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Supporting Information

Oxidative C(sp^3)-H Functionalization of Acetonitrile and Alkanes with Allylic Alcohols Under Metal-Free Conditions

Xue-Qiang Chu, Hua Meng, You Zi, Xiao-Ping Xu,* Shun-Jun Ji*

Key Laboratory of Organic Synthesis of Jiangsu Province, College of Chemistry, Chemical Engineering and Materials Science & Collaborative Innovation Center of Suzhou Nano Science and Technology, Soochow University, Suzhou, 215123, People's Republic of China.

Fax : (+86)-512-65880307; phone: (+86)- 512-65880307; E-mail: xuxp@suda.edu.cn; shunjun@suda.edu.cn

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EXPERIMENTAL SECTION

General Information: Unless otherwise stated, all reagents were purchased from commercial suppliers and used without further purification. All reactions were carried out in air and using undistilled solvent, without need of precautions to exclude air and moisture unless otherwise noted. Melting points were recorded on an Electrothermal digital melting point apparatus. IR spectra were recorded on a FT-IR spectrophotometer using KBr optics. ^{1}H, ^{13}C NMR spectra were recorded in $CDCl_3$ on 400 MHz spectometers. Tetramethylsilane (TMS) served as internal standard for ^{1}H NMR and ^{13}C NMR. High resolution mass spectra were obtained using a commercial apparatus (ESI or EI Source).

General procedure for oxidative addition of acetonitrile to α,α-diaryl allylic alcohols:

α,α-diaryl allylic alcohol **1** (0.3 mmol), nitrile **2** (3 mL) and *tert*-butylperoxybenzoate (0.6 mmol) was stirred at 120 ºC for 12 h. Upon completion of the reaction (indicated by TLC), solvent was removed in vacuum and the residue was purified by flash silica gel column chromatography purification afforded pure product **4** with petroleum ether/ethyl acetate as the eluent.

General procedure for oxidative addition of alkanes to α,α-diaryl allylic alcohols:

α,α-diaryl allylic alcohol **1** (0.3 mmol), alkane **3** (4 mL) and *tert*-butylperoxybenzoate (0.6 mmol) was stirred at 120 ºC for 7 h. Upon completion of the reaction (indicated by TLC), solvent was removed in vacuum and the residue was purified by flash silica gel column chromatography purification to afford pure product **5** with petroleum ether/ethyl acetate as the eluent.

General procedure for the synthesis of 6: 5-oxo-4,5-diphenylpentanenitrile **4aa** (0.5 mmol), concentrated sulfuric acid (0.55 mmol) in 3 mL glacial acetic acid was stirred at refluxing over night. Upon completion of the reaction (indicated by TLC), a saturated aqueous $NaHCO_3$ solution was added and the mixture was extracted with ethyl acetate (5 mL×3). The combined organic extracts were dried with sodium sulfate and concentrated. The pure product **6** was obtained after purification (silica gel, methyl alcohol/chloroform, 1:10).

General procedure for the synthesis of 7: 0.5 mmol of 5-oxo-4,5-diphenylpentanenitrile **4aa** was dissolved in 10.0 mL dry THF. Then 2.5 mmol of $LiAlH_4$ was added at room temperature. After 10 minutes, the reaction mixture was heated to refulx for 1h. Upon completion of the reaction (indicated by TLC), a saturated aqueous NH_4Cl solution was added and the mixture was extracted with ethyl acetate (5 mL×3). The combined organic extracts were dried with sodium sulfate and concentrated. The pure product **7** was obtained after purification (silica gel, petroleum ether/ethyl acetate).

Analytical and spectral data for compounds:

5-oxo-4,5-diphenylpentanenitrile (4aa): Yield = 87% (65 mg). Yellow soild (M.p. 83.1–83.8 °C). IR (KBr) ν = 2938, 2246, 1667, 1595, 1448, 1263, 1199, 988, 754, 694, 661 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.98–7.93 (m, 2H), 7.52–7.46 (m, 1H), 7.41–7.36 (m, 2H), 7.35–7.29 (m, 4H), 7.27–7.23 (m, 1H), 4.73 (t, J = 7.2 Hz, 1H), 2.49–2.35 (m, 2H), 2.30–2.15 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 198.4, 137.7, 136.2, 133.5, 129.6, 129.0, 128.8, 128.3, 128.0, 119.5, 52.1, 29.2, 15.4 ppm. HRMS m/z: calcd for $C_{17}H_{16}NO$ $[M+H]^+$ 250.1232, found: 250.1229.

4,5-bis(4-fluorophenyl)-5-oxopentanenitrile (4ba): Yield = 81% (72 mg). Yellow oil. IR (KBr) ν = 2955, 2924, 2246, 1684, 1595, 1507, 1257, 1222, 1152, 830, 766 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 8.00–7.93 (m, 2H), 7.30–7.25 (m, 2H), 7.12–6.97 (m, 4H), 4.69 (t, J = 7.2 Hz, 1H), 2.49–2.38 (m, 2H), 2.31–2.20 (m, 1H), 2.20–2.09 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 196.7, 166.0 (d, $J_{C\text{-}F}$ = 254.5 Hz), 162.5 (d, $J_{C\text{-}F}$ = 246.1 Hz), 133.3 (d, $J_{C\text{-}F}$ = 3.3 Hz), 132.3 (d, $J_{C\text{-}F}$ = 3.1 Hz), 131.7 (d, $J_{C\text{-}F}$ = 9.4 Hz), 129.9 (d, $J_{C\text{-}F}$ = 8.1 Hz), 119.3, 116.7 (d, $J_{C\text{-}F}$ = 21.5 Hz), 116.1 (d, $J_{C\text{-}F}$ = 21.8 Hz), 51.2, 29.2, 15.3 ppm. HRMS m/z: calcd for $C_{17}H_{14}F_2NO$ $[M+H]^+$ 286.1043, found: 286.1051.

4,5-bis(4-chlorophenyl)-5-oxopentanenitrile (4ca): Yield = 82% (79 mg). Yellow oil. IR (KBr) ν = 2969, 2926, 2246, 1679, 1587, 1489, 1399, 1091, 1031, 806, 743 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.89–7.83 (m, 2H), 7.41–7.35 (m, 2H), 7.34–7.29 (m, 2H), 7.25–7.19 (m, 2H), 4.67 (t, J = 7.2 Hz, 1H), 2.49–2.37 (m, 2H), 2.31–2.20 (m, 1H), 2.19–2.08 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 196.8, 140.3, 135.9, 134.3, 134.2, 130.4, 130.0, 129.6, 129.3, 119.2, 51.4, 29.0, 15.4 ppm. HRMS m/z: calcd for $C_{17}H_{14}Cl_2NO$ $[M+H]^+$ 318.0452, found: 318.0450.

4,5-bis(4-bromophenyl)-5-oxopentanenitrile (4da): Yield = 77% (93 mg). Yellow oil. IR (KBr) ν = 2938, 2245, 1678, 1583, 1486, 1395, 1257, 1173, 1070, 1009, 802, 733 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.81–7.75 (m, 2H), 7.57–7.52 (m, 2H), 7.49–7.44 (m, 2H), 7.18–7.14 (m, 2H), 4.65 (t, J = 7.2 Hz, 1H), 2.49–2.37 (m, 2H), 2.30–2.20 (m, 1H), 2.18–2.08 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.0, 136.4, 134.6, 132.9, 132.3, 130.5, 129.9, 129.1, 122.4, 119.2, 51.5, 28.9, 15.4 ppm. HRMS m/z: calcd for $C_{17}H_{14}Br_2NO$ $[M+H]^+$ 405.9442, found: 405.9436.

5-oxo-4,5-dip-tolylpentanenitrile (4ea): Yield = 69% (58 mg). Yellow oil. IR (KBr) ν = 2942, 2867, 2244, 1673, 1605, 1510, 1261, 1174, 962, 808, 756 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.88–7.83 (m, 2H), 7.20–7.15 (m, 4H), 7.14–7.09 (m, 2H), 4.67 (t, J = 7.1 Hz, 1H), 2.47–2.36 (m, 2H), 2.34 (s, 3H), 2.28 (s, 3H), 2.27–2.10 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 198.1, 144.3, 137.7, 134.9, 133.7, 130.3, 129.5, 129.1, 128.2, 119.6, 51.6, 29.2, 21.8, 21.2, 15.4 ppm. HRMS m/z: calcd for $C_{19}H_{20}NO$ $[M+H]^+$ 278.1545, found: 278.1540.

4,5-bis(4-methoxyphenyl)-5-oxopentanenitrile (4fa): Yield = 58% (61 mg). Yellow oil. IR (KBr) ν = 2957, 2838, 2244, 1668, 1597, 1509, 1246, 1165, 1027, 832, 817 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.98–7.91 (m, 2H), 7.25–7.19 (m, 2H), 6.89–6.82 (m, 4H), 4.63 (t, J = 7.2 Hz, 1H), 3.82 (s, 3H), 3.76 (s, 3H), 2.46–2.35 (m, 2H), 2.30–2.19 (m, 1H), 2.19–2.08 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.1, 163.8, 159.2, 131.4, 130.1, 129.3, 129.2, 119.7, 115.0, 114.0, 55.7, 55.5, 50.9, 29.2, 15.4 ppm. HRMS m/z: calcd for $C_{19}H_{20}NO_3$ $[M+H]^+$ 310.1443, found: 310.1431.

5-oxo-4,5-bis(3-(trifluoromethyl)phenyl)pentanenitrile (4ga): Yield = 71% (83 mg). Yellow oil. IR (KBr) ν = 2970, 2901, 2248, 1687, 1327, 1252, 1164, 1119, 804, 692 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 8.21 (s, 1H),

8.11 (d, J = 7.9 Hz, 1H), 7.79 (d, J = 7.8 Hz, 1H), 7.60–7.47 (m, 5H), 4.82 (t, J = 7.3 Hz, 1H), 2.59–2.42 (m, 2H), 2.35–2.17 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 196.5, 138.1, 136.2, 132.4, 132.1, 132.0 (d, $J_{C\text{-}F}$ = 0.9 Hz), 131.9, 131.7 (d, $J_{C\text{-}F}$ = 0.9 Hz), 131.6, 130.4, 130.3 (dd, $J_{C\text{-}F}$ = 7.2, 3.4 Hz), 129.8, 125.9 (dd, $J_{C\text{-}F}$ = 7.5, 3.8 Hz), 125.4 (dd, $J_{C\text{-}F}$ = 7.4, 3.7 Hz), 124.9 (dd, $J_{C\text{-}F}$ = 7.2, 3.7 Hz), 119.0, 51.94, 29.12, 15.42 ppm. HRMS m/z: calcd for $C_{19}H_{14}F_6NO$ $[M+H]^+$ 386.0980, found: .386.0979

5-(4-(benzyloxy)phenyl)-5-oxo-4-phenylpentanenitrile (4ha) and **4-(4-(benzyloxy)phenyl)-5-oxo-5-phenylpentanenitrile (4ha'):** Yield = 72% (3.7:1, 78 mg). Yellow oil. IR (KBr) ν = 3029, 2931, 2244, 1671, 1597, 1508, 1248, 1165, 1002, 738, 697 cm^{-1}. The ^{1}H NMR spectrum of the isolated product showed a 3.7:1 mixture of **4ha** and its isomer **4ha'**. ^{1}H NMR (400MHz, $CDCl_3$): δ = 7.97–7.91 (m, 2H), 7.40–7.35 (m, 4H), 7.35–7.20 (m, 6H), 6.97–6.89 (m, 2H), 5.08–4.98 (m, 2H), 4.67 (t, J = 7.2 Hz, 1H), 2.48–2.33 (m, 2H), 2.28–2.12 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) major product **4ha**: δ = 196.8, 162.9, 138.17, 136.2, 133.4, 131.4, 129.6, 128.9, 128.4, 128.2, 127.9, 127.6, 119.6, 114.8, 70.3, 51.7, 29.3, 15.4 ppm. HRMS m/z: calcd for $C_{24}H_{22}NO_2$ $[M+H]^+$ 356.1651, found: 356.1650.

5-(3,4-dimethylphenyl)-5-oxo-4-phenylpentanenitrile (4ia) and **4-(3,4-dimethylphenyl)-5-oxo-5-phenylpentanenitrile (4ia'):** Yield = 73% (1.9:1, 62 mg). Yellow oil. IR (KBr) ν = 2920, 2850, 2244, 1673, 1603, 1448, 1259, 1132, 983, 731, 700 cm^{-1}. The ^{1}H NMR spectrum of the isolated product showed a 1.9:1 mixture of **4ia** and its isomer **4ia'**. ^{1}H NMR (400MHz, $CDCl_3$): δ = 7.99–7.93 (m, 0.7H), 7.75–7.73 (m, 0.6H), 7.71–7.66 (m, 0.6H), 7.51–7.45 (m, 0.4H), 7.41–7.35 (m, 0.7H), 7.34–7.28 (m, 2.6H), 7.25–7.20 (m, 0.7H), 7.15–7.01 (m, 1.7H), 4.71 (t, J = 7.3 Hz, 0.65H), 4.68–4.62 (t, J = 7.3 Hz, 0.35H), 2.48–2.34 (m, 2H), 2.30–2.13 (m, 8H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) **4ia** and its isomer **4ia'**: δ = 198.5, 198.2, 143.2, 138.1, 137.9, 137.2, 136.4, 136.2, 135.0, 134.0, 133.4, 130.7, 130.1, 130.0, 129.5, 129.2, 129.0, 128.8, 128.3, 127.9, 126.8, 125.8, 119.6, 119.6, 51.9, 51.7, 29.2, 29.2, 20.2, 20.0, 20.0, 19.6, 15.4, 15.4 ppm. HRMS m/z: calcd for $C_{19}H_{20}NO$ $[M+H]^+$ 278.1545, found: 278.1550.

4-(4-bromophenyl)-5-oxo-5-phenylpentanenitrile (4ja) and **5-(4-bromophenyl)-5-oxo-4-phenylpentanenitrile (4ja'):** Yield = 65% (2.7:1, 65 mg). Yellow oil. IR (KBr) ν = 2923, 2851, 2245, 1678, 1582, 1486, 1477, 1258, 1072, 1009, 807, 701 cm^{-1}. The ^{1}H NMR spectrum of the isolated product showed a 2.7:1 mixture of **4ja** and its isomer **4ja'**. ^{1}H NMR (400MHz, $CDCl_3$): δ = 7.95–7.90 (m, 1.4H), 7.82–7.78 (m, 0.5H), 7.55–7.49 (m, 1.2H), 7.48–7.44 (m, 1.5H), 7.43–7.38 (m, 1.5H), 7.36–7.30 (m, 0.6H), 7.28–7.25 (m, 0.9H), 7.21–7.17 (m, 1.4H), 4.72 (t, J = 7.2 Hz, 0.73H), 4.65 (t, J = 7.1 Hz, 0.27H), 2.52–2.36 (m, 2H), 2.32–2.11 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) **4ja** and its isomer **4ja'**: δ = 198.0, 197.4, 137.4, 136.7, 136.2, 135.9, 134.8, 133.8, 132.8, 132.2, 130.5, 130.0, 129.8, 129.0, 128.3, 128.2, 122.15, 119.3, 52.2, 51.4, 29.0, 15.4, 15.3 ppm. HRMS m/z: calcd for $C_{17}H_{15}BrNO$ $[M+H]^+$ 328.0337, found: 328.0341.

5-oxo-5-phenyl-4-(3-(trifluoromethyl)phenyl)pentanenitrile (4ka) and **5-oxo-4-phenyl-5-(3-(trifluoromethyl)phenyl)pentanenitrile (4ka'):** Yield = 79% (3.5:1, 76 mg). Yellow oil. IR (KBr) ν = 2963, 2920, 2247, 1681, 1448, 1327, 1164, 1121, 1073, 802, 701, 686 cm^{-1}. The ^{1}H NMR spectrum of the isolated product showed a 3.5:1 mixture of **4ka** and its isomer **4ka'**. ^{1}H NMR (400MHz, $CDCl_3$): δ = 8.21–7.93 (m, 1.9H), 7.76–7.71 (m, 0.3H), 7.60–7.51 (m, 3.3H), 7.49–7.40 (m, 2.4H), 7.37–7.32 (m, 0.5H), 7.31–7.26 (m, 0.6H), 4.85 (t, J = 7.4 Hz, 0.78H), 4.70 (t, J = 7.4 Hz, 0.22H), 2.58–2.38 (m, 2H), 2.34–2.13 (m, 2H). ppm. ^{13}C NMR (100 MHz, $CDCl_3$) major product **4ka**: δ = 197.8, 138.8, 135.8, 133.9, 132.1, 131.81, 130.1, 129.9, 129.1, 129.0, 128.3, 125.0 (m), 119.1, 51.6, 29.3, 15.5 ppm. HRMS m/z: calcd for $C_{18}H_{15}F_3NO$ $[M+H]^+$ 318.1106, found: 318.1114.

5-oxo-5-phenyl-4-(pyridin-3-yl)pentanenitrile (4la): Yield = 59% (45 mg). Yellow oil. IR (KBr) ν = 2958, 2923, 2853, 2245, 1678, 1595, 1447, 1424, 1264, 1236, 1176, 1026, 801, 705, 686 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 8.66 (d, J = 1.9 Hz, 1H), 8.56–8.50 (m, 1H), 7.99–7.92 (m, 2H), 7.67–7.60 (m, 1H), 7.57–7.52 (m, 1H), 7.47–7.40 (m, 2H), 7.29–7.26 (m, 1H), 4.82 (t, J = 7.4 Hz, 1H), 2.59–2.40 (m, 2H), 2.37–2.28 (m, 1H), 2.22–2.12 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.7, 149.9, 149.4, 135.7, 135.5, 134.0, 133.7, 129.1, 129.0, 124.4, 119.0, 49.2, 29.2, 15.5 ppm. HRMS m/z: calcd for $C_{16}H_{15}N_2O$ $[M+H]^+$ 251.1184, found: 251.1180.

5-(2-fluorophenyl)-5-oxo-4-phenylpentanenitrile (4ma) and **4-(2-fluorophenyl)-5-oxo-5-phenylpentanenitrile (4ma'):** Yield = 82% (2.6:1, 65 mg). Yellow oil. IR (KBr) ν = 2969, 2926, 2245, 1681, 1608, 1481, 1449, 1275, 1227, 759, 700 cm^{-1}. The ^1H NMR spectrum of the isolated product showed a 2.6:1 mixture of **4ma** and its isomer **4ma'**. ^1H NMR (400MHz, $CDCl_3$): δ = 7.97–7.92 (m, 0.5H), 7.78–7.72 (m, 0.7H), 7.54–7.37 (m, 1.9H), 7.32–7.27 (m, 1.5H), 7.26–7.21 (m, 2.1H), 7.17–7.00 (m, 2.3H), 5.06 (t, J = 7.2 Hz, 0.28H), 4.64 (t, J = 7.2 Hz, 0.72H), 2.56–2.46 (m, 1H), 2.42–2.35 (m, 1H), 2.31–2.08 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) major product **4ma**: δ = 197.5 (d, $J_{C\text{-}F}$ = 4.4 Hz), 161.2 (d, $J_{C\text{-}F}$ = 253.3 Hz), 136.6, 134.9 (d, $J_{C\text{-}F}$ = 9.0 Hz), 133.7, 131.2 (d, $J_{C\text{-}F}$ = 2.5 Hz), 129.3, 128.7 (d, $J_{C\text{-}F}$ = 0.5 Hz), 128.1, 124.7 (d, $J_{C\text{-}F}$ = 3.5 Hz), 119.4, 116.9 (d, $J_{C\text{-}F}$ = 23.7 Hz), 56.1 (d, $J_{C\text{-}F}$ = 6.6 Hz), 28.9, 15.4 ppm. HRMS m/z: calcd for $C_{17}H_{15}FNO$ $[M+H]^+$ 268.1138, found: 268.1144.

5-(2-chlorophenyl)-4-(4-chlorophenyl)-5-oxopentanenitrile (4na): Yield = 49% (47 mg). Yellow oil. IR (KBr) ν = 2967, 2919, 2246, 1697, 1490, 1432, 1091, 1014, 809, 741 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.39–7.32 (m, 2H), 7.31–7.26 (m, 2H), 7.23–7.17 (m, 1H), 7.17–7.11 (m, 3H), 4.61 (t, J = 7.4 Hz, 1H), 2.61–2.41 (m, 2H), 2.34–2.24 (m, 1H), 2.22–2.10 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 201.4, 138.7, 134.4, 132.0, 130.8, 130.7, 130.1, 129.7, 129.2, 127.0, 119.2, 55.5, 28.0, 15.4 ppm. HRMS m/z: calcd for $C_{17}H_{14}Cl_2NO$ $[M+H]^+$ 318.0452, found: 318.0453.

2-(2-benzoyl-2-phenyltetrahydro-2*H*-pyran-3-yl)acetonitrile (4pa): Yield = 33% (35 mg). White soild (M.p. 93.2–94.8 °C). IR (KBr) ν = 2924, 2853, 2245, 1674, 1274, 1222, 843, 759, 707, 631 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.90–7.81 (m, 2H), 7.47–7.42 (m, 1H), 7.40–7.31 (m, 5H), 7.30–7.25 (m, 2H), 3.94–3.84 (m, 1H), 3.45–3.33 (m, 1H), 3.23–3.13 (m, 1H), 2.42–2.35 (m, 1H), 2.22–2.13 (m, 1H), 2.11–2.01 (m, 1H), 1.98–1.83 (m, 2H), 1.79–1.69 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 201.9, 140.0, 135.1, 133.3, 130.6, 129.0, 128.7, 128.2, 126.0, 119.8, 86.7, 65.4, 46.1, 25.8, 25.6, 20.0 ppm. HRMS m/z: calcd for $C_{20}H_{20}NO_2$ $[M+H]^+$ 306.1494, found: 306.1495.

2-(2-(4-chlorobenzoyl)-2-(4-chlorophenyl)tetrahydro-2*H*-pyran-3-yl)acetonitrile (4qa): Yield = 35% (47 mg). Yellow oil. IR (KBr) ν = 2955, 2934, 2246, 1680, 1585, 1488, 1400, 1243, 1090, 1012, 850, 751 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.85–7.79 (m, 2H), 7.38–7.33 (m, 2H), 7.29–7.24 (m, 4H), 3.97–3.88 (m, 1H), 3.41–3.32 (m, 1H), 3.19–3.09 (m, 1H), 2.37–2.30 (m, 1H), 2.22–2.14 (m, 1H), 2.03–1.97 (m, 1H), 1.93–1.85 (m, 2H), 1.78–1.71 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 200.2, 140.1, 138.3, 134.9, 132.9, 132.0, 129.4, 128.7, 127.4, 119.4, 86.2, 77.6, 77.2, 76.9, 65.6, 45.9, 25.7, 25.5, 19.9 ppm. HRMS m/z: calcd for $C_{20}H_{18}Cl_2NO_2$ $[M+H]^+$ 374.0715, found: 374.0712.

2-(2-(4-methylbenzoyl)-2-p-tolyltetrahydro-2*H*-pyran-3-yl)acetonitrile (4ra): Yield = 29% (30 mg). Yellow oil. IR (KBr) ν = 2926, 2856, 2244, 1674, 1604, 1254, 1182, 1077, 1018, 805, 733, 618 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.78 (d, J = 8.3 Hz, 2H), 7.22–7.12 (m, 4H), 7.07 (d, J = 8.1 Hz, 2H), 3.92–3.84 (m, 1H), 3.42–3.33 (m, 1H), 3.21–3.11 (m, 1H), 2.45–2.40 (m, 1H), 2.34 (s, 3H), 2.32 (s, 3H), 2.18–2.12 (m, 1H), 2.06–1.98 (m, 1H), 1.96–1.84 (m, 2H), 1.74–1.67 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 201.6, 144.1, 138.4, 137.2, 132.6,

130.7, 129.6, 128.9, 125.9, 120.0, 86.6, 77.6, 77.2, 76.9, 65.4, 46.2, 25.8, 25.6, 21.9, 21.3, 20.0 ppm. HRMS m/z: calcd for $C_{22}H_{24}NO_2$ $[M+H]^+$ 334.1807, found: 334.1808.

1-(3-oxo-2,3-diphenylpropyl)cyclopropanecarbonitrile (4ab): Yield = 25% (20 mg). Yellow oil. IR (KBr) ν = 2923, 2852, 2234, 1678, 1596, 1447, 1252, 1210, 757, 698 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 8.02–7.98 (m, 2H), 7.53–7.47 (m, 1H), 7.43–7.38 (m, 2H), 7.36–7.29 (m, 4H), 7.26–7.21 (m, 1H), 4.98 (dd, J = 7.9, 6.6 Hz, 1H), 2.54–2.45 (m, 1H), 1.91–1.82 (m, 1H), 1.17–1.091H), 0.99–0.92 (m 1H), 0.91–0.84 (m, 1H), 0.39–0.32 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 198.8, 138.4, 136.3, 133.5, 129.4, 129.0, 128.8, 128.4, 127.9, 123.5, 77.6, 77.2, 76.9, 52.2, 38.7, 14.7, 13.8, 8.5 ppm. HRMS m/z: calcd for $C_{19}H_{18}NO$ $[M+H]^+$ 276.1388, found: 276.1389.

2-(3-oxo-2,3-diphenylpropyl)malononitrile (4af): Yield = 72% (70 mg). Yellow oil. IR (KBr) ν = 2918, 2854, 2255, 1677, 1596, 1447, 1262, 1175, 951, 758, 695 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.96–7.91 (m, 2H), 7.54–7.49 (m, 1H), 7.42–7.34 (m, 4H), 7.32–7.29 (m, 3H), 4.81 (t, J = 7.6 Hz, 1H), 3.67 (dd, J = 8.6, 7.5 Hz, 1H), 2.87–2.77 (m, 1H), 2.62–2.53 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.0, 136.0, 135.4, 134.0, 130.2, 129.2, 129.0, 128.9, 128.2, 112.6, 112.4, 50.7, 34.5, 20.9 ppm. HRMS m/z: calcd for $C_{18}H_{15}N_2O$ $[M+H]^+$ 275.1184, found: 275.1181.

methyl 2-cyano-5-oxo-4,5-diphenylpentanoate (4ag): Yield = 71% (dr = 1:1, 67 mg). Yellow oil. IR (KBr) ν = 2956, 2901, 2250, 1746, 1678, 1447, 1258, 1176, 757, 697 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.95 (d, J = 7.8 Hz, 2H), 7.52–7.46 (m, 1H), 7.41–7.37 (m, 2H), 7.36–7.28 (m, 5H), 4.91–4.79 (m, 1H), 3.76 (s, 1.5H), 3.73 (s, 1.5H), 3.69–3.63 (m, 0.5H), 3.30–3.24 (m, 0.5H), 2.92–2.83 (m, 0.5H), 2.69–2.55 (m, 1H), 2.41–2.32 (m, 0.5H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 198.0, 197.7, 166.5, 166.3, 137.5, 136.7, 135.9, 135.9, 133.6, 133.5, 129.8, 129.6, 129.1, 129.0, 128.9, 128.8, 128.4, 128.4, 128.4, 128.1, 116.4, 116.4, 53.7, 53.7, 51.0, 50.9, 35.6, 35.5, 33.5, 33.4 ppm. HRMS m/z: calcd for $C_{19}H_{18}NO_3$ $[M+H]^+$ 308.1287, found: 308.1295.

2-benzoyl-5-oxo-4,5-diphenylpentanenitrile (4ah): Yield = 53% (dr = 1:1, 56 mg). Yellow oil. IR (KBr) ν = 2925, 2854, 2248, 1678, 1596, 1447, 1265, 1001, 757, 693 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 8.14–8.09 (m, 1H), 8.03–7.99 (m, 1H), 7.96–7.92 (m, 1H), 7.69–7.65 (m, 1H), 7.60–7.56 (m, 1H), 7.54–7.49 (m, 1H), 7.45–7.36 (m, 5H), 7.31–7.26 (m, 2H), 7.26–7.18 (m, 2H), 5.04–4.84 (m, 1H), 4.65–4.56 (m, 0.5H), 4.13–4.06 (m, 0.5H), 2.99–2.89 (m, 0.5H), 2.72–2.56 (m, 1H), 2.30–2.22 (m, 0.5H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 198.8, 197.9, 190.8, 190.7, 138.0, 137.1, 136.0, 135.9 134.9, 134.7, 133.9, 133.8, 133.8, 133.6, 129.9, 129.7, 129.4, 129.3, 129.2, 129.1, 129.0, 128.9, 128.9, 128.6, 128.2, 128.1, 117.4, 117.3, 51.6, 51.3, 39.3, 38.2, 34.4, 33.9 ppm. HRMS m/z: calcd for $C_{24}H_{20}NO_2$ $[M+H]^+$ 354.1494, found: 354.1494.

3-cyclohexyl-1,2-diphenylpropan-1-one (5aa): Yield = 96% (87 mg). White soild (M.p. 64.2–65.6 ºC). IR (KBr) ν = 2922, 2848, 1673, 1596, 1493, 1445, 1228, 999, 941, 758, 733, 695, 652 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.99–7.94 (m, 2H), 7.51–7.45 (m, 1H), 7.42–7.36 (m, 2H), 7.32–7.25 (m, 4H), 7.22–7.16 (m, 1H), 4.72 (t, J = 7.3 Hz, 1H), 2.17–2.07 (m, 1H), 1.85–1.79 (m, 1H), 1.74–1.60 (m, 5H), 1.26–1.10 (m, 4H), 0.99–0.88 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 200.3, 140.2, 137.2, 133.0, 129.1, 128.8, 128.7, 128.5, 127.1, 50.7, 41.9, 35.5, 33.8 33.5, 26.7, 26.4, 26.4 ppm. HRMS m/z: calcd for $C_{21}H_{25}O$ $[M+H]^+$ 293.1905, found: 293.1906.

3-cyclohexyl-1,2-bis(4-fluorophenyl)propan-1-one (5ba): Yield = 64% (63 mg). Colorless oil. IR (KBr) ν = 2922, 2850, 1681, 1505, 1408, 1225, 1154, 831, 770 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 8.01–7.95 (m, 2H), 7.28–7.23 (m, 2H), 7.11–7.04 (m, 2H), 7.01–6.94 (m, 2H), 4.65 (t, J = 7.4 Hz, 1H), 2.13–2.02 (m, 1H), 1.84–1.77 (m, 1H), 1.72–1.62 (m, 5H), 1.20–1.08 (m, 4H), 0.98–0.87 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 198.6, 165.8 (d, $J_{C\text{-}F}$ = 253.6 Hz), 162.0 (d, $J_{C\text{-}F}$ = 244.2 Hz), 135.6 (d, $J_{C\text{-}F}$ = 3.2 Hz), 133.3 (d, $J_{C\text{-}F}$ = 3.1 Hz), 131.4 (d,

$J_{C\text{-}F}$ = 9.2 Hz), 129.9 (d, $J_{C\text{-}F}$ = 7.9 Hz), 116.1 (d, $J_{C\text{-}F}$ = 8.7 Hz), 115.8 (d, $J_{C\text{-}F}$ = 9.2 Hz), 49.8, 41.9, 35.4, 33.8, 33.4, 26.7, 26.3, 26.3 ppm. HRMS m/z: calcd for $C_{21}H_{23}F_2O$ $[M+H]^+$ 329.1717, found: 329.1716.

1,2-bis(4-chlorophenyl)-3-cyclohexylpropan-1-one (5ca): Yield = 84% (93 mg). Colorless oil. IR (KBr) ν = 2920, 2849, 1681, 1588, 1488, 1210, 1091, 1013, 812, 744 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.91–7.85 (m, 2H), 7.40–7.35 (m, 2H), 7.28–7.19 (m, 4H), 4.62 (t, J = 7.3 Hz, 1H), 2.11–2.01 (m, 1H), 1.83–1.75 (m, 1H), 1.72–1.60 (m, 5H), 1.21–1.08 (m, 4H), 0.99–0.86 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 198.7, 139.7, 138.3, 135.1, 133.1, 130.2, 129.7, 129.3, 129.1, 77.6, 77.2, 76.9, 50.0, 41.7, 35.4, 33.8, 33.3, 26.6, 26.3, 26.3 ppm. HRMS m/z: calcd for $C_{21}H_{23}Cl_2O$ $[M+H]^+$ 361.1126, found: 361.1116.

1,2-bis(4-bromophenyl)-3-cyclohexylpropan-1-one (5da): Yield = 88% (118 mg). Colorless oil. IR (KBr) ν = 2919, 2849, 1680, 1584, 1485, 1395, 1172, 1070, 1009, 937, 784, 734 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.82–7.77 (m, 2H), 7.57–7.51 (m, 2H), 7.44–7.38 (m, 2H), 7.18–7.13 (m, 2H), 4.60 (t, J = 7.3 Hz, 1H), 2.09–1.99 (m, 1H), 1.83–1.75 (m, 1H), 1.71–1.59 (m, 5H), 1.20–1.06 (m, 4H), 0.99–0.84 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 198.8, 138.8, 135.5, 132.3, 132.1, 130.3, 130.1, 128.4, 121.3, 50.1, 41.6, 35.4, 33.8, 33.3, 26.6, 26.3, 26.3 ppm. HRMS m/z: calcd for $C_{21}H_{23}Br^{79}Br^{81}O$ $[M+H]^+$ 451.0095, found: 451.0093.

3-cyclohexyl-1,2-dip-tolylpropan-1-one (5ea): Yield = 83% (85 mg). Colorless oil. IR (KBr) ν = 2919, 2849, 1676, 1606, 1447, 1258, 1175, 936, 791, 760 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.88 (d, J = 8.1 Hz, 2H), 7.18 (d, J = 7.9 Hz, 4H), 7.08 (d, J = 7.9 Hz, 2H), 4.66 (t, J = 7.3 Hz, 1H), 2.34 (s, 3H), 2.27 (s, 3H), 2.13–2.03 (m, 1H), 1.85–1.78 (m, 1H), 1.70–1.61 (m, 5H), 1.20–1.08 (m, 4H), 0.98–0.86 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 200.0, 143.7, 137.4, 136.6, 134.6, 129.7, 129.4, 129.0, 128.2, 50.1, 41.8, 35.5, 33.8, 33.5, 26.7, 26.4, 26.3, 21.8, 21.2 ppm. HRMS m/z: calcd for $C_{23}H_{29}O$ $[M+H]^+$ 321.2218, found: 321.2220.

3-cyclohexyl-1,2-bis(4-methoxyphenyl)propan-1-one (5fa): Yield = 75% (103 mg). Colorless oil. IR (KBr) ν = 2920, 2847, 1670, 1598, 1508, 1248, 1165, 1030, 828, 712 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.98–7.91 (m, 2H), 7.25–7.19 (m, 2H), 6.89–6.82 (m, 4H), 4.63 (t, J = 7.2 Hz, 1H), 3.82 (s, 3H), 3.76 (s, 3H), 2.46–2.35 (m, 2H), 2.30–2.19 (m, 1H), 2.19–2.08 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.1, 163.8, 159.2, 131.4, 130.1, 129.3, 129.2, 119.7, 115.0, 114.0, 55.7, 55.5, 50.9, 29.2, 15.4 ppm. HRMS m/z: calcd for $C_{23}H_{29}O_3$ $[M+H]^+$ 353.2117, found: 353.2107.

3-cyclohexyl-1,2-bis(3-(trifluoromethyl)phenyl)propan-1-one (5ga): Yield = 87% (111 mg). Colorless oil. IR (KBr) ν = 2924, 2853, 1688, 1449, 1326, 1164, 1122, 1072, 803, 702 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 8.23 (s, 1H), 8.13 (d, J = 7.9 Hz, 1H), 7.77 (d, J = 7.8 Hz, 1H), 7.57 (t, J = 7.8 Hz, 2H), 7.53–7.47 (m, 2H), 7.47–7.41 (m, 1H), 4.78 (t, J = 7.3 Hz, 1H), 2.19–2.10 (m, 1H), 1.86–1.78 (m, 1H), 1.77–1.62 (m, 5H), 1.23–1.10 (m, 4H), 1.01–0.91 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 198.3, 140.5, 137.2, 131.8 (d, $J_{C\text{-}F}$ = 0.5 Hz), 131.8 (d, $J_{C\text{-}F}$ = 1.0 Hz), 131.7, 131.4 (d, $J_{C\text{-}F}$ = 2.7 Hz), 131.1 (d, $J_{C\text{-}F}$ = 1.2 Hz), 129.8 (d, $J_{C\text{-}F}$ = 3.6 Hz), 129.7 (d, $J_{C\text{-}F}$ = 8.1 Hz), 125.6 (m), 125.2 (m), 124.4 (m), 122.6 (d, $J_{C\text{-}F}$ = 34.2 Hz), 50.7, 41.9, 35.5, 33.7, 33.4, 26.6, 26.3, 26.2 ppm. HRMS m/z: calcd for $C_{23}H_{23}F_6O$ $[M+H]^+$ 429.1653, found: 429.1652.

1-(4-(benzyloxy)phenyl)-3-cyclohexyl-2-phenylpropan-1-one (5ha) and **2-(4-(benzyloxy)phenyl)-3-cyclohexyl-1-phenylpropan-1-one (5ha'):** Yield = 59% (7.6:1, 71 mg). White soild (mixture). IR (KBr) ν = 2920, 2850, 1665, 1600, 1452, 1251, 1172, 1020, 834, 743, 697 cm^{-1}. The ^1H NMR spectrum of the isolated product showed a 7.6:1 mixture of **5ha** and its isomer **5ha'**. ^1H NMR (400MHz, $CDCl_3$): δ = 8.00–7.94 (m, 2H), 7.40–7.31 (m, 5H), 7.29 (d, J = 1.9 Hz, 2H), 7.26 (d, J = 8.4 Hz, 2H), 7.21–7.15 (m, 1H), 6.97–6.88 (m, 2H), 5.05 (s, 1.7H), 4.99 (s, 0.3H), 4.67 (t, J = 7.3 Hz, 1H), 2.15–2.05 (m, 1H), 1.86–1.62 (m, 1H),

1.21–1.10 (m, 4H), 0.98–0.87 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) major product **5ha**: δ = 198.8, 162.6, 140.6, 136.4, 131.1, 130.3, 129.0, 128.9, 128.4, 128.4, 127.7, 127.0, 114.7, 70.3, 50.3, 42.0, 35.5, 33.8, 33.5, 26.7, 26.4, 26.3 ppm. HRMS m/z: calcd for $C_{28}H_{31}O_2$ $[M+H]^+$ 399.2324, found: 399.2322.

3-cyclohexyl-1-(3,4-dimethylphenyl)-2-phenylpropan-1-one (5ia) and **3-cyclohexyl-2-(3,4-dimethylphenyl)-1-phenylpropan-1-one (5ia'):** Yield = 80% (2.3:1, 76 mg). Colorless oil. IR (KBr) ν = 2919, 2849, 1676, 1604, 1405, 1242, 1122, 735, 699 cm^{-1}. The ^{1}H NMR spectrum of the isolated product showed a 2.3:1 mixture of **5ia** and its isomer **5ia'**. ^{1}H NMR (400MHz, $CDCl_3$): δ = 8.00–7.95 (m, 0.6H), 7.77–7.75 (s, 0.6H), 7.74–7.69 (m, 0.7H), 7.49–7.44 (m, 0.3H), 7.41–7.35 (m, 0.6H), 7.32–7.24 (m, 3H), 7.20–7.11 (m, 1.4H), 7.05–7.02 (m, 0.8H), 4.70 (t, J = 7.2 Hz, 0.7H), 4.65 (t, J = 7.2 Hz, 0.3H), 2.26 (s, 2H), 2.25 (s, 2H), 2.20 (s, 1H), 2.18 (s, 1H), 2.16–2.06 (m, 1H), 1.85–1.77 (m, 1H), 1.72–1.59 (m, 5H), 1.25–1.09 (m, 4H), 0.97–0.86 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) **5ia** and its isomer **5ia'**: δ = 200.4, 200.1, 142.6, 140.5, 137.6, 137.2, 137.1, 135.3, 135.0, 132.9, 130.3, 130.0, 129.9, 129.4, 129.0, 128.9, 128.7, 128.4, 126.9, 126.6, 125.9, 50.4, 50.3, 42.0, 41.9, 35.6, 35.5, 33.8, 33.7, 33.5, 33.5, 26.7, 26.4, 26.3, 20.1, 20.0, 19.6 ppm. HRMS m/z: calcd for $C_{23}H_{29}O$ $[M+H]^+$ 321.2218, found: 321.2213.

2-(4-bromophenyl)-3-cyclohexyl-1-phenylpropan-1-one (5ja) and **1-(4-bromophenyl)-3-cyclohexyl-2-phenylpropan-1-one (5ja'):** Yield = 87% (3.2:1, 120 mg). White soild (mixture). IR (KBr) ν = 2919, 2849, 1676, 1582, 1446, 1070, 1010, 973, 823, 718, 685 cm^{-1}. The ^{1}H NMR spectrum of the isolated product showed a 3.2:1 mixture of **5ja** and its isomer **5ja'**. ^{1}H NMR (400MHz, $CDCl_3$): δ = 7.98–7.91 (m, 1.5H), 7.85–7.80 (m, 0.5H), 7.53–7.48 (m, 1.3H), 7.44–7.38 (m, 3H), 7.30–7.25 (m, 1H), 7.22–7.16 (m, 1.7H), 4.69 (t, J = 7.4 Hz, 0.76H), 4.63 (t, J = 7.3 Hz, 0.24H), 2.14–2.02 (m, 1H), 1.81 (d, J = 12.8 Hz, 1H), 1.72–1.60 (m, 5H), 1.22–1.08 (m, 4H), 0.98–0.88 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) major product **5ja**: δ = 199.9, 139.1, 136.8, 133.2, 132.1, 130.2, 128.8, 128.8, 121.1, 50.0, 41.7, 35.4, 33.8, 33.3, 26.6, 26.3, 26.3 ppm. HRMS m/z: calcd for $C_{21}H_{24}BrO$ $[M+H]^+$ 371.1011, found: 371.1003.

3-cyclohexyl-1-phenyl-2-(3-(trifluoromethyl)phenyl)propan-1-one (5ka) and **3-cyclohexyl-2-phenyl-1-(3-(trifluoromethyl)phenyl)propan-1-one (5ka'):** Yield = 90% (4:1, 104 mg). Colorless oil. IR (KBr) ν = 2922, 2852, 1682, 1447, 1326, 1163, 1096, 700, 686 cm^{-1}. The ^{1}H NMR spectrum of the isolated product showed a 4:1 mixture of **5ka** and its isomer **5ka'**. ^{1}H NMR (400MHz, $CDCl_3$): δ = 8.25–7.94 (m, 2H), 7.74–7.50 (m, 3H), 7.48–7.38 (m, 3H), 7.31–7.18 (m, 1H), 4.81 (t, J = 7.3 Hz, 0.8H), 4.68 (t, J = 7.3 Hz, 0.2H), 2.20–2.07 (m, 1H), 1.86–1.62 (m, 6H), 1.21–1.08 (m, 4H), 1.00–0.88 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) major product **3ka**: δ = 199.7, 141.1, 136.8, 133.4, 131.8 (d, $J_{C\text{-}F}$ = 0.8 Hz), 129.5, 129.3, 128.9, 128.8, 128.4, 125.2 (m), 124.1 (m), 50.3, 42.1, 35.6, 33.7, 33.4, 26.6, 26.3, 26.3 ppm. HRMS m/z: calcd for $C_{22}H_{24}F_3O$ $[M+H]^+$ 361.1779, found: 361.1765.

3-cyclohexyl-1-phenyl-2-(pyridin-3-yl)propan-1-one (5la): Yield = 52% (46 mg). White soild (M.p. 92.4–93.7 ^{o}C). IR (KBr) ν = 2919, 2850, 1670, 1446, 1232, 1057, 1027, 742, 707, 692 cm^{-1}. ^{1}H NMR (400MHz, $CDCl_3$): δ = 8.59 (d, J = 1.9 Hz, 1H), 8.46 (dd, J = 4.7, 1.2 Hz, 1H), 7.97 (d, J = 7.3 Hz, 2H), 7.70–7.64 (m, 1H), 7.57–7.50 (m, 1H), 7.47–7.40 (m, 2H), 7.26–7.20 (m, 1H), 4.78 (t, J = 7.4 Hz, 1H), 2.16–2.05 (m, 1H), 1.83 (d, J = 12.6 Hz, 1H), 1.76–1.60 (m, 5H), 1.22–1.08 (m, 4H), 1.00–0.90 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 199.6, 150.1, 148.5, 136.6, 135.7, 135.7, 133.5, 128.9, 128.7, 124.0, 47.7, 41.76, 35.4, 33.8, 33.2, 26.6, 26.3, 26.2 ppm. HRMS m/z: calcd for $C_{20}H_{24}NO$ $[M+H]^+$ 294.1858, found: 294.2863.

3-cyclohexyl-1-(2-fluorophenyl)-2-phenylpropan-1-one (5ma) and

3-cyclohexyl-2-(2-fluorophenyl)-1-phenylpropan-1-one (5ma'): Yield = 86% (2.5:1, 80 mg). Colorless oil. IR (KBr) ν = 2921, 2850, 1682, 1608, 1448, 1273, 1212, 939, 757, 696 cm^{-1}. The ^1H NMR spectrum of the isolated product showed a 2.5:1 mixture of **5ma** and its isomer **5ma'**. ^1H NMR (400MHz, $CDCl_3$): δ = 8.01–7.97 (m, 0.6H), 7.71–7.65 (m, 0.7H), 7.51–7.46 (m, 0.4H), 7.43–7.36 (m, 1.3H), 7.27–7.23 (m, 2.9H), 7.21–7.15 (m, 1.1H), 7.13–7.09 (m, 0.8H), 7.06–7.00 (m, 1.2H), 5.13 (t, J = 7.3 Hz, 0.3H), 4.64 (t, J = 7.3 Hz, 0.7H), 2.15–2.06 (m, 1H), 1.86–1.80 (m, 1H), 1.74–1.60 (m, 5H), 1.20–1.08 (m, 4H), 0.98–0.87 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) major product **5ma**: δ = 199.74, 199.70, 161.1 (d, $J_{C\text{-}F}$ = 252.1Hz), 160.2 (d, $J_{C\text{-}F}$ = 242.9 Hz), 139.2, 136.7, 134.1 (d, $J_{C\text{-}F}$ = 8.9 Hz), 133.2, 131.2 (d, $J_{C\text{-}F}$ = 2.8Hz), 129.3 (d, $J_{C\text{-}F}$ = 3.7Hz), 128.8, 128.7 (d, $J_{C\text{-}F}$ = 0.5Hz), 127.1, 126.6 (d, $J_{C\text{-}F}$ = 12.8Hz), 124.8 (d, $J_{C\text{-}F}$ = 3.6Hz), 124.5 (d, $J_{C\text{-}F}$ = 3.4 Hz), 116.7 (d, $J_{C\text{-}F}$ = 23.7 Hz), 115.7 (d, $J_{C\text{-}F}$ = 22.8 Hz), 55.0, 54.9, 41.4, 40.9, 35.6, 35.4, 33.8, 33.7, 33.4, 33.2, 26.7, 26.7, 26.4, 26.3 ppm. HRMS m/z: calcd for $C_{21}H_{24}FO$ $[M+H]^+$ 311.1811, found: 311.1806.

1-(2-chlorophenyl)-2-(4-chlorophenyl)-3-cyclohexylpropan-1-one (5na): Yield = 90% (108 mg). Colorless oil. IR (KBr) ν = 2921, 2850, 1698, 1589, 1489, 1432, 1263, 1090, 1014, 810, 742 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.37–7.33 (m, 1H), 7.32–7.27 (m, 1H), 7.27–7.22 (m, 2H), 7.20–7.12 (m, 3H), 7.11–7.06 (m, 1H), 4.52 (dd, J = 8.7, 6.3 Hz, 1H), 2.07–1.98 (m, 1H), 1.81–1.74 (m, 2H), 1.70–1.59 (m, 4H), 1.18–1.08 (m, 4H), 0.99–0.88 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 203.7, 139.9, 136.9, 133.3, 131.5, 130.6, 130.5, 130.2, 129.1, 129.1, 126.9, 54.6, 40.2, 35.0, 34.1, 32.9, 26.7, 26.3, 26.2 ppm. HRMS m/z: calcd for $C_{21}H_{23}Cl_2O$ $[M+H]^+$ 361.1126, found: 361.1110.

3-cyclopentyl-1,2-diphenylpropan-1-one (5ab): Yield = 52% (43 mg). Yeild soild (M.p. 72.8–74.1 ºC). IR (KBr) ν = 2950, 2903, 1667, 1491, 1446, 1271, 1200, 1029, 743, 694, 666 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 8.01–7.94 (m, 2H), 7.50–7.45 (m, 1H), 7.41–7.36 (m, 2H), 7.34 – 7.25 (m, 4H), 7.22–7.16 (m, 1H), 4.63 (t, J = 7.3 Hz, 1H), 2.23–2.15 (m, 1H), 1.93–1.79 (m, 2H), 1.71–1.64 (m, 2H), 1.61–1.53 (m, 2H), 1.50–1.41 (m, 2H), 1.19–1.09 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 200.4, 140.0, 137.2, 133.0, 129.0, 128.8, 128.7, 128.5, 127.1, 52.8, 40.6, 38.0, 33.1, 32.8, 25.3, 25.3 ppm. HRMS m/z: calcd for $C_{20}H_{23}O$ $[M+H]^+$ 279.1749, found: 279.1748.

3-cycloheptyl-1,2-diphenylpropan-1-one (5ac): Yield = 80% (74 mg). Colorless oil. IR (KBr) ν = 2919, 2851, 1680, 1492, 1271, 1112, 755, 696 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 8.00–7.94 (m, 2H), 7.50–7.44 (m, 1H), 7.42–7.35 (m, 2H), 7.33–7.25 (m, 4H), 7.21–7.16 (m, 1H), 4.68 (t, J = 7.3 Hz, 1H), 2.18–2.09 (m, 1H), 2.02–1.89 (m, 1H), 1.82–1.73 (m, 2H), 1.59–1.39 (m, 9H), 1.27–1.20 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 200.4, 140.1, 137.2, 133.0, 129.0, 128.8, 128.7, 128.5, 127.1, 51.3, 42.3, 36.8, 35.0, 34.5, 28.8, 28.7, 26.4, 26.3 ppm. HRMS m/z: calcd for $C_{22}H_{27}O$ $[M+H]^+$ 307.2062, found: 307.2061.

3-cyclooctyl-1,2-diphenylpropan-1-one (5ad): Yield = 79% (78 mg). Colorless oil. IR (KBr) ν = 2914, 2853, 1681, 1446, 1210, 1073, 756, 696 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$): δ = 7.92–7.87 (m, 2H), 7.43–7.38 (m, 1H), 7.34–7.29 (m, 2H), 7.25–7.18 (m, 4H), 7.14–7.08 (m, 1H), 4.61 (t, J = 7.3 Hz, 1H), 2.10–2.01 (m, 1H), 1.85–1.75 (m, 1H), 1.57–1.30 (m, 15H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 200.4, 140.1, 137.2, 133.0, 129.0, 128.8, 128.7, 128.5, 127.1, 51.3, 42.1, 34.9, 32.5, 32.1, 27.6, 27.5, 26.3, 25.4, 25.4 ppm. HRMS m/z: calcd for $C_{23}H_{29}O$ $[M+H]^+$ 321.2218, found: 321.2223.

Product (5ae-1) and product (5ae'-2): Yield = 88% (**5ae**-1/**5ae'**-2 = 5/1, 96 mg). White soild (mixture). IR (KBr) ν = 2893, 2845, 1670, 1493, 1447, 1270, 1100, 959, 756, 694 cm^{-1}. ^1H NMR (400MHz, $CDCl_3$) major product **5ae**-1: δ = 7.95–7.91 (m, 2H), 7.44–7.39 (m, 1H), 7.35–7.31 (m, 2H), 7.23–7.17 (m, 4H), 7.11–7.05 (m, 1H),

4.72–4.67 (m, 1H), 2.49–2.41 (m, 1H), 1.83–1.46 (m, 14H), 1.34–1.27 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) major product **5ae**-1: δ = 200.0, 141.5, 137.1, 133.0, 129.1, 128.9, 128.8, 128.3, 126.9, 48.6, 47.7, 43.0, 37.1, 33.3, 28.8 ppm. HRMS m/z: calcd for $C_{25}H_{29}O$ $[M+H]^+$ 345.2218, found: 345.2224.

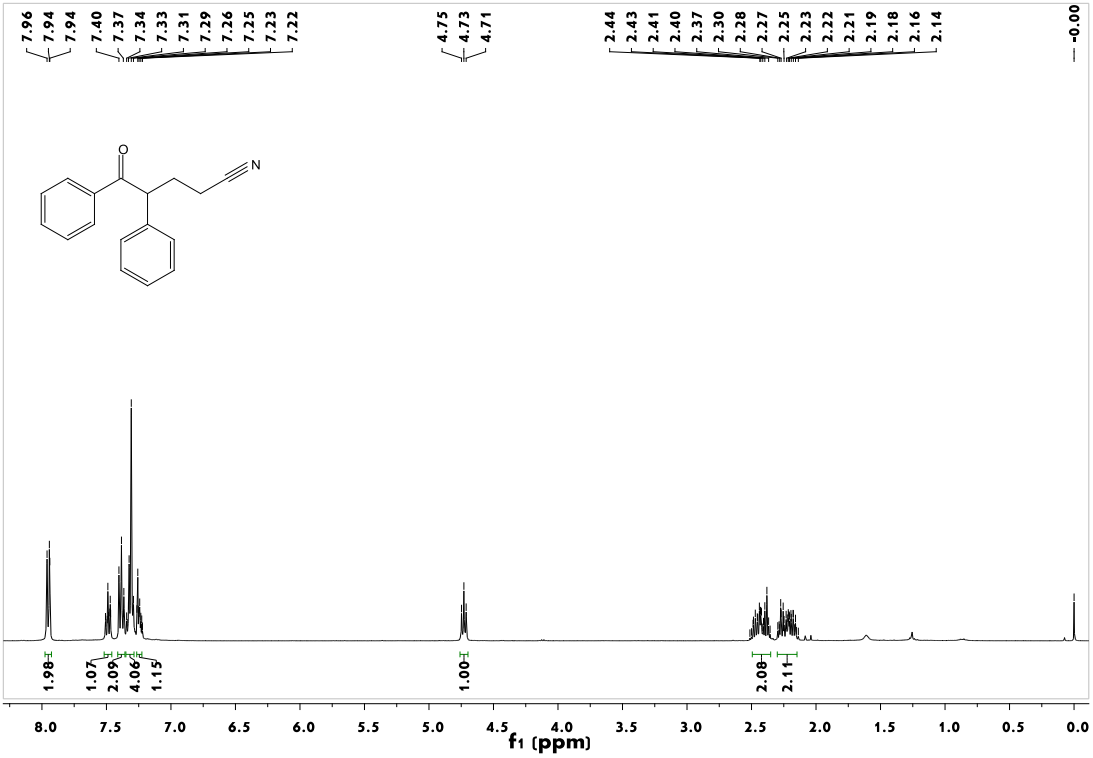
product (5af): Yield = 28% (2/3 = 8/3, 26 mg). Colorless oil. IR (KBr) ν = 2956, 2926, 2870, 1680, 1447, 1205, 1175, 756, 696 cm^{-1}. The ^{1}H NMR spectrum of the isolated product showed a mixture. ^{1}H NMR (400MHz, $CDCl_3$): δ = 7.94–7.85 (m, 2H), 7.43–7.37 (m, 1H), 7.35–7.28 (m, 2H), 7.26–7.18 (m, 4H), 7.14–7.09 (m, 1H), 4.69–4.43 (m, 1H), 2.26–2.17 (m, 0.4H), 2.11–2.02 (m, 0.4H), 1.85 (t, *J* = 7.0 Hz, 0.6H), 1.74–1.64 (m, 0.4H), 1.53–1.44 (m, 0.6H), 1.36–1.00 (m, 5.6H), 0.87–0.83 (m, 1H), 0.82–0.76 (m, 3H), 0.74–0.68 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 200.5, 200.4, 200.2, 140.4, 140.2, 139.8, 137.3, 137.2, 137.2, 137.1, 133.0, 129.1, 129.0, 129.0, 128.8, 128.8, 128.8, 128.7, 128.7, 128.6, 128.5, 128.5, 128.4, 128.4, 127.1, 127.1, 51.3, 51.2, 51.2, 41.9, 41.1, 39.8, 39.5, 38.0, 37.7, 30.6, 30.3, 25.5, 25.4, 20.1, 20.0, 19.8, 14.6, 14.5, 10.7, 10.7 ppm. HRMS m/z: calcd for $C_{20}H_{25}O$ $[M+H]^+$ 281.1905, found: 281.1902.

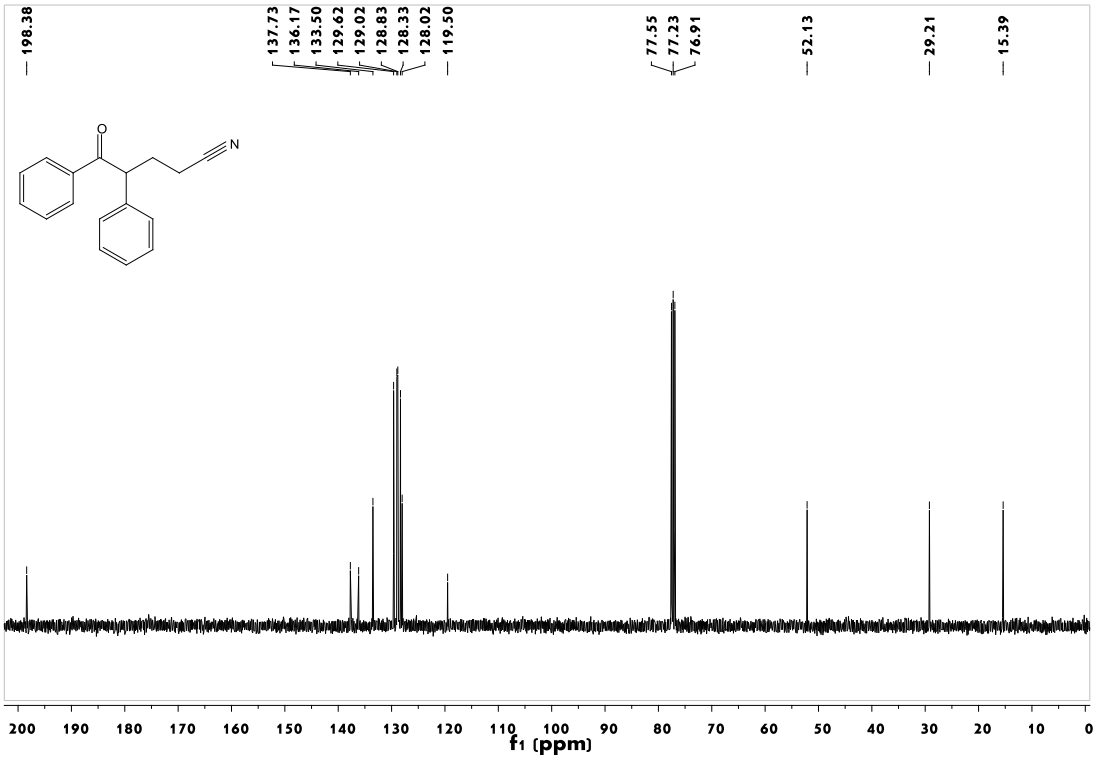
product (5ag): Yield = 76% (2/3 = 6/4, 70 mg). Colorless oil. IR (KBr) ν = 2955, 2925, 1681, 1493, 1447, 1206, 1002, 756, 696 cm^{-1}. The ^{1}H NMR spectrum of the isolated product showed a mixture. ^{1}H NMR (400MHz, $CDCl_3$): δ = 7.93–7.86 (m, 2H), 7.42–7.36 (m, 1H), 7.34–7.28 (m, 2H), 7.26–7.16 (m, 4H), 7.14–7.08 (m, 1H), 4.68–4.43 (m, 1H), 2.27–2.17 (m, 0.4H), 2.13–1.99 (m, 0.4H), 1.85 (t, *J* = 7.0 Hz, 0.6H), 1.74–1.62 (m, 0.5H), 1.52–1.44 (m, 0.5H), 1.33–1.03 (m, 7.6H), 0.87–0.68 (m, 6H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 200.4, 200.4, 200.3, 200.2, 140.4, 140.2, 140.1, 139.8, 137.3, 137.3, 137.2, 137.1, 133.0, 133.0, 129.1, 129.0, 129.0, 129.0, 128.8, 128.8, 128.7, 128.5, 128.5, 128.4, 128.4, 127.1, 127.1, 51.3, 51.3, 51.2, 51.2, 42.0, 41.1, 38.2, 38.0, 37.2, 36.9, 36.4, 36.3, 35.6, 35.6, 30.9, 30.5, 29.2, 29.1, 26.0, 23.2, 23.1, 20.1, 19.9, 19.7, 19.6, 14.7, 14.6, 14.4, 14.3, 10.6, 10.6 ppm. HRMS m/z: calcd for $C_{21}H_{27}O$ $[M+H]^+$ 295.2062, found: 295.2062.

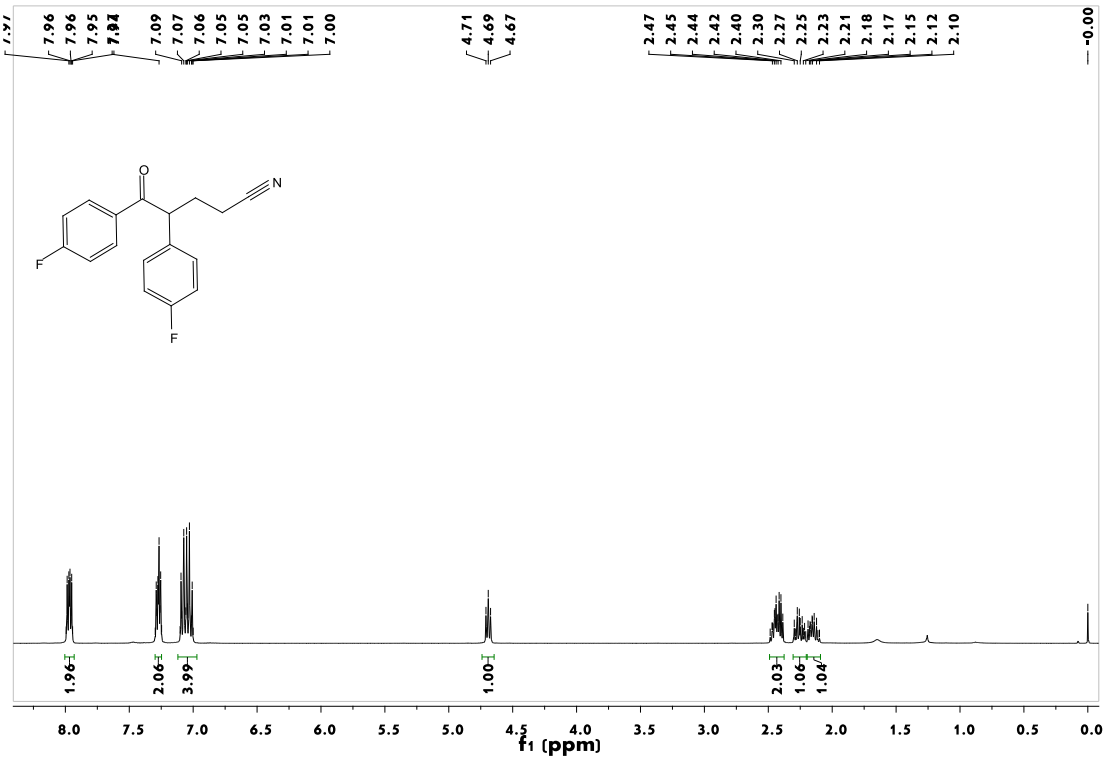
5,6-diphenyl-3,4-dihydropyridin-2(1*H*)-one (6): Yield = 50% (63 mg). White soild (M.p. 224.7–226.3 °C). IR (KBr) ν = 3195, 3080, 1665, 1638, 1384, 1291, 1215, 824, 759, 653 cm^{-1}. ^{1}H NMR (400MHz, $CDCl_3$): δ = 7.26–7.21 (m, 3H), 7.18–7.13 (m, 3H), 7.14–7.09 (m, 2H), 7.02–6.98 (m, 2H), 6.95 (s, 1H), 2.91–2.84 (m, 2H), 2.74–2.67 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 171.2, 140.1, 135.8, 133.0, 129.2, 128.8, 128.7, 128.7, 128.2, 126.4, 115.4, 77.6, 77.2, 76.9, 31.0, 28.1 ppm. HRMS m/z: calcd for $C_{17}H_{16}NO$ $[M+H]^+$ 250.1232, found: 250.1238.

2,3-diphenylpiperidine (7): Yield = 79% (78 mg). Yellow oil. IR (KBr) ν = 3289, 3026, 2935, 2866, 1678, 1451, 1043, 758, 699 cm^{-1}. ^{1}H NMR (400MHz, $CDCl_3$): δ = 7.35–7.20 (m, 8H), 7.19–7.12 (m, 2H), 4.71 (d, *J* = 7.8 Hz, 1H), 2.88–2.77 (m, 1H), 2.54–2.38 (m, 2H), 2.16 (s, 1H), 1.59–1.39 (m, 2H), 1.20–1.11 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 142.8, 141.2, 129.0, 128.7, 128.4, 127.9, 127.1, 127.1, 78.5, 77.6, 77.2, 76.9, 54.1, 41.5, 30.4, 29.0 ppm. HRMS m/z: calcd for $C_{17}H_{20}N$ $[M+H]^+$ 238.1596, found: 238.1594.

The ^{1}H , ^{13}C spectra of compounds:



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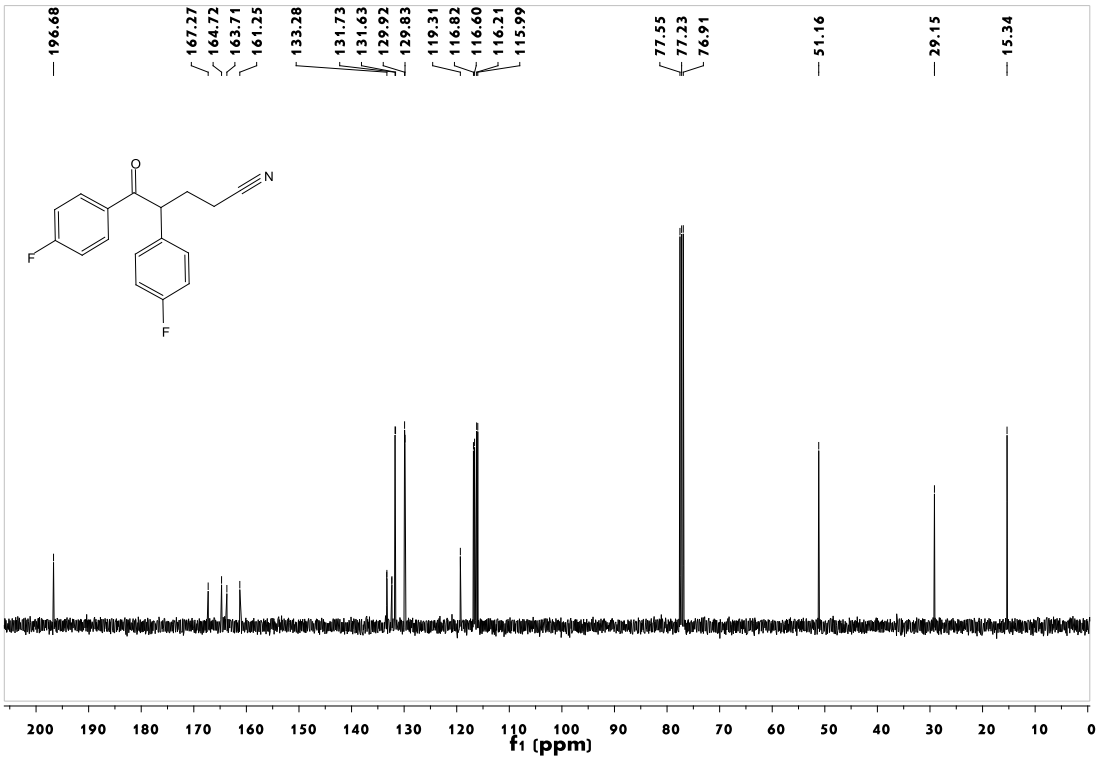
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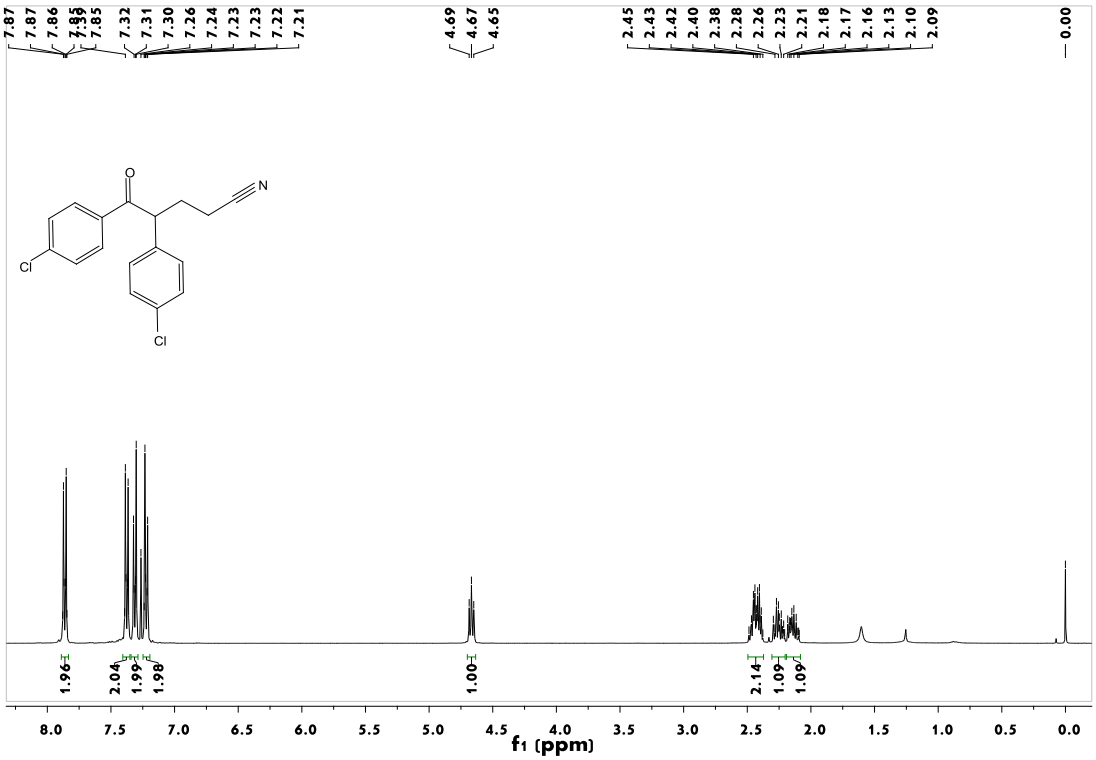
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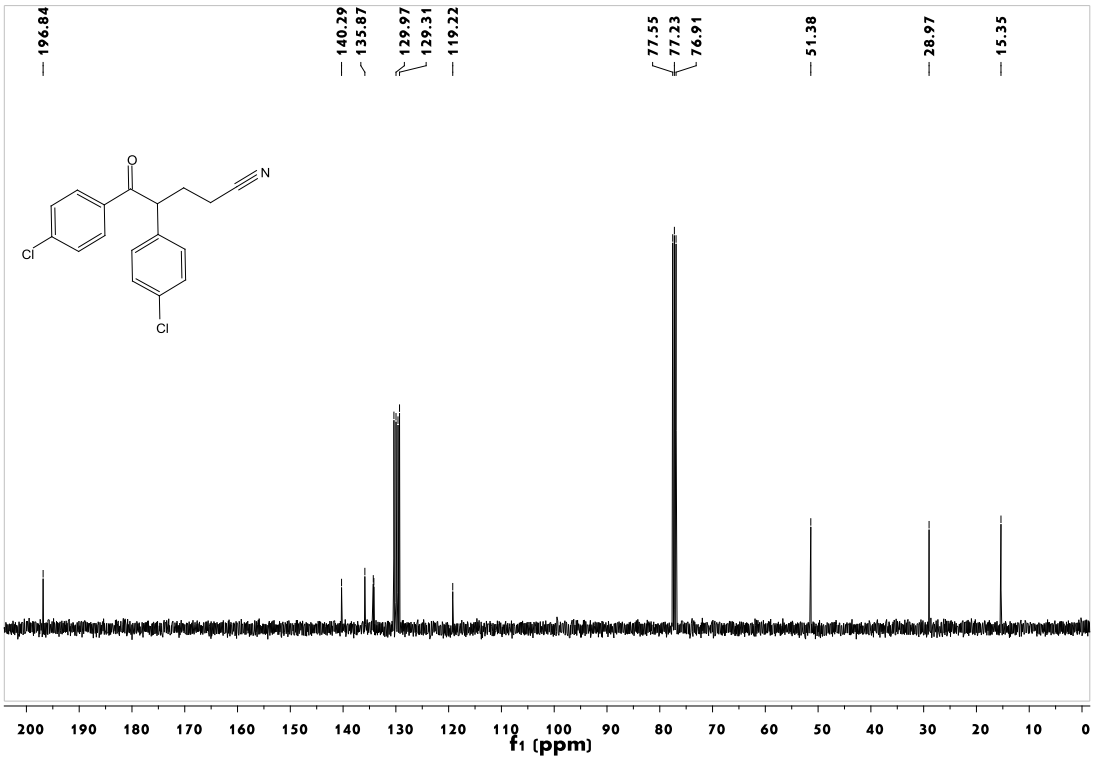
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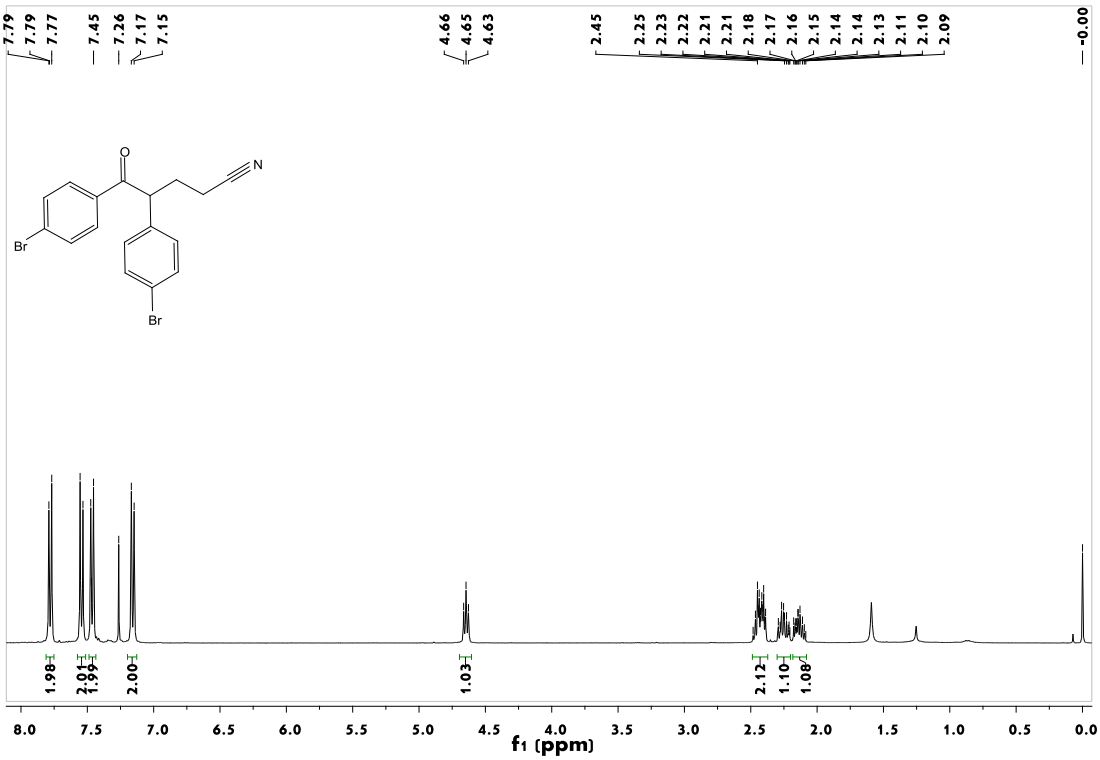
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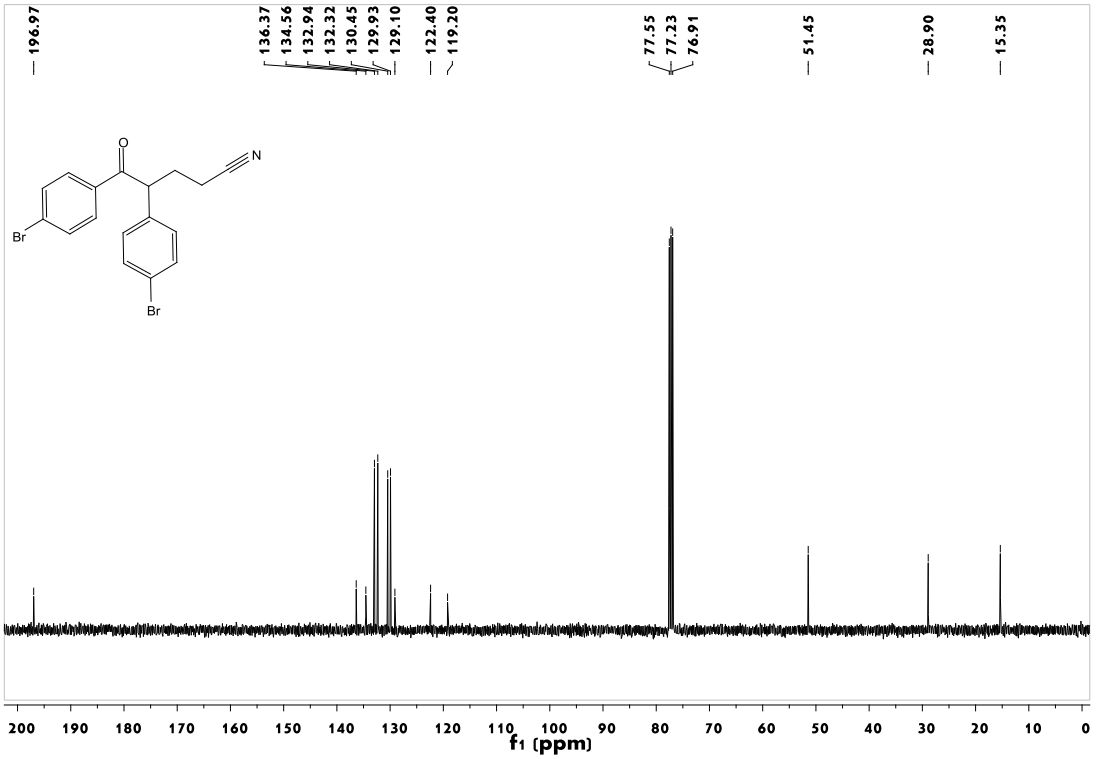
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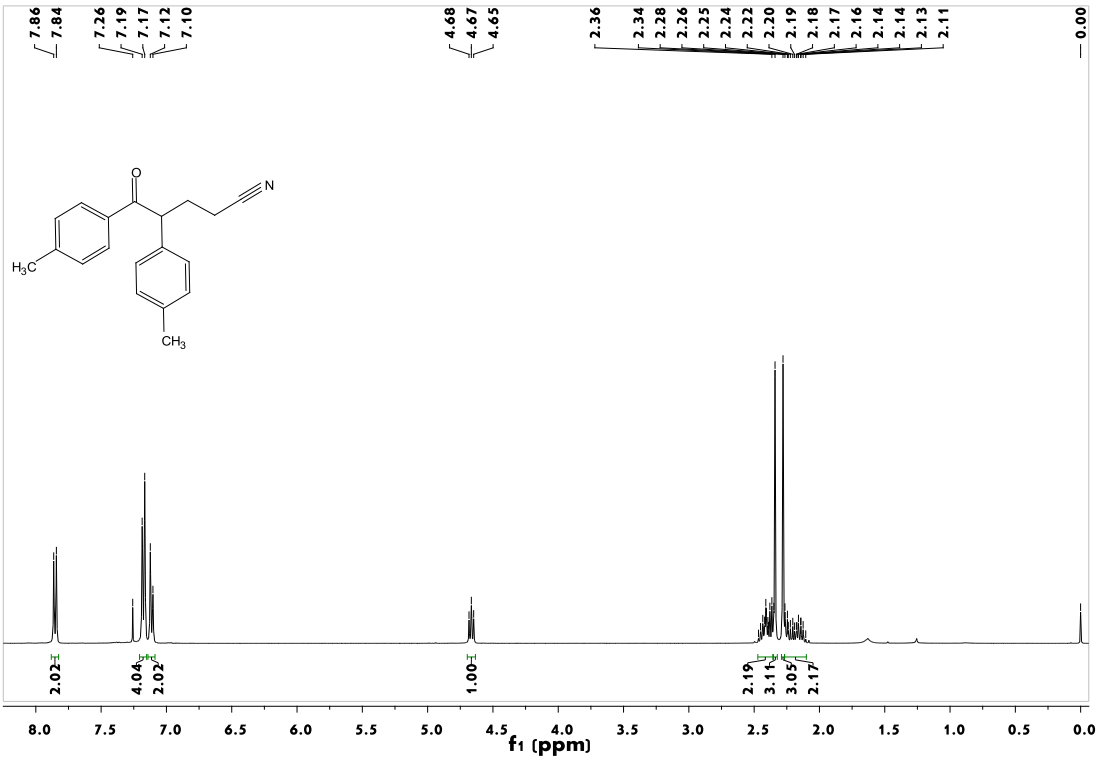
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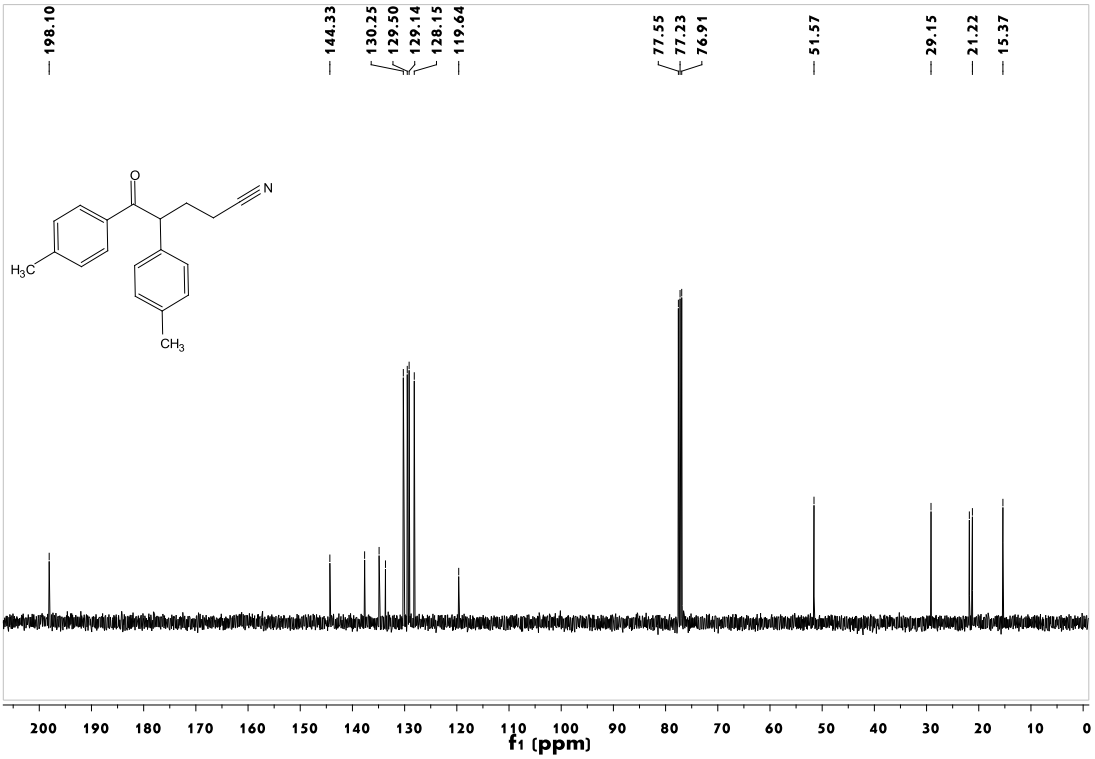
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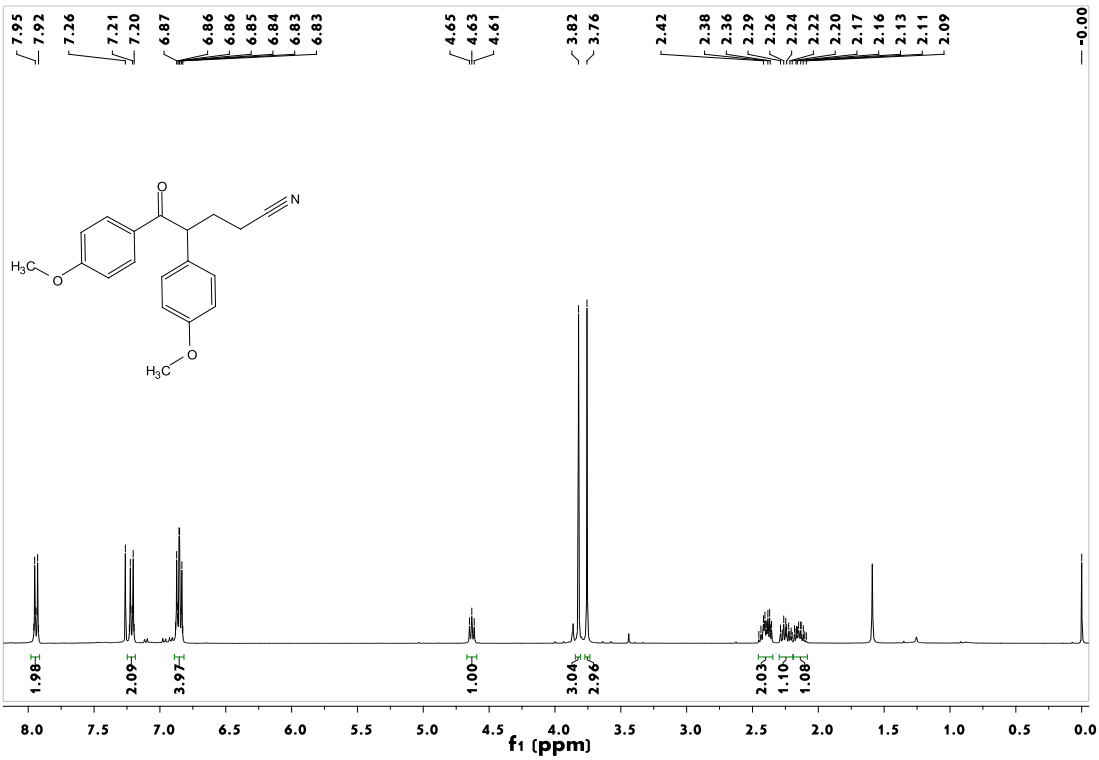
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2.16
2.13
2.11
2.09
-0.00
O
N
H3C
O
O
H3C
1.98
2.09
3.97
1.00
3.04
2.96
2.03
1.10
1.08
8.0
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7.0
6.5
6.0
5.5
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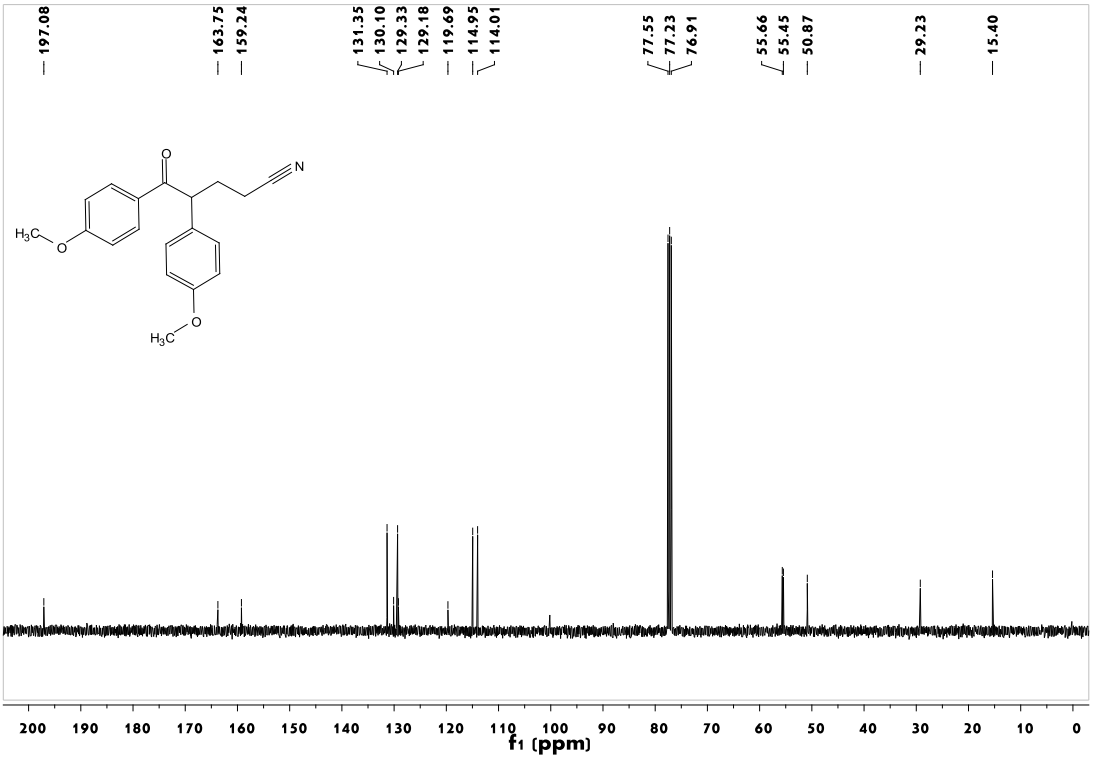
f1 (ppm)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114.01
77.55
77.23
76.91
55.66
55.45
50.87
29.23
15.40
O
N
H3C
O
O
H3C
200
190
180
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130
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110
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90
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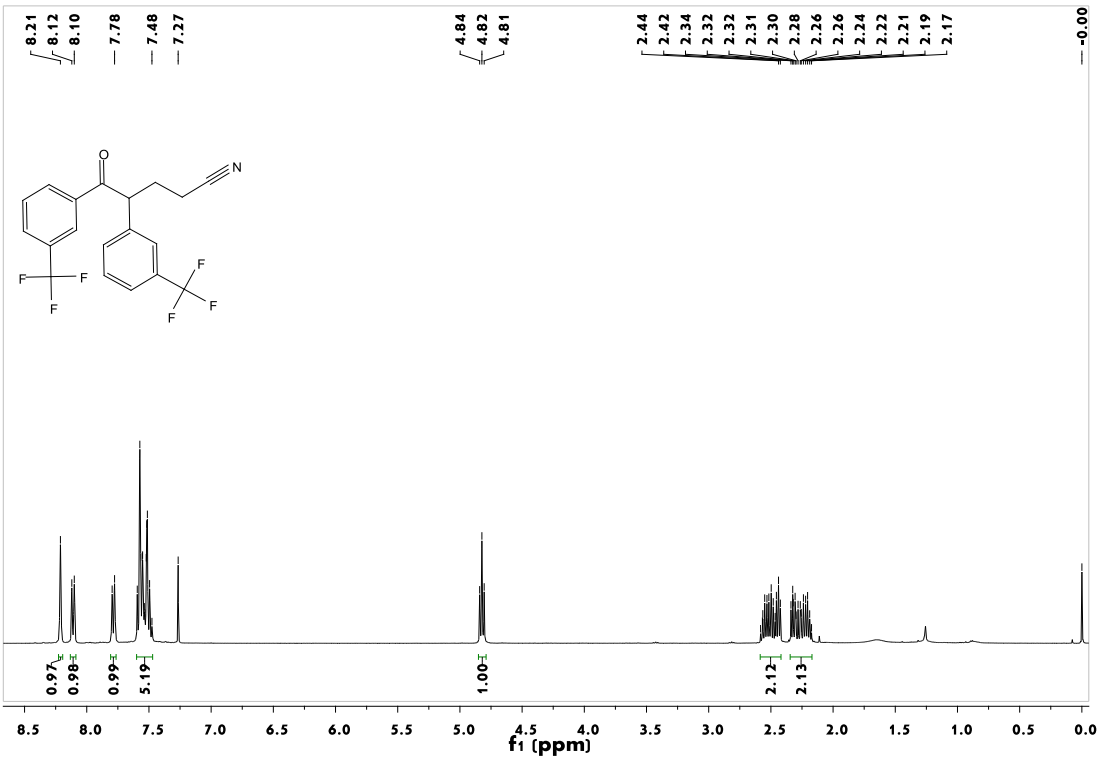
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2.34
2.32
2.32
2.31
2.30
2.28
2.26
2.26
2.24
2.22
2.21
2.19
2.17
0.00
O
N
F
F
F
F
F
F
0.97
0.98
0.99
5.19
1.00
2.12
2.13
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
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1.5
1.0
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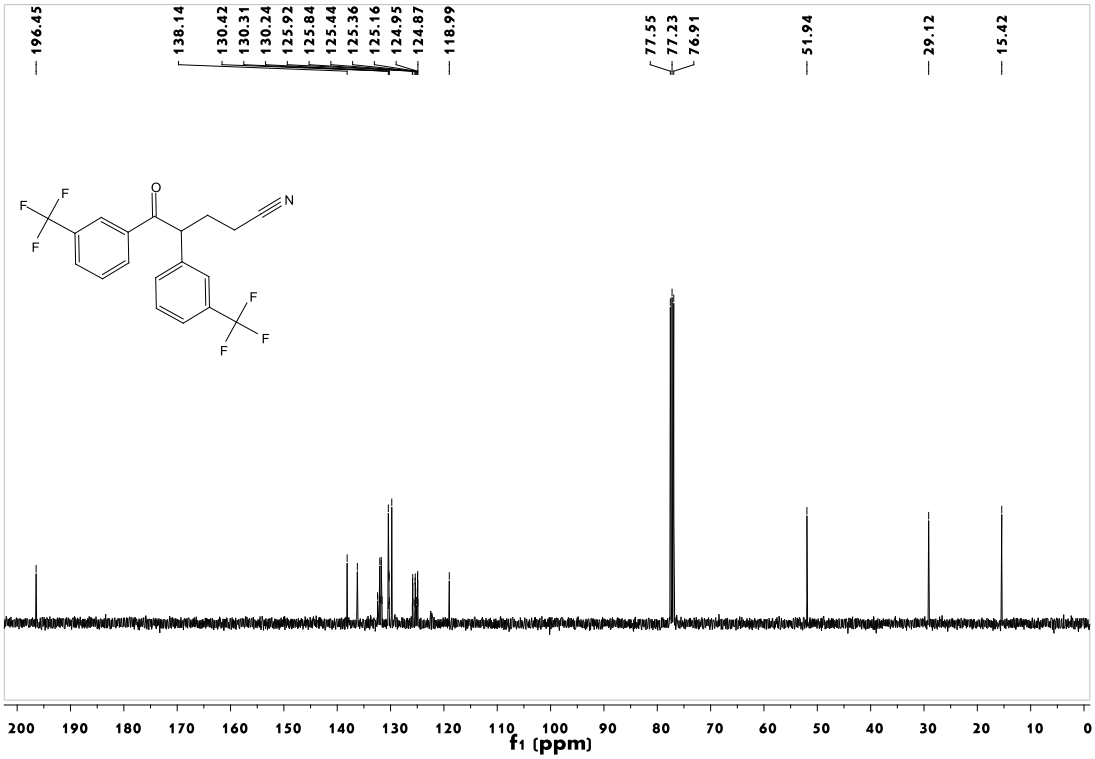
0.0
f1 (ppm)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125.16
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124.87
118.99
77.55
77.23
76.91
51.94
29.12
15.42
O
N
F
F
F
F
F
F
200
190
180
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50
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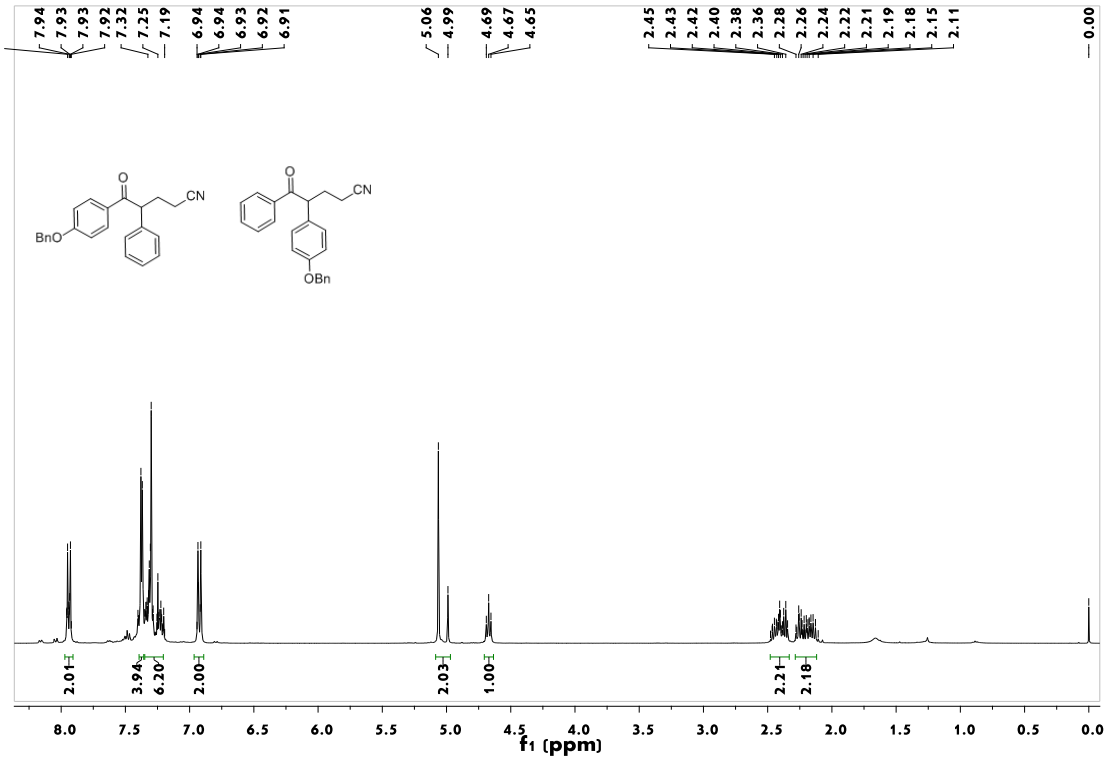
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7.92
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6.94
6.94
6.93
6.92
6.91
5.06
4.99
4.69
4.67
4.65
2.45
2.43
2.42
2.40
2.38
2.36
2.28
2.26
2.24
2.22
2.21
2.19
2.18
2.15
2.11
0.00
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OBn
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1.00
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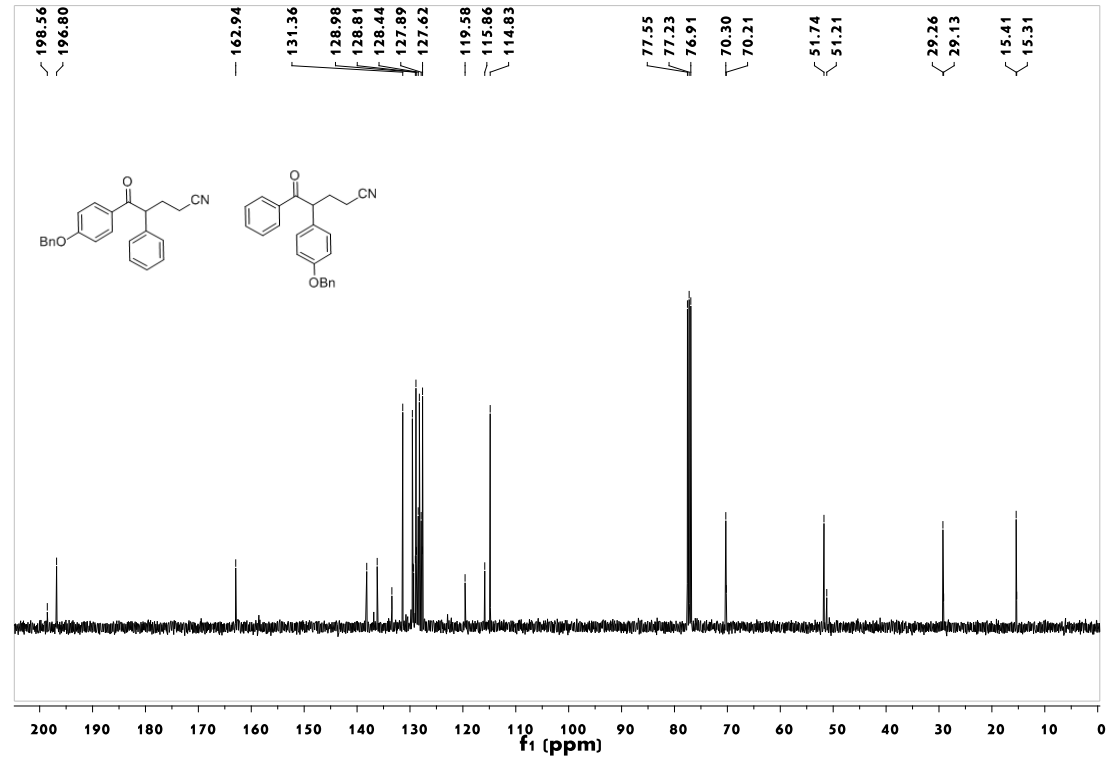
2.18
f1 (ppm)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115.86
114.83
77.55
77.23
76.91
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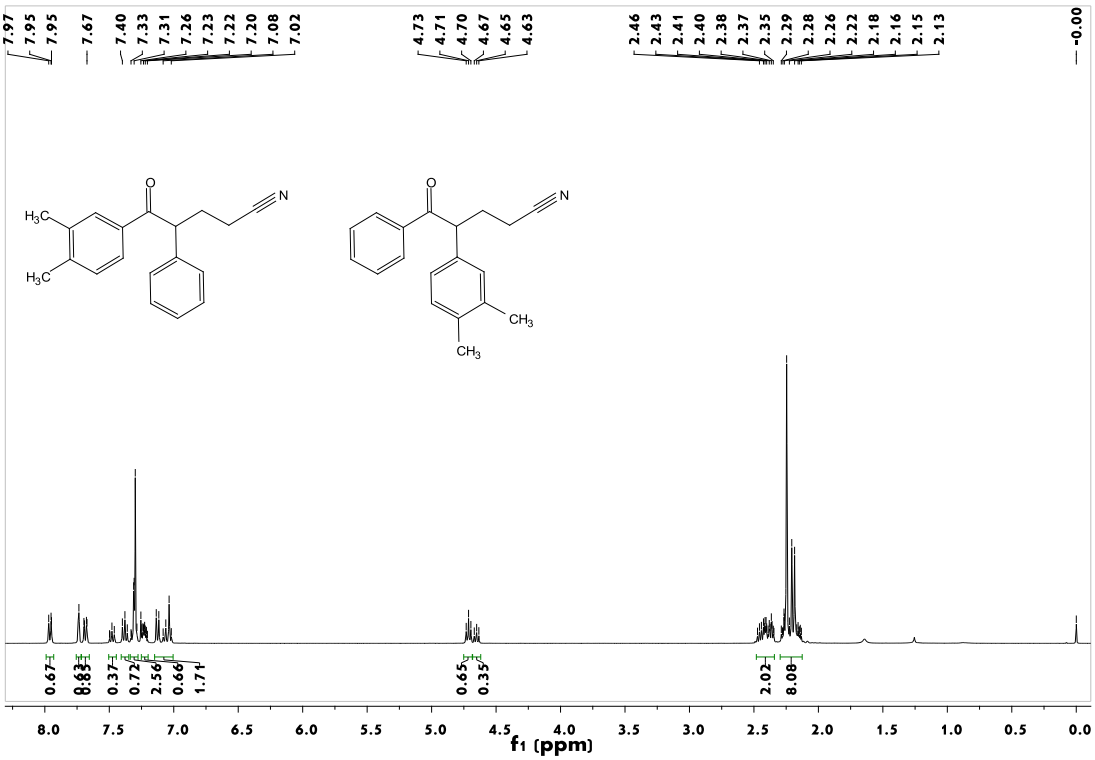
51.21
29.26
29.13
15.41
15.31
BnO
CN
OBn
f1 (ppm)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7.22
7.20
7.08
7.02
4.73
4.71
4.70
4.67
4.65
4.63
2.46
2.43
2.41
2.40
2.38
2.37
2.35
2.29
2.28
2.26
2.22
2.18
2.16
2.15
2.13
-0.00
O
N
H3C
H3C
CH3
CH3
0.67
0.37
0.72
2.56
0.66
1.71
0.65
0.35
2.02
8.08
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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3.5
3.0
2.5
2.0
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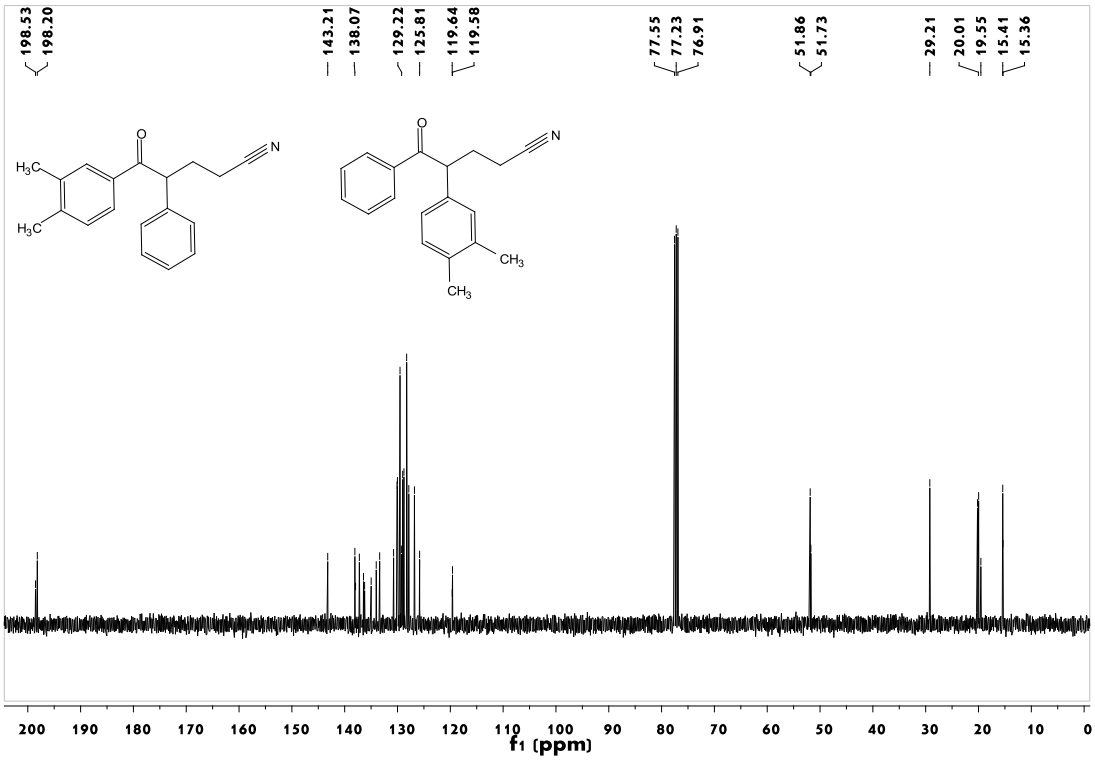
1.0
0.5
0.0
f1 (ppm)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129.22
125.81
119.64
119.58
77.55
77.23
76.91
51.86
51.73
29.21
20.01
19.55
15.41
15.36
O
N
H3C
H3C
CH3
CH3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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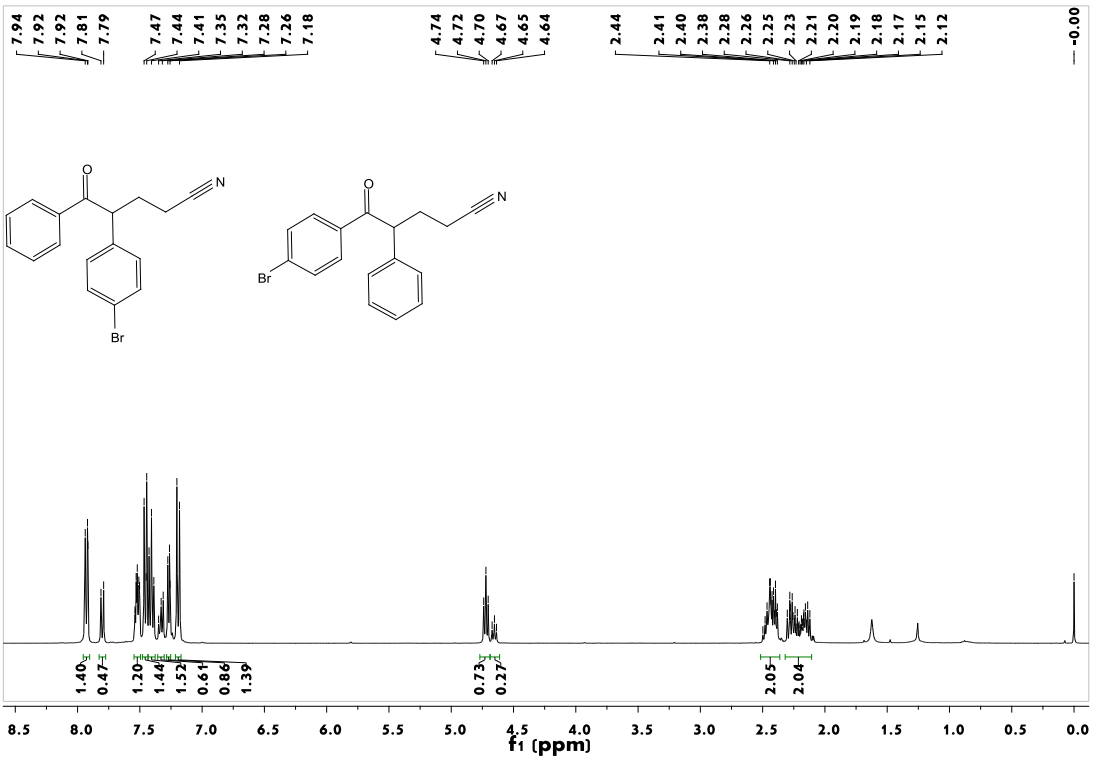
50
40
30
20
10
0
f1 (ppm)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7.92
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7.41
7.35
7.32
7.28
7.26
7.18
4.74
4.72
4.70
4.67
4.65
4.64
2.44
2.41
2.40
2.38
2.28
2.26
2.25
2.23
2.21
2.20
2.19
2.18
2.17
2.15
2.12
-0.00
O
N
Br
O
N
Br
1.40
0.47
1.20
1.44
1.52
0.61
0.86
1.39
0.73
0.27
2.05
2.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
2.0
1.5
1.0
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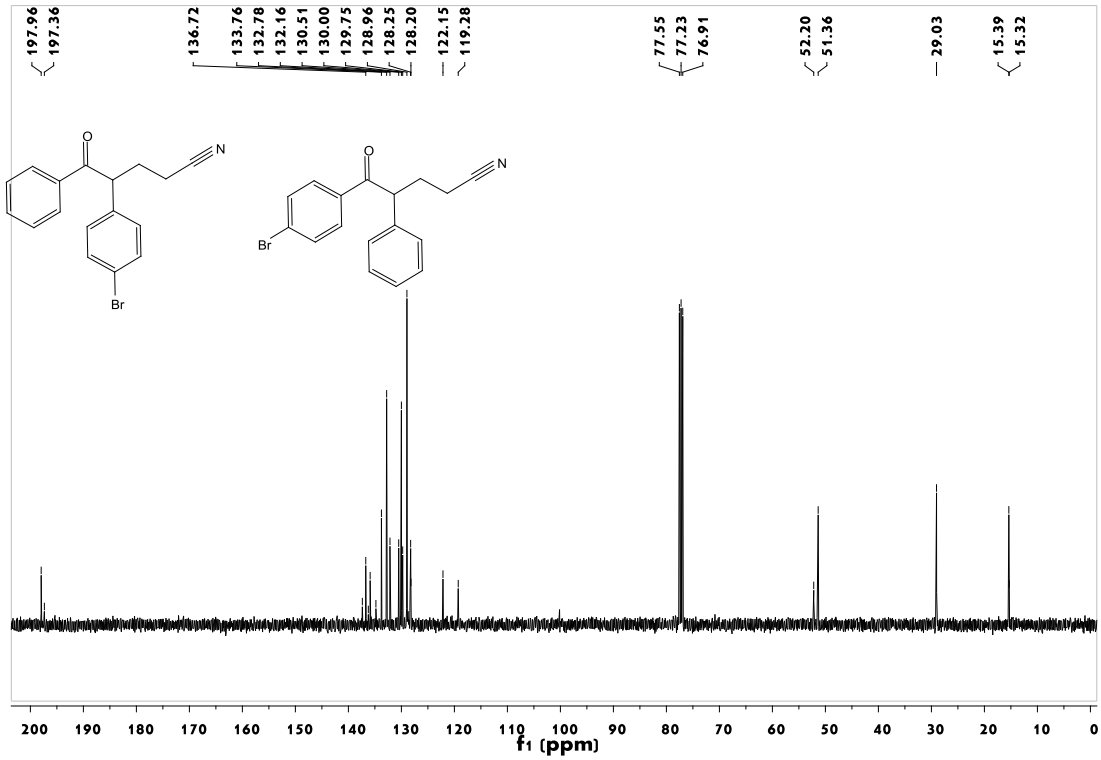
0.0
f1 (ppm)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128.25
128.20
122.15
119.28
77.55
77.23
76.91
52.20
51.36
29.03
15.39
15.32
O
N
Br
O
N
Br
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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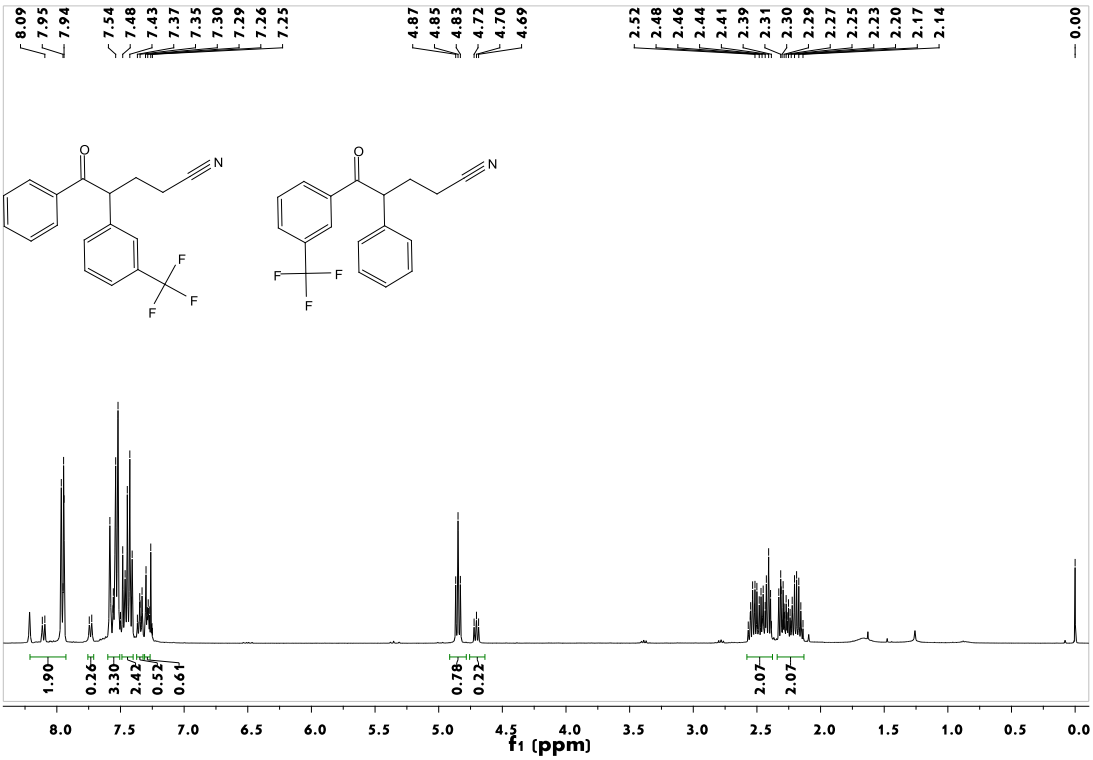
50
40
30
20
10
0
f1 (ppm)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7.43
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7.35
7.30
7.29
7.26
7.25
4.87
4.85
4.83
4.72
4.70
4.69
2.52
2.48
2.46
2.44
2.41
2.39
2.31
2.30
2.29
2.27
2.25
2.23
2.20
2.17
2.14
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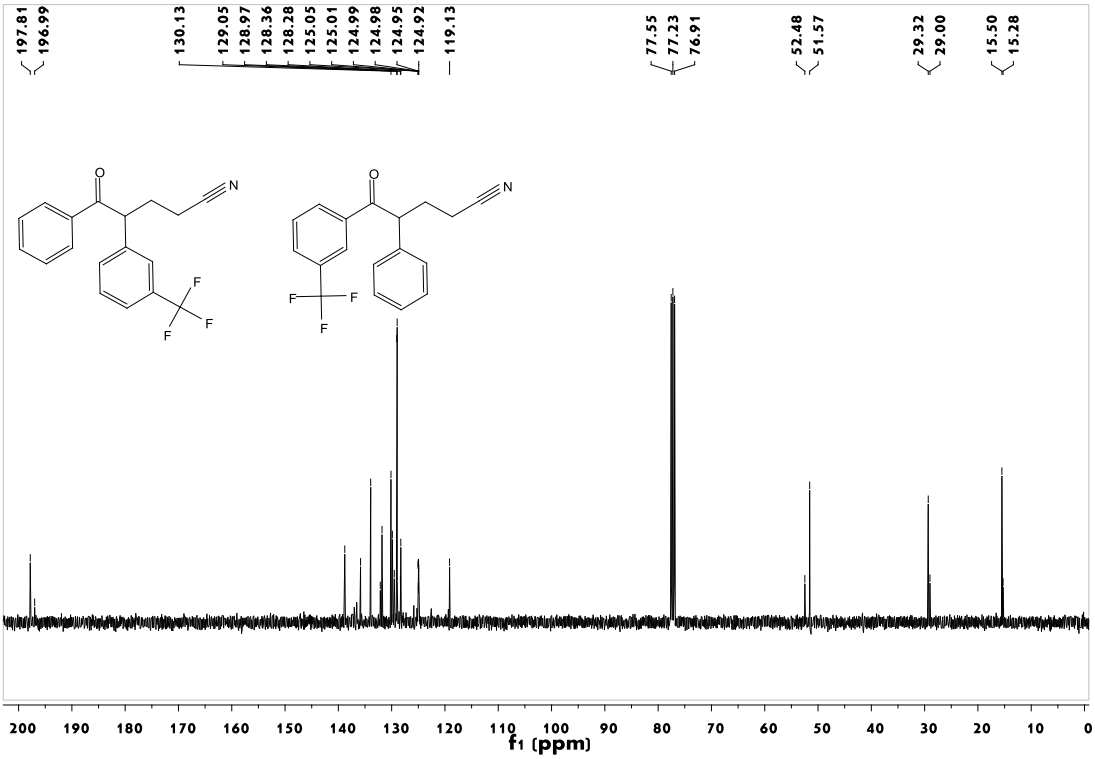
3.30
2.42
0.52
0.61
0.78
0.22
2.07
2.07
f1 (ppm)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124.98
124.95
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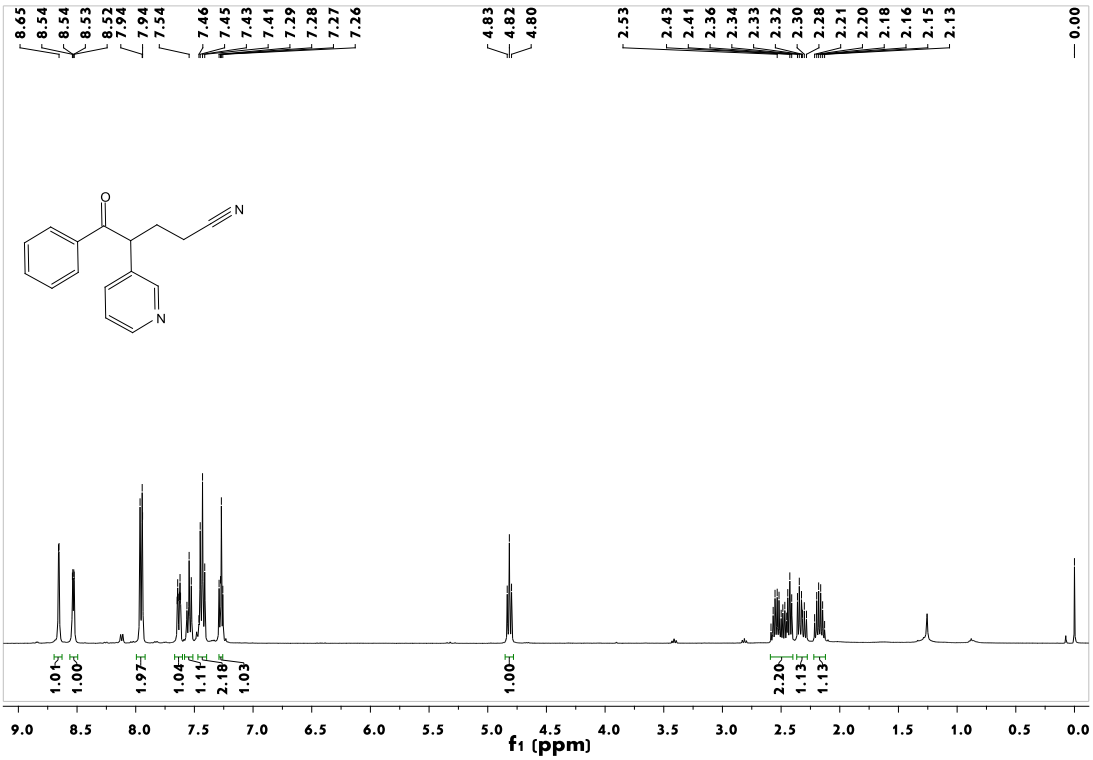
77.23
76.91
52.48
51.57
29.32
29.00
15.50
15.28
f1 (ppm)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7.94
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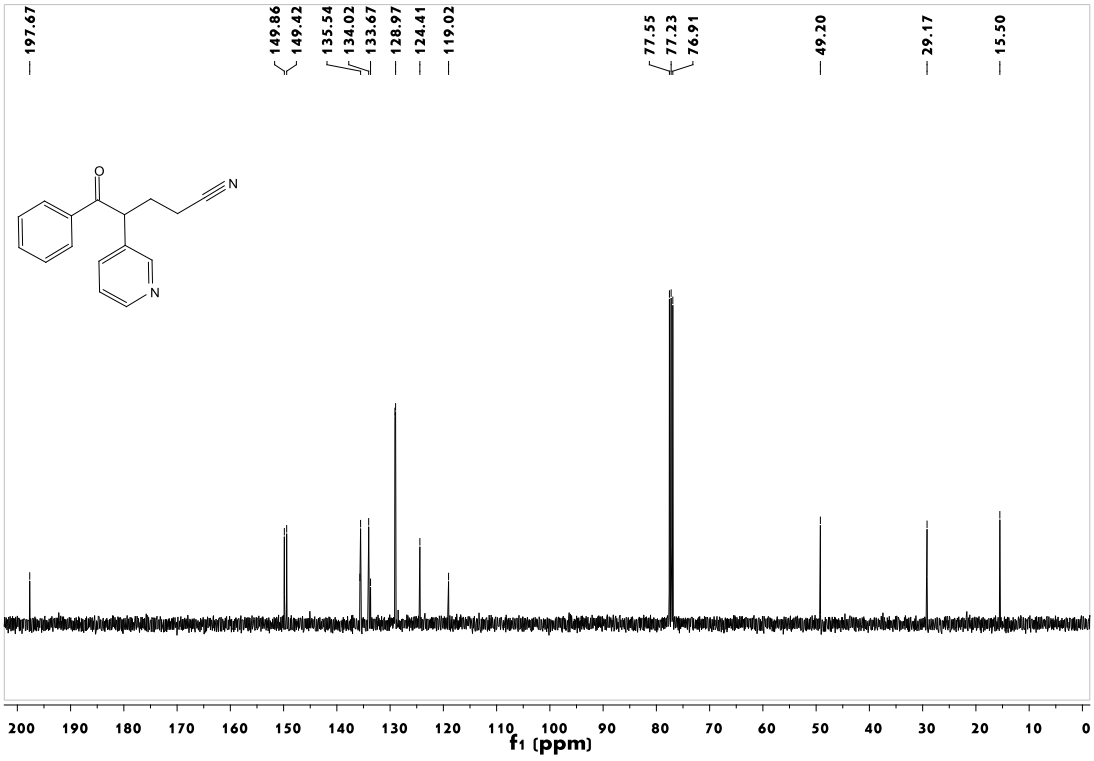
7.28
7.27
7.26
4.83
4.82
4.80
2.53
2.43
2.41
2.36
2.34
2.33
2.32
2.30
2.28
2.21
2.20
2.18
2.16
2.15
2.13
0.00
O
N
N
1.01
1.00
1.97
1.04
1.11
2.18
1.03
1.00
2.20
1.13
1.13
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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124.41
119.02
77.55
77.23
76.91
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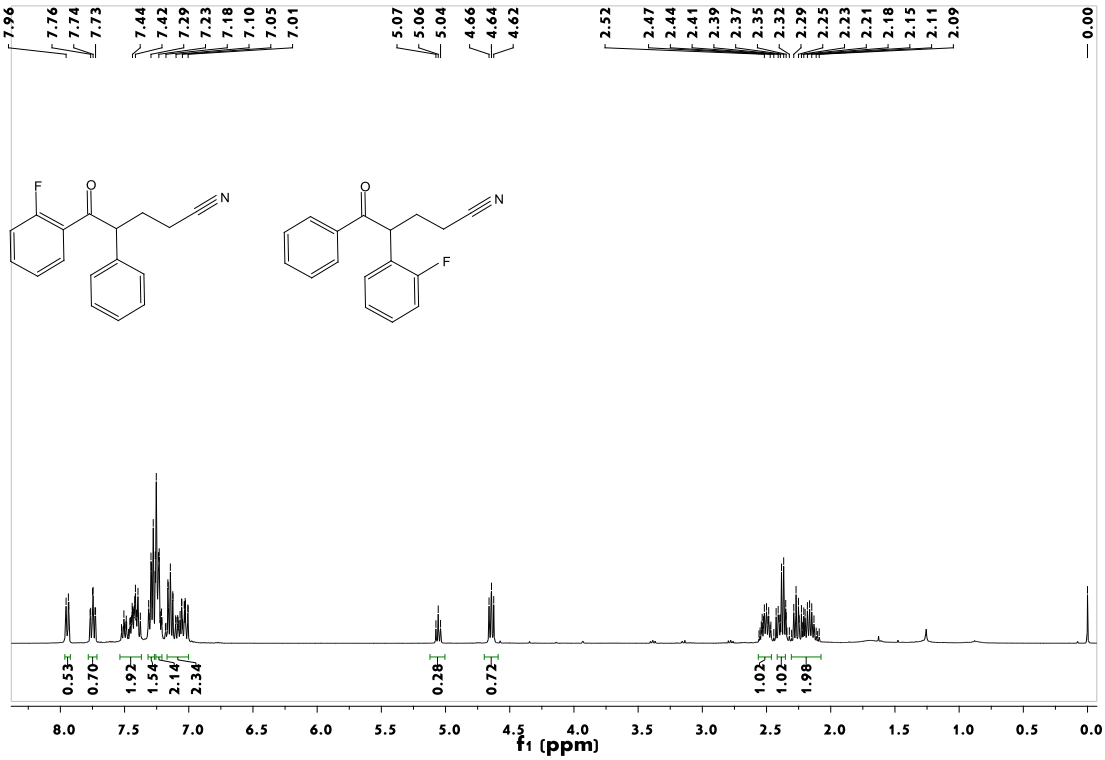
29.17
15.50
O
N
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.10
7.05
7.01
5.07
5.06
5.04
4.66
4.64
4.62
2.52
2.47
2.44
2.41
2.39
2.37
2.35
2.32
2.29
2.25
2.23
2.21
2.18
2.15
2.11
2.09
0.00
F
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N
O
N
F
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0.70
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1.54
2.14
2.34
0.28
0.72
1.02
1.02
1.98
8.0
7.5
7.0
6.5
6.0
5.5
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
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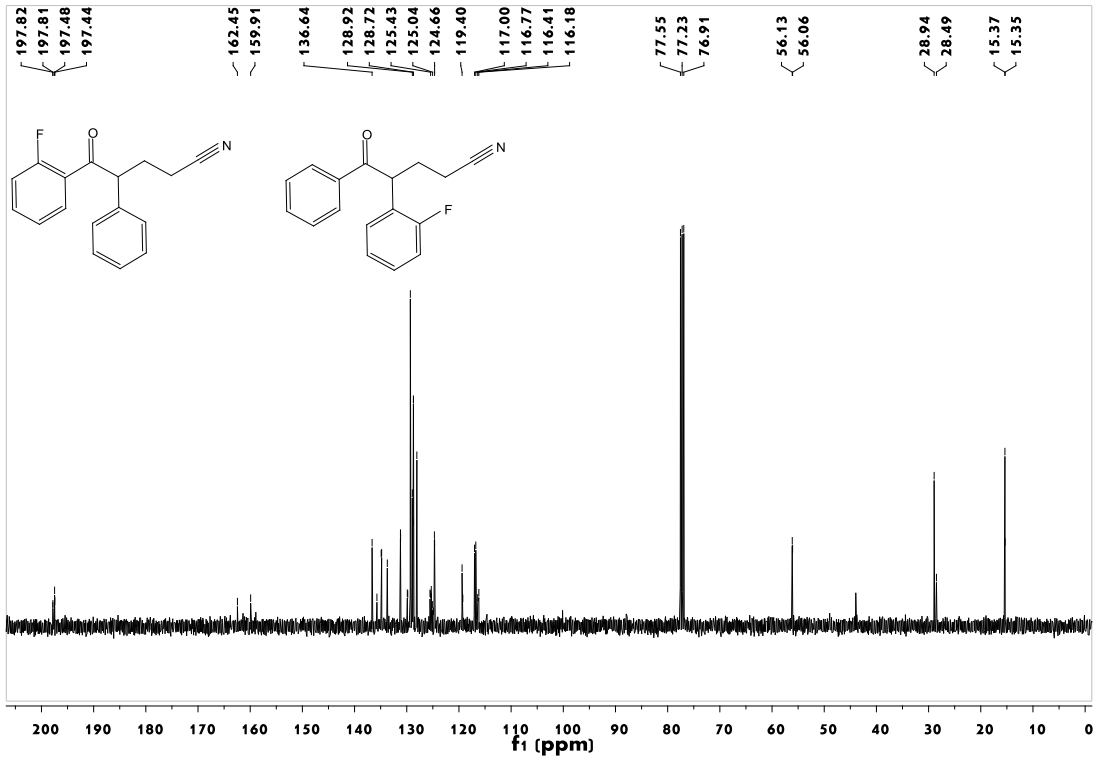
0.0
f1 (ppm)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159.91
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128.92
128.72
125.43
125.04
124.66
119.40
117.00
116.77
116.41
116.18
77.55
77.23
76.91
56.13
56.06
28.94
28.49
15.37
15.35
F
O
N
O
N
F
200
190
180
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130
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110
100
90
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70
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50
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30
20
10
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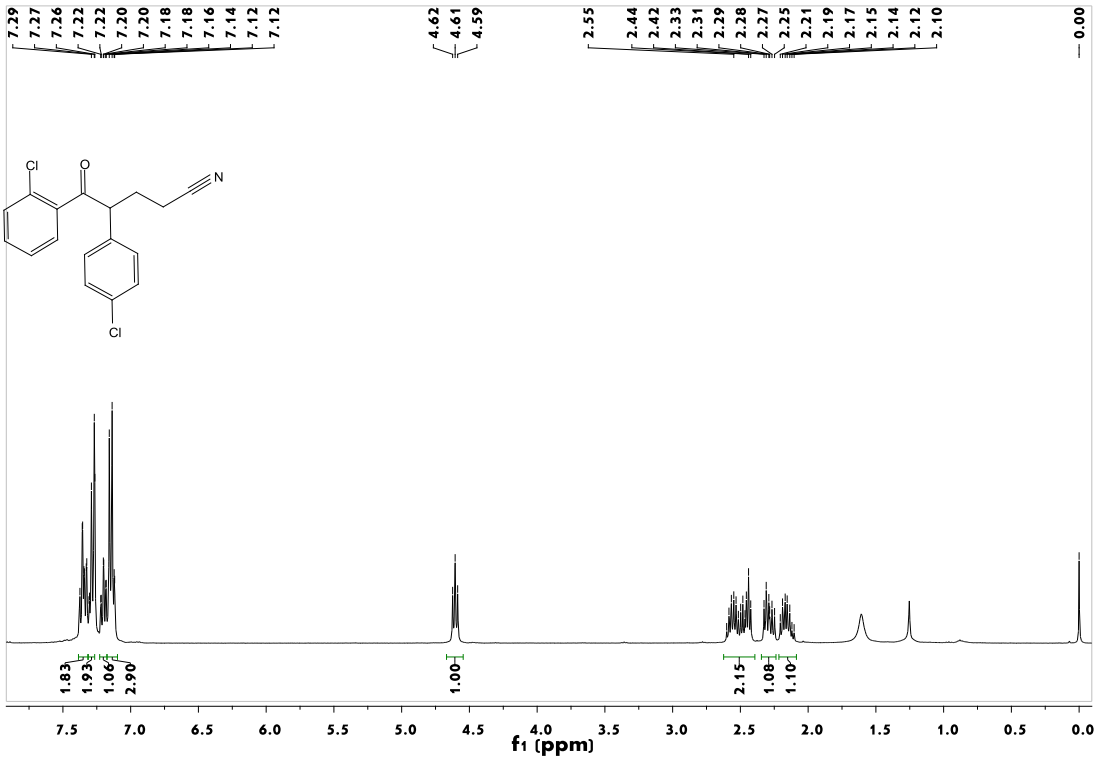
f1 (ppm)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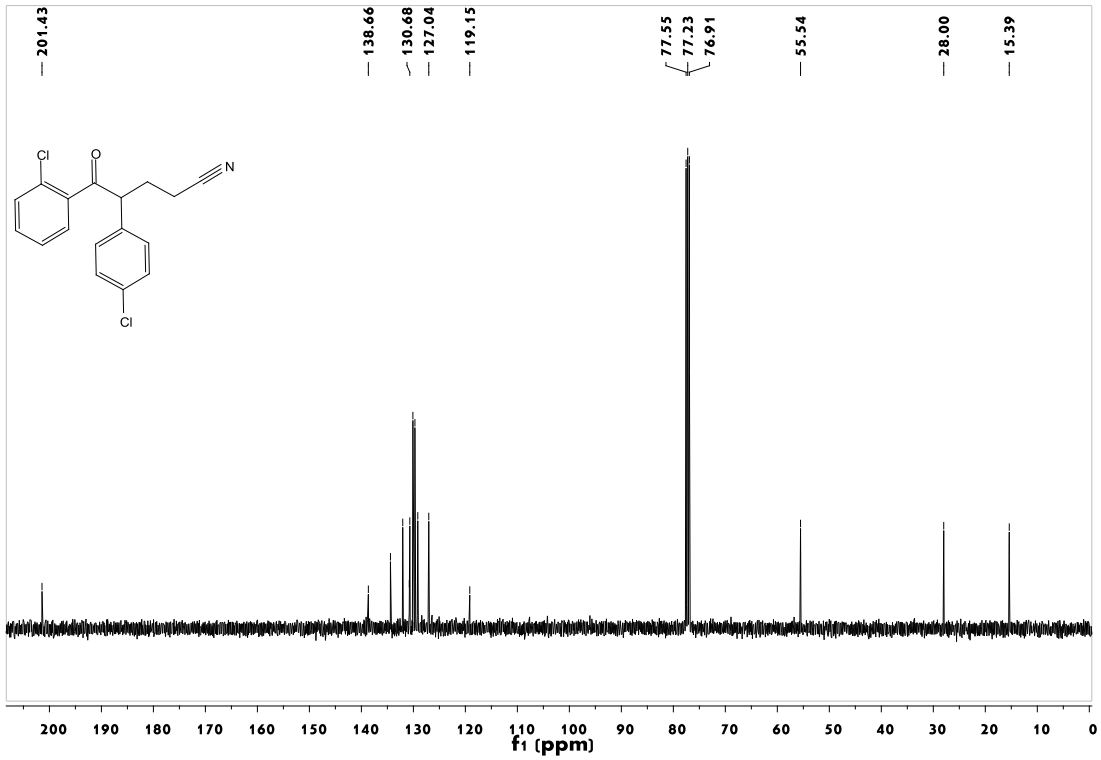
4.62 4.61 4.59
2.55 2.44 2.42 2.33 2.31 2.29 2.28 2.27 2.25 2.21 2.19 2.17 2.15 2.14 2.12 2.10
0.00
Cl
O
N
Cl
1.83 1.93 1.06 2.90
1.00
2.15 1.08 1.10
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.23
76.91
55.54
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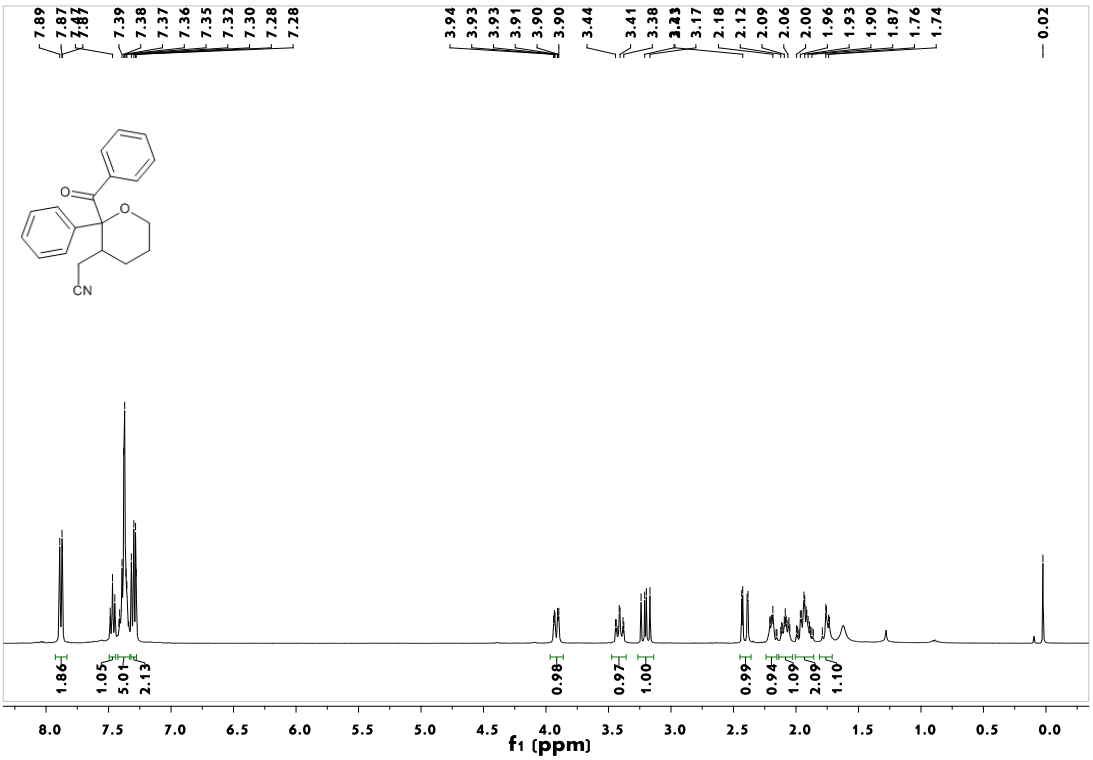
15.39
Cl
O
N
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.32
7.30
7.28
3.94
3.93
3.91
3.90
3.44
3.41
3.38
3.17
2.18
2.12
2.09
2.06
2.00
1.96
1.93
1.90
1.87
1.76
1.74
0.02
O
O
CN
1.86
1.05
5.01
2.13
0.98
0.97
1.00
0.99
0.94
1.09
2.09
1.10
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
1.5
1.0
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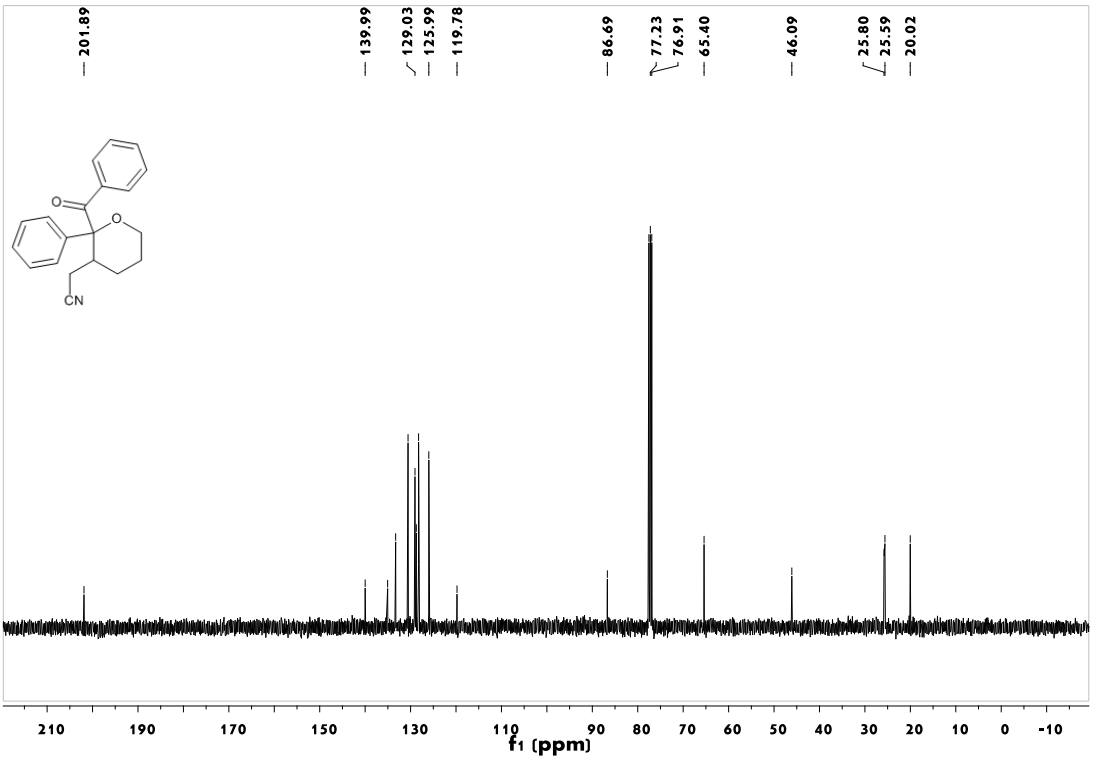
0.0
f1 (ppm)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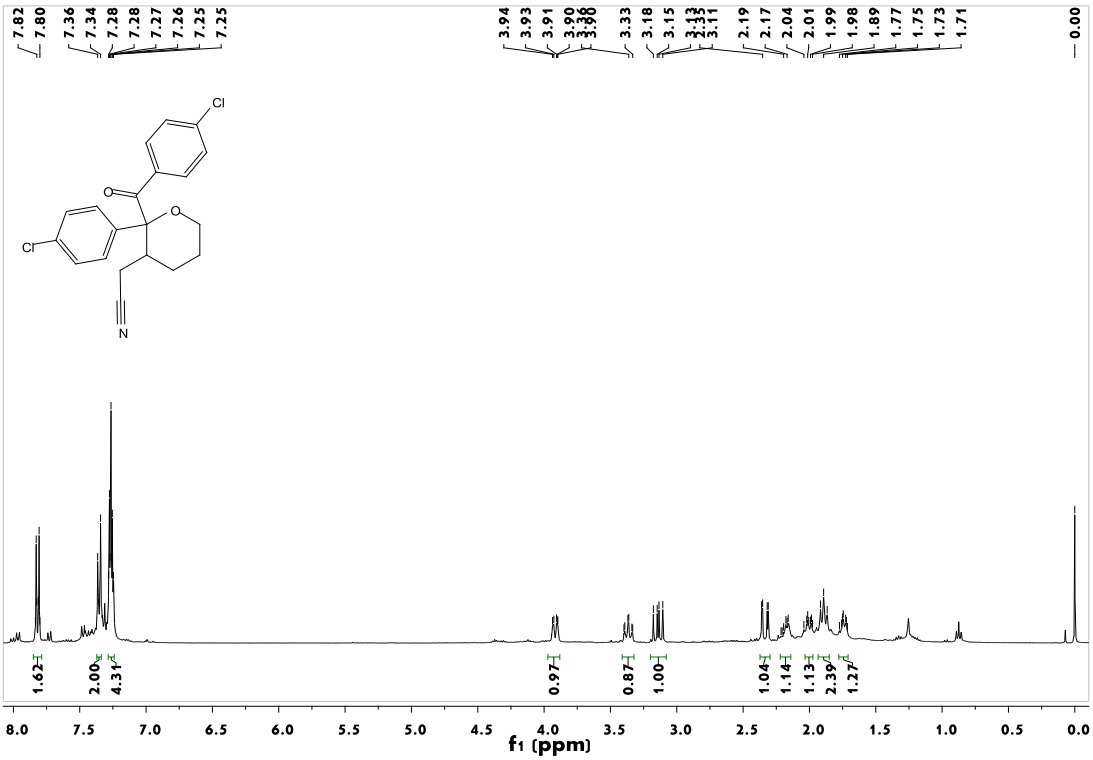
76.91
65.40
46.09
25.80
25.59
20.02
O
O
CN
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.80
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7.34
7.28
7.28
7.27
7.26
7.25
7.25
3.94
3.93
3.91
3.90
3.33
3.18
3.15
3.11
2.19
2.17
2.04
2.01
1.99
1.98
1.89
1.77
1.75
1.73
1.71
0.00
Cl
O
O
Cl
N
1.62
2.00
4.31
0.97
0.87
1.00
1.04
1.14
1.13
2.39
1.27
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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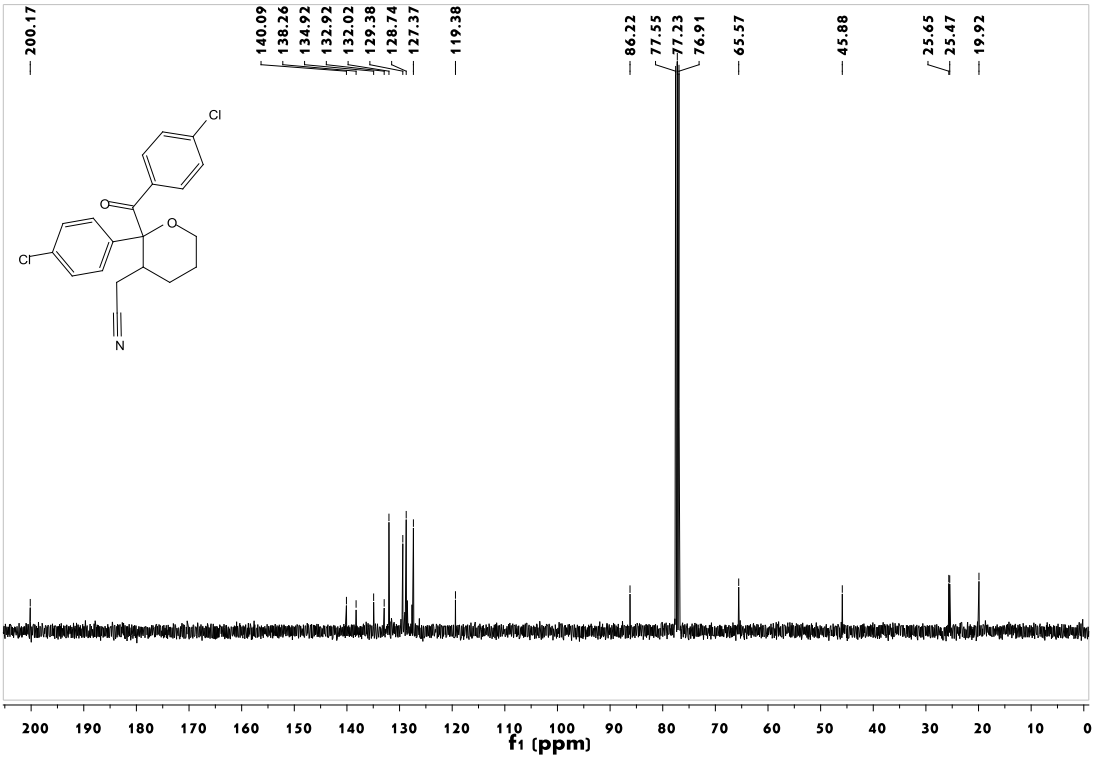
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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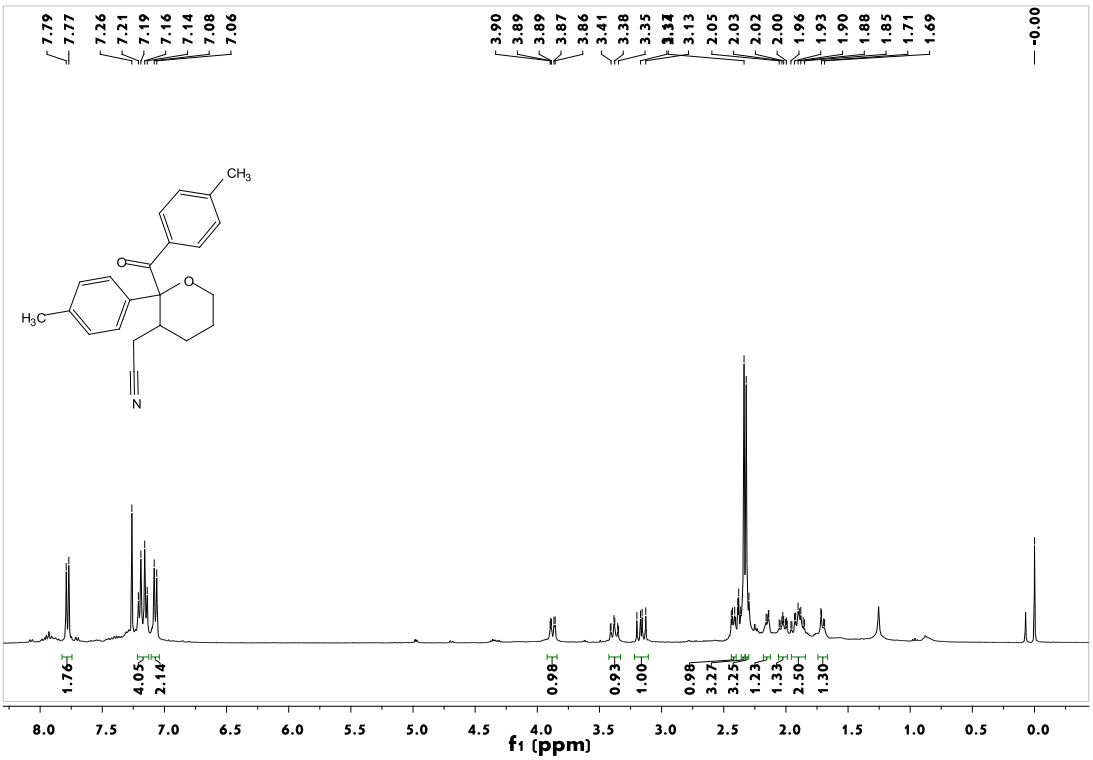
132.92
132.02
129.38
128.74
127.37
119.38
86.22
77.55
77.23
76.91
65.57
45.88
25.65
25.47
19.92
Cl
O
O
Cl
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.77
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7.21
7.19
7.16
7.14
7.08
7.06
3.90
3.89
3.89
3.87
3.86
3.41
3.38
3.35
3.13
2.05
2.03
2.02
2.00
1.96
1.93
1.90
1.88
1.85
1.71
1.69
-0.00
CH3
O
O
H3C
N
1.76
4.05
2.14
0.98
0.93
1.00
0.98
3.27
3.25
1.23
1.33
2.50
1.30
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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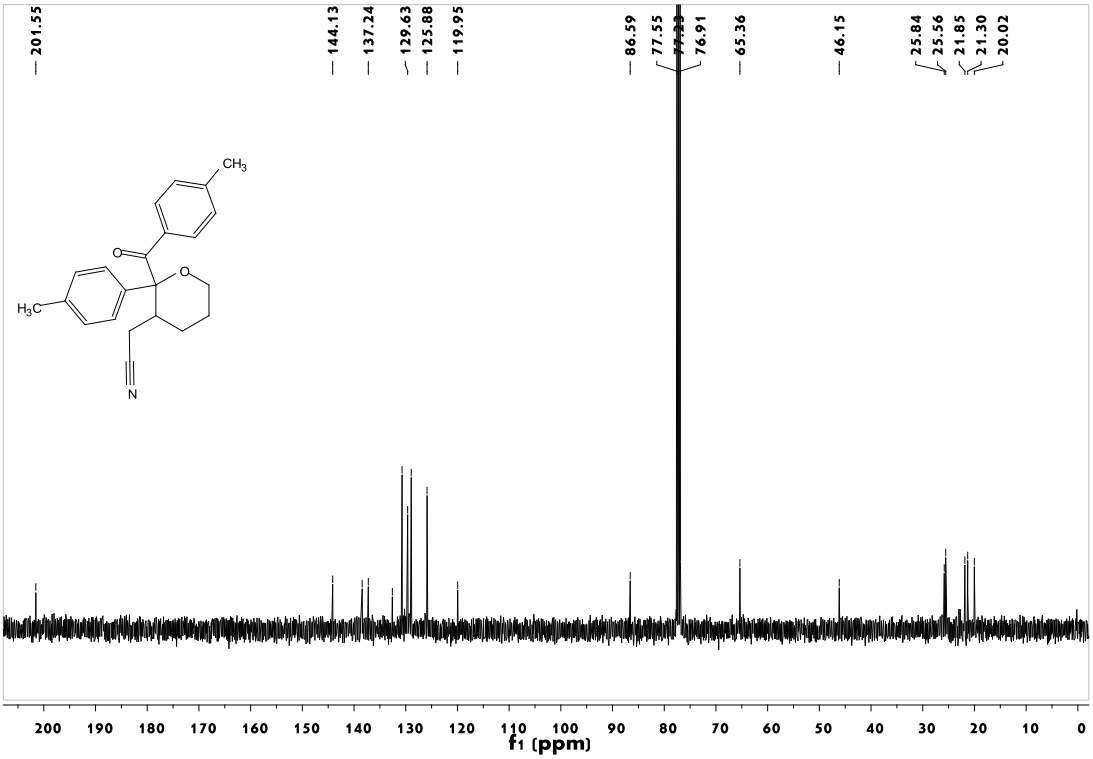
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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119.95
86.59
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76.91
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25.56
21.85
21.30
20.02
CH3
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H3C
N
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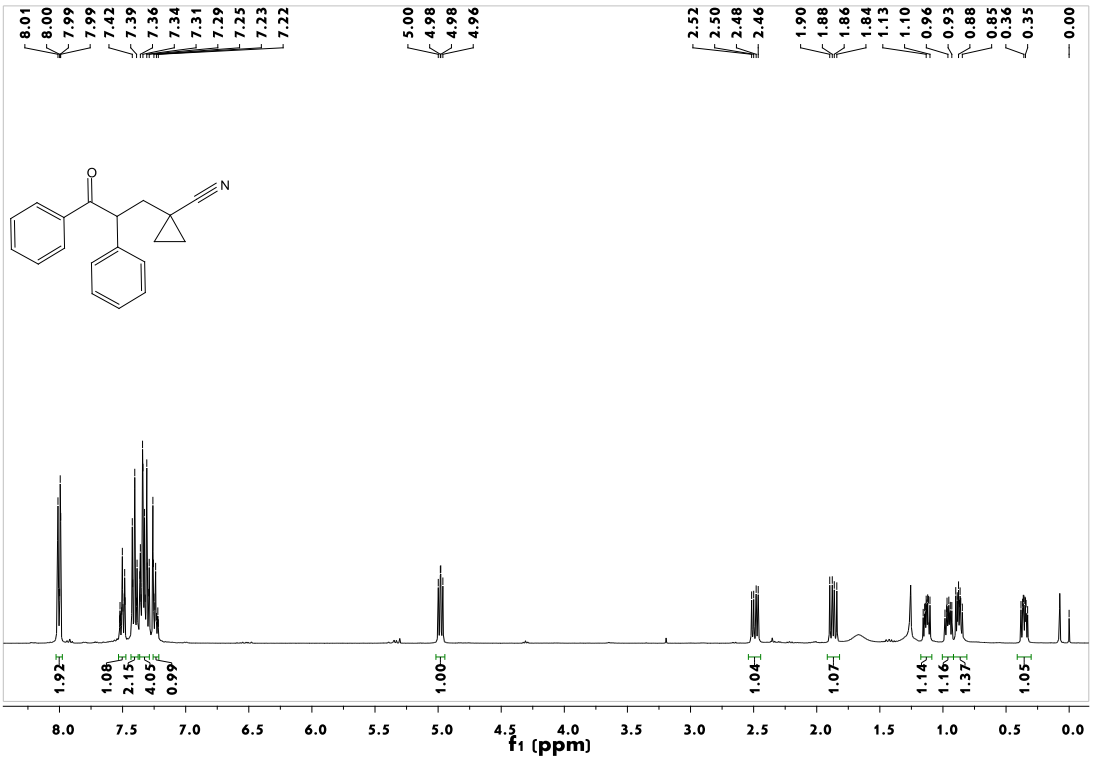
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O
N
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1.37
1.05
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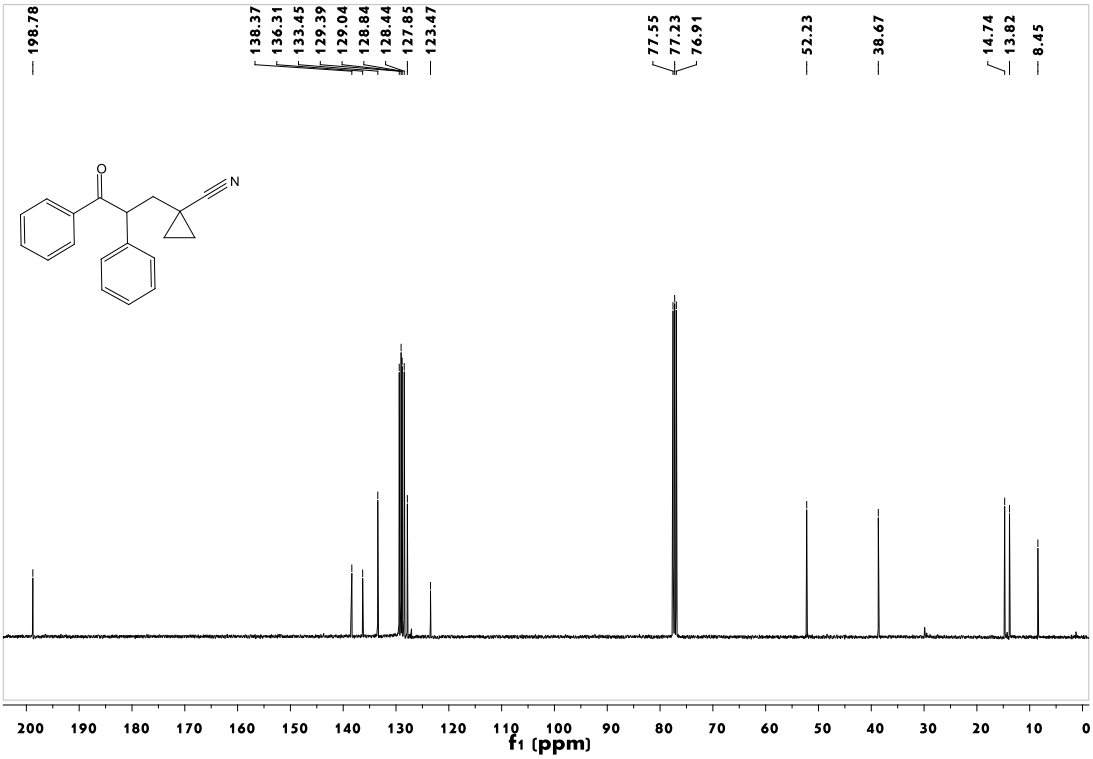
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52.23
38.67
14.74
13.82
8.45
O
N
200
190
180
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90
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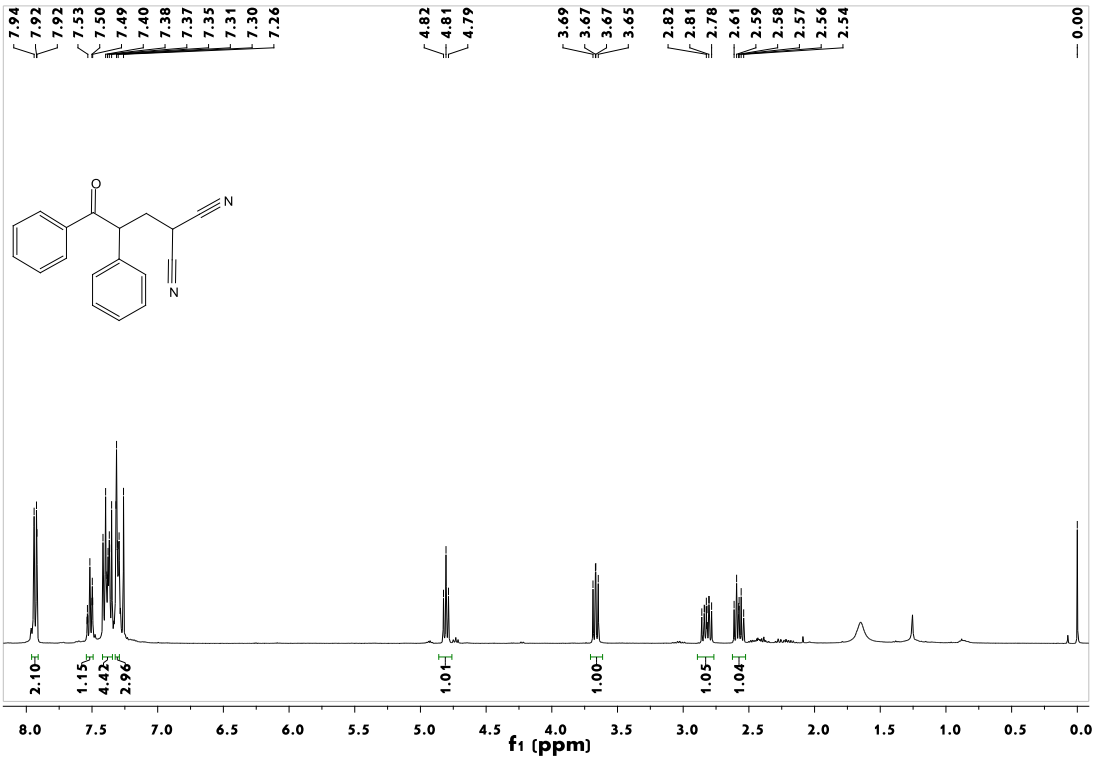
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4.79
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3.67
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2.82
2.81
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2.59
2.58
2.57
2.56
2.54
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N
N
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1.00
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1.04
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7.0
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6.0
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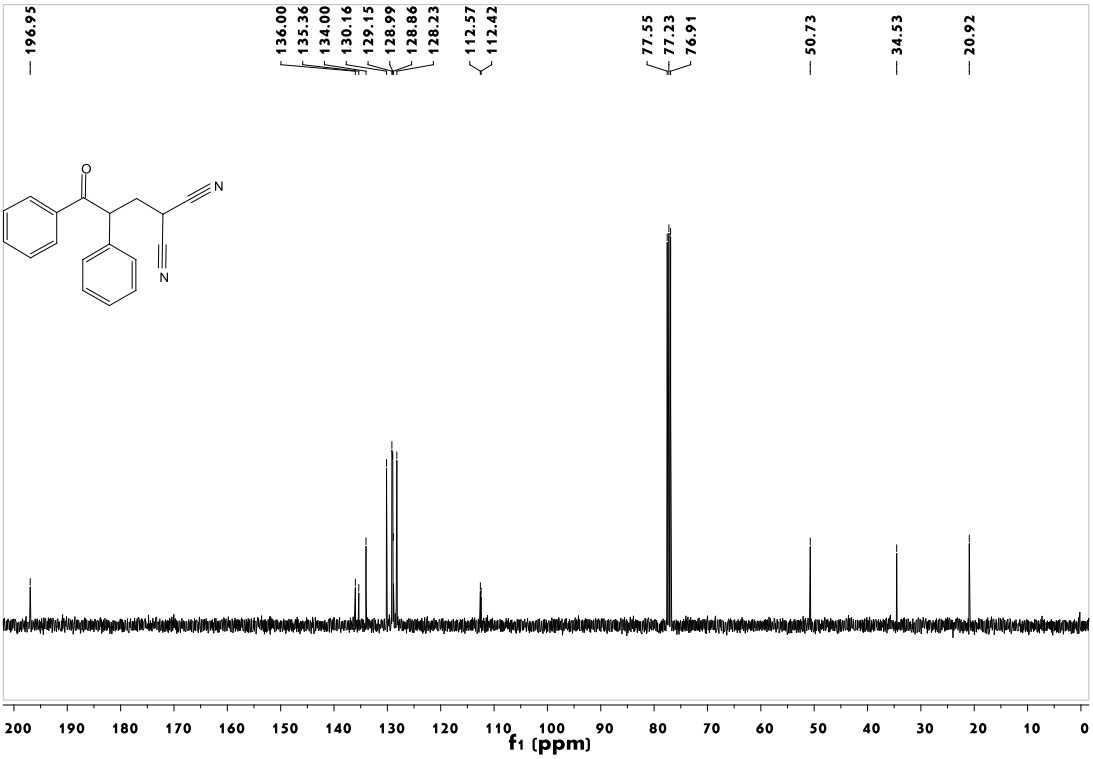
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76.91
50.73
34.53
20.92
O
N
N
200
190
180
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120
110
100
90
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50
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10
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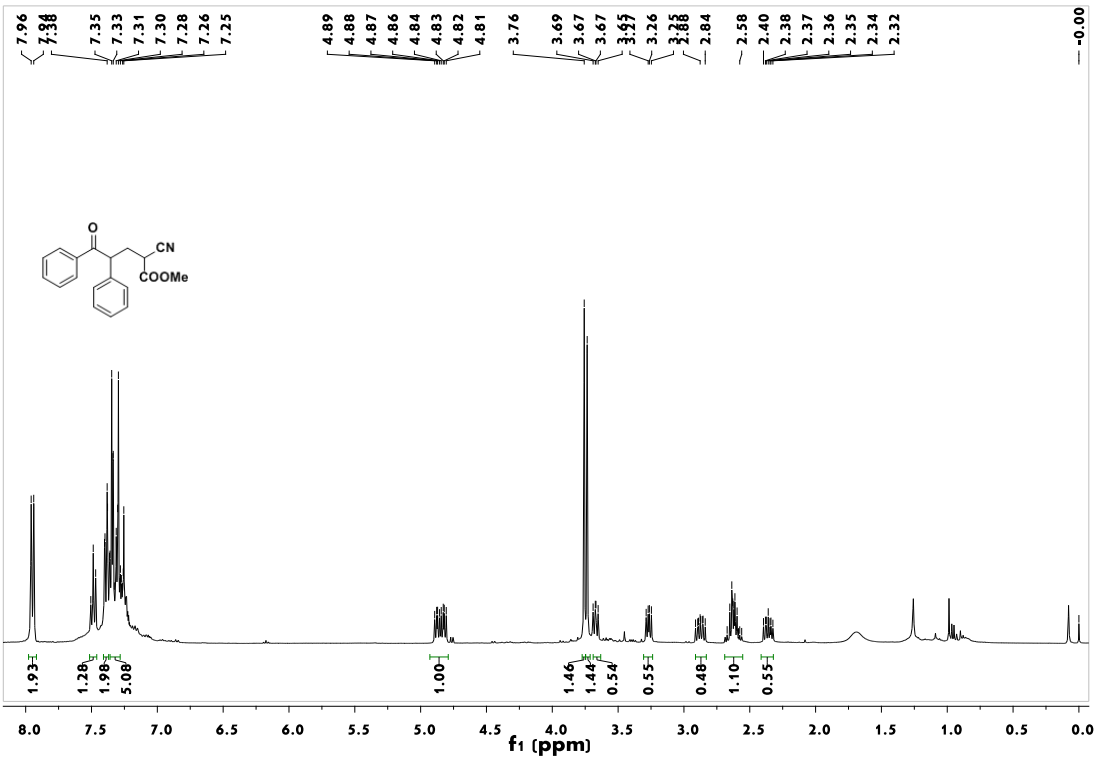
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4.86
4.84
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4.81
3.76
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3.67
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2.40
2.38
2.37
2.36
2.35
2.34
2.32
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O
CN
COOMe
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1.28
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1.44
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1.10
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7.0
6.5
6.0
5.5
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1.0
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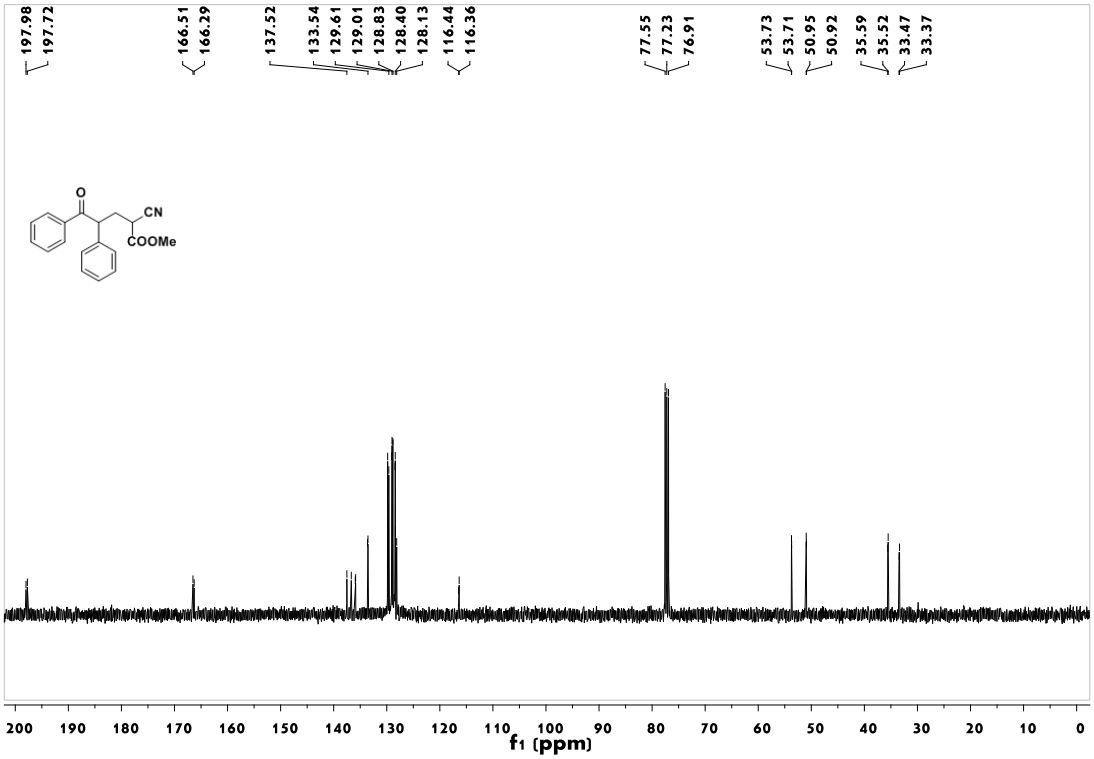
f1 (ppm)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116.36
77.55
77.23
76.91
53.73
53.71
50.95
50.92
35.59
35.52
33.47
33.37
O
CN
COOMe
200
190
180
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30
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10
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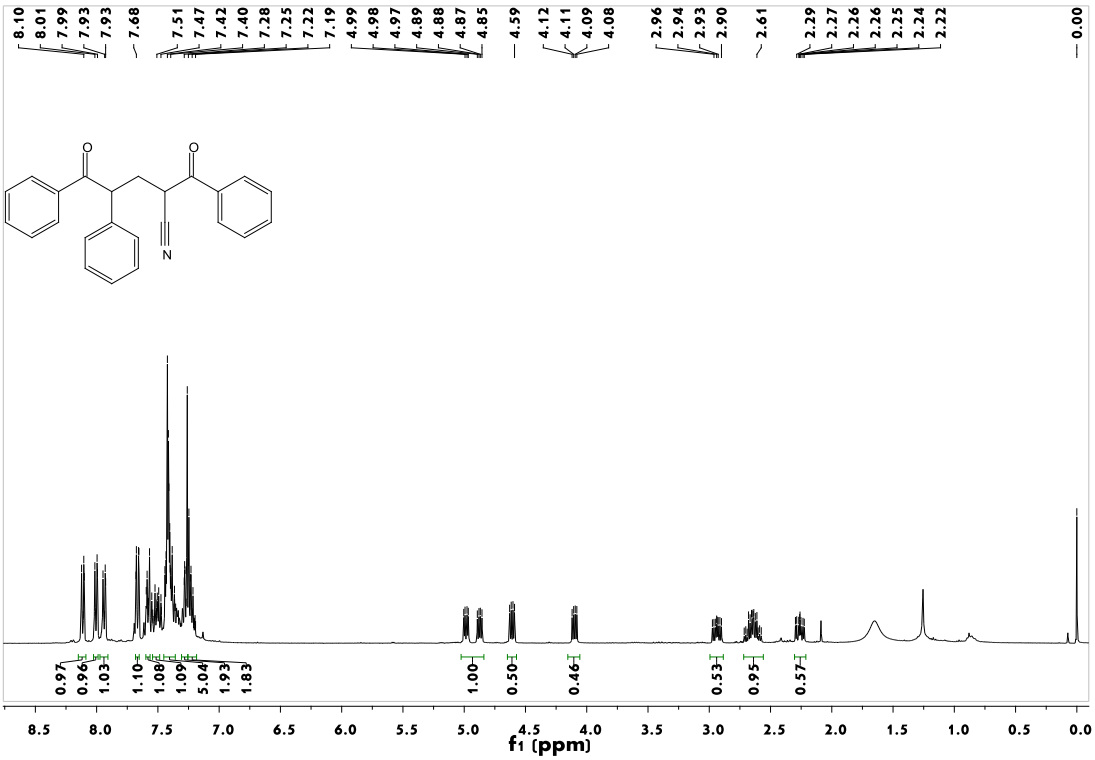
f1 (ppm)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7.19
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4.98
4.97
4.89
4.88
4.87
4.85
4.59
4.12
4.11
4.09
4.08
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2.90
2.61
2.29
2.27
2.26
2.26
2.25
2.24
2.22
0.00
O
O
N
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0.96
1.03
1.10
1.08
1.09
5.04
1.93
1.83
1.00
0.50
0.46
0.53
0.95
0.57
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.0
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1.0
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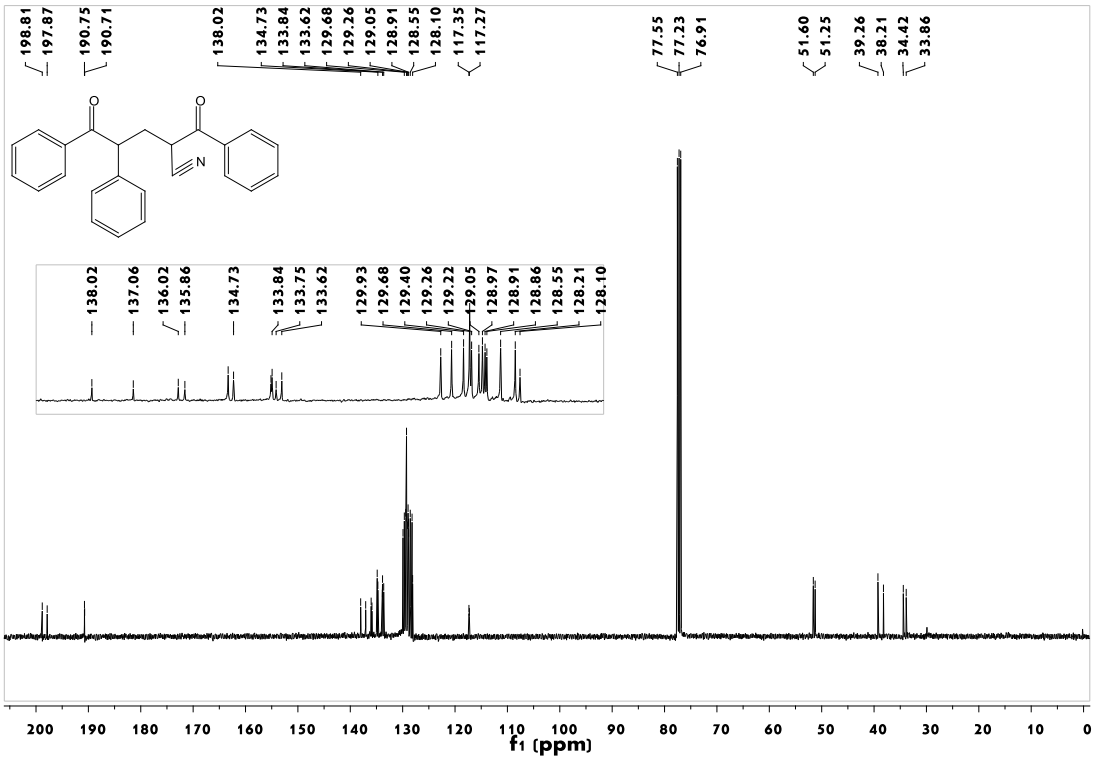
f1 (ppm)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77.55
77.23
76.91
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51.25
39.26
38.21
34.42
33.86
O
O
N
138.02
137.06
136.02
135.86
134.73
133.84
133.75
133.62
129.93
129.68
129.40
129.26
129.22
129.05
128.97
128.91
128.86
128.55
128.21
128.10
200
190
180
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150
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50
40
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10
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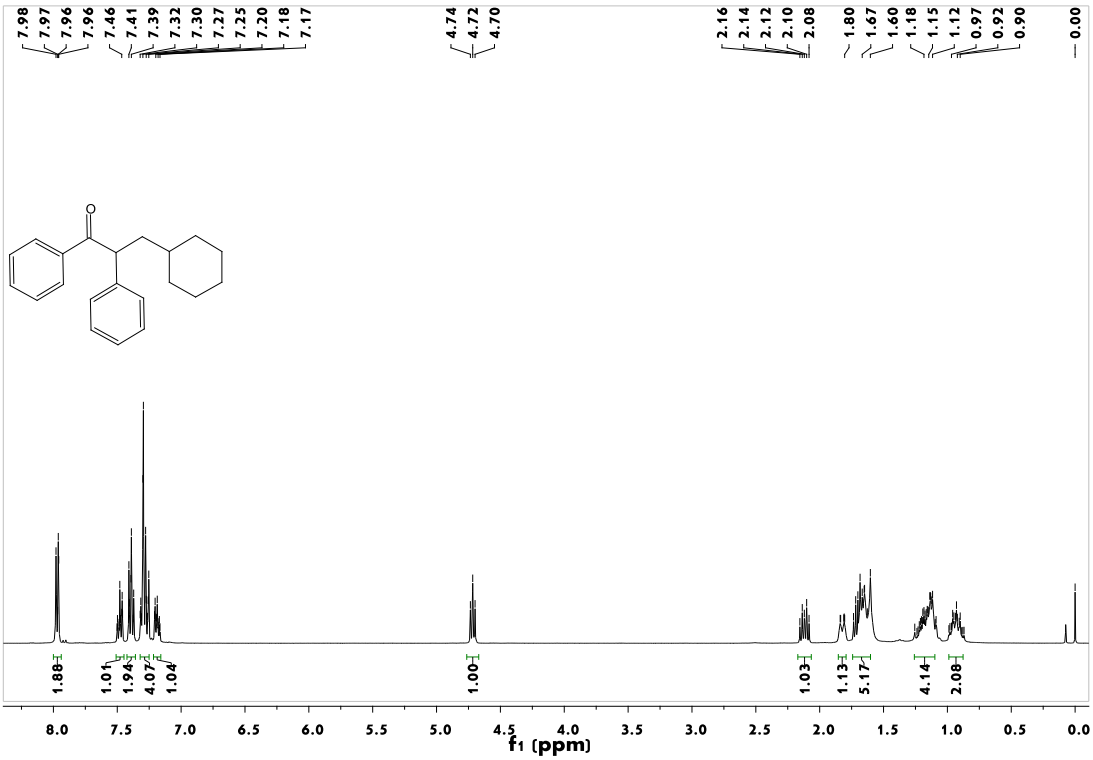
f1 (ppm)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7.17
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4.72
4.70
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2.14
2.12
2.10
2.08
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1.60
1.18
1.15
1.12
0.97
0.92
0.90
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O
1.88
1.01
1.94
4.07
1.04
1.00
1.03
1.13
5.17
4.14
2.08
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
2.0
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1.0
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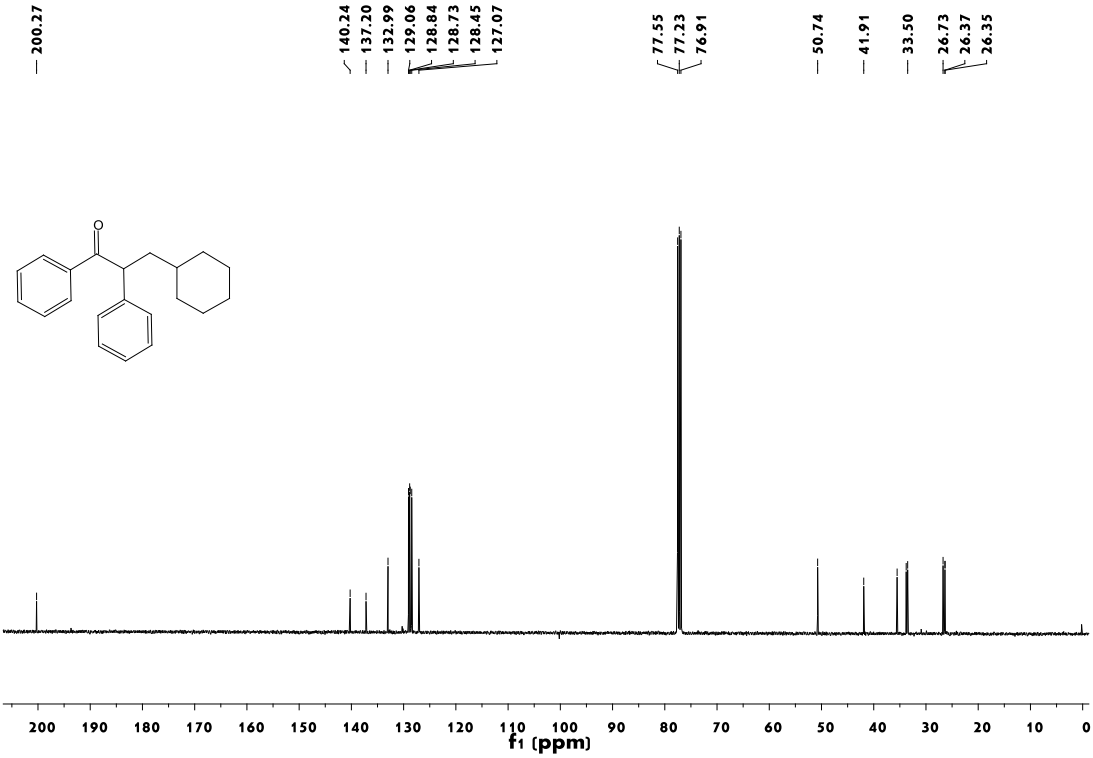
0.0
f1 (ppm)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128.45
127.07
77.55
77.23
76.91
50.74
41.91
33.50
26.73
26.37
26.35
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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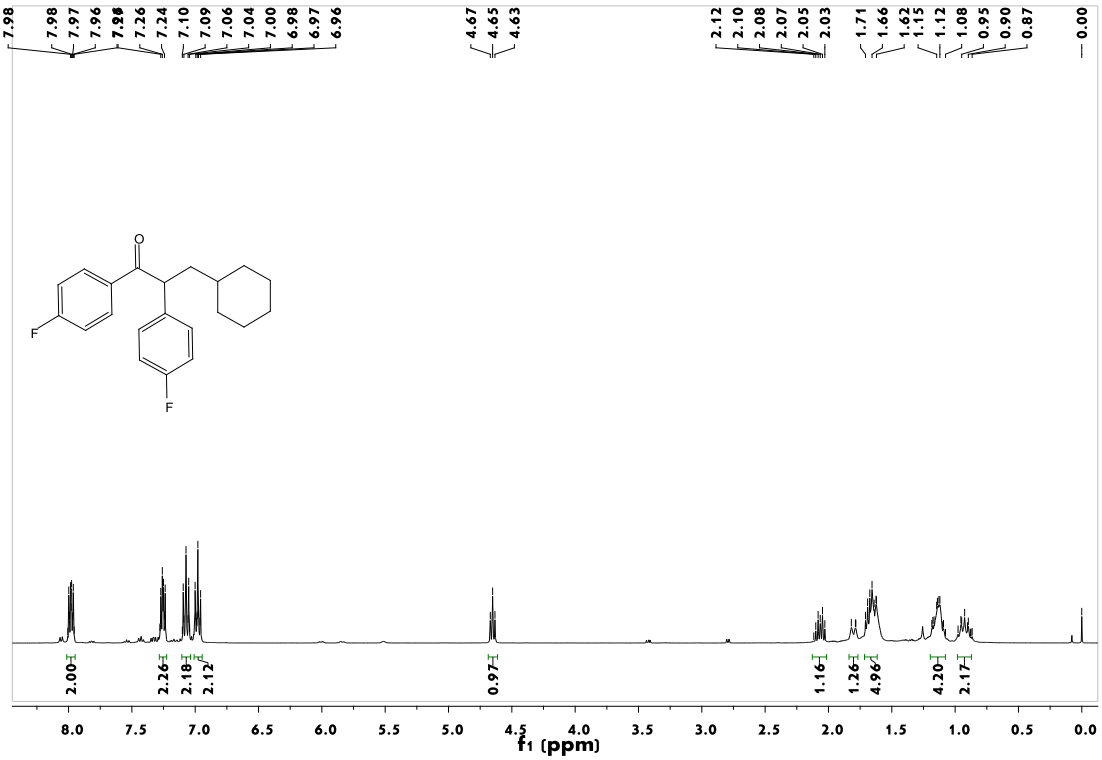
50
40
30
20
10
0
f1 (ppm)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6.98
6.97
6.96
4.67
4.65
4.63
2.12
2.10
2.08
2.07
2.05
2.03
1.71
1.66
1.62
1.15
1.12
1.08
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0.90
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0.00
O
F
F
2.00
2.26
2.18
2.12
0.97
1.16
1.26
4.96
4.20
2.17
8.0
7.5
7.0
6.5
6.0
5.5
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2.0
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1.0
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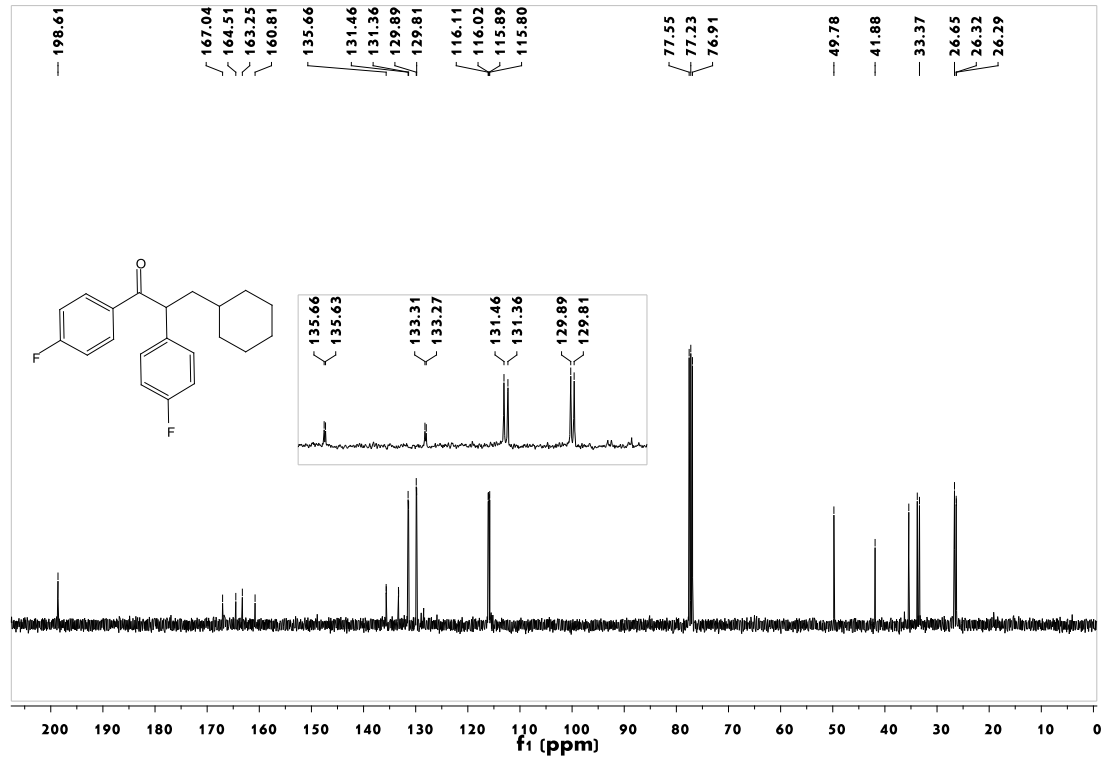
f1 (ppm)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129.81
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115.89
115.80
77.55
77.23
76.91
49.78
41.88
33.37
26.65
26.32
26.29
O
F
F
135.66
135.63
133.31
133.27
131.46
131.36
129.89
129.81
200
190
180
170
160
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100
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60
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40
30
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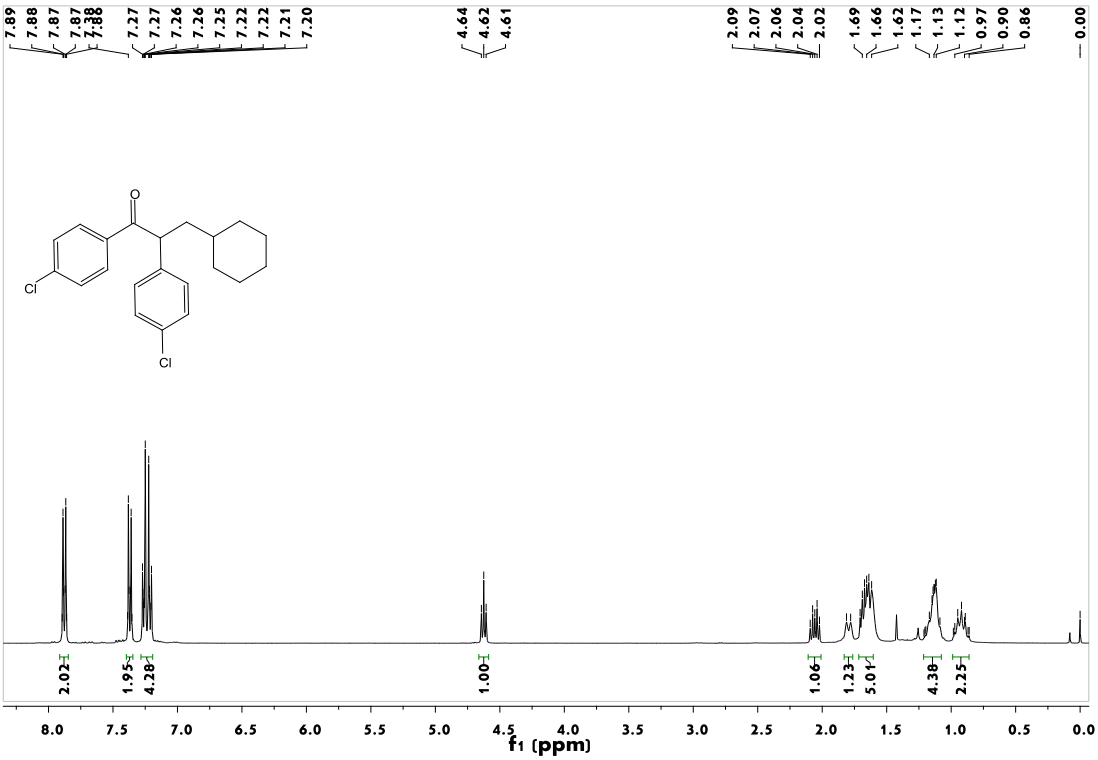
0
f1 (ppm)

bn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4.62
4.61
2.09
2.07
2.06
2.04
2.02
1.69
1.66
1.62
1.17
1.13
1.12
0.97
0.90
0.86
0.00
O
Cl
Cl
2.02
1.95
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1.00
1.06
1.23
5.01
4.38
2.25
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7.0
6.5
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5.5
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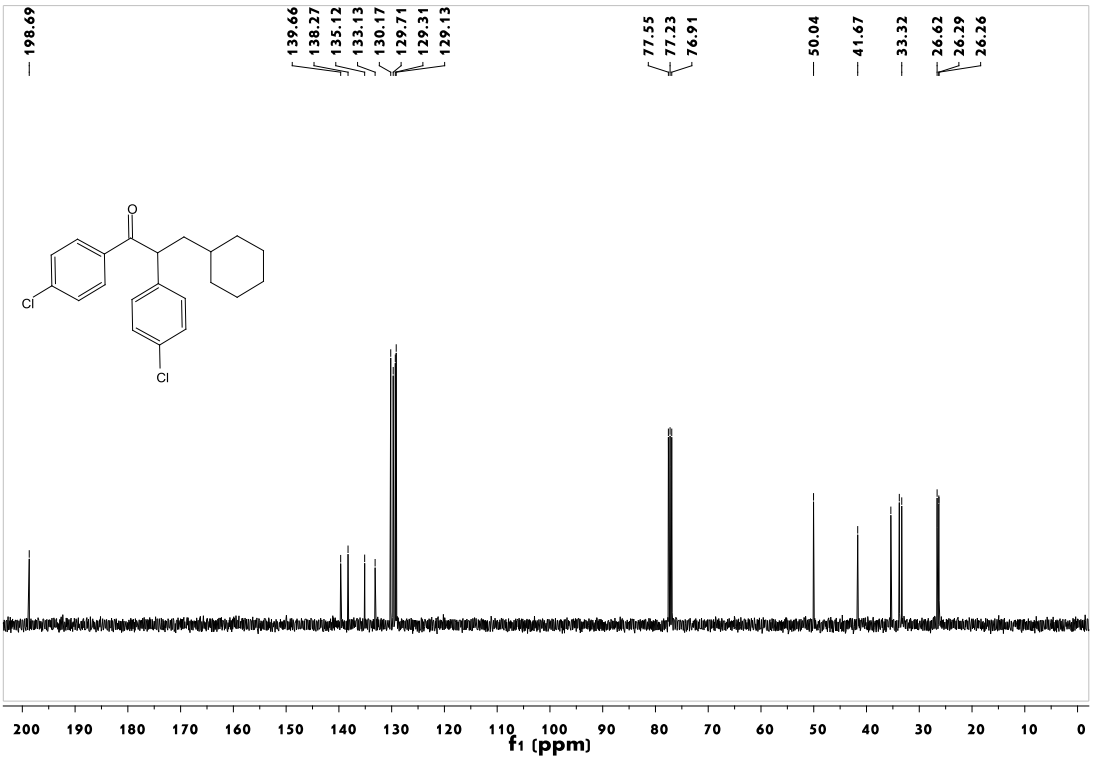
f1 (ppm)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77.23
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50.04
41.67
33.32
26.62
26.29
26.26
O
Cl
Cl
200
190
180
170
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150
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130
120
110
100
90
80
70
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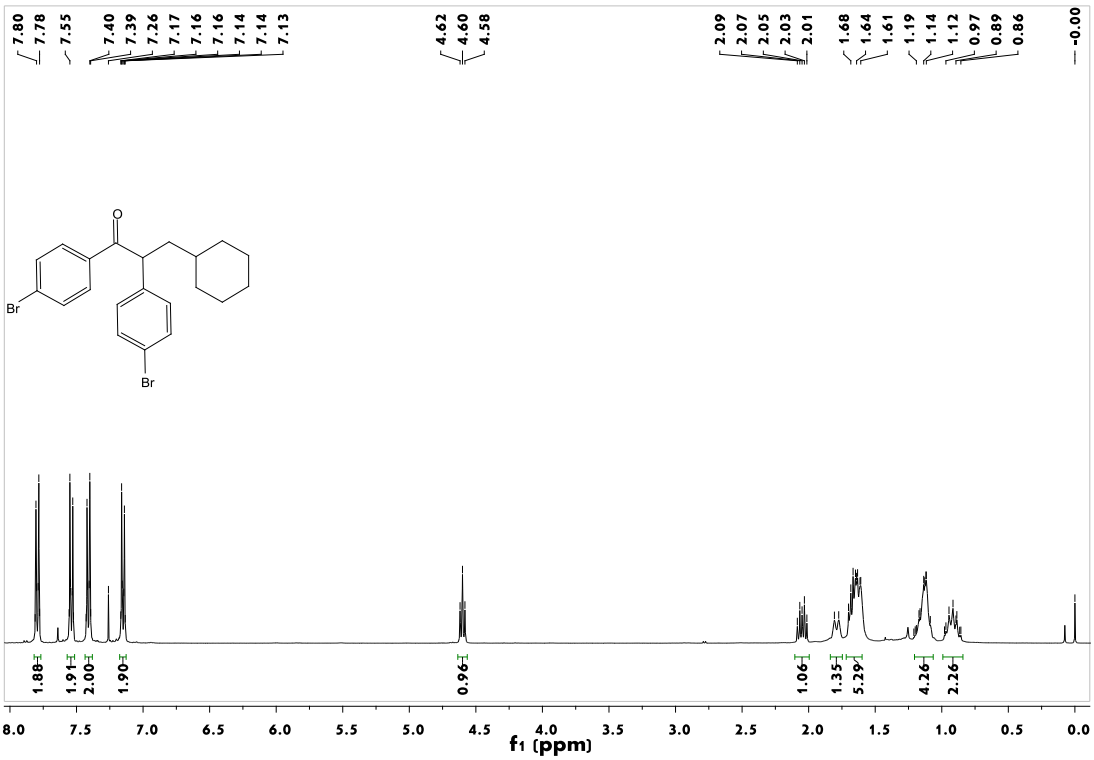
50
40
30
20
10
0
f1 (ppm)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7.14
7.13
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4.60
4.58
2.09
2.07
2.05
2.03
2.01
1.68
1.64
1.61
1.19
1.14
1.12
0.97
0.89
0.86
-0.00
O
Br
Br
1.88
1.91
2.00
1.90
0.96
1.06
1.35
5.29
4.26
2.26
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
1.5
1.0
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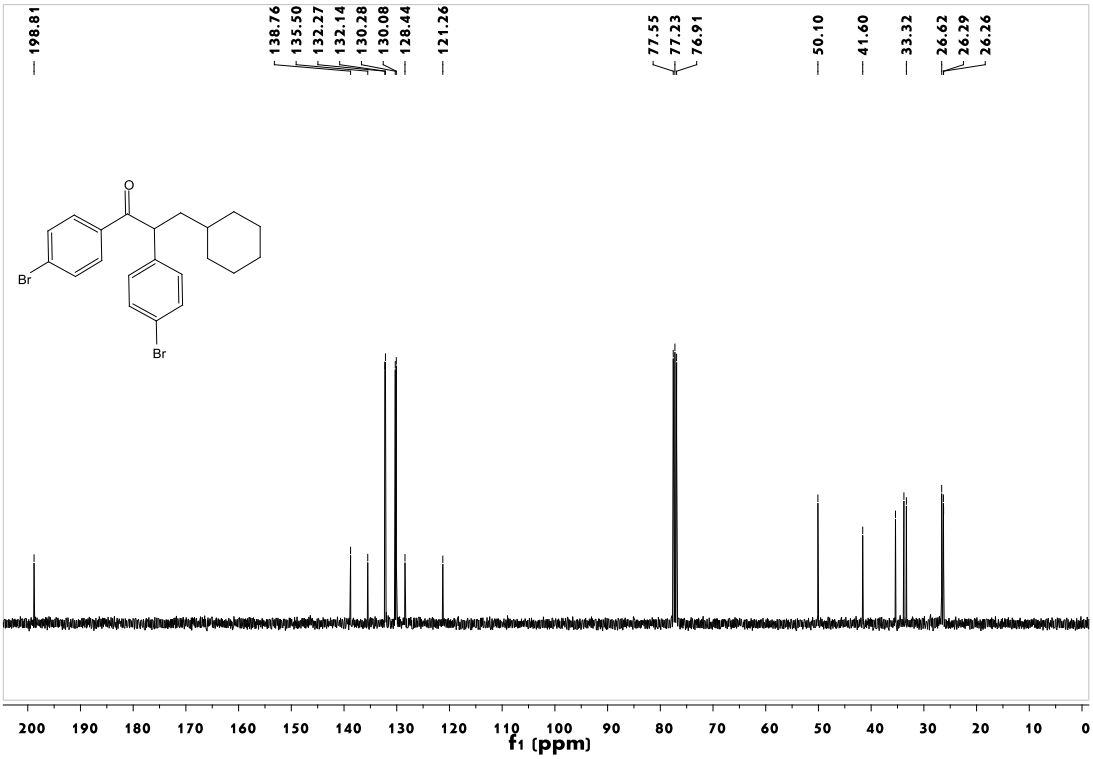
0.0
f1 (ppm)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77.23
76.91
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41.60
33.32
26.62
26.29
26.26
O
Br
Br
200
190
180
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150
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130
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110
100
90
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70
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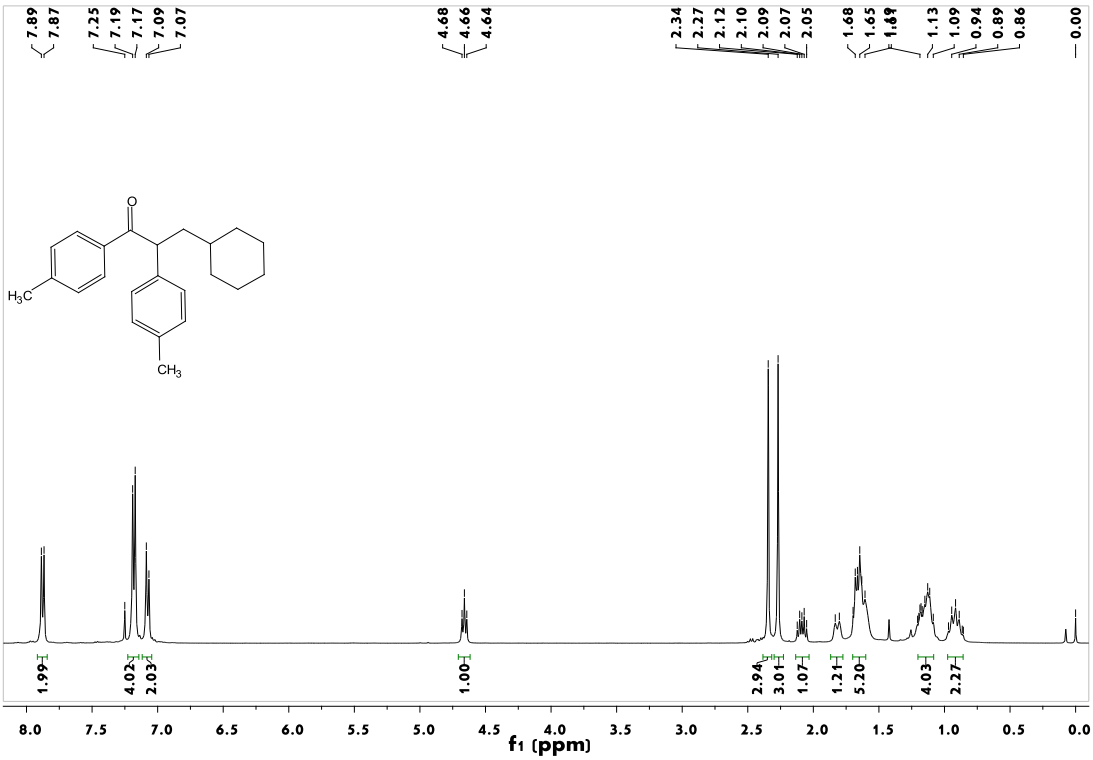
50
40
30
20
10
0
f1 (ppm)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2.10
2.09
2.07
2.05
1.68
1.65
1.13
1.09
0.94
0.89
0.86
0.00
O
H3C
CH3
1.99
4.02
2.03
1.00
2.94
3.01
1.07
1.21
5.20
4.03
2.27
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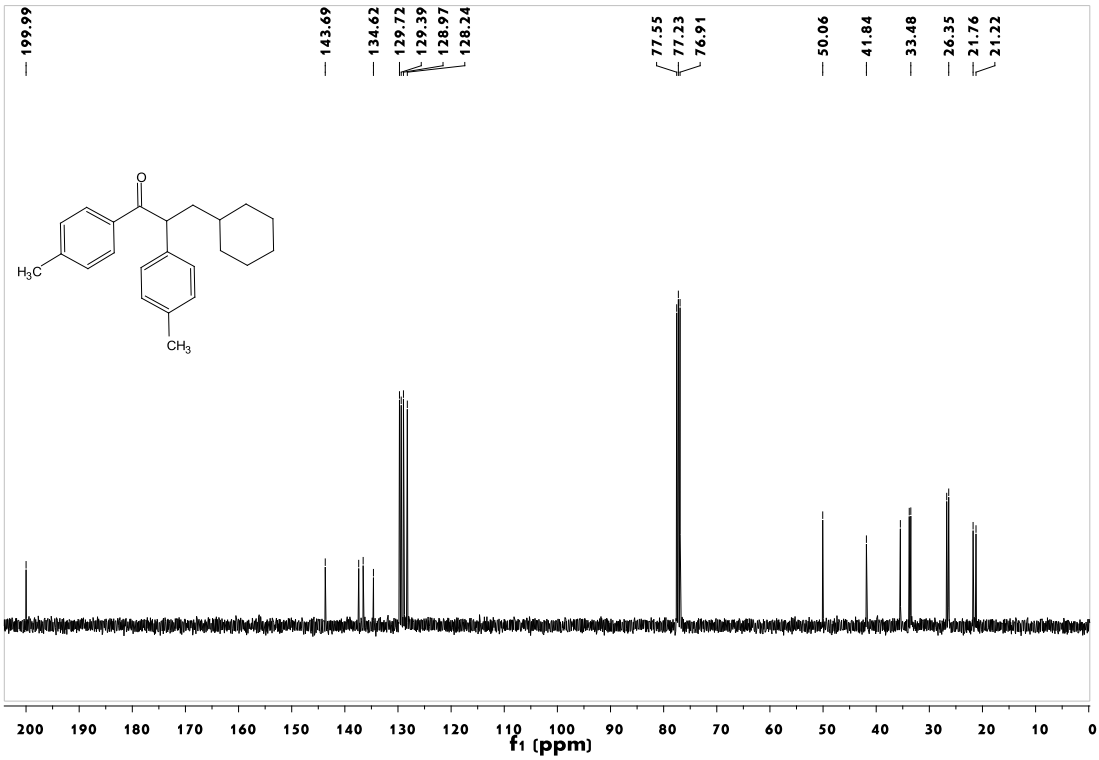
f1 (ppm)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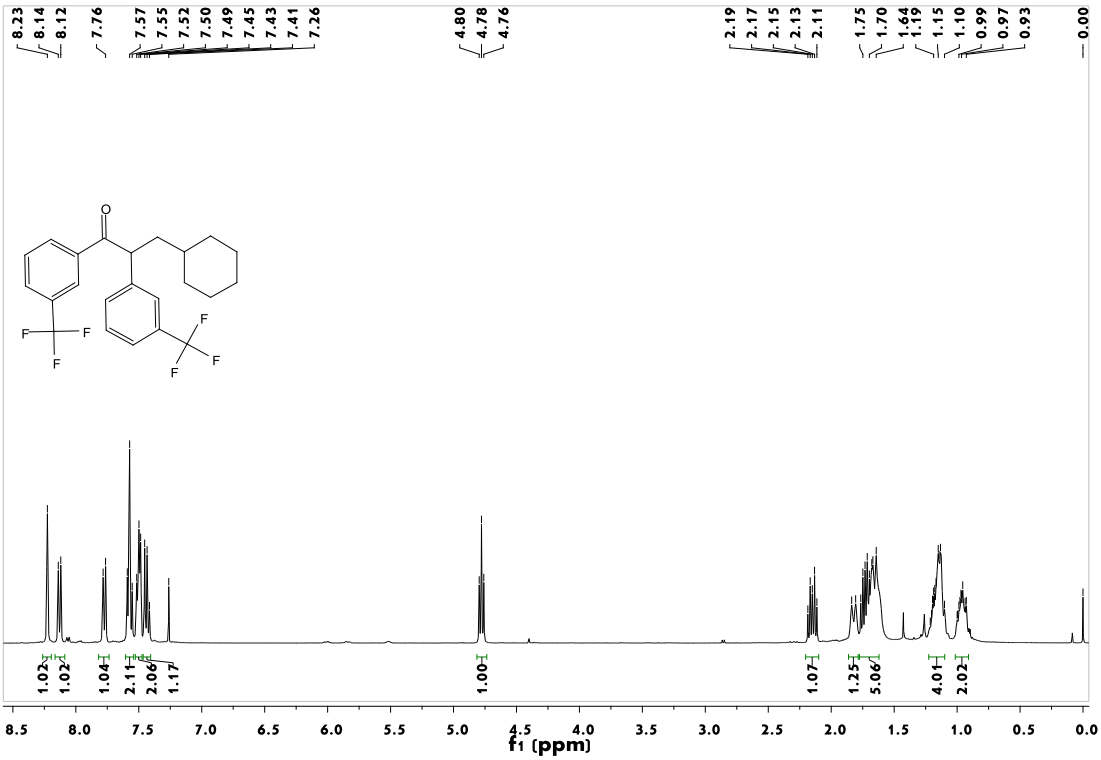
21.22
O
H3C
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.41
7.26
4.80
4.78
4.76
2.19
2.17
2.15
2.13
2.11
1.75
1.70
1.64
1.19
1.15
1.10
0.99
0.97
0.93
0.00
O
F
F
F
F
F
F
1.02
1.02
1.04
2.11
2.06
1.17
1.00
1.07
1.25
5.06
4.01
2.02
8.5
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7.5
7.0
6.5
6.0
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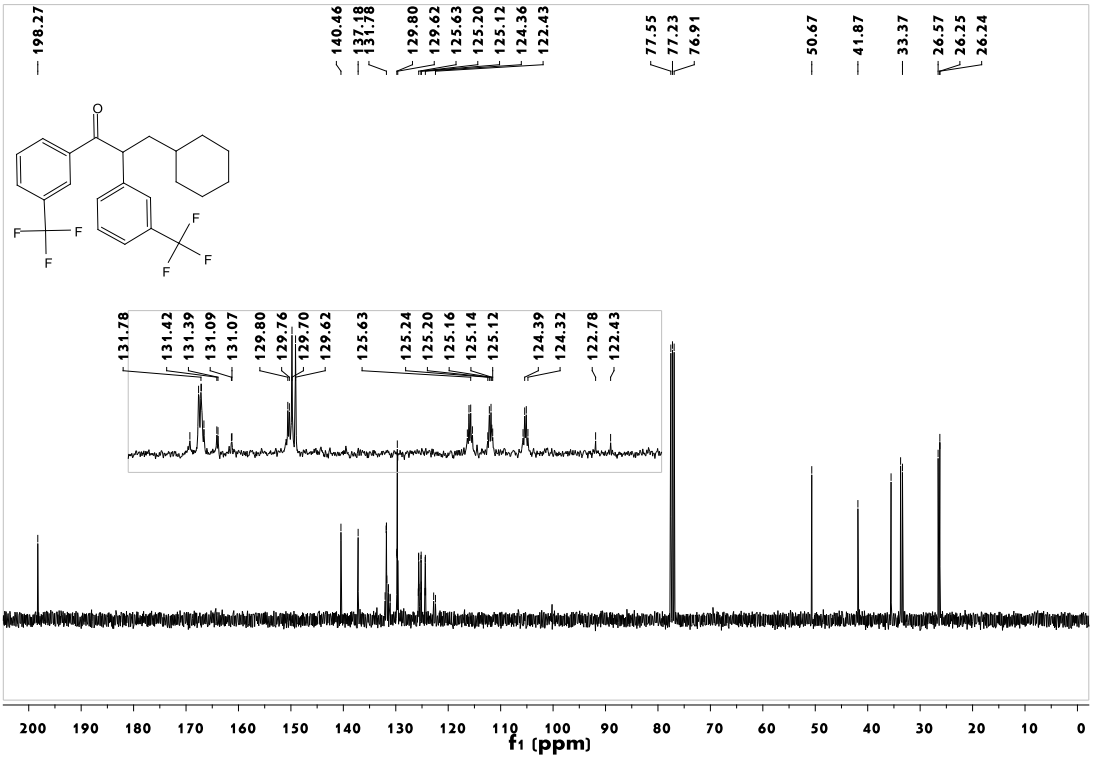
0.0
f1 (ppm)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76.91
50.67
41.87
33.37
26.57
26.25
26.24
O
F
F
F
F
F
F
131.78
131.42
131.39
131.09
131.07
129.80
129.76
129.70
129.62
125.63
125.24
125.20
125.16
125.14
125.12
124.39
124.32
122.78
122.43
200
190
180
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160
150
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130
120
110
100
90
80
70
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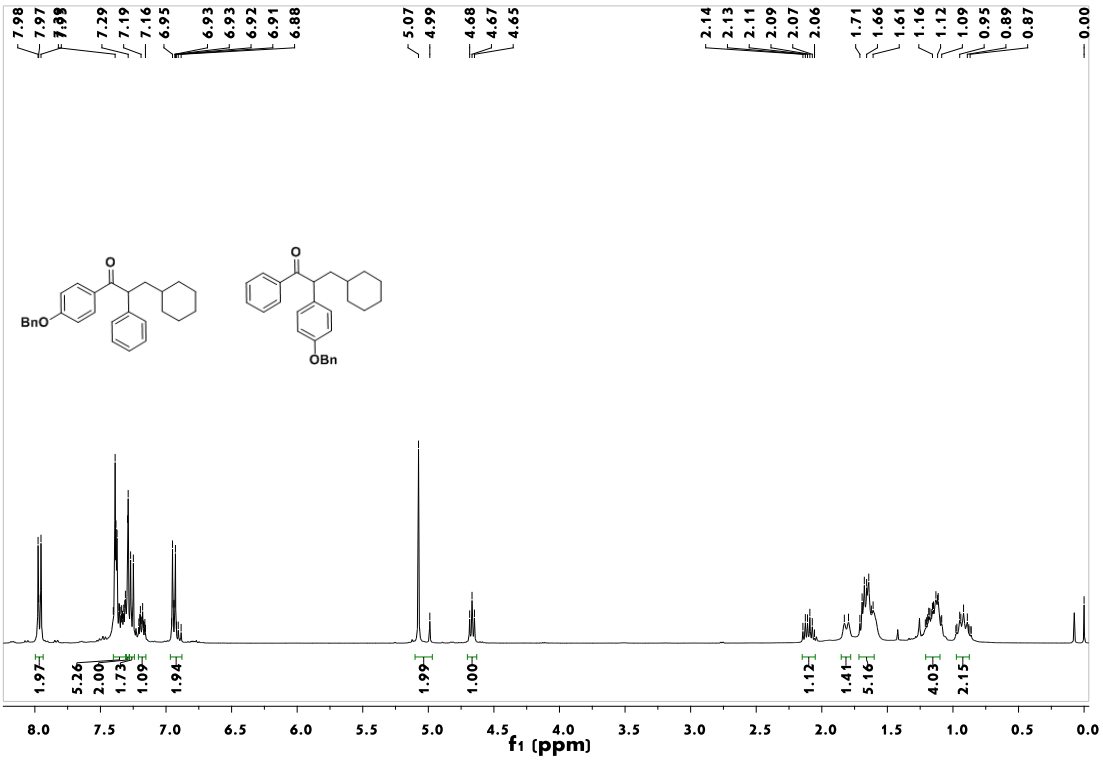
50
40
30
20
10
0
f1 (ppm)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6.88
5.07
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4.67
4.65
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2.13
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2.06
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1.09
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0.00
BnO
OBn
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2.00
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1.99
1.00
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6.5
6.0
5.5
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1.0
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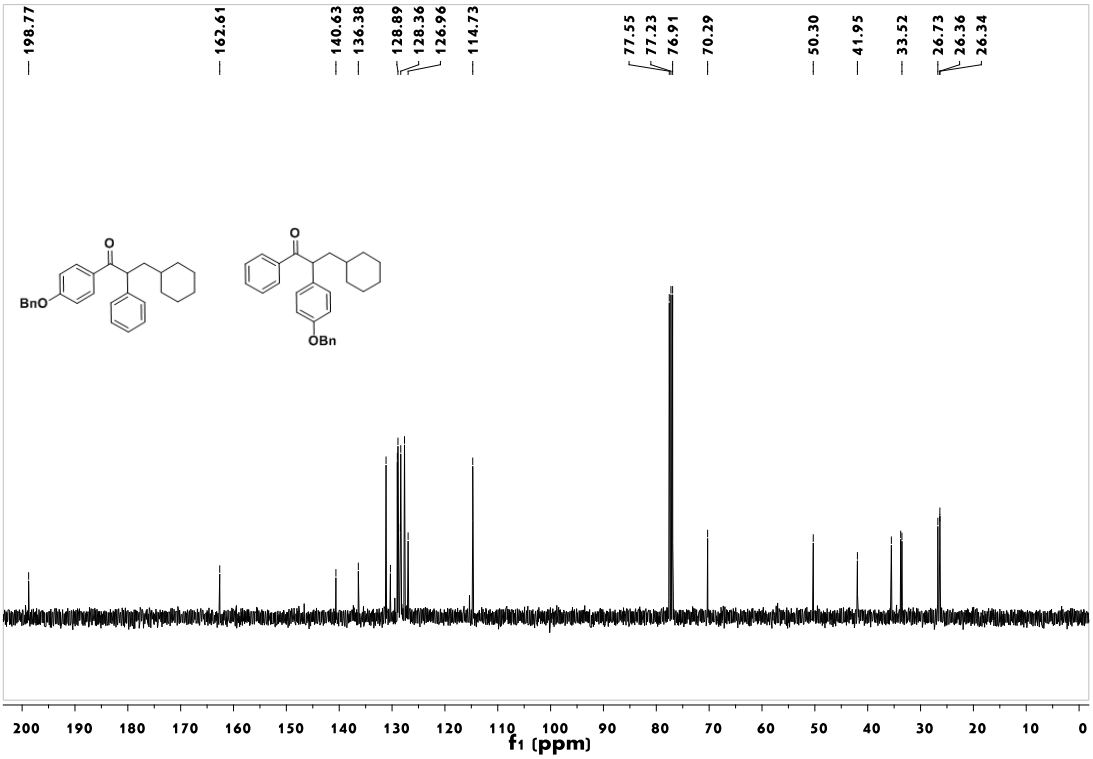
f1 (ppm)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77.23
76.91
70.29
50.30
41.95
33.52
26.73
26.36
26.34
BnO
OBn
200
190
180
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130
120
110
100
90
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70
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50
40
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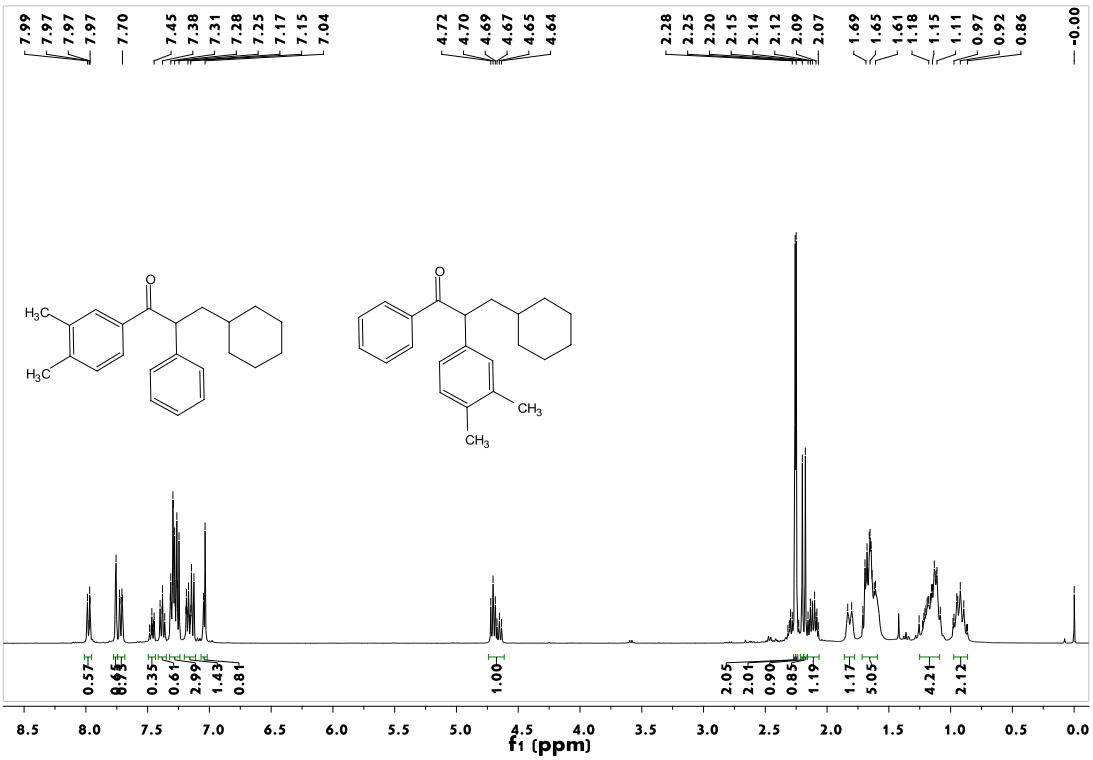
f1 (ppm)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7.25
7.17
7.15
7.04
4.72
4.70
4.69
4.67
4.65
4.64
2.28
2.25
2.20
2.15
2.14
2.12
2.09
2.07
1.69
1.65
1.61
1.18
1.15
1.11
0.97
0.92
0.86
-0.00
H3C
H3C
O
CH3
CH3
0.57
0.35
0.61
2.99
1.43
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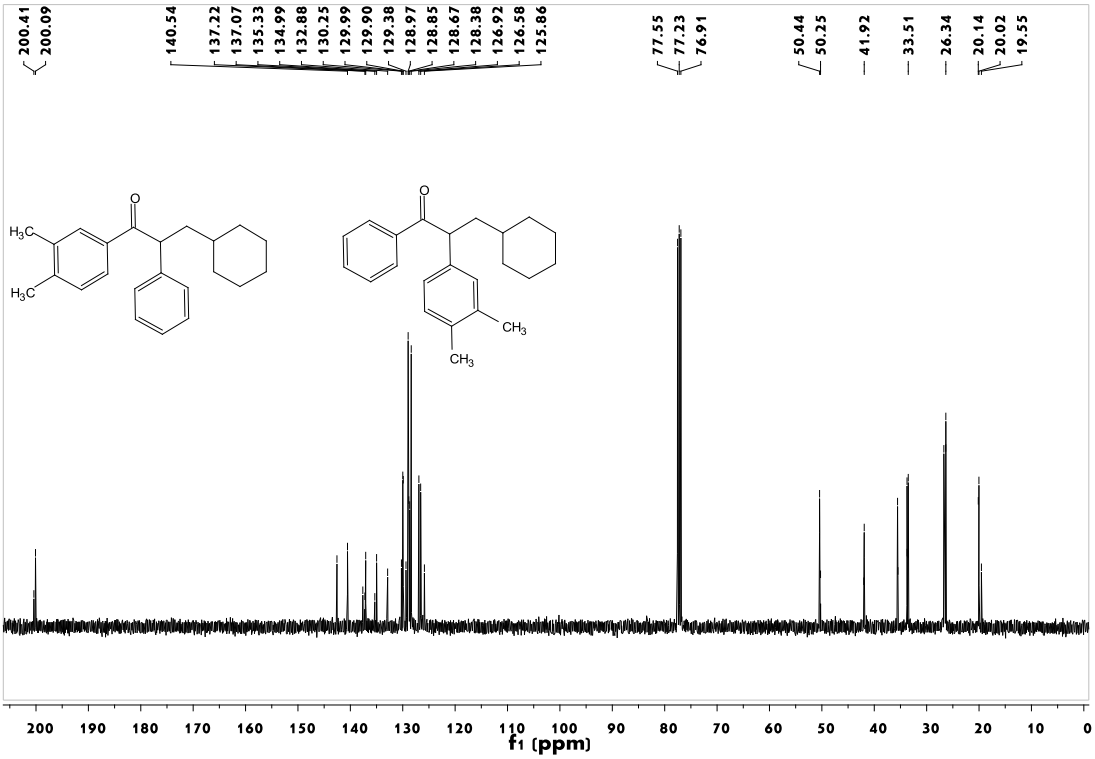
1.00
2.05
2.01
0.90
0.85
1.19
1.17
5.05
4.21
2.12
f1 (ppm)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129.38
128.97
128.85
128.67
128.38
126.92
126.58
125.86
77.55
77.23
76.91
50.44
50.25
41.92
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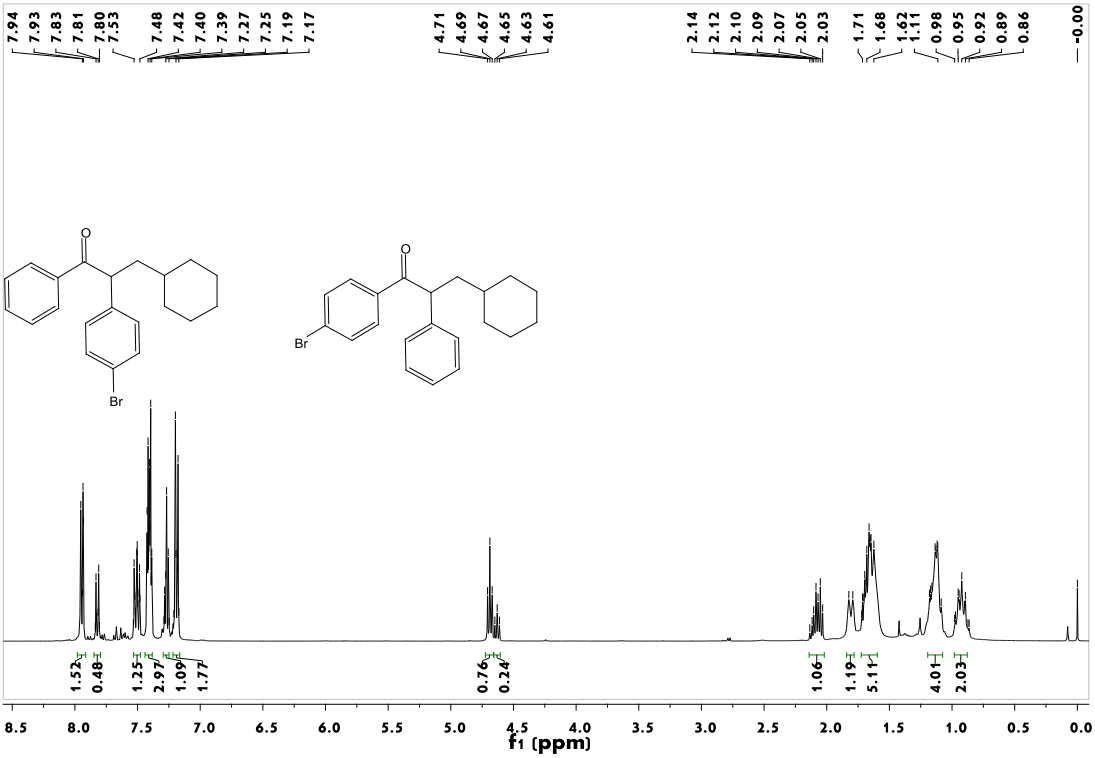
26.34
20.14
20.02
19.55
H3C
H3C
O
CH3
CH3
f1 (ppm)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7.39
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7.25
7.19
7.17
4.71
4.69
4.67
4.65
4.63
4.61
2.14
2.12
2.10
2.09
2.07
2.05
2.03
1.71
1.68
1.62
1.11
0.98
0.95
0.92
0.89
0.86
-0.00
O
Br
O
Br
1.52
0.48
1.25
2.97
1.09
1.77
0.76
0.24
1.06
1.19
5.11
4.01
2.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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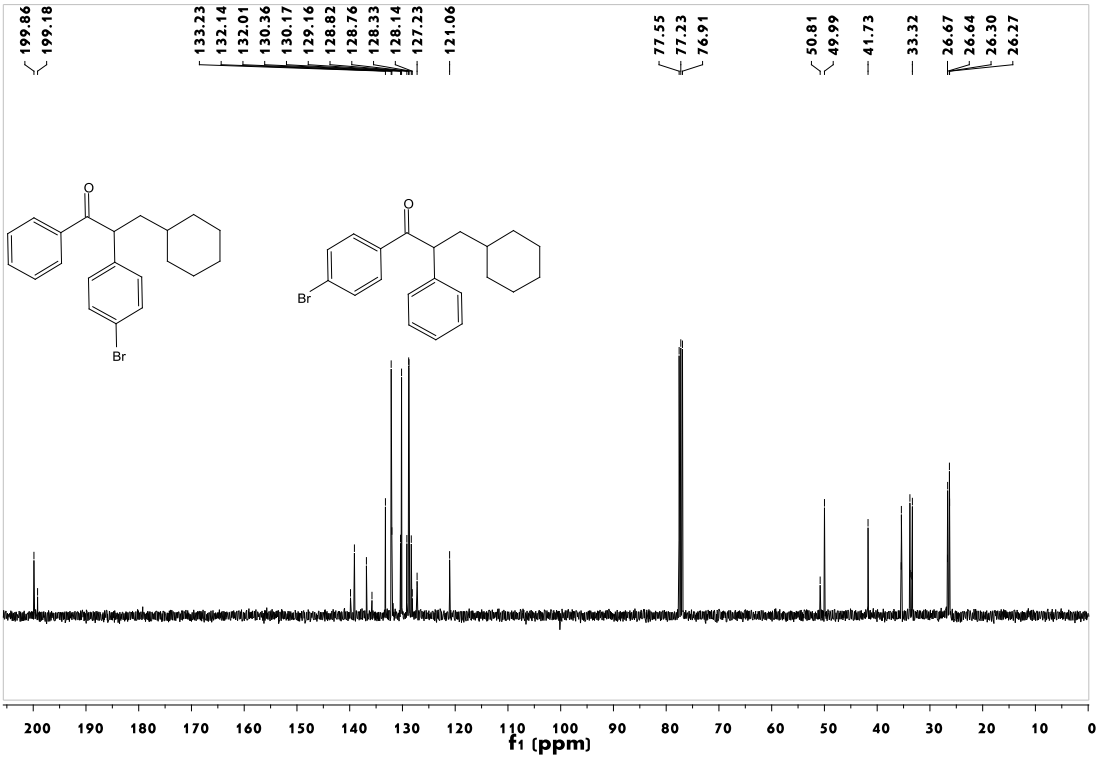
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.16
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128.76
128.33
128.14
127.23
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77.55
77.23
76.91
50.81
49.99
41.73
33.32
26.67
26.64
26.30
26.27
O
Br
O
Br
200
190
180
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150
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130
120
110
100
90
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50
40
30
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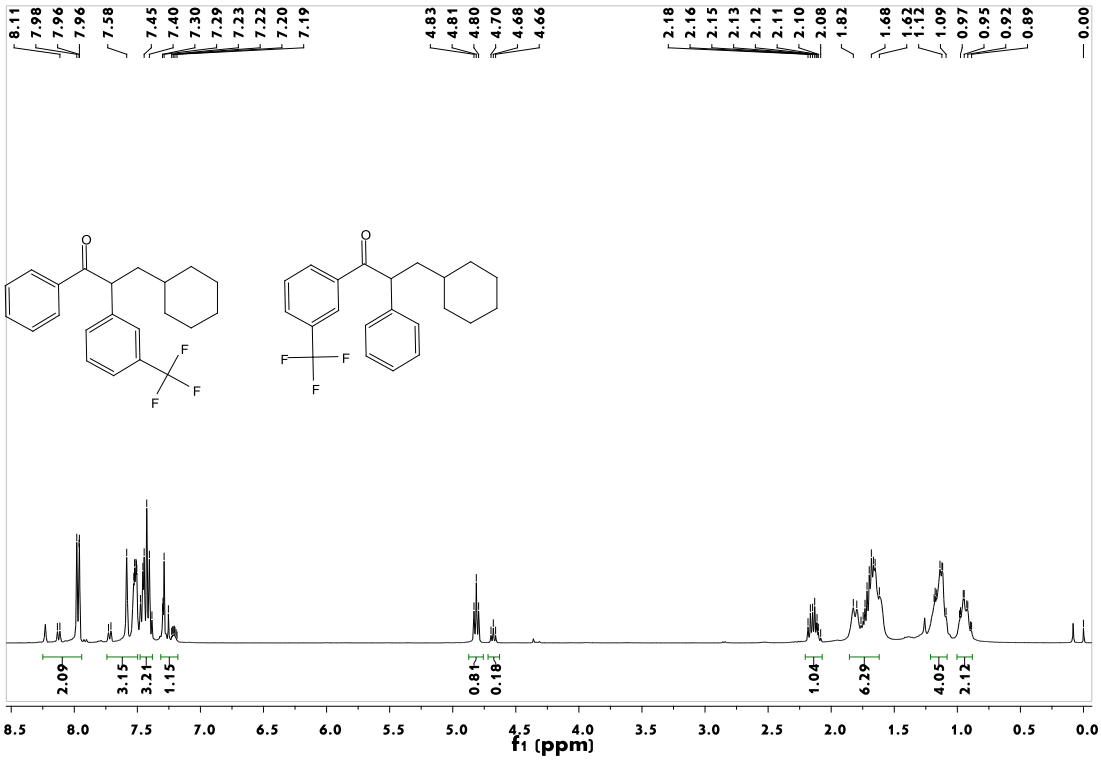
0
f1 (ppm)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7.30
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7.23
7.22
7.20
7.19
4.83
4.81
4.80
4.70
4.68
4.66
2.18
2.16
2.15
2.13
2.12
2.11
2.10
2.08
1.82
1.68
1.62
1.12
1.09
0.97
0.95
0.92
0.89
0.00
2.09
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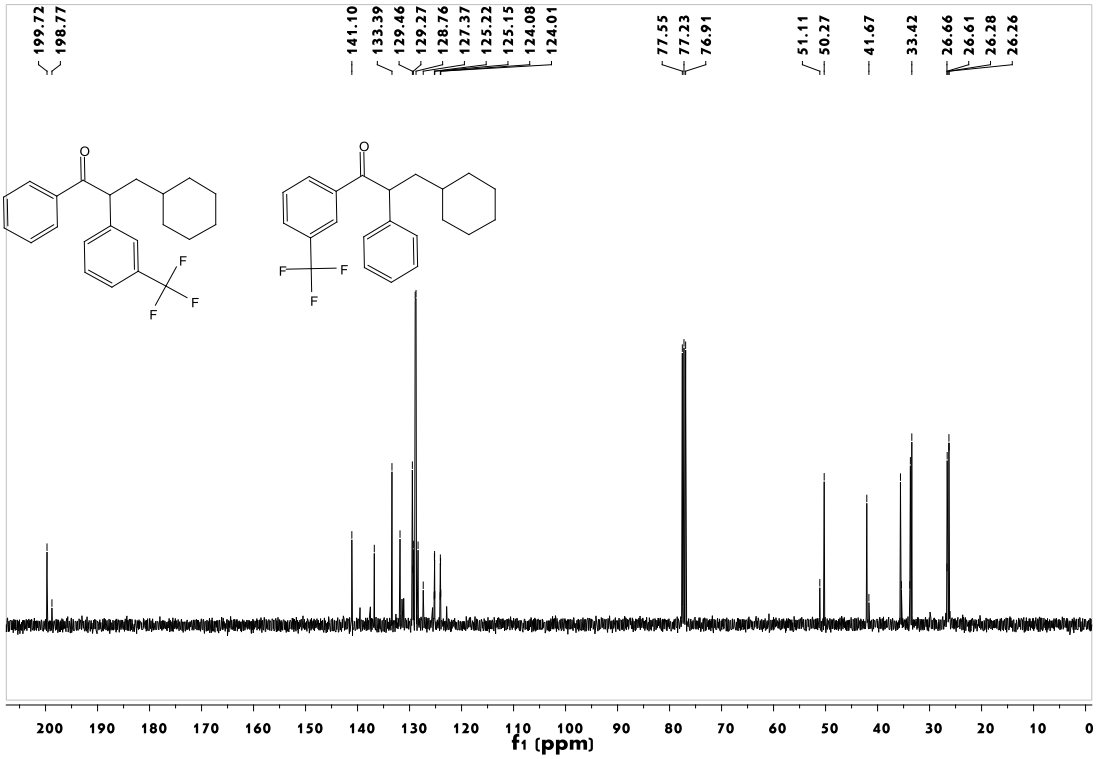
3.21
1.15
0.81
0.18
1.04
6.29
4.05
2.12
f1 (ppm)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129.27
128.76
127.37
125.22
125.15
124.08
124.01
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77.23
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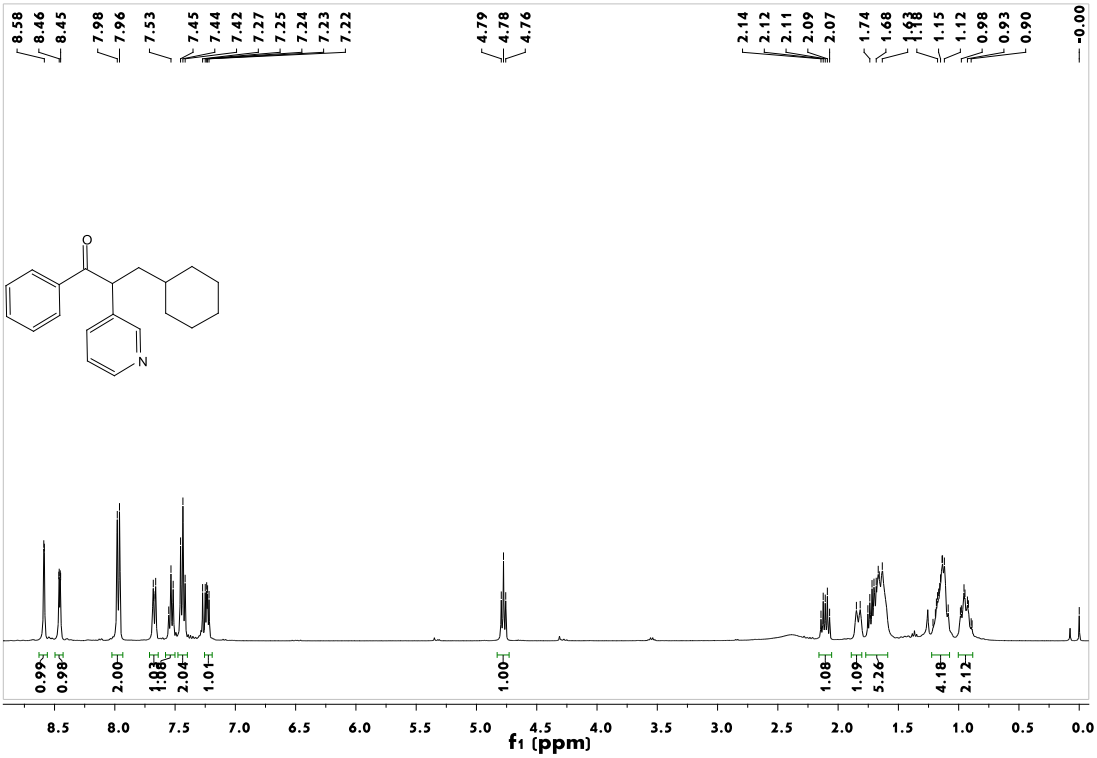
51.11
50.27
41.67
33.42
26.66
26.61
26.28
26.26
f1 (ppm)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8.46
8.45
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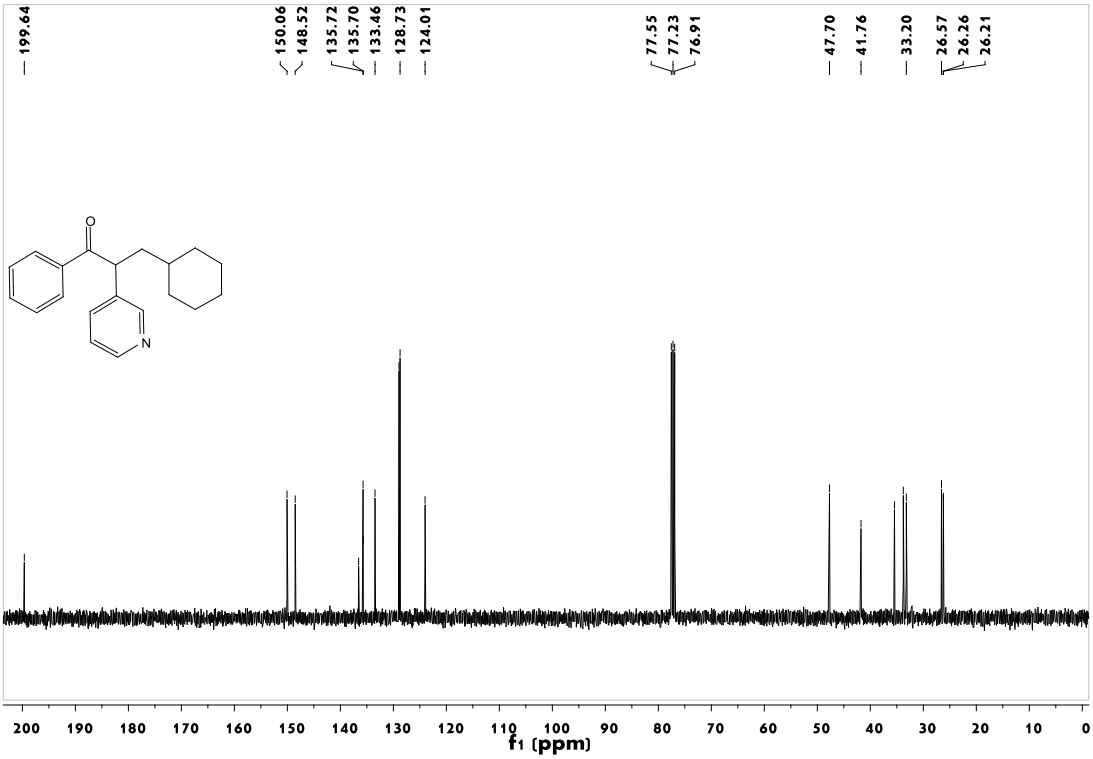
7.53
7.45
7.44
7.42
7.27
7.25
7.24
7.23
7.22
4.79
4.78
4.76
2.14
2.12
2.11
2.09
2.07
1.74
1.68
1.15
1.12
0.98
0.93
0.90
-0.00
0.99
0.98
2.00
2.04
1.01
1.00
1.08
1.09
5.26
4.18
2.12
f1 (ppm)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133.46
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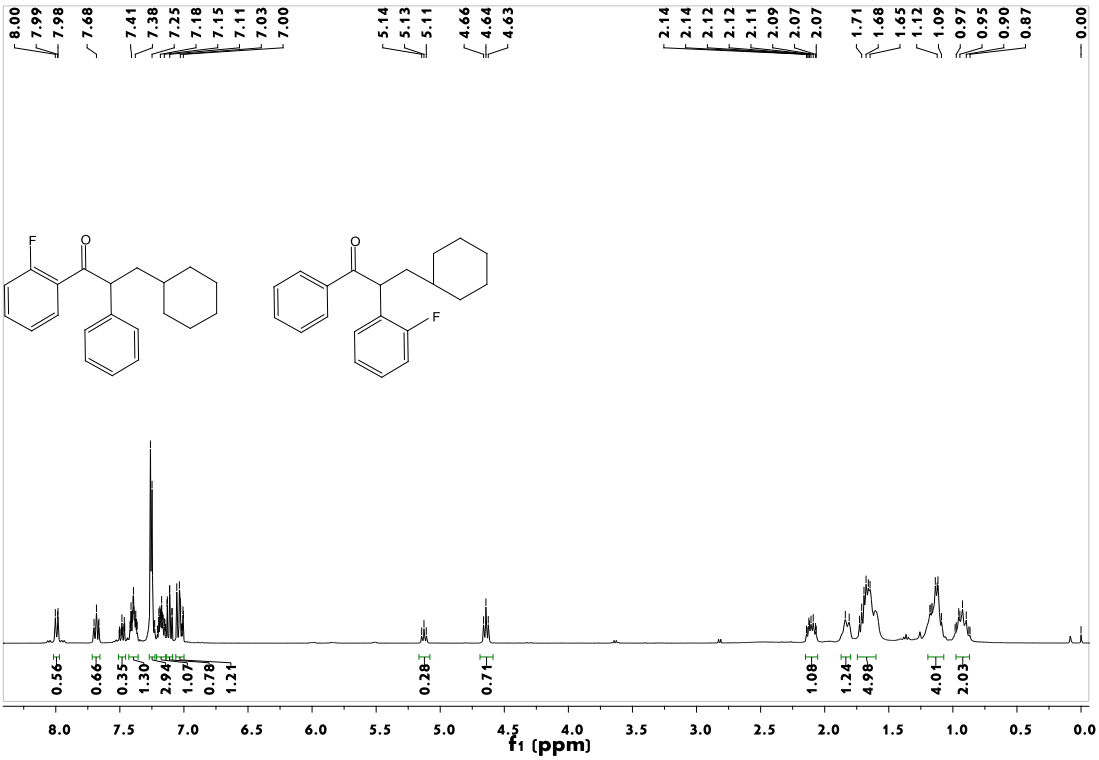
124.01
77.55
77.23
76.91
47.70
41.76
33.20
26.57
26.26
26.21
f1 (ppm)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7.99
7.98
7.68
7.41
7.38
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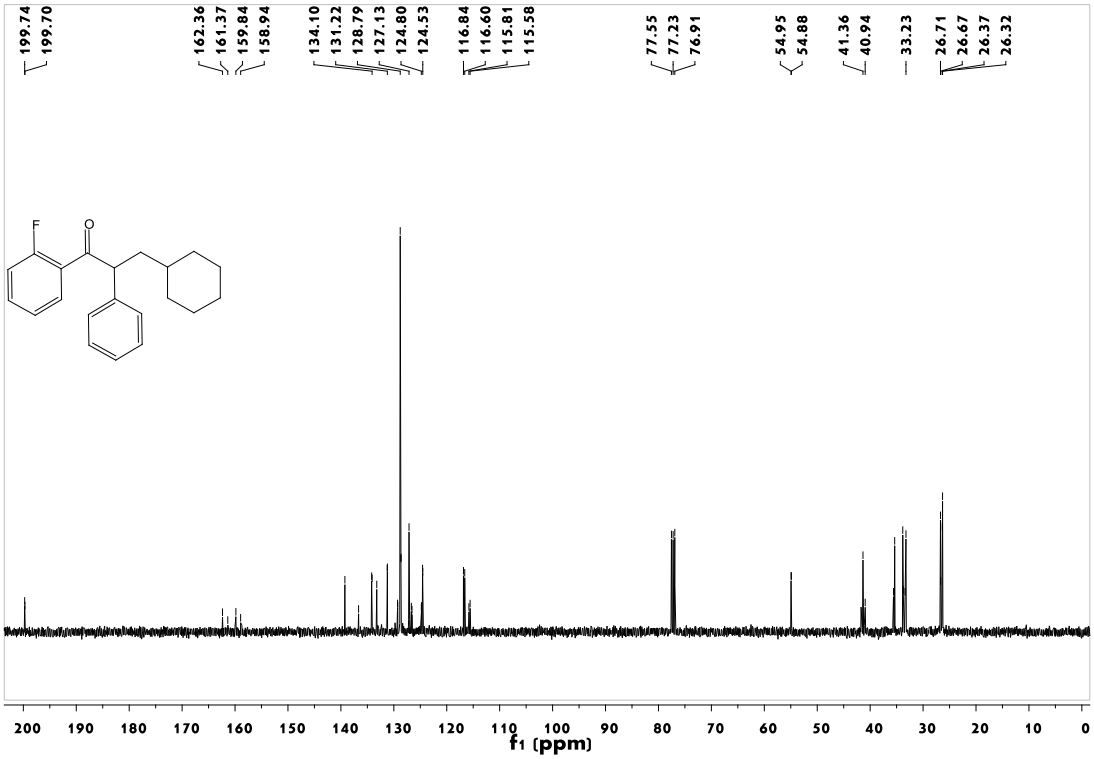
7.11
7.03
7.00
5.14
5.13
5.11
4.66
4.64
4.63
2.14
2.14
2.12
2.12
2.11
2.09
2.07
2.07
1.71
1.68
1.65
1.12
1.09
0.97
0.95
0.90
0.87
0.00
F
O
O
F
0.56
0.66
0.35
1.30
2.94
1.07
0.78
1.21
0.28
0.71
1.08
1.24
4.98
4.01
2.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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124.80
124.53
116.84
116.60
115.81
115.58
77.55
77.23
76.91
54.95
54.88
41.36
40.94
33.23
26.71
26.67
26.37
26.32
F
O
200
190
180
170
160
150
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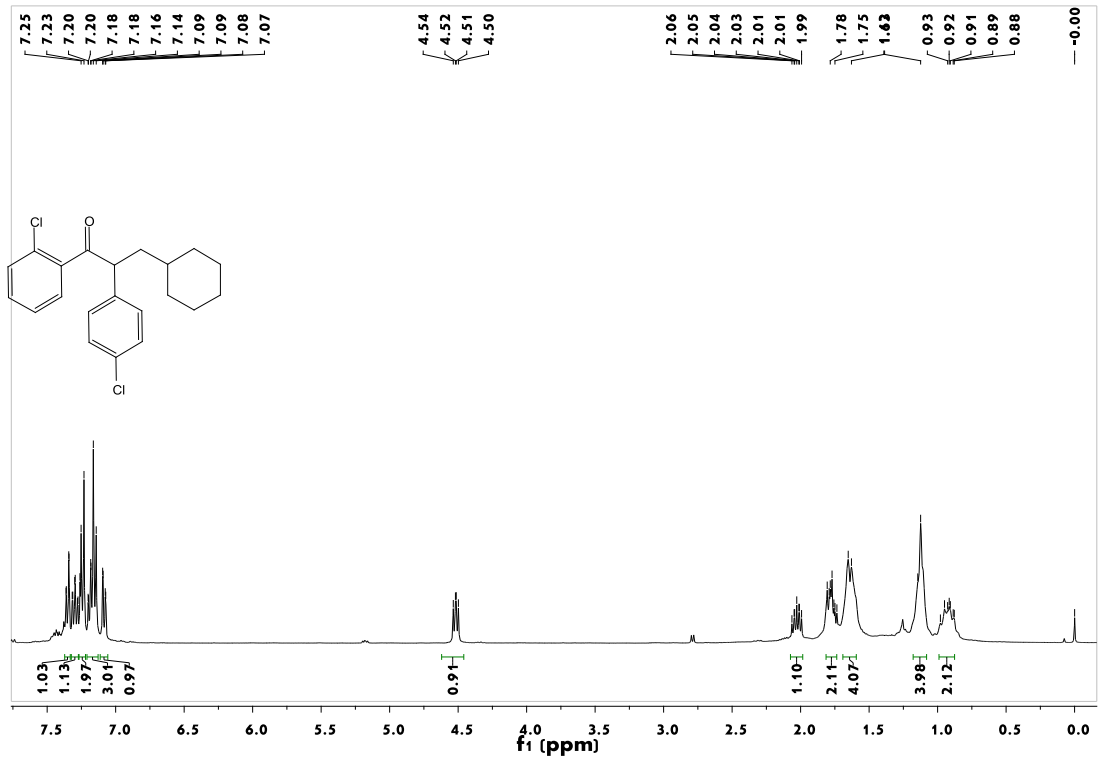
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.18
7.16
7.14
7.09
7.09
7.08
7.07
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4.52
4.51
4.50
2.06
2.05
2.04
2.03
2.01
2.01
1.99
1.78
1.75
0.93
0.92
0.91
0.89
0.88
-0.00
Cl
O
Cl
1.03
1.13
1.97
3.04
0.97
0.91
1.10
2.11
4.07
3.98
2.12
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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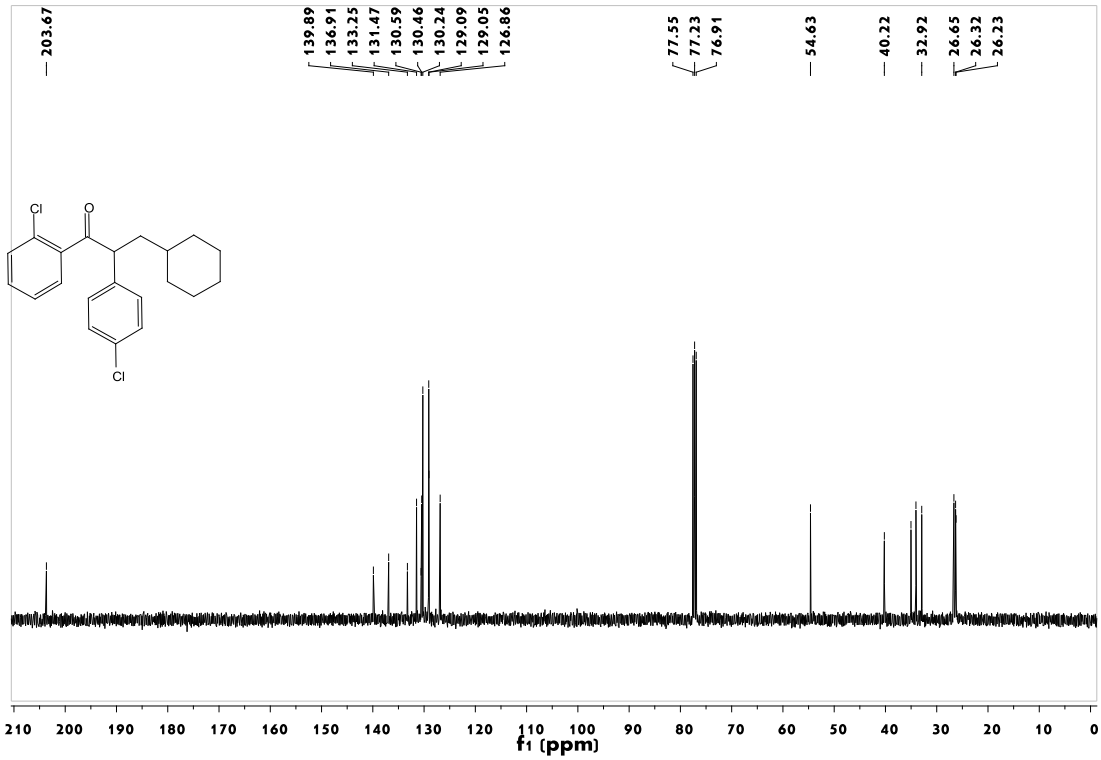
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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130.24
129.09
129.05
126.86
77.55
77.23
76.91
54.63
40.22
32.92
26.65
26.32
26.23
Cl
O
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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50
40
30
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10
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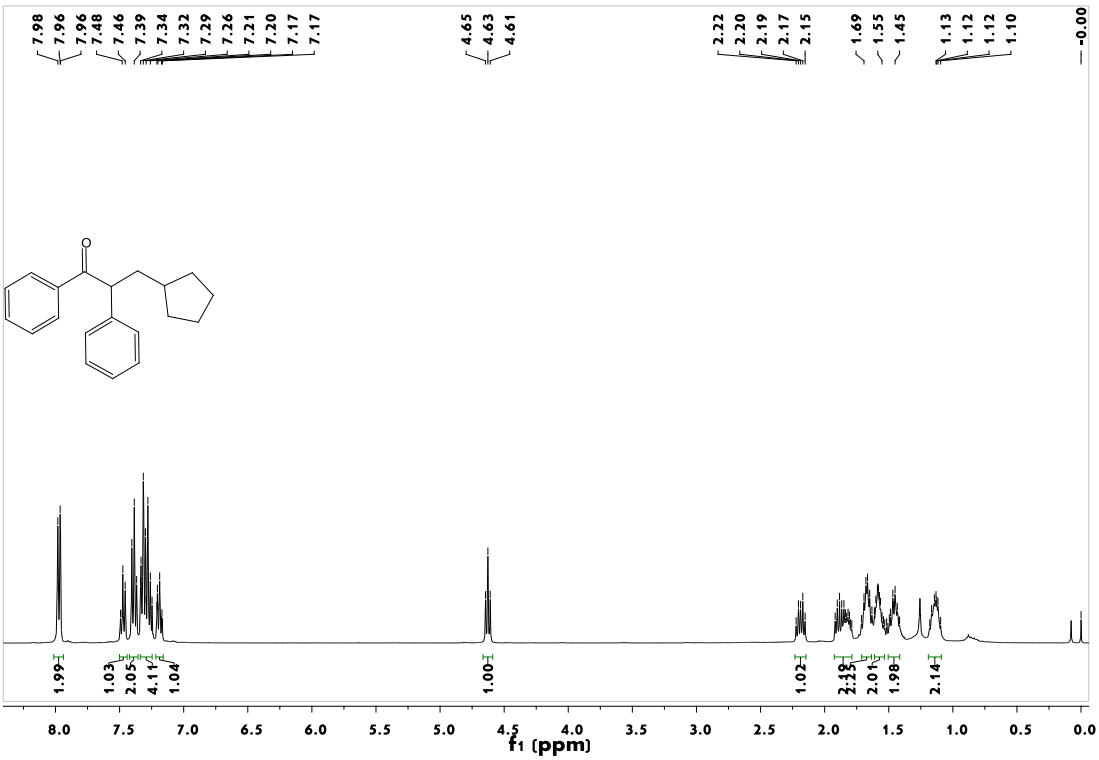
f1 (ppm)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7.96
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7.39
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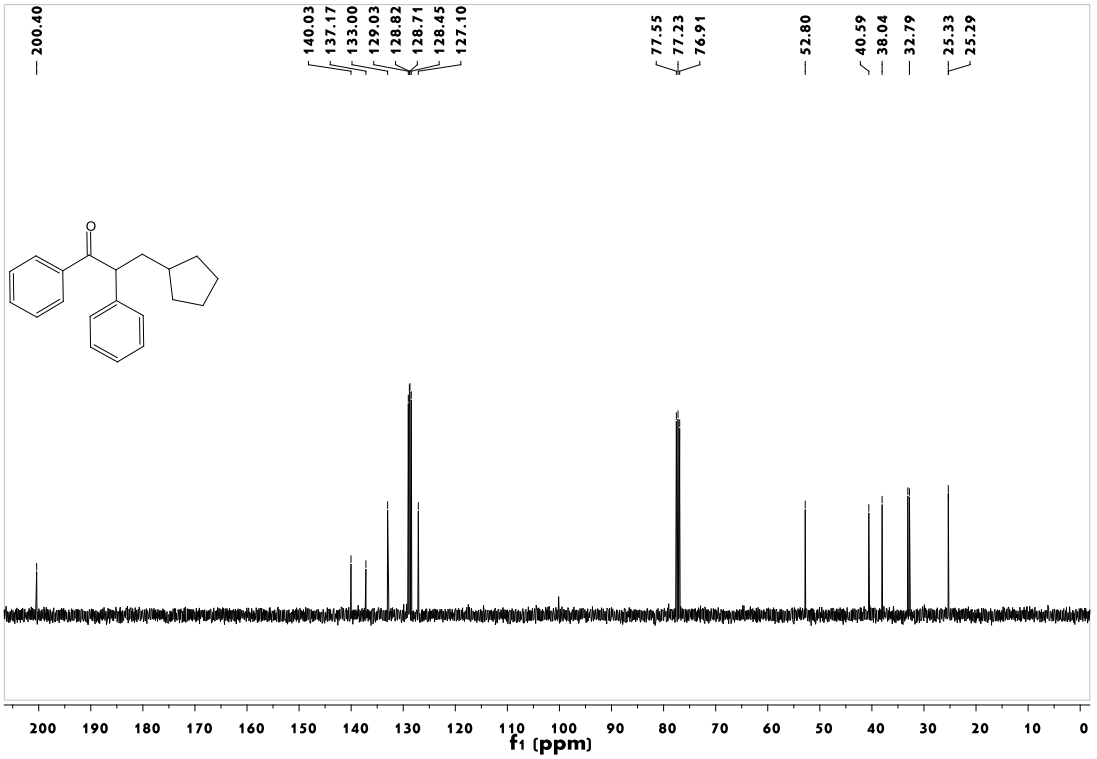
7.32
7.29
7.26
7.21
7.20
7.17
7.17
4.65
4.63
4.61
2.22
2.20
2.19
2.17
2.15
1.69
1.55
1.45
1.13
1.12
1.12
1.10
-0.00
O
1.99
1.03
2.05
4.11
1.04
1.00
1.02
2.18
2.15
2.01
1.98
2.14
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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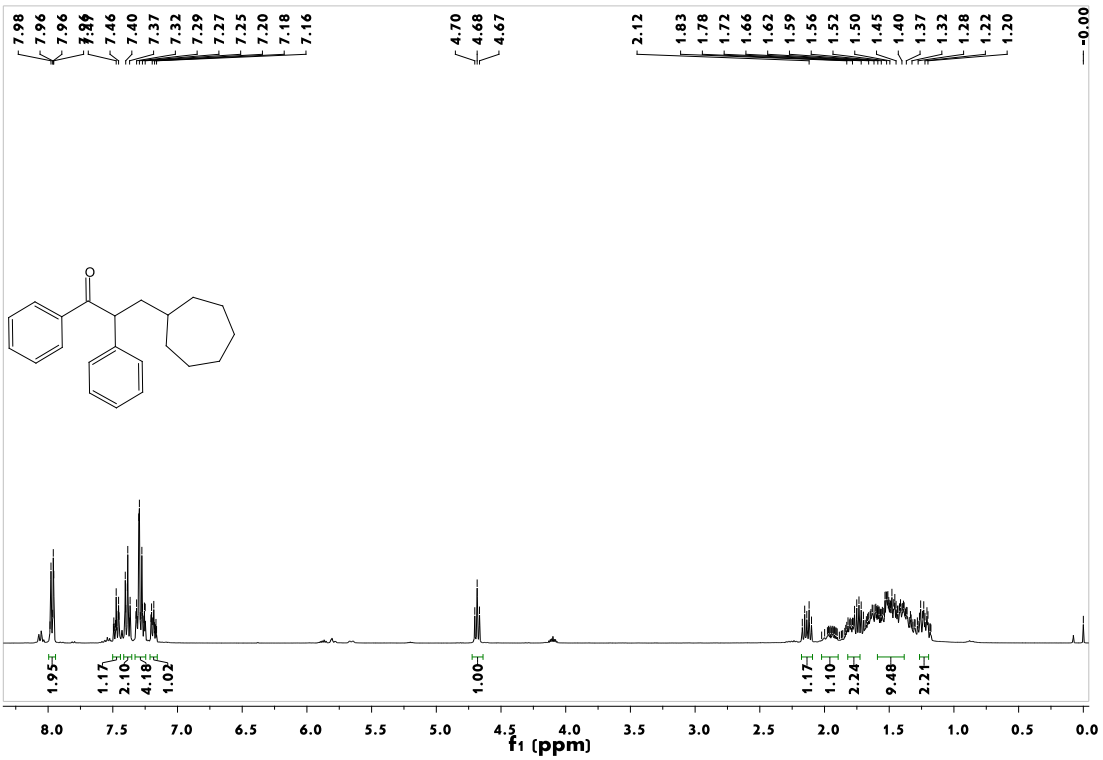
127.10
77.55
77.23
76.91
52.80
40.59
38.04
32.79
25.33
25.29
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.96
7.96
7.46
7.40
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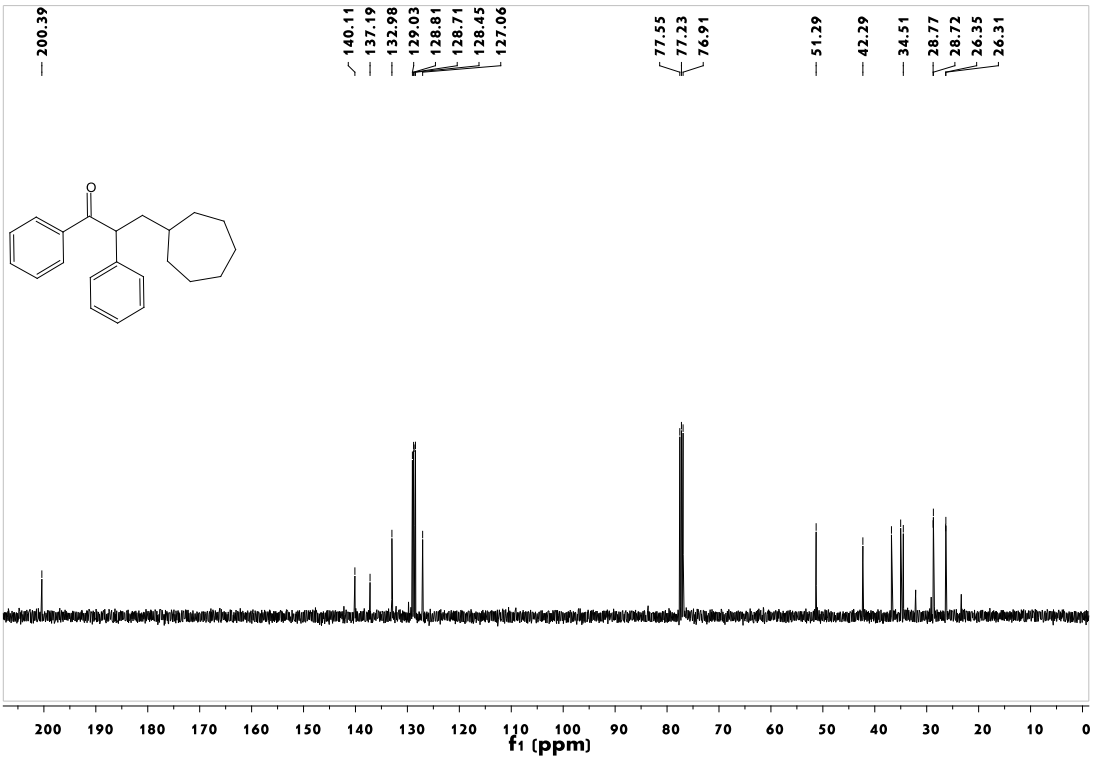
7.32
7.29
7.27
7.25
7.20
7.18
7.16
4.70
4.68
4.67
2.12
1.83
1.78
1.72
1.66
1.62
1.59
1.56
1.52
1.50
1.45
1.40
1.37
1.32
1.28
1.22
1.20
0.00
1.95
1.17
2.10
4.18
1.02
1.00
1.17
1.10
2.24
9.48
2.21
f1 (ppm)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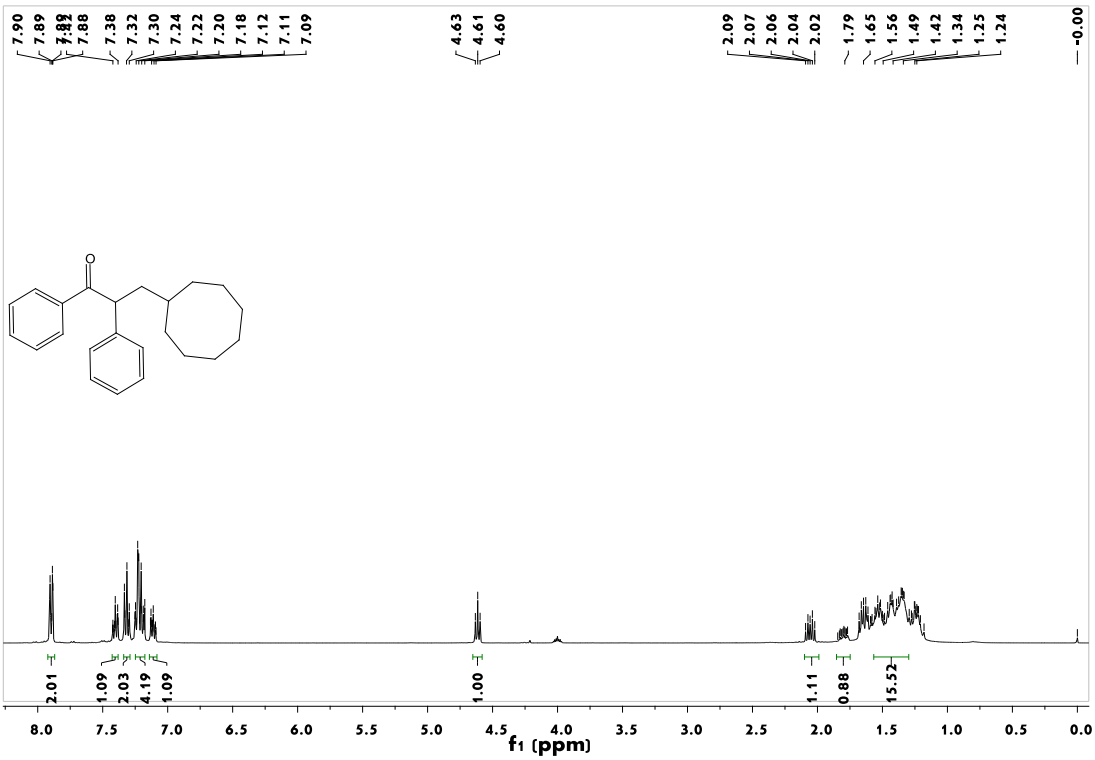
76.91
51.29
42.29
34.51
28.77
28.72
26.35
26.31
f1 (ppm)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7.32
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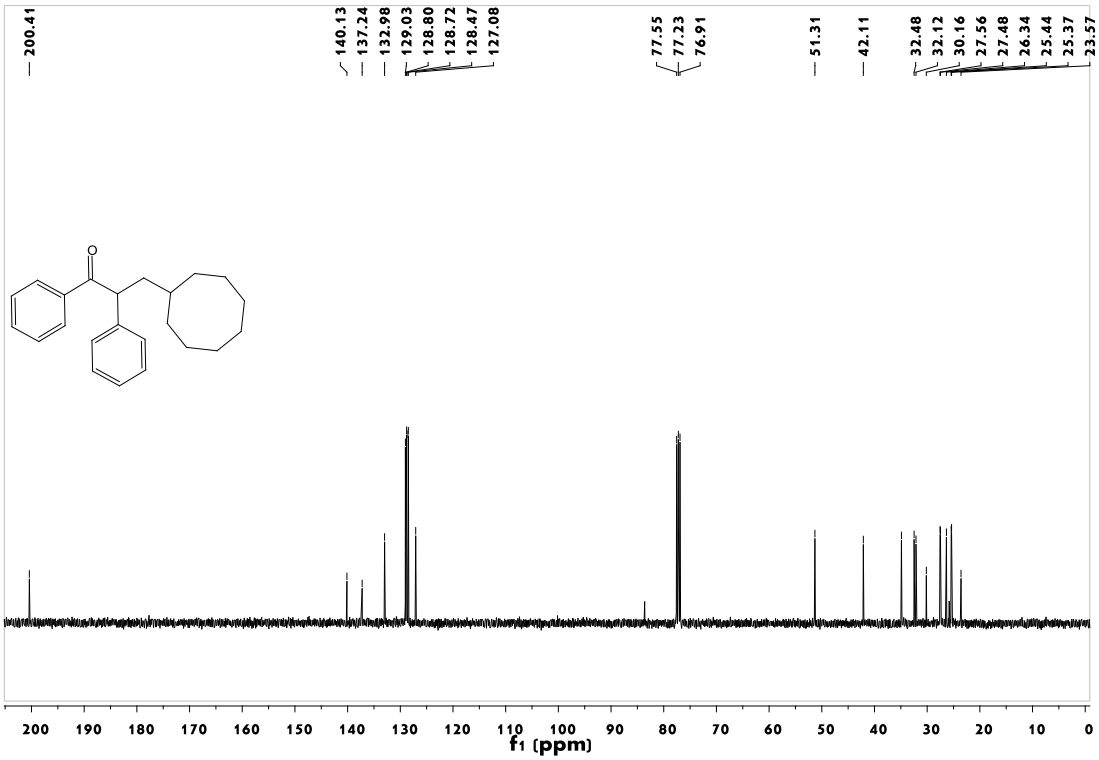
7.24
7.22
7.20
7.18
7.12
7.11
7.09
4.63
4.61
4.60
2.09
2.07
2.06
2.04
2.02
1.79
1.65
1.56
1.49
1.42
1.34
1.25
1.24
-0.00
O
2.01
1.09
2.03
4.19
1.09
1.00
1.11
0.88
15.52
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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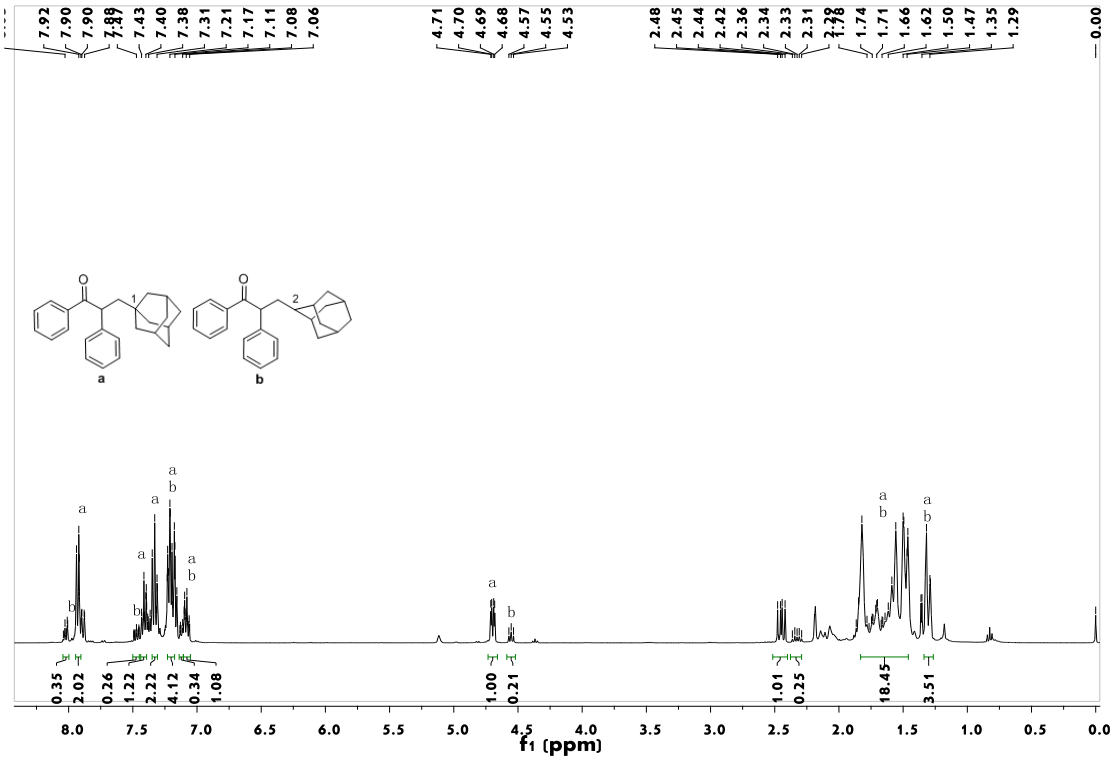
128.80
128.72
128.47
127.08
77.55
77.23
76.91
51.31
42.11
32.48
32.12
30.16
27.56
27.48
26.34
25.44
25.37
23.57
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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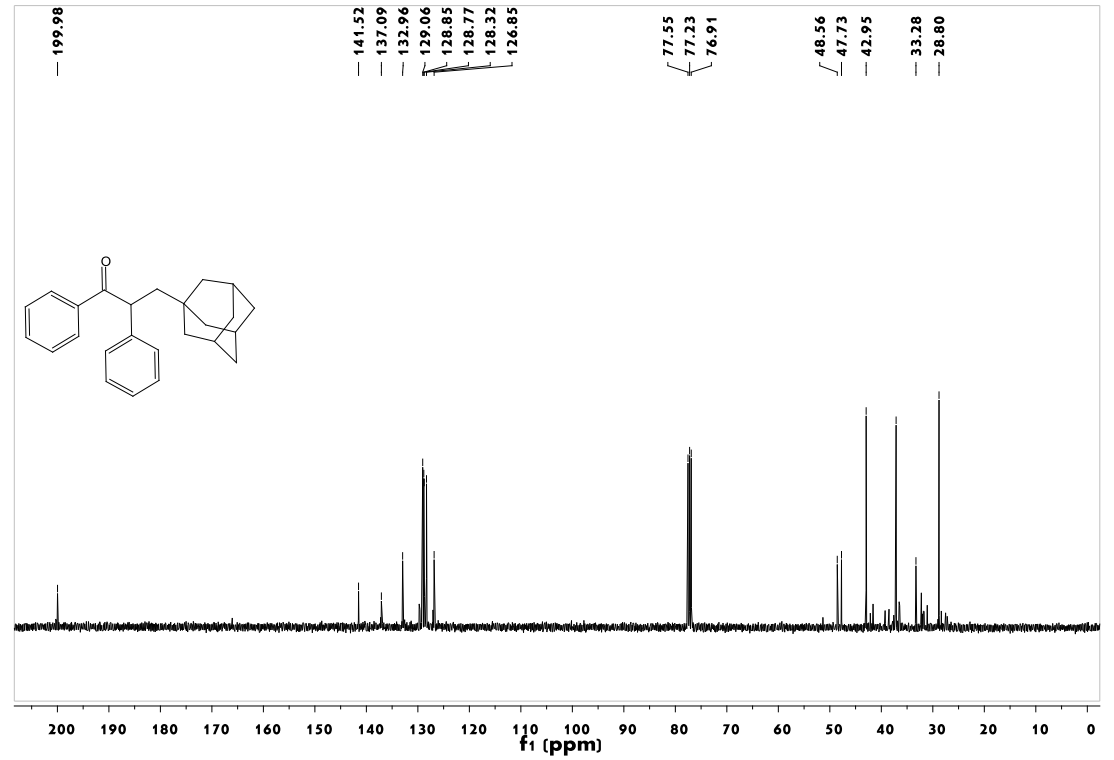
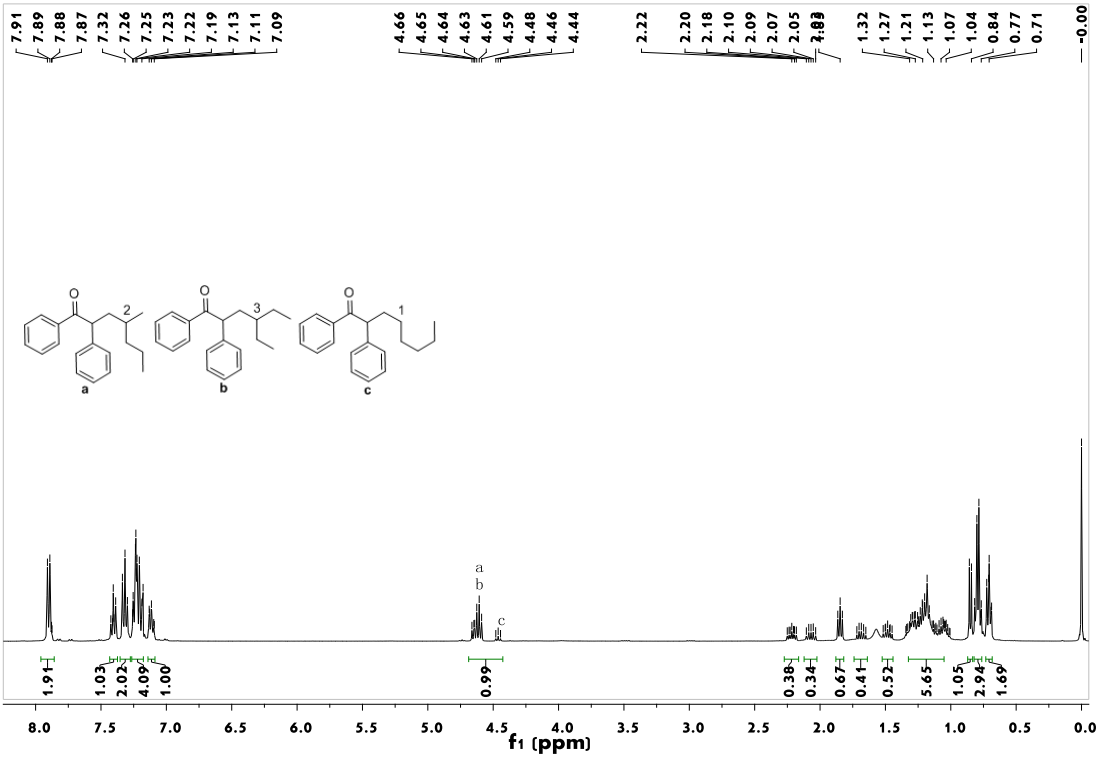
4.71 4.70 4.69 4.68 4.57 4.55 4.53
2.48 2.45 2.44 2.42 2.36 2.34 2.33 2.31 2.29 1.78 1.74 1.71 1.66 1.62 1.50 1.47 1.35 1.29
0.00
a
b
0.35 2.02 0.26 1.22 2.22 4.12 0.34 1.08 1.00 0.21 1.01 0.25 18.45 3.51
f1 (ppm)


199.98
141.52 137.09 132.96 129.06 128.85 128.77 128.32 126.85
77.55 77.23 76.91
48.56 47.73 42.95 33.28 28.80
f1 (ppm)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7.19
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7.11
7.09
4.66
4.65
4.64
4.63
4.61
4.59
4.48
4.46
4.44
2.22
2.20
2.18
2.10
2.09
2.07
2.05
1.32
1.27
1.21
1.13
1.07
1.04
0.84
0.77
0.71
-0.00
a
b
c
1.91
1.03
2.02
4.09
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0.67
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1.05
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1.69
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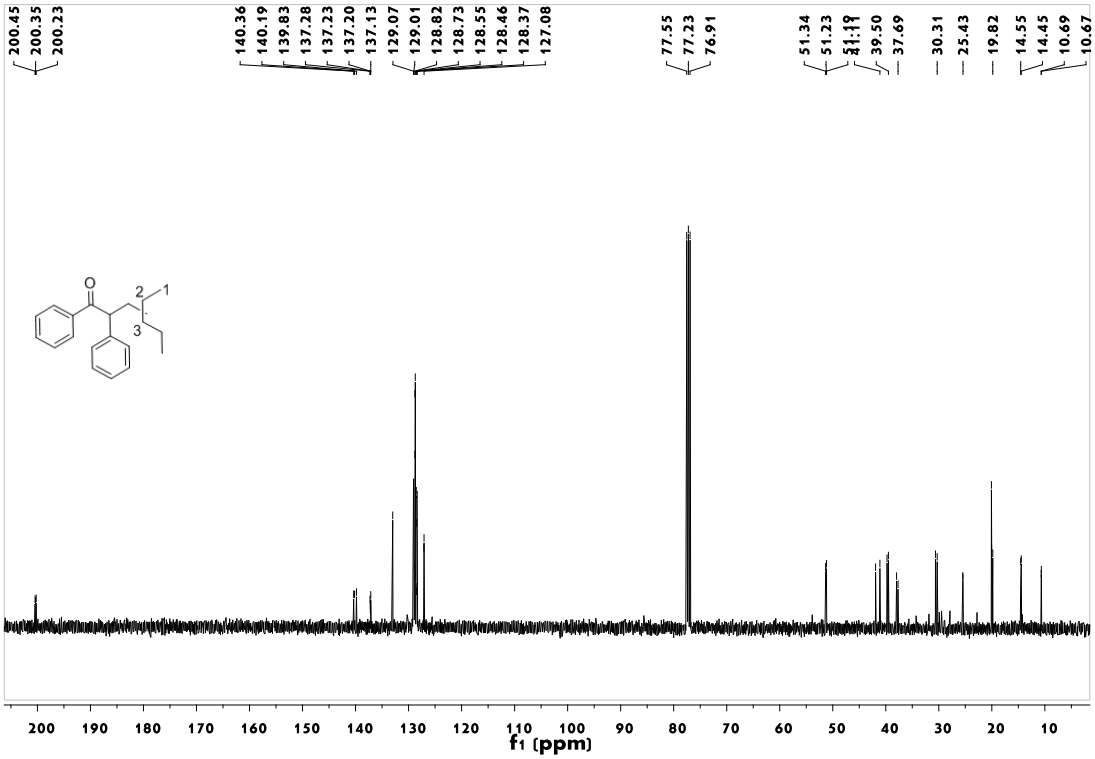
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137.13
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128.73
128.55
128.46
128.37
127.08
77.55
77.23
76.91
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51.23
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30.31
25.43
19.82
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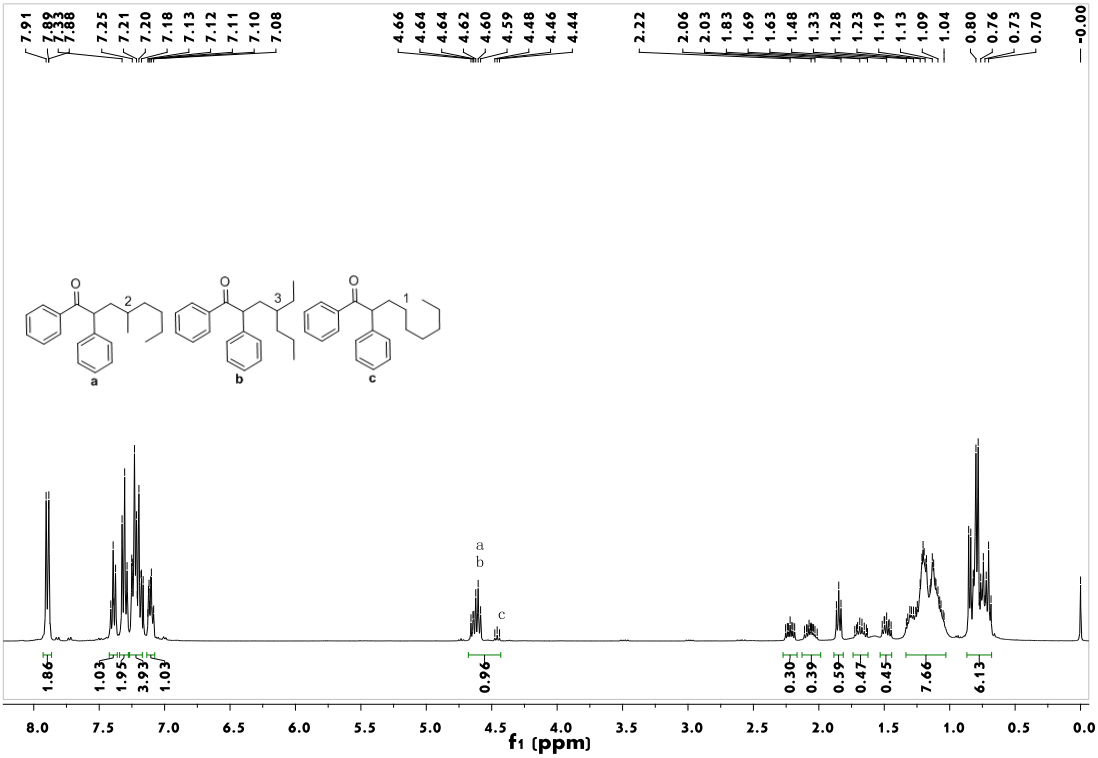
14.45
10.69
10.67
f1 (ppm)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7.12
7.11
7.10
7.08
4.66
4.64
4.64
4.62
4.60
4.59
4.48
4.46
4.44
2.22
2.06
2.03
1.83
1.69
1.63
1.48
1.33
1.28
1.23
1.19
1.13
1.09
1.04
0.80
0.76
0.73
0.70
-0.00
a
b
c
1.86
1.03
1.95
3.93
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0.59
0.47
0.45
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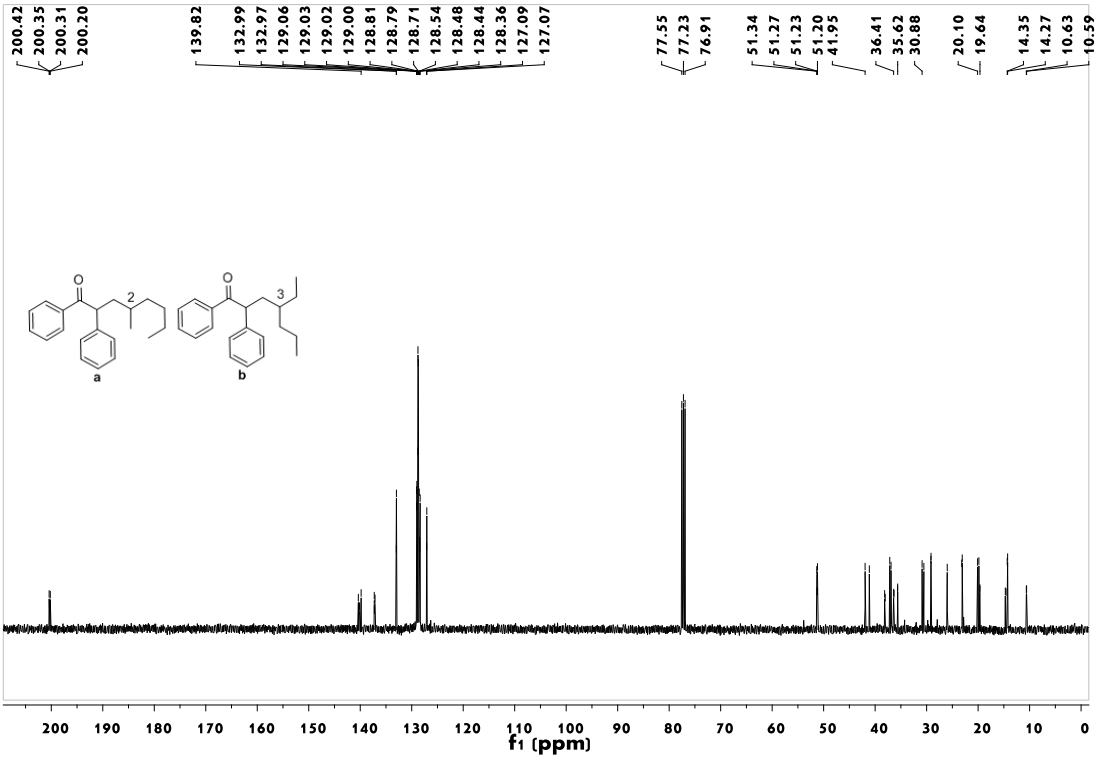
6.13
f1 (ppm)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128.54
128.48
128.44
128.36
127.09
127.07
77.55
77.23
76.91
51.34
51.27
51.23
51.20
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19.64
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14.27
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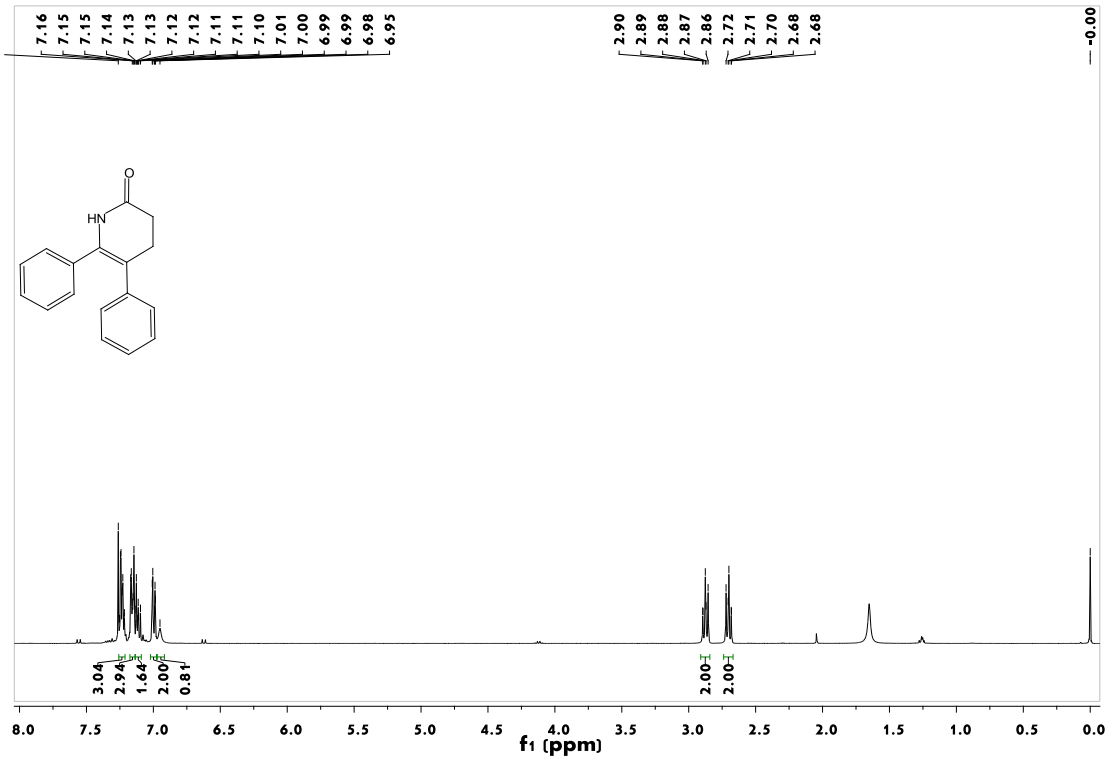
f1 (ppm)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7.11
7.10
7.01
7.00
6.99
6.99
6.98
6.95
2.90
2.89
2.88
2.87
2.86
2.72
2.71
2.70
2.68
2.68
-0.00
O
HN
3.04
2.94
1.64
2.00
0.81
2.00
2.00
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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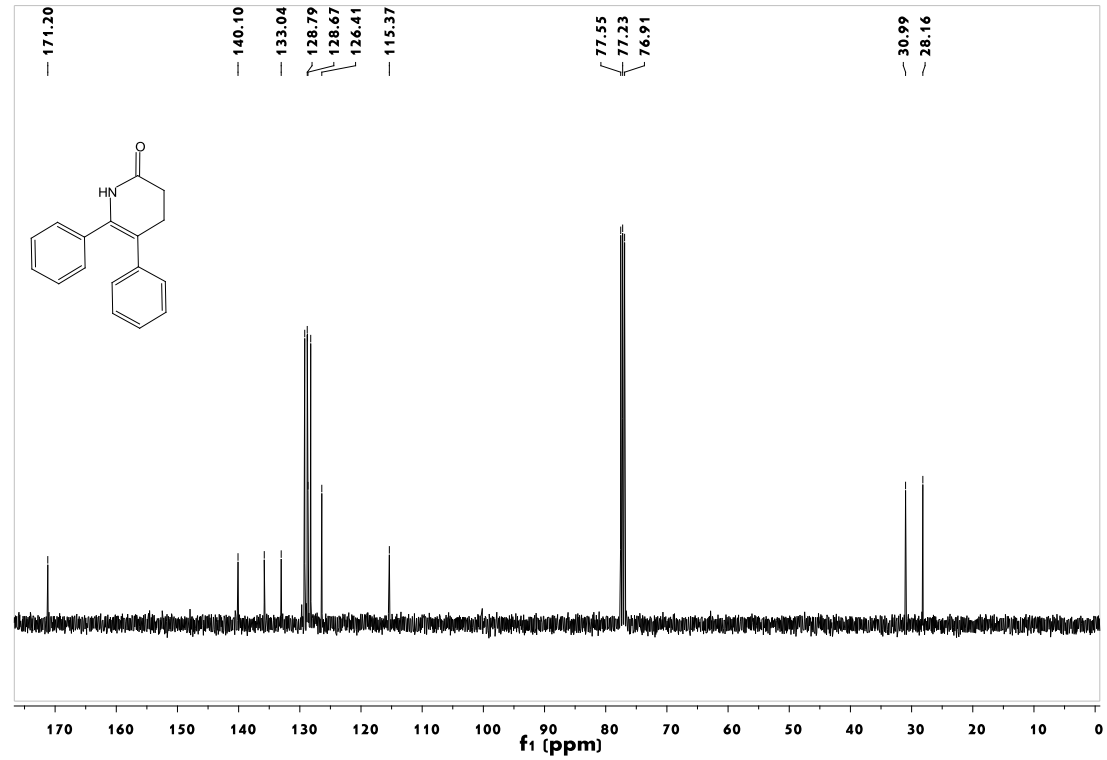
f1 (ppm)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128.79
128.67
126.41
115.37
77.55
77.23
76.91
30.99
28.16
O
HN
170
160
150
140
130
120
110
100
90
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70
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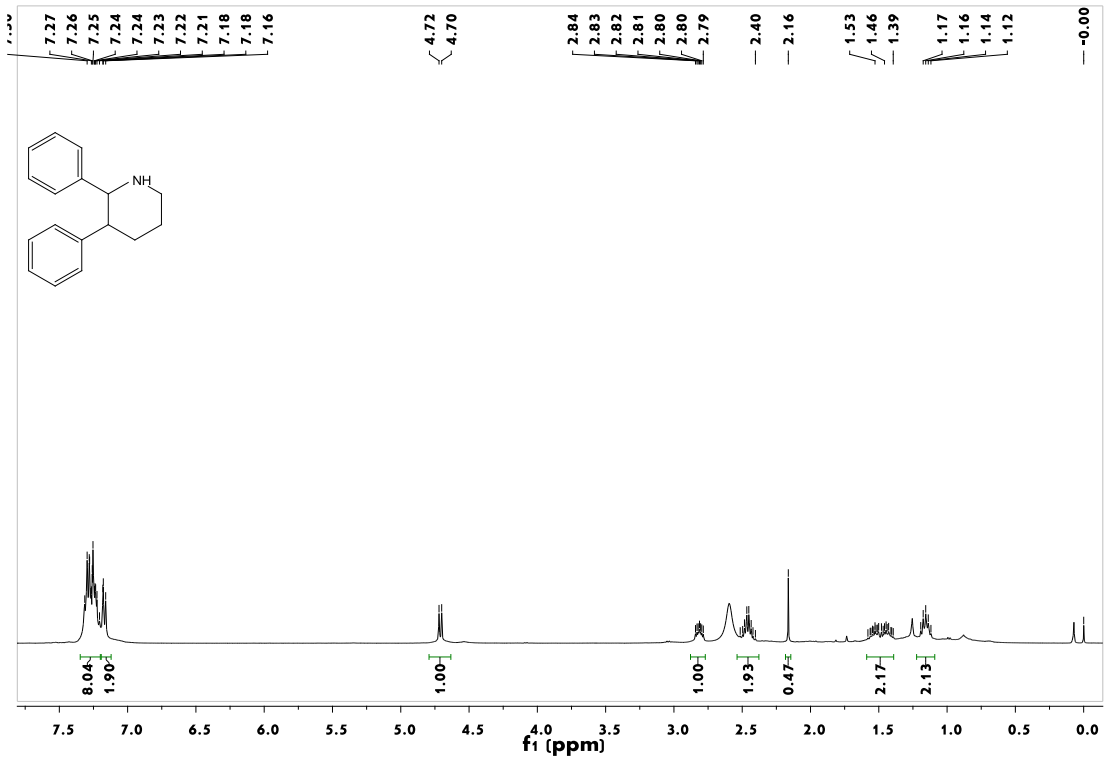
50
40
30
20
10
0
f1 (ppm)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7.24
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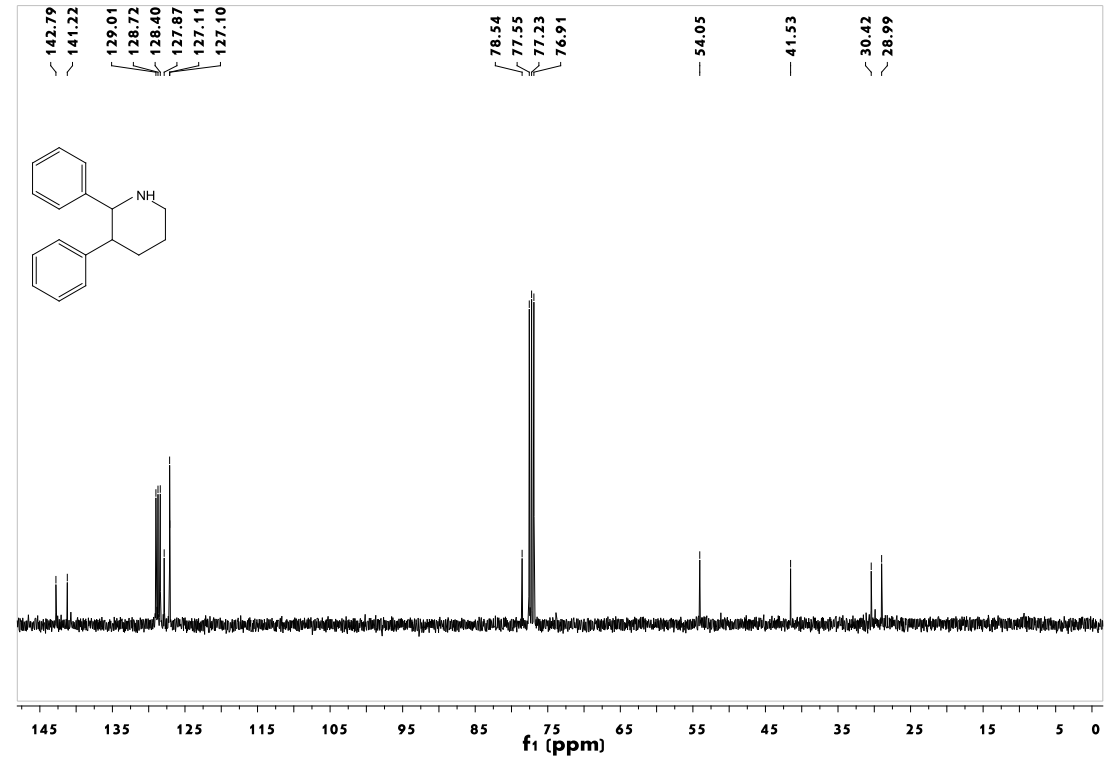
7.21
7.18
7.16
4.72
4.70
2.84
2.83
2.82
2.81
2.80
2.80
2.79
2.40
2.16
1.53
1.46
1.39
1.17
1.16
1.14
1.12
0.00
NH
8.04
1.90
1.00
1.00
1.93
0.47
2.17
2.13
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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141.22
129.01
128.72
128.40
127.87
127.11
127.10
78.54
77.55
77.23
76.91
54.05
41.53
30.42
28.99
NH
145
135
125
115
105
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)