Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Facile and Practical Hydrodehalogenations of Organic Halides Enabled by Calcium Hydride and Palladium Chloride

Jingjing Gui,[+,a] Xin Cai,[+,a] Lingyun Chen,[+,a] Yuxin Zhou,[+,a] Wenjing Zhu,[a] Yuanrui Jiang,[a] Min Hu,[a] Xiaobei Chen,[b,*] Yanwei Hu[a,*] and Shilei Zhang [a,*]

[a]Jiangsu Key Laboratory of Neuropsychiatric Diseases and College of Pharmaceutical Sciences, Soochow University, 199 Ren'ai Road, Suzhou, Jiangsu, 215123, China

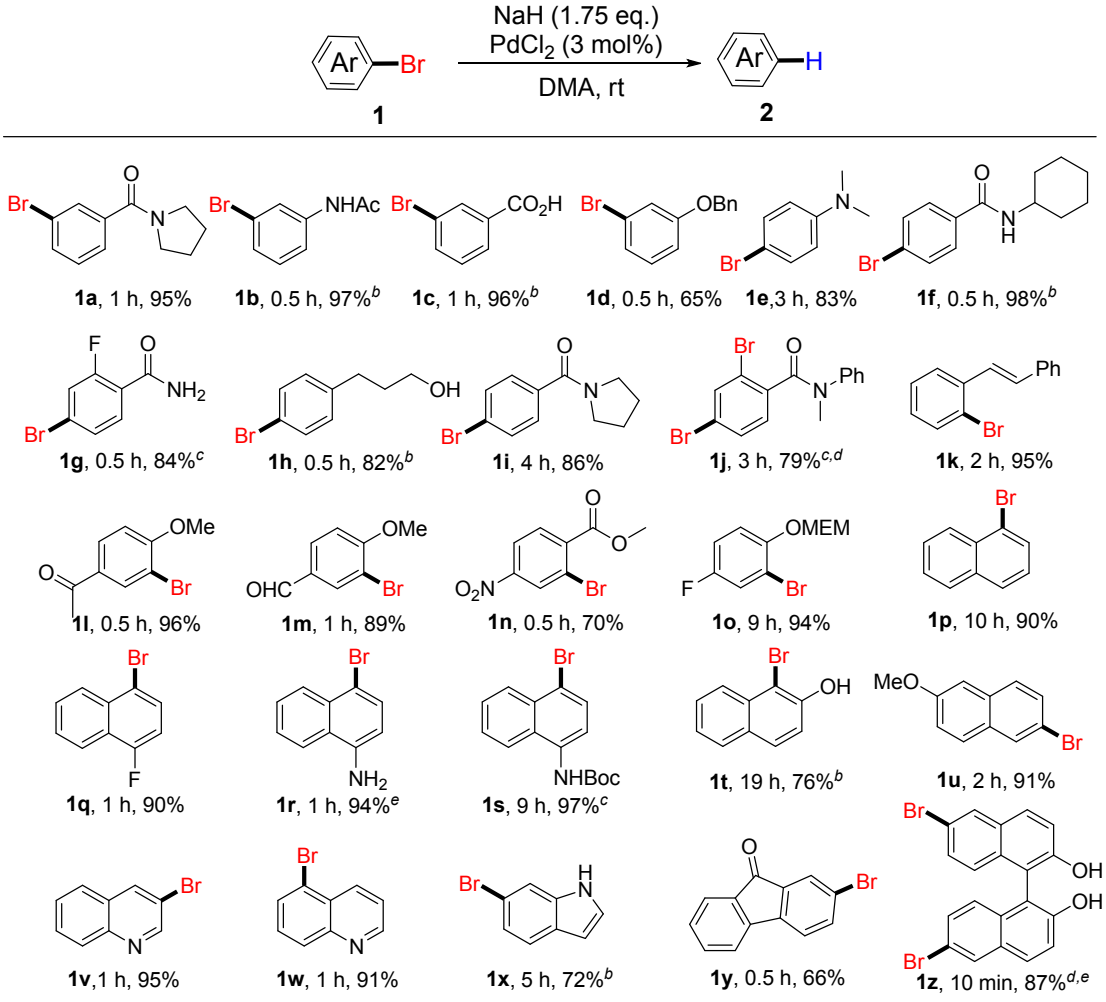
[b]State Key Laboratory of Bioreactor Engineering, and Shanghai Key Laboratory of New Drug Design, School of Pharmacy, East China University of Science & Technology, Shanghai 200237, China

1. General Information

^{1}H and ^{13}C NMR spectra were obtained from a solution in $CDCl_3$ or d^6-DMSO with TMS as internal standard using a 600/151 MHz ($^{1}H/^{13}C$) or 400/101 MHz ($^{1}H/^{13}C$) spectrometer. Spin multiplicity are reported as singlet (s), doublet (d), triplet (t), doublet of doublet (dd) and multiplet (m). Coupling constant *J* is given in Hertz (Hz). Mass spectra were obtained in ESI mode. High-resolution mass spectra (HRMS) were obtained on a Q Exactive Plus orbitrap mass analyzer (Thermo Fisher Scientific) and are given in m/z. Chemicals, reagents and solvents were purchased from commercial suppliers and used without special instructions. Thin layer chromatography (TLC) was performed on silica gel HSGF254 plates. Column chromatography was performed using 200-300 Mesh silica gel. Visualization of spots on TLC plate was accomplished with UV light (254 nm).

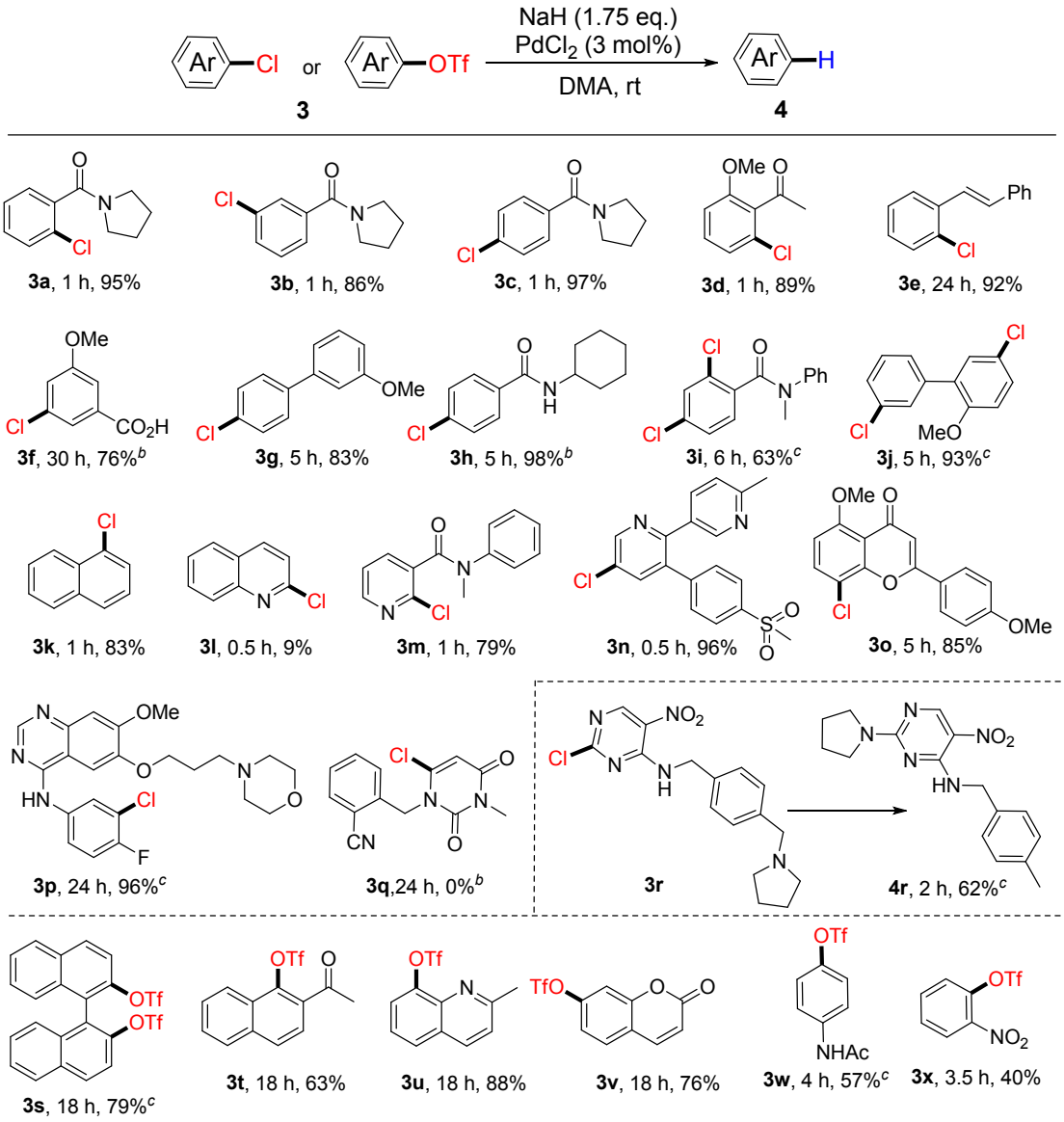
2. The use of NaH for hydrodehalogenation

Scheme S1 Scope of hydrodehalogenation of aryl bromides.[a]



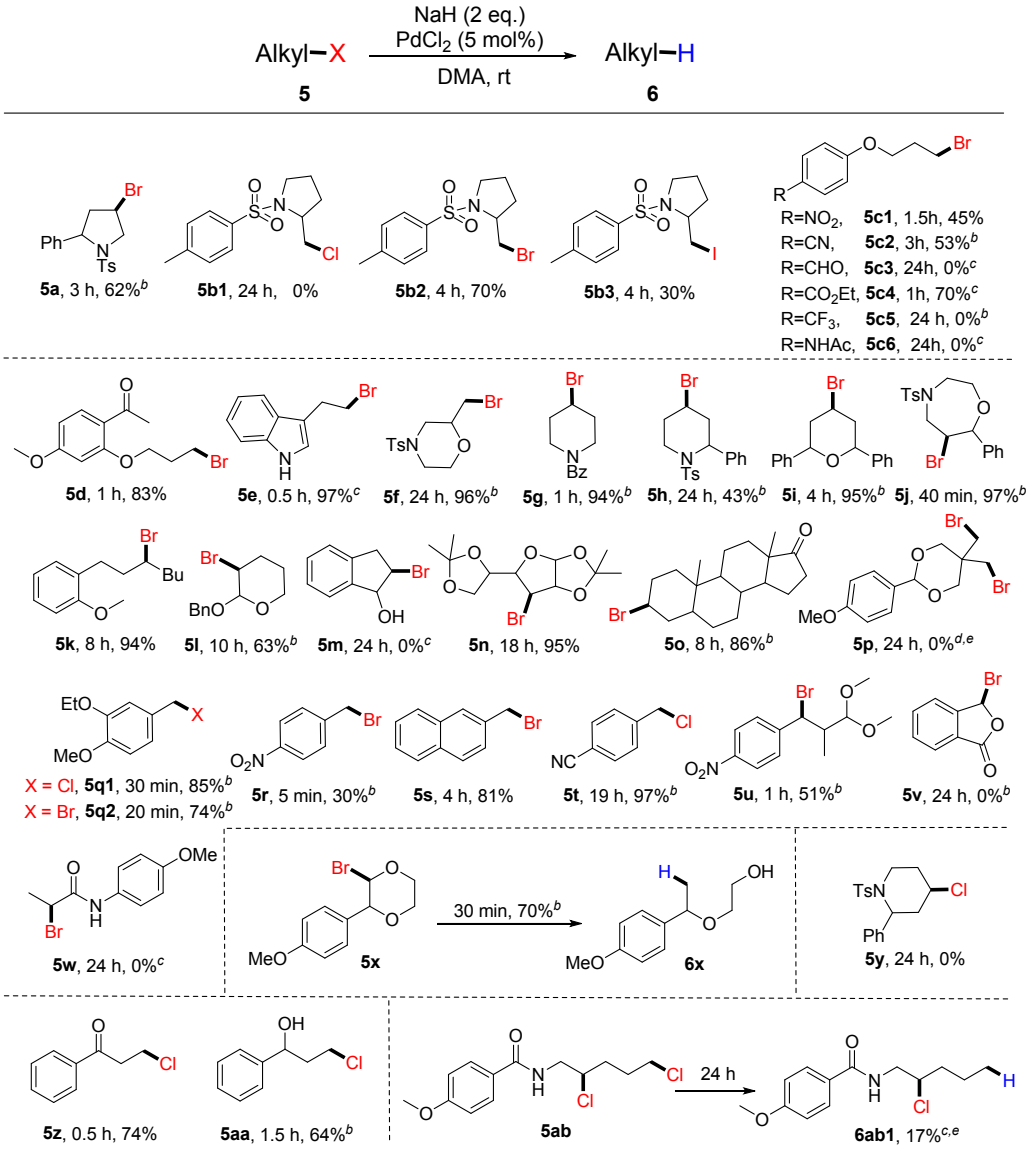
[a]Reaction conditions unless otherwise specified: NaH (0.875 mmol, 1.75 equiv.) and $PdCl_2$ (0.015 mmol, 3 mol %) in DMA (0.5 mL) was stirred for 5 min under N_2 before **1** (0.5 mmol) in DMA (0.5 mL) was added, and then the reaction was stirred at rt for the specified time. [b]NaH (3.0 equiv.) was used. [c]NaH (4.0 equiv.) was used. [d]$PdCl_2$ (10 mol %) was used. [e]NaH (5.0 equiv.) was used.

Scheme S2 Scope of hydrodehalogenation of aryl chlorides and aryl triflates.[a]



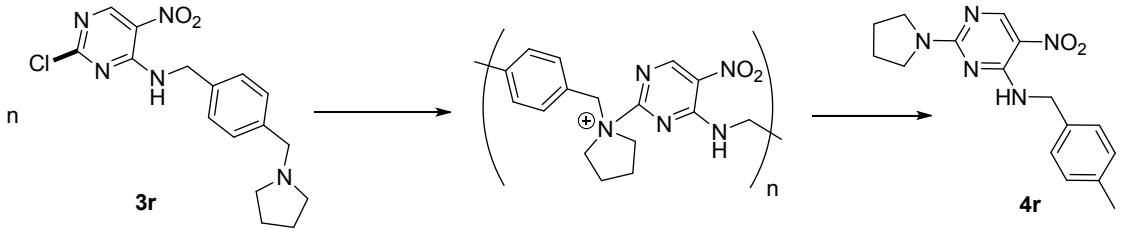
[a]Reaction conditions unless otherwise specified: NaH (0.875 mmol, 1.75 equiv.) and $PdCl_2$ (0.015 mmol, 3 mol %) in DMA (0.5 mL) was stirred for 5 min under N_2 before **3** (0.5 mmol) in DMA (0.5 mL) was added, and then the reaction was stirred at rt for the specified time. [b]NaH (3.0 equiv.) was used. [c]NaH (4.0 equiv.) and $PdCl_2$ (10 mol %) were used.

Scheme S3 Scope of hydrodehalogenation of alkyl halides.

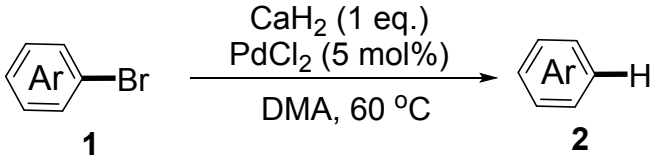


[a]Reaction conditions unless otherwise specified: NaH (1.0 mmol, 2.0 equiv.) and $PdCl_2$ (0.025 mmol, 5 mol %) in DMA (0.5 mL) was stirred for 5 min under N_2 before **5** (0.5 mmol) in DMA (0.5 mL) was added, and then the reaction was stirred at rt for the specified time. [b]NaH (3.0 equiv.) was used. [c]NaH (4.0 equiv.) was used. [d]NaH (6.0 equiv.) was used. [e]$PdCl_2$ (10 mol %) was used.

3. The proposed mechanism for the generation of product 4r

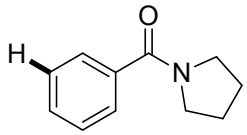


4. General procedure for hydrodehalogenation of aryl bromides



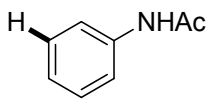
1 **2**

A mixture of $PdCl_2$ (4.4 mg, 0.025 mmol, 5 mol %) and calcium hydride (21 mg, 0.5 mmol, 1 equiv) in DMA (0.5 mL) was stirred for 5 min under N_2 before **1** (0.5 mmol) in DMA (0.5 mL) was added through syringe, and the mixture was stirred at 60 °C for the specified time. After the reaction was completed monitored with TLC, a saturated NH_4Cl aqueous solution was added to quench the reaction and the resulting mixture was extracted with EtOAc. The combined organic layers were washed with water and brine and dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography to give desired product **2**.



2a

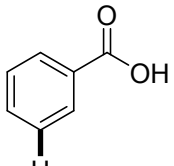
Phenyl(pyrrolidin-1-yl)methanone (**2a**). The title compound was prepared according to the general procedure at 60 °C for 11 h, as described above in 96% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (dd, *J* = 7.0, 2.5 Hz, 2H), 7.41 – 7.30 (m, 3H), 3.64 (t, *J* = 7.0 Hz, 2H), 3.41 (t, *J* = 6.6 Hz, 2H), 1.94 (dd, *J* = 13.6, 6.6 Hz, 2H), 1.86 (dd, *J* = 13.0, 6.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 137.3, 129.8, 128.3, 127.1, 49.7, 46.2, 26.5, 24.5. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{11}H_{14}NO$ 176.1, found 176.1.



2b

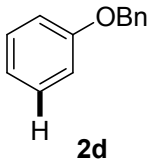
***N*-Phenylacetamide (2b)**. The title compound was prepared according to the general

procedure (1.5 equiv of CaH_2 was used) at 60 °C for 4 h, as described above in 96% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.8 Hz, 2H), 7.41 (s, 1H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.10 (t, *J* = 7.2 Hz, 1H), 2.17 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.8, 168.8, 138.1, 129.0, 124.4, 120.2, 120.1, 24.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_8H_{10}NO$ 136.1, found 136.1.



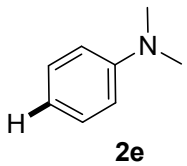
2c

Benzoic acid (2c). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 13 h, as described above in 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 7.5 Hz, 2H), 7.63 (t, *J* = 7.3 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.7, 134.0, 130.3, 129.5, 128.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_7H_7O_2$ 123.0, found 123.1.



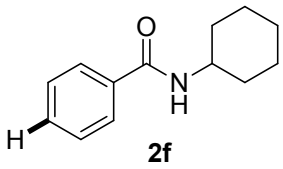
2d

(Benzyloxy)benzene (2d). The title compound was prepared according to the general procedure at 60 °C for 23 h, as described above in 62% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.44 (m, 2H), 7.44 – 7.38 (m, 2H), 7.37 – 7.27 (m, 3H), 7.05 – 6.95 (m, 3H), 5.09 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.9, 137.2, 129.6, 128.7, 128.1, 127.6, 121.1, 115.0, 70.0. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{13}H_{13}O$ 185.1, found 185.1.



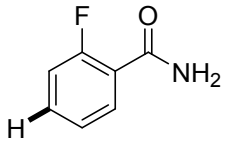
2e

***N,N*-Dimethylaniline (2e)**. The title compound was prepared according to the general procedure at 60 °C for 8 h, as described above in 75% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.22 (m, 2H), 6.80 – 6.70 (m, 3H), 2.96 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.8, 129.2, 116.7, 112.8, 40.7. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_8H_{12}N$ 122.1, found 122.1.



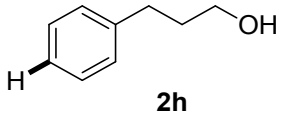
2f

***N*-Cyclohexylbenzamide (2f)**. The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 13 h, as described above in 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.68(m, 2H), 7.52 – 7.36 (m, 3H), 5.97 (s, 1H), 4.05 – 3.90 (m, 1H), 2.10 – 1.96 (m, 2H), 1.83 – 1.70 (m, 2H), 1.50 – 1.35 (m, 2H), 1.33 – 1.10 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.8, 134.0, 131.8, 128.6, 125.9, 49.0, 33.3, 25.7, 25.0. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{13}H_{18}NO$ 204.1, found 204.2.



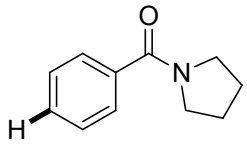
2g

2-Fluorobenzamide (2g). The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 was used) at 60 °C for 4 h, as described above in 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 – 8.07 (m, 1H), 7.53 – 7.45 (m, 1H), 7.29 – 7.23 (m, 1H), 7.17 – 7.09 (m, 1H), 6.82 – 6.30 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.2 (d, J = 3.0 Hz), 161.1 (d, J = 248.5 Hz), 134.0 (d, J = 10.1 Hz), 132.4 (d, J = 2.0 Hz), 124.9 (d, J = 4.0 Hz), 120.3 (d, J = 11.1 Hz), 116.2 (d, J = 24.2 Hz). LR-MS (ESI): m/z $[M+H]^+$ calcd for C_7H_7FNO 140.1, found 140.1.



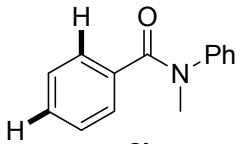
2h

3-Phenylpropan-1-ol (2h). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 6 h, as described above in 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.27 (m, 2H), 7.24 – 7.16 (m, 3H), 3.68 (t, *J* = 6.3 Hz, 2H), 2.72 (t, *J* = 7.6 Hz, 2H), 1.99 – 1.82 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.9, 128.5, 128.5, 125.9, 62.3, 34.3, 32.2. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_9H_{13}O$ 137.1, found 137.1.



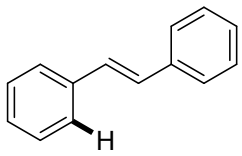
2i

Phenyl(pyrrolidin-1-yl)methanone (2i, the same compound as 2a). The title compound was prepared according to the general procedure at 60 °C for 4 h, as described above in 98% yield.



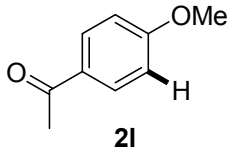
2j

***N*-Methyl-N-phenylbenzamide (2j)**. The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 and 10 mol % of $PdCl_2$ was used) at 60 °C for 9 h, as described above in 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.27 (m, 2H), 7.25 – 7.19 (m, 3H), 7.19 – 7.09 (m, 3H), 7.07 – 7.00 (m, 2H), 3.50 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.7, 145.0, 136.0, 129.7, 129.2, 128.8, 127.8, 127.0, 126.6, 38.5. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{14}NO$ 212.1, found 212.2.



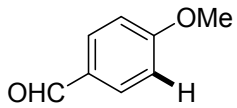
2k

1,2-Diphenylethene (2k). The title compound was prepared according to the general procedure at 60 °C for 4 h, as described above in 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.50 (m, 4H), 7.37 – 7.33 (m, 4H), 7.27 – 7.22 (m, 2H), 7.12 – 7.08 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 137.3, 128.7, 128.7, 127.6, 126.5. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{13}$ 181.1, found 181.1.



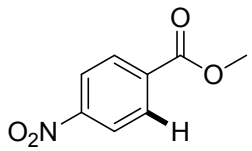
2l

1-(4-Methoxyphenyl)ethan-1-one (2l). The title compound was prepared according to the general procedure at 60 °C for 8 h, as described above in 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, J = 8.6 Hz, 2H), 6.93 (d, J = 8.6 Hz, 2H), 3.87 (s, 3H), 2.56 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 196.9, 163.6, 130.7, 130.5, 113.8, 55.6, 26.5. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_9H_{11}O_2$ 151.1, found 151.1.



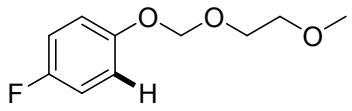
2m

4-Methoxybenzaldehyde (2m). The title compound was prepared according to the general procedure at 60 °C for 10 h, as described above in 85% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.89 (s, 1H), 7.84 (d, J = 8.6 Hz, 2H), 7.01 (d, J = 8.5 Hz, 2H), 3.89 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 190.9, 164.7, 132.1, 130.1, 114.4, 55.7. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_8H_9O_2$ 137.1, found 137.1.



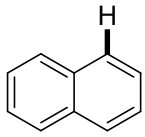
2n

Methyl 4-nitrobenzoate (2n). The title compound was prepared according to the general procedure at 60 °C for 48 h, as described above in 60% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.6 Hz, 2H), 8.21 (d, *J* = 8.6 Hz, 2H), 3.98 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.3, 150.7, 135.6, 130.8, 123.7, 53.0. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_8H_8NO_4$ 182.0, found 182.0.



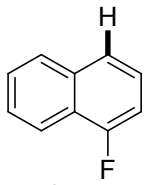
2o

1-Fluoro-4-(2-methoxyethoxy)benzene (2o). The title compound was prepared according to the general procedure at 60 °C for 10 h, as described above in 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 – 6.87 (m, 4H), 5.22 (s, 2H), 3.88 – 3.76 (m, 2H), 3.61 – 3.53 (m, 2H), 3.37 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.1 (d, *J* = 240.1 Hz), 153.5, 117.7 (d, *J* = 7.5 Hz), 115.9 (d, *J* = 22.7 Hz), 94.2, 71.7, 67.7, 59.1. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_{14}FO_3$ 201.1, found 201.1.



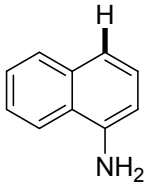
2p

Naphthalene (2p). The title compound was prepared according to the general procedure at 60 °C for 24 h, as described above in 89% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.81 (m, 4H), 7.54 – 7.44 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 133.6, 128.0, 126.0.



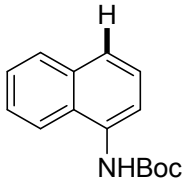
2q

1-Fluoronaphthalene (2q). The title compound was prepared according to the general procedure at 60 °C for 5 h, as described above in 73% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 – 8.08 (m, 1H), 7.89 – 7.83 (m, 1H), 7.69 – 7.60 (m 1H), 7.60 – 7.50 (m, 2H), 7.46 – 7.36 (m, 1H), 7.21 – 7.11 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.9 (d, J = 252.2 Hz), 135.0, 127.6 (d, J = 3.0 Hz), 126.8, 126.3, 125.7 (d, J = 9.0 Hz) 123.9, 123.8 (d, J = 4.5 Hz), 120.7, 120.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_8F$ 147.1, found 147.1.



2r

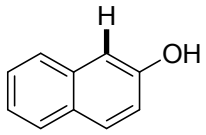
Naphthalen-1-amine (2r). The title compound was prepared according to the general procedure (3.0 equiv of CaH_2 was used) at 60 °C for 18 h, as described above in 82% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.78 (m, 2H), 7.55 – 7.40 (m, 2H), 7.37 – 7.27 (m, 2H), 6.80 (d, J = 5.3 Hz, 1H), 4.04 (br, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.2, 134.5, 128.7, 126.4, 125.9, 125.0, 123.8, 120.9, 119.1, 109.8. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_{10}N$ 144.1, found 144.1.



2s

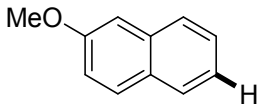
***Tert*-Butyl naphthalen-1-ylcarbamate (2s)**. The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 was used) at 60 °C for 9 h, as described above in 96% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.82 (m, 3H),

7.66 – 7.60(m, 1H), 7.55 – 7.42 (m, 3H), 6.85 (s, 1H), 1.56 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.6, 134.2, 133.1, 128.8, 126.6, 126.1, 126.0, 125.9, 124.6, 120.6, 118.7, 110.1, 80.8, 28.5. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{18}NO_2$ 244.1, found 244.1.



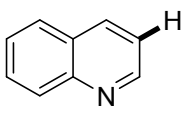
2t

Naphthalen-2-ol (2t). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 19 h, as described above in 79% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.72 (m, 2H), 7.69 (d, *J* = 8.2 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.15 (s, 1H), 7.11 (dd, *J* = 8.8, 2.1 Hz, 1H), 5.02 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.4, 134.7, 130.0, 129.1, 127.9, 126.7, 126.5, 123.8, 117.9, 109.7. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_9O$ 145.1, found 145.1. LR-MS (ESI): m/z 145.1 $[M+H]^+$.



2u

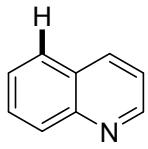
2-Methoxynaphthalene (2u). The title compound was prepared according to the general procedure at 60 °C for 5 h, as described above in 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.71 (m, 3H), 7.45 (t, *J* = 7.4 Hz, 1H), 7.34 (t, *J* = 7.3 Hz, 1H), 7.19 – 7.11 (m, 2H), 3.93 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 157.7, 134.7, 129.5, 129.1, 127.8, 126.9, 126.5, 123.7, 118.8, 105.9, 55.4. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{11}H_{11}O$ 159.1, found 159.1.



2v

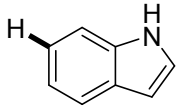
Quinoline (2v). The title compound was prepared according to the general procedure

at 60 °C for 8 h, as described above in 66% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (s, 1H), 8.24 – 8.04 (m, 2H), 7.87 – 7.64 (m, 2H), 7.62 – 7.48 (m, 1H), 7.46 – 7.31 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.5, 148.4, 136.2, 129.6, 128.4, 127.9, 126.6, 121.2. LR-MS (ESI): m/z $[M+H]^+$ calcd for C_9H_8N 130.1, found 130.1.



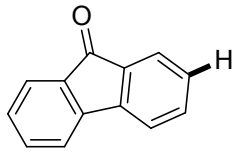
2w

Quinoline (2w, the same compound as 2v). The title compound was prepared according to the general procedure at 60 °C for 8 h, as described above in 80% yield.



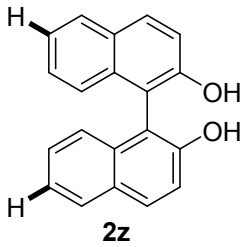
2x

1*H*-Indole (2x). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 5 h, as described above in 86% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (br, 1H), 7.68 (d, J = 7.8 Hz, 1H), 7.41 (d, J = 8.0 Hz, 1H), 7.25 – 7.19 (m, 2H), 7.18 – 7.10 (m, 1H), 6.63 – 6.43 (m, 1H). ^{13}C NMR (151 MHz,$CDCl_3$) δ 135.9, 127.9, 124.3, 122.1, 120.8, 119.9, 111.2, 102.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for C_8H_8N 118.1, found 118.1.



2y

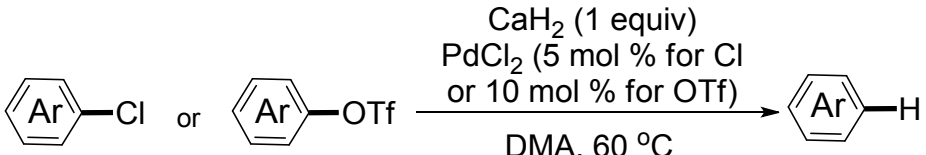
9*H*-Fluoren-9-one (2y). The title compound was prepared according to the general procedure at 60 °C for 4 h, as described above in 89% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 7.3 Hz, 2H), 7.43-7.39 (m, 4H), 7.23 (t, J = 7.2 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 193.8, 144.4, 134.7, 134.1, 129.0, 124.2, 120.3. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{13}H_9O$ 181.1, found 181.1.



2z

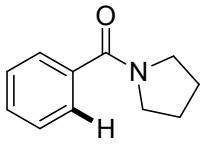
1,1'-Bi-2-naphthol (2z). The title compound was prepared according to the general procedure (3.0 equiv of CaH_2 and 10 mol % of $PdCl_2$ was used) at 60 °C for 5 h, as described above in 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.93 (m, 2H), 7.93 – 7.86 (m, 2H), 7.41 – 7.35 (m, 4H), 7.34 – 7.29 (m, 2H), 7.18 – 7.09 (m, 2H), 5.05 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.9, 133.6, 131.5, 129.6, 128.5, 127.6, 124.3, 124.2, 117.9, 111.0. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{20}H_{15}O_2$ 287.1, found 287.1.

5. General procedure for hydrodehalogenation of aryl chlorides and aryl triflates



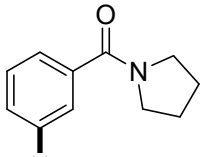
3 **4**

A mixture of $PdCl_2$ ('4.4 mg, 0.025 mmol, 5 mol %' for Cl, or '8.8 mg, 0.05 mmol, 10 mol %' for OTf) and calcium hydride (21 mg, 0.5 mmol, 1 equiv) in DMA (0.5 mL) was stirred for 5 min under N_2 before **3** (0.5 mmol) in DMA (0.5 mL) was added through syringe, and then the mixture was stirred at 60 °C for the specified time. After the reaction was completed monitored with TLC, a saturated NH_4Cl aqueous solution was added to quench the reaction and the resulting mixture was extracted with EtOAc. The combined organic layers were washed with water and brine and dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography to give desired product **4**.



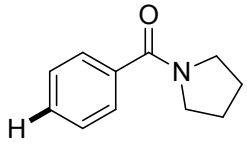
4a

Phenyl(pyrrolidin-1-yl)methanone (4a, the same compound as 2a). The title compound was prepared according to the general procedure at 60 °C for 4 h, as described above in 83% yield.



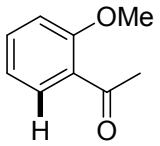
4b

Phenyl(pyrrolidin-1-yl)methanone (4b, the same compound as 2a). The title compound was prepared according to the general procedure at 60 °C for 4 h, as described above in 95% yield.



4c

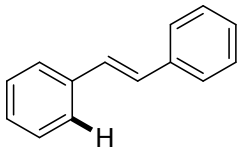
Phenyl(pyrrolidin-1-yl)methanone (4c, the same compound as 2a). The title compound was prepared according to the general procedure at 60 °C for 4 h, as described above in 99% yield.



4d

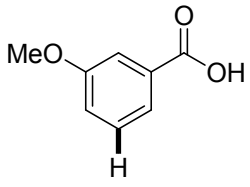
1-(2-Methoxyphenyl)ethan-1-one (4d). The title compound was prepared according to the general procedure at 60 °C for 6 h, as described above in 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 7.1 Hz, 1H), 7.46 (t, J = 7.3 Hz, 1H), 7.04 – 6.94 (m, 2H), 3.91 (s, 3H), 2.61 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 200.0, 159.0, 133.8,

130.5, 128.4, 120.7, 111.7, 55.6, 32.0. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_9H_{11}O_2$ 151.1, found 151.1.



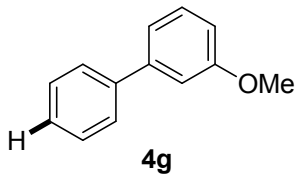
4e

1,2-Diphenylethene (4e, the same compound as 2k). The title compound was prepared according to the general procedure at 60 °C for 24 h, as described above in 87% yield.



4f

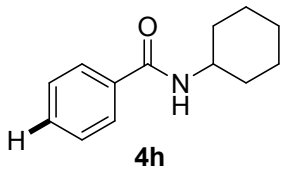
3-Methoxybenzoic acid (4f). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 24 h, as described above in 50% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.5 Hz, 1H), 7.63 (s, 1H), 7.39 (t, *J* = 7.9 Hz, 1H), 7.17 (d, *J* = 7.7 Hz, 1H), 3.88 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.4, 159.7, 130.7, 129.7, 122.8, 120.6, 114.5, 55.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_8H_9O_3$ 153.1, found 153.1.



4g

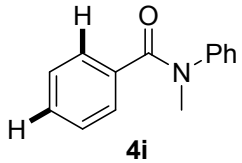
3-Methoxy-1,1'-biphenyl (4g). The title compound was prepared according to the general procedure at 60 °C for 4 h, as described above in 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.54 (m, 2H), 7.50 – 7.41 (m, 2H), 7.40 – 7.32 (m, 2H), 7.23 – 7.16 (m, 1H), 7.14 (s, 1H), 6.91 (d, *J* = 7.4 Hz, 1H), 3.88 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.0, 142.9, 141.2, 129.9, 128.9, 127.5, 127.3, 119.8, 113.0, 112.8, 55.4.

LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{13}H_{13}O$ 185.1, found 185.1.



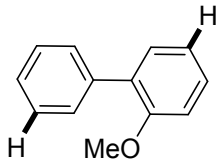
4h

***N*-Cyclohexylbenzamide (4h, the same compound as 2f)**. The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 4 h, as described above in 97% yield.



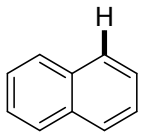
4i

***N*-Methyl-N-phenylbenzamide (4i, the same compound as 2j)**. The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 and 10 mol % of $PdCl_2$ was used) at 60 °C for 24 h, as described above in 90% yield.



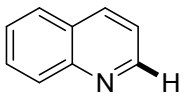
4j

2-Methoxy-1,1'-biphenyl (4j). The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 and 10 mol % of $PdCl_2$ was used) at 60 °C for 6 h, as described above in 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.56 (m, 2H), 7.49 – 7.40 (m, 2H), 7.40 – 7.32 (m, 2H), 7.22 – 7.16 (m, 1H), 7.15 – 7.11 (m, 1H), 6.94 – 6.87 (m, 1H), 3.87 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.1, 142.9, 141.2, 129.9, 128.9, 127.5, 127.3, 119.8, 113.0, 112.8, 55.4. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{13}H_{13}O$ 185.1, found 185.1.



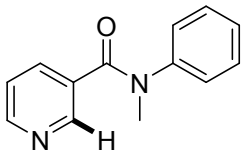
4k

Naphthalene (4k, the same compound as 2p). The title compound was prepared according to the general procedure at 60 °C for 4 h, as described above in 97% yield.



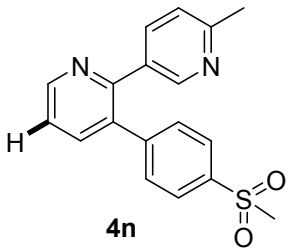
4l

Quinoline (4l, the same compound as 2v). The title compound was prepared according to the general procedure at 60 °C for 3 h, as described above in 87% yield.



4m

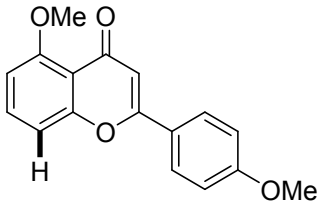
***N*-Methyl-*N*-phenylnicotinamide (4m)**. The title compound was prepared according to the general procedure at 60 °C for 9 h, as described above in 94% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 – 8.42 (m, 2H), 7.61 (d, *J* = 7.5 Hz, 1H), 7.31 – 7.22 (m, 2H), 7.22 – 7.16 (m, 1H), 7.15 – 7.09 (m, 1H), 7.09 – 7.01 (m, 2H), 3.52 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.2, 150.3, 149.7, 144.2, 136.2, 131.9, 129.6, 127.3, 127.1, 122.7, 38.4. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{13}H_{13}N_2O$ 213.1, found 213.1.



4n

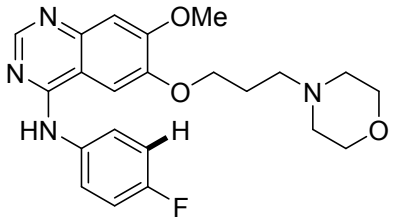
6'-Methyl-3-(4-(methylsulfonyl)phenyl)-2,3'-bipyridine (4n). The title compound was prepared according to the general procedure at 60 °C for 3 h, as described above

in 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 3.7 Hz, 1H), 8.41 (s, 1H), 7.89 (d, *J* = 8.2 Hz, 2H), 7.74 (d, *J* = 7.5 Hz, 1H), 7.64 – 7.58 (m, 1H), 7.44 – 7.37 (m, 3H), 7.10 (d, *J* = 8.0 Hz, 1H), 3.09 (s, 3H), 2.54 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.3, 154.4, 150.1, 149.8, 145.3, 139.8, 138.7, 137.5, 134.5, 132.3, 130.6, 127.9, 122.8, 122.7, 44.6, 24.4. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{18}H_{17}N_2O_2S$ 325.1, found 325.2.



4o

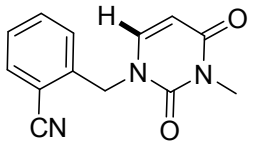
5-Methoxy-2-(4-methoxyphenyl)-4H-chromen-4-one (4o). The title compound was prepared according to the general procedure at 60 °C for 5 h, as described above in 86% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.02 (d, *J* = 8.7 Hz, 2H), 7.69 (t, *J* = 8.4 Hz, 1H), 7.27 (d, *J* = 8.4 Hz, 1H), 7.11 (d, *J* = 8.8 Hz, 2H), 6.99 (d, *J* = 8.3 Hz, 1H), 6.77 (s, 1H), 3.86 (s, 3H), 3.85 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 176.4, 161.9, 160.1, 159.0, 157.5, 134.1, 127.8, 122.9, 114.5, 113.7, 109.9, 107.1, 106.9, 56.1, 55.5. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{15}O_4$ 283.1, found 283.1.



4p

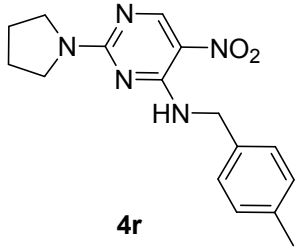
***N*-(4-Fluorophenyl)-7-methoxy-6-(3-morpholinopropoxy)quinazolin-4-amine (4p)**. The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 and 10 mol % of $PdCl_2$ was used) at 60 °C for 24 h, as described above in 87% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.51 (s, 1H), 8.42 (s, 1H), 7.88 – 7.70 (m, 3H), 7.27 – 7.10 (m, 3H), 4.25 – 4.12 (m, 2H), 4.00 – 3.86 (m, 3H), 3.67 – 3.50 (m, 4H), 2.68 – 2.44 (m, 6H), 2.07 – 1.92 (m, 2H). ^{13}C NMR (151 MHz, DMSO-d_6) δ

158.3 (d, J = 241.6 Hz), 156.4, 154.3, 152.8, 148.2, 146.9, 140.5, 135.7, 124.4 (d, J = 7.5 Hz), 115.0 (d, J = 22.6 Hz), 108.7, 107.3, 102.7, 67.1, 66.2, 55.8, 55.0, 53.4, 25.9. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{22}H_{26}FN_4O_3$ 413.1989, found 413.1994.



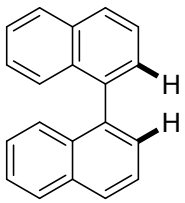
4q

2-((1-Methyl-2,6-dioxo-1,2,3,6-tetrahydropyridin-3-yl)methyl)benzonitrile (4q). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 4 h, as described above in 75% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 7.6 Hz, 1H), 7.64 (t, J = 7.5 Hz, 1H), 7.58 (d, J = 7.6 Hz, 1H), 7.47 (t, J = 7.4 Hz, 1H), 7.40 (d, J = 7.9 Hz, 1H), 5.82 (d, J = 7.9 Hz, 1H), 5.13 (s, 2H), 3.35 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.0, 151.9, 142.1, 139.0, 133.6, 133.30, 130.1, 129.2, 117.7, 112.0, 102.4, 51.0, 28.0. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{13}H_{12}N_3O_2$ 242.0930, found 242.0931.



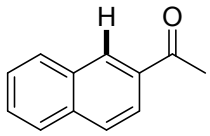
4r

***N*-(4-Methylbenzyl)-5-nitro-2-(pyrrolidin-1-yl)pyrimidin-4-amine (4r).** The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 was used) at 60 °C for 8 h, as described above in 53% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.01 (s, 1H), 8.72 (s, 1H), 7.31 – 7.24 (m, 2H), 7.18 – 7.10 (m, 2H), 4.71 (d, J = 5.7 Hz, 2H), 3.76 – 3.64 (m, 2H), 3.62 – 3.52 (m, 2H), 2.34 (s, 3H), 2.05 – 1.91 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.3, 157.9, 155.6, 137.3, 135.1, 129.5, 127.8, 120.4, 47.6, 47.2, 44.3, 25.6, 25.3, 21.2. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{20}N_5O_2$ 314.1617, found 314.1621.



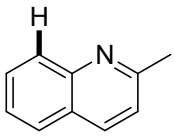
4s

1,1'-Binaphthalene (4s). The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 was used) at 60 °C for 3 h, as described above in 85% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.98 (m, 4H), 7.64 (t, *J* = 7.5 Hz, 2H), 7.53 (dd, *J* = 12.3, 6.9 Hz, 4H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.34 – 7.26 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.6, 133.7, 133.0, 128.3, 128.0, 126.7, 126.1, 126.0, 125.5. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{20}H_{15}$ 255.1, found 255.1.



4t

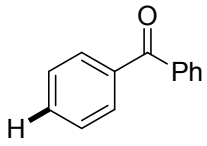
1-(Naphthalen-2-yl)ethan-1-one (**4t**). The title compound was prepared according to the general procedure at 60 °C for 1.5 h, as described above in 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.47 (s, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 7.9 Hz, 1H), 7.92 – 7.86 (m, 2H), 7.58 (dt, *J* = 14.7, 6.9 Hz, 2H), 2.73 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 198.1, 135.6, 134.5, 132.5, 130.2, 129.5, 128.5, 128.4, 127.8, 126.8, 123.9, 26.7. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{11}O$ 171.1, found 171.1.



4u

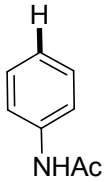
2-Methylquinoline (4u). The title compound was prepared according to the general procedure at 60 °C for 3.5 h, as described above in 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (t, *J* = 9.4 Hz, 2H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.27 (d, *J* = 7.7 Hz, 1H), 2.76 (s, 3H). ^{13}C NMR (151 MHz,

$CDCl_3$) δ 158.9, 147.7, 136.2, 129.4, 128.5, 127.5, 126.5, 125.7, 122.0, 25.3. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_{10}N$ 144.1, found 144.1.



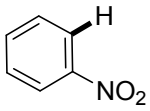
4v

2*H*-Chromen-2-one (4v). The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 and 15 mol % of $PdCl_2$ was used) at 60 °C for 6.5 h, as described above in 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.81 (m, 5H),7.51 – 7.49 (m, 5H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 196.7, 137.6, 132.4, 130.0, 128.3. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{13}H_{11}O$ 183.1, found 183.1.



4w

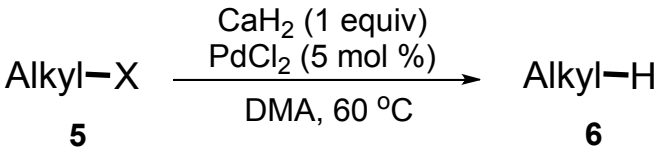
***N*-Phenylacetamide** (**4w, the same compound as 2b**). The title compound was prepared according to the general procedure at 60 °C for 4 h, as described above in 69% yield.



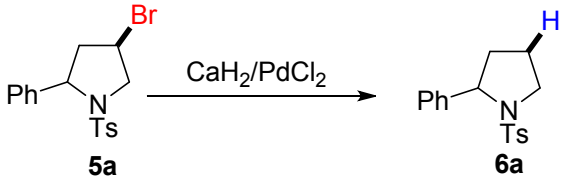
4x

Nitrobenzene (4x). The title compound was prepared according to the general procedure at 60 °C for 3.5 h, as described above in 50% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, J = 8.0 Hz, 2H), 7.69 (t, J = 7.4 Hz, 1H), 7.53 (t, J = 8.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.2, 134.7, 129.4, 123.5. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_6H_6NO_2$ 124.0, found 124.0.

6. General procedure for hydrodehalogenation of alkyl halides

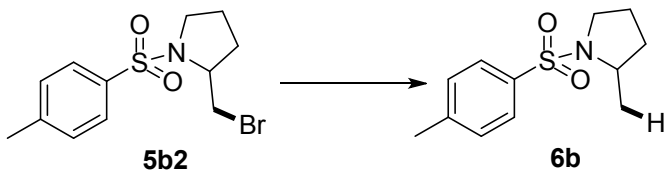


A mixture of $PdCl_2$ (4.4 mg, 0.025 mmol, 5 mol %) and calcium hydrogen (21 mg, 0.5 mmol, 1 equiv) in DMA (0.5 mL) was stirred for 5 min under N_2 before **5** (0.5 mmol) in DMA (0.5 mL) was added through syringe, and then the mixture was stirred at 60 °C for the specified time. After the reaction was completed monitored with TLC, a saturated NH_4Cl aqueous solution was added to quench the reaction and the resulting mixture was extracted with EtOAc. The combined organic layers were washed with water and brine and dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography to give desired product **6**.



5a **6a**

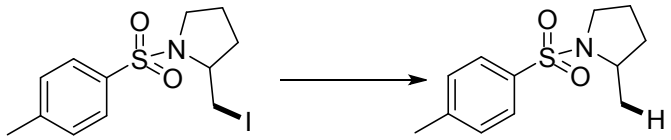
Phenyl-1-tosylpyrrolidine (6a). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 6 h, as described above in 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 8.0 Hz, 2H), 7.34 – 7.27 (m, 6H), 7.25 – 7.20 (m, 1H), 4.782 – 4.73 (m, 1H), 3.67 – 3.58 (m, 1H), 3.50 – 3.37 (m, 1H), 2.43 (s, 3H), 2.03 – 1.93 (m, 1H), 1.91 – 1.76 (m, 2H), 1.71 – 1.62 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.4, 143.2, 135.2, 129.7, 128.4, 127.6, 127.1, 126.2, 63.4, 49.5, 35.9, 24.1, 21.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{20}NO_2S$ 302.1, found 302.1.



5b2 **6b**

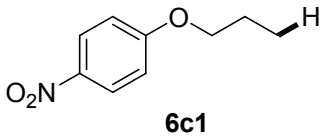
2-Methyl-1-tosylpyrrolidine (6b). The title compound was prepared according to the

general procedure at 60 °C for 19 h, as described above in 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 7.9 Hz, 2H), 3.74 – 3.66 (m, 1H), 3.48 – 3.39 (m, 1H), 3.17 – 3.10 (m, 1H), 2.42 (s, 3H), 1.88 – 1.73 (m, 1H), 1.73 – 1.62 (m, 1H), 1.56-1.44 (m, 2H), 1.31 (d, *J* = 6.3 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.3, 135.1, 129.7, 127.6, 56.2, 49.2, 33.6, 24.1, 23.0, 21.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{18}NO_2S$ 240.1, found 240.1.



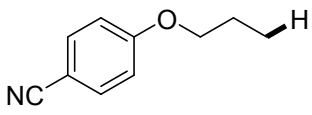
5b3 **6b**

2-Methyl-1-tosylpyrrolidine (6b). The title compound was prepared according to the general procedure at 60 °C for 19 h, as described above in 70% yield.



6c1

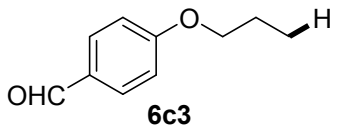
1-Nitro-4-propoxybenzene (6c1). The title compound was prepared according to the general procedure at 60 °C for 24 h, as described above in 57% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 9.0 Hz, 2H), 6.94 (d, *J* = 9.0 Hz, 2H), 4.01 (t, *J* = 6.4 Hz, 2H), 1.92 – 1.77 (m, 2H), 1.06 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.4, 141.4, 126.0, 114.5, 70.5, 22.5, 10.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_9H_{12}NO_3$ 182.1, found 182.1.



6c2

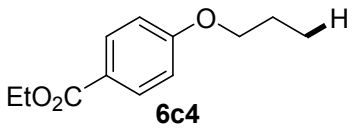
4-Propoxybenzonitrile (6c2). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 24 h, as described above in 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.5 Hz, 2H), 6.91 (d, *J* = 8.5 Hz, 2H), 3.93 (t, *J* = 6.5 Hz, 2H), 1.80 (dt, *J* = 13.9, 7.0 Hz, 2H), 1.02 (t, *J* = 7.4 Hz,

3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.5, 133.9, 119.3, 115.2, 103.6, 69.9, 22.4, 10.4. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_{12}NO$ 162.1, found 162.1.



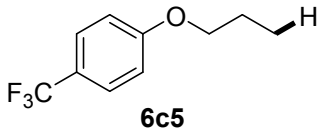
6c3

4-Propoxybenzaldehyde (6c3). The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 was used) at 60 °C for 24 h, as described above in 58% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.86 (s, 1H), 7.81 (d, *J* = 8.5 Hz, 2H), 6.98 (d, *J* = 8.5 Hz, 2H), 3.99 (t, *J* = 6.5 Hz, 2H), 1.88 – 1.76 (m, 2H), 1.04 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 190.9, 164.4, 132.1, 129.9, 114.9, 70.0, 22.6, 10.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_{13}O_2$ 165.1, found 165.1.



6c4

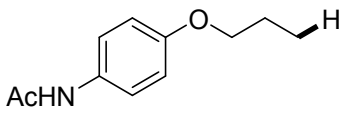
Ethyl 4-propoxybenzoperoxoate (6c4). The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 was used) at 60 °C for 11 h, as described above in 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.7 Hz, 2H), 6.90 (d, *J* = 8.7 Hz, 2H), 4.34 (q, *J* = 7.1 Hz, 2H), 3.97 (t, *J* = 6.5 Hz, 2H), 1.89-1.76 (m, 2H), 1.38 (t, *J* = 7.1 Hz, 3H), 1.04 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 163.0, 131.6, 122.8, 114.1, 69.8, 60.7, 22.6, 14.5, 10.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{17}O_3$ 209.1, found 209.1.



6c5

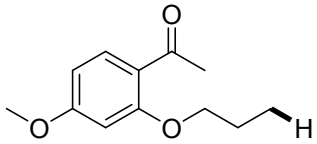
1-Propoxy-4-(trifluoromethyl)benzene (6c5). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 9 h, as described above in 64% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.5 Hz, 2H), 6.95 (d, *J* = 8.5 Hz, 2H), 3.96 (t, *J* = 6.5 Hz, 2H), 1.88 – 1.78 (m, 2H), 1.05 (t, *J* = 7.4

Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.8, 127.4, 127.0, 127.0, 126.96, 126.94, 125.6, 123.8, 123.1, 122.9, 122.6, 122.4, 114.6, 69.9, 25.3, 22.6, 10.6. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_{12}F_3O$ 205.0840, found 205.0842.



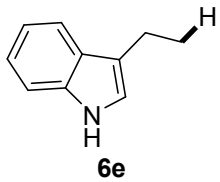
6c6

***N*-(4-Propoxyphenyl)acetamide (6c6)**. The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 was used) at 60 °C for 24 h, as described above in 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (s, 1H), 7.36 (d, *J* = 8.9 Hz, 2H), 6.82 (d, *J* = 8.9 Hz, 2H), 3.88 (t, *J* = 6.6 Hz, 2H), 2.12 (s, 3H), 1.84 – 1.73 (m, 2H), 1.02 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.5, 156.1, 131.0, 122.1, 114.9, 69.9, 24.4, 22.7, 10.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{11}H_{16}NO_2$ 194.1, found 194.1.



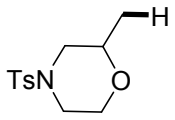
6d

1-(4-Methoxy-2-propoxyphenyl)ethan-1-one (6d). The title compound was prepared according to the general procedure at 60 °C for 3 h, as described above in 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.7 Hz, 1H), 6.51 (d, *J* = 8.7 Hz, 1H), 6.43 (s, 1H), 4.00 (t, *J* = 6.3 Hz, 2H), 3.85 (s, 3H), 2.60 (s, 3H), 1.95 – 1.82 (m, 2H), 1.09 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 198.0, 164.6, 160.8, 132.8, 121.3, 105.1, 98.9, 70.2, 55.6, 32.3, 22.6, 11.0. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{17}O_3$ 209.1178, found 209.1179.



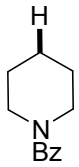
6e

3-Ethyl-1*H*-indole (6e). The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 was used) at 60 °C for 3 h, as described above in 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (br, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.20 (t, *J* = 7.4 Hz, 1H), 7.12 (t, *J* = 7.4 Hz, 1H), 6.98 (s, 1H), 2.80 (q, *J* = 7.5 Hz, 2H), 1.34 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.5, 127.6, 122.0, 120.6, 119.2, 119.1, 119.0, 111.2, 18.5, 14.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_{12}N$ 146.1, found 146.1.



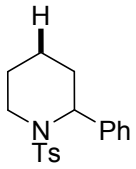
6f

2-Methyl-4-tosylmorpholine (6f). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 36 h, as described above in 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.6 Hz, 2H), 7.34 (d, *J* = 7.4 Hz, 2H), 3.87 (m, 1H), 3.72-3.63 (m, 2H), 3.57-3.49 (m, 2H), 2.44 (s, 3H), 2.42-2.35 (m, 1H), 2.01 (m, 1H), 1.13 (d, *J* = 8.2 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.0, 132.3, 129.9, 128.0, 71.5, 66.0, 51.7, 45.4, 21.7, 18.8. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{18}NO_3S$ 256.1, found 256.1.



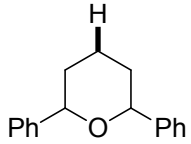
6g

Phenyl(piperidin-1-yl)methanone (6g). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 3 h, as described above in 94% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.40 (m, 1H), 7.39 – 7.37 (m, 4H), 3.82 – 3.62 (m, 2H), 3.42 – 3.24 (m, 2H), 1.76 – 1.63 (m, 4H), 1.57 – 1.41 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.4, 136.6, 129.4, 128.5, 126.9, 48.9, 43.2, 26.7, 25.7, 24.7. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{16}NO$ 190.1, found 190.1.



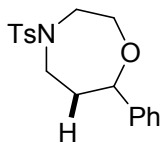
6h

2-Phenyl-1-tosylpiperidine (6h). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 24 h, as described above in 68% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.71(m, 2H), 7.38 – 7.27 (m, 6H), 7.25 – 7.20(m, 1H), 5.31 – 5.21 (m, 1H), 3.92 – 3.78 (m, 1H), 3.07 – 2.95 (m, 1H), 2.44 (s, 3H), 2.26 – 2.16 (m, 1H), 1.72 – 1.62 (m, 1H), 1.55 – 1.46 (m, 1H), 1.45 – 1.36 (m, 2H), 1.35 – 1.28 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.1, 139.0, 138.8, 129.8, 128.7, 127.14, 127.11, 126.9, 55.4, 42.0, 27.4, 24.4, 21.7, 19.1. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{18}H_{22}NO_2S$ 316.1, found 316.2.



6i

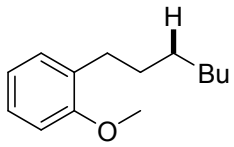
2,6-Diphenyltetrahydro-2*H*-pyran (6i). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 24 h, as described above in 82% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.42 (m, 4H), 7.35 (t, J = 7.4 Hz, 4H), 7.29 – 7.27 (m, 1H), 7.25 – 7.22 (m, 1H), 4.63 – 4.55 (m, 2H), 2.10 – 2.00 (m, 1H), 1.98 – 1.90 (m, 2H), 1.90 – 1.81 (m, 1H), 1.69 – 1.58 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.6, 128.3, 127.3, 125.9, 80.3, 34.0, 24.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{19}O$ 239.1, found 239.2.



6j

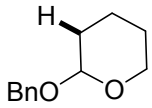
7-Phenyl-4-tosyl-1,4-oxazepane (6j). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 8 h, as described

above in 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.64 (m, 2H), 7.37 – 7.29 (m, 4H), 7.29 – 7.27 (m, 2H), 7.25 – 7.21 (m, 1H), 4.71 – 4.64 (m, 1H), 4.13 – 4.06 (m, 1H), 3.81 – 3.67 (m, 2H), 3.65 – 3.57 (m, 1H), 3.39 – 3.29 (m, 1H), 3.27 – 3.19 (m, 1H), 2.44 (s, 3H), 2.37 – 3.36 (m, 1H), 2.09 – 1.97 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.5, 143.0, 136.1, 129.9, 128.6, 127.5, 127.2, 125.7, 81.6, 70.1, 51.8, 46.4, 37.9, 21.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{18}H_{22}NO_3S$ 332.1, found 332.1.



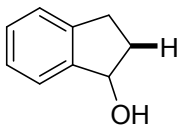
6k

1-Heptyl-2-methoxybenzene (6k). The title compound was prepared according to the general procedure at 60 °C for 6 h, as described above in 96% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 – 7.09 (m, 2H), 6.93 – 6.81 (m, 2H), 3.83 (s, 3H), 2.66 – 2.55 (m, 2H), 1.61 – 1.53 (m, 2H), 1.317 – 1.24 (m, 8H), 0.92 – 0.83 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 157.6, 131.5, 129.9, 126.9, 120.4, 110.3, 55.4, 32.0, 30.3, 30.0, 29.8, 29.4, 22.9, 14.3. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{23}O$ 207.2, found 207.2.



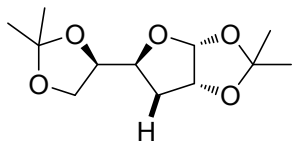
6l

2-(Benzyloxy)tetrahydro-2*H*-pyran (6l). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 19 h, as described above in 66% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.27 (m, 5H), 4.79 (d, J = 11.9 Hz, 1H), 4.71 (s, 1H), 4.51 (d, J = 11.9 Hz, 1H), 3.98 – 3.88 (m, 1H), 3.61 – 3.50 (m, 1H), 1.95 – 1.82 (m, 1H), 1.80 – 1.70 (m, 1H), 1.69 – 1.64 (m, 1H), 1.64 – 1.60(m, 1H), 1.58 – 1.50 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.4, 128.5, 127.9, 127.6, 97.9, 69.0, 62.3, 30.7, 25.6, 19.5. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{17}O_2$ 193.1, found 193.2.



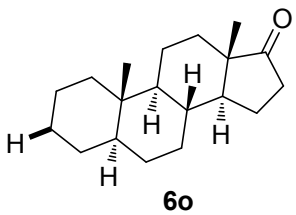
6m

2,3-Dihydro-1*H*-inden-1-ol (6m). The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 was used) at 60 °C for 3 h, as described above in 67% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 5.2 Hz, 1H), 7.31-7.21 (m, 3H), 5.30-5.18 (s, 1H), 3.11 – 3.01 (m, 1H), 2.87 – 2.77 (m, 1H), 2.56-2.43 (m, 1H), 2.00-1.87 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.1, 143.4, 128.4, 126.8, 125.0, 124.3, 76.5, 36.0, 29.9. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_9H_{11}O$ 135.1, found 135.1.



6n

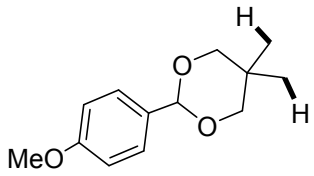
(3a*R*,5*S*,6a*R*)-5-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxole (6n). The title compound was prepared according to the general procedure at 60 °C for 24 h, as described above in 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.81 (s, 1H), 4.75 (t, *J* = 3.7 Hz, 1H), 4.19 – 4.06 (m, 3H), 3.86 – 3.77 (m, 1H), 2.22 – 2.13 (m, 1H), 1.85 – 1.71 (m, 1H), 1.51 (s, 3H), 1.42 (s, 3H), 1.33 (d, *J* = 15.3 Hz, 7H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 112.7, 110.2, 103.5, 80.7, 80.7, 75.2, 65.6, 43.9, 26.8, 26.7, 26.5, 25.4. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{21}O_5$ 245.1, found 245.2.



6o

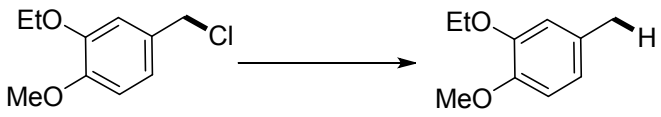
(5*R*,8*R*,9*S*,10*S*,13*S*,14*S*)-10,13-dimethyltetradecahydro-1*H*-cyclopenta[*a*]phenanthren-17(2*H*)-one (6o). The title compound was prepared

according to the general procedure (1.5 equiv of CaH_2 was used) for 8 h, as described above in 86% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.49 – 2.36 (m, 1H), 2.12 – 1.98 (m, 1H), 1.99 – 1.86 (m, 1H), 1.83 – 1.72 (m, 2H), 1.71 – 1.62 (m, 3H), 1.56 – 1.44 (m, 3H), 1.44 – 1.37 (m, 1H), 1.14 – 1.16 (m, 9H), 1.10 – 1.00 (m, 1H), 0.99 – 0.87 (m, 2H), 0.87 – 0.83 (m, 3H), 0.82 – 0.77 (m, 3H), 0.76 – 0.67 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 221.5, 54.8, 51.6, 47.8, 47.0, 38.6, 36.4, 35.8, 35.1, 31.6, 31.0, 29.0, 28.7, 26.7, 22.1, 21.7, 20.0, 13.8, 12.2. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{19}H_{31}O$ 275.2, found 275.2.



6p

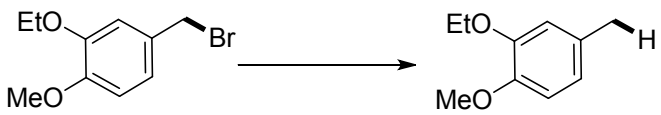
2-(4-Methoxyphenyl)-5,5-dimethyl-1,3-dioxane (6p). The title compound was prepared according to the general procedure (3.0 equiv of CaH_2 and 10 mol % of $PdCl_2$ was used) at 60 °C for 24 h, as described above in 79% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, J = 8.4 Hz, 2H), 6.89 (d, J = 8.4 Hz, 2H), 5.35 (s, 1H), 3.80 (s, 3H), 3.70 (dd, J = 46.8, 10.8 Hz, 4H), 1.29 (s, 3H), 0.79 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.1, 131.2, 127.5, 113.8, 101.8, 77.8, 55.4, 30.3, 23.2, 22.0. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{13}H_{19}O_3$ 223.1, found 223.1.



5q1 **6q**

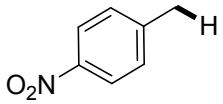
2-Ethoxy-1-methoxy-4-methylbenzene (6q). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 3.5 h, as described above in 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.77 (d, J = 7.9 Hz, 1H), 6.73 – 6.67 (m, 2H), 4.08 (q, J = 7.0 Hz, 2H), 3.84 (s, 3H), 2.29 (s, 3H), 1.46 (t, J = 7.0 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.2, 147.3, 130.5, 120.9, 114.1, 111.7, 64.3, 56.2, 21.1, 15.0. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_{15}O_2$ 167.1, found

167.1.



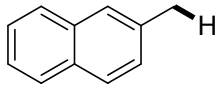
5q2 **6q**

2-Ethoxy-1-methoxy-4-methylbenzene (6q). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 40 min, as described above in 71% yield.



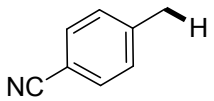
6r

1-Methyl-4-nitrobenzene (6r). The title compound was prepared according to the general procedure at 60 °C for 24 h, as described above in 57% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 7.7 Hz, 2H), 7.31 (d, *J* = 7.7 Hz, 2H), 2.46 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.3, δ 146.1, 129.9, 123.7, 21.7. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_7H_8NO_2$ 138.1, found 138.1.



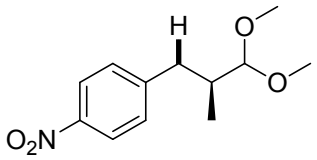
6s

2-Methylnaphthalene (6s). The title compound was prepared according to the general procedure (2.0 equiv of NaH at rt instead of 1.0 equiv of CaH_2 at 60 °C was used) for 4 h, as described above in 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.8 Hz, 1H), 7.90 – 7.88 (m, 2H), 7.77 (s, 1H), 7.63 – 7.53 (m, 2H), 7.48 (d, *J* = 8.3 Hz, 1H), 2.68 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 135.9, 133.8, 131.8, 128.2, 127.8, 127.7, 127.4, 127.0, 126.0, 125.1, 21.8. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{11}H_{11}$ 143.1, found 143.1.



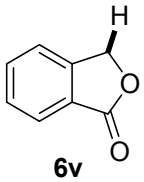
6t

4-Methylbenzonitrile (6t). The title compound was prepared according to the general procedure at 60 °C for 1 h, as described above in 94% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 2.42 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.8, 132.2, 129.9, 119.2, 109.4, 22.0. LR-MS (ESI): m/z $[M+H]^+$ calcd for C_8H_8N 118.1, found 118.1.



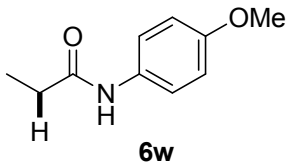
6u

(*S*)-1-(3,3-dimethoxy-2-methylpropyl)-4-nitrobenzene (6u). The title compound was prepared according to the general procedure at 60 °C for 5 h, as described above in 54% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 4.06 (d, *J* = 5.9 Hz, 1H), 3.40 (s, 3H), 3.38 (s, 3H), 3.00 (dd, *J* = 13.4, 4.2 Hz, 1H), 2.46 (dd, *J* = 13.2, 9.7 Hz, 1H), 2.15 – 1.98 (m, 1H), 0.85 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.0, 146.6, 130.1, 123.6, 108.2, 54.9, 54.3, 38.1, 38.0, 14.3. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{18}NO_4$ 240.1, found 240.1.



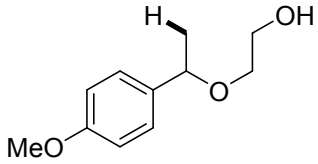
6v

Isobenzofuran-1(3*H*)-one (6v). The title compound was prepared according to the general procedure at 60 °C for 3 h, as described above in 67% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.6 Hz, 1H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.57 – 7.47 (m, 2H), 5.33 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.2, 146.6, 134.1, 129.1, 125.8, 122.2, 69.8. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_8H_7O_2$ 135.0, found 135.0.



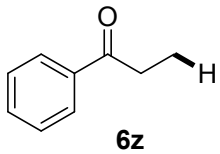
6w

N-(4-Methoxyphenyl)propionamide (6w). The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 was used) at 60 °C for 4 h, as described above in 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.8 Hz, 2H), 7.28 (s, 1H), 6.84 (d, *J* = 8.8 Hz, 2H), 3.78 (s, 3H), 2.36 (q, *J* = 7.5 Hz, 2H), 1.23 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.2, 156.4, 131.3, 121.9, 114.2, 55.6, 30.6, 9.9. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_{14}NO_2$ 180.1, found 180.1.



6x

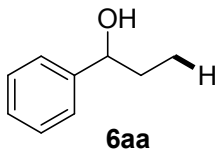
2-(1-(4-Methoxyphenyl)ethoxy)ethan-1-ol (6x). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 6 h, as described above in 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (d, *J* = 8.4 Hz, 2H), 6.89 (d, *J* = 8.4 Hz, 2H), 4.41 (d, *J* = 6.4 Hz, 1H), 3.81 (s, 3H), 3.74 – 3.64 (m, 2H), 3.46 – 3.35 (m, 2H), 1.45 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.2, 135.6, 127.5, 114.0, 78.1, 69.6, 62.1, 55.4, 23.9. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{11}H_{17}O_3$ 197.1, found 197.1.



6z

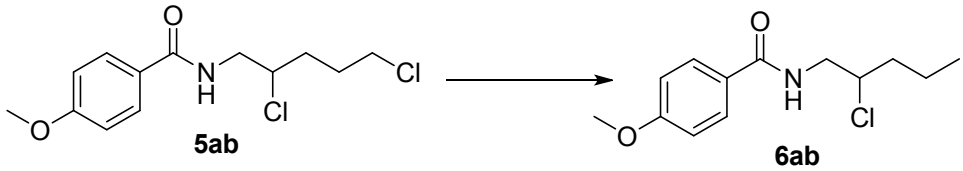
Propiophenone (6z). The title compound was prepared according to the general procedure at 60 °C for 22 h, as described above in 67% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.6 Hz, 2H), 7.55 (t, *J* = 7.1 Hz, 1H), 7.46 (t, *J* = 7.4 Hz, 2H), 3.01 (q, *J* = 7.1 Hz, 2H), 1.23 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 200.9, 137.0, 133.0, 128.7, 128.1, 31.9, 8.3. LR-MS (ESI): m/z $[M+H]^+$ calcd for

$C_9H_{11}O$ 135.1, found 135.1.



6aa

1-Phenylpropan-1-ol (6aa). The title compound was prepared according to the general procedure (1.5 equiv of CaH_2 was used) at 60 °C for 24 h, as described above in 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 3.9 Hz, 4H), 7.31 – 7.27 (m, 1H), 4.69 – 4.54 (m, 1H), 1.85 – 1.70 (m, 2H), 0.92 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 128.5, 127.6, 126.1, 76.1, 32.0, 10.3. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_9H_{13}O$ 137.1, found 137.1.



5ab **6ab**

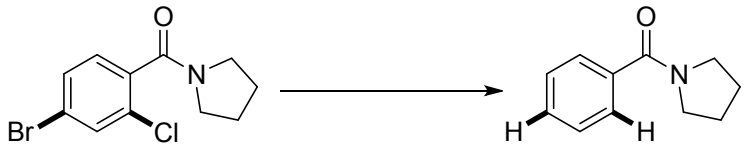
***N*-(2-Chloropentyl)-4-methoxybenzamide (6ab).** The title compound was prepared according to the general procedure (2.0 equiv of CaH_2 and 10 mol % of $PdCl_2$ was used) at 60 °C for 24 h, as described above in 45% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.5 Hz, 2H), 6.90 (d, *J* = 8.5 Hz, 2H), 4.72 – 4.63 (m, 1H), 4.15 – 4.02 (m, 1H), 3.84 (s, 3H), 3.69 – 3.56 (m, 1H), 1.77 – 1.65 (m, 1H), 1.63 – 1.35 (m, 3H), 0.98 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.9, 162.0, 129.9, 120.8, 113.7, 79.9, 60.1, 55.4, 37.7, 18.6, 14.1. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{13}H_{19}ClNO_2$ 256.1104, found 256.1106.

7. Complete or selective hydrodehalogenation by applying DMA or THF as solvent respectively

7.1. Complete hydrodehalogenation by using DMA as solvent

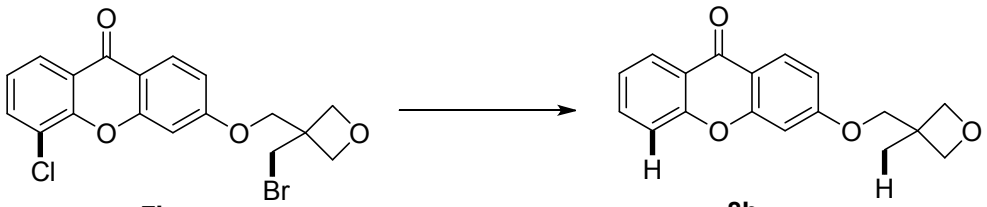
A mixture of $PdCl_2$ (8.8 mg, 0.05 mmol, 10 mol %) and calcium hydride (42 mg, 1.0 mmol, 2 equiv) in DMA (0.5 mL) was stirred for 5 min under N_2 before **7** (0.5 mmol)

in DMA (0.5 mL) was added through syringe, and then the reaction was stirred at 60 °C for the specified time. After the reaction was completed monitored with TLC, a saturated NH_4Cl aqueous solution was added to quench the reaction and the resulting mixture was extracted with EtOAc. The combined organic layers were washed with water and brine and dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography to give desired product **8**.



7a **8a**

Phenyl(pyrrolidin-1-yl)methanone (**8a, the same compound as 2a**). The title compound was prepared according to the general procedure at 60 °C for 3 h, as described above in 88% yield.



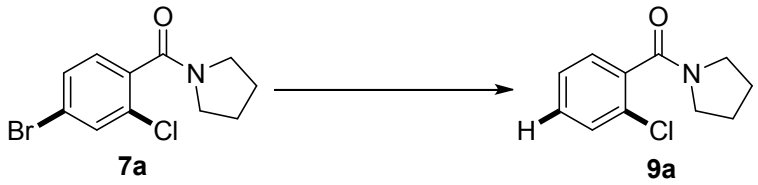
7b **8b**

3-((3-Methyloxetan-3-yl)methoxy)-9H-xanthen-9-one (8b). The title compound was prepared according to the general procedure at 60 °C for 10 h, as described above in 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, J = 7.7 Hz, 1H), 8.27 (d, J = 8.7 Hz, 1H), 7.71 (t, J = 7.4 Hz, 1H), 7.47 (d, J = 8.2 Hz, 1H), 7.38 (t, J = 7.3 Hz, 1H), 6.99 (d, J = 8.7 Hz, 1H), 6.94 (s, 1H), 4.72 – 4.61 (m, 2H), 4.57 – 4.47 (m, 2H), 4.17 (s, 2H), 1.48 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.4, 164.5, 158.1, 156.3, 134.5, 128.5, 126.8, 124.0, 122.1, 117.8, 116.2, 113.6, 101.0, 79.7, 73.4, 39.7, 21.3. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{18}H_{17}O_4$ 297.1127, found 297.1132.

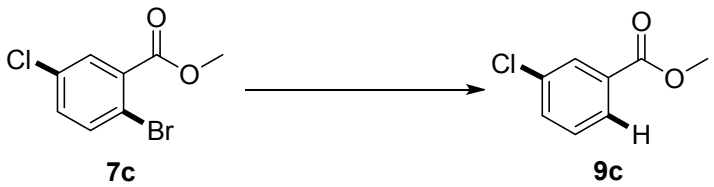
7.2. Selective hydrodehalogenation by using THF as solvent

A mixture of $PdCl_2$ (4.4 mg, 0.025 mmol, 5 mol %) and calcium hydride (21 mg, 0.5

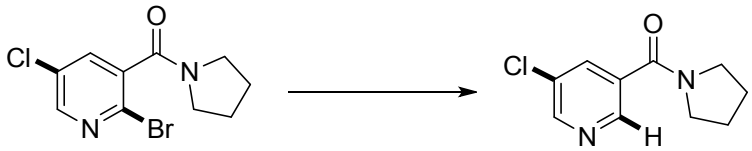
mmol, 1 equiv) in THF (0.5 mL) was stirred for 5 min under N_2 before **7** (0.5 mmol) in THF (0.5 mL) was added through syringe, and then the reaction was stirred at 60 °C for the specified time. After the reaction was completed monitored with TLC, a saturated NH_4Cl aqueous solution was added to quench the reaction and the resulting mixture was extracted with EtOAc. The combined organic layers were washed with water and brine and dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography to give desired product **9**.



(2-Chlorophenyl)(pyrrolidin-1-yl)methanone (9a). The title compound was prepared according to the general procedure at 60 °C for 7 h, as described above in 86% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.35 (m, 1H), 7.35 – 7.27 (m, 3H), 3.66 (t, *J* = 6.7 Hz, 2H), 3.26 – 3.10 (m, 2H), 2.0 – 1.81 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.9, 137.5, 130.2, 130.1, 129.8, 127.6, 127.3, 48.0, 45.6, 26.0, 24.7. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{11}H_{13}ClNO$ 210.1, found 210.1.

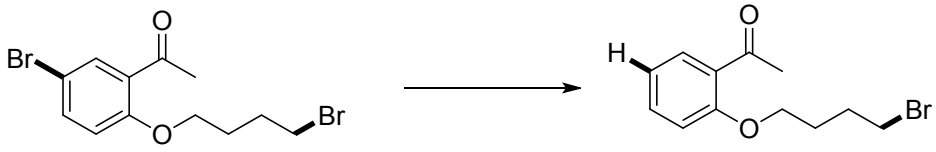


Methyl 3-chlorobenzoate (9c). The title compound was prepared according to the general procedure at 60 °C for 17 h, as described above in 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.92 (d, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.38 (t, *J* = 7.7 Hz, 1H), 3.93 (s, 3H).^{13}C NMR (151 MHz, $CDCl_3$) δ 162.0, 136.4, 129.3, 125.8, 120.4, 67.0. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_8H_8ClO_2$ 171.0, found 171.0.



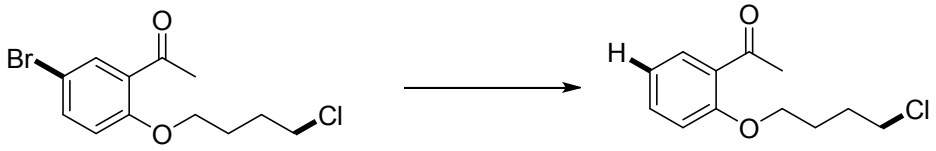
7d **9d**

(5-Chloropyridin-3-yl)(pyrrolidin-1-yl)methanone (9d). The title compound was prepared according to the general procedure at 60 °C for 10 h, as described above in 96% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, *J* = 10.9 Hz, 2H), 7.85 (s, 1H), 3.64 (t, *J* = 6.5 Hz, 2H), 3.45 (t, *J* = 6.1 Hz, 2H), 2.08 – 1.85 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.6, 149.9, 145.9, 134.9, 133.9, 132.2, 49.7, 46.6, 26.5, 24.5. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_{12}ClN_2O$ 211.0638, found 211.0639.



7e **9e**

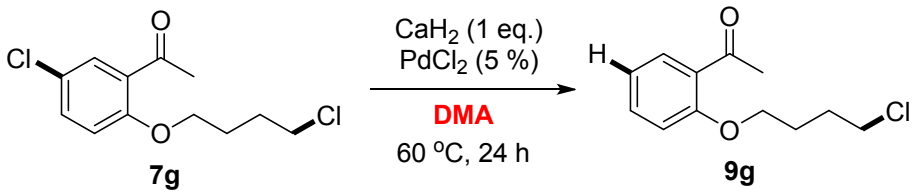
1-(2-(4-Bromobutoxy)phenyl)ethan-1-one (9e). The title compound was prepared according to the general procedure at 60 °C for 5 h, as described above in 82% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.5 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 6.98 (t, *J* = 7.4 Hz, 1H), 6.93 (d, *J* = 8.3 Hz, 1H), 4.09 (t, *J* = 4.9 Hz, 2H), 3.48 (t, *J* = 5.5 Hz, 2H), 2.61 (s, 3H), 2.13 – 1.92 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 199.9, 158.2, 133.7, 130.5, 128.5, 120.8, 112.3, 67.7, 44.7, 32.1, 29.5, 26.8. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{16}BrO_2$ 271.0, found 271.0.



7f **9f**

1-(2-(4-Chlorobutoxy)phenyl)ethan-1-one (9f). The title compound was prepared according to the general procedure at 60 °C for 24 h, as described above in 84% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.5 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 6.99 (t, *J* = 7.3 Hz, 1H), 6.94 (d, *J* = 8.3 Hz, 1H), 4.20 – 4.04 (m, 2H), 3.68 – 3.54 (m, 2H), 2.62 (s, 3H), 2.09 – 1.97 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.8, 158.2,

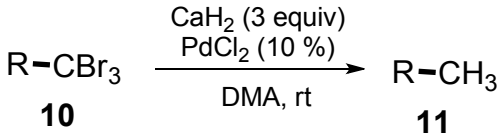
133.7, 130.5, 128.5, 120.7, 112.3, 67.5, 33.3, 32.1, 29.6, 27.9. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{16}ClO_2$ 227.0839, found 227.0842.



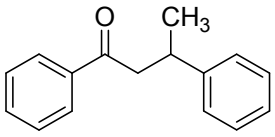
1-(2-(4-Chlorobutoxy)phenyl)ethan-1-one (9g, the same compound as 9f). The title compound was prepared according to the general procedure in DMA at 60 °C for 24 h, as described above in 86% yield.

8. General procedure for the reduction of trihalomethyl groups

8.1. The complete dehalogenation of trihalomethyl groups by using DMA as solvent

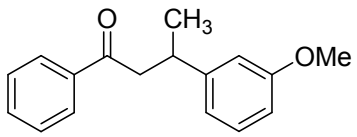


A mixture of $PdCl_2$ (8.8 mg, 0.05 mmol, 10 mol %) and calcium hydride (63 mg, 1.5 mmol, 3 equiv) in DMA (1.0 mL) was stirred at room temperature under N_2 for 10 min until the mixture turned black. Compound **10** (0.5 mmol) in DMA (1.0 mL) was added through syringe, and the mixture was stirred at room temperature for specified time. After the reaction was completed monitored with TLC, a saturated NH_4Cl aqueous solution was added to quench the reaction and the resulting mixture was extracted with EtOAc. The combined organic layers were washed with water and brine and dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography to give desired methyl prouct **11**.



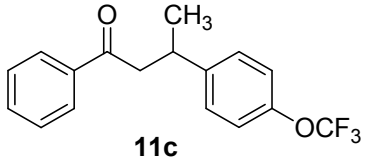
11a

1,3-Diphenylbutan-1-one (11a). The title compound was prepared according to the general procedure in 42% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 – 7.93 (m, 2H), 7.57 – 7.53 (m, 1H), 7.47 – 7.43 (m, 2H), 7.34 – 7.28 (m, 4H), 7.22 – 7.19 (m, 1H), 3.59 – 3.46 (m, 1H), 3.31 (dd, *J* = 16.5, 5.7 Hz, 1H), 3.20 (dd, *J* = 16.5, 8.3 Hz, 1H), 1.35 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.2, 146.7, 137.3, 133.1, 128.67, 128.65, 128.2, 127.0, 126.4, 47.1, 35.7, 22.0. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{17}O$ 225.1, found 225.1.



11b

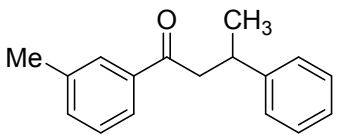
3-(3-Methoxyphenyl)-1-phenylbutan-1-one (11b). The title compound was prepared according to the general procedure in 43% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.56 – 7.53 (m, 1H), 7.46 – 7.42 (m, 2H), 7.26 – 7.21 (m, 1H), 6.87 (d, *J* = 7.5 Hz, 1H), 6.82 (s, 1H), 6.76 – 6.74 (m, 1H), 3.80 (s, 3H), 3.51 – 3.46 (m, 1H), 3.30 (dd, *J* = 16.4, 5.5 Hz, 1H), 3.17 (dd, *J* = 16.5, 8.4 Hz, 1H), 1.33 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 199.2, 159.8, 148.5, 137.3, 133.1, 129.7, 128.7, 128.2, 119.4, 113.1, 111.4, 55.3, 47.1, 35.7, 21.9. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{19}O_2$ 255.1, found 255.1.



11c

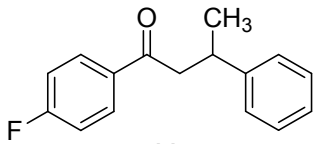
1-Phenyl-3-(4-(trifluoromethoxy)phenyl)butan-1-one (11c). The title compound was prepared according to the general procedure in 50% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, *J* = 7.6 Hz, 2H), 7.55 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.29 (d, *J* = 8.3 Hz, 2H), 7.13 (d, *J* = 8.1 Hz, 2H), 3.60 – 3.48 (m, 1H), 3.28 (dd, *J* = 16.7, 6.2 Hz, 1H), 3.19 (dd, *J* = 16.7, 7.7 Hz, 1H), 1.34 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR

(101 MHz, $CDCl_3$): δ 198.8, 147.7 (d, J = 1.8 Hz), 145.4, 137.2, 133.2, 128.7, 128.3, 128.2, 121.2, 47.0, 35.0, 22.1. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{16}F_3O_2$ 309.1102, found 309.1100.



11d

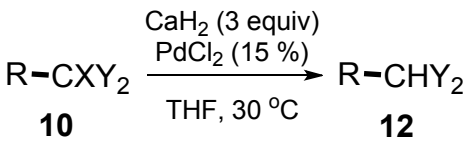
3-Phenyl-1-(m-tolyl)butan-1-one (**11d**). The title compound was prepared according to the general procedure in 54% yield. ^1H NMR (400 MHz, $CDCl_3$): δ 7.75 – 7.73 (m, 2H), 7.38 – 7.27 (m, 6H), 7.23 – 7.19 (m, 1H), 3.55 – 3.48 (m, 1H), 3.30 (dd, J = 16.4, 5.6 Hz, 1H), 3.19 (dd, J = 16.5, 8.3 Hz, 1H), 2.41 (s, 3H), 1.35 (d, J = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 199.4, 146.8, 138.5, 137.4, 133.8, 128.74, 128.65, 128.6, 127.0, 126.4, 125.4, 47.2, 35.7, 22.0, 21.5. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{19}O$ 239.1, found 239.1.



11e

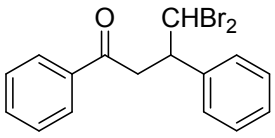
1-(4-Fluorophenyl)-3-phenylbutan-1-one (11e). The title compound was prepared according to the general procedure in 54% yield. ^1H NMR (400 MHz, $CDCl_3$): δ 7.96 – 7.81 (m, 2H), 7.31 – 7.18 (m, 4H), 7.16 – 7.13 (m, 1H), 7.07 – 7.03 (m, 2H), 3.46 – 7.40 (m, 1H), 3.22 (dd, J = 16.4, 5.7 Hz, 1H), 3.10 (dd, J = 16.4, 8.1 Hz, 1H), 1.29 (d, J = 6.8 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 197.6, 165.8 (d, J = 254.5 Hz), 146.5, 133.8 (d, J = 2.7 Hz), 130.8 (d, J = 9.3 Hz), 128.7, 127.0, 126.5, 115.8 (d, J = 21.8 Hz), 47.1, 35.8, 22.0. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{16}FO$ 243.1, found 243.1.

8.2. The mono-dehalogenation of trihalomethyl groups by using THF as solvent



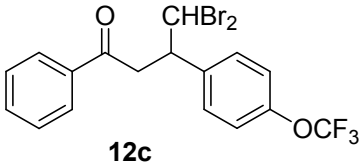
10 **12**

A mixture of $PdCl_2$ (13.3 mg, 0.075 mmol, 15 mol %) and calcium hydride (63 mg, 1.5 mmol, 3 equiv) in THF (1.0 mL) was stirred at room temperature under N_2 for 5 min until the mixture turned black. Compound **10** (0.5 mmol) in THF (0.5 mL) was added through syringe, and the mixture was stirred at 30 °C for specified time. After the reaction was completed monitored with TLC, a saturated NH_4Cl aqueous solution was added to quench the reaction and the resulting mixture was extracted with EtOAc. The combined organic layers were washed with water and brine and dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography to give desired dihalomethyl prouct **12**.



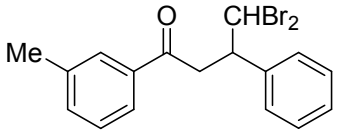
12a

4,4-Dibromo-1,3-diphenylbutan-1-one (**12a**). The title compound was prepared according to the general procedure at 30 °C for 5 h, as described above in 55% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 7.6 Hz, 2H), 7.59 (t, *J* = 7.3 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.39 – 7.30 (m, 5H), 6.05 (d, *J* = 4.0 Hz, 1H), 4.24 – 4.20 (m, 1H), 3.79 (d, *J* = 6.3 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 196.9, 138.9, 136.7, 133.6, 128.9, 128.8, 128.6, 128.2, 128.1, 51.8, 51.3, 41.0. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{15}Br_2O$ 382.9469, found 382.9471.



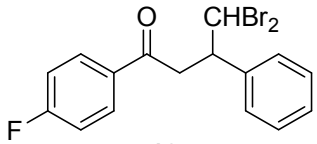
12c

4,4-Dibromo-1-phenyl-3-(4-(trifluoromethoxy)phenyl)butan-1-one (**12c**). The title compound was prepared according to the general procedure at 30 °C for 5 h, as described above in 68% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 7.6 Hz, 2H), 7.60 (t, *J* = 7.3 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.18 (d, *J* = 8.1 Hz, 2H), 6.03 (d, *J* = 3.7 Hz, 1H), 4.29 – 4.14 (m, 1H), 3.83 – 3.70 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 196.6, 149.0, 137.4, 136.5, 133.8, 130.4, 128.9, 128.2, 120.9, 51.0, 50.5, 41.2. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{14}Br_2F_3O_2$ 466.9292, found 466.9303.



12d

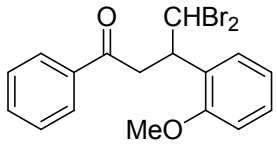
4,4-Dibromo-3-phenyl-1-(*m*-tolyl)butan-1-one (**12d**). The title compound was prepared according to the general procedure at 30 °C for 5 h, as described above in 57% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 – 7.78 (d, *J* = 6.9 Hz, 2H), 7.39 – 7.30 (m, 7H), 6.07 (d, *J* = 4.0 Hz, 1H), 4.24 – 4.20 (m, 1H), 3.79 – 3.77 (m, 2H), 2.42 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 197.1, 138.9, 138.6, 136.8, 134.3, 128.9, 128.7, 128.7, 128.6, 128.1, 125.4, 51.9, 51.3, 41.1, 21.5. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{17}Br_2O$ 396.9626, found 396.9632.



12e

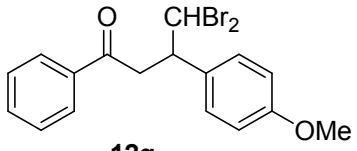
4,4-Dibromo-1-(4-fluorophenyl)-3-phenylbutan-1-one (**12e**). The title compound was prepared according to the general procedure at 30 °C for 5 h, as described above in 67% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 – 7.99 (m, 2H), 7.38 – 7.31 (m, 5H), 7.16 – 7.12 (m, 2H), 6.04 (d, *J* = 4.0 Hz, 1H), 4.22 – 4.18 (m, 1H), 3.75 (d, *J* = 5.8 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 195.3, 166.1 (d, *J* = 255.5 Hz), 138.8,

133.2 (d, J = 2.8 Hz), 130.9 (d, J = 9.3 Hz), 128.7 (d, J = 24.5Hz), 128.2, 116.0 (d, J = 21.9 Hz), 51.7, 51.3, 40.9. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{14}Br_2FO$ 400.9375, found 400.9378.



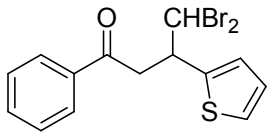
12f

4,4-Dibromo-3-(2-methoxyphenyl)-1-phenylbutan-1-one (**12f**). The title compound was prepared according to the general procedure at 30 °C for 11 h, as described above in 74% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (d, J = 7.6 Hz, 2H), 7.58 (t, J = 7.3 Hz, 1H), 7.48 (t, J = 7.6 Hz, 2H), 7.34 – 7.14 (m, 2H), 6.89 – 6.87 (m, 2H), 6.20 (d, J = 4.7 Hz, 1H), 4.64 – 4.55 (m, 1H), 3.99 – 3.91 (m, 1H), 3.89 (s, 3H), 3.83 – 3.77 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 197.2, 157.2, 137.0, 133.4, 129.0, 128.9, 128.8, 128.2, 127.1, 120.6, 110.9, 55.7, 51.4, 46.3, 39.2. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{17}Br_2O_2$ 412.9575, found 412.9579.



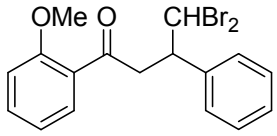
12g

4,4-Dibromo-3-(4-methoxyphenyl)-1-phenylbutan-1-one (**12g**). The title compound was prepared according to the general procedure at 30 °C for 5 h, as described above in 65% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, J = 7.6 Hz, 2H), 7.58 (t, J = 7.3 Hz, 1H), 7.47 (t, J = 7.6 Hz, 2H), 7.29 (d, J = 8.5 Hz, 2H), 6.86 (d, J = 8.5 Hz, 2H), 6.01 (d, J = 3.8 Hz, 1H), 4.22 – 4.07 (m, 1H), 3.78 (s, 3H), 3.77 – 3.69 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 197.1, 159.3, 136.8, 133.5, 130.9, 130.0, 128.8, 128.2, 114.0, 55.3, 52.6, 50.6, 41.0. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{17}Br_2O_2$ 412.9575, found 412.9580.



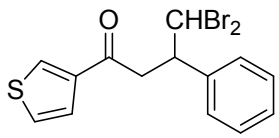
12h

4,4-Dibromo-1-phenyl-3-(thiophen-2-yl)butan-1-one (**12h**). The title compound was prepared according to the general procedure at 30 °C for 19 h, as described above in 62% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.22 – 7.14 (m, 1H), 7.02 – 7.00 (m, 1H), 6.94 – 6.86 (m, 1H), 6.03 (d, *J* = 3.1 Hz, 1H), 4.48 – 4.44 (m, 1H), 3.68 (d, *J* = 6.2 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 196.5, 141.4, 136.6, 133.7, 128.9, 128.3, 127.1, 126.8, 125.2, 51.3, 46.9, 42.8. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{13}Br_2OS$ 388.9033, found 388.9034.



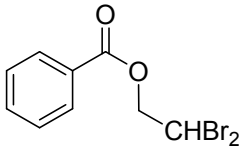
12i

4,4-Dibromo-1-(2-methoxyphenyl)-3-phenylbutan-1-one (**12i**). The title compound was prepared according to the general procedure at 30 °C for 4 h, as described above in 61% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 – 7.53 (m, 1H), 7.48 – 7.45 (m, 1H), 7.33 – 7.27 (m, 5H), 6.99 – 6.94 (m, 2H), 6.03 (d, *J* = 4.2 Hz, 1H), 4.17 – 4.09 (m, 1H), 3.94 (s, 3H), 3.89 – 3.72 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 199.3, 158.6, 139.2, 133.9, 130.5, 129.1, 128.4, 128.0, 127.9, 120.9, 111.7, 55.8, 52.0, 51.6, 46.4. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{17}Br_2O_2$ 412.9575, found 412.9579.



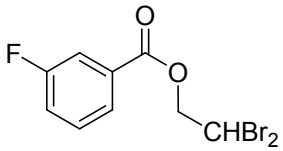
12j

4,4-Dibromo-3-phenyl-1-(thiophen-3-yl)butan-1-one (**12j**). The title compound was prepared according to the general procedure at 30 °C for 12 h, as described above in 51% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 – 8.12 (m, 1H), 7.55 – 7.53 (m, 1H), 7.38 – 7.27 (m, 6H), 6.04 (d, *J* = 4.0 Hz, 1H), 4.23 – 4.14 (m, 1H), 3.77 – 3.58 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 191.2, 142.0, 138.8, 132.4, 128.9, 128.6, 128.2, 127.0, 126.7, 51.7, 51.2, 42.1. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{13}Br_2OS$ 388.9033, found 388.9035.



12k

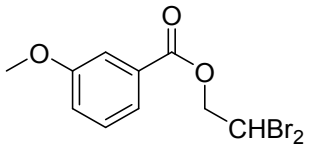
2,2-Dibromoethyl benzoate (**12k**). The title compound was prepared according to the general procedure at 30 °C for 14 h, as described above in 64% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09 (d, *J* = 7.6 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 5.86 (t, *J* = 6.2 Hz, 1H), 4.80 (d, *J* = 6.3 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 165.6, 133.8, 130.0, 129.2, 128.7, 77.4, 77.2, 77.0, 69.6, 39.8. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_9H_9Br_2O_2$ 308.8949, found 308.8958.



12l

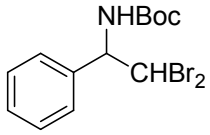
2,2-Dibromoethyl-3-fluorobenzoate (12l). The title compound was prepared according to the general procedure at 30 °C for 2 h, as described above in 72% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.7 Hz, 1H), 7.76 (d, *J* = 9.0 Hz, 1H), 7.46 (dd, *J* = 13.6, 7.8 Hz, 1H), 7.35 – 7.28 (m, 1H), 5.85 (t, *J* = 6.2 Hz, 1H), 4.81 (d, *J* = 6.2 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.3 (d, *J* = 1.5 Hz), 162.5 (d, *J* = 247.6 Hz), 131.1 (d, *J* = 7.5 Hz), 130.2 (d, *J* = 7.5 Hz), 125.6 (d, *J* = 3.0 Hz), 120.7 (d, *J* = 21.1 Hz), 116.8 (d, *J* = 22.6 Hz), 69.7, 39.3. HRMS (ESI): m/z $[M+H]^+$ calcd for

$C_9H_8Br_2FO_2$ 326.8855, found 326.8862.



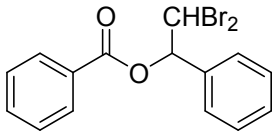
12m

2,2-Dibromoethyl-3-methoxybenzoate (12m). The title compound was prepared according to the general procedure at 30 °C for 14 h, as described above in 69% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.6 Hz, 1H), 7.59 (s, 1H), 7.38 (t, *J* = 8.0 Hz, 1H), 7.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 5.86 (t, *J* = 6.3 Hz, 1H), 4.80 (d, *J* = 6.3 Hz, 2H), 3.87 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.3, 159.6, 130.3, 129.6, 122.3, 120.0, 114.4, 69.5, 55.5, 39.6. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_{11}Br_2O_3$ 338.9054, found 338.9056.



12n

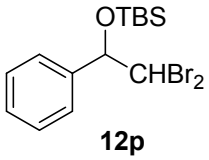
***tert*-Butyl (2,2-dibromo-1-phenylethyl)carbamate (12n).** The title compound was prepared according to the general procedure at 30 °C for 4 h, as described above in 76% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (m, 5H), 5.97 (m, 1H), 5.49 (m, 1H), 5.34 (br, 1H), 1.47 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 154.9, 137.3, 128.5, 127.2, 80.5, 61.5, 50.1, 28.3. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{13}H_{18}Br_2NO_2$ 379.9684, found 379.9689.



12o

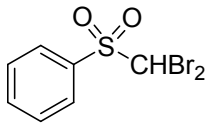
2,2-Dibromo-1-phenylethyl benzoate (12o). The title compound was prepared according to the general procedure at 30 °C for 1 h, as described above in 79% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 7.7 Hz, 2H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.39

(dd, J = 9.1, 6.3 Hz, 4H), 7.31 – 7.23 (m, 3H), 6.29 (d, J = 4.9 Hz, 1H), 5.84 (d, J = 4.9 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.7, 135.6, 133.6, 130.0, 129.3, 129.2, 128.6, 128.5, 127.6, 78.7, 45.7. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{13}Br_2O_2$ 384.9262, found 384.9265.



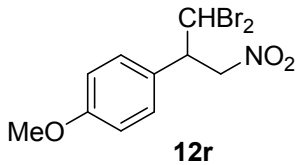
12p

***tert*-Butyl(2,2-dibromo-1-phenylethoxy)dimethylsilane (12p)**. The title compound was prepared according to the general procedure at 30 °C for 1.5 h, as described above in 76% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.58 (m, 2H), 7.56 (d, J = 4.3 Hz, 3H), 5.85 (d, J = 5.2 Hz, 1H), 5.16 (d, J = 5.1 Hz, 1H), 1.12 (s, 9H), 0.37 (s, 3H), 0.08 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.5, 134.3, 133.8, 133.2, 85.7, 57.3, 31.4, 24.0, 1.1, 0.8. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{23}Br_2OSi$ 394.9864, found 394.9868.



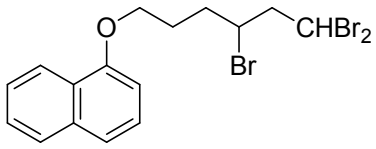
12q

[(Dibromomethyl)sulfonyl]benzene (**12q**). The title compound was prepared according to the general procedure at 30 °C for 2 h, as described above in 61% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (d, J = 7.7 Hz, 2H), 7.78 (t, J = 7.4 Hz, 1H), 7.64 (t, J = 7.7 Hz, 2H), 6.26 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 135.5, 132.3, 131.3, 129.3, 50.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_7H_7Br_2O_2S$ 314.9, found 314.9.



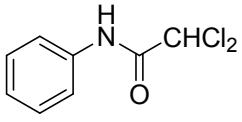
12r

1-(1,1-Dibromo-3-nitropropan-2-yl)-4-methoxybenzene (12r). The title compound was prepared according to the general procedure at 30 °C for 5 h, as described above in 49% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26 (d, *J* = 8.4 Hz, 2H), 6.90 (d, *J* = 8.5 Hz, 2H), 5.83 (d, *J* = 4.4 Hz, 1H), 5.14 (dd, *J* = 13.5, 4.9 Hz, 1H), 4.97 (dd, *J* = 13.4, 9.6 Hz, 1H), 4.24 (dt, *J* = 9.2, 4.5 Hz, 1H), 3.81 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.1, 129.5, 126.5, 114.4, 76.7, 55.3, 53.1, 46.4. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_{12}Br_2NO_3$ 353.9163, found 353.9164.



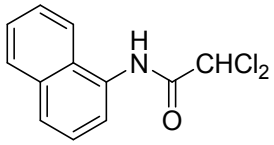
12s

1-[(4,6,6-Tribromohexyl)oxy]naphthalene (12s). The title compound was prepared according to the general procedure at 30 °C for 2 h, as described above in 58% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (t, *J* = 2.2 Hz, 1H), 7.81 (t, *J* = 2.2 Hz, 1H), 7.51–7.48 (m, 2H), 7.44 (d, *J* = 8.2 Hz, 1H), 7.37 (t, *J* = 7.9 Hz, 1H), 6.80 (d, *J* = 7.4 Hz, 1H), 5.93 (dd, *J* = 9.6, 3.8 Hz, 1H), 4.29 – 4.25 (m, 1H), 4.19 (d, *J* = 4.8 Hz, 2H), 2.95 – 2.81 (m, 2H), 2.25 (m, 2H), 2.19 – 2.07 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.5, 134.5, 127.5, 126.4, 125.8, 125.6, 125.2, 122.0, 120.4, 104.6, 67.0, 66.9, 51.6, 36.6, 36.0, 27.5. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{18}Br_3O$ 464.8887, found 464.8889.



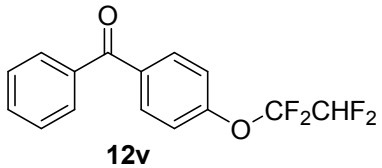
12t

2,2-Dichloro-*N*-phenylacetamide (12t). The title compound was prepared according to the general procedure at 30 °C for 1 h, as described above in 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.56 (d, *J* = 7.5 Hz, 2H), 7.37 (t, *J* = 7.2 Hz, 2H), 7.20 (t, *J* = 7.1 Hz, 1H), 6.10 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.0, 136.4, 129.3, 125.8, 120.4, 67.0. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_8H_8Cl_2NO$ 204.0, found 204.1.



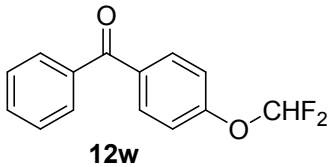
12u

2,2-Dichloro-*N*-(naphthalen-1-yl)acetamide (12u). The title compound was prepared according to the general procedure at 30 °C for 1 h, as described above in 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 7.90-7.85 (m, 3H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.62 – 7.45 (m, 3H), 6.17 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.6, 134.1, 130.5, 128.9, 127.3, 127.1, 126.9, 126.4, 125.6, 121.2, 120.2, 67.1. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{10}Cl_2NO$ 254.0, found 254.0.



12v

Phenyl[4-(1,1,2,2-tetrafluoroethoxy)phenyl]methanone (12v). The title compound was prepared according to the general procedure at 30 °C for 18 h, as described above in 57% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.6 Hz, 2H), 7.80 (d, *J* = 7.3 Hz, 2H), 7.61 (t, *J* = 7.3 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 2H), 5.95 (t, *J* = 53.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.3, 152.0, 137.2, 135.6, 132.7, 131.9, 130.0, 128.4, 121.0. HRMS (ESI): m/z $[M+Na]^+$ calcd for $C_{15}H_{10}F_4NaO_2$ 321.0515, found 321.0522.



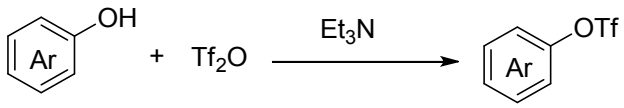
12w

[4-(Difluoromethoxy)phenyl](phenyl)methanone (12w)[1]. The title compound was prepared according to the general procedure at 30 °C for 18 h, as described above in 68% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.1 Hz, 2H), 7.77 (d, *J* = 7.3 Hz, 2H), 7.59 (t, *J* = 7.1 Hz, 1H), 7.48 (t, *J* = 7.3 Hz, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 6.63 (t,

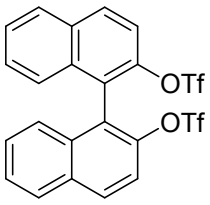
J = 73.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.3, 154.3 (t, J = 6.1 Hz), 137.4, 134.5, 132.6, 132.2, 129.9, 128.4, 118.6, 115.4 (t, J = 524.5 Hz). LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{10}F_2NaO_2$ 271.1, found 271.1.

9. The procedures for the preparation of some substrates

Procedure 1: the preparation of aryl triflates (for: **3s-x**)

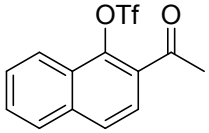


To a solution of phenol (2.0 mmol, 1.0 equiv), DMAP (3.0 mmol, 1.5 equiv) and Et_3N (2.4 mmol, 1.2 equiv) in CH_2Cl_2 (8 mL) at 0 °C was added Tf_2O (2.4 mmol, 1.2 equiv) dropwise within 15 min. Then the reaction was raised to room temperature and stirred until completion of the reaction monitored by TLC. Water was added to quench the reaction and the resulting mixture was extracted with CH_2Cl_2 for three times. The combined organic layers were washed with water and brine and dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography to give desired product **3s-x**.



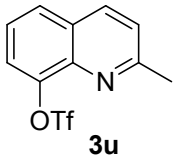
3s

[1,1'-Binaphthalene]-2,2'-diyl bis(trifluoromethanesulfonate) (3s). The title compound was prepared according to the general procedure in 85% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 9.1 Hz, 2H), 8.01 (d, J = 8.2 Hz, 2H), 7.60 (dd, J = 15.2, 8.3 Hz, 4H), 7.41 (t, J = 7.6 Hz, 2H), 7.26 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.3, 133.1, 132.3, 132.0, 128.3, 127.9, 127.3, 126.7, 123.4, 118.1 (q, J = 215.1 Hz), 114.9. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{22}H_{13}F_6O_6S_2$ 551.0, found 551.1.



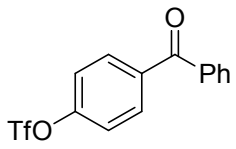
3t

2-Acetylnaphthalen-1-yl trifluoromethanesulfonate (3t). The title compound was prepared according to the general procedure in 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 7.7 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.70 (m, 3H), 2.73 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.3, 142.0, 136.0, 130.0, 128.9, 128.6, 128.5, 127.9, 126.6, 124.4, 122.3, 118.5 (q, *J* = 215.1 Hz), 29.7. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{13}H_{10}F_3O_4S$ 319.0, found 319.0.



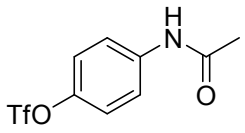
3u

2-Methylquinolin-8-yl trifluoromethanesulfonate (3u). The title compound was prepared according to the general procedure in 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.5 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.57 (d, *J* = 7.5 Hz, 1H), 7.48 (t, *J* = 7.9 Hz, 1H), 7.39 (d, *J* = 8.5 Hz, 1H), 2.79 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.8, 145.6, 140.4, 135.7, 128.0, 127.8, 124.9, 123.5, 120.9, 118.9 (q, *J* = 214.1 Hz), 25.5. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{11}H_9F_3NO_3S$ 292.0, found 292.1.



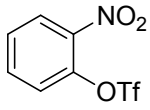
3v

4-Benzoylphenyl trifluoromethanesulfonate (3v). The title compound was prepared according to the general procedure in 89% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.6 Hz, 2H), 7.80 (d, *J* = 7.6 Hz, 2H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 2H), 7.41 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.8, 151.9, 137.6, 136.7, 133.0, 132.1, 130.0, 128.5, 121.4, 117.6 (t, *J* = 215.1 Hz). LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{10}F_3O_4S$ 331.0, found 331.0.



3w

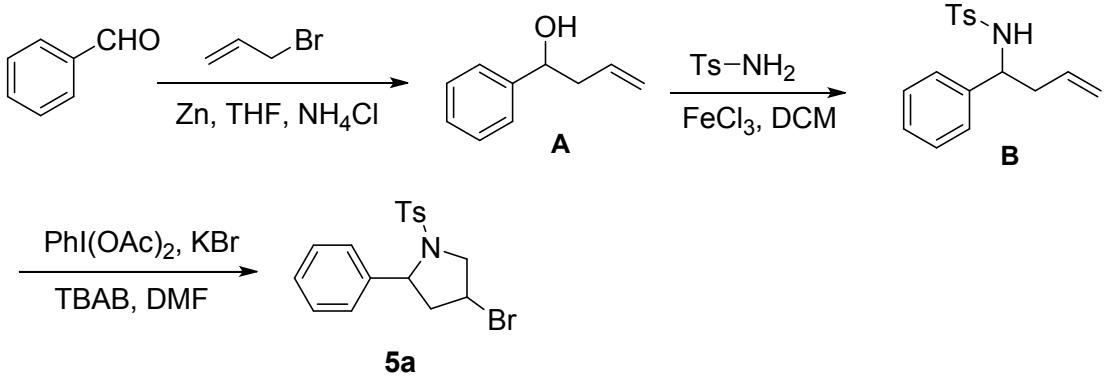
4-Acetamidophenyl trifluoromethanesulfonate (3w). The title compound was prepared according to the general procedure in 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 8.8 Hz, 2H), 7.33 (s, 1H), 7.22 (d, J = 8.9 Hz, 2H), 2.20 (s, 3H). LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_9H_9F_3NO_4S$ 284.0, found 284.1.



3x

2-Nitrophenyl trifluoromethanesulfonate (3x). The title compound was prepared according to the general procedure in 60% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, J = 7.8 Hz, 1H), 7.77 (t, J = 7.5 Hz, 1H), 7.60 (t, J = 7.8 Hz, 1H), 7.48 (d, J = 8.2 Hz, 1H). LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_7H_5F_3NO_5S$ 272.0, found 272.0.

Procedure 2 (for: **5a**)



5a

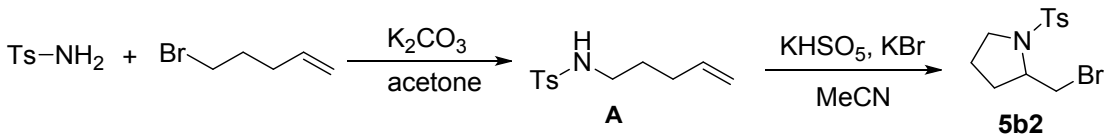
To a suspension of zinc (1.3 g, 20 mmol, 2.0 equiv) in THF (10 mL) at 0 °C was added a solution of allyl bromide (1.2 g, 10 mmol, 1.0 equiv) in THF (80 mL) dropwise. The resulting suspension was stirred for 0.5 h, followed by the addition of a solution of benzaldehyde (1.2 g, 10 mmol, 1.0 equiv) in THF (10 mL) slowly. The reaction mixture was stirred for another 1.5 h, and an aqueous ammonium chloride solution (saturated, 100 mL) was added dropwise. The mixture was extracted with DCM for three times. The organic layers were combined and washed with brine, dried

over $MgSO_4$, filtered and the solvent removed under reduced pressure to give the title compound **A** (1.02 g, 70%) as a colourless oil, which was pure enough to be used in the next step without further purification.

To a stirred solution of **A** (740 mg, 5 mmol , 1.0 equiv) in anhydrous DCM (50 mL) under N_2 was added *p*-toluenesulfonamide (1.1 g, 6.5 mmol, 1.3 equiv) and $FeCl_3$ (162 mg, 1.0 mmol, 0.2 equiv) successively at room temperature. After stirred at room temperature for 1 h, the reaction was quenched by addition of H_2O and then extracted with DCM. The combined organic layer was washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel to afford the corresponding product **B** (902 mg, 60%).

A solution of **B** (1.5 g, 5 mmol) in anhydrous DMF (20 mL) was treated with $PhI(OAc)_2$ (2.42 g, 7.5 mmol, 1.5 equiv), TBAB (805 mg, 2.5 mmol, 0.5 equi) and KBr (2.38 g, 20 mmol, 4.0 equiv). The reaction mixture was stirred at room temperature under N_2 for 5 h, and then quenched with saturated solution of $Na_2S_2O_3$. The mixture was extracted with DCM for three times, dried over anhydrous Na_2SO_4, and the crude product was purified by flash column chromatography to provide the corresponding product **5a** (1.48 g, 78%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, J = 7.2 Hz, 2H), 7.35-7.25 (m, 4H), 7.28-7.26 (m, 1H), 7.26 – 7.21 (m, 2H), 4.74 (t, J = 7.6 Hz, 1H), 4.21-4.13 (m, 1H), 3.88 – 3.78 (m, 1H), 3.64 (t, J = 10.2 Hz, 1H), 292-2.82 (m, 1H), 2.42 (s, 3H), 2.27-2.16 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.9, 141.3, 135.4, 129.9, 128.7, 127.8, 127.5, 126.6, 63.3, 57.4, 46.6, 40.3, 21.7. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{19}BrNO_2S$ 380.0, found 380.0.

Procedure 3 (for: **5b1-5b3**)

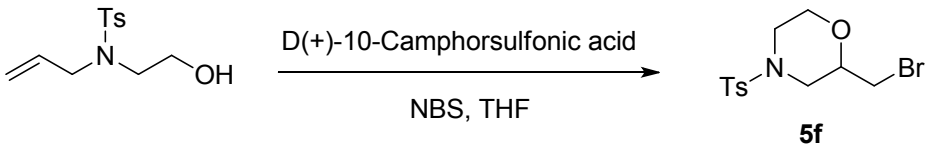


$TsNH_2$ (1.71 g, 10 mmol) was dissolved in acetone (50 mL), followed by the addition of K_2CO_3 (2.76 g, 20 mmol, 2.0 equiv) and 5-bromopent-1-ene (1.63 g, 11 mmol, 1.1

equiv) to the solution. The reaction mixture was refluxed for 6 h. The resulting mixture was quenched with water and extracted with EtOAc for three times. The combined organic layers were washed with water and brine and dried over sodium sulfate, and concentrated under reduced pressure. The crude product was purified by column chromatography to give desired product **A** (2.17 g, 91%).

A solution of **A** (1.20 g, 5 mmol), potassium monopersulfate triple salt (2.02 g, 12 mmol, 1.2 equiv) and KBr (2.56 g, 12 mmol, 1.2 equiv) in MeCN (25 mL) was stirred at room temperature for 7 h. The resulting mixture was quenched with $NaHCO_3$ (aq) and extracted with EtOAc for three times. The combined organic layers were washed with water and brine and dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography to give desired product **5b2** (1.29 g, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.8 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 3.85-3.73 (m, 2H), 3.51-3.43(m, 1H), 3.41-3.31 (m, 1H), 3.20-3.12 (m, 1H), 2.44 (s, 3H), 1.99 – 1.90 (m, 1H), 1.89-1.80 (m, 1H), 1.79 – 1.70 (m, 1H), 1.57-1.52 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.9, 134.1, 130.0, 127.7, 60.5, 49.9, 36.2, 30.4, 23.9, 21.7. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{17}BrNO_2S$ 318.0, found 318.0.

Procedure 4 (for: **5f**)

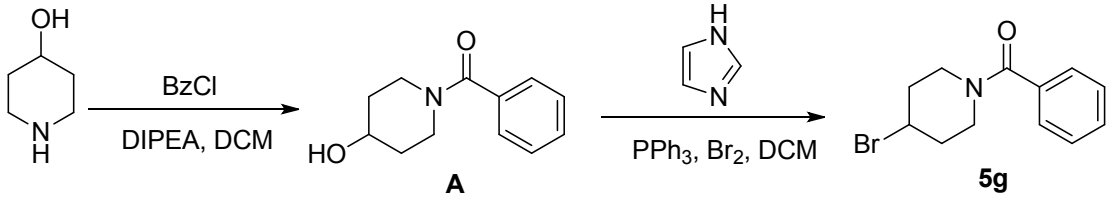


5f

To a solution of *N*-allyl-N-(2-hydroxyethyl)-4-methylbenzenesulfonamide (892 mg, 3.5 mmol) and D(+)-10-Camphorsulfonic acid (81 mg, 0.35 mmol, 0.1 equiv) in THF (10 mL), NBS (685 mg, 3.85 mmol, 1.1 equiv) was added by small portions at 0°C. Then the reaction mixture was stirred at 0°C for 5 h. And the resulting mixture was quenched with $NaHCO_3$ (aq) and extracted with EtOAc, the combined organic layers were washed with water and brine and dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography to give the desired product **5f** (931 mg, 93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d,

J = 8.0 Hz, 2H), 7.35 (d, *J* = 7.9 Hz, 2H), 4.00-3.95 (m, 1H), 3.80 – 3.66 (m, 3H), 3.53-3.46 (m, 1H), 3.38-3.26 (m, 2H), 2.48 – 2.40 (m, 4H), 2.27-2.17 (m 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.5, 132.4, 130.2, 128.2, 74.4, 66.4, 49.2, 45.6, 31.7, 21.9. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{17}BrNO_3S$ 334.0, found 334.1.

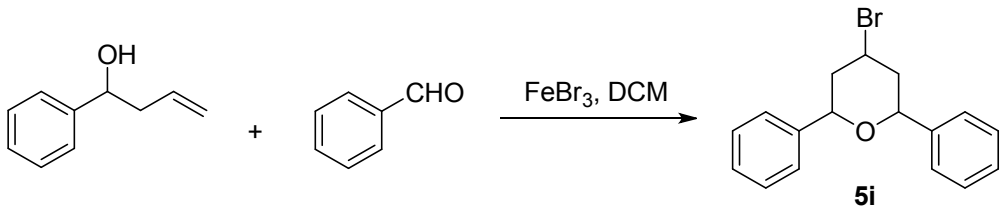
Procedure 5 (for: **5g**)



BzCl (564 mg, 4 mmol, 1.0 equiv) was added slowly to a mixture of 4-hydroxypiperidine (606 mg, 6 mmol, 1.5 equiv), DIPEA (1.29 g, 10 mmol, 2.5 equiv) in DCM (8 mL) at 0 °C. The reaction mixture was warmed to room temperature. After stirred for 2 h, the mixture was added water and extracted with DCM for three times, the combined organic layers were washed with brine and dried over anhydrous Na_2SO_4, and the crude product was purified by flash column chromatography to provide the corresponding product **A** (780 mg, 95%).

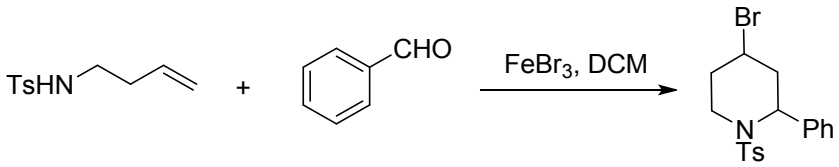
A (451 mg, 2.2 mmol) in DCM (10 mL) was treated with imidazole (150 mg, 2.2 mmol, 1.0 equiv), PPh_3 (577 mg, 2.2 mmol, 1.0 equiv) and Br_2 (352 mg, 2.2 mmol, 1.0 equiv) at rt. The reaction mixture was stirred overnight at room temperature. The resulting brown suspension was added DCM (10 mL) and washed with $Na_2S_2O_3$ (saturated) and brine. The organic phase was dried over Na_2SO_4 and filtered, concentrated under reduced pressure, and the residue was purified by flash chromatography to afford the corresponding product **5g** (340 mg, 58%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.4-7.36 (m, 5H), 4.49 – 4.38 (m, 1H), 4.04 – 3.31 (m, 4H), 2.29-1.84 (dd, *J* = 79.6, 26.4 Hz, 5H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.6, 135.8, 129.9, 128.7, 127.0, 49.0, 46.0, 40.4, 36.3, 35.4. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{15}BrNO$ 268.0, found 268.1.

Procedure 6 (for: **5i**, **5h**, **5y**)



5i

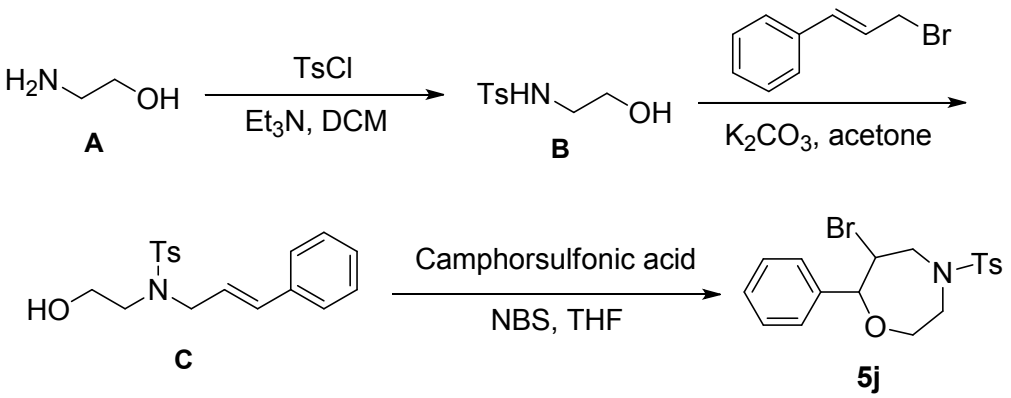
To a solution of 1-phenylbut-3-en-1-ol (740 mg, 5 mmol) and PhCHO (530 mg, 5 mmol, 1.0 equiv) in DCM (25 mL) at 0 °C was added $FeBr_3$ (1.48 g, 5 mmol, 1.0 equiv). The reaction mixture was stirred at 0 °C for 10 min. Water was added to quench the reaction and stirred at 0 °C for another 5 min. The mixture was filtered and the filtrate was extracted with DCM for three times. The combined organic layers were washed with water and brine and dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography to give the desired product **5i** (630 mg, 40%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46–7.40 (m, 4H), 7.40–7.33 (m, 4H), 7.33–7.27 (m, 2H), 4.63-4.54 (m, 2H), 4.53-4.42 (m, 1H), 2.61-2.53 (m, 2H), 2.13 (q, J = 12.1 Hz, 2H). ^{13}C NMR (151 MHz, cdcl$_3$) δ 141.4, 128.6, 127.9, 126.0, 79.9, 46.3, 45.3. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{18}BrO$ 317.1, found 317.1.



5h

4-Bromo-2-phenyl-1-tosylpiperidine (5h). The title compound was prepared according to procedure 6 as described above in 62% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.1 Hz, 2H), 7.37 – 7.28 (m, 6H), 7.26-7.21 (m, 1H), 5.38-5.30 (m, 1H), 4.08 – 3.96 (m, 1H), 3.96.3.85 (m, 1H), 3.08 – 2.98 (m, 1H), 2.89-2.78 (m, 1H), 2.44 (s, 3H), 2.11 – 1.96 (m, 2H), 1.79 – 1.70 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.7, 138.0, 137.3, 130.0, 129.0, 127.5, 127.0, 126.6, 56.8, 43.8, 42.3, 38.6, 36.0, 21.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{18}H_{21}BrNO_2S$ 394.0, found 394.1.

Procedure 7 (for: **5j**)



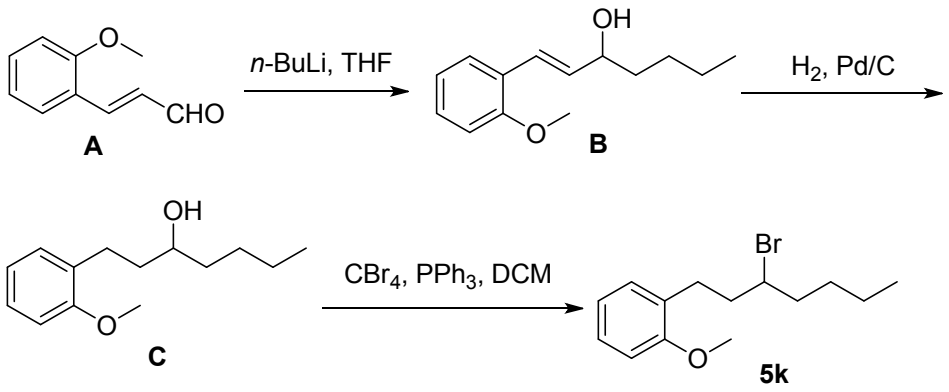
To a solution of **A** (610 mg，10 mmol, 1.0 equiv) in 50 mL of CH_2Cl_2 was added Et_3N (3.03 g, 30 mmol, 3.0 equiv) and TsCl (2.28 g, 12 mmol, 1.2 equiv), and the reaction was stirred at 0 °C for 0.5 h. The resulting solution was warmed slowly to room temperature and stirred for another 16 h. The product was washed with water and extracted with DCM for three times. the combined organic layers were dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The crude product was purified by column chromatography to give the desired product **B**.

N-(2-Hydroxyethyl)-4-methylbenzenesulfonamide **B** (1.08 g, 5 mmol, 1.0 equiv) and K_2CO_3 (6.9 g, 50 mmol, 10.0 equiv) was dissolved in 50 mL of acetone. Cinnamyl bromide (1.28 g, 6.5 mmol, 1.3 equiv) was then added via syringe, and the resulting mixture was stirred at room temperature for 16 h and filtered, the filtrate was then removed in vacuo, and the residue was dissolved in CH_2Cl_2 and washed with water; the organic layer was dried over Na_2SO_4, filtered, and concentrated in vacuo. The residue was purified by column chromatography to give the desired product **C**.

C (662 mg, 2 mmol, 1.0 equiv) was dissolved in 20 mL THF at 0 °C. (±)-CSA (46.4 mg, 0.2 mmol, 0.1 equiv) was added, followed by NBS (392 mg, 2.2 mmol, 1.1 equiv). The mixture was then stirred at 0 °C for 12 h. The reaction was warmed slowly to room temperature and was stirred for additional 5 h. The reaction was quenched by adding 5 mL of saturated $NaHCO_3$ solution to the reaction mixture. The product was then extracted with EtOAc for three times, and the combined organic layers were dried over Na_2SO_4, filtered, and concentrated in vacuo. The crude product was purified by column chromatography to give desired product **5j** (589 mg, 72%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.82-7.72 (m', 2H), 7.41 – 7.31 (m, 5H), 7.31-7.26 (m,

2H), 4.51 (d, J = 9.4 Hz, 1H), 4.22 – 4.09 (m, 2H), 4.07 – 3.95 (m, 1H), 3.86 – 3.70 (m, 2H), 3.60-3.38 (m, 2H), 2.46 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.9, 139.7, 136.1, 130.1, 128.7, 128.5, 127.4, 127.2, 88.8, 70.0, 53.5, 53.0, 50.4, 21.7. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{18}H_{21}BrNO_3S$ 410.0, found 410.0.

Procedure 8 (for: **5k**)



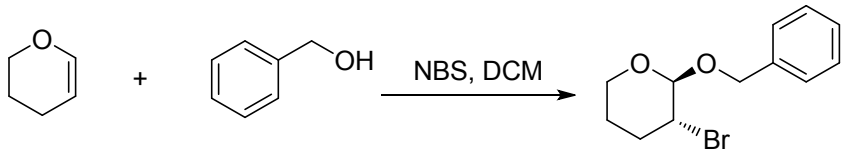
A solution of **A** (1.7 g, 10.4 mmol, 1.0 equiv) in THF (50 mL) under N_2 was cooled to -78 °C. *n*-BuLi (1.6 M, 6.5 mL, 10.4 mmol, 1.0 equiv) was added dropwise, and the resulting mixture was gradually warm to rt and stirred for 1 h at rt. The reaction was then cooled to 0 °C, and a saturated aqueous ammonium chloride (10 mL) was added to quench the reaction. The organic phase was separated, and the aqueous layer was extracted with diethyl ether (2 × 15 mL). The combined organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by silica gel flash chromatography to give the desired product **B** (1.65 g, 72%).

The above product **B** (1.1 g, 5 mmol) was dissolved in MeOH (25 mL), and Pd/C (110 mg, 10% W/W) was added as a catalyst. The reactor was loaded with H_2 balloon and stirred at rt for 5 h. After completion of the reaction monitored by TLC, the solution was filtered to remove Pd/C. The resulting filtrate was evaporated under reduced pressure to give the desired product **C**.

To a solution of the above product **C** (666 mg, 3 mmol) and PPh_3 (1.02 g, 3.9 mmol, 1.3 equiv) in DCM (6 mL) was added CBr_4 (1.30 g, 3.9 mmol, 1.3 equiv) by small portions at 0 °C. Then the reaction mixture was stirred at 0°C for 1 h. The resulting

mixture was purified by column chromatography directly to give the desired product **5k** (670 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.14 (m, 2H), 6.93 – 6.82 (m, 2H), 4.07 – 3.98 (m, 1H), 3.83 (s, 3H), 2.96 – 2.85 (m, 1H), 2.78 – 2.67 (m, 1H), 2.15-2.04 (m, 2H), 1.89-1.80 (m, 2H), 1.55-1.46 (m, 1H), 1.45 – 1.23 (m, 3H), 0.91 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 157.6, 130.2, 129.6, 127.4, 120.5, 110.4, 58.7, 55.3, 39.1, 39.0, 29.8, 28.7, 22.3, 14.1. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{22}BrO$ 285.1, found 285.1.

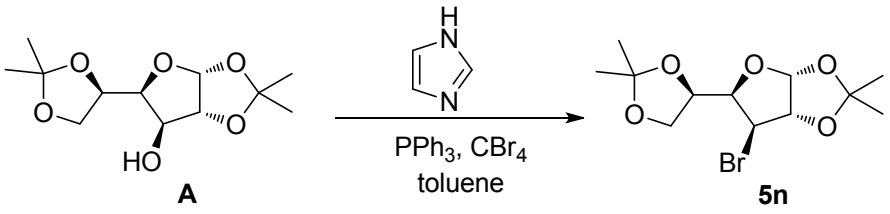
Procedure 9 (for: **5l**)



5l
dr > 5:1

A solution of benzyl alcohol (540 mg, 5 mmol) and NBS (1.07 g, 6 mmol, 1.2 equiv) in DCM (30 mL) was cooled to -10 °C under N_2. A solution of 3,4-dihydro-2*H*-pyran (462 mg, 5.5 mmol, 1.1 equiv) in DCM (5 mL) was added dropwise. The resulting mixture was gradually warmed to 0 °C and stirred for 3 h, and then warmed to rt and stirred overnight. The reaction was quenched with saturated aqueous $Na_2S_2O_3$ and extracted with DCM for three times. The combined organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by silica gel flash chromatography to give the desired product **5l** (810 mg，60%, dr > 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.27 (m, 5H), 4.87 – 4.76 (m, 1H), 4.74 – 4.66 (m, 1H), 4.64 – 4.53 (m, 1H), 4.07 – 4.00 (m, 1H), 3.99 – 3.91 (m, 1H), 3.66 – 3.52 (m, 1H), 2.48 – 2.36 (m, 1H), 2.03 – 1.86 (m, 2H), 1.57 – 1.50 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 137.5, 128.6, 128.1, 128.0, 100.2, 69.8, 62.6, 49.4, 30.1, 23.3. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{16}BrO_2$ 271.0, found 271.0.

Procedure 10 (for: **5n**)

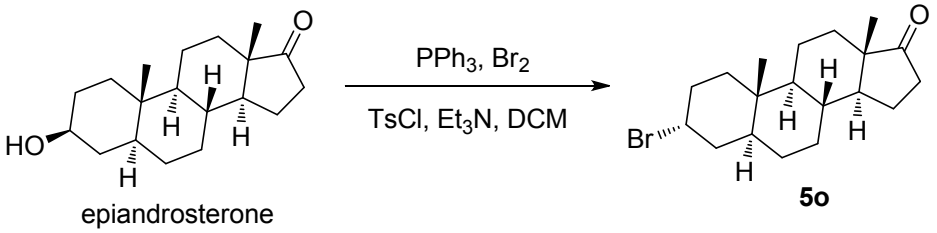


A **5n**

Ref: Org. Biomol. Chem., 2011, 9, 3415

Carbon tetrabromide (14.92 g, 45 mmol, 2.25 equiv) was added to the solution of diacetone-α-D-glucose **A** (5.21 g, 20 mmol), triphenylphosphine (5.24 g, 20 mmol, 1.0 equiv) and imidazole (2.72 g, 40 mmol, 2.0 equiv) in toluene (200 mL). The brown mixture was reflux for 3 h, followed by the addition of $NaHCO_3$ (aq., 50 mL). The organic layer was seperated and washed with aqueous $Na_2S_2O_3$, water and brine sequentially, dried over $MgSO_4$, and concentrated to give a yellow oil. The yellow oil was purified by flash chromatography to give the desired iodide **5n** as a white solid (1.51 g, 23%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.82 (d, J = 3.1 Hz, 1H), 4.68 (t, J = 3.5 Hz, 1H), 4.40 – 4.32 (m, 1H), 4.25-4.19 (m, 1H), 4.106-4.04(m, 2H), 3.94-3.86 (m, 1H), 1.58 (s, 3H), 1.48 (s, 3H), 1.38 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 111.4, 109.8, 105.7, 80.6, 78.8, 76.9, 67.3, 35.3, 26.9, 26.6, 26.3, 25.3. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{20}BrO_5$ 323.0, found 323.1.

Procedure 11 (for: **5o**)



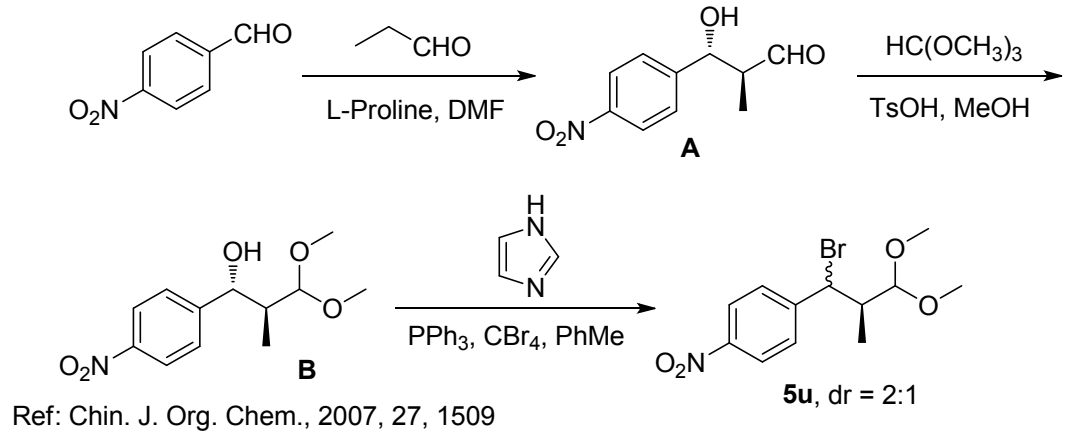
epiandrosterone **5o**

Ref: Chem. Sci., 2018, 9, 4529

To a solution of PPh_3 (1.31 g, 5 mmol, 2.5 eq) in DCM (40 mL) at 0 ºC was added Br_2 (480 mg, 3 mmol, 1.5 equiv) dropwise, followed by the addition of Et_3N (303 mg, 3.0 mmol, 1.5 equiv) and TsCl (76 mg, 0.4 mmol, 0.2 equiv), and the reaction was stirred for 10 min. A solution of epiandrosterone (580 mg, 2 mmol) in DCM (10 mL) was

added dropwise within 10 min and then allowed to stir overnight at room temperature. The reaction was quenched with water, extracted twice with DCM, and the combined organic layers were washed with aqueous $NaHSO_3$, dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The resulting mixture was purified by column chromatography to give the desired product **5o** (485 mg, 69%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.70-4.62 (m, 1H), 2.43-2.32 (m, 1H), 2.07 – 1.95 (m, 1H), 1.94-1.82 (m, 3H), 1.77 – 1.67 (m, 4H), 1.67-1.57 (m, 2H), 1.51 – 1.37 (m, 4H), 1.25-1.14 (m, 5H), 1.06-0.93 (m, 1H), 0.87-0.81 (m, 1H), 0.79 (s, 3H), 0.74 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 221.5, 55.8, 54.1, 51.5, 47.9, 40.3, 37.3, 36.5, 36.0, 35.1, 33.0, 31.6, 31.1, 30.8, 27.7, 21.9, 20.2, 14.0, 12.5. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{19}H_{30}BrO$ 353.1, found 353.2.

Procedure 12 (for: **5u**)



Ref: Chin. J. Org. Chem., 2007, 27, 1509

To a solution of freshly distilled propionaldehyde (1.16 g, 20 mmol, 2.0 equiv) in DMF (35 mL) at 0 °C was added 4-nitrobenzaldehyde (1.5 g, 10 mmol) and L-Proline (230 mg, 2 mmol, 0.2 equiv). After 5 h, the resulting solution was diluted with ethyl acetate and washed successively with water and brine. The combined aqueous layers were back-extracted with 3 portions of dichloromethane. The organic layers were combined, dried over anhydrous Na_2SO_4, and then concentrated.

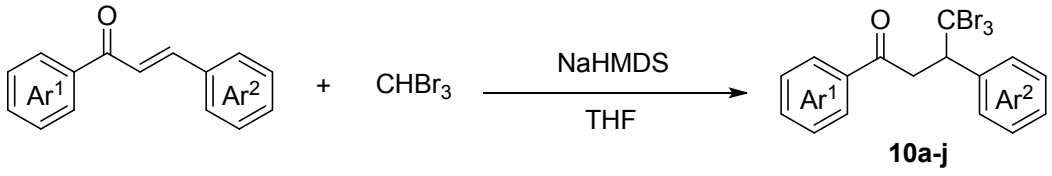
To a solution of the above crude product **A** in MeOH (20 mL) were added triethyl orthoformate (1.59 g, 15 mmol, 1.5 equiv) and *p*-toluenesulfonic acid (172 mg, 1 mmol, 0.1 equiv). After 1 h of stirring at rt, the reaction was quenched with H_2O and extracted with EtOAc. The combined organic layers were washed with brine, dried

over Na_2SO_4 and concentrated. The residue was purified by flash column chromatography to give the desired acetal product **B** (1.57 g, 61%).

CBr_4 (4.15 g, 12.5 mmol, 2.5 equiv) was added to the solution of the above acetal **B** (1.27 g, 5 mmol), triphenylphosphine (1.96 g, 7.5 mmol, 1.5 equiv) and imidazole (680 mg, 10 mmol, 2.0 equiv) in toluene (40 mL). The brown mixture was reflux for 3 h, followed by the addition of $NaHCO_3$ (aq.). The organic layer was seperated and washed with $Na_2S_2O_3$ (aq.), water and brine, dried over $MgSO_4$, and concentrated to give a yellow oil. The yellow oil was purified by flash chromatography to give the desired product **5u** as a yellow oil (1.43g, 90%, dr = 2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.3 Hz, 2H), 7.64 – 7.49 (m, 2H), 5.33 (d, *J* = 4.7 Hz, 0.69H), 5.04 (d, *J* = 9.0 Hz, 0.35H), 4.50 (d, *J* = 3.7 Hz, 0.34H), 4.12 (d, *J* = 6.4 Hz, 0.62H), 3.55 – 3.38 (m, 4H), 3.30 (s, 2H), 2.57 – 2.47 (m, 1H), 2.16 – 2.06 (m, 1H), 1.06 (d, *J* = 6.6 Hz, 2H), 0.83 (d, *J* = 6.9 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.1, 147.6, 147.5, 147.46, 129.3, 129.26, 123.9, 123.7, 106.8, 106.6, 56.7, 56.5, 55.9, 55.8, 54.5, 54.2, 44.2, 44.1, 10.8. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{12}H_{17}BrNO_4$ 318.0, found 318.1.

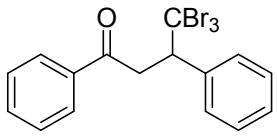
Procedure 13: the preparation of various trihalomethyl substrates

I) Compounds 10a-j



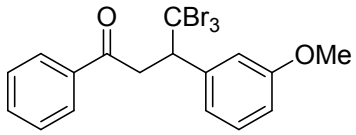
10a-j

To a solution of chalcone (3 mmol, 1 equiv) in dry THF (8 mL) at -60 °C under N_2 was added $CHBr_3$ (4.5 mmol, 1.5 equiv) in THF (1 mL), then NaHMDS (6 mmol, 2 equiv) was added slowly *via* syringe. The reaction was stirred at -60 °C for 10-20 min and then quenched with water, extracted for three times with ethyl acetate, the organic layers were combined, washed with saturated brine, dried over anhydrous sodium sulfate, concentrated under reduced pressure, and the residue was purified by column chromatography to give the desired product **10a-j**.



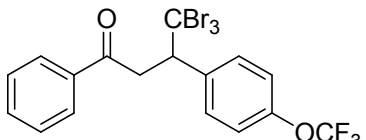
10a

4,4,4-Tribromo-1,3-diphenylbutan-1-one (10a). The title compound was prepared according to the general procedure in 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96-7.94 (m, 2H), 7.64-7.62 (m, 2H), 7.57-7.55 (m, 1H), 7.48-7.44 (m, 2H), 7.35-7.32 (m, 3H), 4.71 (dd, *J* = 7.7, 4.1 Hz, 1H), 4.03-4.01 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 195.5, 138.2, 136.6, 133.6, 130.4, 128.8, 128.6, 128.22, 128.17, 62.9, 50.5, 43.8. HRMS(ESI): m/z $[M + Na]^+$ calcd for $C_{16}H_{13}Br_3NaO$ 482.8394, found 482.8395.



10b

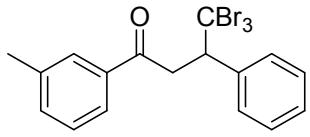
4,4,4-Tribromo-3-(3-methoxyphenyl)-1-phenylbutan-1-one (10b). The title compound was prepared according to the general procedure in 79% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, *J* = 7.6 Hz, 2H), 7.63-7.52 (m, 1H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.29-7.14 (m, 3H), 6.92-6.86 (m, 1H), 4.69 (dd, *J* = 8.0, 3.6 Hz, 1H), 4.00-3.97 (m, 2H), 3.79 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 195.4, 159.1, 139.7, 136.5, 133.5, 129.0, 128.8, 128.2, 122.8, 116.5, 113.5, 62.8, 55.3, 50.1, 43.9. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{16}Br_3O_2$ 490.9, found 490.9.



10c

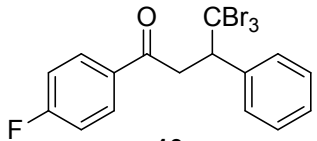
4,4,4-Tribromo-1-phenyl-3-(4-(trifluoromethoxy)phenyl)butan-1-one (10c). The title compound was prepared according to the general procedure in 43% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, *J* = 7.6 Hz, 2H), 7.66 (d, *J* = 8.5 Hz, 2H), 7.59 (t,

J = 7.3 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.17 (d, *J* = 8.2 Hz, 2H), 4.73 (dd, *J* = 8.6, 3.0 Hz, 1H), 4.11-3.91 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 195.3, 149.3 (d, *J* =1.4 Hz), 136.8, 136.4, 133.8, 131.8, 128.9, 128.2, 120.4, 62.2, 49.5, 43.8. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{13}Br_3F_3O_2$ 544.8, found 544.8.



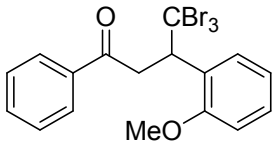
10d

4,4,4-Tribromo-3-phenyl-1-(m-tolyl)butan-1-one (10d). The title compound was prepared according to the general procedure in 71% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76-7.75 (m, 2H), 7.65-7.63 (m, 2H), 7.39-7.33 (m, 5H), 4.71 (dd, *J* = 7.6, 4.1 Hz, 1H), 4.01-3.99 (m 2H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 195.7, 138.7, 138.3, 136.6, 134.3, 130.4, 128.72, 128.70, 128.6, 128.2, 125.4, 63.0, 50.5, 43.9, 21.5. LR-MS (ESI): m/z $[M+Na]^+$ calcd for $C_{17}H_{15}Br_3NaO$ 496.9, found 496.9.



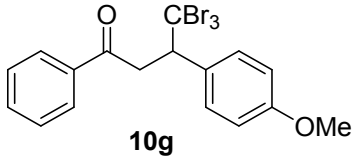
10e

4,4,4-Tribromo-1-(4-fluorophenyl)-3-phenylbutan-1-one (10e). The title compound was prepared according to the general procedure in 86% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99-7.96 (m, 2H), 7.64-7.61 (m, 2H), 7.34-7.26 (m, 3H), 7.12 (t, *J* = 8.4 Hz, 2H), 4.70 (dd, *J* = 6.9, 4.8 Hz, 1H), 4.02-3.98 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 194.0, 166.0 (d, *J* = 255.5 Hz), 138.1, 133.0 (d, *J* = 3.1 Hz), 130.9 (d, *J* = 9.4 Hz), 130.3, 128.7, 128.2, 116.0 (d, *J* = 22.0 Hz), 63.0, 50.3, 43.7. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{13}Br_3FO$ 478.8, found 478.9.



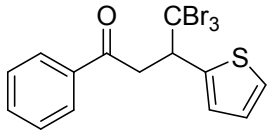
10f

4,4,4-Tribromo-1-(2-methoxyphenyl)-3-phenylbutan-1-one (**10f**). The title compound was prepared according to the general procedure in 62% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.65 (d, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.3 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.31-7.28 (m, 1H), 6.91 (t, *J* = 7.6 Hz, 2H), 5.44-5.42 (m, 1H), 4.06-3.93 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 195.8, 158.5, 136.7, 133.4, 129.6, 128.8, 128.2, 127.4, 127.1, 120.3, 111.6, 56.1, 53.1, 50.6, 44.0. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{16}Br_3O_2$ 490.9, found 490.9.



10g

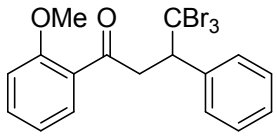
4,4,4-Tribromo-3-(4-methoxyphenyl)-1-phenylbutan-1-one (**10g**). The title compound was prepared according to general procedure in 45% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, *J* = 6.1 Hz, 2H), 7.54-7.46 (m, 5H), 6.85 (d, *J* = 7.0 Hz, 2H), 4.64 (s, 1H), 3.99 (d, *J* = 3.8 Hz, 2H), 3.78 (s, 3H);^{13}C NMR (151 MHz, $CDCl_3$): δ 195.7, 159.7, 136.6, 133.5, 131.5, 130.1, 128.8, 128.2, 113.5, 62.4, 55.3, 52.0, 43.7. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{16}Br_3O_2$ 490.9, found 490.9.



10h

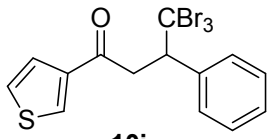
4,4,4-Tribromo-1-phenyl-3-(thiophen-2-yl)butan-1-one (10h). The title compound was prepared according to the general procedure in 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, *J* = 7.6 Hz, 2H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.26-7.24 (m, 2H), 6.97-6.88 (m, 1H), 5.01 (t, *J* = 5.8 Hz, 1H), 3.96 (d, *J* = 5.9 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 195.2, 140.4, 136.5, 133.7, 129.7, 128.9, 128.3,

126.3, 125.9, 59.2, 50.3, 45.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{12}Br_3OS$ 466.8, found 466.8.



10i

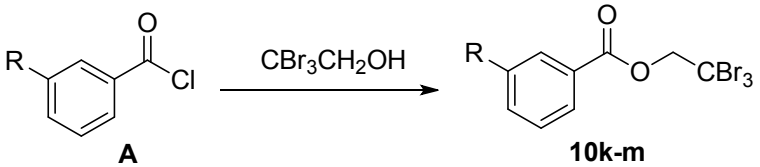
4,4,4-Tribromo-1-(2-methoxyphenyl)-3-phenylbutan-1-one (**10i**). The title compound was prepared according to the general procedure in 62% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51-7.49 (m, 2H), 7.41-7.36 (m, 2H), 7.27-7.25 (m, 3H), 6.97-6.79 (m, 2H), 4.54 (dd, *J* = 8.1, 3.2 Hz, 1H), 4.00-3.97 (m, 2H), 3.89 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 198.4, 159.0, 138.8, 134.4, 131.1, 131.0, 128.9, 128.4, 128.3, 121.4, 112.1, 63.7, 56.3, 51.3, 49.4. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{17}H_{16}Br_3O_2$ 490.9, found 490.9.



10j

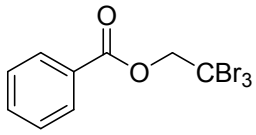
4,4,4-Tribromo-3-phenyl-1-(thiophen-3-yl)butan-1-one (**10j**). The title compound was prepared according to the general procedure in 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12-8.10 (m, 1H), 7.62-7.60 (m, 2H), 7.51 (d, *J* = 4.8 Hz, 1H), 7.40-7.27 (m, 4H), 4.67 (dd, *J* = 7.6, 4.3 Hz, 1H), 3.95-3.87 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 189.7, 141.8, 138.1, 132.5, 130.3, 128.7, 128.2, 127.0, 126.7, 62.8, 50.3, 44.9. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{12}Br_3OS$ 466.8, found 466.8.

II) Compounds 10k-m



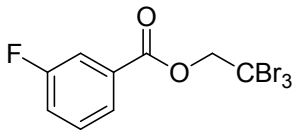
A **10k-m**

To a solution of 2,2,2-tribromoethanol (592 mg, 2.1 mmol, 1.05 equiv), diisopropylethylamine (388 mg, 3.0 mmol, 1.5 equiv) and DMAP (0.2 mmol, 0.1 equiv) in DCM (15 mL) was added acyl chloride **A** (2.0 mmol, 1.0 equiv) slowly, then the reaction was stirred at rt for 1 h. The reaction was quenched with 5% aqueous $NaHCO_3$ and extracted with DCM for three times, the organic layers were combined, washed with saturated brine, dried over anhydrous sodium sulfate, concentrated under reduced pressure, and the residue was purified by column chromatography to give the desired product **10k-m**.



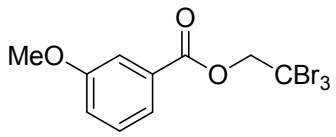
10k

2,2,2-Tribromoethyl benzoate (10k). The title compound was prepared according to the general procedure in 79% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 7.6 Hz, 1H), 7.64 (t, J = 7.4 Hz, 1H), 7.51 (t, J = 7.6 Hz, 1H), 5.17 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.7, 133.8, 130.1, 128.8, 128.6, 77.3, 35.8. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_9H_8Br_3O_2$ 386.8, found 386.7.



10l

2,2,2-Tribromoethyl-3-fluorobenzoate (10l). The title compound was prepared according to the general procedure in 72% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 7.6 Hz, 1H), 7.84 (d, J = 8.8 Hz, 1H), 7.49 (dd, J = 13.5, 7.7 Hz, 1H), 7.34 (t, J = 7.4 Hz, 1H), 5.16 (s, 2H). LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_9H_7Br_3FO_2$ 404.8, found 404.8.

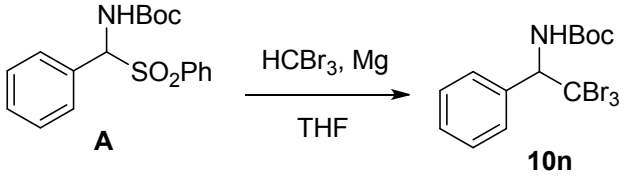


10m

2,2,2-Tribromoethyl-3-methoxybenzoate (10m). The title compound was prepared according to the general procedure in 69% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78

(d, J = 7.5 Hz, 1H), 7.68 (s, 1H), 7.41 (t, J = 7.9 Hz, 1H), 7.17 (d, J = 7.9 Hz, 1H), 5.16 (s, 2H), 3.88 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.3, 159.6, 130.3, 129.6, 122.3, 120.0, 114.4, 69.5, 55.5, 39.6. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_{10}Br_3O_3$ 416.8, found 416.7.

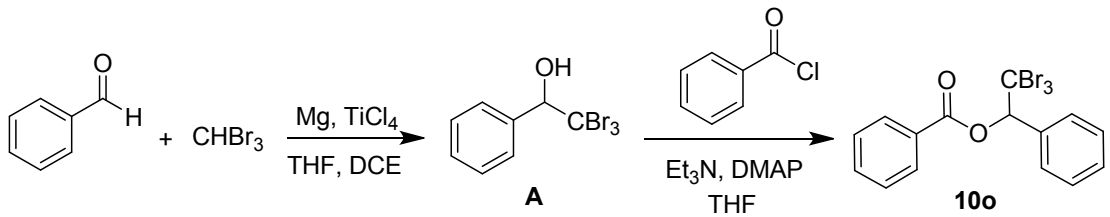
III) Compound 10n



A **10n**

A solution of **A** (347 mg, 1 mmol) in THF (5 mL) was added Mg (192 mg, 8 mmol) and $HCBr_3$ (5.56 g, 22 mmol) at 0 °C. The reaction was stirred and warmed to rt within 2 h. Aqueous NH_4Cl was added to quench the reaction, and extracted with EtOAc for three times, the organic layers were combined, washed with saturated brine, dried over anhydrous sodium sulfate, concentrated under reduced pressure, and the residue was purified by column chromatography to give the desired product **10n**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, J = 6.2 Hz, 2H), 7.39 – 7.38 (m, 3H), 5.79 – 5.53 (m, 1H), 1.45 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 154.3, 135.9, 129.8, 129.1, 128.1, 81.0, 70.0, 50.7, 28.4. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{13}H_{17}Br_3NO_2$ 457.9, found 457.9.

IV) Compound 10o



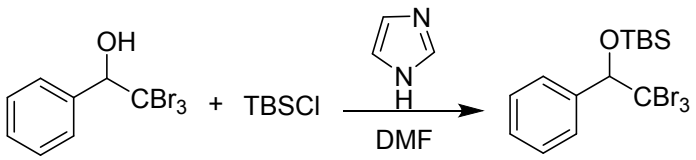
A **10o**

A mixture of Mg (576 mg, 24.0 mmol, 6.0 equiv), 1,2-dichloroethane (40 mL) and $TiCl_4$ (2 mL) was stirred at -30 °C under N_2 for 1 min, followed by the addition of aldehyde (424 mg, 4.0 mmol, 1.0 equiv) and $HCBr_3$ (6 mL), and stirred for 10 min before THF (6 mL) was added. The reaction was stirred at -30 °C for another 5 h. Aqueous NH_4Cl was added to quench the reaction, and extracted with DCM for three

times, the organic layers were combined, washed with saturated brine, dried over anhydrous sodium sulfate, concentrated under reduced pressure, and the residue was purified by column chromatography to give the desired product **A**.

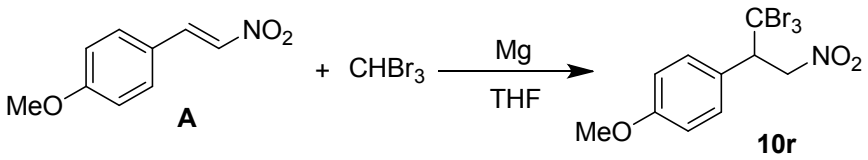
To a solution of above **A** (1.0 mmol, 1.0 equiv), DMAP (0.5 mmol, 0.5 equiv) and Et_3N (4.0 mmol, 4.0 equiv) was added benzoyl chloride (4.0 mmol, 4.0 equiv). The reaction was stirred at rt for 5 h. Water was added to quench the reaction, and extracted with EtOAc for three times, the organic layers were combined, washed with saturated brine, dried over anhydrous sodium sulfate, concentrated under reduced pressure, and the residue was purified by column chromatography to give the desired product **10o** in 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, J = 7.5 Hz, 2H), 7.80 (d, J = 7.0 Hz, 2H), 7.63 (t, J = 6.9 Hz, 1H), 7.51 (t, J = 7.0 Hz, 2H), 7.45 – 7.35 (m, 3H), 6.60 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.0, 133.8, 133.7, 130.1, 130.0, 129.7, 129.0, 128.6, 127.8, 84.3, 45.2. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{12}Br_3O_2$ 462.8, found 462.8.

V) Compound 10p



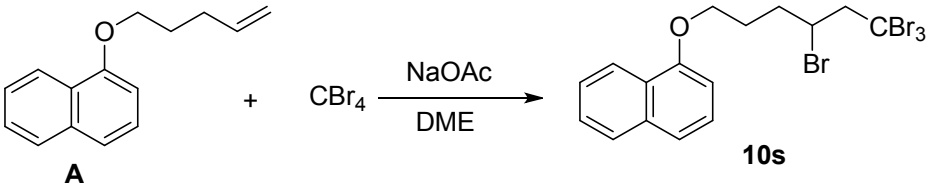
A solution of 2,2,2-tribromo-1-phenylethanol (359 mg, 1 mmol) in DMF (0.5 mL) at 0 °C was added imidazole (544 mg, 8.0 mmol, 8.0 equiv) and TBSCl (904 mg, 6.0 mmol, 6.0 equiv). The reaction was warmed to rt and stirred for 3 h. Water was added to quench the reaction, and extracted with EtOAc for three times, the organic layers were combined, washed with saturated brine, dried over sodium sulfate, concentrated under reduced pressure, and the residue was purified by column chromatography to give the desired product **10p** in 66% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 7.0 Hz, 2H), 7.74 – 7.65 (m, 3H), 5.40 (s, 1H), 1.27 (s, 9H), 0.53 (s, 3H), 0.10 (s, 3H). LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{22}Br_3OSi$ 472.9, found 472.9.

VI) Compound 10r



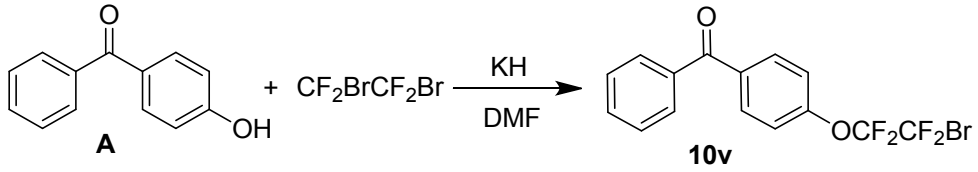
A solution of **A** (358 mg, 2.0 mmol, 1.0 equiv) in THF (9 mL) was added Mg (384 mg, 16.0 mmol, 8.0 equiv). The reaction was cooled to 0 °C and $CHBr_3$ (11.1 g, 44 mmol, 22 equiv) was added within 10 min. The reaction was stirred at 0 °C for 30 min and then warmed to rt gradually. When the reaction was completed monitored by TLC, it was filtered and the filtrate was added ice-water, and extracted with EtOAc for three times, the organic layers were combined, washed with saturated brine, dried over sodium sulfate, concentrated under reduced pressure, and the residue was purified by column chromatography to give the desired product **10r** in 71% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49 (d, *J* = 8.5 Hz, 2H), 6.91 (d, *J* = 8.5 Hz, 2H), 5.40 (dd, *J* = 13.3, 3.3 Hz, 1H), 5.10 (dd, *J* = 13.0, 10.7 Hz, 1H), 4.67 (dd, *J* = 10.3, 3.3 Hz, 1H), 3.82 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.6, 131.4, 125.9, 114.1, 78.0, 64.0, 55.4, 44.2. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{10}H_{11}Br_3NO_3$ 431.8, found 431.8.

VII) Compound 10s

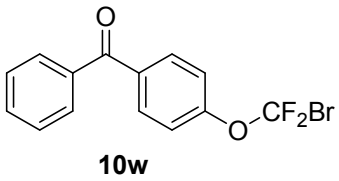


A solution of CBr_4 (10.0 mmol, 2.0 equiv) and NaOAc (7.5 mmol, 1.5 equiv) in 1,2-dimethoxyethane (20 mL) was added **A** (5.0 mmol, 1.0 equiv) under N_2. The reaction was refluxed until completion monitored by TLC. The reaction was quenched with water and extracted with methyl *tert*-butyl ether for three times, the organic layers were combined, washed with saturated brine, dried over sodium sulfate, concentrated under reduced pressure, and the residue was purified by column chromatography to give the desired product **10s** in 69% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 7.8 Hz, 1H), 7.79 (d, *J* = 7.5 Hz, 1H), 7.51 – 7.40 (m, 3H), 7.37 (t, *J* = 7.8 Hz, 1H), 6.81 (d, *J* = 7.4 Hz, 1H), 4.35 (dd, *J* = 8.4, 4.2 Hz, 1H), 4.27 – 4.16 (m, 2H), 3.92 (dd, *J* = 16.1, 4.1 Hz, 1H), 3.62 (dd, *J* = 16.1, 5.2 Hz, 1H), 2.53 (ddd, *J* = 14.4, 10.6, 3.7 Hz, 1H), 2.34 – 2.11 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.5, 134.5, 127.5, 126.4, 125.8, 125.6, 125.2, 122.0, 120.4, 104.6, 77.3, 77.0, 76.7, 67.0, 66.9, 51.6, 36.6, 36.0, 27.5. LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{17}Br_4O$ 544.8, found 544.8.

VIII) Compound 10v-w

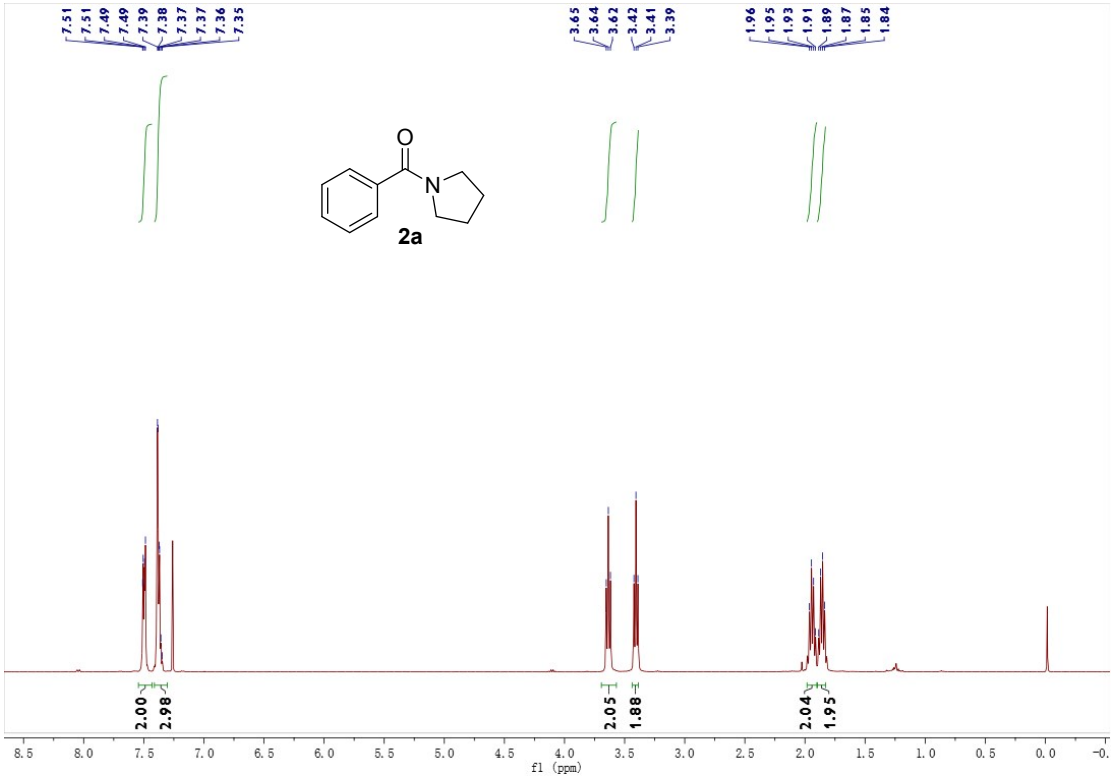


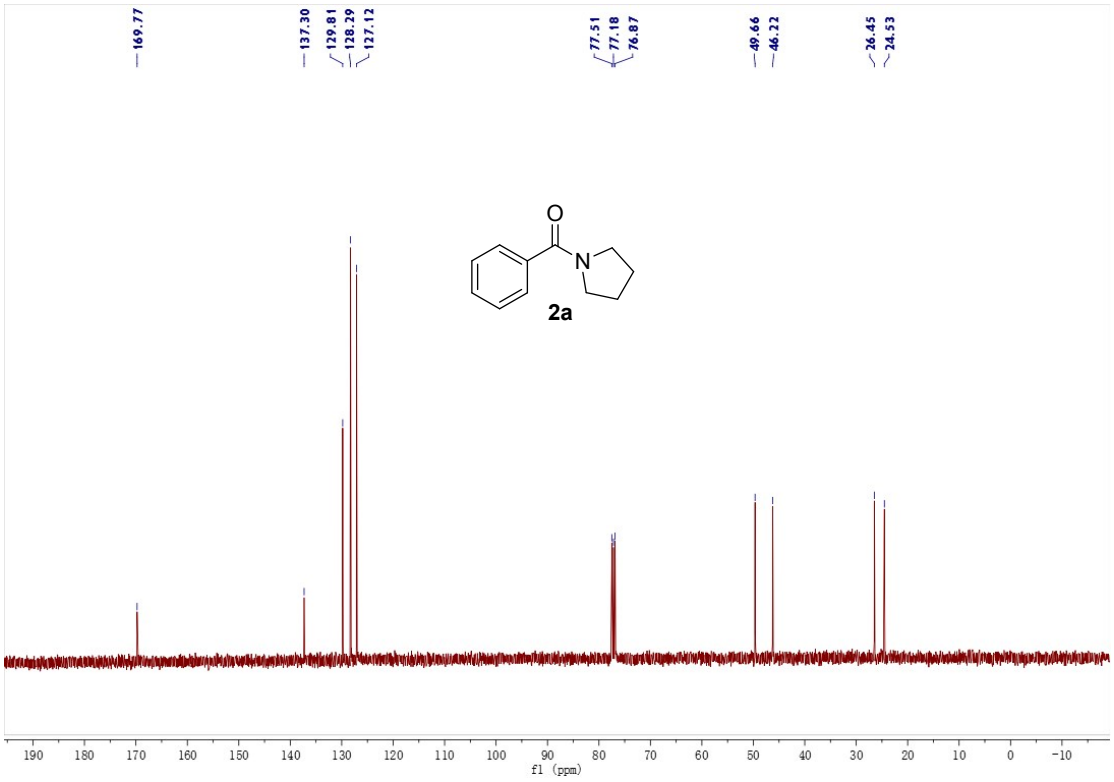
A suspension of KH (3.15 mmol, 1.05 equiv) in DMF (2 mL) was added **A** (3.0 mmol, 1.0 equiv) in portions within 30 min at 10 °C. Then 1,2-dibromotetrafluoroethane was added, and the resulting mixture was heated at 120 °C until completion monitored by TLC. The reaction was quenched with water and extracted with EtOAc for three times, the organic layers were combined, washed with saturated brine, dried over sodium sulfate, concentrated under reduced pressure, and the residue was purified by column chromatography to give the desired product **10v** in 79% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.5 Hz, 2H), 7.80 (d, *J* = 7.4 Hz, 2H), 7.62 (t, *J* = 7.3 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.35 (d, *J* = 8.3 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 195.2, 151.9, 137.2, 136.0, 132.8, 131.9, 130.0, 128.5, 121.1, 116.2 (t, *J* = 51.3 Hz), 113.6 (t, *J* = 43.8 Hz). LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{15}H_{10}BrF_4O_2$ 377.0, found 377.0.

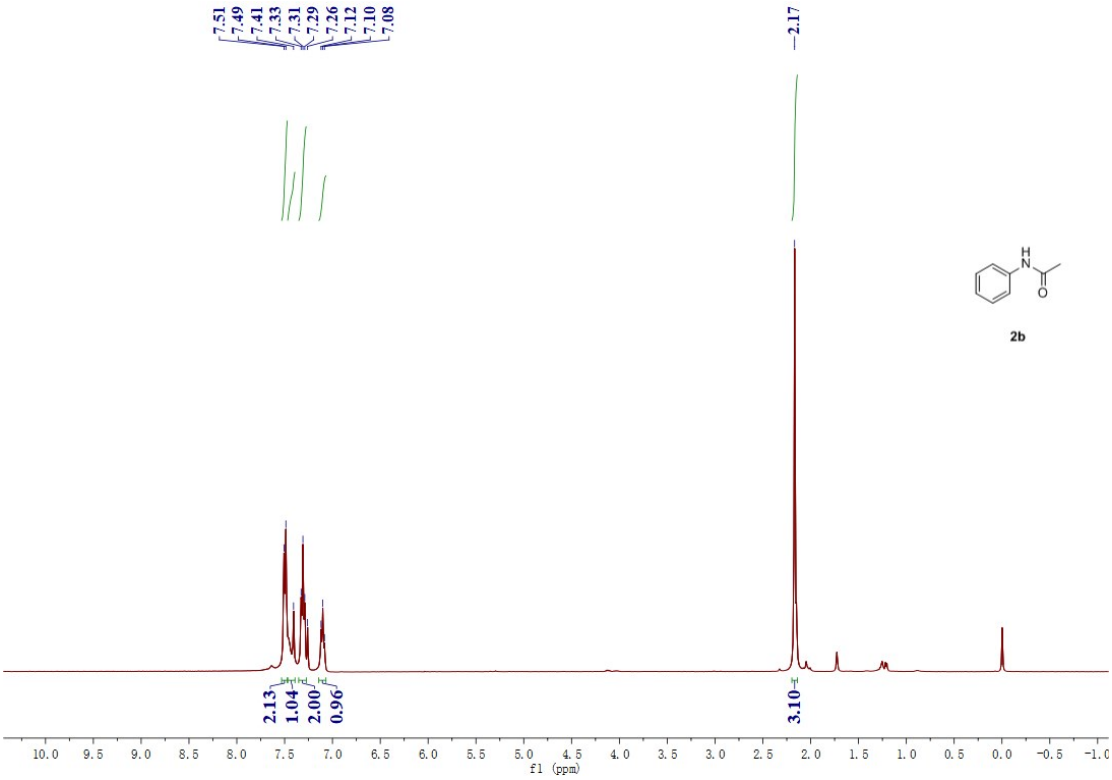


[4-(Bromodifluoromethoxy)phenyl](phenyl)methanone (10w). The title compound was prepared according to the general procedure in 73% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.9 (d, *J* = 8.6 Hz, 2H), 7.8 (d, *J* = 7.4 Hz, 2H), 7.6 (t, *J* = 7.3 Hz, 1H), 7.5 (t, *J* = 7.5 Hz, 2H), 7.4 (d, *J* = 8.3 Hz, 2H). LR-MS (ESI): m/z $[M+H]^+$ calcd for $C_{14}H_{10}BrF_2O_2$ 327.0, found 327.0.

10. ^{1}H and ^{13}C NMR spectra of products



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7.29
7.26
7.12
7.10
7.08
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2b
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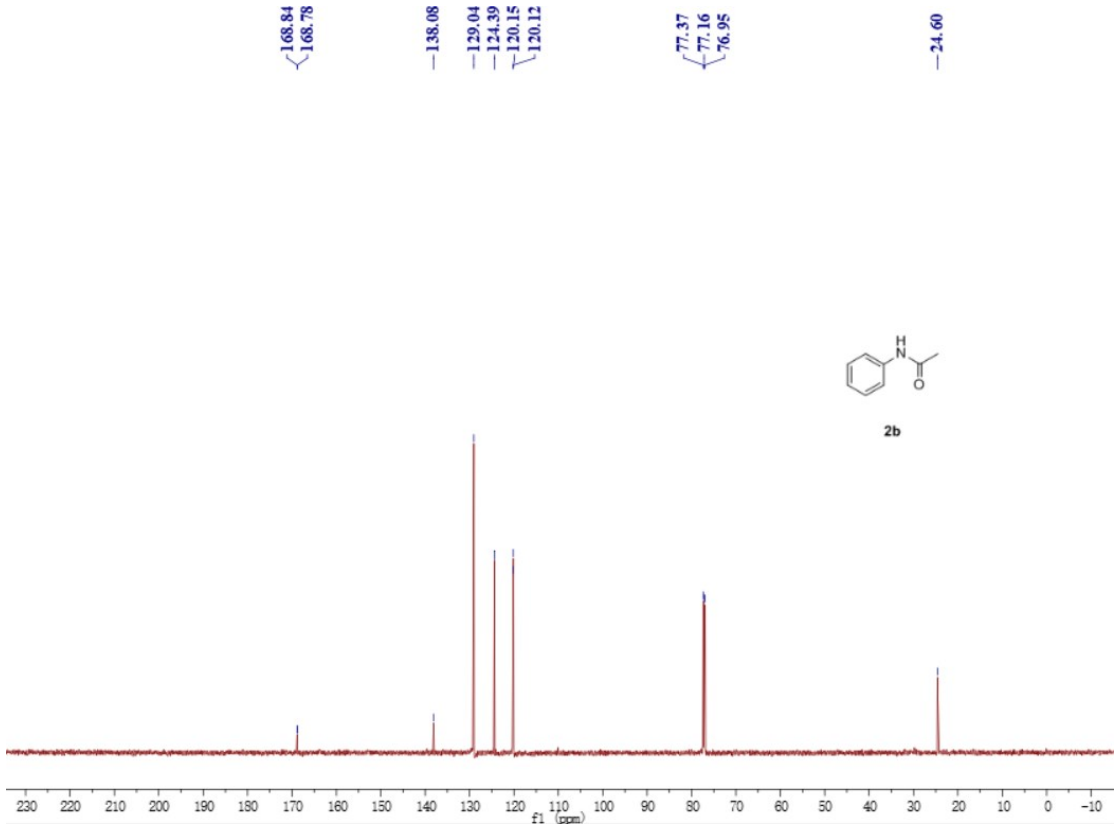
2.00
0.96
3.10
f1 (ppm)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124.39
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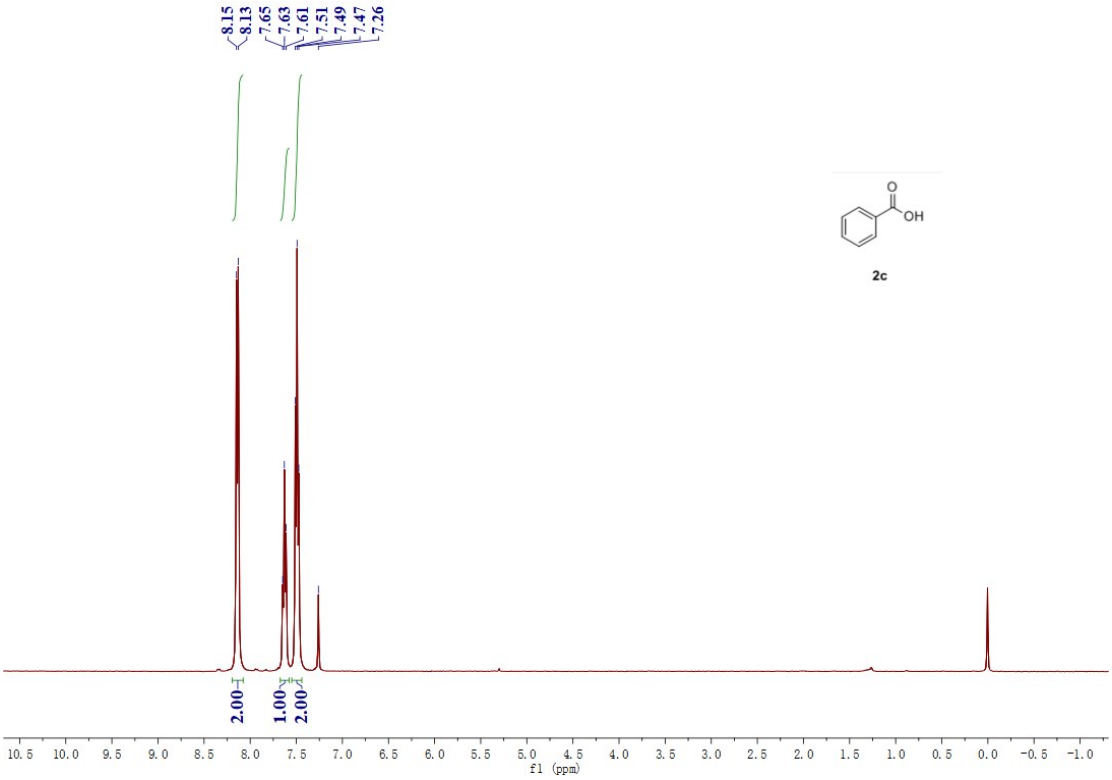
120.12
77.37
77.16
76.95
24.60
2b
f1 (ppm)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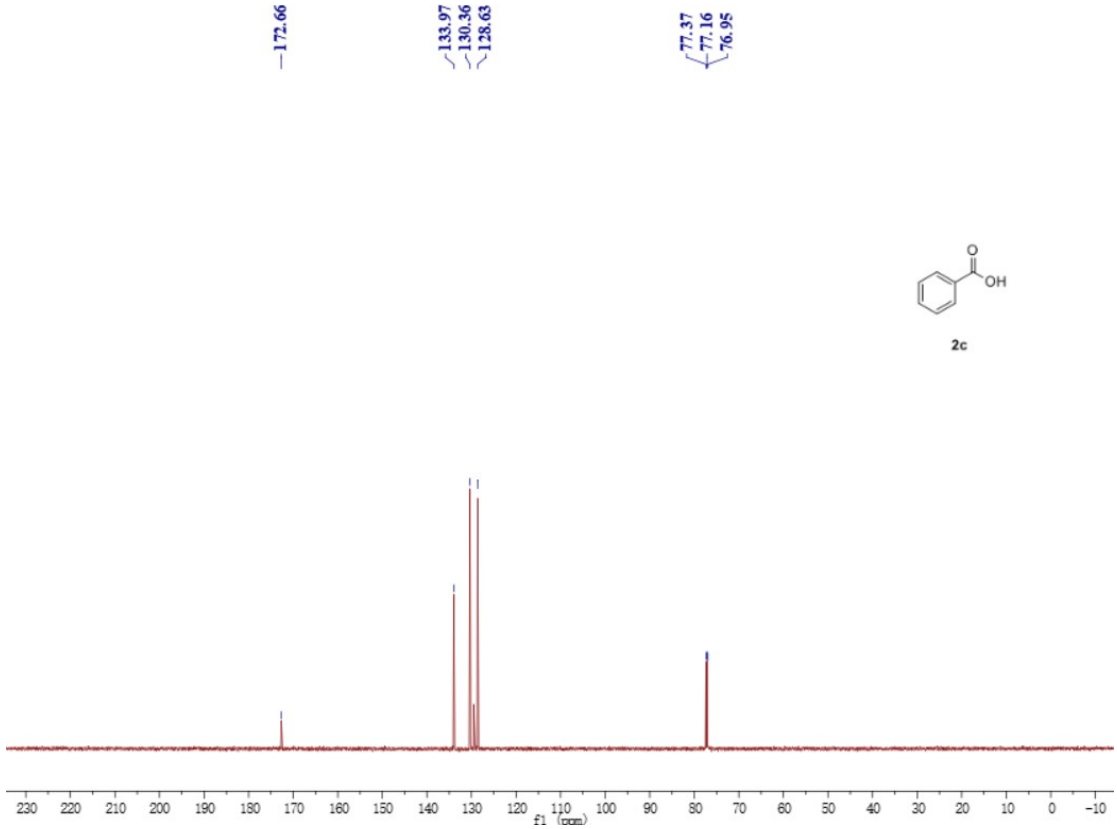
1.00
2.00
f1 (ppm)

2c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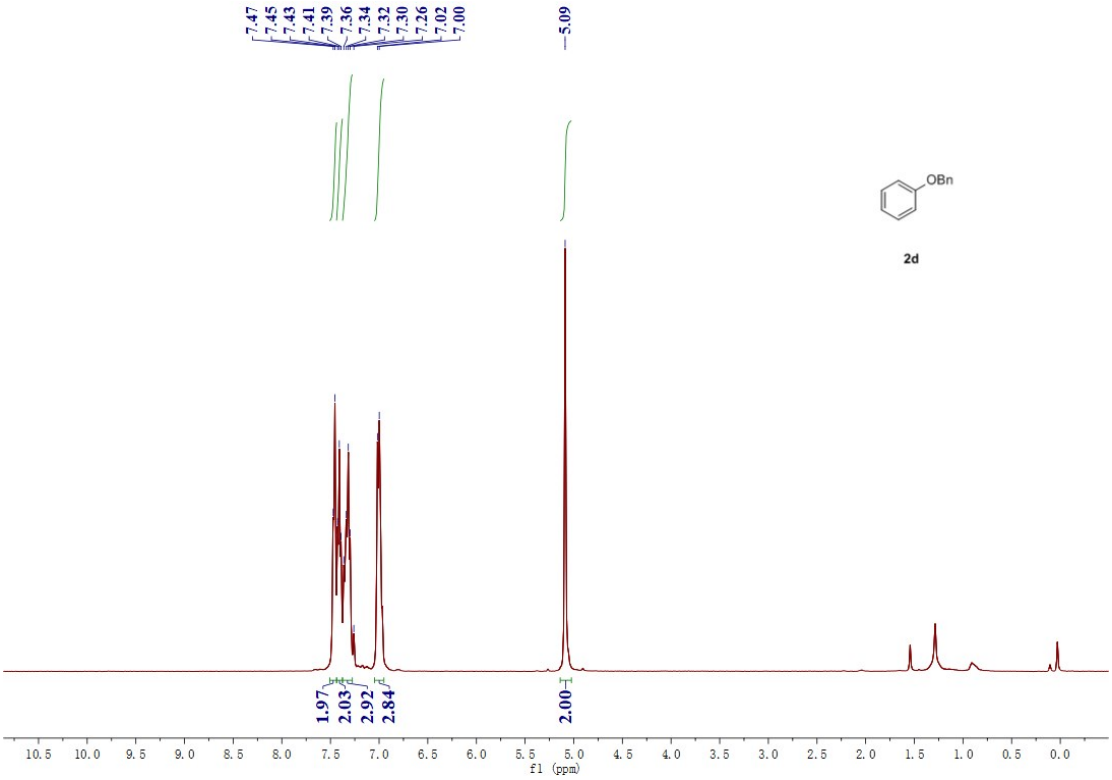
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7.32
7.30
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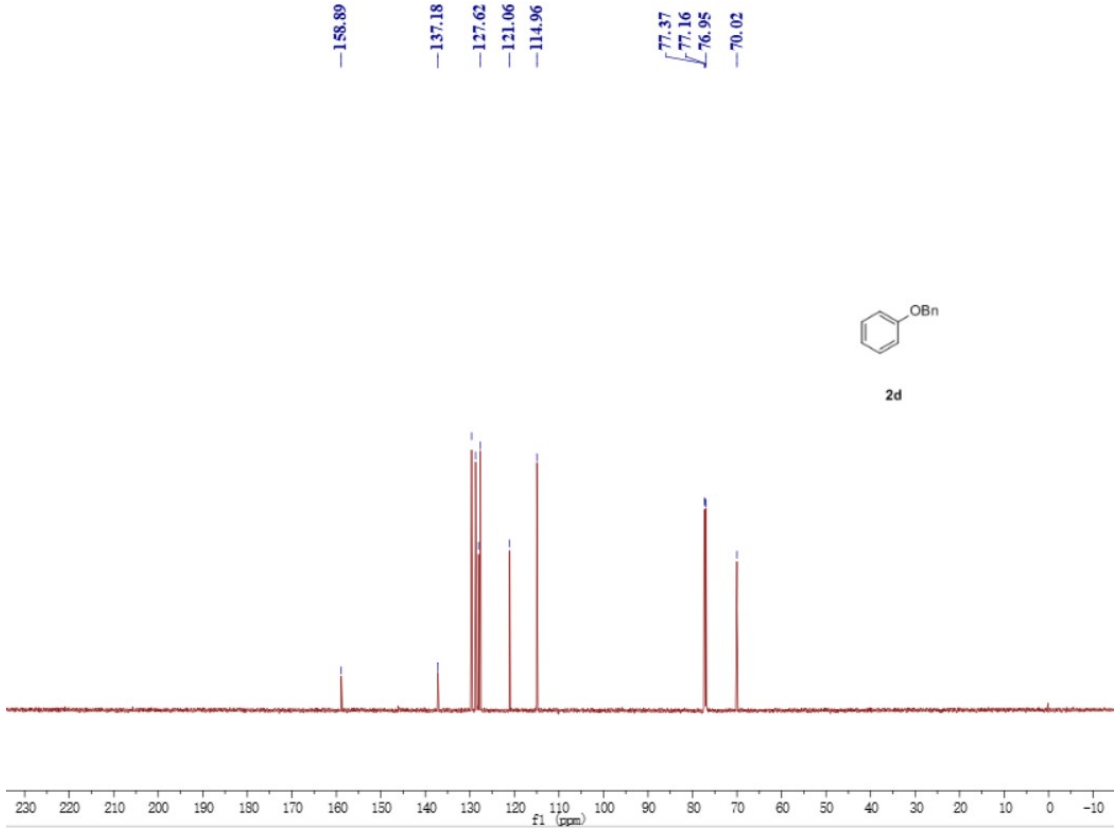
2.03
2.92
2.84
2.00
f1 (ppm)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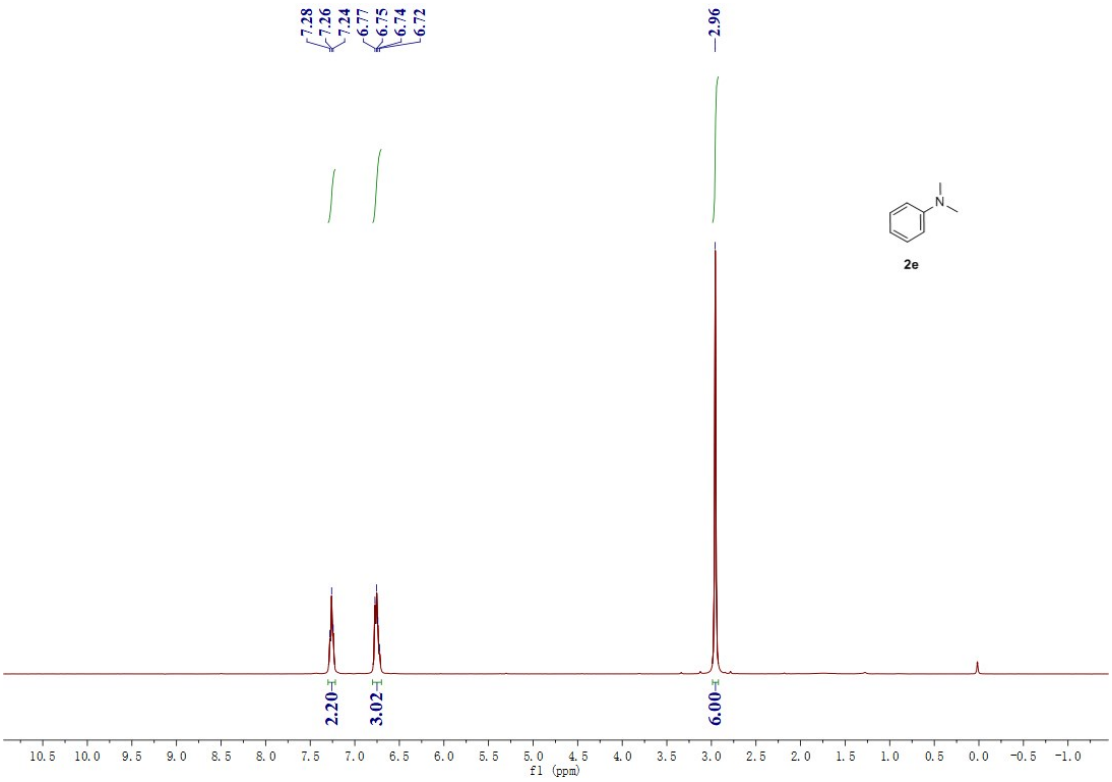
2d
f1 (ppm)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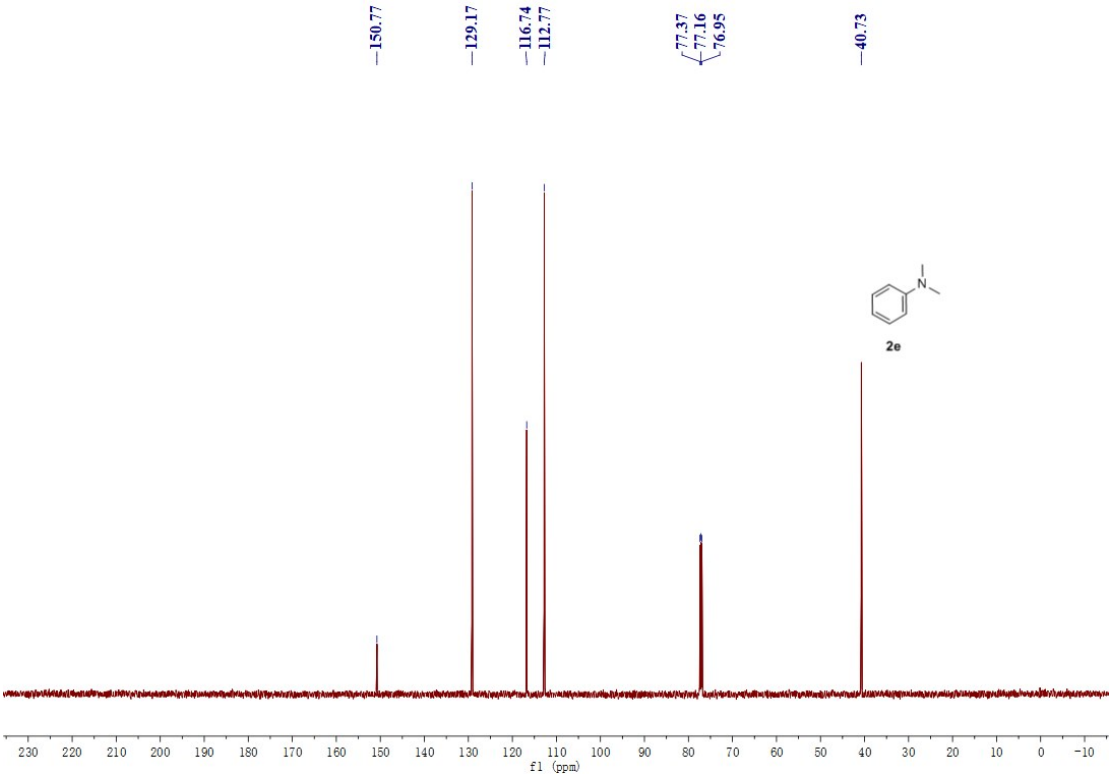
3.02
6.00
f1 (ppm)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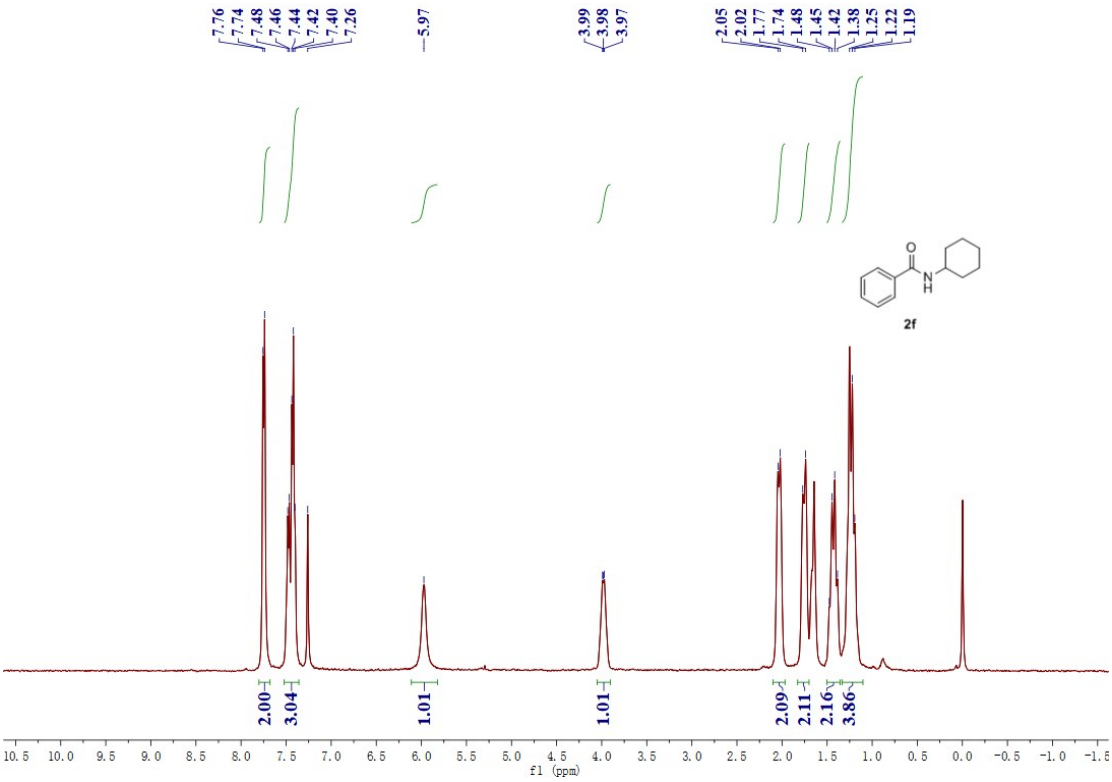
2e
f1 (ppm)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3.99
3.98
3.97
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2.02
1.77
1.74
1.48
1.45
1.42
1.38
1.25
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1.01
2.09
2.11
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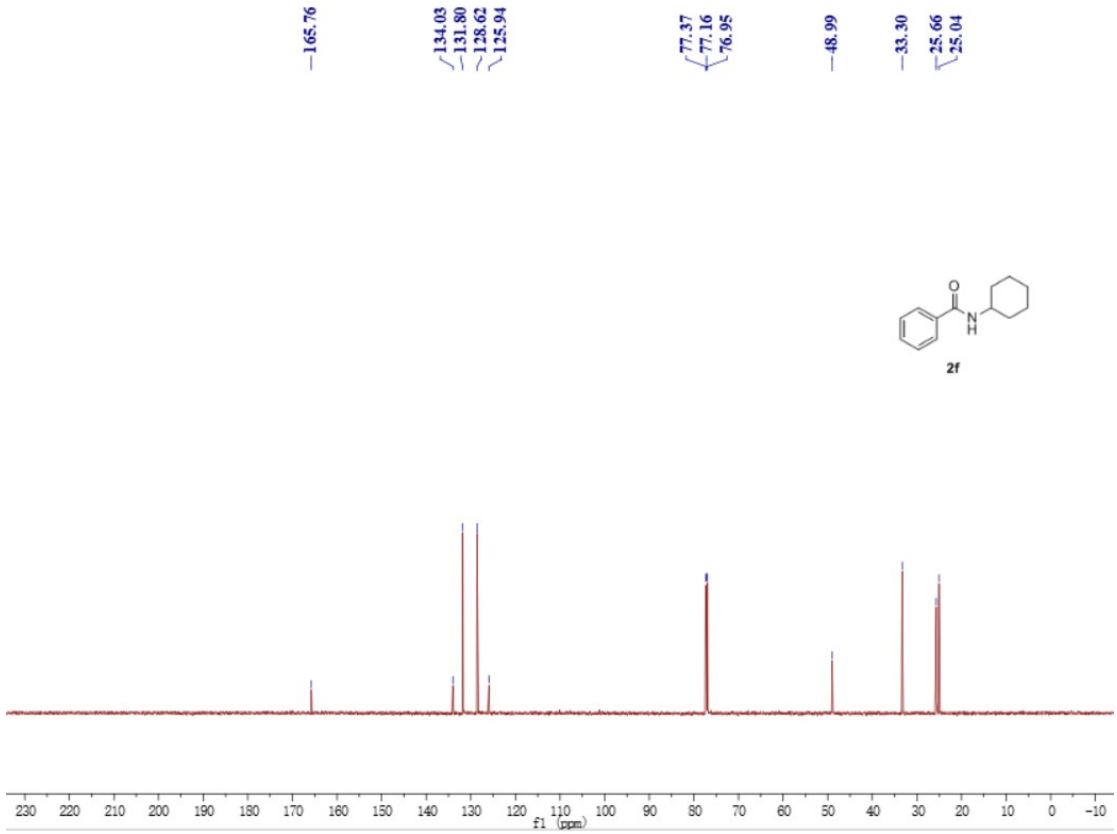
3.86
f1 (ppm)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33.30
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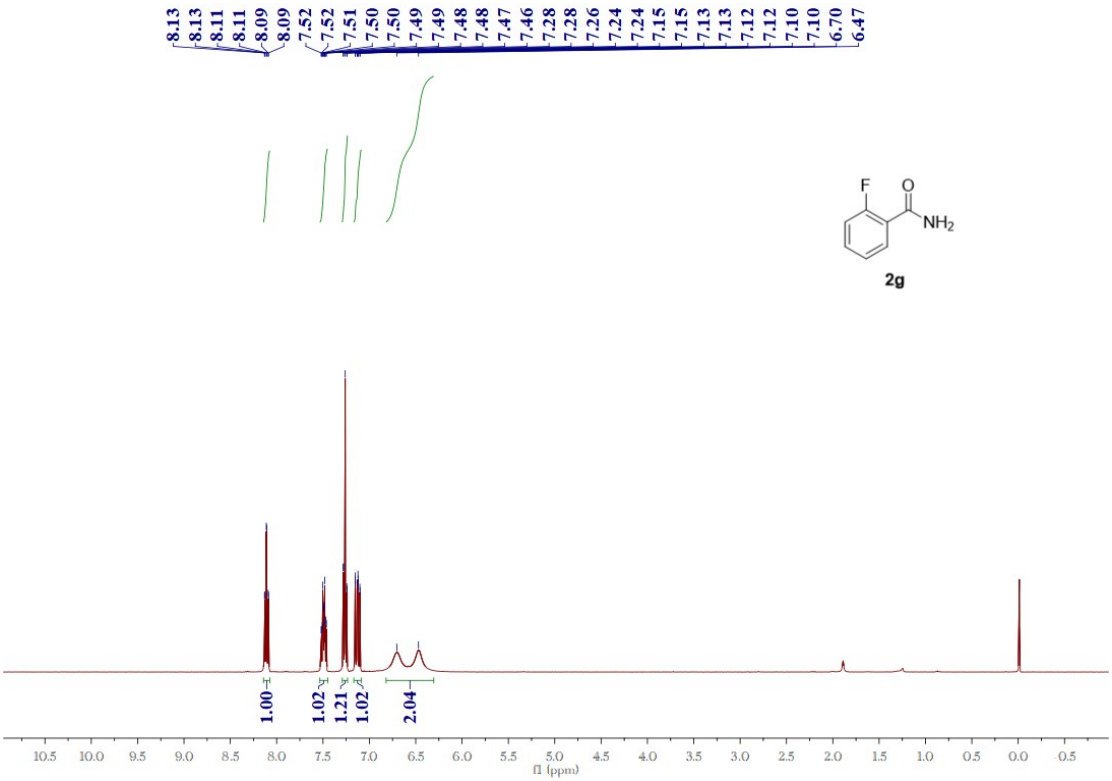
2f
f1 (ppm)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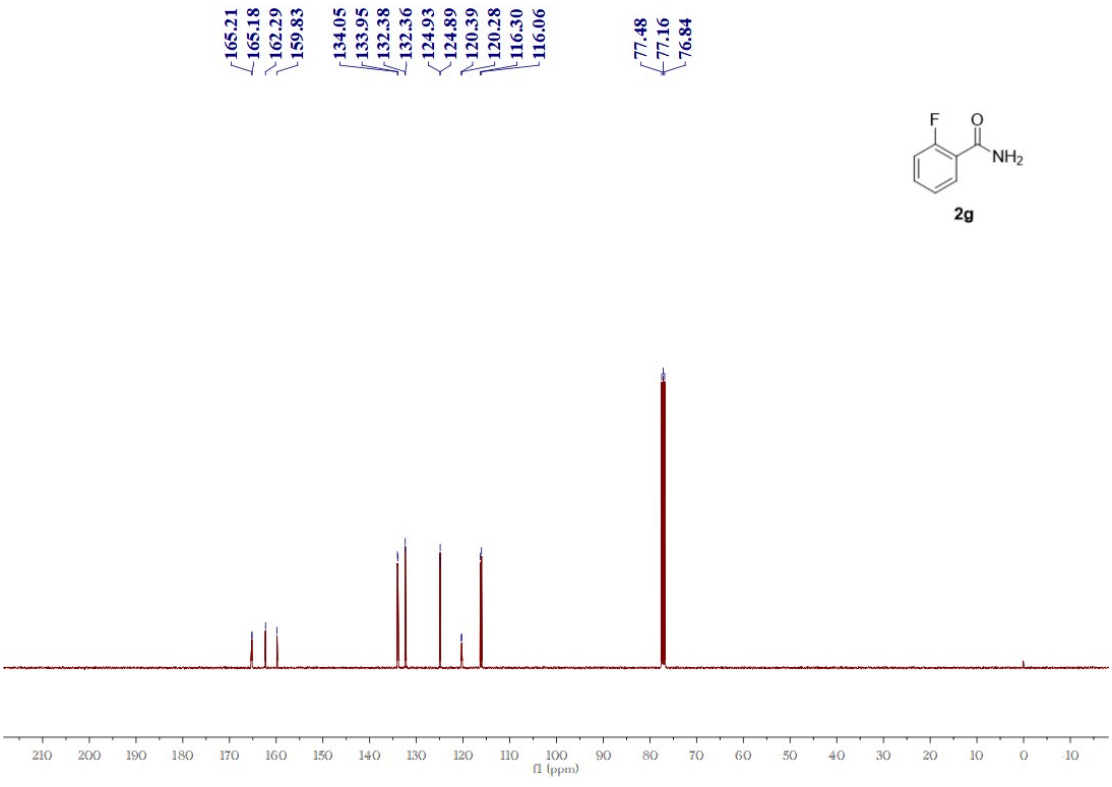
2.04
f1 (ppm)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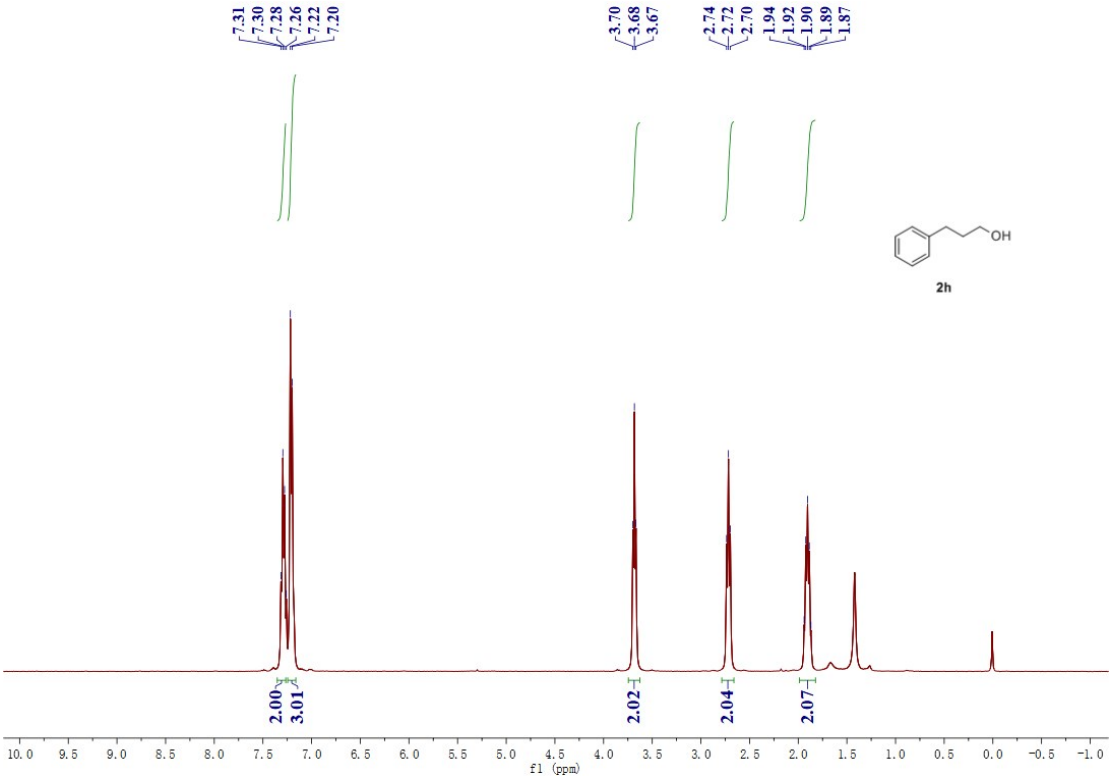
76.84
F
O
NH2
2g
f1 (ppm)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OH
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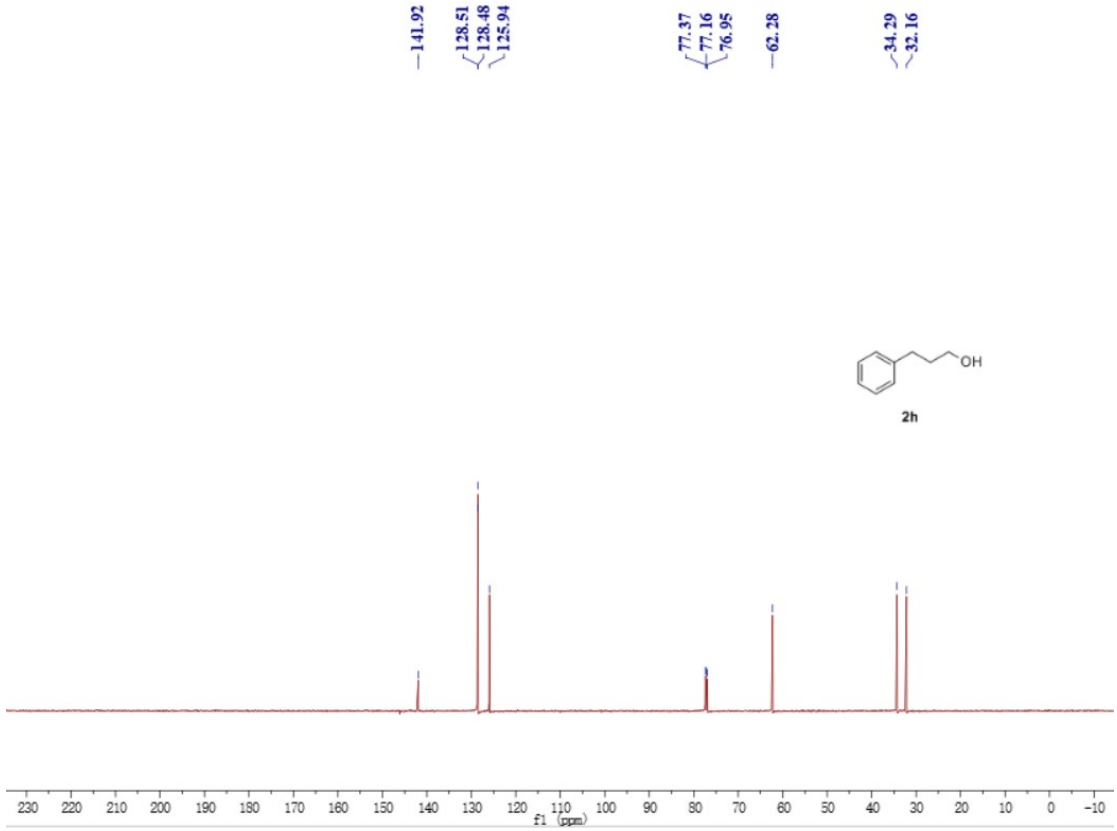
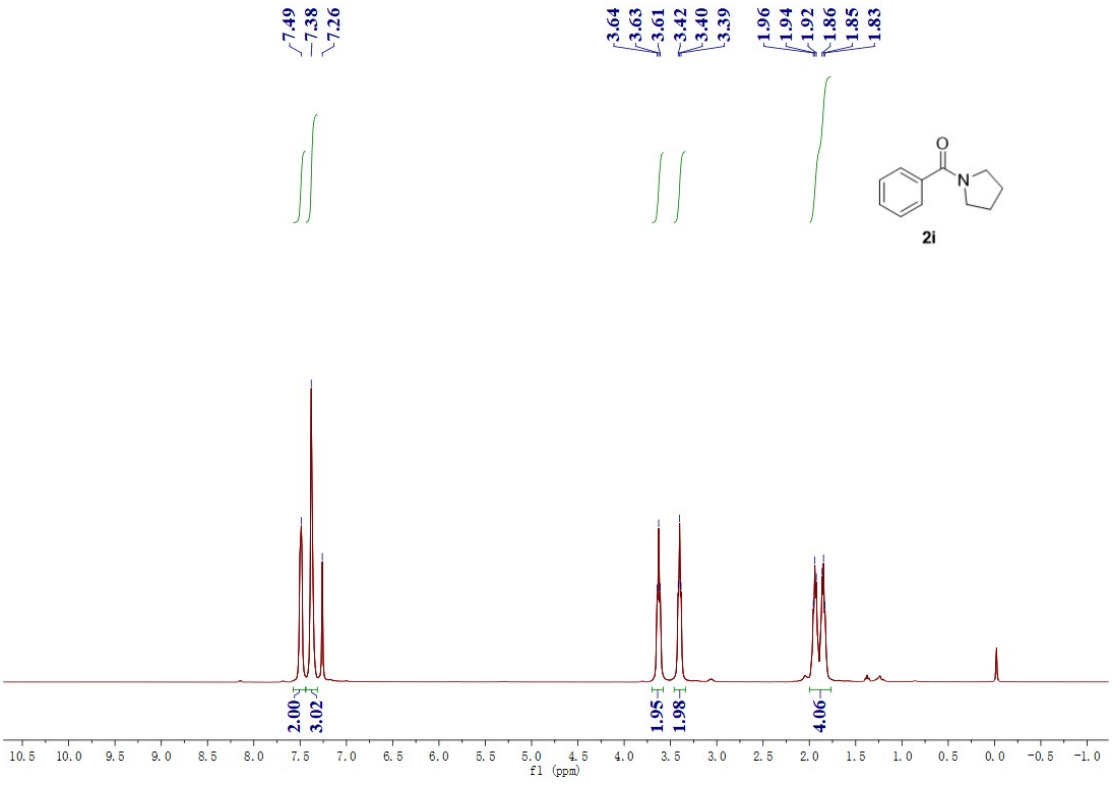
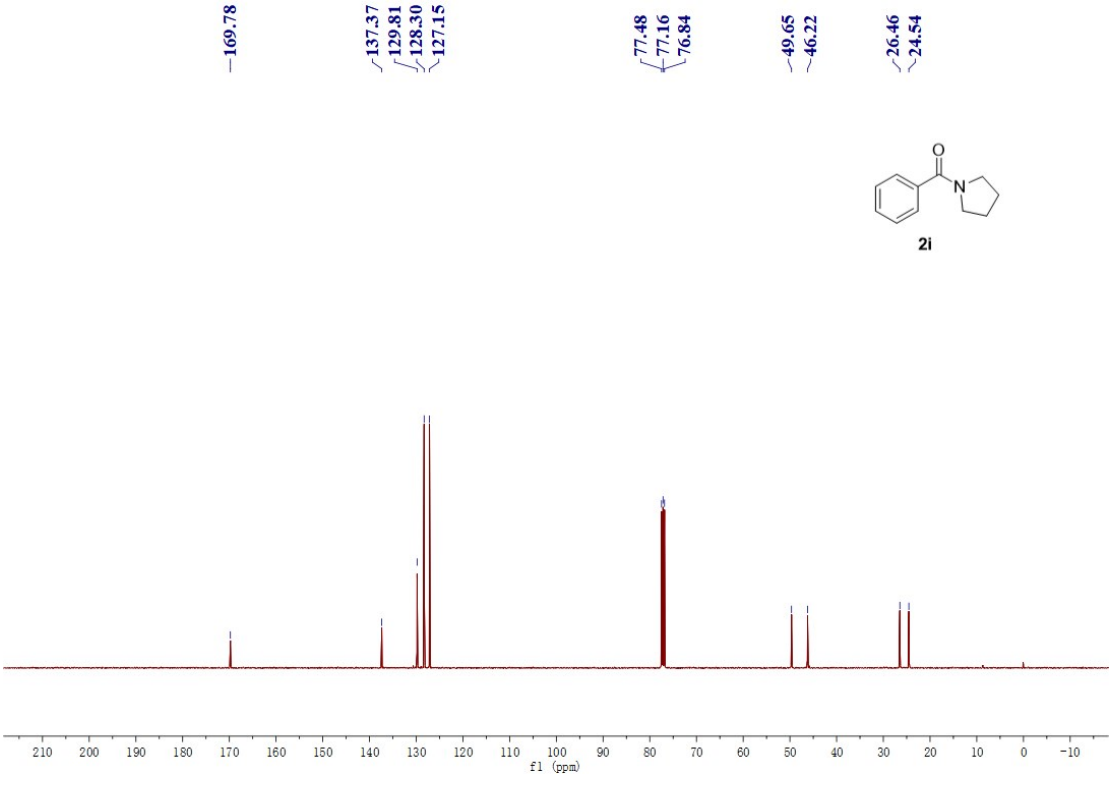
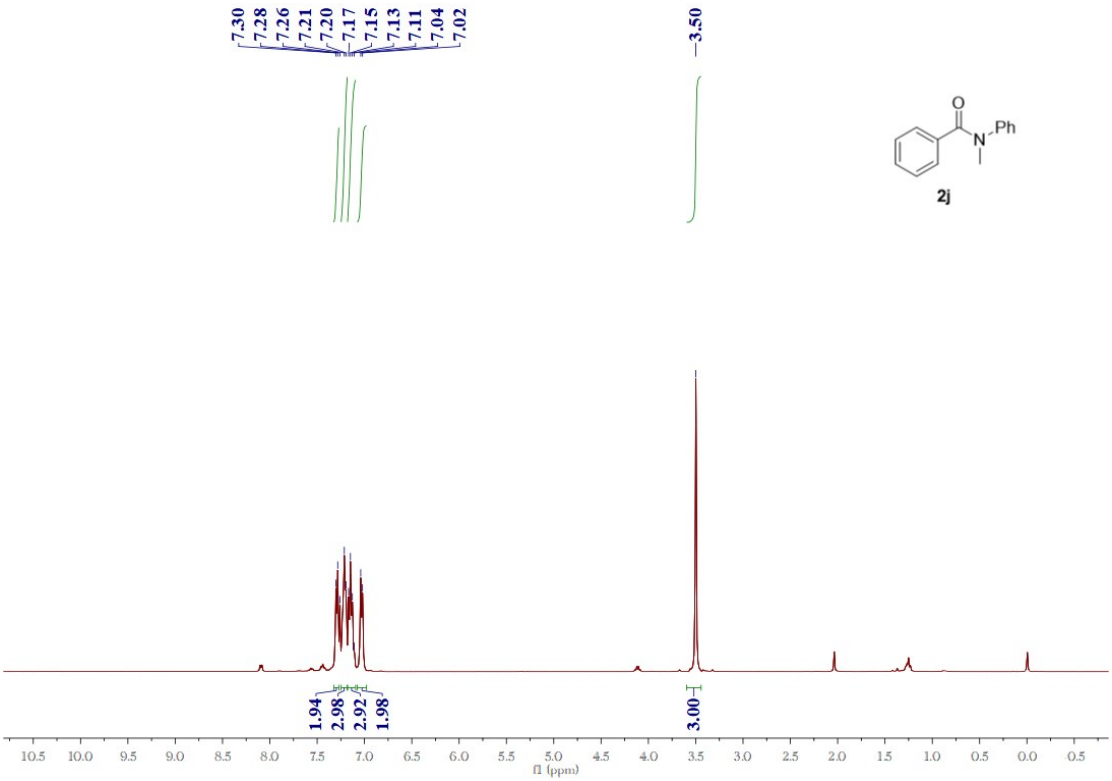
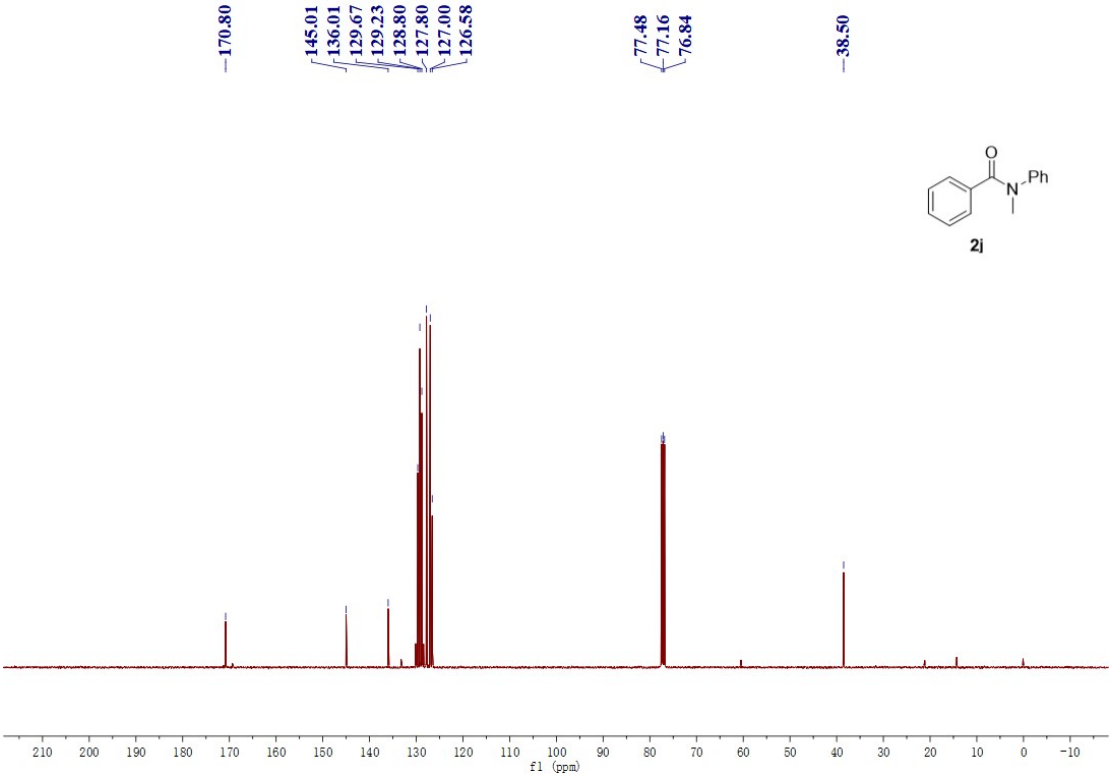
3.01
2.02
2.04
2.07
f1 (ppm)

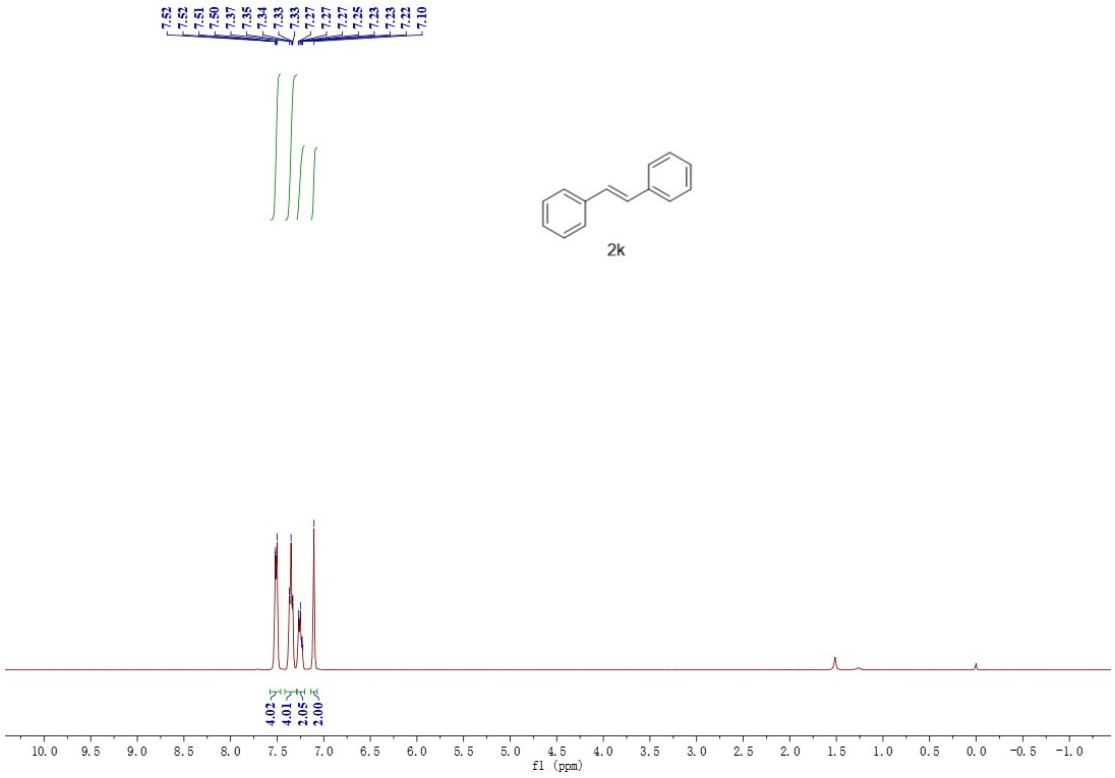

141.92
128.51
128.48
125.94
77.37
77.16
76.95
62.28
34.29
32.16
OH
2h
f1 (ppm)

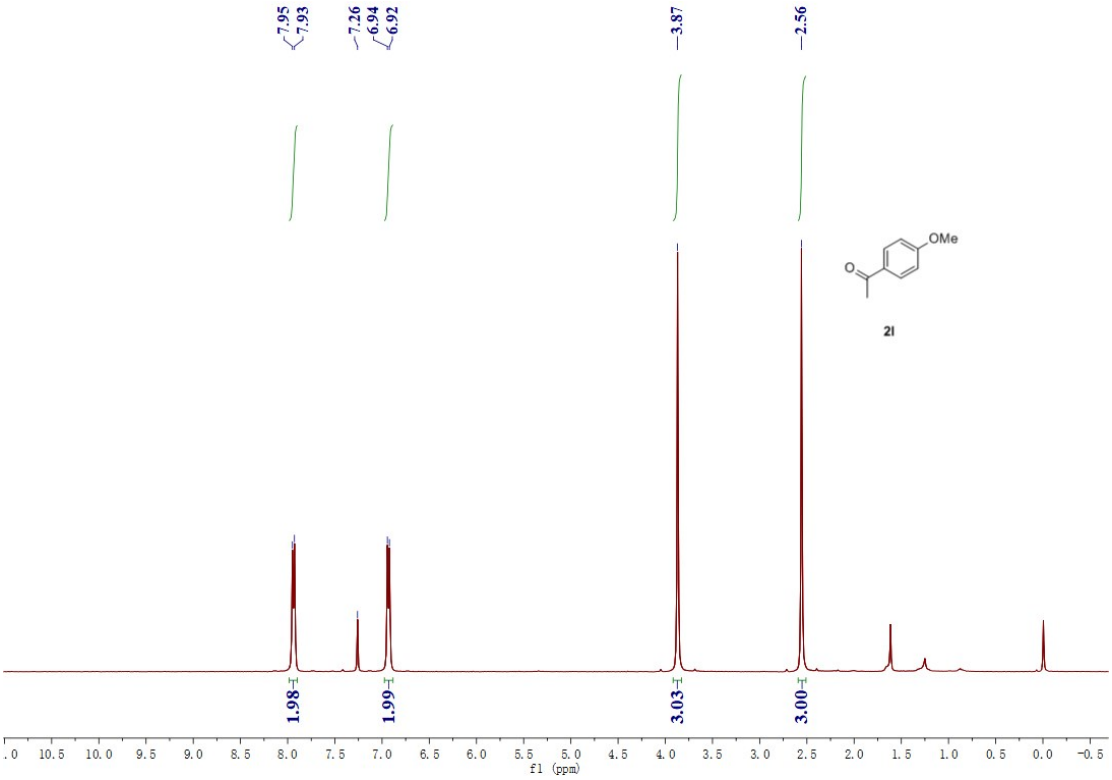

7.49
7.38
7.26
3.64
3.63
3.61
3.42
3.40
3.39
1.96
1.94
1.92
1.86
1.85
1.83
2i
2.00
3.02
1.95
1.98
4.06
f1 (ppm)

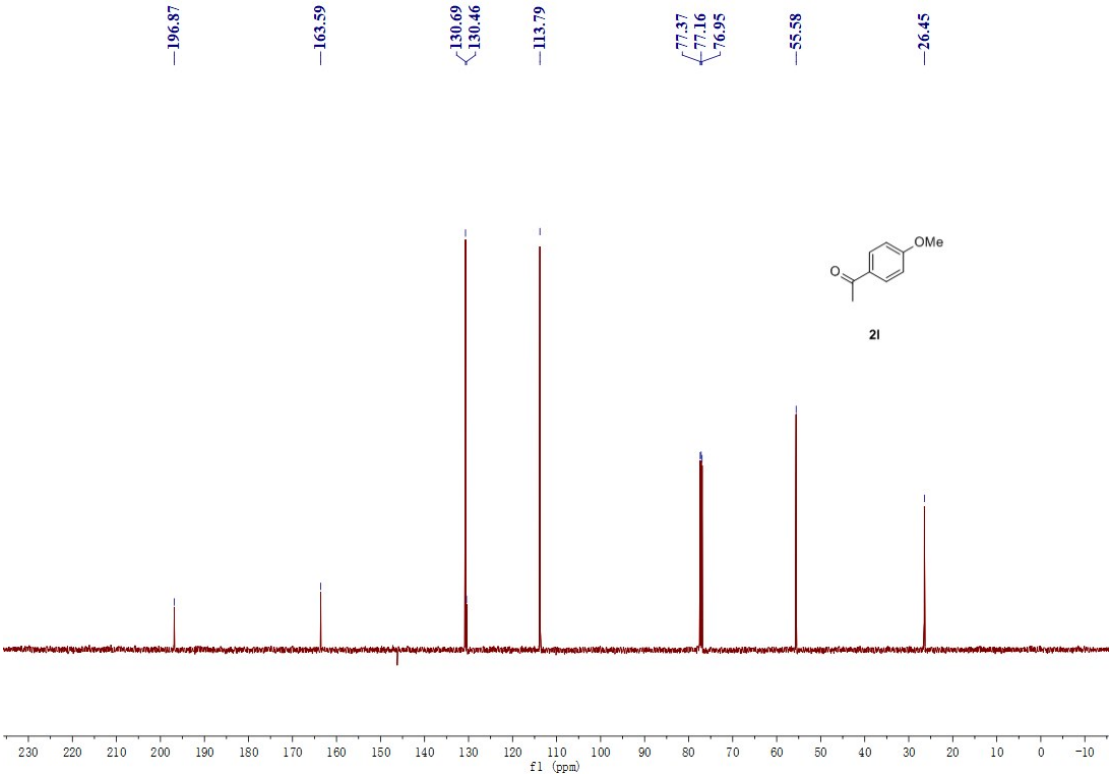

169.78
137.37
129.81
128.30
127.15
77.48
77.16
76.84
49.65
46.22
26.46
24.54
2i
f1 (ppm)

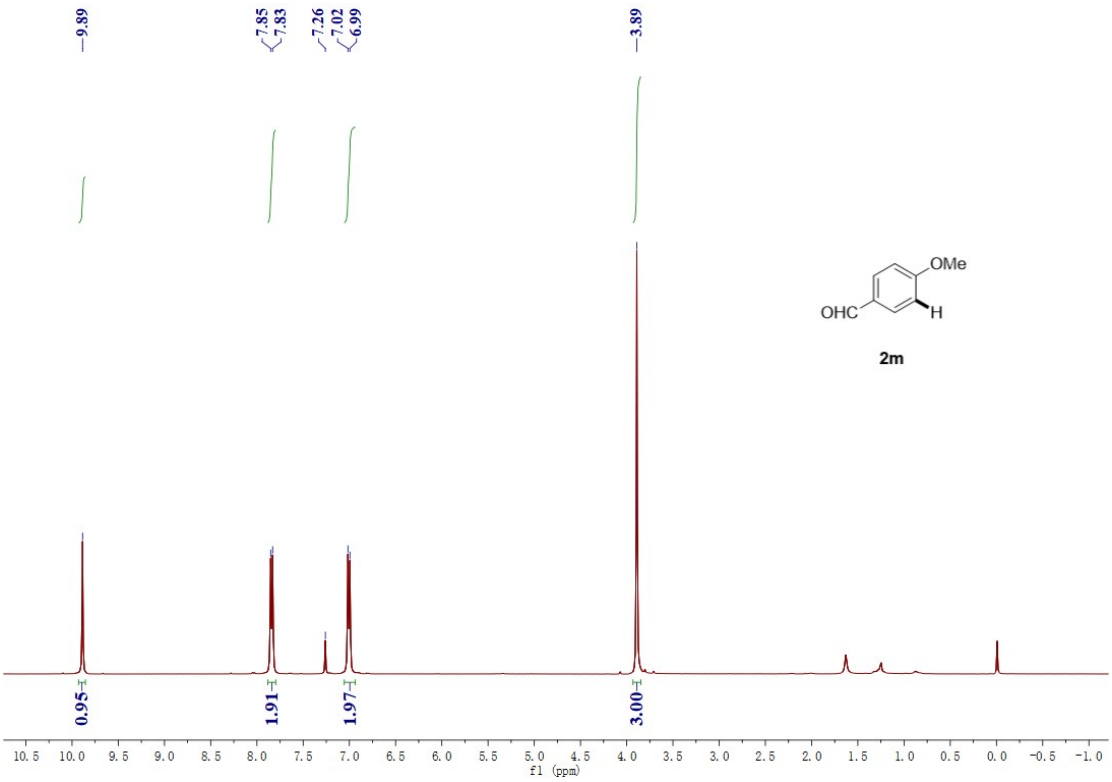

7.30
7.28
7.26
7.21
7.20
7.17
7.15
7.13
7.11
7.04
7.02
3.50
O
N
Ph
2j
1.94
2.98
2.92
1.98
3.00
f1 (ppm)

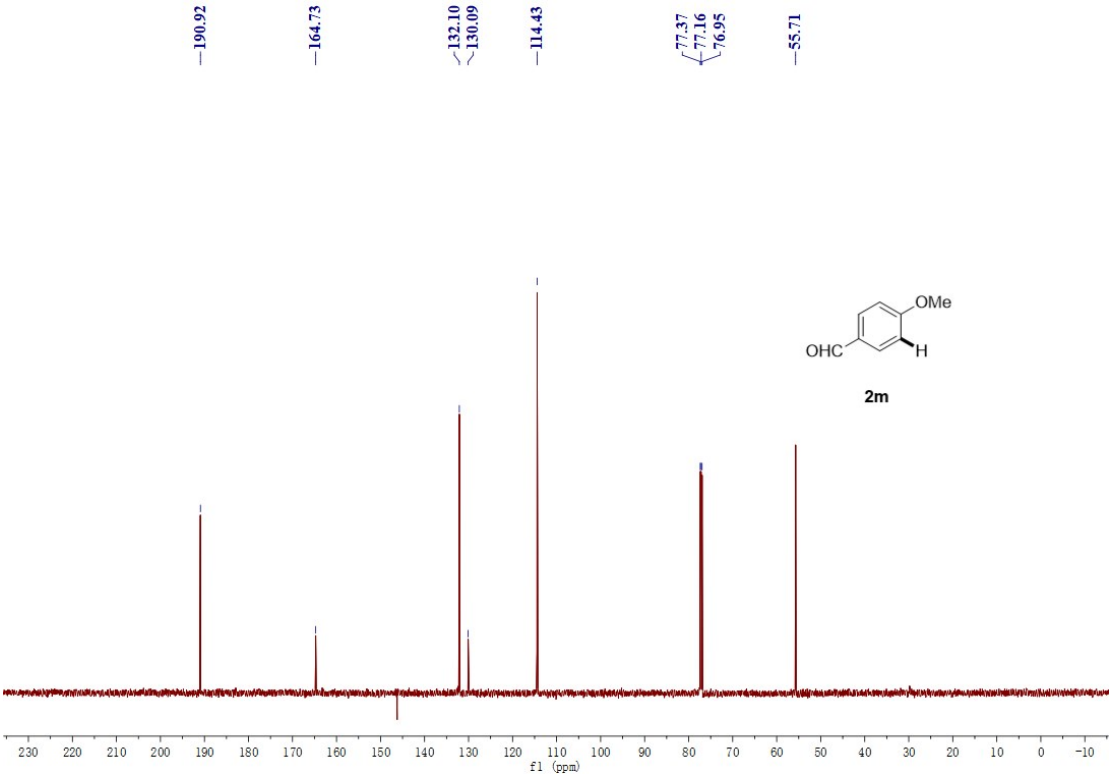

170.80
145.01
136.01
129.67
129.23
128.80
127.80
127.00
126.58
77.48
77.16
76.84
38.50
O
N
Ph
2j
f1 (ppm)

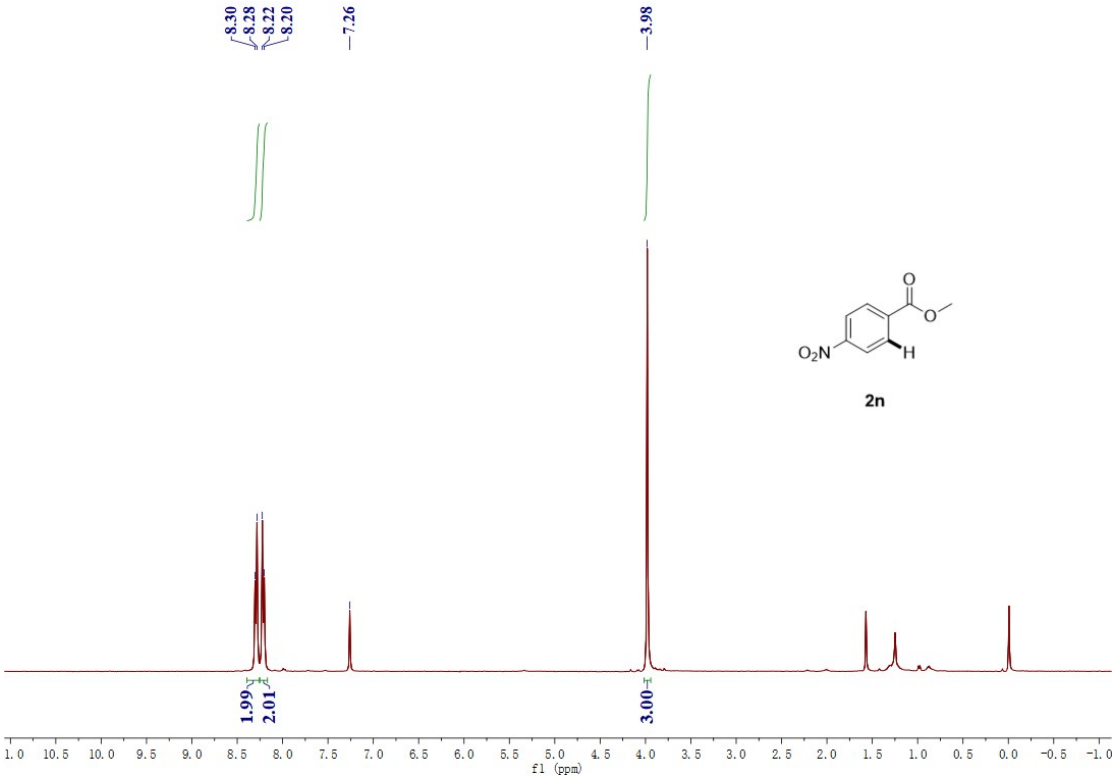

7.52
7.52
7.51
7.50
7.37
7.35
7.34
7.33
7.33
7.27
7.27
7.27
7.25
7.23
7.23
7.22
7.10
2k
4.02
4.01
2.05
2.00
f1 (ppm)
137.32
128.68
128.66
127.60
126.50
77.22
77.00
76.79
2k
f1 (ppm)

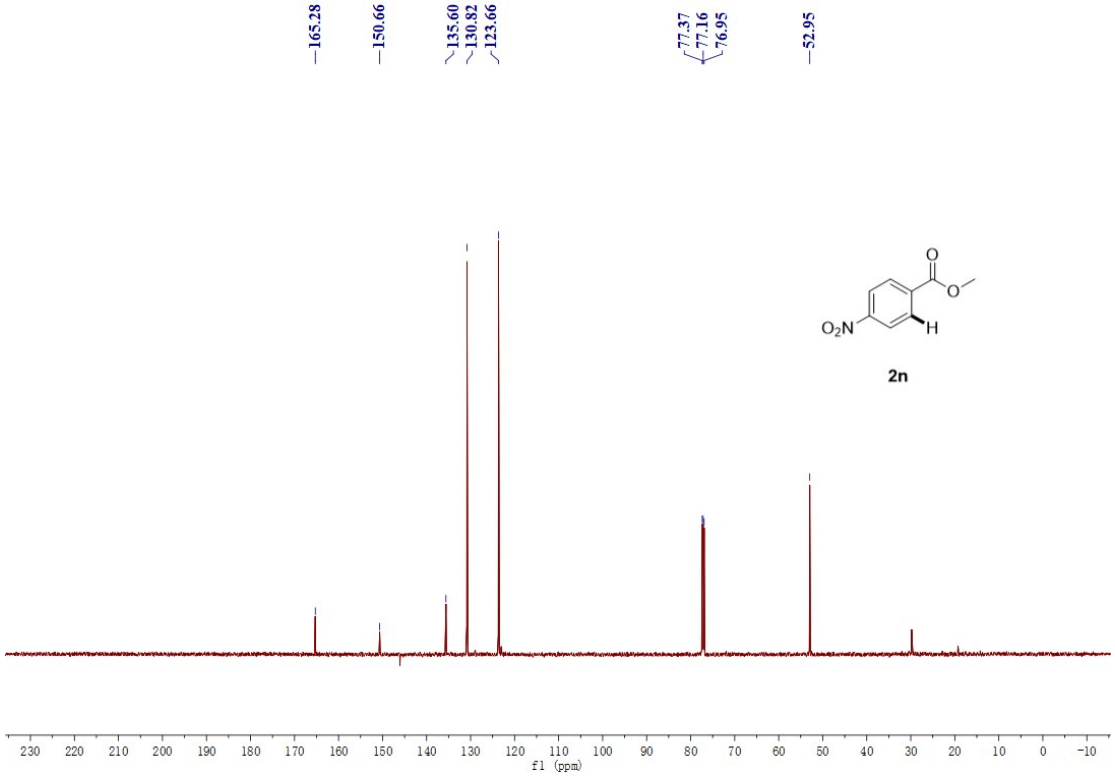

7.95
7.93
7.26
6.94
6.92
3.87
2.56
OMe
O
2l
1.98
1.99
3.03
3.00
f1 (ppm)

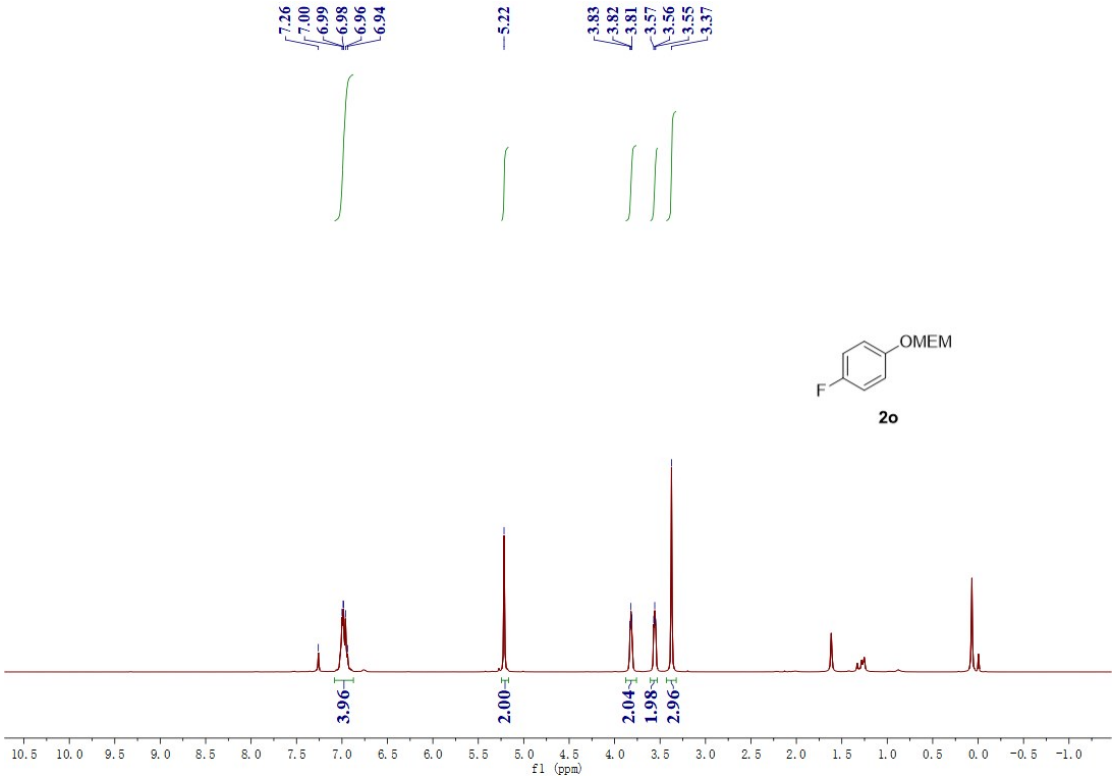

196.87
163.59
130.69
130.46
113.79
77.37
77.16
76.95
55.58
26.45
OMe
O
2l
f1 (ppm)

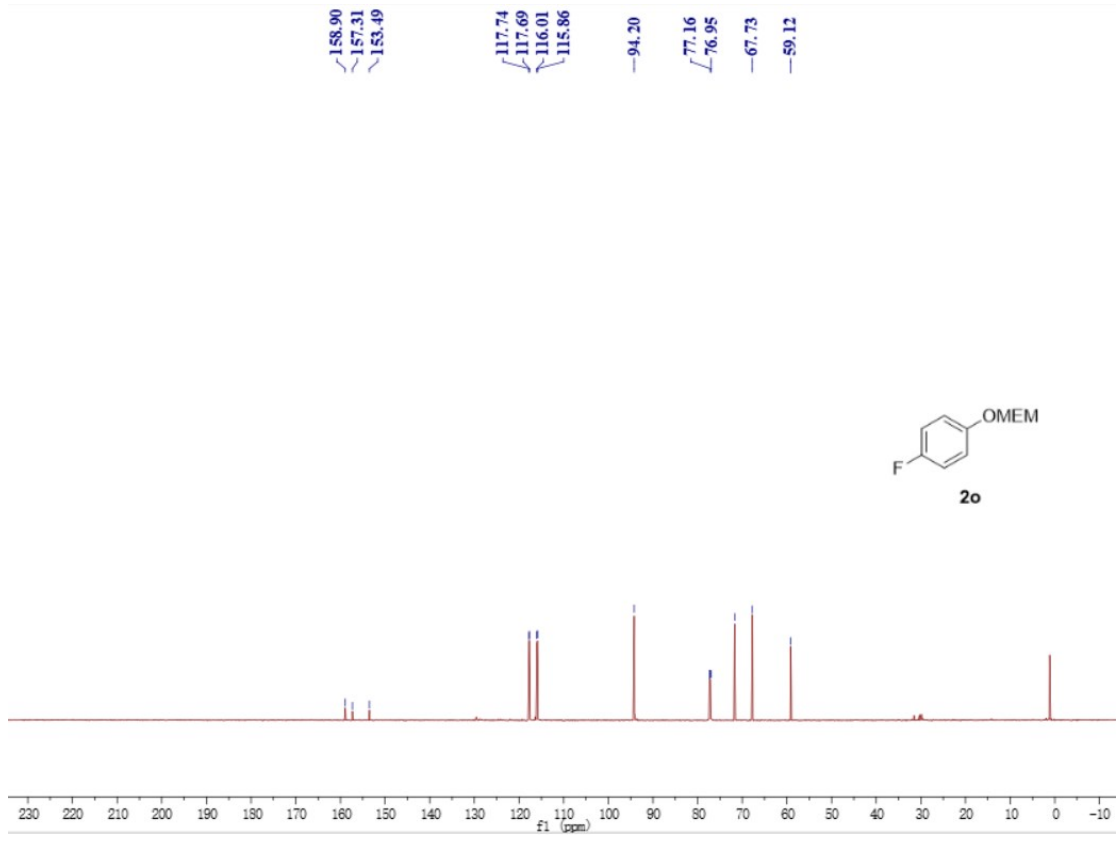

9.89
7.85
7.83
7.26
7.02
6.99
3.89
OMe
OHC
H
2m
0.95
1.91
1.97
3.00
f1 (ppm)

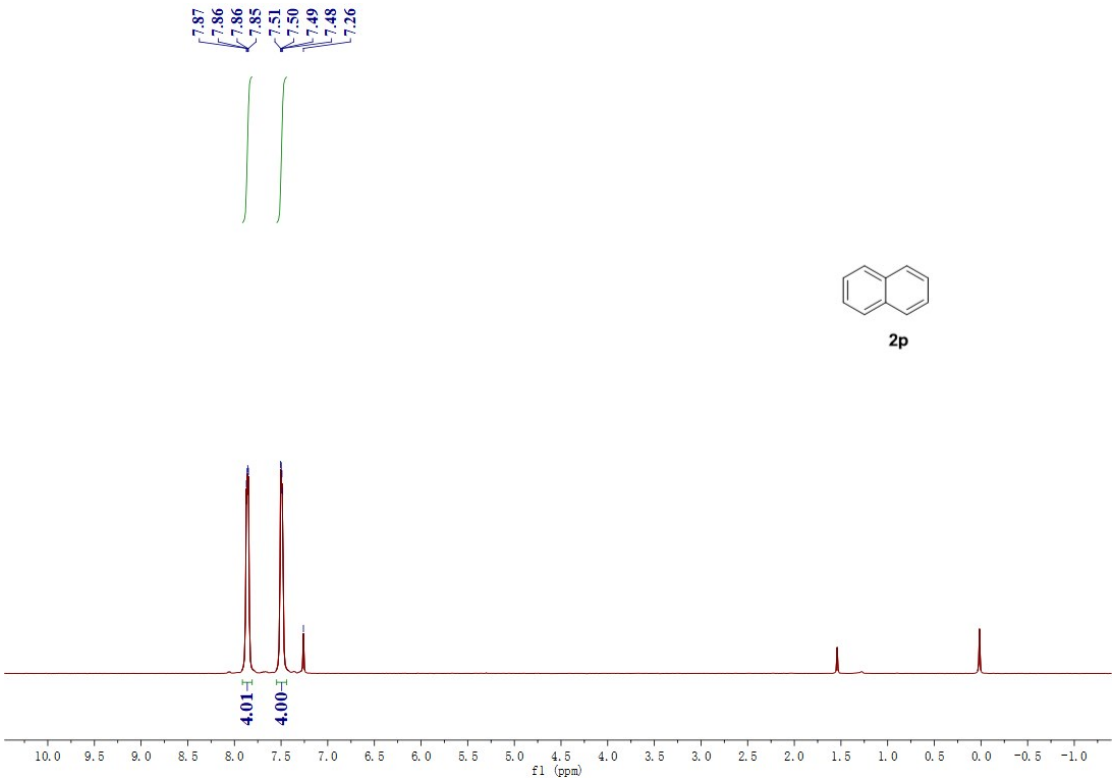

190.92
164.73
132.10
130.09
114.43
77.37
77.16
76.95
55.71
OMe
OHC
H
2m
f1 (ppm)

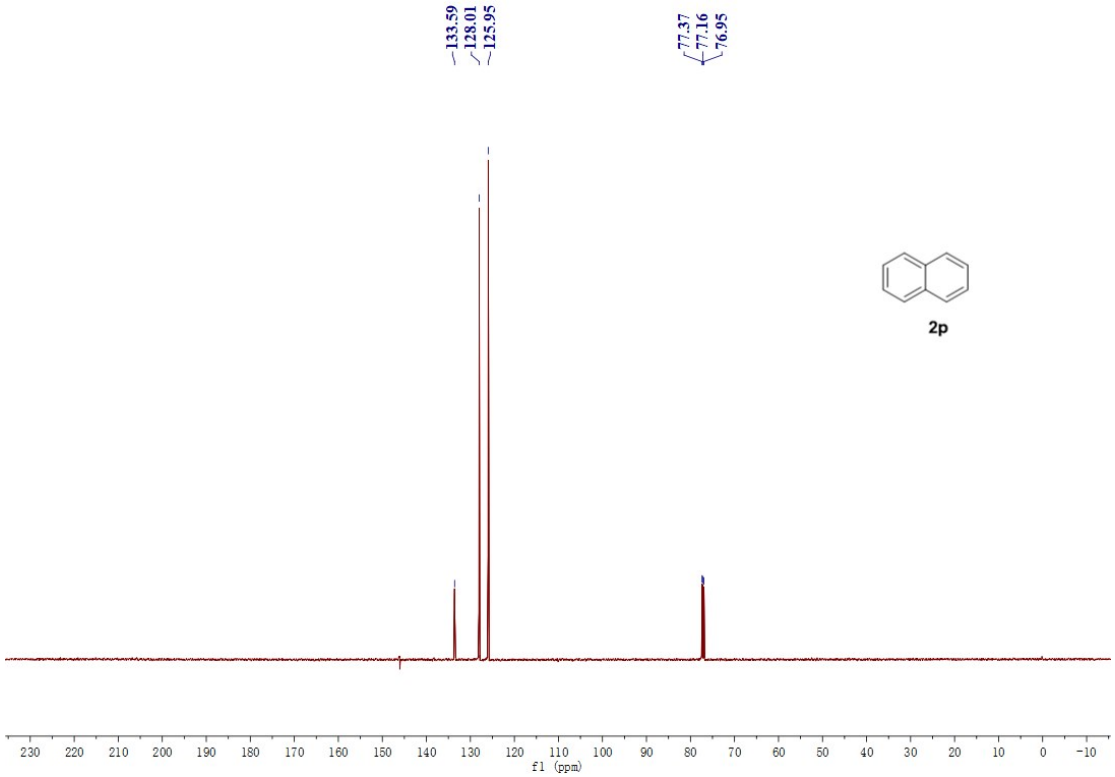

8.30
8.28
8.22
8.20
7.26
3.98
1.99
2.01
3.00
f1 (ppm)

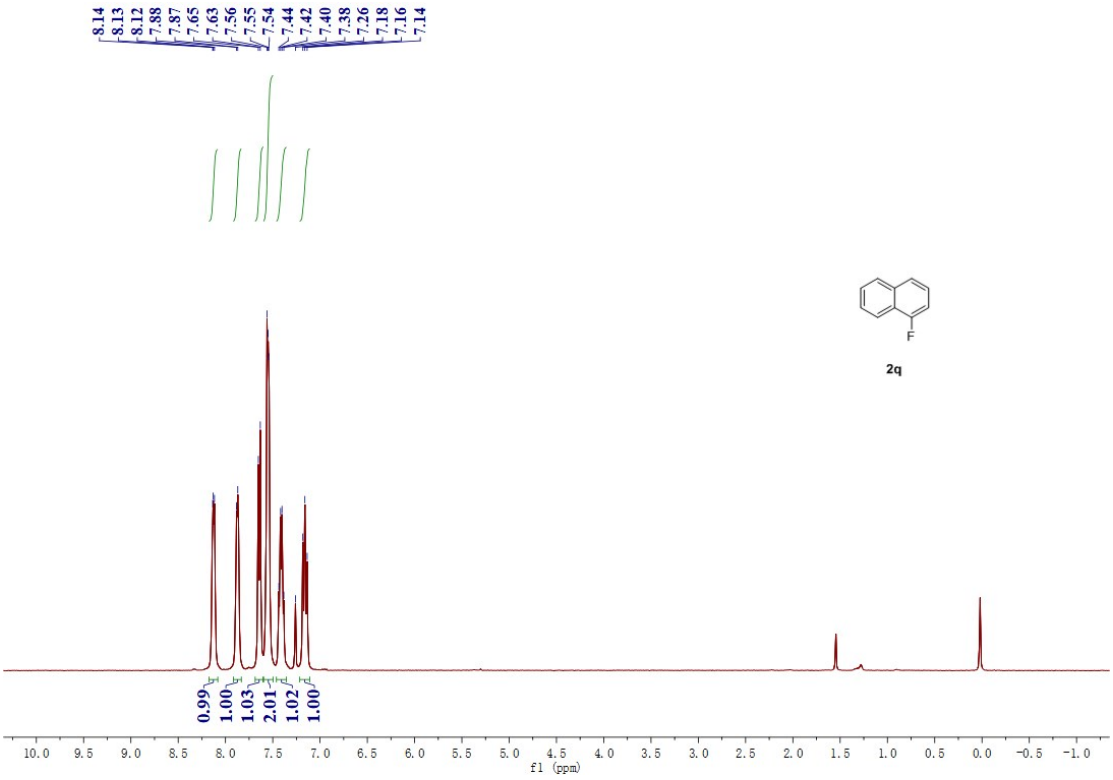

165.28
150.66
135.60
130.82
123.66
77.37
77.16
76.95
52.95
f1 (ppm)

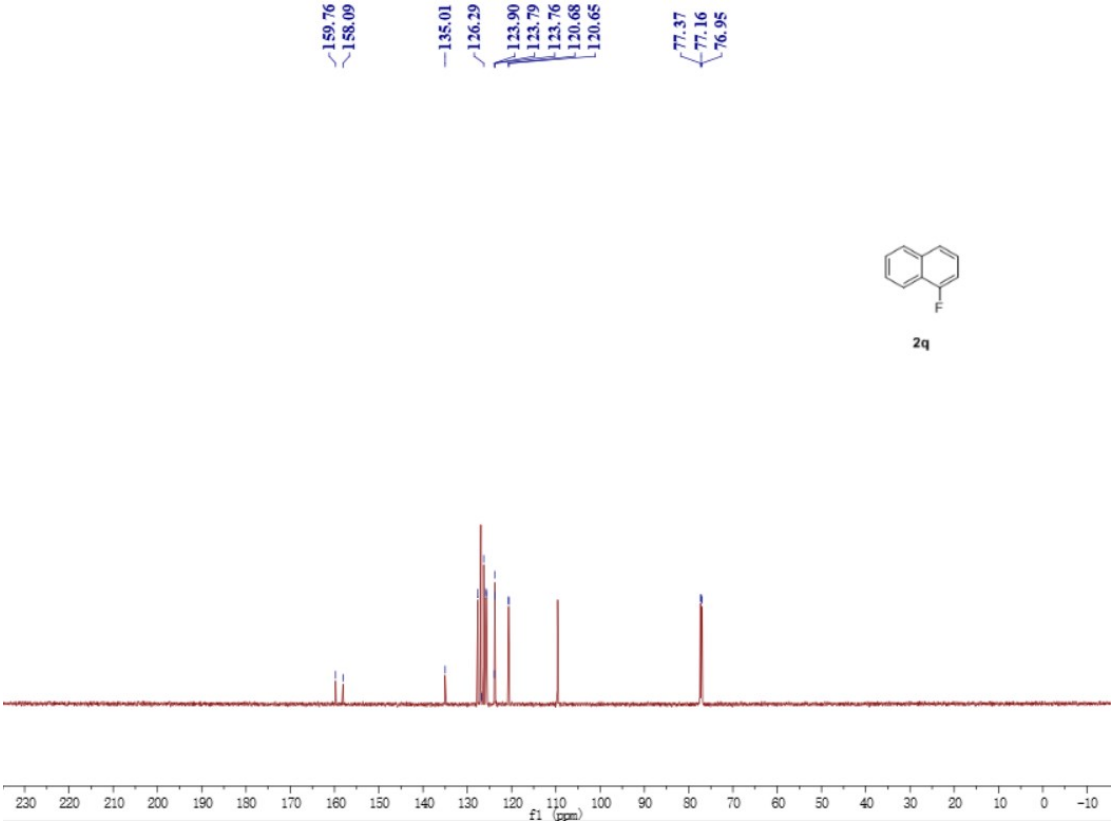

7.26
7.00
6.99
6.98
6.96
6.94
5.22
3.83
3.82
3.81
3.57
3.56
3.55
3.37
OMEM
F
2o
3.96
2.00
2.04
1.98
2.96
f1 (ppm)

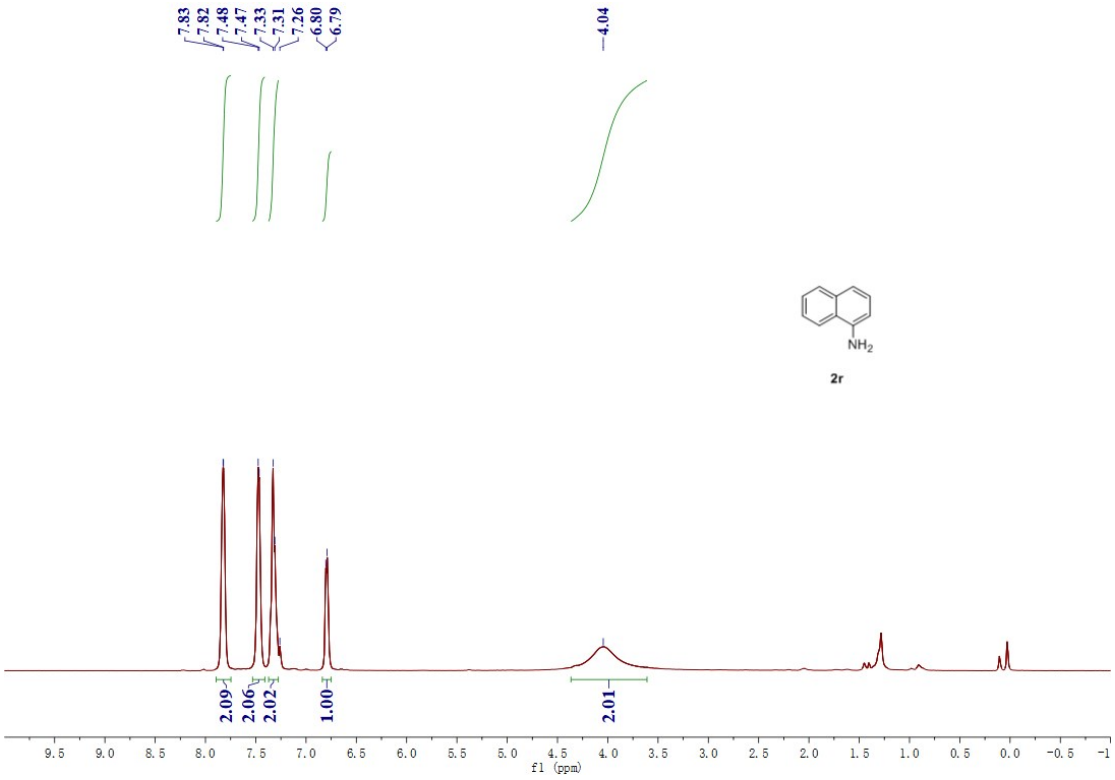

158.90
157.31
153.49
117.74
117.69
116.01
115.86
94.20
77.16
76.95
67.73
59.12
OMEM
F
2o
f1 (ppm)

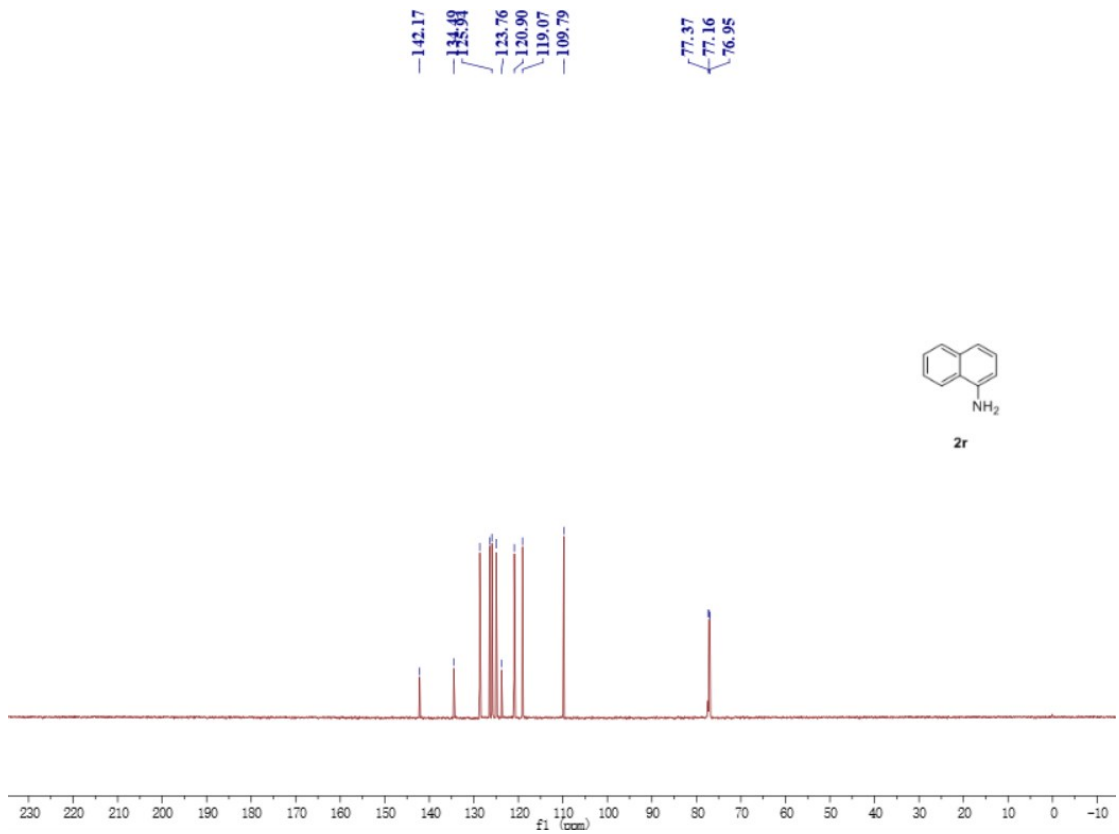

7.87
7.86
7.86
7.85
7.51
7.50
7.49
7.48
7.26
2p
4.01
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

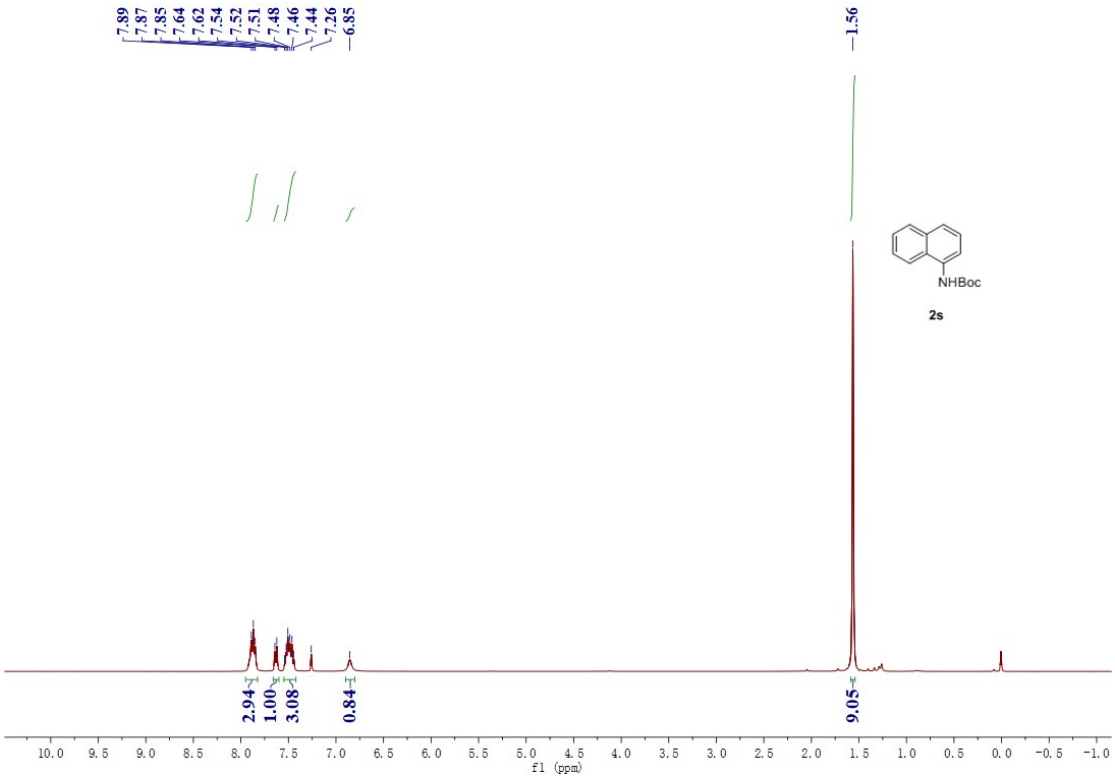

133.59
128.01
125.95
77.37
77.16
76.95
2p
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

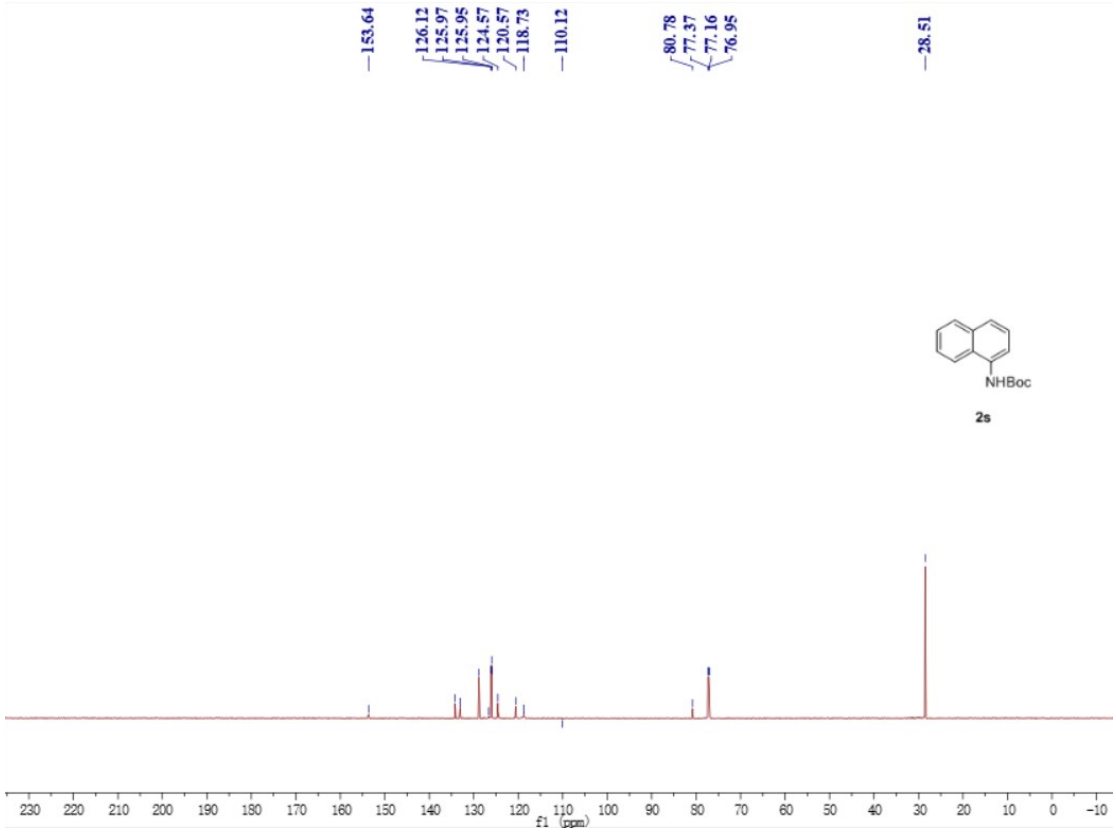

8.14
8.13
8.12
7.88
7.87
7.65
7.63
7.56
7.55
7.54
7.44
7.42
7.40
7.38
7.26
7.18
7.16
7.14
F
2q
0.99
1.00
1.03
2.01
1.02
1.00
f1 (ppm)

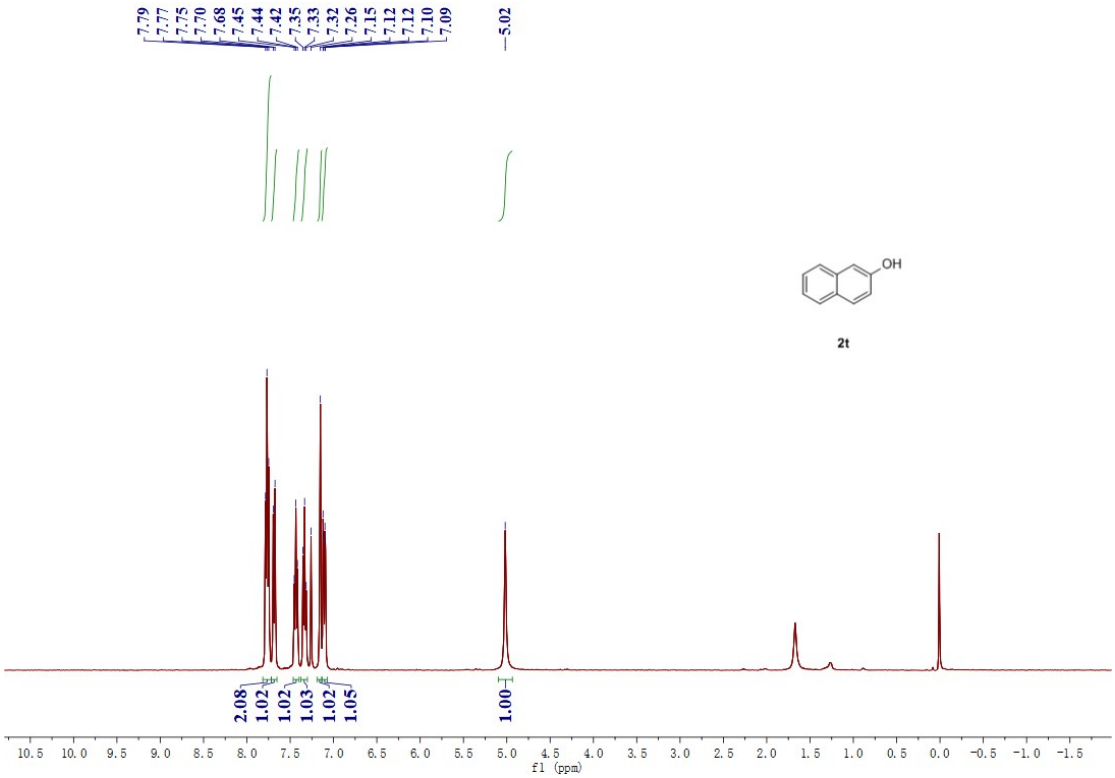

159.76
158.09
135.01
126.29
123.90
123.79
123.76
120.68
120.65
77.37
77.16
76.95
F
2q
f1 (ppm)

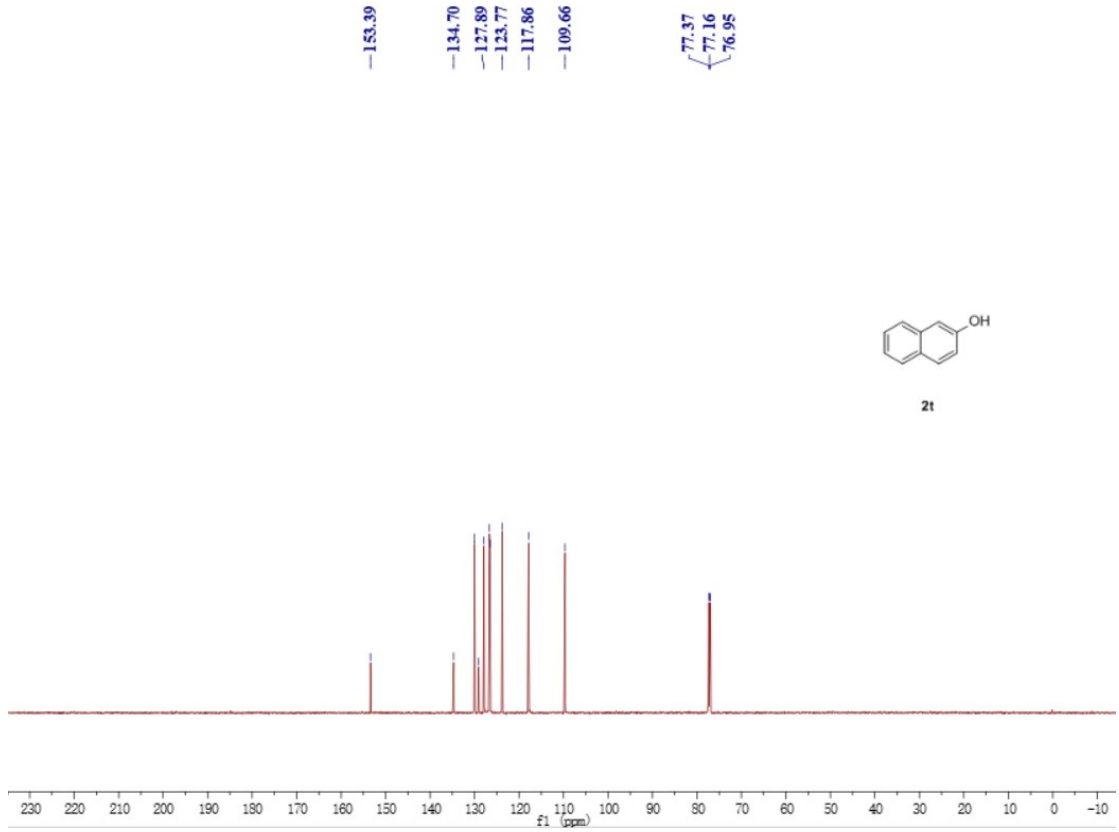

7.83
7.82
7.48
7.47
7.33
7.31
7.26
6.80
6.79
4.04
NH2
2r
2.09
2.06
2.02
1.00
2.01
f1 (ppm)

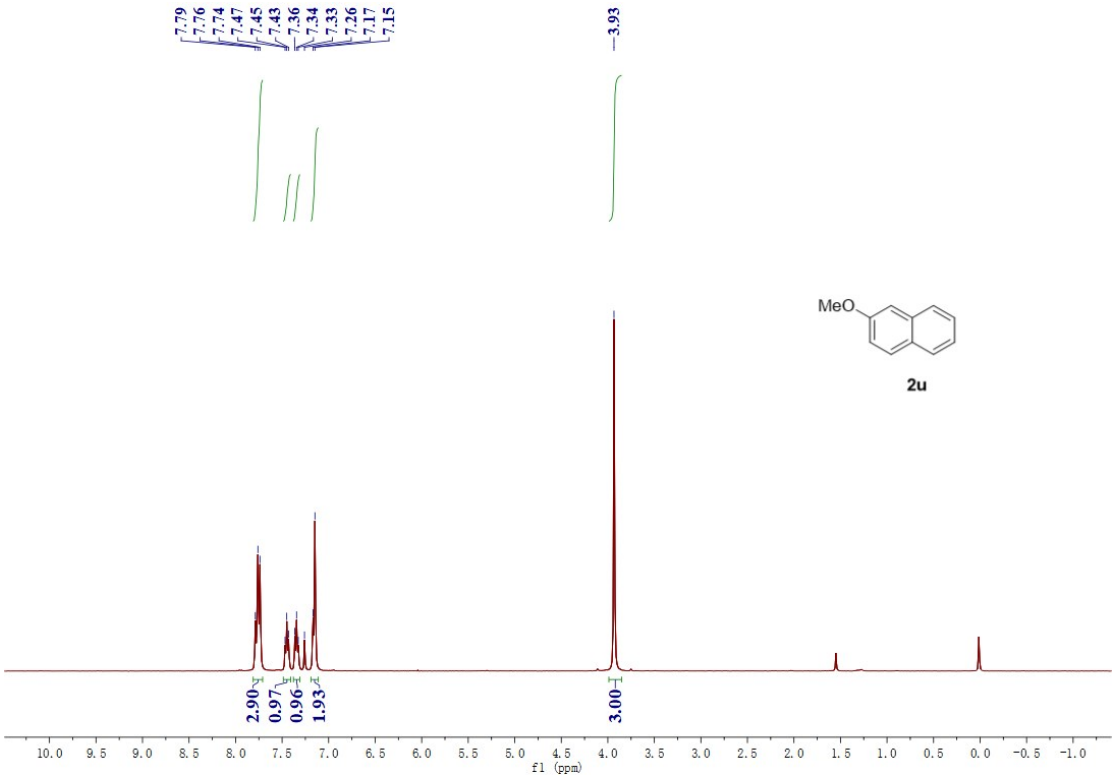

142.17
123.76
120.90
119.07
109.79
77.37
77.16
76.95
NH2
2r
f1 (ppm)

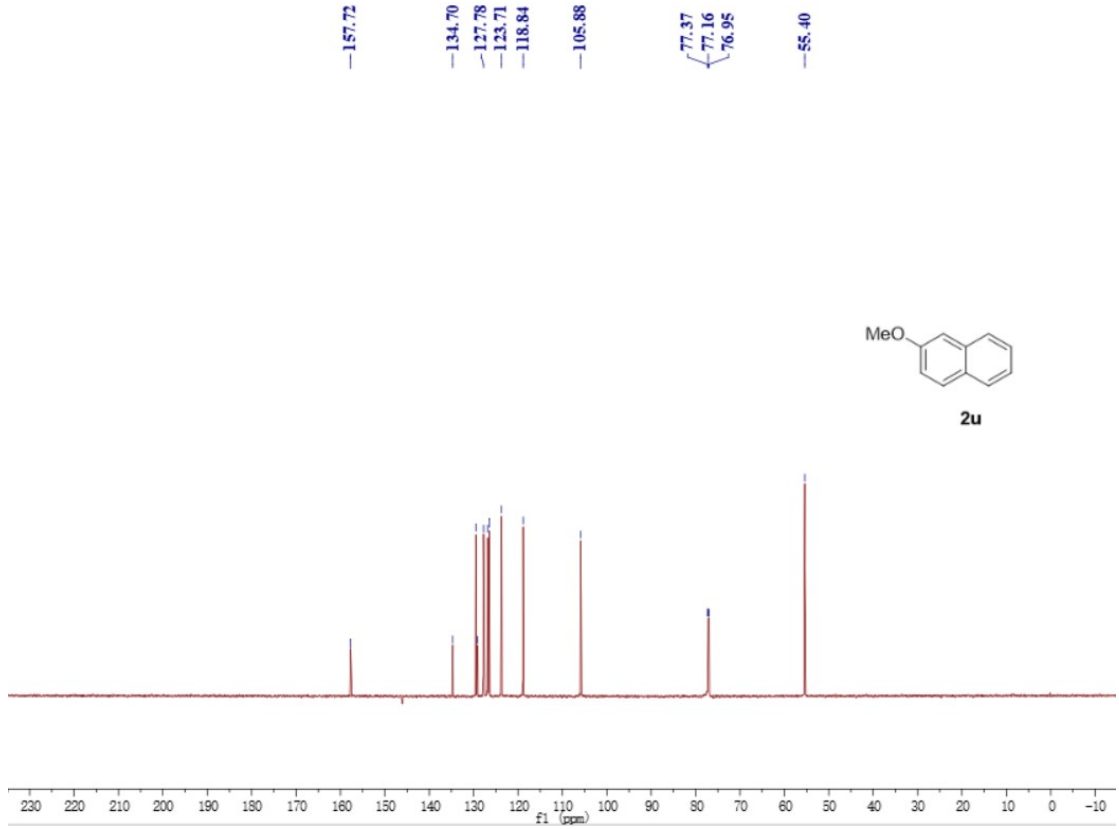

7.89
7.87
7.85
7.64
7.62
7.54
7.52
7.51
7.48
7.46
7.44
7.26
6.85
1.56
NHBoc
2s
2.94
1.00
3.08
0.84
9.05
f1 (ppm)

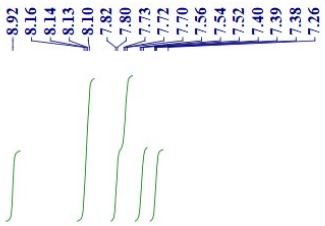

153.64
126.12
125.97
125.95
124.57
120.57
118.73
110.12
80.78
77.37
77.16
76.95
28.51
NHBoc
2s
f1 (ppm)


7.79
7.77
7.75
7.70
7.68
7.45
7.44
7.42
7.35
7.33
7.32
7.26
7.15
7.12
7.12
7.10
7.09
5.02
OH
2t
2.08
1.02
1.02
1.03
1.02
1.05
1.00
f1 (ppm)

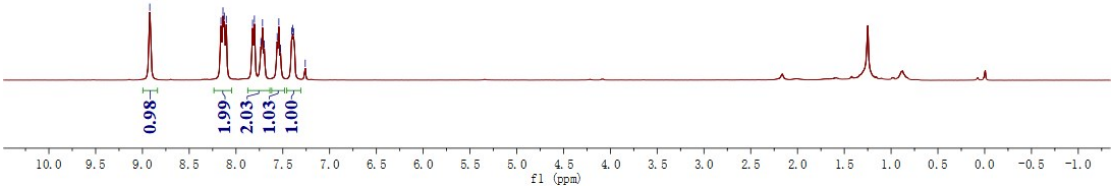

153.39
134.70
127.89
123.77
117.86
109.66
77.37
77.16
76.95
OH
2t
f1 (ppm)


7.79
7.76
7.74
7.47
7.45
7.43
7.36
7.34
7.33
7.26
7.17
7.15
3.93
MeO
2u
2.90
0.97
0.96
1.93
3.00
f1 (ppm)


157.72
134.70
127.78
123.71
118.84
105.88
77.37
77.16
76.95
55.40
MeO
2u
f1 (ppm)

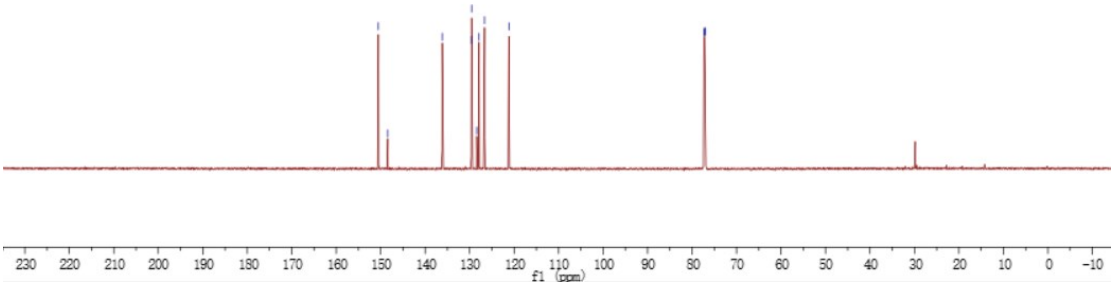

8.92
8.16
8.14
8.13
8.10
7.82
7.80
7.73
7.72
7.70
7.56
7.54
7.52
7.40
7.39
7.38
7.26

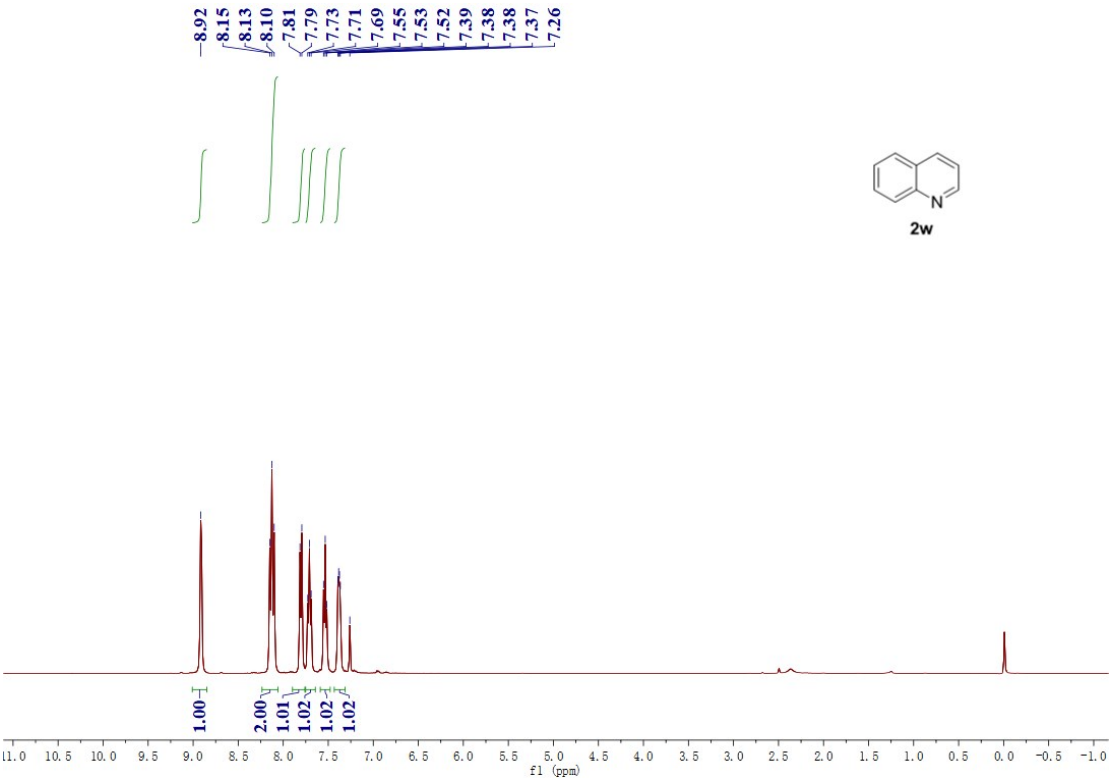
2v

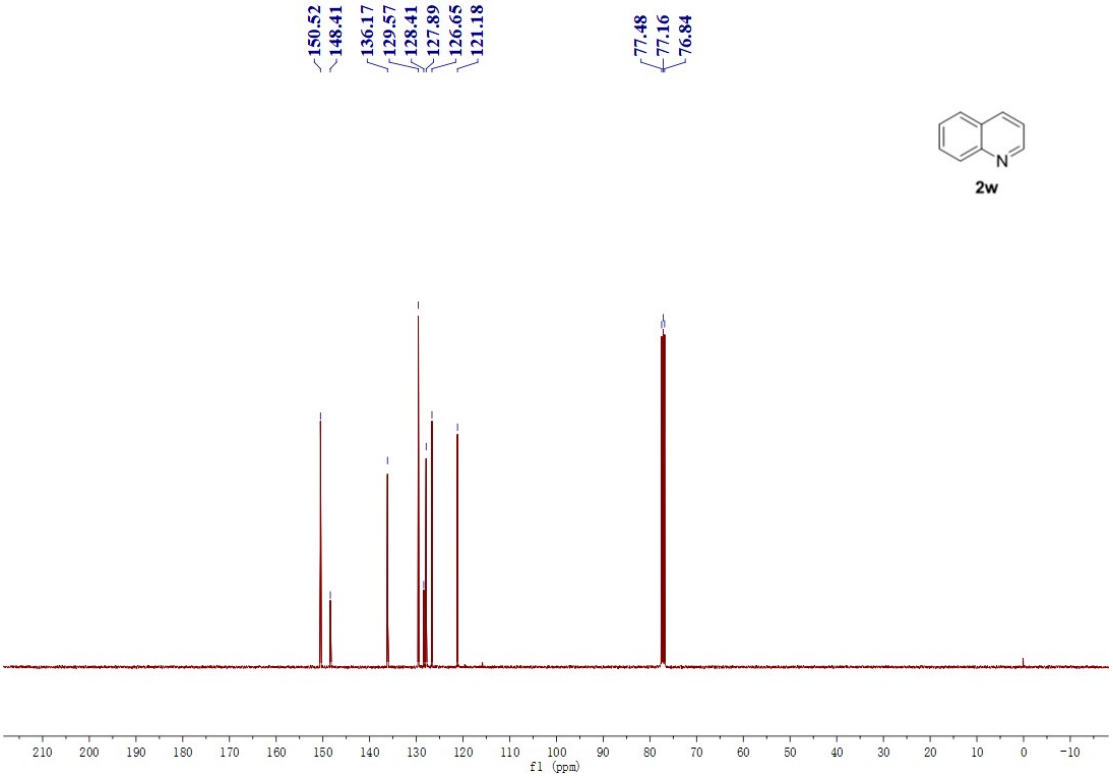

0.98
1.99
2.03
1.03
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

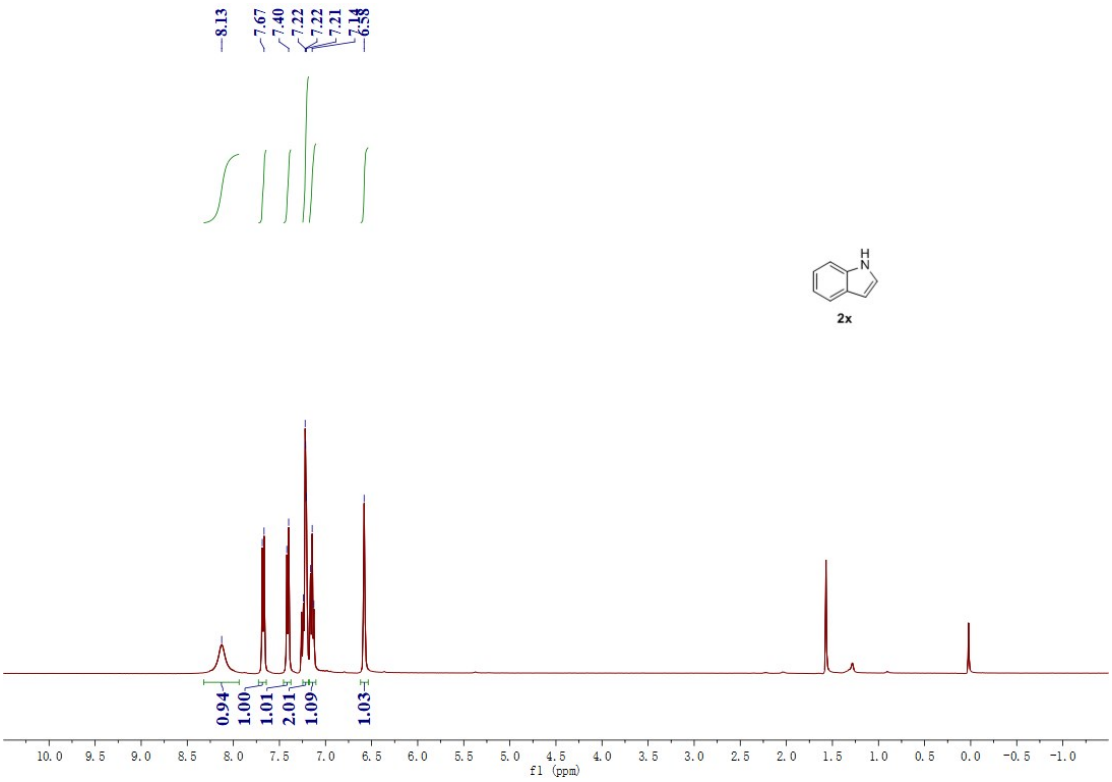

150.53
148.42
136.15
126.65
121.18
77.37
77.16
76.95

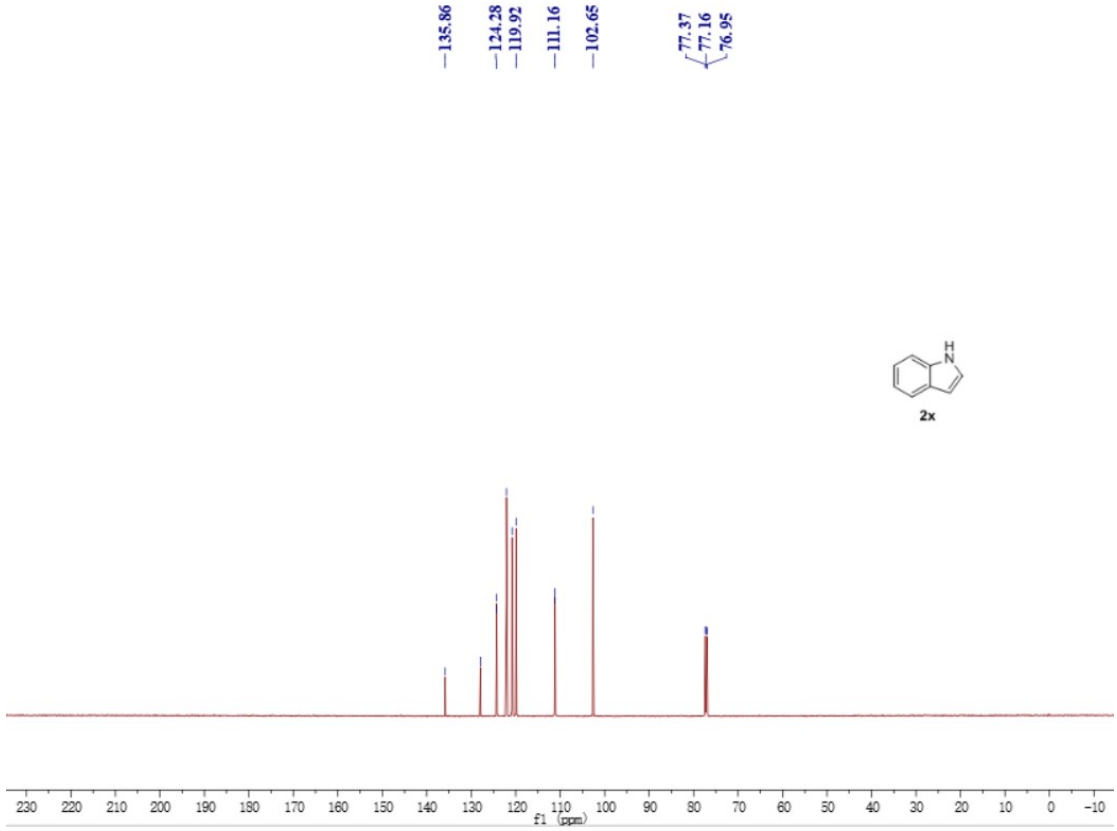
2v

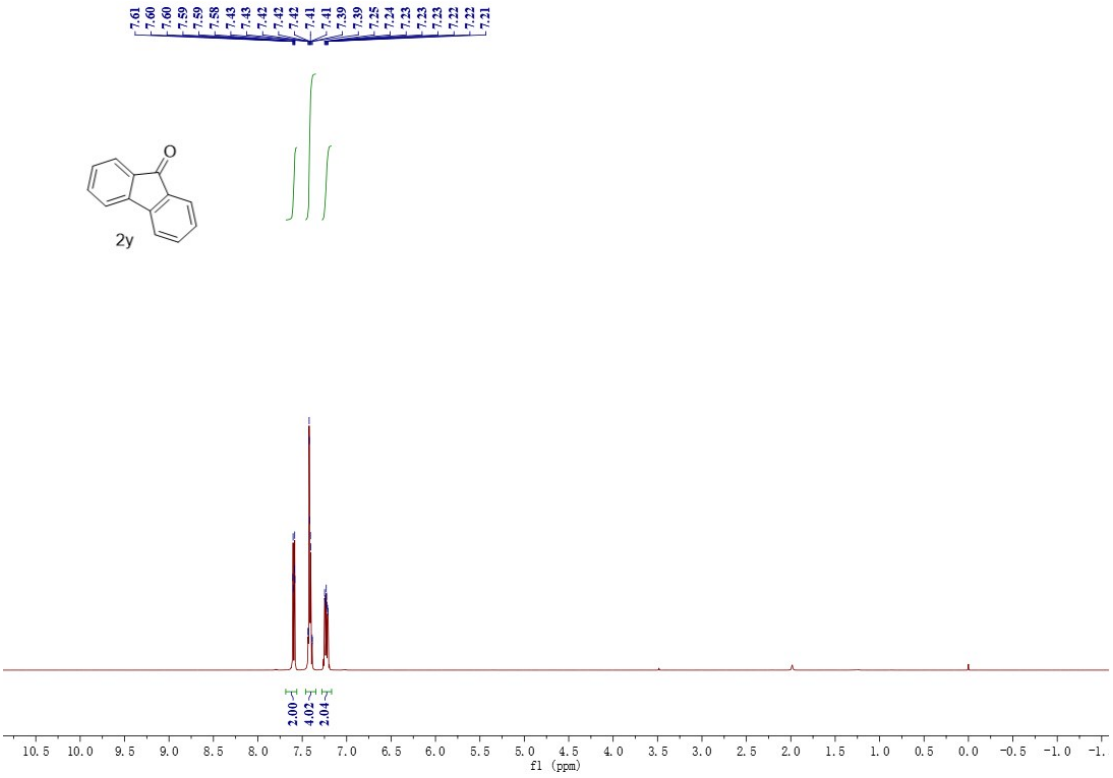

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

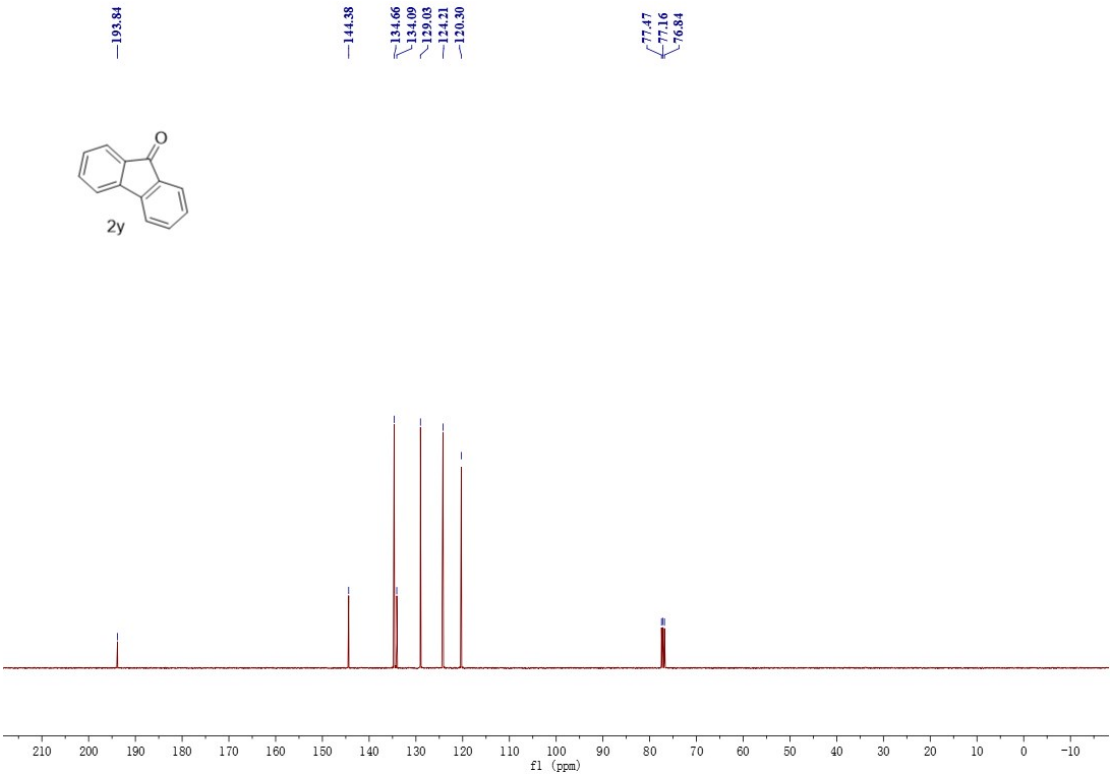

8.92
8.15
8.13
8.10
7.81
7.79
7.73
7.71
7.69
7.55
7.53
7.52
7.39
7.38
7.38
7.37
7.26
2w
1.00
2.00
1.01
1.02
1.02
1.02
f1 (ppm)

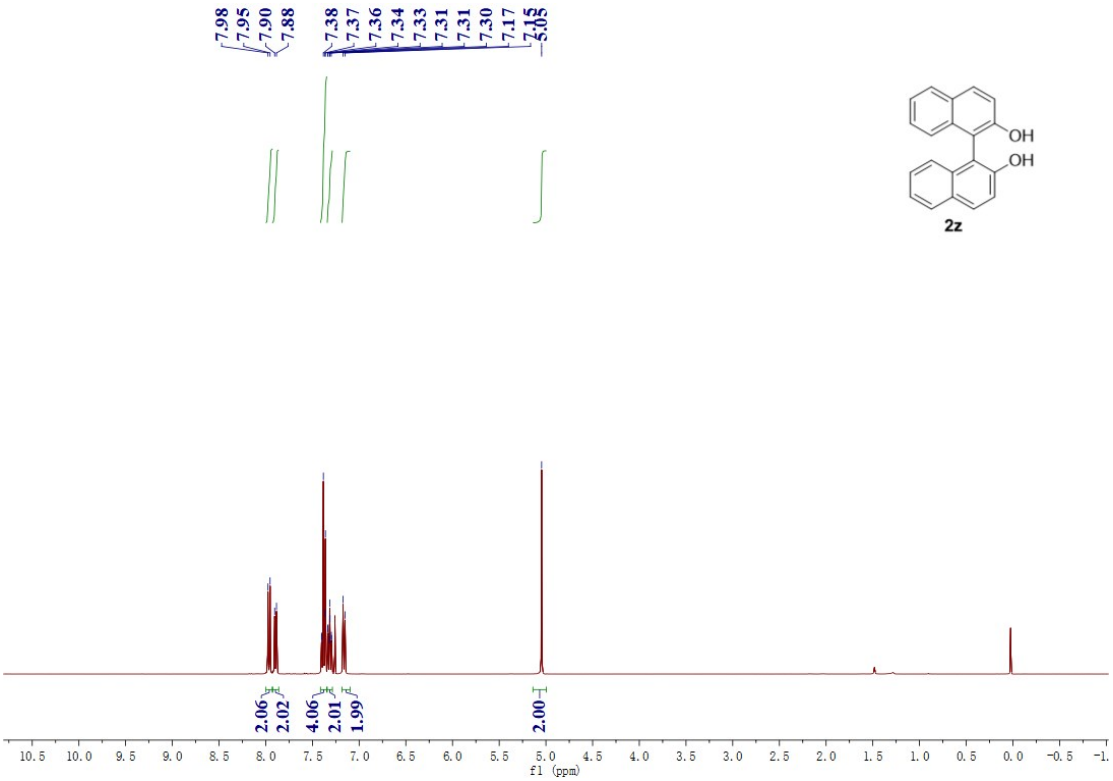

150.52
148.41
136.17
129.57
128.41
127.89
126.65
121.18
77.48
77.16
76.84
2w
f1 (ppm)

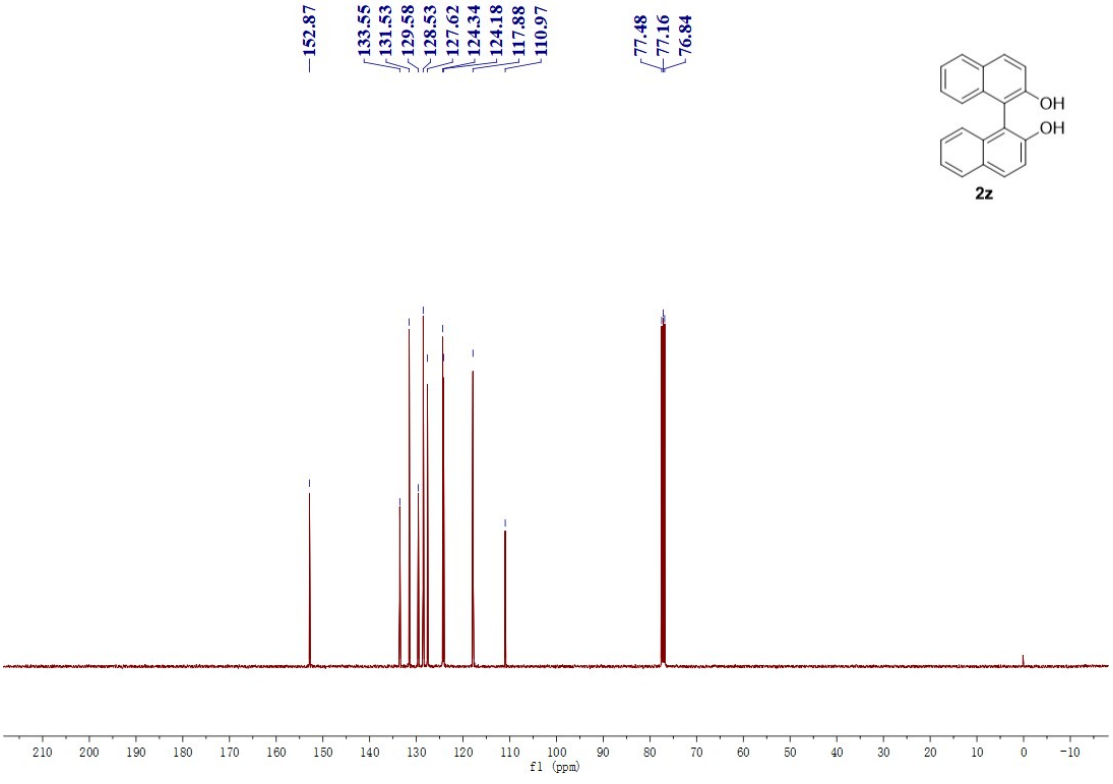

8.13
7.67
7.40
7.22
7.22
7.21
6.58
2x
0.94
1.00
1.01
2.01
1.09
1.03
f1 (ppm)

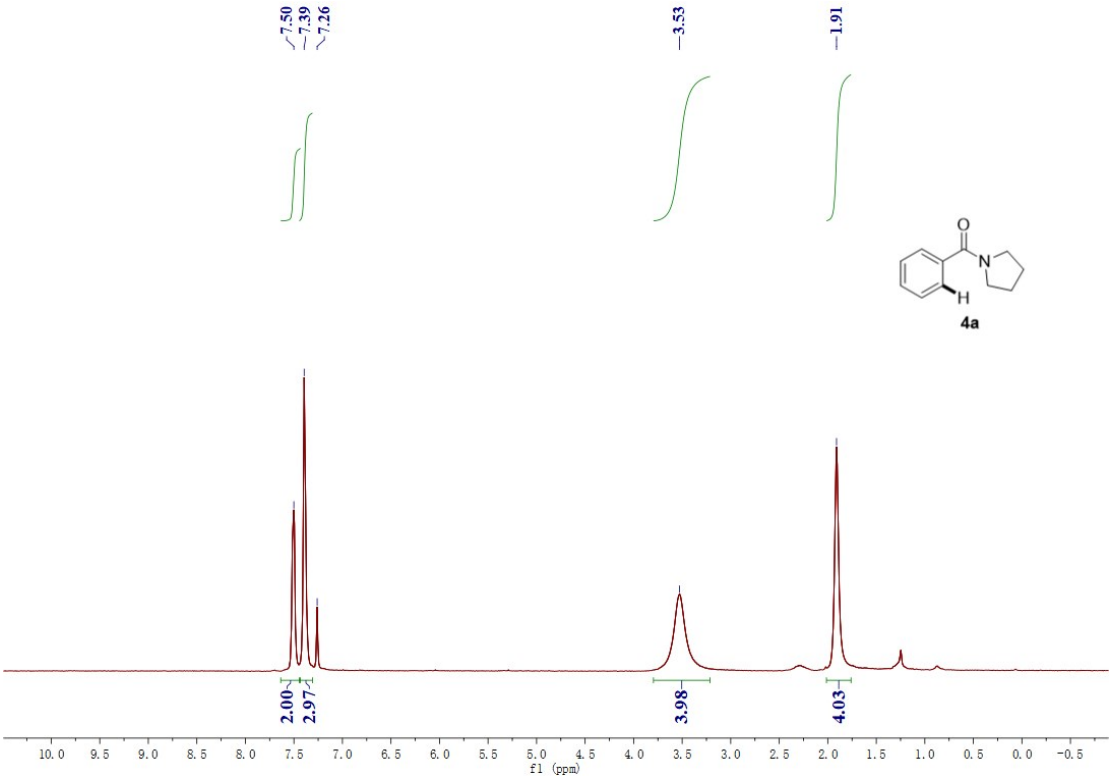

135.86
124.28
119.92
111.16
102.65
77.37
77.16
76.95
2x
f1 (ppm)


7.61
7.60
7.60
7.59
7.59
7.58
7.43
7.43
7.42
7.42
7.42
7.41
7.41
7.39
7.39
7.25
7.24
7.23
7.23
7.23
7.22
7.22
7.21
O
2y
2.00
4.02
2.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.
f1 (ppm)


193.84
144.38
134.66
134.09
129.03
124.21
120.30
77.47
77.16
76.84
O
2y
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.98
7.95
7.90
7.88
7.38
7.37
7.36
7.34
7.33
7.31
7.31
7.30
7.17
7.15
5.05
OH
OH
2z
2.06
2.02
4.06
2.01
1.99
2.00
f1 (ppm)


152.87
133.55
131.53
129.58
128.53
127.62
124.34
124.18
117.88
110.97
77.48
77.16
76.84
OH
OH
2z
f1 (ppm)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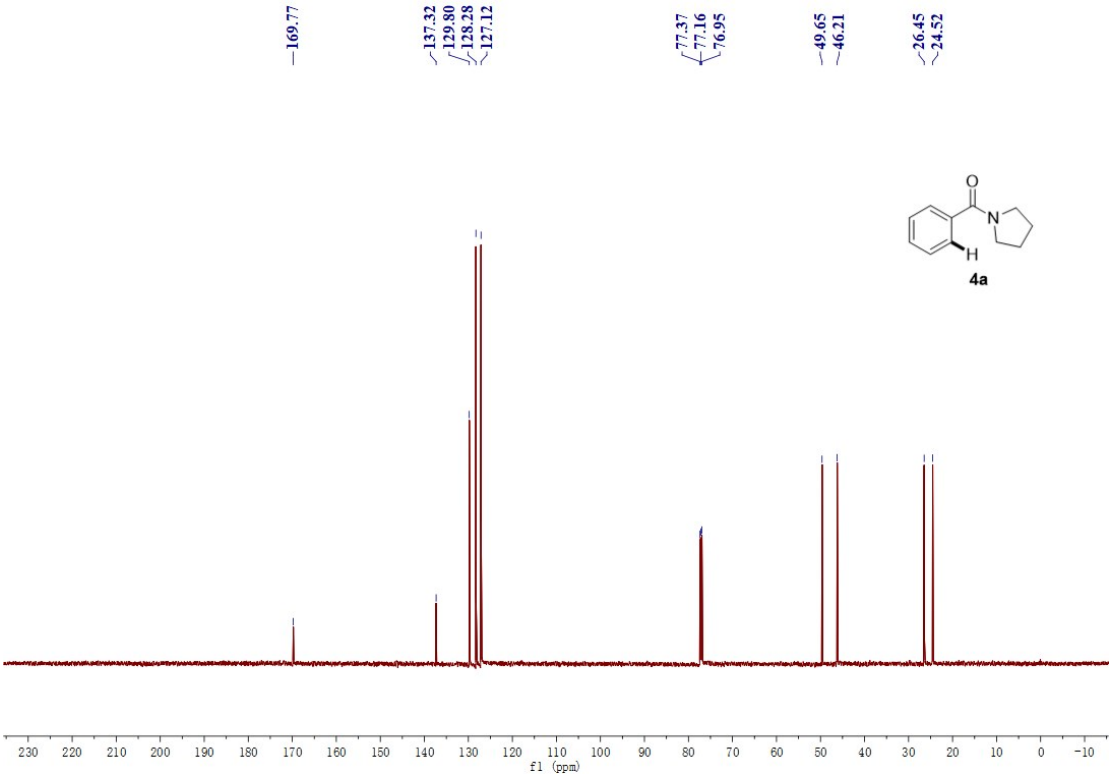
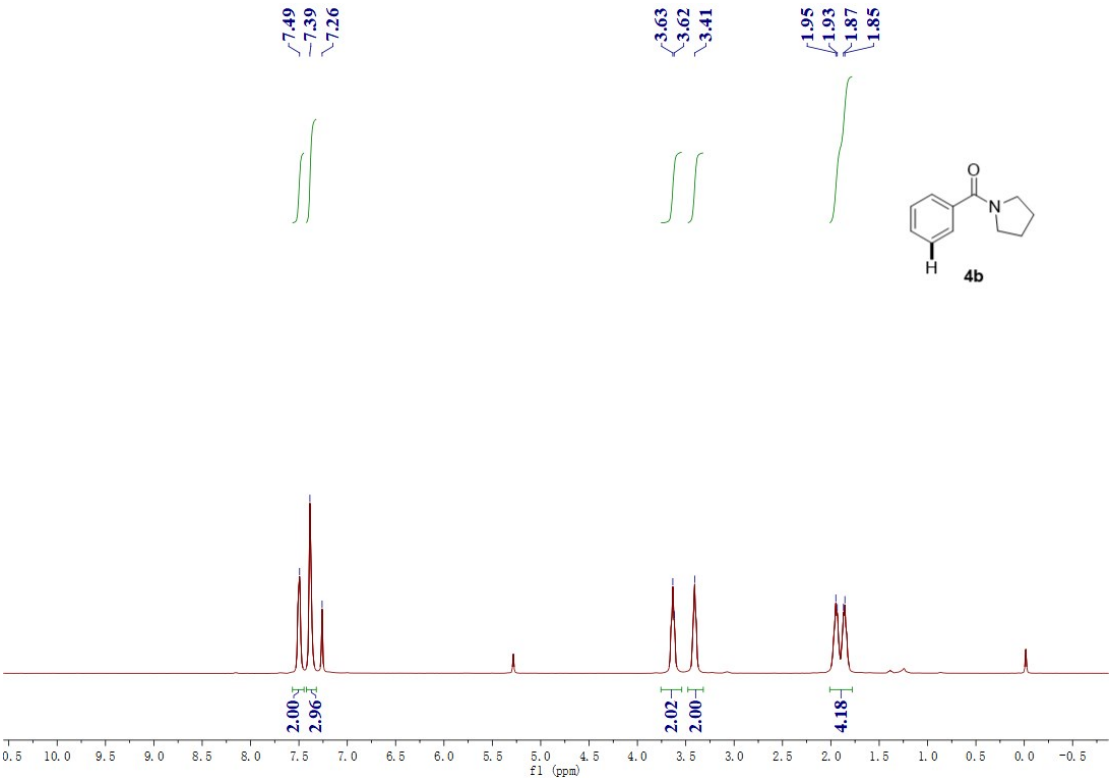
7.39
7.26
3.53
1.91
2.00
2.97
3.98
4.03
f1 (ppm)

4a


169.77
137.32
129.80
128.28
127.12
77.37
77.16
76.95
49.65
46.21
26.45
24.52
f1 (ppm)

4a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7.39
7.26
3.63
3.62
3.41
1.95
1.93
1.87
1.85
4b
2.00
2.96
2.02
2.00
4.18
f1 (ppm)

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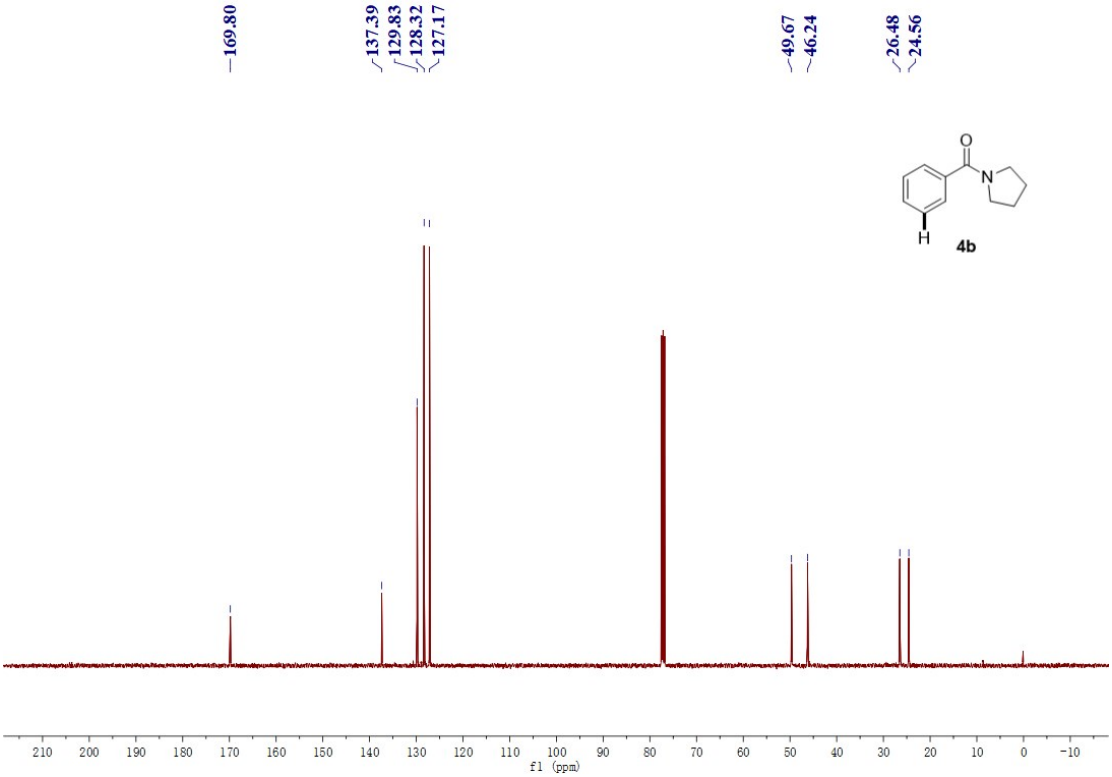
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137.39
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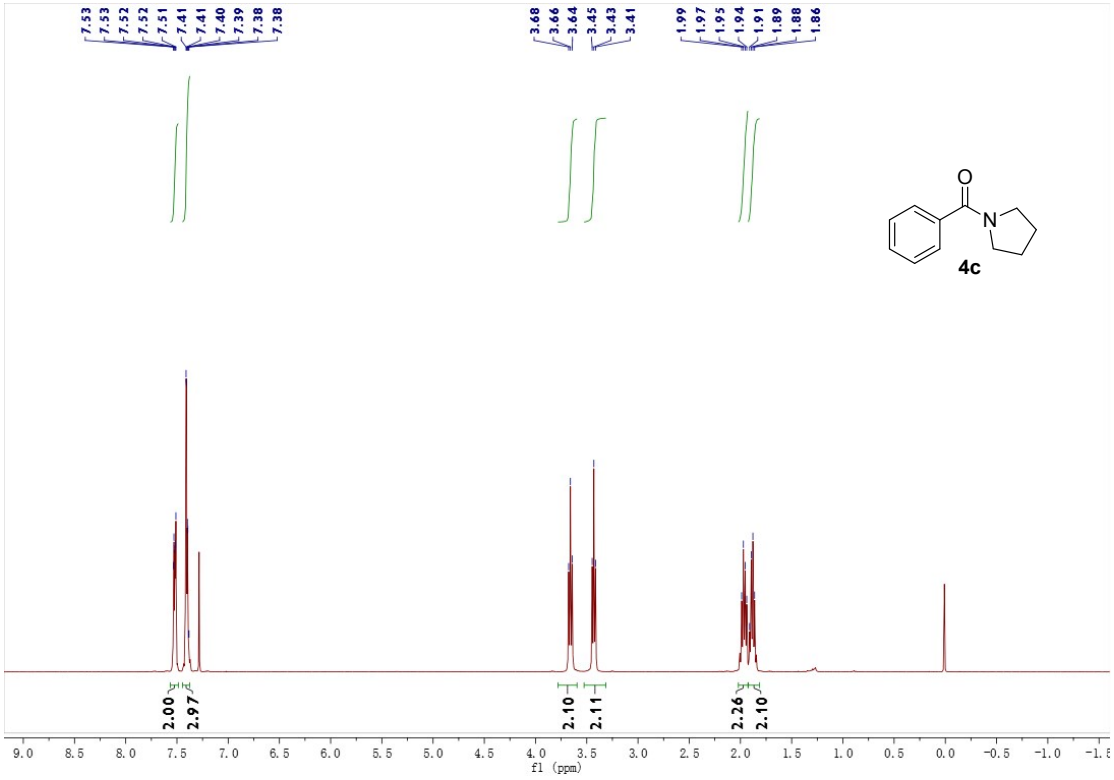
127.17
49.67
46.24
26.48
24.56
4b
f1 (ppm)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7.52
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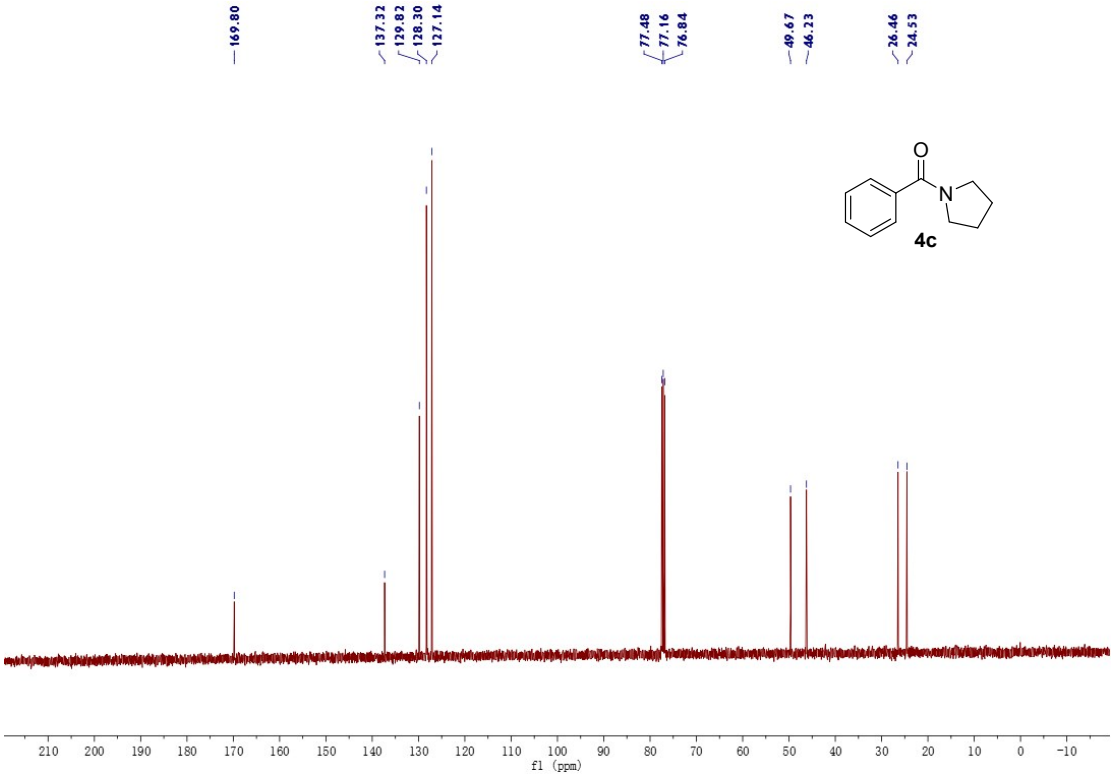
7.41
7.41
7.40
7.39
7.38
7.38
3.68
3.66
3.64
3.45
3.43
3.41
1.99
1.97
1.95
1.94
1.91
1.89
1.88
1.86
O
N
4c
2.00
2.97
2.10
2.11
2.26
2.10
f1 (ppm)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137.32
129.82
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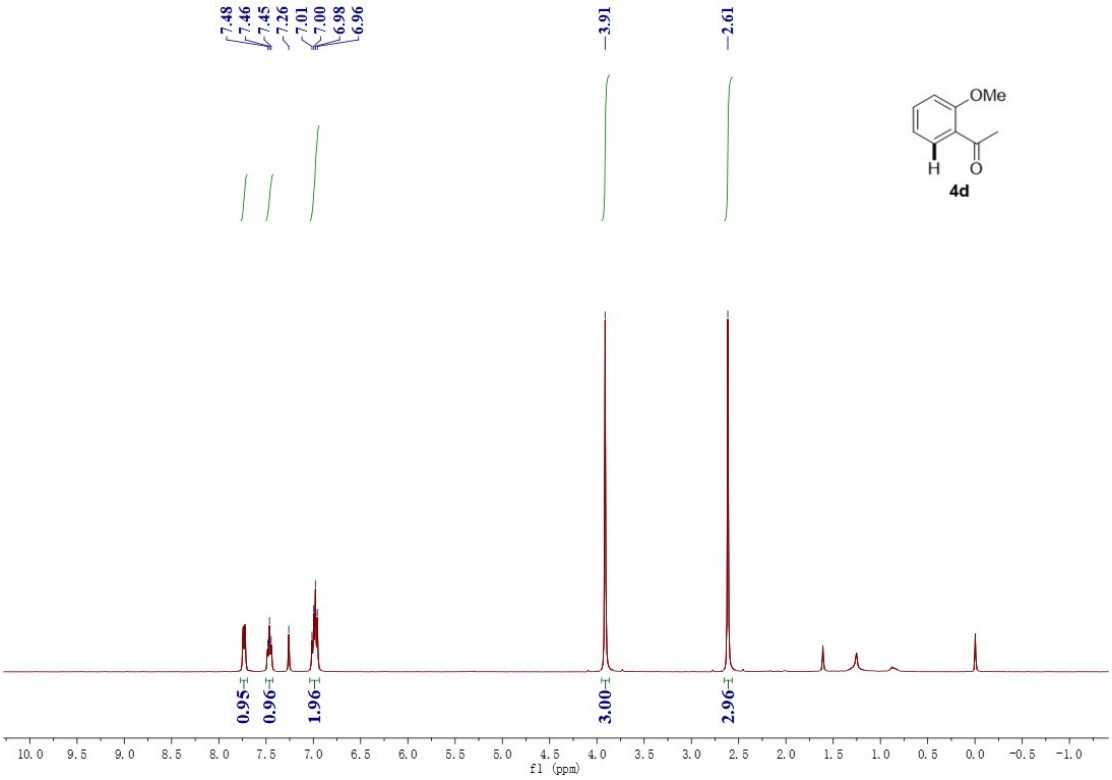
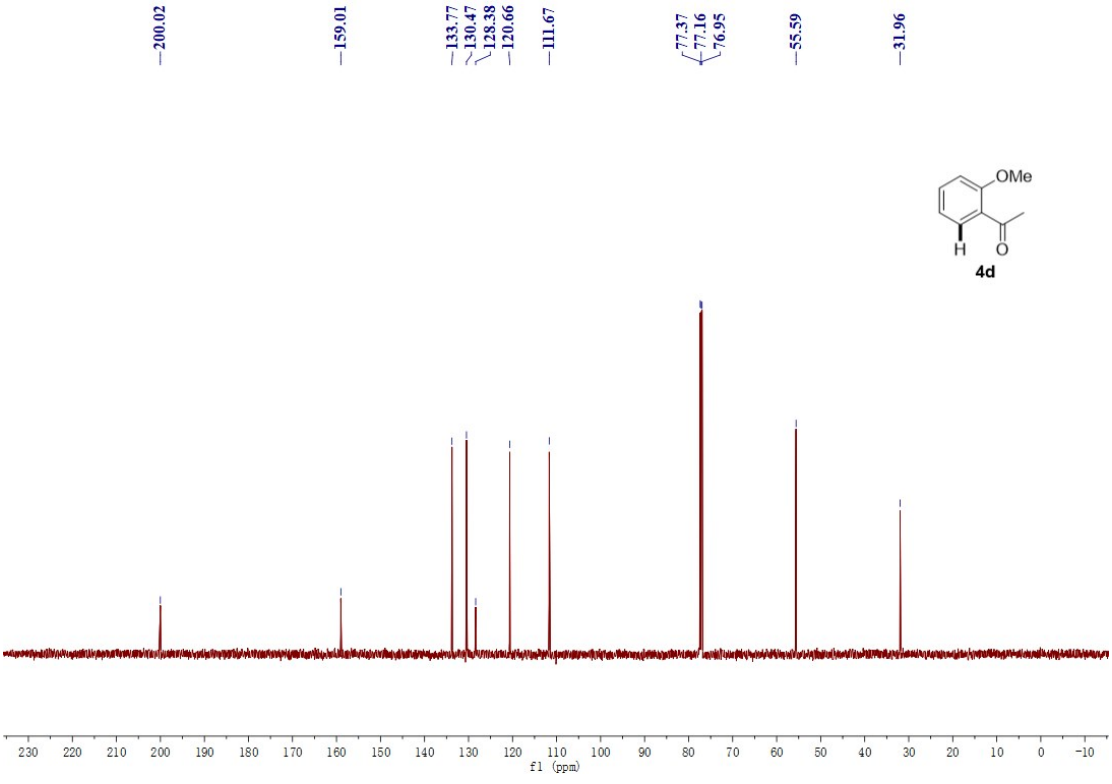
76.84
49.67
46.23
26.46
24.53
O
N
4c
f1 (ppm)


7.48
7.46
7.45
7.26
7.01
7.00
6.98
6.96
3.91
2.61
OMe
H
O
4d
0.95
0.96
1.96
3.00
2.96
f1 (ppm)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159.01
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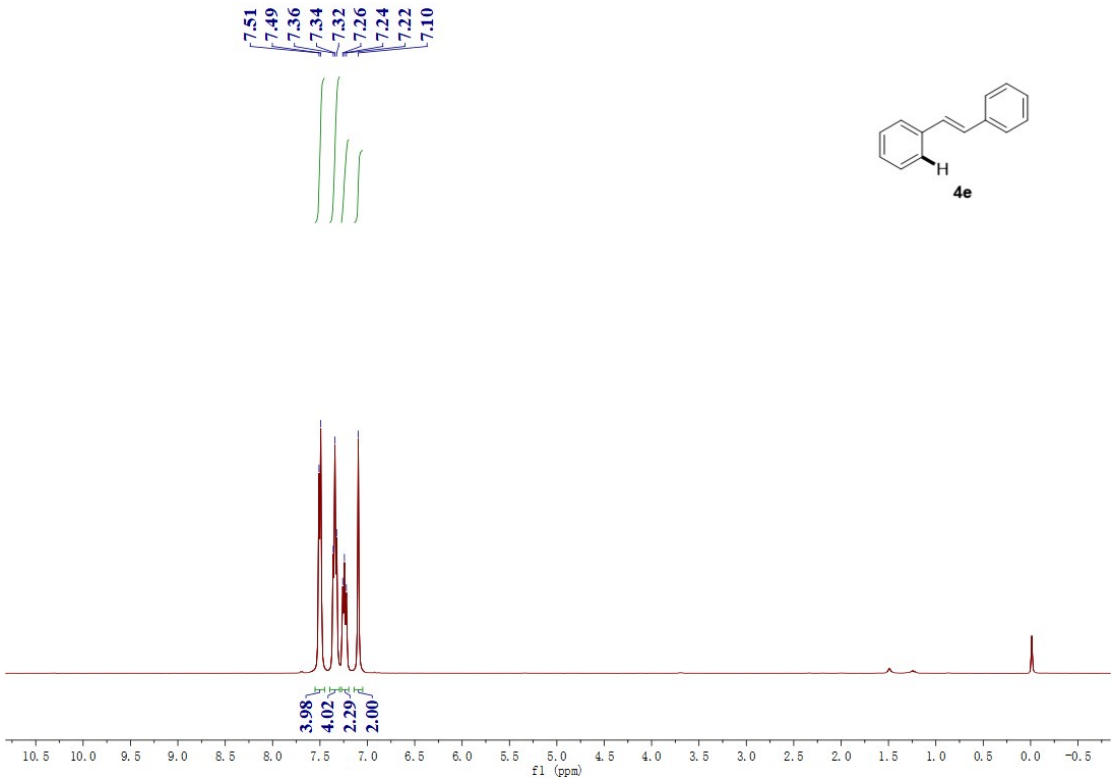
77.37
77.16
76.95
55.59
31.96
OMe
H
O
4d
f1 (ppm)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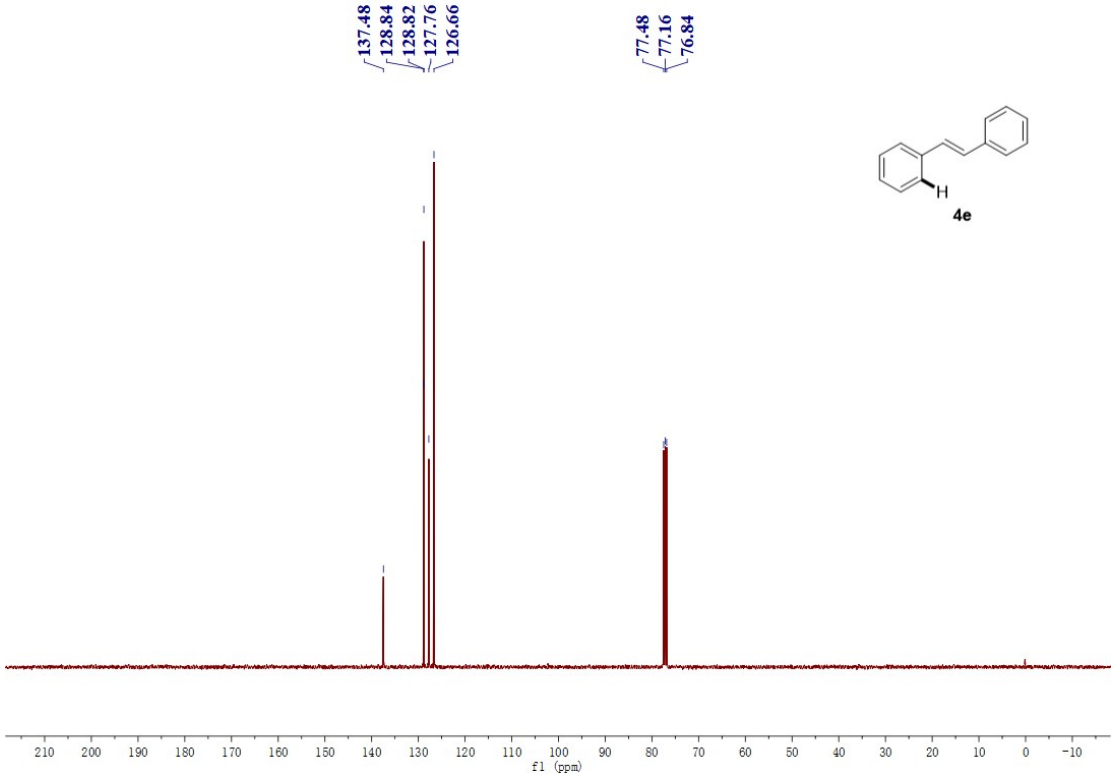
7.49
7.36
7.34
7.32
7.26
7.24
7.22
7.10
H
4e
3.98
4.02
2.29
2.00
f1 (ppm)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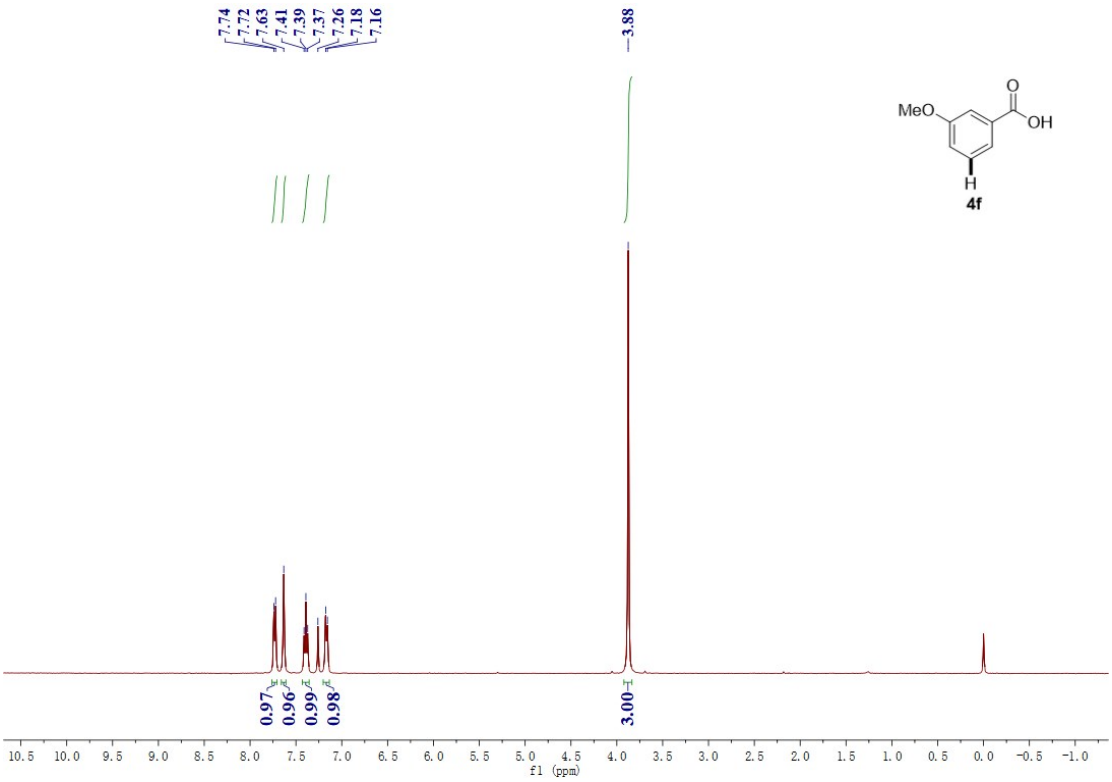
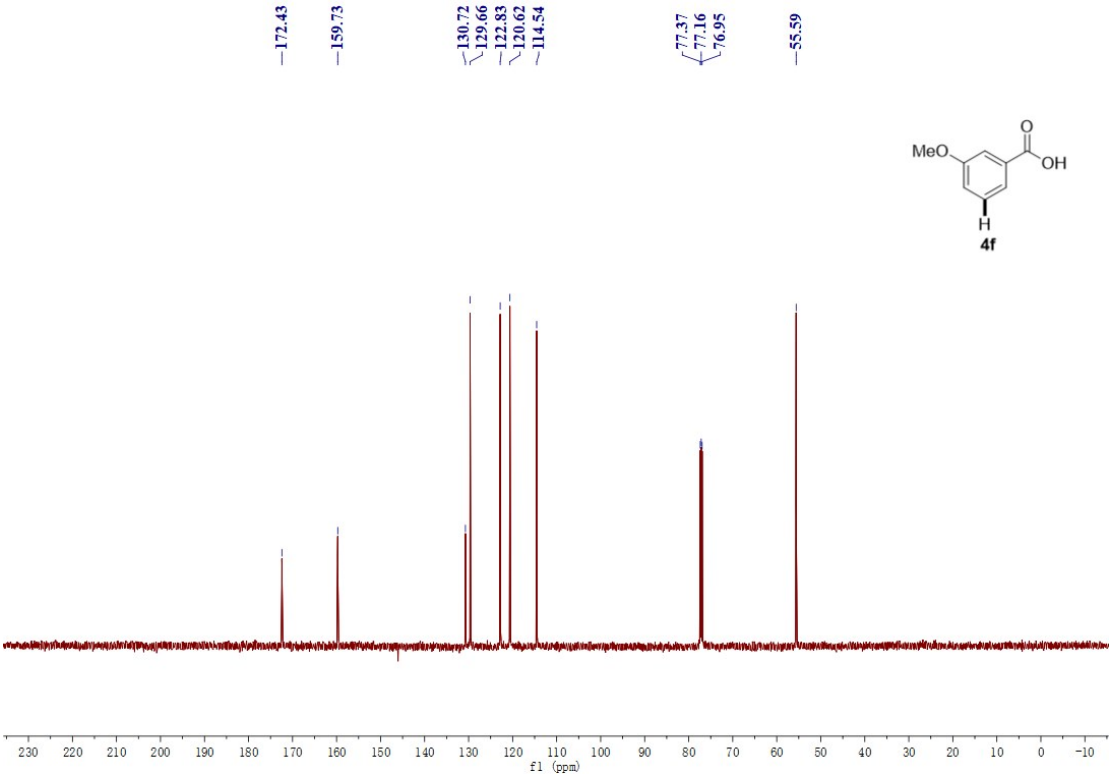
128.84
128.82
127.76
126.66
77.48
77.16
76.84
H
4e
f1 (ppm)


7.74
7.72
7.63
7.41
7.39
7.37
7.26
7.18
7.16
3.88
MeO
O
OH
H
4f
0.97
0.96
0.99
0.98
3.00
f1 (ppm)


172.43
159.73
130.72
129.66
122.83
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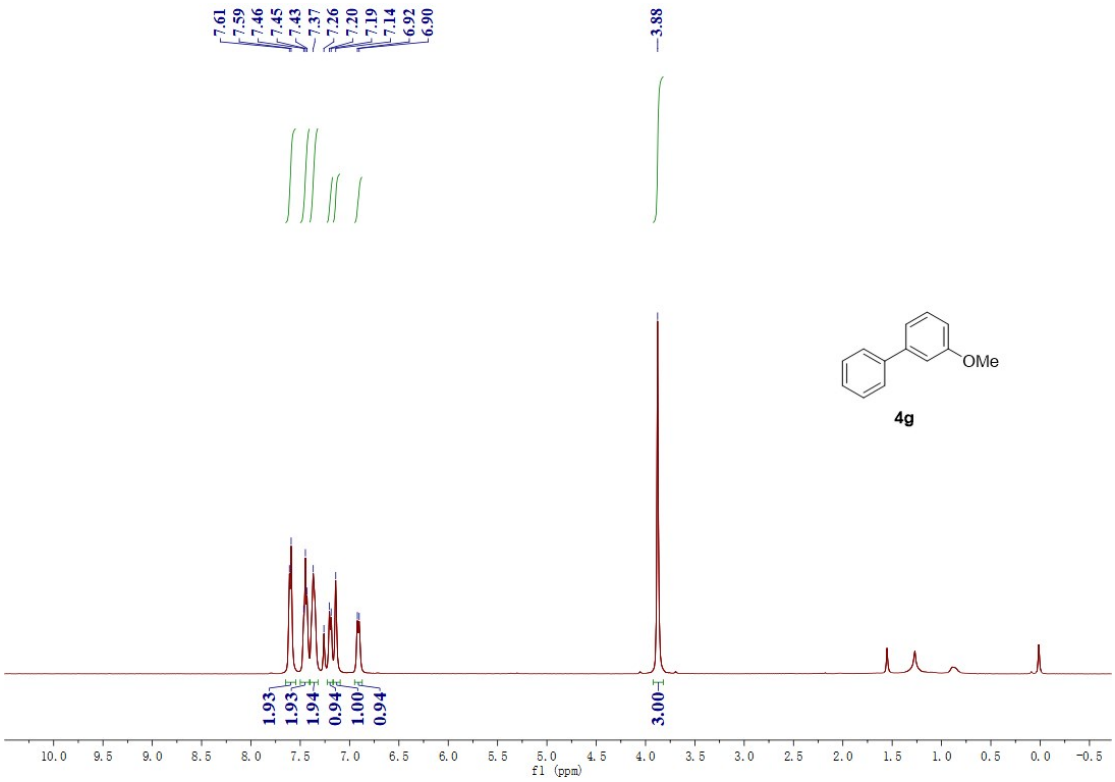
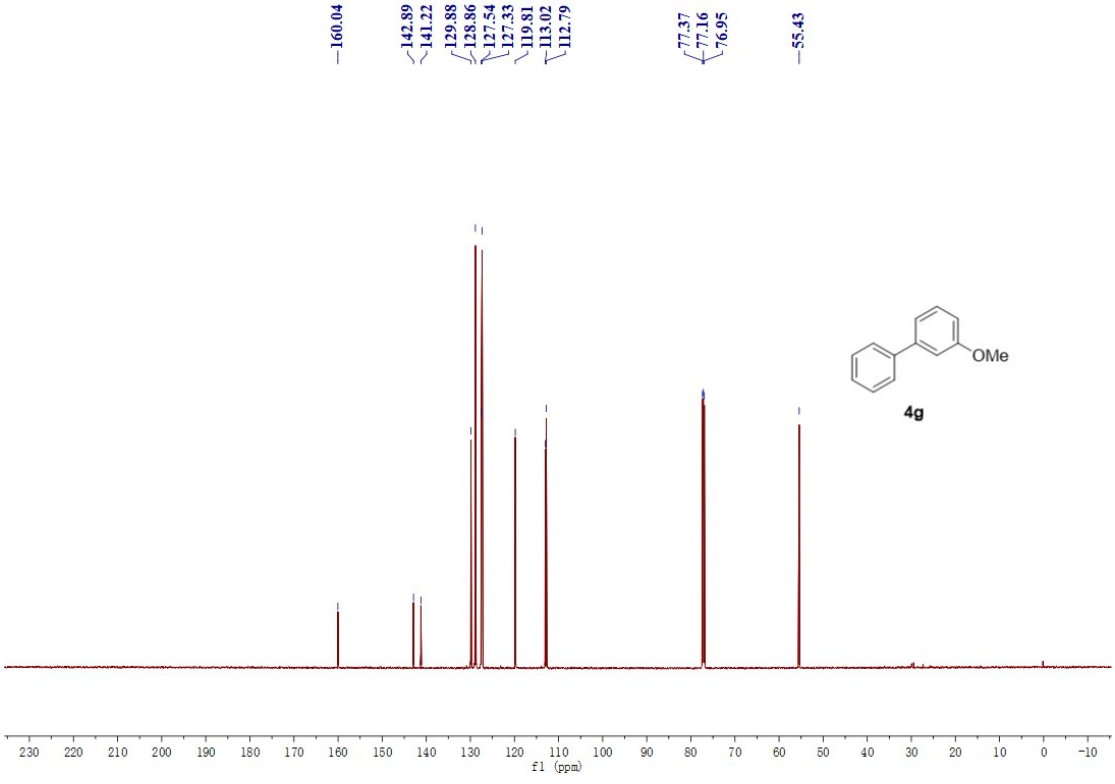
114.54
77.37
77.16
76.95
55.59
MeO
O
OH
H
4f
f1 (ppm)


7.61
7.59
7.46
7.45
7.43
7.37
7.26
7.20
7.19
7.14
6.92
6.90
3.88
OMe
4g
1.93
1.93
1.94
0.94
1.00
0.94
3.00
f1 (ppm)


160.04
142.89
141.22
129.88
128.86
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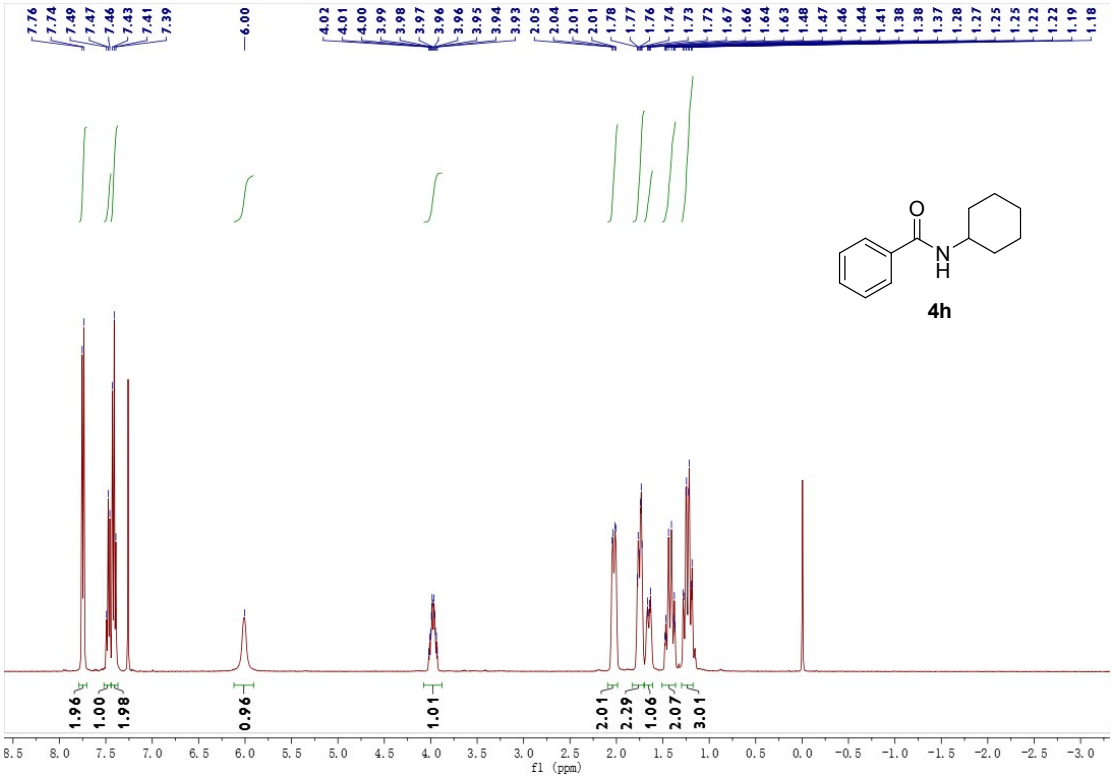
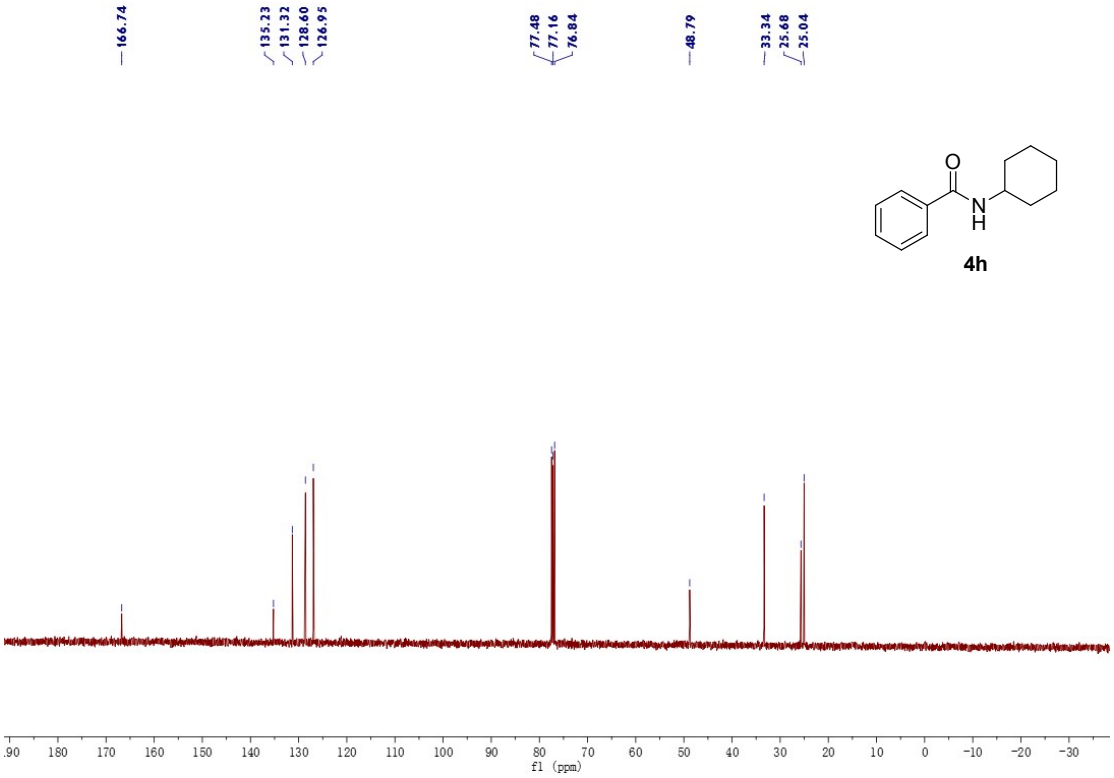
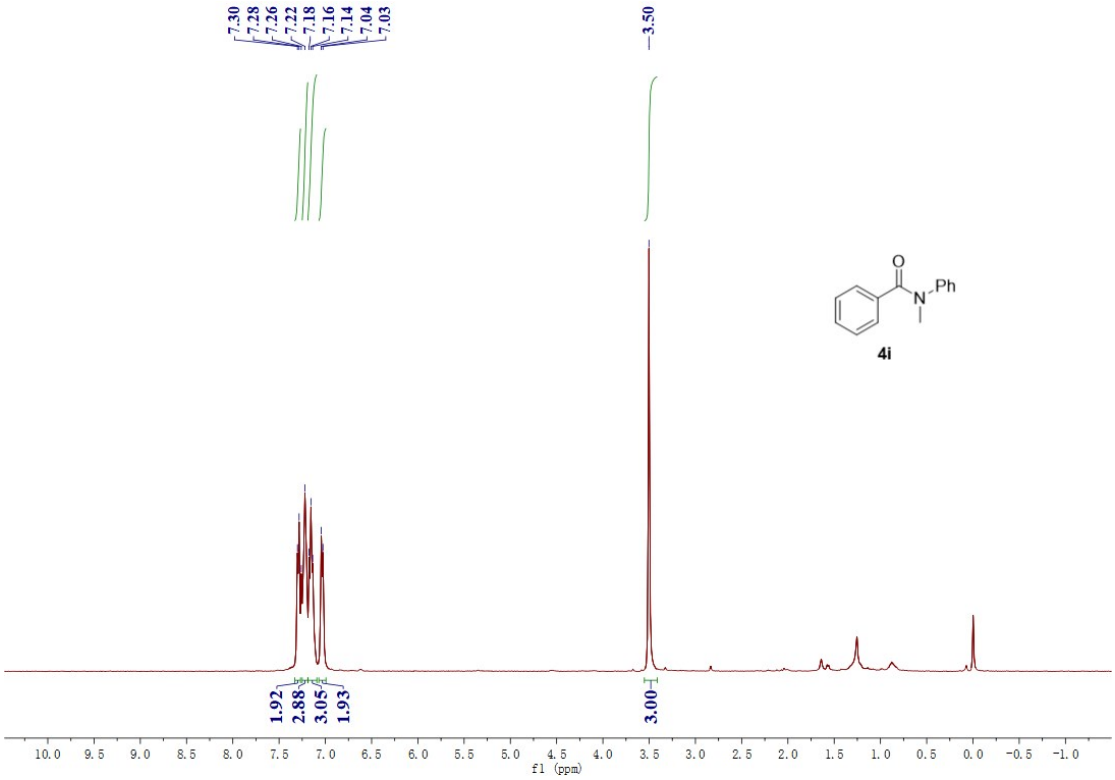
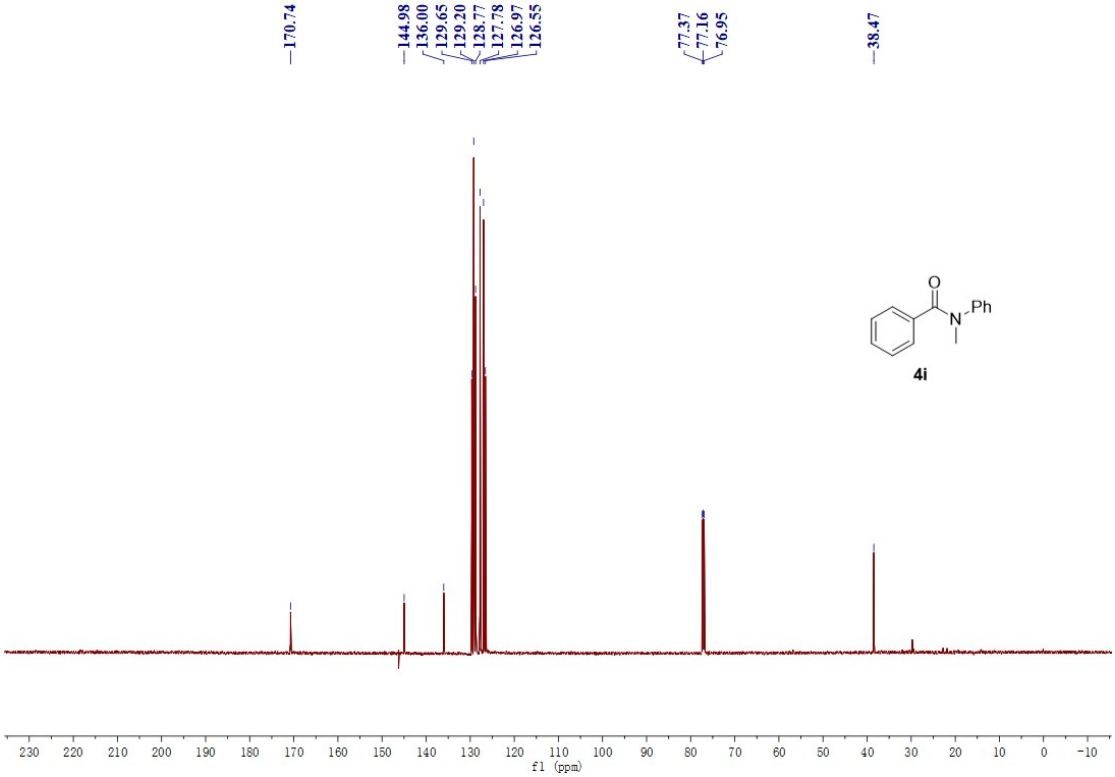
127.33
119.81
113.02
112.79
77.37
77.16
76.95
55.43
OMe
4g
f1 (ppm)


7.76 7.74 7.49 7.47 7.46 7.43 7.41 7.39
6.00
4.02 4.01 4.00 3.99 3.98 3.97 3.96 3.96 3.95 3.94 3.93
2.05 2.04 2.01 2.01 1.78 1.77 1.76 1.74 1.73 1.72 1.67 1.66 1.64 1.63 1.48 1.47 1.46 1.44 1.41 1.38 1.38 1.37 1.28 1.27 1.25 1.25 1.22 1.22 1.19 1.18
O
N
H
4h
1.96 1.00 1.98 0.96 1.01 2.01 2.29 1.06 2.07 3.01
f1 (ppm)


166.74
135.23 131.32 128.60 126.95
77.48 77.16 76.84
48.79
33.34 25.68 25.04
O
N
H
4h
f1 (ppm)


7.30
7.28
7.26
7.22
7.18
7.16
7.14
7.04
7.03
3.50
O
N
Ph
4i
1.92
2.88
3.05
1.93
3.00
f1 (ppm)


170.74
144.98
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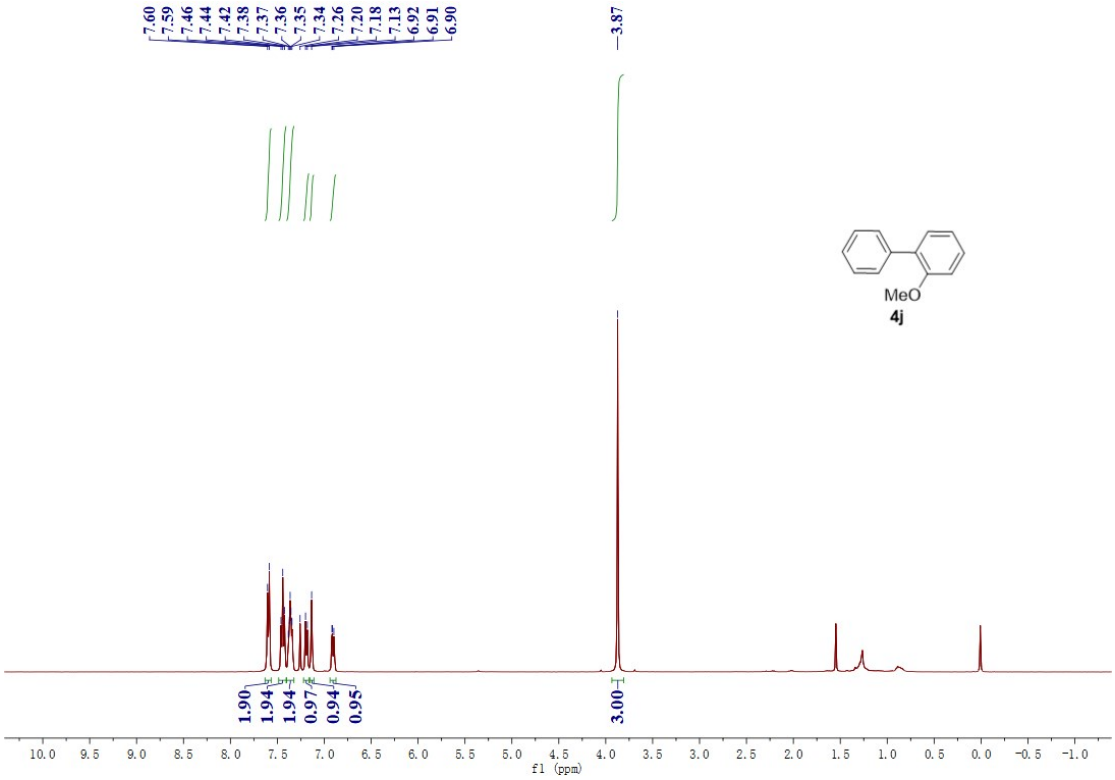
129.20
128.77
127.78
126.97
126.55
77.37
77.16
76.95
38.47
O
N
Ph
4i
f1 (ppm)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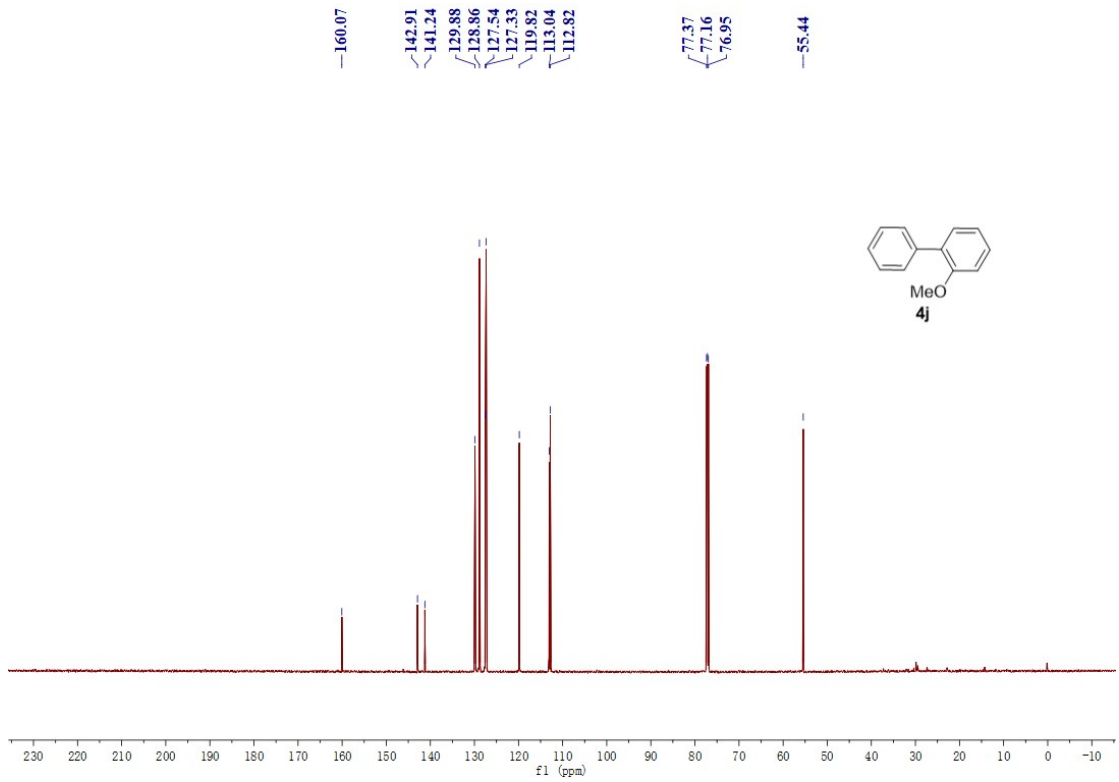
7.46
7.44
7.42
7.38
7.37
7.36
7.35
7.34
7.26
7.20
7.18
7.13
6.92
6.91
6.90
3.87
MeO
4j
1.90
1.94
1.94
0.97
0.94
0.95
3.00
f1 (ppm)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142.91
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129.88
128.86
127.54
127.33
119.82
113.04
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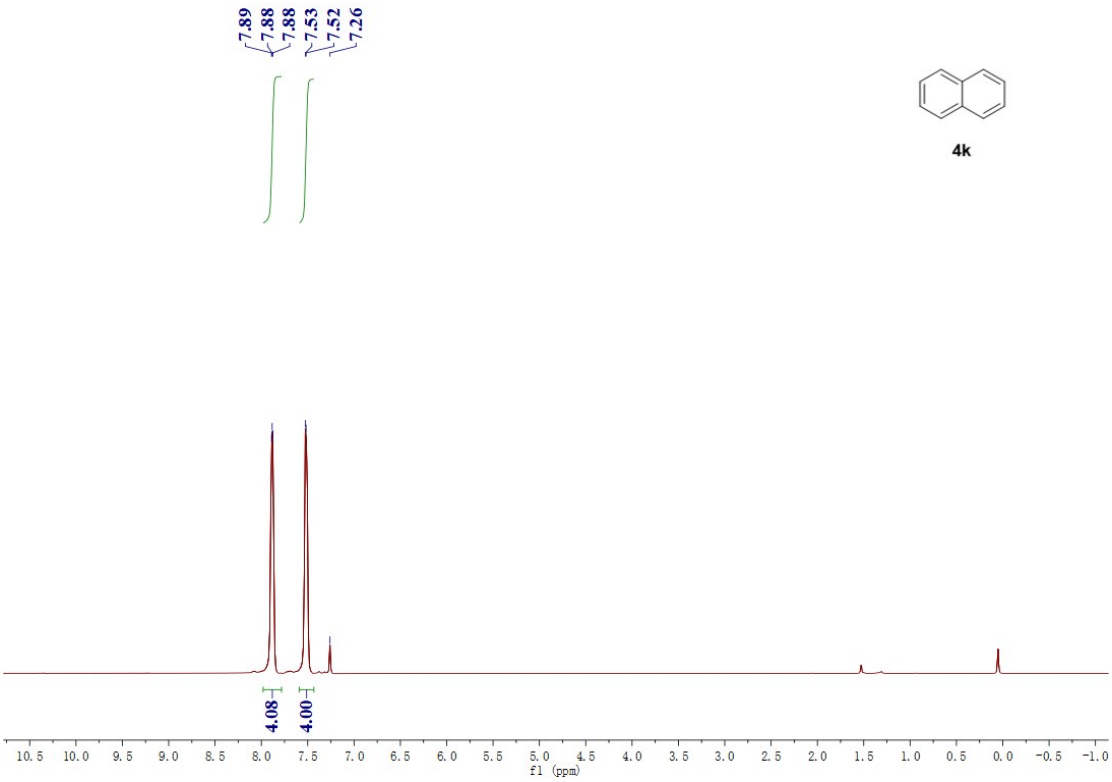
77.37
77.16
76.95
55.44
MeO
4j
f1 (ppm)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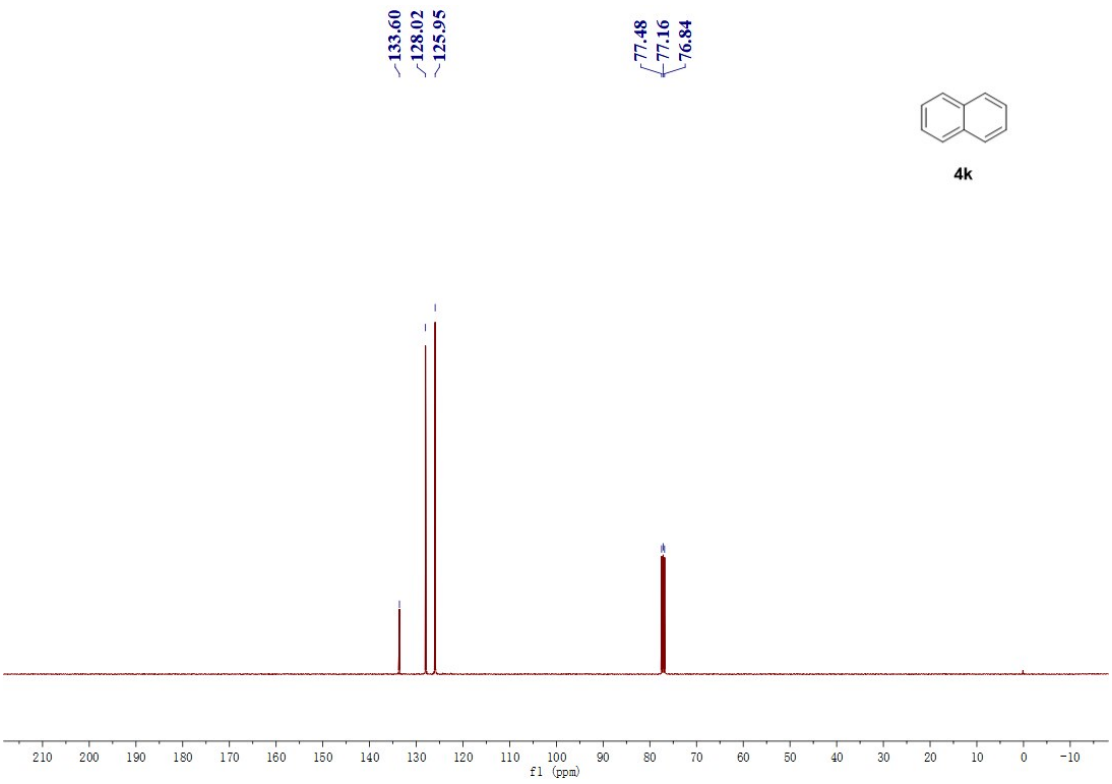
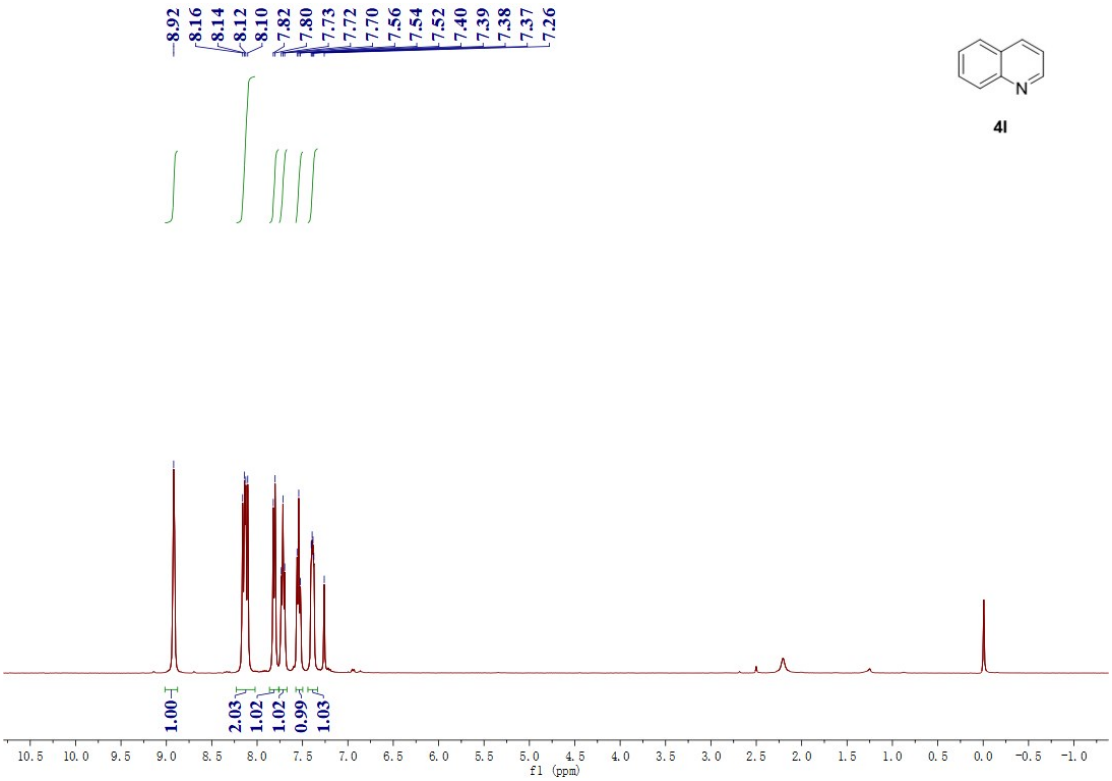
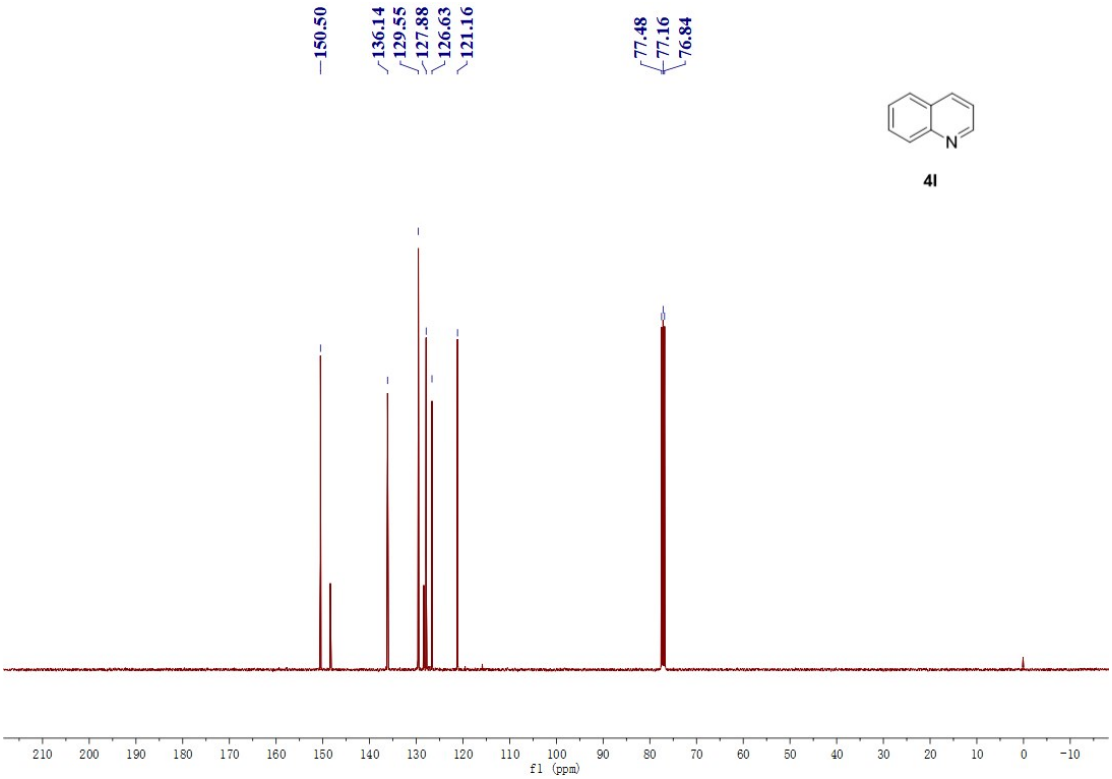
7.88
7.88
7.53
7.52
7.26
4k
4.08
4.00
f1 (ppm)


133.60
128.02
125.95
77.48
77.16
76.84
4k
f1 (ppm)


8.92
8.16
8.14
8.12
8.10
7.82
7.80
7.73
7.72
7.70
7.56
7.54
7.52
7.40
7.39
7.38
7.37
7.26
4l
1.00
2.03
1.02
1.02
0.99
1.03
f1 (ppm)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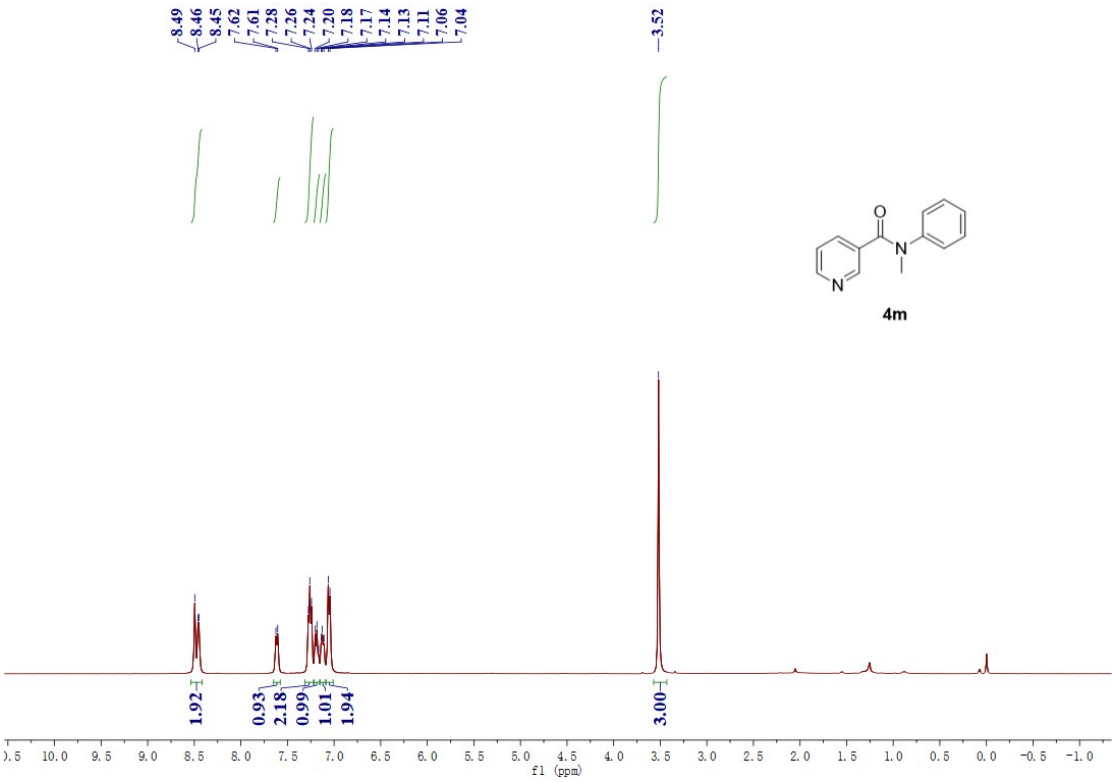
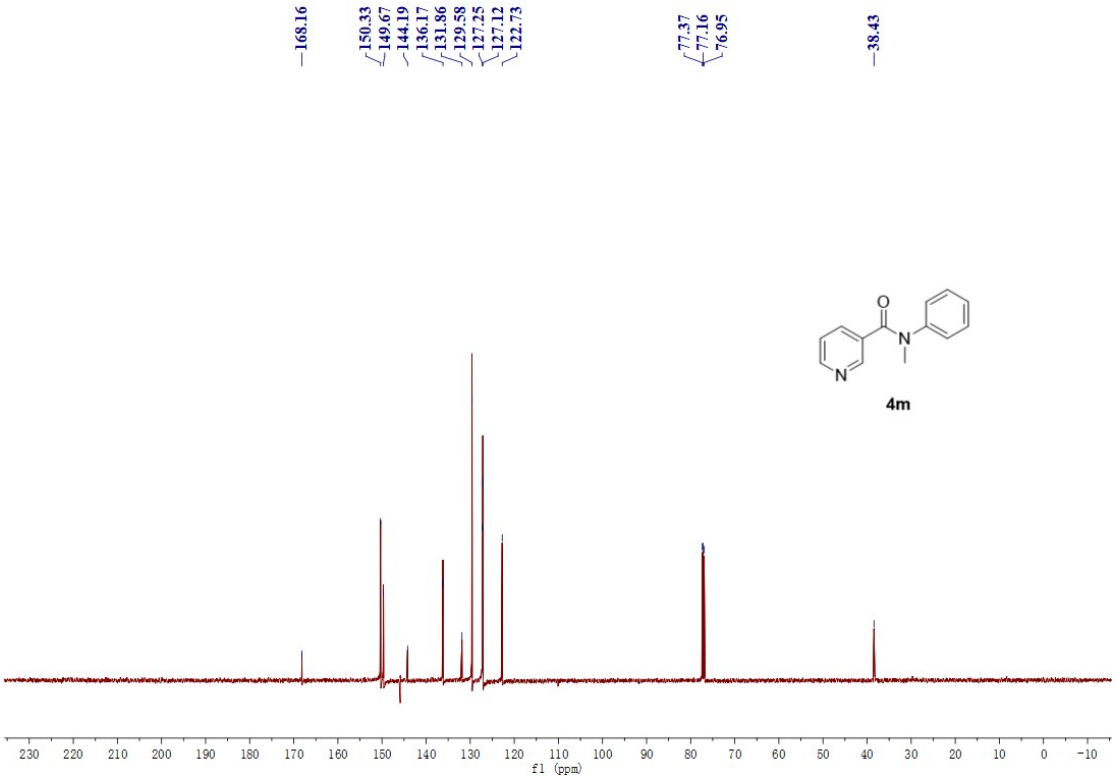
129.55
127.88
126.63
121.16
77.48
77.16
76.84
4l
f1 (ppm)


8.49
8.46
8.45
7.62
7.61
7.28
7.26
7.24
7.20
7.18
7.17
7.14
7.13
7.11
7.06
7.04
3.52
1.92
0.93
2.18
0.99
1.01
1.94
3.00
f1 (ppm)

4m


168.16
150.33
149.67
144.19
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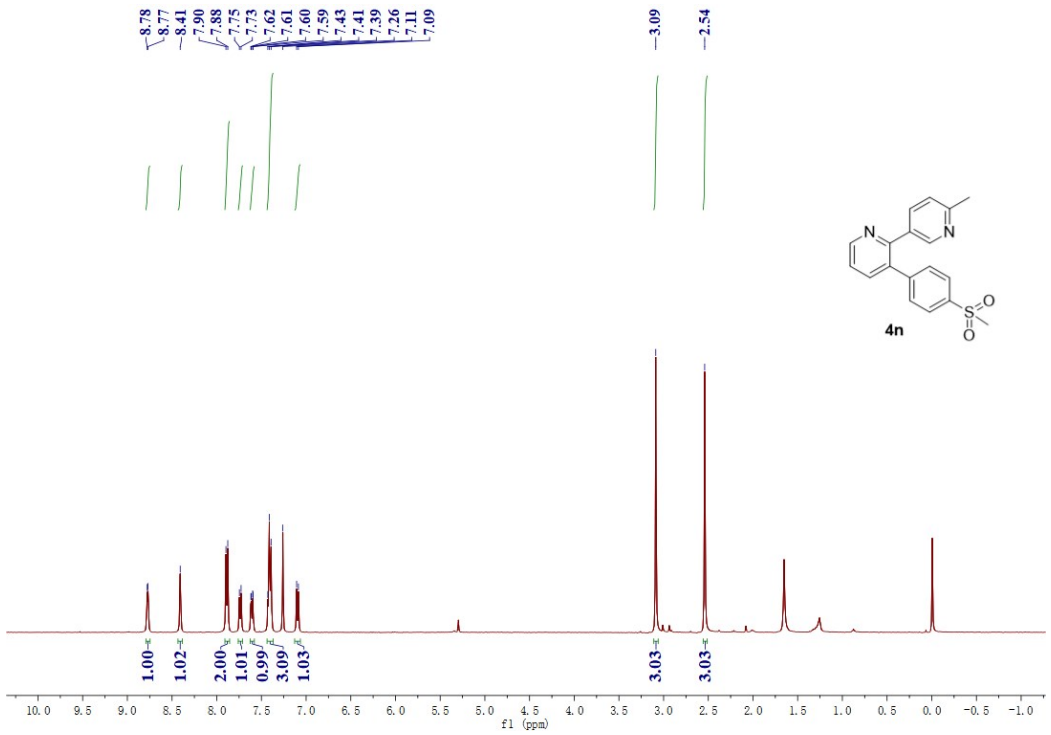
131.86
129.58
127.25
127.12
122.73
77.37
77.16
76.95
38.43
f1 (ppm)

4m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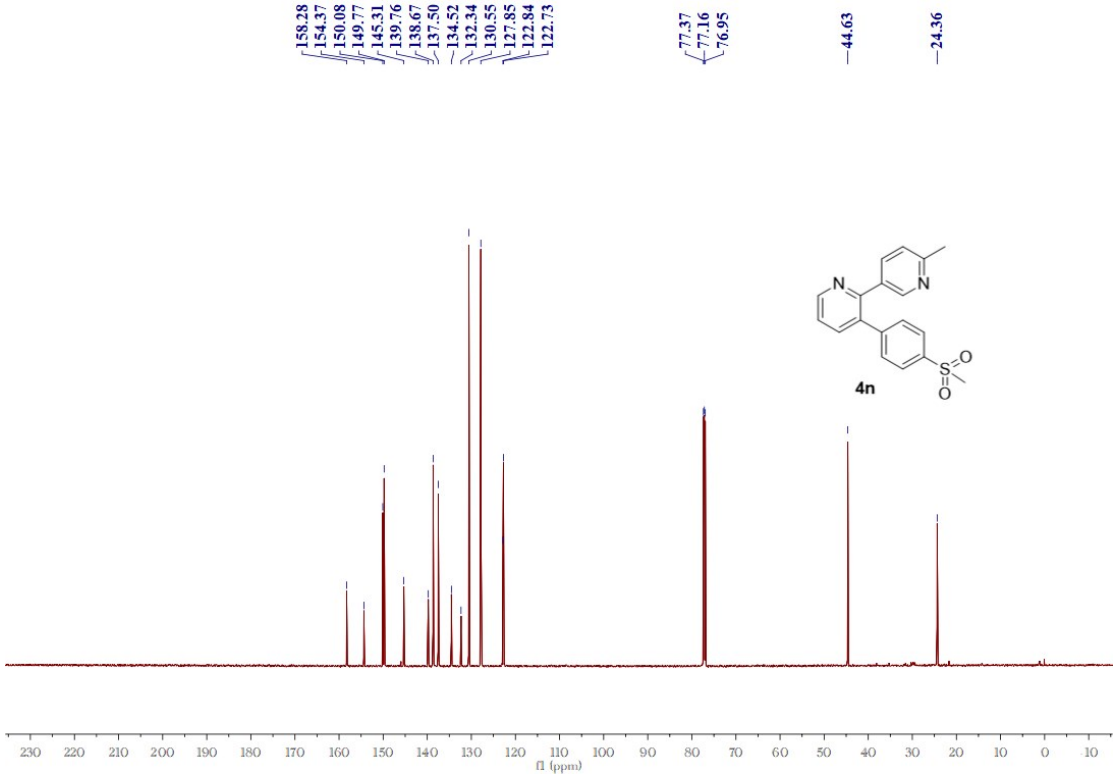
7.75
7.73
7.62
7.61
7.60
7.59
7.43
7.41
7.39
7.26
7.11
7.09
3.09
2.54
4n
1.00
1.02
2.00
1.01
0.99
3.09
1.03
3.03
3.03
f1 (ppm)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134.52
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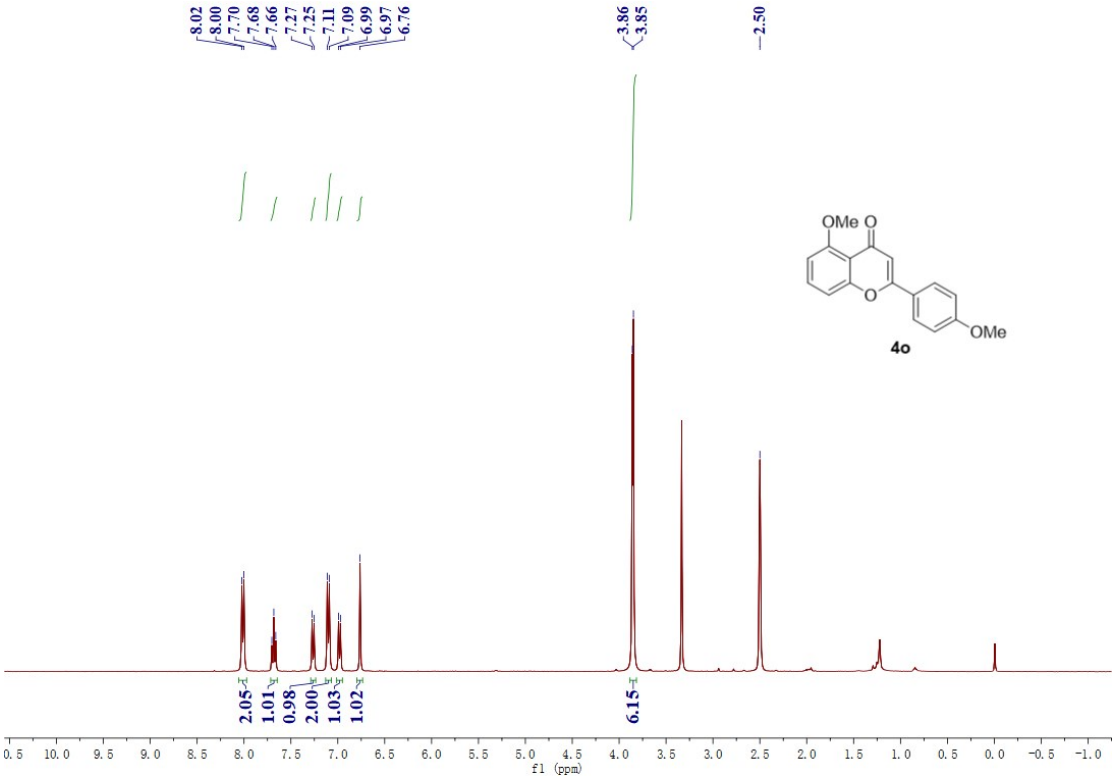
76.95
44.63
24.36
4n
f1 (ppm)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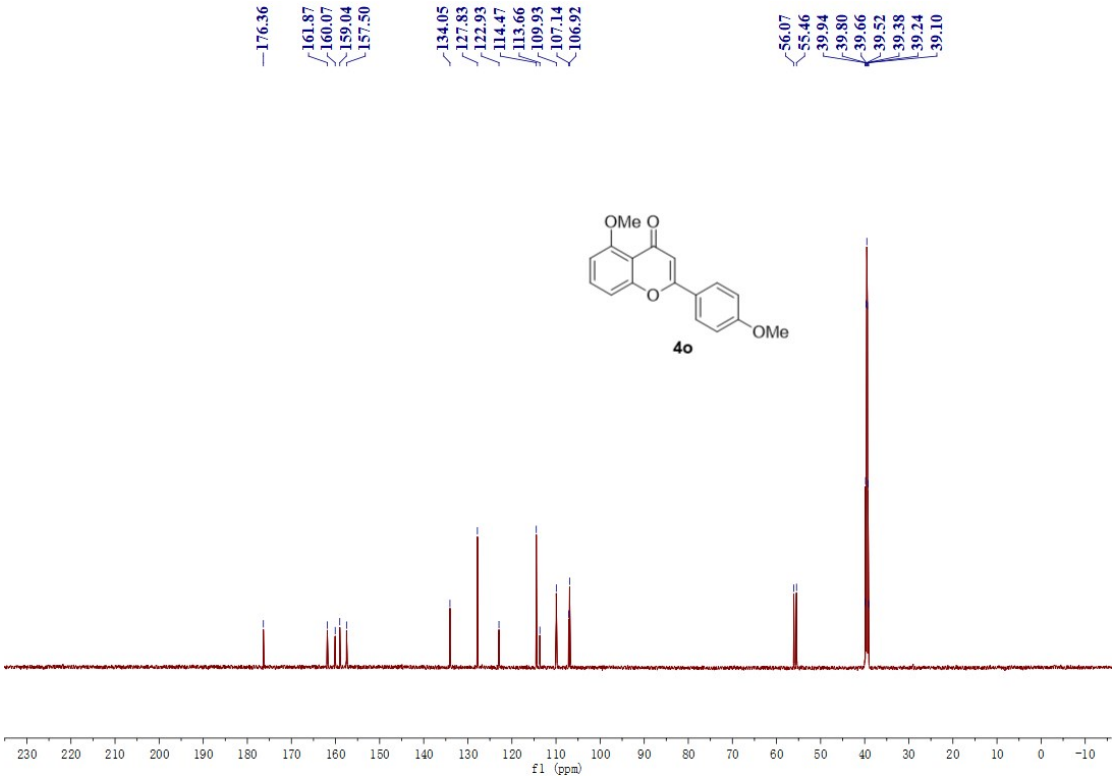
7.27
7.25
7.11
7.09
6.99
6.97
6.76
3.86
3.85
2.50
OMe O
O
OMe
4o
2.05
1.01
0.98
2.00
1.03
1.02
6.15
f1 (ppm)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159.04
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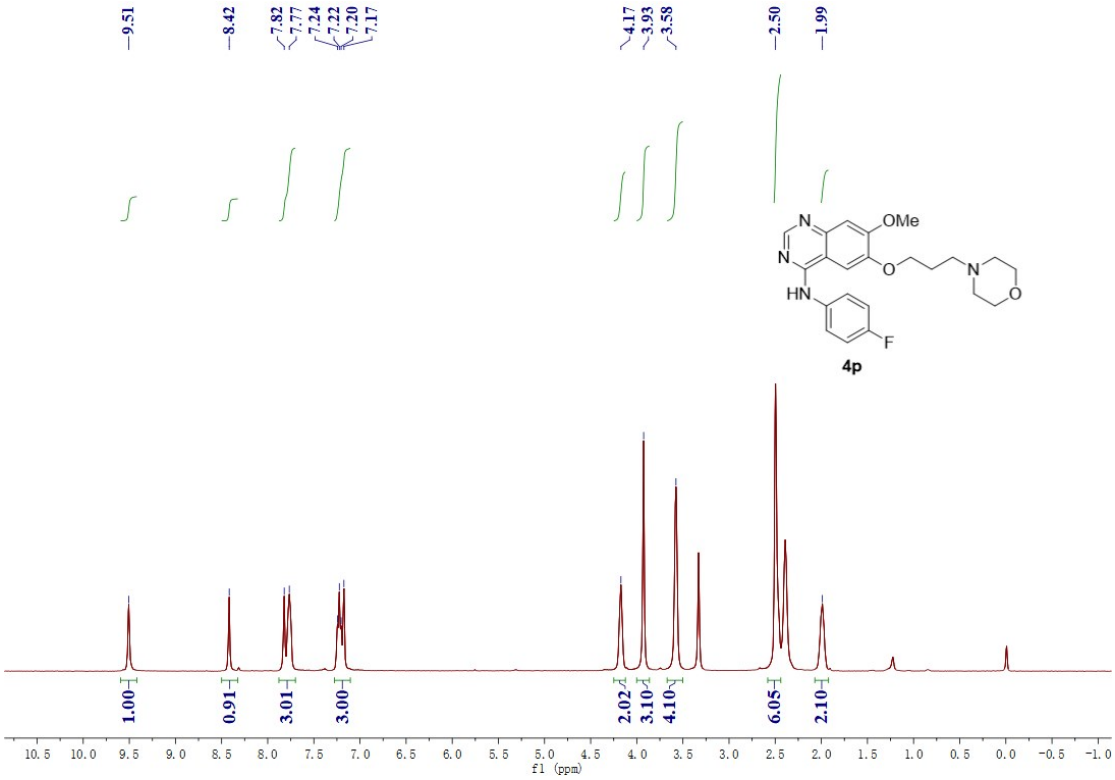
134.05
127.83
122.93
114.47
113.66
109.93
107.14
106.92
56.07
55.46
39.94
39.80
39.66
39.52
39.38
39.24
39.10
OMe O
O
OMe
4o
f1 (ppm)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7.82
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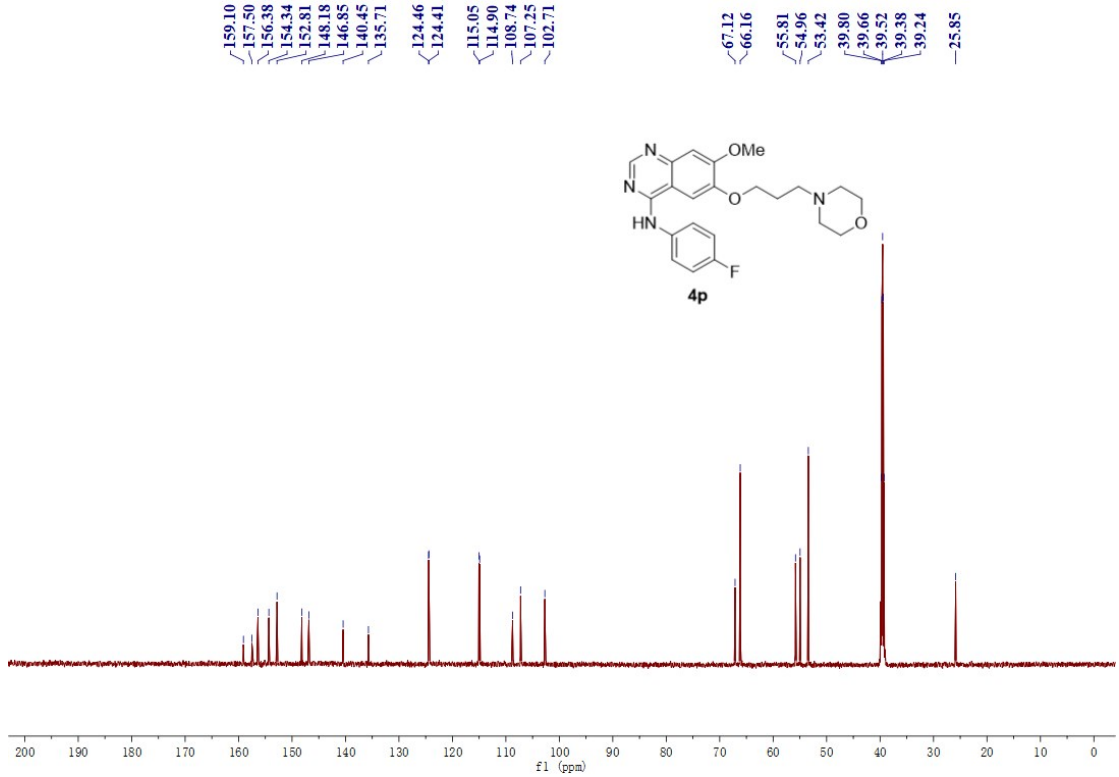
7.24
7.22
7.20
7.17
4.17
3.93
3.58
2.50
1.99
OMe
N
N
O
N
O
HN
F
4p
1.00
0.91
3.01
3.00
2.02
3.10
4.10
6.05
2.10
f1 (ppm)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135.71
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124.41
115.05
114.90
108.74
107.25
102.71
67.12
66.16
55.81
54.96
53.42
39.80
39.66
39.52
39.38
39.24
25.85
OMe
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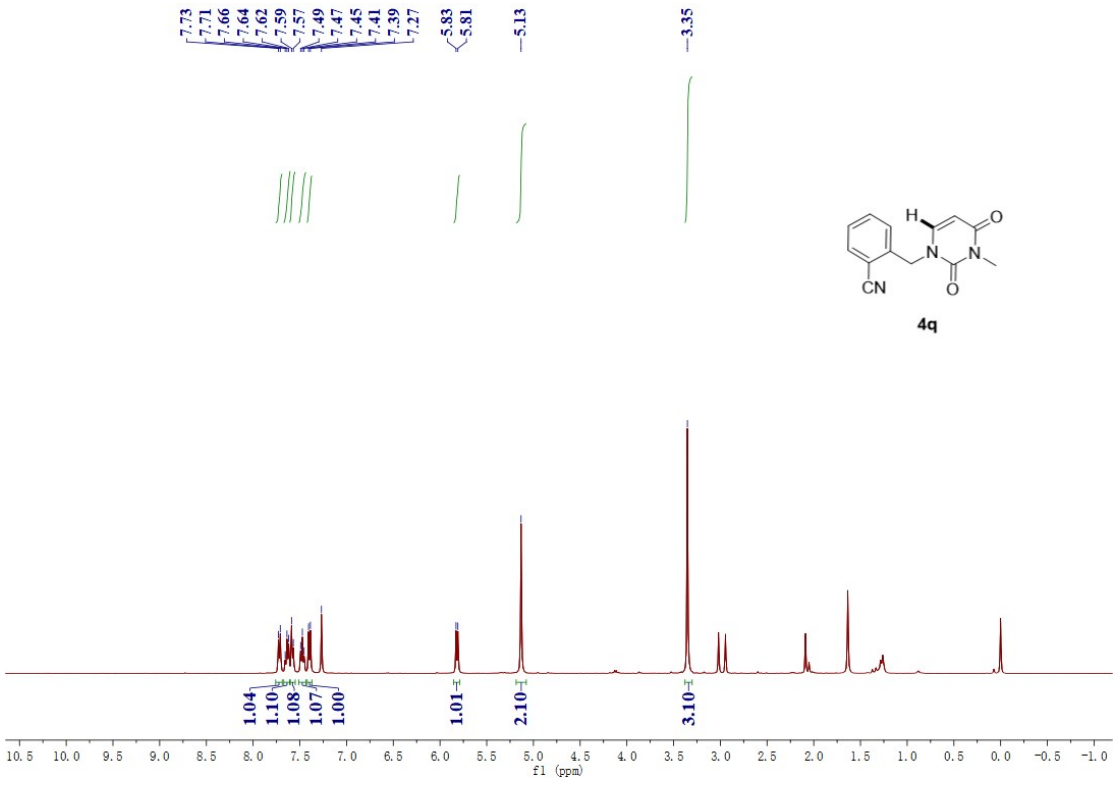
N
O
N
O
HN
F
4p
f1 (ppm)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7.57
7.49
7.47
7.45
7.41
7.39
7.27
5.83
5.81
5.13
3.35
H
O
N
N
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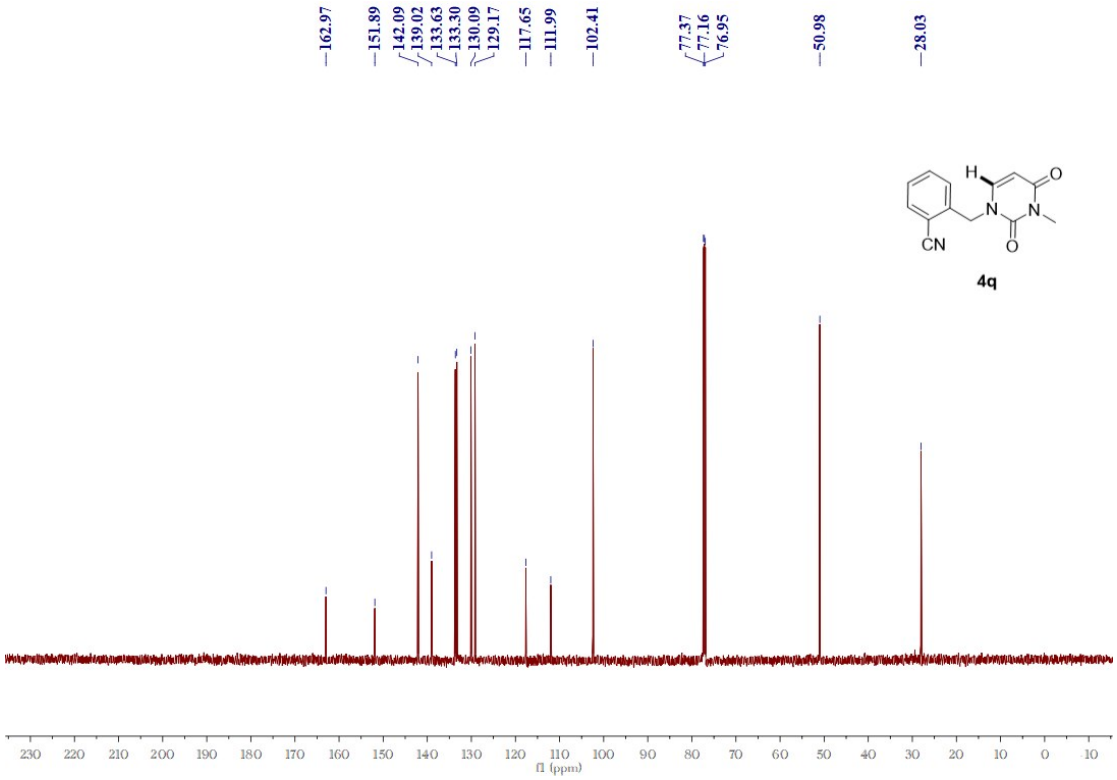
CN
4q
1.04
1.10
1.08
1.07
1.00
1.01
2.10
3.10
f1 (ppm)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139.02
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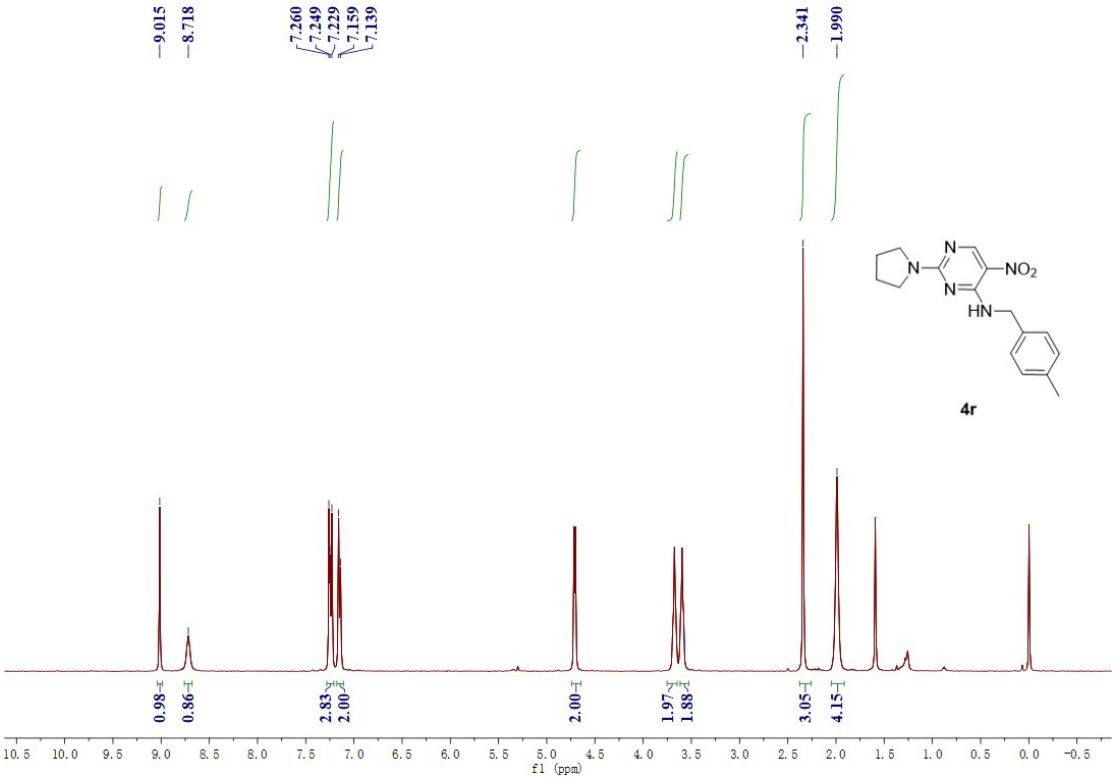
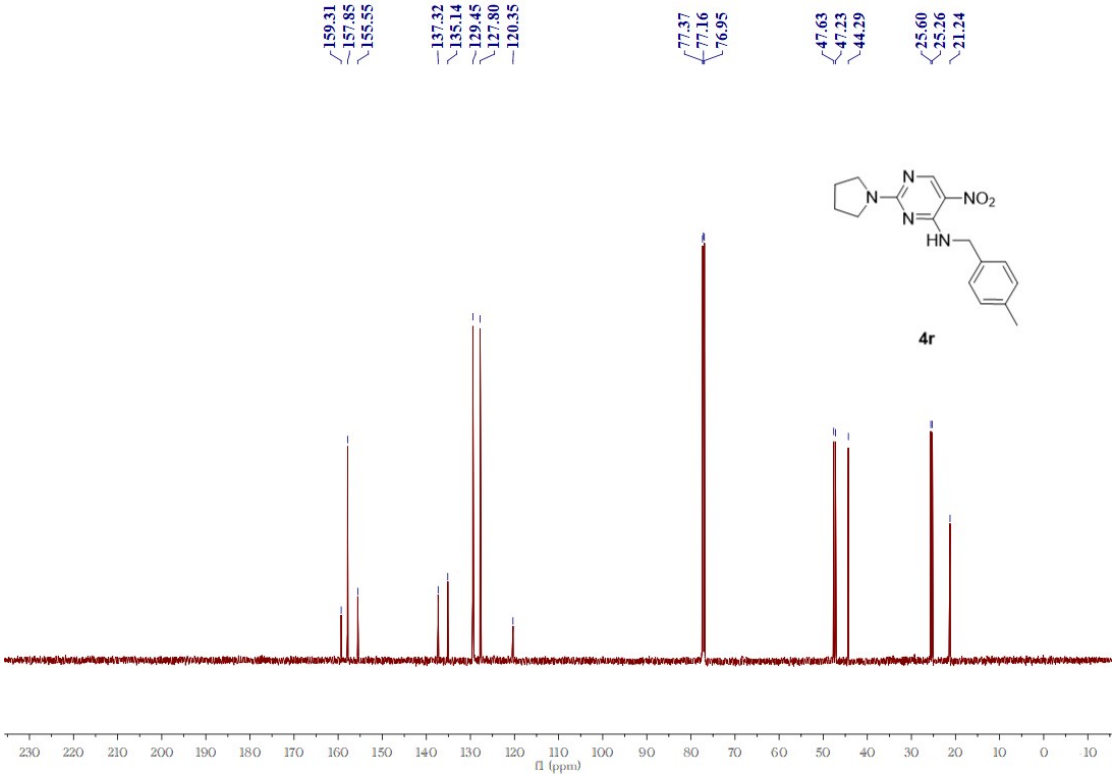
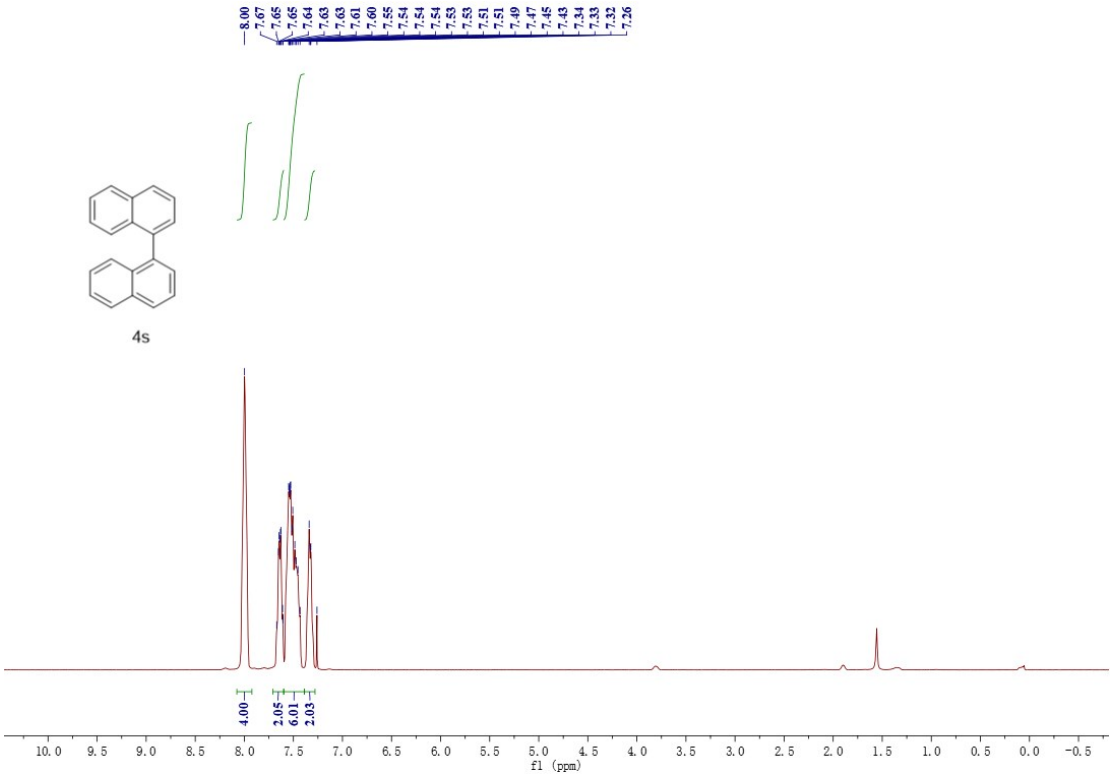
133.30
130.09
129.17
117.65
111.99
102.41
77.37
77.16
76.95
50.98
28.03
H
O
N
N
O
CN
4q
f1 (ppm)


9.015
8.718
7.260
7.249
7.229
7.159
7.139
2.341
1.990
0.98
0.86
2.83
2.00
2.00
1.97
1.88
3.05
4.15
f1 (ppm)
4r


159.31
157.85
155.55
137.32
135.14
129.45
127.80
120.35
77.37
77.16
76.95
47.63
47.23
44.29
25.60
25.26
21.24
f1 (ppm)
4r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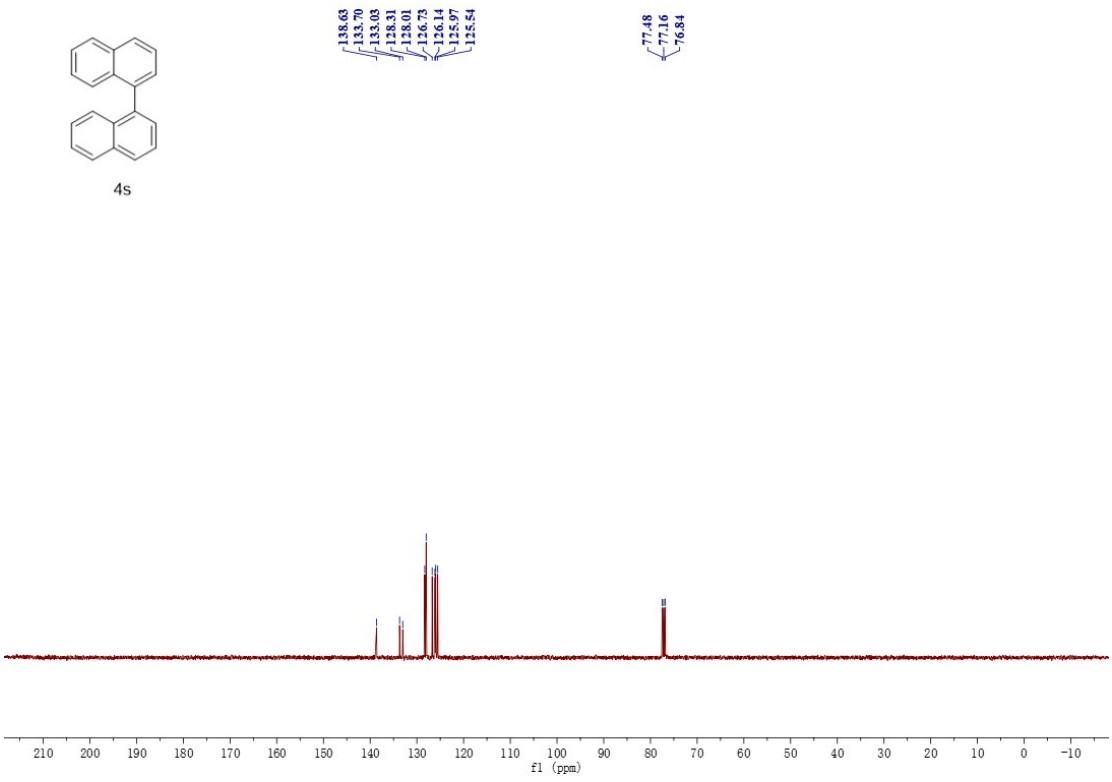
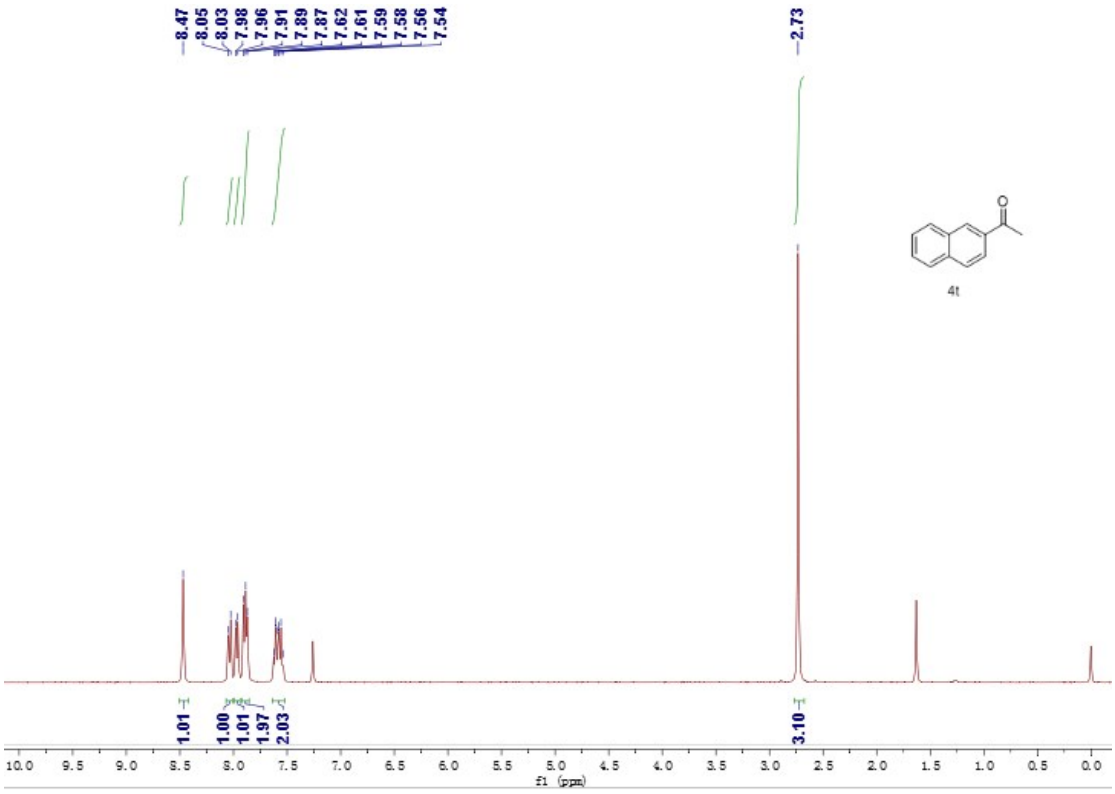
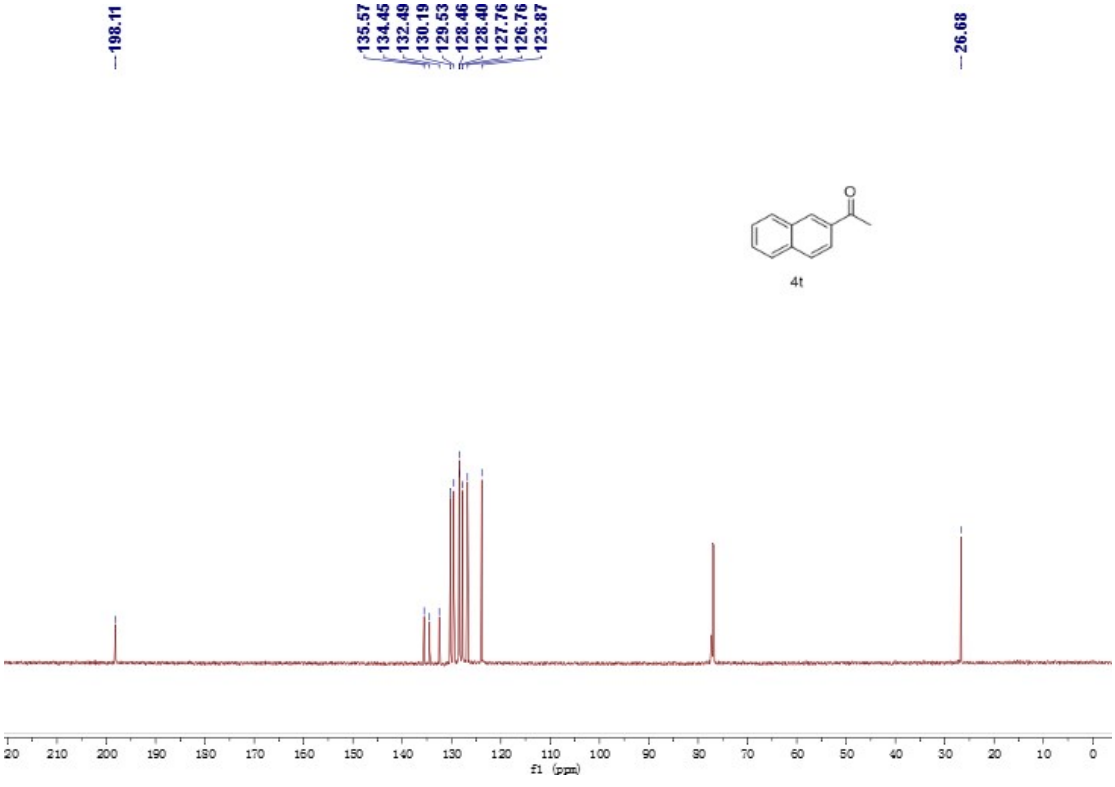
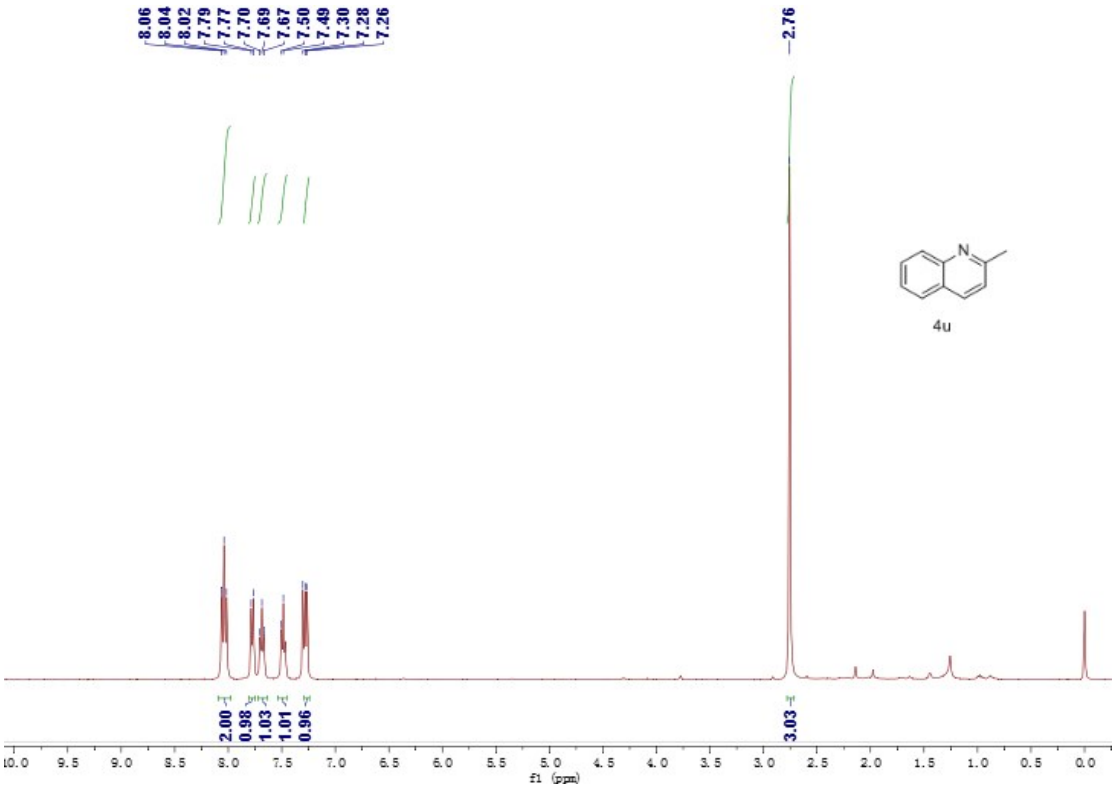
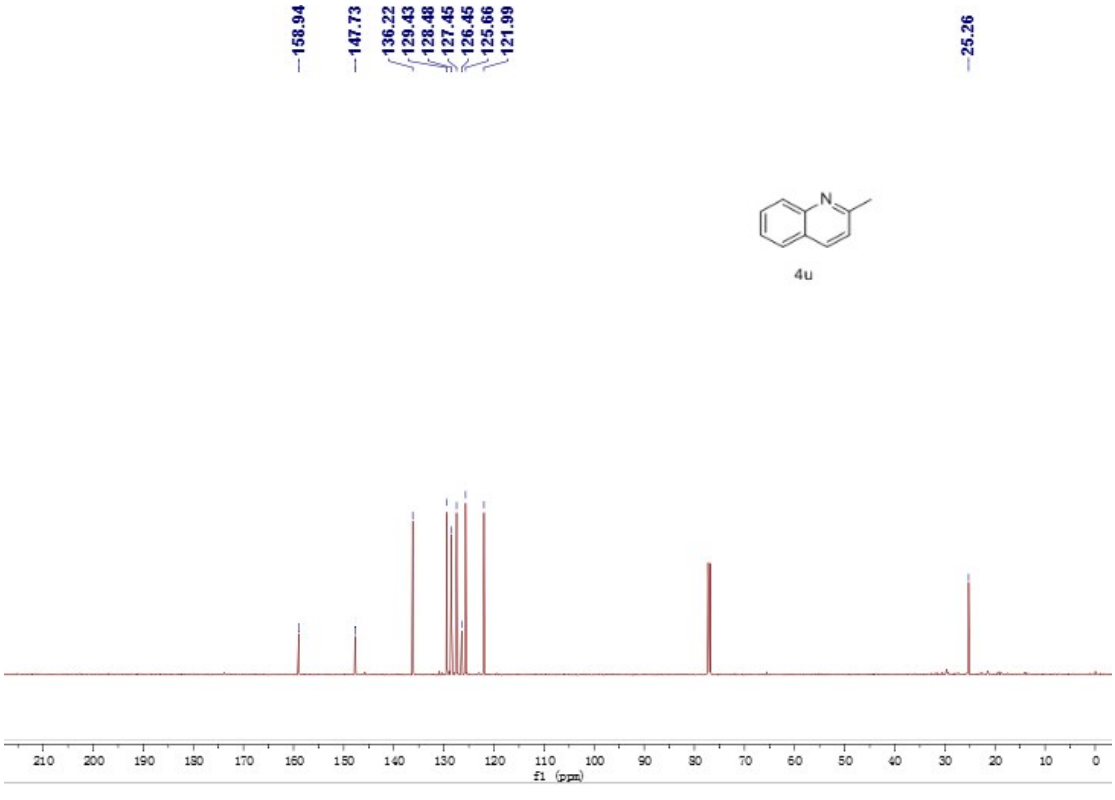
7.67
7.65
7.65
7.64
7.63
7.63
7.61
7.60
7.55
7.54
7.54
7.54
7.53
7.53
7.51
7.51
7.49
7.47
7.45
7.43
7.34
7.33
7.32
7.26
4s
4.00
2.05
6.01
2.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

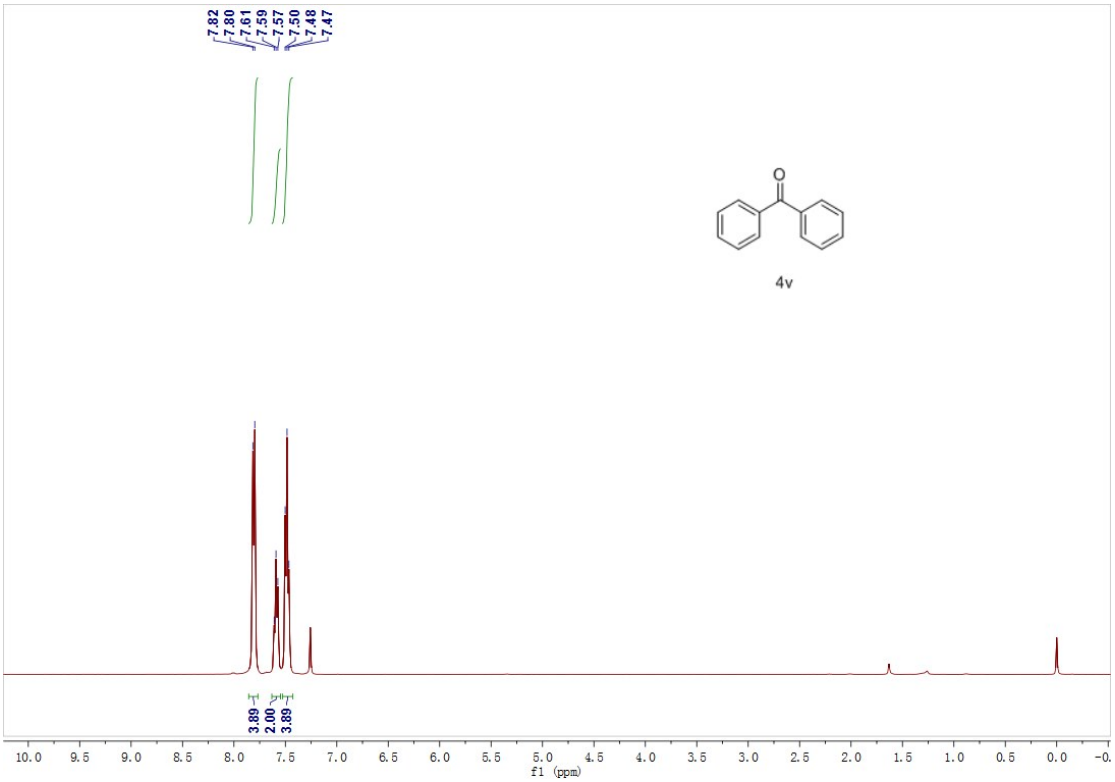

138.63
133.70
133.03
128.31
128.01
126.73
126.14
125.97
125.54
77.48
77.16
76.84
4s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

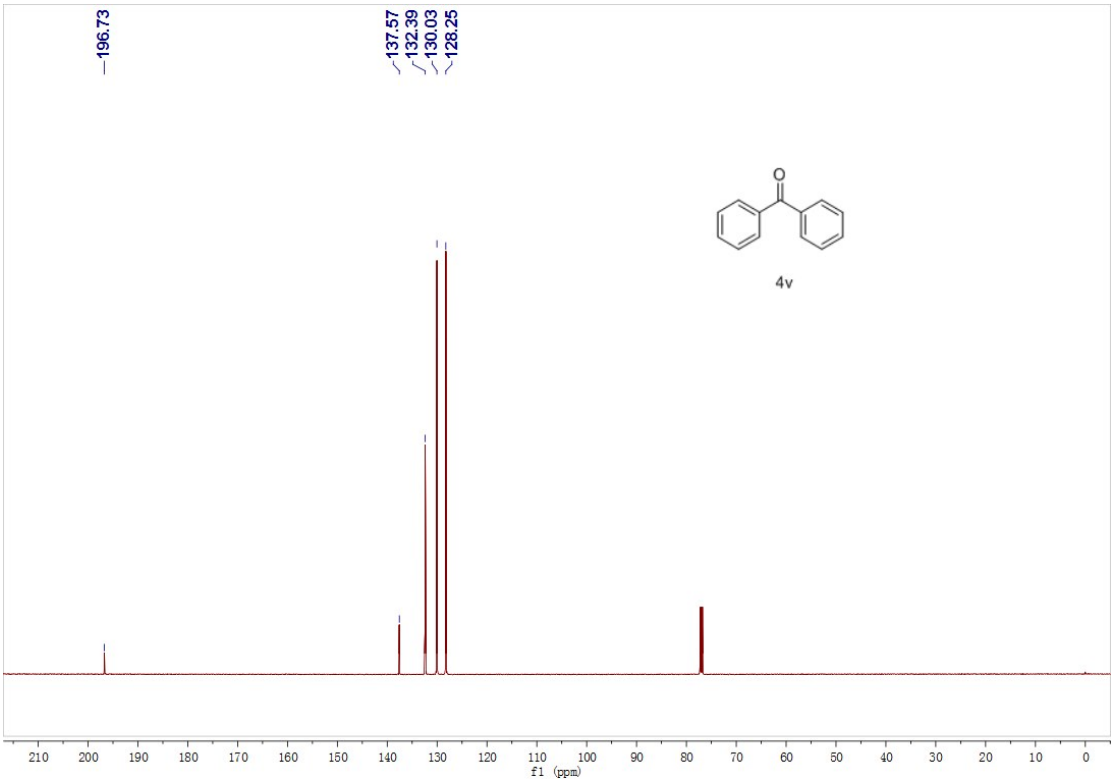

8.47
8.05
8.03
7.98
7.96
7.91
7.89
7.87
7.62
7.61
7.59
7.58
7.56
7.54
2.73
1.01
1.00
1.01
1.97
2.03
3.10
f1 (ppm)
4t

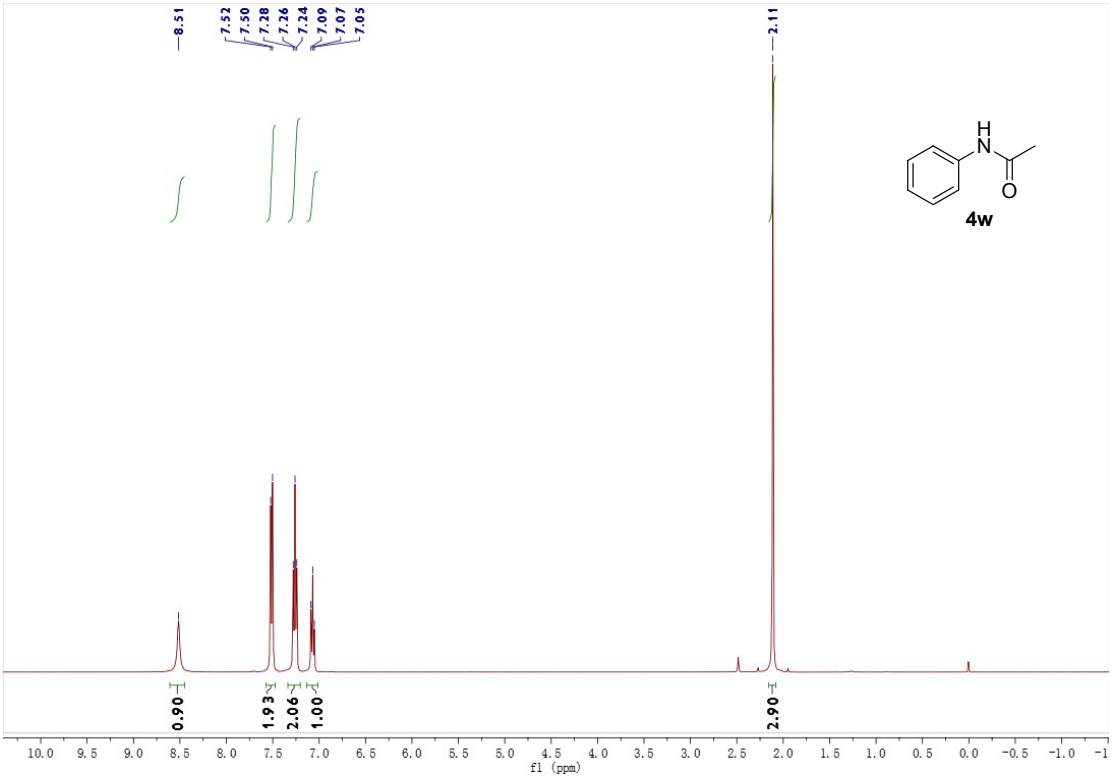

198.11
135.57
134.45
132.49
130.19
129.53
128.46
128.40
127.76
126.76
123.87
26.68
f1 (ppm)
4t

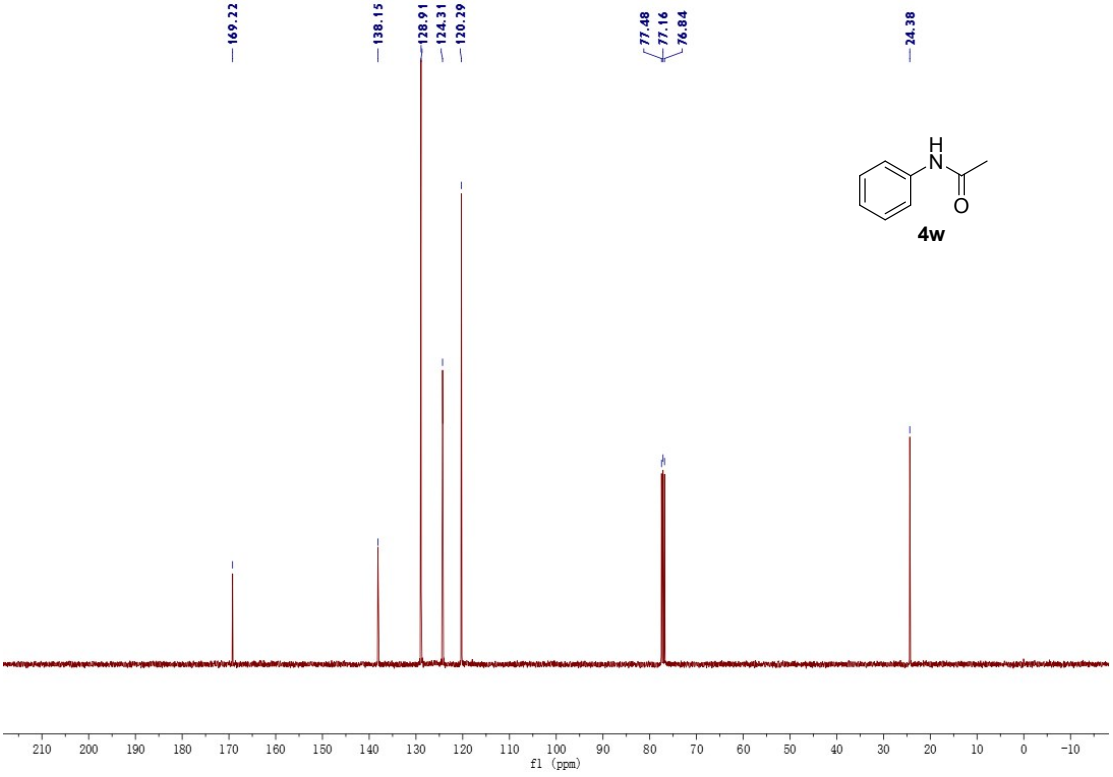

8.06
8.04
8.02
7.79
7.77
7.70
7.69
7.67
7.50
7.49
7.30
7.28
7.26
2.76
4u
2.00
0.98
1.03
1.01
0.96
3.03
f1 (ppm)

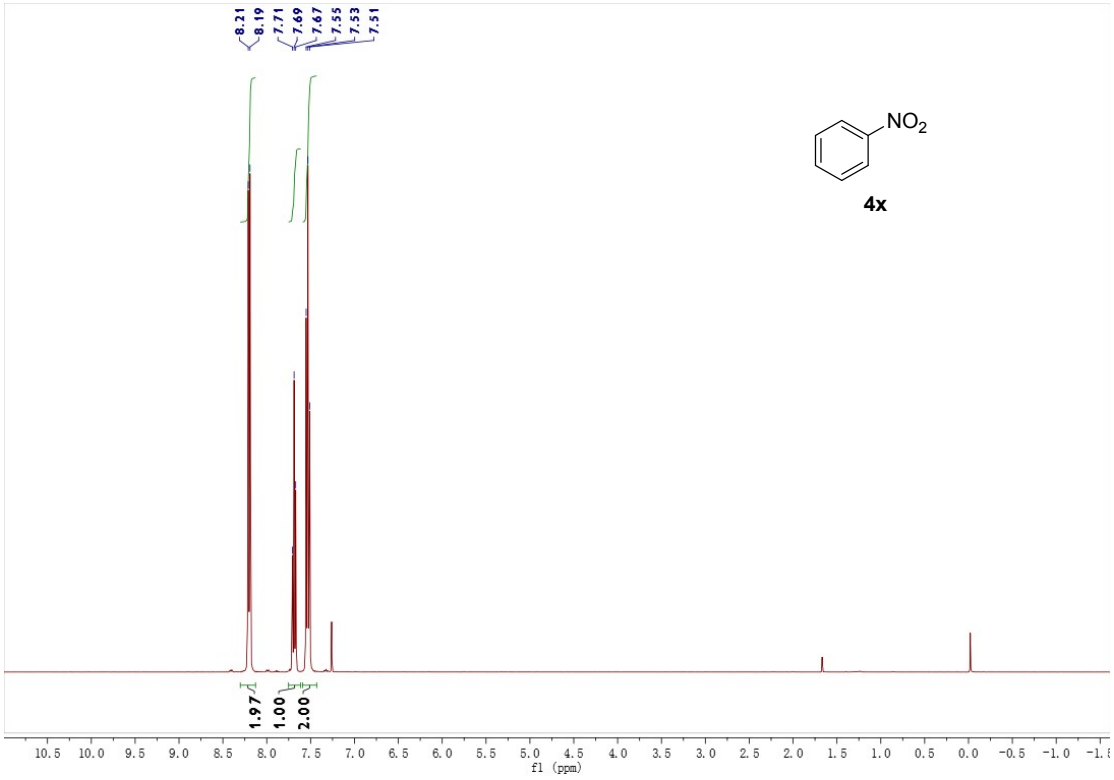

158.94
147.73
136.22
129.43
128.48
127.45
126.45
125.66
121.99
25.26
4u
f1 (ppm)

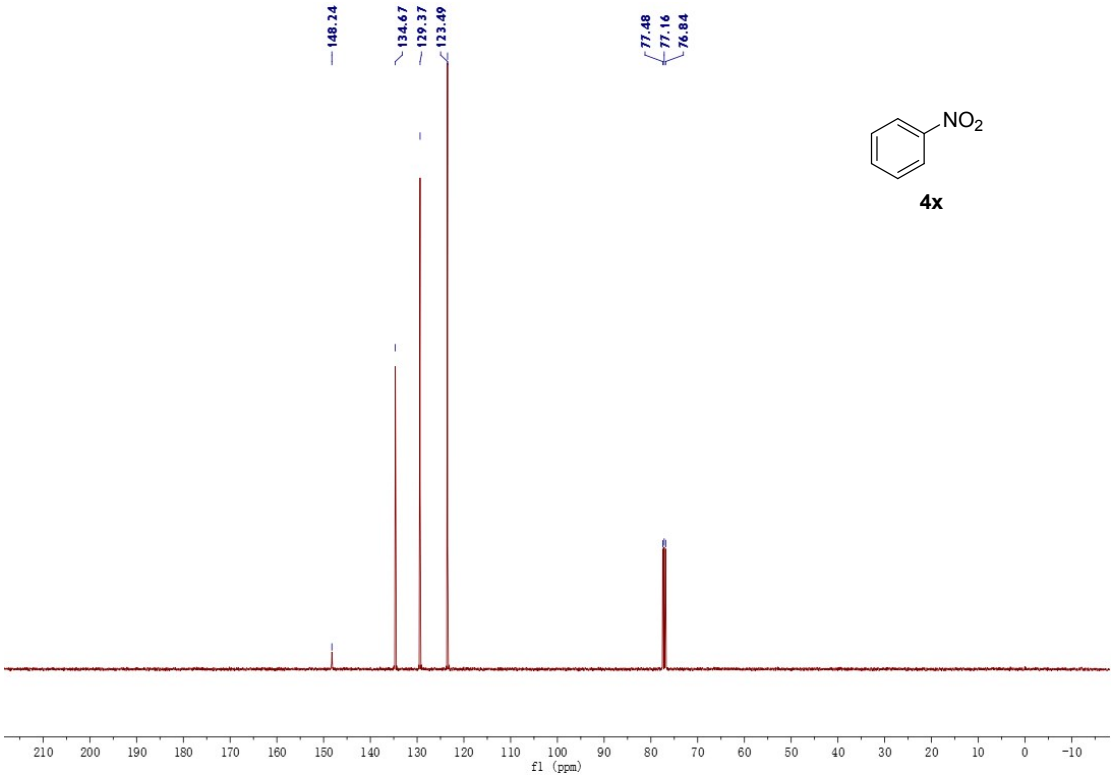

7.82
7.80
7.61
7.59
7.57
7.50
7.48
7.47
4v
3.89
2.00
3.89
f1 (ppm)

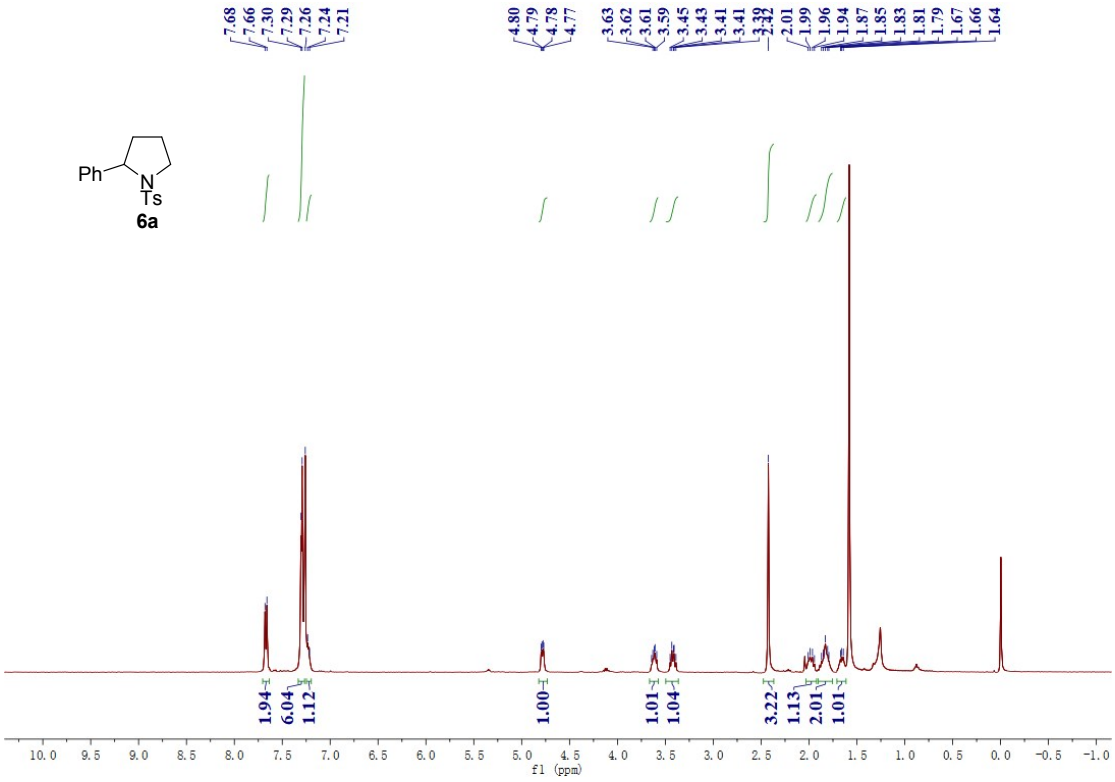

196.73
137.57
132.39
130.03
128.25
4v
f1 (ppm)

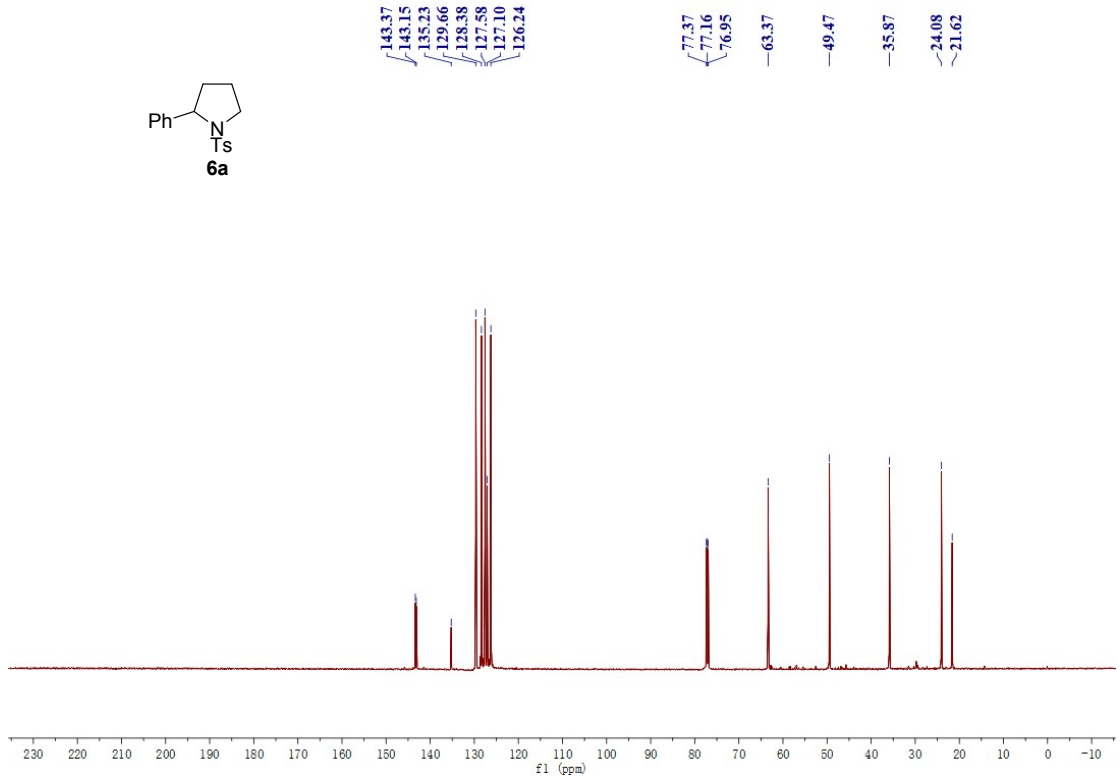

8.51
7.52
7.50
7.28
7.26
7.24
7.09
7.07
7.05
2.11
0.90
1.93
2.06
1.00
2.90
f1 (ppm)
4w

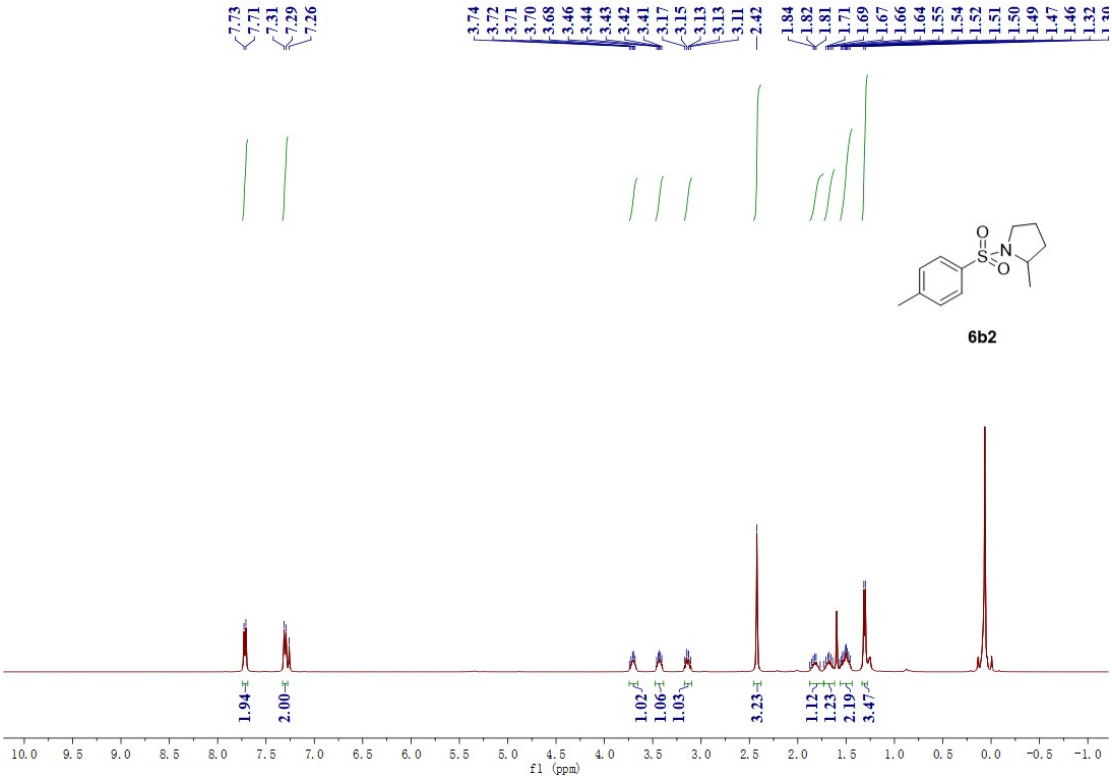

169.22
138.15
128.91
124.31
120.29
77.48
77.16
76.84
24.38
f1 (ppm)
4w

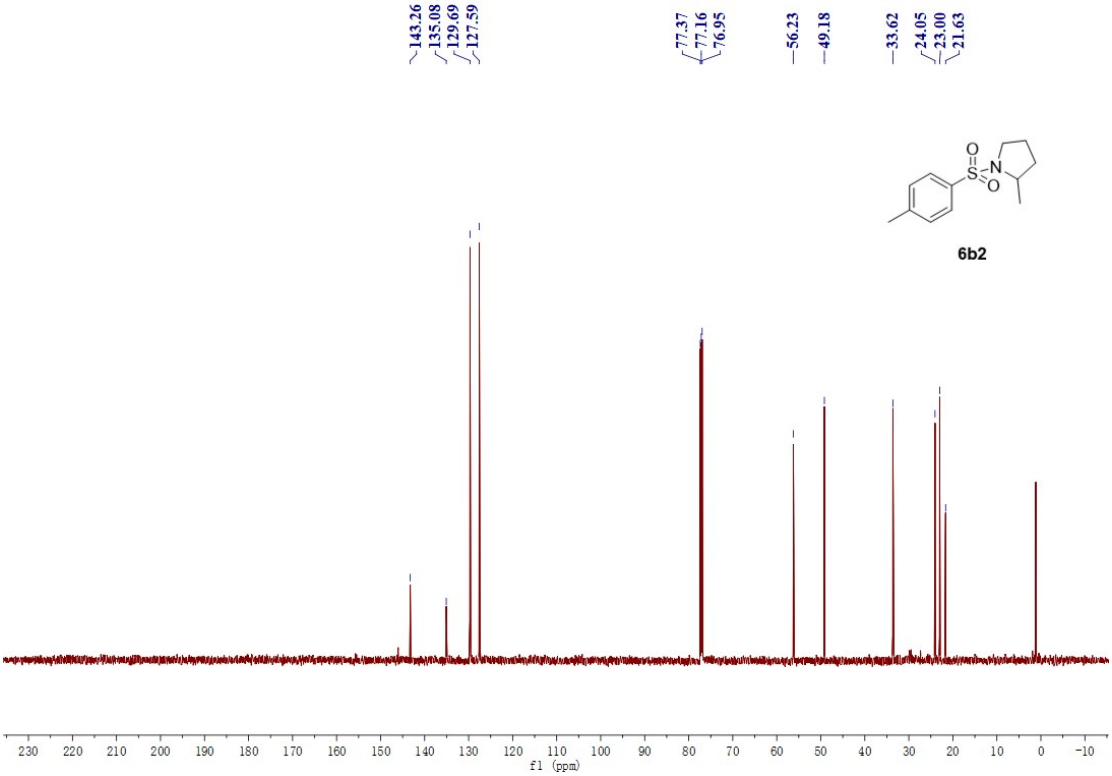

8.21
8.19
7.71
7.69
7.67
7.55
7.53
7.51
NO2
4x
1.97
1.00
2.00
f1 (ppm)

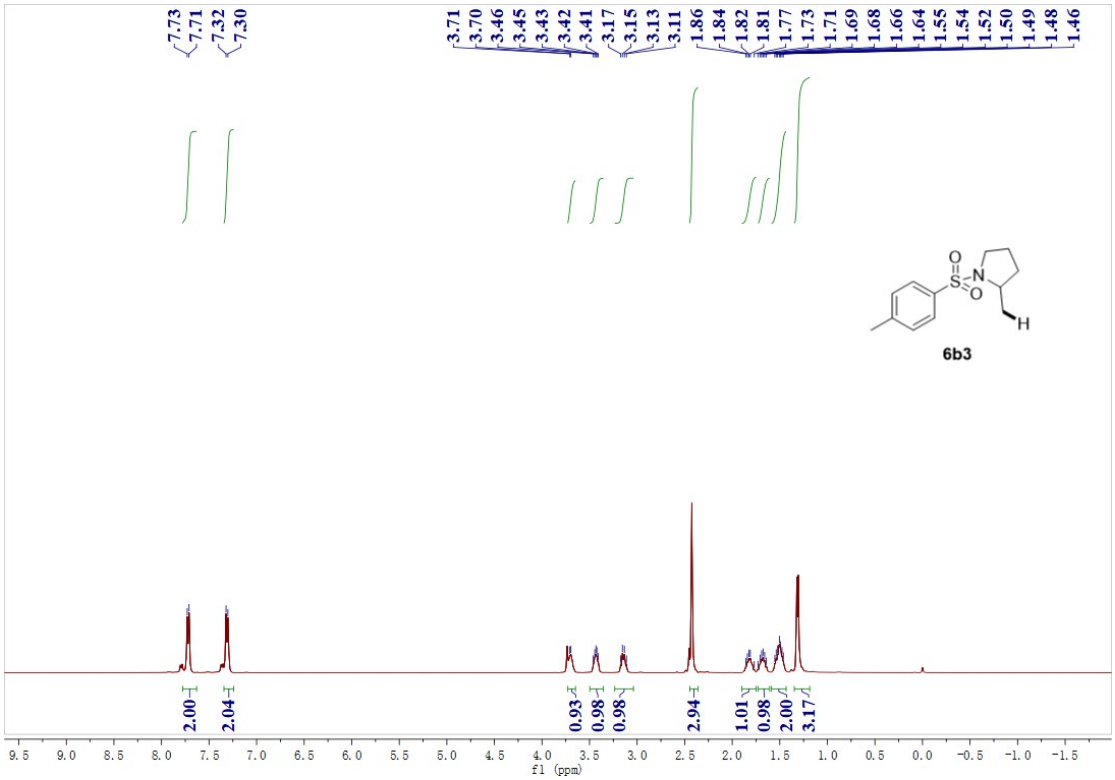

148.24
134.67
129.37
123.49
77.48
77.16
76.84
NO2
4x
f1 (ppm)

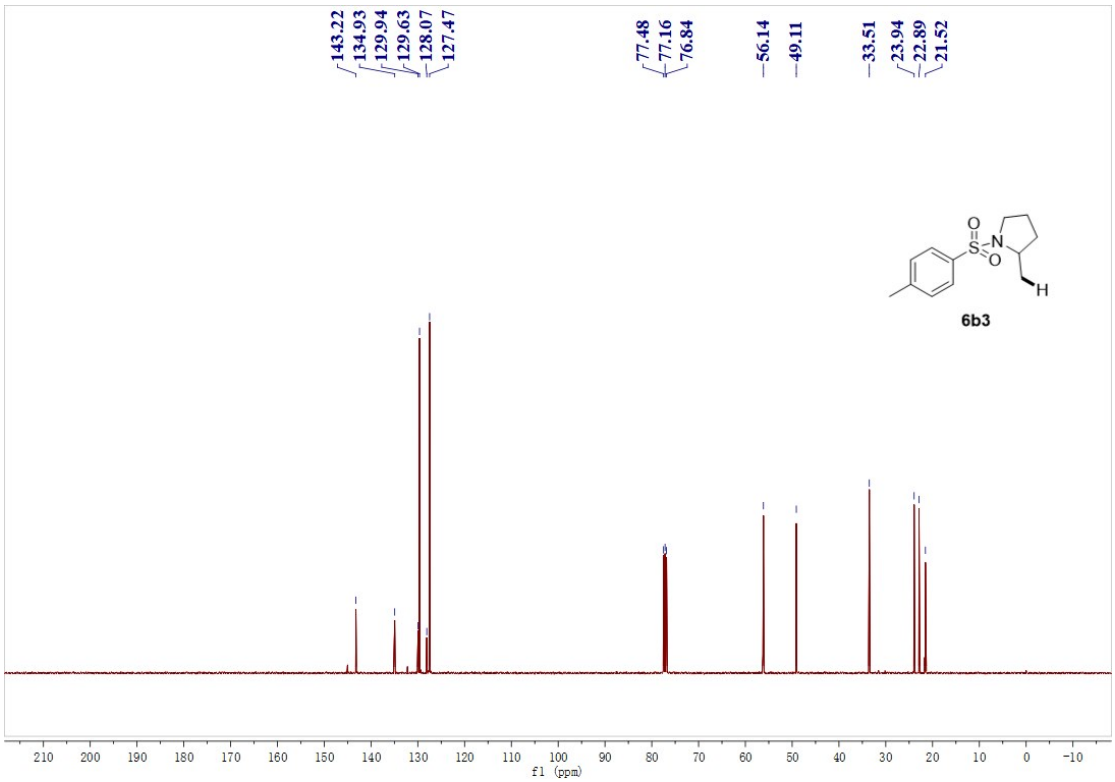

7.68
7.66
7.30
7.29
7.26
7.24
7.21
4.80
4.79
4.78
4.77
3.63
3.62
3.61
3.59
3.45
3.43
3.41
3.41
2.01
1.99
1.96
1.94
1.87
1.85
1.83
1.81
1.79
1.67
1.66
1.64
Ph
N
Ts
6a
1.94
6.04
1.12
1.00
1.01
1.04
3.22
1.13
2.01
1.01
f1 (ppm)

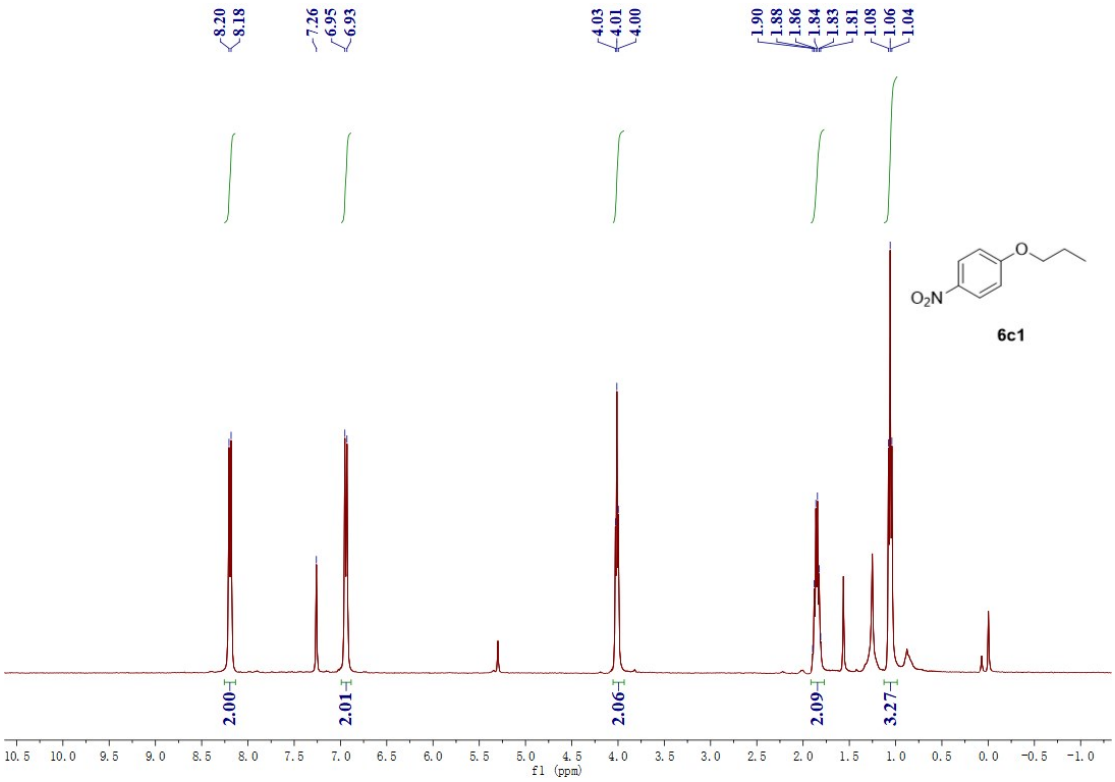

143.37
143.15
135.23
129.66
128.38
127.58
127.10
126.24
77.37
77.16
76.95
63.37
49.47
35.87
24.08
21.62
Ph
N
Ts
6a
f1 (ppm)


7.73
7.71
7.31
7.29
7.26
3.74
3.72
3.71
3.70
3.68
3.46
3.44
3.43
3.42
3.41
3.17
3.15
3.13
3.13
3.11
2.42
1.84
1.82
1.81
1.71
1.69
1.67
1.66
1.64
1.55
1.54
1.52
1.51
1.50
1.49
1.47
1.46
1.32
6b2
1.94
2.00
1.02
1.06
1.03
3.23
1.12
1.23
2.19
3.47
f1 (ppm)


143.26
135.08
129.69
127.59
77.37
77.16
76.95
56.23
49.18
33.62
24.05
23.00
21.63
6b2
f1 (ppm)


7.73
7.71
7.32
7.30
3.71
3.70
3.46
3.45
3.43
3.42
3.41
3.17
3.15
3.13
3.11
1.86
1.84
1.82
1.81
1.77
1.73
1.71
1.69
1.68
1.66
1.64
1.55
1.54
1.52
1.50
1.49
1.48
1.46
6b3
2.00
2.04
0.93
0.98
0.98
2.94
1.01
0.98
2.00
3.17
f1 (ppm)


143.22
134.93
129.94
129.63
128.07
127.47
77.48
77.16
76.84
56.14
49.11
33.51
23.94
22.89
21.52
6b3
f1 (ppm)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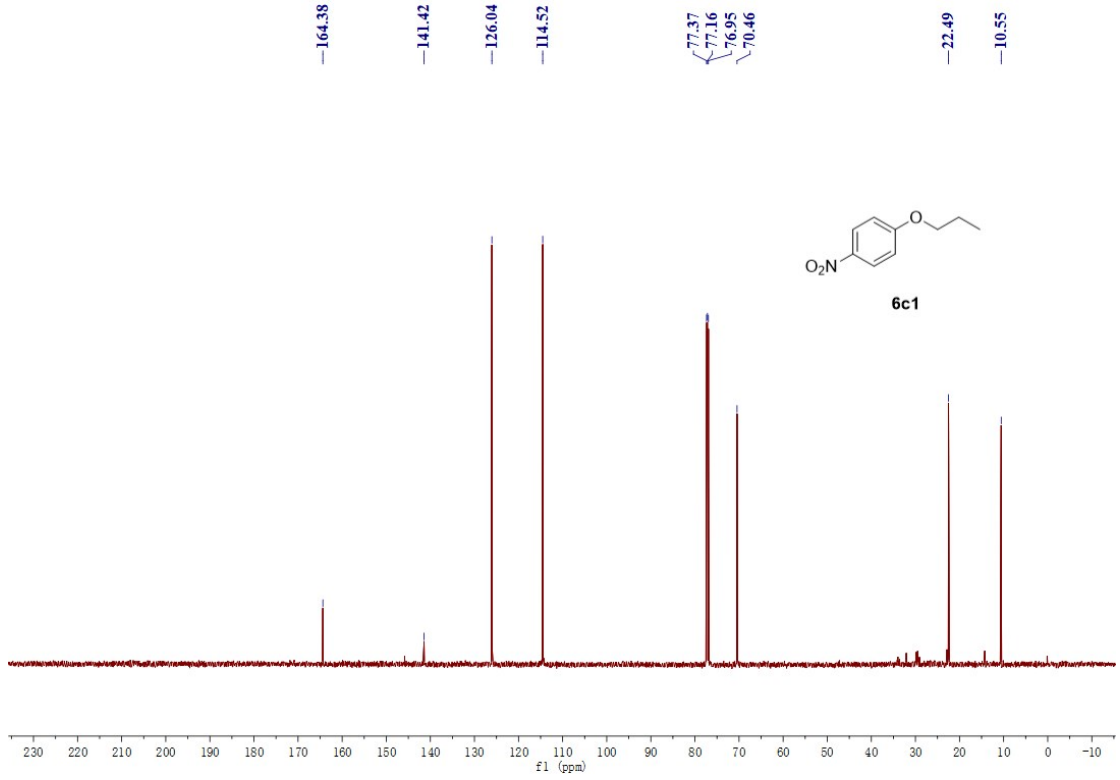
8.18
7.26
6.95
6.93
4.03
4.01
4.00
1.90
1.88
1.86
1.84
1.83
1.81
1.08
1.06
1.04
O2N
O
6c1
2.00
2.01
2.06
2.09
3.27
f1 (ppm)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141.42
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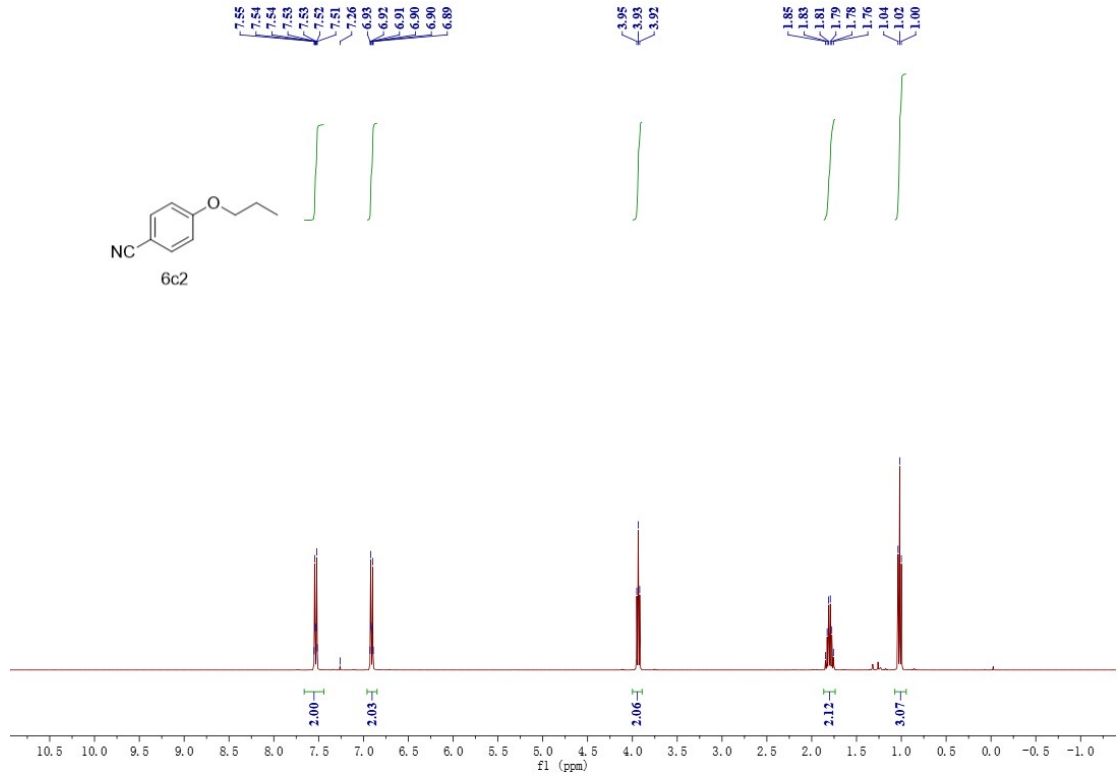
114.52
77.37
77.16
76.95
70.46
22.49
10.55
O2N
O
6c1
f1 (ppm)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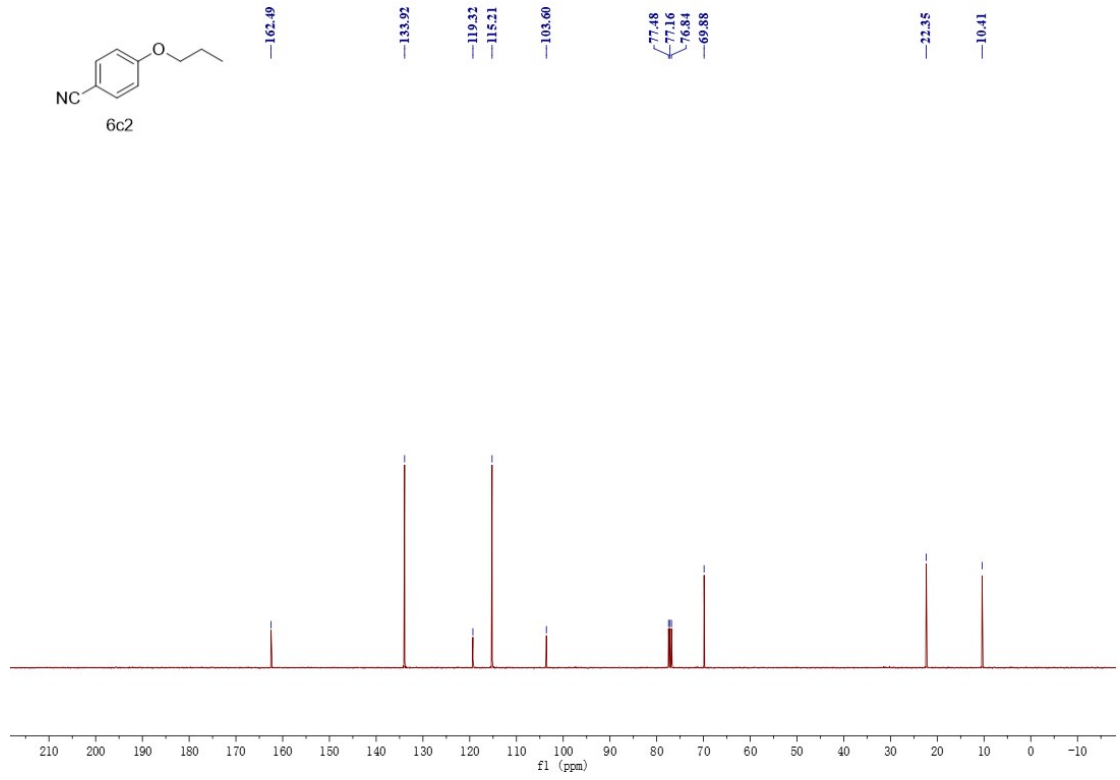
7.54
7.54
7.53
7.53
7.52
7.51
7.26
6.93
6.92
6.91
6.90
6.90
6.89
3.95
3.93
3.92
1.85
1.83
1.81
1.79
1.78
1.76
1.04
1.02
1.00
NC
O
6c2
2.00
2.03
2.06
2.12
3.07
f1 (ppm)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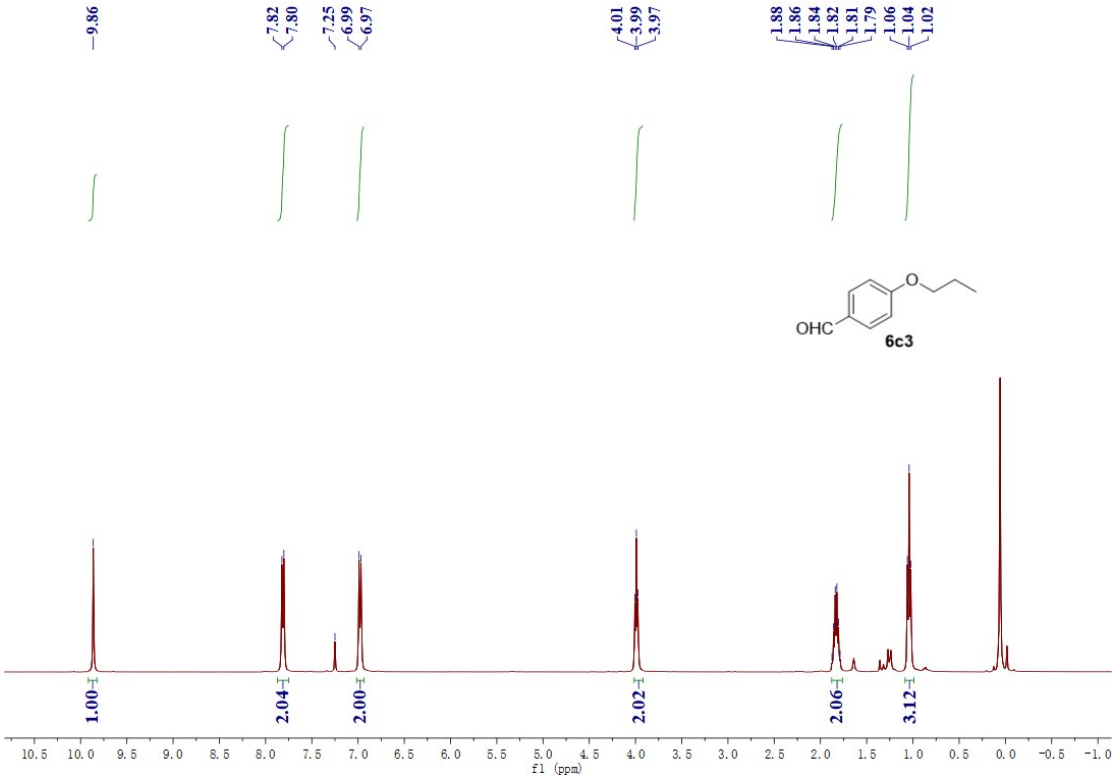
133.92
119.32
115.21
103.60
77.48
77.16
76.84
69.88
22.35
10.41
NC
O
6c2
f1 (ppm)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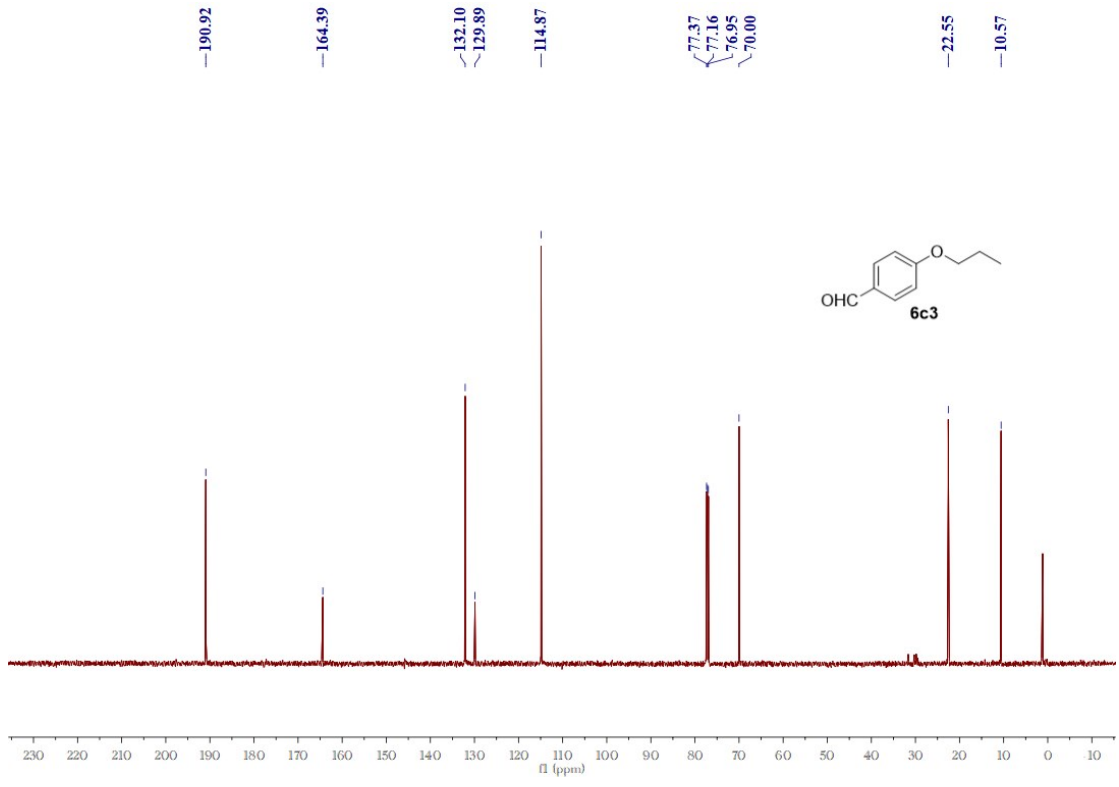
7.82
7.80
7.25
6.99
6.97
4.01
3.99
3.97
1.88
1.86
1.84
1.82
1.81
1.79
1.06
1.04
1.02
OHC
O
6c3
1.00
2.04
2.00
2.02
2.06
3.12
f1 (ppm)


190.92
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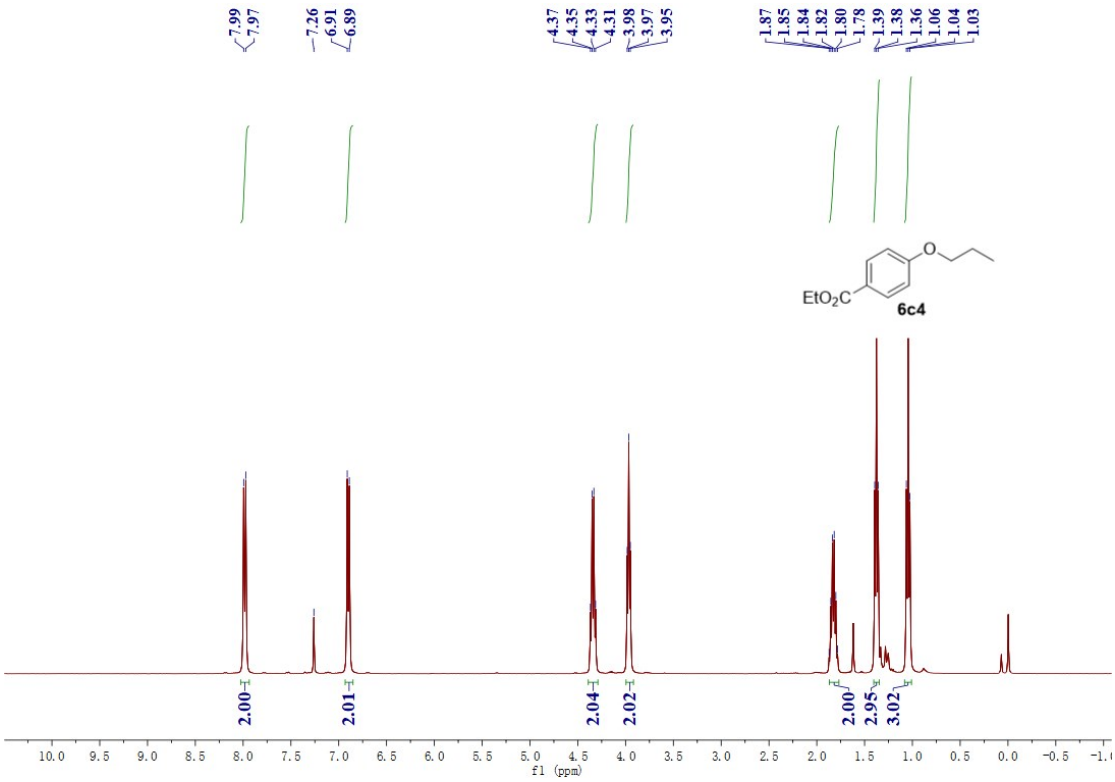
77.37
77.16
76.95
70.00
22.55
10.57
OHC
O
6c3
f1 (ppm)


7.99
7.97
7.26
6.91
6.89
4.37
4.35
4.33
4.31
3.98
3.97
3.95
1.87
1.85
1.84
1.82
1.80
1.78
1.39
1.38
1.36
1.06
1.04
1.03
EtO2C
6c4
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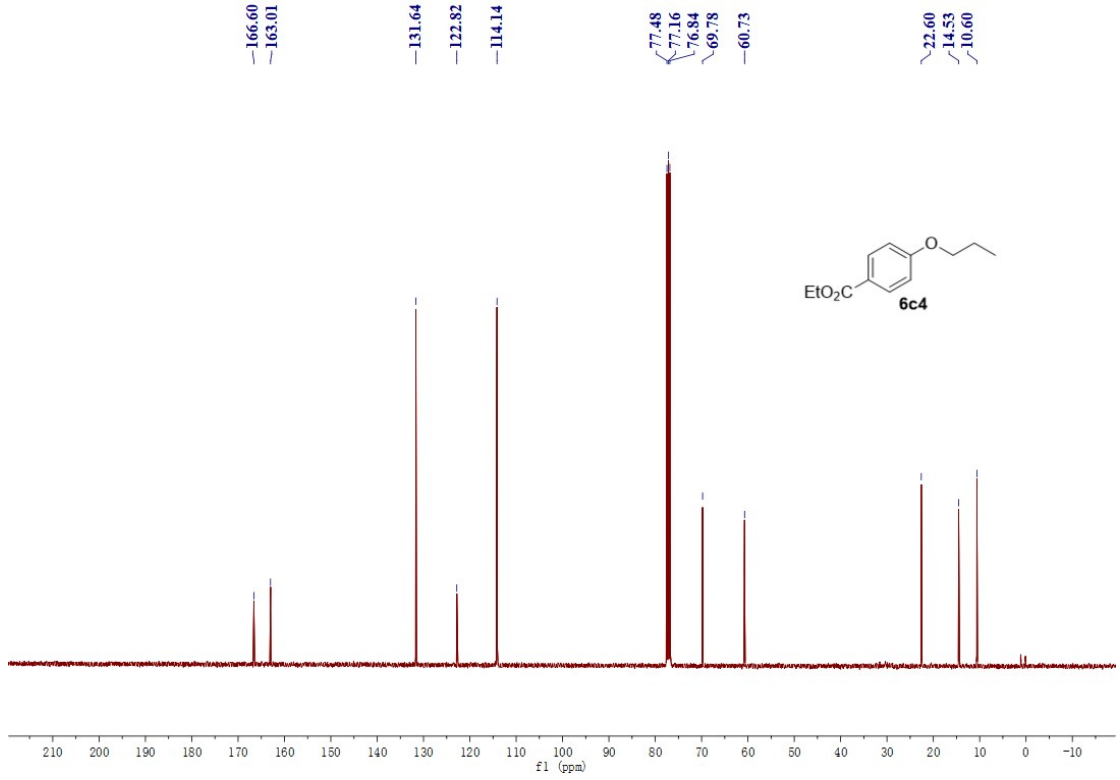
2.01
2.04
2.02
2.00
2.95
3.02
f1 (ppm)


166.60
163.01
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122.82
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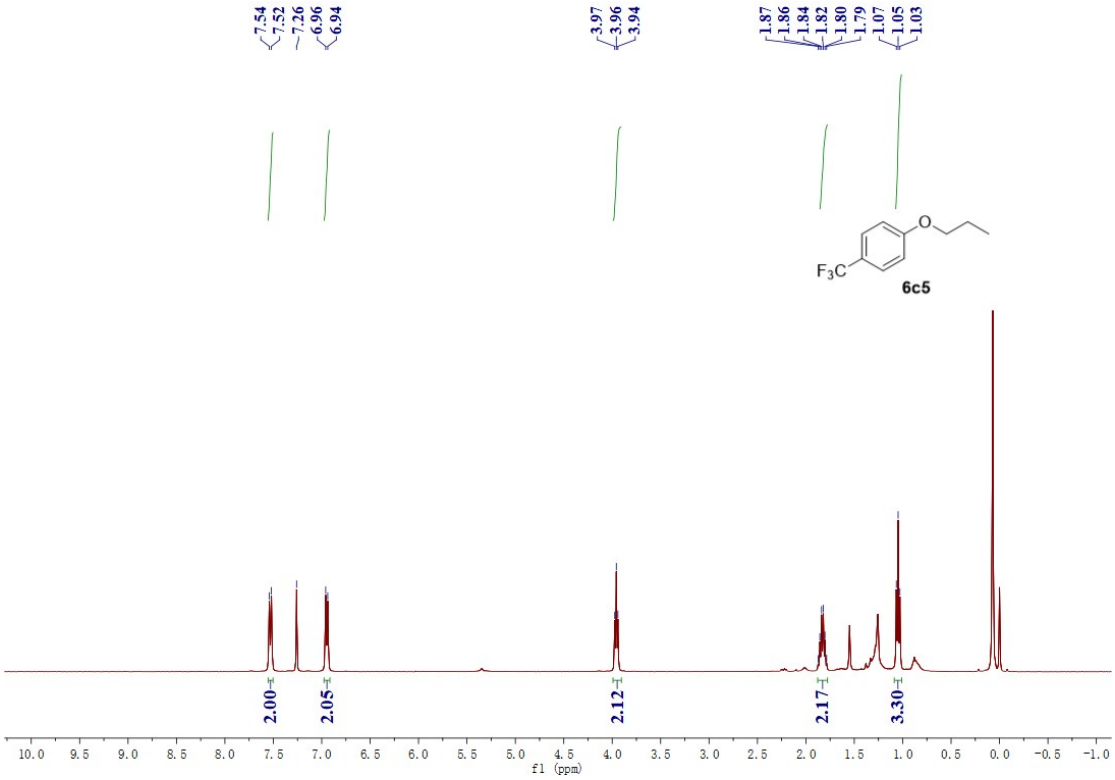
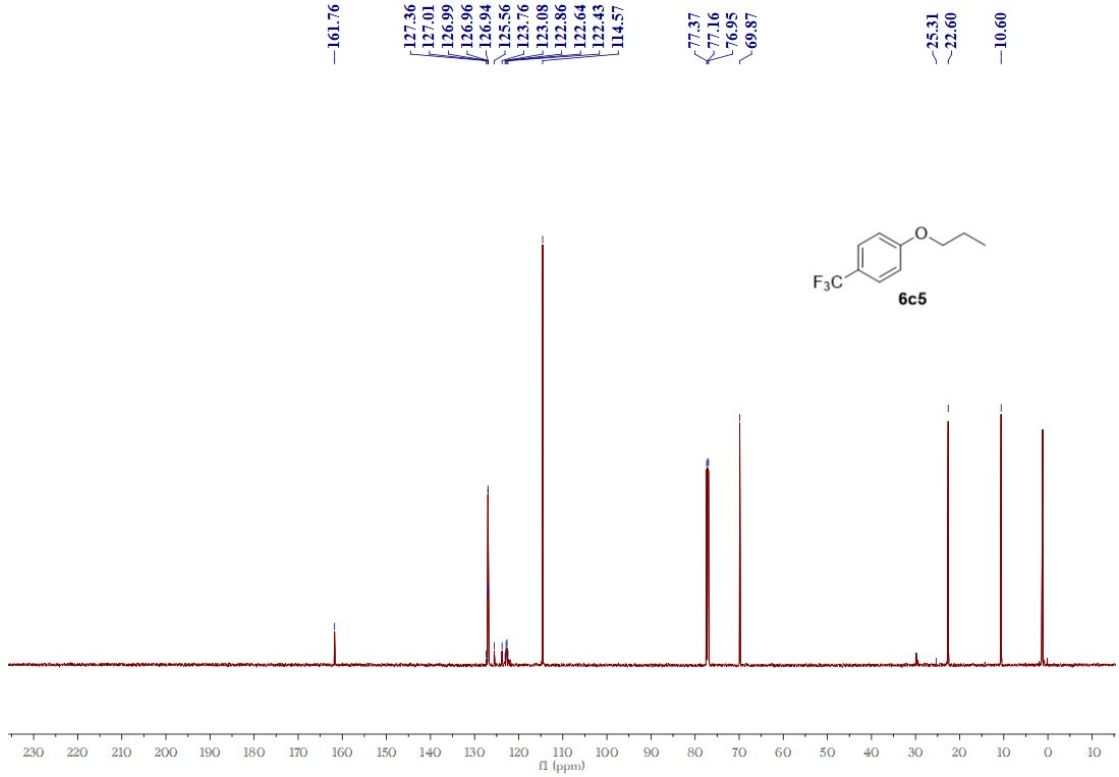
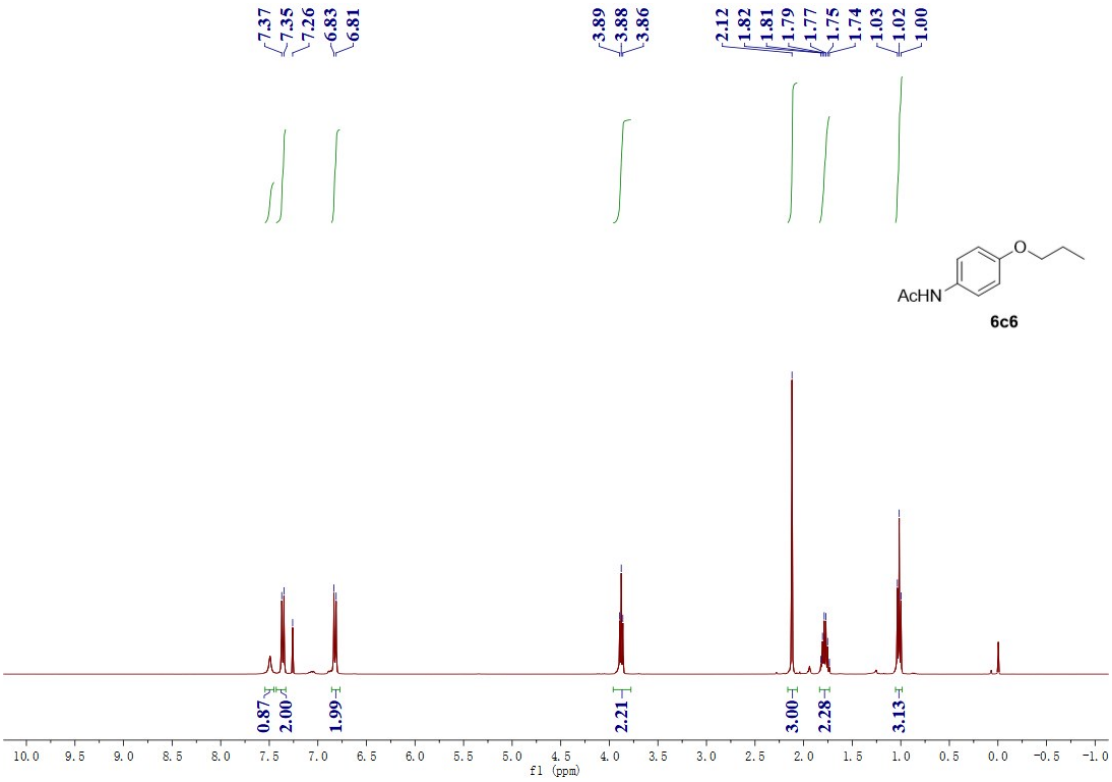
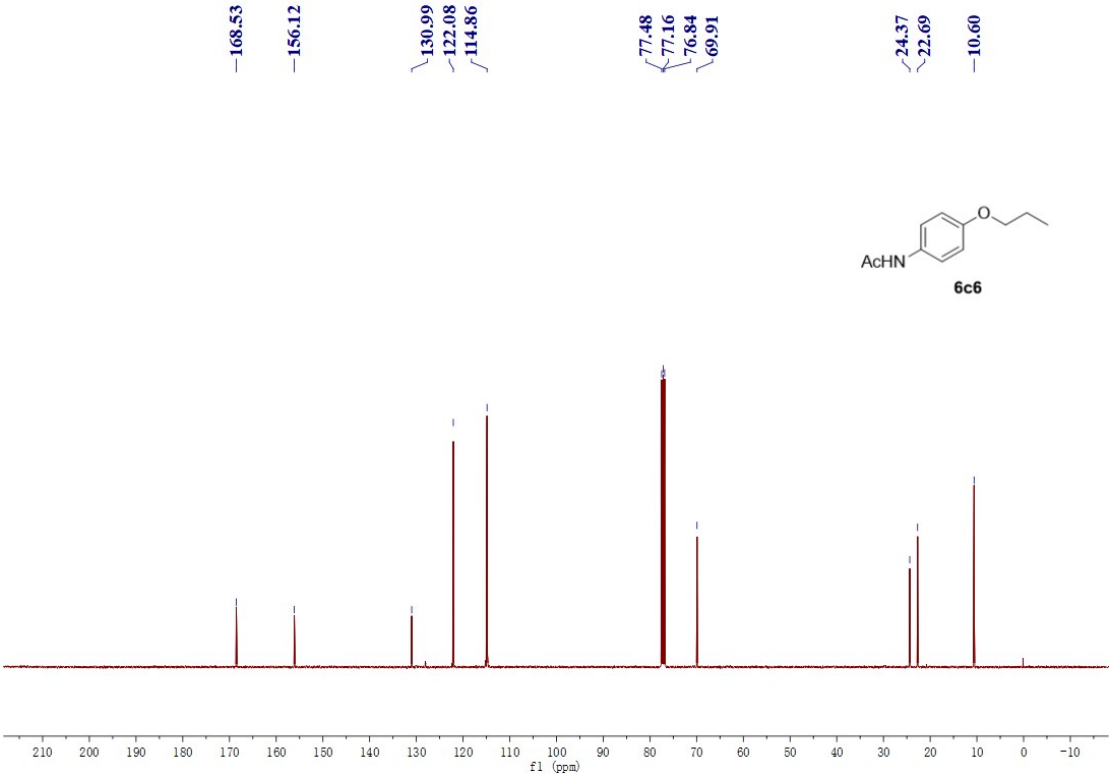
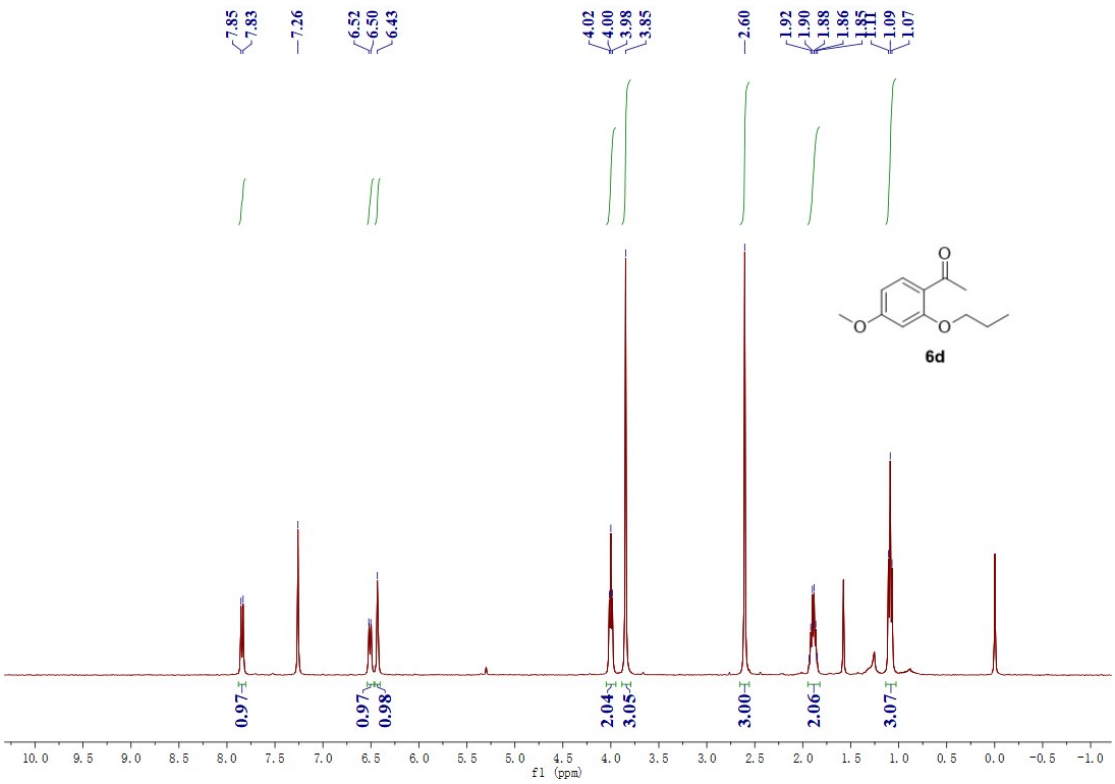
76.84
69.78
60.73
22.60
14.53
10.60
EtO2C
6c4
f1 (ppm)


7.54
7.52
7.26
6.96
6.94
3.97
3.96
3.94
1.87
1.86
1.84
1.82
1.80
1.79
1.07
1.05
1.03
F3C
O
6c5
2.00
2.05
2.12
2.17
3.30
f1 (ppm)


161.76
127.36
127.01
126.99
126.96
126.94
125.56
123.76
123.08
122.86
122.64
122.43
114.57
77.37
77.16
76.95
69.87
25.31
22.60
10.60
F3C
O
6c5
f1 (ppm)


7.37
7.35
7.26
6.83
6.81
3.89
3.88
3.86
2.12
1.82
1.81
1.79
1.77
1.75
1.74
1.03
1.02
1.00
AcHN
O
6c6
0.87
2.00
1.99
2.21
3.00
2.28
3.13
f1 (ppm)


168.53
156.12
130.99
122.08
114.86
77.48
77.16
76.84
69.91
24.37
22.69
10.60
AcHN
O
6c6
f1 (ppm)


7.85
7.83
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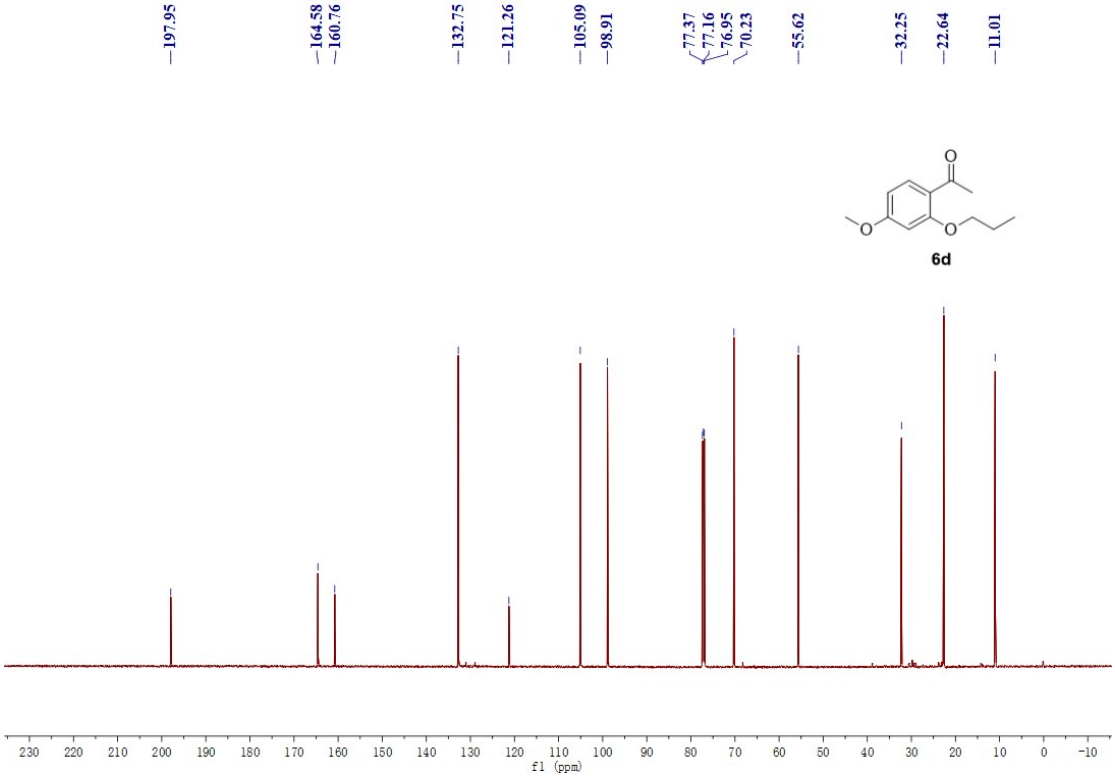
6.52
6.50
6.43
4.02
4.00
3.98
3.85
2.60
1.92
1.90
1.88
1.86
1.85
1.11
1.09
1.07
6d
0.97
0.97
0.98
2.04
3.05
3.00
2.06
3.07
f1 (ppm)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98.91
77.37
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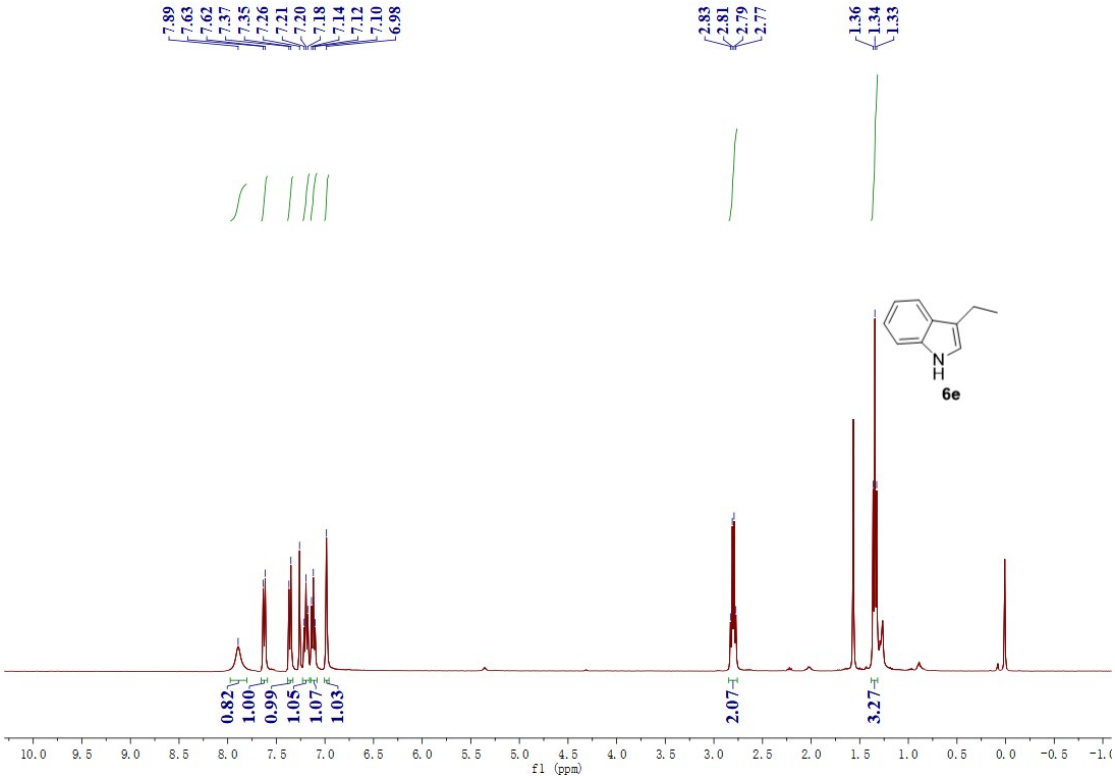
76.95
70.23
55.62
32.25
22.64
11.01
6d
f1 (ppm)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7.62
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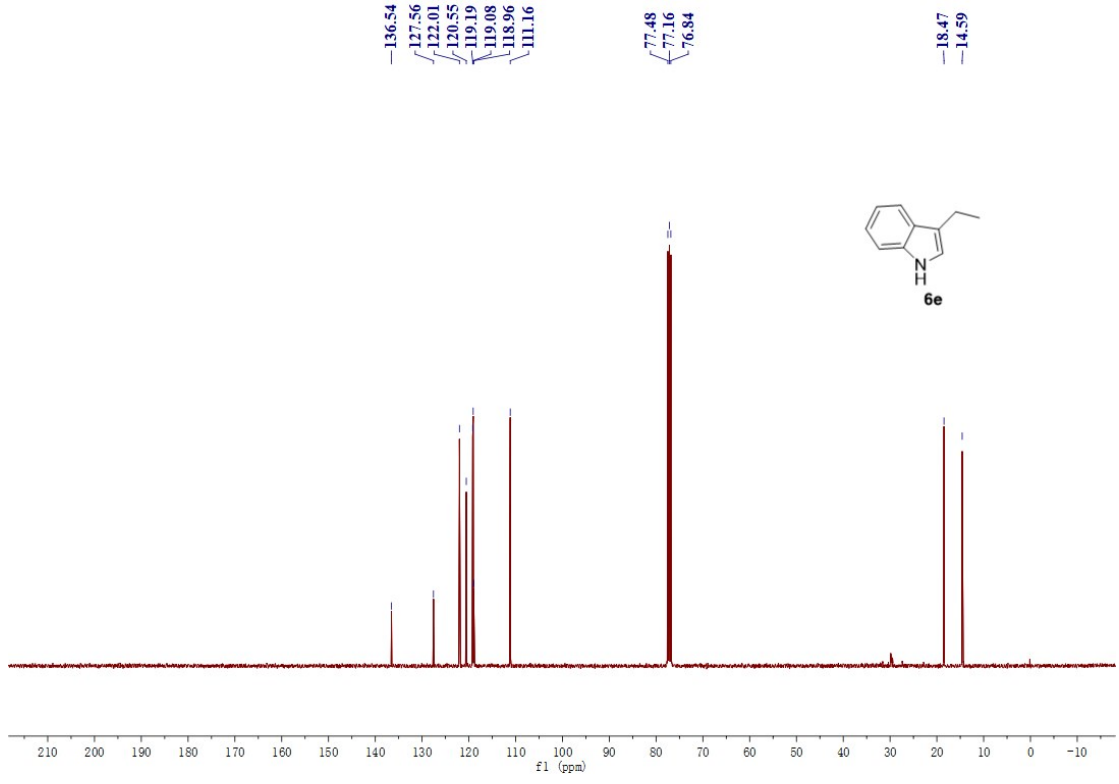
7.26
7.21
7.20
7.18
7.14
7.12
7.10
6.98
2.83
2.81
2.79
2.77
1.36
1.34
1.33
6e
0.82
1.00
0.99
1.05
1.07
1.03
2.07
3.27
f1 (ppm)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111.16
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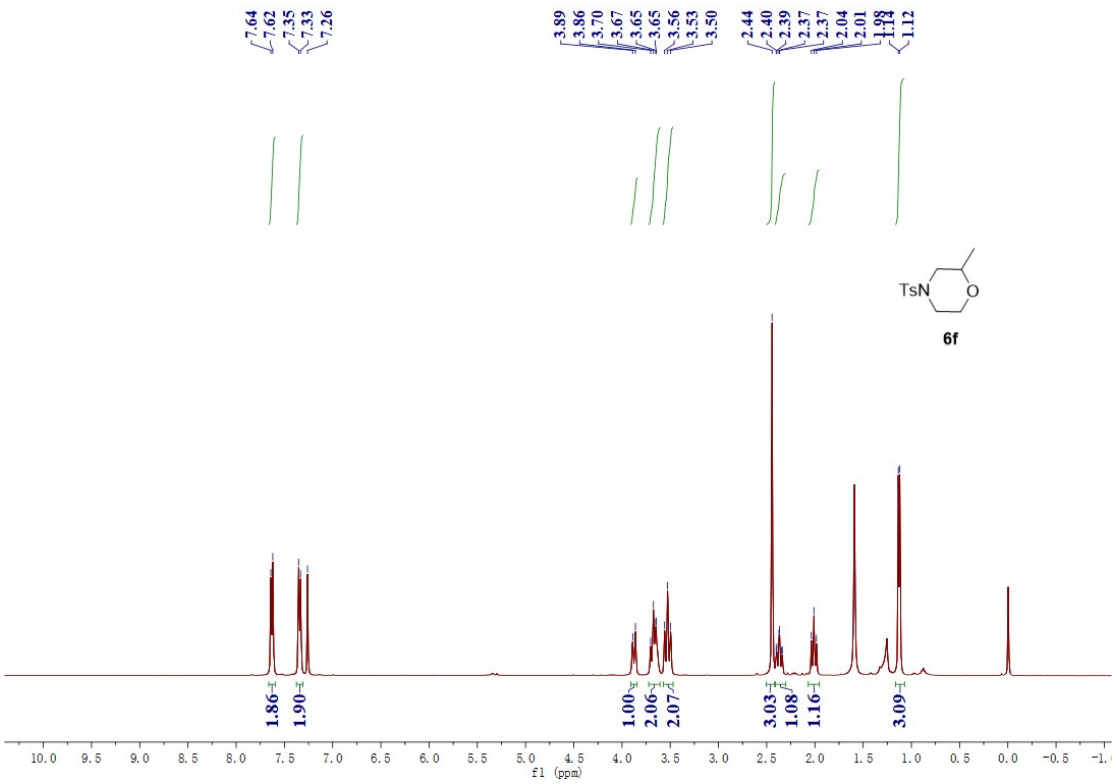
77.16
76.84
18.47
14.59
6e
f1 (ppm)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3.70
3.67
3.65
3.65
3.56
3.53
3.50
2.44
2.40
2.39
2.37
2.37
2.04
2.01
1.98
1.14
1.12
TsN
O
6f
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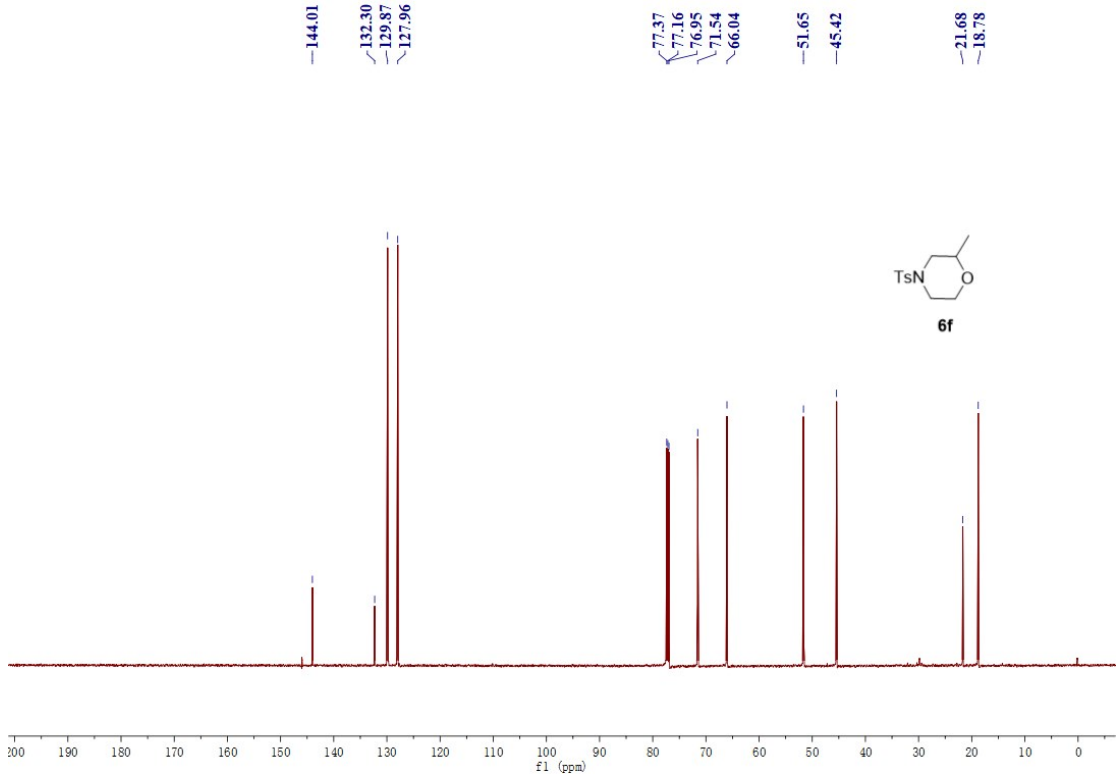
1.90
1.00
2.06
2.07
3.03
1.08
1.16
3.09
f1 (ppm)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71.54
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51.65
45.42
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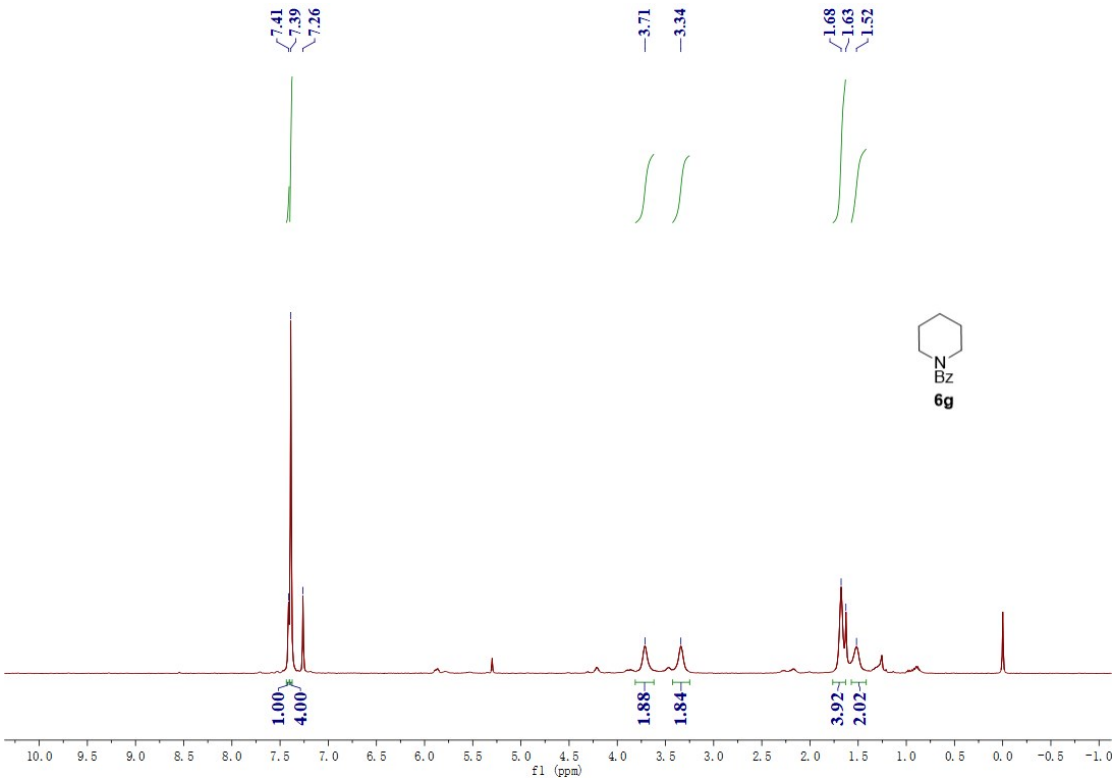
18.78
TsN
O
6f
f1 (ppm)


7.41
7.39
7.26
3.71
3.34
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1.63
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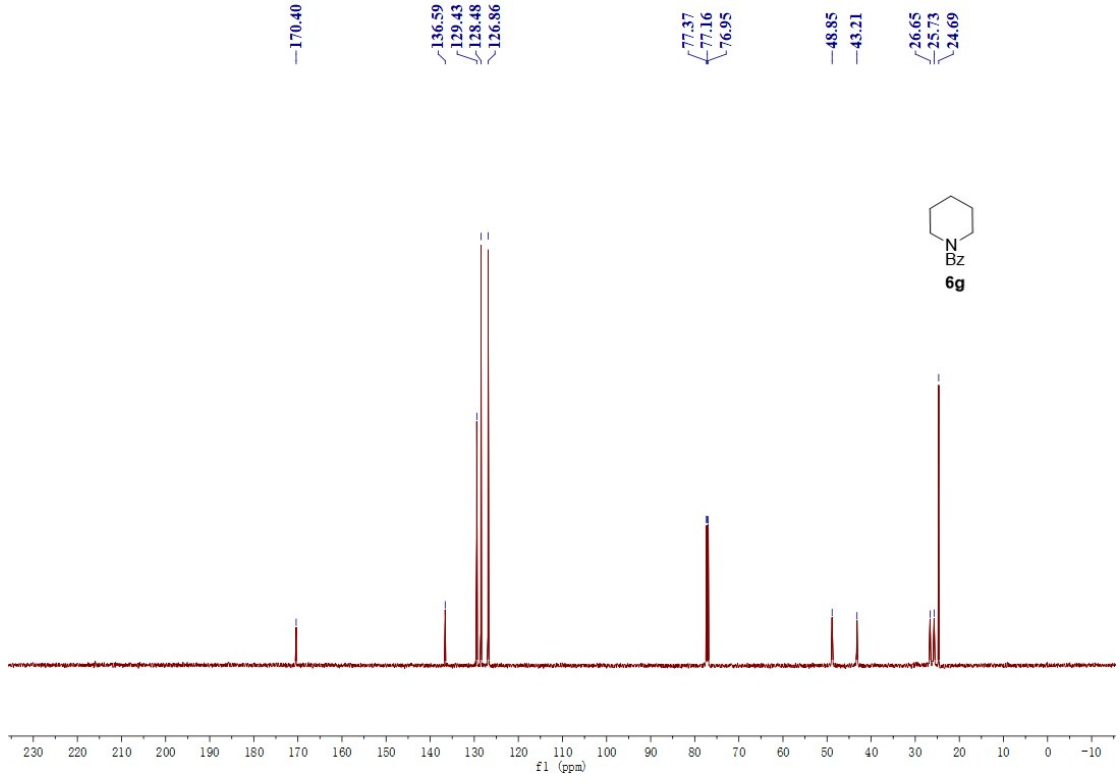
Bz
6g
1.00
4.00
1.88
1.84
3.92
2.02
f1 (ppm)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43.21
26.65
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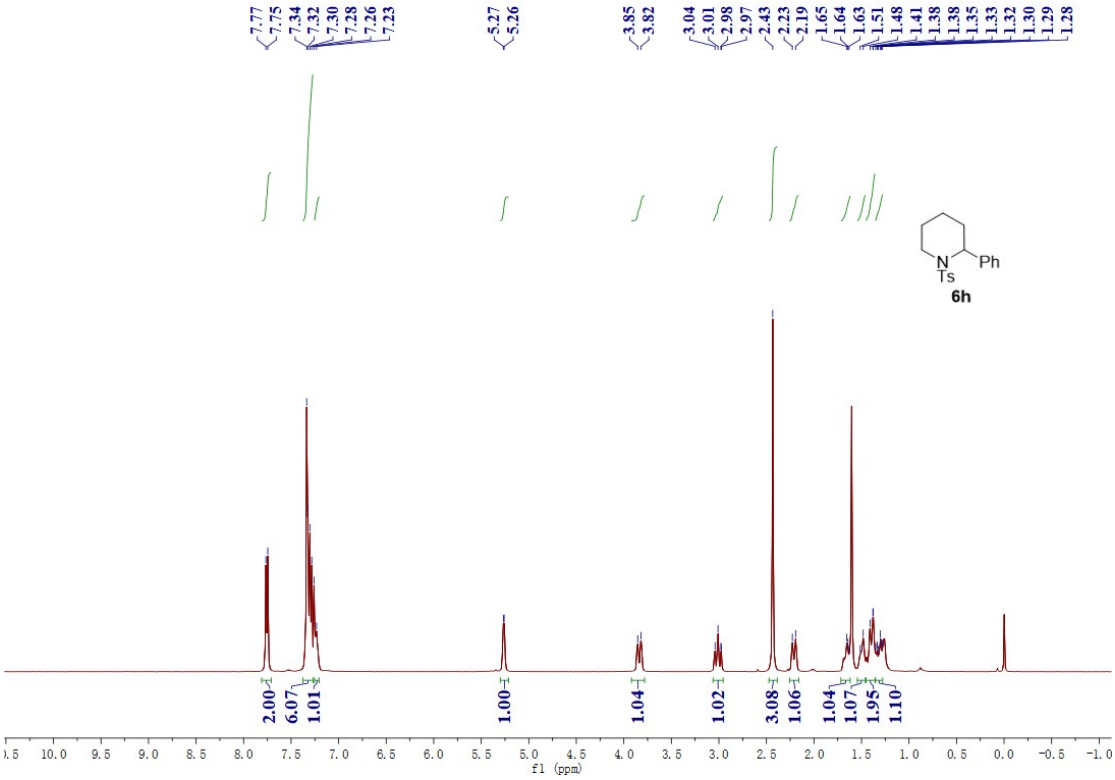
24.69
N
Bz
6g
f1 (ppm)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7.75
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7.28
7.26
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5.27
5.26
3.85
3.82
3.04
3.01
2.98
2.97
2.43
2.23
2.19
1.65
1.64
1.63
1.51
1.48
1.41
1.38
1.38
1.35
1.33
1.32
1.30
1.29
1.28
N
Ts
Ph
6h
2.00
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1.01
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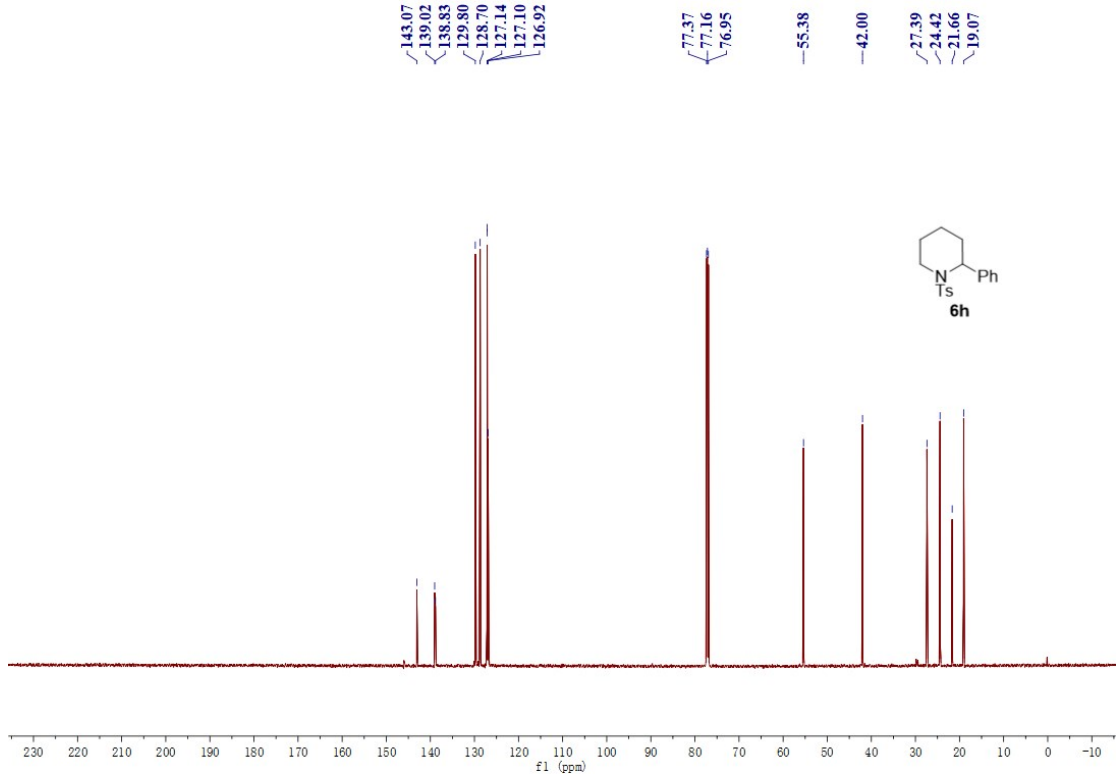
1.04
1.02
3.08
1.06
1.04
1.07
1.95
1.10
f1 (ppm)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139.02
138.83
129.80
128.70
127.14
127.10
126.92
77.37
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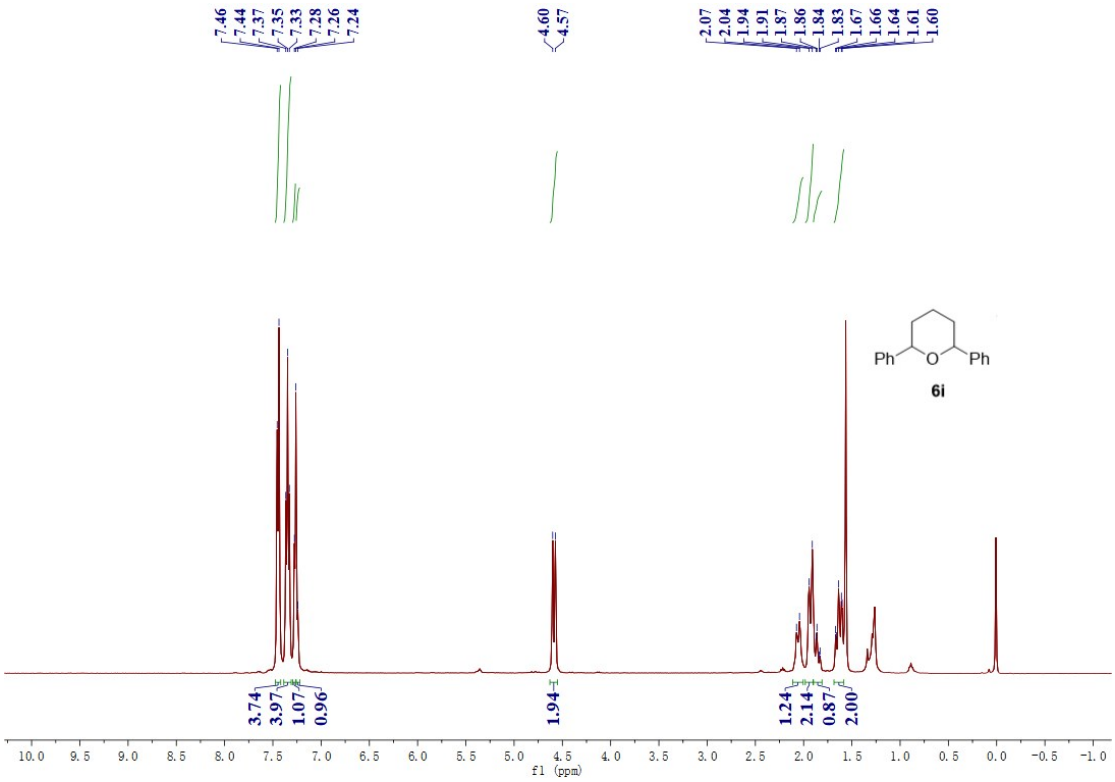
76.95
55.38
42.00
27.39
24.42
21.66
19.07
N
Ts
Ph
6h
f1 (ppm)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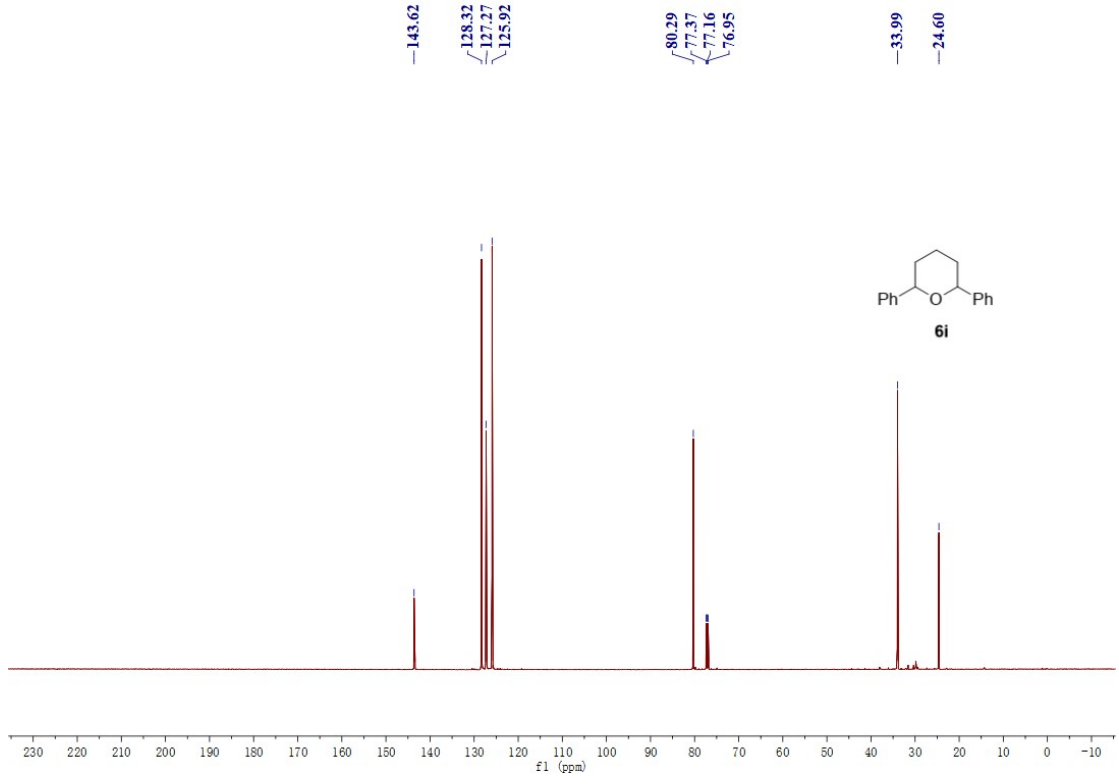
7.35
7.33
7.28
7.26
7.24
4.60
4.57
2.07
2.04
1.94
1.91
1.87
1.86
1.84
1.83
1.67
1.66
1.64
1.61
1.60
Ph
O
Ph
6i
3.74
3.97
1.07
0.96
1.94
1.24
2.14
0.87
2.00
f1 (ppm)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128.32
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77.37
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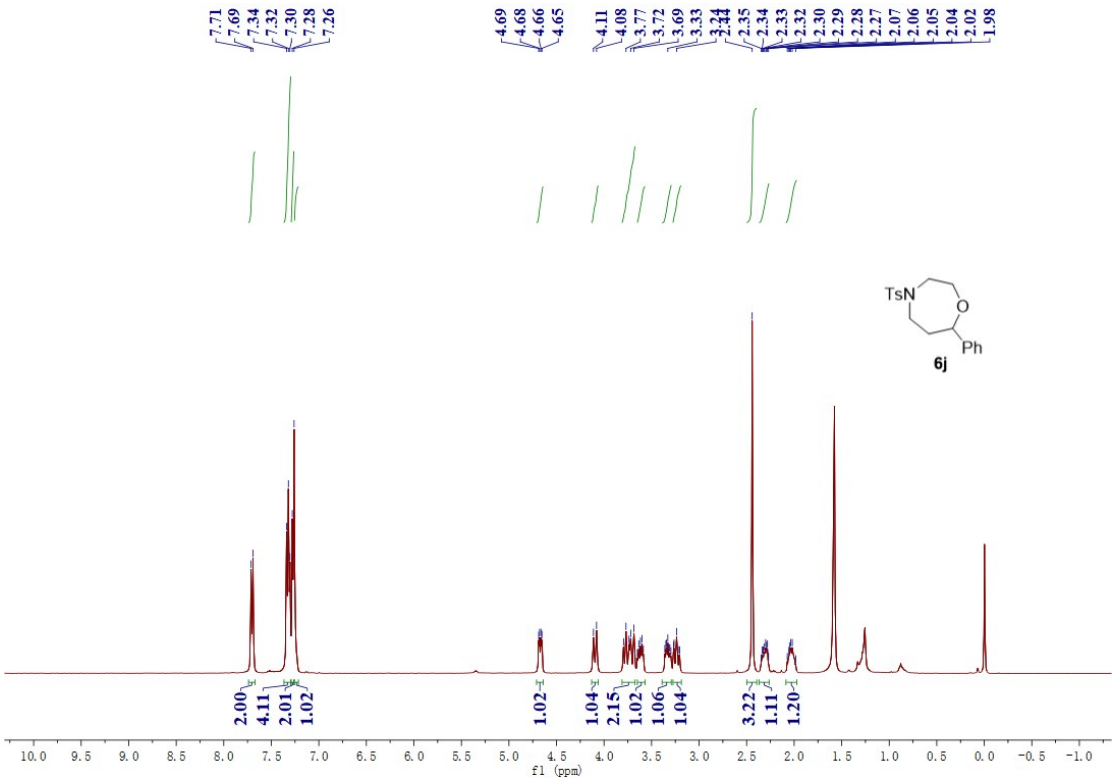
76.95
33.99
24.60
Ph
O
Ph
6i
f1 (ppm)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7.69
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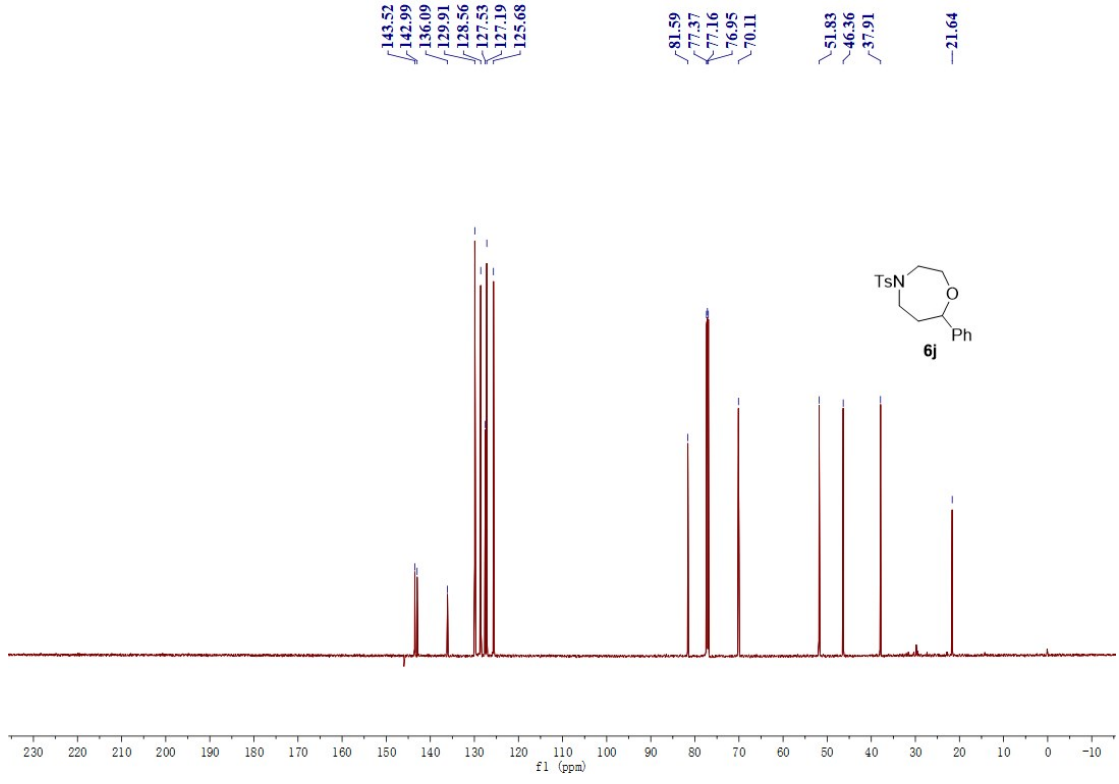
7.30
7.28
7.26
4.69
4.68
4.66
4.65
4.11
4.08
3.77
3.72
3.69
3.33
2.35
2.34
2.33
2.32
2.30
2.29
2.28
2.27
2.07
2.06
2.05
2.04
2.02
1.98
TsN
O
Ph
6j
2.00
4.11
2.01
1.02
1.02
1.04
2.15
1.02
1.06
1.04
3.22
1.11
1.20
f1 (ppm)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127.53
127.19
125.68
81.59
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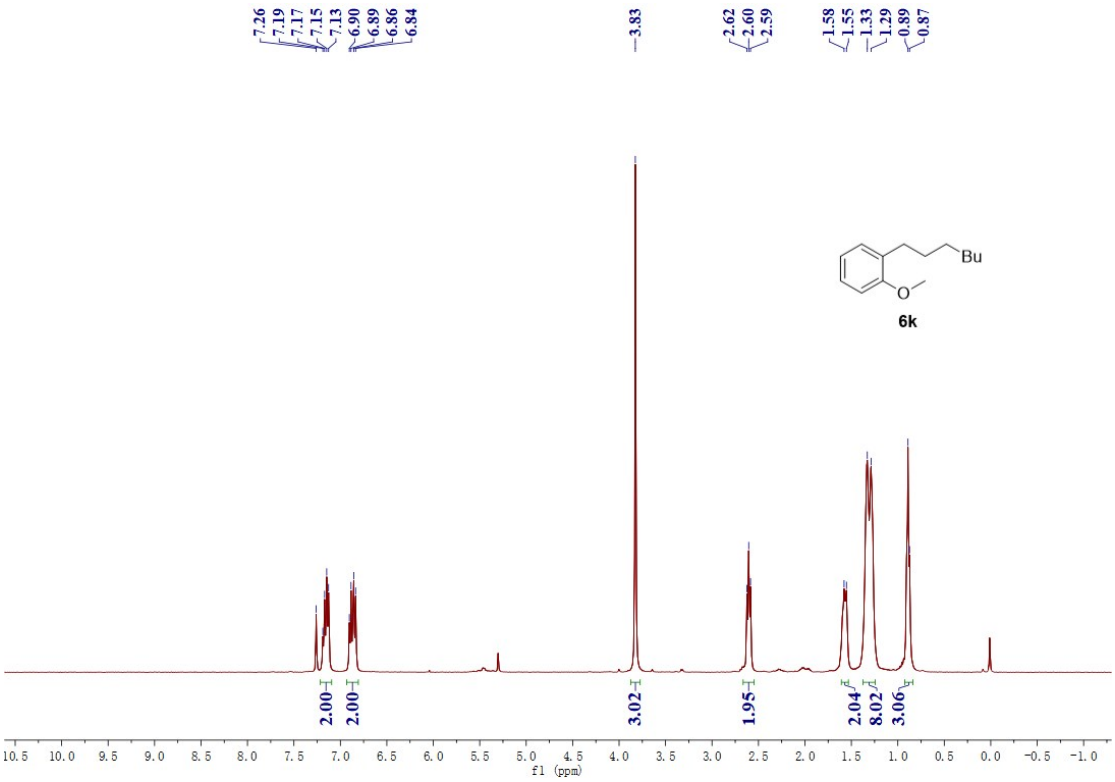
76.95
70.11
51.83
46.36
37.91
21.64
TsN
O
Ph
6j
f1 (ppm)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7.19
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7.15
7.13
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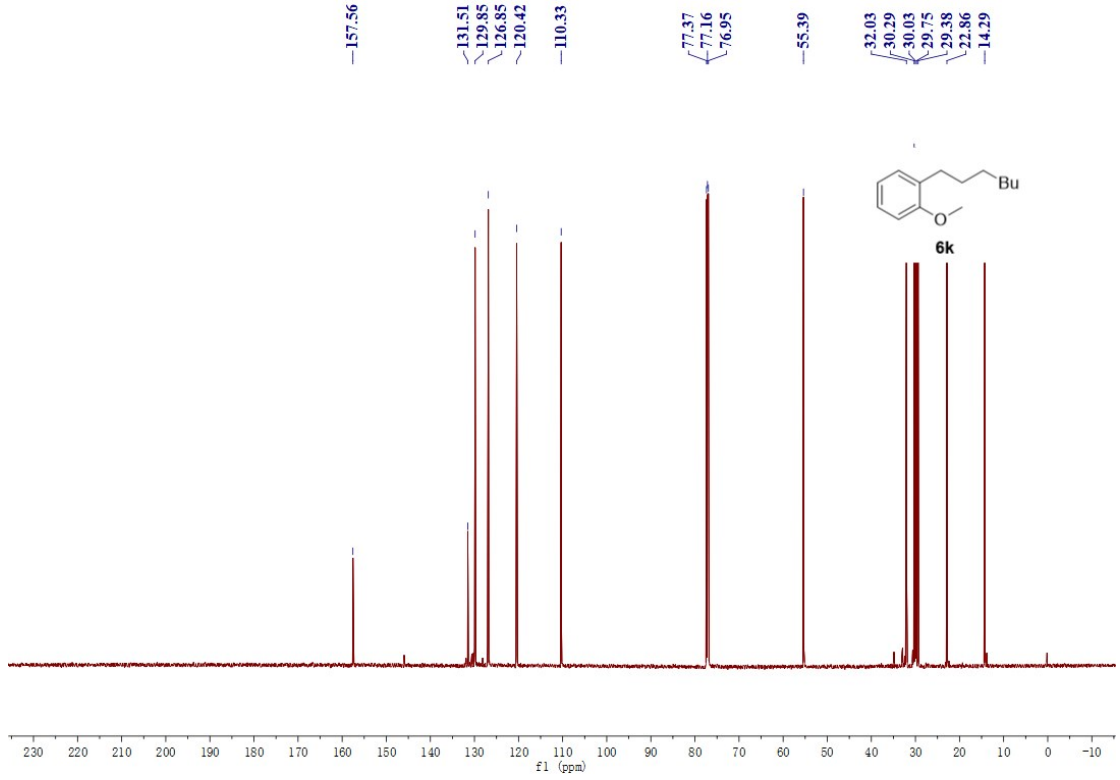
6.89
6.86
6.84
3.83
2.62
2.60
2.59
1.58
1.55
1.33
1.29
0.89
0.87
Bu
O
6k
2.00
2.00
3.02
1.95
2.04
8.02
3.06
f1 (ppm)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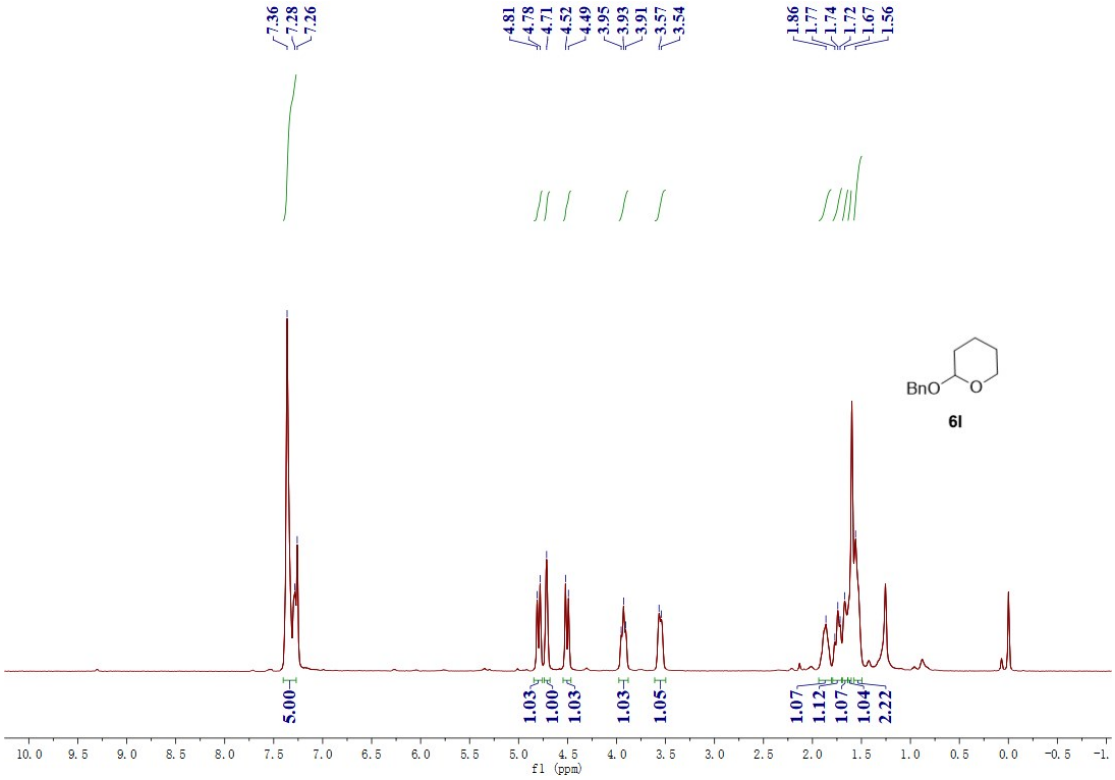
30.29
30.03
29.75
29.38
22.86
14.29
Bu
O
6k
f1 (ppm)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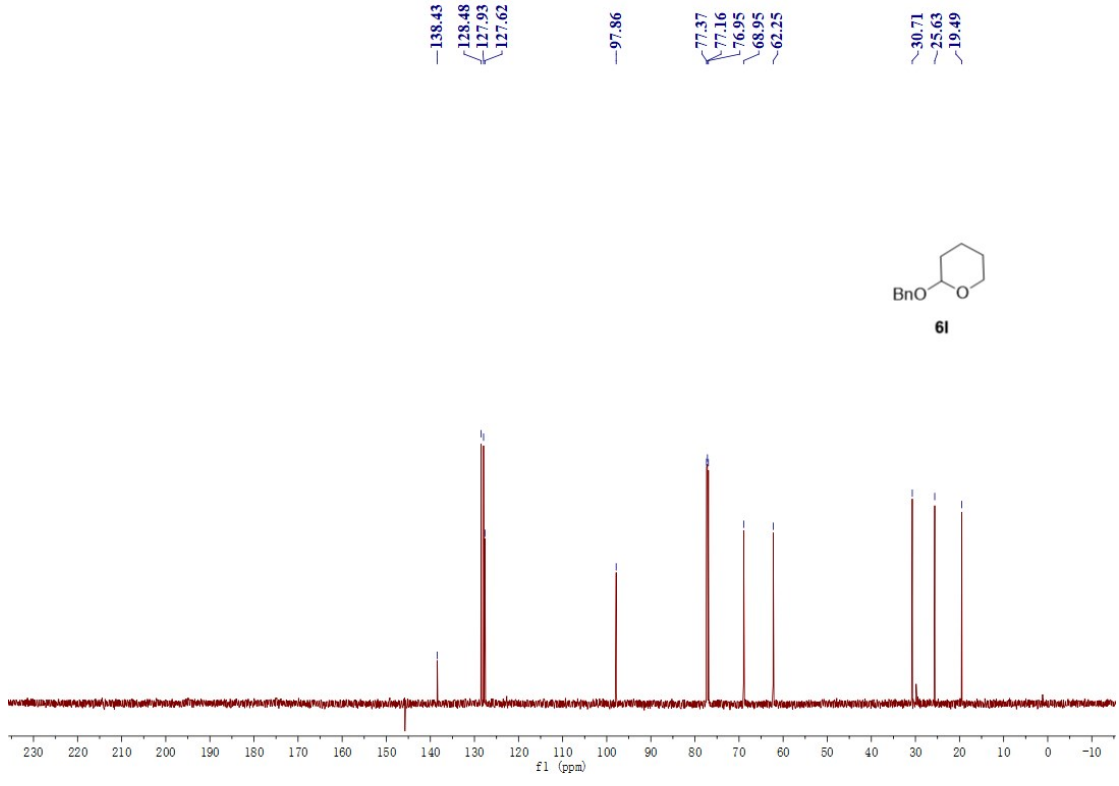
3.91
3.57
3.54
1.86
1.77
1.74
1.72
1.67
1.56
BnO
O
6l
5.00
1.03
1.00
1.03
1.03
1.05
1.07
1.12
1.07
1.04
2.22
f1 (ppm)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127.62
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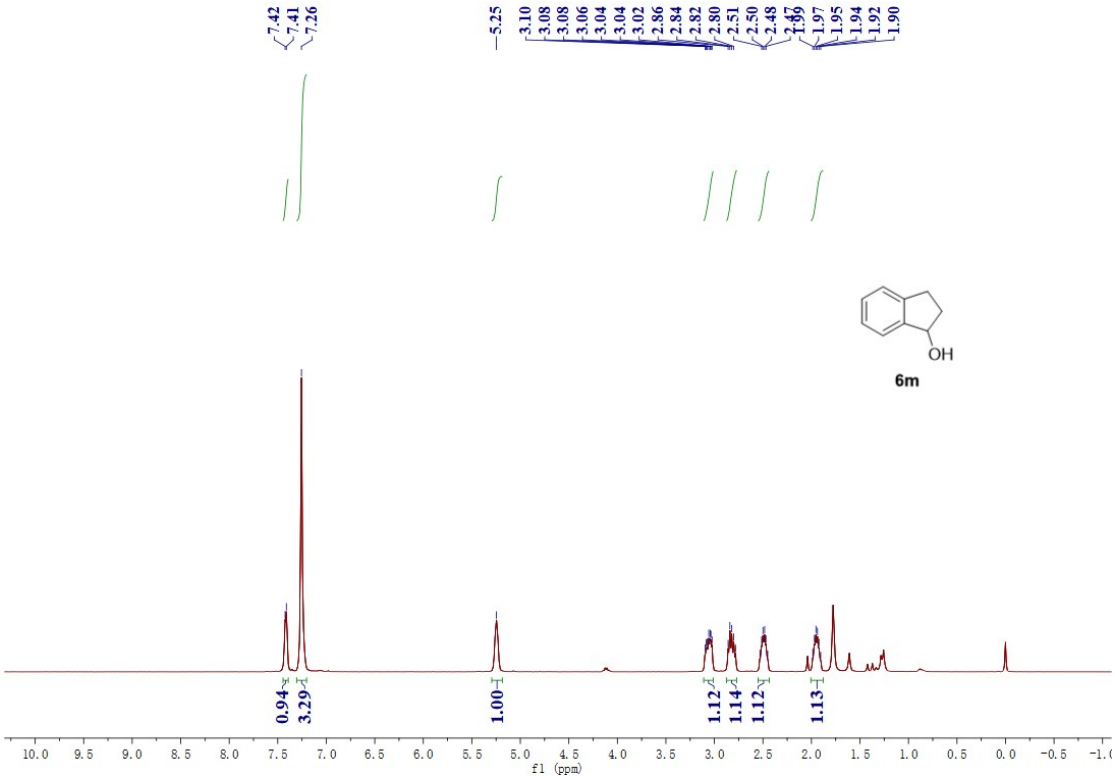
76.95
68.95
62.25
30.71
25.63
19.49
BnO
O
6l
f1 (ppm)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7.41
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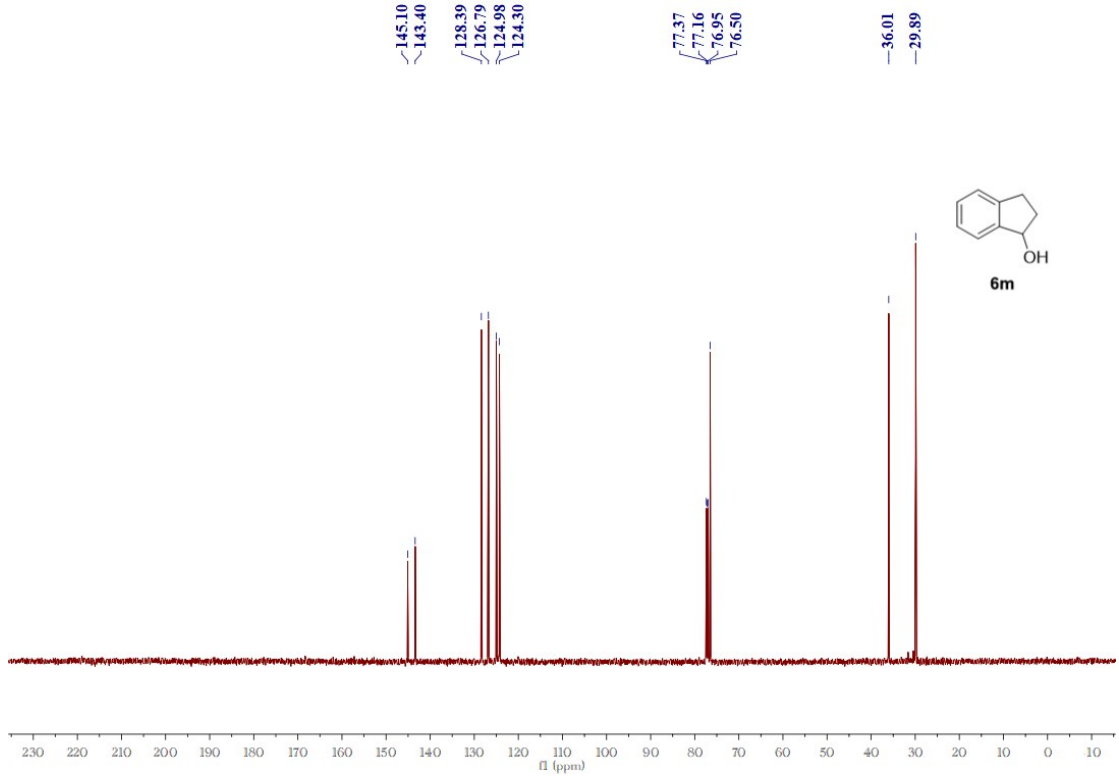
3.10
3.08
3.08
3.06
3.04
3.04
3.02
2.86
2.84
2.82
2.80
2.51
2.50
2.48
1.97
1.95
1.94
1.92
1.90
OH
6m
0.94
3.29
1.00
1.12
1.14
1.12
1.13
f1 (ppm)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128.39
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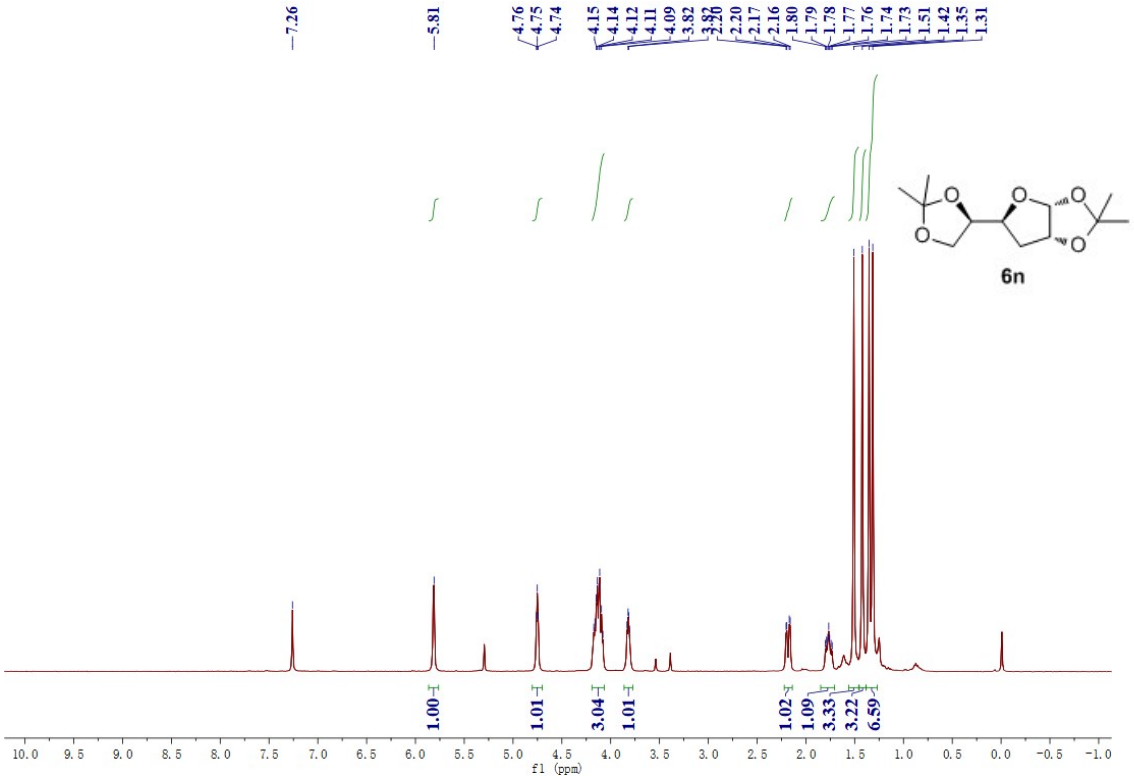
124.30
77.37
77.16
76.95
76.50
36.01
29.89
OH
6m
f1 (ppm)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4.75
4.74
4.15
4.14
4.12
4.11
4.09
3.82
2.20
2.17
2.16
1.80
1.79
1.78
1.77
1.76
1.74
1.73
1.51
1.42
1.35
1.31
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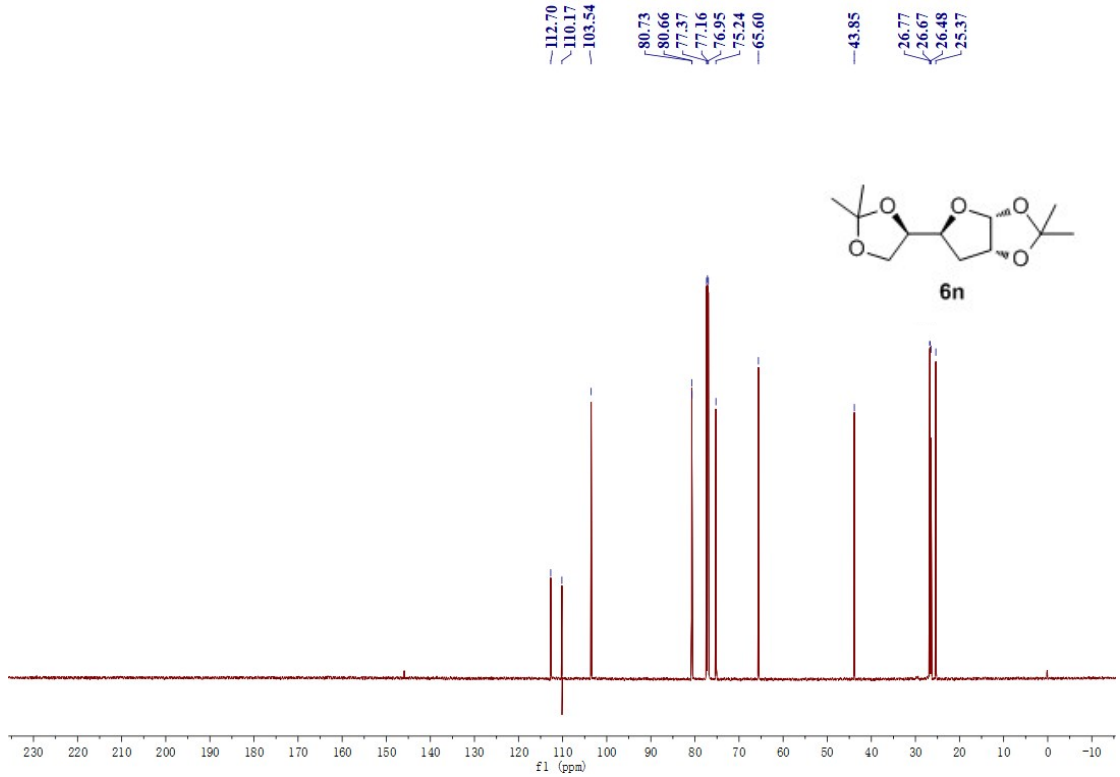
1.01
3.04
1.01
1.02
1.09
3.33
3.22
6.59
f1 (ppm)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80.66
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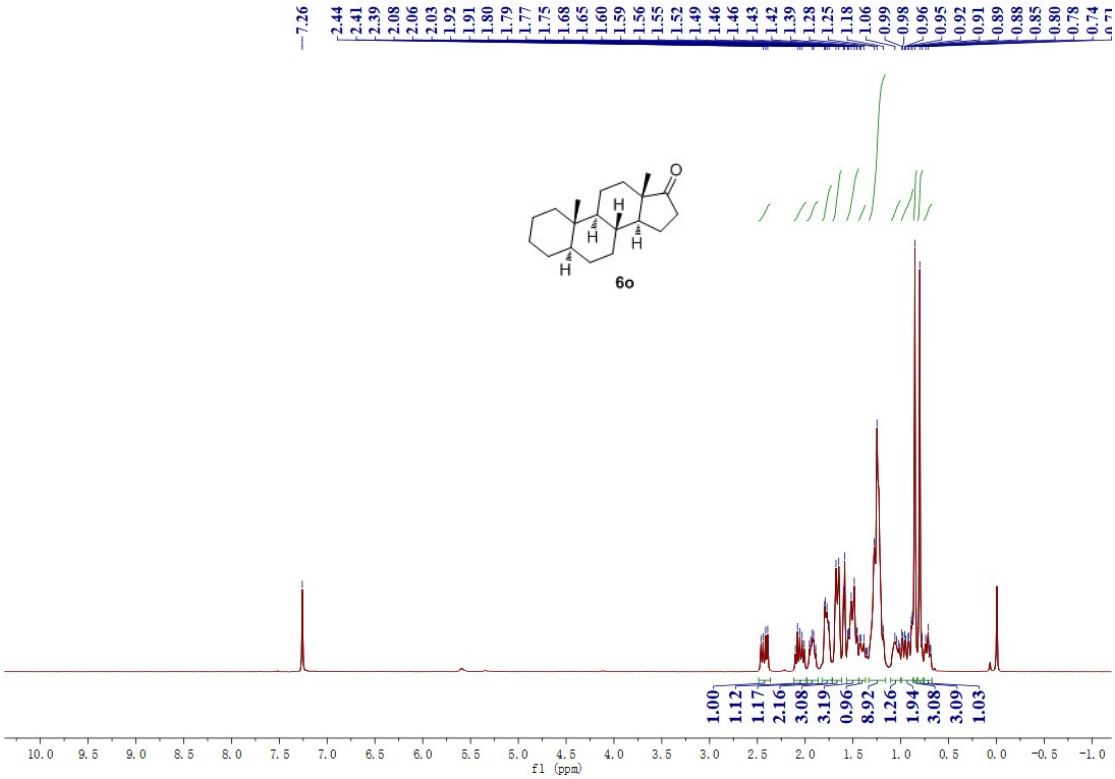
43.85
26.77
26.67
26.48
25.37
6n
f1 (ppm)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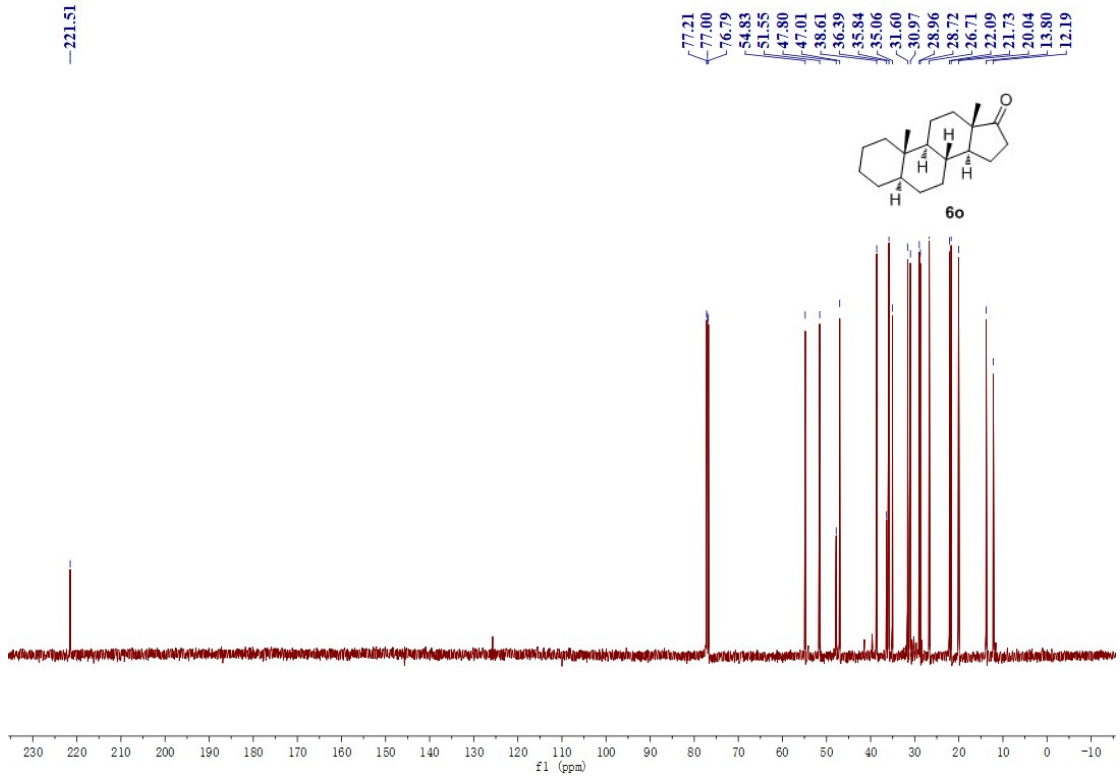
2.39
2.08
2.06
2.03
1.92
1.91
1.80
1.79
1.77
1.75
1.68
1.65
1.60
1.59
1.56
1.55
1.52
1.49
1.46
1.46
1.43
1.42
1.39
1.28
1.25
1.18
1.06
0.99
0.98
0.96
0.95
0.92
0.91
0.89
0.88
0.85
0.80
0.78
0.74
O
H
H
H
6o
1.00
1.12
1.17
2.16
3.08
3.19
0.96
8.92
1.26
1.94
3.08
3.09
1.03
f1 (ppm)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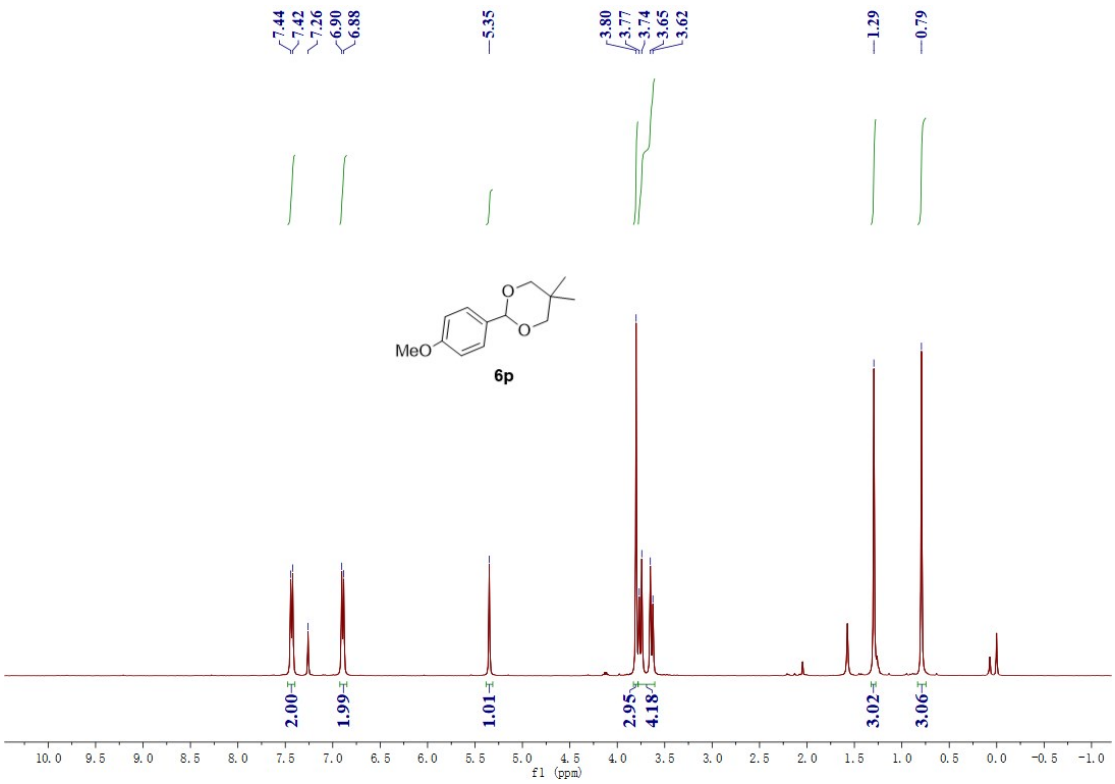
47.80
47.01
38.61
36.39
35.84
35.06
31.60
30.97
28.96
28.72
26.71
22.09
21.73
20.04
13.80
12.19
O
H
H
H
6o
f1 (ppm)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7.26
6.90
6.88
5.35
3.80
3.77
3.74
3.65
3.62
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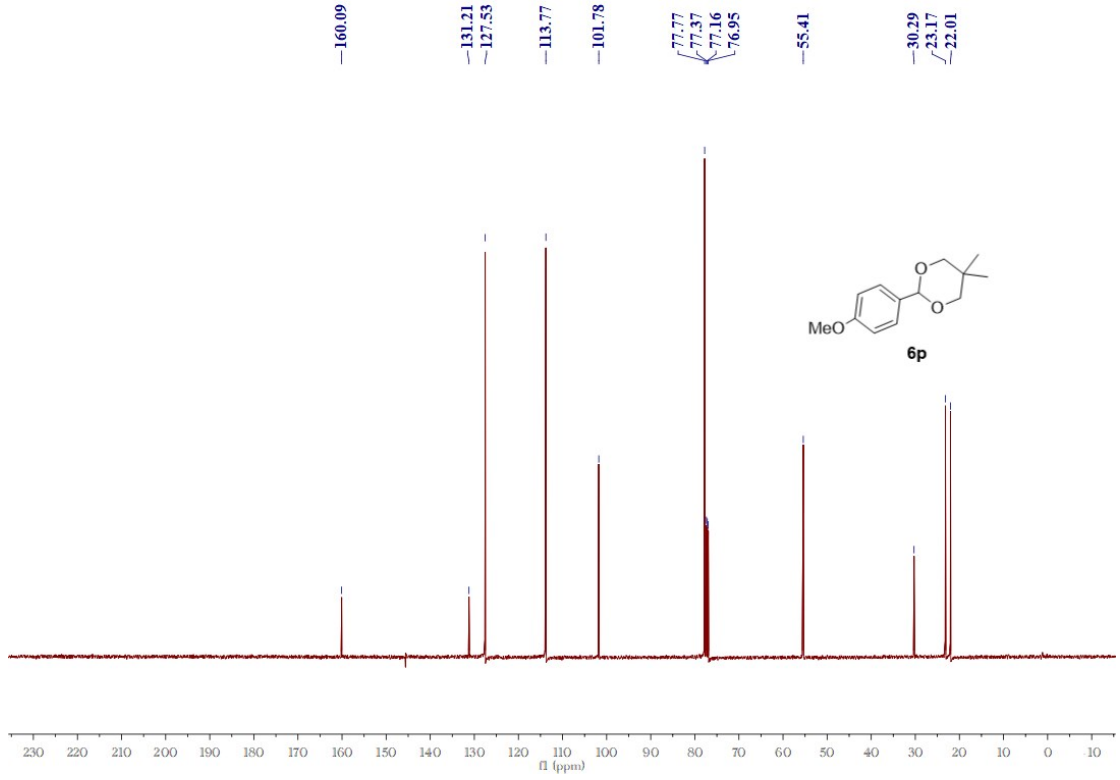
MeO
6p
2.00
1.99
1.01
2.95
4.18
3.02
3.06
f1 (ppm)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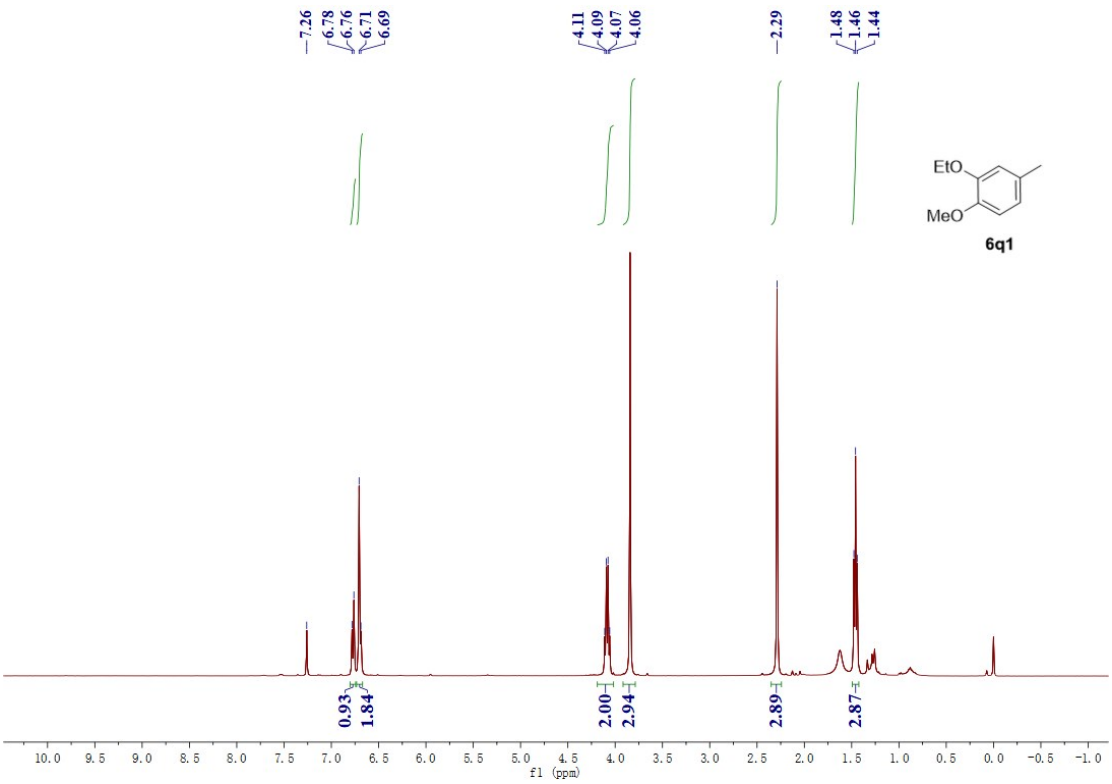
77.16
76.95
55.41
30.29
23.17
22.01
MeO
6p
f1 (ppm)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6.71
6.69
4.11
4.09
4.07
4.06
2.29
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EtO
MeO
6q1
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2.00
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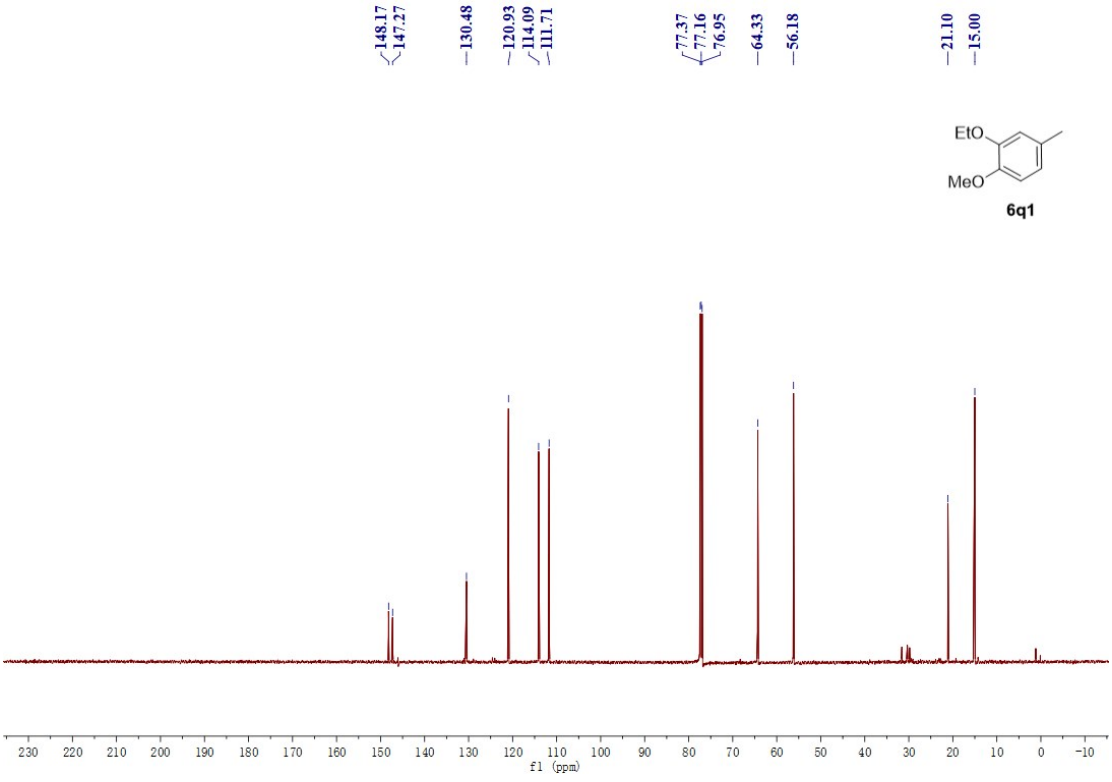
2.87
f1 (ppm)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76.95
64.33
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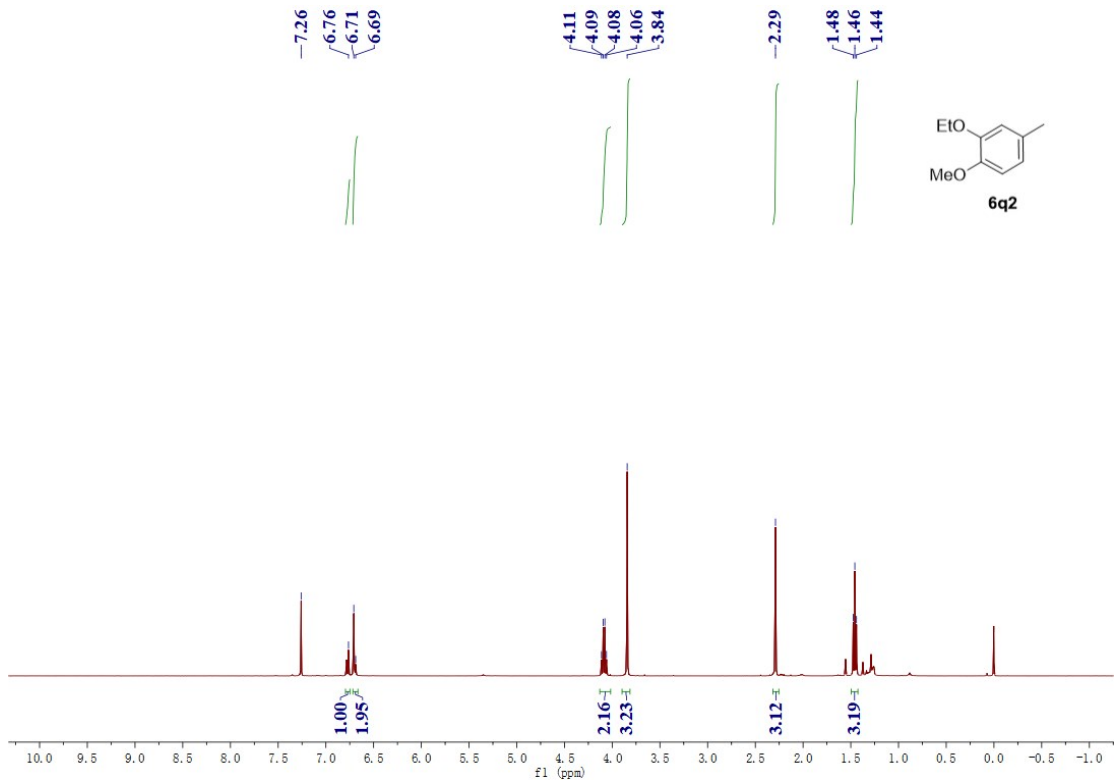
21.10
15.00
EtO
MeO
6q1
f1 (ppm)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4.11
4.09
4.08
4.06
3.84
2.29
1.48
1.46
1.44
EtO
MeO
6q2
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1.95
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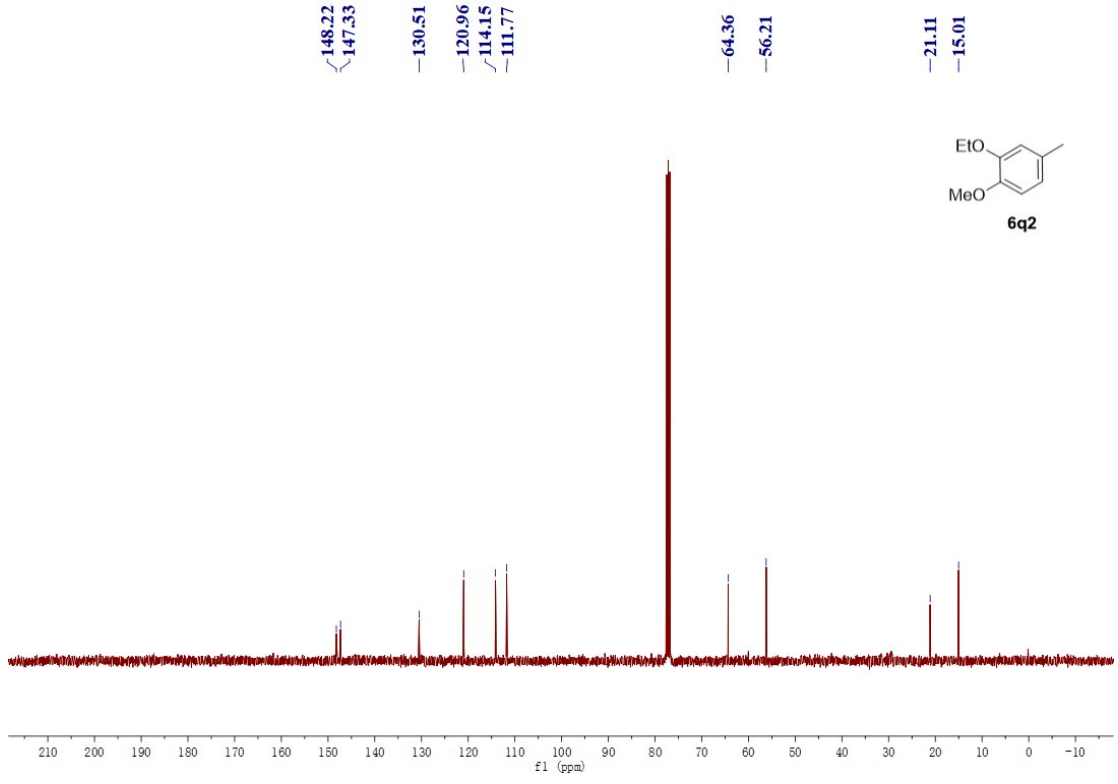
3.23
3.12
3.19
f1 (ppm)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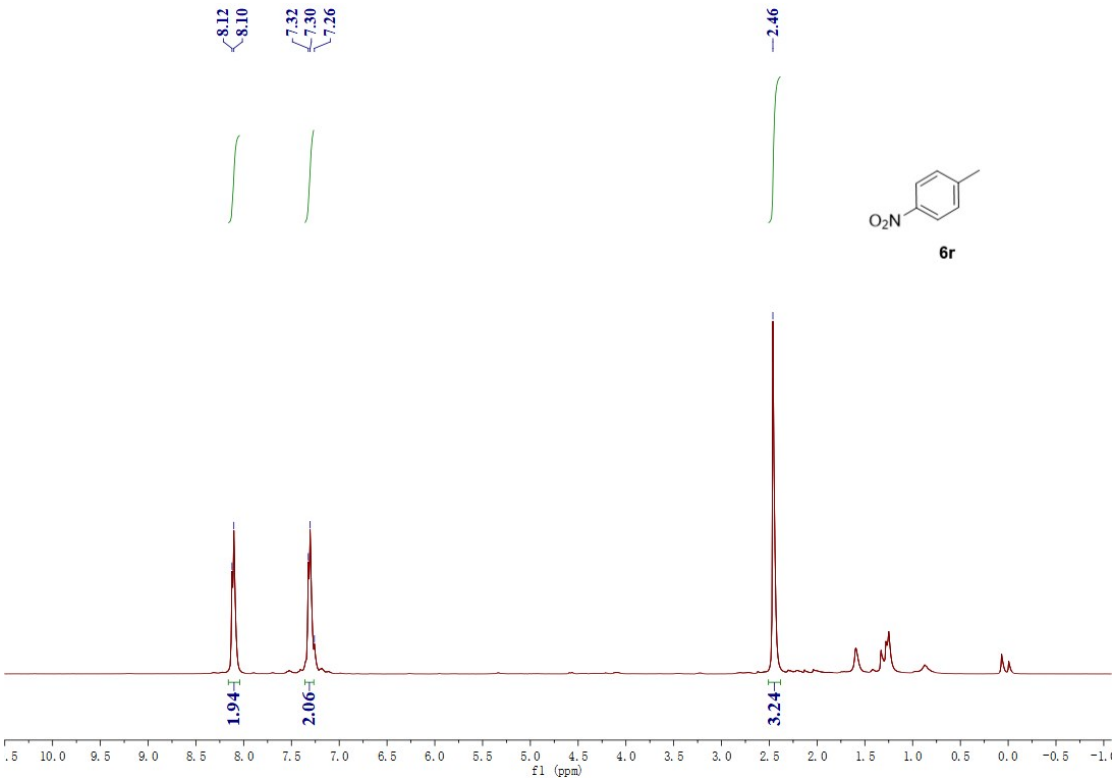
111.77
64.36
56.21
21.11
15.01
EtO
MeO
6q2
f1 (ppm)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8.10
7.32
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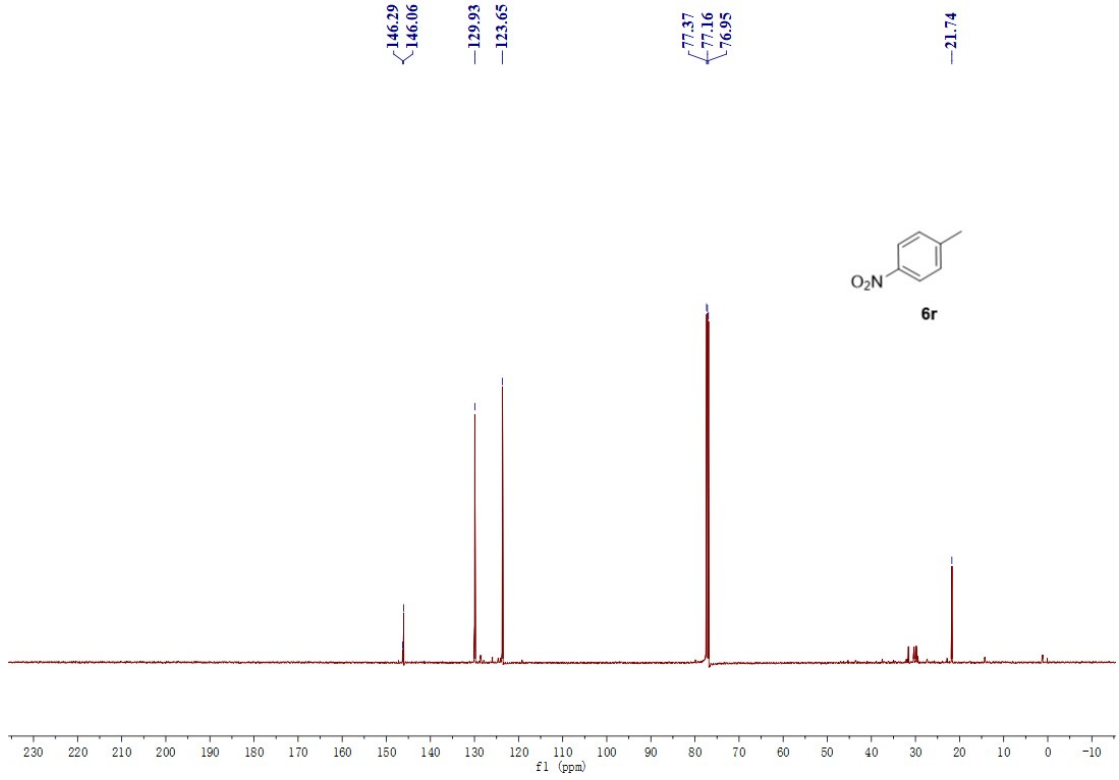
7.26
2.46
O2N
6r
1.94
2.06
3.24
f1 (ppm)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146.06
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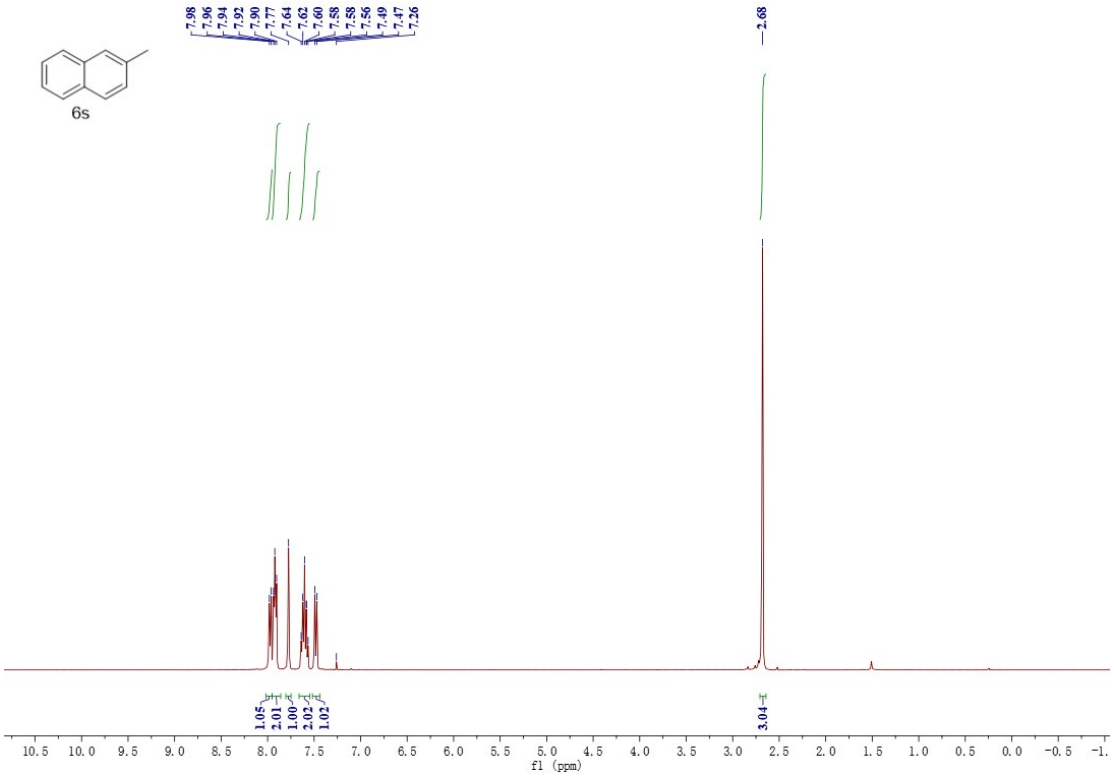
123.65
77.37
77.16
76.95
21.74
O2N
6r
f1 (ppm)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7.92
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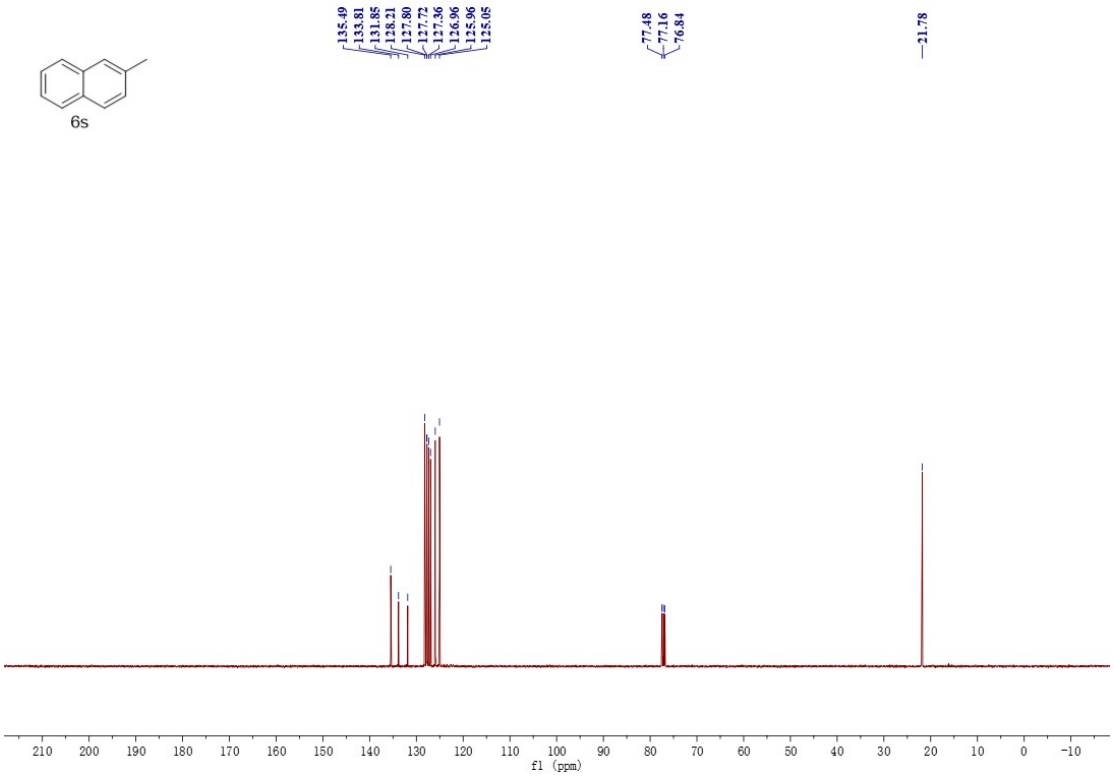
7.62
7.60
7.58
7.58
7.56
7.49
7.47
7.26
2.68
6s
1.05
2.01
1.00
2.02
1.02
3.04
f1 (ppm)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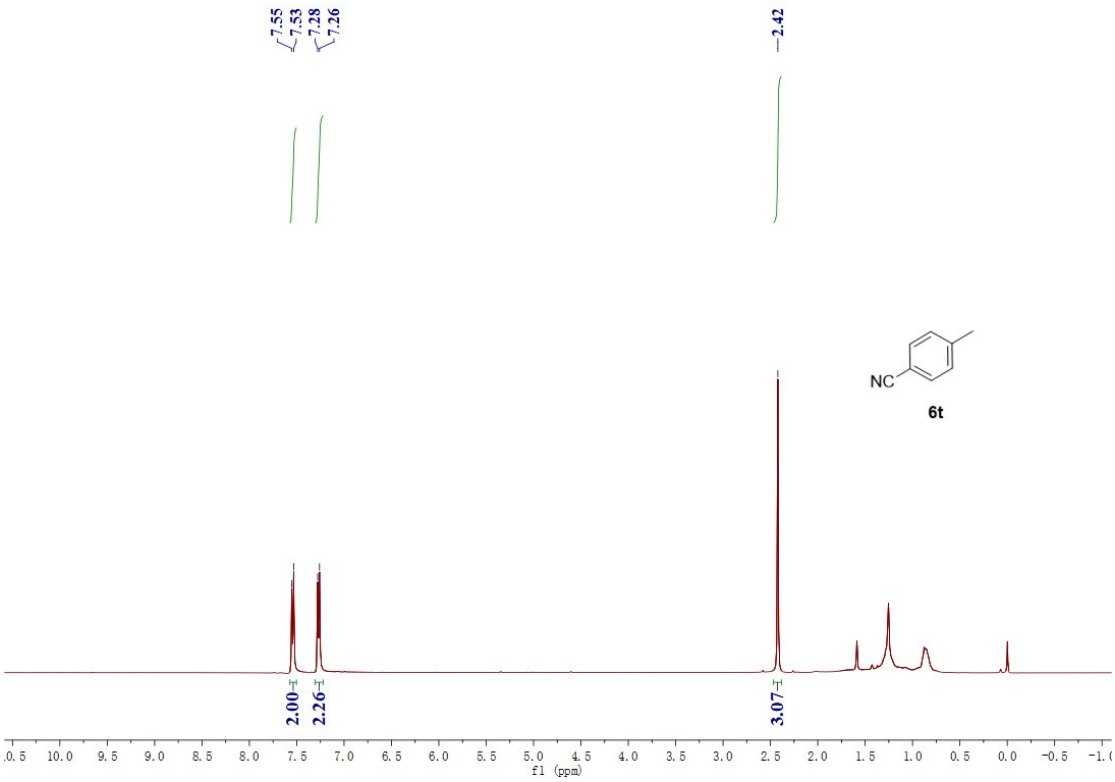
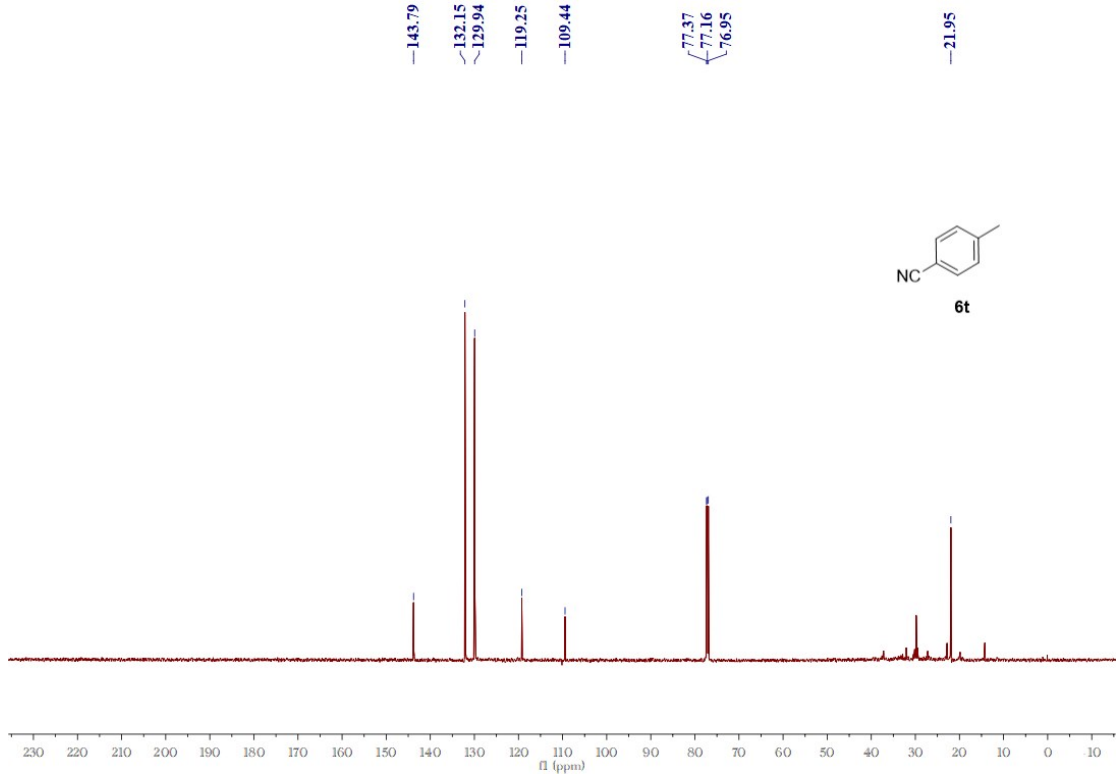
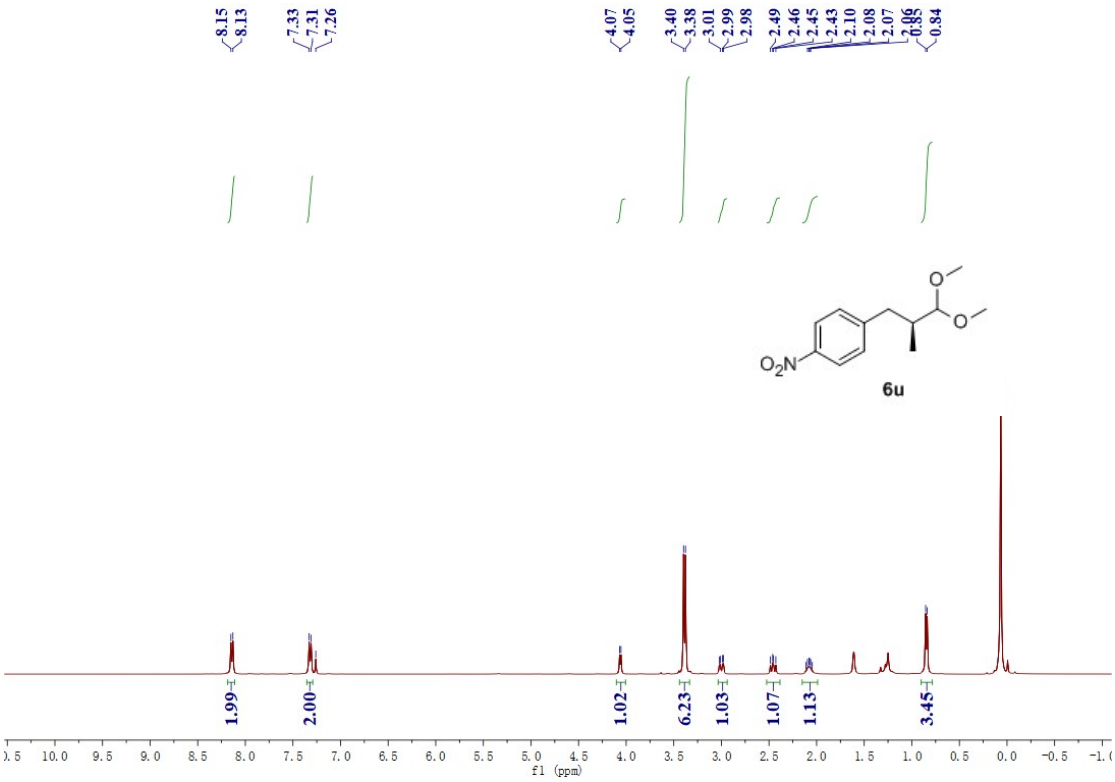
133.81
131.85
128.21
127.80
127.72
127.36
126.96
125.96
125.05
77.48
77.16
76.84
21.78
6s
f1 (ppm)


7.55
7.53
7.28
7.26
2.42
NC
6t
2.00
2.26
3.07
f1 (ppm)


143.79
132.15
129.94
119.25
109.44
77.37
77.16
76.95
21.95
NC
6t
f1 (ppm)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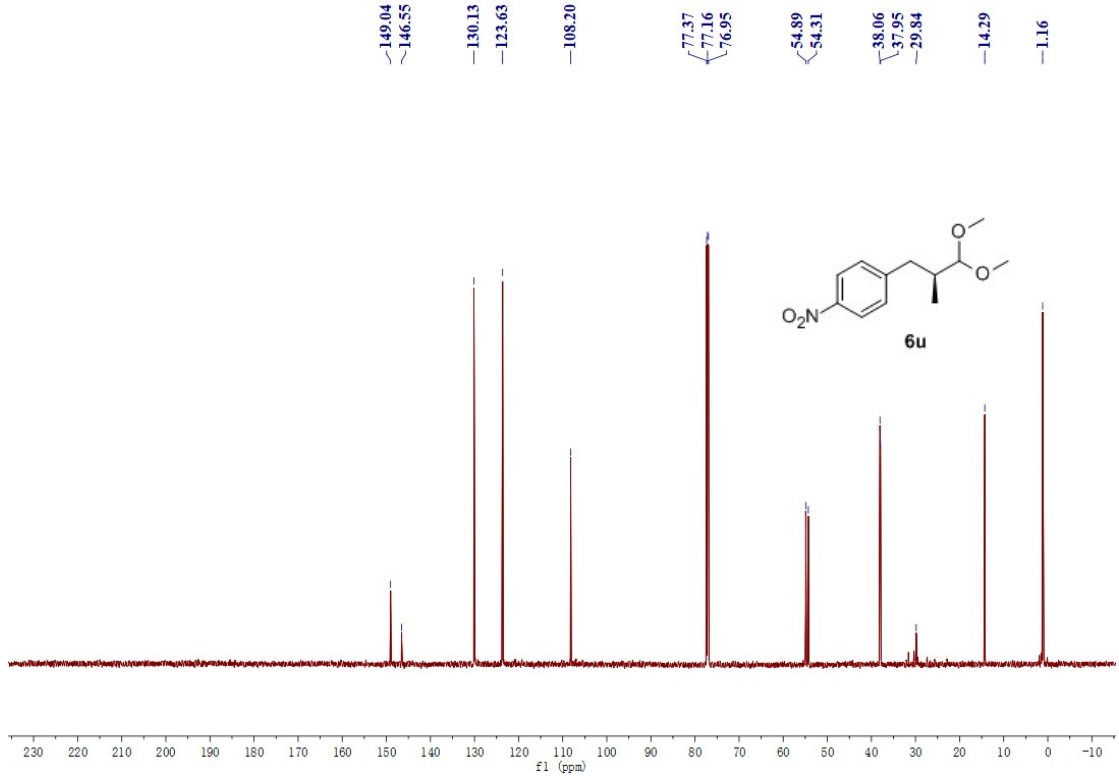
7.31
7.26
4.07
4.05
3.40
3.38
3.01
2.99
2.98
2.49
2.46
2.45
2.43
2.10
2.08
2.07
2.06
0.85
0.84
O2N
O
O
6u
1.99
2.00
1.02
6.23
1.03
1.07
1.13
3.45
f1 (ppm)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146.55
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123.63
108.20
77.37
77.16
76.95
54.89
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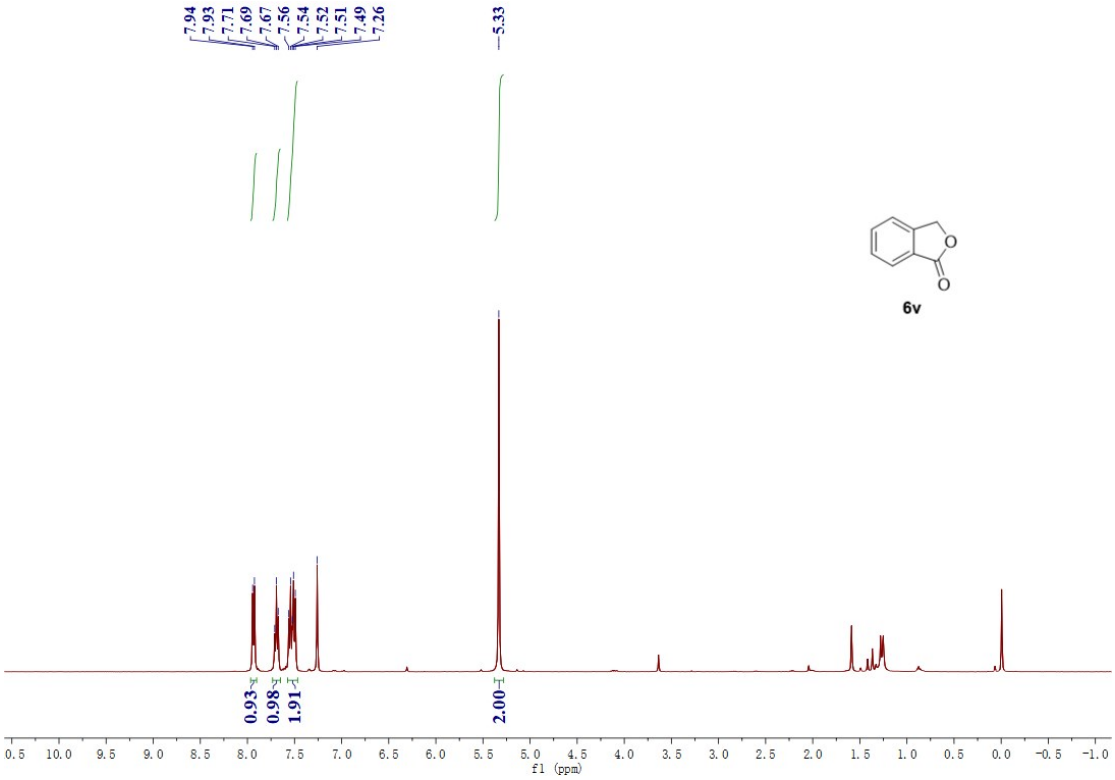
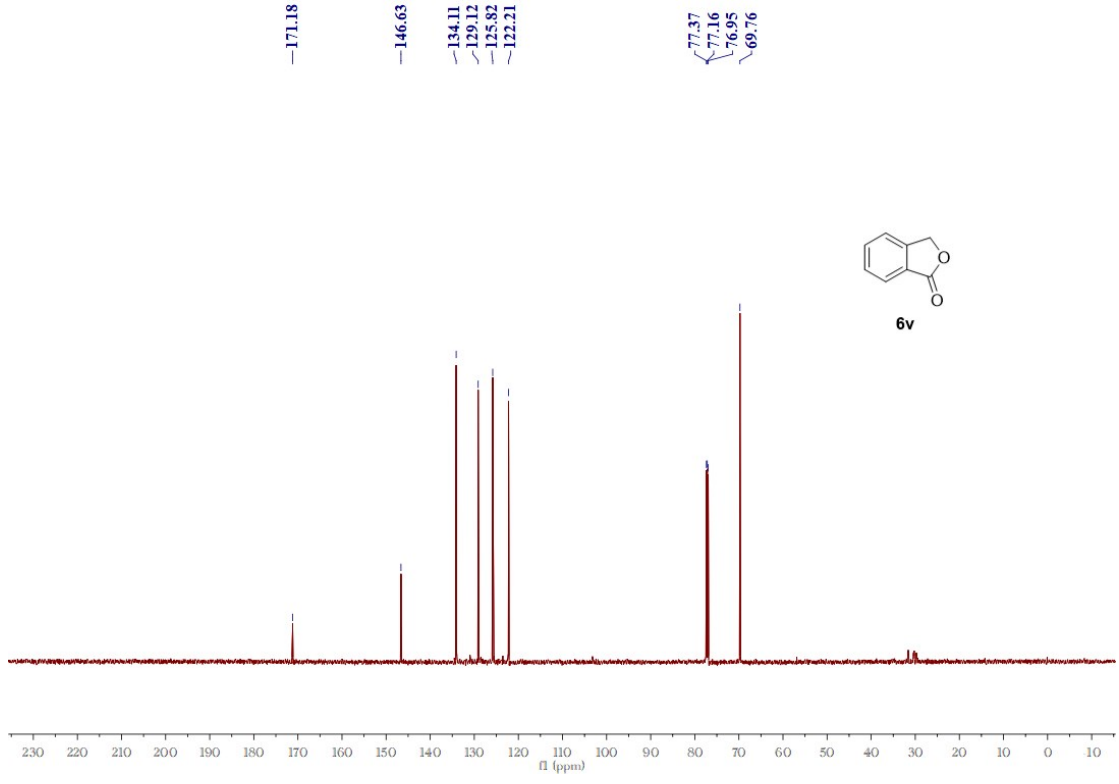
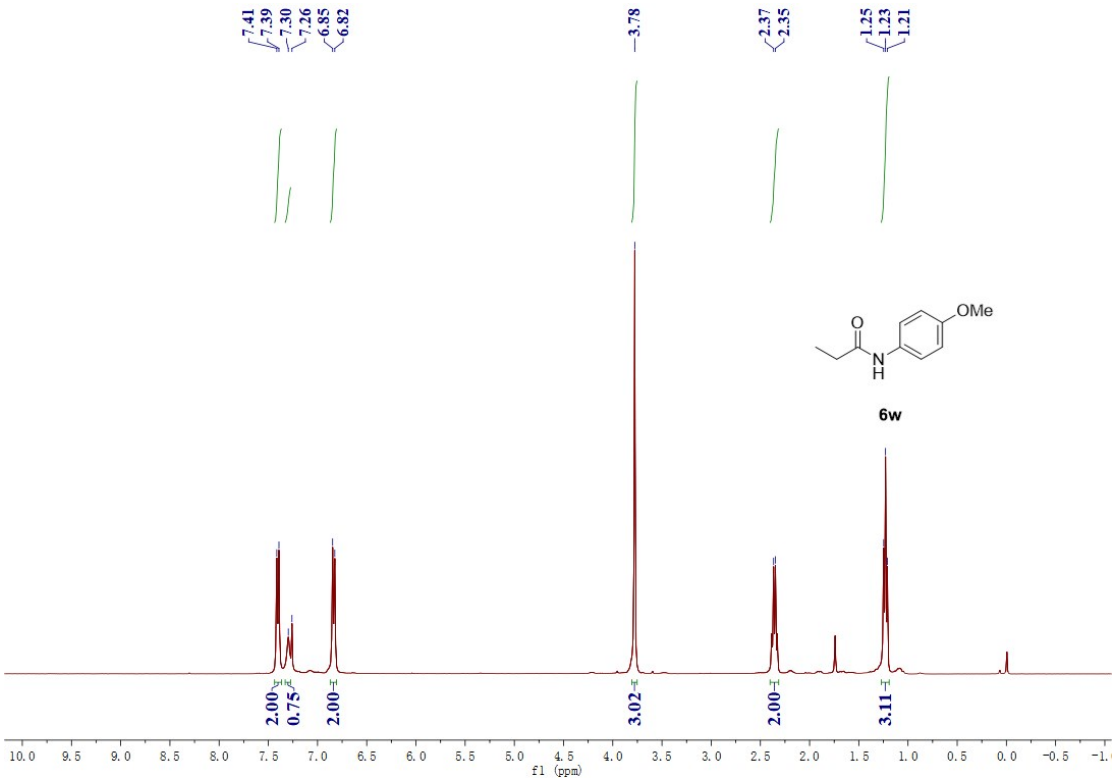
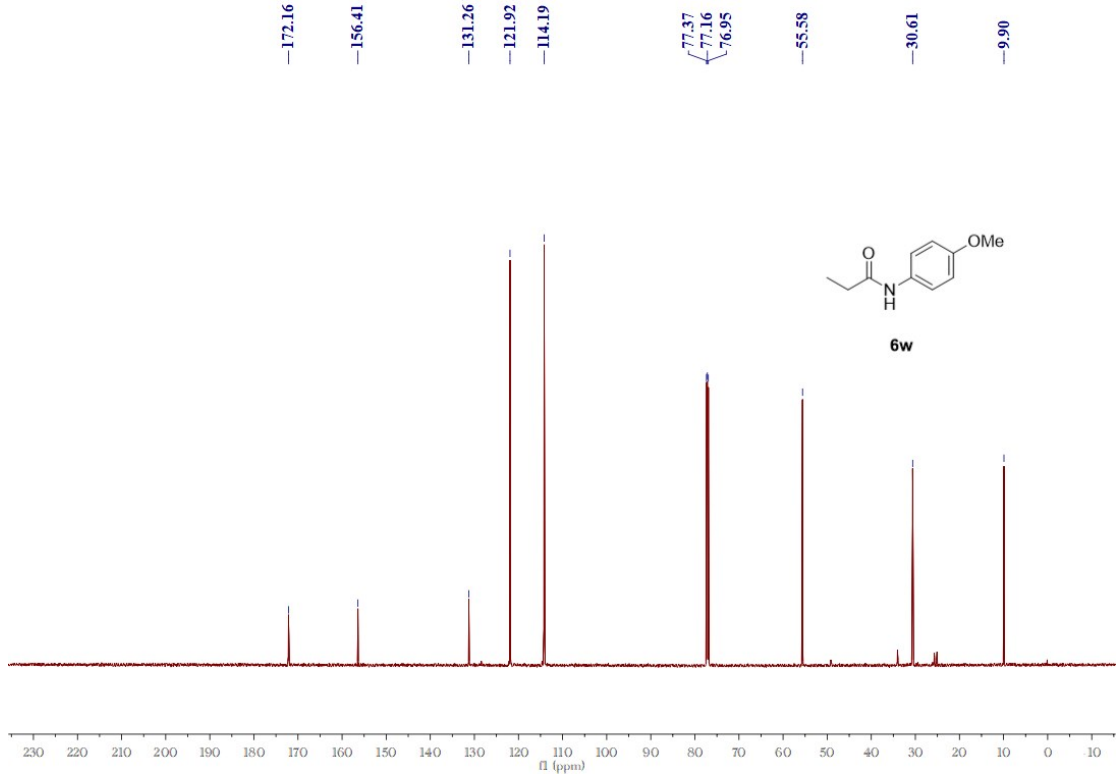
38.06
37.95
29.84
14.29
11.16
O2N
O
O
6u
f1 (ppm)


7.94
7.93
7.71
7.69
7.67
7.56
7.54
7.52
7.51
7.49
7.26
5.33
6v
0.93
0.98
1.91
2.00
f1 (ppm)


171.18
146.63
134.11
129.12
125.82
122.21
77.37
77.16
76.95
69.76
6v
f1 (ppm)


7.41
7.39
7.30
7.26
6.85
6.82
3.78
2.37
2.35
1.25
1.23
1.21
OMe
O
N
H
6w
2.00
0.75
2.00
3.02
2.00
3.11
f1 (ppm)


172.16
156.41
131.26
121.92
114.19
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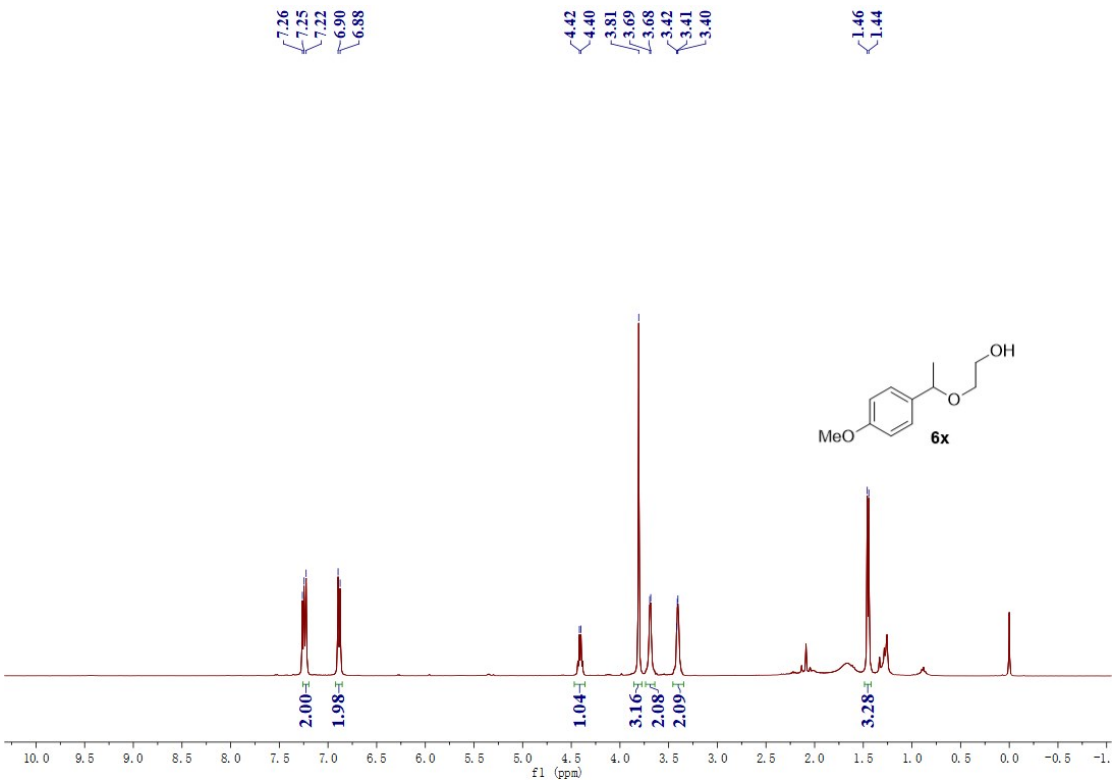
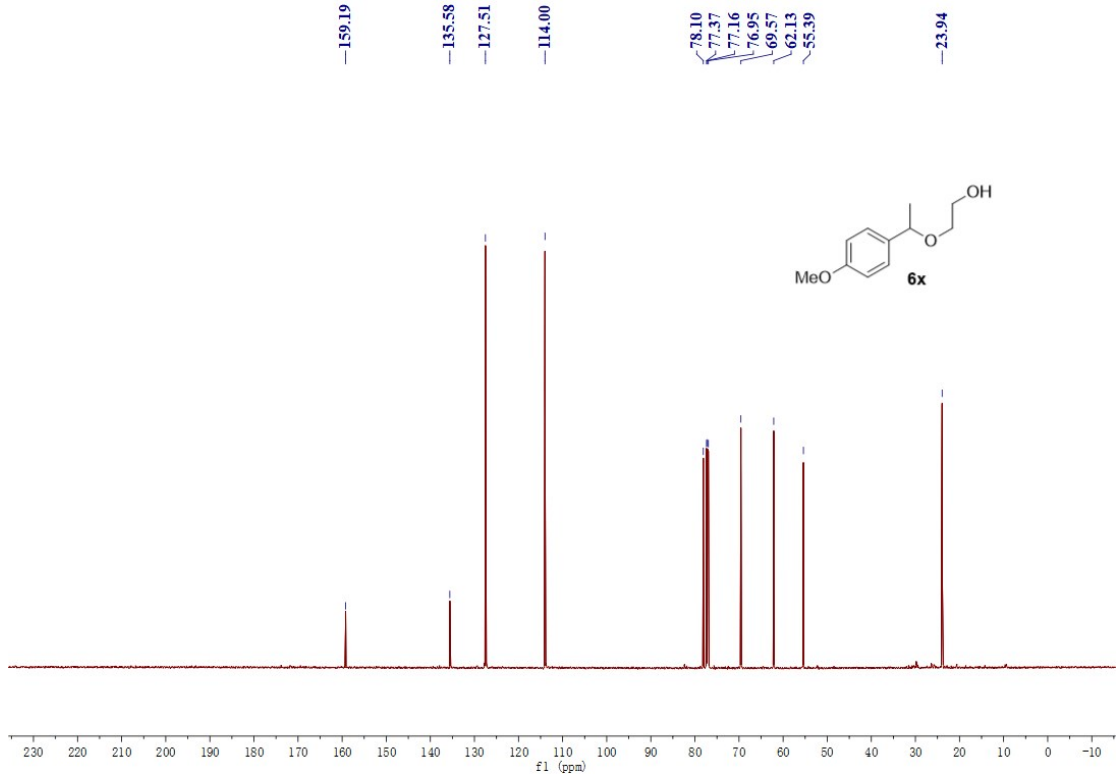
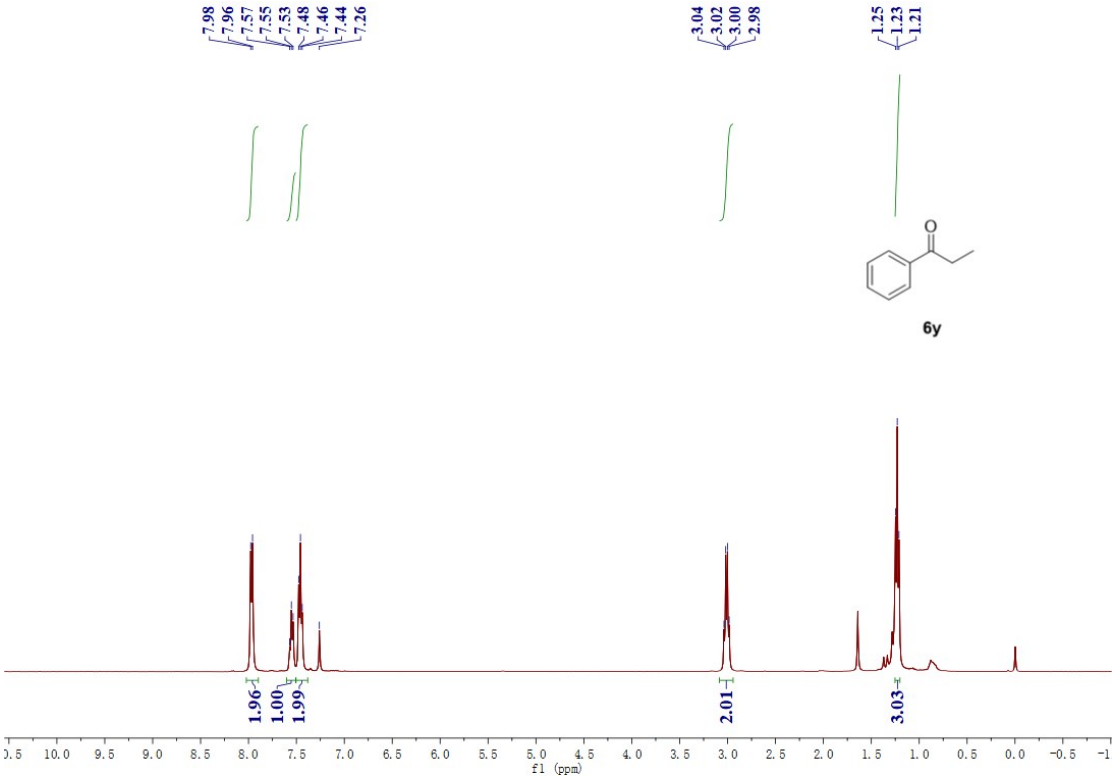
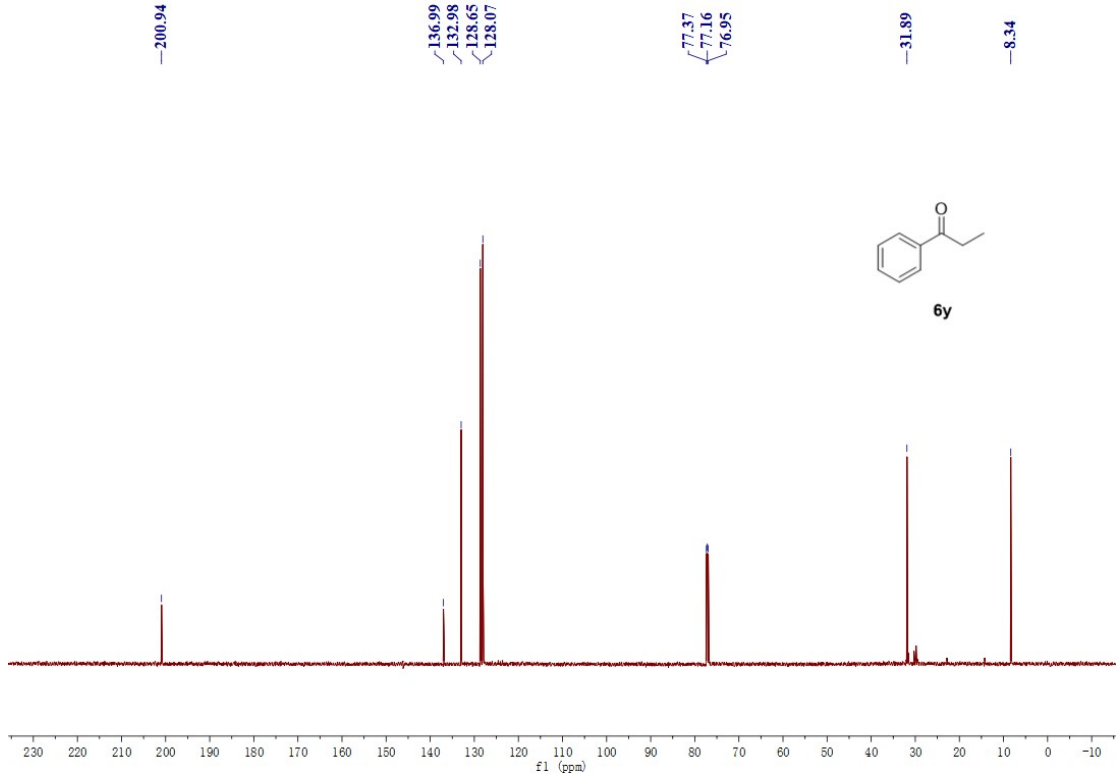
77.16
76.95
55.58
30.61
9.90
OMe
O
N
H
6w
f1 (ppm)


7.26
7.25
7.22
6.90
6.88
4.42
4.40
3.81
3.69
3.68
3.42
3.41
3.40
1.46
1.44
OH
O
MeO
6x
2.00
1.98
1.04
3.16
2.08
2.09
3.28
f1 (ppm)


159.19
135.58
127.51
114.00
78.10
77.37
77.16
76.95
69.57
62.13
55.39
23.94
OH
O
MeO
6x
f1 (ppm)


7.98
7.96
7.57
7.55
7.53
7.48
7.46
7.44
7.26
3.04
3.02
3.00
2.98
1.25
1.23
1.21
O
6y
1.96
1.00
1.99
2.01
3.03
f1 (ppm)


200.94
136.99
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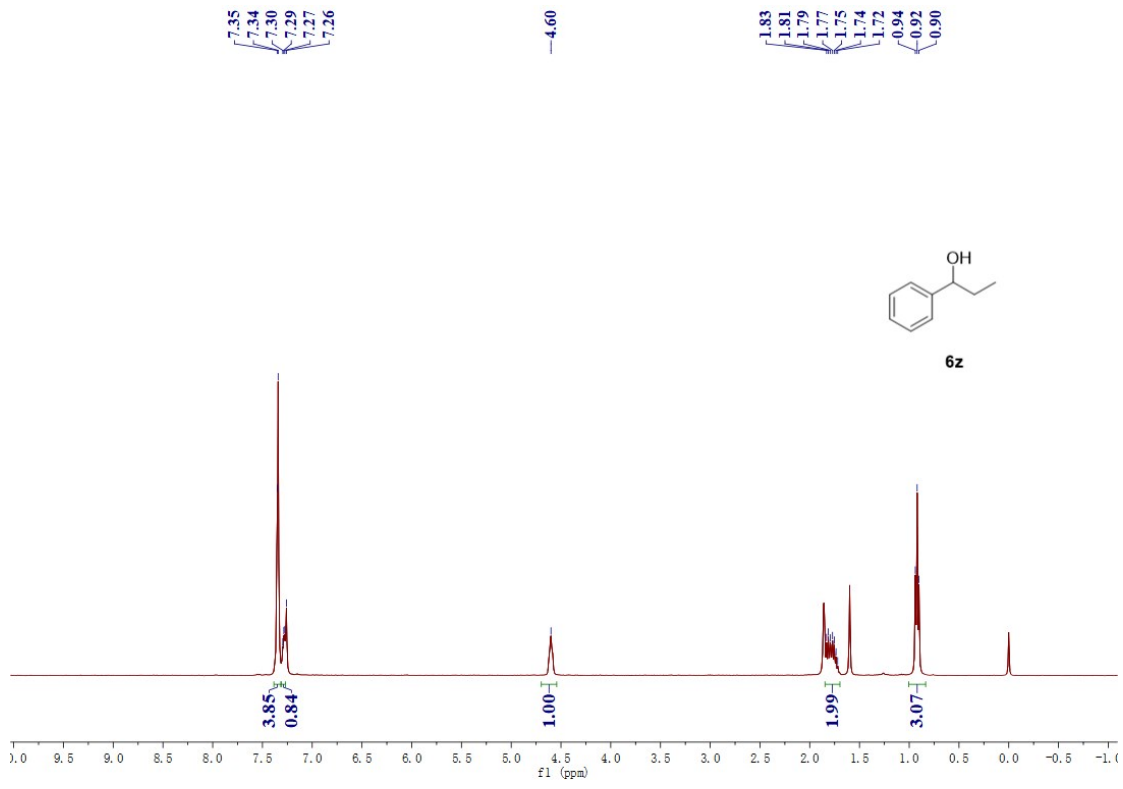
128.65
128.07
77.37
77.16
76.95
31.89
8.34
O
6y
f1 (ppm)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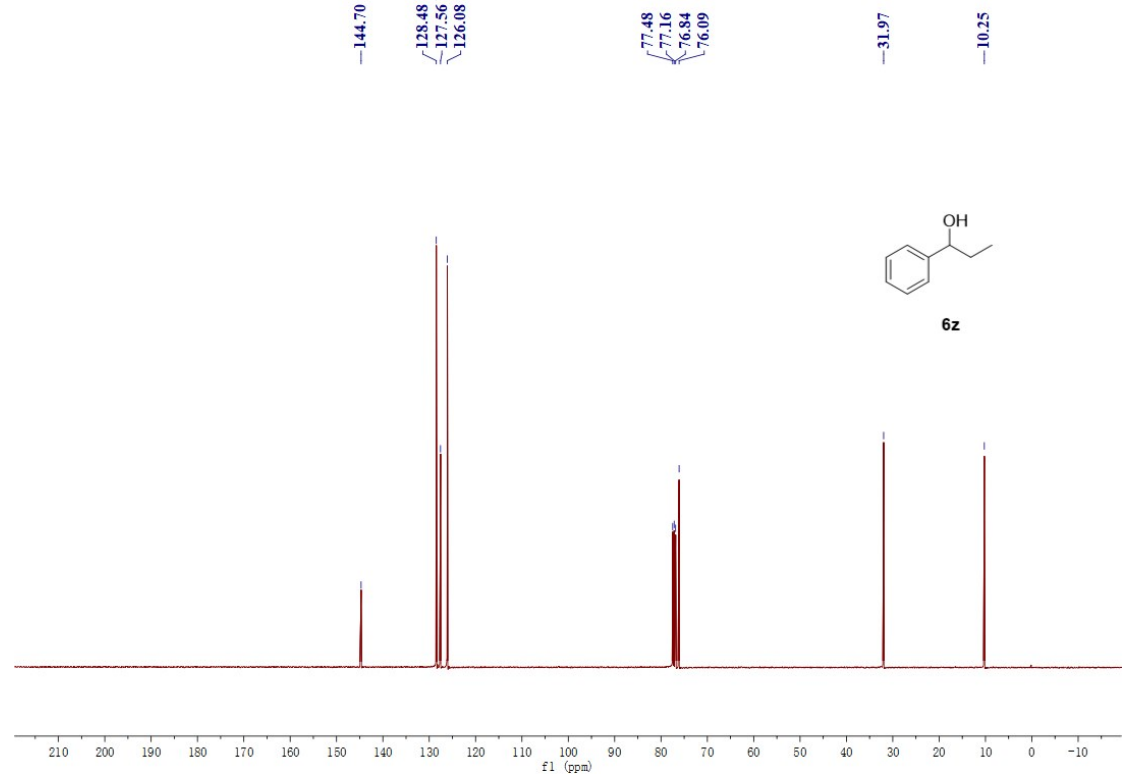
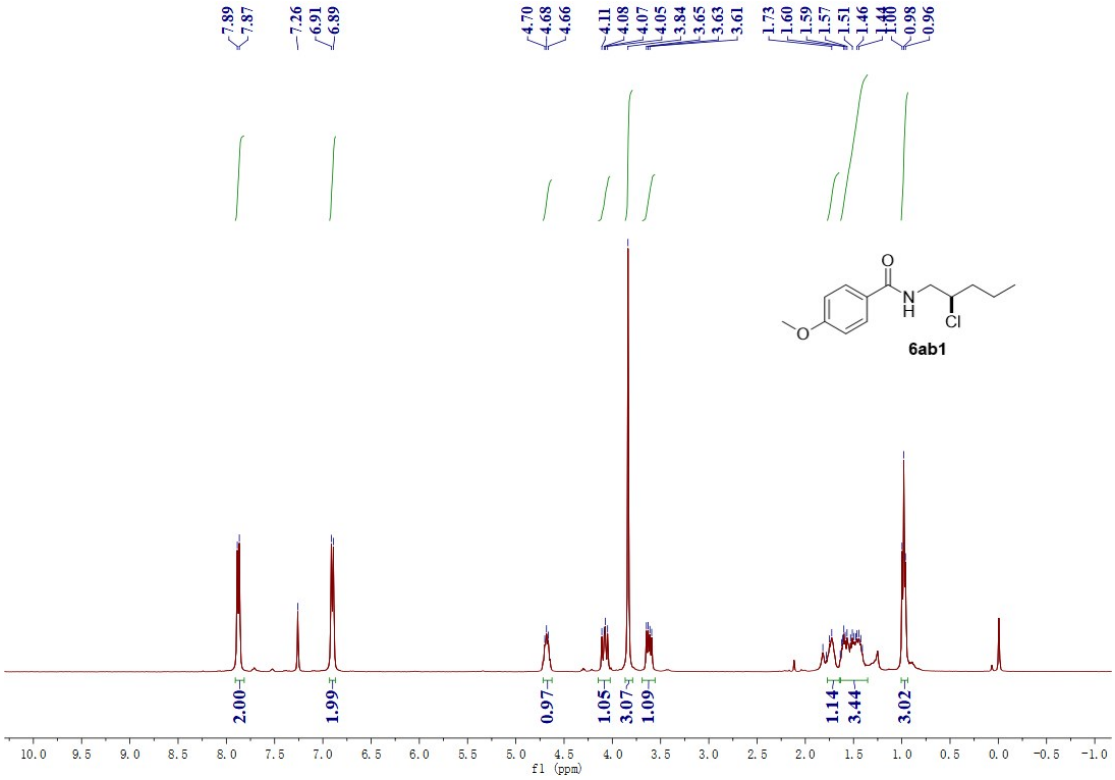
7.34
7.30
7.29
7.27
7.26
4.60
1.83
1.81
1.79
1.77
1.75
1.74
1.72
0.94
0.92
0.90
OH
6z
3.85
0.84
1.00
1.99
3.07
f1 (ppm)


144.70
128.48
127.56
126.08
77.48
77.16
76.84
76.09
31.97
10.25
OH
6z
f1 (ppm)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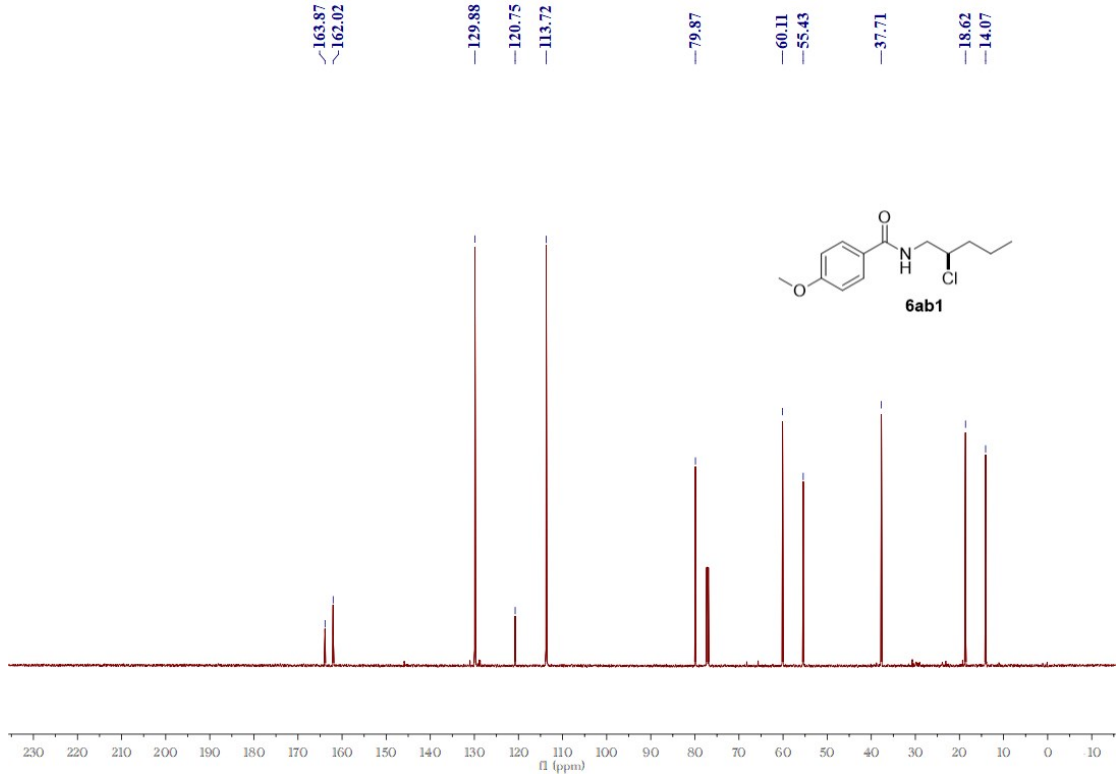
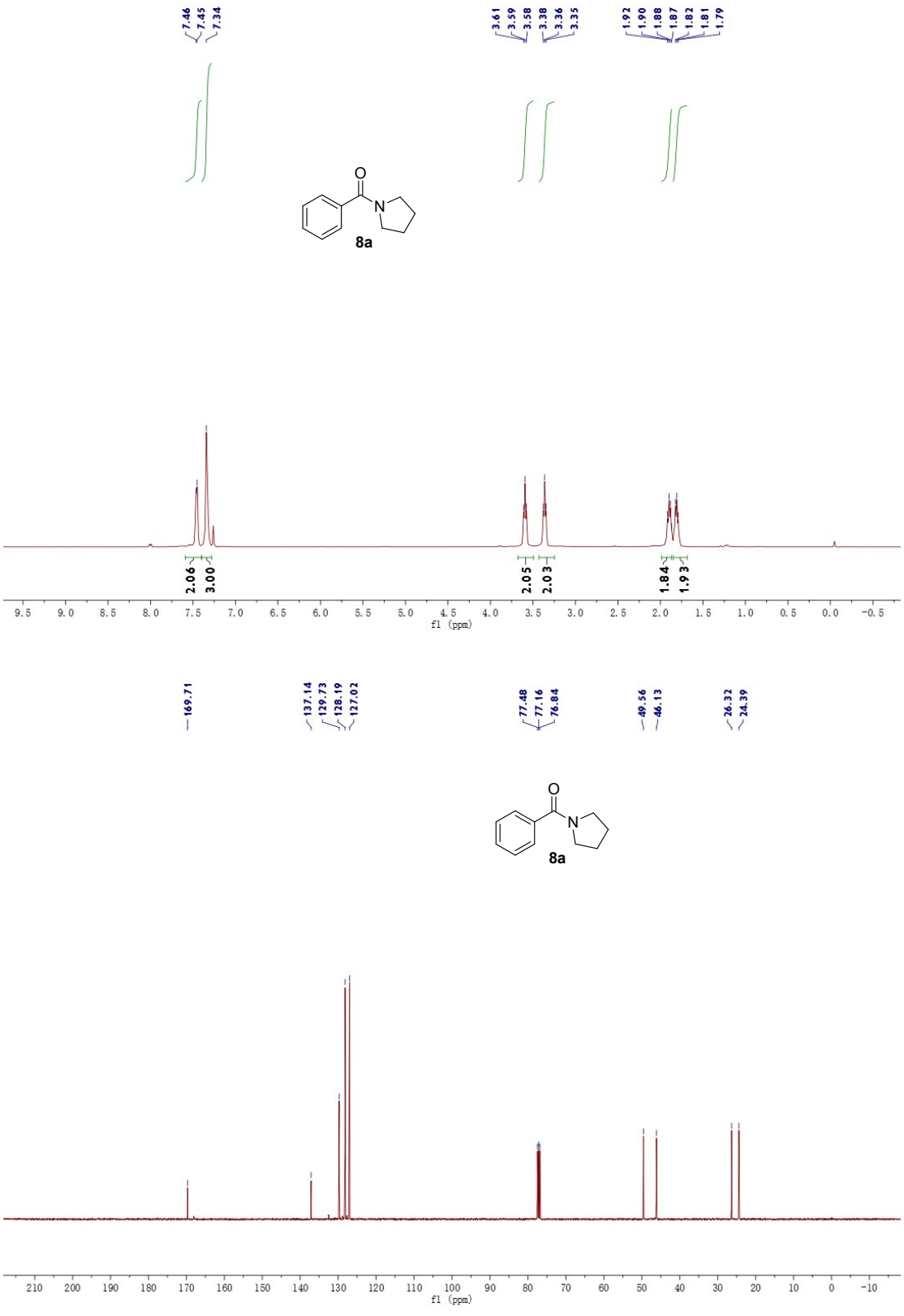
7.26
6.91
6.89
4.70
4.68
4.66
4.11
4.08
4.07
4.05
3.84
3.65
3.63
3.61
1.73
1.60
1.59
1.57
1.51
1.46
0.98
0.96
O
N
H
Cl
O
6ab1
2.00
1.99
0.97
1.05
3.07
1.09
1.14
3.44
3.02
f1 (ppm)


163.87
162.02
129.88
120.75
113.72
79.87
60.11
55.43
37.71
18.62
14.07
O
N
H
Cl
O
6ab1
f1 (ppm)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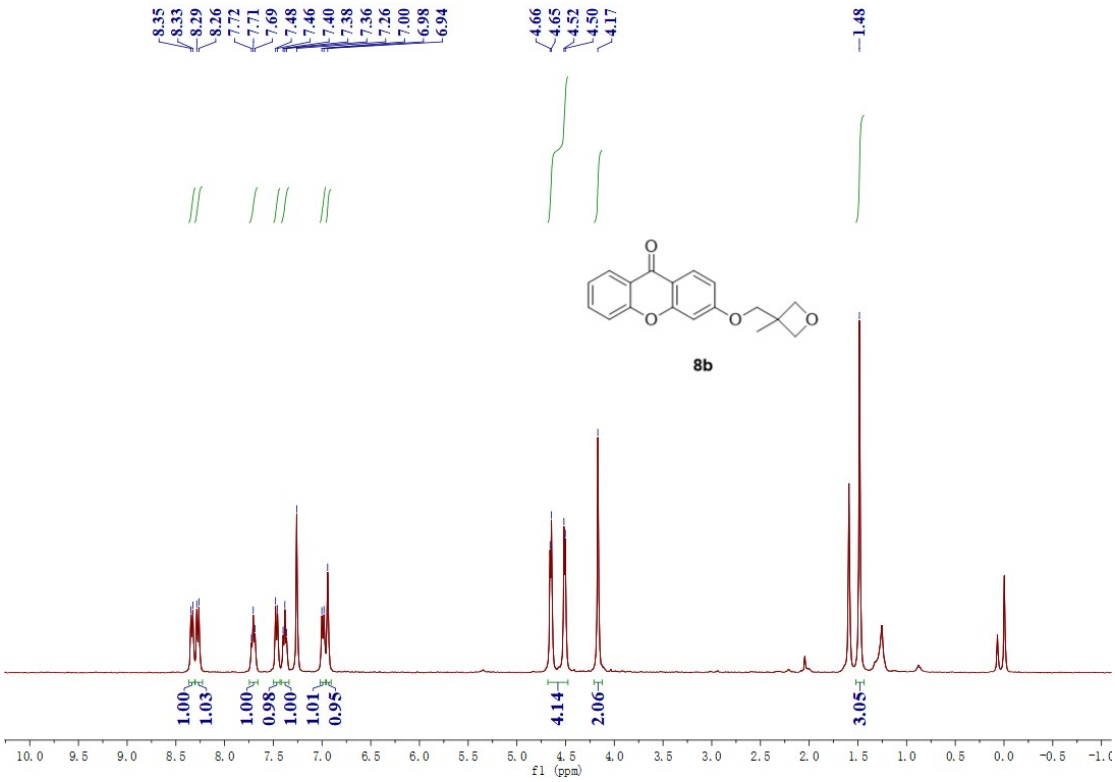
7.45
7.34
3.61
3.59
3.58
3.38
3.36
3.35
1.92
1.90
1.88
1.87
1.82
1.81
1.79
O
N
8a
2.06
3.00
2.05
2.03
1.84
1.93
f1 (ppm)
169.71
137.14
129.73
128.19
127.02
77.48
77.16
76.84
49.56
46.13
26.32
24.39
O
N
8a
f1 (ppm)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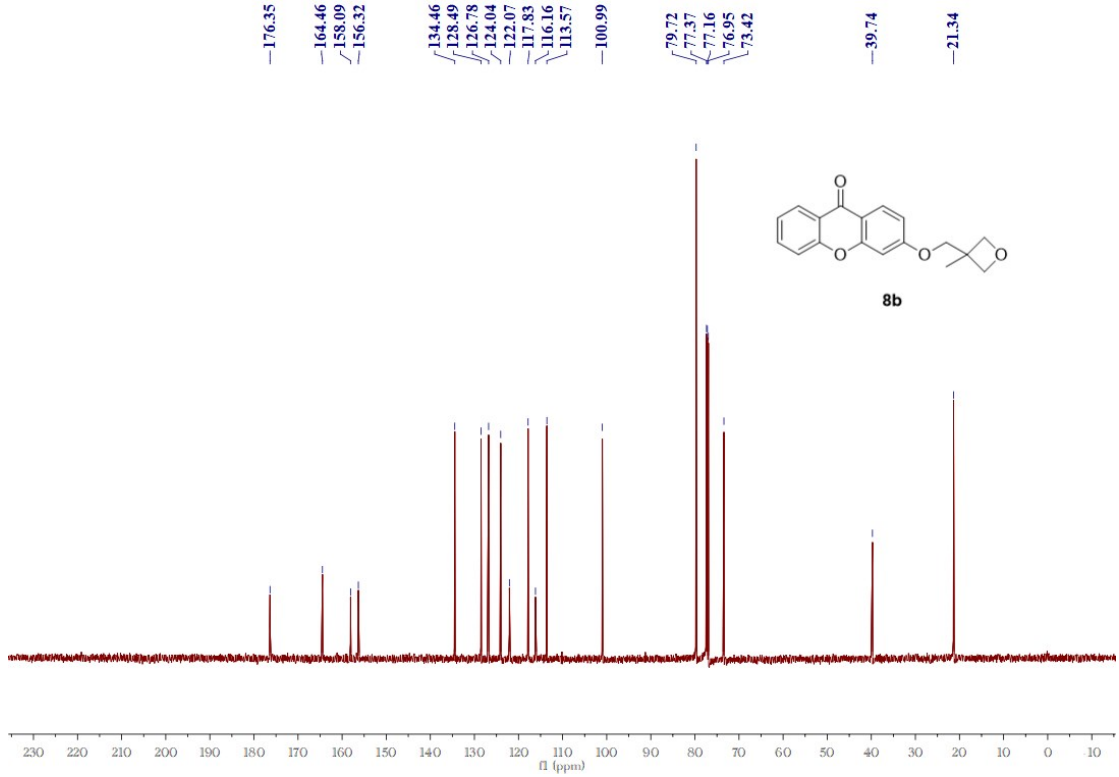
7.46
7.40
7.38
7.36
7.26
7.00
6.98
6.94
4.66
4.65
4.52
4.50
4.17
1.48
8b
1.00
1.03
1.00
0.98
1.00
1.01
0.95
4.14
2.06
3.05
f1 (ppm)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156.32
134.46
128.49
126.78
124.04
122.07
117.83
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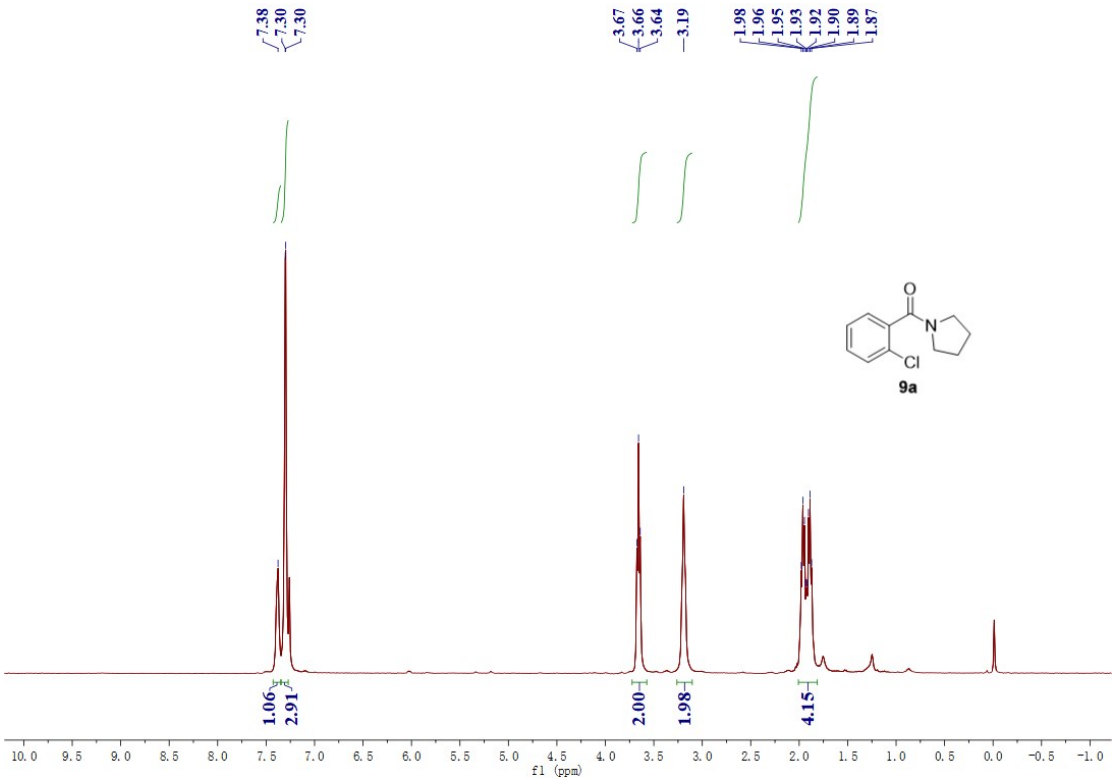
113.57
100.99
79.72
77.37
77.16
76.95
73.42
39.74
21.34
8b
f1 (ppm)


7.38
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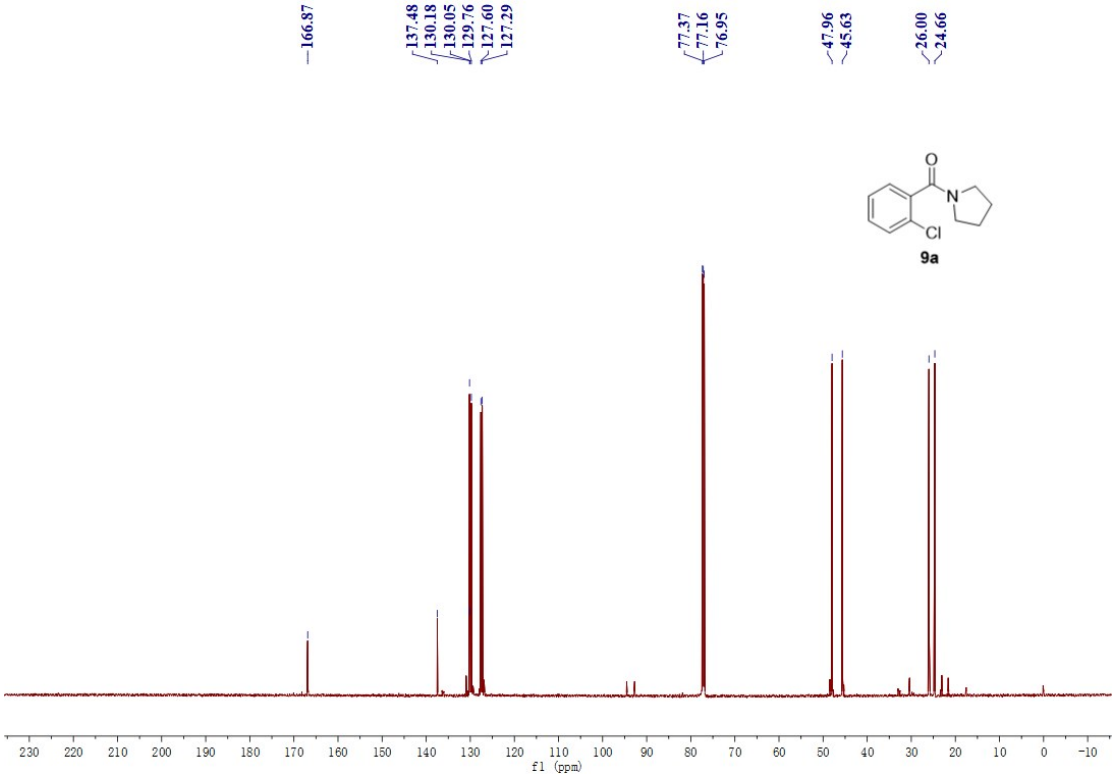
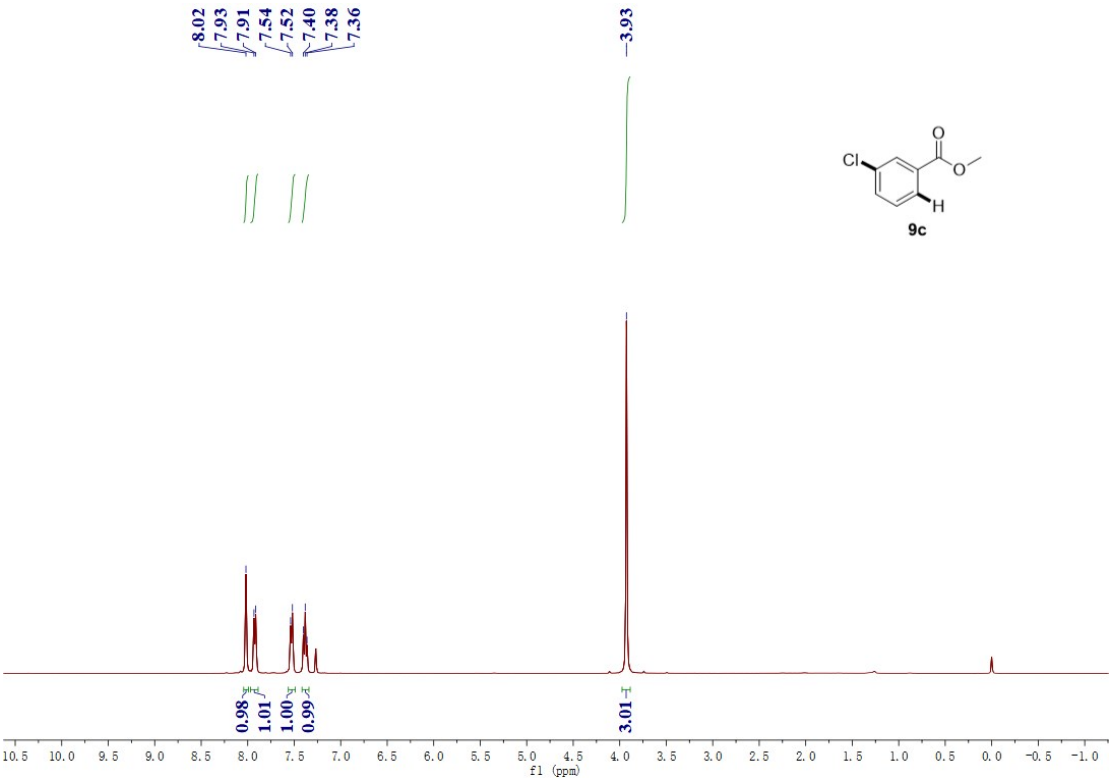
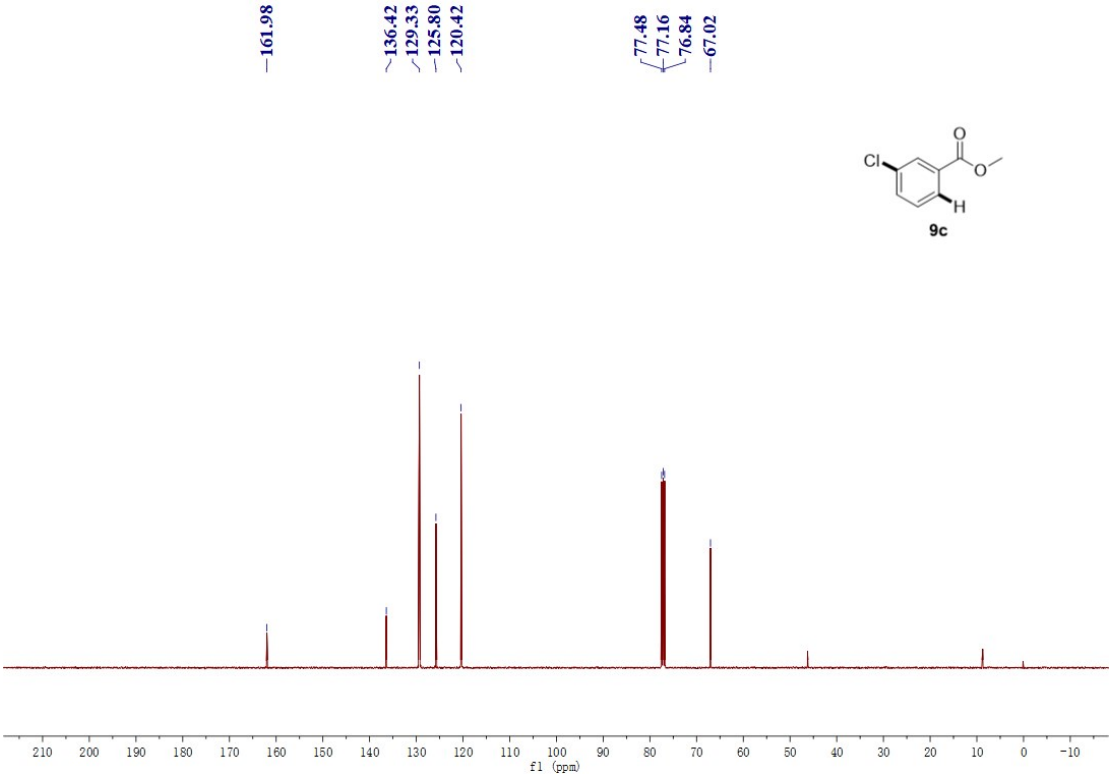
7.30
3.67
3.66
3.64
3.19
1.98
1.96
1.95
1.93
1.92
1.90
1.89
1.87
1.06
2.91
2.00
1.98
4.15
f1 (ppm)
9a


166.87
137.48
130.18
130.05
129.76
127.60
127.29
77.37
77.16
76.95
47.96
45.63
26.00
24.66
f1 (ppm)
9a


8.02
7.93
7.91
7.54
7.52
7.40
7.38
7.36
3.93
Cl
O
O
H
9c
0.98
1.01
1.00
0.99
3.01
f1 (ppm)


161.98
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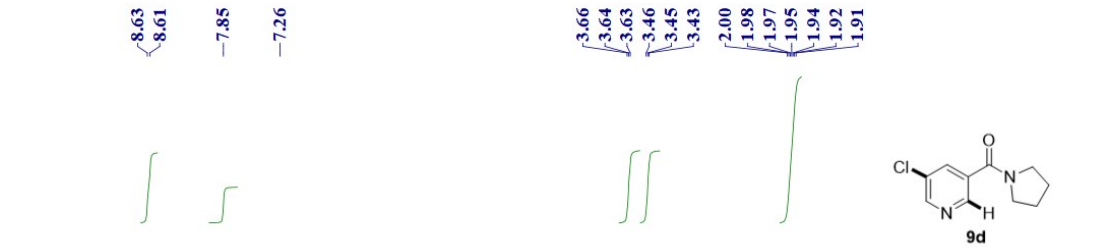
120.42
77.48
77.16
76.84
67.02
Cl
O
O
H
9c
f1 (ppm)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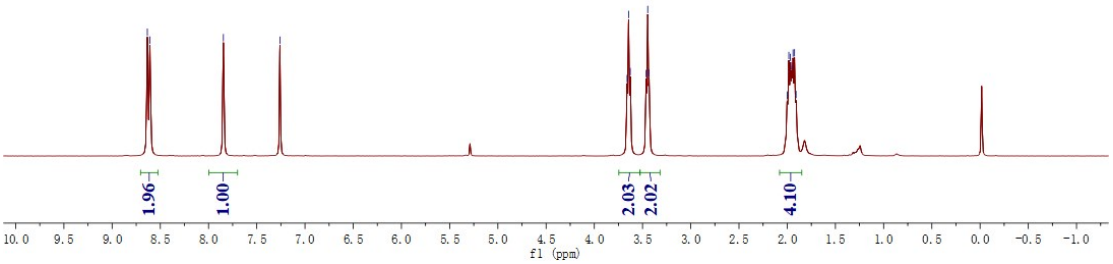
7.26
3.66
3.64
3.63
3.46
3.45
3.43
2.00
1.98
1.97
1.95
1.94
1.92
1.91
Cl
O
N
N
H
9d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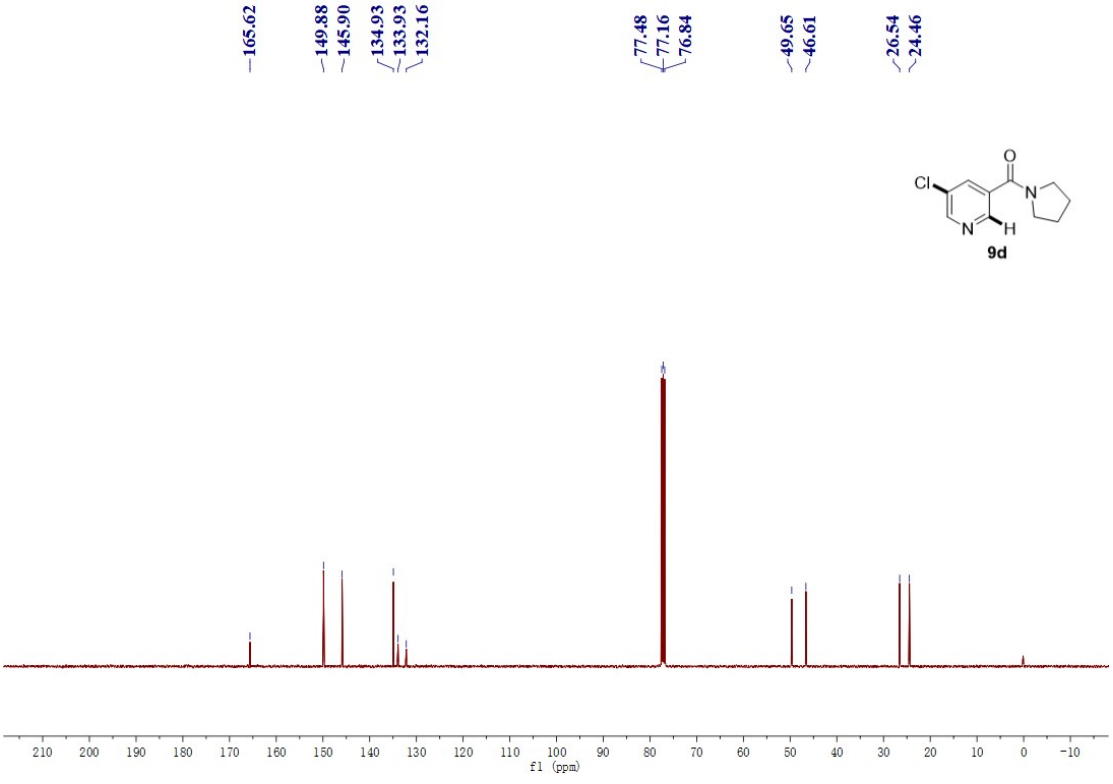
2.02
4.10
f1 (ppm)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133.93
132.16
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77.16
76.84
49.65
46.61
26.54
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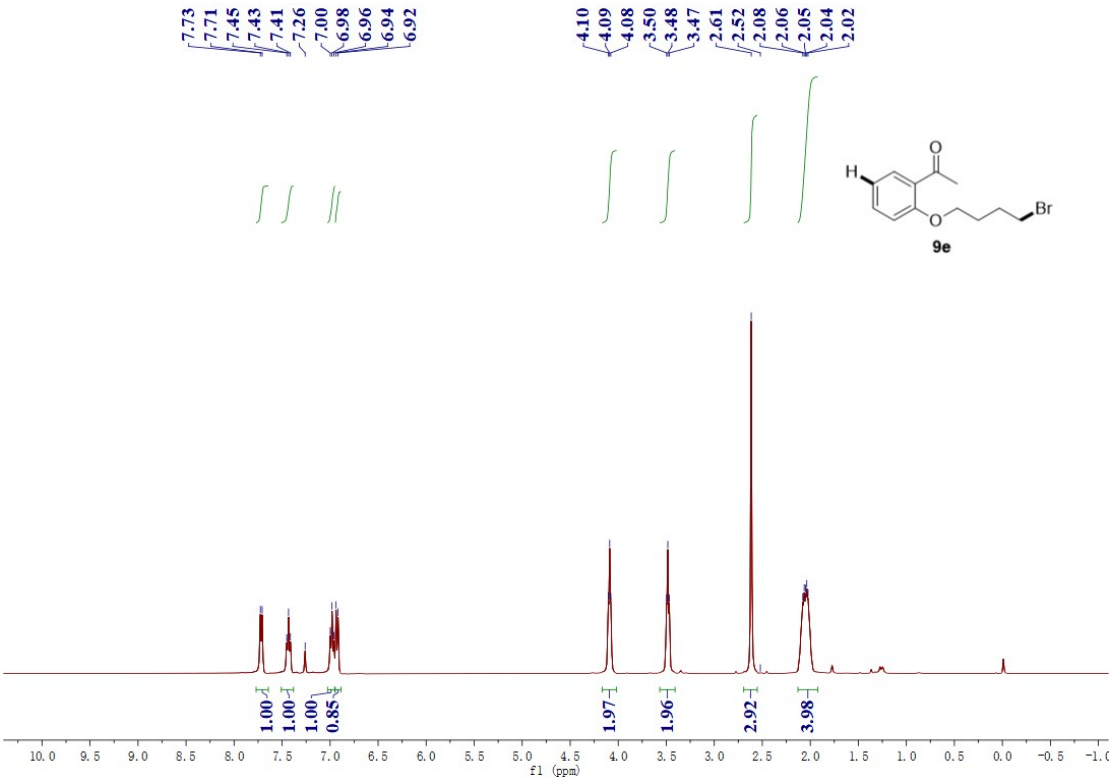
Cl
O
N
N
H
9d
f1 (ppm)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7.41
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7.00
6.98
6.96
6.94
6.92
4.10
4.09
4.08
3.50
3.48
3.47
2.61
2.52
2.08
2.06
2.05
2.04
2.02
O
H
Br
O
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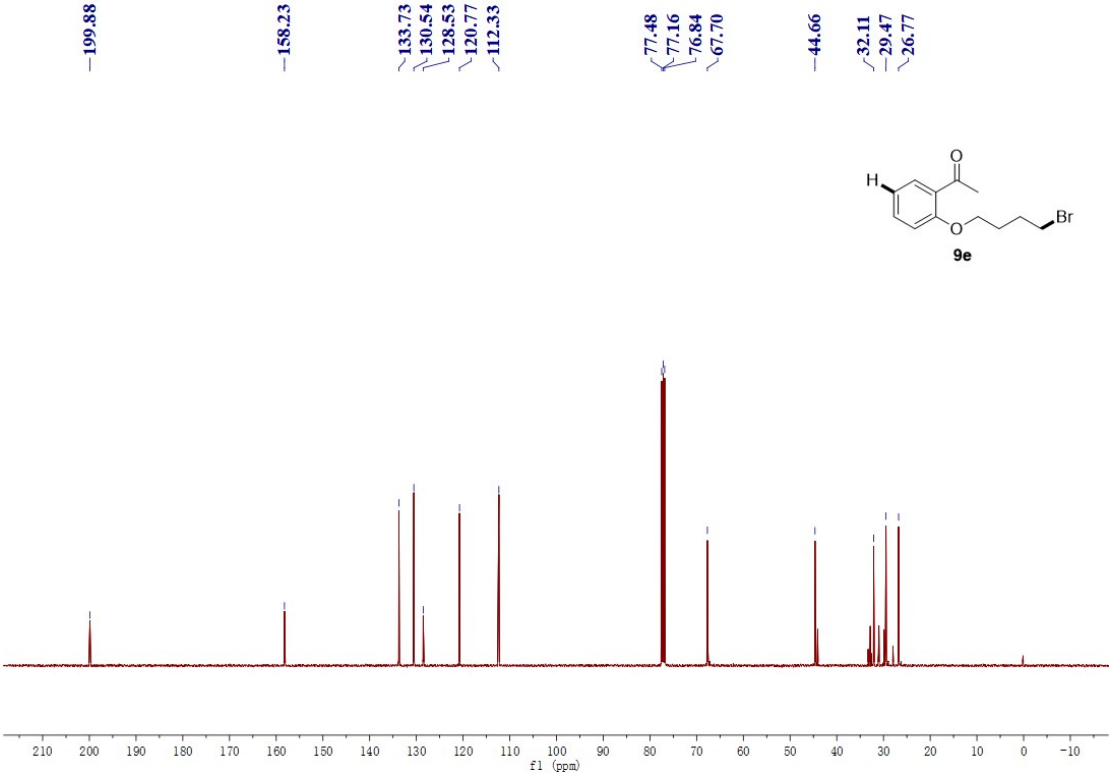
1.00
1.00
1.00
0.85
1.97
1.96
2.92
3.98
f1 (ppm)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128.53
120.77
112.33
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77.16
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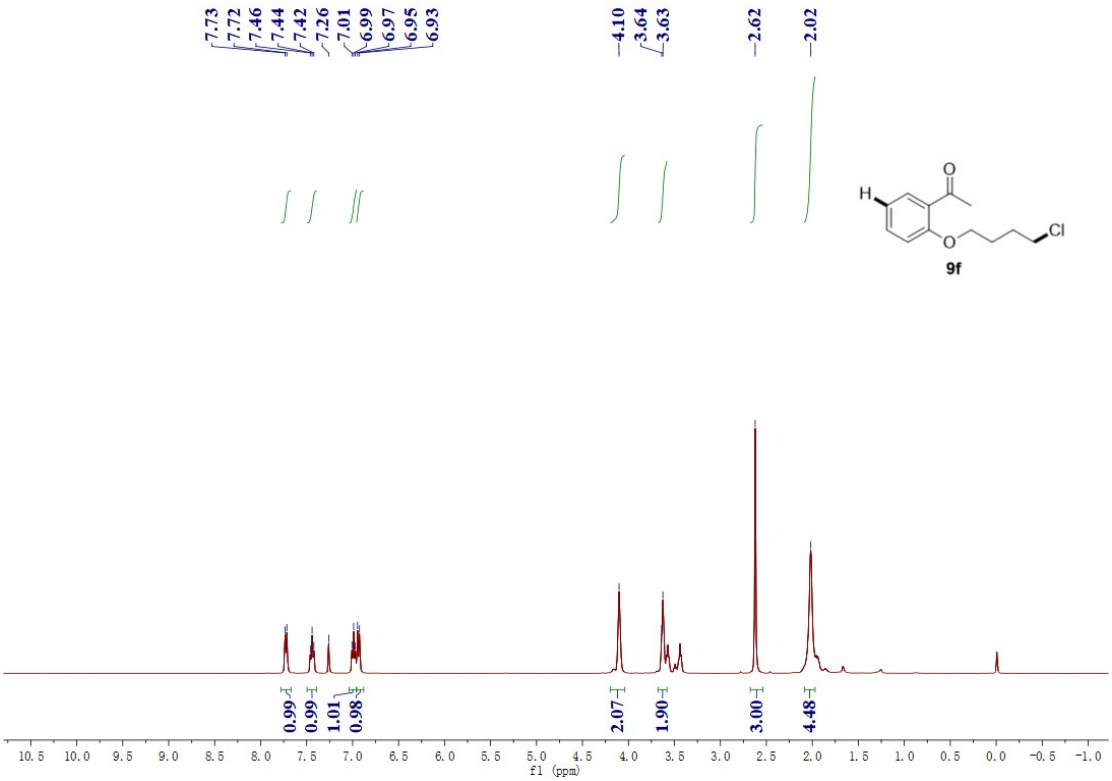
67.70
44.66
32.11
29.47
26.77
O
H
Br
O
9e
f1 (ppm)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7.42
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7.01
6.99
6.97
6.95
6.93
4.10
3.64
3.63
2.62
2.02
O
H
O
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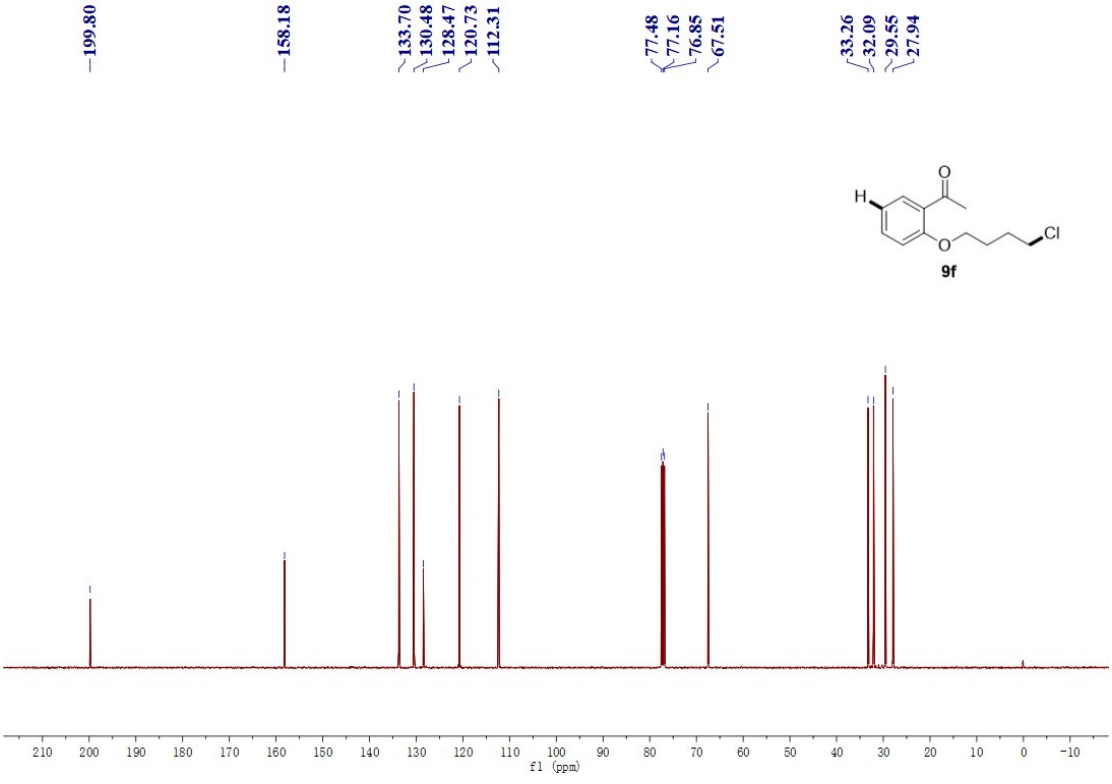
9f
0.99
0.99
1.01
0.98
2.07
1.90
3.00
4.48
f1 (ppm)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128.47
120.73
112.31
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77.16
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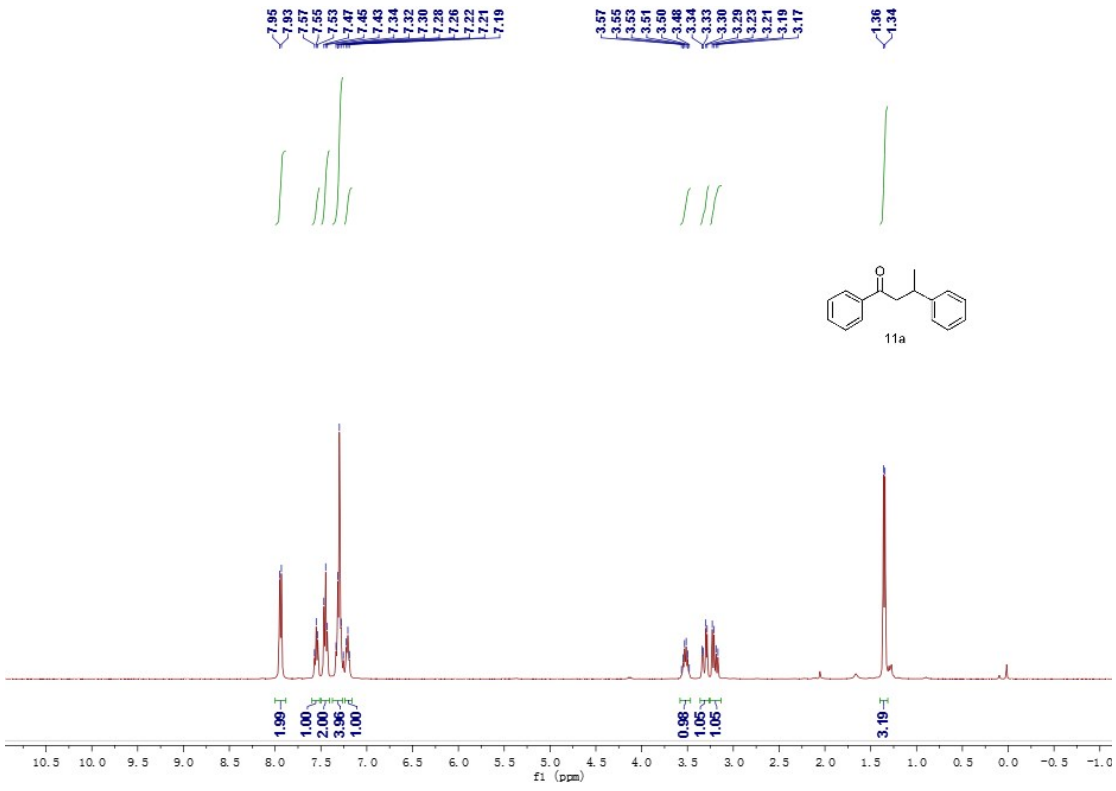
67.51
33.26
32.09
29.55
27.94
O
H
O
Cl
9f
f1 (ppm)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7.45
7.43
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7.32
7.30
7.28
7.26
7.22
7.21
7.19
3.57
3.55
3.53
3.51
3.50
3.48
3.34
3.33
3.30
3.29
3.23
3.21
3.19
3.17
1.36
1.34
11a
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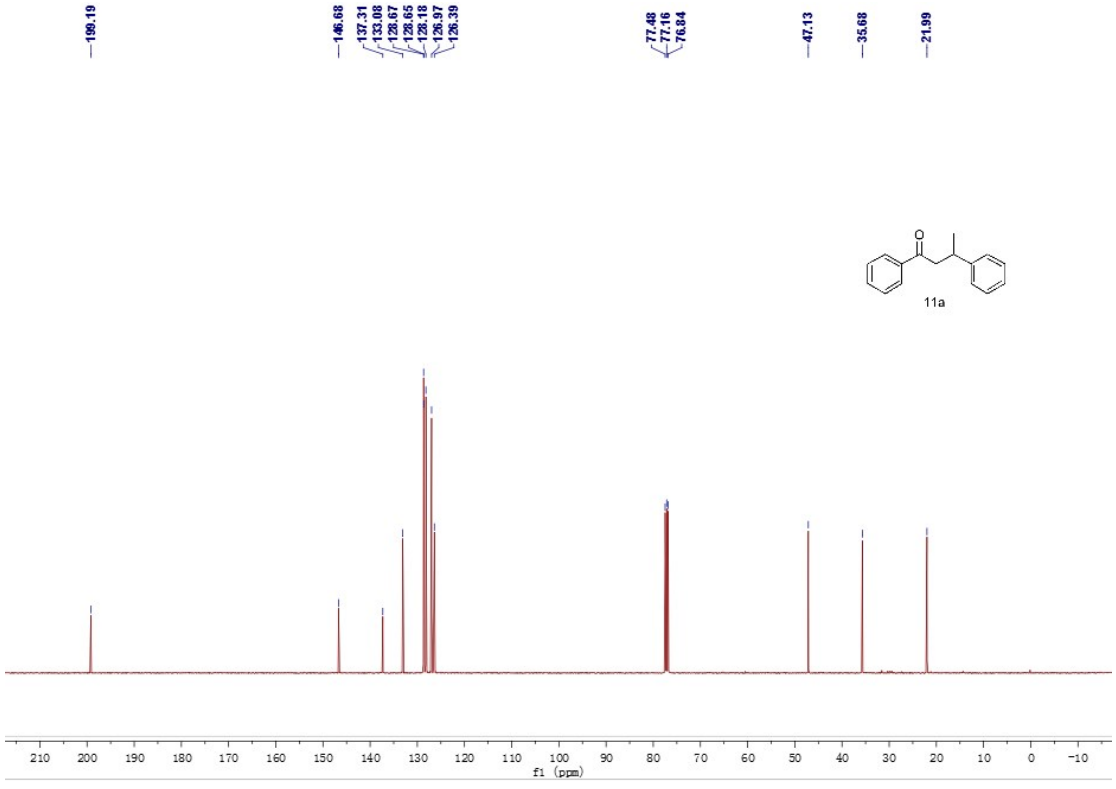
1.00
2.00
3.96
1.00
0.98
1.05
1.05
3.19
f1 (ppm)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128.18
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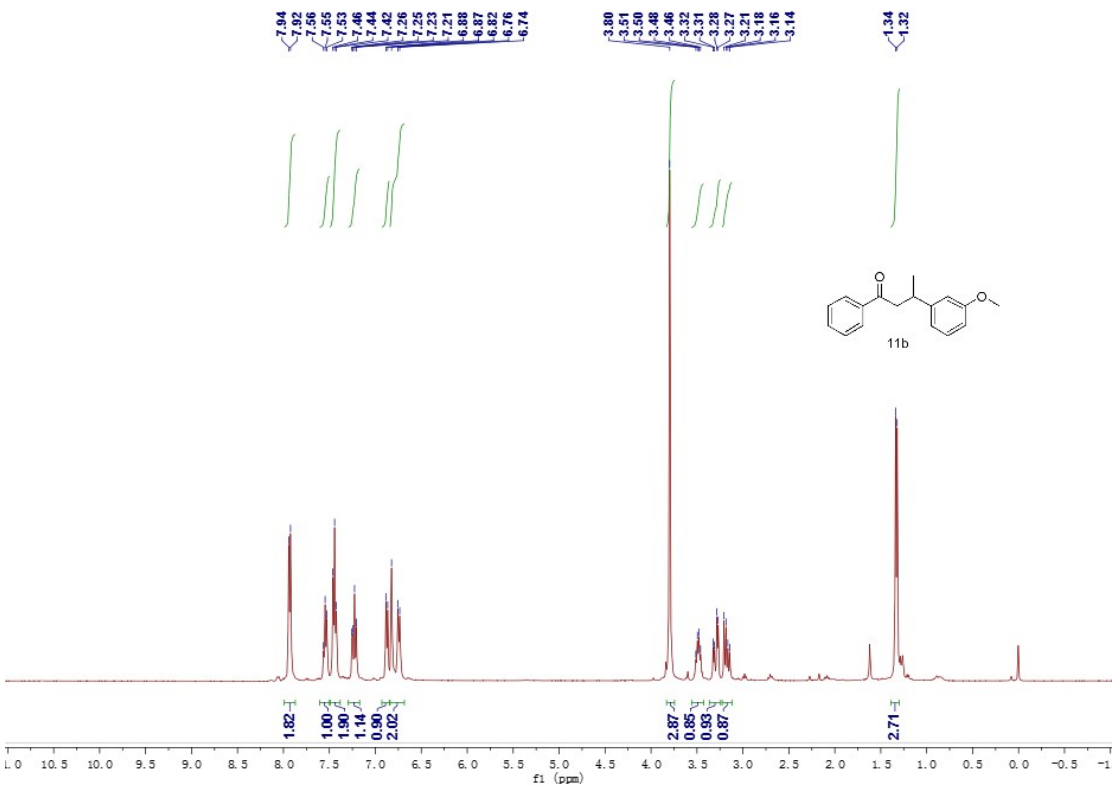
77.48
77.16
76.84
47.13
35.68
21.99
11a
f1 (ppm)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6.88
6.87
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3.51
3.50
3.48
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3.31
3.28
3.27
3.21
3.18
3.16
3.14
1.34
1.32
11b
1.82
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1.14
0.90
2.02
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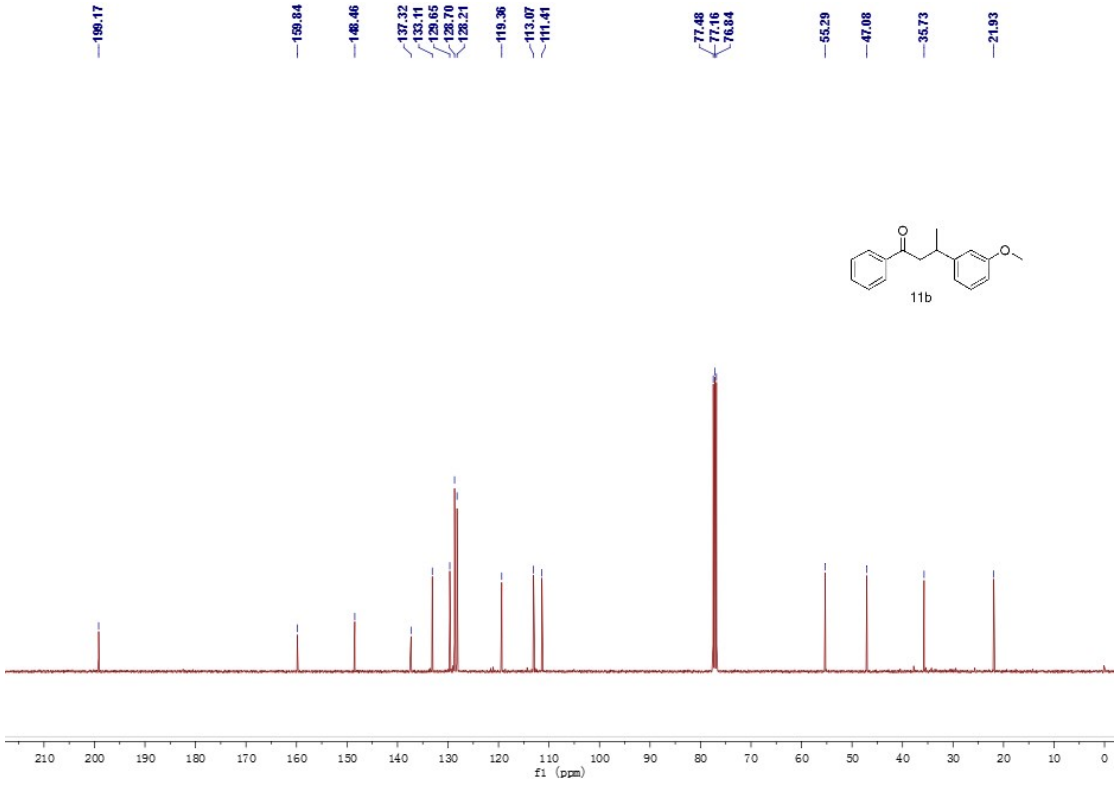
0.85
0.93
0.87
2.71
f1 (ppm)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128.70
128.21
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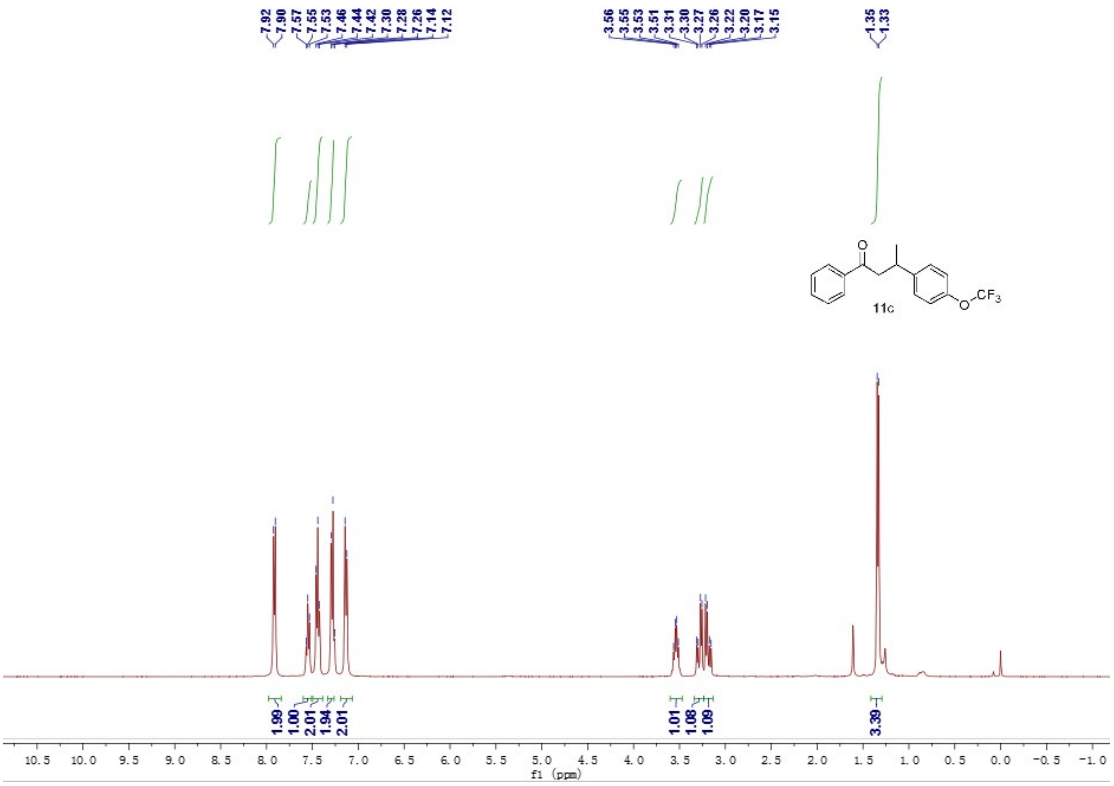
77.16
76.84
55.29
47.08
35.73
21.93
11b
f1 (ppm)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7.26
7.14
7.12
3.56
3.55
3.53
3.51
3.31
3.30
3.27
3.26
3.22
3.20
3.17
3.15
1.35
1.33
O
CF3
11c
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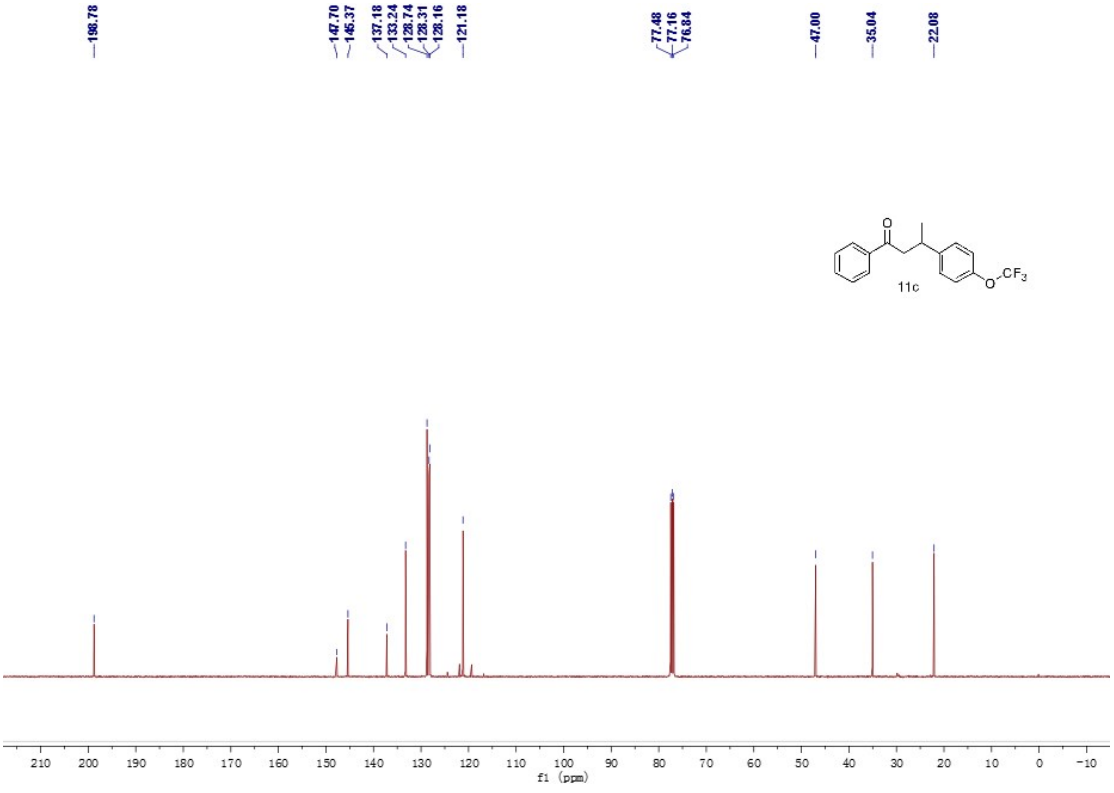
1.00
2.01
1.94
2.01
1.01
1.08
1.09
3.39
f1 (ppm)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47.00
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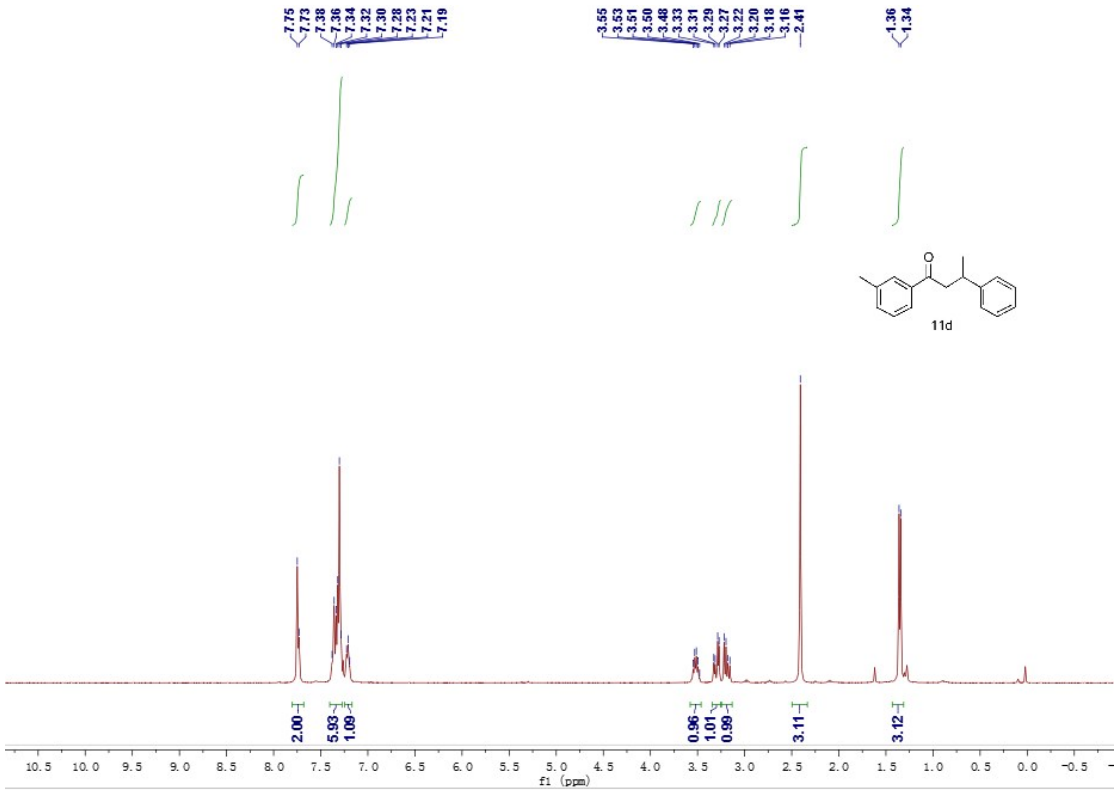
22.08
O
CF3
11c
f1 (ppm)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3.51
3.50
3.48
3.33
3.31
3.29
3.27
3.22
3.20
3.18
3.16
2.41
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1.34
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2.00
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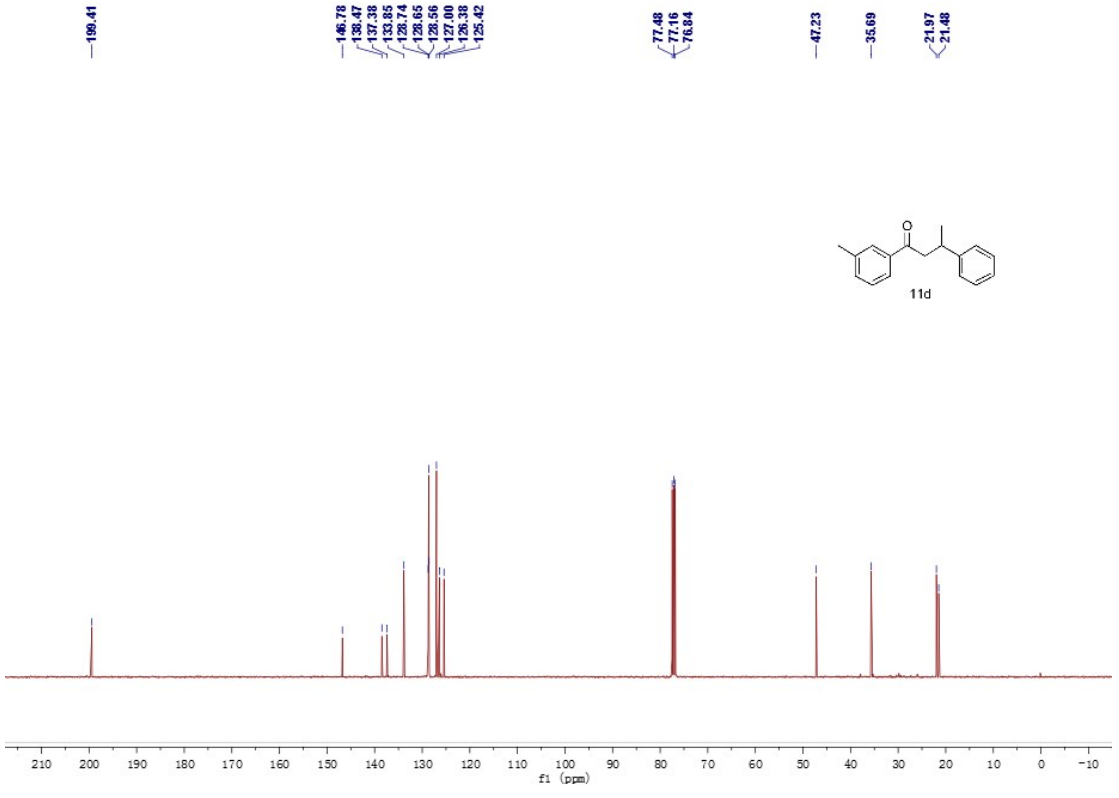
1.09
0.96
1.01
0.99
3.11
3.12
f1 (ppm)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128.56
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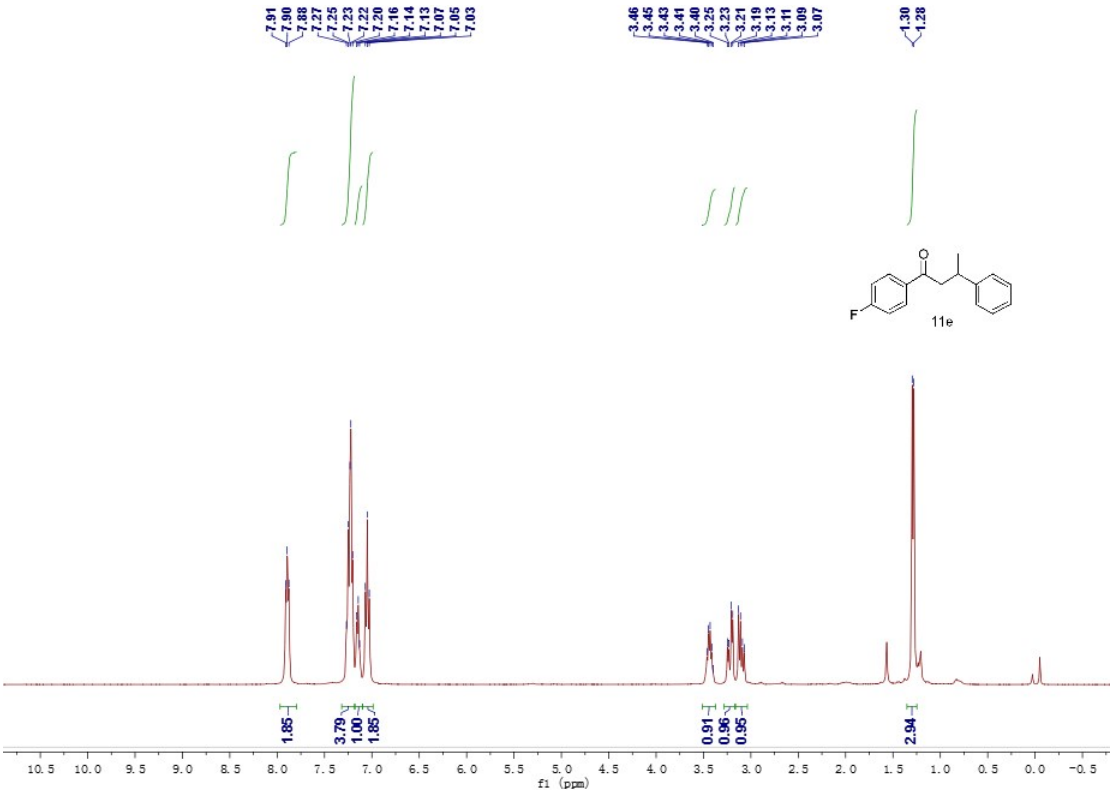
47.23
35.69
21.97
21.48
11d
f1 (ppm)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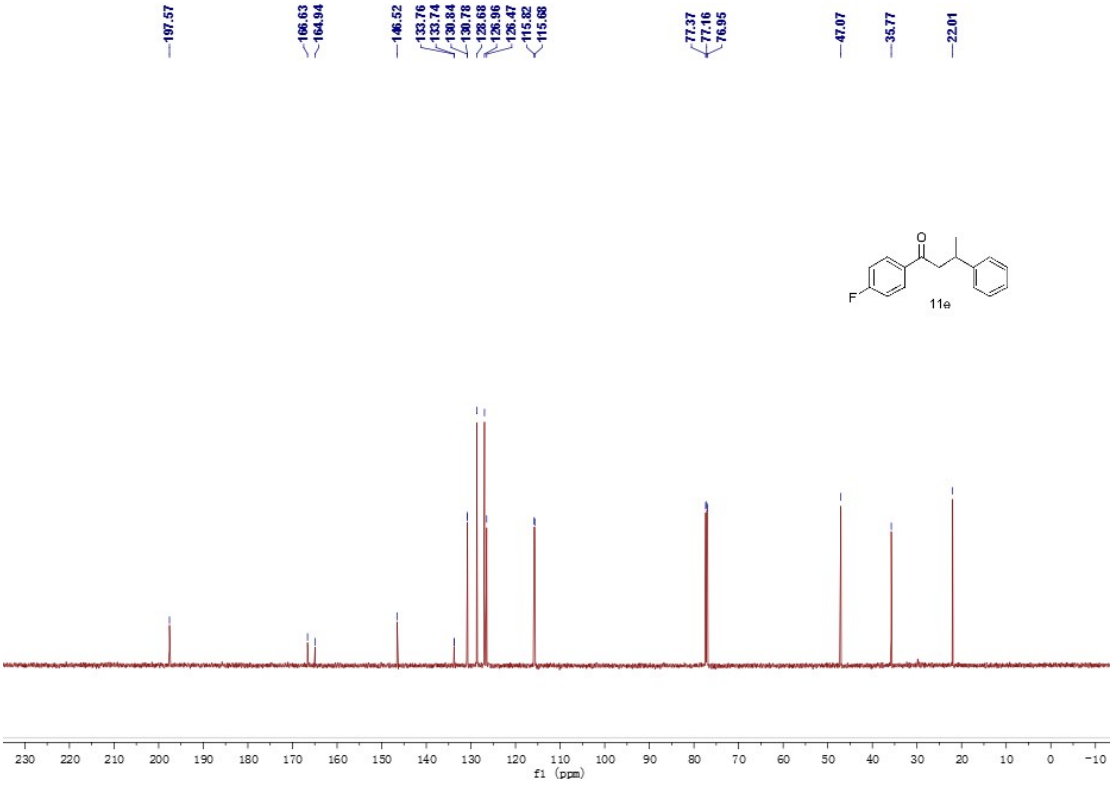
7.20
7.16
7.14
7.13
7.07
7.05
7.03
3.46
3.45
3.43
3.41
3.40
3.25
3.23
3.21
3.19
3.13
3.11
3.09
3.07
1.30
1.28
F
O
11e
1.85
3.79
1.00
1.85
0.91
0.96
0.95
2.94
f1 (ppm)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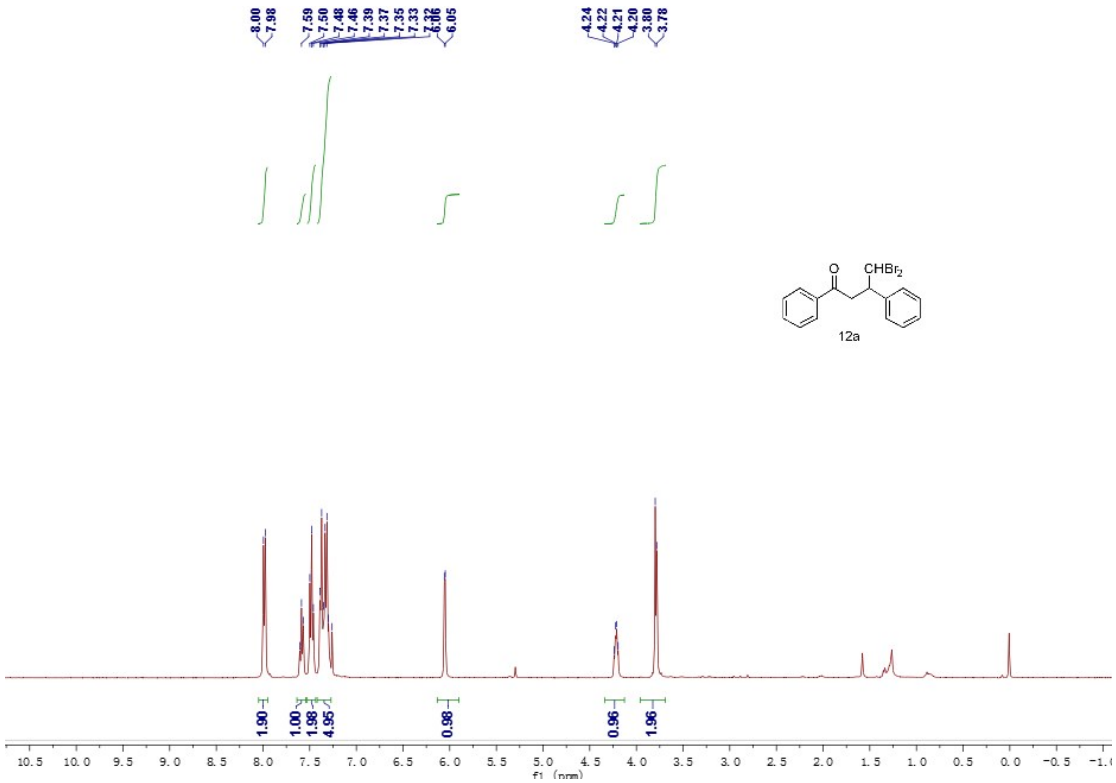
77.37
77.16
76.95
47.07
35.77
22.01
F
O
11e
f1 (ppm)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7.37
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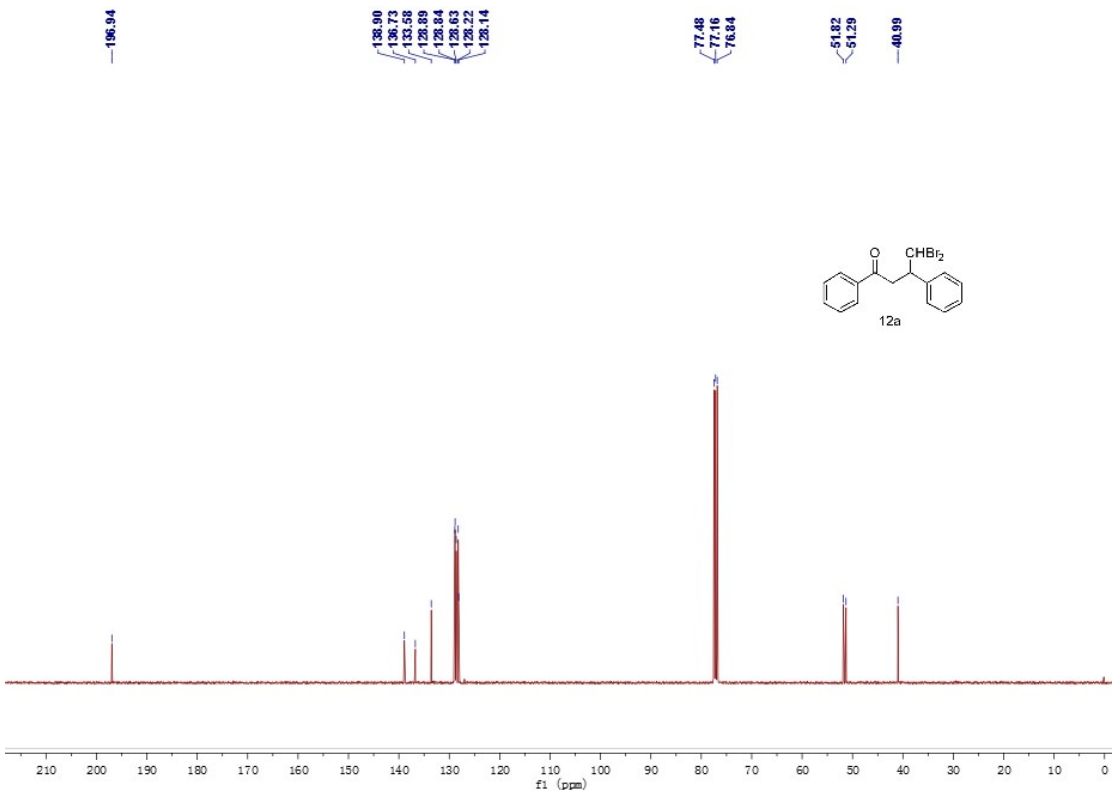
7.33
7.32
6.06
6.05
4.24
4.22
4.21
4.20
3.80
3.78
O
CHBr2
12a
1.90
1.00
1.98
4.95
0.98
0.96
1.96
f1 (ppm)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128.84
128.63
128.22
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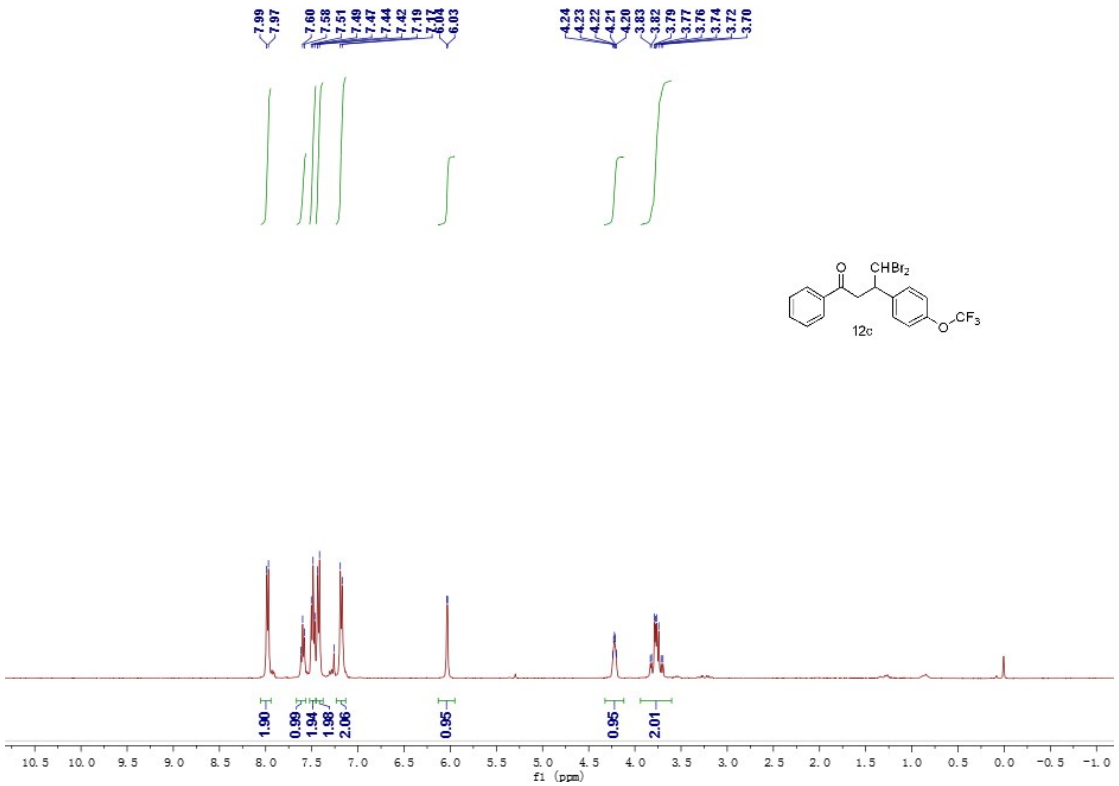
77.16
76.84
51.82
51.29
40.99
O
CHBr2
12a
f1 (ppm)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7.44
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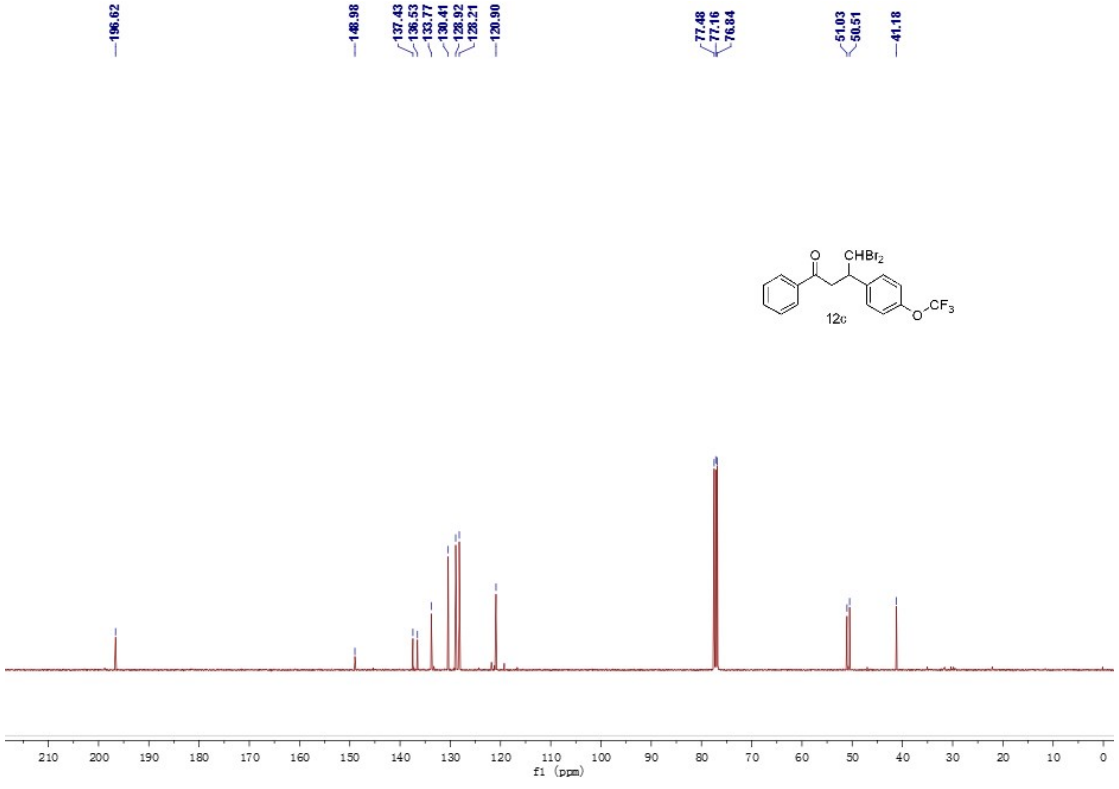
7.19
7.17
6.04
6.03
4.24
4.23
4.22
4.21
4.20
3.83
3.82
3.79
3.77
3.76
3.74
3.72
3.70
CHBr2
CF3
12c
1.90
0.99
1.94
1.98
2.06
0.95
0.95
2.01
f1 (ppm)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77.16
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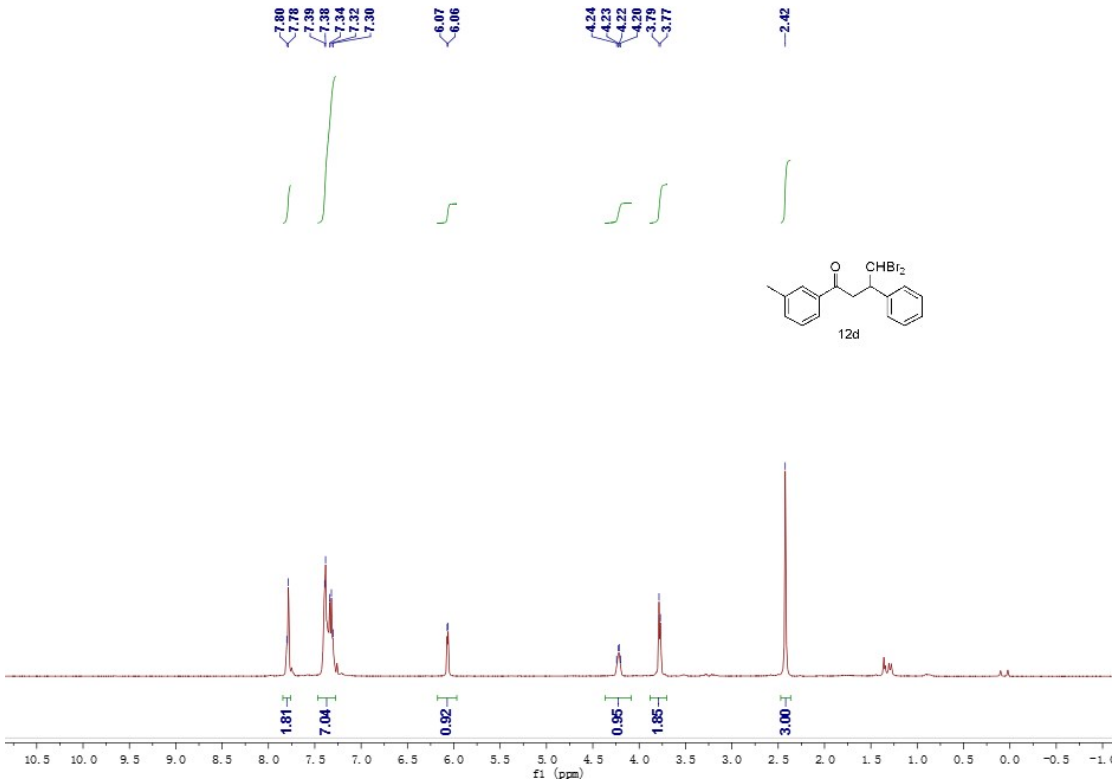
41.18
CHBr2
CF3
12c
f1 (ppm)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7.34
7.32
7.30
6.07
6.06
4.24
4.23
4.22
4.20
3.79
3.77
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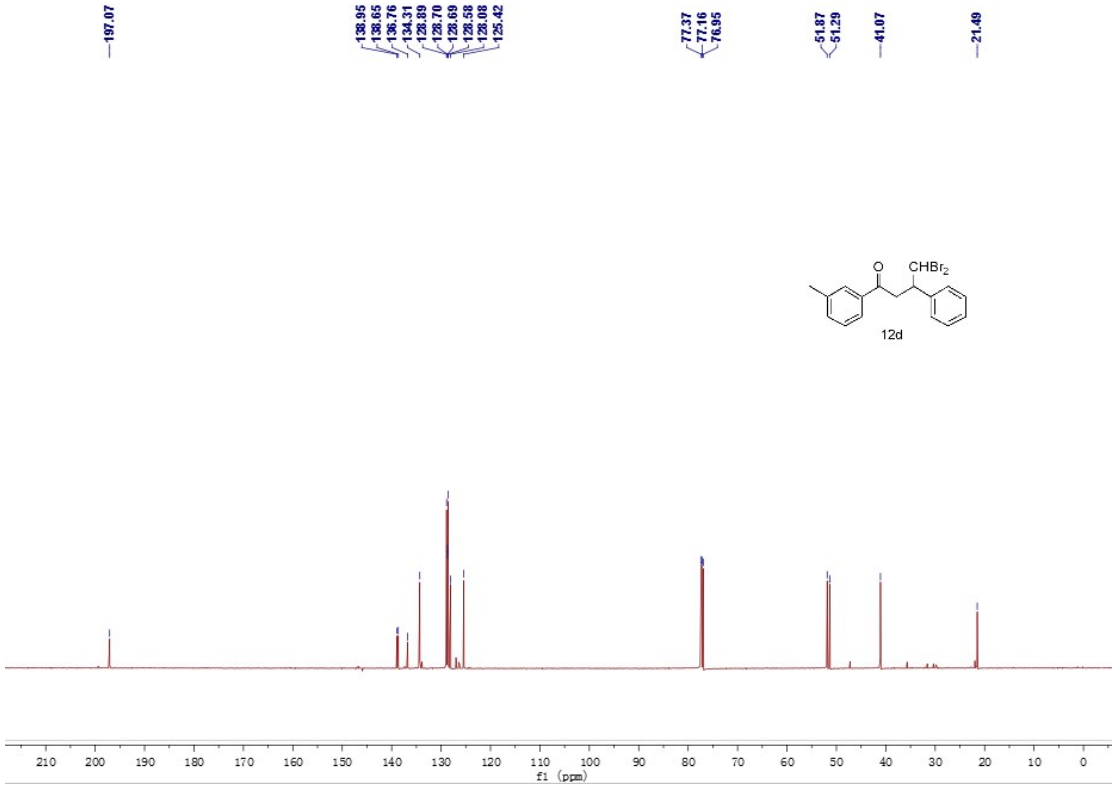
O
CHBr2
12d
1.81
7.04
0.92
0.95
1.85
3.00
f1 (ppm)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128.89
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128.69
128.58
128.08
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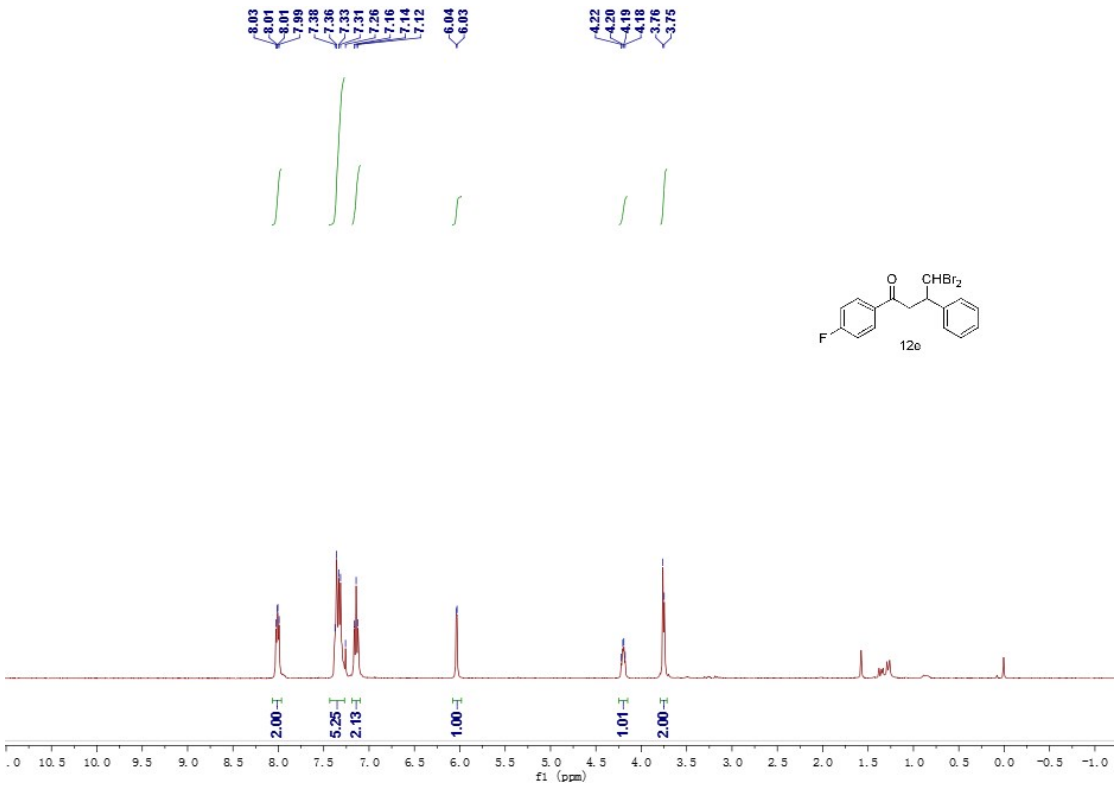
77.16
76.95
51.87
51.29
41.07
21.49
O
CHBr2
12d
f1 (ppm)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7.31
7.26
7.16
7.14
7.12
6.04
6.03
4.22
4.20
4.19
4.18
3.76
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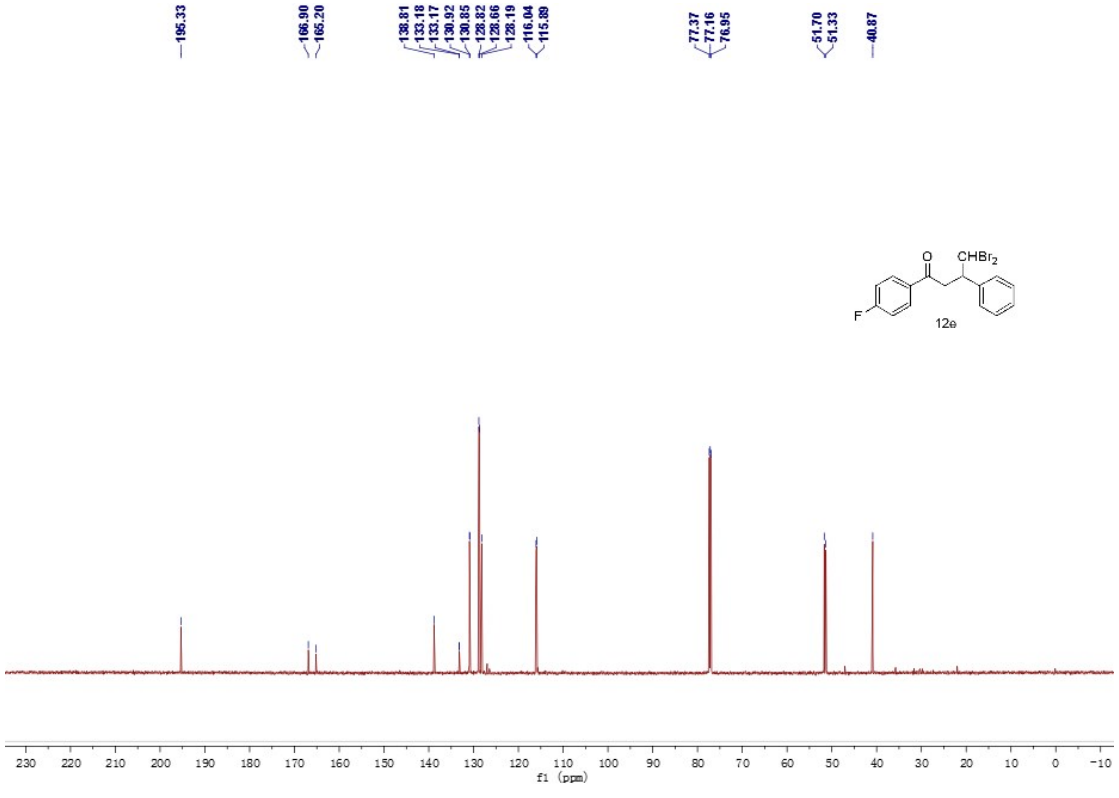
CHBr2
F
12e
2.00
5.25
2.13
1.00
1.01
2.00
f1 (ppm)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128.19
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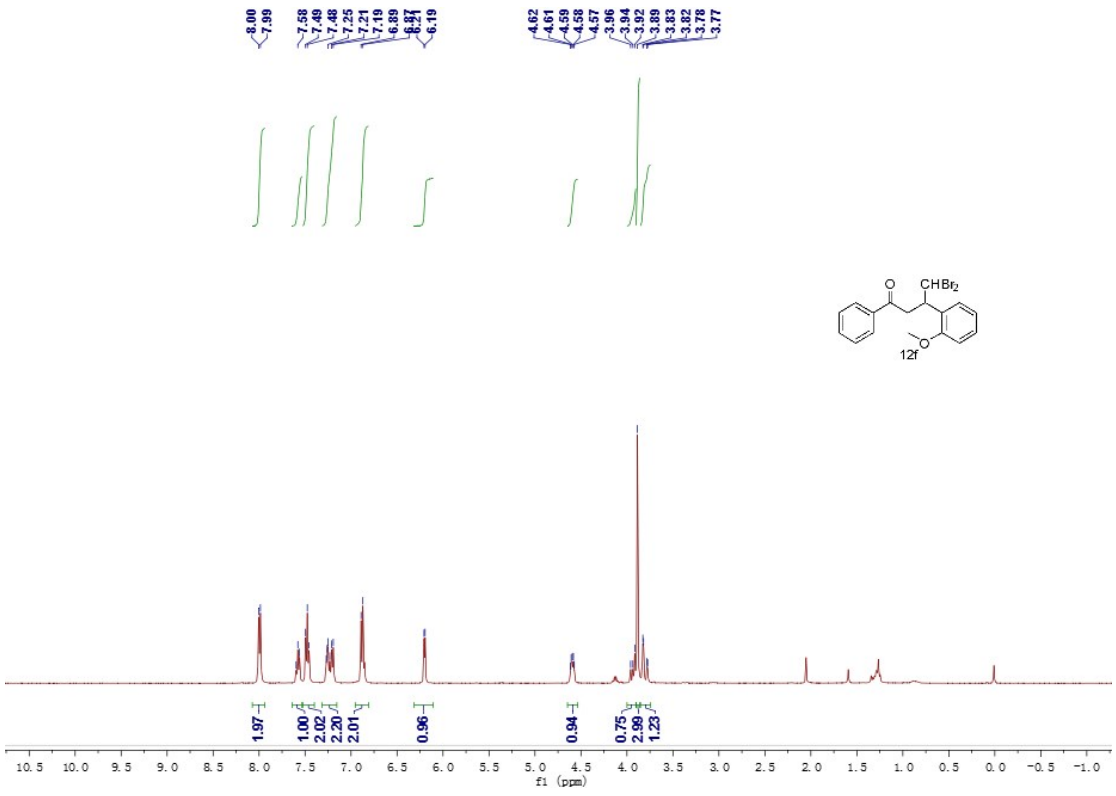
77.16
76.95
51.70
51.33
40.87
O
CHBr2
F
12e
f1 (ppm)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7.19
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6.87
6.19
4.62
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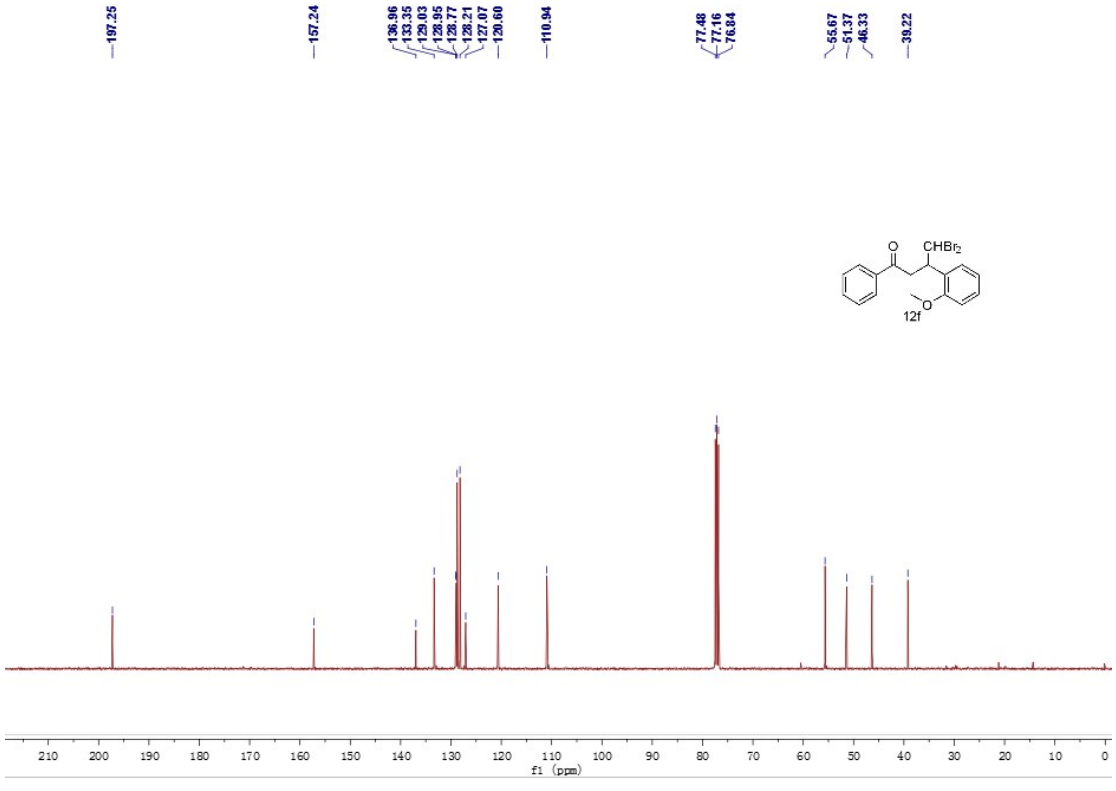
4.59
4.58
4.57
3.96
3.94
3.92
3.89
3.83
3.82
3.78
3.77
CHBr2
O
O
12f
1.97
1.00
2.02
2.20
2.01
0.96
0.94
0.75
2.99
1.23
f1 (ppm)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128.21
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76.84
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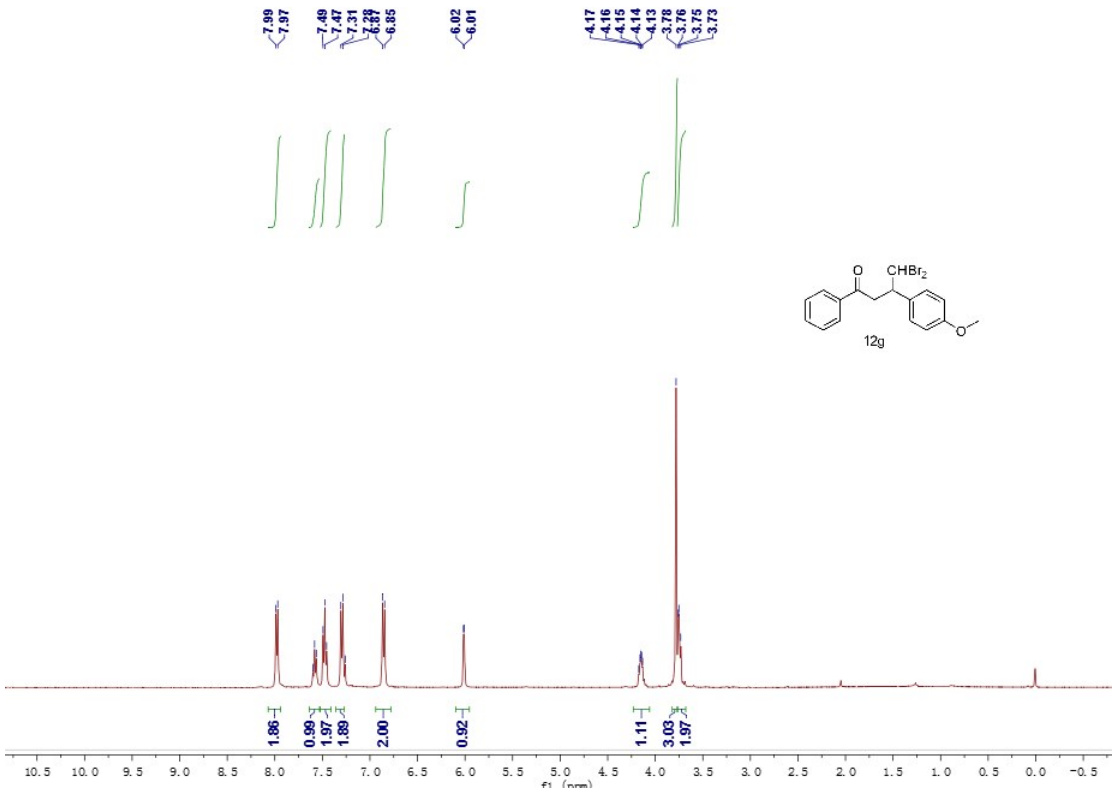
46.33
39.22
CHBr2
O
O
12f
f1 (ppm)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4.15
4.14
4.13
3.78
3.76
3.75
3.73
O
CHBr2
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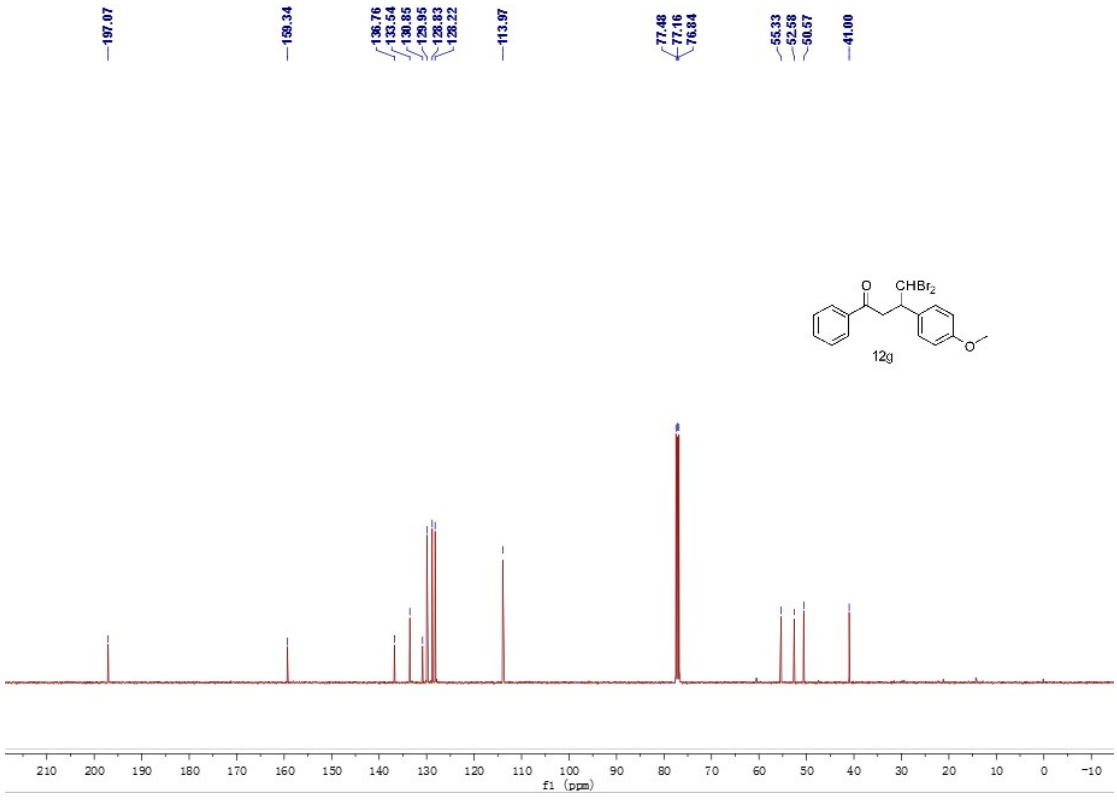
0.99
1.97
1.89
2.00
0.92
1.11
3.03
1.97
f1 (ppm)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76.84
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52.58
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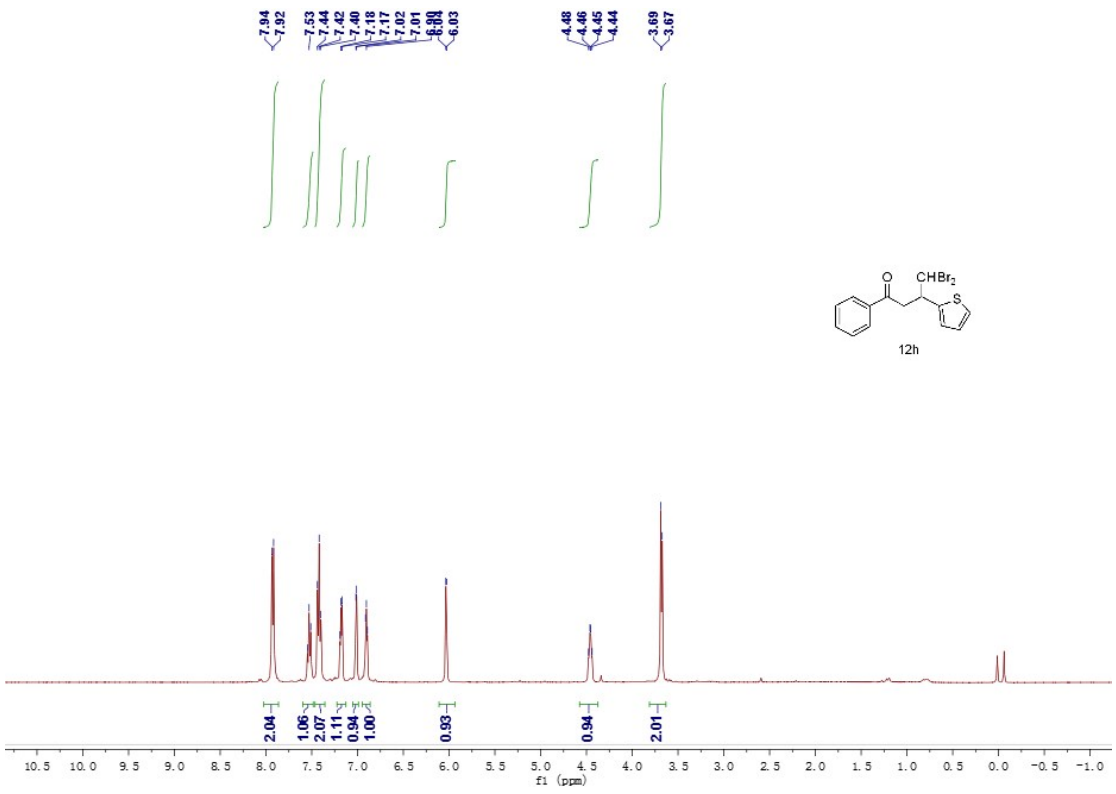
41.00
O
CHBr2
O
12g
f1 (ppm)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7.17
7.02
7.01
6.04
6.03
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4.46
4.45
4.44
3.69
3.67
CHBr2
S
12h
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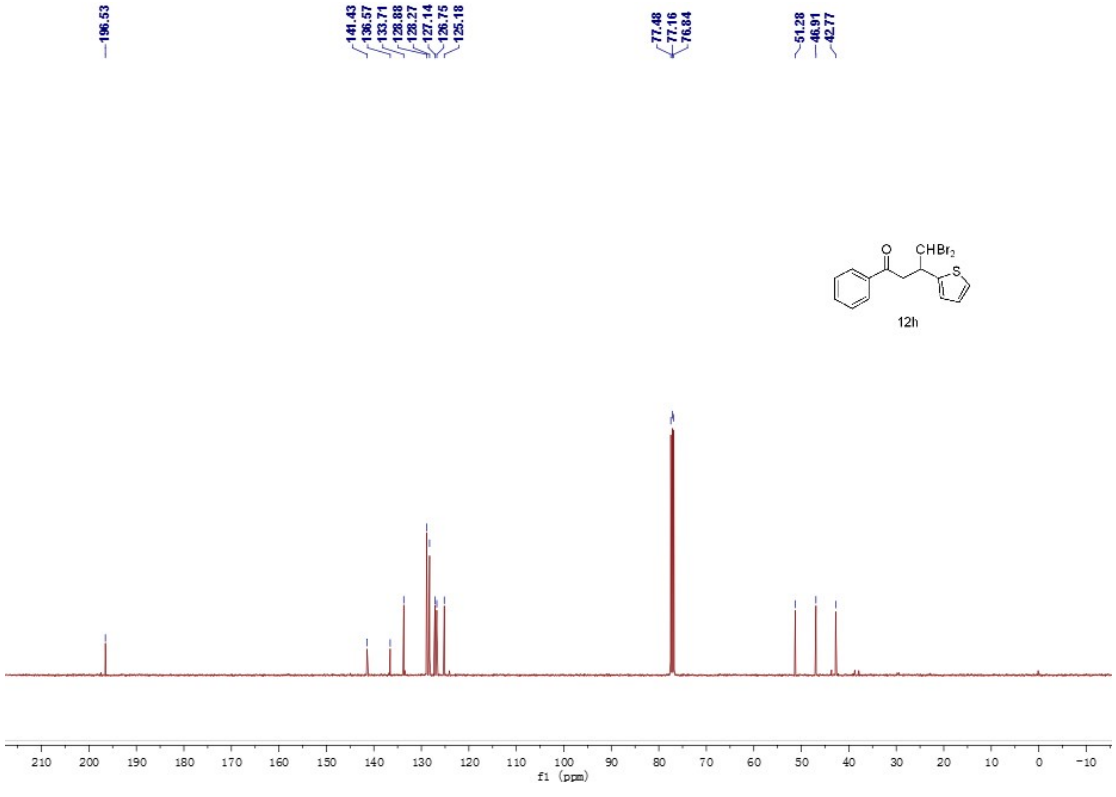
1.06
2.07
1.11
0.94
1.00
0.93
0.94
2.01
f1 (ppm)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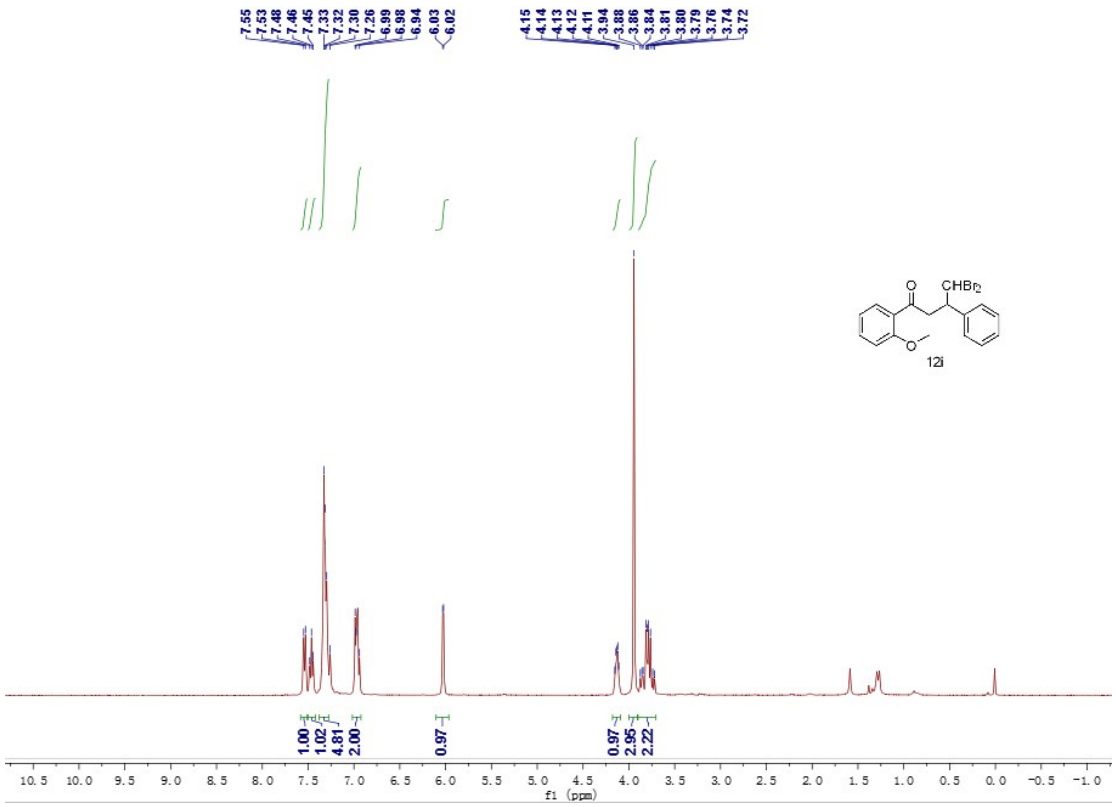
42.77
CHBr2
S
12h
f1 (ppm)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6.94
6.03
6.02
4.15
4.14
4.13
4.12
4.11
3.94
3.88
3.86
3.84
3.81
3.80
3.79
3.76
3.74
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12i
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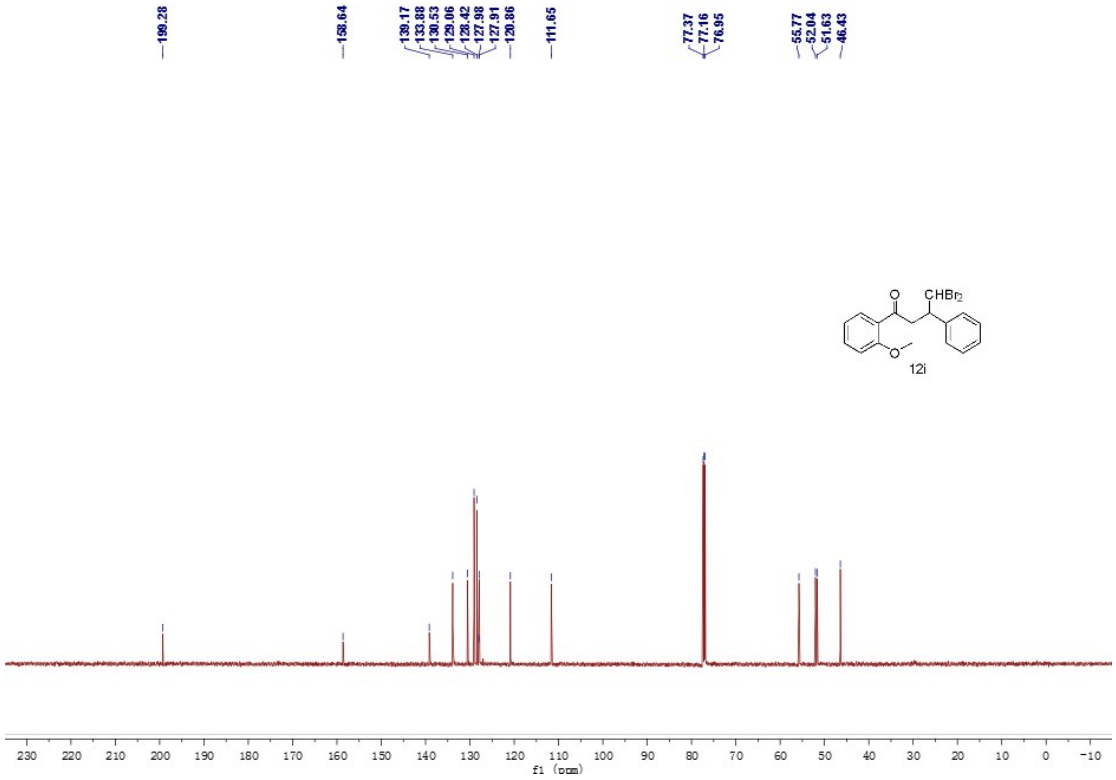
4.81
2.00
0.97
0.97
2.95
2.22
f1 (ppm)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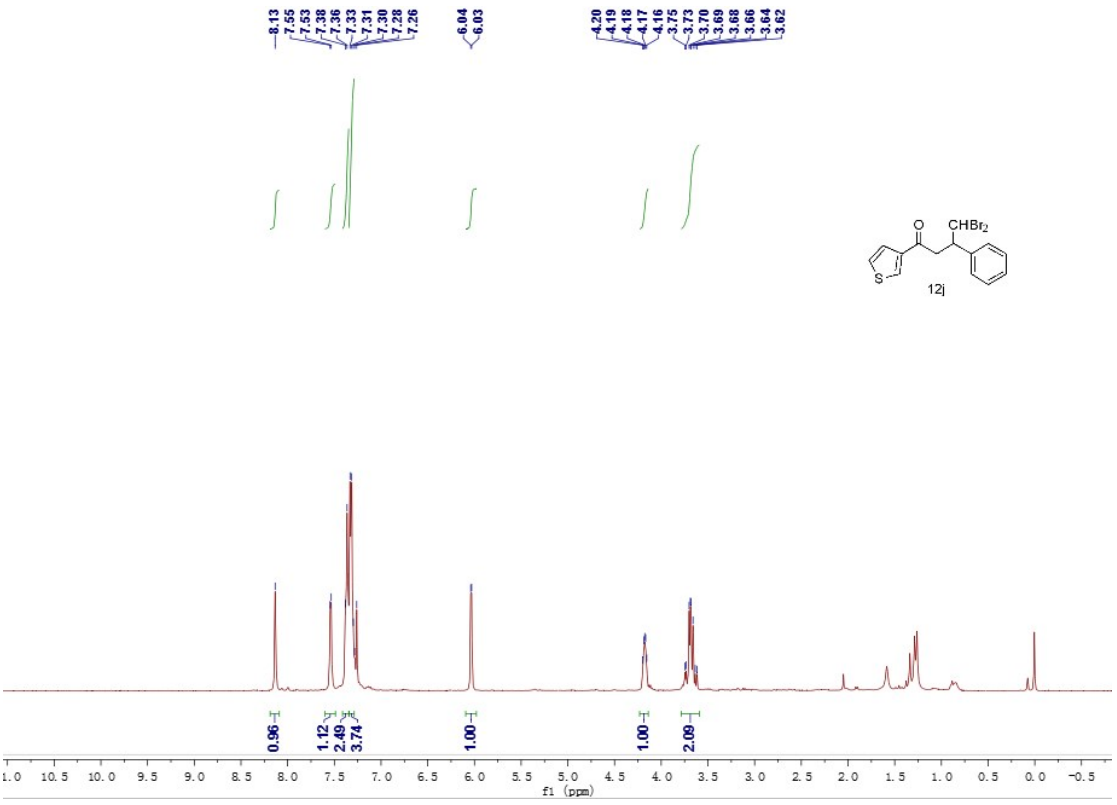
77.16
76.95
55.77
52.04
51.63
46.43
CHBr2
12i
f1 (ppm)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7.26
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6.03
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4.19
4.18
4.17
4.16
3.75
3.73
3.70
3.69
3.68
3.66
3.64
3.62
O
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S
12j
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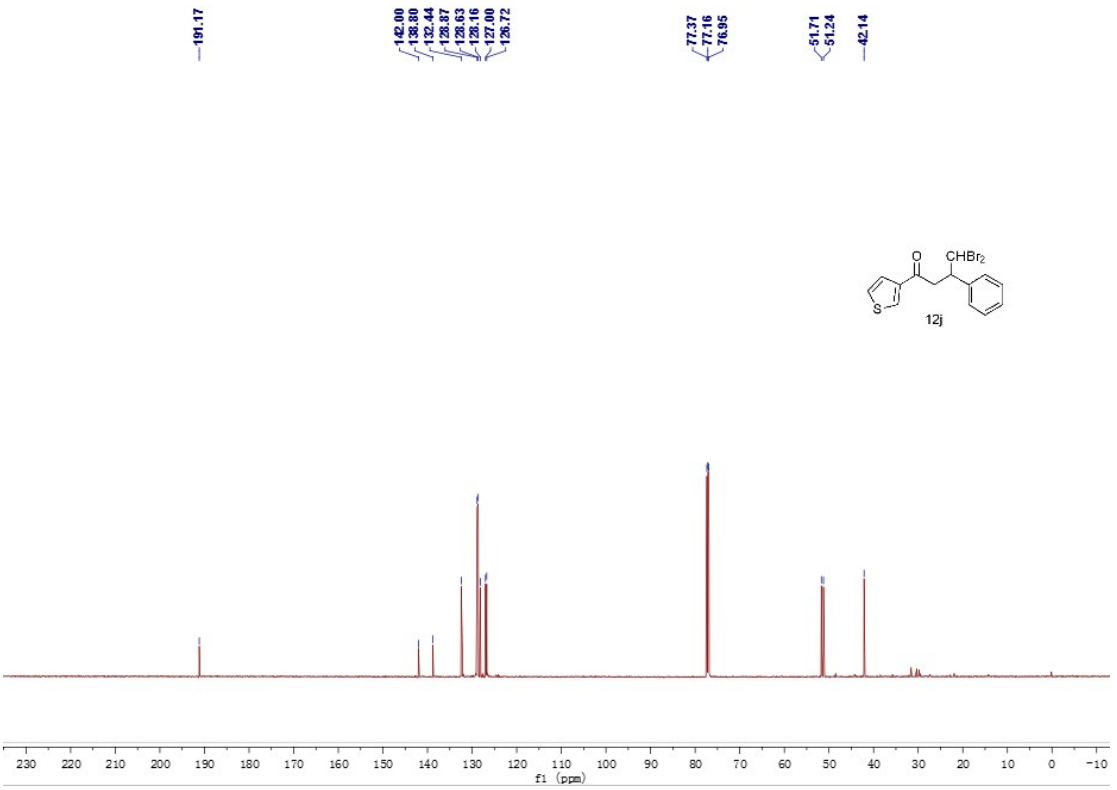
1.12
2.49
3.74
1.00
1.00
2.09
f1 (ppm)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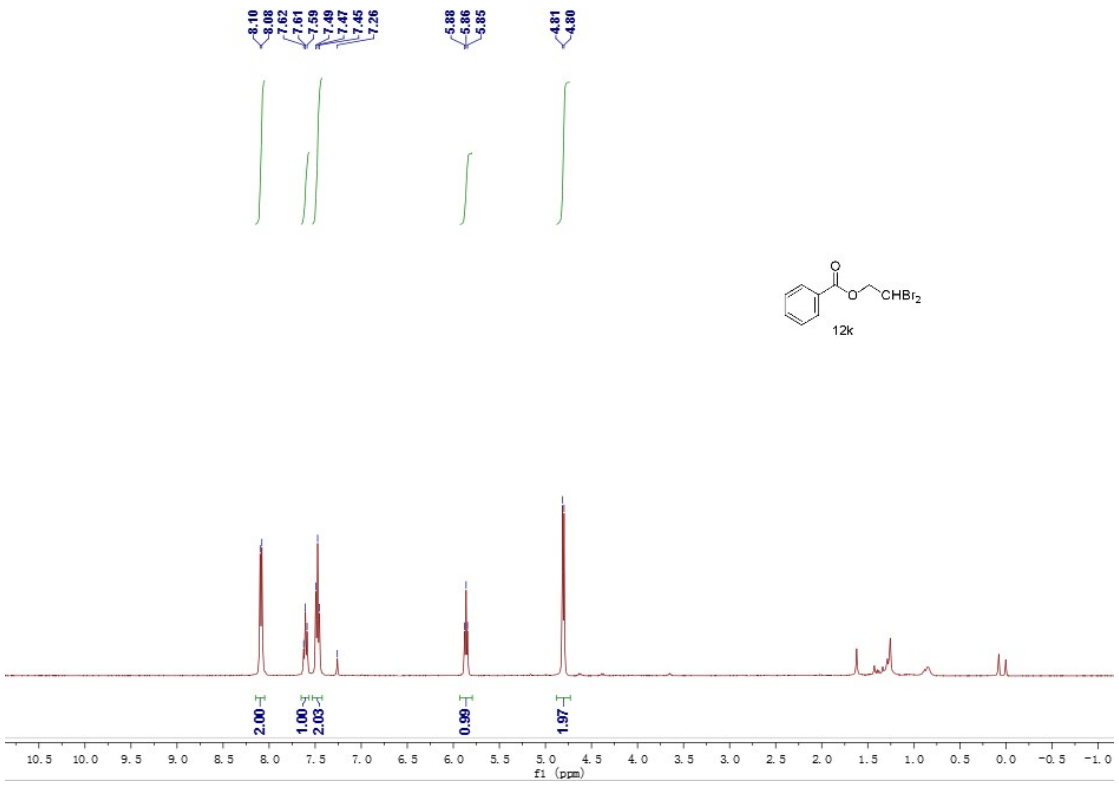
77.16
76.95
51.71
51.24
42.14
O
CHBr2
S
12j
f1 (ppm)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8.08
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7.61
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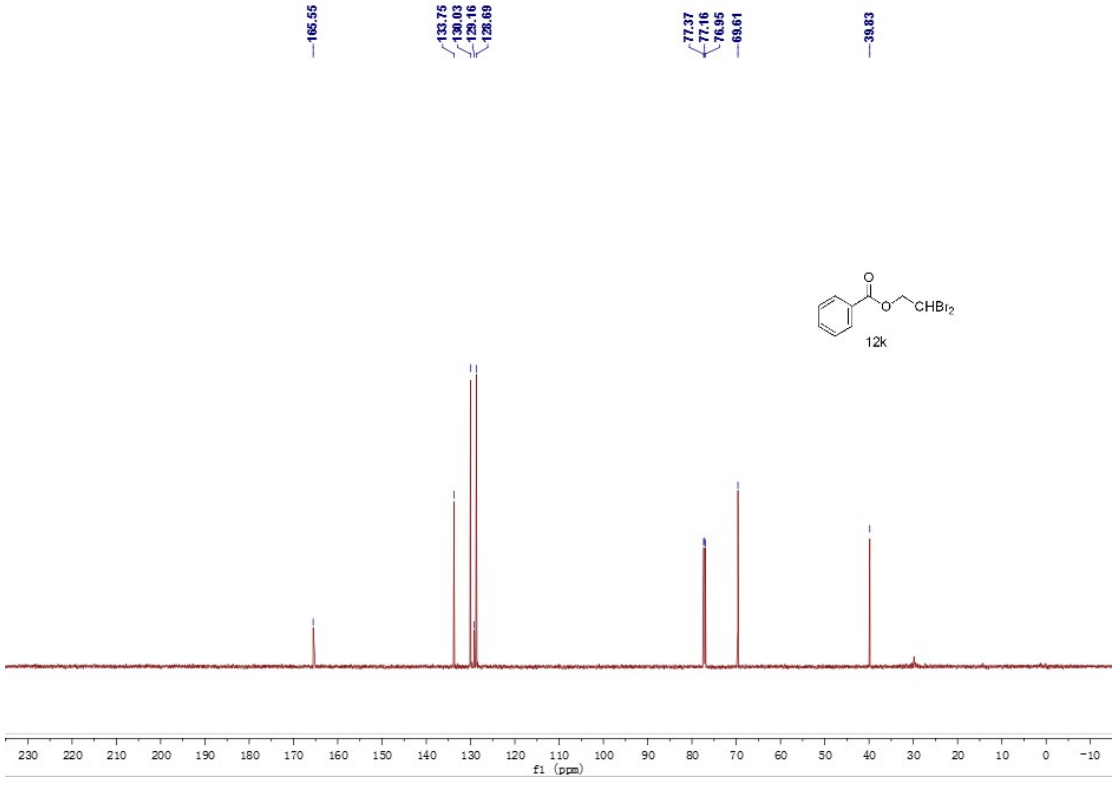
7.49
7.47
7.45
7.26
5.88
5.86
5.85
4.81
4.80
CHBr2
12k
2.00
1.00
2.03
0.99
1.97
f1 (ppm)


165.55
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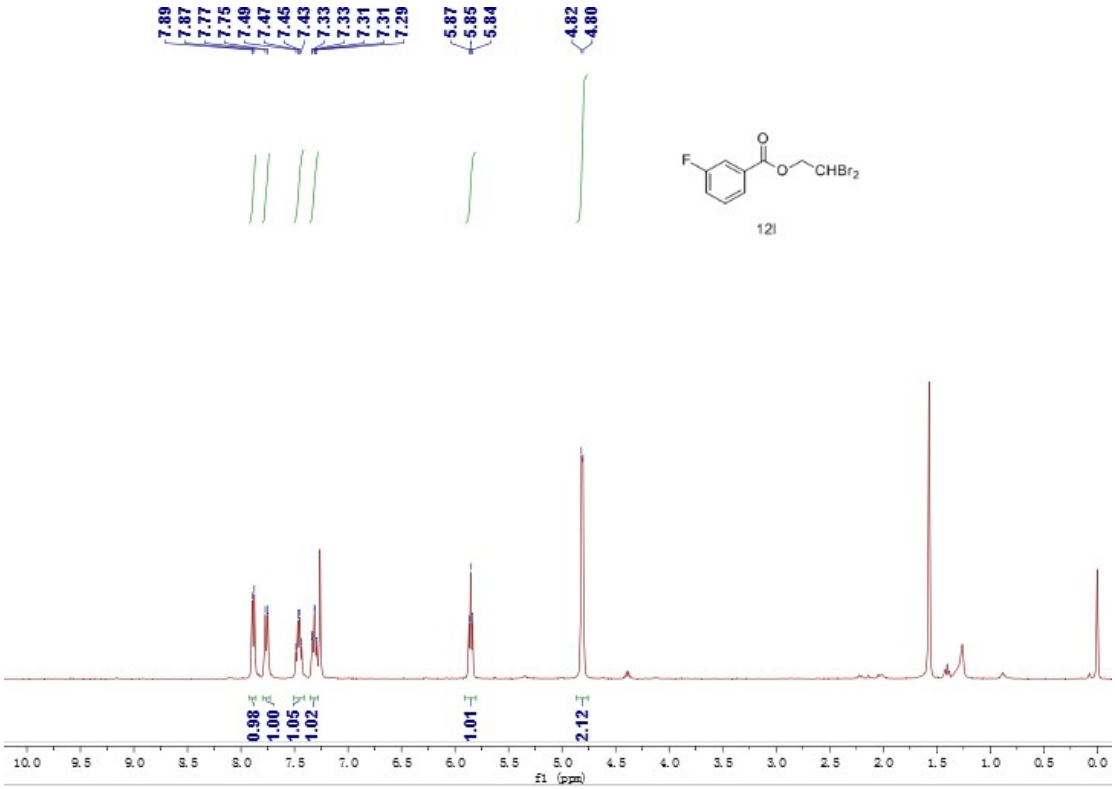
77.37
77.16
76.95
69.61
39.83
CHBr2
12k
f1 (ppm)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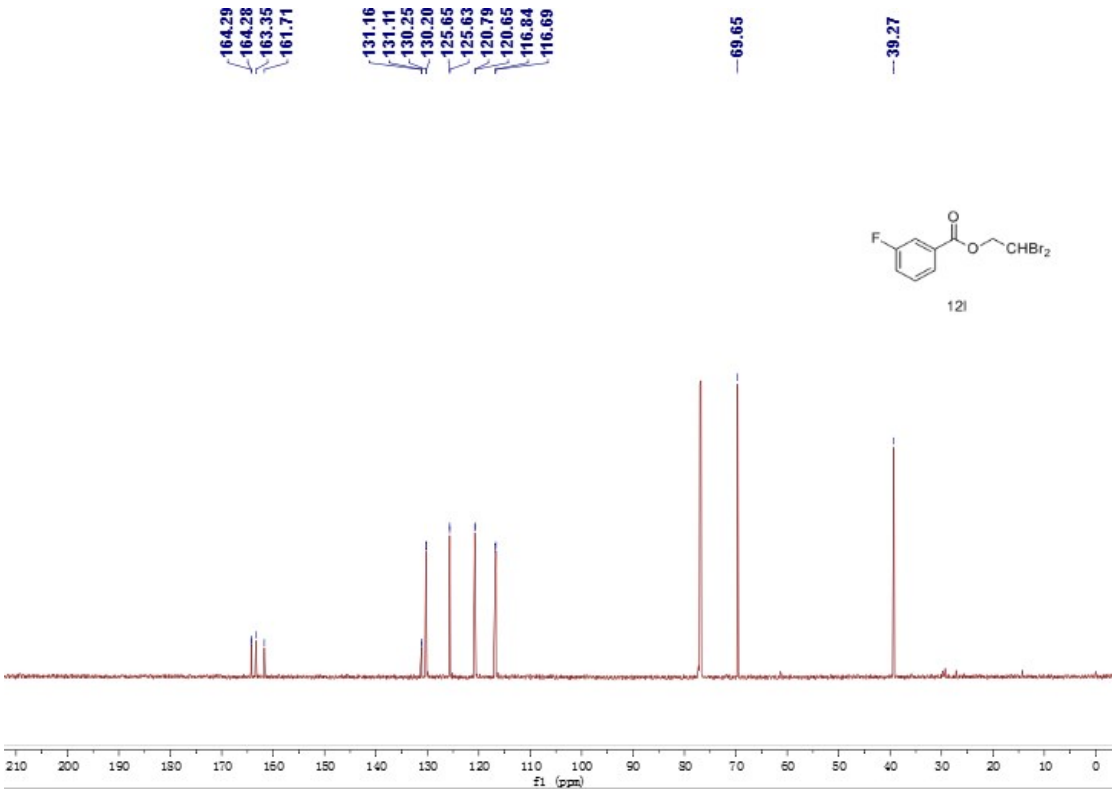
7.33
7.33
7.31
7.31
7.29
5.87
5.85
5.84
4.82
4.80
F
O
O
CHBr2
12l
0.98
1.00
1.05
1.02
1.01
2.12
f1 (ppm)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130.20
125.65
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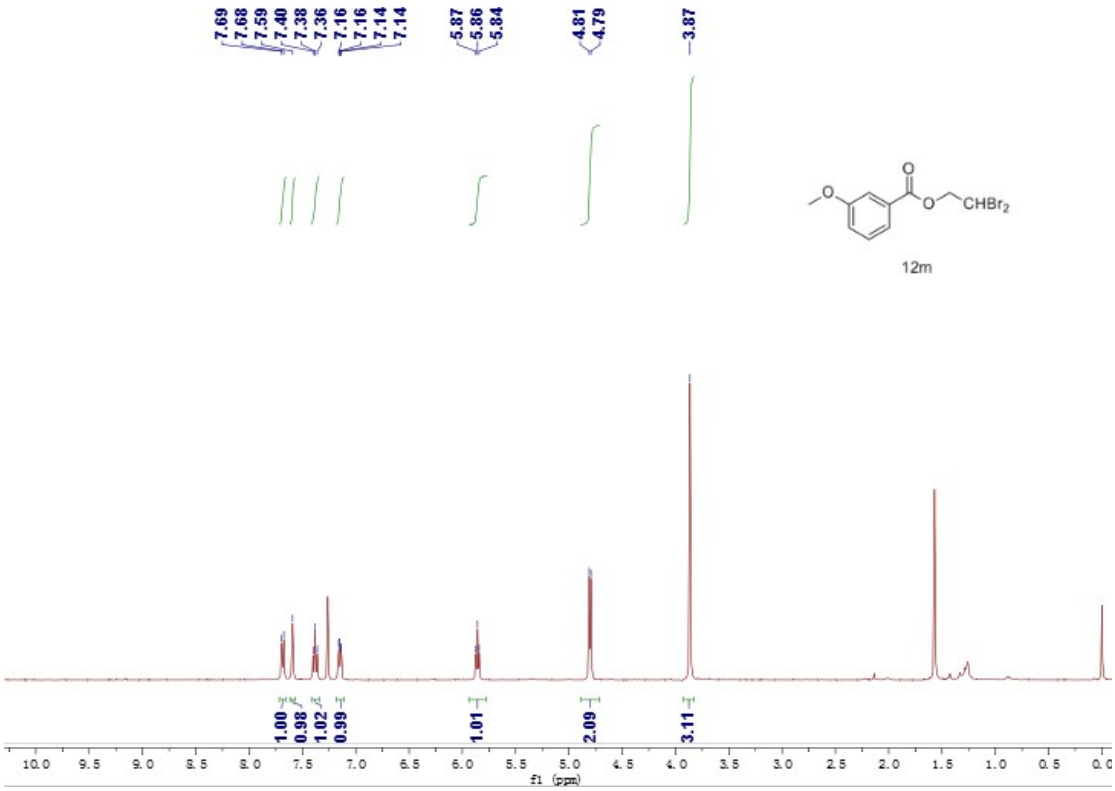
120.65
116.84
116.69
69.65
39.27
F
O
O
CHBr2
12l
f1 (ppm)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7.14
7.14
5.87
5.86
5.84
4.81
4.79
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O
O
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12m
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1.02
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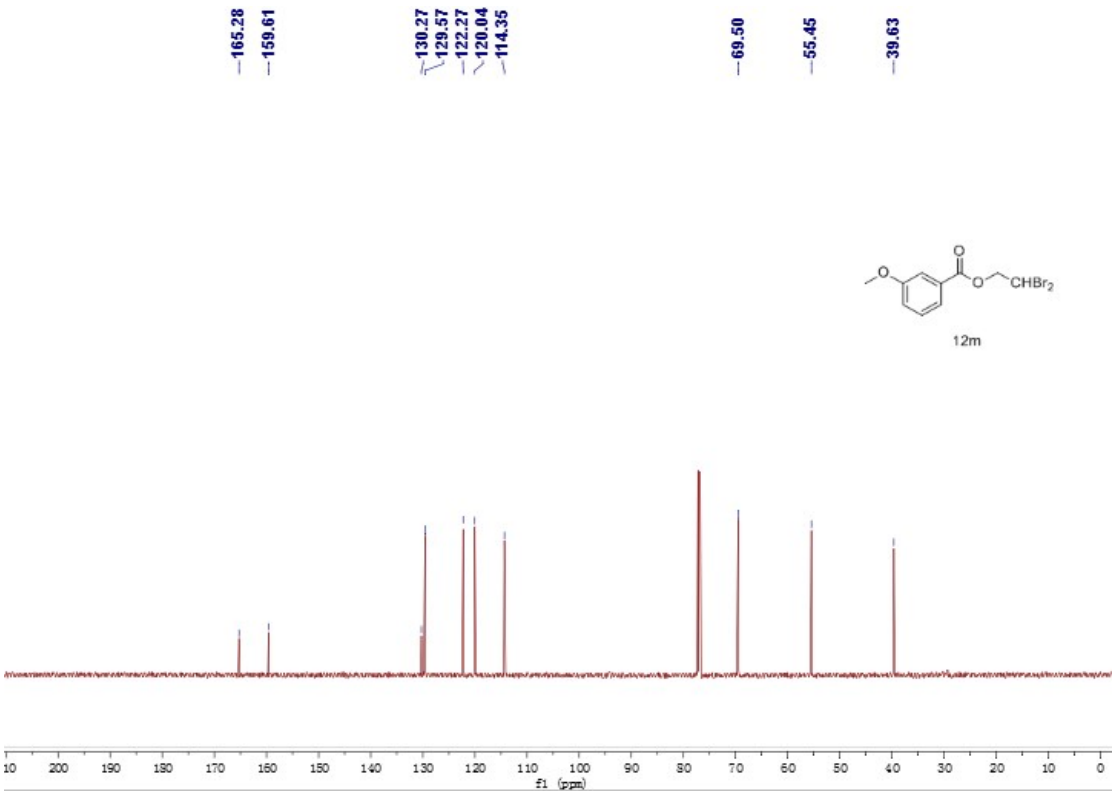
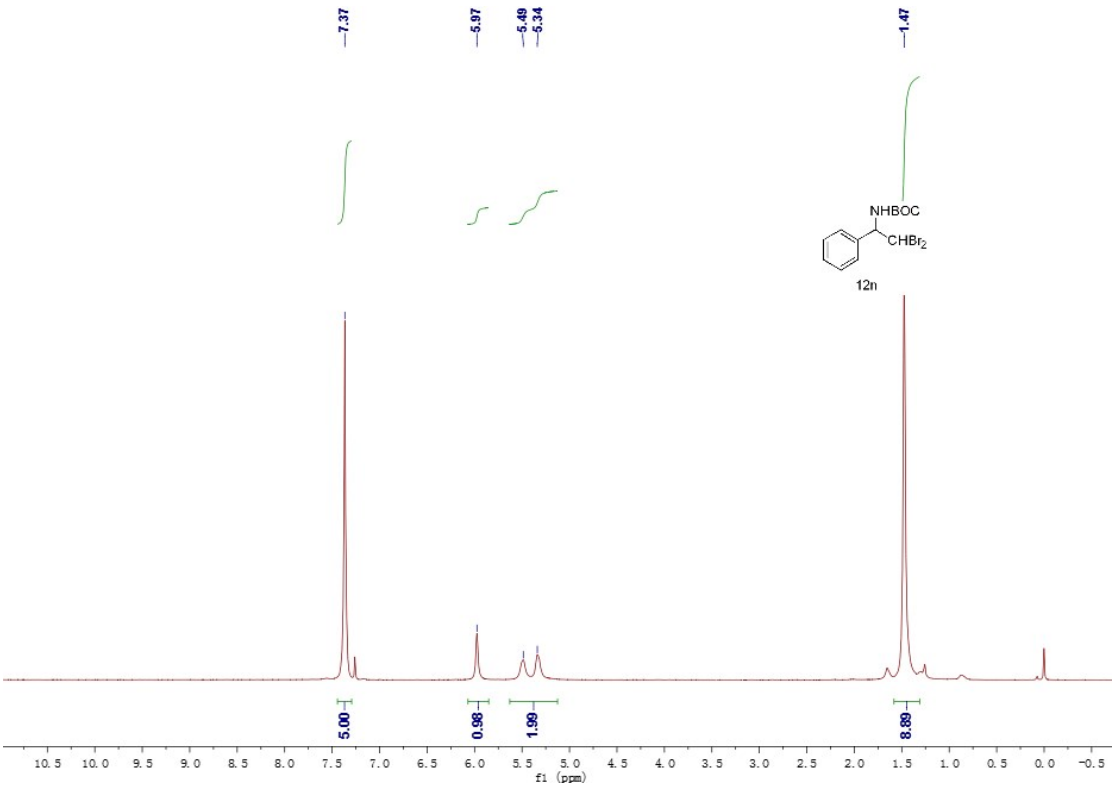
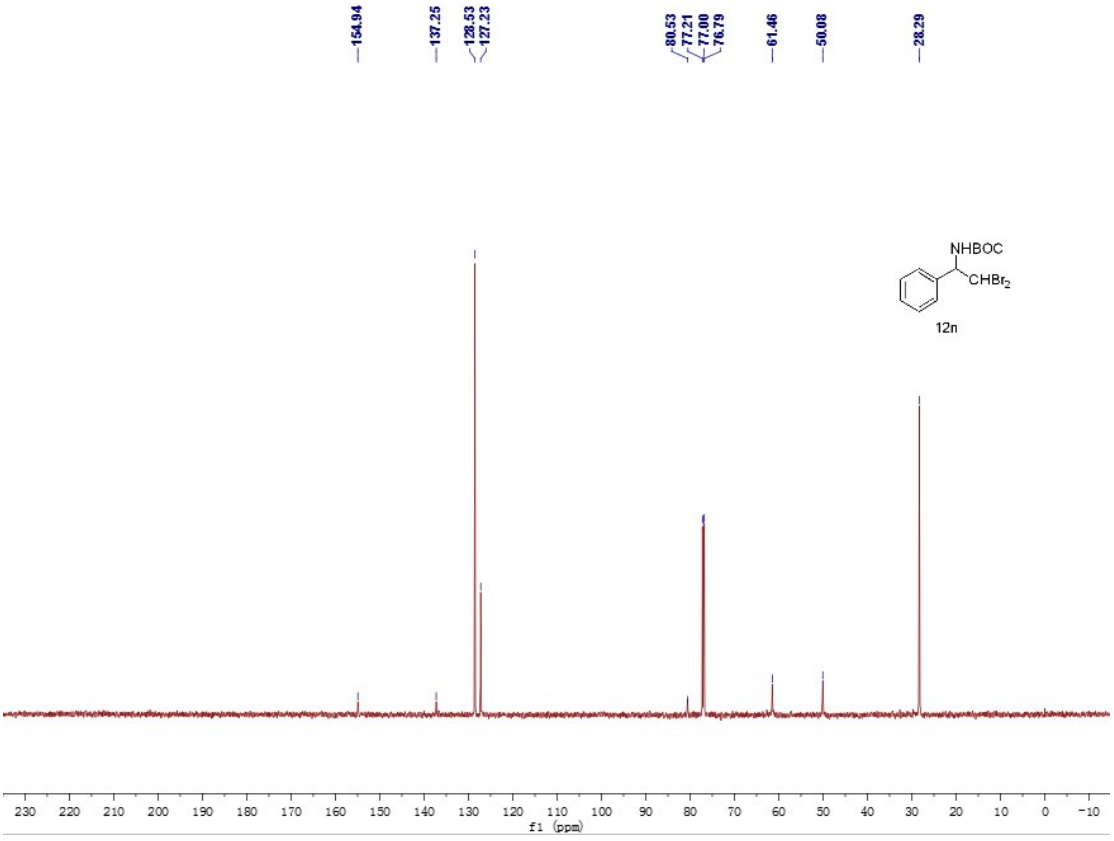
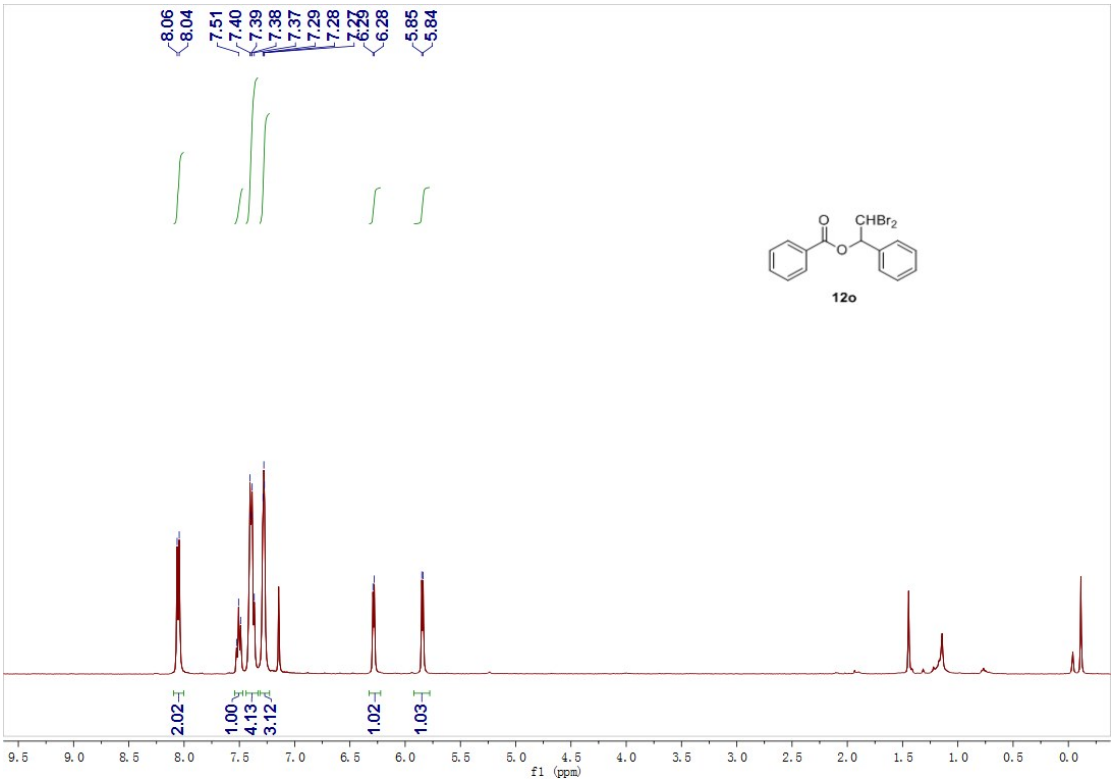
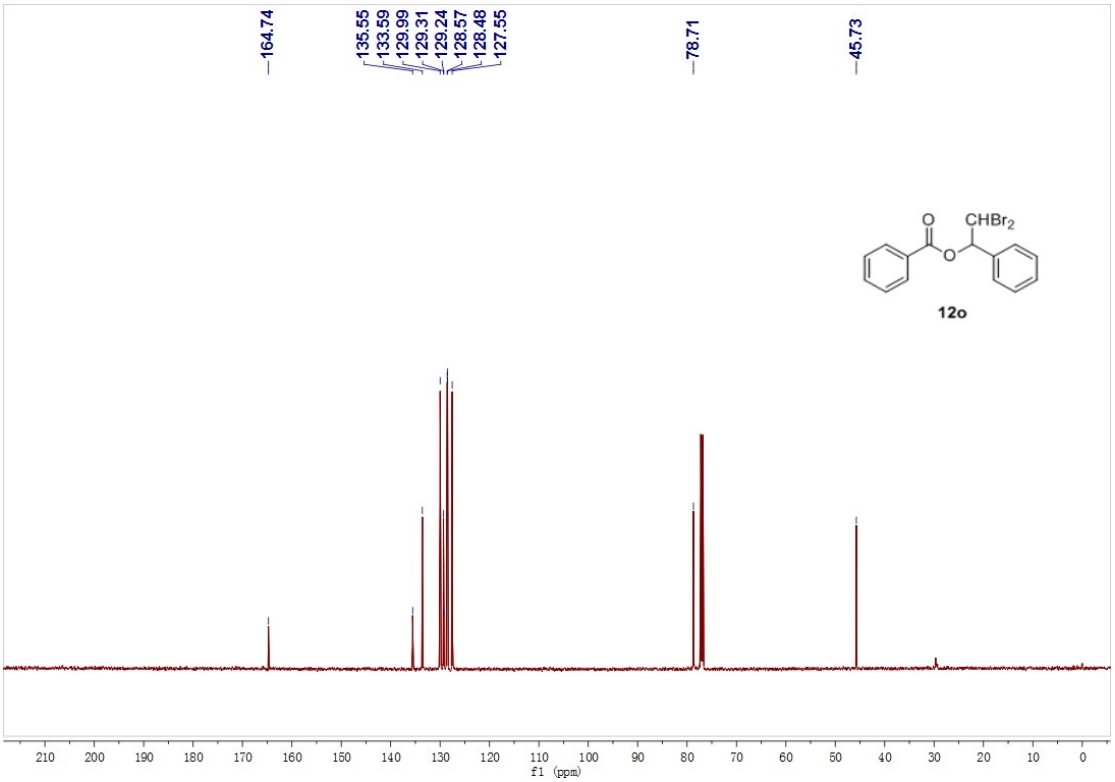
1.01
2.09
3.11
f1 (ppm)

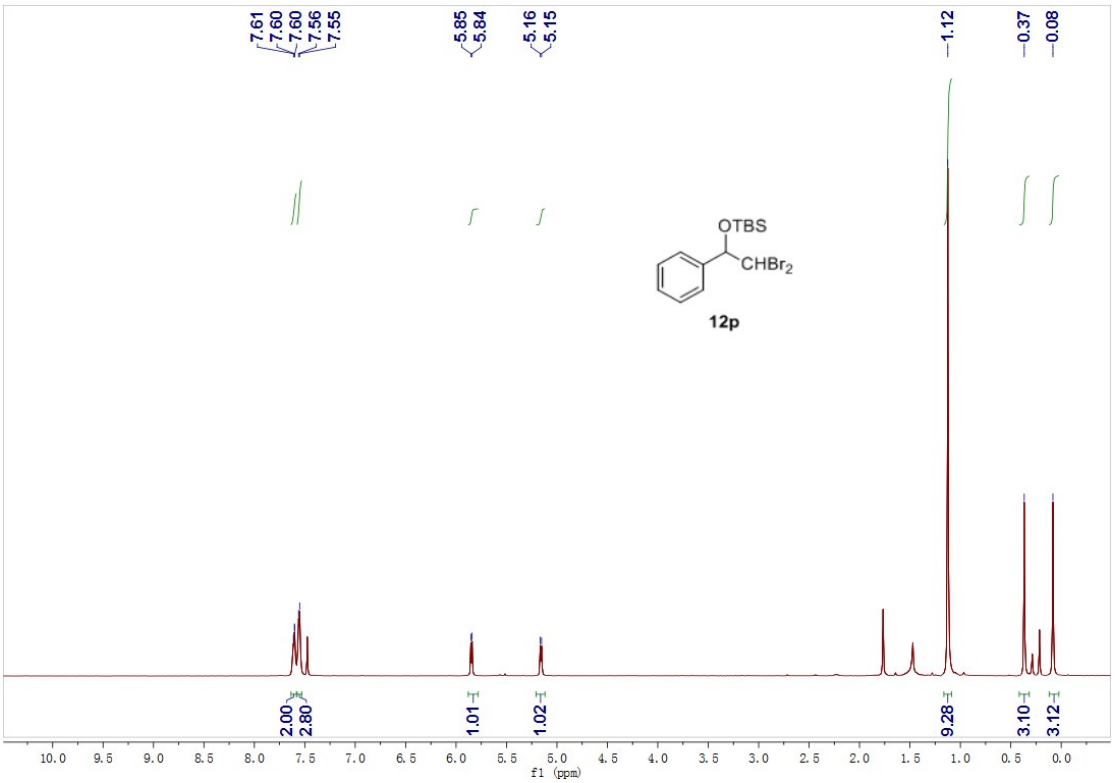

165.28
159.61
130.27
129.57
122.27
120.04
114.35
69.50
55.45
39.63
O
O
CHBr2
12m
f1 (ppm)

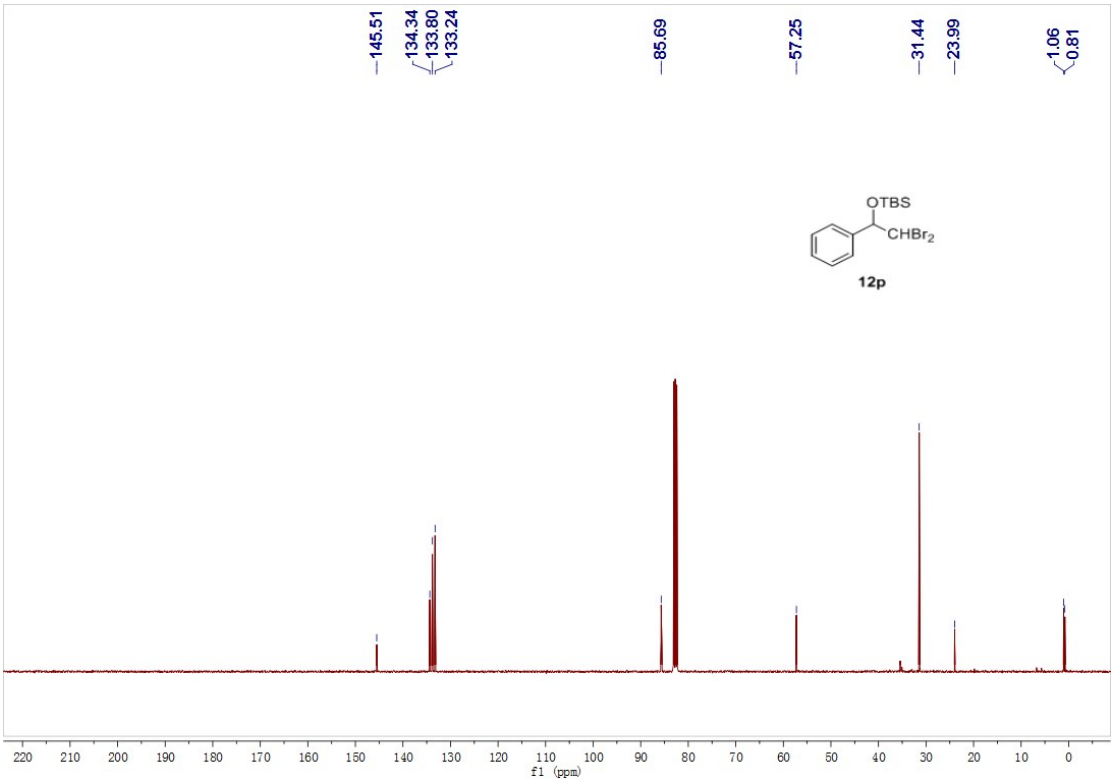

7.37
5.97
5.49
5.34
1.47
NHBOC
CHBr2
12n
5.00
0.98
1.99
8.89
f1 (ppm)

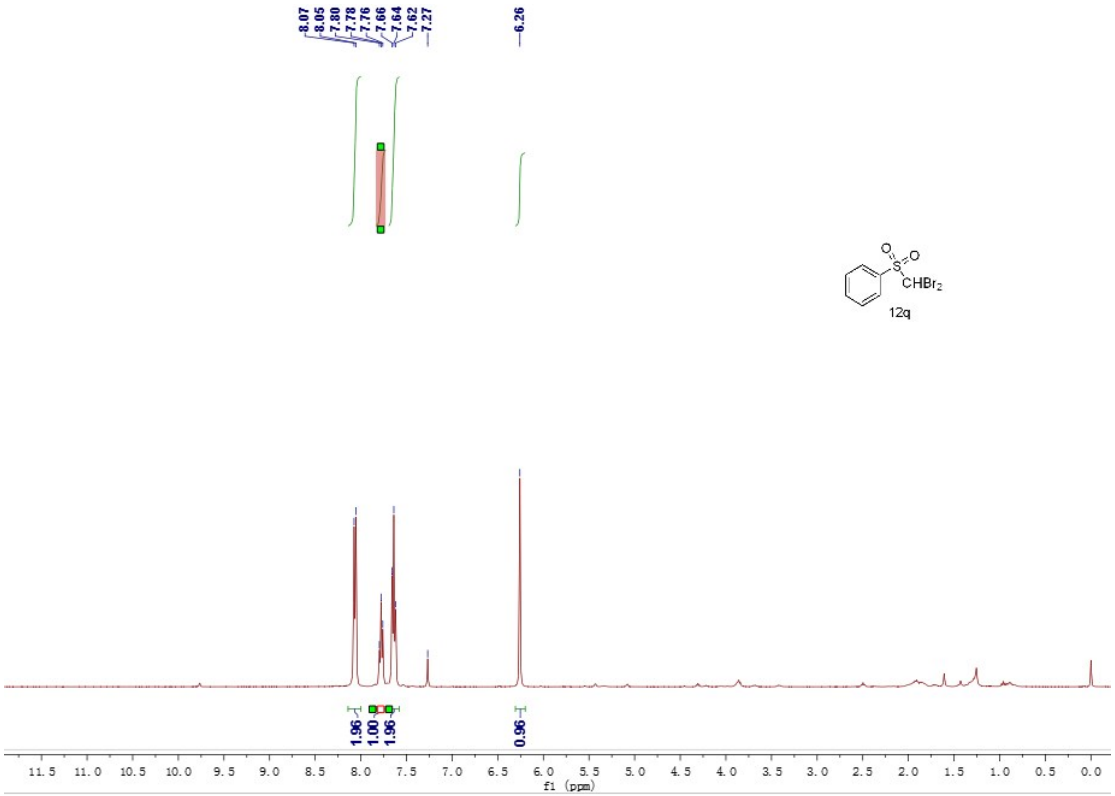

154.94
137.25
128.53
127.23
80.53
77.21
77.00
76.79
61.46
50.08
28.29
NHBOC
CHBr2
12n
f1 (ppm)

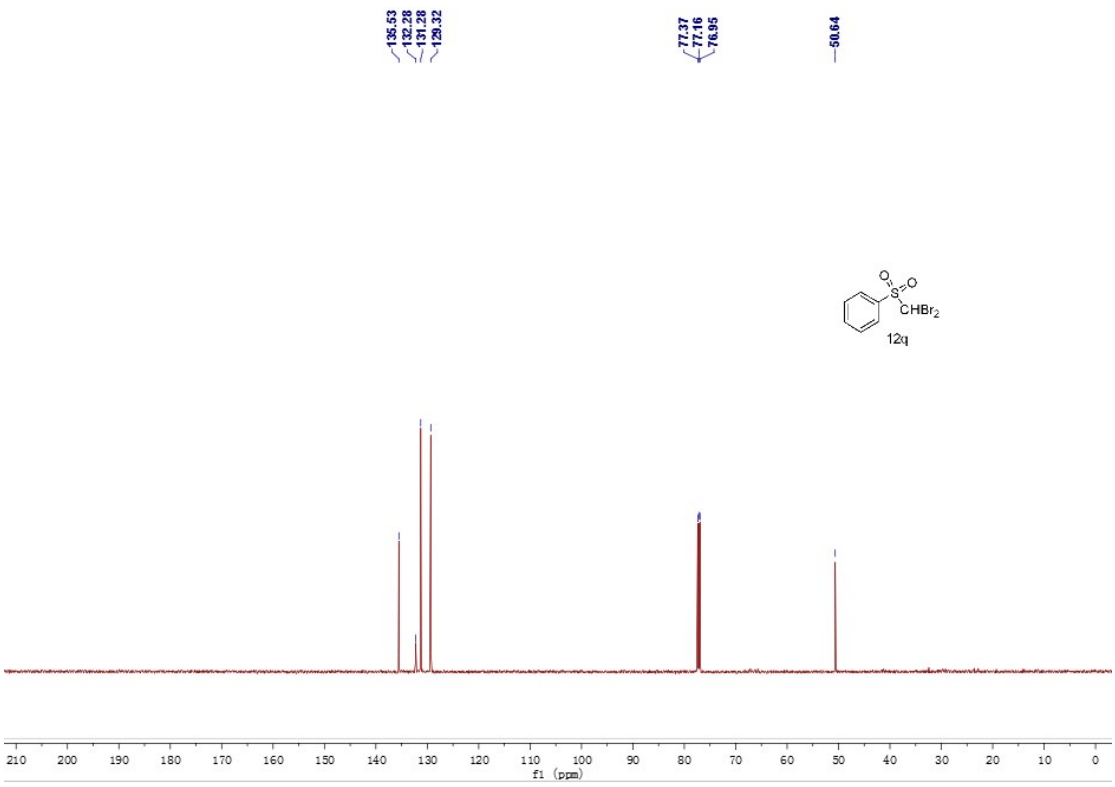

8.06
8.04
7.51
7.40
7.39
7.38
7.37
7.29
7.28
6.29
6.28
5.85
5.84
CHBr2
O
O
12o
2.02
1.00
4.13
3.12
1.02
1.03
f1 (ppm)

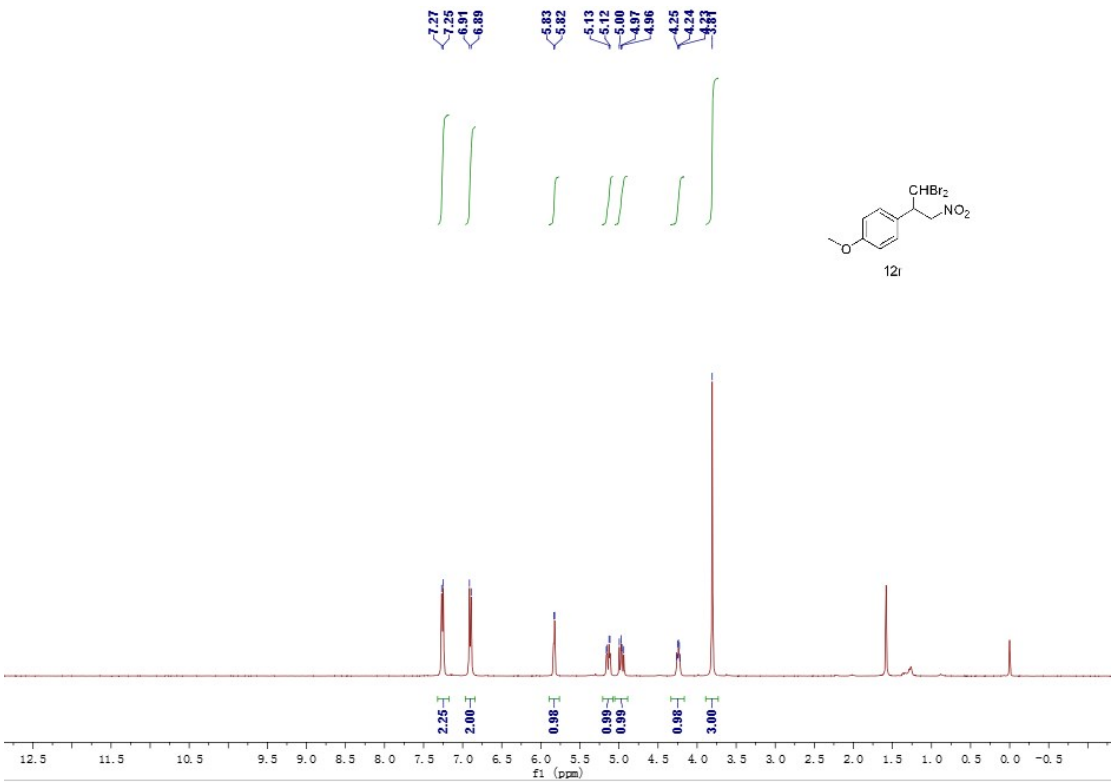

164.74
135.55
133.59
129.99
129.31
129.24
128.57
128.48
127.55
78.71
45.73
CHBr2
O
O
12o
f1 (ppm)

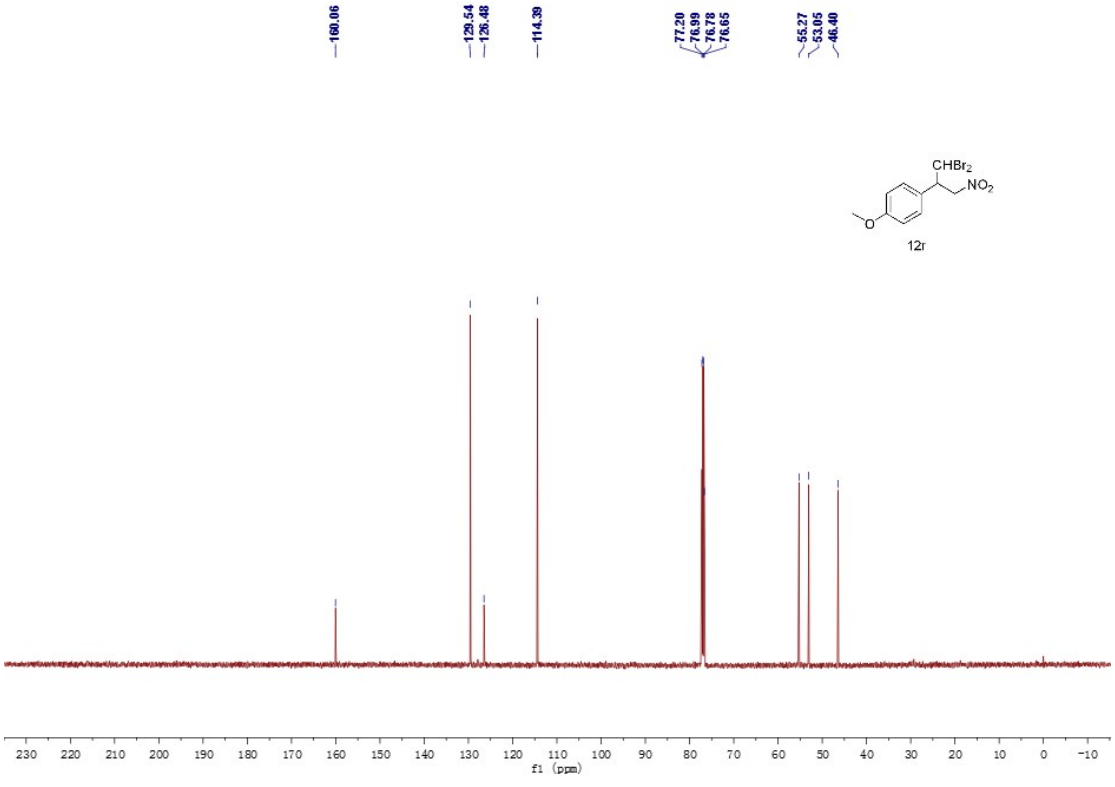

7.61
7.60
7.60
7.56
7.55
5.85
5.84
5.16
5.15
1.12
0.37
0.08
OTBS
CHBr2
12p
2.00
2.80
1.01
1.02
9.28
3.10
3.12
f1 (ppm)

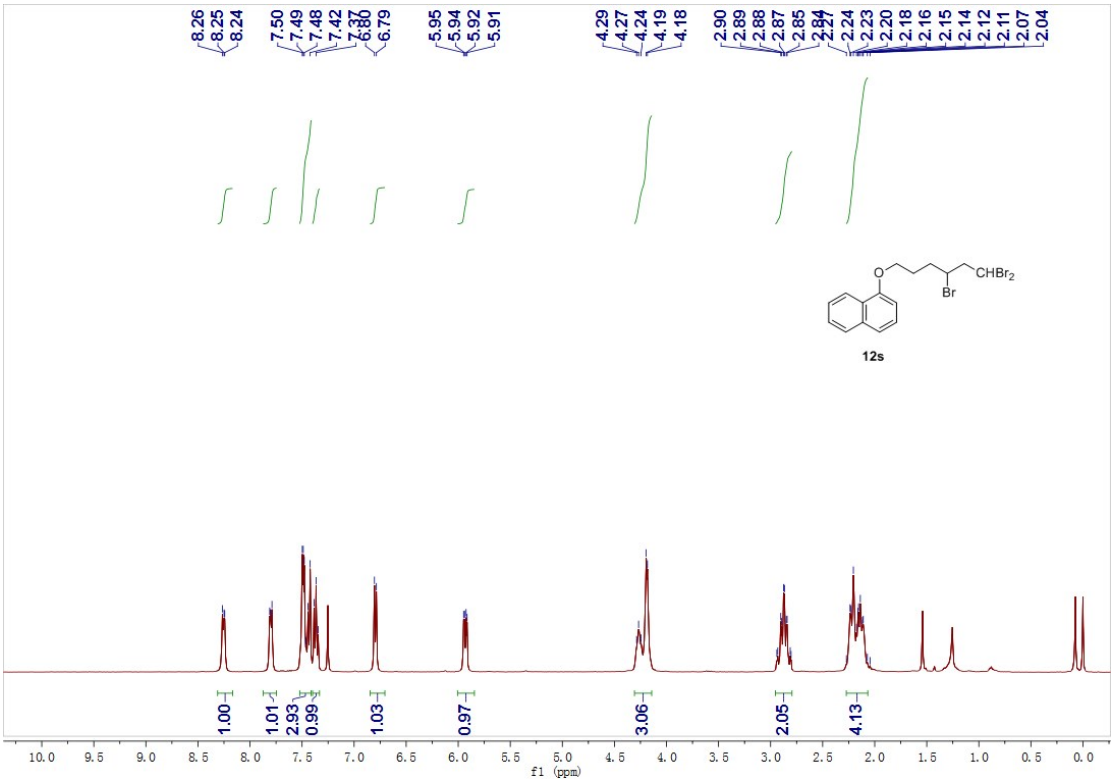

145.51
134.34
133.80
133.24
85.69
57.25
31.44
23.99
1.06
0.81
OTBS
CHBr2
12p
f1 (ppm)

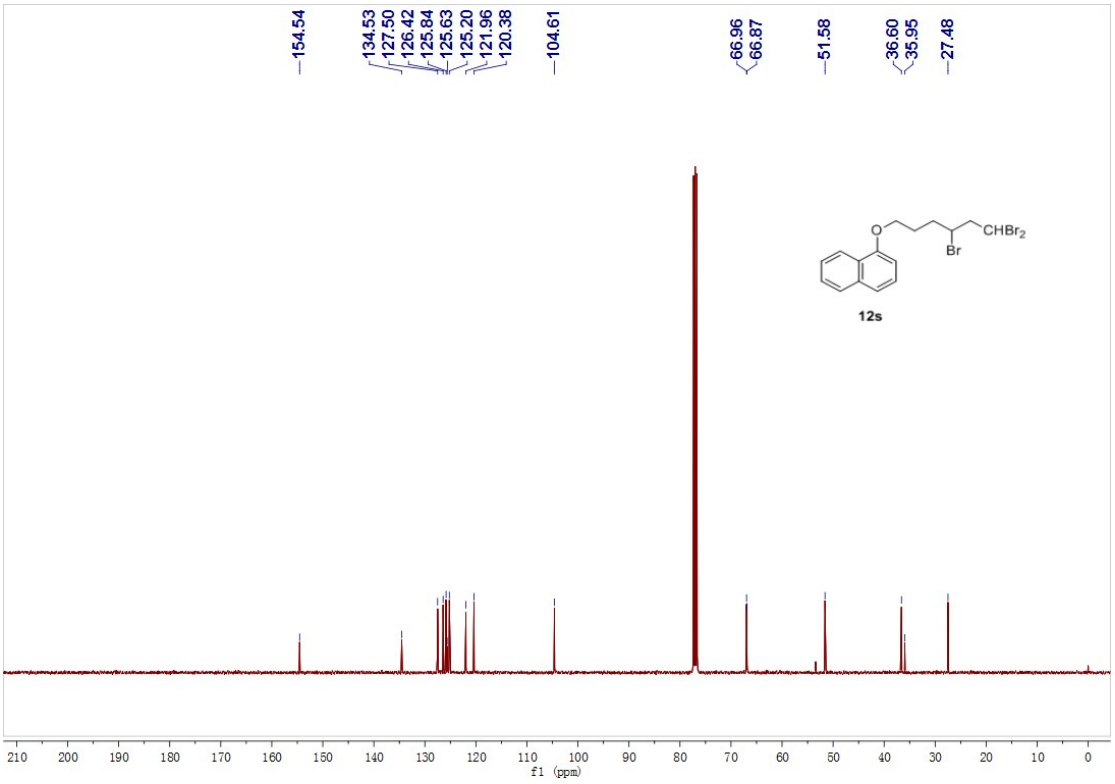

8.07
8.05
7.80
7.78
7.76
7.66
7.64
7.62
7.27
6.26
CHBr2
12q
1.96
1.00
1.96
0.96
f1 (ppm)

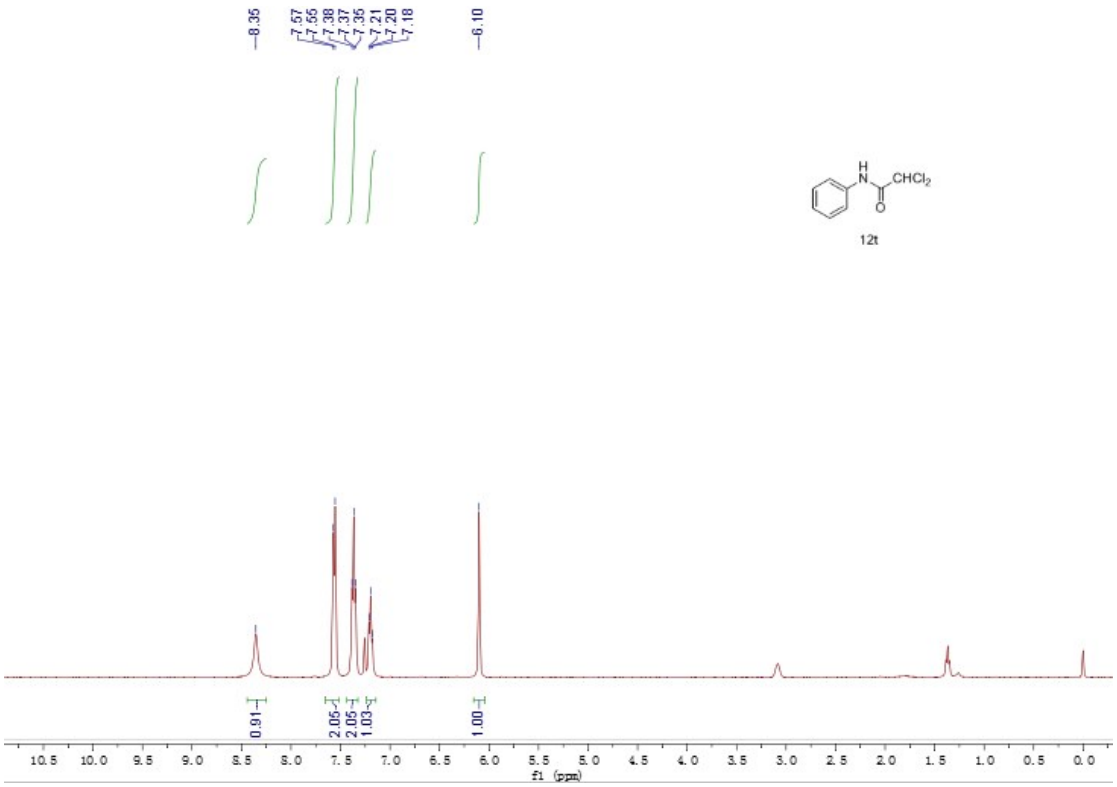

135.53
132.28
131.28
129.32
77.37
77.16
76.95
50.64
CHBr2
12q
f1 (ppm)

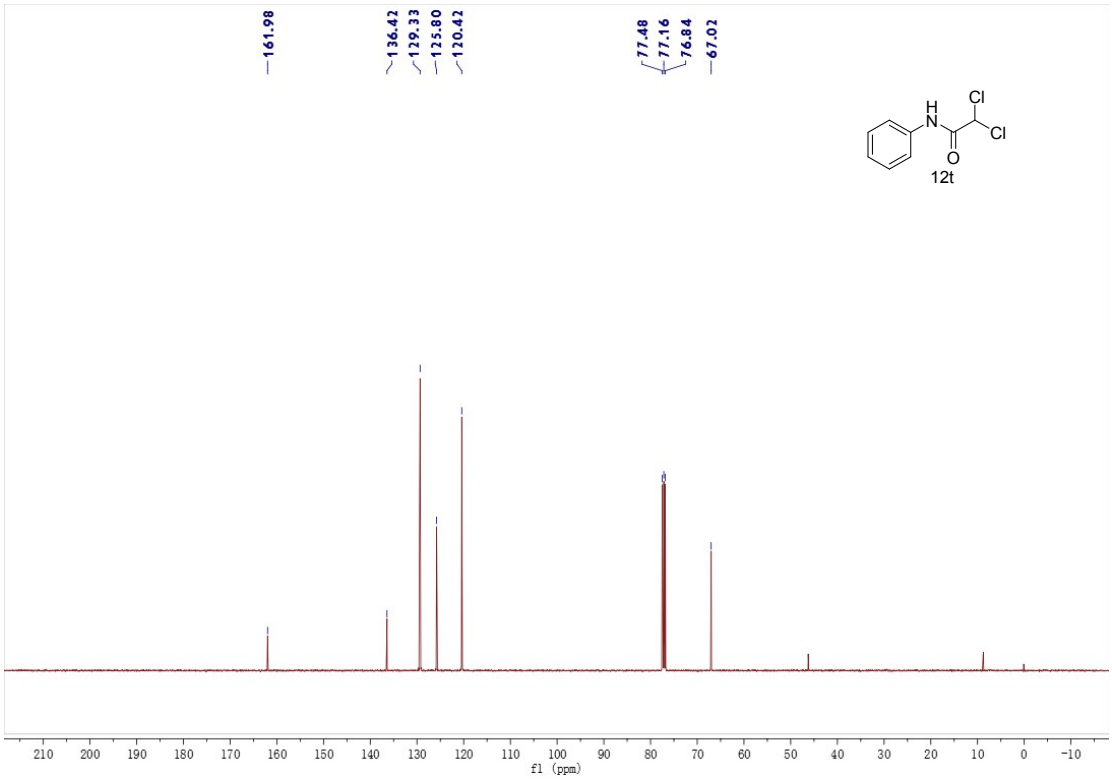

7.27
7.25
6.91
6.89
5.83
5.82
5.13
5.12
5.00
4.97
4.96
4.25
4.24
4.21
4.17
CHBr2
NO2
O
12r
2.25
2.00
0.98
0.99
0.99
0.98
3.00
f1 (ppm)


160.06
129.54
126.48
114.39
77.20
76.99
76.78
76.65
55.27
53.05
46.40
CHBr2
NO2
O
12r
f1 (ppm)

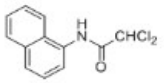

8.26
8.25
8.24
7.50
7.49
7.48
7.42
7.37
6.80
6.79
5.95
5.94
5.92
5.91
4.29
4.27
4.24
4.19
4.18
2.90
2.89
2.88
2.87
2.85
2.24
2.23
2.20
2.18
2.16
2.15
2.14
2.12
2.11
2.07
2.04
O
CHBr2
Br
12s
1.00
1.01
2.93
0.99
1.03
0.97
3.06
2.05
4.13
f1 (ppm)


154.54
134.53
127.50
126.42
125.84
125.63
125.20
121.96
120.38
104.61
66.96
66.87
51.58
36.60
35.95
27.48
O
CHBr2
Br
12s
f1 (ppm)

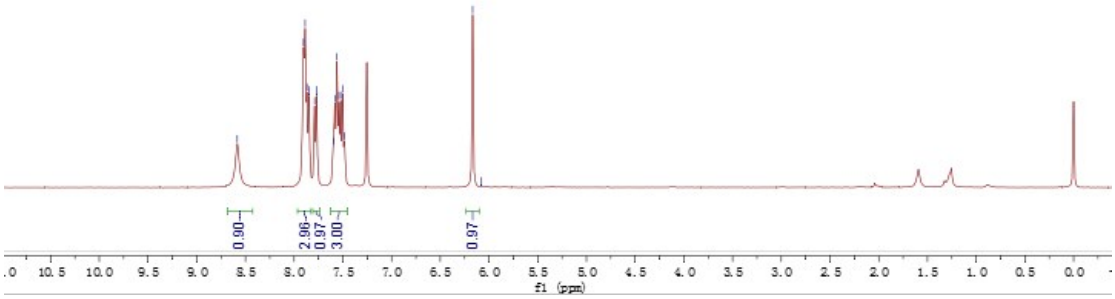

8.35
7.57
7.55
7.38
7.37
7.35
7.21
7.20
7.18
6.10
CHCl2
12t
0.91
2.05
2.05
1.03
1.00
f1 (ppm)


161.98
136.42
129.33
125.80
120.42
77.48
77.16
76.84
67.02
Cl
Cl
12t
f1 (ppm)


8.58
7.90
7.89
7.87
7.85
7.79
7.77
7.60
7.58
7.56
7.54
7.52
7.50
7.48
6.17
6.08

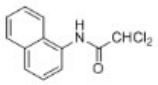

H
N
CHCl2
O

12u


0.90
2.96
0.97
3.00
0.97
f1 (ppm)

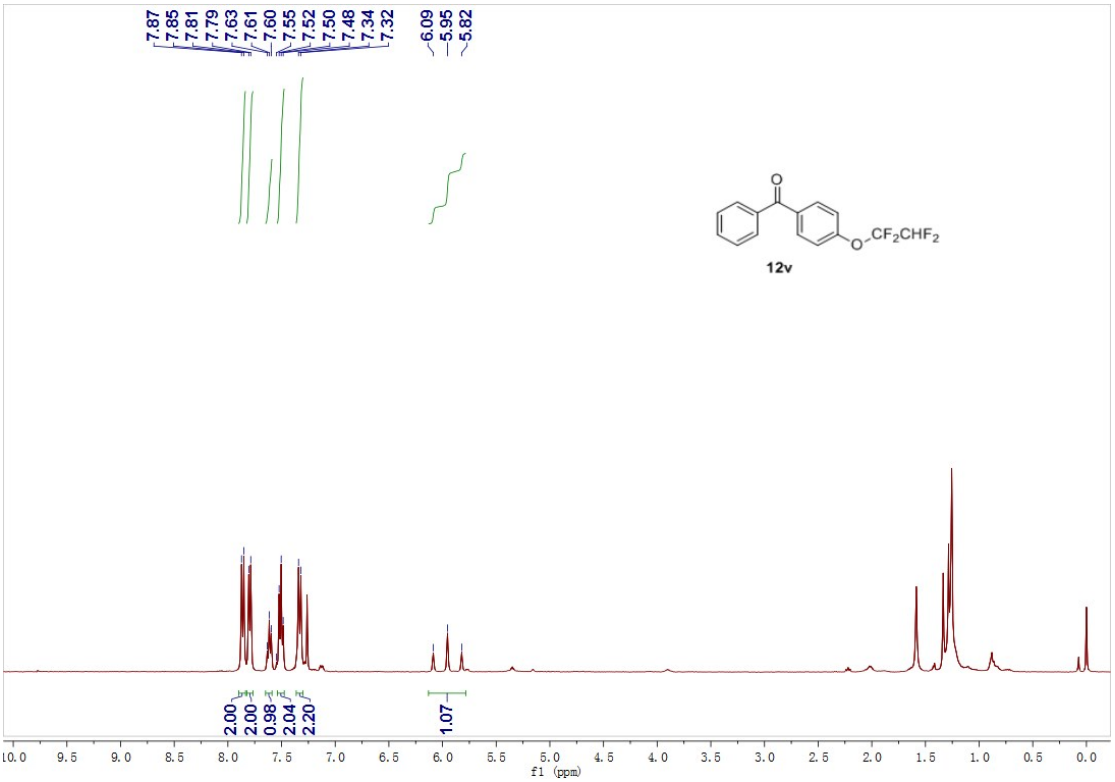

162.56
134.11
130.49
128.92
127.25
127.12
126.94
126.40
125.61
121.17
120.17

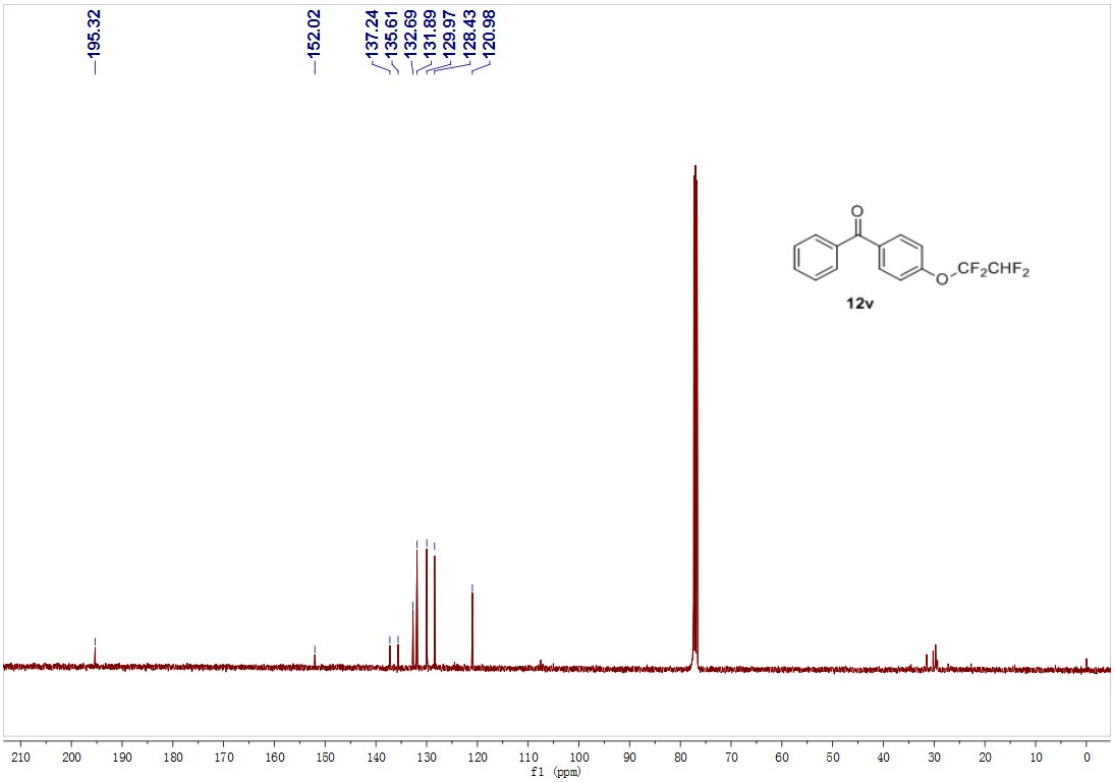

67.13

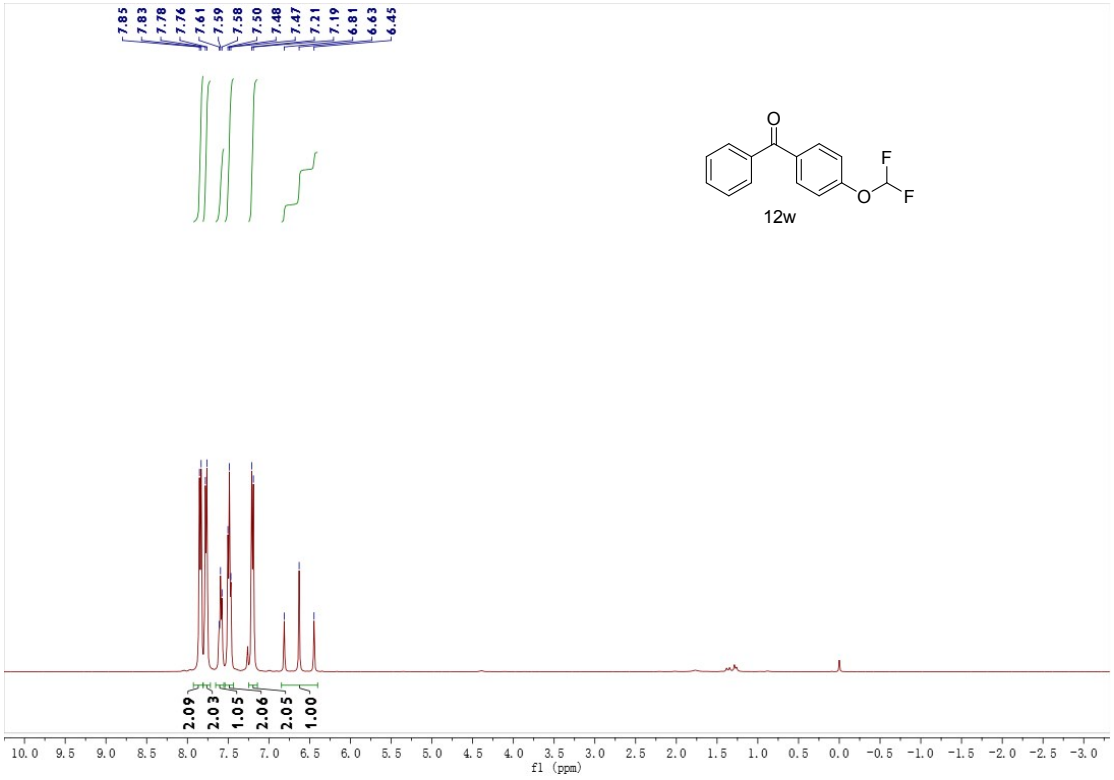

H
N
CHCl2
O

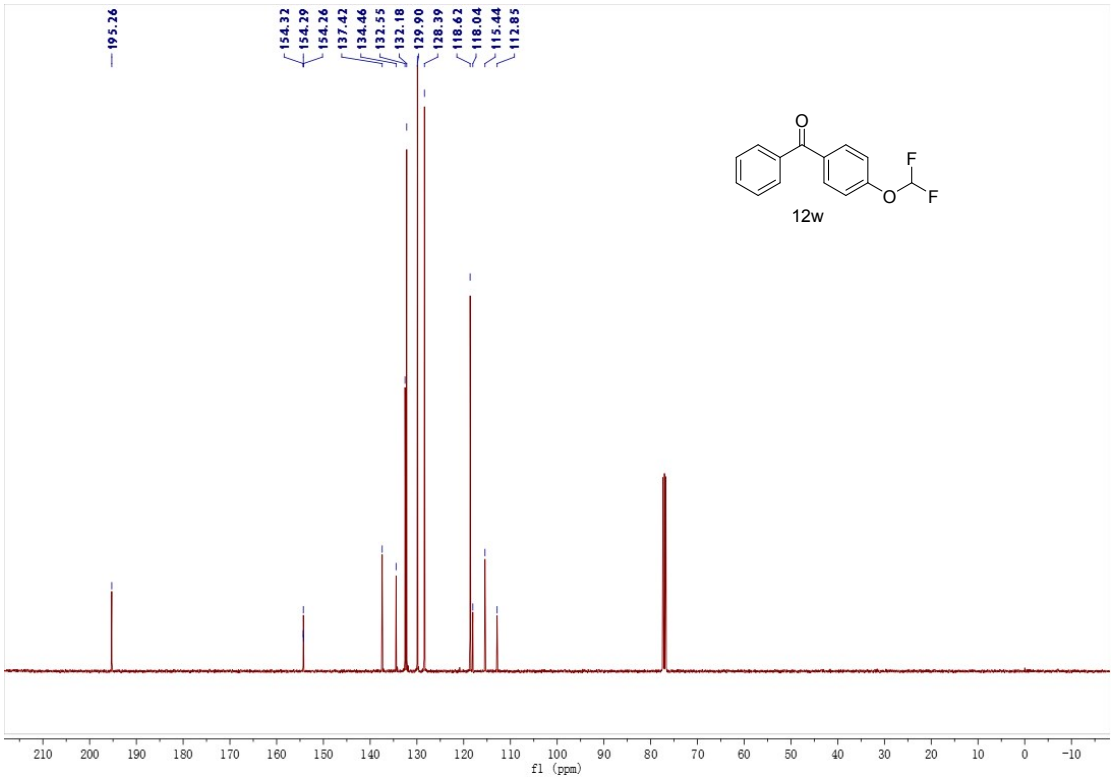
12u

f1 (ppm)

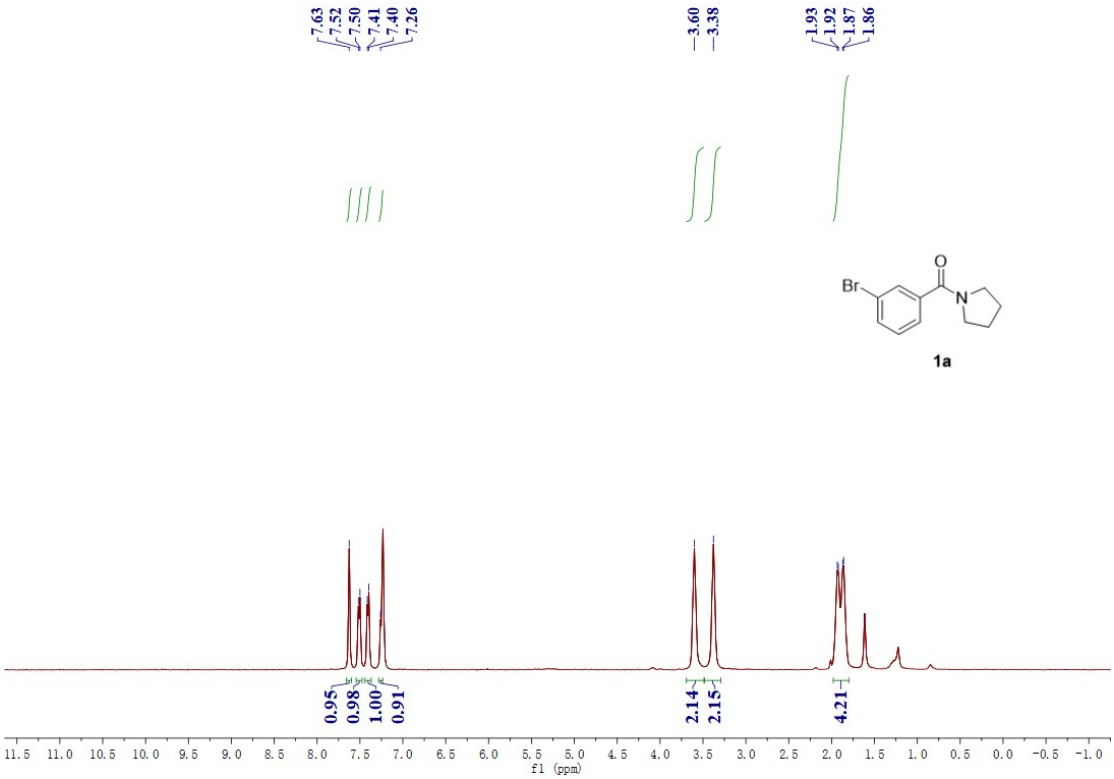

7.87
7.85
7.81
7.79
7.63
7.61
7.60
7.55
7.52
7.50
7.48
7.34
7.32
6.09
5.95
5.82
O
O
CF2CHF2
12v
2.00
2.00
0.98
2.04
2.20
1.07
f1 (ppm)

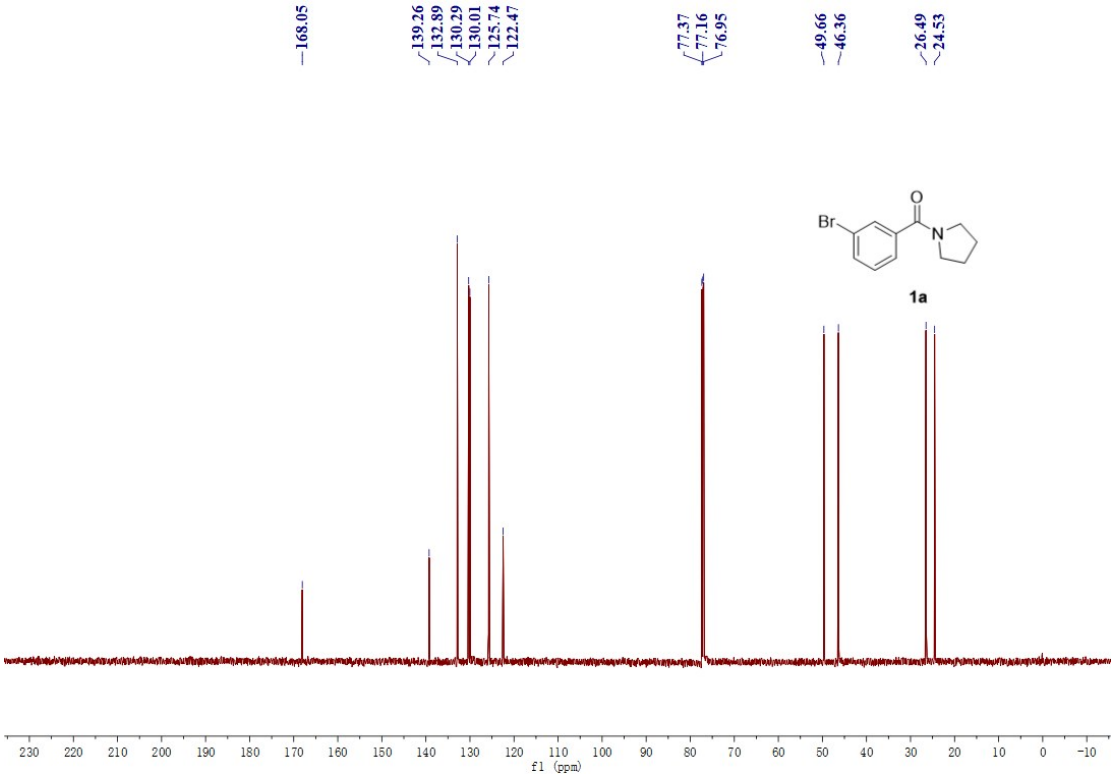

195.32
152.02
137.24
135.61
132.69
131.89
129.97
128.43
120.98
O
O
CF2CHF2
12v
f1 (ppm)

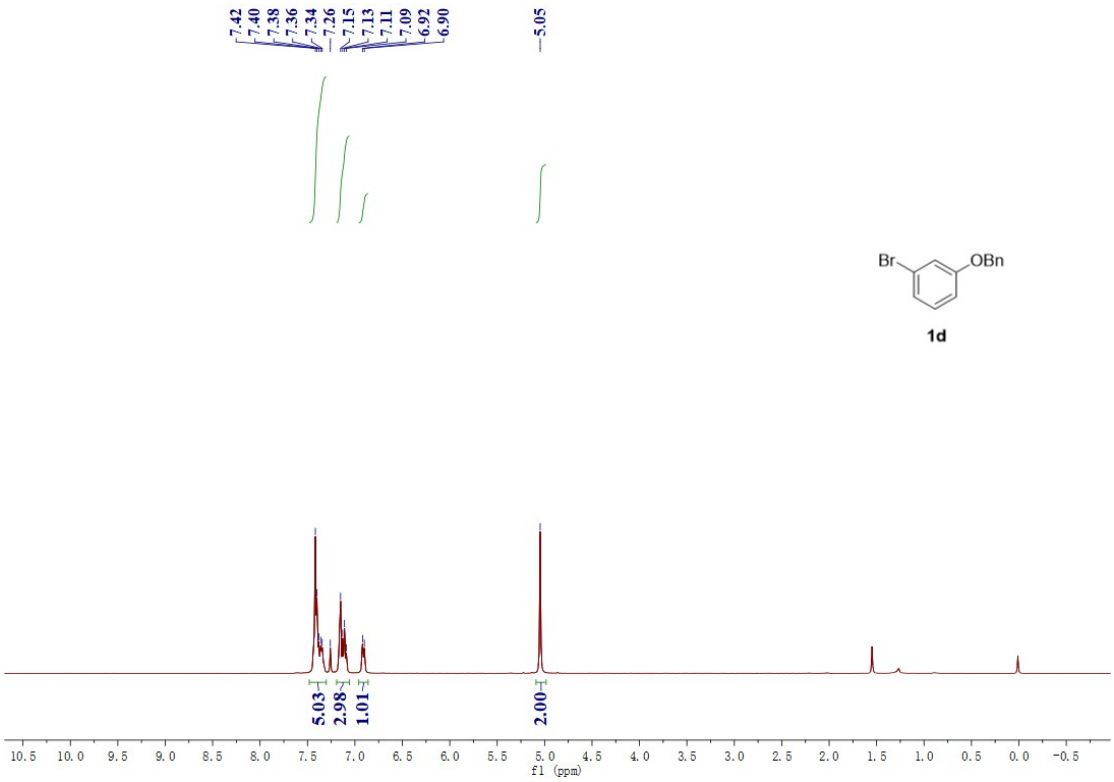

7.85
7.83
7.78
7.76
7.61
7.59
7.58
7.50
7.48
7.47
7.21
7.19
6.81
6.63
6.45
O
F
O
F
12w
2.09
2.03
1.05
2.06
2.05
1.00
f1 (ppm)

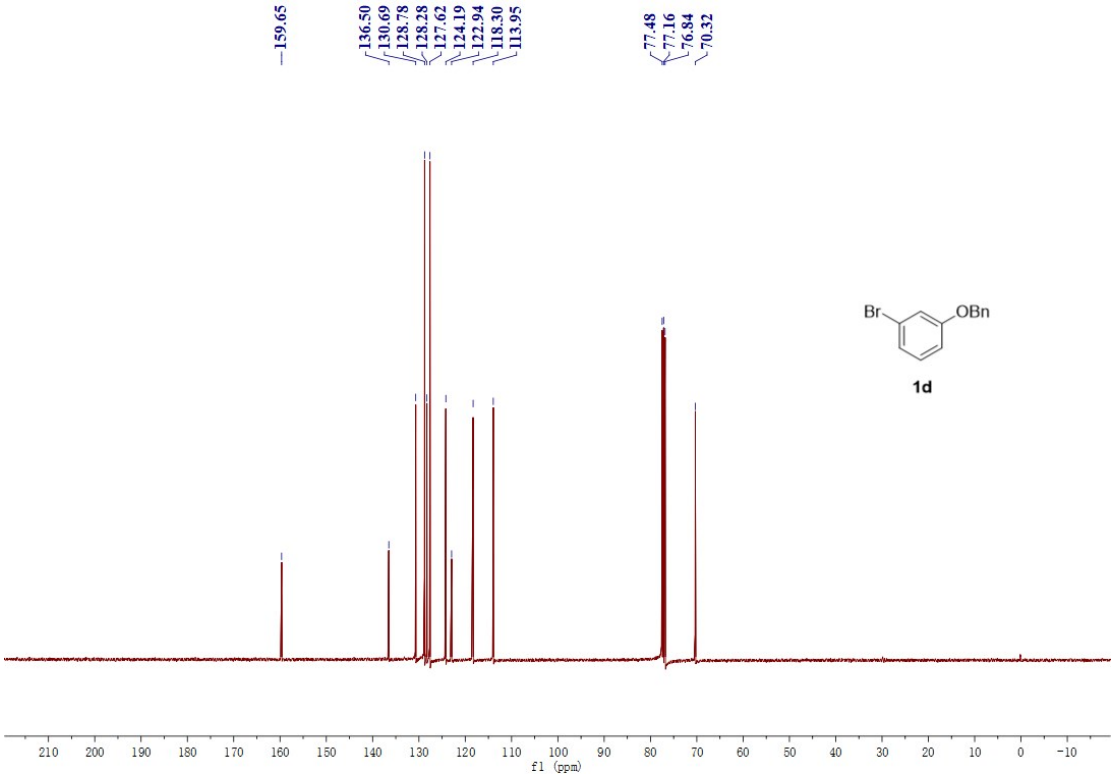

195.26
154.32
154.29
154.26
137.42
134.46
132.55
132.18
129.90
128.39
118.62
118.04
115.44
112.85
O
F
O
F
12w
f1 (ppm)

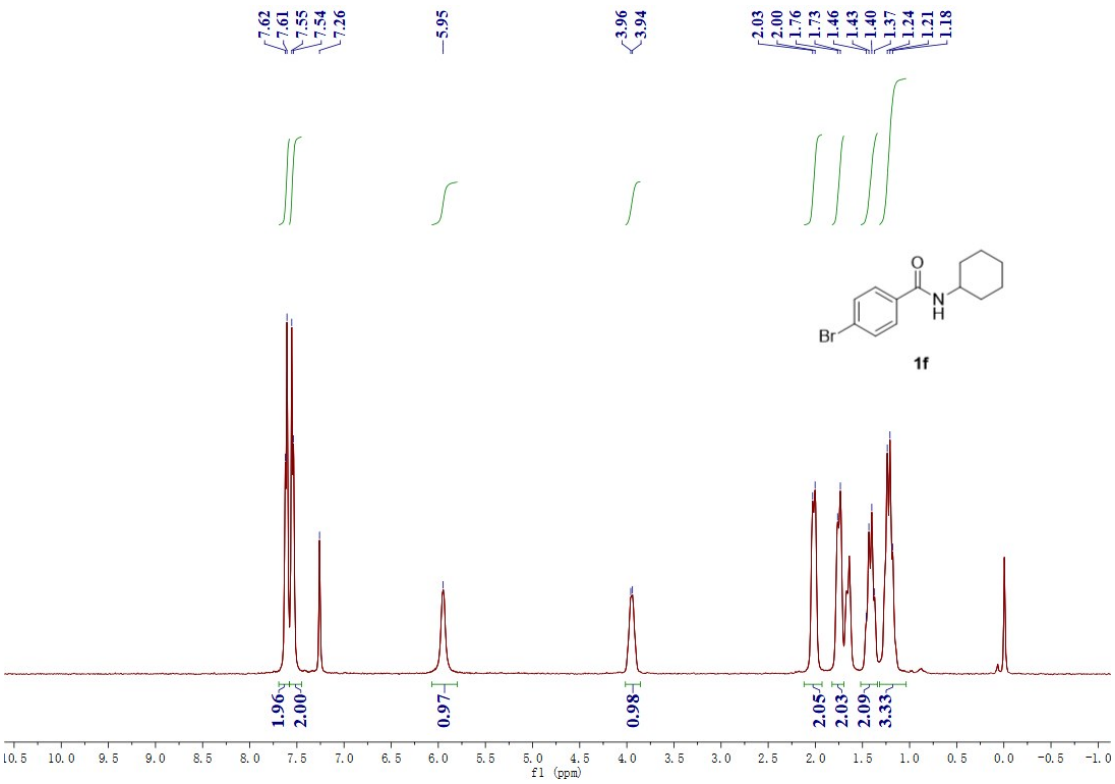
11. ^{1}H and ^{13}C NMR spectra of some substrates

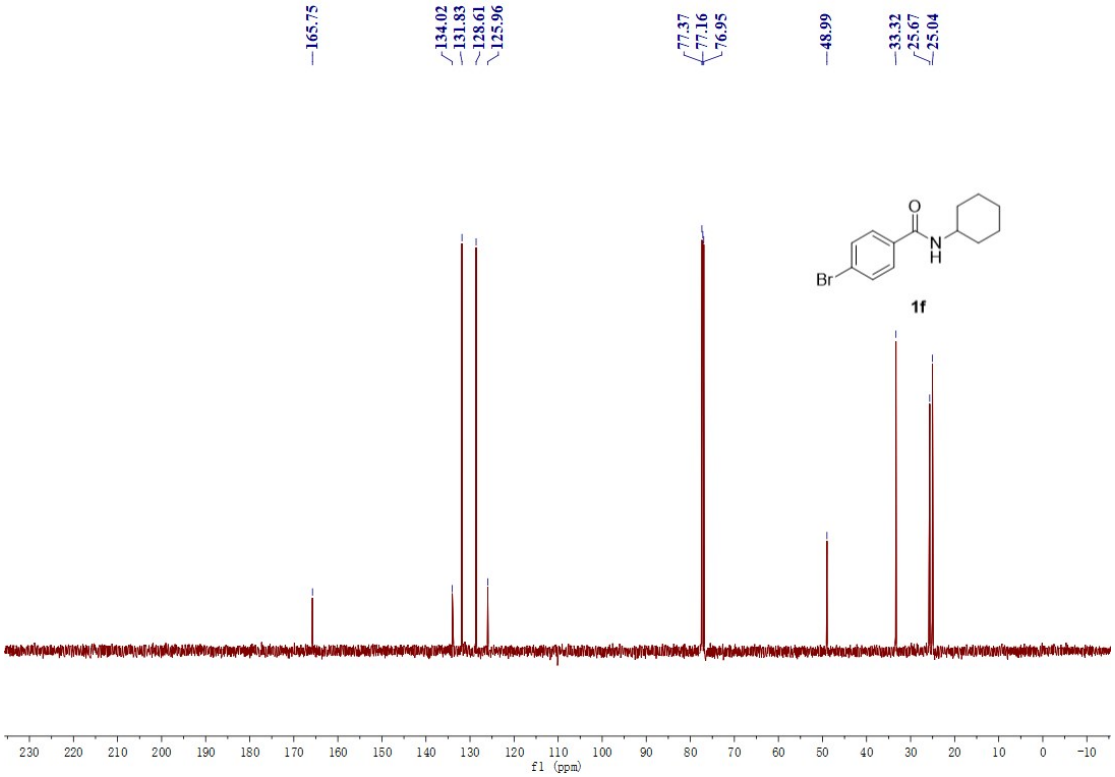


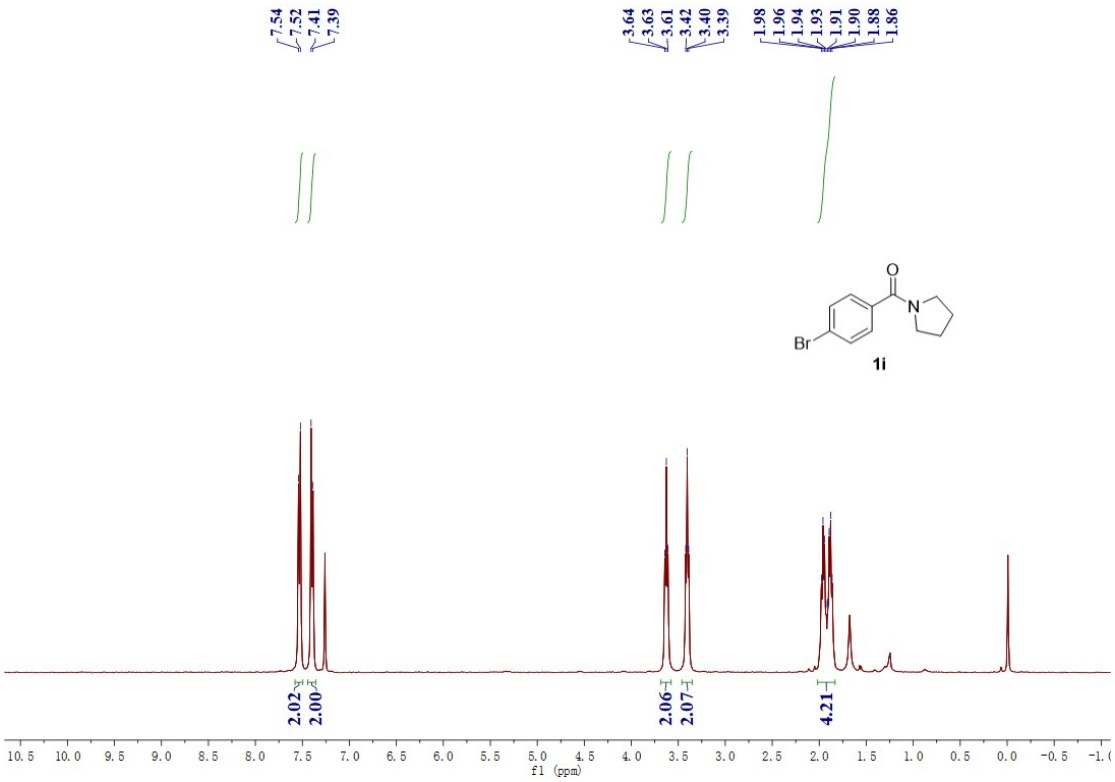


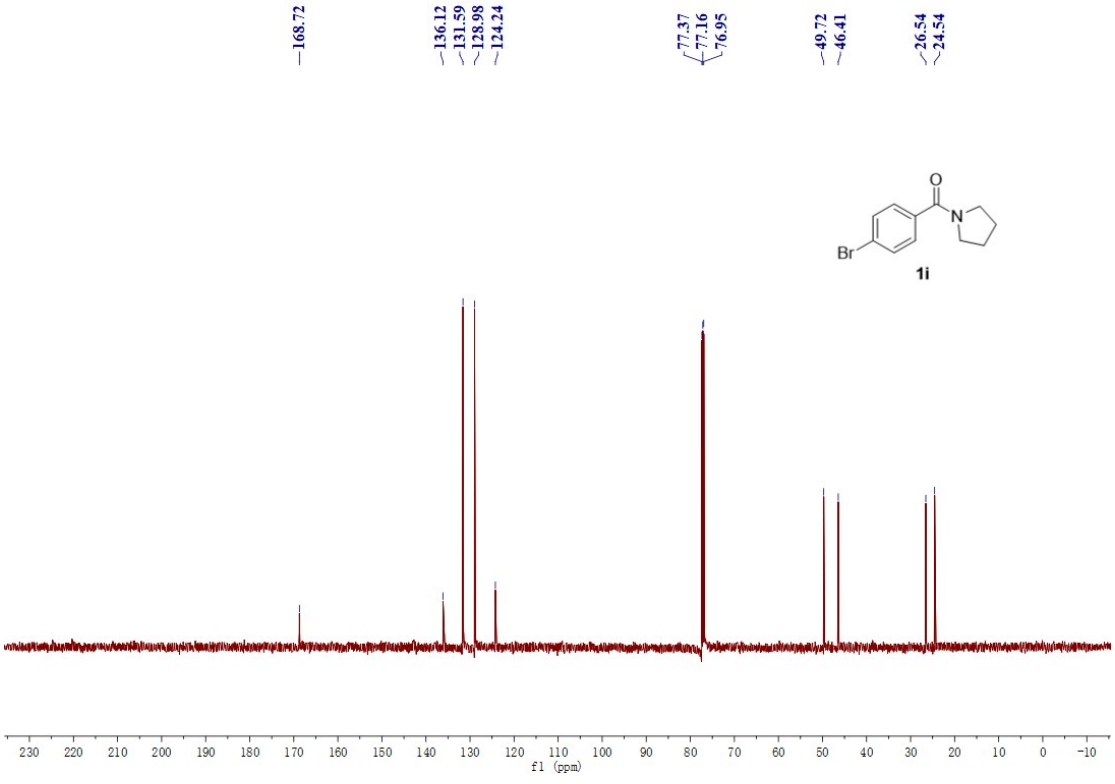

7.42
7.40
7.38
7.36
7.34
7.26
7.15
7.13
7.11
7.09
6.92
6.90
5.05
Br
OBn
1d
5.03
2.98
1.01
2.00
f1 (ppm)

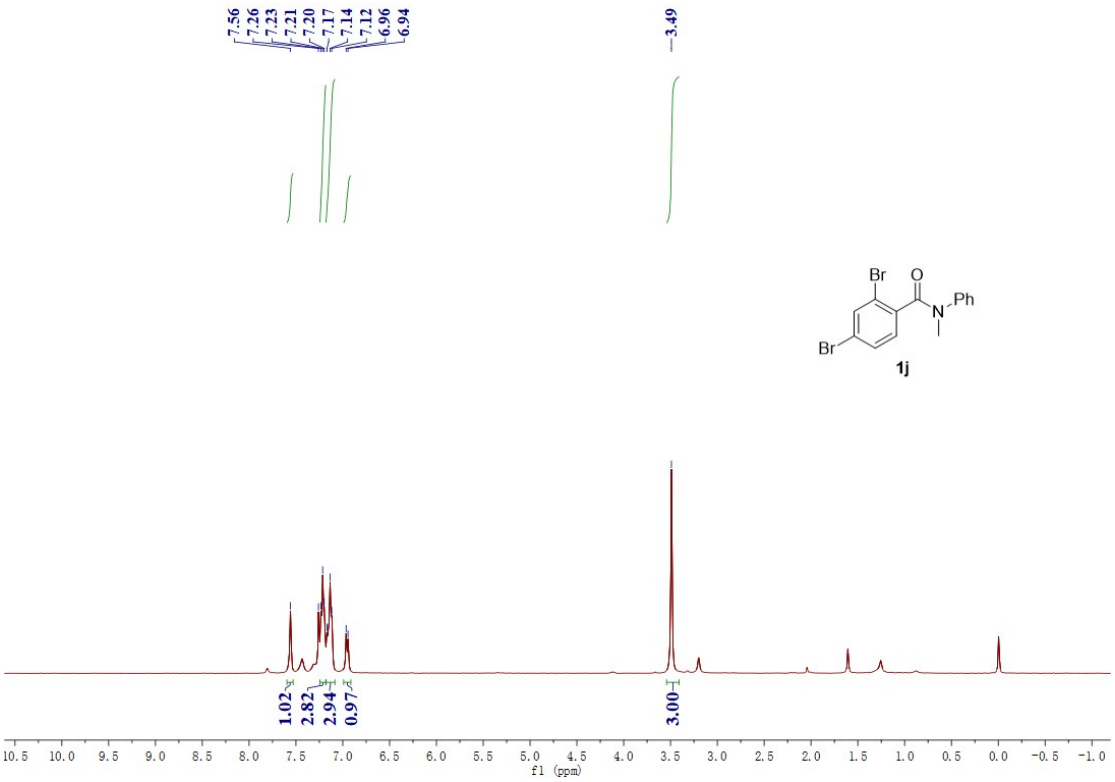

159.65
136.50
130.69
128.78
128.28
127.62
124.19
122.94
118.30
113.95
77.48
77.16
76.84
70.32
Br
OBn
1d
f1 (ppm)

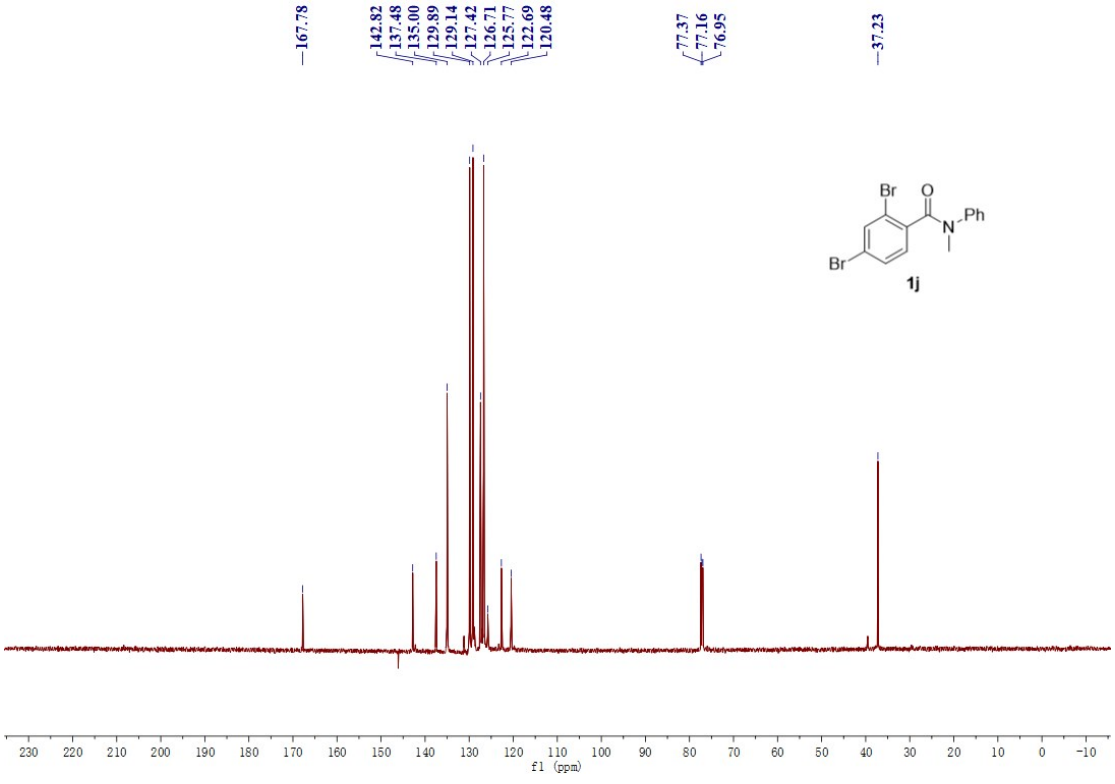

7.62
7.61
7.55
7.54
7.26
5.95
3.96
3.94
2.03
2.00
1.76
1.73
1.46
1.43
1.40
1.37
1.24
1.21
1.18
O
N
H
Br
1f
1.96
2.00
0.97
0.98
2.05
2.03
2.09
3.33
f1 (ppm)

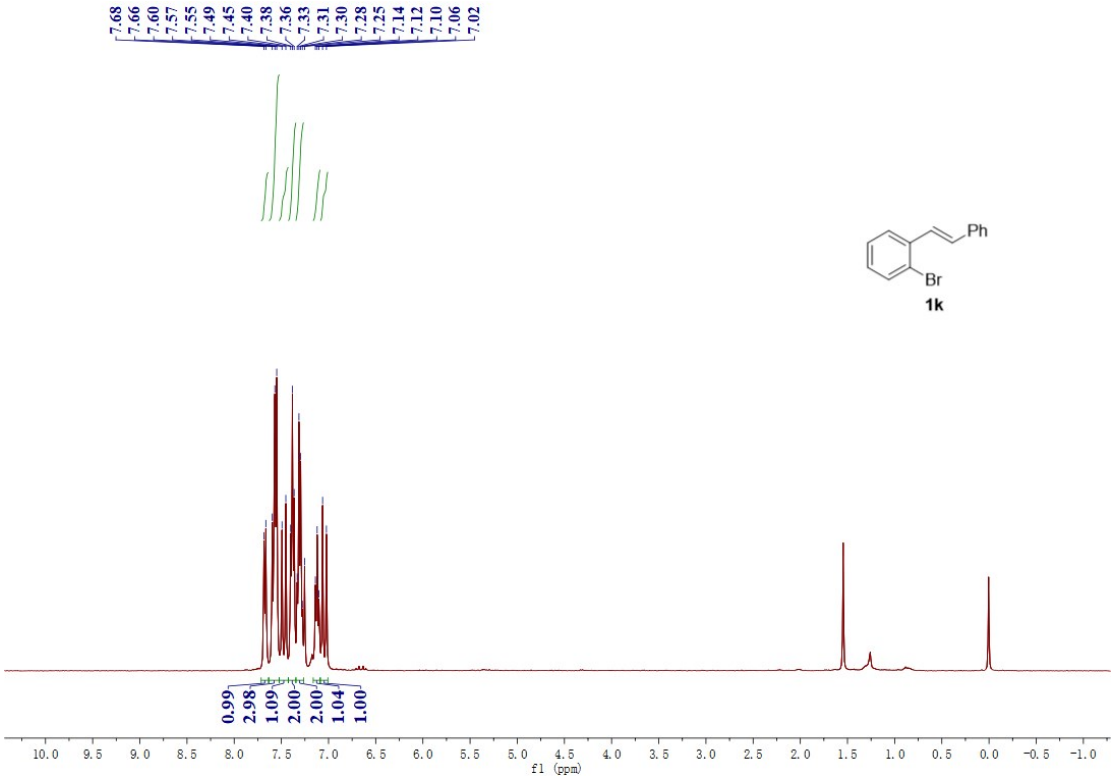

165.75
134.02
131.83
128.61
125.96
77.37
77.16
76.95
48.99
33.32
25.67
25.04
O
N
H
Br
1f
f1 (ppm)

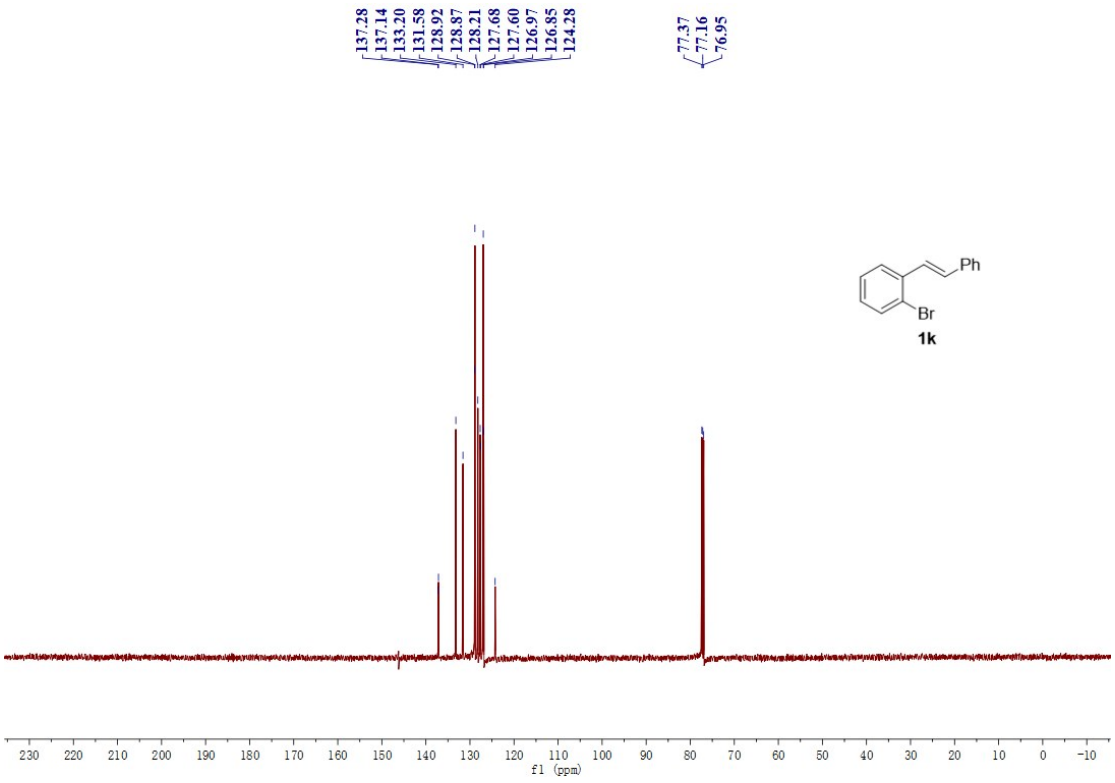

7.54
7.52
7.41
7.39
3.64
3.63
3.61
3.42
3.40
3.39
1.98
1.96
1.94
1.93
1.91
1.90
1.88
1.86
O
N
Br
1i
2.02
2.00
2.06
2.07
4.21
f1 (ppm)

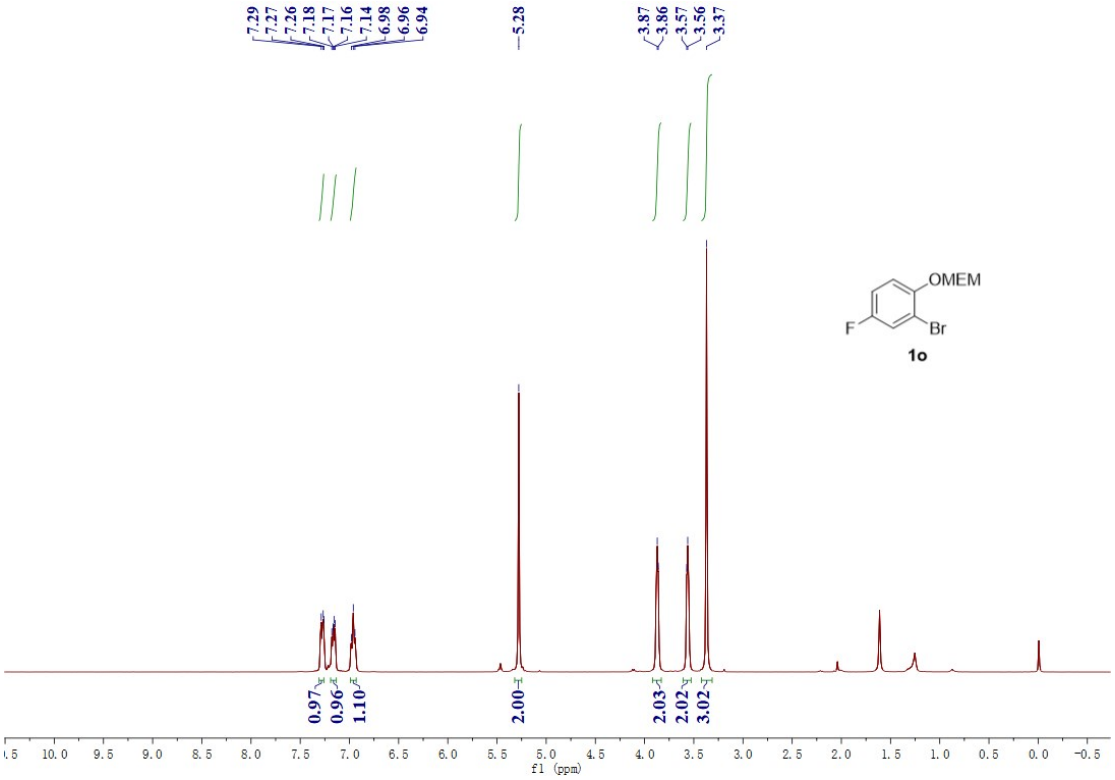

168.72
136.12
131.59
128.98
124.24
77.37
77.16
76.95
49.72
46.41
26.54
24.54
O
N
Br
1i
f1 (ppm)

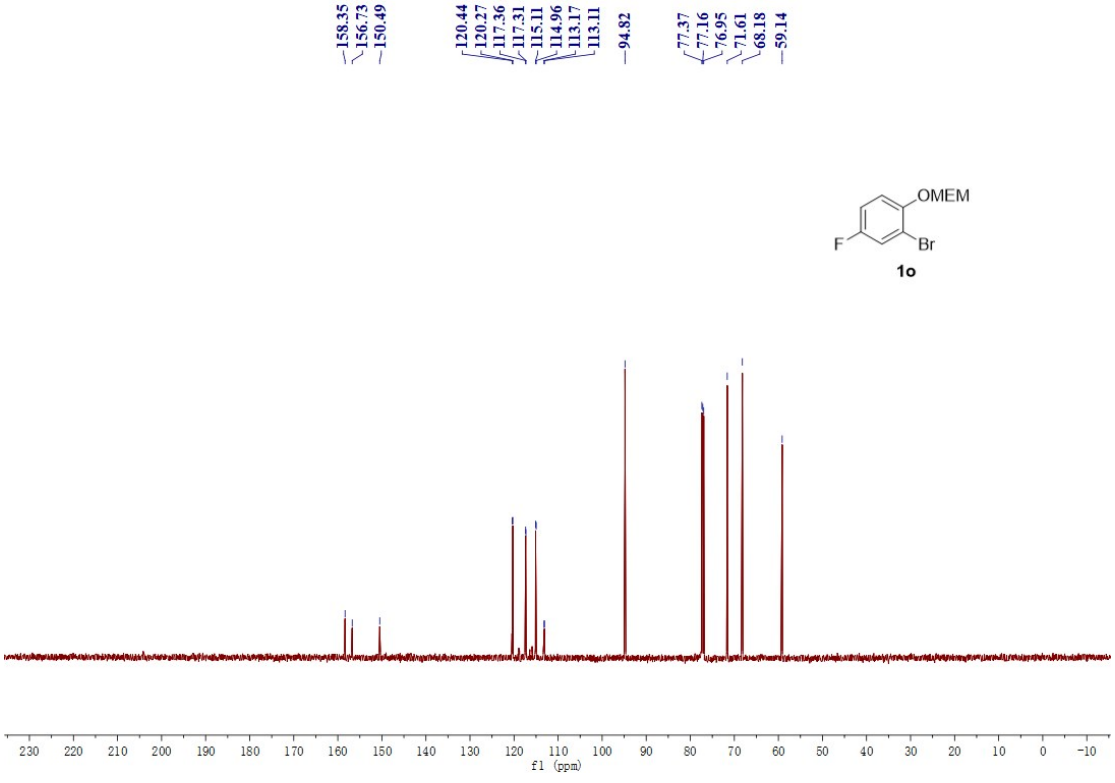

7.56
7.26
7.23
7.21
7.20
7.17
7.14
7.12
6.96
6.94
3.49
Br
O
N
Ph
Br
1j
1.02
2.82
2.94
0.97
3.00
f1 (ppm)

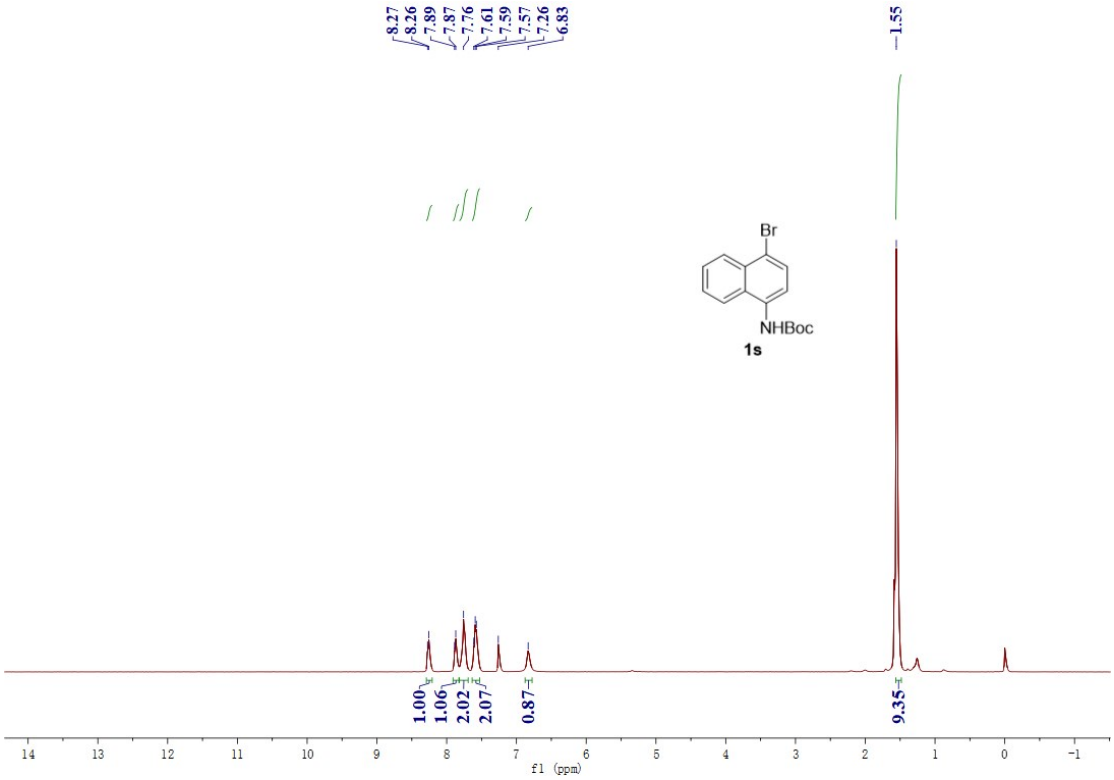

167.78
142.82
137.48
135.00
129.89
129.14
127.42
126.71
125.77
122.69
120.48
77.37
77.16
76.95
37.23
Br
O
N
Ph
Br
1j
f1 (ppm)

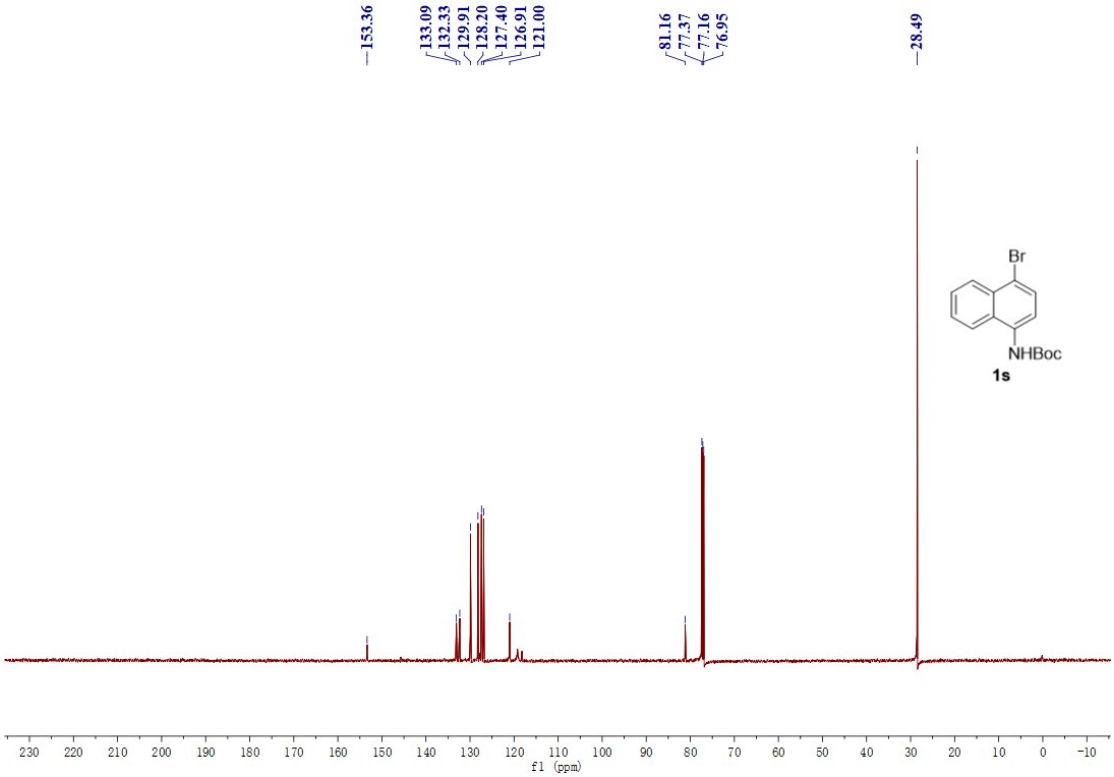

7.68
7.66
7.60
7.57
7.55
7.49
7.45
7.40
7.38
7.36
7.33
7.31
7.30
7.28
7.25
7.14
7.12
7.10
7.06
7.02
Ph
Br
1k
0.99
2.98
1.09
2.00
2.00
1.04
1.00
f1 (ppm)

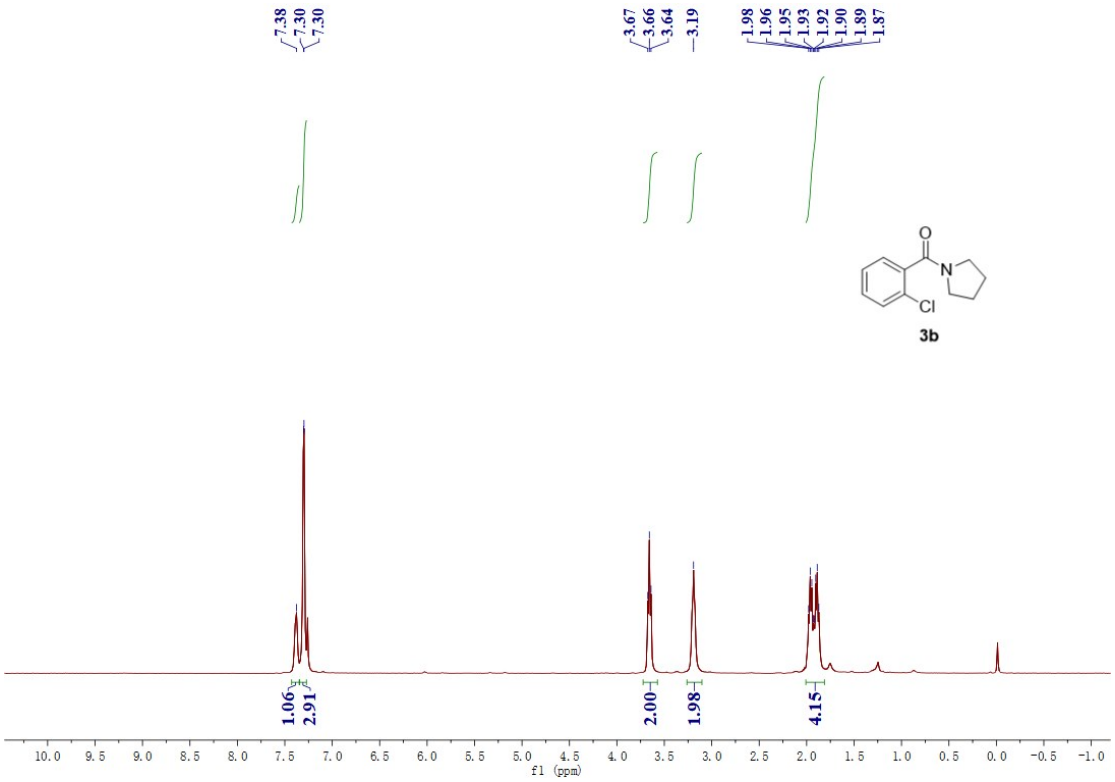

137.28
137.14
133.20
131.58
128.92
128.87
128.21
127.68
127.60
126.97
126.85
124.28
77.37
77.16
76.95
Ph
Br
1k
f1 (ppm)

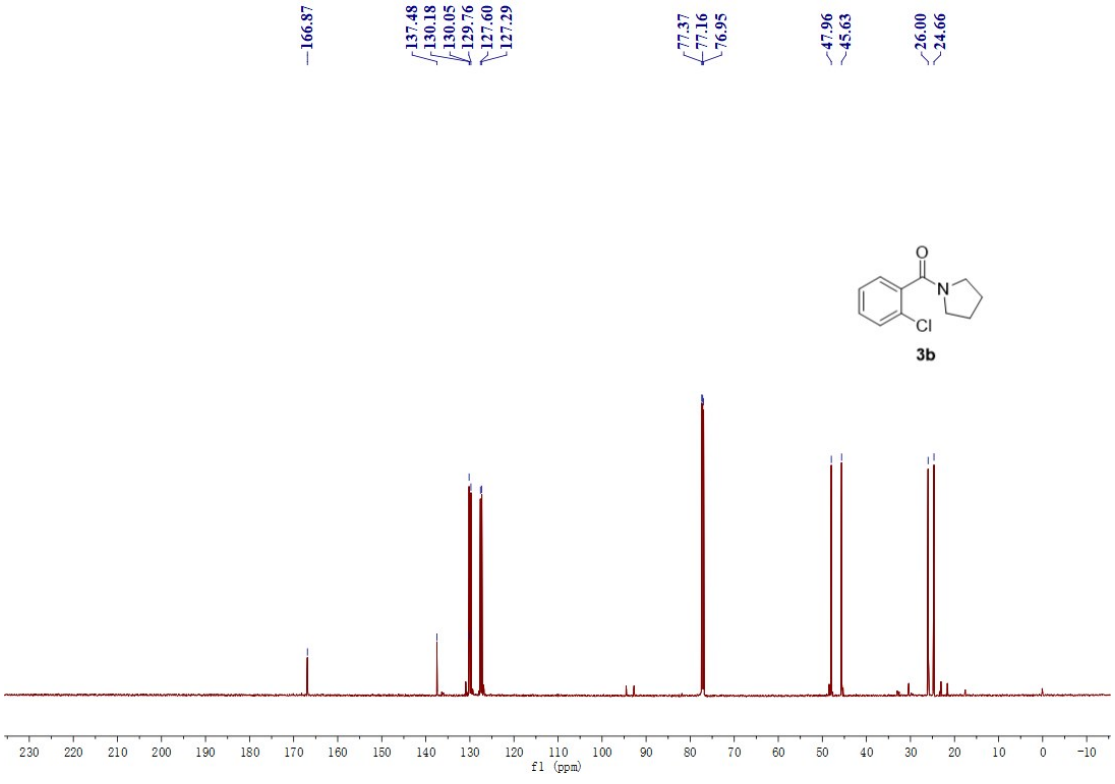

7.29
7.27
7.26
7.18
7.17
7.16
7.14
6.98
6.96
6.94
5.28
3.87
3.86
3.57
3.56
3.37
OMEM
F
Br
1o
0.97
0.96
1.10
2.00
2.03
2.02
3.02
f1 (ppm)


158.35
156.73
150.49
120.44
120.27
117.36
117.31
115.11
114.96
113.17
113.11
94.82
77.37
77.16
76.95
71.61
68.18
59.14
OMEM
F
Br
1o
f1 (ppm)


8.27
8.26
7.89
7.87
7.76
7.61
7.59
7.57
7.26
6.83
1.55
Br
NHBoc
1s
1.00
1.06
2.02
2.07
0.87
9.35
f1 (ppm)


153.36
133.09
132.33
129.91
128.20
127.40
126.91
121.00
81.16
77.37
77.16
76.95
28.49
Br
NHBoc
1s
f1 (ppm)


7.38
7.30
7.30
3.67
3.66
3.64
3.19
1.98
1.96
1.95
1.93
1.92
1.90
1.89
1.87
O
N
Cl
3b
1.06
2.91
2.00
1.98
4.15
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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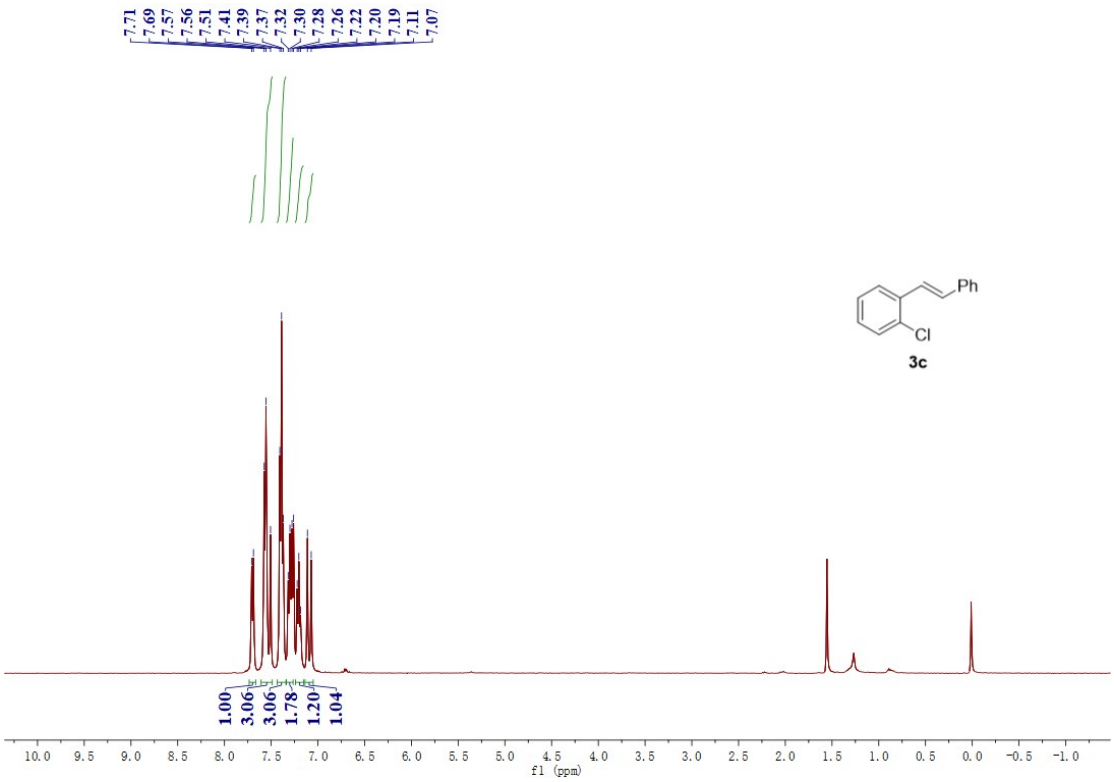
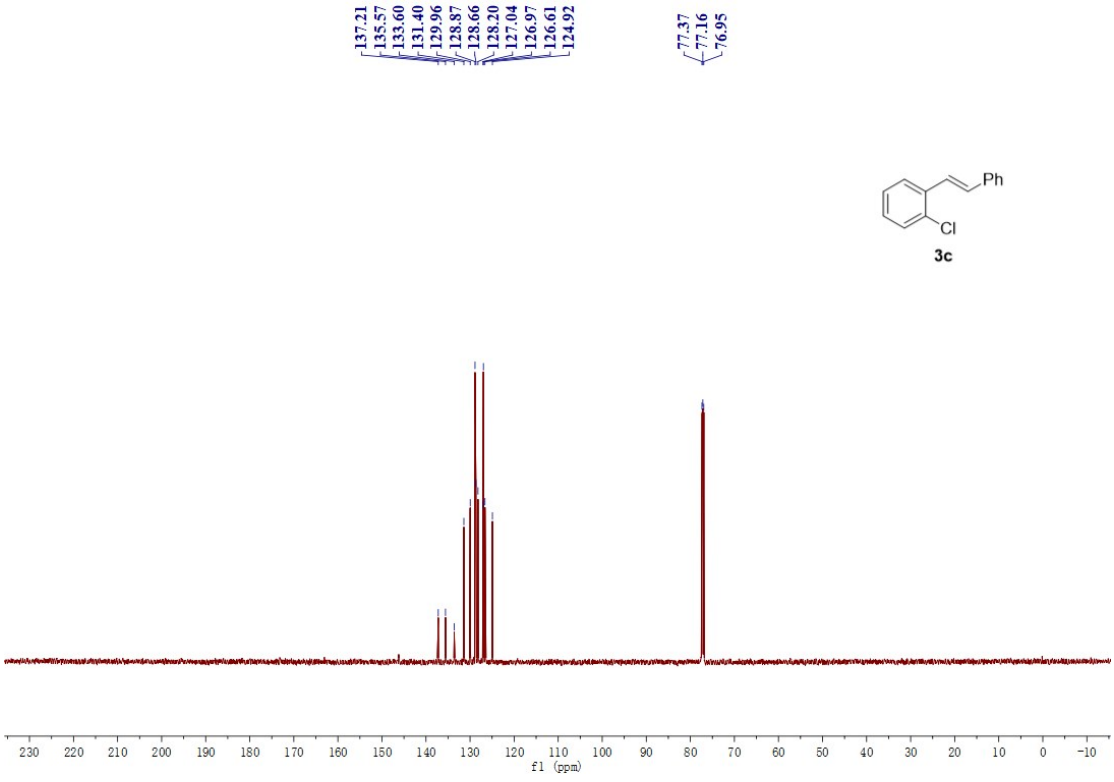
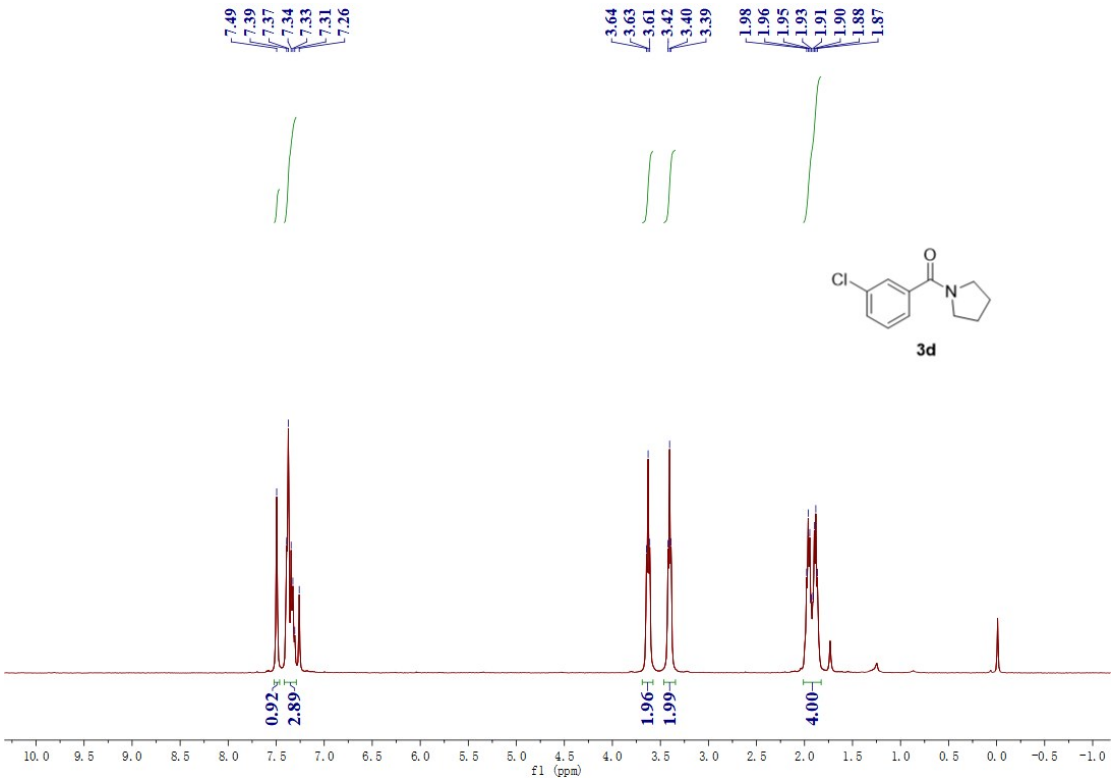
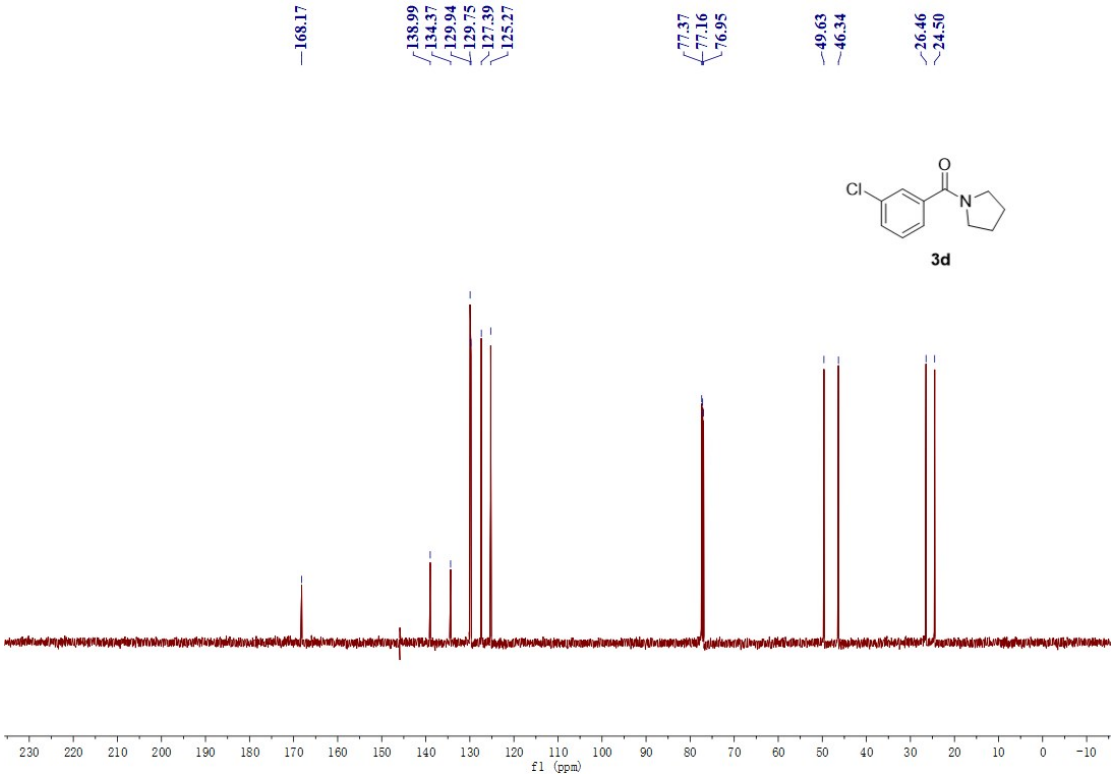
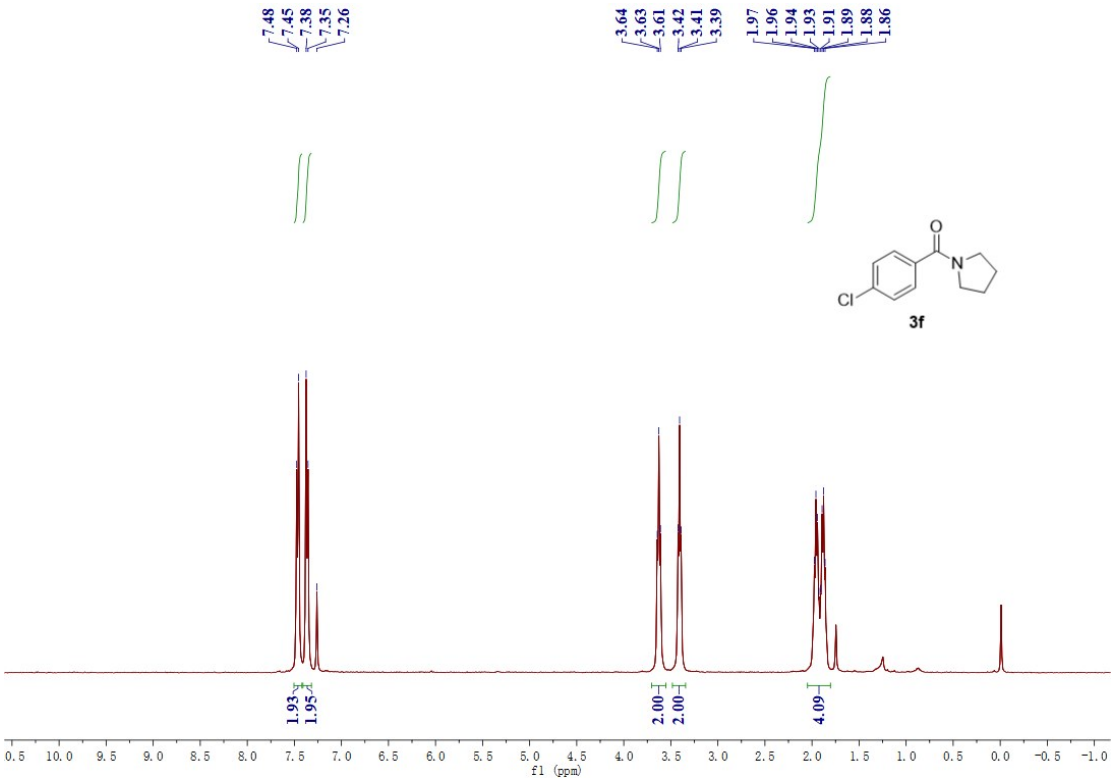
130.18
130.05
129.76
127.60
127.29
77.37
77.16
76.95
47.96
45.63
26.00
24.66
O
N
Cl
3b
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.71
7.69
7.57
7.56
7.51
7.41
7.39
7.37
7.32
7.30
7.28
7.26
7.22
7.20
7.19
7.11
7.07
Ph
Cl
3c
1.00
3.06
3.06
1.78
1.20
1.04
f1 (ppm)


137.21
135.57
133.60
131.40
129.96
128.87
128.66
128.20
127.04
126.97
126.61
124.92
77.37
77.16
76.95
Ph
Cl
3c
f1 (ppm)


7.49
7.39
7.37
7.34
7.33
7.31
7.26
3.64
3.63
3.61
3.42
3.40
3.39
1.98
1.96
1.95
1.93
1.91
1.90
1.88
1.87
Cl
O
N
3d
0.92
2.89
1.96
1.99
4.00
f1 (ppm)


168.17
138.99
134.37
129.94
129.75
127.39
125.27
77.37
77.16
76.95
49.63
46.34
26.46
24.50
Cl
O
N
3d
f1 (ppm)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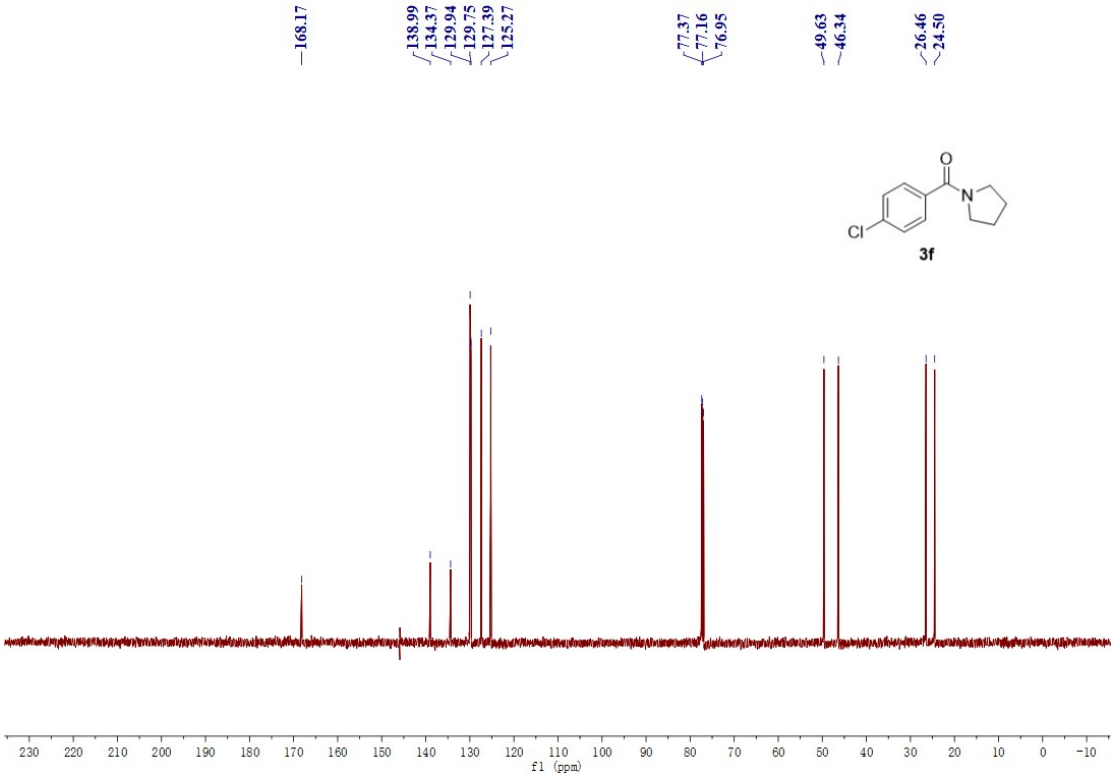
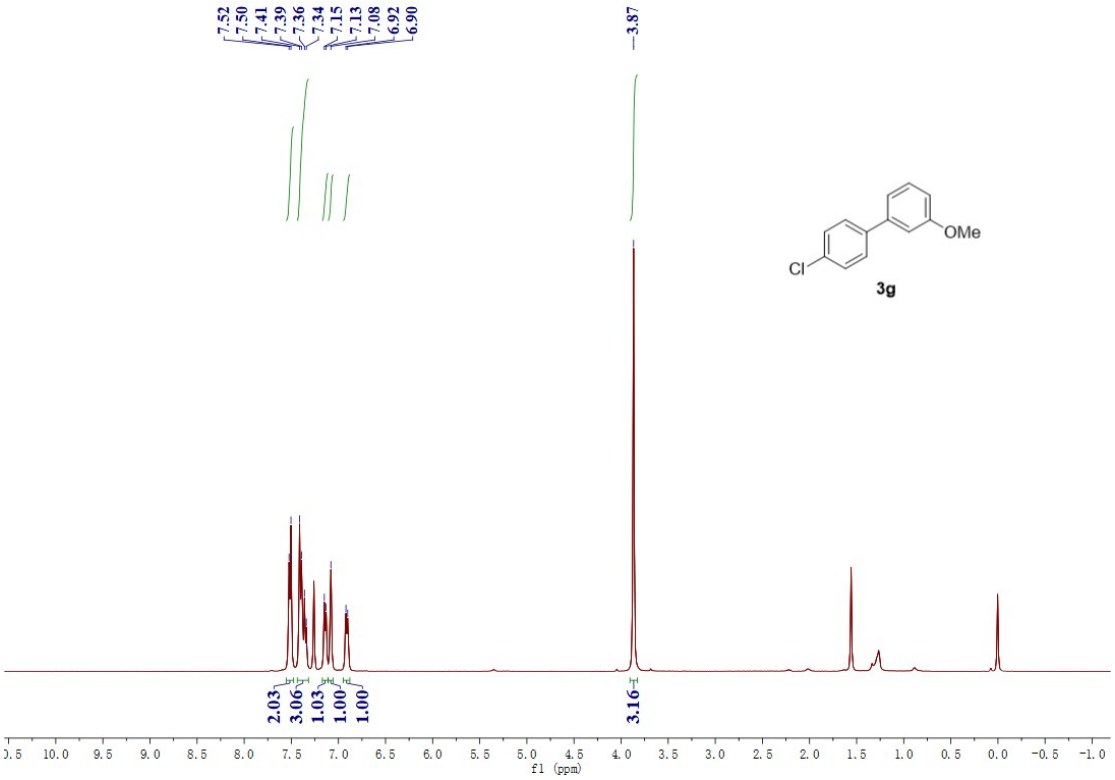
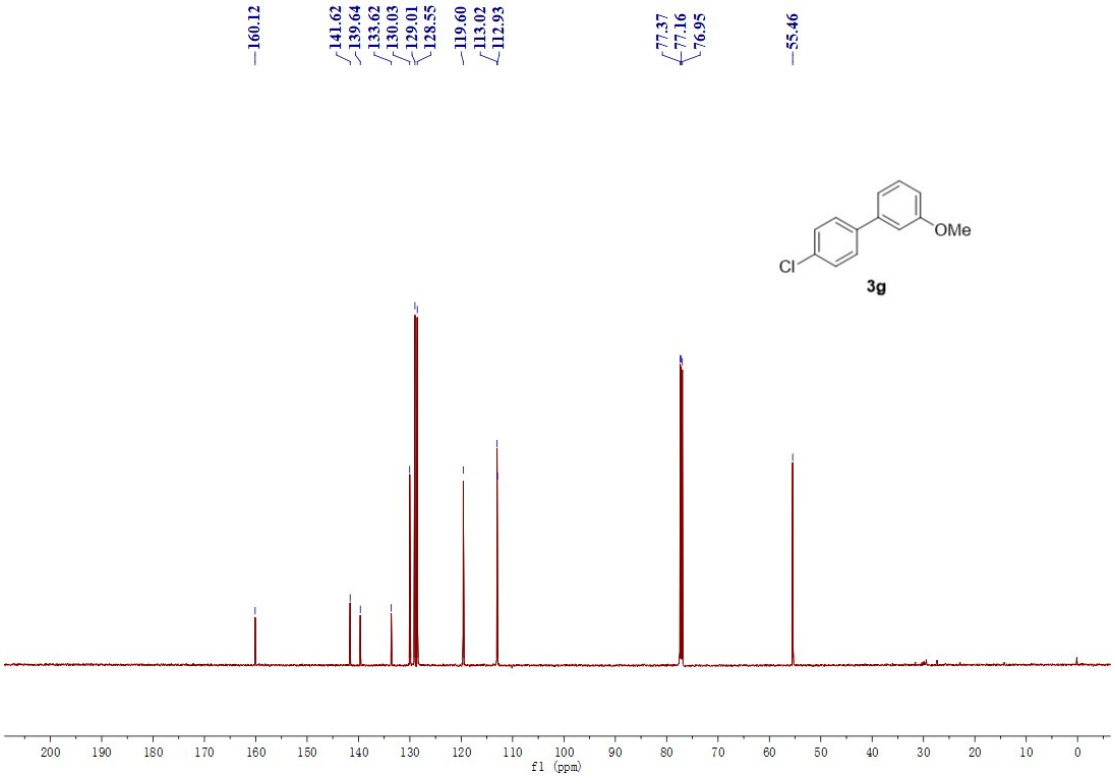
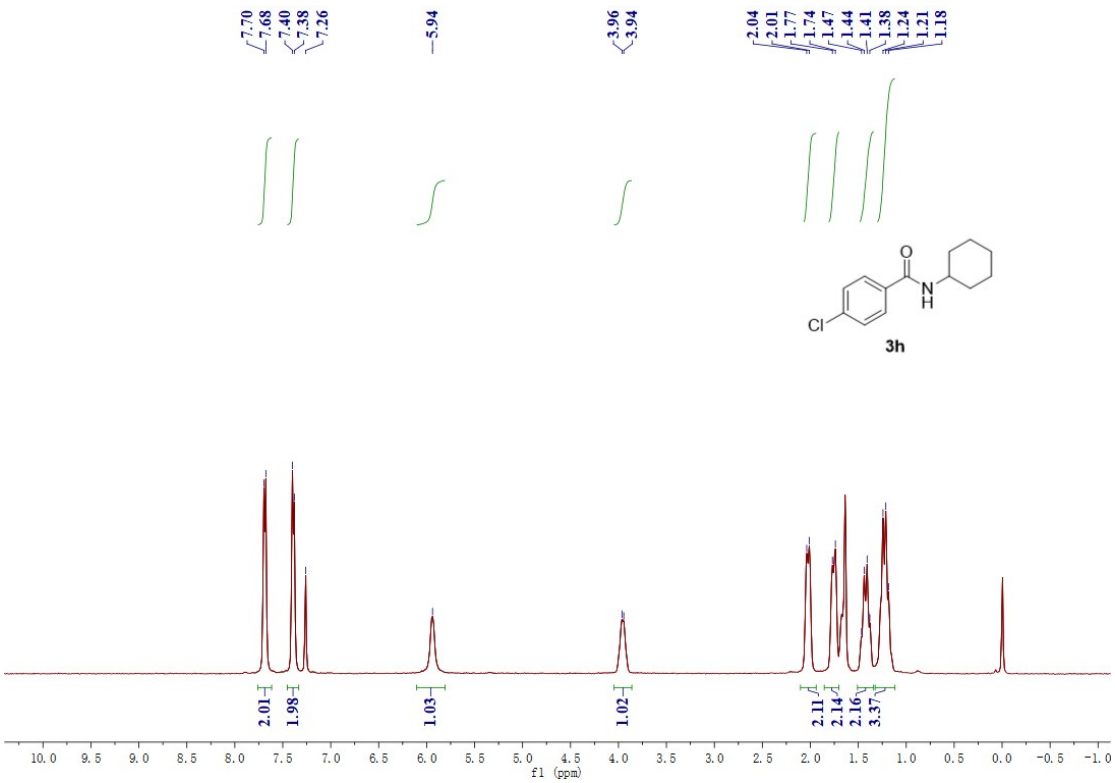
7.45
7.38
7.35
7.26
3.64
3.63
3.61
3.42
3.41
3.39
1.97
1.96
1.94
1.93
1.91
1.89
1.88
1.86
O
N
Cl
3f
1.93
1.95
2.00
2.00
4.09
f1 (ppm)


168.17
138.99
134.37
129.94
129.75
127.39
125.27
77.37
77.16
76.95
49.63
46.34
26.46
24.50
O
N
Cl
3f
f1 (ppm)


7.52
7.50
7.41
7.39
7.36
7.34
7.15
7.13
7.08
6.92
6.90
3.87
OMe
Cl
3g
2.03
3.06
1.03
1.00
1.00
3.16
f1 (ppm)


160.12
141.62
139.64
133.62
130.03
129.01
128.55
119.60
113.02
112.93
77.37
77.16
76.95
55.46
OMe
Cl
3g
f1 (ppm)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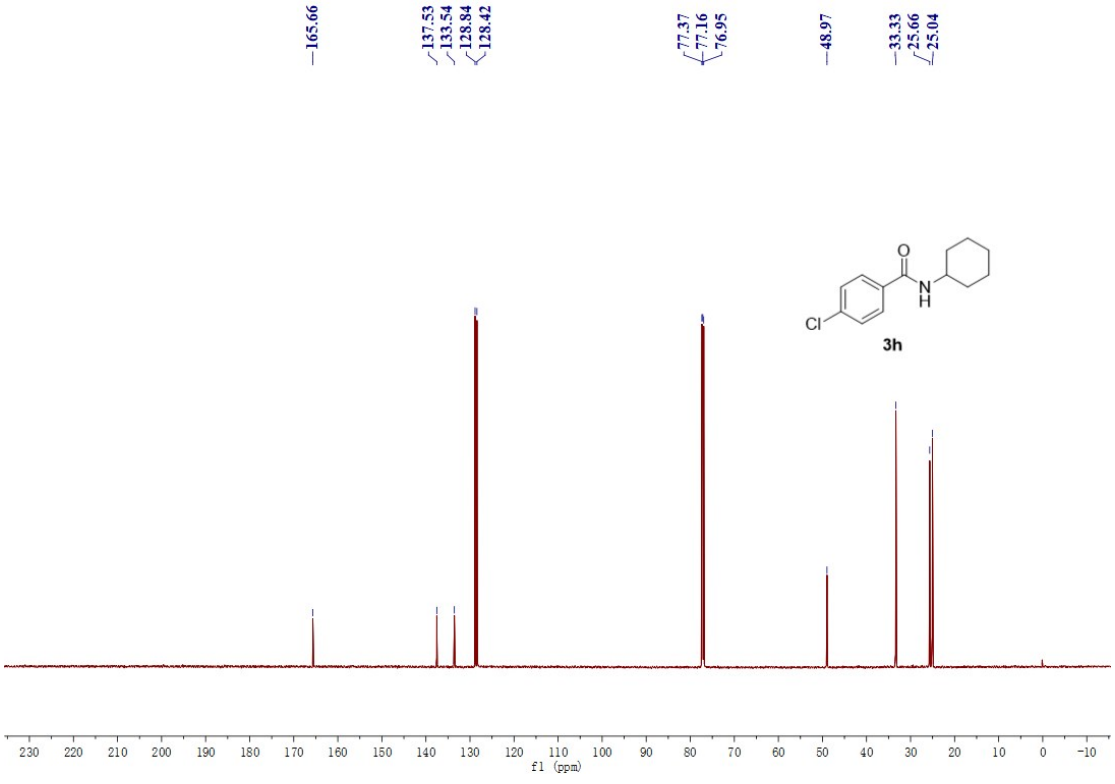
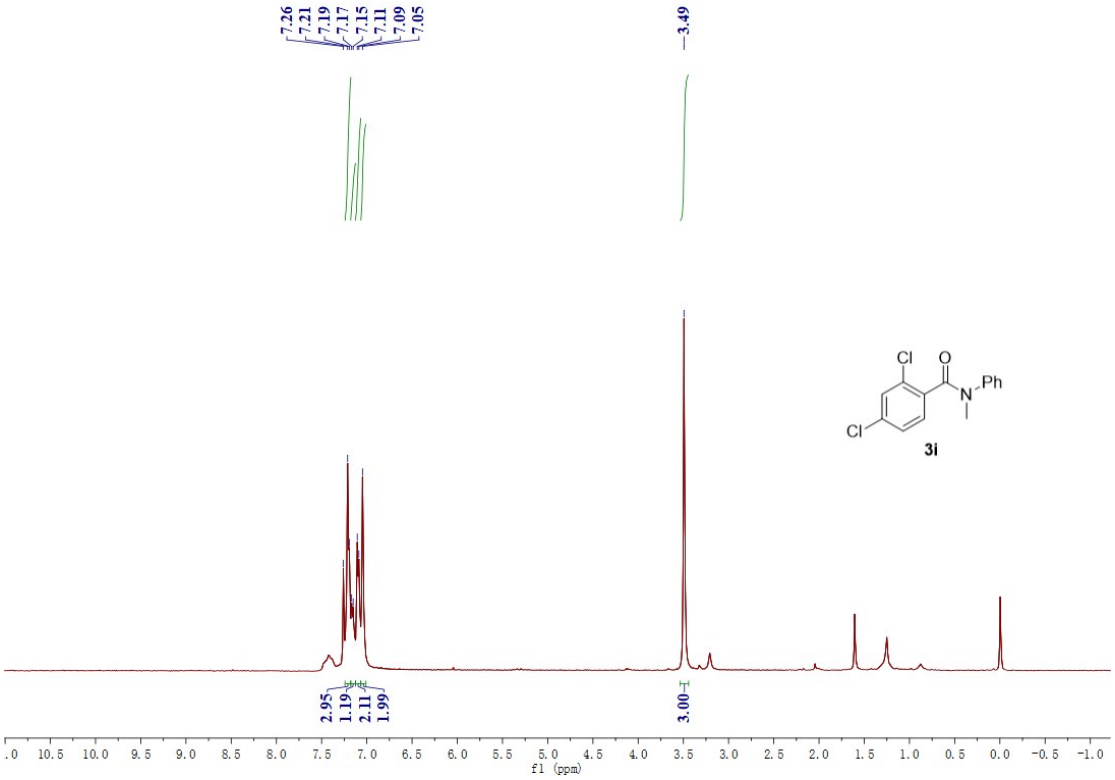
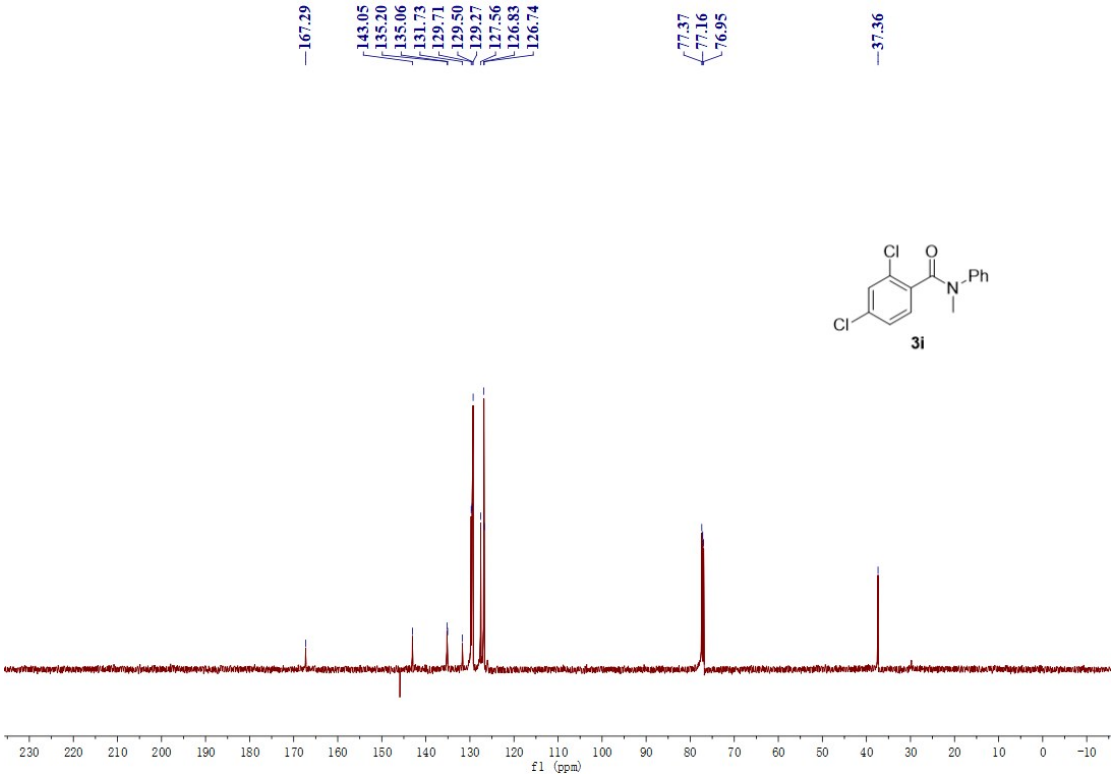
7.68
7.40
7.38
7.26
5.94
3.96
3.94
2.04
2.01
1.77
1.74
1.47
1.44
1.41
1.38
1.24
1.21
1.18
O
N
H
Cl
3h
2.01
1.98
1.03
1.02
2.11
2.14
2.16
3.37
f1 (ppm)


165.66
137.53
133.54
128.84
128.42
77.37
77.16
76.95
48.97
33.33
25.66
25.04
O
N
H
Cl
3h
f1 (ppm)


7.26
7.21
7.19
7.17
7.15
7.11
7.09
7.05
3.49
Cl
O
N
Ph
Cl
3i
2.95
1.19
2.11
1.99
3.00
f1 (ppm)


167.29
143.05
135.20
135.06
131.73
129.71
129.50
129.27
127.56
126.83
126.74
77.37
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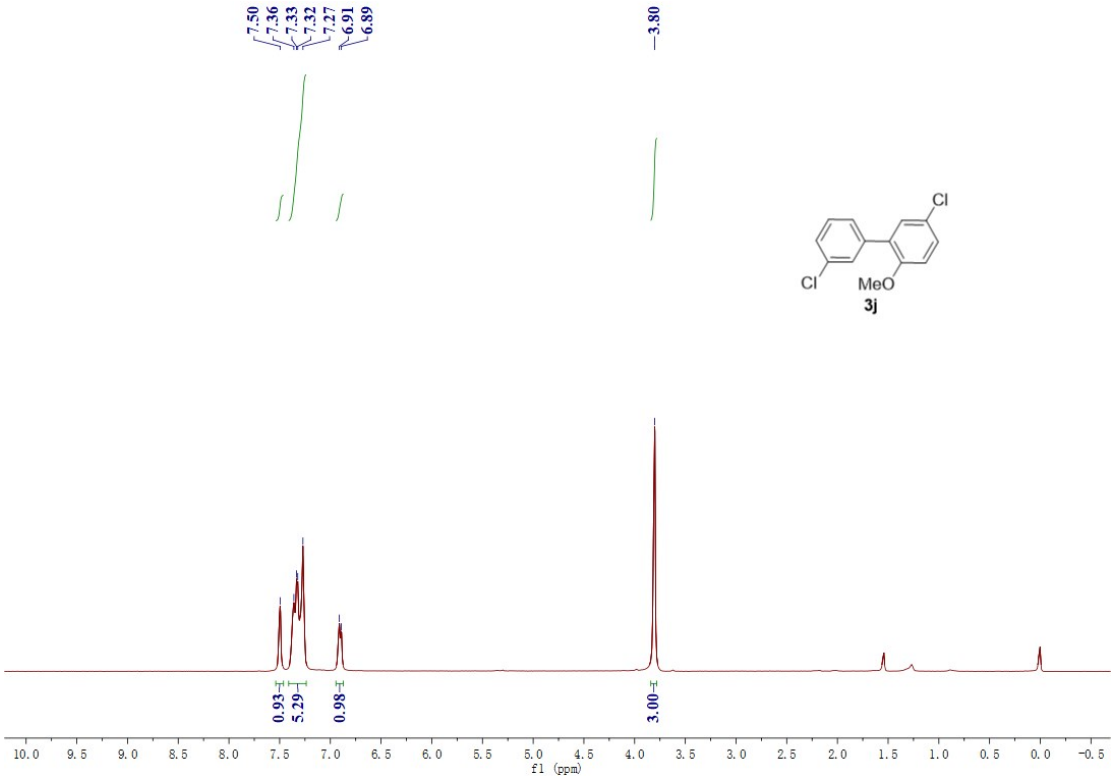
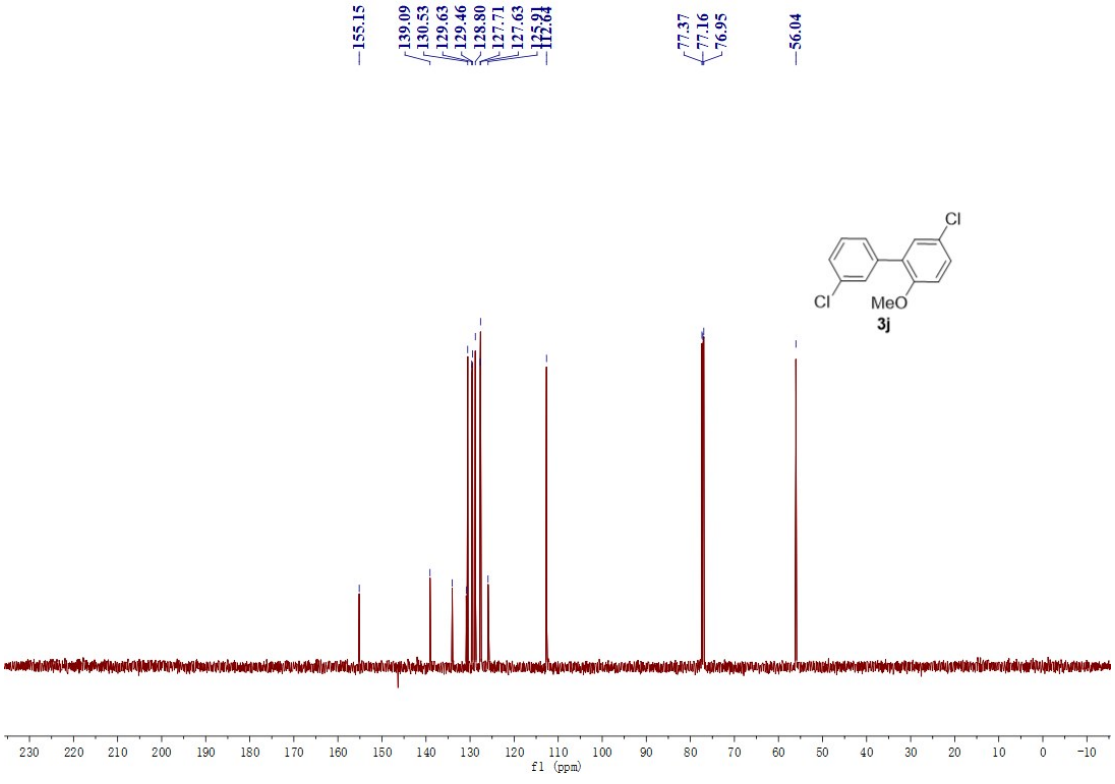
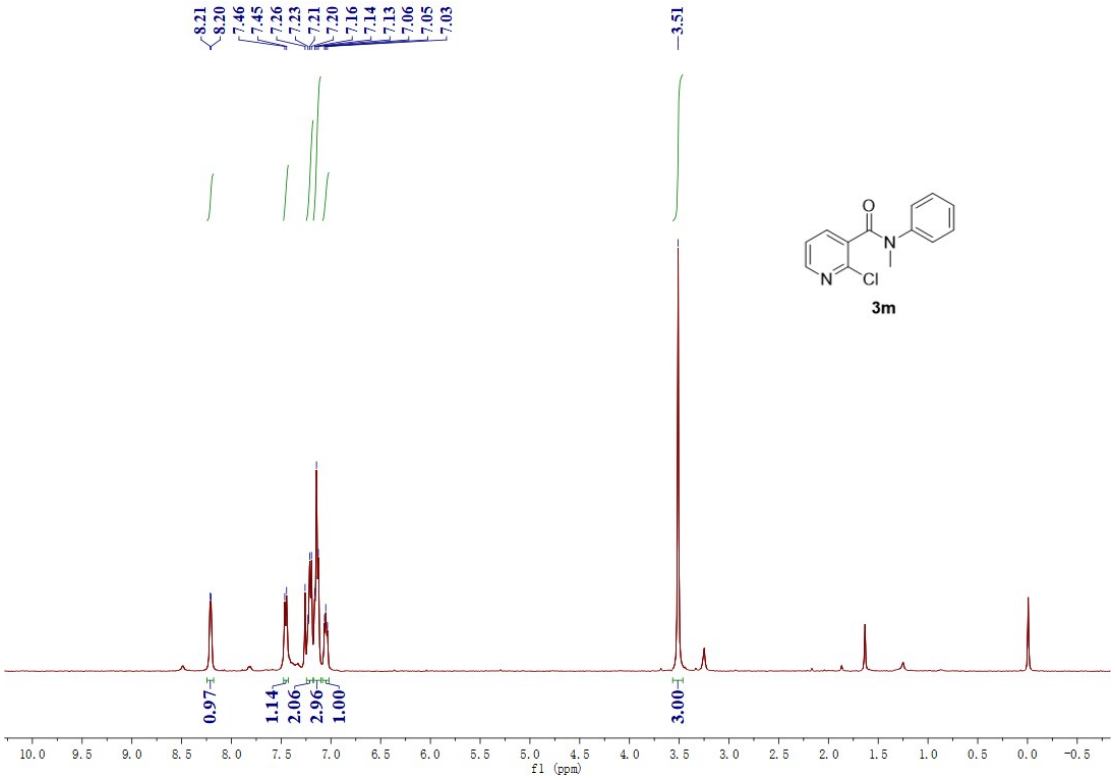
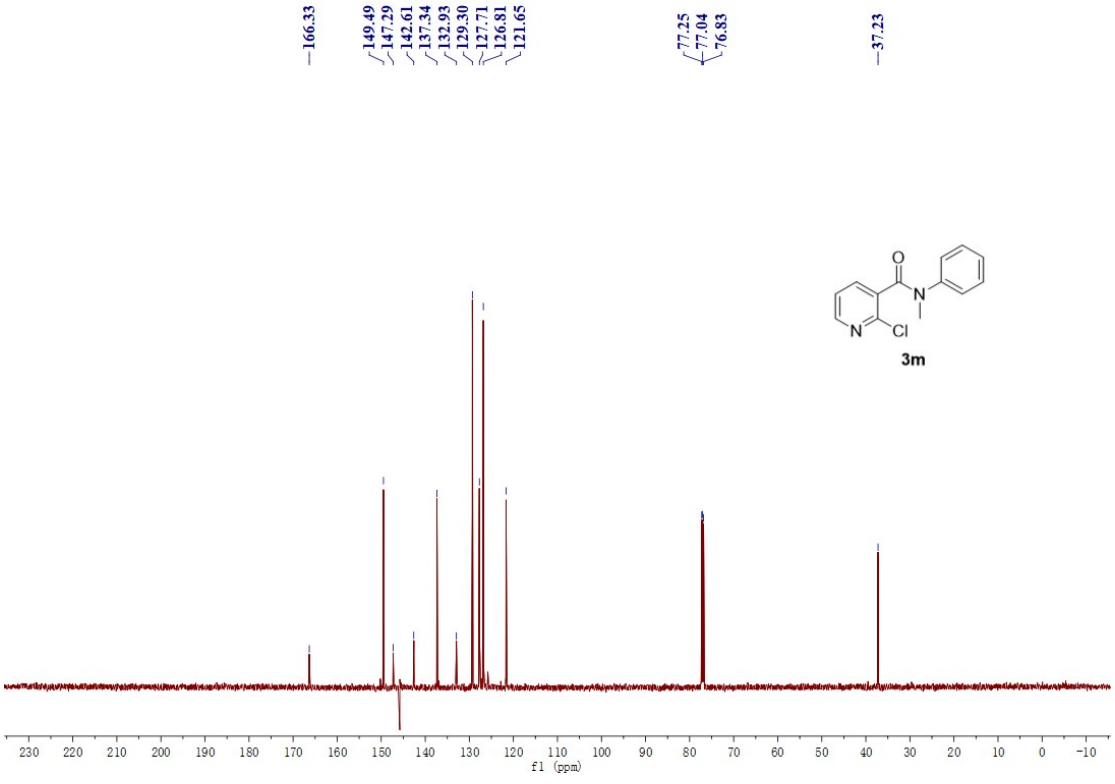
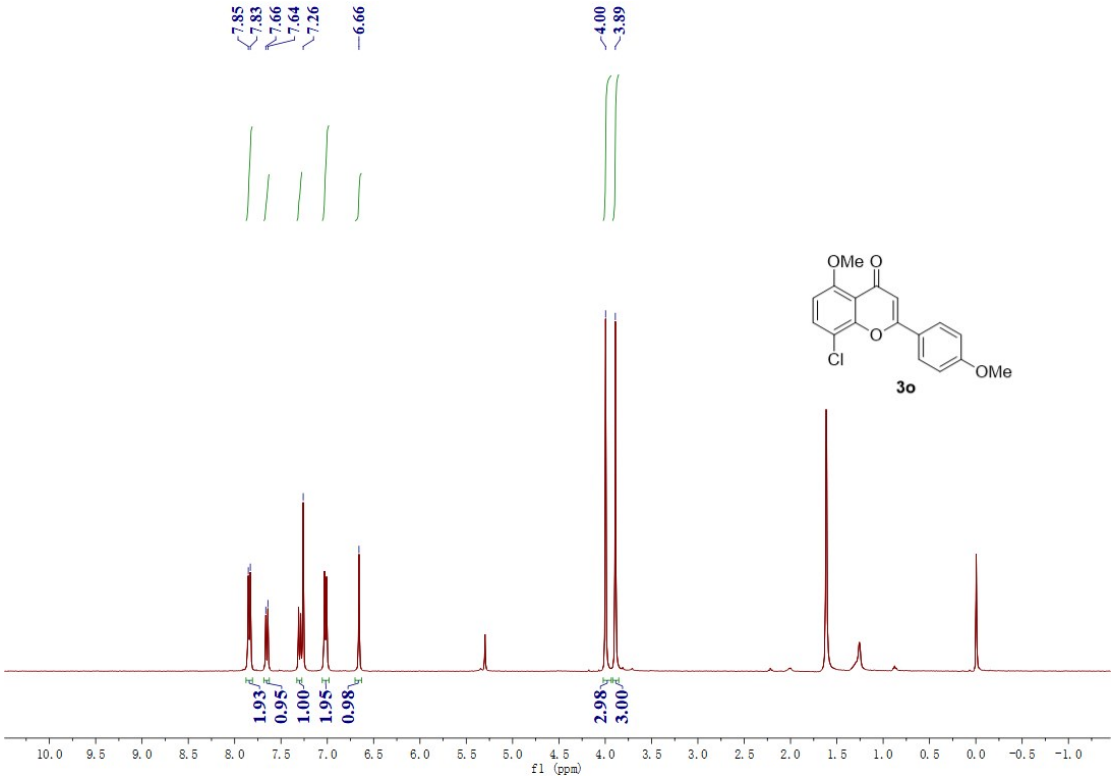
37.36
Cl
O
N
Ph
Cl
3i
f1 (ppm)

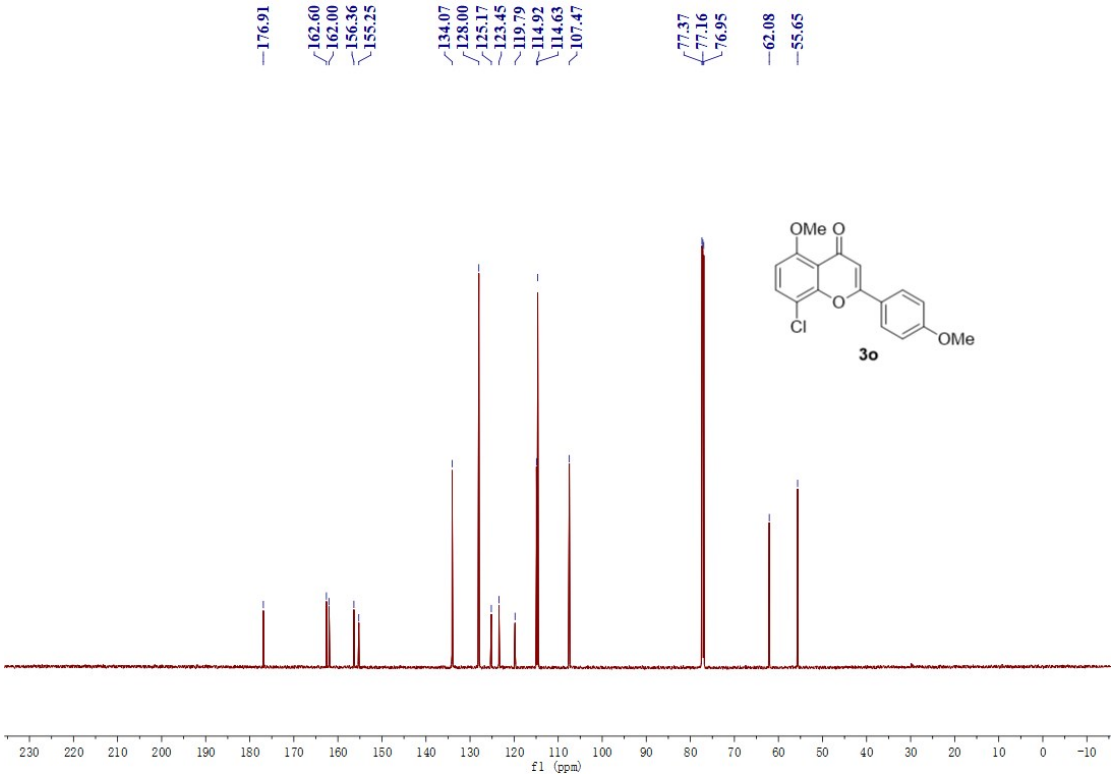

7.50
7.36
7.33
7.32
7.27
6.91
6.89
3.80
Cl
Cl
MeO
3j
0.93
5.29
0.98
3.00
f1 (ppm)

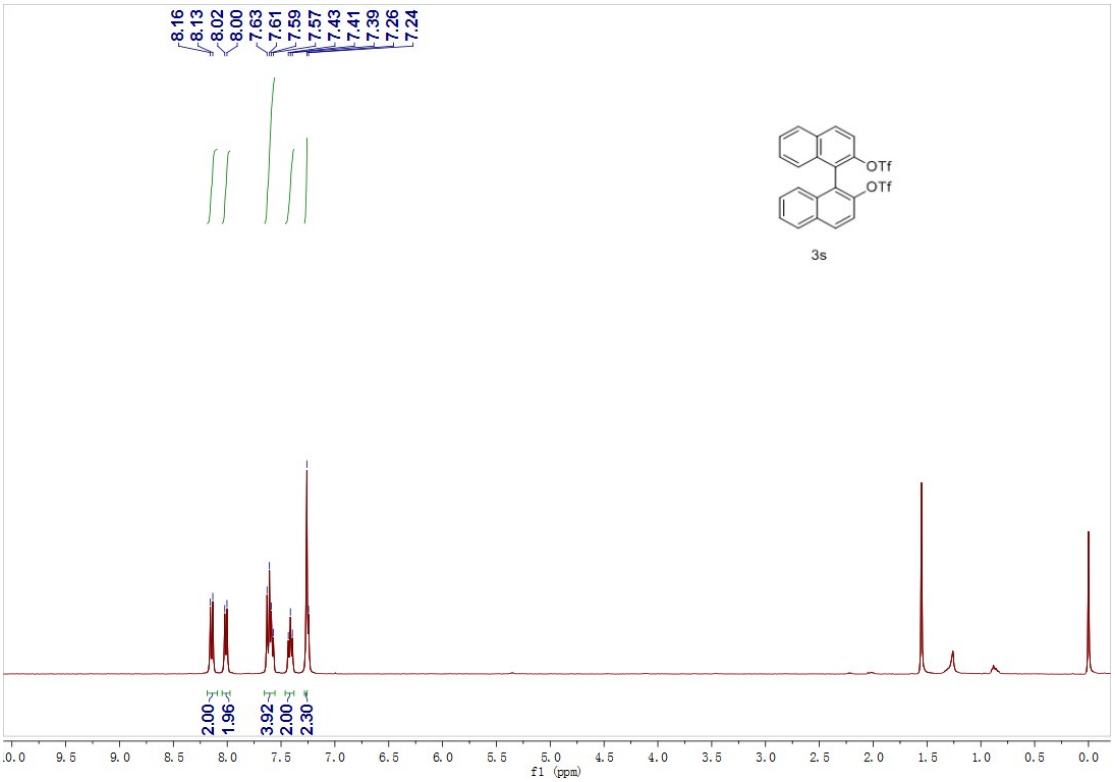

155.15
139.09
130.53
129.63
129.46
128.80
127.71
127.63
77.37
77.16
76.95
56.04
Cl
Cl
MeO
3j
f1 (ppm)

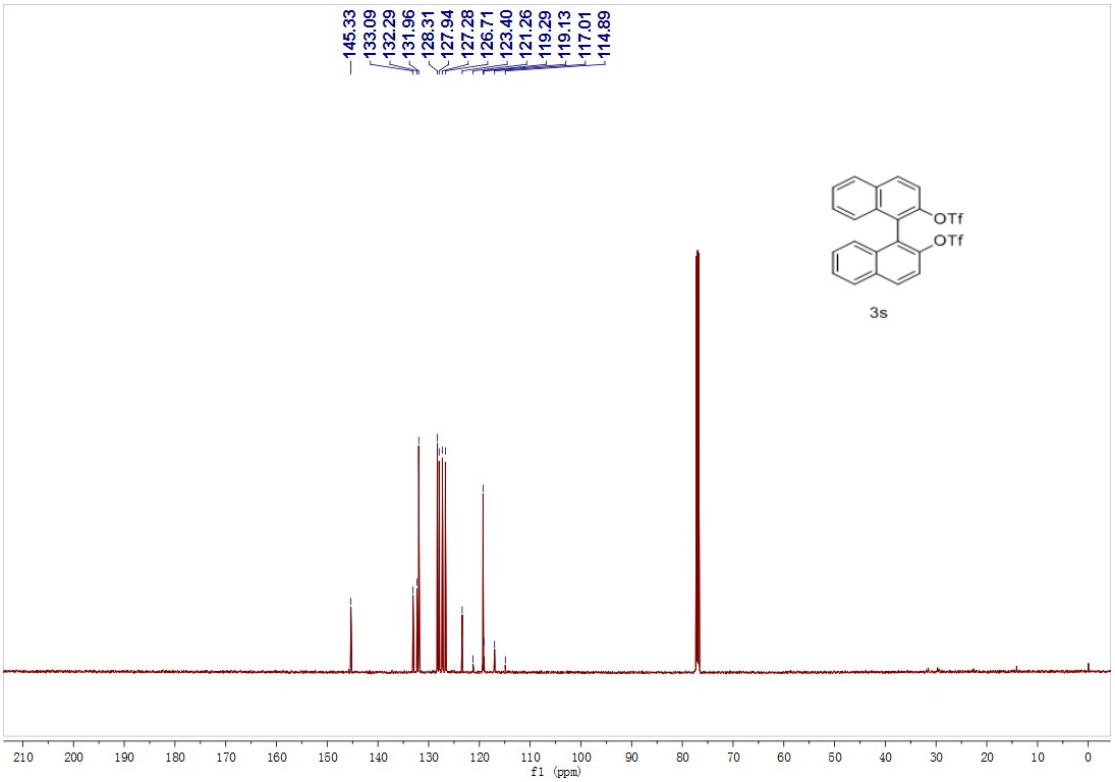

8.21
8.20
7.46
7.45
7.26
7.23
7.21
7.20
7.16
7.14
7.13
7.06
7.05
7.03
3.51
0.97
1.14
2.06
2.96
1.00
3.00
f1 (ppm)
3m

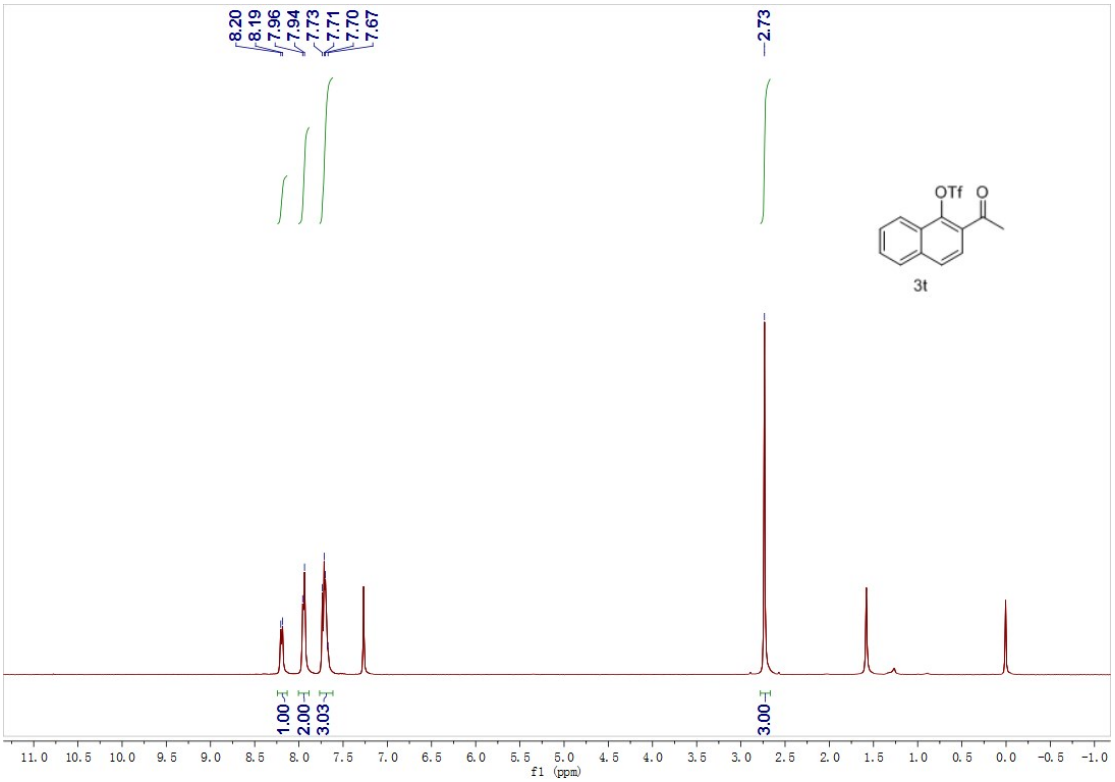

166.33
149.49
147.29
142.61
137.34
132.93
129.30
127.71
126.81
121.65
77.25
77.04
76.83
37.23
f1 (ppm)
3m

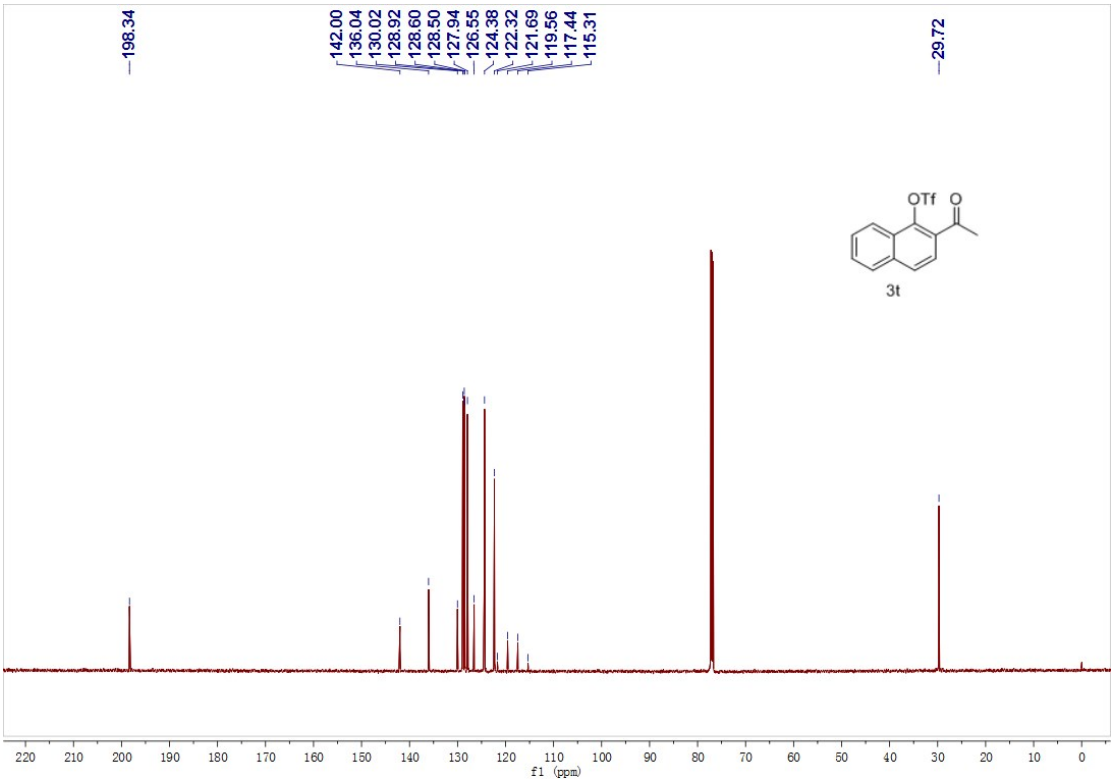

7.85
7.83
7.66
7.64
7.26
6.66
4.00
3.89
OMe O
Cl
O
OMe
3o
1.93
0.95
1.00
1.95
0.98
2.98
3.00
f1 (ppm)

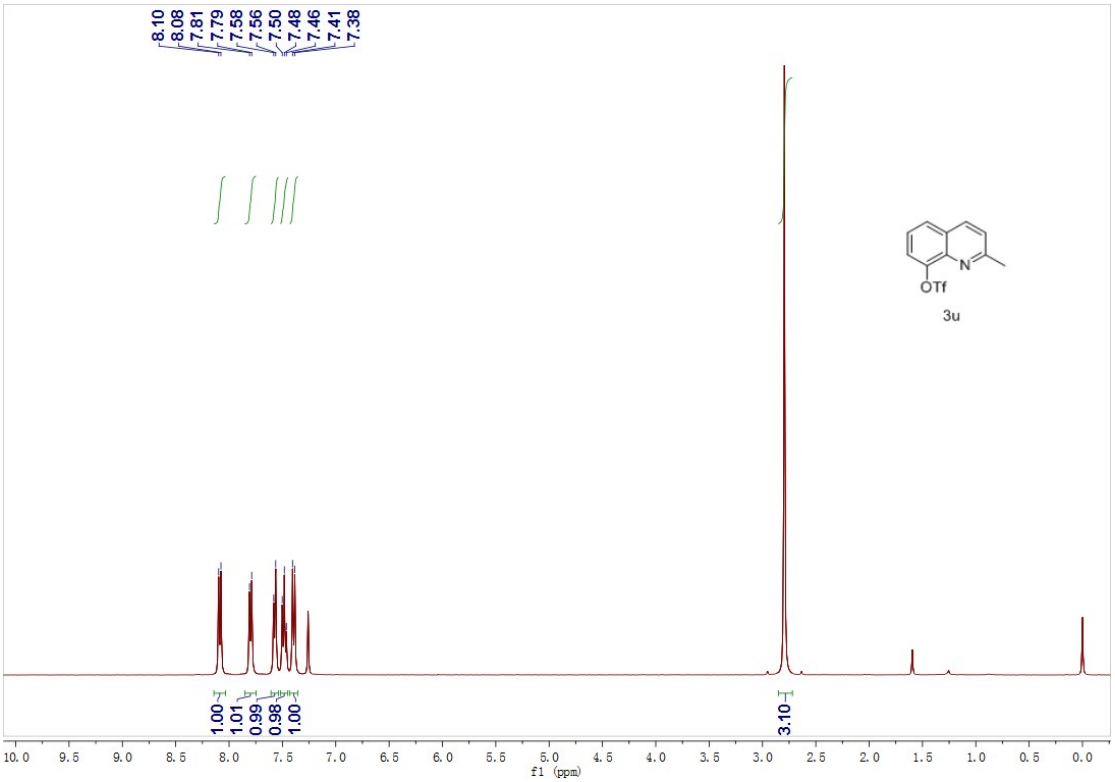

176.91
162.60
162.00
156.36
155.25
134.07
128.00
125.17
123.45
119.79
114.92
114.63
107.47
77.37
77.16
76.95
62.08
55.65
OMe O
Cl
O
OMe
3o
f1 (ppm)


8.16
8.13
8.02
8.00
7.63
7.61
7.59
7.57
7.43
7.41
7.39
7.26
7.24
OTf
OTf
3s
2.00
1.96
3.92
2.00
2.30
f1 (ppm)


145.33
133.09
132.29
131.96
128.31
127.94
127.28
126.71
123.40
121.26
119.29
119.13
117.01
114.89
OTf
OTf
3s
f1 (ppm)


8.20
8.19
7.96
7.94
7.73
7.71
7.70
7.67
2.73
OTf
O
3t
1.00
2.00
3.03
3.00
f1 (ppm)


198.34
142.00
136.04
130.02
128.92
128.60
128.50
127.94
126.55
124.38
122.32
121.69
119.56
117.44
115.31
29.72
OTf
O
3t
f1 (ppm)


8.10
8.08
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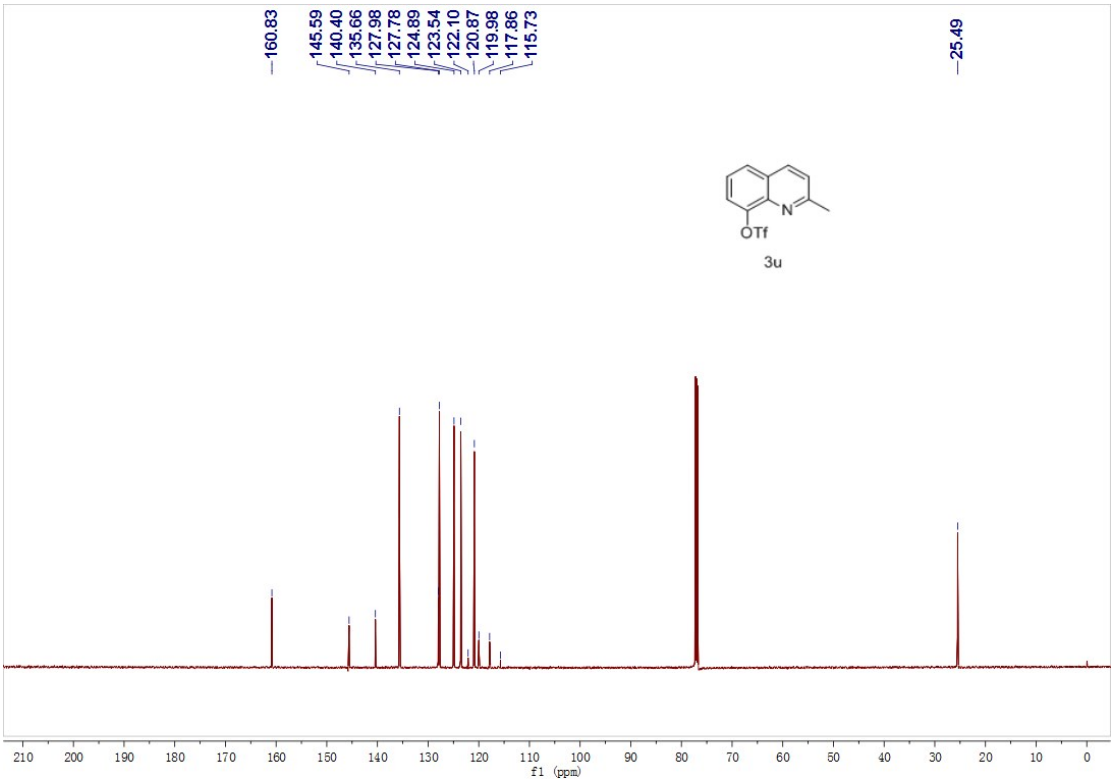
7.79
7.58
7.56
7.50
7.48
7.46
7.41
7.38
OTf
3u
1.00
1.01
0.99
0.98
1.00
3.10
f1 (ppm)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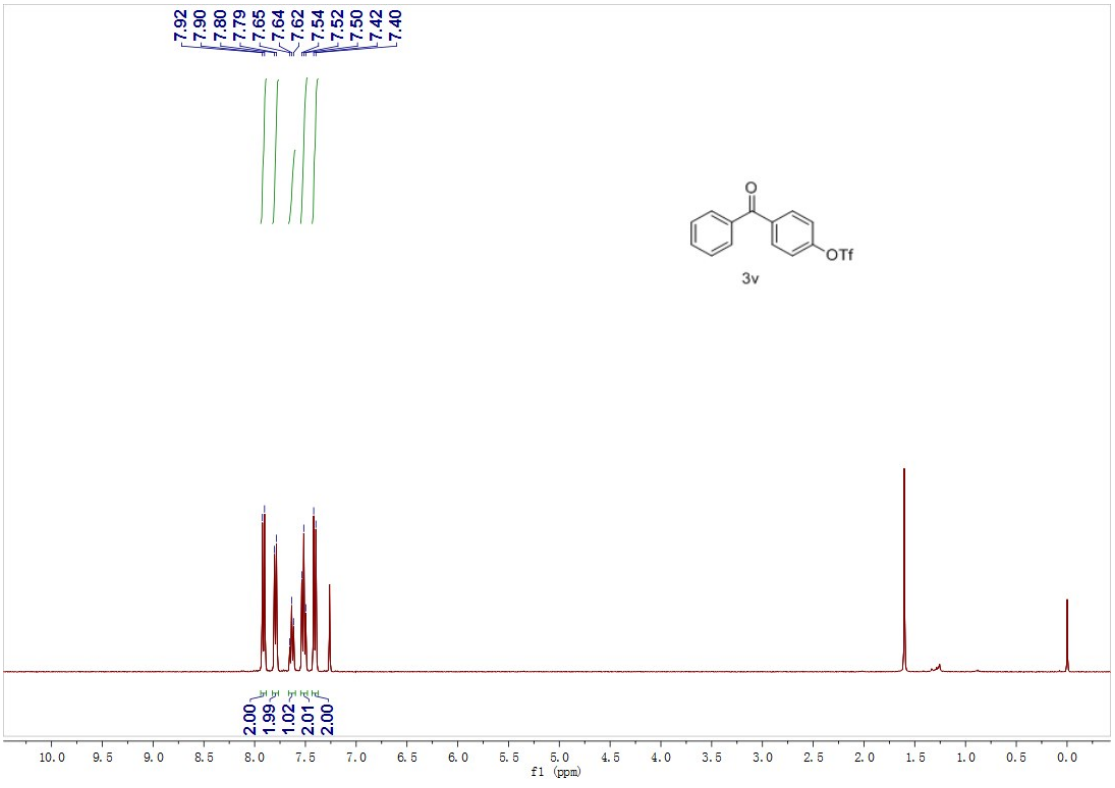
123.54
122.10
120.87
119.98
117.86
115.73
25.49
OTf
3u
f1 (ppm)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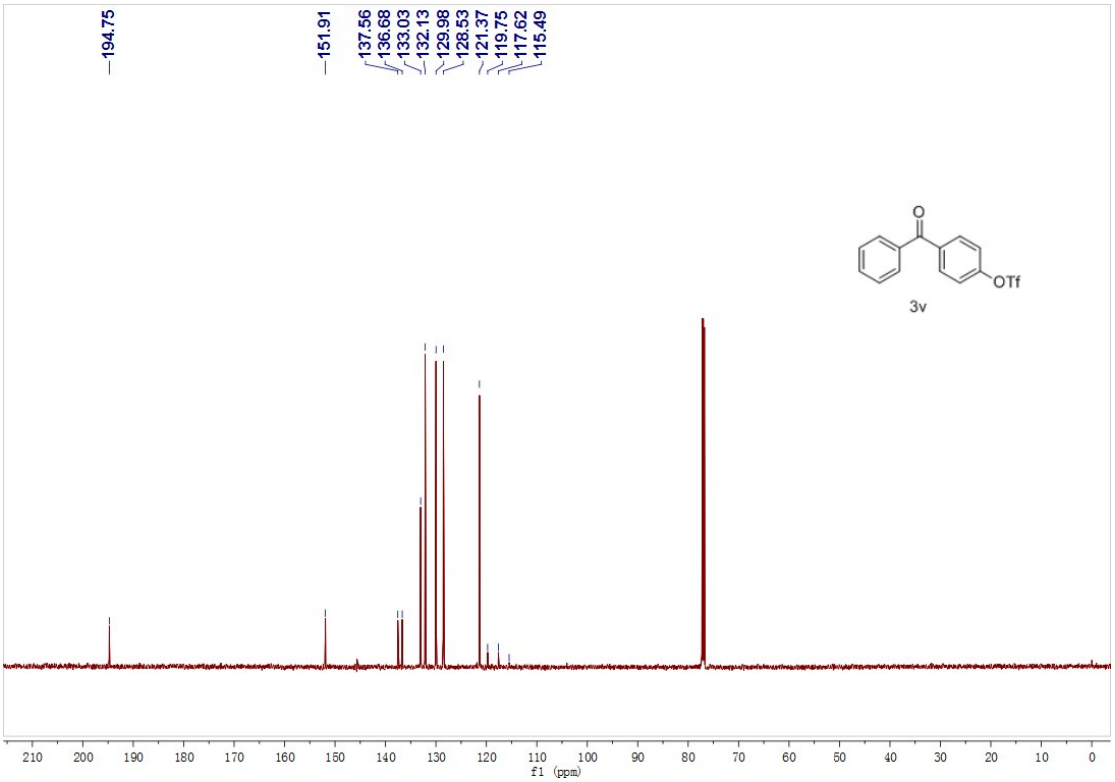
7.90
7.80
7.79
7.65
7.64
7.62
7.54
7.52
7.50
7.42
7.40
O
OTf
3v
2.00
1.99
1.02
2.01
2.00
f1 (ppm)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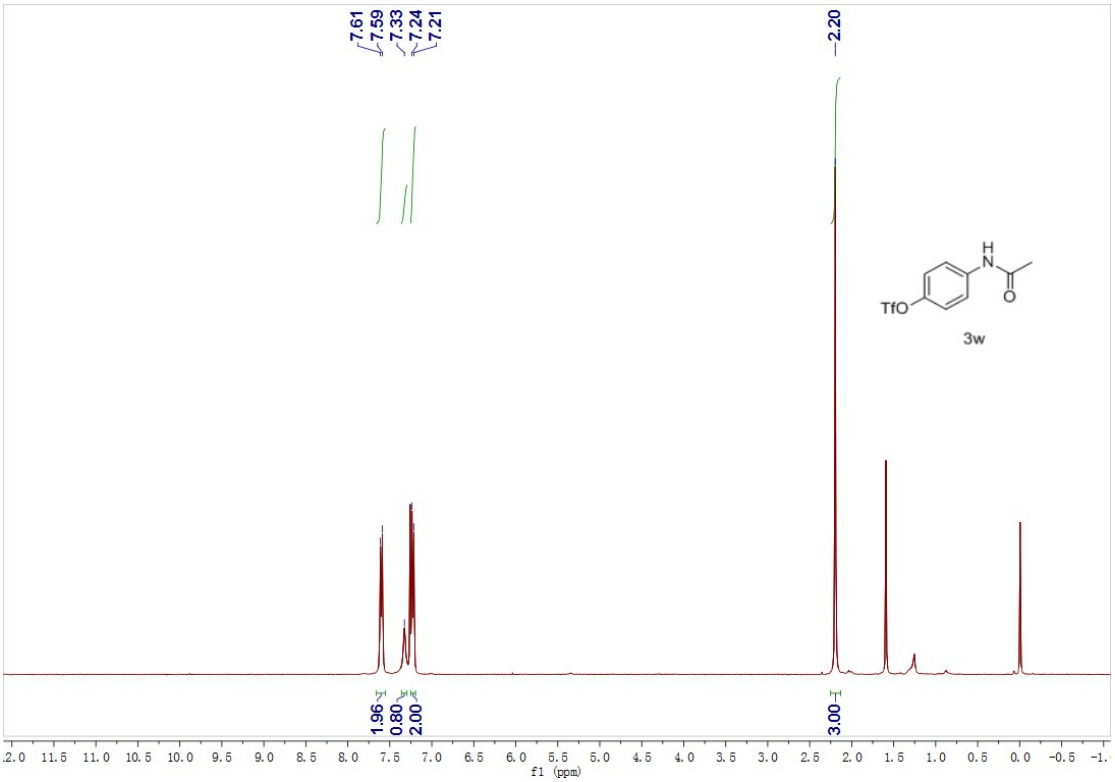
133.03
132.13
129.98
128.53
121.37
119.75
117.62
115.49
O
OTf
3v
f1 (ppm)


7.61
7.59
7.33
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TfO
H
N
O
3w
1.96
0.80
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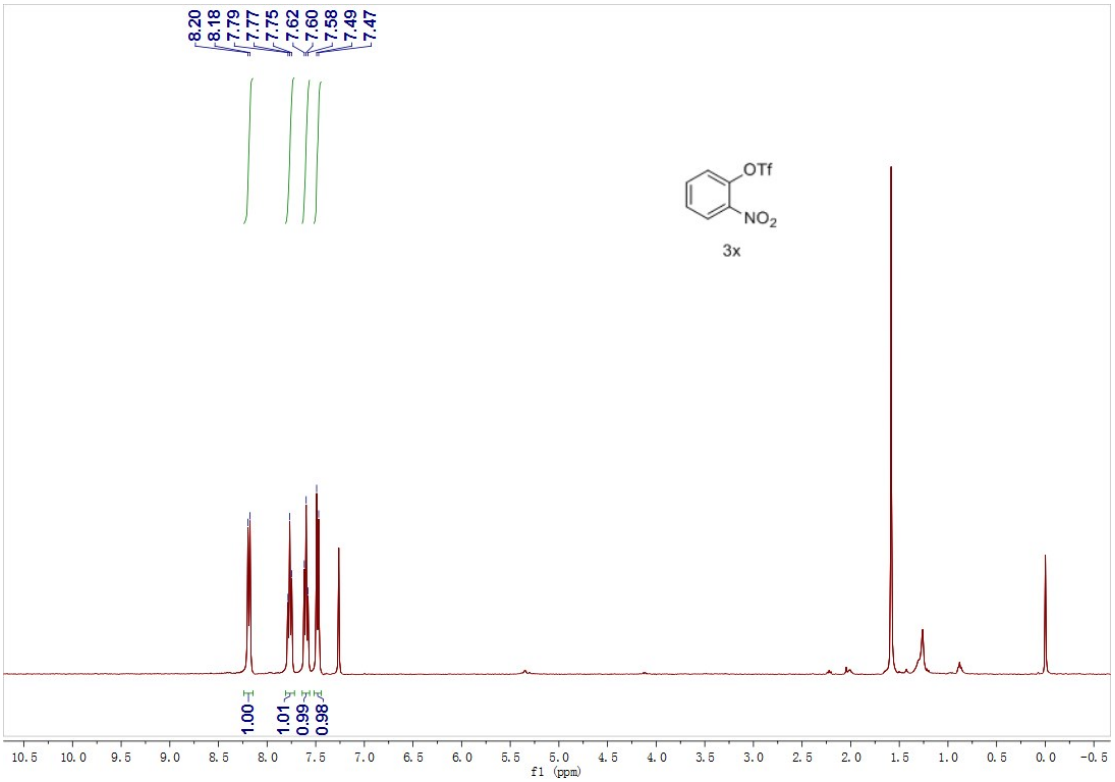
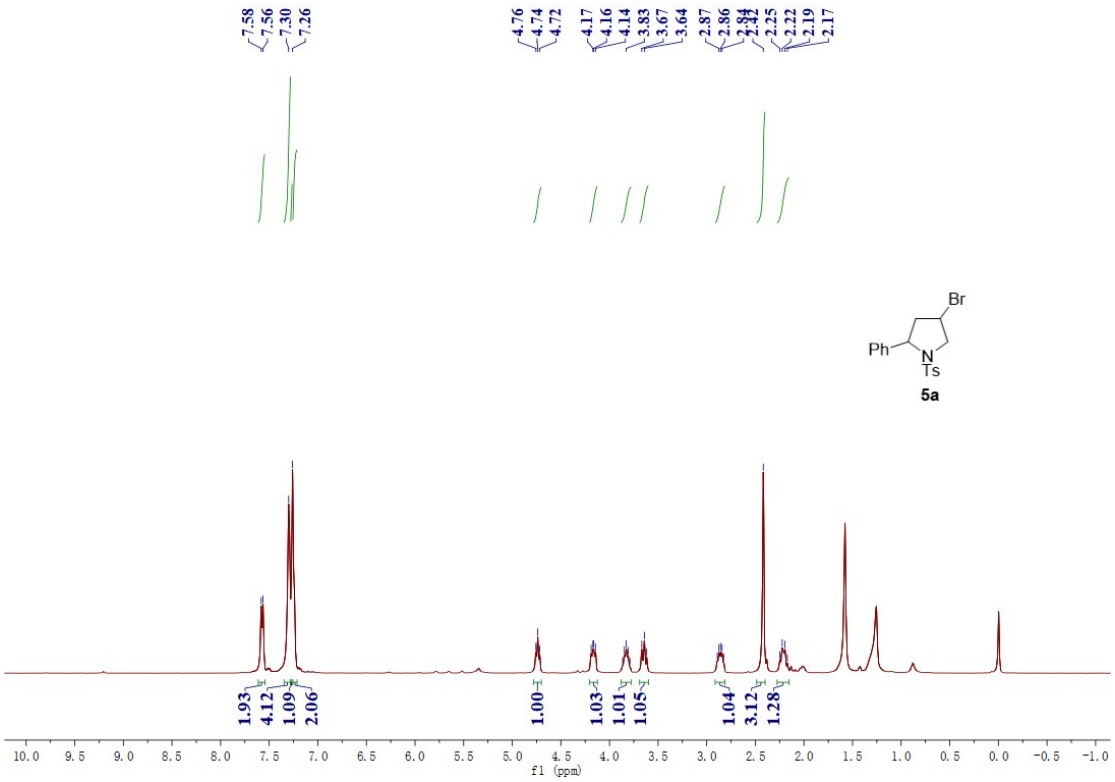
3.00
f1 (ppm)


8.20
8.18
7.79
7.77
7.75
7.62
7.60
7.58
7.49
7.47
OTf
NO2
3x
1.00
1.01
0.99
0.98
f1 (ppm)


7.58
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7.26
4.76
4.74
4.72
4.17
4.16
4.14
3.83
3.67
3.64
2.87
2.86
2.84
2.25
2.22
2.19
2.17
Br
Ph
N
Ts
5a
1.93
4.12
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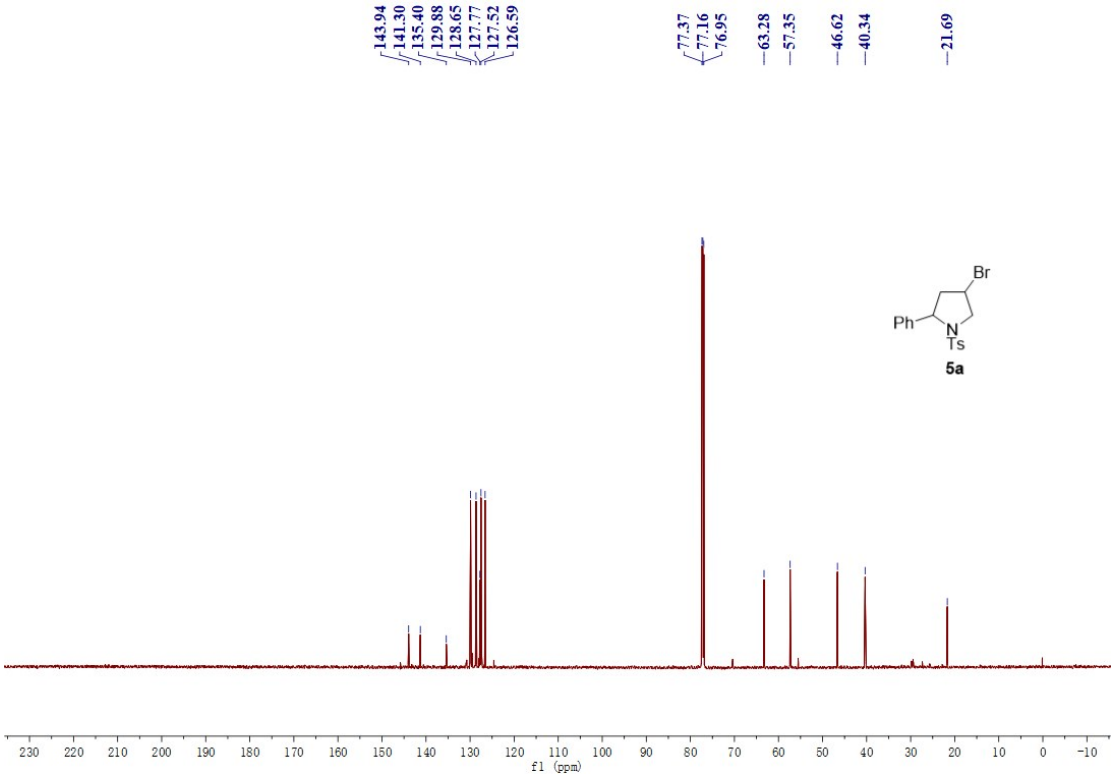
2.06
1.00
1.03
1.01
1.05
1.04
3.12
1.28
f1 (ppm)


143.94
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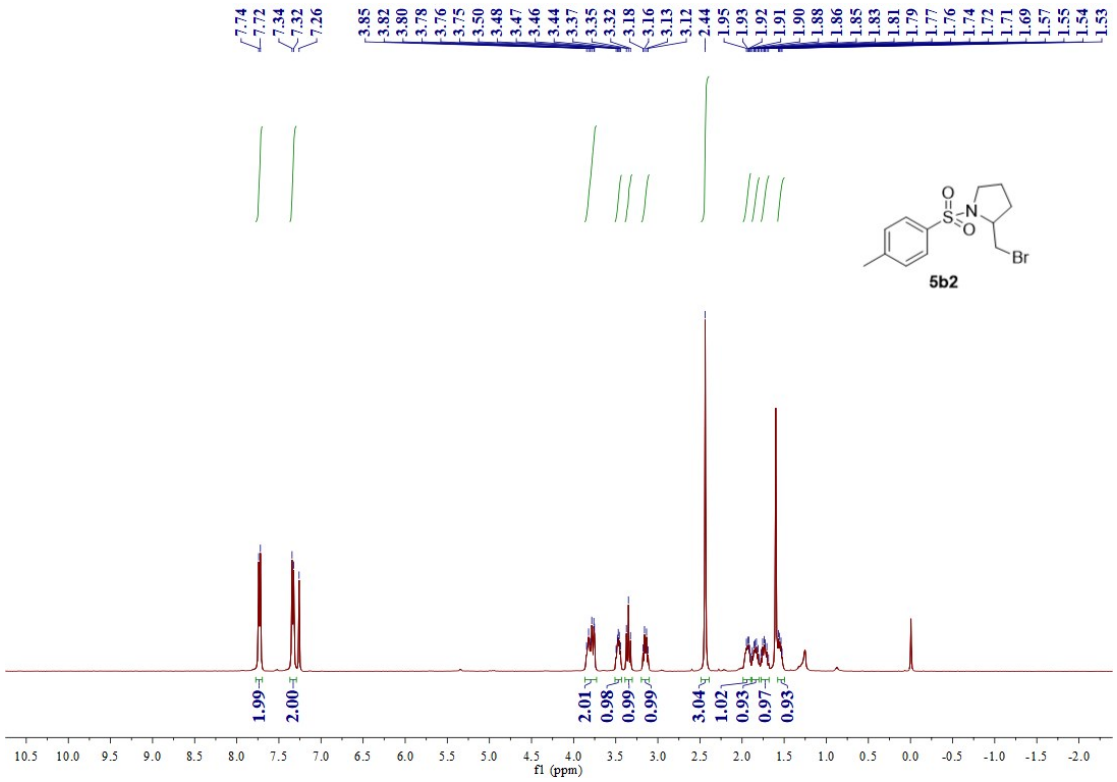
128.65
127.77
127.52
126.59
77.37
77.16
76.95
63.28
57.35
46.62
40.34
21.69
Br
Ph
N
Ts
5a
f1 (ppm)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7.34
7.32
7.26
3.85
3.82
3.80
3.78
3.76
3.75
3.50
3.48
3.47
3.46
3.44
3.37
3.35
3.32
3.18
3.16
3.13
3.12
2.44
1.95
1.93
1.92
1.91
1.90
1.88
1.86
1.85
1.83
1.81
1.79
1.77
1.76
1.74
1.72
1.71
1.69
1.57
1.55
1.54
1.53
O
S
N
O
Br
5b2
1.99
2.00
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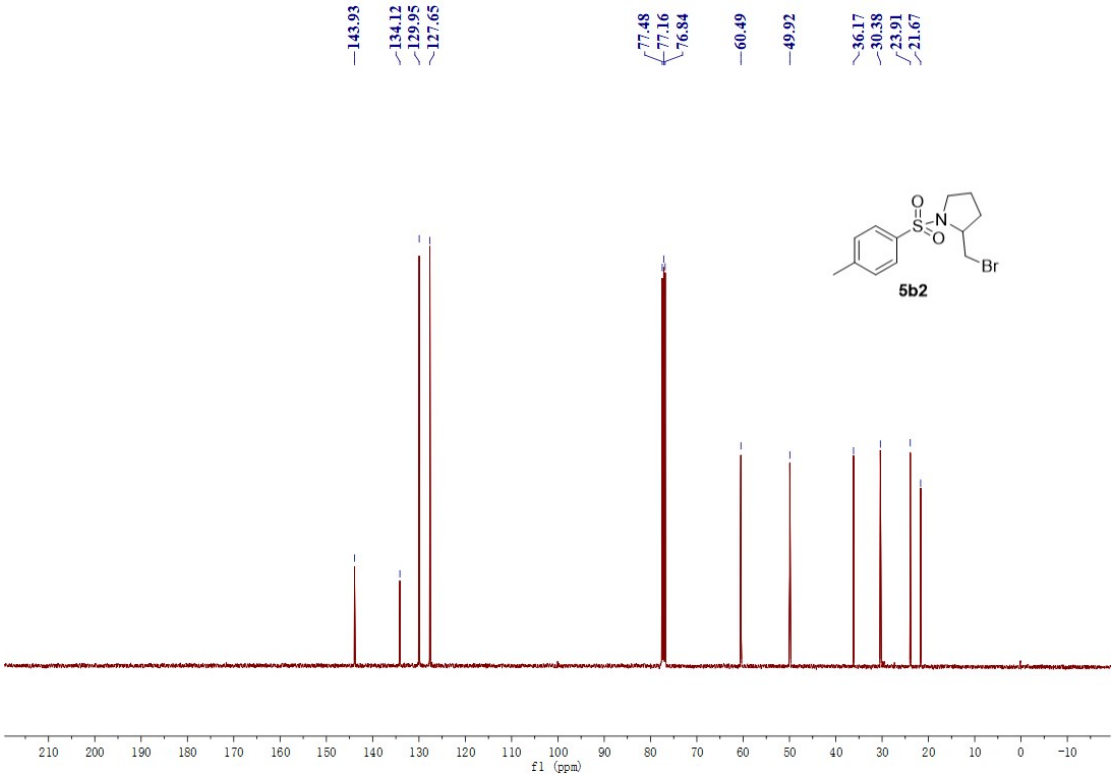
0.98
0.99
0.99
3.04
1.02
0.93
0.97
0.93
f1 (ppm)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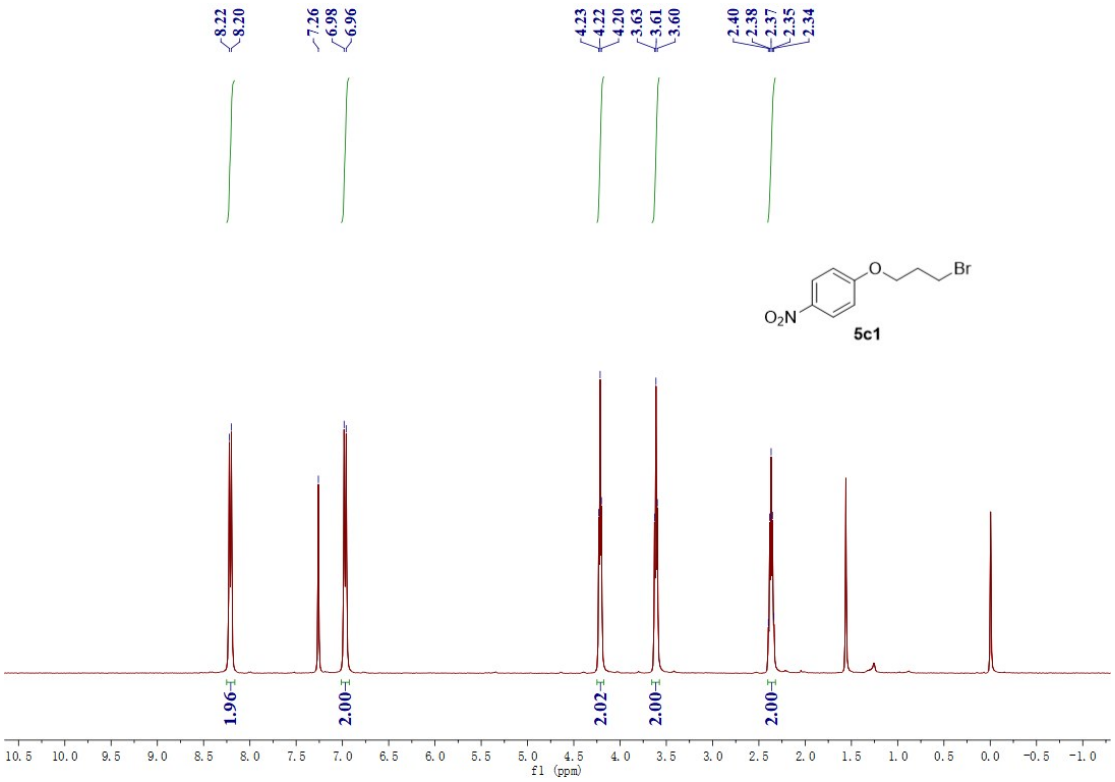
134.12
129.95
127.65
77.48
77.16
76.84
60.49
49.92
36.17
30.38
23.91
21.67
O
S
N
O
Br
5b2
f1 (ppm)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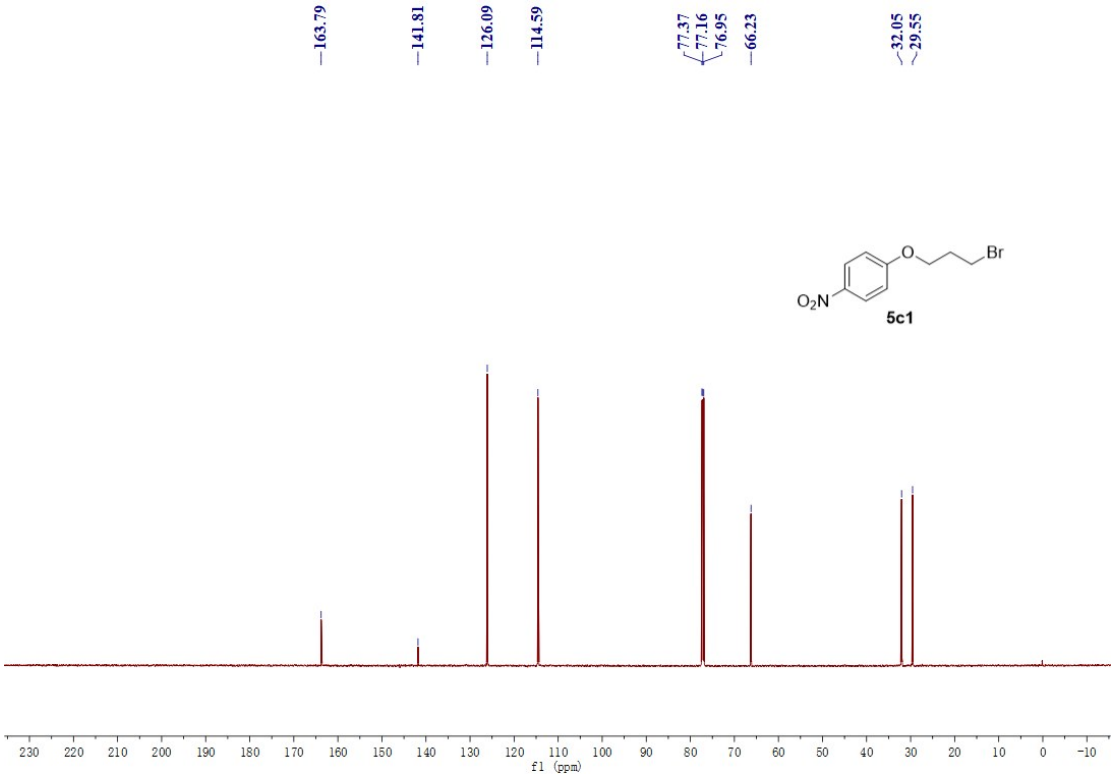
8.20
7.26
6.98
6.96
4.23
4.22
4.20
3.63
3.61
3.60
2.40
2.38
2.37
2.35
2.34
O
Br
O2N
5c1
1.96
2.00
2.02
2.00
2.00
f1 (ppm)


163.79
141.81
126.09
114.59
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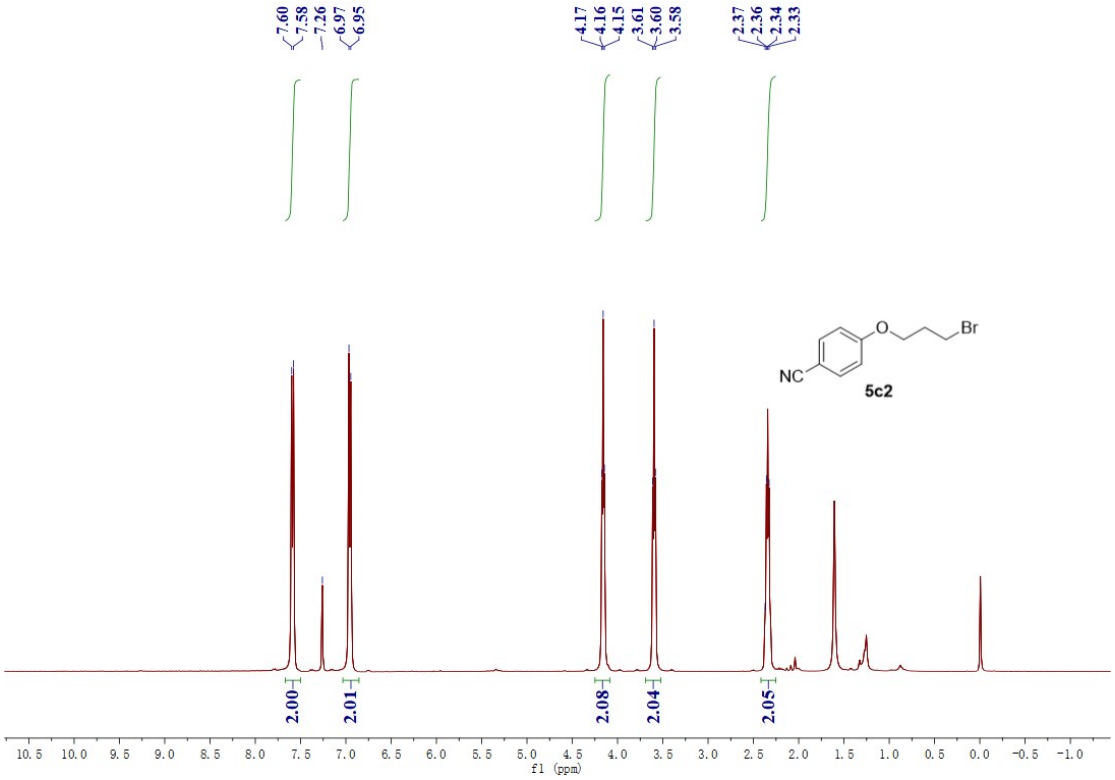
77.16
76.95
66.23
32.05
29.55
O
Br
O2N
5c1
f1 (ppm)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7.58
7.26
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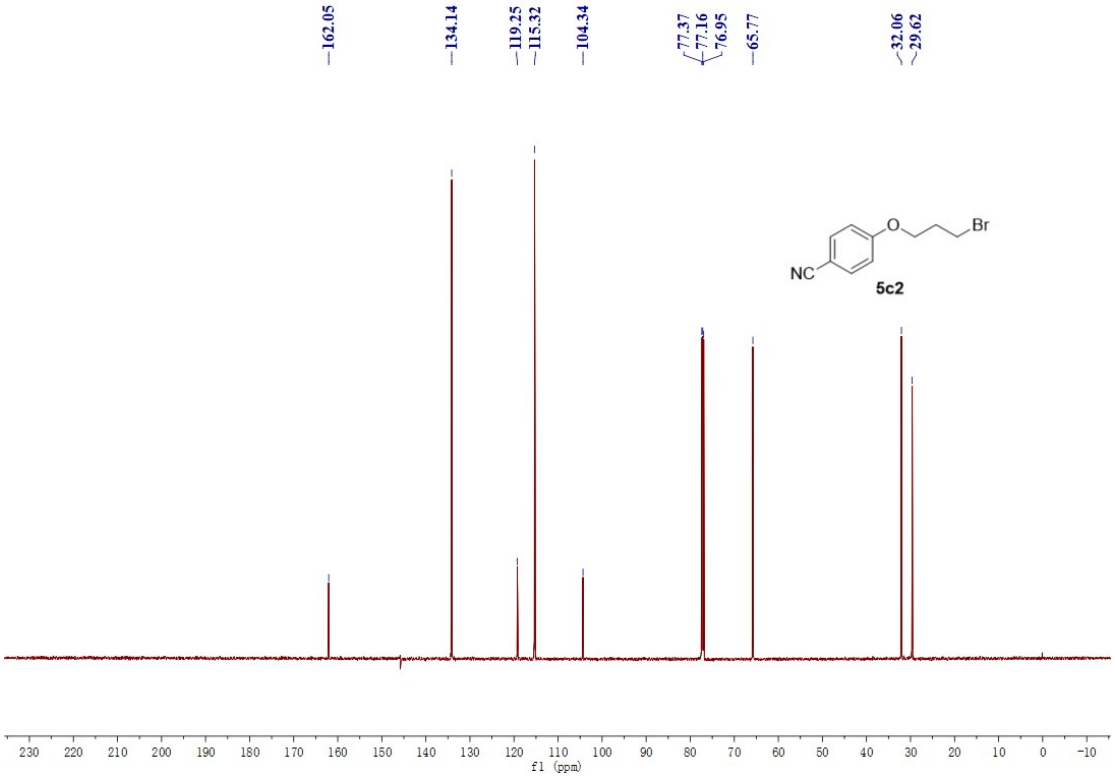
6.95
4.17
4.16
4.15
3.61
3.60
3.58
2.37
2.36
2.34
2.33
NC
O
Br
5c2
2.00
2.01
2.08
2.04
2.05
f1 (ppm)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134.14
119.25
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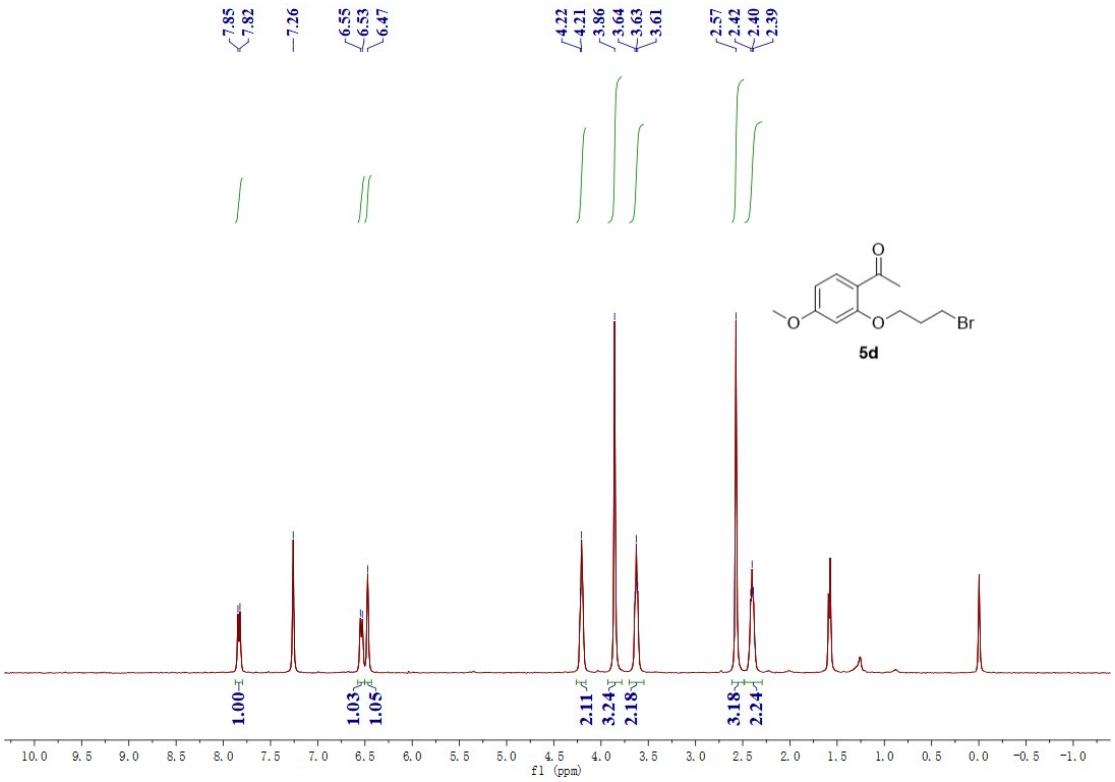
104.34
77.37
77.16
76.95
65.77
32.06
29.62
NC
O
Br
5c2
f1 (ppm)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7.82
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6.53
6.47
4.22
4.21
3.86
3.64
3.63
3.61
2.57
2.42
2.40
2.39
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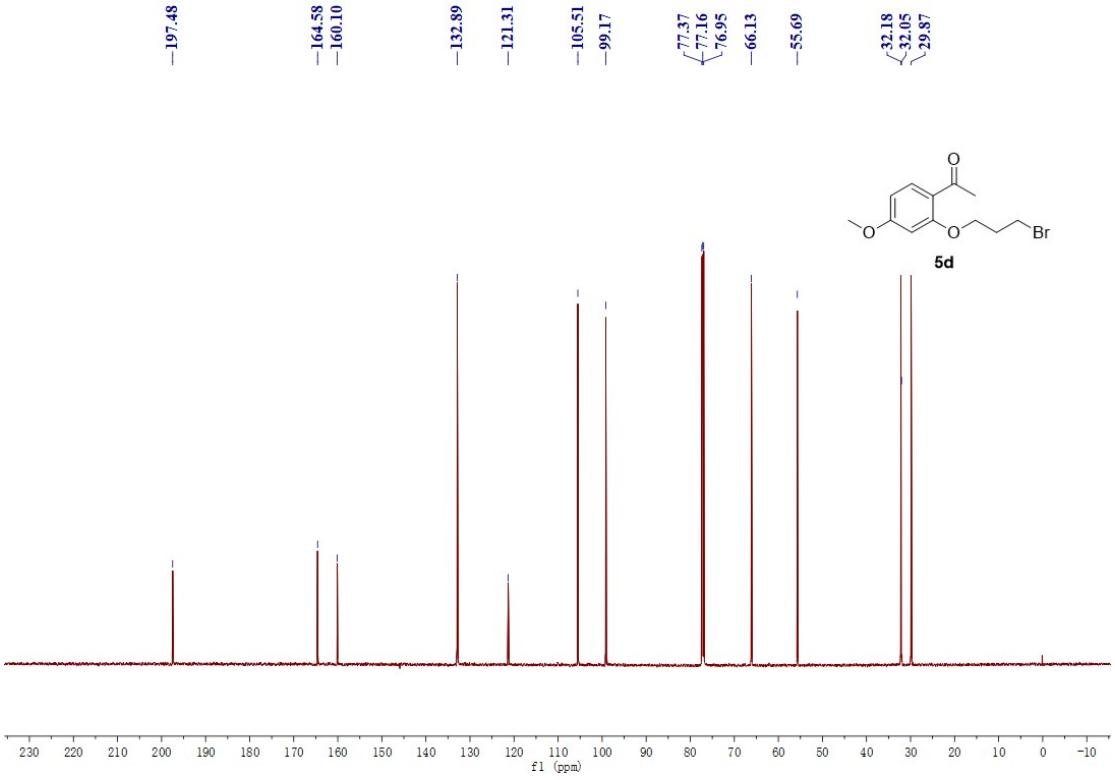
O
O
Br
5d
1.00
1.03
1.05
2.11
3.24
2.18
3.18
2.24
f1 (ppm)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105.51
99.17
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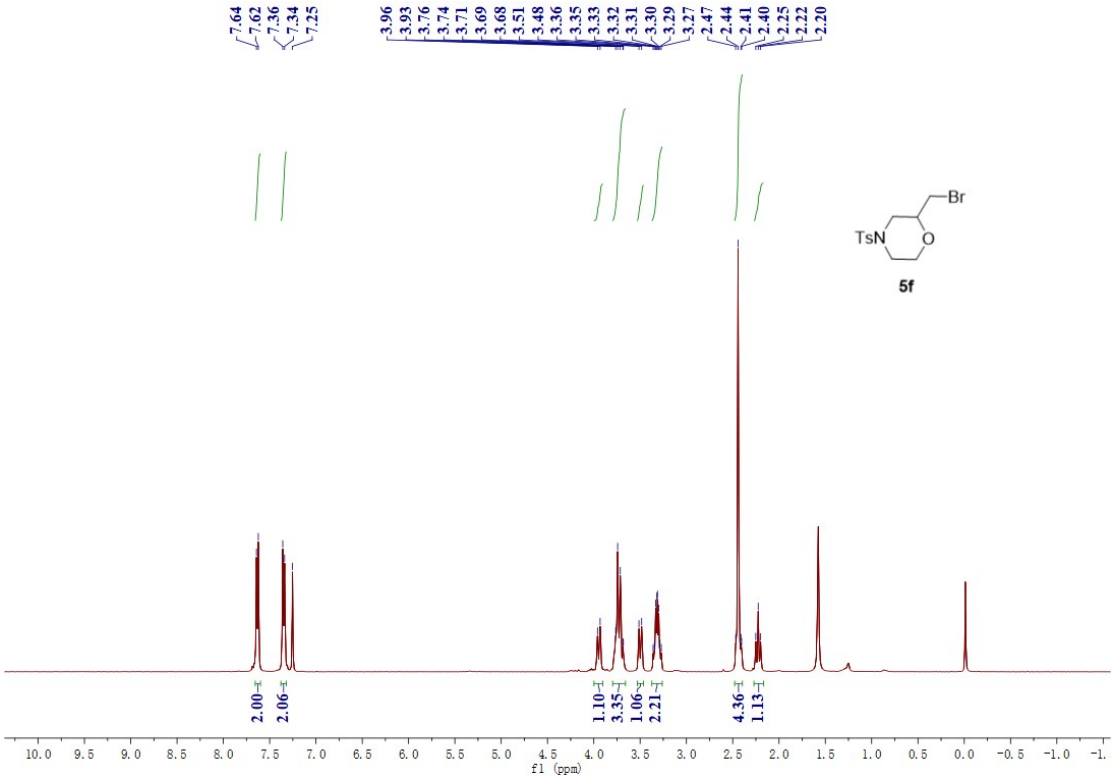
66.13
55.69
32.18
32.05
29.87
O
O
O
Br
5d
f1 (ppm)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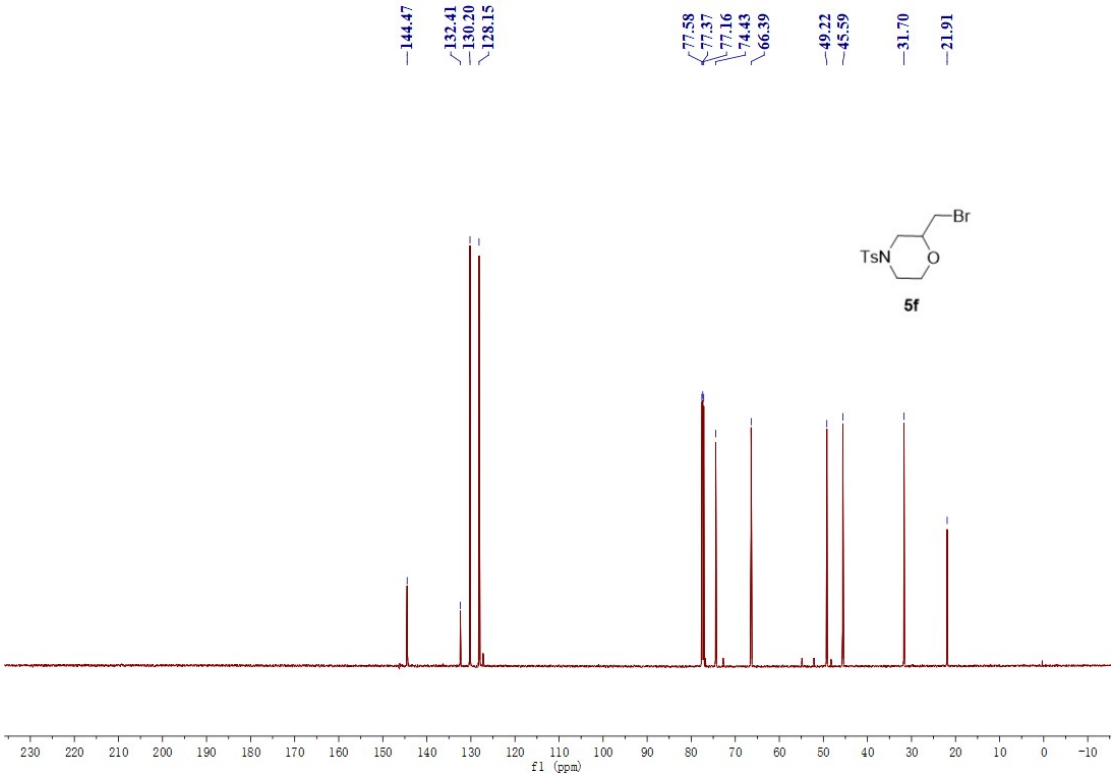
3.93
3.76
3.74
3.71
3.69
3.68
3.51
3.48
3.36
3.35
3.33
3.32
3.31
3.30
3.29
3.27
2.47
2.44
2.41
2.40
2.25
2.22
2.20
Br
TsN
O
5f
2.00
2.06
1.10
3.35
1.06
2.21
4.36
1.13
f1 (ppm)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132.41
130.20
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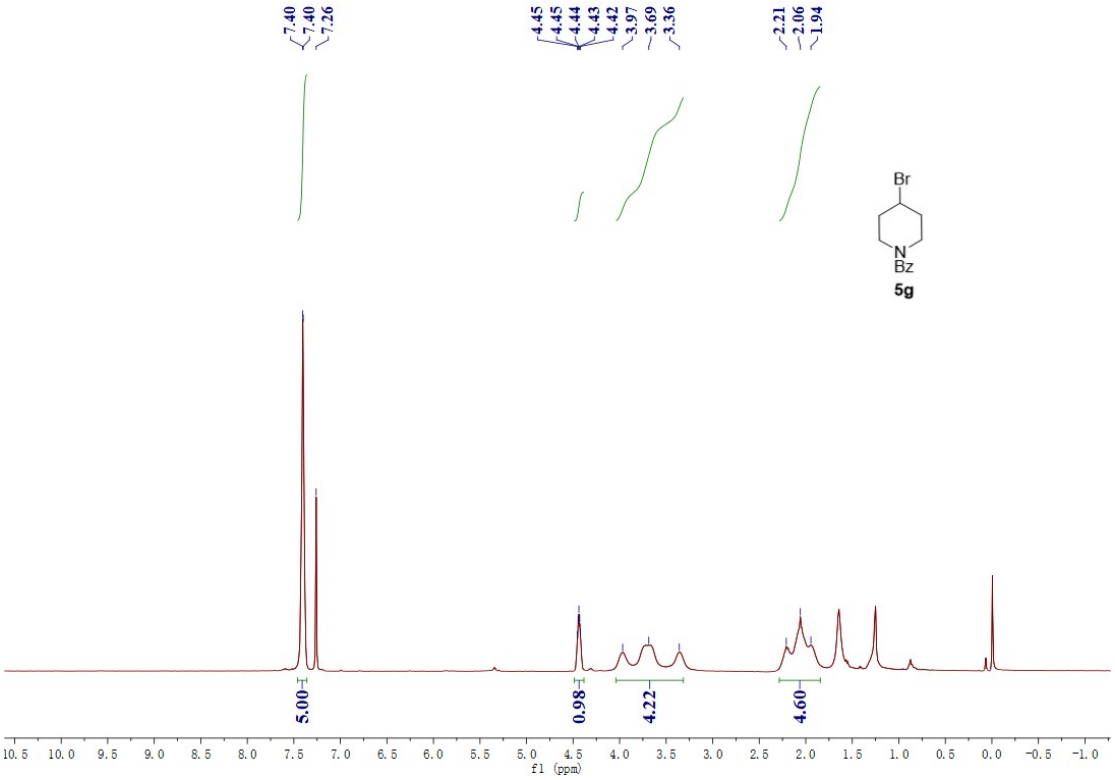
77.58
77.37
77.16
74.43
66.39
49.22
45.59
31.70
21.91
Br
TsN
O
5f
f1 (ppm)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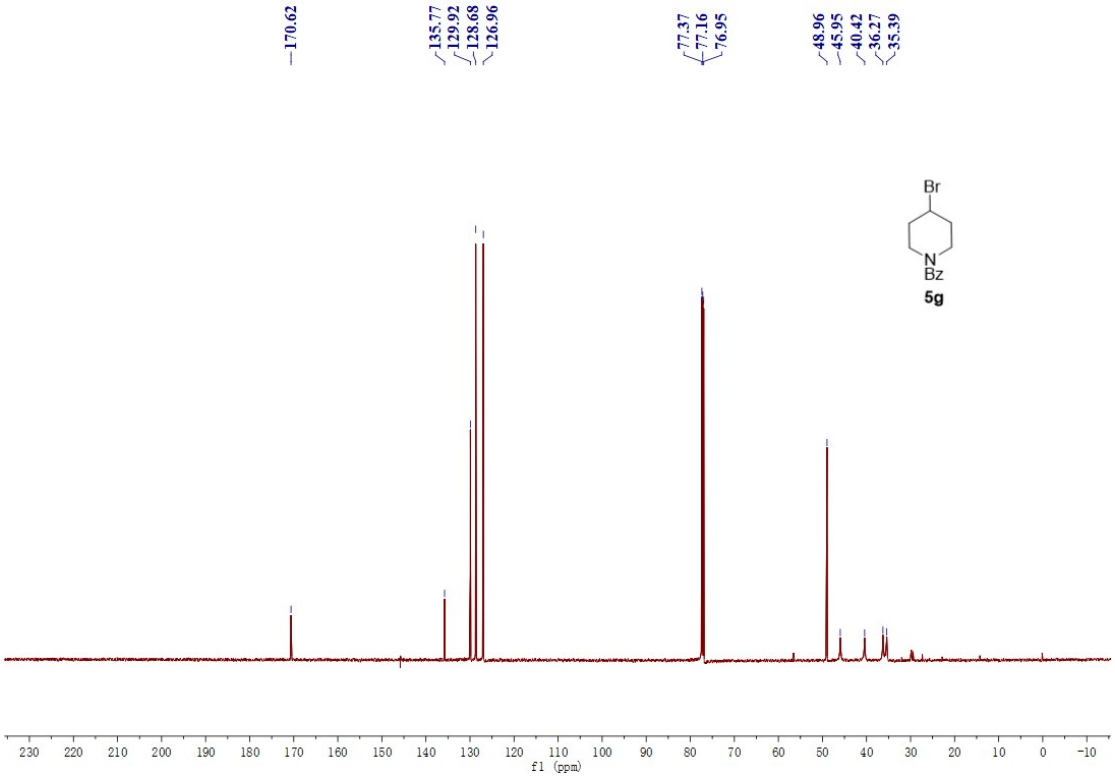
7.40
7.26
4.45
4.45
4.44
4.43
4.42
3.97
3.69
3.36
2.21
2.06
1.94
Br
N
Bz
5g
5.00
0.98
4.22
4.60
f1 (ppm)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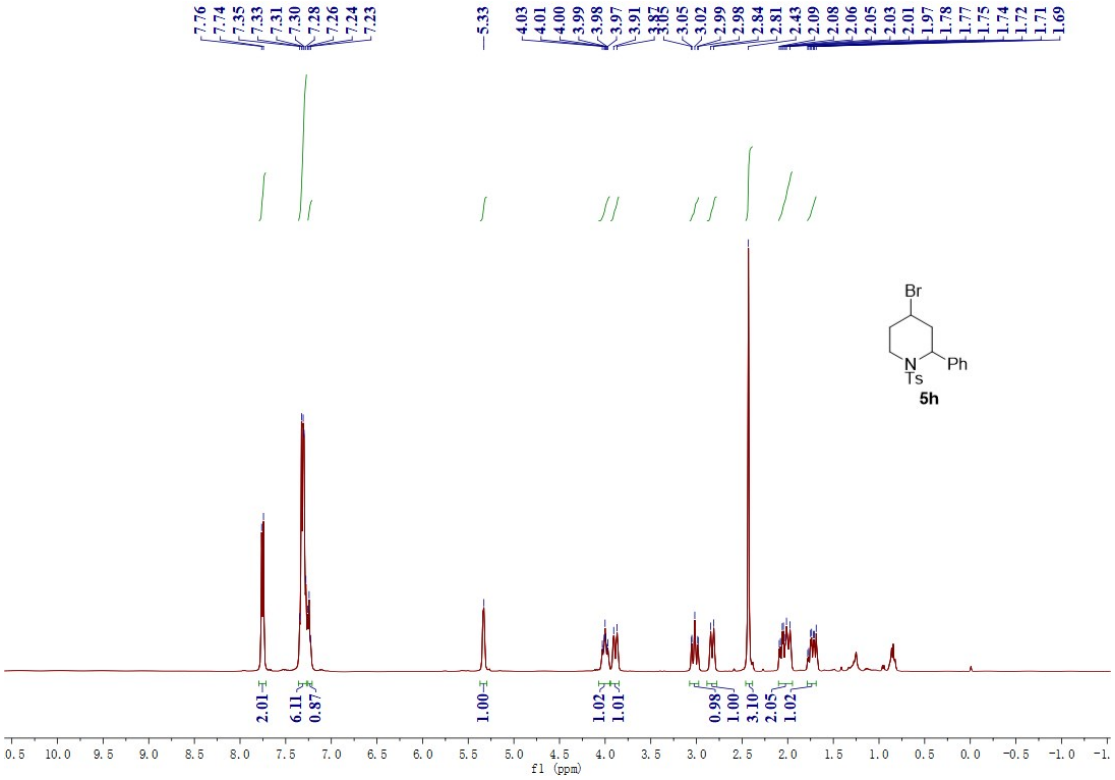
35.39
Br
N
Bz
5g
f1 (ppm)


7.76
7.74
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7.33
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7.26
7.24
7.23
5.33
4.03
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3.99
3.98
3.97
3.91
3.87
3.85
3.05
3.02
2.99
2.98
2.84
2.81
2.43
2.09
2.08
2.06
2.05
2.03
2.01
1.97
1.78
1.77
1.75
1.74
1.72
1.71
1.69
Br
N
Ts
Ph
5h
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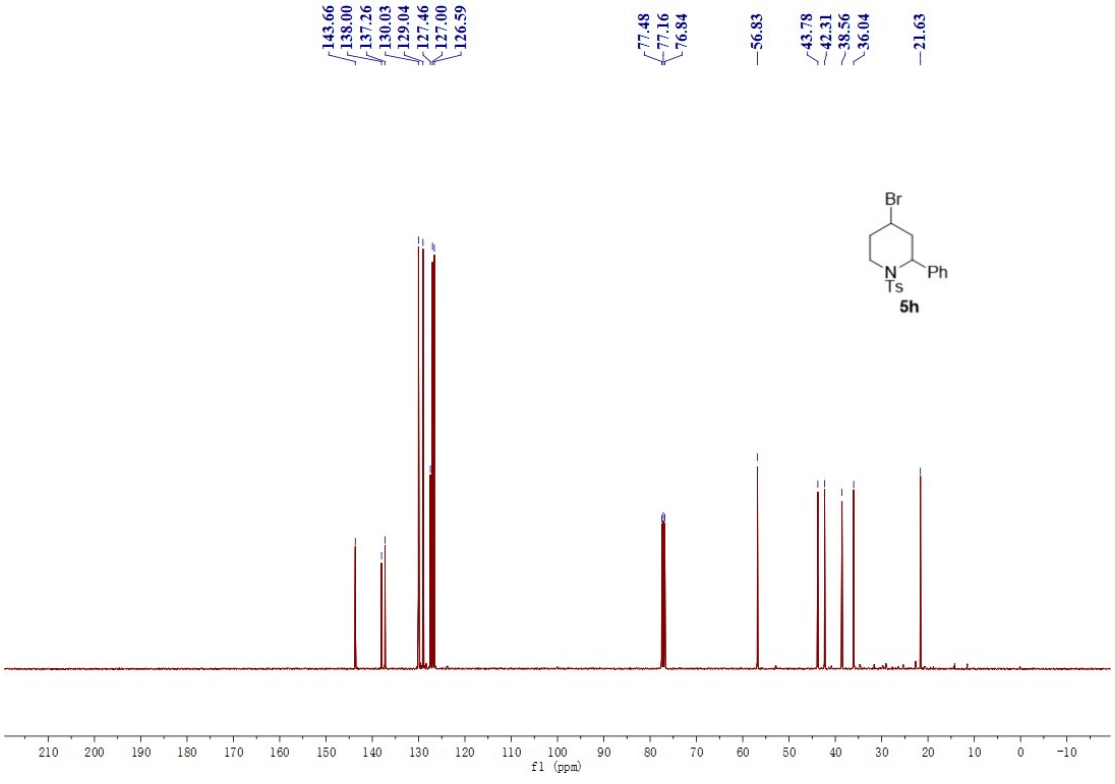
6.11
0.87
1.00
1.02
1.01
0.98
1.00
3.10
2.05
1.02
f1 (ppm)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129.04
127.46
127.00
126.59
77.48
77.16
76.84
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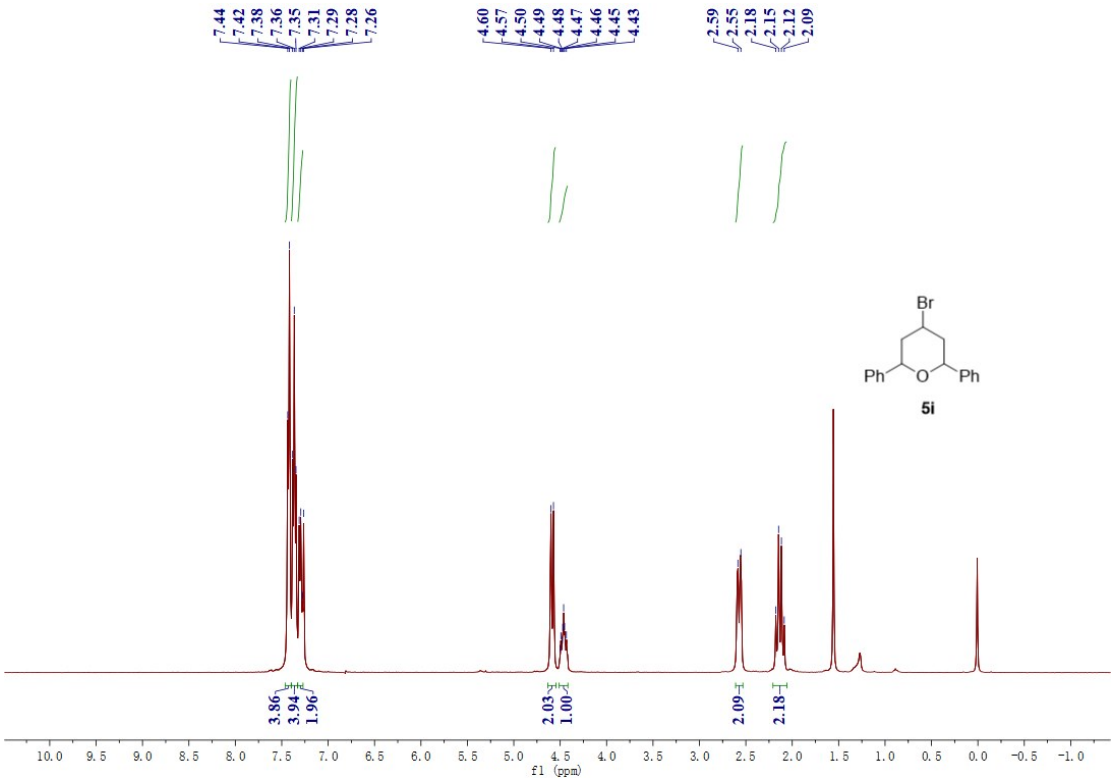
43.78
42.31
38.56
36.04
21.63
Br
N
Ts
Ph
5h
f1 (ppm)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7.28
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4.50
4.49
4.48
4.47
4.46
4.45
4.43
2.59
2.55
2.18
2.15
2.12
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Ph
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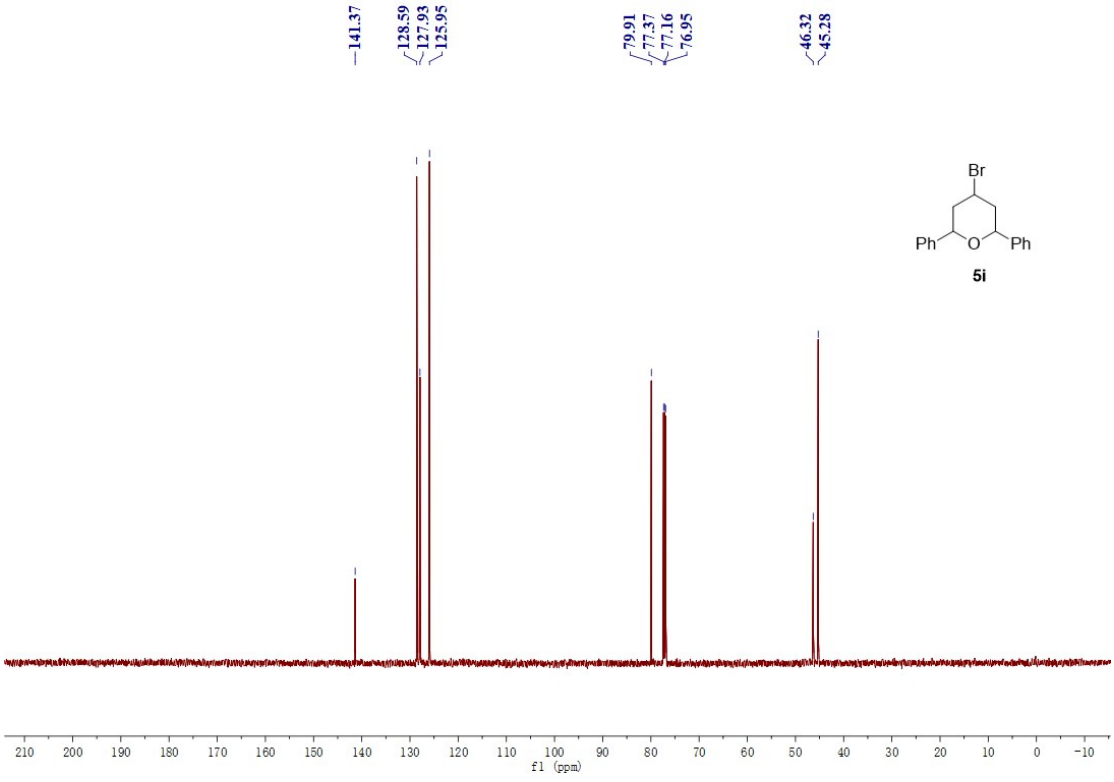
Ph
5i
3.86
3.94
1.96
2.03
1.00
2.09
2.18
f1 (ppm)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76.95
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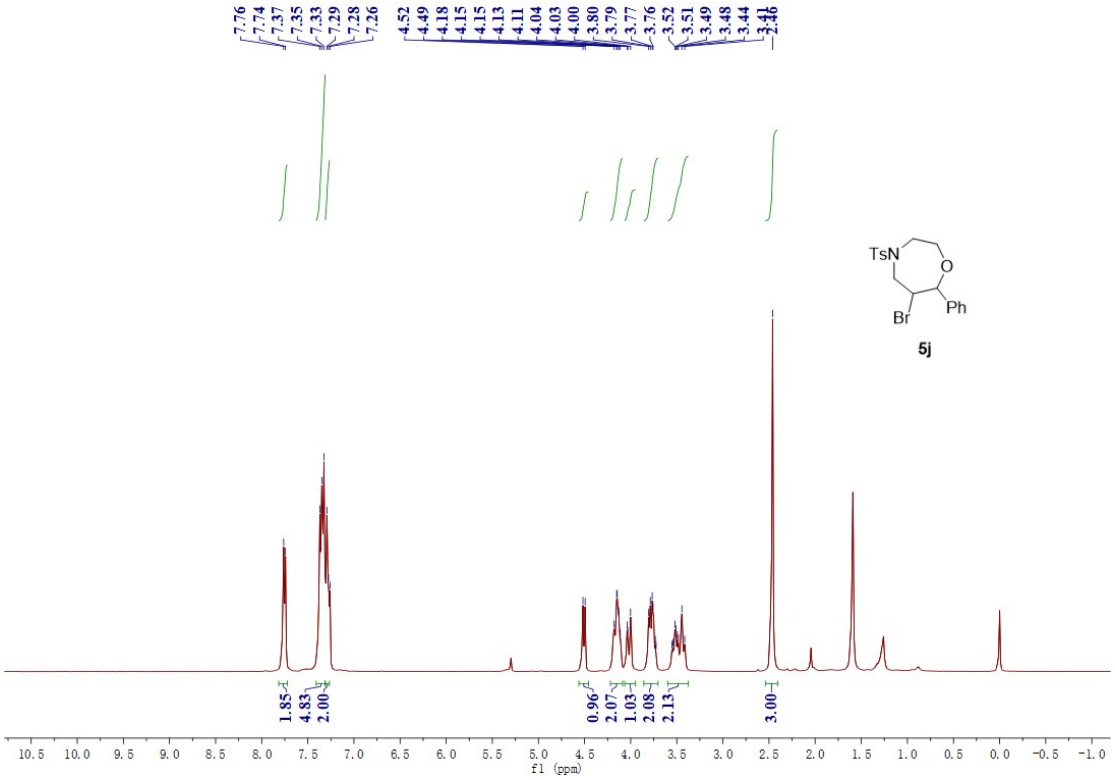
Br
Ph
O
Ph
5i
f1 (ppm)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7.35
7.33
7.29
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7.26
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4.49
4.18
4.15
4.15
4.13
4.11
4.04
4.03
4.00
3.80
3.79
3.77
3.76
3.52
3.51
3.49
3.48
3.44
3.41
2.46
TsN
O
Br
Ph
5j
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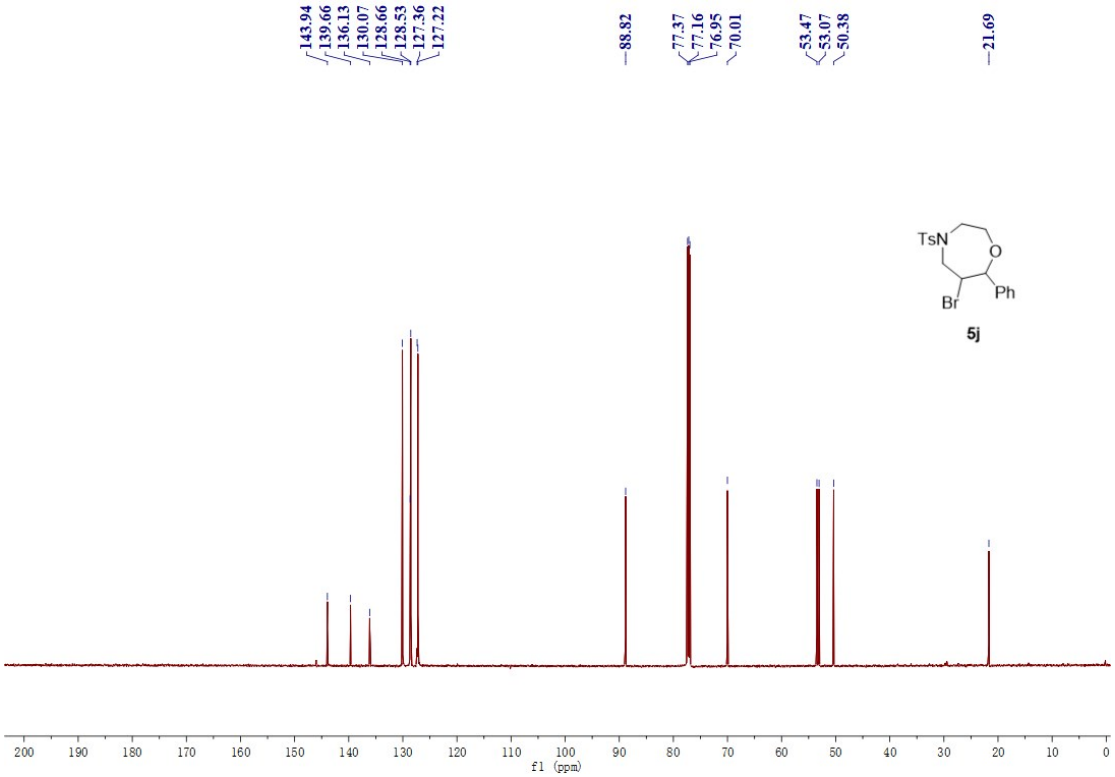
4.83
2.00
0.96
2.07
1.03
2.08
2.13
3.00
f1 (ppm)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127.22
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77.37
77.16
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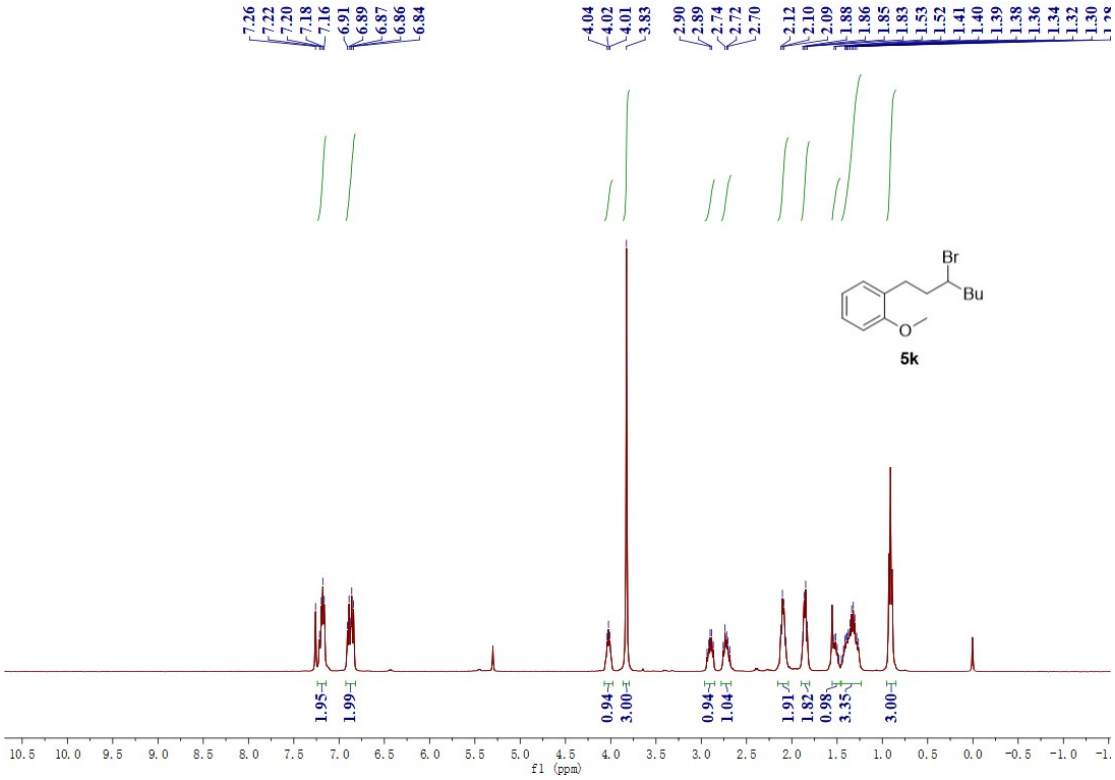
53.47
53.07
50.38
21.69
TsN
O
Br
Ph
5j
f1 (ppm)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7.18
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6.87
6.86
6.84
4.04
4.02
4.01
3.83
2.90
2.89
2.74
2.72
2.70
2.12
2.10
2.09
1.88
1.86
1.85
1.83
1.53
1.52
1.41
1.40
1.39
1.38
1.36
1.34
1.32
1.30
Br
Bu
O
5k
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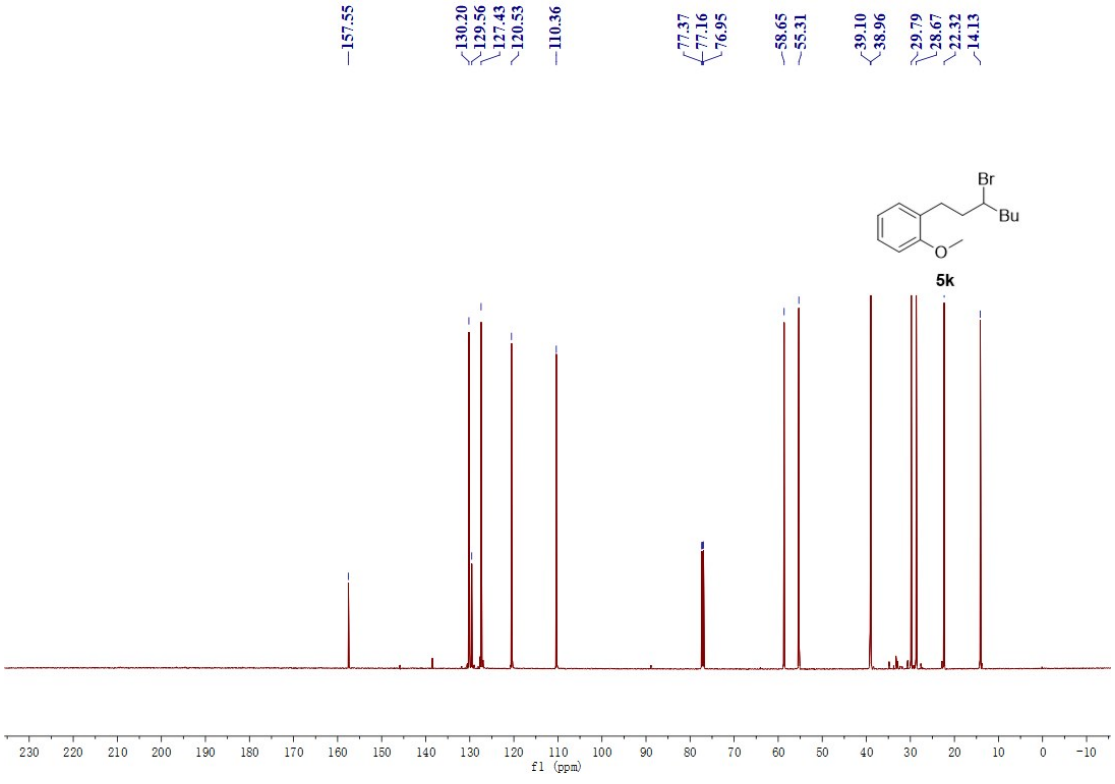
1.99
0.94
3.00
0.94
1.04
1.91
1.82
0.98
3.35
3.00
f1 (ppm)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76.95
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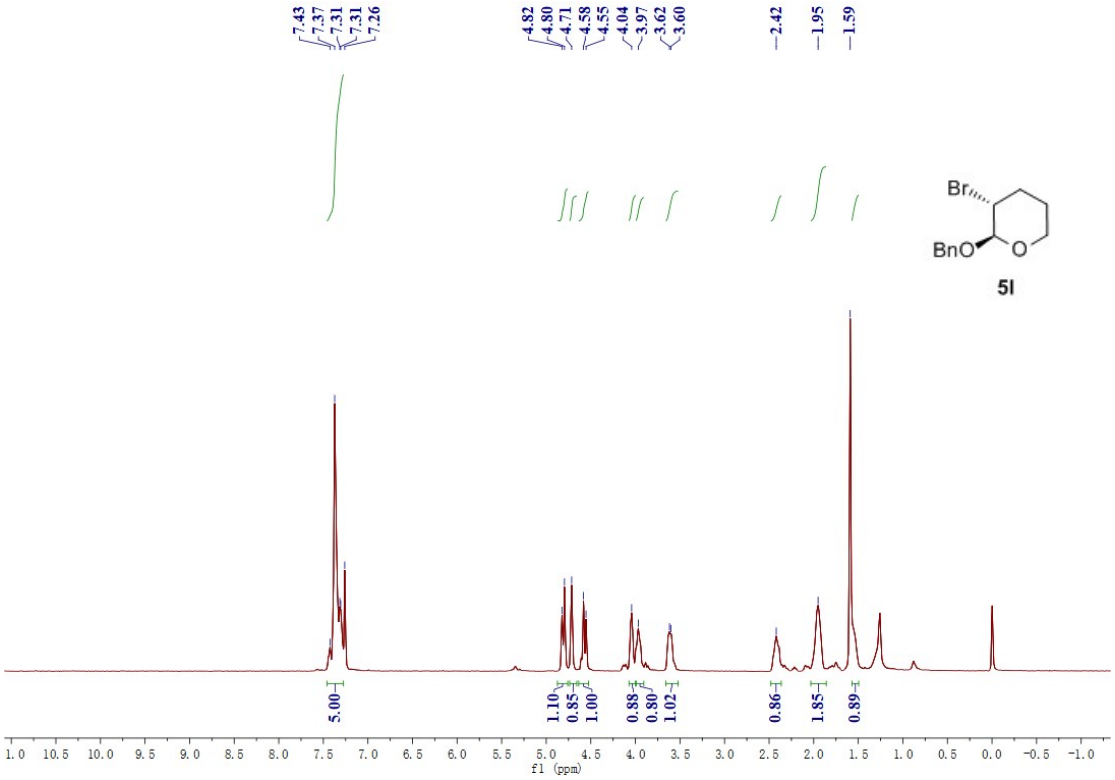
39.10
38.96
29.79
28.67
22.32
14.13
Br
Bu
O
5k
f1 (ppm)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4.71
4.58
4.55
4.04
3.97
3.62
3.60
2.42
1.95
1.59
Br
BnO
O
5l
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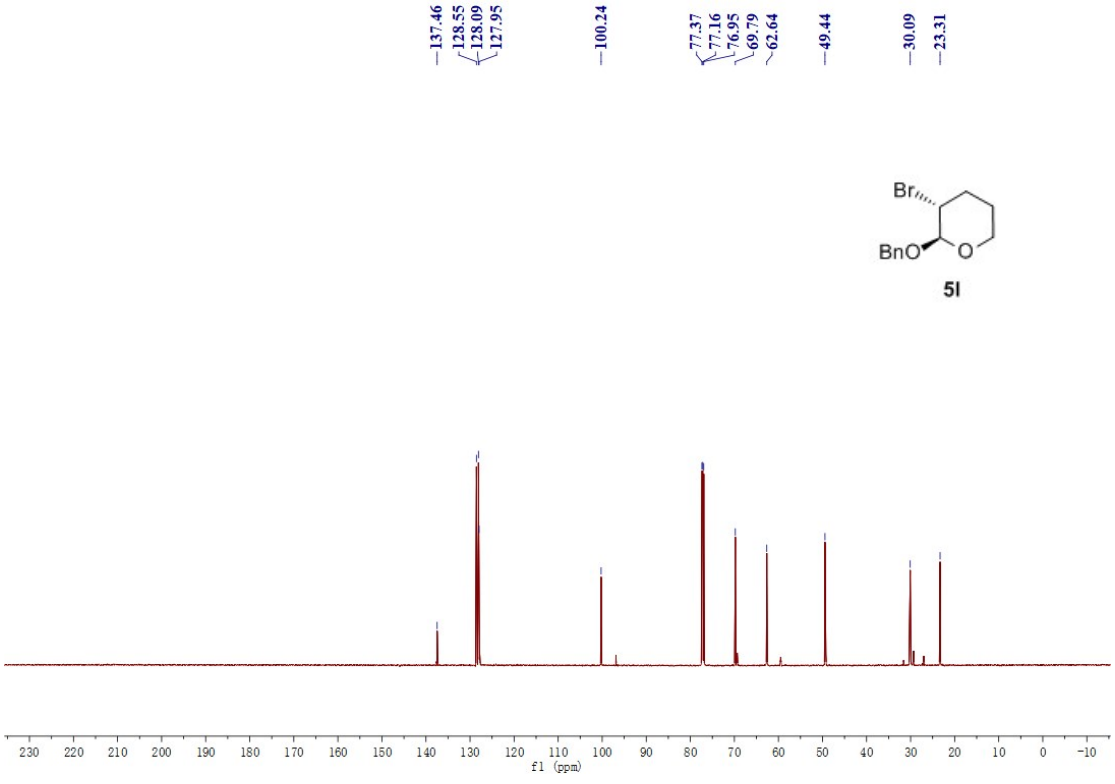
1.10
0.85
1.00
0.88
0.80
1.02
0.86
1.85
0.89
f1 (ppm)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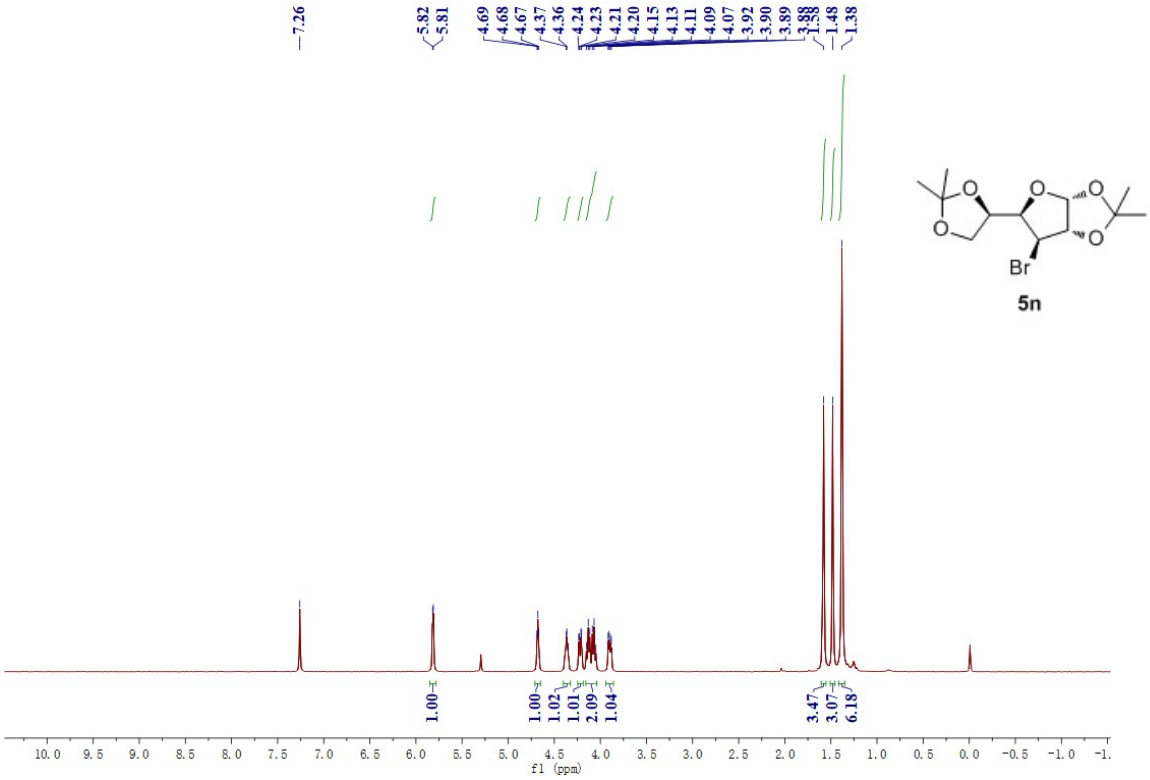
69.79
62.64
49.44
30.09
23.31
Br
BnO
O
5l
f1 (ppm)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4.67
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4.24
4.23
4.21
4.20
4.15
4.13
4.11
4.09
4.07
3.92
3.90
3.89
1.48
1.38
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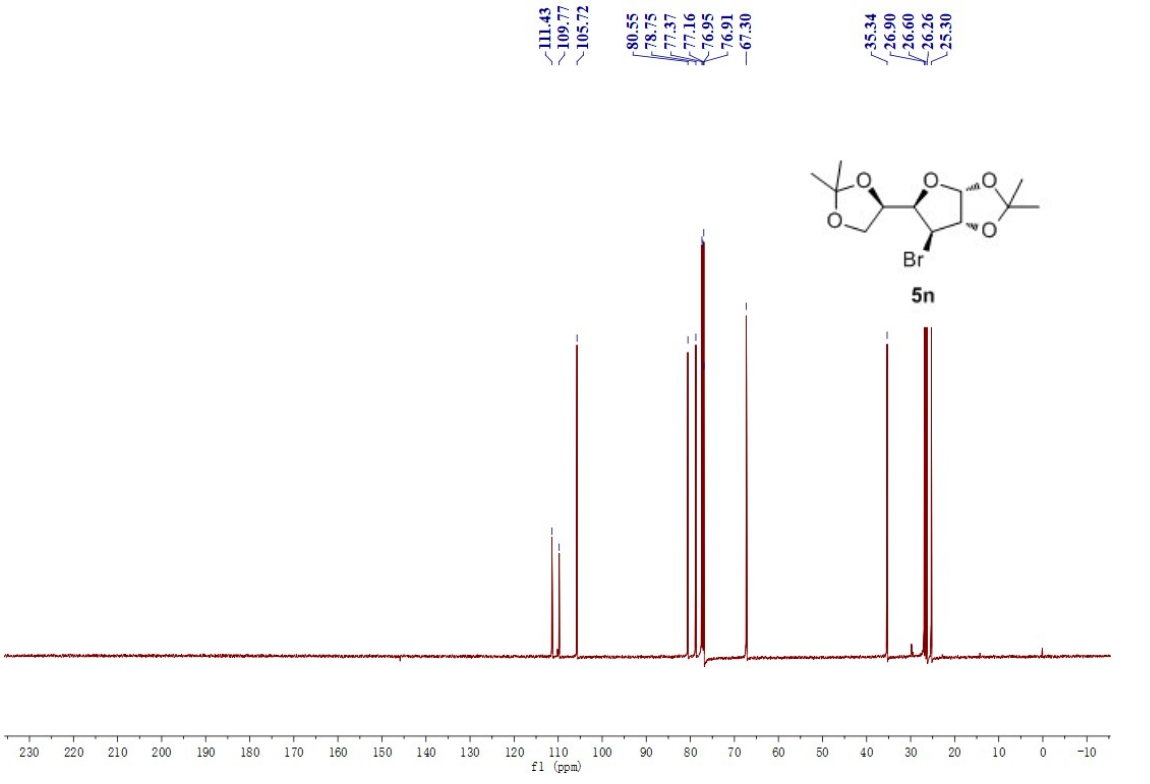
1.00
1.02
1.01
2.09
1.04
3.47
3.07
6.18
f1 (ppm)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67.30
35.34
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26.26
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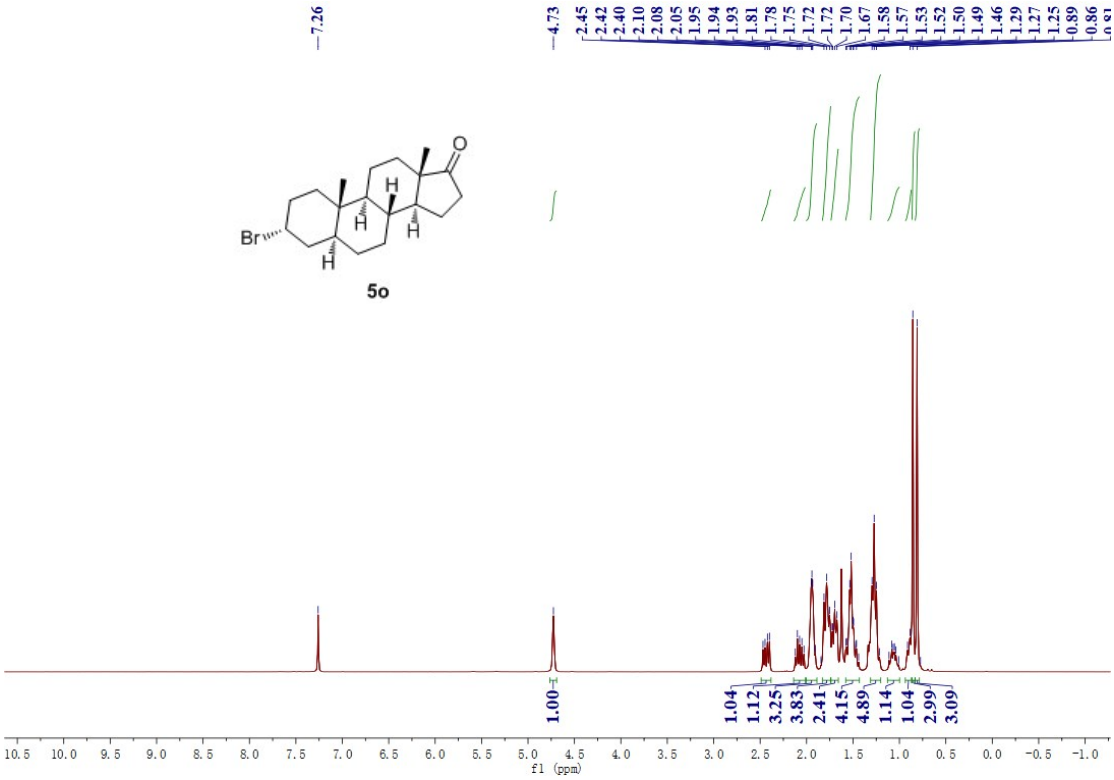
5n
f1 (ppm)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2.40
2.10
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1.95
1.94
1.93
1.81
1.78
1.75
1.72
1.72
1.70
1.67
1.58
1.57
1.53
1.52
1.50
1.49
1.46
1.29
1.27
1.25
0.89
0.86
Br
H
H
H
O
5o
1.00
1.04
1.12
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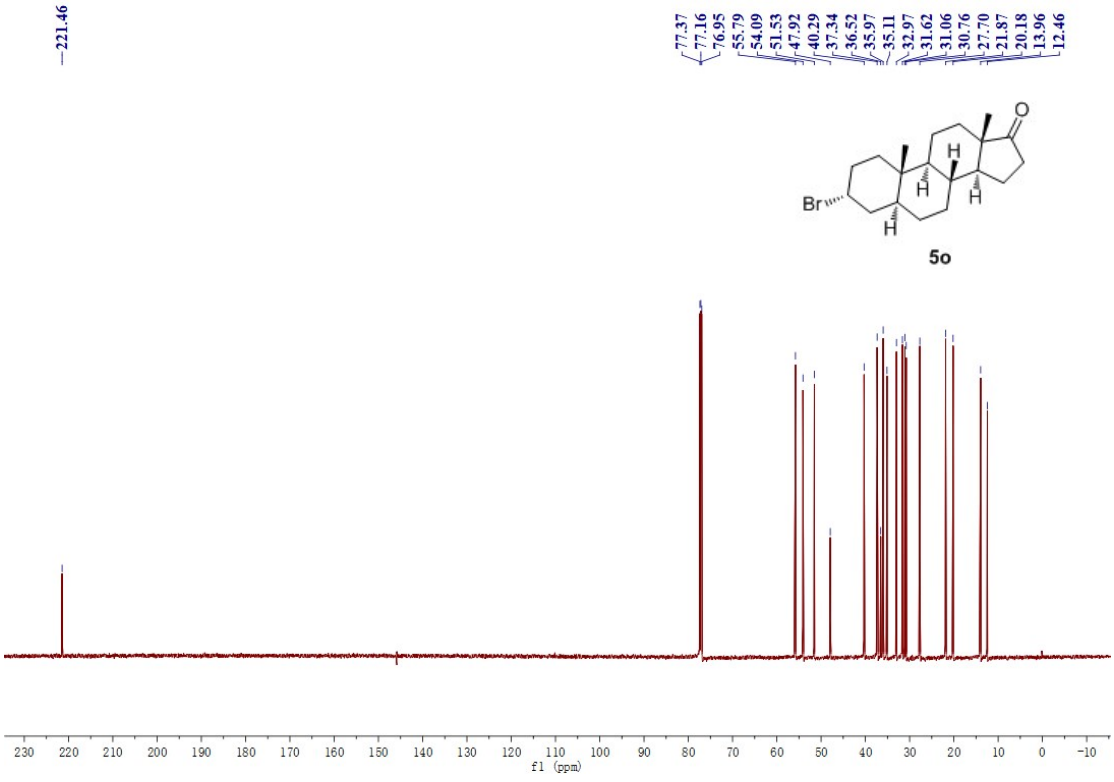
3.83
2.41
4.15
4.89
1.14
1.04
2.99
3.09
f1 (ppm)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35.11
32.97
31.62
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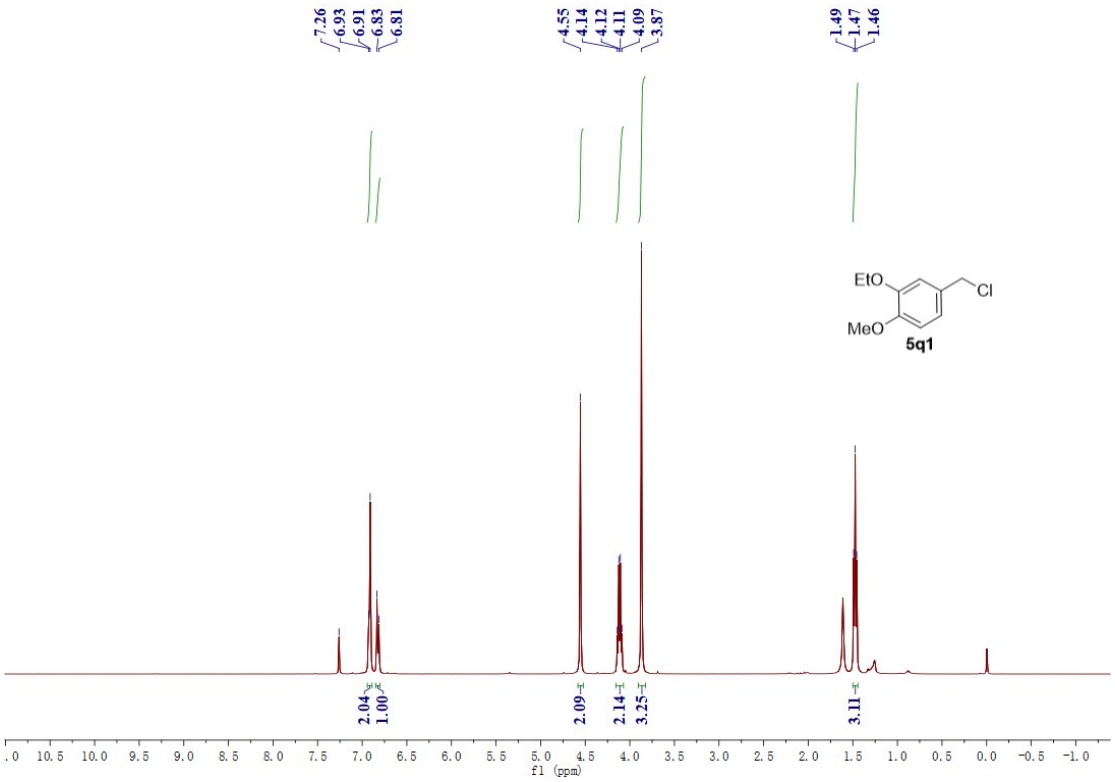
27.70
21.87
20.18
13.96
12.46
Br
H
H
H
O
5o
f1 (ppm)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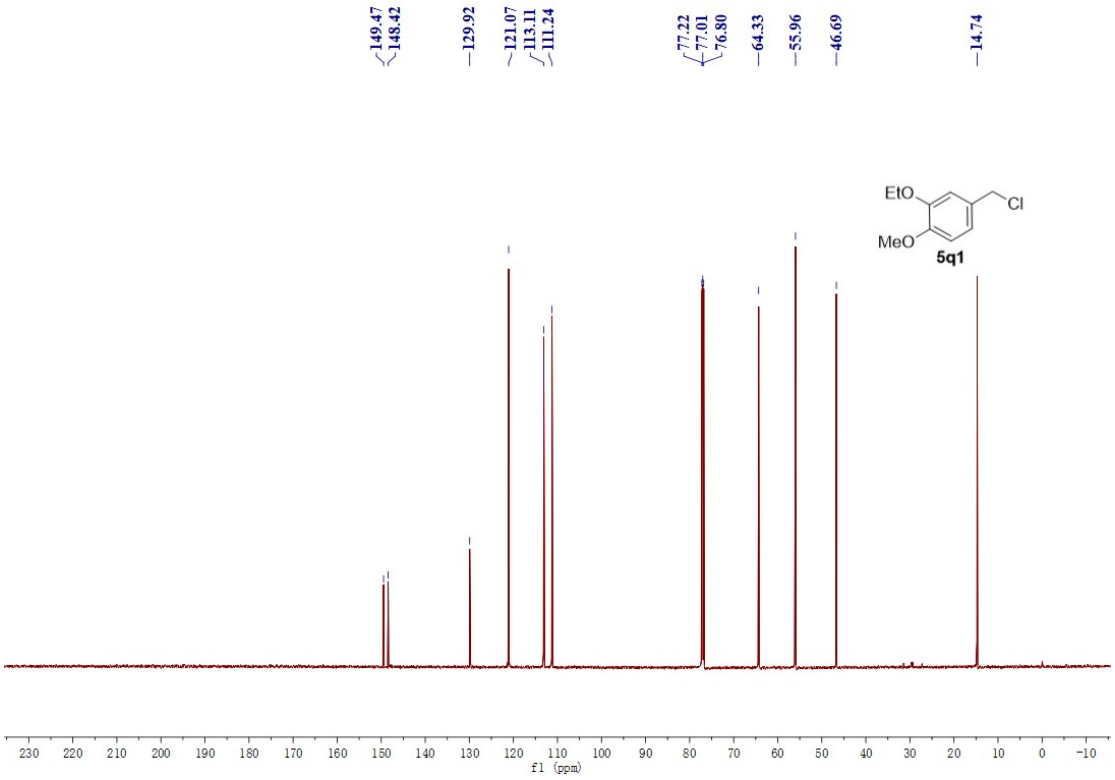
6.91
6.83
6.81
4.55
4.14
4.12
4.11
4.09
3.87
1.49
1.47
1.46
EtO
Cl
MeO
5q1
2.04
1.00
2.09
2.14
3.25
3.11
f1 (ppm)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113.11
111.24
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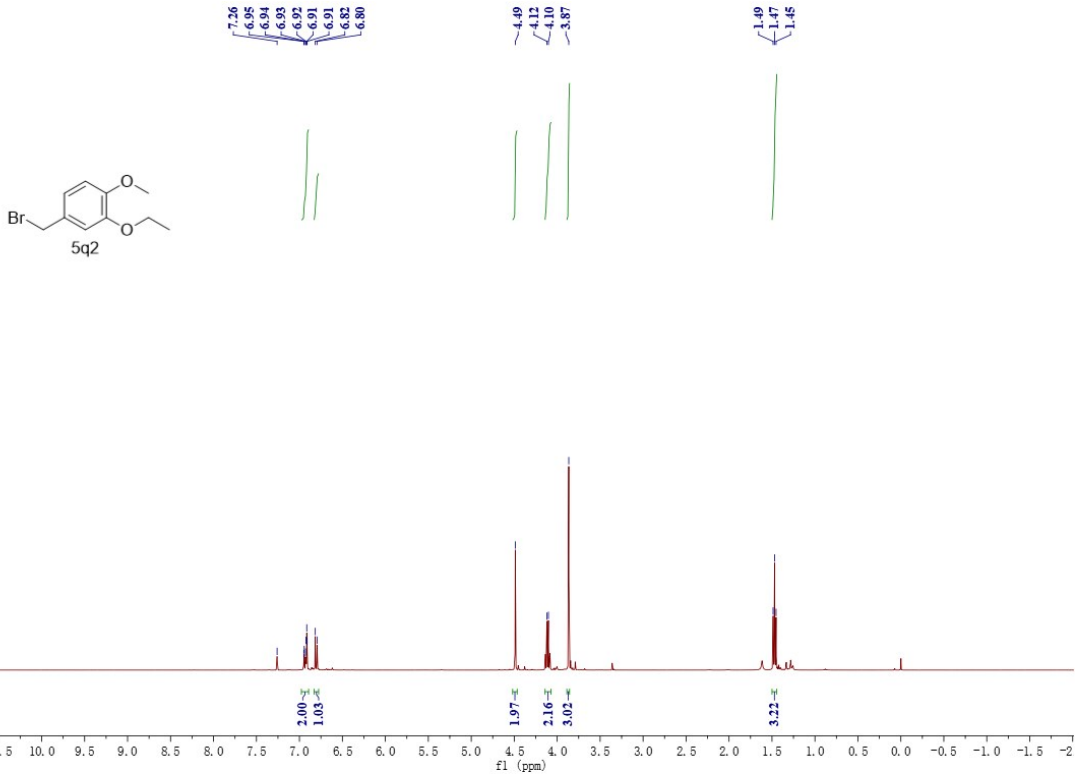
76.80
64.33
55.96
46.69
14.74
EtO
Cl
MeO
5q1
f1 (ppm)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6.95
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6.93
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6.91
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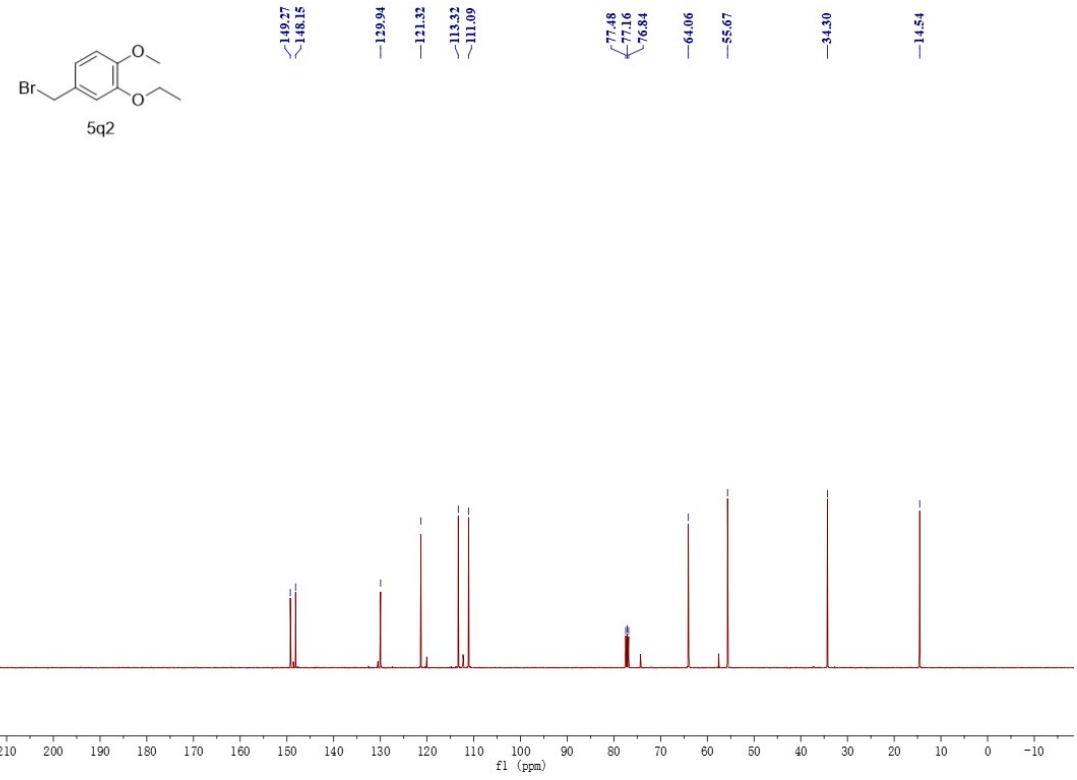
6.82
6.80
4.49
4.12
4.10
3.87
1.49
1.47
1.45
Br
O
O
5q2
2.00
1.03
1.97
2.16
3.02
3.22
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2
f1 (ppm)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121.32
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77.48
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76.84
64.06
55.67
34.30
14.54
Br
O
O
5q2
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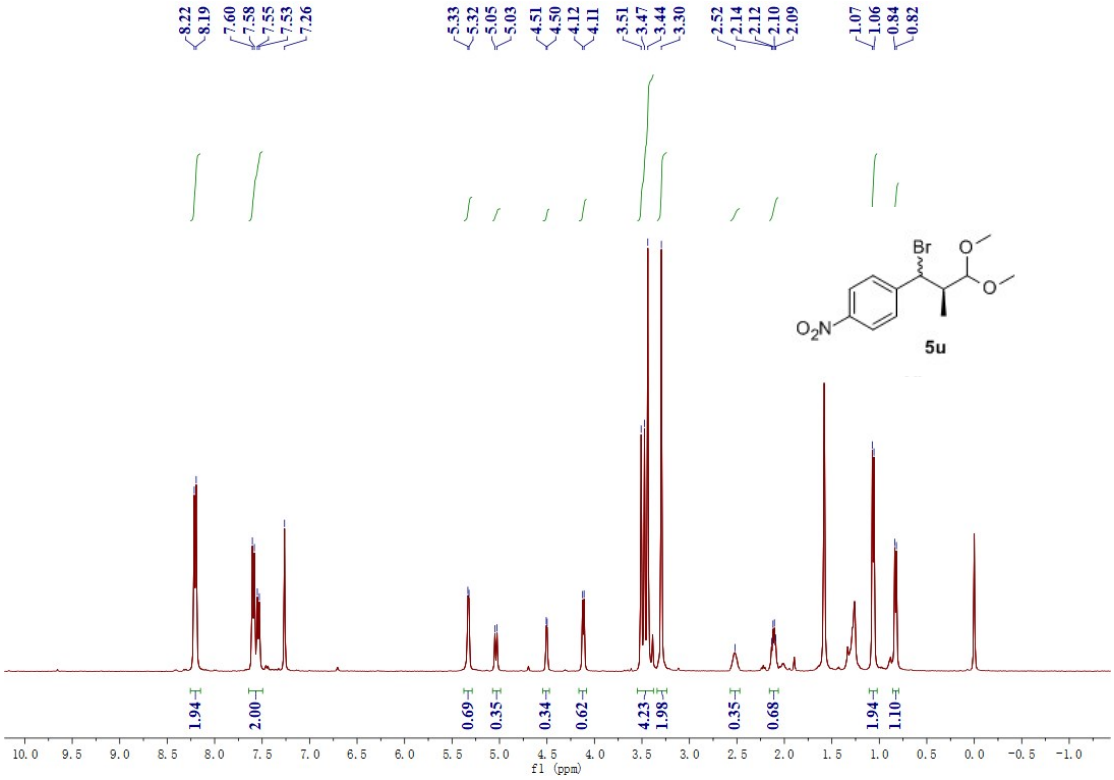
f1 (ppm)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5.33
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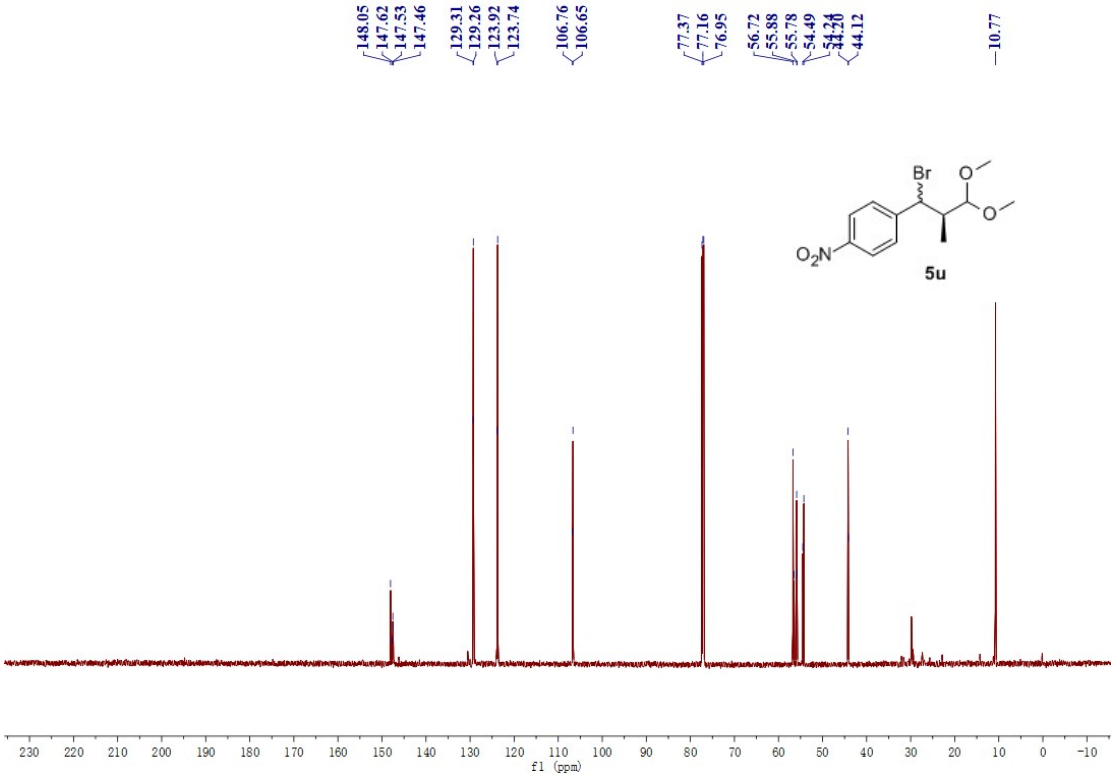
5.05
5.03
4.51
4.50
4.12
4.11
3.51
3.47
3.44
3.30
2.52
2.14
2.12
2.10
2.09
1.07
1.06
0.84
0.82
Br
O
O
O2N
5u
1.94
2.00
0.69
0.35
0.34
0.62
4.23
1.98
0.35
0.68
1.94
1.10
f1 (ppm)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123.74
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106.65
77.37
77.16
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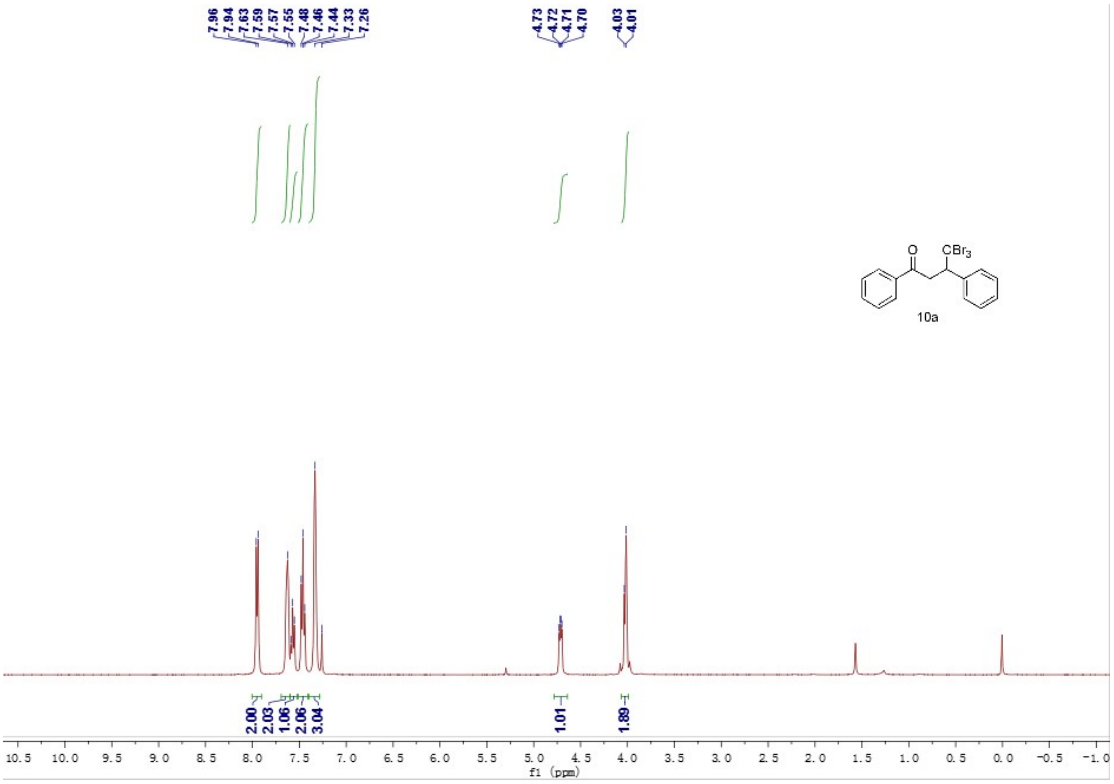
55.88
55.78
54.49
44.12
10.77
Br
O
O
O2N
5u
f1 (ppm)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7.46
7.44
7.33
7.26
4.73
4.72
4.71
4.70
4.03
4.01
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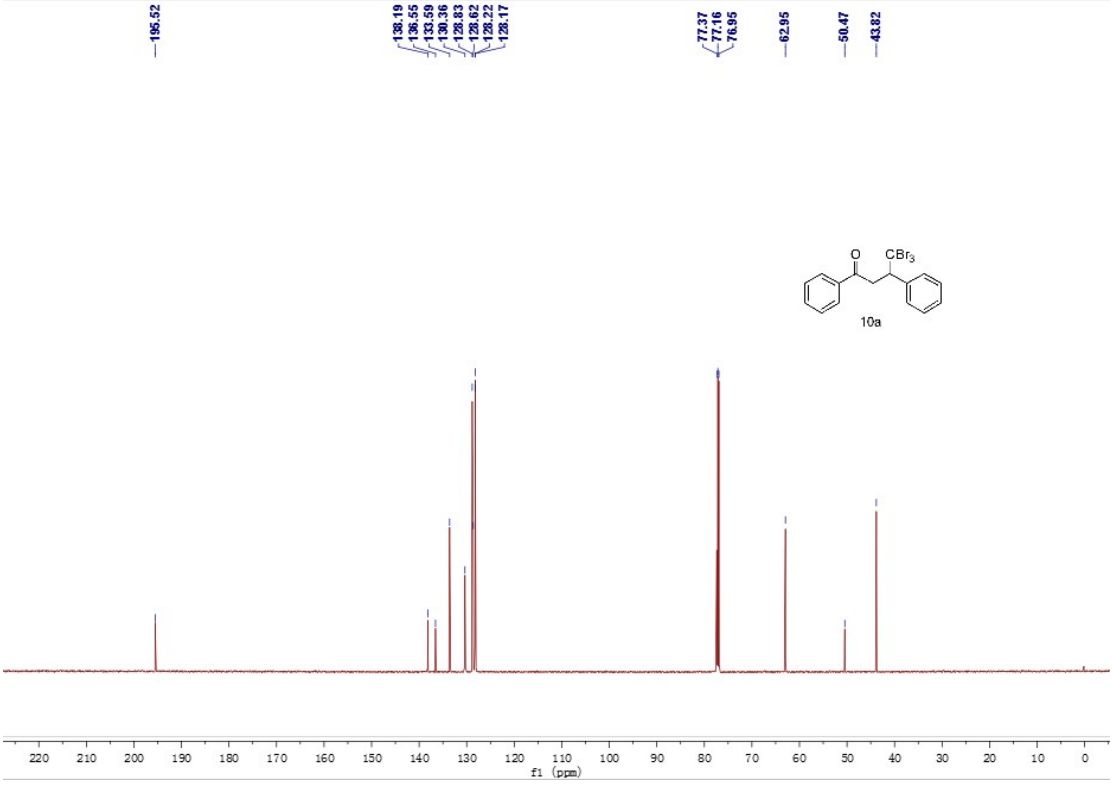
10a
2.00
2.03
1.06
2.06
3.04
1.01
1.89
f1 (ppm)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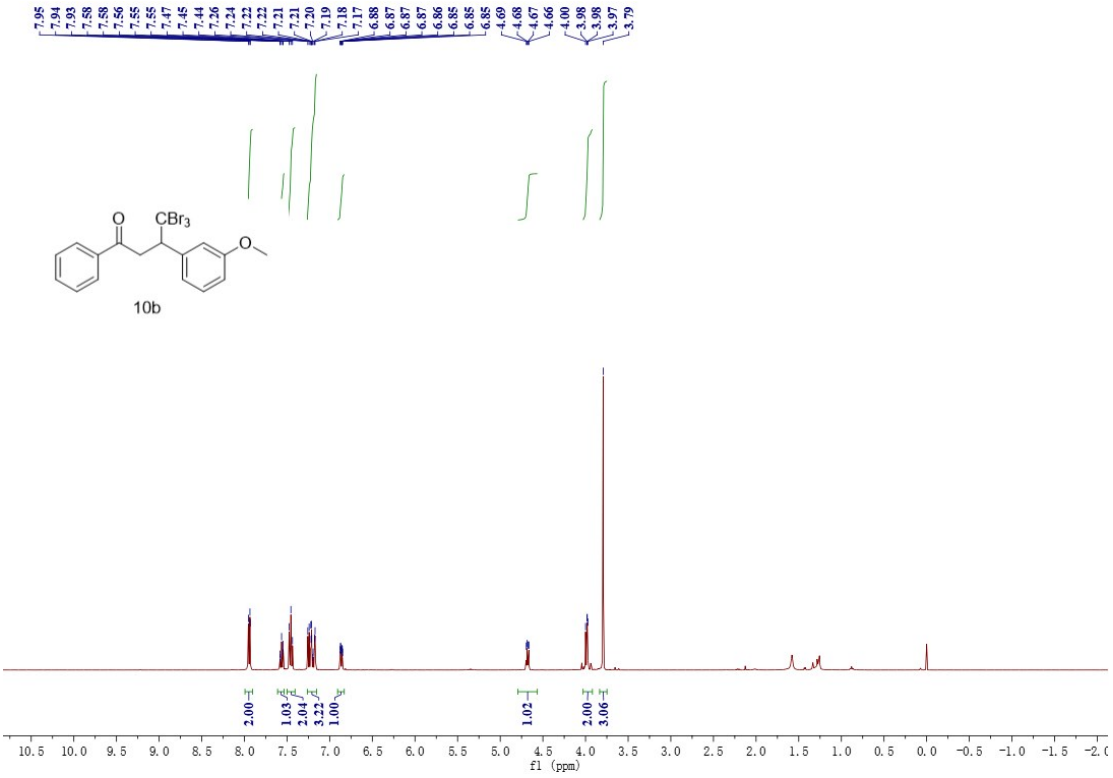
77.16
76.95
62.95
50.47
43.82
O
CBr3
10a
f1 (ppm)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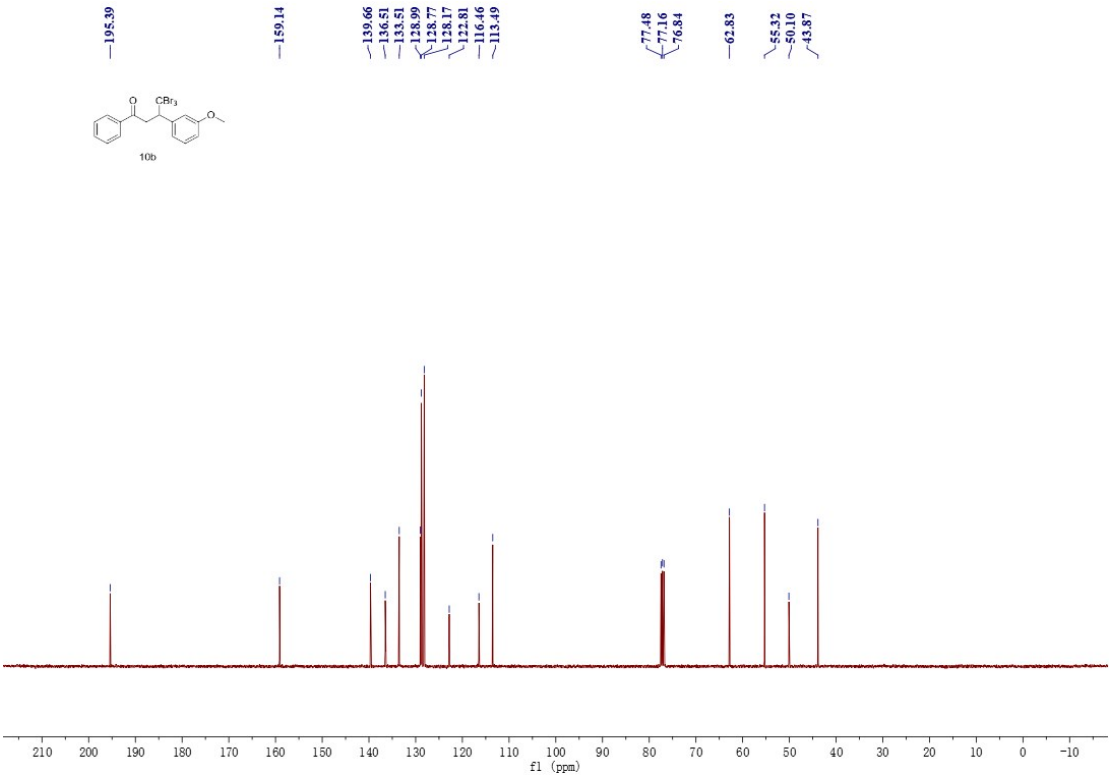
7.26
7.24
7.22
7.22
7.21
7.21
7.20
7.19
7.18
7.17
6.88
6.87
6.87
6.87
6.86
6.85
6.85
6.85
4.69
4.68
4.67
4.66
4.00
3.98
3.98
3.97
3.79
O
CBr3
O
10b
2.00
1.03
2.04
3.22
1.00
1.02
2.00
3.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)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128.17
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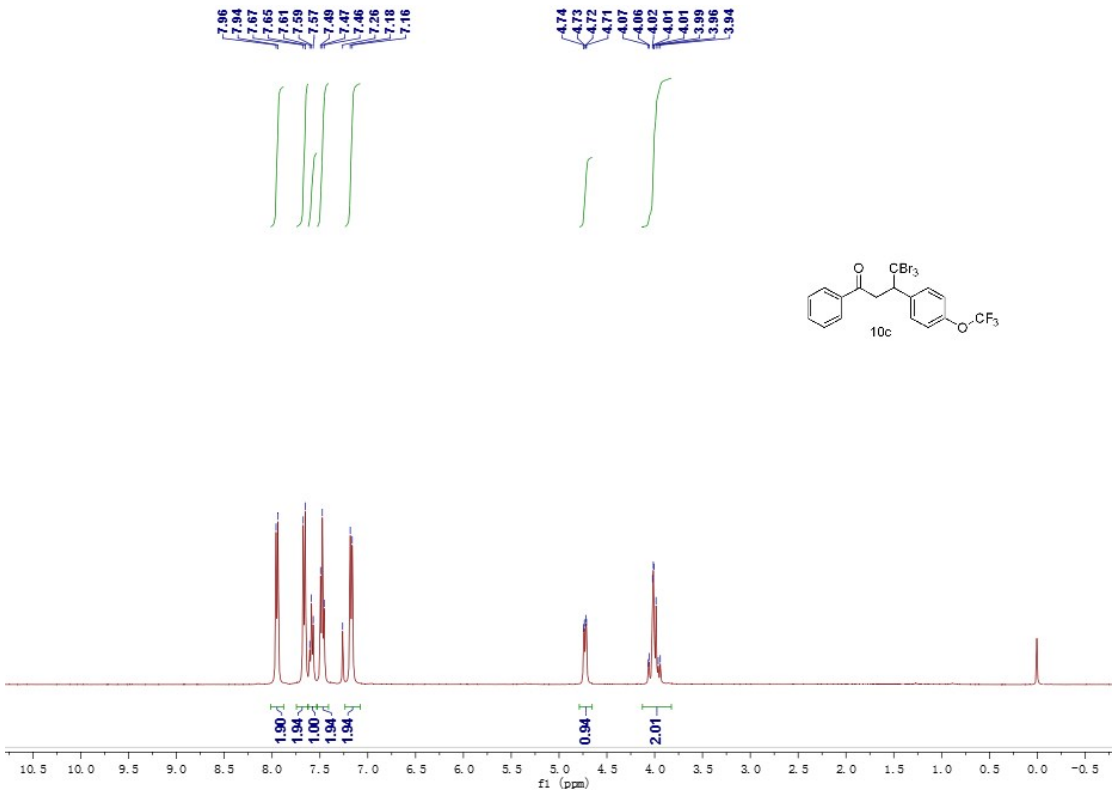
116.46
113.49
77.48
77.16
76.84
62.83
55.32
50.10
43.87
O
CBr3
O
10b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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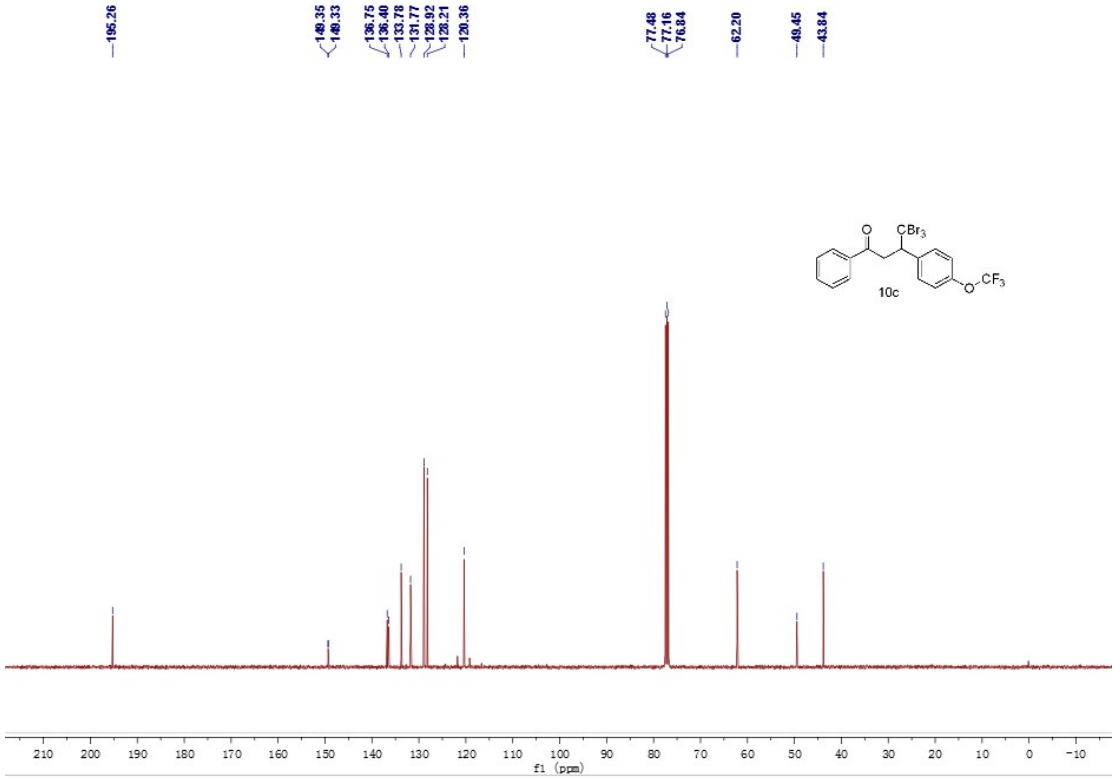
7.94
7.67
7.65
7.61
7.59
7.57
7.49
7.47
7.46
7.26
7.18
7.16
4.74
4.73
4.72
4.71
4.07
4.06
4.02
4.01
4.01
3.99
3.96
3.94
CBr3
O
CF3
O
10c
1.90
1.94
1.00
1.94
1.94
0.94
2.01
f1 (ppm)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133.78
131.77
128.92
128.21
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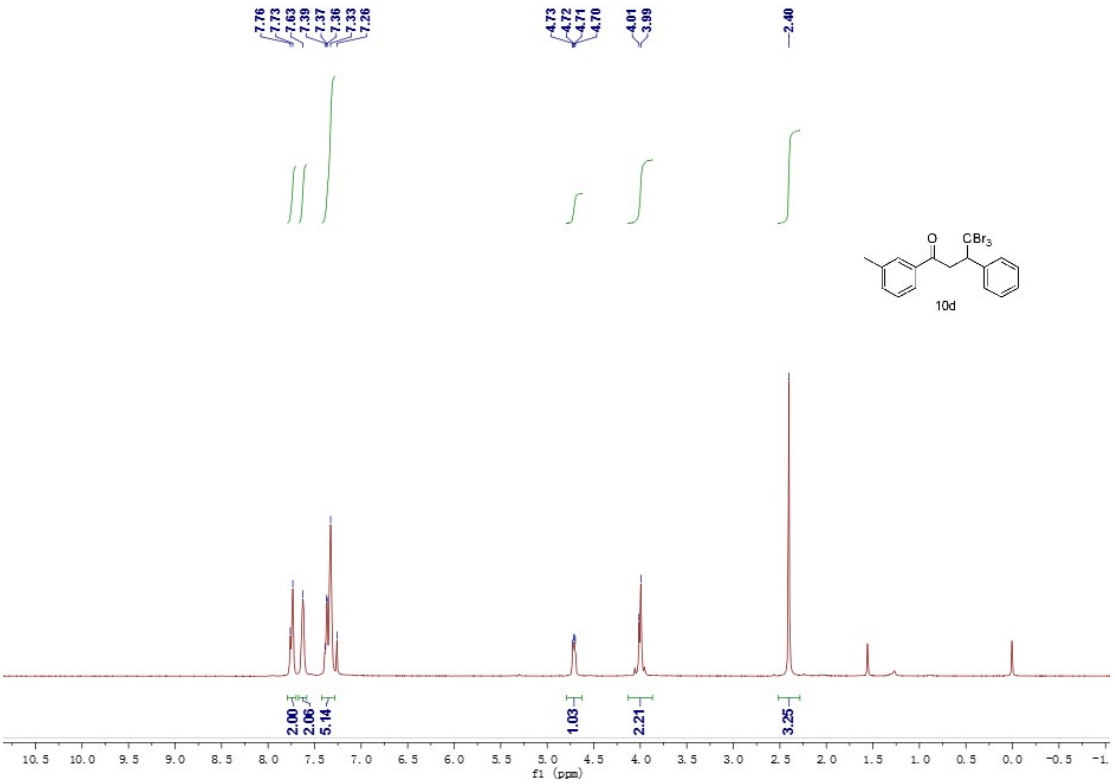
77.16
76.84
62.20
49.45
43.84
CBr3
O
CF3
O
10c
f1 (ppm)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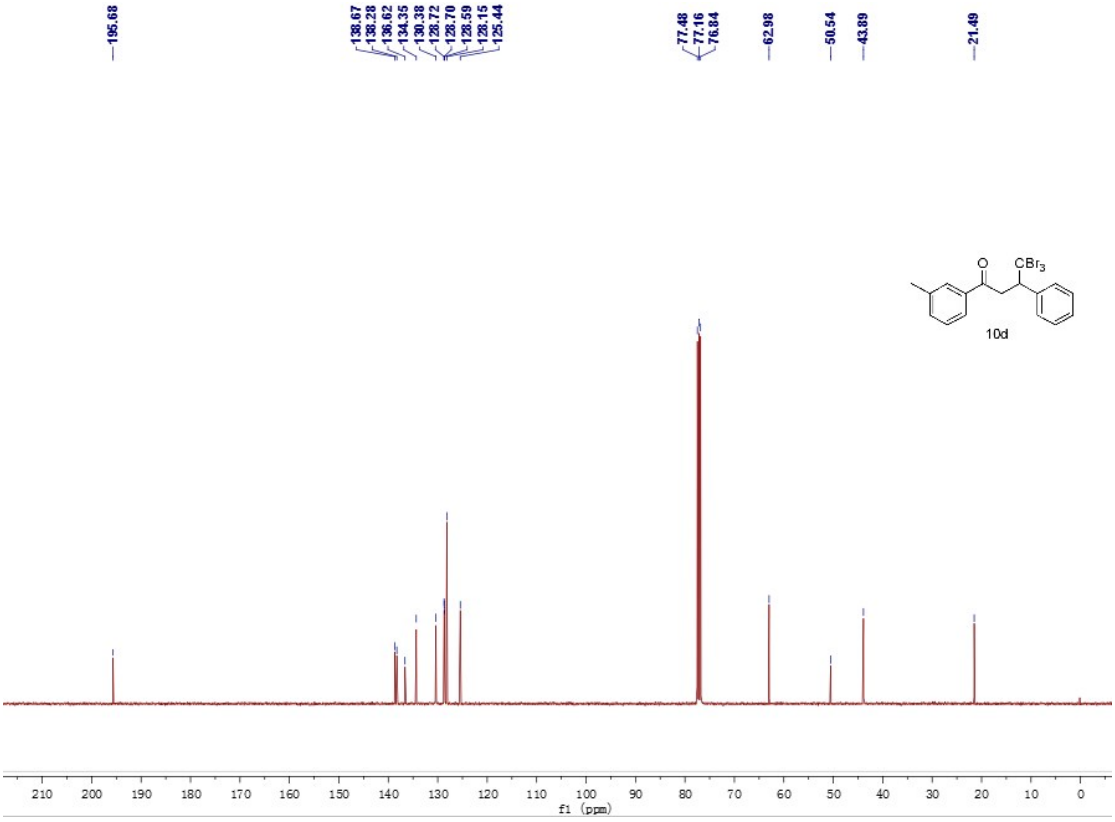
7.63
7.39
7.37
7.36
7.33
7.26
4.73
4.72
4.71
4.70
4.01
3.99
2.40
O
CBr3
10d
2.00
2.06
5.14
1.03
2.21
3.25
f1 (ppm)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130.38
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128.70
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128.15
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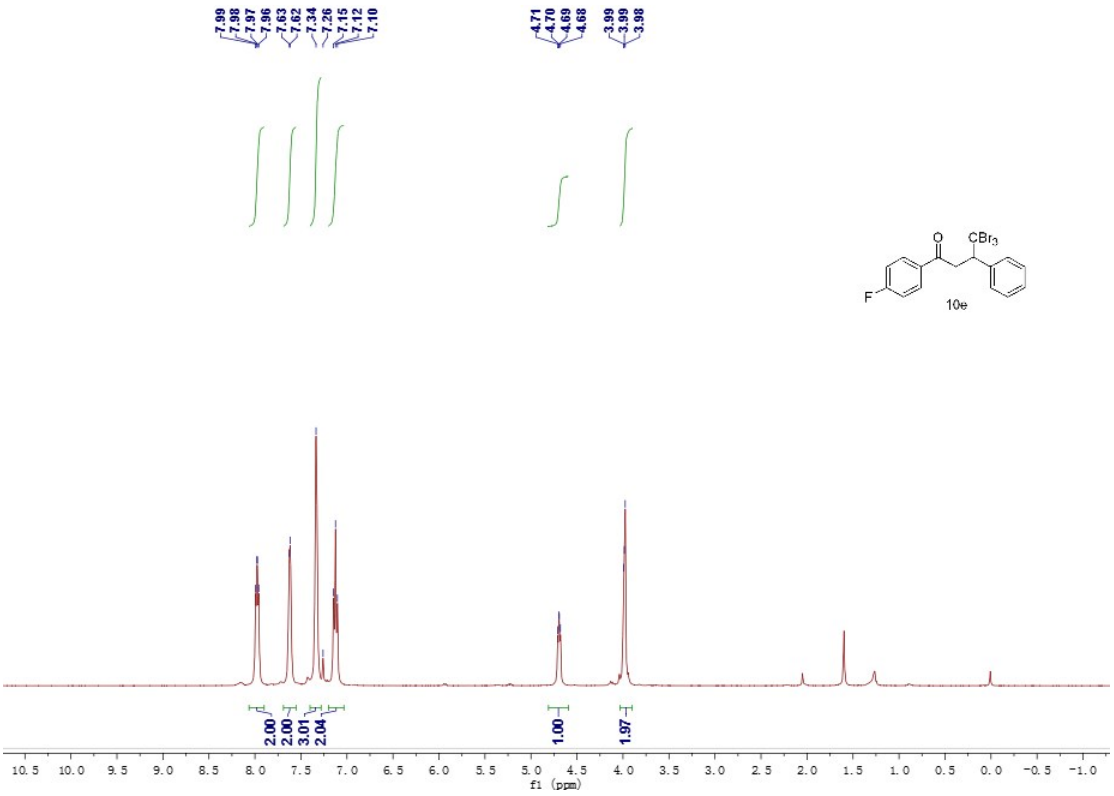
77.16
76.84
62.98
50.54
43.89
21.49
O
CBr3
10d
f1 (ppm)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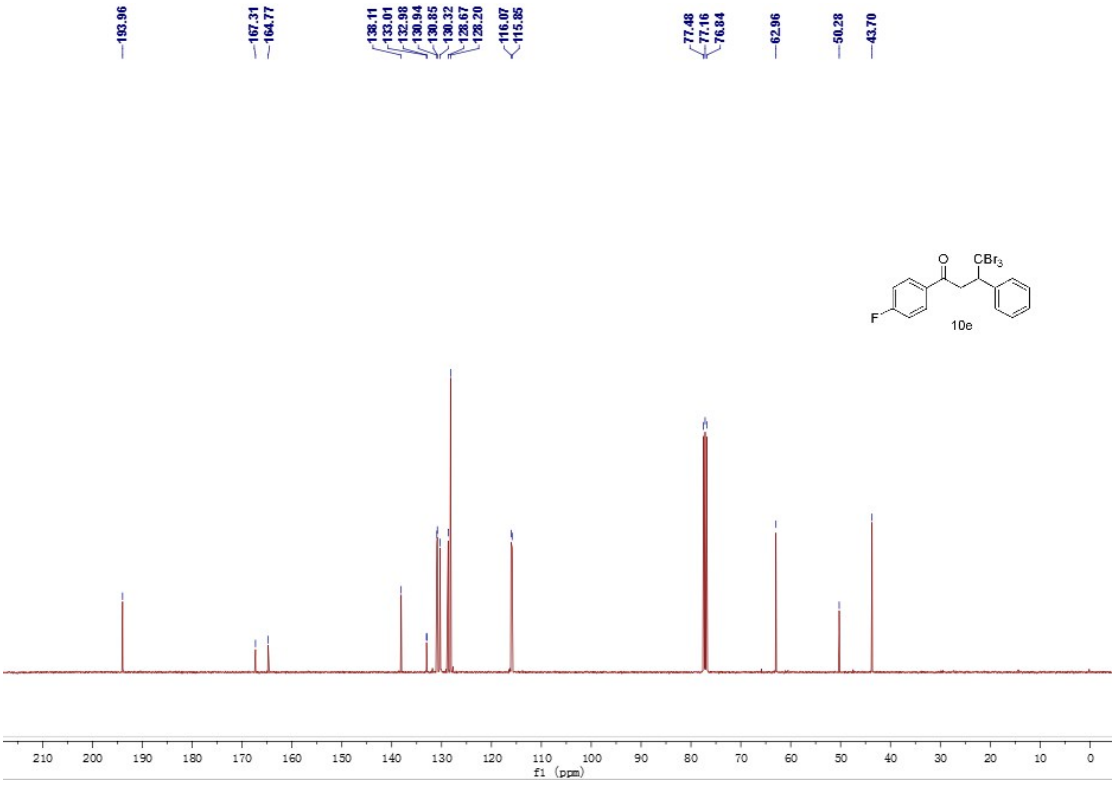
7.96
7.63
7.62
7.34
7.26
7.15
7.12
7.10
4.71
4.70
4.69
4.68
3.99
3.99
3.98
O
CBr3
F
10e
2.00
2.00
3.01
2.04
1.00
1.97
f1 (ppm)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128.20
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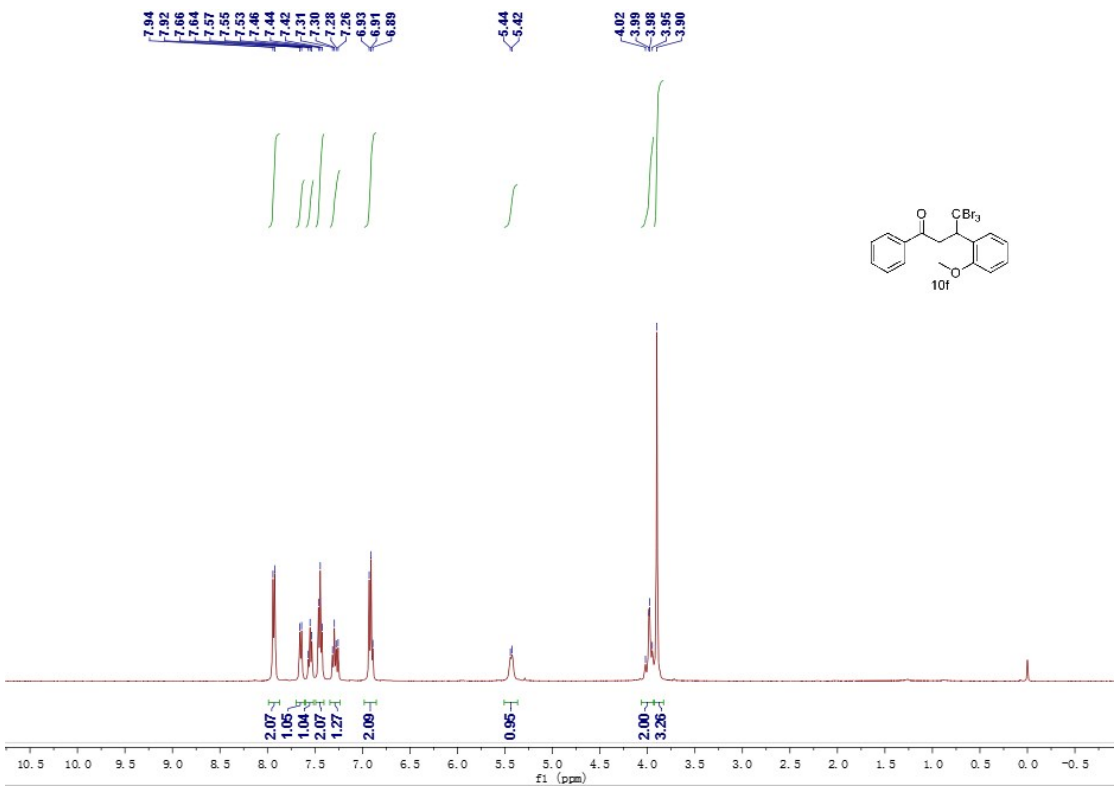
77.16
76.84
62.96
50.28
43.70
O
CBr3
F
10e
f1 (ppm)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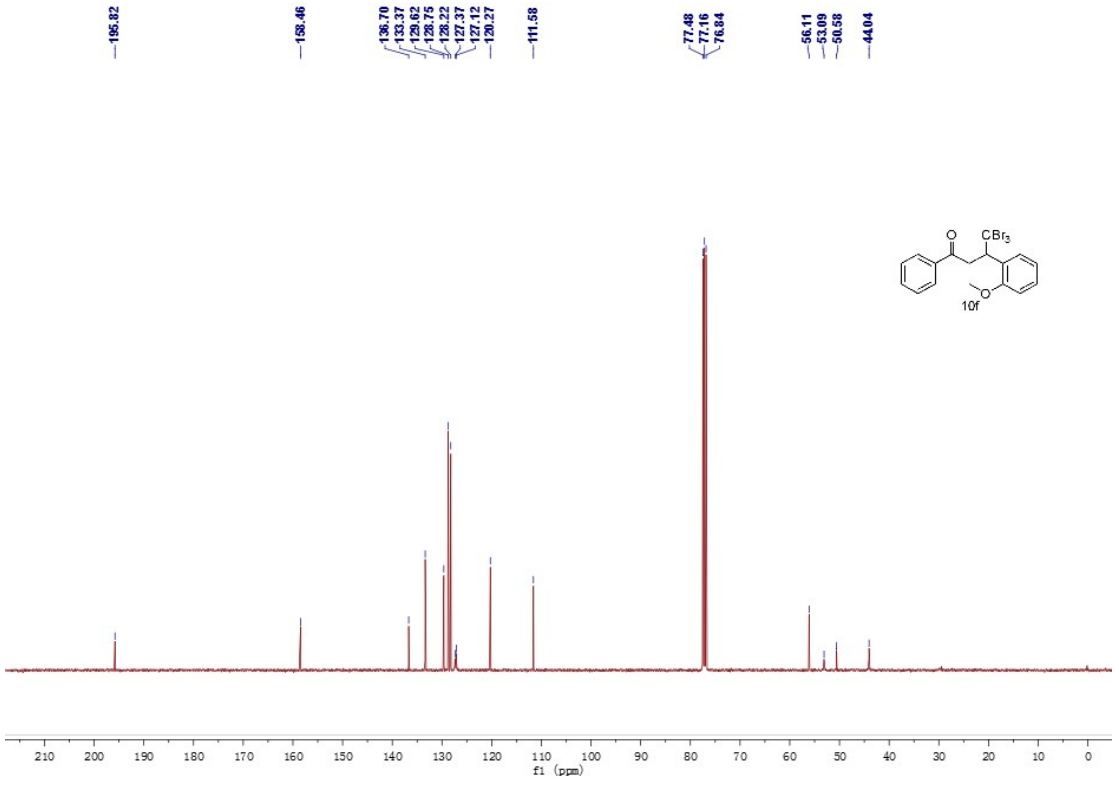
7.53
7.46
7.44
7.42
7.31
7.30
7.28
7.26
6.93
6.91
6.89
5.44
5.42
4.02
3.99
3.98
3.95
3.90
CBr3
O
O
10f
2.07
1.05
1.04
2.07
1.27
2.09
0.95
2.00
3.26
f1 (ppm)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128.22
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127.12
120.27
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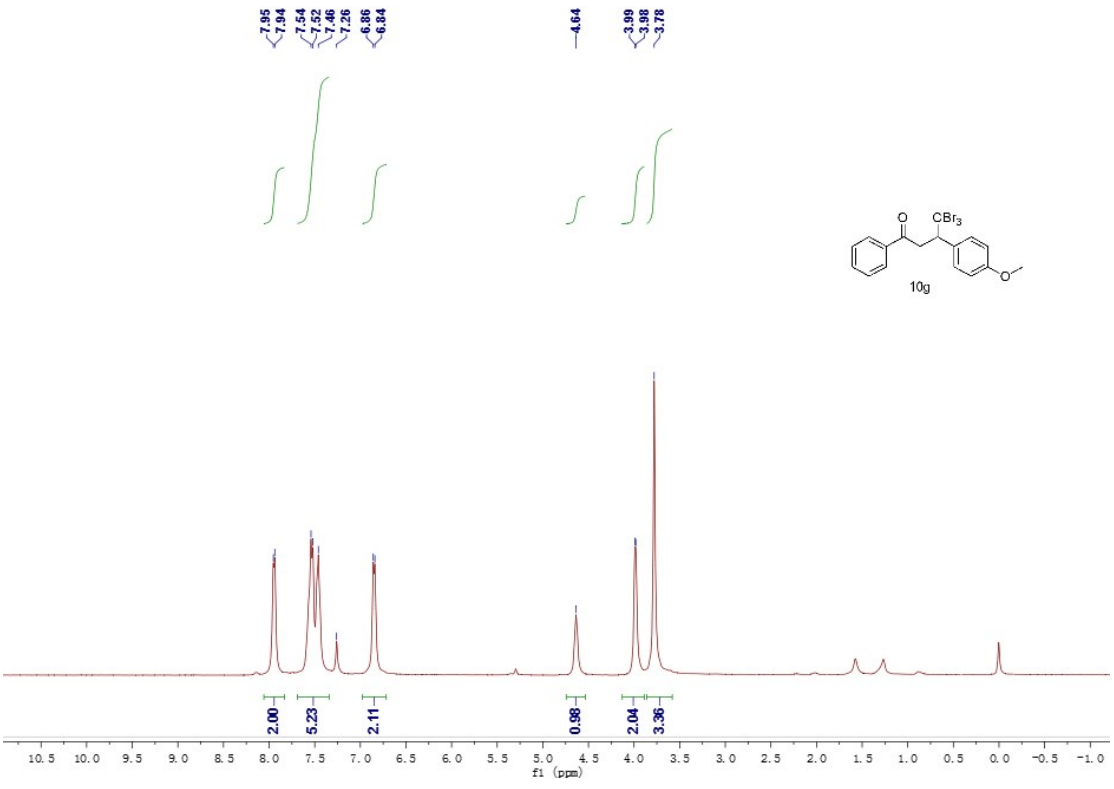
76.84
56.11
53.09
50.58
44.04
CBr3
O
O
10f
f1 (ppm)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7.94
7.54
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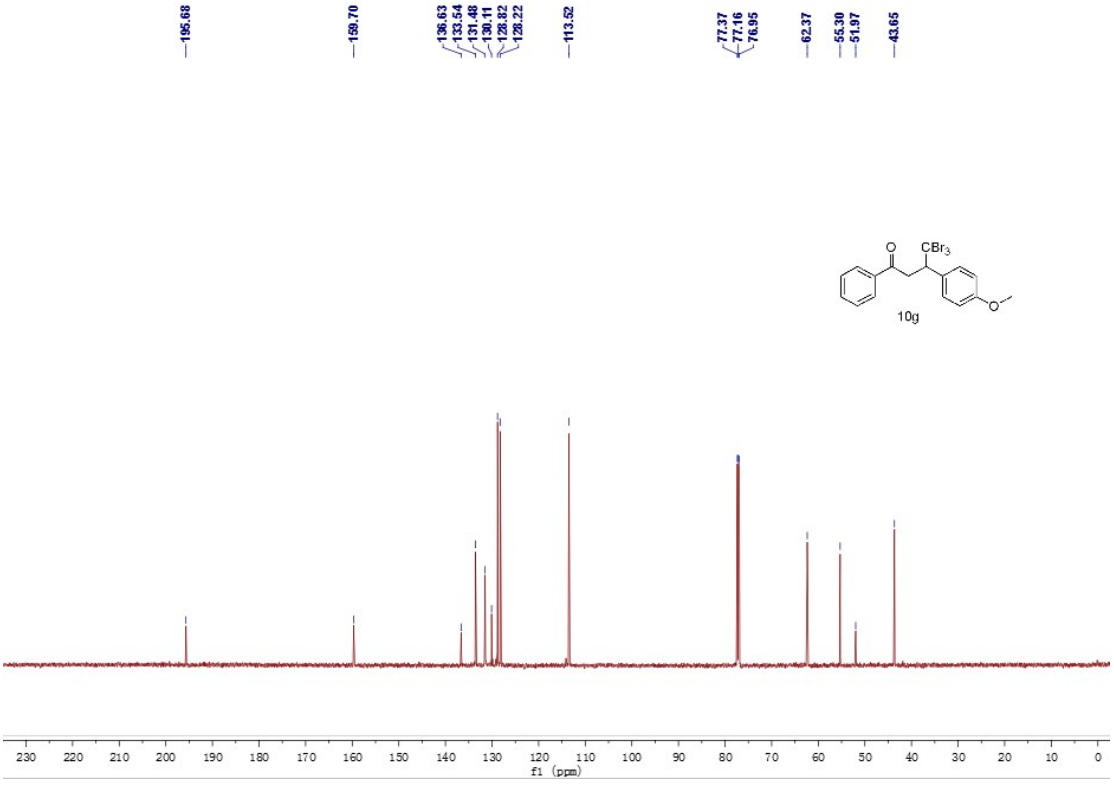
7.46
7.26
6.86
6.84
4.64
3.99
3.98
3.78
CBr3
O
O
10g
2.00
5.23
2.11
0.98
2.04
3.36
f1 (ppm)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128.22
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77.16
76.95
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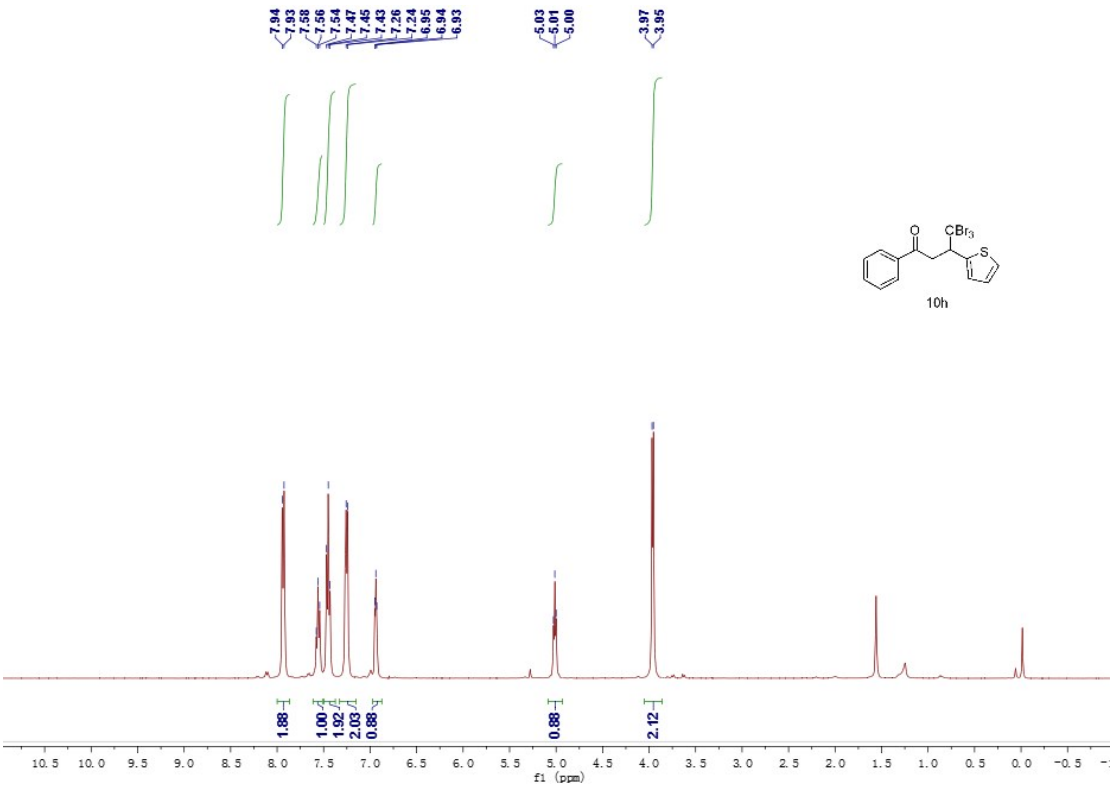
43.65
CBr3
O
O
10g
f1 (ppm)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7.93
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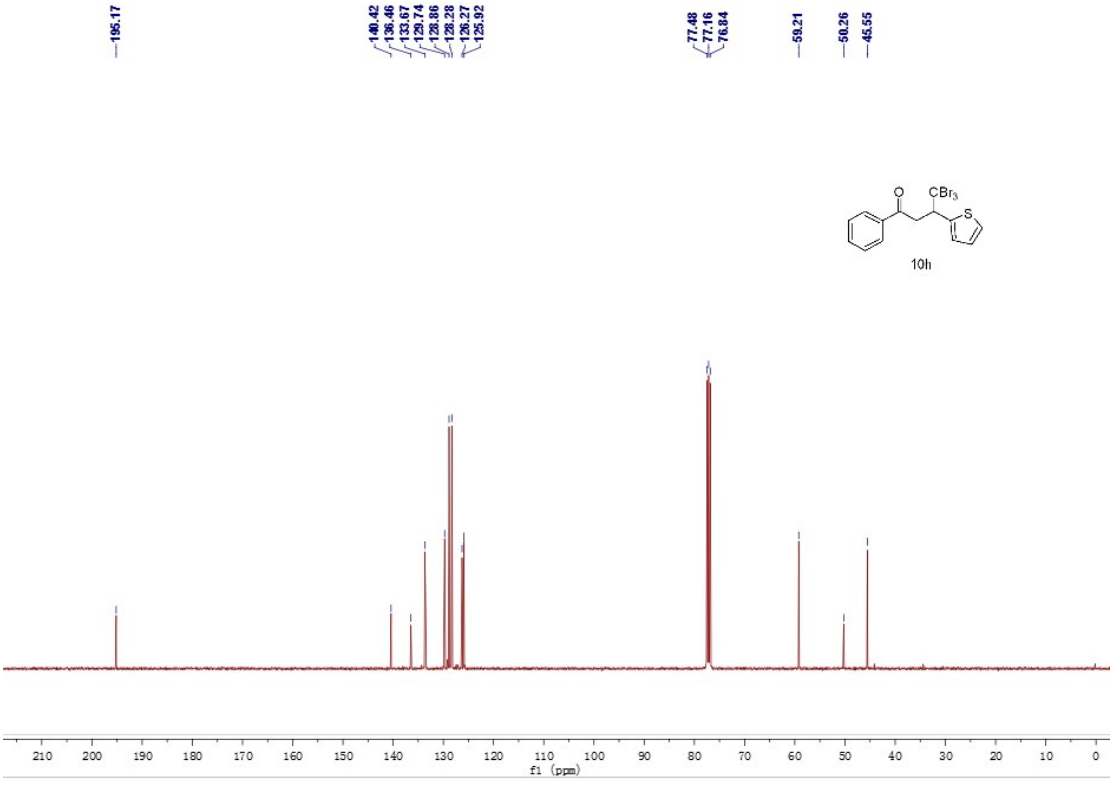
7.47
7.45
7.43
7.26
7.24
6.95
6.94
6.93
5.03
5.01
5.00
3.97
3.95
O
CBr3
S
10h
1.88
1.00
1.92
2.03
0.88
0.88
2.12
f1 (ppm)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128.86
128.28
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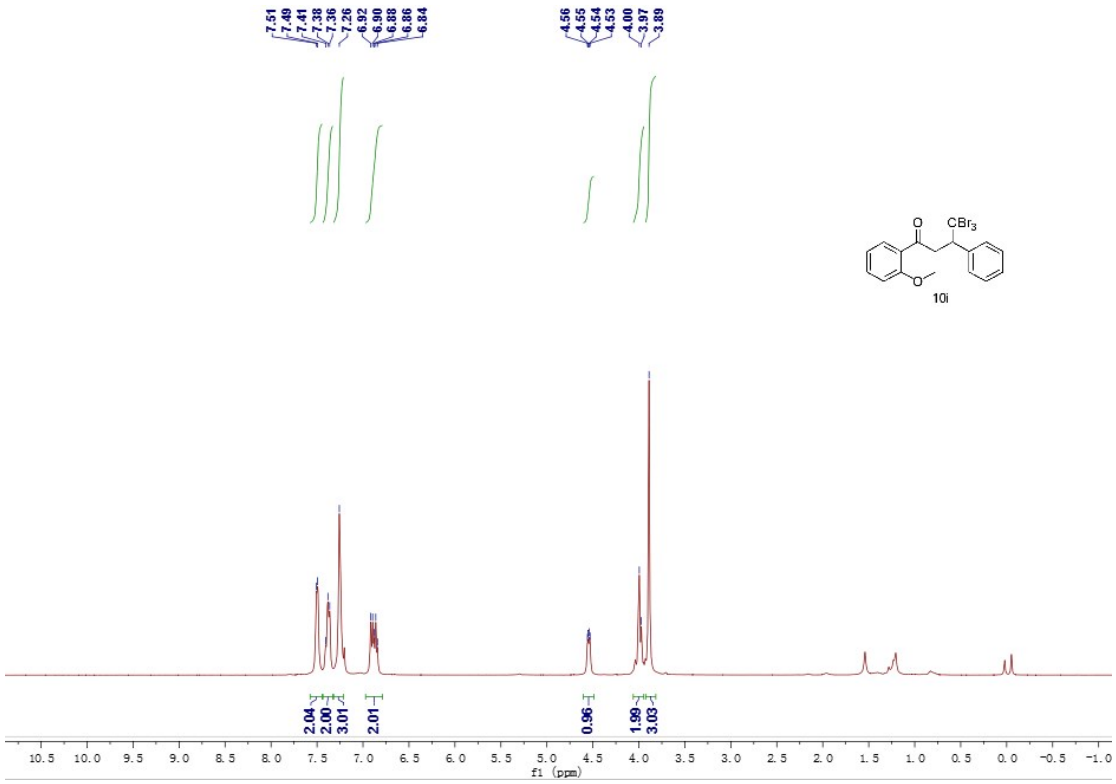
77.16
76.84
59.21
50.26
45.55
O
CBr3
S
10h
f1 (ppm)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7.36
7.26
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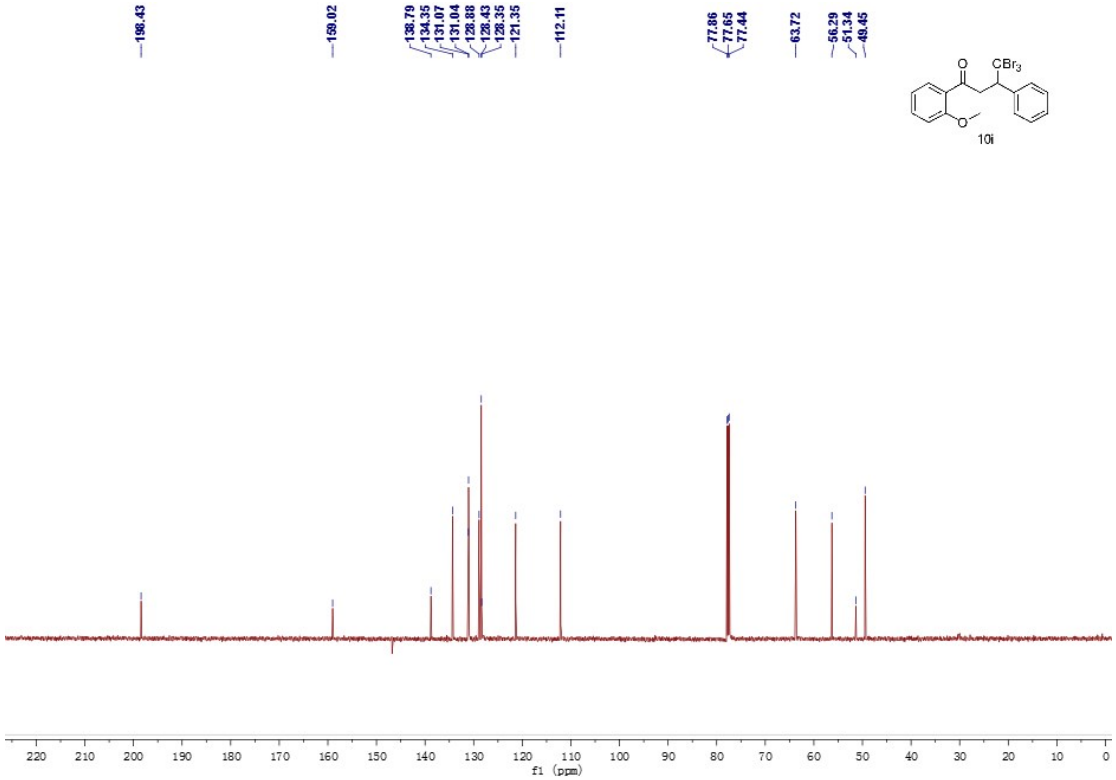
6.90
6.88
6.86
6.84
4.56
4.55
4.54
4.53
4.00
3.97
3.89
O
CBr3
O
10i
2.04
2.00
3.01
2.01
0.96
1.99
3.03
f1 (ppm)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131.04
128.88
128.43
128.35
121.35
112.11
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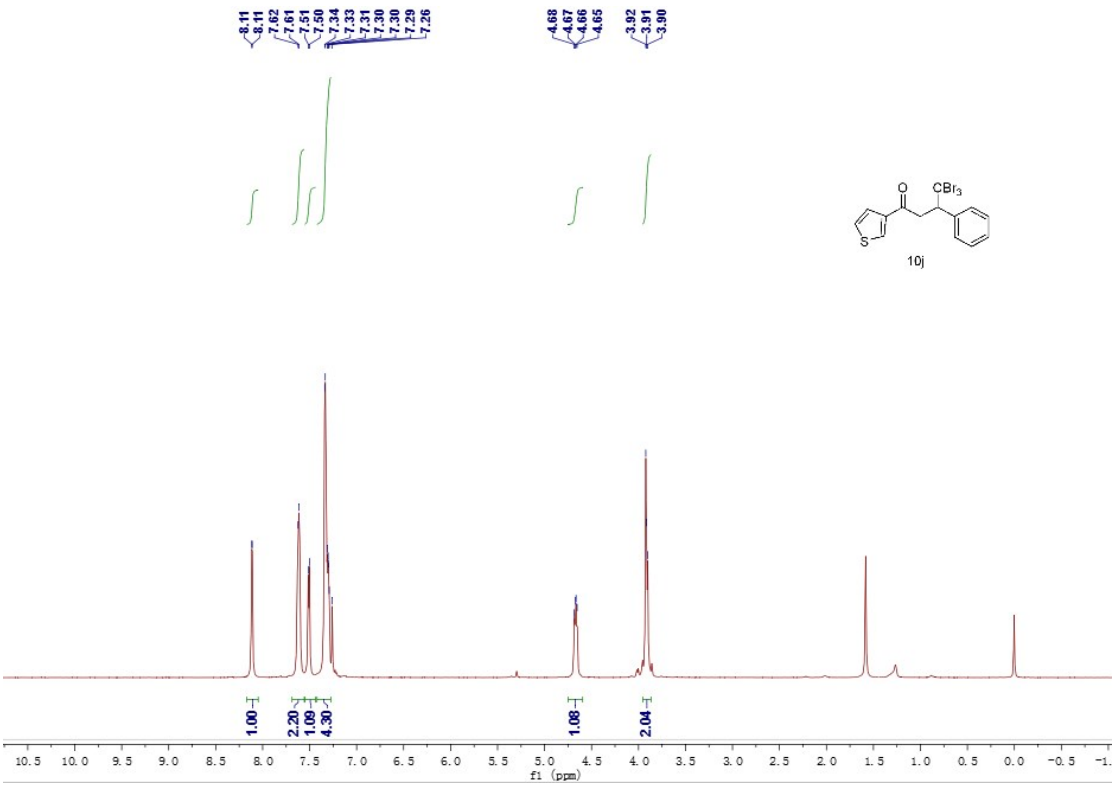
77.44
63.72
56.29
51.34
49.45
O
CBr3
O
10i
f1 (ppm)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7.50
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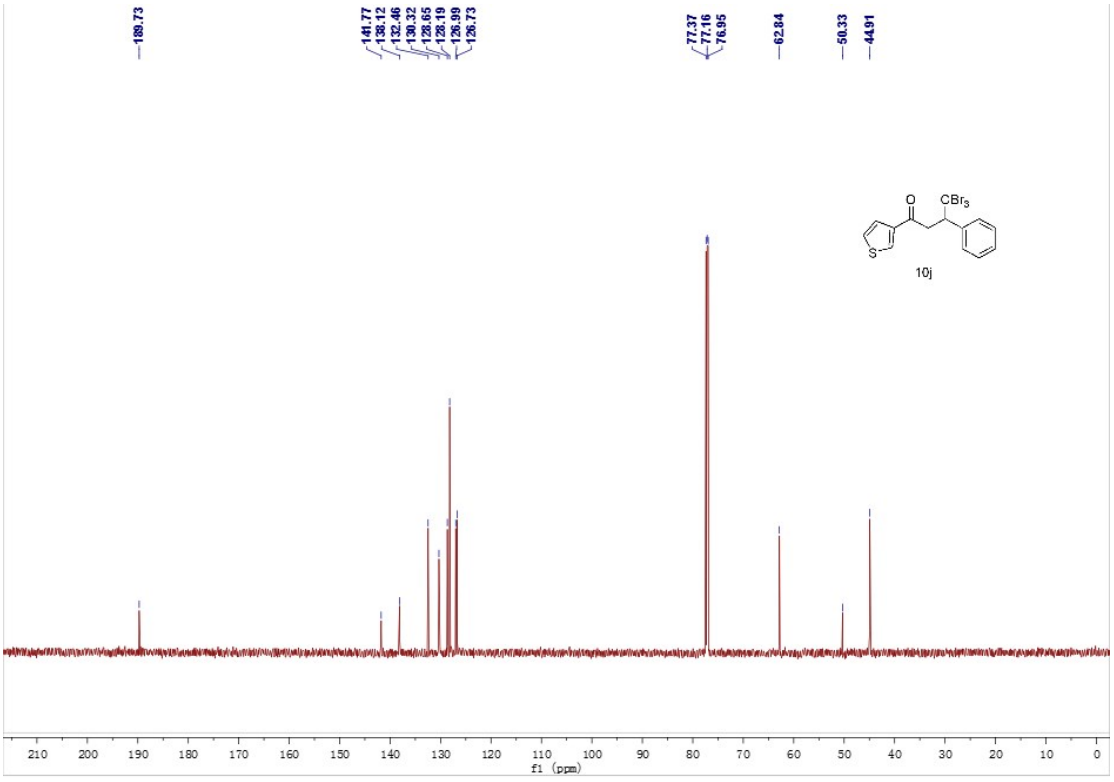
7.33
7.31
7.30
7.30
7.29
7.26
4.68
4.67
4.66
4.65
3.92
3.91
3.90
O
CBr3
S
10j
1.00
2.20
1.09
4.30
1.08
2.04
f1 (ppm)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77.16
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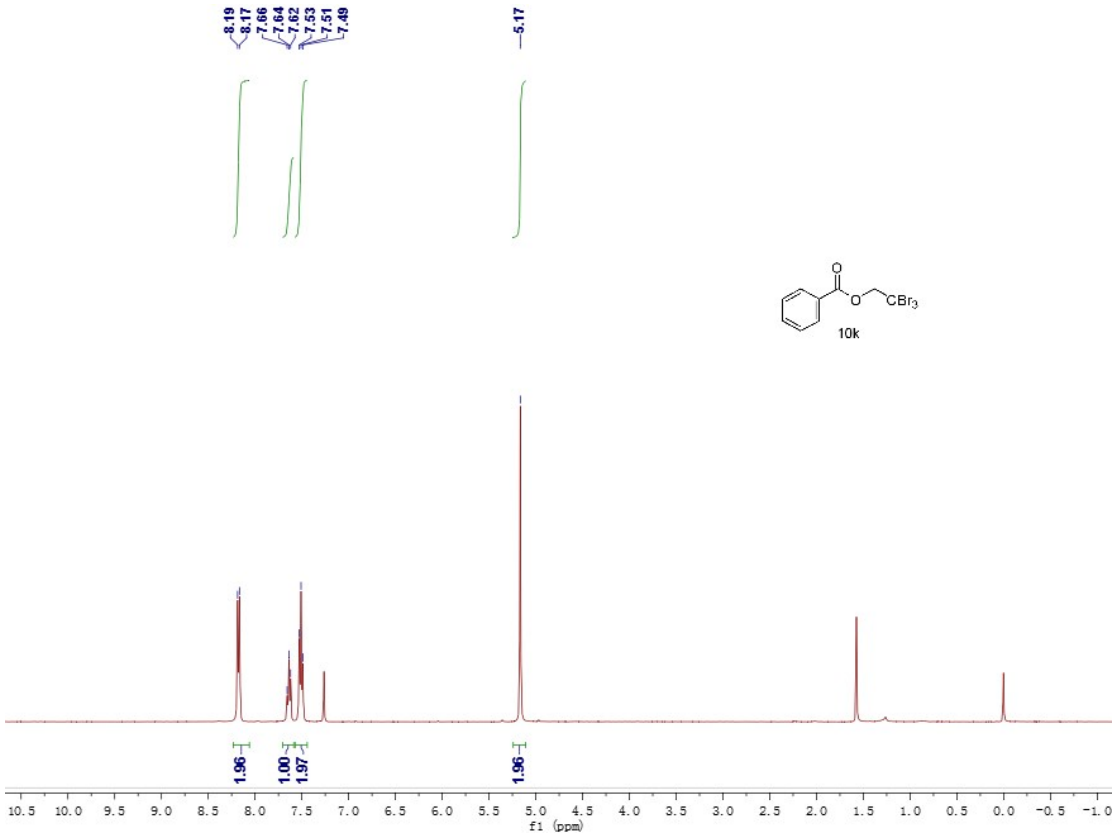
44.91
O
CBr3
S
10j
f1 (ppm)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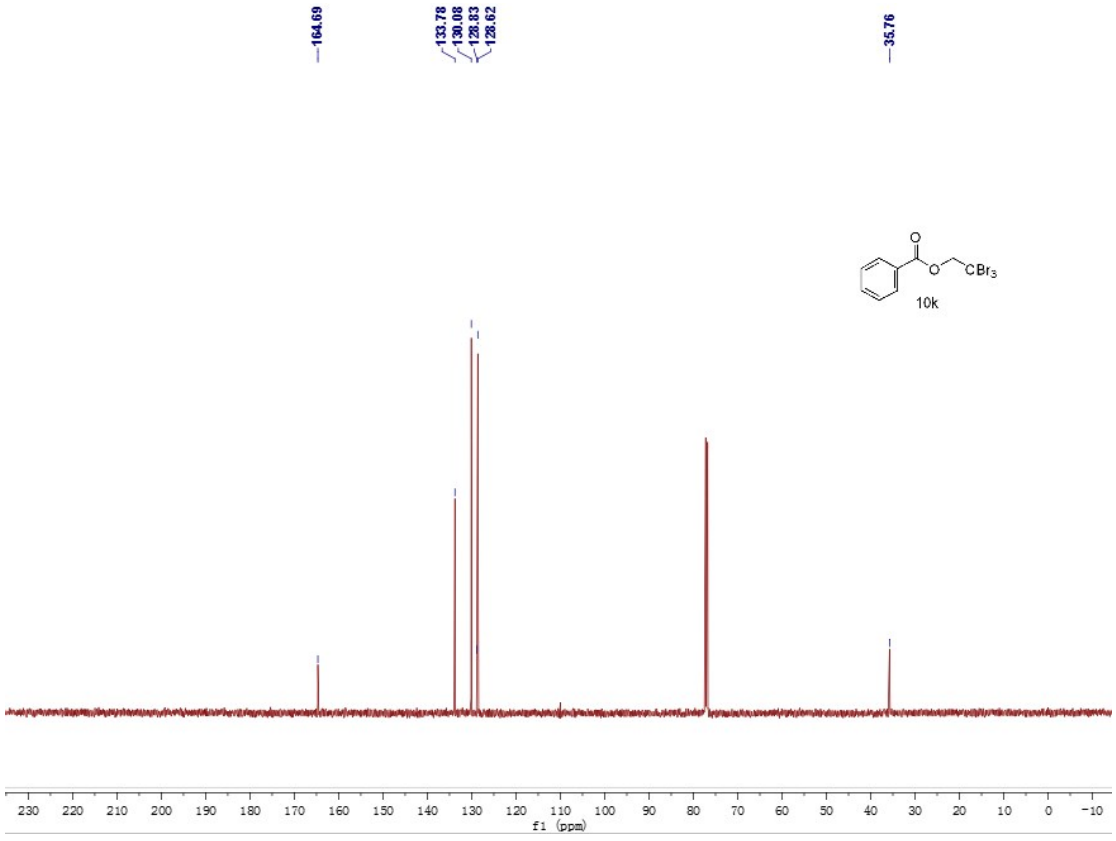
7.53
7.51
7.49
5.17
CBr3
10k
1.96
1.00
1.97
1.96
f1 (ppm)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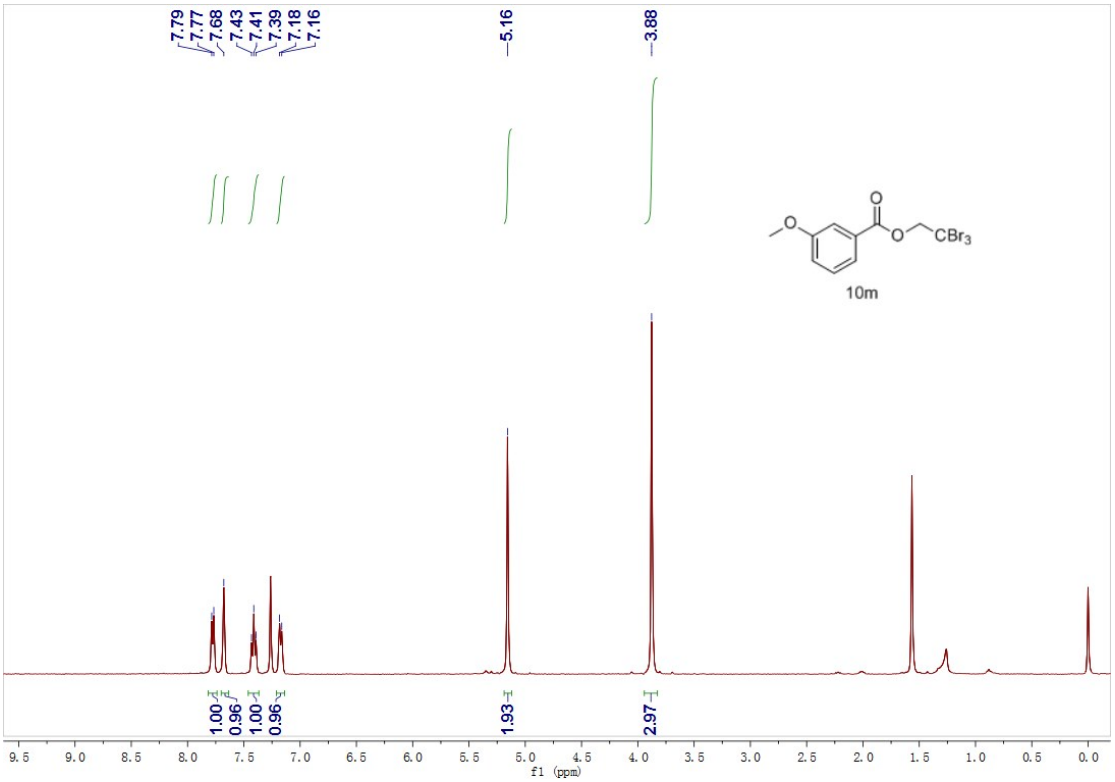
128.62
35.76
CBr3
10k
f1 (ppm)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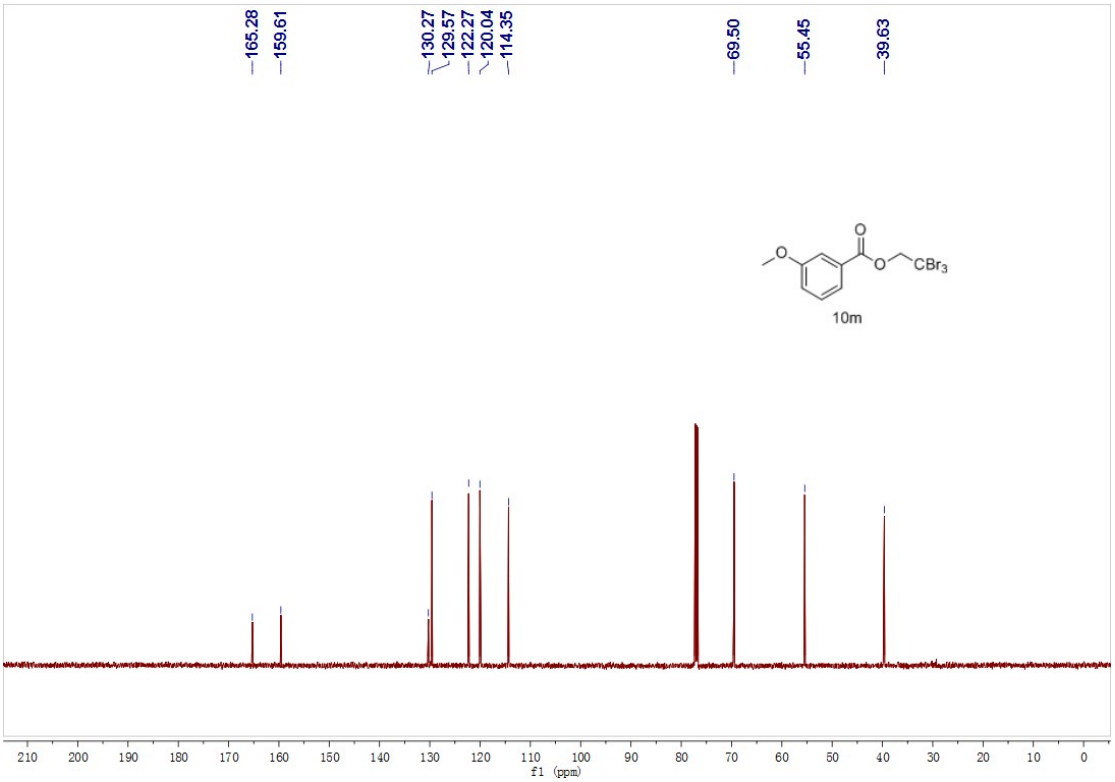
5.16
3.88
10m
1.00
0.96
1.00
0.96
1.93
2.97
f1 (ppm)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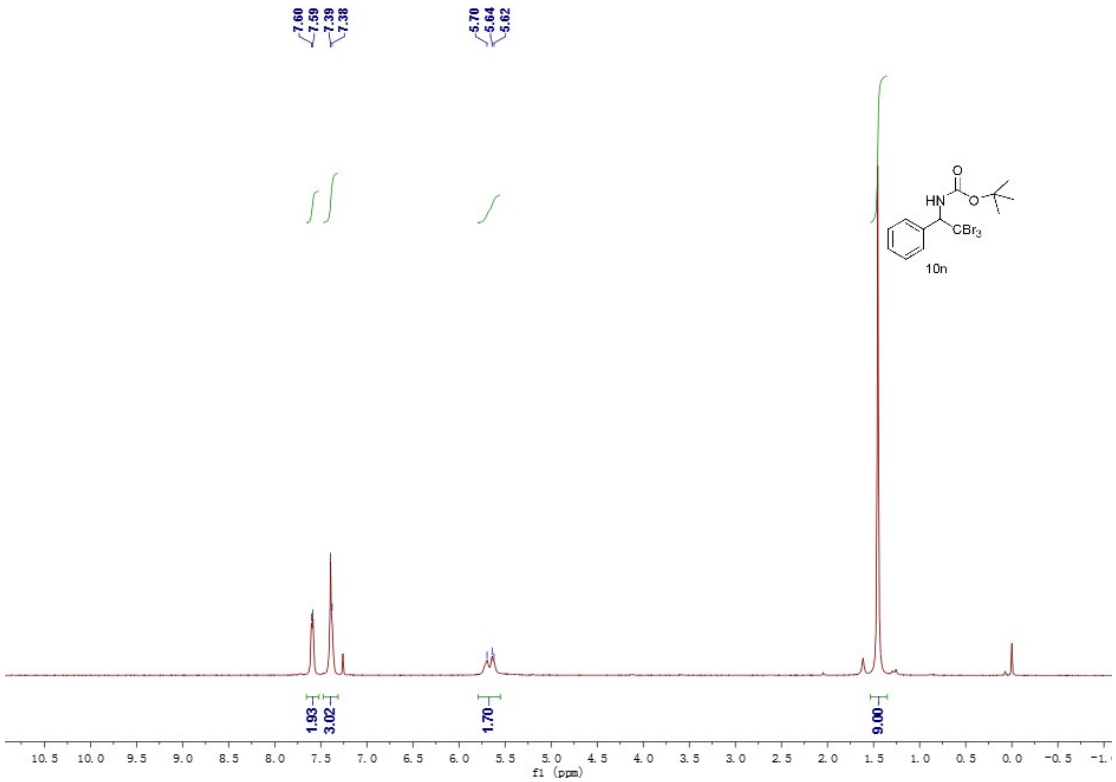
120.04
114.35
69.50
55.45
39.63
10m
f1 (ppm)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7.59
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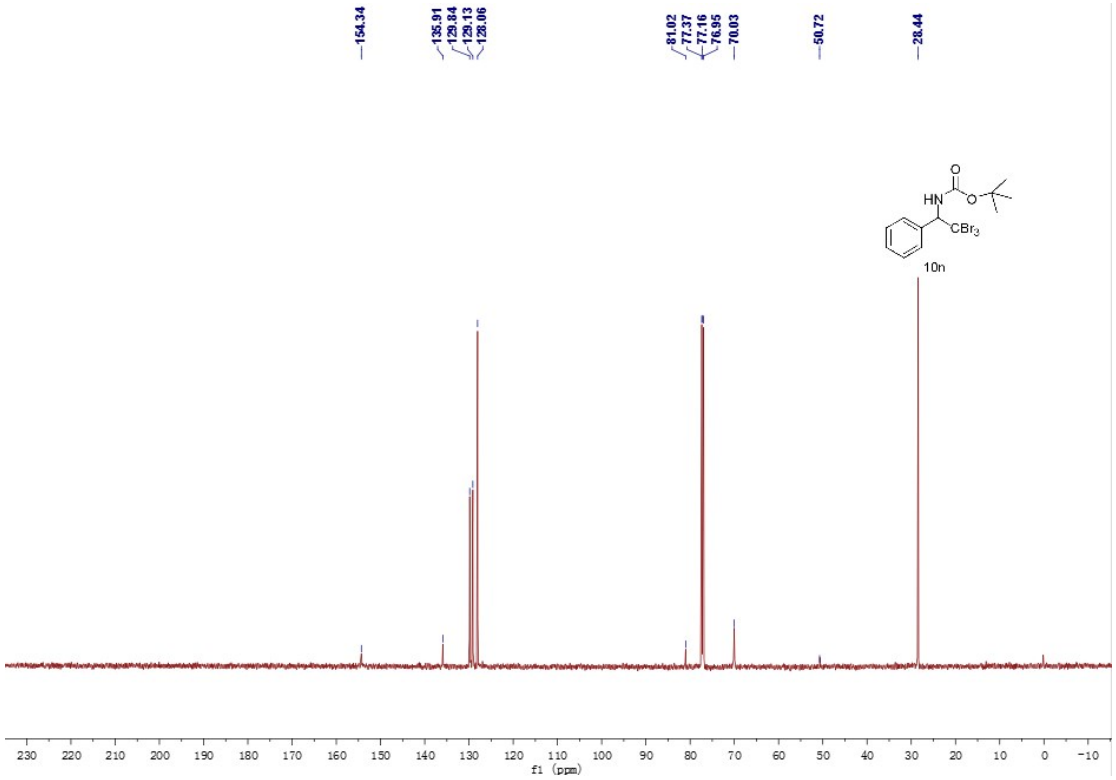
5.62
HN
O
CBr3
10n
1.93
3.02
1.70
9.00
f1 (ppm)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129.13
128.06
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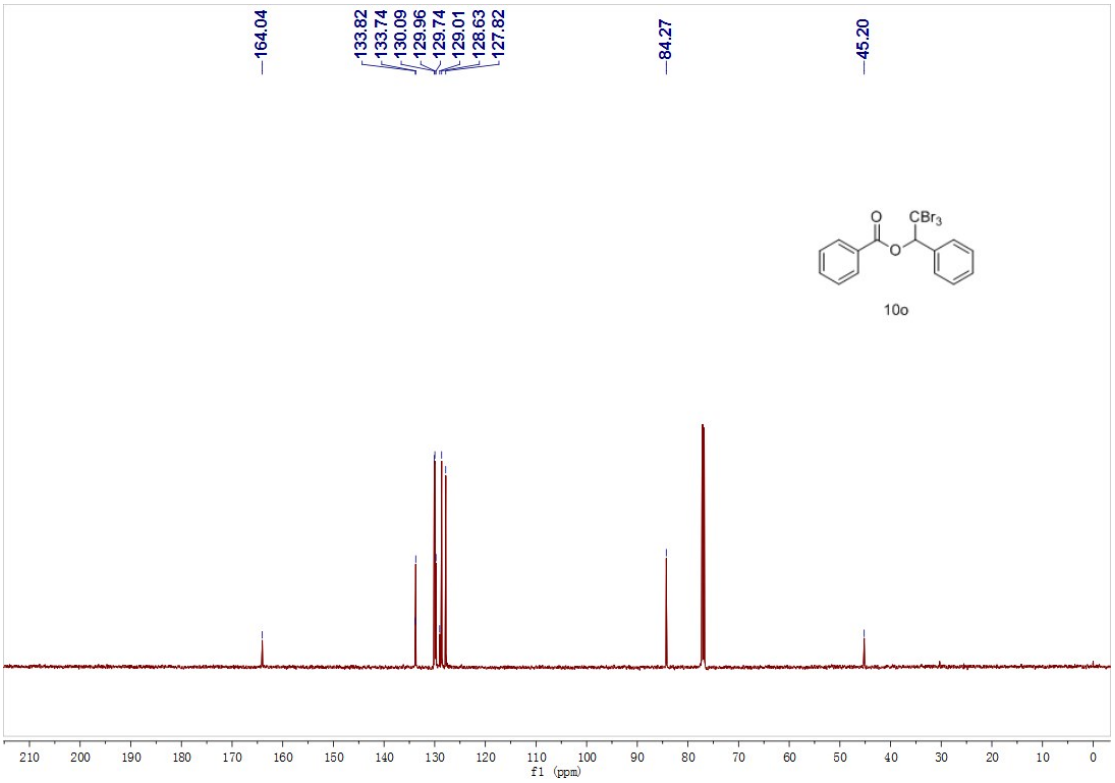
77.16
76.95
70.03
50.72
28.44
HN
O
CBr3
10n
f1 (ppm)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129.74
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127.82
84.27
45.20
O
CBr3
O
10o
210
200
190
180
170
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130
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100
90
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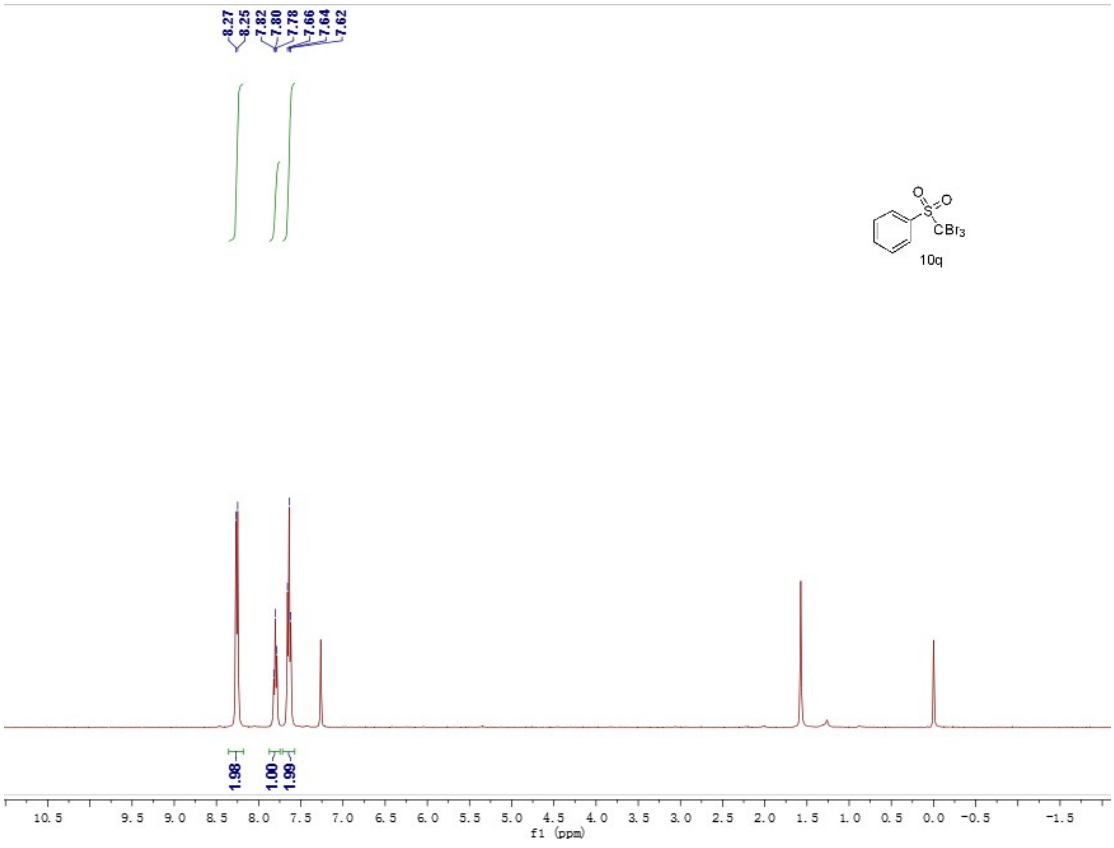
60
50
40
30
20
10
0
f1 (ppm)


8.27
8.25
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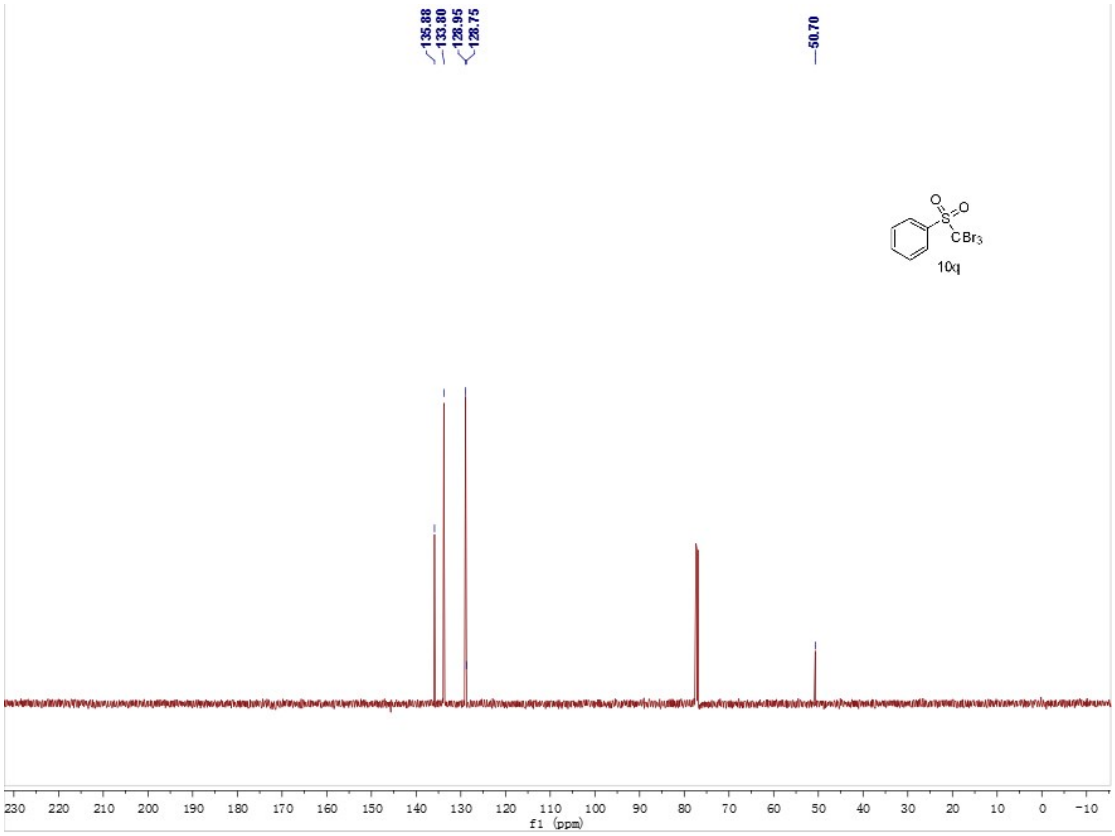
7.80
7.78
7.66
7.64
7.62
CBr3
10q
1.98
1.00
1.99
f1 (ppm)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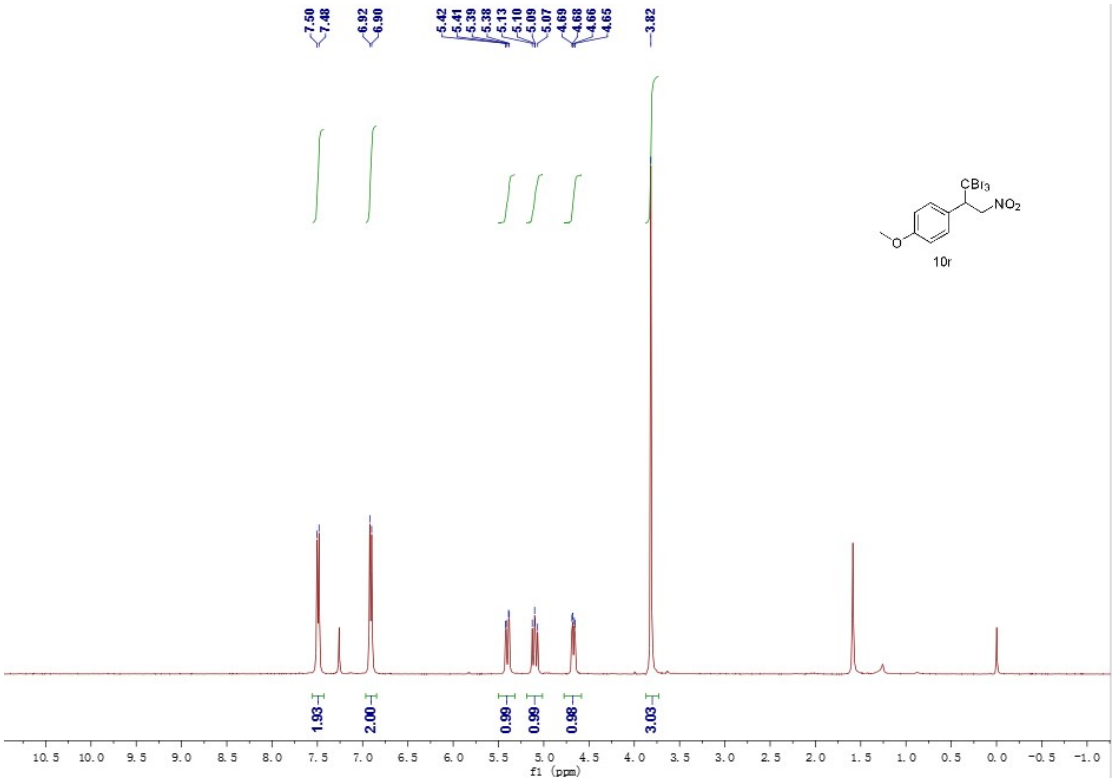
CBr3
10q
f1 (ppm)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5.38
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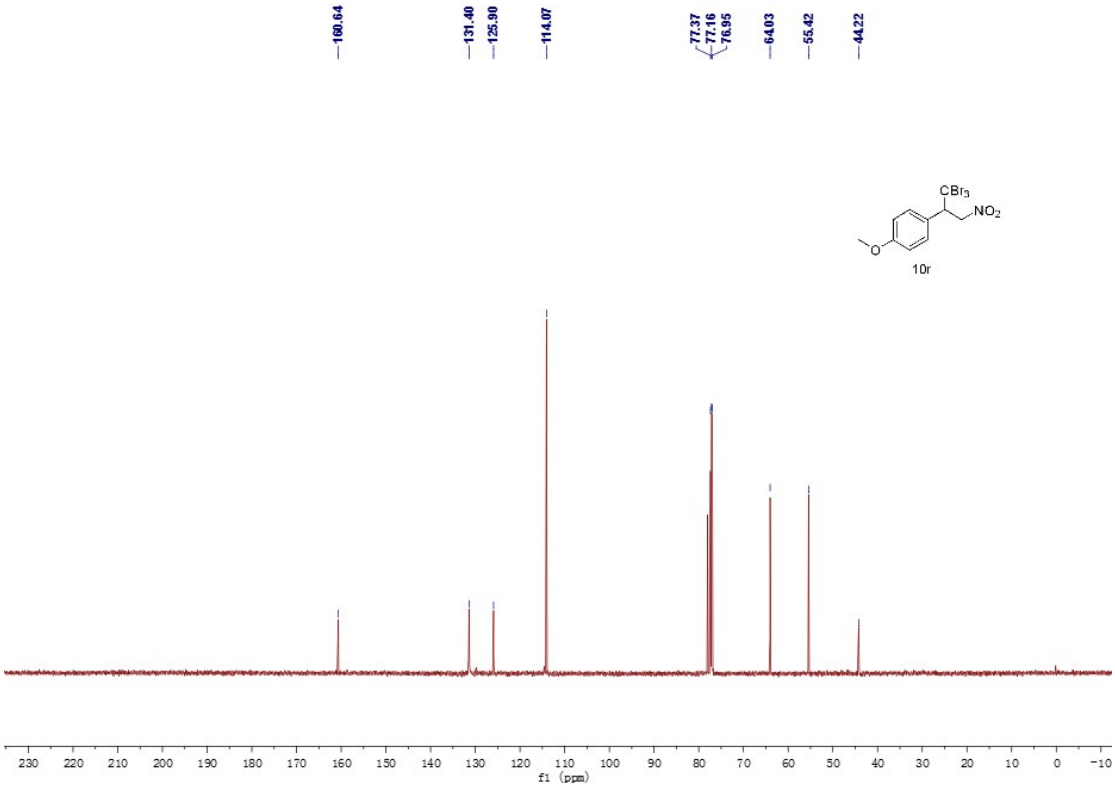
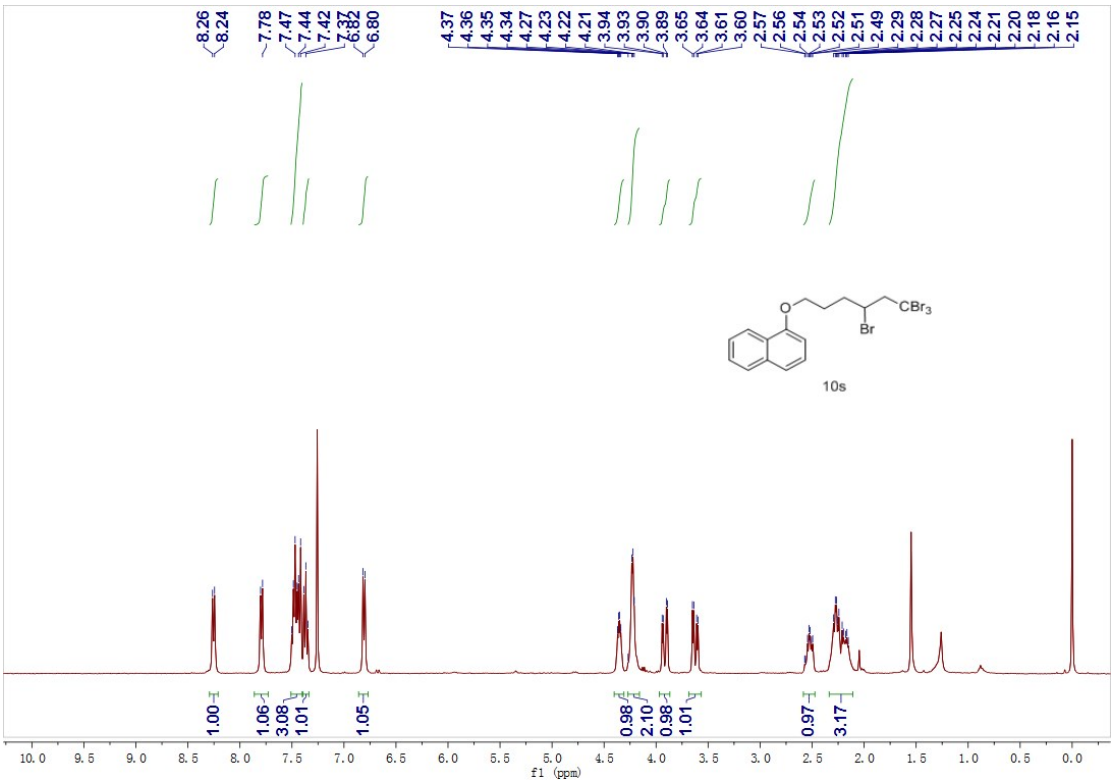
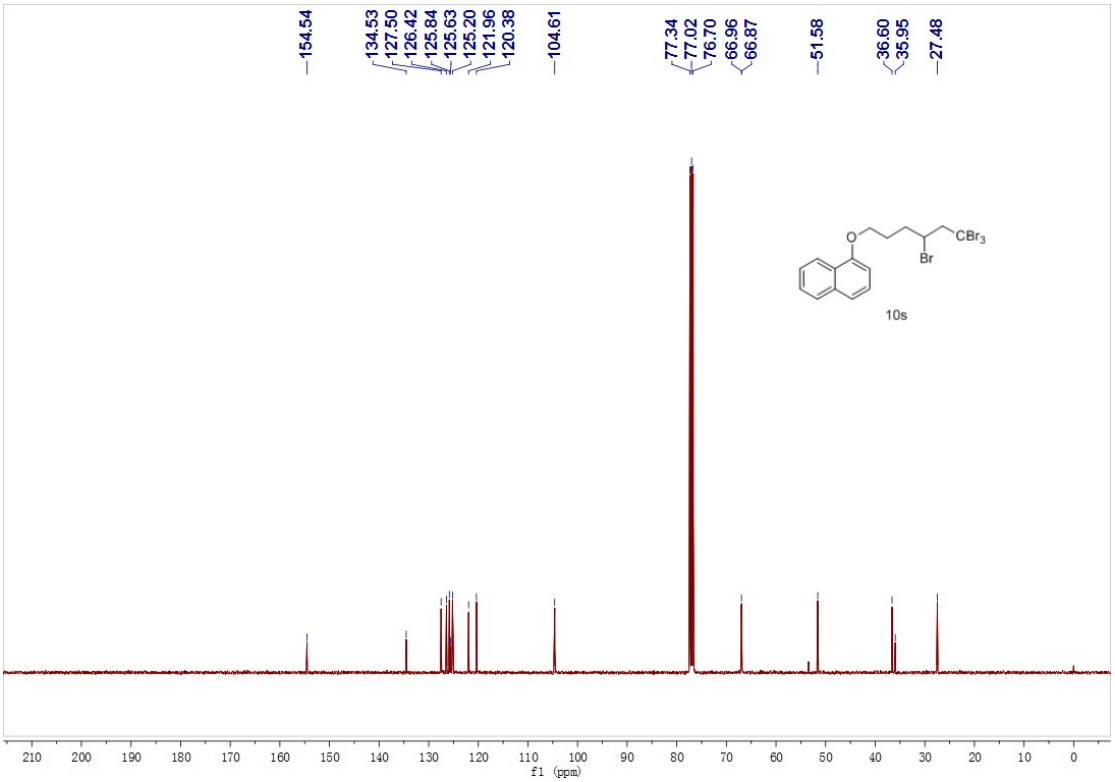
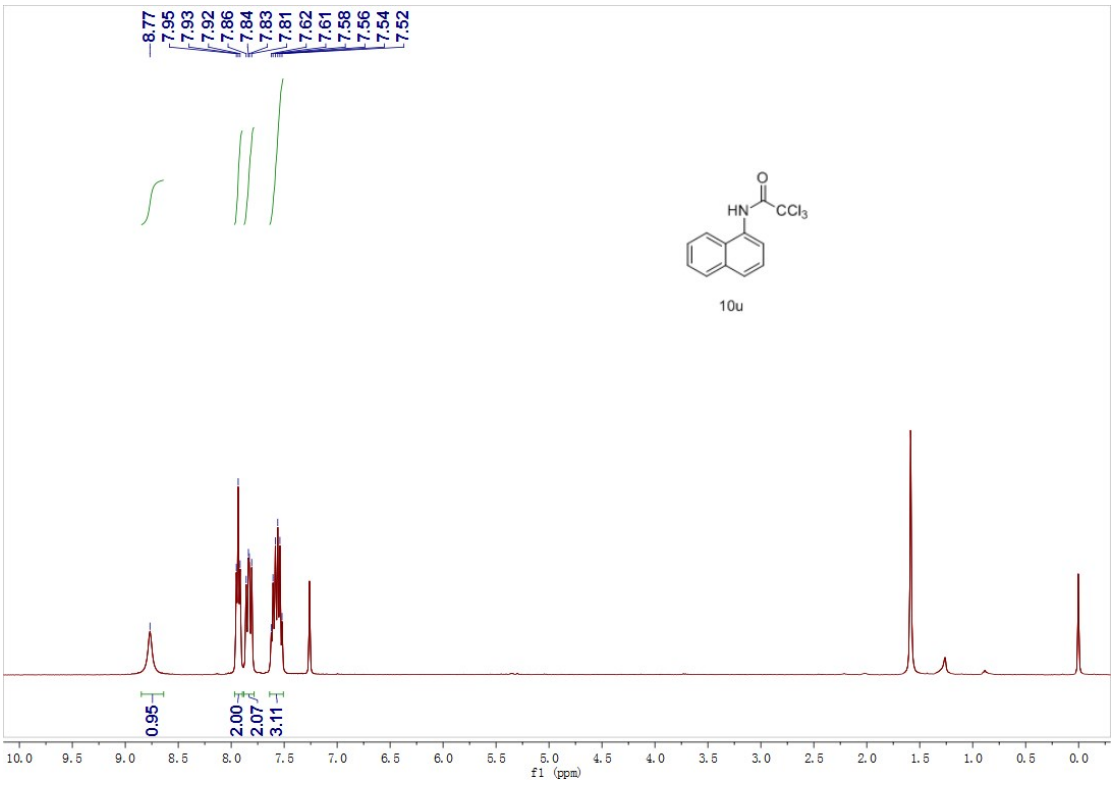
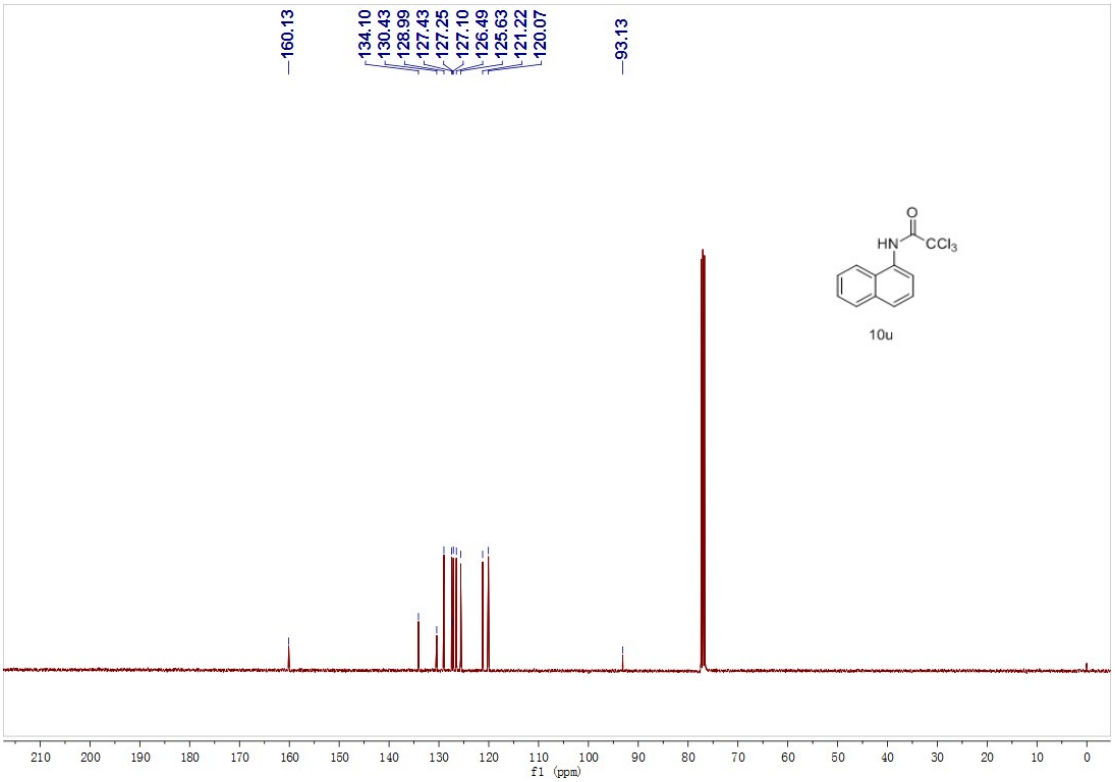
5.09
5.07
4.69
4.68
4.66
4.65
3.82
CBr3
NO2
O
10r
1.93
2.00
0.99
0.99
0.98
3.03
f1 (ppm)

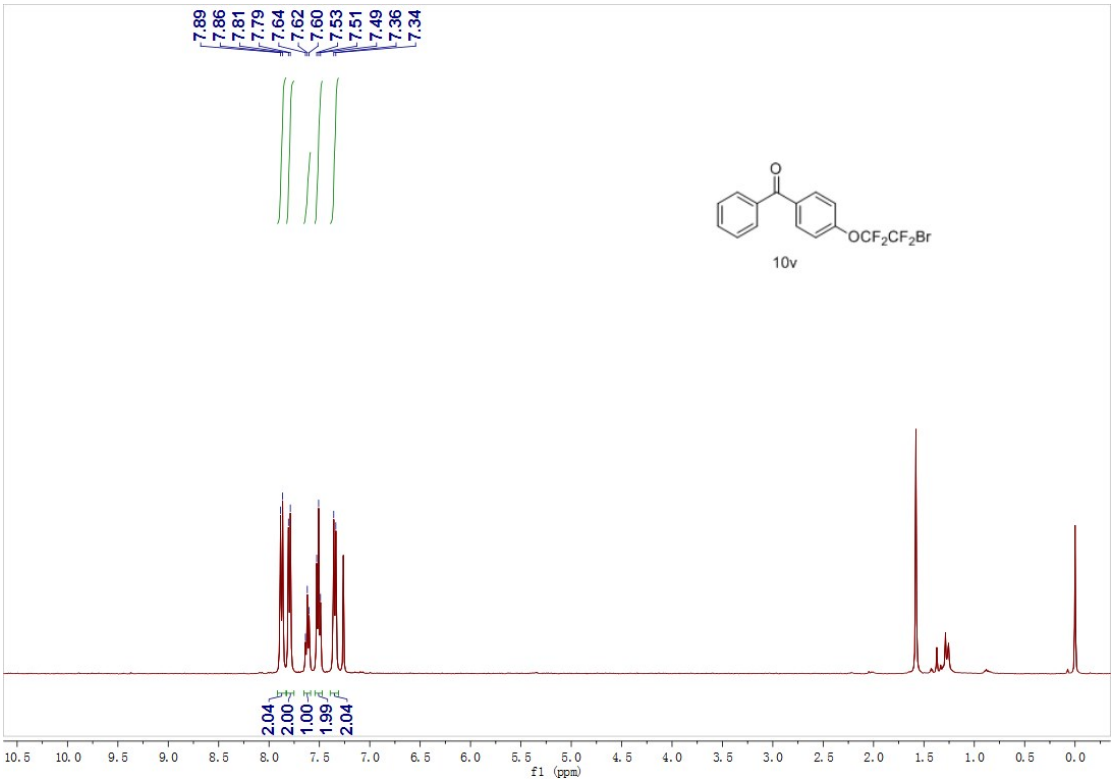

160.64
131.40
125.90
114.07
77.37
77.16
76.95
64.03
55.42
44.22
CBr3
NO2
O
10r
f1 (ppm)

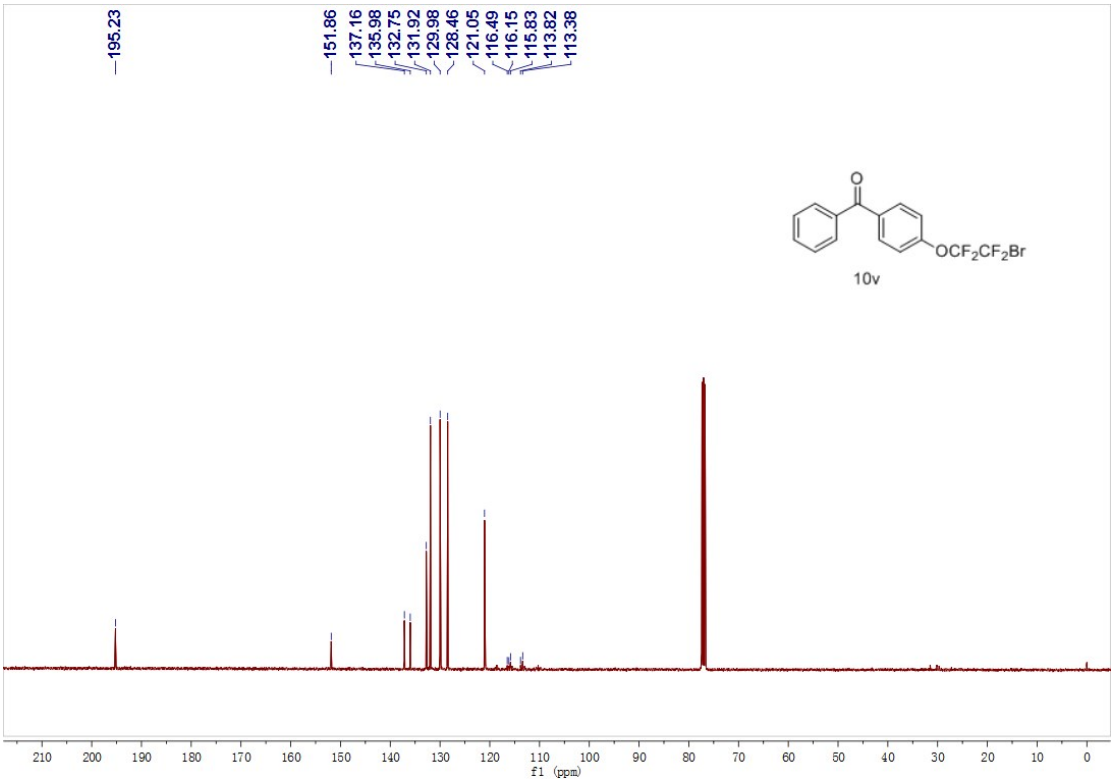

8.26
8.24
7.78
7.47
7.44
7.42
7.37
6.82
6.80
4.37
4.36
4.35
4.34
4.27
4.23
4.22
4.21
3.94
3.93
3.90
3.89
3.65
3.64
3.61
3.60
2.57
2.56
2.54
2.53
2.52
2.51
2.49
2.29
2.28
2.27
2.25
2.24
2.21
2.20
2.18
2.16
2.15
CBr3
Br
10s
1.00
1.06
3.08
1.01
1.05
0.98
2.10
0.98
1.01
0.97
3.17
f1 (ppm)


154.54
134.53
127.50
126.42
125.84
125.63
125.20
121.96
120.38
104.61
77.34
77.02
76.70
66.96
66.87
51.58
36.60
35.95
27.48
CBr3
Br
10s
f1 (ppm)


8.77
7.95
7.93
7.92
7.86
7.84
7.83
7.81
7.62
7.61
7.58
7.56
7.54
7.52
HN
O
CCl3
10u
0.95
2.00
2.07
3.11
f1 (ppm)


160.13
134.10
130.43
128.99
127.43
127.25
127.10
126.49
125.63
121.22
120.07
93.13
HN
O
CCl3
10u
f1 (ppm)


7.89
7.86
7.81
7.79
7.64
7.62
7.60
7.53
7.51
7.49
7.36
7.34
O
OCF2CF2Br
10v
2.04
2.00
1.00
1.99
2.04
f1 (ppm)


195.23
151.86
137.16
135.98
132.75
131.92
129.98
128.46
121.05
116.49
116.15
115.83
113.82
113.38
O
OCF2CF2Br
10v
f1 (ppm)