Electronic Supplementary Information for

Integration of CO_2 Capture, Activation, and Conversion in a Ternary Acetylglucosyl 2-Methyl-imidazolium Modified Pd Catalyst

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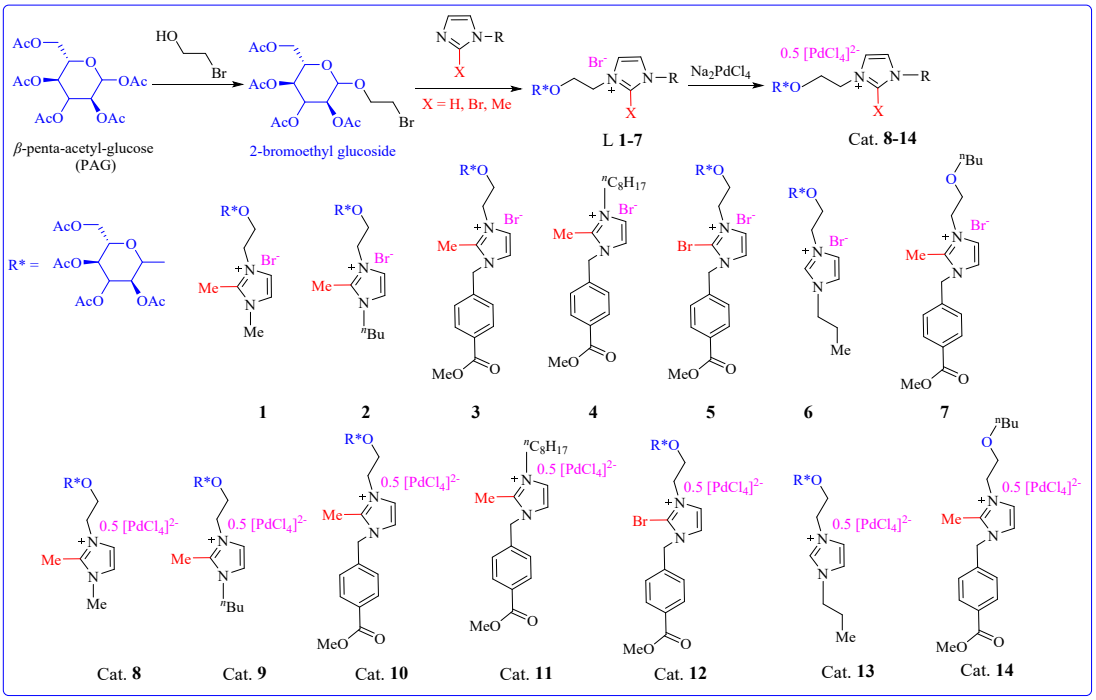
1. Experimental Section

1.1 General

All NMR spectra were tested with Bruker Advance III 400 NMR spectrometer. Chemical shifts were given in ppm. Melting points were determined on X-5 melting point instrument. FT-IR spectra were tested on an Avatar Nicholet FT-IR spectrometer in neat with the smart OMNI-transmission accessories or KBr pellets by standard method, and frequencies were reported as cm^{-1}. HPLC/HR-MS (ESI) spectra were acquired using a Waters G2-XS QTOF mass spectrometer, and the samples were dissolved in methanol.

All reagents were supplied commercially from Sinopharm Chemical Reagent Limited Corporation or Shanghai Aladdin Biochemical Technology Co., Ltd., and were used as received unless otherwise noted. Nitrogen gas (N_2, 99.999%) and dilute CO_2 (CO_2/N_2, Vol/Vol = 15:85) were purchased from Ganzhou Shengda Gas Co., Ltd. Flash column chromatography was performed over silica gel (300-400 mesh).

1.2 Synthesis and Characterization of Imidazolium Salts



Scheme S1. The synthesis and structures of imidazolium salts **1-14**.

Synthesis of R-Im-Br 1-7.

β-Penta-acetyl-glucose (PAG, 12.00 g, 30 mmol) and bromoethanol (4.2 g, 34 mmol) were dissolved in DCM (100 mL) and treated with $BF_3{\cdot}OEt_2$ (6.6 g, 46 mmol). The reaction was stirred at R.T. for 6 h and washed with a solution of $NaHCO_3$ and saturated salt water. The organic layer was dried over $MgSO_4$ and then concentrated. The solid was crystallized from ethanol to give colorless crystals 2-bromoethyl glucoside (7.8 g, 56%). The 2-bromoethyl glucoside (1.0 equivalent) and *N*-alkylated imidazole (3.0 equivalent) were dissolved in dry acetonitrile, and the resulting solution was heated at 110 °C for 48 h. After cooling, acetonitrile was removed by rotary evaporation. Purification by column chromatography on silica with dichloromethane/methanol (V:V = 20:1 to 10:1) afforded products R-Im-Br **1-7** (84-96 %) as pale yellow solids.[1]

Synthesis of $Im\text{-}PdCl_4$ 8-14.

In a 100 mL round-bottom flask, R-Im-Br **1** (0.17 g, 0.30 mmol) were dissolved in 50.0 mL of dichloromethane, and aqueous solution of potassium tetrachloropalladate (0.1 $g{\cdot}mL^{-1}$, 7.6 mL) was added in the flask and the mixture was stirred at room temperature overnight. The

solution was washed twice with ultrapure water, then removed by rotary evaporation and dried under vacuum to get the product Im-$PdCl_4$ **8** (0.17 g, 99%) as a reddish brown solid. R-Im-$PdCl_4$ **9-14** were prepared in a similar method of that for R-Im-$PdCl_4$ **8**. The R-Im-$PdCl_4$ **8-14** absorbs moisture easily and followed the trend of the other palladium salts, being reddish brown.

1-[2-(2,3,4,6-tetra-O-acetyl-*β*-D-glucopyranosyloxy)-ethyl]-2,3-dimethyl-imidazolium bromide (1)

Pale yellow solid, 89%, M_p: 105 – 107 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, J = 1.9 Hz, 1H), 7.55 (d, J = 1.9 Hz, 1H), 5.13 (dd, J = 11.0, 8.0 Hz, 1H), 4.98 (t, J = 9.7 Hz, 1H), 4.83 (dd, J = 9.5, 8.1 Hz, 1H), 4.68 (dd, J = 15.0, 3.0 Hz, 1H), 4.52 (d, J = 8.0 Hz, 2H), 4.22 (dd, J = 12.4, 4.8 Hz, 2H), 4.14 – 4.00 (m, 2H), 3.91 (s, 3H), 3.72 (ddd, J = 10.1, 4.7, 2.0 Hz, 1H), 2.70 (s, 3H), 2.07 (s, 3H), 2.01 – 1.88 (m, 9H);^{13}C NMR (101 MHz, $CDCl_3$): δ 170.1, 169.3, 168.9, 168.8, 144.5, 122.0, 120.9, 99.5, 77.3, 77.0, 76.7, 71.8, 70.8, 70.4, 67.6, 67.5, 61.0, 53.2, 47.8, 35.3, 20.2, 20.2, 19.9, 19.9, 10.1.FT-IR (KBr): 3417, 2958, 1748, 1632, 1592, 1541, 1429, 1375, 1228, 1039, 909, 697, 601, 431 cm^{-1}. LC–HR/MS (ESI-QTOF) m/z: $[M-Br]^+$ calcd for $C_{21}H_{31}N_2O_{10}$, 471.1973; found, 471.1980.

1-[2-(2,3,4,6-tetra-O-acetyl-*β*-D-glucopyranosyloxy)-ethyl]-2-methyl-3-butyl-imidazolium bromide (2)

Pale yellow solid, 91%, M_p: 123 – 128 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, J = 2.1 Hz, 1H), 7.43 (d, J = 2.1 Hz, 1H), 5.09 (t, J = 9.5 Hz, 1H), 4.92 (t, J = 9.7 Hz, 1H), 4.78 (dd, J = 9.7, 8.0 Hz, 1H), 4.66 (ddd, J = 14.6, 5.3, 2.9 Hz, 1H), 4.55 (dd, J = 7.8, 3.1 Hz, 1H), 4.51 (d, J = 8.0 Hz, 1H), 4.19 (ddd, J = 12.3, 7.0, 4.1 Hz, 2H), 4.14 – 4.04 (m, 3H), 4.01 (dd, J = 12.4, 2.2 Hz, 1H), 3.70 (ddd, J = 10.1, 4.9, 2.2 Hz, 1H), 2.67 (s, 3H), 2.02 (s, 3H), 1.94 (s, 3H), 1.89 (d, J = 6.6 Hz, 6H), 1.76 (dt, J = 20.9, 7.5 Hz, 2H), 1.43 – 1.27 (m, 2H), 0.91 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 170.5, 169.8, 169.5, 169.4, 144.3, 122.6, 121.8, 100.2, 77.3, 77.0, 76.7, 72.5, 71.8, 71.0, 68.1, 67.7, 61.6, 53.4, 49.4, 49.3, 31.4, 20.9, 20.5, 20.5, 19.7, 13.5, 11.5. FT-IR (KBr): 3408, 2961, 2937, 2876, 1749, 1634, 1586, 1533, 1431, 1376, 1231, 1167, 1040, 909, 752, 675, 600, 557, 490 cm^{-1}. LC–HR/MS (ESI-QTOF) m/z: $[M-Br]^+$ calcd for $C_{24}H_{37}N_2O_{10}$, 513.2443; found, 513.2446.

1-[2-(2,3,4,6-tetra-O-acetyl-*β*-D-glucopyranosyloxy)-ethyl]-2-methyl-3-[4-(methoxycarbonyl)phenyl]-imidazolium bromide (3)

Pale yellow solid, 86%, M_p: 100 – 102 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, J = 8.3 Hz, 2H), 7.78 (d, J = 1.8 Hz, 1H), 7.62 (d, J = 1.8 Hz, 1H), 7.29 (d, J = 8.3 Hz, 2H), 5.53 (dd, J = 43.3, 15.7 Hz, 2H), 5.02 (t, J = 9.5 Hz, 1H), 4.83 (t, J = 9.7 Hz, 1H), 4.66 (dd, J = 9.6, 8.1 Hz, 1H), 4.47 (d, J = 8.0 Hz, 1H), 4.08 (dt, J = 12.4, 6.2 Hz, 2H), 3.98 – 3.89 (m, 2H), 3.75 (s, 3H), 3.64 (ddd, J = 10.1, 4.5, 2.2 Hz, 1H), 2.57 (s, 3H), 1.90 (s, 3H), 1.90 (s, 3H), 1.85 (s, 3H), 1.83 (s, 3H), 1.77 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 170.0, 169.3, 168.91, 168.9, 165.6, 144.6, 137.5, 130.0, 129.8, 127.5, 121.7, 121.4, 99.5, 77.3, 77.0, 76.7, 71.8, 71.1, 70.4, 67.6, 67.3, 61.1, 51.7, 51.1, 48.1, 20.2, 20.2, 19.9, 19.9, 10.5. FT-IR (KBr): 3416, 2957, 2929, 2858, 1753, 1723, 1615, 1584, 1531, 1434, 1374, 1283, 1226, 1111, 1039, 963, 909, 746, 672, 600, 539 cm^{-1}. LC–HR/MS (ESI-QTOF) m/z: $[M\text{-}Br]^+$ calcd for $C_{29}H_{37}N_2O_{12}$, 605.2346; found, 605.2349.

1-(*n*-octyl)-2-methyl-3-[4-(methoxycarbonyl)phenyl]-imidazolium bromide (4)

Pale yellow solid, 84%, M_p: 86 – 88 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, J = 2.0 Hz, 1H), 7.97 (d, J = 8.3 Hz, 2H), 7.74 (d, J = 2.0 Hz, 1H), 7.52 (d, J = 8.3 Hz, 2H), 5.86 (s, 2H), 4.28 (t, J = 7.4 Hz, 2H), 3.89 (s, 3H), 2.80 (s, 3H), 1.86 – 1.76 (m, 2H), 1.32 – 1.20 (m, 10H), 0.85 (t, J = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.4, 142.9, 137.7, 129.5, 129.4, 127.3, 121.7, 120.9, 77.3, 77.00, 76.7, 53.0, 51.4, 50.8, 48.8, 48.1, 30.7, 28.9, 28.1, 28.1, 25.4, 21.6, 13.1, 10.4. FT-IR (KBr): 3425, 3089, 3039, 2929, 2857, 1724, 1613, 1579, 1525, 1436, 1380, 1279, 1186, 1109, 1020, 964, 739, 540 cm^{-1}. LC–HR/MS (ESI-QTOF) m/z: $[M\text{-}Br]^+$ calcd for $C_{21}H_{31}N_2O_2$, 343.2380; found, 343.2383.

1-[2-(2,3,4,6-tetra-O-acetyl-*β*-D-glucopyranosyloxy)-ethyl]-2-bromo-3-[4-(methoxycarbonyl)phenyl]-imidazolium bromide (5)

Pale yellow solid, 96%, M_p: 112 – 116 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (d, J = 1.7 Hz, 1H), 7.90 (d, J = 1.8 Hz, 1H), 7.83 (d, J = 8.2 Hz, 2H), 7.37 (d, J = 8.2 Hz, 2H), 5.51 (q, J = 15.1 Hz, 2H), 5.00 (t, J = 9.5 Hz, 1H), 4.81 (t, J = 9.7 Hz, 1H), 4.72 – 4.64 (m, 1H), 4.52 (d, J = 8.0 Hz, 1H), 4.44 (s, 2H), 4.13 – 3.99 (m, 2H), 3.94 (d, J = 11.8 Hz, 2H), 3.71 (s, 3H), 3.68 – 3.63 (m, 1H), 1.88 (s, 3H), 1.84 – 1.73 (m, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 170.2, 169.5, 169.0, 169.0, 165.7, 136.7, 130.5, 130.0, 129.9, 128.3, 124.8, 123.9, 122.9, 99.6, 77.3,

77.0, 76.7, 72.0, 71.3, 70.5, 67.7, 66.2, 61.2, 53.0, 51.9, 50.3, 49.5, 20.4, 20.4, 20.1, 20.1. FT-IR (KBr): 3421, 2955, 1752, 1616, 1571, 1514, 1436, 1374, 1286, 1277, 1111, 1039, 908, 741, 675, 601, 538 cm^{-1}. LC–HR/MS (ESI-QTOF) m/z: $[M-Br]^+$ calcd for $C_{28}H_{34}BrN_2O_{12}$, 669.1295; found, 669.1297.

1-[2-(2,3,4,6-tetra-O-acetyl-*β*-D-glucopyranosyloxy)-ethyl]-3-propyl-imidazolium bromide (6)

Pale yellow solid, 88%, M_p: 86 – 88 °C. ^1H NMR (400 MHz, $CDCl_3$): δ 9.34 (s, 1H), 7.36 (d, J = 13.4 Hz, 2H), 4.85 (t, J = 9.5 Hz, 1H), 4.67 (t, J = 9.7 Hz, 1H), 4.60 – 4.52 (m, 1H), 4.43 (d, J = 8.0 Hz, 1H), 4.39 – 4.28 (m, 2H), 3.97 (t, J = 7.2 Hz, 2H), 3.90 (dd, J = 12.1, 4.4 Hz, 2H), 3.85 – 3.72 (m, 2H), 3.60 – 3.53 (m, 1H), 1.73 (s, 3H), 1.68 (s, 3H), 1.67 – 1.61 (m, 8H), 0.64 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 169.8, 169.0, 168.8, 168.6, 135.7, 122.6, 121.2, 99.4, 77.3, 77.0, 76.7, 71.5, 70.9, 70.3, 67.3, 66.9, 60.9, 50.6, 48.9, 22.7, 20.0, 20.0, 19.7, 19.7, 9.9. FT-IR (KBr): 3420, 2968, 2887, 1750, 1632, 1565, 1435, 1375, 1229, 1169, 1040, 909, 600, 540 cm^{-1}. LC–HR/MS (ESI-QTOF) m/z: $[M-Br]^+$ calcd for $C_{22}H_{33}N_2O_{10}$, 485.2130; found, 485.2137.

3-(2-butoxyethyl)-1-(4-(methoxycarbonyl)benzyl)-2-methyl-1H-imidazol-3-ium bromide (7)

Pale yellow solid, 89%. ^1H NMR (400 MHz, $CDCl_3$): δ 8.02 (d, J = 8.3 Hz, 2H), 7.85 (d, J = 2.0 Hz, 1H), 7.81 (d, J = 2.0 Hz, 1H), 7.36 (d, J = 8.3 Hz, 2H), 4.52 – 4.47 (m, 2H), 3.91 (s, 3H), 3.78 – 3.73 (m, 2H), 3.36 (t, J = 6.5 Hz, 2H), 2.71 (s, 3H), 1.44 – 1.36 (m, 3H), 1.33 – 1.26 (m, 1H), 1.19 (dt, J = 22.1, 7.4 Hz, 3H), 0.82 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 166.1, 144.7, 138.4, 130.3, 130.2, 127.6, 122.3, 122.0, 119.7, 77.3, 77.0, 76.7, 52.1, 51.5, 48.9, 31.3, 19.0, 13.6, 10.8. FT-IR (KBr): 3487, 3415, 3130, 3070, 2955, 2870, 1735, 1631, 1586, 1424, 1292, 1191, 1111, 1020, 834, 776, 745, 687, 557, 420 cm^{-1}.

1-[2-(2,3,4,6-tetra-O-acetyl-*β*-D-glucopyranosyloxy)-ethyl]-2,3-dimethyl-imidazolium tetratetrachloropalladate (8)

Reddish brown solid, 99%, M_p: 96 – 98 °C. ^1H NMR (400 MHz, $CDCl_3$): δ 7.76 (d, J = 2.1 Hz, 1H), 7.57 (d, J = 2.0 Hz, 1H), 5.19 (t, J = 9.5 Hz, 1H), 5.03 (t, J = 9.7 Hz, 1H), 4.92 (dd, J = 9.6, 8.0 Hz, 1H), 4.81 – 4.64 (m, 3H), 4.37 (dt, J = 8.7, 4.2 Hz, 1H), 4.27 (dd, J = 12.5, 4.6 Hz, 1H), 4.22 – 4.10 (m, 2H), 4.06 (s, 3H), 3.80 (ddd, J = 10.0, 4.5, 2.2 Hz, 1H), 2.93 (s,

3H), 2.10 (s, 3H), 2.02 – 1.96 (m, 9H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 170.6, 169.9, 169.5, 145.1, 128.5, 123.0, 122.2, 121.1, 100.3, 77.3, 77.0, 76.7, 72.5, 71.8, 71.1, 68.1, 67.8, 61.6, 49.3, 36.4, 20.9, 20.5, 20.5, 11.6. FT-IR (KBr): 3436, 3139, 2961, 2360, 1747, 1589, 1537, 1513, 1429, 1369, 1223, 1169, 1120, 1037, 957, 800, 748, 697 cm^{-1}. LC–HR/MS (ESI-QTOF) m/z: $[M\text{-}PdCl_4]^+$ calcd for $C_{21}H_{31}N_2O_{10}$, 471.1973; found, 471.1980.

1-[2-(2,3,4,6-tetra-O-acetyl-*β*-D-glucopyranosyloxy)-ethyl]-2-methyl-3-butyl-imidazolium tetratetrachloropalladate (9)

Reddish brown solid, 98%, M_p: 120 – 122 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, J = 2.0 Hz, 1H), 7.52 (d, J = 2.0 Hz, 1H), 5.16 (d, J = 9.5 Hz, 1H), 5.00 (t, J = 9.7 Hz, 1H), 4.89 (dd, J = 9.5, 8.1 Hz, 1H), 4.73 (dd, J = 18.8, 5.8 Hz, 3H), 4.39 (s, 1H), 4.34 – 4.28 (m, 2H), 4.28 – 4.22 (m, 2H), 4.12 (dd, J = 12.4, 1.9 Hz, 1H), 3.81 (dd, J = 10.1, 2.3 Hz, 1H), 2.91 (s, 3H), 2.07 (s, 3H), 2.00 – 1.94 (m, 9H), 1.93 – 1.87 (m, 2H), 1.45 (dq, J = 14.7, 7.3 Hz, 2H), 1.45 (dq, J = 14.7, 7.3 Hz, 2H), 0.99 (t, J = 7.3 Hz, 3H), 0.99 (t, J = 7.3 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 170.6, 169.9, 169.5, 144.4, 122.7, 121.9, 100.3, 77.3, 77.0, 76.7, 72.5, 71.9, 71.1, 68.1, 67.6, 61.7, 49.6, 49.4, 31.5, 20.9, 20.5, 20.5, 19.8, 13.6, 11.5. FT-IR (KBr): 3597, 3513, 3177, 3134, 2960, 2936, 2874, 1753, 1626, 1585, 1530, 1433, 1375, 1227, 1169, 1126, 1037, 908, 749, 698 cm^{-1}. LC–HR/MS (ESI-QTOF) m/z: $[M\text{-}PdCl_4]^+$ calcd for $C_{24}H_{37}N_2O_{10}$, 513.2443; found, 513.2446.

1-[2-(2,3,4,6-tetra-O-acetyl-*β*-D-glucopyranosyloxy)-ethyl]-2-methyl-3-[4-(methoxycarbonyl)phenyl]-imidazolium tetratetrachloropalladate (10)

Reddish brown solid, 98%, M_p: 93 – 95 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (d, J = 8.4 Hz, 2H), 7.82 (d, J = 2.2 Hz, 1H), 7.49 (d, J = 2.2 Hz, 1H), 7.47 (d, J = 8.4 Hz, 2H), 5.74 (d, J = 2.7 Hz, 2H), 5.22 (t, J = 9.5 Hz, 1H), 5.08 – 5.00 (m, 1H), 4.93 (dd, J = 9.7, 8.0 Hz, 1H), 4.83 (t, J = 4.9 Hz, 2H), 4.70 (d, J = 8.0 Hz, 1H), 4.42 (dt, J = 10.6, 4.4 Hz, 1H), 4.30 – 4.22 (m, 2H), 4.16 (dd, J = 12.5, 2.2 Hz, 1H), 3.94 (s, 3H), 3.79 (ddd, J = 10.1, 4.6, 2.2 Hz, 1H), 3.00 (s, 3H), 2.08 (s, 3H), 2.02 (s, 3H), 2.01 (s, 3H), 2.00 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 170.5, 169.9, 169.5, 169.4, 166.2, 145.2, 137.3, 131.0, 130.6, 128.4, 122.8, 122.3, 100.2, 77.3, 77.0, 76.7, 72.4, 71.9, 71.0, 68.1, 67.3, 61.6, 52.7, 52.3, 49.5, 20.9, 20.8, 20.5, 20.5, 11.8. FT-IR (KBr): 3452, 3141, 2954, 1752, 1615, 1585, 1529, 1434, 1376, 1285, 1227, 1111, 1038, 908, 744, 699 cm^{-1}. LC–HR/MS (ESI-QTOF) m/z: $[M\text{-}PdCl_4]^+$ calcd for

$C_{29}H_{37}N_2O_{12}$, 605.2346; found, 605.2349.

1-(*n*-octyl)-2-methyl-3-[4-(methoxycarbonyl)phenyl[-imidazolium tetratetrachloropalladate (11)

Reddish brown solid, 99%, M_p: 104 – 106 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, J = 8.2 Hz, 2H), 7.46 (d, J = 1.6 Hz, 1H), 7.41 (d, J = 8.3 Hz, 3H), 5.78 (s, 2H), 4.32 (t, J = 7.5 Hz, 2H), 3.90 (s, 3H), 2.95 (s, 3H), 1.91 – 1.78 (m, 2H), 1.39 – 1.15 (m, 11H), 0.86 (t, J = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 166.2, 144.0, 138.3, 130.5, 130.4, 128.1, 122.5, 121.7, 77.3, 77.0, 76.7, 52.7, 52.2, 49.5, 31.5, 29.4, 28.9, 28.9, 26.4, 22.5, 13.9, 11.9. FT-IR (KBr): 3440, 3158, 3115, 3093, 2953, 2934, 2853, 2382, 1953, 1728, 1656, 1613, 1580, 1530, 1465, 1439, 1379, 1358, 1352, 1278, 1186, 1165, 1109, 1020, 965, 871,838, 805, 782, 751, 733, 703 cm^{-1}. LC–HR/MS (ESI-QTOF) m/z: $[M\text{-}PdCl_4]^+$ calcd for $C_{21}H_{31}N_2O_2$, 343.2380; found, 343.2383.

1-[2-(2,3,4,6-tetra-O-acetyl-*β*-D-glucopyranosyloxy)-ethyl]-2-bromo-3-[4-(methoxycarbonyl)phenyl]-imidazolium tetratetrachloropalladate (12)

Reddish brown solid, 99%, M_p: 94 – 97 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 – 8.09 (m, 3H), 7.75 (d, J = 2.2 Hz, 1H), 7.55 (d, J = 8.2 Hz, 2H), 5.81 (s, 2H), 5.20 (t, J = 9.5 Hz, 1H), 5.03 (t, J = 9.8 Hz, 1H), 4.94 (dd, J = 9.5, 8.1 Hz, 1H), 4.86 (t, J = 4.8 Hz, 2H), 4.76 (d, J = 8.0 Hz, 1H), 4.49 (dd, J = 10.6, 5.6 Hz, 1H), 4.38 – 4.30 (m, 1H), 4.25 (dd, J = 12.5, 4.4 Hz, 1H), 4.18 (dd, J = 12.4, 2.0 Hz, 1H), 3.92 (s, 3H), 3.85 – 3.79 (m, 1H), 2.07 (s, 3H), 2.00 (s, 3H), 1.98 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 170.6, 170.0, 169.6, 169.5, 166.2, 136.4, 131.4, 130.7, 129.0, 126.2, 124.9, 121.8, 100.3, 77.3, 77.0, 76.7, 72.5, 72.0, 71.0, 68.1, 66.4, 61.6, 54.9, 52.4, 51.8, 20.9, 20.5. FT-IR (KBr): 3449, 3104, 2958, 2851, 1752, 1720, 1642, 1614, 1570, 1507, 1434, 1371, 1285, 1258, 1225, 1185, 1038, 964, 911, 873, 841, 801, 735, 697 cm^{-1}. LC–HR/MS (ESI-QTOF) m/z: $[M\text{-}PdCl_4]^+$ calcd for $C_{28}H_{34}BrN_2O_{12}$, 669.1295; found, 669.1297.

1-[2-(2,3,4,6-tetra-O-acetyl-*β*-D-glucopyranosyloxy)-ethyl]-3-propyl-imidazolium tetratetrachloropalladate (13)

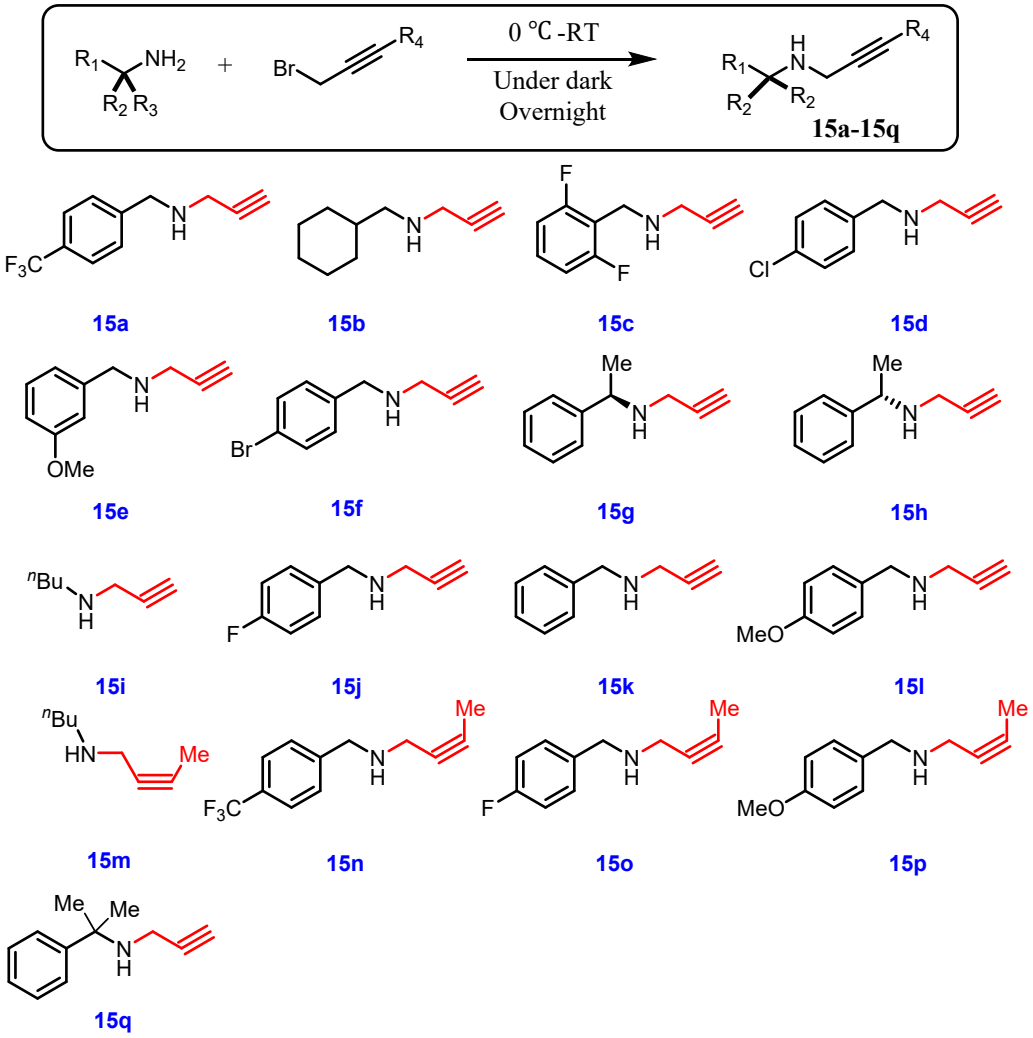
Reddish brown solid, 99%, M_p: 94 – 97 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.20 (s, 1H), 7.54 (s, 1H), 7.32 (s, 1H), 5.21 (t, J = 9.5 Hz, 1H), 5.05 (t, J = 9.7 Hz, 2H), 4.97 (dd, J = 9.5, 8.1 Hz, 1H), 4.85 (dd, J = 13.1, 6.4 Hz, 1H), 4.70 (d, J = 8.0 Hz, 1H), 4.40 (ddd, J = 17.7,

12.0, 5.3 Hz, 4H), 4.33 – 4.26 (m, 1H), 4.16 (dd, *J* = 12.3, 1.6 Hz, 1H), 3.87 – 3.78 (m, 1H), 2.10 (s, 3H), 2.04 (s, 3H), 2.02 (t, *J* = 6.6 Hz, 8H), 1.02 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 170.5, 169.9, 169.7, 169.4, 137.1, 123.6, 121.0, 100.4, 77.3, 77.0, 76.7, 72.4, 71.7, 71.1, 68.6, 68.1, 61.6, 51.7, 50.2, 23.5, 20.8, 20.8, 20.5, 10.8. FT-IR (KBr): 3484, 3136, 3098, 3055, 2967, 2881, 1752, 1628, 1564, 1523, 1440, 1375, 1227, 1167, 1062, 1039, 957, 909, 842, 799, 755, 697 cm^{-1}. LC–HR/MS (ESI-QTOF) m/z: $[M\text{-}PdCl_4]^+$ calcd for $C_{22}H_{33}N_2O_{10}$, 485.2130; found, 485.2137.

3-(2-butoxyethyl)-1-(4-(methoxycarbonyl)benzyl)-2-methyl-1H-imidazol-3-ium tetratetrachloropalladate (14)

Reddish brown solid, 99%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (d, *J* = 8.0 Hz, 2H), 7.50 (s, 1H), 7.33 (d, *J* = 7.9 Hz, 3H), 4.56 (s, 2H), 3.90 (s, 3H), 3.79 (s, 2H), 3.40 (t, *J* = 6.4 Hz, 2H), 2.91 (s, 3H), 1.48 – 1.35 (m, 3H), 1.27 – 1.22 (m, 4H), 0.83 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 166.3, 145.4, 138.6, 130.5, 130.4, 127.8, 122.1, 122.1, 77.3, 77.0, 76.7, 71.1, 68.4, 52.5, 52.2, 49.5, 31.6, 31.5, 29.6, 19.2, 13.8, 11.9. FT-IR (KBr): 3439, 3114, 3089, 2959, 2932, 2872, 1723, 1615, 1583, 1521, 1454, 1420, 1283, 1185, 1121, 1106, 1018, 833, 796, 750, 543, 417.

1.3 Synthesis and Characterization of Propargyl Amines



Scheme S2. The synthesis and structures of propargyl amines **15a-15q**.

Synthesis of propargyl amines **15a-15q**.[2] For the preparation of propargyl amines, propargyl halide (1.0 mmol) was added dropwise to the corresponding amine (3.0 mmol) at 0 °C in dark and warm up to room temperature slowly, the reaction was stirred for 12-24 h. Then, NaOH and dichloromethane were added. After extraction of the aqueous layer with dichloromethane, washed with saturate brine, dried with $MgSO_4$ and the solvent was removed. The crude was purified by flash column chromatography (silica gel, V_{PE}/V_{EA} = 20:1).

N-(4-(trifluoromethyl)benzyl)prop-2-yn-1-amine (**15a**), ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.58 (d, J = 8.1 Hz, 2H), 7.47 (d, J = 8.0 Hz, 2H), 3.95 (s, 2H), 3.42 (d, J = 2.4 Hz, 2H), 2.27 (t, J = 2.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 143.52, 128.57, 125.58, 125.34, 122.88, 81.69, 71.84, 51.60, 37.32.[3]

N-(cyclohexylmethyl)prop-2-yn-1-amine (**15b**), ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.40 – 3.34 (m, 2H), 2.49 (d, J = 6.7 Hz, 2H), 2.18 (t, J = 2.1 Hz, 1H), 1.76 – 1.61 (m, 5H), 1.41 (dtd, J = 14.0, 7.0, 3.5 Hz, 1H), 1.30 – 1.09 (m, 4H), 0.97 – 0.85 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 82.45, 71.01, 55.51, 38.41, 37.89, 31.37, 26.61, 26.00.[4]

N-(2,6-difluorobenzyl)prop-2-yn-1-amine (**15c**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.22 (ddd, J = 13.1, 7.5, 4.2 Hz, 1H), 6.92 – 6.84 (m, 2H), 3.96 (s, 2H), 3.44 (d, J = 2.4 Hz, 2H), 2.23 (t, J = 2.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.04, 160.58, 129.07, 115.29, 111.45 – 110.99, 81.66, 71.50, 39.65, 37.65.[2]

N-(4-chlorobenzyl)prop-2-yn-1-amine (**15d**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.28 (s, 4H), 3.84 (s, 2H), 3.40 (d, J = 2.4 Hz, 2H), 2.26 (t, J = 2.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 137.79, 132.80, 129.68, 128.48, 81.78, 71.69, 51.37, 37.17.[5]

N-(3-methoxybenzyl)prop-2-yn-1-amine (**15e**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.26 (t, J = 8.0 Hz, 1H), 6.95 (d, J = 7.1 Hz, 2H), 6.86 – 6.80 (m, 1H), 3.88 (s, 2H), 3.83 (s, 3H), 3.45 (d, J = 2.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 159.80, 141.05, 129.42, 120.69, 81.97, 71.70, 55.19, 52.24, 37.29.[2]

N-(4-bromobenzyl)prop-2-yn-1-amine (**15f**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.49 – 7.44 (m, 2H), 7.25 (d, J = 8.3 Hz, 2H), 3.86 (s, 2H), 3.43 (d, J = 2.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 138.39, 131.52, 130.12, 120.98, 81.82, 71.76, 51.49, 37.25.[6]

(R)-*N*-(1-phenylethyl)prop-2-yn-1-amine (**15g**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.46 – 7.16 (m, 5H), 4.05 (q, J = 6.6 Hz, 1H), 3.39 (dd, J = 17.1, 2.4 Hz, 1H), 3.19 (dd, J = 17.1, 2.4 Hz, 1H), 2.30 – 2.09 (m, 1H), 1.40 (t, J = 5.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 144.47, 128.52, 127.22, 126.90,82.31, 71.30, 56.36, 35.91, 23.93.[7]

(S)-*N*-(1-phenylethyl)prop-2-yn-1-amine (**15h**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.44 – 7.20 (m, 5H), 4.05 (q, J = 6.6 Hz, 1H), 3.39 (dd,J = 17.1,2.5Hz,1H), 3.19 (dd, J = 17.1, 2.4Hz,1H), 2.20 (dd, J = 37.3, 34.9 Hz, 1H), 1.40 (d, J = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 144.51, 128.54, 127.23, 126.92, 82.35, 71.36, 56.36, 35.91, 23.96.[8]

N-(prop-2-yn-1-yl)butan-1-amine (**15i**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.38 (d, J = 2.4 Hz, 2H), 2.72 – 2.58 (m, 2H), 2.16 (t, J = 2.4 Hz, 1H), 1.44 (qd, J = 6.9, 2.7 Hz, 2H), 1.32 (dq, J = 14.1, 7.0 Hz, 2H), 0.88 (t, J = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 82.30, 71.11, 48.35, 38.13, 31.90, 20.38, 13.91.[6]

N-(4-fluorobenzyl)prop-2-yn-1-amine (**15j**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.34 – 7.27 (m, 2H), 7.04 – 6.96 (m, 2H), 3.84 (s, 2H), 3.40 (d, J = 2.4 Hz, 2H), 2.25 (t, J = 2.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.28, 160.84, 135.13, 135.10, 130.01, 129.93, 115.31, 115.10, 81.93, 71.65, 51.42, 37.19.[3]

N-benzylprop-2-yn-1-amine (**15k**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.36 – 7.29 (m, 4H), 7.28 – 7.22 (m, 1H), 3.87 (s, 2H), 3.42 (d, J = 2.4 Hz, 2H), 2.26 (t, J = 2.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 139.43, 128.45, 127.19, 82.11, 71.62, 52.29, 37.35.[2]

N-(4-methoxybenzyl)prop-2-yn-1-amine (**15l**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.31 – 7.26 (m, 2H), 6.91 – 6.86 (m, 2H), 3.83 (s, 2H), 3.81 (s, 3H), 3.42 (d, J = 2.4 Hz, 2H), 2.28 (t, J = 2.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 158.82, 131.45, 129.64, 113.85, 82.11, 71.56, 55.26, 51.62, 37.14.[6]

N-butylbut-2-yn-1-amine (**15m**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.96 (dd, J = 4.6, 2.2 Hz, 2H), 2.27 (t, J = 7.1 Hz, 2H), 1.42 (t, J = 2.4 Hz, 3H), 1.14 (s, 1H), 1.12 – 1.02 (m, 2H), 1.02 – 0.89 (m, 2H), 0.55 (t, J = 7.3 Hz, 3H).[2]

N-(4-(trifluoromethyl)benzyl)but-2-yn-1-amine (**15n**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.58 (d, J = 8.0 Hz, 2H), 7.47 (d, J = 8.1 Hz, 2H), 3.92 (s, 2H), 3.37 (q, J = 2.3 Hz, 2H), 1.84 (t, J = 2.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 143.84, 128.51, 125.59, 125.26, 79.50, 77.34, 77.02, 76.75, 51.86, 37.85, 3.42.[2]

N-(4-fluorobenzyl)but-2-yn-1-amine (**15o**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.30 (d, J = 8.5, 5.6 Hz, 2H), 7.00 (t, J = 8.7 Hz, 2H), 3.82 (s, 2H), 3.35 (q, J = 2.3 Hz, 2H), 1.84 (t, J = 2.3 Hz, 3H), 1.62 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.16, 160.72, 135.38, 135.34, 129.90, 129.82, 115.19, 114.98, 79.24, 76.97, 51.66, 37.69, 3.44.[2]

N-(4-methoxybenzyl)but-2-yn-1-amine (**15p**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.15 (d, J = 8.5 Hz, 2H), 6.75 (d, J = 8.6 Hz, 2H), 3.67 (s, 2H), 3.63 (d, J = 0.7 Hz, 3H), 3.27 – 3.19 (m, 2H), 1.73 (t, J = 2.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 158.72, 131.81, 129.58, 113.78, 79.13, 77.19, 55.22, 51.89, 37.69, 3.52.[9]

N-(2-phenylpropan-2-yl)prop-2-yn-1-amine (**15q**). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.46 (dd, J = 8.3, 1.1 Hz, 2H), 7.37 (dd, J = 10.4, 5.0 Hz, 2H), 7.29 – 7.23 (m, 1H), 3.13 (d, J = 2.5 Hz, 2H), 2.20 (t, J = 2.5 Hz, 1H), 1.51 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 146.5, 128.3, 126.5, 125.7, 83.1, 70.7, 56.2, 32.6, 29.4.

2 Catalytic Section

2.1 Optimization of the Reaction Conditions

Table S1 Optimization of bases in reactions [a]

Entry	Base	Solvent	T (°C)/t (h)	Yields (%)[b]	TOF (h^{-1})
1	NaO^{t}Bu	DMF	70/1 (2)	60 (100)	60 (100)
2	NaO^{t}Bu	MeCN	70/6	45	7.5
3	NaO^{t}Bu	MeOH	70/6	56	9.5
4	NaO^{t}Bu	EtOH	70/1 (2)	96 (100)	96 (100)
5	NaO^{t}Bu	Dioxane	70/6	15	2.5
6	NaO^{t}Bu	THF	70/6	33	5.5
7	NaO^{t}Bu	DMSO	70/1	100 (93[c])	100 (930)
8	KOH	DMSO	70/2	65[c]	325
9	NaOH	DMSO	70/2	52[c]	260
10	NaOAc	DMSO	70/2	57[c]	285
11	$Na_3PO_4 \cdot 12H_2O$	DMSO	70/2	49[c]	245
12	Na_2CO_3	DMSO	70/2	63[c]	315
13	$NaHCO_3$	DMSO	70/2	38[c]	190
14	K_2CO_3	DMSO	70/2	83[c]	415
15	Et_3N	DMSO	70/2	N.R.[d]	/
16	Base-free	DMSO	70/2	N.R.	/
17	NaO^{t}Bu	DMSO	60/1	43[c]	860

[a]The reactions were carried out with **13a** (0.1 mmol), Cat. **10** (1.0 mol %), dilute CO_2 (bubbling), NaO^{t}Bu (0.15 mmol), DMSO (2.0 mL) and stirred at 70 °C, unless noted otherwise. [b]Determined by ^{1}H NMR. [c]Catalyst (0.1 mol %). [d]N.R. = no reaction. [e]Catalyst (0.05 mol %) at 60 °C for 1 h.

Table S2 Screening of the reaction temperatures [a]

Entry	T (°C)/t (h)	Yields (%)[b]	TOF (h^{-1})
1	RT	74	74
2	30	85	85
3	40	89	89
4	50	97	97
5	60	100	100
6	70	100	100
7	80	86	86
8	90	74	74

[a]The reactions were carried out with **13a** (0.1 mmol), Cat. **9** (1.0 mol %), dilute CO_2 (bubbling), NaO^{t}Bu (0.15 mmol), DMSO (2.0 mL) and stirred at different temperatures for 1.0 hour, unless noted otherwise. [b]Determined by ^{1}H NMR.

2.2 Comparison of Turnover Frequency with Other Reported Catalysts

Table S3 Comparison with the TOFs of previously catalytic systems [a]

Entry	Catalyst	T (°C)/t (h)	*P* (atm)[b]	TOF (h^{-1})	Ref.
1	AcGlu-Im-$PdCl_4$ **10**	60/0.5	0.15	1440	Herein
2	CuI/DBU	50/4	1.0	2	[10]
3	AgOAc	25/7	1.0	7	[11]
4	$AgNO_3$/DBU	60/2	1.0	94	[12]
5	$CoBr_2$/TBD	80/9	1.0	1	[13]
6	$ZnCl_2(TBD)_2$	60/12	1.0	2	[14]
7	Ag_{27}-MOF	25/6	1.0	16	[15]
8	TOS-Ag_4	25/24	1.0	4	[16]
9	Zn_{116}	70/12	1.0	31	[17]
10	PdSCS	50/0.33	1.0	60	[18]
11	Ag@TpPa-1	60/18	1.0	17	[19]
12	Ag@2,6-FPP-TAPT	50/2	1.0	964	[20]
13	Cu_2O@ZIF-8	40/6	1.0	3.3	[21]
14	Cu^{I}/Cu^{II}-MOF	30/0.17	1.0	230	[22]
15	Pd@BBA-2	40/2	1.0	43.68	[23]
15	AuCl(IPr)	40/15	1.0	3.03	[24]
16	AgCl(IPr)	40/15	1.0	3.03	[25]
17	[Au]	RT/24	air	5.33	[26]
18	Ag-HMP-2	60/20	1.0	10.6	[27]
19	Ag-MOF-1	RT/24	1.0	0.56	[28]
20	2G*n*[TEG][Au]	RT/24	1.0	1.77	[29]

[a]TOF is calculated directly using the optimal conditions given in the literature.

2.3 General Procedure for Pd-catalyzed Carboxylative Cyclization of CO_2 with Propargyl Amines.

The carboxylative cyclization of dilute CO_2 with *N*-(4-(trifluoromethyl)benzyl)prop-2-yn-1-amine (**15a**) into 5-methylene-3-(4-(trifluoromethyl)benzyl)oxazolidin-2-one (**16a**) was carried out in DMSO. AcGlu-Im-$PdCl_4$ (1.0 mol%), **15a** (13.5 mg, 0.05 mmol), and NaO^{t}Bu (3.6 mg, 0.075 mmol) were added to DMSO (2.0 mL) in the reaction tube (10 mL). dilute CO_2 (bubbling, CO_2/N_2, Vol/Vol = 15:85) was introduced into the reaction mixture with stirring using a long hollow needle (φ 0.7 × 200 mm). The reaction mixture was stirred in a preheated 60 °C oil bath for 1.0 h. After the reaction stopped, the mixture was transferred to ethyl acetate solution (10 mL) and water (5.0 mL), the mixture was stirred for 10 min, then extracted with ethyl acetate (3 × 5.0 mL). The combined organic layers were dried over Mg_2SO_4 and filtered, the organic solution was concentrated in vacuo to give the crude product, and the yield was determined by ^{1}H NMR, the pure **16a** was purified by flash chromatograph (V_{PE} : V_{EA} = 30:1 – 20:1).

2.4 NMR Data of 2-Oxazolidinones 16a-16q.

5-methylene-3-(4-(trifluoromethyl)benzyl)oxazolidin-2-one (16a)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63 (d, J = 8.1 Hz, 2H), 7.41 (d, J = 8.0 Hz, 2H), 4.78 (dd, J = 5.8, 2.6 Hz, 1H), 4.53 (s, 2H), 4.28 (dt, J = 3.2, 2.2 Hz, 1H), 4.05 (t, J = 2.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.7, 148.5, 139.1, 128.4, 126.0, 87.3, 47.4.[3]

3-(cyclohexylmethyl)-5-methyleneoxazolidin-2-one (16b)

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.74 (q, J = 2.7 Hz, 1H), 4.28 (dd, J = 5.2, 2.2 Hz, 1H), 4.17 (t, J = 2.4 Hz, 2H), 3.13 (d, J = 7.3 Hz, 2H), 1.77 – 1.65 (m, 5H), 1.59 (dtd, J = 15.0, 7.4, 3.8 Hz, 1H), 1.28 – 1.17 (m, 3H), 0.97 (td, J = 11.7, 6.2 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.9, 149.21, 86.3, 50.2, 48.7, 36.0, 30.5, 26.2, 25.6.[30]

3-(2,6-difluorobenzyl)-5-methyleneoxazolidin-2-one (16c)

Light yellow liquid, 99%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 (tt, J = 8.4, 6.5 Hz, 1H), 7.02 – 6.88 (m, 2H), 4.74 (dd, J = 5.6, 2.7 Hz, 1H), 4.63 (s, 2H), 4.27 (dd, J = 5.3, 2.2 Hz, 1H), 4.10 (t, J = 2.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.9, 162.8, 160.4, 160.4, 154.9, 148.8, 130.7, 130.63, 130.5, 111.8, 111.7, 111.6, 111.5, 110.7, 110.5, 86.8, 47.4, 35.2, 35.2, 35.1, 31.5, 30.1, 1.0. LC–HR/MS (ESI-QTOF) m/z: $[M-H]^+$ calcd for $C_{11}H_8F_2NO_2$, 224.0601; found, 224.0603.

3-(4-chlorobenzyl)-5-methyleneoxazolidin-2-one (16d)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 – 7.27 (m, 2H), 7.24 – 7.16 (m, 2H), 4.72 (dd, J = 5.6, 2.7 Hz, 1H), 4.41 (s, 2H), 4.24 (dd, J = 5.3, 2.2 Hz, 1H), 4.01 (t, J = 2.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.5, 148.6, 134.0, 133.5, 129.4, 129.0, 86.9, 47.1, 47.1.[3]

3-(3-methoxybenzyl)-5-methyleneoxazolidin-2-one (16e)

Yellow oil, 86%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27 (dd, J = 10.3, 5.4 Hz, 1H), 6.91 – 6.76 (m, 3H), 4.72 (dd, J = 5.7, 2.7 Hz, 1H), 4.42 (d, J = 3.5 Hz, 2H), 4.24 (dt, J = 3.0, 2.2 Hz, 1H), 4.03 (t, J = 2.4 Hz, 2H), 3.80 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.1, 155.6, 149.0, 136.6, 130.0, 120.3, 113.7, 113.6, 86.7, 55.3, 47.8, 47.3. LC–HR/MS (ESI-QTOF) m/z: $[M-H]^+$ calcd for $C_{12}H_{12}NO_3$, 218.0895; found, 218.0893.

3-(4-bromobenzyl)-5-methyleneoxazolidin-2-one (16f)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 – 7.43 (m, 2H), 7.21 – 7.11 (m, 2H), 4.75 (dd, J = 5.7, 2.6 Hz, 1H), 4.42 (s, 2H), 4.26 (dt, J = 3.2, 2.2 Hz, 1H), 4.03 (t, J = 2.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.6, 148.7, 134.1, 132.1, 129.8, 122.3, 87.0, 47.2, 47.2, 47.1.[31]

(R)-5-methylene-3-(1-phenylethyl)oxazolidin-2-one (16g)

Light yellow liquid, 100%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 (qdd, J = 6.9, 5.4, 1.8 Hz, 5H), 5.27 (q, J = 7.1 Hz, 1H), 4.72 (dd, J = 5.6, 2.7 Hz, 1H), 4.29 – 4.21 (m, 1H), 4.12 (dt, J = 14.2, 2.4 Hz, 1H), 3.79 (dt, J = 14.2, 2.4 Hz, 1H), 1.61 (d, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.1, 149.3, 138.9, 128.9, 128.2, 127.0, 86.5, 51.4, 43.7, 16.4. LC–HR/MS (ESI-QTOF) m/z: $[M-H]^+$ calcd for $C_{12}H_{12}NO_2$, 202.0946; found, 202.0948.

(S)-5-methylene-3-(1-phenylethyl)oxazolidin-2-one (16h)

Yellow oil, 100%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 – 7.29 (m, 5H), 5.27 (q, J = 7.1 Hz, 1H), 4.72 (q, J = 2.7 Hz, 1H), 4.23 (dd, J = 5.3, 2.2 Hz, 1H), 4.12 (dt, J = 14.2, 2.4 Hz, 1H), 3.79 (dt, J = 14.2, 2.4 Hz, 1H), 1.61 (d, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.1, 149.3, 138.9, 128.9, 128.2, 127.0, 86.5, 51.4, 43.7, 16.4. LC–HR/MS (ESI-QTOF) m/z: $[M-H]^+$ calcd for $C_{12}H_{12}NO_2$, 202.0946; found, 202.0948.

3-butyl-5-methyleneoxazolidin-2-one (16i)

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.75 (q, J = 2.7 Hz, 1H), 4.29 (dd, J = 5.2, 2.2 Hz, 1H), 4.17 (t, J = 2.4 Hz, 2H), 3.31 (t, J = 7.3 Hz, 2H), 1.60 – 1.51 (m, 2H), 1.36 (dd, J = 15.1, 7.4 Hz, 2H), 0.96 (t, J = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.6, 149.2, 86.3, 47.8, 43.5, 29.3, 19.8, 13.6.[32]

3-(4-fluorobenzyl)-5-methyleneoxazolidin-2-one (16j)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30 – 7.24 (m, 2H), 7.12 – 6.97 (m, 2H), 4.74 (dd, J = 5.7, 2.7 Hz, 1H), 4.44 (s, 2H), 4.26 (dt, J = 3.1, 2.2 Hz, 1H), 4.03 (t, J = 2.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 161.4, 155.6, 148.8, 130.9, 129.9, 115.9, 86.9, 47.2, 47.1.[3]

3-benzyl-5-methyleneoxazolidin-2-one (16k)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 – 7.23 (m, 5H), 4.74 (dd, J = 5.7, 2.7 Hz, 1H), 4.47 (s, 2H), 4.25 (dt, J = 3.1, 2.2 Hz, 1H), 4.03 (t, J = 2.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.7 , 149.0 , 135.0, 129.0, 128.3, 128.2, 86.8, 47.9, 47.2.[3]

3-(4-methoxybenzyl)-5-methyleneoxazolidin-2-one (16l)

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.26 – 7.16 (m, 2H), 6.95 – 6.85 (m, 2H), 4.73 (dd, J = 5.7, 2.7 Hz, 1H), 4.41 (s, 2H), 4.24 (dt, J = 3.0, 2.2 Hz, 1H), 4.01 (t, J = 2.4 Hz, 2H), 3.81 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 159.6, 155.6, 149.1, 129.6, 127.0, 114.3, 86.6, 55.3, 47.2.[3]

(E)-3-butyl-5-ethylideneoxazolidin-2-one (16m)

Light yellow liquid, 100%. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 4.53 (qd, J = 6.9, 4.8 Hz, 1H), 4.02 (dd, J = 4.4, 2.2 Hz, 2H), 3.22 (t, J = 7.3 Hz, 2H), 1.61 (dt, J = 6.9, 2.2 Hz, 3H), 1.51 – 1.42 (m, 2H), 1.31 – 1.22 (m, 2H), 0.87 (t, J = 7.3 Hz, 3H). LC–HR/MS (ESI-QTOF) m/z: $[M-H]^+$ calcd for $C_9H_{14}NO_2$, 168.1103; found, 168.1101.

(E)-5-ethylidene-3-(4-(trifluoromethyl)benzyl)oxazolidin-2-one (16n)

Light yellow liquid, 83%. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.61 (d, J = 8.1 Hz, 2H), 7.45 (d, J = 8.0 Hz, 2H), 4.78 (dd, J = 4.3, 3.2 Hz, 1H), 4.63 (s, 2H), 3.71 (dq, J = 3.7, 1.8 Hz, 2H), 1.87 (dd, J = 3.0, 1.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 156.1, 141.2, 139.3, 128.3, 126.0, 125.9, 125.9, 125.8, 98.1, 47.4, 47.2, 9.9. LC–HR/MS (ESI-QTOF) m/z: $[M-H]^+$ calcd for $C_{13}H_{11}F_3NO_2$, 271.0820; found, 271.0822.[33]

(E)-5-ethylidene-3-(4-fluorobenzyl)oxazolidin-2-one (16o)

Light yellow liquid, 86%. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.26 (dt, J = 4.8, 4.1 Hz, 2H), 7.11 – 7.01 (m, 2H), 4.66 – 4.53 (m, 1H), 4.45 (s, 2H), 3.97 (p, J = 2.1 Hz, 2H), 1.68 (ddd, J = 9.6, 5.9, 3.7 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.8, 161.3, 156.0, 141.5, 131.0, 131.0, 130.0, 129.9, 116.0, 115.8, 97.8, 47.2, 47.0, 10.0. LC–HR/MS (ESI-QTOF) m/z: $[M-H]^+$ calcd for $C_{12}H_{11}FNO_2$, 221.0852; found, 221.0850.

(E)-5-ethylidene-3-(4-methoxybenzyl)oxazolidin-2-one (16p)

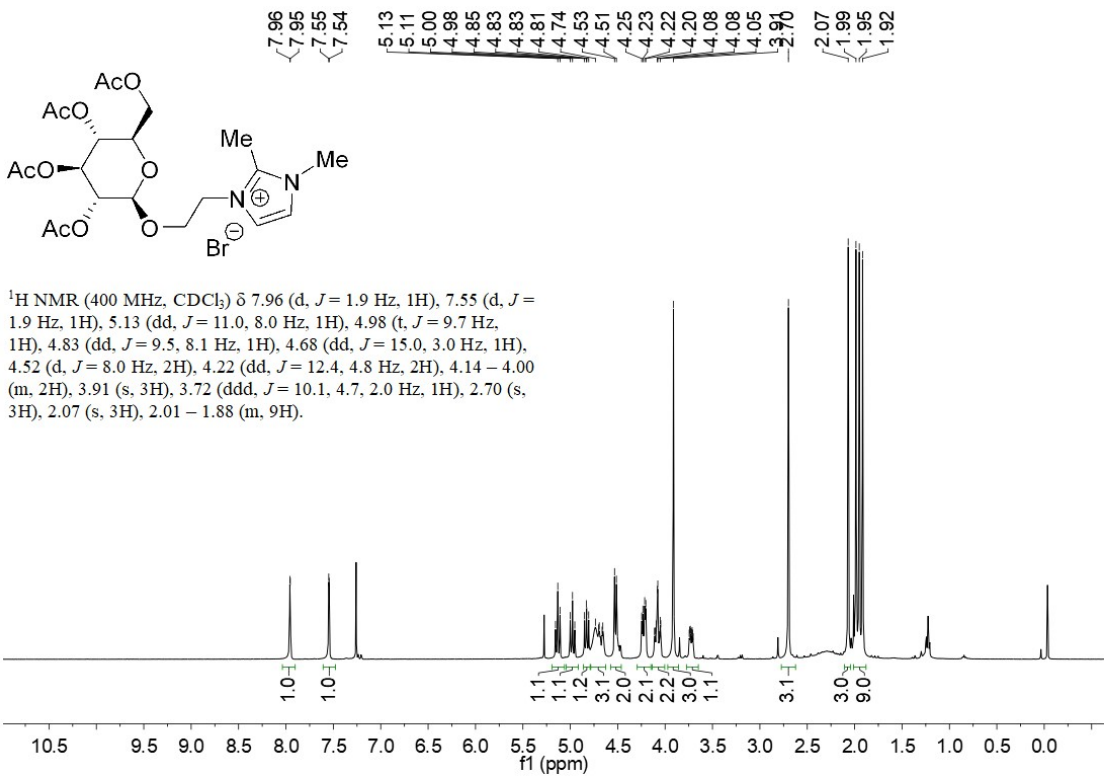
Light yellow liquid, 99%. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.21 (d, J = 8.6 Hz, 2H), 6.90 (d, J = 8.6 Hz, 2H), 4.56 (qt, J = 6.9, 2.0 Hz, 1H), 4.41 (s, 2H), 3.99 – 3.91 (m, 2H), 3.82 (s, 3H), 1.68 (dt, J = 6.9, 2.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 159.5, 156.0, 141.8, 129.6, 127.2, 114.3, 97.5, 55.3, 47.3, 46.9, 9.9. LC–HR/MS (ESI-QTOF) m/z: $[M-H]^+$ calcd for $C_{13}H_{14}NO_3$, 232.1052; found, 232.1050.[33]

5-methylene-3-(2-phenylpropan-2-yl)oxazolidin-2-one (16q)

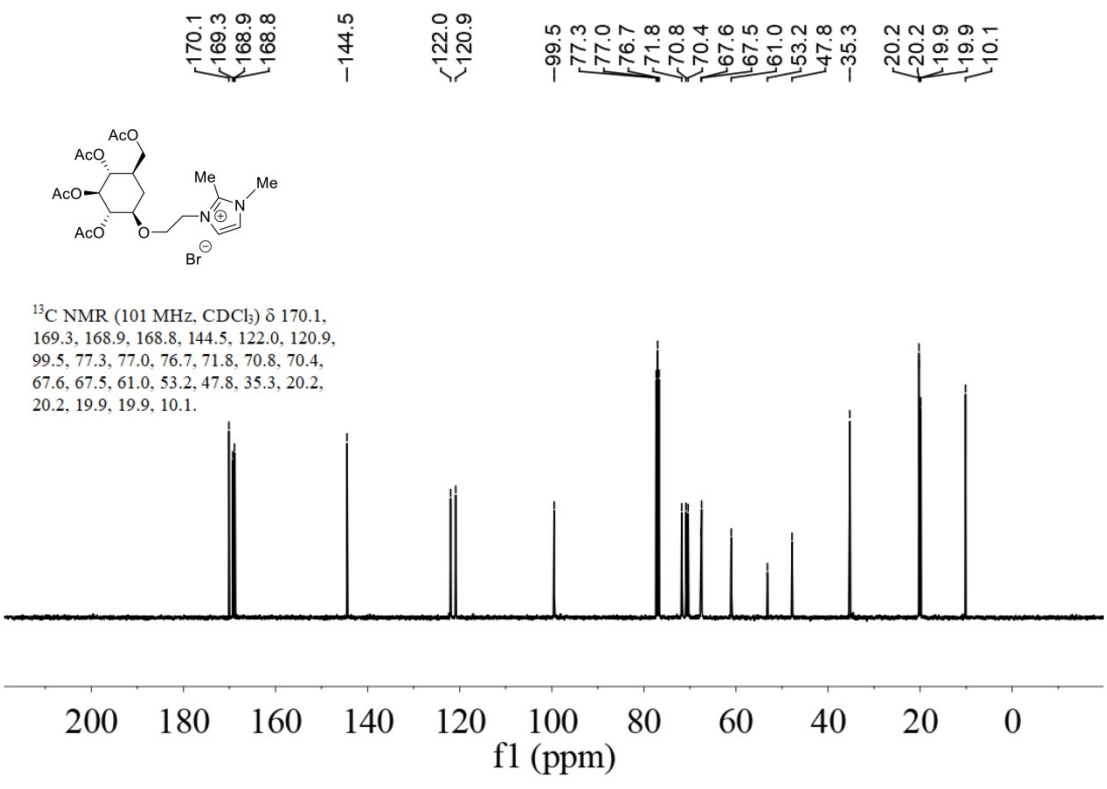
Light yellow liquid, 100%. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.36 (dd, J = 10.0, 3.4 Hz, 4H), 7.32 – 7.26 (m, 1H), 4.66 (dd, J = 5.3, 2.6 Hz, 1H), 4.17 (dd, J = 4.8, 2.2 Hz, 1H), 4.07 (t, J =

2.3 Hz, 2H), 1.80 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 154.2, 148.9, 144.7, 128.7, 127.4, 125.1, 85.6, 77.3, 77.0, 76.7, 58.9, 47.4, 27.4.

2.5 NMR, FT-IR and HR-MS Spectra of Imidazolium Salts

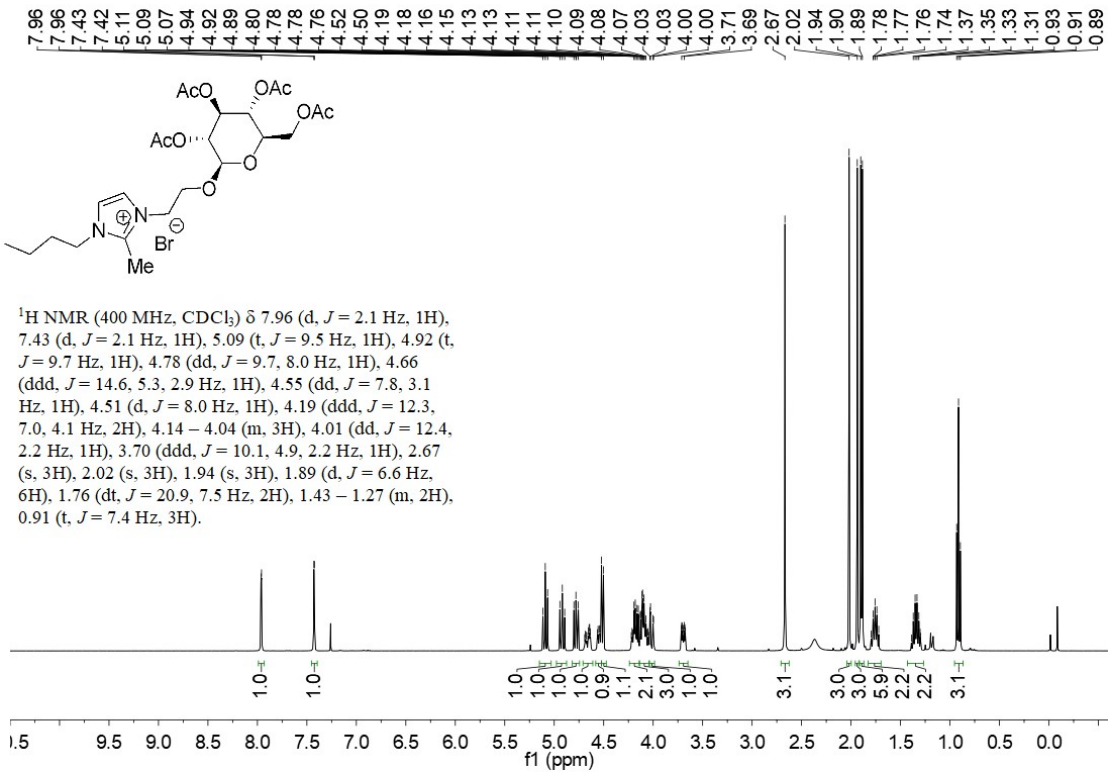


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 1.9 Hz, 1H), 7.55 (d, J = 1.9 Hz, 1H), 5.13 (dd, J = 11.0, 8.0 Hz, 1H), 4.98 (t, J = 9.7 Hz, 1H), 4.83 (dd, J = 9.5, 8.1 Hz, 1H), 4.68 (dd, J = 15.0, 3.0 Hz, 1H), 4.52 (d, J = 8.0 Hz, 2H), 4.22 (dd, J = 12.4, 4.8 Hz, 2H), 4.14 – 4.00 (m, 2H), 3.91 (s, 3H), 3.72 (ddd, J = 10.1, 4.7, 2.0 Hz, 1H), 2.70 (s, 3H), 2.07 (s, 3H), 2.01 – 1.88 (m, 9H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 169.3, 168.9, 168.8, 144.5, 122.0, 120.9, 99.5, 77.3, 77.0, 76.7, 71.8, 70.8, 70.4, 67.6, 67.5, 61.0, 53.2, 47.8, 35.3, 20.2, 20.2, 19.9, 19.9, 10.1.

Figure S1. The ^{1}H and ^{13}C NMR spectra of AcGlu-Im-Br **1** in $CDCl_3$.



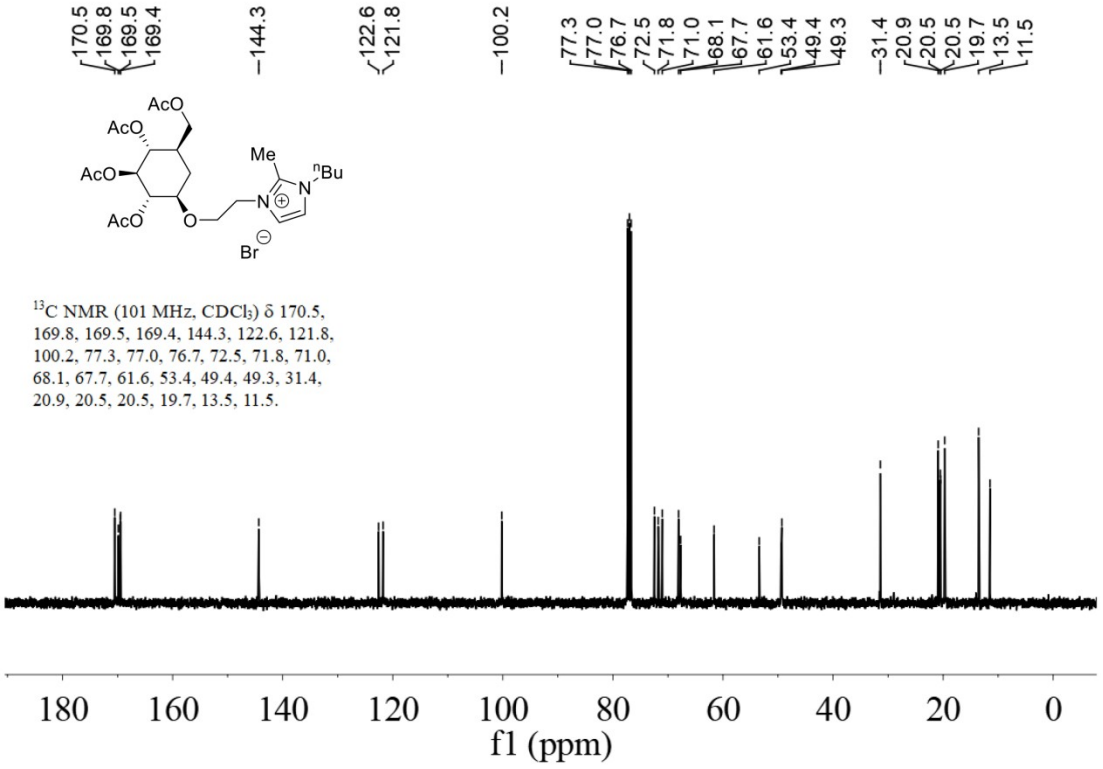


Figure S2. The ^{1}H and ^{13}C NMR spectra of AcGlu-Im-Br **2** in $CDCl_3$.

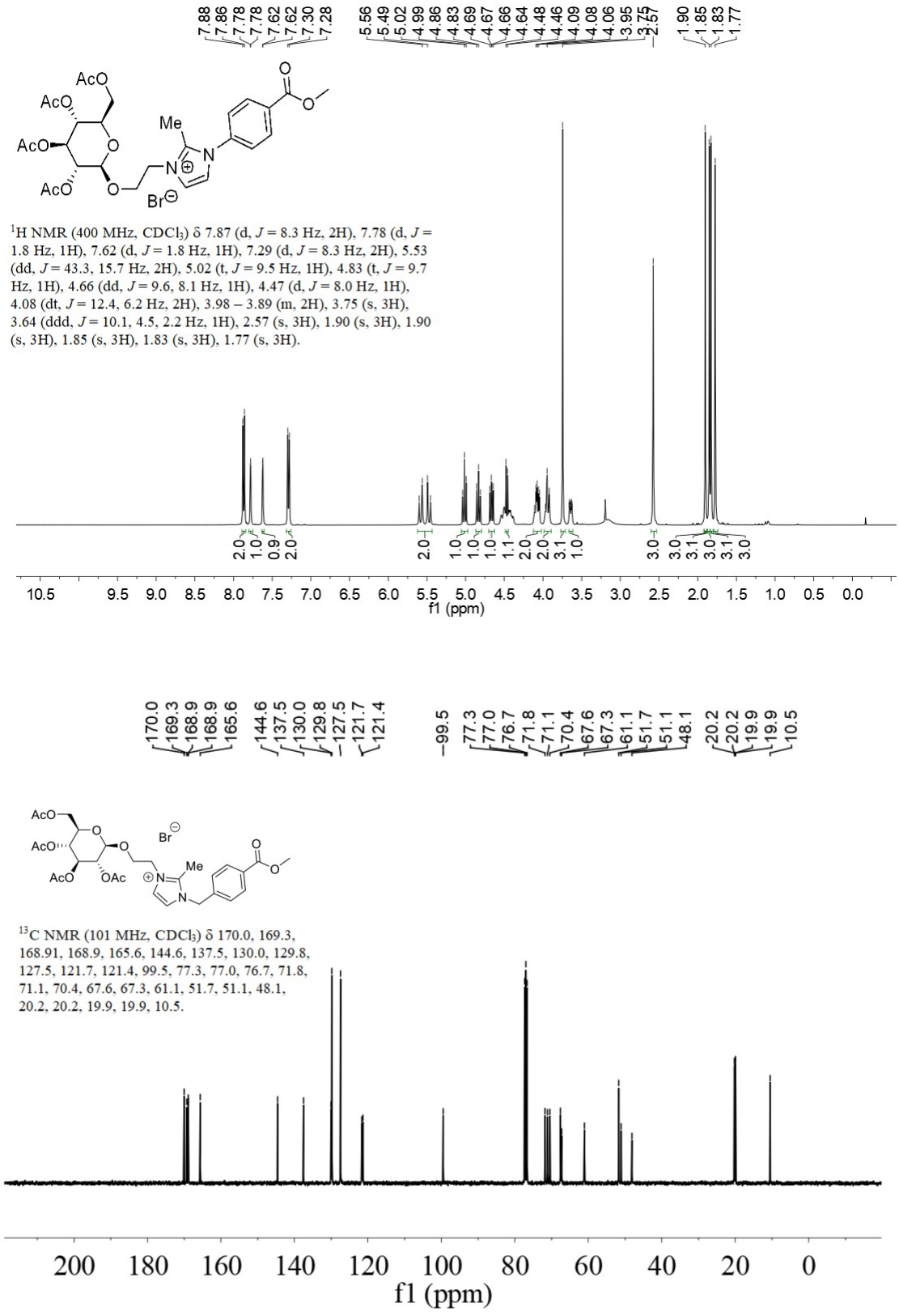
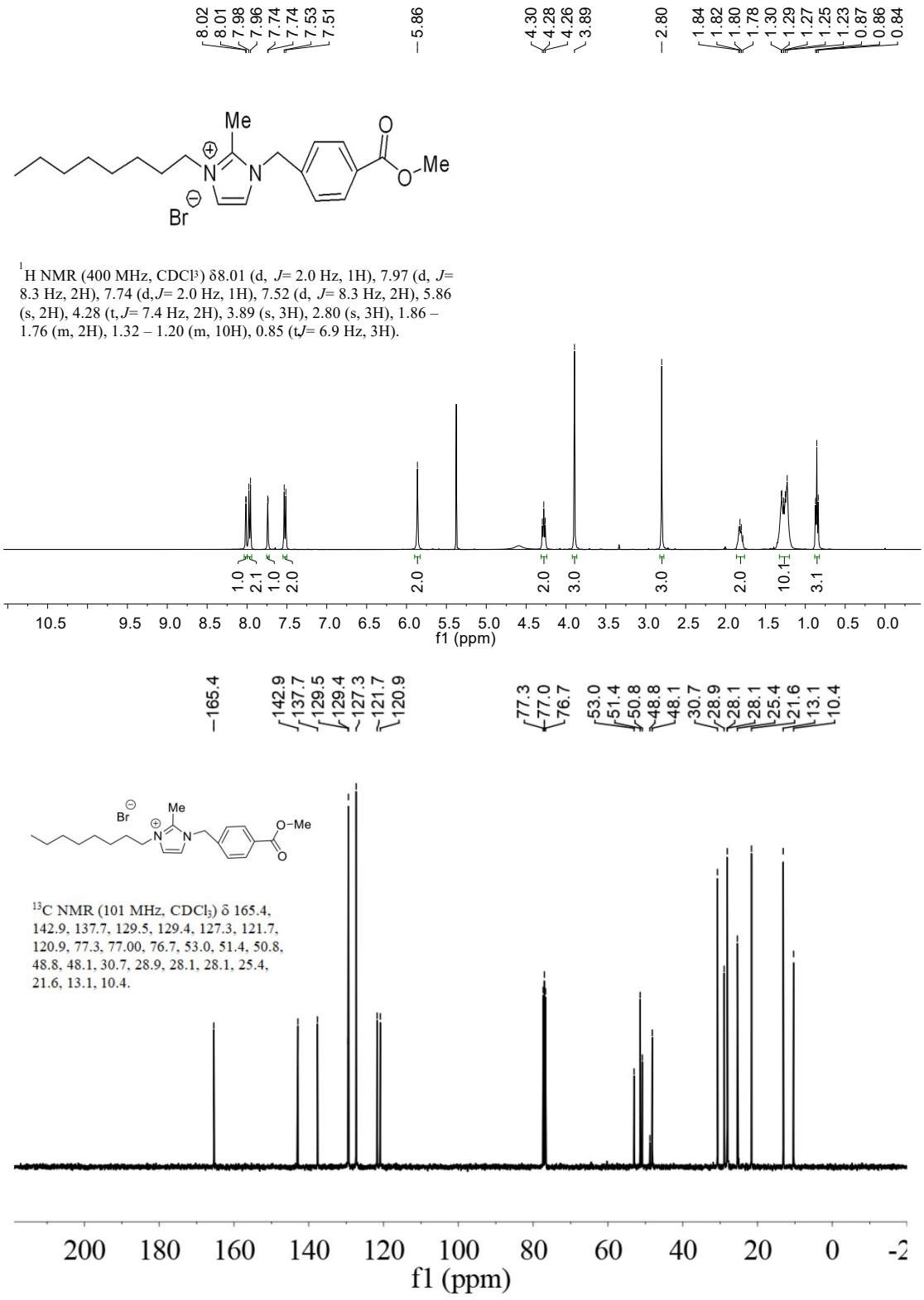


Figure S3. The [1]H and [13]C NMR spectra of AcGlu-Im-Br **3** in $CDCl_3$.



^{1}H NMR (400 MHz, CDCl^{3}) δ8.01 (d, *J*= 2.0 Hz, 1H), 7.97 (d, *J*= 8.3 Hz, 2H), 7.74 (d,*J*= 2.0 Hz, 1H), 7.52 (d, *J*= 8.3 Hz, 2H), 5.86 (s, 2H), 4.28 (t, *J*= 7.4 Hz, 2H), 3.89 (s, 3H), 2.80 (s, 3H), 1.86 – 1.76 (m, 2H), 1.32 – 1.20 (m, 10H), 0.85 (t,*J*= 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.4, 142.9, 137.7, 129.5, 129.4, 127.3, 121.7, 120.9, 77.3, 77.00, 76.7, 53.0, 51.4, 50.8, 48.8, 48.1, 30.7, 28.9, 28.1, 28.1, 25.4, 21.6, 13.1, 10.4.

Figure S4. The ^{1}H and ^{13}C NMR spectra of Octyl-Im-Br **4** in $CDCl_3$**.**

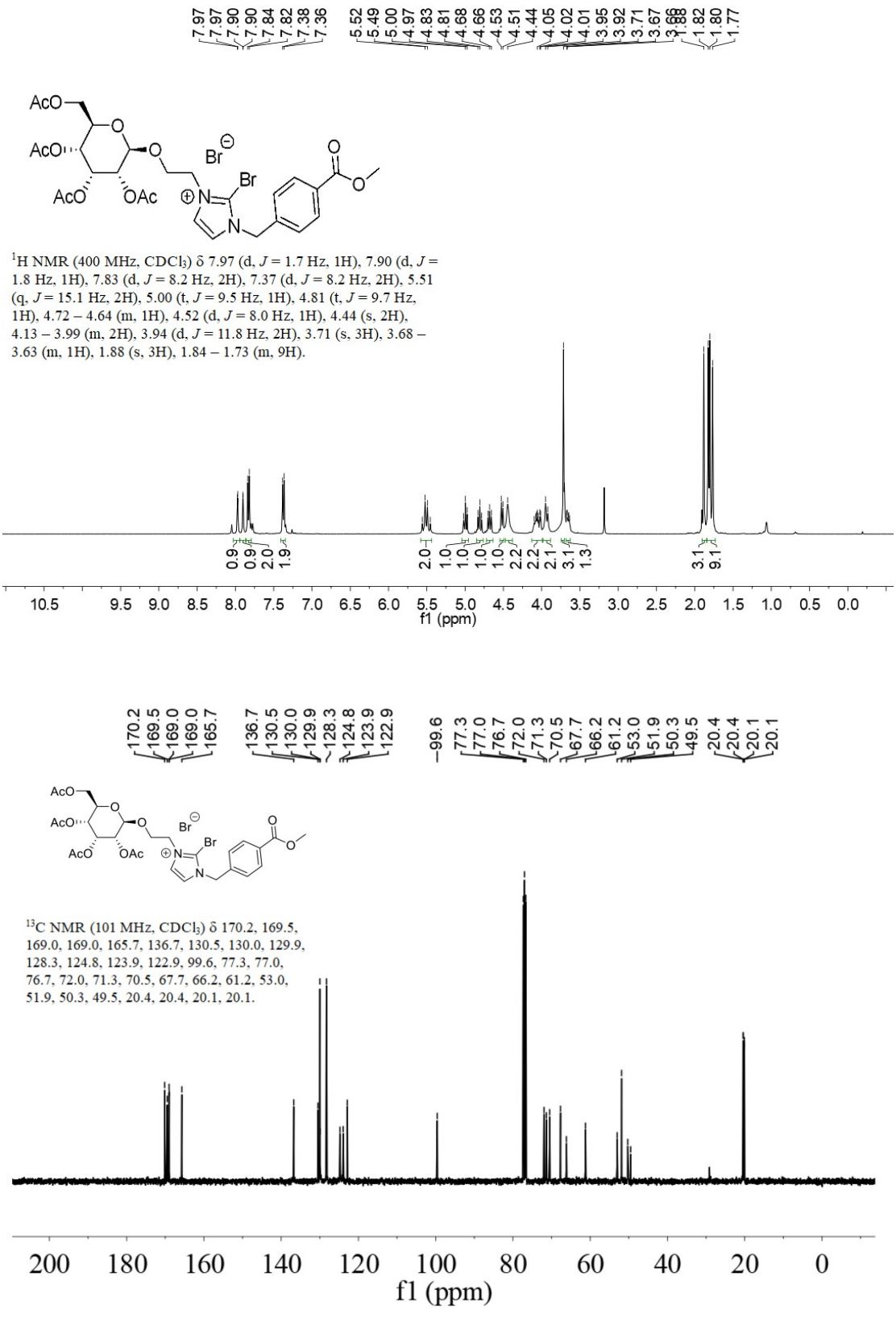


Figure S5. The [1]H and [13]C NMR spectra of AcGlu-Im-Br **5** in $CDCl_3$.

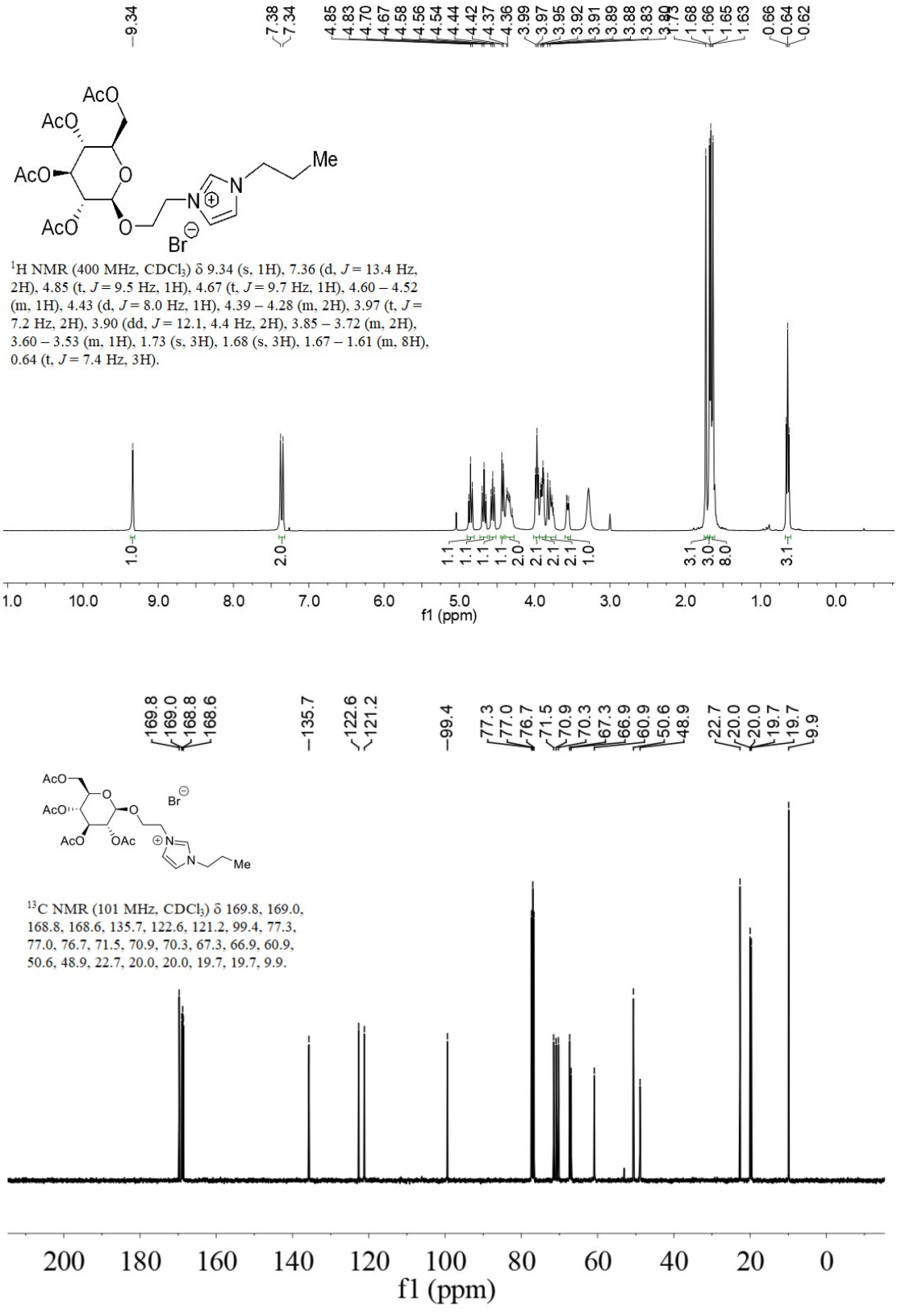


Figure S6. The ^{1}H and ^{13}C NMR spectra of AcGlu-Im-Br **6** in $CDCl_3$.

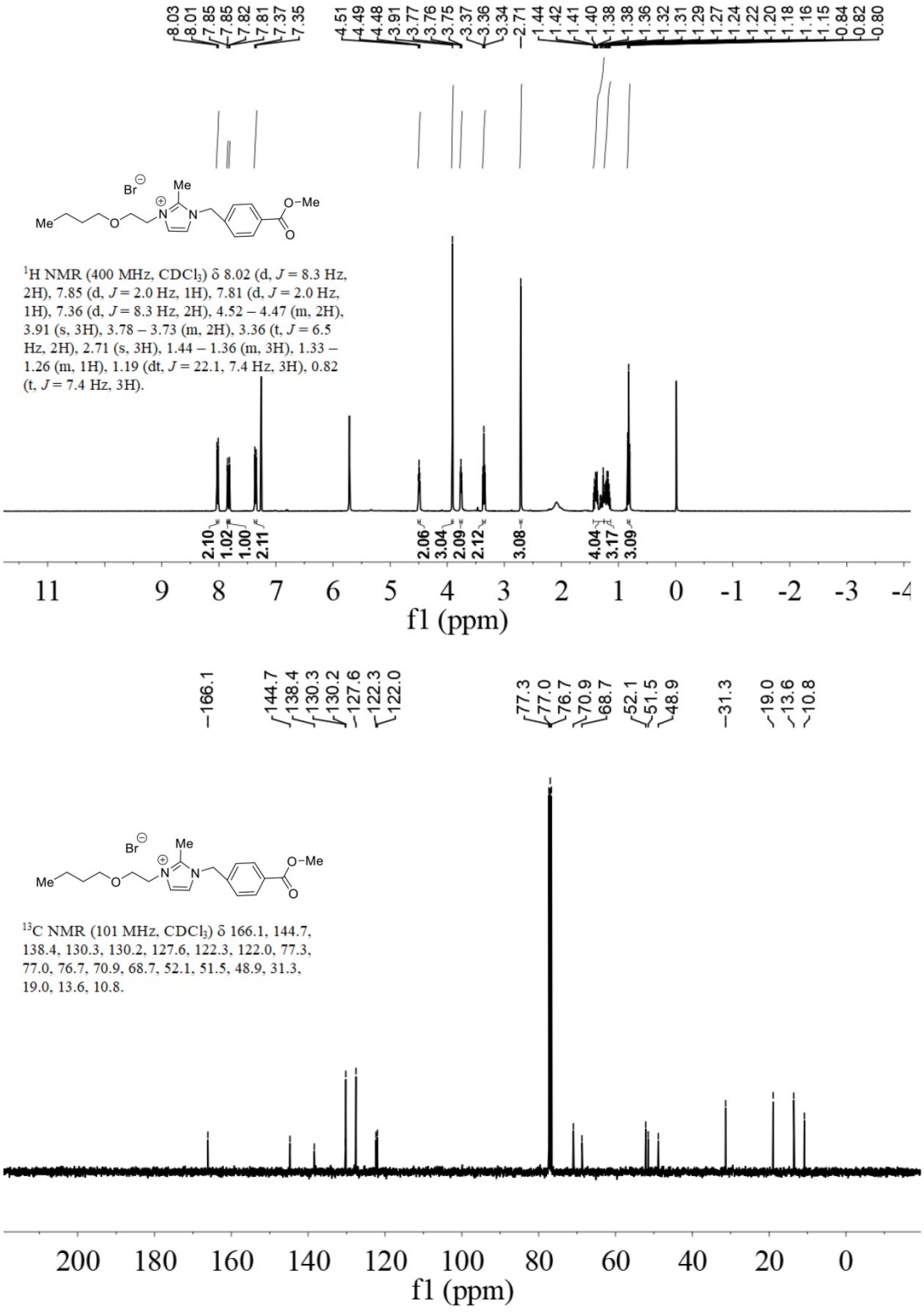


Figure S7. The ^{1}H and ^{13}C NMR spectra of BOE-Im-Br **7** in $CDCl_3$.

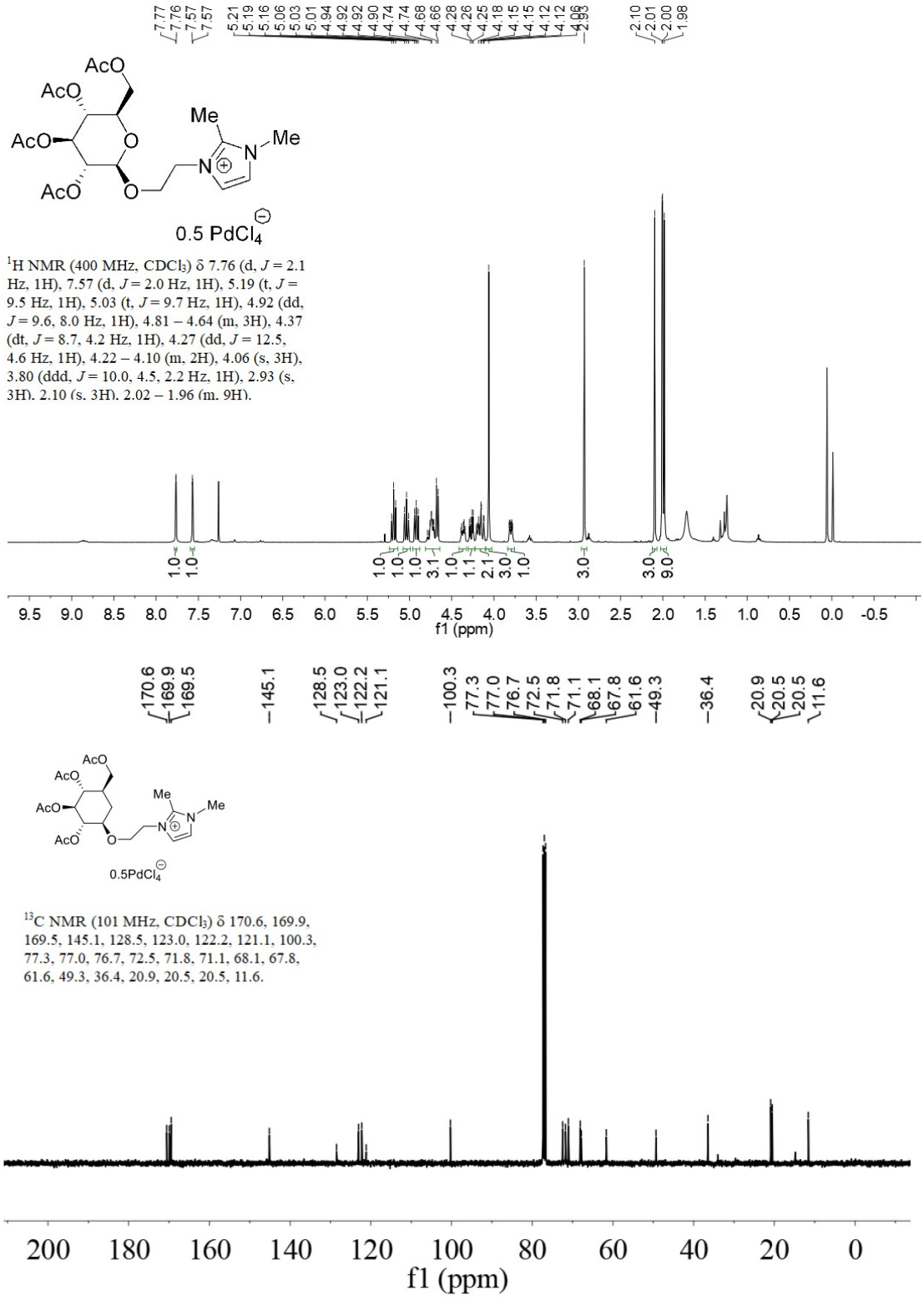


Figure S8. ^{1}H and ^{13}C NMR spectra of AcGlu-Im-$PdCl_4$ **8** in $CDCl_3$.

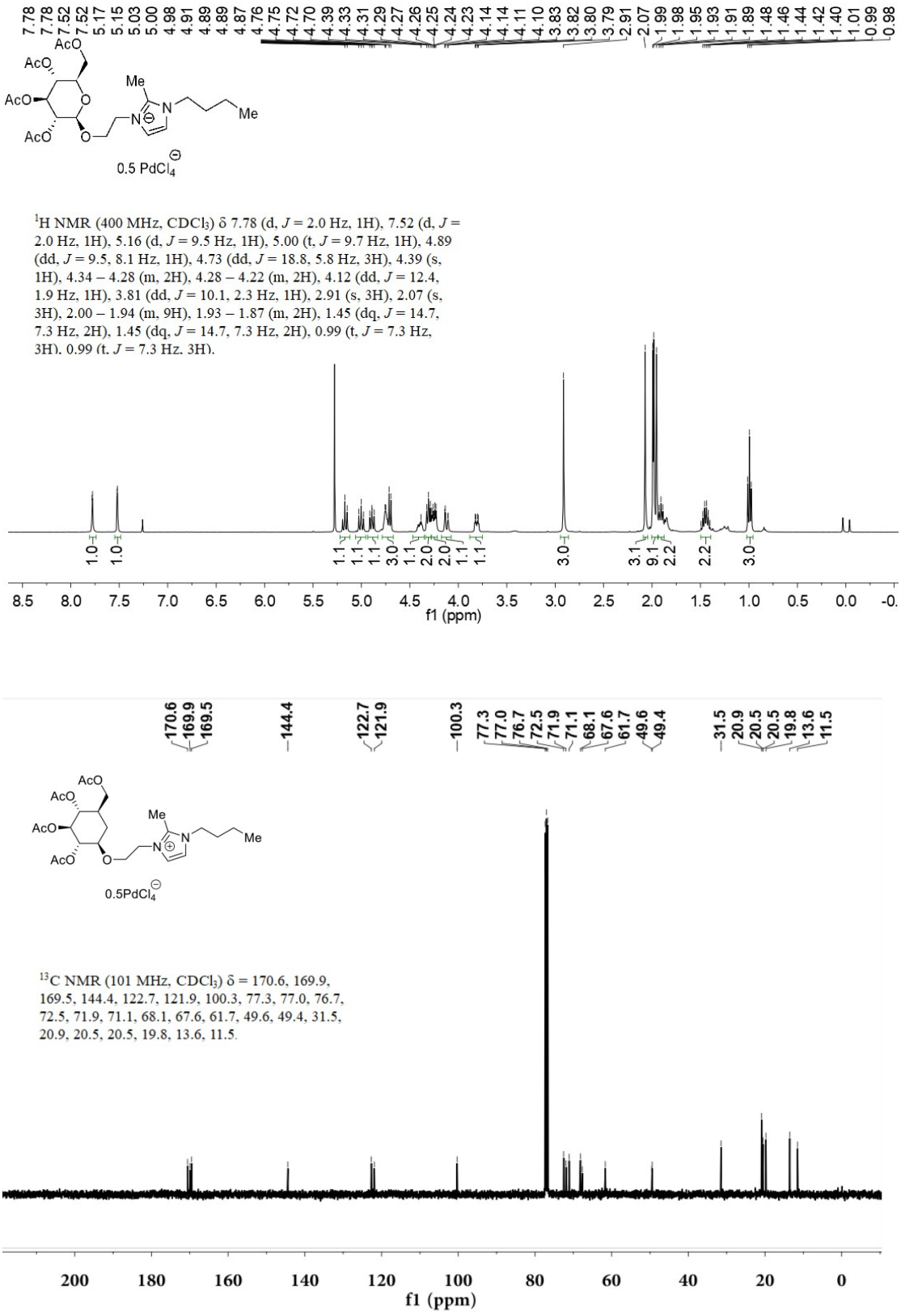
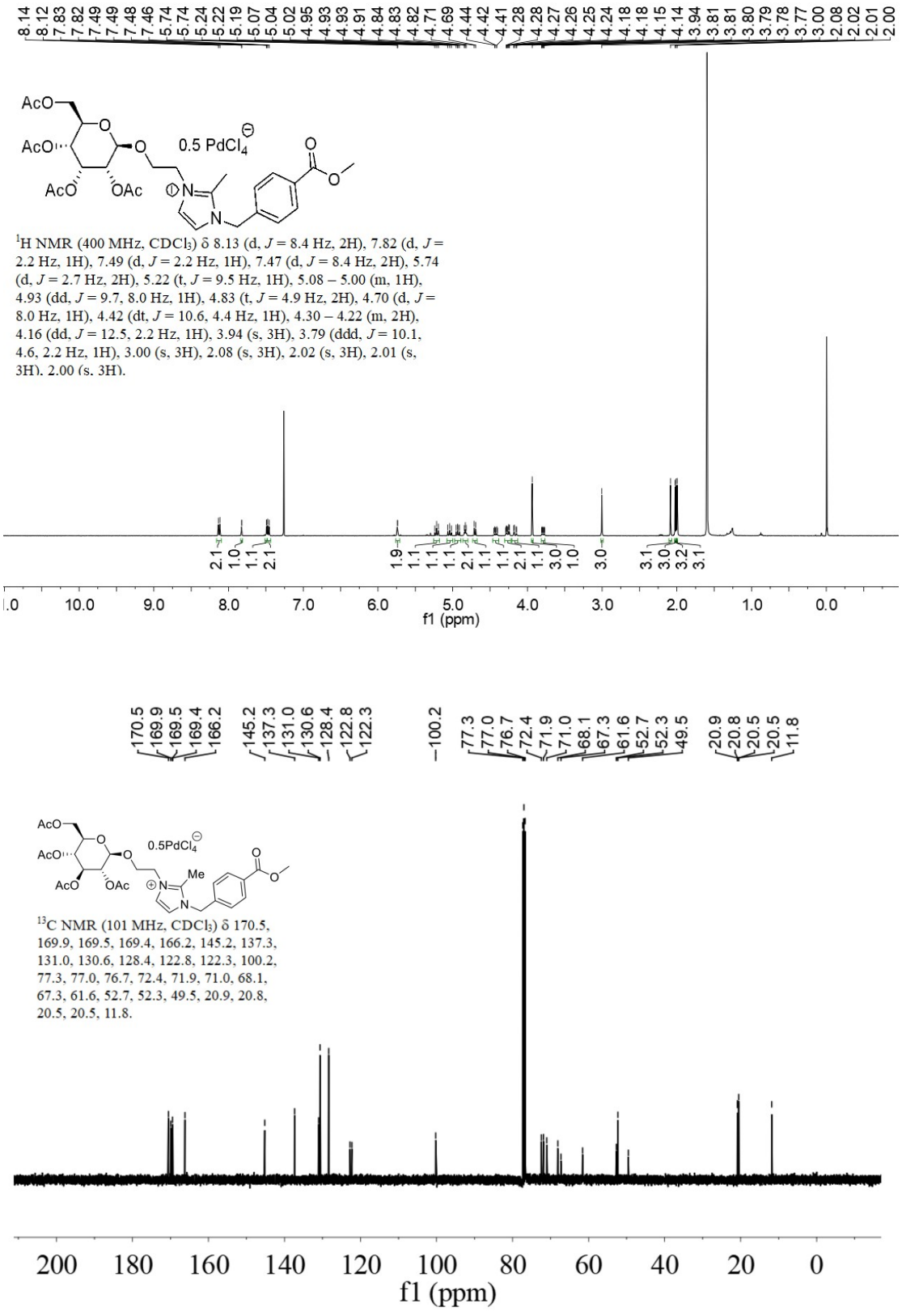


Figure S9. ^{1}H and ^{13}C NMR spectra of AcGlu-Im-$PdCl_4$ **9** in $CDCl_3$.



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.4 Hz, 2H), 7.82 (d, *J* = 2.2 Hz, 1H), 7.49 (d, *J* = 2.2 Hz, 1H), 7.47 (d, *J* = 8.4 Hz, 2H), 5.74 (d, *J* = 2.7 Hz, 2H), 5.22 (t, *J* = 9.5 Hz, 1H), 5.08 – 5.00 (m, 1H), 4.93 (dd, *J* = 9.7, 8.0 Hz, 1H), 4.83 (t, *J* = 4.9 Hz, 2H), 4.70 (d, *J* = 8.0 Hz, 1H), 4.42 (dt, *J* = 10.6, 4.4 Hz, 1H), 4.30 – 4.22 (m, 2H), 4.16 (dd, *J* = 12.5, 2.2 Hz, 1H), 3.94 (s, 3H), 3.79 (ddd, *J* = 10.1, 4.6, 2.2 Hz, 1H), 3.00 (s, 3H), 2.08 (s, 3H), 2.02 (s, 3H), 2.01 (s, 3H), 2.00 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5, 169.9, 169.5, 169.4, 166.2, 145.2, 137.3, 131.0, 130.6, 128.4, 122.8, 122.3, 100.2, 77.3, 77.0, 76.7, 72.4, 71.9, 71.0, 68.1, 67.3, 61.6, 52.7, 52.3, 49.5, 20.9, 20.8, 20.5, 20.5, 11.8.

Figure S10. ^{1}H and ^{13}C NMR spectra of AcGlu-Im-$PdCl_4$ **10** in $CDCl_3$.

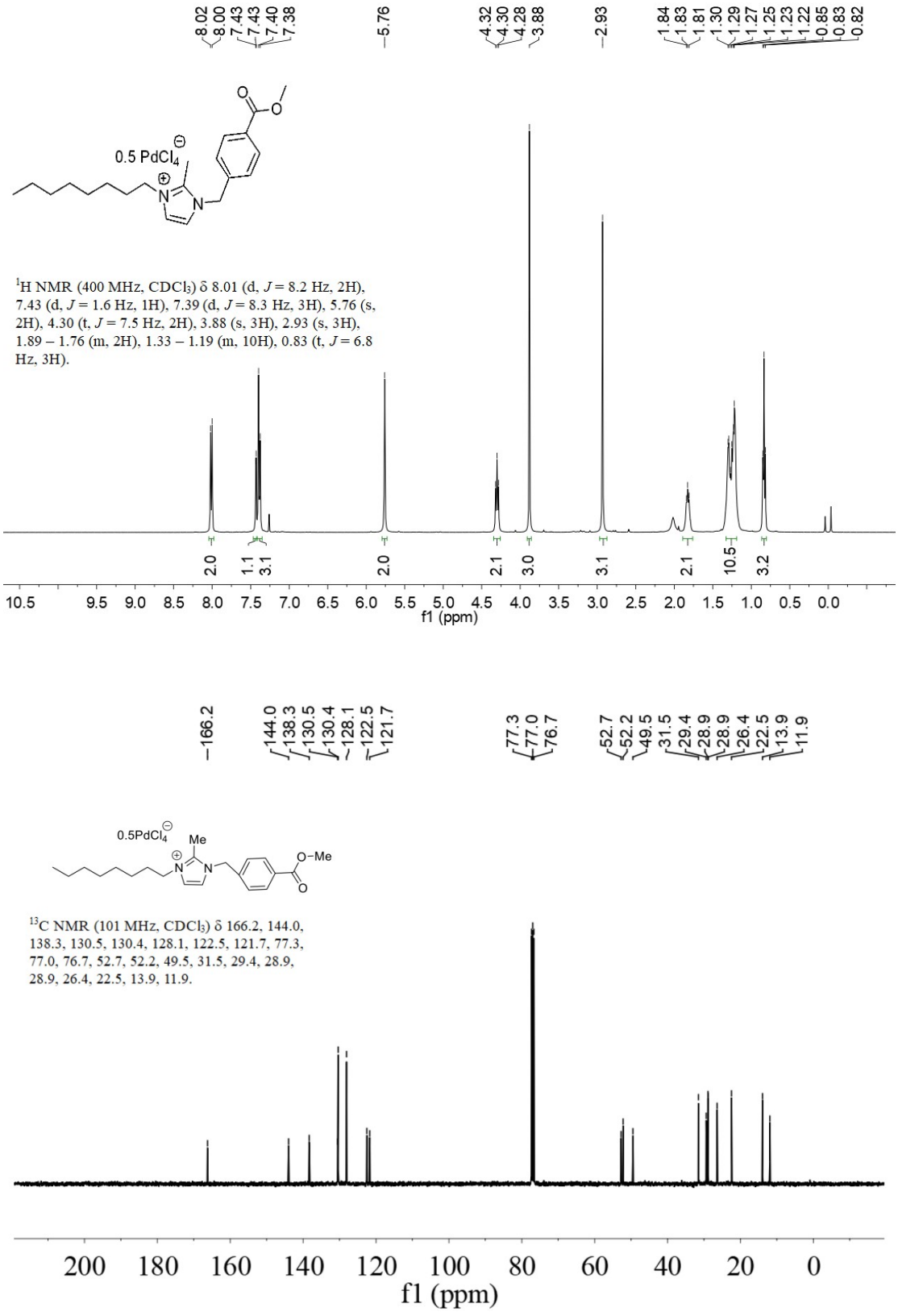


Figure S11. ^{1}H and ^{13}C NMR spectra of Octyl-Im-$PdCl_4$ **11** in $CDCl_3$.

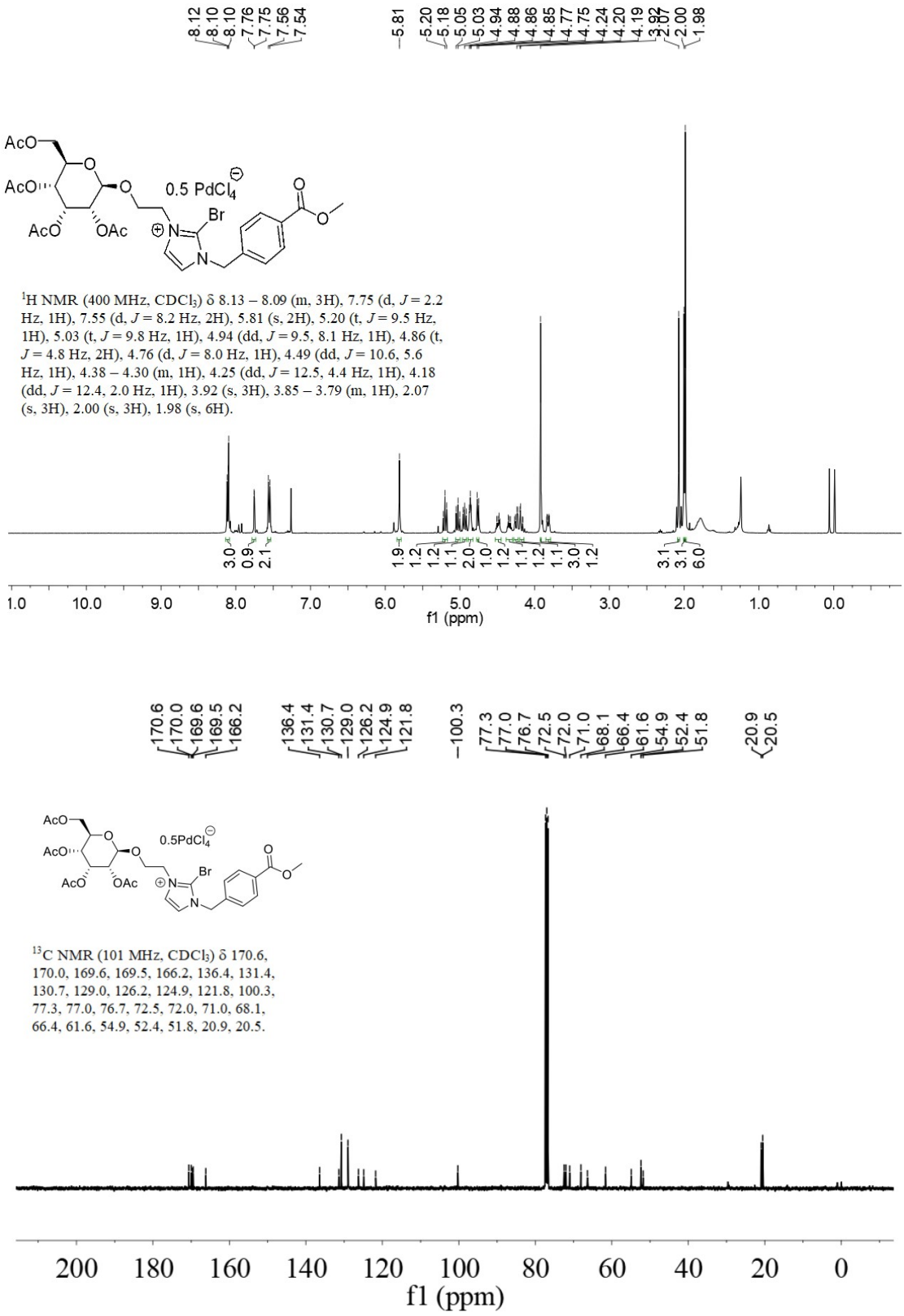


Figure S12. ^{1}H and ^{13}C NMR spectra of AcGlu-Im-$PdCl_4$ **12** in $CDCl_3$.

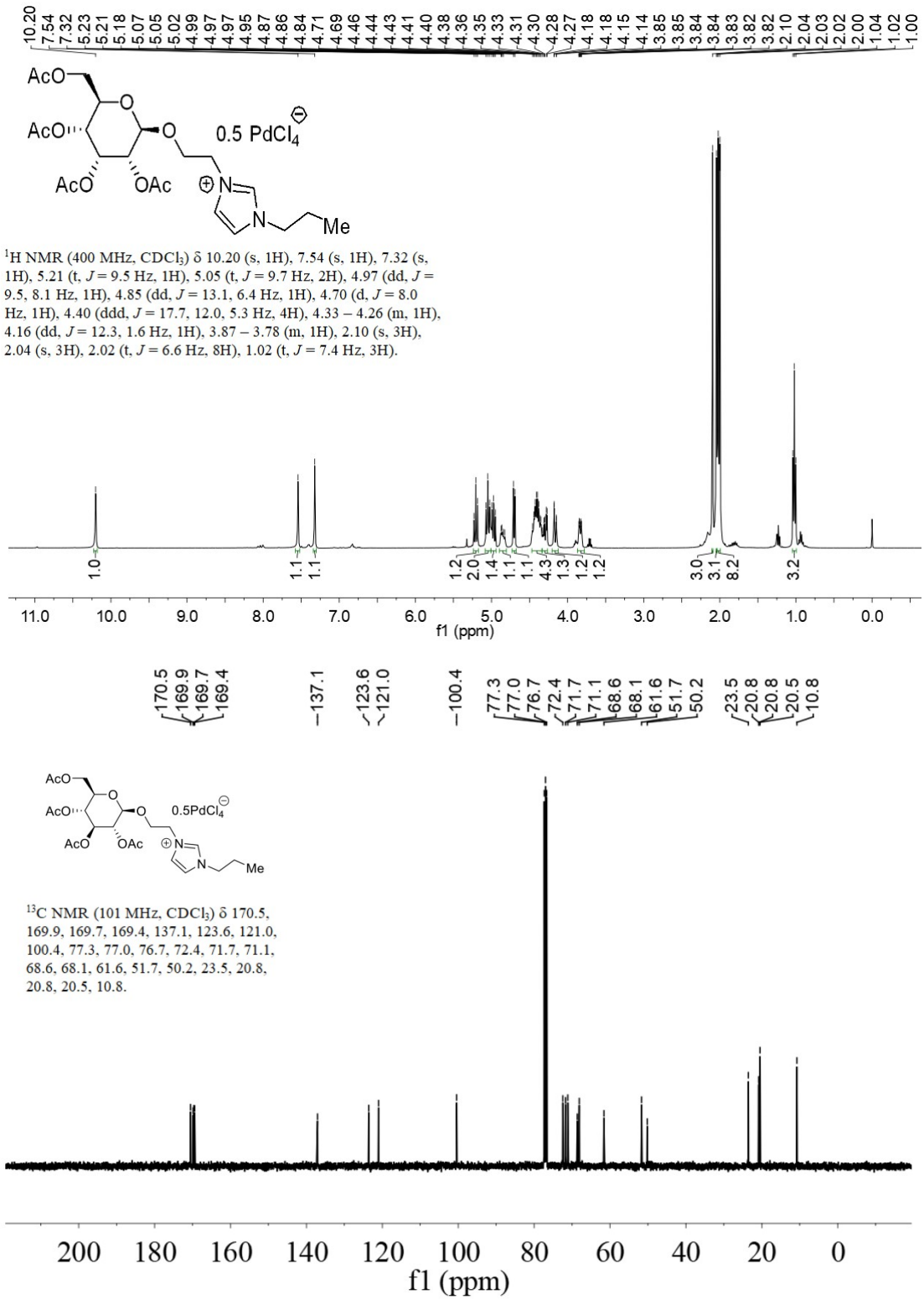


Figure S13. [1]H and [13]C NMR spectra of AcGlu-Im-$PdCl_4$ **13** in $CDCl_3$.

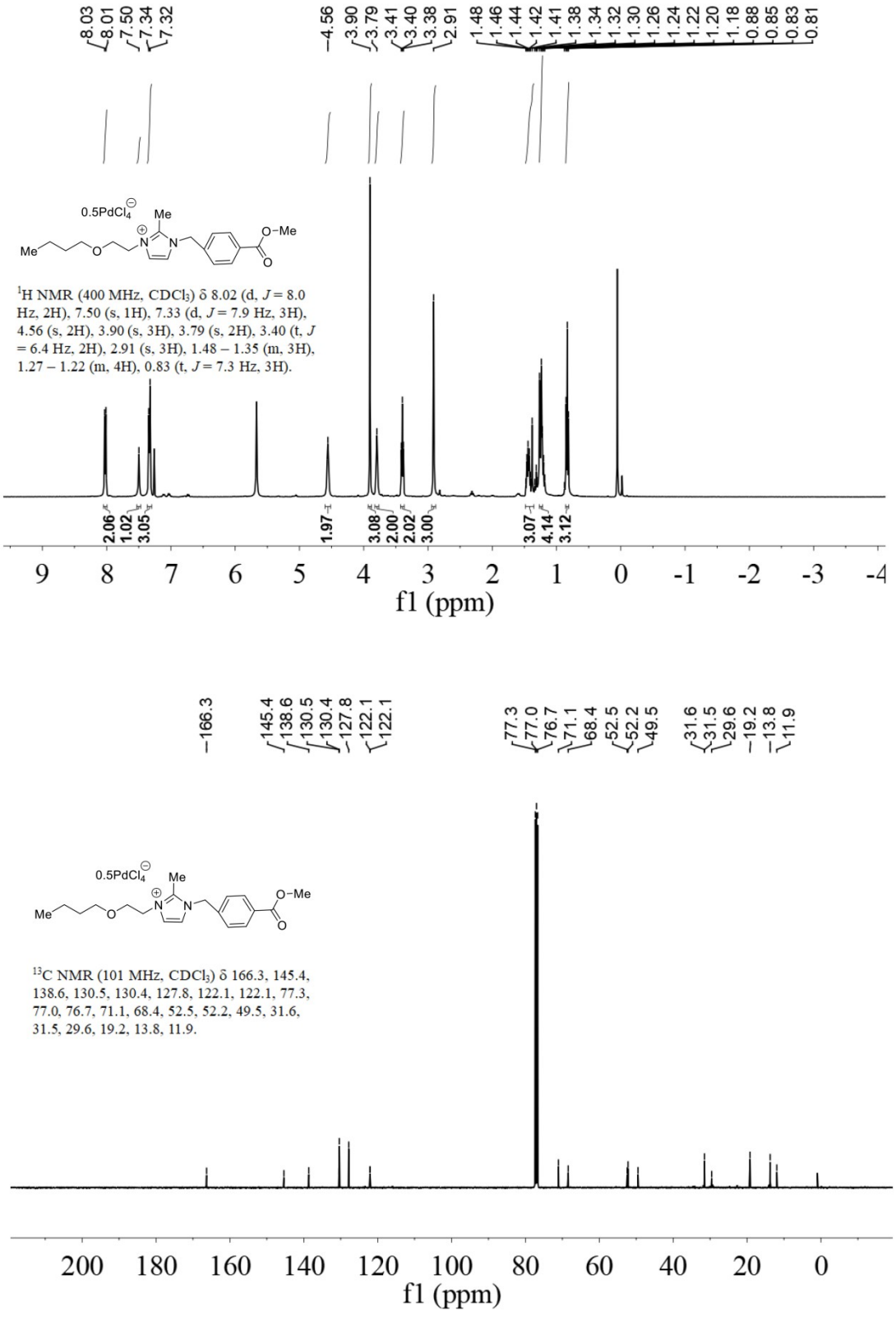


Figure S14. ^{1}H and ^{13}C NMR spectra of BOE-Im-$PdCl_4$ **14** in $CDCl_3$.

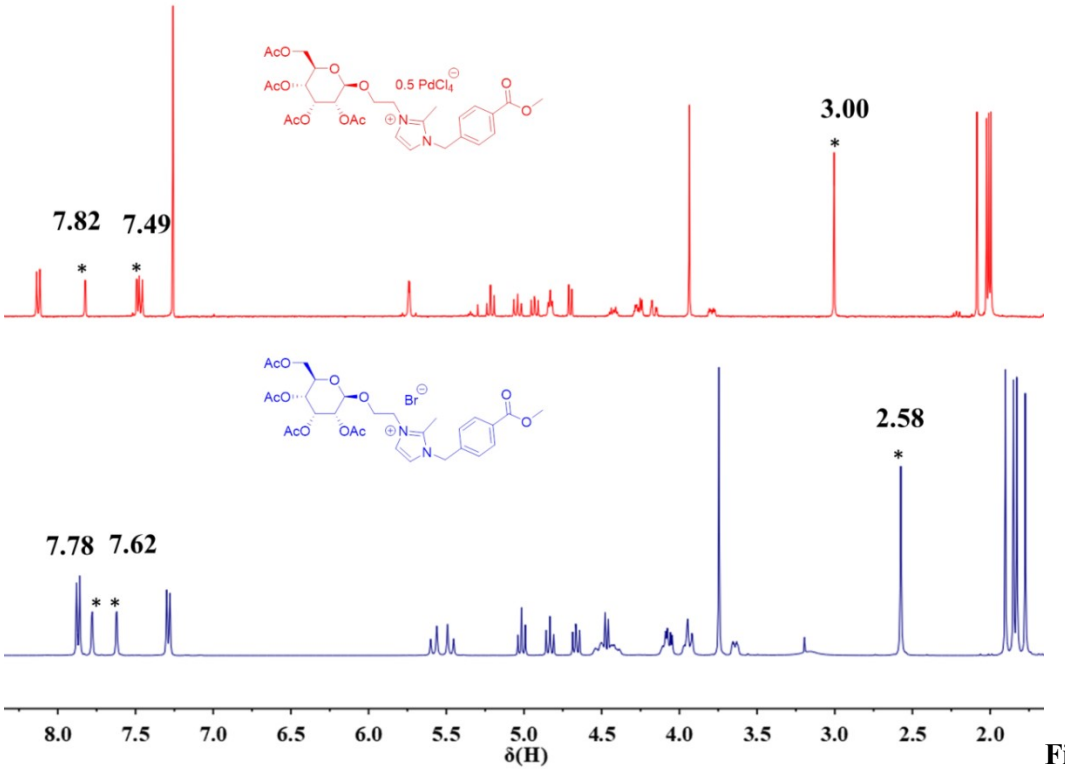


Figure S15. ^{1}H NMR spectra of AcGlu-Im-Br **3** and AcGlu-Im-$PdCl_4$ **10** in $CDCl_3$.

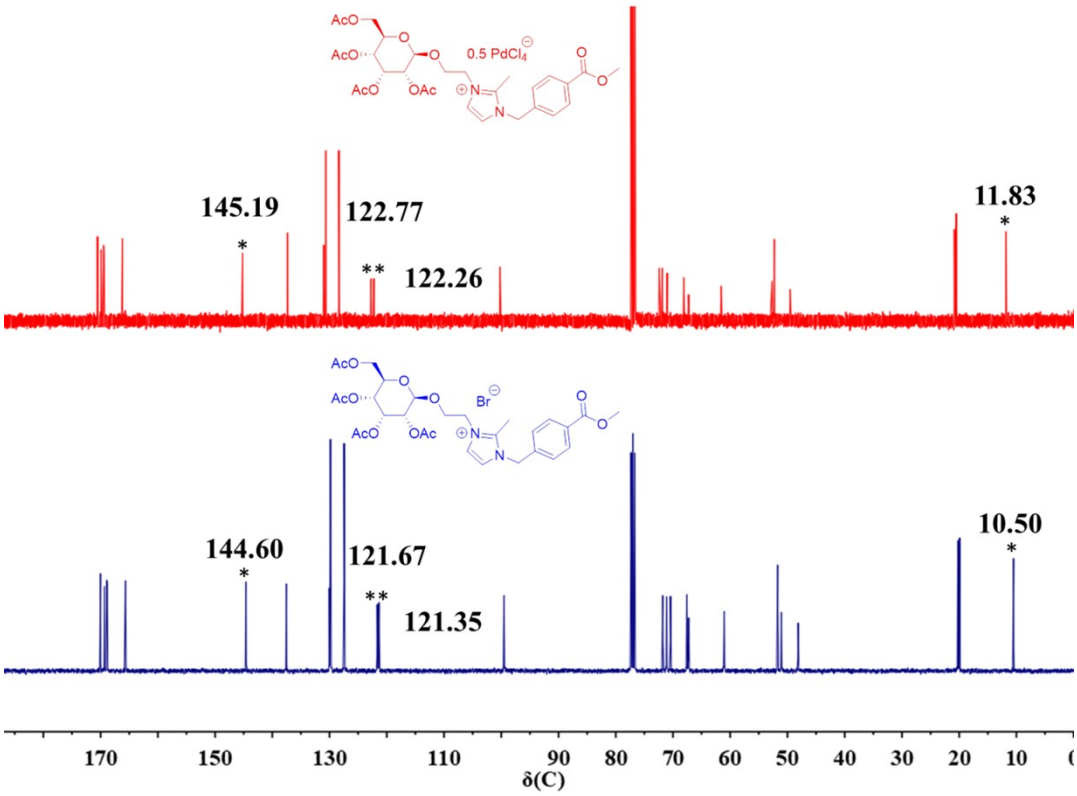


Figure S16. ^{13}C NMR spectra of AcGlu-Im-Br **3** and AcGlu-Im-$PdCl_4$ **10** in $CDCl_3$.

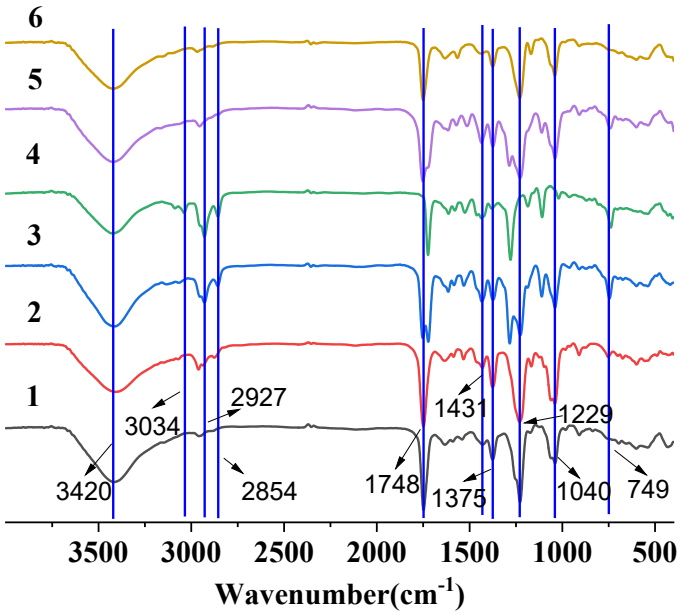


Figure S17. FT-IR spectra of Im-Br **1-6**.

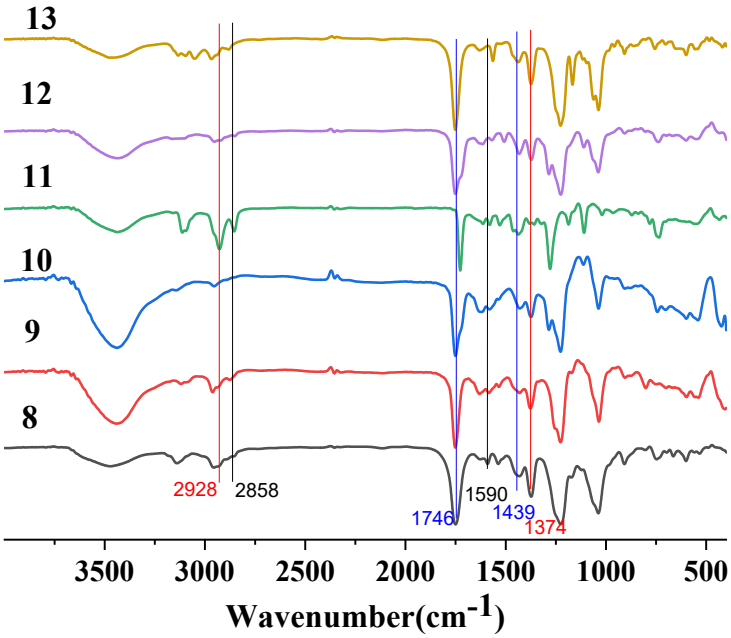


Figure S18. FT-IR spectra of Im-$PdCl_4$ **8-13**.

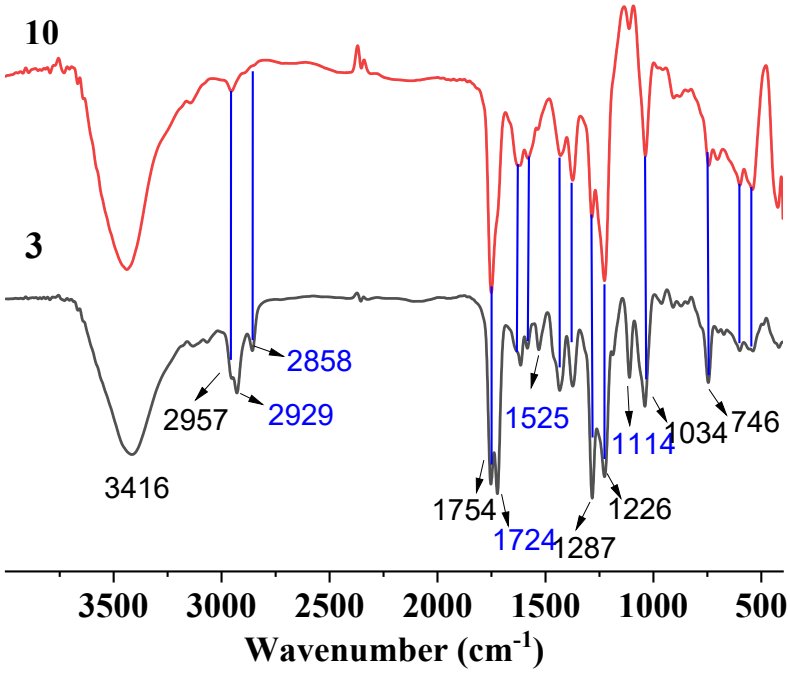


Figure S19. FT-IR spectra of AcGlu-Im-Br **3** and AcGlu-Im-$PdCl_4$ **10**.

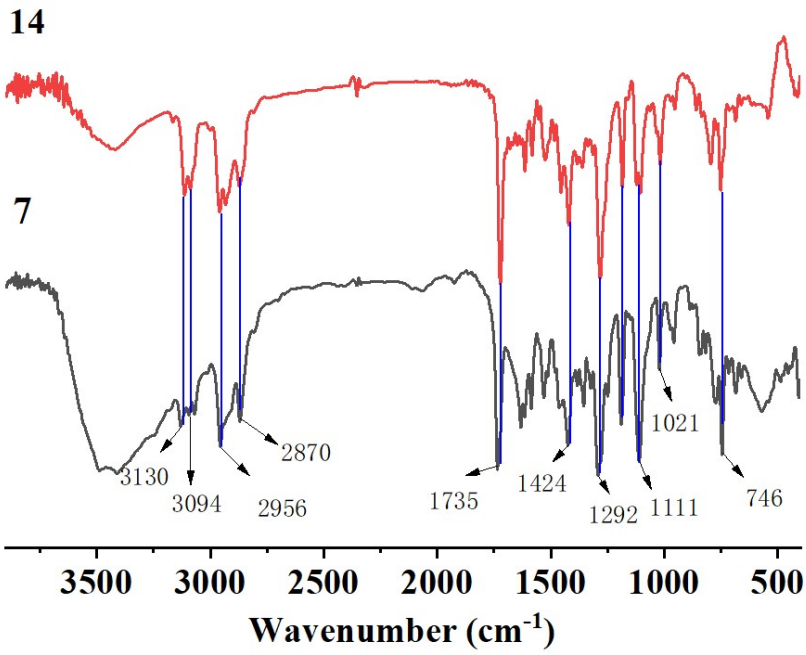


Figure S20. FT-IR spectra of BOE-Im-Br **7** and BOE-Im-$PdCl_4$ **14**.

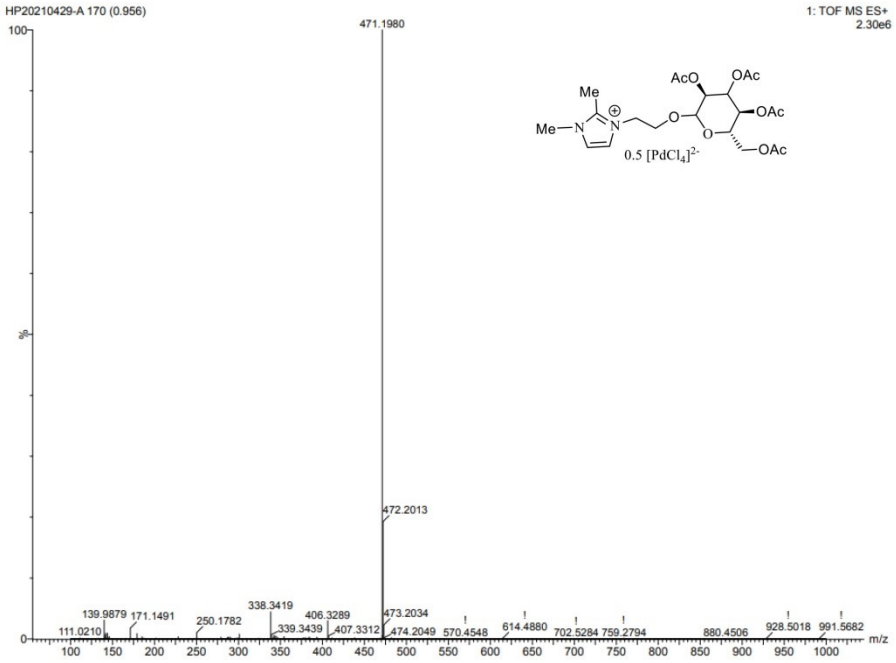


Figure S21. HR-MS spectra of AcGlu-Im-$PdCl_4$ **8**.

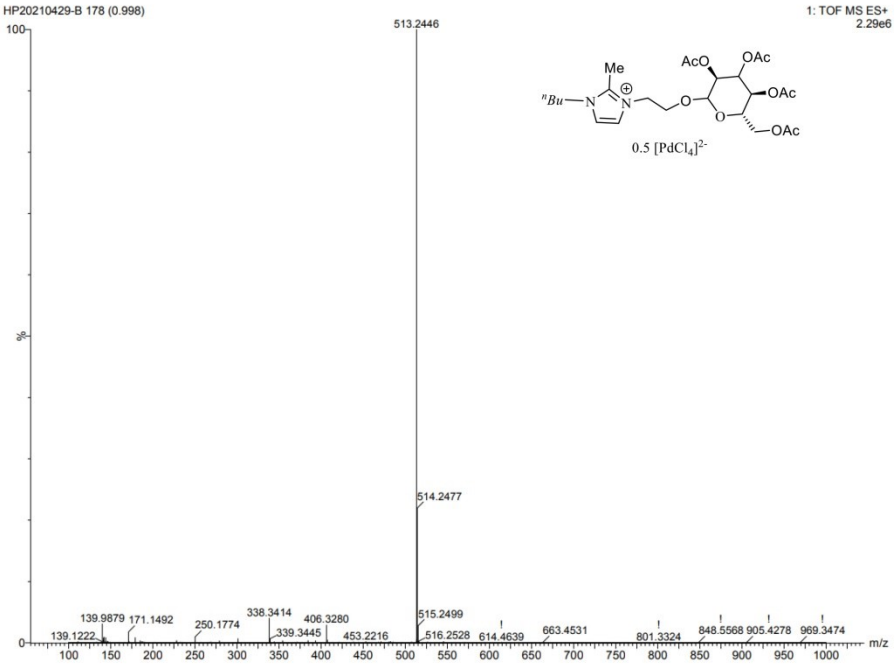


Figure S22. HR-MS spectra of AcGlu-Im-$PdCl_4$ **9**.

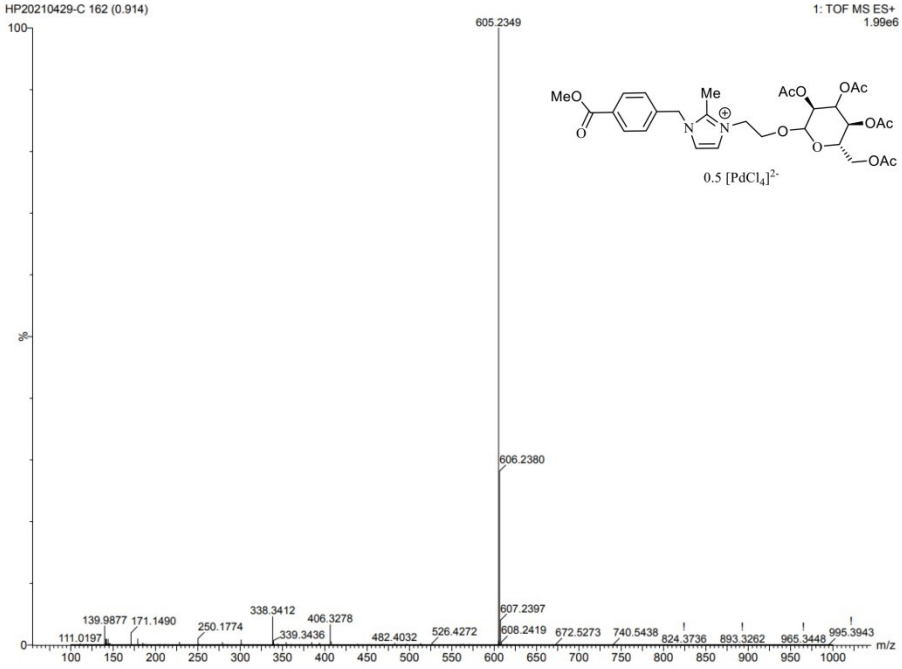


Figure S23. HR-MS spectra of AcGlu-Im-$PdCl_4$ **10**.

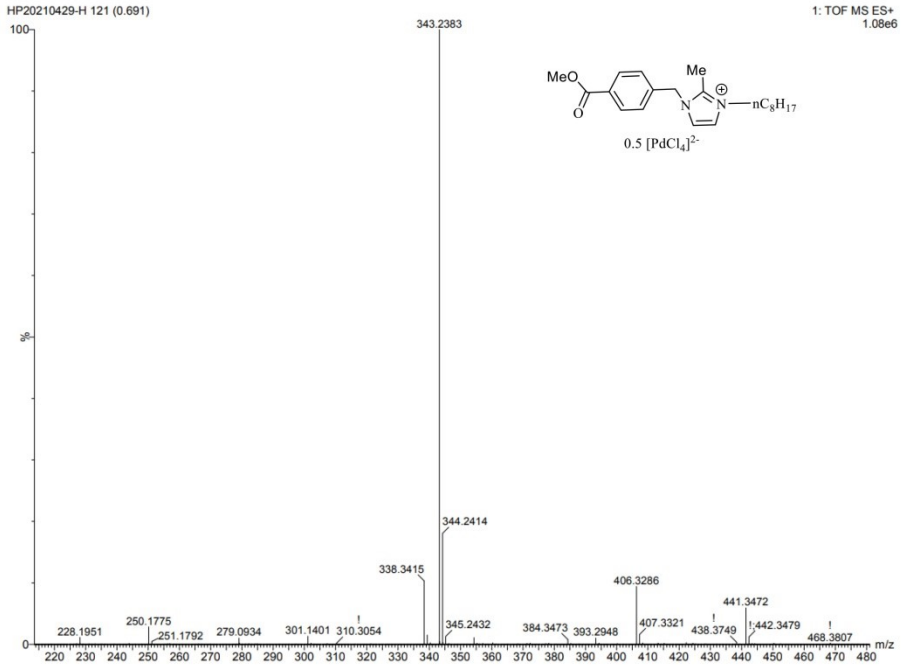


Figure S24. HR-MS spectra of Octyl-Im-$PdCl_4$ **11**.

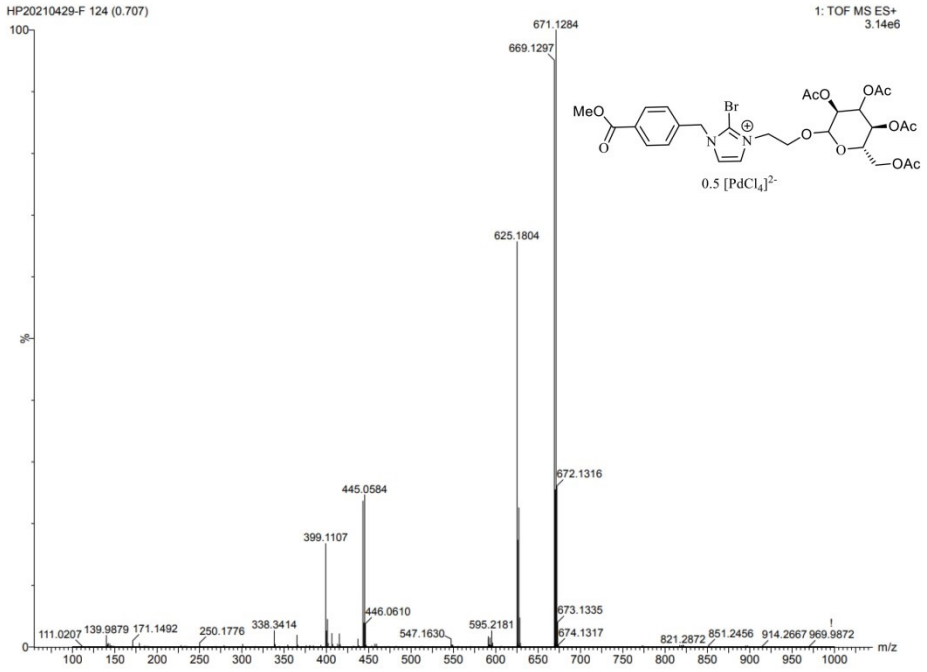


Figure S25. HR-MS spectra of Octyl-Im-$PdCl_4$ **12**.

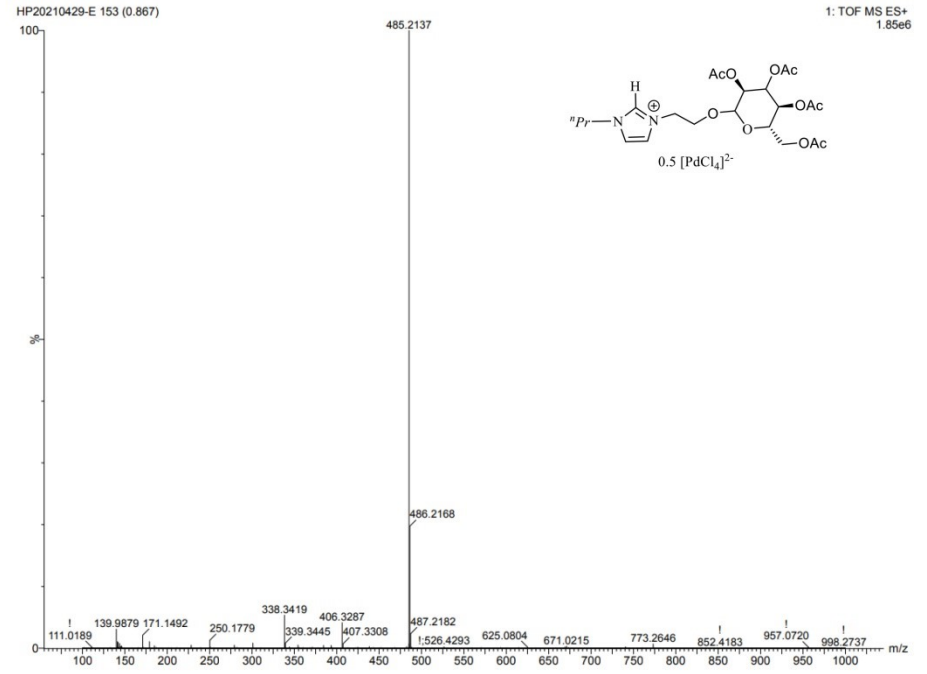


Figure S26. HR-MS spectra of AcGlu-Im-$PdCl_4$ **13**.

Formula Predictor Result	C19 H27 N2 O3
Mass	332.20789
Error Margin	10 ppm
DBE Range	Not Used
Electron Ions	Both configurations
HC Ratio	Not Used
Nitrogen Rule	Not Used

#	Score	Pred. (M)	Pred. m/z	Meas. m/z	Diff. (mDa)	Formulae (M)	Ion	Diff. (ppm)	Iso Score	DBE
4	53.46	331.20217	332.20944	332.20789	-1.55	C19 H27 N2 O3	[M+H]+	-4.666	54.48	7.5

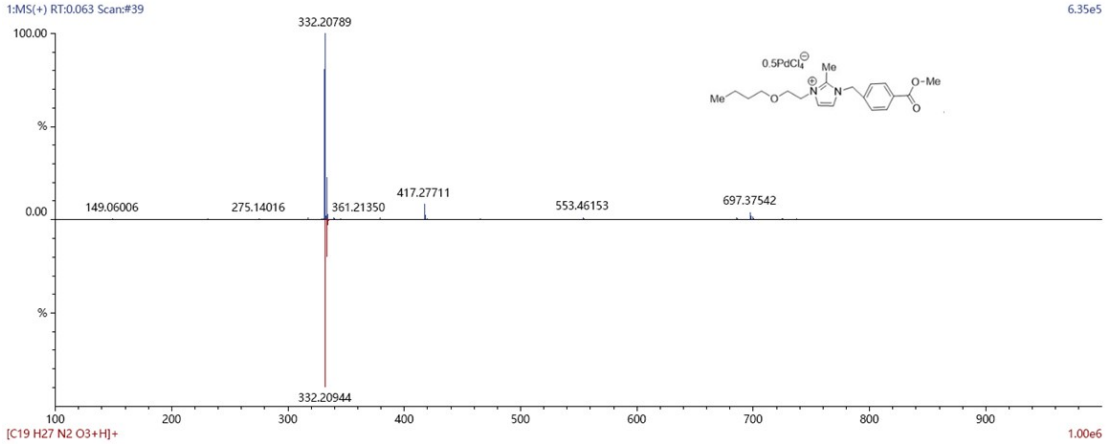


Figure S27. HR-MS spectra of BOE-Im-$PdCl_4$ **14**.

2.6 NMR Spectra of Mechanisms

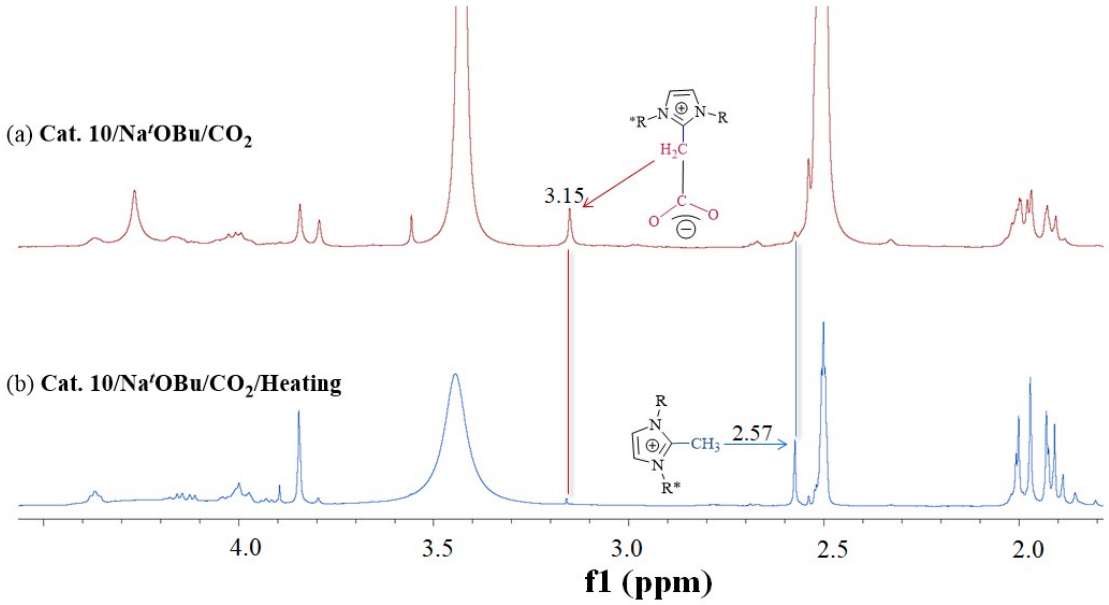


Figure S28. ^{1}H NMR spectrum of (a) Cat. **10**/Na^{t}OBu/CO_2 in DMSO-d_6 and (b) Cat. **10**/Na^{t}OBu/CO_2/Heating at 70 °C for 20 min in DMSO-d_6.

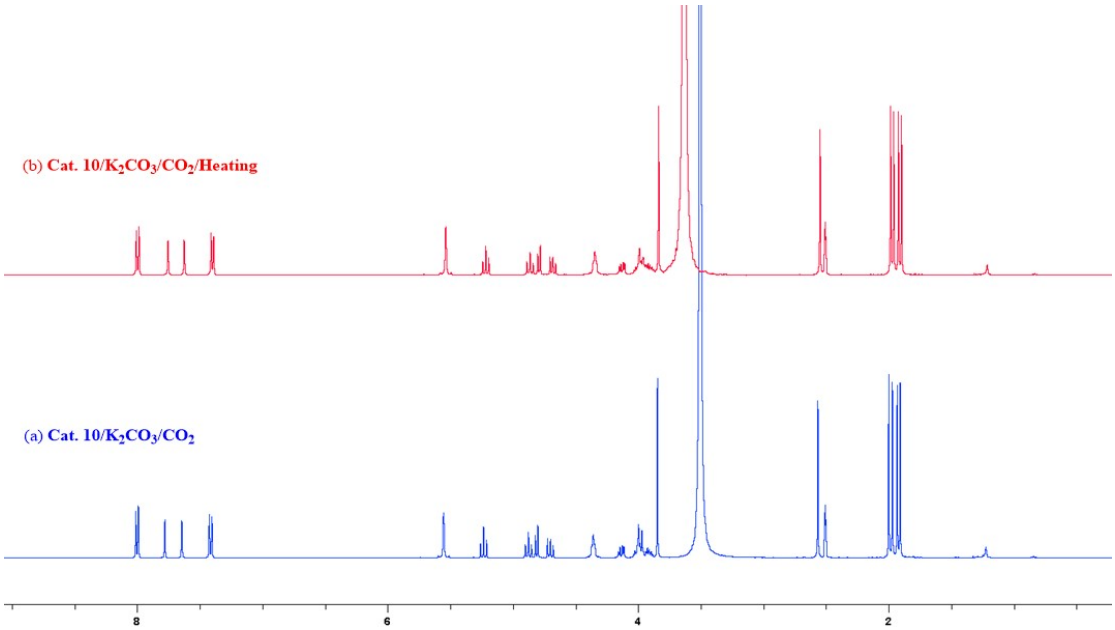


Figure S29. ^{1}H NMR spectra of (a) Cat. **10**/K_2CO_3/CO_2 at R.T. and (b) Cat. **10**/K_2CO_3/CO_2/Heating at 35 °C for 1.0 h in DMSO-d_6.

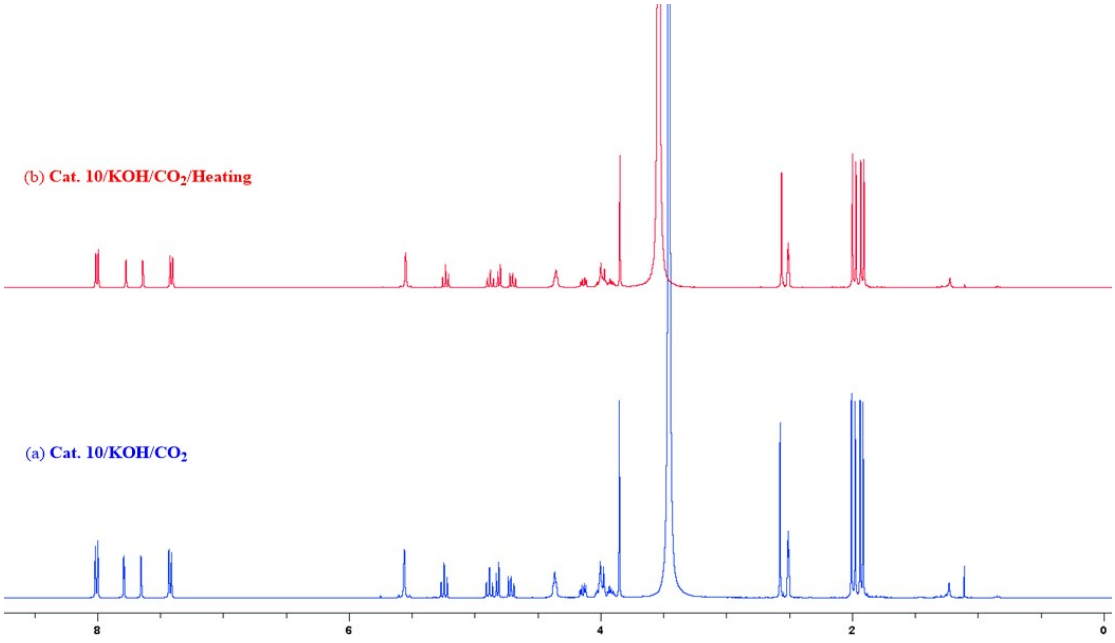
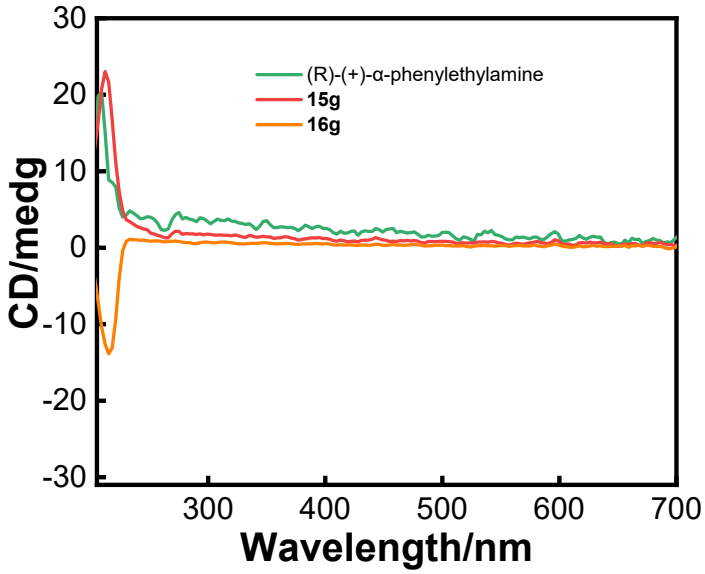


Figure S30. ^{1}H NMR spectra of (a) Cat. **10**/KOH/CO_2 at R.T. and (b) Cat. **10**/KOH/CO_2/Heating at 35 °C for 1.0 h in DMSO-d_6.



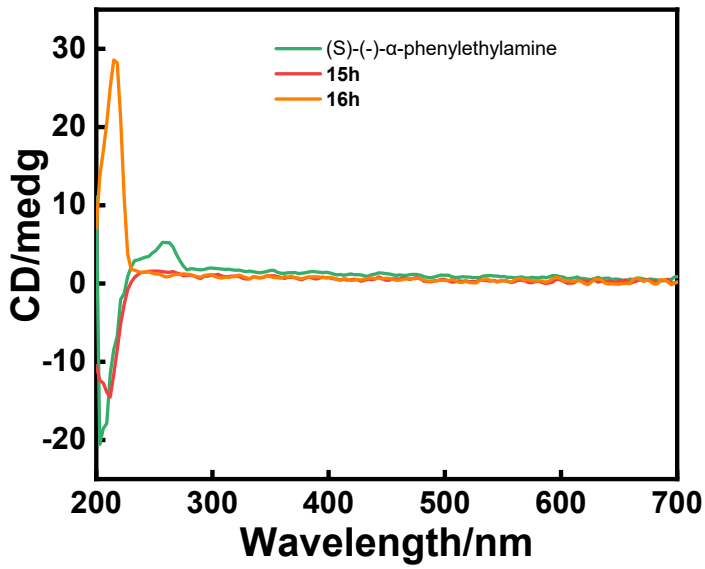


Figure S31. The circular dichroism spectrum of (R)-(+)-α-phenylethylamine, (S)-(-)-α-phenylethylamine, **15g**, **15h**, **16g**, and **16h**.

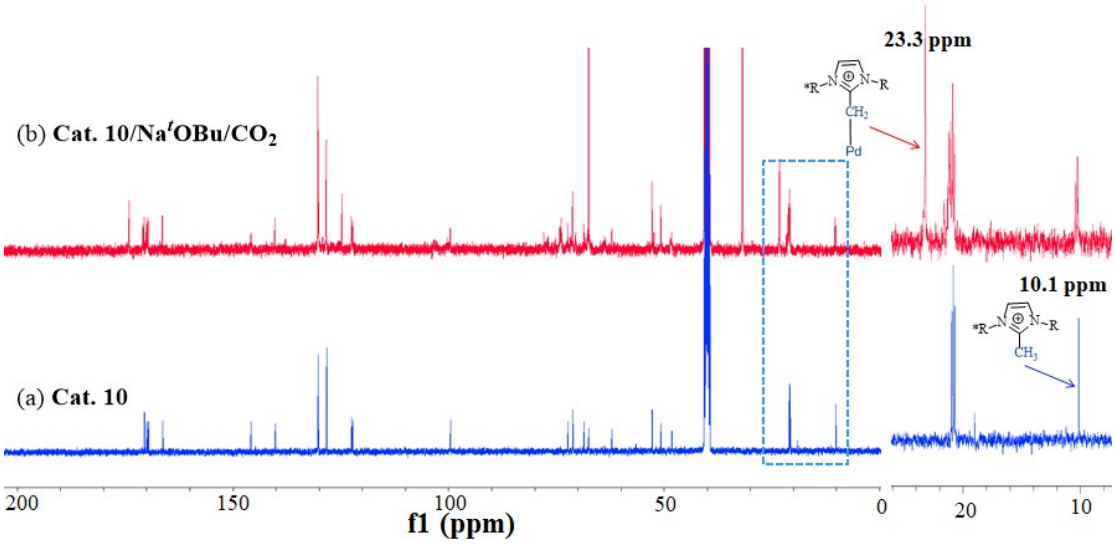


Figure S32. ^{13}C NMR spectrum of (a) Cat. **10** and (b) Cat. **10**/NaᵗOBu/CO_2.

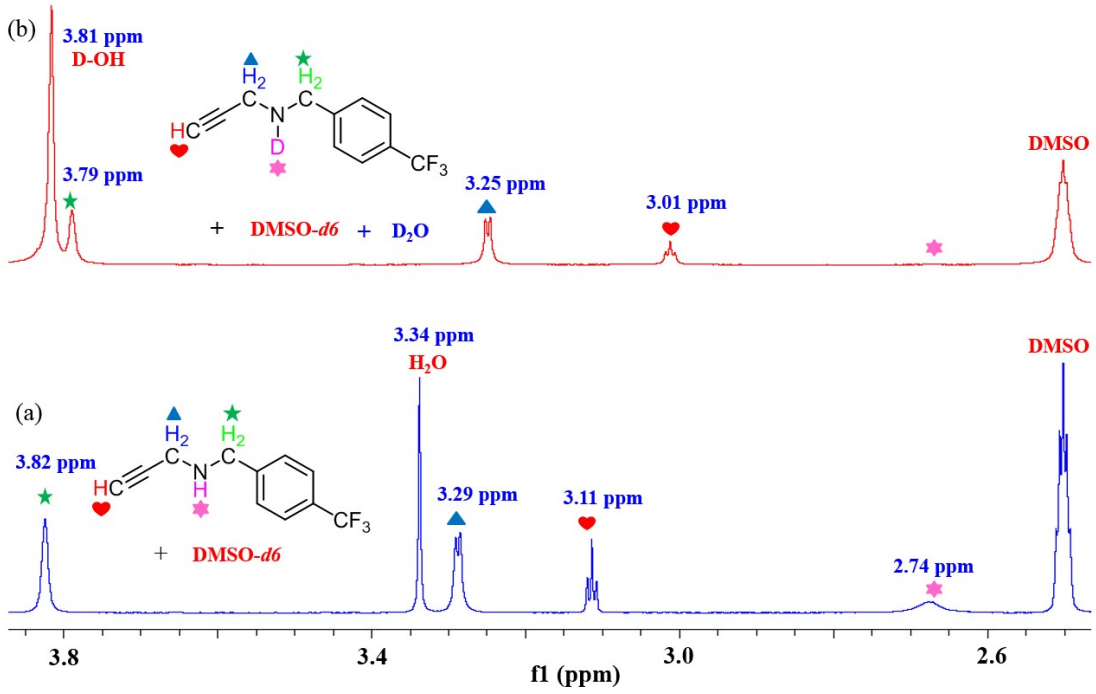


Figure S33. ^{1}H NMR spectra of (a) **15a** and (b) D_2O exchange experiment of **15a**/D_2O (two drops) in DMSO-d_6.

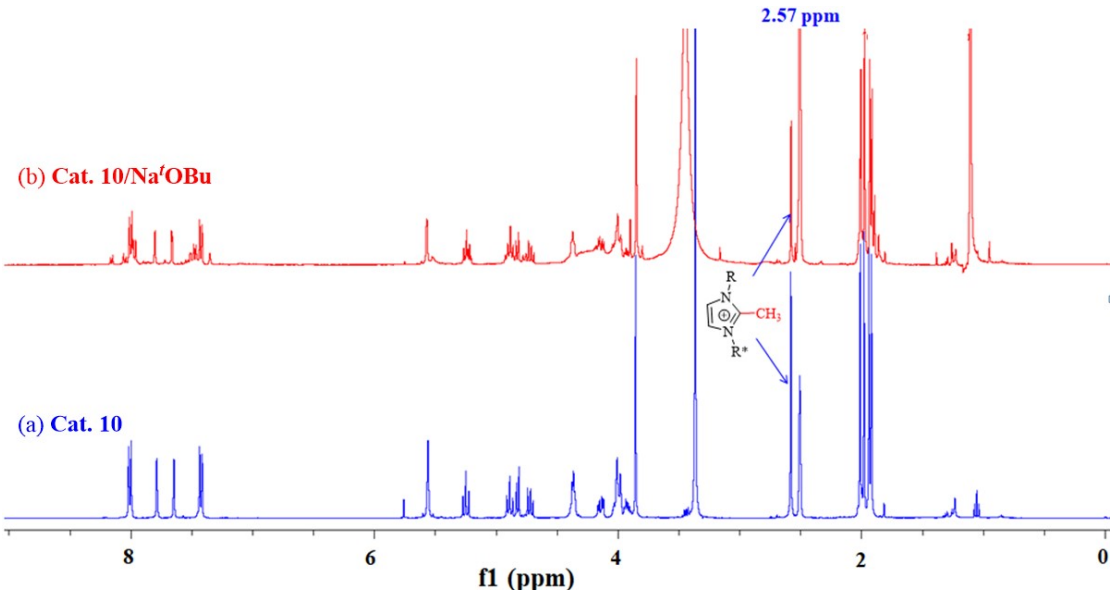


Figure S34. ^{1}H NMR spectra of (a) Cat. **10** and (b) Cat. **10**/Na^{t}OBu in DMSO-d_6.

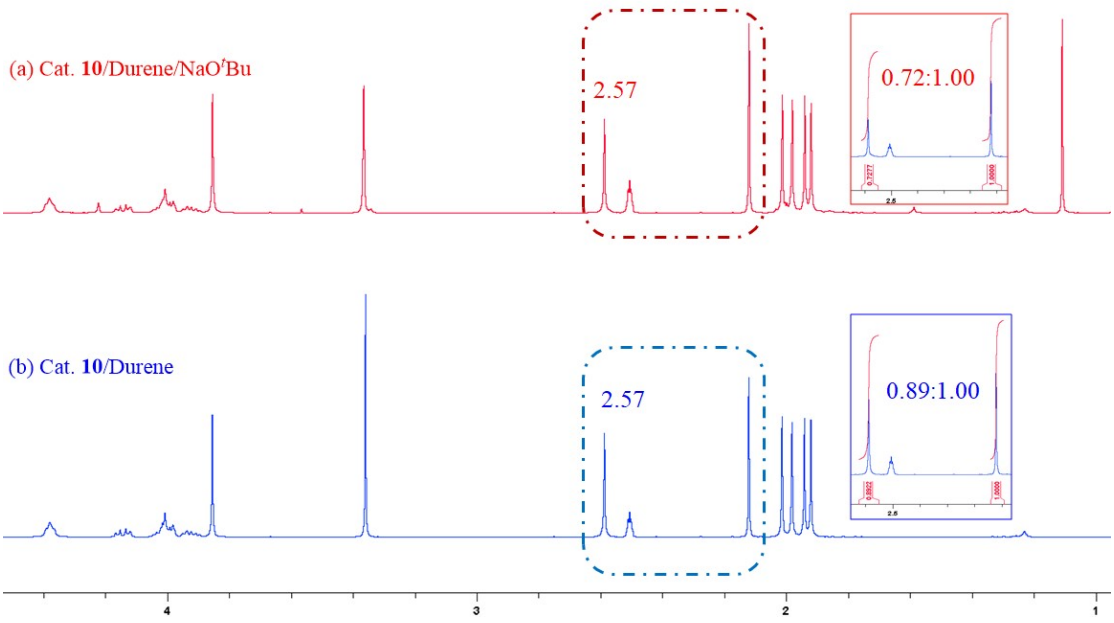


Figure S35. (a) ^{1}H NMR spectra of Cat. **10** with internal standard durene. (b) ^{1}H NMR spectra of Cat. **10**/NaO^{t}Bu with internal standard durene.

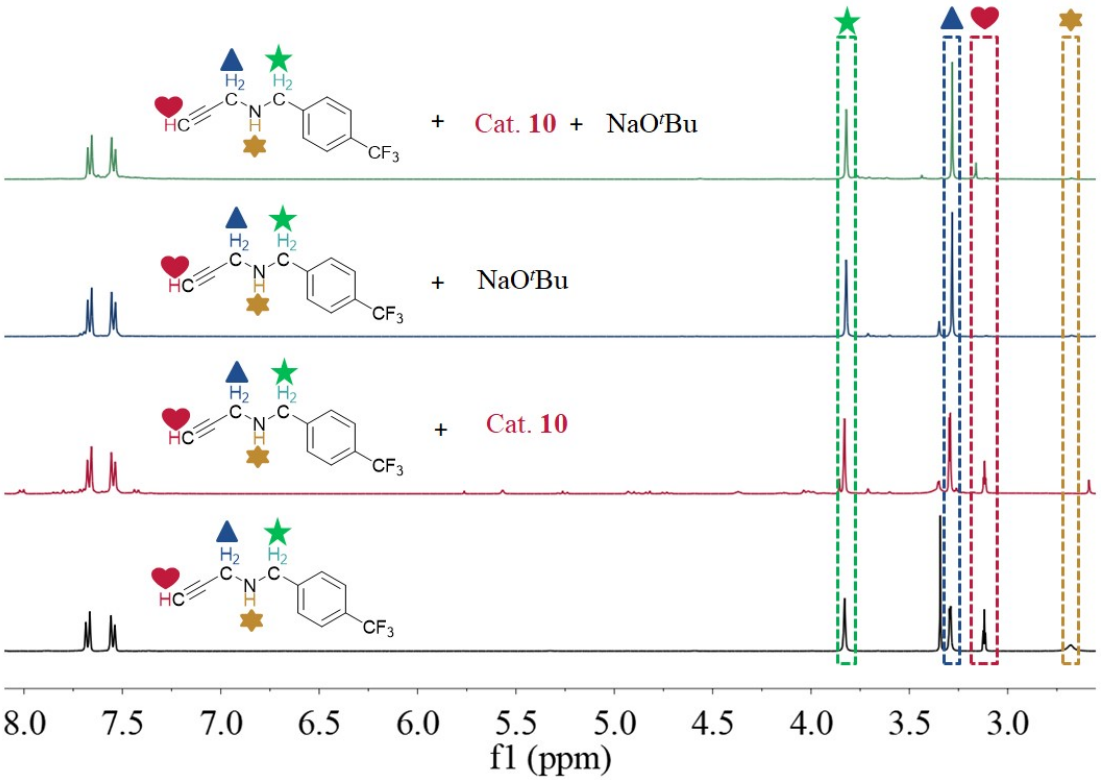


Figure S36. Activation of propargylamine **15a** by different systems in DMSO-d_6.

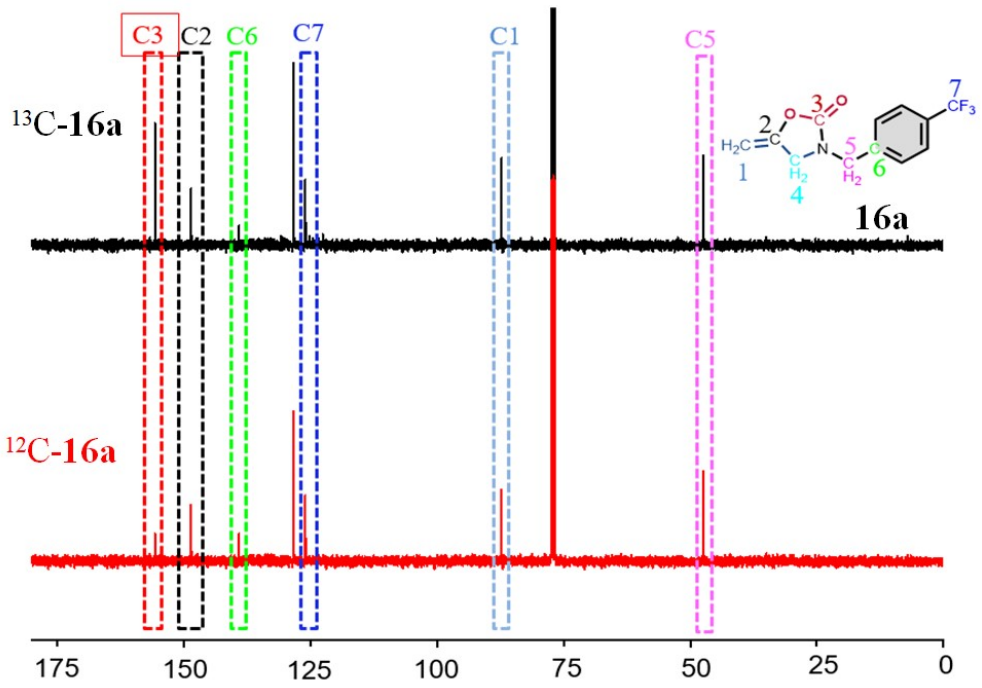


Figure S37. The ^{13}C NMR comparison spectra of ^{13}C-isotope-labeling experiments for **16a**.

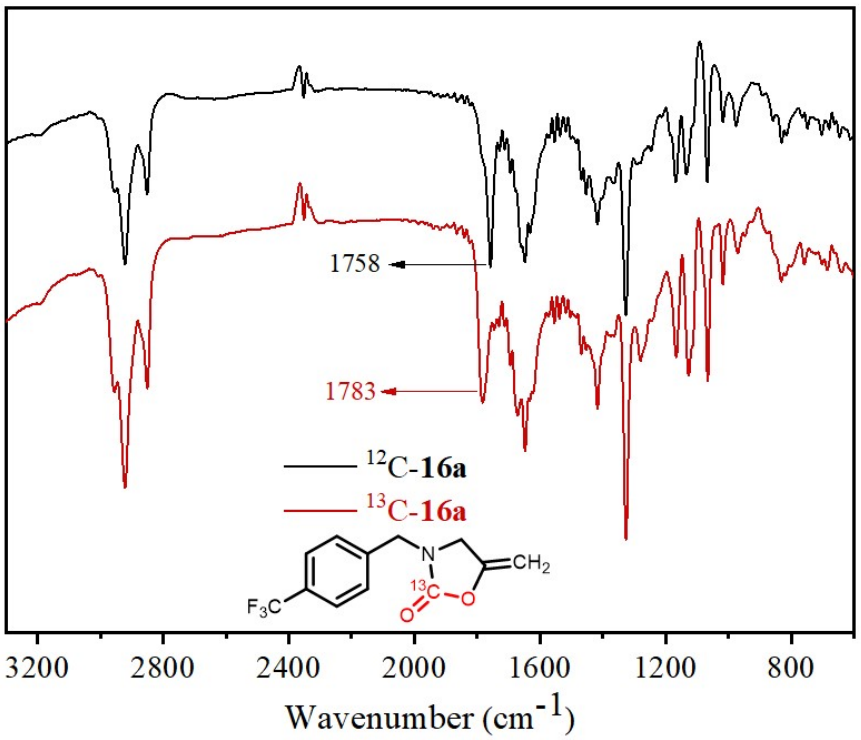
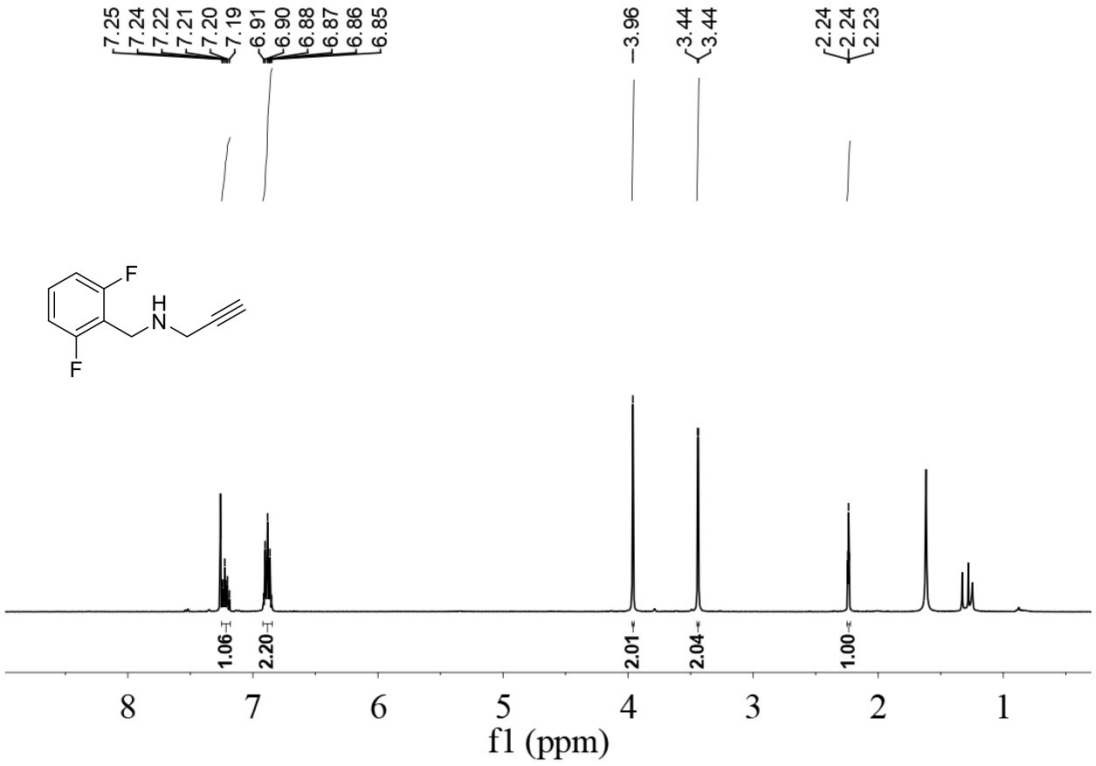
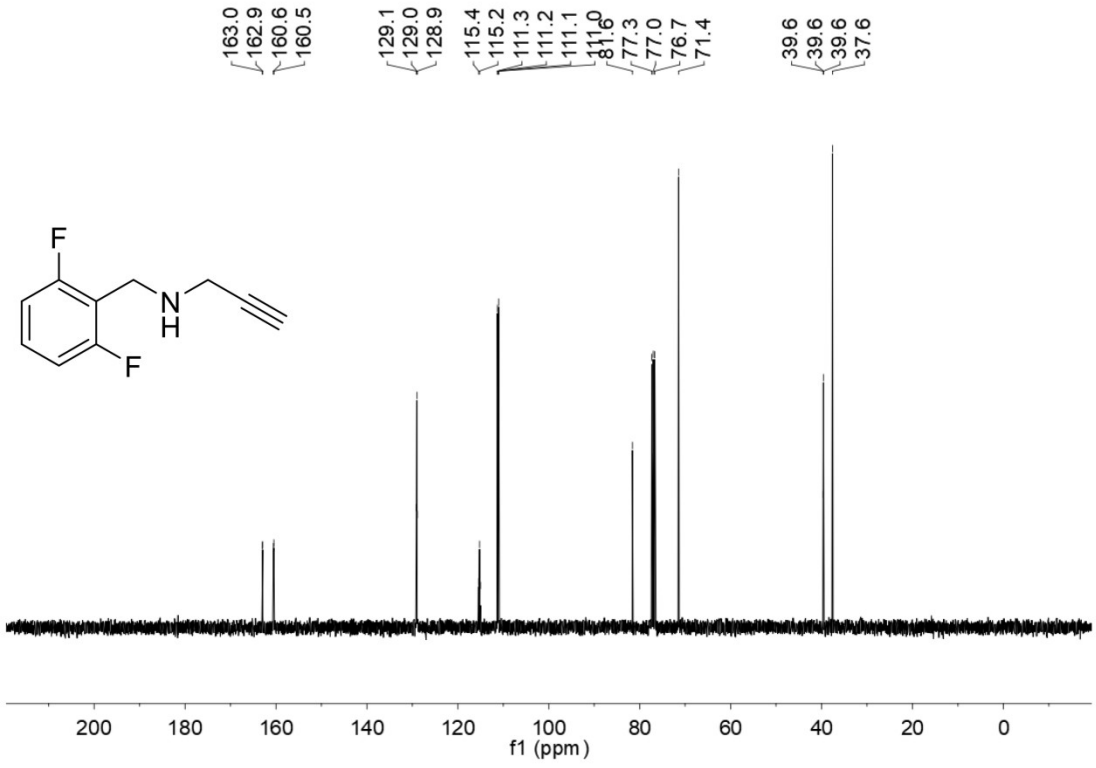
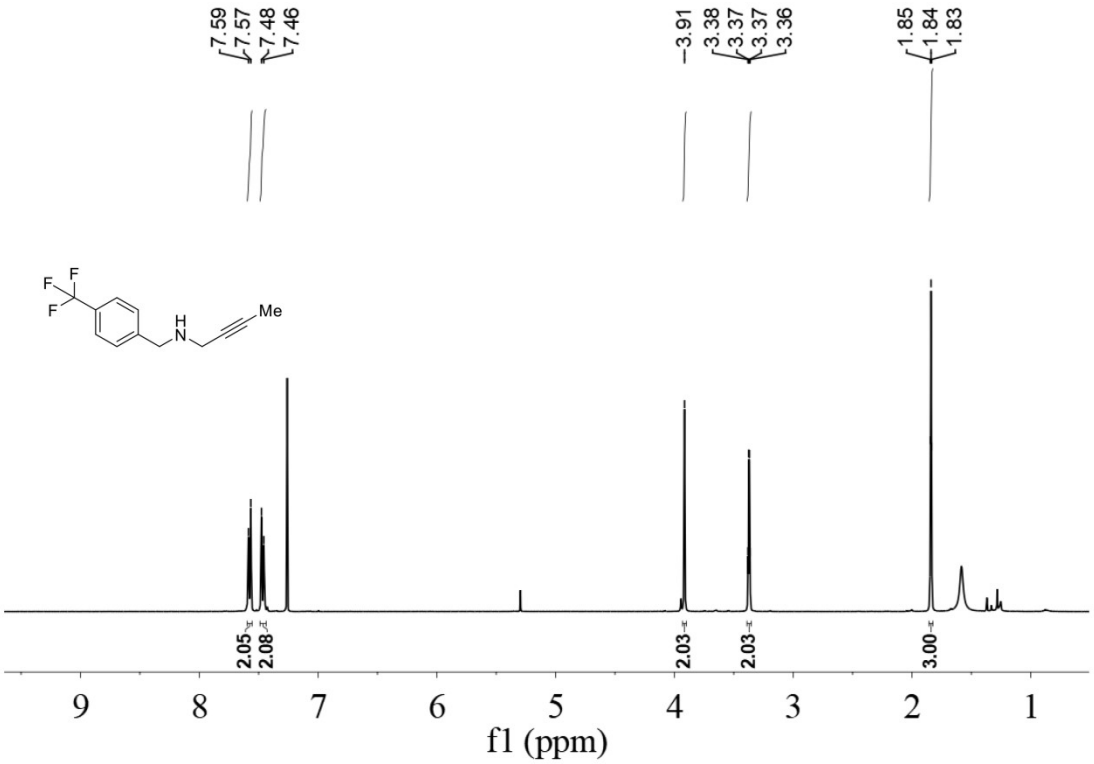


Figure S38. The FT-IR spectra of ^{13}C-isotope-labeling experiments for **16a**.

2.7 NMR Spectra of Propargyl Amines and 2-Oxazolidinones



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7.48
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3.37
3.37
3.36
1.85
1.84
1.83
F
F
F
H
N
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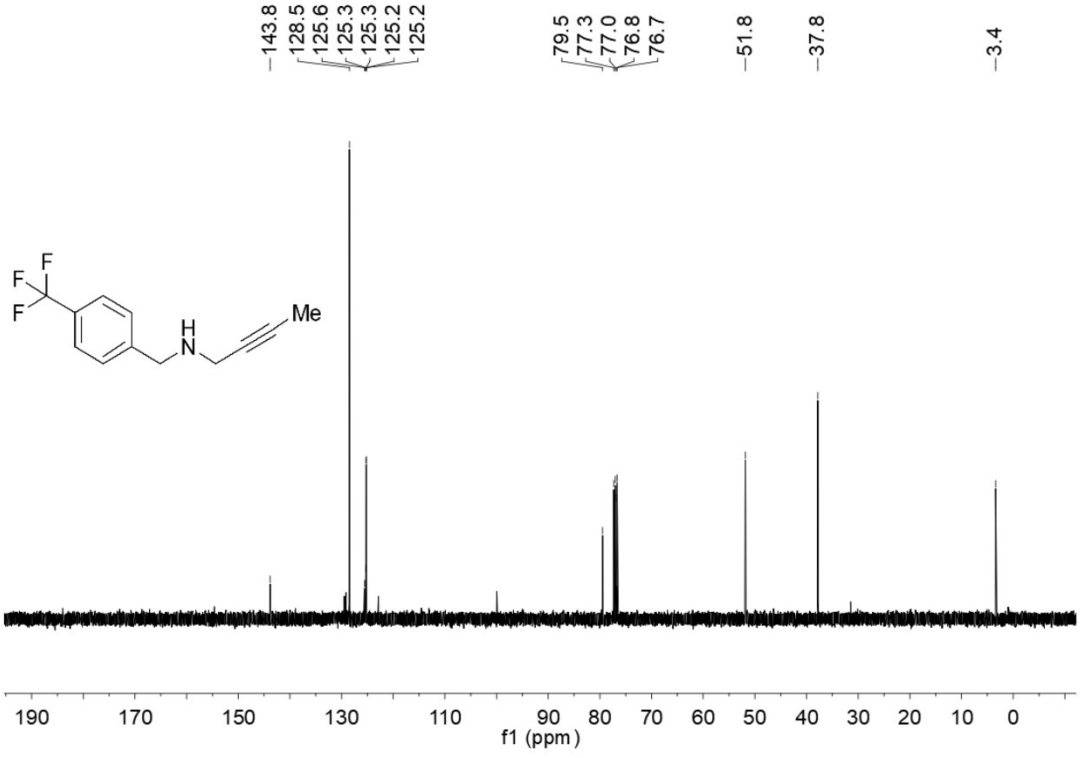
7
6
5
4
3
2
1
f1 (ppm)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125.3
125.2
125.2
79.5
77.3
77.0
76.8
76.7
51.8
37.8
3.4
F
F
F
H
N
Me
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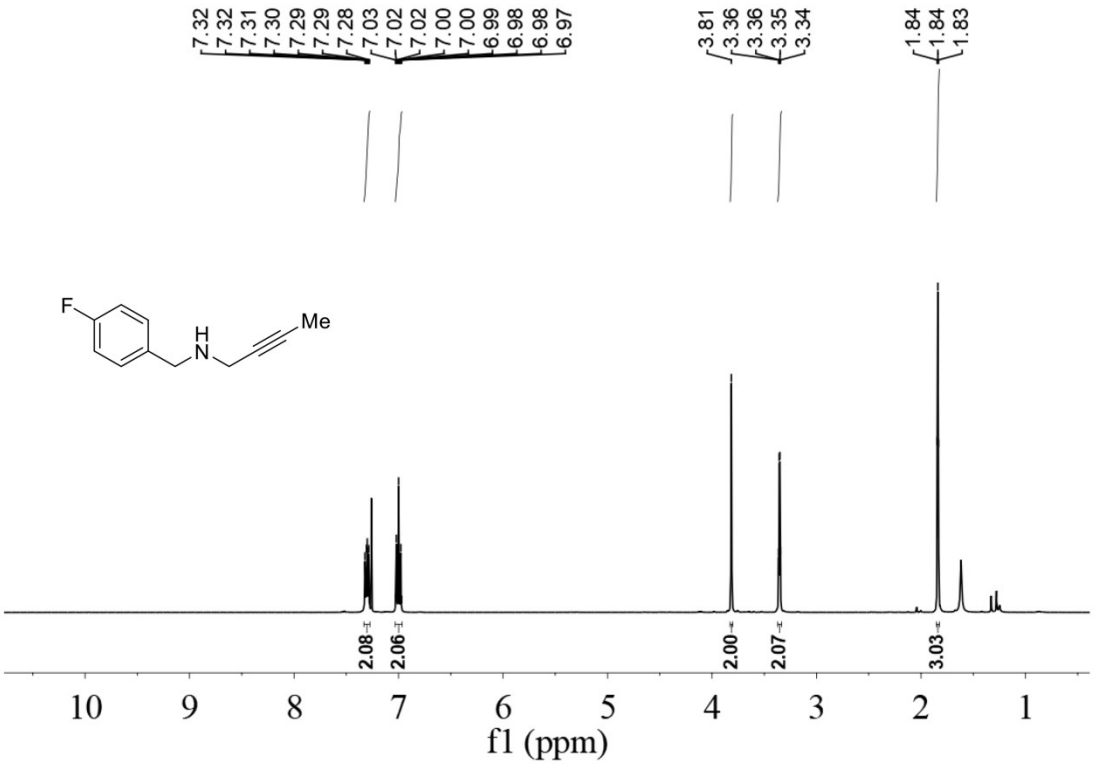
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.02
7.02
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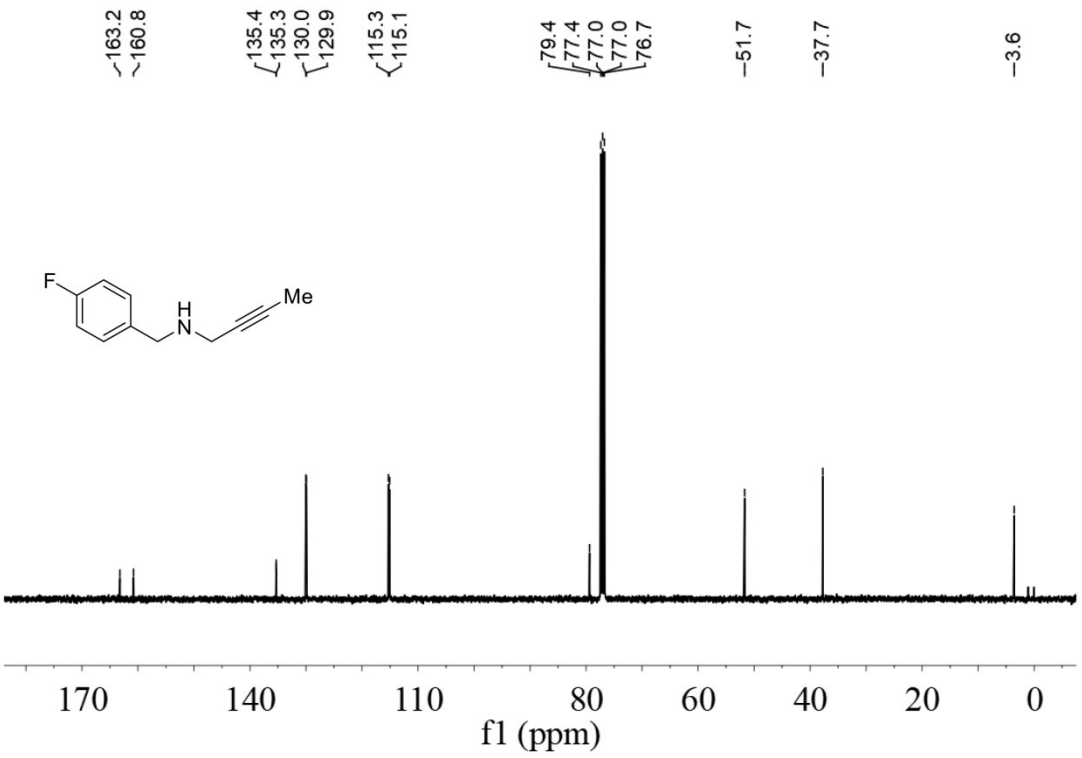
6.98
6.98
6.97
3.81
3.36
3.36
3.35
3.34
1.84
1.84
1.83
F
H
N
Me
2.08
2.06
2.00
2.07
3.03
10
9
8
7
6
5
4
3
2
1
f1 (ppm)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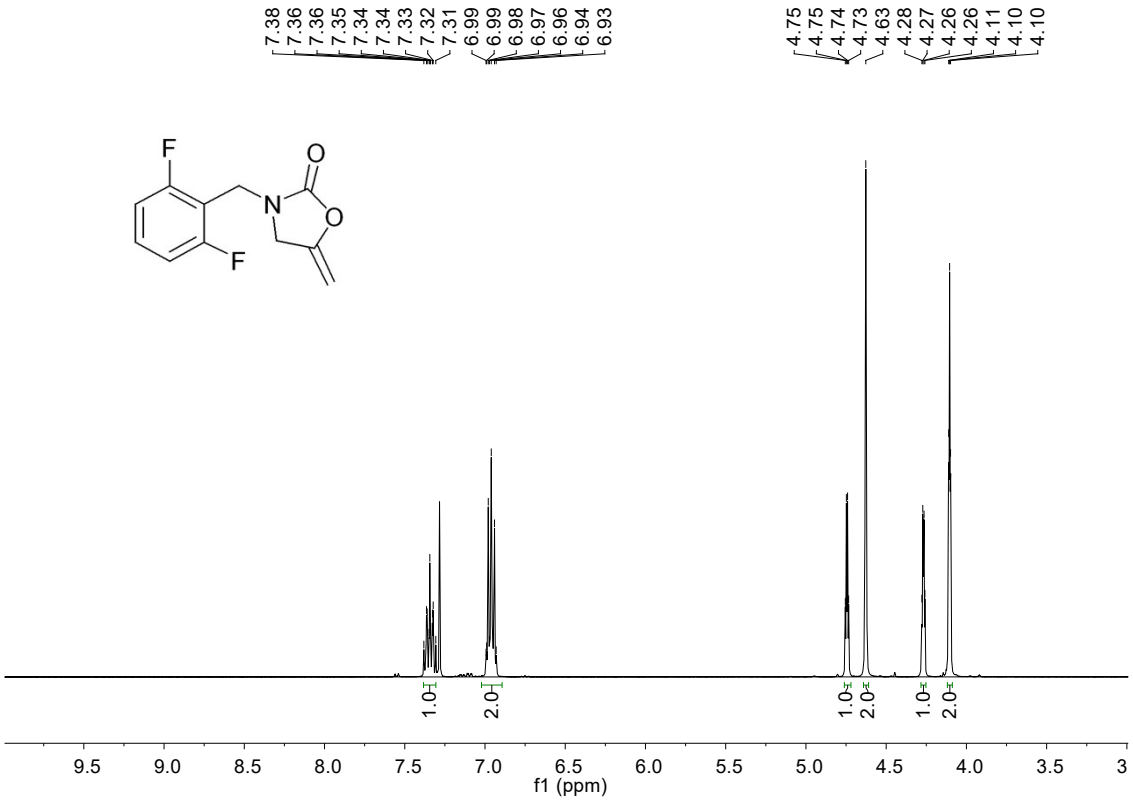
135.4
135.3
130.0
129.9
115.3
115.1
79.4
77.4
77.0
77.0
76.7
51.7
37.7
3.6
F
H
N
Me
170
140
110
80
60
40
20
0
f1 (ppm)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6.97
6.96
6.94
6.93
4.75
4.75
4.74
4.73
4.63
4.28
4.27
4.26
4.26
4.11
4.10
4.10
F
O
N
O
F
1.0
2.0
1.0
2.0
1.0
2.0
9.5
9.0
8.5
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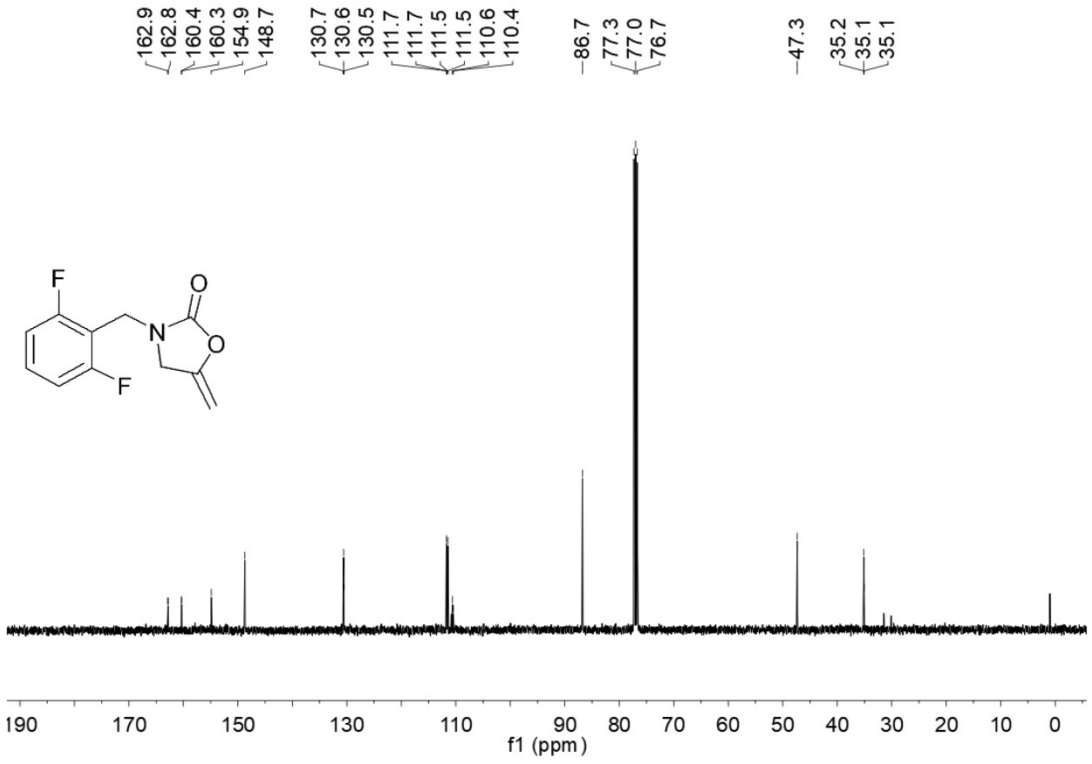
5.0
4.5
4.0
3.5
3
f1 (ppm)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130.6
130.5
111.7
111.7
111.5
111.5
110.6
110.4
86.7
77.3
77.0
76.7
47.3
35.2
35.1
35.1
F
O
N
O
F
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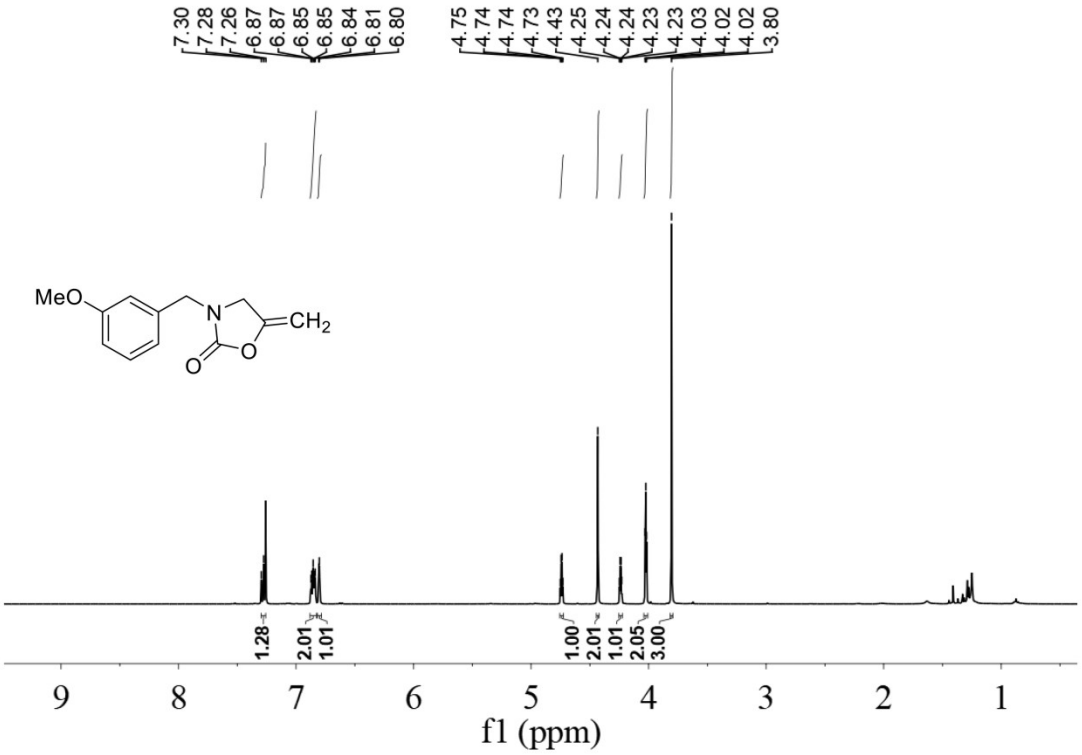
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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4.73
4.43
4.25
4.24
4.24
4.23
4.23
4.03
4.02
4.02
3.80
MeO
N
O
O
CH2
1.28
2.01
1.01
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1.01
2.05
3.00
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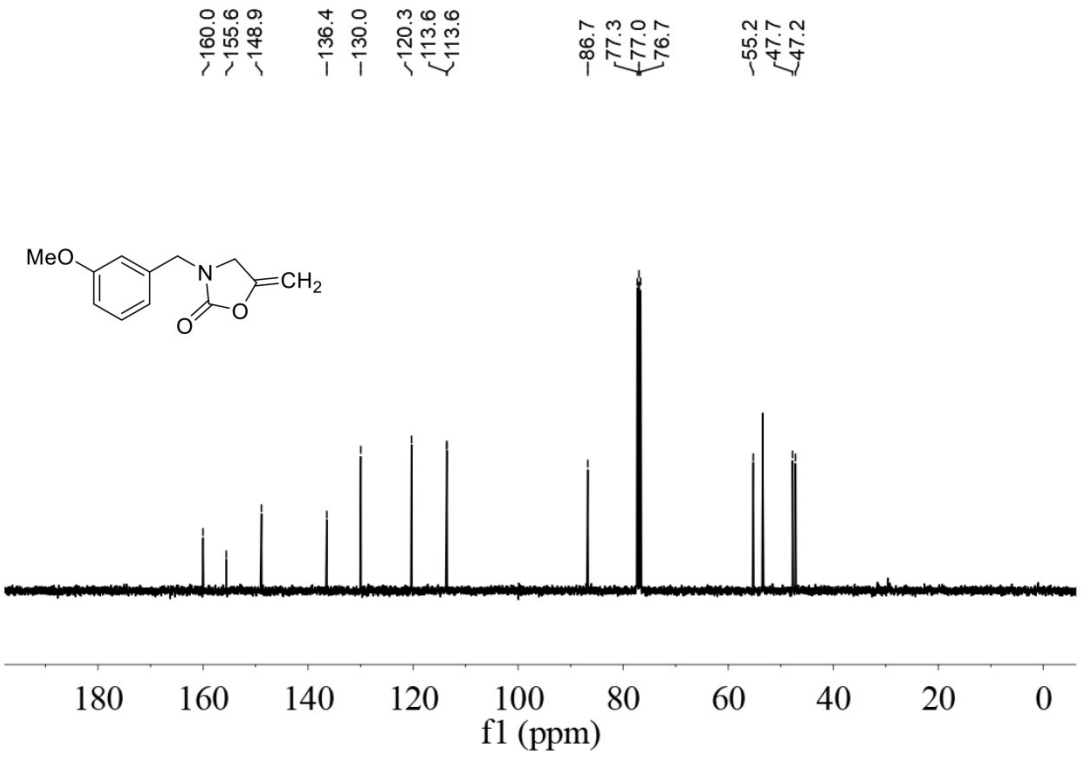
6
5
4
3
2
1
f1 (ppm)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77.0
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55.2
47.7
47.2
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O
O
CH2
180
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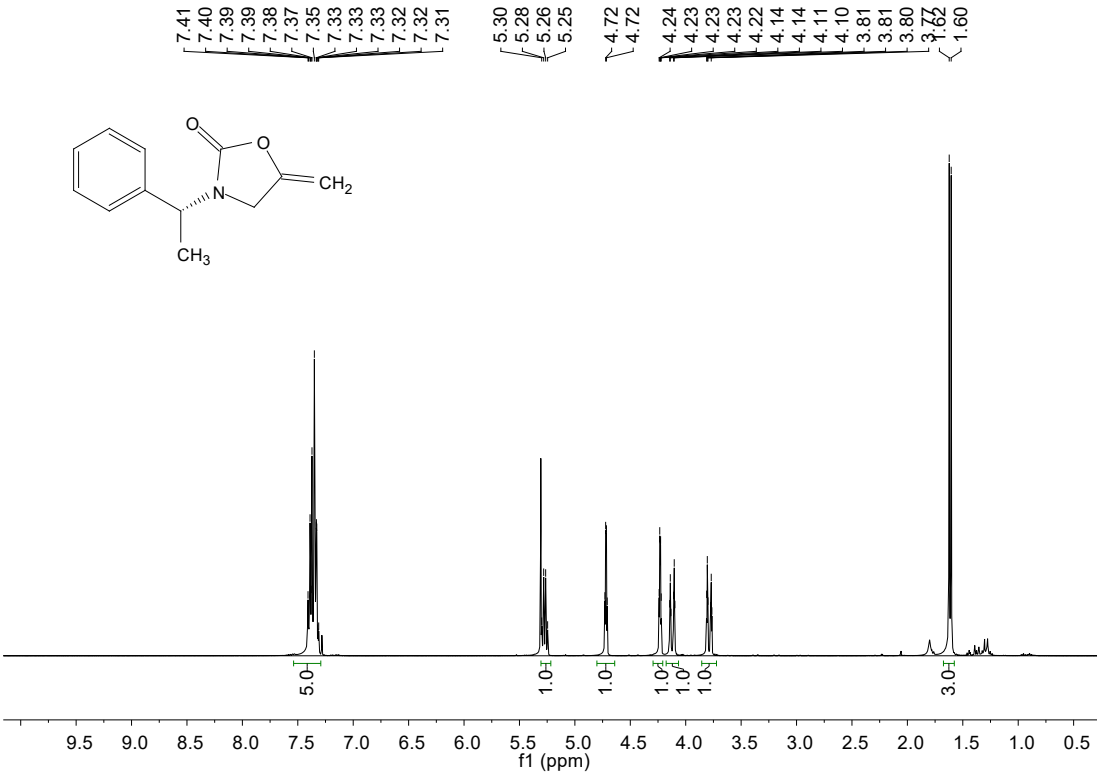
140
120
100
80
60
40
20
0
f1 (ppm)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7.32
7.31
5.30
5.28
5.26
5.25
4.72
4.72
4.24
4.23
4.23
4.23
4.22
4.14
4.11
4.10
3.81
3.81
3.80
3.77
1.62
1.60
O
O
N
CH2
CH3
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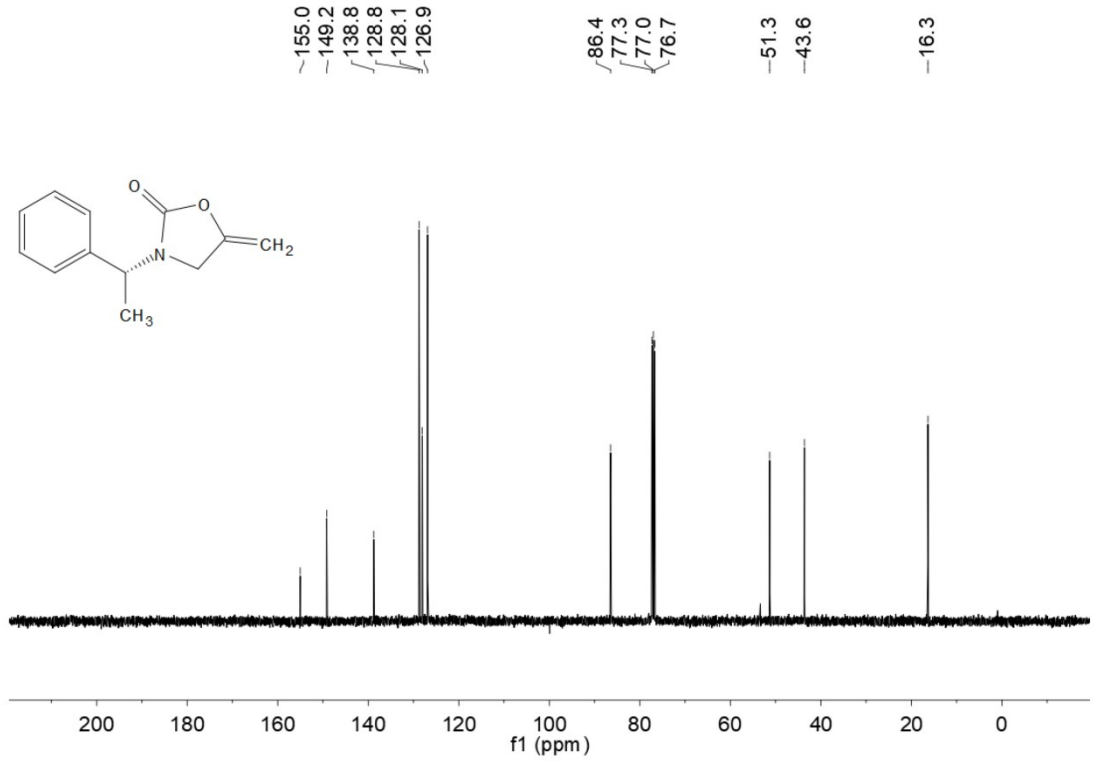
1.0
1.0
1.0
1.0
1.0
3.0
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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128.1
126.9
86.4
77.3
77.0
76.7
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43.6
16.3
O
O
N
CH2
CH3
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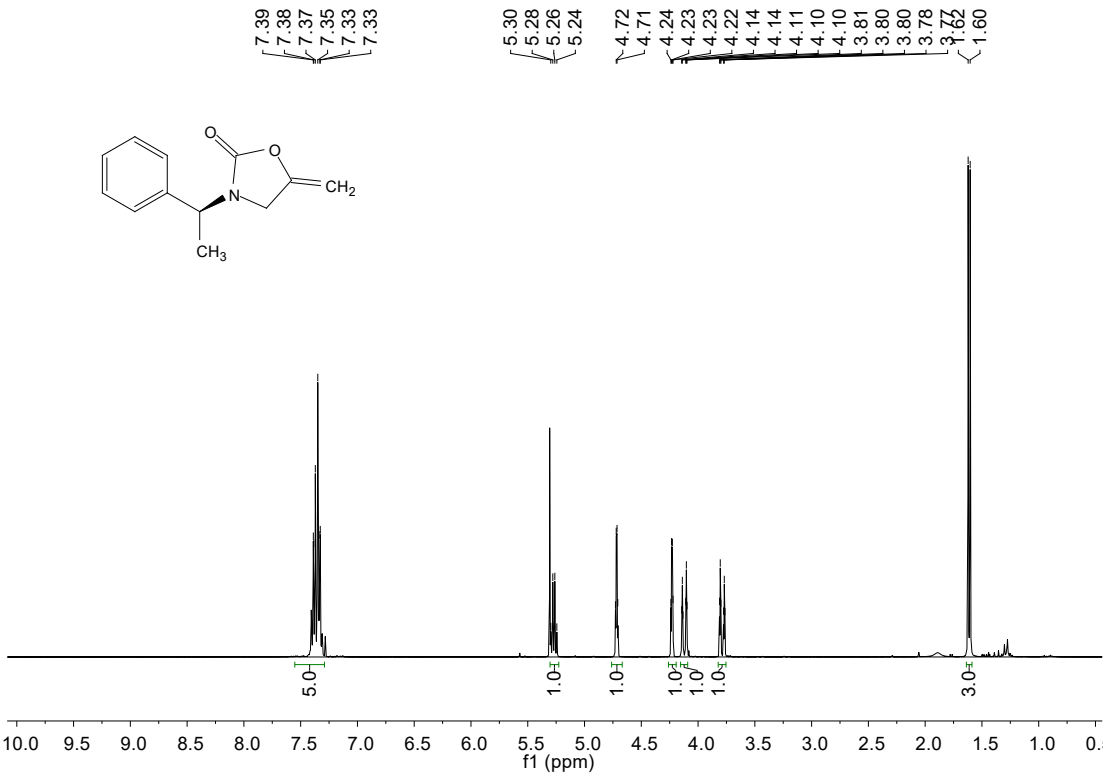
f1 (ppm)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4.23
4.23
4.22
4.14
4.14
4.11
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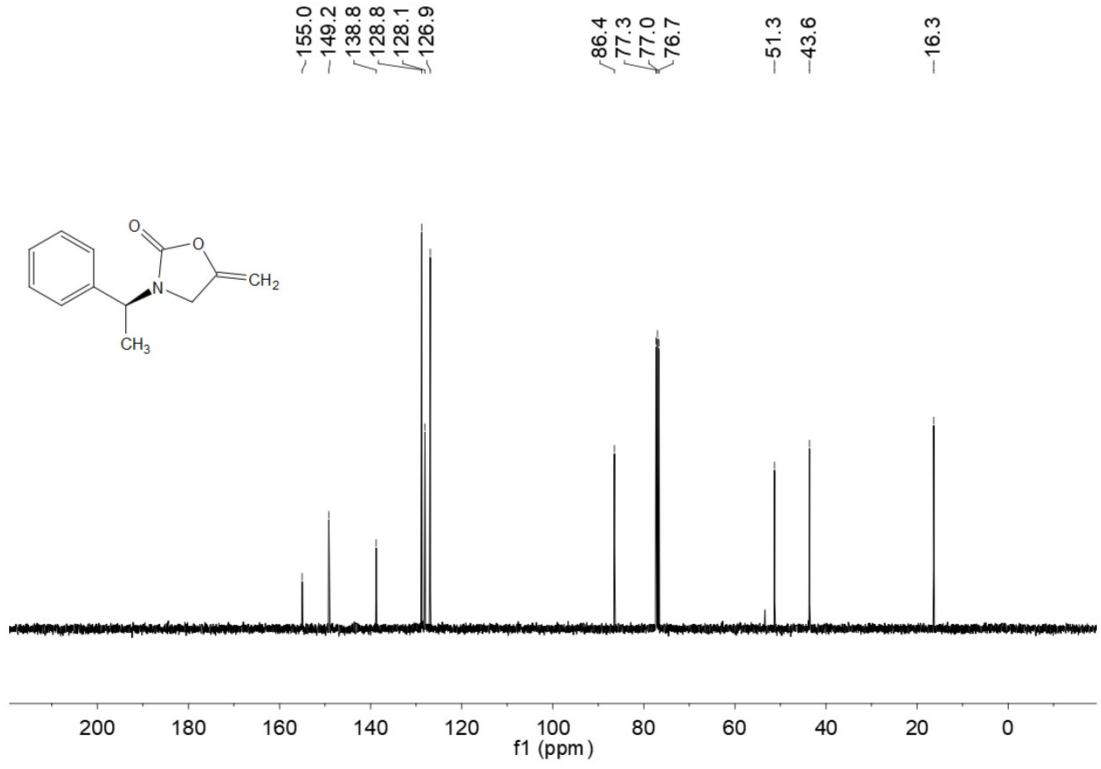
4.10
3.81
3.80
3.80
3.78
3.77
3.62
1.60
O
O
N
CH2
CH3
5.0
1.0
1.0
1.0
1.0
1.0
3.0
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)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128.1
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86.4
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76.7
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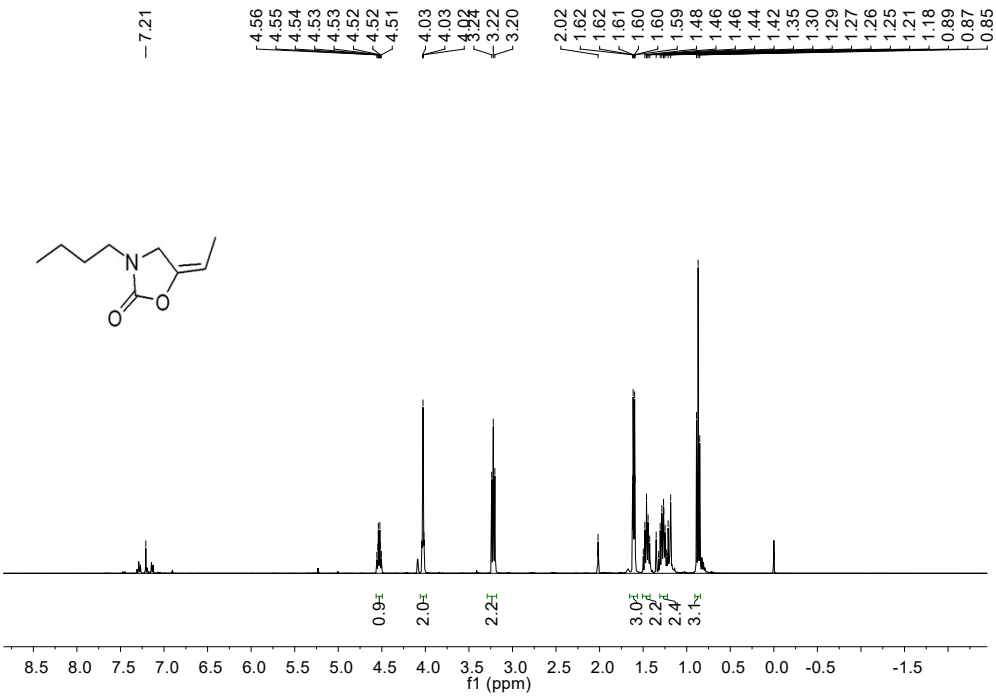
16.3
O
O
N
CH2
CH3
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)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3.22
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2.02
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1.62
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1.60
1.59
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1.46
1.44
1.42
1.35
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1.27
1.26
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1.18
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0.87
0.85
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O
O
0.9
2.0
2.2
3.0
2.2
2.4
3.1
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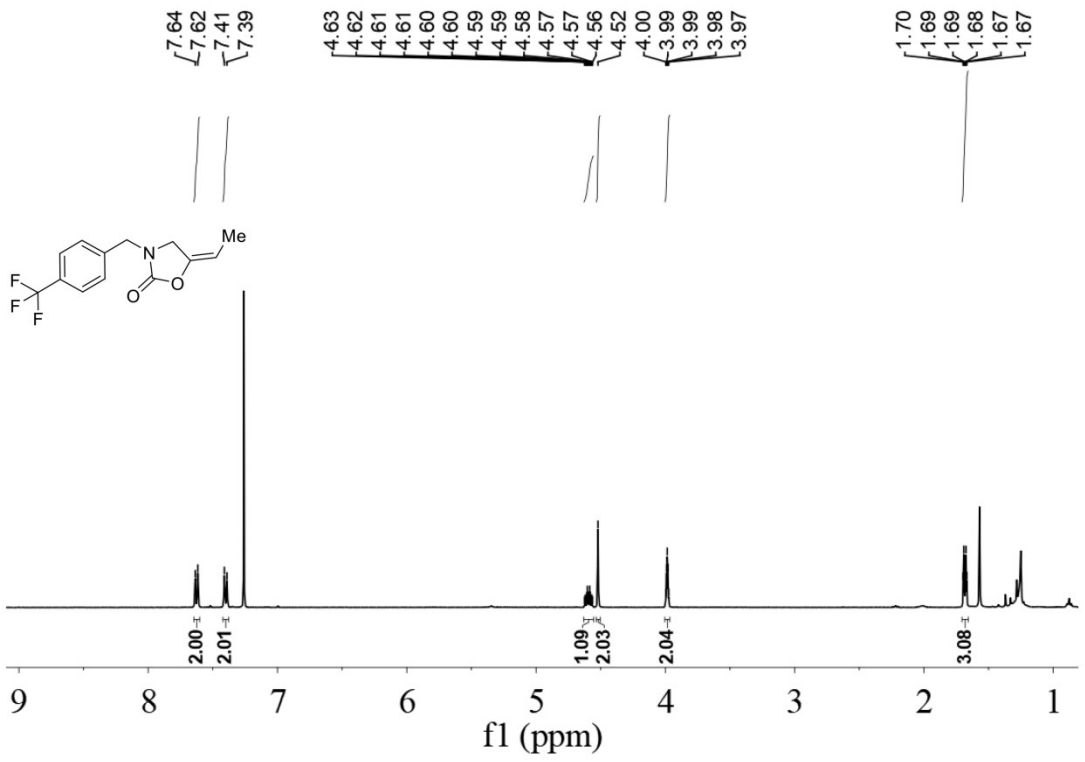
f1 (ppm)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4.56
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3.98
3.97
1.70
1.69
1.69
1.68
1.67
1.67
Me
N
O
O
F
F
F
2.00
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2.04
3.08
9
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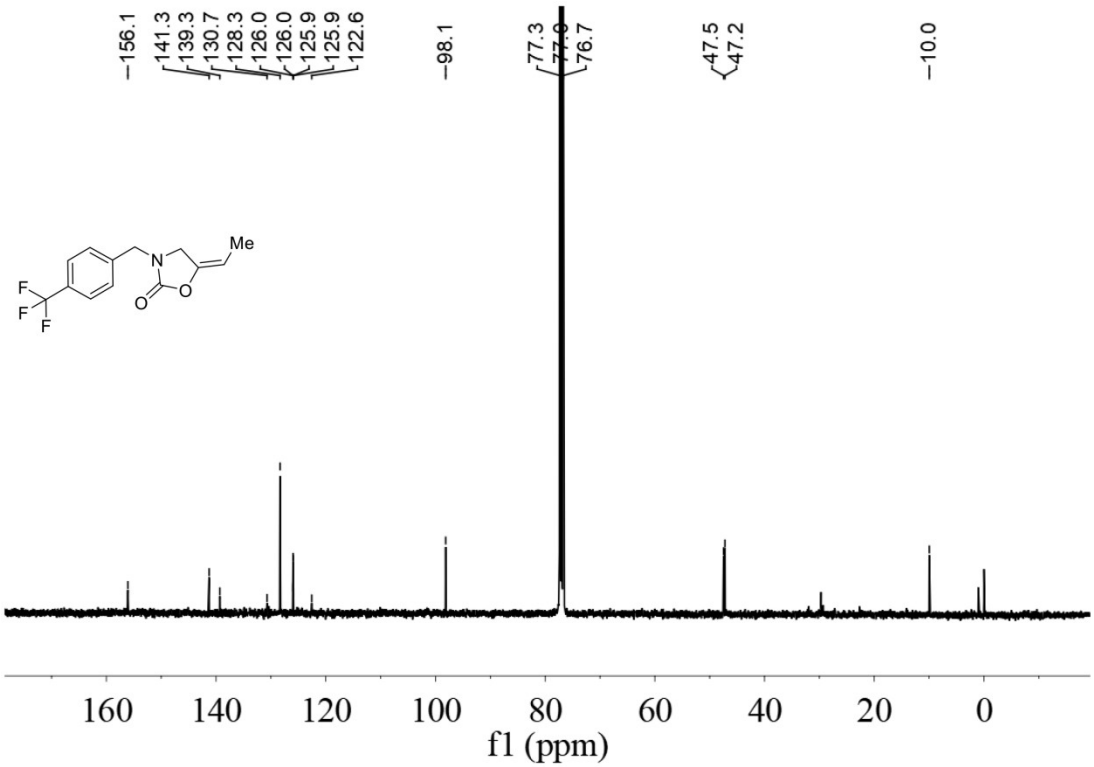
7
6
5
4
3
2
1
f1 (ppm)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77.0
76.7
47.5
47.2
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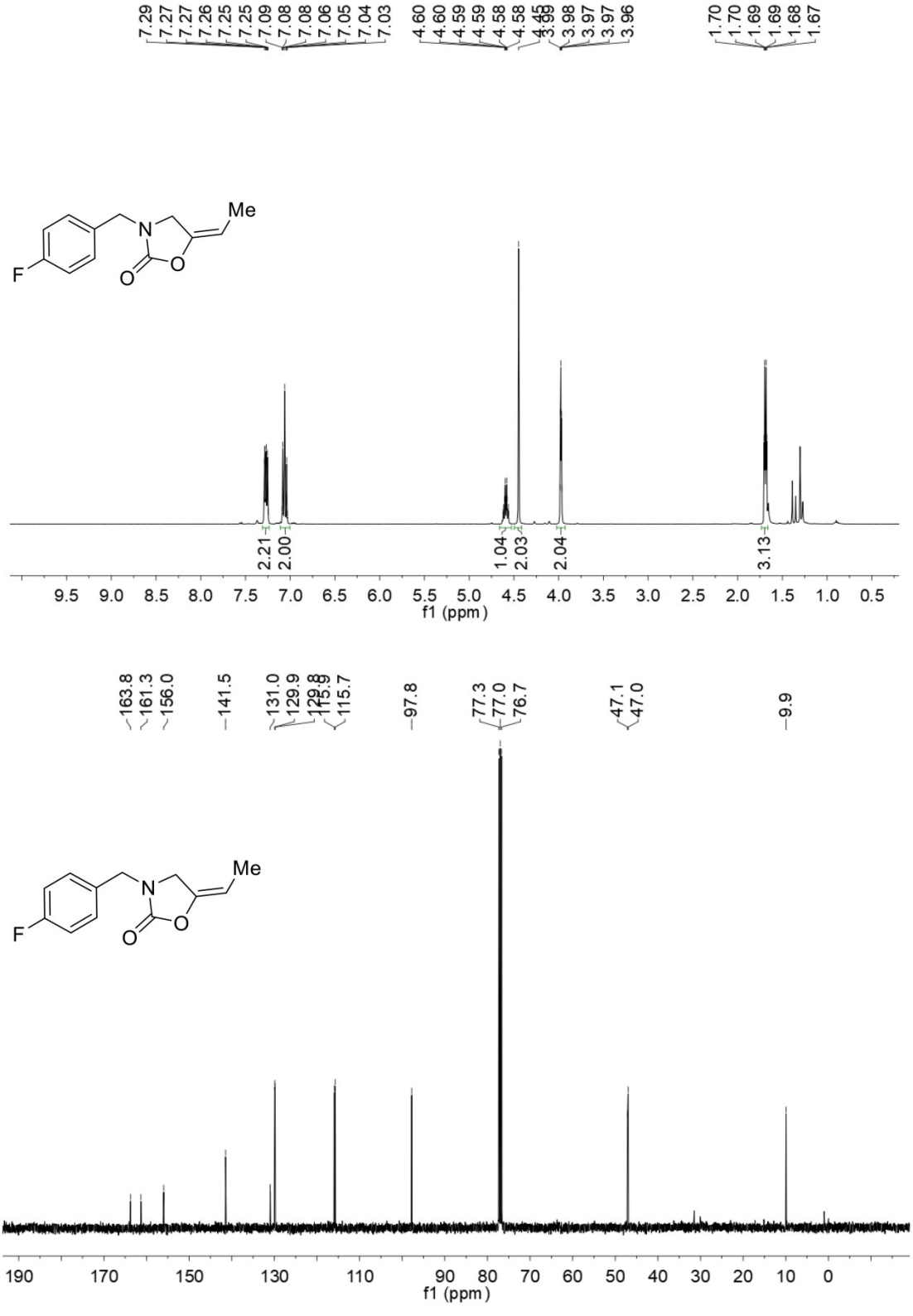
O
O
F
F
F
160
140
120
100
80
60
40
20
0
f1 (ppm)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4.58
4.58
4.45
3.98
3.97
3.97
3.96
1.70
1.70
1.69
1.69
1.68
1.67
Me
N
O
O
F
2.21
2.00
1.04
2.03
2.04
3.13
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)
163.8
161.3
156.0
141.5
131.0
129.9
115.7
97.8
77.3
77.0
76.7
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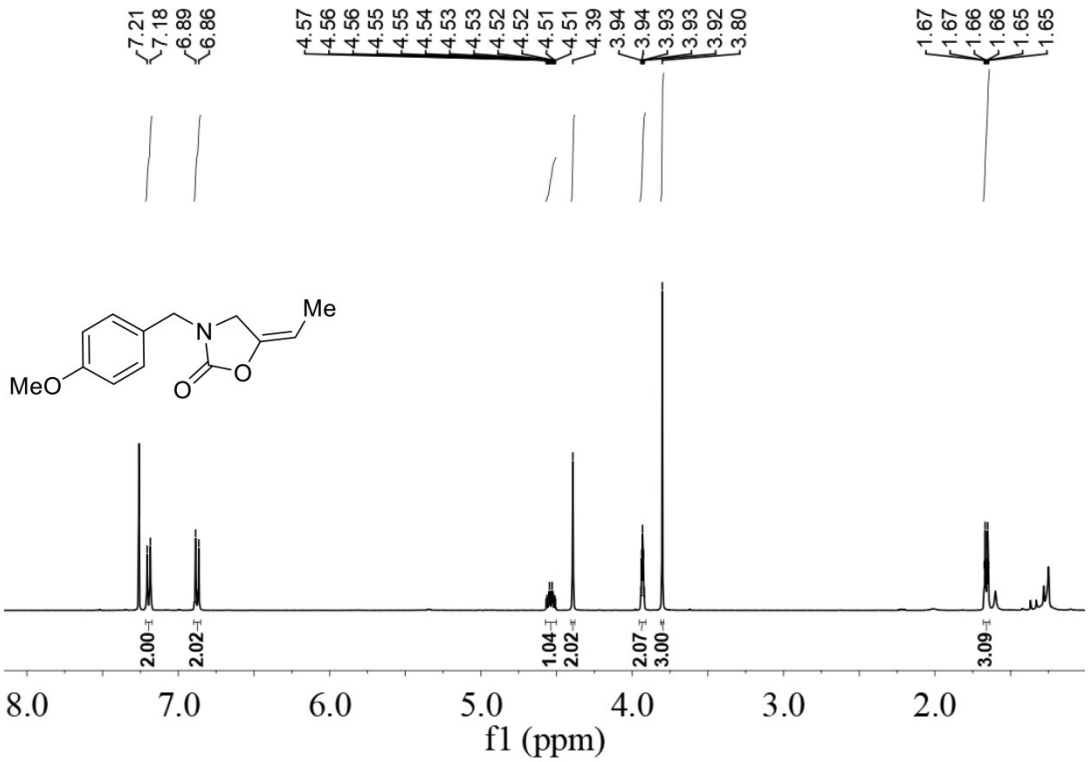
47.0
9.9
Me
N
O
O
F
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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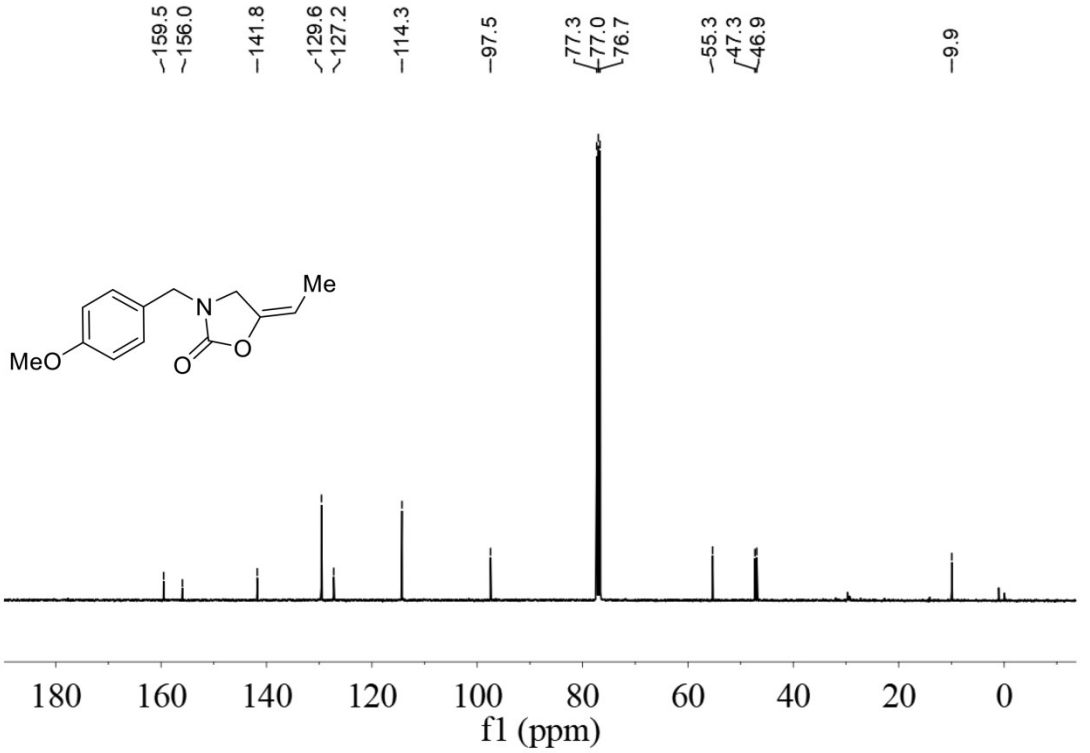
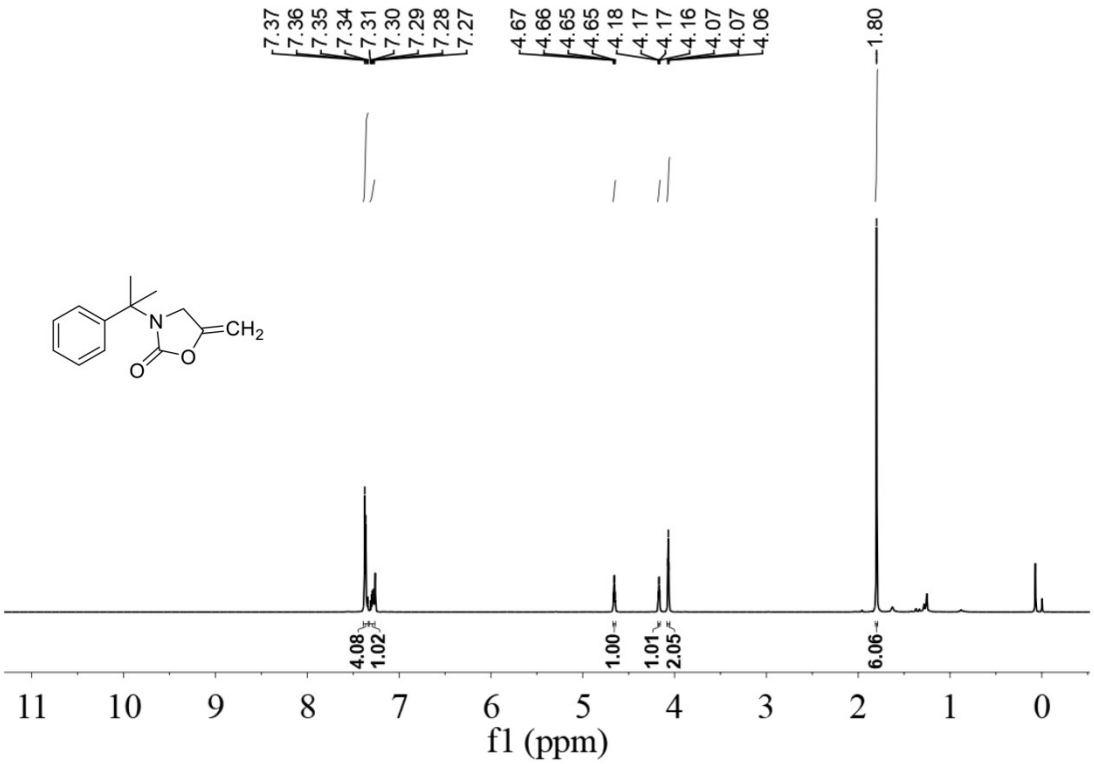
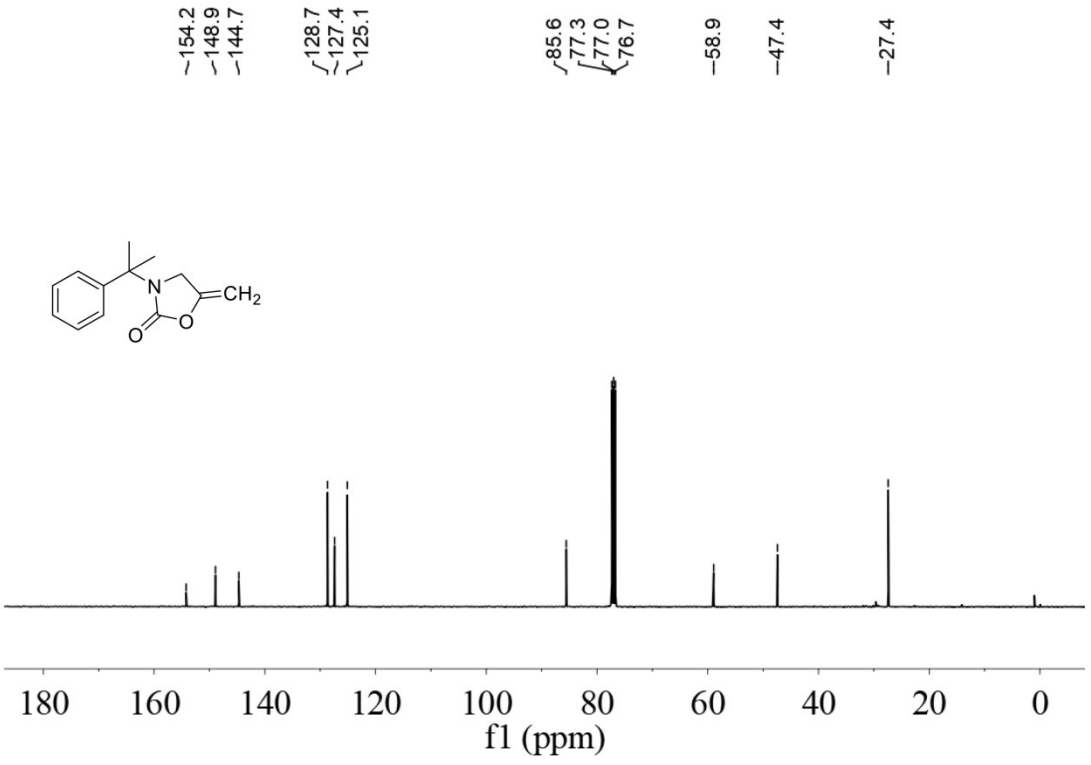
4.51
4.51
4.39
3.94
3.94
3.93
3.93
3.92
3.80
1.67
1.67
1.66
1.66
1.65
1.65
Me
N
O
O
MeO
2.00
2.02
1.04
2.02
2.07
3.00
3.09
8.0
7.0
6.0
5.0
4.0
3.0
2.0
f1 (ppm)


159.5
156.0
141.8
129.6
127.2
114.3
97.5
77.3
77.0
76.7
55.3
47.3
46.9
9.9
Me
N
O
O
MeO
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


7.37
7.36
7.35
7.34
7.31
7.30
7.29
7.28
7.27
4.67
4.66
4.65
4.65
4.18
4.17
4.17
4.16
4.07
4.07
4.06
1.80
4.08
1.02
1.00
1.01
2.05
6.06
11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


154.2
148.9
144.7
128.7
127.4
125.1
85.6
77.3
77.0
76.7
58.9
47.4
27.4
180 160 140 120 100 80 60 40 20 0
f1 (ppm)

3. Notes and references

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