Supporting information

for

Pd(II)-catalyzed synthesis of aryl ketones in water

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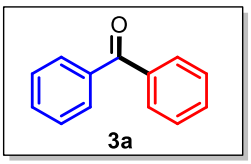
1. General information

All the chemicals and reagents including starting materials used for the reactions were purchased from commercial suppliers like Sigma Aldrich, TCI, SRL, BLD Pharm, Spectrochem, etc. and used without further purification. The progress of the reaction was monitored through thin layer chromatography on Merck Kieselgel silica gel 60 F_{254} plates using short wave UV light (λ = 254 nm). The products were purified by column chromatography using silica gel (60-120 mesh). The identification of the purified products was carried out by NMR (^{1}H and ^{13}C) spectroscopy. The NMR spectra were recorded on a 400 MHz JEOL ECZ NMR spectrophotometer (400 MHz for ^{1}H and 100 MHz for ^{13}C NMR spectroscopy) or on Bruker Avance III 500 MHz FTNMR spectrometer (500 MHz for ^{1}H and 125 MHz for ^{13}C NMR spectroscopy). Chemical shifts for both ^{1}H (δ_H) and ^{13}C (δ_C) NMR are assigned in parts per million (ppm) using TMS (0 ppm) as the internal reference, $CDCl_3$ and DMSO-d_6 as the solvent ($CDCl_3$: δ_H = 7.25 ppm and δ_C = 77.1 ppm; DMSO-d_6: δ_H = 2.5 ppm, DMSO-d_6 absorbed water = 3.3 ppm and δ_C = 40.0 ppm). The coupling constants, J are given in hertz and the multiplicities of the signals are assigned as: s = singlet, d = doublet, dd = doublet of doublet, t = triplet, br = broad and m = multiplet. High-resolution mass spectra were recorded on an ESI-Q-TOF mass spectrometer. Melting points (mp) were determined by JSGW Digital Melting Point Apparatus and are uncorrected.

2. ^{1}H and ^{13}C NMR spectral analysis of the aryl ketones

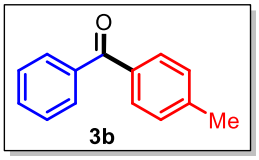
Benzophenone (3a)[1]



3a

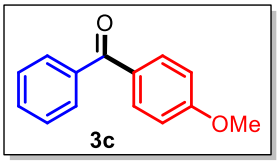
Colourless oil (90 mg, 99%); ^{1}H NMR (600 MHz, $CDCl_3$): δ_H (ppm) 7.85-7.81 (m, 4H), 7.63-7.59 (m, 2H), 7.52-7.49 (m, 4H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ_C (ppm) 196.8, 137.6, 132.4, 130.1, 128.3.

Phenyl(*p*-tolyl)methanone (3b)[1]



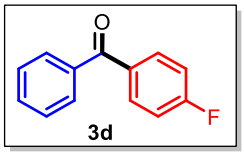
Colourless oil (97 mg, 99%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.79-7.76 (m, 2H), 7.73-7.69 (m, 2H), 7.59-7.53 (m, 1H), 7.48-7.43 (m, 2H), 7.29-7.25 (m, 2H), 2.42 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 196.6, 143.4, 138.0, 134.9, 132.3, 130.4, 130.0, 129.1, 128.3, 21.8.

(4-Methoxyphenyl)(phenyl)methanone (3c)[1]



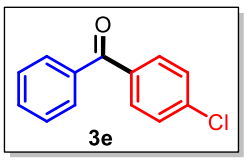
White solid (105 mg, 99%); mp 61-62 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ_H (ppm) 7.83 (d, J = 8.8 Hz, 2H), 7.76 (d, J = 7.1 Hz, 2H), 7.57 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.5 Hz, 2H), 6.97 (d, J = 8.8 Hz, 2H), 3.89 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 195.7, 163.3, 138.4, 132.7, 132.0, 130.2, 129.8, 128.3, 113.6, 55.6.

(4-Fluorophenyl)(phenyl)methanone (3d)[1]



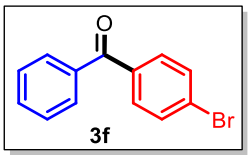
White solid (88 mg, 88%); mp 48-49 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.85-7.80 (m, 2H), 7.77-7.73 (m, 2H), 7.60-7.55 (m, 1H), 7.49-7.44 (m, 2H), 7.17-7.10 (m, 2H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 195.4, 165.5 (d, $^{1}J_{C-F}$ = 253 Hz), 137.5, 133.8 (d, $^{4}J_{C-F}$ = 3 Hz), 132.8 (d, $^{3}J_{C-F}$ = 9 Hz), 132.6, 130.0, 128.5, 115.6 (d, $^{2}J_{C-F}$ = 22 Hz); ^{19}F NMR (376 MHz, $CDCl_3$): δ_F (ppm) -105.8.

(4-Chlorophenyl)(phenyl)methanone (3e)[1]



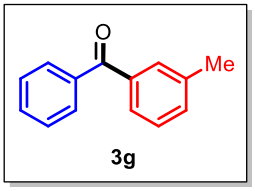
White solid (91 mg, 73%); mp 75-76 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.78-7.72 (m, 4H), 7.62-7.56 (m, 1H), 7.50-7.43 (m, 4H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ_C (ppm) 195.6, 139.0, 137.3, 136.0, 132.7, 131.5, 130.0, 128.7, 128.5.

(4-Bromophenyl)(phenyl)methanone (3f)[2]



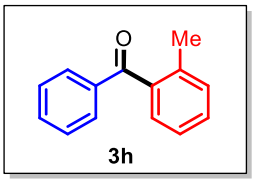
White solid (108 mg, 83%); mp 76-77 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.78-7.74 (m, 2H), 7.69-7.57 (m, 5H), 7.51-7.45 (m, 2H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ_C (ppm) 195.8, 137.2, 136.4, 132.8, 131.71, 131.67, 130.0, 128.5, 127.6.

Phenyl(*m*-tolyl)methanone (3g)[1]



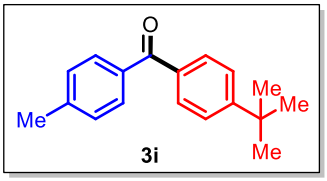
Colourless oil (97 mg, 99%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.81-7.77 (m, 2H), 7.62 (s, 1H), 7.59-7.54 (m, 2H), 7.49-7.43 (m, 2H), 7.40-7.32 (m, 2H), 2.40 (s, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ_C (ppm) 197.1, 138.2, 137.8, 137.7, 133.3, 132.5, 130.6, 130.1, 128.3, 128.2, 127.5, 21.5.

Phenyl(*o*-tolyl)methanone (3h)[1]



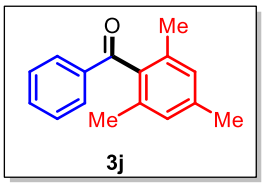
Colourless oil (97 mg, 99%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.82-7.78 (m, 2H), 7.59-7.54 (m, 1H), 7.47-7.41 (m, 2H), 7.38 (td, J = 7.4, 1.6 Hz, 1H), 7.32-7.21 (m, 3H), 2.33 (s, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ_C (ppm) 198.8, 138.7, 137.8, 136.8, 133.3, 131.1, 130.4, 130.2, 128.64, 128.58, 125.3, 20.1.

(4-(tert-butyl)phenyl)(*p*-tolyl)methanone (3i)[1]



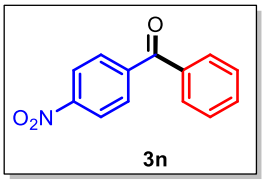
Colourless oil (106 mg, 84%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.73 (t, J = 7.9 Hz, 4H), 7.48 (dd, J = 8.5, 2.0 Hz, 2H), 7.26 (d, J = 8.3 Hz, 2H), 2.43 (s, 3H), 1.36 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 196.3, 155.9, 143.0, 135.3, 135.2, 130.3, 130.1, 129.0, 125.2, 35.2, 31.2, 21.7.

mesityl(phenyl)methanone (3j)[3]



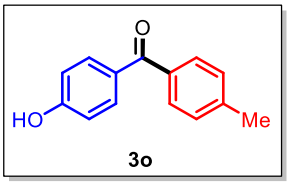
Yellow oil (62 mg, 55%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.70 (d, J = 7.1 Hz, 2H), 7.46-7.41 (m, 1H), 7.39-7.34 (m, 2H), 6.91 (s, 2H), 2.33 (s, 3H), 2.09 (s, 6H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 178.8, 137.9, 137.7, 134.4, 131.1, 128.7, 128.4, 127.7, 21.2, 19.7.

(4-nitrophenyl)(phenyl)methanone (3n)[2]



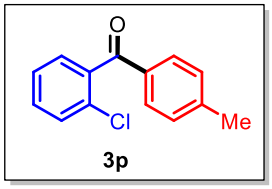
White solid (108 mg, 95%); mp 134-135 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 8.35-8.29 (m, 2H), 7.94-7.89 (m, 2H), 7.81-7.75 (m, 2H), 7.67-7.60 (m, 1H), 7.54-7.47 (m, 2H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 194.9, 149.9, 143.0, 136.4, 133.6, 130.8, 130.2, 128.8, 123.6.

(4-hydroxyphenyl)(*p*-tolyl)methanone (3o)[4]



White solid (105 mg, 99%); mp 156-157 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 10.35 (s, 1H), 7.63-7.51 (m, 4H), 7.31-7.26 (m, 2H), 6.87-6.82 (m, 2H), 2.35 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6): δ_C (ppm) 194.5, 162.3, 142.6, 135.8, 132.9, 129.9, 129.4, 128.7, 115.7, 21.6.

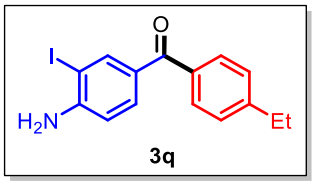
(2-chlorophenyl)(*p*-tolyl)methanone (3p)[5]



3p

Pale yellow oil (75 mg, 65%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.72-7.68 (m, 2H), 7.46-7.38 (m, 2H), 7.38-7.33 (m, 2H), 7.27-7.22 (m, 2H), 2.41 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 195.0, 144.9, 138.9, 134.1, 131.3, 131.0, 130.3, 130.1, 129.5, 129.1, 127.2, 126.7, 21.9.

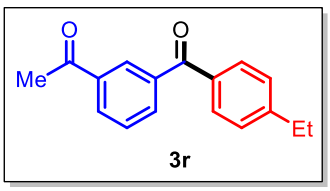
(4-amino-3-iodophenyl)(4-ethylphenyl)methanone (3q)



3q

Yellow oil (130 mg, 74%); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 7.68 (d, J = 8.1 Hz, 1H), 7.63-7.59 (m, 2H), 7.33 (d, J = 8.4 Hz, 2H), 7.07 (d, J = 2.0 Hz, 1H), 6.57 (dd, J = 8.1, 2.1 Hz, 1H), 5.49 (s, 2H), 2.64 (q, J = 7.6 Hz, 2H), 1.16 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6): δ_C (ppm) 195.9, 149.6, 149.3, 139.2, 138.7, 135.2, 130.4, 128.4, 119.1, 115.1, 88.9, 28.7, 15.8; HRMS (ESI/Q-TOF) m/z: [M + H]$^{+}$ calcd for $C_{15}H_{14}INO$, 352.0198; found, 352.2708.

1-(3-(4-ethylbenzoyl)phenyl)ethan-1-one (3r)

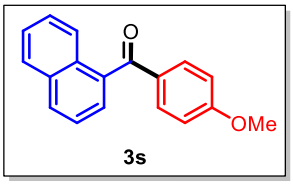


3r

Colourless oil (120 mg, 95%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 8.33-8.30 (m, 1H), 8.16-8.12 (m, 1H), 7.96-7.92 (m, 1H), 7.71 (d, J = 8.1 Hz, 2H), 7.56 (dd, J = 11.3, 4.1 Hz,

1H), 7.29 (d, J = 7.9 Hz, 2H), 2.71 (q, J = 7.6 Hz, 2H), 2.62 (s, 3H), 1.26 (t, J = 7.6 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ_C (ppm) 197.5, 195.7, 150.1, 138.5, 137.2, 134.6, 134.3, 131.6, 130.5, 129.7, 128.8, 128.1, 29.1, 26.9, 15.3; HRMS (ESI/Q-TOF) m/z: $[M]^+$ calcd for $C_{17}H_{16}O_2$, 252.1150; found, 252.2738.

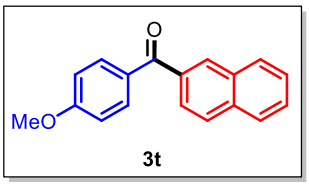
(4-methoxyphenyl)(naphthalen-1-yl)methanone (3s)[6]



3s

Colourless oil (88 mg, 67%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 8.02-7.95 (m, 2H), 7.91-7.88 (m, 1H), 7.87-7.83 (m, 2H), 7.56-7.44 (m, 4H), 6.93-6.89 (m, 2H), 3.84 (s, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ_C (ppm) 196.8, 163.9, 137.1, 133.8, 132.9, 131.2, 131.0, 130.8, 128.5, 127.1, 126.9, 126.5, 125.8, 124.5, 113.8, 55.6.

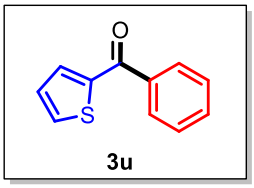
(4-methoxyphenyl)(naphthalen-2-yl)methanone (3t)[6]



3t

Colourless oil (108 mg, 82%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 8.22 (s, 1H), 7.94-7.86 (m, 6H), 7.61-7.50 (m, 2H), 7.00-6.96 (m, 2H), 3.87 (s, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ_C (ppm) 195.7, 163.3, 135.6, 135.1, 132.7, 132.4, 131.3, 130.5, 129.4, 128.3, 128.2, 127.9, 126.9, 126.0, 113.7, 55.6.

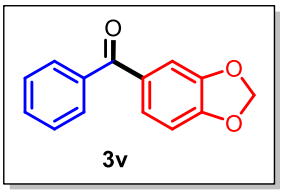
phenyl(thiophen-2-yl)methanone (3u)[7]



3u

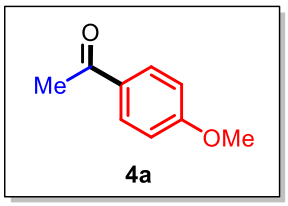
Colourless oil (91 mg, 97%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.86-7.83 (m, 2H), 7.70 (dd, J = 5.0, 1.1 Hz, 1H), 7.62 (dd, J = 3.8, 1.1 Hz, 1H), 7.60-7.54 (m, 1H), 7.50-7.45 (m, 2H), 7.14 (dd, J = 4.9, 3.8 Hz, 1H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ_C (ppm) 188.4, 143.7, 138.2, 135.0, 134.4, 132.4, 129.3, 128.5, 128.1.

benzo[*d*][1,3]dioxol-5-yl(phenyl)methanone (3v)[7]



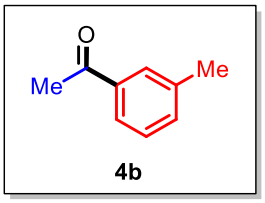
Colourless oil (112 mg, 99%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.71 (ddd, J = 7.0, 3.0, 1.6 Hz, 2H), 7.54-7.49 (m, 1H), 7.45-7.40 (m, 2H), 7.34-7.31 (m, 2H), 6.82-6.79 (m, 1H), 6.00 (s, 2H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 195.2, 151.6, 148.0, 138.2, 132.1, 131.9, 129.8, 128.3, 127.0, 109.9, 107.8, 102.0.

1-(4-methoxyphenyl)ethan-1-one (4a)[8]



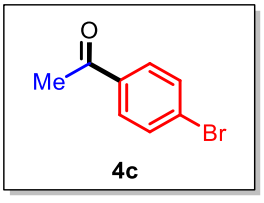
Colourless oil (62 mg, 83%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.95-7.86 (m, 2H), 6.93-6.87 (m, 2H), 3.84 (s, 3H), 2.52 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 196.9, 163.6, 130.7, 130.4, 113.7, 55.5, 26.4

1-(*m*-tolyl)ethan-1-one (4b)[8]



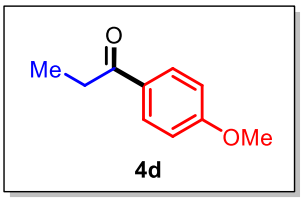
Yellow oil (37 mg, 55%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.77-7.72 (m, 2H), 7.38-7.31 (m, 2H), 2.58 (s, 3H), 2.40 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 198.5, 138.4, 137.2, 134.0, 128.9, 128.5, 125.7, 26.8, 21.4.

1-(4-bromophenyl)ethan-1-one (4c)[8]



Colourless oil (35 mg, 35%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.83-7.78 (m, 2H), 7.61-7.57 (m, 2H), 2.57 (s, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ_C (ppm) 197.2, 135.9, 132.0, 129.9, 128.4, 26.6.

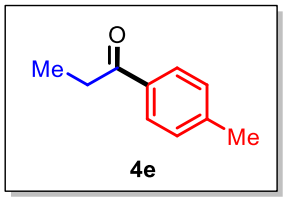
1-(4-methoxyphenyl)propan-1-one (4d)[9]



4d

Colourless oil (81 mg, 99%); ^{1}H NMR (500 MHz, $CDCl_3$): δ_H (ppm) 7.96-7.93 (m, 2H), 6.95-6.91 (m, 2H), 3.86 (s, 3H), 2.95 (q, J = 7.3 Hz, 2H), 1.21 (t, J = 7.3 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ_C (ppm) 199.6, 163.4, 130.3, 130.1, 113.7, 55.5, 31.5, 8.5.

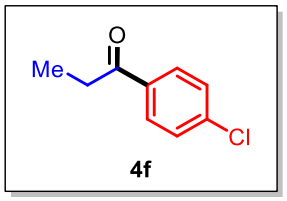
1-(*p*-tolyl)propan-1-one (4e)[10]



4e

Colourless oil (52 mg, 70%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.87-7.83 (m, 2H), 7.25-7.21 (m, 2H), 2.96 (q, J = 7.3 Hz, 2H), 2.38 (s, 3H), 1.20 (t, J = 7.3 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ_C (ppm) 200.6, 143.7, 134.5, 129.3, 128.2, 31.7, 21.7, 8.4.

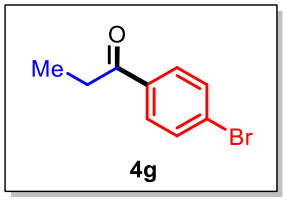
1-(4-chlorophenyl)propan-1-one (4f)[10]



4f

Colourless oil (44 mg, 52%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.91-7.87 (m), 7.43-7.39 (m), 2.96 (q, J = 7.2 Hz), 1.20 (t, J = 7.2 Hz); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ_C (ppm) 199.7, 139.4, 135.2, 129.5, 129.0, 31.9, 8.2.

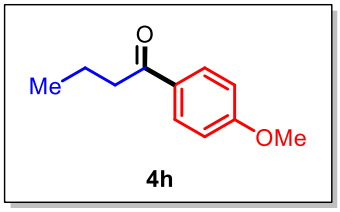
1-(4-bromophenyl)propan-1-one (4g)[11]



4g

Colourless oil (33 mg, 31%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.84-7.79 (m, 2H), 7.61-7.56 (m, 2H), 2.96 (q, J = 7.2 Hz, 2H), 1.20 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 199.8, 135.7, 131.9, 129.6, 128.1, 31.9, 8.2.

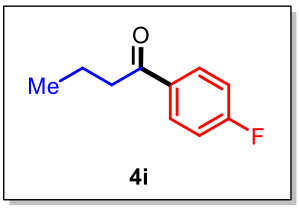
1-(4-methoxyphenyl)butan-1-one (4h)[12]



4h

Colourless oil (88 mg, 99%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.92-7.88 (m, 2H), 6.90-6.86 (m, 2H), 3.81 (s, 3H), 2.87-2.82 (m, 2H), 1.76-1.66 (m, 2H), 0.95 (t, J = 7.4 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 199.1, 163.4, 130.3, 130.2, 113.7, 55.5, 40.2, 18.1, 14.0.

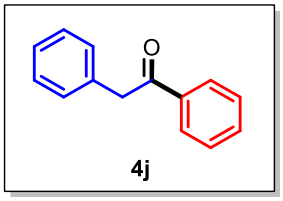
1-(4-fluorophenyl)butan-1-one (4i)[12]



4i

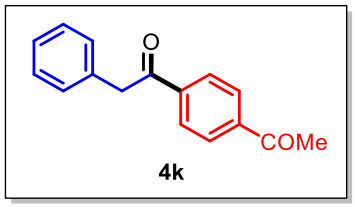
Colourless oil (55 mg, 66%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 8.00-7.94 (m, 2H), 7.14-7.07 (m, 2H), 2.93-2.87 (m, 2H), 1.80-1.69 (m, 2H), 0.99 (t, J = 7.4 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 198.9, 165.7 (d, $^{1}J_{C-F}$ = 253 Hz), 133.6 (d, $^{4}J_{C-F}$ = 3 Hz), 130.7 (d, $^{3}J_{C-F}$ = 9 Hz), 115.7 (d, $^{2}J_{C-F}$ = 22 Hz), 40.5, 17.8, 14.0; ^{19}F NMR (376 MHz, $CDCl_3$): δ_F (ppm) -105.6.

1,2-diphenylethan-1-one (4j)[2]



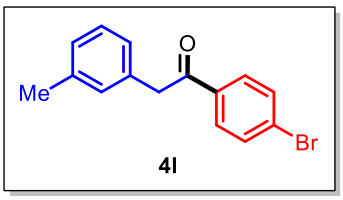
White solid (96 mg, 98%); mp 55-56 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ_H (ppm) 8.01 (d, J = 7.4 Hz, 2H), 7.57-7.52 (m, 1H), 7.45 (t, J = 7.7 Hz, 2H), 7.35-7.30 (m, 2H), 7.25 (dd, J = 12.4, 7.7 Hz, 3H), 4.28 (s, 2H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 197.7, 136.7, 134.6, 133.3, 129.6, 128.8, 128.74, 128.71, 127.0, 45.6.

1-(4-acetylphenyl)-2-phenylethan-1-one (4k)[13]



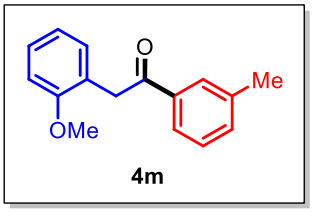
White solid (61 mg, 51%); mp 135-136 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 8.08-8.04 (m, 2H), 8.03-7.98 (m, 2H), 7.35-7.28 (m, 2H), 7.28-7.22 (m, 3H), 4.29 (s, 2H), 2.62 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 197.5, 197.2, 140.2, 139.8, 134.0, 129.5, 128.89, 128.88, 128.6, 127.2, 46.0, 26.9.

1-(4-bromophenyl)-2-(*m*-tolyl)ethan-1-one (4l)



Yellow oil (77 mg, 53%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.89-7.82 (m, 2H), 7.62-7.54 (m, 2H), 7.28-7.16 (m, 1H), 7.10-7.00 (m, 3H), 4.19 (s, 2H), 2.31 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 196.8, 138.5, 135.4, 134.1, 132.0, 130.3, 130.1, 128.8, 128.4, 127.9, 126.5, 45.6, 21.5; HRMS (ESI/Q-TOF) m/z: $[M]^+$ calcd for $C_{15}H_{13}BrO$, 288.0150; found, 288.6530.

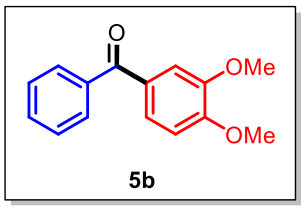
2-(2-methoxyphenyl)-1-(*m*-tolyl)ethan-1-one (4m)



4m

Sticky white solid (94 mg, 78%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.88-7.82 (m, 2H), 7.38-7.31 (m, 2H), 7.26 (td, J = 8.0, 1.7 Hz, 1H), 7.18 (dd, J = 7.4, 1.6 Hz, 1H), 6.95-6.90 (m, 1H), 6.90-6.87 (m, 1H), 4.27 (s, 2H), 3.79 (s, 3H), 2.41 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 198.3, 157.3, 138.3, 137.1, 133.8, 131.1, 129.0, 128.5, 128.4, 125.8, 123.9, 120.7, 110.7, 55.5, 40.1, 21.5; HRMS (ESI/Q-TOF) m/z: $[M]^+$ calcd for $C_{16}H_{16}O_2$, 240.1150; found, 240.0879.

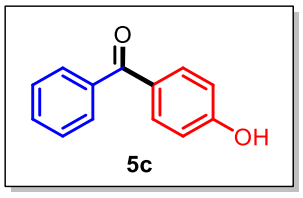
(3,4-dimethoxyphenyl)(phenyl)methanone (5b)[14]



5b

Colourless oil (111 mg, 92%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.77-7.68 (m, 2H), 7.61-7.50 (m, 1H), 7.49-7.37 (m, 3H), 7.34 (dd, J = 8.4, 2.1 Hz, 1H), 6.85 (d, J = 8.5 Hz, 1H), 3.92 (s, 3H), 3.90 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 195.6, 153.1, 149.1, 138.3, 132.0, 130.2, 129.8, 128.2, 125.6, 112.1, 109.8, 56.2, 56.1.

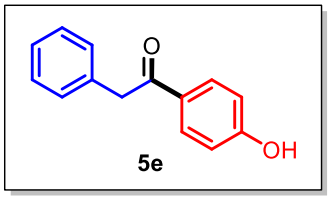
(4-hydroxyphenyl)(phenyl)methanone (5c)[2]



5c

White solid (96 mg, 97%); mp 125-126 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 10.40 (s, 1H), 7.64-7.60 (m, 4H), 7.57 (dt, J = 2.8, 1.8 Hz, 1H), 7.52-7.46 (m, 2H), 6.88-6.84 (m, 2H); ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6): δ_C (ppm) 194.8, 162.5, 138.6, 133.0, 132.3, 129.7, 128.9, 128.4, 115.8.

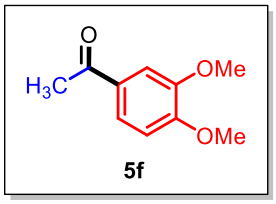
1-(4-hydroxyphenyl)-2-phenylethan-1-one (5e)[13]



5e

Pale yellow solid (81 mg, 76%); mp 143-144 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 10.36 (s, 1H), 7.91-7.87 (m, 2H), 7.28-7.15 (m, 5H), 6.84-6.79 (m, 2H), 4.22 (s, 2H); ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6): δ_C (ppm) 196.3, 162.6, 136.2, 131.6, 130.1, 128.8, 128.4, 126.9, 115.8, 44.8.

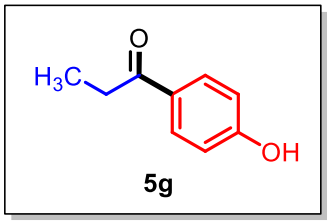
1-(3,4-dimethoxyphenyl)ethan-1-one (5f)[15]



5f

Colourless oil (88 mg, 98%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.48 (dd, J = 8.3, 2.0 Hz, 1H), 7.42 (d, J = 2.0 Hz, 1H), 6.79 (d, J = 8.4 Hz, 1H), 3.84 (d, J = 4.9 Hz, 6H), 2.47 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 196.9, 153.3, 148.9, 130.4, 123.4, 110.0, 109.9, 56.1, 56.0, 26.2.

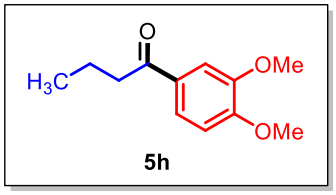
1-(4-hydroxyphenyl)propan-1-one (5g)[16]



5g

White solid (75 mg, 99%); mp 146-147 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 10.28 (s, 1H), 7.83-7.77 (m, 2H), 6.82-6.76 (m, 2H), 2.88 (q, J = 7.2 Hz, 2H), 1.00 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6): δ_C (ppm) 199.1, 162.3, 130.8, 128.7, 115.7, 31.1, 8.9.

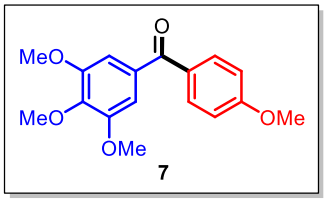
1-(3,4-dimethoxyphenyl)butan-1-one (5h)[17]



5h

White solid (103 mg, 99%); mp 66-67 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.57 (dd, J = 8.4, 2.0 Hz, 1H), 7.51 (d, J = 2.0 Hz, 1H), 6.86 (d, J = 8.4 Hz, 1H), 3.92 (s, 3H), 3.91 (s, 3H), 2.91-2.86 (m, 2H), 1.79-1.69 (m, 2H), 0.98 (t, J = 7.4 Hz, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 199.3, 153.1, 149.0, 130.4, 122.8, 110.1, 110.0, 56.1, 56.0, 40.1, 18.2, 14.0.

(4-methoxyphenyl)(3,4,5-trimethoxyphenyl)methanone (7)[18]



7

Colourless oil (145 mg, 96%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm) 7.79-7.75 (m, 2H), 6.97 (s, 2H), 6.94-6.90 (m, 2H), 3.88 (s, 3H), 3.83 (s, 3H), 3.83 (s, 6H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ_C (ppm) 194.8, 163.2, 152.9, 141.5, 133.4, 132.5, 130.2, 113.6, 107.4, 61.0, 56.3, 55.6.

3. References

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4. ^{1}H and ^{13}C NMR spectra of the aryl ketones

Figure S1. ^{1}H NMR (600 MHz) Spectrum of **3a** in $CDCl_3$ at 298K.

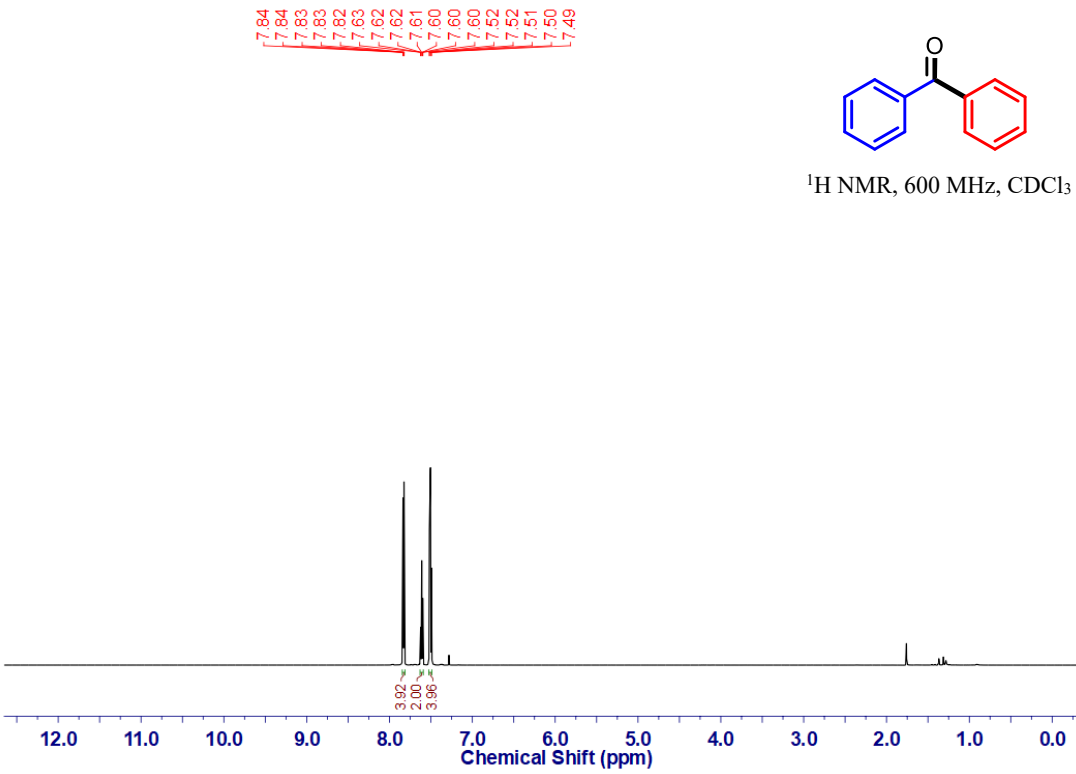


Figure S2. $^{13}C\{^{1}H\}$ NMR (151 MHz) Spectrum of **3a** in $CDCl_3$ at 298K.

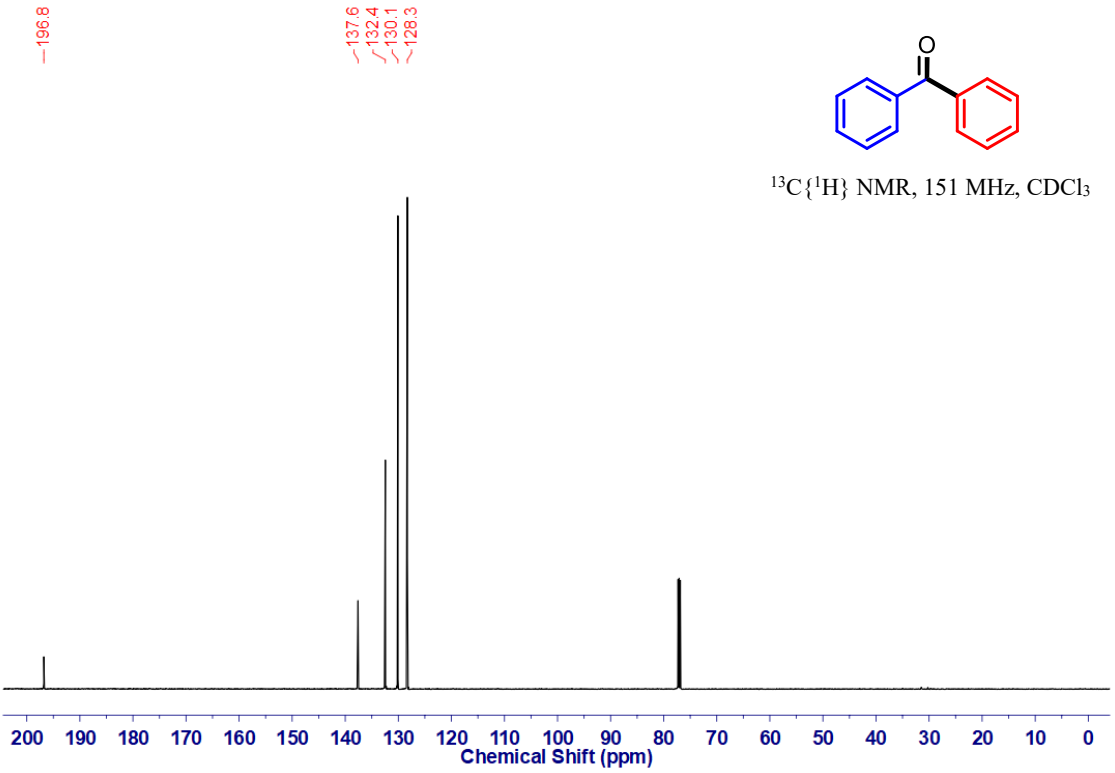


Figure S3. ^{1}H NMR (400 MHz) Spectrum of **3b** in $CDCl_3$ at 298K.

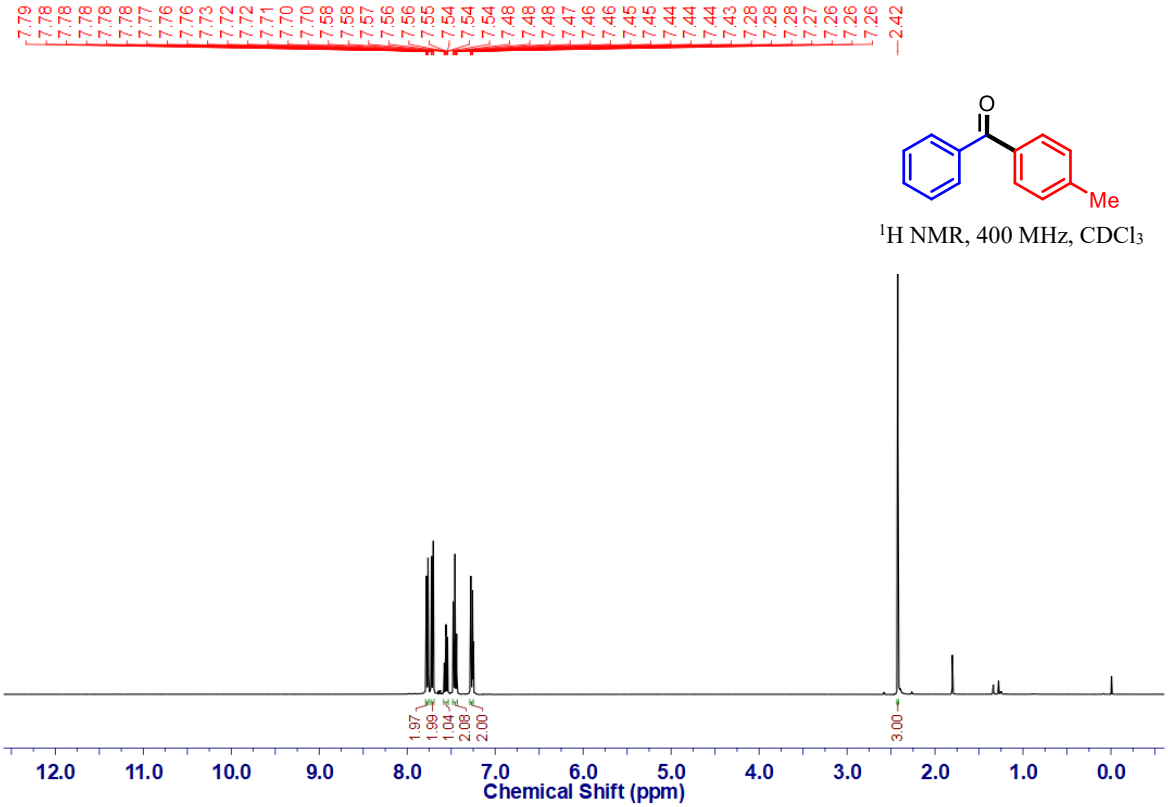


Figure S4. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3b** in $CDCl_3$ at 298K.

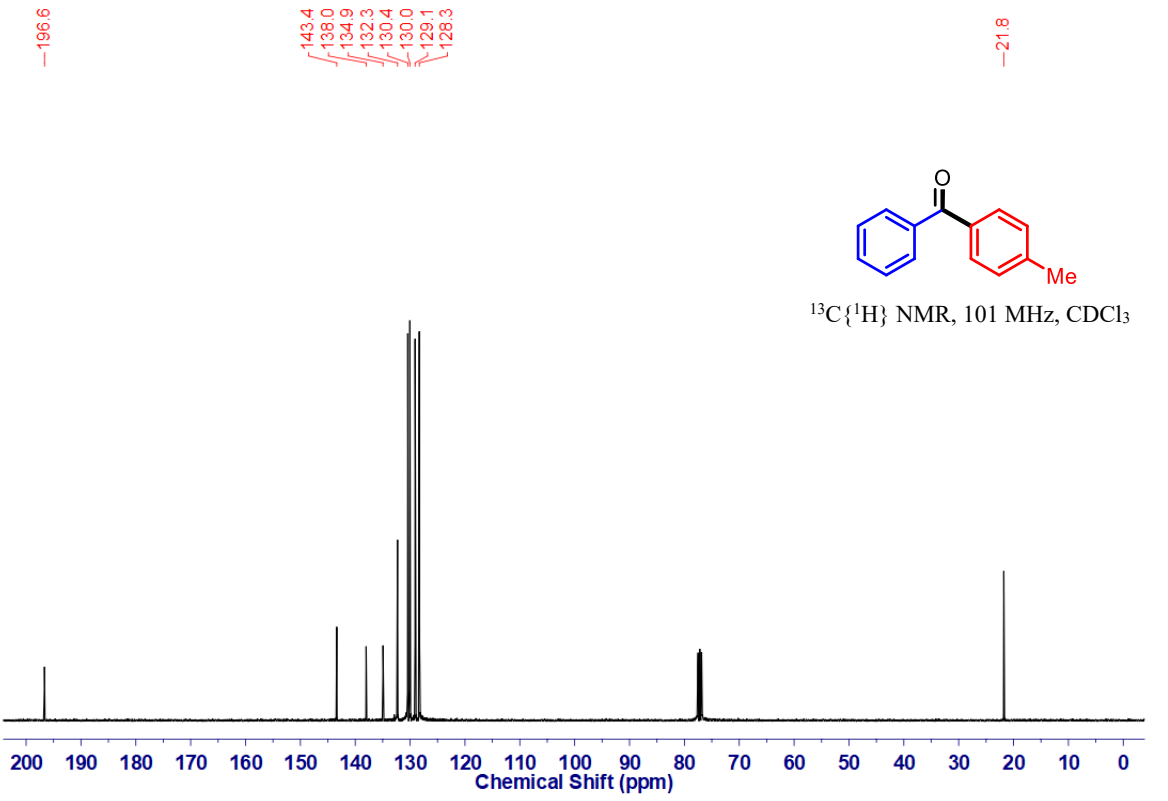


Figure S5. ^{1}H NMR (500 MHz) Spectrum of **3c** in $CDCl_3$ at 298K.

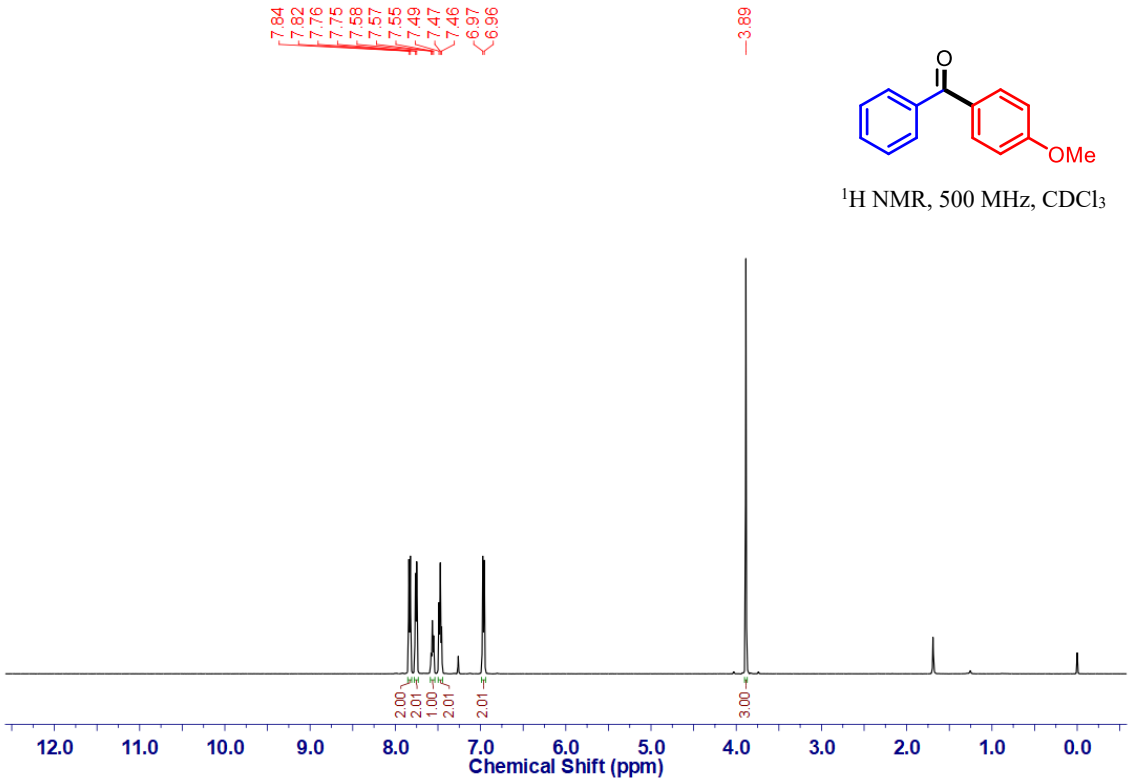


Figure S6. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3c** in $CDCl_3$ at 298K.

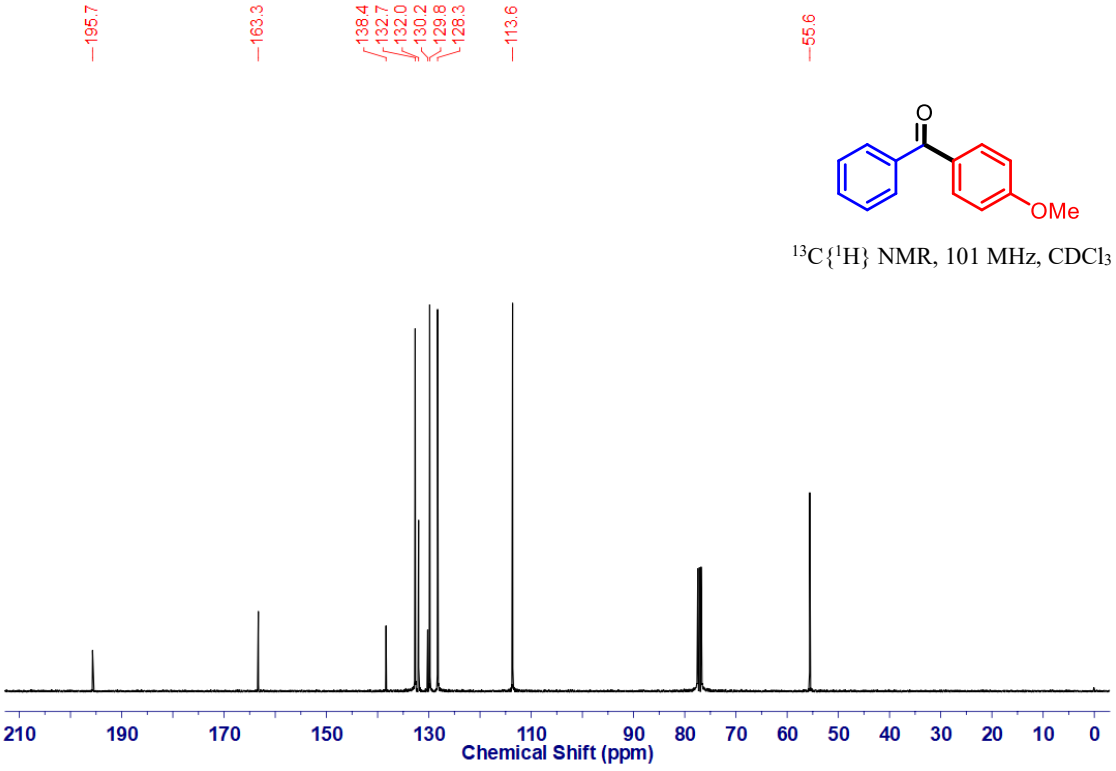
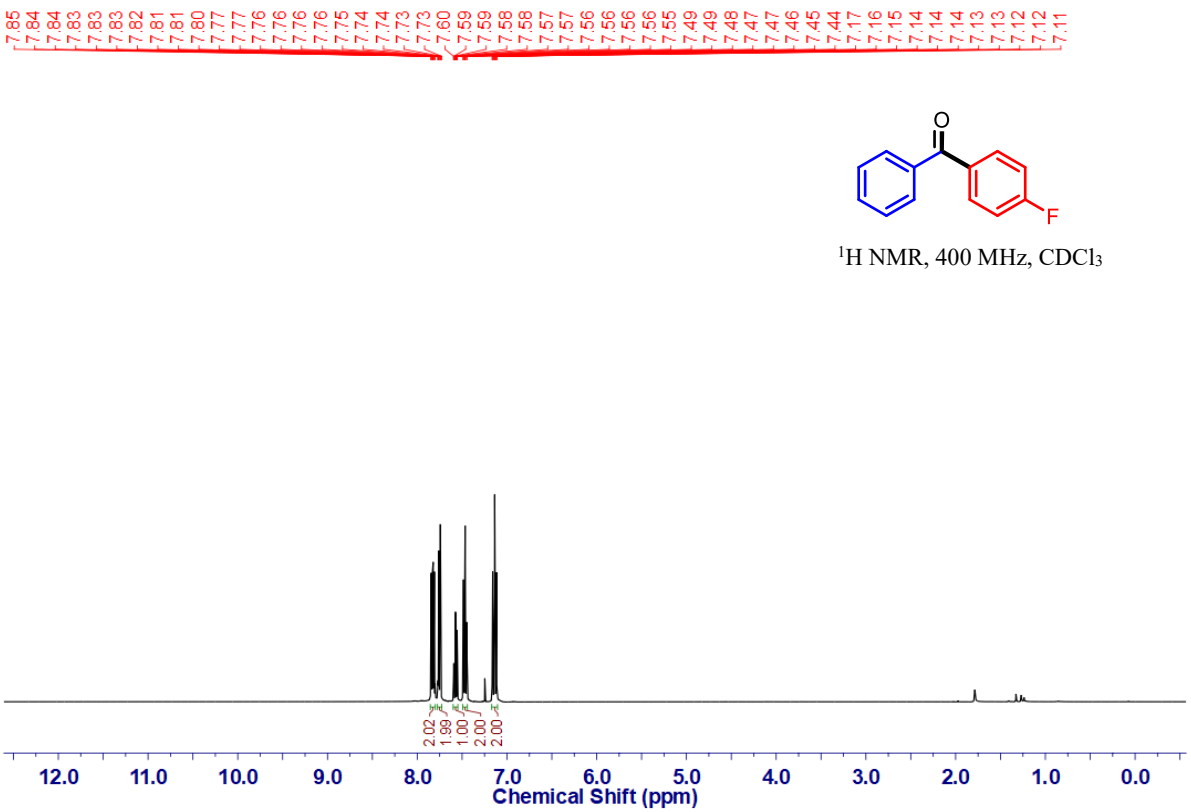
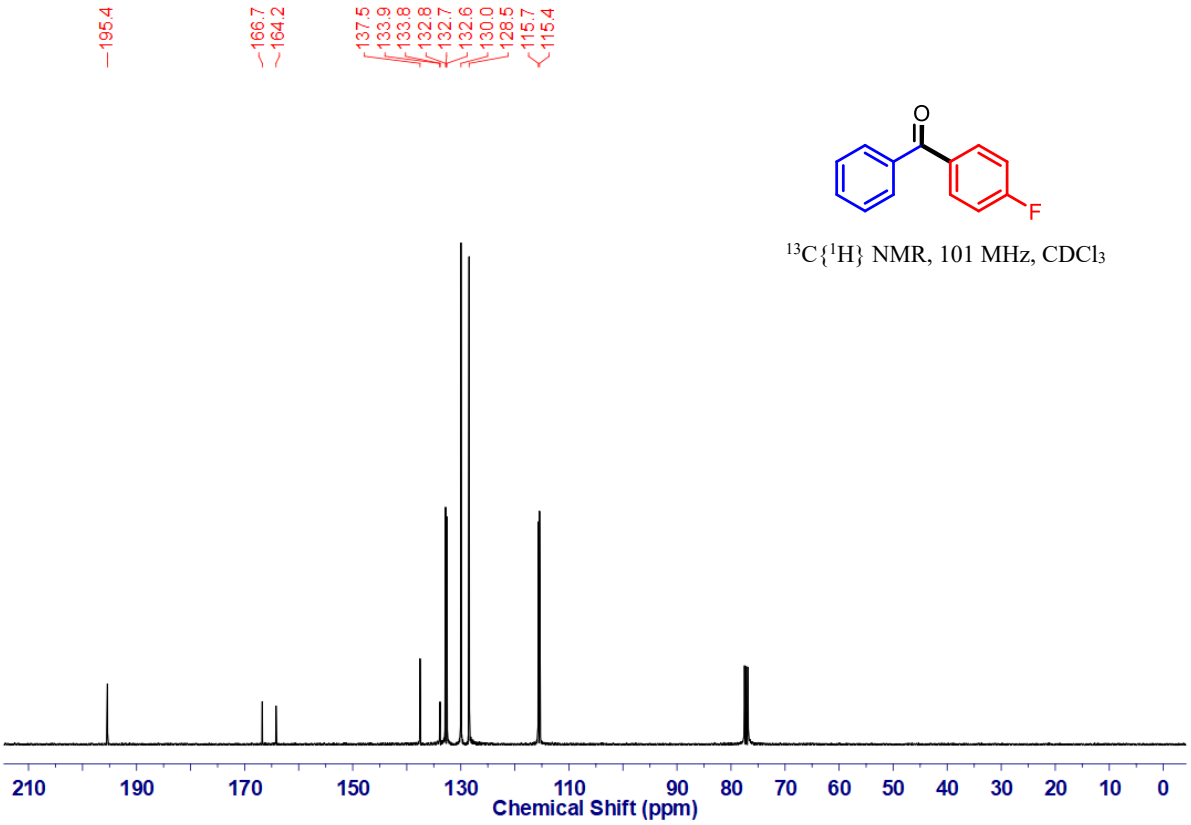


Figure S7. ^{1}H NMR (400 MHz) Spectrum of **3d** in $CDCl_3$ at 298K.



^{1}H NMR, 400 MHz, $CDCl_3$

Figure S8. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3d** in $CDCl_3$ at 298K.



$^{13}C\{^{1}H\}$ NMR, 101 MHz, $CDCl_3$

Figure S9. ^{19}F NMR (376 MHz) Spectrum of **3d** in $CDCl_3$ at 298K.

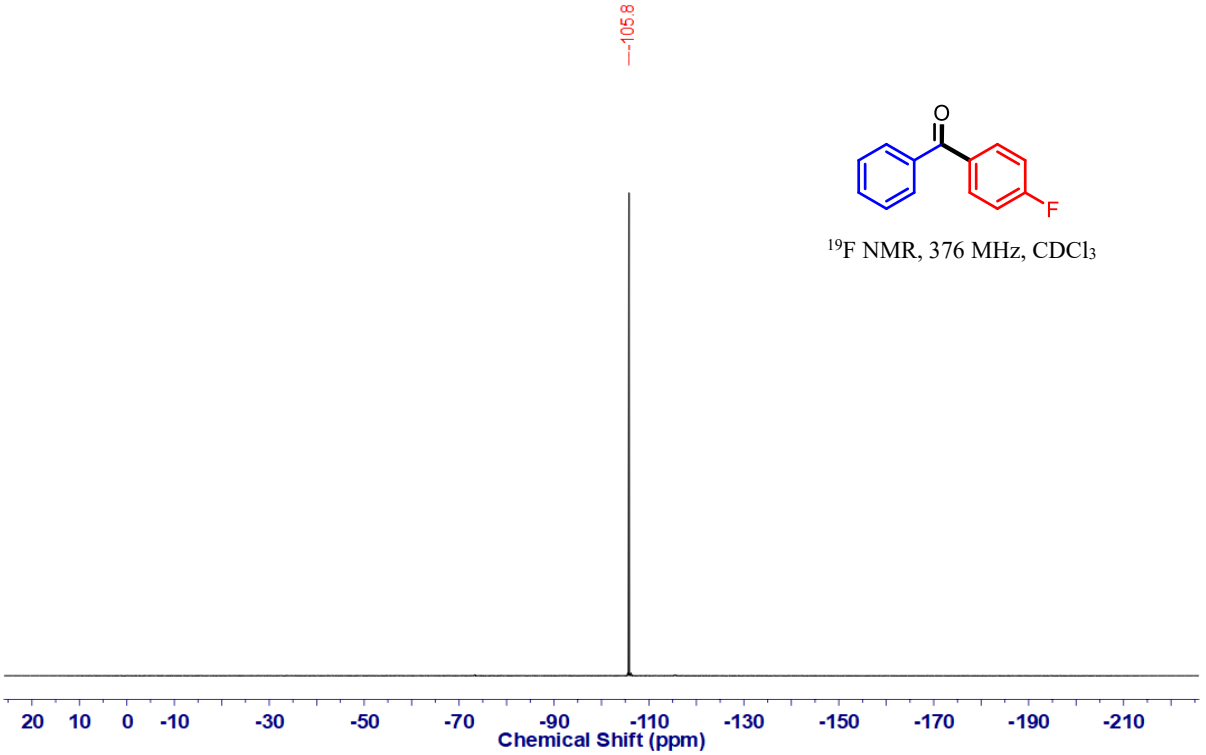


Figure S10. ^{1}H NMR (400 MHz) Spectrum of **3e** in $CDCl_3$ at 298K.

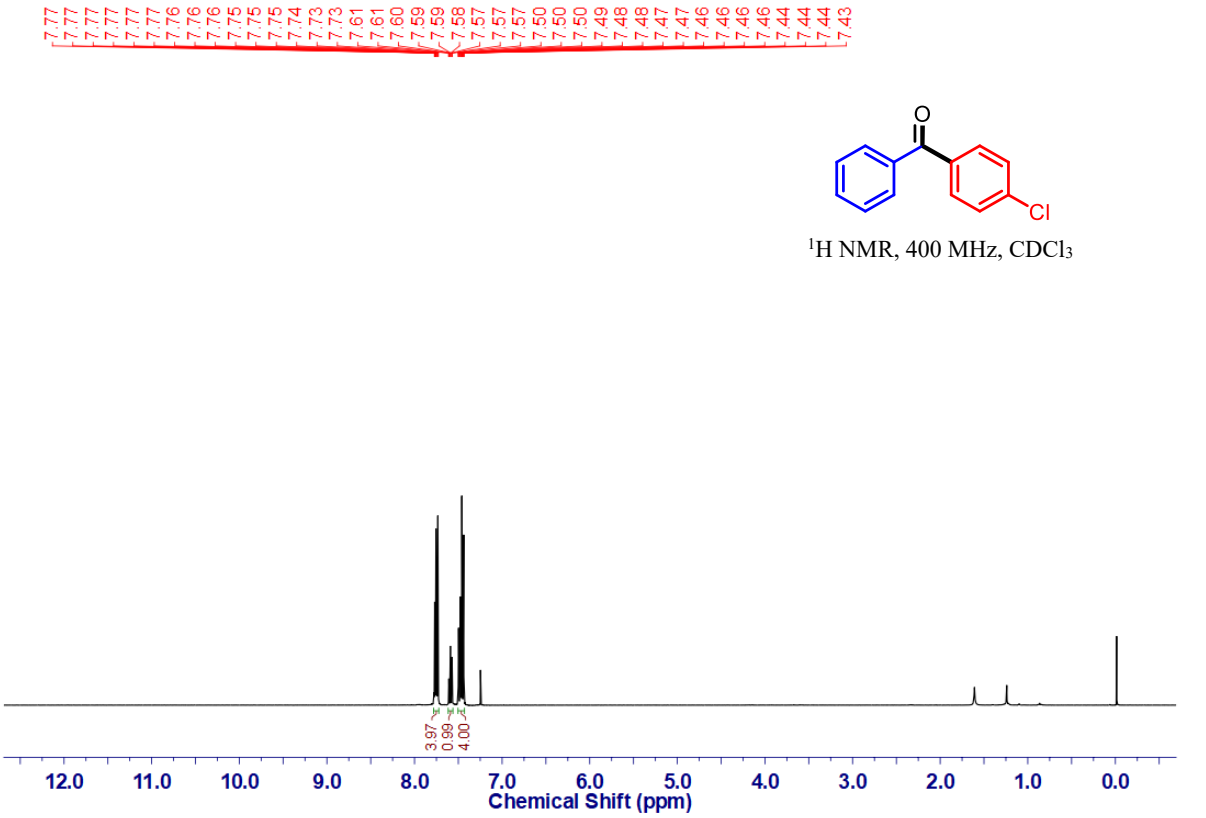


Figure S11. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3e** in $CDCl_3$ at 298K.

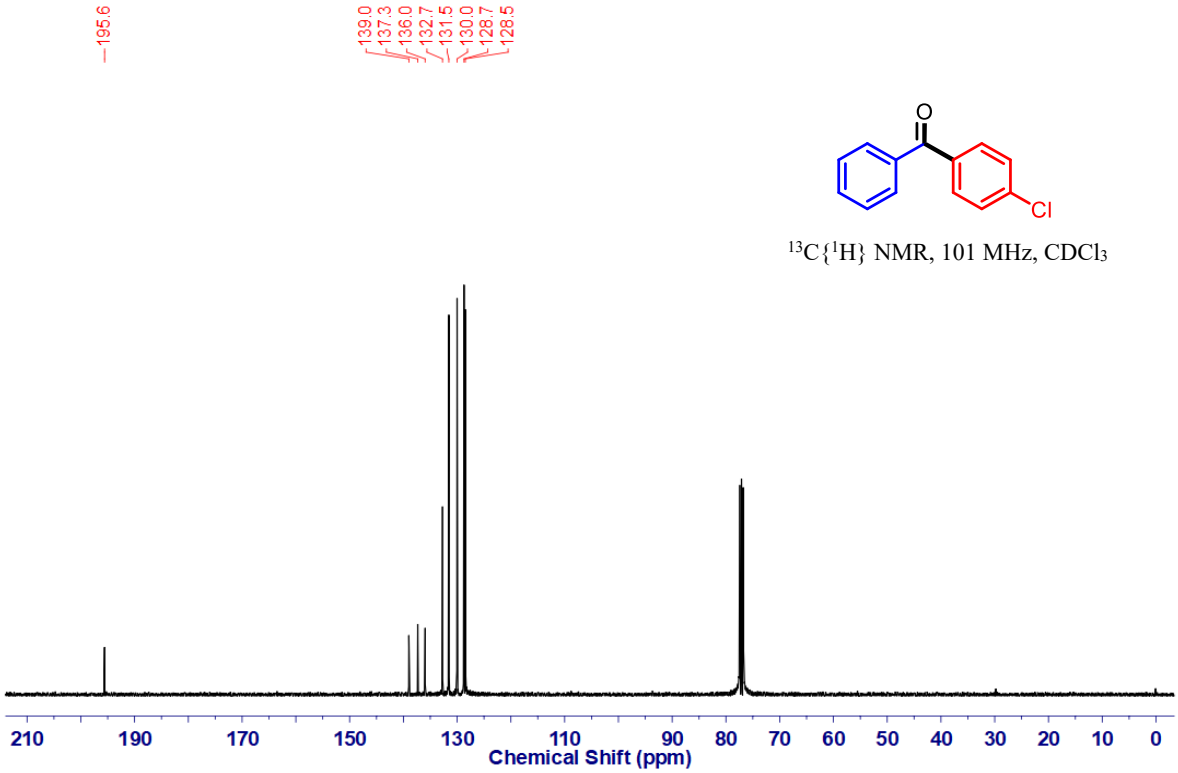


Figure S12. ^{1}H NMR (400 MHz) Spectrum of **3f** in $CDCl_3$ at 298K.

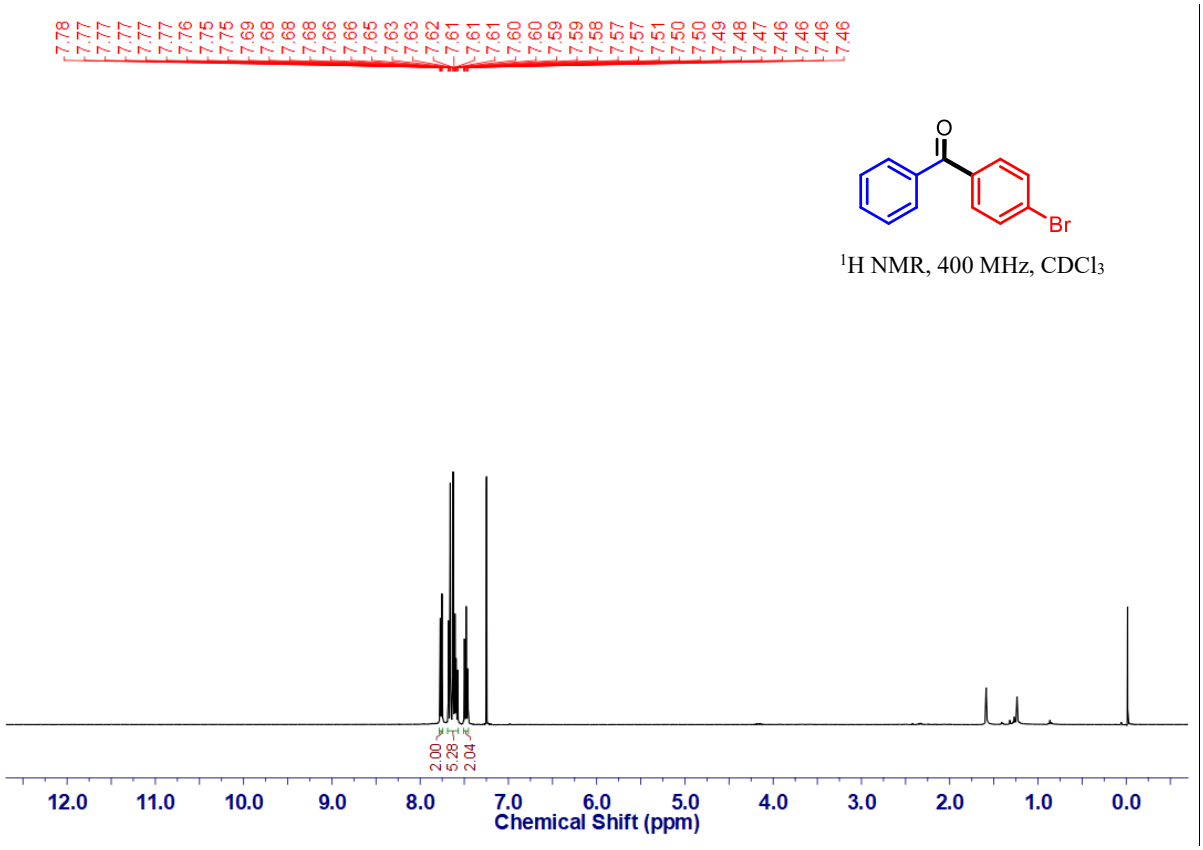


Figure S13. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3f** in $CDCl_3$ at 298K.

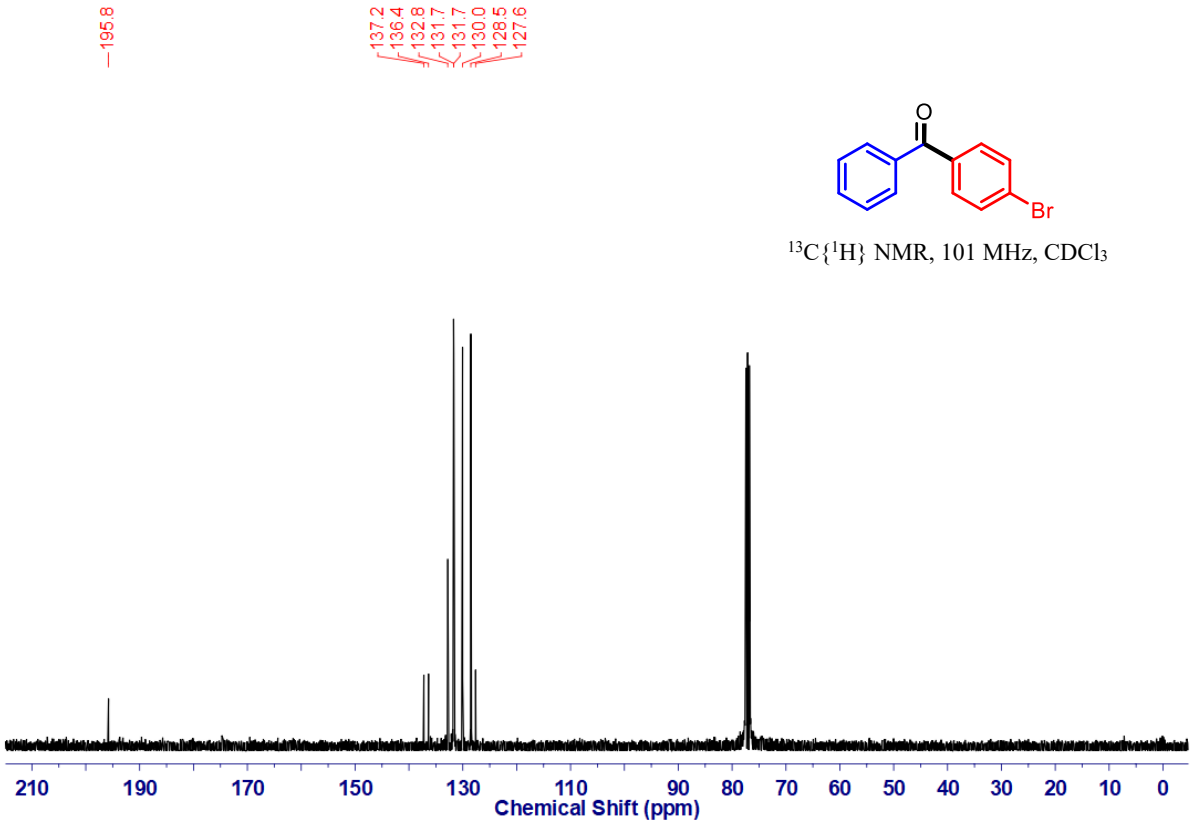


Figure S14. ^{1}H NMR (400 MHz) Spectrum of **3g** in $CDCl_3$ at 298K.

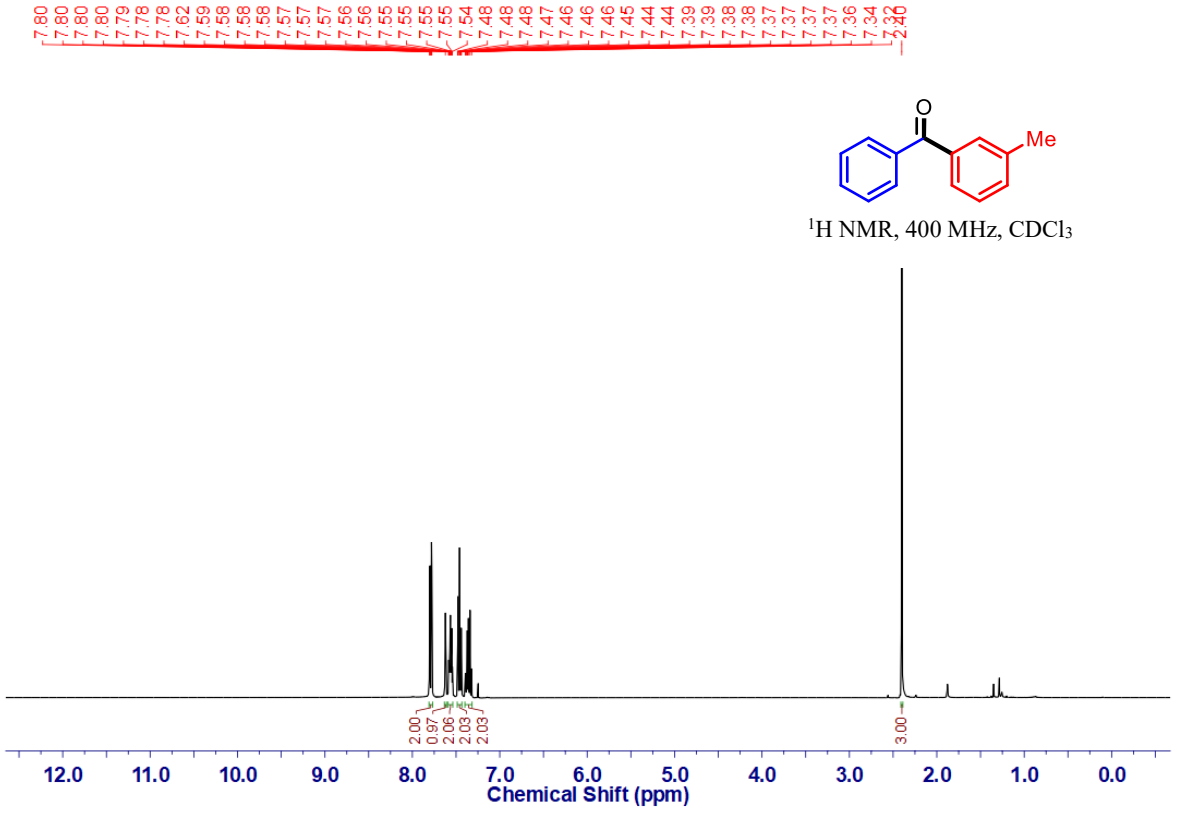


Figure S15. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3g** in $CDCl_3$ at 298K.

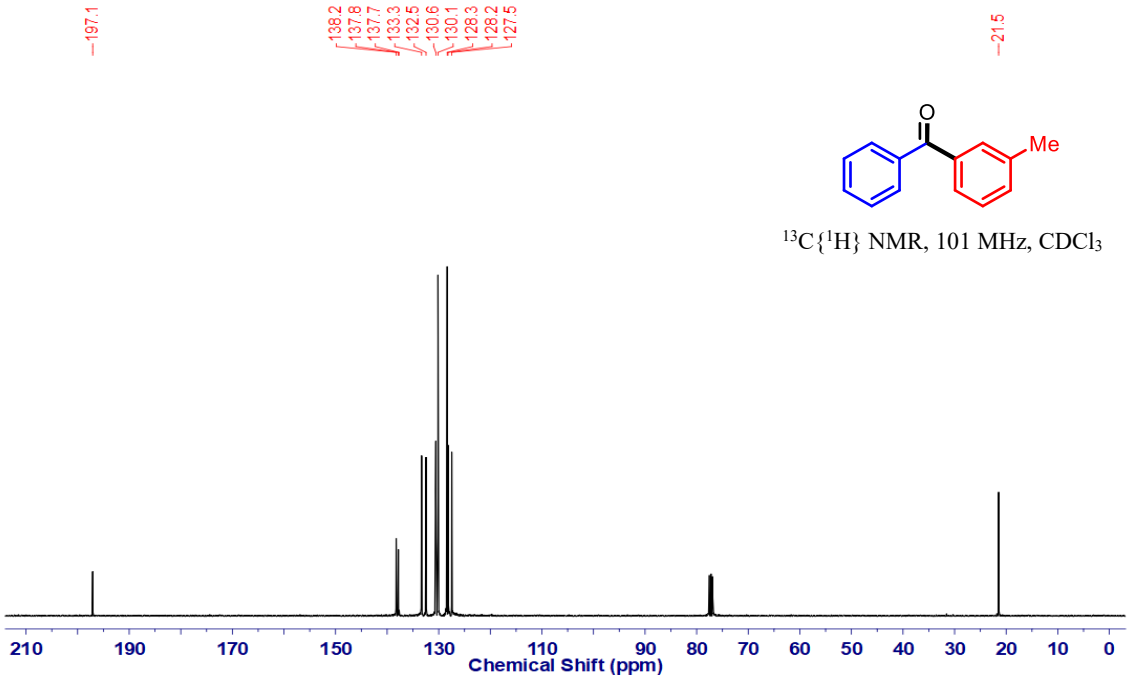


Figure S16. ^{1}H NMR (400 MHz) Spectrum of **3h** in $CDCl_3$ at 298K.

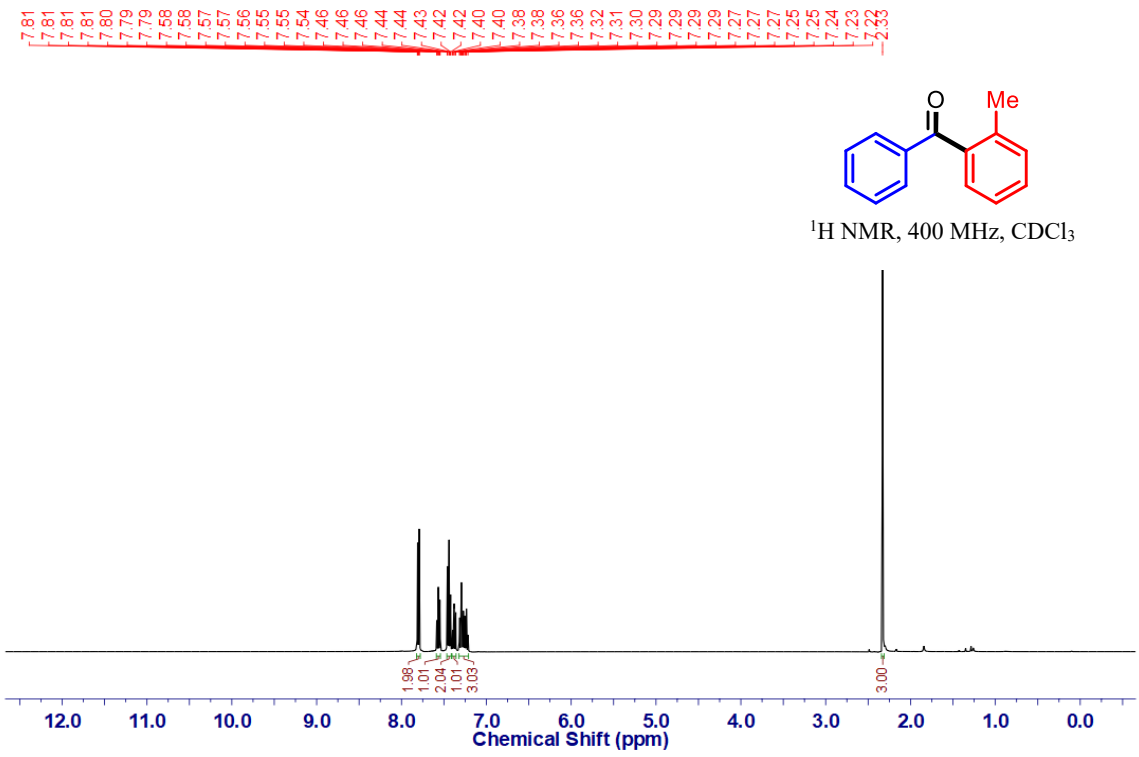


Figure S17. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3h** in $CDCl_3$ at 298K.

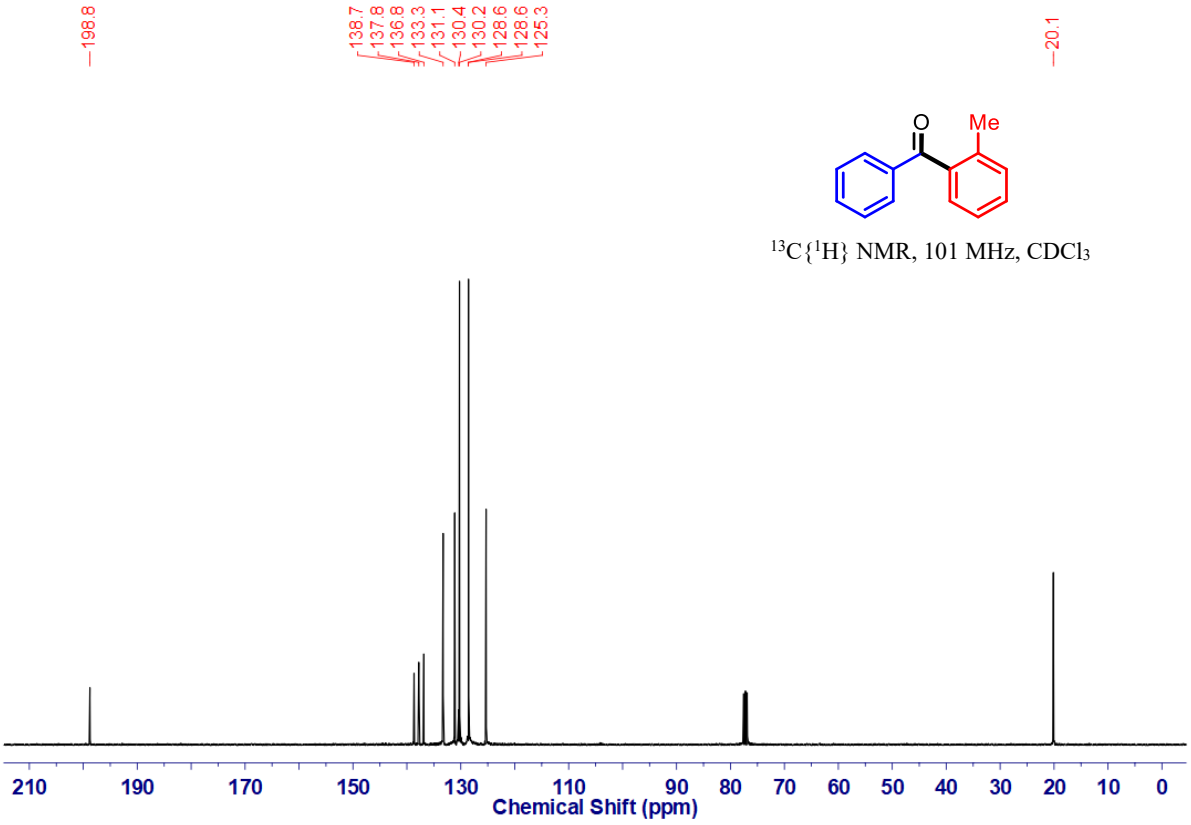


Figure S18. ^{1}H NMR (400 MHz) Spectrum of **3i** in $CDCl_3$ at 298K.

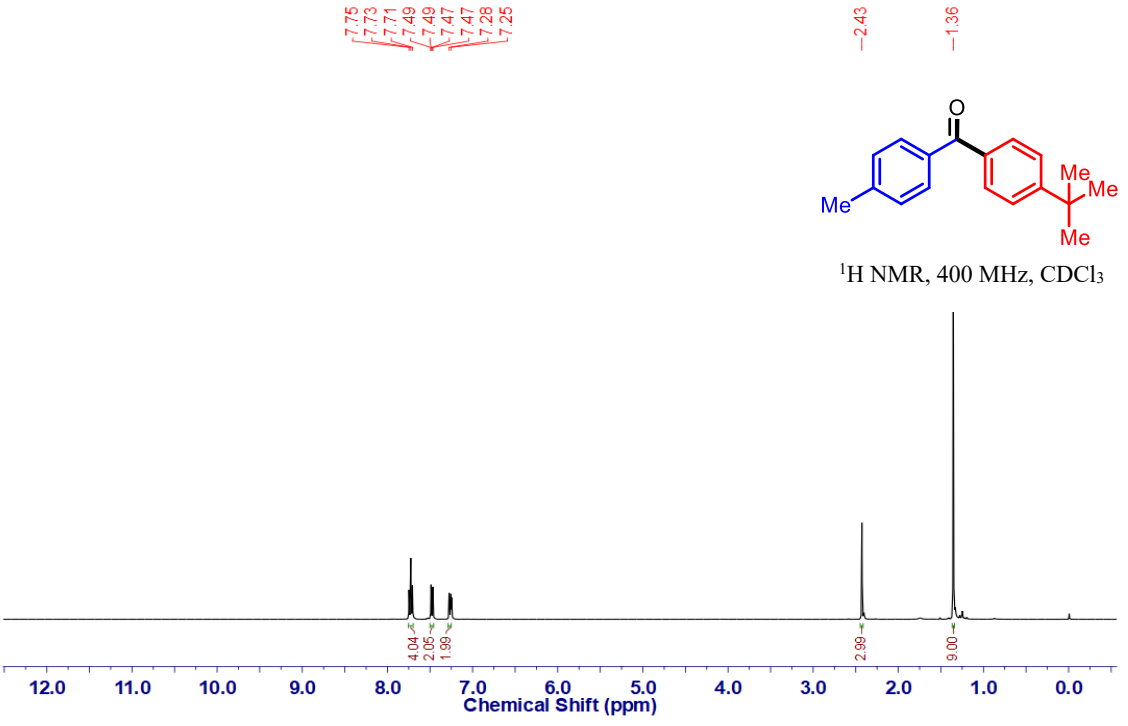


Figure S19. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3i** in $CDCl_3$ at 298K.

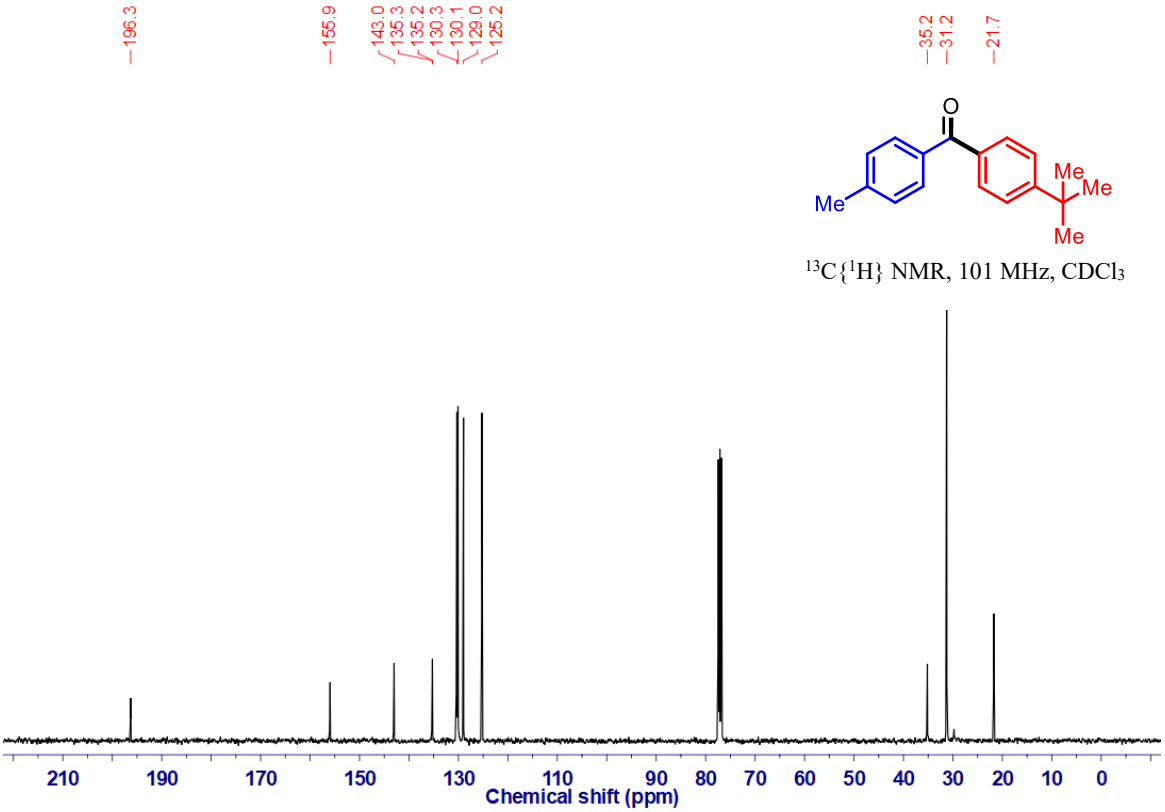


Figure S20. ^{1}H NMR (400 MHz) Spectrum of **3j** in $CDCl_3$ at 298K.

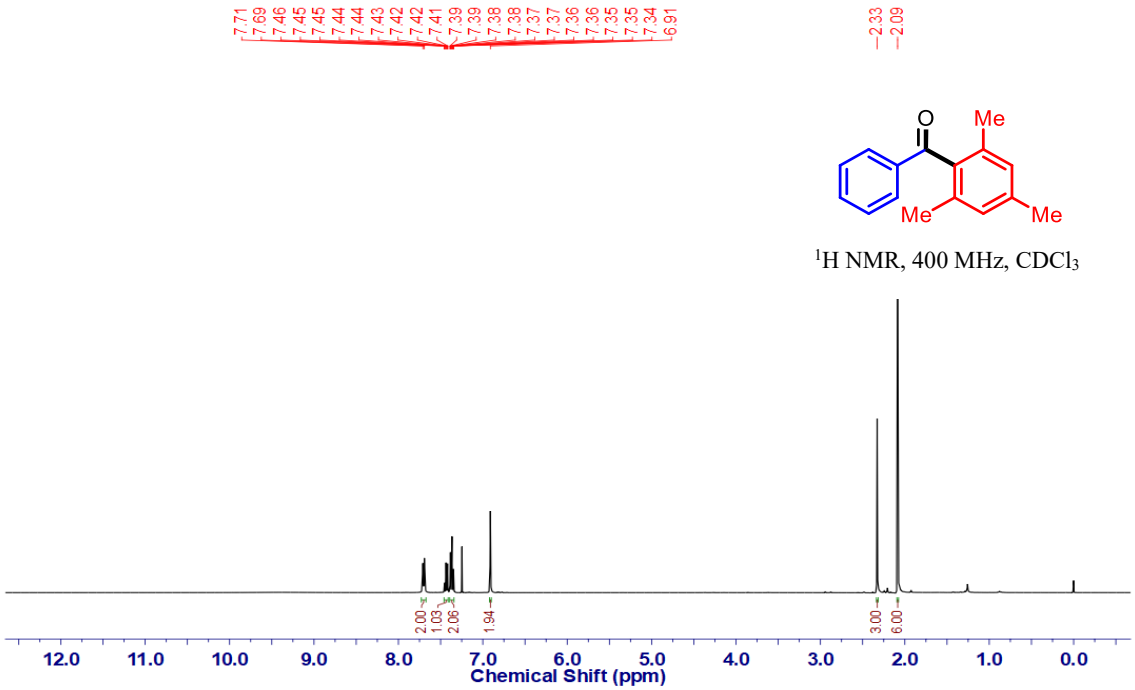


Figure S21. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3j** in $CDCl_3$ at 298K.

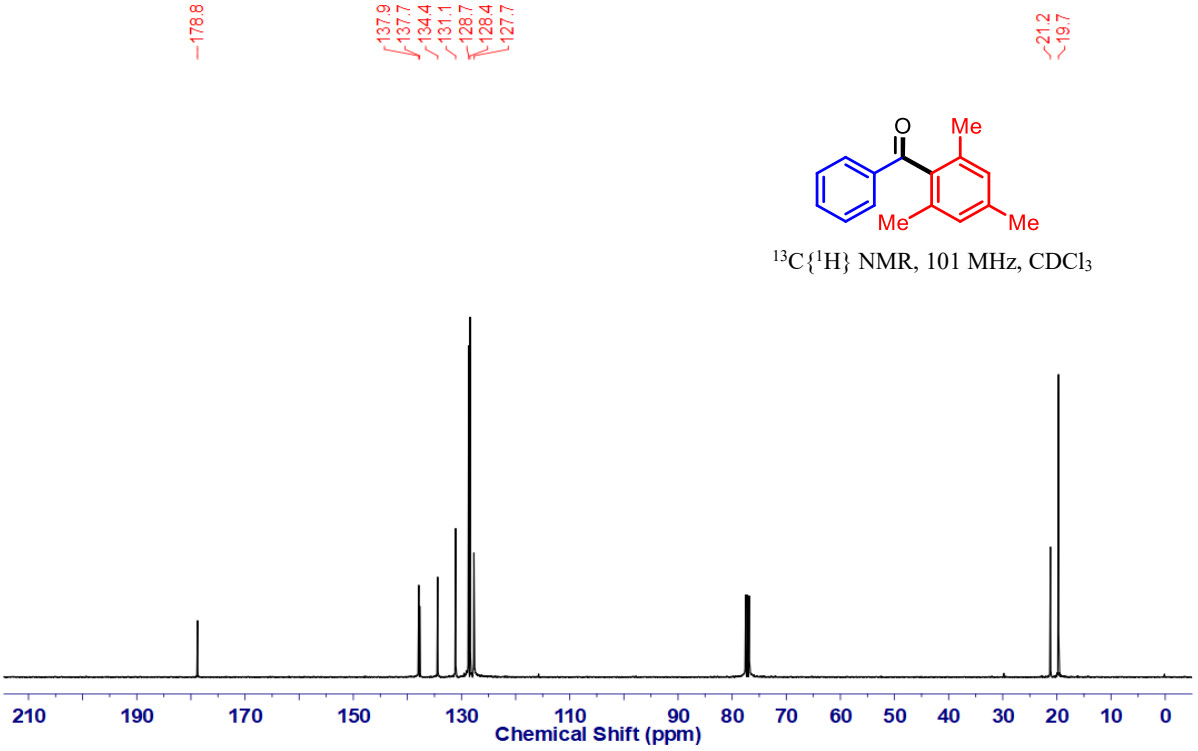


Figure S22. ^{1}H NMR (400 MHz) Spectrum of **3n** in $CDCl_3$ at 298K.

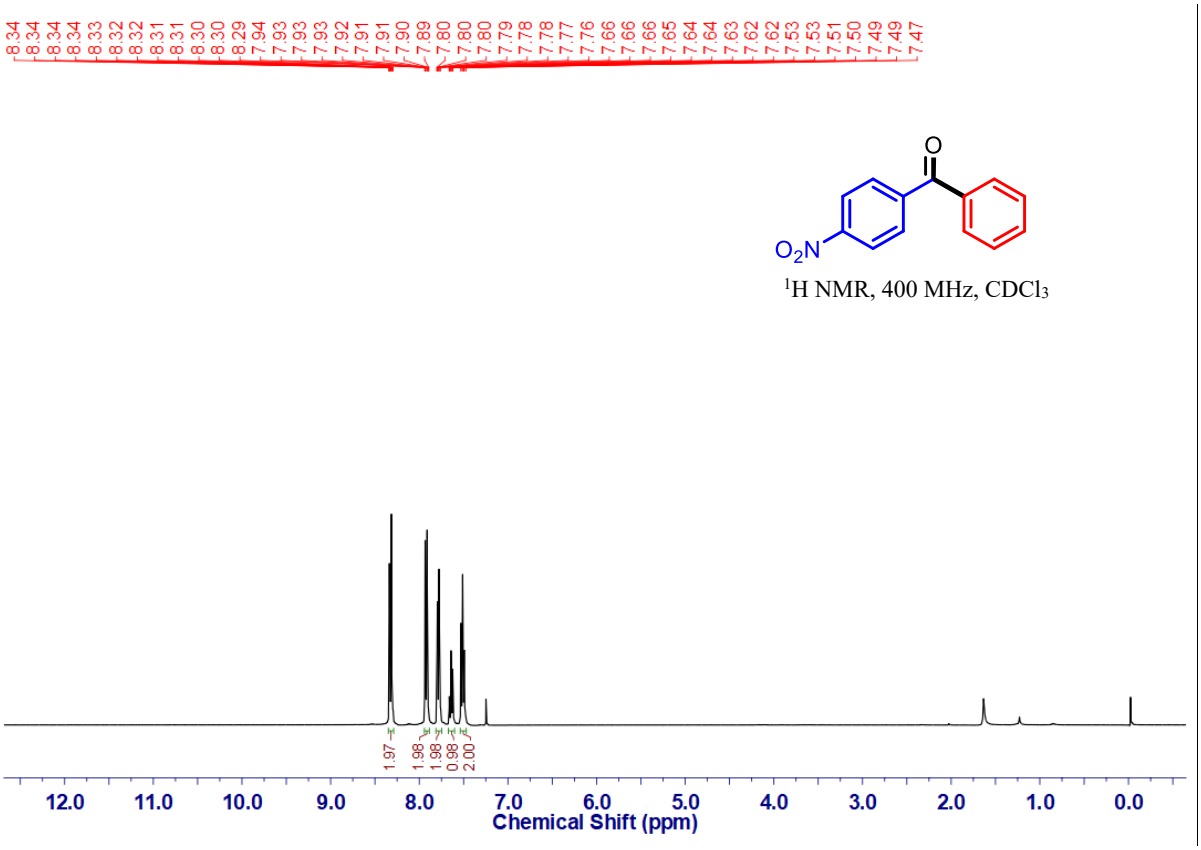


Figure S23. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3n** in $CDCl_3$ at 298K.

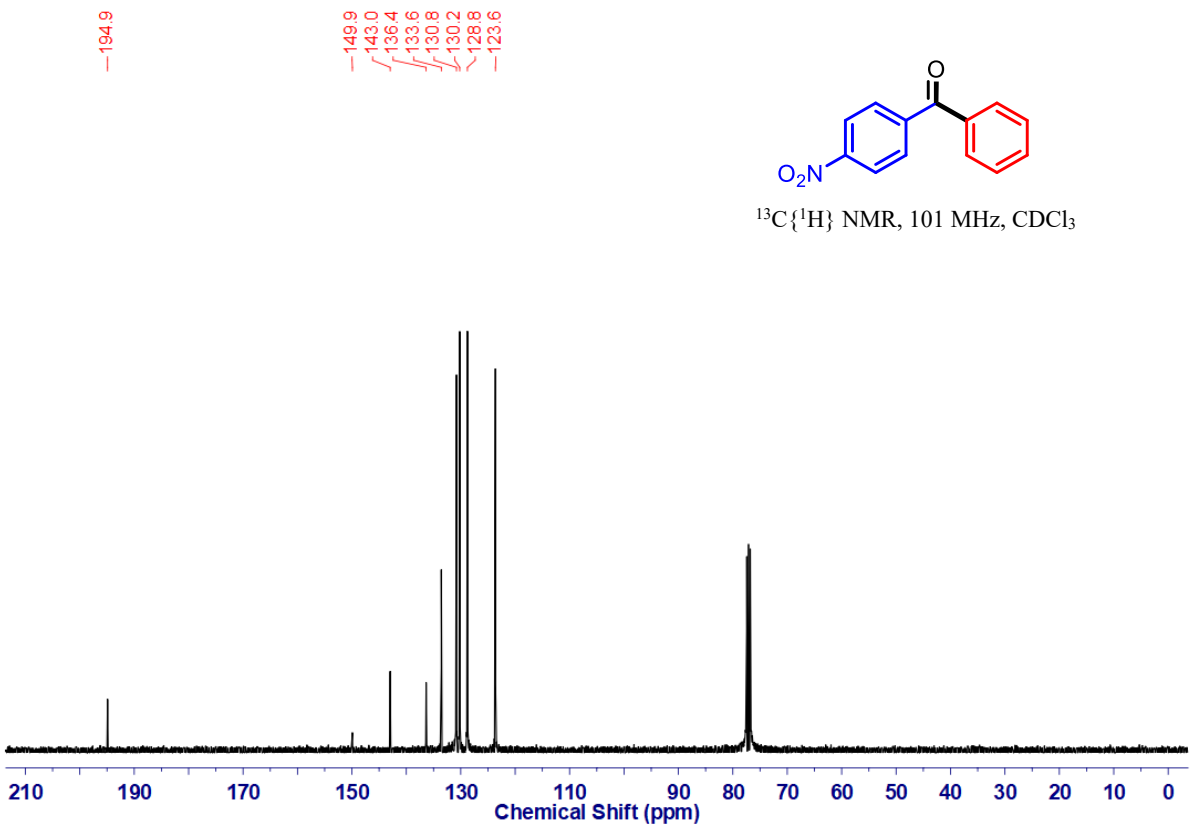


Figure S24. ^{1}H NMR (400 MHz) Spectrum of **3o** in DMSO-d_6 at 298K.

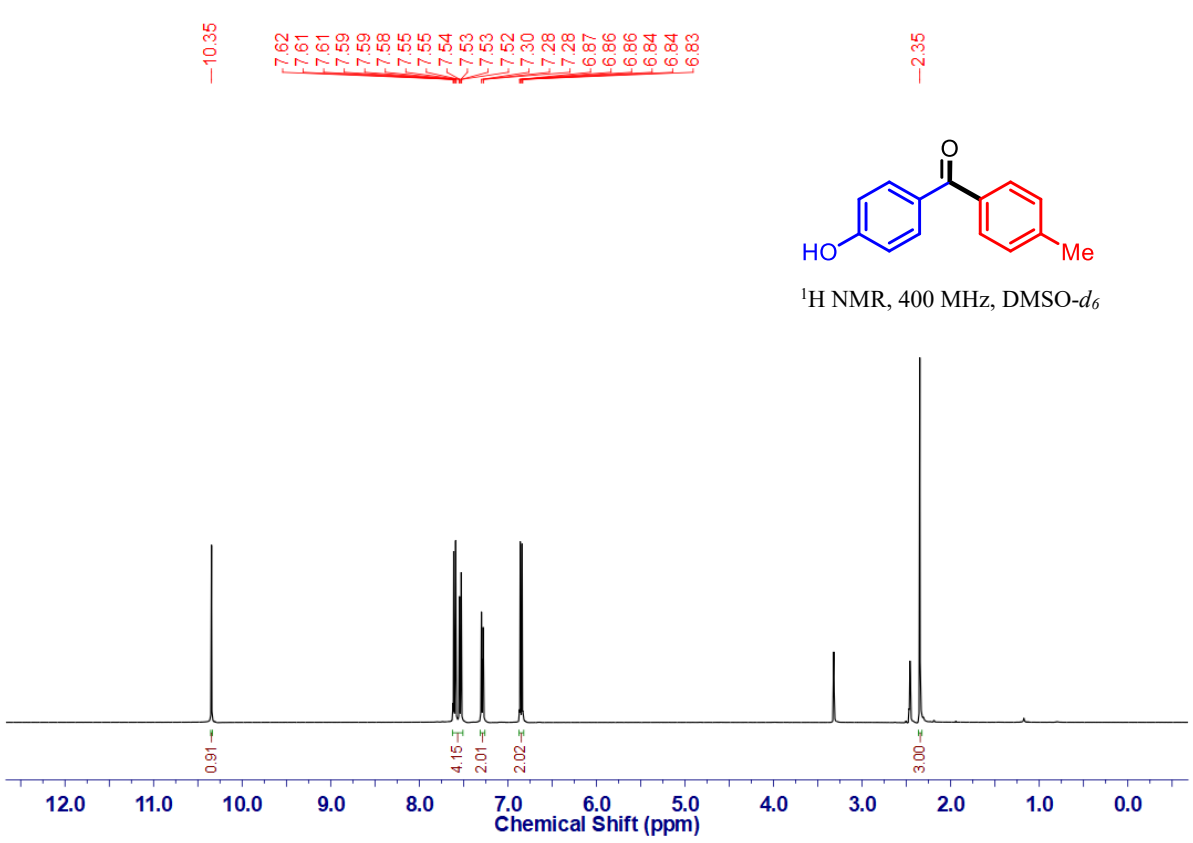


Figure S25. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3o** in DMSO-d_6 at 298K.

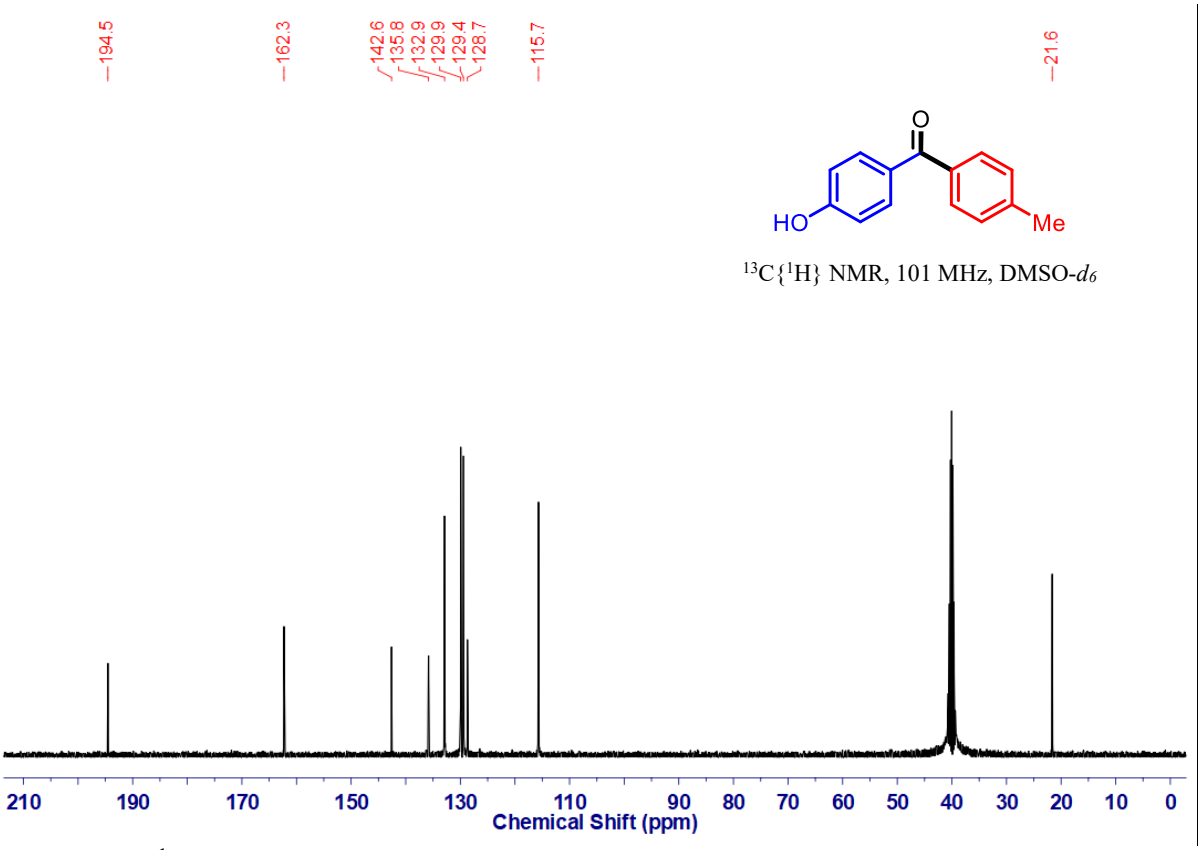


Figure S26. ^{1}H NMR (400 MHz) Spectrum of **3p** in $CDCl_3$ at 298K.

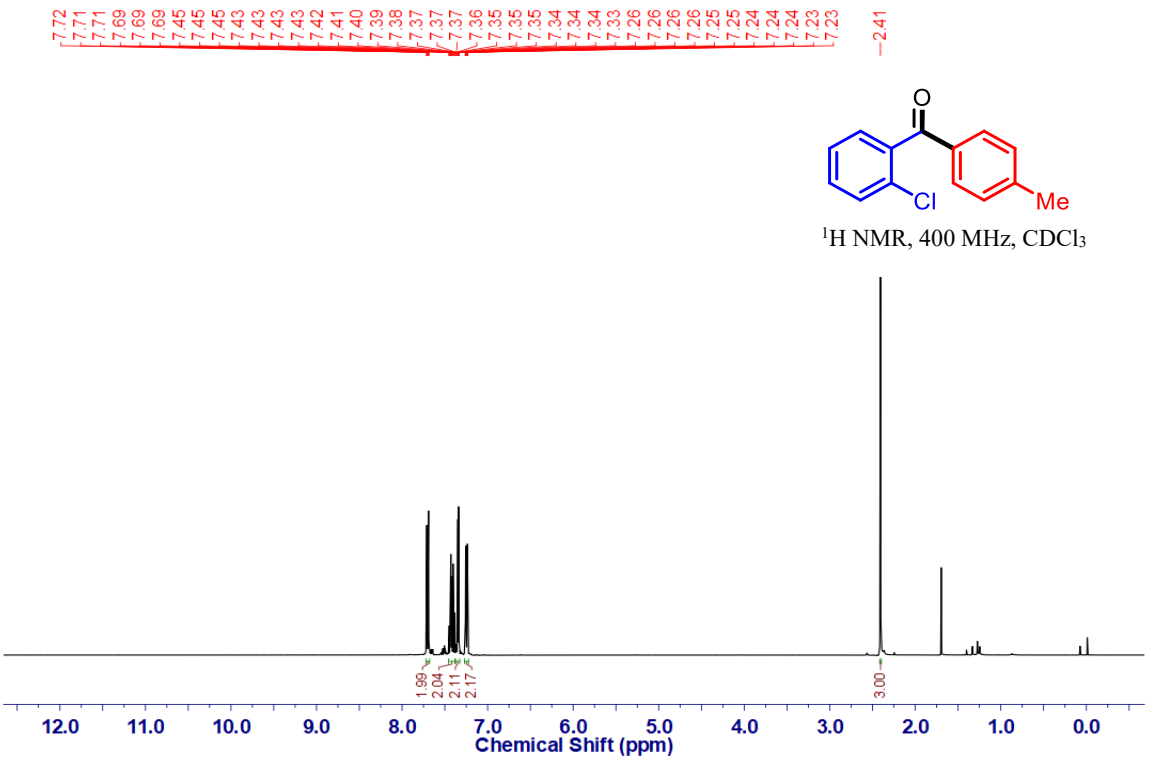


Figure S27. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3p** in $CDCl_3$ at 298K.

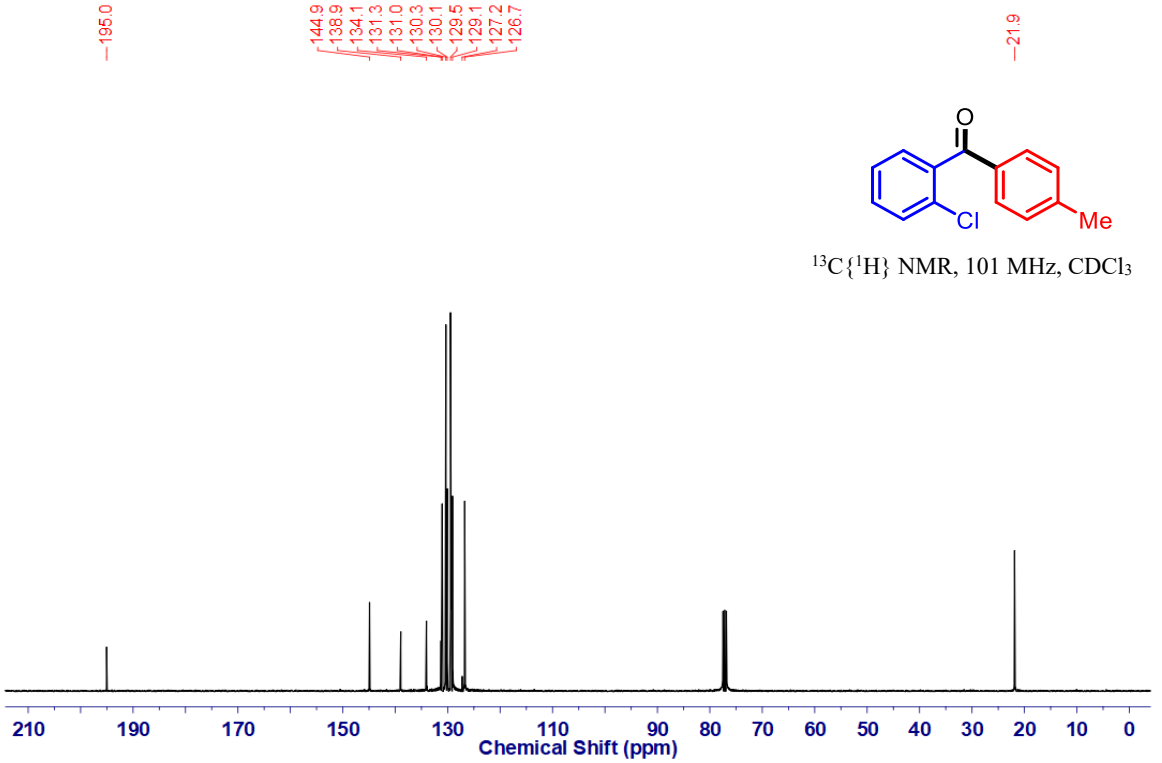


Figure S28. ^{1}H NMR (400 MHz) Spectrum of **3q** in DMSO-d_6 at 298K.

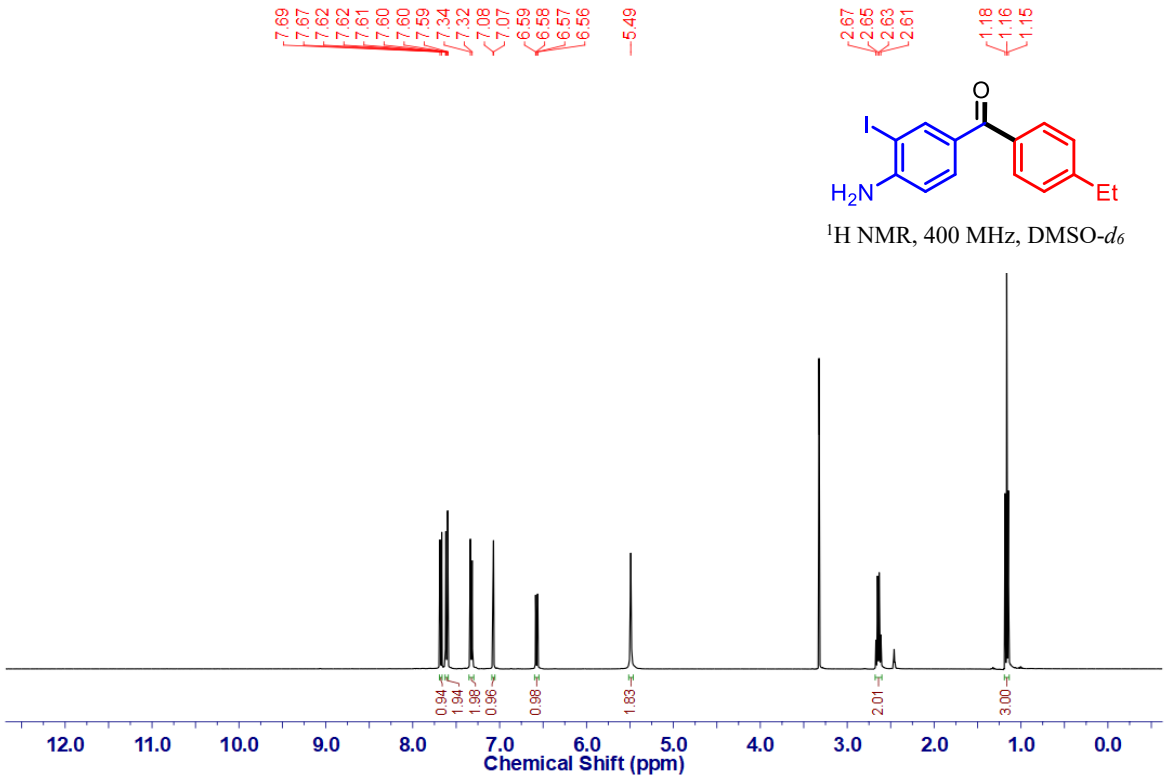


Figure S29. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3q** in DMSO-d_6 at 298K.

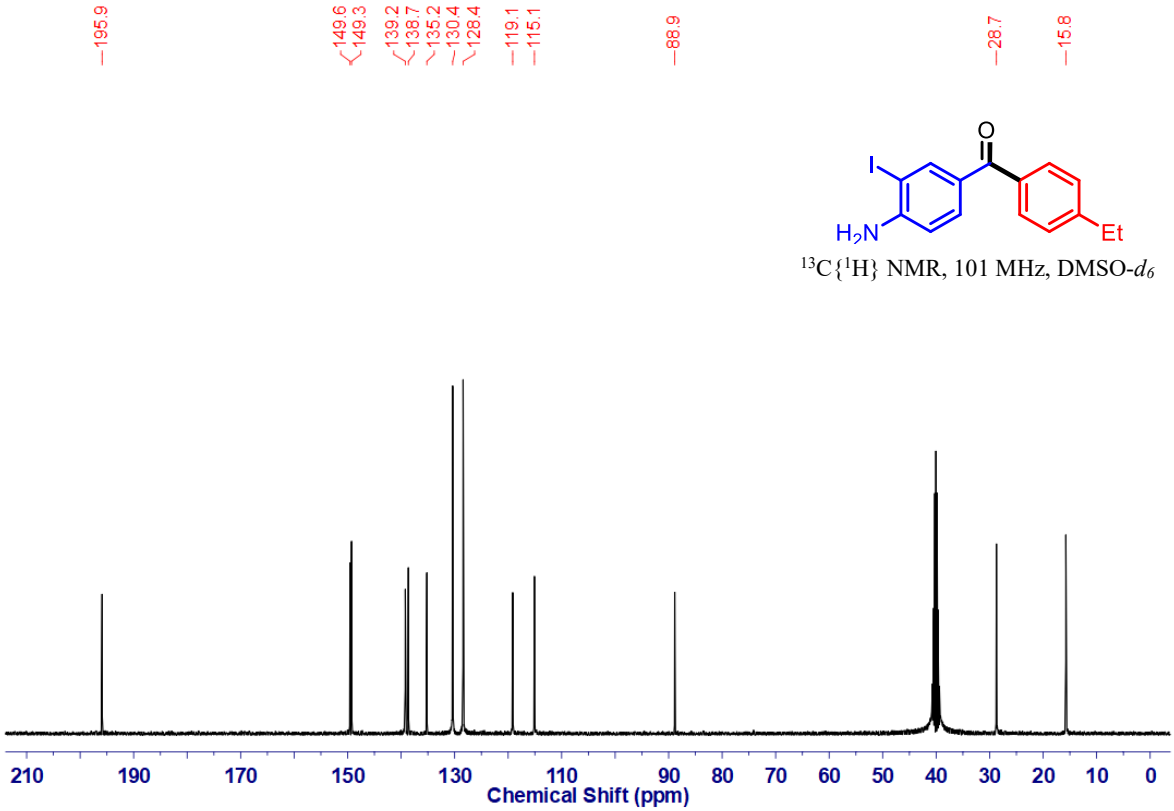


Figure S30. ^{1}H NMR (400 MHz) Spectrum of **3r** in $CDCl_3$ at 298K.

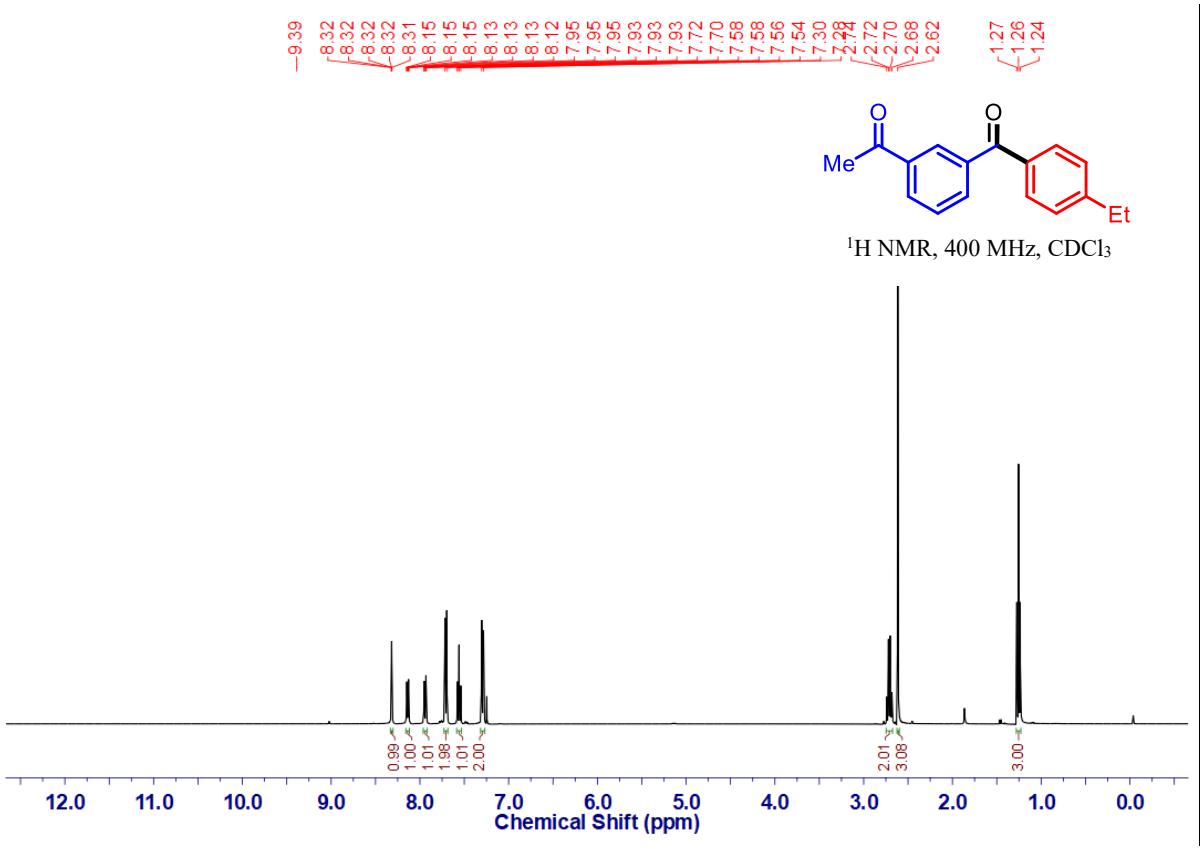


Figure S31. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3r** in $CDCl_3$ at 298K.

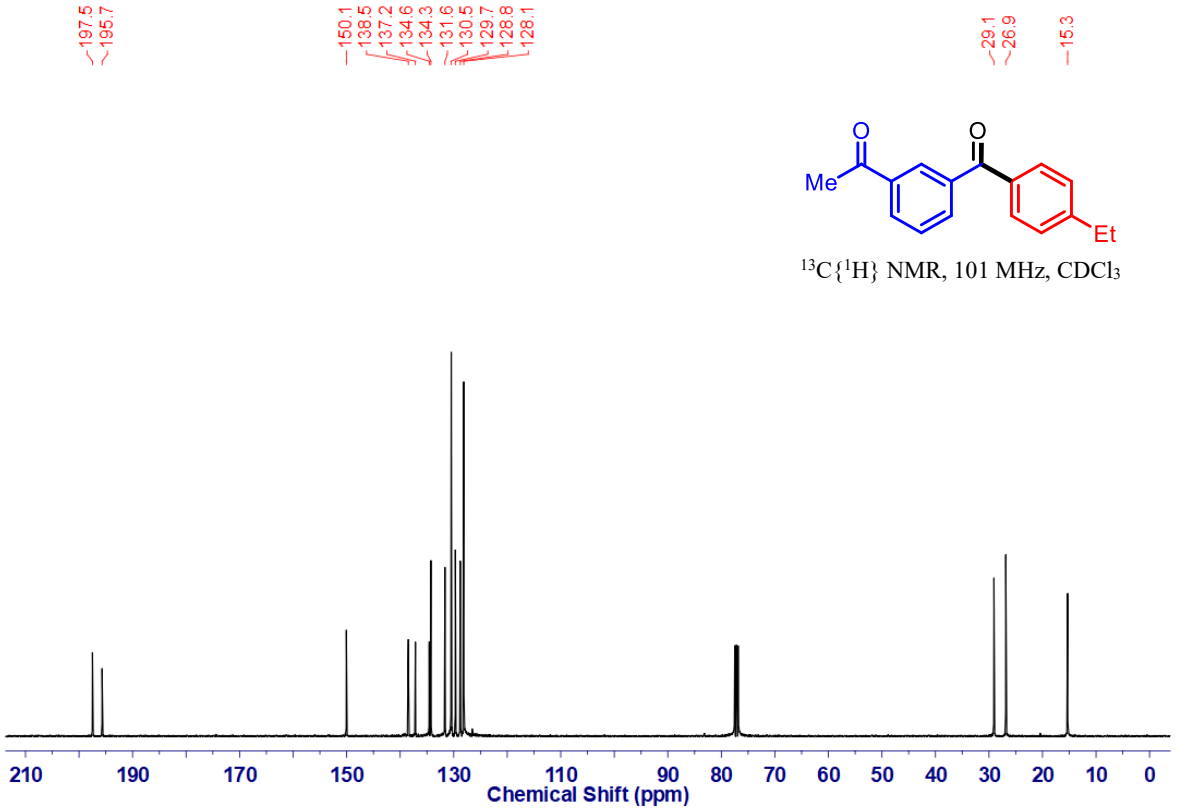


Figure S32. ^{1}H NMR (400 MHz) Spectrum of **3s** in $CDCl_3$ at 298K.

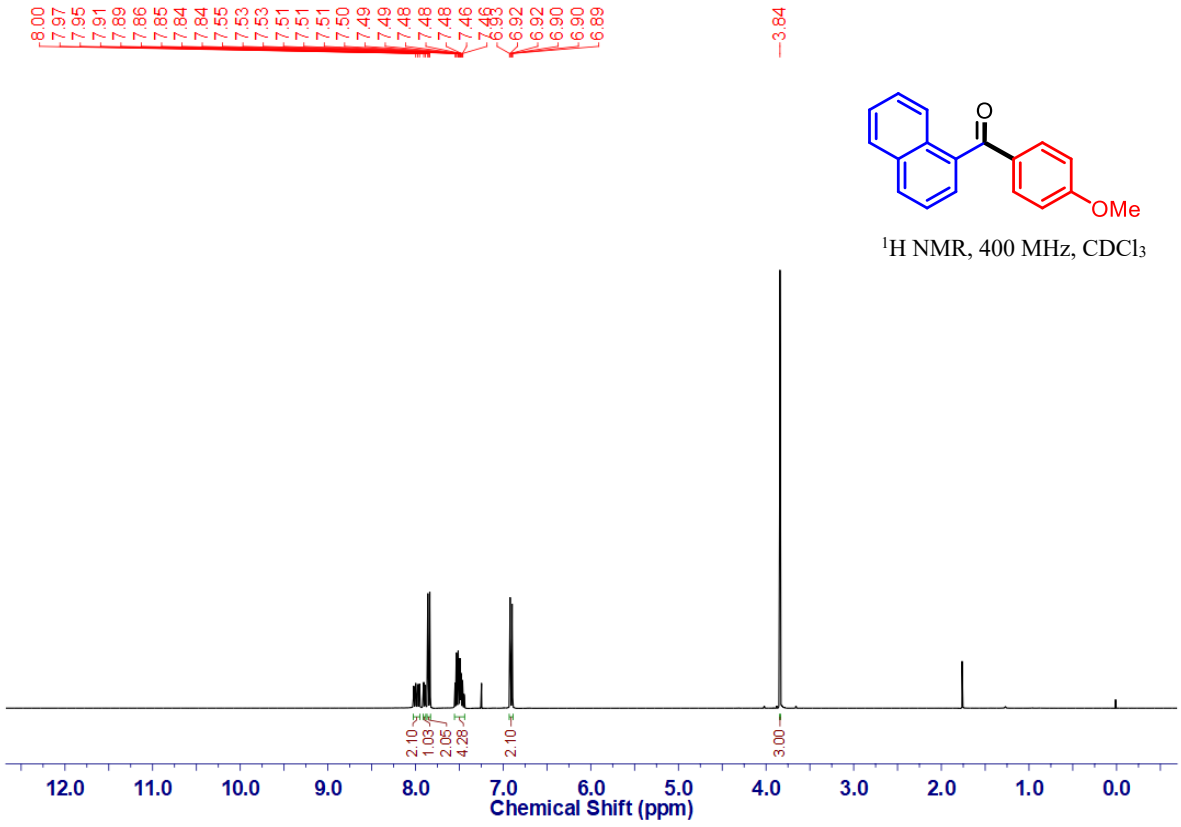


Figure S33. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3s** in $CDCl_3$ at 298K.

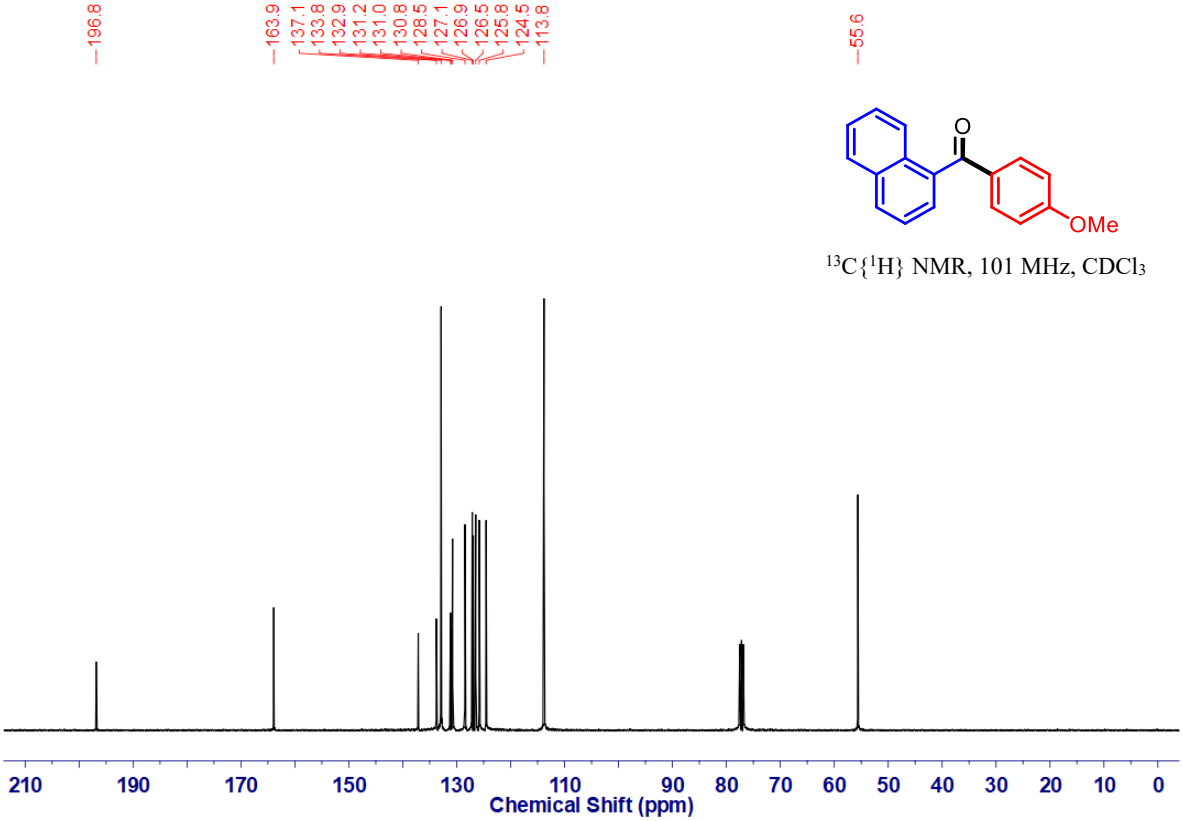


Figure S34. ^{1}H NMR (400 MHz) Spectrum of **3t** in $CDCl_3$ at 298K.

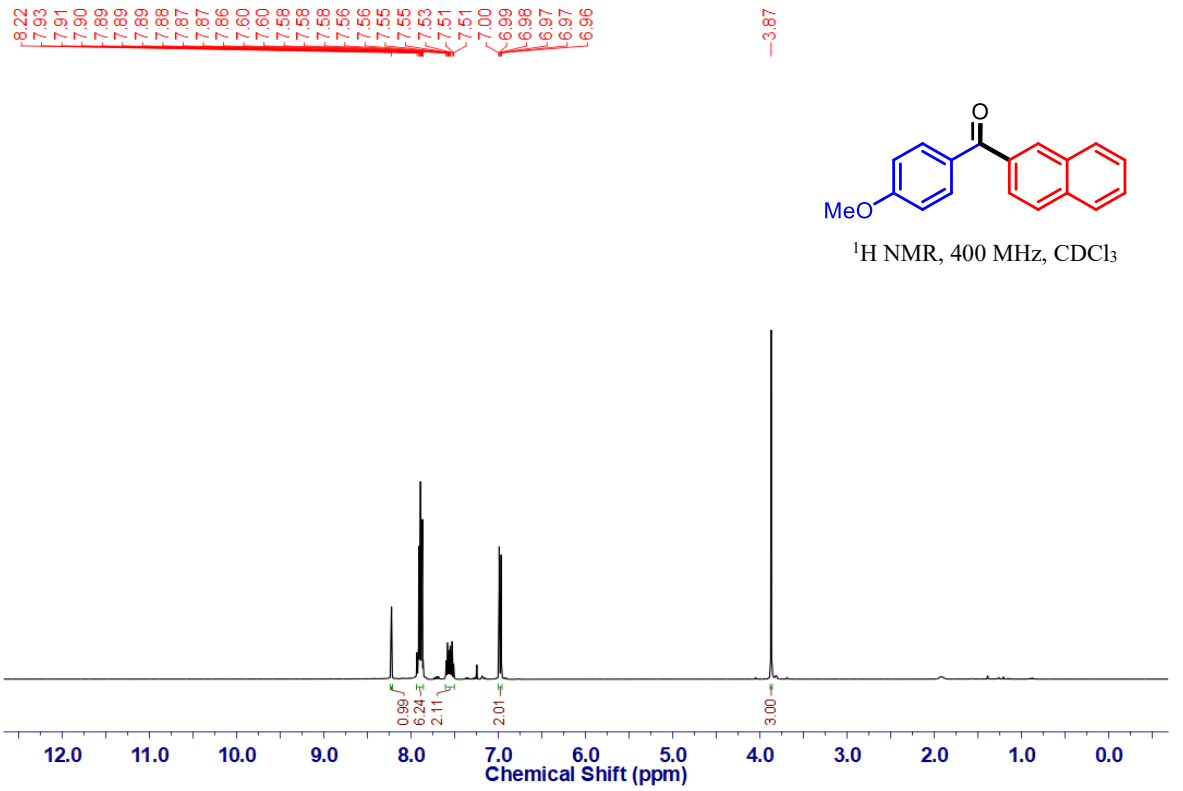


Figure S35. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3t** in $CDCl_3$ at 298K.

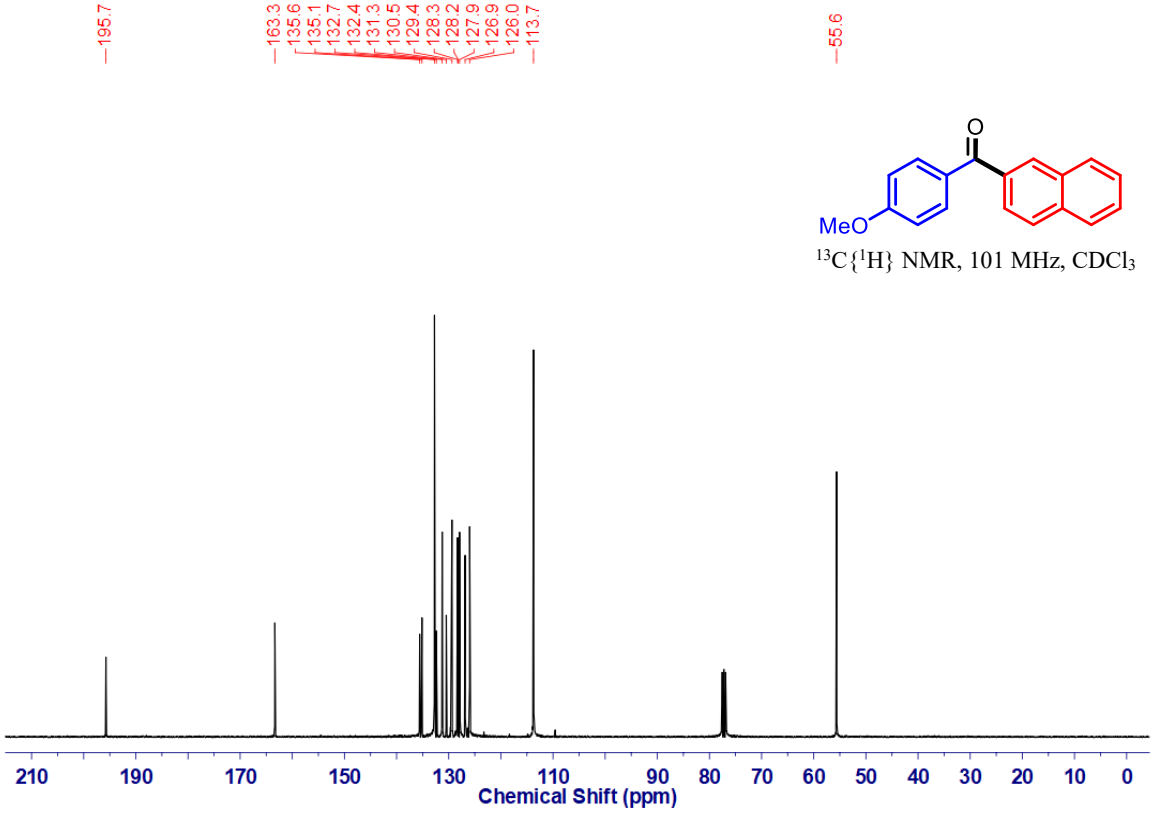


Figure S36. ^{1}H NMR (400 MHz) Spectrum of **3u** in $CDCl_3$ at 298K.

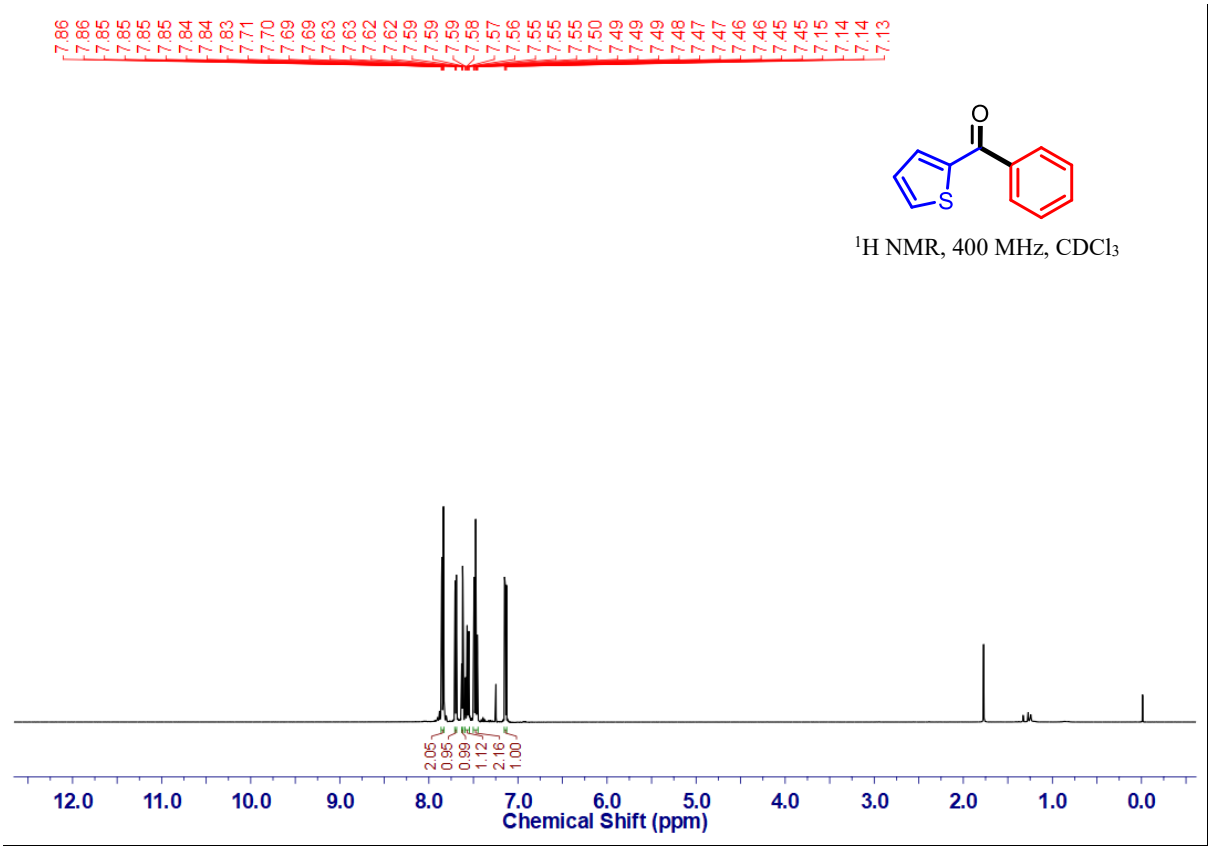


Figure S37. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3u** in $CDCl_3$ at 298K.

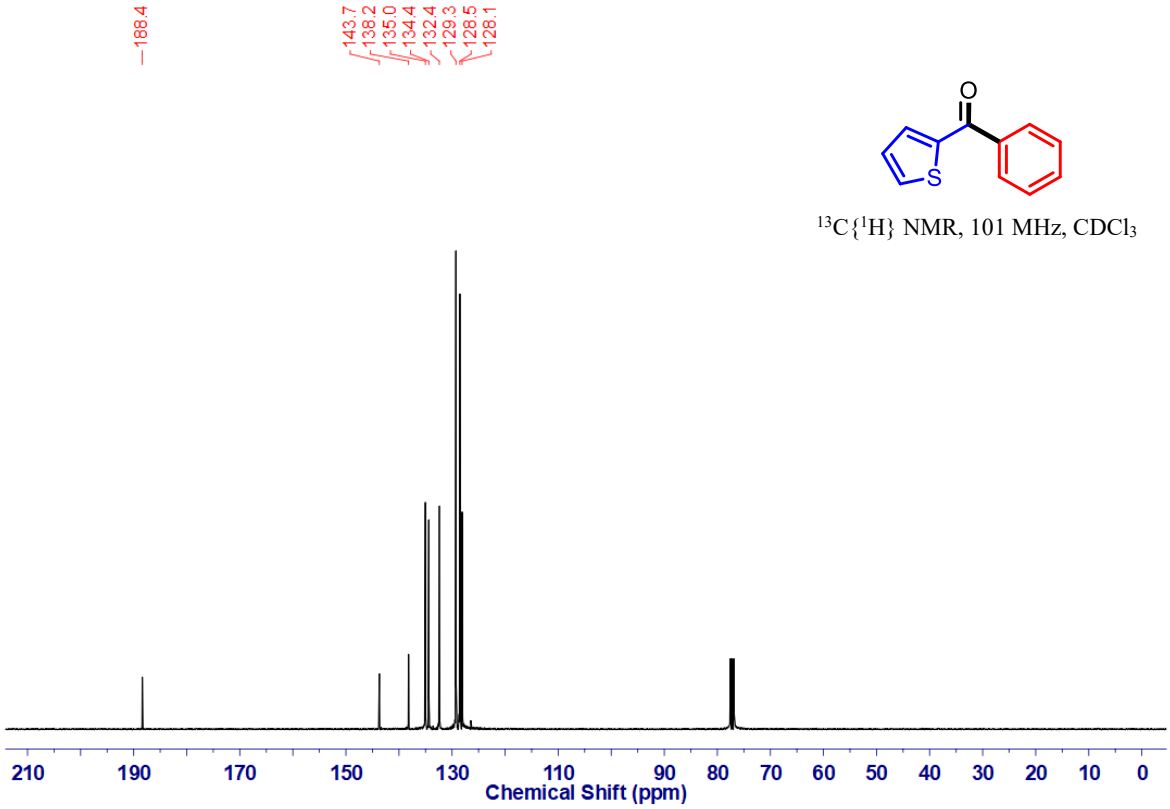


Figure S38. ^{1}H NMR (400 MHz) Spectrum of **3v** in $CDCl_3$ at 298K.

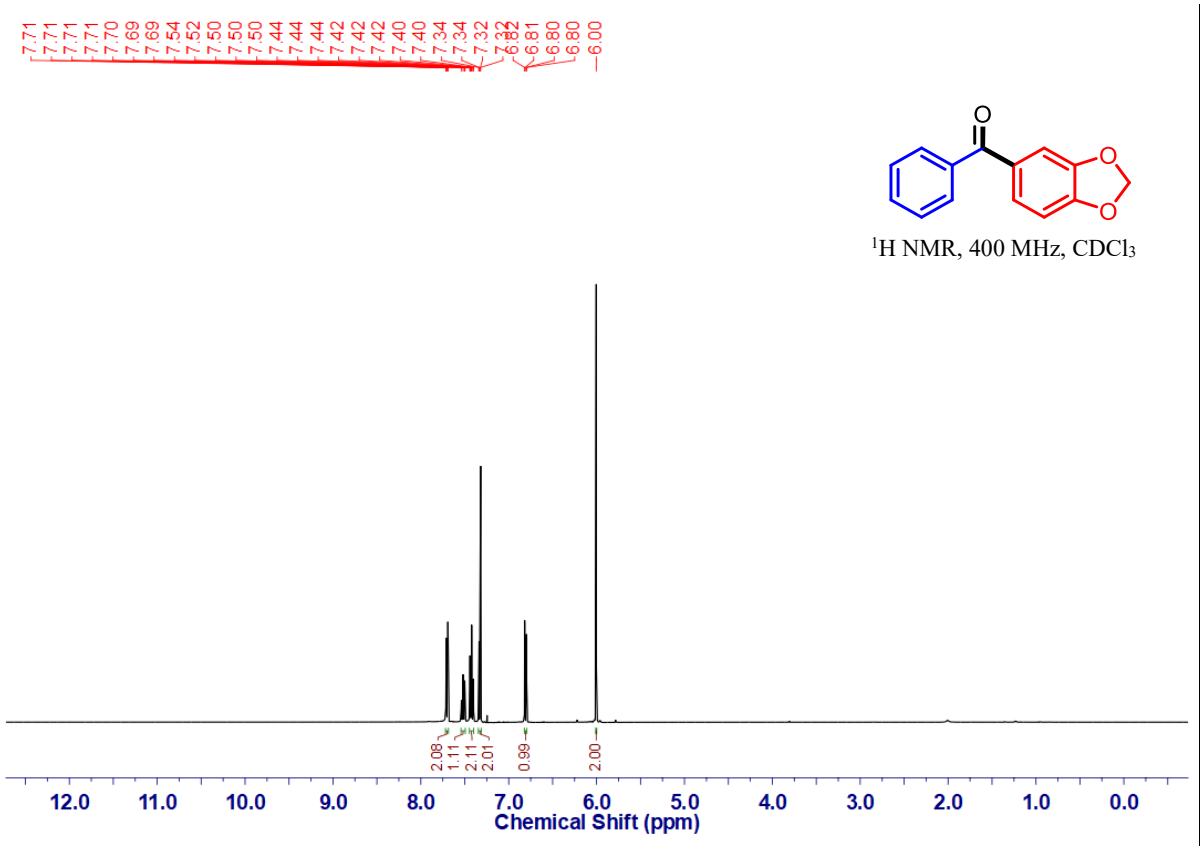


Figure S39. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **3v** in $CDCl_3$ at 298K.

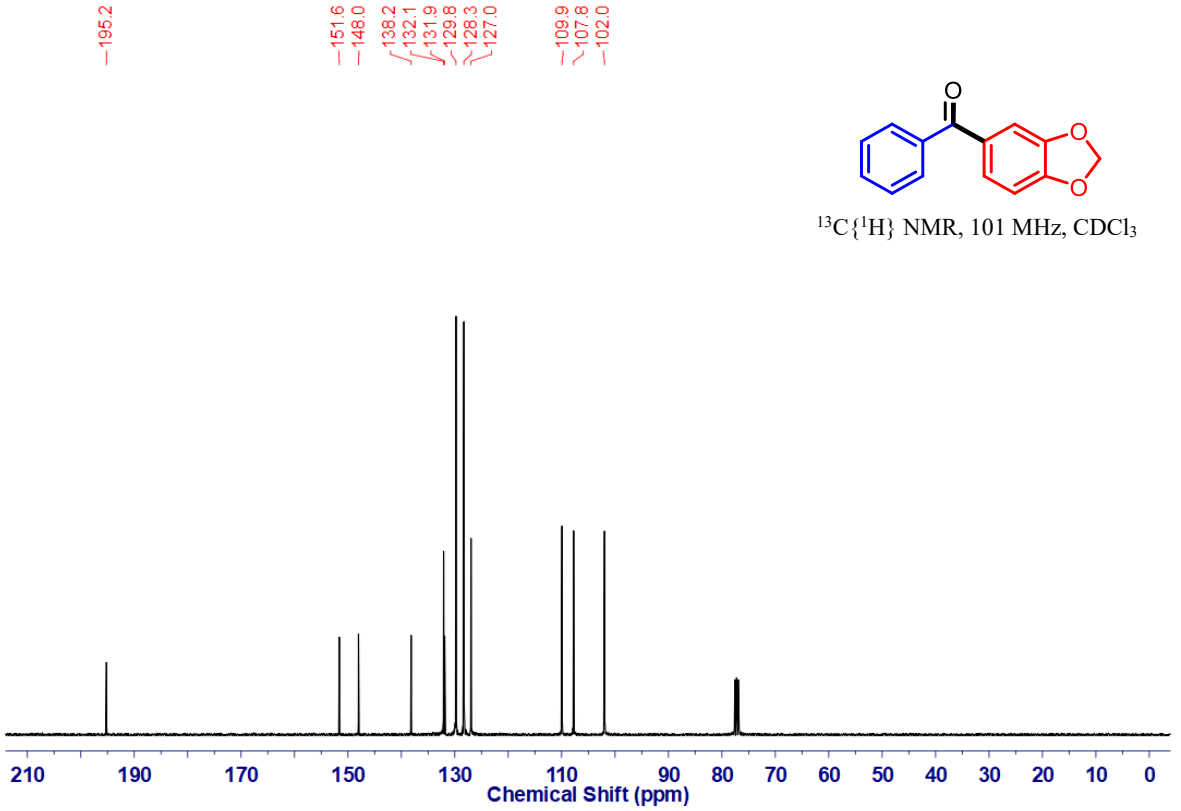


Figure S40. ^{1}H NMR (400 MHz) Spectrum of **4a** in $CDCl_3$ at 298K.

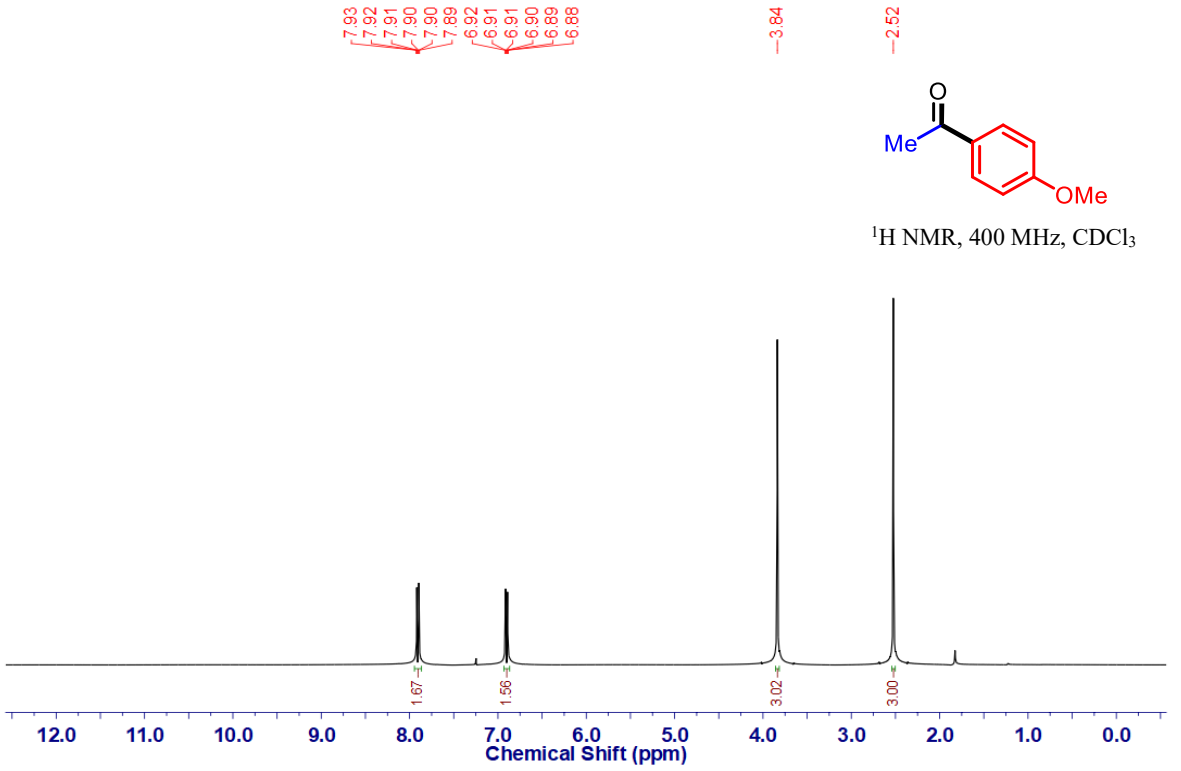


Figure S41. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **4a** in $CDCl_3$ at 298K.

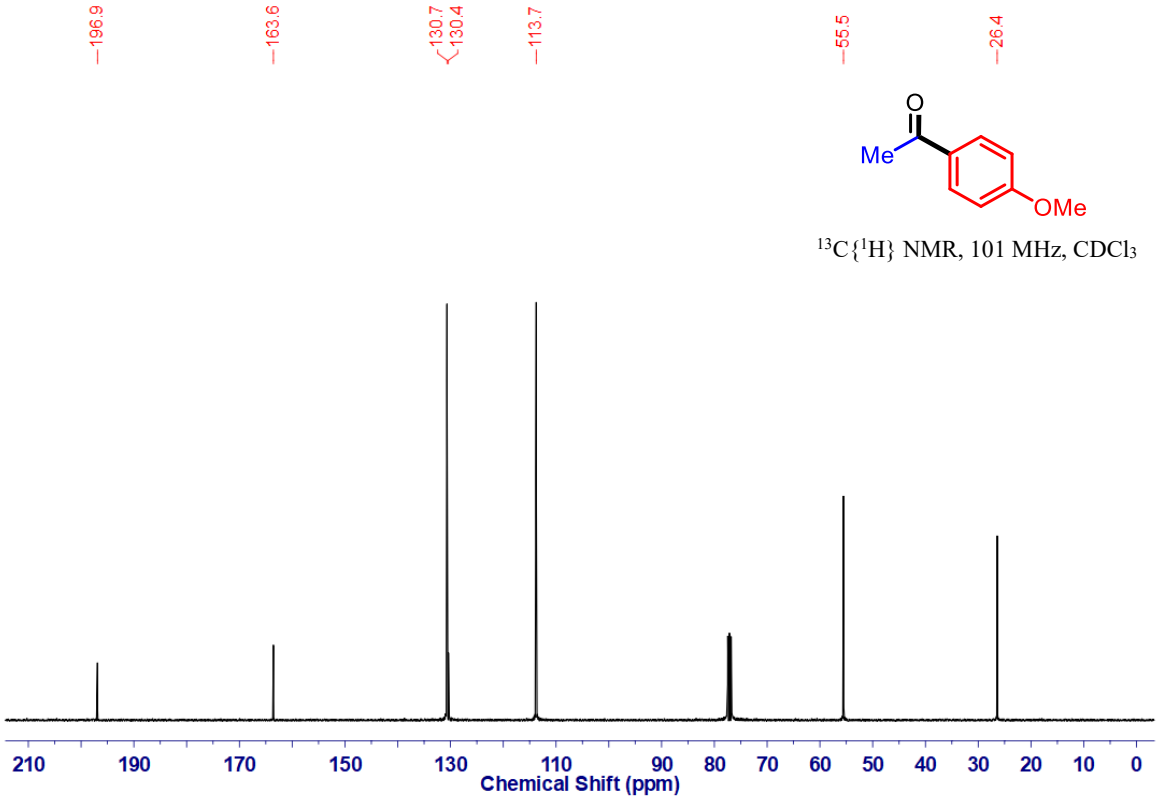


Figure S42. ^{1}H NMR (400 MHz) Spectrum of **4b** in $CDCl_3$ at 298K.

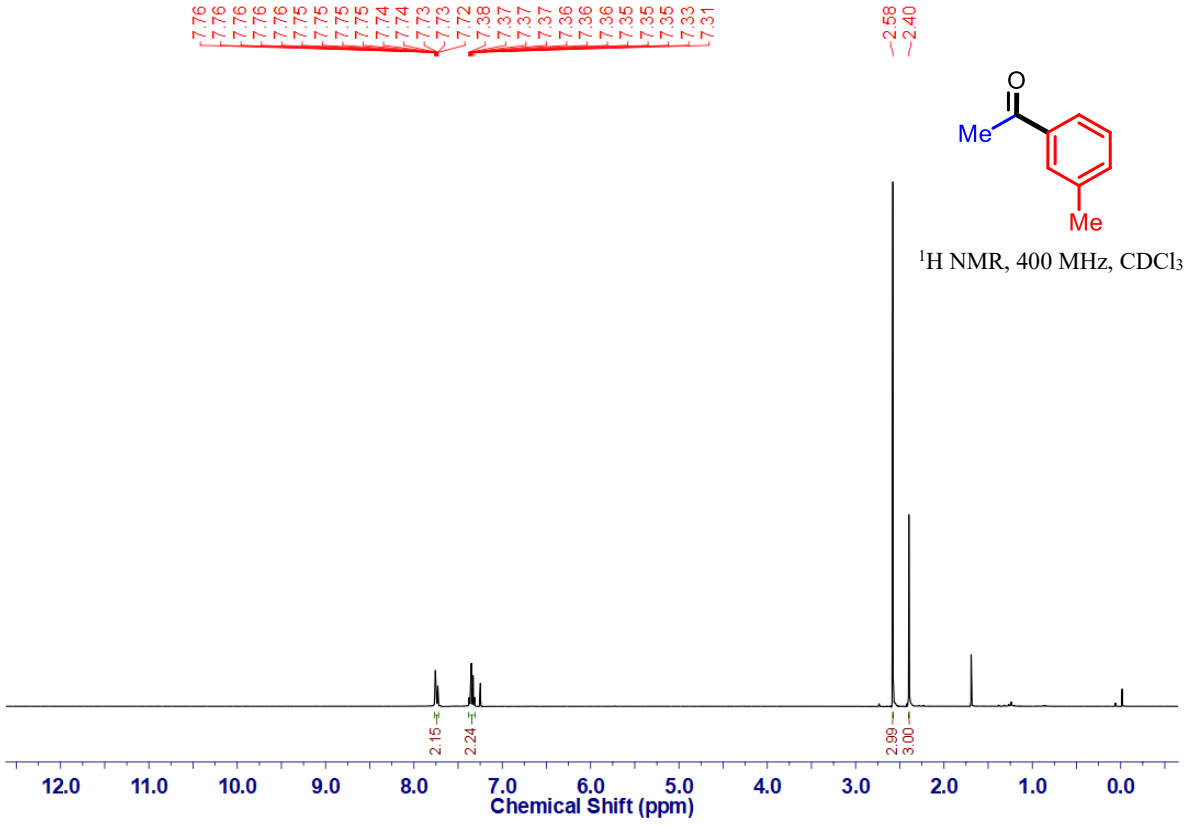


Figure S43. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **4b** in $CDCl_3$ at 298K.

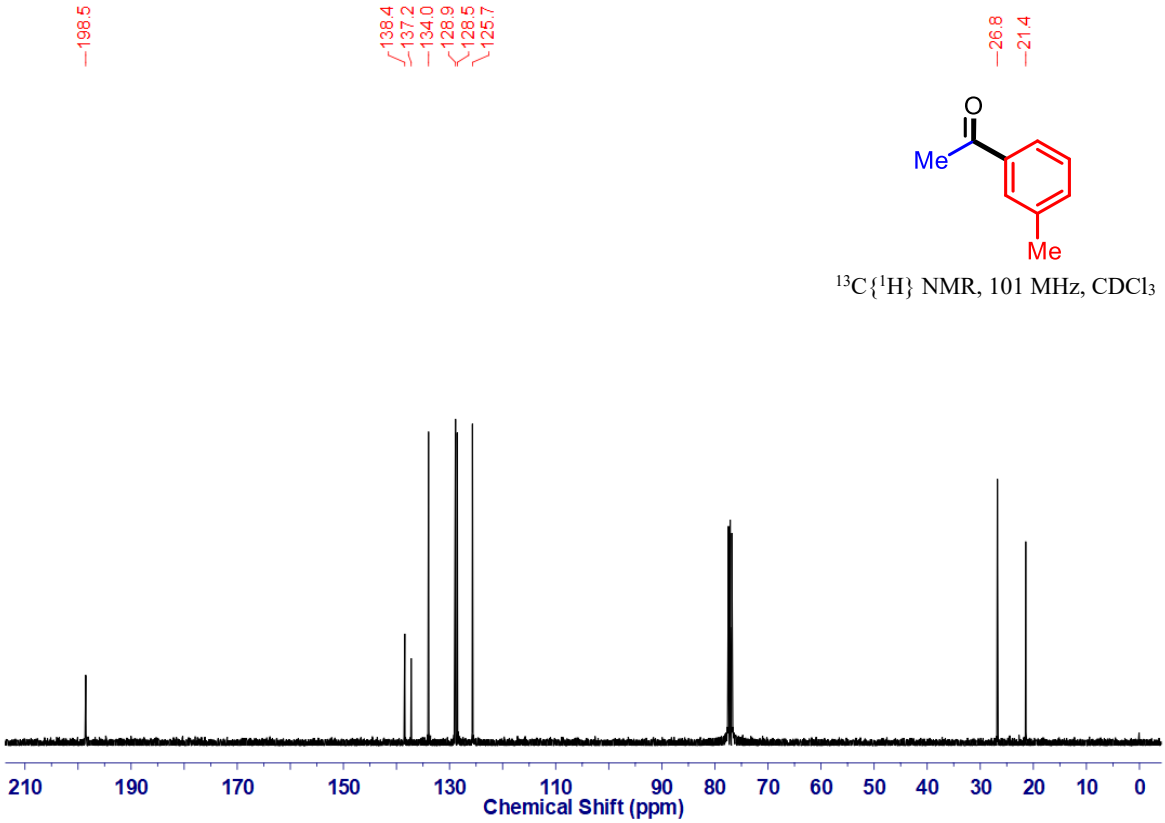


Figure S44. ^{1}H NMR (400 MHz) Spectrum of **4c** in $CDCl_3$ at 298K.

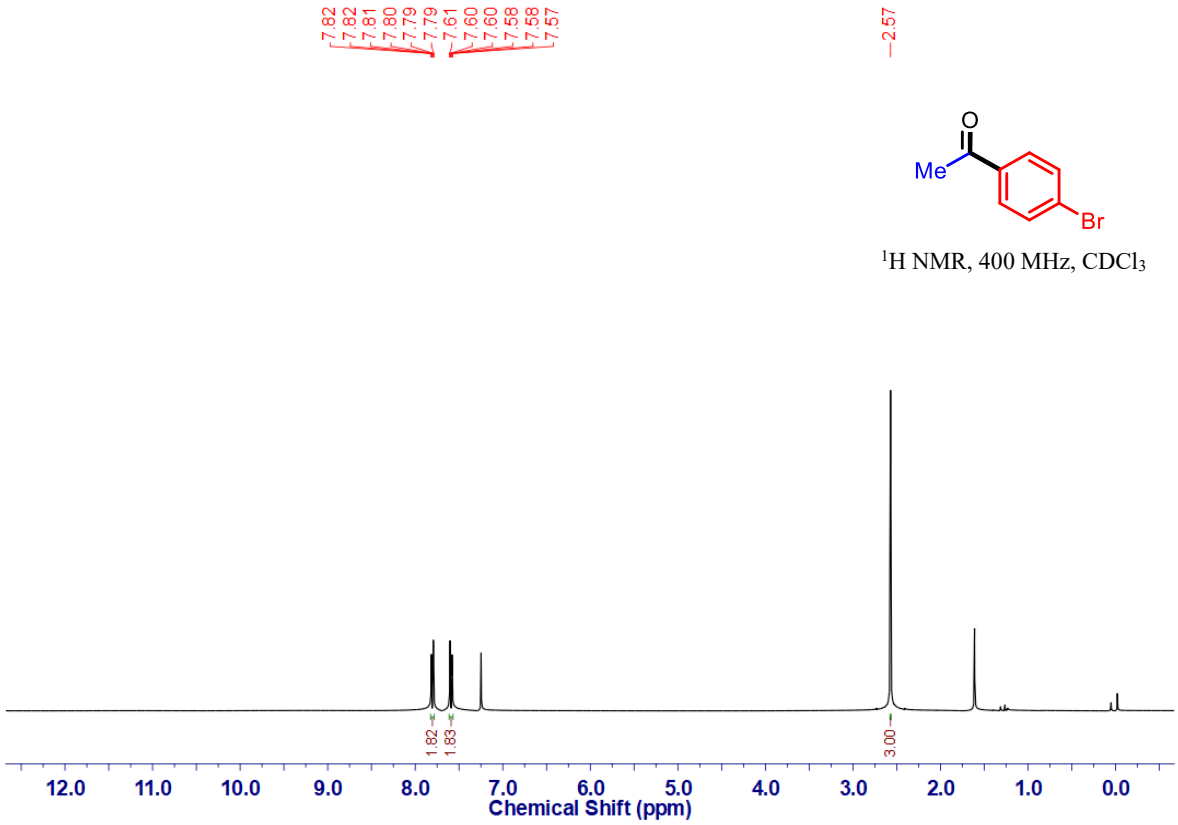


Figure S45. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **4c** in $CDCl_3$ at 298K.

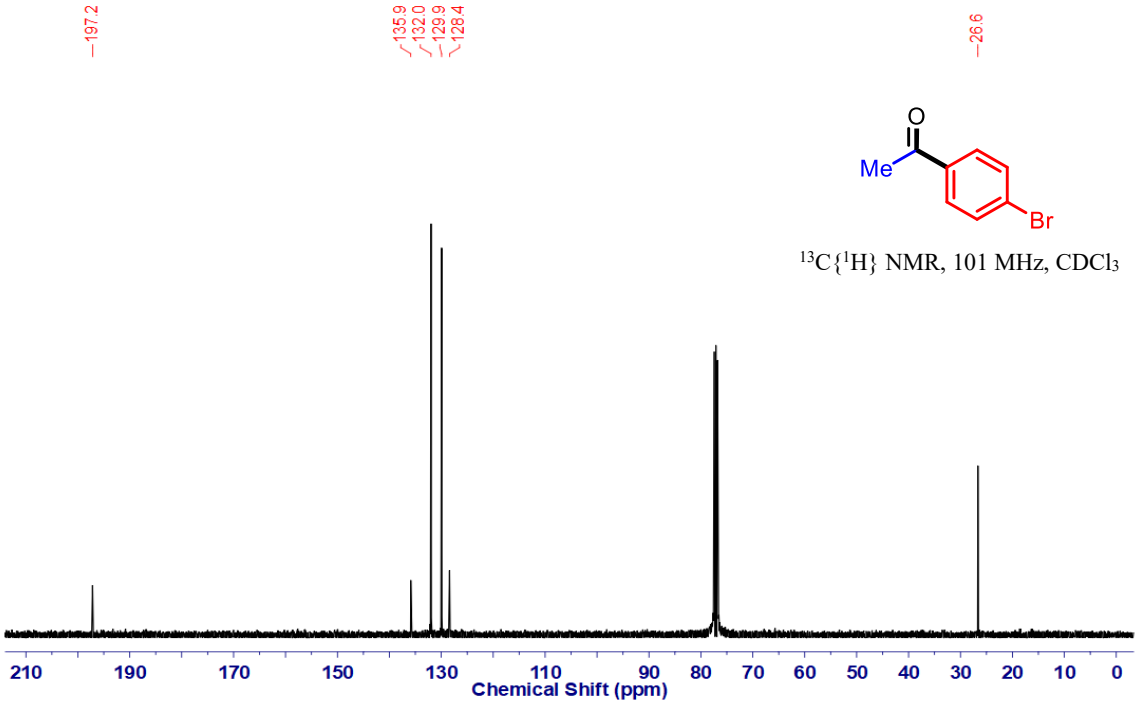


Figure S46. ^{1}H NMR (500 MHz) Spectrum of **4d** in $CDCl_3$ at 298K.

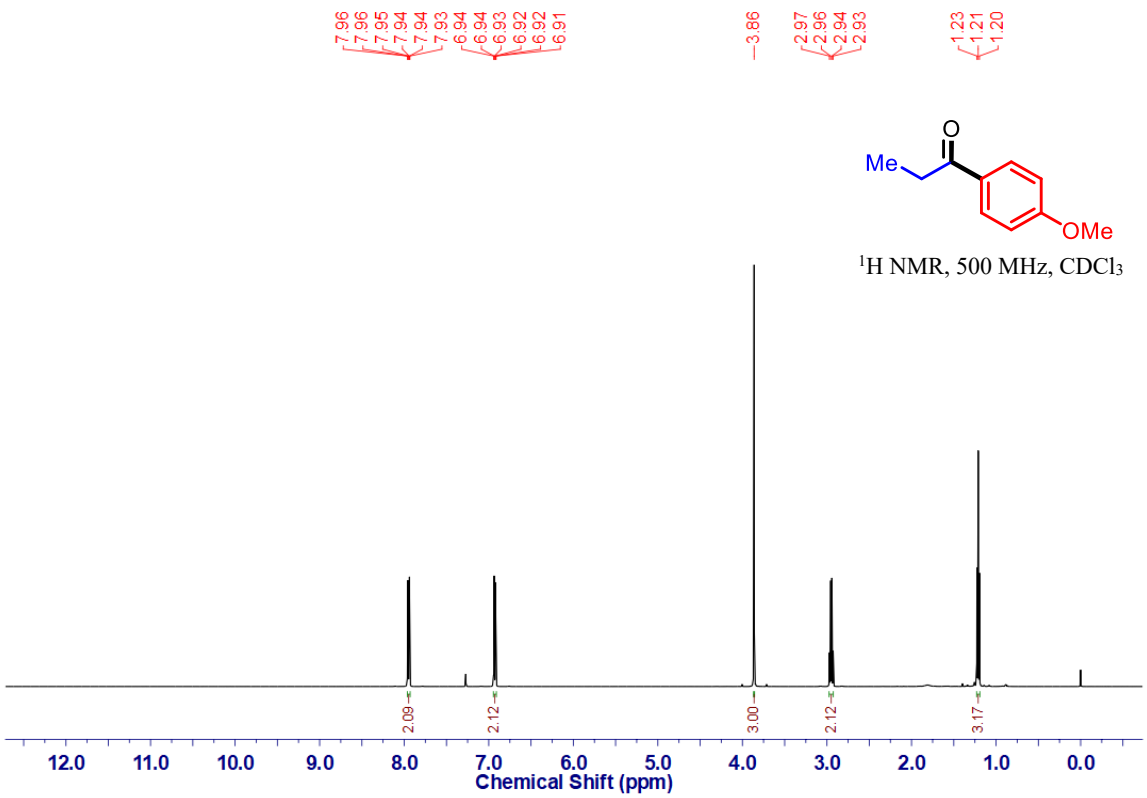


Figure S47. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **4d** in $CDCl_3$ at 298K.

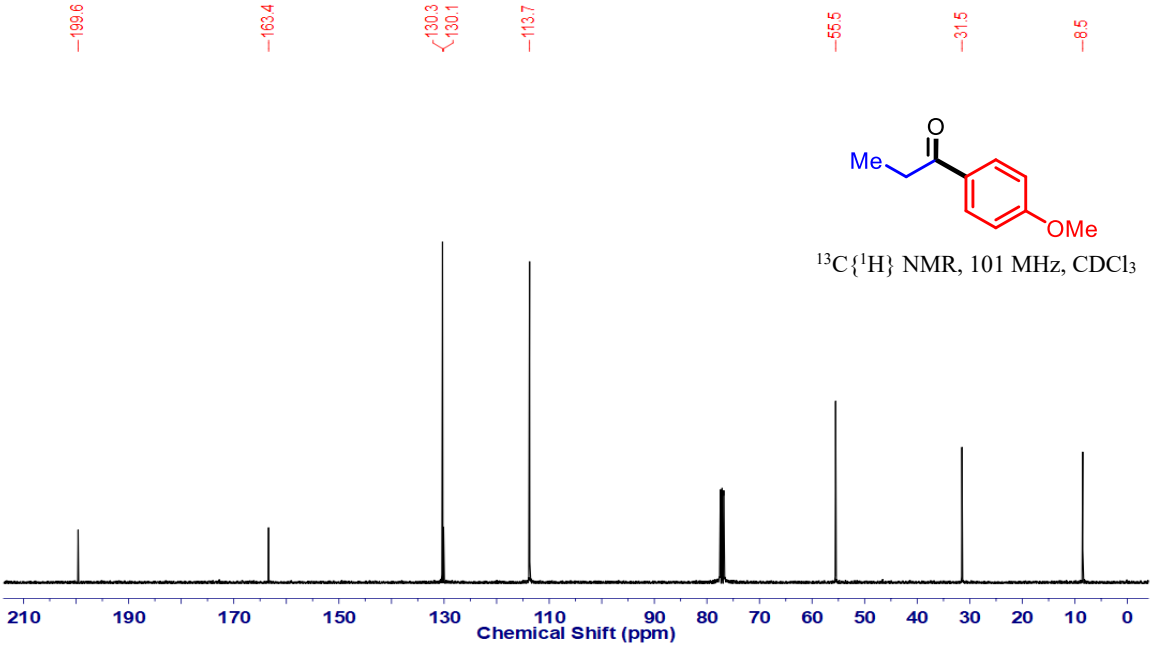


Figure S48. ^{1}H NMR (400 MHz) Spectrum of **4e** in $CDCl_3$ at 298K.

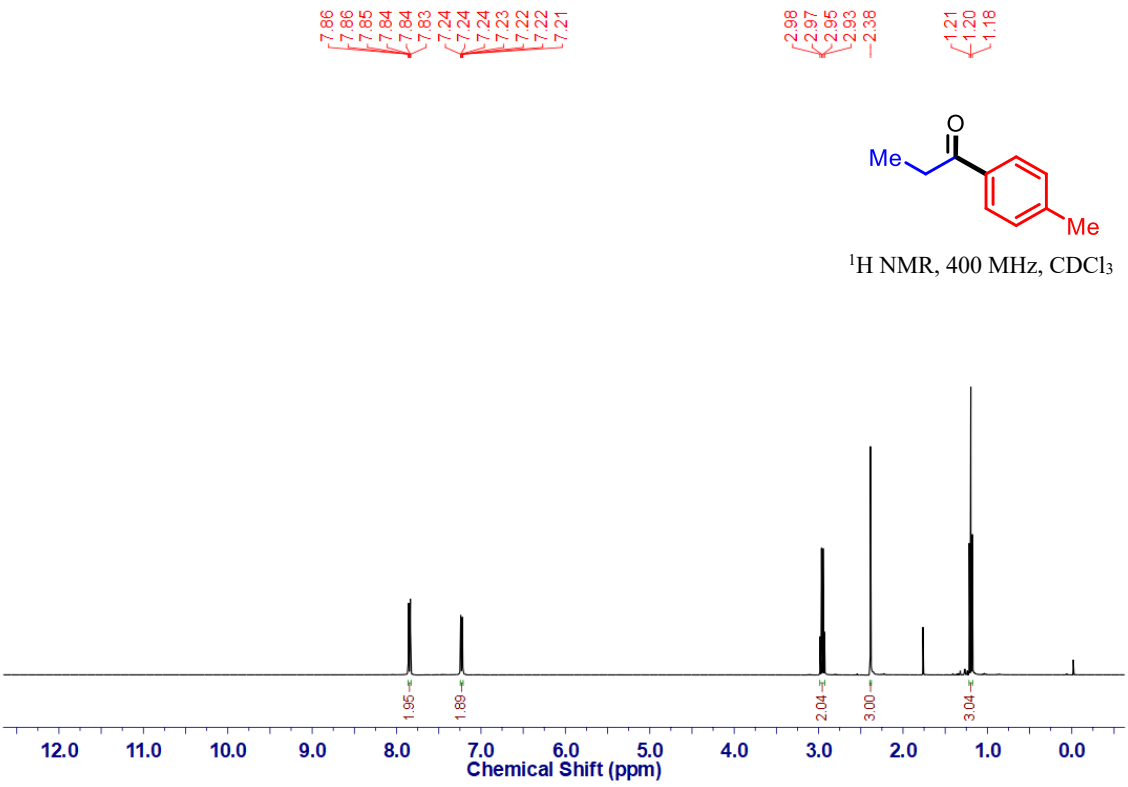


Figure S49. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **4e** in $CDCl_3$ at 298K.

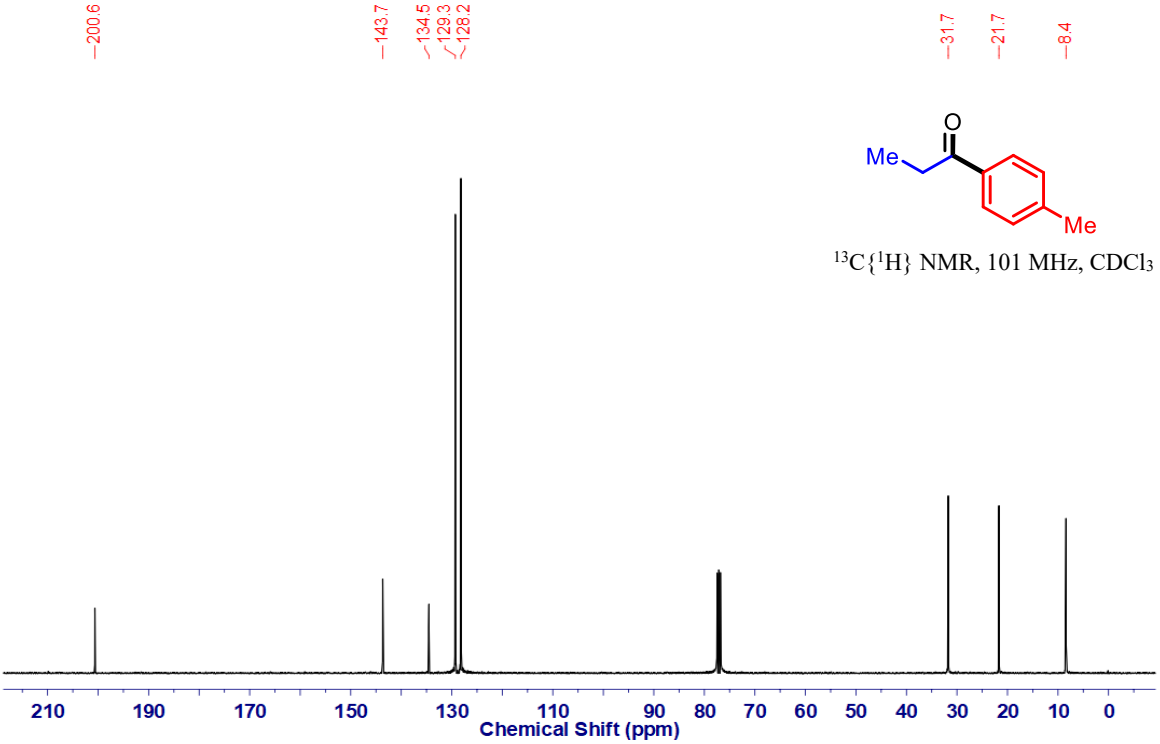


Figure S50. ^{1}H NMR (400 MHz) Spectrum of **4f** in $CDCl_3$ at 298K.

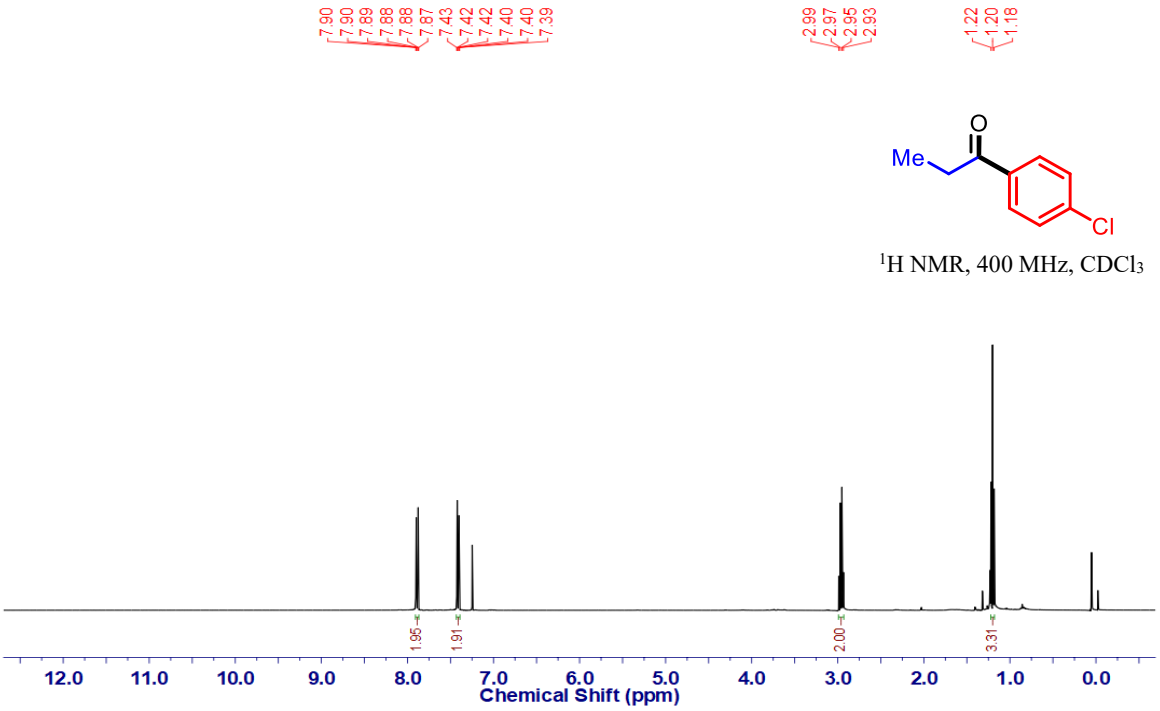


Figure S51. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **4f** in $CDCl_3$ at 298K.

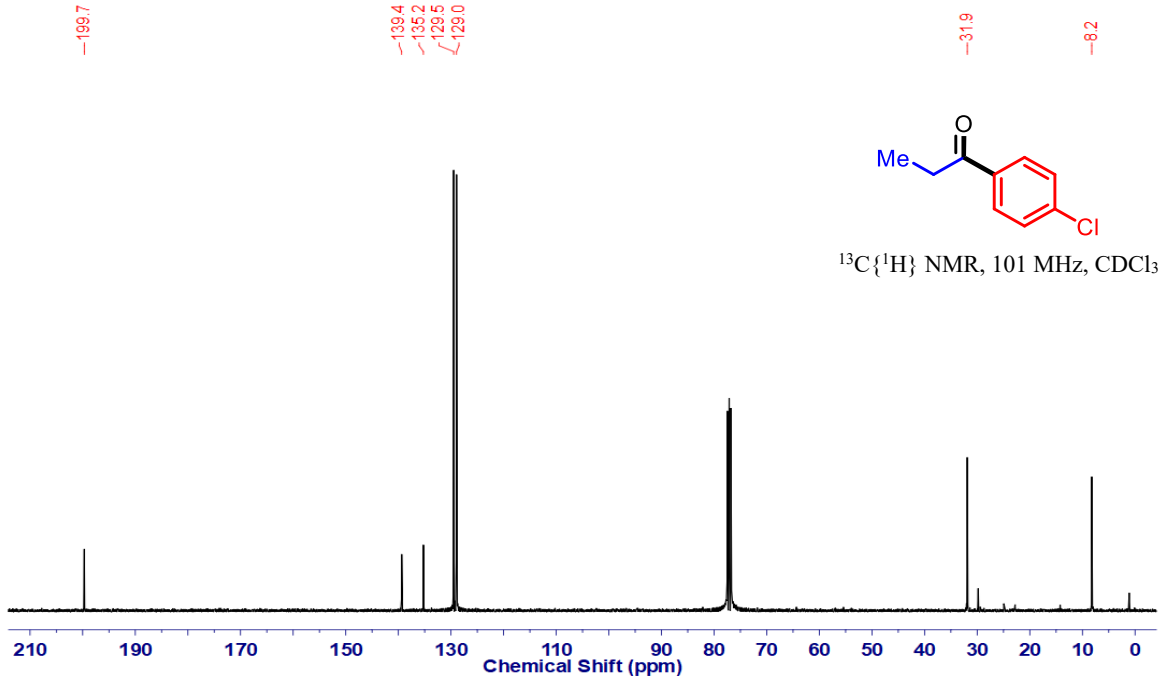


Figure S52. ^{1}H NMR (400 MHz) Spectrum of **4g** in $CDCl_3$ at 298K.

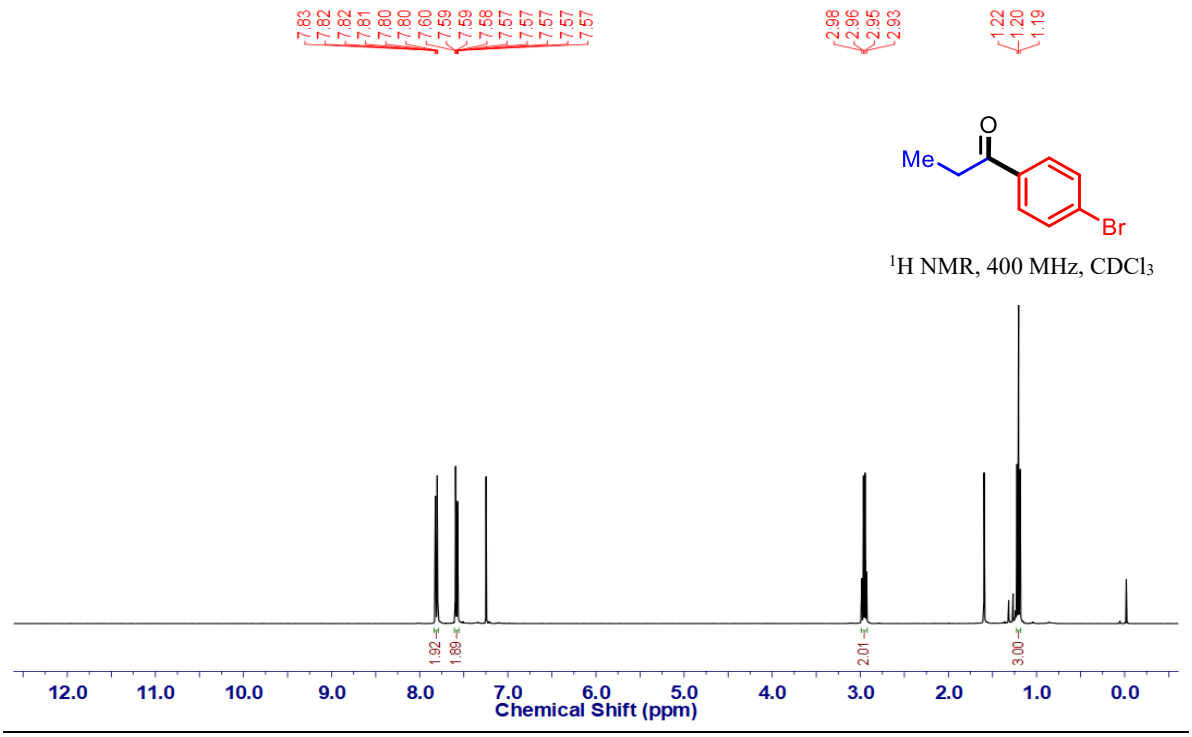


Figure S53. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **4g** in $CDCl_3$ at 298K.

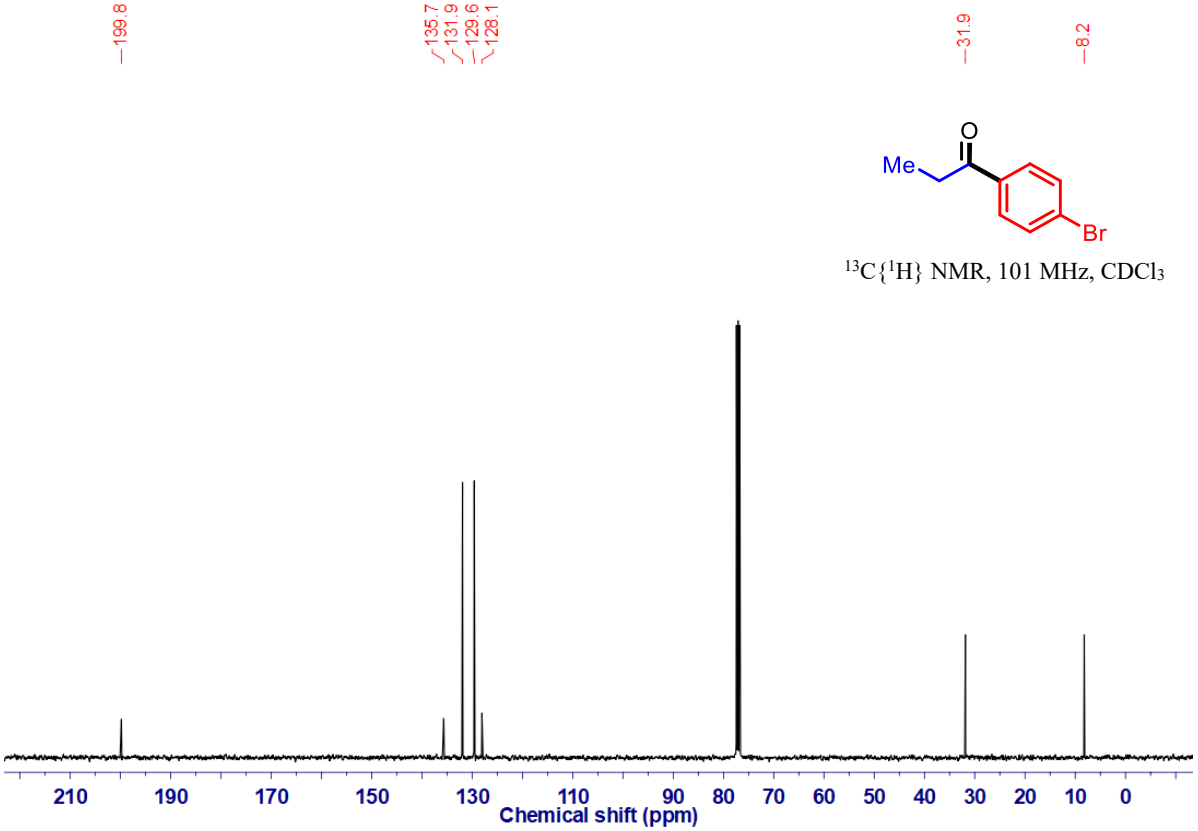


Figure S54. ^{1}H NMR (400 MHz) Spectrum of **4h** in $CDCl_3$ at 298K.

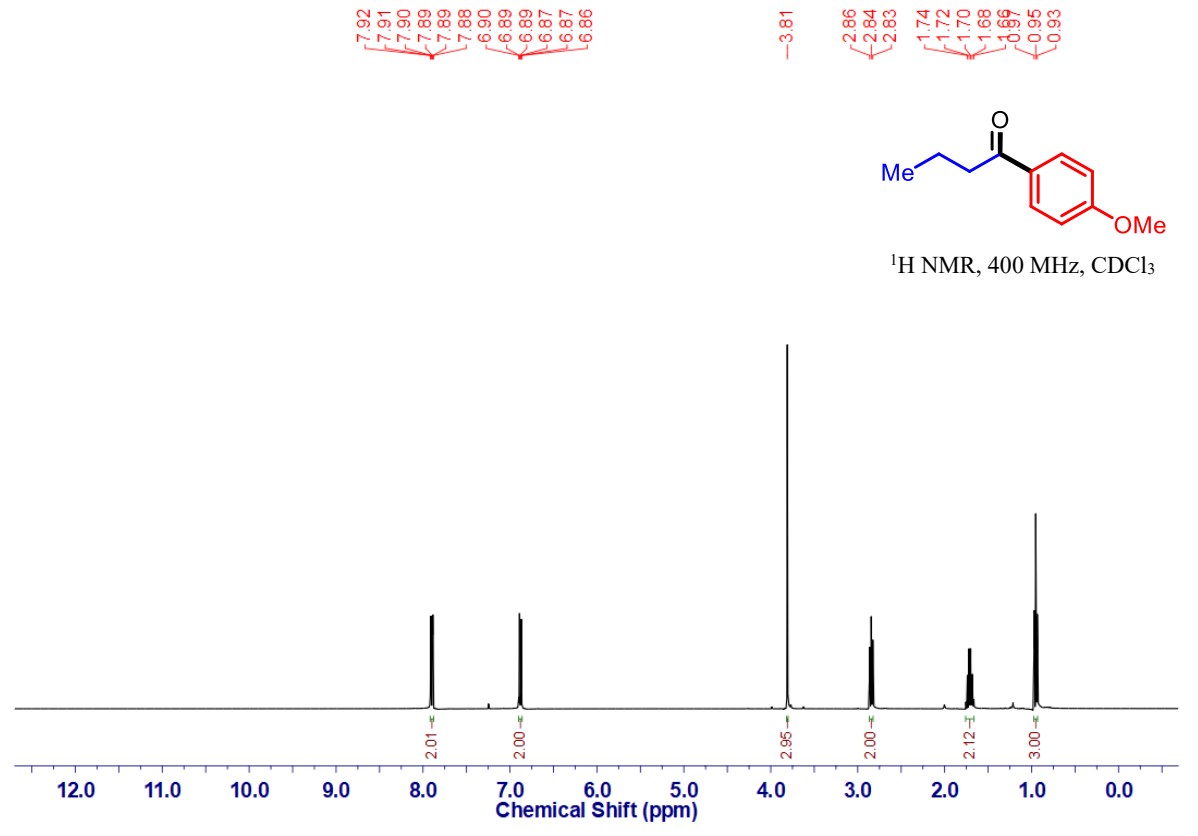


Figure S55. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **4h** in $CDCl_3$ at 298K.

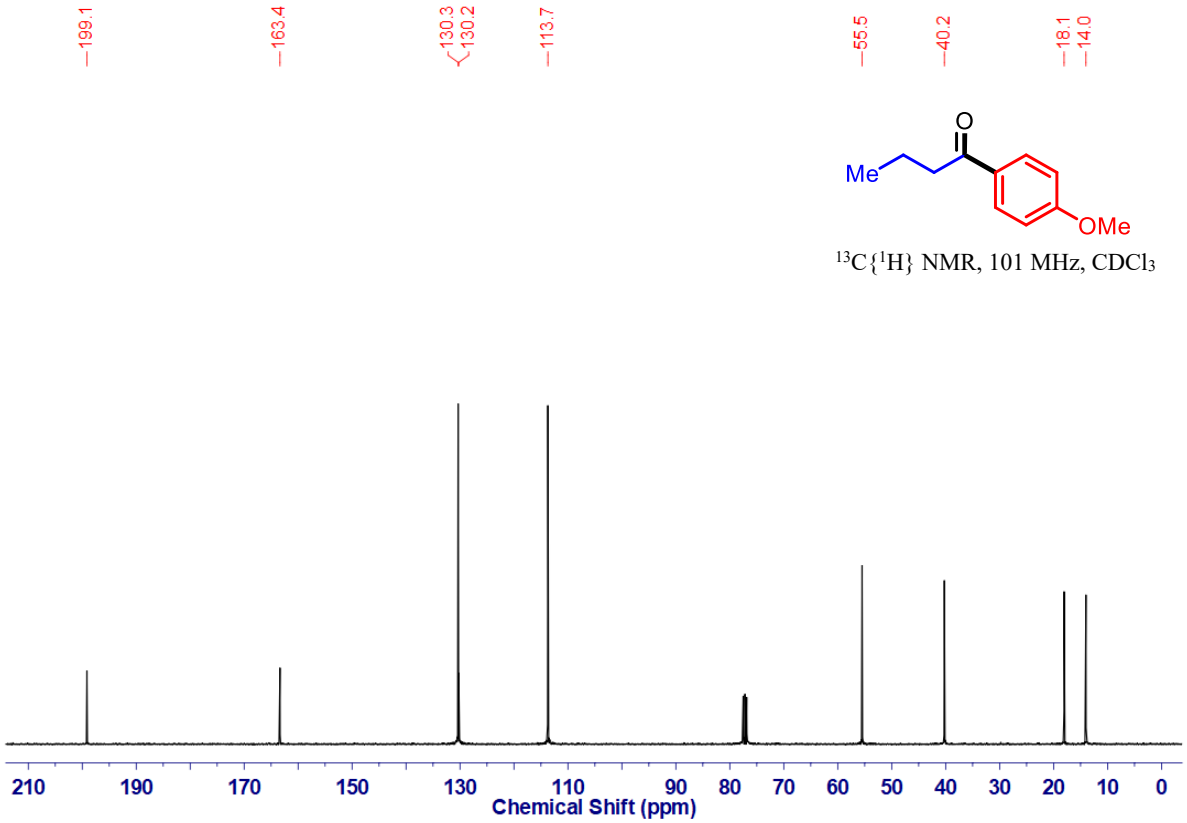


Figure S56. ^{1}H NMR (400 MHz) Spectrum of **4i** in $CDCl_3$ at 298K.

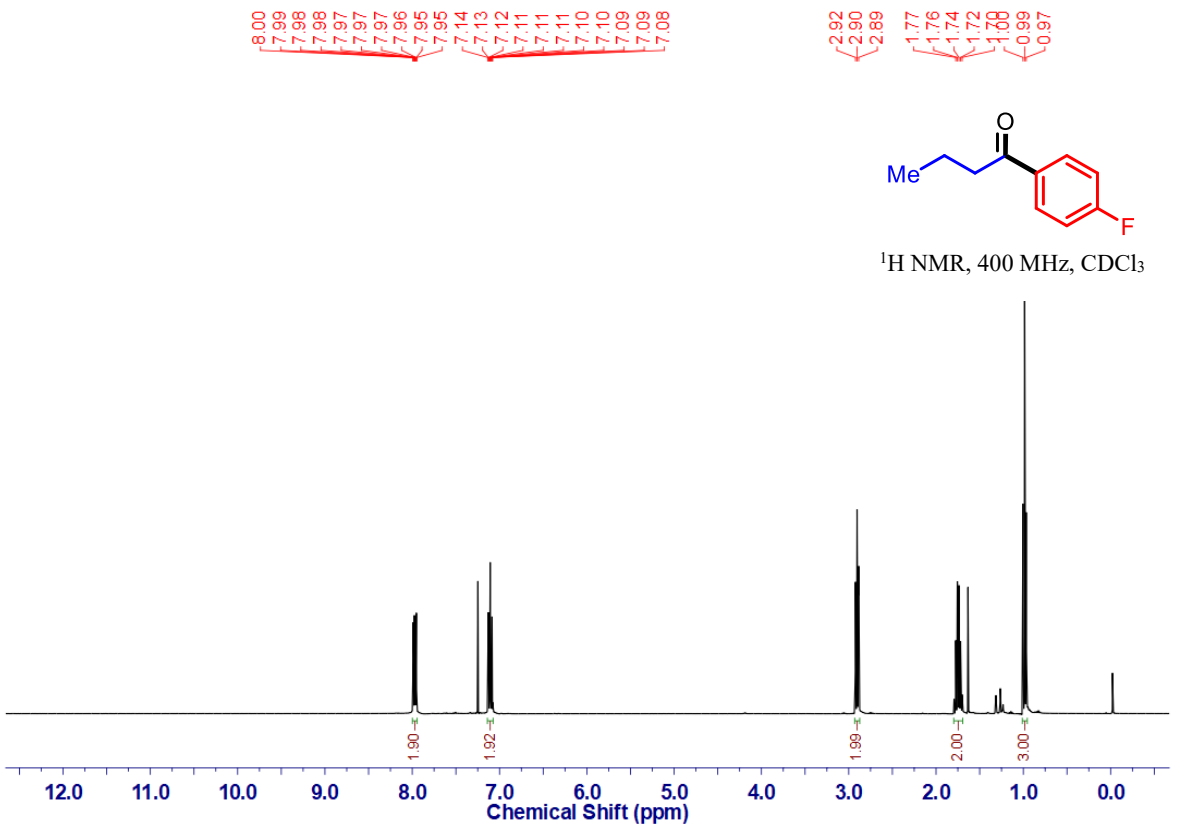


Figure S57. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **4i** in $CDCl_3$ at 298K.

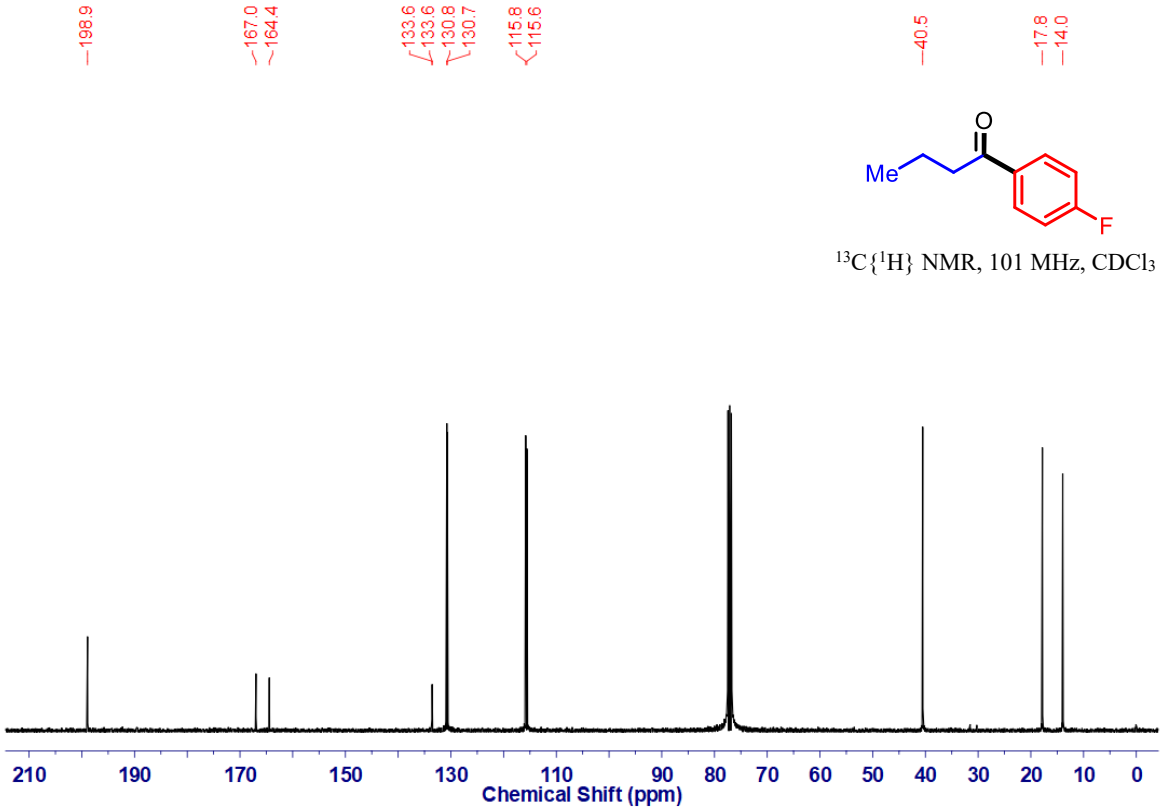


Figure S58. ^{19}F NMR (376 MHz) Spectrum of **4i** in $CDCl_3$ at 298K.

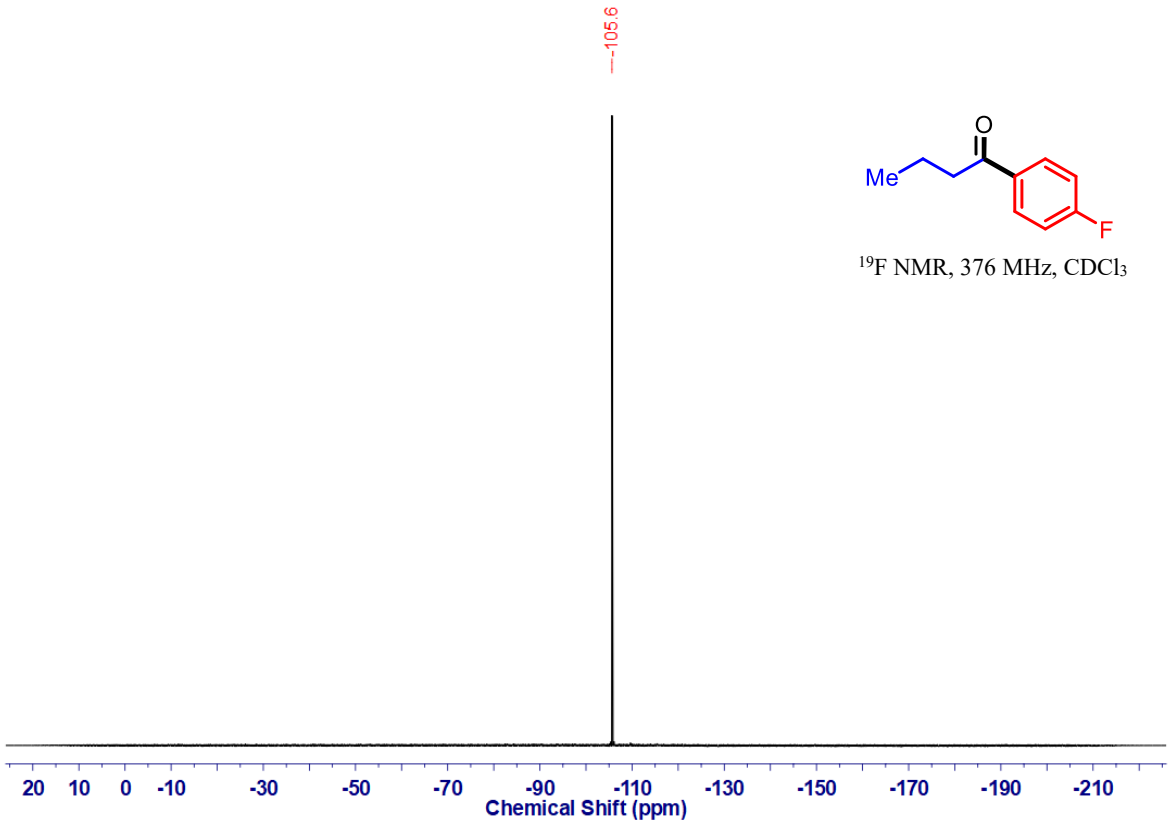


Figure S59. ^{1}H NMR (500 MHz) Spectrum of **4j** in $CDCl_3$ at 298K.

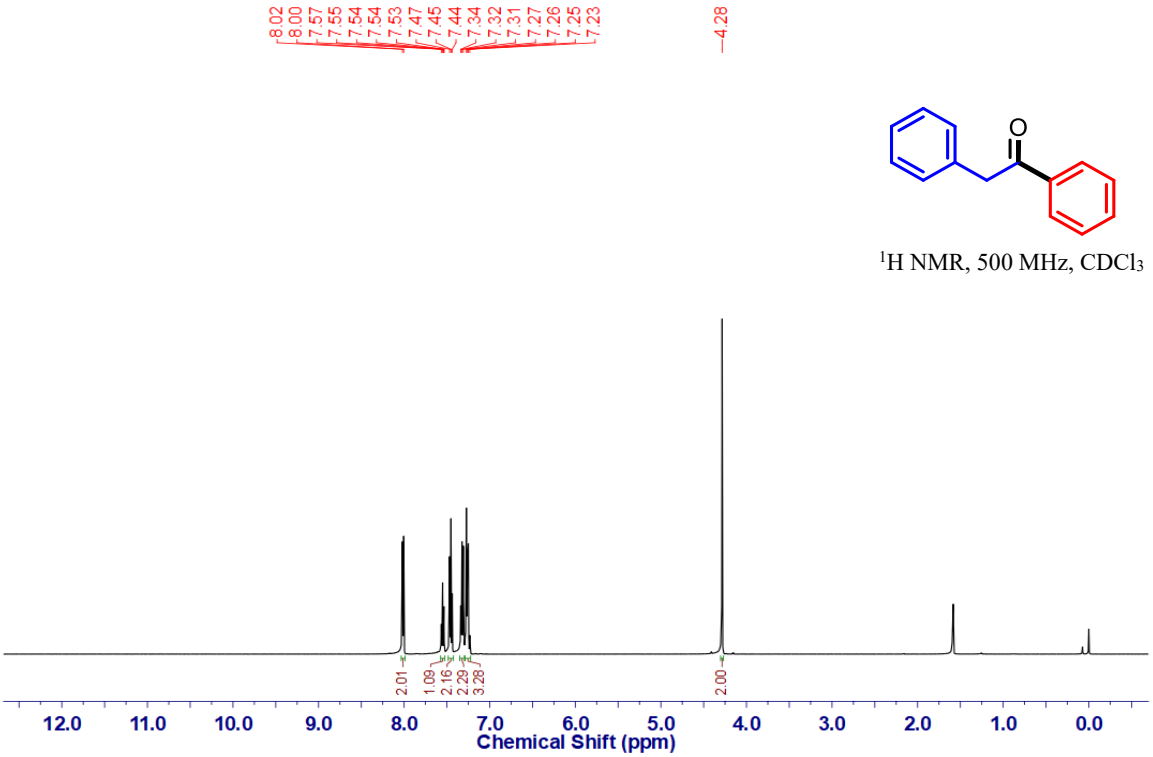


Figure S60. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **4j** in $CDCl_3$ at 298K.

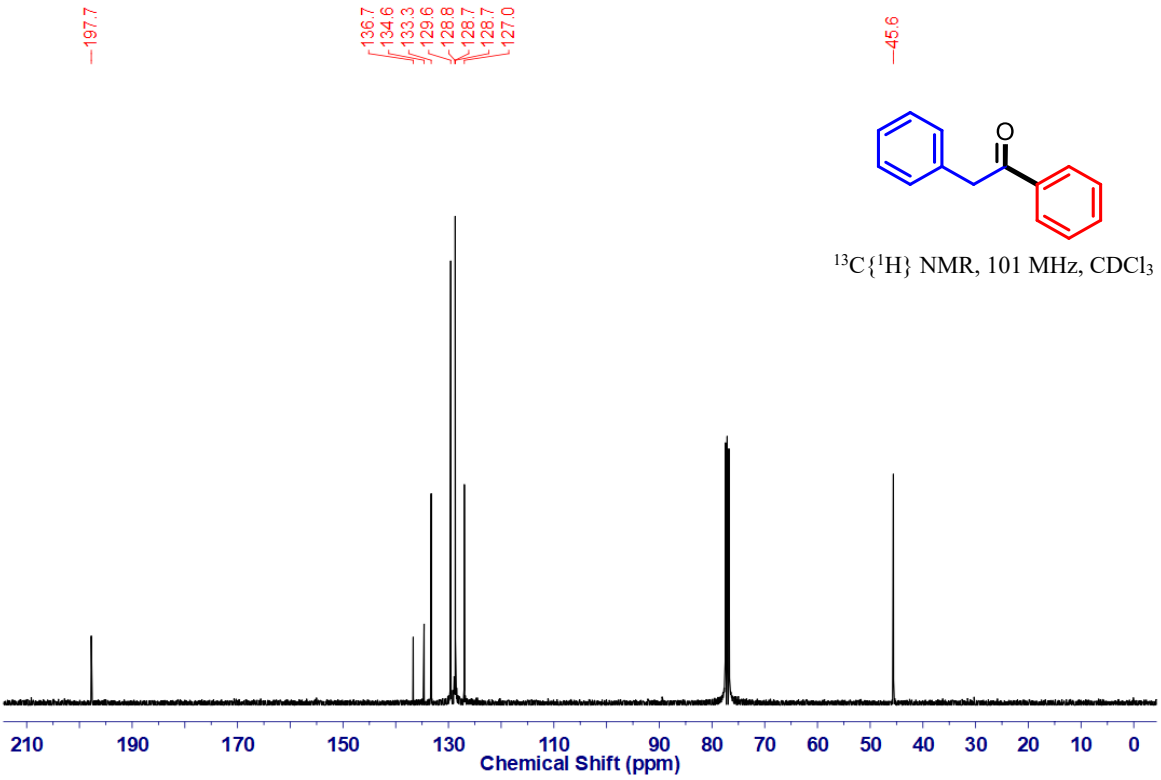
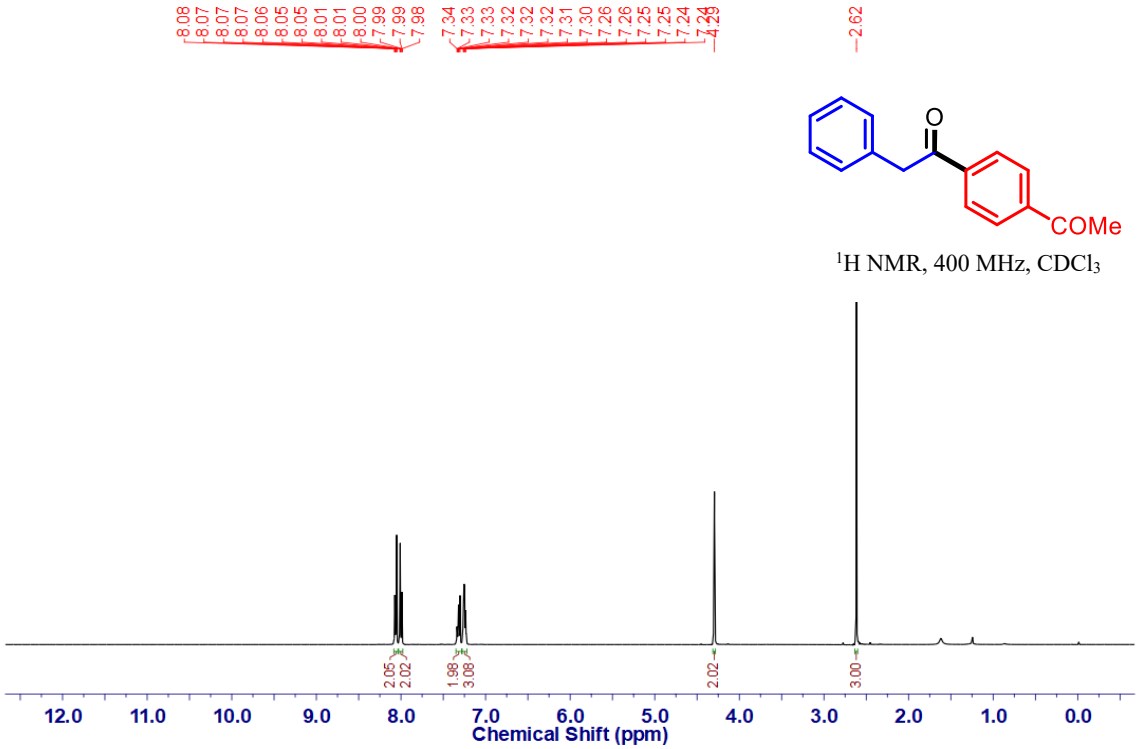
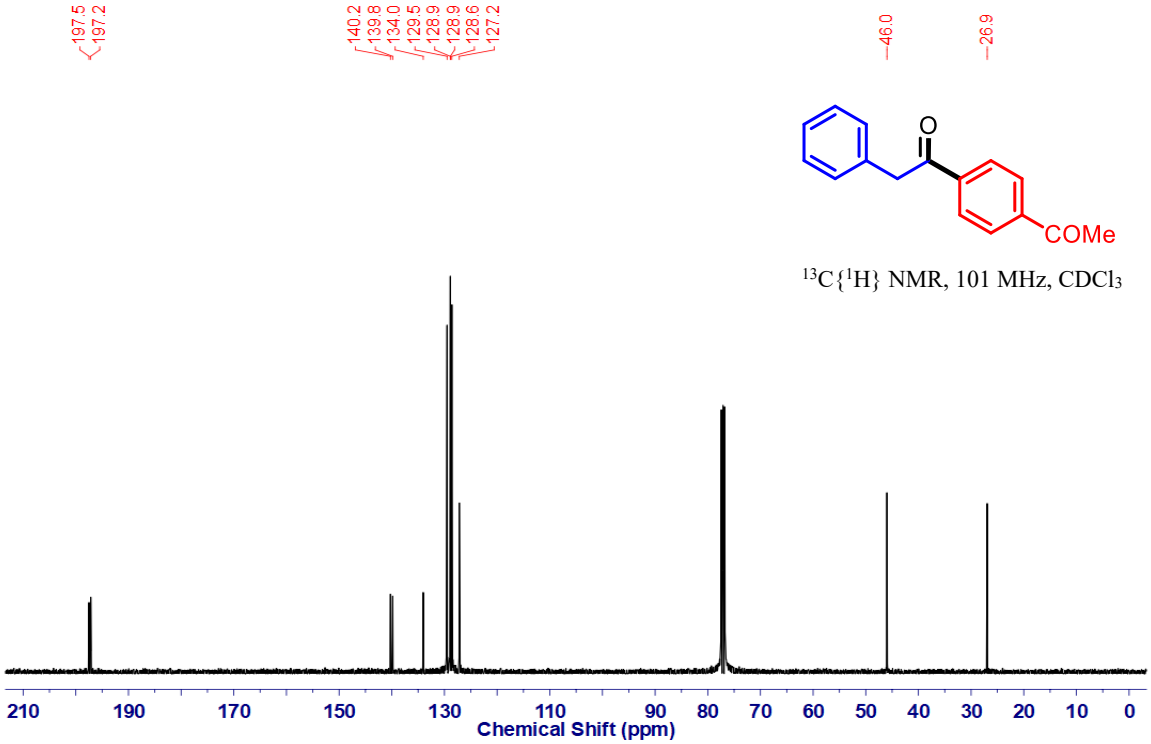


Figure S61. ^{1}H NMR (400 MHz) Spectrum of **4k** in $CDCl_3$ at 298K.



^{1}H NMR, 400 MHz, $CDCl_3$

Figure S62. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **4k** in $CDCl_3$ at 298K.



$^{13}C\{^{1}H\}$ NMR, 101 MHz, $CDCl_3$

Figure S63. ^{1}H NMR (400 MHz) Spectrum of **4l** in $CDCl_3$ at 298K.

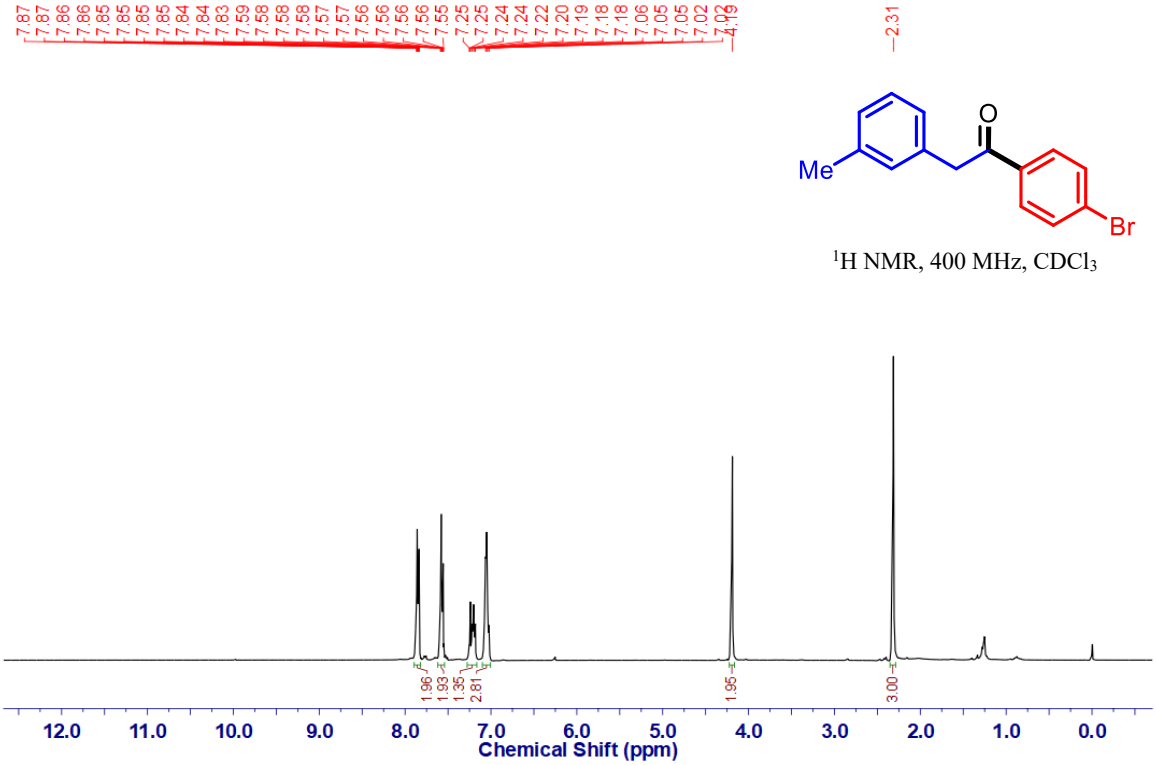


Figure S64. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **4l** in $CDCl_3$ at 298K.

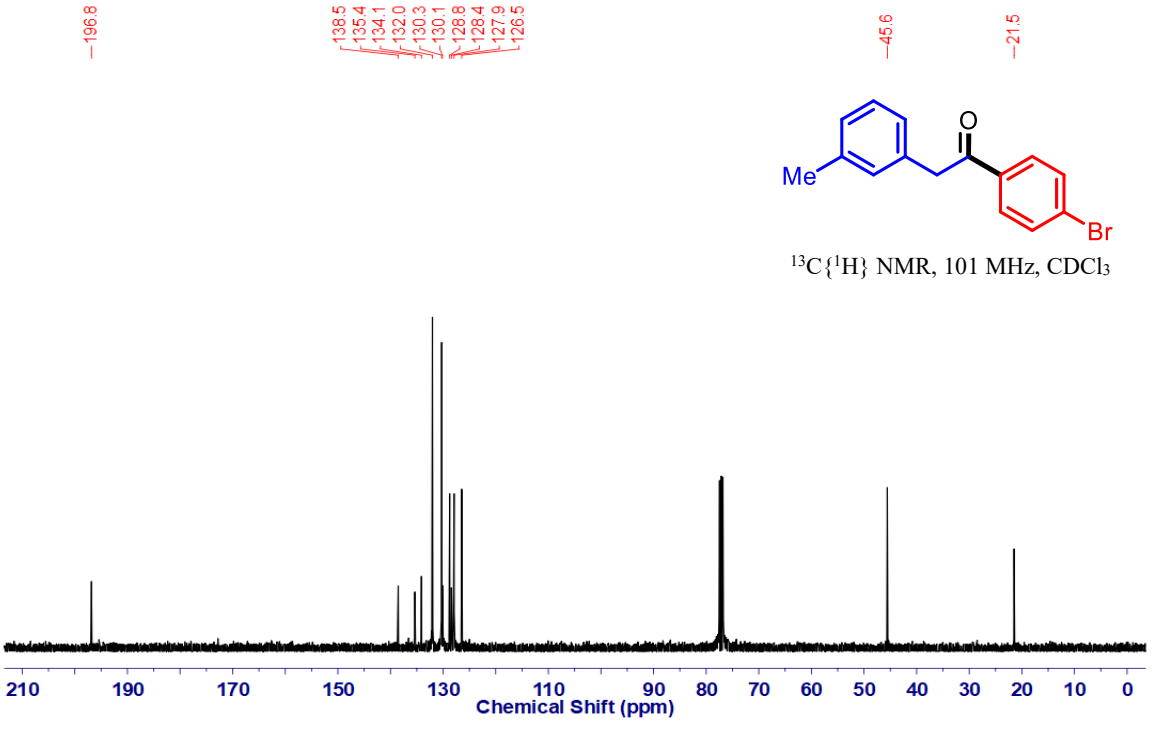


Figure S65. ^{1}H NMR (400 MHz) Spectrum of **4m** in $CDCl_3$ at 298K.

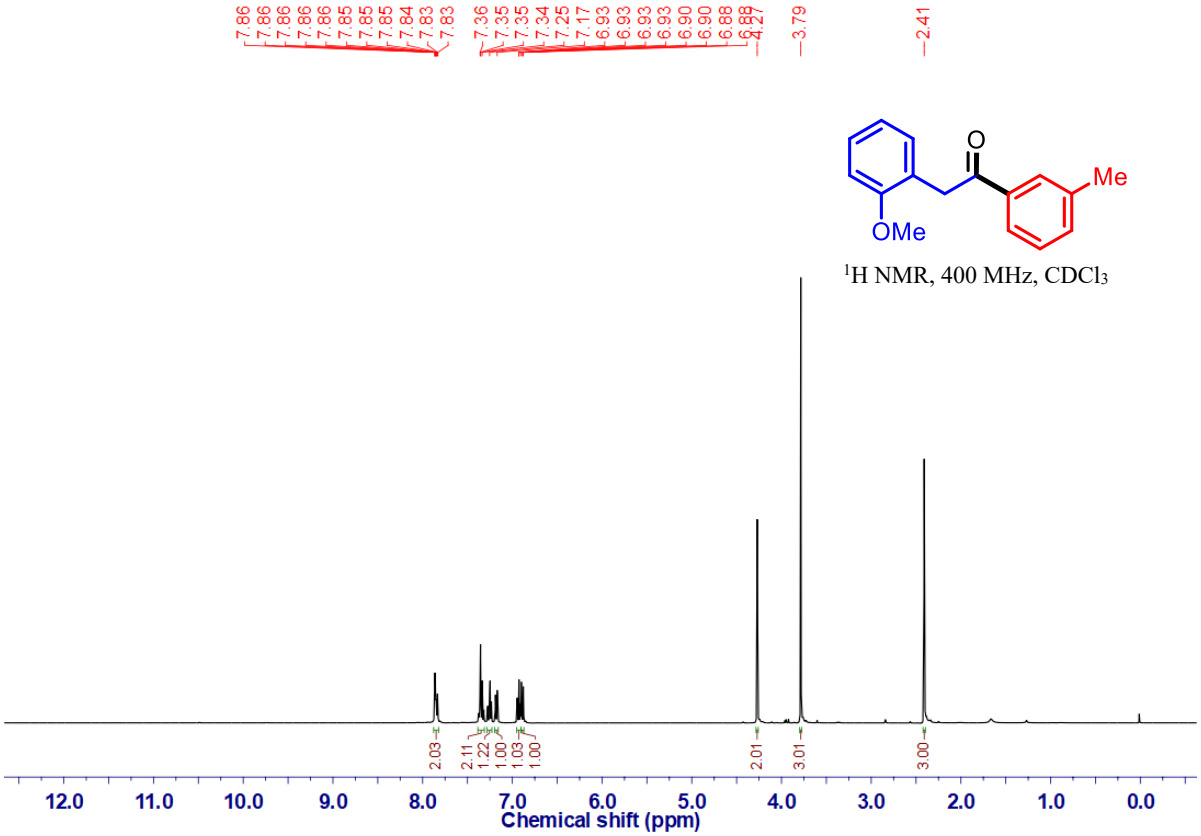


Figure S66. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **4m** in $CDCl_3$ at 298K.

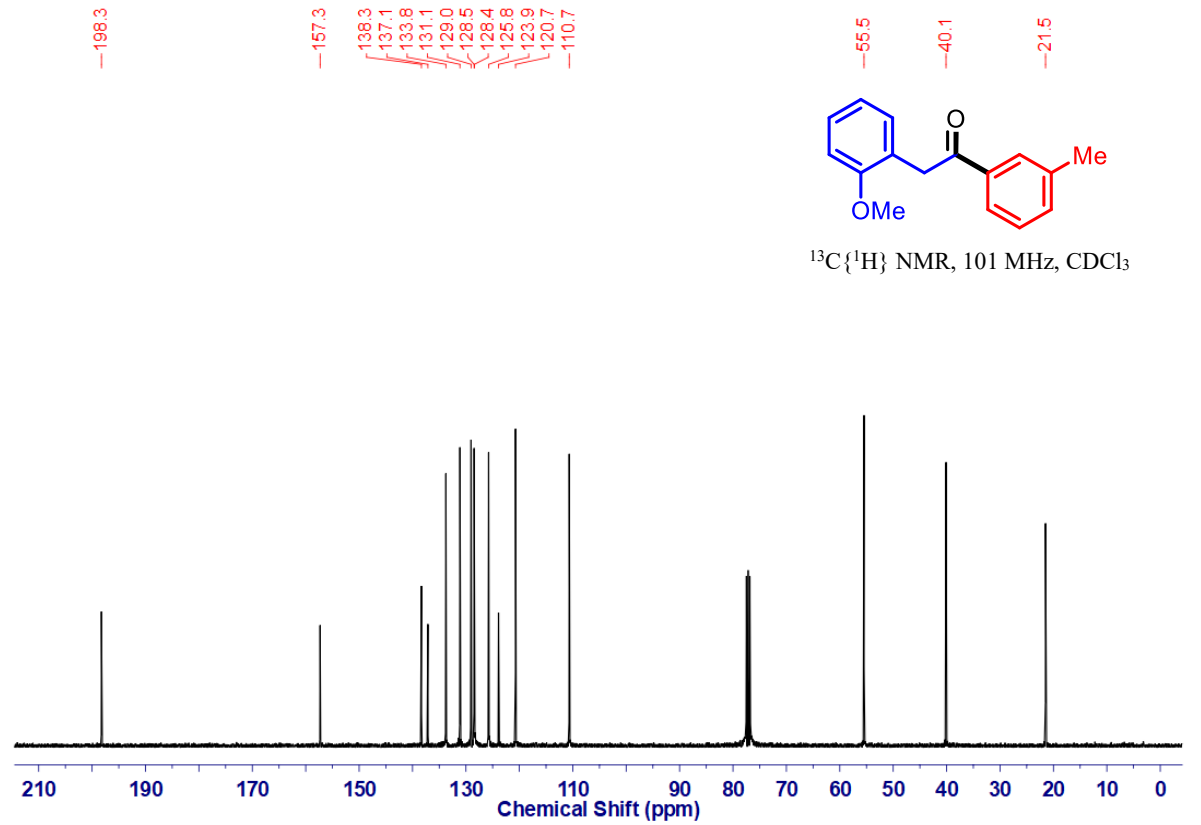


Figure S67. ^{1}H NMR (400 MHz) Spectrum of **5b** in $CDCl_3$ at 298K.

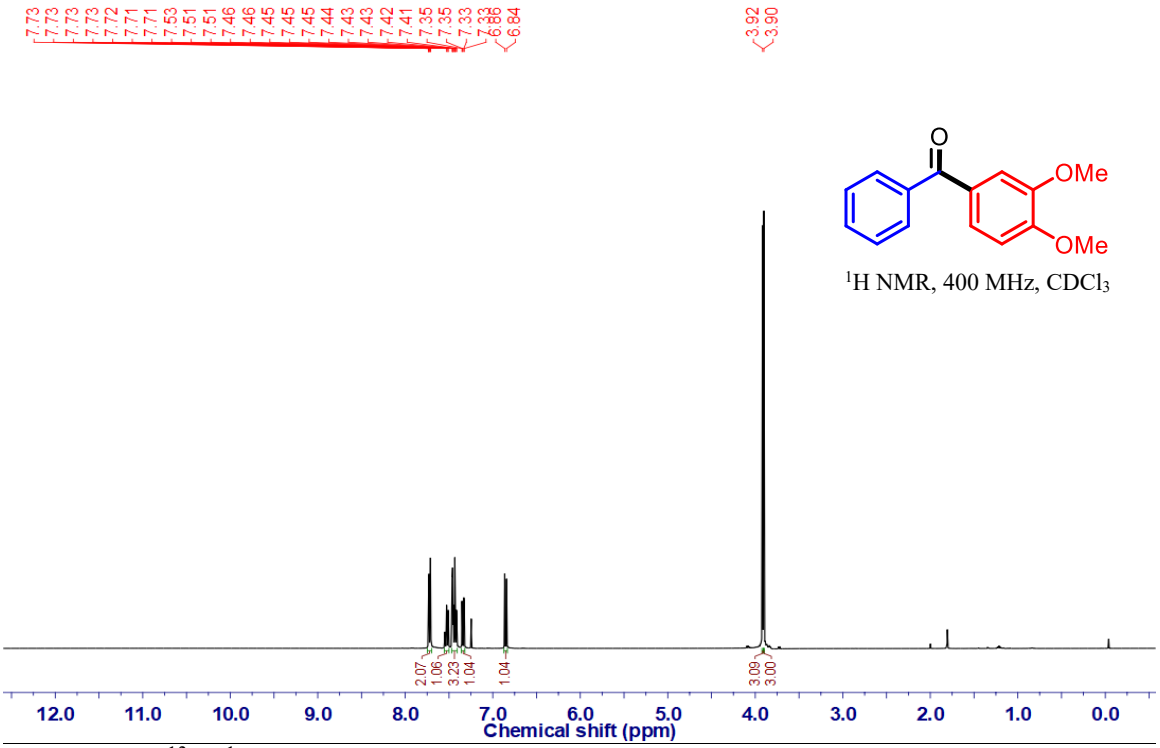


Figure S68. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **5b** in $CDCl_3$ at 298K.

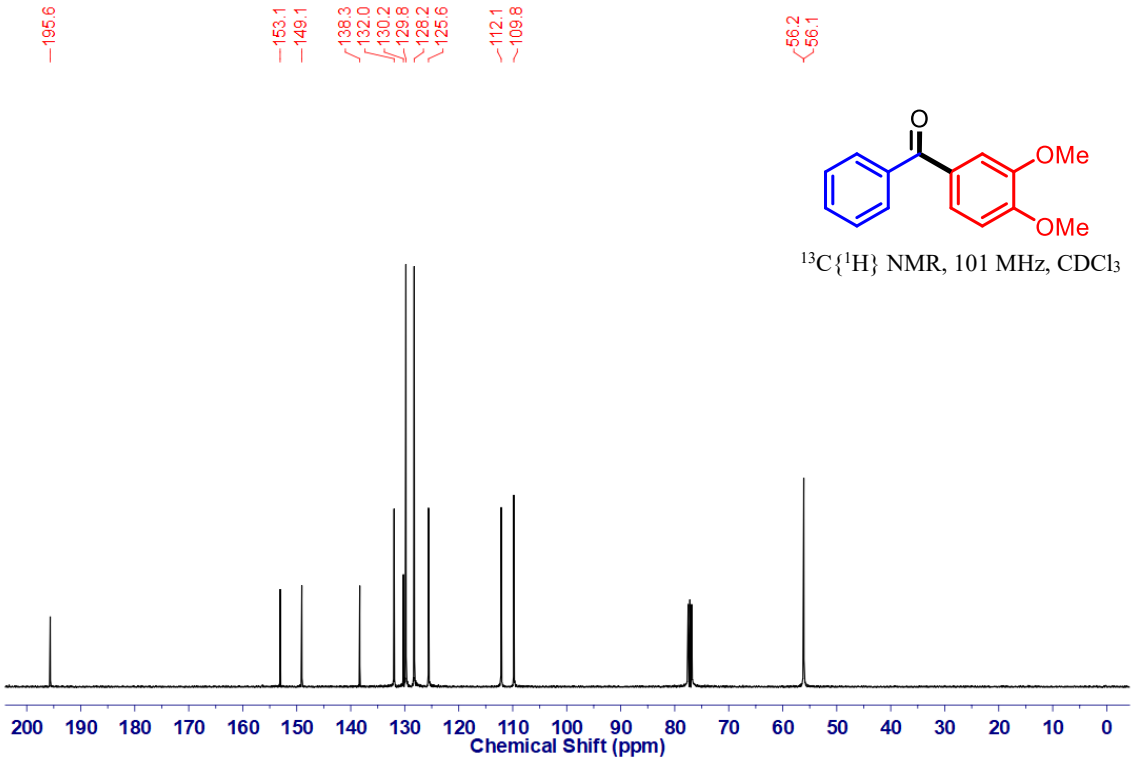


Figure S69. ^{1}H NMR (400 MHz) Spectrum of **5c** in DMSO-d_6 at 298K.

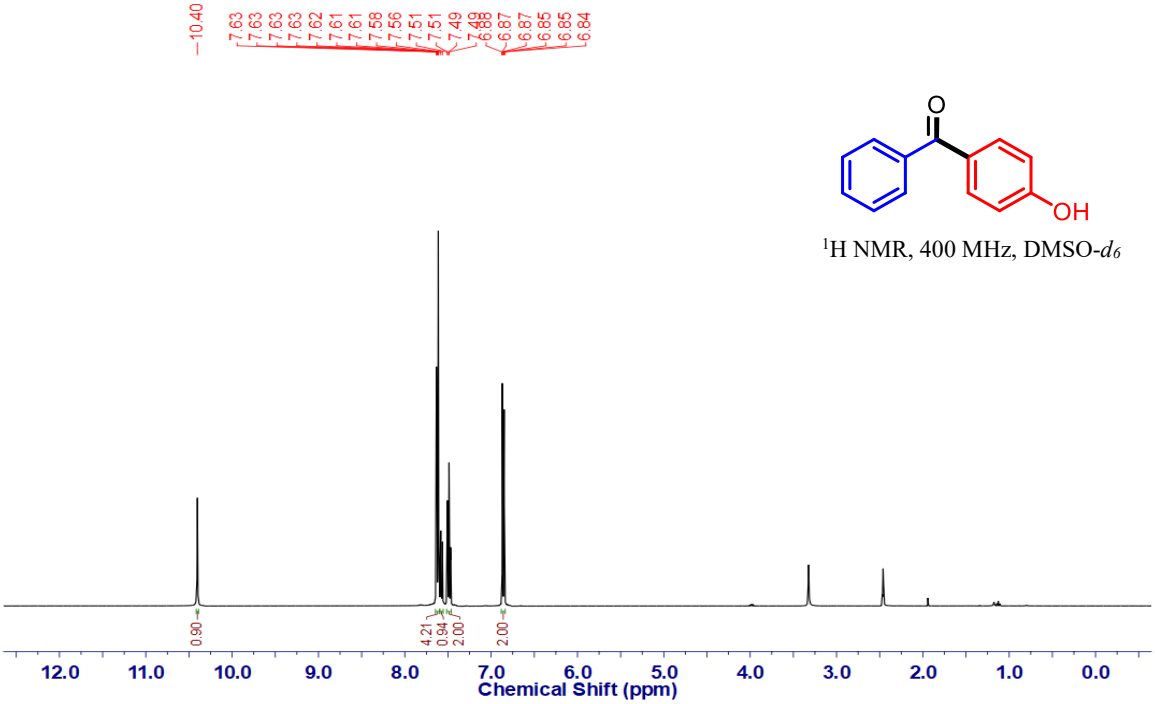


Figure S70. ^{13}C{^{1}H} NMR (101 MHz) Spectrum of **5c** in DMSO-d_6 at 298K.

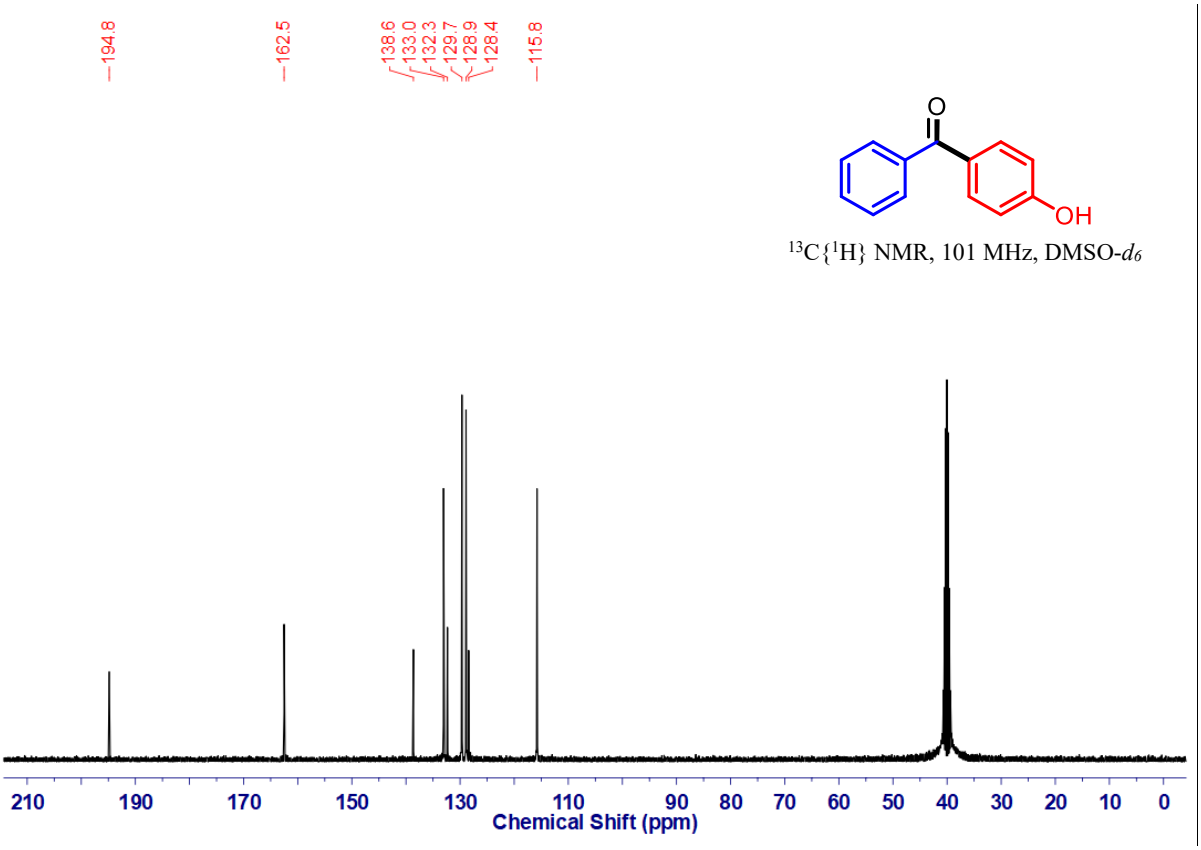
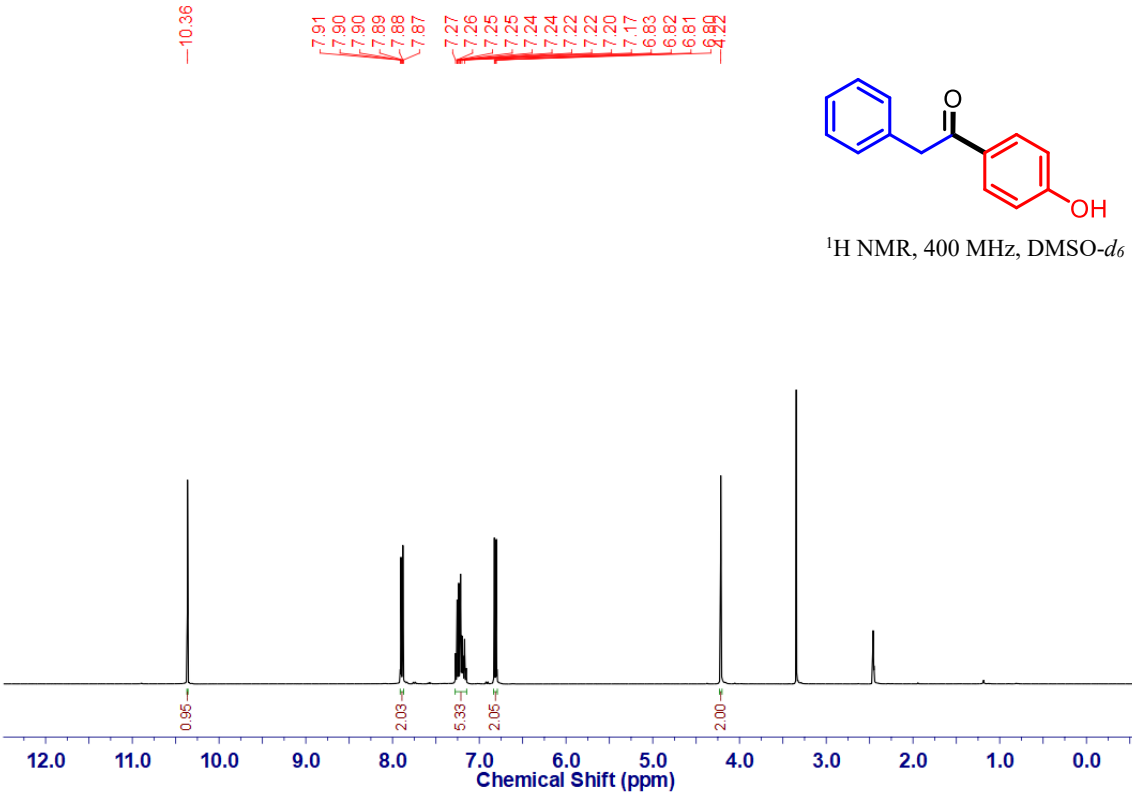
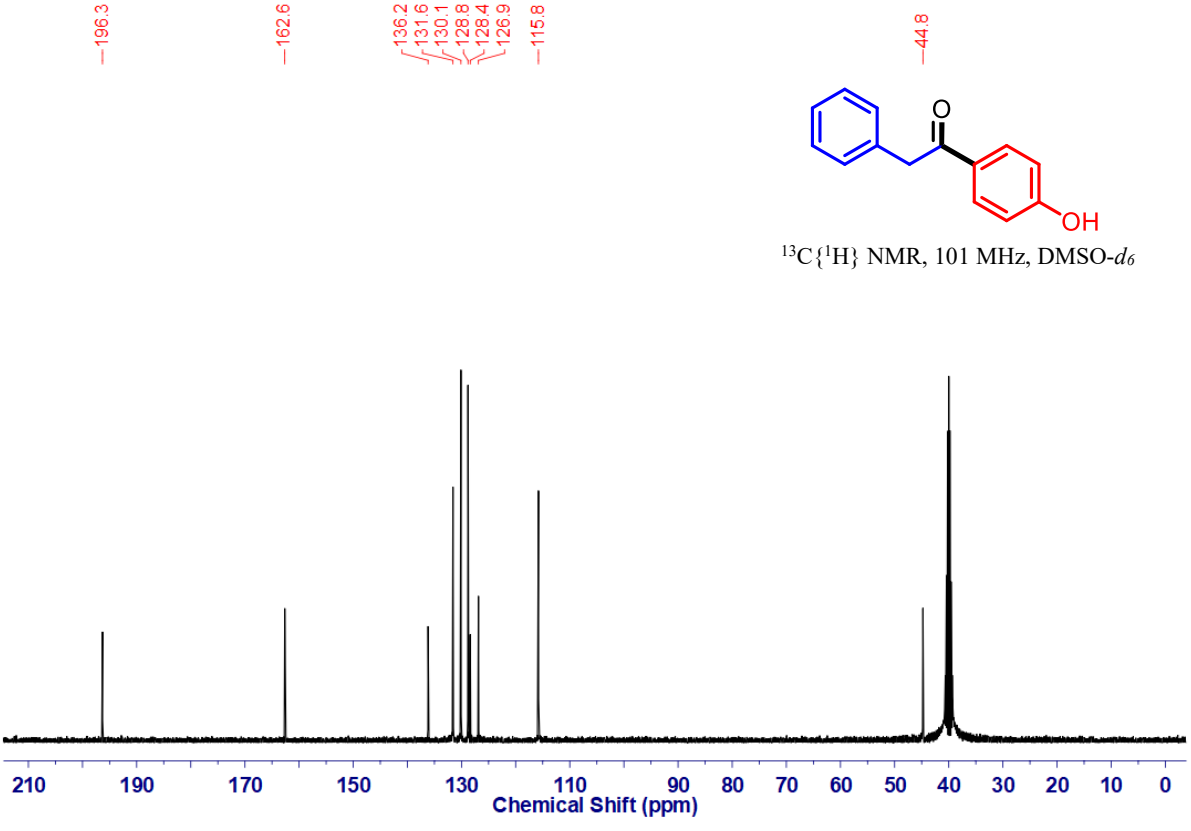


Figure S71. ^{1}H NMR (400 MHz) Spectrum of **5e** in DMSO-d_6 at 298K.



^{1}H NMR, 400 MHz, DMSO-d_6

Figure S72. ^{13}C{^{1}H} NMR (101 MHz) Spectrum of **5e** in DMSO-d_6 at 298K.



^{13}C{^{1}H} NMR, 101 MHz, DMSO-d_6

Figure S73. ^{1}H NMR (400 MHz) Spectrum of **5f** in $CDCl_3$ at 298K.

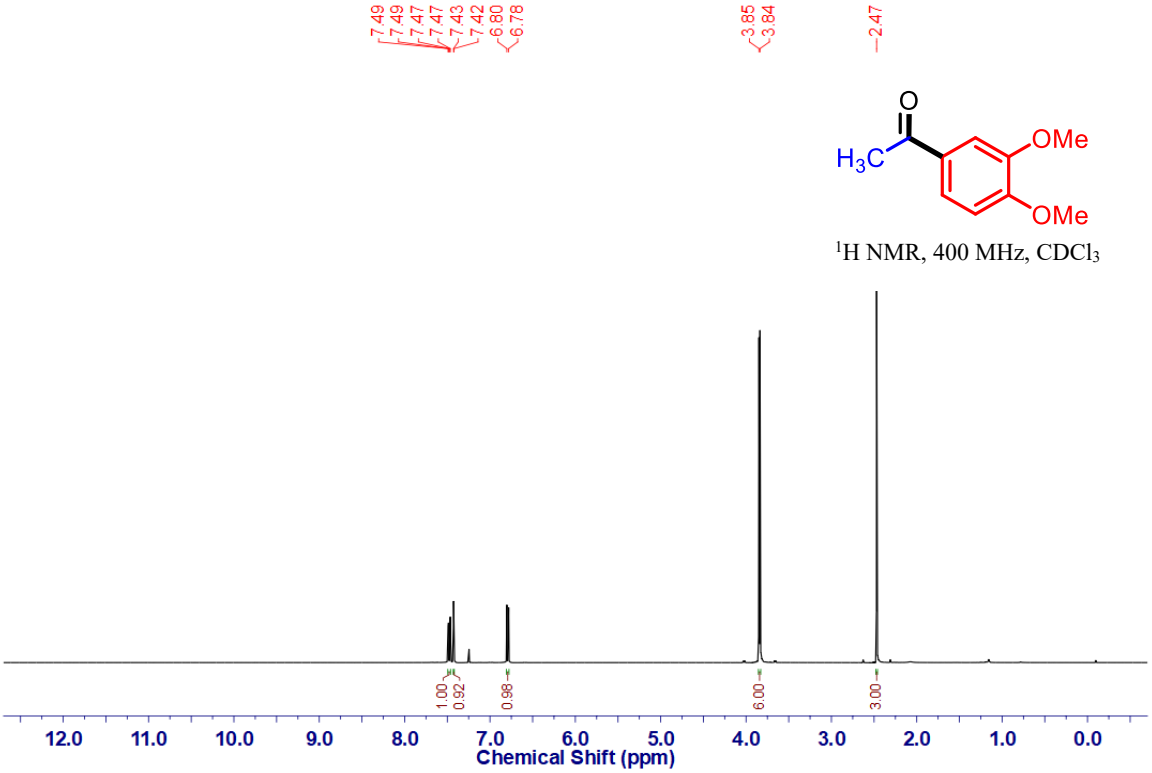


Figure S74. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **5f** in $CDCl_3$ at 298K.

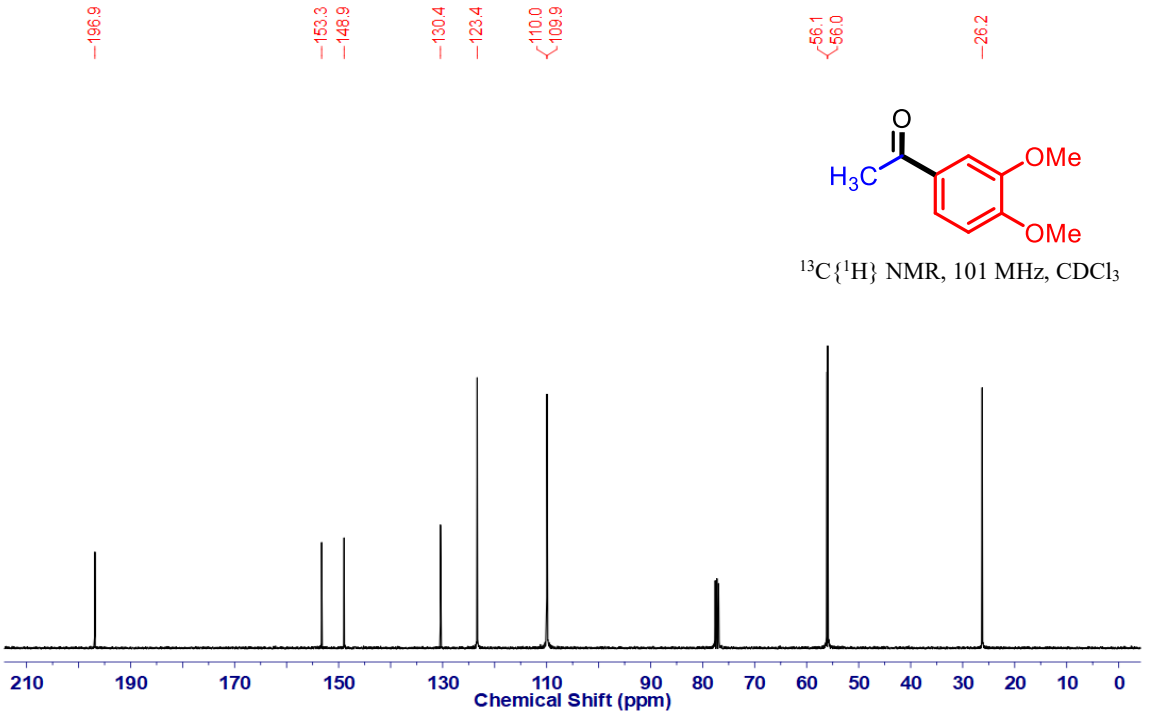
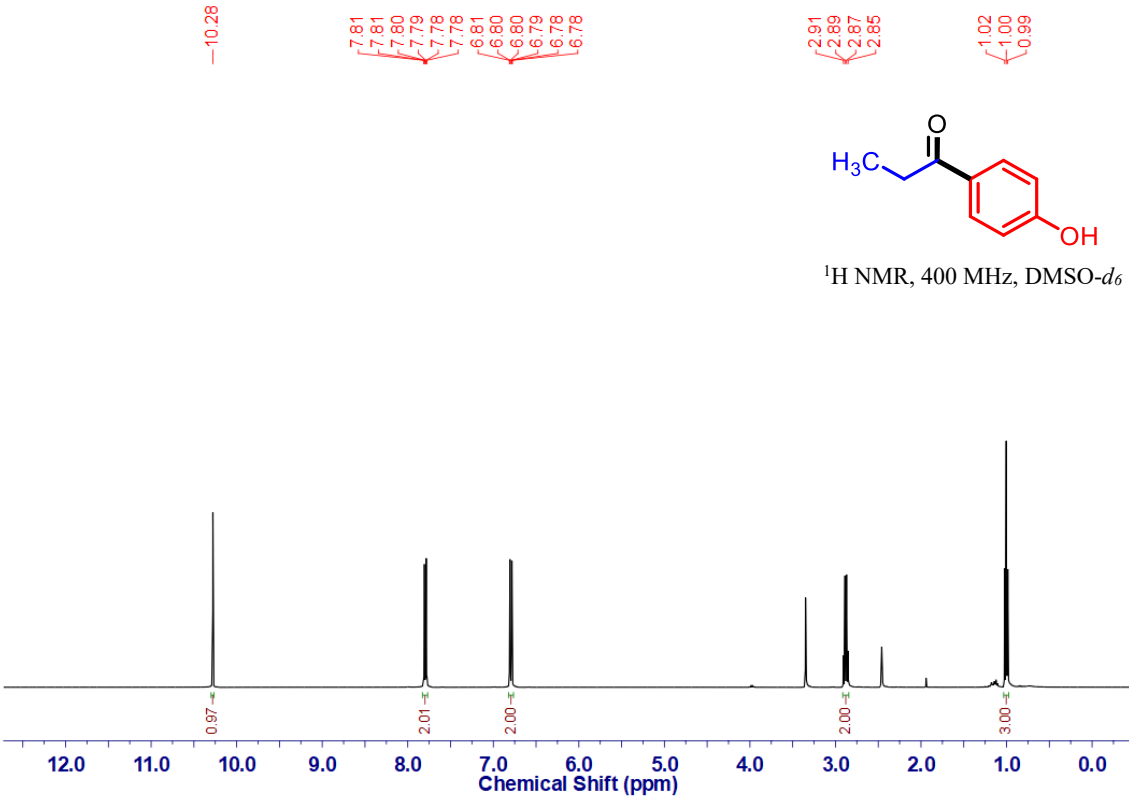
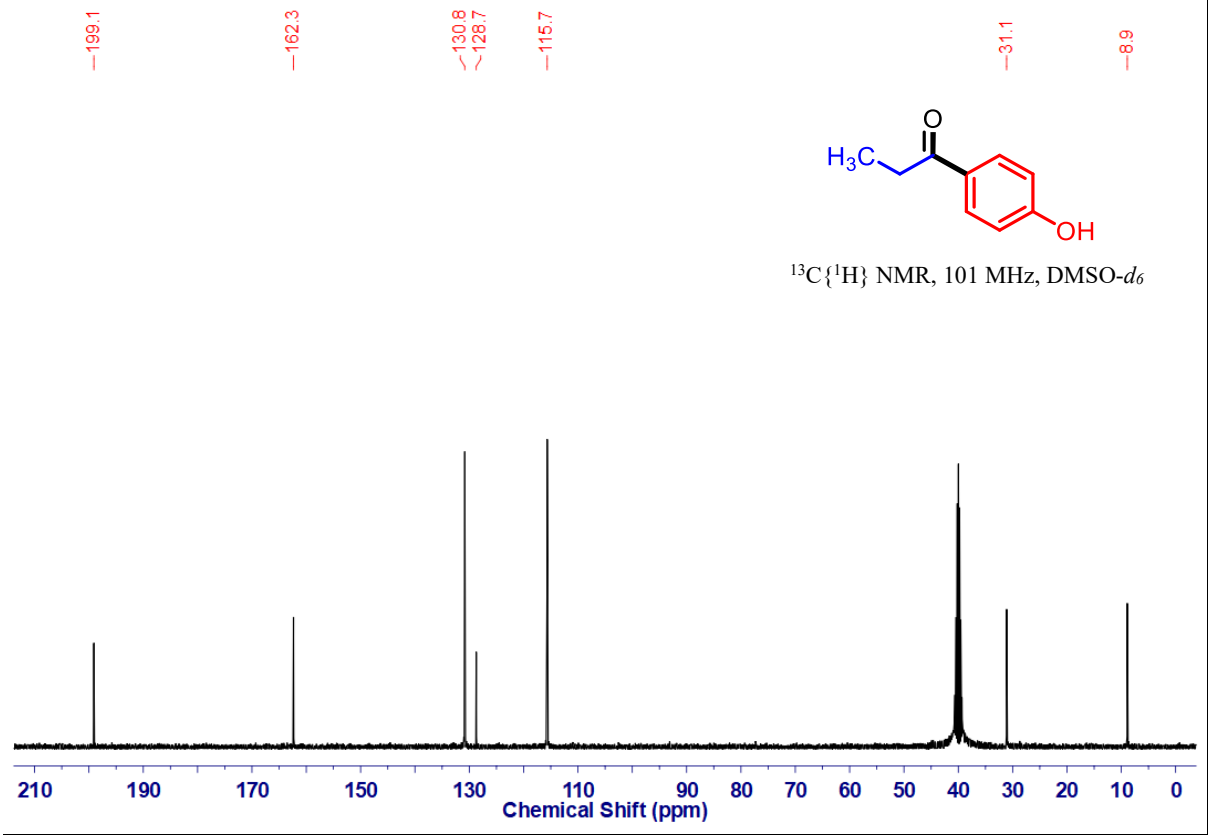


Figure S75. ^{1}H NMR (400 MHz) Spectrum of **5g** in DMSO-d_6 at 298K.



^{1}H NMR, 400 MHz, DMSO-d_6

Figure S76. ^{13}C{^{1}H} NMR (101 MHz) Spectrum of **5g** in DMSO-d_6 at 298K.



^{13}C{^{1}H} NMR, 101 MHz, DMSO-d_6

Figure S77. ^{1}H NMR (400 MHz) Spectrum of **5h** in $CDCl_3$ at 298K.

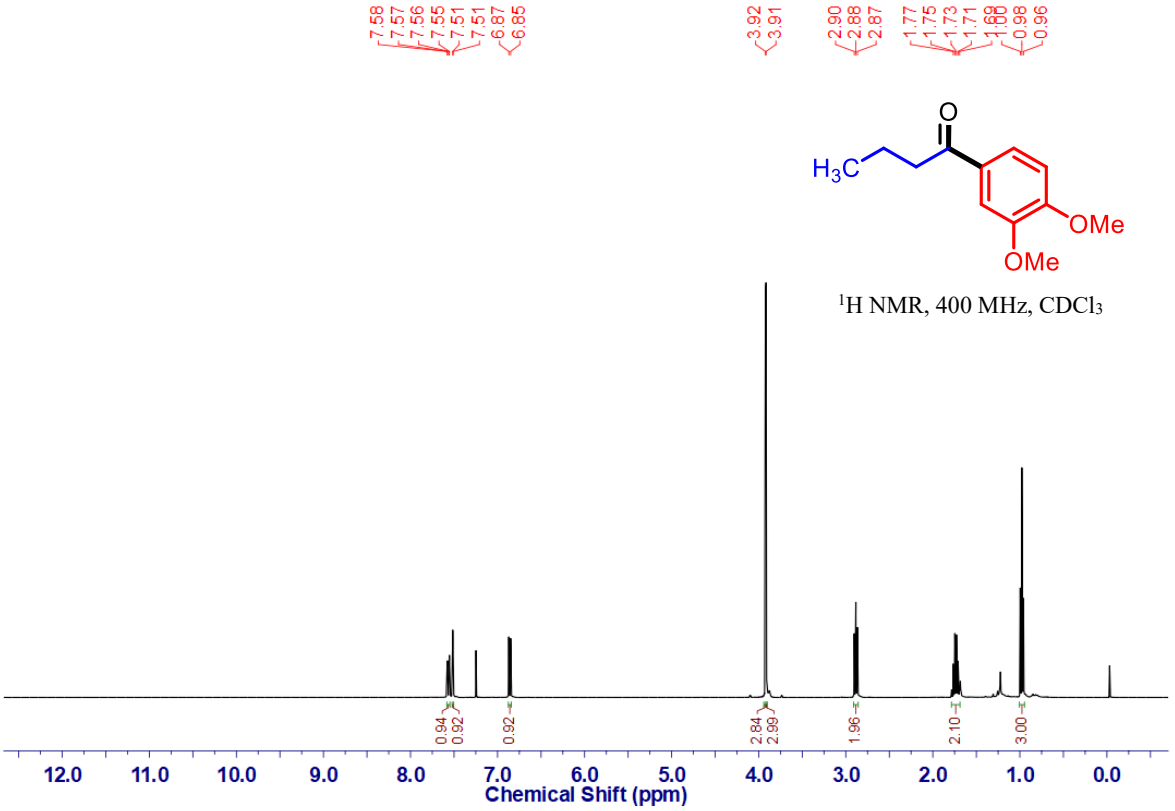


Figure S78. ^{13}C{^{1}H} NMR (101 MHz) Spectrum of **5h** in $CDCl_3$ at 298K.

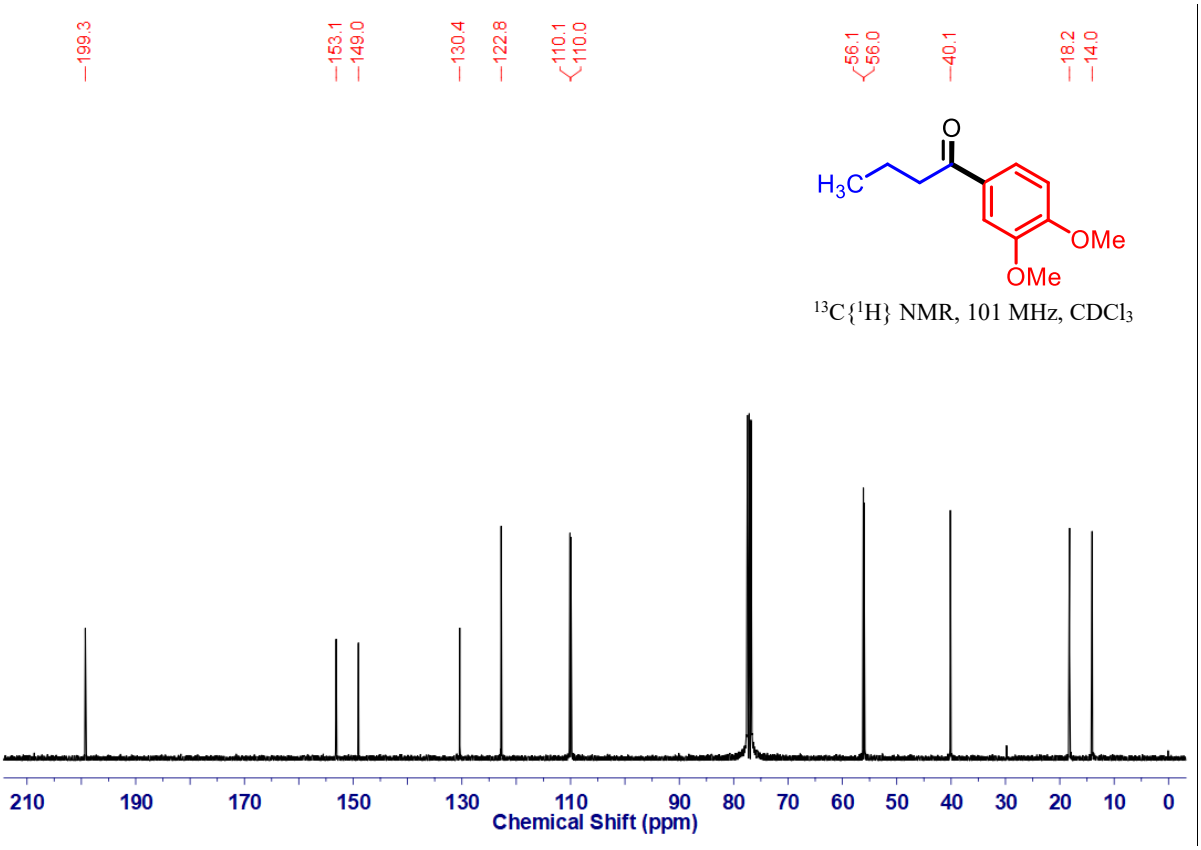


Figure S79. ^{1}H NMR (400 MHz) Spectrum of **7** in $CDCl_3$ at 298K.

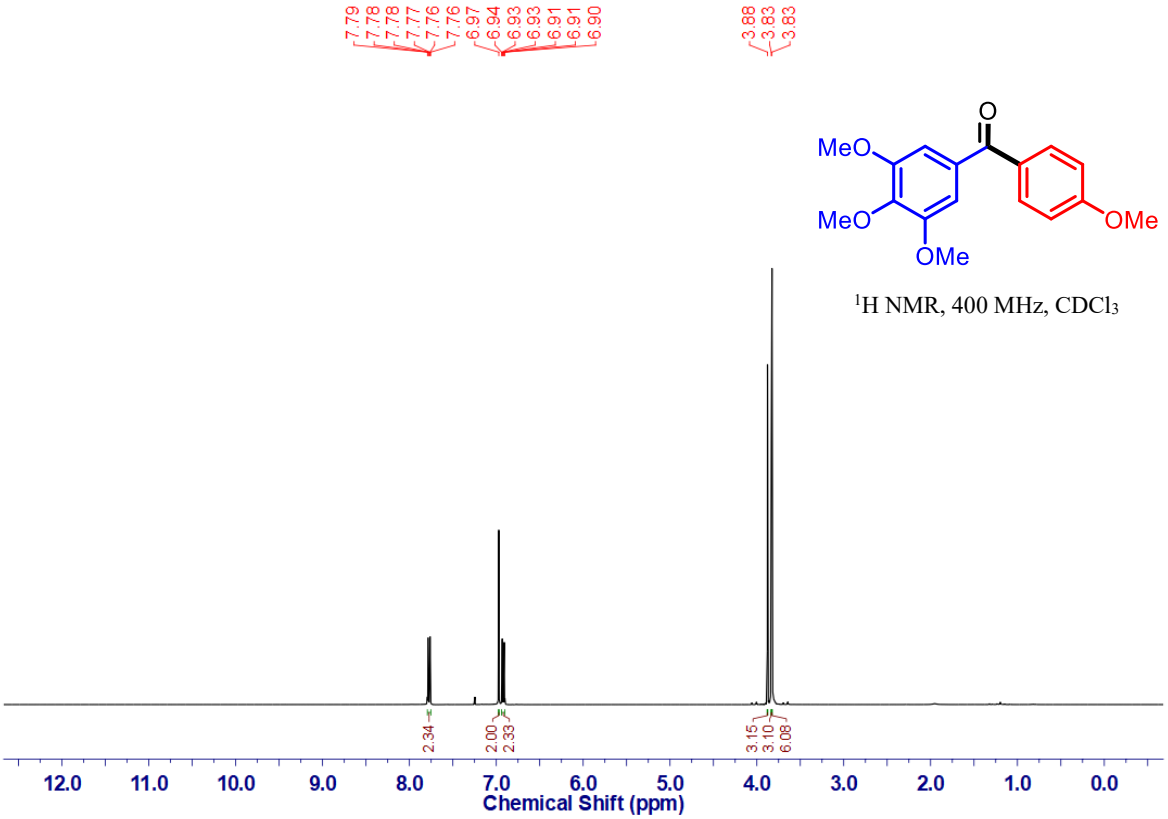


Figure S80. $^{13}C\{^{1}H\}$ NMR (101 MHz) Spectrum of **7** in $CDCl_3$ at 298K.

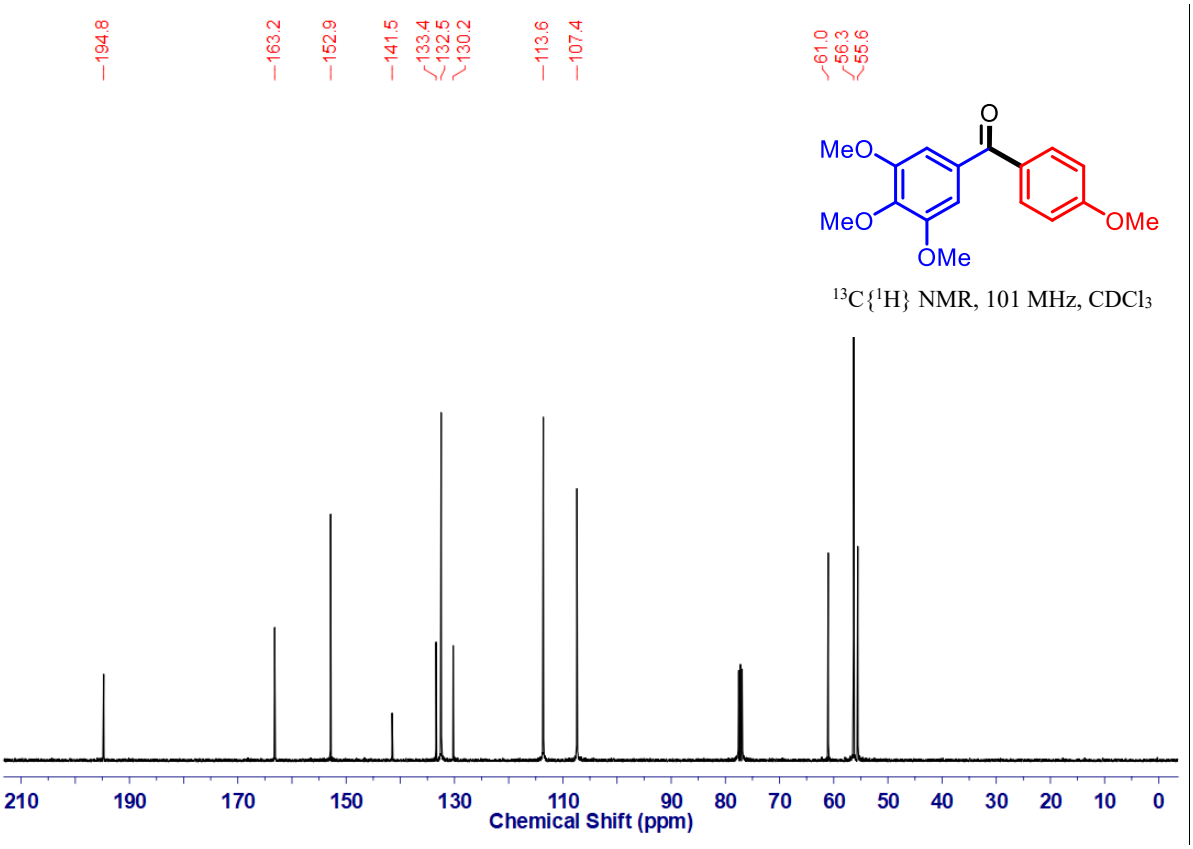


Figure S81. HRMS spectrum of **3q** in methanol solvent.

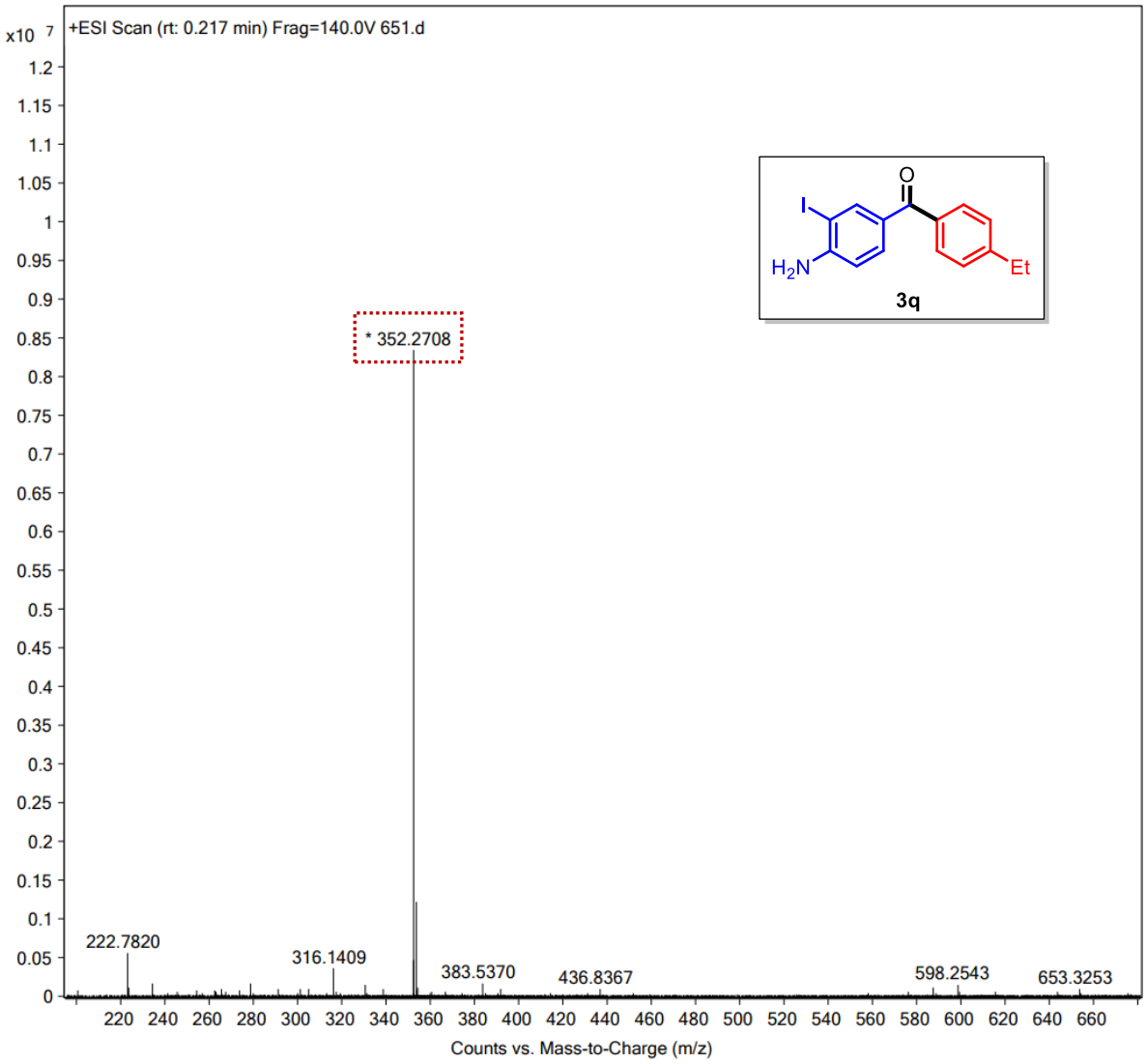


Figure S82. HRMS spectrum of **3r** in methanol solvent.

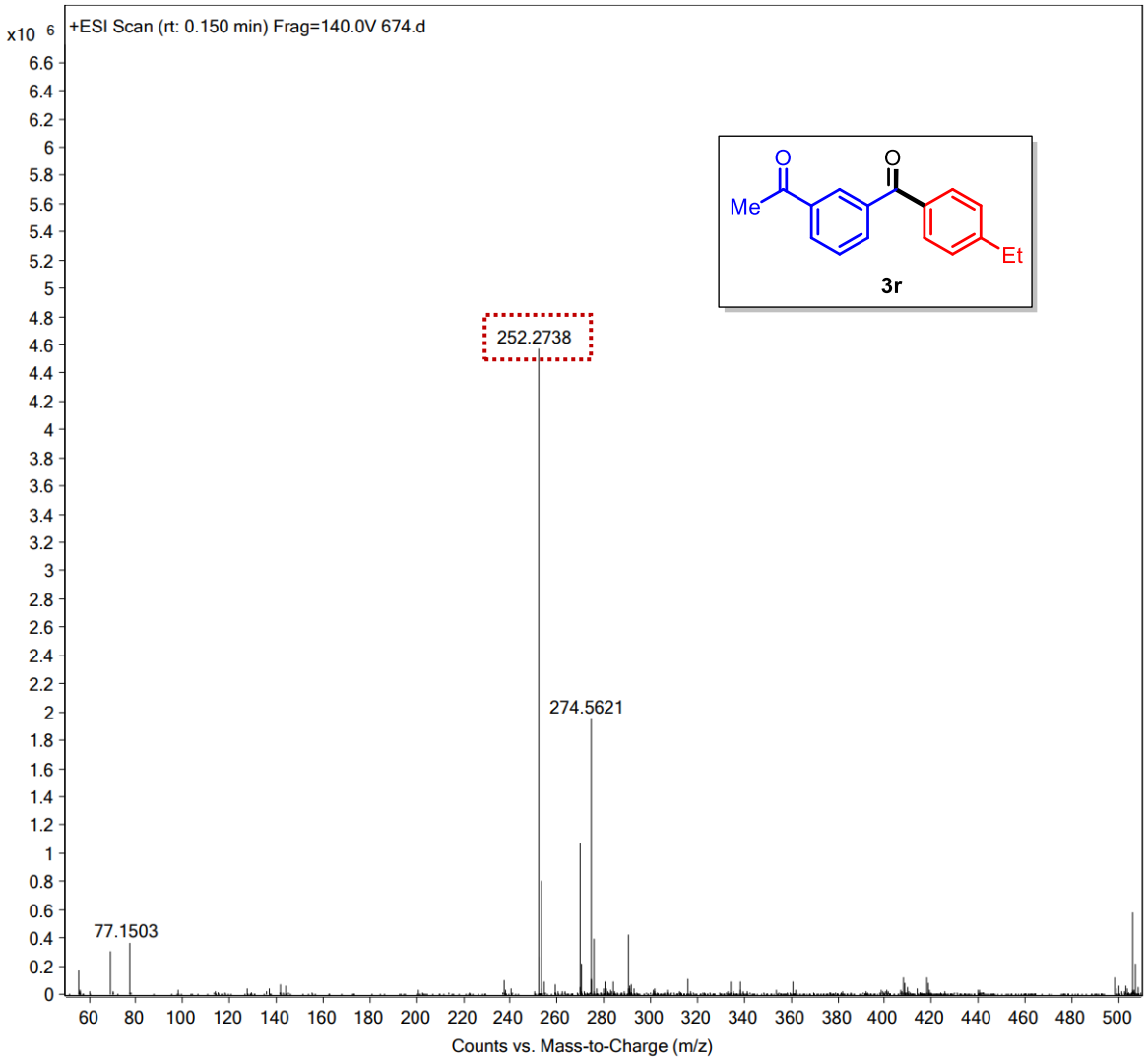


Figure S83. HRMS spectrum of **4l** in methanol solvent.

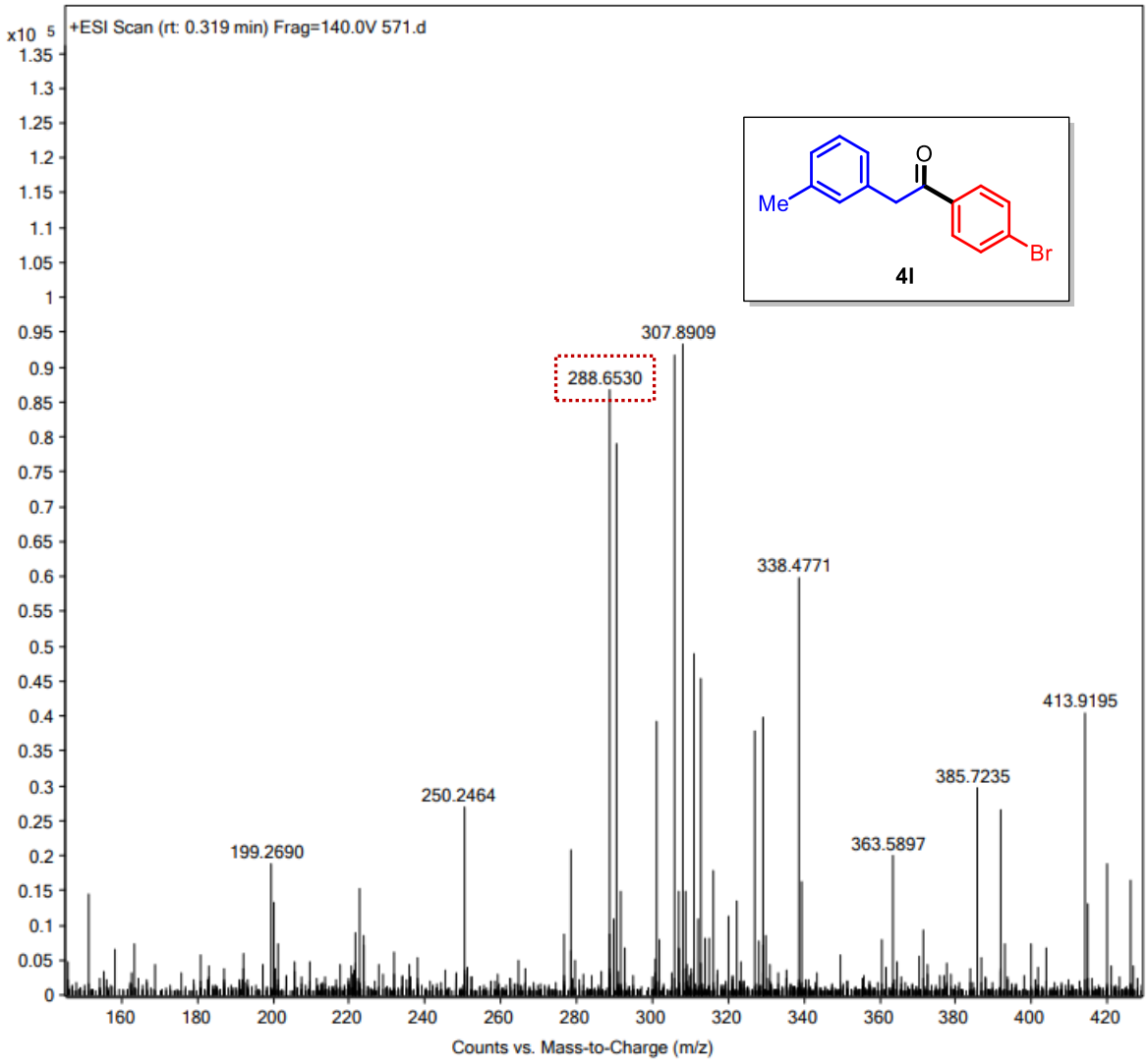


Figure S84. HRMS spectrum of **4m** in methanol solvent.