Supporting information

H_2O_2-Mediated Room Temperature Synthesis of 2-Arylacetophenones from Arylhydrazines and Vinyl Azides in Water

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General Information

Commercially available materials were used as received. Purifications of all the desired products were performed by chromatography (silica gel 200-300 mesh). NMR spectra were recorded on a 400 MHz spectrometer, data are reported as follows: chemical shift, integration, multiplicity (s=singlet, d=doublet, t=triplet, q=quartet, m=multiplet). Chemical shifts (δ) were reported in ppm and the coupling constants J are given in Hz. For ^{1}H NMR, DMSO-d_6 (δ = 2.50) or $CDCl_3$ (δ = 7.26) was used as internal standard. For ^{13}C NMR, DMSO-d_6 (δ = 39.5) or $CDCl_3$ (δ = 77.16) was used as internal standard. HRMS data was obtained using Agilent Technologies 6224 TOF LC/MS. Melting points were measured on a BÜCHI B-540 melting point apparatus and uncorrected. The starting material of vinyl azides **2** were prepared according to the reported methods.[1-3]

General procedures for synthesis of compounds 3aa-3ap and 3ba-3ra

A mixture of arylhydrazines **1**(1.2 mmol, 1.2 equiv), vinyl azides **2** (1.0 mmol), H_2O_2 (4.0 mmol) and PEG-800 (0.05 mmol) in water (10 mL) was stirred at room temperature for 4h. Upon completion of the reaction, the resulting mixture was diluted with saturated NaCl solution (5 mL) and extracted with EtOAc (3×10 mL). The combined organic phase was dried with anhydrous Na_2SO_4, concentrated and purified by chromatography (petroleum ether/ethylacetate = 30:1) on silica gel to afford the desired products 2-aryl acetophenones **3aa-3ap** and **3ba-3ra**.

Typical procedures for control experiments

(a)Typical procedure for radical trapping experiment

A mixture of p-tolylhydrazine **(1h)**(1.2 mmol, 1.2 equiv), α-phenylvinyl azide **(2a)** (1.0 mmol), H_2O_2 (4.0 mmol), PEG-800 (0.05 mmol) and TEMPO (2.0 mmol) in water (10 mL) was stirred at room temperature for 4h. Upon completion of the reaction, the resulting mixture was diluted with saturated NaCl solution (5 mL) and extracted with EtOAc (3×10 mL). The combined organic phase was dried with anhydrous Na_2SO_4, concentrated and purified by chromatography on silica gel, the desired product **(3ha)** was obtained in 15% yield (petroleum ether/ethylacetate = 30:1).

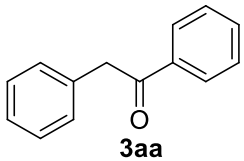
(b) Typical procedure for solely treated with p-tolylhydrazine under the standard condition

A mixture of p-tolylhydrazine **(1h)**(1.0 mmol), H_2O_2 (4.0 mmol), PEG-800 (0.05 mmol) in H_2O (10 mL) was stirred at room temperature for 4h. Upon completion of the reaction, the resulting mixture was detected by GC-MS.

(c) Typical procedure for studying the role of H_2O_2

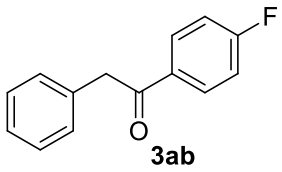
A mixture of p-tolylhydrazine **(2h)** (1.2 mmol, 1.2 equiv), α-phenylvinyl azide **(2a)** (1.0 mmol), and PEG-800 (0.05 mmol) in water (10 mL) was stirred at room temperature for 4h. Then the resulting mixture was detected by LC-MS, no desired product **(3ha)** was detected.

Characterization of Synthesized Compounds 3aa-3ap and 3ba-3ra



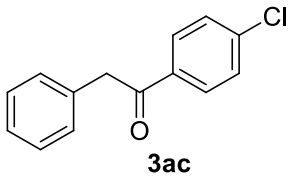
3aa

1,2-Diphenylethanone(3aa)[4]: Yellow oil, yield 85%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 8.02 (m, 2H), 7.57 (tt, *J* = 7.4, 1.2 Hz, 1H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.36 – 7.32 (m, 2H), 7.29 – 7.24 (m, 3H), 4.30 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.78, 136.66, 134.63, 133.31, 129.59, 128.80, 128.77, 128.74, 127.02, 45.62. HRMS (ESI): m/z calcd for $C_{14}H_{13}O$ $[M+H]^+$: 197.0961, found: 197.0965.



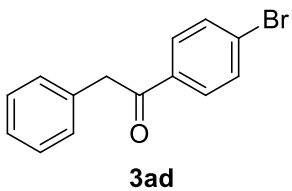
3ab

1-(4-Fuorophenyl)-2-phenylethanone(3ab)[4]: Yellow solid, m.p. 93.3 – 93.8 °C, yield 81%, ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.13 (q, *J* = 5.2 Hz, 2H), 7.36 (tt, *J* = 8.8, 2.4 Hz, 2H), 7.31 – 7.29 (m, 3H), 7.25 – 7.21 (m, 2H), 4.39 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 196.28, 165.03 (d, *J* =250 Hz), 134.99, 133.06 (d, *J* = 3 Hz), 131.38 (d, *J* = 10 Hz), 129.69, 128.30, 126.51, 115.75 (d, *J* = 19 Hz), 44.64. HRMS (ESI): m/z calcd for $C_{14}H_{12}FO$ $[M+H]^+$: 215.0867, found: 215.0861.



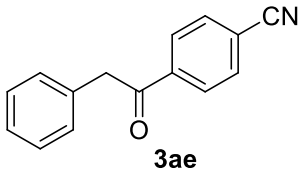
3ac

1-(4-Chlorophenyl)-2-phenylethanone(3ac)[4]: White solid, m.p. 97.8 – 98.3 °C, yield 82%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.4 Hz, 2H), 7.46 (d, *J* = 8.4 Hz, 2H), 7.36 (t, *J* = 7.2 Hz, 2H), 7.31 – 7.27 (m, 3H), 4.29 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.55, 139.78, 135.05, 134.34, 130.19, 129.51, 129.11, 128.91, 127.18, 45.70. HRMS (ESI): m/z calcd for $C_{14}H_{12}ClO$ $[M+H]^+$: 231.0571, found: 231.0570.



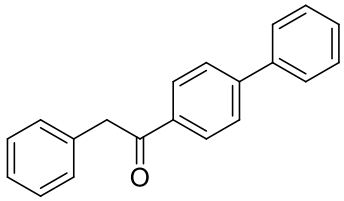
3ad

1-(4-Bromophenyl)-2-phenylethanone (3ad)[4]: White solid, m.p. 101.1 – 101.6 °C, yield 85%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.8 Hz, 2H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.33 (t, *J* = 7.2 Hz, 2H), 7.28 – 7.24 (m, 3H), 4.25 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.78, 135.39, 134.28, 132.12, 130.30, 129.51, 128.92, 128.53, 127.20, 45.68. HRMS (ESI): m/z calcd for $C_{14}H_{12}BrO$ $[M+H]^+$: 275.0066, found: 275.0068.



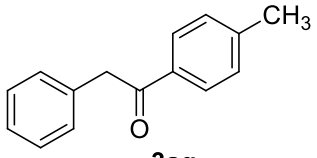
3ae

4-(2-Phenylacetyl)benzonitrile (3ae) [4]: White solid, m.p. 98.0 – 99.7 °C, yield 81%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.4 Hz, 2H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.37 – 7.33 (m, 2H), 7.31 – 7.24 (m, 3H), 4.29 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.18, 139.51, 133.45, 132.38, 129.39, 129.03, 128.92, 127.34, 117.79, 116.53, 45.77. HRMS (ESI): m/z calcd for $C_{15}H_{11}NO$ $[M+H]^+$: 221.0841, found: 221.0848..



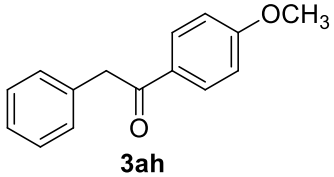
3af

1-([1,1'-Biphenyl]-4-yl)-2-phenylethanone (3af) [6]: Light yellow solid, m.p. 89.6 – 90.1 °C, yield 89%,^{1}H NMR (400 MHz, DMSO-d_6) δ 8.13 (d, *J* = 8.8 Hz, 2H), 7.83 (d, *J* = 8.8 Hz, 2H), 7.74 (d, *J* = 7.2 Hz, 2H), 7.52 – 7.48 (m, 2H), 7.42 (t, *J* = 7.2 Hz, 1H), 7.34 – 7.28 (m, 4H), 7.26 – 7.21 (m, 1H), 4.42 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 197.22, 144.60, 138.83, 135.14, 129.66, 129.15, 129.08, 128.40, 128.33, 126.98, 126.91, 126.49, 44.73. HRMS (ESI): m/z calcd for $C_{20}H_{17}O$ $[M+H]^+$: 273.1274, found: 273.1271.



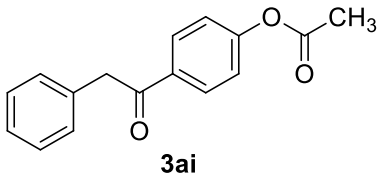
3ag

2-Phenyl-1-(p-tolyl)ethanone (3ag) [4]: Yellow solid, m.p. 95.6 – 96.1 °C, yield 89%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.0 Hz, 2H), 7.36 (t, *J* = 7.4 Hz, 2H), 7.31 – 7.28 (m, 5H), 4.30 (s, 2H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.44, 144.12, 134.90, 134.23, 129.57, 129.46, 128.90, 128.77, 126.94, 45.55, 21.78. HRMS (ESI): m/z calcd for $C_{15}H_{15}O$ $[M+H]^+$: 211.1117, found: 211.1120.



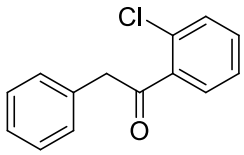
3ah

1-(4-Methoxyphenyl)-2-phenylethanone (3ah) [4]: White solid, m.p. 101.2 – 102.1 °C, yield 88%, ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.03 (d, *J* = 8.8 Hz, 2H), 7.32 – 7.25 (m, 4H), 7.22 (tt, *J* = 7.0, 2.0 Hz, 1 H), 7.04 (d, *J* = 8.8 Hz, 2H), 4.31 (s, 2H), 3.84 (s, 3H); ^{13}C NMR(100 MHz, $CDCl_3$) δ 196.37, 163.65, 135.11, 131.09, 129.77, 129.52, 128.78, 126.91, 113.92, 55.61, 45.41. HRMS (ESI): m/z calcd for $C_{15}H_{15}O_2$ $[M+H]^+$: 227.1067, found: 227.1070.



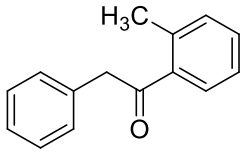
3ai

4-(2-Phenylacetyl)phenyl acetate (3ai): Yellow solid, m.p. 81.2 – 81.6 °C, yield 86%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* =8.4 Hz, 2H), 7.33 (t, *J* = 7.2 Hz, 2H), 7.27 – 7.24 (m, 3H),7.19 (d, *J* =8.8 Hz, 2H), 4.27 (s, 2H), 2.32 (s, 3H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 196.45, 168.96, 154.47, 134.44, 134.25, 130.39, 129.53, 128.85, 127.09, 121.96, 45.63, 21.28. HRMS (ESI): m/z calcd for $C_{16}H_{15}O_3$ $[M+H]^+$: 255.1016, found: 255.1017.



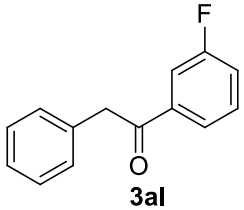
3aj

1-(2-Chlorophenyl)-2-phenylethanone (3aj) [4]: Yellow oil, yield 75%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.44 (td, *J* = 7.2, 2.0 Hz, 1H), 7.33 – 7.29 (m, 2H), 7.26 – 7.22 (m, 3H), 4.29 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.20, 138.64, 133.98, 132.12, 130.33, 129.82, 129.59, 129.05, 128.34, 127.30, 126.76, 48.63. HRMS (ESI): m/z calcd for $C_{14}H_{12}ClO$ $[M+H]^+$: 231.0571, found: 231.0568.



3ak

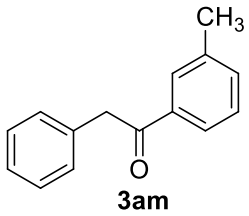
2-Phenyl-1-(o-tolyl)ethanone (3ak) [4]: Yellow oil, yield 78%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (dd, J = 7.6, 0.8 Hz, 1H), 7.41 (td, J = 7.6, 1.2 Hz, 1H), 7.34 – 7.26 (m, 4H), 7.24 – 7.20 (m, 3H), 4.29 (s, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 201.61, 137.67, 137.09, 134.96, 131.54, 131.21, 129.69, 128.72, 128.28, 126.47, 125.81, 47.74, 20.58. HRMS (ESI): m/z calcd for $C_{15}H_{15}O$ $[M+H]^+$: 211.1117, found: 211.1120.



3al

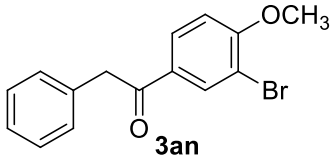
1-(3-Fluorophenyl)-2-phenylethanone (3al)[14]: Yellow solid, m.p. 81.3 – 81.8 °C, yield 83%, ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.07 – 8.05 (m, 2H), 7.65 (tt, *J* = 7.4, 2.0 Hz, 1H), 7.55 (t, *J* =7.6

Hz, 2H), 7.38 – 7.32 (m, 1H), 7.14 – 7.04 (m, 3H), 4.46 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 197.14, 162.06 (d, *J* = 242 Hz), 137.94 (d, *J* = 8 Hz), 136.26, 133.36, 130.00 (d, *J* = 8 Hz), 128.76, 128.31, 126.00 (d, *J* = 3 Hz), 116.65 (d, *J* = 22 Hz), 113.28 (d, *J* = 21 Hz), 44.21. HRMS (ESI): m/z calcd for $C_{14}H_{12}FO$ $[M+H]^+$: 215.0867, found: 215.0865.



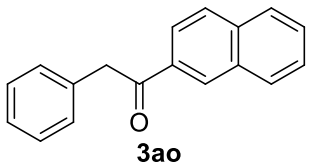
3am

2-Phenyl-1-(*m*-tolyl)ethanone (3am)[5]: White solid, m.p. 98.1 – 98.6 °C, yield 86%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.8 Hz, 2H), 7.38 – 7.31 (m, 4H), 7.28 – 7.23 (m, 3H), 4.28 (s, 2H), 2.41(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.01, 138.60, 136.81, 134.79, 134.08, 129.61, 129.23, 128.79, 128.63, 126.99, 126.02, 45.65, 21.52. HRMS (ESI): m/z calcd for $C_{15}H_{15}O$ $[M+H]^+$: 211.1117, found: 211.1119.



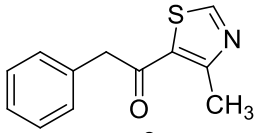
3an

1-(3-Bromo-4-methoxyphenyl)-2-phenylethanone (3an)[15]: White solid, m.p. 115.2 – 115.5 °C, yield 88%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 2.0 Hz, 1H), 7.96 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.33 (t, *J* = 7.2 Hz, 2H), 7.27 – 7.24 (m, 3H), 6.91 (d, *J* = 8.4 Hz, 1H), 4.22 (s, 2H), 3.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.27, 159.72, 134.55, 134.21, 130.67, 130.01, 129.49, 128.85, 127.07, 112.11, 111.24, 56.60, 45.36. HRMS (ESI): m/z calcd for $C_{15}H_{14}BrO_2$ $[M+H]^+$: 305.0172, found: 305.0175.



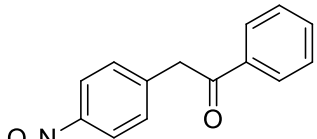
3ao

1-(Naphthalen-2-yl)-2-phenylethanone (3ao)[6]: Light yellow solid, m.p. 78.3 – 78.7 °C, yield 89%, ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.30 (s, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 8.03 – 8.02 (m, 2H), 8.00 (d, *J* = 7.6 Hz, 1H), 7.70 – 7.61 (m, 2H), 7.33 – 7.35 (m, 2H), 7.32 (d, *J* = 2.0 H, 2H), 7.25 – 7.21 (m, 1H), 4.53 (s, 2H); ^{13}C NMR (100 MHz, DMSO) δ 197.69, 135.28, 135.07, 133.64, 132.23, 130.50, 129.82, 129.66, 128.76, 128.36, 127.69, 127.01, 126.52, 123.90, 44.69. HRMS (ESI): m/z calcd for $C_{18}H_{15}O$ $[M+H]^+$: 247.1117, found: 247.1112.



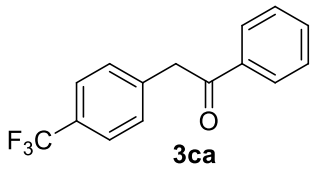
3ap

1-(4-Methylthiazol-5-yl)-2-phenylethanone (3ap): Yellow solid, m.p. 65.2 – 65.7 °C, yield 85%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (s, 1H), 7.33 (t, *J* = 7.4 Hz, 2H), 7.27 – 7.23 (m, 3H), 4.26 (s, 2H), 2.68 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 190.97, 158.44, 156.94, 134.26, 130.41, 129.79, 128.30, 126.76, 48.84, 18.03. HRMS (ESI): m/z calcd for $C_{12}H_{12}NOS$ $[M+H]^+$: 218.0634, found: 218.0630.



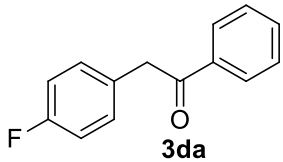
3ba

2-(4-Nitrophenyl)-1-phenylethanone (3ba)[7]: Light yellow solid, m.p. 137.8 – 138.4 °C, yield 88%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* =8.8 Hz, 2H), 8.03 – 8.00 (m, 2H), 7.61 (tt, J = 7.4, 1.6 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.43 (d, *J* =8.8 Hz, 2H), 4.42 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.12, 147.16, 142.17, 136.26, 133.86, 130.77, 129.00, 128.55, 123.85, 45.05. HRMS (ESI): m/z calcd for $C_{14}H_{12}NO_3$ $[M+H]^+$: 242.0812, found: 242.0808.



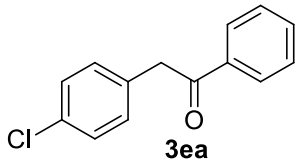
3ca

1-Phenyl-2-(4-(trifluoromethyl)phenyl)ethanone (3ca)[8]: White solid, m.p. 97.1 – 97.8 °C, yield 86%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 8.01 (m, 2H), 7.61 – 7.58 (m, 3H), 7.49 (t, *J* =7.6 Hz, 2H), 7.39 (d, *J* =8.0 Hz, 2H), 4.36 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 197.06, 140.17, 136.25, 133.44, 130.77, 128.79, 128.31, 127.22 (d, *J* = 32 Hz), 124.40 (d, *J* = 270 Hz), 124.97 (q, *J* = 4.0 Hz), 44.34. HRMS (ESI): m/z calcd for $C_{15}H_{12}$ F_3O $[M+H]^+$: 265.0835, found: 265.0838.



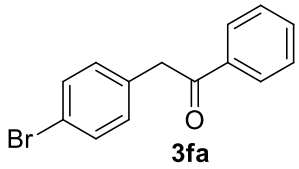
3da

2-(4-Fluorophenyl)-1-phenylethanone (3da) [5]: Light yellow solid, m.p. 100.1 – 100.4 °C, yield 88%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (dd, *J* = 8.4, 1.4 Hz, 2H), 7.58 (tt, *J* = 7.2, 1.6 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.24 – 7.21(m, 2H), 7.02 (t, *J* = 8.4 Hz, 2H), 4.27 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.54, 162.05 (d, *J* = 244 Hz), 136.60, 133.45, 131.18 (d, *J* = 8 Hz), 130.27(d, *J* = 3 Hz), 128.86, 128.66, 115.67 (d, *J* = 22 Hz), 44.66. HRMS (ESI): m/z calcd for $C_{14}H_{12}FO$ $[M+H]^+$: 215.0867, found: 215.0870.



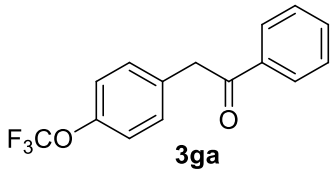
3ea

2-(4-Chlorophenyl)-1-phenylethanone (3ea) [5]: Light yellow solid, m.p. 111.2 – 112.0 °C, yield 90%, ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.05 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.66 (tt, *J* = 7.6, 1.6 Hz, 1H), 7.55 (t, *J* =7.6 Hz, 2H), 7.02 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.8 Hz, 2H), 4.43 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 197.30, 136.22, 134.17, 133.31, 131.66, 131.18, 128.73, 128.27, 128.12, 43.84. HRMS (ESI): m/z calcd for $C_{14}H_{12}ClO$ $[M+H]^+$: 231.0571, found: 231.0574.



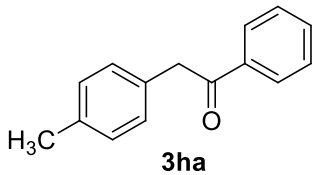
3fa

2-(4-Bromophenyl)-1-phenylethanone (3fa)[9]: Light yellow solid, m.p. 139.5 – 140.2 °C, yield 87%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.58 (tt, *J* = 7.6, 1.6 Hz, 1H), 7.49 – 7.44 (m, 4H), 7.14 (d, *J* = 8.4, 2H), 4.25 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.14, 136.49, 133.56, 133.52, 131.87, 131.40, 128.87, 128.65, 121.10, 44.88. HRMS (ESI): m/z calcd for $C_{14}H_{12}BrO$ $[M+H]^+$: 275.0066, found: 275.0065.



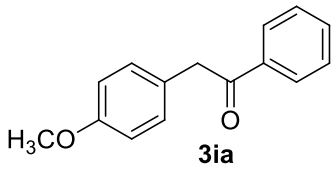
3ga

1-Phenyl-2-(4-(trifluoromethoxy)phenyl)ethanone (3ga) [5]: White solid, m.p. 121.2 – 121.8 °C, yield 85%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 8.01 (m, 2H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.29 (d, *J* = 8.8 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 4.30 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.17, 148.33, 136.51, 133.57, 133.28, 131.08, 128.89, 128.63, 121.26, 120.60 (d, *J* = 255 Hz), 44.62. HRMS (ESI): m/z calcd for $C_{15}H_{12}F_3O_2$ $[M+H]^+$: 281.0784, found: 281.0789.



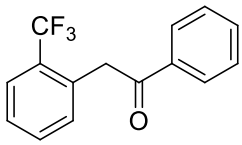
3ha

1-Phenyl-2-(p-tolyl)ethanone (3ha) [5]: Yellow solid, m.p. 81.2 – 81.6 °C, yield 83%, ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.03 (dd, J = 8.2, 1.0 Hz, 2H), 7.63 (tt, J = 7.4, 1.6 Hz, 1H), 7.52 (t, J = 7.6 Hz, 2H), 7.12 (q, J = 8.2 Hz, 4H), 4.32 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 197.81, 136.30, 135.50, 133.20, 131.97, 129.49, 128.92, 128.72, 128.40, 44.34, 20.63. HRMS (ESI): m/z calcd for $C_{15}H_{15}O$ $[M+H]^+$: 211.1117, found: 211.1117.



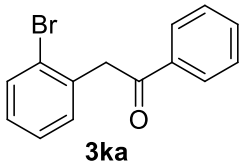
3ia

2-(4-Methoxyphenyl)-1-phenylethanone (3ia)[4]: White solid, m.p. 86.7 – 87.1 °C, yield 80%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (dd, J = 8.4, 1.2Hz, 2H), 7.55 (tt, J = 7.4, 1.2Hz, 1H), 7.46 (t, J = 7.6 Hz, 2H), 7.18 (d, J = 8.8 Hz, 2H), 8.87 (d, J = 8.8 Hz, 2H), 4.23(s, 2H), 3.79(s, 3H); ^{13}C NMR(100 MHz, $CDCl_3$) δ 198.07, 158.72, 136.81, 136.77, 133.22, 130.60, 128.75, 126.67, 114.31, 55.40, 44.79. HRMS (ESI): m/z calcd for $C_{15}H_{15}O_2$ $[M+H]^+$: 227.1067, found: 227.1066.



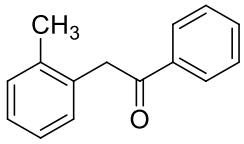
3ja

1-Phenyl-2-(2-(trifluoromethyl)phenyl)ethanone (3ja)[7]: Yellow solid, m.p. 63.4 – 64.1 °C, yield 78%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 8.02 (m, 2H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.61 (tt, *J* = 7.6, 1.6 Hz, 1H), 7.55 – 7.48 (m, 3H), 7.41 (t, *J* = 7.6, 1.6 Hz, 1H), 7.32 (d, *J* = 7.6, 1.6 Hz, 1H), 4.52 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.49, 136.55, 133.49, 133.29, 132.98, 131.94, 129.12 (d, *J* = 30 Hz), 128.86, 128.38, 127.32, 126.25(q, *J* = 5 Hz), 124.53 (d, *J* = 272 Hz), 120.45, 42.57.HRMS (ESI): m/z calcd for $C_{15}H_{12}F_3O$ $[M+H]^+$: 265.0835, found: 265.0832.



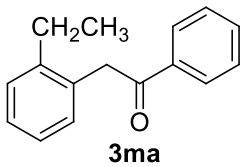
3ka

2-(2-Bromophenyl)-1-phenylethanone (3ka)[13]: Yellow oil, yield 76%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 – 8.04 (m, 2H), 7.61 – 7.58 (m, 2H), 7.50 (t, *J* = 7.6, 1.6 Hz, 2H), 7.32 – 7.24 (m, 2H), 7.16 (td, *J* = 7.6, 1.6 Hz, 1H), 4.47 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.48, 136.76, 135.12, 133.44, 132.92, 131.83, 128.87, 128.83, 128.47, 127.66, 125.23, 45.91. HRMS (ESI): m/z calcd for $C_{14}H_{12}BrO$ $[M+H]^+$: 275.0066, found: 275.0068.



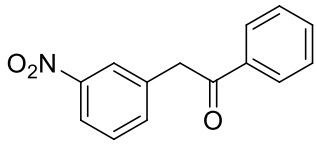
3la

1-Phenyl-2-(o-tolyl)ethanone (3la)[10]: Light yellow solid, m.p. 61.2 – 61.7 °C, yield 76%, ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.08 – 8.06 (m, 2H), 7.66 (tt, J = 7.4, 1.2Hz, 1H), 7.55 (t, J = 7.6 Hz, 2H), 7.18 – 7.12 (m, 4H), 4.44(s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 197.58, 136.87, 136.64, 134.19, 133.26, 130.58, 129.83, 128.75, 128.16, 126.73, 125.70, 43.06, 19.27. HRMS (ESI): m/z calcd for $C_{14}H_{15}O$ $[M+H]^+$: 211.1117, found: 211.1114.



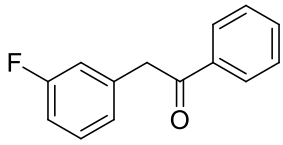
3ma

2-(2-Ethylphenyl)-1-phenylethanone (3ma)[12]: Yellow oil, yield 74%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.06 (m, 2H), 7.63 (tt, *J* = 7.4, 1.2 Hz, 1H), 7.53 (t, *J* = 7.4 Hz, 2H), 7.30 – 7.29 (m, 2H), 7.23 – 7.16 (m, 2H), 4.38 (s, 2H), 2.65 (q, *J* = 7.6 Hz, 2H), 1.25 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.94, 142.66, 137.01, 133.28, 132.79, 130.69, 128.79, 128.58, 128.46, 127.53, 126.13, 42.97, 26.08, 14.85. HRMS (ESI): m/z calcd for $C_{16}H_{17}O$ $[M+H]^+$: 225.1274, found: 225.1275.



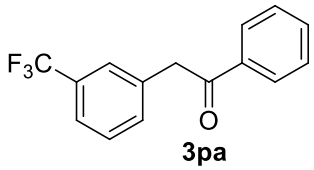
3na

2-(3-Nitrophenyl)-1-phenylethanone (3na)[11]: Yellow solid, m.p. 58.7 – 59.3 °C, yield 85%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 – 8.12 (m, 2H), 8.03 – 8.01 (m, 2H), 7.63 – 7.59 (m, 2H), 7.50 (dt, *J* = 8.0, 3.6 Hz, 3H), 4.42 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.23, 148.41, 136.47, 136.22, 136.18, 133.81, 129.49, 128.97, 128.48, 124.84, 122.18, 44.64. HRMS (ESI): m/z calcd for $C_{14}H_{12}NO_3$ $[M+H]^+$: 242.0812, found: 242.0815.



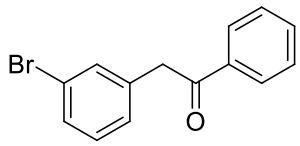
3oa

2-(3-Fluorophenyl)-1-phenylethanone (3oa) [5]: Light yellow oil, yield 87%, ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.07 – 8.05 (m, 2H), 7.65 (tt, *J* = 7.4, 1.6 Hz, 1H), 7.55 (t, *J* =7.6 Hz, 2H), 7.38 – 7.32 (m, 1H), 7.15 – 7.04 (m, 3H), 4.46 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 197.14, 162.06 (d, *J* = 242.0 Hz), 137.94 (d, *J* = 8.0 Hz), 136.26, 133.36, 130.00(d, *J* = 8.0 Hz), 128.76, 128.31, 126.00 (d, *J* = 3.0 Hz), 116.65 (d, *J* = 12.0 Hz), 113.28(d, *J* = 21.0 Hz), 44.21. HRMS (ESI): m/z calcd for C14H12FO $[M+H]^+$: 215.0867, found: 215.0864.



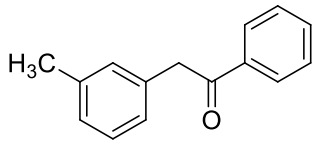
3pa

1-Phenyl-2-(3-(trifluoromethyl)phenyl)ethanone (3pa) [5]: Yellow solid, m.p. 78.6 – 79.3 °C, yield 84%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 8.01 (m, 2H), 7.60 (tt, J = 8.0, 1.2 Hz, 1H), 7.54 – 7.45 (m, 6H), 4.36 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.79, 136.48, 135.48, 133.65, 133.24, 131.03 (d, *J* = 33 Hz), 129.13, 128.76 (d, *J* = 35 Hz), 126.55 (d, *J* = 4 Hz), 123.98 (d, *J* = 4 Hz), 124.21 (d, *J* = 270 Hz), 120.15, 45.02. HRMS (ESI): m/z calcd for $C_{15}H_{12}F_3O$ $[M+H]^+$: 265.0835, found: 265.0834.



3qa

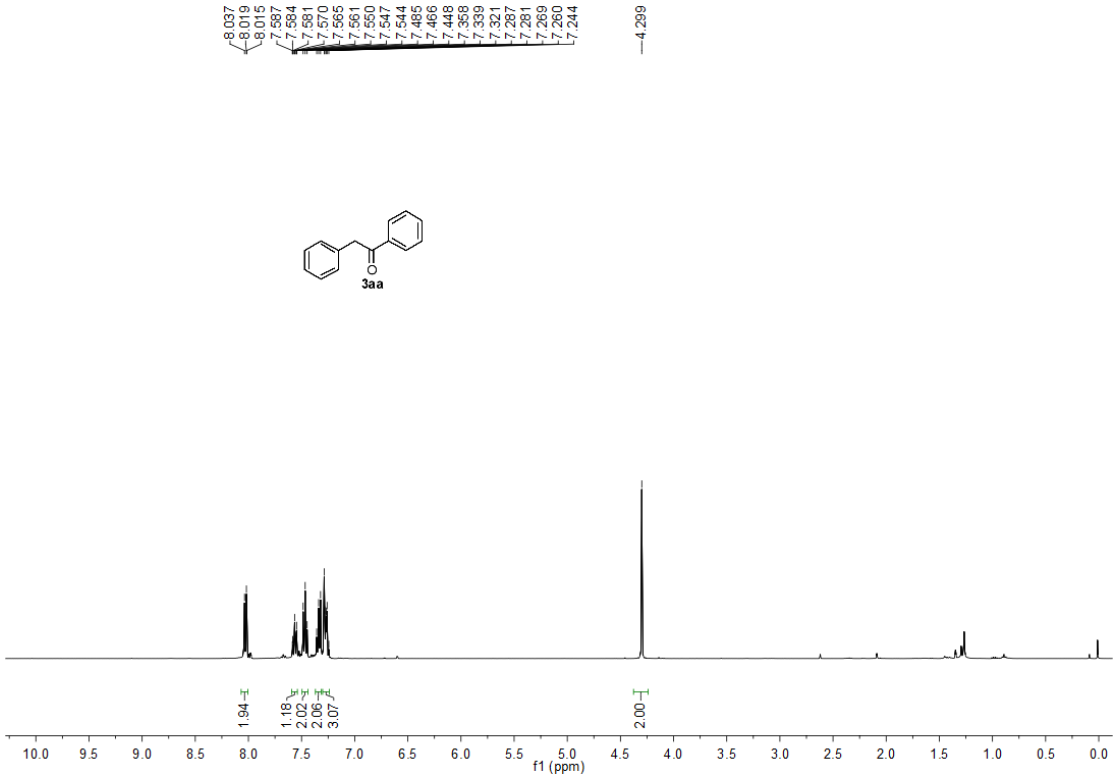
2-(3-Bromophenyl)-1-phenylethanone (3qa) [5]: Light yellow solid, m.p. 95.6 – 96.3 °C, yield 86%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (*d*, J = 7.2 Hz, 2H), 7.58 (t, J = 7.4 Hz 1H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.43 (s, 1H), 7.41 – 7.38 (m, 1H), 7.20 (d, *J* = 4.8 Hz, 2H), 4.25 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.83, 136.77, 136.38, 133.47, 132.61, 130.17, 130.10, 128.80, 128.55, 128.33, 122.65, 44.84. HRMS (ESI): m/z calcd for $C_{14}H_{12}BrO$ $[M+H]^+$: 275.0066, found: 275.0065.

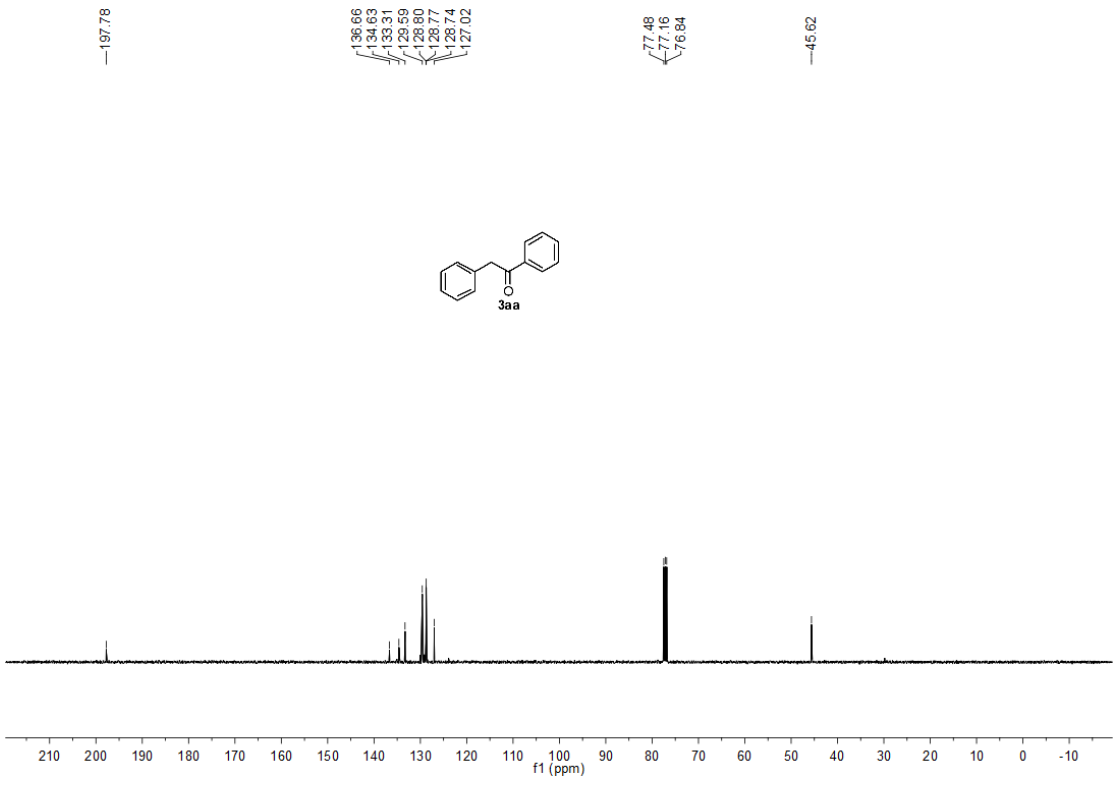


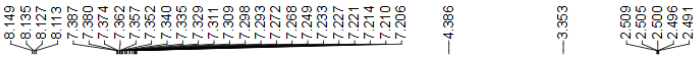
3ra

1-Phenyl-2-(*m*-tolyl)ethanone (3ra) [5]: Yellow oil, yield 85%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.06 (m, 2H), 7.60 (tt, *J* = 7.4, 1.2 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 2H), 7.27 (t, *J* = 7.4 Hz, 1H), 7.14 – 7.11 (m, 3H), 4.30 (s, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.84, 138.37, 136.70, 134.51, 133.21, 130.25, 128.97, 128.71, 128.64, 127.75, 126.57, 45.52, 21.47. HRMS (ESI): m/z calcd for $C_{15}H_{15}O$ $[M+H]^+$: 211.1117, found: 211.1116.

^{1}H and ^{13}C NMR Spectra of Products for Control Experiments



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7.309
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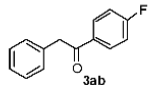
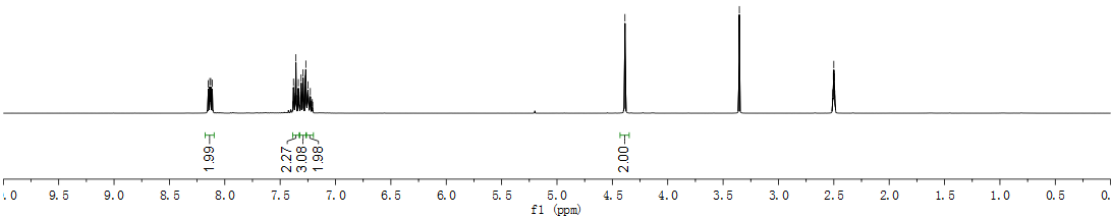
2.500
2.496
2.491


F
O
3ab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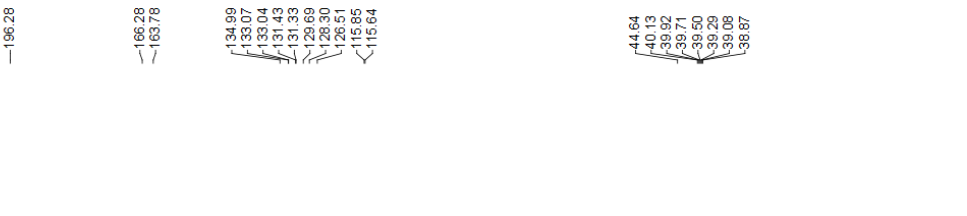
2.27
3.08
1.98
2.00
f1 (ppm)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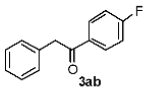
39.50
39.29
39.08
38.87


F
O
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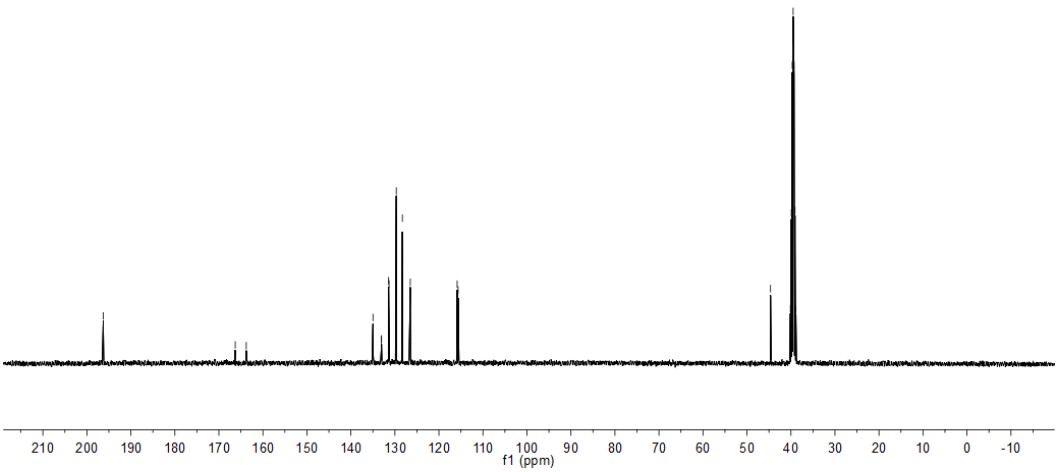
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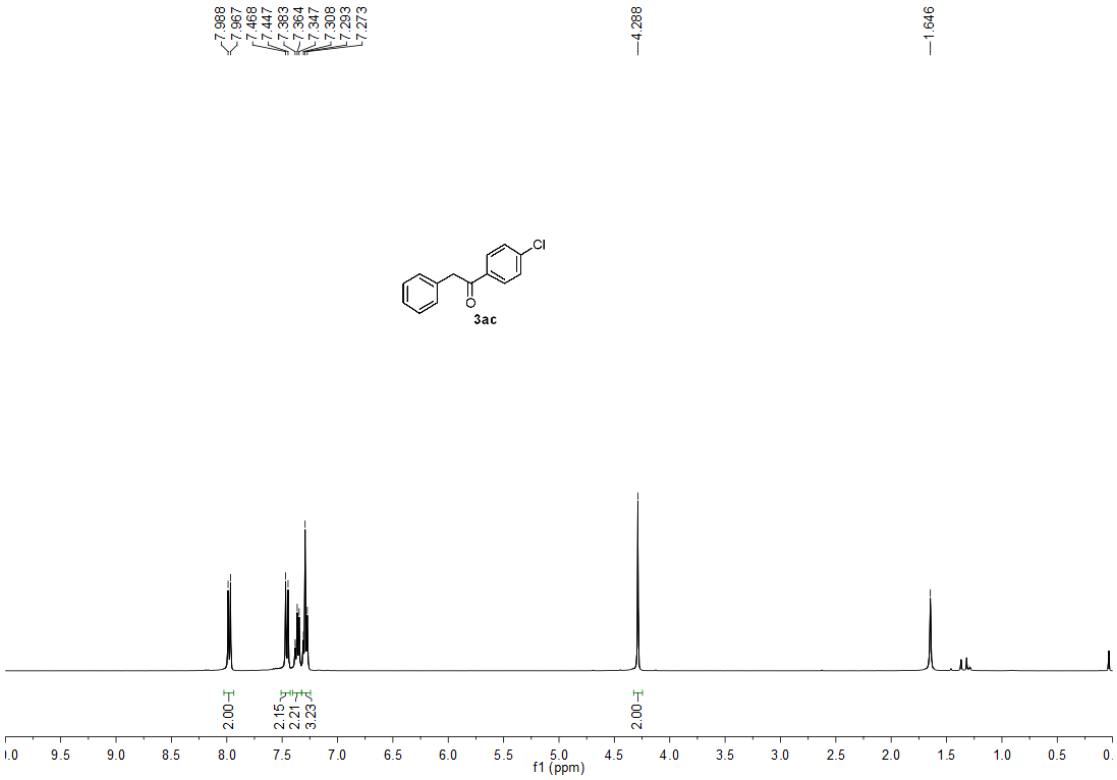
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2.15
2.21
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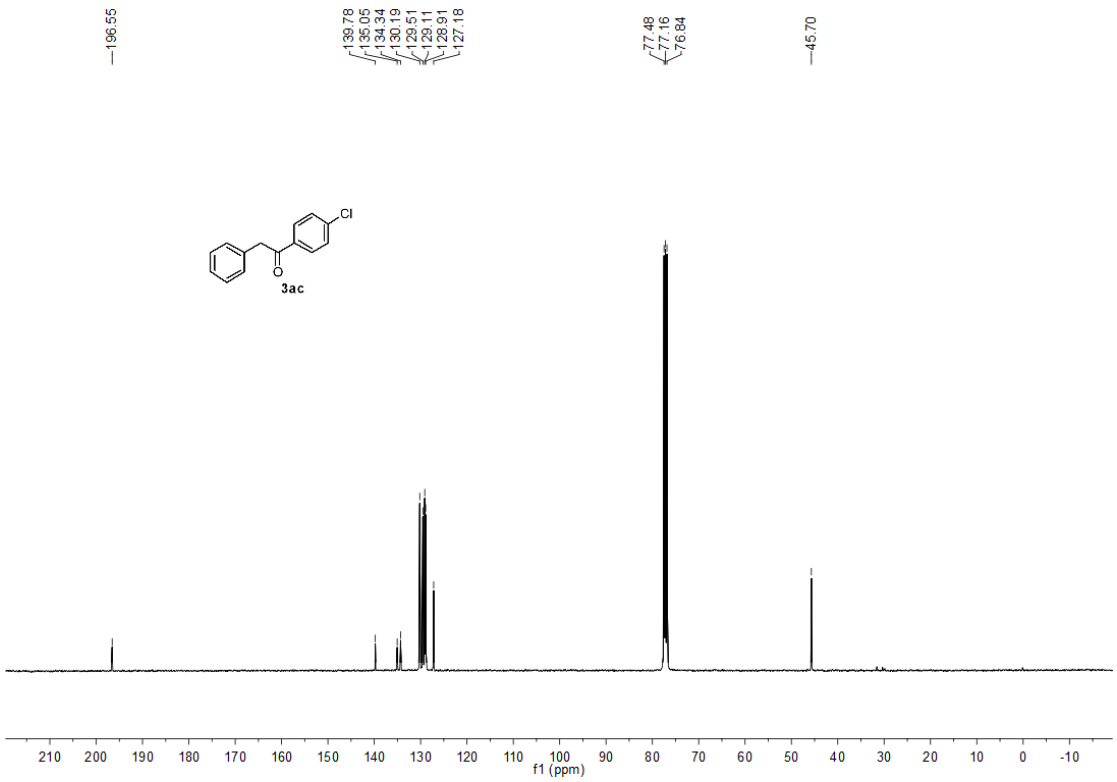
2.00
f1 (ppm)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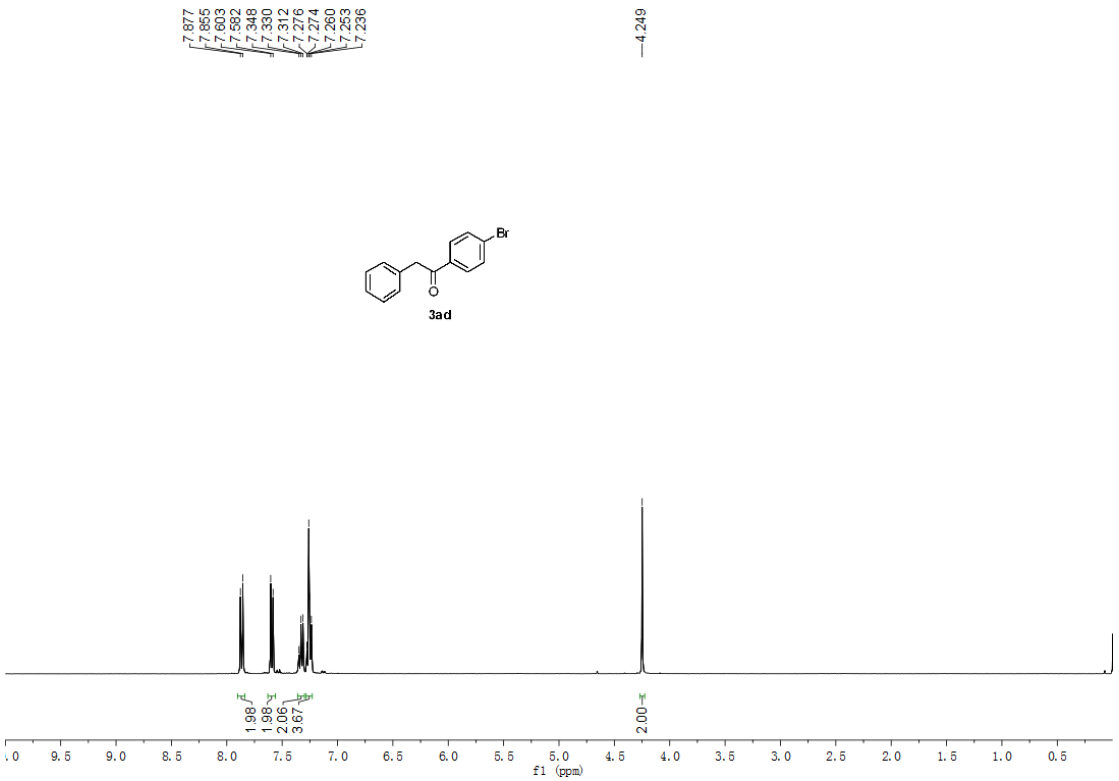
Cl
O
3ac
f1 (ppm)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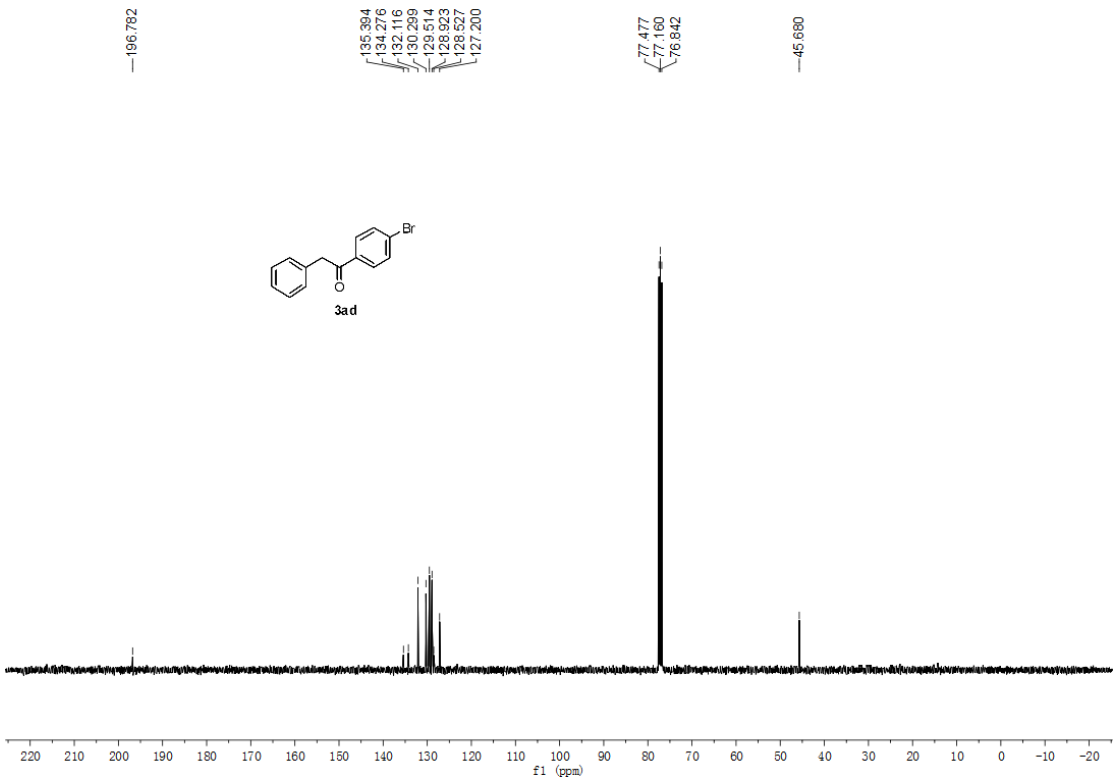
7.855
7.603
7.582
7.348
7.330
7.312
7.276
7.274
7.260
7.253
7.236
4.249
Br
O
3ad
1.98
1.98
2.06
3.67
2.00
f1 (ppm)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135.394
134.276
132.116
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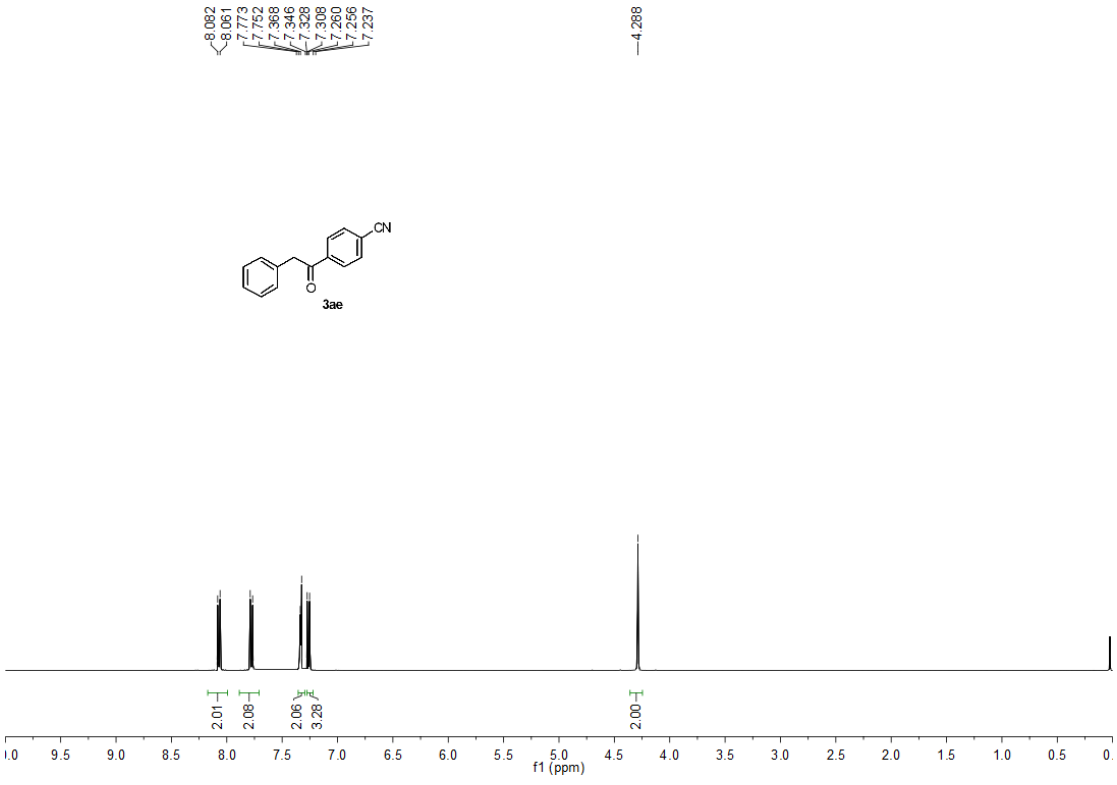
128.527
127.200
77.477
77.160
76.842
45.680
Br
O
3ad
f1 (ppm)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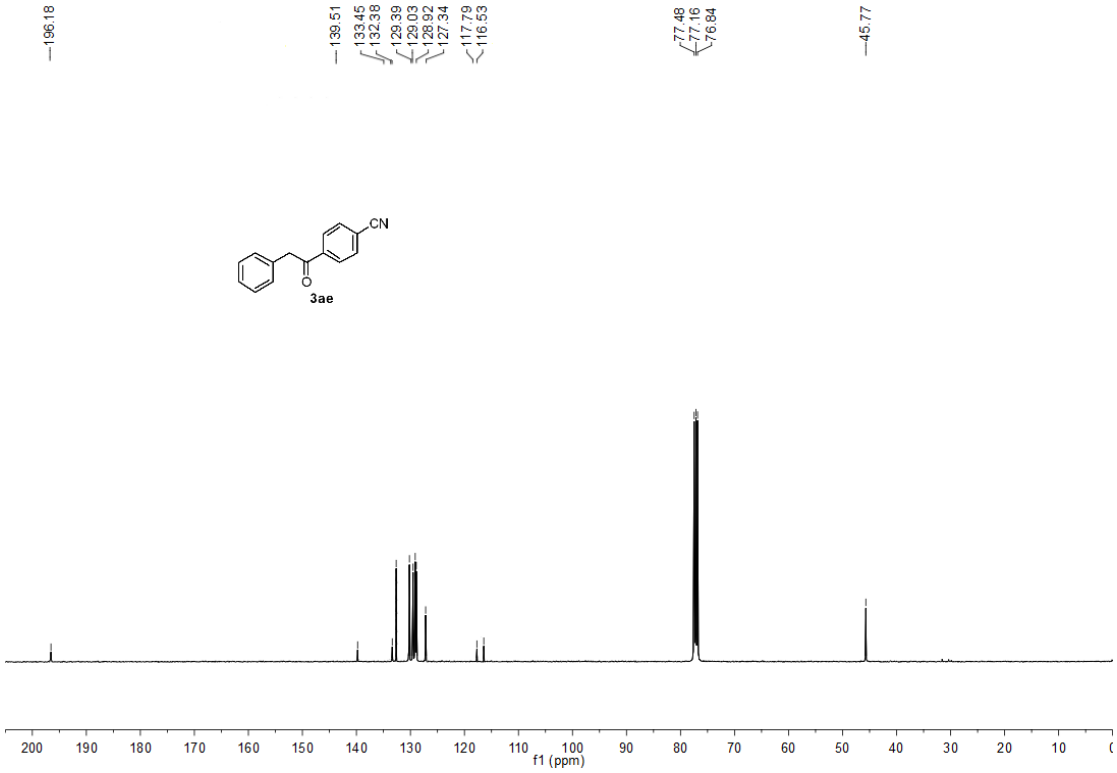
8.061
7.773
7.752
7.368
7.346
7.328
7.308
7.260
7.256
7.237
4.288
CN
O
3ae
2.01
2.08
2.06
3.28
2.00
f1 (ppm)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132.38
129.39
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127.34
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116.53
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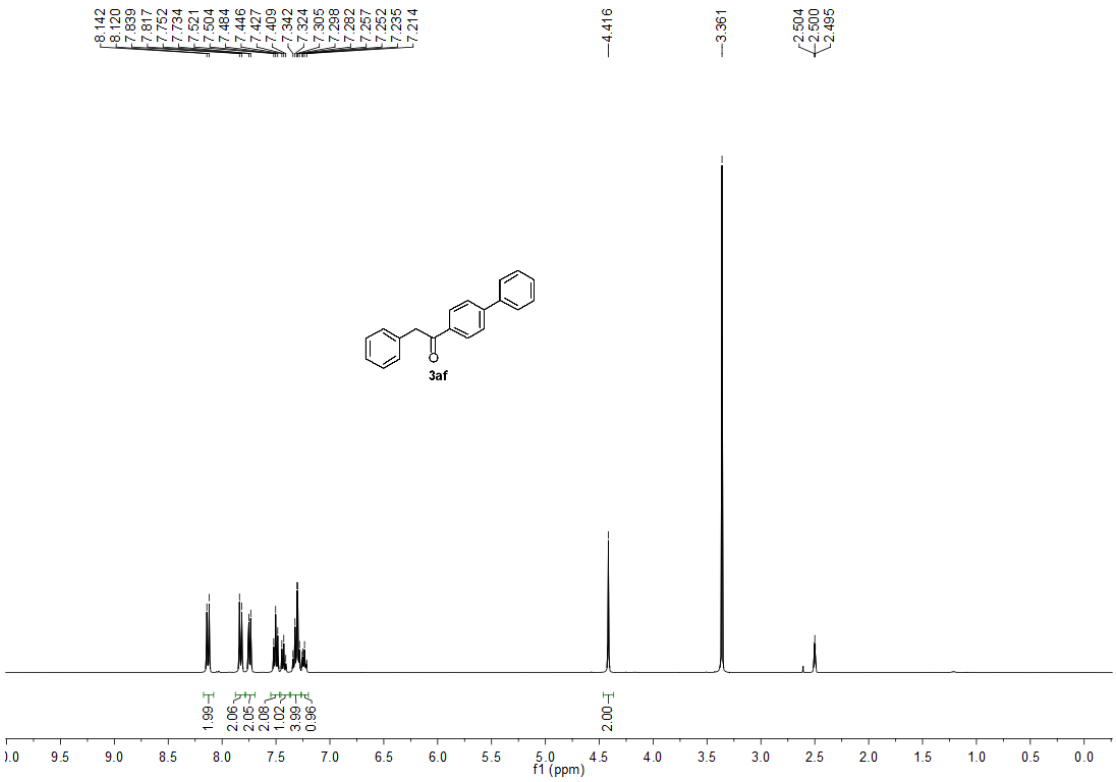
77.16
76.84
45.77
CN
O
3ae
f1 (ppm)


8.142
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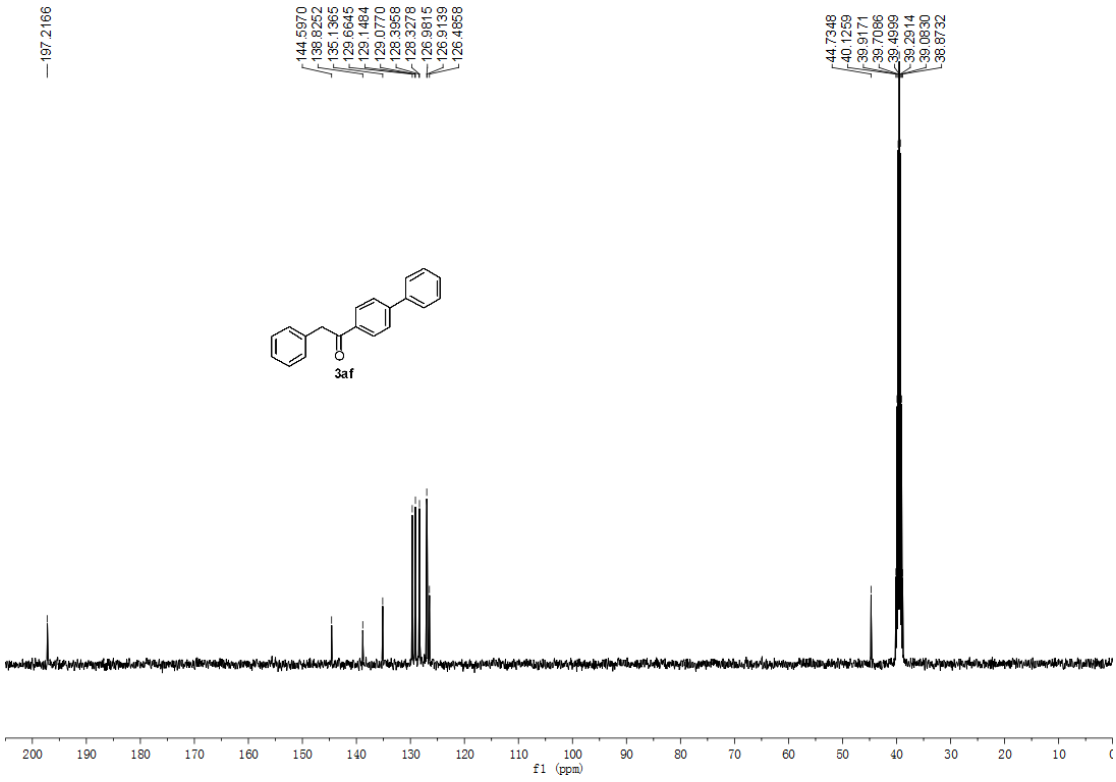
7.752
7.734
7.521
7.504
7.484
7.446
7.427
7.409
7.342
7.324
7.305
7.298
7.282
7.257
7.252
7.235
7.214
4.416
3.361
2.504
2.500
2.495
3af
1.99
2.06
2.05
2.08
1.02
3.99
0.96
2.00
f1 (ppm)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138.8252
135.1365
129.6645
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129.0770
128.3958
128.3278
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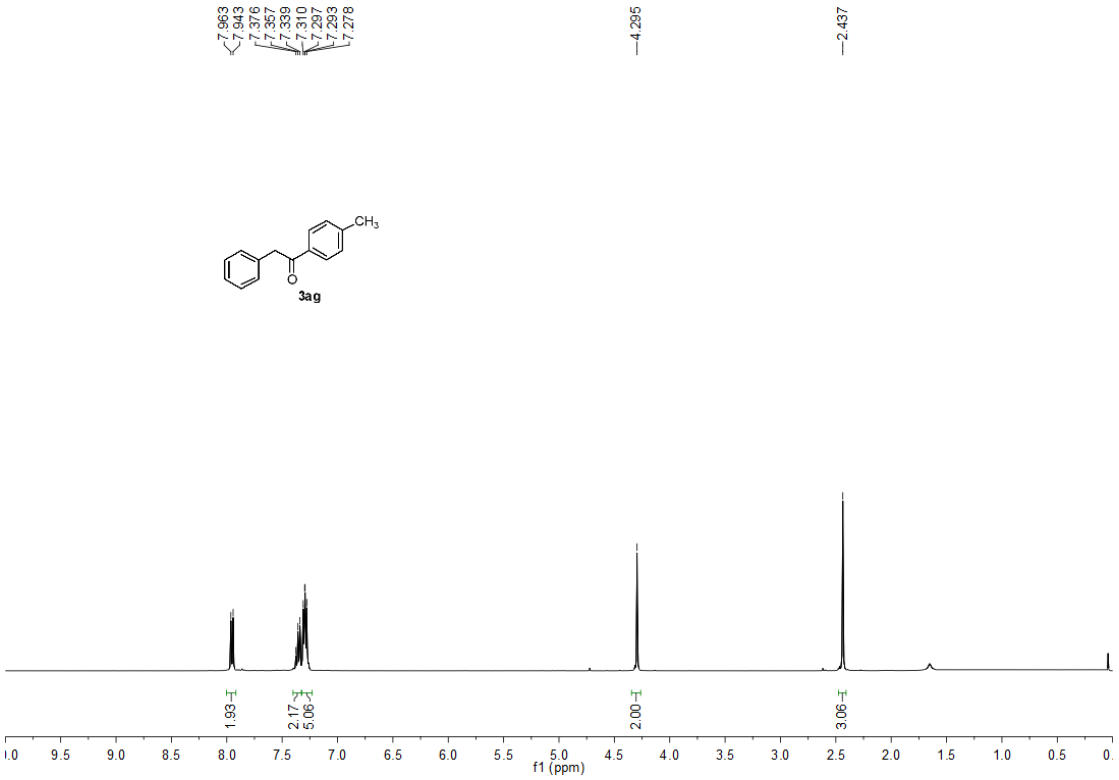
126.9139
126.4858
44.7348
40.1259
39.9171
39.7086
39.4999
39.2914
39.0830
38.8732
3af
f1 (ppm)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7.943
7.376
7.357
7.339
7.310
7.297
7.293
7.278
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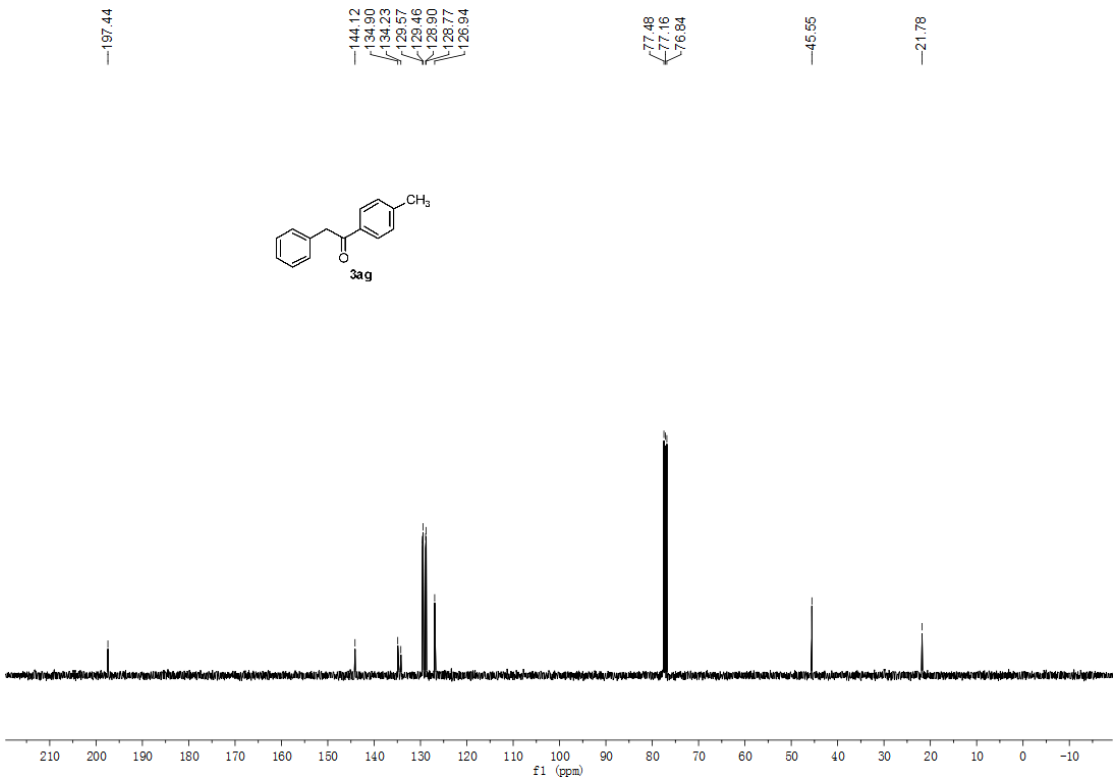
2.437
CH3
O
3ag
1.93
2.17
5.06
2.00
3.06
f1 (ppm)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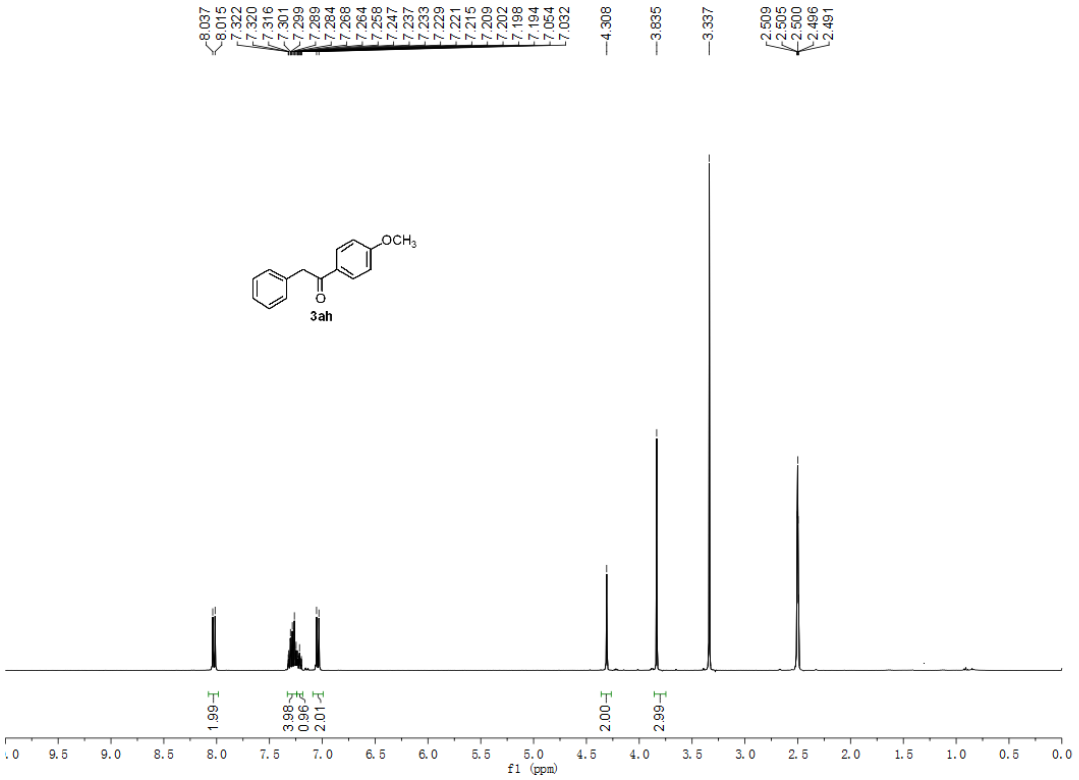
144.12
134.90
134.23
129.57
129.46
128.90
128.77
126.94
77.48
77.16
76.84
45.55
21.78
CH3
O
3ag
f1 (ppm)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7.316
7.301
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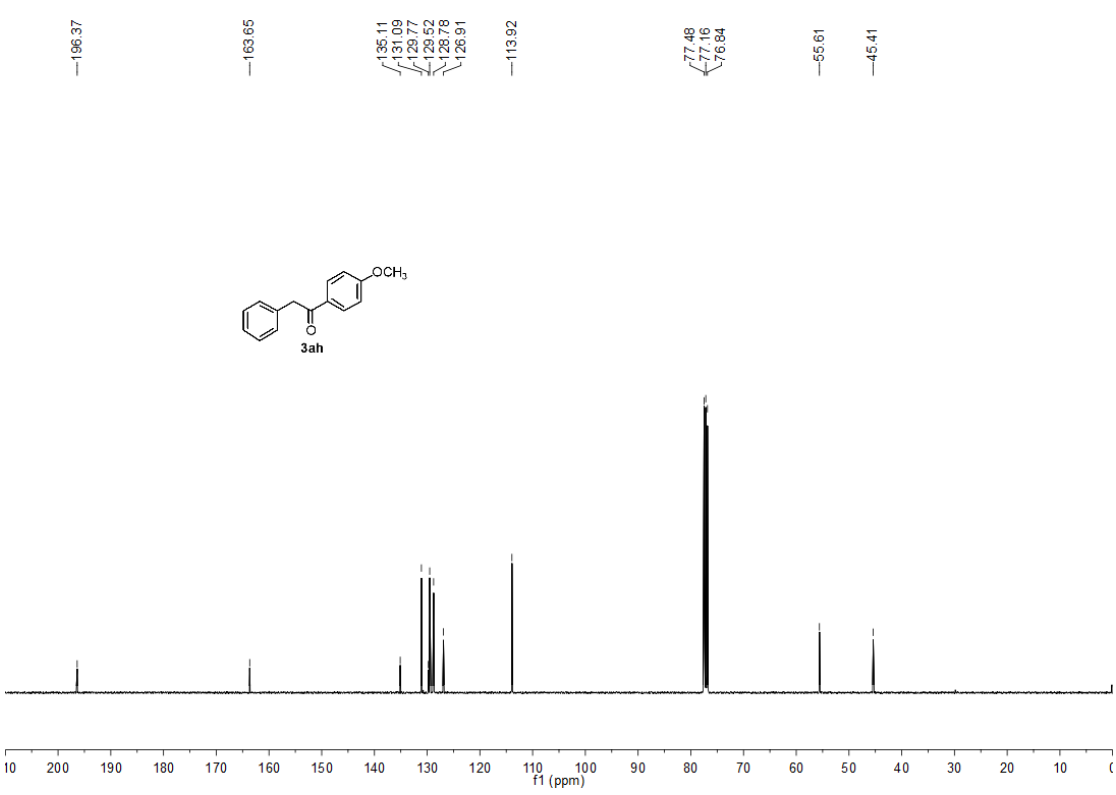
7.289
7.284
7.268
7.264
7.258
7.247
7.237
7.233
7.229
7.221
7.215
7.209
7.202
7.198
7.194
7.054
7.032
4.308
3.835
3.337
2.509
2.505
2.500
2.496
2.491
OCH3
O
3ah
1.99
3.98
0.96
2.01
2.00
2.99
f1 (ppm)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163.65
135.11
131.09
129.77
129.52
128.78
126.91
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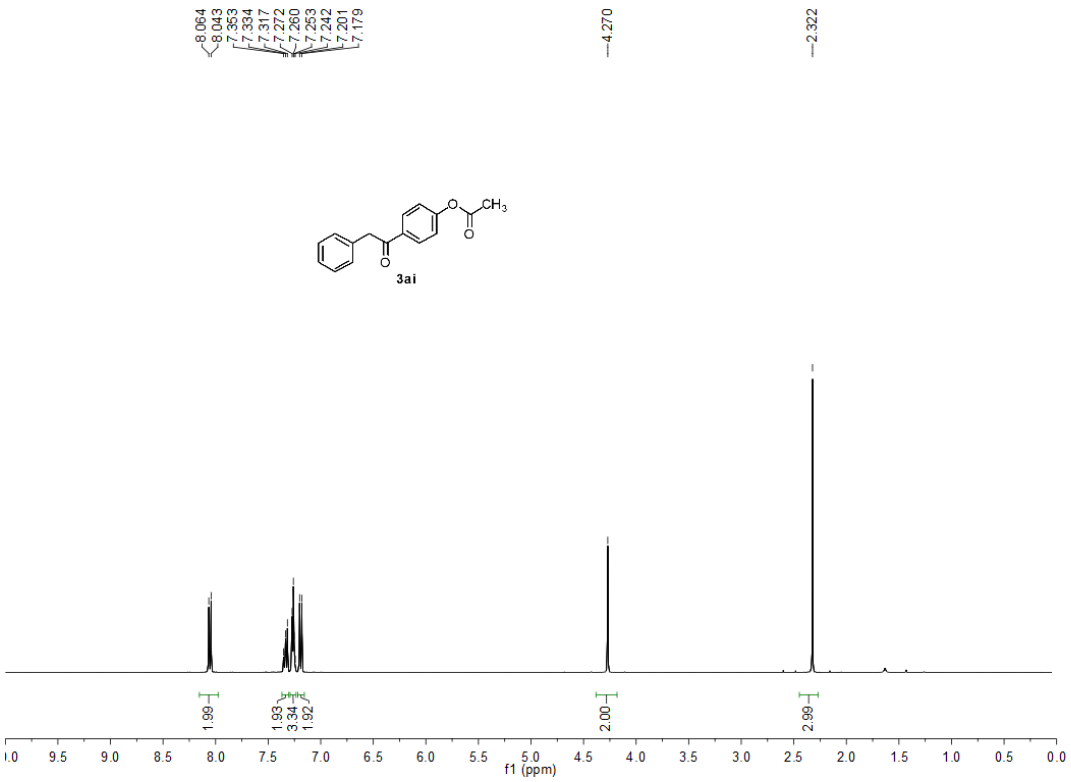
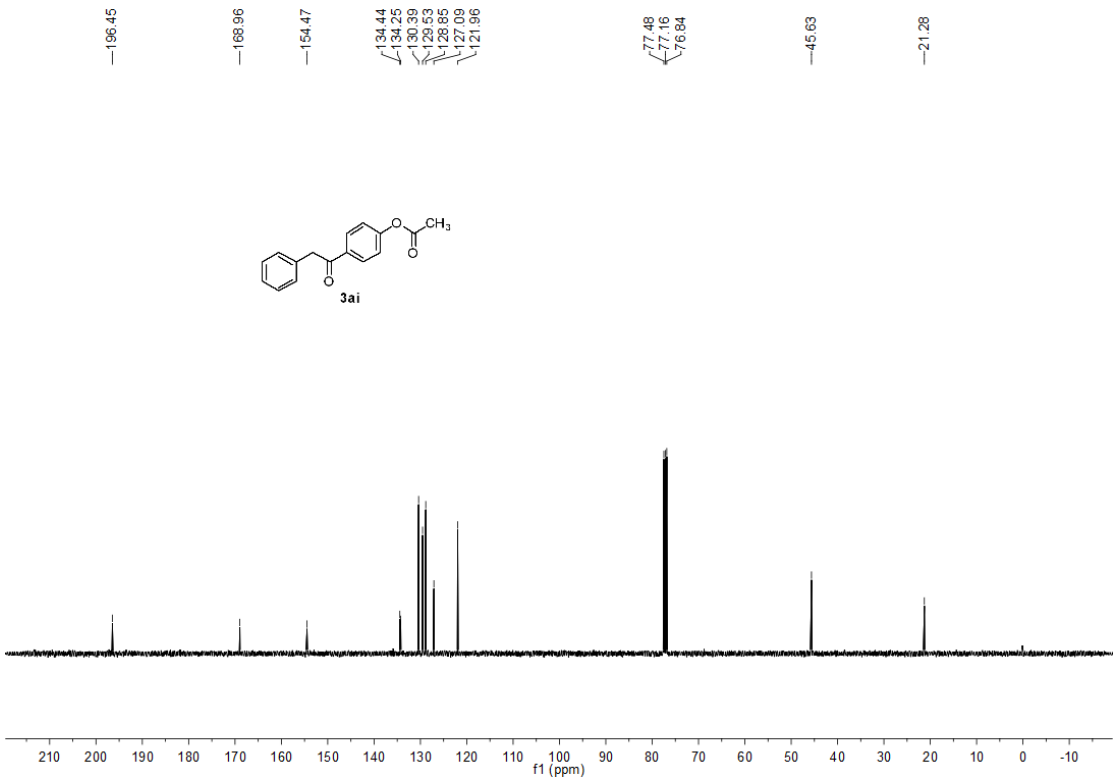
77.48
77.16
76.84
55.61
45.41
OCH3
O
3ah
f1 (ppm)


8.064
8.043
7.353
7.334
7.317
7.272
7.260
7.253
7.242
7.201
7.179
4.270
2.322
3ai
1.99
1.93
3.34
1.92
2.00
2.99
f1 (ppm)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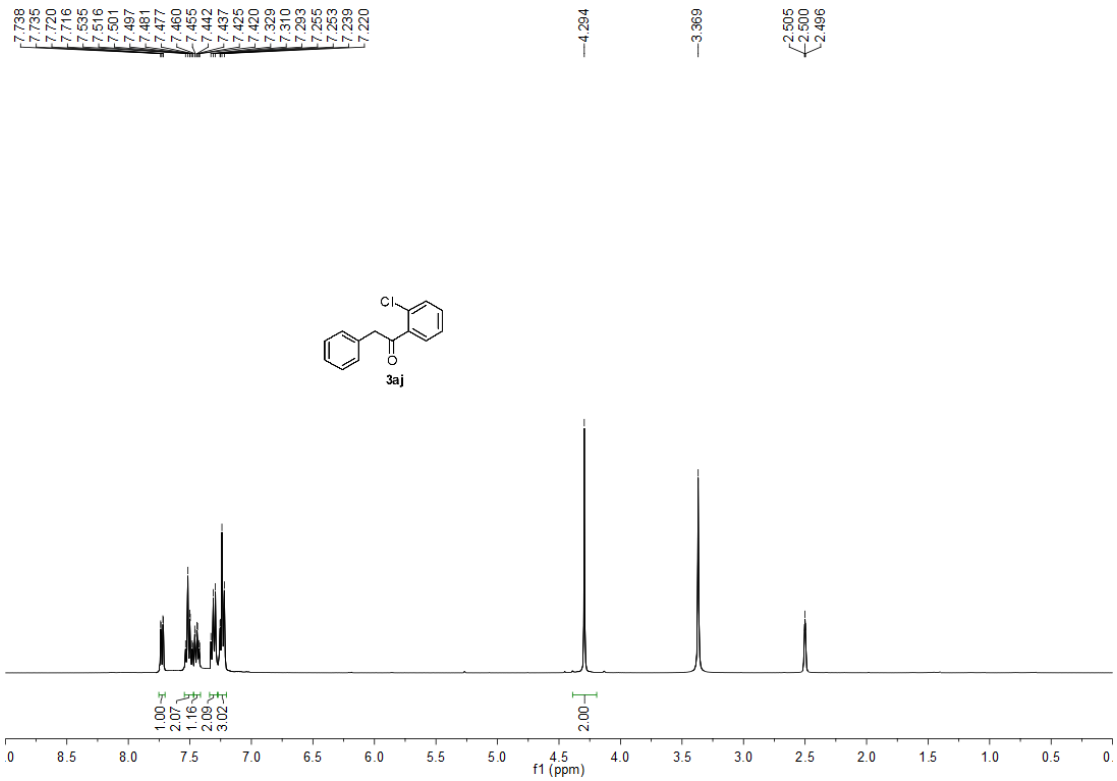
168.96
154.47
134.44
134.25
130.39
129.53
128.85
127.09
121.96
77.48
77.16
76.84
45.63
21.28
3ai
f1 (ppm)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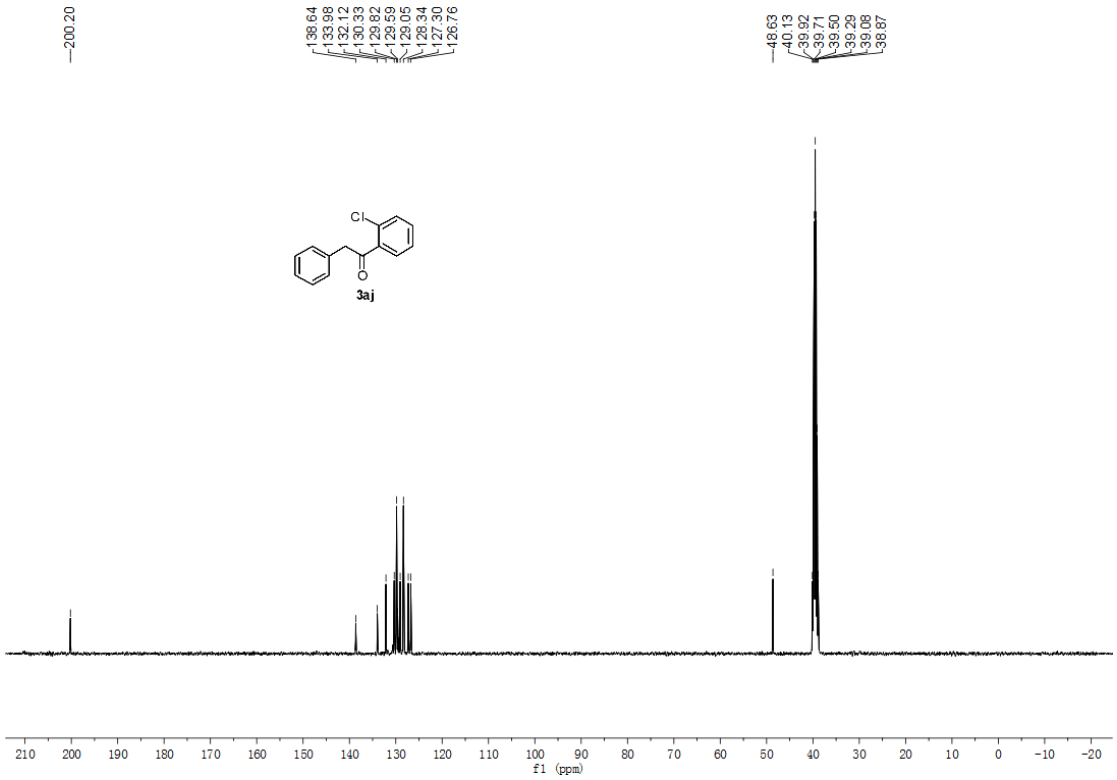
7.735
7.720
7.716
7.535
7.516
7.501
7.497
7.481
7.477
7.460
7.455
7.442
7.437
7.425
7.420
7.329
7.310
7.293
7.255
7.253
7.239
7.220
4.294
3.369
2.505
2.500
2.496
Cl
O
3aj
1.00
2.07
1.16
2.09
3.02
2.00
f1 (ppm)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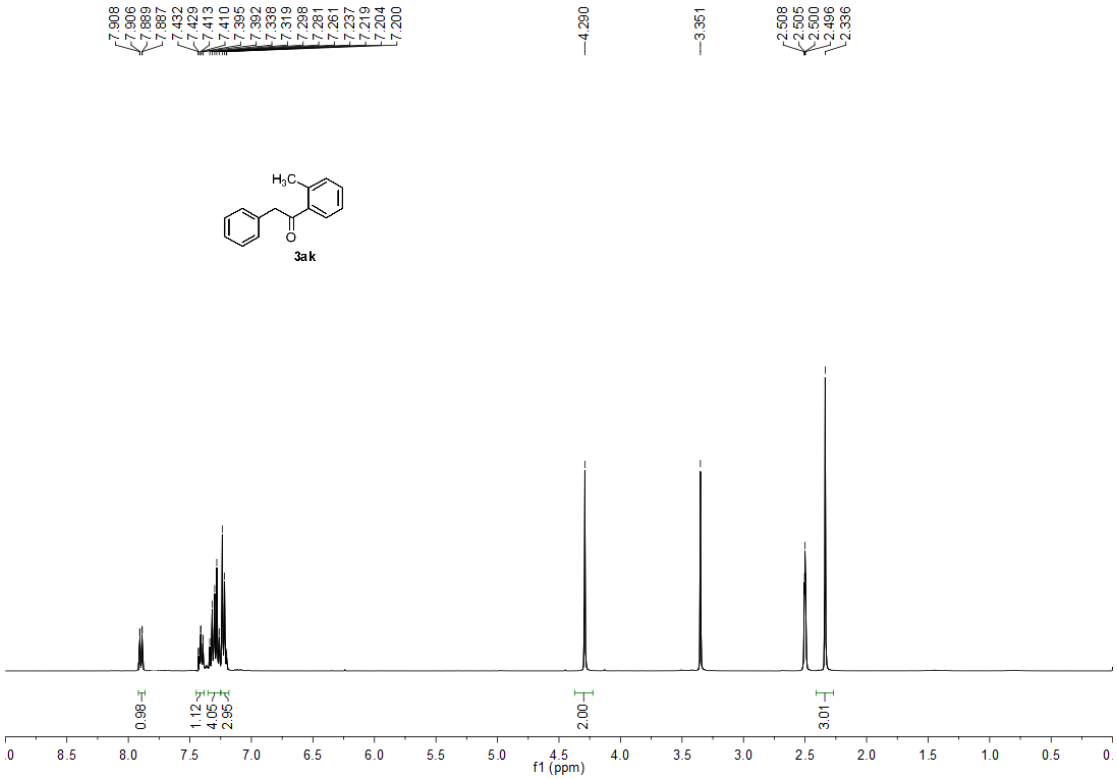
138.64
133.98
132.12
130.33
129.82
129.59
129.05
128.34
127.30
126.76
48.63
40.13
39.92
39.71
39.50
39.29
39.08
38.87
Cl
O
3aj
f1 (ppm)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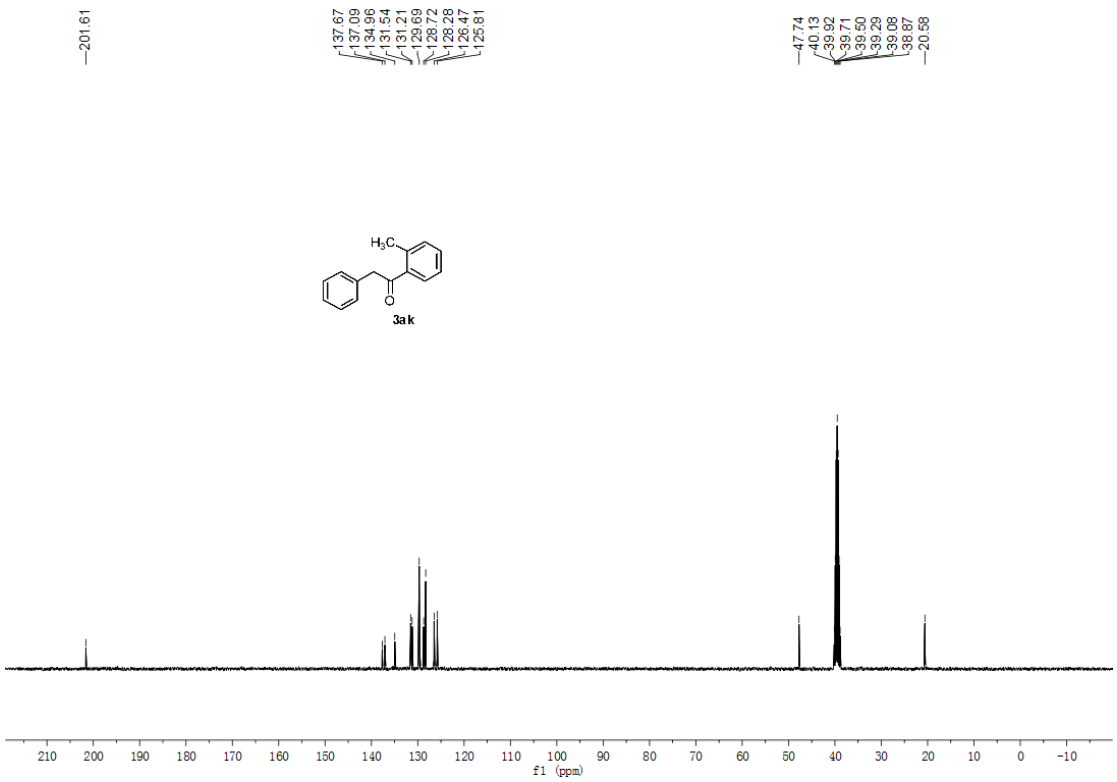
7.410
7.395
7.392
7.338
7.319
7.298
7.281
7.261
7.237
7.219
7.204
7.200
4.290
3.351
2.508
2.505
2.500
2.496
2.336
H3C
O
3ak
0.98
1.12
4.05
2.95
2.00
3.01
f1 (ppm)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128.72
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126.47
125.81
47.74
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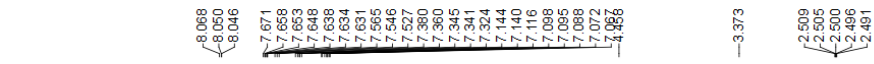
39.71
39.50
39.29
39.08
38.87
20.58
H3C
O
3ak
f1 (ppm)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7.546
7.527
7.380
7.360
7.345
7.341
7.324
7.144
7.140
7.116
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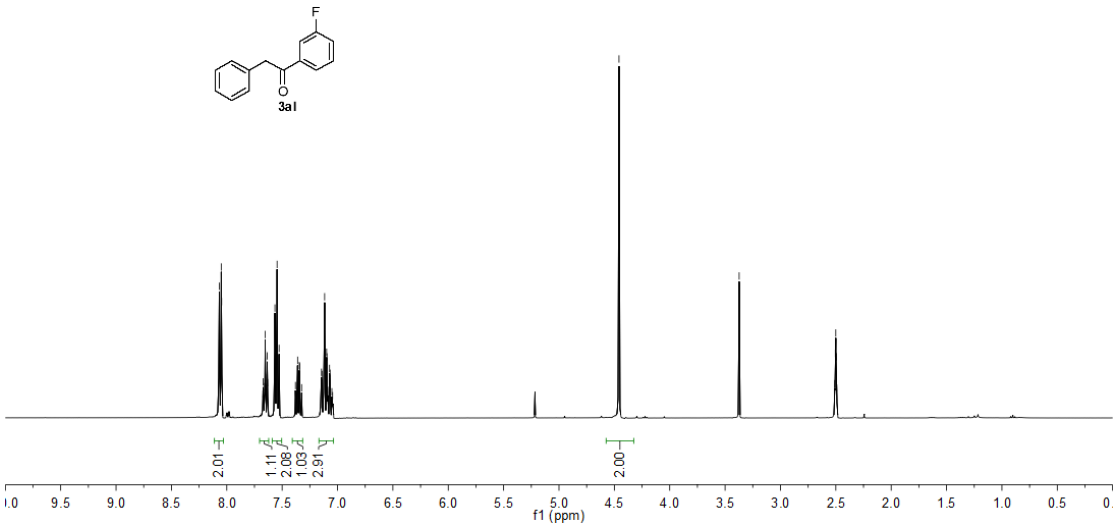
7.072
7.067
4.458
3.373
2.509
2.505
2.500
2.496
2.491


F
O
3al
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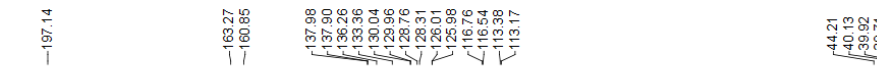
1.11
2.08
1.03
2.91
2.00
f1 (ppm)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128.31
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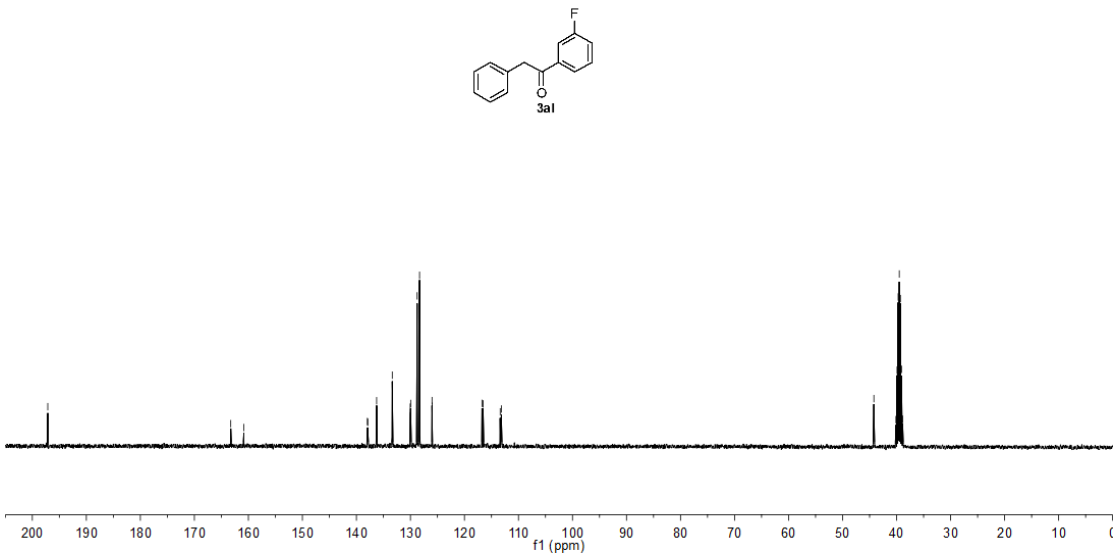
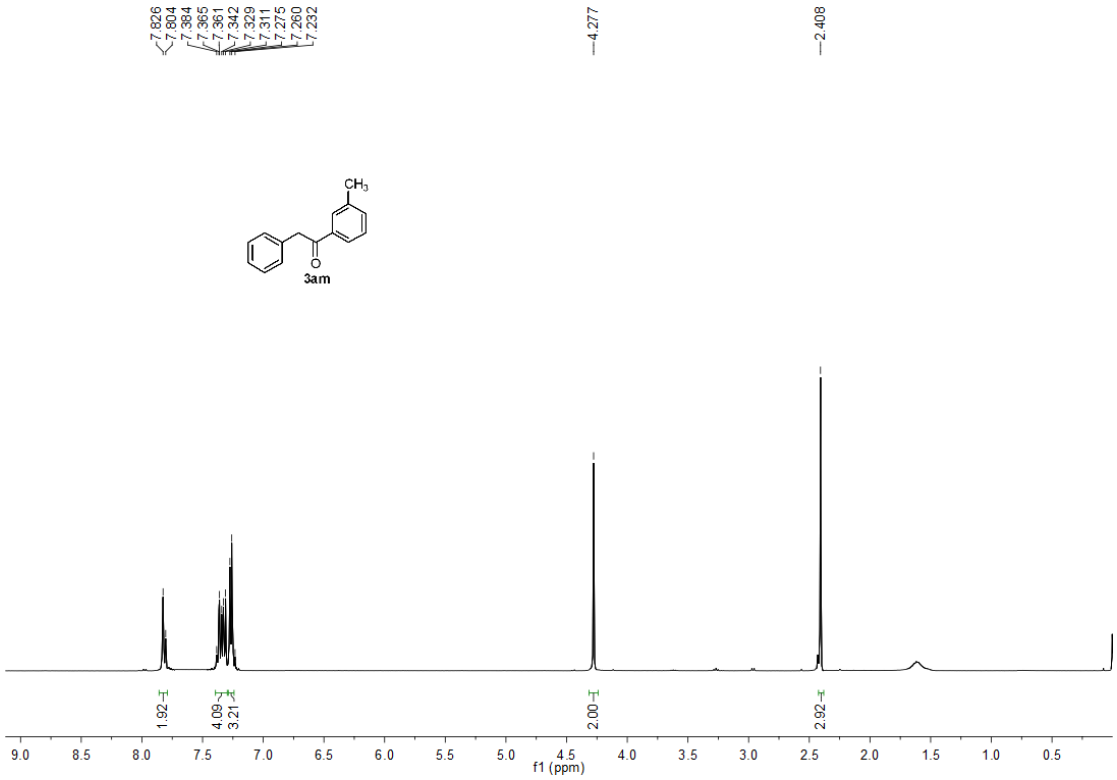
39.92
39.71
39.50
39.29
39.08
38.87


F
O
3al
f1 (ppm)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7.311
7.275
7.260
7.232
4.277
2.408
CH3
O
3am
1.92
4.09
3.21
2.00
2.92
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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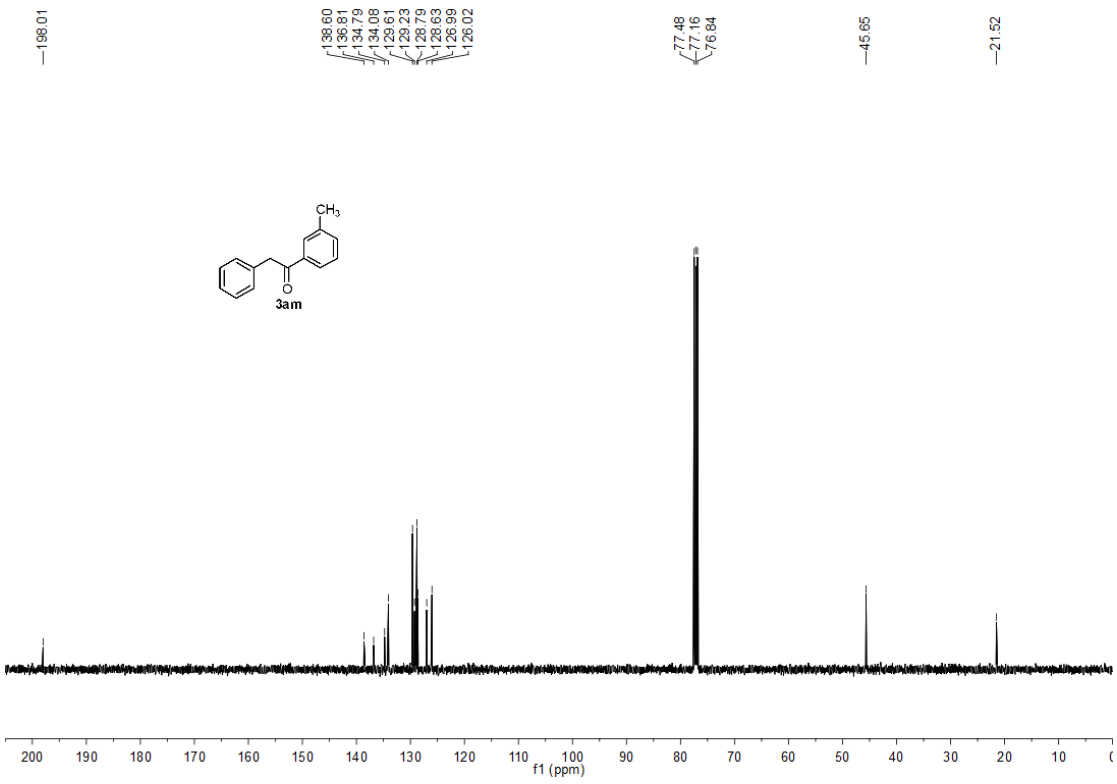
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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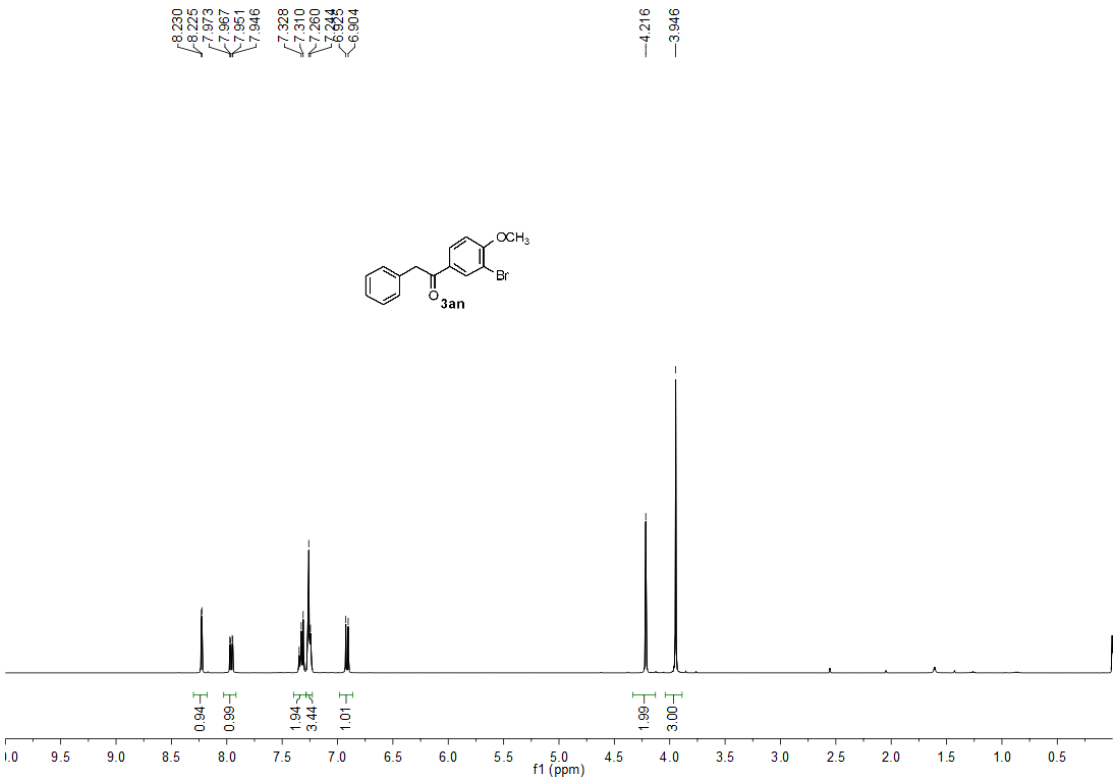
134.08
129.61
129.23
128.79
128.63
126.99
126.02
77.48
77.16
76.84
45.65
21.52
CH3
O
3am
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.310
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7.244
6.925
6.904
4.216
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Br
O
3an
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0.99
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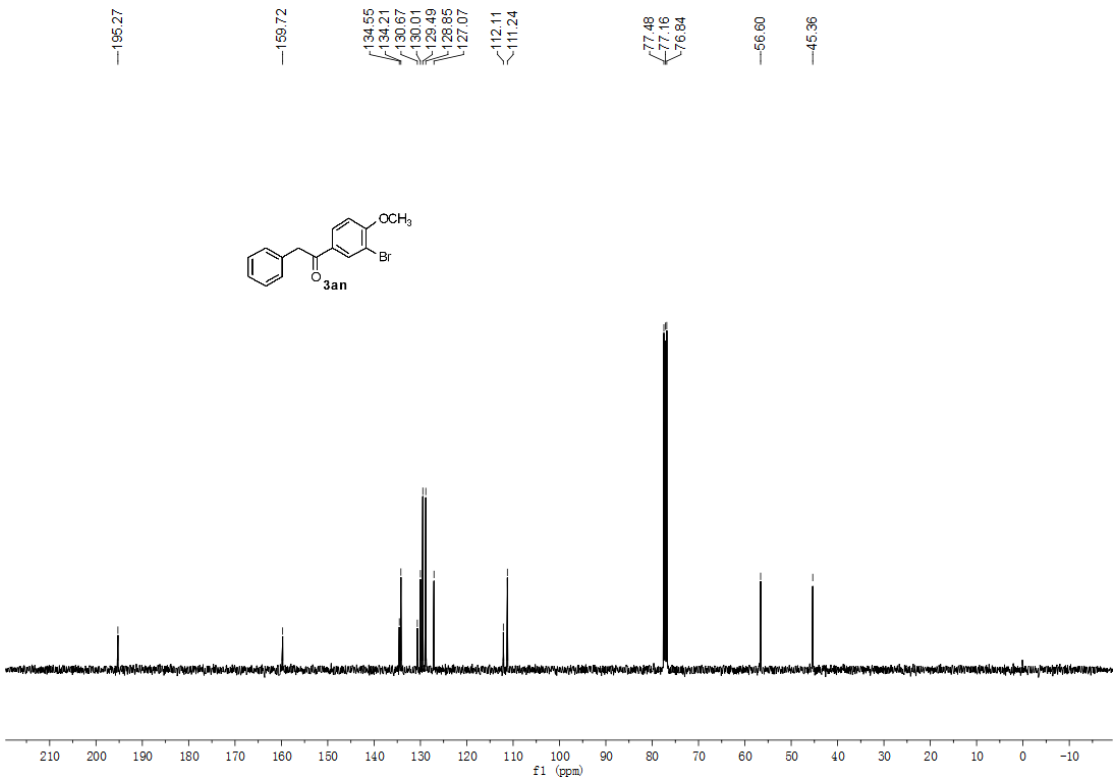
1.01
1.99
3.00
f1 (ppm)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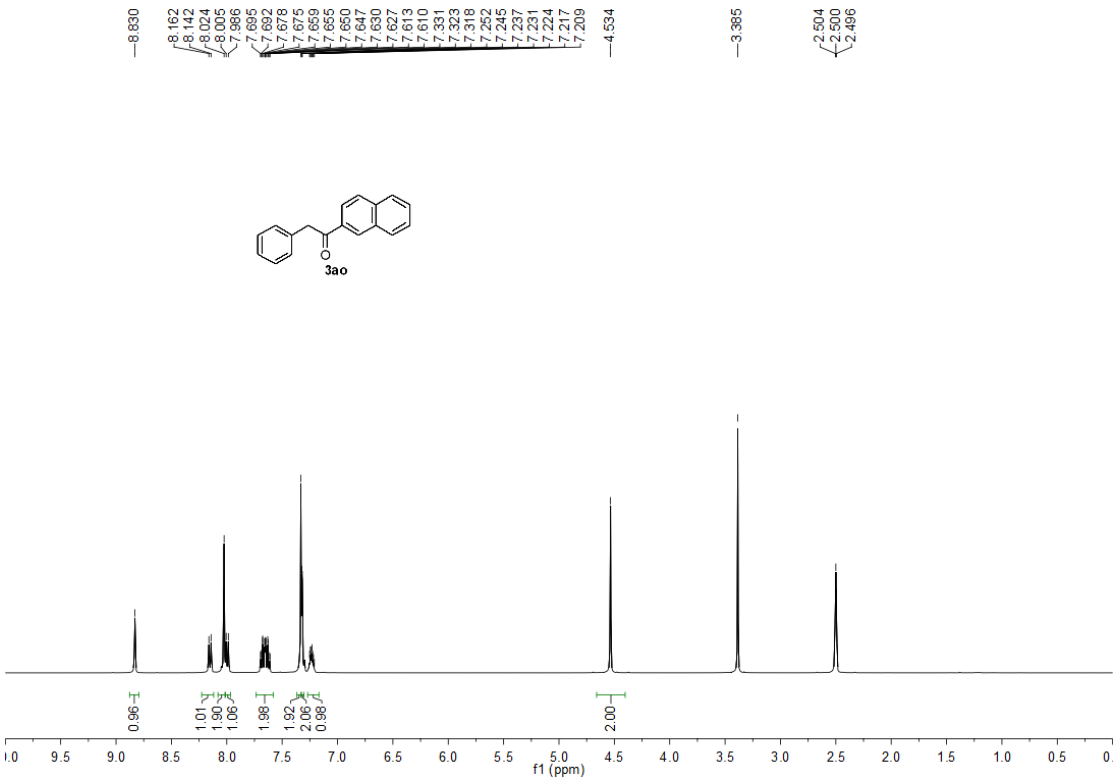
Br
O
3an
f1 (ppm)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7.647
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7.627
7.613
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7.331
7.323
7.318
7.252
7.245
7.237
7.231
7.224
7.217
7.209
4.534
3.385
2.504
2.500
2.496
3ao
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1.01
1.90
1.06
1.98
1.92
2.06
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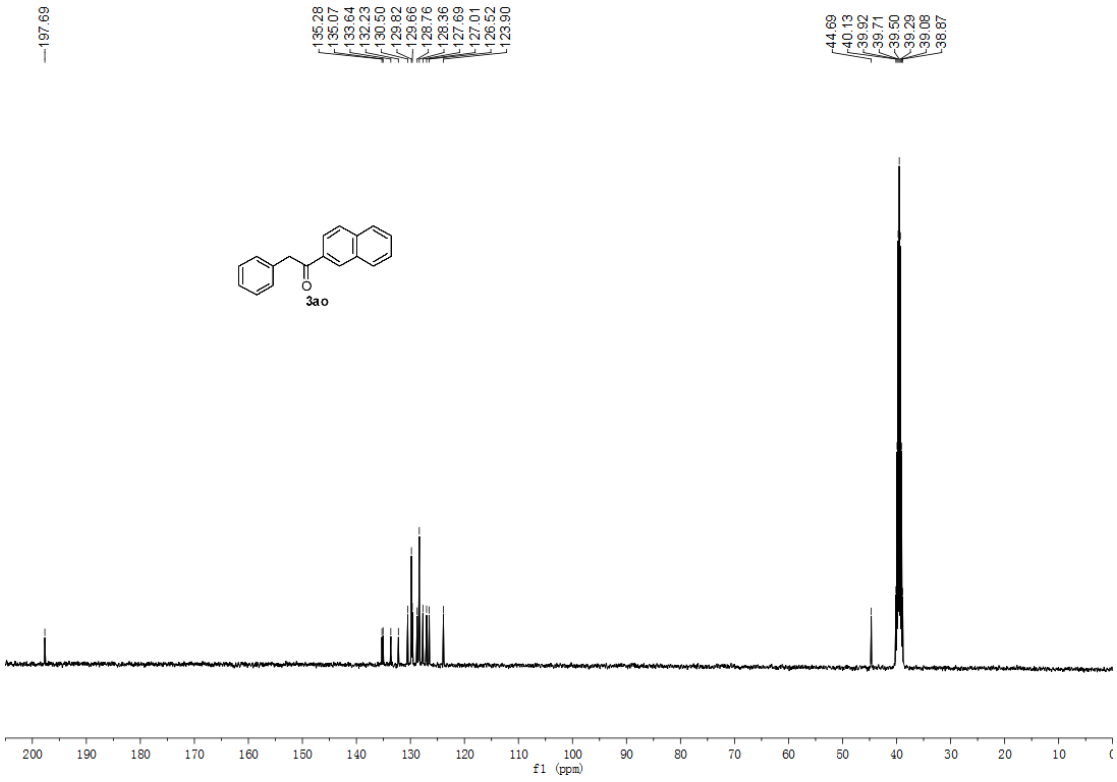
2.00
f1 (ppm)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129.66
128.76
128.36
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127.01
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40.13
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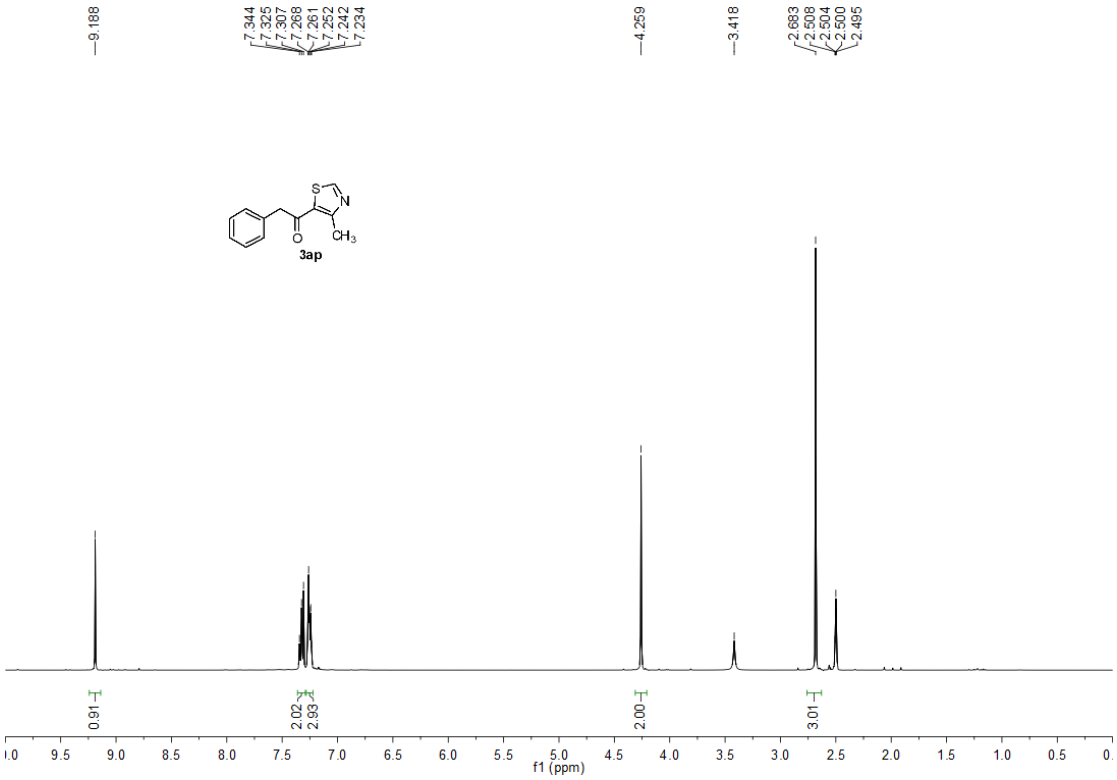
39.71
39.50
39.29
39.08
38.87
3ao
f1 (ppm)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7.268
7.261
7.252
7.242
7.234
4.259
3.418
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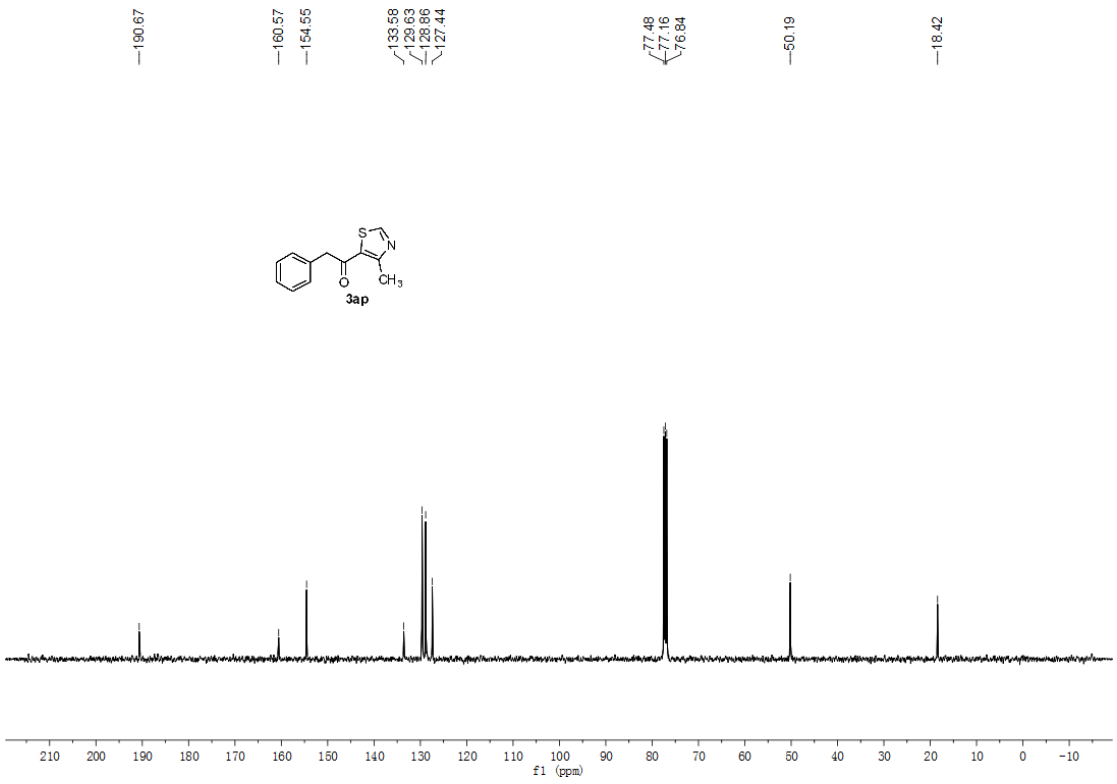
2.504
2.500
2.495
3ap
0.91
2.02
2.93
2.00
3.01
f1 (ppm)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77.48
77.16
76.84
50.19
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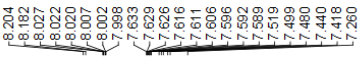
f1 (ppm)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8.182
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8.022
8.020
8.007
8.002
7.998
7.633
7.629
7.626
7.616
7.611
7.606
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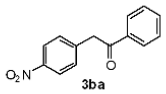
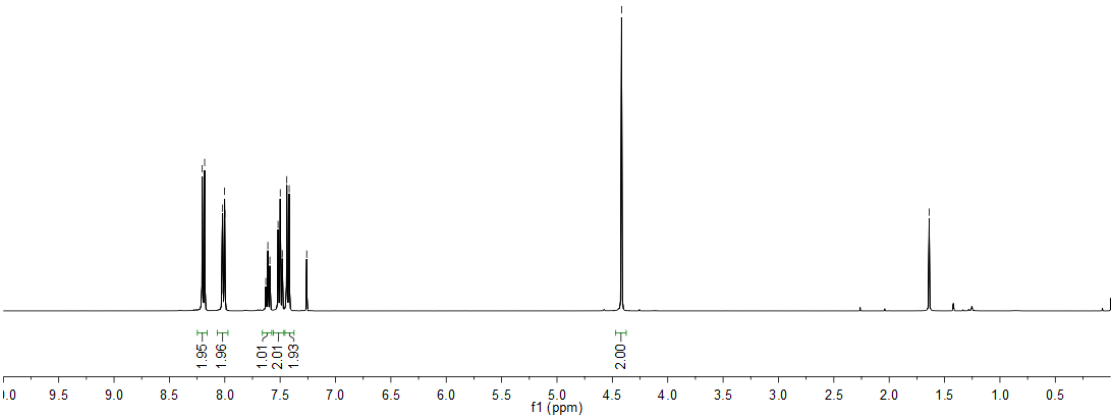
7.589
7.519
7.499
7.480
7.440
7.418
7.260
4.417
1.639


O2N
O
3ba


1.95
1.96
1.01
2.01
1.93
2.00
f1 (ppm)


196.12
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129.00
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123.85
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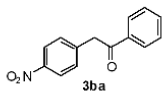
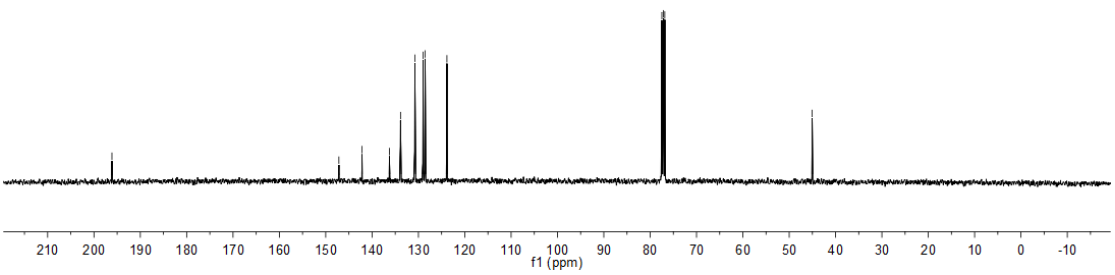
77.16
76.84
45.05


O2N
O
3ba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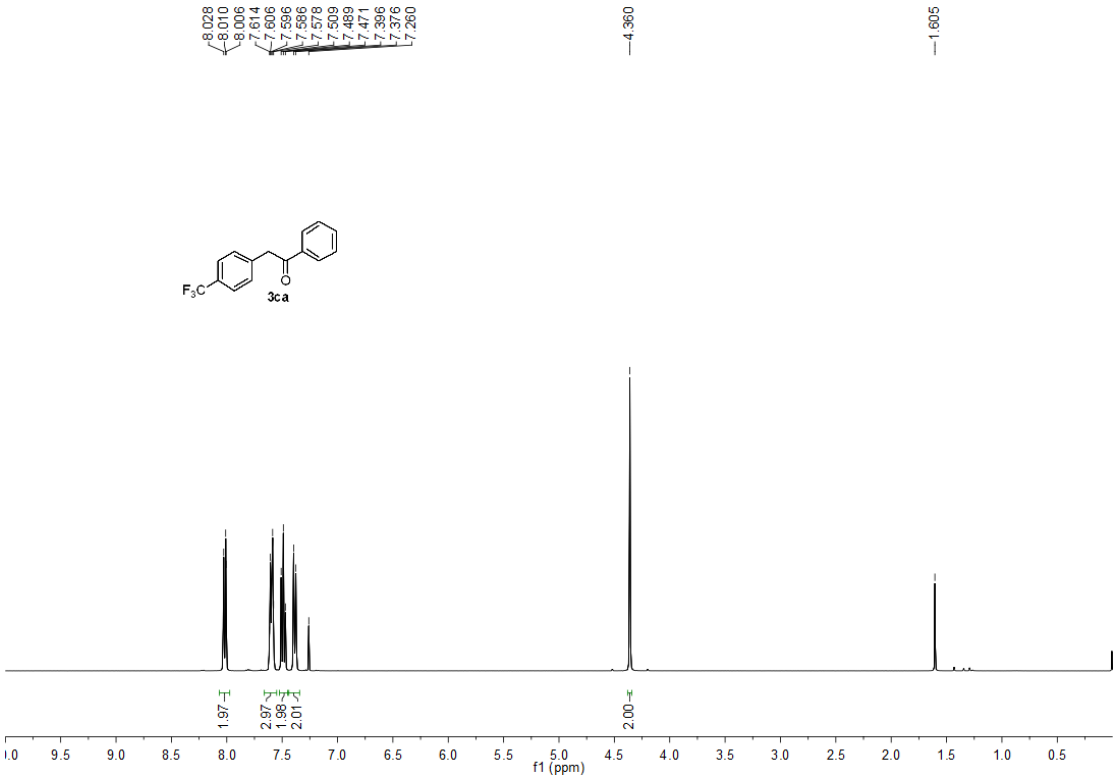
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7.471
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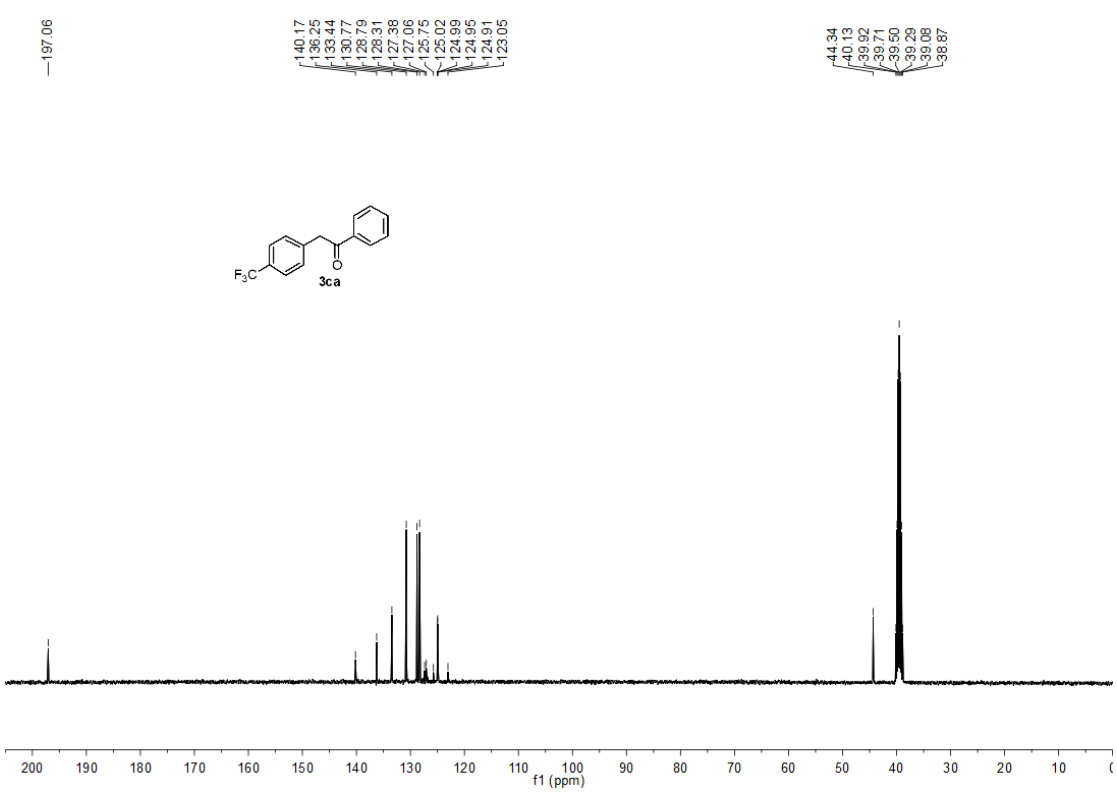
1.605
3ca
1.97
2.97
1.98
2.01
2.00
f1 (ppm)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39.71
39.50
39.29
39.08
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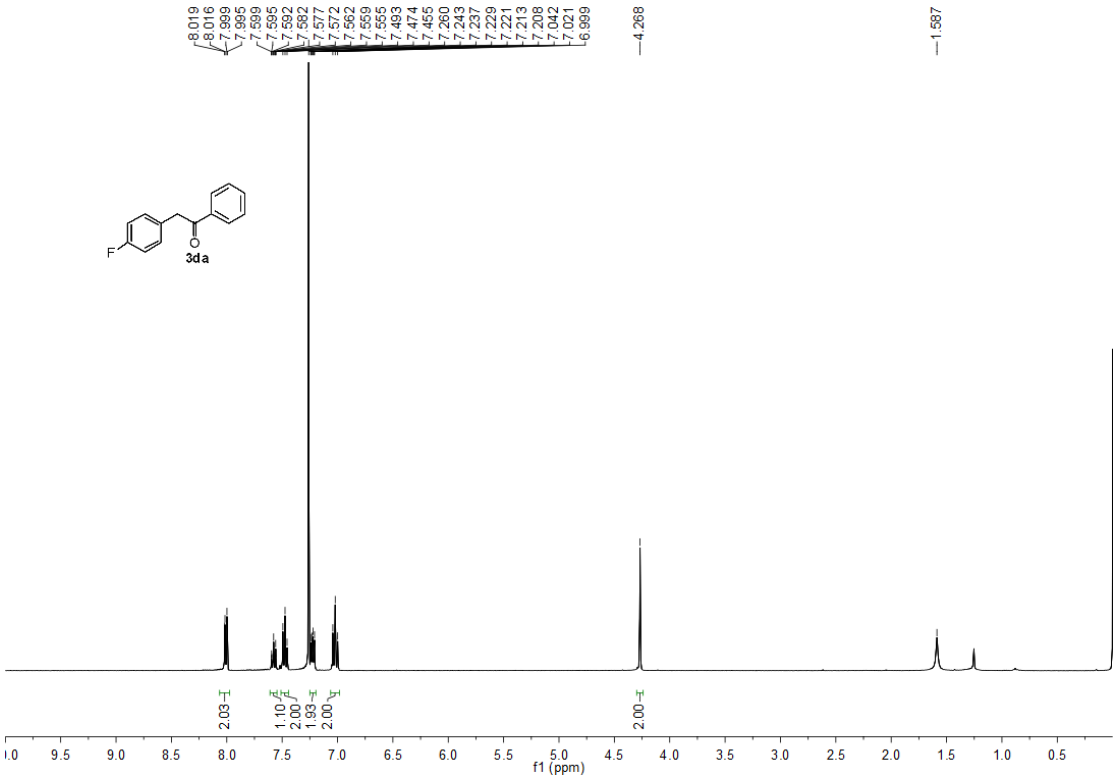
3ca
f1 (ppm)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7.455
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7.243
7.237
7.229
7.221
7.213
7.208
7.042
7.021
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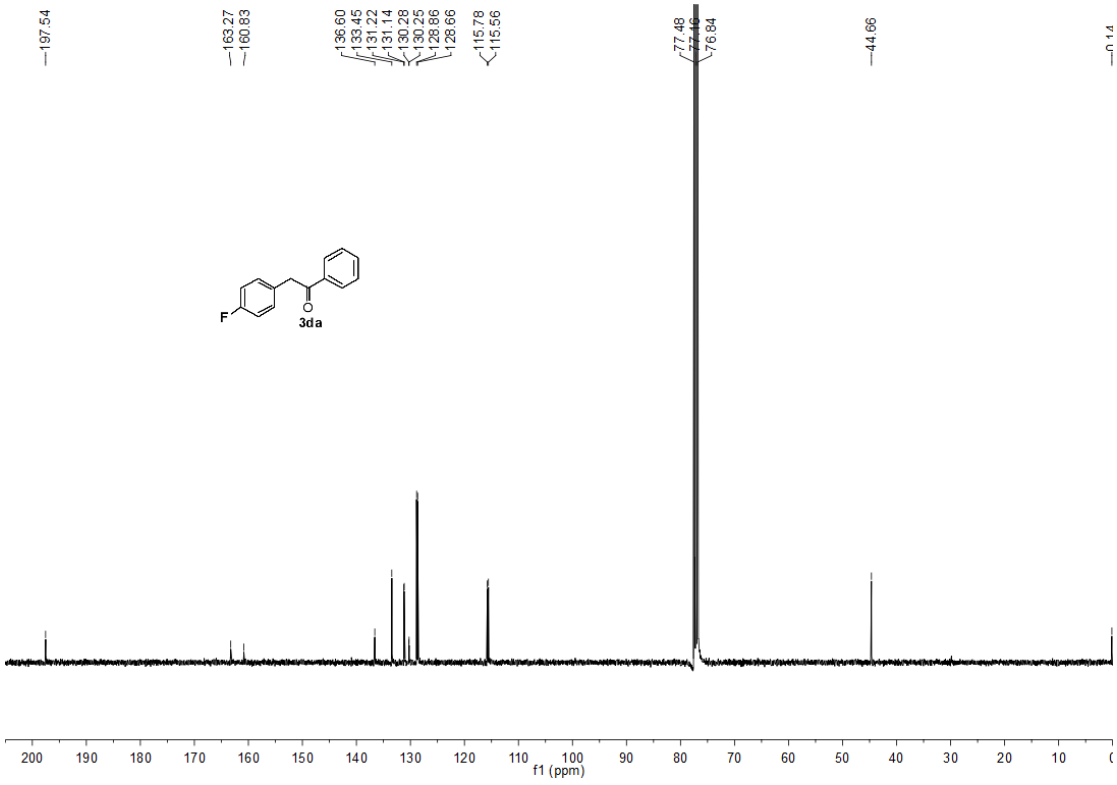
F
O
3da
2.03
1.10
2.00
1.93
2.00
2.00
f1 (ppm)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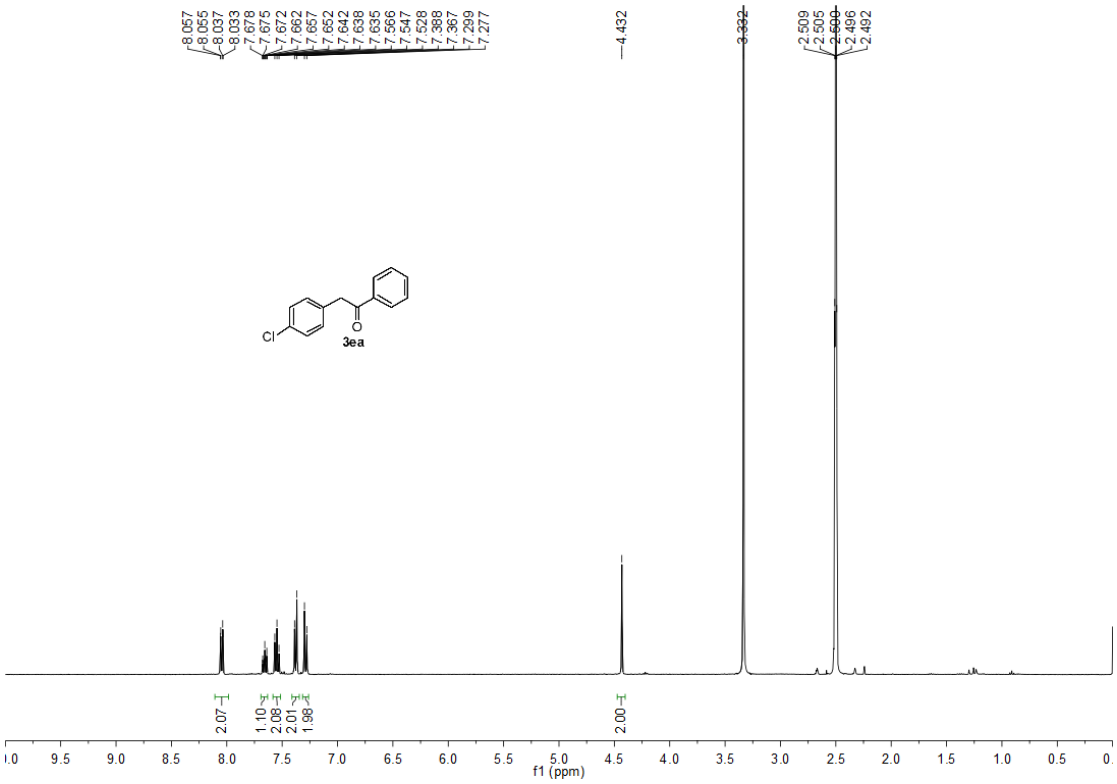
76.84
44.66
F
O
3da
f1 (ppm)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7.635
7.566
7.547
7.528
7.388
7.367
7.299
7.277
4.432
3.332
2.509
2.505
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2.496
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Cl
O
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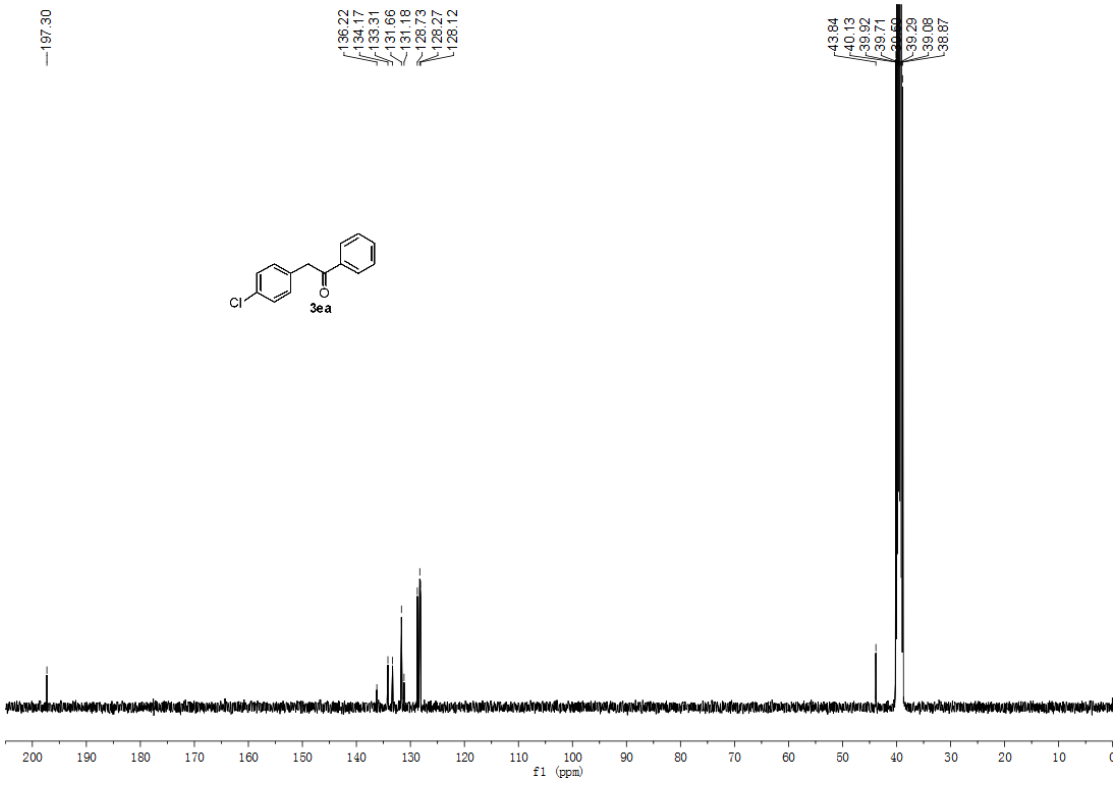
2.08
2.01
1.98
2.00
f1 (ppm)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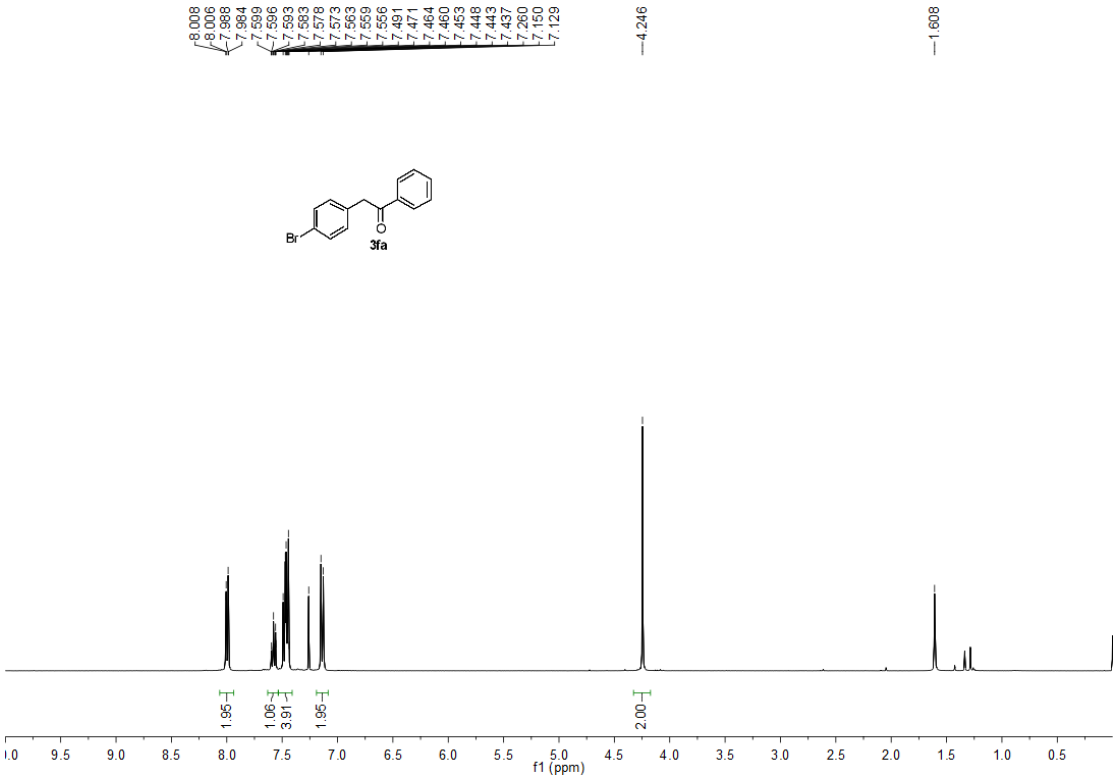
39.29
39.08
38.87
Cl
O
3ea
f1 (ppm)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7.556
7.491
7.471
7.464
7.460
7.453
7.448
7.443
7.437
7.260
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Br
O
3fa
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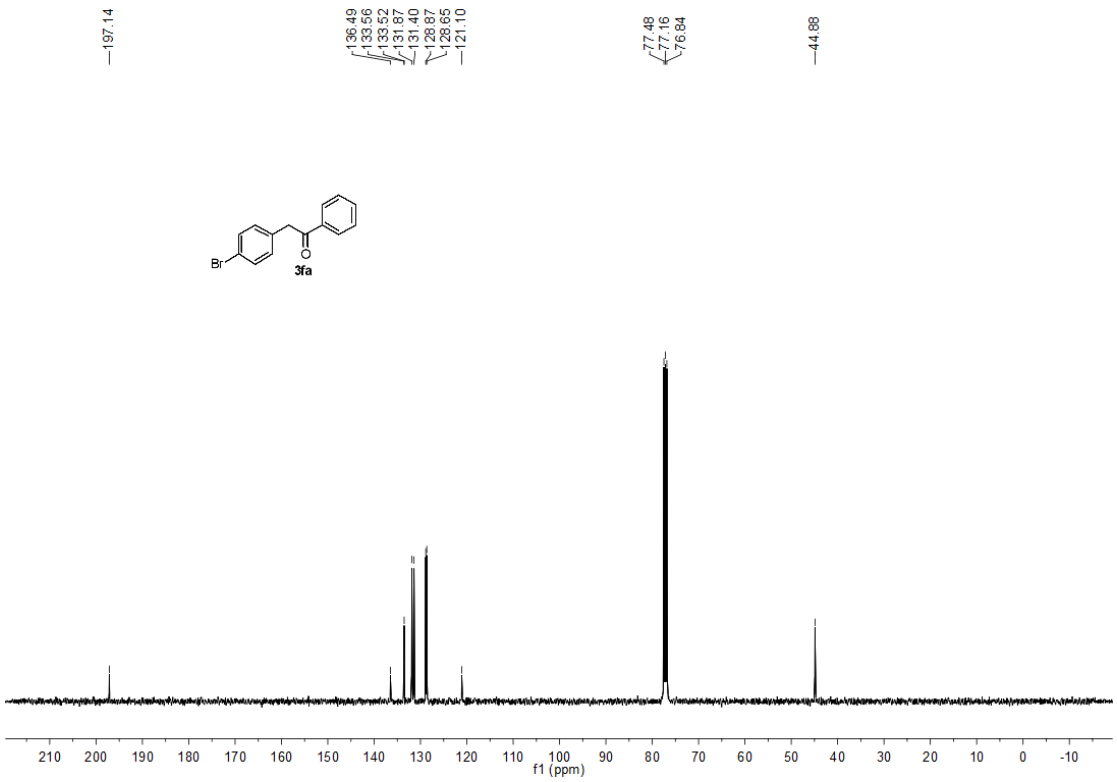
1.06
3.91
1.95
2.00
f1 (ppm)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44.88
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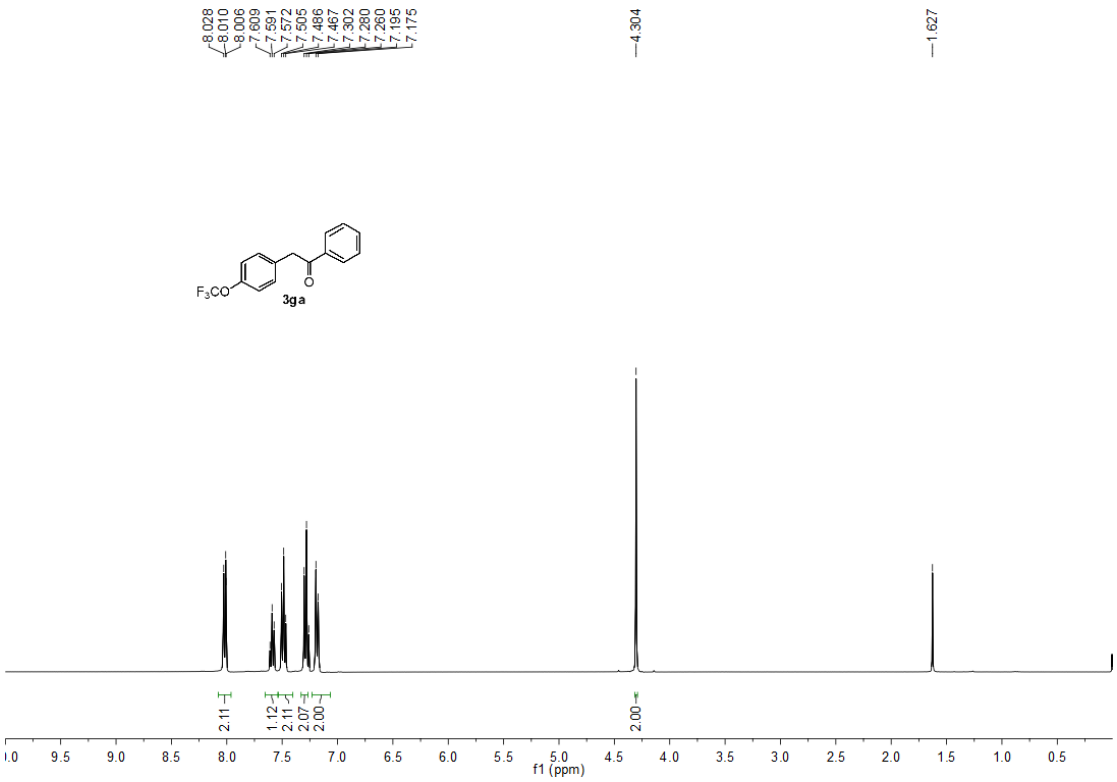
O
3fa
f1 (ppm)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7.175
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O
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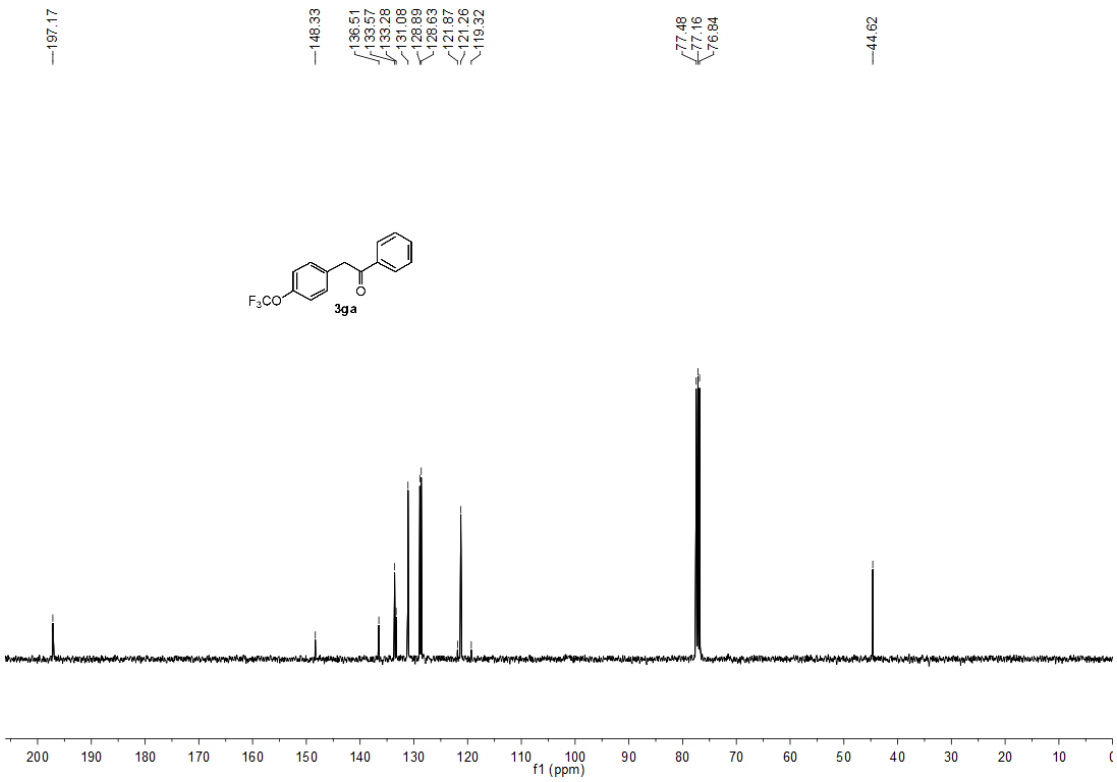
2.11
1.12
2.11
2.07
2.00
2.00
f1 (ppm)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77.16
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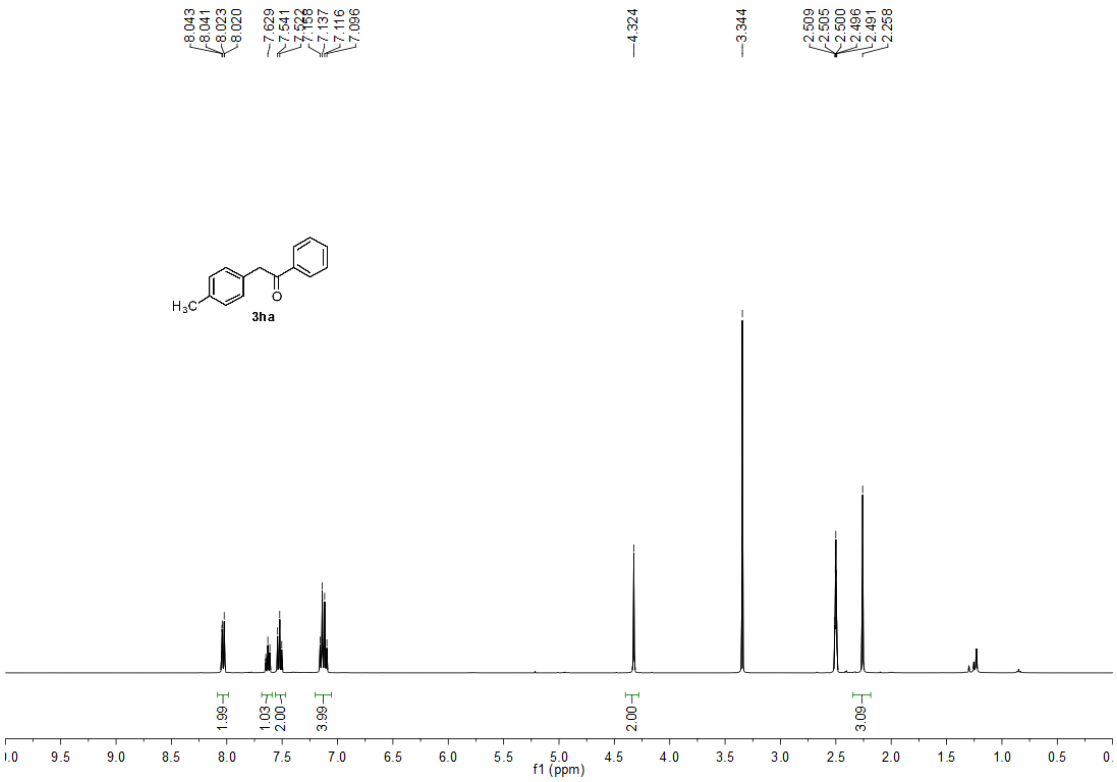
44.62
F3CO
O
3ga
f1 (ppm)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3.344
2.509
2.505
2.500
2.496
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H3C
O
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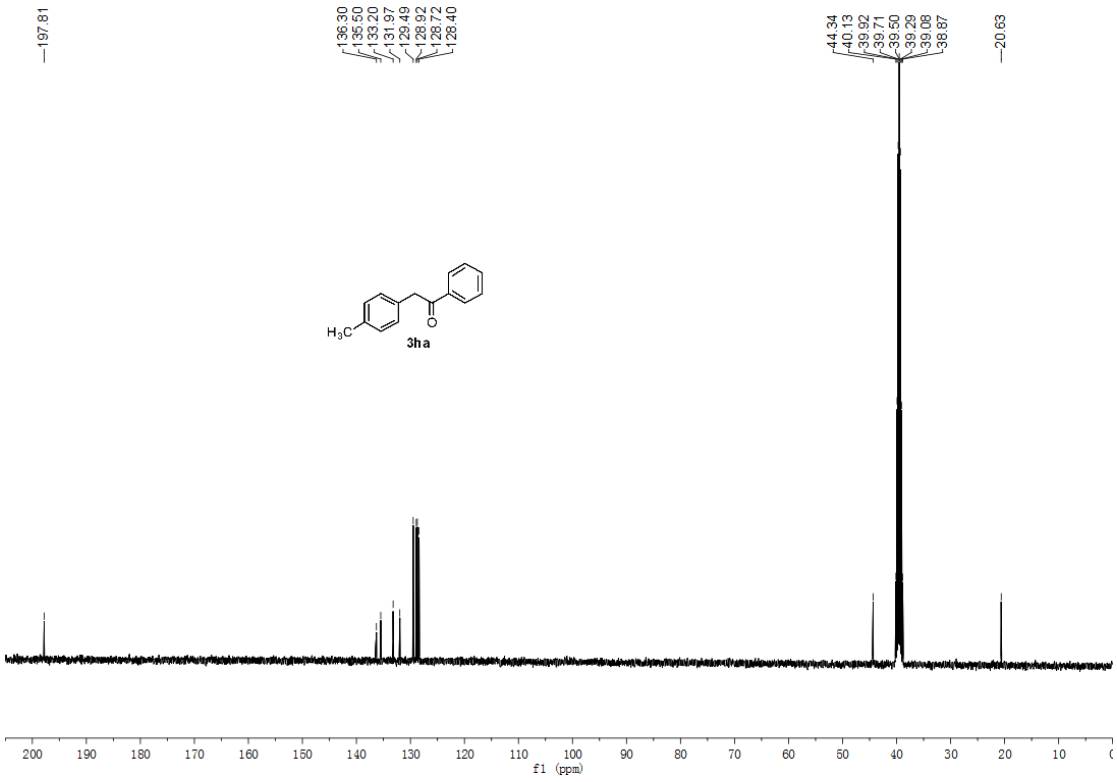
1.03
2.00
3.99
2.00
3.09
f1 (ppm)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39.08
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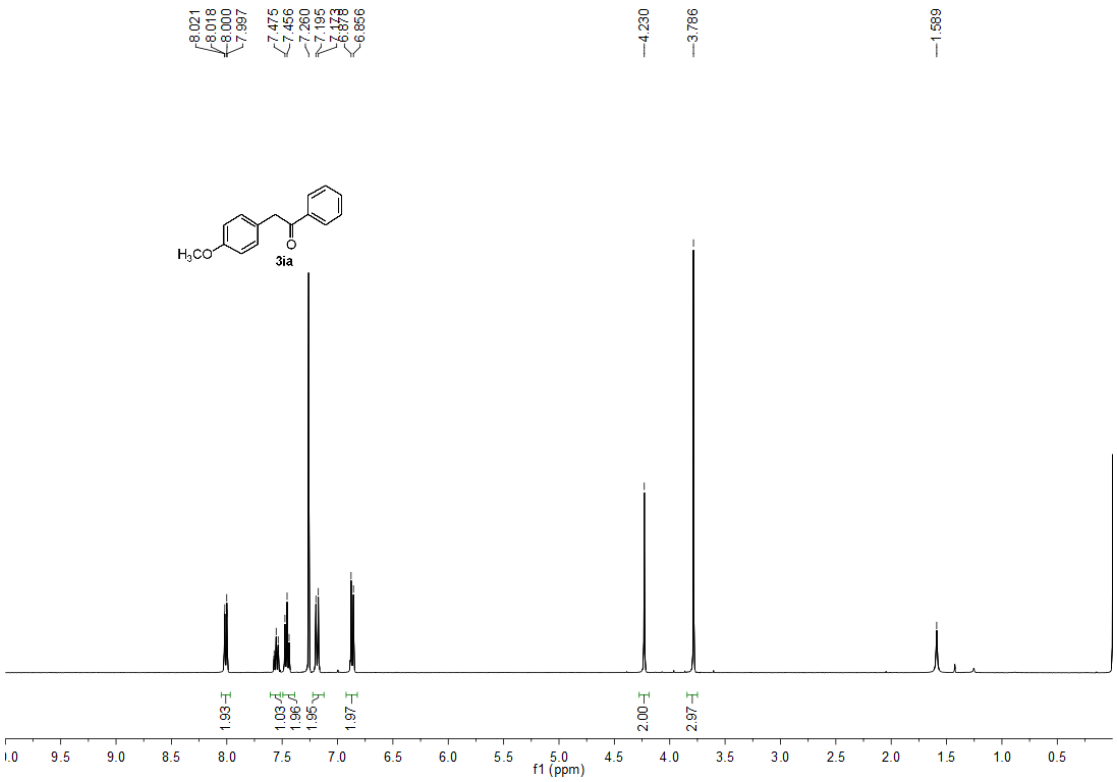
20.63
H3C
O
3ha
f1 (ppm)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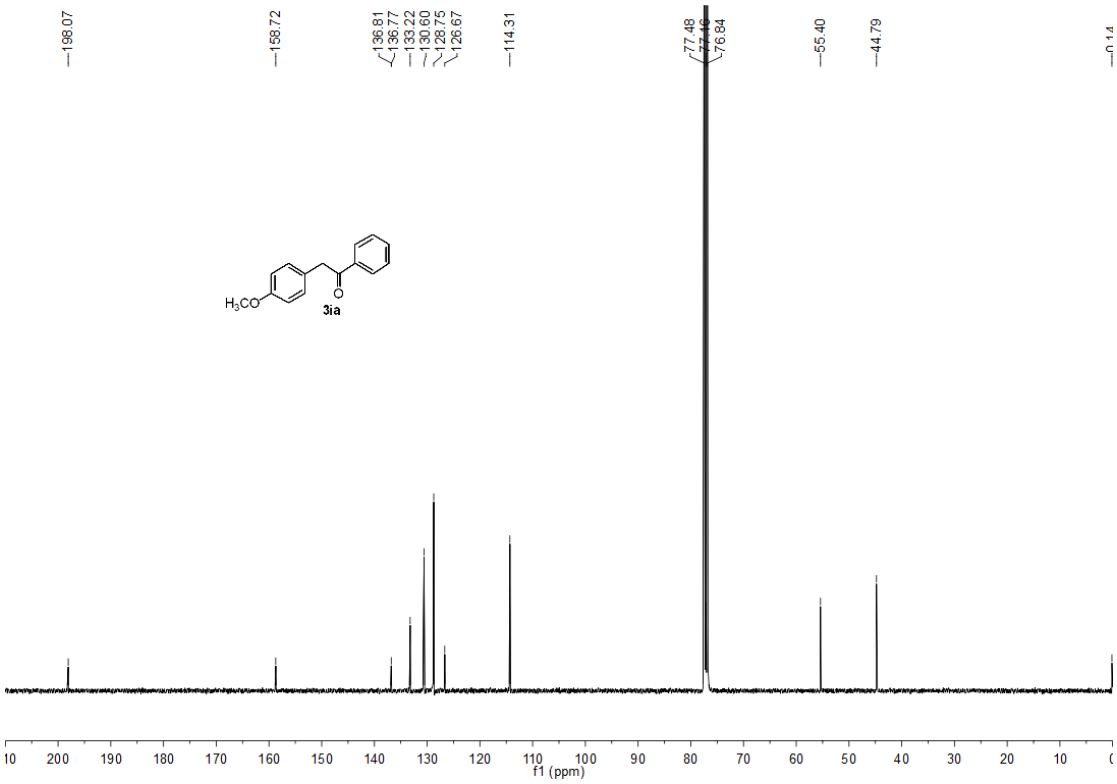
1.97
2.00
2.97
f1 (ppm)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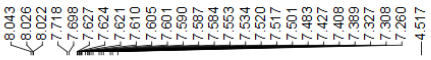
H3CO
3ia
f1 (ppm)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7.587
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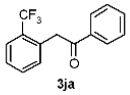
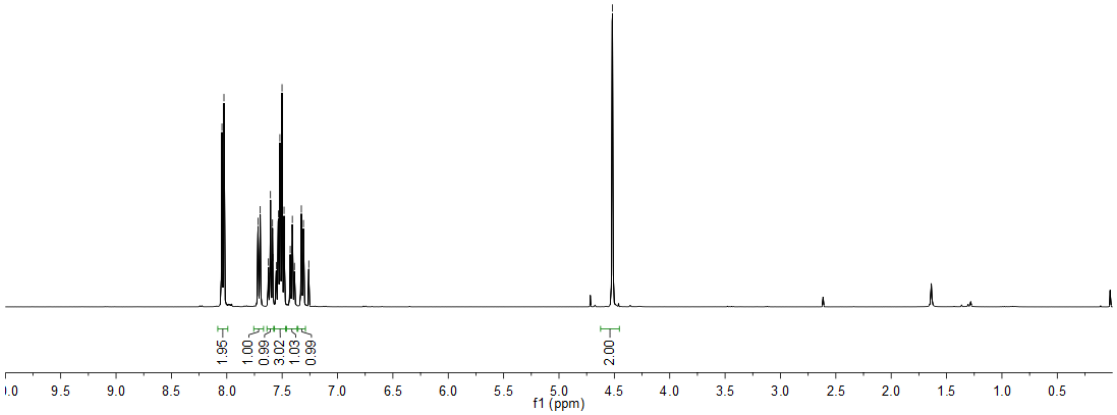

CF3
O

3ja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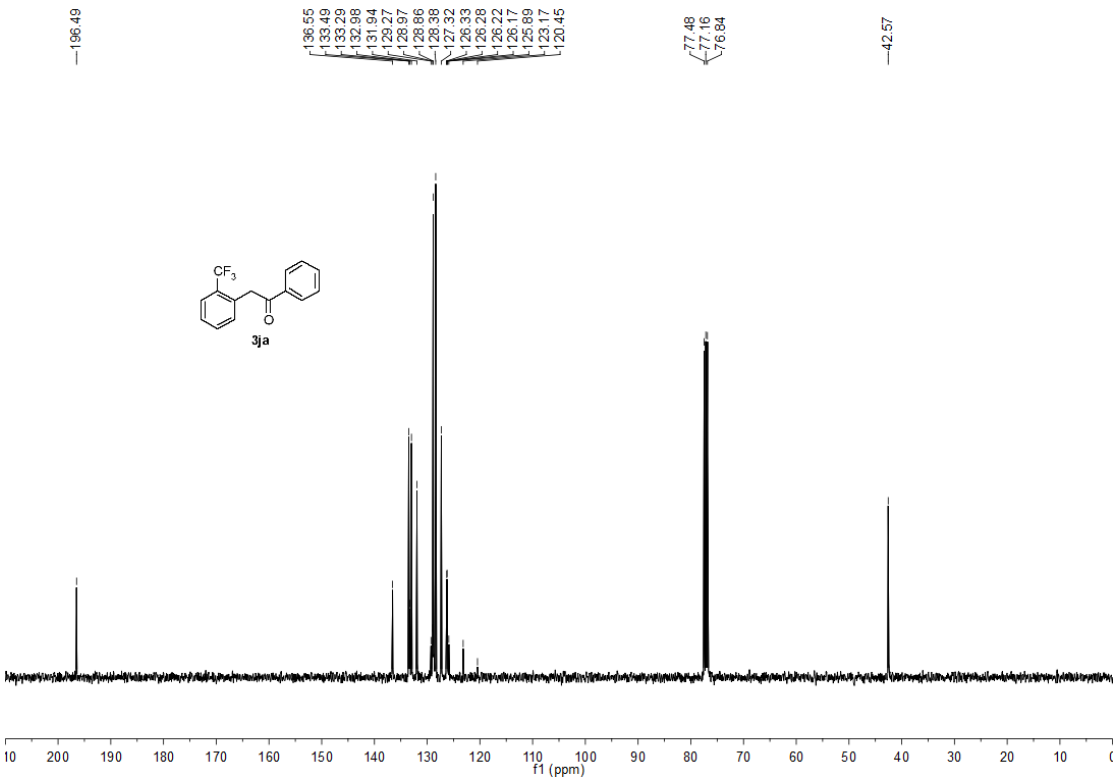
2.00
f1 (ppm)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126.33
126.28
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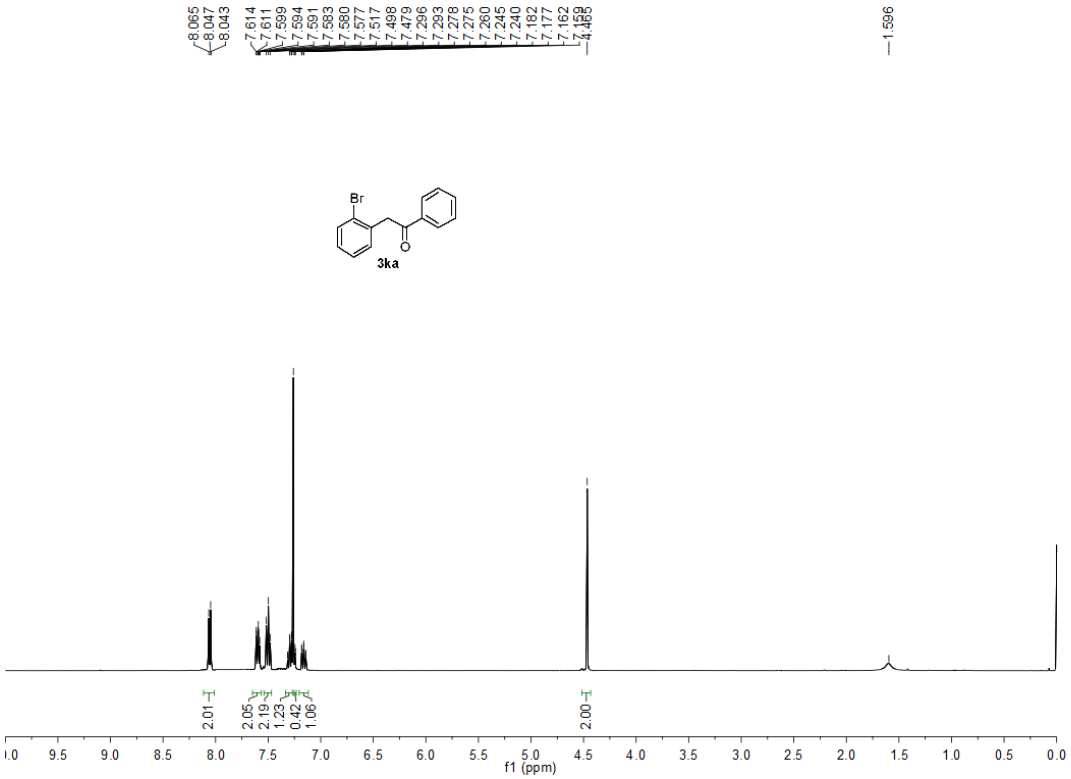
123.17
120.45
77.48
77.16
76.84
42.57
f1 (ppm)

CF3
O

3ja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7.293
7.278
7.275
7.260
7.245
7.240
7.182
7.177
7.162
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O
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0.42
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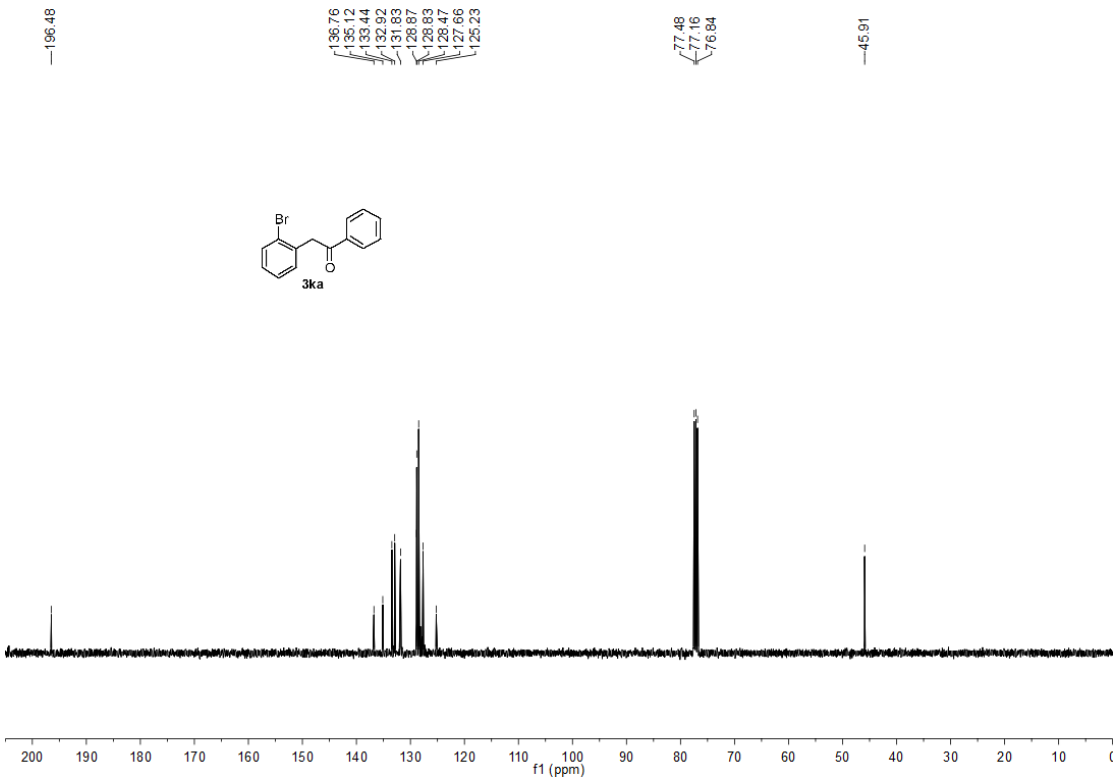
2.00
f1 (ppm)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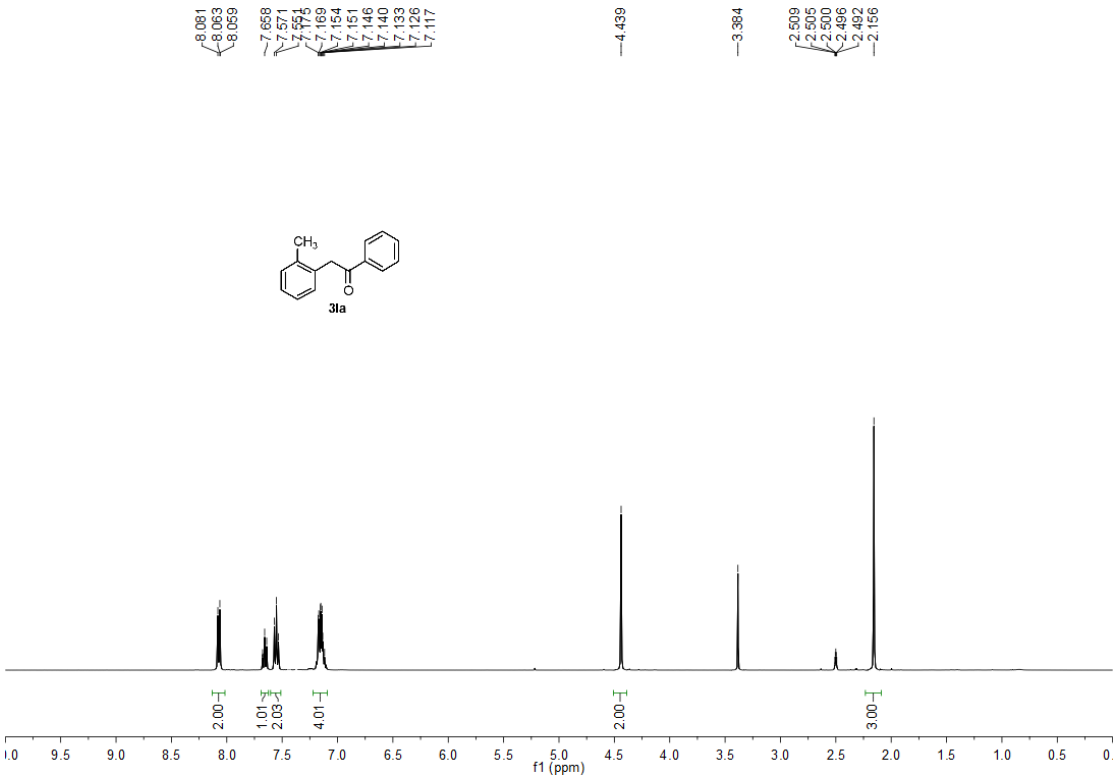
77.48
77.16
76.84
45.91
Br
O
3ka
f1 (ppm)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7.117
4.439
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2.509
2.505
2.500
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CH3
O
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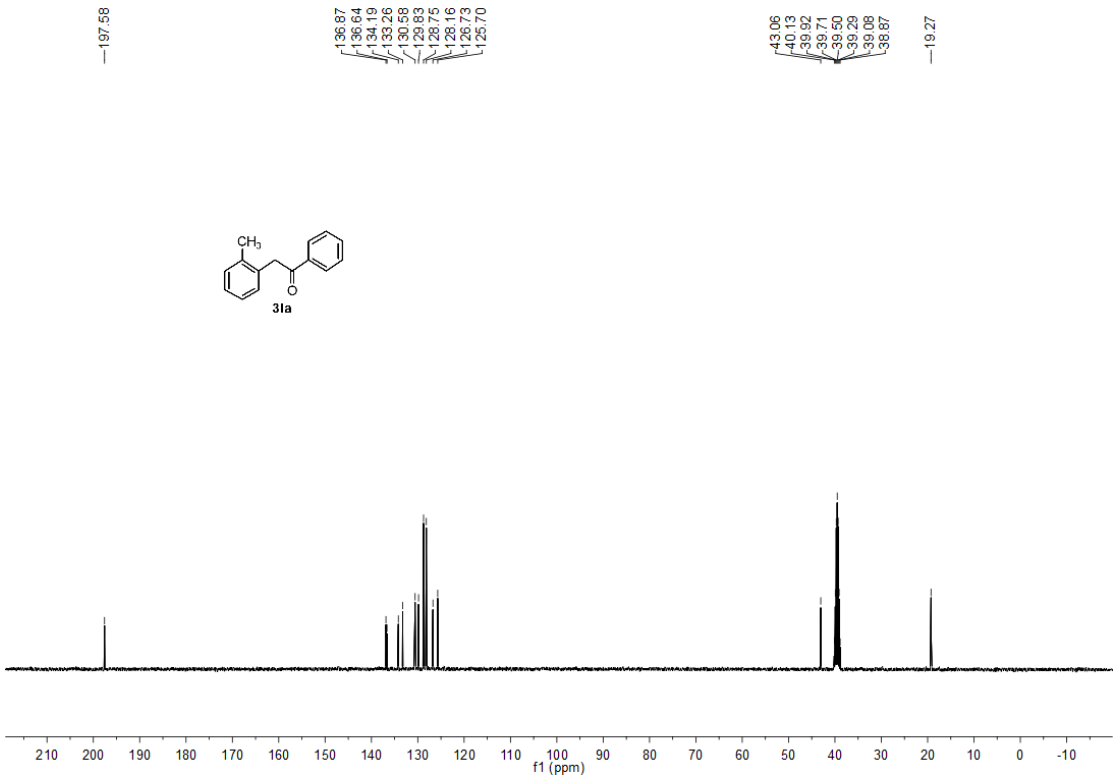
3.00
f1 (ppm)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39.29
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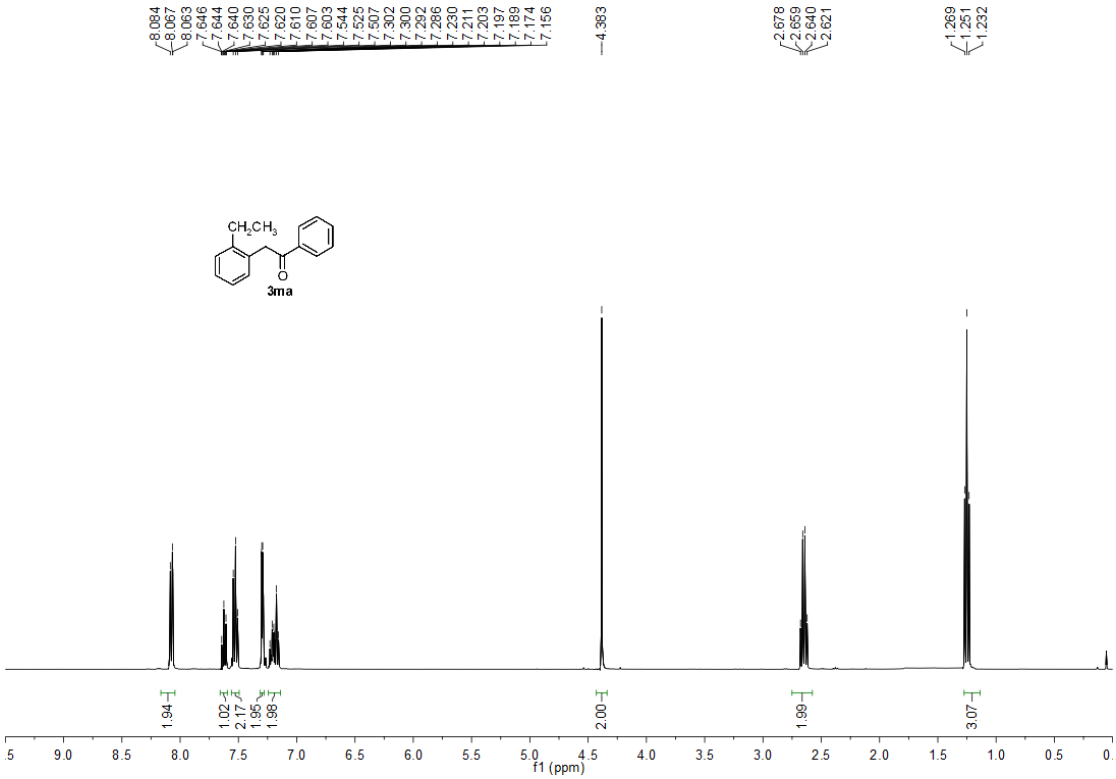
19.27
CH3
O
3la
f1 (ppm)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7.174
7.156
4.383
2.678
2.659
2.640
2.621
1.269
1.251
1.232
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1.98
2.00
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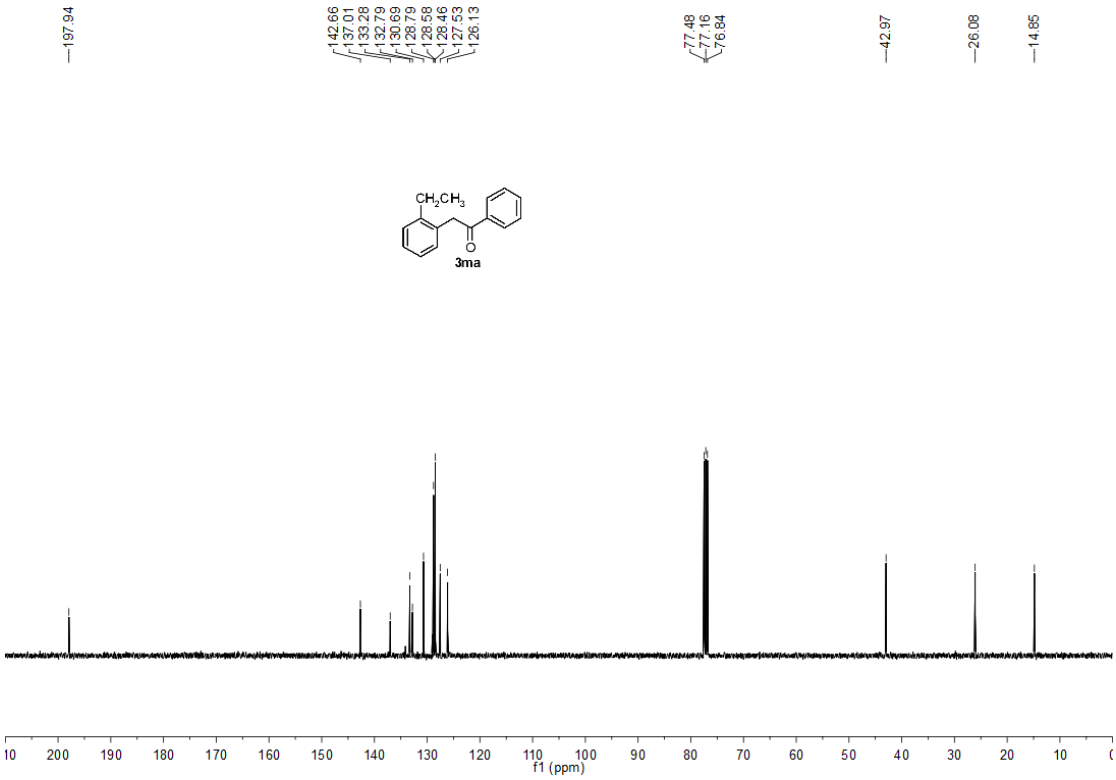
3.07
f1 (ppm)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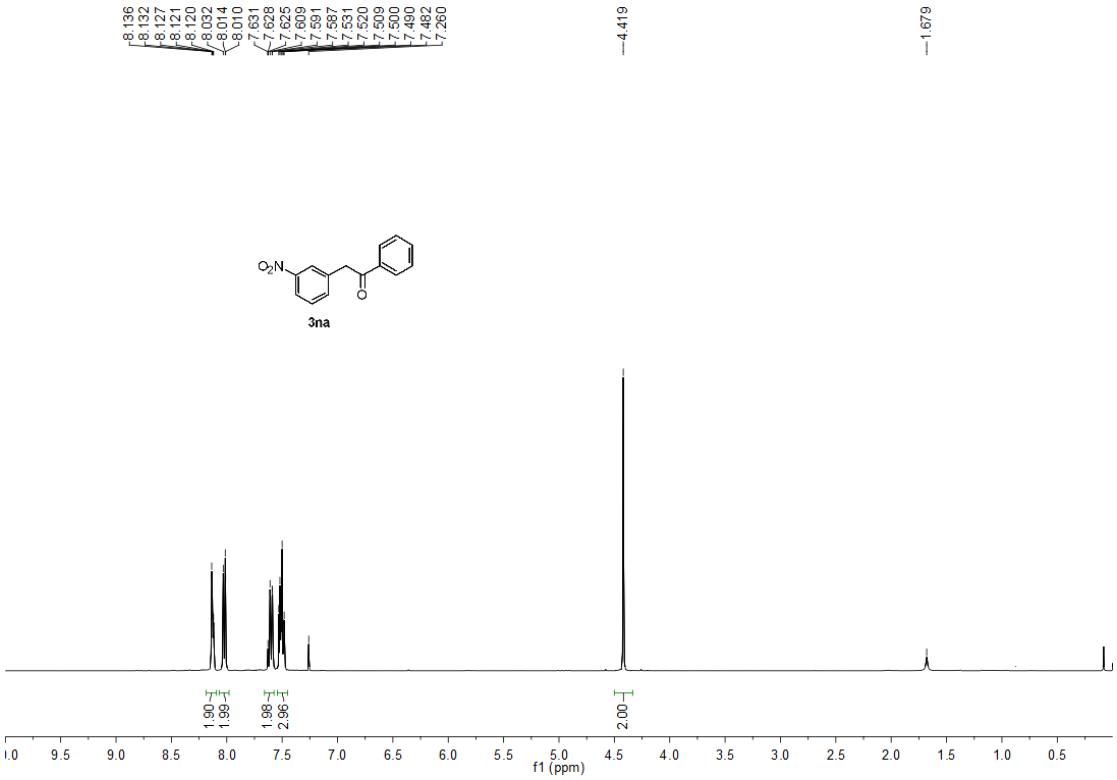
42.97
26.08
14.85
CH2CH3
O
3ma
f1 (ppm)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7.587
7.531
7.520
7.509
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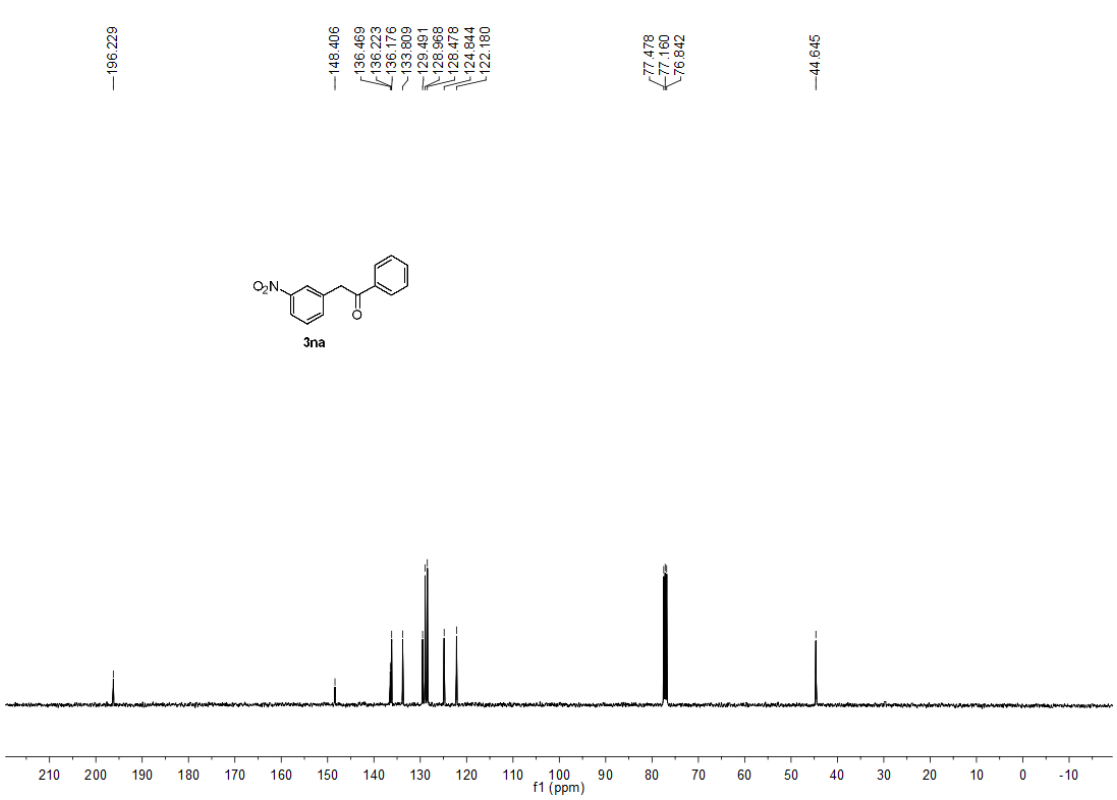
2.00
f1 (ppm)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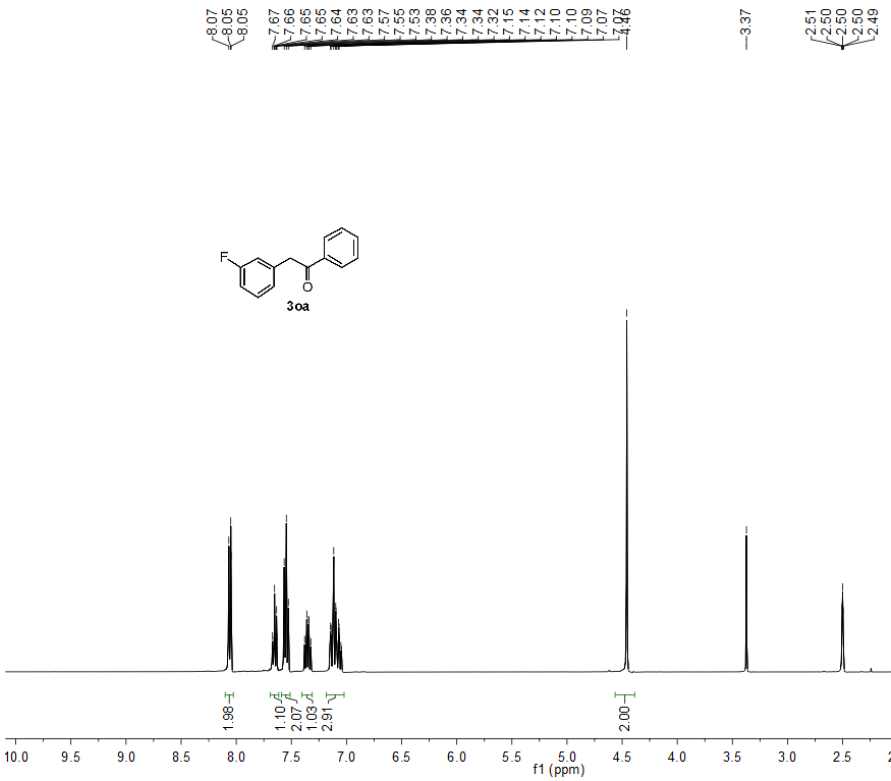
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7.07
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4.06
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2.51
2.50
2.50
2.50
2.49
F
O
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1.98
1.10
2.07
1.03
2.91
2.00
10.0 9.5 9.0 8.5 8.0 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
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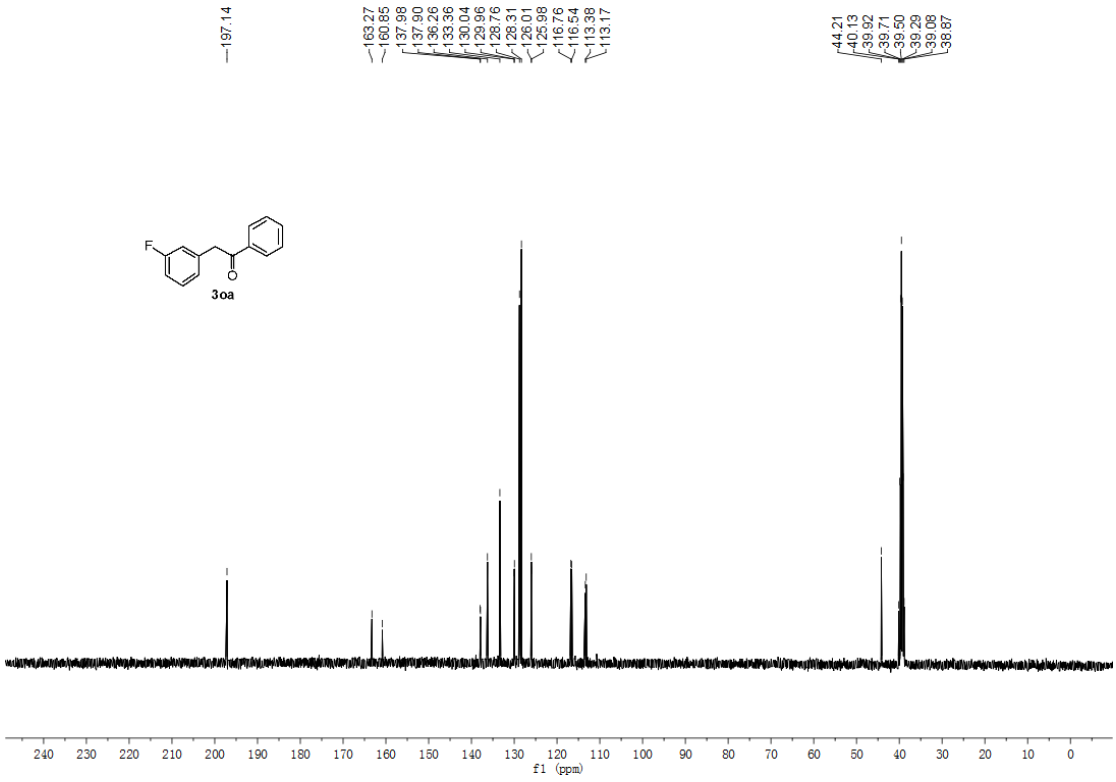
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116.54
113.38
113.17
44.21
40.13
39.92
39.71
39.50
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38.87
F
O
3oa
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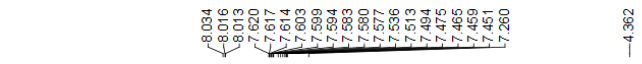
f1 (ppm)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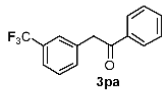
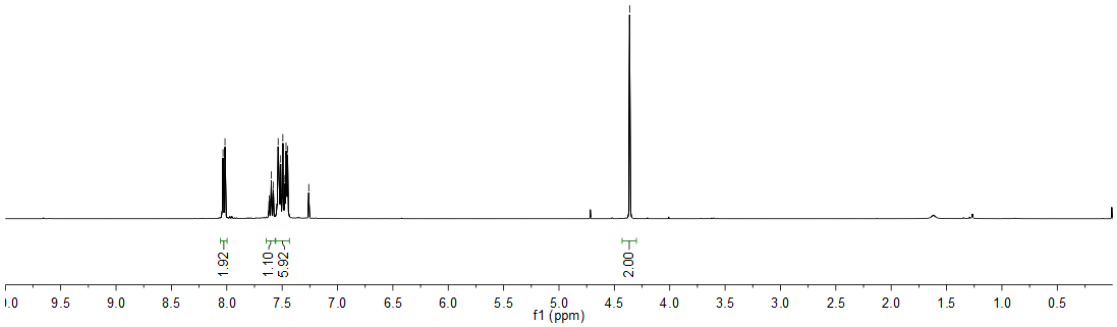

F3C
O

3pa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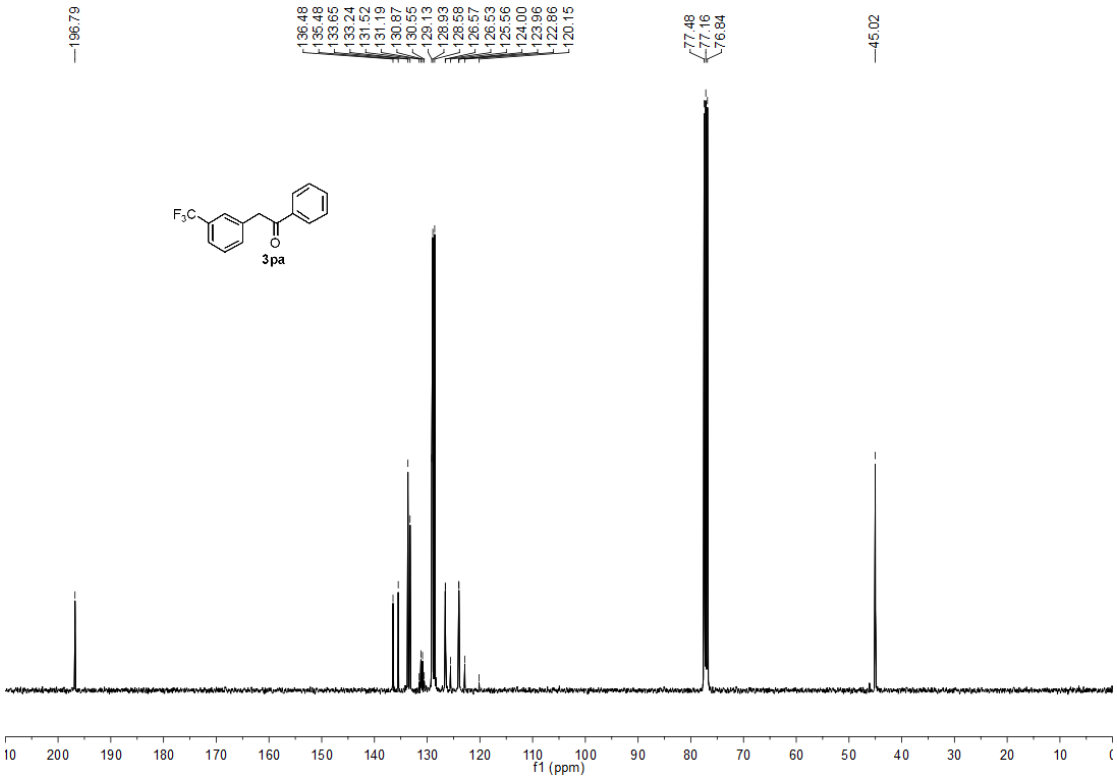
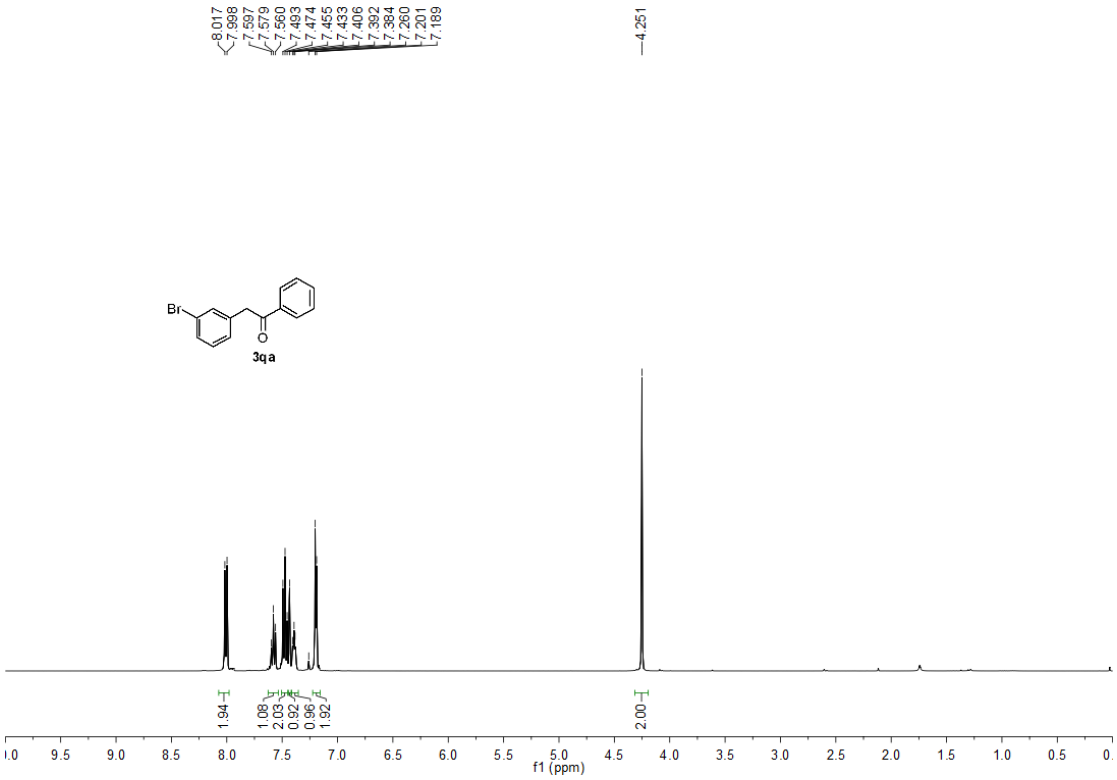

196.79
136.48
135.48
133.65
133.24
131.52
131.19
130.87
130.55
129.13
128.93
128.58
126.57
126.53
125.56
124.00
123.96
122.86
120.15
77.48
77.16
76.84
45.02
F3C
O
f1 (ppm)

3pa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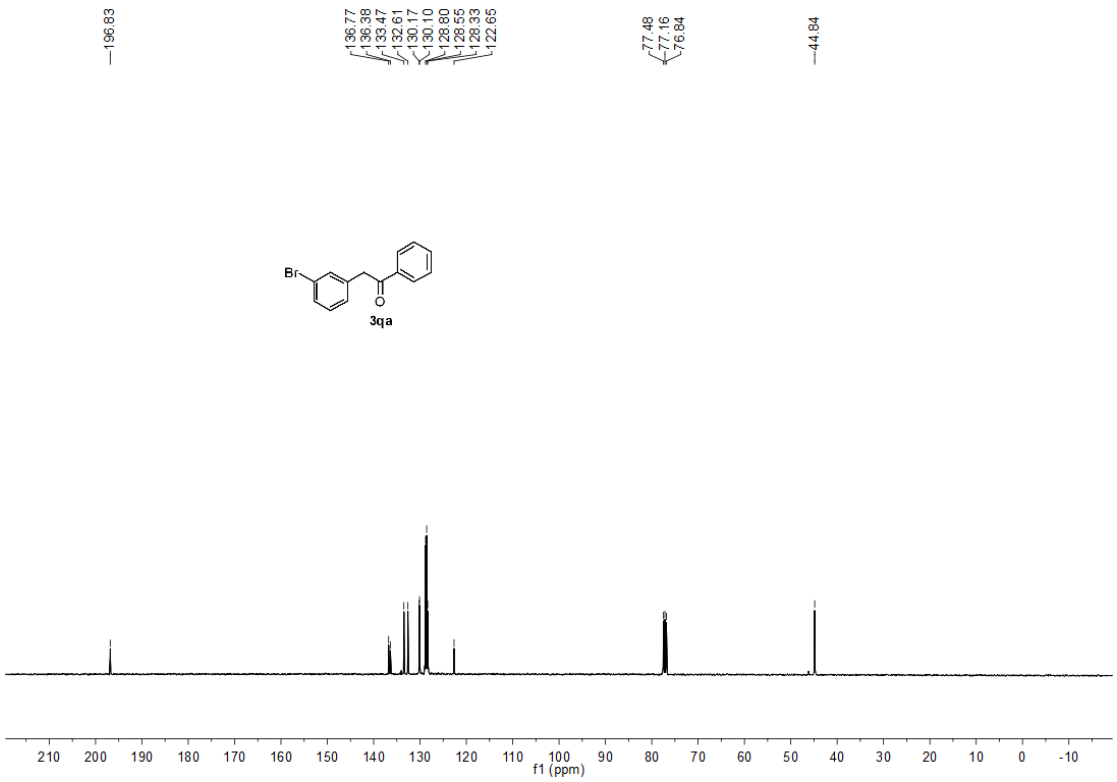
7.597
7.579
7.560
7.493
7.474
7.455
7.433
7.406
7.392
7.384
7.260
7.201
7.189
4.251
Br
O
3qa
1.94
1.08
2.03
0.92
0.96
1.92
2.00
f1 (ppm)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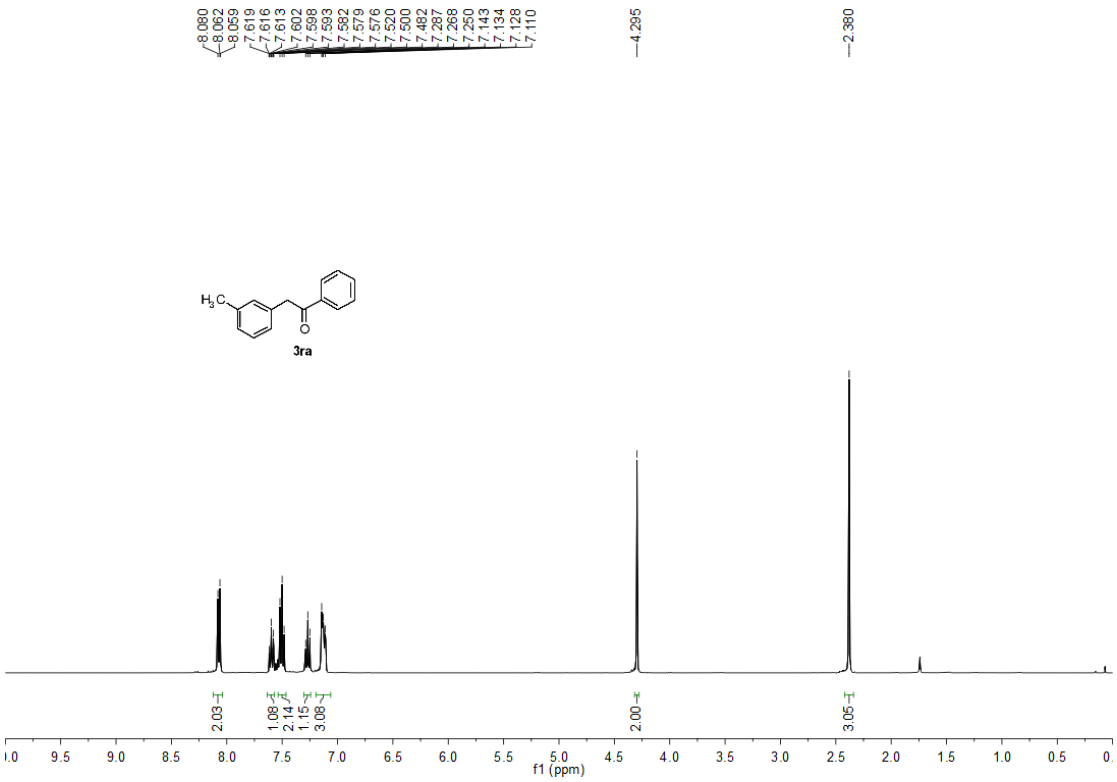
136.38
133.47
132.61
130.17
130.10
128.80
128.55
128.33
122.65
77.48
77.16
76.84
44.84
Br
O
3qa
f1 (ppm)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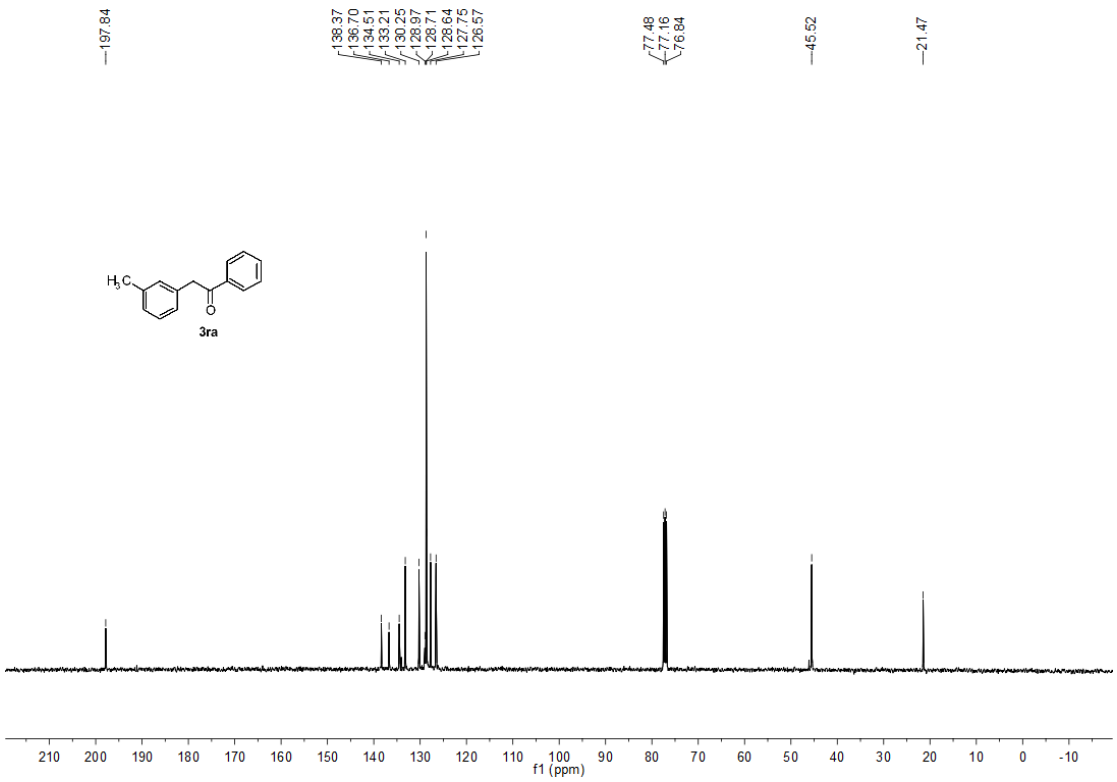
8.062
8.059
7.619
7.616
7.613
7.602
7.598
7.593
7.582
7.579
7.576
7.520
7.500
7.482
7.287
7.268
7.250
7.143
7.134
7.128
7.110
4.295
2.380
3ra
2.03
1.08
2.14
1.15
3.08
2.00
3.05
f1 (ppm)


197.84
138.37
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133.21
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128.71
128.64
127.75
126.57
77.48
77.16
76.84
45.52
21.47
3ra
f1 (ppm)

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