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Supporting Information

Palladium-Catalyzed Synthesis of Aldehydes from Aryl Halides and *tert*-Butyl Isocyanide using Formate salts as a Hydride Donor

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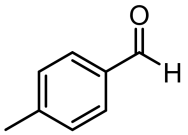
General information:

All reactants and reagents were purchased from commercial suppliers. All anhydrous solvents used in the reactions were dried and freshly distilled. TLC was performed on silica HSGF254 plates. Melting points were determined with a digital melting-point apparatus. ^{1}H and ^{13}C NMR spectra were obtained at 400/101 or 600/125 MHz, respectively. NMR spectra were run in a solution of deuterated chloroform ($CDCl_3$) or DMSO-d_6 and were reported in parts per million (ppm). LRMS analyses were carried out on an electrospray ionization (ESI) apparatus using time-of-flight (TOF) mass spectrometry.

Typical experimental procedure for reductive formylation reaction of aryl halides:

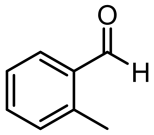
Into a 15 mL sealed tube was added aryl halides (0.7 mmol), *tert*-butyl isocyanide (0.84 mmol, 95 μL), $Pd(OAc)_2$ (0.032 mmol, 7 mg), dppe (0.063 mmol, 25 mg), HCO_2Na (1.4 mmol, 95 mg) and anhydrous DMSO (3.0 mL). The mixture was stirred at 120 °C under nitrogen. After completion of the reaction indicated by TLC, the mixture was extracted with Et_2O (3×10 mL). The combined organic layer was dried over Na_2SO_4, and the filtrate was then concentrated under vacuum. The residue was purified by column chromatography on silica gel using petroleum ether (30—60 °C)/Et_2O as eluent to provide the pure desired product.

4-Methylbenzaldehyde (2a):[1]



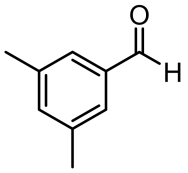
Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 95% (80 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.96 (s, 1H), 7.77 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 7.9 Hz, 2H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.1, 145.6, 134.2, 129.9, 129.8, 22.0. LRMS (ESI): *m/z* calcd for C_8H_8O $[M + H]^+$, 121.1; found, 121.0.

2-Methylbenzaldehyde (2b):[1]



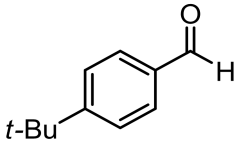
Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 65% (55 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.98 (s, 1H), 7.67 (d, *J* = 7.1 Hz, 2H), 7.45–7.38 (m, 2H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.6, 139.0, 136.5, 135.4, 130.1, 128.9, 127.3, 21.3. LRMS (ESI): *m/z* calcd for C_8H_8O $[M + H]^+$, 121.1; found, 121.0.

3,5-Dimethylbenzaldehyde (2c):[2]



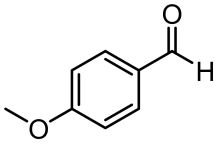
Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 84% (79 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.84 (s, 1H), 7.38 (s, 2H), 7.15 (s, 1H), 2.28 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.8, 138.8, 136.6, 136.2, 127.6, 21.1. LRMS (ESI): *m/z* calcd for $C_9H_{10}O$ $[M + H]^+$, 135.1; found, 134.9.

4-*tert*-Butylbenzaldehyde (2d):[3]



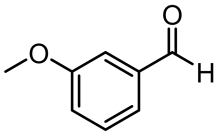
Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 90% (102 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.97 (s, 1H), 7.81 (d, *J* = 8.4 Hz, 2H), 7.54 (d, *J* = 8.3 Hz, 2H), 1.34 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.1, 158.5, 134.2, 129.8, 126.1, 35.4, 31.1. LRMS (ESI): *m/z* calcd for $C_{11}H_{14}O$ $[M + H]^+$, 163.1; found, 163.0.

4-Methoxybenzaldehyde (**2e**):[1]



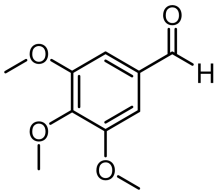
Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 66% (63 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.78 (s, 1H), 7.74 (d, *J* = 8.6 Hz, 2H), 6.90 (d, *J* = 8.4 Hz, 2H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.8, 164.6, 132.0, 129.9, 114.3, 55.6. LRMS (ESI): *m/z* calcd for $C_8H_8O_2$ $[M + H]^+$, 137.0; found, 136.9.

3-Methoxybenzaldehyde (2f):[1]



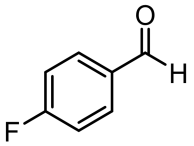
Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 61% (58 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.97 (s, 1H), 7.47–7.42 (m, 2H), 7.39 (s, 1H), 7.18 (d, *J*= 6.6 Hz, 1H), 3.86 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.3, 160.2, 137.9, 130.1, 123.6, 121.6, 112.1, 55.6. LRMS (ESI): *m/z* calcd for $C_8H_8O_2$ $[M + H]^+$, 137.2; found, 137.0.

3,4,5-Trimethoxybenzaldehyde (2g):[4]



Prepared from corresponding aryl iodide for 6 h. White solid. Yield: 80% (93 mg). M.p 68- 70 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.88 (s, 1H), 7.14 (s, 2H), 3.94(s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 191.2, 153.7, 143.6, 131.8, 106.8, 61.1, 56.4. LRMS (ESI): *m/z* calcd for $C_{10}H_{12}O_4$ $[M + H]^+$, 167.1; found, 167.1.

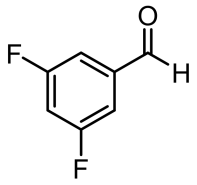
4-Fluorobenzaldehyde (2h):[5]



Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 85% (74 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.98 (s, 1H), 7.95–7.89 (m, 2H), 7.22 (t, *J* = 8.6 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 190.6 (s), 166.6 (d, *J* = 256.7 Hz), 133.1 (d, *J* = 2.7 Hz), 132.3 (d, *J* = 9.7 Hz), 116.4 (d, *J* = 22.3 Hz). LRMS (ESI):

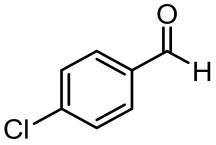
m/z calcd for C_7H_5FO [M + H]$^+$, 125.0; found, 124.9.

3,5-Difluorobenzaldehyde (2i):[6]



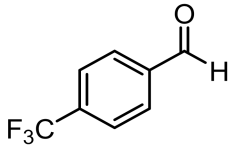
Prepared from corresponding aryl iodide for 6 h. Colorless oil. Yield: 55% (55 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.96 (s, 1H), 7.45–7.38 (dd, *J* = 6.9, 1.9 Hz, 2H), 7.10 (tt, *J* = 8.4, 2.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.5 (t, *J* = 2.5 Hz), 163.5 (dd, *J* = 252.5, 11.5 Hz), 139.29 (s), 112.3 (m), 109.9 (t, *J* = 25.5 Hz). LRMS (ESI): *m/z* calcd for $C_7H_4F_2O$ [M + H]$^+$, 143.0; found, 143.0.

4-Chlorobenzaldehyde (2j):[5]



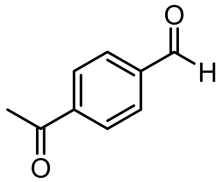
prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 70% (69 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.98 (s, 1H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.51 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.0, 141.1, 134.8, 131.0, 129.6. LRMS (ESI): *m/z* calcd for C_7H_5ClO [M + H]$^+$, 141.0; found, 141.0.

4-(Trifluoromethyl)benzaldehyde (2k):[3]



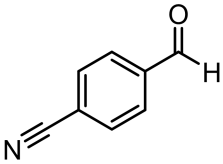
Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 73% (89 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.11 (s, 1H), 8.02 (d, *J* = 7.9 Hz, 2H), 7.82 (d, *J* = 8.1 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 191.1 (s), 138.7 (d, *J* = 1.0 Hz), 135.6 (q, *J* = 32.7 Hz), 129.9 (s), 126.1 (q, *J* = 3.8 Hz),123.5 (q, *J* = 272.9 Hz). LRMS (ESI): *m/z* calcd for $C_8H_5F_3O$ [M + H]$^+$, 175.0; found, 175.0.

4-Acetylbenzaldehyde (2l):[5]



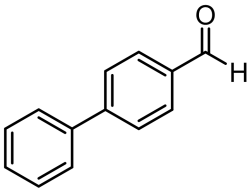
Prepared from corresponding aryl iodide for 24 h. Colorless oil. Yield: 64% (66 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.12 (s, 1H), 8.11 (d, *J* = 8.1 Hz, 2H), 7.99 (d, *J* = 8.4 Hz, 2H), 2.67 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 197.6, 191.8, 141.3, 139.2, 130.0, 129.0, 27.1. LRMS (ESI): *m/z* calcd for $C_9H_8O_2$ [M + H]$^+$, 149.1; found, 149.0.

4-Formylbenzonitrile (2m):[1]



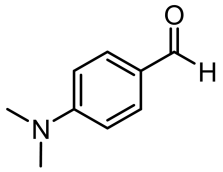
Prepared from corresponding aryl iodide for 6 h. Colorless oil. Yield: 49% (45 mg). ^{1}H NMR ($CDCl^3$, 400 MHz) δ 10.03 (s, 1H), 7.94 (d, *J* = 8.3 Hz, 2H), 7.79 (d, *J* = 8.2 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.8, 138.8, 133.0, 129.9, 117.8, 117.6. LRMS (ESI): *m/z* calcd for C_8H_5NO $[M + H]^+$, 132.0; found,132.0.

Biphenyl-4-carbaldehyde (2n):[1]



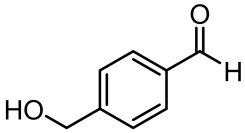
Prepared from corresponding aryl iodide for 6 h. White solid. Yield: 77% (98 mg). Mp. 55–56 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.00 (s, 1H), 7.89 (d, *J* = 8.1 Hz, 2H), 7.69 (d, *J* = 8.2 Hz, 2H), 7.58 (d, *J* = 7.6 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.38 (t, *J* = 7.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.9, 147.0, 139.6, 135.1, 130.2, 129.0, 128.5, 127.6, 127.3. LRMS (ESI): *m/z* calcd for $C_{13}H_{10}O$ $[M + H]^+$, 183.1; found, 183.0.

4-(dimethylamino)benzaldehyde (2o):[1]



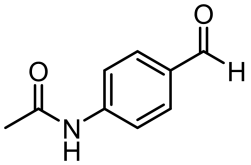
Prepared from corresponding aryl iodide for 6 h. White solid. Yield: 90% (94 mg). M.p 69–71 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.73 (s, 1H), 7.73 (d, *J* = 7.7 Hz, 2H), 6.69 (d, *J* = 7.5 Hz, 2H), 3.08 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.4, 154.4, 132.1, 125.3, 111.1, 40.2. LRMS (ESI): *m/z* calcd for $C_9H_{11}NO$ $[M + H]^+$, 150.1; found, 150.1.

4-Hydroxymethylbenzaldehyde (2p):[7]



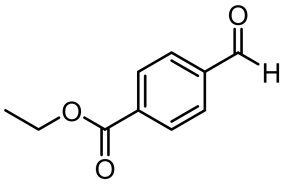
Prepared from corresponding aryl iodide for 6 h. Colorless oil. Yield: 94% (90 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.90 (s, 1H), 7.79 (d, *J* = 7.9 Hz, 2H), 7.47 (d, *J* = 7.9 Hz, 2H), 4.73 (s, 2H), 3.69 ((brs, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.52, 148.27, 135.32, 130.00, 126.92, 64.16. LRMS (ESI): *m/z* calcd for $C_8H_8O_2$ $[M + H]^+$, 137.1; found, 137.1.

N-(4-formylphenyl)acetamide (2q):[8]



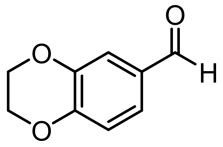
Prepared from corresponding aryl iodide for 6 h. Yellow solid. Yield: 82% (94 mg). M.p 155–157 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.91 (s, 1H), 8.07 (s, 1H), 7.83 (d, *J* = 8.5 Hz, 2H), 7.72 (d, *J* = 8.4 Hz, 2H), 2.23 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.3, 169.1, 143.8, 132.3, 131.3, 119.4, 24.9. LRMS (ESI): *m/z* calcd for $C_9H_9NO_2$ $[M + H]^+$, 164.1; found, 164.0.

Ethyl-4-formylbenzoate (2r):[1]



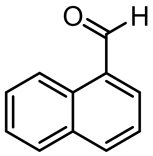
Prepared from corresponding aryl iodide for 6 h. Colorless liquid. Yield: 91% (113 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.09 (s, 1H), 8.19 (d, *J* = 8.4 Hz, 2H), 7.94 (d, *J* = 8.6 Hz, 2H), 4.41 (q, *J* = 7.1 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.8, 165.6, 139.1, 135.5, 130.2, 129.6, 61.7, 14.3. LRMS (ESI): *m/z* calcd for $C_{10}H_{10}O_3$ $[M + H]^+$, 179.1; found, 179.0.

2,3-Dihydrobenzo[b][1,4]dioxine-6-carbaldehyde (2s):[9]



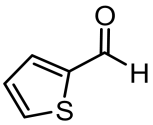
Prepared from corresponding aryl iodide for 3 h. White solid. Yield: 73% (84 mg). M.p 51–53 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.80 (s, 1H), 7.38 (d, *J* = 5.9 Hz, 2H), 6.96 (d, *J* = 8.7 Hz, 1H), 4.32 (d, *J* = 3.9 Hz, 2H), 4.28 (d, *J* = 4.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.8, 149.3, 143.9, 130.6, 124.2, 118.3, 117.8, 64.7, 64.0. LRMS (ESI): *m/z* calcd for $C_9H_8O_3$ $[M + H]^+$, 165.1; found, 165.0.

1-Naphthaldehyde (2t):[1]



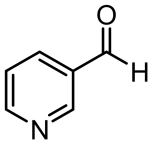
Prepared from corresponding aryl iodide for 3 h. Yellow oil. Yield: 80% (87 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.36 (s, 1H), 9.24 (d, *J* = 8.6 Hz, 1H), 8.05 (d, *J* = 8.2 Hz, 1H), 7.93 (d, *J* = 6.9 Hz, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.66 (t, *J* = 7.7 Hz, 1H), 7.57 (q, *J* = 7.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.7, 136.8, 135.4, 133.8, 131.4, 130.6, 129.4, 128.6, 127.0, 124.9. LRMS (ESI): *m/z* calcd for $C_{11}H_8O$ $[M + H]^+$, 157.1; found, 157.0.

Thiophene-2-carbaldehyde (2u):[1]



Prepared from corresponding aryl iodide for 8 h. Yellow oil. Yield: 38% (30 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.95 (s, 1H), 7.80–7.77 (m, 2H), 7.22 (t, *J* = 4.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 183.1, 144.0, 136.5, 135.2, 128.4. LRMS (ESI): *m/z* calcd for C_5H_4OS $[M + H]^+$, 113.0; found, 113.0.

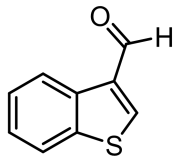
Pyridine-3-carbaldehyde(2v):[1]



Prepared from corresponding aryl iodide for 3 h. Yellow oil. Yield: 69% (52 mg) ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.14 (s, 1H), 9.11 (s, 1H), 8.87 (d, *J* = 4.6 Hz, 1H), 8.20 (dt, *J* = 7.9, 1.9 Hz, 1H), 7.52 (dd, *J* = 7.7, 5.0

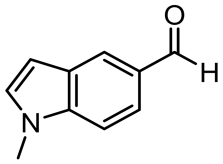
Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.8, 154.7, 152.0, 135.9, 131.4, 124.2. LRMS (ESI): *m/z* calcd for C_6H_5NO [M + H]$^+$, 108.0; found, 108.0.

Benzo[b]thiophene-3-carbaldehyde (2w):[3]



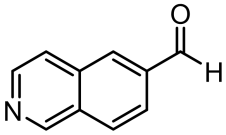
Prepared from corresponding aryl bromide for 30 h. Yellow solid. Yield: 57% (65 mg). M.p 49–50 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 10.13 (s, 1H), 8.68 (d, *J* = 7.7 Hz, 1H), 8.31 (s, 1H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.48 (dt, *J* = 22.8, 7.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 185.5, 143.4, 140.5, 136.5, 135.2, 126.2, 124.9, 122.5. LRMS (ESI): *m/z* calcd for C_9H_6OS [M + H]+, 163.0; found, 162.9.

1-Methyl-1H-indole-5-carbaldehyde (2x):[10]



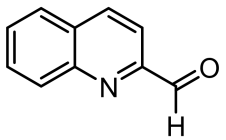
Prepared from corresponding aryl iodide for 6 h. White solid. Yield: 36% (40 mg). M.p 79–81 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 8.15 (s, 1H), 7.80 (d, *J* = 8.6 Hz, 1H), 7.40 (d, *J* = 8.6 Hz, 1H), 7.15 (d, *J* = 3.1 Hz, 1H), 6.65 (d, *J* = 3.0 Hz, 1H), 3.84 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 192.7, 140.1, 130.9, 129.4, 128.3, 126.6, 122.0, 109.9, 103.4, 33.3. LRMS (ESI): *m/z* calcd for $C_{10}H_9NO$ [M + H]$^+$, 160.1; found, 159.9.

Isoquinoline-6-carbaldehyde (2y):[11]



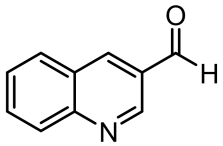
Prepared from corresponding aryl iodide for 3 h. Yellow solid. Yield: 87% (96 mg). M.p 73–75 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.37 (s, 1H), 9.31 (s, 1H), 8.96 (d, *J* = 6.0 Hz, 1H), 8.69 (d, *J* = 6.0 Hz, 1H), 8.20 (t, *J* = 8.2 Hz, 2H), 7.75 (dd, *J* = 8.0, 7.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.7, 153.0, 146.4, 140.0, 134.9, 133.4, 130.7, 128.8, 126.7, 117.9. LRMS (ESI): *m/z* calcd for $C_{10}H_7NO$ [M + H]$^+$, 158.1; found, 158.0.

Quinoline-2-carbaldehyde (2z):[1]



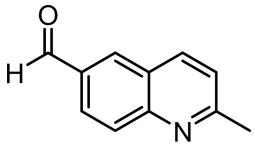
Prepared from corresponding aryl bromide for 30 h. Yellow solid. Yield: 68% (75 mg). M.p 69–71 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.23 (s, 1H), 8.31 (d, *J* = 8.4 Hz, 1H), 8.25 (d, *J* = 8.5 Hz, 1H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.2 Hz, 1H), 7.83 (dd, *J* = 8.3, 7.1 Hz, 1H), 7.69 (t, *J* = 7.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.9, 152.7, 148.0, 137.5, 130.6, 130.5, 130.2, 129.3, 128.0, 117.5. LRMS (ESI): *m/z* calcd for $C_{10}H_7NO$ [M + H]$^+$, 158.1; found, 158.0.

Quinoline-3-carbaldehyde (2aa):[1]



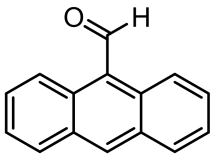
Prepared from corresponding aryl bromide for 30 h. Yellow solid. Yield: 76% (84 mg). M.p 70–72 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.22 (s, 1H), 9.34 (s, 1H), 8.60 (s, 1H), 8.16 (d, *J* = 8.5 Hz, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.86 (dd, *J* = 8.4, 7.0 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.8, 150.6, 149.2, 140.3, 132.8, 129.8, 129.5, 128.6, 128.0, 127.1. LRMS (ESI): *m/z* calcd for $C_{10}H_7NO$ [M + H]$^+$, 158.1; found, 158.0.

2-Methylquinoline-6-carbaldehyde (2bb):[13]



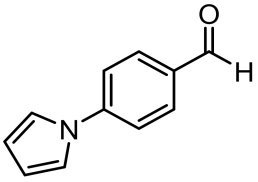
Prepared from corresponding aryl bromide for 30 h. White solid. Yield: 87% (104 mg). M.p 73–75 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.10 (s, 1H), 8.23 (s, 1H), 8.12 (m, 2H), 8.04 (d, *J* = 8.7 Hz, 1H), 7.34 (d, *J* = 8.4 Hz, 1H), 2.74 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.5, 162.4, 150.6, 137.4, 133.7, 133.4, 129.9, 126.9, 125.9, 123.2, 25.72. LRMS (ESI): *m/z* calcd for $C_{11}H_9NO$ [M + H]$^+$, 172.1; found, 172.0.

Anthracene-9-carbaldehyde (2cc):[14]



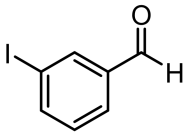
Prepared from corresponding aryl bromide for 30 h. Yellow solid. Yield: 56% (81 mg). M.p 113–114 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.36 (s, 1H), 8.85 (d, *J* = 9.0 Hz, 2H), 8.47 (s, 1H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.58 (t, *J* = 7.8 Hz, 2H), 7.45 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.9, 135.2, 132.0, 130.9, 129.3, 129.0, 125.6, 124.5,123.5. LRMS (ESI): *m/z* calcd for $C_{11}H_9NO$ [M + H]$^+$, 207.1; found, 206.9.

4-(1H-pyrrol-1-yl)benzaldehyde (2dd):[15]



Prepared from corresponding aryl iodide for 6 h. Brown solid. Yield: 92% (110 mg). M.p 92–94 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.98 (s, 1H), 7.94 (d, *J* = 8.4 Hz, 2H), 7.53 (d, *J* = 8.4 Hz, 2H), 7.19 (s, 2H), 6.41 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.9, 145.0, 133.3, 131.5, 119.7, 119.1, 112.0. LRMS (ESI): *m/z* calcd for $C_{11}H_9NO$ [M + H]$^+$, 172.1; found, 172.1.

3-Iodobenzaldehyde (2ee):[16]



Prepared from 1,3-diiodobenzene for 12 h. Yellow solid. Yield: 45% (73 mg). M.p 58–59 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.92 (s, 1H), 8.21 (s, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.33 – 7.18 (m, 1H), 7.35 – 7.26 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 190.8, 143.3, 138.6, 138.1, 130.8, 129.0, 94.8.

LRMS (ESI): *m/z* calcd for C_7H_5IO $[M + H]^+$, 232.9; found, 233.0.

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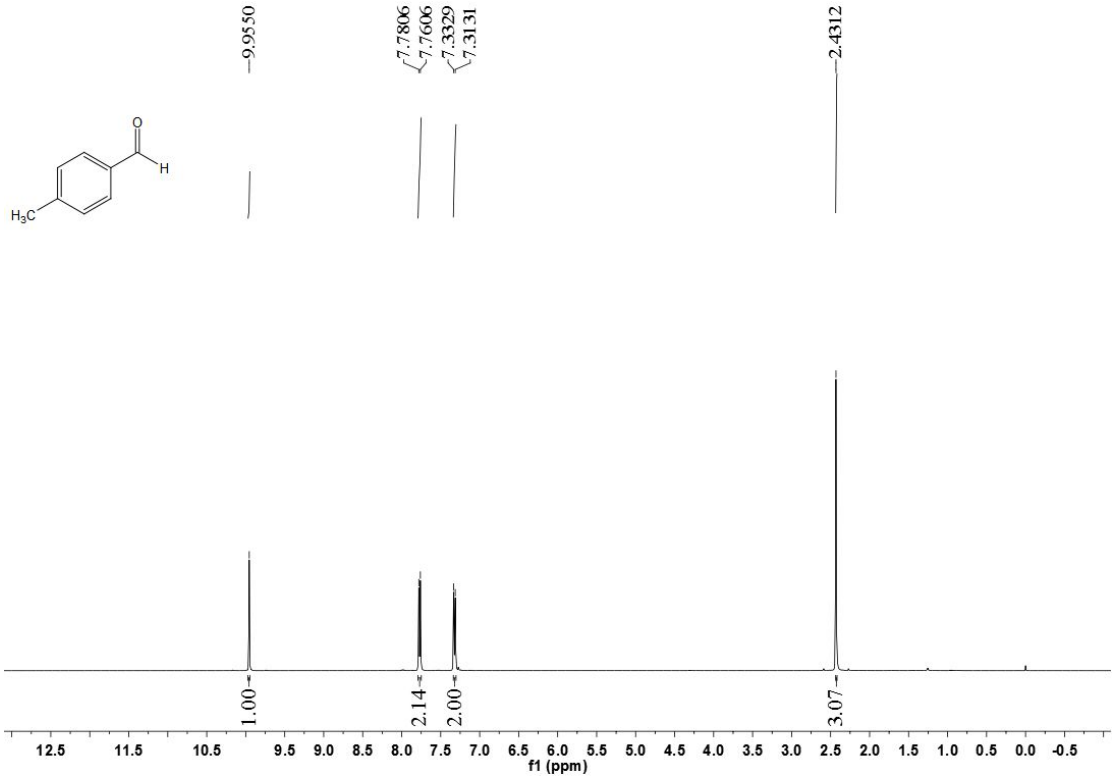
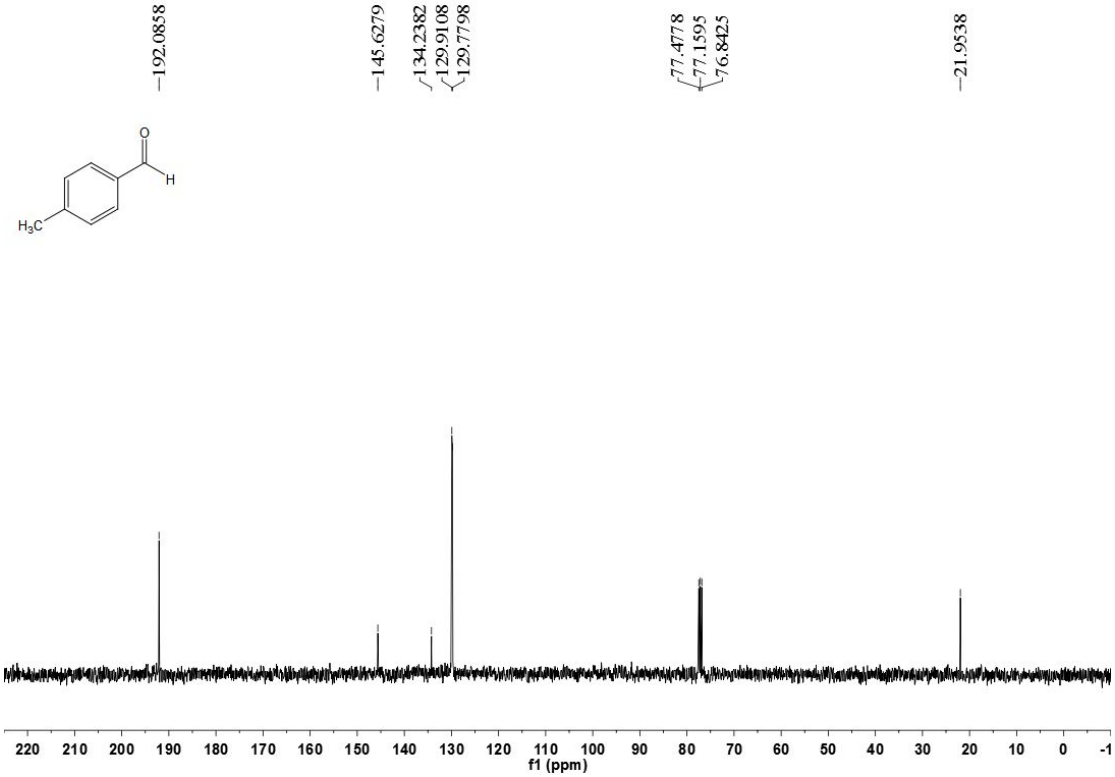
Spectra data for NMR of aldehydes

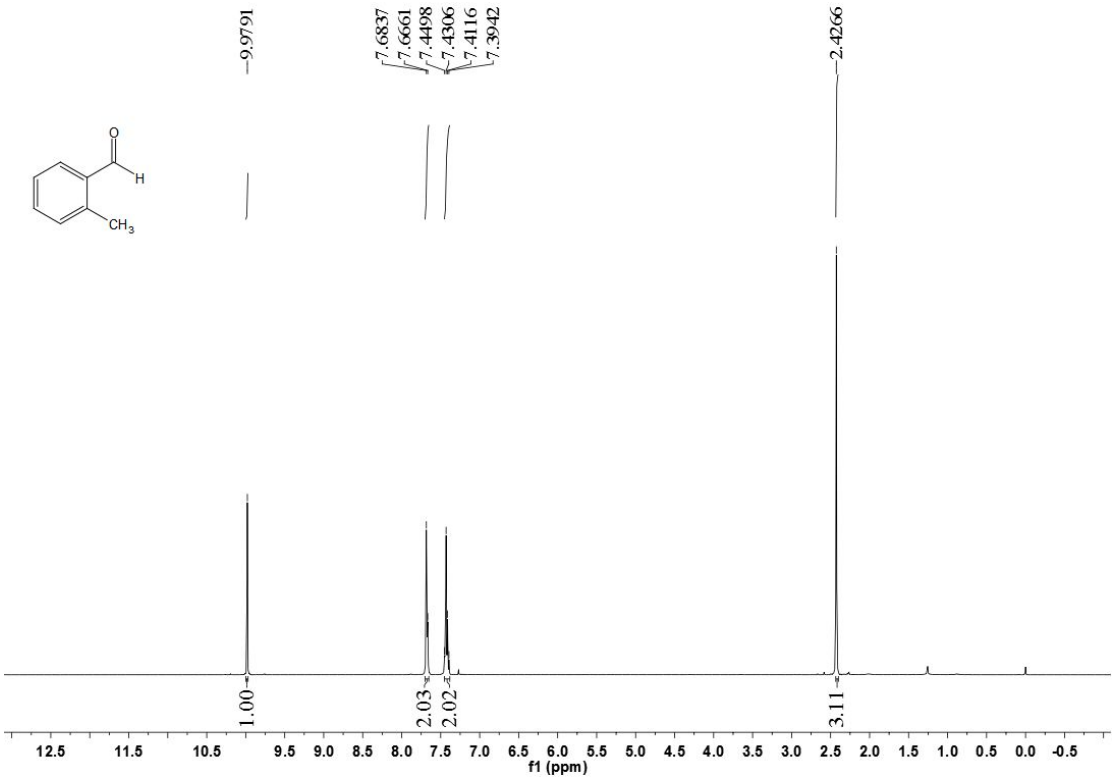
^{1}H NMR spectrum of compound **2a**



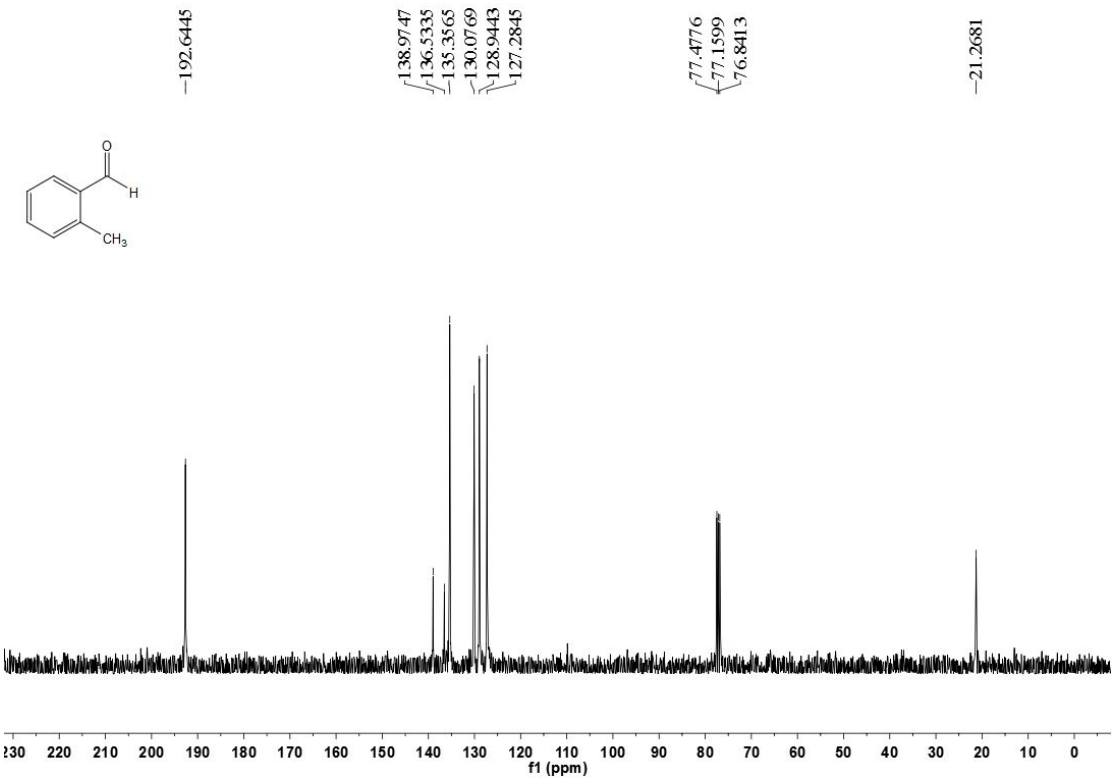
^{13}C NMR spectrum of compound **2a**



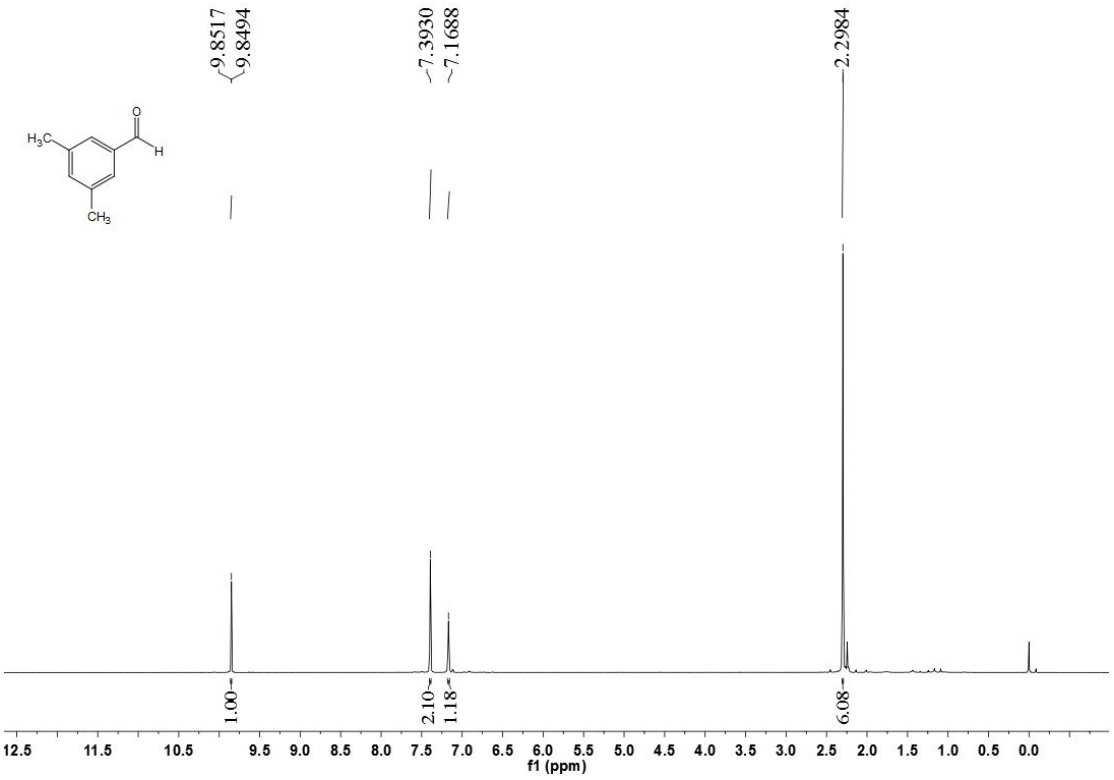
^{1}H NMR spectrum of compound **2b**



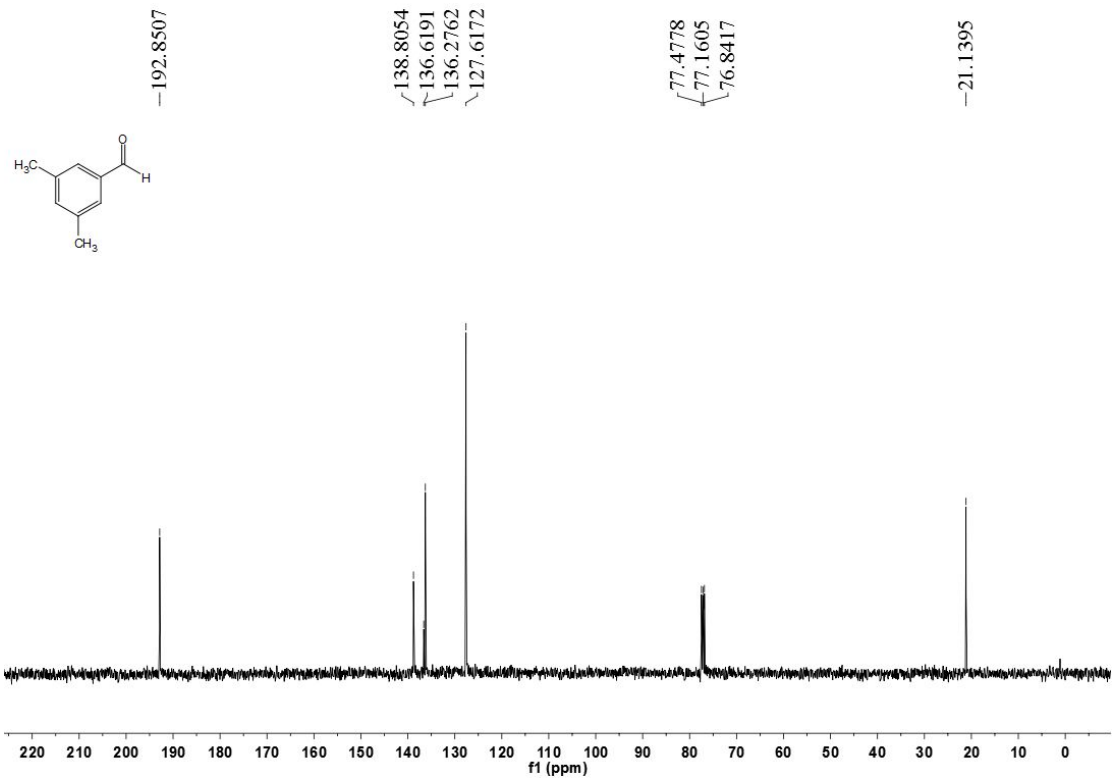
^{13}C NMR spectrum of compound **2b**



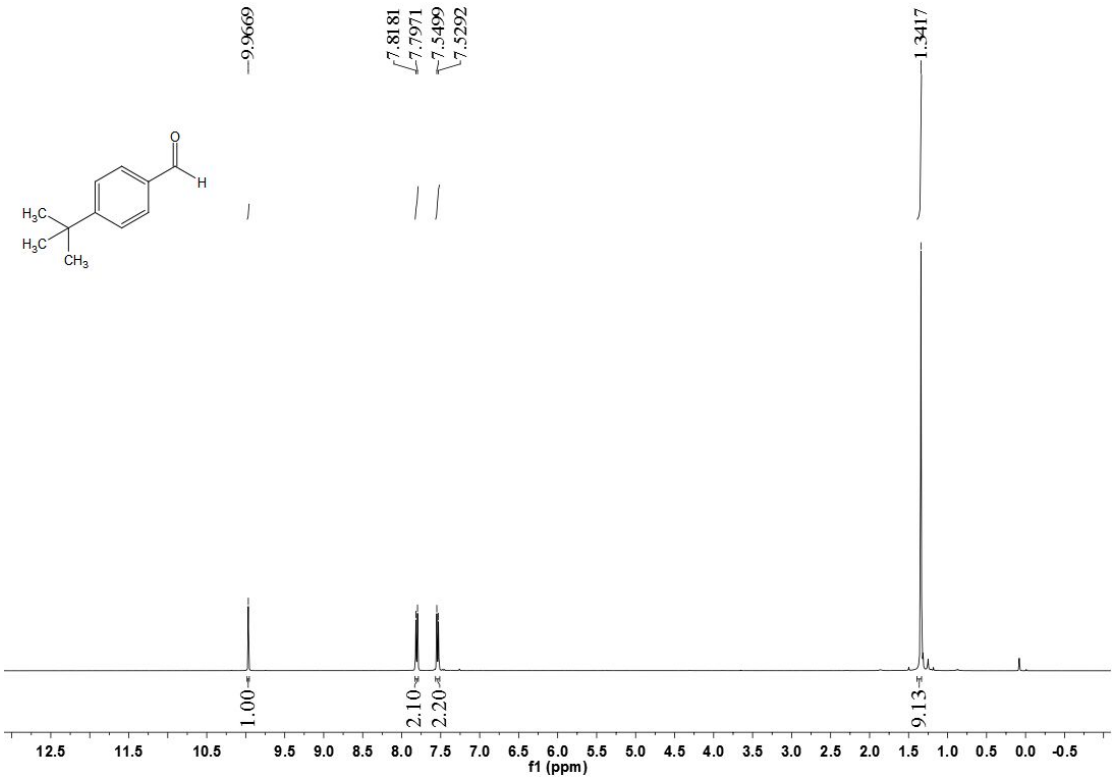
^{1}H NMR spectrum of compound **2c**



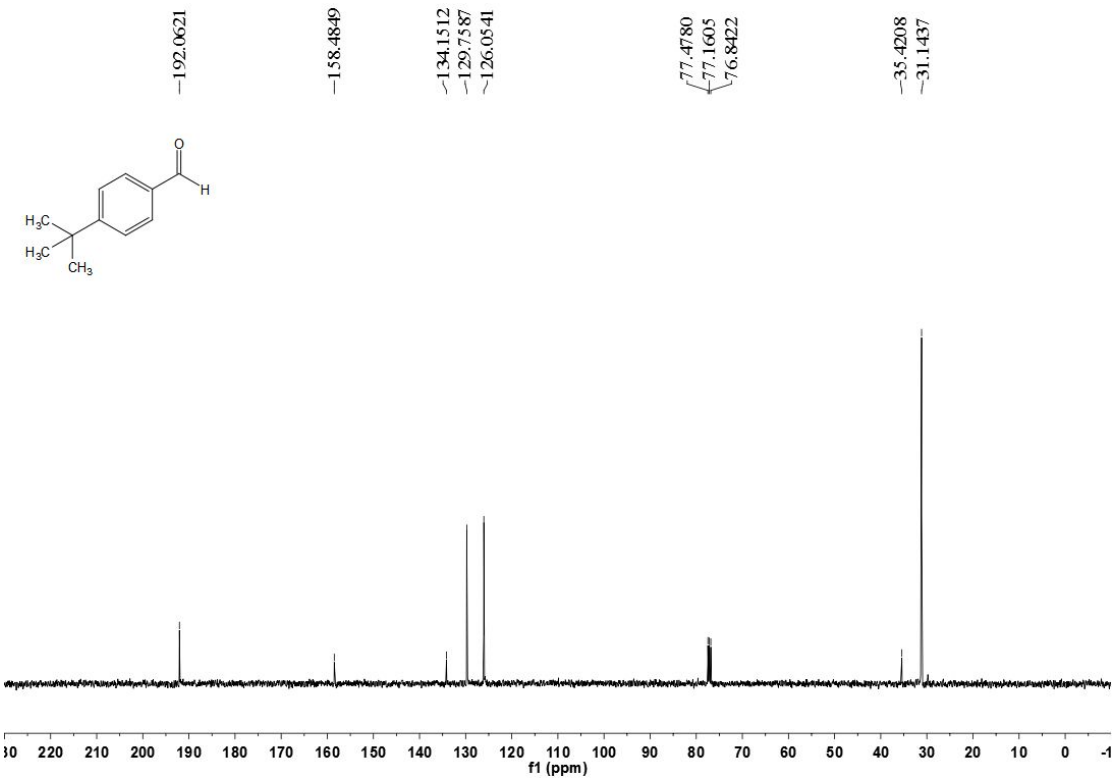
^{13}C NMR spectrum of compound **2c**



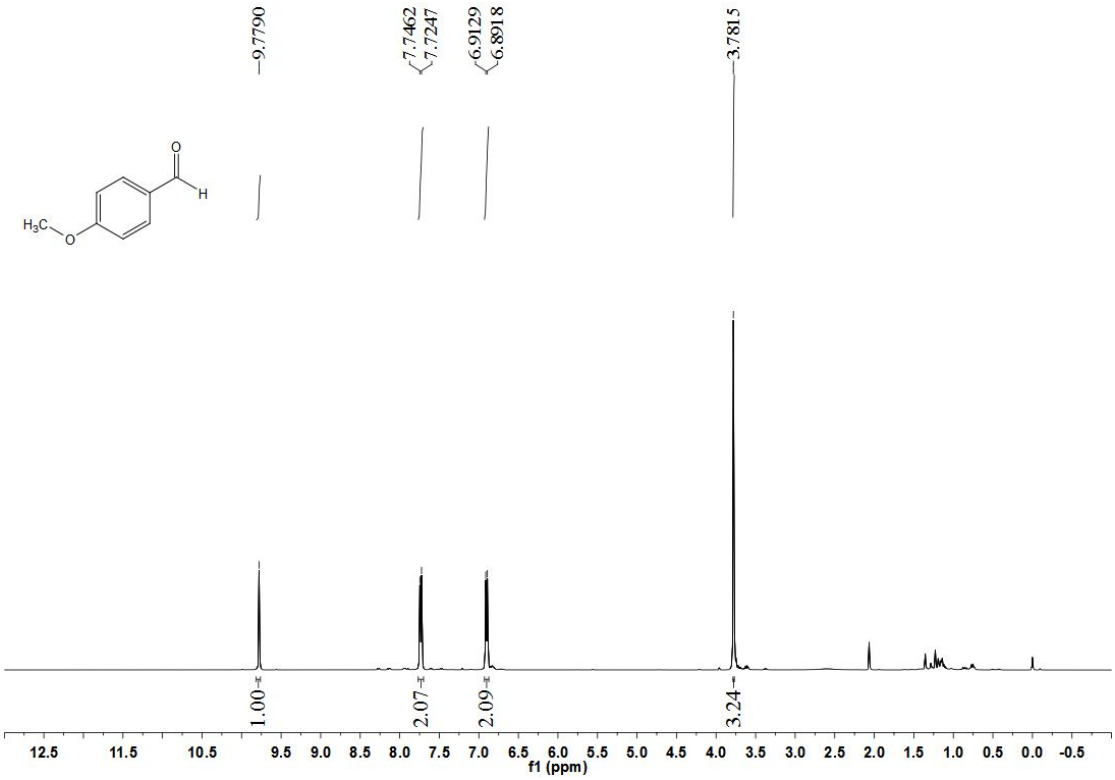
^{1}H NMR spectrum of compound **2d**



^{13}C NMR spectrum of compound **2d**



^{1}H NMR spectrum of compound **2e**



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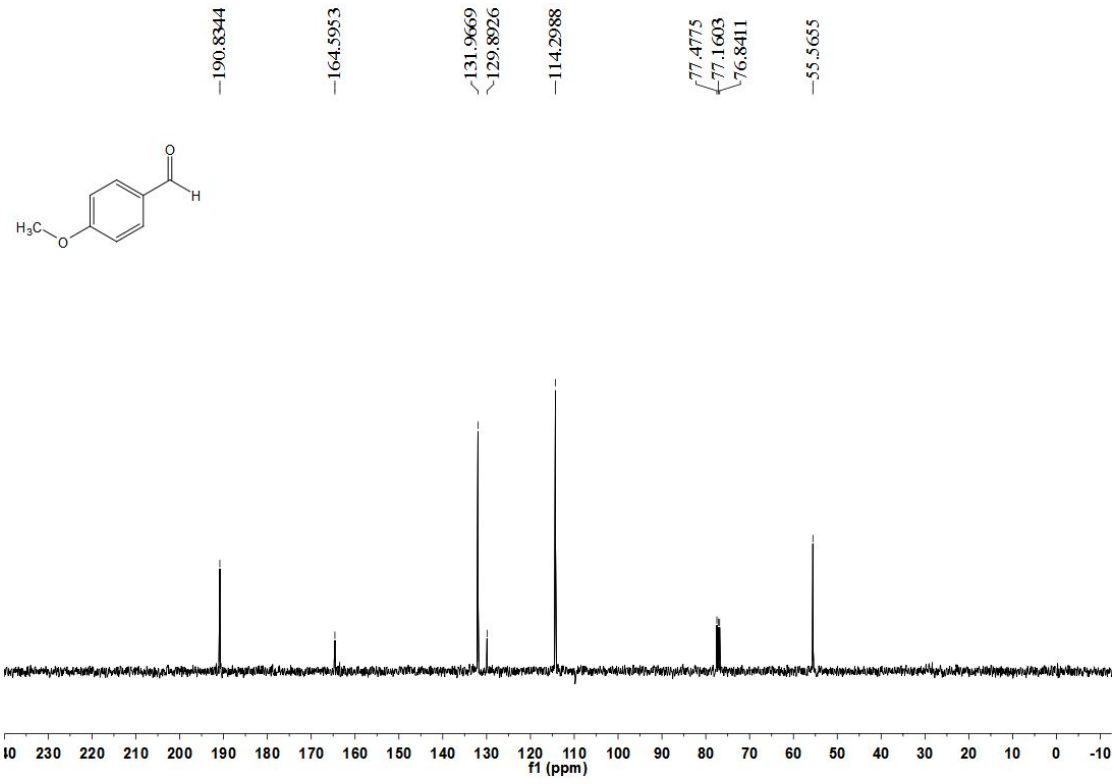
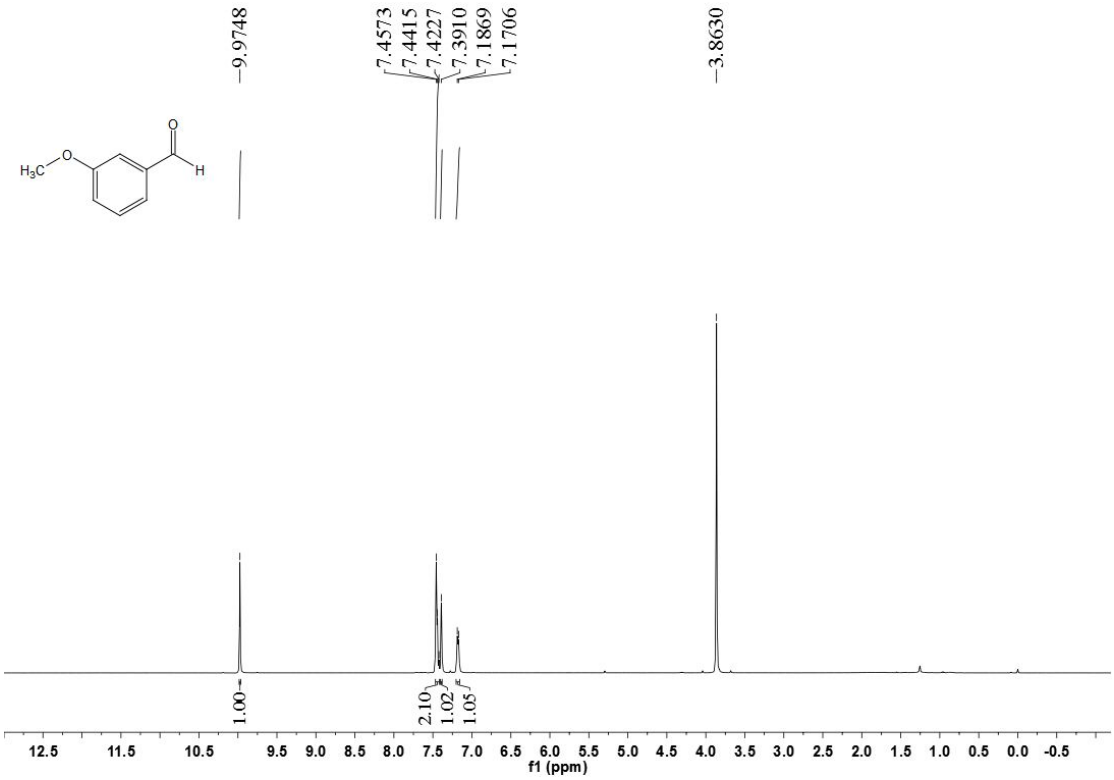
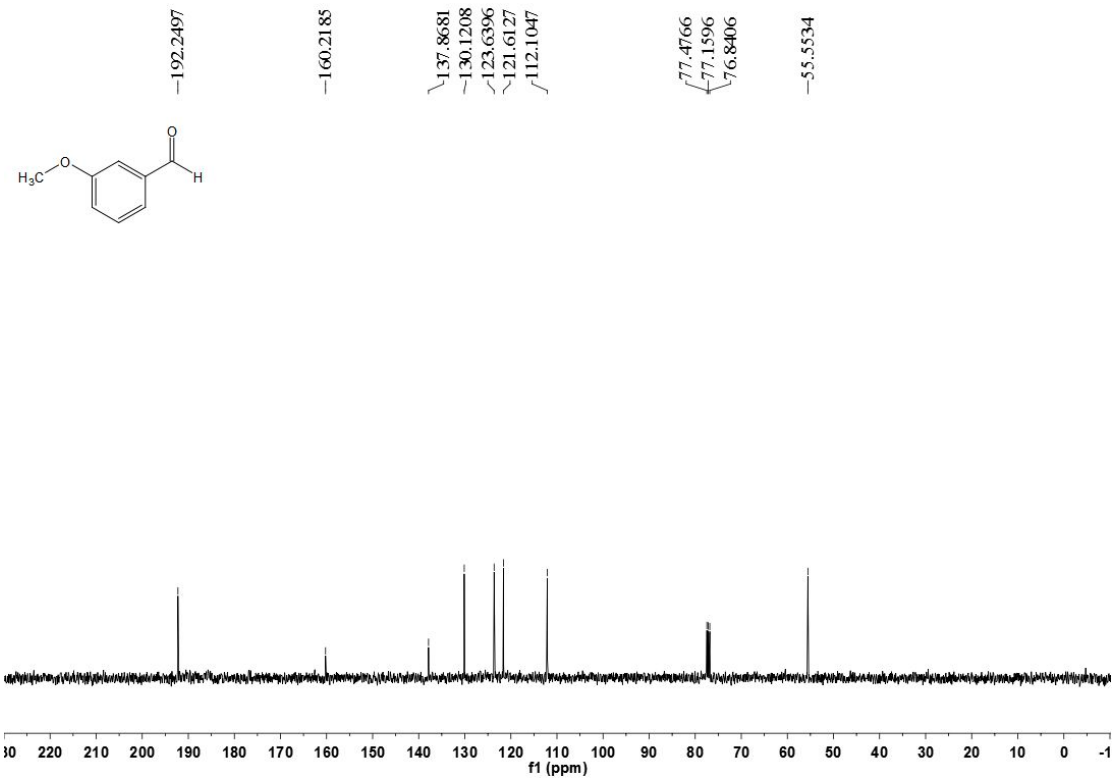


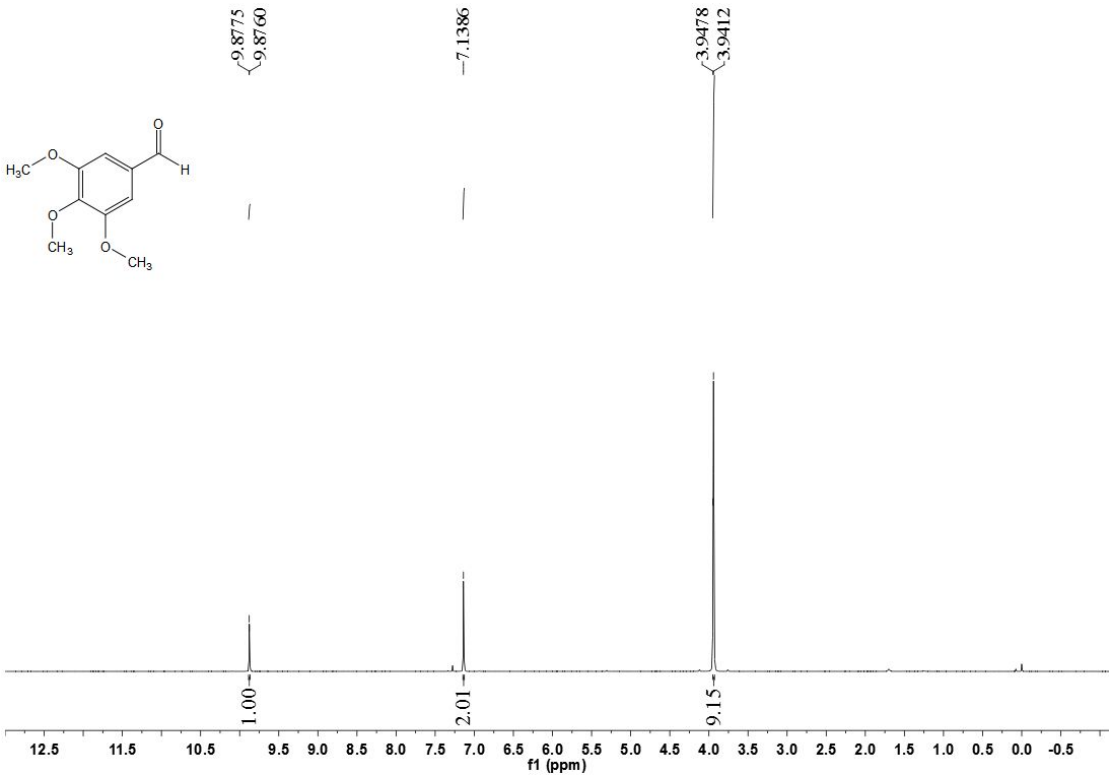
^{1}H NMR spectrum of compound **2f**



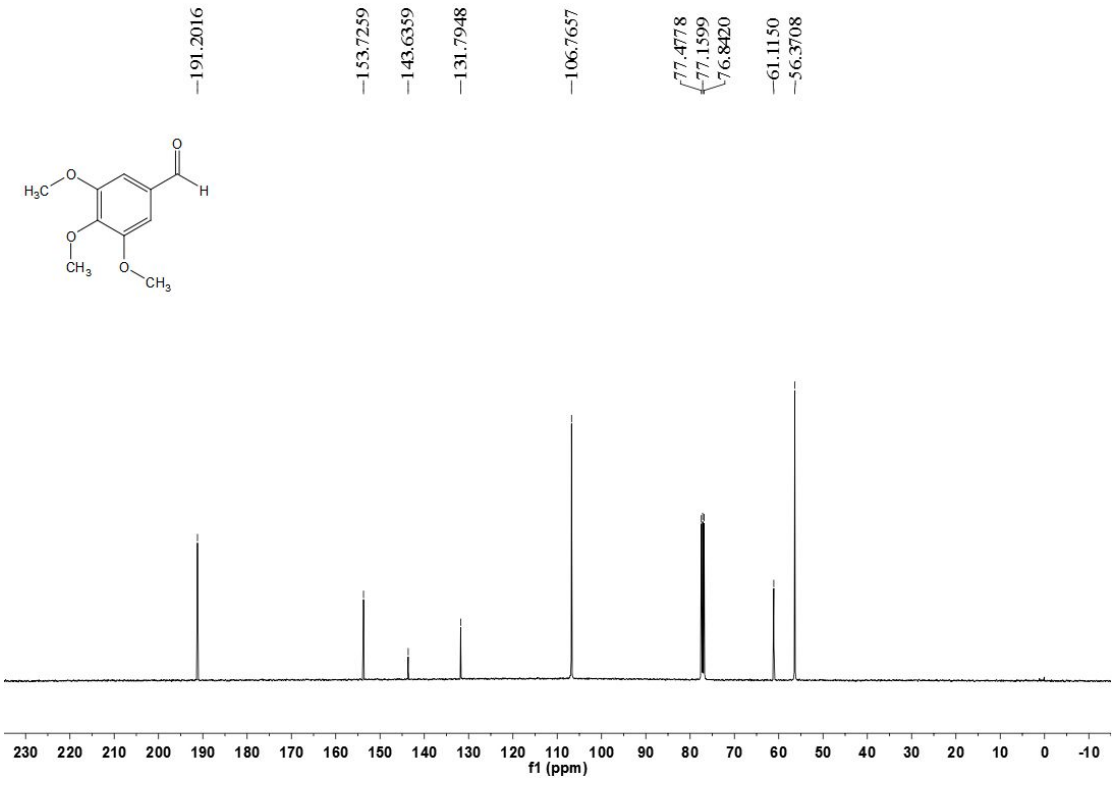
^{13}C NMR spectrum of compound **2f**



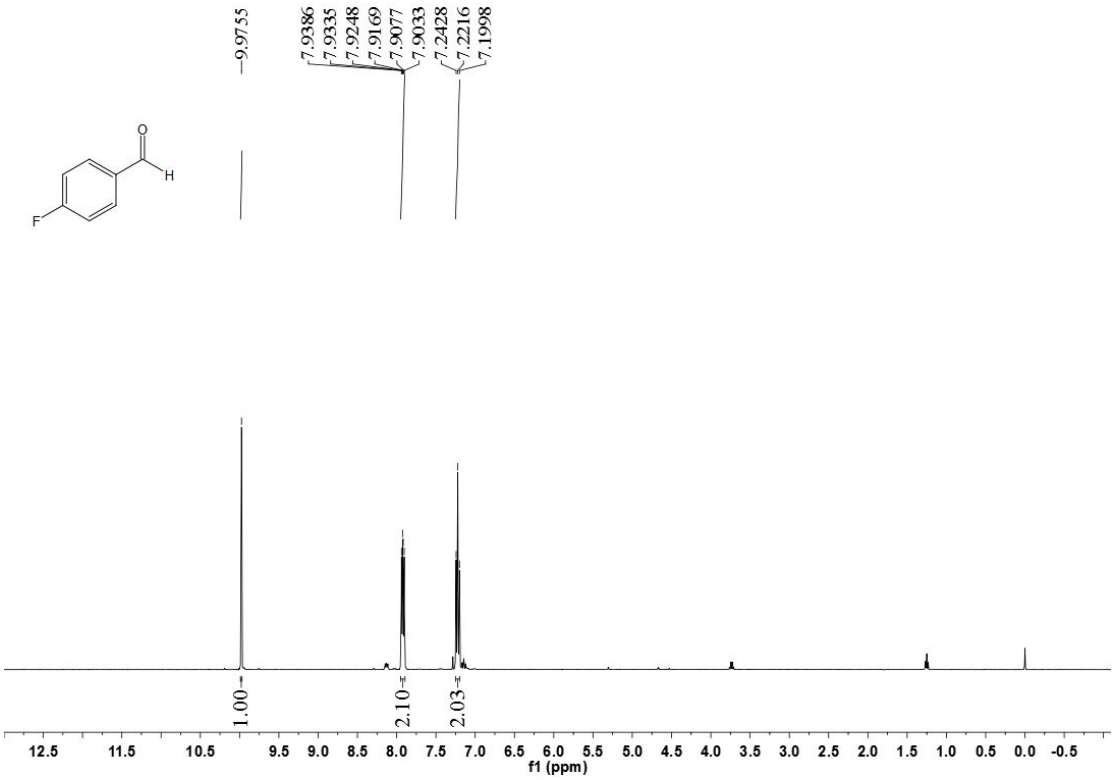
^{1}H NMR spectrum of compound **2g**



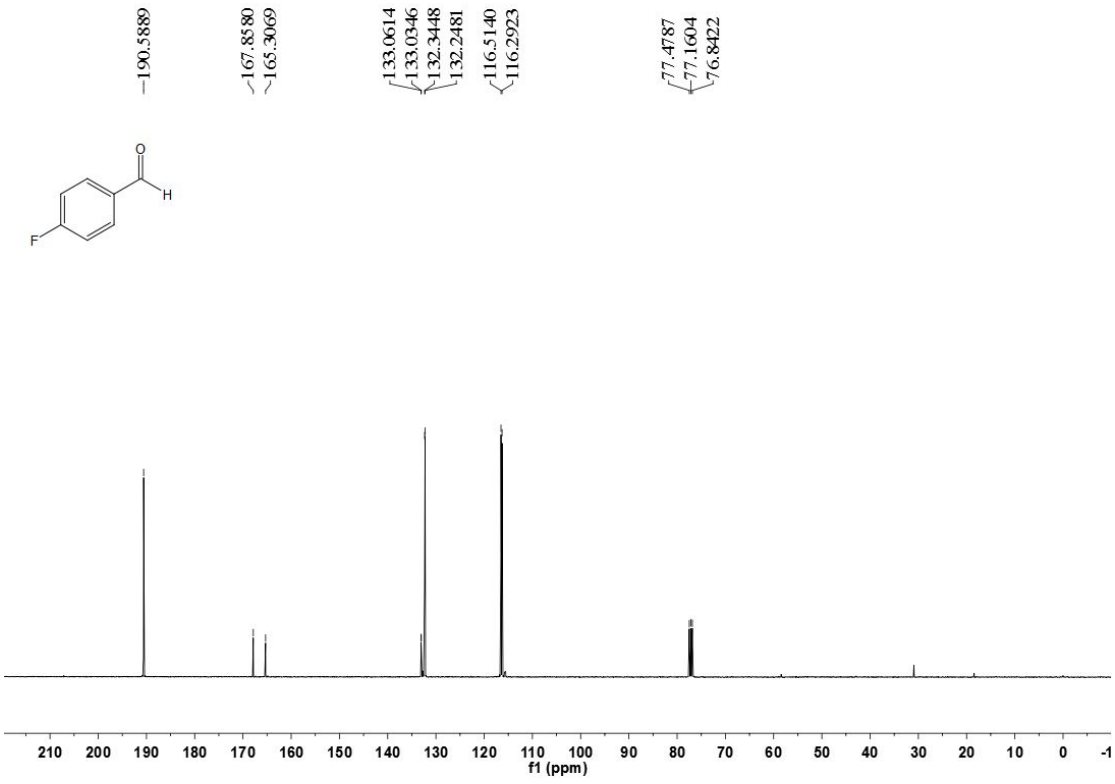
^{13}C NMR spectrum of compound **2g**



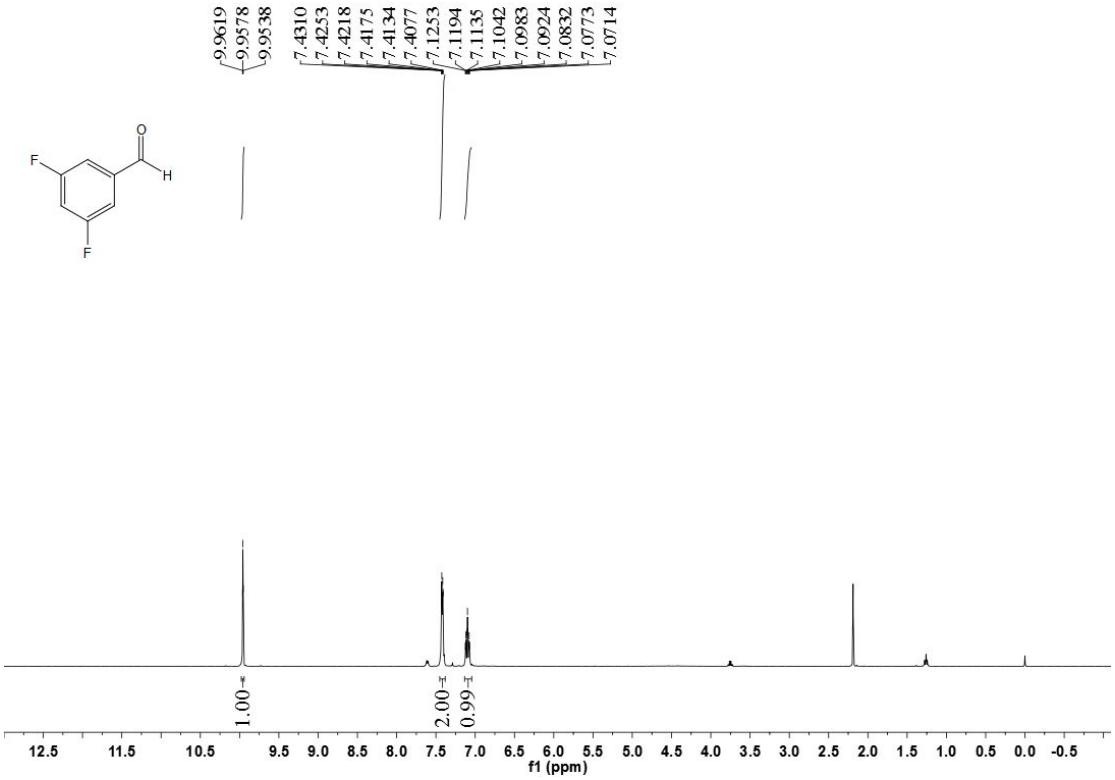
^{1}H NMR spectrum of compound **2h**



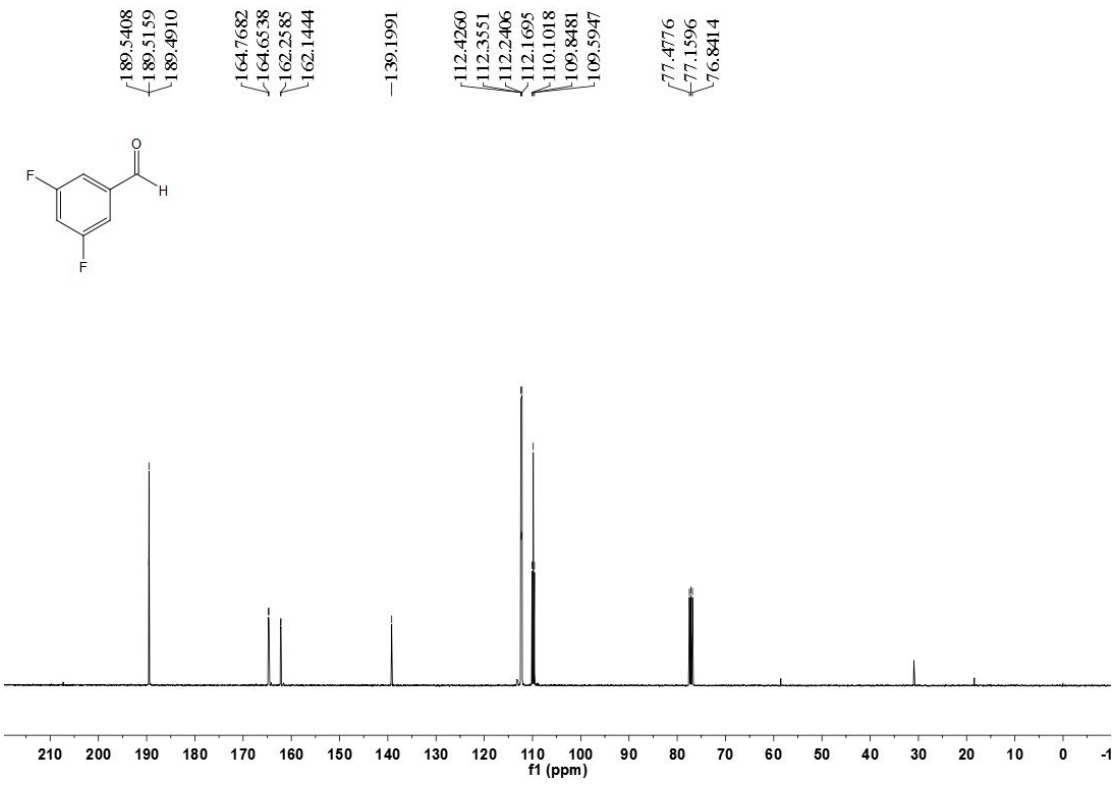
^{13}C NMR spectrum of compound **2h**



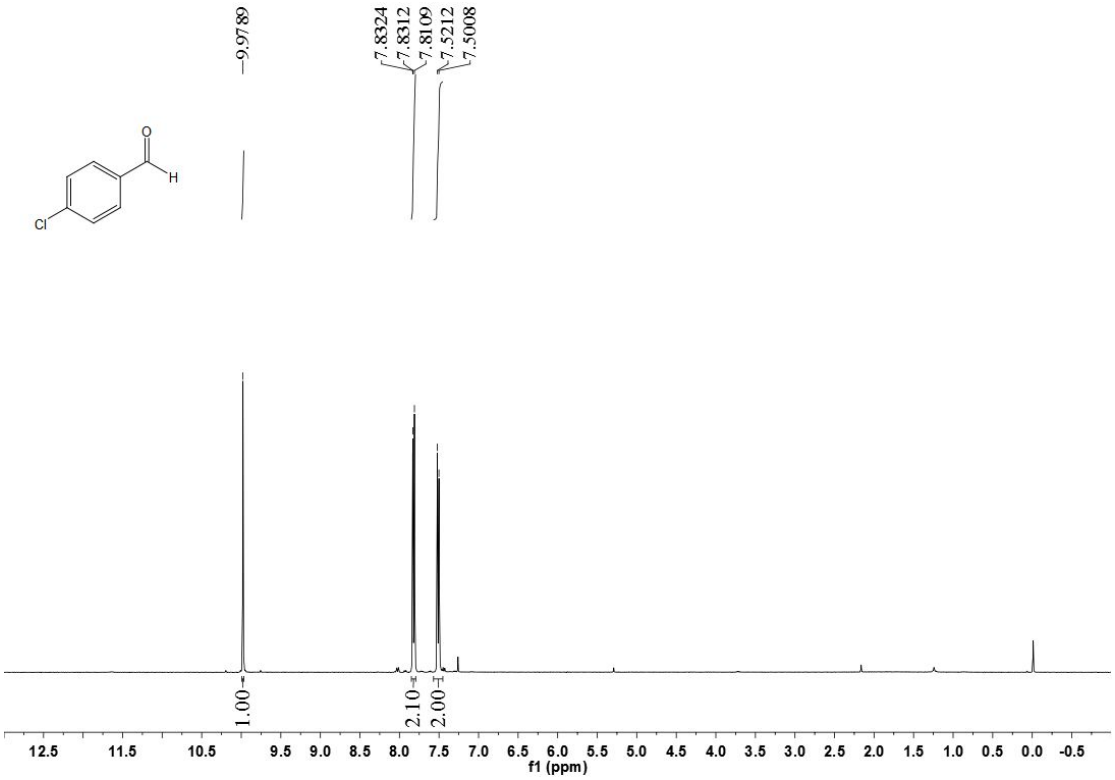
^{1}H NMR spectrum of compound **2i**



^{13}C NMR spectrum of compound **2i**



^{1}H NMR spectrum of compound **2j**



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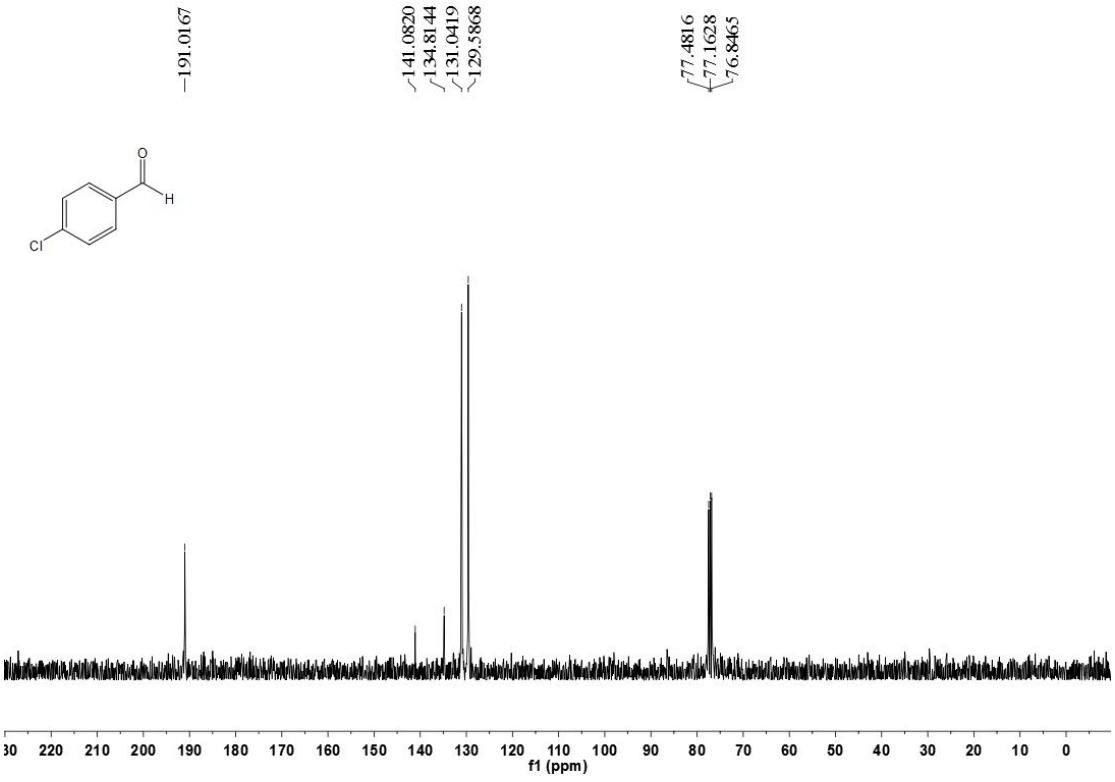
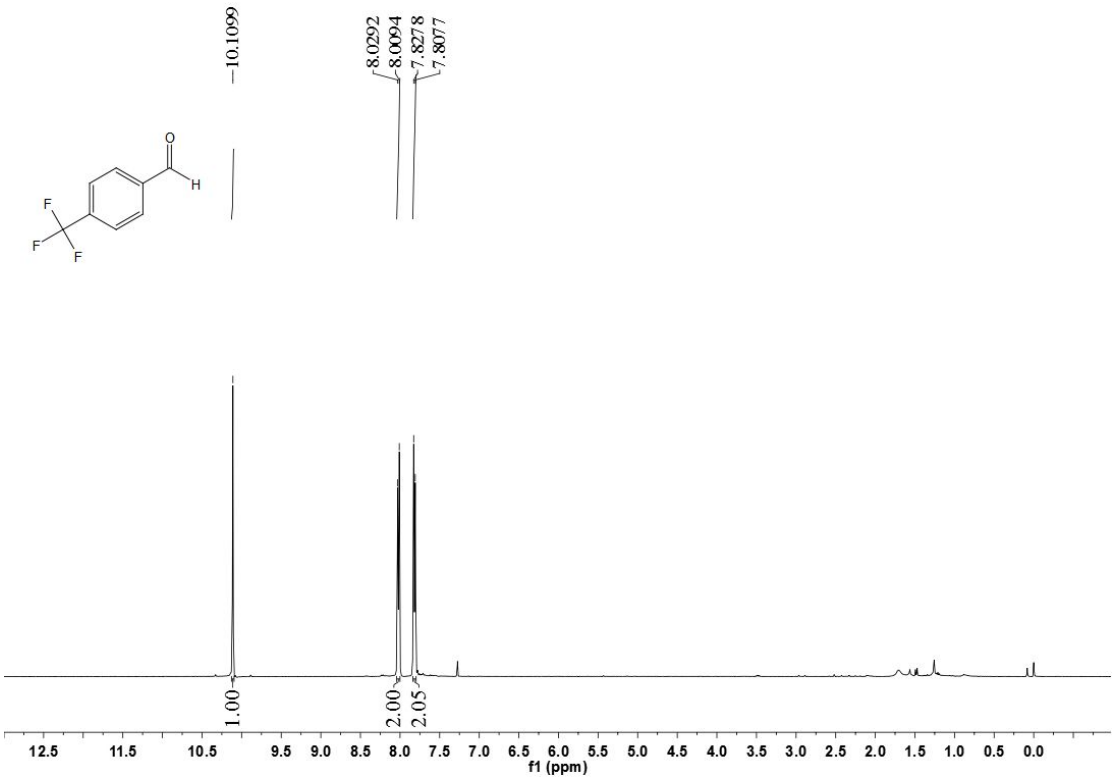
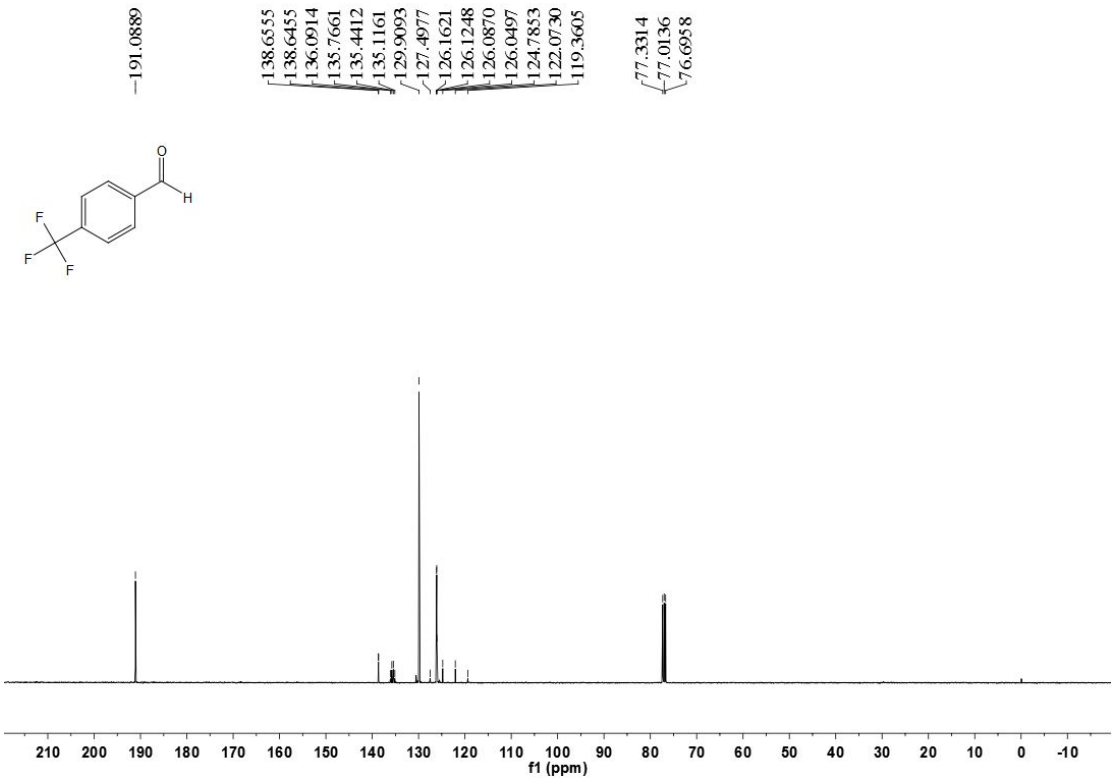


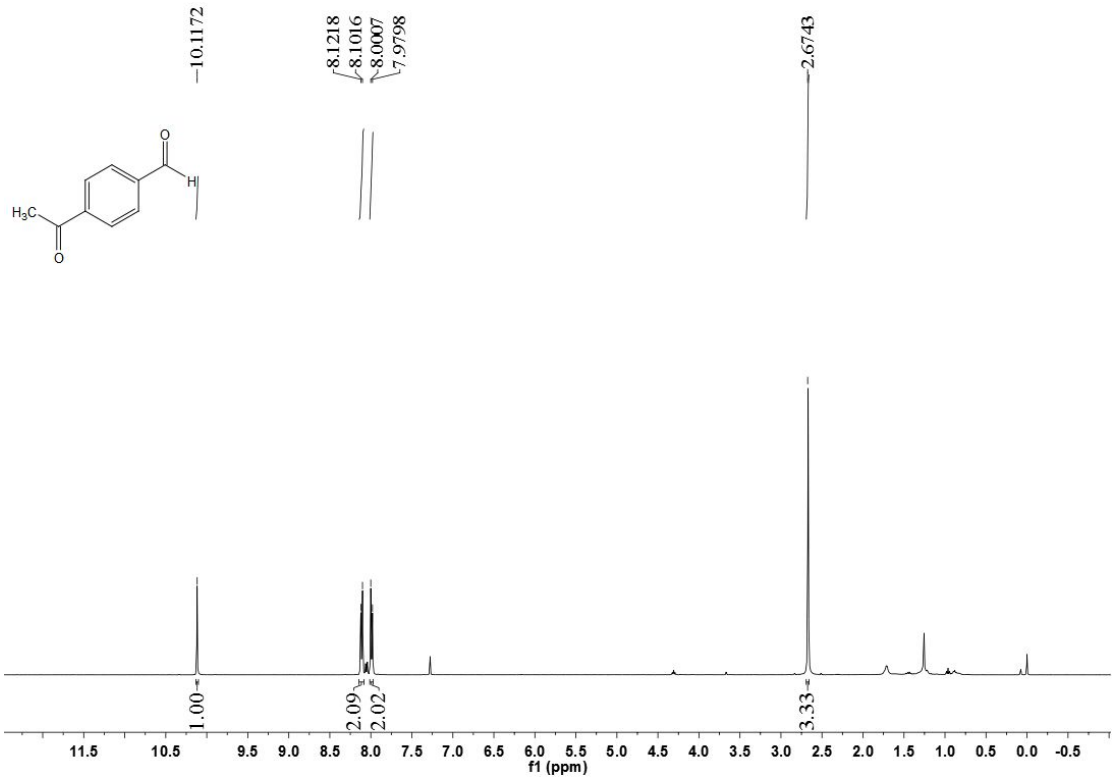
^{1}H NMR spectrum of compound **2k**



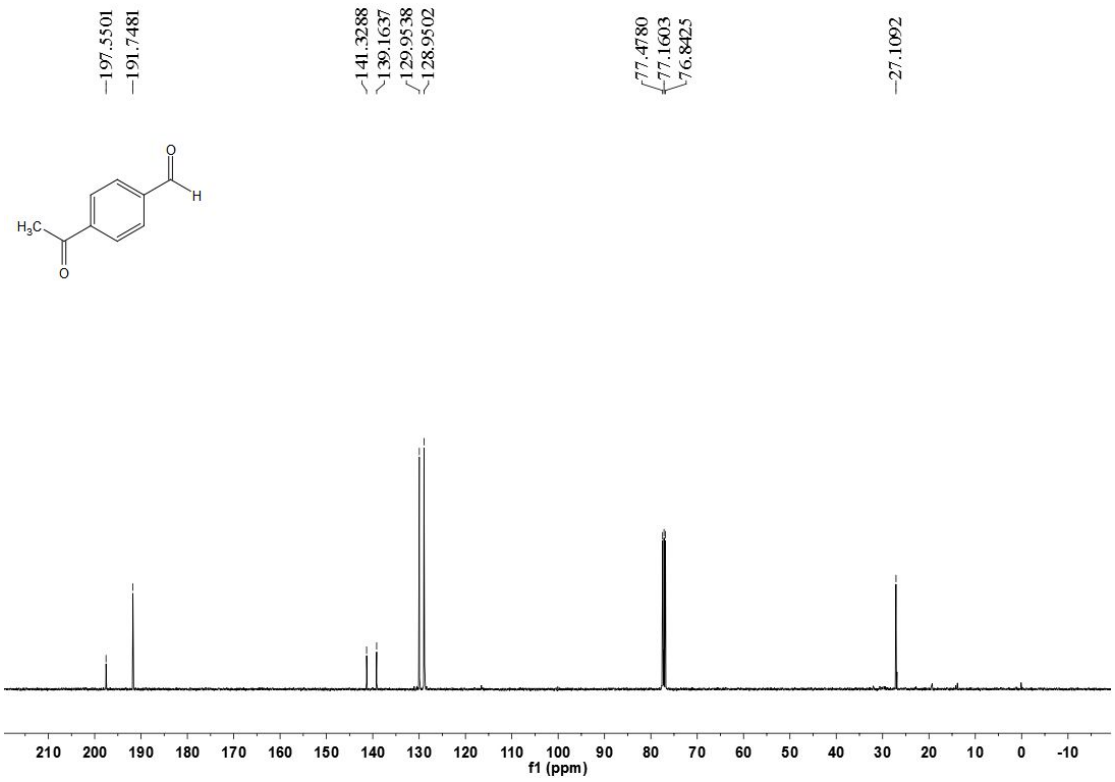
^{13}C NMR spectrum of compound **2k**



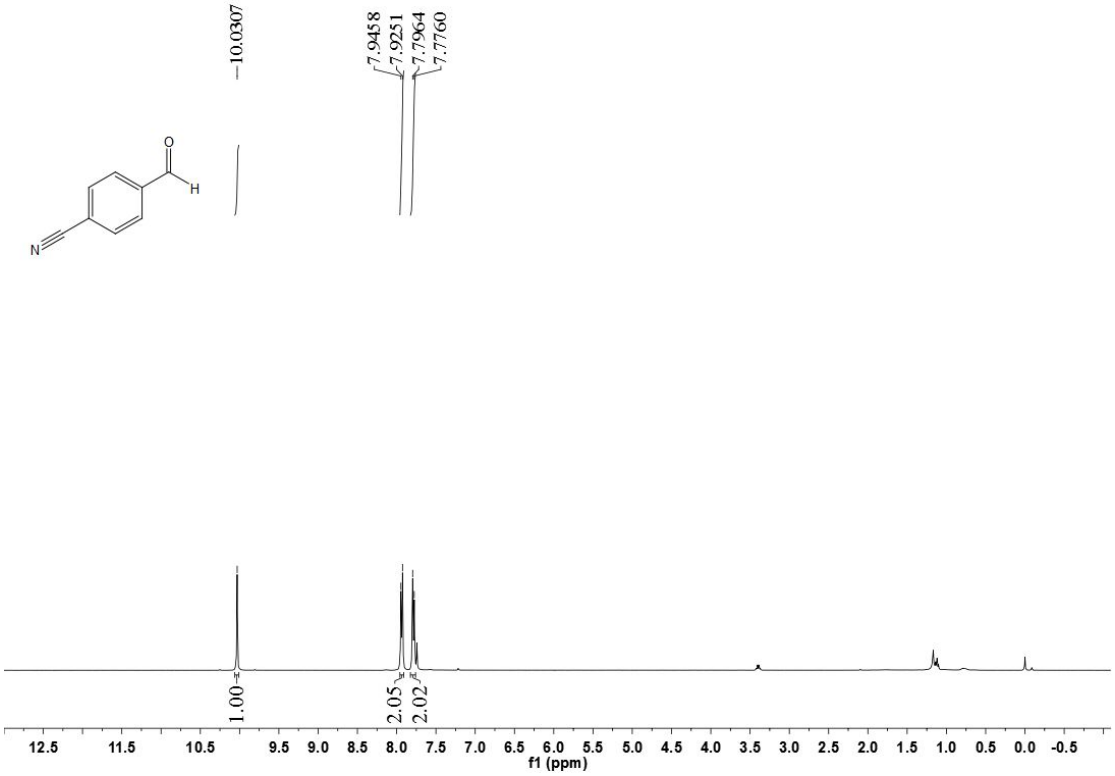
^{1}H NMR spectrum of compound **2l**



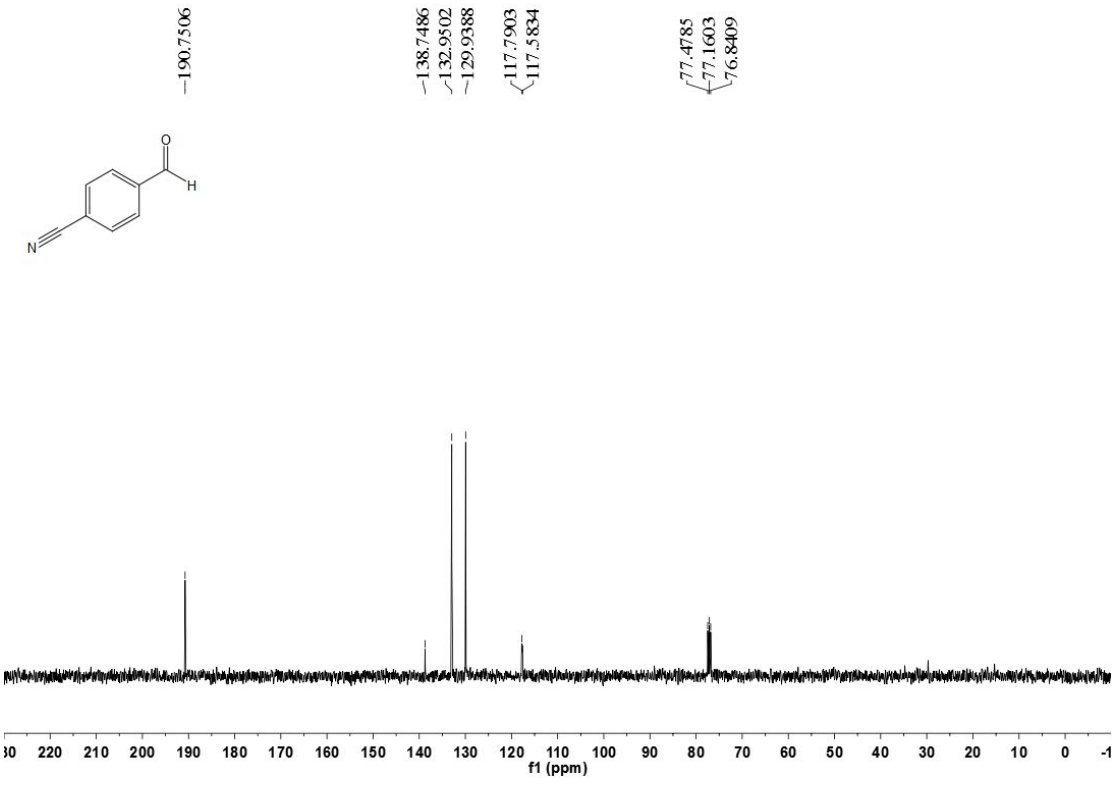
^{13}C NMR spectrum of compound **2l**



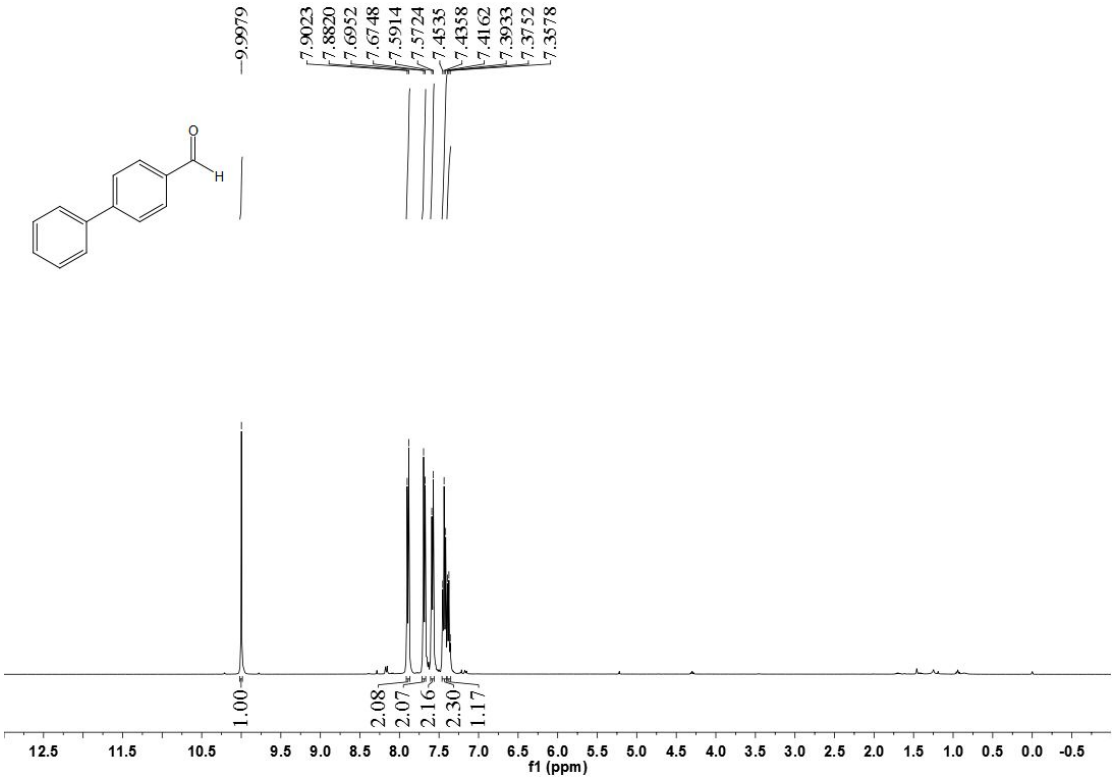
^{1}H NMR spectrum of compound **2m**



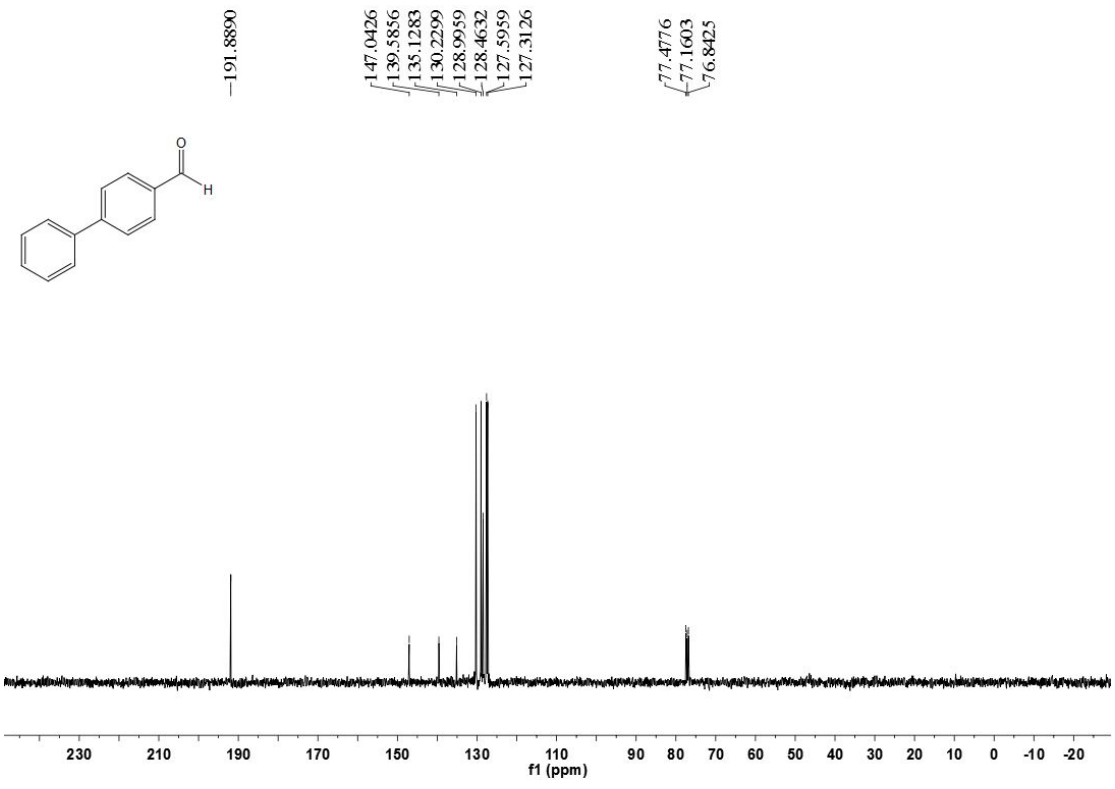
^{13}C NMR spectrum of compound **2m**



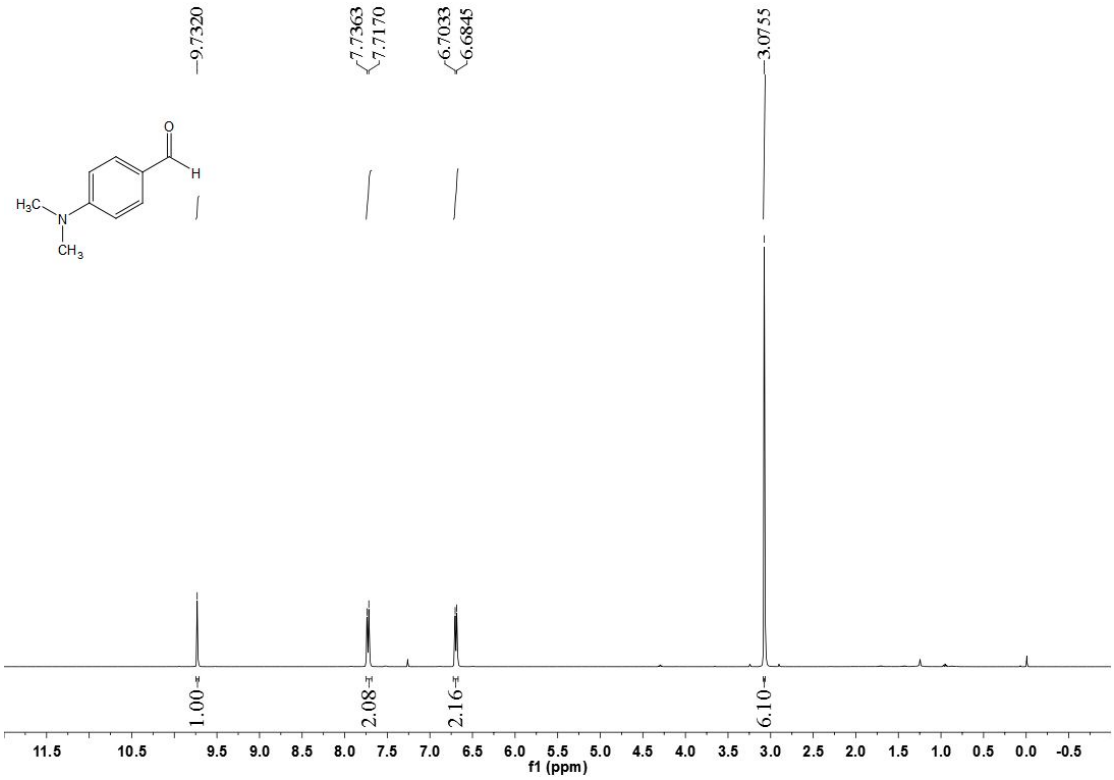
^{1}H NMR spectrum of compound **2n**



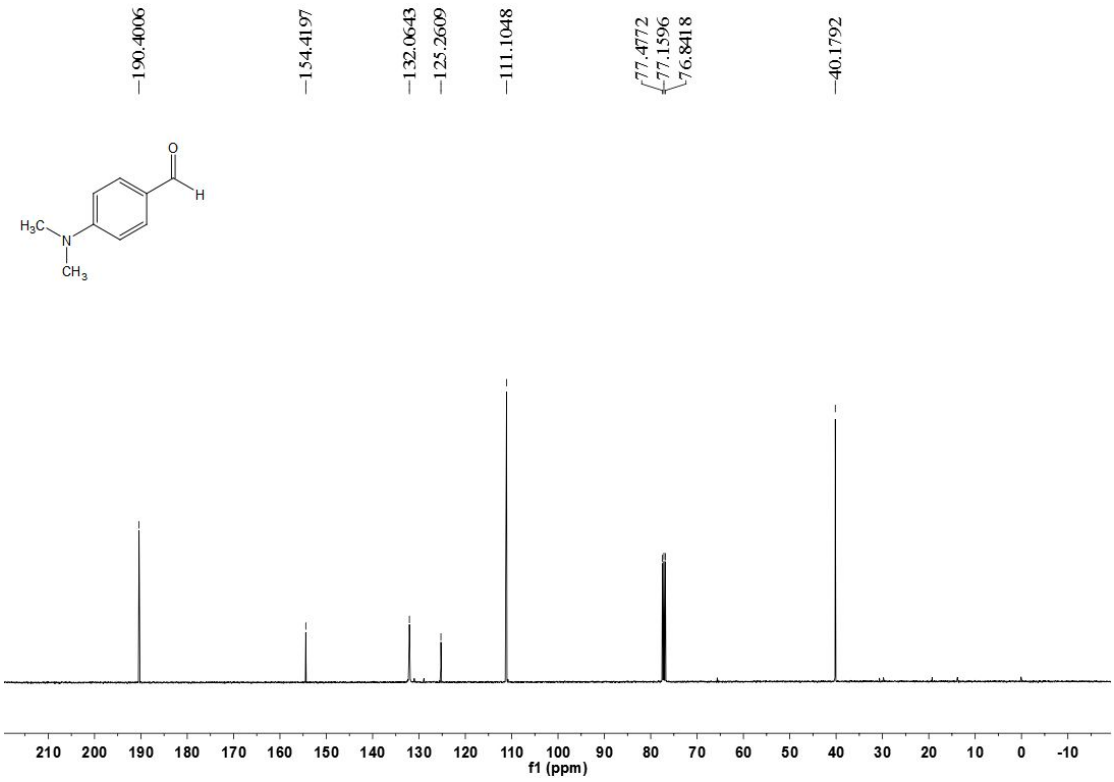
^{13}C NMR spectrum of compound **2n**



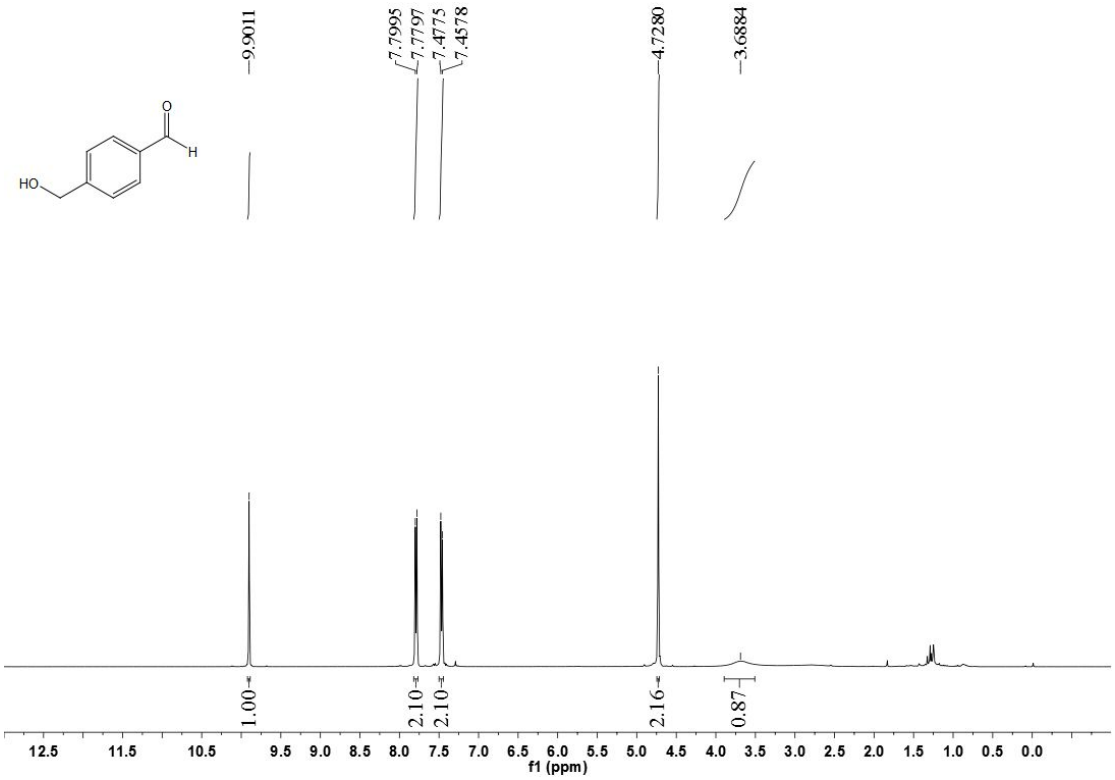
^{1}H NMR spectrum of compound **2o**



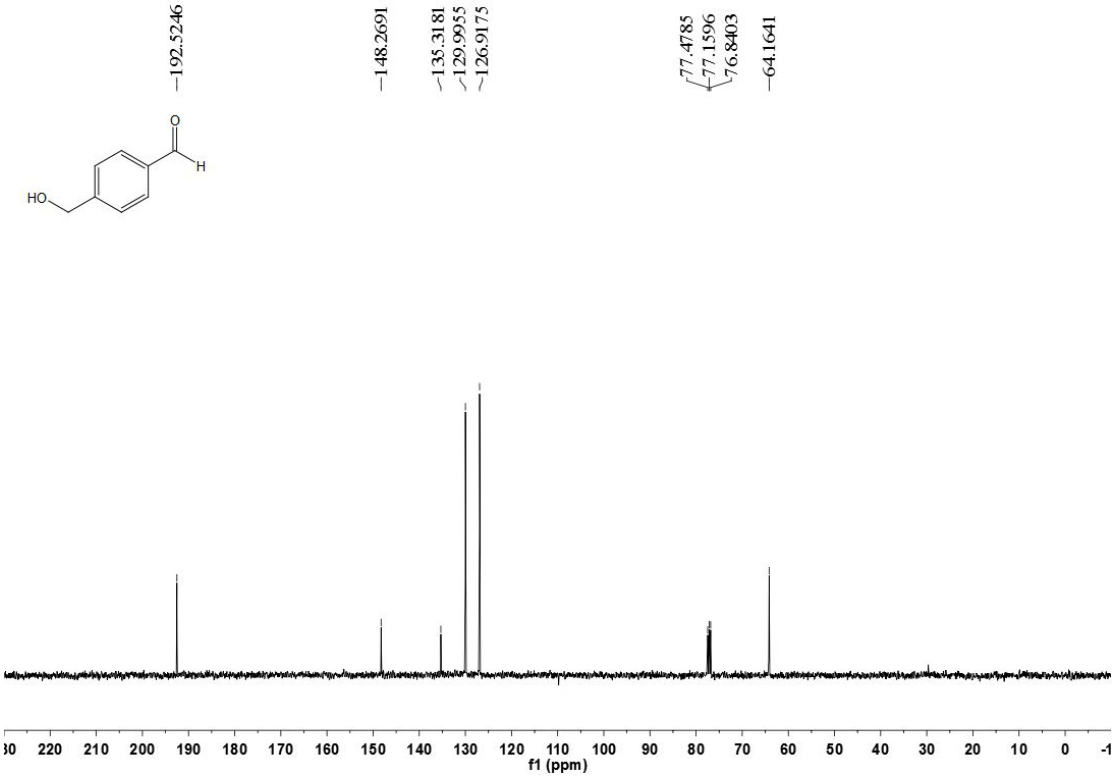
^{13}C NMR spectrum of compound **2o**



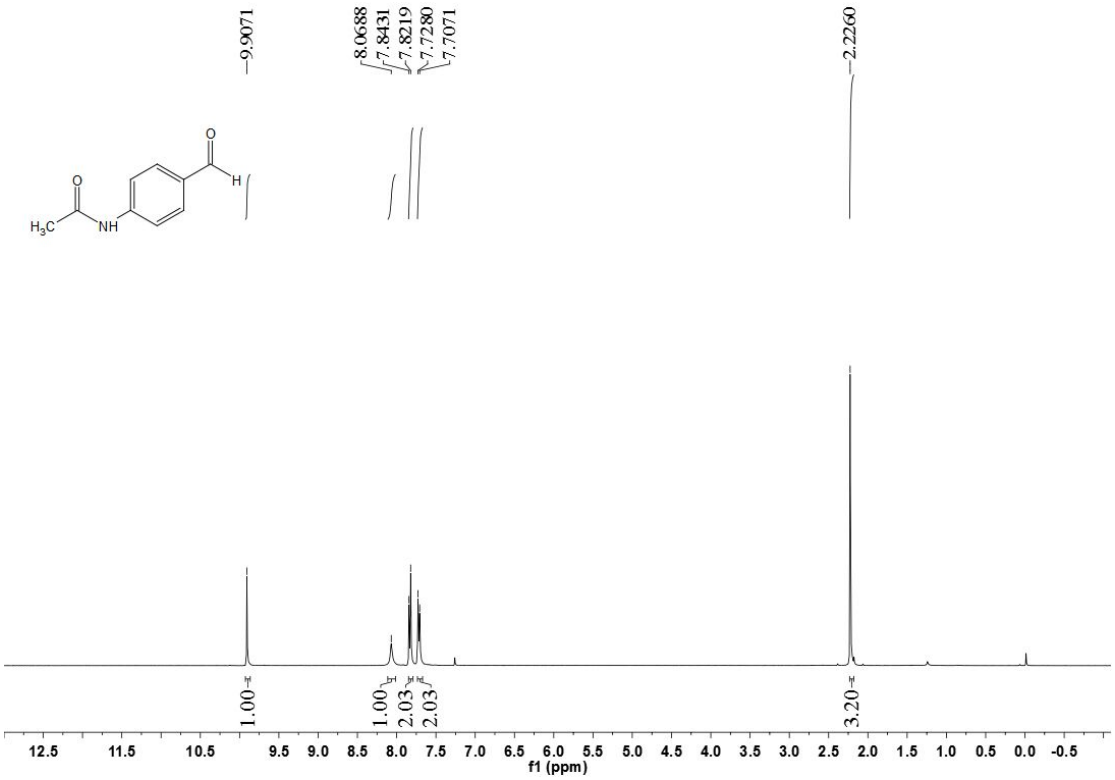
^{1}H NMR spectrum of compound **2p**



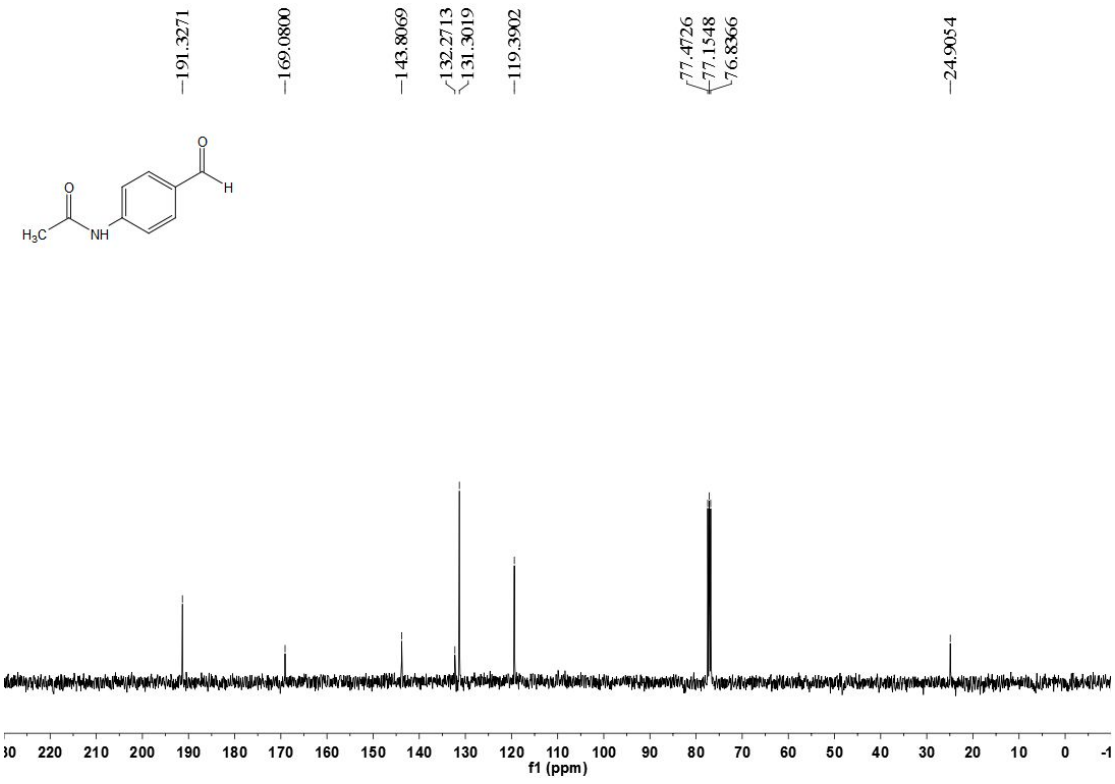
^{13}C NMR spectrum of compound **2p**



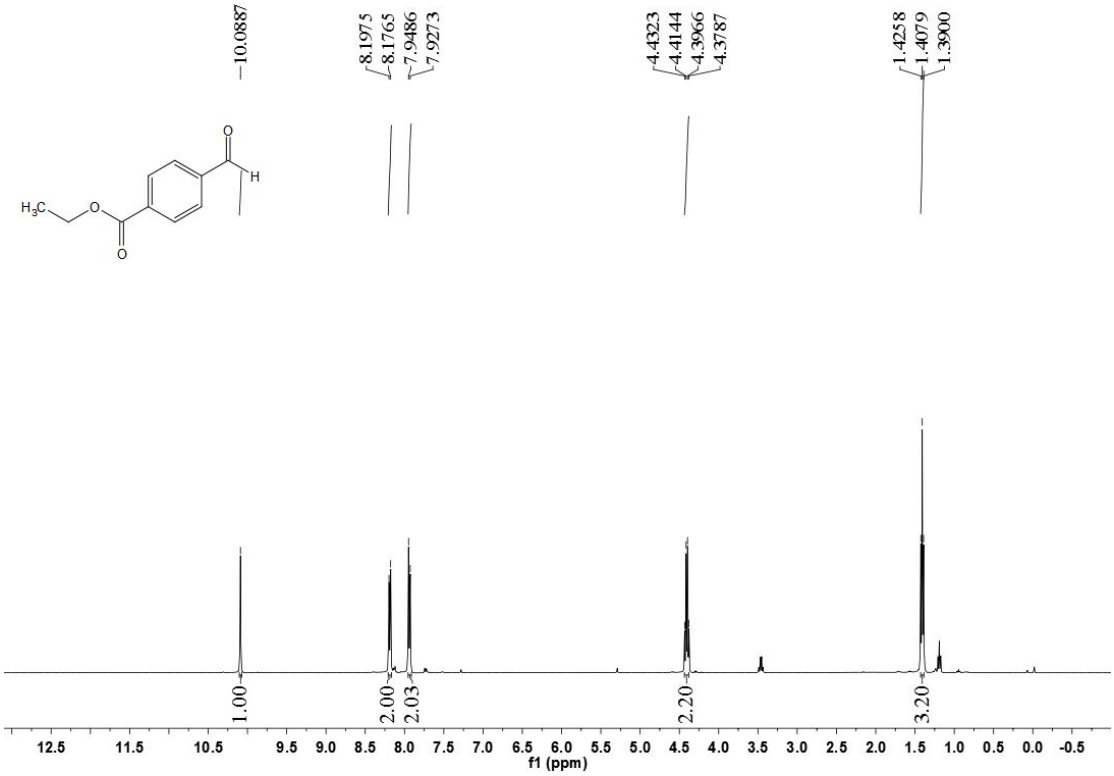
^{1}H NMR spectrum of compound **2q**



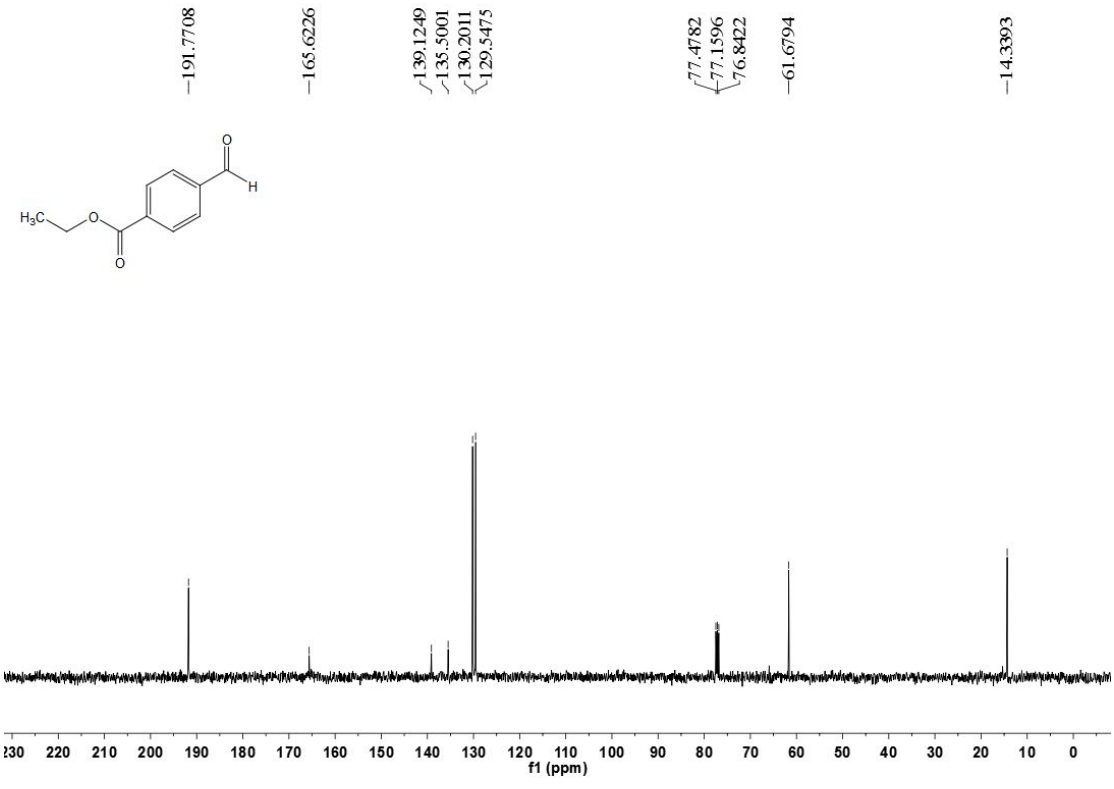
^{13}C NMR spectrum of compound **2q**



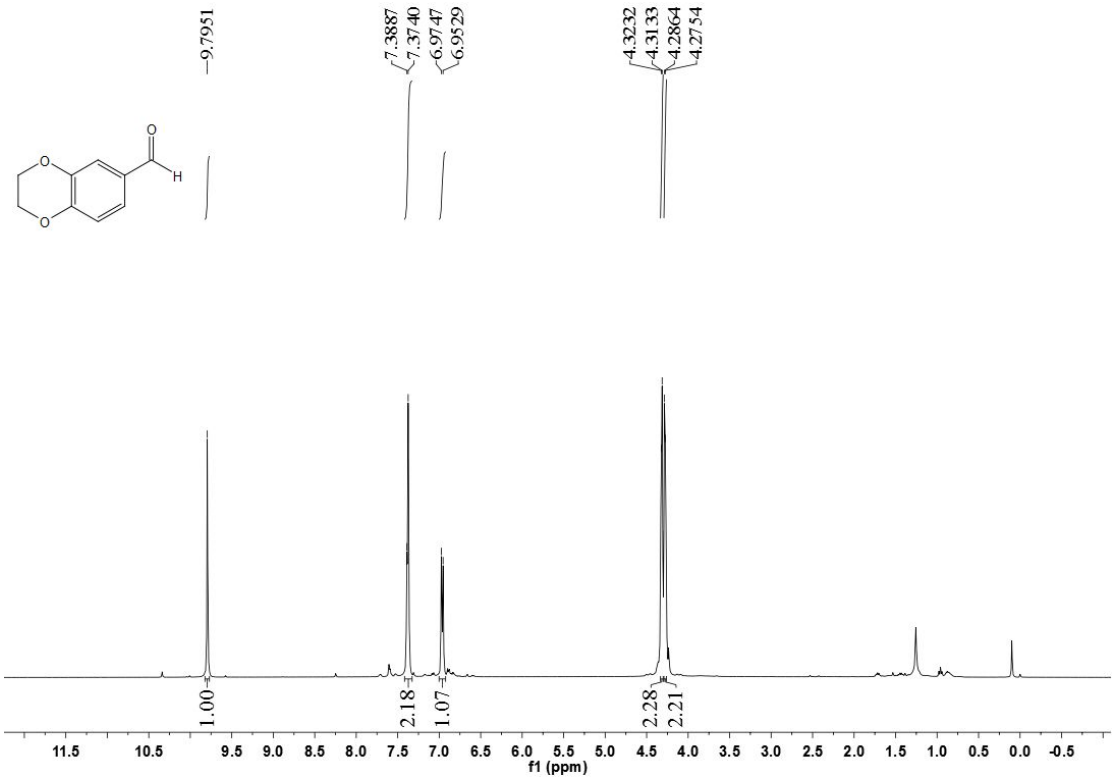
^{1}H NMR spectrum of compound **2r**



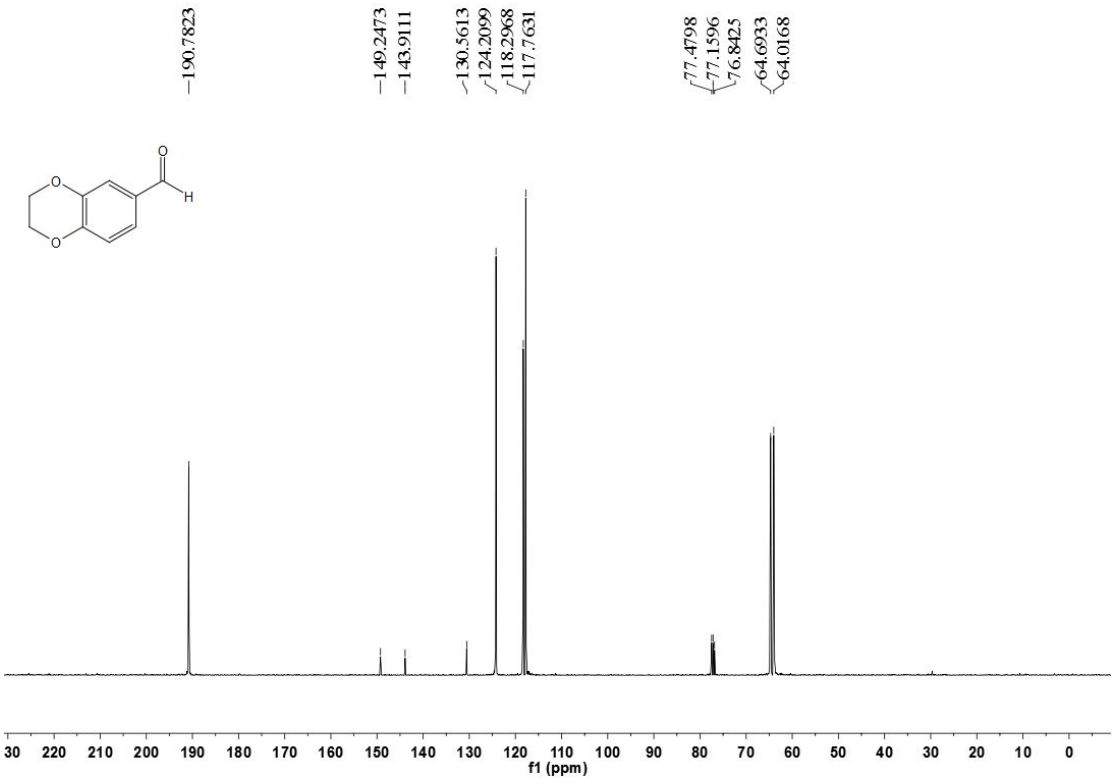
^{13}C NMR spectrum of compound **2r**



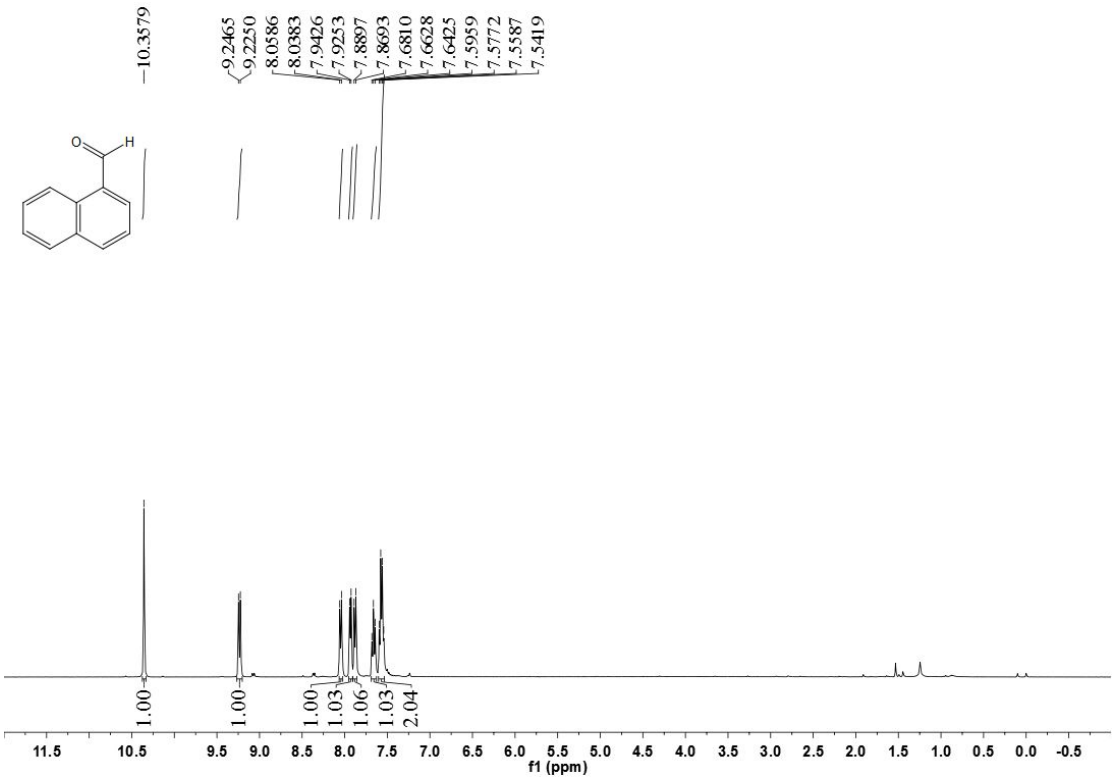
^{1}H NMR spectrum of compound **2s**



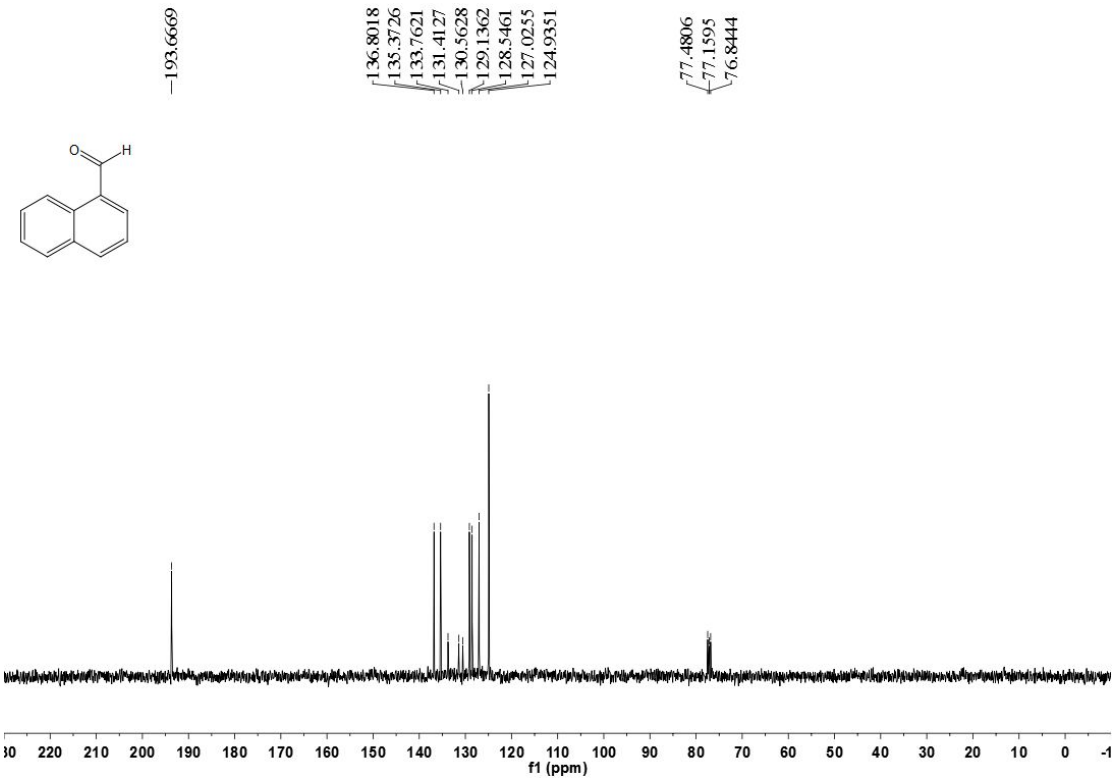
^{13}C NMR spectrum of compound **2s**



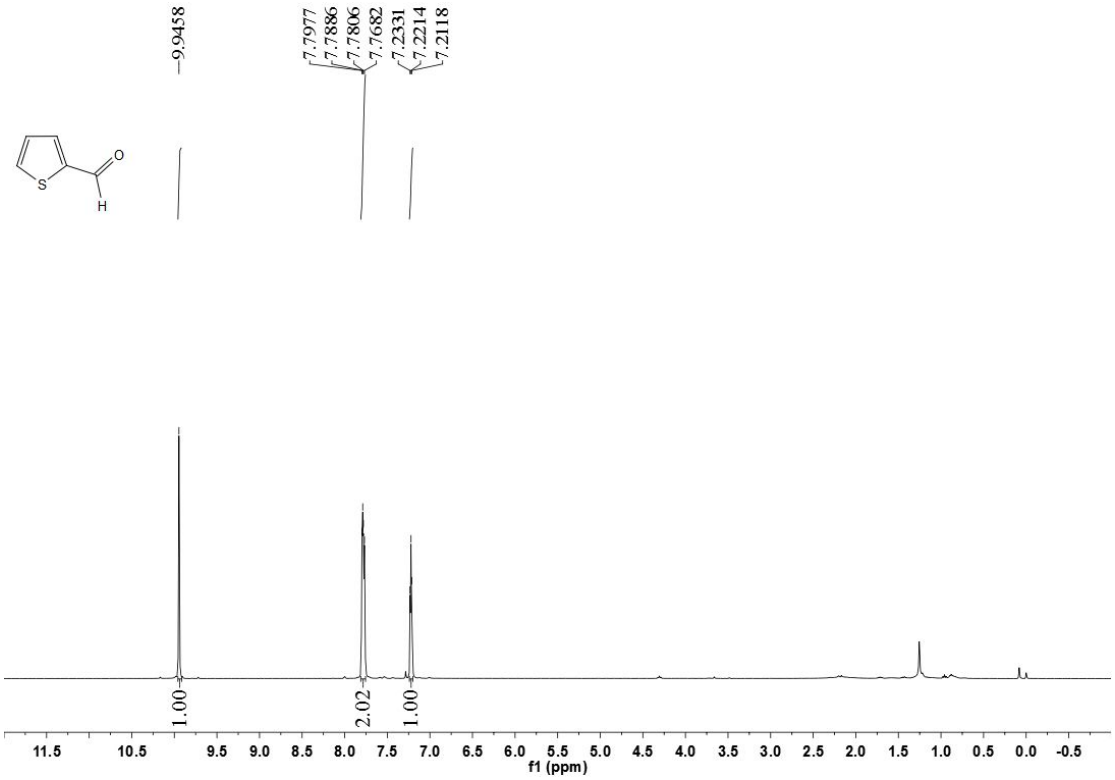
^{1}H NMR spectrum of compound **2t**



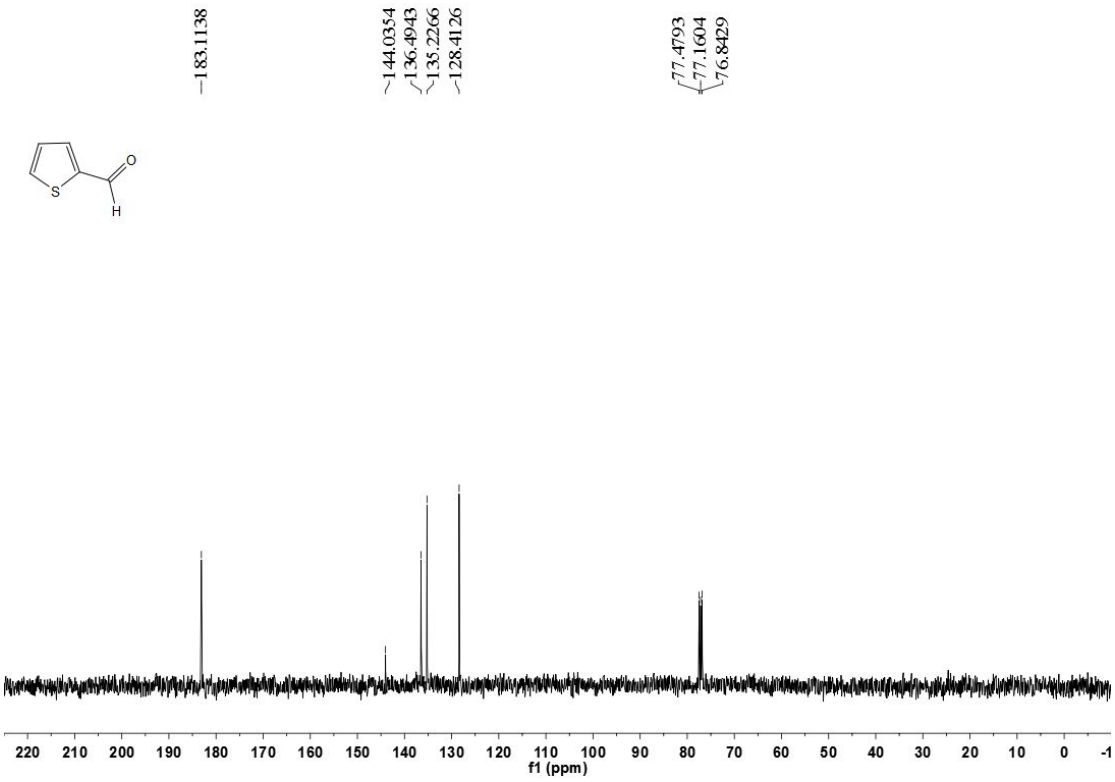
^{13}C NMR spectrum of compound **2t**



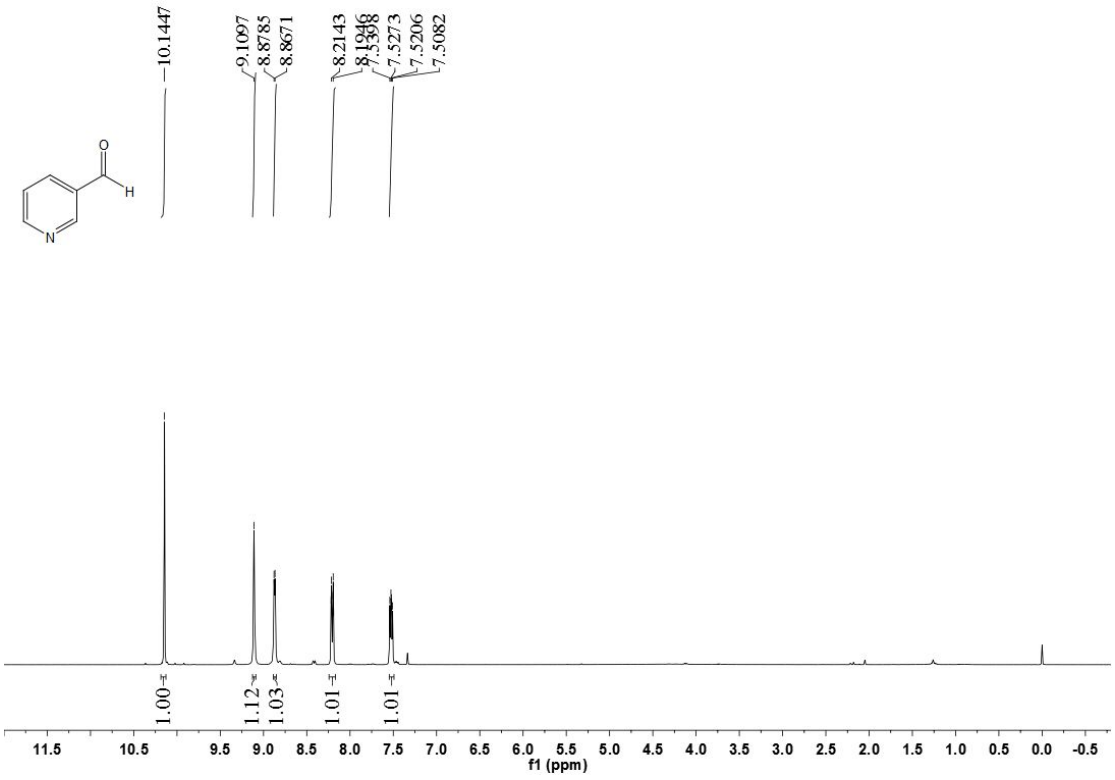
^{1}H NMR spectrum of compound **2u**



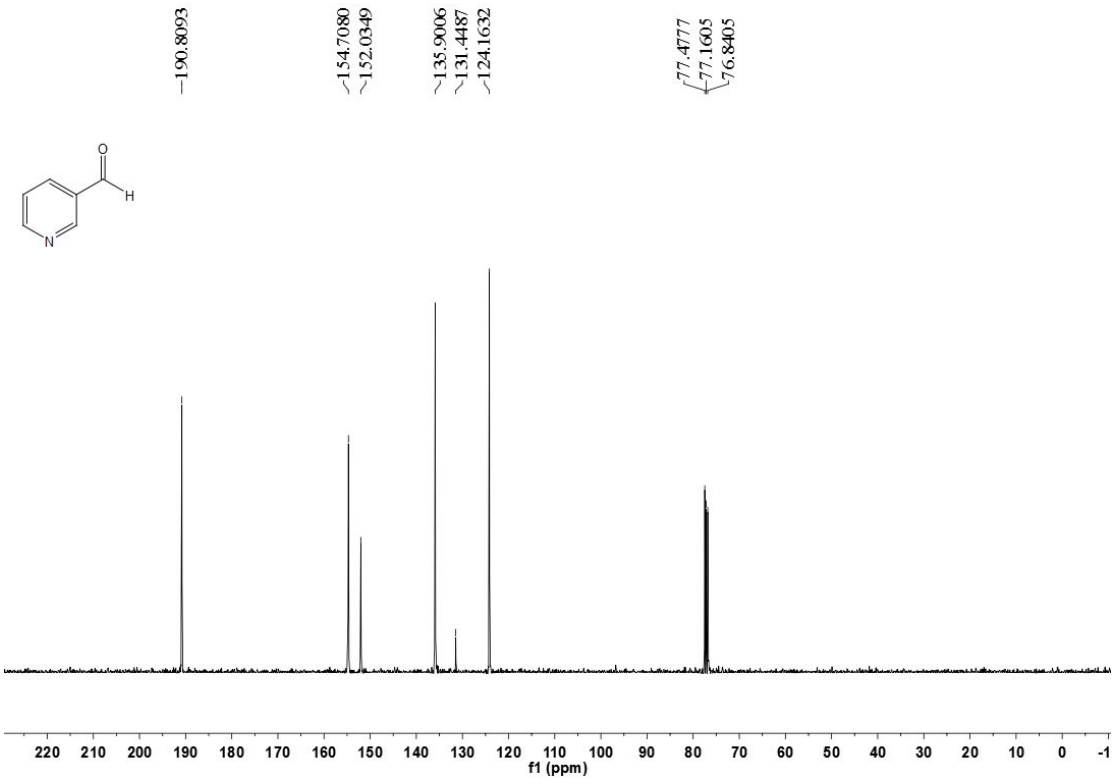
^{13}C NMR spectrum of compound **2u**



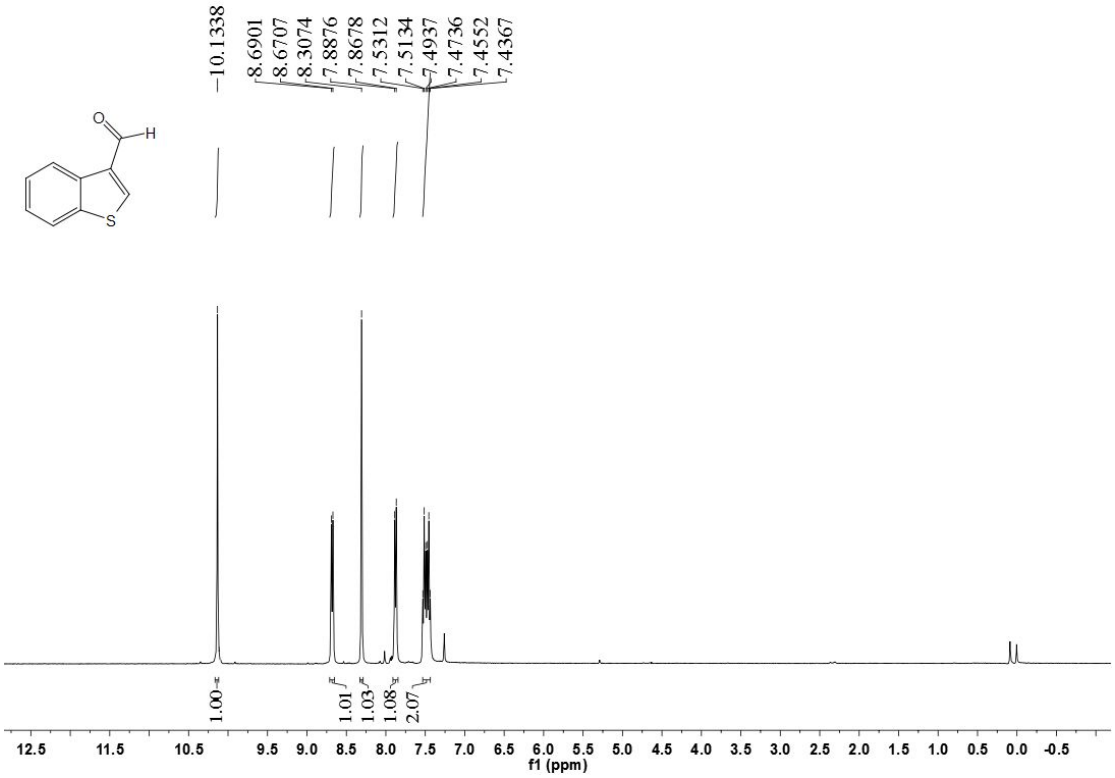
^{1}H NMR spectrum of compound **2v**



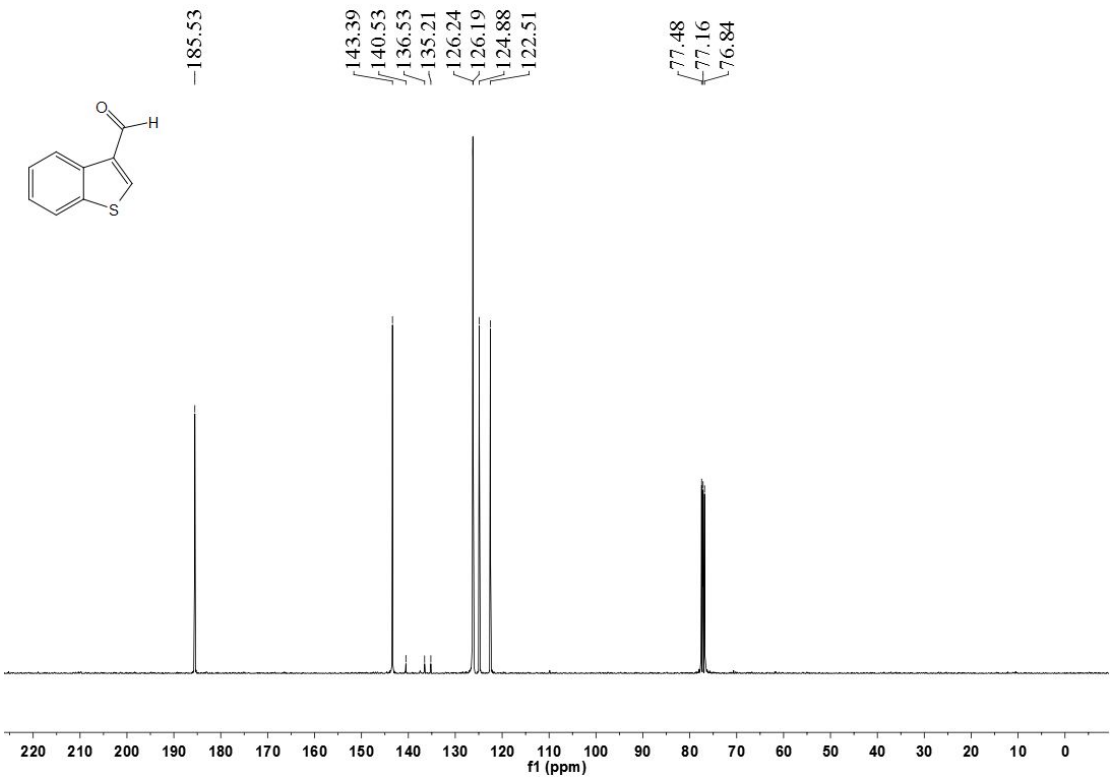
^{13}C NMR spectrum of compound **2v**



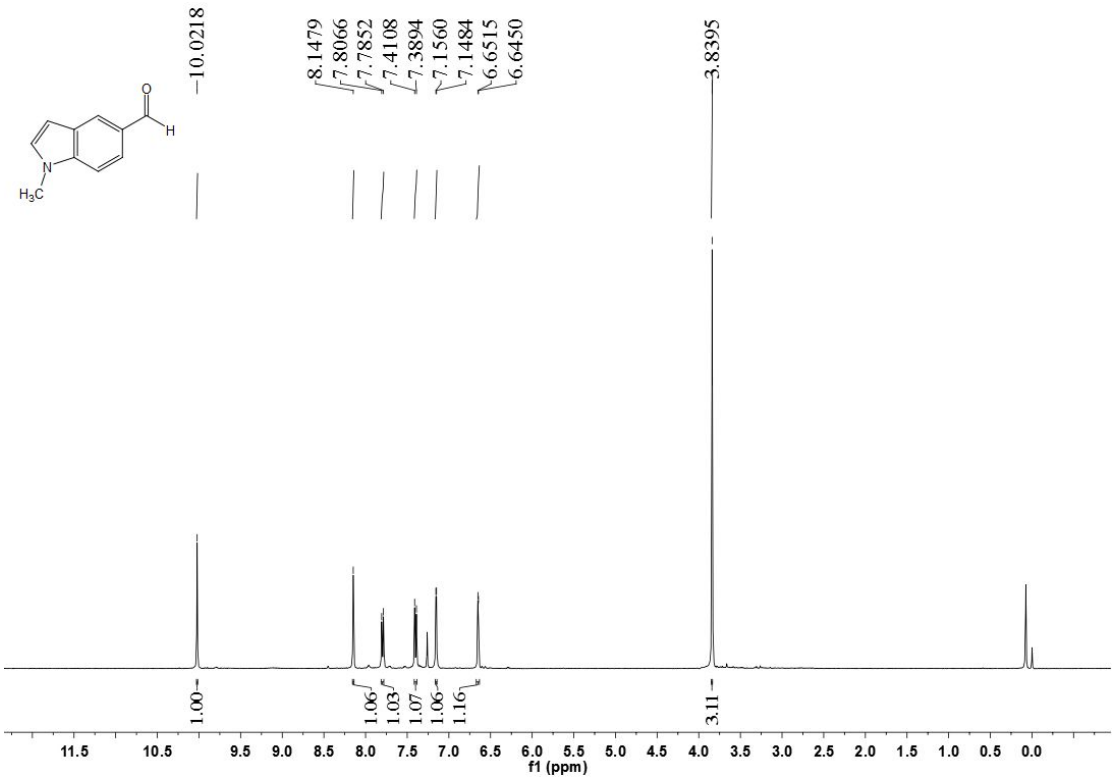
^{1}H NMR spectrum of compound **2w**



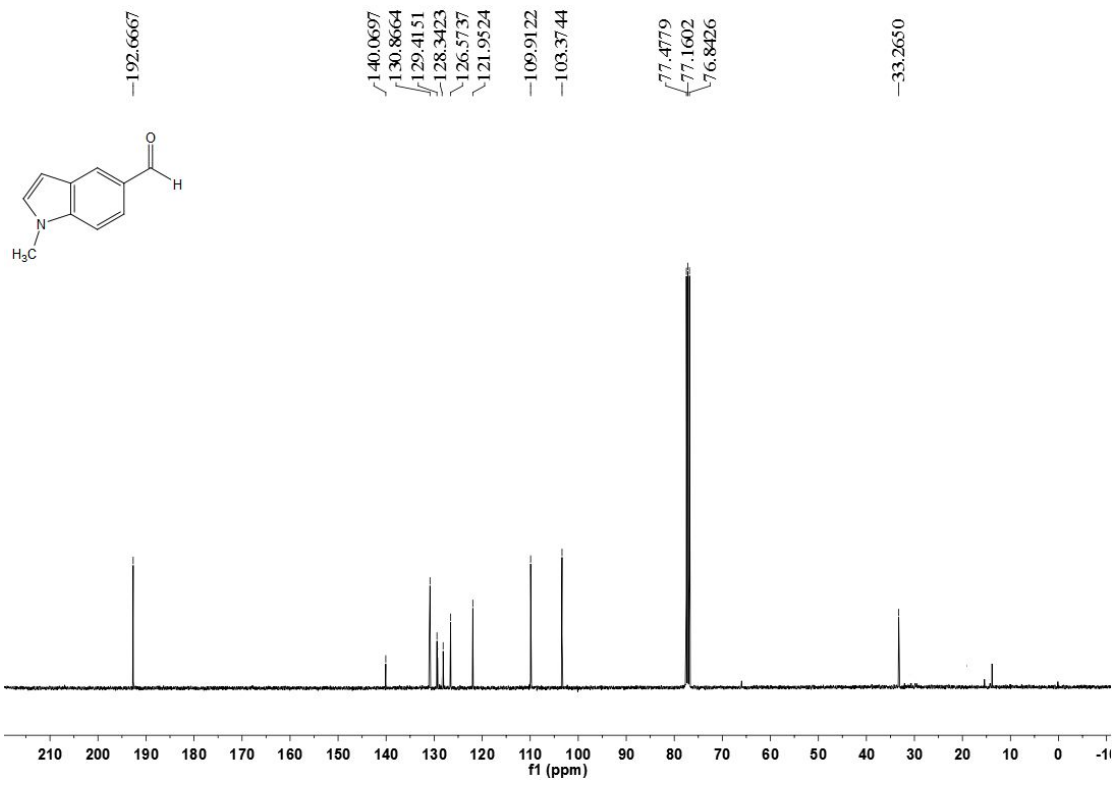
^{13}C NMR spectrum of compound **2w**



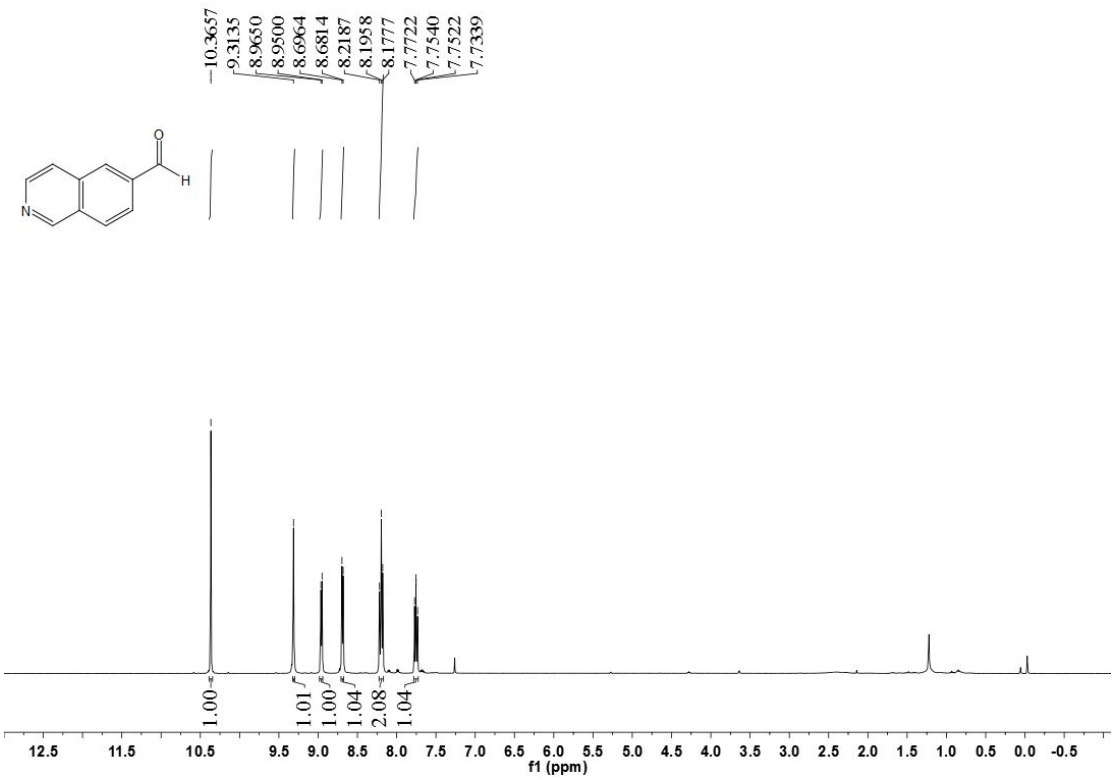
^{1}H NMR spectrum of compound **2x**



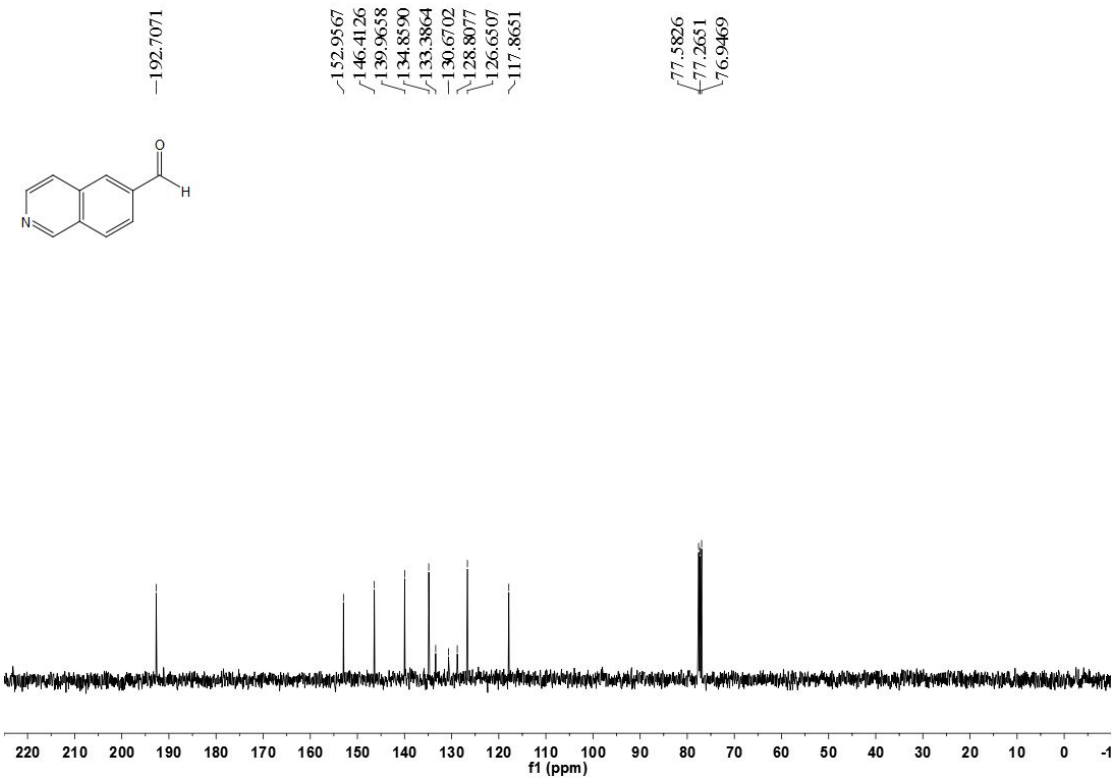
^{13}C NMR spectrum of compound **2x**



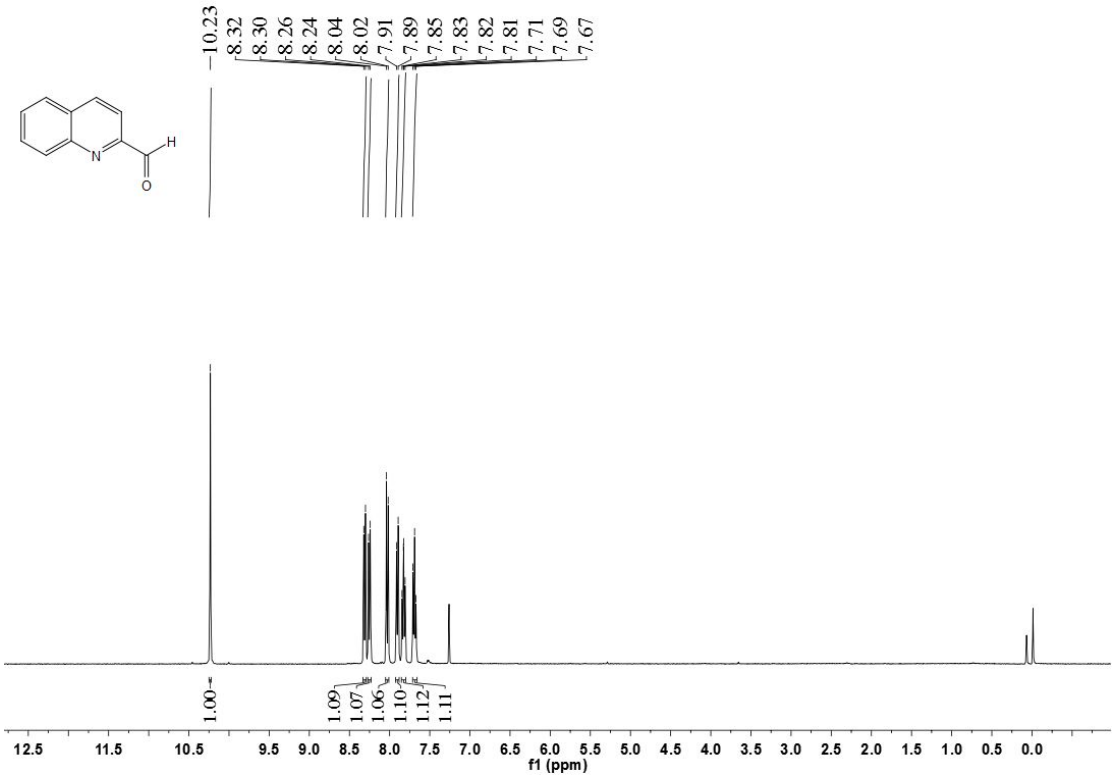
^{1}H NMR spectrum of compound **2y**



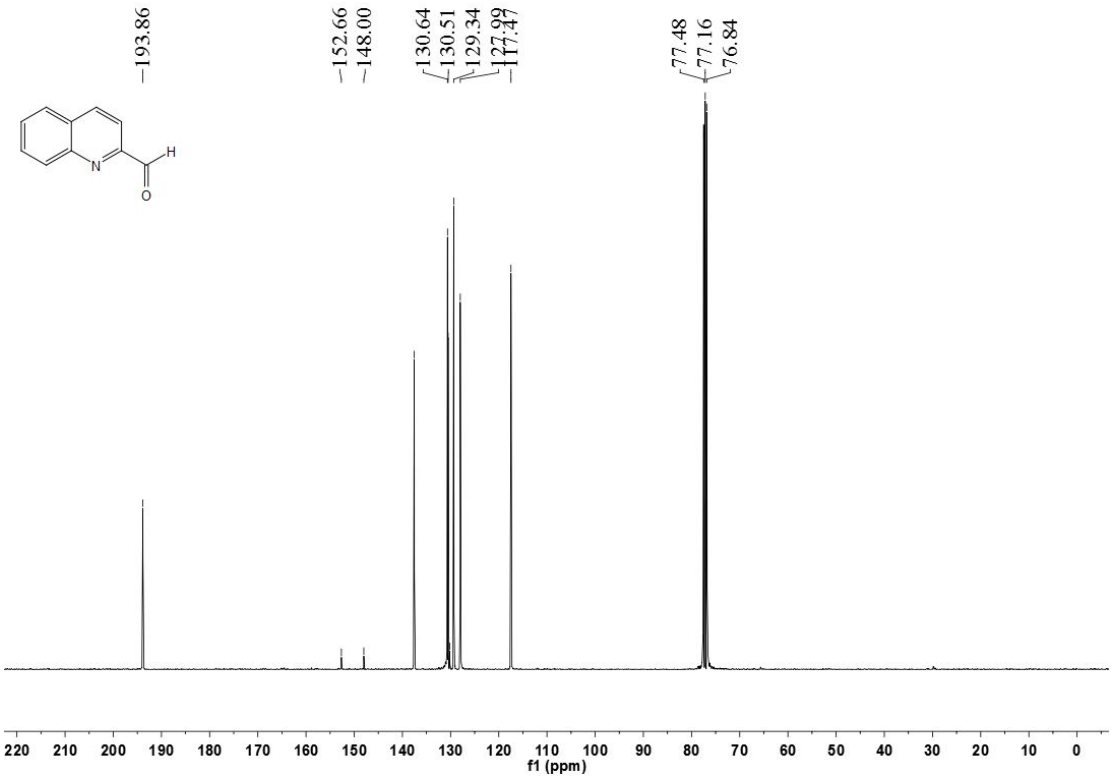
^{13}C NMR spectrum of compound **2y**



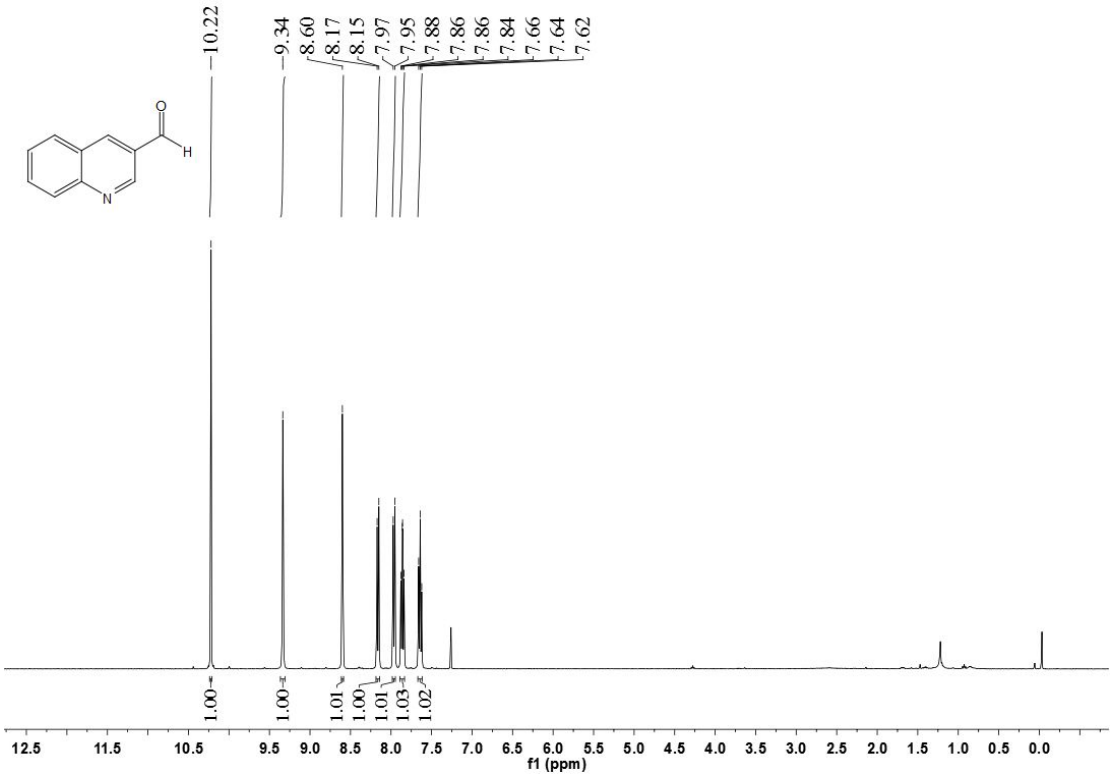
^{1}H NMR spectrum of compound **2z**



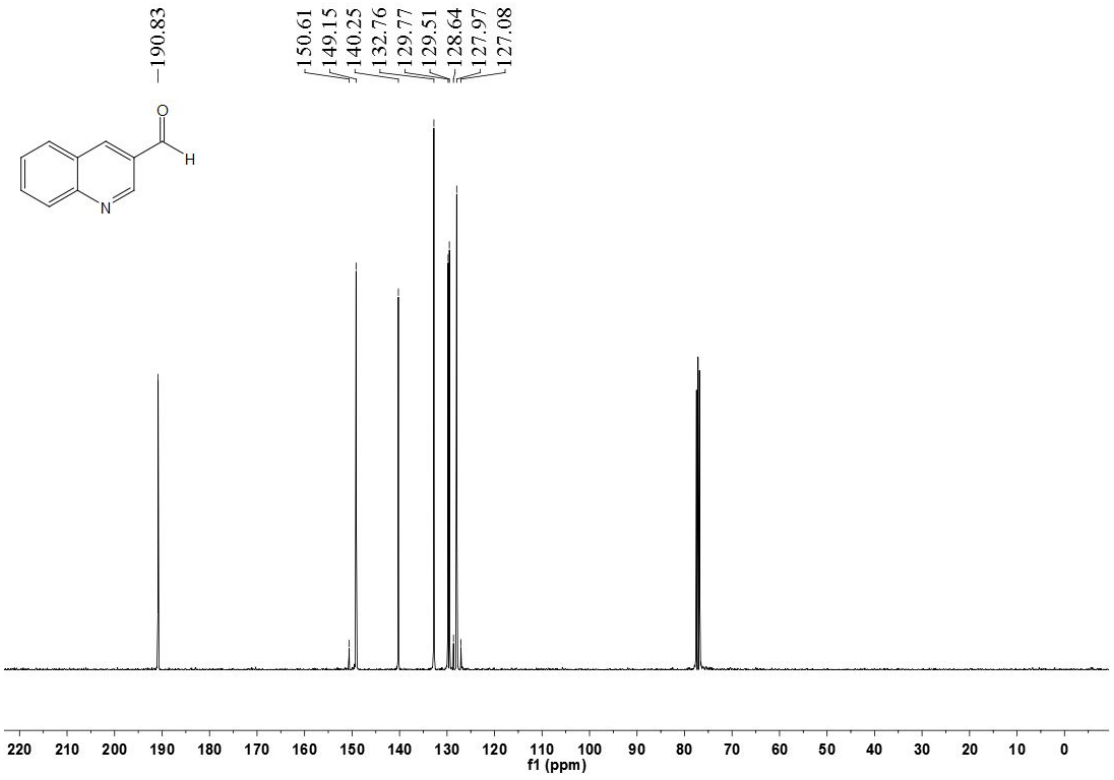
^{13}C NMR spectrum of compound **2z**



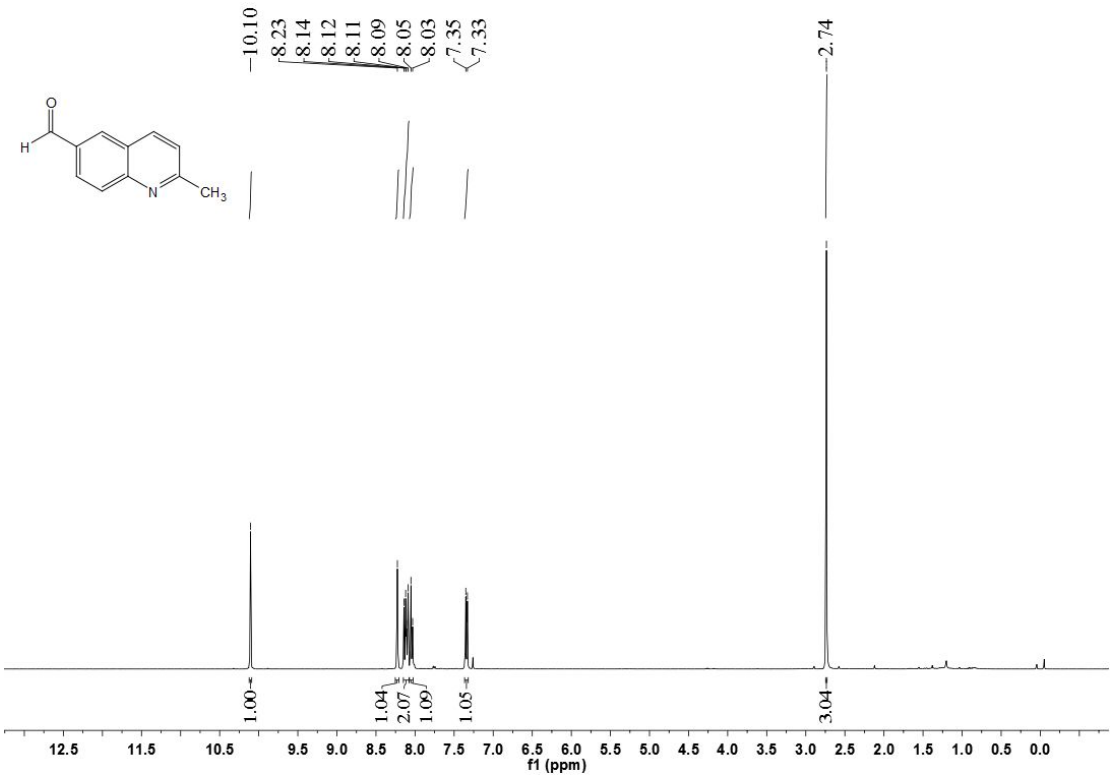
^{1}H NMR spectrum of compound **2aa**



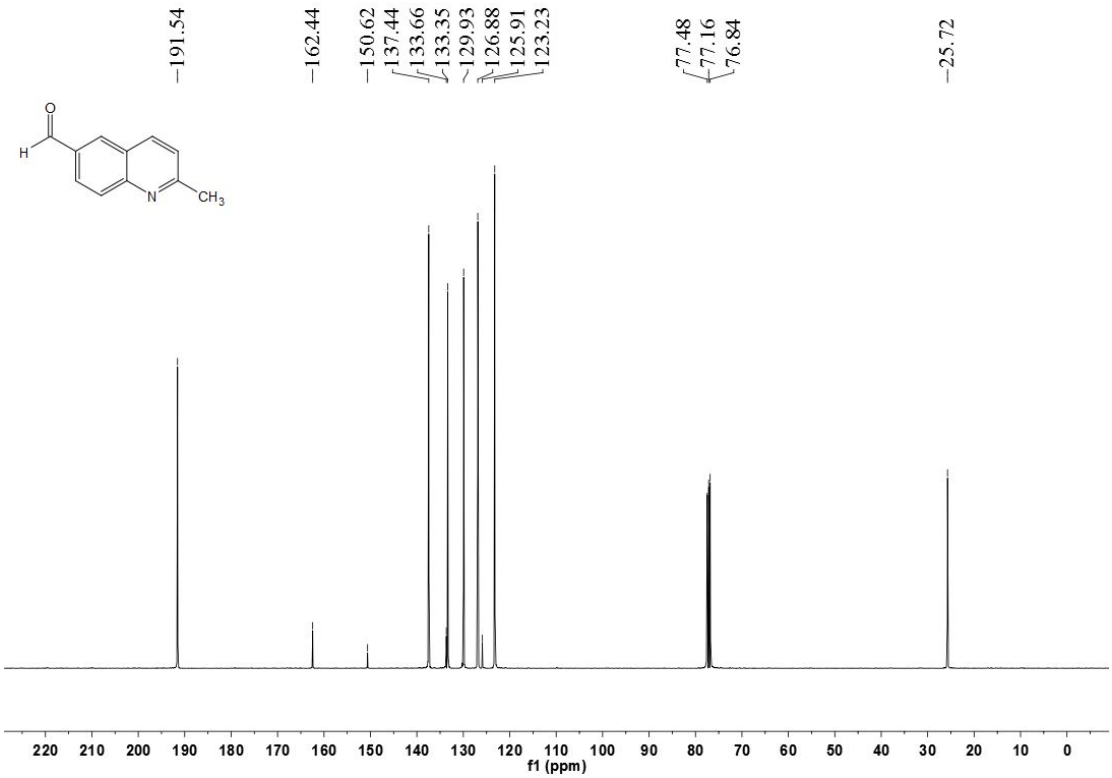
^{13}C NMR spectrum of compound **2aa**



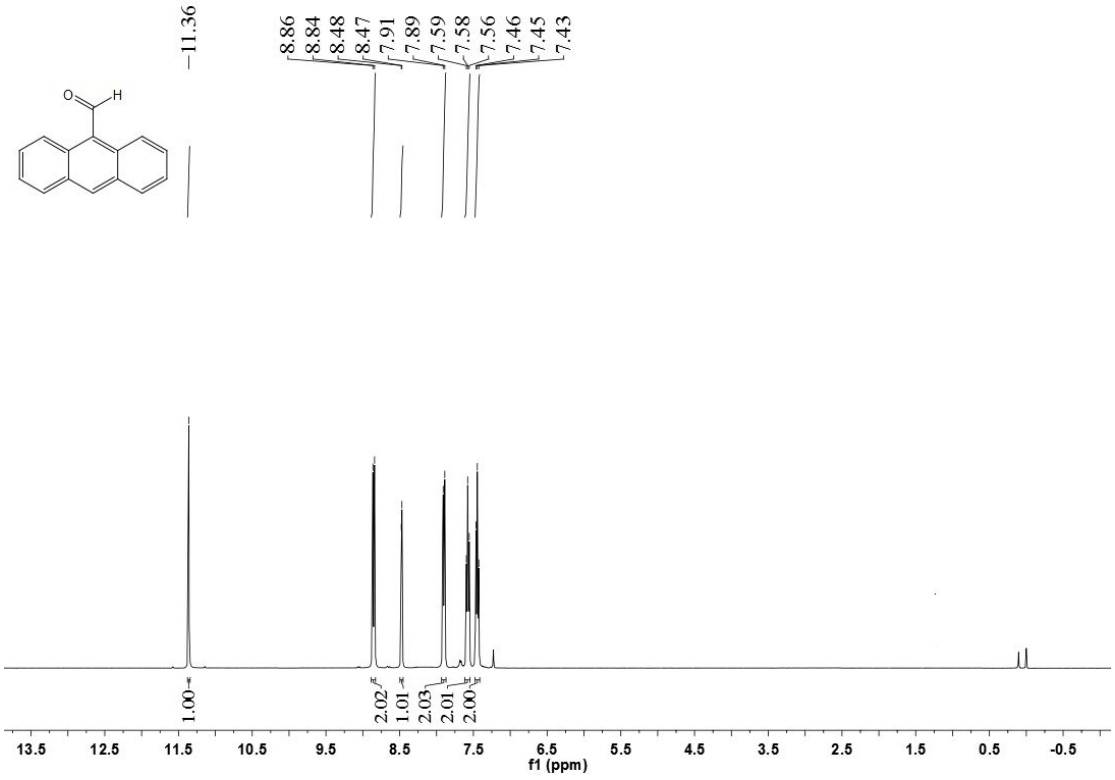
^{1}H NMR spectrum of compound **2bb**



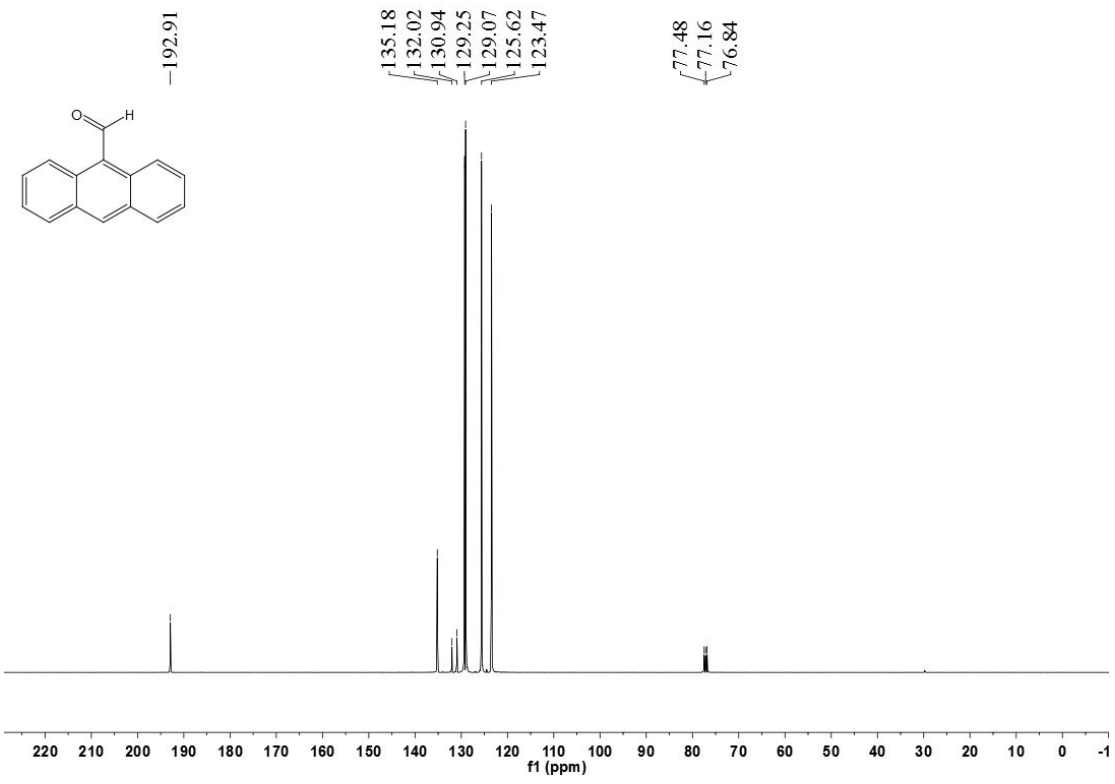
^{13}C NMR spectrum of compound **2bb**



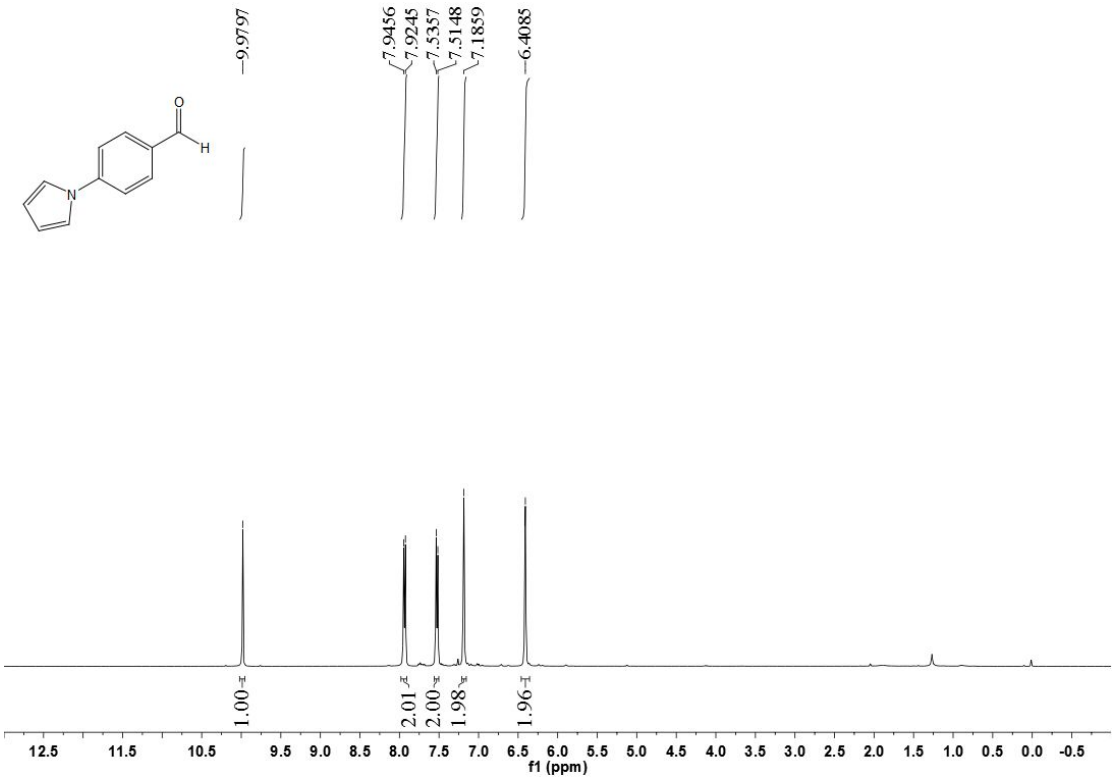
^{1}H NMR spectrum of compound **2cc**



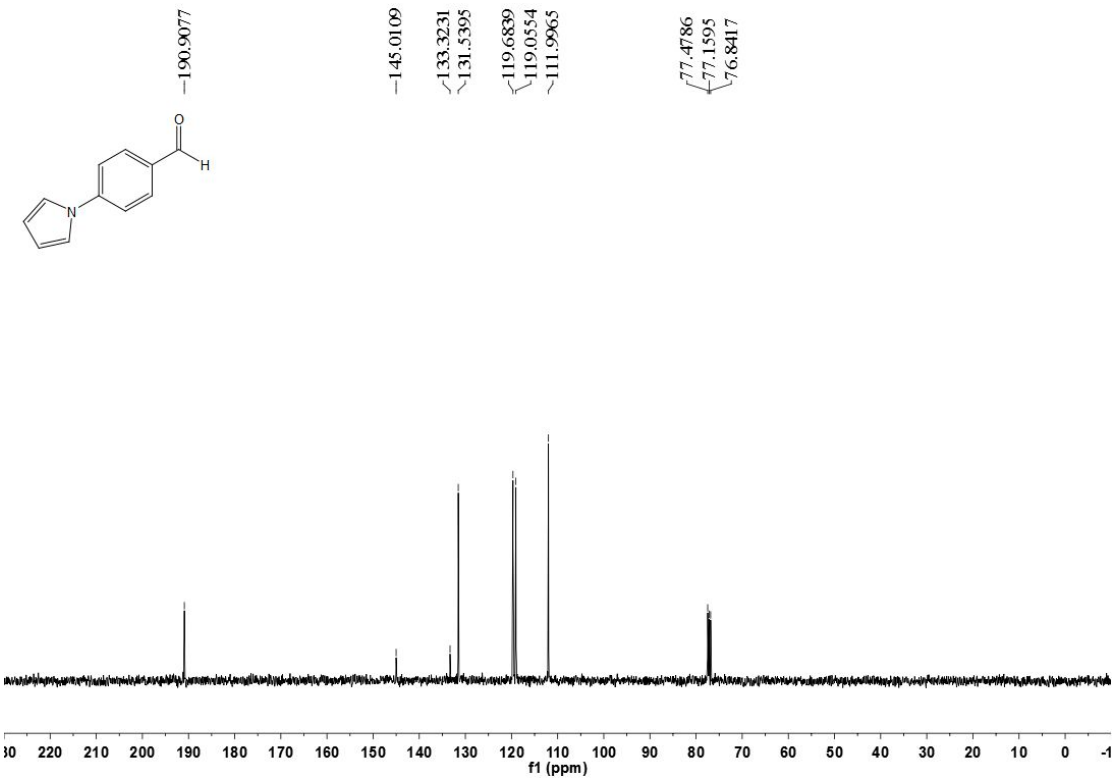
^{13}C NMR spectrum of compound **2cc**



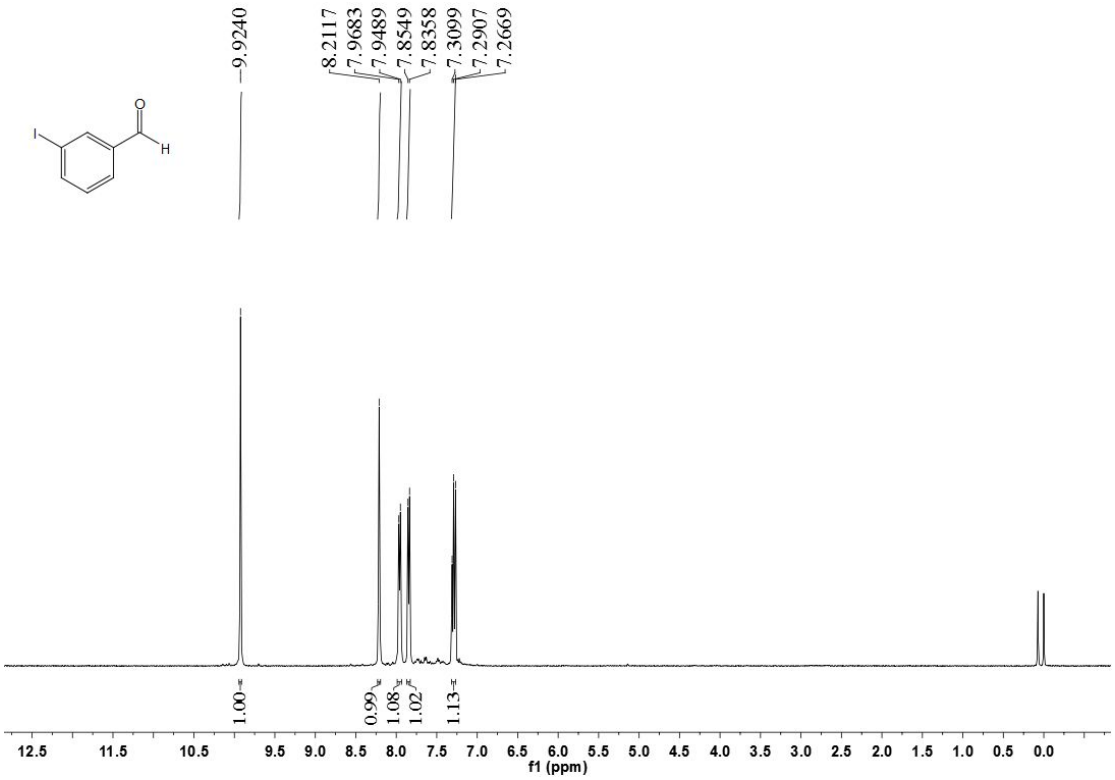
^{1}H NMR spectrum of compound **2dd**



^{13}C NMR spectrum of compound **2dd**



^{1}H NMR spectrum of compound **2ee**



^{13}C NMR spectrum of compound **2ee**