Electronic Supplementary Information

Palladium- Assisted Multicomponent Cyclization of Aromatic Aldehydes, Arylamines and Terminal Olefins under Molecular Oxygen: An Assembly of 1,4-Dihydropyridines

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I. General

Melting points were measured with a BÜCHI B-545 melting point instrument and were uncorrected. ^{1}H and ^{13}C NMR spectra were recorded using a Bruker Avance 400 MHz NMR spectrometer. The chemical shifts are referenced to $CDCl_3$ at δ 7.260 and 77.00, respectively, chloroform is solvent with TMS as the internal standard. Mass spectra were recorded on a Shimadzu GCMS-QP5050A spectrometer at an ionization voltage of 70 eV equipped with a DB-WAX capillary column (internal diameter: 0.25 mm, length: 30 m). HRMS was carried out on a MAT 95 XP (Thermo). Elemental analyses were performed with a Vario EL elemental analyzer. TLC was performed using commercially prepared 100-400 mesh silica gel plates (GF_{254}), and visualization was effected at 254 nm. All the other chemicals were purchased from Aldrich Chemicals. Commercial reagents were used without further purification.

II. General experimental procedure

$PdCl_2$ (10 mol %), aldehyde (1 mmol), amine (1 mmol), olefin (2 mmol), TBAB (0.5 equiv) and CH_3CN (2 mL) were added into a 25 mL Schlenk tube equipped with a balloon in sequence. The tube was then put into a 75 ^{o}C oil bath under magnetic stirring for 12 h. After the reaction, the mixture was diluted with water and extracted with diethyl ether (15 mL×3). The combined extract was dried with anhydrous $MgSO_4$. The solvent was evaporated to dryness under reduced pressure, and the crude product was separated by column chromatography to give products **4**, which were further recrystalized from ethyl acetate/ petroleum ether.

III. X-ray crystal structure of complex 4a and 4q

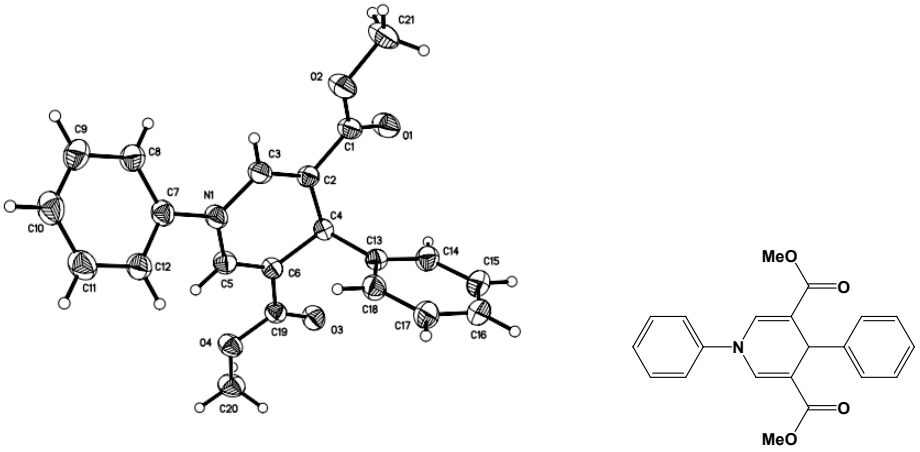


Figure ESI1. X-ray crystal structure of complex **4a**

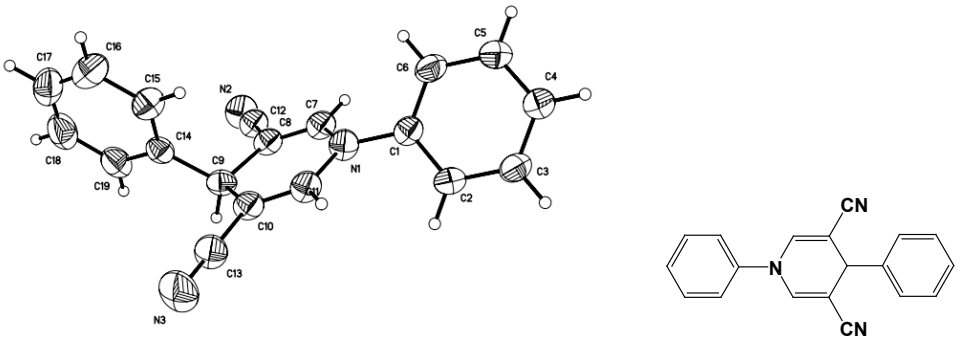
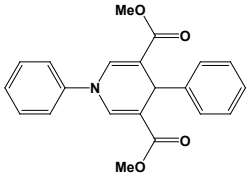


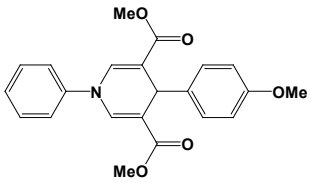
Figure ESI2. X-ray crystal structure of complex **4q**

Ⅳ. Characterization data for all products



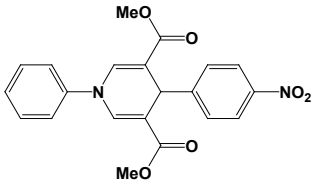
Dimethyl 1,4-diphenyl-1,4-dihydropyridine-3,5-dicarboxylate (4a)[1]

m.p. 186-188 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.68 (s, 2H), 7.46 (t, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 7.6 Hz, 2H), 7.32-7.26 (m, 5H), 7.18 (t, *J* = 7.2 Hz, 1H), 4.97 (s, 1H), 3.66 (s, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.1, 145.9, 143.2, 135.7, 129.9, 128.2, 126.7, 126.4, 120.8, 110.8, 51.4, 37.6 ppm; HRMS EI (m/z): calcd for $C_{21}H_{19}O_4N$, 349.1314; found, 349.1307; IR(KBr): 3028, 2950, 2849, 1708, 1591, 1496, 1439, 1277, 1209, 1074, 753, 695 cm^{-1}.



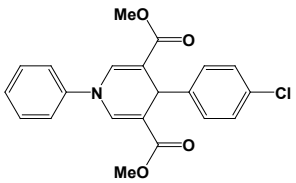
Dimethyl 4-(4-methoxyphenyl)-1-phenyl-1,4-dihydropyridine-3,5-dicarboxylate (4b)

m.p. 165-168 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.66 (s, 2H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.29 (t, *J* = 6.6 Hz, 5H), 6.81 (d, *J* = 8.4 Hz, 2H), 4.92 (s, 1H), 3.76 (s, 3H), 3.66 (s, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.1, 158.2, 143.1, 138.4, 135.4, 129.9, 129.1, 126.3, 120.6, 113.5, 110.9, 55.1, 51.4, 36.6 ppm; HRMS EI (m/z): calcd for $C_{22}H_{21}O_5N$, 379.1420; found, 379.1411; IR(KBr): 2951, 2841, 1708, 1592, 1503, 1438, 1348, 1209, 1074, 831, 738 cm^{-1}.



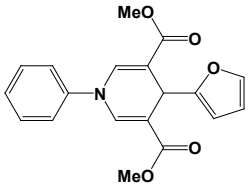
Dimethyl 4-(4-nitrophenyl)-1-phenyl-1,4-dihydropyridine-3,5-dicarboxylate (4c)

m.p. 162-165 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.13 (dd, *J* = 8.4 Hz, 2H), 7.72(s, 2H), 7.57 (d, *J* = 8.8 Hz, 2H), 7.48 (t, *J* =7.0 Hz, 2H), 7.32 (d, *J* = 7.6 Hz, 3H), 5.12 (s, 1H), 3.66 (s, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.6, 153.0, 146.7, 142.8, 136.5, 130.1, 129.2, 126.9, 123.5, 120.8, 109.5, 51.6, 38.0 ppm; HRMS EI (m/z): calcd for $C_{21}H_{18}O_6N_2$, 394.1165; found, 394.1161; IR(KBr): 3065, 2952, 2848, 1708, 1591, 1519, 1345, 1279, 1210, 1075, 832, 752 cm^{-1}.



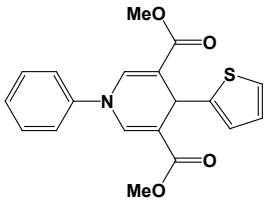
Dimethyl 4-(4-chlorophenyl)-1-phenyl-1,4-dihydropyridine-3,5-dicarboxylate (4d)

m.p. 152-154 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.68 (s, 2H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.34-7.28 (m, 5H), 7.23 (d, *J* = 8.4 Hz, 2H), 4.97 (s, 1H), 3.65 (s, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.7, 144.3, 142.8, 135.7, 132.2, 129.8, 129.5, 128.2, 126.4, 120.5, 110.2, 51.3, 37.0 ppm; HRMS EI (m/z): calcd for $C_{21}H_{18}O_4NCl$, 383.0924; found, 383.0914; IR(KBr): 3055, 2951, 2846, 1709, 1591, 1494, 1278, 1209, 1078, 831, 760, 699 cm^{-1}.



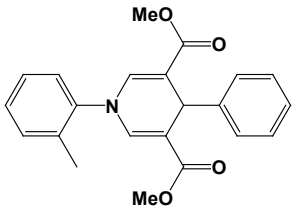
Dimethyl 4-(furan-2-yl)-1-phenyl-1,4-dihydropyridine-3,5-dicarboxylate (4e)

Reddish-brown oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.67 (s, 2H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.31-7.27 (m, 4H), 6.28-6.26 (m, 1H), 6.14 (d, *J* = 3.2 Hz, 1H), 5.15 (s, 1H), 3.73 (s, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.0, 156.9, 143.1, 141.4, 136.7, 129.9, 126.5, 120.9, 110.4, 107.4, 105.7, 51.6, 31.1 ppm; HRMS EI (m/z): calcd for $C_{19}H_{17}O_5N$, 339.1107; found, 339.1097; IR(KBr): 2951, 1709, 1591, 1497, 1437, 1350, 1276, 1205, 1074, 805, 750, 695 cm^{-1}.



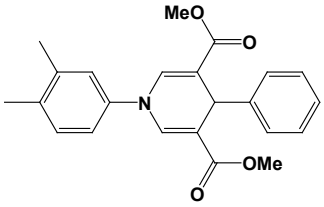
Dimethyl 1-phenyl-4-(thiophen-2-yl)-1,4-dihydropyridine-3,5-dicarboxylate (4f)

m.p. 140-142 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.65 (s, 2H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.32-7.27 (m, 3H), 7.12 (dd, *J* = 4.8 Hz, 1H), 6.94 (d, *J* = 3.2 Hz, 1H), 6.90-6.88 (m, 1H), 5.31 (s, 1H), 3.73 (s, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.0, 150.0, 143.0, 135.9, 129.9, 126.8, 126.6, 124.3, 124.1, 121.1, 110.0, 51.6, 32.1 ppm; HRMS EI (m/z): calcd for $C_{19}H_{17}O_4NS$, 355.0878; found, 355.0875; IR(KBr): 2950, 2850, 1708, 1589, 1497, 1437, 1348, 1277, 1207, 1073, 759, 697 cm^{-1}.



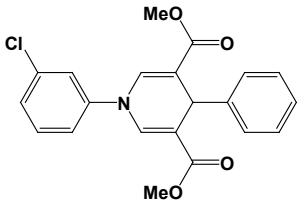
Dimethyl 4-phenyl-1-o-tolyl-1,4-dihydropyridine-3,5-dicarboxylate (4g)

m.p. 155-157 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.44 (d, *J* = 7.2 Hz, 2H), 7.34 (s, 2H), 7.31-7.28 (m, 5H), 7.25-7.16 (m, 2H), 5.01 (s, 1H), 3.62 (s, 6H), 2.36 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.1, 146.2, 142.5, 137.6, 133.9, 131.7, 128.4, 128.1, 127.4, 126.5, 126.0, 108.8, 51.3, 37.2, 17.9 ppm; HRMS EI (m/z): calcd for $C_{22}H_{21}O_4N$, 363.1471; found, 363.1466; IR(KBr): 3027, 2951, 1708, 1585, 1495, 1440, 1339, 1276, 1206, 1076, 729, 702 cm^{-1}.



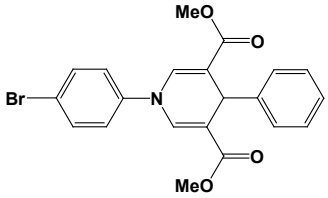
Dimethyl 1-(3,4-dimethylphenyl)-4-phenyl-1,4-dihydropyridine-3,5-dicarboxylate (4h)

m.p. 114-117 ºC ; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.62 (s, 2H), 7.37 (d, *J* = 6.8 Hz, 2H), 7.27 (t, *J* = 7.6 Hz, 2H), 7.20-7.15 (m, 2H), 7.03 (t, *J* = 10.8 Hz, 2H), 4.96 (s, 1H), 3.65 (s, 6H), 2.32 (s, 3H), 2.29 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.3, 146.1, 141.1, 138.5, 136.1, 135.1, 130.7, 128.2, 126.6, 122.1, 118.2, 110.3, 51.4, 37.5, 19.9, 19.2 ppm; HRMS EI (m/z): calcd for $C_{23}H_{23}O_4N$, 377.1627; found, 377.1618; IR(KBr): 2948, 2921, 1709, 1584, 1503, 1441, 1248, 1208, 1075, 751, 720 cm^{-1}.



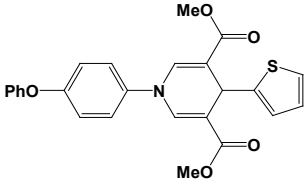
Dimethyl 1-(3-chlorophenyl)-4-phenyl-1,4-dihydropyridine-3,5-dicarboxylate (4i)

m.p. 167-170 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.65 (s, 2H), 7.41-7.35 (m, 3H), 7.32-7.26 (m, 4H), 7.19 (t, *J* = 8.2 Hz, 2H), 4.97 (s, 1H), 3.67 (s, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.8, 145.4, 144.0, 135.6, 134.9, 130.9, 128.2, 128.1, 126.7, 126.3, 120.8, 118.5, 111.5, 51.5, 37.5 ppm; HRMS EI (m/z): calcd for $C_{21}H_{18}O_4NCl$, 383.0924; found, 383.0922; IR(KBr): 3067, 3028, 2951, 2846, 1710, 1590, 1483, 1439, 1275, 1210, 1073, 747, 695 cm^{-1}.



Dimethyl 1-(4-bromophenyl)-4-phenyl-1,4-dihydropyridine-3,5-dicarboxylate (4j)

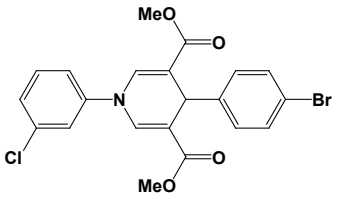
m.p. 203-205 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.61 (s, 2H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 7.2 Hz, 2H), 7.26 (t, *J* = 7.2 Hz, 2H), 7.16 (d, *J* = 8.8 Hz, 3H), 4.96 (s, 1H), 3.64 (s, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.8, 145.4, 142.0, 135.0, 132.9, 128.1(d), 126.7, 122.0, 119.4, 111.2, 51.4, 37.4 ppm; HRMS EI (m/z): calcd for $C_{21}H_{18}O_4NBr$, 427.0419; found, 427.0415 IR(KBr): 3067, 2949, 1708, 1594, 1490, 1435, 1275, 1209, 1079, 828, 749 cm^{-1}.



Dimethyl 1-(4-phenoxyphenyl)-4-(thiophen-2-yl)-1,4-dihydropyridine-3,5-dicarboxylate (4k)

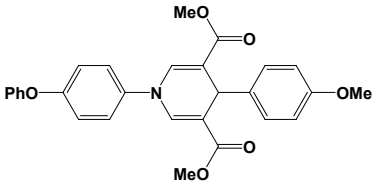
Reddish-brown oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.58 (s, 2H), 7.37 (t, *J* = 8.0 Hz, 2H), 7.24 (d,

J = 8.8 Hz, 1H), 7.17-7.12 (m, 2H), 7.07-7.02 (m, 4H), 6.95-6.89 (m, 3H), 5.31 (s, 1H), 3.73 (s, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.9, 156.7, 156.1, 150.1, 138.4, 136.2, 129.9, 126.8, 124.2, 124.0, 123.8, 123.0, 119.8, 119.0, 109.7, 51.6, 32.0 ppm; MS (ESI) m/z: 446 ([M-H]$^-$). Anal. Calcd for $C_{25}H_{21}NO_5S$: C, 67.10; H, 4.73; N, 3.13. Found: C, 66.89; H, 4.81; N, 3.17; IR(KBr): 3068, 2951, 2849, 1708, 1587, 1499, 1276, 1220, 1072, 840, 696 cm^{-1}.



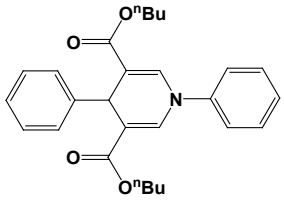
Dimethyl 4-(4-bromophenyl)-1-(3-chlorophenyl)-1,4-dihydropyridine-3,5-dicarboxylate (4l)

m.p. 150-152 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.63 (s, 2H), 7.41-7.37 (m, 3H), 7.31-7.27 (m, 2H), 7.24-7.22 (m, 2H), 7.20-7.18 (m, 1H), 4.93 (s, 1H), 3.66 (s, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.6, 144.5, 143.9, 135.7, 135.1, 131.3, 131.0, 130.0, 126.5, 120.8, 120.7, 118.6, 111.0, 51.6, 37.2 ppm; HRMS EI (m/z): calcd for $C_{21}H_{17}O_4NBrCl$, 461.0029; found, 461.0020 IR(KBr): 3071, 2996, 2951, 2846, 1710, 1589, 1482, 1437, 1334, 1275, 1211, 1073, 781, 734 cm^{-1}.



Dimethyl 4-(4-methoxyphenyl)-1-(4-phenoxyphenyl)-1,4-dihydropyridine-3,5-dicarboxylate (4m)

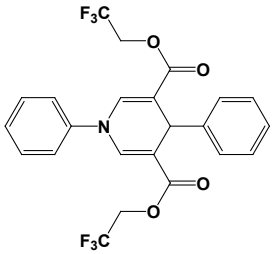
m.p. 181-183 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.59 (s, 2H), 7.37 (t, *J* = 8.0 Hz, 2H), 7.30-7.25 (m, 4H), 7.15 (t, *J* = 7.4 Hz, 1H), 7.09-7.02 (m, 4H), 6.81(d, *J* = 8.8 Hz, 2H), 4.91 (s, 1H), 3.77 (s, 3H), 3.66 (s, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.2, 158.3, 156.8, 155.7, 138.6, 138.4, 135.7, 129.9, 129.1, 123.7, 122.6, 119.9, 118.9, 113.5, 110.6, 55.1, 51.4, 36.5 ppm; MS (ESI) m/z: 470 ([M-H]$^-$). Anal. Calcd for $C_{28}H_{25}NO_6$: C, 71.33; H, 5.34; N, 2.97. Found: C, 71.15; H, 5.39; N, 3.04; IR(KBr): 2950, 2841, 1708, 1590, 1501, 1436, 1337, 1215, 1073, 833, 736 cm^{-1}.



Dibutyl 1,4-diphenyl-1,4-dihydropyridine-3,5-dicarboxylate (4n)

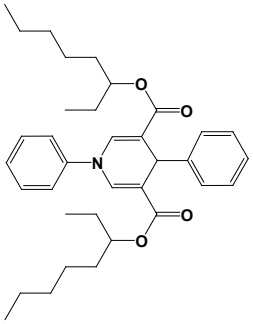
m.p. 78-80 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.67 (s, 2H), 7.46 (t, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 7.2 Hz, 2H), 7.32-7.24 (m, 5H), 7.16 (t, *J* = 7.2 Hz, 1H), 4.96 (s, 1H), 4.14-4.08 (m, 2H), 4.04-3.98 (m, 2H), 1.55 (qui, *J* = 7.1Hz, 4H), 1.31-1.245 (m, 4H), 0.88 (t, *J* = 7.4 Hz, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.8, 146.0, 143.2, 135.5, 129.9, 128.3, 128.0, 126.5, 126.2, 120.6, 111.1, 64.1, 37.7, 30.7, 19.0, 13.6 ppm; HRMS EI (m/z): calcd for $C_{27}H_{31}O_4N$, 433.2253; found, 433.2250; IR(KBr): 3060, 2959, 2872, 1705, 1591, 1497, 1274, 1205, 1073, 754,

696 cm^{-1}.



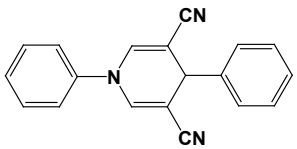
Bis(trifluoromethyl) 1,4-diphenyl-1,4-dihydropyridine-3,5-dicarboxylate (4o)

m.p. 154-157 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.70 (s, 2H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.37-7.23 (m, 7H), 7.19 (t, *J* = 7.2 Hz, 1H), 4.95 (s, 1H), 4.52-4.42 (m, 2H), 4.40-4.31 (m, 2H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.7, 145.0, 142.7, 137.1, 130.1, 128.3, 128.3, 127.1(d), 124.4, 121.6, 121.1, 109.5, 60.8, 60.4, 60.0, 59.7, 37.5 ppm; HRMS EI (m/z): calcd for $C_{23}H_{17}O_4NF_6$, 485.1062; found, 485.1055; IR(KBr): 3074, 2966, 1721, 1587, 1496, 1413, 1282, 1167, 1089, 751, 695 cm^{-1}.



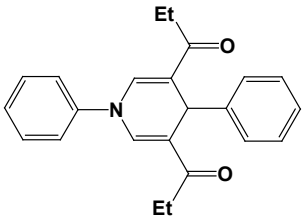
Dioctan-3-yl 1,4-diphenyl-1,4-dihydropyridine-3,5-dicarboxylate (4p)

Reddish-brown oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.69 (s, 2H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.37 (d, *J* = 7.2 Hz, 2H), 7.33-7.24 (m, 5H), 7.16 (t, *J* = 7.4 Hz, 1H), 4.96 (s, 1H), 4.05-3.92 (m, 4H), 1.30-1.23 (m, 16H), 0.92-0.82 (m, 14H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.0(d), 145.9, 143.1, 135.5(d), 129.9, 129.8, 128.2, 128.0, 126.5, 126.2, 120.5, 115.9, 111.1, 66.6(d), 38.8(d), 37.7, 30.4(d), 28.9(d), 23.8, 23.7, 22.9, 14.0, 11.0(d) ppm; MS (ESI) m/z: 544 ([M-H]$^-$). Anal. Calcd for $C_{35}H_{47}NO_4$: C, 77.03; H, 8.68; N, 2.57. Found: C, 76.84; H, 8.73; N, 2.61; IR(KBr): 3061, 2959, 2928, 2865, 1706, 1590, 1497, 1460, 1274, 1202, 1067, 754, 702 cm^{-1}.



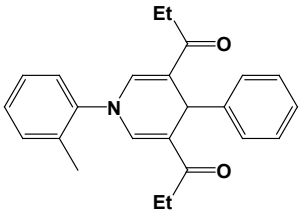
1,4-Diphenyl-1,4-dihydropyridine-3,5-dicarbonitrile (4q)

m.p. 205-207 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.49-7.43 (m, 4H), 7.39-7.34 (m, 4H), 7.18 (d, *J* = 7.6 Hz, 2H), 7.07 (s, 2H), 4.49 (s, 1H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 141.7, 141.0, 137.8, 130.3, 129.3, 128.6, 127.9, 127.6, 120.8, 117.8, 90.9, 40.6 ppm; HRMS EI (m/z): calcd for $C_{19}H_{13}N_3$, 283.1109; found, 283.1103; IR(KBr): 3087, 2923, 2860, 2206, 1668, 1586, 1496, 1347, 1299, 1258, 1167, 1068, 755, 697 cm^{-1}.



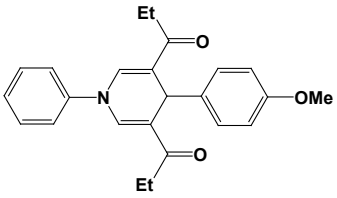
1,1'-(1,4-Diphenyl-1,4-dihydropyridine-3,5-diyl)dipropan-1-one (4r)

m.p. 148-151 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.59 (s, 2H), 7.50 (t, *J* = 8.0 Hz, 2H), 7.39-7.33 (m, 5H), 7.24 (t, *J* = 8.0 Hz, 2H), 7.13 (t, *J* = 7.2 Hz, 1H), 5.24 (s, 1H), 2.60-2.49 (m, 4H), 1.02 (t, *J* =7.2 Hz, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 198.3, 145.5, 143.3, 135.4, 130.1, 128.2(d), 126.8, 126.5, 121.3, 120.1, 35.9, 30.6, 8.4 ppm; HRMS EI (m/z): calcd for $C_{23}H_{23}O_2N$, 345.1729; found, 345.1725; IR(KBr): 3061, 2976, 2934, 1653, 1589, 1495, 1335, 1214, 1179, 1084, 754, 697 cm^{-1}.



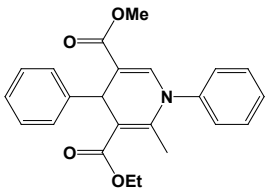
1,1'-[1-(2-Methylphenyl)-4-phenyl-1,4-dihydropyridine-3,5-diyl]dipropanone (4s)

m.p. 135-137 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.43 (d, *J* = 7.6 Hz, 2H), 7.37-7.33 (m, 4H), 7.26 (t, *J* = 7.8 Hz, 4H), 7.14 (t, *J* = 7.4 Hz, 1H), 5.28 (s, 1H), 2.55-2.44 (m, 4H), 2.39 (s, 3H), 1.00 (t, *J* = 7.4 Hz, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 198.2, 145.8, 142.6, 137.3, 134.0, 131.9, 128.7, 128.2, 127.6, 126.3, 126.1, 118.6 35.6, 30.4, 17.9, 8.5 ppm; HRMS EI (m/z): calcd for $C_{24}H_{25}O_2N$, 359.1885; found, 359.1876 IR(KBr): 3065, 3029, 2977, 2935, 1651, 1572, 1494, 1456, 1326, 1221, 1182, 1086, 748, 699 cm^{-1}.



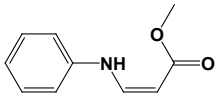
1,1'-[4-(4-Methoxyphenyl)-1-phenyl-1,4-dihydropyridine-3,5-diyl]dipropanone (4t)

m.p. 112-114 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.57 (s, 2H), 7.50 (t, *J* = 7.8 Hz, 2H), 7.37-7.32 (m, 3H), 7.28 (d, *J* = 8.4 Hz, 2H), 6.78 (d, *J* = 8.4 Hz, 2H), 5.17 (s, 1H), 3.74 (s, 3H), 2.58-2.52 (m, 4H), 1.02 (t, *J* = 7.2 Hz, 6H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 198.4, 158.1, 143.4, 138.0, 135.2, 130.1, 129.2, 126.8, 121.2, 120.3, 113.6, 55.1, 35.1, 30.6, 8.4 ppm; HRMS EI (m/z): calcd for $C_{24}H_{25}O_3N$, 375.1834; found, 375.1827; IR(KBr): 3061, 2976, 2937, 2835, 1652, 1596, 1502, 1335, 1251, 1214, 1178, 761, 697 cm^{-1}.



3-ethyl 5-methyl 2-methyl-1,4-diphenyl-1,4-dihydropyridine-3,5-dicarboxylate (4u)

m.p. 143-146 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.47 (t, *J* = 7.4 Hz, 2H), 7.40-7.39 (m, 4H), 7.30-7.24 (m, 4H), 7.17 (t, *J* = 7.2 Hz, 1H), 5.09 (s, 1H), 4.10 (q, *J* =7.2 Hz, 2H), 3.63 (s, 3H), 2.14 (s, 3H), 1.22 (t, *J* = 7.0 Hz, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.9, 167.3, 146.6, 145.6, 142.5, 139.4, 129.8, 128.2, 128.1, 127.9, 127.4, 126.4, 107.8, 107.0, 60.0, 51.2, 38.9, 18.0, 14.2 ppm; MS (EI) m/z: 77, 115, 167, 272, 300, 348, 377. Anal. Calcd for $C_{23}H_{23}NO_4$: C, 73.19; H, 6.14; N, 3.71. Found: C, 73.05; H, 6.21; N, 3.75; IR(KBr): 3028, 2983, 2947, 1701, 1585, 1493, 1443, 1341, 1212, 1072, 757, 702 cm^{-1}.



(Z)-methyl 3-(phenylamino)acrylate

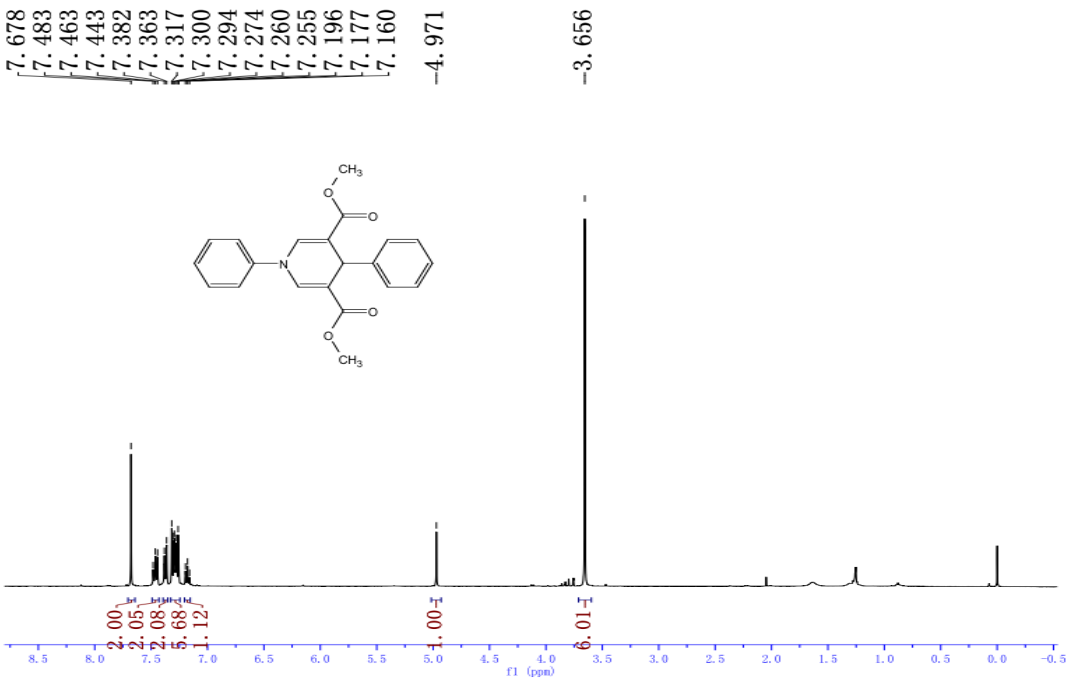
m.p. 149-151 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.87 (s, 1H), 7.30 (t, *J* = 7.4 Hz, 2H), 7.24 (d, *J* = 8.4 Hz, 1H), 7.02-6.95 (m, 3H), 4.85 (d, *J* = 8.0 Hz, 1H), 3.72 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 170.6, 143.1, 140.6, 129.6, 122.6, 115.3, 86.9, 50.6 ppm; MS (EI) m/z: 77, 92, 118, 146, 177. IR(KBr): 3320, 3008, 2952, 1630, 1493, 1440, 1232, 752, 694 cm^{-1}.

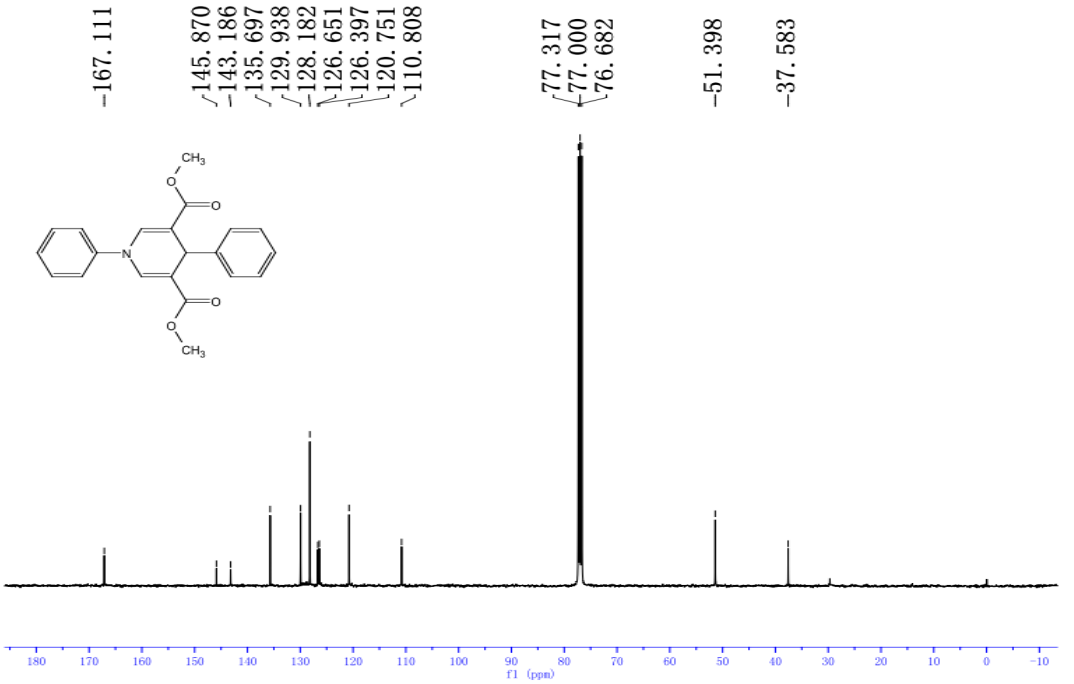
References

[1] B. Cekavicius, A. Sausins, G. Duburs, *Khim. Geterotsikl. Soedin*. **1982**, *8*, 1072-1077.

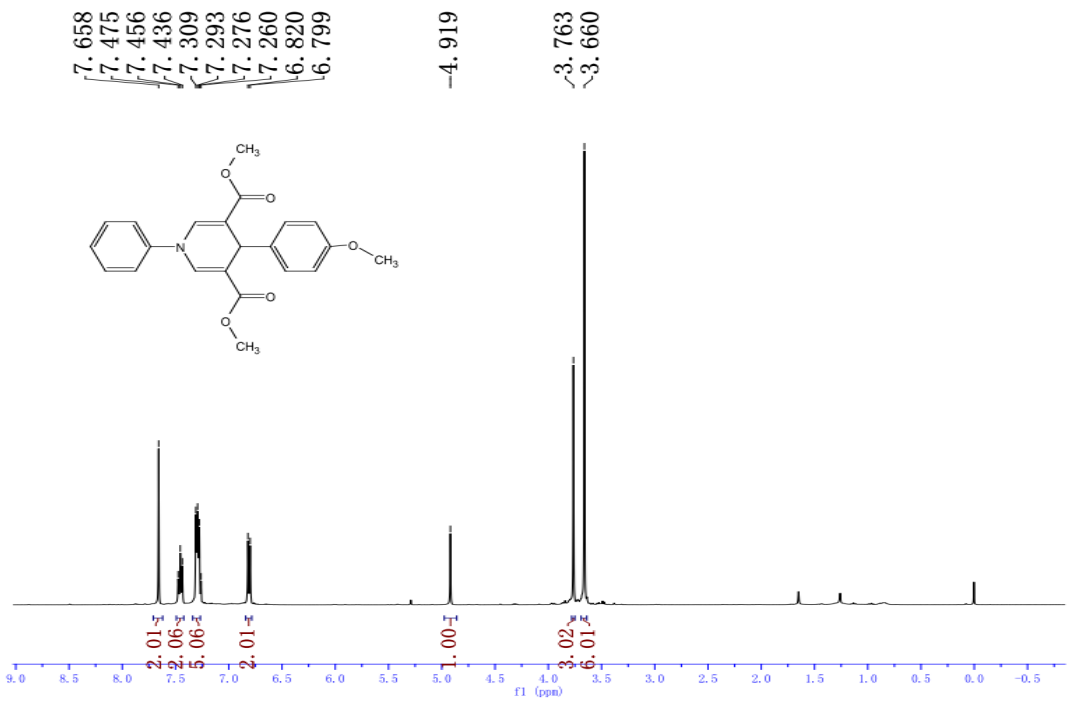
Ⅴ. NMR Spectra

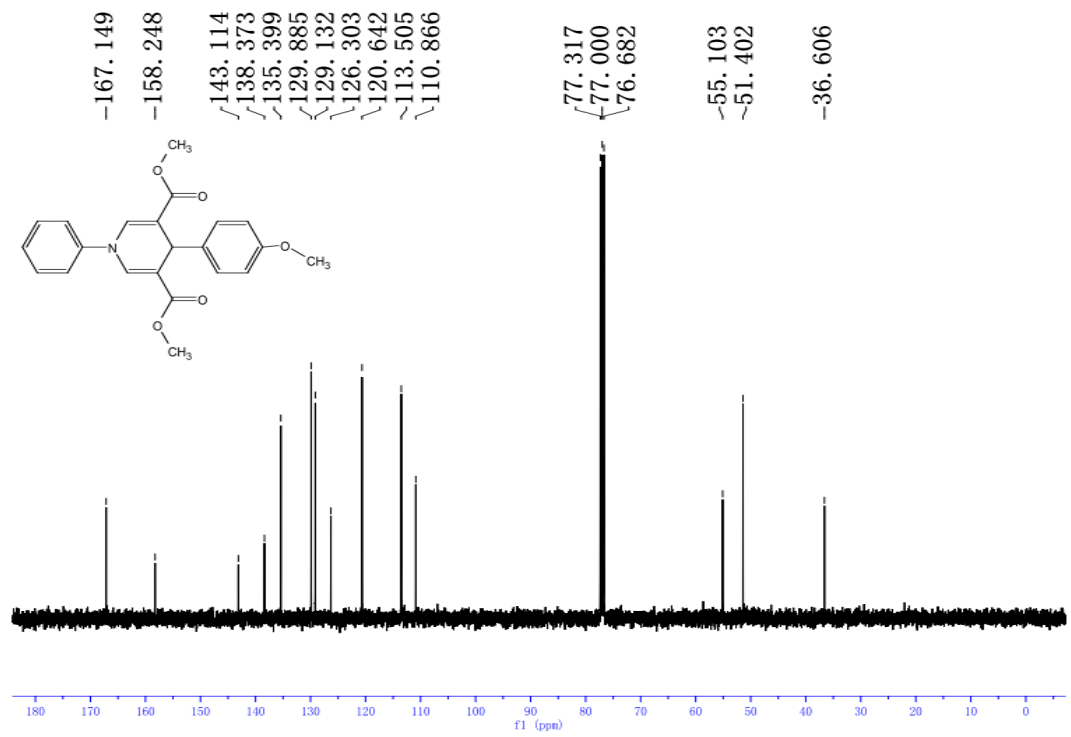
^{1}H NMR and ^{13}C NMR of dimethyl 1,4-diphenyl-1,4-dihydropyridine-3,5-dicarboxylate (4a)



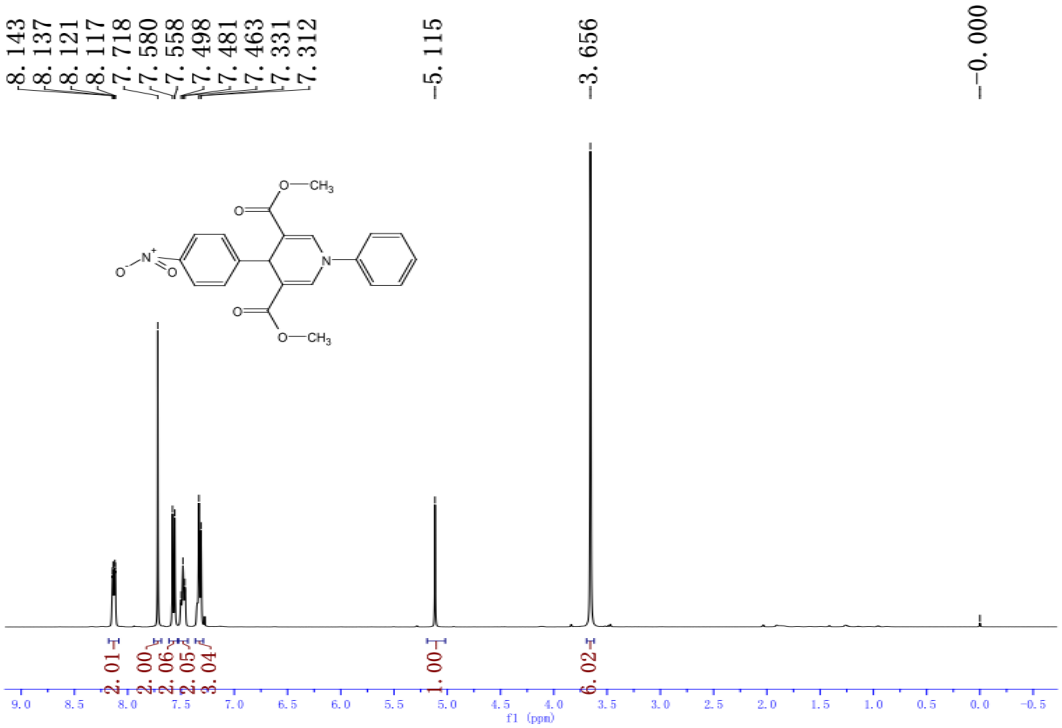


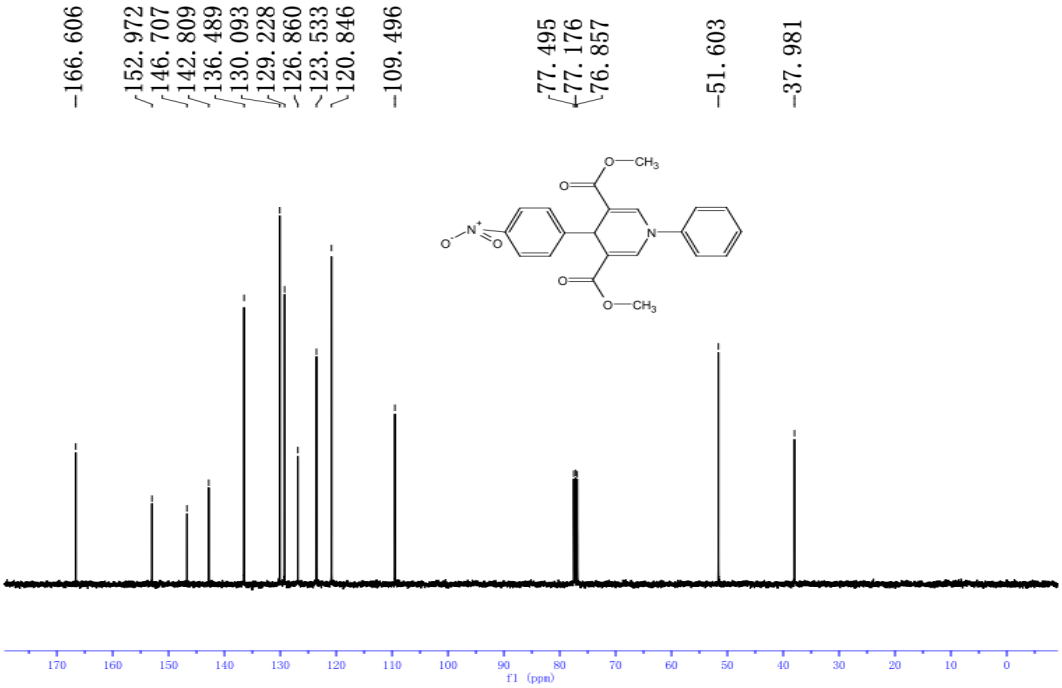
^{1}H NMR and ^{13}C NMR of dimethyl 4-(4-methoxyphenyl)-1-phenyl-1,4-dihydropyridine-3,5-dicarboxylate (4b)



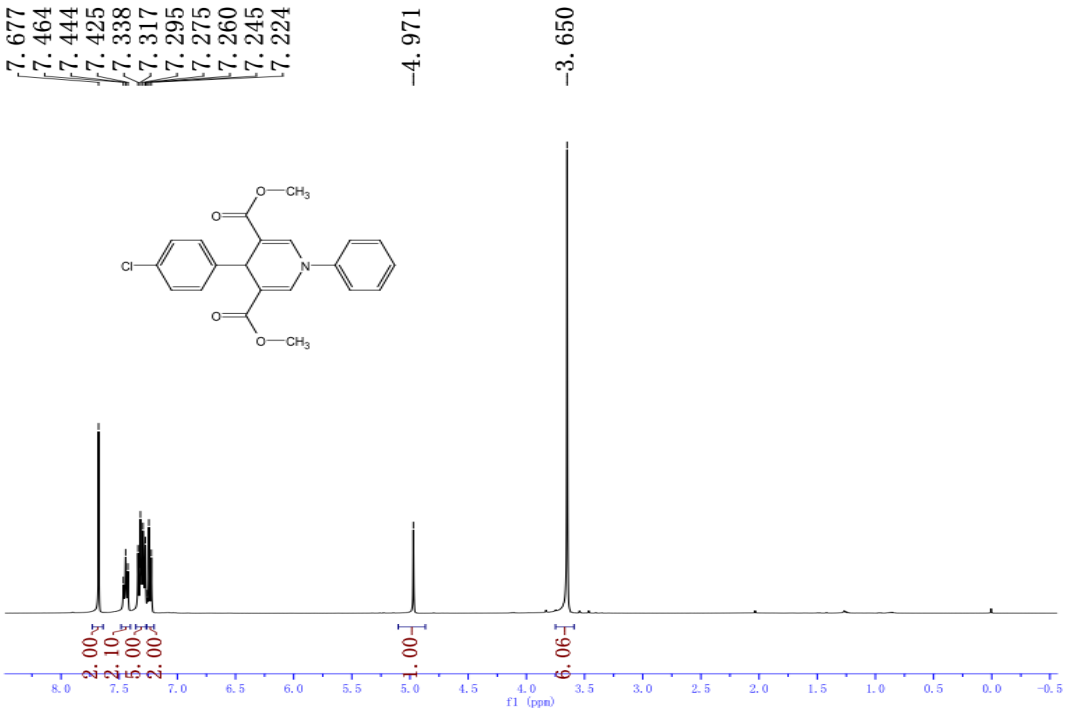


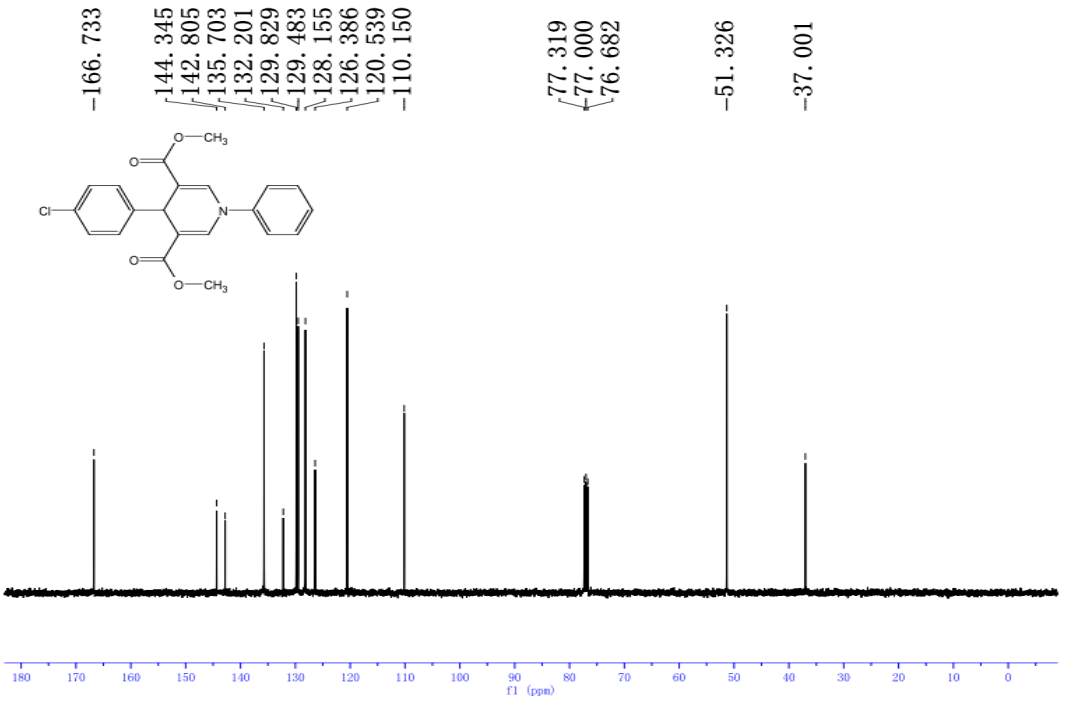
^{1}H NMR and ^{13}C NMR of dimethyl 4-(4-nitrophenyl)-1-phenyl-1,4-dihydropyridine-3,5- dicarboxylate (4c)



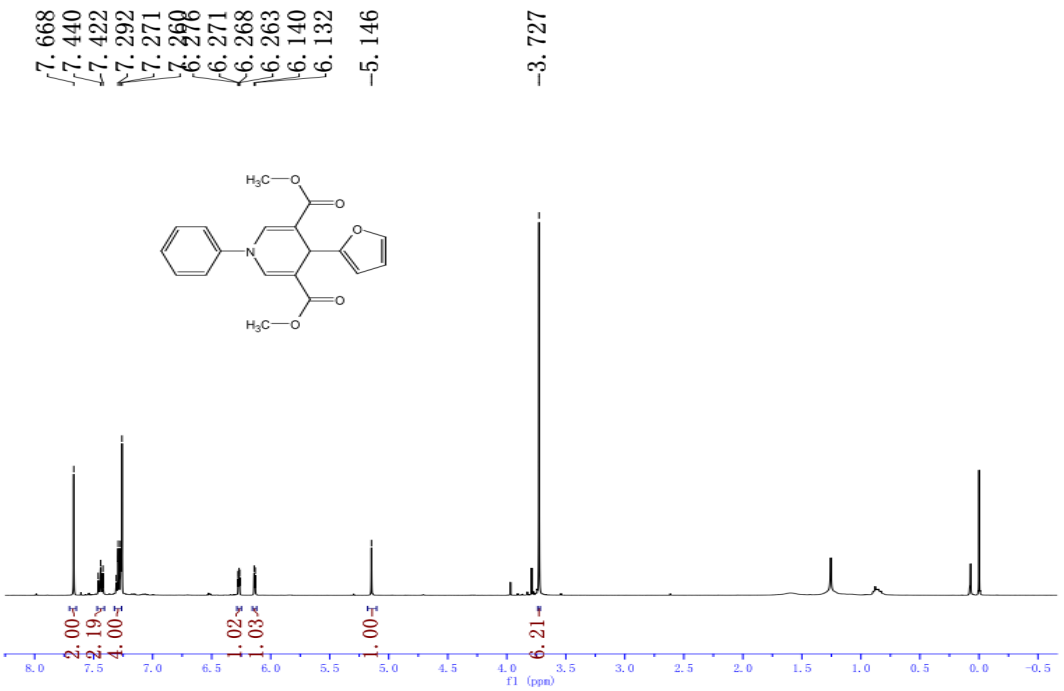


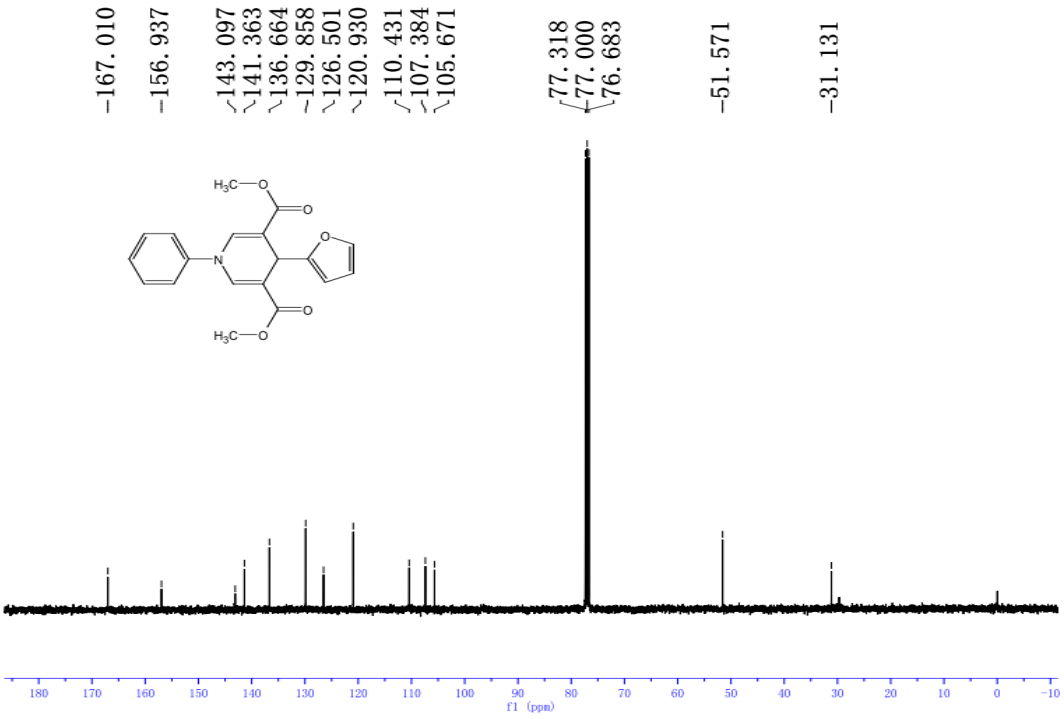
^{1}H NMR and ^{13}C NMR of dimethyl 4-(4-chlorophenyl)-1-phenyl-1,4-dihydropyridine- 3,5-dicarboxylate (4d)



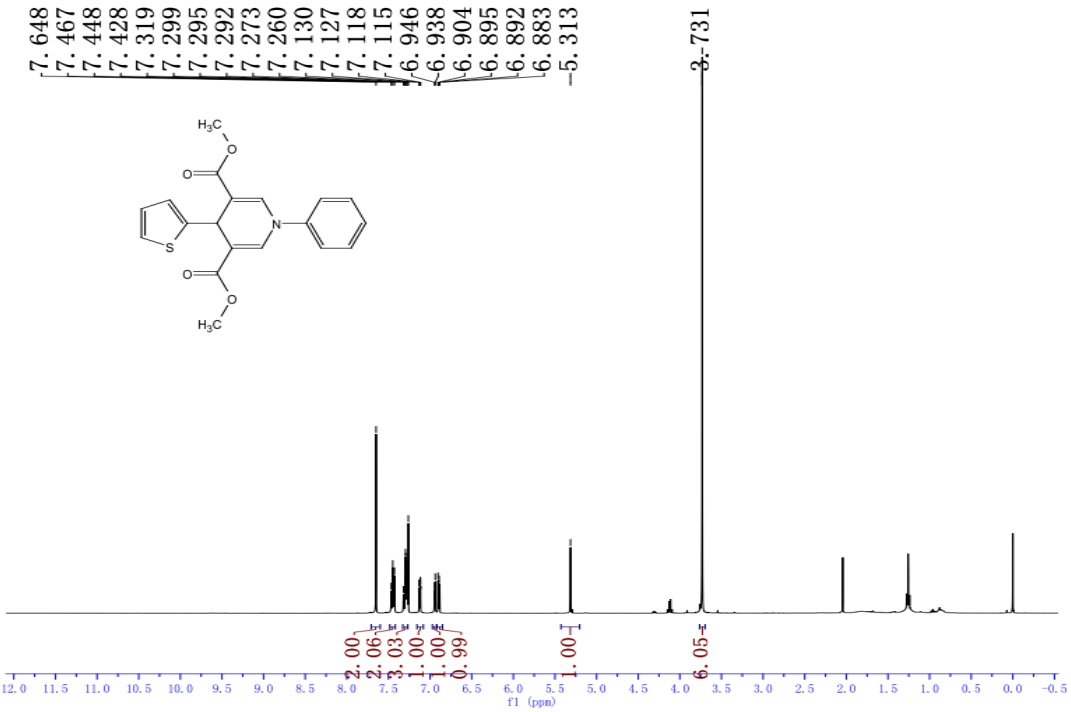


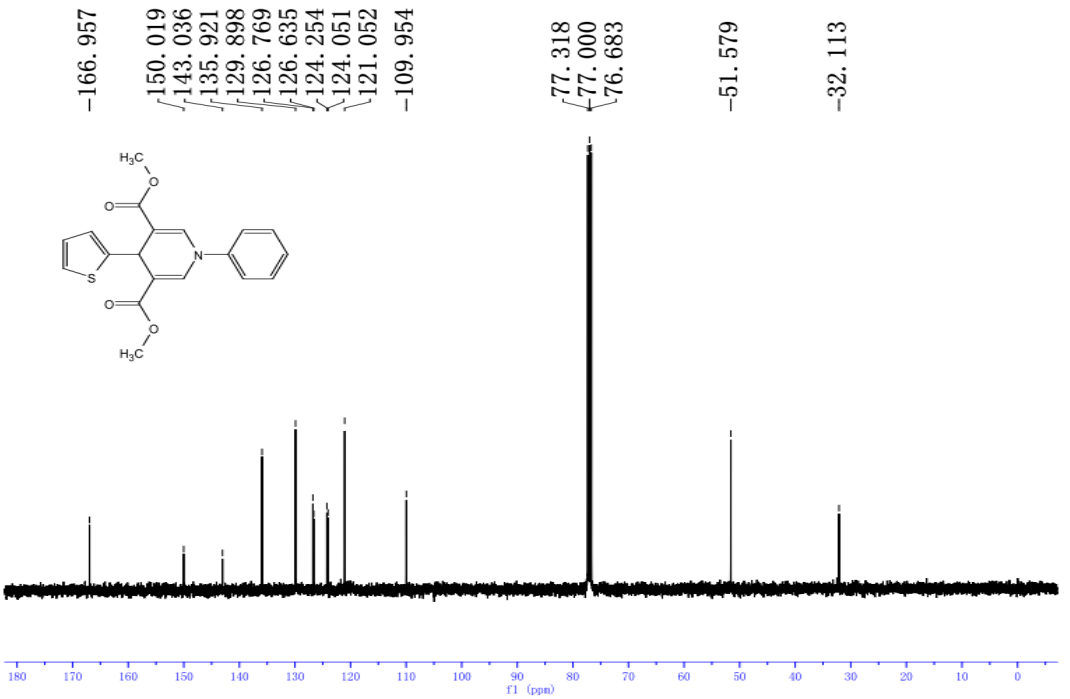
^{1}H NMR and ^{13}C NMR of dimethyl 4-(furan-2-yl)-1-phenyl-1,4-dihydropyridine-3,5-dicarboxylate (4e)



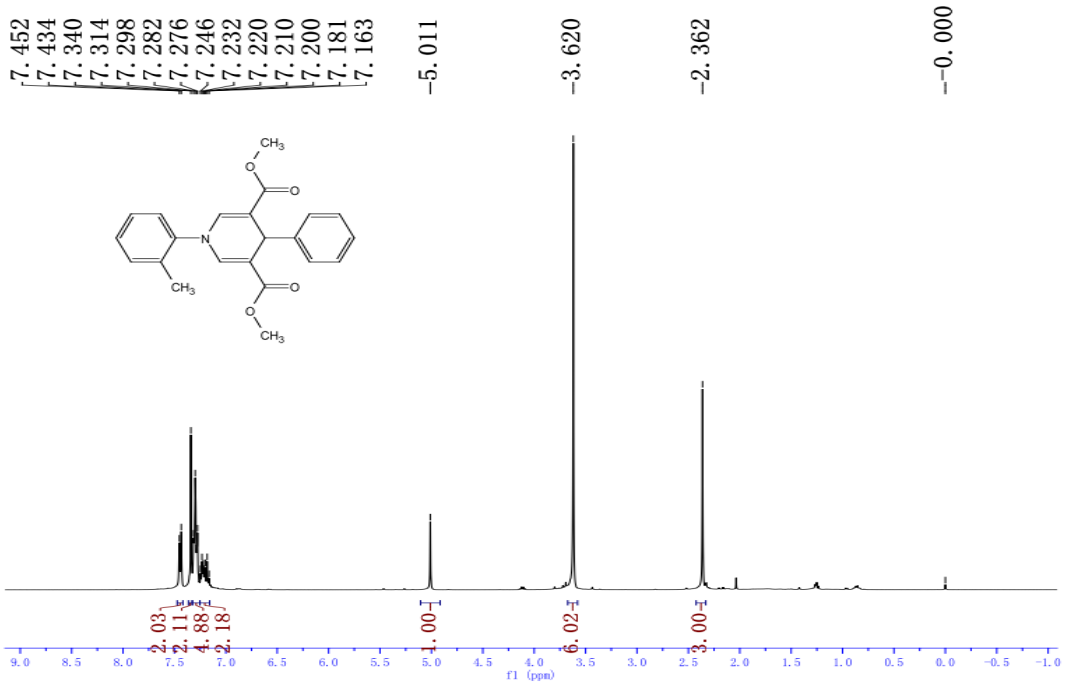


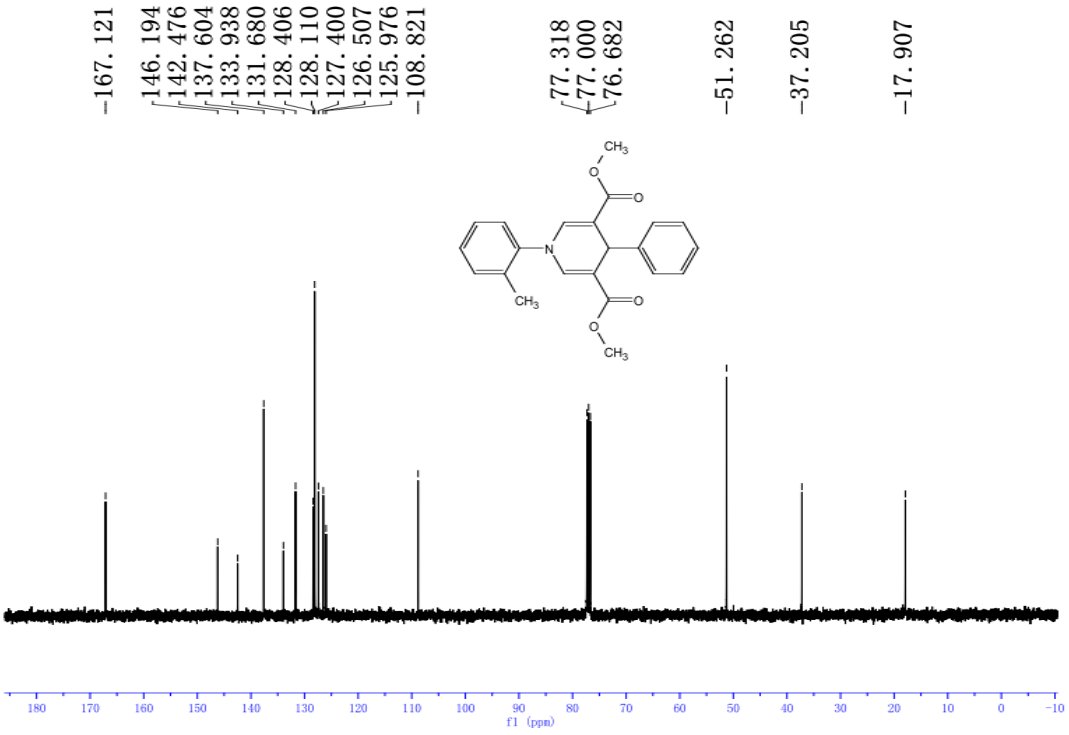
^{1}H NMR and ^{13}C NMR of dimethyl
1-phenyl-4-(thiophen-2-yl)-1,4-dihydropyridine-3,5- dicarboxylate (4f)



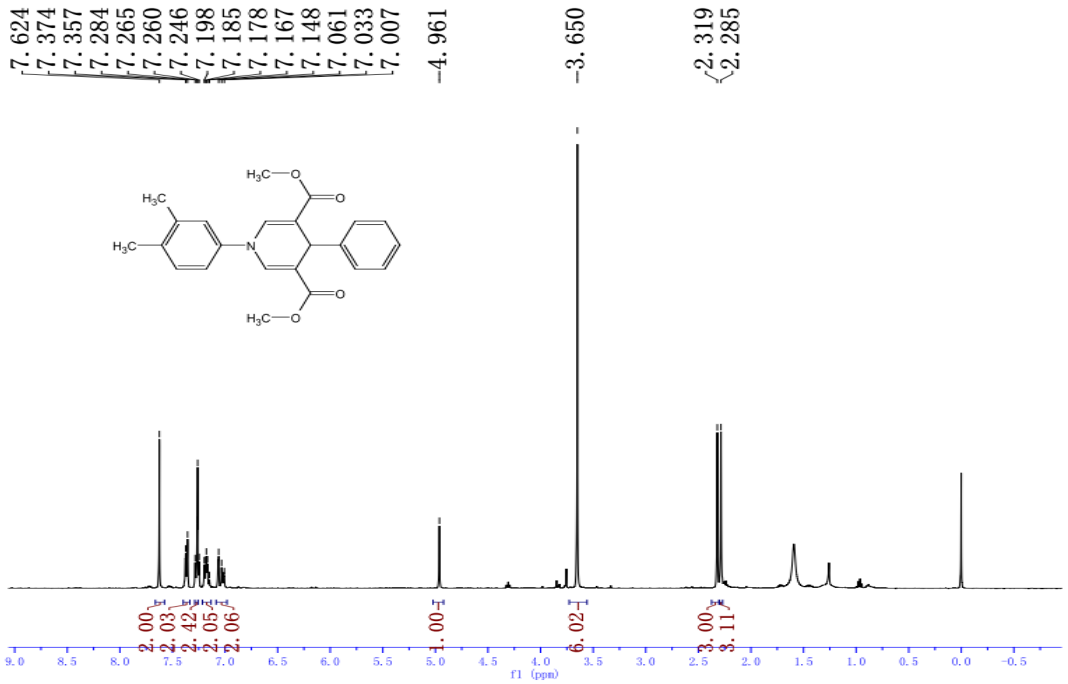


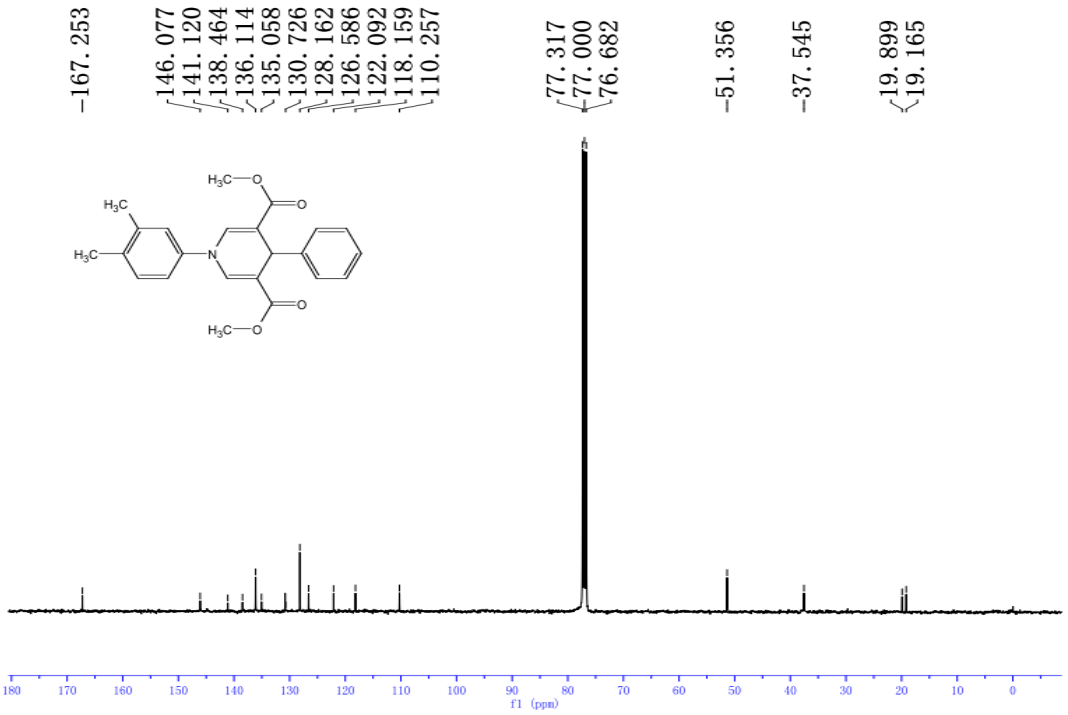
^{1}H NMR and ^{13}C NMR of dimethyl 4-phenyl-1-o-tolyl-1,4-dihydropyridine-3,5- dicarboxylate (4g)



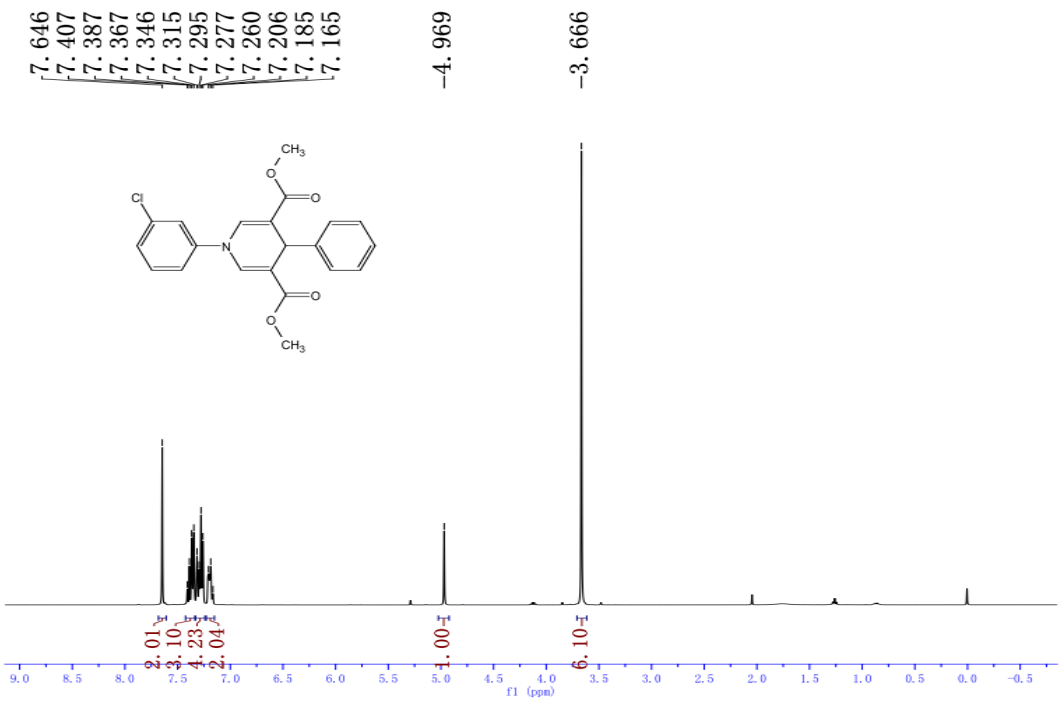


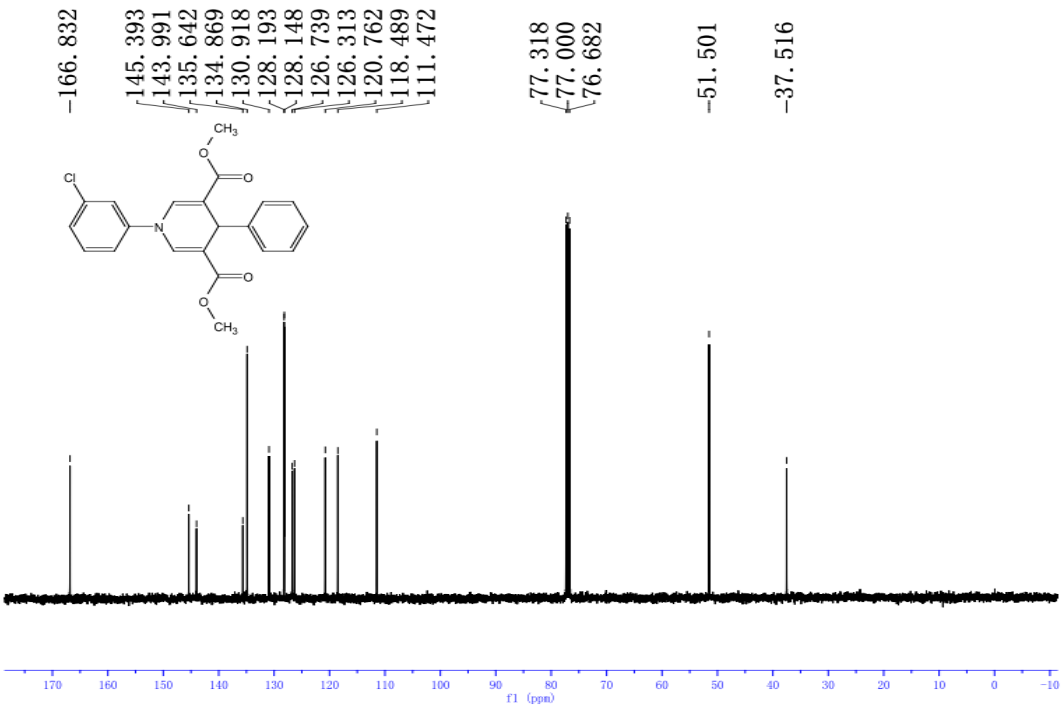
^{1}H NMR and ^{13}C NMR of dimethyl 1-(3,4-dimethylphenyl)-4-phenyl-1,4-dihydropyridine-3,5-dicarboxylate (4h)



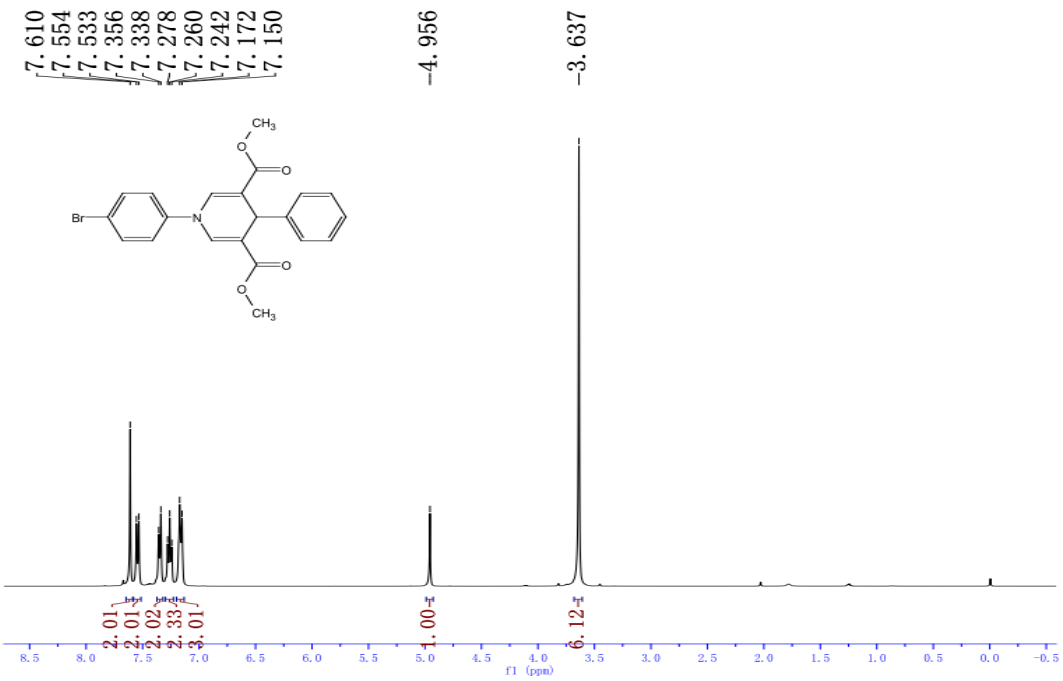


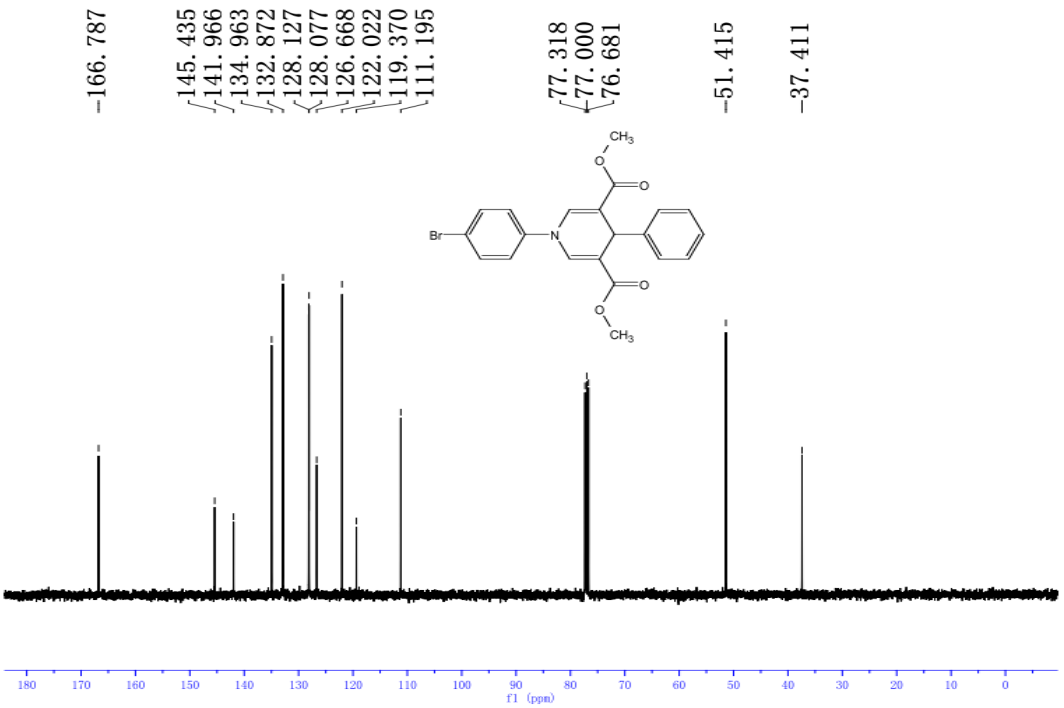
^{1}H NMR and ^{13}C NMR of dimethyl 1-(3-chlorophenyl)-4-phenyl-1,4-dihydropyridine-3,5- dicarboxylate (4i)



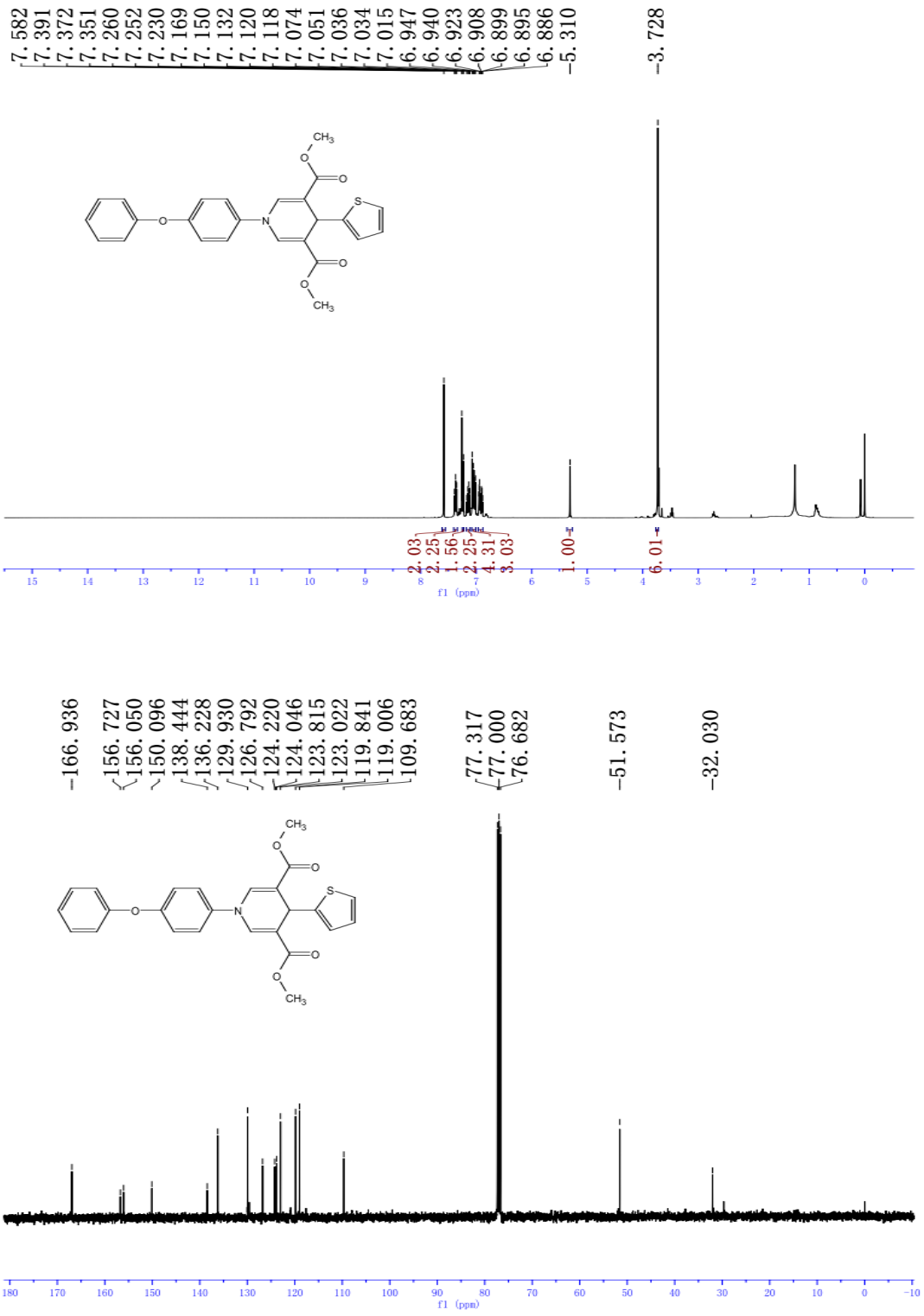


^{1}H NMR and ^{13}C NMR of dimethyl 1-(4-bromophenyl)-4-phenyl-1,4-dihydropyridine-3,5-dicarboxylate (4j)

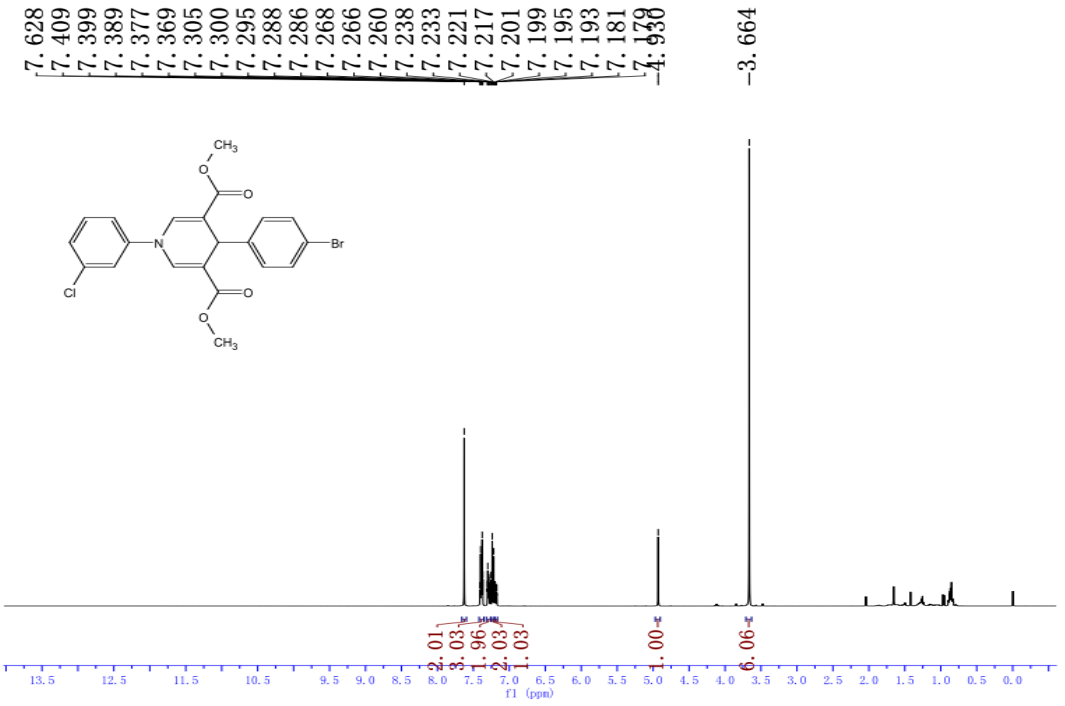


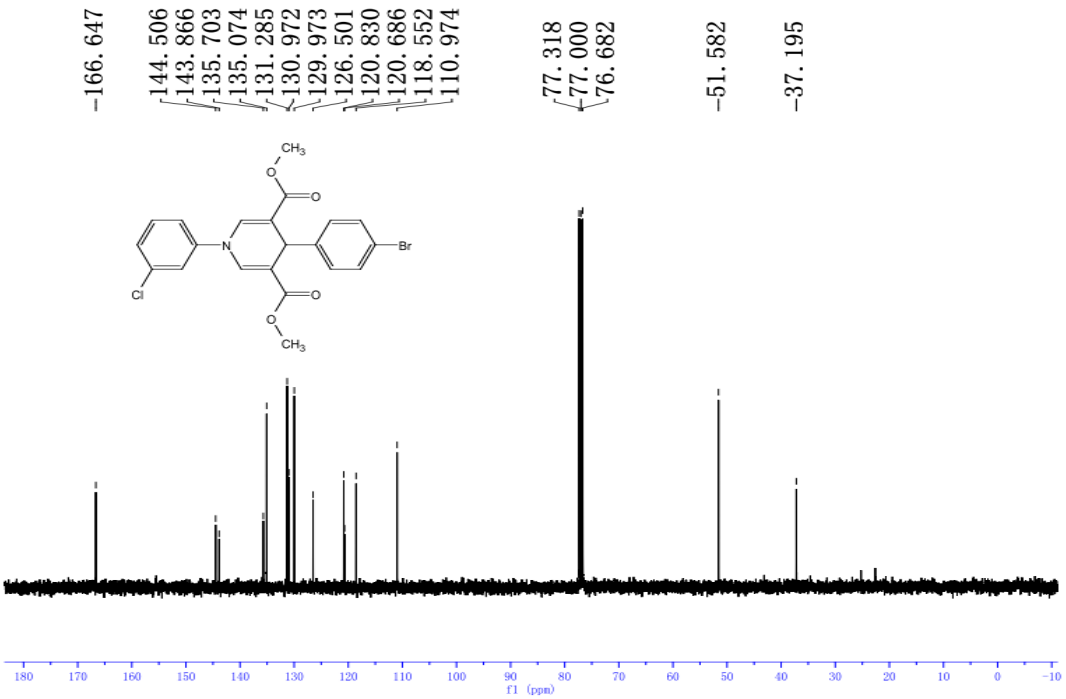


^{1}H NMR and ^{13}C NMR of dimethyl 1-(4-phenoxyphenyl)-4-(thiophen-2-yl)-1,4-dihydropyridine-3,5-dicarboxylate (4k)



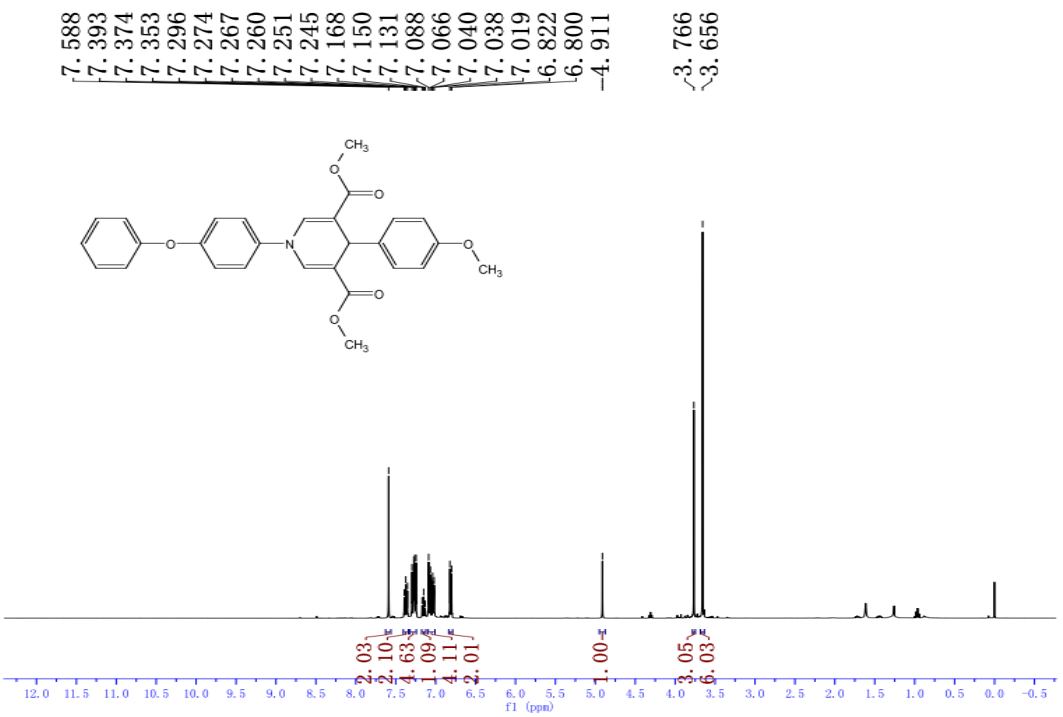
^{1}H NMR and ^{13}C NMR of dimethyl 4-(4-bromophenyl)-1-(3-chlorophenyl)-1,4- dihydropyridine-3,5-dicarboxylate (4l)

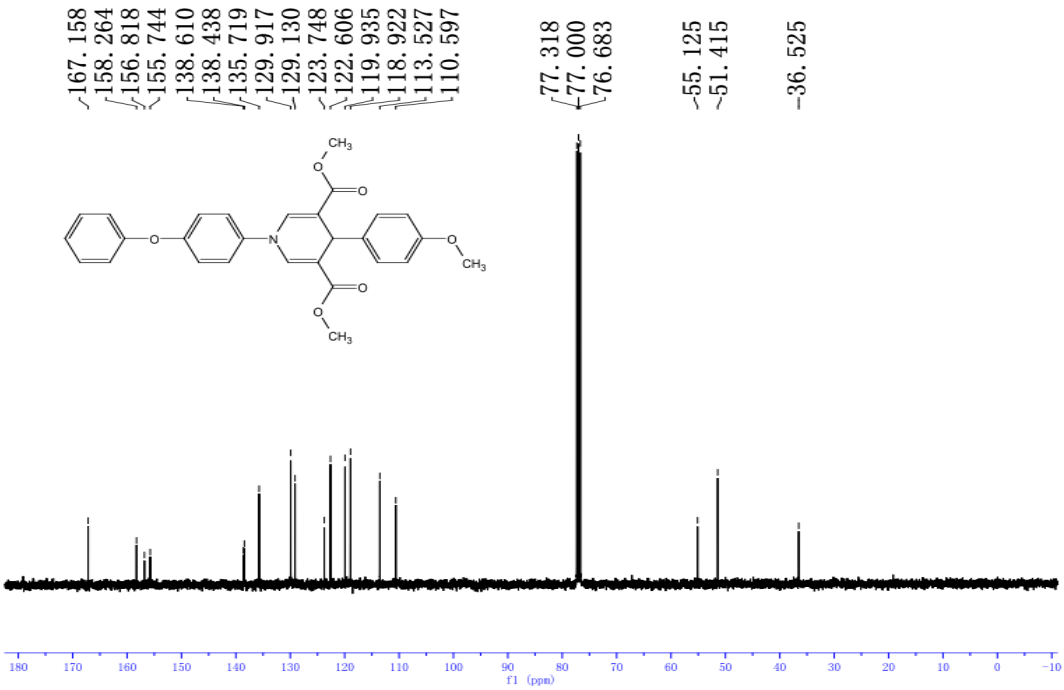




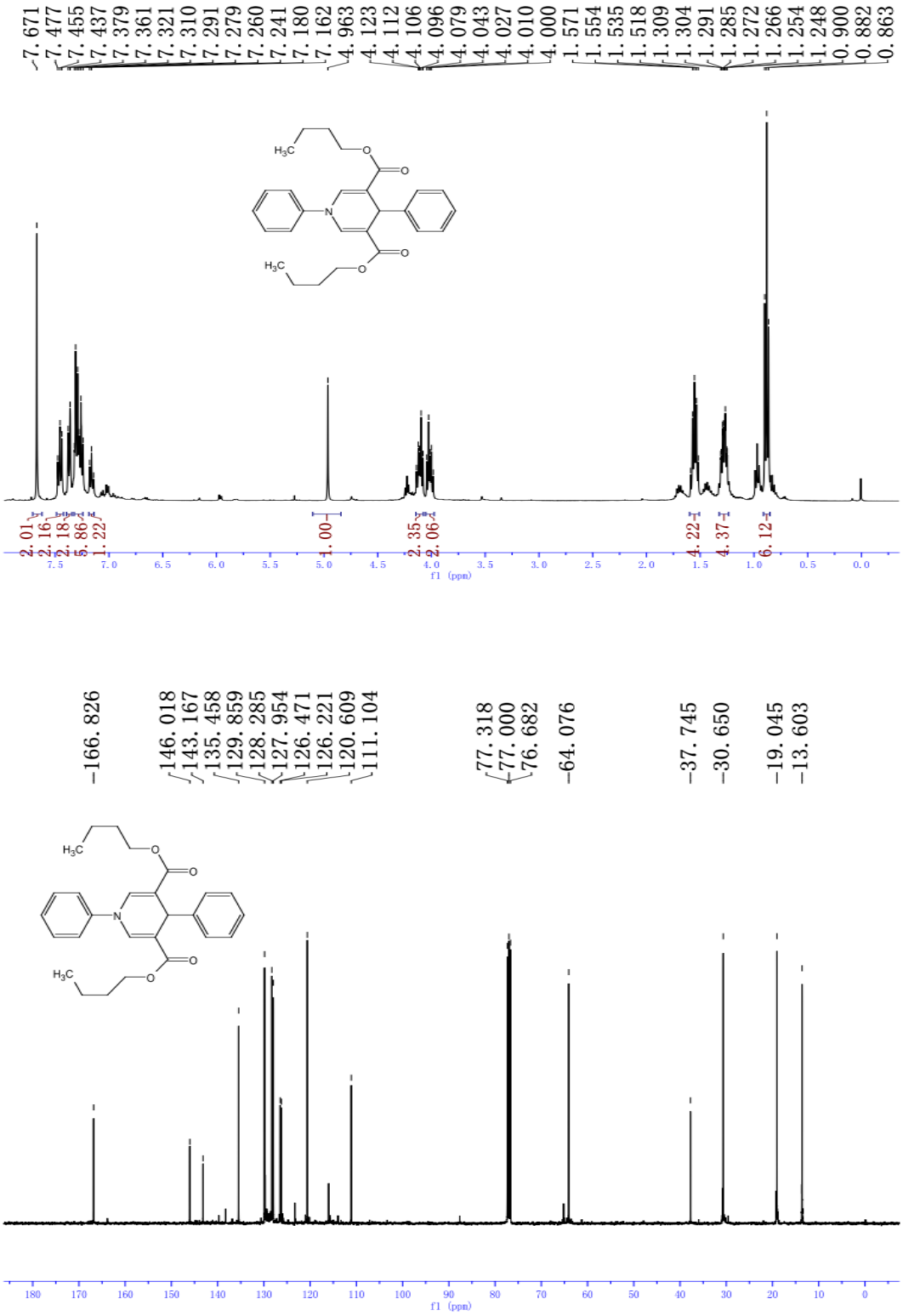
^{1}H NMR and ^{13}C NMR of dimethyl

4-(4-methoxyphenyl)-1-(4-phenoxyphenyl)-1,4-dihydropyridine-3,5-dicarboxylate (4m)

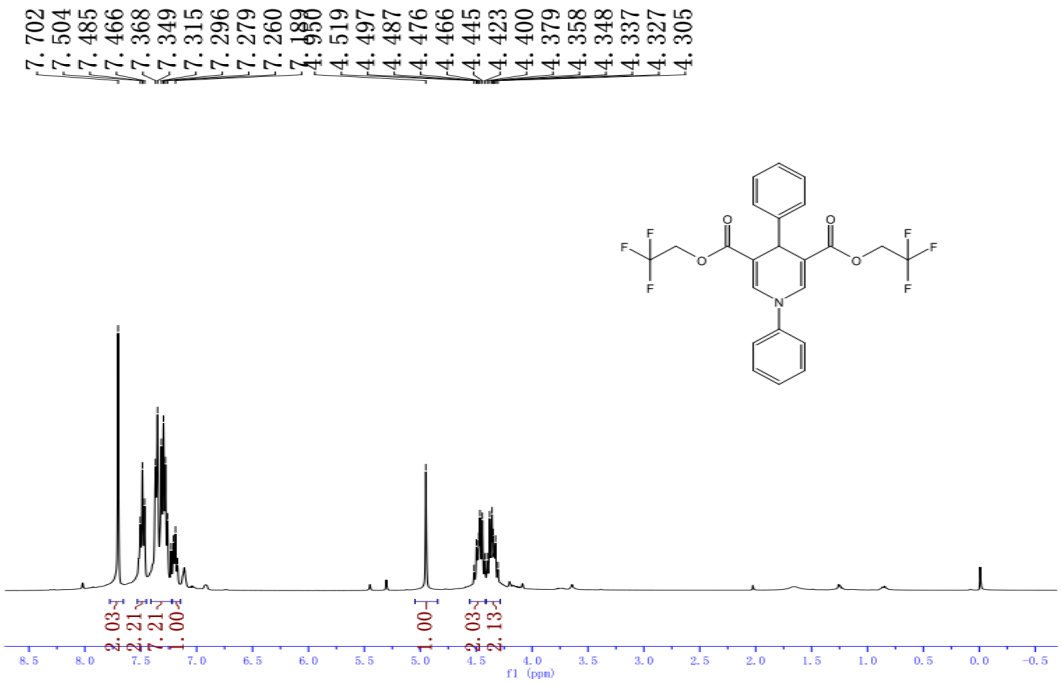


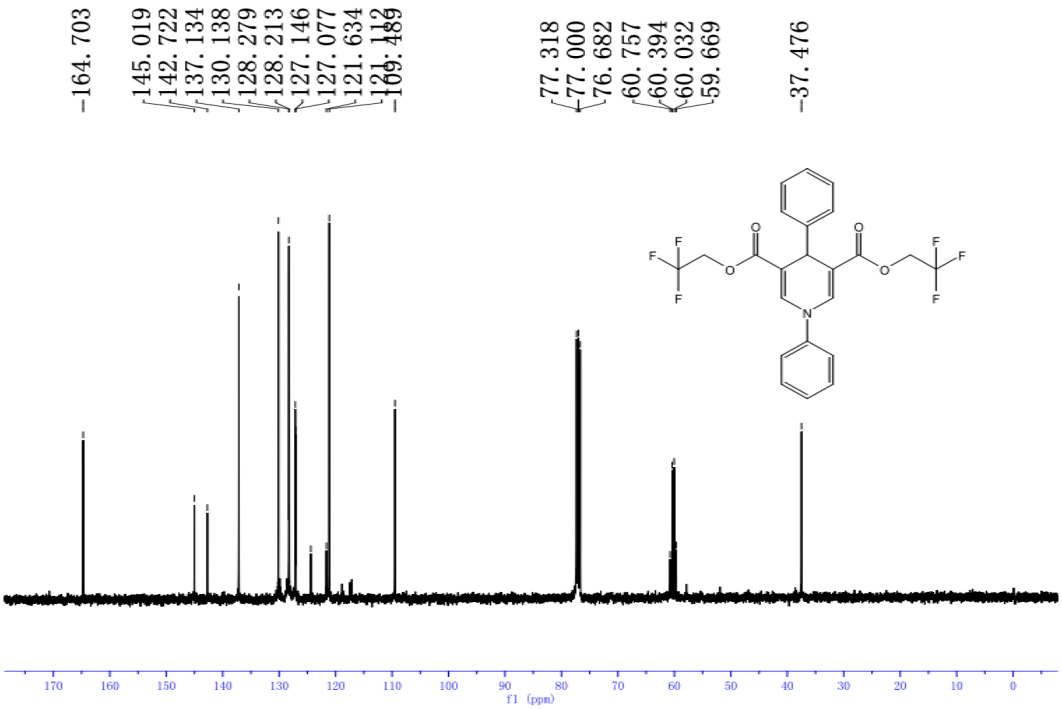


^{1}H NMR and ^{13}C NMR of dibutyl 1,4-diphenyl-1,4-dihydropyridine-3,5-dicarboxylate (4n)

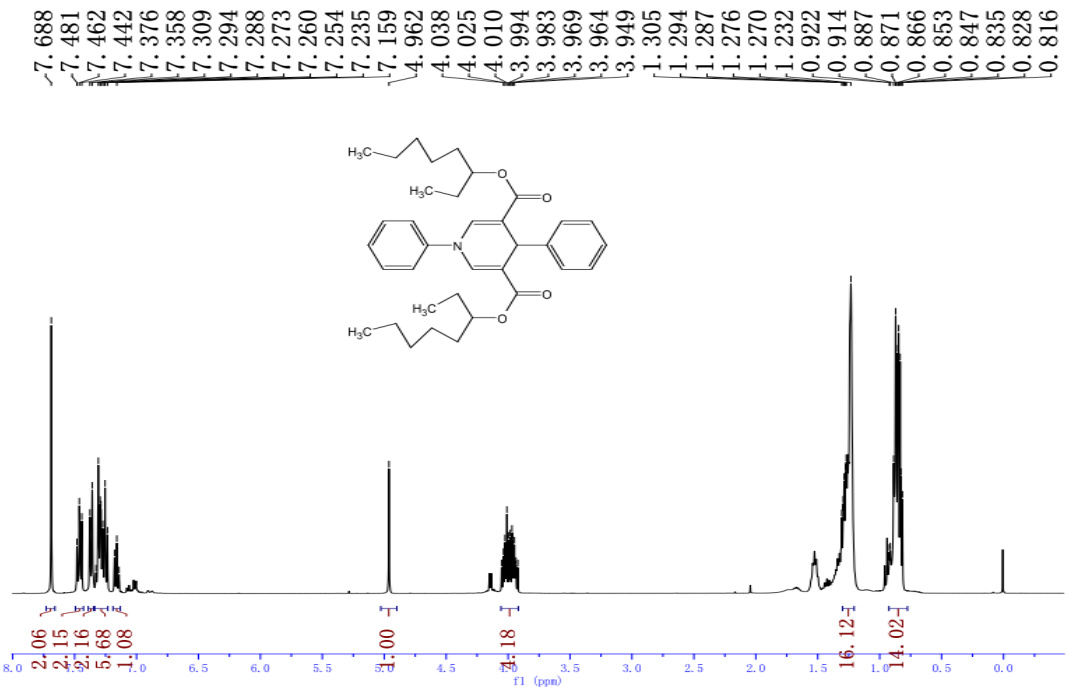


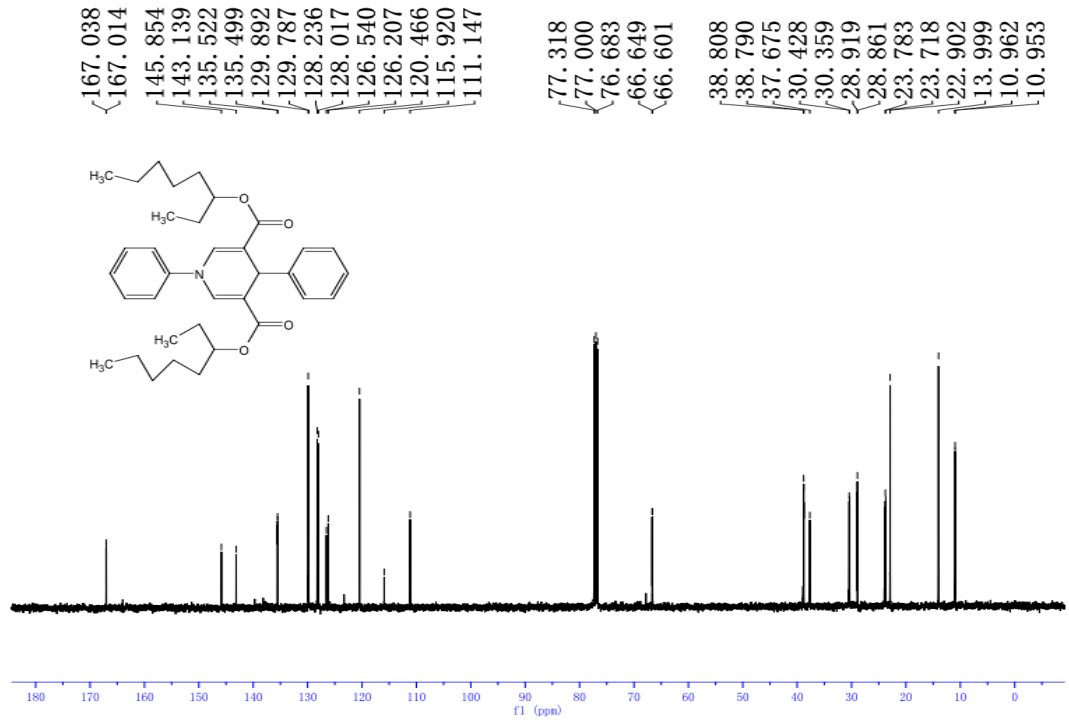
^{1}H NMR and ^{13}C NMR of bis(trifluoromethyl) 1,4-diphenyl-1,4-dihydropyridine-3,5-dicarboxylate (4o)



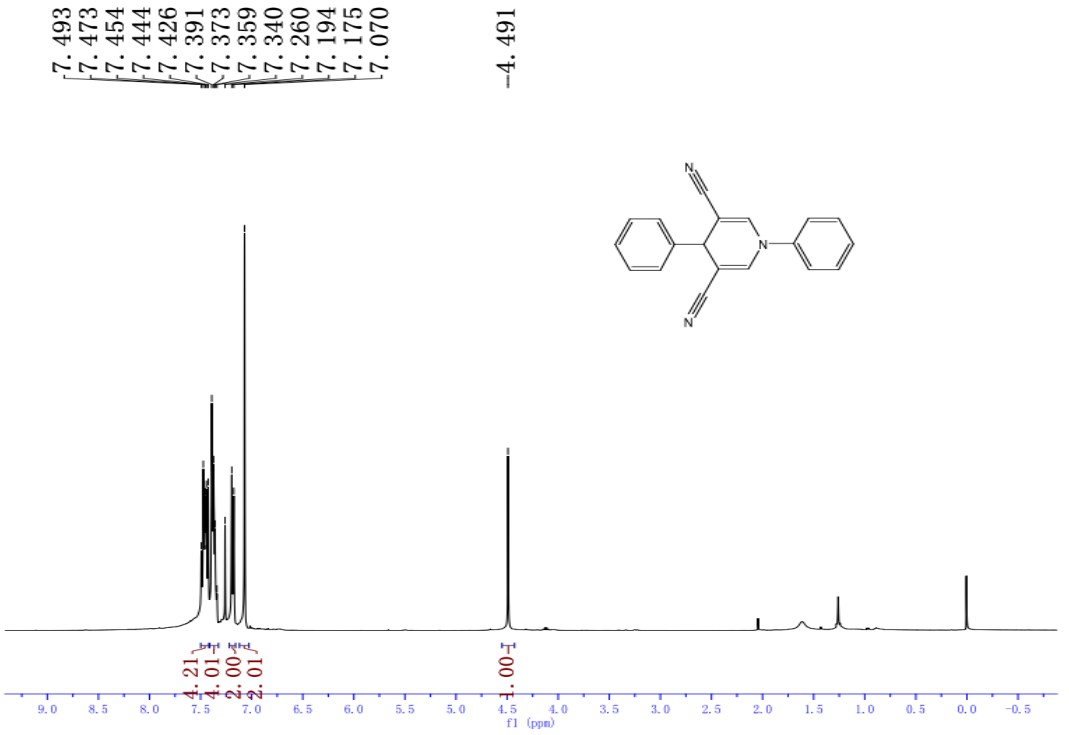


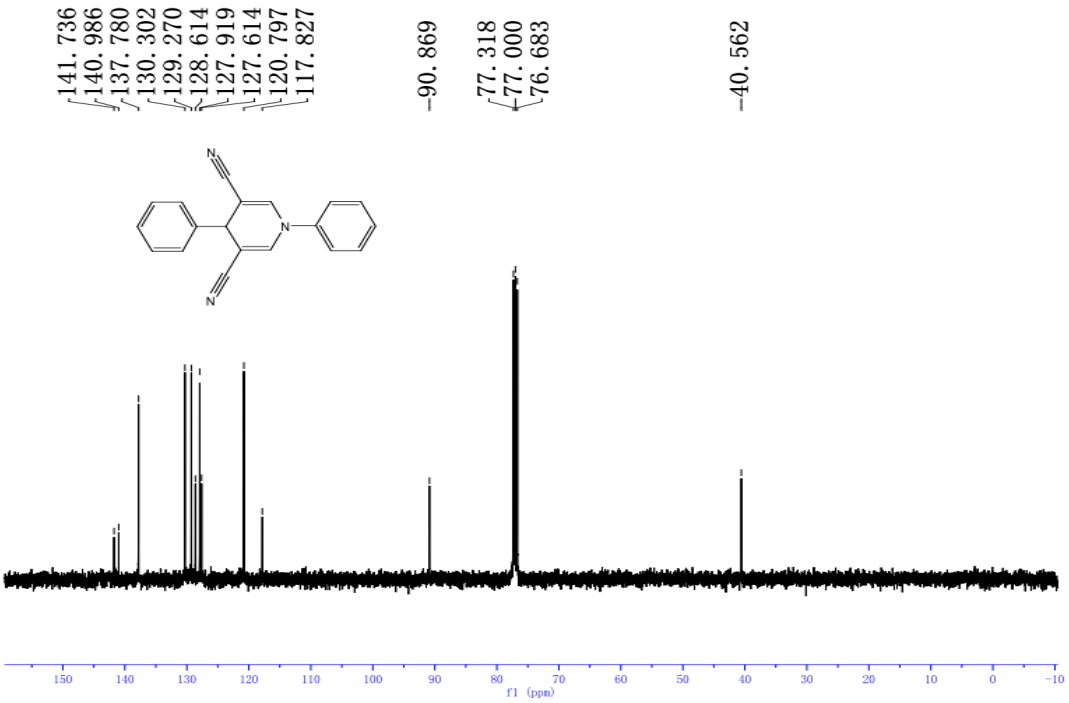
^{1}H NMR and ^{13}C NMR of dioctan-3-yl 1,4-diphenyl-1,4-dihydropyridine-3,5-dicarboxylate (4p)



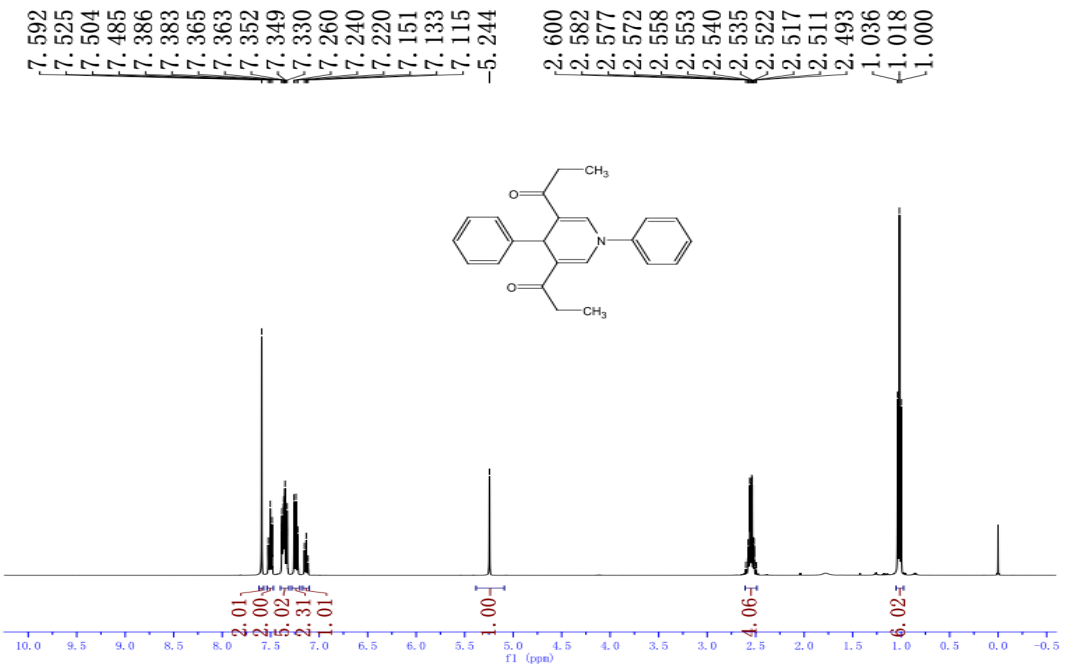


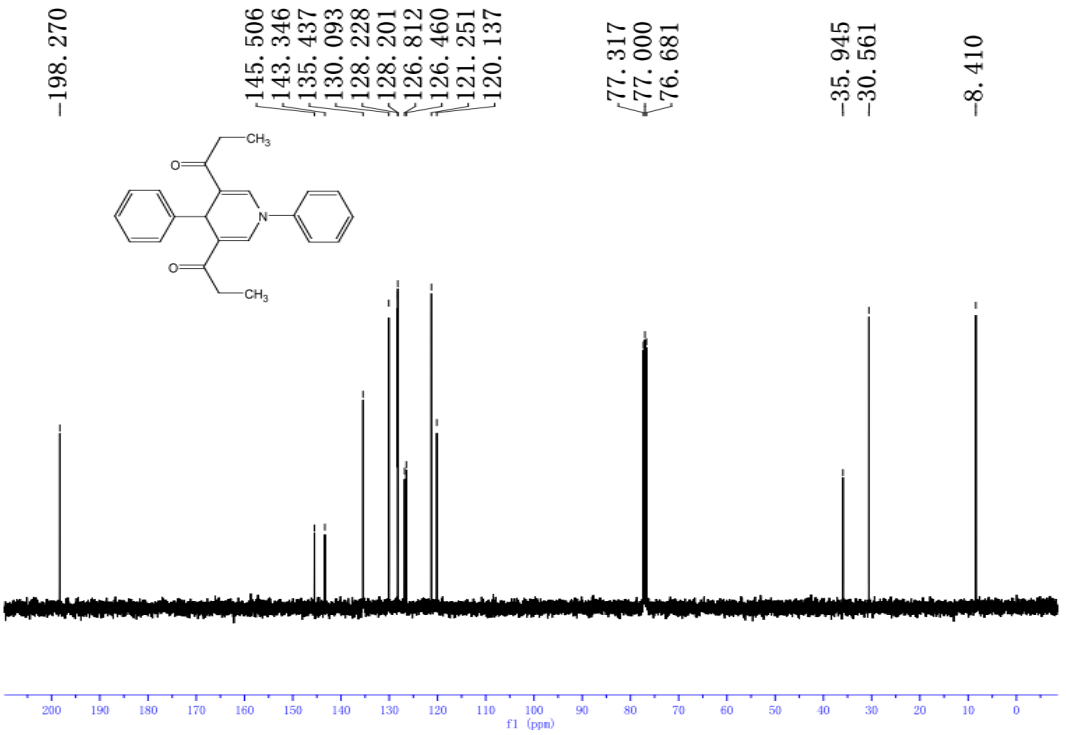
^{1}H NMR and ^{13}C NMR of 1,4-diphenyl-1,4-dihydropyridine-3,5-dicarbonitrile (4q)





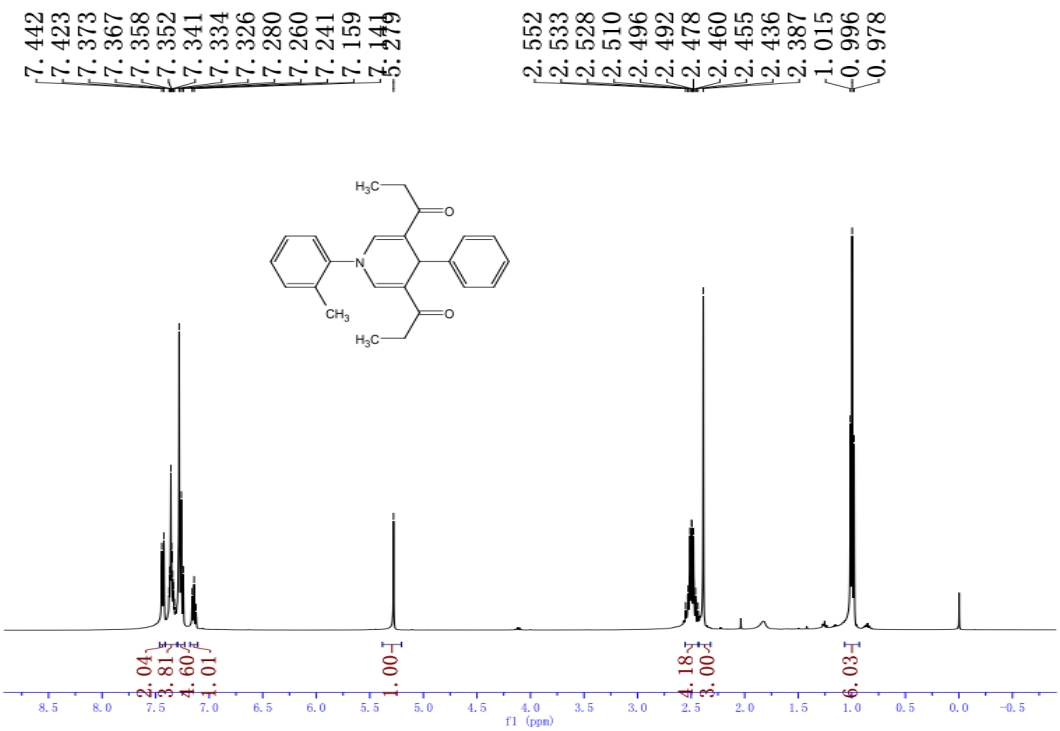
^{1}H NMR and ^{13}C NMR of
1,1'-(1,4-diphenyl-1,4-dihydropyridine-3,5-diyl)dipropan-1-one (4r)

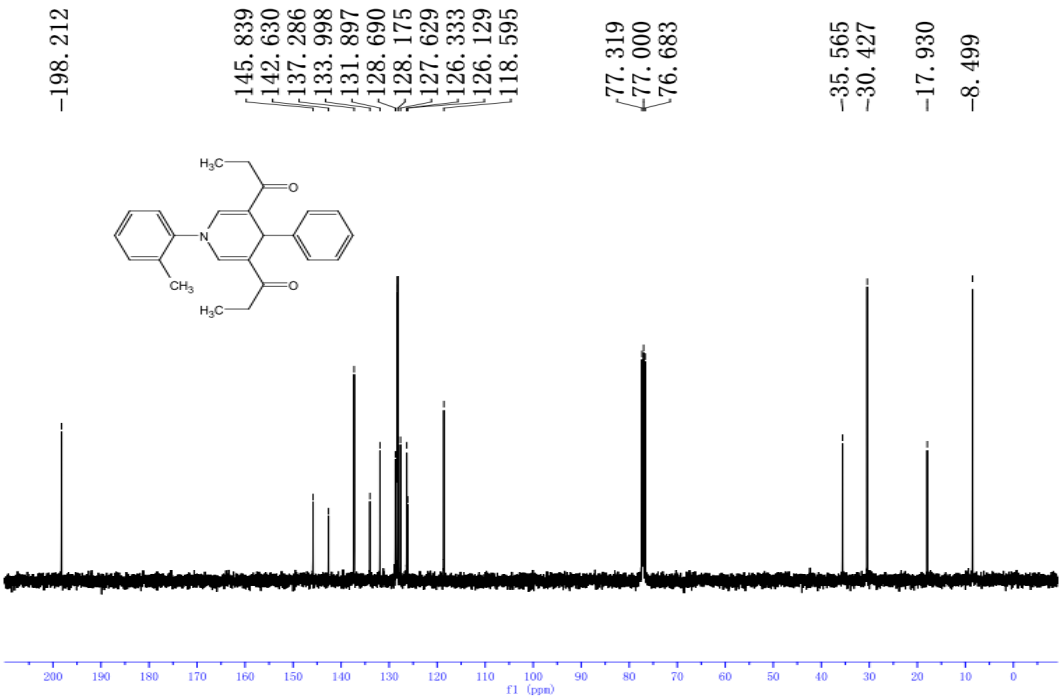




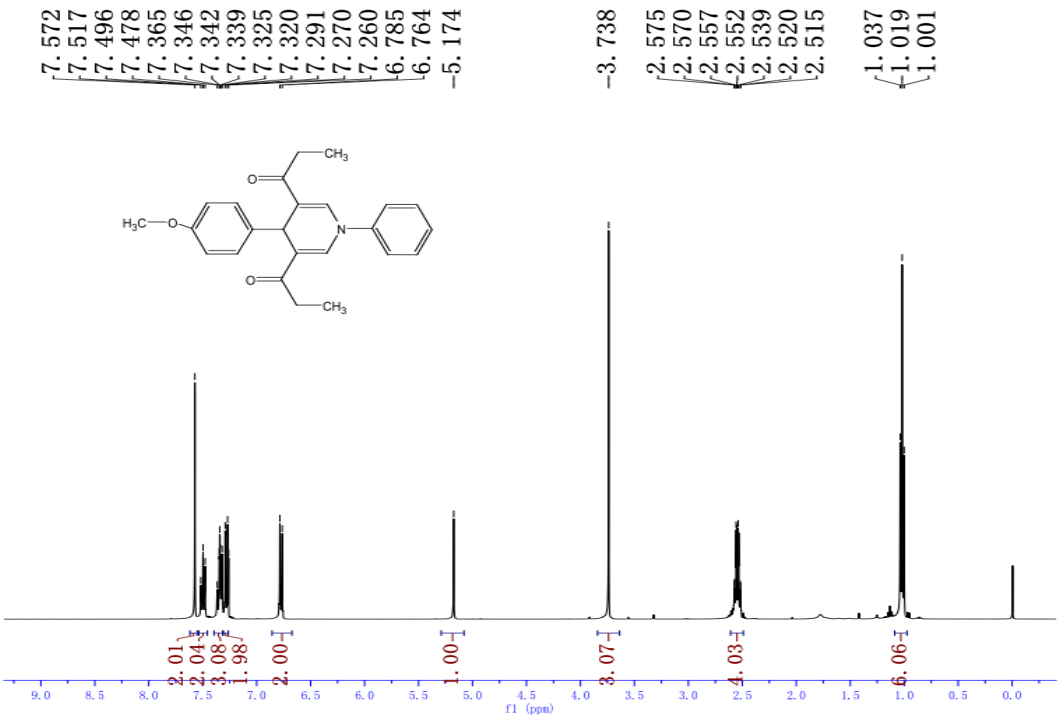
^{1}H NMR and ^{13}C NMR of

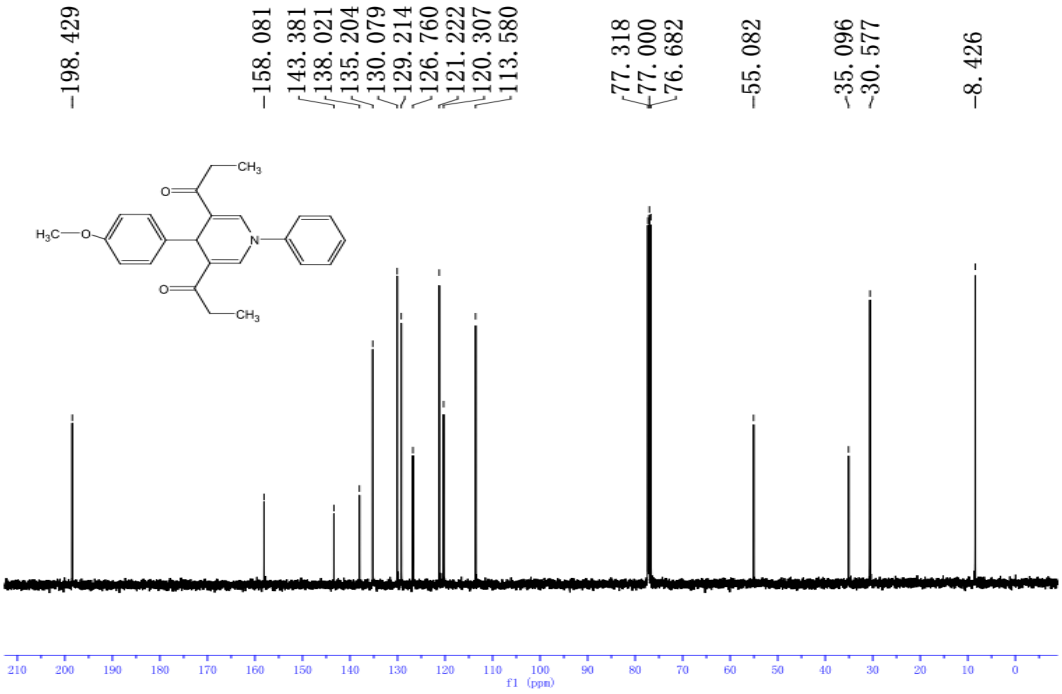
1,1'-[1-(2-methylphenyl)-4-phenyl-1,4-dihydropyridine-3,5- diyl]dipropanone (4s)



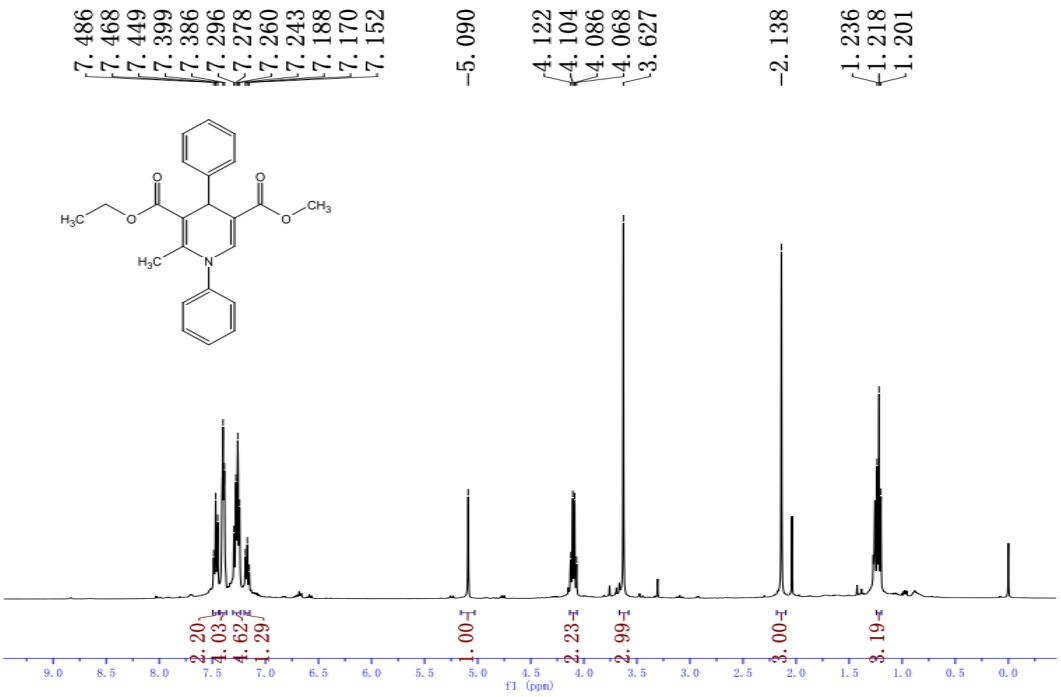


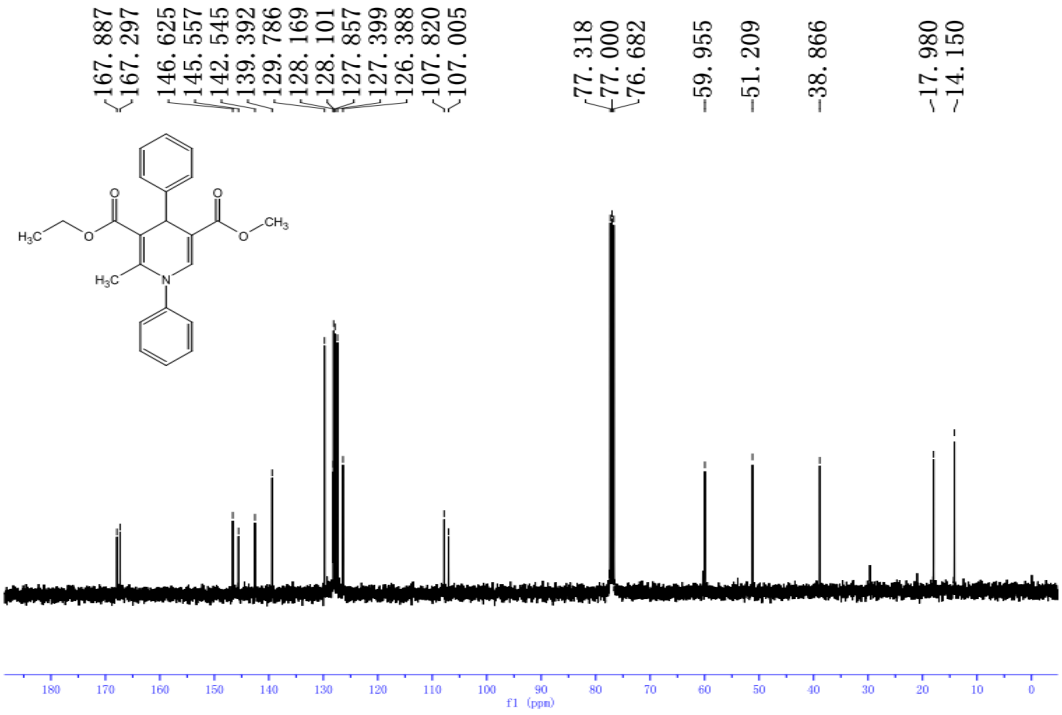
^{1}H NMR and ^{13}C NMR of
1,1'-[4-(4-methoxyphenyl)-1-phenyl-1,4-dihydropyridine-3,5-diyl]dipropanone (4t)





^{1}H NMR and ^{13}C NMR of 3-ethyl 5-methyl 2-methyl-1,4-diphenyl-1,4-dihydropyridine-3,5-dicarboxylate (4u)





^{1}H NMR and ^{13}C NMR of (Z)-methyl 3-(phenylamino)acrylate 7