Metal-free oxidative C(sp^3)–H bond functionalization of alkanes and alkylation-initiated radical 1,2-aryl migration in α,α-diaryl allylic alcohols

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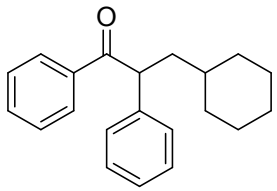
1. General information

All manipulations were carried out under air atmosphere. Commercially available reagents were used as received without purification. Column chromatography was carried out on silica gel (300–400 mesh). Analytical thin–layer chromatography was performed on glass plates of Silica Gel GF–254 with detection by UV. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVANCE 400M spectrometer. The chemical shift references were as follows: (^{1}H) $CDCl_3$, 7.26 ppm ($CHCl_3$); (^{13}C) $CDCl_3$, 77.00 ppm ($CDCl_3$). HRMS spectra were carried out at Micromass Q-Tof instrument (ESI). Melting point determination was taken on a Melt–Temp apparatus (X-4) from Beijing Fukai Electro–optic Instrument Plant and was uncorrected.

2. General procedure for the synthesis of α,α-diaryl allylic alcohols

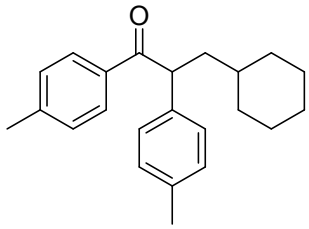
A sealable reaction tube equipped with a magnetic stirrer bar was charged with □,□-Diaryl allylic alcohol (63 mg, 0.3 mmol), DTBP (di-*tert*-butyl peroxide, 0.9 mmol, 170 μL), and cyclohexane (1.0 mL, 15-25 mmol). The rubber septum was then replaced by a Teflon–coated screw cap, and the reaction vessel placed in an oil bath at 120 °C. After stirring the mixture at this temperature for 24 h, it was cooled to room temperature and diluted with ethyl acetate, washed with water, dried over $MgSO_4$. After the solvent was removed under reduced pressure, the residue was purified by column chromatography on silica gel (CH_2Cl_2/hexane = 1:2) to afford the corresponding product, 3-cyclohexyl-1,2-diphenylpropan-1-one (**3ab**, 79 mg, 90% yield).

3. Characterization data for 3

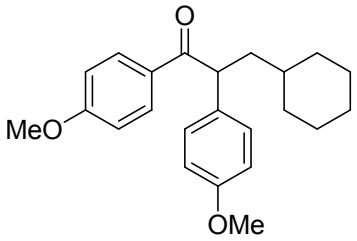


3-cyclohexyl-1,2-diphenylpropan-1-one (3ab): White solid, mp 54–56 °C. Yield: 79 mg (90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.8 Hz, 2H), 7.39 (ddd, *J* = 6.6, 3.8, 1.2 Hz, 1H), 7.30 (dd, *J* = 10.4, 4.7 Hz, 2H), 7.25 – 7.16 (m, 4H), 7.11 (ddd, *J* = 8.5, 3.5, 1.7 Hz, 1H), 4.64 (t, *J* = 7.3 Hz, 1H), 2.09 – 1.99 (m, 1H), 1.75 (d, *J* = 12.6 Hz, 1H), 1.66 – 1.49 (m, 5H), 1.17 – 0.98 (m, 4H), 0.91 – 0.79 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.02, 139.98, 136.92, 132.75, 128.82, 128.59, 128.48,

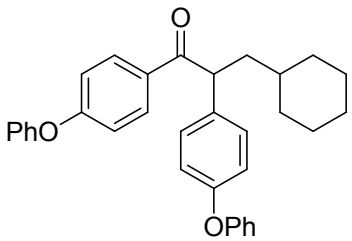
128.19, 126.83, 50.47, 41.67, 35.27, 33.54, 33.25, 26.47, 26.11, 26.10. HRMS (ESI) m/z calcd. for $[C_{21}H_{24}O+Na]^+$ 315.1725, found 315.1722.



3-cyclohexyl-1,2-di-p-tolylpropan-1-one (3bb): Colorless oil. Yield: 82 mg (85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.2 Hz, 2H), 7.17 (dd, *J* = 14.7, 8.1 Hz, 4H), 7.06 (d, *J* = 7.9 Hz, 2H), 4.67 (t, *J* = 7.3 Hz, 1H), 2.31 (s, 3H), 2.24 (s, 3H), 2.10 (dt, *J* = 14.6, 7.5 Hz, 1H), 1.82 (d, *J* = 12.7 Hz, 1H), 1.71 – 1.56 (m, 5H), 1.24 – 1.07 (m, 4H), 0.99 – 0.85 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.61, 143.34, 137.13, 136.22, 134.35, 129.43, 129.08, 128.67, 127.94, 49.79, 41.58, 35.19, 33.50, 33.21, 26.45, 26.07, 26.05, 21.43, 20.90. HRMS (ESI) m/z calcd. for $[C_{23}H_{28}O+Na]^+$ 343.2038, found 343.2036.

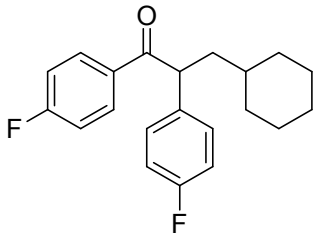


3-cyclohexyl-1,2-bis(4-methoxyphenyl)propan-1-one (3cb): Colorless oil. Yield: 92 mg (87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.94 (m, 2H), 7.27 – 7.19 (m, 2H), 6.89 – 6.79 (m, 4H), 4.63 (t, *J* = 7.4 Hz, 1H), 3.80 (s, 3H), 3.73 (s, 3H), 2.11 – 2.02 (m, 1H), 1.82 (d, *J* = 12.7 Hz, 1H), 1.71 – 1.59 (m, 5H), 1.22 – 1.09 (m, 4H), 0.98 –0.86 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.75, 163.12, 158.32, 132.36, 130.82, 129.84, 129.07, 114.13, 113.61, 55.31, 55.08, 49.05, 41.63, 35.17, 33.55, 33.21, 26.48, 26.12, 26.09. HRMS (ESI) m/z calcd. for $[C_{23}H_{28}O_3+Na]^+$ 375.1936, found 375.1936.

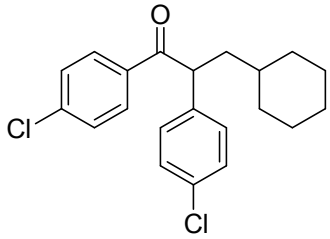


3-cyclohexyl-1,2-bis(4-phenoxyphenyl)propan-1-one (3db): Colorless oil. Yield: 109 mg (76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.95 (m, 2H), 7.40 – 7.34 (m, 2H), 7.33 – 7.28 (m, 2H), 7.27 – 7.23 (m, 2H), 7.21 – 7.15 (m, 1H), 7.11 – 7.02 (m, 3H), 6.99 – 6.89 (m, 6H), 4.66 (t, *J* = 7.3 Hz, 1H),

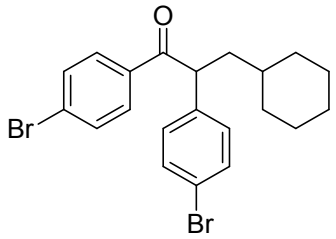
2.10 (dt, *J* = 14.6, 7.5 Hz, 1H), 1.80 (d, *J* = 12.8 Hz, 1H), 1.69 – 1.59 (m, 5H), 1.24 – 1.09 (m, 4H), 1.00 – 0.86 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.60, 161.83, 156.93, 156.14, 155.32, 134.80, 131.36, 130.88, 130.01, 129.68, 129.39, 124.62, 123.29, 120.25, 118.97, 118.94, 117.15, 49.36, 41.77, 35.29, 33.53, 33.27, 26.48, 26.13, 26.10. HRMS (ESI) m/z calcd. for $[C_{33}H_{32}O_3+Na]^+$ 499.2249, found 499.2244.



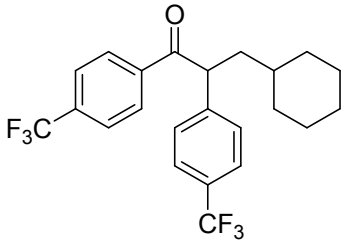
3-cyclohexyl-1,2-bis(4-fluorophenyl)propan-1-one (3eb): White solid, mp 57–59 °C. Yield: 72 mg (73%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (dd, *J* = 8.8, 5.4 Hz, 2H), 7.26 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.06 (t, *J* = 8.6 Hz, 2H), 6.97 (t, *J* = 8.6 Hz, 2H), 4.67 (t, *J* = 7.3 Hz, 1H), 2.12 – 2.03 (m, 1H), 1.81 (d, *J* = 12.7 Hz, 1H), 1.73 – 1.58 (m, 5H), 1.22 – 1.07 (m, 4H), 0.99 – 0.87 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.32, 165.51 (d, *J* = 255.0 Hz), 161.77 (d, *J* = 245.7 Hz), 135.42 (d, *J* = 3.2 Hz), 133.04 (d, *J* = 3.0 Hz), 131.15 (d, *J* = 9.3 Hz), 129.61 (d, *J* = 7.9 Hz), 115.79 (d, *J* = 9.4 Hz), 115.58 (d, *J* = 9.9 Hz), 49.52, 41.64, 35.17, 33.53, 33.11, 26.39, 26.07, 26.04. HRMS (ESI) m/z calcd. for $[C_{21}H_{22}OF_2+Na]^+$ 351.1536, found 351.1528.



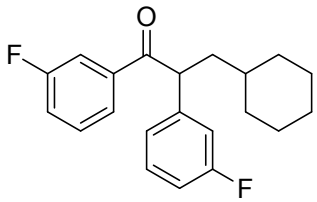
1,2-bis(4-chlorophenyl)-3-cyclohexylpropan-1-one (3fb): Colorless oil. Yield: 87 mg (80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.5 Hz, 2H), 7.28 (d, *J* = 8.5 Hz, 2H), 7.15 (q, *J* = 8.5 Hz, 4H), 4.54 (t, *J* = 7.3 Hz, 1H), 1.97 (dt, *J* = 14.5, 7.4 Hz, 1H), 1.71 (d, *J* = 12.8 Hz, 1H), 1.64 – 1.51 (m, 5H), 1.10 – 1.00 (m, 4H), 0.90 – 0.77 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.42, 139.41, 138.03, 134.88, 132.89, 129.93, 129.46, 129.06, 128.89, 49.80, 41.43, 35.15, 33.54, 33.08, 26.38, 26.05, 26.02. HRMS (ESI) m/z calcd. for $[C_{21}H_{22}OCl_2+Na]^+$ 383.0945, found 383.0937.



1,2-bis(4-bromophenyl)-3-cyclohexylpropan-1-one (3gb): Colorless oil. Yield: 113 mg (84%).[1]H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.3 Hz, 2H), 7.53 (d, *J* = 8.4 Hz, 2H), 7.43 – 7.39 (m, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 4.62 (t, *J* = 7.2 Hz, 1H), 2.10 – 2.02 (m, 1H), 1.80 (d, *J* = 12.7 Hz, 1H), 1.71 – 1.59 (m, 5H), 1.21 – 1.07 (m, 4H), 0.98 – 0.86 (m, 2H). [13]C NMR (100 MHz, $CDCl_3$) δ 198.44, 138.49, 135.21, 131.98, 131.84, 130.00, 129.80, 128.14, 120.98, 49.81, 41.33, 35.10, 33.50, 33.04, 26.34, 26.01, 25.99. HRMS (ESI) m/z calcd. for $[C_{21}H_{22}OBr_2+Na]^+$ 470.9935, found 470.9931.

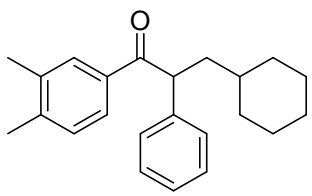


3-cyclohexyl-1,2-bis(4-(trifluoromethyl)phenyl)propan-1-one (3hb): Colorless oil. Yield: 92 mg (72%).[1]H NMR (400 MHz, $CDCl_3$) δ 8.26 (s, 1H), 8.16 (d, *J* = 7.9 Hz, 1H), 7.76 (d, *J* = 7.8 Hz, 1H), 7.62 (s, 1H), 7.59 – 7.52 (m, 2H), 7.49 (d, *J* = 7.8 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 1H), 4.83 (t, *J* = 7.3 Hz, 1H), 2.18 (dt, *J* = 14.5, 7.4 Hz, 1H), 1.84 (d, *J* = 12.6 Hz, 1H), 1.79 – 1.60 (m, 5H), 1.24 – 1.10 (m, 4H), 1.02 – 0.93 (m, 2H). [13]C NMR (100 MHz, $CDCl_3$) δ 198.04, 140.32, 137.02, 131.60, 129.51 (dd, *J* = 6.7, 3.1 Hz), 129.46, 129.37, 125.41 (q, *J* = 3.8 Hz), 124.97 (q, *J* = 3.8 Hz), 124.12 (q, *J* = 3.7 Hz), 122.42 (d, *J* = 35.5 Hz), 50.48, 41.69, 35.35, 33.50, 33.15, 26.34, 26.02, 26.01. HRMS (ESI) m/z calcd. for $[C_{23}H_{22}OF_6+Na]^+$ 451.1473, found 451.1476.

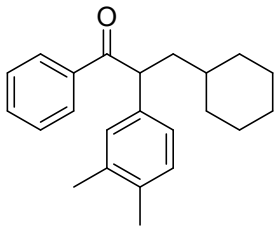


3-cyclohexyl-1,2-bis(3-fluorophenyl)propan-1-one (3ib): Colorless oil. Yield: 69 mg (70%). [1]H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.8 Hz, 1H), 7.56 – 7.52 (m, 1H), 7.30 – 7.23 (m, 1H), 7.16 – 7.05 (m, 2H), 6.98 (d, *J* = 7.8 Hz, 1H), 6.95 – 6.90 (m, 1H), 6.81 – 6.76 (m, 1H), 4.57 (t, *J* = 7.3 Hz, 1H), 2.05 – 1.95 (m, 1H), 1.74 – 1.68 (m, 1H), 1.64 – 1.47 (m, 5H), 1.11 – 0.97 (m, 4H), 0.89 – 0.77

(m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.17 (d, *J* = 1.9 Hz), 164.11 (d, *J* = 23.2 Hz), 161.65 (d, *J* = 24.6 Hz), 141.93 (d, *J* = 7.2 Hz), 138.75 (d, *J* = 6.0 Hz), 130.31 (d, *J* = 8.3 Hz), 130.19 (d, *J* = 7.6 Hz), 124.21 (d, *J* = 2.9 Hz), 123.89 (d, *J* = 2.8 Hz), 119.95 (d, *J* = 21.5 Hz), 115.27 (d, *J* = 22.4 Hz), 115.00 (d, *J* = 21.7 Hz), 114.00 (d, *J* = 21.1 Hz), 50.34 (d, *J* = 1.1 Hz), 41.49, 35.21, 33.46, 33.11, 26.36, 26.03, 26.00. HRMS (ESI) m/z calcd. for $[C_{21}H_{22}OF_2+H]^+$ 329.1717, found 329.1714.

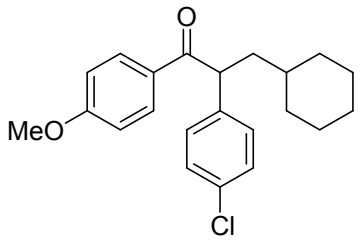


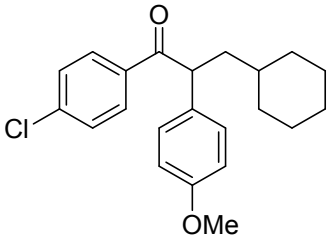
3jb



3jb'

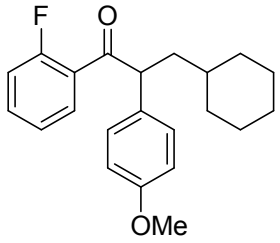
3-cyclohexyl-1-(3,4-dimethylphenyl)-2-phenylpropan-1-one (3jb) and 3-cyclohexyl-2-(3,4-dimethylphenyl)-1-phenylpropan-1-one (3jb'): Colorless oil. Yield: 79 mg (82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.85 (m, 0.66H), 7.68 – 7.59 (m, 1.33H), 7.34 – 7.11 (m, 3.60H), 7.06 – 6.90 (m, 2.40H), 4.65 – 4.58 (m, 0.66H), 4.58– 4.52 (m, 0.33H), 2.12 (s, 2H), 2.10 (s, 2H), 2.07 (s, 1H), 2.04 (s, 1H), 2.03 – 1.97 (m, 1H), 1.72 (d, *J* = 12.6 Hz, 1H), 1.62 – 1.45 (m, 5H), 1.18 – 0.94 (m, 4H), 0.90 – 0.75 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.00, 199.68, 142.20, 140.28, 137.35, 136.92, 136.73, 134.99, 134.72, 132.55, 129.96, 129.68, 129.60, 129.07, 128.67, 128.53, 128.35, 128.07, 126.62, 126.28, 125.57, 50.15, 49.97, 41.72, 41.65, 35.28, 35.21, 33.45, 33.23, 26.43, 26.05, 19.80, 19.71, 19.68, 19.22. HRMS (ESI) m/z calcd. for $[C_{23}H_{28}O+Na]^+$ 343.2038, found 343.2036.

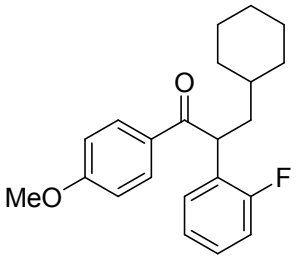




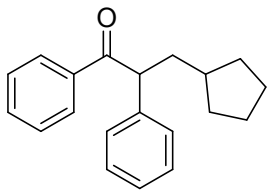
2-(4-chlorophenyl)-3-cyclohexyl-1-(4-methoxyphenyl)propan-1-one(3kb) and 1-(4-chlorophenyl) -3-cyclohexyl-2-(4-methoxyphenyl)propan-1-one(3kb'): Colorless oil. Yield: 73 mg (68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.93 (m, 1.86H), 7.91 – 7.88 (m, 0.14H), 7.34 (d, *J* = 8.6 Hz, 0.14H), 7.27 – 7.22 (m, 3.72H), 7.19 (d, *J* = 8.7 Hz, 0.14H), 6.90 – 6.85 (m, 1.86H), 6.83 – 6.80 (m, 0.14H), 4.66 (t, *J* = 7.3 Hz, 0.93H), 4.59 (t, *J* = 7.3 Hz, 0.07H), 3.80 (s, 2.79H), 3.73 (s, 0.21H), 2.13 – 2.02 (m, 1H), 1.80 (d, *J* = 12.8 Hz, 1H), 1.71 – 1.57 (m, 5H), 1.21 – 1.07 (m, 4H), 0.98 – 0.85 (m, 2H). ^{13}C NMR

(100 MHz, $CDCl_3$) δ 198.88, 198.09, 163.33, 158.49, 139.00, 138.79, 135.15, 132.52, 131.52, 130.79, 129.95, 129.52, 129.45, 129.08, 128.84, 128.71, 114.28, 113.71, 55.32, 55.06, 49.60, 49.21, 41.58, 41.41, 35.18, 35.09, 33.51, 33.11, 26.40, 26.05, 26.02. HRMS (ESI) m/z calcd. for $[C_{22}H_{25}ClO_2+Na]^+$ 379.1441, found 379.1446.



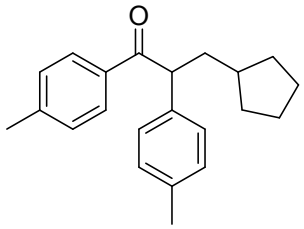


3-cyclohexyl-1-(2-fluorophenyl)-2-(4-methoxyphenyl)propan-1-one(3lb) and 3-cyclohexyl-2- (2-fluorophenyl)-1-(4-methoxyphenyl)propan-1-one(3lb'): Colorless oil. Yield: 79 mg (77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.84 (m, 1.34H), 7.55 (td, *J* = 7.6, 1.8 Hz, 0.33H), 7.21 – 7.13 (m, 1H), 7.05 (d, *J* = 8.6 Hz, 0.67H), 7.01 – 6.82 (m, 2.67H), 6.73 – 6.68 (m, 1.33H), 6.67 – 6.62 (m, 0.67H), 4.98 (t, *J* = 7.3 Hz, 0.67H), 4.48 (t, *J* = 7.4 Hz, 0.33H), 3.58 (s, 2H), 3.53 (s, 1H), 1.98 (td, *J* = 14.1, 7.0 Hz, 1H), 1.77 – 1.67 (m, 1H), 1.58 – 1.43 (m, 5H), 1.08 – 0.95 (m, 4H), 0.85 – 0.72 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.27 (d, *J* = 4.4 Hz), 197.63 (d, *J* = 1.2 Hz), 163.27, 161.91, 160.92, 159.39, 158.50, 158.38, 133.65 (d, *J* = 8.9 Hz), 130.82 (d, *J* = 2.8 Hz), 130.52, 129.32 (d, *J* = 11.3 Hz), 128.86 (d, *J* = 3.7 Hz), 128.17 (d, *J* = 8.3 Hz), 127.20 (d, *J* = 15.1 Hz), 126.27 (d, *J* = 12.9 Hz), 124.38 (d, *J* = 3.4 Hz), 124.13 (d, *J* = 3.4 Hz), 116.26 (d, *J* = 23.9 Hz), 115.21 (d, *J* = 23.0 Hz), 113.83, 113.57, 55.04, 54.75, 53.64, 53.58, 40.91, 40.83, 40.81, 40.68, 35.27, 34.92, 33.52, 33.33, 33.09, 32.82, 26.35, 26.31, 26.02, 25.96. HRMS (ESI) m/z calcd. for $[C_{22}H_{25}FO_2+Na]^+$ 363.1736, found 363.1738.

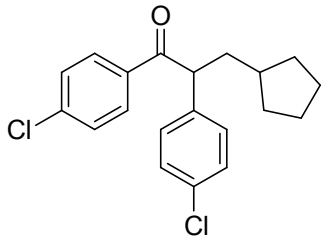


3-cyclopentyl-1,2-diphenylpropan-1-one (3aa): Colorless oil. Yield: 63 mg (76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (dd, *J* = 5.3, 3.3 Hz, 2H), 7.47 (ddd, *J* = 6.6, 3.9, 1.3 Hz, 1H), 7.41 – 7.36 (m, 2H), 7.35 – 7.26 (m, 4H), 7.21 – 7.16 (m, 1H), 4.63 (t, *J* = 7.3 Hz, 1H), 2.19 (dt, *J* = 14.3, 7.3 Hz, 1H), 1.94 – 1.79 (m, 2H), 1.72 – 1.42 (m, 6H), 1.20 – 1.08 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.14, 139.80, 136.94, 132.76, 128.79, 128.59, 128.48, 128.22, 126.87, 52.56, 40.36, 37.80, 32.87, 32.56,

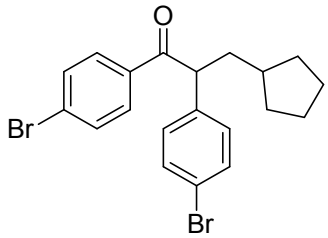
25.09, 25.06. HRMS (ESI) m/z calcd. for $[C_{20}H_{22}O+Na]^+$ 301.1568, found 301.1566.



3-cyclopentyl-1,2-di-p-tolylpropan-1-one (3ba): Colorless oil. Yield: 65 mg (71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.2 Hz, 2H), 7.10 (dd, *J* = 13.8, 8.0 Hz, 4H), 6.99 (d, *J* = 7.9 Hz, 2H), 4.49 (t, *J* = 7.3 Hz, 1H), 2.24 (s, 3H), 2.17 (s, 3H), 2.07 (dt, *J* = 14.2, 7.3 Hz, 1H), 1.82 – 1.69 (m, 2H), 1.64 – 1.32 (m, 6H), 1.09 – 0.99 (m, 6.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.83, 143.42, 136.97, 136.34, 134.40, 129.44, 129.12, 128.71, 128.02, 51.93, 40.28, 37.78, 32.87, 32.53, 25.08, 25.04, 21.49, 20.95. HRMS (ESI) m/z calcd. for $[C_{22}H_{26}O+Na]^+$ 329.1881, found 329.1879.

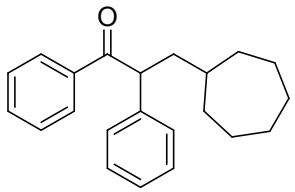


1,2-bis(4-chlorophenyl)-3-cyclopentylpropan-1-one (3fa): Colorless oil. Yield: 73 mg (70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.6 Hz, 2H), 7.30 (d, *J* = 8.6 Hz, 2H), 7.21 – 7.13 (m, 4H), 4.45 (t, *J* = 7.3 Hz, 1H), 2.11 – 2.01 (m, 1H), 1.82 – 1.69 (m, 2H), 1.60 – 1.35 (m, 6H), 1.11 – 0.98 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.59, 139.47, 137.90, 134.93, 132.98, 129.96, 129.51, 129.08, 128.92, 51.94, 40.17, 37.69, 32.89, 32.49, 25.08, 25.05. HRMS (ESI) m/z calcd. for $[C_{20}H_{20}OCl_2+H]^+$ 347.0969, found 347.0973.

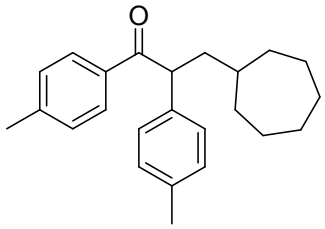


1,2-bis(4-bromophenyl)-3-cyclopentylpropan-1-one (3ga): Colorless oil. Yield: 94 mg (72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (dd, *J* = 8.8, 2.0 Hz, 2H), 7.54 (dd, *J* = 8.8, 2.1 Hz, 2H), 7.41 (dd, *J* = 8.7, 2.1 Hz, 2H), 7.18 – 7.14 (m, 2H), 4.51 (t, *J* = 7.3 Hz, 1H), 2.17 – 2.08 (m, 1H), 1.88 – 1.76 (m, 2H), 1.67 – 1.43 (m, 6H), 1.17 – 1.08 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.69, 138.39, 135.31, 132.03, 131.92, 130.06, 129.88, 128.23, 121.09, 52.00, 40.10, 37.68, 32.89, 32.48, 25.08, 25.04.

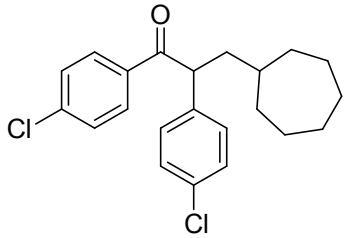
HRMS (ESI) m/z calcd. for $[C_{20}H_{20}OBr_2+Na]^+$ 456.9779, found 456.9776.



3-cycloheptyl-1,2-diphenylpropan-1-one (3ac): Colorless oil. Yield: 84 mg (91%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.5 Hz, 2H), 7.35 (t, *J* = 7.2 Hz, 1H), 7.27 (t, *J* = 7.5 Hz, 2H), 7.24 – 7.15 (m, 4H), 7.08 (t, *J* = 7.0 Hz, 1H), 4.60 (t, *J* = 7.2 Hz, 1H), 2.11 – 2.01 (m, 1H), 1.76 – 1.62 (m, 2H), 1.59 – 1.21 (m, 10H), 1.20 – 1.08 (dd, *J* = 20.4, 10.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.04, 139.86, 136.93, 132.69, 128.76, 128.53, 128.42, 128.17, 126.79, 51.03, 42.05, 36.53, 34.75, 34.25, 28.50, 28.45, 26.08, 26.05. HRMS (ESI) m/z calcd. for $[C_{22}H_{26}O+Na]^+$ 329.1881, found 329.1879.

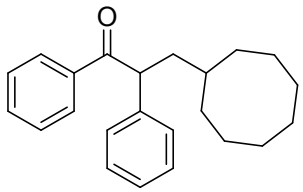


3-cycloheptyl-1,2-di-p-tolylpropan-1-one (3bc): Colorless oil. Yield: 87 mg (87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.1 Hz, 2H), 7.09 (t, *J* = 8.5 Hz, 4H), 6.98 (d, *J* = 8.0 Hz, 2H), 4.55 (t, *J* = 7.3 Hz, 1H), 2.24 (s, 3H), 2.17 (s, 3H), 2.03 (dt, *J* = 14.5, 7.4 Hz, 1H), 1.74 – 1.67 (m, 1H), 1.66 – 1.22 (m, 11H), 1.18 – 1.07 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.78, 143.39, 137.07, 136.28, 134.44, 129.45, 129.11, 128.69, 128.01, 50.43, 42.00, 36.52, 34.79, 34.27, 28.55, 28.49, 26.10, 26.07, 21.48, 20.94. HRMS (ESI) m/z calcd. for $[C_{24}H_{30}O+Na]^+$ 357.2194, found 357.2192.

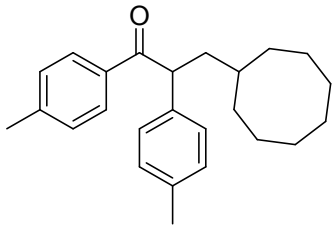


1,2-bis(4-chlorophenyl)-3-cycloheptylpropan-1-one (3fc): Colorless oil. Yield: 92 mg (82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.6 Hz, 2H), 7.28 (d, *J* = 8.6 Hz, 2H), 7.15 (q, *J* = 8.6 Hz, 4H), 4.51 (t, *J* = 7.3 Hz, 1H), 2.00 (dt, *J* = 14.3, 7.3 Hz, 1H), 1.71 – 1.65 (m, 1H), 1.64 – 1.58 (m, 1H), 1.57 – 1.34 (m, 8H), 1.30 – 1.22 (m, 2H), 1.18 – 1.07 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.55, 138.43, 136.98, 133.95, 131.92, 128.94, 128.51, 128.08, 127.90, 49.42, 40.88, 35.49, 33.86, 33.12,

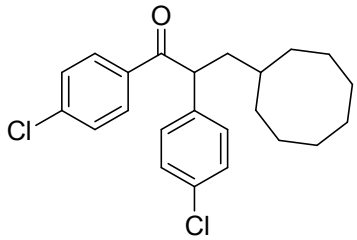
27.49, 27.42, 25.11, 25.06. HRMS (ESI) m/z calcd. for $[C_{22}H_{24}OCl_2+H]^+$ 375.1282, found 375.1286.



3-cyclooctyl-1,2-diphenylpropan-1-one (3ad): Colorless oil. Yield: 89 mg (93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 5.2, 3.4 Hz, 2H), 7.32 (ddd, *J* = 6.4, 3.8, 1.2 Hz, 1H), 7.27 – 7.20 (m, 4H), 7.16 (dd, *J* = 10.3, 4.8 Hz, 2H), 7.08 – 7.02 (m, 1H), 4.60 (t, *J* = 7.3 Hz, 1H), 2.05 (dt, *J* = 14.4, 7.3 Hz, 1H), 1.67 – 1.59 (m, 2H), 1.53 – 1.16 (m, 14H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.98, 139.84, 136.93, 132.64, 128.71, 128.47, 128.38, 128.14, 126.75, 51.00, 41.85, 34.58, 32.17, 31.83, 27.26, 27.17, 26.05, 25.13, 25.06. HRMS (ESI) m/z calcd. for $[C_{23}H_{28}O+Na]^+$ 343.2038, found 343.2035.

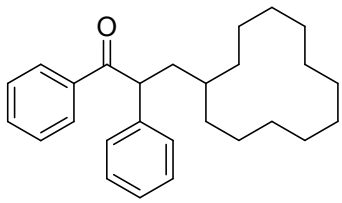


3-cyclooctyl-1,2-di-p-tolylpropan-1-one (3bd): Colorless oil. Yield: 94 mg (90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.2 Hz, 2H), 7.09 (d, *J* = 8.1 Hz, 2H), 7.04 (d, *J* = 8.1 Hz, 2H), 6.95 (d, *J* = 7.9 Hz, 2H), 4.54 (t, *J* = 7.3 Hz, 1H), 2.19 (s, 3H), 2.13 (s, 3H), 2.03 (dt, *J* = 14.4, 7.3 Hz, 1H), 1.64 – 1.56 (m, 2H), 1.55 – 1.47 (m, 3H), 1.44 – 1.15 (m, 11H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.66, 143.28, 137.05, 136.18, 134.42, 129.38, 129.05, 128.61, 127.95, 50.38, 41.76, 34.59, 32.14, 31.81, 27.29, 27.21, 26.03, 25.14, 25.06, 21.39, 20.87. HRMS (ESI) m/z calcd. for $[C_{25}H_{32}O+Na]^+$ 371.2351, found 371.2349.

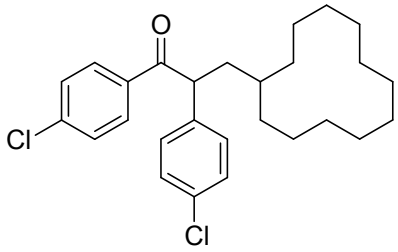


1,2-bis(4-chlorophenyl)-3-cyclooctylpropan-1-one (3fd): Colorless oil. Yield: 97 mg (83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.6 Hz, 2H), 7.37 (d, *J* = 8.6 Hz, 2H), 7.30 – 7.19 (m, 4H), 4.60 (t, *J* = 7.3 Hz, 1H), 2.08 (dt, *J* = 14.2, 7.2 Hz, 1H), 1.72 – 1.63 (m, 3H), 1.60 – 1.37 (m, 10H), 1.34 – 1.25 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.57, 139.43, 137.98, 134.98, 132.92, 129.92, 129.52,

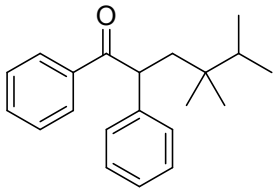
129.06, 128.91, 50.42, 41.71, 34.58, 32.37, 31.75, 27.26, 27.19, 26.09, 25.17, 25.12. HRMS (ESI) m/z calcd. for $[C_{23}H_{26}OCl_2+Na]^+$ 389.1439, found 389.1440.



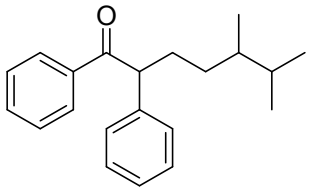
3-cyclododecyl-1,2-diphenylpropan-1-one (3ae): Colorless oil. Yield: 74 mg (65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 8.4, 1.0 Hz, 2H), 7.35 (ddd, *J* = 6.5, 3.8, 1.2 Hz, 1H), 7.29 – 7.22 (m, 4H), 7.17 (dd, *J* = 10.3, 4.8 Hz, 2H), 7.10 – 7.05 (m, 1H), 4.60 (t, *J* = 7.4 Hz, 1H), 2.05 – 1.94 (m, 1H), 1.73 – 1.63 (m, 1H), 1.33 – 1.07 (m, 21H), 1.05 – 0.92 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.15, 139.87, 137.05, 132.65, 128.71, 128.49, 128.41, 128.22, 126.81, 51.02, 39.11, 31.28, 29.45, 28.86, 24.68, 24.34, 23.84, 23.54, 23.42, 23.01, 22.82, 21.46, 21.45. HRMS (ESI) m/z calcd. for $[C_{27}H_{36}O+Na]^+$ 399.2664, found 399.2660.



1,2-bis(4-chlorophenyl)-3-cyclododecylpropan-1-one (3be): Colorless oil. Yield: 74 mg (61%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91– 7.86(m, 2H), 7.38 – 7.33 (m, 2H), 7.27 – 7.22 (m, 4H), 4.60 (t, *J* = 7.4 Hz, 1H), 2.04 (dt, *J* = 13.0, 6.3 Hz, 1H), 1.76 – 1.68 (m, 1H), 1.41 – 1.15 (m, 21H), 1.14 – 0.99 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.57, 139.37, 138.02, 135.04, 132.91, 129.87, 129.51, 128.99, 128.86, 50.37, 38.98, 31.38, 29.29, 28.91, 24.72, 24.42, 23.89, 23.46, 23.35, 23.00, 22.82, 21.45, 21.39. HRMS (ESI) m/z calcd. for $[C_{27}H_{34}OCl_2+H]^+$ 445.2065, found 445.2069.



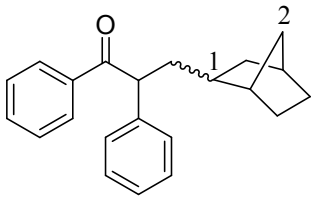
3af



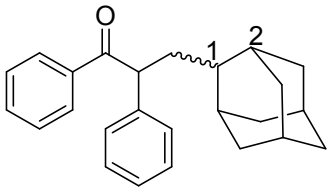
3af'

4,4,5-trimethyl-1,2-diphenylhexan-1-one (3af) and 5,6-dimethyl-1,2-diphenylheptan-1-one (3af'): Colorless oil. Yield: 60 mg (68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (ddd, *J* = 6.4, 5.8, 4.3

Hz, 2H), 7.43 – 7.37 (m, 1H), 7.34 – 7.28 (m, 2H), 7.27 – 7.16 (m, 4H), 7.13 – 7.05 (m, 1H), 4.65 (dd, *J* = 8.8, 2.9 Hz, 0.69H), 4.60 (t, *J* = 7.4 Hz, 0.24H), 4.46 – 4.40 (m, 0.07H), 2.58 (dd, *J* = 14.1, 8.8 Hz, 0.69H), 2.00 (dt, *J* = 13.7, 7.5 Hz, 0.24H), 1.70 – 1.62 (m, 0.24H), 1.58– 1.38 (m, 2.12H), 1.24– 1.14 (m, 1.01H), 0.88 – 0.79 (m, 1.55H), 0.78 – 0.68 (m, 7.19H), 0.67 – 0.61 (m, 2.45H). HRMS (ESI) m/z calcd. for $[C_{21}H_{26}O+Na]^+$ 317.1881, found 317.1882.

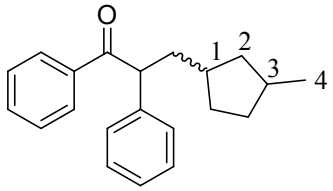


3-((1R,4S)-bicyclo[2.2.1]heptan-2-yl)-1,2-diphenylpropan-1-one (3ag, C1) and 3-((1R,4S)-bicyclo[2.2.1]heptan-7-yl)-1,2-diphenylpropan-1-one (3ag, C2): White solid. Yield: 65 mg (71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.96 (m, 2H), 7.52 – 7.46 (m, 1H), 7.43 – 7.37 (m, 2H), 7.35 – 7.27 (m, 4H), 7.23 – 7.17 (m, 1H), 4.64 (t, *J* = 7.3 Hz, 0.5H), 4.60 (dd, *J* = 7.9, 6.7 Hz, 0.5H), 2.29 – 2.17 (m, 1.5H), 2.09 – 2.06 (m, 0.5H), 1.99 – 1.85 (m, 1.5H), 1.67 – 1.57 (m, 0.5H), 1.54 – 1.39 (m, 2.5H), 1.38 – 1.22 (m, 2.5H), 1.16 – 0.91 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.31, 200.11, 139.92, 139.68, 137.00, 136.96, 132.76, 132.72, 128.80, 128.60, 128.47, 128.45, 128.33, 128.20, 126.85, 126.84, 51.51, 51.43, 41.37, 41.00, 41.00, 40.75, 39.65, 39.53, 38.17, 37.97, 36.59, 35.48, 35.28, 29.89, 28.61. HRMS (ESI) m/z calcd. for $[C_{22}H_{24}O+Na]^+$ 327.1725, found 327.1721.



3-((1r,3r,5r,7r)-adamantan-2-yl)-1,2-diphenylpropan-1-one(3ah, C1) and 3-((3r,5r,7r)-adamantan-1-yl)-1,2-diphenylpropan-1-one(3ah, C2): White solid. Yield: 67 mg (65%).^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.99 (m, 1.72H), 7.98 – 7.95 (m, 0.28H), 7.48 – 7.41 (m, 1H), 7.40 – 7.34 (m, 2H), 7.34 – 7.27 (m, 2H), 7.24 (dt, *J* = 11.0, 3.2 Hz, 2H), 7.20 – 7.10 (m, 1H), 4.78 (dd, *J* = 9.1, 3.0 Hz, 0.86H), 4.64 (t, *J* = 7.2 Hz, 0.14H), 2.54 (dd, *J* = 14.1, 9.2 Hz, 0.86H), 2.46 – 2.37 (m, 0.14H), 1.97 – 1.84 (m, 3H), 1.82 – 1.71 (m, 1H), 1.69 – 1.33 (m, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.94,

199.60, 141.25, 140.04, 136.95, 136.80, 132.65, 128.77, 128.54, 128.52, 128.47, 128.41, 128.11, 128.02, 126.78, 126.55, 51.07, 48.30, 47.45, 42.67, 41.88, 38.97, 38.94, 38.22, 37.07, 36.85, 32.99, 32.00, 31.75, 31.55, 31.41, 28.66, 28.52, 28.35, 28.07, 27.92. HRMS (ESI) m/z calcd. for $[C_{25}H_{28}O+Na]^+$ 367.2038, found 367.2041.

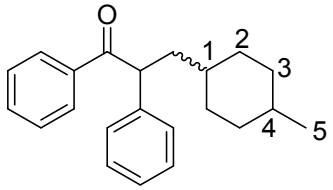


3-(3-methylcyclopentyl)-1,2-diphenylpropan-1-one(3ai, C1),

3-(2-methylcyclopentyl)-1,2-diphenylpropan-1-one(3ai, C2),

3-(1-methylcyclopentyl)-1,2-diphenylpropan-1-one(3ai, C3),

4-cyclopentyl-1,2-diphenylbutan-1-one(3ai, C4): Colorless oil. Yield: 65 mg (74%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 – 7.87 (m, 2H), 7.41 – 7.35 (m, 1H), 7.33 – 7.14 (m, 6H), 7.12 – 7.04 (m, 1H), 4.65 (dd, *J* = 8.3, 3.7 Hz, 0.5H), 4.59 (dd, *J* = 9.7, 4.9 Hz, 0.08H), 4.52 (dd, *J* = 8.6, 5.2 Hz, 0.40H), 4.43 (dd, *J* = 13.0, 6.3 Hz, 0.02H), 2.63 – 2.45 (m, 0.58H), 2.15 – 2.06 (m, 0.42H), 1.95 – 1.56 (m, 2.80H), 1.51 – 1.45 (m, 2.20H), 1.38 – 1.03 (m, 3.40H), 0.99 – 0.59 (m, 3.60H). HRMS (ESI) m/z calcd. for $[C_{21}H_{24}O+Na]^+$ 315.1725, found 315.1722.



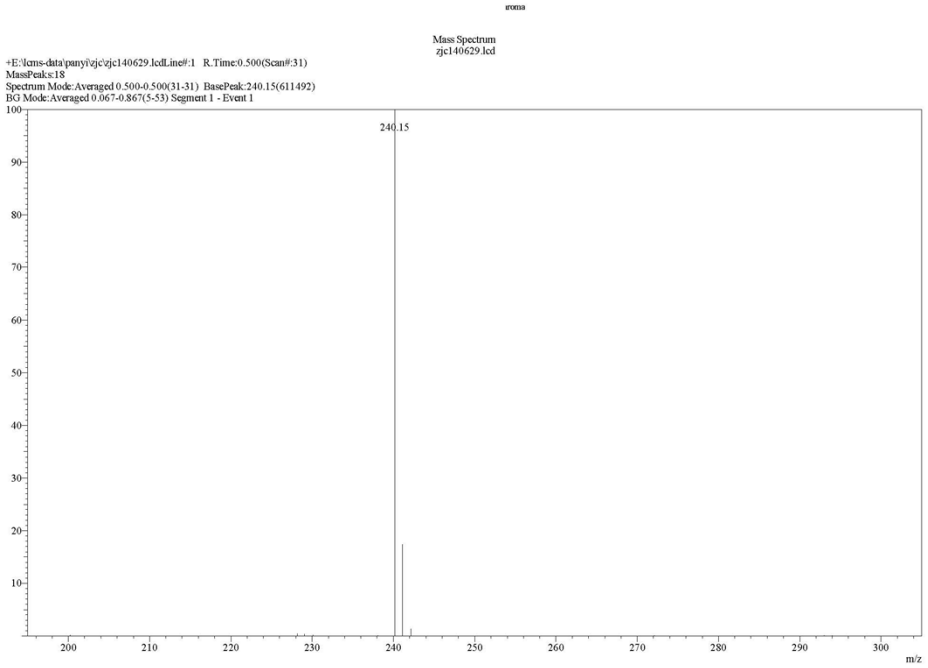
3-(4-methylcyclohexyl)-1,2-diphenylpropan-1-one(3aj, C1), 3-(3-methylcyclohexyl)-1,2-diphenylpropan-1-one(3aj, C2), 3-(2-methylcyclohexyl)-1,2-diphenylpropan-1-one(3aj, C3),

3-(1-methylcyclohexyl)-1,2-diphenylpropan-1-one(3aj, C4),

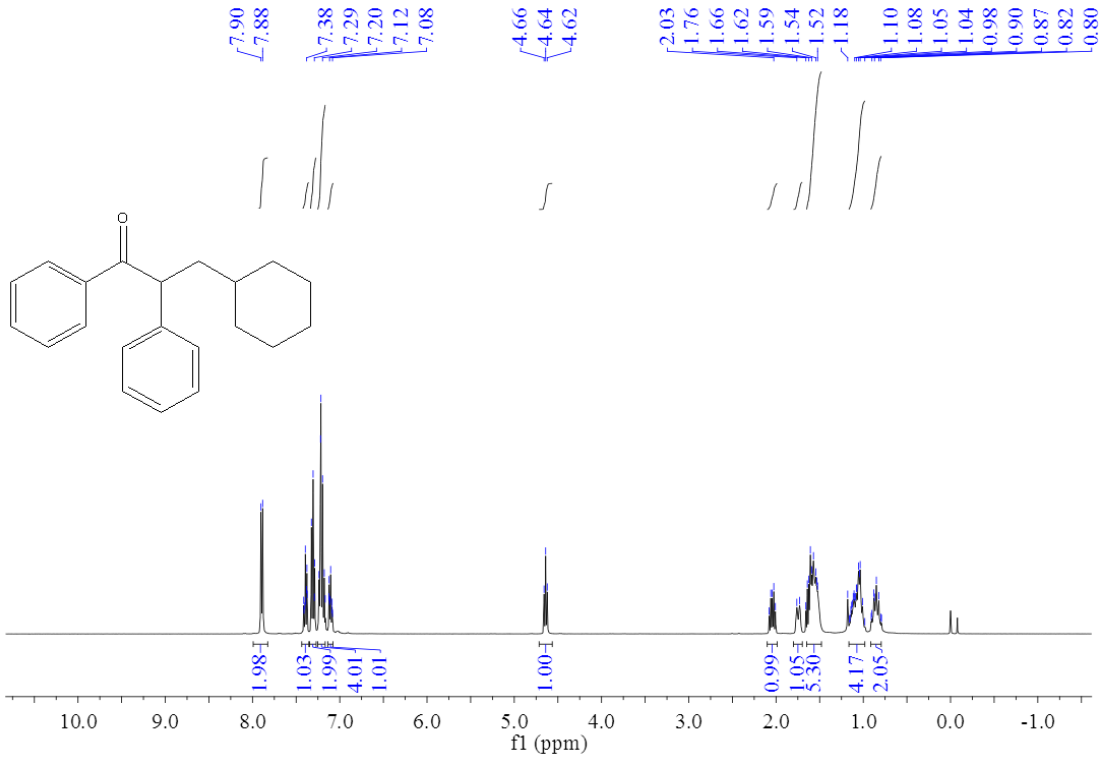
4-cyclohexyl-1,2-diphenylbutan-1-one(3aj, C5): Colorless oil. Yield: 80 mg (87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 9.1, 7.6 Hz, 2H), 7.36 – 7.29 (m, 1H), 7.28 – 7.19 (m, 4H), 7.14 (dd, *J* = 14.8, 7.4 Hz, 2H), 7.08 – 6.99 (m, 1H), 4.69 – 4.54 (m, 1H), 2.71 – 2.51 (m, 0.46H), 2.27 – 1.97 (m, 0.62H), 1.76 – 1.46 (m, 3H), 1.34 – 1.05 (m, 7H), 0.91 (s, 0.35H), 0.80 – 0.62 (m, 3.48H), 0.48 (dt, *J* =

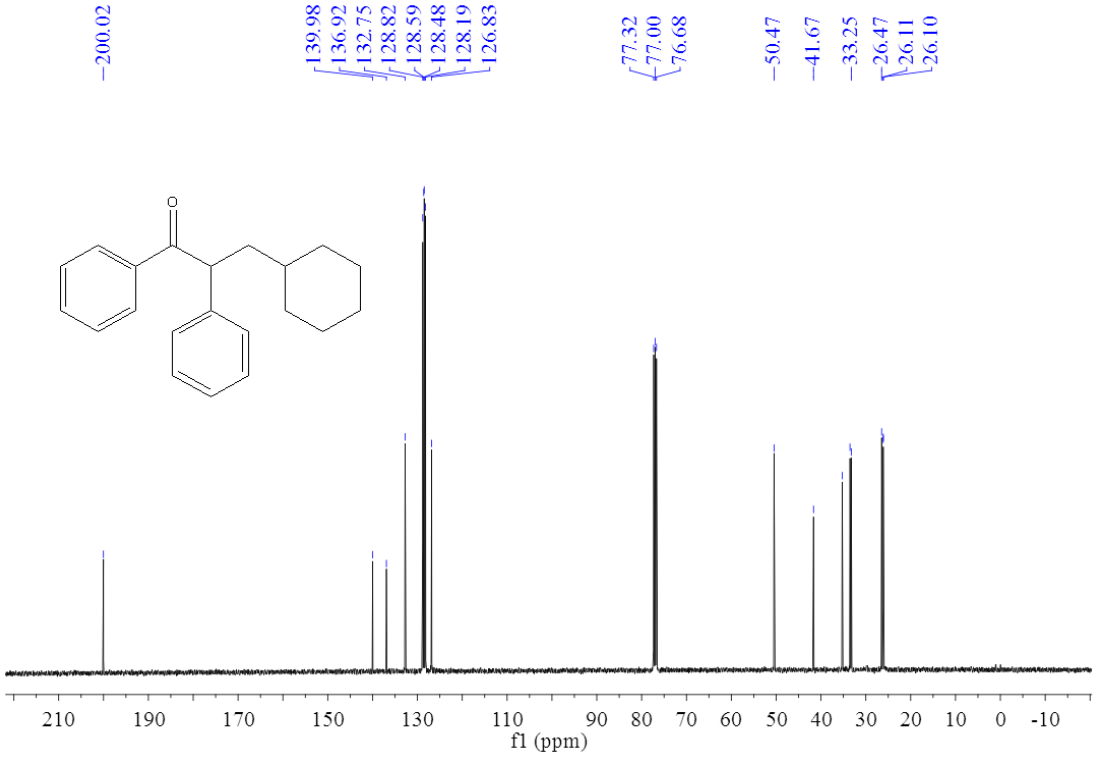
23.2, 11.7 Hz, 0.23H). HRMS (ESI) m/z calcd. for $[C_{22}H_{26}O+Na]^+$ 329.1881, found 329.1886.

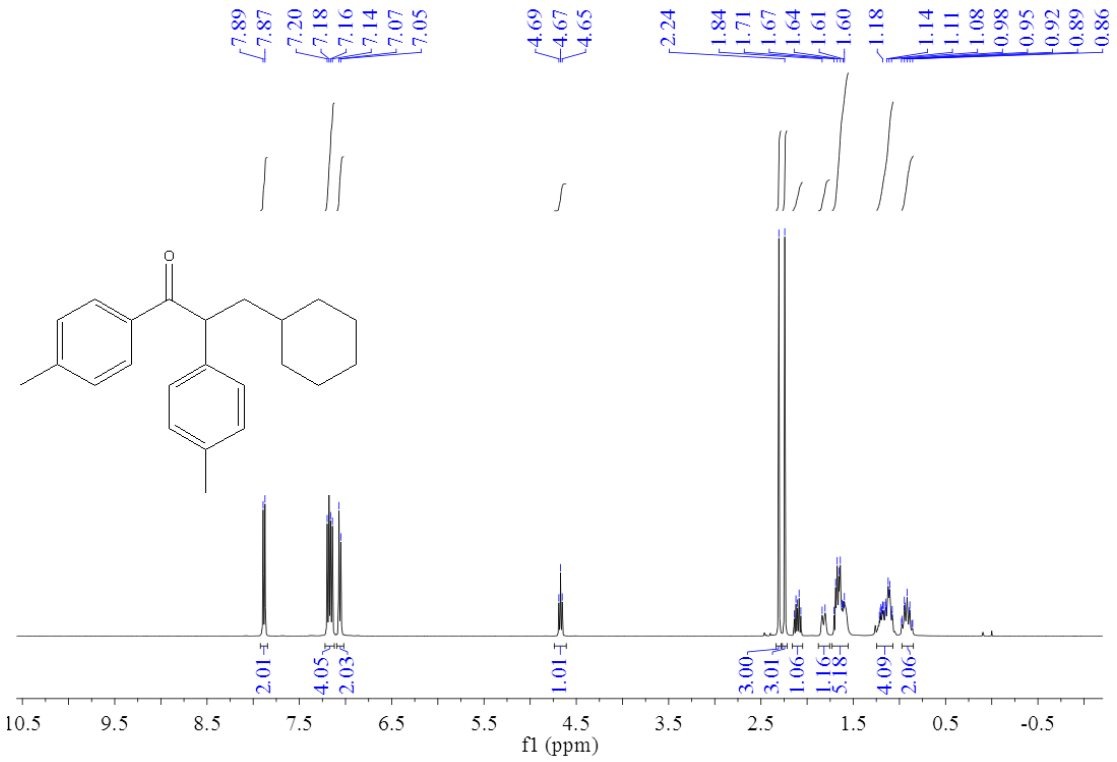
4. Mass spectrum of TEMPO-cyclohexane adduct



5. ^{1}H and ^{13}C NMR spectra of 3



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1.71
1.67
1.64
1.61
1.60
1.18
1.14
1.11
1.08
0.98
0.95
0.92
0.89
0.86
O
2.01
4.05
2.03
1.01
3.00
3.01
1.06
1.16
5.18
4.09
2.06
10.5
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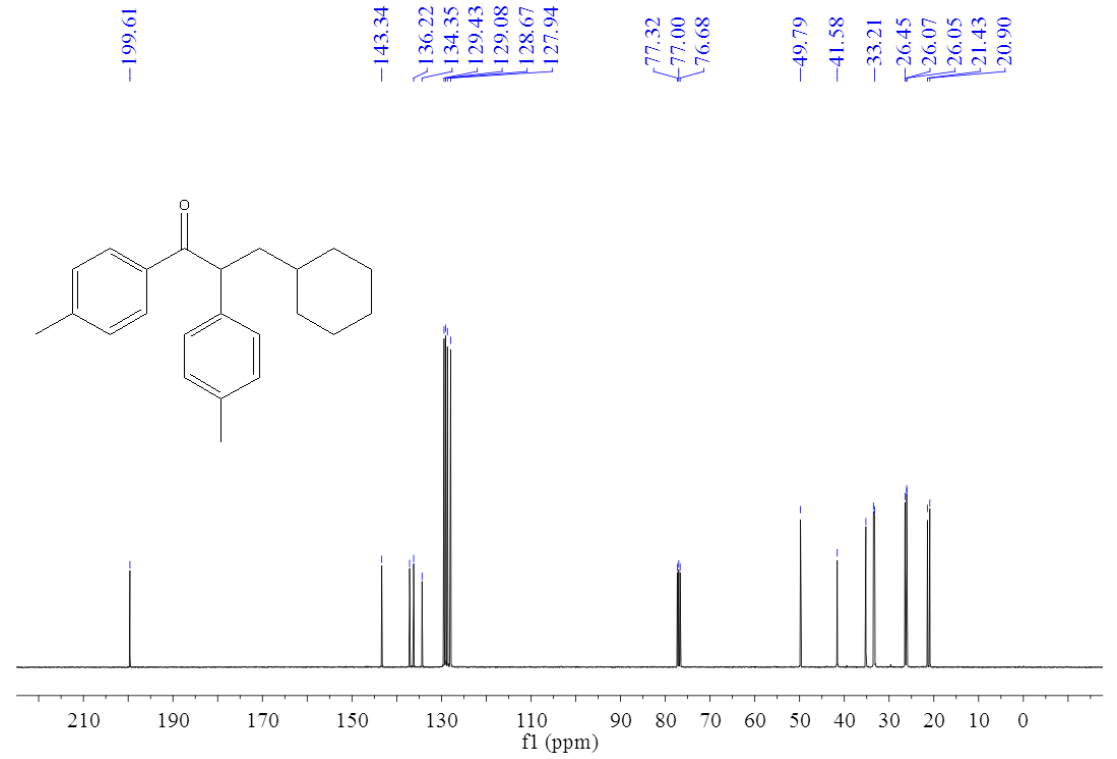
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26.05
21.43
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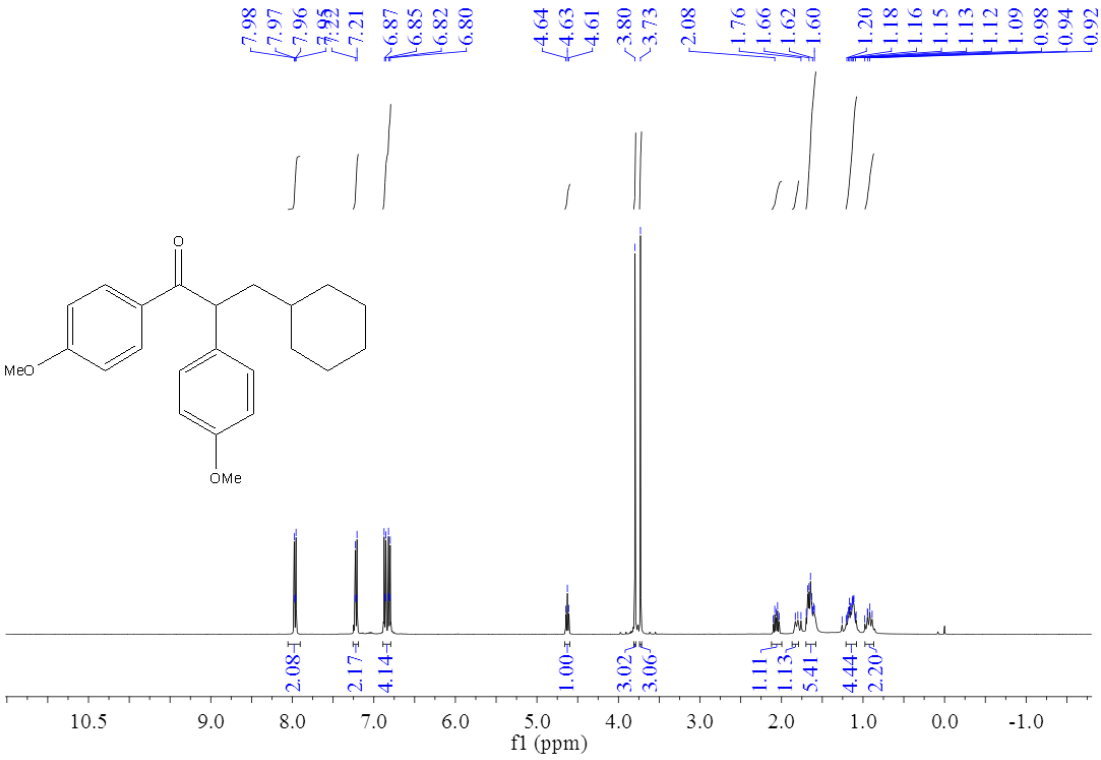
f1 (ppm)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1.62
1.60
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1.18
1.16
1.15
1.13
1.12
1.09
0.98
0.94
0.92
MeO
OMe
2.08
2.17
4.14
1.00
3.02
3.06
1.11
1.13
5.41
4.44
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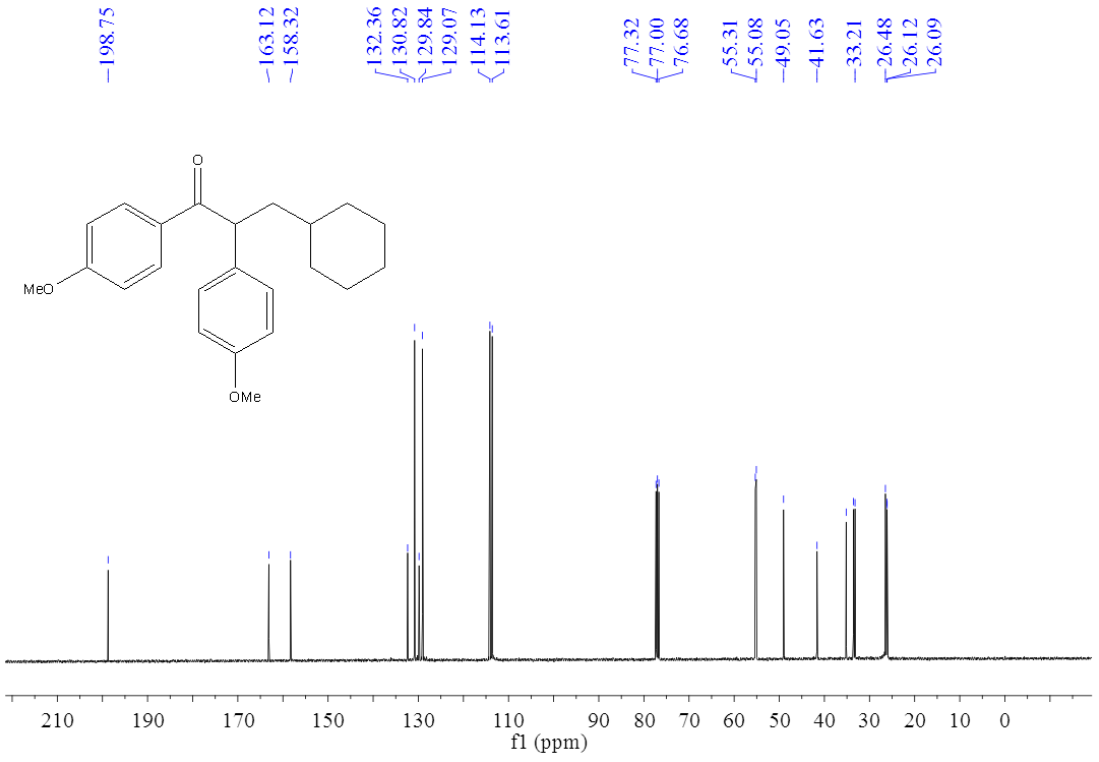
f1 (ppm)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41.63
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26.48
26.12
26.09
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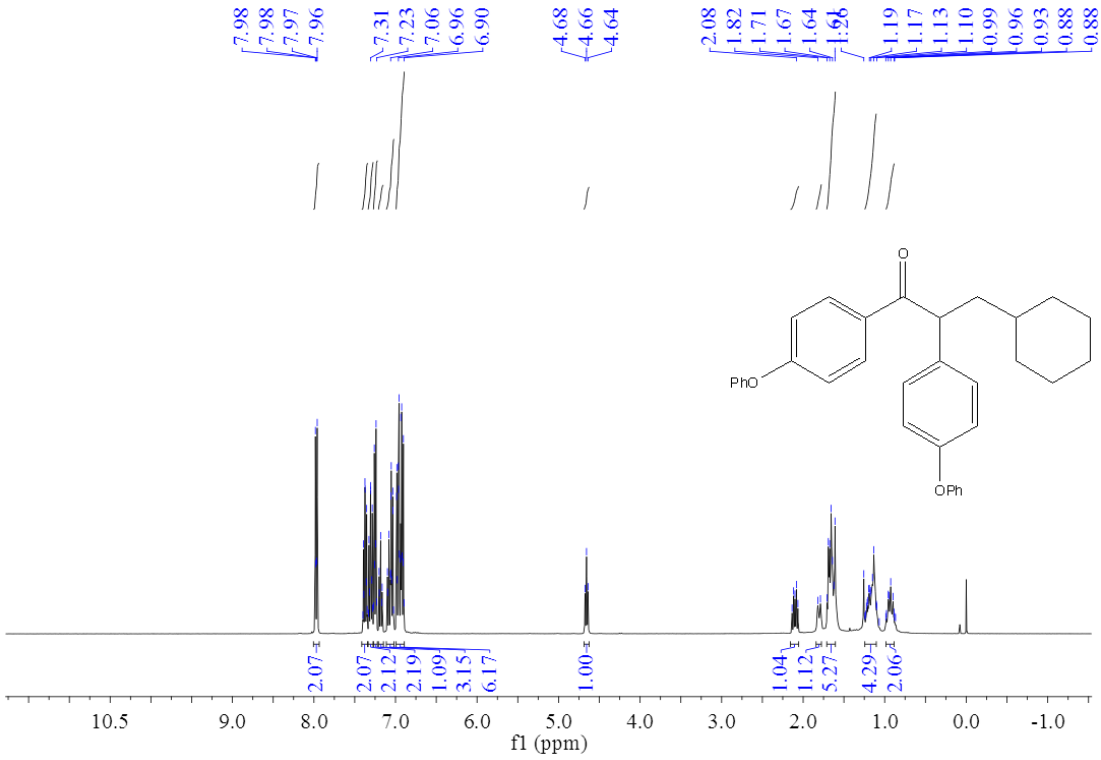
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1.17
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0.93
0.88
0.88
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OPh
2.07
2.07
2.12
2.19
1.09
3.15
6.17
1.00
1.04
1.12
5.27
4.29
2.06
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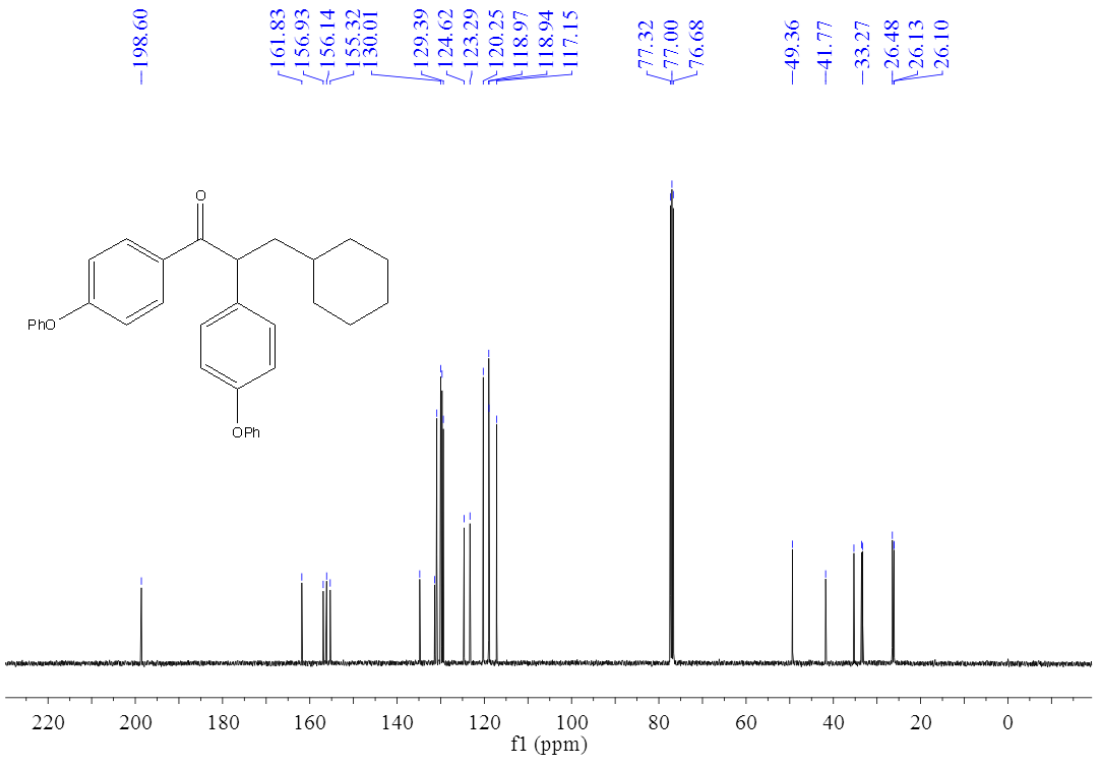
f1 (ppm)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118.94
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77.32
77.00
76.68
49.36
41.77
33.27
26.48
26.13
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OPh
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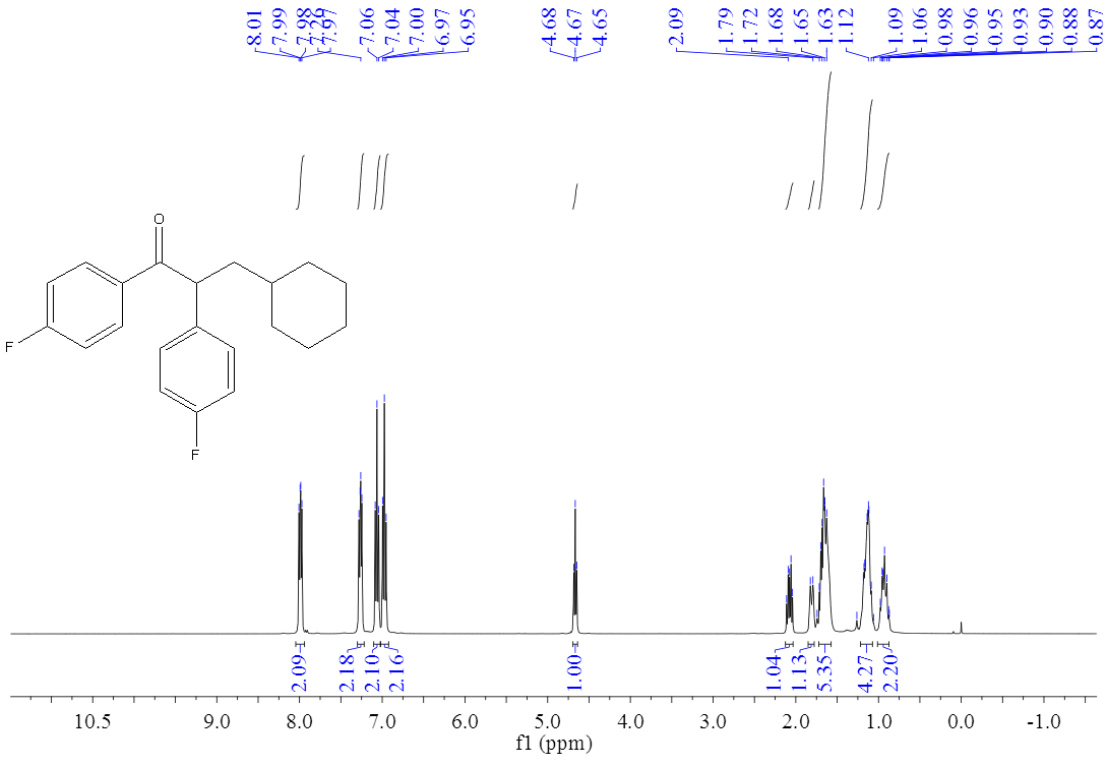
f1 (ppm)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0.93
0.90
0.88
0.87
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F
F
2.09
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2.10
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1.04
1.13
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4.27
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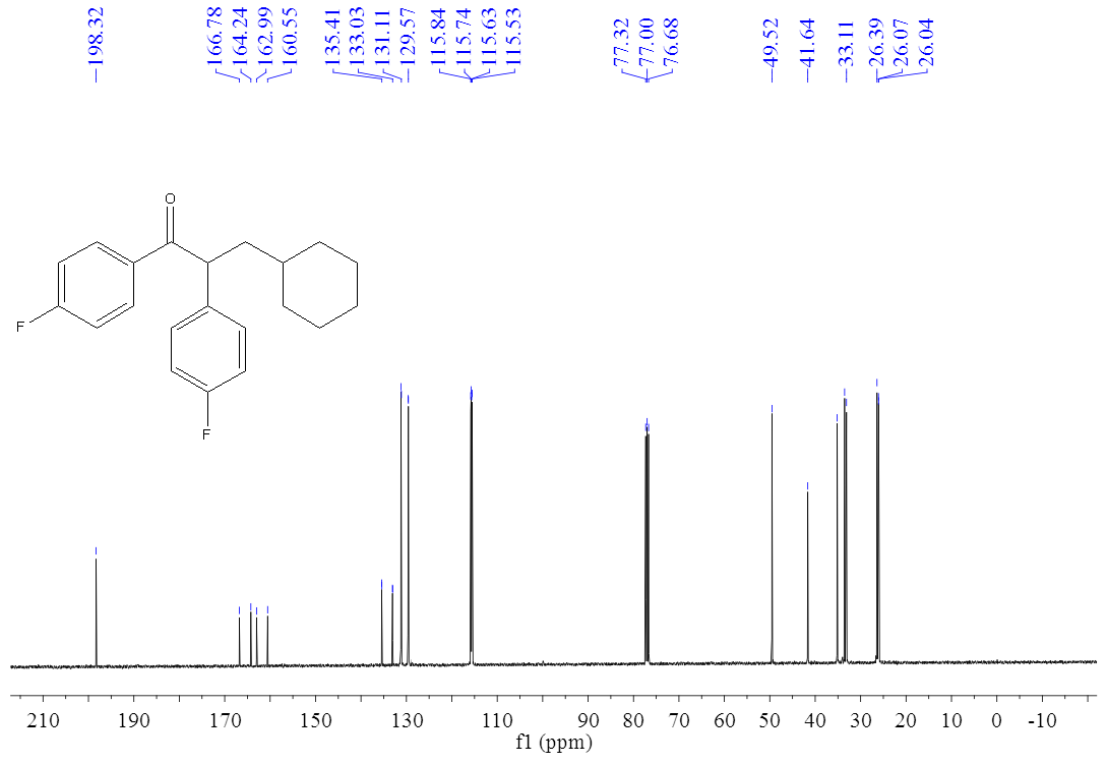
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76.68
49.52
41.64
33.11
26.39
26.07
26.04
O
F
F
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80
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30
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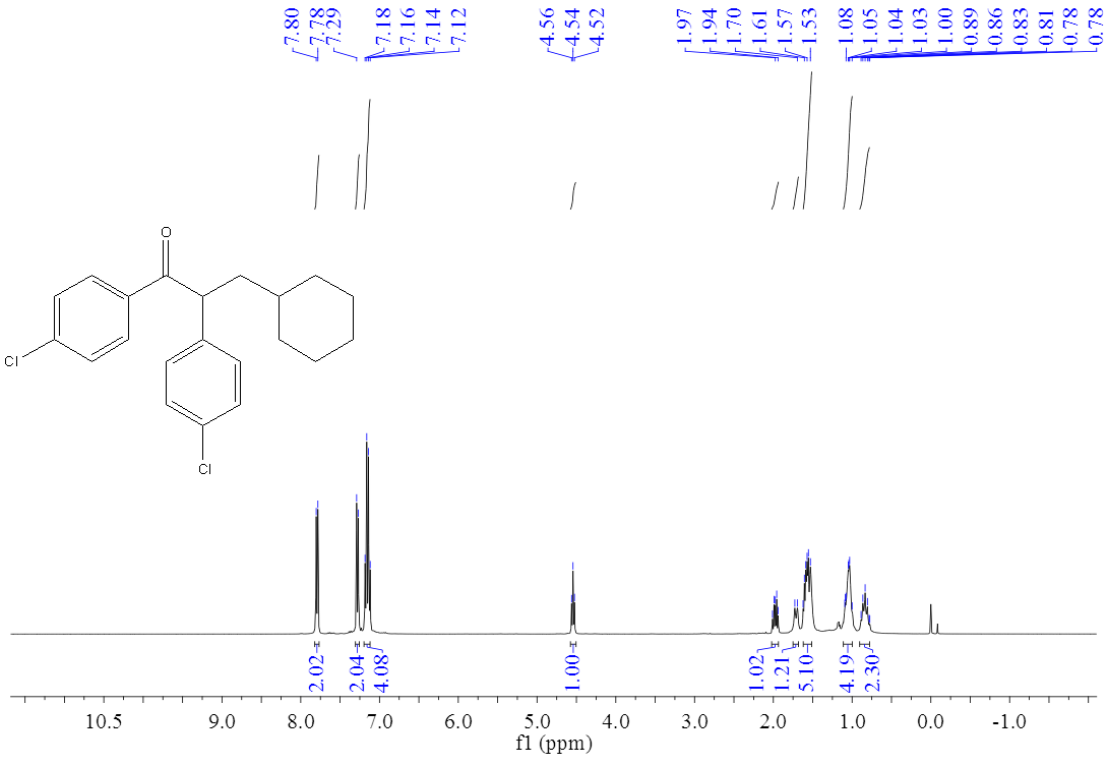
f1 (ppm)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0.78
0.78
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Cl
Cl
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2.04
4.08
1.00
1.02
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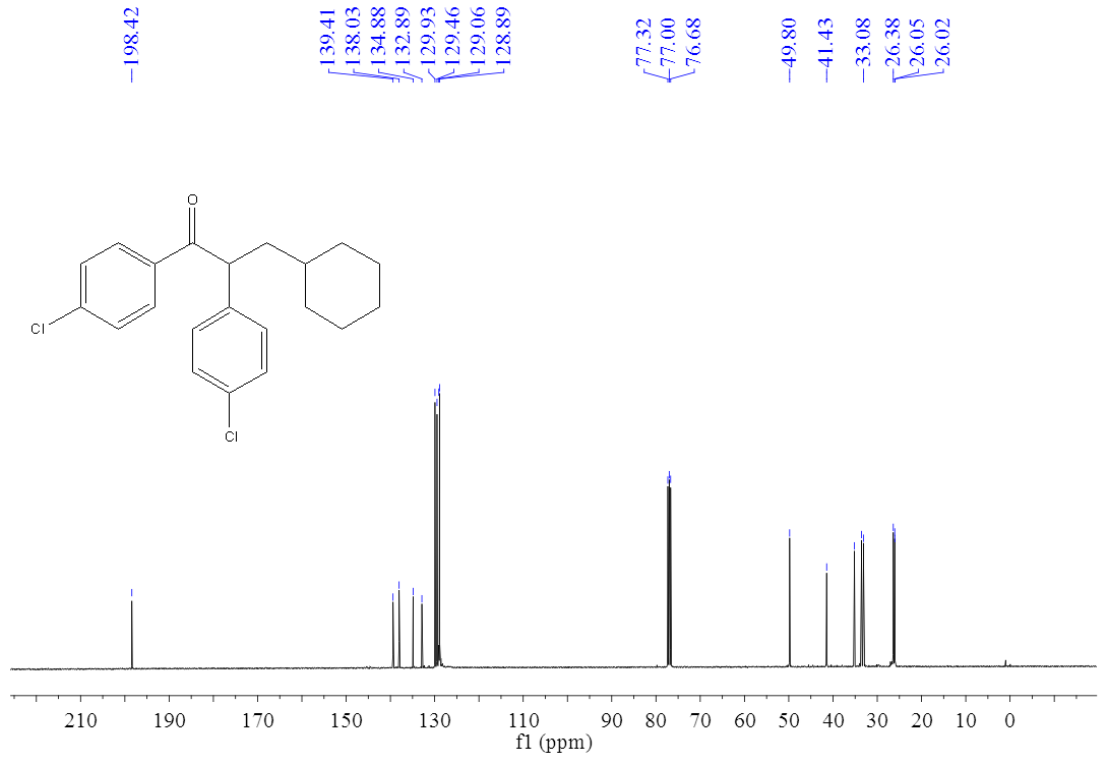
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26.02
O
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Cl
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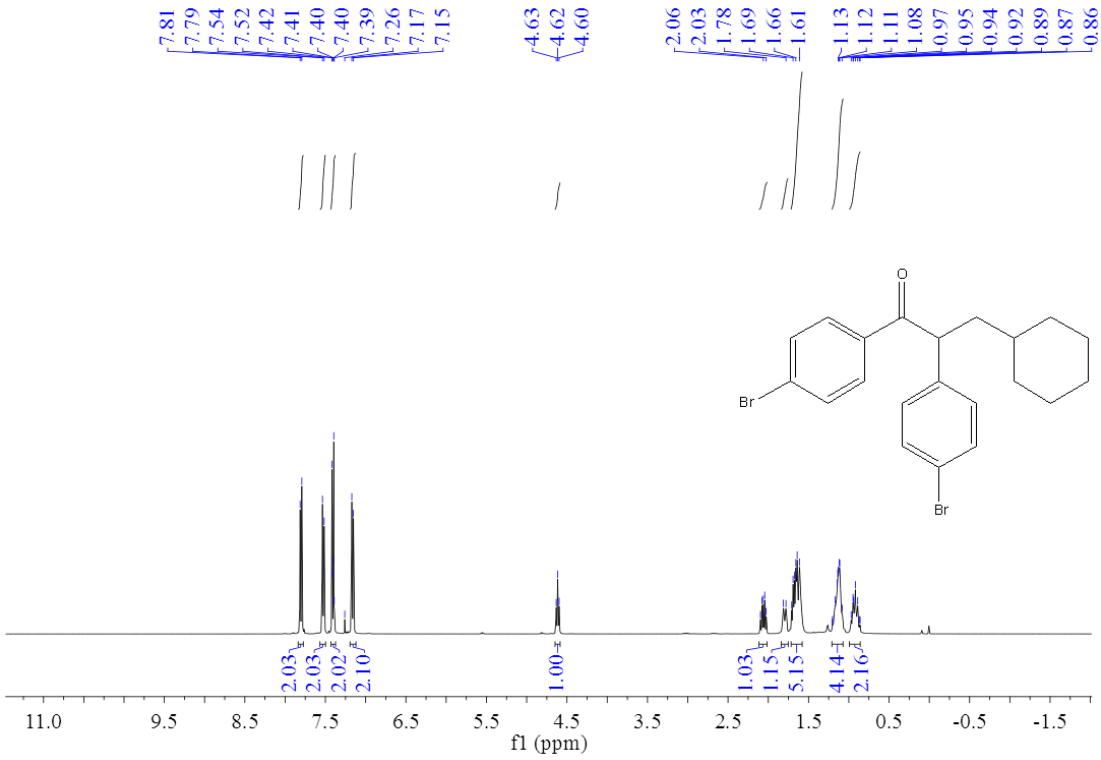
f1 (ppm)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1.11
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0.94
0.92
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0.86
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Br
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2.02
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1.03
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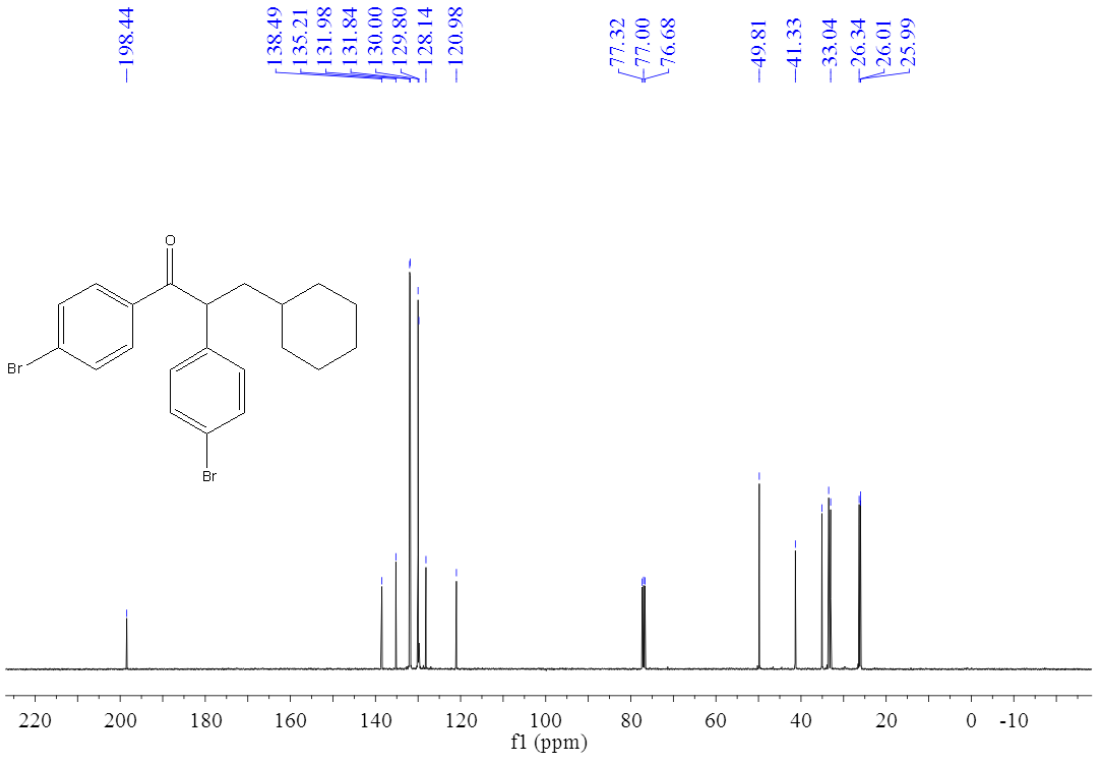
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26.34
26.01
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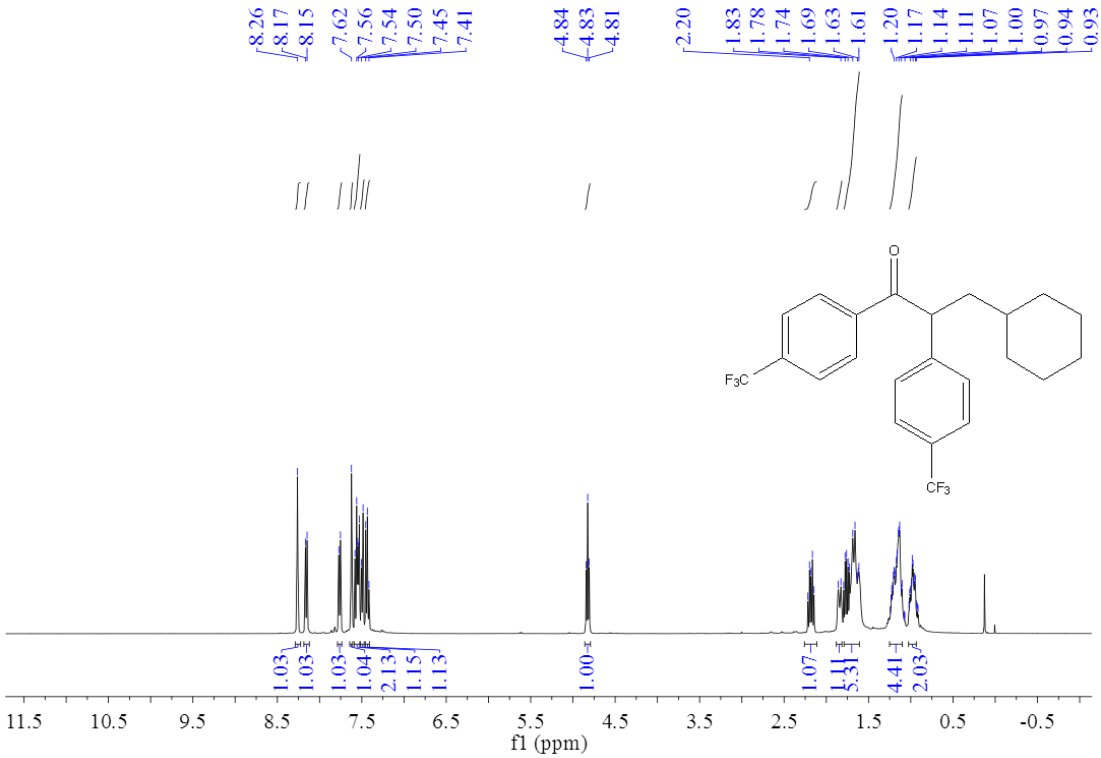
f1 (ppm)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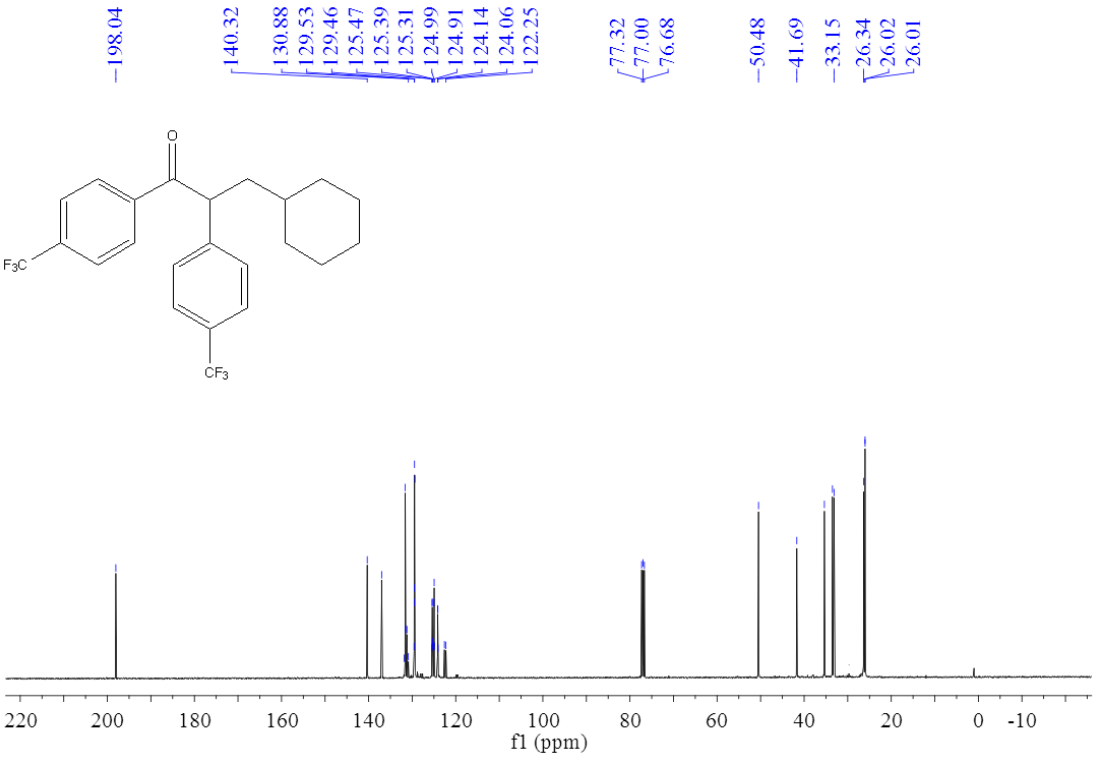
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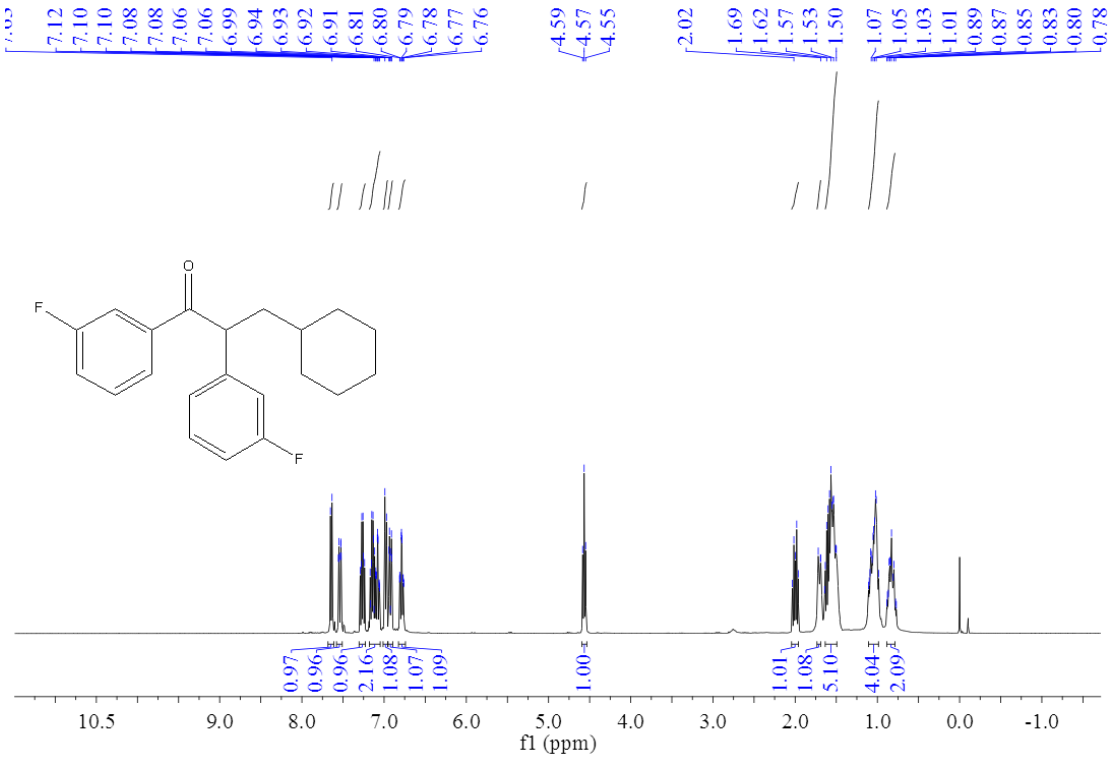
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F
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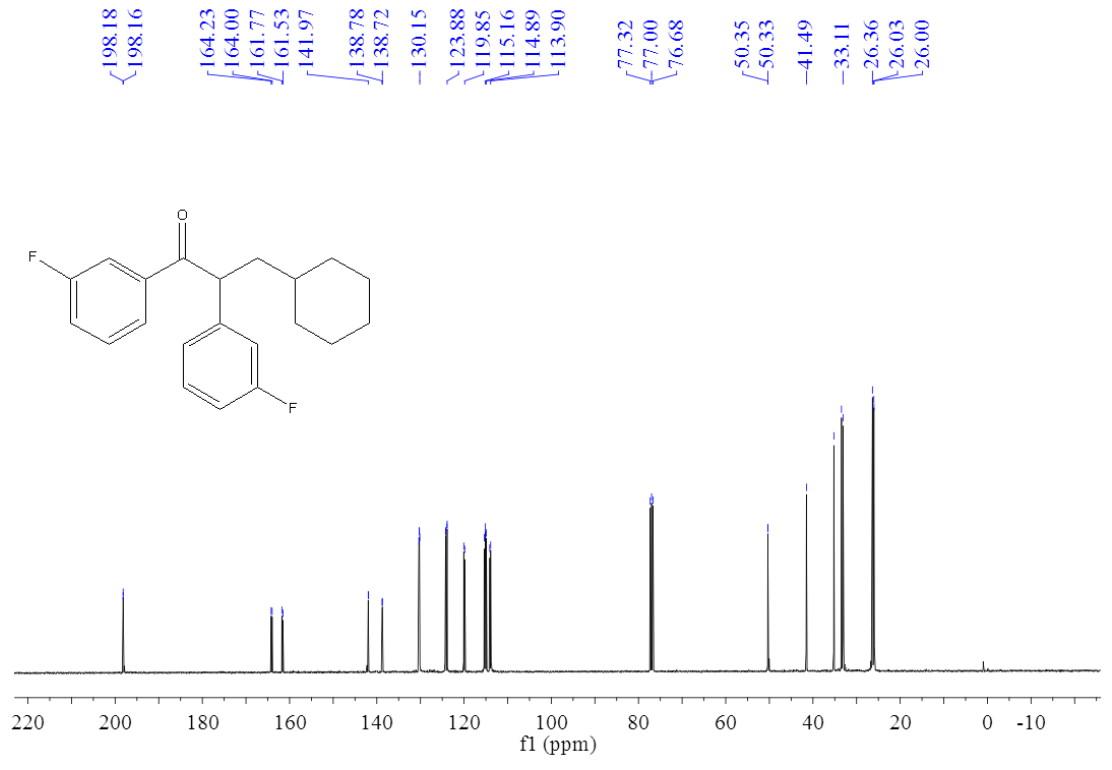
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33.11
26.36
26.03
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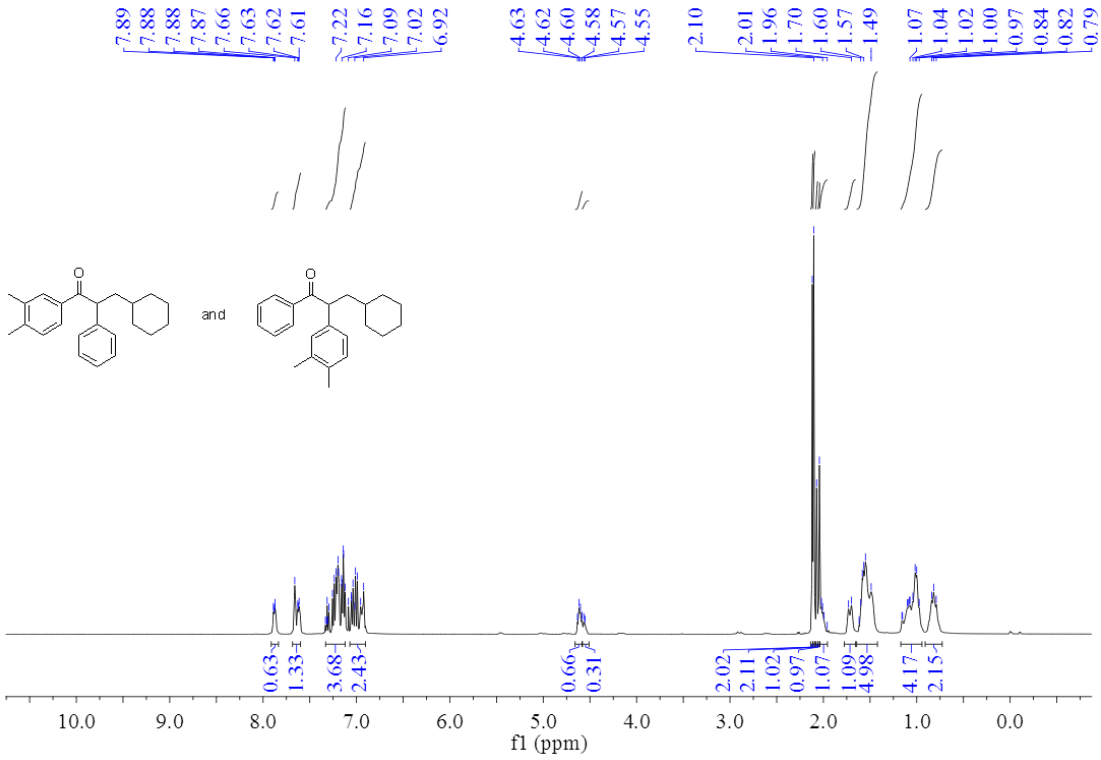
f1 (ppm)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4.55
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1.49
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1.04
1.02
1.00
0.97
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0.82
0.79
and
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0.31
2.02
2.11
1.02
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1.07
1.09
4.98
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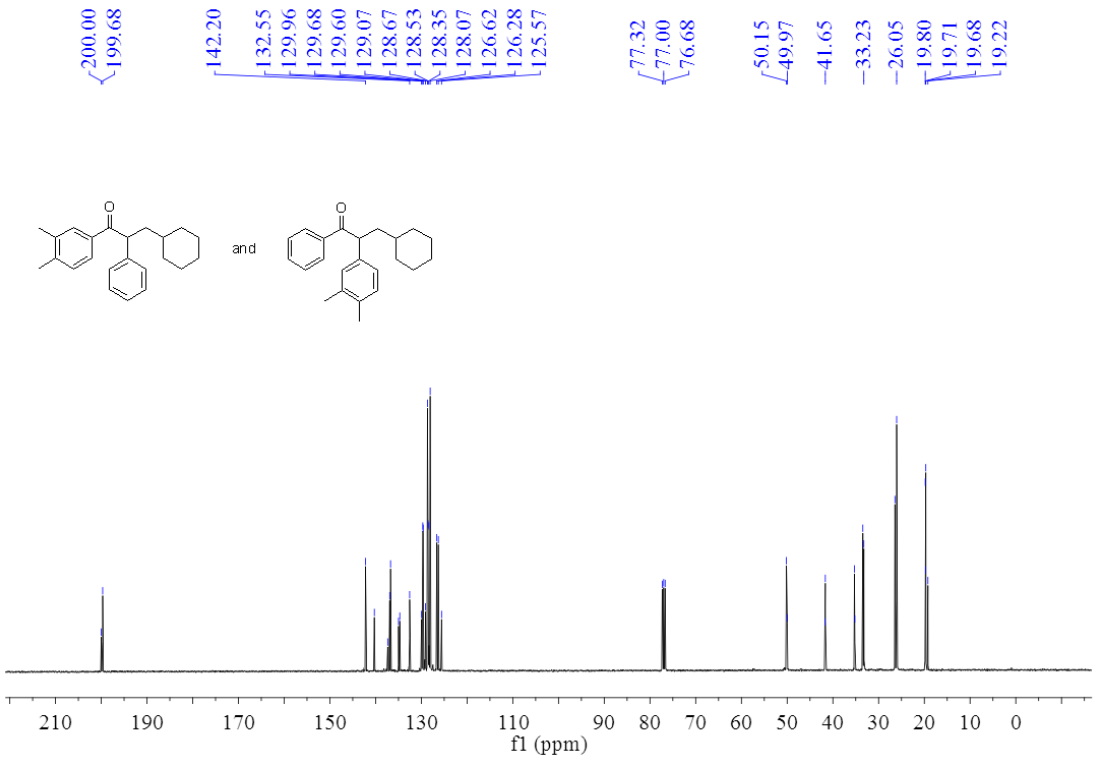
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77.00
76.68
50.15
49.97
41.65
33.23
26.05
19.80
19.71
19.68
19.22
and
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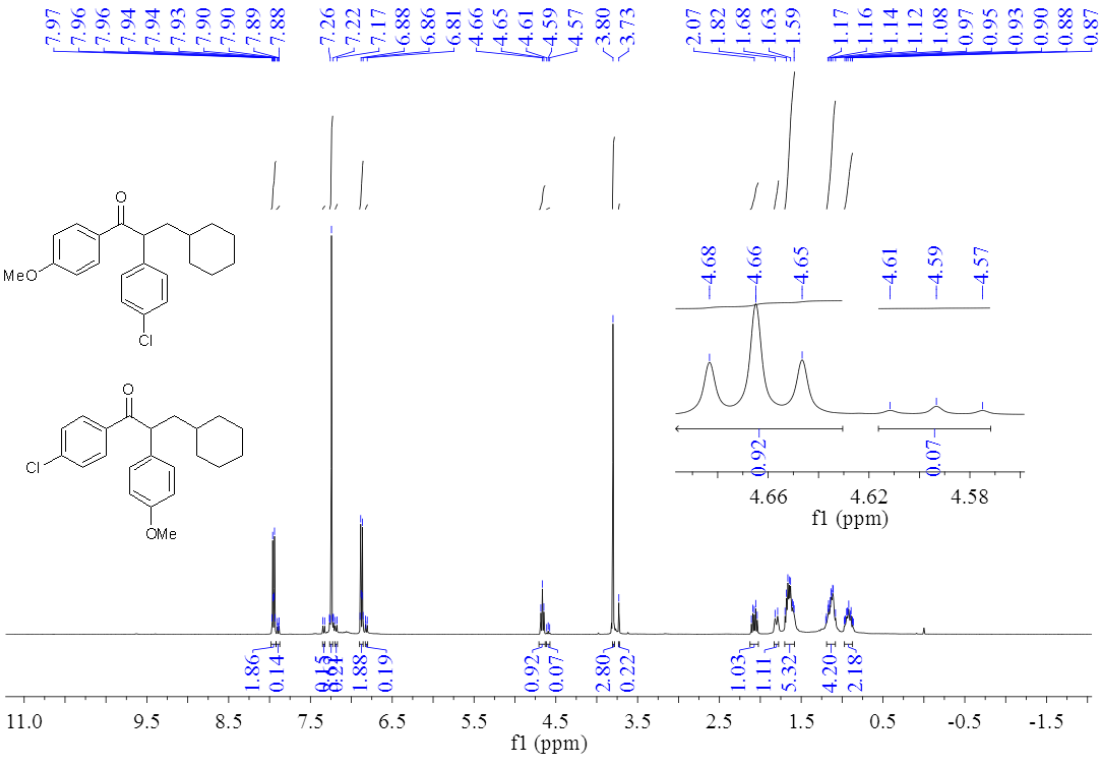
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6.86
6.81
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4.65
4.61
4.59
4.57
3.80
3.73
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1.68
1.63
1.59
1.17
1.16
1.14
1.12
1.08
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0.95
0.93
0.90
0.88
0.87
MeO
Cl
Cl
OMe
4.68
4.66
4.65
4.61
4.59
4.57
0.92
0.07
4.66
4.62
4.58
f1 (ppm)
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0.14
1.88
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0.92
0.07
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5.32
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2.18
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8.5
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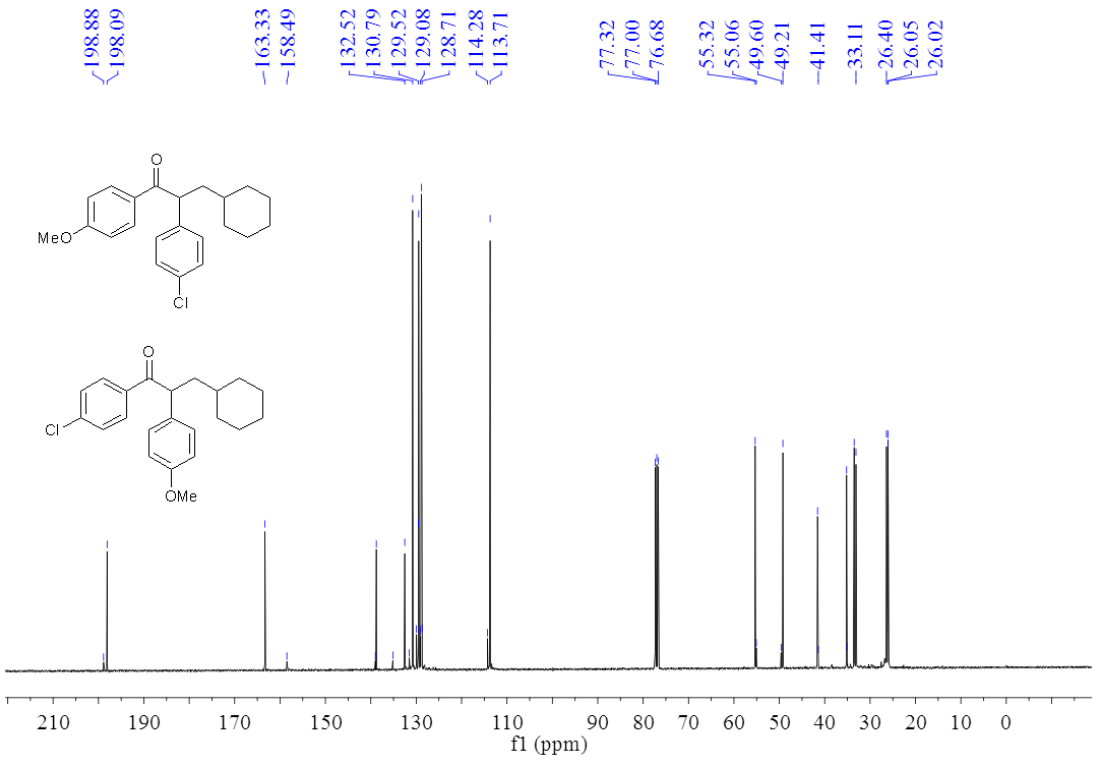
f1 (ppm)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41.41
33.11
26.40
26.05
26.02
MeO
Cl
Cl
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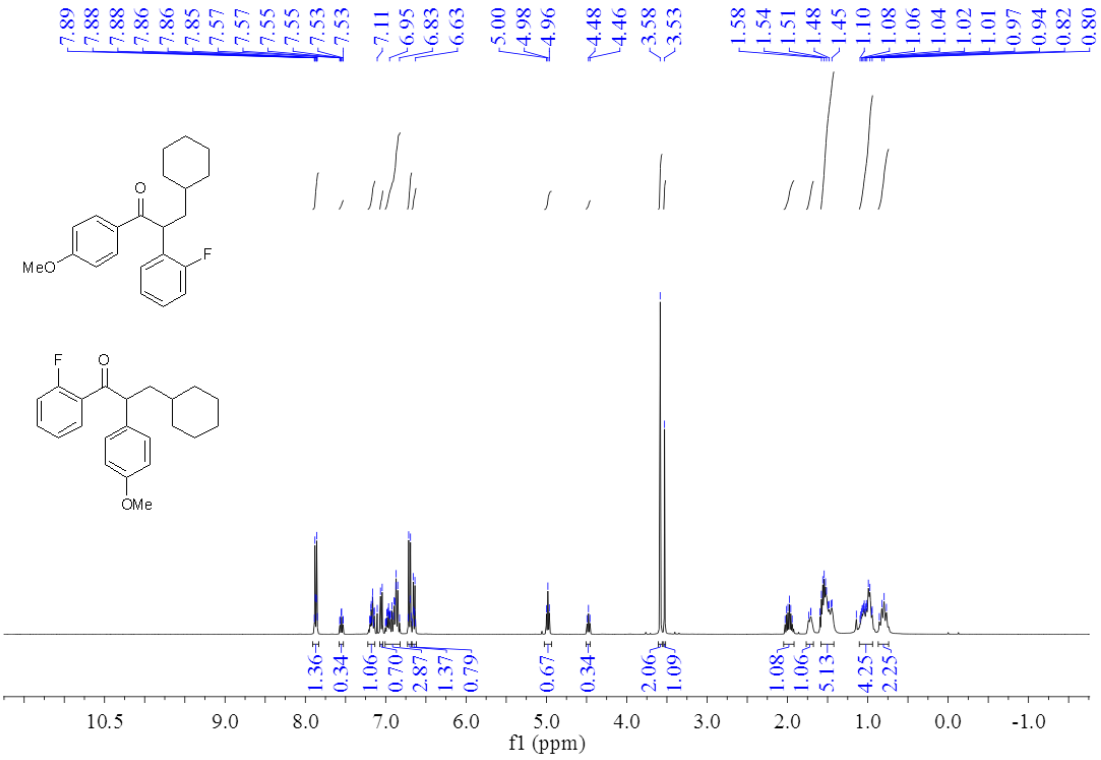
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1.02
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0.94
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0.80
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O
F
F
O
OMe
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0.34
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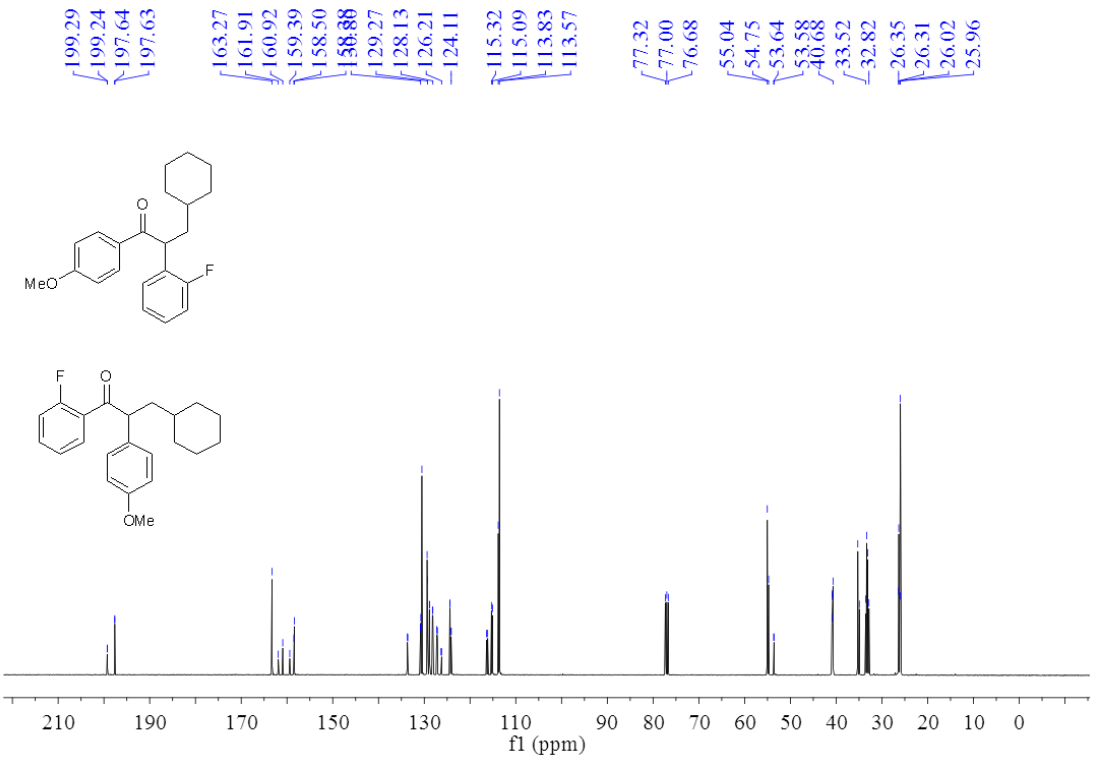
f1 (ppm)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O
F
F
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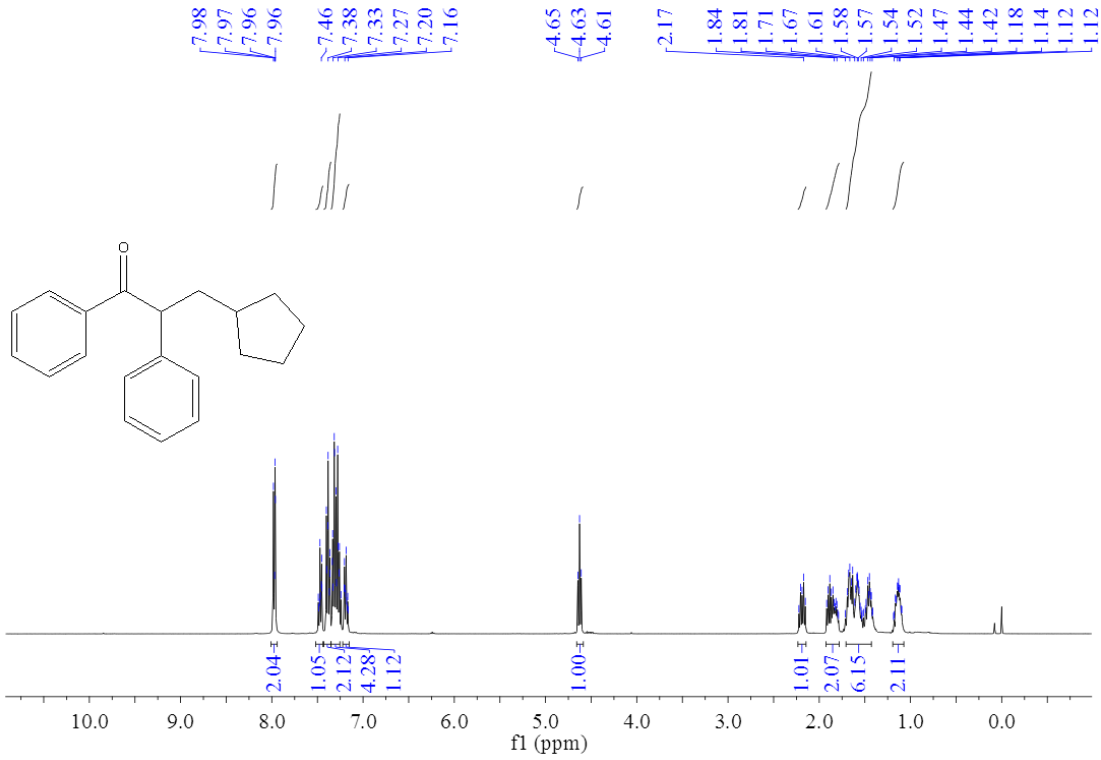
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1.54
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1.12
1.12
O
2.04
1.05
2.12
4.28
1.12
1.00
1.01
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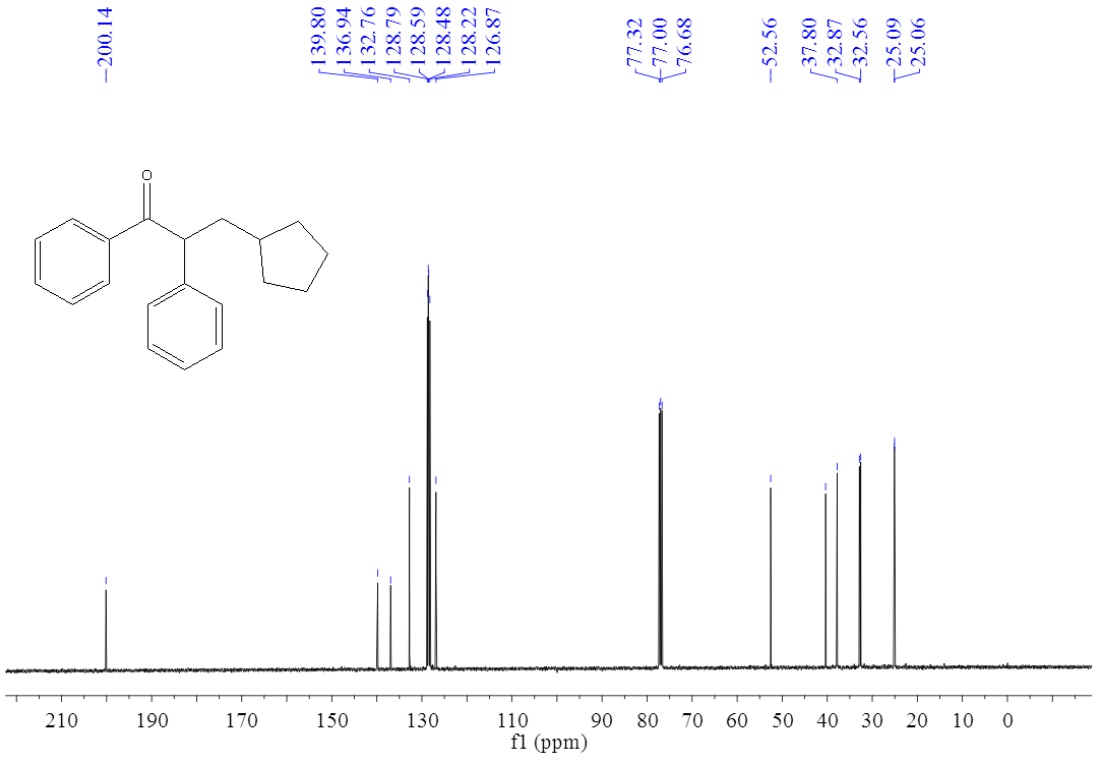
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32.87
32.56
25.09
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50
40
30
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10
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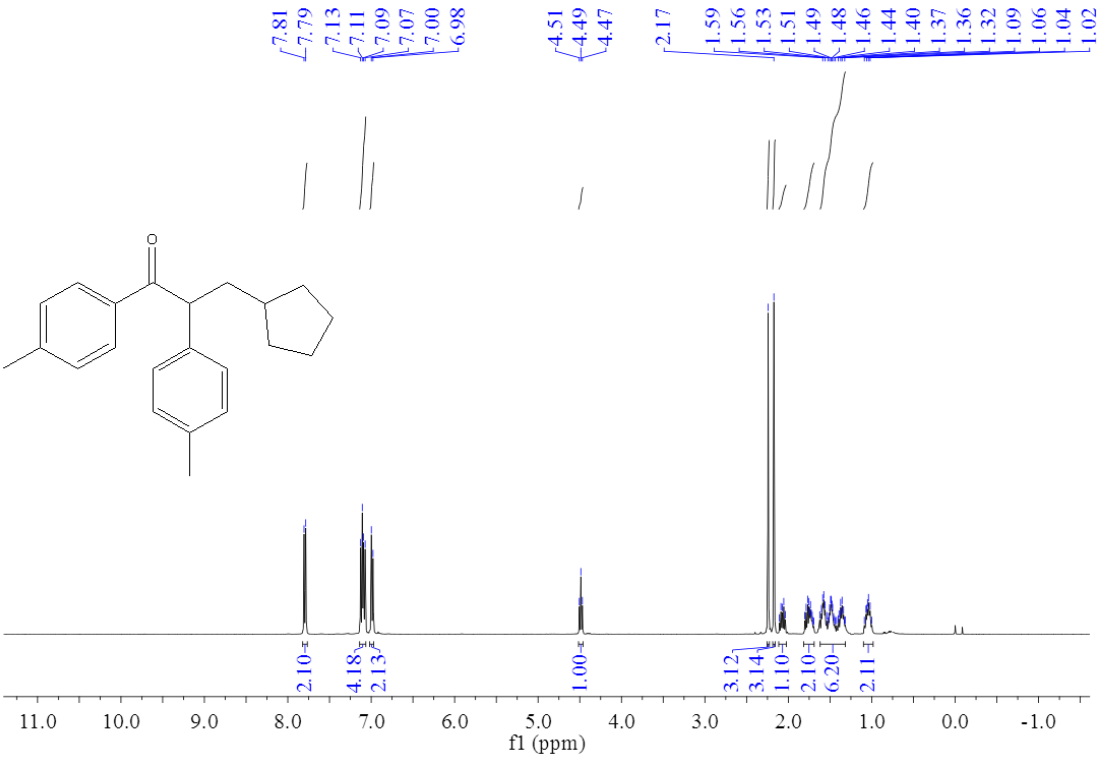
f1 (ppm)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1.56
1.53
1.51
1.49
1.48
1.46
1.44
1.40
1.37
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1.32
1.09
1.06
1.04
1.02
O
2.10
4.18
2.13
1.00
3.12
3.14
1.10
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2.11
11.0
10.0
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1.0
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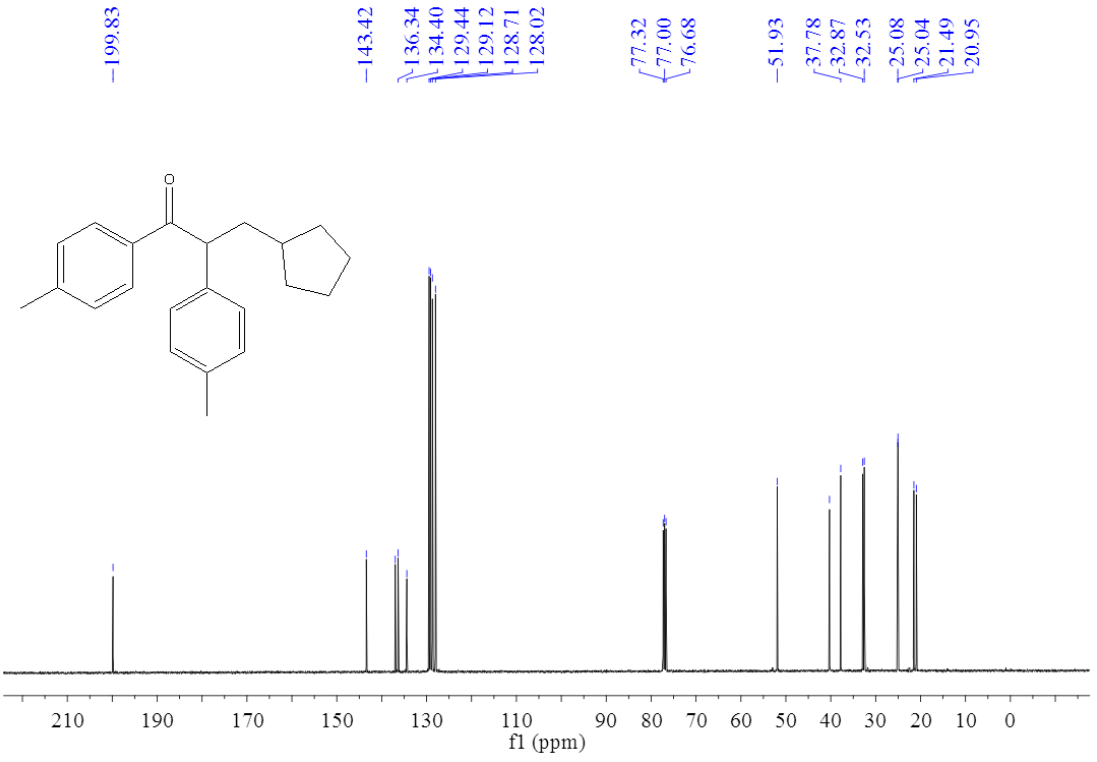
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32.53
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25.04
21.49
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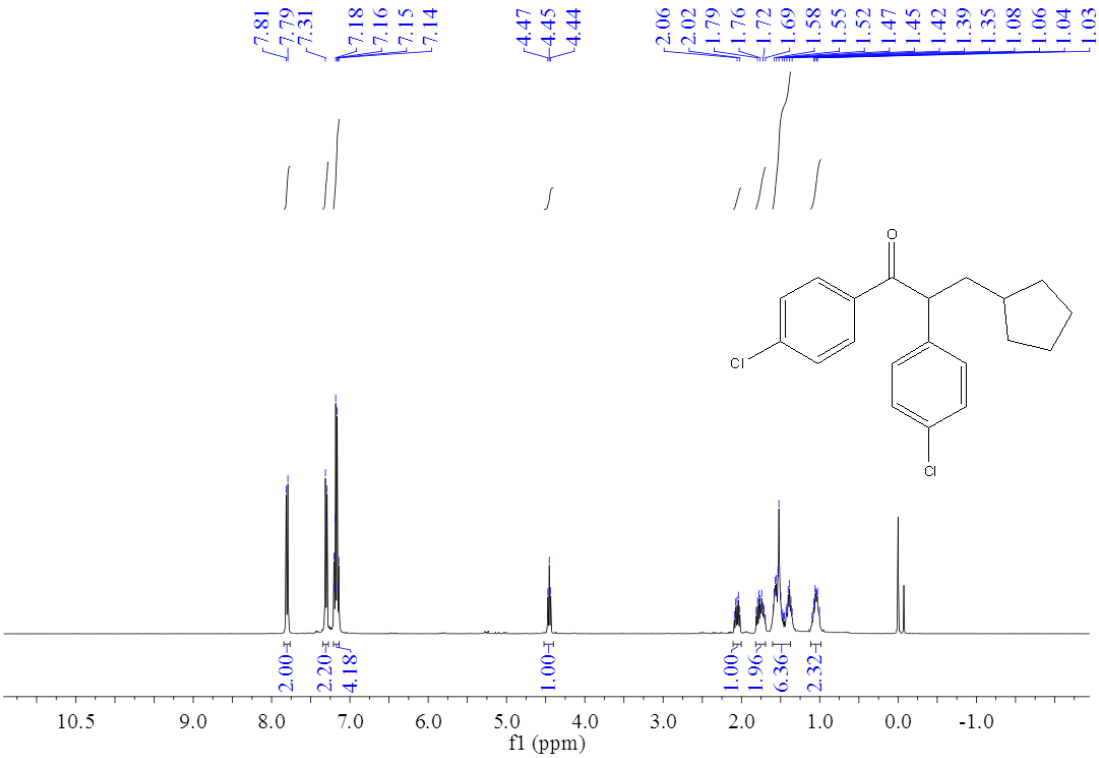
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4.44
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2.02
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1.52
1.47
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1.35
1.08
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1.04
1.03
O
Cl
Cl
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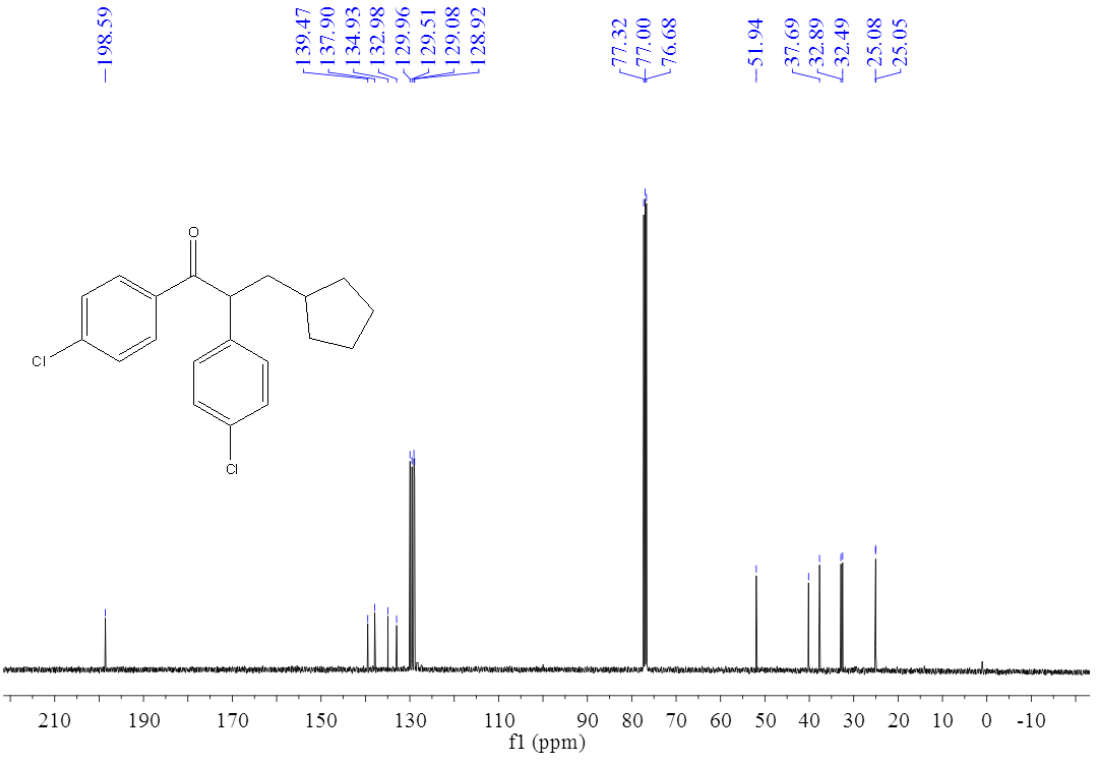
f1 (ppm)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32.49
25.08
25.05
O
Cl
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80
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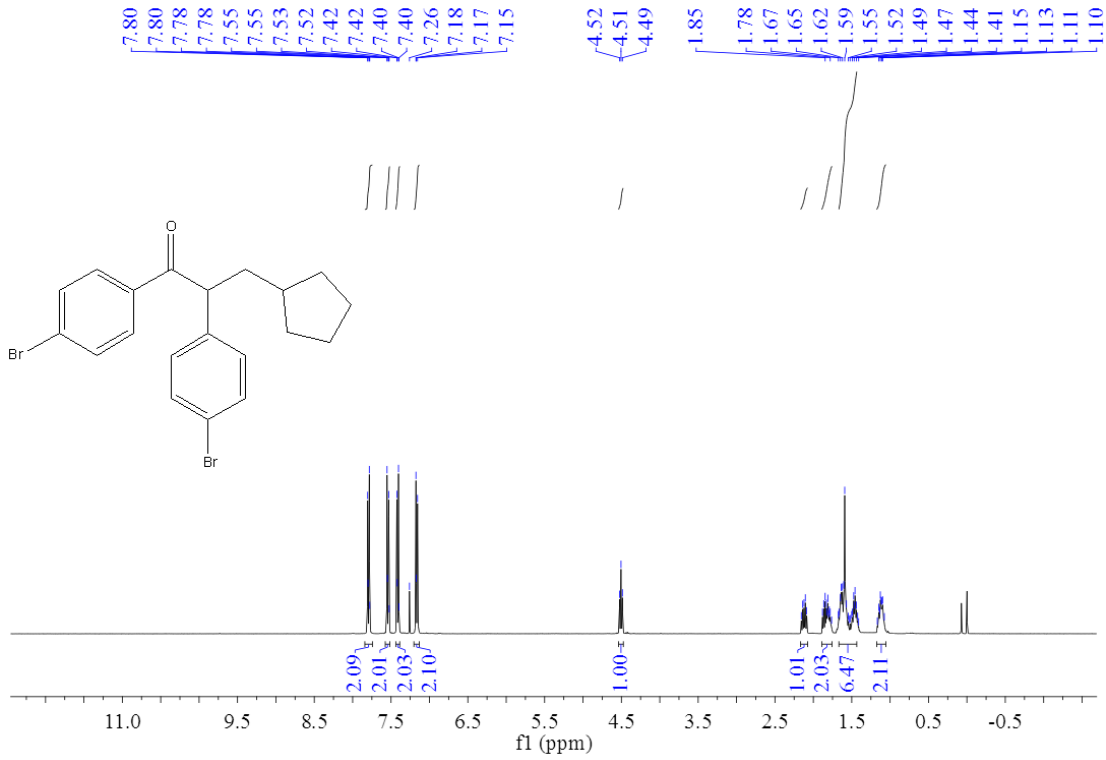
f1 (ppm)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1.10
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Br
Br
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2.03
2.10
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1.01
2.03
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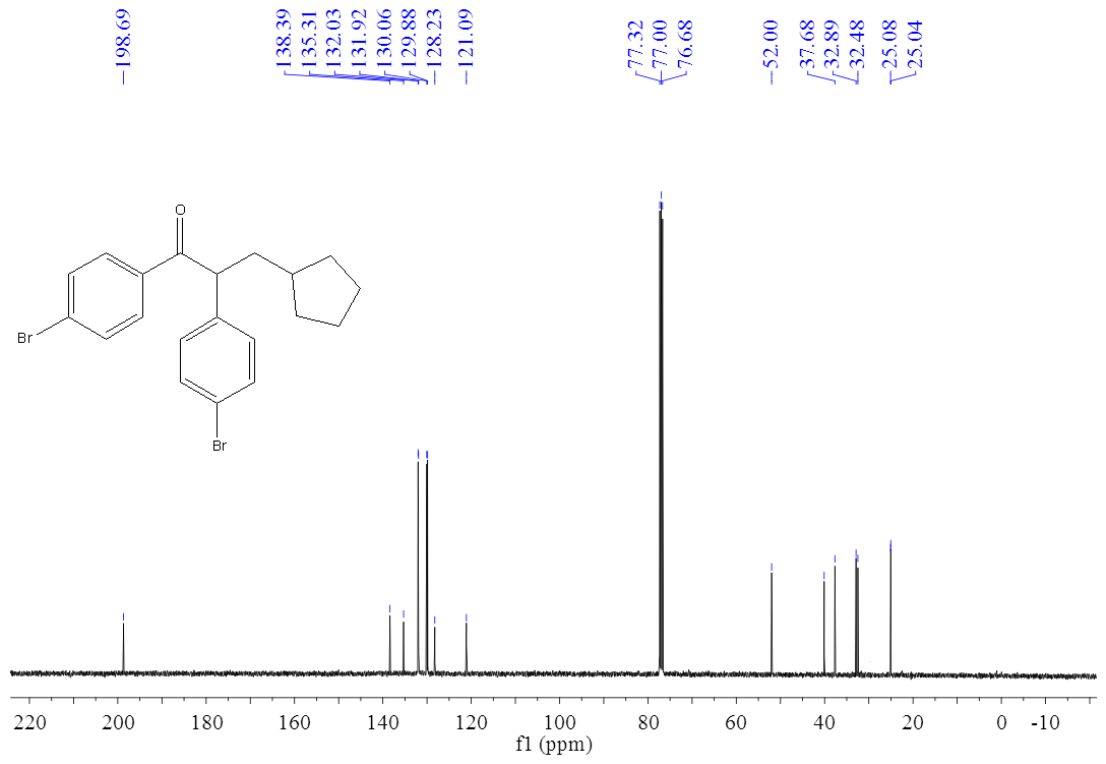
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Br
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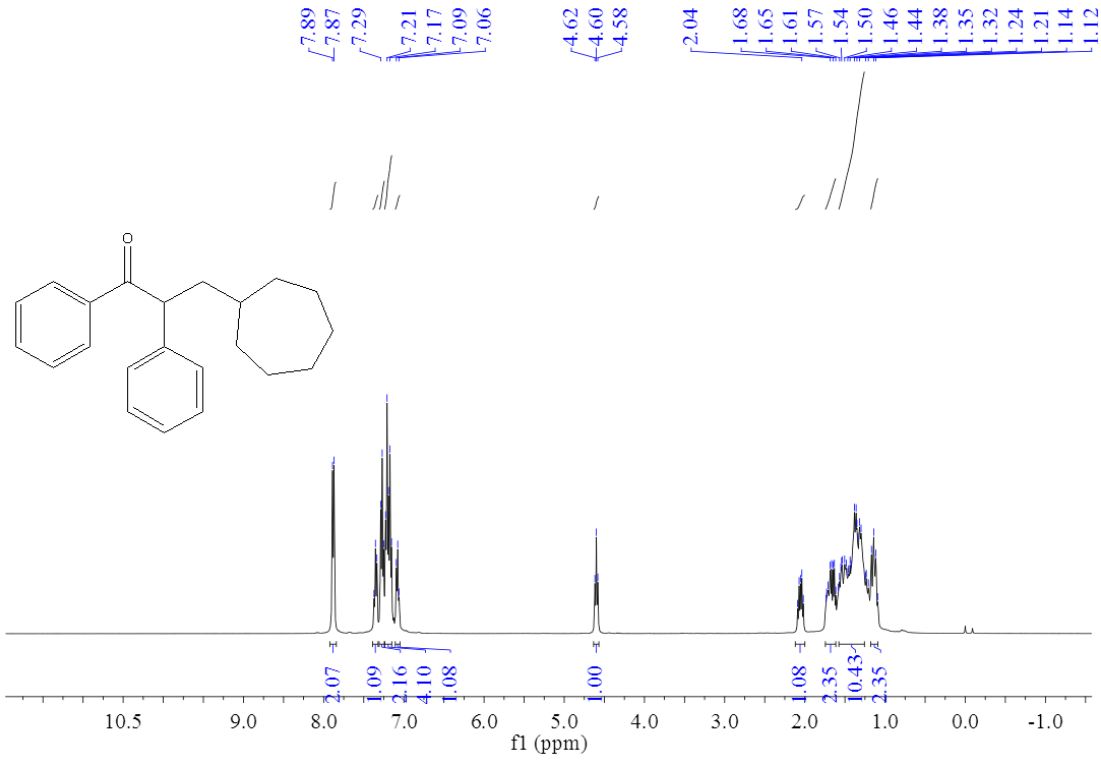
f1 (ppm)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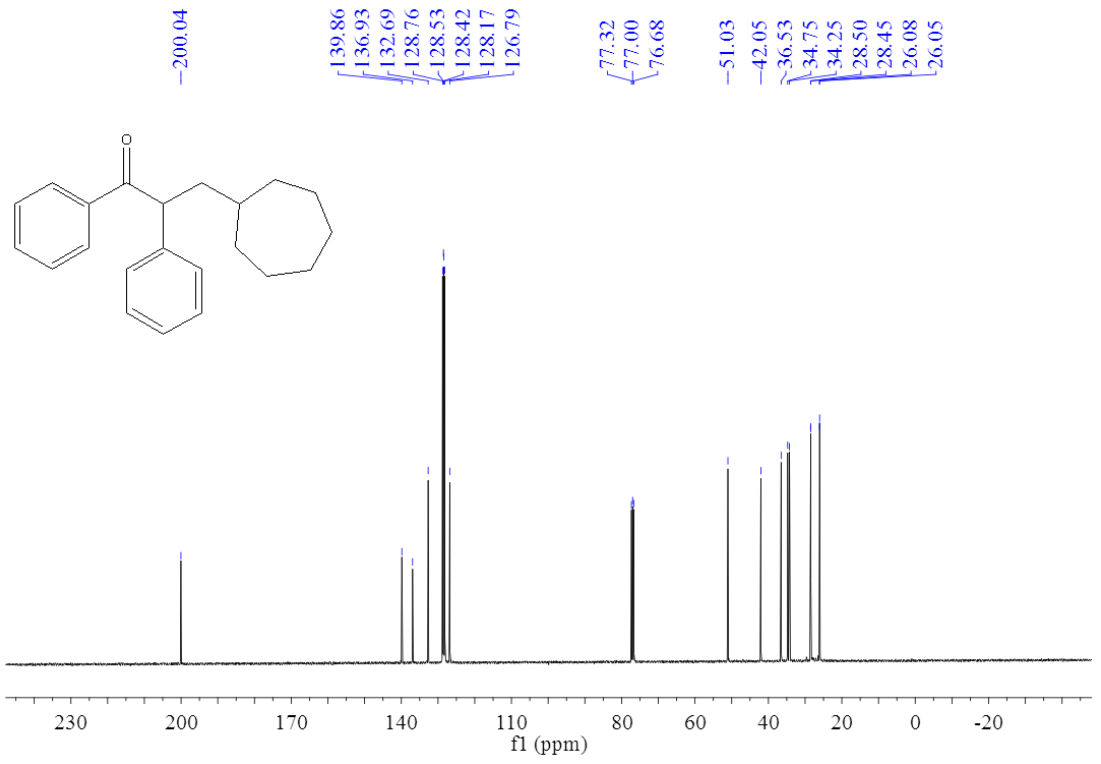
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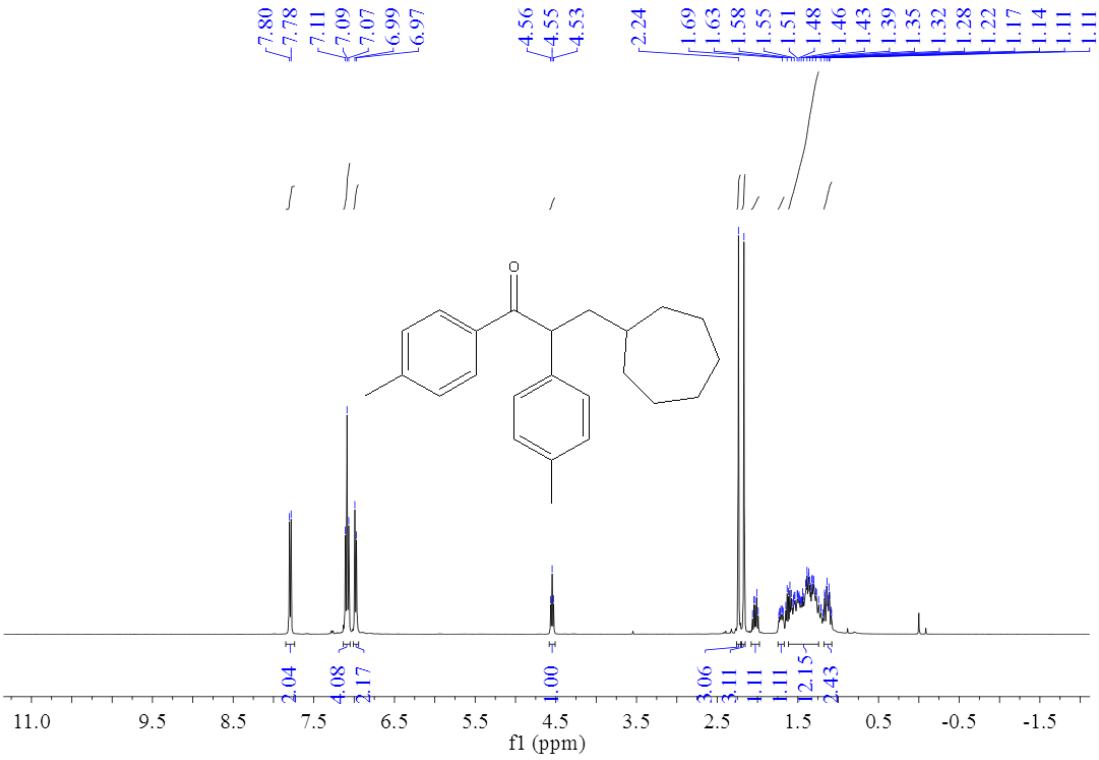
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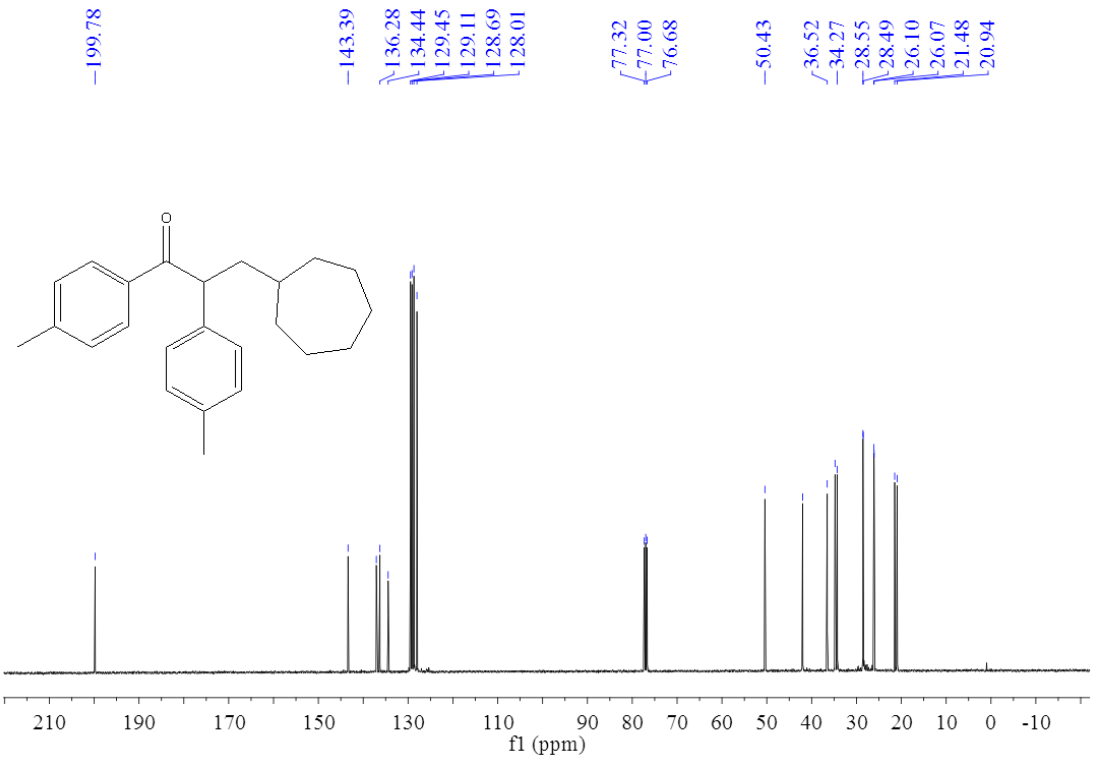
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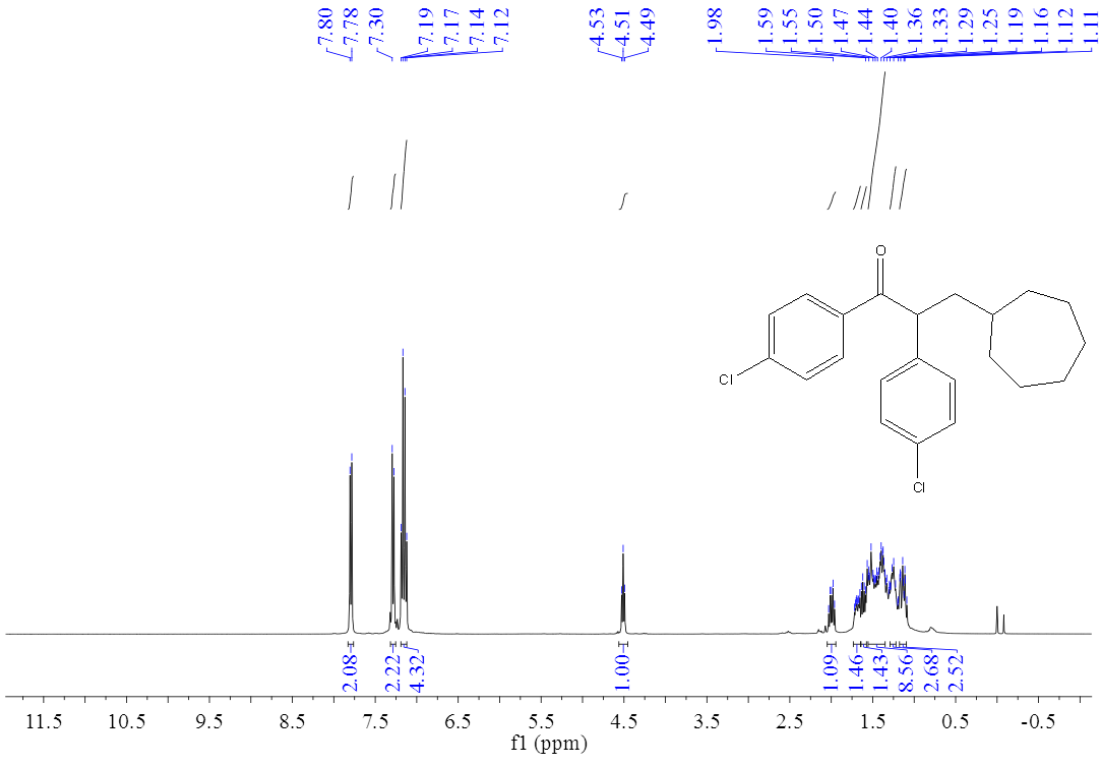
f1 (ppm)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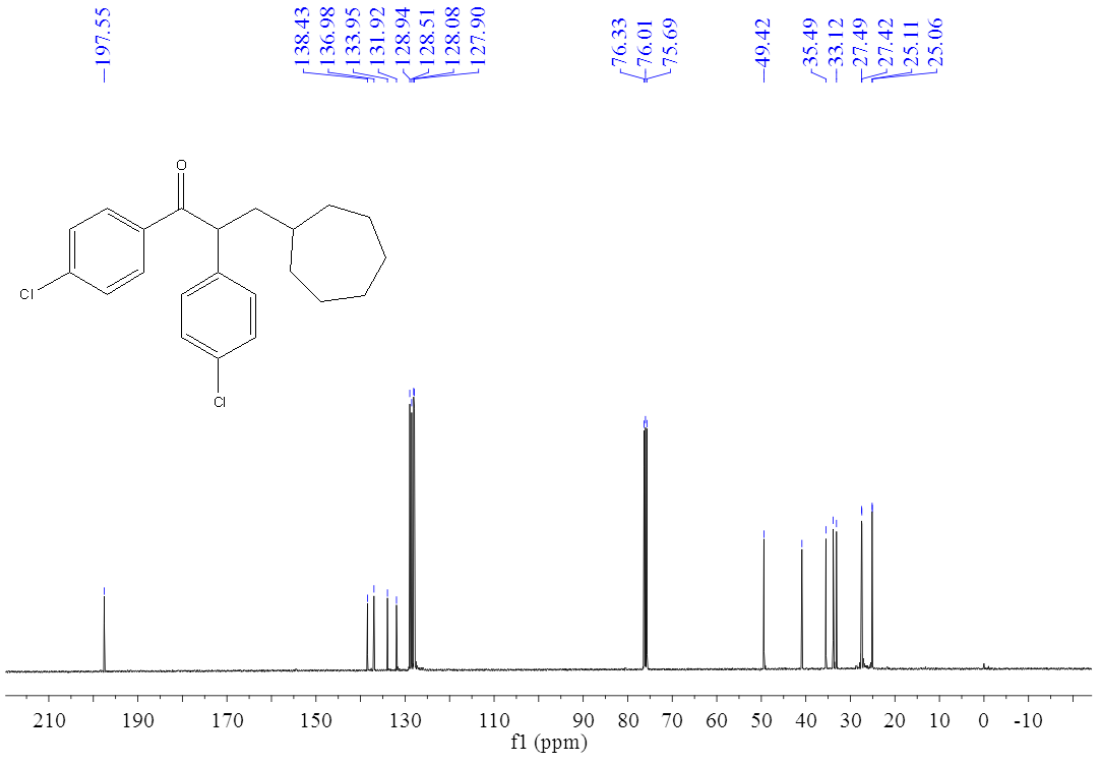
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25.06
O
Cl
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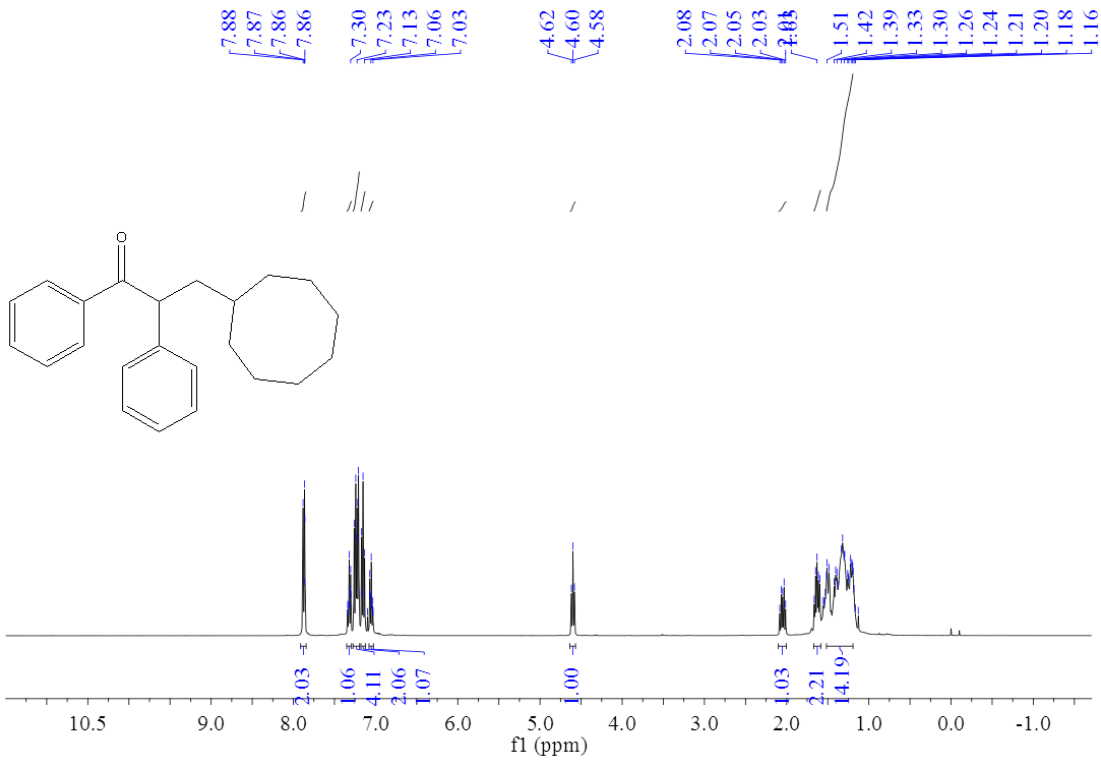
f1 (ppm)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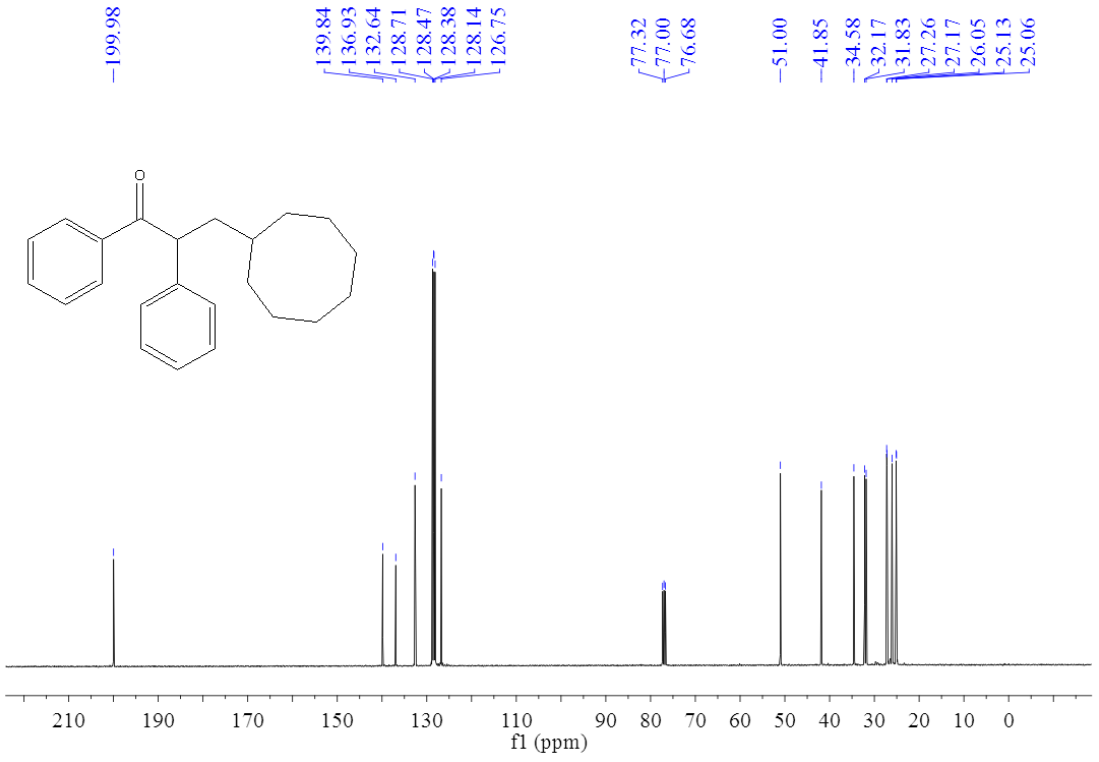
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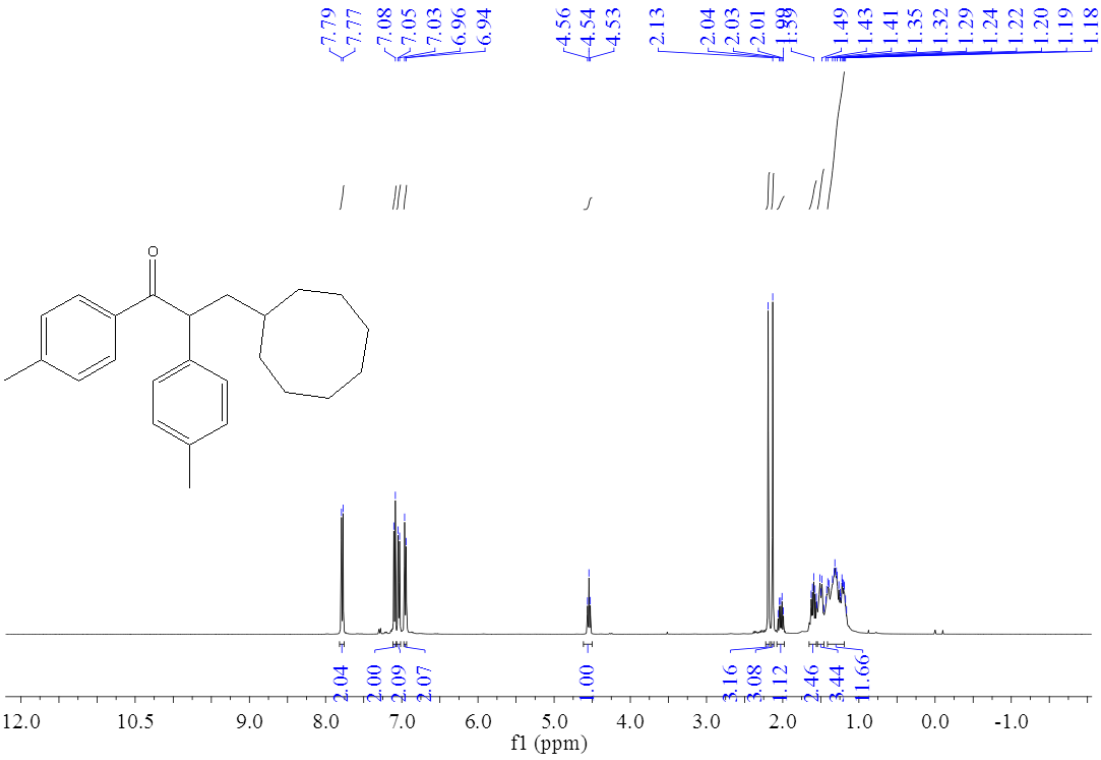
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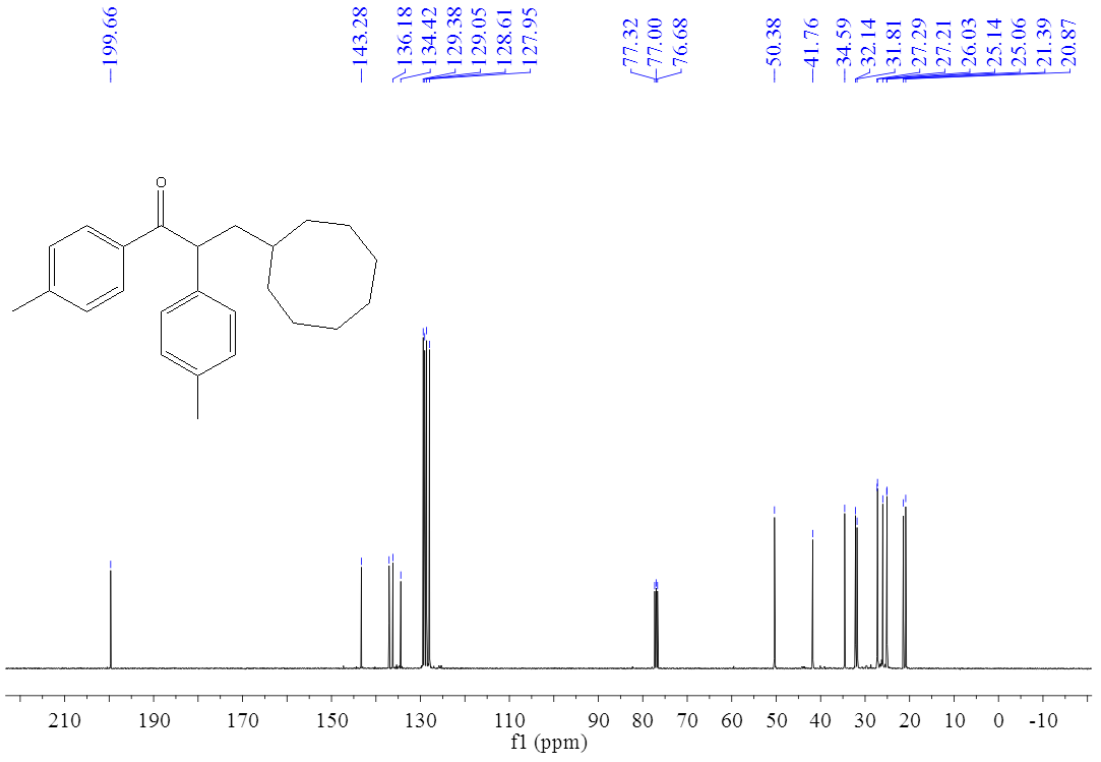
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50.38
41.76
34.59
32.14
31.81
27.29
27.21
26.03
25.14
25.06
21.39
20.87
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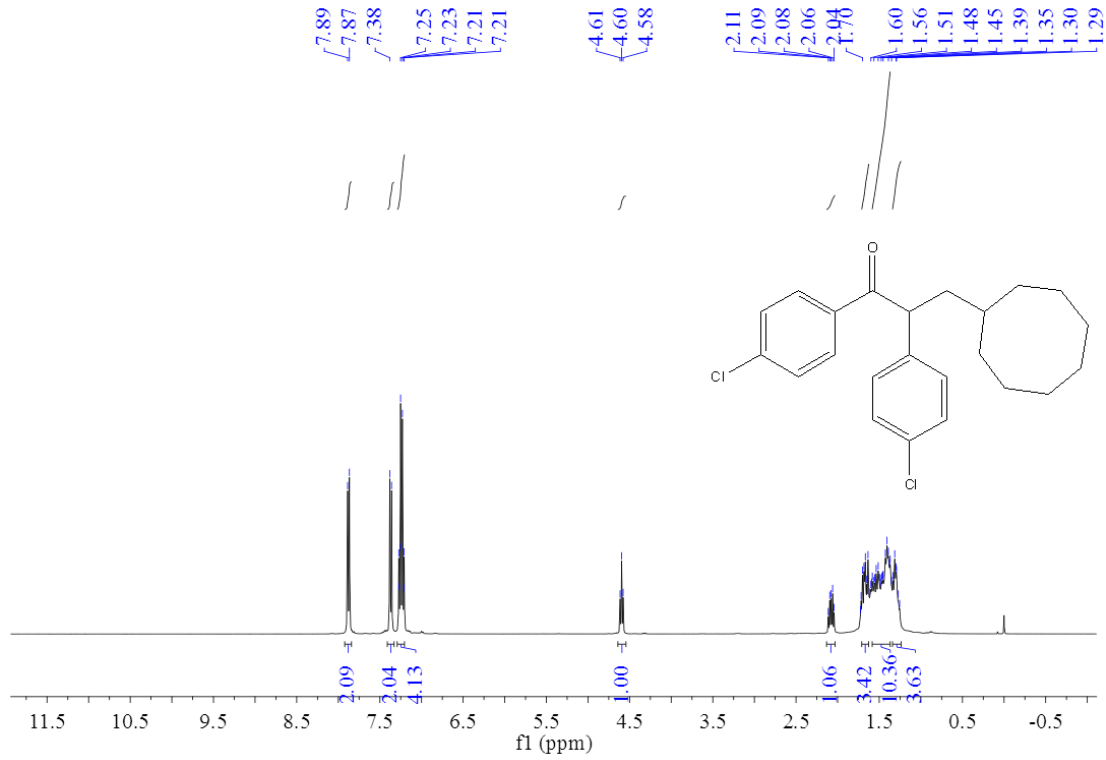
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4.58
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2.08
2.06
2.04
1.70
1.60
1.56
1.51
1.48
1.45
1.39
1.35
1.30
1.29
O
Cl
Cl
2.09
2.04
4.13
1.00
1.06
3.42
10.36
3.63
11.5
10.5
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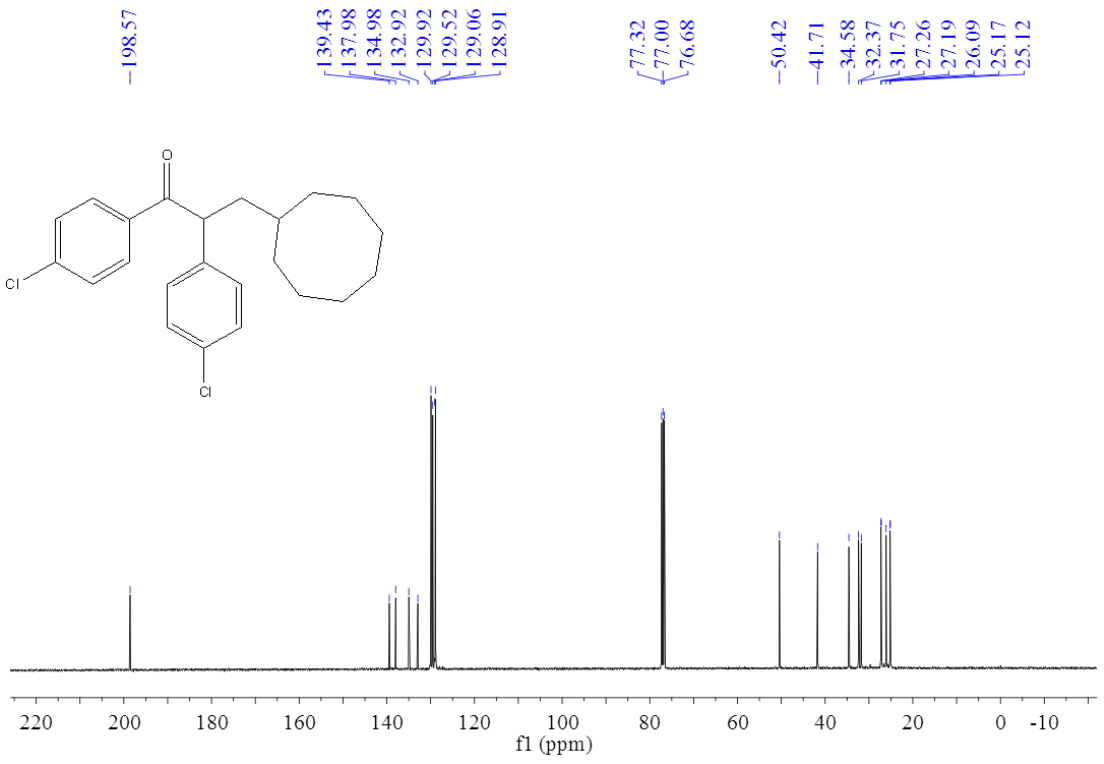
f1 (ppm)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41.71
34.58
32.37
31.75
27.26
27.19
26.09
25.17
25.12
O
Cl
Cl
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200
180
160
140
120
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80
60
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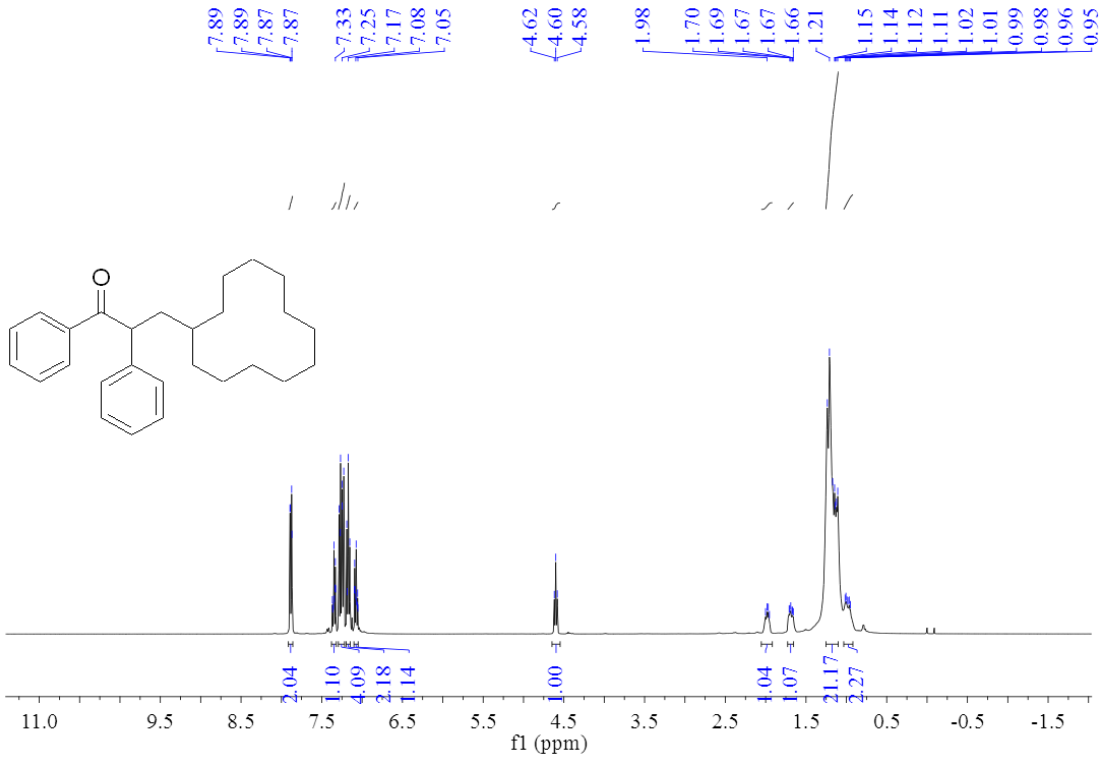
0
-10
f1 (ppm)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1.66
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1.15
1.14
1.12
1.11
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0.95
2.04
1.10
4.09
2.18
1.14
1.00
1.04
1.07
21.17
2.27
11.0
9.5
8.5
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4.5
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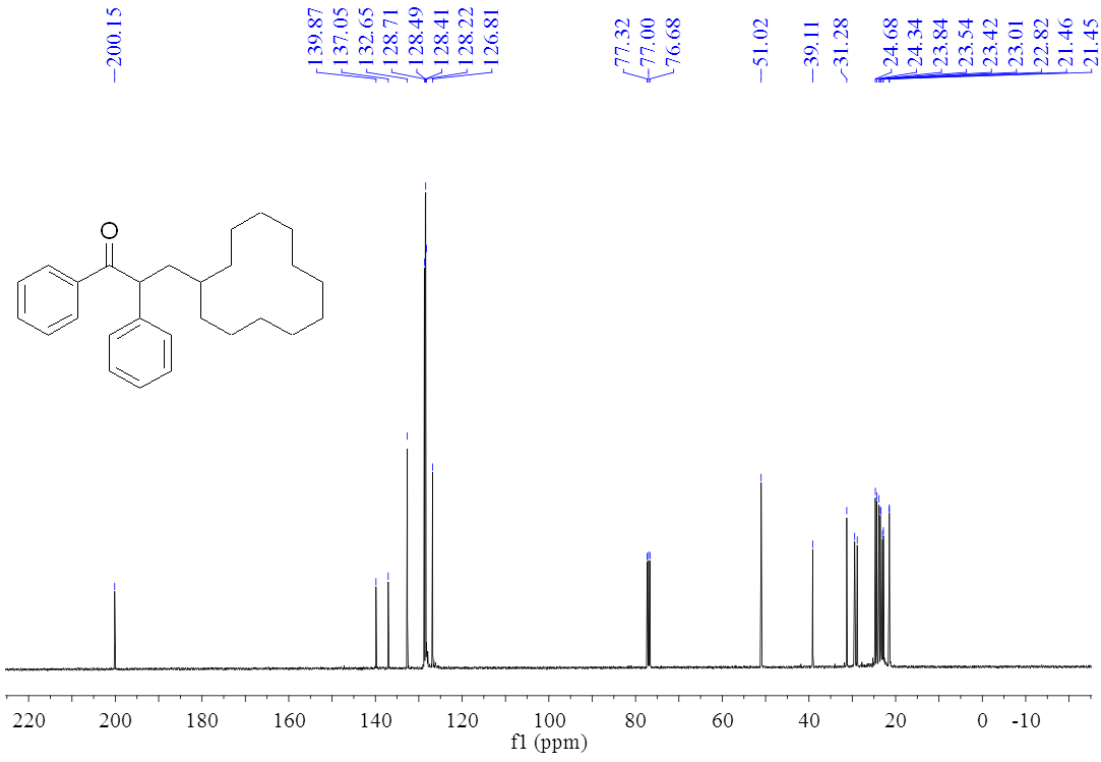
f1 (ppm)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51.02
39.11
31.28
24.68
24.34
23.84
23.54
23.42
23.01
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200
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160
140
120
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80
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0
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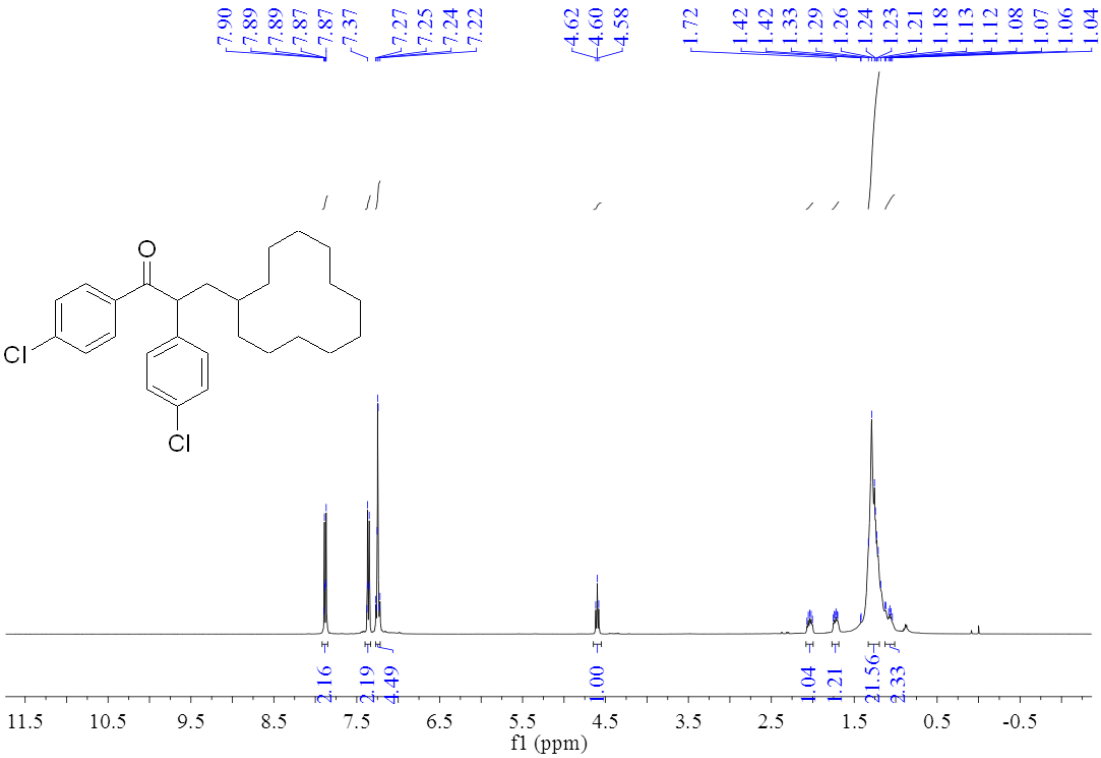
f1 (ppm)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4.58
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1.42
1.33
1.29
1.26
1.24
1.23
1.21
1.18
1.13
1.12
1.08
1.07
1.06
1.04
O
Cl
Cl
2.16
2.19
4.49
1.00
1.04
1.21
21.56
2.33
11.5
10.5
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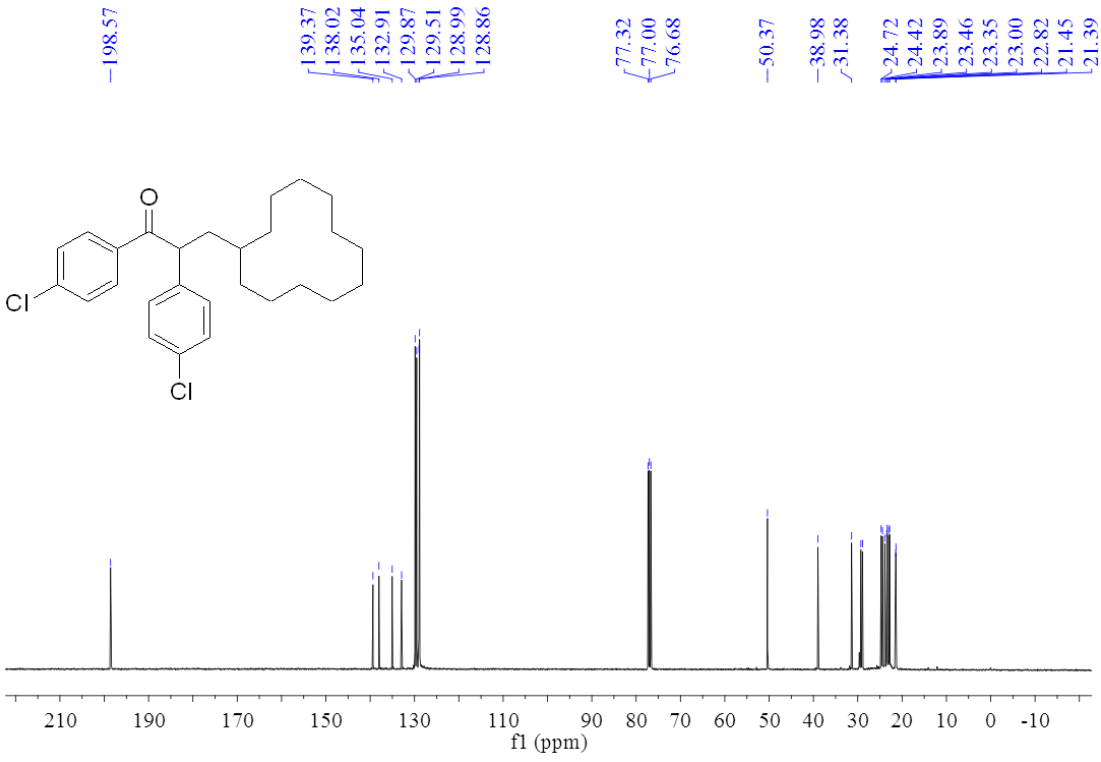
f1 (ppm)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38.98
31.38
24.72
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23.89
23.46
23.35
23.00
22.82
21.45
21.39
O
Cl
Cl
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150
130
110
90
80
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60
50
40
30
20
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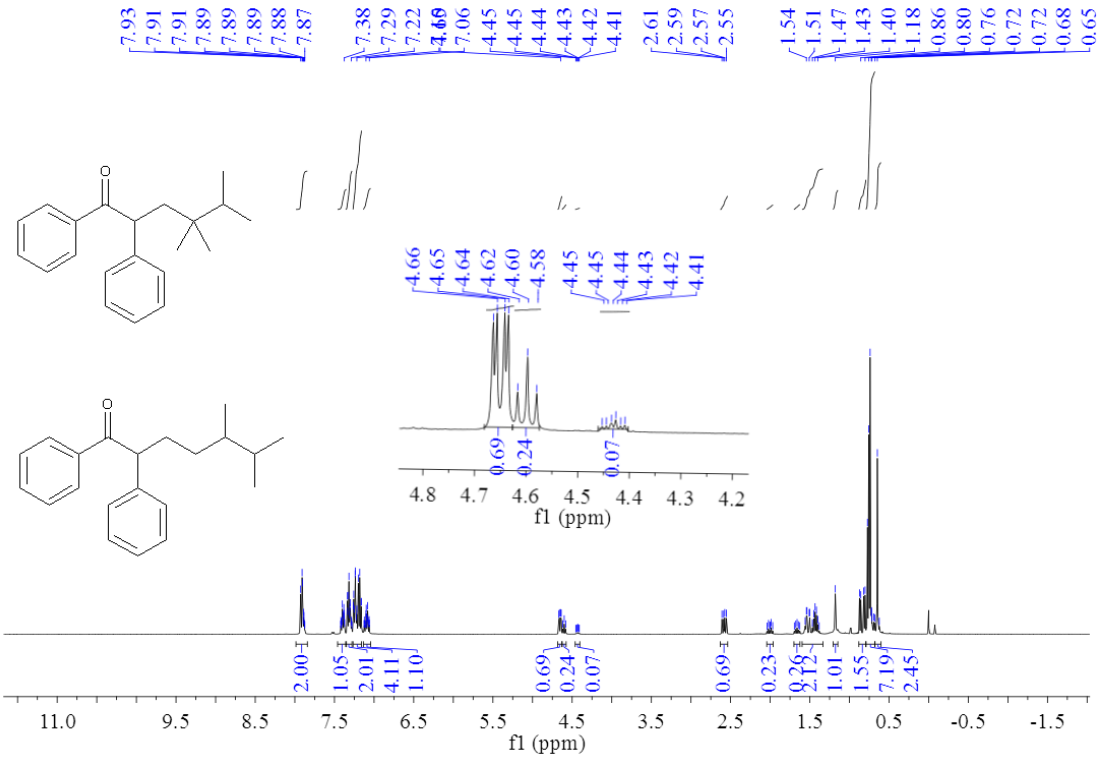
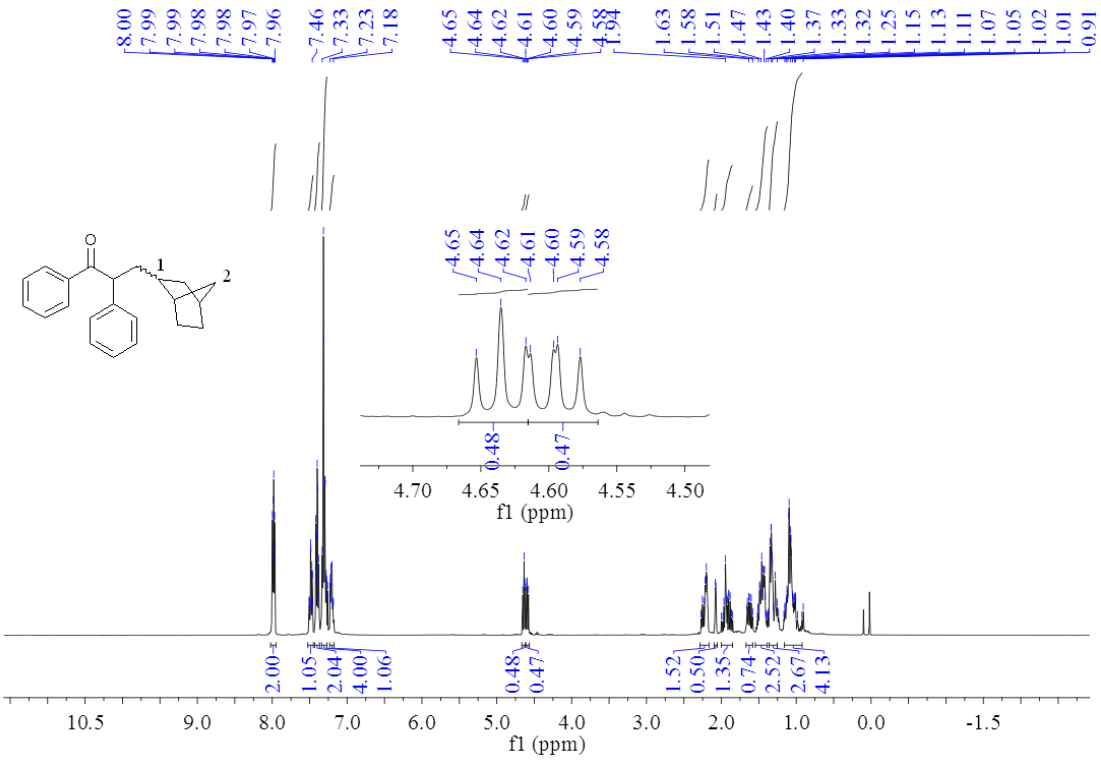
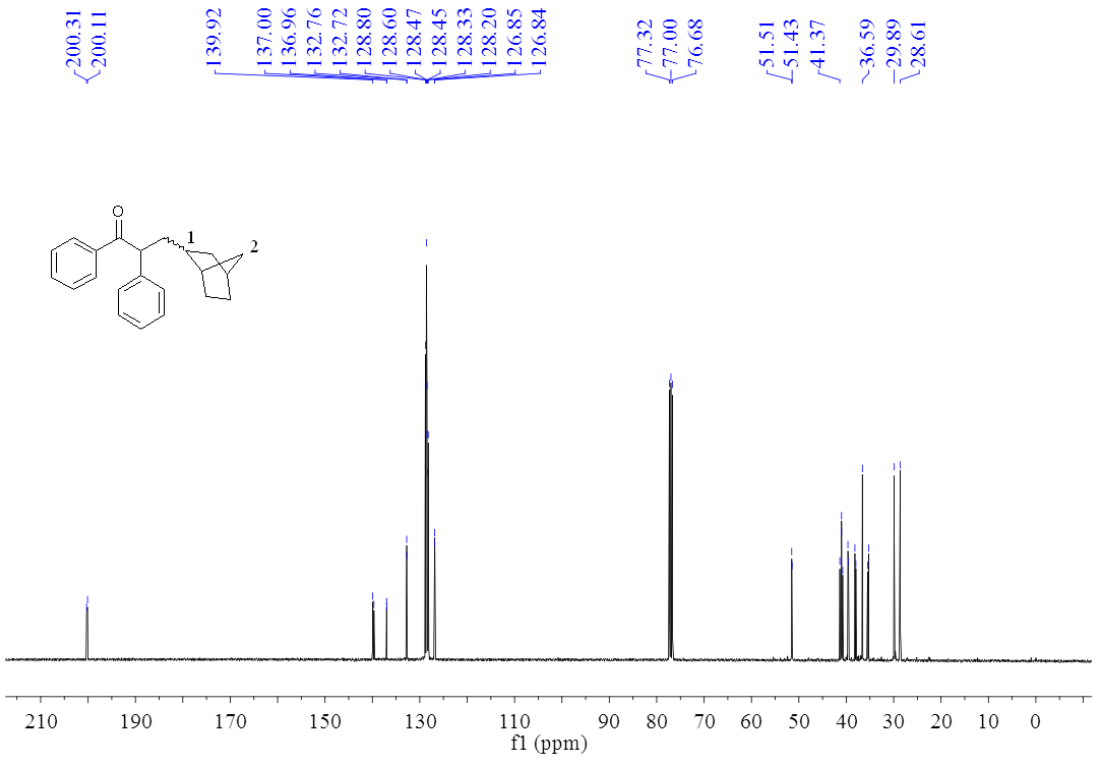
0
-10
f1 (ppm)


f1 (ppm)


1
2
f1 (ppm)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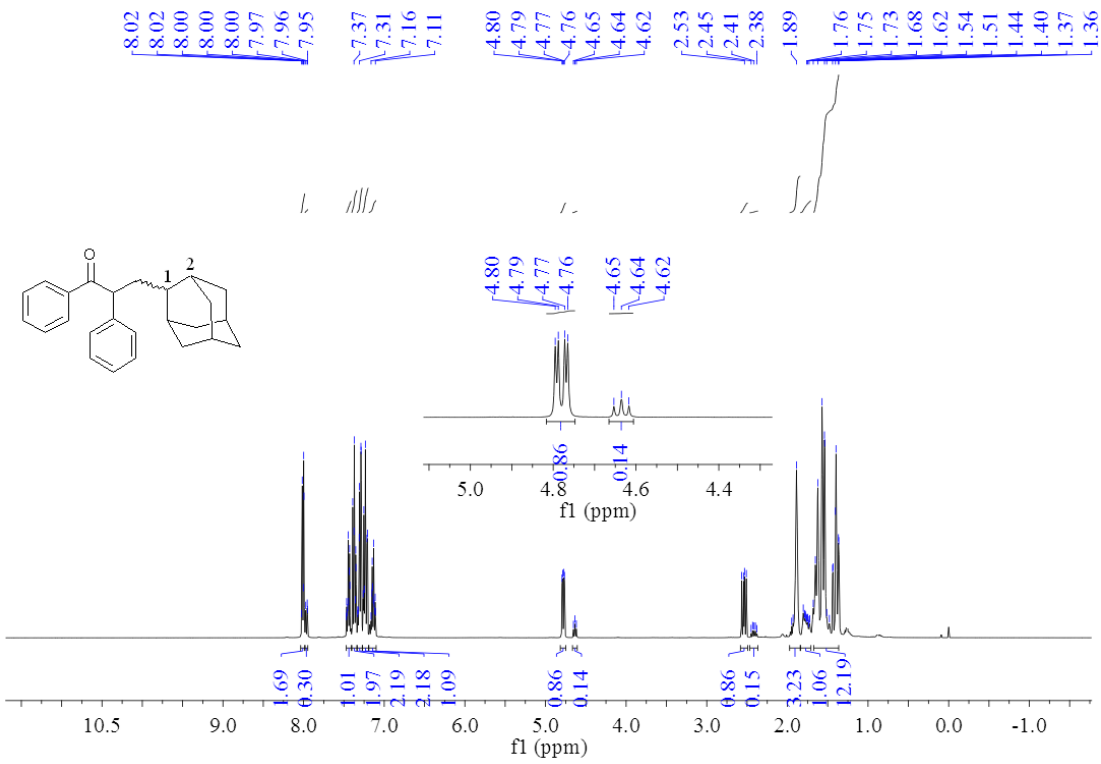
128.47
128.45
128.33
128.20
126.85
126.84
77.32
77.00
76.68
51.51
51.43
41.37
36.59
29.89
28.61
O
1
2
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.95
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7.31
7.16
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4.80
4.79
4.77
4.76
4.65
4.64
4.62
2.53
2.45
2.41
2.38
1.89
1.76
1.75
1.73
1.68
1.62
1.54
1.51
1.44
1.40
1.37
1.36
O
1
2
1.69
6.30
1.01
1.97
2.19
2.18
1.09
0.86
0.14
0.86
0.15
3.23
1.06
12.19
10.5
9.0
8.0
7.0
6.0
5.0
4.0
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f1 (ppm)
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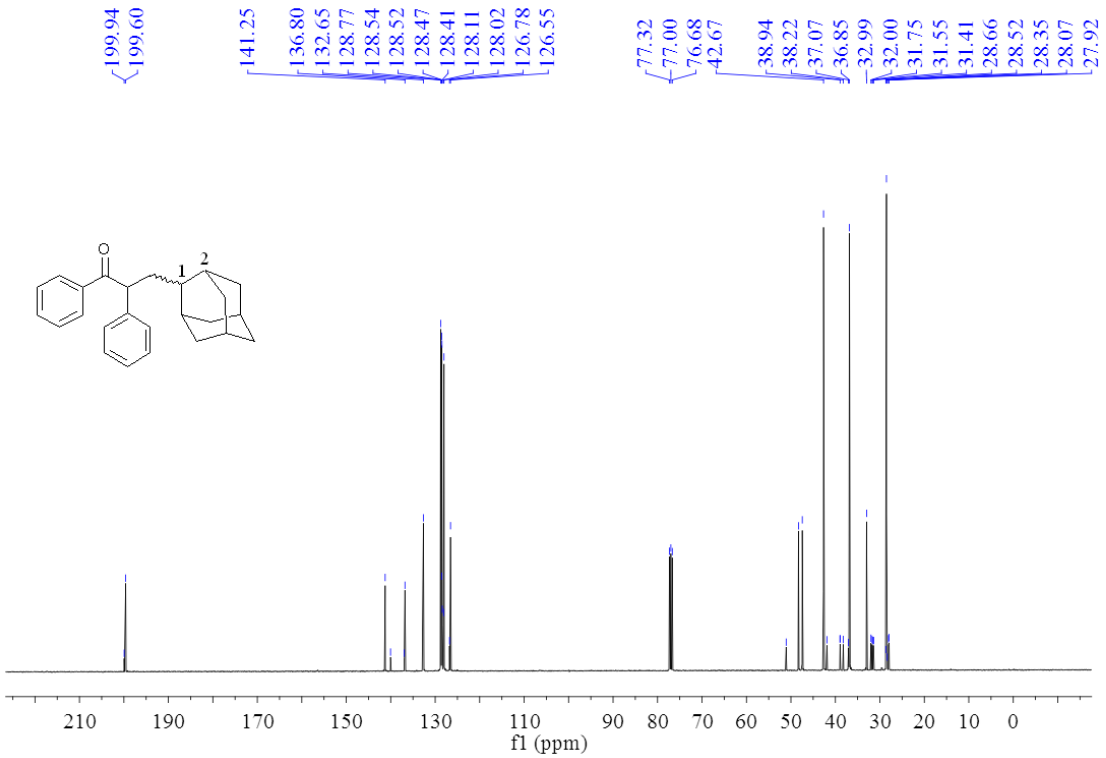
4.8
4.6
4.4
f1 (ppm)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126.55
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77.00
76.68
42.67
38.94
38.22
37.07
36.85
32.99
32.00
31.75
31.55
31.41
28.66
28.52
28.35
28.07
27.92
1
2
210
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170
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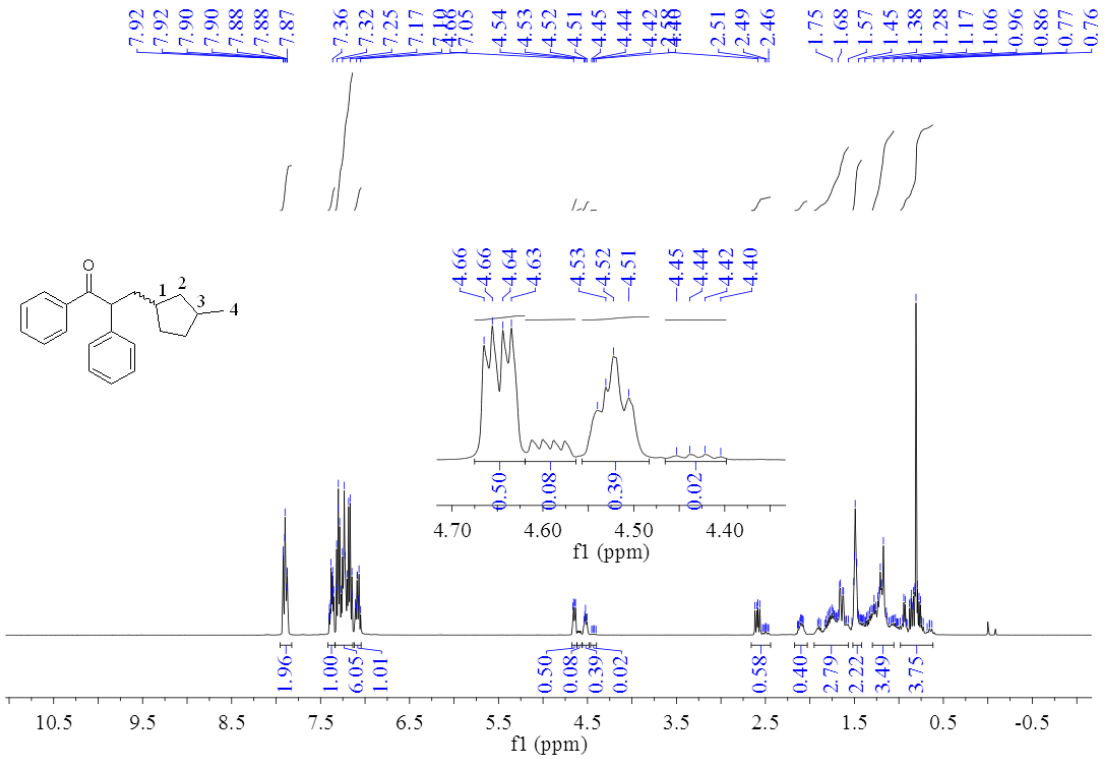
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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4.53
4.52
4.51
4.45
4.44
4.42
2.51
2.49
2.46
1.75
1.68
1.57
1.45
1.38
1.28
1.17
1.06
0.96
0.86
0.77
0.76
1
2
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4
4.66
4.66
4.64
4.63
4.53
4.52
4.51
4.45
4.44
4.42
4.40
0.50
0.08
0.39
0.02
4.70
4.60
4.50
4.40
f1 (ppm)
1.96
1.00
6.05
1.01
0.50
0.08
0.39
0.02
0.58
0.40
2.79
2.22
3.49
3.75
10.5
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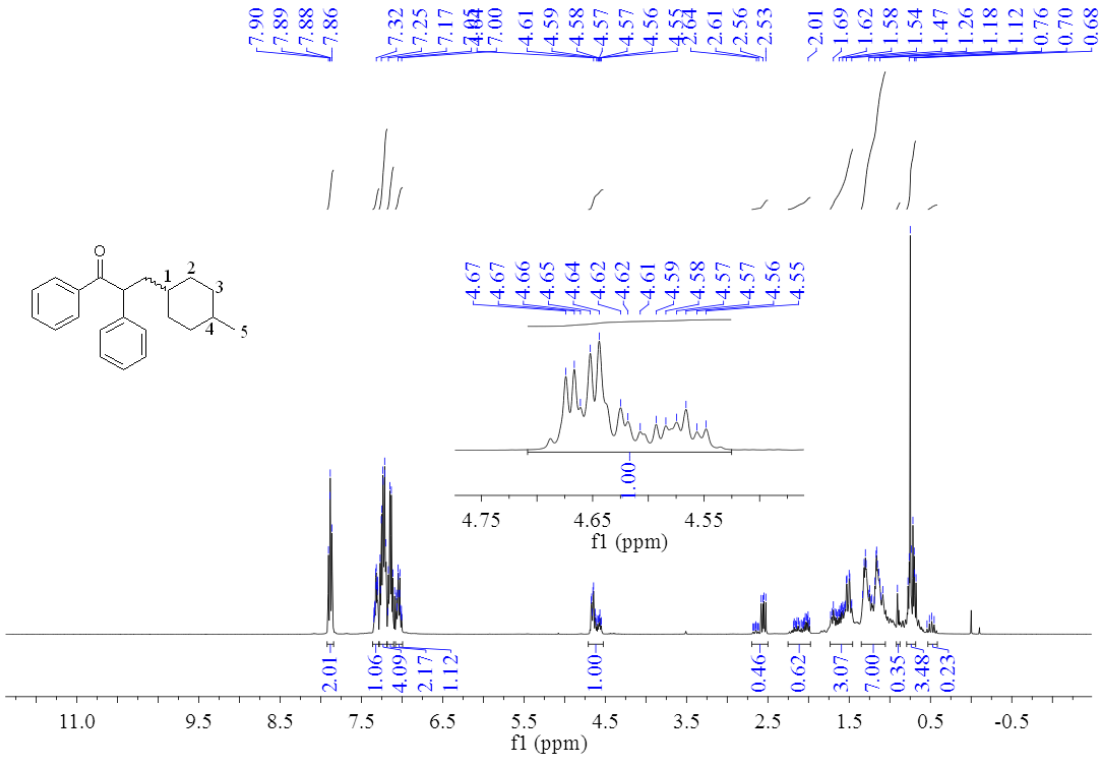
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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4.61
4.59
4.58
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4.57
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2.56
2.53
2.01
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1.62
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1.54
1.47
1.26
1.18
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0.70
0.68
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2
3
4
5
4.67
4.67
4.66
4.65
4.64
4.62
4.62
4.61
4.59
4.58
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1.00
4.75
4.65
4.55
f1 (ppm)
2.01
1.06
4.09
2.17
1.12
1.00
0.46
0.62
3.07
7.00
0.35
3.48
0.23
11.0
9.5
8.5
7.5
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5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)