Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Photocatalytic dehydrations for Ritter reaction

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Contents

1. General Information

- Chemicals were purchased from Alfa Aesar, Bidepharm, and TCI, they were used without further purification unless otherwise noted. Solvents were purified using a solvent-purification system (VSPS-8, Vigor).
- Analytical thin-layer chromatography was carried out with silica gel pre-coated glass plates (TLC-Silica gel GF254, coating thickness: 0.25 mm) purchased from Xinnuo Chemical (Yantai, China). Chromatographic purification of the products was performed on silica gel 200-300 mesh. Visualization of the developed TLC plates was performed with ultraviolet irradiation (254 nm) or by staining with basic potassium permanganate solution.
- ^{1}H- and ^{13}C- NMR spectra were recorded at ambient temperature on a Shimadzu Avance 400/500 Spectrometer. The chemical shifts are reported in ppm downfield of tetramethylsilane (TMS) and referenced to residual solvent peaks resonance as the internal standard. The order of citation in parentheses is a) multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, m = multiplet), b) coupling constants, c) number of protons. Coupling constants (*J*) are reported in Hertz (Hz).
- IR spectra were taken on a Vertex 70 spectrophotometer and reported as wave numbers (cm^{-1}).
- High-resolution mass spectra (HRMS) were obtained with the mass analyzer of an orbitrap. The calculated values are based on the most abundant isotope.
- The SGW X-4 was used to measure the melting point of solids.
- The GC-MS TQ8040 was used in the detection of the reaction mixture.
- The fluorescence quenching experiment was conducted by using an Edinburgh instruments FS5.
- Photochemical experiments were performed magnetically stirred in 10 mL glass tubes, sealed with a rubber septum (Figure S1). The tubes were irradiated with blue light using a LED lamp with a power output of 100 W (see the below picture). All distances from the light source to the irradiation vessel are 2 cm and a fan is used to keep the reaction temperature at 45 ± 5 °C.

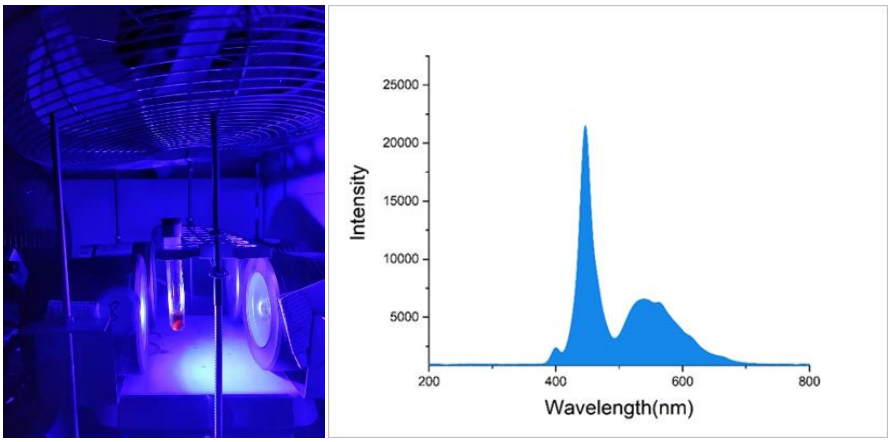
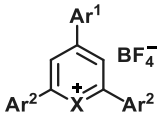


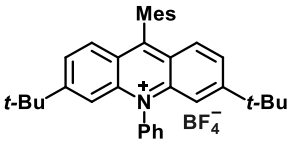
Figure S1 The spectrum of blue LEDs (100 W) employed in the reaction.

2. Experimental Procedures

2.1 Preparation for the photocatalysts



PC1: X = O, Ar^1 = Ar^2 = Ph
PC2: X = O, Ar^1 = Ar^2 = 4-MeC_6H_4
PC3: X = O, Ar^1 = Ar^2 = 4-$MeOC_6H_4$
PC4: X = O, Ar^1 = Ar^2 = 4-BrC_6H_4r
PC5: X = S, Ar^1 = Ar^2 = Ph
PC6: X = O, Ar^1 = Mes, Ar^2 = Ph

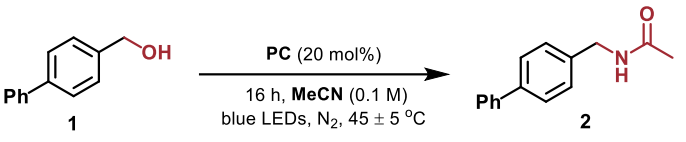


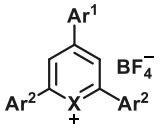
PC8

PC1-PC5 were synthesized according to the literature procedure.[1] **PC6** and **PC8** were synthesized according to the literature procedure.[2]

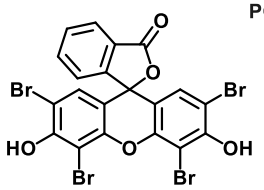
2.2 Optimization of the reaction conditions

Table S1 Screening of photocatalysts.[a]

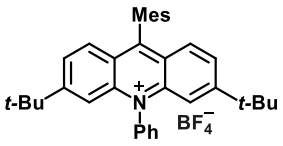




PC1: X = O, Ar^1 = Ar^2 = Ph
PC2: X = O, Ar^1 = Ar^2 = 4-MeC_6H_4
PC3: X = O, Ar^1 = Ar^2 = 4-$MeOC_6H_4$
PC4: X = O, Ar^1 = Ar^2 = 4-BrC_6H_4r
PC5: X = S, Ar^1 = Ar^2 = Ph
PC6: X = O, Ar^1 = Mes, Ar^2 = Ph



PC7



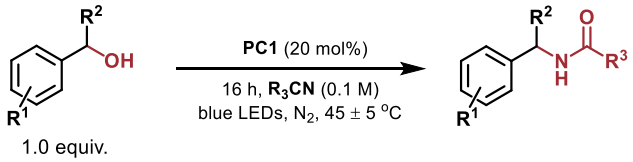
PC8

Entry	Catalyst	Yield (%)[b]
1	**PC1**	76 (87)[c]
2	**PC1**	65[d]
3	**PC1**	20[e]
4	**PC2**	52
5	**PC3**	72
6	**PC4**	63
7	**PC5**	30
8	**PC6**	67
9	**PC7**	trace

10	**PC8**	trace
11	**PC1**	69[f]
12	**PC1**	65[g]
13	**PC1**	NR[h]
14	**PC1**	NR[i]
15	/	NR

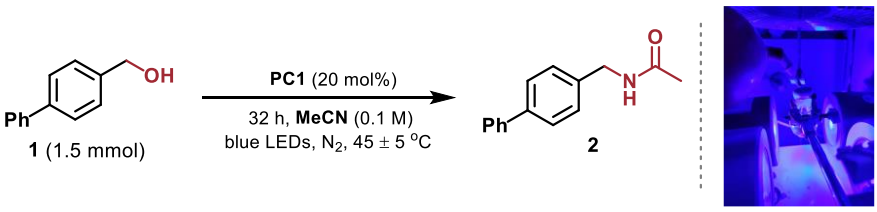
[a]**1** (0.2 mmol), **PC** (20 mol%), MeCN (2.0 mL), irradiation with 100 W blue LEDs, NR denotes no reaction; [b]yield of isolated products; [c]NMR yield in parentheses; [d]in 40W Blue LEDs; [e]in 10W Blue LEDs; [f]in 0.2 M MeCN; [g]with 10 mol% **PC1**; [h]no illumination at 45 °C; [i]no illumination at 120 °C.

2.3 The general procedure of the reaction



General Procedure A: In a nitrogen atmosphere, to a dry glass tube equipped with a stirring bar, the specified benzyl alcohol (0.2 mmol, 1.0 equiv.), **PC1** (0.04 mmol, 20 mol%, 15.8 mg), and the specified nitrile solvent (2.0 mL) were added. The mixture was stirred for overnight under a 100 W blue LED lamp. The distance from the light source to the irradiation glass tubes was 2 cm and a fan was used to keep the reaction temperature at 45 ± 5 °C (the heat source is from irradiation of LED lamp). Upon completion, the solvent was removed and the residue was subjected to silica gel chromatography to afford the desired product.

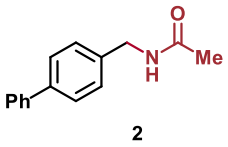
2.4 Large-scale reaction



In a nitrogen-filled glovebox, a dry tube equipped with a magnetic stirring bar was charged sequentially with **1** (1.5 mmol, 276.0 mg), **PC1** (0.3 mmol, 79.2 mg), and MeCN (15.0 mL). The vial was closed and removed from the glovebox. The resulting mixture was allowed to stir at about 45 °C under two blue LEDs irradiation for 32 h. Upon completion, the solvent was

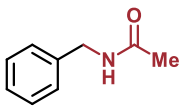
removed under vacuum and the residue was subjected to silica gel chromatography. The desired product **2** (182.3 mg, 0.810 mmol, 54%) was obtained after purification (PE/EA/acetone = 4:1:1).

3. Compound Characterization Data



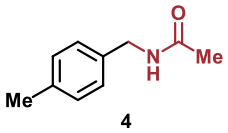
2

***N*-([1,1'-biphenyl]-4-ylmethyl)acetamide (2):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (34.2 mg, 0.152 mmol, 76%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.59 – 7.52 (m, 4H), 7.47 – 7.41 (m, 2H), 7.38 – 7.31 (m, 3H), 5.92 (s, 1H), 4.46 (d, *J* = 5.7 Hz, 2H), 2.04 (d, *J* = 1.3 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 170.1, 140.8, 140.7, 137.4, 128.9, 128.4, 127.6, 127.5, 127.2, 43.6, 23.4. These data are in agreement with those reported previously in the literature.[3]



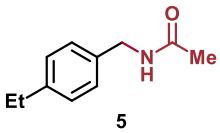
3

***N*-benzylacetamide (3):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (13.4 mg, 0.090 mmol, 45%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.36 – 7.32 (m, 2H), 7.30 – 7.26 (m, 3H), 5.77 (s, 1H), 4.42 (d, *J* = 5.7 Hz, 2H), 2.01 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 170.0, 138.3, 128.9, 128.0, 127.7, 43.9, 23.4. These data are in agreement with those reported previously in the literature.[4]



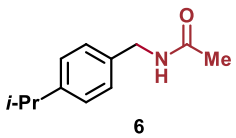
4

***N*-(4-methylbenzyl)acetamide (4):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (18.9 mg, 0.116 mmol, 58%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.18 – 7.13 (m, 4H), 5.87 (s, 1H), 4.37 (d, *J* = 4.5 Hz, 2H), 2.33 (s, 3H), 2.00 (d, *J* = 1.3 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 170.0, 137.4, 135.3, 129.5, 128.0, 43.6, 23.4, 21.2. These data are in agreement with those reported previously in the literature.[4]



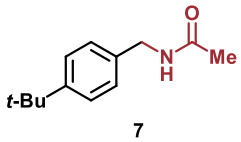
5

***N*-(4-ethylbenzyl)acetamide (5):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (17.7 mg, 0.100 mmol, 50%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.20 – 7.15 (m, 4H), 5.90 (s, 1H), 4.37 (d, *J* = 5.6 Hz, 2H), 2.63 (d, *J* = 7.5 Hz, 2H), 1.99 (d, *J* = 1.2 Hz, 3H), 1.22 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 167.0, 143.8, 135.5, 128.3, 128.1, 43.6, 28.6, 23.4, 15.8. These data are in agreement with those reported previously in the literature.[5]



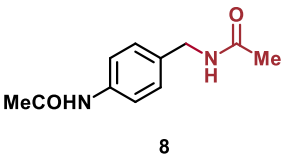
6

***N*-(4-isopropylbenzyl)acetamide (6):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (21.8 mg, 0.114 mmol, 57%). **Melting point**: 101 – 102 °C. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.24 – 7.16 (m, 4H), 5.83 (s, 1H), 4.38 (d, *J* = 5.6 Hz, 2H), 2.93 – 2.86 (m, 1H), 2.00 (s, 3H), 1.24 (d, *J* = 6.9 Hz, 6H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 167.0, 148.5, 135.7, 128.1, 126.9, 43.7, 33.9, 24.1, 23.4. **IR (ATR)**: 3283, 2959, 1650, 1546, 1372, 1257, 1017, 702, 566 cm^{-1}. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{12}H_{18}NO^+$ 192.1383, found 192.1383.



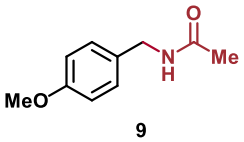
7

***N*-(4-(tert-butyl)benzyl)acetamide (7):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (22.6 mg, 0.110 mmol, 55%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.36 (d, *J* = 8.1 Hz, 2H), 7.22 (d, *J* = 8.1 Hz, 2H), 5.84 (s, 1H), 4.39 (d, *J* = 5.6 Hz, 2H), 2.00 (s, 3H), 1.31 (s, 9H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 167.0, 150.7, 135.3, 127.8, 125.8, 43.6, 34.6, 31.4, 23.4. These data are in agreement with those reported previously in the literature.[6]



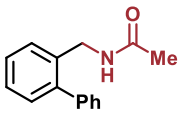
8

***N*-(4-(acetamidomethyl)phenyl)acetimide (8):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (23.5 mg, 0.114 mmol, 57%). **^{1}H NMR** (500 MHz, Methanol-d_4) δ 7.50 (d, *J* = 8.5 Hz, 2H), 7.23 (d, *J* = 8.3 Hz, 2H), 4.30 (s, 2H), 2.11 (s, 3H), 1.97 (s, 3H). **^{13}C NMR** (126 MHz, Methanol-d_4) δ 173.1, 171.6, 139.0, 135.7, 129.1, 121.2, 43.8, 23.8, 22.5. These data are in agreement with those reported previously in the literature.[7]



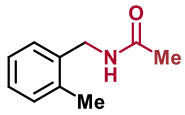
9

***N*-(4-methoxybenzyl)acetamide (9):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (24.7 mg, 0.138 mmol, 69%). **^{1}H NMR** (500 MHz, Methanol-d_4) δ 7.21 (d, *J* = 8.5 Hz, 2H), 6.87 (d, *J* = 8.6 Hz, 2H), 5.71 (s, 1H), 4.36 (d, *J* = 5.6 Hz, 2H), 3.80 (s, 3H), 2.01 (d, *J* = 0.6 Hz, 3H). **^{13}C NMR** (126 MHz, Methanol-d_4) δ 169.9, 159.2, 130.4, 129.4, 114.2, 55.4, 43.4, 23.4. These data are in agreement with those reported previously in the literature.[6]



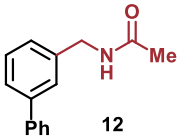
10

***N*-([1,1'-biphenyl]-2-ylmethyl)acetamide (10):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (27.0 mg, 0.120 mmol, 60%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.45 – 7.40 (m, 3H), 7.39 – 7.36 (m, 1H), 7.35 – 7.32 (m, 2H), 7.31 – 7.28 (m, 2H), 7.26 (d, *J* = 1.8 Hz, 1H), 5.56 (s, 1H), 4.40 (d, *J* = 5.6 Hz, 2H), 1.89 (d, *J* = 0.7 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.8, 141.8, 140.8, 135.5, 130.3, 129.1, 128.9, 128.5, 127.9, 127.6, 127.4, 41.7, 23.2. These data are in agreement with those reported previously in the literature.[8]



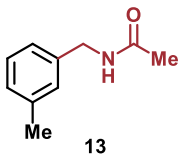
11

***N*-(2-methylbenzyl)acetamide (11):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (20.5 mg, 0.126 mmol, 63%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.25 – 7.15 (m, 4H), 5.71 (s, 1H), 4.41 (d, *J* = 5.3 Hz, 2H), 2.32 (s, 3H), 2.00 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.9, 136.6, 135.9, 130.7, 128.7, 128.0, 126.3, 42.0, 23.3, 19.1. These data are in agreement with those reported previously in the literature.[9]



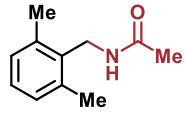
12

***N*-([1,1'-biphenyl]-3-ylmethyl)acetamide (12):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (24.8 mg, 0.110 mmol, 55%). **Melting point**: 105 – 106 °C. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.59 – 7.56 (m, 2H), 7.52 – 7.48 (m, 2H), 7.46 – 7.40 (m, 3H), 7.38 – 7.33 (m, 1H), 7.30 – 7.24 (m, 1H), 5.83 (s, 1H), 4.50 (d, *J* = 5.7 Hz, 2H), 2.04 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 170.1, 141.9, 140.9, 138.9, 129.3, 129.0, 127.6, 127.3, 126.9, 126.9, 126.6, 44.0, 23.5. **IR (ATR)**: 3301, 2922, 1639, 1538, 1374, 1086, 760, 697 cm^{-1}. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{15}H_{16}NO^+$ 226.1226, found 226.1227.



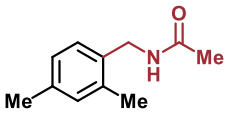
13

***N*-(3-methylbenzyl)acetamide (13):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (17.3 mg, 0.106 mmol, 53%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.24 – 7.21 (m, 1H), 7.14 – 7.03 (m, 3H), 5.74 (s, 1H), 4.39 (d, *J* = 5.7 Hz, 2H), 2.35 (s, 3H), 2.02 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 170.0, 138.6, 138.2, 128.8, 128.4, 125.0, 43.9, 23.5, 21.5. These data are in agreement with those reported previously in the literature.[9]



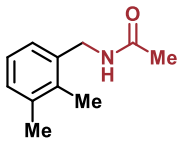
14

***N*-(2,6-dimethylbenzyl)acetamide (14):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (25.8 mg, 0.146 mmol, 73%). **Melting point**: 146 – 147 °C. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.11 – 7.09 (m, 1H), 7.03 (d, *J* = 7.5 Hz, 2H), 5.42 (s, 1H), 4.43 (d, *J* = 4.6 Hz, 2H), 2.34 (s, 6H), 1.94 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 170.0, 137.6, 133.9, 128.5, 128.0, 38.5, 23.1, 19.8. **IR (ATR)**: 3251, 2922, 1630, 1551, 1374, 1220, 1095, 768, 574 cm^{-1}. **HRMS** (ESI) *m/z*: [M+H]$^+$ calcd. for $C_{11}H_{16}NO^+$ 178.1226, found 178.1227.



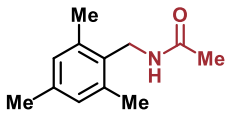
15

***N*-(2,4-dimethylbenzyl)acetamide (15):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (23.7 mg, 0.134 mmol, 67%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.11 (d, *J* = 7.6 Hz, 1H), 6.99 (d, *J* = 13.2 Hz, 2H), 5.66 (s, 1H), 4.37 (d, *J* = 5.3 Hz, 2H), 2.29 (d, *J* = 7.2 Hz, 6H), 1.99 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.8, 137.7, 136.5, 132.9, 131.5, 129.0, 126.9, 41.8, 23.3, 21.1, 19.0. These data are in agreement with those reported previously in the literature.[10]



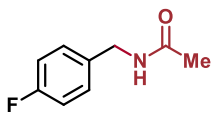
16

***N*-(2,3-dimethylbenzyl)acetamide (16):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (19.1 mg, 0.108 mmol, 54%). **Melting point**: 142 – 143 °C. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.14 – 7.06 (m, 3H), 5.64 (s, 1H), 4.43 (d, *J* = 5.2 Hz, 2H), 2.29 (s, 3H), 2.21 (s, 3H), 1.99 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.7, 137.6, 135.7, 135.4, 129.7, 127.0, 125.8, 42.8, 23.3, 20.6, 15.0. **IR (ATR)**: 3677, 2921, 1630, 1539, 1282, 1028, 725, 604 cm^{-1}. **HRMS** (ESI) *m/z*: [M+H]$^+$ calcd. for $C_{11}H_{16}NO^+$ 178.1226, found 178.1229.



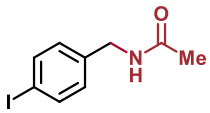
17

***N*-(2,4,6-trimethylbenzyl)acetamide (17):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (28.2 mg, 0.148 mmol, 74%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 6.87 (s, 2H), 5.42 (s, 1H), 4.39 (d, *J* = 4.6 Hz, 2H), 2.31 (s, 6H), 2.26 (s, 3H), 1.95 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 170.0, 137.7, 137.5, 131.0, 129.3, 38.2, 23.1, 21.0, 19.7. These data are in agreement with those reported previously in the literature.[11]



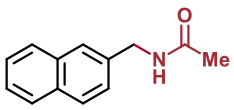
18

***N*-(4-fluorobenzyl)acetamide (18):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (10.4 mg, 0.062 mmol, 31%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.27 – 7.24 (m, 2H), 7.03 – 7.00 (m, 2H), 5.87 (s, 1H), 4.39 (d, *J* = 5.8 Hz, 2H), 2.02 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 170.1, 162.3 (d, *J* = 245.7 Hz), 134.2 (d, *J* = 3.2 Hz), 129.6 (d, *J* = 8.1 Hz), 115.7 (d, *J* = 21.4 Hz)., 43.1, 23.4. These data are in agreement with those reported previously in the literature.[5]



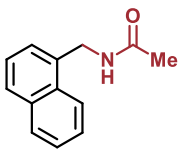
19

***N*-(4-iodobenzyl)acetamide (19):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (22.0 mg, 0.080 mmol, 40%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.01 (d, *J* = 8.3 Hz, 2H), 5.84 (s, 1H), 4.35 (d, *J* = 5.9 Hz, 2H), 2.01 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 170.1, 138.1, 137.9, 129.9, 93.0, 43.3, 23.4. These data are in agreement with those reported previously in the literature.[5]



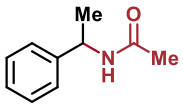
20

***N*-(naphthalen-2-ylmethyl)acetamide (20):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (29.9 mg, 0.150 mmol, 75%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.84 – 7.76 (m, 3H), 7.69 (s, 1H), 7.49 – 7.43 (m, 2H), 7.39 – 7.35 (m, 1H), 6.00 (s, 1H), 4.56 (d, *J* = 5.8 Hz, 2H), 2.03 (d, *J* = 1.4 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 170.1, 135.8, 133.4, 132.8, 128.7, 127.8, 126.5, 126.4, 126.08, 126.05, 44.0, 23.4. These data are in agreement with those reported previously in the literature.[12]



21

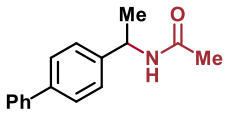
***N*-(naphthalen-1-ylmethyl)acetamide (21):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (33.0 mg, 0.166 mmol, 83%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.99 – 7. 95 (m, 1H), 7.90 – 7.82 (m, 1H), 7.81 – 7.75 (m, 1H), 7.56 – 7.45 (m, 2H), 7.42 – 7.36 (m, 2H), 5.97 (s, 1H), 4.80 (d, *J* = 5.4 Hz, 2H), 1.94 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.9, 133.9, 133.6, 131.5, 128.9, 128.7, 126.8, 126.7, 126.1, 125.5, 123.6, 41.9, 23.2. These data are in agreement with those reported previously in the literature.[13]



22

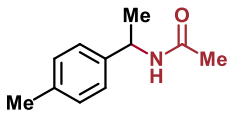
***N*-(1-phenylethyl)acetamide (22):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (15.3 mg, 0.094 mmol, 47%). **^{1}H NMR** (500 MHz,

Chloroform-*d*) δ 7.37 – 7.30 (m, 4H), 7.29 – 7.26 (m, 1H), 5.74 (s, 1H), 5.16 – 5.10 (m, 1H), 1.98 (s, 3H), 1.49 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.2, 143.3, 128.8, 127.6, 126.4, 48.9, 23.6, 21.8. These data are in agreement with those reported previously in the literature.[14]



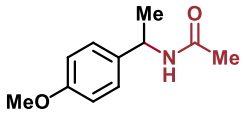
23

***N*-(1-([1,1'-biphenyl]-4-yl)ethyl)acetamide (23):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (34.4 mg, 0.144 mmol, 72%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.57 – 7.54 (m, 4H), 7.45 – 7.41 (m, 2H), 7.38 (d, *J* = 8.2 Hz, 2H), 7.36 – 7.32 (m, 1H), 5.76 (s, 1H), 5.20 – 5.15 (m, 1H), 2.00 (s, 3H), 1.52 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.3, 142.3, 140.8, 140.5, 128.9, 127.6, 127.4, 127.2, 126.8, 48.6, 23.6, 21.8. These data are in agreement with those reported previously in the literature.[15]



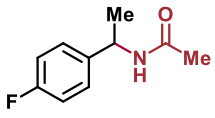
24

***N*-(1-(*p*-tolyl)ethyl)acetamide (24):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (19.1 mg, 0.108 mmol, 54%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.21 (d, *J* = 8.1 Hz, 2H), 7.15 (d, *J* = 7.2 Hz, 2H), 5.73 (s, 1H), 5. 12 – 5.06 (m, 1H), 2.33 (s, 3H), 1.97 (s, 3H), 1.47 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.2, 140.3, 137.2, 129.5, 126.3, 48.6, 23.6, 21.8, 21.2. These data are in agreement with those reported previously in the literature.[16]



25

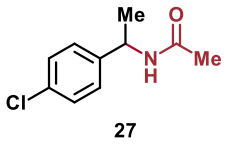
***N*-(1-(4-methoxyphenyl)ethyl)acetamide (25):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (20.8 mg, 0.108 mmol, 54%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.25 (d, *J* = 8.6 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 5.67 (s, 1H), 5.11 – 5.06 (m, 1H), 3.80 (s, 3H), 1.97 (s, 3H), 1.47 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.1, 159.0, 135.4, 127.6, 114.1, 55.4, 48.3, 23.7, 21.7. These data are in agreement with those reported previously in the literature.[16]



26

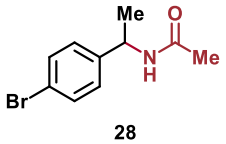
***N*-(1-(4-fluorophenyl)ethyl)acetamide (26):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (16.3 mg, 0.090 mmol, 45%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.29 – 7.26 (m, 2H), 7.03 – 6.99 (m, 2H), 5.87 (s, 1H), 5.12 – 5.07 (m, 1H), 1.97 (s, 3H), 1.46 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.3, 162.1 (d, *J* = 245.3 Hz), 139.2 (d, *J* = 3.3 Hz), 127.9 (d, *J* = 8.2 Hz), 115.5 (d, *J* = 21.5 Hz), 48.2, 23.5,

21.9. These data are in agreement with those reported previously in the literature.[14]



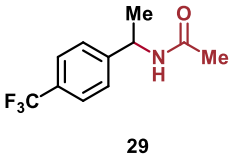
27

***N*-(1-(4-chlorophenyl)ethyl)acetamide (27):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (26.1 mg, 0.132 mmol, 66%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.28 (d, *J* = 6.7 Hz, 2H), 7.24 (d, *J* = 8.5 Hz, 2H), 5.95 (s, 1H), 5.11 – 5.05 (m, 1H), 1.97 (s, 3H), 1.45 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 169.4, 141.9, 133.1, 128.8, 127.7, 48.3, 23.5, 21.8. These data are in agreement with those reported previously in the literature.[14]



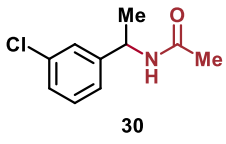
28

***N*-(1-(4-bromophenyl)ethyl)acetamide (28):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (29.0 mg, 0.120 mmol, 60%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.45 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 5.82 (s, 1H), 5.09 – 5.04 (m, *J* = 7.2 Hz, 1H), 1.98 (s, 3H), 1.45 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.3, 142.4, 131.8, 128.1, 121.2, 48.4, 23.5, 21.8. These data are in agreement with those reported previously in the literature.[14]



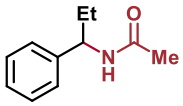
29

***N*-(1-(4-(trifluoromethyl)phenyl)ethyl)acetamide (29):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (15.2 mg, 0.066 mmol, 33%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 8.1 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 5.83 (s, 1H), 5.18 – 5.12 (m, 1H), 2.00 (s, 3H), 1.49 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.4, 147.5, 129.7 (d, *J* = 32.4 Hz), 126.6, 125.8 (q, *J* = 3.8 Hz), 124.2 (d, *J* = 272.1 Hz)., 48.7, 23.5, 22.0. These data are in agreement with those reported previously in the literature.[17]



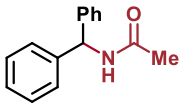
30

***N*-(1-(3-chlorophenyl)ethyl)acetamide (30):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (23.8 mg, 0.120 mmol, 60%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.34 – 7.29 (m, 2H), 7.24 – 7.16 (m, 2H), 6.02 (s, 1H), 5.39 – 5.34 (m, 1H), 1.97 (s, 3H), 1.46 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.2, 140.6, 133.0, 130.3, 128.6, 127.3, 127.2, 47.4, 23.5, 21.0. These data are in agreement with those reported previously in the literature.[17]



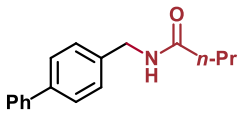
31

***N*-(1-phenylpropyl)acetamide (31):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (15.6 mg, 0.088 mmol, 44%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.36 – 7.31 (m, 2H), 7.29 – 7.26 (m, 3H), 5.84 (s, 1H), 4.90 – 4.85 (m, 1H), 1.98 (s, 3H), 1.85 – 1.78 (m, 2H), 0.88 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.4, 142.2, 128.8, 127.5, 126.8, 55.1, 29.2, 23.6, 10.9. These data are in agreement with those reported previously in the literature.[16]



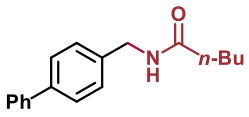
32

***N*-benzhydrylacetamide (32):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (16.7 mg, 0.074 mmol, 37%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.35 – 7.27 (m, 6H), 7.24 – 7.21 (m, 4H), 6.25 (d, *J* = 8.0 Hz, 1H), 6.06 (d, *J* = 8.0 Hz, 1H), 2.07 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 169.2, 141.6, 128.8, 127.6, 127.6, 57.1, 23.6. These data are in agreement with those reported previously in the literature.[14]



33

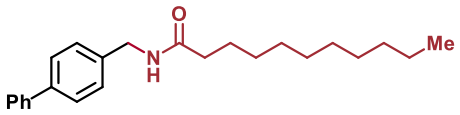
***N*-([1,1'-biphenyl]-4-ylmethyl)butyramide (33):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a yellow solid (29.9 mg, 0.118 mmol, 59%). **Melting point**: 155 – 156 °C. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.60 – 7.54 (m, 4H), 7.45 – 7.42 (m, 2H), 7.36 – 7.33 (m, 3H), 5.81 (s, 1H), 4.49 (d, *J* = 5.7 Hz, 2H), 2.21 (t, *J* = 7.5 Hz, 2H), 1.75 – 1.67 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 173.0, 140.8, 140.6, 137.6, 128.9, 128.4, 127.6, 127.5, 127.2, 43.4, 38.9, 19.3, 14.0. **IR (ATR)**: 3288, 2923, 1631, 1546, 1280, 1209, 751, 686 cm^{-1}. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{17}H_{20}NO^+$ 254.1539, found 254.1539.



34

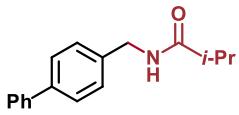
***N*-([1,1'-biphenyl]-4-ylmethyl)pentanamide (34):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a yellow solid (27.2 mg, 0.102 mmol, 51%). **Melting point**: 164 – 165 °C. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.59 – 7.54 (m, 4H), 7.45 – 7.42 (m, 2H), 7.36 – 7.33 (m, 3H), 5.84 (s, 1H), 4.47 (d, *J* = 5.7 Hz, 2H), 2.27 – 2.21 (m, 2H), 1.69 – 1.63 (m, 2H), 1.40 – 1.33 (m, 2H), 0.92 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 173.2, 140.8, 140.6, 137.6, 128.9, 128.4, 127.6, 127.5, 127.2, 43.4, 36.7, 28.0, 22.6, 14.0. **IR (ATR)**: 3669, 2989, 1631, 1380, 1231, 1066, 750, 687 cm^{-1}. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd.

for $C_{18}H_{22}NO^+$ 268.1696, found 268.1698.



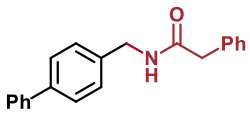
35

***N*-([1,1'-biphenyl]-4-ylmethyl)undecanamide (35):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a yellow solid (31.7 mg, 0.090 mmol, 45%). **Melting point**: 139 – 140 °C. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.59 – 7.55 (m, 4H), 7.46 – 7.42 (m, 2H), 7.36 – 7.33 (m, 3H), 5.79 (s, 1H), 4.48 (d, *J* = 5.7 Hz, 2H), 2.25 – 2.20 (m, 2H), 1.70 – 1.64 (m, 2H), 1.35 – 1.20 (m, 14H), 0.87 (t, *J* = 6.6 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 173.2, 140.8, 140.6, 137.6, 128.9, 128.4, 127.6, 127.5, 127.2, 65.2, 43.4, 37.0, 32.0, 29.6, 29.49, 29.46, 29.4, 25.9, 22.8, 14.3. **IR (ATR)**: 3246, 2989, 1631, 1550, 1373, 1280, 996, 752, 687 cm^{-1}. **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd. for $C_{24}H_{33}NONa^+$ 374.2454, found 374.2455.



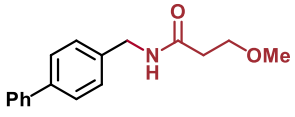
36

***N*-([1,1'-biphenyl]-4-ylmethyl)isobutyramide (36):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a yellow solid (26.8 mg, 0.106 mmol, 53%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.58 – 7.55 (m, 4H), 7.46 – 7.43 (m, 2H), 7.37 – 7.33 (m, 3H), 5.80 (s, 1H), 4.48 (d, *J* = 5.7 Hz, 2H), 2.45 – 2.36 (m, 1H), 1.20 (d, *J* = 6.9 Hz, 6H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 177.0, 140.8, 140.6, 137.7, 128.9, 128.4, 127.6, 127.5, 127.2, 43.3, 35.9, 19.8. These data are in agreement with those reported previously in the literature.[18]



37

***N*-([1,1'-biphenyl]-4-ylmethyl)-2-phenylacetamide (37):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (37.3 mg, 0.124 mmol, 62%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.57 – 7.51 (m, 4H), 7.45 – 7.41 (m, 2H), 7.37 (d, *J* = 1.6 Hz, 3H), 7.31 – 7.28 (m, 3H), 7.25 (d, *J* = 5.8 Hz, 2H), 5.73 (s, 1H), 4.46 (d, *J* = 5.9 Hz, 2H), 3.66 (s, 2H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 171.1, 140.8, 140.6, 137.3, 134.9, 129.6, 129.3, 128.9, 128.1, 127.6, 127.54, 127.50, 127.2, 44.0, 43.4. These data are in agreement with those reported previously in the literature.[18]



38

***N*-([1,1'-biphenyl]-4-ylmethyl)-3-methoxypropanamide (38):** Following the general procedure A, the title product was obtained after purification by column chromatography (PE/EA = 5:1 – 2:1) as a white solid (27.4 mg, 0.102 mmol, 51%). **Melting point:** 121 – 122 °C. **^{1}H NMR** (500 MHz, Chloroform-*d*)

δ 7.59 – 7.55 (m, 4H), 7.46 – 7.42 (m, 2H), 7.37 – 7.33 (m, 3H), 6.58 (s, 1H), 4.50 (d, *J* = 5.8 Hz, 2H), 3.68 (t, *J* = 5.8 Hz, 2H), 3.37 (s, 3H), 2.53 (t, *J* = 5.7 Hz, 2H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 171.6, 140.9, 140.5, 137.6, 128.9, 128.1, 127.52, 127.45, 127.2, 68.8, 59.0, 43.2, 37.2. **IR (ATR)**: 3288, 2920, 1633, 1539, 1495, 1120, 858, 751, 686 cm^{-1}. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{17}H_{20}NO_2^+$ 270.1489, found 270.1490.

4. Mechanism Exploration

4.1 Stern-Volmer emission quenching experiment

The specified amount of the quencher was added to 3 mL of a 1 mM solution of **PC1** in a degassed mixture of MeCN. Luminescence intensities were recorded using an Edinburgh instruments FS5 spectrofluorometer excited at 420 nm. All luminescence measurements were recorded using a quartz cuvette (fluorescence quartz cuvette, 10*10 mm, 3.5 mL). Quenching was analyzed by plotting I_0/I according to the Stern-Volmer relationship: $I_0/I = k_q\tau_0[Q]+1$ where I_0 represents the integral of the luminescence over the range of 400 to 650 nm in the absence of a quencher, I is the integral of luminescence over the range of 400 to 650 nm in the presence of a quencher, k_q represents the quenching rate constant, [Q] is the concentration of a given quencher.

Entry	Quencher Concentration	Concentration of **PC1**
1	0 M	1 mM
2	2.0×10^{-3} M	1 mM
3	4.0×10^{-3} M	1 mM
4	6.0×10^{-3} M	1 mM
5	8.0×10^{-3} M	1 mM
6	10.0×10^{-3} M	1 mM

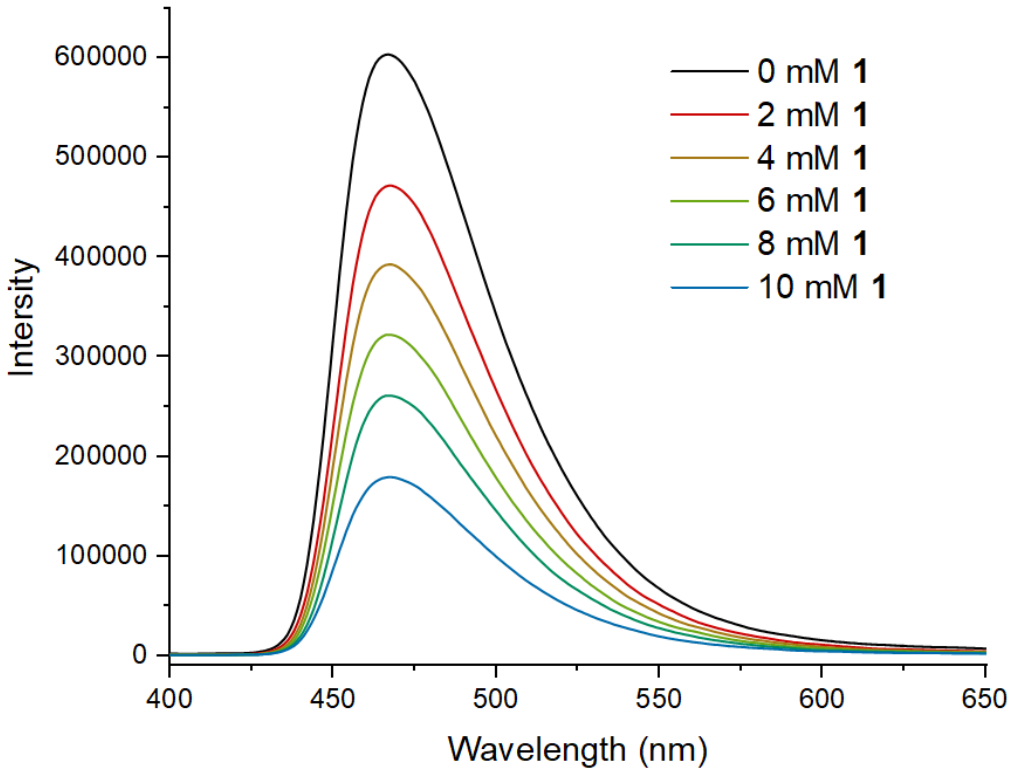


Figure S2 Fluorescence emission spectrum of **PC1** (1 mM) at different concentrations of **1**.

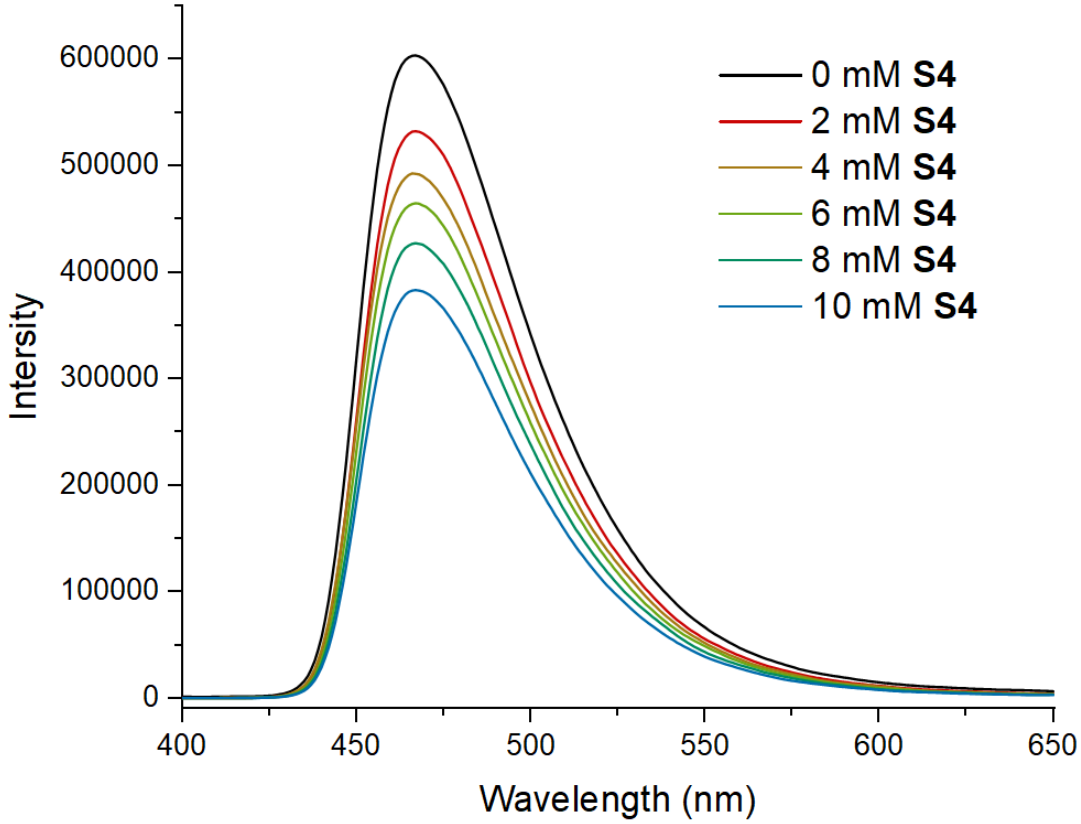
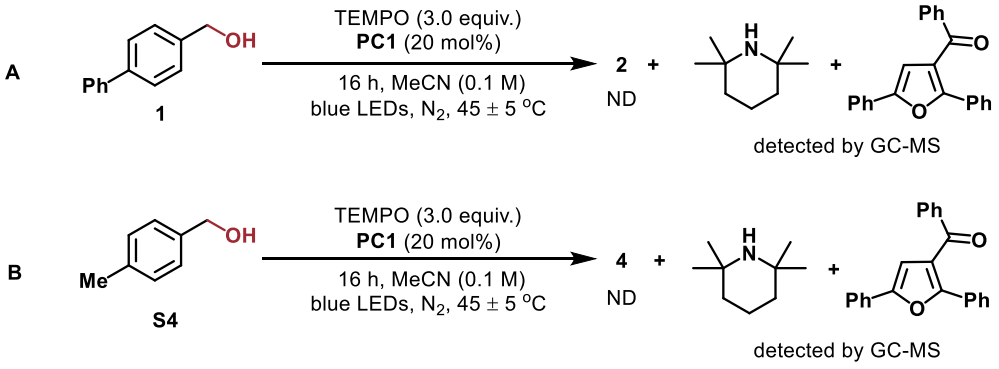


Figure S3 Fluorescence emission spectrum of **PC1** (1 mM) at different concentrations of **S4**.

4.2 Radical trapping experiments



In a nitrogen atmosphere, to a dry glass tube equipped with a stirring bar, **1** (36.8 mg, 0.20 mmol, 1.0 equiv.) or **S4** (24.4 mg, 0.20 mmol, 1.0 equiv.), TEMPO (83.8 mg, 0.60 mmol, 3.0 equiv.), **PC1** (15.8 mg, 0.04 mmol, 20 mol%) and MeCN (2.0 mL) were added. Then the mixture was stirred for overnight under a 100 W blue LED lamp, where the distance from the light source to the irradiation glass tubes was 2 cm. And a fan was used to keep the reaction temperature at 45 ± 5 °C (the heat source is from irradiation of LED lamp). Upon completion, as monitored by TLC and GC-MS, product **4** was not observed.

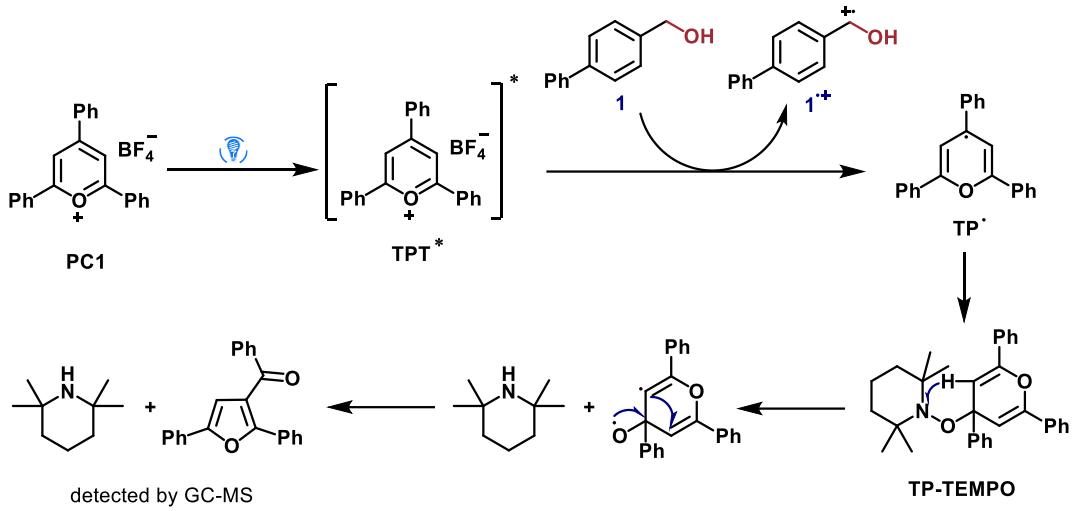


Figure S4 The possible generation path of the trapped products.

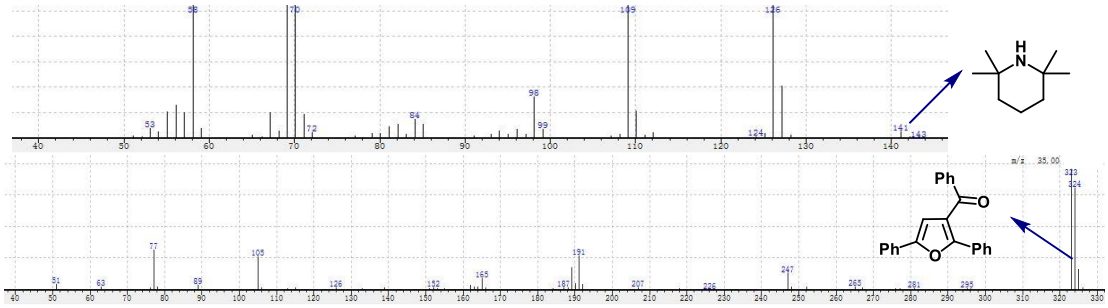


Figure S5 The **TP** radical trapped product was detected by GC-MS in reaction **A**.

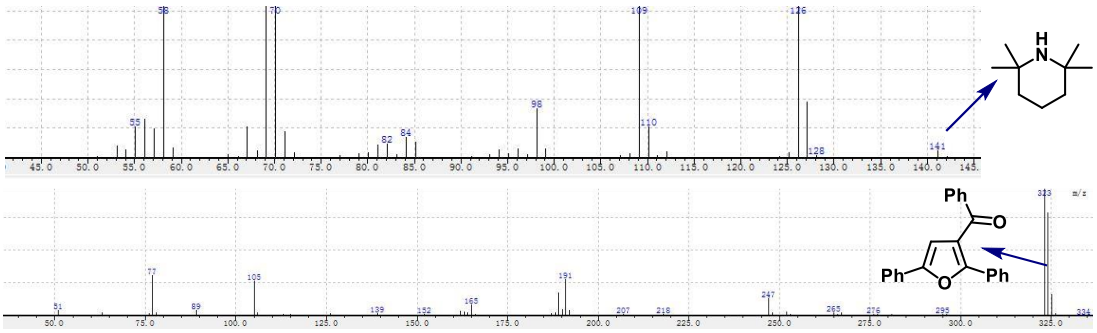


Figure S6 The **TP** radical trapped product was detected by GC-MS in reaction **B**.

4.3 Computational results

To gain more insight into the reaction mechanism, we carried out density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations. The geometries were optimized in MeCN solvent with the implicit solvent model SMD[19] at M06-2X[20]/def-TZVP[21] level. Harmonic vibrational frequency analyses were performed at the same level to verify the nature of stationary points (no imaginary frequency for minima and only one imaginary frequency for

transition states). The energies were further improved by M06-2X/def2-TZVP single-point calculations with solvent effects of MeCN accounted by the SMD solvent model. Harmonic vibration frequencies at M06-2X/def-TZVP level were used to correct the singlet-point energies to free energies at 298.15 K, which are used in the main text. A factor of 1.89 kcal/mol was employed for the standard state change from 1 atm to 1 M by adding it to the above free energies. The vertical excitation energies of the photocatalyst were calculated at TD[22]-B3LYP/def2-TZVP level with solvent effects of MeCN accounted by the SMD solvent model. The B3LYP method gave a vertical absorption energy that is more consistent with the experimental results of UV-Vis for **PC1**.[1] Generally, M06-2X method has good accuracy in calculating the structures and energies for the organic reaction system. Therefore, the choice of calculation method is reasonable here. All DFT and TD-DFT calculations were carried out by using Gaussian 16 program.[23]

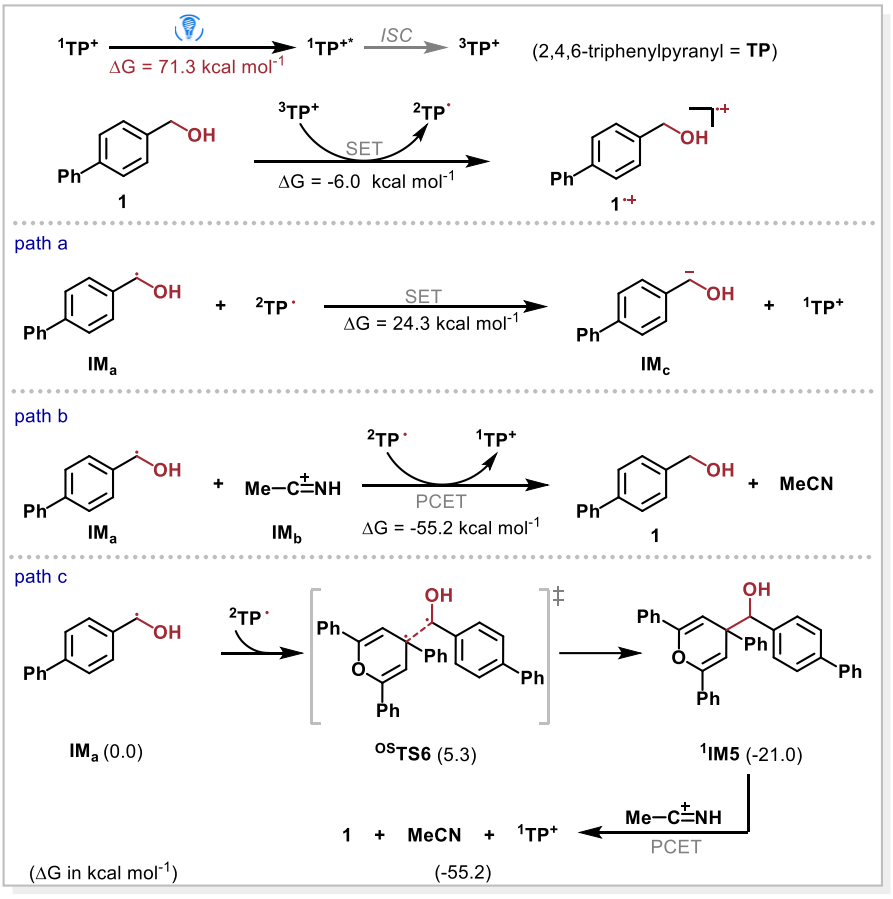


Figure S7 Three pathways for regenerating **PC1** from ^{2}**TP**$^\bullet$ were considered. In path a, **IM$_a$** quenches ^{2}**TP**$^\bullet$ directly. Because the process is endergonic by 24.3 kcal mol^{-1}, we excluded the pathway. In path b, **IM$_a$**, **IM$_b$**, and ^{2}**TP**$^\bullet$ undergo direct proton-coupled electron transfer (PCET). In path c, **IM$_a$** and ^{2}**TP**$^\bullet$ first undergo radical-crossing to give ^{1}**IM5**, which then undergoes PCET

with **IM$_b$**. Both paths b and c are thermodynamically feasible, being exergonic by 55.2 kcal mol^{-1}. However, we were not able to characterize the kinetic barriers of the PCET processes.

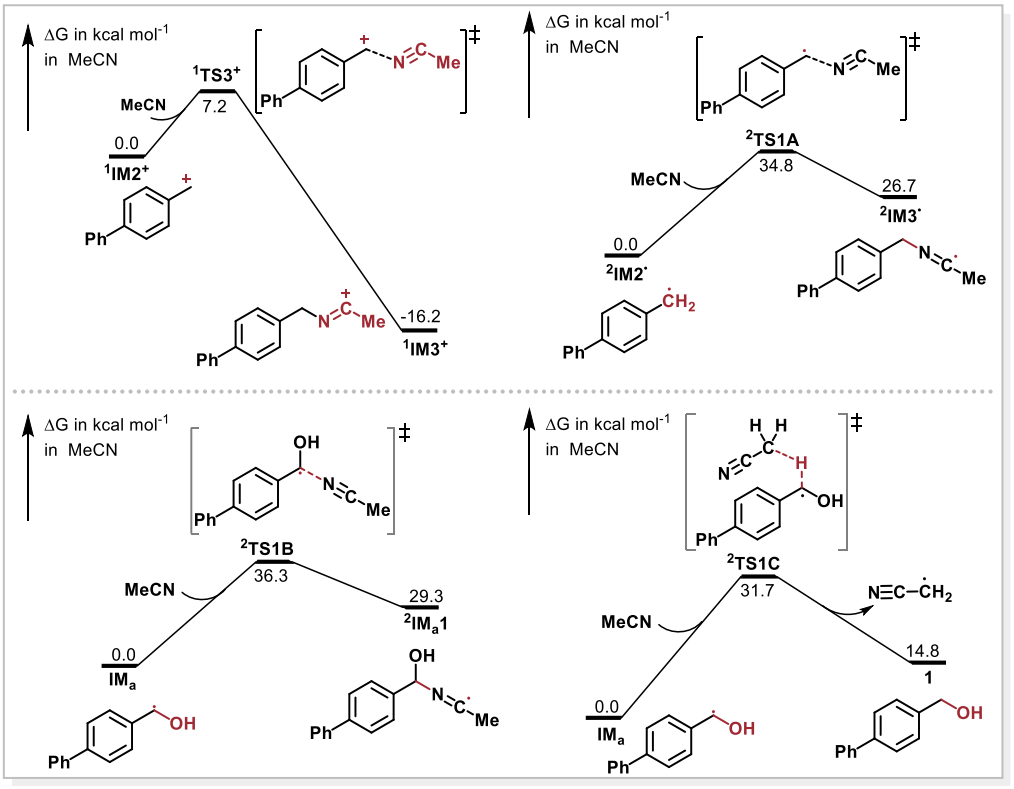


Figure S8 Comparing the kinetic barriers for MeCN attacking various possible intermediates. It can be observed that the attack of MeCN to **^{1}IM2$^+$** is most favorable, which is presented in **Figure 1** in the main text.

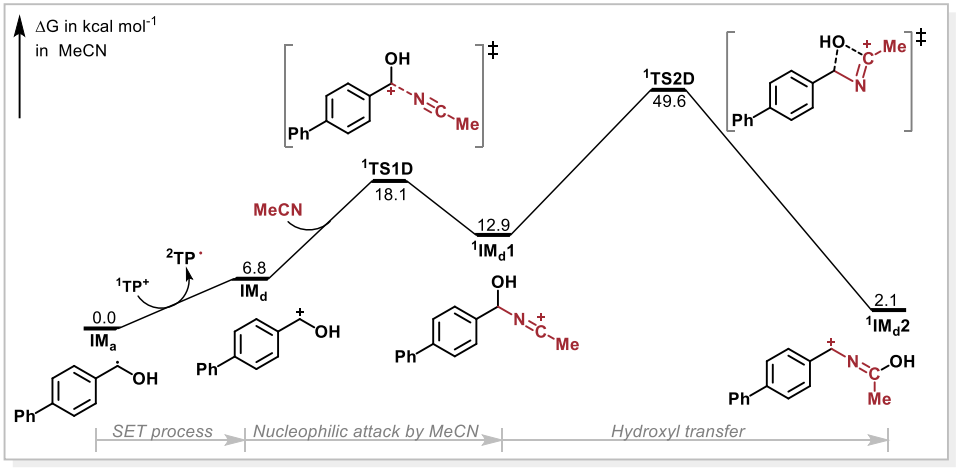


Figure S9 Free energy profile of SET from **IM$_a$** to **^{1}TP$^+$** and its following reaction processes. It can be observed that the pathway is unfavorable.

Cartesian Coordinates in Å, SCF Energies and Free Energies (in a.u.) at 298.15 K for the Optimized Structures [BSI= TZVP, BSII= def2-TZVP)]

1

M06-2X/BSI SCF energy in MeCN:

-577.796154 a.u.

M06-2X/BSII SCF energy in MeCN:

-577.819364 a.u.

M06-2X/BSII free energy in MeCN:

-577.641517 a.u.

C	3.681937	-1.251256	0.375269
C	2.295833	-1.168917	0.400581
C	1.642248	0.002219	0.006304
C	2.415365	1.089288	-0.411552
C	3.801583	1.007200	-0.434857
C	4.440623	-0.163491	-0.042166
H	4.170672	-2.165352	0.690303
H	1.715121	-2.016369	0.745358
H	1.927770	2.000385	-0.737997
H	4.383415	1.858083	-0.768178
H	5.521649	-0.227643	-0.061166
C	0.160891	0.088657	0.028511
C	-0.483620	1.281409	0.375450
C	-0.627913	-1.014425	-0.297389
C	-1.866247	1.360554	0.393883
H	0.103926	2.149284	0.650938
C	-2.016269	-0.933942	-0.279528
H	-0.155027	-1.945672	-0.586994
C	-2.649777	0.253913	0.065823
H	-2.347053	2.292294	0.673784
H	-2.611394	-1.798442	-0.542680
C	-4.149382	0.382031	0.094491
H	-4.460769	0.700630	1.095464
H	-4.453830	1.164441	-0.609474
O	-4.745509	-0.858521	-0.245819
H	-5.702048	-0.742920	-0.231721

^{1}TP$^+$

M06-2X/BSI SCF energy in MeCN:

-961.672109 a.u.

M06-2X/BSII SCF energy in MeCN:

-961.715407 a.u.

M06-2X/BSII free energy in MeCN:

-961.428581 a.u.

C	0.523116	-1.178620	-0.011009
C	0.540767	1.170456	-0.040916
C	-0.827326	1.211418	-0.005578
C	-1.555861	0.014685	0.014845
C	-0.846761	-1.193356	0.020548
H	-1.323486	2.169896	-0.000738
H	-1.362542	-2.138563	0.089767
C	-3.025097	0.024380	0.050090
C	-3.712009	1.073632	0.670057
C	-3.749902	-1.016966	-0.539651
C	-5.097430	1.073814	0.706316
H	-3.165758	1.874648	1.151893
C	-5.135523	-1.002160	-0.515343
H	-3.232867	-1.823974	-1.043636
C	-5.811133	0.039685	0.110593
H	-5.620943	1.881097	1.202442
H	-5.689008	-1.803503	-0.988016
H	-6.893880	0.045613	0.134272
C	1.411386	-2.339552	0.005220
C	2.771434	-2.177252	0.288829
C	0.904549	-3.615640	-0.260418
C	3.608495	-3.280779	0.312680
H	3.172058	-1.193690	0.495927
C	1.749723	-4.712811	-0.235570
H	-0.140247	-3.756123	-0.504181
C	3.100390	-4.548776	0.052237
H	4.659419	-3.151271	0.537408
H	1.353974	-5.697793	-0.447243
H	3.757648	-5.409268	0.070557
C	1.445777	2.317747	-0.073785
C	0.982673	3.561313	-0.513331
C	2.774023	2.173040	0.338633
C	1.842352	4.647556	-0.535150
H	-0.037442	3.677874	-0.856702
C	3.624722	3.266281	0.317001

H	3.135288	1.214301	0.687710
C	3.161517	4.503050	-0.119091
H	1.483747	5.607414	-0.883981
H	4.650323	3.154192	0.644590
H	3.829839	5.355011	-0.136415
O	1.168073	-0.009093	-0.047111

^{3}TP^{+}

M06-2X/BSI SCF energy in MeCN:

-961.574656 a.u.

M06-2X/BSII SCF energy in MeCN:

-961.618595 a.u.

M06-2X/BSII free energy in MeCN:

-961.338236 a.u.

C	-0.581760	1.184627	0.008862
C	-0.582034	-1.184611	-0.009909
C	0.810862	-1.185065	-0.007436
C	1.561785	-0.000211	-0.000242
C	0.811091	1.184750	0.007265
H	1.312690	-2.142124	-0.033744
H	1.313128	2.141661	0.034785
C	3.030321	-0.000317	-0.000089
C	3.745701	-1.052552	0.584930
C	3.745831	1.051907	-0.584979
C	5.132870	-1.051216	0.582015
H	3.218019	-1.866737	1.067221
C	5.132996	1.050591	-0.581754
H	3.218216	1.866071	-1.067386
C	5.833450	-0.000309	0.000213
H	5.668502	-1.870282	1.046047
H	5.668728	1.869654	-1.045678
H	6.916354	-0.000304	0.000334
C	-1.420388	2.336000	0.045983
C	-2.828278	2.176961	0.082985
C	-0.882075	3.648601	0.038054
C	-3.651136	3.281360	0.112578
H	-3.255708	1.184455	0.092334
C	-1.718814	4.739844	0.067486
H	0.186847	3.805558	0.008762
C	-3.105214	4.566129	0.103914
H	-4.725034	3.150406	0.142161
H	-1.299365	5.737367	0.060907
H	-3.756844	5.430444	0.126004
C	-1.420812	-2.335735	-0.046330
C	-0.882739	-3.648532	-0.037444
C	-2.828752	-2.176465	-0.083637
C	-1.719647	-4.739598	-0.066075
H	0.186166	-3.805549	-0.008150
C	-3.651756	-3.280719	-0.112409
H	-3.255990	-1.183885	-0.093821
C	-3.106047	-4.565619	-0.102674
H	-1.300420	-5.737207	-0.058772
H	-4.725634	-3.149660	-0.142201
H	-3.757859	-5.429812	-0.124107
O	-1.270566	0.000127	-0.001570

^{2}TP$^{\bullet}$

M06-2X/BSI SCF energy in MeCN:

-961.811787 a.u.

M06-2X/BSII SCF energy in MeCN:

-961.854167 a.u.

M06-2X/BSII free energy in MeCN:

-961.572155 a.u.

C	-0.529459	1.190126	-0.034854
C	-0.545568	-1.183817	-0.053221
C	0.811613	-1.208413	-0.019850
C	1.573358	-0.012552	-0.011184
C	0.828882	1.193134	-0.012328
H	1.301067	-2.171115	-0.010429
H	1.332992	2.146293	0.047442
C	3.034339	-0.020762	0.025079
C	3.747415	-1.147148	0.470948
C	3.777725	1.099506	-0.385744
C	5.133463	-1.150520	0.503022
H	3.214811	-2.023073	0.818827
C	5.163517	1.092423	-0.348007
H	3.269450	1.979009	-0.760449
C	5.853220	-0.031749	0.095374
H	5.655356	-2.031163	0.858036
H	5.709402	1.968742	-0.676662
H	6.935720	-0.035914	0.122620
C	-1.409676	2.358956	-0.002870

C	-2.787521	2.196948	0.189686
C	-0.903280	3.656482	-0.168020
C	-3.629149	3.300811	0.230066
H	-3.199590	1.204450	0.312010
C	-1.748640	4.752206	-0.123155
H	0.153181	3.815491	-0.342540
C	-3.116697	4.582315	0.076308
H	-4.691555	3.155177	0.383209
H	-1.339043	5.746369	-0.253634
H	-3.774262	5.442145	0.107155
C	-1.441844	-2.341102	-0.064884
C	-0.959805	-3.630272	-0.331886
C	-2.807996	-2.175121	0.194075
C	-1.817951	-4.717240	-0.322823
H	0.086418	-3.787262	-0.561104
C	-3.662707	-3.269554	0.197738
H	-3.199461	-1.187977	0.400448
C	-3.174243	-4.544399	-0.057837
H	-1.428047	-5.705525	-0.533599
H	-4.715924	-3.122549	0.403817
H	-3.842234	-5.396735	-0.055668
O	-1.225280	0.007761	-0.066660

1$^{\bullet+}$

M06-2X/BSI SCF energy in MeCN:

-577.569791 a.u.

M06-2X/BSII SCF energy in MeCN:

-577.594138 a.u.

M06-2X/BSII free energy in MeCN:

-577.417163 a.u.

C	3.639174	-1.316486	0.215364
C	2.267123	-1.240694	0.218569
C	1.610134	0.001726	0.002580
C	2.410306	1.154711	-0.226701
C	3.781004	1.062164	-0.246971
C	4.402647	-0.169727	-0.021640
H	4.129489	-2.262983	0.400723
H	1.691091	-2.130764	0.428601
H	1.943530	2.108760	-0.426841
H	4.379952	1.941793	-0.442213
H	5.483386	-0.236140	-0.031153
C	0.178971	0.090216	0.016207
C	-0.481889	1.342246	0.208968
C	-0.632165	-1.070821	-0.166167
C	-1.842615	1.415461	0.226863
H	0.096961	2.237761	0.384279
C	-1.997567	-0.985396	-0.165225
H	-0.167632	-2.029754	-0.346990
C	-2.627156	0.255482	0.035216
H	-2.338026	2.364308	0.395606
H	-2.603796	-1.865957	-0.324890
C	-4.108268	0.389443	0.052700
H	-4.393155	0.845692	1.010786
H	-4.388791	1.104589	-0.732913
O	-4.719466	-0.863700	-0.134875
H	-5.675460	-0.737654	-0.134577

^{2}TS1$^{\bullet+}$

M06-2X/BSI SCF energy in MeCN:

-1155.363239 a.u.

M06-2X/BSII SCF energy in MeCN:

-1155.409373 a.u.

M06-2X/BSII free energy in MeCN:

-1155.033097 a.u.

C	-3.986085	1.643467	-0.714965
C	-2.633763	1.618055	-1.029964
C	-1.665390	1.810443	-0.039414
C	-2.091263	2.010718	1.277816
C	-3.444009	2.036303	1.591864
C	-4.397175	1.855945	0.596333
H	-4.720890	1.500172	-1.498181
H	-2.329133	1.471812	-2.059611
H	-1.359099	2.131460	2.067529
H	-3.752983	2.189408	2.618879
H	-5.452222	1.875048	0.840758
C	-0.218507	1.782397	-0.367876
C	0.696063	2.549086	0.356526
C	0.270977	0.949687	-1.380086
C	2.057708	2.463080	0.099572
H	0.345777	3.218162	1.133069
C	1.628748	0.876188	-1.648426
H	-0.414804	0.327605	-1.943727

C	2.536777	1.626509	-0.903008
H	2.754443	3.053995	0.683634
H	1.986574	0.217271	-2.431316
C	4.008358	1.567861	-1.194782
H	4.247912	2.088917	-2.123795
H	4.584742	2.007322	-0.379893
O	4.394721	0.182091	-1.372457
H	5.322938	0.136136	-1.659467
C	-3.814098	-1.697346	0.755072
C	-2.461041	-1.622961	1.045887
C	-1.503904	-1.871140	0.052017
C	-1.943795	-2.175100	-1.243891
C	-3.298428	-2.235630	-1.533484
C	-4.237609	-2.001489	-0.534893
H	-4.541029	-1.515746	1.537060
H	-2.146924	-1.400621	2.058272
H	-1.223514	-2.337613	-2.036070
H	-3.621798	-2.459593	-2.542439
H	-5.295634	-2.051251	-0.761381
C	-0.067239	-1.781508	0.347447
C	0.869703	-2.546074	-0.378052
C	0.405794	-0.885934	1.331981
C	2.214860	-2.387371	-0.168280
H	0.526287	-3.268659	-1.106527
C	1.748677	-0.710028	1.540674
H	-0.300942	-0.282557	1.887696
C	2.684410	-1.466428	0.799897
H	2.933850	-2.967372	-0.735541
H	2.102223	0.006224	2.270532
C	4.094208	-1.232270	0.900019
H	4.755866	-2.070150	0.656827
H	4.206019	-0.587224	-0.200741
O	4.504910	-0.423420	1.924485
H	5.471433	-0.410867	1.960291

IM_a

M06-2X/BSI SCF energy in MeCN:

-577.157557 a.u.

M06-2X/BSII SCF energy in MeCN:

-577.182034 a.u.

M06-2X/BSII free energy in MeCN:

-577.015102 a.u.

C	3.643661	-1.255535	0.340695
C	2.257797	-1.179069	0.364490
C	1.596077	0.002062	0.006120
C	2.372249	1.104289	-0.373040
C	3.758223	1.027653	-0.393006
C	4.401718	-0.152738	-0.037490
H	4.133909	-2.178001	0.628125
H	1.683283	-2.040337	0.683978
H	1.886456	2.024381	-0.675473
H	4.337583	1.891390	-0.696565
H	5.482968	-0.212548	-0.054643
C	0.120579	0.082601	0.025583
C	-0.538221	1.285979	0.339083
C	-0.672096	-1.038018	-0.270900
C	-1.911131	1.368623	0.358599
H	0.044604	2.163577	0.592990
C	-2.049185	-0.974309	-0.260627
H	-0.193355	-1.973369	-0.536997
C	-2.714286	0.237799	0.057639
H	-2.395259	2.304352	0.615058
H	-2.633637	-1.851828	-0.506114
C	-4.109253	0.340163	0.080725
H	-4.622038	1.262582	0.321491
O	-4.858121	-0.745524	-0.206093
H	-5.796345	-0.523007	-0.150338

$^1IM1^+$

M06-2X/BSI SCF energy in MeCN:

-578.202670 a.u.

M06-2X/BSII SCF energy in MeCN:

-578.225155 a.u.

M06-2X/BSII free energy in MeCN:

-578.033077 a.u.

C	3.701365	-1.233276	0.430674
C	2.317565	-1.185713	0.327637
C	1.671016	0.002882	-0.021900
C	2.443355	1.141124	-0.268026
C	3.827229	1.091456	-0.167290
C	4.460909	-0.095472	0.182914
H	4.187086	-2.159959	0.711149

H	1.733416	-2.073351	0.539810
H	1.959750	2.066386	-0.558157
H	4.412087	1.980435	-0.369612
H	5.540354	-0.133414	0.262584
C	0.192457	0.055796	-0.127246
C	-0.508308	1.198428	0.268196
C	-0.525869	-1.035971	-0.627606
C	-1.889915	1.248587	0.171018
H	0.029564	2.048555	0.669216
C	-1.905737	-0.988020	-0.726545
H	0.002673	-1.920215	-0.961525
C	-2.596228	0.154999	-0.325406
H	-2.425464	2.138461	0.482485
H	-2.453484	-1.834277	-1.125594
C	-4.077391	0.199760	-0.397322
H	-4.485458	1.206475	-0.395731
H	-4.502937	-0.416126	-1.183467
O	-4.610021	-0.468042	0.872446
H	-5.587857	-0.396822	0.955646
H	-4.192255	-0.089296	1.679039

^{1}TS2$^+$

M06-2X/BSI SCF energy in MeCN:

-578.184465 a.u.

M06-2X/BSII SCF energy in MeCN:

-578.206552 a.u.

M06-2X/BSII free energy in MeCN:

-578.020622 a.u.

C	3.676097	-1.284275	0.408401
C	2.299795	-1.220148	0.253106
C	1.674874	0.001703	-0.021566
C	2.459967	1.153771	-0.145357
C	3.837496	1.081874	-0.005255
C	4.448309	-0.135352	0.275882
H	4.147103	-2.232365	0.635930
H	1.706078	-2.117798	0.373663
H	1.995916	2.103404	-0.381129
H	4.435831	1.977200	-0.118410
H	5.523812	-0.188509	0.391595
C	0.212197	0.074952	-0.178447
C	-0.484745	1.232069	0.224065
C	-0.496489	-1.009639	-0.734428
C	-1.845451	1.306264	0.080372
H	0.055631	2.055147	0.671861
C	-1.857064	-0.944329	-0.884083
H	0.041150	-1.887017	-1.068168
C	-2.561575	0.219158	-0.482077
H	-2.390429	2.187971	0.396705
H	-2.408582	-1.768467	-1.321105
C	-3.934813	0.297572	-0.644361
H	-4.465048	1.215062	-0.424557
H	-4.474167	-0.483771	-1.163838
O	-4.932022	-0.504664	1.221900
H	-4.598027	-0.035158	1.998753
H	-4.684684	-1.430097	1.355981

^{1}IM2$^+$

M06-2X/BSI SCF energy in MeCN:

-501.746984 a.u.

M06-2X/BSII SCF energy in MeCN:

-501.767522 a.u.

M06-2X/BSII free energy in MeCN:

-501.601860 a.u.

C	-3.224955	1.155058	0.343640
C	-1.840285	1.162367	0.332931
C	-1.129177	0.000072	0.000227
C	-1.839890	-1.162356	-0.332896
C	-3.224558	-1.155336	-0.344283
C	-3.919415	-0.000212	-0.000481
H	-3.764719	2.051366	0.621616
H	-1.310470	2.061817	0.619806
H	-1.309744	-2.061683	-0.619545
H	-3.764008	-2.051749	-0.622527
H	-5.002483	-0.000319	-0.000740
C	0.334234	0.000173	0.000512
C	1.044543	-1.184645	0.319808
C	1.044546	1.185032	-0.318577
C	2.406204	-1.190555	0.325183
H	0.500315	-2.078249	0.592289
C	2.406214	1.190756	-0.324530
H	0.500344	2.078742	-0.590752
C	3.135753	0.000004	0.000030

H	2.960569	-2.085173	0.583084
H	2.960530	2.085398	-0.582448
C	4.494599	-0.000262	-0.001135
H	5.051461	-0.896779	0.249420
H	5.051327	0.896047	-0.252762

H_2O

M06-2X/BSI SCF energy in MeCN:

-76.432148 a.u.

M06-2X/BSII SCF energy in MeCN:

-76.434481 a.u.

M06-2X/BSII free energy in MeCN:

-76.428356 a.u.

O	0.000000	0.117778	0.000000
H	0.762452	-0.471111	0.000000
H	-0.762452	-0.471114	0.000000

MeCN

M06-2X/BSI SCF energy in MeCN:

-132.751984 a.u.

M06-2X/BSII SCF energy in MeCN:

-132.757537 a.u.

M06-2X/BSII free energy in MeCN:

-132.731833 a.u.

C	0.000000	0.000000	0.278776
N	0.000000	0.000000	1.426234
C	0.000000	0.000000	-1.174149
H	0.000000	1.027019	-1.537134
H	0.889425	-0.513510	-1.537134
H	-0.889425	-0.513510	-1.537134

^{1}TS3$^+$

M06-2X/BSI SCF energy in MeCN:

-634.501110 a.u.

M06-2X/BSII SCF energy in MeCN:

-634.526649 a.u.

M06-2X/BSII free energy in MeCN:

-634.322273 a.u.

C	4.073507	1.597203	0.523506
C	2.757596	1.182507	0.663078
C	2.303022	0.035188	0.003678
C	3.197279	-0.690031	-0.791128
C	4.516253	-0.280047	-0.916278
C	4.956750	0.865641	-0.262902
H	4.409615	2.494776	1.027454
H	2.073348	1.767624	1.265161
H	2.868052	-1.592729	-1.290762
H	5.202600	-0.858048	-1.522425
H	5.985725	1.187383	-0.366026
C	0.902509	-0.404165	0.145627
C	0.246003	-1.034856	-0.928413
C	0.215371	-0.197286	1.357339
C	-1.057720	-1.443804	-0.800690
H	0.764595	-1.175072	-1.867374
C	-1.086966	-0.606429	1.494934
H	0.725652	0.266293	2.191023
C	-1.747071	-1.242828	0.417927
H	-1.574132	-1.918231	-1.626817
H	-1.620544	-0.459172	2.426611
C	-3.061516	-1.679133	0.560439
H	-3.534790	-2.258912	-0.220711
H	-3.550521	-1.641373	1.524521
C	-4.841944	1.014367	-0.388086
N	-4.377817	0.023307	-0.048439
C	-5.433823	2.266436	-0.817436
H	-4.730225	2.792927	-1.461401
H	-6.351312	2.059566	-1.367264
H	-5.658839	2.875243	0.057501

^{1}IM3$^+$

M06-2X/BSI SCF energy in MeCN:

-634.541493 a.u.

M06-2X/BSII SCF energy in MeCN:

-634.568367 a.u.

M06-2X/BSII free energy in MeCN:

-634.359514 a.u.

C	4.214496	1.519216	0.174720

C	2.864322	1.255477	0.363229
C	2.320953	0.022180	-0.006407
C	3.163672	-0.940579	-0.568443
C	4.514078	-0.676306	-0.755295
C	5.044312	0.554389	-0.385116
H	4.617625	2.483407	0.459720
H	2.222327	2.020029	0.784617
H	2.764623	-1.909710	-0.843838
H	5.154983	-1.436612	-1.184928
H	6.097492	0.760141	-0.531754
C	0.877929	-0.259097	0.194959
C	0.161709	-1.017350	-0.735808
C	0.206845	0.223670	1.321257
C	-1.184901	-1.285832	-0.545356
H	0.658924	-1.389586	-1.623242
C	-1.141224	-0.042317	1.511835
H	0.747287	0.794649	2.066391
C	-1.842464	-0.798753	0.579678
H	-1.729615	-1.873627	-1.275684
H	-1.648127	0.328974	2.395195
C	-3.308790	-1.085043	0.782942
H	-3.595459	-2.060018	0.390975
H	-3.599886	-1.009729	1.829490
C	-4.719384	0.653519	-0.500883
N	-4.110320	-0.117638	0.070736
C	-5.488140	1.629893	-1.225054
H	-4.801319	2.357886	-1.658141
H	-6.045714	1.120153	-2.011190
H	-6.171383	2.119108	-0.530315

^{1}TS4$^+$

M06-2X/BSI SCF energy in MeCN:

-843.719033 a.u.

M06-2X/BSII SCF energy in MeCN:

-843.753012 a.u.

M06-2X/BSII free energy in MeCN:

-843.480366 a.u.

C	4.533174	-0.211155	1.503759
C	3.235583	-0.632004	1.244427
C	2.677506	-0.477030	-0.027413
C	3.451244	0.109130	-1.032629
C	4.749261	0.528384	-0.772523
C	5.294647	0.370543	0.496504
H	4.947348	-0.331291	2.497448
H	2.644307	-1.067026	2.041639
H	3.042136	0.221247	-2.029793
H	5.338063	0.973600	-1.565265
H	6.306764	0.698521	0.699182
C	1.288960	-0.921557	-0.302791
C	0.460366	-0.186256	-1.158290
C	0.777189	-2.078908	0.286563
C	-0.841097	-0.590709	-1.405533
H	0.833117	0.721470	-1.617567
C	-0.530744	-2.482283	0.042827
H	1.407232	-2.679230	0.931621
C	-1.352419	-1.737437	-0.798599
H	-1.476712	-0.000227	-2.057095
H	-0.915036	-3.382107	0.509741
C	-2.792915	-2.125651	-1.015631
H	-3.046227	-2.112813	-2.075453
H	-2.992100	-3.129466	-0.639074
C	-3.812772	-0.405396	0.479362
N	-3.742604	-1.245877	-0.361972
C	-4.808373	0.488774	1.085664
H	-4.909277	0.258155	2.145597
H	-4.485037	1.525241	0.978828
H	-5.755757	0.340718	0.572352
O	-2.389535	0.005816	1.380752
H	-2.045404	0.907075	1.063395
H	-1.681717	-0.650240	1.237762
C	-1.259157	3.329998	-0.019226
N	-1.597570	2.342708	0.451209
C	-0.828526	4.576505	-0.617731
H	0.242151	4.698582	-0.456751
H	-1.040685	4.551885	-1.686084
H	-1.367220	5.401858	-0.153594

IM_b

M06-2X/BSI SCF energy in MeCN:

-133.154937 a.u.

M06-2X/BSII SCF energy in MeCN:

-133.161225 a.u.

M06-2X/BSII free energy in MeCN:

-133.126684 a.u.

C	0.167049	0.000662	0.000298
N	1.301514	-0.000230	-0.000087
C	-1.266602	-0.000140	-0.000056
H	-1.610602	0.114975	1.028698
H	-1.610308	0.833051	-0.614680
H	-1.608762	-0.949398	-0.414772
H	2.316391	-0.000149	-0.000088

^{1}IM4

M06-2X/BSI SCF energy in MeCN:

-710.564645 a.u.

M06-2X/BSII SCF energy in MeCN:

-710.594642 a.u.

M06-2X/BSII free energy in MeCN:

-710.370021 a.u.

C	-5.084178	0.720245	0.761324
C	-3.707758	0.889997	0.687870
C	-2.909046	-0.031944	0.004961
C	-3.527732	-1.129407	-0.601060
C	-4.903931	-1.299859	-0.525892
C	-5.688173	-0.375538	0.155093
H	-5.685322	1.442381	1.300606
H	-3.246164	1.737716	1.180478
H	-2.929027	-1.846280	-1.150638
H	-5.365695	-2.153224	-1.007757
H	-6.761531	-0.508344	0.212868
C	-1.438579	0.150563	-0.076484
C	-0.574484	-0.946683	-0.043416
C	-0.877999	1.425697	-0.185373
C	0.801257	-0.775802	-0.119169
H	-0.981044	-1.945962	0.060985
C	0.497448	1.593010	-0.259880
H	-1.523458	2.295379	-0.225350
C	1.356975	0.496300	-0.229708
H	1.454304	-1.638833	-0.079011
H	0.910448	2.592487	-0.346257
C	2.845370	0.700698	-0.372292
H	3.097183	0.719189	-1.439518
H	3.112240	1.687671	0.018667
C	4.862194	-0.307617	0.187716
N	3.605217	-0.340545	0.305442
C	5.769202	-1.307615	0.828683
H	6.465150	-0.804021	1.503527
H	5.185213	-2.033584	1.387560
H	6.355092	-1.823838	0.064608
O	5.465859	0.663361	-0.544430
H	6.425825	0.543919	-0.537669

^{1}TS5

M06-2X/BSI SCF energy in MeCN:

-1288.374032 a.u.

M06-2X/BSII SCF energy in MeCN:

-1288.425931 a.u.

M06-2X/BSII free energy in MeCN:

-1288.002037 a.u.

C	-3.706110	1.057030	1.902249
C	-2.356123	1.031581	1.576659
C	-1.839545	1.887783	0.600766
C	-2.708799	2.787922	-0.023514
C	-4.057822	2.815593	0.303715
C	-4.563789	1.945723	1.263745
H	-4.090381	0.372727	2.649434
H	-1.704422	0.314266	2.060817
H	-2.325345	3.479696	-0.764177
H	-4.715358	3.521174	-0.189815
H	-5.617764	1.961621	1.513245
C	-0.409712	1.818644	0.210825
C	-0.014400	2.072924	-1.104573
C	0.578174	1.479909	1.142247
C	1.323204	2.001468	-1.473629
H	-0.759712	2.305956	-1.855939
C	1.912455	1.413936	0.771724
H	0.303340	1.289800	2.173134
C	2.301756	1.675485	-0.540980
H	1.606584	2.188945	-2.503421
H	2.663251	1.156633	1.511696
C	3.758495	1.604839	-0.933327
H	3.849951	1.705109	-2.016990
H	4.303142	2.433384	-0.475461
C	5.504387	0.196648	0.011651
N	4.330974	0.336276	-0.515741
C	6.463450	1.312065	0.257086

H	7.386571	0.914050	0.669409
H	6.673386	1.841612	-0.672858
H	6.029021	2.025220	0.960159
O	5.888553	-1.003961	0.360654
H	5.056211	-1.660443	0.137607
C	-4.466989	-0.327055	-1.664933
C	-3.122973	-0.548467	-1.397393
C	-2.723499	-1.583550	-0.546007
C	-3.708558	-2.392889	0.025991
C	-5.054285	-2.170623	-0.240892
C	-5.439397	-1.136545	-1.085966
H	-4.756778	0.488656	-2.316762
H	-2.375131	0.107262	-1.829383
H	-3.420943	-3.211279	0.675663
H	-5.802961	-2.812079	0.208348
H	-6.488302	-0.961339	-1.291737
C	-1.288586	-1.786682	-0.230713
C	-0.885863	-2.197171	1.045983
C	-0.299026	-1.549885	-1.184941
C	0.456220	-2.357195	1.350488
H	-1.631220	-2.367071	1.814591
C	1.047653	-1.713409	-0.877337
H	-0.581146	-1.245028	-2.186443
C	1.442427	-2.115680	0.393006
H	0.746802	-2.662299	2.350969
H	1.799955	-1.532044	-1.635290
C	2.901647	-2.256059	0.769303
H	3.098060	-1.552582	1.596380
H	3.063871	-3.260718	1.176941
O	3.774186	-2.024327	-0.301602
H	3.804245	-0.766896	-0.549740

2

M06-2X/BSI SCF energy in MeCN:

-710.591836 a.u.

M06-2X/BSII SCF energy in MeCN:

-710.621186 a.u.

M06-2X/BSII free energy in MeCN:

-710.397392 a.u.

C	-4.986966	0.577210	0.245022
C	-3.639450	0.912131	0.272774
C	-2.658408	-0.050515	0.018058
C	-3.064683	-1.357916	-0.264400
C	-4.412168	-1.692963	-0.289918
C	-5.379068	-0.726713	-0.036069
H	-5.732310	1.335885	0.451046
H	-3.345576	1.927336	0.512233
H	-2.320871	-2.114840	-0.483599
H	-4.707361	-2.710161	-0.517482
H	-6.430011	-0.987709	-0.057296
C	-1.218556	0.307158	0.045628
C	-0.264543	-0.588841	0.528215
C	-0.778326	1.552872	-0.414317
C	1.084883	-0.254973	0.552811
H	-0.578391	-1.554840	0.906308
C	0.567181	1.882270	-0.390713
H	-1.493800	2.262719	-0.812690
C	1.517258	0.983358	0.094132
H	1.802775	-0.968481	0.939880
H	0.888761	2.850026	-0.761627
C	2.975428	1.399633	0.104212
H	3.266683	1.686745	-0.907635
H	3.095999	2.277154	0.740423
C	4.324608	-0.615686	-0.224615
N	3.890509	0.384243	0.572806
C	5.238574	-1.626224	0.420390
H	6.139051	-1.721725	-0.186321
H	5.512722	-1.360334	1.440151
H	4.733412	-2.593348	0.425557
O	3.992481	-0.700994	-1.401343
H	4.160931	0.385016	1.544892

^{os}TS6

M06-2X/BSI SCF energy in MeCN:

-1538.987371 a.u.

M06-2X/BSII SCF energy in MeCN:

-1539.052777 a.u.

M06-2X/BSII free energy in MeCN:

-1538.578825 a.u.

C	0.938827	-1.163225	0.739428
C	0.487970	1.052920	1.435540
C	1.706983	1.456482	1.005609
C	2.594950	0.561583	0.343739

C	2.156805	-0.791043	0.277094
H	1.962243	2.496673	1.132471
H	2.773579	-1.551385	-0.177482
C	3.928417	0.975027	-0.095525
C	4.422678	2.265746	0.169466
C	4.755216	0.114338	-0.844249
C	5.671414	2.668877	-0.287678
H	3.843744	2.965565	0.756942
C	6.001197	0.519678	-1.291754
H	4.419209	-0.883549	-1.093695
C	6.471768	1.802834	-1.021375
H	6.019705	3.669435	-0.060238
H	6.608639	-0.170273	-1.865447
H	7.445386	2.118030	-1.374912
C	0.336520	-2.496696	0.671476
C	-1.023781	-2.655859	0.962568
C	1.074107	-3.617774	0.268784
C	-1.632188	-3.898403	0.838038
H	-1.610270	-1.799341	1.266890
C	0.461487	-4.854398	0.148035
H	2.131467	-3.530243	0.052878
C	-0.895719	-5.001891	0.426931
H	-2.688573	-3.998303	1.058953
H	1.046750	-5.711106	-0.163021
H	-1.369846	-5.970540	0.328241
C	-0.539189	1.880972	2.076118
C	-0.422140	3.276586	2.132930
C	-1.686818	1.282348	2.607519
C	-1.416220	4.042296	2.718321
H	0.441891	3.772129	1.708809
C	-2.682547	2.057140	3.190870
H	-1.799302	0.207200	2.564905
C	-2.553680	3.437907	3.250192
H	-1.308527	5.119547	2.751960
H	-3.563591	1.574865	3.597142
H	-3.330861	4.041475	3.702277
O	0.098507	-0.252965	1.320860
C	-5.281261	-1.088847	0.475224
C	-4.084087	-0.473722	0.135054
C	-3.364842	-0.874271	-0.998069
C	-3.888260	-1.912704	-1.778044
C	-5.084312	-2.529679	-1.435169
C	-5.787069	-2.122304	-0.306654
H	-5.815678	-0.766965	1.361198
H	-3.688666	0.311526	0.769347
H	-3.363490	-2.230310	-2.671155
H	-5.472097	-3.327637	-2.057148
H	-6.719128	-2.604736	-0.039160
C	-2.074443	-0.238586	-1.339238
C	-1.048269	-0.981357	-1.951185
C	-1.829058	1.114439	-1.057488
C	0.175722	-0.417823	-2.223968
H	-1.204675	-2.031991	-2.167653
C	-0.610723	1.700036	-1.333392
H	-2.613438	1.717749	-0.613407
C	0.437275	0.943259	-1.918391
H	0.963253	-1.018320	-2.666561
H	-0.447606	2.746055	-1.106157
C	1.723654	1.456891	-2.090051
H	2.517029	0.877550	-2.546013
O	1.957038	2.765229	-1.852464
H	2.912643	2.928259	-1.843251

^{1}IM5

M06-2X/BSI SCF energy in MeCN:

-1539.034171 a.u.

M06-2X/BSII SCF energy in MeCN:

-1539.096689 a.u.

M06-2X/BSII free energy in MeCN:

-1538.620691 a.u.

C	-1.249546	1.411902	0.682617
C	-0.892234	-0.834453	1.287965
C	-1.541227	-1.276092	0.213482
C	-2.079539	-0.372979	-0.858891
C	-1.864885	1.057284	-0.443625
H	-1.644411	-2.344482	0.077522
H	-2.217882	1.834814	-1.109503
C	-3.578609	-0.596534	-1.114687
C	-4.334853	-1.475650	-0.342659
C	-4.217721	0.103223	-2.143380
C	-5.691982	-1.657466	-0.593195
H	-3.870731	-2.019712	0.470427
C	-5.571305	-0.076364	-2.393614
H	-3.658600	0.804684	-2.752417
C	-6.314687	-0.961409	-1.619629
H	-6.260847	-2.345868	0.020132

H	-6.046573	0.477430	-3.194214
H	-7.370752	-1.102573	-1.814243
C	-0.997677	2.800025	1.122539
C	0.080138	3.080432	1.965300
C	-1.817962	3.847629	0.696548
C	0.341040	4.386803	2.359188
H	0.717631	2.274811	2.305787
C	-1.552162	5.150754	1.090444
H	-2.676202	3.641462	0.068899
C	-0.471114	5.425806	1.922059
H	1.183194	4.591980	3.008711
H	-2.198282	5.953293	0.756434
H	-0.268091	6.443639	2.231496
C	-0.277304	-1.682398	2.330720
C	0.131986	-2.986737	2.041681
C	-0.092453	-1.183163	3.621848
C	0.692194	-3.781409	3.031296
H	0.027845	-3.376638	1.036390
C	0.470958	-1.981613	4.608948
H	-0.396809	-0.170643	3.853079
C	0.862391	-3.282795	4.318865
H	1.008221	-4.789620	2.793041
H	0.603531	-1.584544	5.607945
H	1.304001	-3.903547	5.088699
O	-0.725870	0.500268	1.563606
C	6.412782	-0.766316	-0.179176
C	5.047038	-0.894695	-0.395575
C	4.408863	-0.150276	-1.391884
C	5.175565	0.726112	-2.165063
C	6.541207	0.854651	-1.947833
C	7.165369	0.108938	-0.954260
H	6.888837	-1.345981	0.602443
H	4.466626	-1.565861	0.226785
H	4.702592	1.298323	-2.954444
H	7.120486	1.533685	-2.561789
H	8.230463	0.209086	-0.785010
C	2.949398	-0.287486	-1.622342
C	2.170693	0.818188	-1.971395
C	2.318447	-1.528856	-1.502815
C	0.805026	0.686523	-2.184430
H	2.632119	1.794241	-2.064588
C	0.953041	-1.657765	-1.712404
H	2.904233	-2.407370	-1.258587
C	0.178466	-0.549601	-2.049133
H	0.219466	1.558293	-2.454595
H	0.482174	-2.628616	-1.623031
C	-1.315101	-0.663243	-2.207738
H	-1.643068	0.084956	-2.936231
O	-1.615656	-1.968778	-2.669640
H	-2.572416	-2.032976	-2.789503

IM_c

M06-2X/BSI SCF energy in MeCN:

-577.259190 a.u.

M06-2X/BSII SCF energy in MeCN:

-577.283237 a.u

M06-2X/BSII free energy in MeCN:

-577.120029 a.u.

C	3.645613	-1.306496	0.215542
C	2.261736	-1.220144	0.222443
C	1.590481	0.002048	-0.001365
C	2.410449	1.130165	-0.222547
C	3.794546	1.041278	-0.214517
C	4.432381	-0.177452	0.000917
H	4.116474	-2.266666	0.395403
H	1.687973	-2.115950	0.426270
H	1.954871	2.091568	-0.425292
H	4.382555	1.934900	-0.392535
H	5.513019	-0.245663	0.002372
C	0.134360	0.094072	-0.002053
C	-0.550835	1.326735	0.195801
C	-0.698143	-1.031041	-0.207197
C	-1.912133	1.430587	0.208166
H	0.024552	2.229767	0.373516
C	-2.069335	-0.966451	-0.214470
H	-0.241157	-1.996299	-0.403205
C	-2.778348	0.280694	0.010871
H	-2.372950	2.396979	0.388751
H	-2.640691	-1.865574	-0.414849
C	-4.136380	0.373279	0.053976
H	-4.665006	1.303410	0.224764
O	-4.968710	-0.741225	-0.124664
H	-4.756315	-1.400322	0.548718

^{2}IM2•

M06-2X/BSI SCF energy in MeCN:

-501.922700 a.u.

M06-2X/BSII SCF energy in MeCN:

-501.942607 a.u.

M06-2X/BSII free energy in MeCN:

-501.779492 a.u.

C	-3.256017	1.148084	0.352445
C	-1.867828	1.148683	0.353068
C	-1.150249	0.000007	0.000007
C	-1.867787	-1.148686	-0.353069
C	-3.255978	-1.148115	-0.352491
C	-3.956859	-0.000025	-0.000036
H	-3.792187	2.045643	0.636335
H	-1.335598	2.044331	0.650523
H	-1.335532	-2.044326	-0.650501
H	-3.792118	-2.045687	-0.636395
H	-5.039942	-0.000039	-0.000052
C	0.328464	0.000025	0.000032
C	1.051948	-1.156099	0.337392
C	1.051938	1.156126	-0.337299
C	2.429204	-1.161639	0.340574
H	0.518619	-2.055608	0.621439
C	2.429210	1.161688	-0.340500
H	0.518633	2.055664	-0.621306
C	3.169916	0.000024	-0.000015
H	2.966627	-2.062383	0.614885
H	2.966621	2.062446	-0.614788
C	4.572852	-0.000064	-0.000100
H	5.125996	-0.891920	0.262373
H	5.125995	0.891812	-0.262565

^{2}TS1A

M06-2X/BSI SCF energy in MeCN:

-634.634361 a.u.

M06-2X/BSII SCF energy in MeCN:

-634.659656 a.u.

M06-2X/BSII free energy in MeCN:

-634.455933 a.u.

C	3.989615	-1.609411	0.258264
C	2.637743	-1.320119	0.127978
C	2.199541	-0.000588	-0.024411
C	3.155691	1.020034	-0.041177
C	4.507215	0.730159	0.090770
C	4.930465	-0.585823	0.240624
H	4.308142	-2.637442	0.382294
H	1.913507	-2.125372	0.164025
H	2.840158	2.047673	-0.177723
H	5.232482	1.534629	0.067941
H	5.984770	-0.811851	0.342658
C	0.757386	0.309003	-0.165282
C	0.214542	1.477155	0.383259
C	-0.100805	-0.556271	-0.854511
C	-1.131903	1.768641	0.250613
H	0.853053	2.155523	0.937062
C	-1.447310	-0.266452	-0.990253
H	0.297586	-1.456683	-1.307508
C	-1.992358	0.907018	-0.446331
H	-1.533349	2.674600	0.691191
H	-2.092088	-0.945362	-1.537981
C	-3.416629	1.177437	-0.530369
H	-3.723128	2.200461	-0.352299
H	-3.950049	0.683561	-1.335681
C	-4.433870	-0.788533	0.856212
N	-4.188634	0.368170	0.944705
C	-4.448876	-2.056136	0.125988
H	-3.630497	-2.683445	0.482133
H	-5.387058	-2.585653	0.286840
H	-4.315774	-1.864513	-0.944127

^{2}IM3$^{\cdot}$

M06-2X/BSI SCF energy in MeCN:

-634.649967 a.u.

M06-2X/BSII SCF energy in MeCN:

-634.675566 a.u.

M06-2X/BSII free energy in MeCN:

-634.468701 a.u.

C	-4.142585	1.536357	0.456665
C	-2.779641	1.272301	0.421864
C	-2.303721	0.031813	-0.012311
C	-3.229491	-0.936451	-0.411447

C	-4.592319	-0.671985	-0.376150
C	-5.054380	0.565454	0.057861
H	-4.493322	2.500876	0.803439
H	-2.078824	2.029800	0.752640
H	-2.879328	-1.897615	-0.769110
H	-5.294628	-1.432196	-0.696129
H	-6.117296	0.771684	0.085163
C	-0.847606	-0.251077	-0.047995
C	-0.355956	-1.517858	0.269423
C	0.067955	0.746929	-0.400217
C	1.008230	-1.780256	0.236885
H	-1.042248	-2.302724	0.564786
C	1.427305	0.481635	-0.432660
H	-0.290496	1.733307	-0.670037
C	1.914400	-0.786449	-0.117022
H	1.371949	-2.768384	0.495523
H	2.122197	1.266279	-0.714796
C	3.395404	-1.056095	-0.157686
H	3.588797	-2.104788	0.061885
H	3.794488	-0.822888	-1.148664
C	4.767687	0.746449	0.647651
N	4.090521	-0.247378	0.872580
C	5.189216	1.537703	-0.533962
H	4.785779	2.548272	-0.454061
H	6.276434	1.616760	-0.558945
H	4.835863	1.082443	-1.465151

^{2}TS1B

M06-2X/BSI SCF energy in MeCN:

-709.867920 a.u.

M06-2X/BSII SCF energy in MeCN:

-709.897130 a.u.

M06-2X/BSII free energy in MeCN:

-709.689101 a.u.

C	4.205087	0.853492	1.060340
C	2.833641	0.639459	1.024212
C	2.260454	-0.159785	0.030130
C	3.100498	-0.738389	-0.926345
C	4.471903	-0.523281	-0.889974
C	5.030197	0.273670	0.103057
H	4.629279	1.481971	1.834087
H	2.199009	1.112255	1.764498
H	2.680368	-1.377990	-1.693521
H	5.107003	-0.986168	-1.635631
H	6.099825	0.441402	0.131012
C	0.795903	-0.387485	-0.007811
C	0.117474	-0.503592	-1.226564
C	0.056634	-0.503585	1.175793
C	-1.251165	-0.705725	-1.260353
H	0.664245	-0.409261	-2.157283
C	-1.312866	-0.704916	1.147569
H	0.565194	-0.444140	2.130820
C	-1.986734	-0.804811	-0.074516
H	-1.765310	-0.772919	-2.213142
H	-1.869687	-0.785744	2.072719
C	-3.441761	-0.852575	-0.140696
H	-3.855908	-1.206533	-1.081679
O	-4.040238	-1.352447	0.984518
H	-4.992519	-1.196457	0.917867
C	-3.372376	1.809079	-0.327983
N	-4.064428	0.847082	-0.212810
C	-2.079374	2.485212	-0.490558
H	-2.107625	3.484320	-0.056601
H	-1.277616	1.908214	-0.020133
H	-1.868435	2.580440	-1.557288

^{1}IM$_a$1

M06-2X/BSI SCF energy in MeCN:

-709.880817 a.u.

M06-2X/BSII SCF energy in MeCN:

-709.910332 a.u.

M06-2X/BSII free energy in MeCN:

-709.700181 a.u.

C	4.483549	-0.384389	1.249821
C	3.106923	-0.507942	1.115325
C	2.454196	-0.018970	-0.019724
C	3.216726	0.596681	-1.016198
C	4.593257	0.720244	-0.880992
C	5.232160	0.230155	0.252397
H	4.971486	-0.762872	2.139865
H	2.531027	-0.972101	1.907199
H	2.731128	0.966060	-1.911732
H	5.168862	1.194255	-1.666806
H	6.305788	0.326643	0.357804

C	0.983020	-0.149288	-0.162888
C	0.232901	0.856749	-0.774614
C	0.315038	-1.284101	0.309695
C	-1.143963	0.734538	-0.906890
H	0.726066	1.750229	-1.138289
C	-1.059178	-1.406421	0.178722
H	0.880322	-2.086468	0.768612
C	-1.798527	-0.396634	-0.432899
H	-1.713107	1.525116	-1.383444
H	-1.563397	-2.295415	0.537503
C	-3.295376	-0.507380	-0.534777
H	-3.678297	0.225626	-1.252554
O	-3.632808	-1.810396	-0.918644
H	-4.593902	-1.896807	-0.868788
C	-4.108266	0.905300	1.228068
N	-3.904542	-0.221595	0.793562
C	-3.874544	2.297226	0.777726
H	-4.633271	2.971753	1.171383
H	-2.901029	2.622947	1.152967
H	-3.864920	2.350759	-0.316138

^{2}TS1C

M06-2X/BSI SCF energy in MeCN:

-709.868388 a.u.

M06-2X/BSII SCF energy in MeCN:

-709.897478 a.u.

M06-2X/BSII free energy in MeCN:

-709.696354 a.u.

C	-4.585837	1.583311	0.145255
C	-3.222098	1.350383	0.025735
C	-2.719092	0.046060	0.011577
C	-3.619219	-1.018020	0.120347
C	-4.982769	-0.784316	0.240218
C	-5.471717	0.517180	0.253145
H	-4.956474	2.601088	0.161928
H	-2.539549	2.189597	-0.038160
H	-3.251150	-2.036843	0.092416
H	-5.665817	-1.621750	0.315806
H	-6.535292	0.699334	0.346434
C	-1.262944	-0.203716	-0.116452
C	-0.655248	-1.265160	0.562770
C	-0.462758	0.612019	-0.921242
C	0.703617	-1.501198	0.440033
H	-1.250756	-1.903012	1.205022
C	0.899164	0.380518	-1.043695
H	-0.913996	1.428611	-1.472449
C	1.496445	-0.685558	-0.370485
H	1.159012	-2.327257	0.975262
H	1.501733	1.017019	-1.679225
C	2.953687	-0.919579	-0.435714
H	3.243166	-1.961776	-0.282787
O	3.546482	-0.321560	-1.536881
H	4.482238	-0.560844	-1.562486
C	5.331453	0.839552	0.861060
N	6.285315	1.064380	0.248194
C	4.140735	0.513235	1.542317
H	4.247465	-0.155812	2.388774
H	3.420232	1.317648	1.644902
H	3.429606	-0.352443	0.573034

$NCCH_2^{\bullet}$

M06-2X/BSI SCF energy in MeCN:

-132.086344 a.u.

M06-2X/BSII SCF energy in MeCN:

-132.092118 a.u.

M06-2X/BSII free energy in MeCN:

-132.081902 a.u.

C	0.193437	0.000004	0.000121
N	1.351799	0.000002	-0.000063
C	-1.194976	0.000002	-0.000009
H	-1.726631	-0.939981	-0.000114
H	-1.726726	0.939934	-0.000114

IM_d

M06-2X/BSI SCF energy in MeCN:

-577.005903 a.u.

M06-2X/BSII SCF energy in MeCN:

-577.031378 a.u

M06-2X/BSII free energy in MeCN:

-576.860700 a.u.

C	3.624688	-1.237951	0.362570
C	2.239389	-1.173242	0.378925
C	1.581440	0.004127	0.007032
C	2.341018	1.110927	-0.387089
C	3.725648	1.037267	-0.415654
C	4.370920	-0.135307	-0.038301
H	4.122984	-2.150253	0.665964
H	1.668178	-2.032579	0.708128
H	1.847353	2.023384	-0.698621
H	4.302132	1.895873	-0.736653
H	5.452426	-0.189672	-0.056718
C	0.108199	0.076442	0.027432
C	-0.539354	1.276642	0.360025
C	-0.659993	-1.062620	-0.290508
C	-1.912764	1.343598	0.376603
H	0.042778	2.148059	0.627947
C	-2.029626	-1.009335	-0.280568
H	-0.163013	-1.982557	-0.568411
C	-2.673295	0.201505	0.055663
H	-2.420893	2.263679	0.641381
H	-2.614769	-1.883593	-0.536247
C	-4.068855	0.320523	0.082410
H	-4.541093	1.264261	0.349827
O	-4.821108	-0.677191	-0.209254
H	-5.771703	-0.454529	-0.153800

^{1}TS1D

M06-2X/BSI SCF energy in MeCN:

-709.753354 a.u.

M06-2X/BSII SCF energy in MeCN:

-709.784045 a.u

M06-2X/BSII free energy in MeCN:

-709.574507 a.u.

C	-4.389514	1.110874	-1.081188
C	-3.041246	0.782399	-1.047913
C	-2.521217	0.021354	0.002724
C	-3.382706	-0.404477	1.017350
C	-4.731783	-0.079081	0.979728
C	-5.239299	0.680125	-0.068635
H	-4.775930	1.709122	-1.897242
H	-2.383732	1.136704	-1.832792
H	-3.000374	-1.011315	1.829448
H	-5.389038	-0.424732	1.768195
H	-6.291690	0.934440	-0.096554
C	-1.081654	-0.328199	0.037805
C	-0.391987	-0.385601	1.253773
C	-0.390788	-0.608195	-1.148400
C	0.952057	-0.710551	1.284722
H	-0.906953	-0.155591	2.177789
C	0.952107	-0.932844	-1.125760
H	-0.917190	-0.588575	-2.094131
C	1.624519	-0.986789	0.095315
H	1.487702	-0.744419	2.226650
H	1.475018	-1.155171	-2.047381
C	3.036356	-1.341959	0.161880
H	3.463931	-1.574664	1.131072
O	3.551224	-1.907148	-0.890525
H	4.447149	-2.247460	-0.715706
C	4.268593	1.490036	0.202634
N	3.879555	0.414492	0.189062
C	4.764567	2.848479	0.217469
H	4.939692	3.172233	-0.808082
H	4.021099	3.491245	0.688140
H	5.695603	2.880501	0.782344

^{1}IM$_d$1

M06-2X/BSI SCF energy in MeCN:

-709.763722 a.u.

M06-2X/BSII SCF energy in MeCN:

-709.794913 a.u

M06-2X/BSII free energy in MeCN:

-709.582862 a.u.

C	4.400612	1.598490	0.317565
C	3.040388	1.319977	0.335318
C	2.569073	0.050973	-0.011372
C	3.493239	-0.932299	-0.374557
C	4.853313	-0.653056	-0.390532
C	5.311870	0.613103	-0.045107
H	4.748626	2.589696	0.581666
H	2.337218	2.099998	0.602438
H	3.147827	-1.927740	-0.627476
H	5.556780	-1.429064	-0.666655
H	6.372807	0.830510	-0.058007
C	1.115272	-0.244871	0.006838
C	0.543109	-1.077244	-0.956255
C	0.289470	0.308914	0.992415
C	-0.817869	-1.350639	-0.938550
H	1.160157	-1.503305	-1.737834
C	-1.068070	0.039962	1.012874
H	0.719152	0.941920	1.759038
C	-1.621836	-0.793346	0.045263
H	-1.254429	-1.994512	-1.693220
H	-1.695112	0.468191	1.786516
C	-3.092147	-1.108739	0.074459
H	-3.371174	-1.786436	-0.732335
O	-3.476890	-1.546045	1.322555
H	-4.347408	-1.969982	1.267053
C	-4.396623	1.106248	-0.465817
N	-3.835631	0.143237	-0.233879
C	-5.101935	2.322571	-0.759056
H	-5.763677	2.547106	0.078480
H	-4.372880	3.122688	-0.892094
H	-5.680548	2.176360	-1.671777

^{1}TS2D

M06-2X/BSI SCF energy in MeCN:

-709.705651 a.u.

M06-2X/BSII SCF energy in MeCN:

-709.737192 a.u

M06-2X/BSII free energy in MeCN:

-709.524355 a.u.

C	-4.579410	-1.488131	-0.308685
C	-3.208077	-1.279265	-0.368526
C	-2.659421	-0.047644	-0.001574
C	-3.516842	0.968505	0.428570
C	-4.887773	0.757508	0.490295
C	-5.423944	-0.470995	0.121362
H	-4.989415	-2.445937	-0.604972
H	-2.560282	-2.072937	-0.721376
H	-3.107534	1.923425	0.736345
H	-5.537771	1.552850	0.834158
H	-6.493465	-0.634904	0.168897
C	-1.194677	0.176391	-0.066611
C	-0.679720	1.417324	-0.444859
C	-0.301803	-0.854735	0.251243
C	0.690491	1.627140	-0.502854
H	-1.352456	2.222652	-0.712198
C	1.064796	-0.650850	0.191885
H	-0.682888	-1.818992	0.563613
C	1.563991	0.594723	-0.183599
H	1.081930	2.592336	-0.802252
H	1.740523	-1.459970	0.446449
C	3.030016	0.836994	-0.236450
H	3.286209	1.850306	-0.536586
O	3.698518	0.492395	1.043169
H	4.104365	1.267061	1.480171
C	4.561414	-0.532433	-0.210368
N	3.794724	-0.123423	-1.047841
C	5.645339	-1.310379	0.317624
H	6.420564	-0.647327	0.703979
H	5.276592	-1.980065	1.094748
H	6.036141	-1.888611	-0.526165

^{1}IM$_d$2

M06-2X/BSI SCF energy in MeCN:

-709.781150 a.u.

M06-2X/BSII SCF energy in MeCN:

-709.813467 a.u

M06-2X/BSII free energy in MeCN:

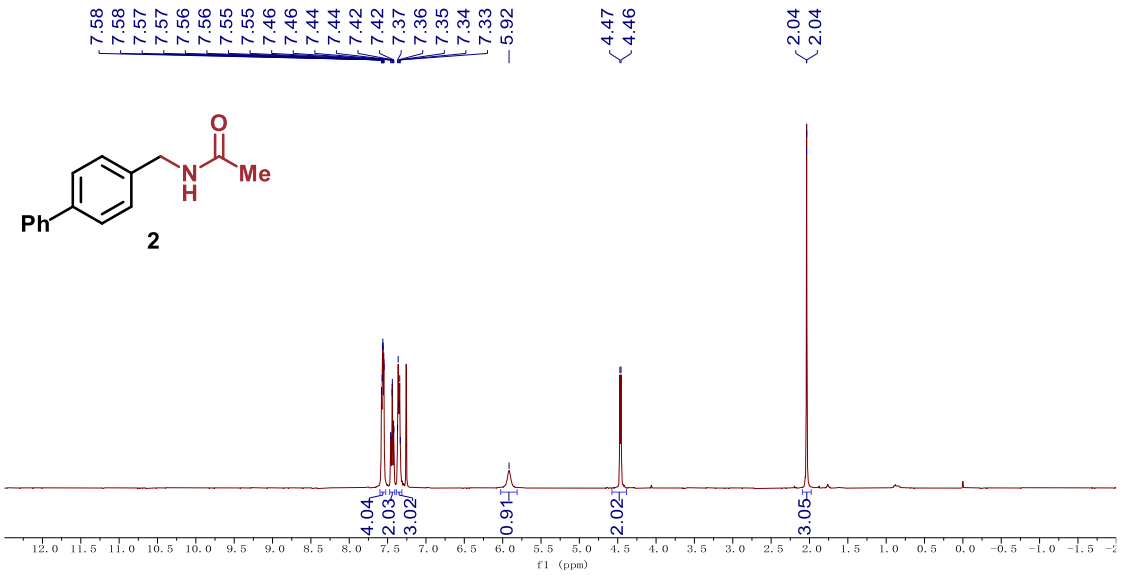
-709.600067 a.u.

C	-4.589962	1.574655	-0.375943
C	-3.235061	1.282062	-0.449175
C	-2.747647	0.055890	0.011670
C	-3.647236	-0.867899	0.551037
C	-5.000823	-0.570752	0.629143

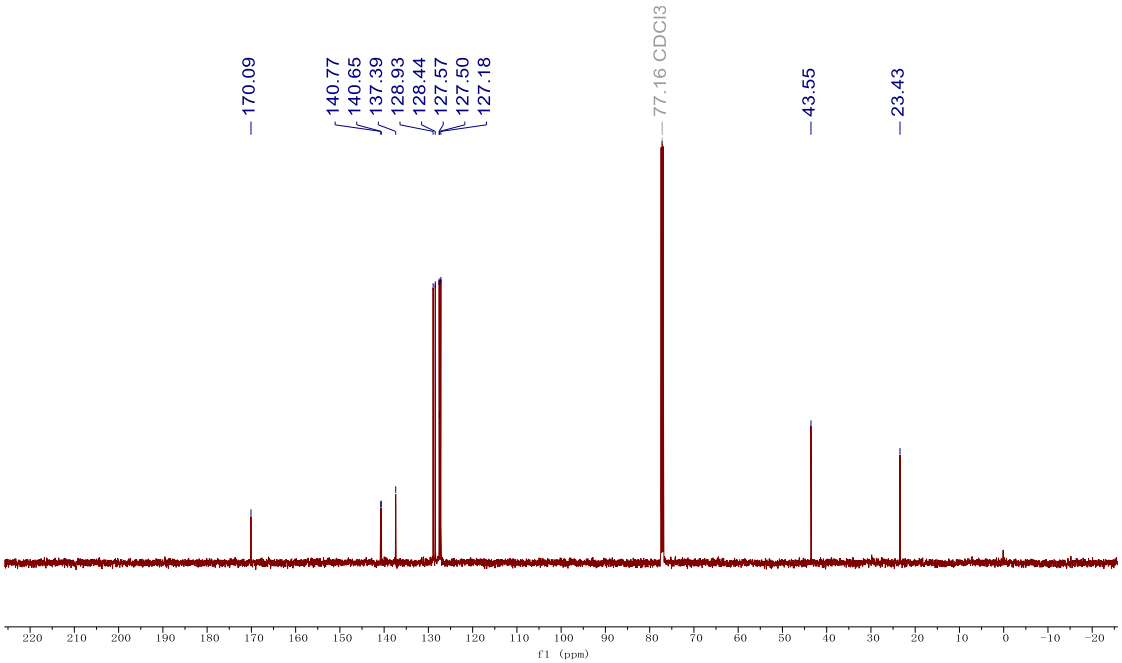
C	-5.476727	0.650209	0.164323
H	-4.954423	2.524598	-0.747215
H	-2.554329	2.001863	-0.887493
H	-3.283652	-1.815671	0.929723
H	-5.684766	-1.292461	1.058582
H	-6.533482	0.880098	0.222840
C	-1.303691	-0.261329	-0.075297
C	-0.878516	-1.564544	-0.350096
C	-0.341368	0.743039	0.112533
C	0.469945	-1.859731	-0.439116
H	-1.607861	-2.346941	-0.516318
C	1.004642	0.455145	0.028234
H	-0.657026	1.752712	0.342786
C	1.417990	-0.852297	-0.249315
H	0.796105	-2.868962	-0.661869
H	1.739809	1.237314	0.178879
C	2.820763	-1.207568	-0.351534
H	3.075858	-2.237879	-0.601334
O	5.132606	1.166908	-0.915003
H	5.835549	1.763476	-0.601837
C	4.667408	0.440751	0.085587
N	3.766911	-0.398454	-0.173216
C	5.222546	0.620836	1.454402
H	5.096788	1.664564	1.748223
H	4.718650	-0.031155	2.161207
H	6.289969	0.391547	1.427654

5. NMR Spectra

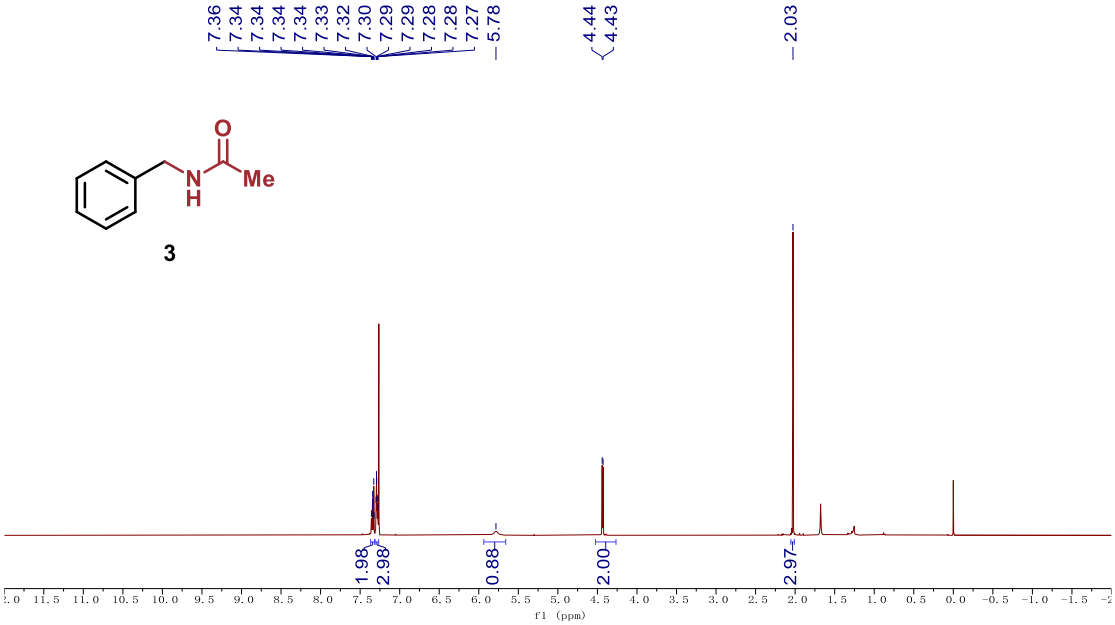
^{1}H NMR of compound **2** (400 MHz in $CDCl_3$)



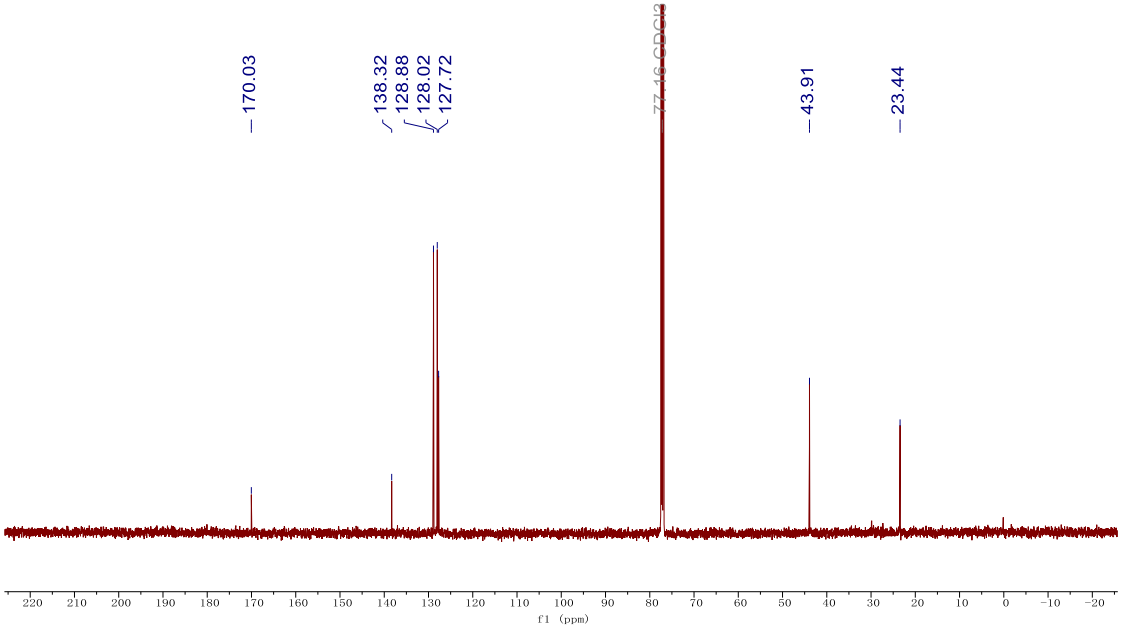
^{13}C NMR of compound **2** (126 MHz in $CDCl_3$)



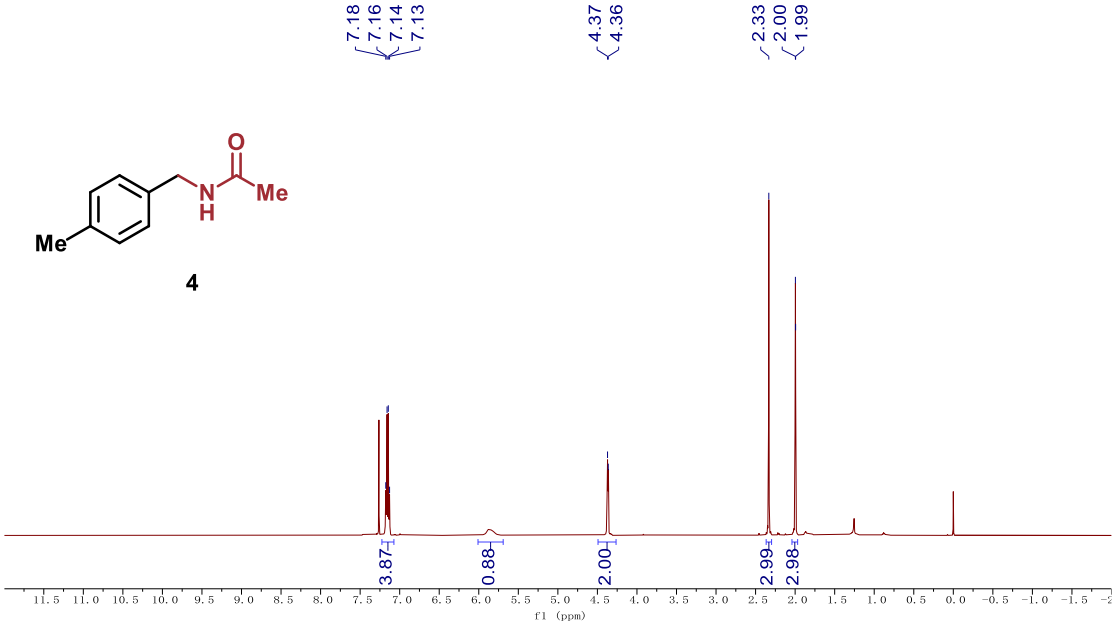
^{1}H NMR of compound **3**(500 MHz in $CDCl_3$)



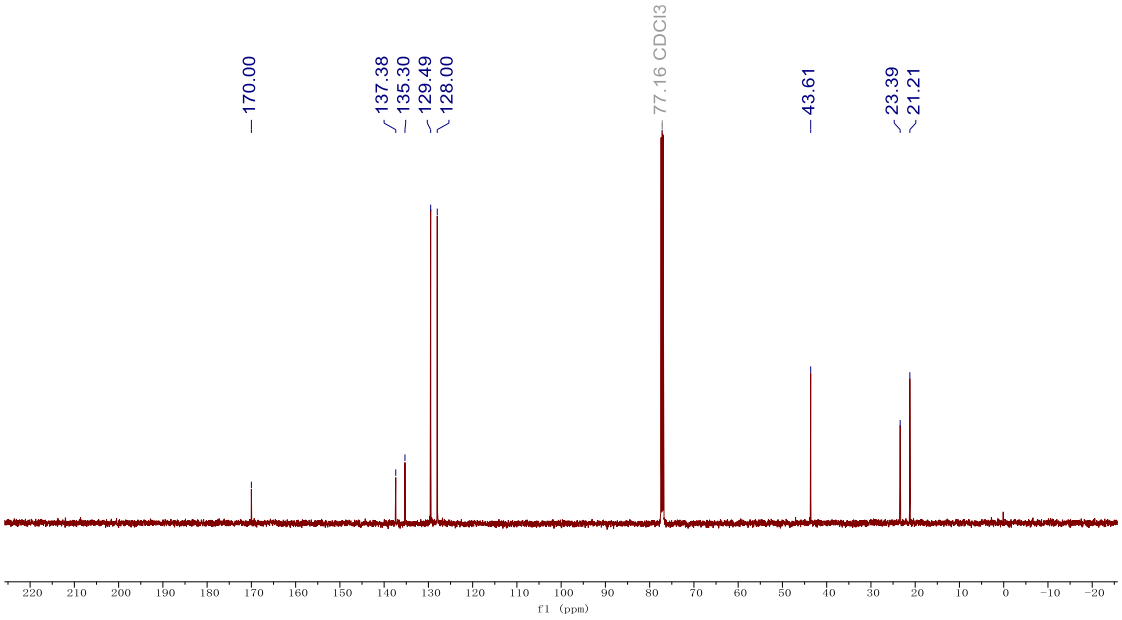
^{13}C NMR of compound **3** (126 MHz in $CDCl_3$)



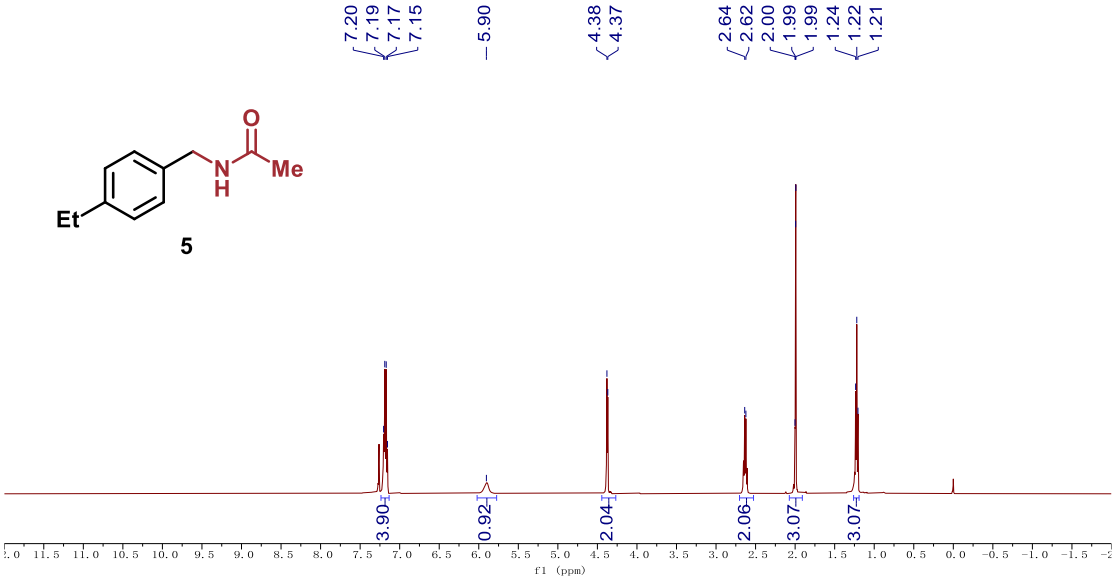
^{1}H NMR of compound **4** (500 MHz in $CDCl_3$)



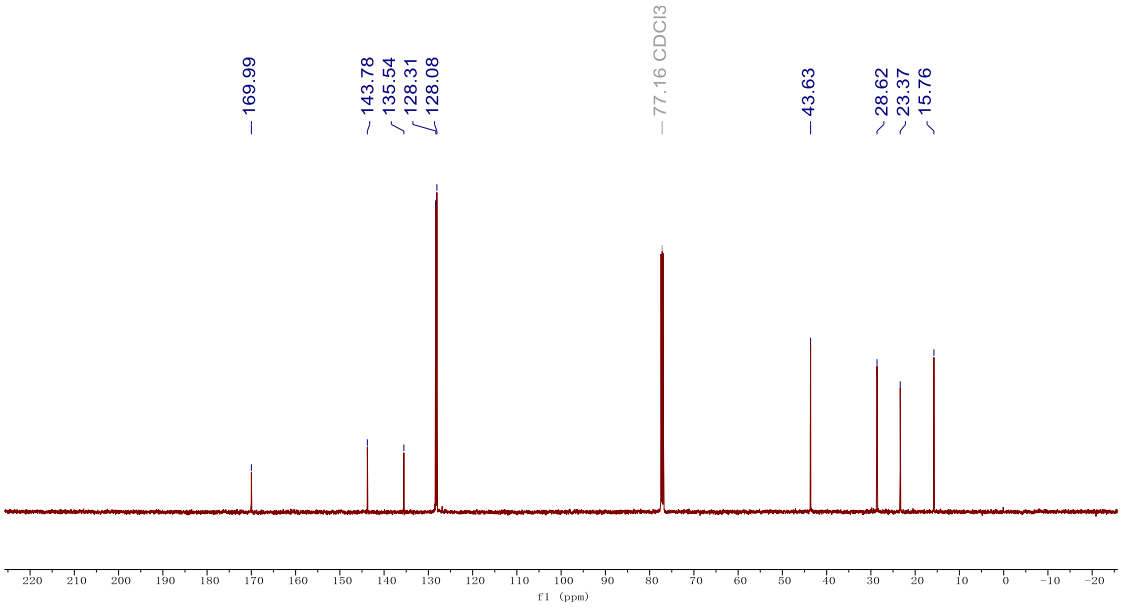
^{13}C NMR of compound **4** (126 MHz in $CDCl_3$)



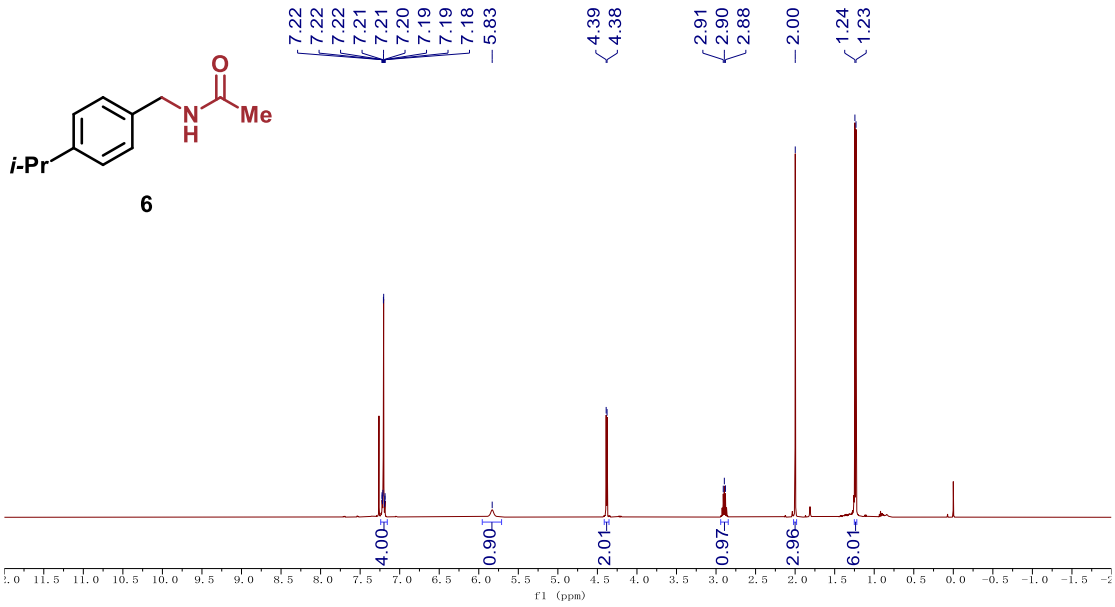
^{1}H NMR of compound **5** (500 MHz in $CDCl_3$)



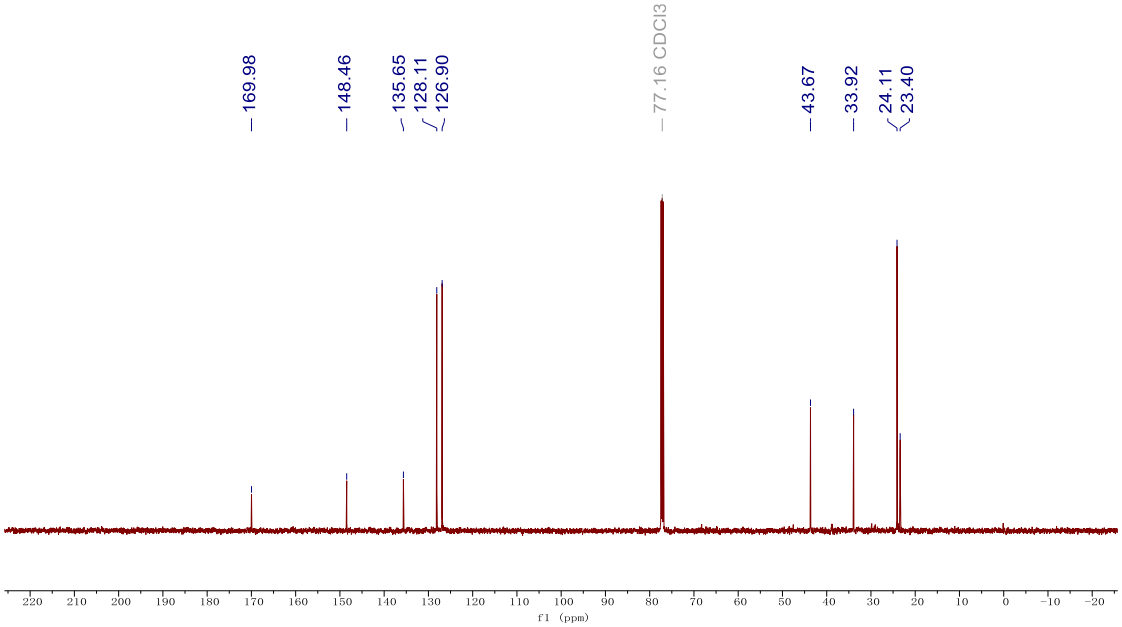
^{13}C NMR of compound **5** (126 MHz in $CDCl_3$)



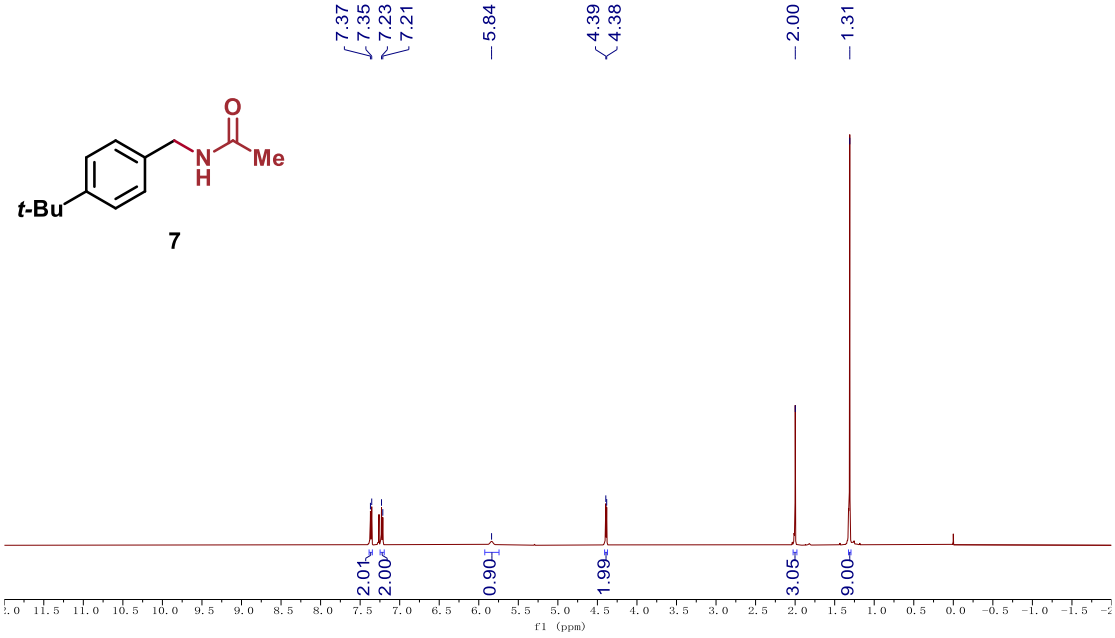
^{1}H NMR of compound **6** (500 MHz in $CDCl_3$)



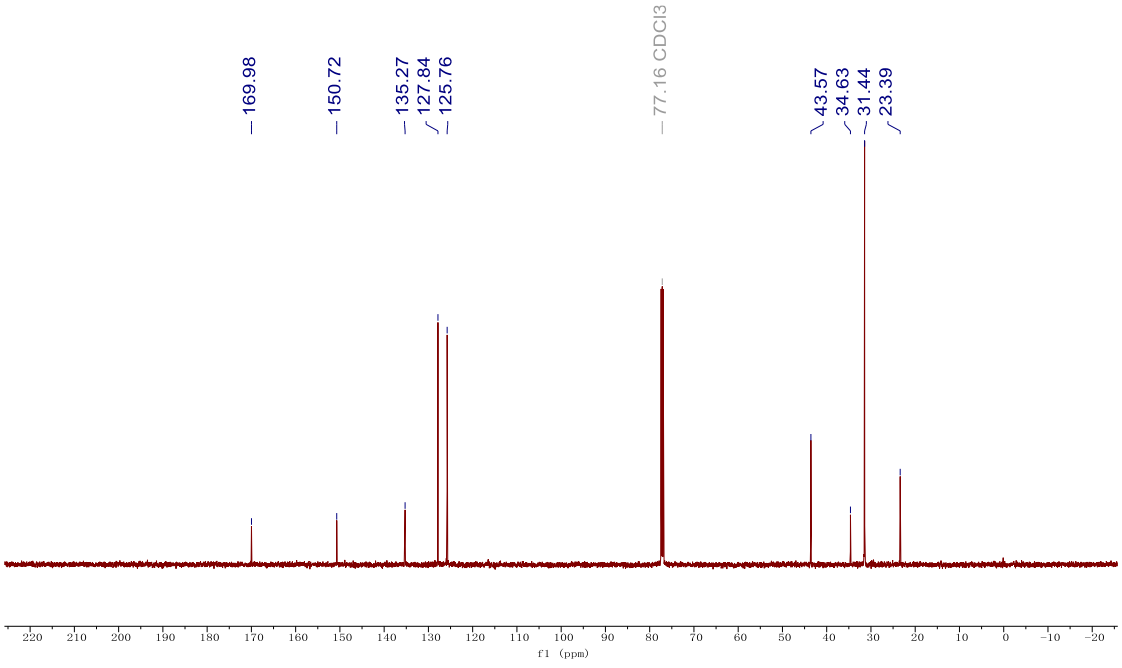
^{13}C NMR of compound **6** (126 MHz in $CDCl_3$)



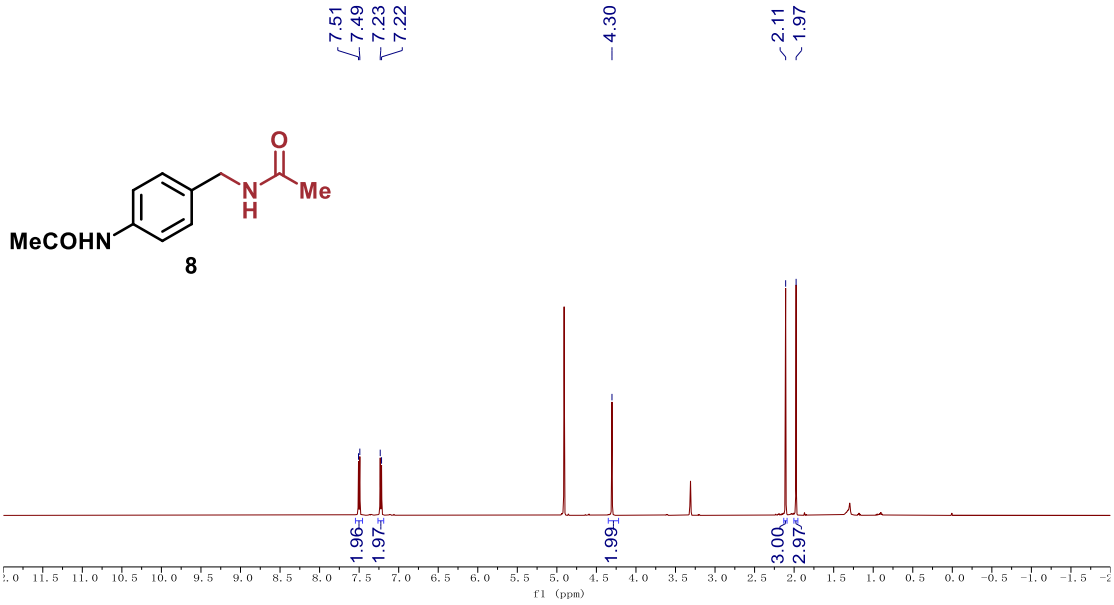
^{1}H NMR of compound **7** (500 MHz in $CDCl_3$)



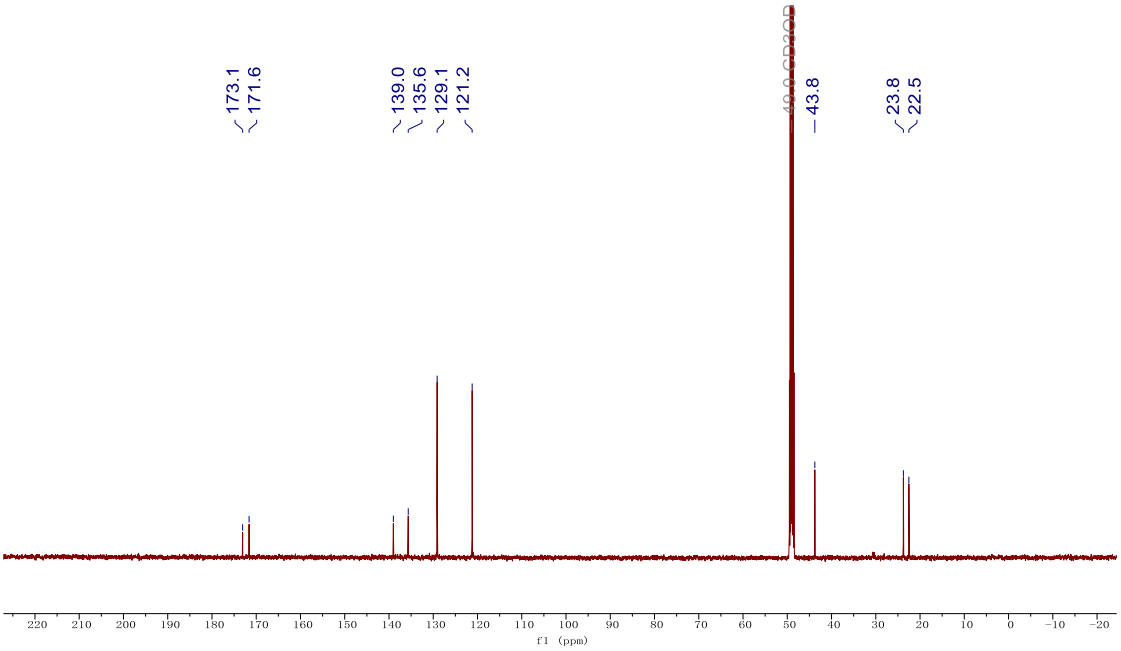
^{13}C NMR of compound **7** (126 MHz in $CDCl_3$)



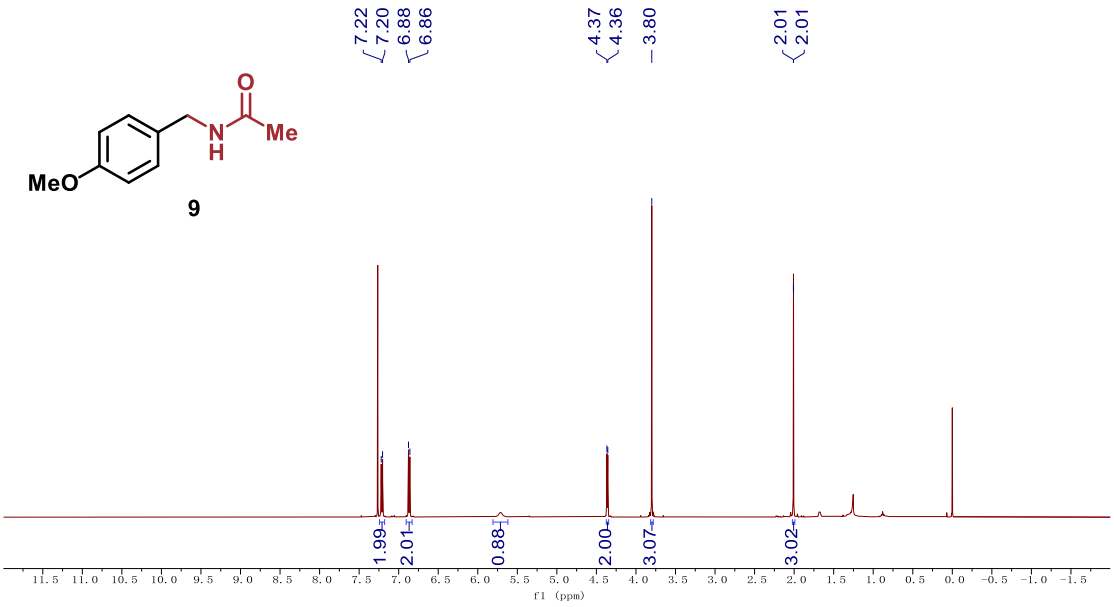
^{1}H NMR of compound **8** (500 MHz in Methanol-d_4)



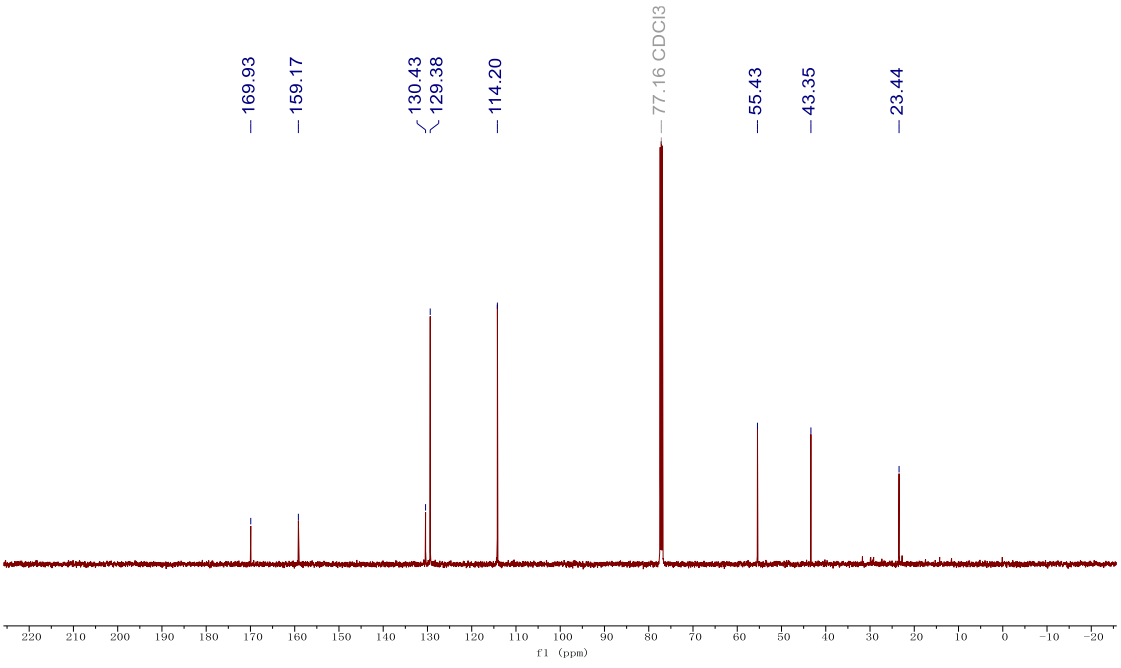
^{13}C NMR of compound **8** (126 MHz in Methanol-d_4)



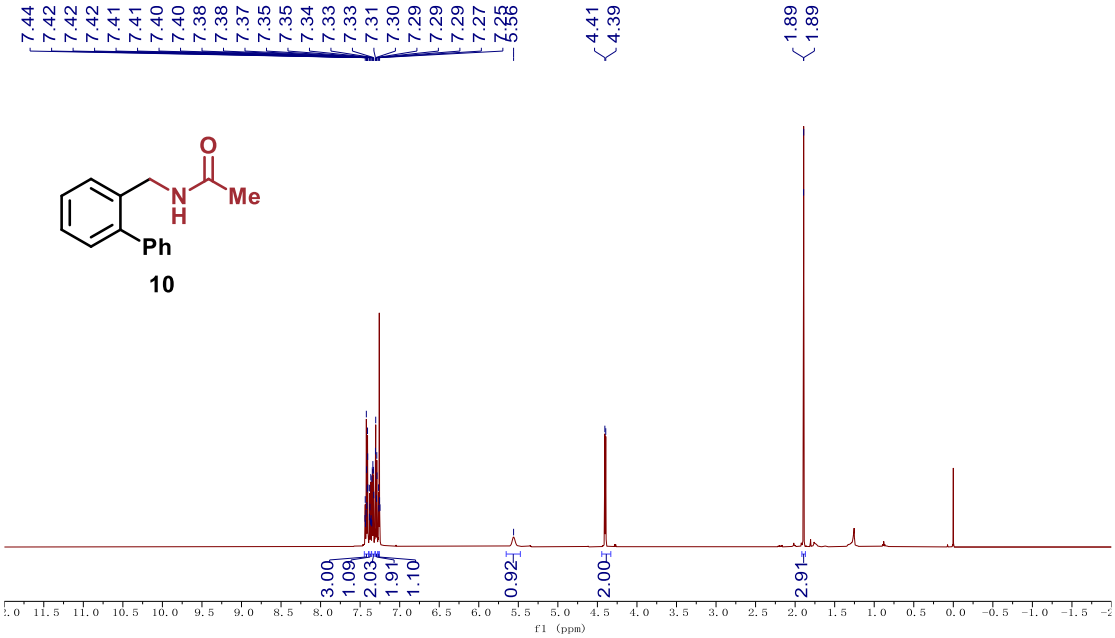
^{1}H NMR of compound **9** (500 MHz in $CDCl_3$)



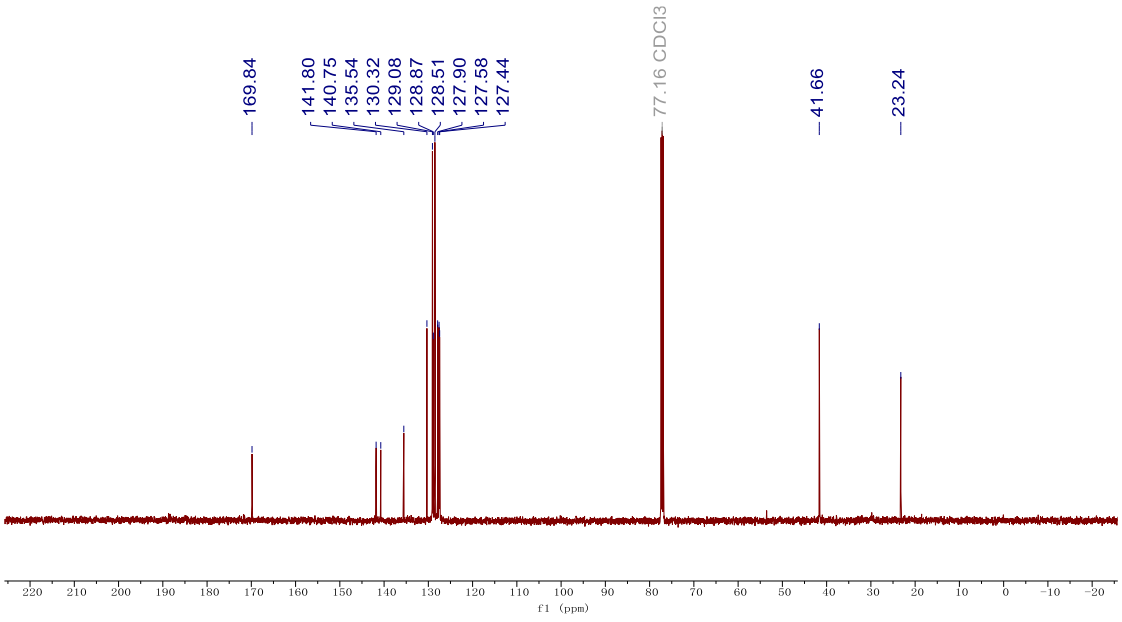
^{13}C NMR of compound **9** (126 MHz in $CDCl_3$)



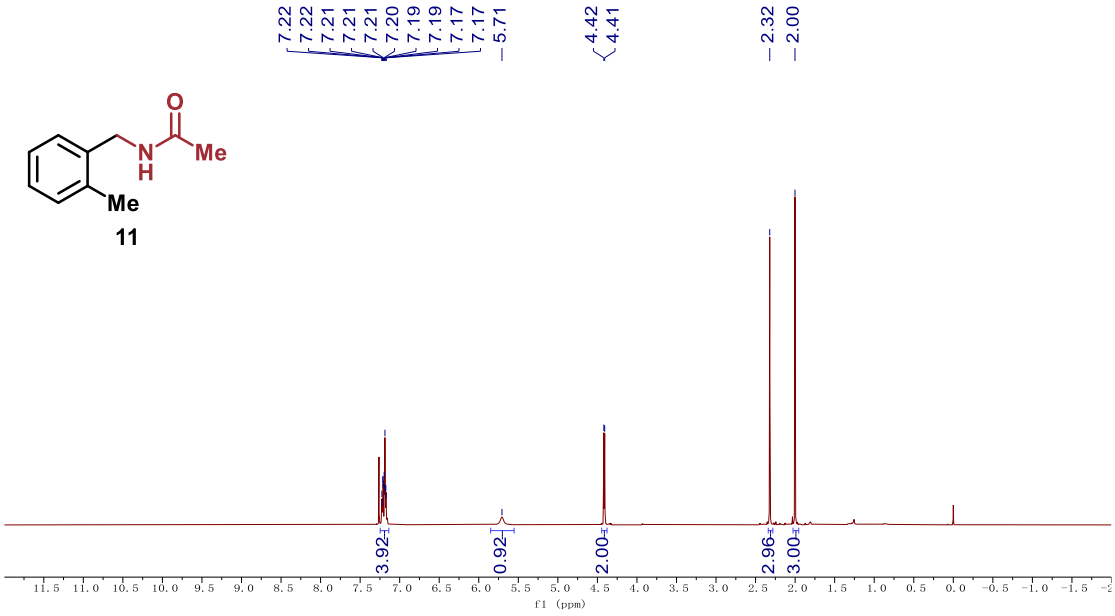
^{1}H NMR of compound **10** (500 MHz in $CDCl_3$)



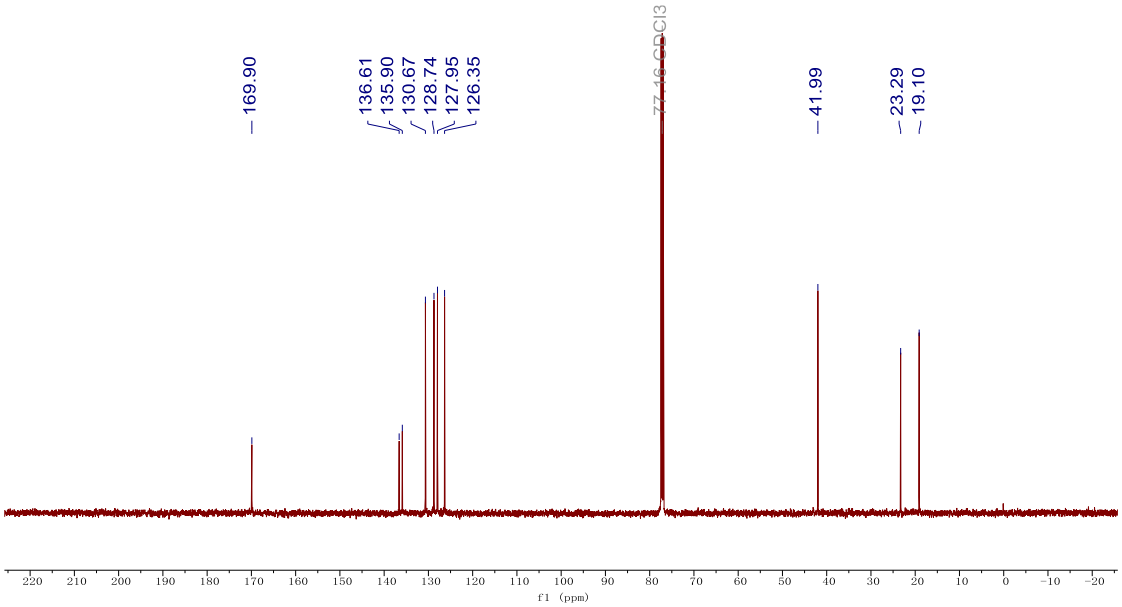
^{13}C NMR of compound **10** (126 MHz in $CDCl_3$)



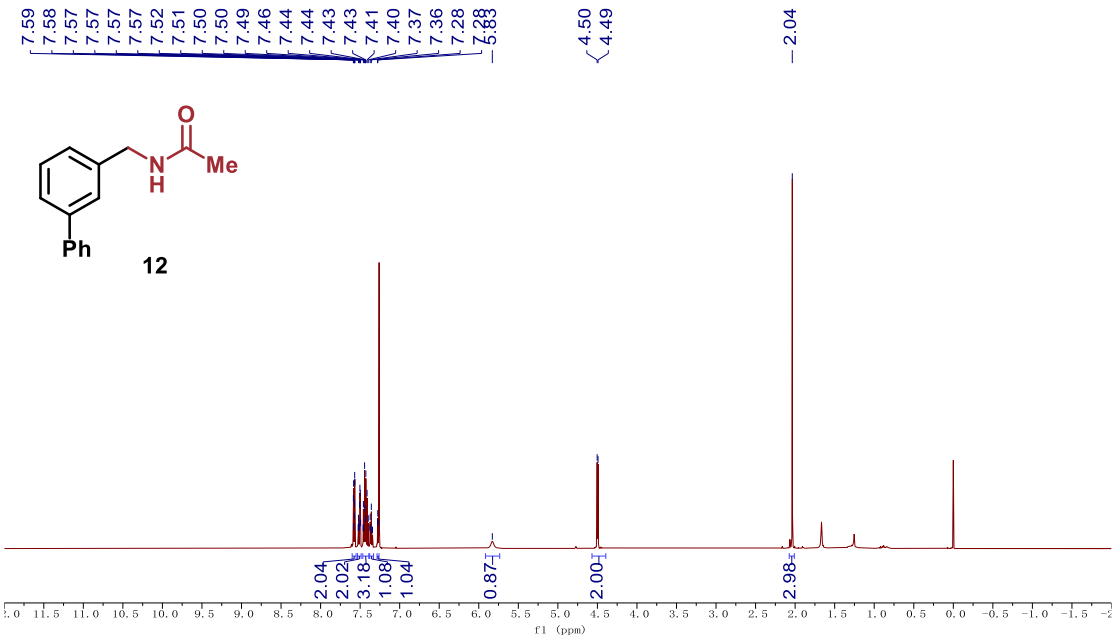
^{1}H NMR of compound **11** (500 MHz in $CDCl_3$)



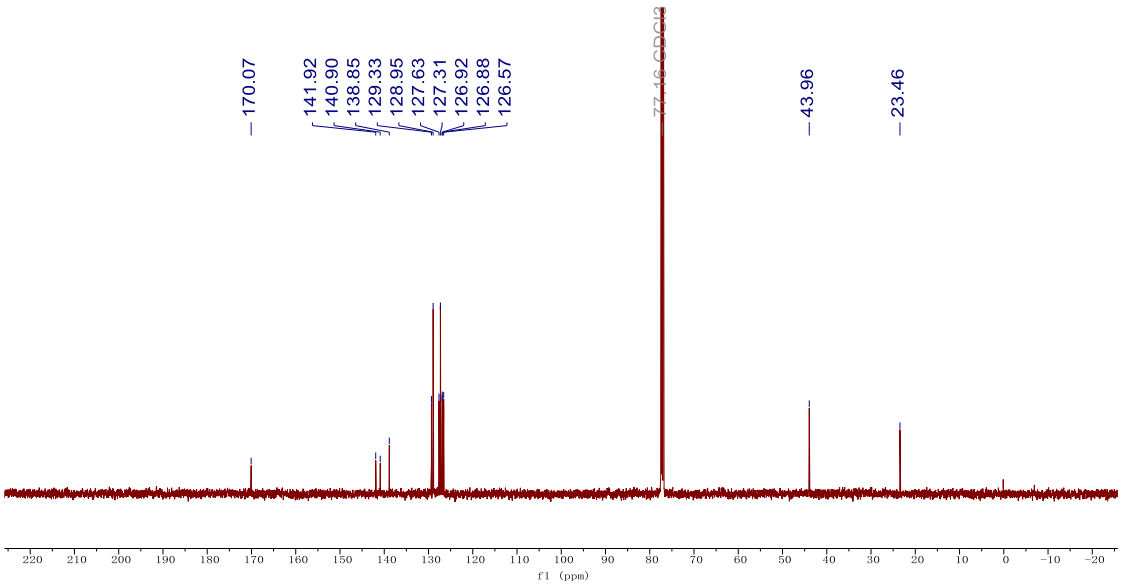
^{13}C NMR of compound **11** (126 MHz in $CDCl_3$)



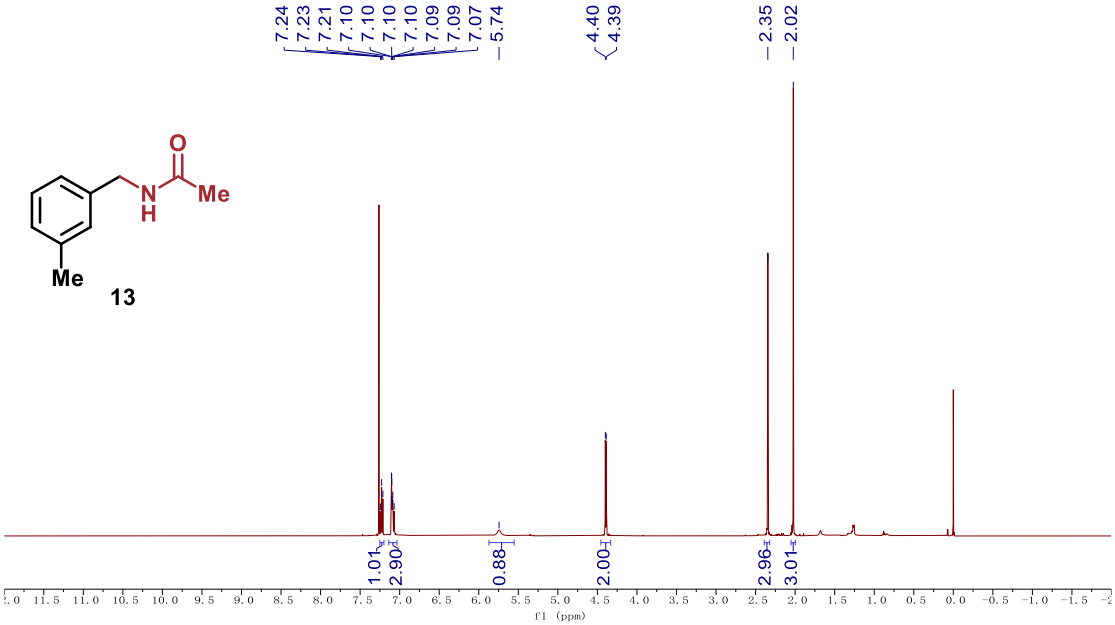
^{1}H NMR of compound **12** (500 MHz in $CDCl_3$)



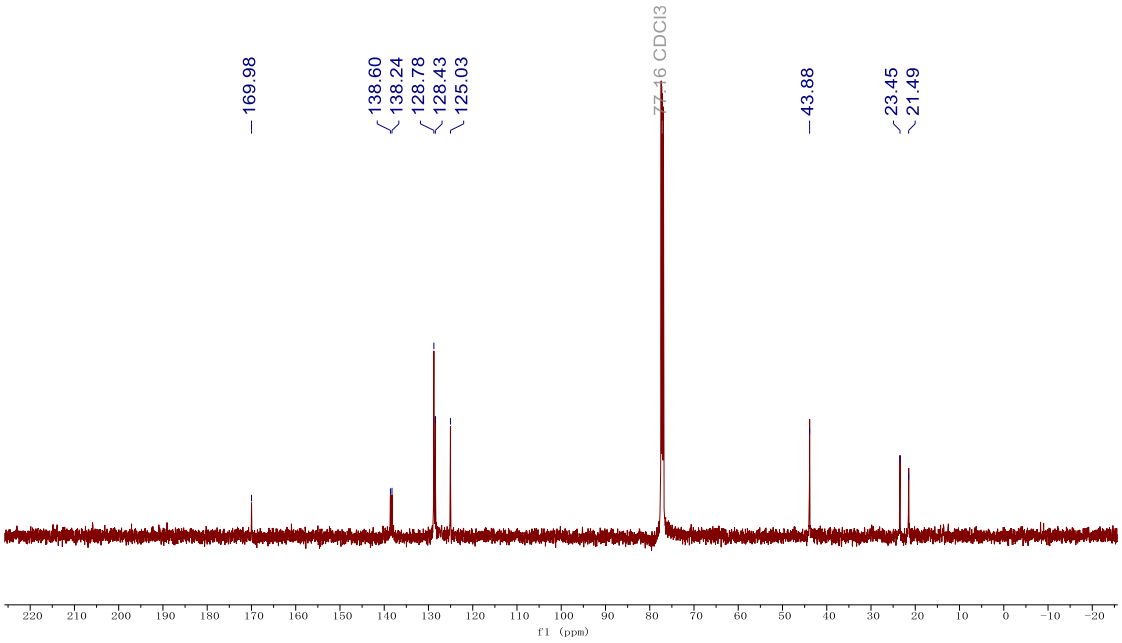
^{13}C NMR of compound **12** (126 MHz in $CDCl_3$)



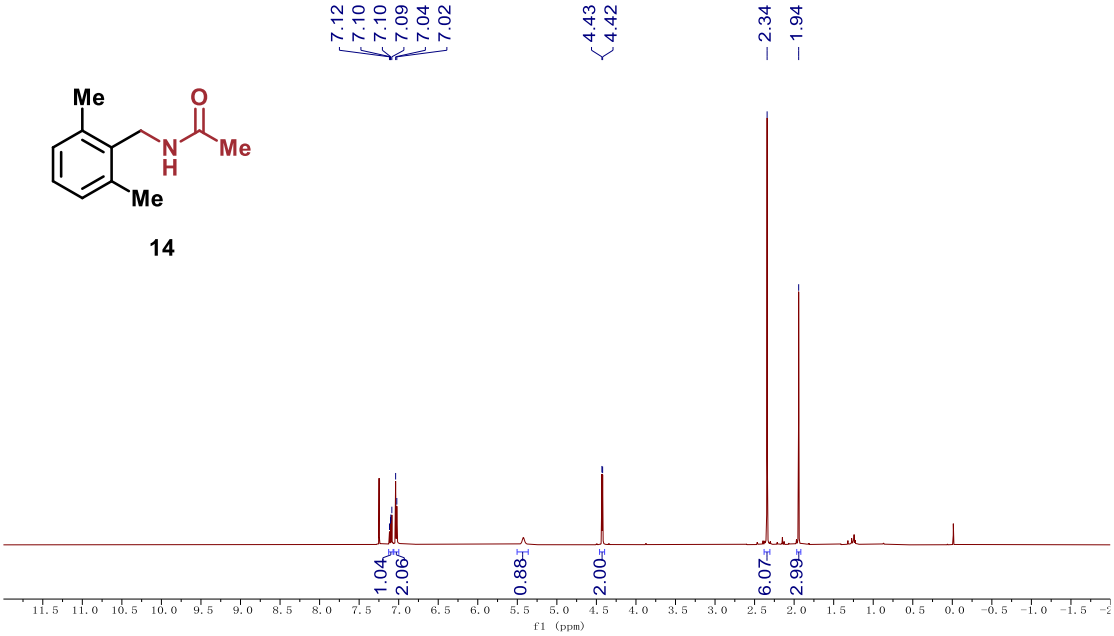
^{1}H NMR of compound **13** (500 MHz in $CDCl_3$)



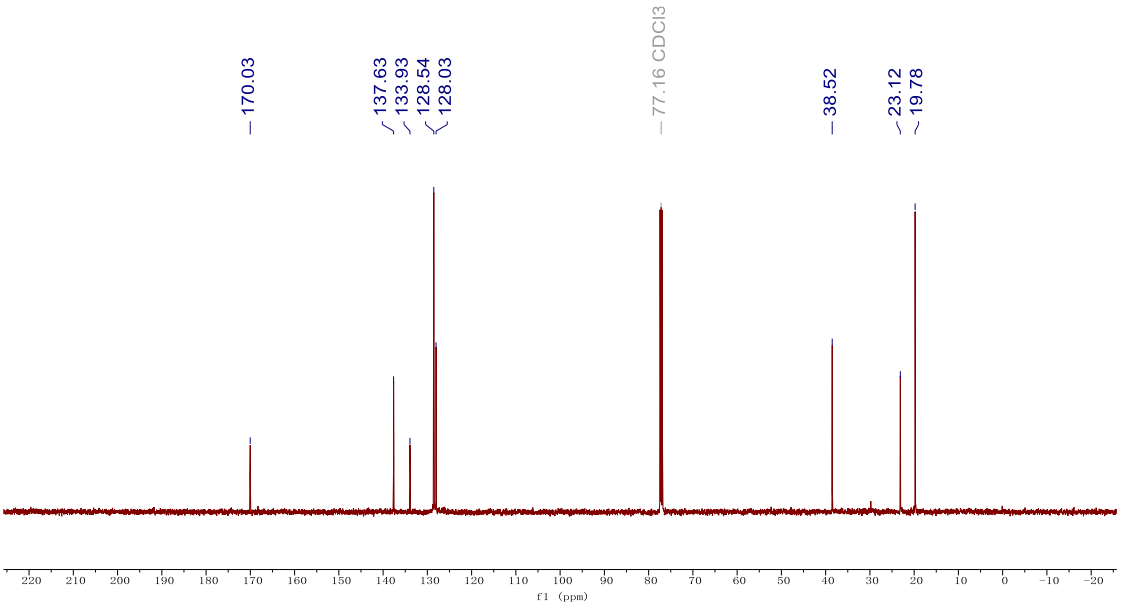
^{13}C NMR of compound **13** (126 MHz in $CDCl_3$)



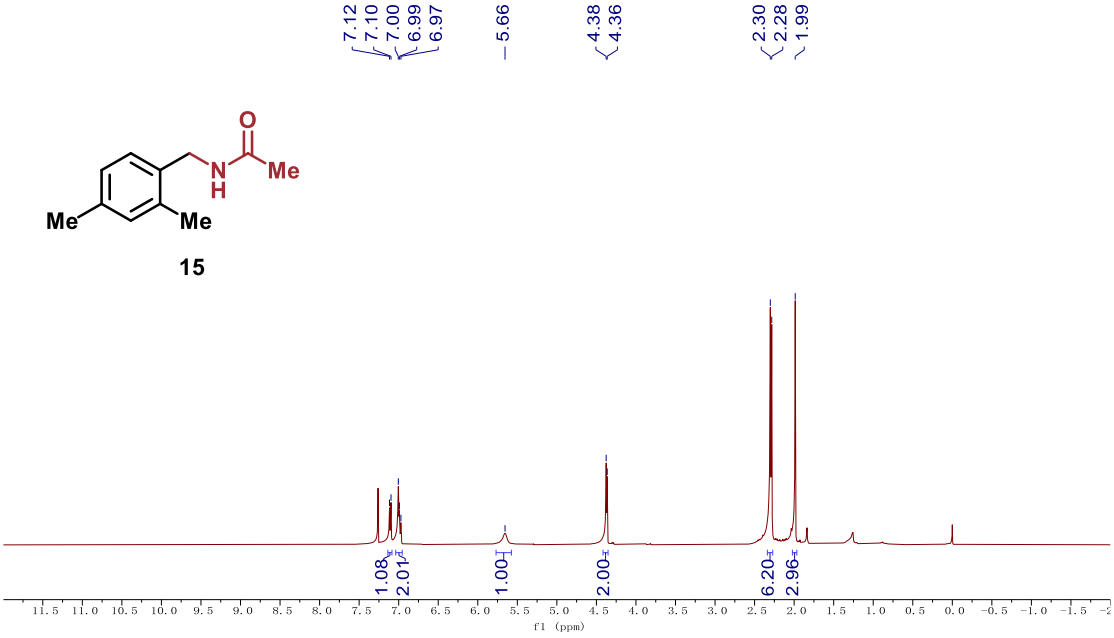
^{1}H NMR of compound **14** (500 MHz in $CDCl_3$)



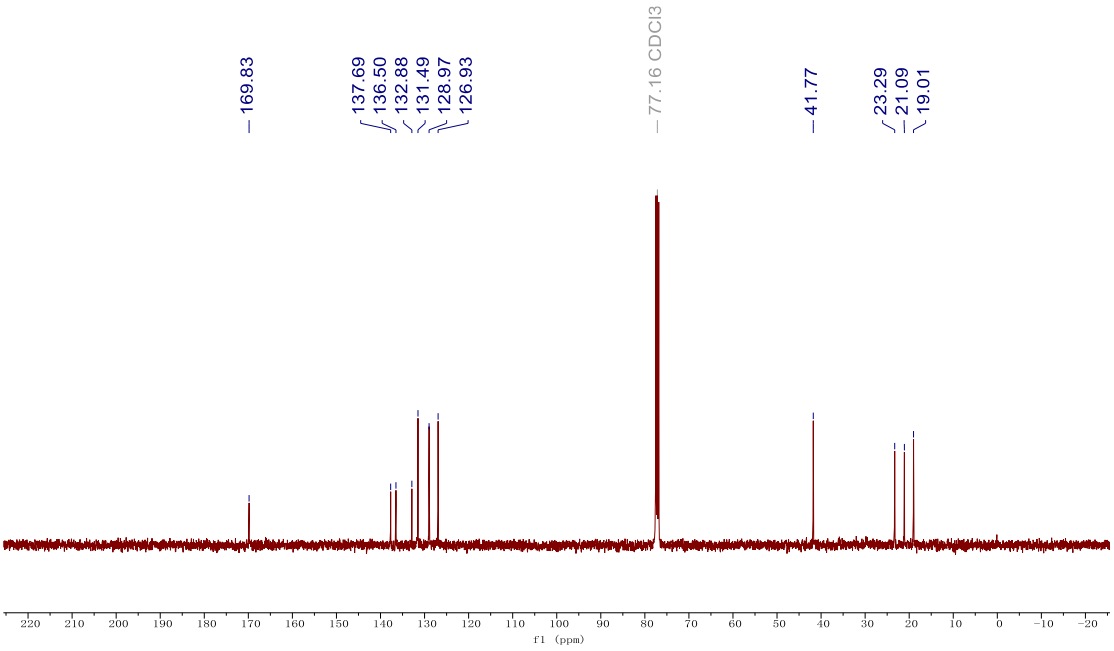
^{13}C NMR of compound **14** (126 MHz in $CDCl_3$)



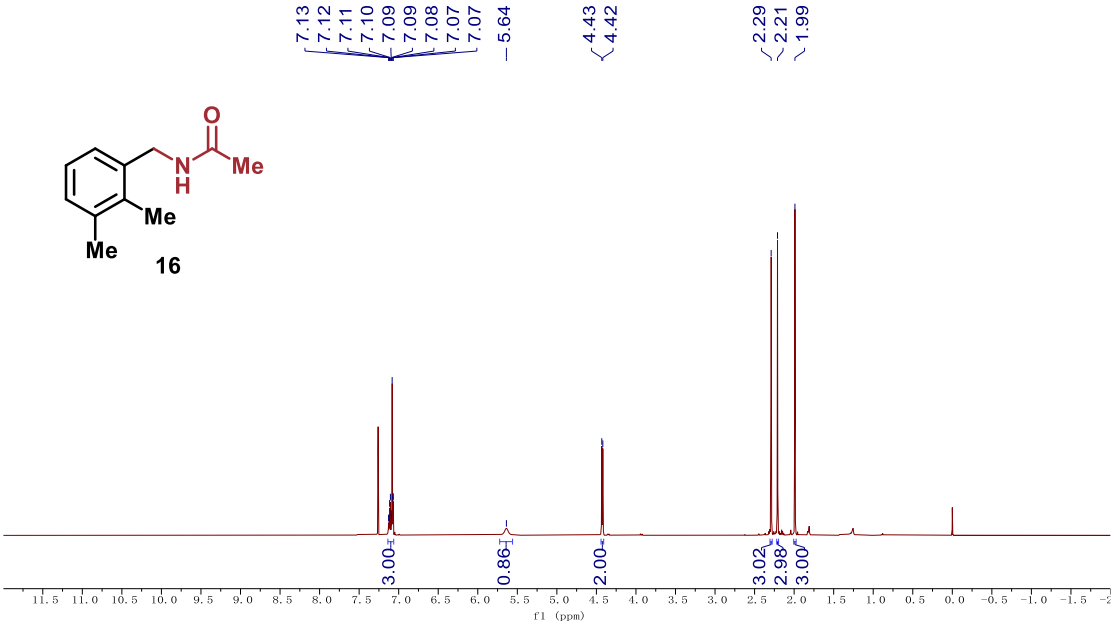
^{1}H NMR of compound **15** (500 MHz in $CDCl_3$)



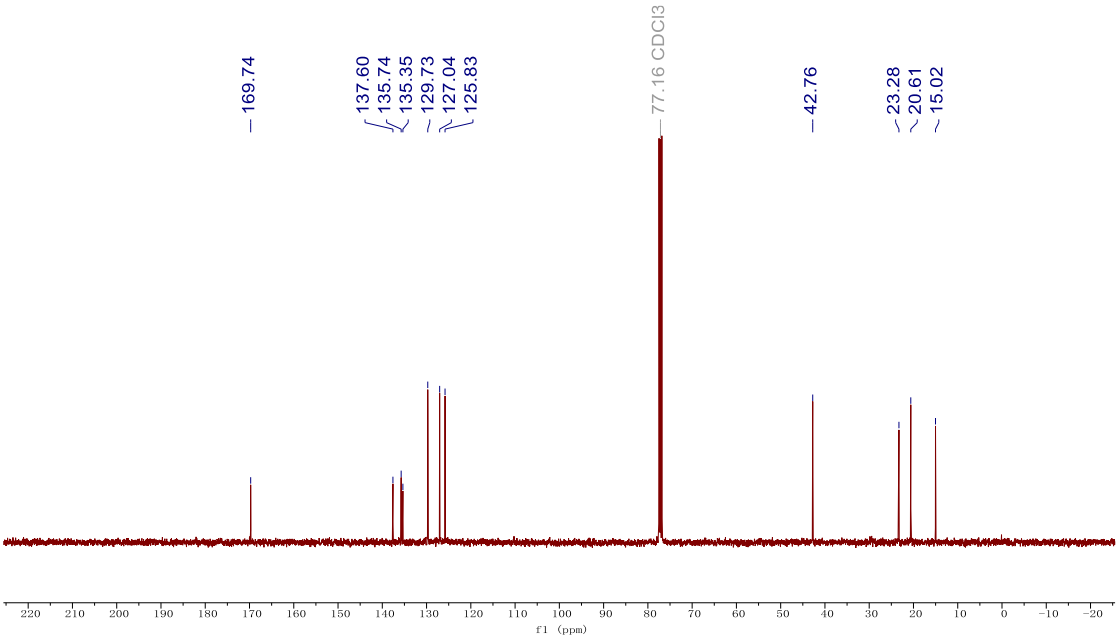
^{13}C NMR of compound **15** (126 MHz in $CDCl_3$)



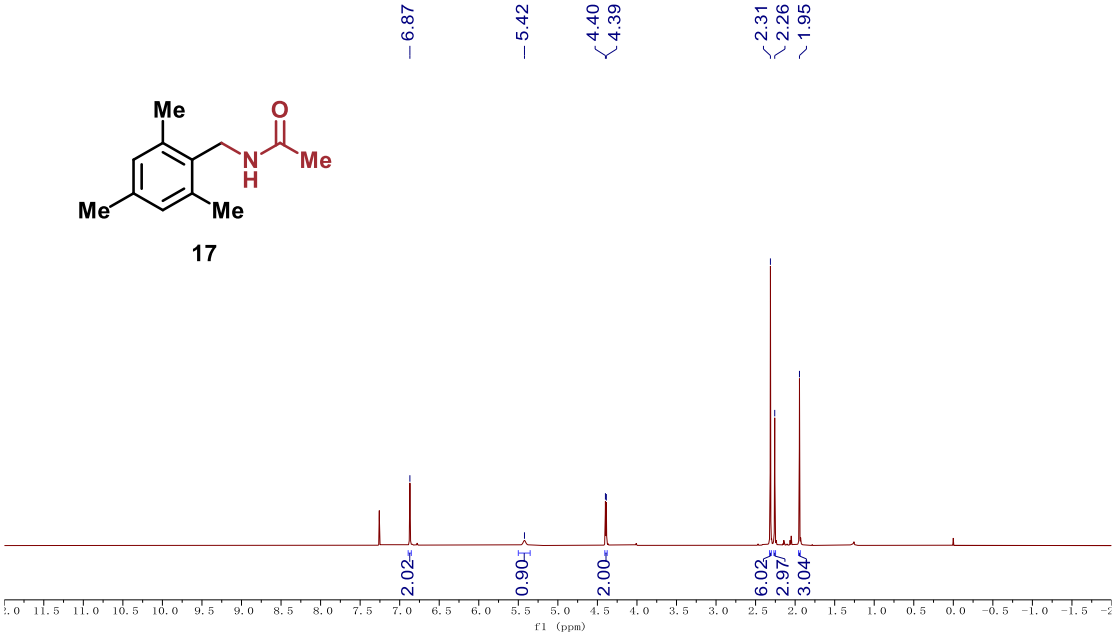
^{1}H NMR of compound **16** (500 MHz in $CDCl_3$)



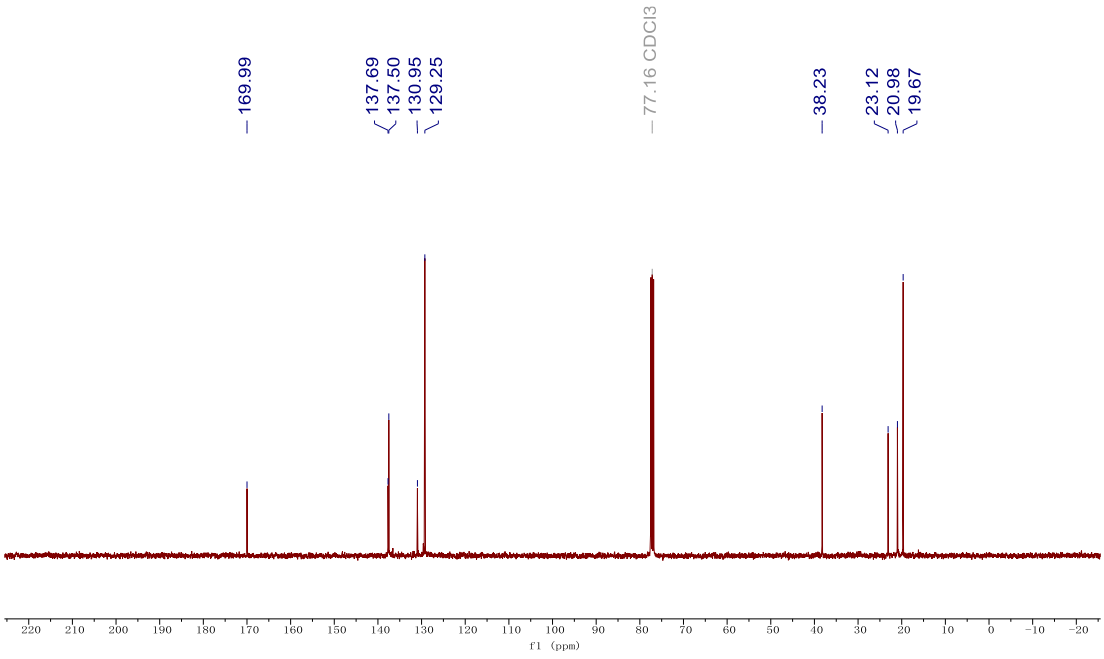
^{13}C NMR of compound **16** (126 MHz in $CDCl_3$)



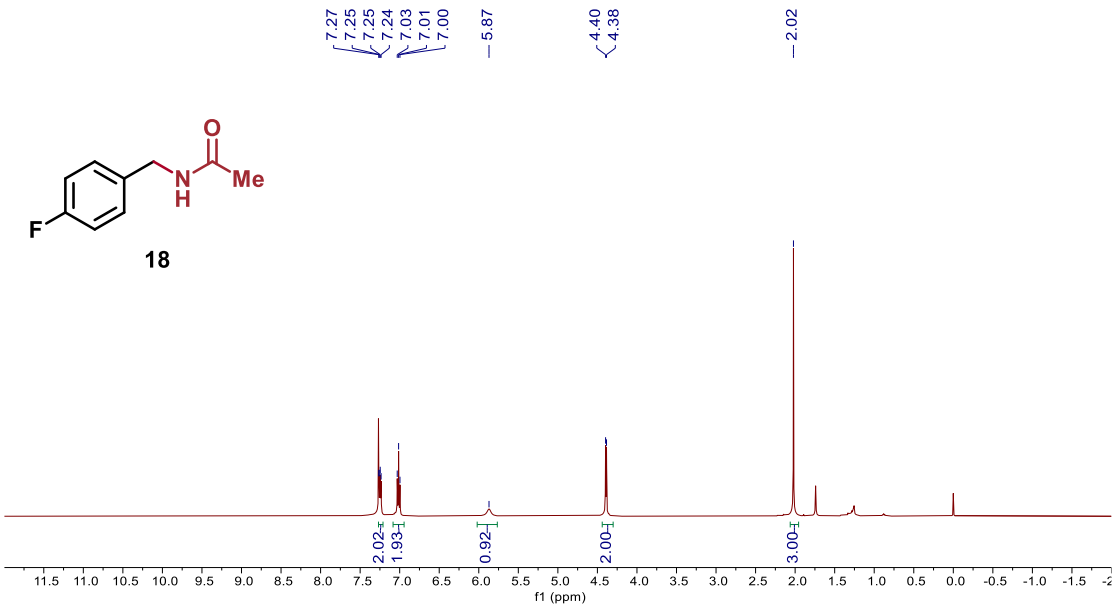
^{1}H NMR of compound **17** (500 MHz in $CDCl_3$)



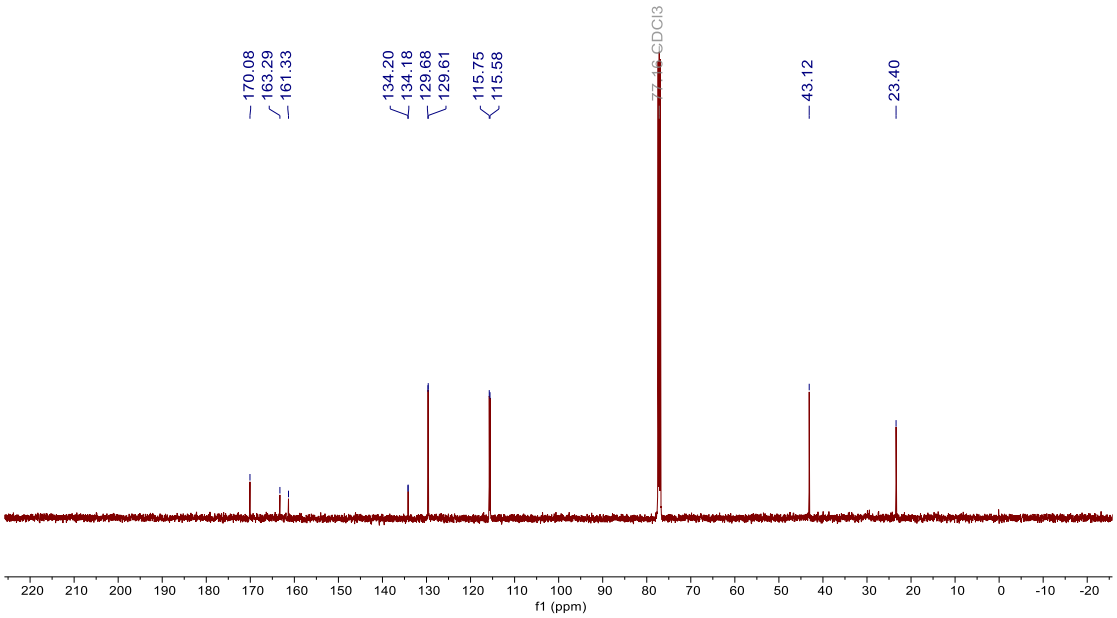
^{13}C NMR of compound **17** (126 MHz in $CDCl_3$)



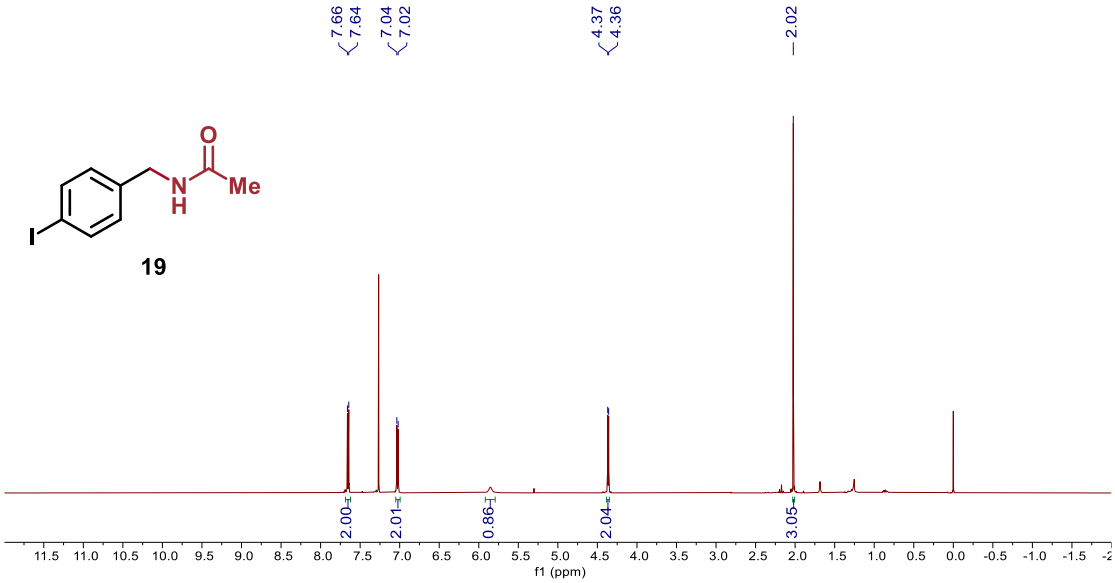
^{1}H NMR of compound **18** (500 MHz in $CDCl_3$)



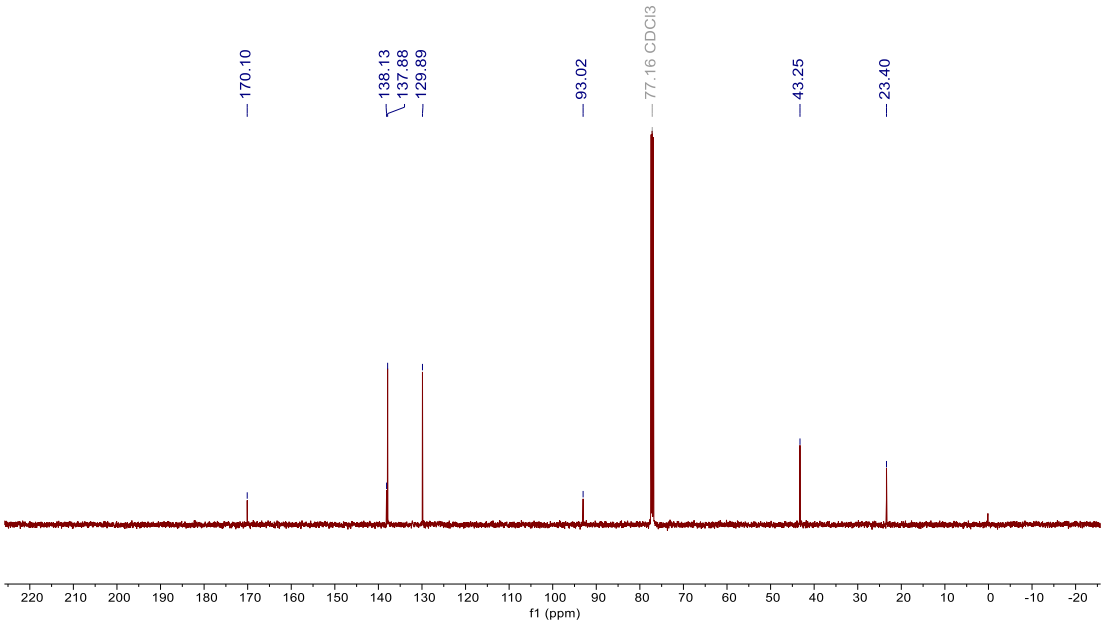
^{13}C NMR of compound **18** (126 MHz in $CDCl_3$)



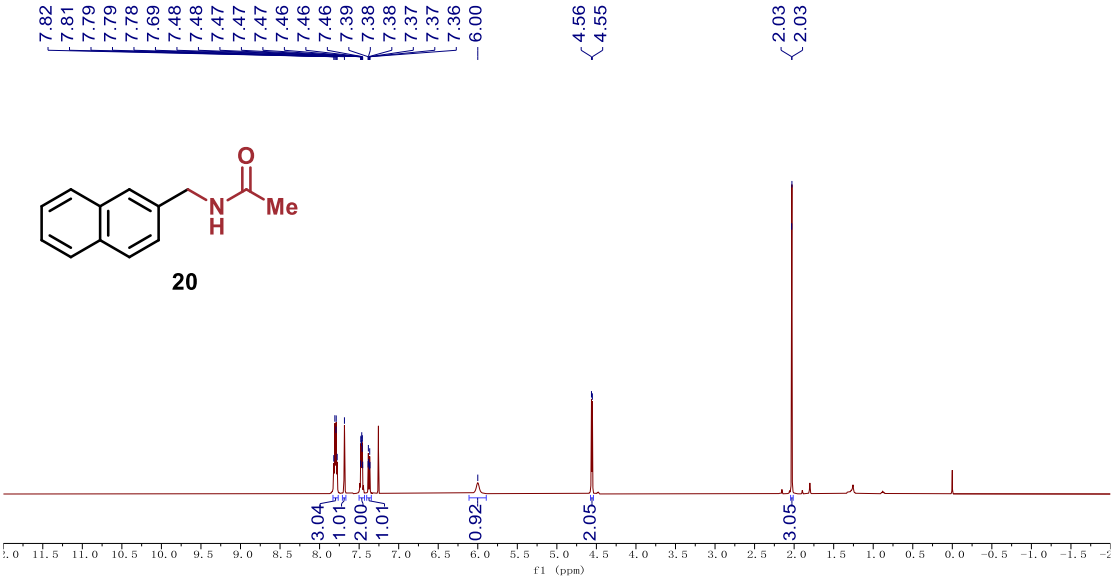
^{1}H NMR of compound **19** (500 MHz in $CDCl_3$)



^{13}C NMR of compound **19** (126 MHz in $CDCl_3$)

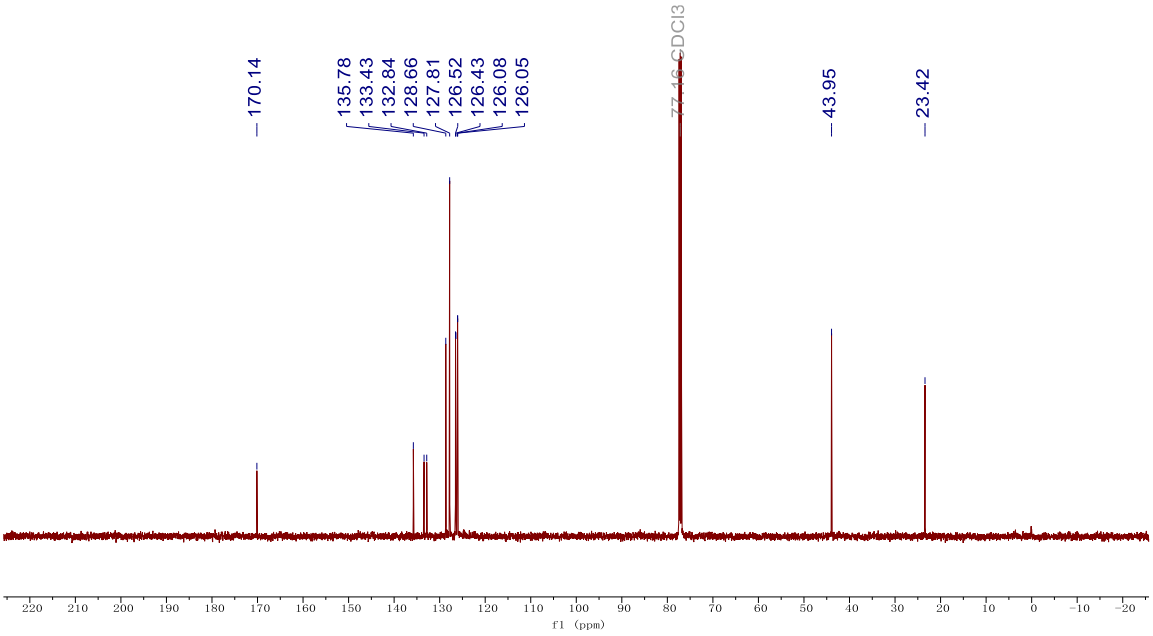


^{1}H NMR of compound **20** (500 MHz in $CDCl_3$)

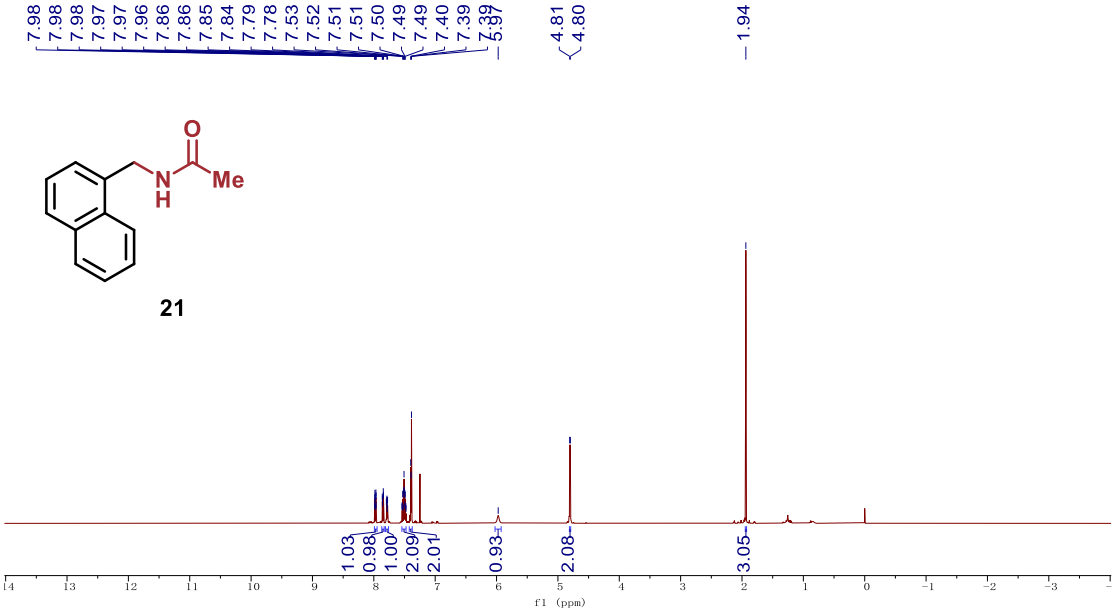


20

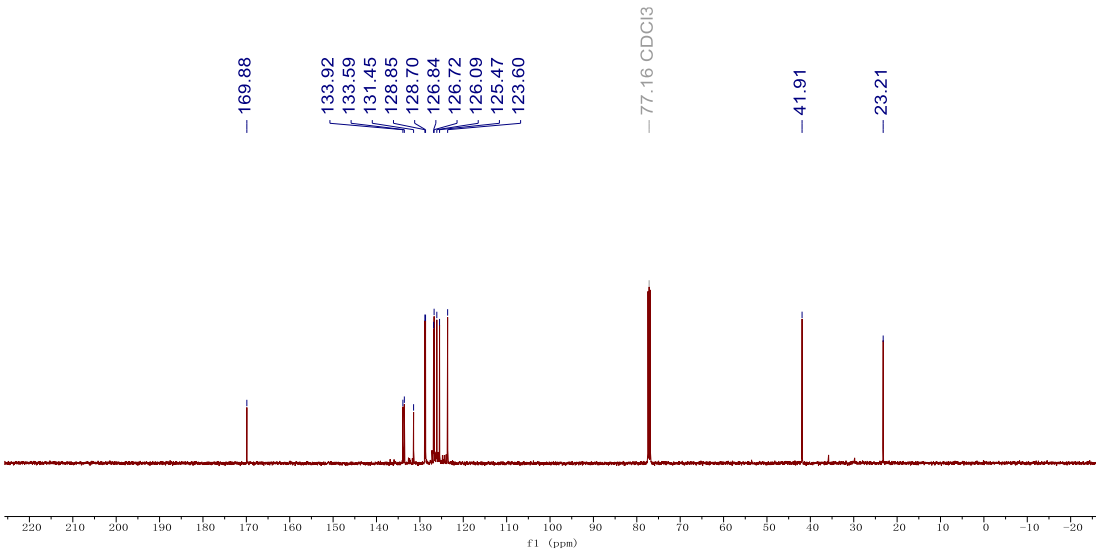
^{13}C NMR of compound **20** (126 MHz in $CDCl_3$)



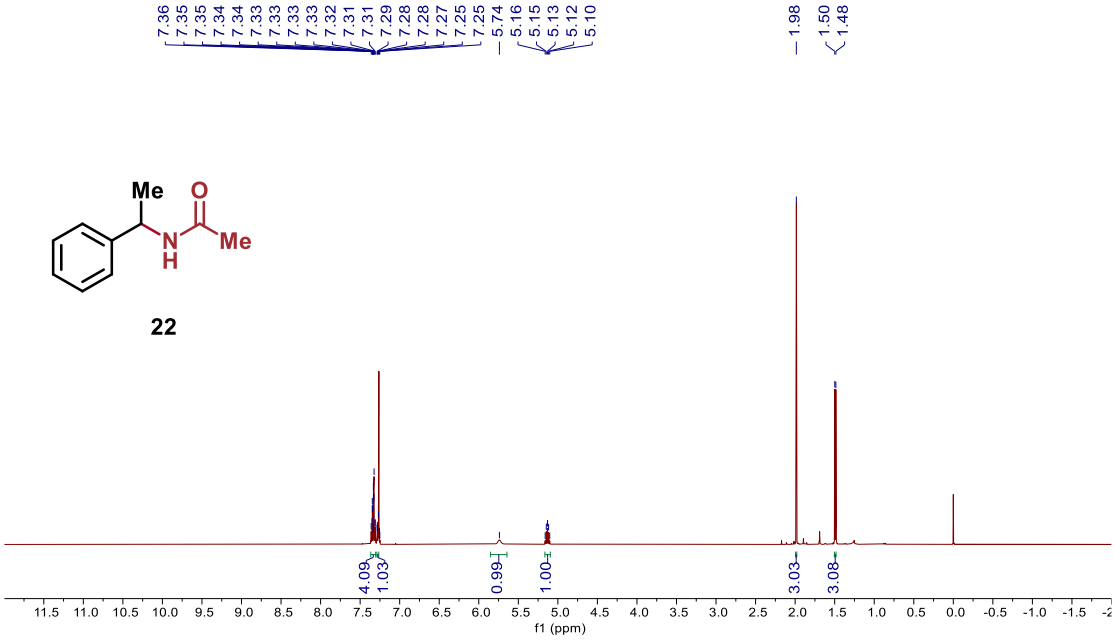
^{1}H NMR of compound **21** (500 MHz in $CDCl_3$)



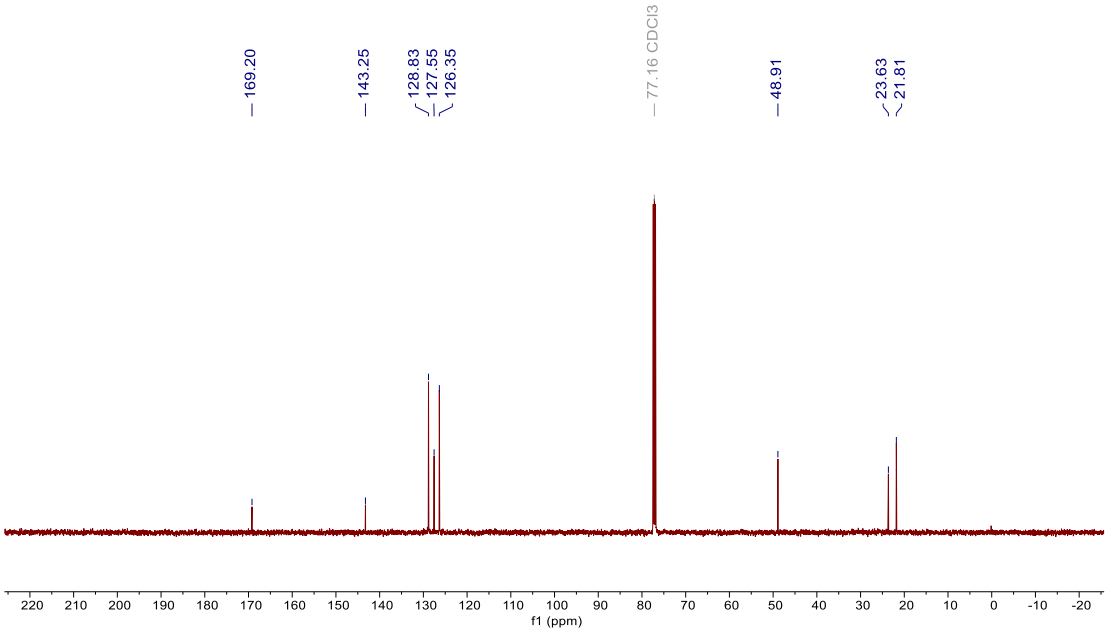
^{13}C NMR of compound **21** (126 MHz in $CDCl_3$)



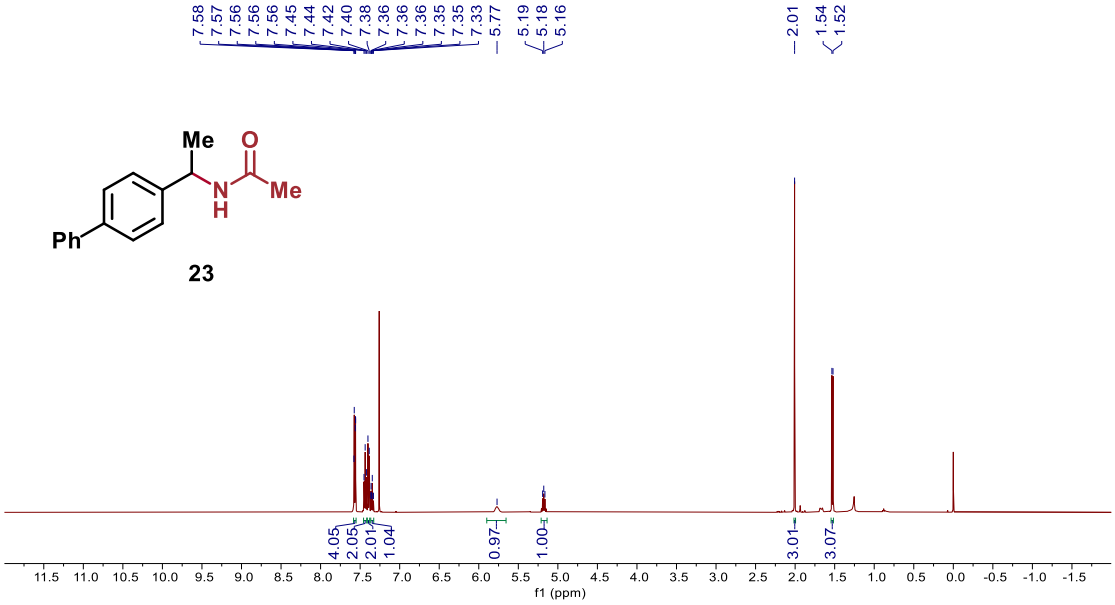
^{1}H NMR of compound **22** (500 MHz in $CDCl_3$)



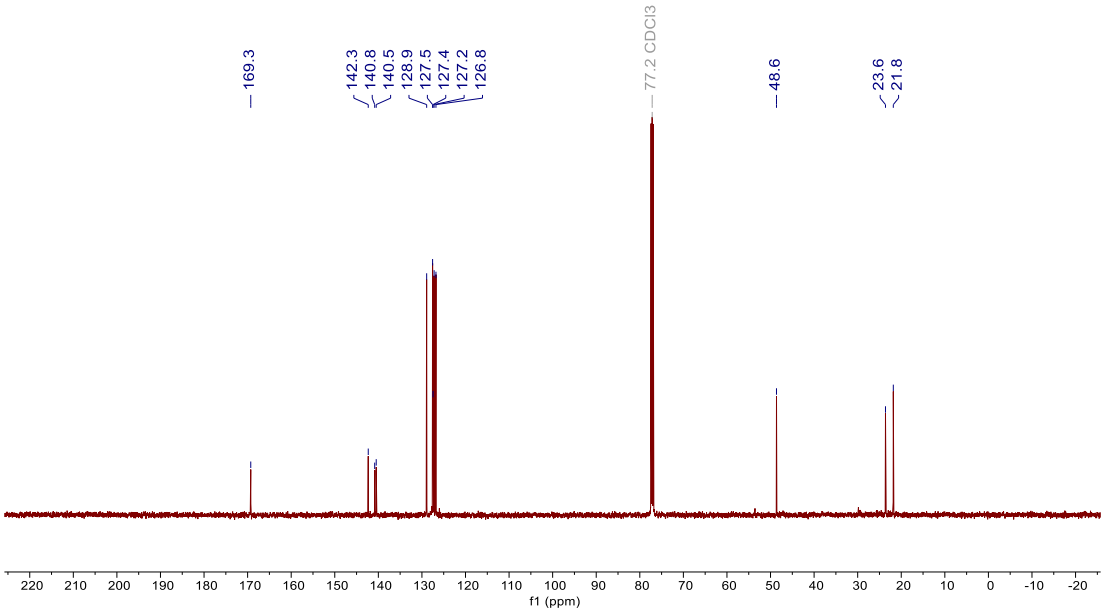
^{13}C NMR of compound **22** (126 MHz in $CDCl_3$)



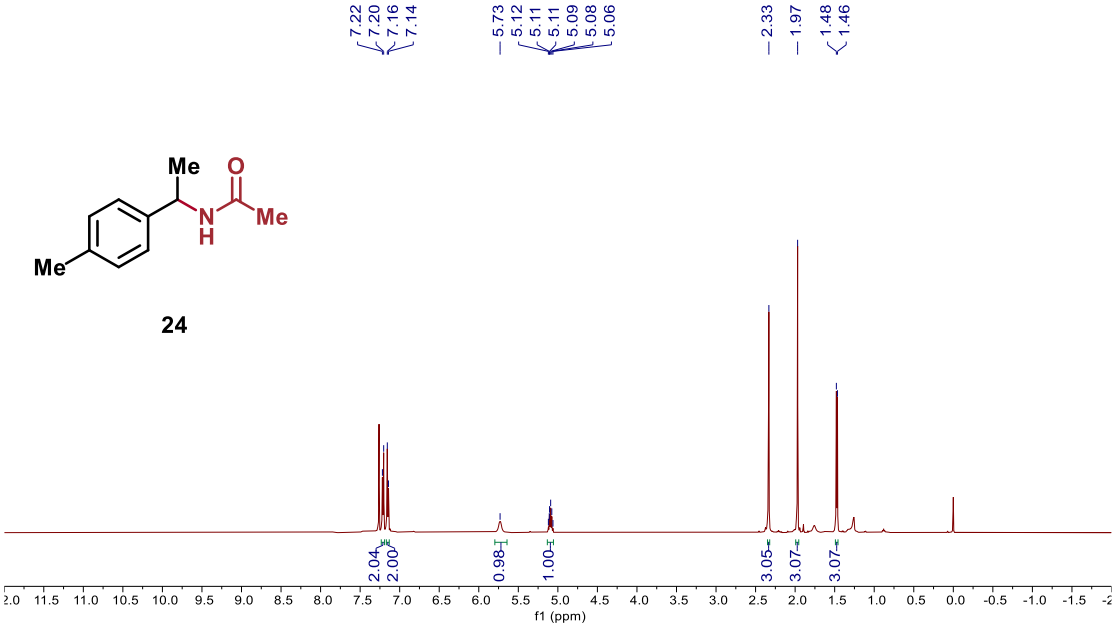
^{1}H NMR of compound **23** (500 MHz in $CDCl_3$)



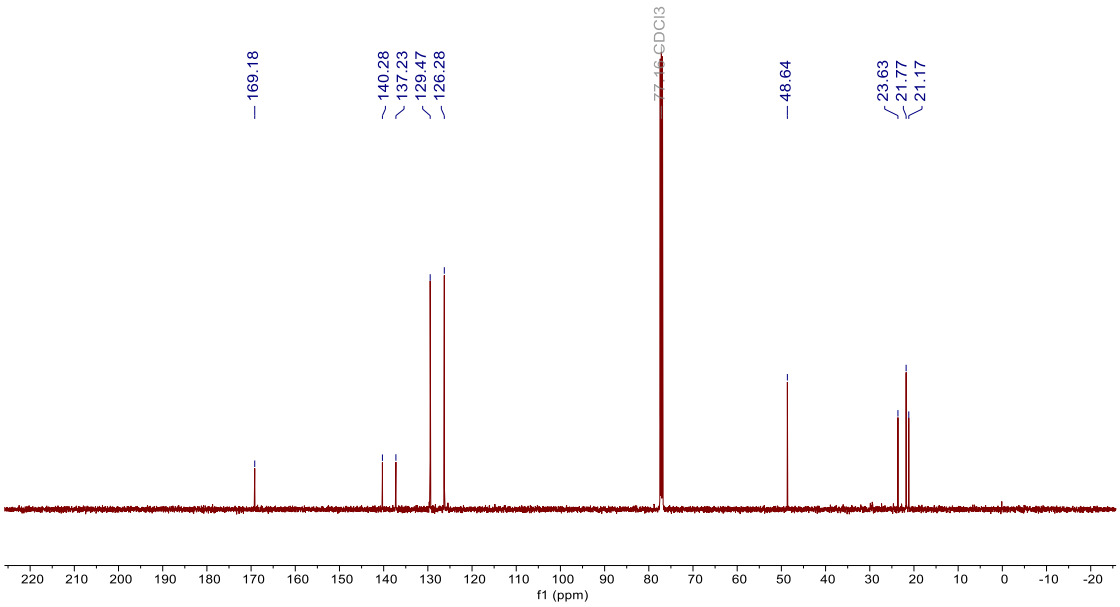
^{13}C NMR of compound **23** (126 MHz in $CDCl_3$)



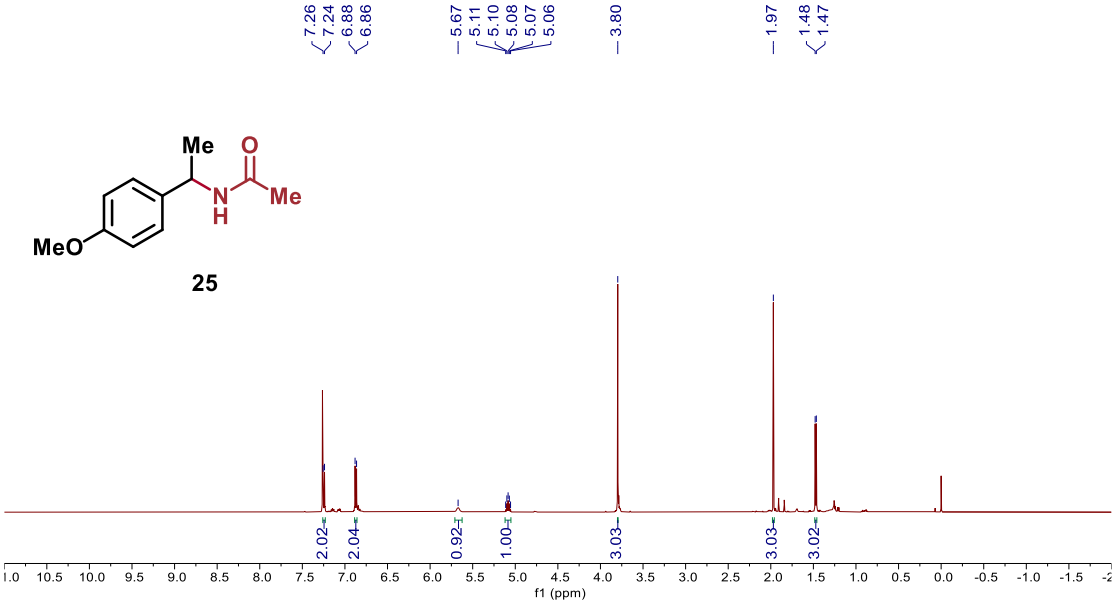
^{1}H NMR of compound **24** (500 MHz in $CDCl_3$)



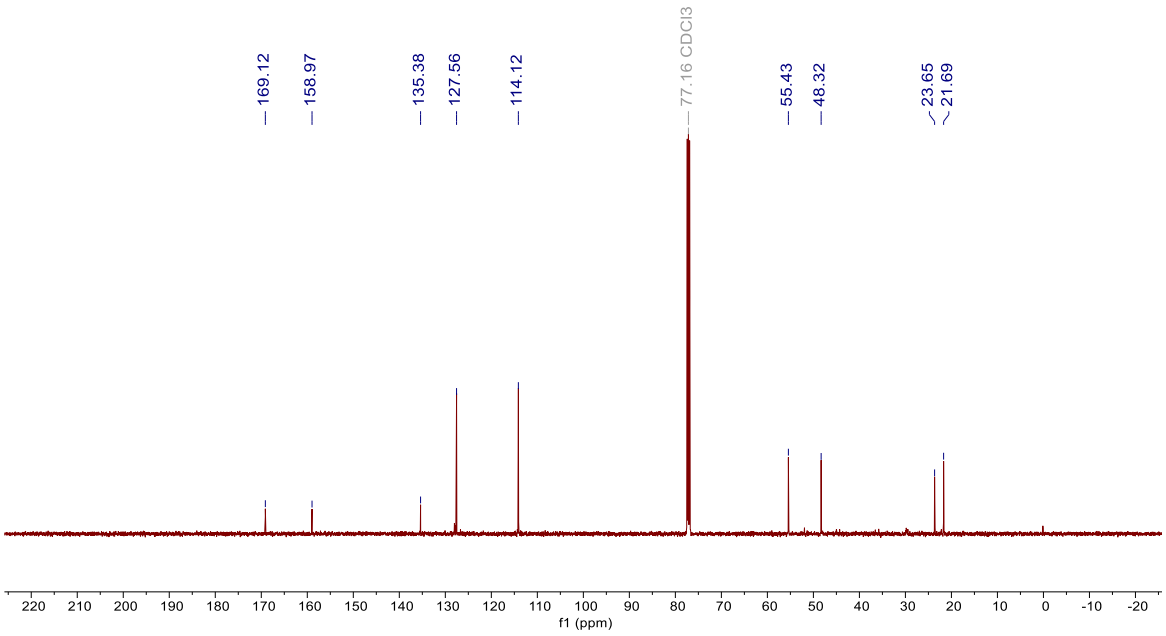
^{13}C NMR of compound **24** (126 MHz in $CDCl_3$)



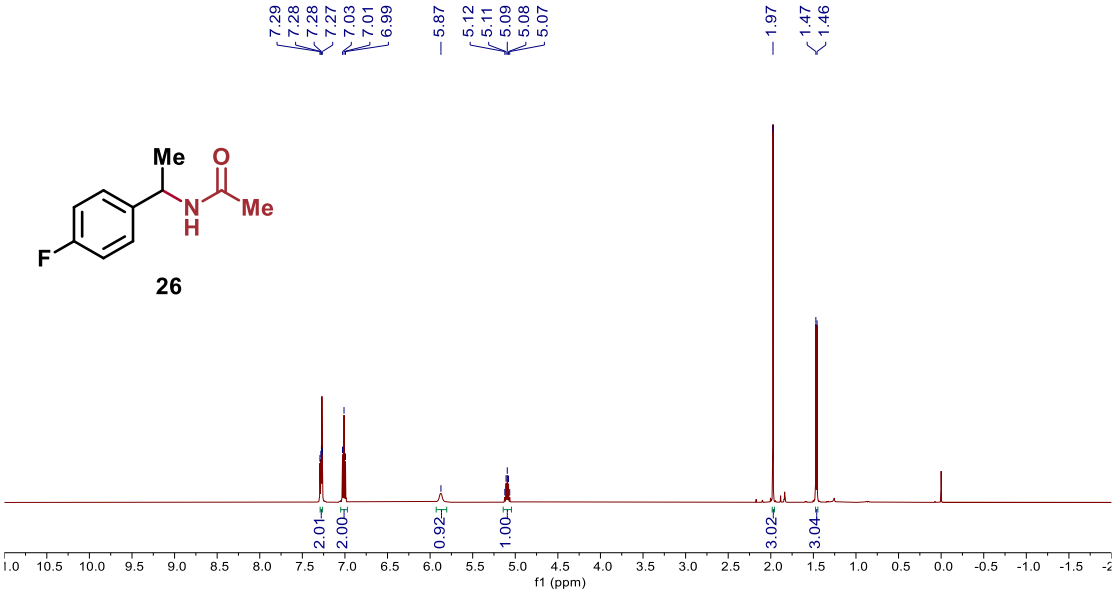
^{1}H NMR of compound **25** (500 MHz in $CDCl_3$)



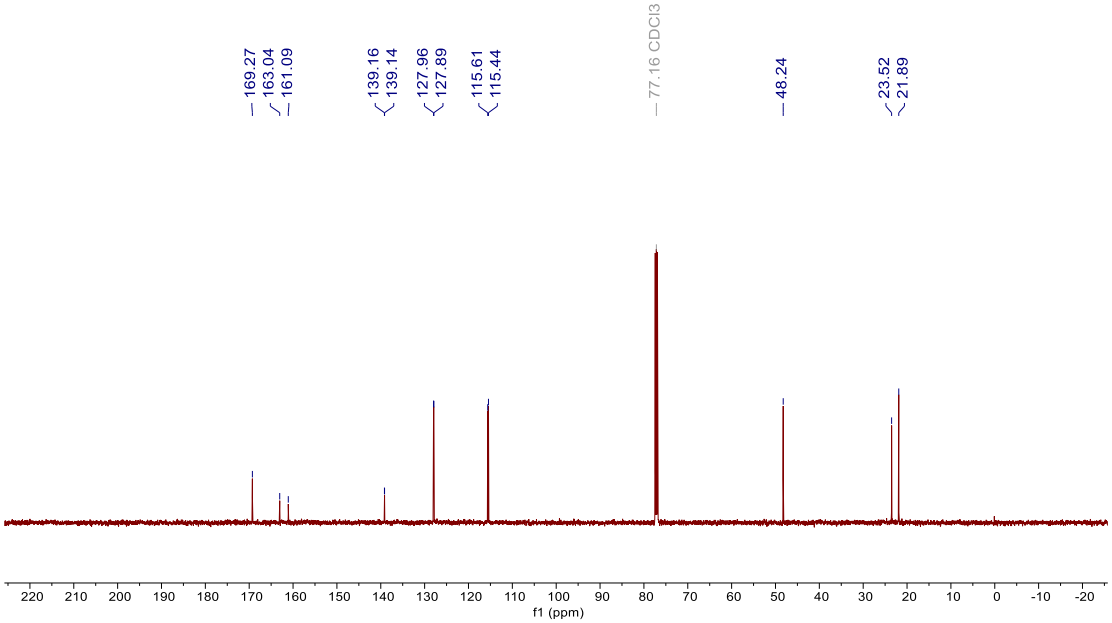
^{13}C NMR of compound **25** (126 MHz in $CDCl_3$)



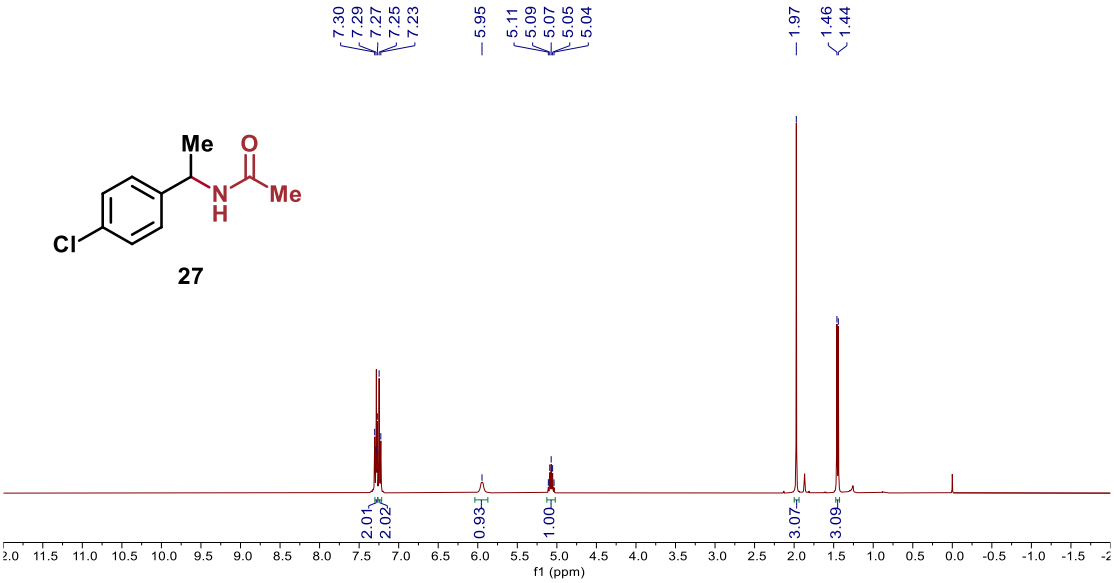
^{1}H NMR of compound **26** (500 MHz in $CDCl_3$)



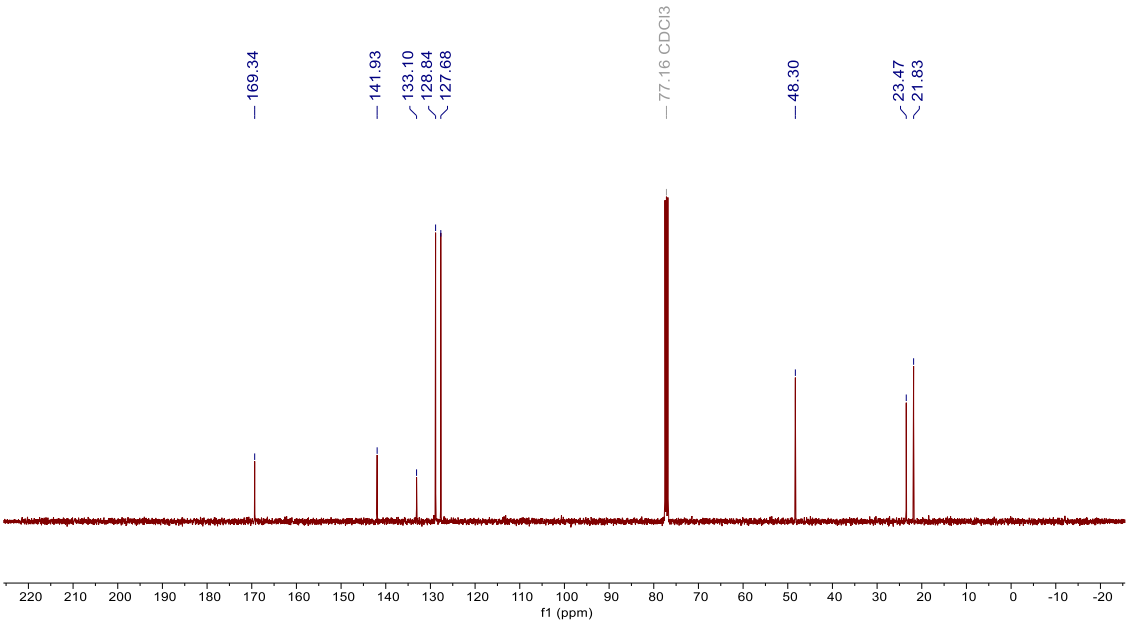
^{13}C NMR of compound **26** (126 MHz in $CDCl_3$)



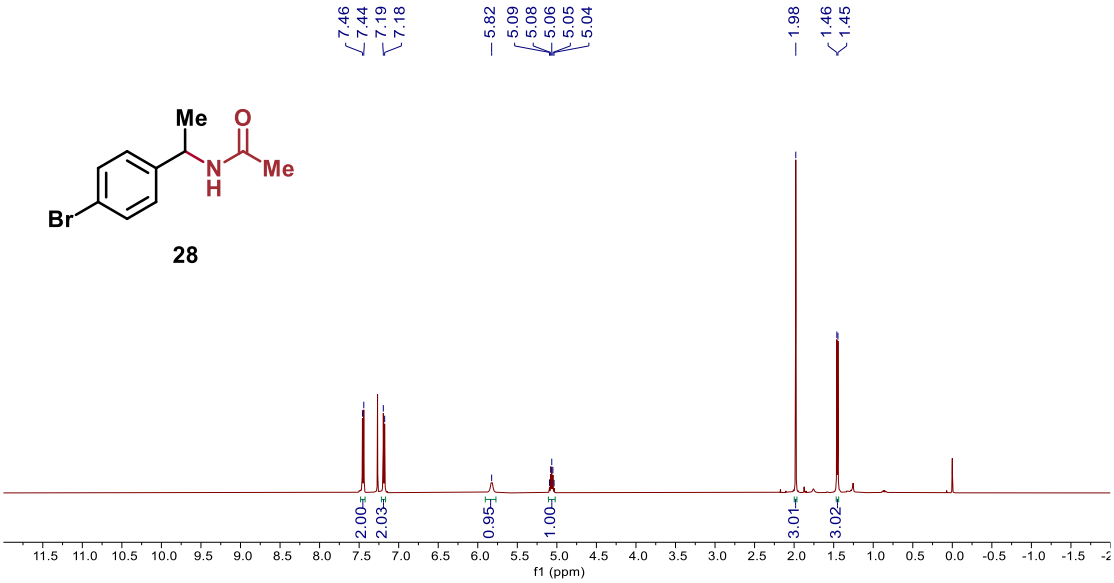
^{1}H NMR of compound **27** (500 MHz in $CDCl_3$)



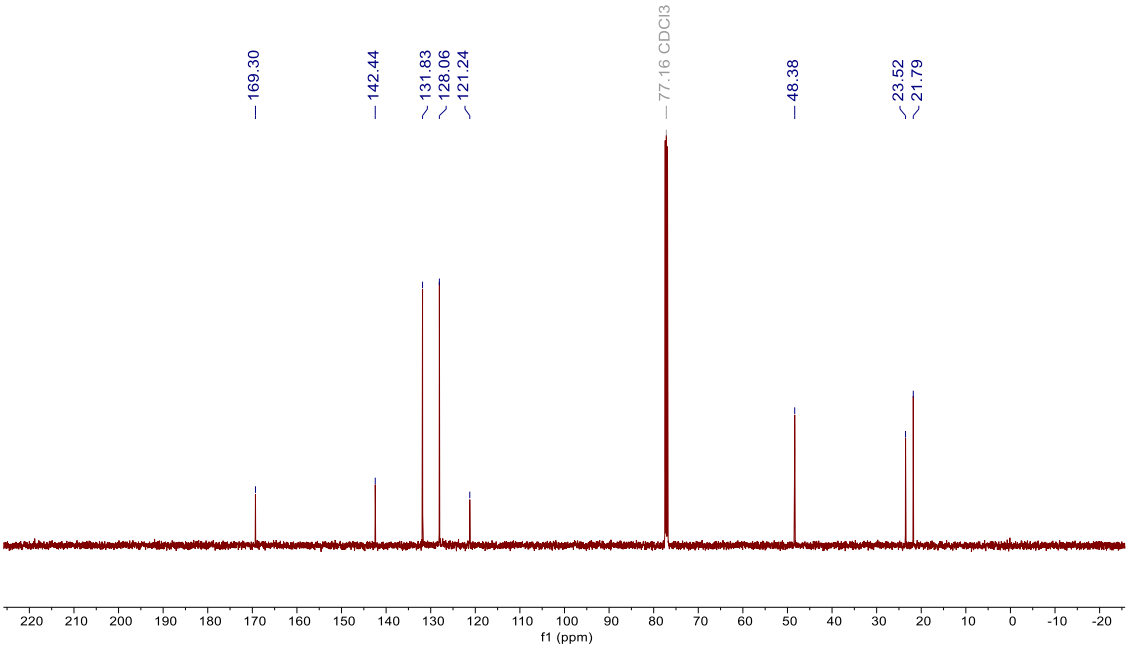
^{13}C NMR of compound **27** (126 MHz in $CDCl_3$)



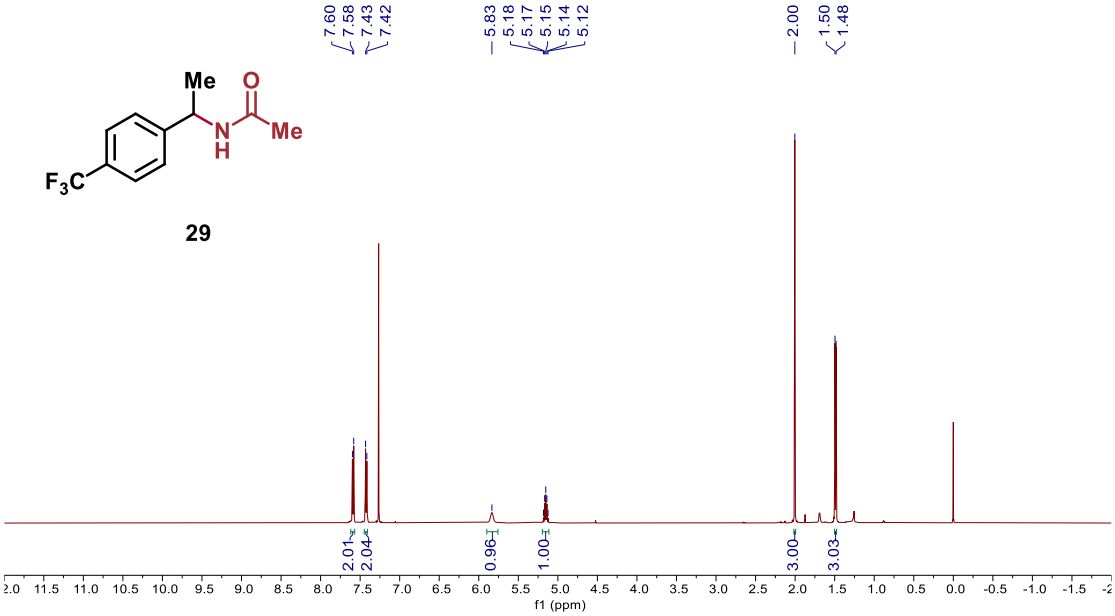
^{1}H NMR of compound **28** (500 MHz in $CDCl_3$)



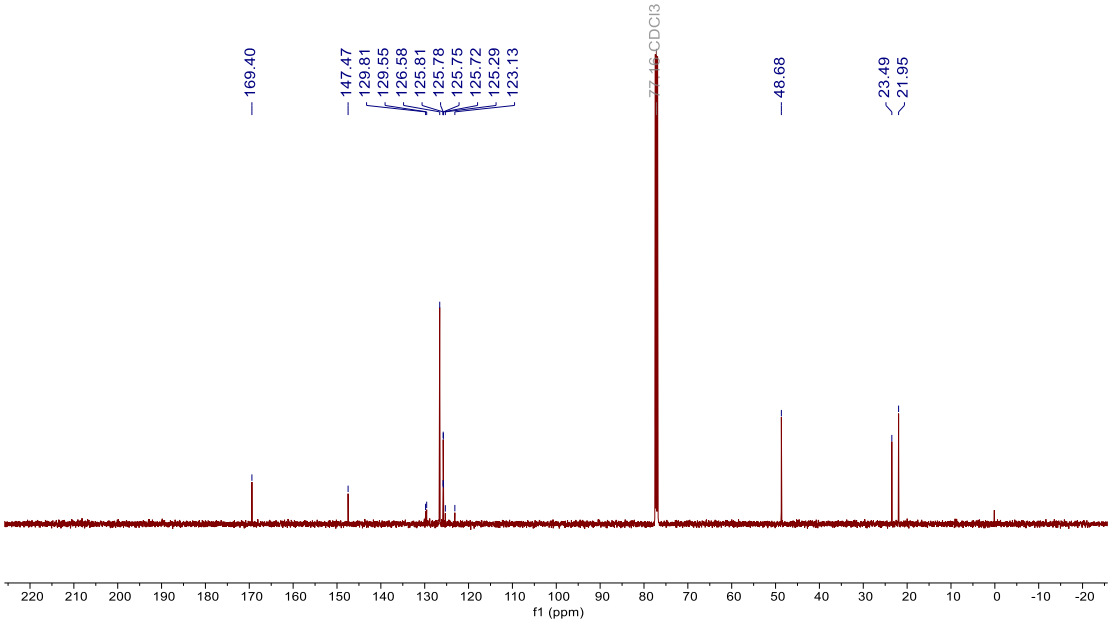
^{13}C NMR of compound **28** (126 MHz in $CDCl_3$)



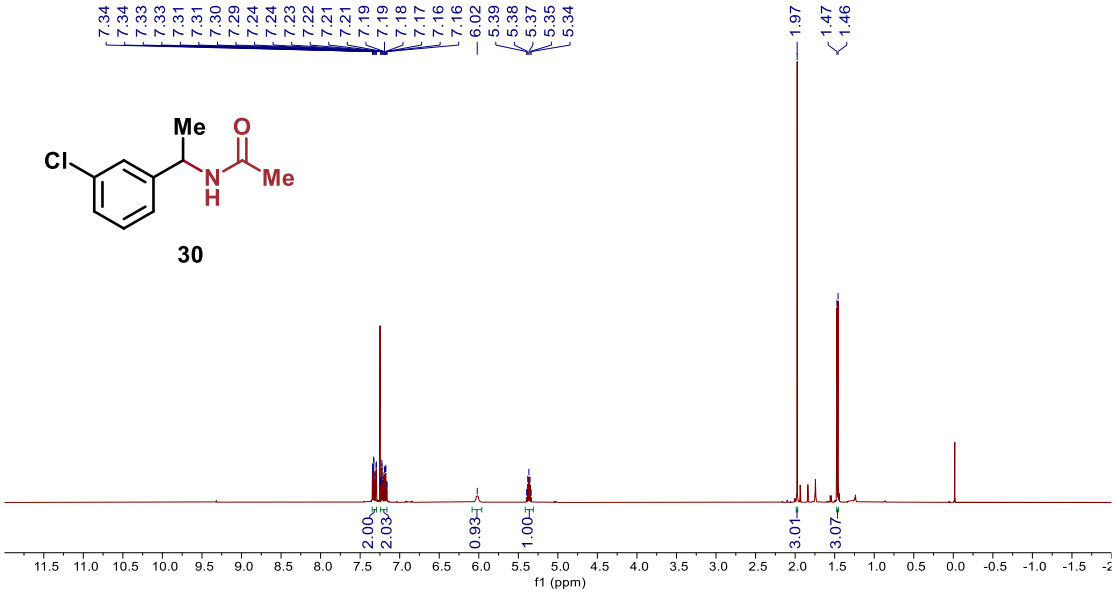
^{1}H NMR of compound **29** (500 MHz in $CDCl_3$)



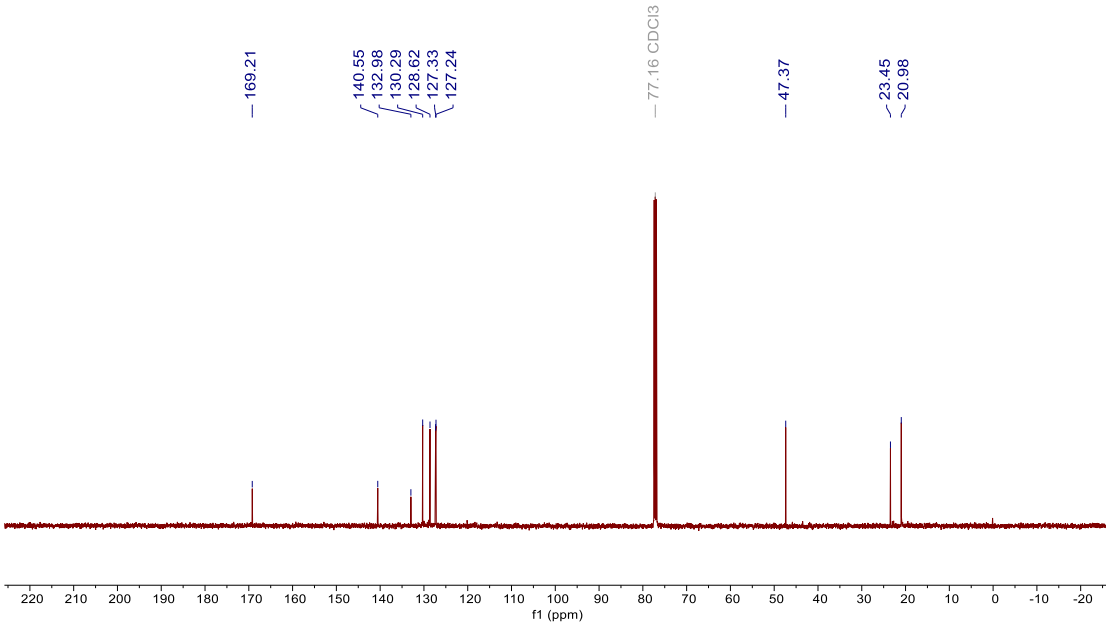
^{13}C NMR of compound **29** (126 MHz in $CDCl_3$)



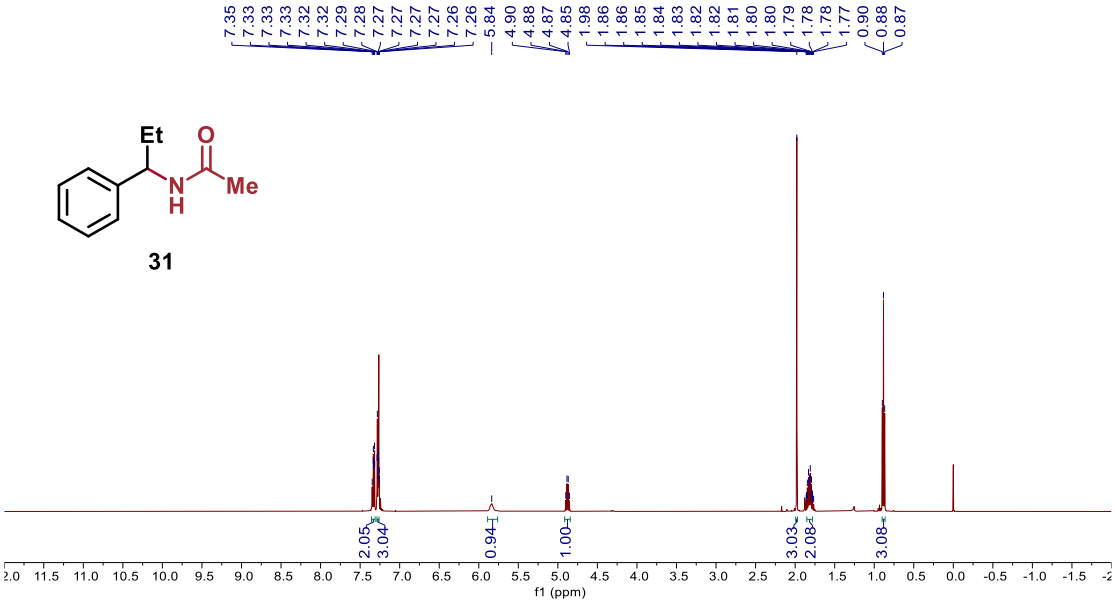
^{1}H NMR of compound **30** (500 MHz in $CDCl_3$)



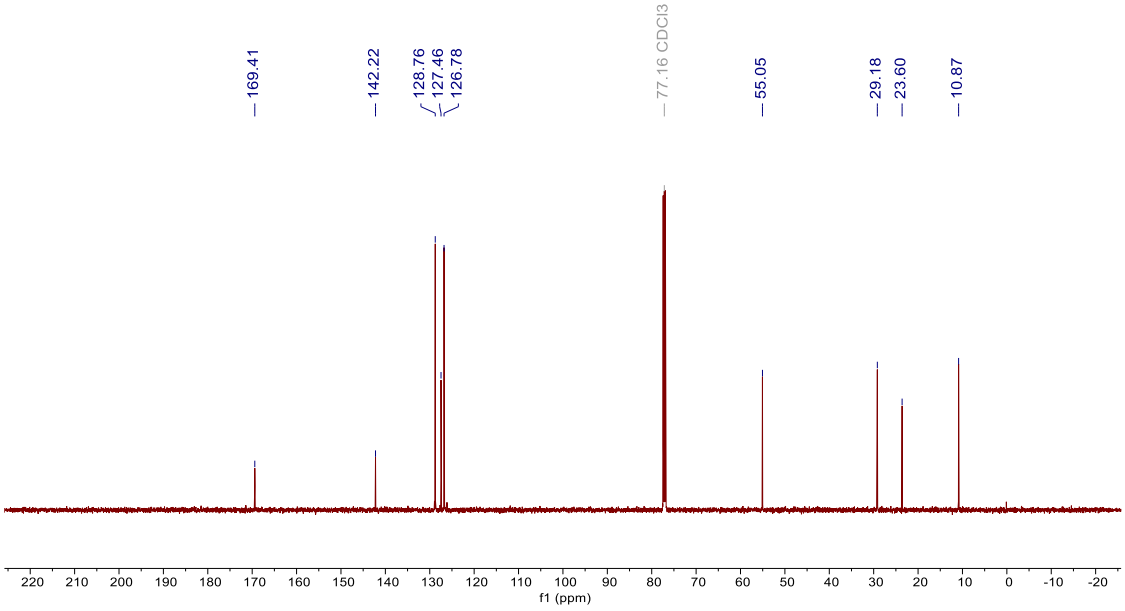
^{13}C NMR of compound **30** (126 MHz in $CDCl_3$)



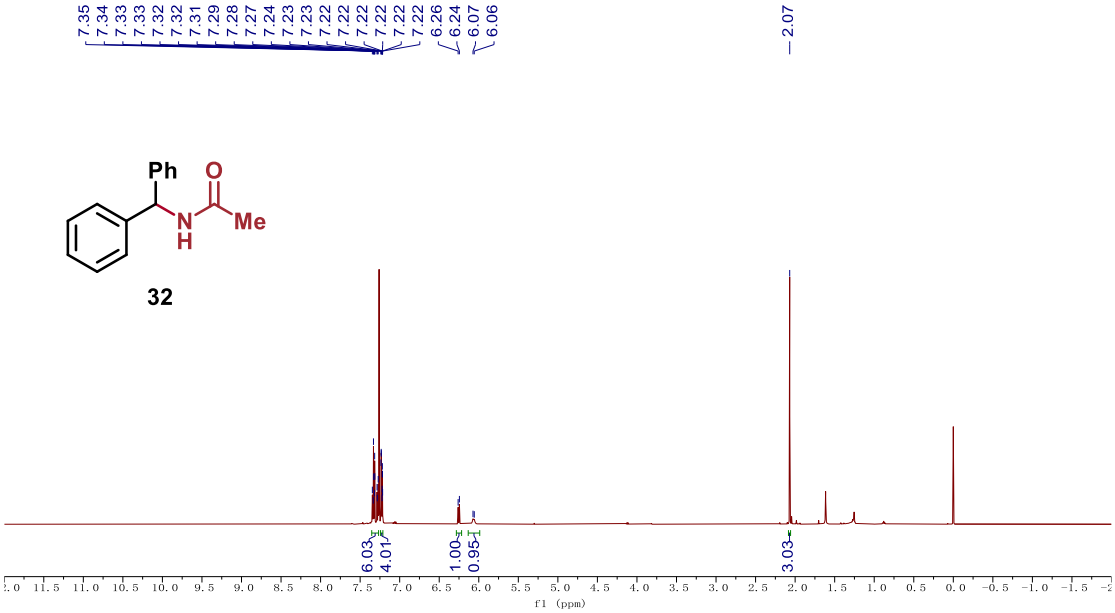
^{1}H NMR of compound **31** (500 MHz in $CDCl_3$)



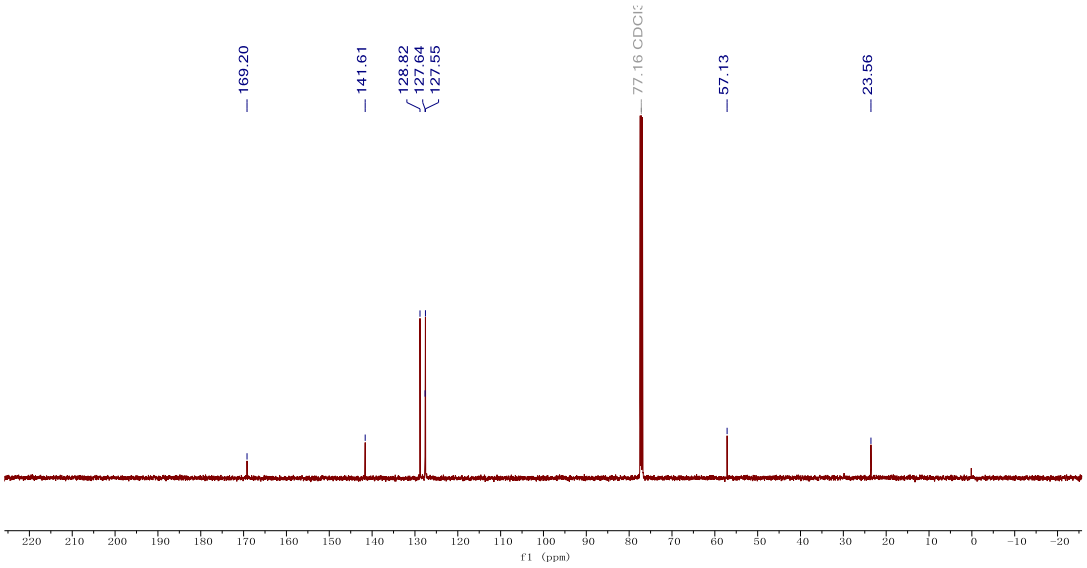
^{13}C NMR of compound **31** (126 MHz in $CDCl_3$)



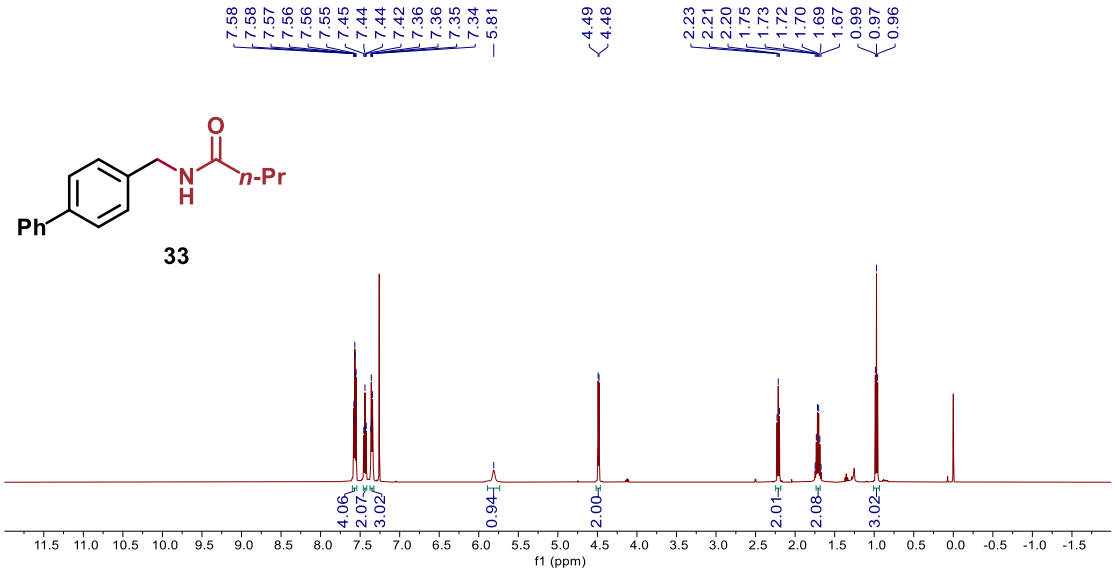
^{1}H NMR of compound **32** (500 MHz in $CDCl_3$)



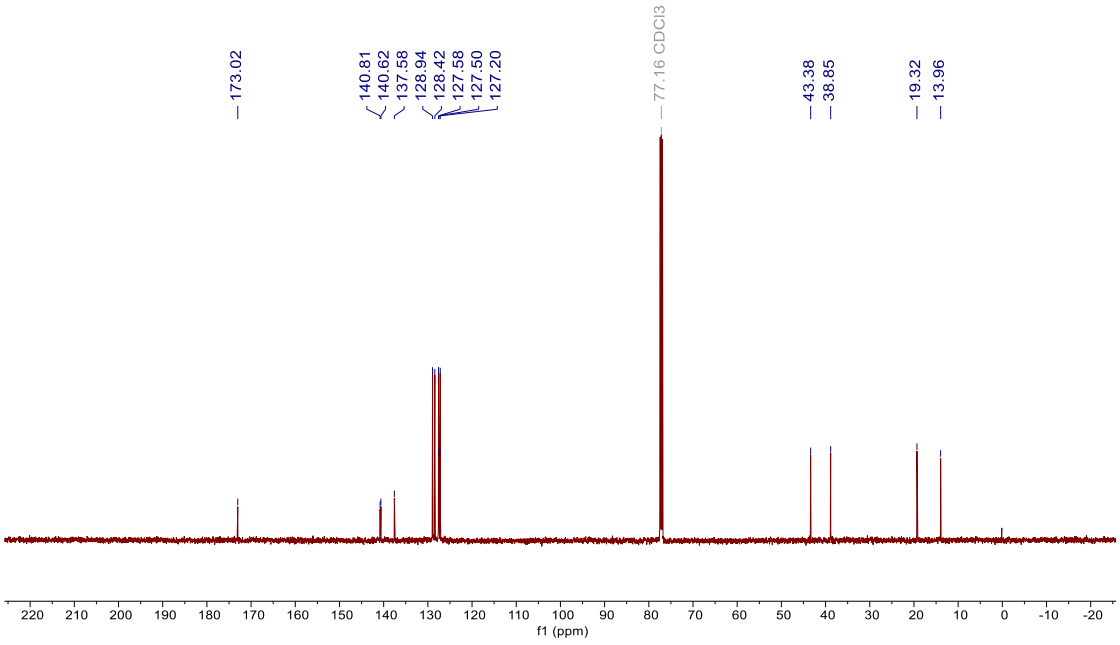
^{13}C NMR of compound **32** (126 MHz in $CDCl_3$)



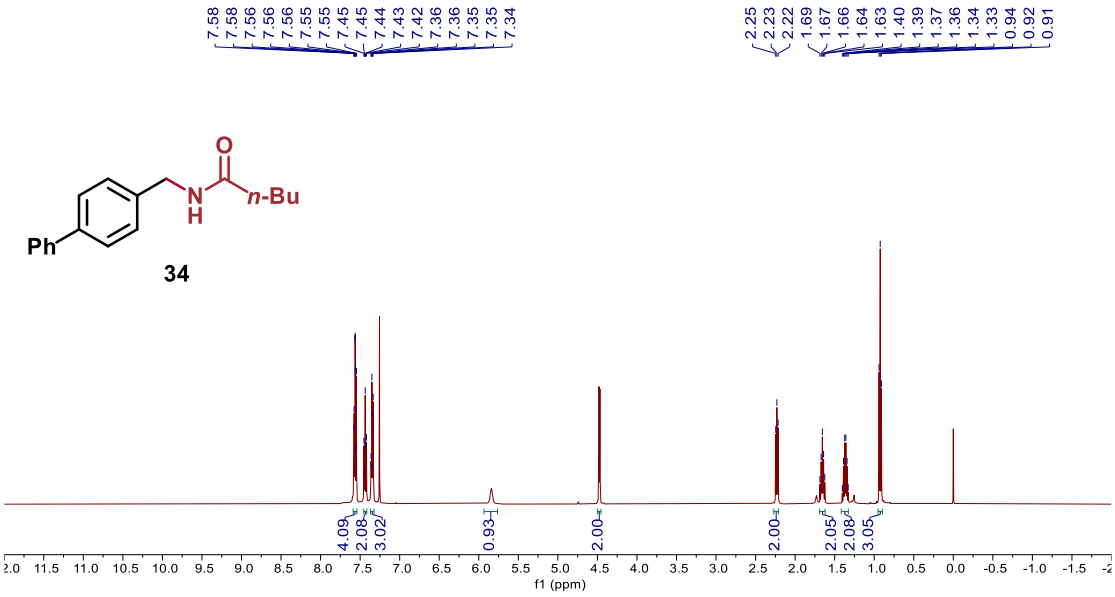
^{1}H NMR of compound **33** (500 MHz in $CDCl_3$)



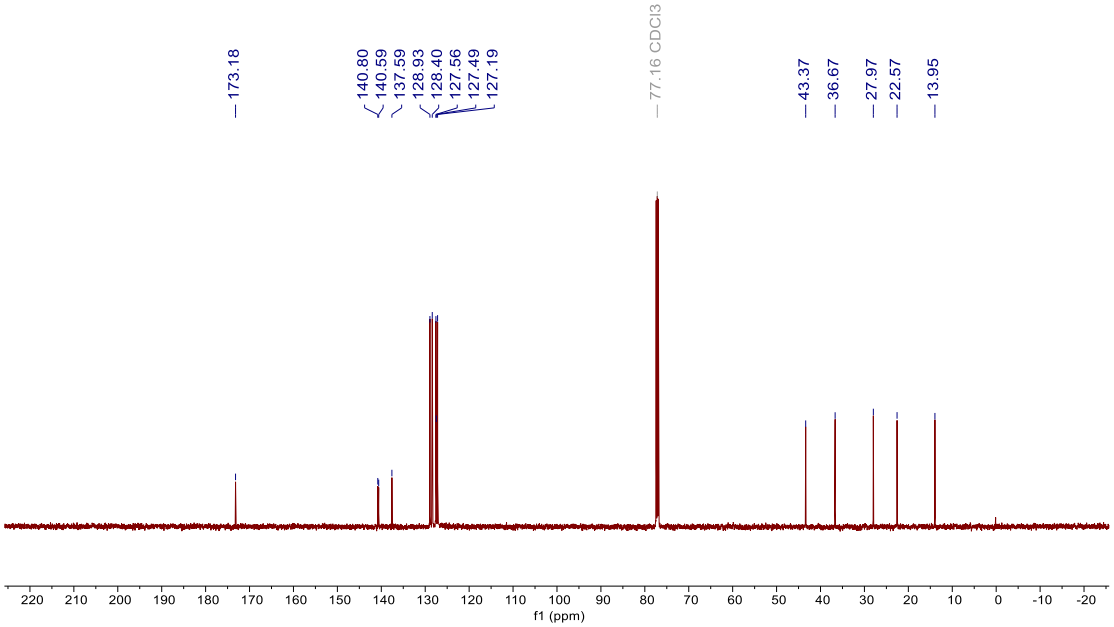
^{13}C NMR of compound **33** (126 MHz in $CDCl_3$)



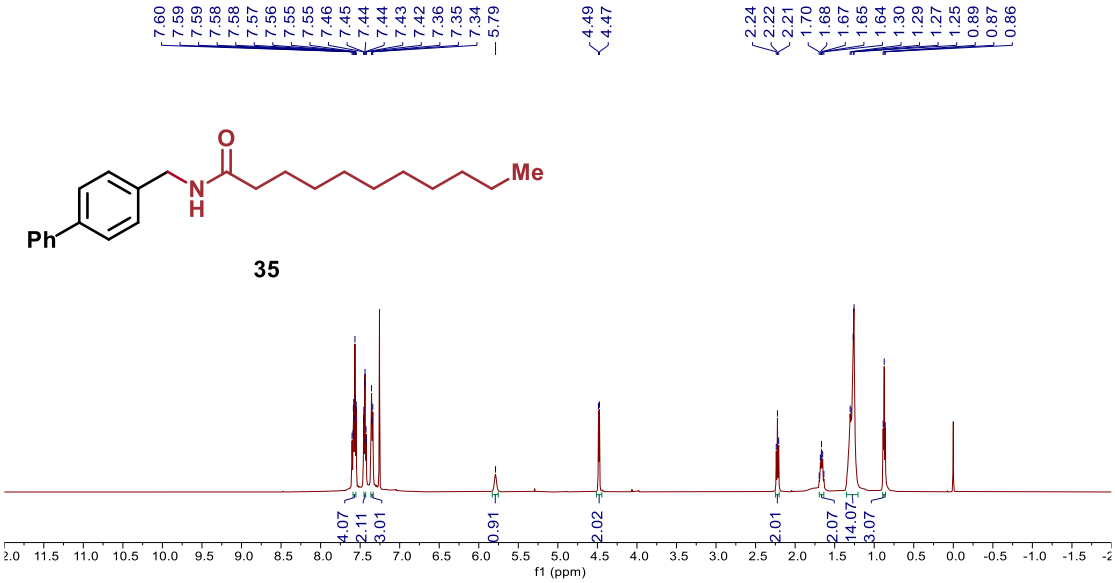
^{1}H NMR of compound **34** (500 MHz in $CDCl_3$)



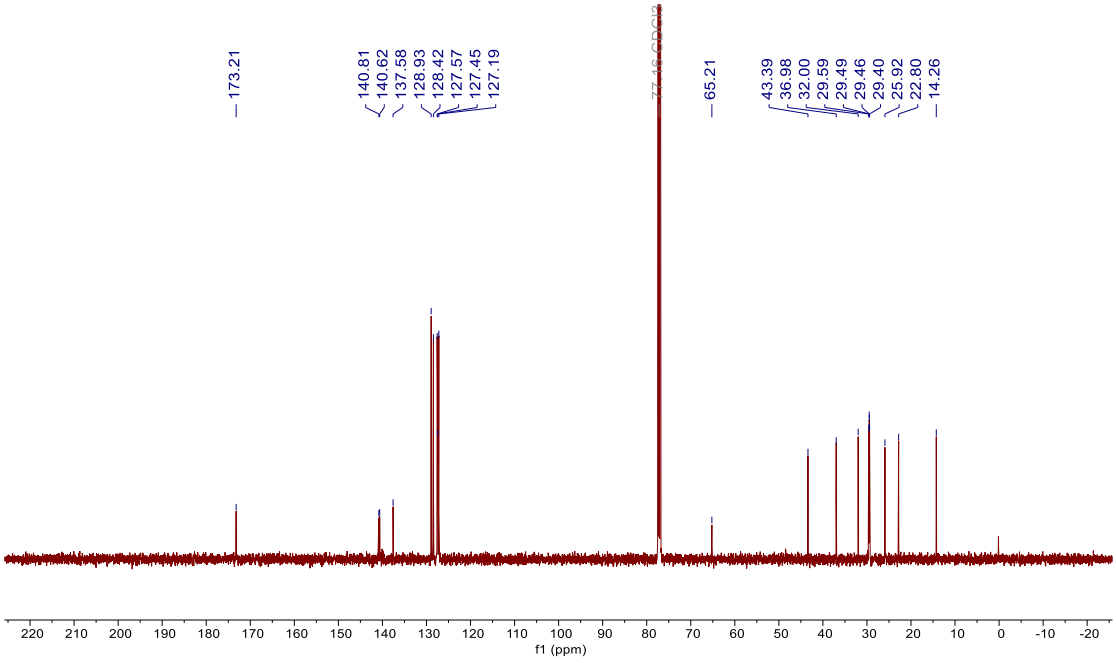
^{13}C NMR of compound **34** (126 MHz in $CDCl_3$)



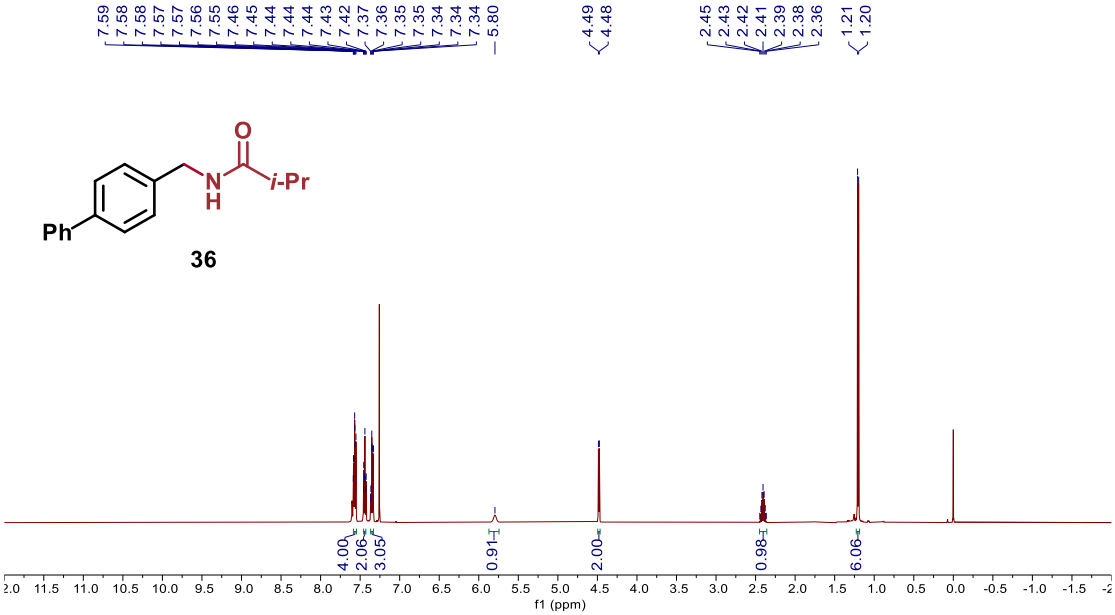
^{1}H NMR of compound **35** (500 MHz in $CDCl_3$)



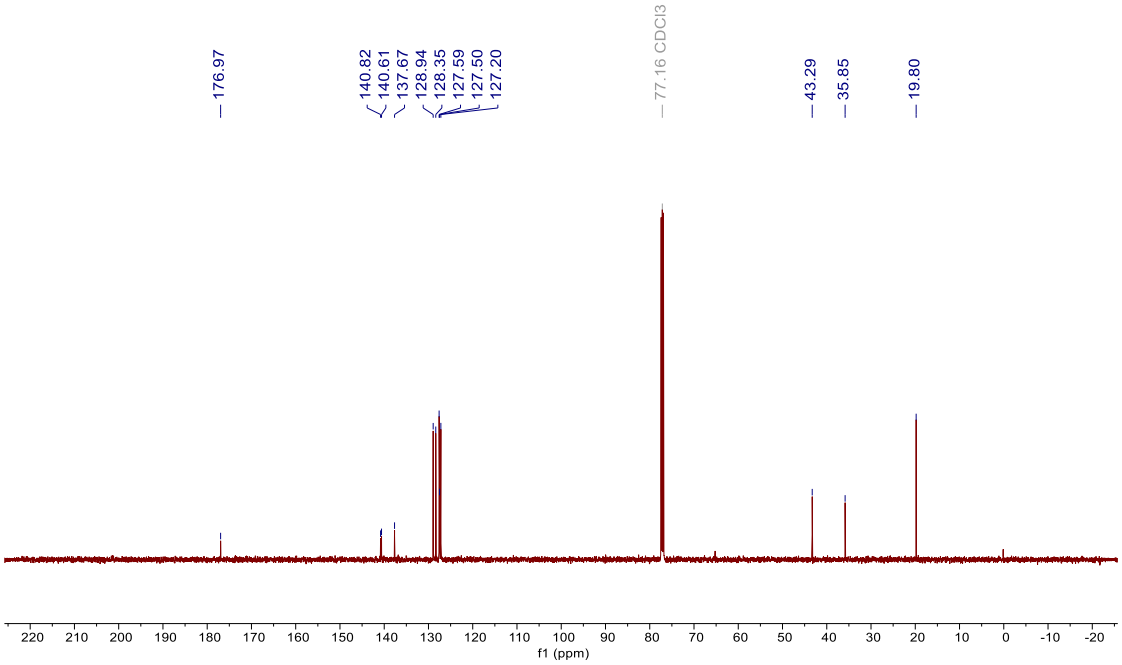
^{13}C NMR of compound **35** (126 MHz in $CDCl_3$)



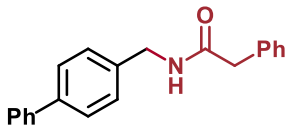
^{1}H NMR of compound **36** (500 MHz in $CDCl_3$)



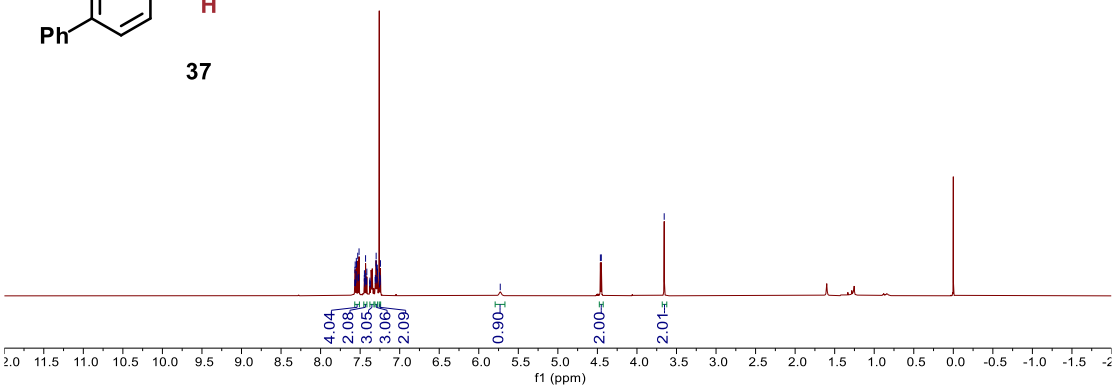
^{13}C NMR of compound **36** (126 MHz in $CDCl_3$)



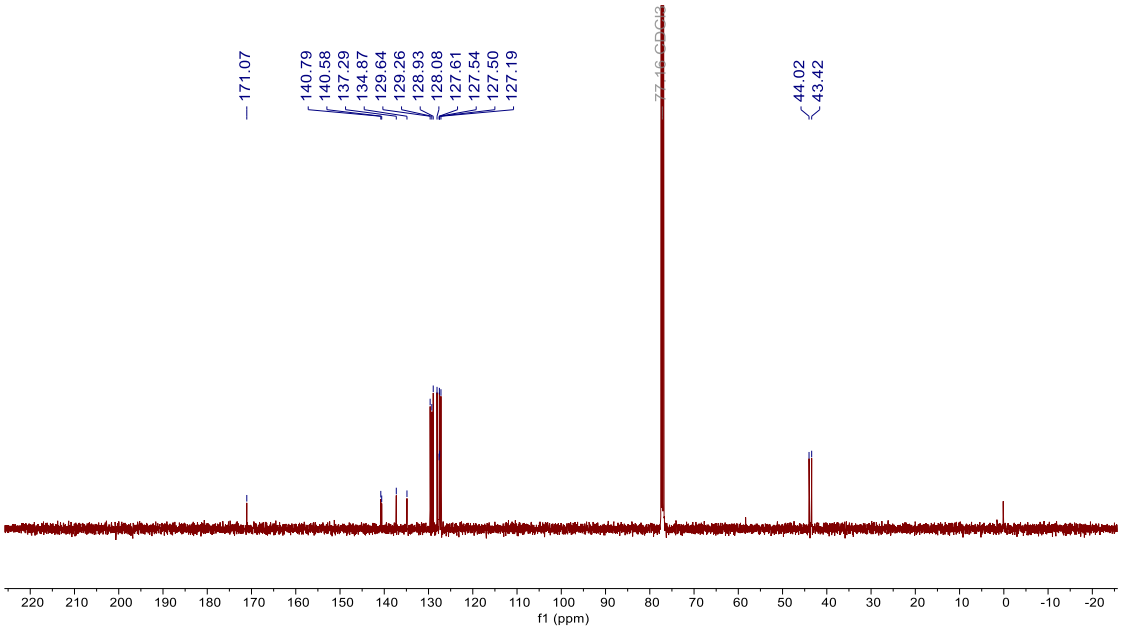
^{1}H NMR of compound **37** (500 MHz in $CDCl_3$)



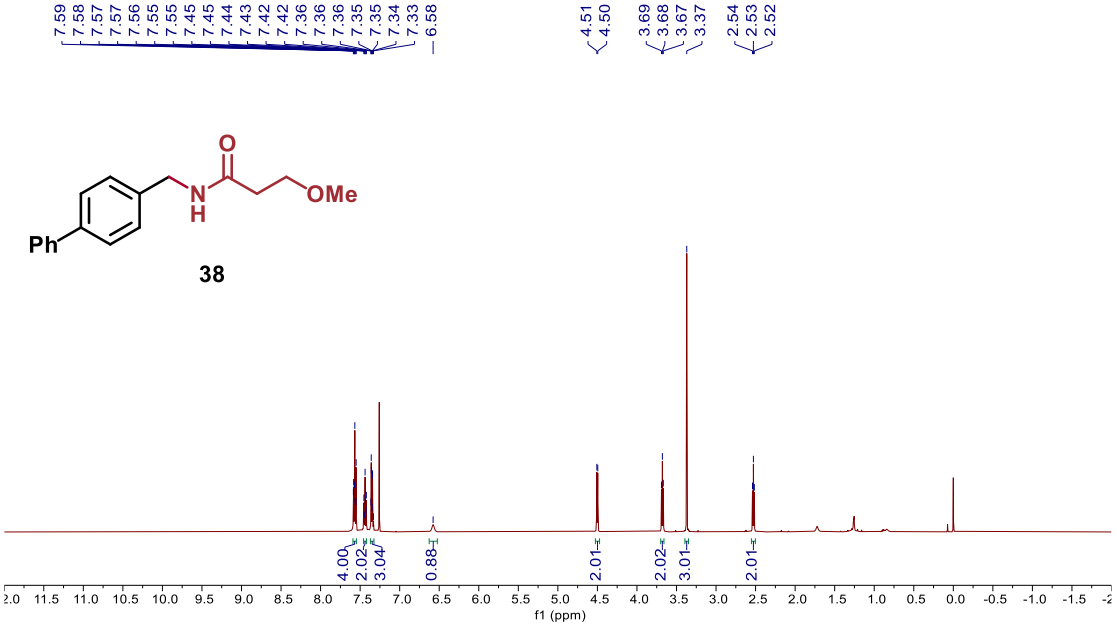
37



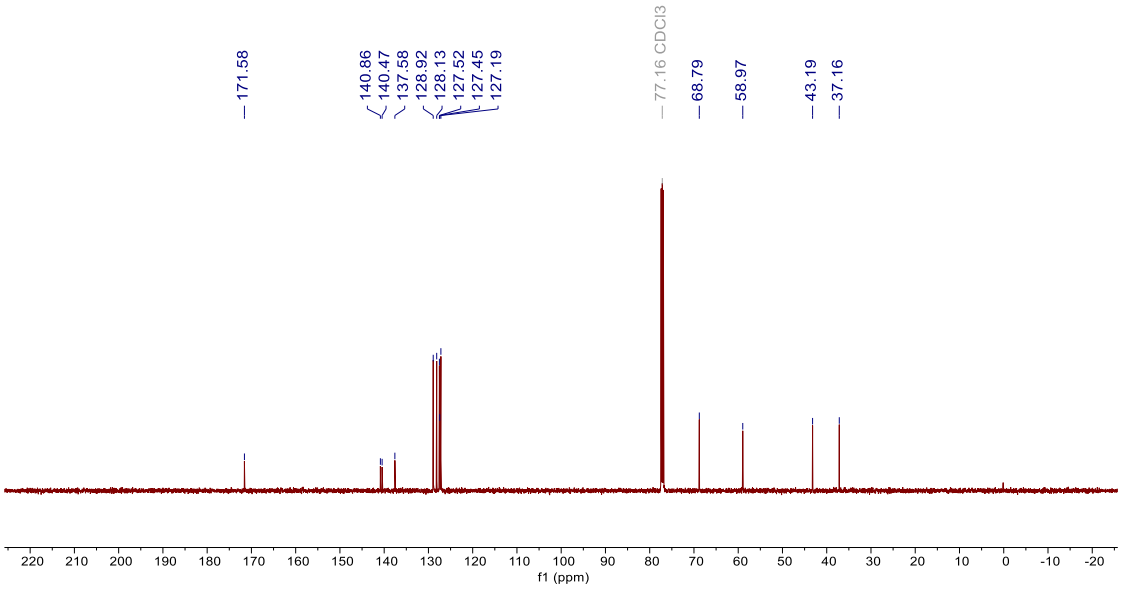
^{13}C NMR of compound **37** (126 MHz in $CDCl_3$)



^{1}H NMR of compound **38** (500 MHz in $CDCl_3$)



^{13}C NMR of compound **38** (126 MHz in $CDCl_3$)



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