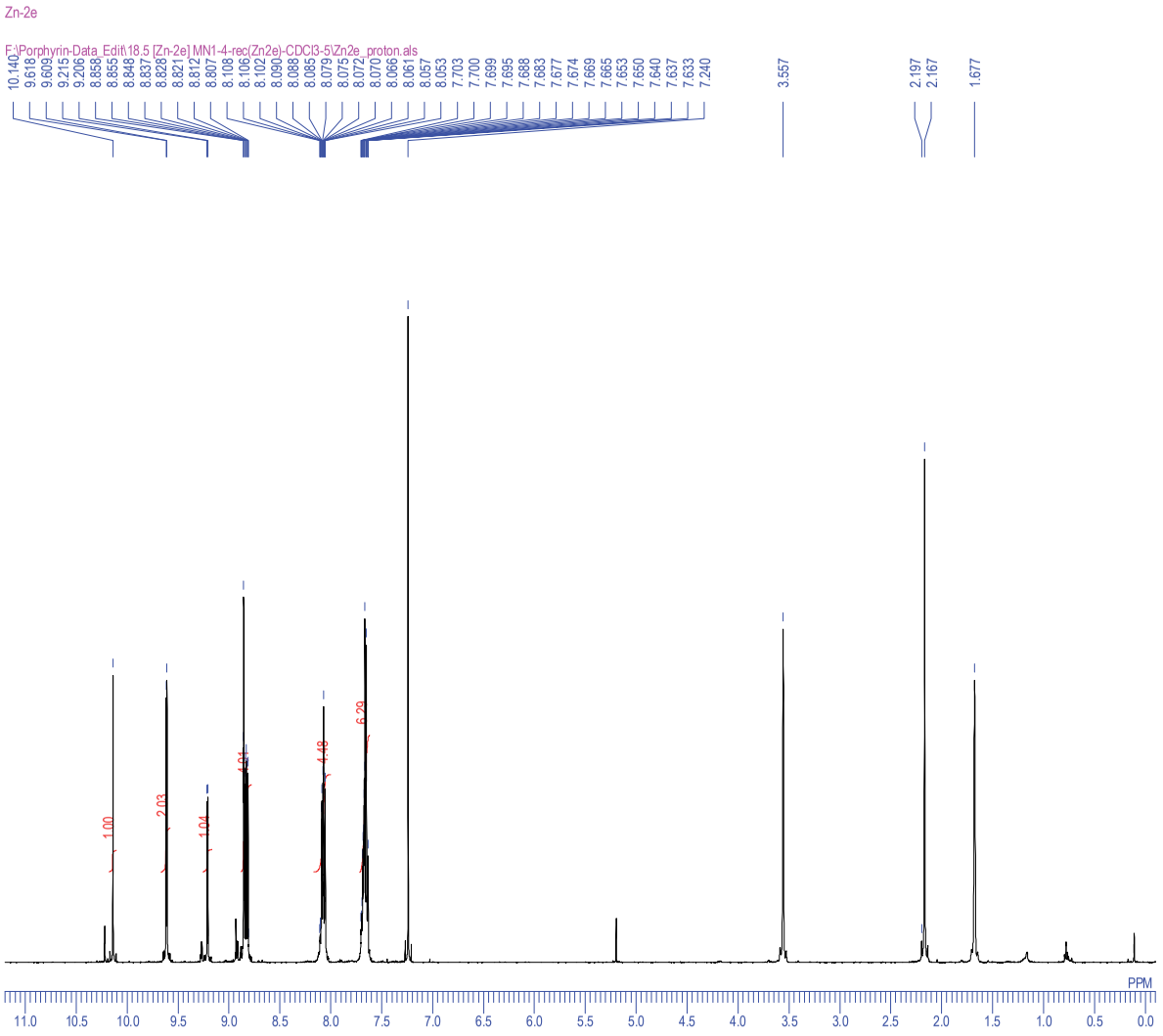
Ph
OSiMe3
Si–Me
OSiMe3
N
N
Br
Zn
Br
N
N
Ph

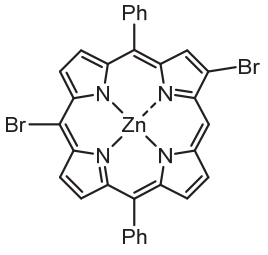
Zn-3e

Zn-3e


single pulse decoupled gated NOE
D:\Porphyrin-Data\18 [Zn-3e]\[Zn-3e]-13C\RT-11-27-13C DPP-BrbetaSimesoBr(Zn)_E13C-1-1•ÒWŒä.als
154.760
150.737
150.699
150.575
150.365
150.222
149.917
149.745
147.848
143.948
142.794
142.642
134.556
134.470
134.060
133.231
133.174
132.973
132.869
132.792
127.596
126.538
126.499
121.980
121.141
106.791
104.474
77.415
77.100
76.776
67.499
67.279
67.060
66.841
66.621
24.888
24.688
24.487
24.287
24.087
3.959
2.024
DFILE RT-11-27-13C DPP-BrbetaSimesoBr(Zn)_E13C-1-1•
COMNT single pulse decoupled gated NOE
DATIM 2019-01-18 16:25:10
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 40000
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.60 usec
IRNUC 1H
CTEMP 23.3 c
SLVNT CDCL3
EXREF 77.10 ppm
BF 1.20 Hz
RGAIN 60
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0
Ph
OSiMe3
Si
Me
OSiMe3
N
N
Br
Zn
Br
N
N
Ph
Zn-3e

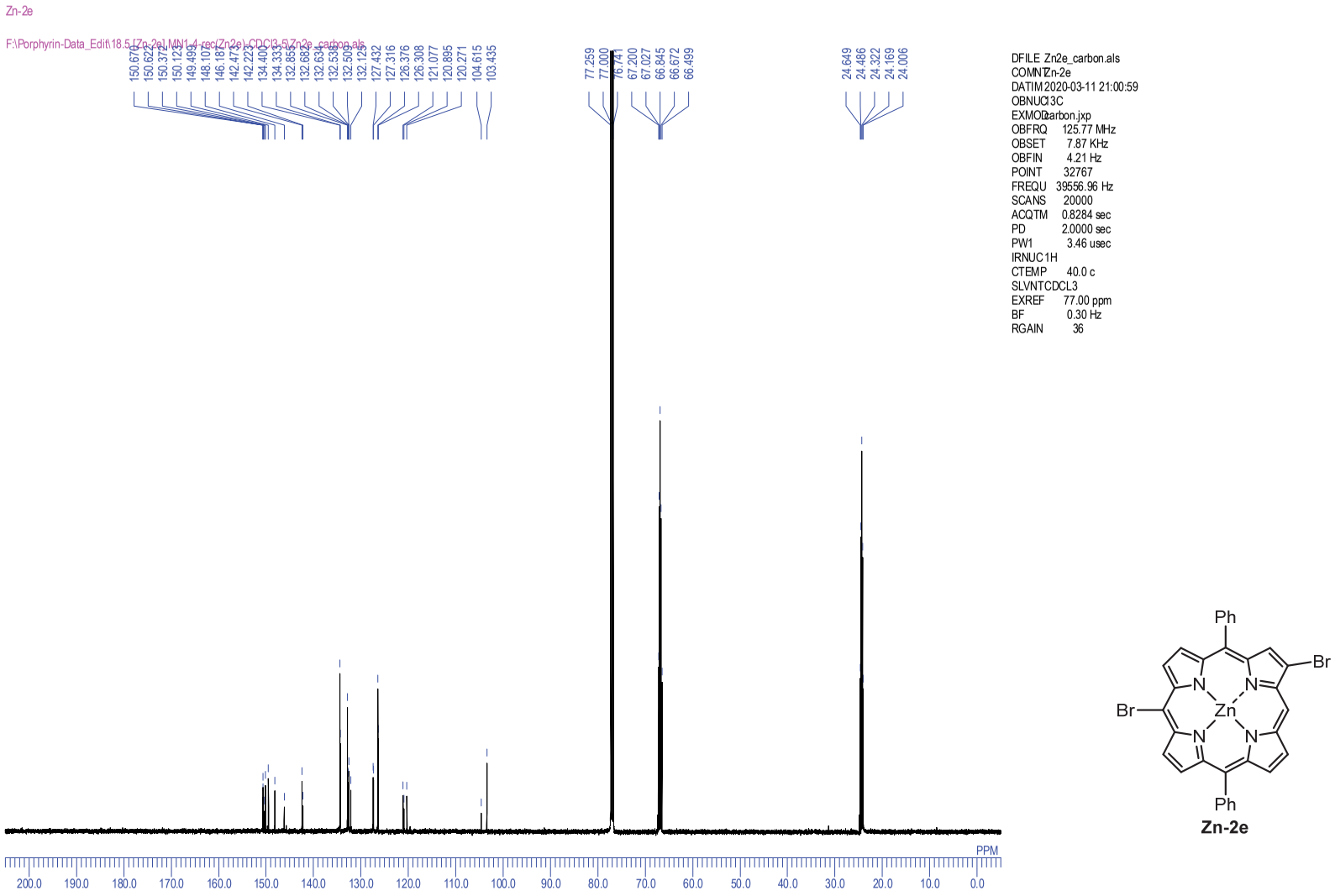
Zn-2e


Zn-2e
F:\Porphyrin-Data_Edit\18.5 [Zn-2e] MN1-4-rec(Zn2e)-CDCl3-5\Zn2e_proton.als
10.140
9.618
9.609
9.215
9.206
8.858
8.855
8.848
8.837
8.826
8.821
8.812
8.807
8.109
8.106
8.102
8.090
8.088
8.085
8.079
8.075
8.072
8.070
8.066
8.061
8.057
8.053
7.703
7.700
7.699
7.695
7.688
7.683
7.677
7.674
7.669
7.665
7.653
7.650
7.640
7.637
7.633
7.240
3.557
2.197
2.167
1.677
DFILE Zn2e_proton.als
COMNT Zn-2e
DATIM 2020-03-11 20:58:02
OBNUC 1H
EXMOD proton.jxp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 32767
FREQU 9384.38 Hz
SCANS 16
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 3.00 usec
IRNUC 1H
CTEMP 40.0 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.30 Hz
RGAIN 56
1.00
2.03
1.04
4.01
4.48
6.29
PPM
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


Ph
Br
N
N
Zn
Br
N
N
Ph

Zn-2e

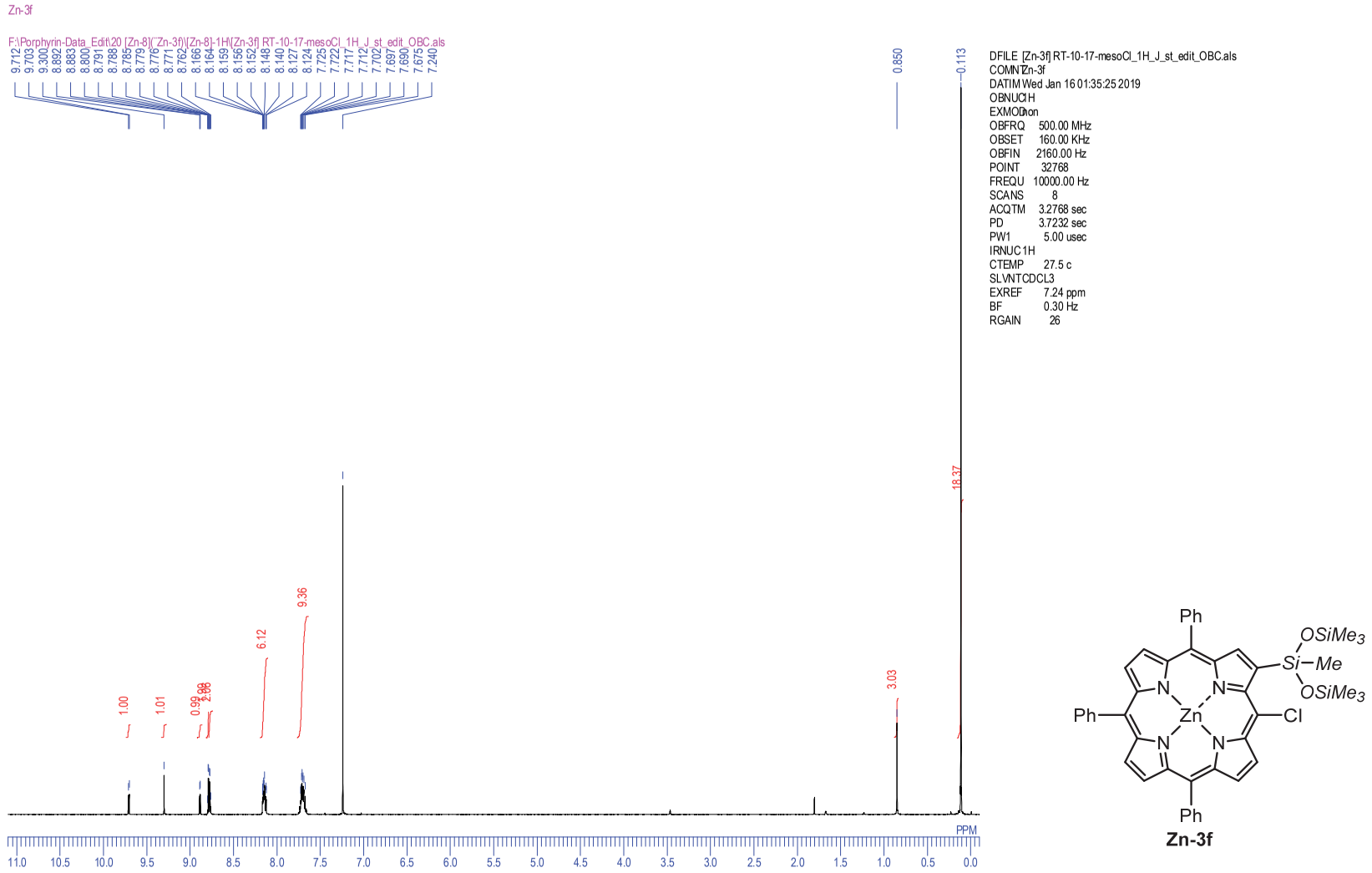
Zn-2e


Zn-2e
F:\Porphyrin-Data_Edit\18.5-[Zn-2e]-MN1-4-rec(Zn2e)-CDCl3-5\Zn2e_carbon.als
150.670
150.622
150.372
150.122
149.493
148.107
146.187
142.477
142.223
134.400
134.333
132.853
132.682
132.634
132.538
132.505
132.123
127.432
127.316
126.376
126.308
121.077
120.895
120.271
104.615
103.435
77.259
77.000
76.741
67.200
67.027
66.845
66.672
66.499
24.649
24.486
24.322
24.169
24.006
DFILE Zn2e_carbon.als
COMNTZn-2e
DATIM2020-03-11 21:00:59
OBNUC13C
EXMOD carbon.jxp
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 32767
FREQU 39556.96 Hz
SCANS 20000
ACQTM 0.8284 sec
PD 2.0000 sec
PW1 3.46 usec
IRNUC1H
CTEMP 40.0 c
SLVNTCDCL3
EXREF 77.00 ppm
BF 0.30 Hz
RGAIN 36
PPM
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0

Ph
Br
N
N
Zn
N
N
Br
Ph

Zn-2e

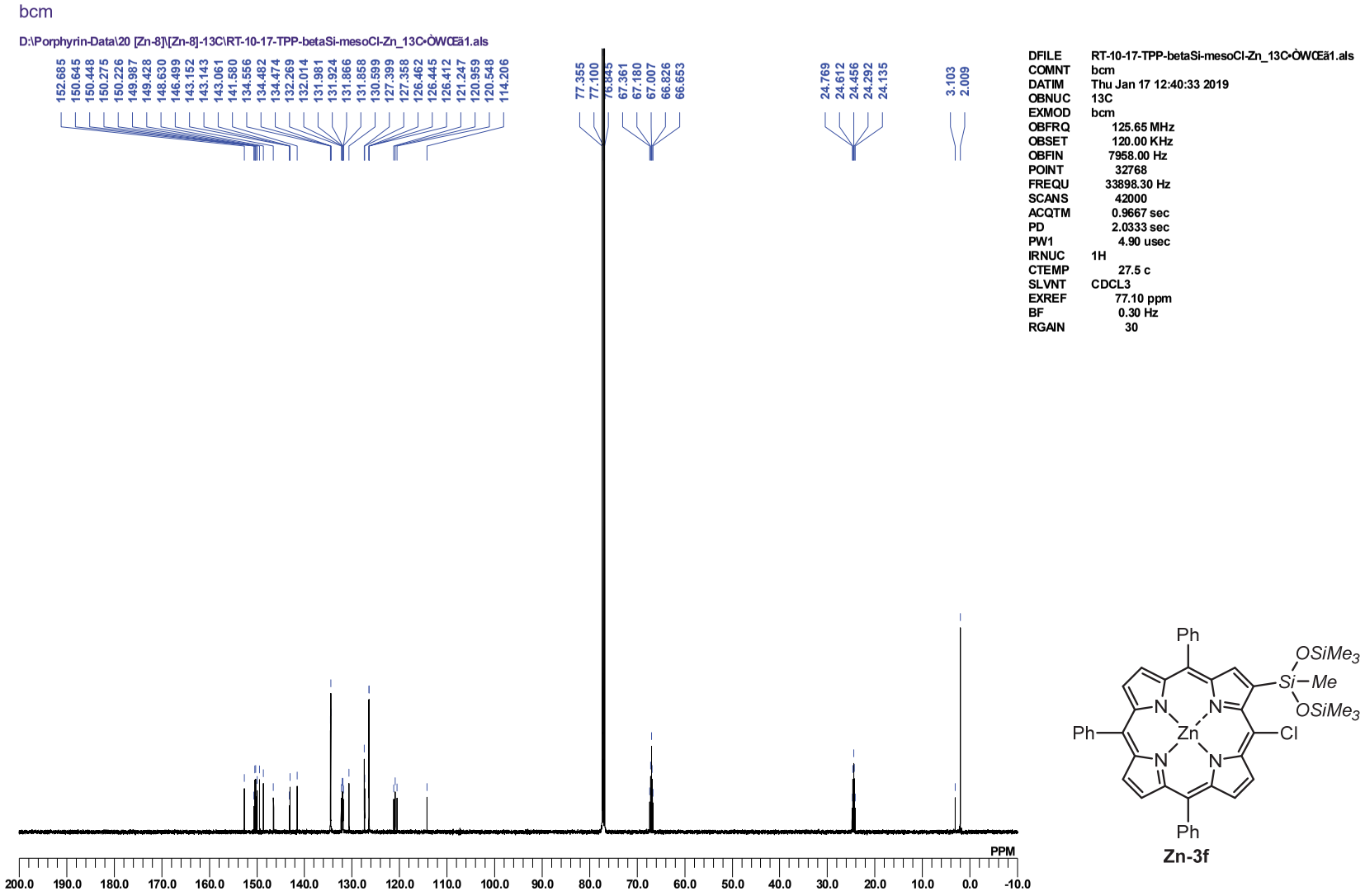
Zn-3f


Zn-3f
F:\Porphyrin-Data_Edit\20 [Zn-8](Zn-3f)\[Zn-8]-1H\[Zn-3f] RT-10-17-mesoCl_1H_J_st_edit_OBC.als
9.712
9.703
9.300
8.892
8.883
8.800
8.791
8.788
8.785
8.779
8.776
8.771
8.762
8.166
8.164
8.159
8.156
8.152
8.148
8.140
8.127
8.124
7.725
7.722
7.717
7.712
7.702
7.697
7.690
7.675
7.240
0.850
0.113
DFILE [Zn-3f] RT-10-17-mesoCl_1H_J_st_edit_OBC.als
COMNTZn-3f
DATIM Wed Jan 16 01:35:25 2019
OBNUCl H
EXMODtion
OBFRQ 500.00 MHz
OBSET 160.00 KHz
OBFIN 2160.00 Hz
POINT 32768
FREQU 10000.00 Hz
SCANS 8
ACQTM 3.2768 sec
PD 3.7232 sec
PW1 5.00 usec
IRNUC 1H
CTEMP 27.5 c
SLVNTCDCL3
EXREF 7.24 ppm
BF 0.30 Hz
RGAIN 26
18.37
9.36
6.12
3.03
1.00
1.01
0.99
2.00
2.00
PPM
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

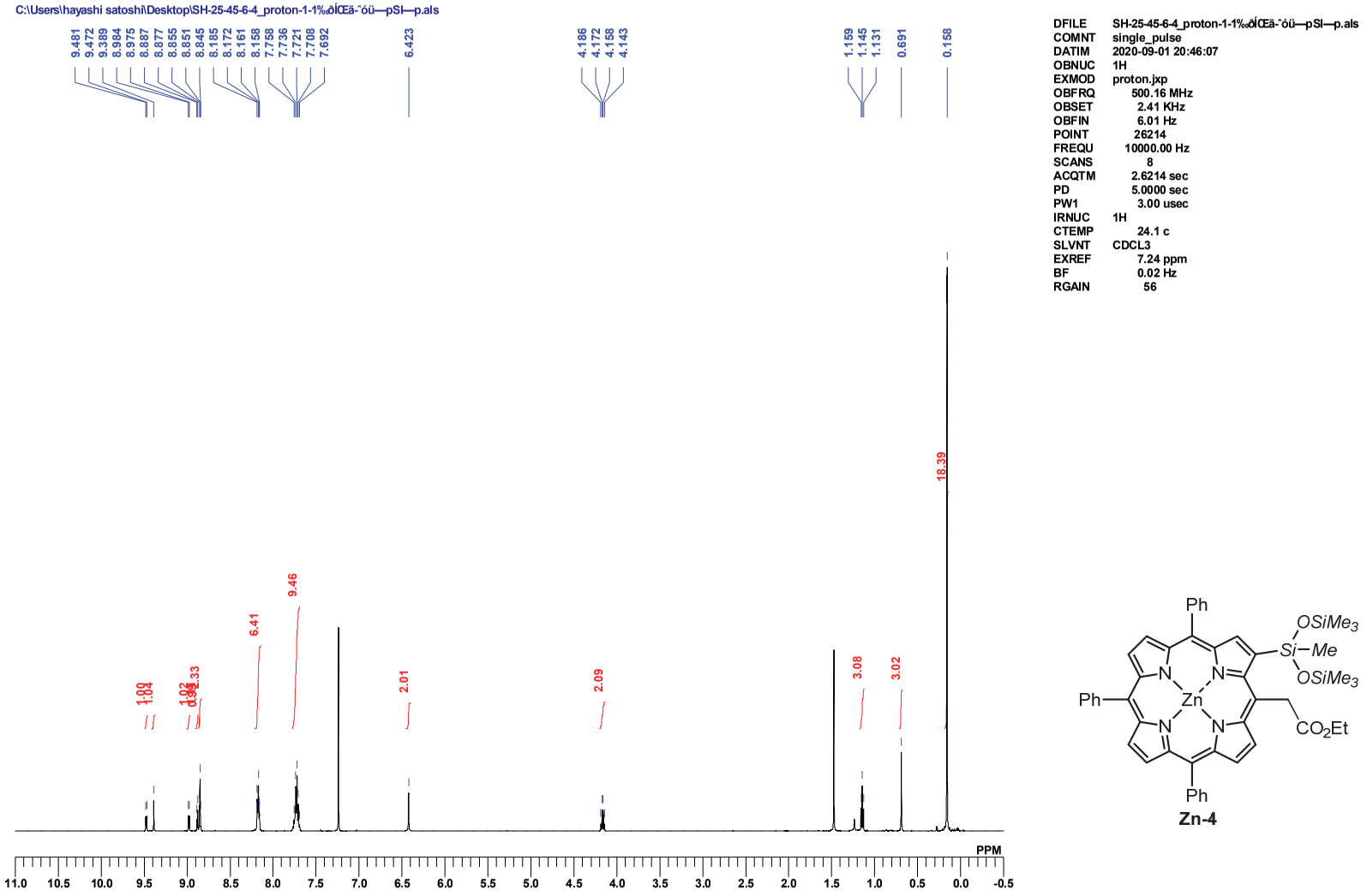
Ph
OSiMe3
Si–Me
OSiMe3
N
N
Zn
Cl
Ph
N
N
Ph

Zn-3f

Zn-3f


bcm
D:\Porphyrin-Data\20 [Zn-8]\[Zn-8]-13C\RT-10-17-TPP-betaSi-mesoCl-Zn_13C•ÒWŒã1.als
152.685 150.645 150.448 150.275 150.226 149.987 149.428 148.630 146.499 143.152 143.143 143.061 141.580 134.556 134.482 134.474 132.269 132.014 131.981 131.924 131.866 131.858 130.599 127.399 127.358 126.462 126.445 126.412 121.247 120.959 120.548 114.206
77.355 77.100 76.845 67.361 67.180 67.007 66.826 66.653
24.769 24.612 24.456 24.292 24.135
3.103 2.009
DFILE RT-10-17-TPP-betaSi-mesoCl-Zn_13C•ÒWŒã1.als
COMNT bcm
DATIM Thu Jan 17 12:40:33 2019
OBNUC 13C
EXMOD bcm
OBFRQ 125.65 MHz
OBSET 120.00 KHz
OBFIN 7958.00 Hz
POINT 32768
FREQU 33898.30 Hz
SCANS 42000
ACQTM 0.9667 sec
PD 2.0333 sec
PW1 4.90 usec
IRNUC 1H
CTEMP 27.5 c
SLVNT CDCL3
EXREF 77.10 ppm
BF 0.30 Hz
RGAIN 30
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0 -10.0
Ph
OSiMe3
Si–Me
OSiMe3
N
N
Ph
Zn
Cl
N
N
Ph
Zn-3f

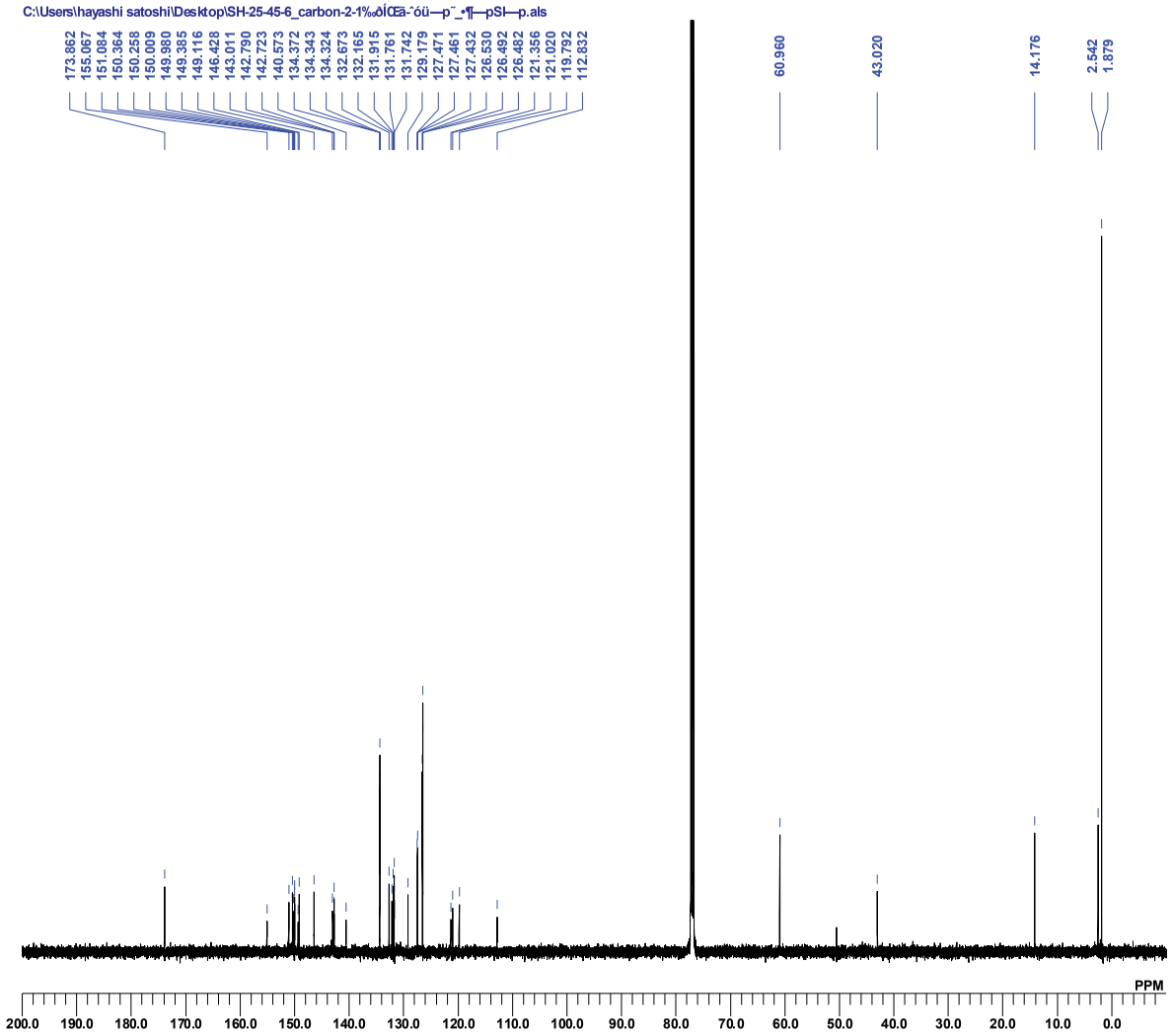
Zn-4


C:\Users\hayashi satoshi\Desktop\SH-25-45-6-4_proton-1-1‰ðÍŒä-ˆóü—pSI—p.als
9.481
9.472
9.389
8.984
8.975
8.887
8.877
8.855
8.851
8.845
8.185
8.172
8.161
8.158
7.758
7.736
7.721
7.708
7.692
6.423
4.186
4.172
4.158
4.143
1.159
1.145
1.131
0.691
0.158
DFILE SH-25-45-6-4_proton-1-1‰ðÍŒä-ˆóü—pSI—p.als
COMNT single_pulse
DATIM 2020-09-01 20:46:07
OBNUC 1H
EXMOD proton.jxp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 10000.00 Hz
SCANS 8
ACQTM 2.6214 sec
PD 5.0000 sec
PW1 3.00 usec
IRNUC 1H
CTEMP 24.1 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.02 Hz
RGAIN 56
1.00
1.04
1.02
0.94
0.93
6.41
9.46
2.01
2.09
3.08
3.02
18.39
PPM
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

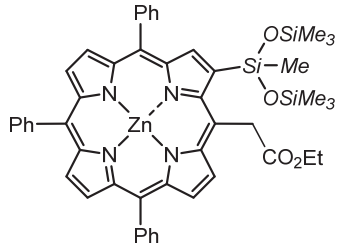
Ph
OSiMe3
Si–Me
OSiMe3
N
N
Ph
Zn
N
N
CO2Et
Ph

Zn-4

Zn-4

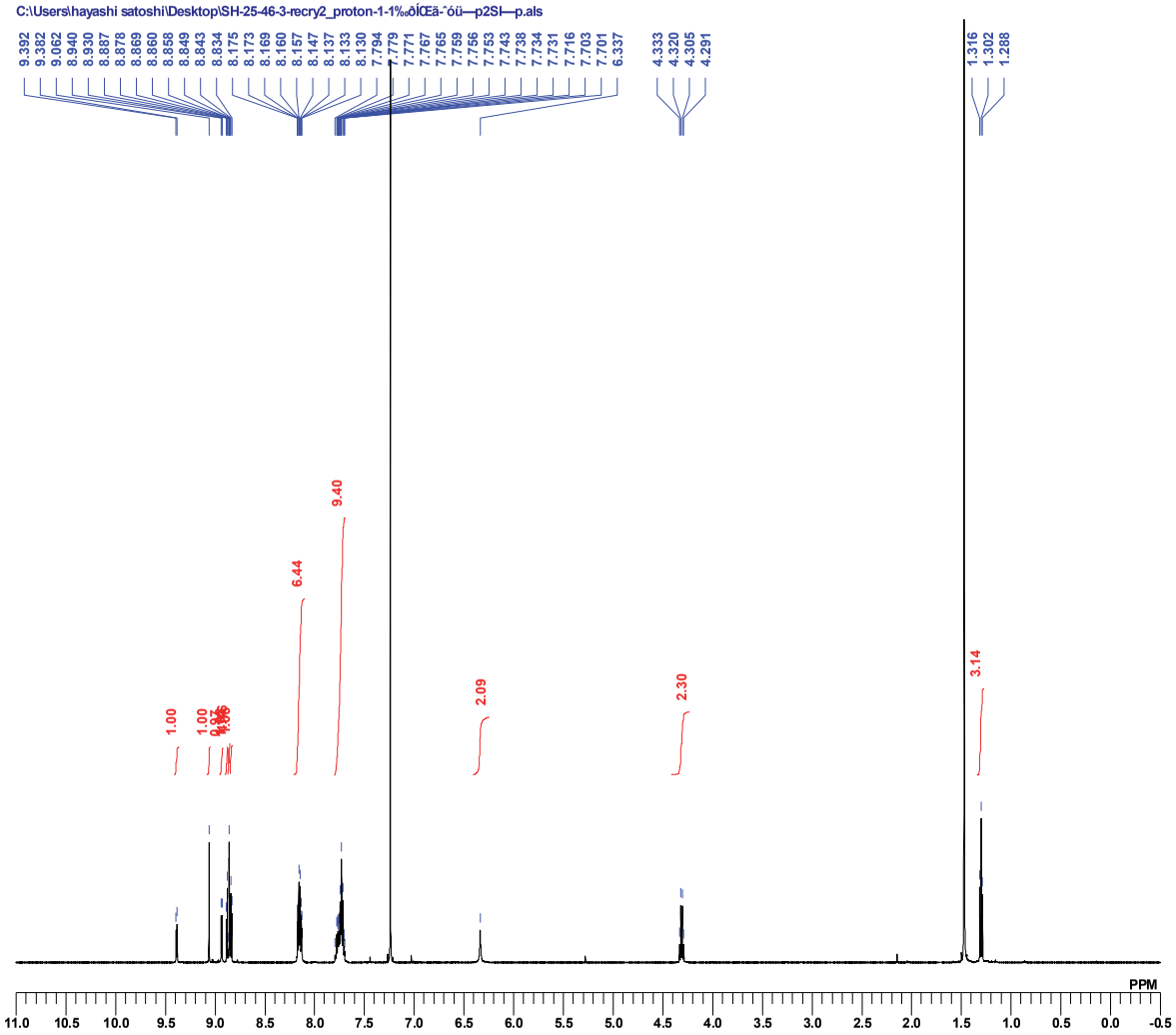


DFILE	SH-25-45-6_carbon-2-1‰ôÍŒã-ˆóü—p¨_•¶—pSI—p.als
COMNT	single pulse decoupled gated NOE
DATIM	2020-08-30 07:15:03
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	26214
FREQU	31645.57 Hz
SCANS	30000
ACQTM	0.8284 sec
PD	2.0000 sec
PW1	3.46 usec
IRNUC	1H
CTEMP	23.5 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.02 Hz
RGAIN	36

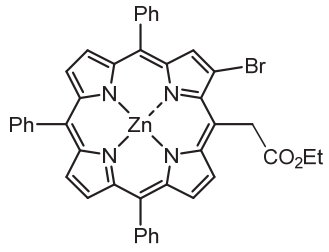


Zn-4

Zn-5

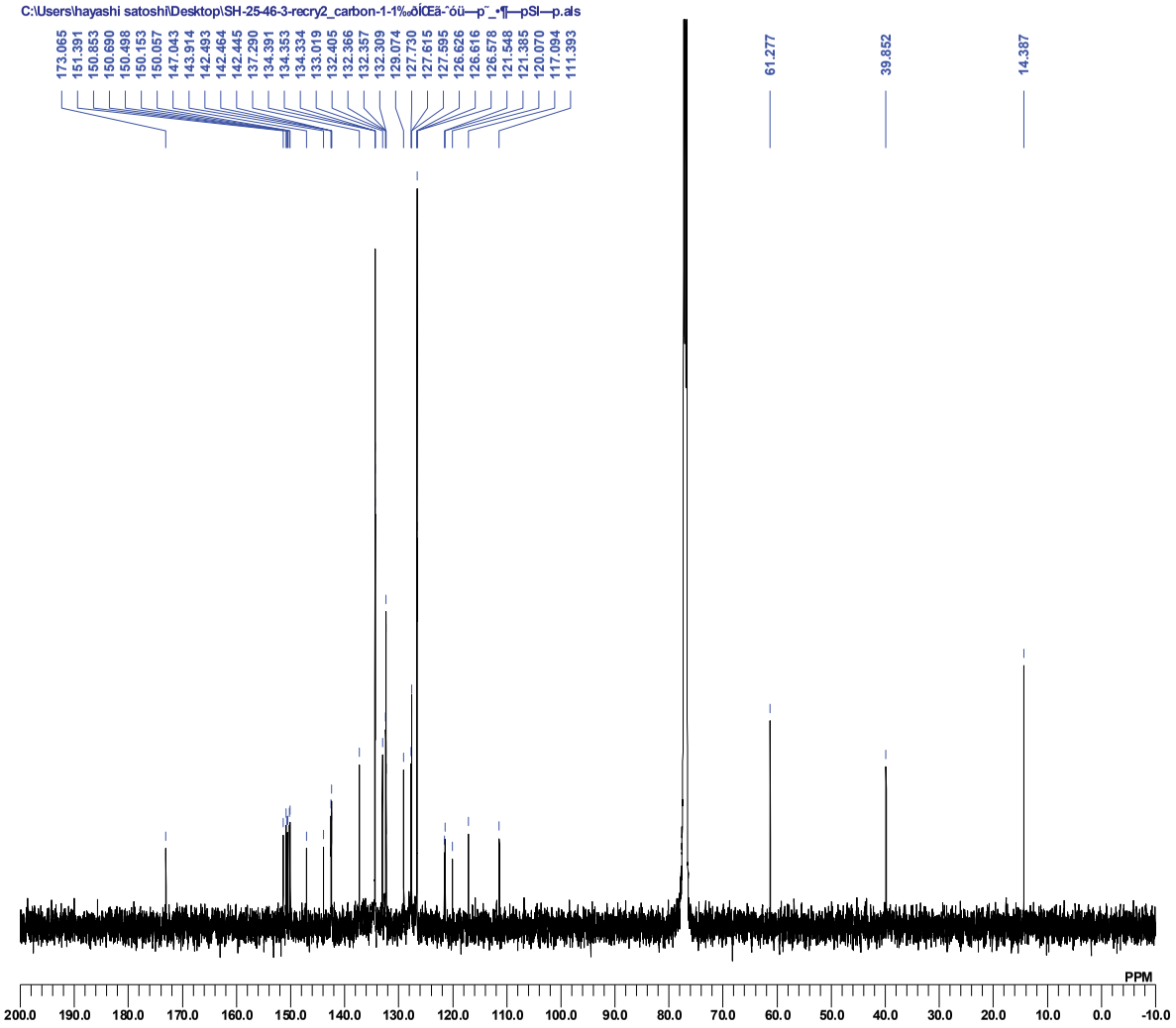


DFILE	SH-25-46-3-recry2_proton-1-1‰ôÍŒä-ˆóü—p2SI—p.als
COMNT	single_pulse
DATIM	2020-09-03 14:30:18
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	26214
FREQU	10000.00 Hz
SCANS	8
ACQTM	2.6214 sec
PD	5.0000 sec
PW1	3.00 usec
IRNUC	1H
CTEMP	24.0 c
SLVNT	CDCL3
EXREF	7.24 ppm
BF	0.02 Hz
RGAIN	66

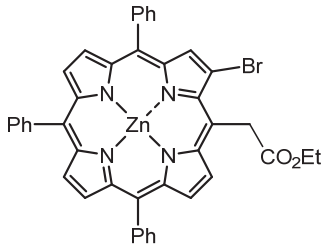


Zn-5

Zn-5

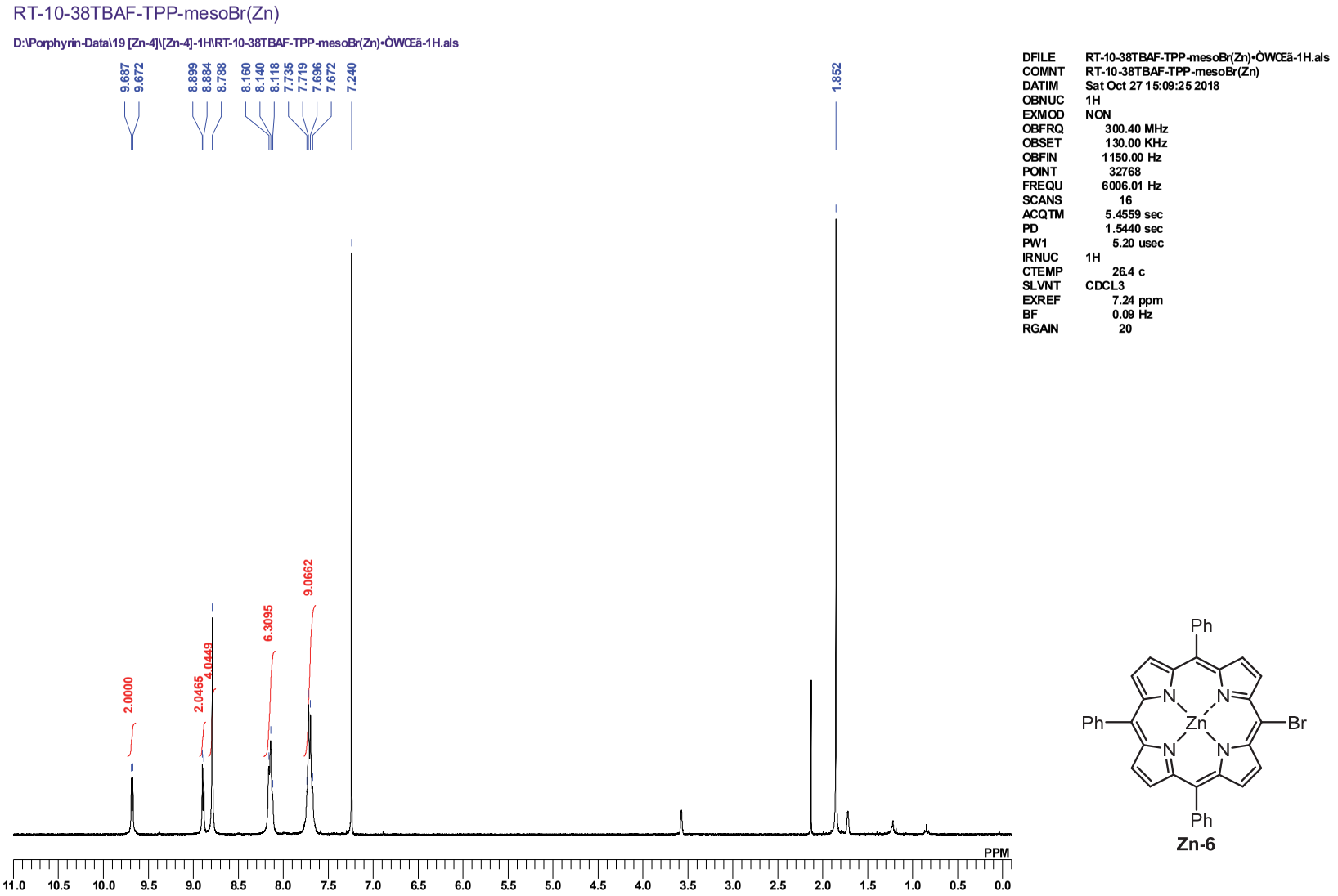


DFILE	SH-25-46-3-recry2_carbon-1-1‰ôÍŒã-ˆóü—p¯_•¶—pSI—p
COMNT	single pulse decoupled gated NOE
DATIM	2020-09-03 14:35:12
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	26214
FREQU	31645.57 Hz
SCANS	26000
ACQTM	0.8284 sec
PD	2.0000 sec
PW1	3.46 usec
IRNUC	1H
CTEMP	24.2 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.72 Hz
RGAIN	36



Zn-5

Zn-6


RT-10-38TBAF-TPP-mesoBr(Zn)
D:\Porphyrin-Data\19 [Zn-4]\[Zn-4]-1H\RT-10-38TBAF-TPP-mesoBr(Zn)•ÒWŒä-1H.als
9.687
9.672
8.899
8.884
8.788
8.160
8.140
8.118
7.735
7.719
7.696
7.672
7.240
1.852
2.0000
2.0465
4.0449
6.3095
9.0662
PPM
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
DFILE RT-10-38TBAF-TPP-mesoBr(Zn)•ÒWŒä-1H.als
COMNT RT-10-38TBAF-TPP-mesoBr(Zn)
DATIM Sat Oct 27 15:09:25 2018
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.00 Hz
POINT 32768
FREQU 6006.01 Hz
SCANS 16
ACQTM 5.4559 sec
PD 1.5440 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 26.4 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.09 Hz
RGAIN 20

Ph
N
N
Ph
Zn
Br
N
N
Ph

Zn-6