Electronic Supplementary Information (ESI)

Catch & release of alkyne-tagged molecules in water by polymer-supported cobalt complex

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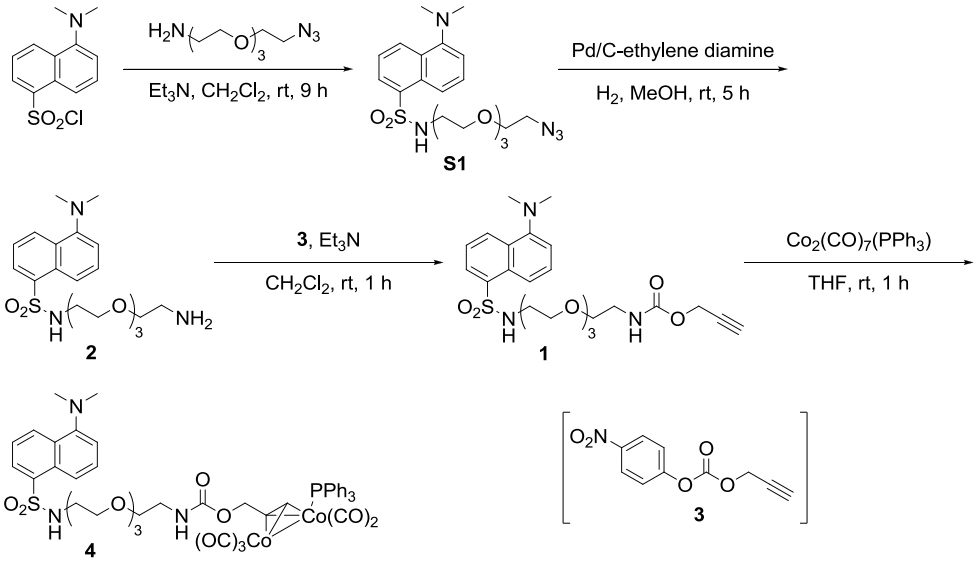
1. General

^{1}H, ^{13}C and ^{31}P NMR spectra were measured on a JEOL JNM-AL400 spectrometer at 400, 100 and 160 MHz, respectively. All chemical shifts were recorded in δ (ppm) relative to tetramethylsilane (TMS), chloroform or H_3PO_4. Infrared spectra were measured on a Thermo Nicolet iS5, and only diagnostic absorptions are listed below. HPLC analysis was performed on DIONEX UltiMate3000 consisting of the followings: pump, DGP-3600; auto-sampler, WPS-3000; flow manager, FLM-3x00; detector, VWD-3x00 measured at 280 nm. ESI-MS was taken on a Bruker micrOTOF-QII-$_{RSL}$. Column chromatography was performed with silica gel N-60 (40-100 μm) purchased from Kanto Chemical Co., Inc. or Chromatorex (N-H type silica gel) purchased from Fuji Silysia Chemical, Ltd. TLC analysis was performed on Silica gel 60 F_{254}-coated glass plates (Merck). Visualization was accomplished by means of ultraviolet (UV) irradiation at 254 nm or by spraying 12-molybdo(VI)phosphoric acid ethanol solution as the developing agent. Water was prepared with a Millipore Milli-Q Advantage A10. Dehydrated tetrahydrofuran (THF), methanol (MeOH) and dichloromethane (CH_2Cl_2) were purchased from Wako Pure Chemical Industries, Ltd. PS-PEG was purchased from HiPep Laboratories Co., Inc. Phosphine ligand supported by PS-PEG was synthesized according to the literature.[1] $Co_2(CO)_8$ was purchased from Kanto Chemical Co., Inc. $Co_2(CO)_7(PPh_3)$ was synthesized according to the literature.[2]

2. Synthesis of 1, 2, 4, 5 and 9

2.1. Synthesis of 1, 2 and 4



2.1.1. Synthesis of S1

To a solution of dansyl chloride (312 mg, 1 mmol) in CH_2Cl_2 was added Et_3N (560 ml, 4 mmol) and 11-azido-3,6,9-trioxaundecan-1-amine (220 µl, 1 mmol) at room temperature. The mixture was stirred for 9 h, then aqueous $NaHCO_3$ was added. After extraction with CH_2Cl_2, the combined organic layer was dried over Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was subjected to column chromatography on N-H type silica gel (hexane/ethyl acetate = 3/1) to give **S1** as a yellow viscous oil (418.3 mg, 93%). IR (neat): 2869, 2098, 1588, 1574, 1454, 1407, 1307, 1140, 1091, 941, 790 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.53 (d, 1H, J = 8.5 Hz), 8.30 (d, 1H, J = 8.8 Hz), 8.24 (dd, 1H, J = 1.2, 7.3 Hz), 7.58-7.49 (m, 2H), 7.18 (d, 1H, J = 7.6 Hz), 5.44 (t, 1H, J = 5.8 Hz), 3.68-3.60 (m, 6H), 3.52-3.48 (m, 2H), 3.40-3.37 (m, 6H), 3.11 (dt, 2H, J = 4.9, 5.8 Hz), 2.89 ppm (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 151.8, 135.0, 130.3, 129.8, 129.6, 129.2, 128.2, 123.1, 118.9, 115.1, 70.6, 70.6, 70.4, 70.3, 70.0, 69.2, 50.7, 45.4, 43.1 ppm; HRMS (ESI^+), Calcd for $[C_{20}H_{29}O_5SN_5 + Na]^+$: m/z = 474.1782, Found: m/z = 474.1784.

2.1.2. Synthesis of 2

To a solution of **S1** (390 mg, 0.86 mmol) in MeOH (10 ml) was added Pd/C-ethylene diamine complex (39 mg) at room temperature under nitrogen. The nitrogen was replaced with hydrogen, and the mixture was stirred for 5 h, then filtered through a pad of Celite. The filtrate was evaporated and the residue was subjected to column chromatography on N-H type silica gel (CH_2Cl_2/MeOH = 95/5) to give **2** as a yellow viscous oil (350.8 mg, 95%). IR (neat): 2865, 1587, 1573, 1453, 1405, 1352, 1310, 1139, 1091, 941, 790, 750 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.49 (d, 1H, *J* = 8.3 Hz), 8.34 (d, 1H, *J* = 8.8 Hz), 8.20 (dd, 1H, *J* = 1.2, 7.3 Hz), 7.54-7.45 (m, 2H), 7.15 (d, 1H, *J* = 7.6 Hz), 3.62-3.56 (m, 4H), 3.52-3.49 (m, 4H), 3.40-3.36 (m, 4H), 3.09 (t, 2H, *J* = 4.9 Hz), 2.85-2.84 ppm (m, 8H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 151.7, 135.6, 129.9, 129.8, 129.6, 128.9, 127.9, 123.1, 119.2, 115.0, 73.1, 70.5, 70.4, 70.2, 70.1, 69.7, 45.4, 43.0, 41.5 ppm; HRMS (ESI^+), Calcd for $[C_{20}H_{31}O_5SN_3 + H]^+$: *m/z* = 426.2057, Found: *m/z* = 426.2053.

2.1.3. Synthesis of 3

To a solution of 4-nitrophenyl chloroformate (1 g, 5 mmol) in THF was added Et_3N (0.8 ml, 5.8 mmol) and 2-propyn-1-ol (290 μl, 4.98 mmol) at 0 °C. The mixture was stirred for 1 h, then the reaction was quenched by addition of aqueous NH_4Cl. After extraction with ethyl acetate, the combined organic layer was dried over Na_2SO_4 and filtered. The filtrate was concentrated *in vacuo* and the residue was subjected to column chromatography on silica gel (hexane/ethyl acetate = 7/1) to give **3** as a colorless solid (905 mg, 82%). IR (neat): 3271, 2134, 1751, 1595, 1519, 1375, 1349, 1262, 1229, 1060, 966, 957, 859, 730 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.28 (d, 2H, *J* = 9.3 Hz), 7.40 (d, 2H, *J* = 9.3 Hz), 4.88 (d, 2H, *J* = 2.2 Hz), 2.62 ppm (t, 1H, *J* = 2.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.1, 151.8, 145.4, 125.2, 121.6, 76.7, 76.0, 56.5 ppm; HRMS (ESI^+), Calcd for $[C_{10}H_7NO_5 + Na]^+$: *m/z* = 244.0216, Found: *m/z* = 244.0218.

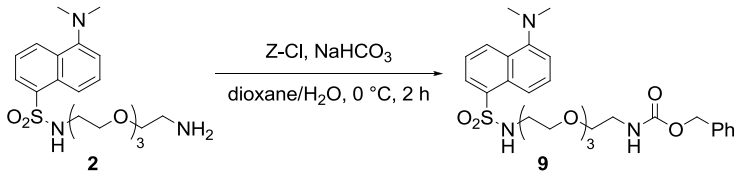
2.1.4. Synthesis of 1

To a solution of **2** (350 mg, 0.82 mmol) in CH_2Cl_2 (10 ml) was added Et_3N (460 µl, 3.3 mmol) and **3** (221 mg, 1 mmol) at room temperature. The solution was stirred for 1 h, followed by addition of aqueous $NaHCO_3$. After extraction with ethyl acetate, the combined organic layer was washed with brine, dried over Na_2SO_4 and filtered. The filtrate was evaporated *in vacuo* and the residue was subjected to column chromatography on silica gel (hexane/ethyl acetate = 3/1) to give **1** as a yellow viscous oil (368.3 mg, 88%). IR (neat): 3267, 2870, 1711, 1588, 1573, 1525, 1455, 1319, 1232, 1139, 1090, 941, 790 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.53 (d, 1H, J = 8.5 Hz), 8.31 (d, 1H, J = 8.5 Hz), 8.24 (dd, 1H, J = 1.5, 7.3 Hz), 7.56-7.49 (m, 2H), 7.18 (d, 1H, J = 7.6 Hz), 5.57-5.49 (m, 2H), 4.65 (d, 2H, J = 2.4 Hz), 3.63-3.54 (m, 6H), 3.50-3.48 (m, 2H), 3.43-3.35 (m, 6H), 3.11 (dt, 2H, J = 4.9, 5.6 Hz), 2.89 (s, 6H), 2.43 ppm (t, 1H, J = 2.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.3, 151.7, 134.9, 130.2, 129.7, 129.5, 129.2, 128.1, 123.0, 118.8, 115.0, 78.3, 74.4, 70.3, 70.2, 70.1, 70.1, 69.8, 69.2, 52.3, 45.4, 43.0, 40.8 ppm; HRMS (ESI^+), Calcd for $[C_{24}H_{33}O_7SN_3 + H]^+$: m/z = 508.2112, Found: m/z = 508.2113.

2.1.5. Synthesis of 4

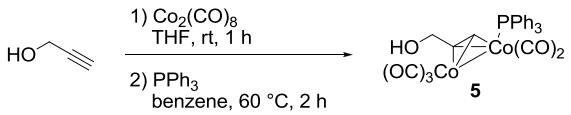
To a solution of **1** (10 mg, 0.02 mmol) in THF (1 ml) was added $Co_2(CO)_7(PPh_3)$ (11.4 mg, 0.02 mmol) at room temperature. The mixture was stirred for 1 h, then concentrated under reduced pressure. The residue was subjected to column chromatography on silica gel (CH_2Cl_2/MeOH = 95/5) and GPC to give **4** [6.1 mg, 75% (based on recovered **1**)] as a dark brown viscous liquid, together with **1** (6.0 mg). IR (neat): 2060, 1997, 1958 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.52 (d, 1H, J = 9.0 Hz), 8.30 (d, 1H, J = 9.0 Hz), 8.23 (dd, 1H, J = 1.2, 7.3), 7.56-7.40 (m, 17H), 7.17 (d, 1H, J = 7.3 Hz), 5.48-5.44 (m, 1H), 5.25-5.16 (m, 2H), 4.74 (d, 1H, J = 14.4 Hz), 4.24 (d, 1H, J = 14.4 Hz), 3.61-3.35 (m, 14H), 3.12-3.06 (m, 2H), 2.88 ppm (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 201.4 (brs), 156.2, 151.9, 135.0, 134.6, 134.2, 132.9, 132.8, 130.4, 129.9, 129.7, 129.4, 128.6, 128.5, 128.3, 123.2, 118.9, 115.2, 71.0, 70.5, 70.3, 70.2, 70.1, 69.2, 65.3, 45.4, 43.0, 40.7 ppm; ^{31}P NMR ($CDCl_3$, 160 MHz): δ 53.9 ppm; HRMS (ESI^+), Calcd for $[C_{24}H_{33}SO_7N_3Co_2(PC_{18}H_{15})(CO)_5 + Na]^+$: m/z = 1050.1253, Found: m/z = 1050.1253.

2.2. Synthesis of 9



To a solution of **2** (85 mg, 0.2 mmol) in dioxane/H_2O (3 ml/3 ml) were added $NaHCO_3$ (51 mg, 0.6 mmol) and benzyl chloroformate (34 μl, 0.24 mmol) at 0 °C. The solution was stirred for 2 h at 0 °C, followed by addition of aqueous NH_4Cl. After extraction with ethyl acetate, the combined organic layer was washed with brine, dried over $MgSO_4$ and filtered. The filtrate was concentrated under reduced pressure and the residue was subjected to column chromatography on silica gel (ethyl acetate) to give **9** as a yellow viscous oil (93.6 mg, 84%). IR (neat): 3311, 2869, 1701, 1587, 1573, 1521, 1454, 1321, 1231, 1140, 1091, 941, 790, 750 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.52 (d, 1H, J = 8.5 Hz), 8.30 (d, 1H, J = 8.5 Hz), 8.23 (d, 1H, J = 7.3 Hz), 7.56-7.48 (m, 2H), 7.36-7.28 (m, 5H), 7.17 (d, 1H, J = 7.3 Hz), 5.47 (brs, 1H), 5.37 (brs, 1H), 5.07 (s, 2H), 3.61-3.34 (m, 14H), 3.08-3.04 (m, 2H), 2.88 ppm (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 156.3, 151.7, 136.5, 135.0, 130.1, 129.7, 129.5, 129.1, 128.3, 128.1, 127.9, 127.9, 123.0, 118.9, 115.0, 70.3, 70.2, 70.0, 70.0, 69.9, 69.2, 66.5, 45.4, 42.9, 40.8 ppm; HRMS (ESI^+), Calcd for $[C_{28}H_{37}N_3O_7S + Na]^+$: m/z =582.2244, Found: m/z = 582.2247.

2.3. Synthesis of 5



To a solution of 2-propyn-1-ol (58 μl, 1 mmol) in THF (5 ml) was added $Co_2(CO)_8$ (342 mg, 1 mmol) at room temperature. The mixture was stirred for 1 h, then concentrated under reduced pressure. The residue was dissolved in benzene (5 ml) and triphenylphosphine (262 mg, 1 mmol) was added to the solution under nitrogen atmosphere. After stirring for 2 h at 60 °C, the reaction mixture was concentrated under reduced pressure. The residue was subjected to column chromatography on silica gel (hexane/ethyl acetate = 3/1) to give **5** (240 mg, 41%) as a brown viscous liquid. IR (neat): 2059, 1994 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.49-7.40 (m, 15H),

5.21 (d, 1H, J = 3.7 Hz), 4.18 (dd, 1H, J = 5.0, 14.2 Hz), 3.90-3.85 (m, 1H), 1.34 ppm (dd, 1H, J = 5.0, 7.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 205.7, 204.6, 201.6, 134.5 (d, J = 42 Hz), 132.9 (d, J = 11 Hz), 130.4, 128.6 (d, J = 11Hz), 92.1, 70.9, 62.8 ppm; ^{31}P NMR ($CDCl_3$, 160 MHz): δ 53.9 ppm; LC-MS (ESI$^+$) [GL Sciences Inertsil ODS-3, H_2O/MeCN (0.1% TFA) = 84/16 (0-10 min) → 75/25 (10-25 min) → 23/77 (25-35 min), 100 μl/min, 280 nm, τ = 33.8 min], Calcd for $[(C_3H_4O)Co_2(PC_{18}H_{15})(CO) + Na]^+$: m/z = 486.9679, Found: m/z = 486.9662, Calcd for $[(C_3H_4O)Co_2(PC_{18}H_{15})(CO)_2 + Na]^+$: m/z = 514.9628, Found: m/z = 514.9604, Calcd for $[(C_3H_4O)Co_2(PC_{18}H_{15})(CO)_3 + Na]^+$: m/z = 542.9577, Found: m/z = 542.9562, Calcd for $[(C_3H_4O)Co_2(PC_{18}H_{15})(CO)_4 + Na]^+$: m/z = 570.9526, Found: m/z = 570.9509, Calcd for $[(C_3H_4O)Co_2(PC_{18}H_{15})(CO)_5 + Na]^+$: m/z = 598.9475, Found: m/z = 598.9459.

3. Reaction of 4 with TFA (Figure 1)

To a solution of triphenylphosphine-cobalt-alkyne complex **4** in 5% MeCN/H_2O (50 μM, 1 ml) was added TFA (50 μl) at 4 °C. The reaction mixture was stirred at 4 °C. Aliquots (5 μl) were taken from the reaction mixture at intervals and subjected to HPLC analysis to monitor the reaction. The conversions and yields of all materials were calculated with reference to standard curves. HPLC [GL Sciences Inertsil ODS-3, H_2O/MeCN (0.1% TFA) = 84/16 (0-10 min) → 75/25 (10-25 min) → 23/77 (25-35 min), 100 μl/min, 280 nm, τ (compound **2**) = 7.0 min, τ (compound **1**) = 19.9 min, τ (compound **4**) = 32.4 min, τ (compound **5**) = 33.8 min].

4. Synthesis of cobalt complexes 7 and 8 (Scheme 3)[3]

4.1. Preparation of complex 7

To a solution of $Co_2(CO)_8$ (30 mg, 0.088 mmol) in THF (0.5 ml) was added phosphine supported on PS-PEG (30 mg, <0.28 mmol/g). After rotation for 3 h in a tube rotator, the mixture was filtered on a glass filter and the beads were washed with THF (10 ml) and MeOH (10 ml). The IR spectrum was directly measured. IR (neat): 2077, 2021, 1985, 1956 cm^{-1}.

4.2. Reaction of alkyne 1 and cobalt complex 7

Cobalt complex **7** supported on PS-PEG (30 mg, <0.28 mmol/g) was added to a solution of **1** (9 mg, 0.018 mmol) in Hepes buffer (pH 7.0) containing 150 mM NaCl, 10 mM Hepes-Na, 0.5% and Triton X-100 (9 ml) at room temperature. The mixture was rotated for 6 h, then centrifuged, and the supernatant was collected. The beads were washed with the same buffer (9 ml × 3), and the IR spectrum was directly measured in a wet condition. IR (neat): 2064, 2012, 2002, 1960 cm^{-1}.

5. Catch & release reaction of alkyne 1 at 4 °C under highly diluted conditions (Scheme 4)

Cobalt complex **7** (10 mg) was added to a solution of **1** (50 μM, 1 ml) in Hepes buffer (pH 7.0) containing 150 mM NaCl, 10 mM Hepes-Na, and 0.5% Triton X-100 at 4 °C. The mixture was rotated for 12 h at the same temperature, then centrifuged. After removal of the supernatant, the beads were washed with Hepes buffer (1 ml × 10). The supernatant and the washing solutions were subjected to fluorescence analysis (excitation: 355 nm, emission: 538 nm) to determine the conversion. To the beads was added 5% TFA solution (1 ml) and the mixture was rotated for 24 h. An aliquot of the supernatant was subjected to HPLC analysis to determine the yields of products. The conversions and yields of all materials were calculated with reference to standard curves. HPLC [GL Sciences Inertsil ODS-3, H_2O/MeCN (0.1% TFA) = 86/14 (0-10 min) → 77/23 (10-25 min), 100 μl/min, 280 nm, τ (compound **2**) = 10.1 min, τ (compound **1**) = 23.8 min].

6. Selective reaction of 1 in the presence of control material 9 (Scheme 5)

Cobalt beads **7** (10 mg) were added to a solution (1 ml) of **1** (50 μM) and **9** (50 μM) in Hepes buffer (pH 7.0) containing 150 mM NaCl, 10 mM Hepes-Na, and 0.5% Triton X-100 at 4 °C. The mixture was rotated for 12 h at the same temperature, then centrifuged. After removal of supernatant, the beads were washed with buffer (1 ml × 10). The supernatant and the washing solutions were subjected to HPLC analysis to determine conversions. To the beads was added 5% TFA in 5% MeCN/H_2O (1 ml) and the mixture was rotated for 24 h. A part of the supernatant was subjected to the HPLC analysis and the yields of all materials were calculated. The conversions and yields of all materials were calculated with reference to standard curves. HPLC [GL Sciences Inertsil ODS-3, H_2O/MeCN (0.1% TFA) = 86/14 (0-10 min) → 77/23 (10-25 min) → 61/39

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(25-35 min), 100 μl/min, 280 nm, τ (compound **2**) = 10.1 min, τ (compound **1**) = 23.8 min, τ (compound **9**) = 31.0 min].

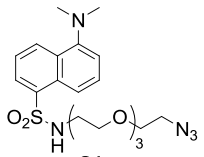
7. References

[1] H. Danjo, D. Tanaka, T. Hayashi and Y. Uozumi, *Tetrahedron*, 1999, **55**, 14341-14352.

[2] S. E. Gibson, C. Johnstone and A. Stevenazzi, *Tetrahedron*, 2002, **58**, 4937-4942.

[3] The cobalt complexes were identified by comparison of their IR spectra with the reported spectra of triphenylphosphine complexes and other analogous complexes. See (a) P. Szabo, L. Fekete and G. Bor, *J. Organomet. Chem.*, 1968, **12**, 245-248; (b) L. M. Bower and M. H. B. Stiddard, *J. Organomet. Chem.*, 1968, **13**, 235-239; (c) G. O. Evans, C. U. Pittman, Jr., R. McMillan, R. T. Beach and R. Jones, *J. Organomet. Chem.*, 1974, **67**, 295-314; (d) R. A. Dubois, P. E. Garrou, K. D. Lavin and H. R. Allcock, *Organometallics*, 1986, **5**, 460-466; (e) A. C. Comely, S. E. Gibson, N. J. Hales, C. Johnstone and A. Stevenazzi, *Org. Biomol. Chem.*, 2003, **1**, 1959-1968.

8. NMR spectra



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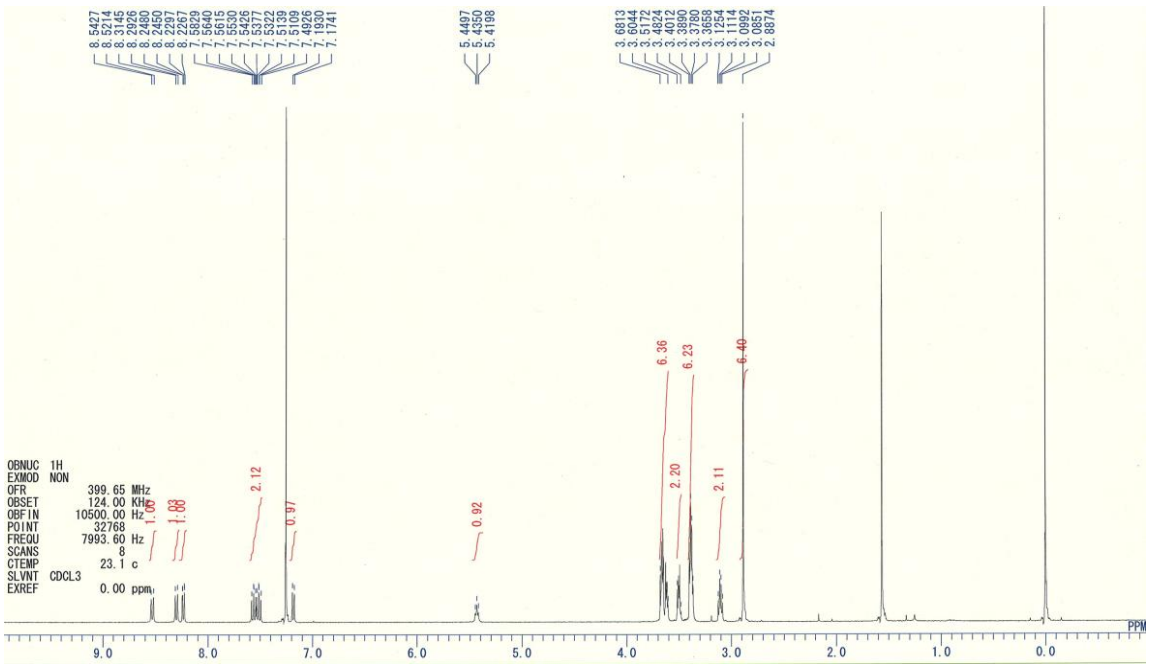

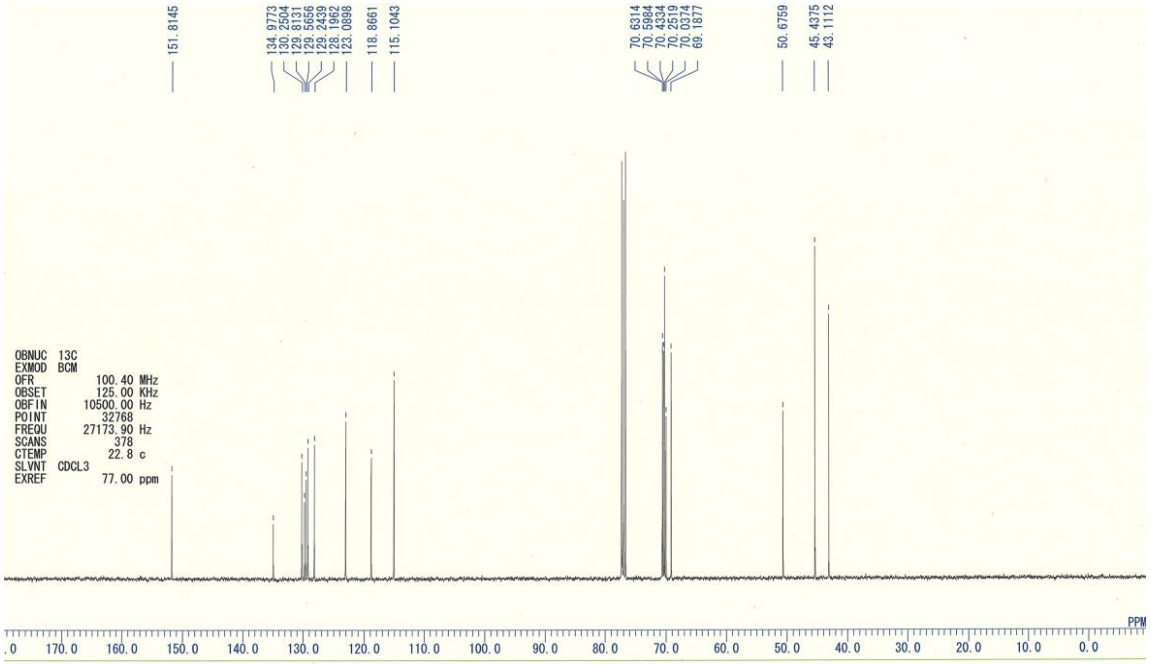

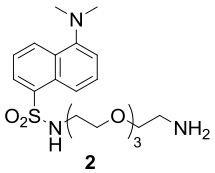

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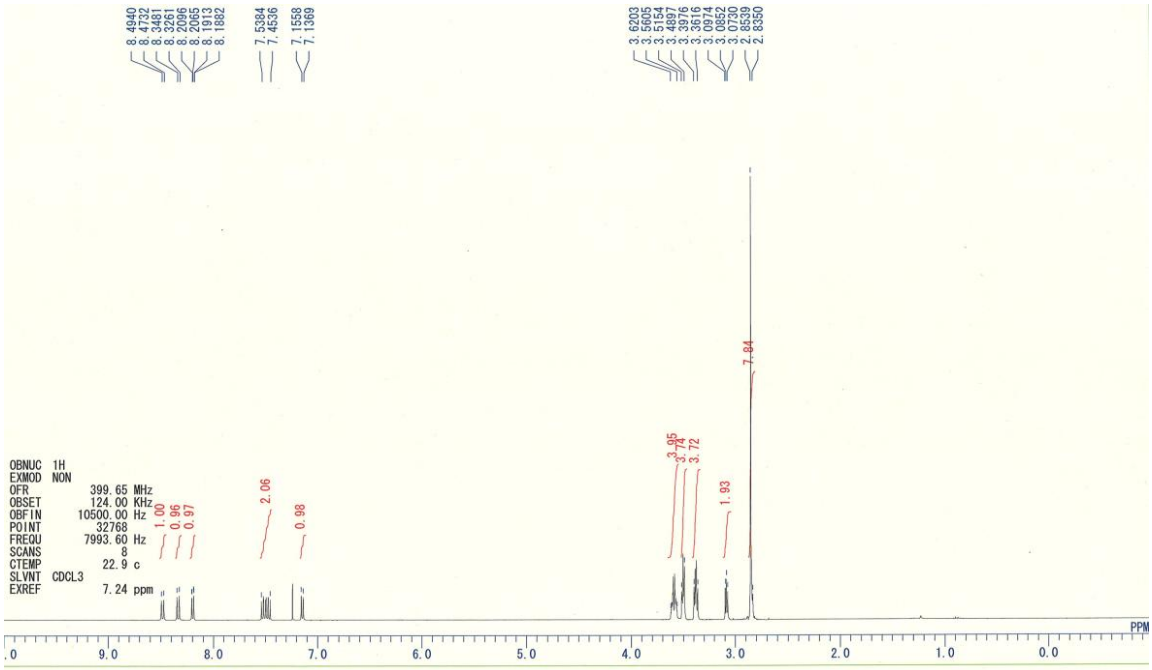
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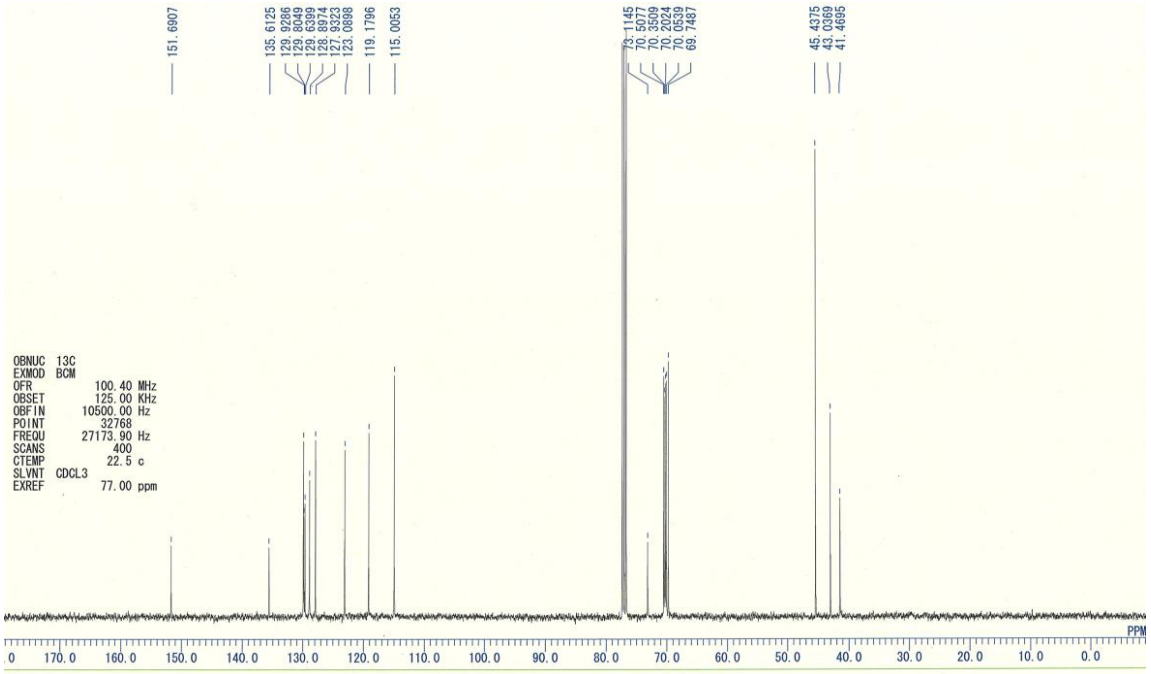
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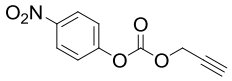

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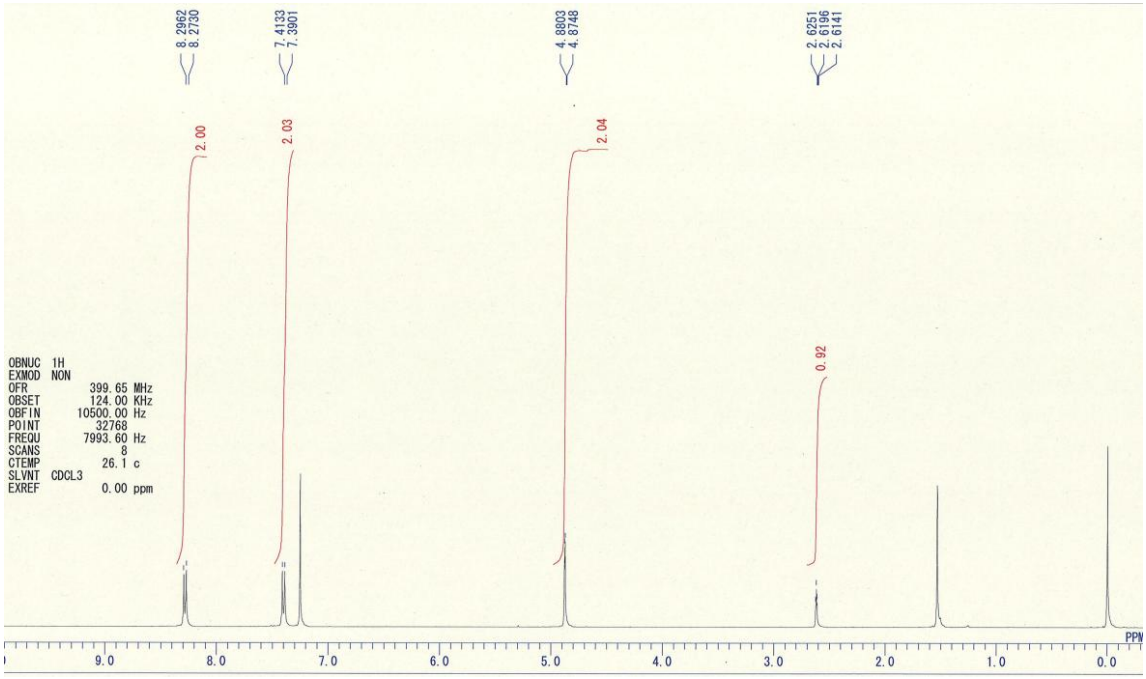
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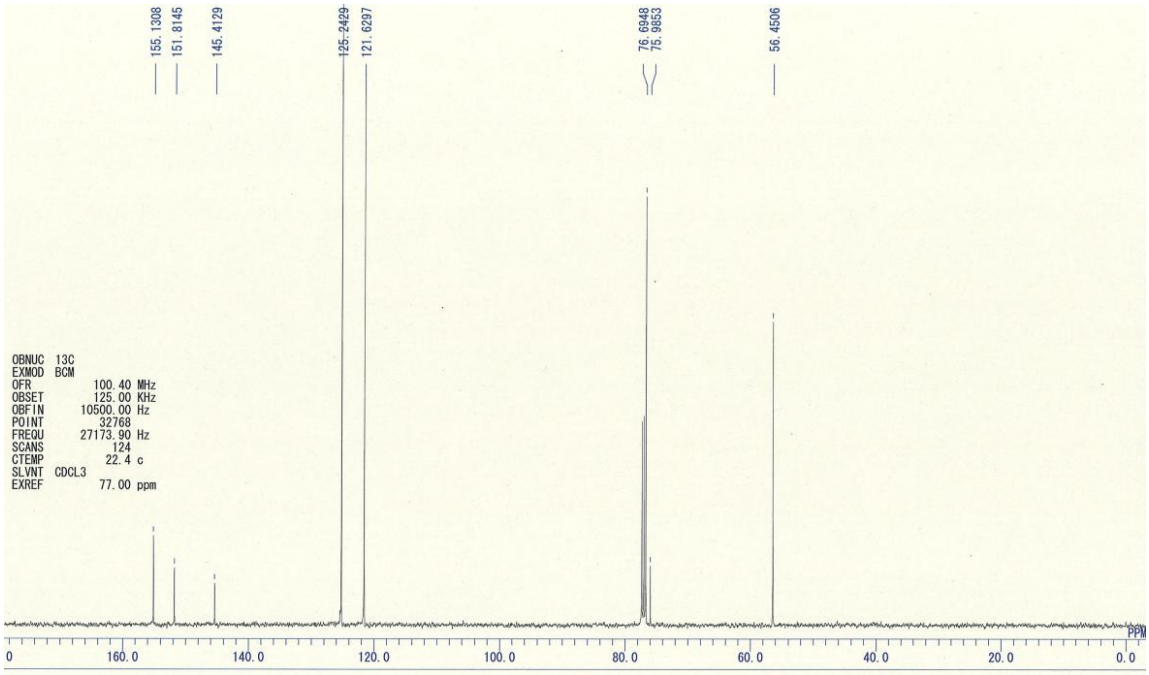
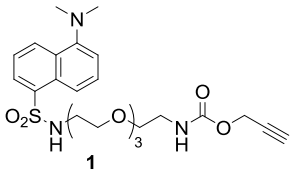
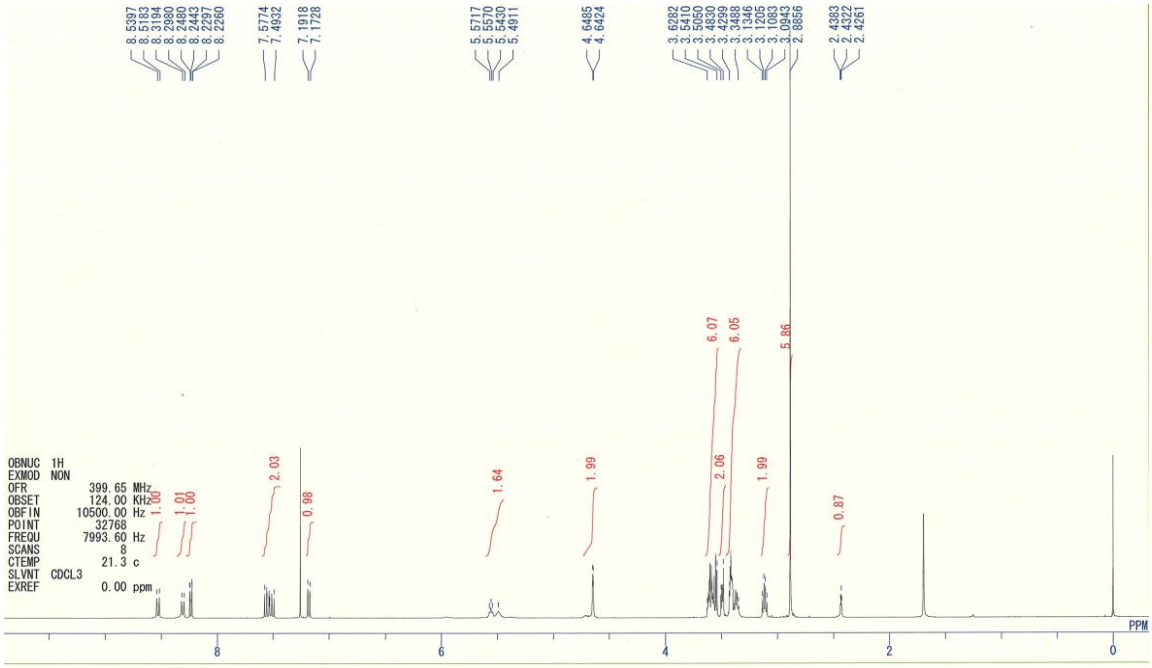
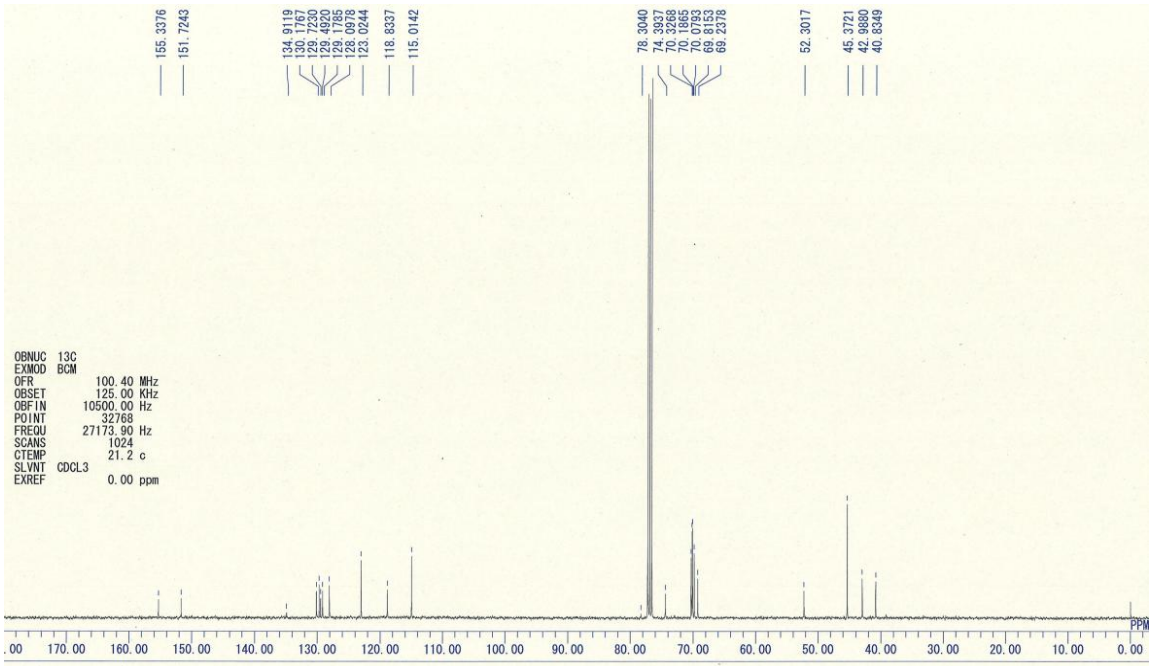
2.6196
2.6141
2.00
2.03
2.04
0.92
OBNUC 1H
EXMOD NON
OFR 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 7993.60 Hz
SCANS 8
CTEMP 26.1 c
SLVNT CDCL3
EXREF 0.00 ppm
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
PPM

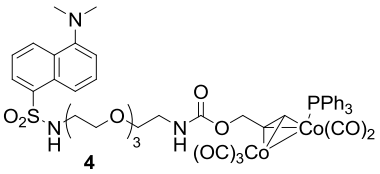

155.1308
151.8145
145.4129
125.2429
121.6297
76.6948
75.9853
56.4506
OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27173.90 Hz
SCANS 124
CTEMP 22.4 c
SLVNT CDCL3
EXREF 77.00 ppm
160.0
140.0
120.0
100.0
80.0
60.0
40.0
20.0
0.0
PPM



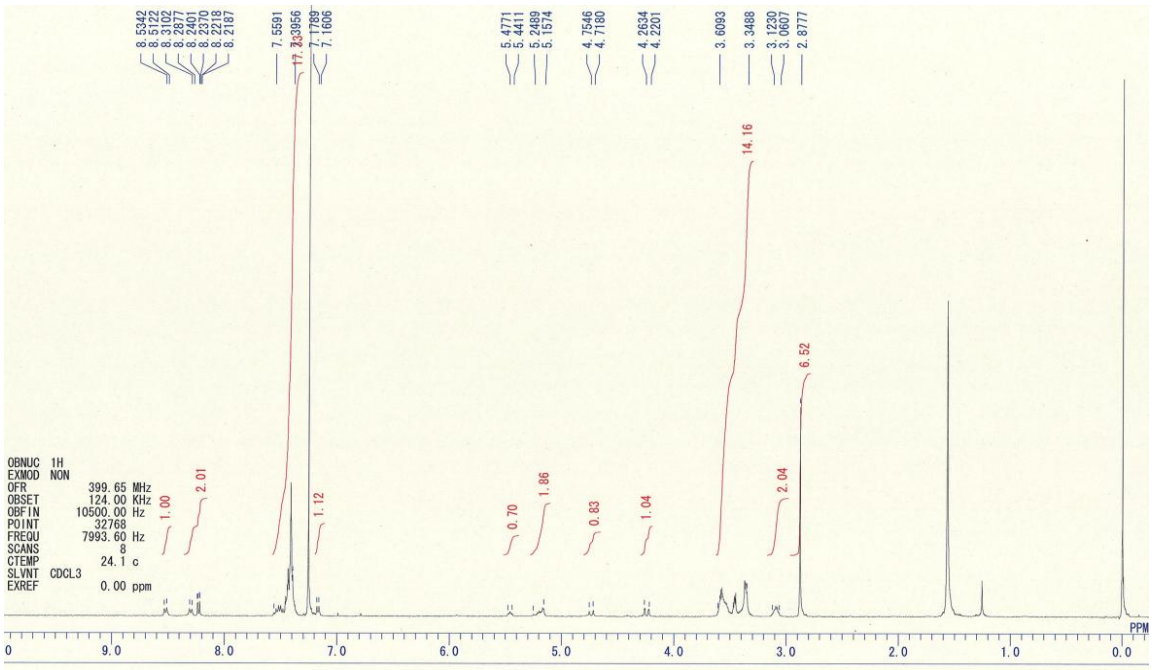
1

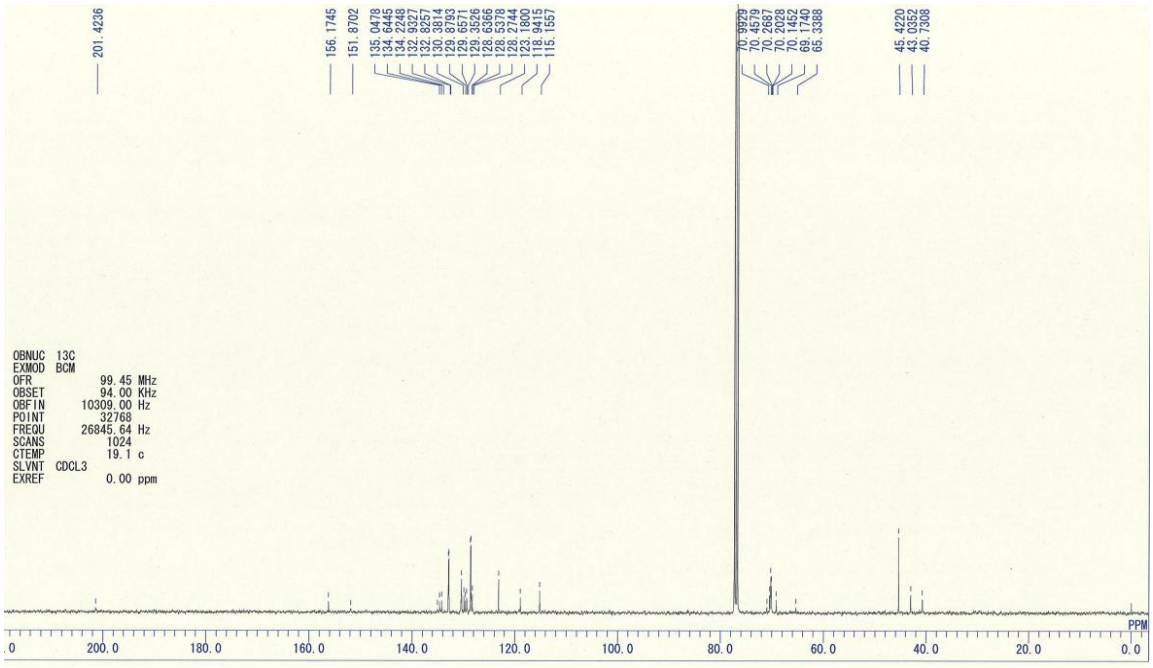

8.5397
8.5163
8.3194
8.2980
8.2460
8.2443
8.2297
8.2260
7.5774
7.4932
7.1918
7.1728
5.5717
5.5570
5.5430
5.4911
4.6485
4.6424
3.6282
3.5410
3.5050
3.4830
3.4299
3.3488
3.1346
3.1205
3.1043
3.0943
2.8856
2.4383
2.4322
2.4261
6.07
6.05
5.86
2.03
1.64
1.99
2.06
1.99
0.87
0.98
1.00
1.01
1.00
OBNUC 1H
EXMOD NON
OFR 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 7993.60 Hz
SCANS 8
CTEMP 21.3 c
SLVNT CDCL3
EXREF 0.00 ppm
PPM
8
6
4
2
0

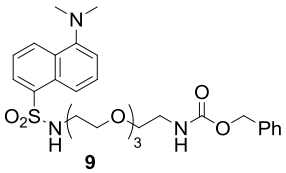

155.3376
151.7243
134.9119
130.1767
129.7230
129.4920
129.1755
128.0978
123.0244
118.8337
115.0142
78.3040
74.3937
70.3268
70.1865
70.0793
69.8153
69.2378
52.3017
45.3721
42.9880
40.8349
OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27173.90 Hz
SCANS 1024
CTEMP 21.2 c
SLVNT CDCL3
EXREF 0.00 ppm
PPM
170.00
160.00
150.00
140.00
130.00
120.00
110.00
100.00
90.00
80.00
70.00
60.00
50.00
40.00
30.00
20.00
10.00
0.00


N
O2S
N
H
O
3
N
H
O
O
PPh3
Co(CO)2
(OC)3Co

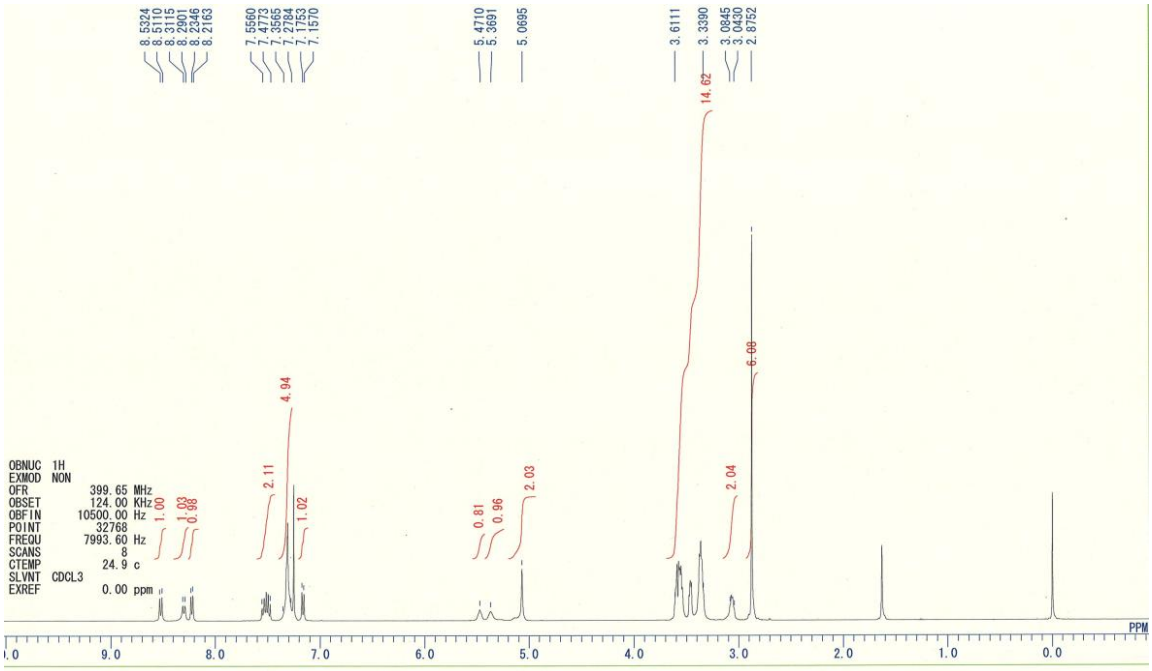
4

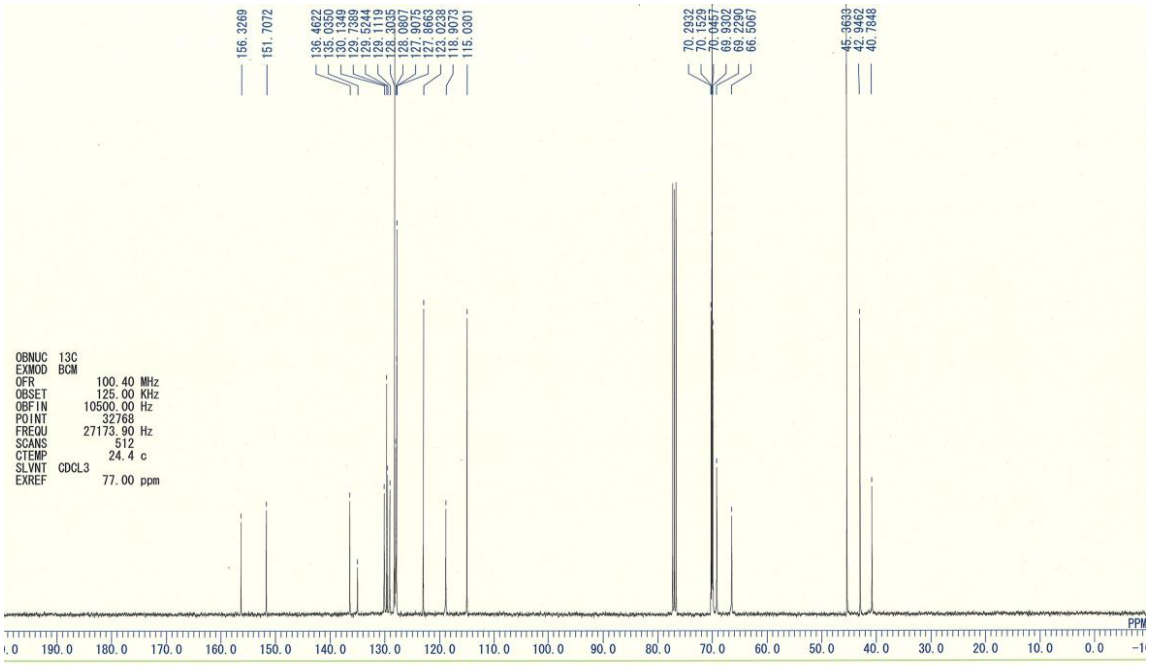

8.5342
8.5122
8.3102
8.2877
8.2401
8.2370
8.2218
8.2187
7.5591
7.3956
7.1789
7.1606
5.4771
5.4411
5.2489
5.1574
4.7546
4.7180
4.2634
4.2201
3.6093
3.3488
3.1230
3.0607
2.8777
14.16
6.52
2.04
1.00
2.01
1.12
0.70
1.86
0.83
1.04
OBNUC 1H
EXMOD NON
OFR 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 7993.60 Hz
SCANS 8
CTEMP 24.1 c
SLVNT CDCL3
EXREF 0.00 ppm
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

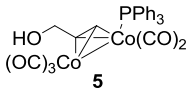

201.4236
156.1745
151.8702
135.0478
134.6445
134.2248
132.9327
132.8257
130.3814
129.8793
129.8571
129.3526
128.6366
128.5378
128.2744
123.1800
118.9415
115.1557
70.9929
70.4579
70.2687
70.2028
70.1452
69.1740
65.3388
45.4220
43.0352
40.7308
OBNUC 13C
EXMOD BCM
OFR 99.45 MHz
OBSET 94.00 KHz
OBFIN 10309.00 Hz
POINT 32768
FREQU 26845.64 Hz
SCANS 1024
CTEMP 19.1 c
SLVNT CDCL3
EXREF 0.00 ppm
PPM
200.0
180.0
160.0
140.0
120.0
100.0
80.0
60.0
40.0
20.0
0.0



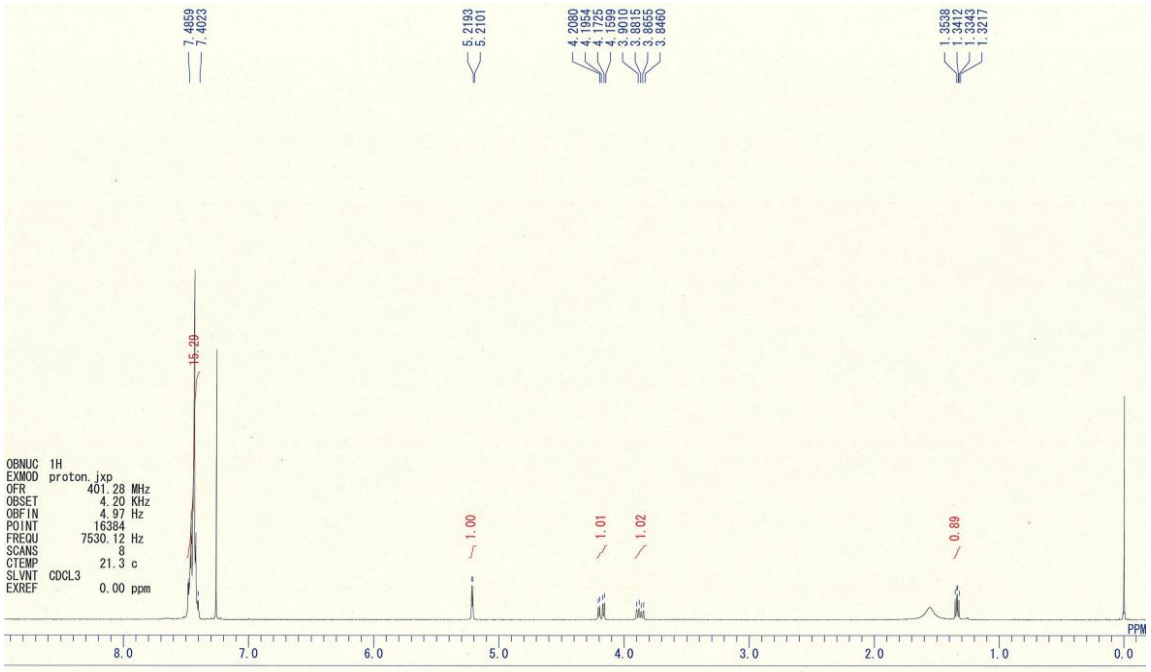
9

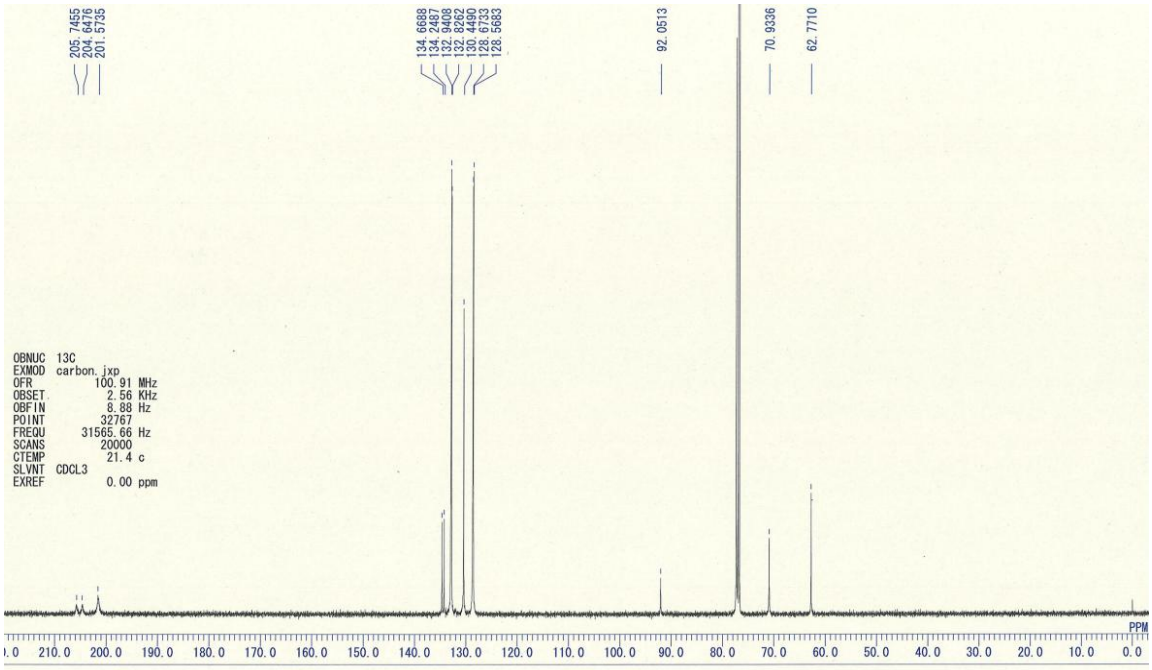

OBNUC 1H
EXMOD NON
OFR 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 7993.60 Hz
SCANS 8
CTEMP 24.9 c
SLVNT CDCL3
EXREF 0.00 ppm


OBNUC 13C
EXMOD BCM
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27173.90 Hz
SCANS 512
CTEMP 24.4 c
SLVNT CDCL3
EXREF 77.00 ppm


PPh3
HO
Co(CO)2
(OC)3Co

5


7.4859
7.4023
5.2193
5.2101
4.2080
4.1954
4.1725
4.1599
3.9010
3.8815
3.8655
3.8460
1.3538
1.3412
1.3343
1.3217
15.29
1.00
1.01
1.02
0.89
OBNUC 1H
EXMOD proton.jxp
OFR 401.28 MHz
OBSET 4.20 KHz
OBFIN 4.97 Hz
POINT 16384
FREQU 7530.12 Hz
SCANS 8
CTEMP 21.3 c
SLVNT CDCL3
EXREF 0.00 ppm
PPM
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


205.7455
204.6476
201.5735
134.6688
134.2487
132.9408
132.8262
130.4490
128.6733
128.5683
92.0513
70.9336
62.7710
OBNUC 13C
EXMOD carbon.jxp
OFR 100.91 MHz
OBSET 2.56 KHz
OBFIN 8.88 Hz
POINT 32767
FREQU 31565.66 Hz
SCANS 20000
CTEMP 21.4 c
SLVNT CDCL3
EXREF 0.00 ppm
PPM
210.0
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