Supporting Information

Oxidative alkylarylation of α-aryl allylic alcohols through direct C-H bond functionalization by photoredox catalysis

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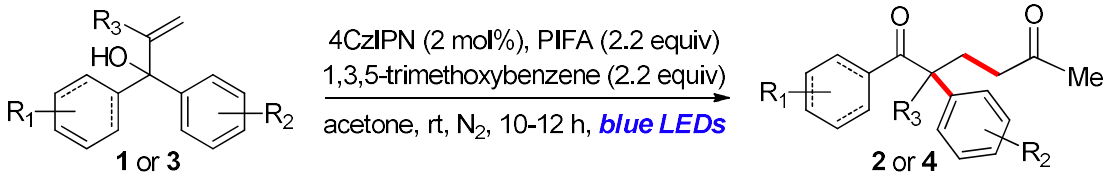
Materials and methods

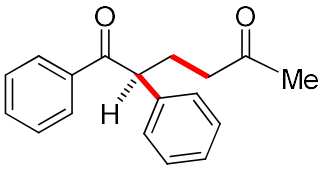
All the chemicals were purchased commercially, and used without further purification. Thin-layer chromatography (TLC) was conducted with 0.25 mm Tsingdao silica gel plates (60F-254) and visualized by exposure to UV light (254 nm) or stained with potassium permanganate. Flash column chromatography was performed using Tsingdao silica gel (60, particle size 0.040–0.063 mm). Reagents were purchased at the highest commercial quality and used without further purification, unless otherwise stated. ^{1}H NMR spectra were recorded on JEOL spectrometers (at 400 MHz) and were reported relative to deuterated solvent signals. Data for ^{1}H NMR spectra were reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz) and integration. ^{13}C NMR spectra were recorded on JEOL Spectrometers (at 100 MHz). Data for ^{13}C NMR spectra were reported in terms of chemical shift. Mass spectrometric data were obtained using Bruker Apex IV RTMS. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad.

General procedure for 1,5-diketone synthesis



A flame-dried round bottom flask was equipped with magnetic stir bar and charged with α-aryl allylic alcohols **1** or **3** (0.143 mmol, 1.0 equiv), $PhI(OCOCF_3)_2$ (0.314 mmol, 2.2 equiv), 1,3,5-trimethoxybenzene (0.314 mmol, 2.2 equiv), 1,2,3,5-tetrakis(carbazol-9-yl)-4,6-dicyanobenzene (4CzIPN) (0.0029 mmol, 0.02 equiv), and acetone (6.0 mL). The reaction mixture was degassed by purging thoroughly with nitrogen for 10 minutes, then irradiated by blue LEDs (18 *W*) under a balloon nitrogen atmosphere at room temperature until the starting material disappeared from the TLC. After that the reaction mixture was directly concentrated under reduced pressure and the crude product was purified by silica gel column chromatography using hexane/EtOAc (6/1 to 3/1) to afford the desired pure product **2** or **4** in 56-92% yields.

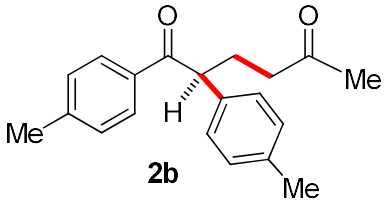
^{1}H and ^{13}C spectra data of compounds 2a-2l, 4a-4x



2a

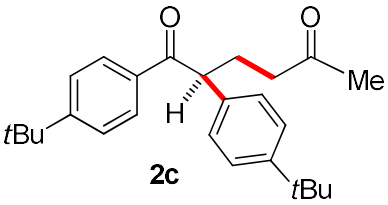
1,2-diphenylhexane-1,5-dione (2a): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.6 Hz, 2H), 7.52-7.43 (m, 1H), 7.40-7.34 (m, 2H), 7.32-7.26 (m, 4H), 7.24-7.18 (m, 1H), 4.67-4.63 (m, 1H), 2.48-2.32 (m, 3H), 2.20-2.04 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.7, 199.6, 139.1, 136.6, 133.1, 129.1, 128.8, 128.6, 128.4, 127.3, 52.3,

41.0, 30.1, 27.7. These data are consistent with literature values, see: X. Chu, H. Meng, Y. Zi, X. Xu and S.-J. Ji, *Chem. Eur. J.,* 2014, **20**, 17198. (Pale yellow solid, 29.6 mg, 78% isolated yield)



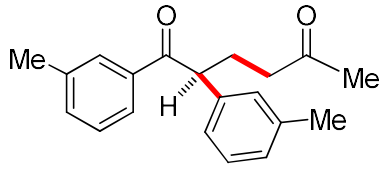
2b

1,2-di-*p*-tolylhexane-1,5-dione (2b): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.6 Hz, 2H), 7.20-7.12 (m, 4H), 7.10-7.06 (m, 2H), 4.58 (t, *J* = 7.2 Hz, 1H), 2.46-2.30 (m, 3H), 2.34 (s, 3H), 2.28 (s, 3H), 2.11-2.05 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.8, 199.3, 143.8, 136.9, 136.2, 134.2, 129.8, 129.3, 128.9, 128.2, 51.8, 41.2, 30.1, 27.7, 21.7, 21.1. These data are consistent with literature values, see: X. Chu, H. Meng, Y. Zi, X. Xu and S.-J. Ji, *Chem. Eur. J.,* 2014, **20**, 17198. (Pale yellow solid, 24.4 mg, 77% isolated yield)



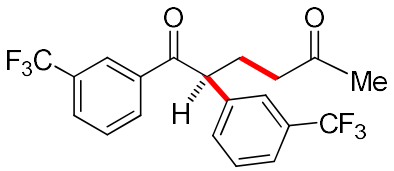
2c

1,2-bis(4-(*tert*-butyl)phenyl)hexane-1,5-dione (2c): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.8 Hz, 2H), 7.41 (d, *J* = 8.8 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 4.62-4.59 (m, 1H), 2.41-2.36 (m, 3H), 2.15-2.08 (m, 4H), 1.30 (s, 9H), 1.27 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.8, 199.3, 156.7, 150.0, 136.0, 134.2, 128.9, 127.9, 126.0, 125.6, 51.6, 41.3, 35.1, 34.5, 31.4, 31.1, 30.1, 27.9; HRMS calculated for $C_{26}H_{34}NaO_2$ ($M + Na^+$): 401.2457, found: 401.2442. (Pale yellow solid, 37.3 mg, 81% isolated yield)



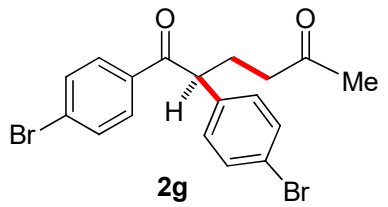
2d

1,2-di-*m*-tolylhexane-1,5-dione (2d): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.01 (m, 2H), 7.32-7.22 (m, 2H), 7.20-7.13 (m, 1H), 7.10-7.04 (m, 2H), 7.03-6.98 (m, 1H), 4.59 (t, *J* = 6.8 Hz, 1H), 2.50-2.32 (m, 3H), 2.35 (s, 3H), 2.29 (s, 3H), 2.13-2.05 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.7, 199.9, 139.1, 138.8, 138.4, 136.8, 133.8, 129.3, 128.9, 128.8, 128.5, 128.1, 126.1, 125.5, 52.2, 41.2, 30.1, 27.8, 21.5, 21.4; HRMS calculated for $C_{20}H_{22}NaO_2$ ($M + Na^+$): 317.1517, found: 317.1525. (Yellow oil, 28.5 mg, 73% isolated yield)



2f

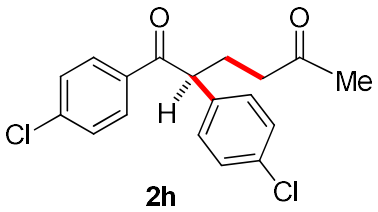
1,2-bis(3-(trifluoromethyl)phenyl)hexane-1,5-dione (2f): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58-7.50 (m, 1H), 7.30-7.20 (m, 4H), 7.16-7.10 (m, 2H), 7.04-7.00 (m, 1H), 4.57 (t, *J* = 6.8 Hz, 1H), 2.48-2.42 (m, 1H), 2.22-2.06 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.2, 203.1, 141.3, 135.7, 133.6, 133.5, 131.5, 130.2, 129.2, 128.8, 127.3, 118.7, 55.8, 40.8, 30.1, 26.3. These data are consistent with literature values, see: X. Chu, H. Meng, Y. Zi, X. Xu and S.-J. Ji, *Chem. Eur. J.,* 2014, **20**, 17198. (Yellow oil, 20.8 mg, 56% isolated yield)



2g

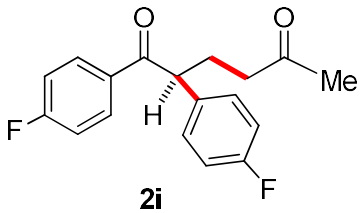
1,2-bis(4-bromophenyl)hexane-1,5-dione (2g): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79

(d, J = 8.4 Hz, 2H), 7.53 (d, J = 8.0 Hz, 2H), 7.43 (d, J = 8.4 Hz, 2H), 7.12 (d, J = 8.0 Hz, 2H), 4.59 (d, J = 7.6 Hz, 2H), 2.45-2.30 (m, 3H), 2.20-2.00 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.4, 198.3, 137.7, 135.0, 132.4, 132.1, 130.3, 130.0, 128.5, 121.6, 51.5, 40.6, 30.2, 27.4. These data are consistent with literature values, see: X. Chu, H. Meng, Y. Zi, X. Xu and S.-J. Ji, *Chem. Eur. J.,* 2014, **20**, 17198. (Pale yellow solid, 25.3 mg, 73% isolated yield)



2h

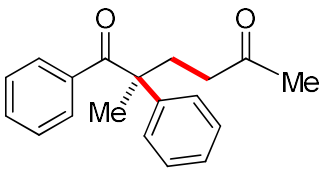
1,2-bis(4-chlorophenyl)hexane-1,5-dione (2h): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, J = 8.0 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 7.27 (d, J = 8.0 Hz, 2H), 7.18 (d, J = 8.0 Hz, 2H), 4.61 (t, J = 7.2 Hz, 1H), 2.42-2.30 (m, 3H), 2.12-2.00 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.4, 198.1, 139.7, 137.2, 134.7, 133.5, 130.2, 129.7, 129.4, 129.0, 51.4, 40.6, 30.2, 27.5. These data are consistent with literature values, see: X. Chu, H. Meng, Y. Zi, X. Xu and S.-J. Ji, *Chem. Eur. J.,* 2014, **20**, 17198. (Yellow solid, 32.1 mg, 89% isolated yield)



2i

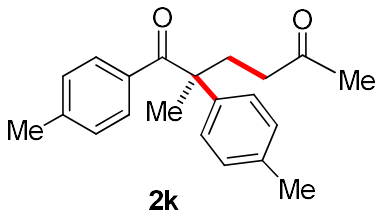
1,2-bis(4-fluorophenyl)hexane-1,5-dione (2i): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.95 (m, 2H), 7.25-7.19 (m, 2H), 7.10-7.03 (m, 2H), 7.02-6.95 (m, 2H), 4.63 (t, J = 7.6 Hz, 1H), 2.45-2.30 (m, 3H), 2.10 (s, 3H), 2.13-2.02 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.6, 198.0, 167.0, 163.3, 160.9, 134.6, 132.8, 131.5, 131.4, 129.9, 129.8, 116.2, 116.0, 115.9, 115.7, 51.2, 40.8, 30.2, 27.7. These data are consistent

with literature values, see: X. Chu, H. Meng, Y. Zi, X. Xu and S.-J. Ji, *Chem. Eur. J.,* 2014, **20**, 17198. (Yellow oil, 30.9 mg, 84% isolated yield)



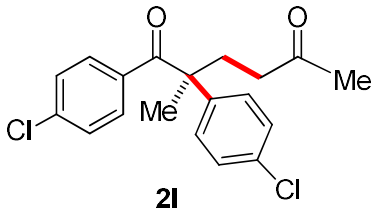
2j

2-methyl-1,2-diphenylhexane-1,5-dione (2j): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.0 Hz, 2H), 7.40-7.33 (m, 3H), 7.31-7.19 (m, 5H), 2.39-2.20 (m, 4H), 2.06 (s, 3H), 1.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.5, 203.1, 143.6, 136.3, 131.9, 129.7, 129.2, 128.1, 127.2, 126.3, 54.0, 39.1, 33.9, 30.0, 24.2; HRMS calculated for $C_{19}H_{20}NaO_2$ ($M + Na^+$): 303.1361, found: 303.1356. (Pale yellow solid, 22.6 mg, 60% isolated yield)



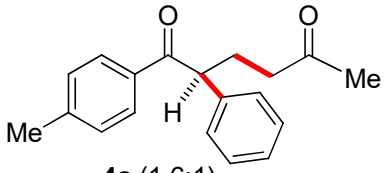
2k

2-methyl-1,2-di-*p*-tolylhexane-1,5-dione (2k): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.6 Hz, 2H), 7.20-7.10 (m, 4H), 7.02 (d, *J* = 8.0 Hz, 2H), 2.40-2.20 (m, 10H), 2.05 (s, 3H), 1.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.7, 202.8, 142.6, 140.9, 136.7, 133.6, 129.9, 129.7, 128.8, 126.2, 53.5, 39.2, 34.0, 30.0, 24.5, 21.5, 21.1; HRMS calculated for $C_{21}H_{24}NaO_2$ ($M + Na^+$): 331.1674, found: 331.1671. (Yellow solid, 26.8 mg, 63% isolated yield)



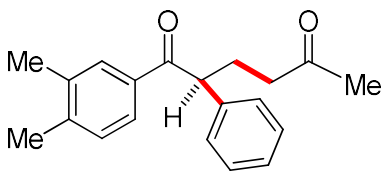
2l

1,2-bis(4-chlorophenyl)-2-methylhexane-1,5-dione (2l): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.8 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.31-7.18 (m, 4H), 2.38-2.10 (m, 4H), 2.08 (s, 3H), 1.56 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.1, 201.3, 142.0, 138.7, 134.0, 133.4, 131.1, 129.5, 128.6, 127.7, 53.6, 38.9, 33.7, 30.1, 24.3; HRMS calculated for $C_{19}H_{18}Cl_2NaO_2$ ($M + Na^+$): 371.0582, found: 371.0575. (Pale yellow solid, 24.0 mg, 56% isolated yield)



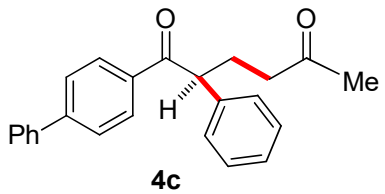
4a (1.6:1)

2-phenyl-1-(*p*-tolyl)hexane-1,5-dione (4a): ^{1}H NMR (400 MHz, $CDCl_3$; the major product is designated by *, minor product denoted by §) δ 7.95 (d, *J* = 8.0 Hz, 0.7H§), 7.85 (d, *J* = 8.0 Hz, 1.3H*), 7.52-7.46 (m, 0.30H§), 7.42-7.35 (m, 0.70H*), 7.32-7.25 (m, 3.0H§), 7.24-7.08 (m, 3.0H*), 4.64-4.59 (m, 1.0H), 2.49-2.32 (m, 5.0H), 2.28 (s, 1.2H), 2.15-2.02 (m, 4.0H); ^{13}C NMR (100 MHz, $CDCl_3$; compounds exist as a mixture of major and minor products) δ 208.7, 199.2, 143.9, 139.3, 134.1, 133.0, 129.8, 129.3, 129.1, 128.9, 128.8, 128.6, 128.3, 128.2, 127.3, 52.1, 51.9, 41.1, 41.0, 30.1, 27.7, 27.6, 21.7, 21.1; HRMS calculated for $C_{19}H_{21}O_2$ ($M + H^+$): 281.1542, found: 281.1528. (Yellow oil, 20.1 mg, 60% isolated yield)



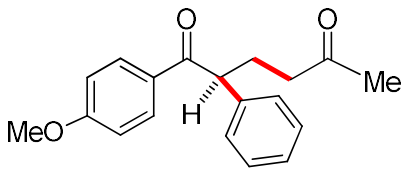
4b: (2.3:1)

1-(3,4-dimethylphenyl)-2-phenylhexane-1,5-dione (4b): ^{1}H NMR (400 MHz, $CDCl_3$; the major product is designated by *, minor product denoted by §) δ 7.95 (d, *J* = 7.6 Hz, 0.6H), 7.42 (s, 0.7H), 7.68 (d, *J* = 7.6 Hz, 0.8H), 7.48-7.44 (m, 0.4H§), 7.39-7.35 (m, 0.8H), 7.28-7.24 (m, 2.4H), 7.22-7.16 (m, 0.8H), 7.14-7.10 (s, 0.8H§), 7.06-6.98 (m, 1.0H), 4.65-4.60 (m, 0.7H*), 4.59-4.54 (m, 0.3H§), 2.47-2.33 (m, 3.0H), 2.25-2.16 (m, 7.0H), 2.13-2.08 (m, 4.0H); ^{13}C NMR (100 MHz, $CDCl_3$; compounds exist as a mixture of major and minor products) δ 208.8, 199.5, 142.7, 139.4, 137.0, 133.0, 130.3, 129.9, 129.8, 129.3, 129.1, 128.8, 128.6, 128.3, 127.2, 126.6, 125.9, 52.0, 51.9, 41.2, 30.0, 27.8, 20.0, 19.9, 19.4. These data are consistent with literature values, see: X. Chu, H. Meng, Y. Zi, X. Xu and S.-J. Ji, *Chem. Eur. J.,* 2014, **20**, 17198. (Pale yellow solid, 22.9 mg, 63% isolated yield)



4c

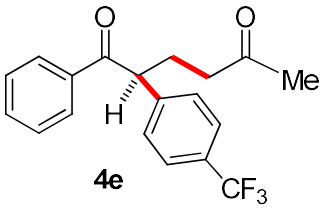
1-([1,1'-biphenyl]-4-yl)-2-phenylhexane-1,5-dione (4c): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.0 Hz, 2H), 7.58-7.48 (m, 5H), 7.42-7.28 (m, 8H), 4.72-4.69 (m, 1H), 2.48-2.40 (m, 3H), 2.20-2.12 (m, 1H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.7, 199.6, 140.6, 140.2, 138.1, 136.7, 133.2, 128.9, 128.8, 128.7, 127.8, 127.4, 127.3, 127.1, 51.9, 41.1, 30.1, 27.7; HRMS calculated for $C_{24}H_{22}NaO_2$ ($M + Na^+$): 365.1517, found: 365.1508. (Pale yellow solid, 34.6 mg, 88% isolated yield)



4d

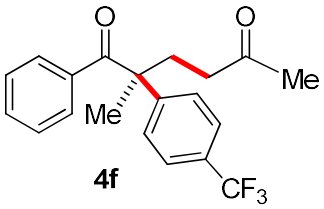
1-(4-methoxyphenyl)-2-phenylhexane-1,5-dione (4d): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.8 Hz, 2H), 7.29-7.27 (m, 4H), 6.86 (d, *J* = 8.4 Hz, 2H), 4.62-4.55 (m,

1H), 3.82 (s, 3H), 2.50-2.31 (m, 3H), 2.16-2.04 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.8, 198.1, 163.4, 139.5, 131.2, 129.6, 129.1, 128.3, 127.2, 113.8, 55.5, 51.9, 41.2, 30.1, 27.8; HRMS calculated for $C_{19}H_{20}NaO_3$ ($M + Na^+$): 319.1310, found: 319.1306. (Yellow oil, 28.2 mg, 82% isolated yield)



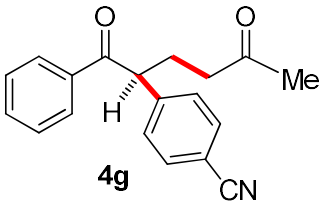
4e

1-phenyl-2-(4-(trifluoromethyl)phenyl)hexane-1,5-dione (4e): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, J = 7.6 Hz, 2H), 7.60-7.50 (m, 3H), 7.46-7.38 (m, 4H), 4.78 (t, J = 6.8 Hz, 1H), 2.45-2.40 (m, 3H), 2.22-2.03 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.3, 199.0, 143.1, 136.3, 133.5, 129.8, 129.5, 128.8, 128.7, 126.1, 126.0, 122.7, 51.8, 40.8, 30.1, 27.7; HRMS calculated for $C_{19}H_{17}F_3NaO_2$ ($M + Na^+$): 357.1078, found: 357.1077. (Pale yellow solid, 27.9 mg, 77% isolated yield)



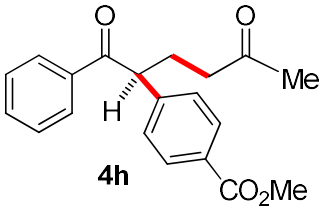
4f

2-methyl-1-phenyl-2-(4-(trifluoromethyl)phenyl)hexane-1,5-dione (4f): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, J = 8.4 Hz, 2H), 7.50-7.38 (m, 5H), 7.30-7.20 (m, 2H), 2.40-2.20 (m, 4H), 2.07 (s, 3H), 1.61 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.0, 202.2, 148.1, 135.7, 132.4, 129.6, 128.4, 127.8, 127.6, 126.6, 126.1, 54.0, 38.9, 33.8, 30.1, 24.5; HRMS calculated for $C_{20}H_{19}F_3NaO_2$ ($M + Na^+$): 371.1235, found: 371.1229. (Pale yellow solid, 32.7 mg, 80% isolated yield)



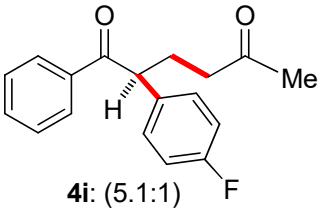
4g

4-(1,5-dioxo-1-phenylhexan-2-yl)benzonitrile (4g): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.6 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.56-7.51 (m, 1H), 7.46-7.38 (m, 4H), 4.81-4.78 (m, 1H), 2.50-2.38 (m, 3H), 2.15-2.02 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.2, 198.7, 144.6, 136.2, 133.7, 132.9, 129.2, 128.9, 128.8, 118.6, 111.3, 51.9, 40.7, 30.2, 27.6; HRMS calculated for $C_{19}H_{17}NNaO_2$ (M + Na^+): 314.1157, found: 314.1149. (Pale yellow solid, 34.1 mg, 92% isolated yield)



4h

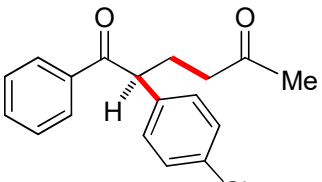
methyl 4-(1,5-dioxo-1-phenylhexan-2-yl)benzoate (4h): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.90 (m, 4H), 7.52-7.47 (m, 1H), 7.42-7.32 (m, 4H), 4.77-4.73 (m, 1H), 3.88 (s, 3H), 2.50-2.38 (m, 3H), 2.19-2.03 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.4, 199.1, 166.8, 144.3, 136.4, 133.3, 130.4, 129.3, 128.8, 128.7, 128.4, 52.2, 52.1, 40.8, 30.2, 27.5; HRMS calculated for $C_{20}H_{21}O_4$ (M + H^+): 325.1440, found: 325.1432. (Pale yellow solid, 25.3 mg, 61% isolated yield)



4i: (5.1:1)

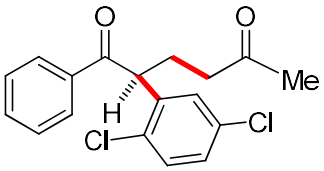
2-(4-fluorophenyl)-1-phenylhexane-1,5-dione (4i): ^{1}H NMR (400 MHz, $CDCl_3$; the major product is designated by *, minor product denoted by §) δ 8.02-7.91 (m, 2.0H),

7.36-7.20 (m, 5.0H), 7.10-6.95 (m, 2H), 4.70-4.65 (m, 0.16H[§]), 4.63-4.59 (m, 0.80H*), 2.49-2.31 (m, 4.0H), 2.21-2.04 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$; compounds exist as a mixture of major and minor products) δ 208.7, 198.0, 164.4, 138.9, 133.2, 132.9, 131.5, 131.4, 129.9, 129.8, 129.2, 128.8, 128.7, 128.3, 127.5, 115.8, 115.6, 52.2, 51.3, 40.9, 31.1, 30.1, 29.8, 27.6. HRMS calculated for $C_{18}H_{18}FO_2$ ($M + H^+$): 285.1291, found: 285.1280. (Pale yellow solid, 27.0 mg, 72% isolated yield)



4j: (8.2:1)

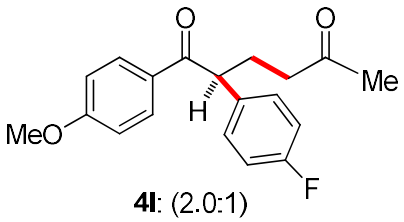
2-(4-chlorophenyl)-1-phenylhexane-1,5-dione (4j): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.6 Hz, 2H), 7.55-7.48 (m, 1H), 7.45-7.37 (m, 2H), 7.30-7.18 (m, 4H), 4.68-4.65 (m, 1H), 2.45-2.30 (m, 3H), 2.15-2.01 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.5, 199.4, 137.6, 136.4, 133.3, 130.3, 129.7, 129.3, 128.8, 128.7, 51.4, 40.8, 30.1, 27.6; HRMS calculated for $C_{18}H_{17}ClNaO_2$ ($M + Na^+$): 323.0815, found: 323.0783. (Pale yellow solid, 32.1 mg, 87% isolated yield)



4k: (1.2:1)

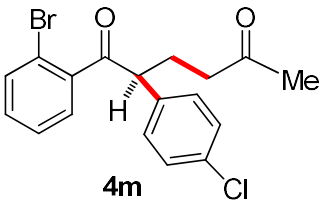
2-(2,5-dichlorophenyl)-1-phenylhexane-1,5-dione (4k): ^{1}H NMR (400 MHz, $CDCl_3$; the major product is designated by *, minor product denoted by [§]) δ 7.96 (d, *J* = 7.6 Hz, 1H), 7.58-7.50 (m, 0.47H[§]), 7.46-7.38 (m, 1H), 7.36-7.20 (m, 4H), 7.20-7.10 (m, 1H), 7.03 (s, 0.53H*), 5.12 (t, *J* = 7.6 Hz, 0.47H*), 4.43 (t, *J* = 6.8 Hz, 0.58H*), 2.55-2.32 (m, 3H), 2.20-1.95 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$; compounds exist as a mixture of major and minor products) δ 208.2, 207.9, 201.5, 198.7, 140.7, 138.7,

136.7, 133.6, 132.8, 131.9, 131.5, 131.3, 131.0, 129.2, 129.0, 128.9, 128.8, 128.7, 127.9, 56.7, 47.8, 40.8, 30.1, 30.0, 27.2, 26.2; HRMS calculated for $C_{18}H_{17}Cl_2O_2$ (M + H^+): 335.0606, found: 335.0591. (Pale yellow solid, 40.7 mg, 75% isolated yield)



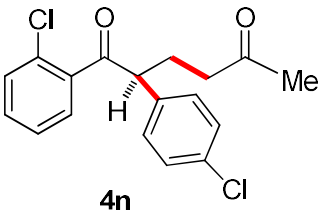
4l: (2.0:1)

2-(4-fluorophenyl)-1-(4-methoxyphenyl)hexane-1,5-dione (4l): ^{1}H NMR (400 MHz, $CDCl_3$; the major product is designated by *, minor product denoted by §) δ 7.99-7.91 (m, 2H), 7.25-7.21 (m, 2H), 7.19-6.90 (m, 4H), 6.88-6.78 (m, 2H), 4.60 (t, *J* = 7.6 Hz, 0.63H*), 4.53 (t, *J* = 7.6 Hz, 0.34H§), 3.78-3.68 (m, 3H), 2.39-2.32 (m, 3H), 2.10-2.01 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$; compounds exist as a mixture of major and minor products) δ 208.6, 198.1, 163.6, 131.5, 131.4, 131.1, 129.9, 129.8, 129.4, 116.0, 115.8, 114.6, 113.9, 93.0, 55.5, 55.3, 51.3, 50.9, 41.0, 40.9, 30.1, 27.9, 27.6; HRMS calculated for $C_{19}H_{19}FNaO_3$ (M + Na^+): 337.1216, found: 337.1207. (Yellow solid, 31.4 mg, 86% isolated yield)



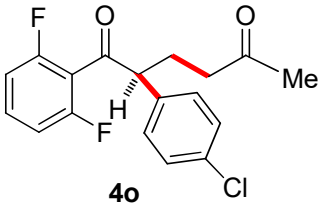
4m

1-(2-bromophenyl)-2-(4-chlorophenyl)hexane-1,5-dione (4m): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (s, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.77 (d, *J* = 7.6 Hz, 1H), 7.62-7.41 (m, 5H), 4.78 (t, *J* = 7.2 Hz, 1H), 2.51-2.40 (m, 3H), 2.20-2.05 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.2, 197.8, 139.4, 136.7, 131.9, 131.7, 129.8, 129.5, 125.7, 125.1, 124.6, 51.9, 40.5, 30.2, 27.6; HRMS calculated for $C_{18}H_{16}BrClNaO_2$ (M + Na^+): 400.9920, found: 400.9912. (Pale yellow solid, 19.8 mg, 56% isolated yield)



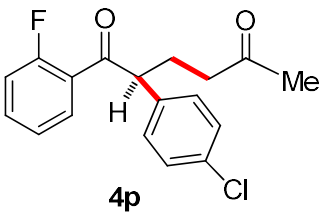
4n

1-(2-chlorophenyl)-2-(4-chlorophenyl)hexane-1,5-dione (4n): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.21 (m, 4H), 7.20-7.06 (m, 4H), 4.52-4.42 (m, 1H), 2.51-2.38 (m, 3H), 2.18-2.02 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.2, 202.7, 139.3, 135.9, 133.6, 131.6, 130.5, 130.4, 130.1, 129.2, 129.0, 126.8, 55.9, 40.8, 30.1, 26.4. These data are consistent with literature values, see: X. Chu, H. Meng, Y. Zi, X. Xu and S.-J. Ji, *Chem. Eur. J.,* 2014, **20**, 17198. (Pale yellow solid, 32.7 mg, 91% isolated yield)



4o

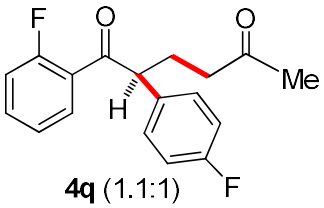
2-(4-chlorophenyl)-1-(2,6-difluorophenyl)hexane-1,5-dione (4o): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.21 (m, 3H), 7.24-7.08 (m, 2H), 7.88-7.80 (m, 2H), 4.26-4.23 (m, 1H), 2.52-2.40 (m, 3H), 2.12 (s, 3H), 2.10-1.98 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.0, 196.7, 160.6, 158.2, 135.4, 133.7, 132.4, 130.0, 129.2, 112.1, 111.9, 58.0, 40.8, 30.1, 26.0; HRMS calculated for $C_{18}H_{15}ClF_2NaO_2$ ($M + Na^+$): 359.0626, found: 359.0612. (Yellow oil, 33.3 mg, 77% isolated yield)



4p

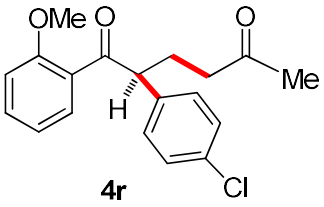
2-(4-chlorophenyl)-1-(2-fluorophenyl)hexane-1,5-dione (4p): ^{1}H NMR (400 MHz,

$CDCl_3$) δ 7.75-7.68 (m, 1H), 7.49-7.40 (m, 1H), 7.30-7.20 (m, 2H), 7.19-7.10 (m, 3H), 7.08-6.99 (m, 1H), 4.52 (t, J = 7.2 Hz, 1H), 2.45-2.38 (m, 3H), 2.14-2.01 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.2, 198.4, 136.6, 134.6, 134.5, 133.4, 131.1, 130.0, 129.1, 125.9, 124.6, 124.6, 116.8, 116.6, 55.8, 55.7, 41.1, 30.1, 27.3; HRMS calculated for $C_{18}H_{16}ClFNaO_2$ ($M + Na^+$): 341.0721, found: 341.0714. (Yellow oil, 30.8 mg, 84% isolated yield)



4q (1.1:1)

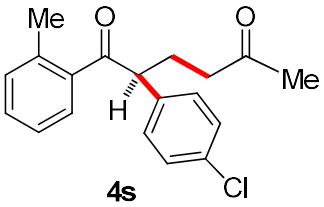
1-(2-fluorophenyl)-2-(4-fluorophenyl)hexane-1,5-dione (4q): ^1H NMR (400 MHz, $CDCl_3$; the major product is designated by *, minor product denoted by §) δ 7.98-7.95 (m, 1H), 7.71-7.67 (m, 0.5H), 7.44-7.39 (m, 0.5H), 7.22-7.11 (m, 3H), 7.07-6.99 (m, 3H), 6.96-6.92 (m, 1H), 4.94-4.90 (m, 0.54H*), 4.52-4.49 (m, 0.46H§), 2.51-2.36 (m, 3H), 2.09-2.04 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$; compounds exist as a mixture of major and minor products) δ 208.3, 208.2, 198.7, 197.4, 17.1, 164.5, 163.4, 162.3, 161.3, 160.9, 159.7, 158.9, 134.5, 134.4, 133.8, 132.5, 131.3, 131.2, 131.1, 130.3, 130.2, 129.3, 129.2, 129.0, 126.0, 125.8, 125.0, 124.9, 124.6, 124.5, 116.8, 116.6, 115.9, 115.8, 115.7, 115.6, 55.7, 55.6, 43.6, 41.1, 40.7, 30.1, 27.4, 26.6; HRMS calculated for $C_{18}H_{17}F_2O_2$ ($M + H^+$): 303.1197, found: 303.1194. (Yellow oil, 19.2 mg, 52% isolated yield)



4r

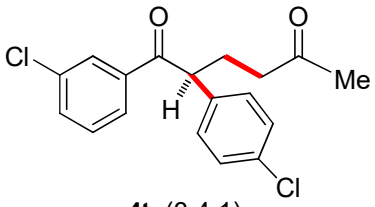
2-(4-chlorophenyl)-1-(2-methoxyphenyl)hexane-1,5-dione (4r): ^1H NMR (400

MHz, $CDCl_3$) δ 7.48-7.35 (m, 2H), 7.24-7.00 (m, 4H), 6.91-6.87 (m, 2H), 4.72-4.61 (m, 1H), 3.84 (s, 3H), 2.50-2.30 (m, 3H), 2.15-1.96 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.4, 202.8, 157.8, 137.6, 133.4, 132.9, 130.6, 130.0, 128.8, 128.6, 120.8, 111.5, 55.7, 55.4, 41.3, 30.0, 27.4; HRMS calculated for $C_{19}H_{19}ClNaO_3$ ($M + Na^+$): 353.0920, found: 353.0906. (Pale yellow solid, 26.0 mg, 67% isolated yield)



4s

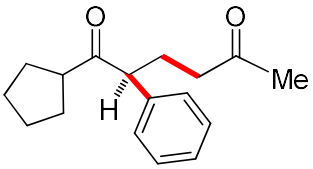
2-(4-chlorophenyl)-1-(o-tolyl)hexane-1,5-dione (4s): ^1H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.0 Hz, 1H), 7.35-7.11 (m, 7H), 4.49 (t, *J* = 7.2 Hz, 1H), 2.48-2.32 (m, 3H), 2.32 (s, 3H), 2.15-2.02 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.4, 203.3, 138.2, 138.2, 136.8, 133.3, 131.9, 131.3, 129.8, 129.2, 128.1, 125.7, 54.4, 40.9, 30.1, 26.9, 21.0; HRMS calculated for $C_{19}H_{19}ClNaO_2$ ($M + Na^+$): 337.0971, found: 337.0962. (Yellow oil, 26.1 mg, 71% isolated yield)



4t: (3.4:1)

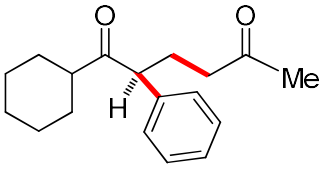
1-(3-chlorophenyl)-2-(4-chlorophenyl)hexane-1,5-dione (4t): ^1H NMR (400 MHz, $CDCl_3$; the major product is designated by *, minor product denoted by §) δ 7.92-7.85 (m, 1.6H*), 7.82-7.78 (m, 0.4H§), 7.50-7.46 (m, 0.4H§), 7.40-7.10 (m, 5.6H), 4.63-4.59 (m, 1H), 2.48-2.30 (m, 3H), 2.15-2.00 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$; compounds exist as a mixture of major and minor products) δ 208.3, 198.1, 197.9, 140.7, 139.8, 134.6, 133.2, 130.4, 130.2, 130.0, 129.7, 129.4, 129.1, 128.8, 128.4, 127.8, 126.9, 126.6, 51.7, 51.6, 40.7, 30.2, 27.5, 27.4; HRMS calculated for

$C_{18}H_{16}Cl_2NaO_2$ (M + Na^+): 357.0425, found: 357.0418. (Yellow solid, 28.9 mg, 80% isolated yield)



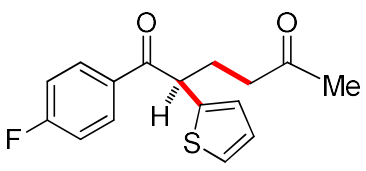
4u

1-cyclopentyl-2-phenylhexane-1,5-dione (4u): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.22 (m, 3H), 7.21-7.16 (m, 2H), 3.82-3.75 (m, 1H), 2.90-2.78 (m, 1H), 2.40-2.20 (m, 3H), 2.08 (s, 3H), 2.00-1.80 (m, 2H); 1.70-1.35 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 212.7, 208.6, 138.5, 129.0, 128.6, 127.4, 57.1, 50.6, 41.1, 30.4, 30.0, 28.8, 26.4, 26.1, 26.0; HRMS calculated for $C_{17}H_{22}NaO_2$ (M + Na^+): 281.1517, found: 281.1535. (Pale yellow solid, 31.5 mg, 82% isolated yield)



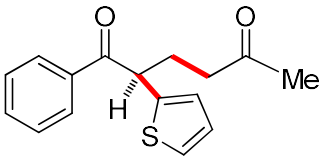
4v

1-cyclohexyl-2-phenylhexane-1,5-dione (4v): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.22 (m, 3H), 7.20-7.15 (m, 2H), 3.87-3.83 (m, 2H), 2.40-2.16 (m, 4H), 2.07 (s, 3H), 1.95-1.70 (m, 3H), 1.68-1.55 (m, 2H); 1.45-1.03 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 213.1, 208.6, 138.4, 129.0, 128.5, 127.4, 55.7, 50.1, 41.1, 30.0, 29.3, 28.2, 26.7, 26.0, 25.8, 25.3; HRMS calculated for $C_{18}H_{25}O_2$ (M + H^+): 273.1855, found: 273.1840. (Pale yellow solid, 26.6 mg, 79% isolated yield)



4w

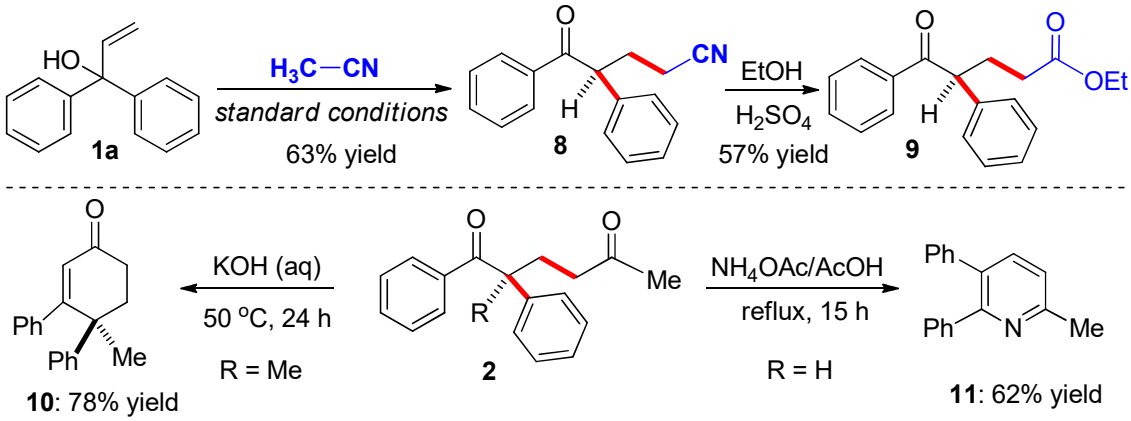
1-(4-fluorophenyl)-2-(thiophen-2-yl)hexane-1,5-dione (4w): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12-8.02 (m, 2H), 7.24-7.19 (m, 1H), 7.16-7.08 (m, 2H), 6.95-6.85 (m, 2H), 4.98 (t, *J* = 7.2 Hz, 1H), 2.52-2.31 (m, 3H), 2.19-2.08 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.5, 197.1, 140.9, 131.6, 131.5, 127.1, 126.1, 125.4, 116.0, 115.8, 46.5, 40.5, 30.2, 28.5; HRMS calculated for $C_{16}H_{15}FNaO_2S$ (M + Na^+): 313.0674, found: 313.0672. (Yellow oil, 23.2 mg, 70% isolated yield)



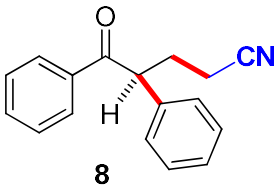
4x

1-phenyl-2-(thiophen-2-yl)hexane-1,5-dione (4x): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.0 Hz, 2H), 7.59-7.50 (m, 1H), 7.50-7.40 (m, 2H), 7.23-7.18 (m, 1H), 6.95-6.86 (m, 2H), 5.02 (t, *J* = 7.2 Hz, 1H), 2.52-2.33 (m, 3H); 2.20-2.02 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.4, 198.7, 141.1, 136.1, 133.4, 128.9, 128.8, 127.0, 126.1, 125.3, 46.5, 40.6, 30.2, 28.6; HRMS calculated for $C_{16}H_{16}NaO_2S$ (M + Na^+): 295.0769, found: 295.0822. (Yellow oil, 30.9 mg, 82% isolated yield)

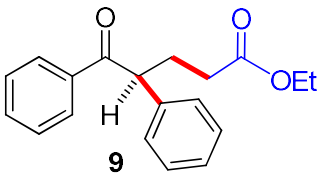
Illustrative synthetic transformations



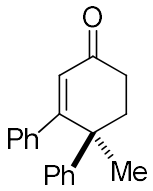
^{1}H and ^{13}C spectra data of compounds 8-11



5-oxo-4,5-diphenylpentanenitrile (8): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, J = 7.2 Hz, 2H), 7.52-7.46 (m, 1H), 7.42-7.38 (m, 2H), 7.36-7.27 (m, 4H), 7.27-7.21 (m, 1H), 4.75-4.72 (m, 1H), 2.52-2.34 (m, 2H); 2.30-2.12 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.3, 137.6, 136.0, 133.4, 129.5, 128.9, 128.7, 128.2, 127.9, 119.4, 52.0, 29.1, 15.3. These data are consistent with literature values, see: X. Chu, H. Meng, Y. Zi, X. Xu and S.-J. Ji, *Org. Chem. Front.,* 2015, **2**, 216. (Pale yellow solid, 24.4 mg, 63% isolated yield)

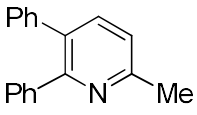


ethyl 5-oxo-4,5-diphenylpentanoate (9): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.4 Hz, 2H), 7.52-7.44 (m, 1H), 7.42-7.35 (m, 2H), 7.33-7.26 (m, 4H), 7.24-7.18 (m, 1H), 4.68 (t, *J* = 7.2 Hz, 1H), 4.10 (q, *J* = 7.6 Hz, 2H); 2.51-2.40 (m, 1H), 2.35-2.26 (m, 2H), 2.21-2.11 (m, 1H), 1.24 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.4, 173.4, 138.9, 136.6, 133.0, 129.1, 128.8, 128.6, 128.4, 127.4, 60.5, 52.5, 31.9, 28.9, 14.3; HRMS calculated for $C_{19}H_{21}O_3$ ($M + H^+$): 297.1491, found: 297.1477. (Pale yellow solid, 16.0 mg, 57% isolated yield)



10

1'-methyl-5',6'-dihydro-[1,1':2',1''-terphenyl]-4'(1'*H*)-one (10): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.43 (m, 2H), 7.41-7.35 (m, 2H), 7.34-7.20 (m, 5H), 7.18-7.00 (m, 2H), 6.43 (m, 1H), 2.40-2.29 (m, 3H), 2.12-2.02 (m, 1H); 1.54 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.0, 166.0, 143.6, 139.1, 129.6, 129.0, 128.8, 128.3, 127.9, 127.0, 126.9, 43.7, 42.0, 34.1, 28.1; HRMS calculated for $C_{19}H_{19}O$ ($M + H^+$): 263.1436, found: 263.1424. (Pale yellow solid, 32.3 mg, 78% isolated yield)



11

6-methyl-2,3-diphenylpyridine (11): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.6 Hz, 1H), 7.38-7.30 (m, 2H), 7.26-7.01 (m, 9H), 2.66 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 156.6, 140.5, 140.1, 138.9, 133.2, 130.0, 129.7, 128.3, 128.0, 127.7, 127.0, 121.8, 24.5. These data are consistent with literature values, see: X. Chu, H. Meng, Y. Zi, X. Xu and S.-J. Ji, *Chem. Eur. J.,* 2014, **20**, 17198. (Pale yellow solid, 30.6 mg, 62% isolated yield)

On-off swithching of the visible light irradiation

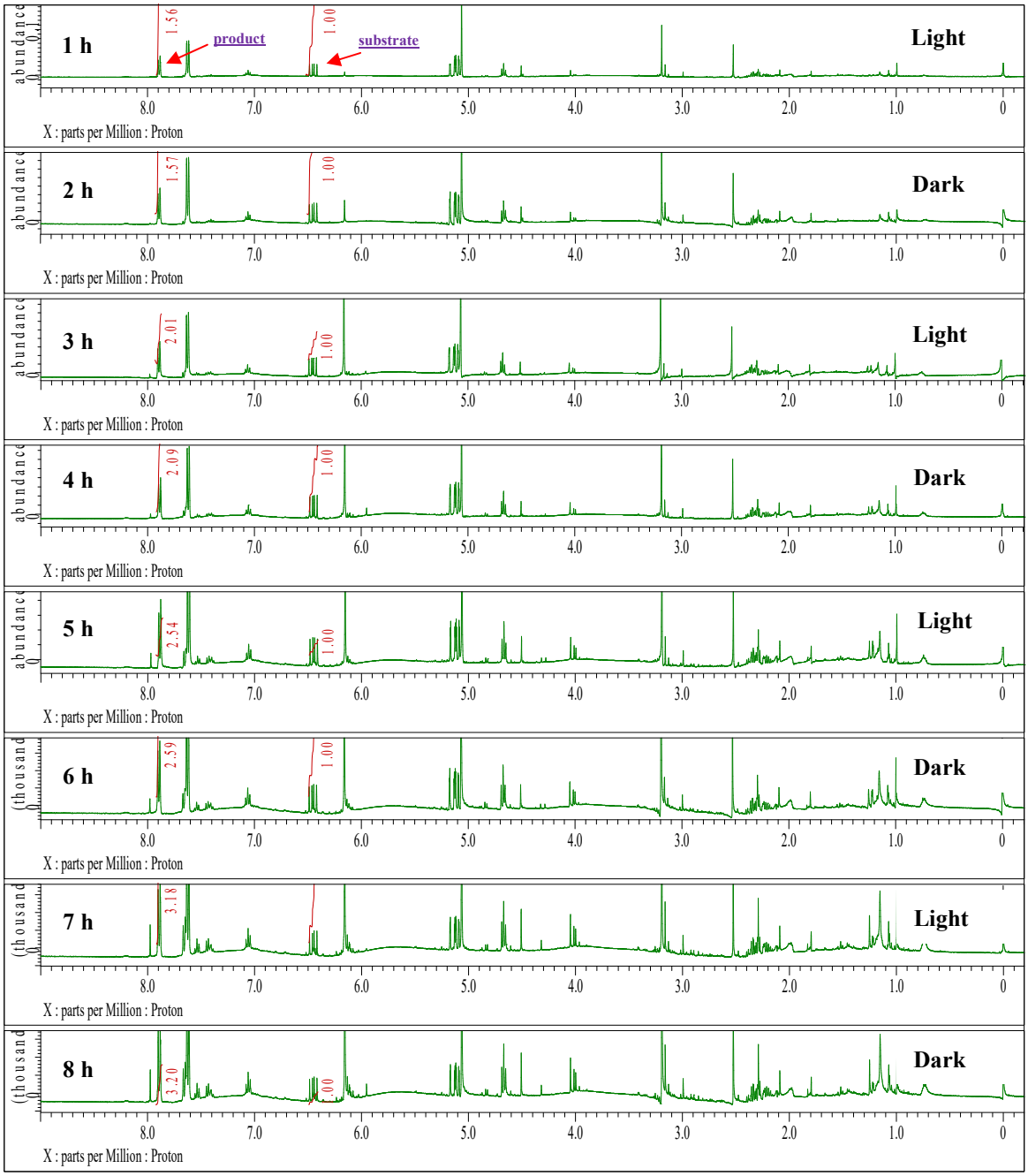


Figure (a). ^{1}H NMR spectra copies of reaction of **1a** and acetone with different reaction time

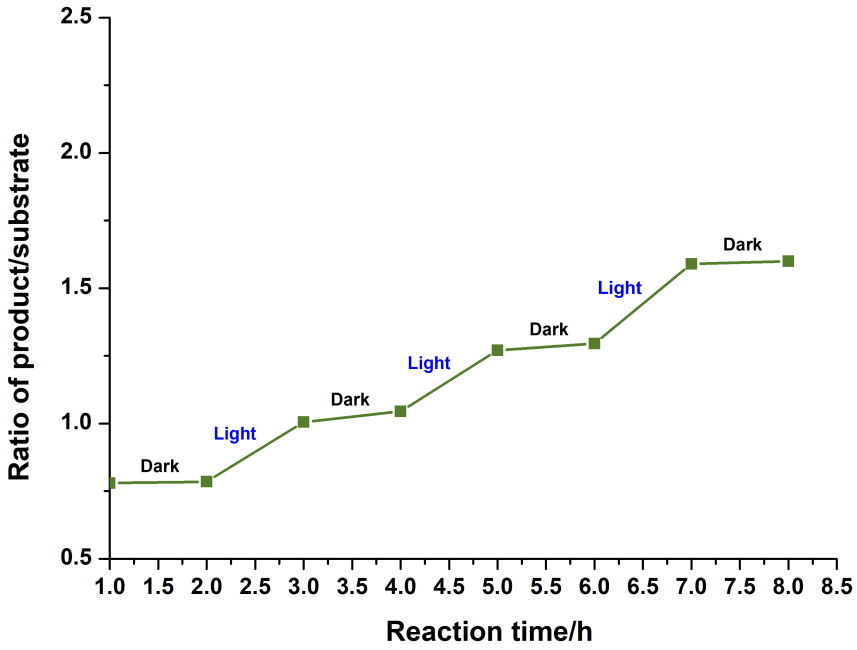


Figure (b). Time profile of visible-light-enabled oxidative alkylarylation of **1a** and acetone

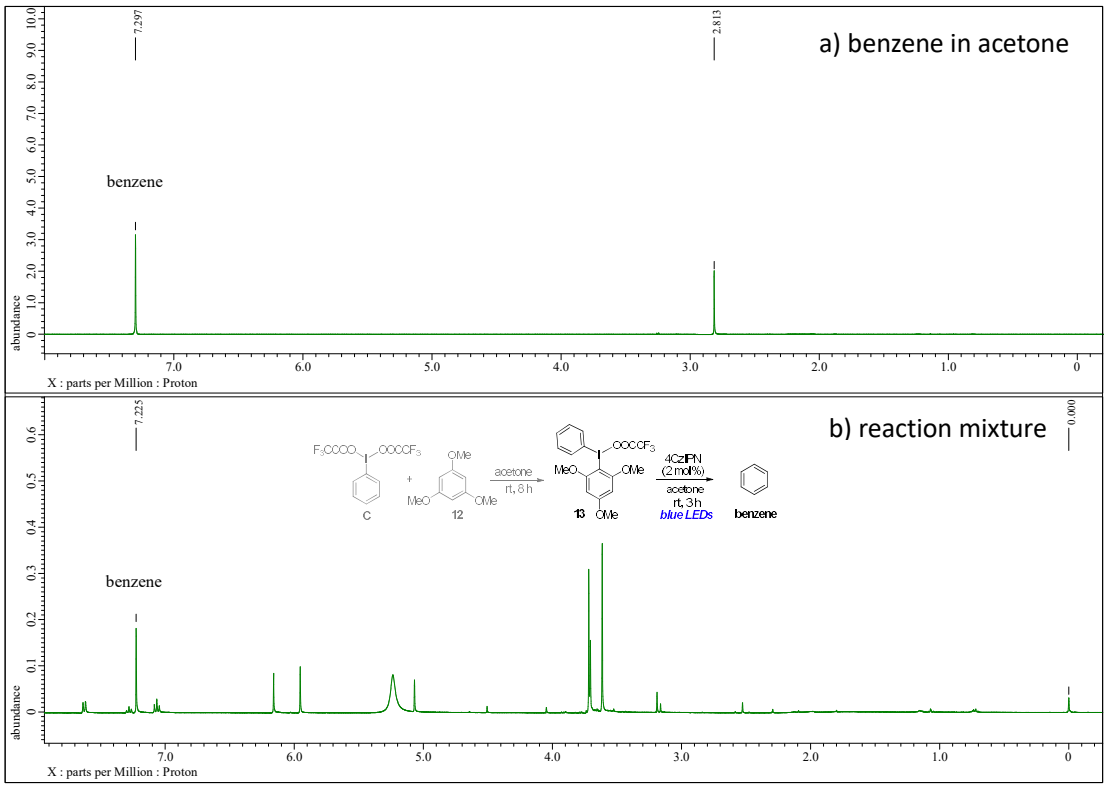
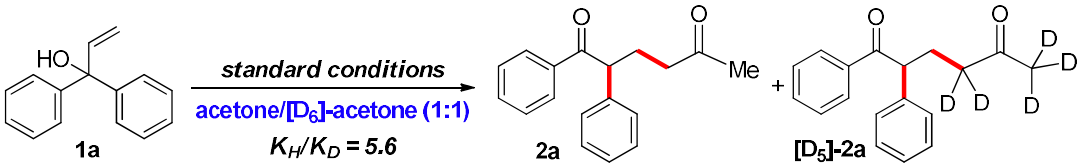
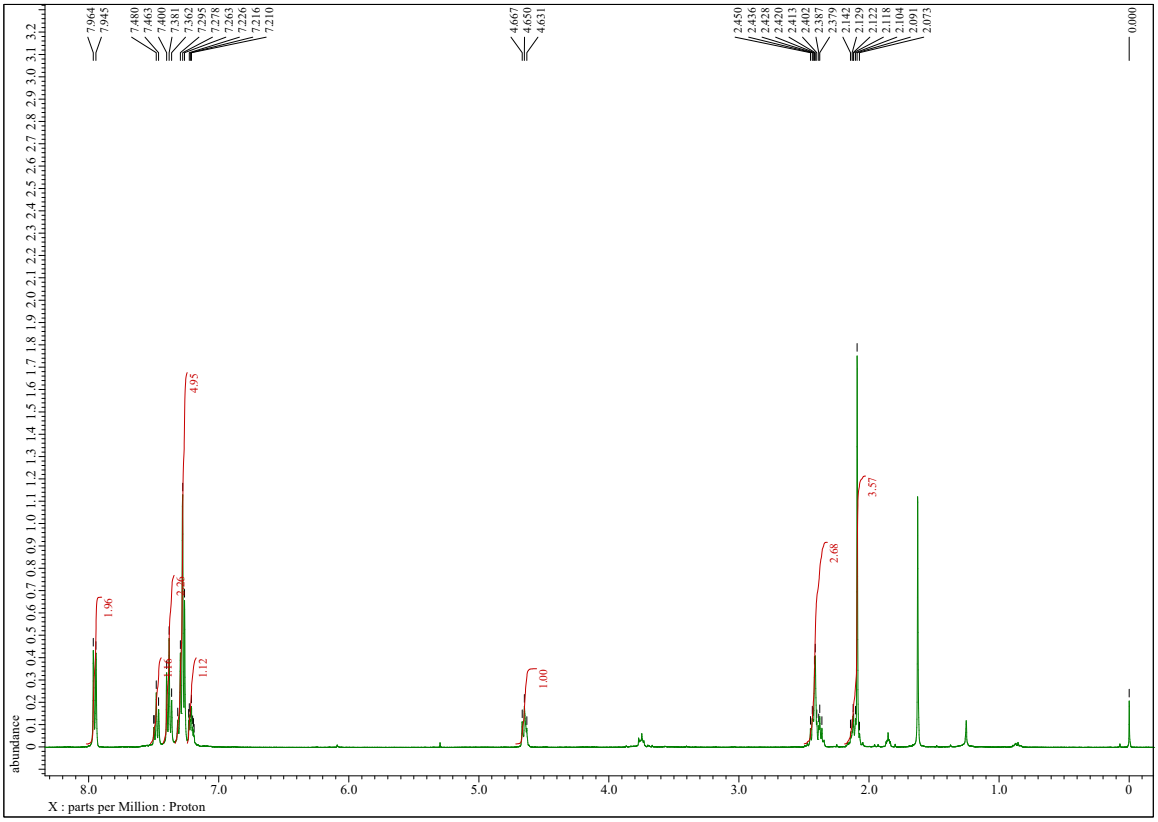


Figure (c). The experiment to confirm the generation of benzene

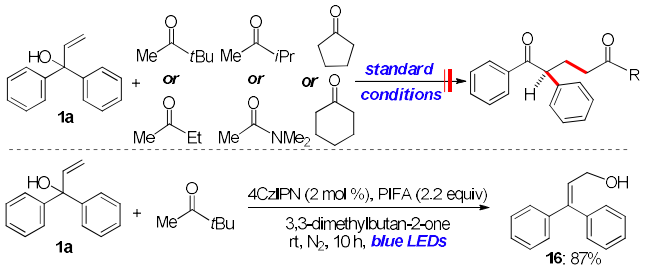
Experiment on kinetic isotope effect





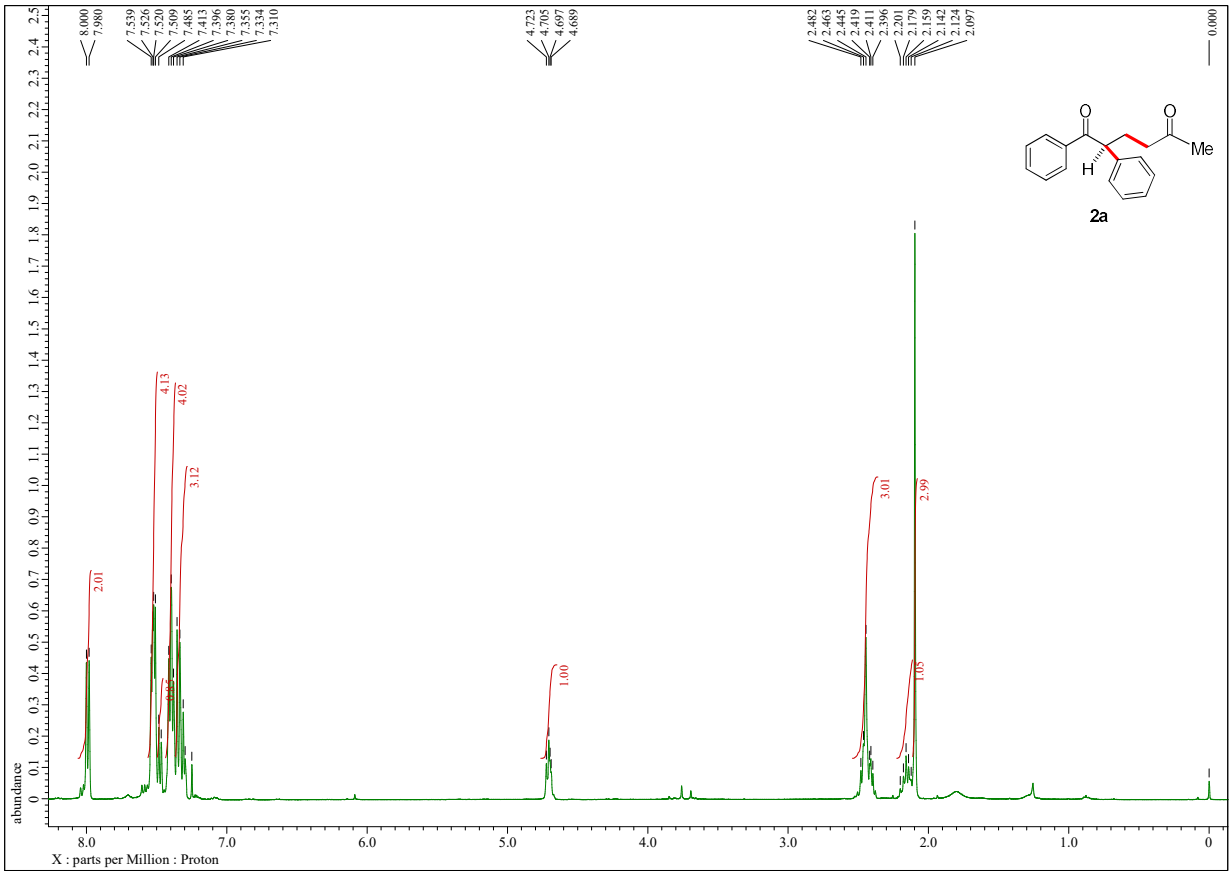
A significant kinetic isotope effect (K_H/K_D = 5.6) was observed in the model reaction, which provided a direct evidence that the event of C-H bond cleavage might have constituted a rate-determining step.

Examinations of other ketones and amides under standard reaction conditions



In this work, other ketones and amides, such as butan-2-one and 3,3-dimethylbutan-2-one, and *N*,*N*-dimethylacetamide, had also been carefully examined. However, we did not obtain the desired products under standard reaction conditions.

Copies of ^{1}H NMR and ^{13}C NMR spectra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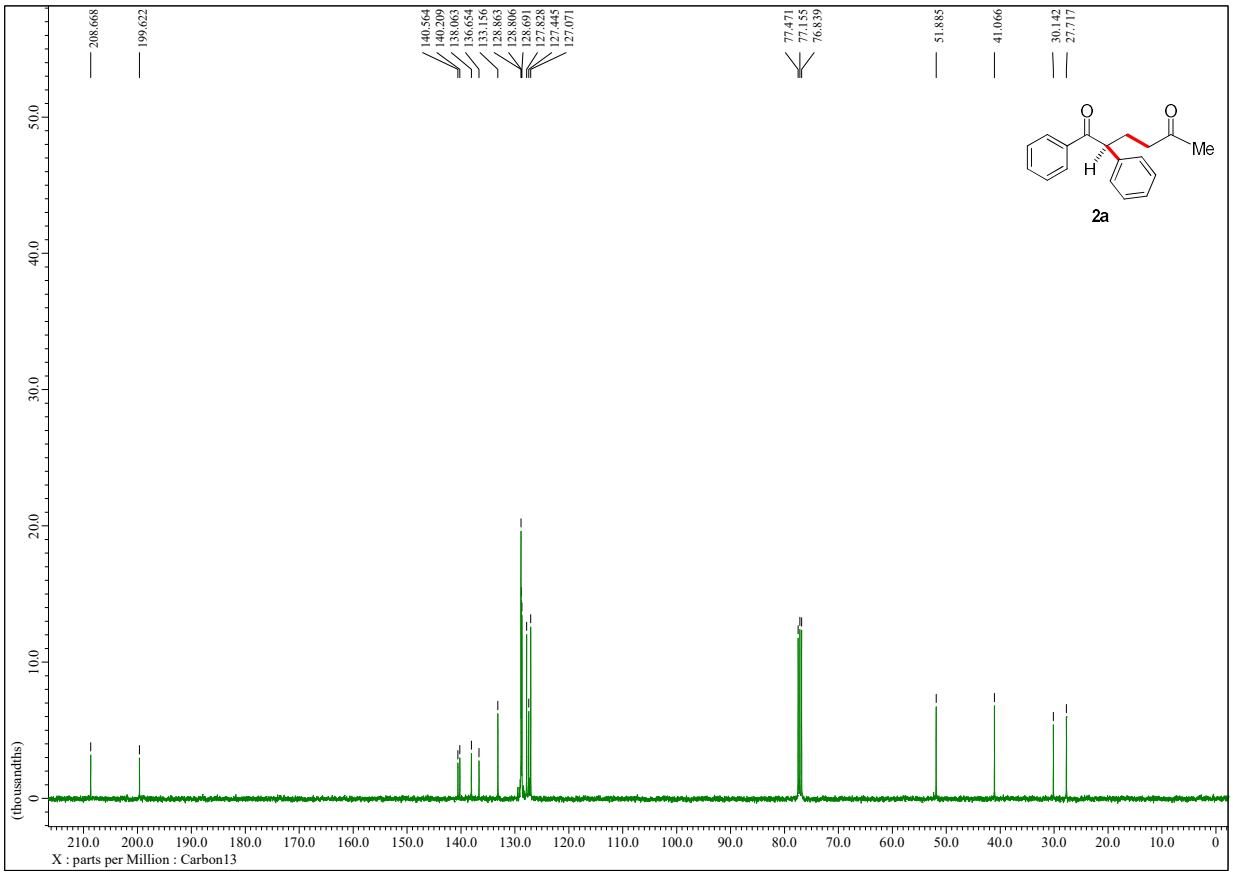
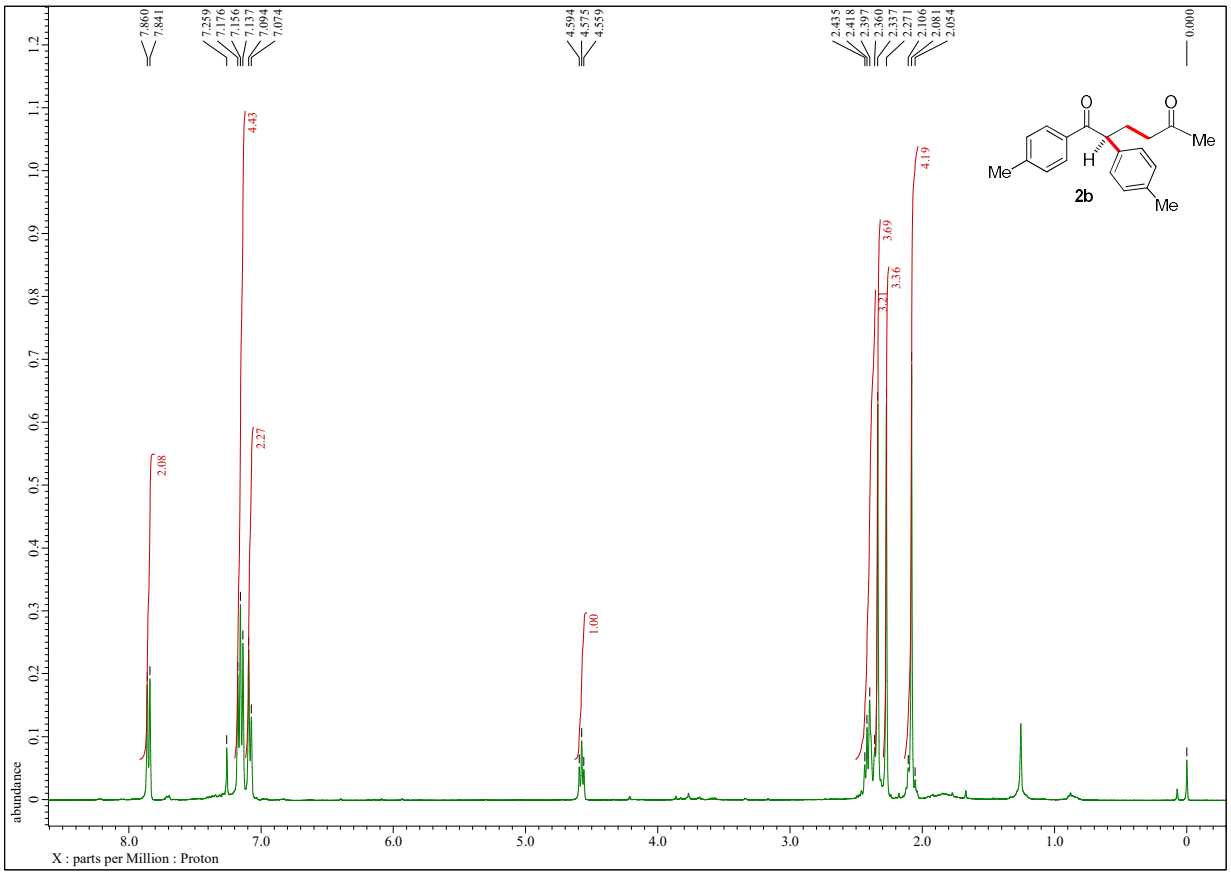
7.980
7.539
7.526
7.520
7.509
7.485
7.413
7.396
7.380
7.355
7.334
7.310
4.723
4.705
4.697
4.689
2.482
2.463
2.445
2.419
2.411
2.396
2.201
2.179
2.159
2.142
2.124
2.097
0.000
4.13
4.02
3.12
2.01
1.00
3.01
2.99
1.05
abundance
X : parts per Million : Proton
O
O
Me
H
2a


208.668
199.622
140.564
140.209
138.063
136.654
133.156
128.863
128.806
128.691
127.828
127.445
127.071
77.471
77.155
76.839
51.885
41.066
30.142
27.717
(thousandths)
X : parts per Million : Carbon13
O
O
Me
H
2a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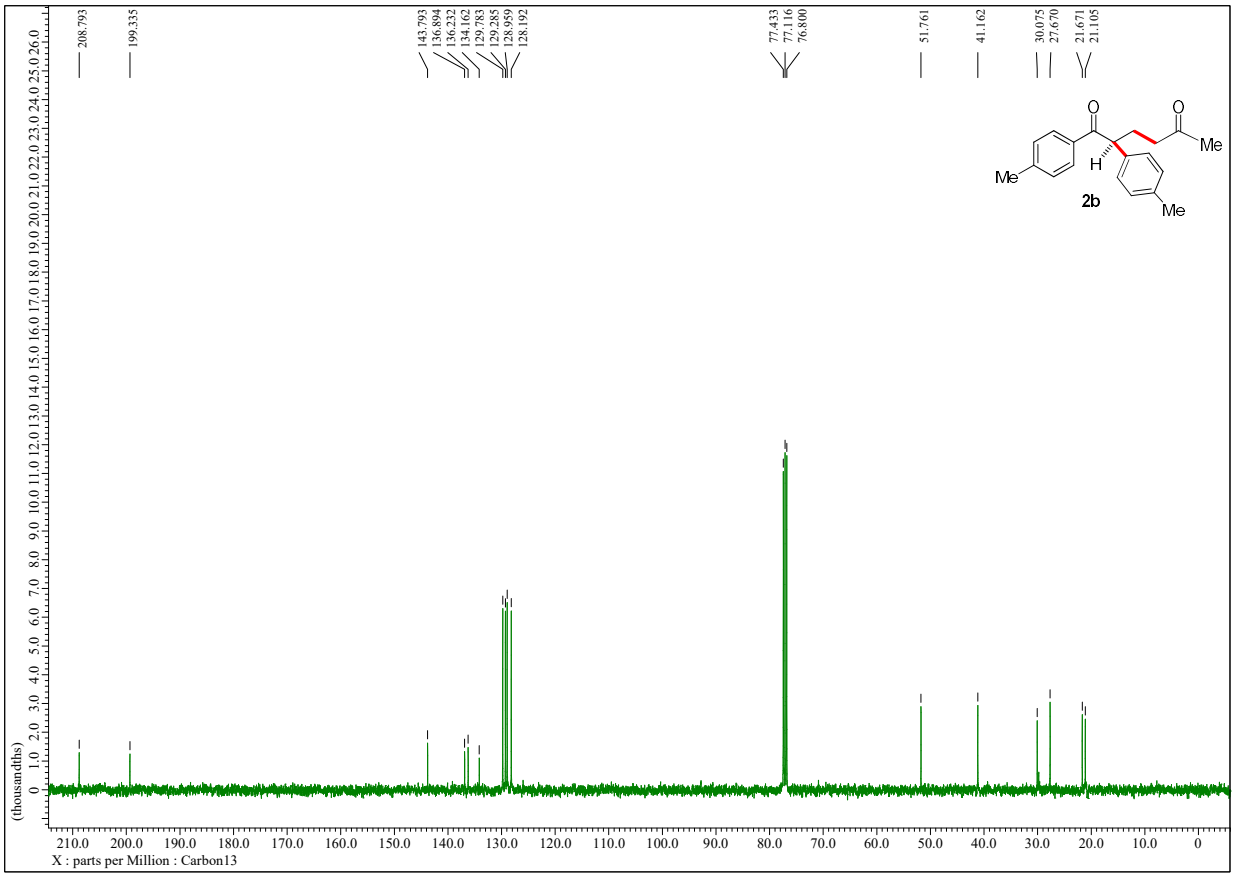
7.841
7.259
7.176
7.156
7.137
7.094
7.074
4.594
4.575
4.559
2.435
2.418
2.397
2.360
2.337
2.271
2.106
2.081
2.054
0.000
4.43
4.19
3.69
3.36
3.21
2.27
2.08
1.00
O
O
Me
H
Me
Me
2b
abundance
X : parts per Million : Proton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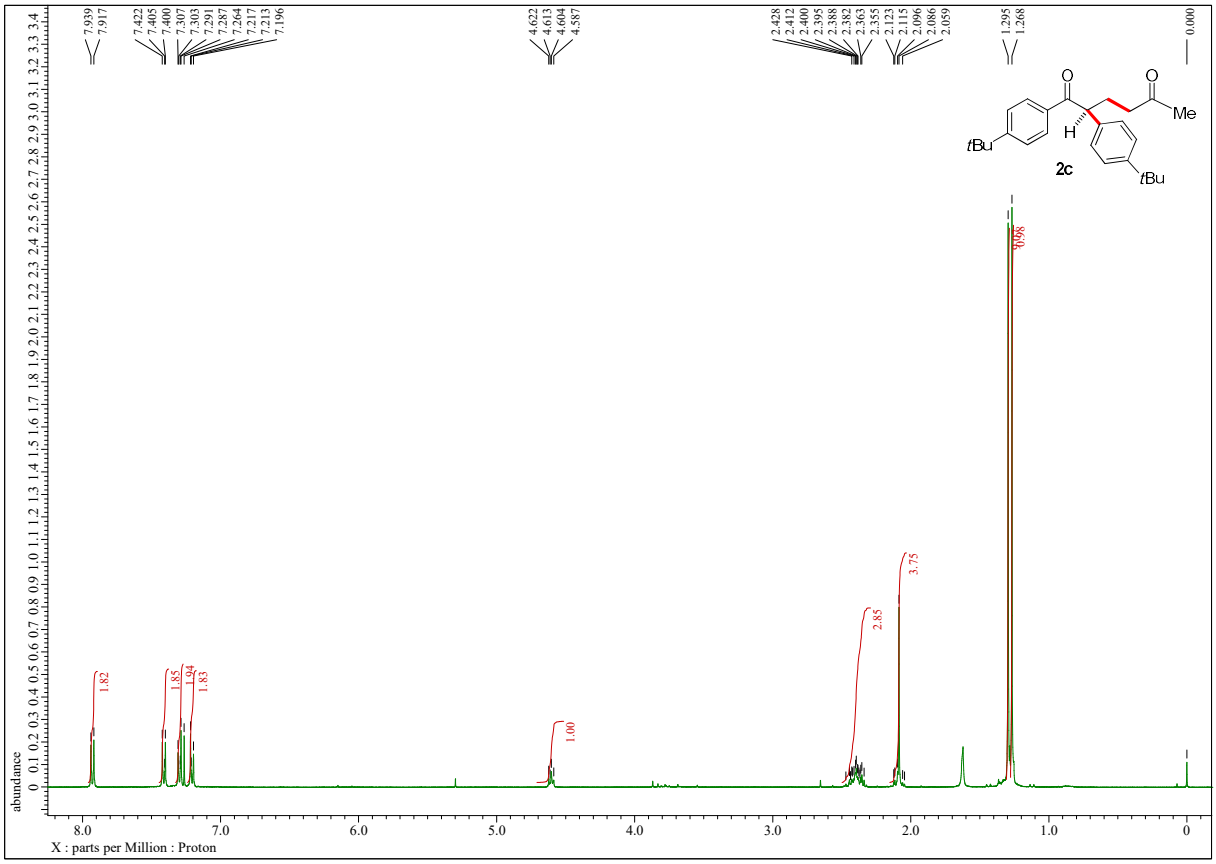
199.335
143.793
136.894
136.232
134.162
129.783
129.285
128.959
128.192
77.433
77.116
76.800
51.761
41.162
30.075
27.670
21.671
21.105
O
O
Me
H
Me
Me
2b
(thousandths)
X : parts per Million : Carbon13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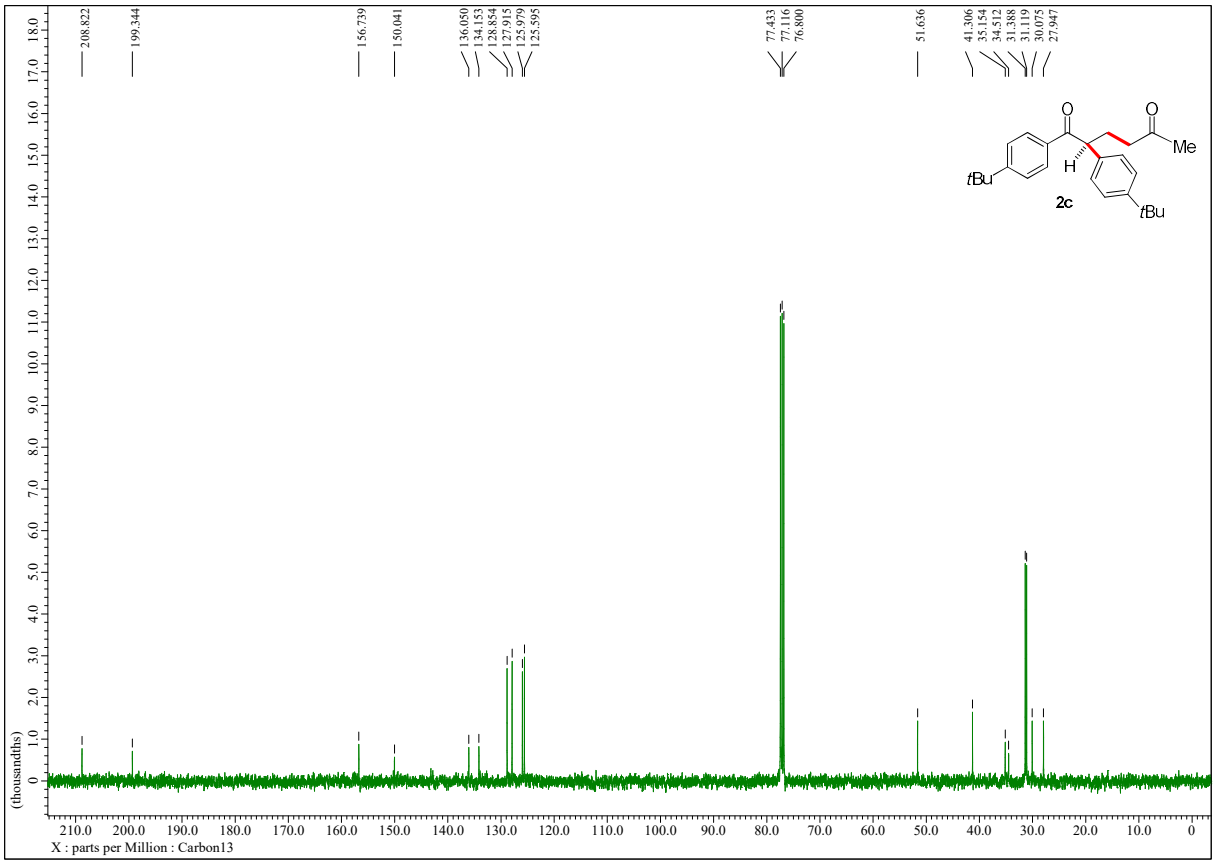
7.917
7.422
7.405
7.400
7.307
7.303
7.291
7.287
7.264
7.217
7.213
7.196
4.622
4.613
4.604
4.587
2.428
2.412
2.400
2.395
2.388
2.382
2.363
2.355
2.123
2.115
2.096
2.086
2.059
1.295
1.268
0.000
1.82
1.85
1.94
1.83
1.00
2.85
3.75
9.00
9.98
O
O
Me
H
tBu
tBu
2c
abundance
X : parts per Million : Proton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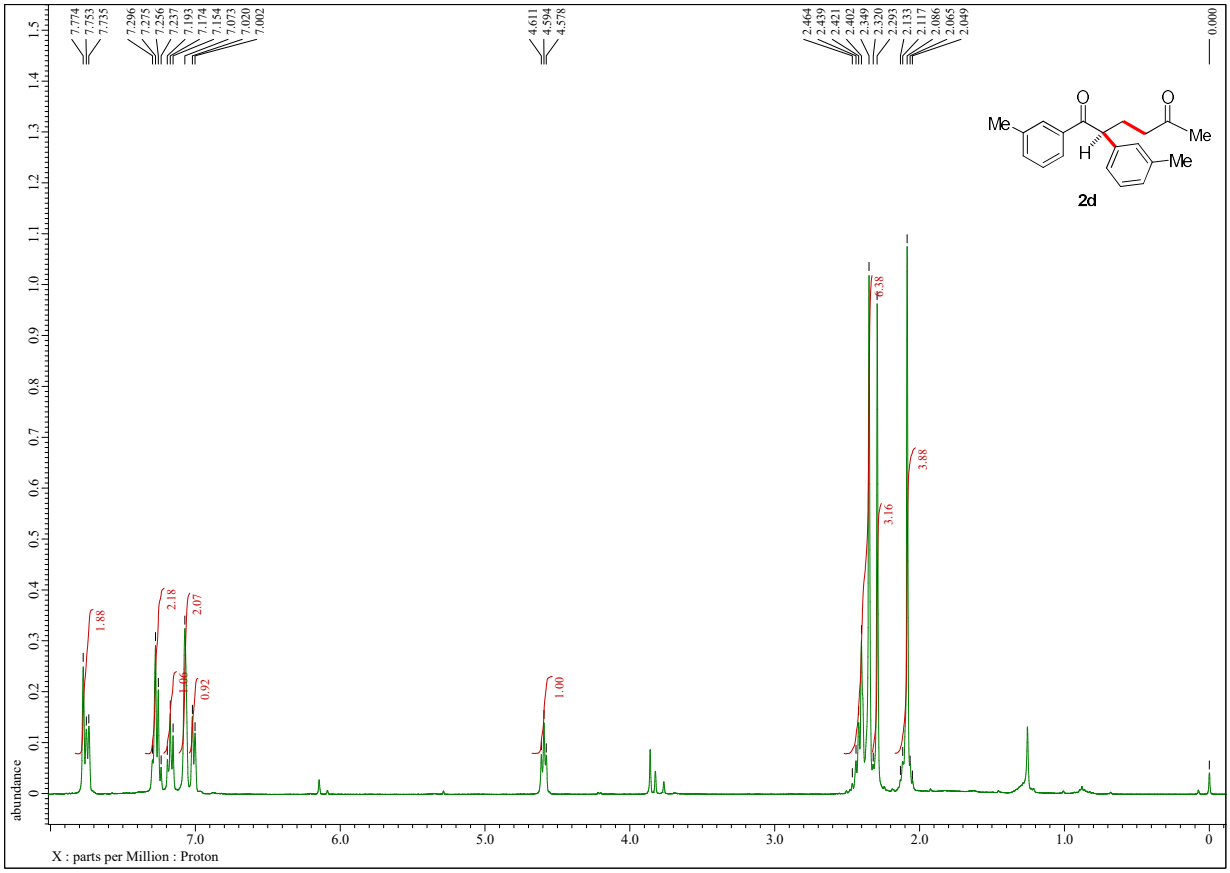
199.344
156.739
150.041
136.050
134.153
128.854
127.915
125.979
125.595
77.433
77.116
76.800
51.636
41.306
35.154
34.512
31.388
31.119
30.075
27.947
O
O
Me
H
tBu
tBu
2c
(thousandths)
X : parts per Million : Carbon13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7.735
7.296
7.275
7.256
7.237
7.193
7.174
7.154
7.073
7.020
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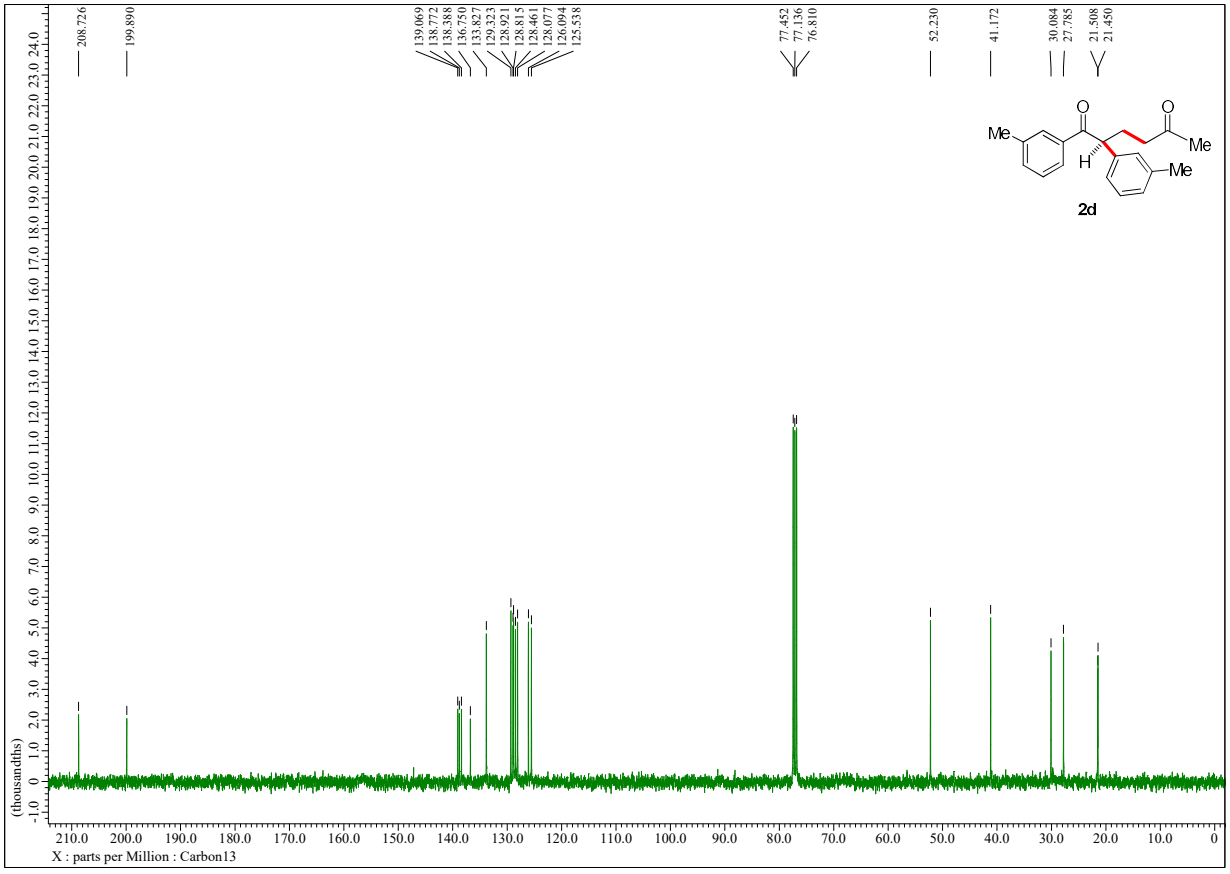
4.594
4.578
2.464
2.439
2.421
2.402
2.349
2.320
2.293
2.133
2.117
2.086
2.065
2.049
0.000
Me
O
O
Me
H
Me
2d
1.88
2.18
2.07
1.06
0.92
1.00
6.38
3.16
3.88
abundance
X : parts per Million : Proton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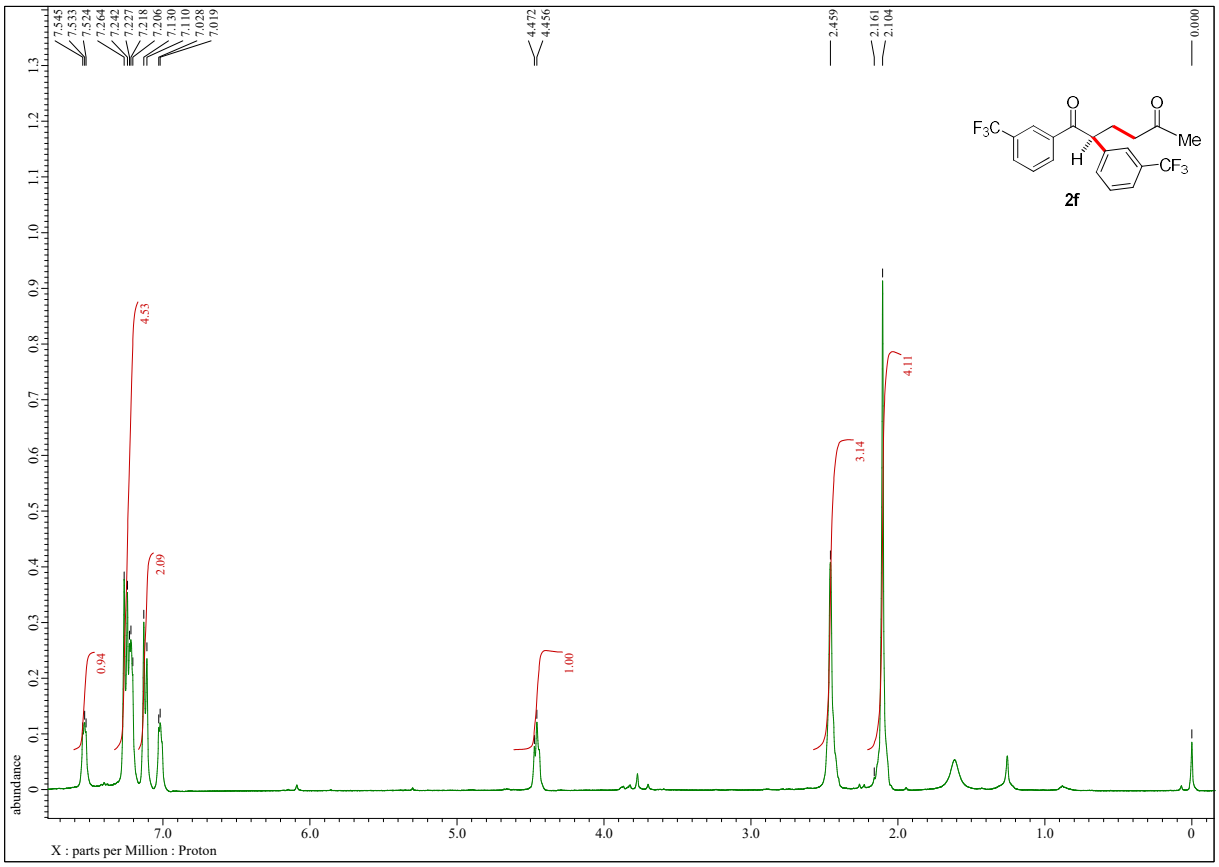
126.094
125.538
77.452
77.136
76.810
52.230
41.172
30.084
27.785
21.508
21.450
Me
O
O
Me
H
Me
2d
(thousandths)
X : parts per Million : Carbon13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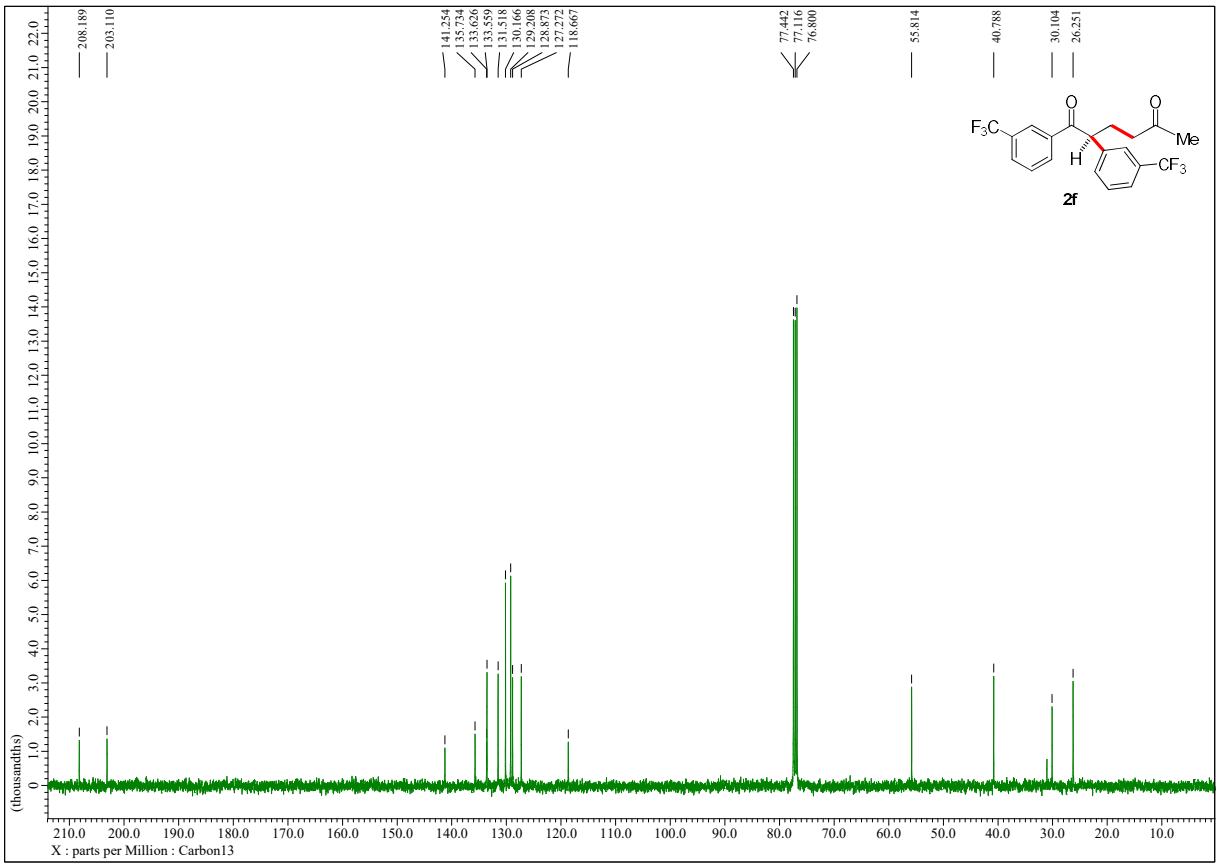
7.524
7.264
7.242
7.227
7.218
7.206
7.130
7.110
7.028
7.019
4.472
4.456
2.459
2.161
2.104
0.000
F3C
O
O
Me
H
CF3
2f
4.53
4.11
3.14
2.09
0.94
1.00
abundance
X : parts per Million : Proton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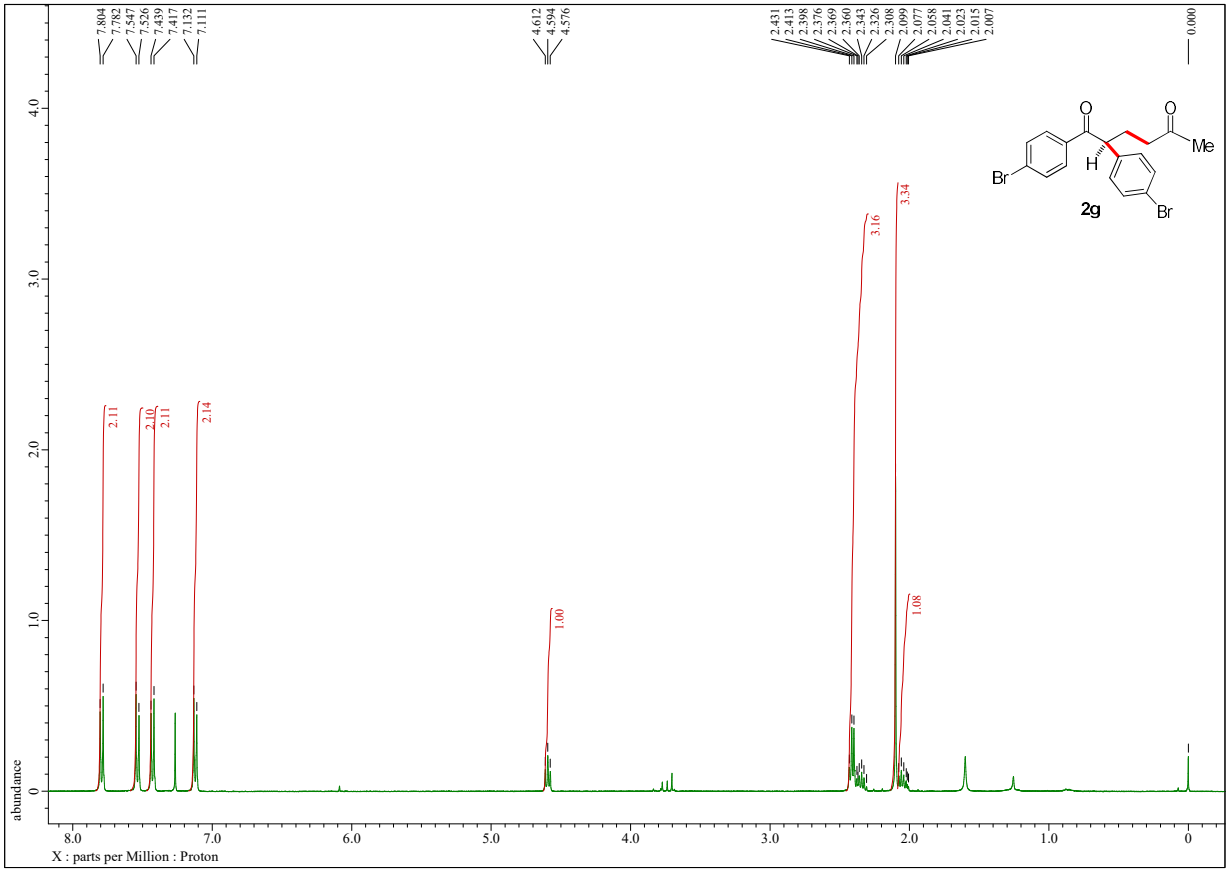
203.110
141.254
135.734
133.626
133.559
131.518
130.166
129.208
128.873
127.272
118.667
77.442
77.116
76.800
55.814
40.788
30.104
26.251
F3C
O
O
Me
H
CF3
2f
(thousandths)
X : parts per Million : Carbon13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7.526
7.439
7.417
7.132
7.111
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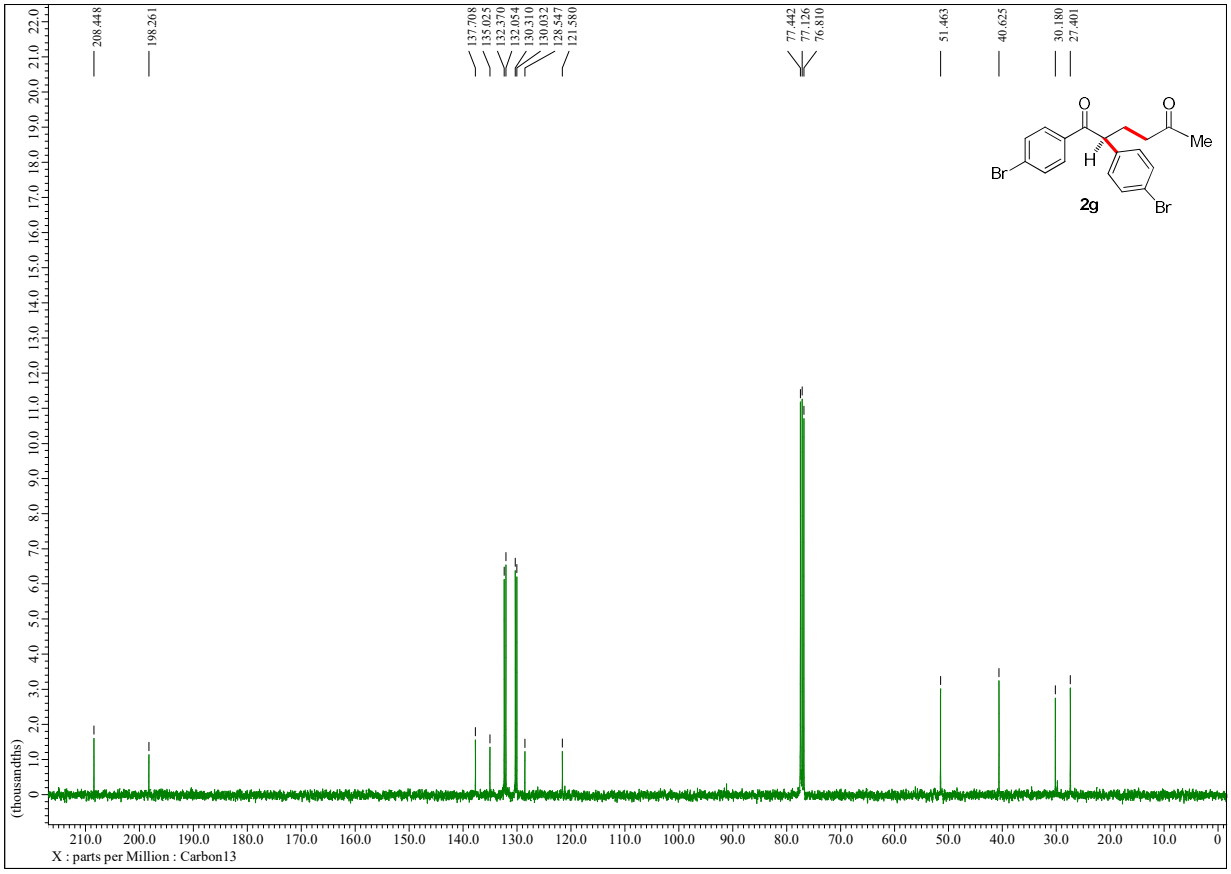
4.594
4.576
2.431
2.413
2.398
2.376
2.369
2.360
2.343
2.326
2.308
2.099
2.077
2.058
2.041
2.023
2.015
2.007
0.000
2.11
2.10
2.11
2.14
1.00
3.16
3.34
1.08
O
O
Me
H
Br
Br
2g
abundance
X : parts per Million : Proton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132.054
130.310
130.032
128.547
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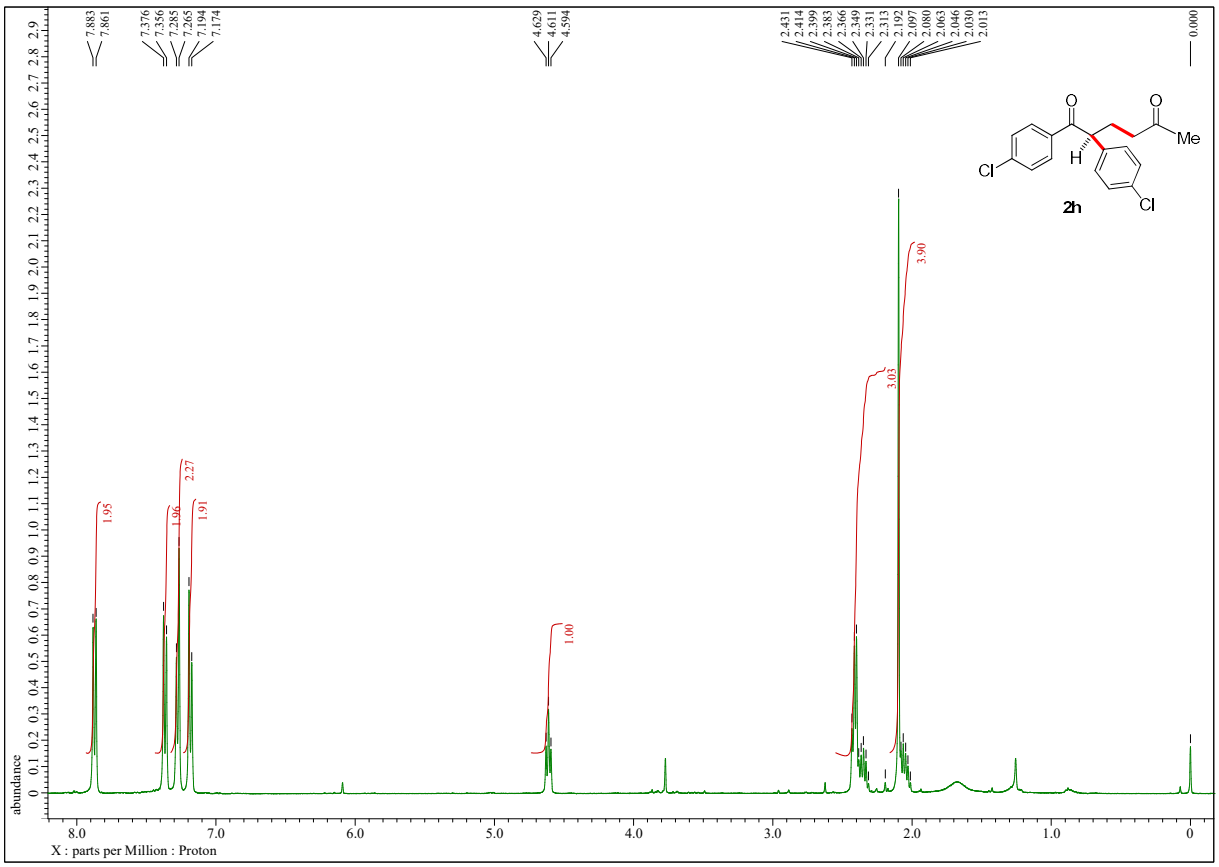
77.442
77.126
76.810
51.463
40.625
30.180
27.401
O
O
Me
H
Br
Br
2g
(thousandths)
X : parts per Million : Carbon13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7.285
7.265
7.194
7.174
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4.611
4.594
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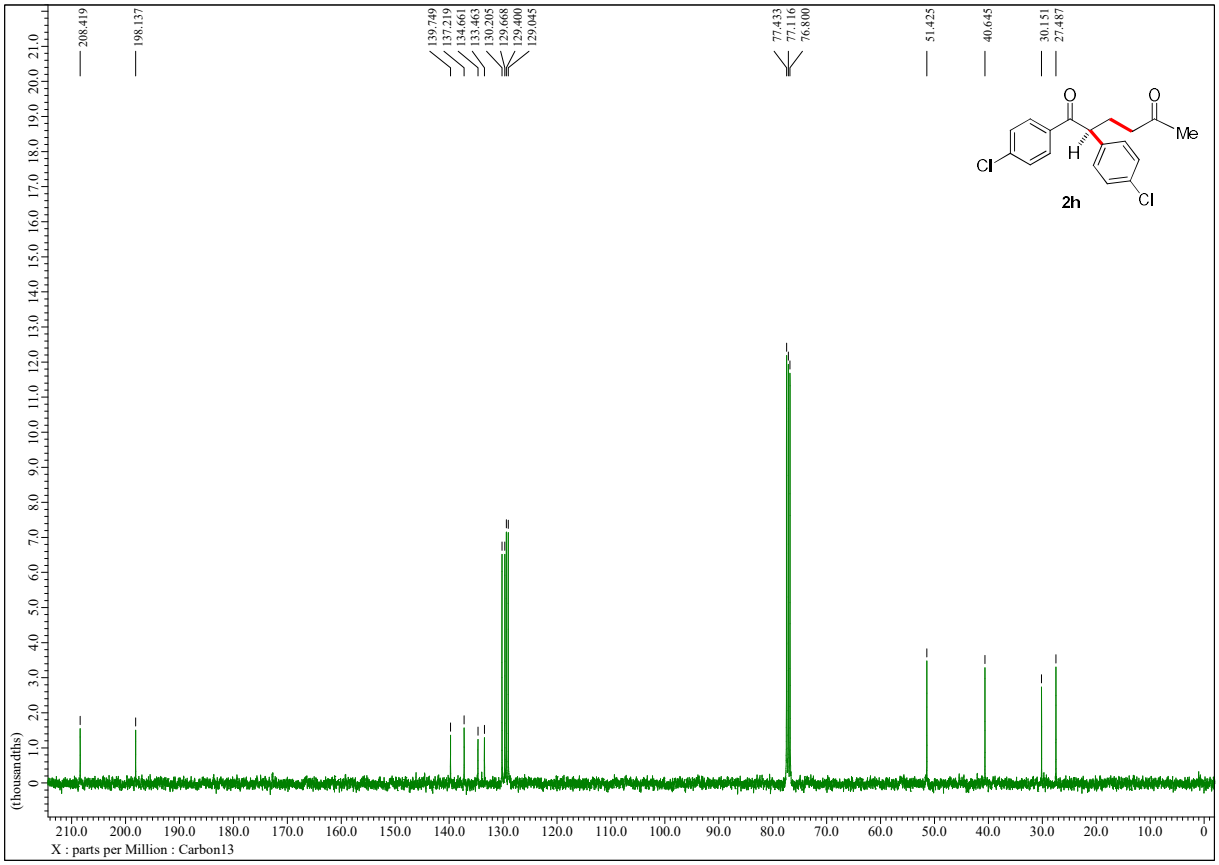
2.414
2.399
2.383
2.366
2.349
2.331
2.313
2.192
2.097
2.080
2.063
2.046
2.030
2.013
0.000
1.95
1.96
2.27
1.91
1.00
3.03
3.90
abundance
X : parts per Million : Proton
O
O
Me
H
Cl
Cl
2h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133.463
130.205
129.668
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129.045
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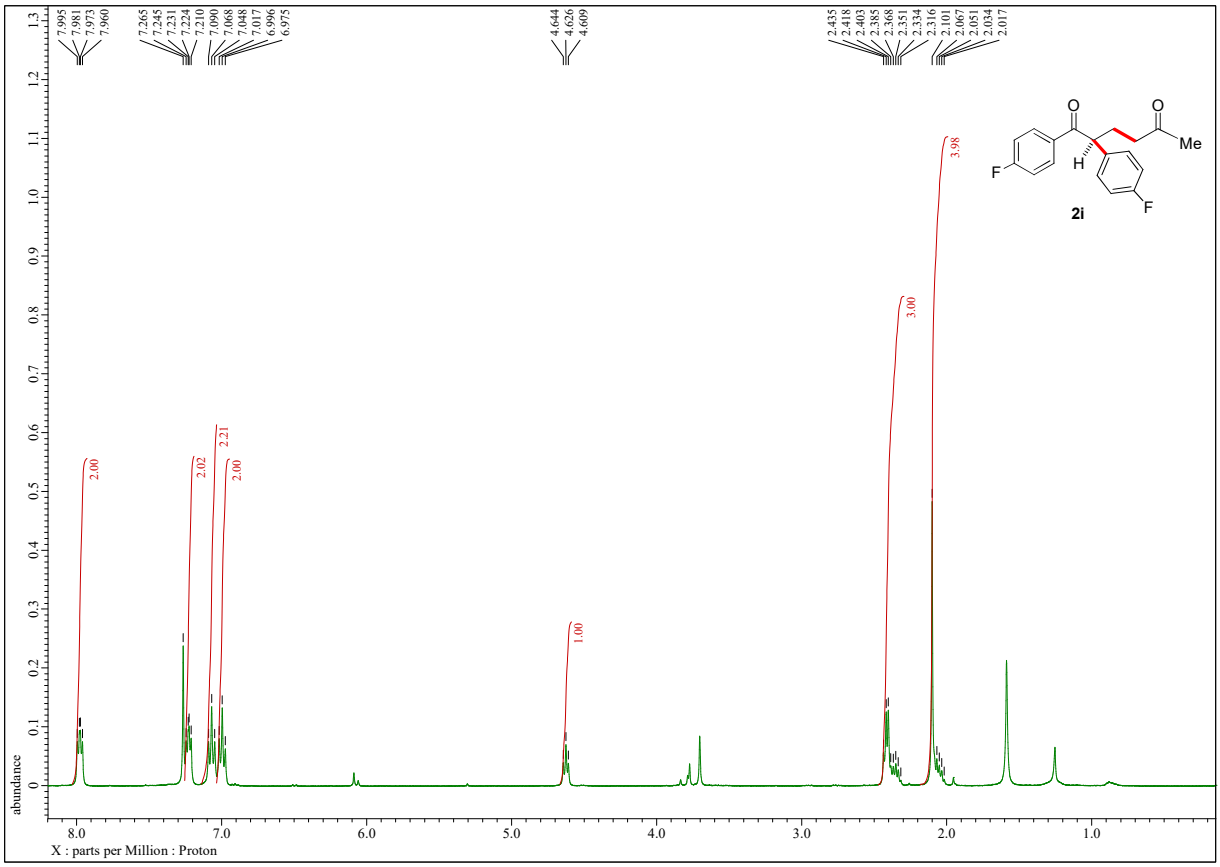
77.116
76.800
51.425
40.645
30.151
27.487
(thousandths)
X : parts per Million : Carbon13
O
O
Me
H
Cl
Cl
2h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7.090
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2.316
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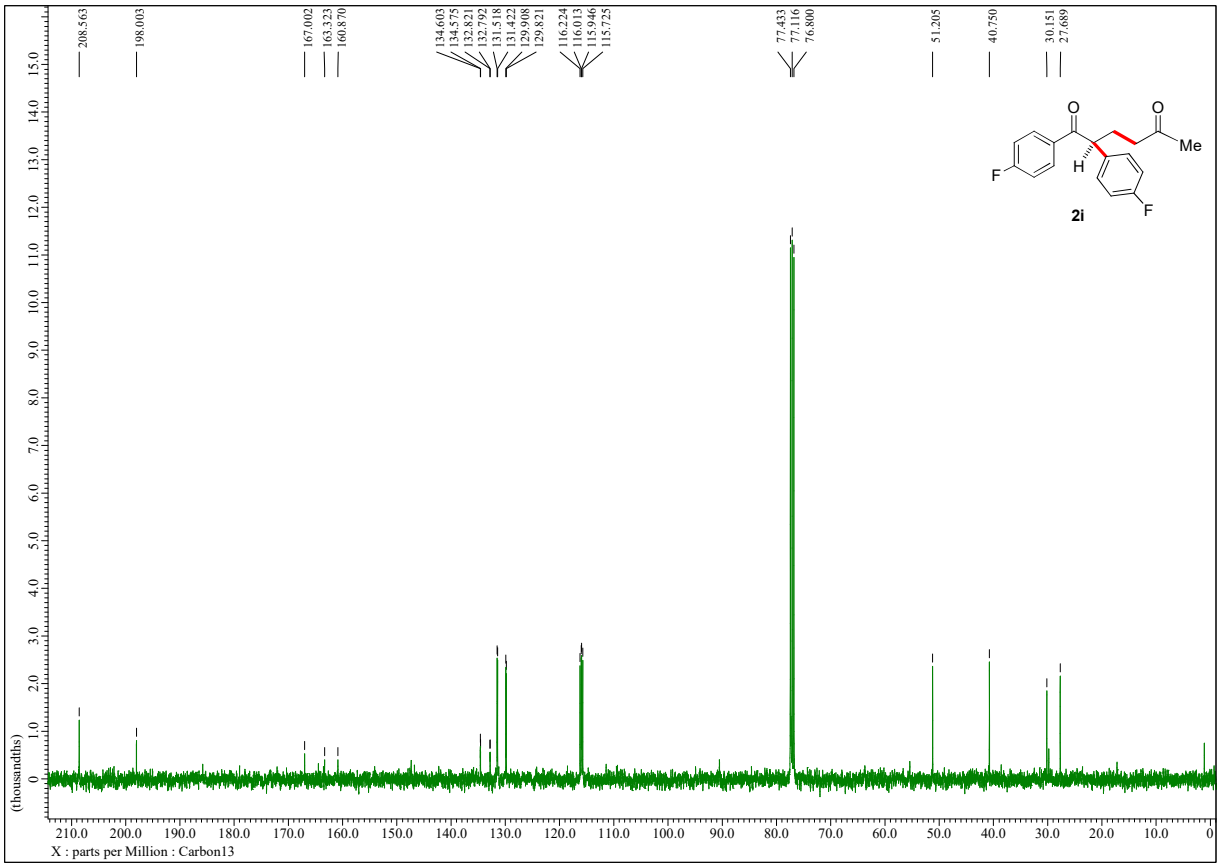
2.067
2.051
2.034
2.017
2.00
2.02
2.21
2.00
1.00
3.00
3.98
O
O
Me
H
F
F
2i
abundance
X : parts per Million : Proton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160.870
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134.575
132.821
132.792
131.518
131.422
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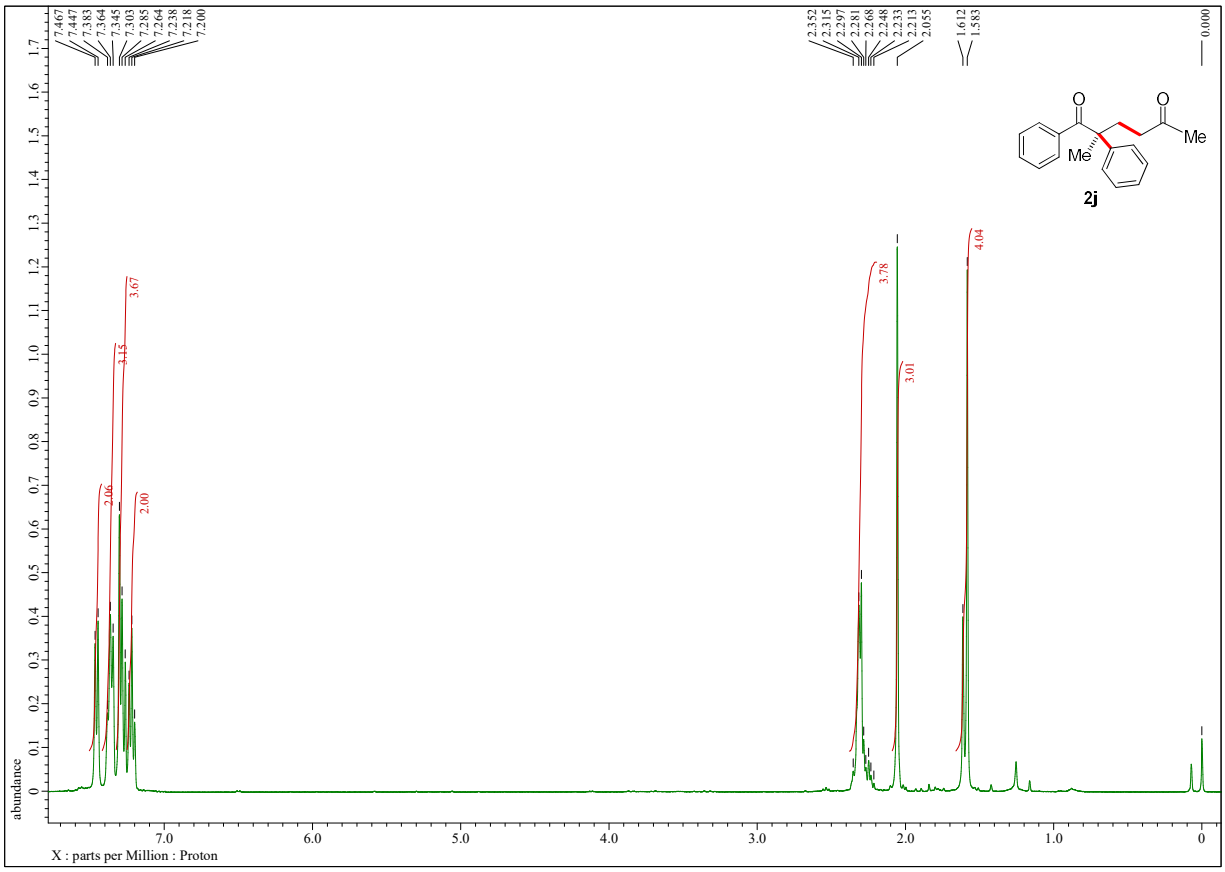
116.224
116.013
115.946
115.725
77.433
77.116
76.800
51.205
40.750
30.151
27.689
O
O
Me
H
F
F
2i
(thousandths)
X : parts per Million : Carbon13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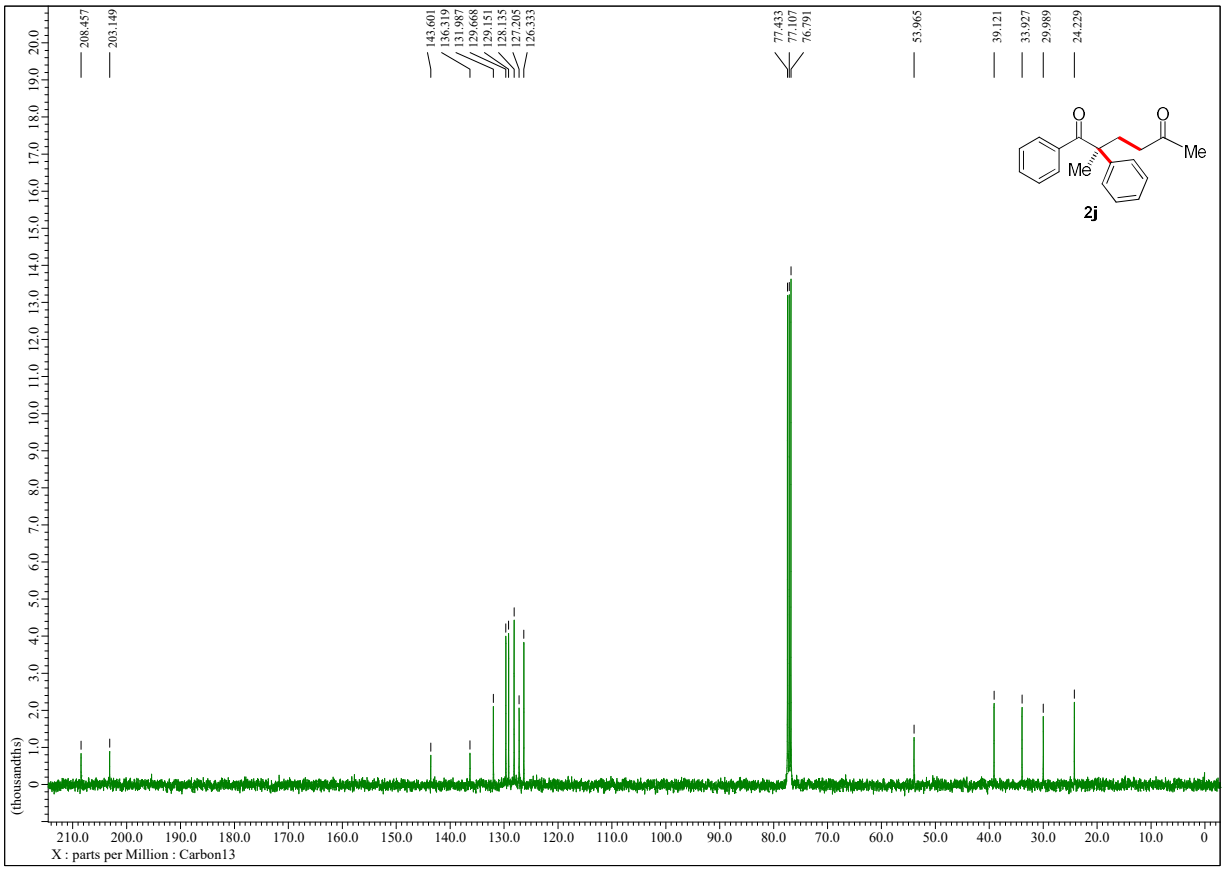
7.447
7.383
7.364
7.345
7.303
7.285
7.264
7.238
7.218
7.200
2.352
2.315
2.297
2.281
2.268
2.248
2.233
2.213
2.055
1.612
1.583
0.000
Me
Me
2j
3.67
3.15
2.06
2.00
3.78
3.01
4.04
abundance
X : parts per Million : Proton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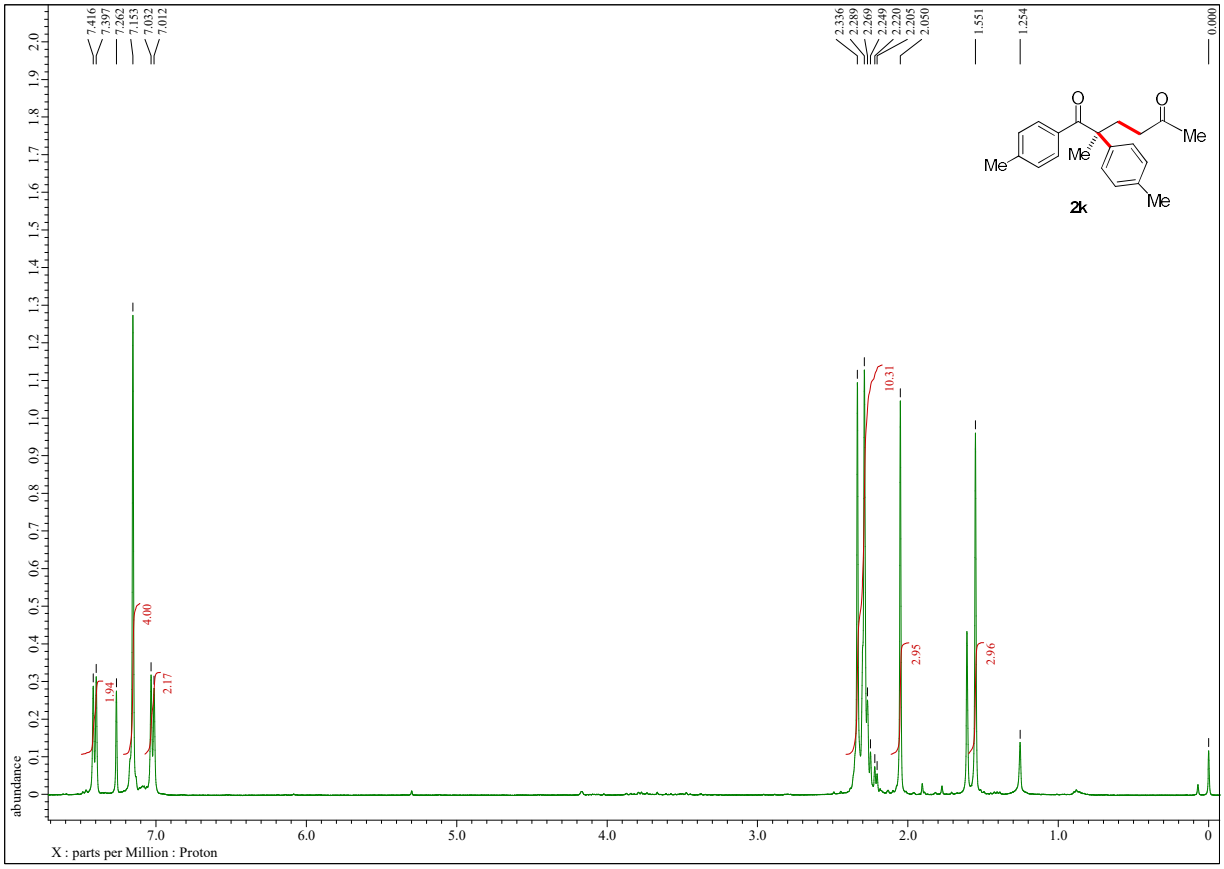
203.149
143.601
136.319
131.987
129.668
129.151
128.135
127.205
126.333
77.433
77.107
76.791
53.965
39.121
33.927
29.989
24.229
Me
Me
2j
(thousandths)
X : parts per Million : Carbon13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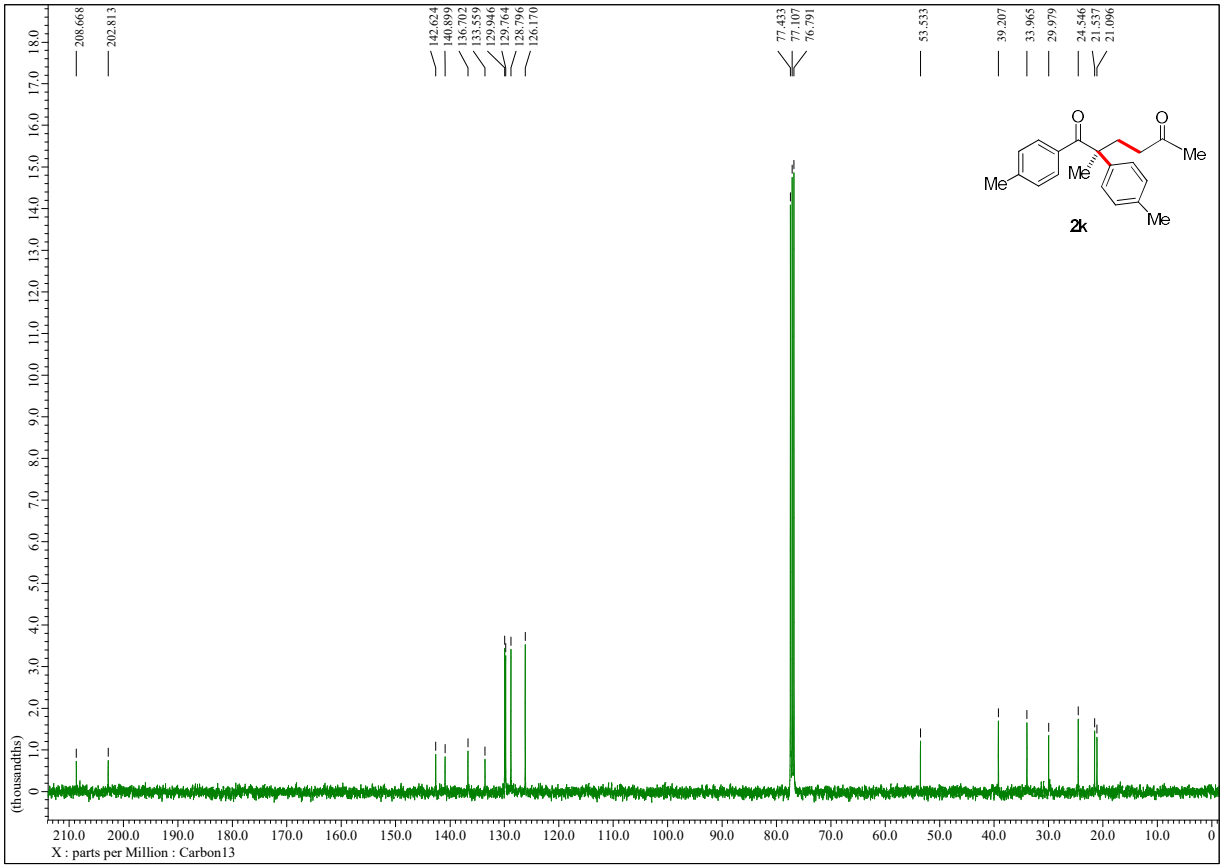
7.397
7.262
7.153
7.032
7.012
2.336
2.289
2.269
2.249
2.220
2.205
2.050
1.551
1.254
0.000
Me
Me
Me
Me
2k
10.31
4.00
2.95
2.96
1.94
2.17
abundance
X : parts per Million : Proton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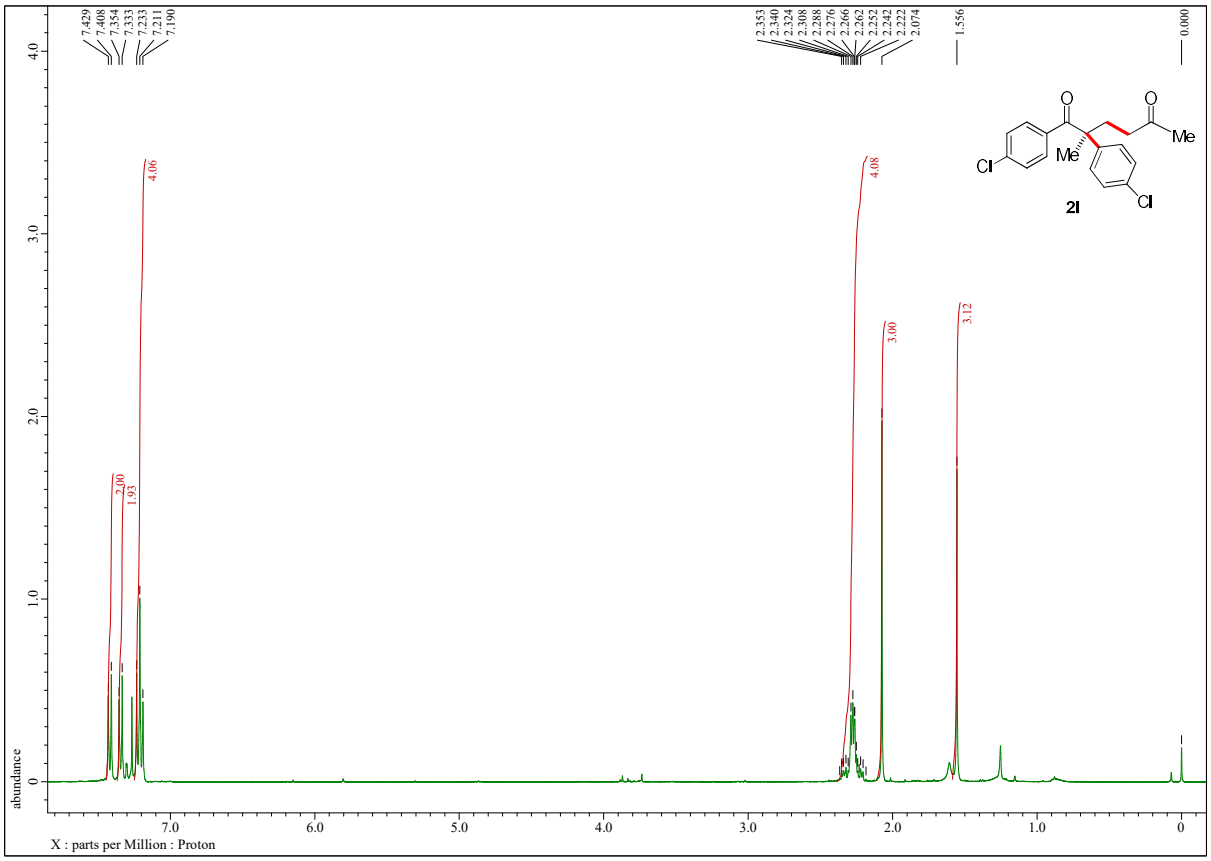
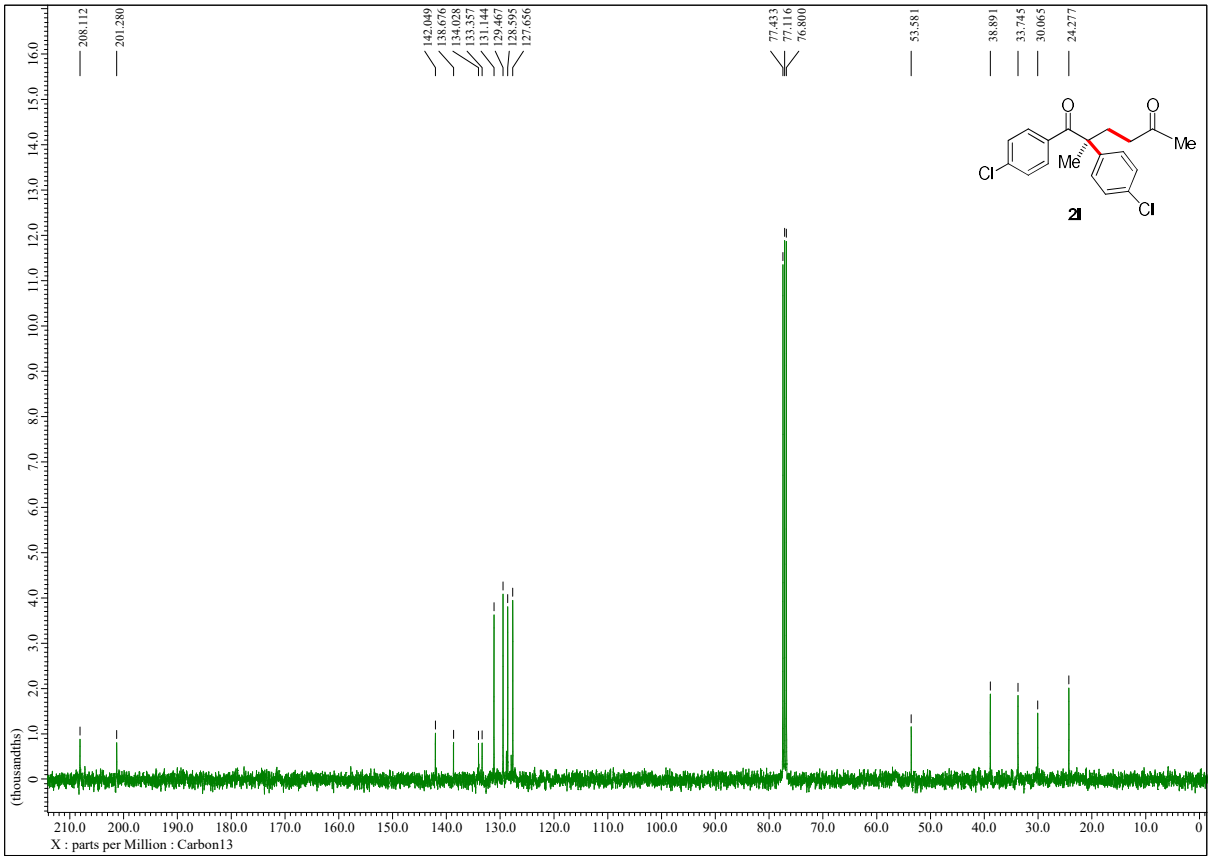
202.813
142.624
140.899
136.702
133.559
129.946
129.764
128.796
126.170
77.433
77.107
76.791
53.533
39.207
33.965
29.979
24.546
21.537
21.096
Me
Me
Me
Me
2k
(thousandths)
X : parts per Million : Carbon13


7.429
7.408
7.354
7.333
7.233
7.211
7.190
2.353
2.340
2.324
2.308
2.288
2.276
2.266
2.262
2.252
2.242
2.222
2.074
1.556
0.000
4.06
4.08
3.00
3.12
2.00
1.93
abundance
X : parts per Million : Proton
Cl
Me
O
Me
Cl
2l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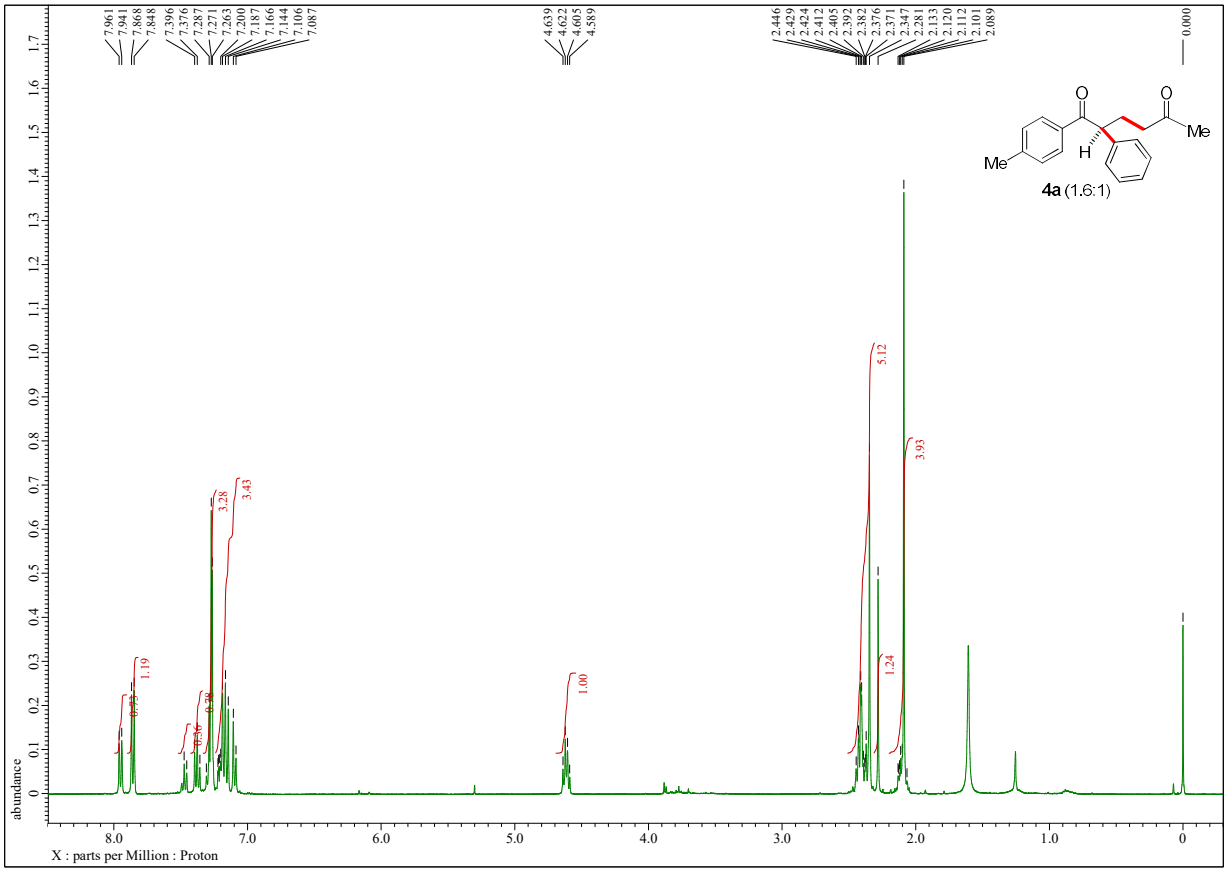
201.280
142.049
138.676
134.028
133.357
131.144
129.467
128.595
127.656
77.433
77.116
76.800
53.581
38.891
33.745
30.065
24.277
(thousandths)
X : parts per Million : Carbon13
Cl
Me
O
Me
Cl
2l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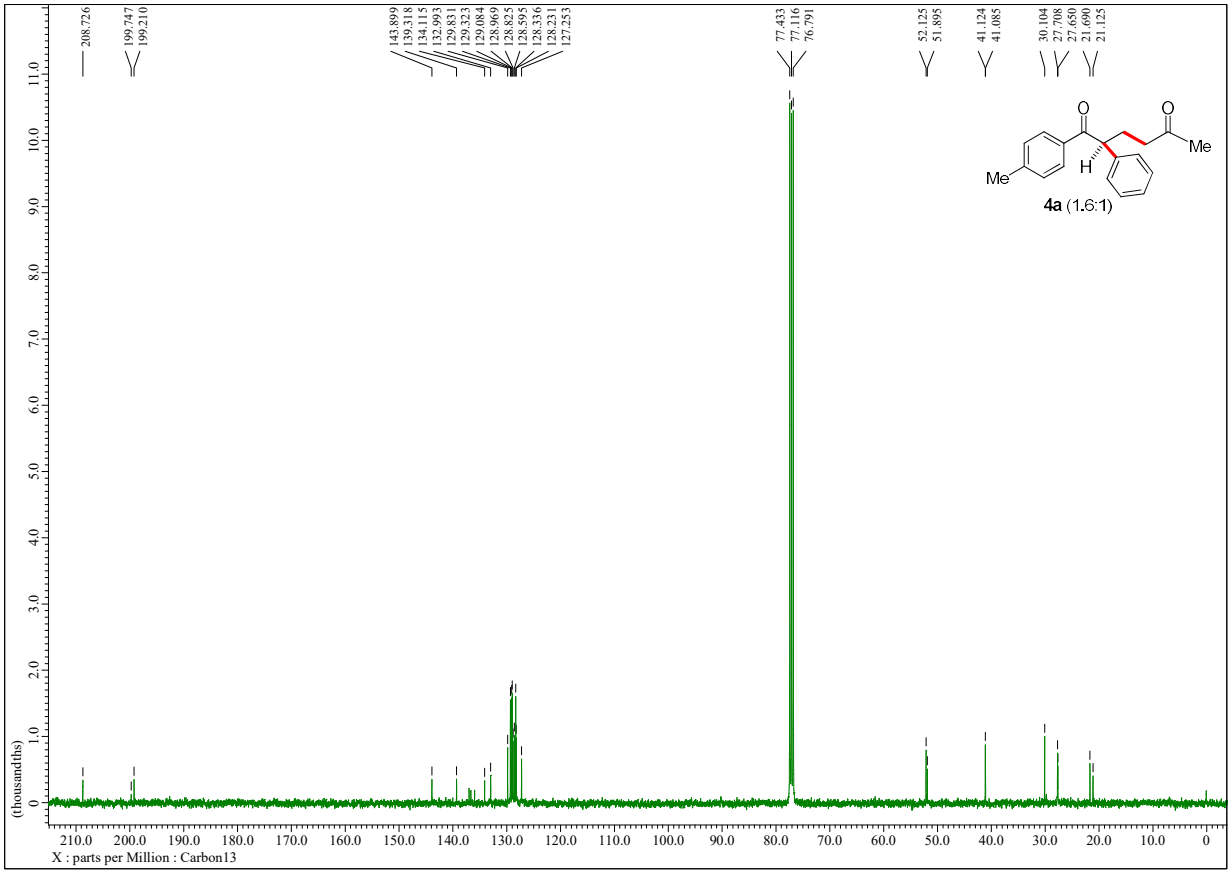
7.941
7.868
7.848
7.396
7.376
7.287
7.271
7.263
7.200
7.187
7.166
7.144
7.106
7.087
4.639
4.622
4.605
4.589
2.446
2.429
2.424
2.412
2.405
2.392
2.382
2.376
2.371
2.347
2.281
2.133
2.120
2.112
2.101
2.069
0.000
Me
O
O
Me
H
4a (1.6:1)
5.12
3.93
3.28
3.43
1.19
1.24
1.00
abundance
X : parts per Million : Proton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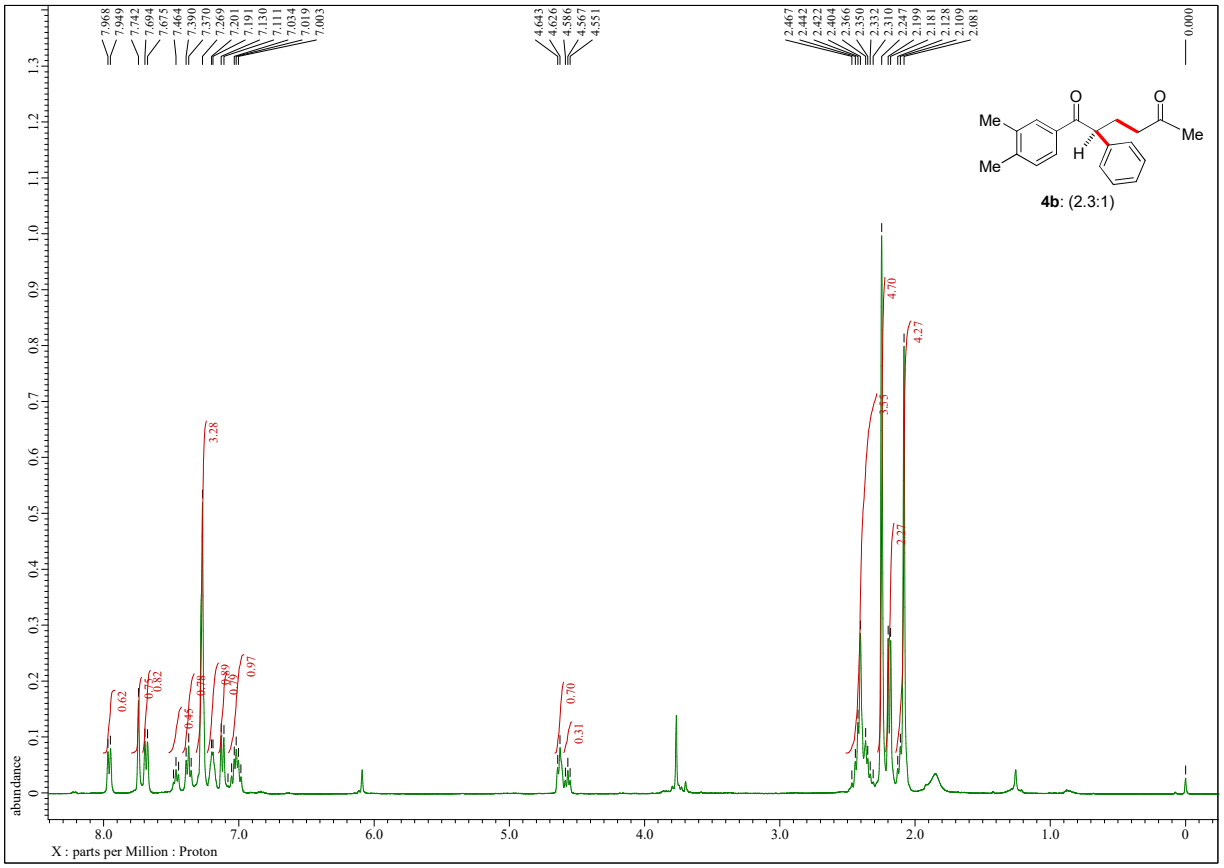
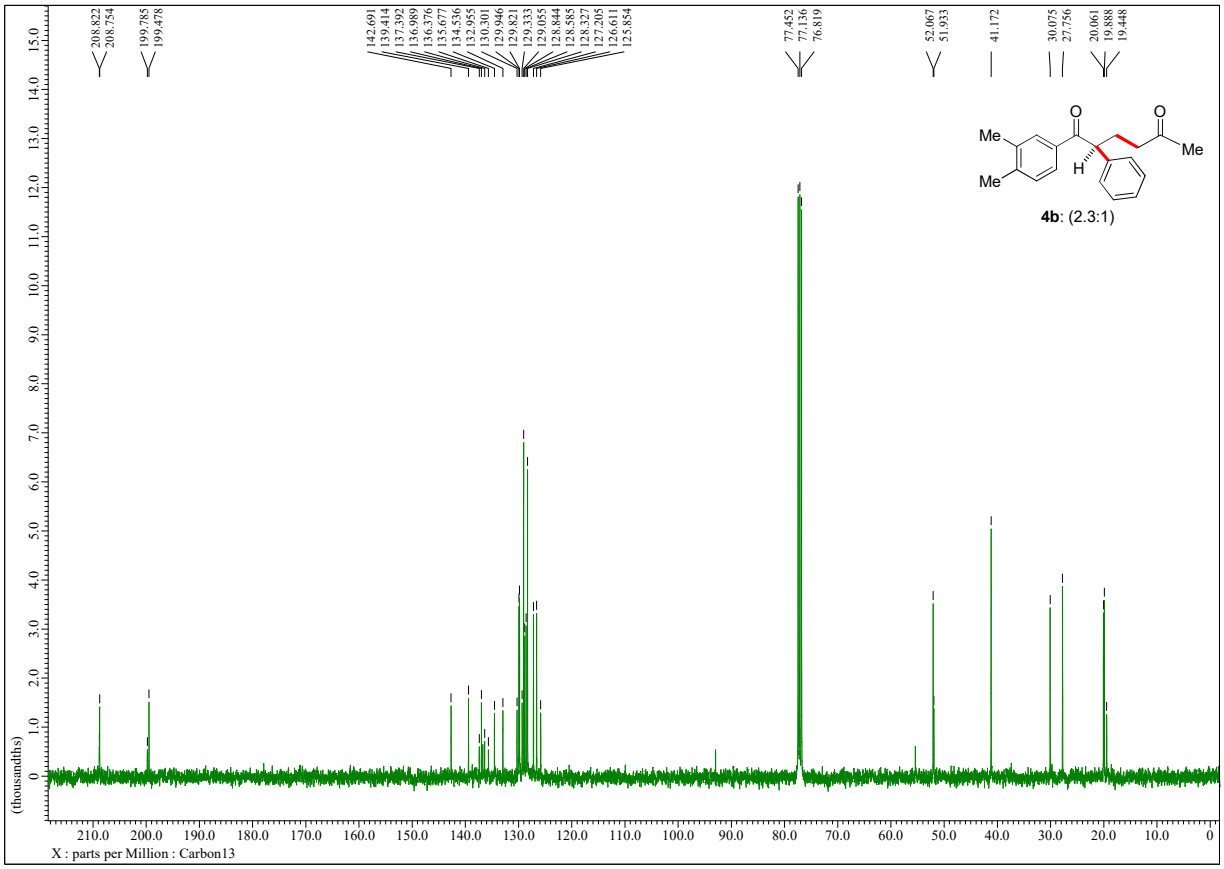
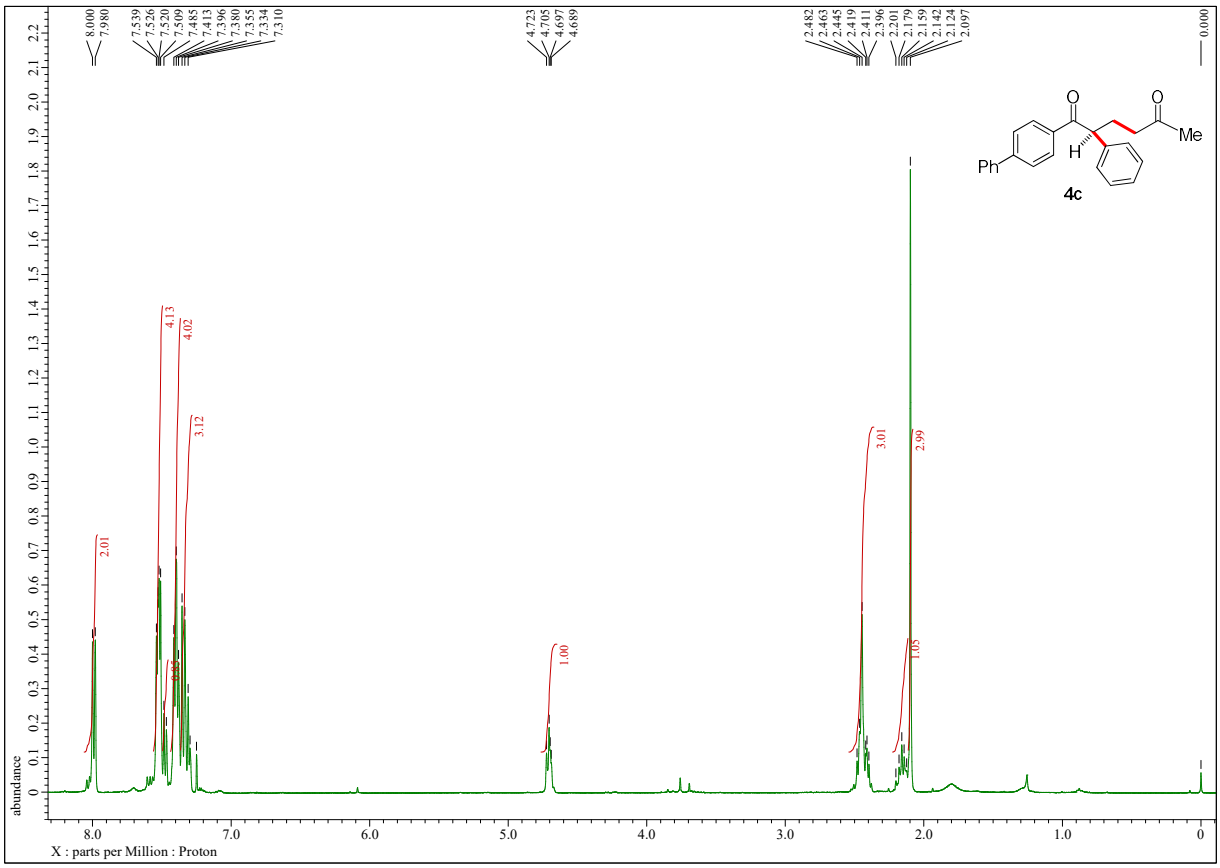
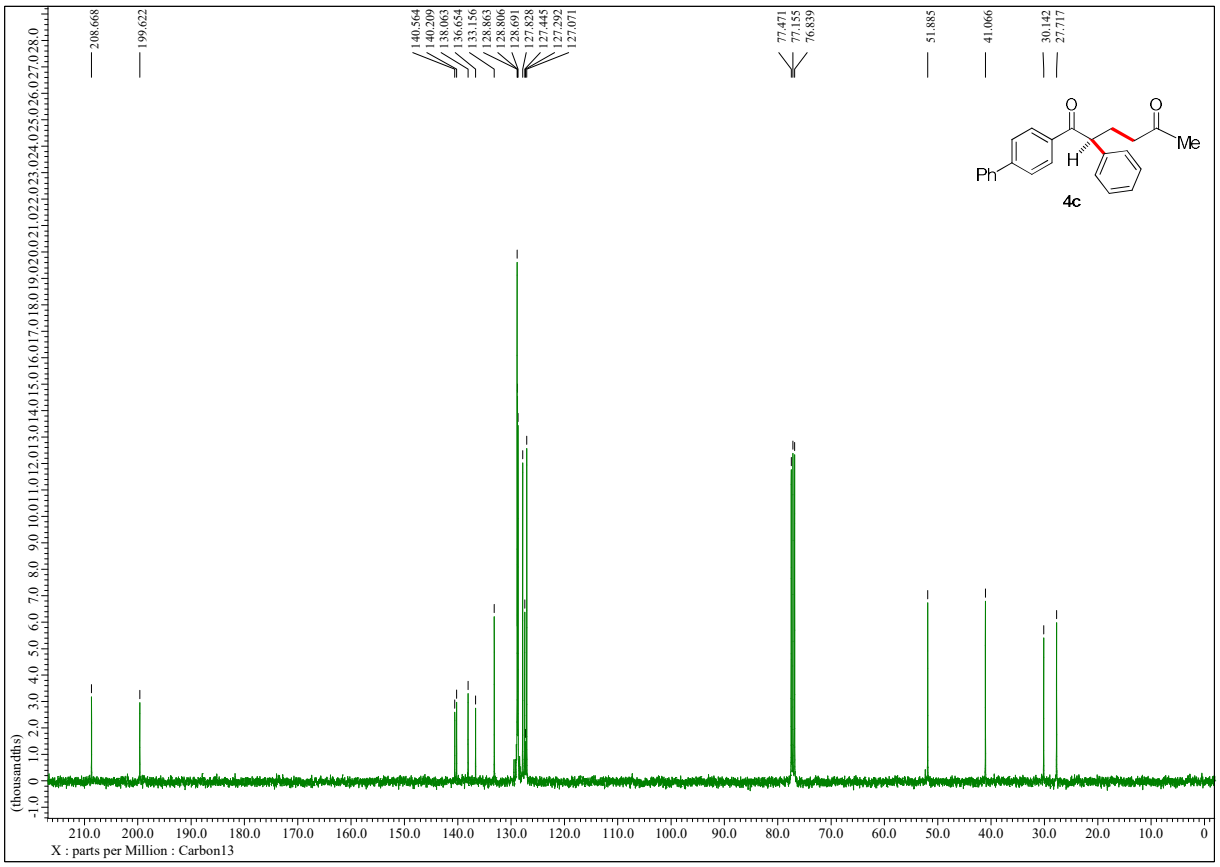
199.747
199.210
143.899
139.318
134.115
132.993
129.831
129.323
129.084
128.969
128.825
128.595
128.336
128.231
127.253
77.433
77.116
76.791
52.125
51.895
41.124
41.085
30.104
27.708
27.650
21.690
21.125
Me
O
O
Me
H
4a (1.6:1)
(thousandths)
X : parts per Million : Carbon13


7.968
7.949
7.742
7.694
7.675
7.464
7.390
7.370
7.269
7.201
7.191
7.130
7.111
7.034
7.019
7.003
4.643
4.626
4.586
4.567
4.551
2.467
2.442
2.422
2.404
2.366
2.350
2.332
2.310
2.247
2.199
2.181
2.128
2.109
2.081
0.000
Me
Me
O
O
H
Me
4b: (2.3:1)
4.70
4.27
3.53
3.28
2.77
0.97
0.89
0.82
0.70
0.62
0.31
abundance
X : parts per Million : Proton


208.822
208.754
199.785
199.478
142.691
139.414
137.392
136.989
136.376
135.677
134.536
132.955
130.301
129.946
129.821
129.333
129.055
128.844
128.585
128.327
127.205
126.611
125.854
77.452
77.136
76.819
52.067
51.933
41.172
30.075
27.756
20.061
19.888
19.448
Me
Me
O
O
H
Me
4b: (2.3:1)
(thousandths)
X : parts per Million : Carbon13


8.000
7.980
7.539
7.526
7.520
7.509
7.485
7.413
7.396
7.380
7.355
7.334
7.310
4.723
4.705
4.697
4.689
2.482
2.463
2.445
2.419
2.411
2.396
2.201
2.179
2.159
2.142
2.124
2.097
0.000
4.13
4.02
3.12
2.01
1.00
3.01
2.99
1.05
abundance
X : parts per Million : Proton
Ph
H
O
O
Me
4c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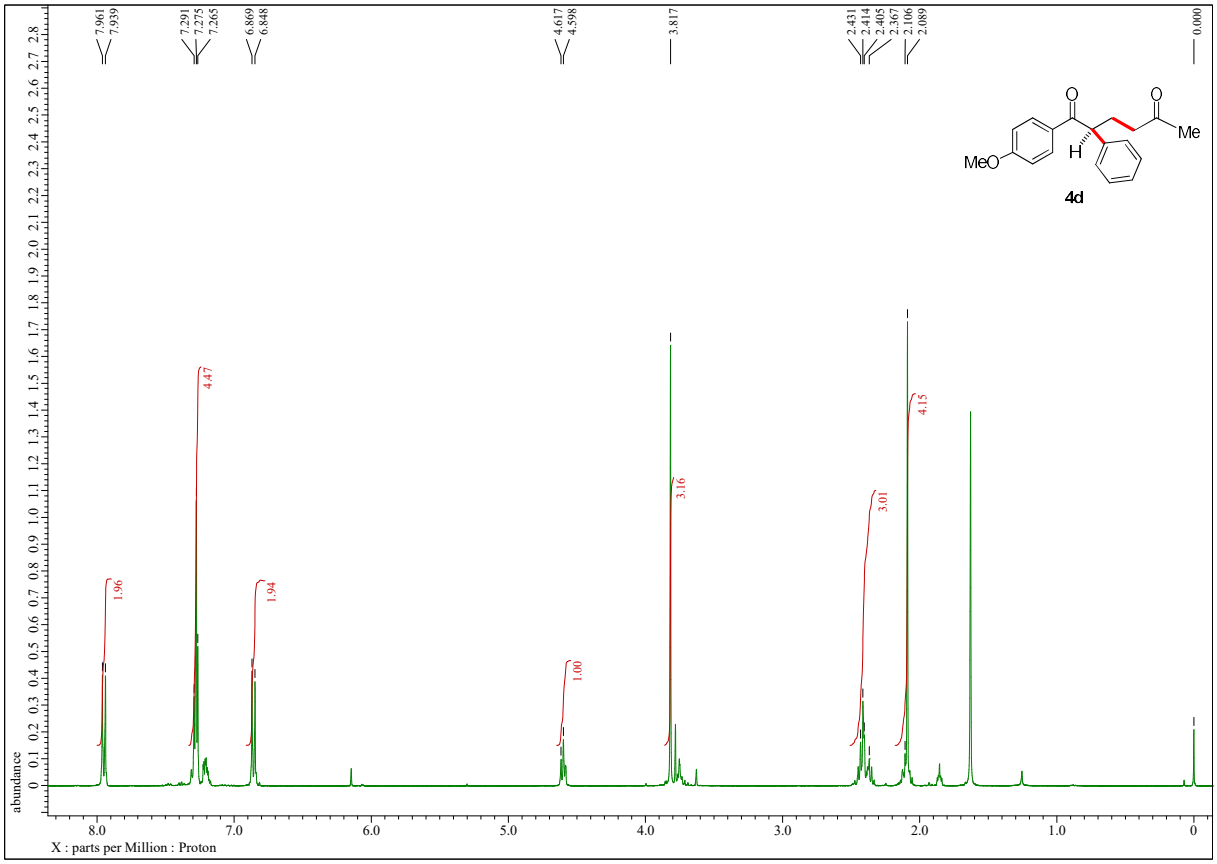
140.564
140.299
138.063
136.654
133.156
128.863
128.806
128.691
127.828
127.445
127.292
127.071
77.471
77.155
76.839
51.885
41.066
30.142
27.717
(thousandths)
X : parts per Million : Carbon13
Ph
H
O
O
Me
4c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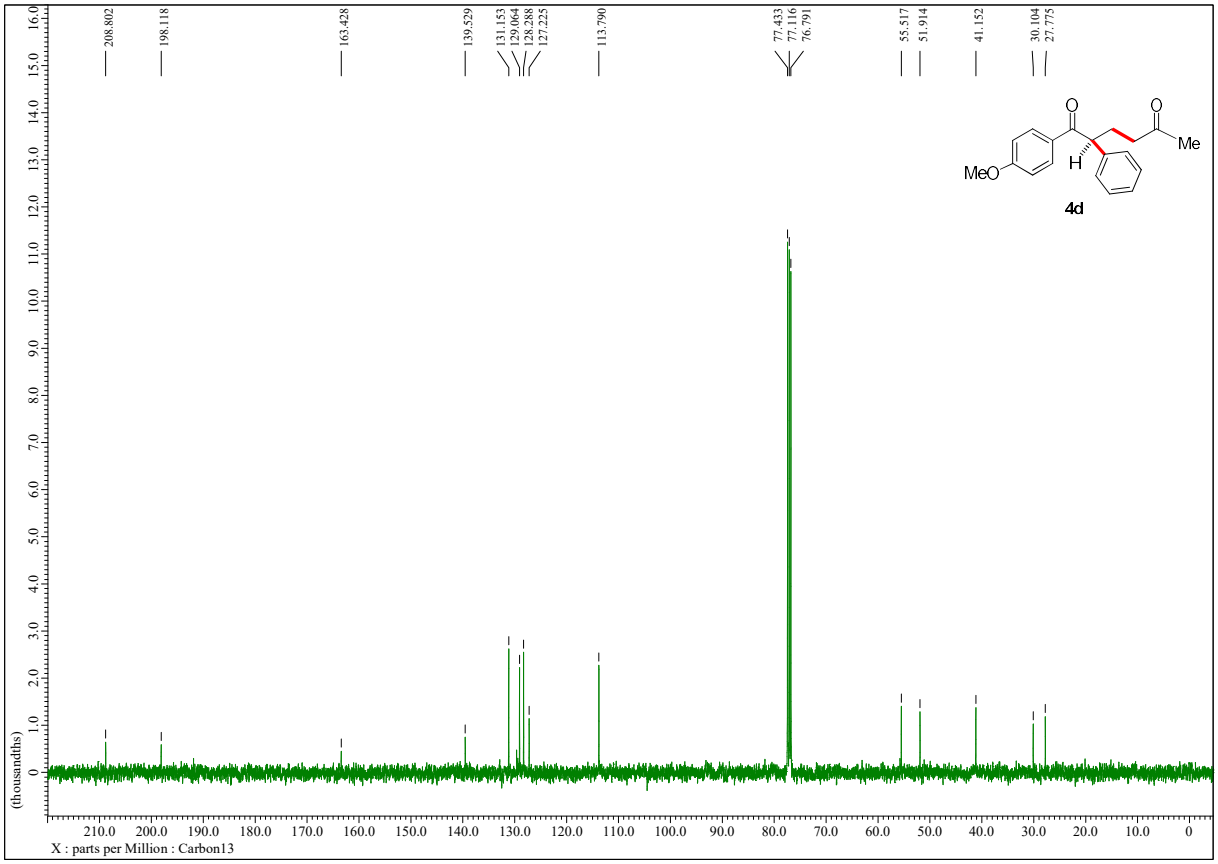
7.939
7.291
7.275
7.265
6.869
6.848
4.617
4.598
3.817
2.431
2.414
2.405
2.367
2.106
2.089
0.000
MeO
H
O
O
Me
4d
1.96
4.47
1.94
1.00
3.16
3.01
4.15
abundance
X : parts per Million : Proton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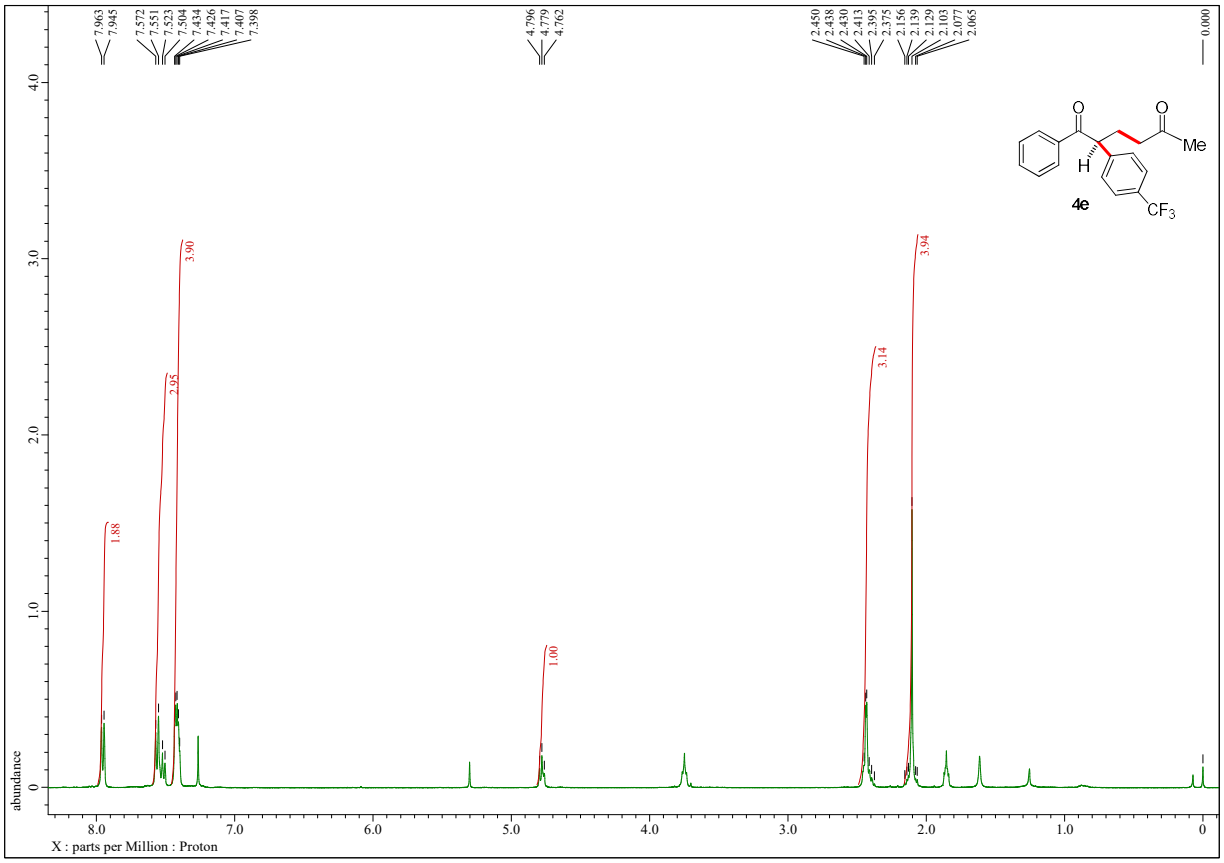
198.118
163.428
139.529
131.153
129.964
128.298
127.225
113.790
77.433
77.116
76.791
55.517
51.914
41.152
30.104
27.775
MeO
H
O
O
Me
4d
(thousandths)
X : parts per Million : Carbon13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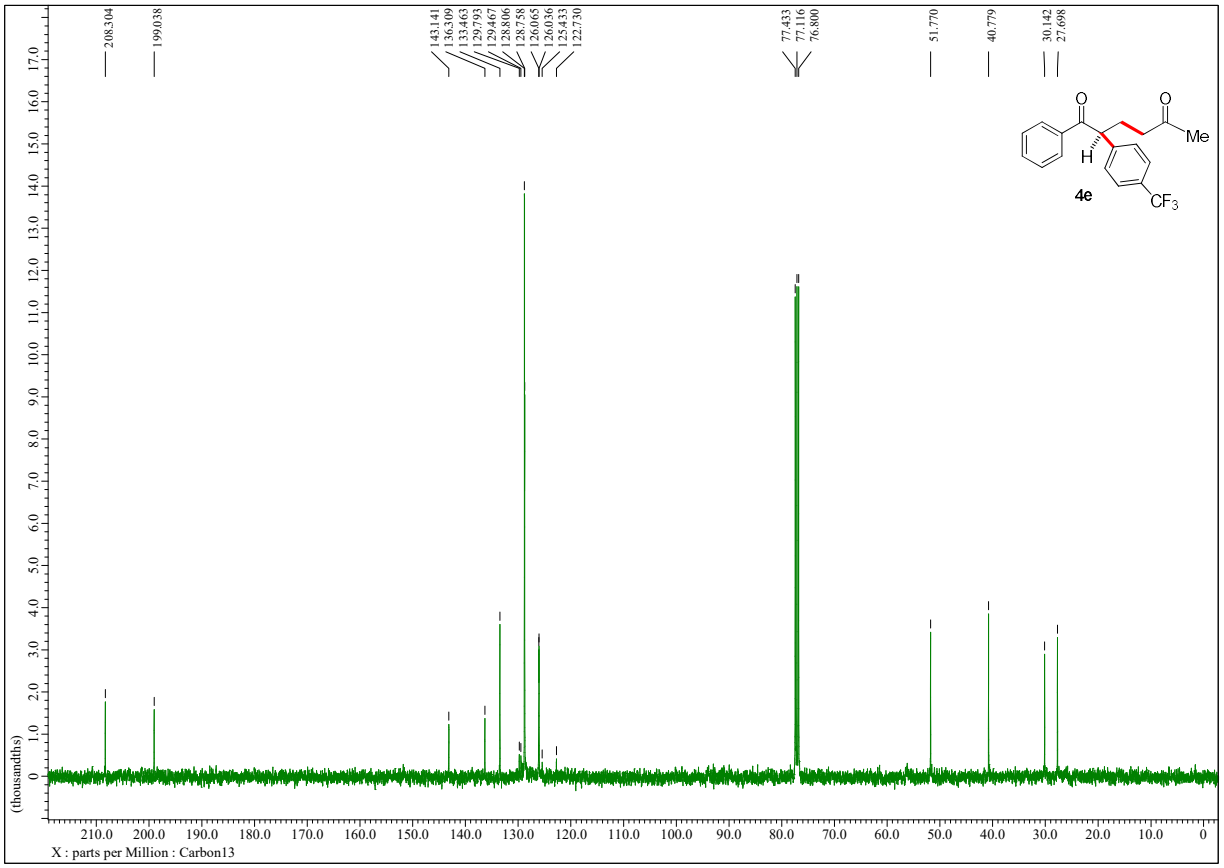
7.945
7.572
7.551
7.523
7.504
7.434
7.426
7.417
7.407
7.398
4.796
4.779
4.762
2.450
2.438
2.430
2.413
2.395
2.375
2.156
2.139
2.129
2.103
2.077
2.065
0.000
1.88
2.95
3.90
1.00
3.14
3.94
Me
H
4e
CF3
abundance
X : parts per Million : Proton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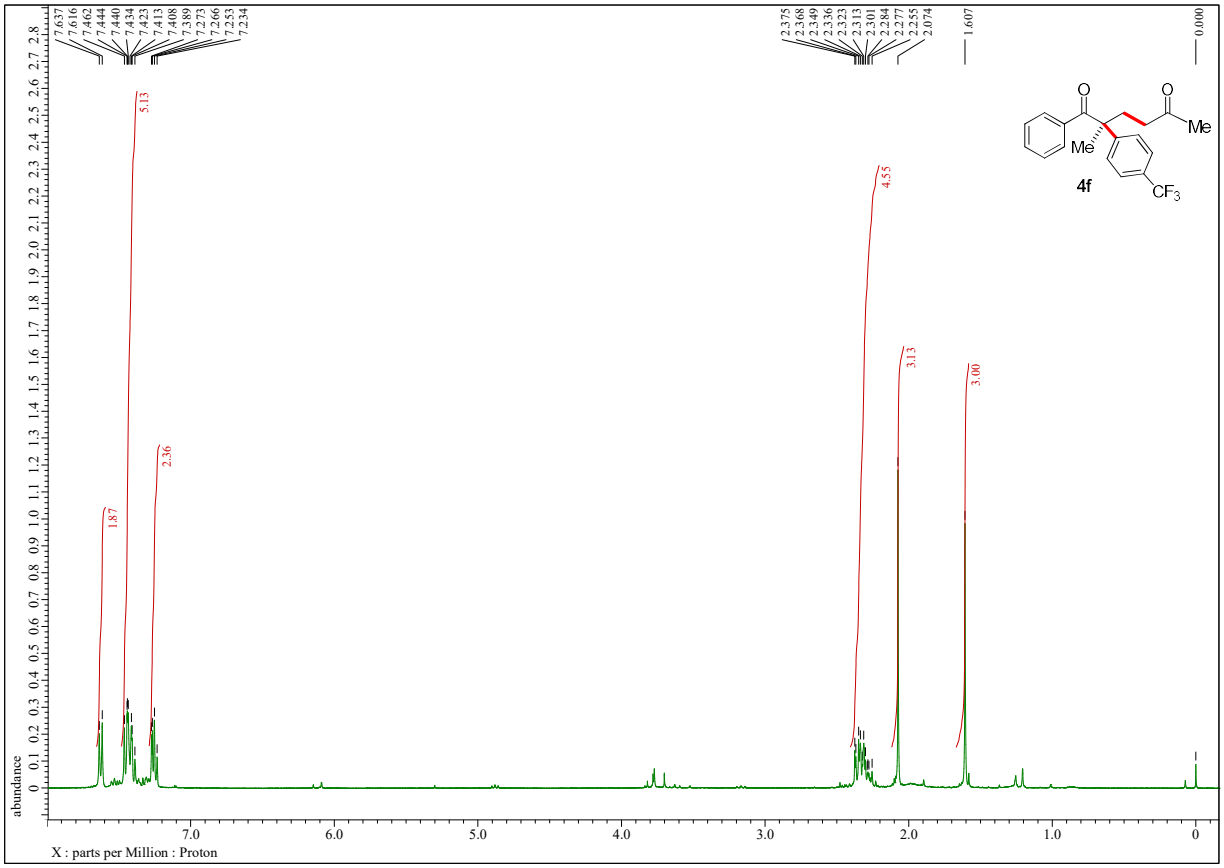
199.038
143.141
136.309
133.463
129.793
129.467
128.806
128.758
126.065
126.036
125.433
122.730
77.433
77.116
76.800
51.770
40.779
30.142
27.698
Me
H
4e
CF3
(thousandths)
X : parts per Million : Carbon13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7.616
7.462
7.444
7.440
7.434
7.423
7.413
7.408
7.389
7.273
7.266
7.253
7.234
2.375
2.368
2.349
2.336
2.323
2.313
2.301
2.284
2.277
2.255
2.074
1.607
0.000
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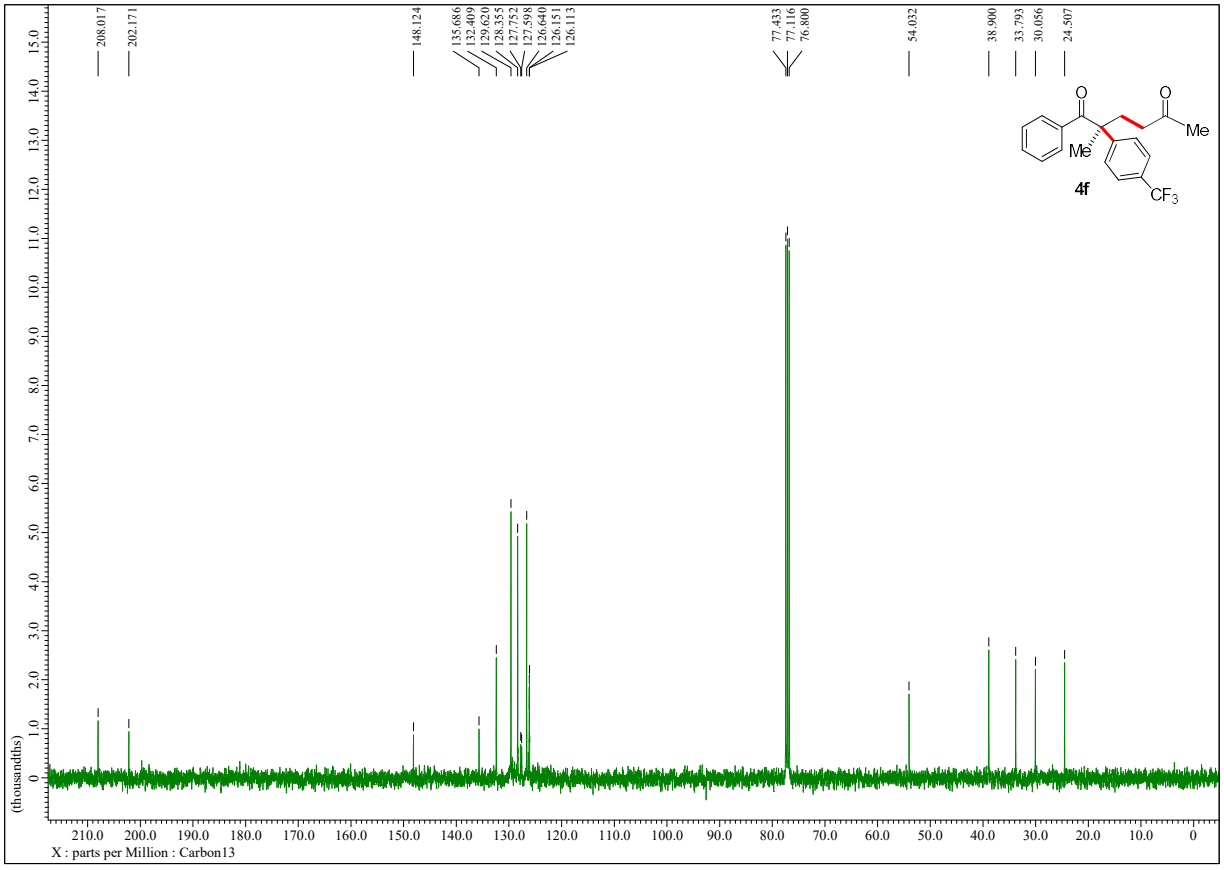
4.55
3.13
3.00
2.36
1.87
Me
Me
4f
CF3
abundance
X : parts per Million : Proton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202.171
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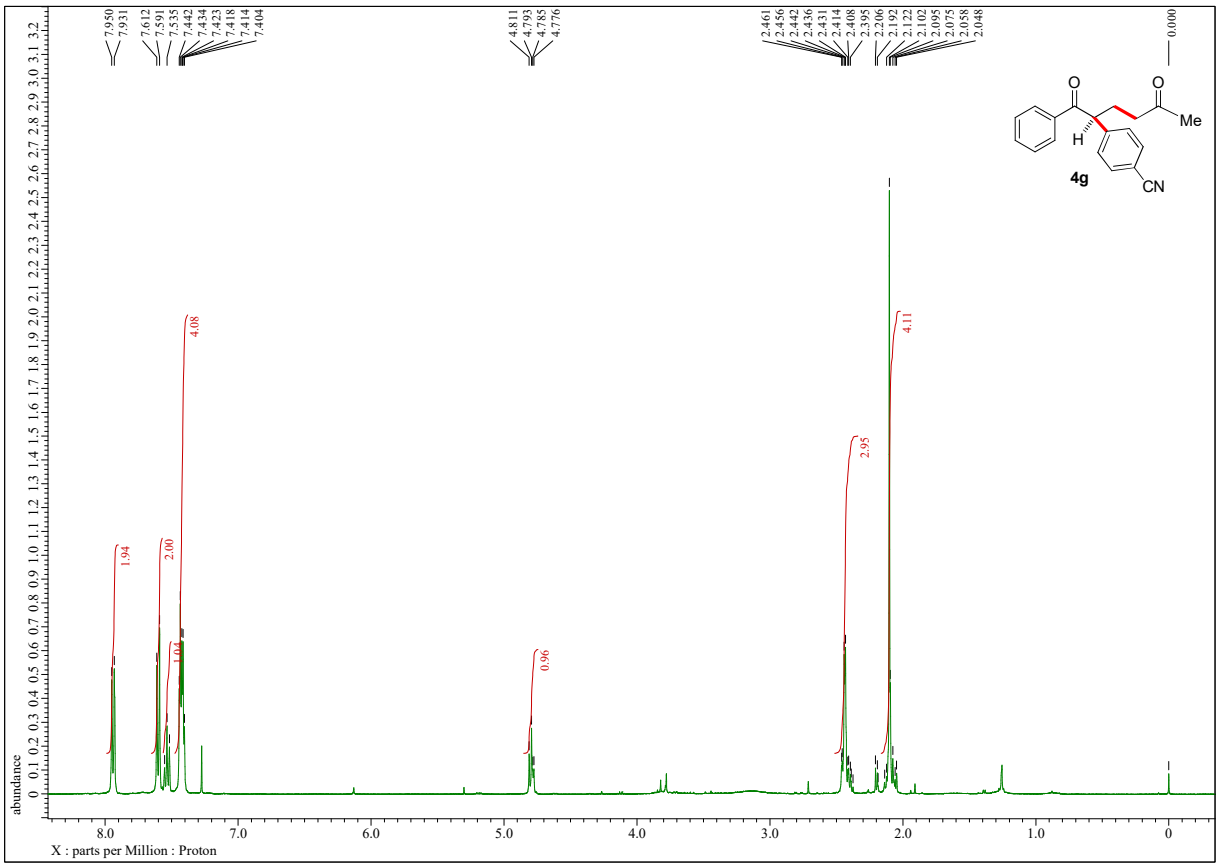
135.686
132.409
129.620
128.355
127.752
127.598
126.640
126.151
126.113
77.433
77.116
76.800
54.032
38.900
33.793
30.056
24.507
Me
Me
4f
CF3
(thousandths)
X : parts per Million : Carbon13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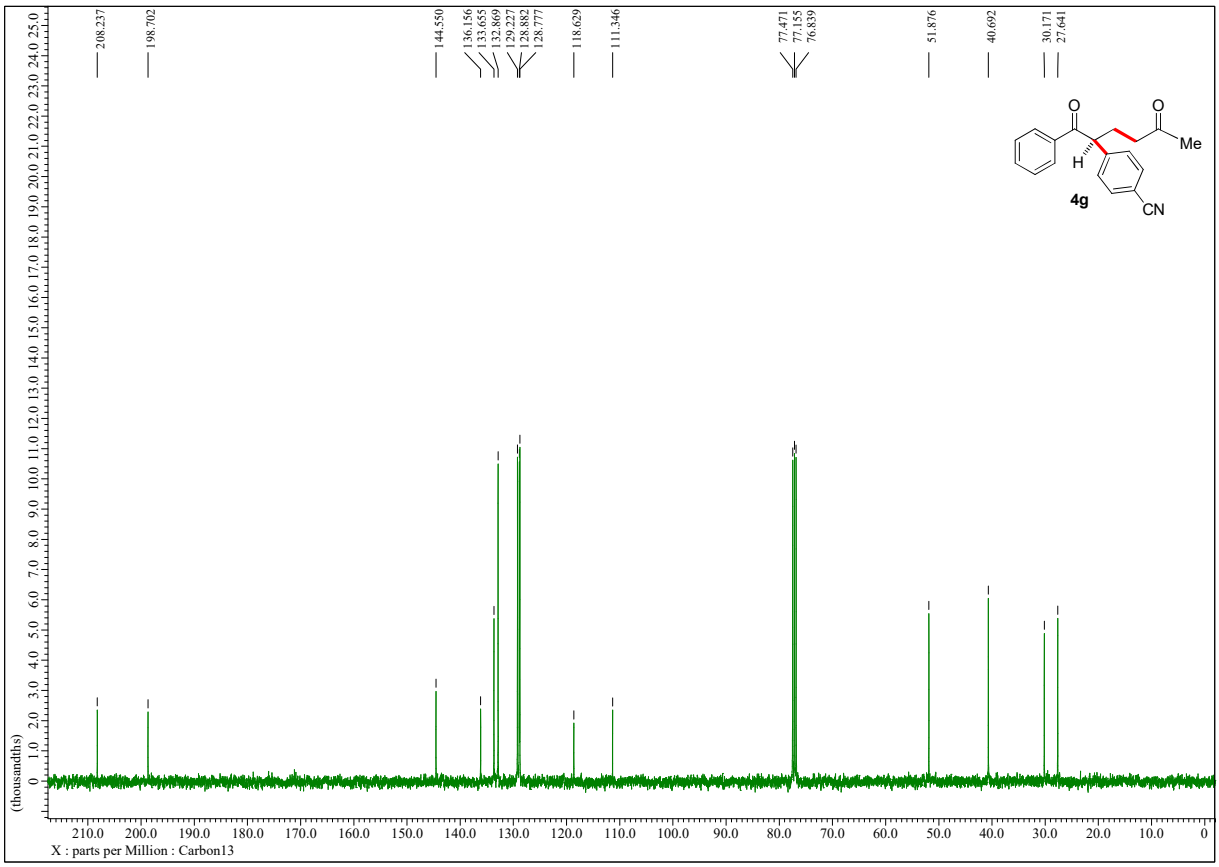
7.931
7.612
7.591
7.535
7.442
7.434
7.423
7.418
7.414
7.404
4.811
4.793
4.785
4.776
2.461
2.456
2.442
2.436
2.431
2.414
2.408
2.395
2.206
2.192
2.122
2.102
2.095
2.075
2.058
2.048
0.000
1.94
2.00
1.04
4.08
0.96
2.95
4.11
O
O
Me
H
CN
4g
abundance
X : parts per Million : Proton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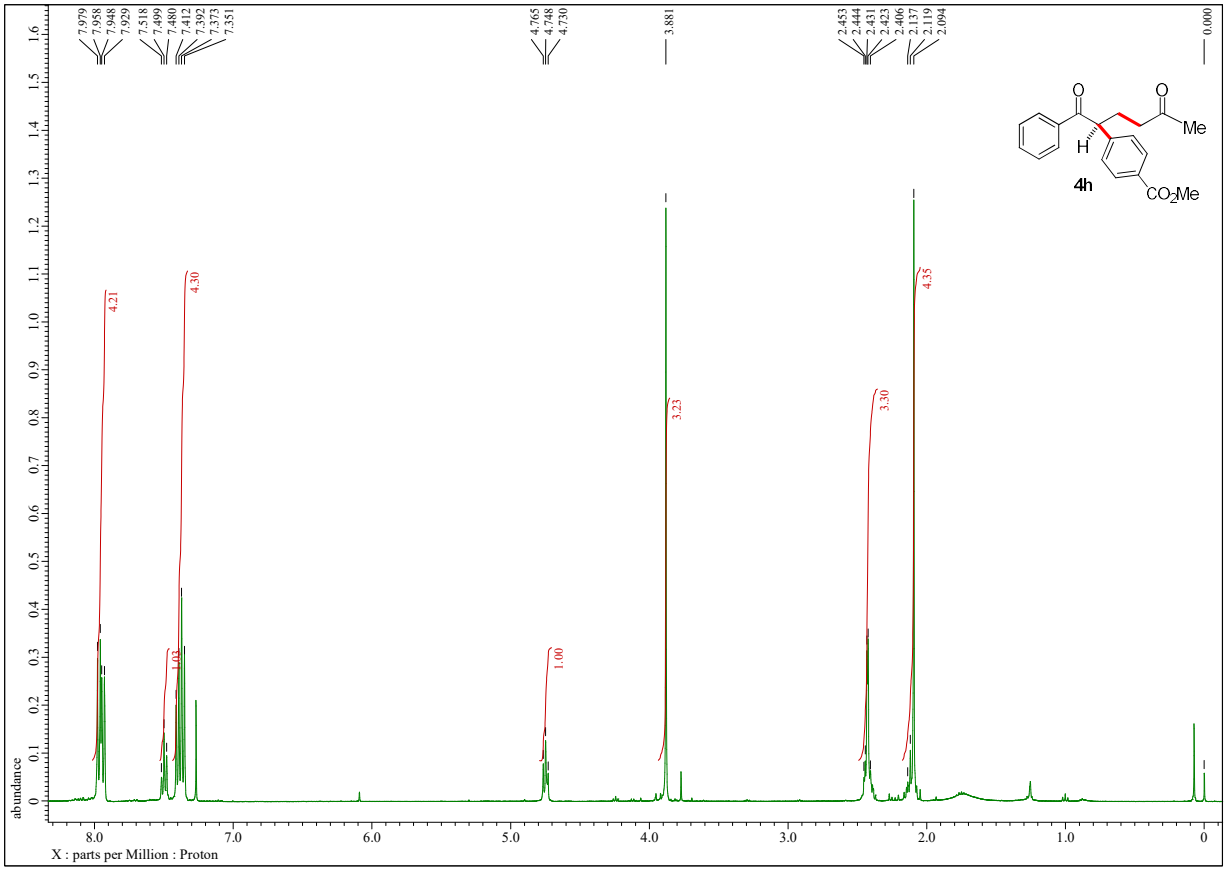
132.869
129.227
128.882
128.777
118.629
111.346
77.471
77.155
76.839
51.876
40.692
30.171
27.641
O
O
Me
H
CN
4g
(thousandths)
X : parts per Million : Carbon13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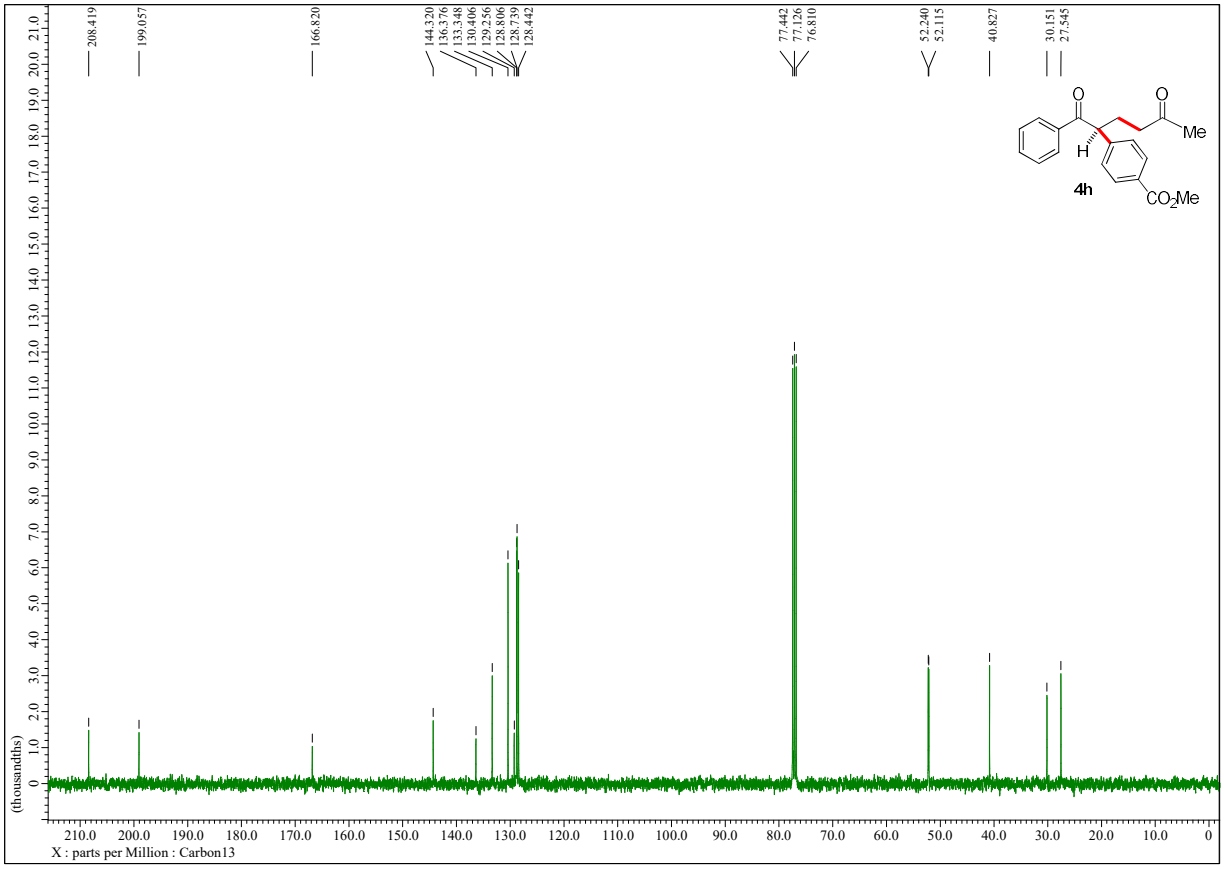
7.929
7.518
7.499
7.480
7.412
7.392
7.373
7.351
4.765
4.748
4.730
3.881
2.453
2.444
2.431
2.423
2.406
2.137
2.119
2.094
0.000
4.21
4.30
1.03
1.00
3.23
3.30
4.35
abundance
X : parts per Million : Proton
Me
H
4h
CO2Me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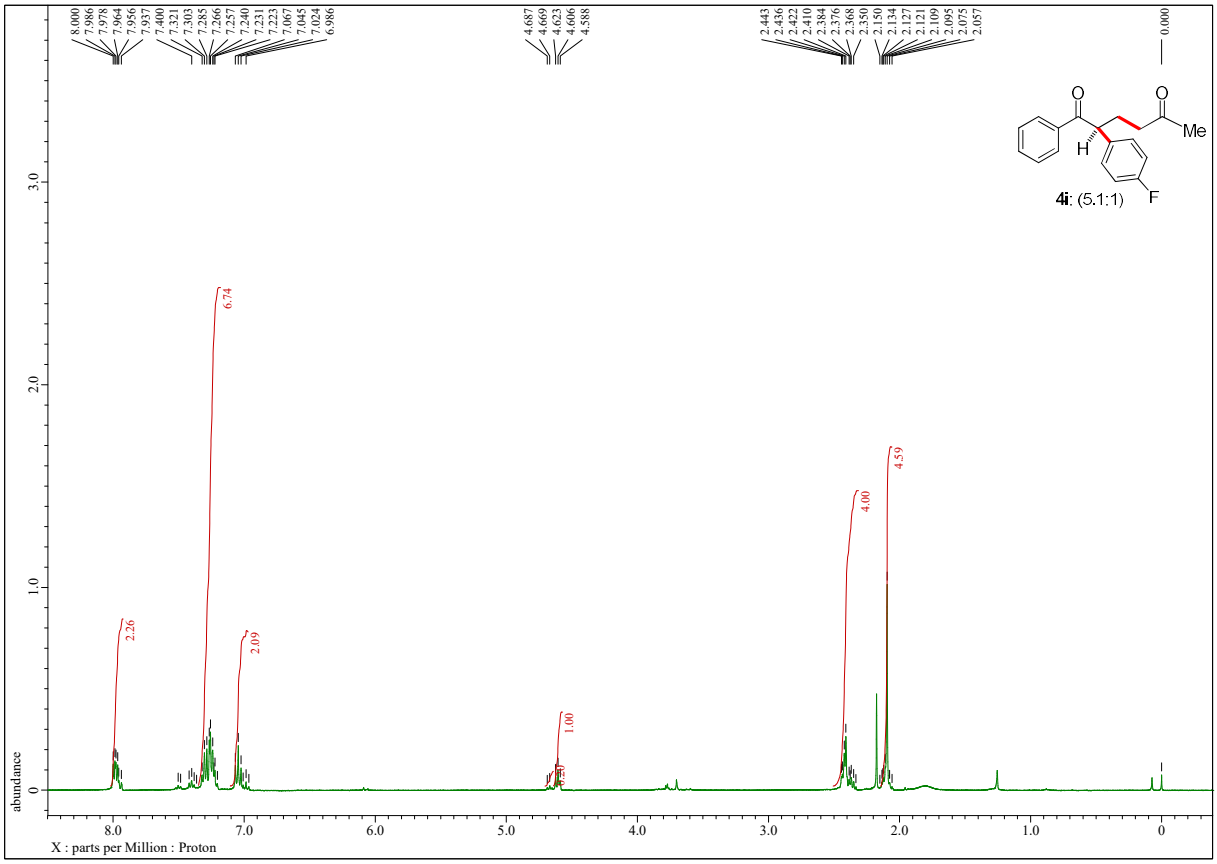
144.320
136.376
133.348
130.406
129.256
128.806
128.739
128.442
77.442
77.126
76.810
52.240
52.115
40.827
30.151
27.545
(thousandths)
X : parts per Million : Carbon13
Me
H
4h
CO2Me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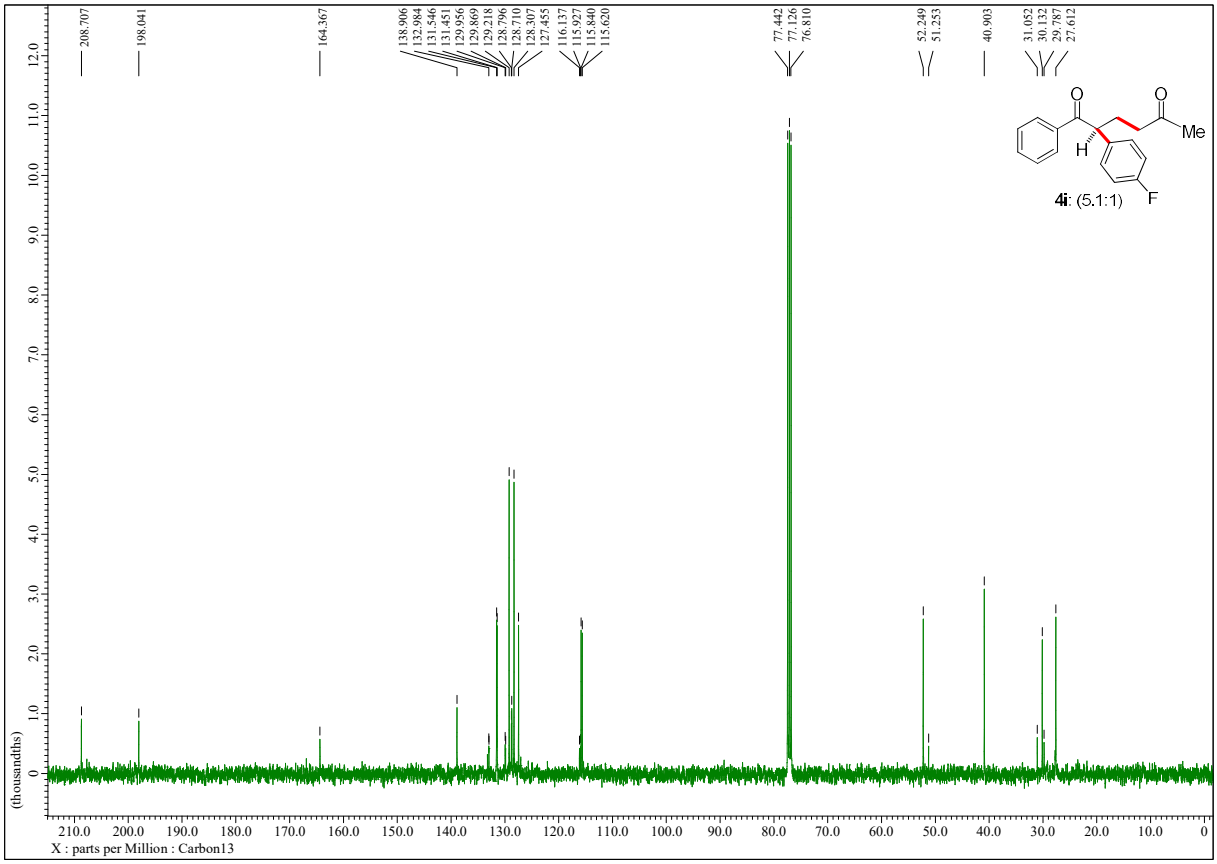
7.956
7.937
7.400
7.321
7.303
7.285
7.266
7.257
7.240
7.231
7.223
7.067
7.045
7.024
6.986
4.687
4.669
4.623
4.606
4.588
2.443
2.436
2.422
2.410
2.384
2.376
2.368
2.350
2.150
2.134
2.127
2.121
2.109
2.095
2.075
2.057
0.000
6.74
2.26
2.09
1.00
4.00
4.59
O
O
Me
H
F
4i: (5.1:1)
abundance
X : parts per Million : Proton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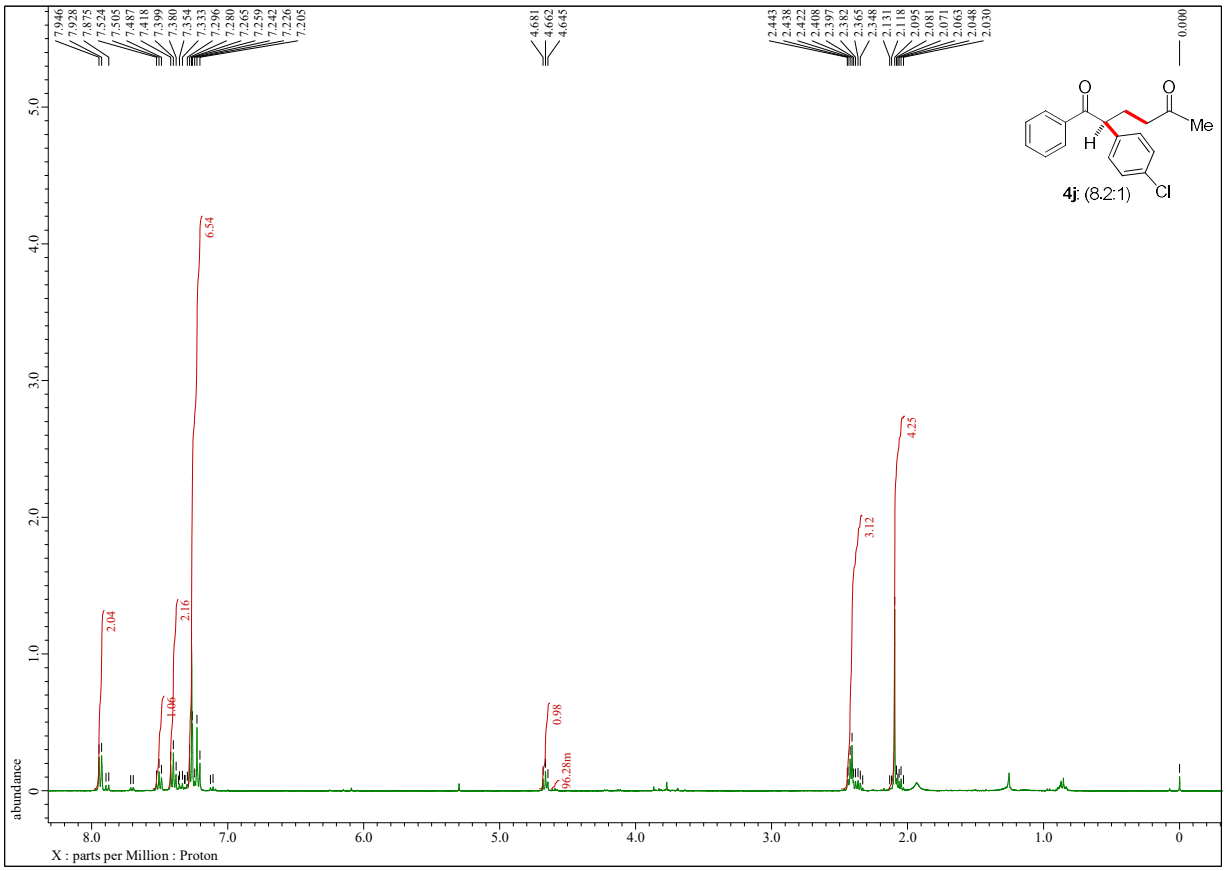
138.906
132.984
131.546
131.451
129.956
129.869
129.218
128.796
128.710
128.307
127.455
116.137
115.927
115.840
115.620
77.442
77.126
76.810
52.249
51.253
40.903
31.052
30.132
29.787
27.612
O
O
Me
H
F
4i: (5.1:1)
(thousandths)
X : parts per Million : Carbon13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7.487
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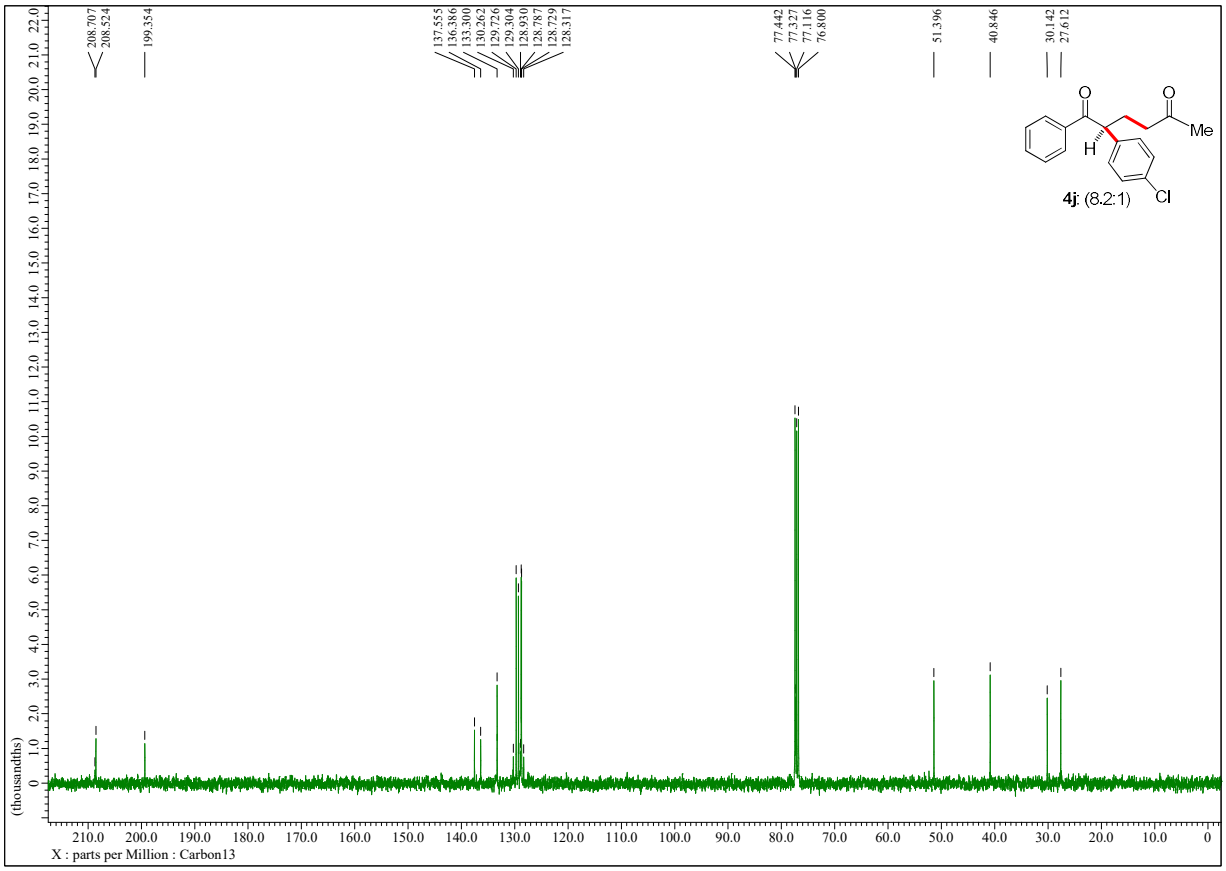
7.399
7.380
7.354
7.333
7.296
7.280
7.265
7.259
7.242
7.226
7.205
4.681
4.662
4.645
2.443
2.438
2.422
2.408
2.397
2.382
2.365
2.348
2.131
2.118
2.095
2.081
2.071
2.063
2.048
2.030
0.000
6.54
4.25
3.12
2.04
2.16
1.06
0.98
96.28m
abundance
X : parts per Million : Proton
O
O
Me
H
Cl
4j: (8.2:1)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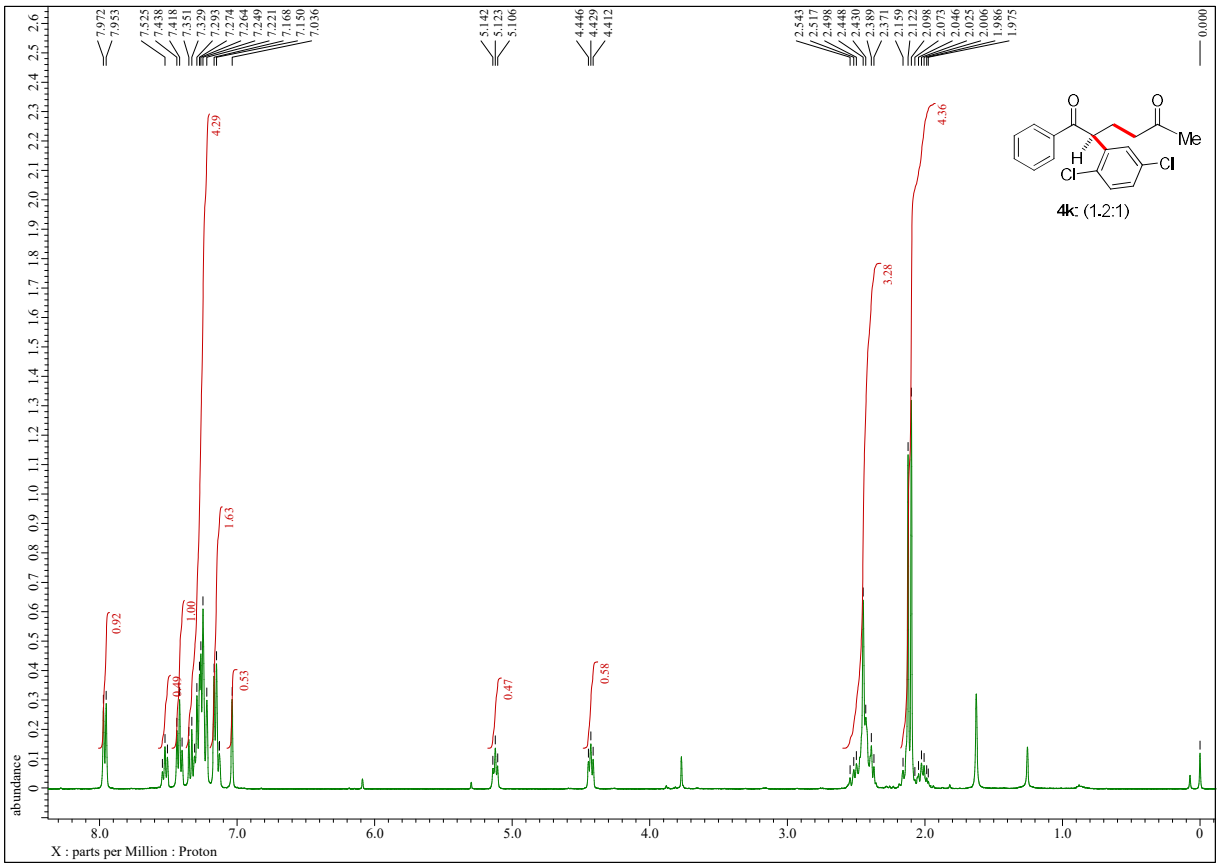
208.524
199.354
137.555
136.386
133.300
130.262
129.726
129.304
128.930
128.787
128.729
128.317
77.442
77.327
77.116
76.800
51.396
40.846
30.142
27.612
(thousandths)
X : parts per Million : Carbon13
O
O
Me
H
Cl
4j: (8.2:1)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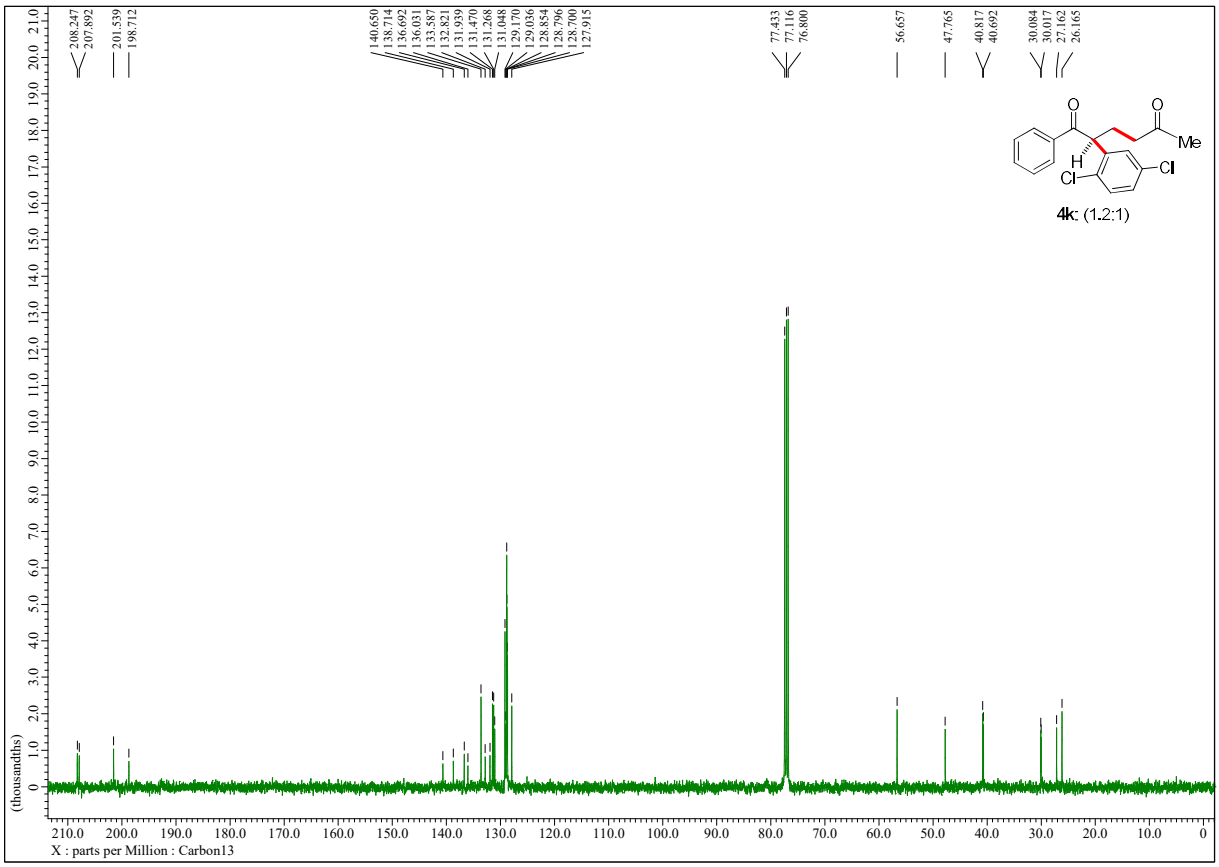
7.293
7.274
7.264
7.249
7.221
7.168
7.150
7.036
5.142
5.123
5.106
4.446
4.429
4.412
2.543
2.517
2.498
2.448
2.430
2.389
2.371
2.159
2.122
2.098
2.073
2.046
2.025
2.006
1.986
1.975
0.000
4.29
4.36
3.28
1.63
1.00
0.92
0.49
0.53
0.47
0.58
abundance
X : parts per Million : Proton
Me
Cl
H
Cl
4k: (1.2:1)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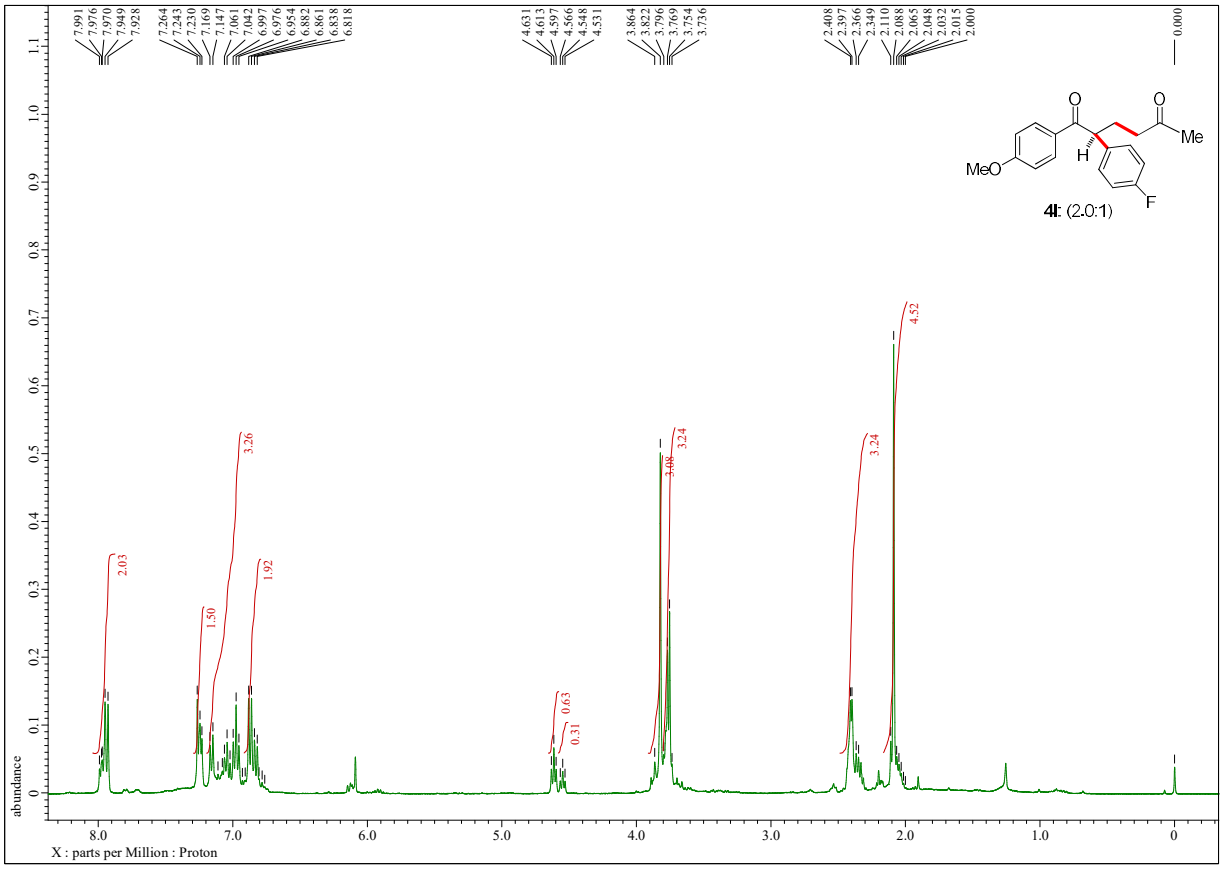
198.712
140.650
138.714
136.692
136.031
133.587
132.821
131.699
131.470
131.268
131.048
129.170
129.036
128.854
128.796
128.700
127.915
77.433
77.116
76.800
56.657
47.765
40.817
40.692
30.084
30.017
27.162
26.165
(thousandths)
X : parts per Million : Carbon13
Me
Cl
H
Cl
4k: (1.2:1)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7.976
7.970
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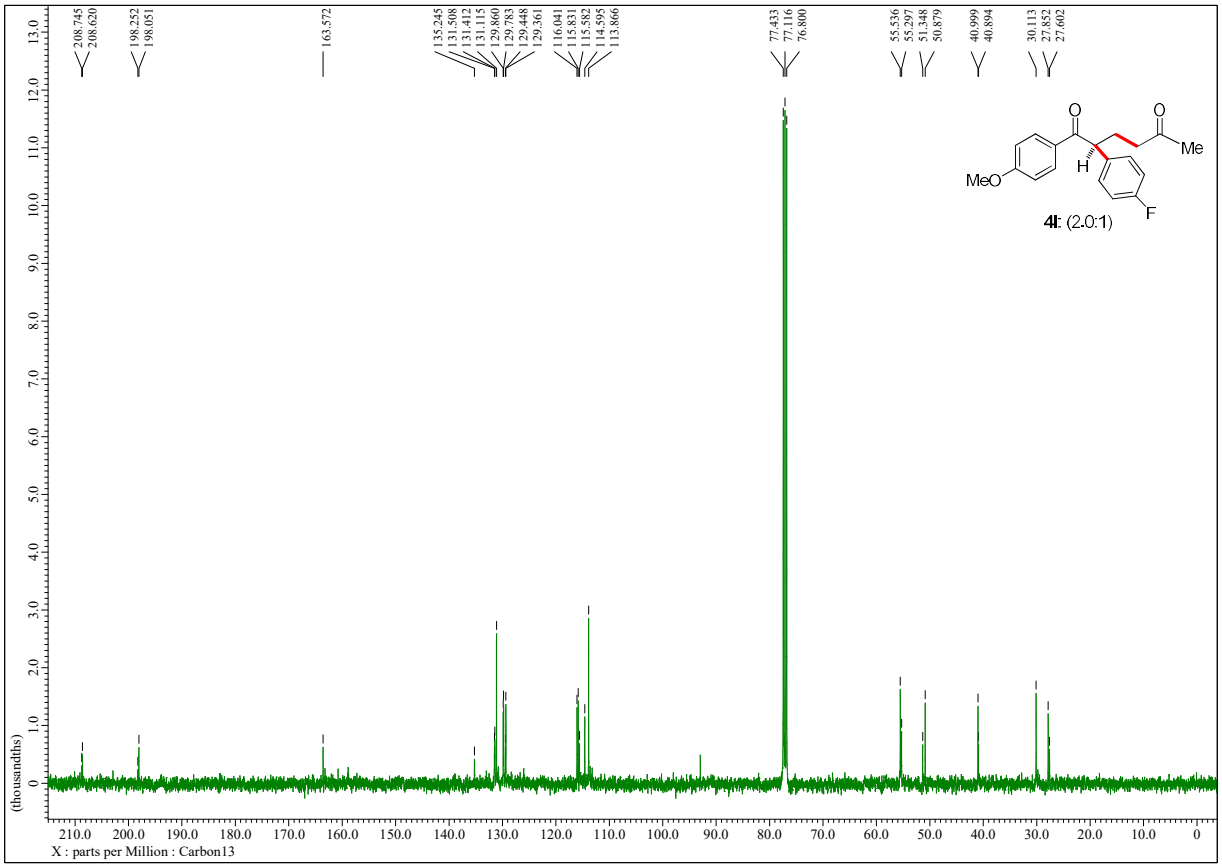
7.928
7.264
7.243
7.230
7.169
7.147
7.061
7.042
6.997
6.976
6.954
6.882
6.861
6.838
6.818
4.631
4.613
4.597
4.566
4.548
4.531
3.864
3.822
3.796
3.769
3.754
3.736
2.408
2.397
2.366
2.349
2.110
2.088
2.065
2.048
2.032
2.015
2.000
0.000
O
O
Me
MeO
H
F
4l: (2.0:1)
2.03
1.50
3.26
1.92
0.63
0.31
3.08
3.24
3.24
4.52
abundance
X : parts per Million : Proton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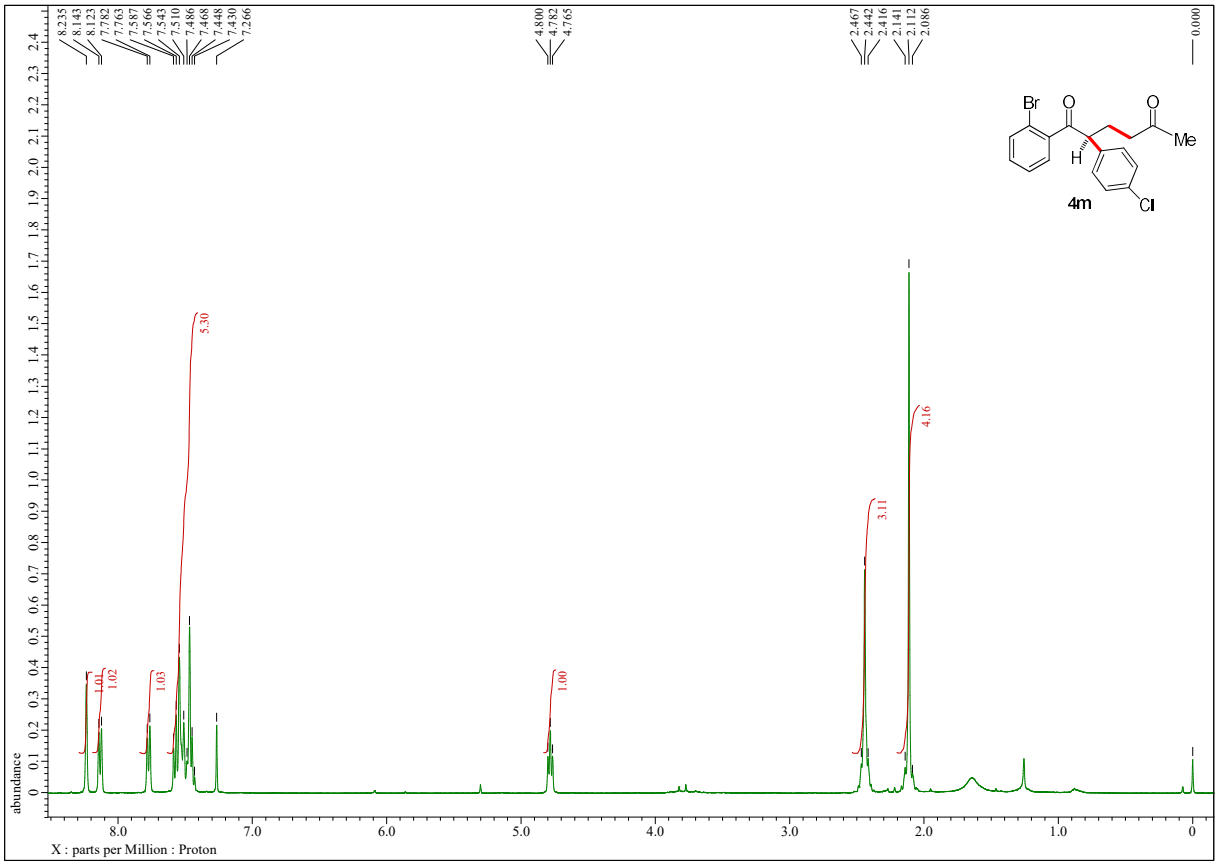
198.252
198.051
163.572
135.245
131.508
131.412
131.115
129.860
129.783
129.448
129.361
116.041
115.831
115.582
114.595
113.866
77.433
77.116
76.800
55.536
55.297
51.348
50.879
40.999
40.894
30.113
27.852
27.602
O
O
Me
MeO
H
F
4l: (2.0:1)
(thousandths)
X : parts per Million : Carbon13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8.123
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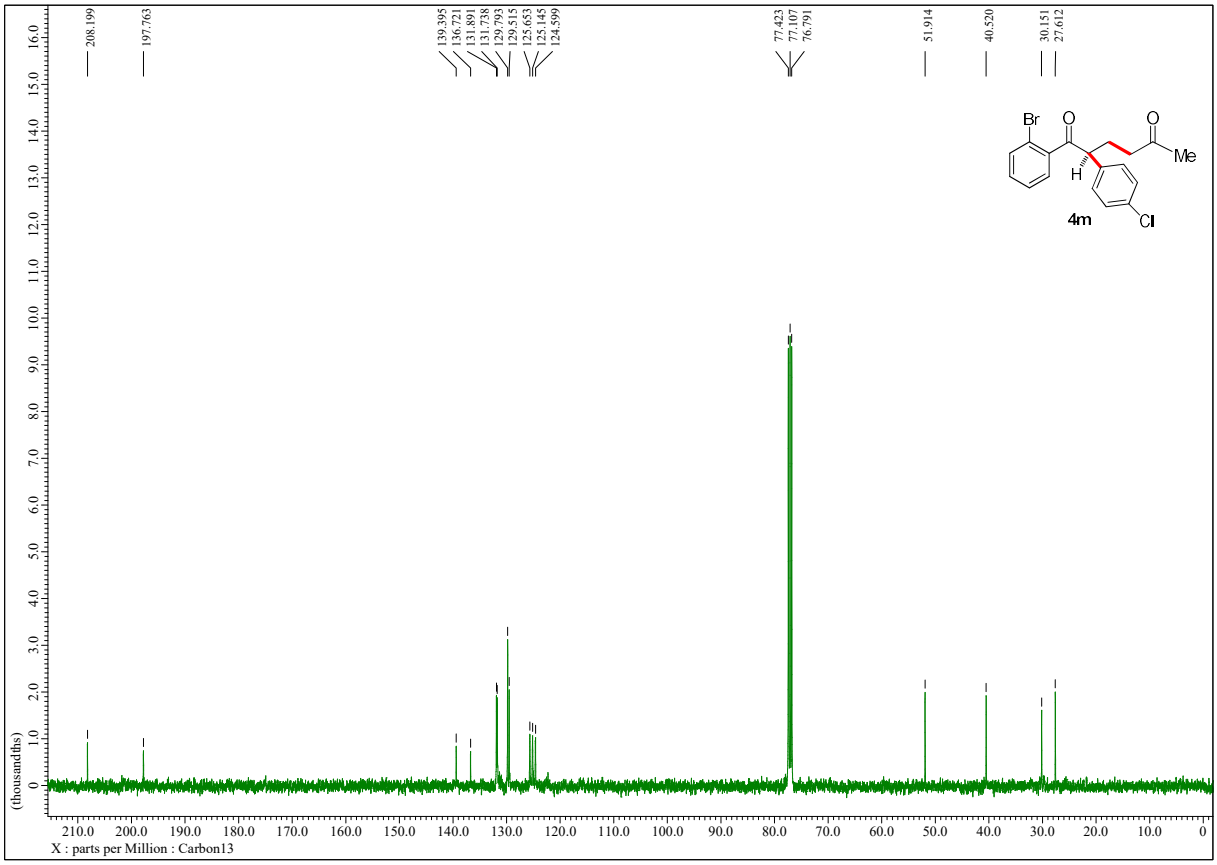
7.763
7.587
7.566
7.543
7.510
7.486
7.468
7.448
7.430
7.266
4.800
4.782
4.765
2.467
2.442
2.416
2.141
2.112
2.086
0.000
Br
O
O
Me
H
Cl
4m
5.30
4.16
3.11
1.01
1.02
1.03
1.00
abundance
X : parts per Million : Proton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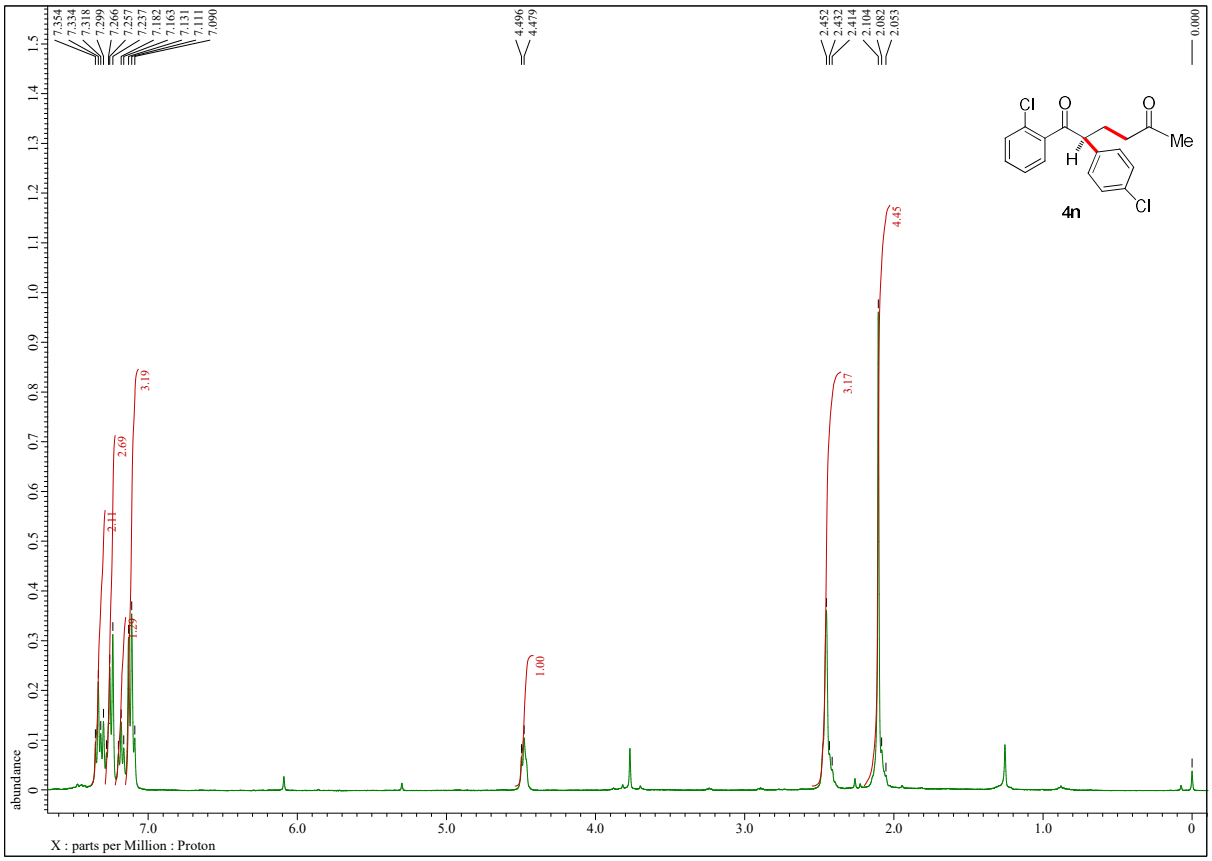
136.721
131.891
131.738
129.793
129.515
125.653
125.145
124.599
77.423
77.107
76.791
51.914
40.520
30.151
27.612
Br
O
O
Me
H
Cl
4m
(thousandths)
X : parts per Million : Carbon13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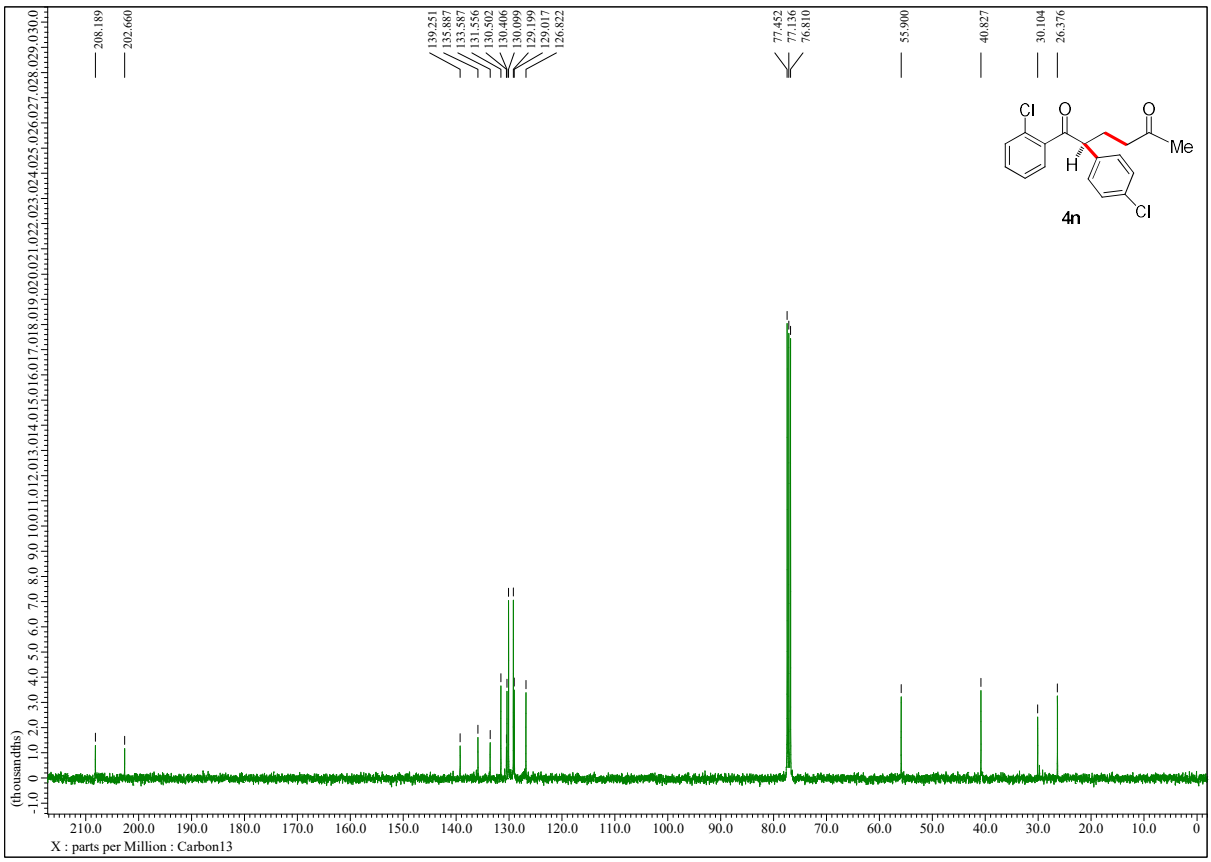
7.334
7.318
7.299
7.266
7.257
7.237
7.182
7.163
7.131
7.111
7.090
4.496
4.479
2.452
2.432
2.414
2.104
2.082
2.053
0.000
Cl
O
O
Me
H
Cl
4n
4.45
3.19
3.17
2.69
2.11
1.00
abundance
X : parts per Million : Proton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202.660
139.251
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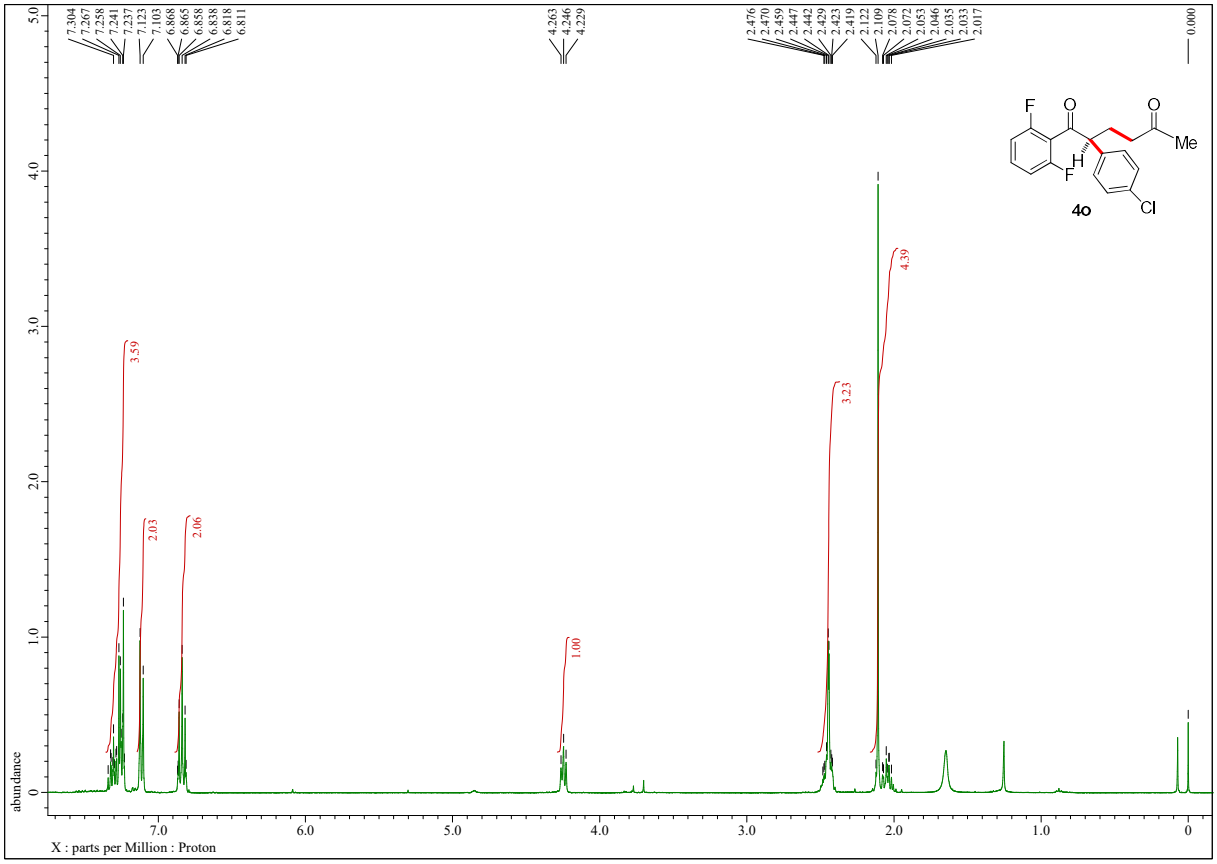
133.587
131.556
130.502
130.406
130.099
129.199
129.017
126.822
77.452
77.136
76.810
55.900
40.827
30.104
26.376
Cl
O
O
Me
H
Cl
4n
(thousandths)
X : parts per Million : Carbon13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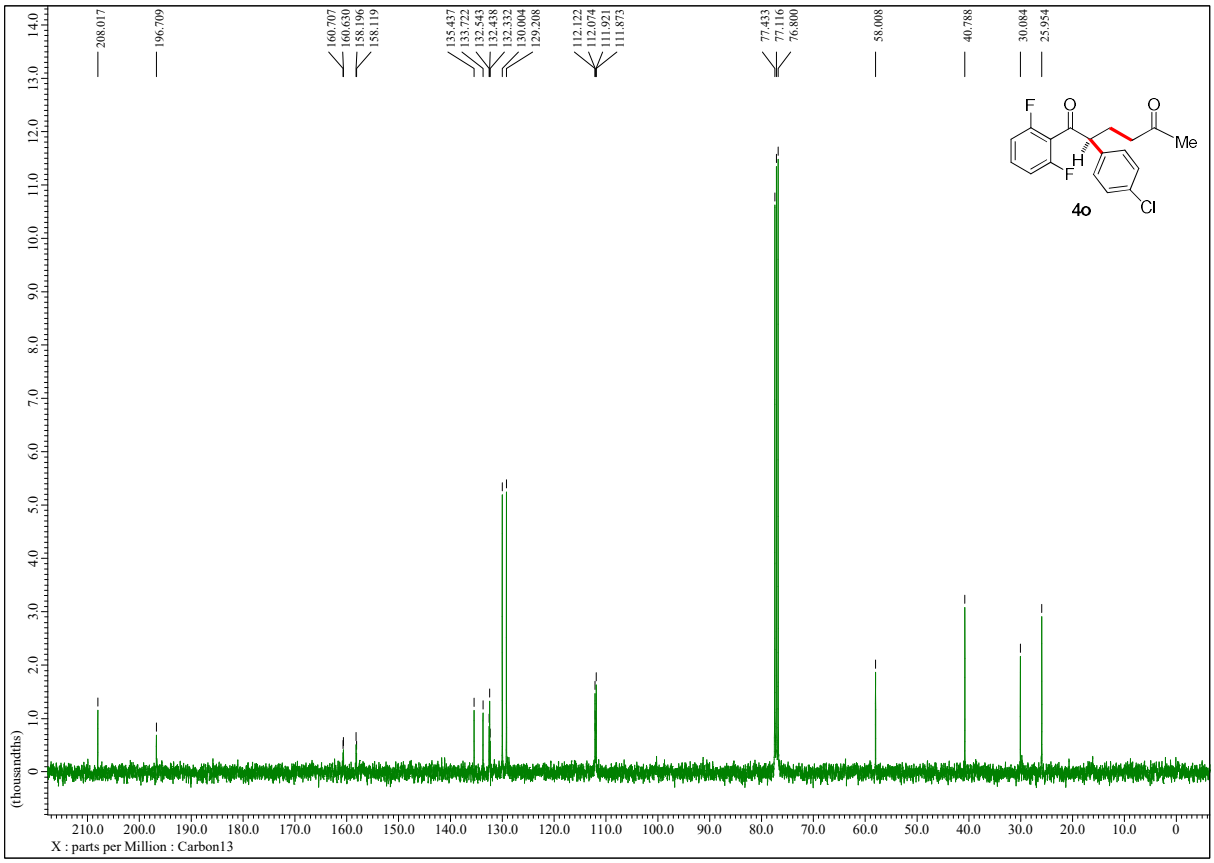
7.267
7.258
7.241
7.237
7.123
7.103
6.868
6.865
6.858
6.838
6.818
6.811
4.263
4.246
4.229
2.476
2.470
2.459
2.447
2.442
2.429
2.423
2.419
2.122
2.109
2.078
2.072
2.053
2.046
2.035
2.033
2.017
0.000
3.59
2.03
2.06
1.00
3.23
4.39
F
O
O
Me
H
F
Cl
4o
abundance
X : parts per Million : Proton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160.630
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158.119
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133.722
132.543
132.438
132.332
130.004
129.208
112.122
112.074
111.921
111.873
77.433
77.116
76.800
58.008
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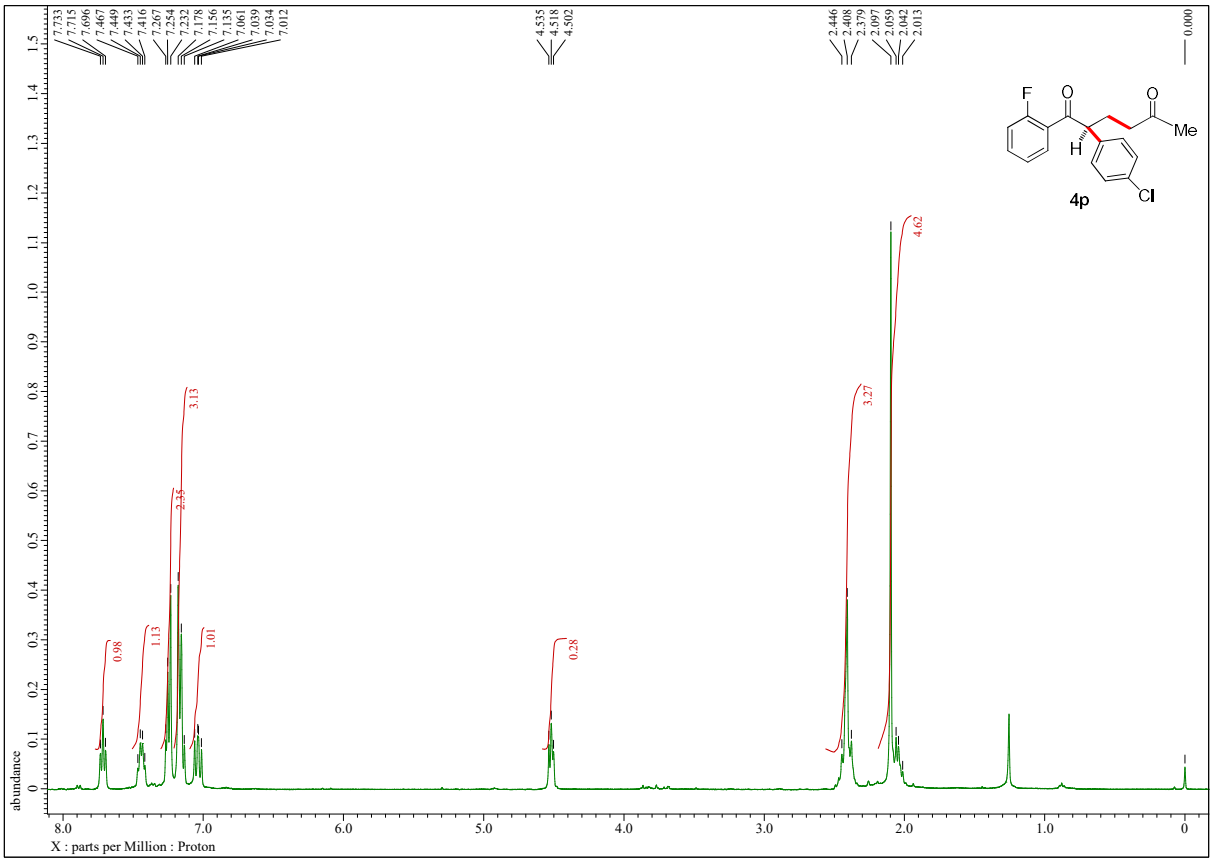
30.084
25.954
F
O
O
Me
H
F
Cl
4o
(thousandths)
X : parts per Million : Carbon13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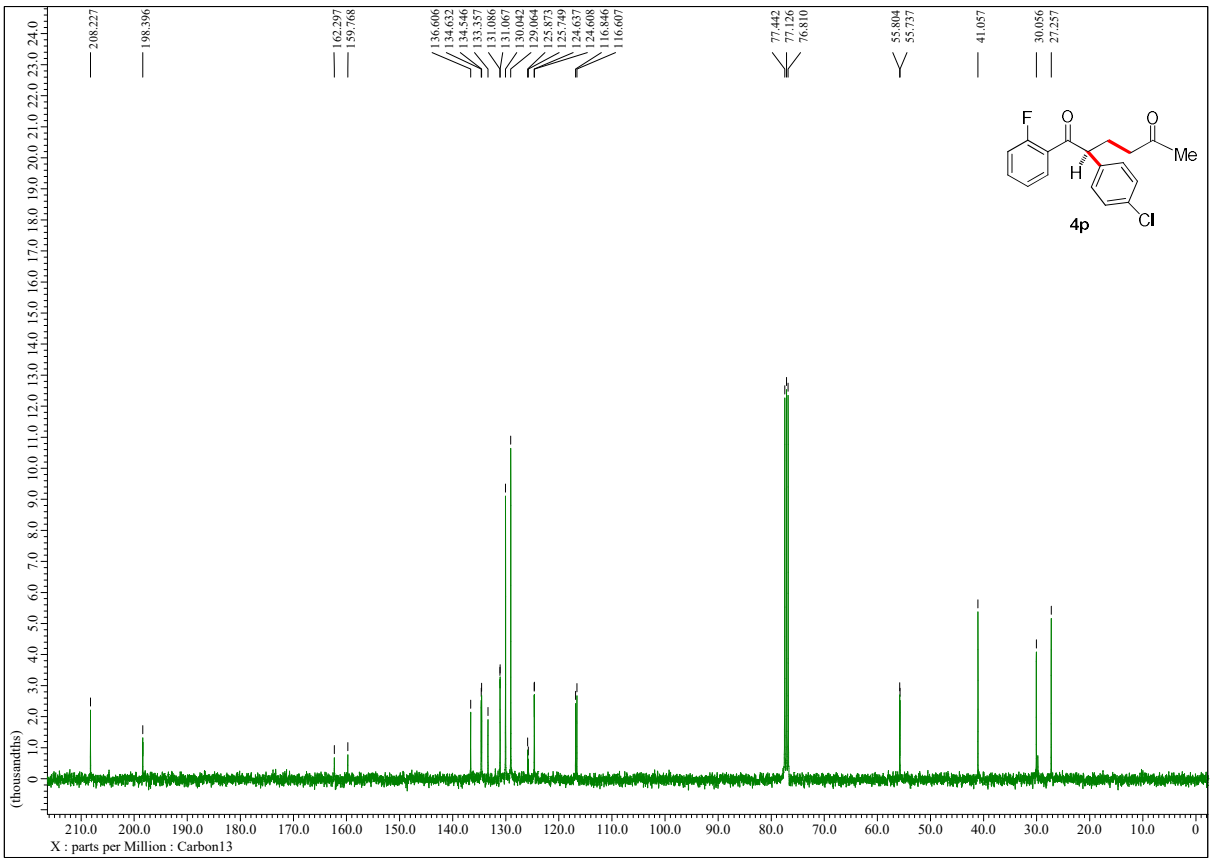
7.696
7.467
7.449
7.433
7.416
7.267
7.254
7.232
7.178
7.156
7.135
7.061
7.039
7.034
7.012
4.535
4.518
4.502
2.446
2.408
2.379
2.097
2.059
2.042
2.013
0.000
F
O
O
Me
H
Cl
4p
4.62
3.27
3.13
2.35
1.13
1.01
0.98
0.28
abundance
X : parts per Million : Proton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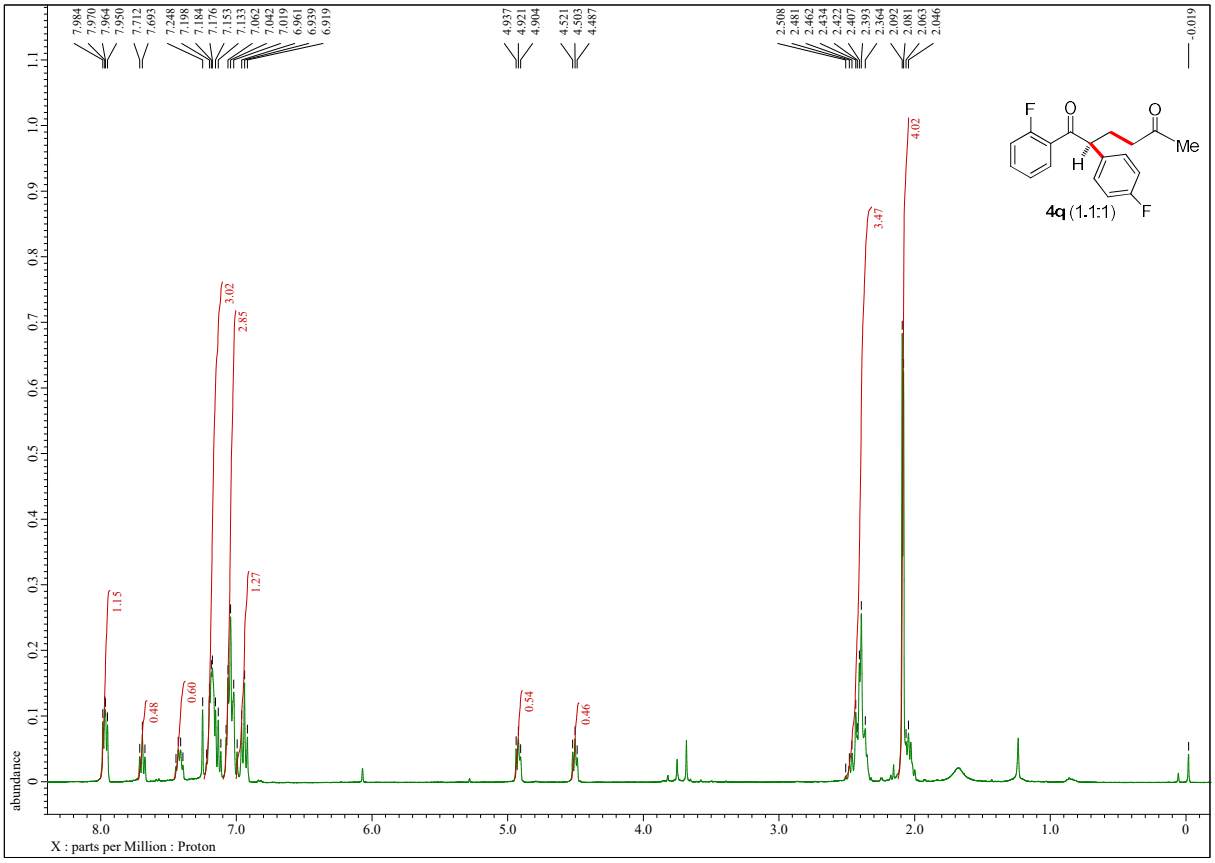
134.632
134.546
133.357
131.086
131.067
130.042
129.064
125.873
125.749
124.637
124.608
116.846
116.607
77.442
77.126
76.810
55.804
55.737
41.057
30.056
27.257
F
O
O
Me
H
Cl
4p
(thousandths)
X : parts per Million : Carbon13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7.950
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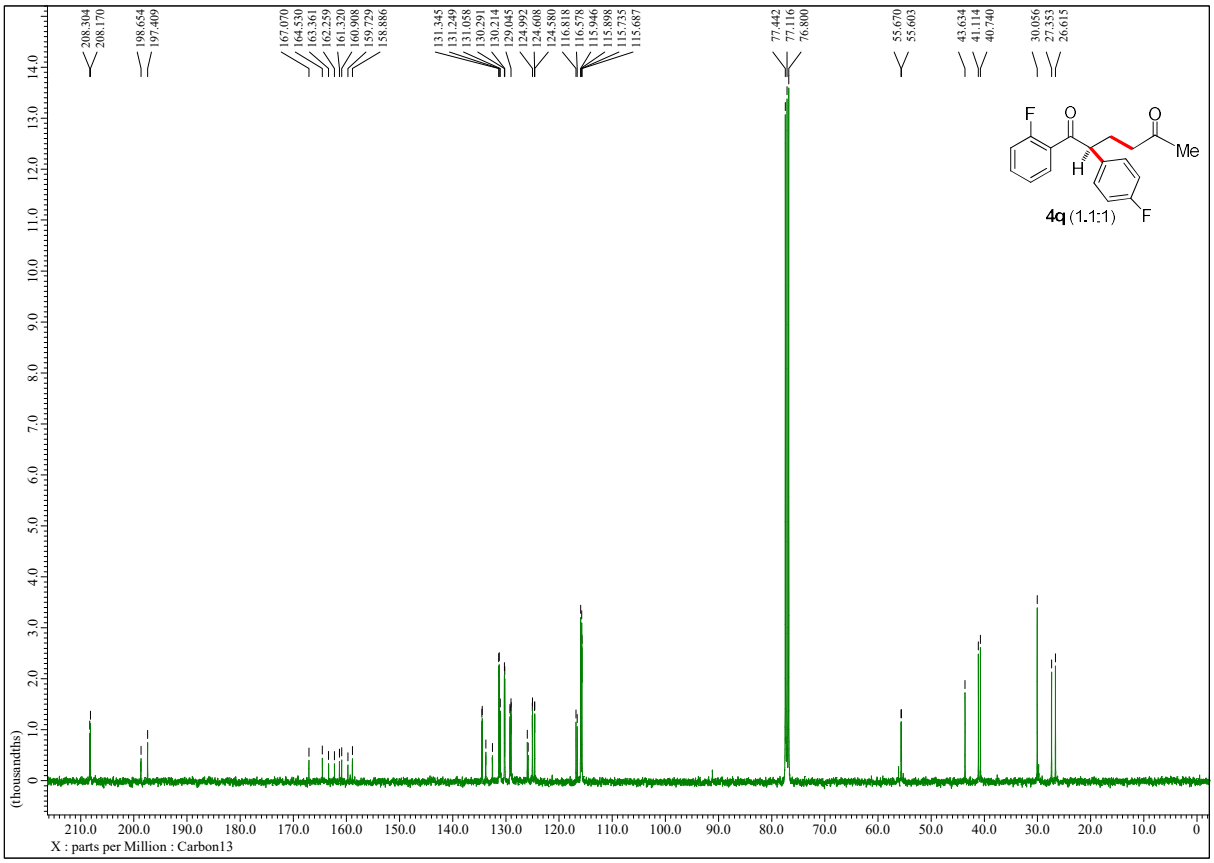
7.693
7.248
7.198
7.184
7.176
7.153
7.133
7.062
7.042
7.019
6.961
6.939
6.919
4.937
4.921
4.904
4.521
4.503
4.487
2.508
2.481
2.462
2.434
2.422
2.407
2.393
2.364
2.092
2.081
2.063
2.046
-0.019
1.15
0.48
0.60
3.02
2.85
1.27
0.54
0.46
3.47
4.02
F
O
O
Me
H
F
4q (1.1:1)
abundance
X : parts per Million : Proton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163.361
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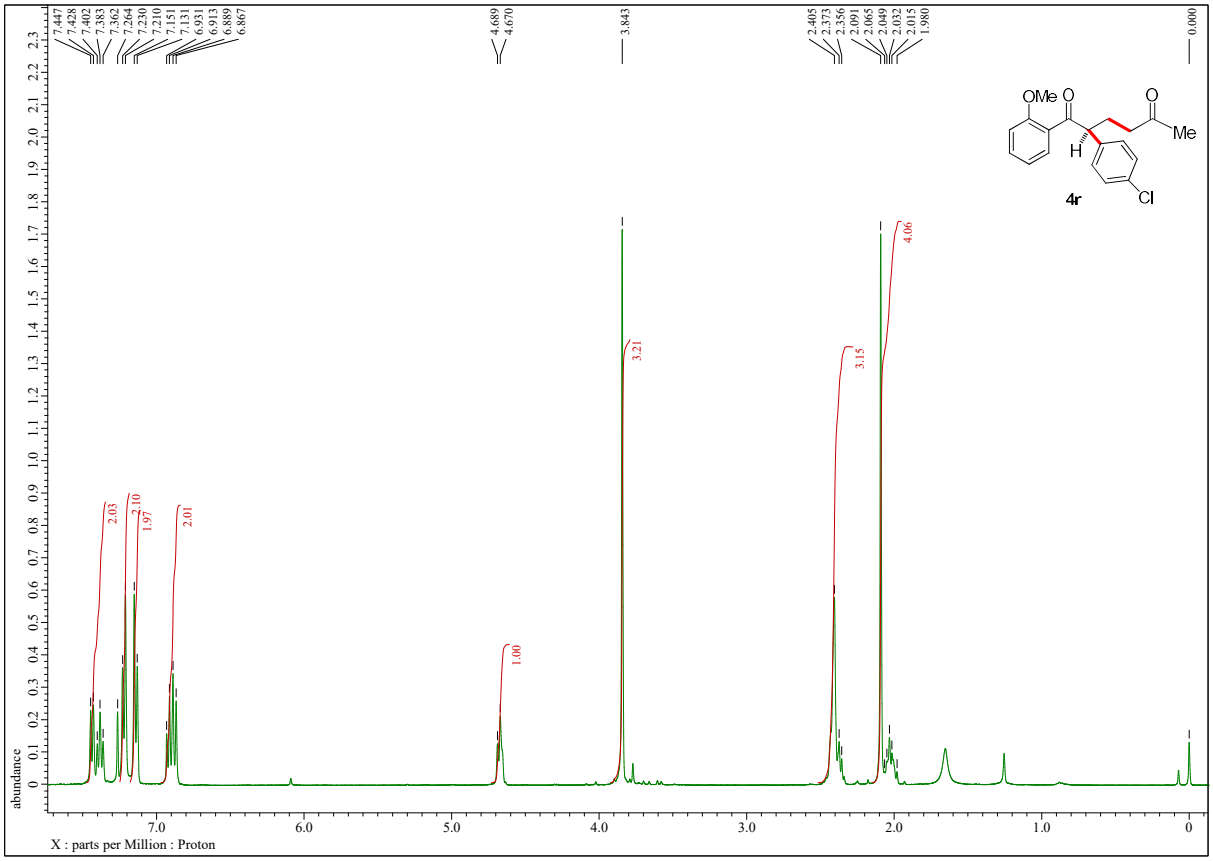
160.908
159.729
158.886
131.345
131.249
131.058
130.291
130.214
129.045
124.992
124.608
124.580
116.818
116.578
115.946
115.898
115.735
115.687
77.442
77.116
76.800
55.670
55.603
43.634
41.114
40.740
30.056
27.353
26.615
F
O
O
Me
H
F
4q (1.1:1)
(thousandths)
X : parts per Million : Carbon13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7.230
7.210
7.151
7.131
6.931
6.913
6.889
6.867
4.689
4.670
3.843
2.405
2.373
2.356
2.091
2.065
2.049
2.032
2.015
1.980
0.000
OMe
O
O
Me
H
Cl
4r
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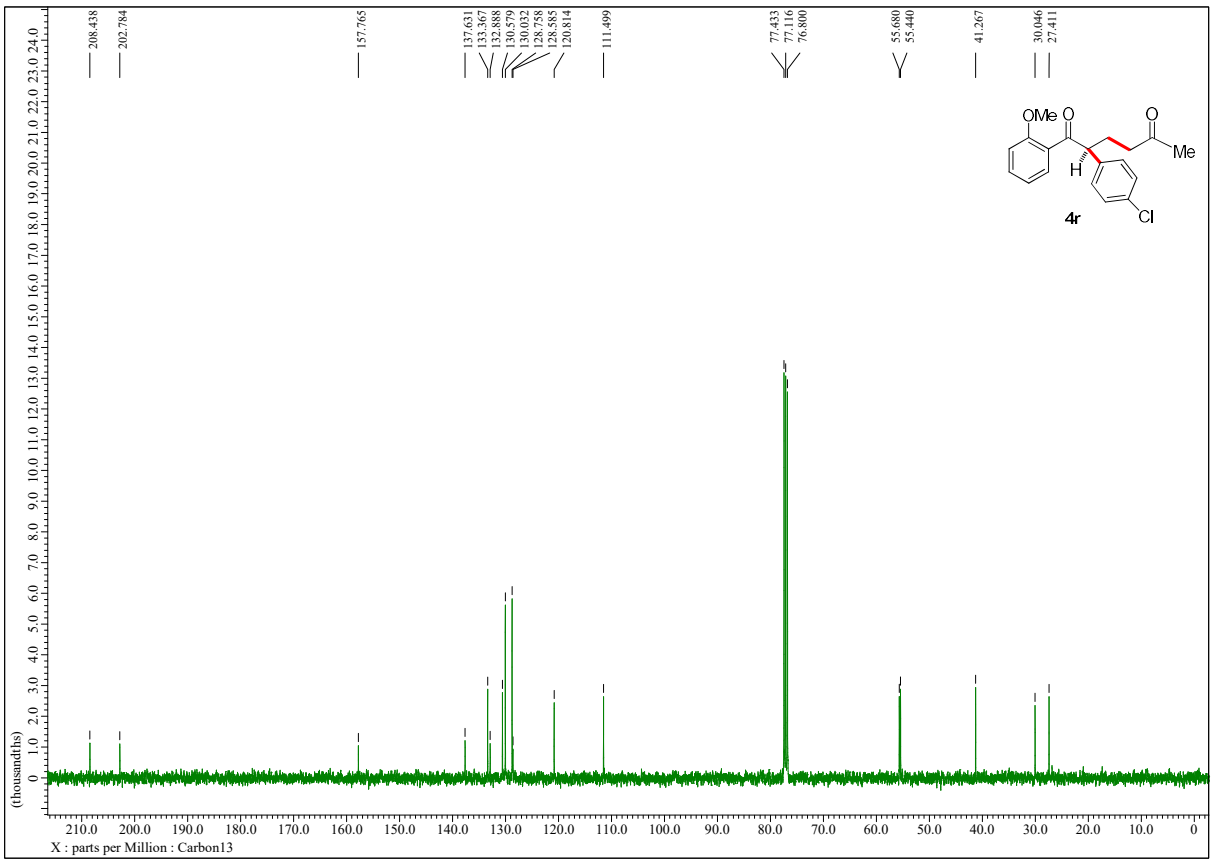
2.10
1.97
2.01
1.00
3.21
3.15
4.06
abundance
X : parts per Million : Proton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157.765
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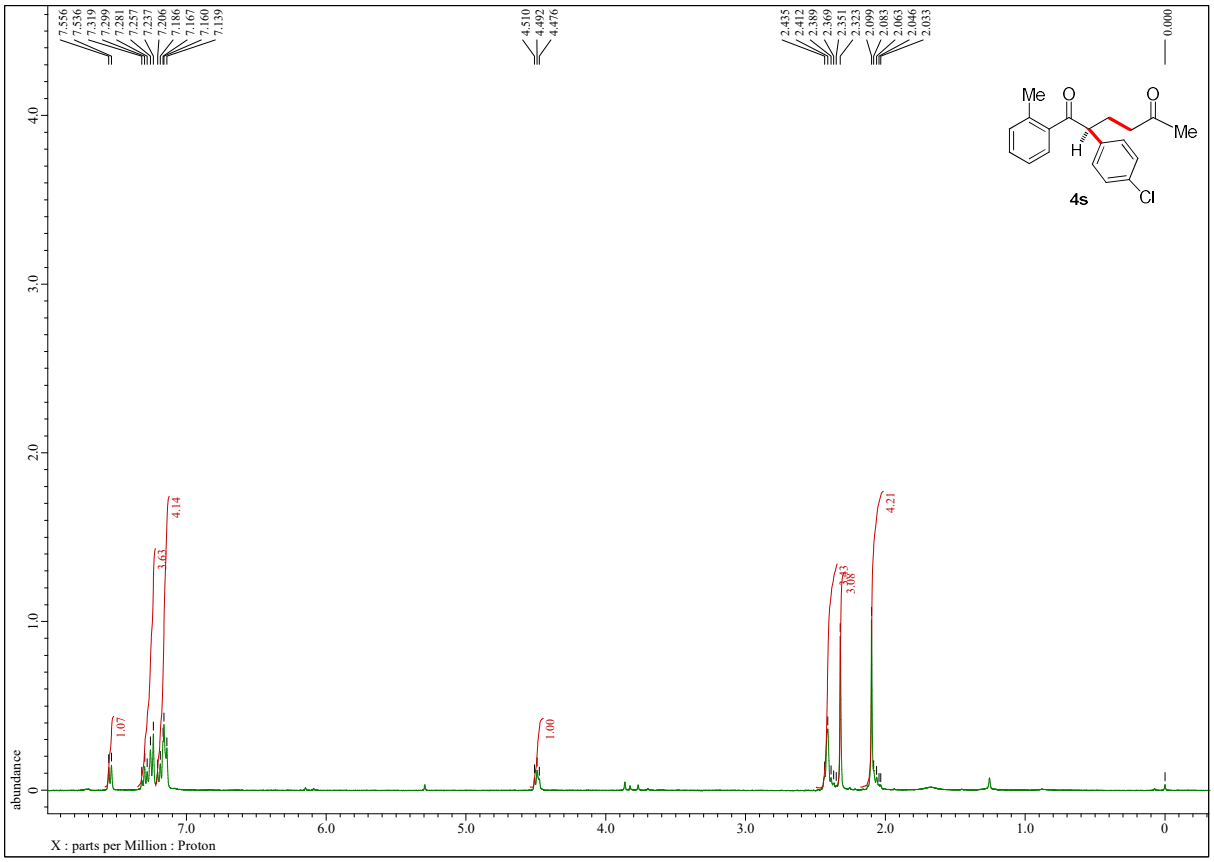
133.367
132.888
130.579
130.032
128.758
128.585
120.814
111.499
77.433
77.116
76.800
55.680
55.440
41.267
30.046
27.411
OMe
O
O
Me
H
Cl
4r
(thousandths)
X : parts per Million : Carbon13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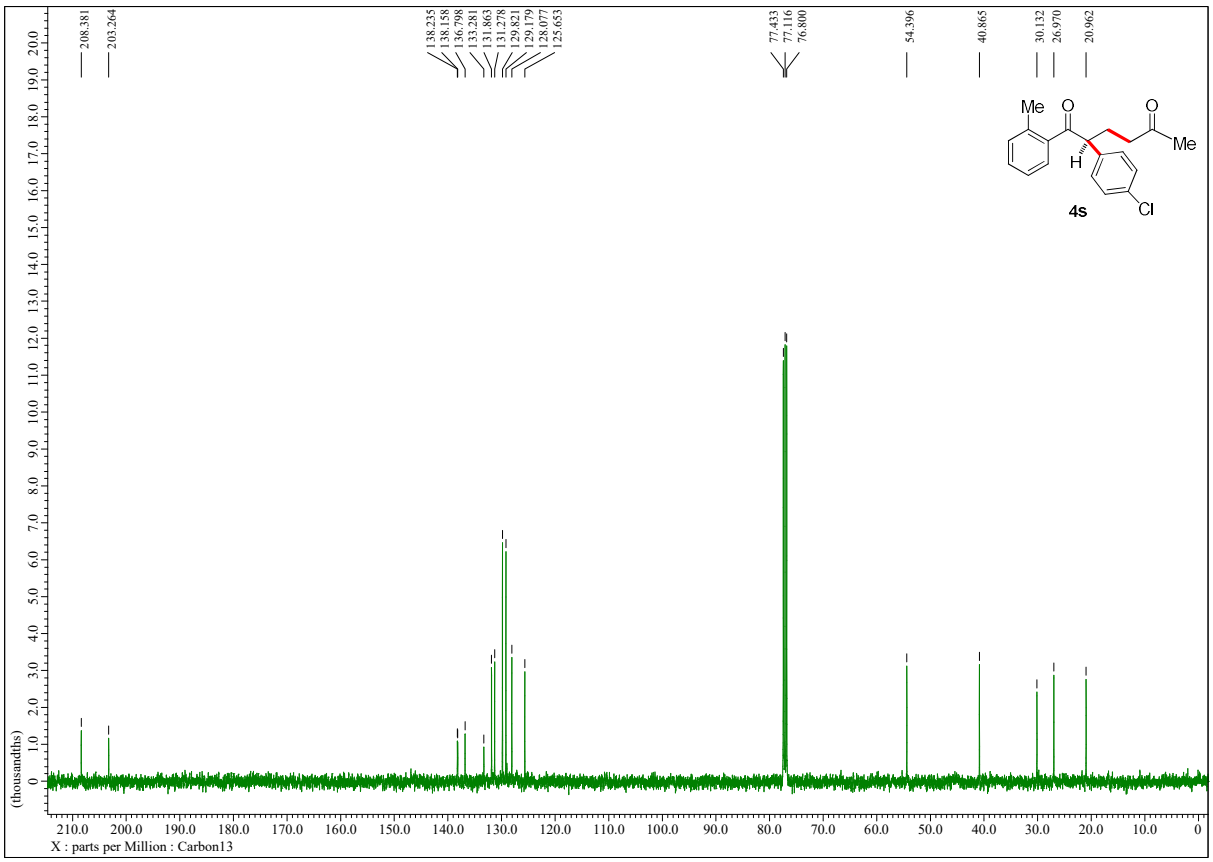
7.206
7.186
7.167
7.160
7.139
4.510
4.492
4.476
2.435
2.412
2.389
2.369
2.351
2.323
2.099
2.083
2.063
2.046
2.033
0.000
Me
O
O
Me
H
Cl
4s
4.14
3.63
4.21
3.08
1.07
1.00
abundance
X : parts per Million : Proton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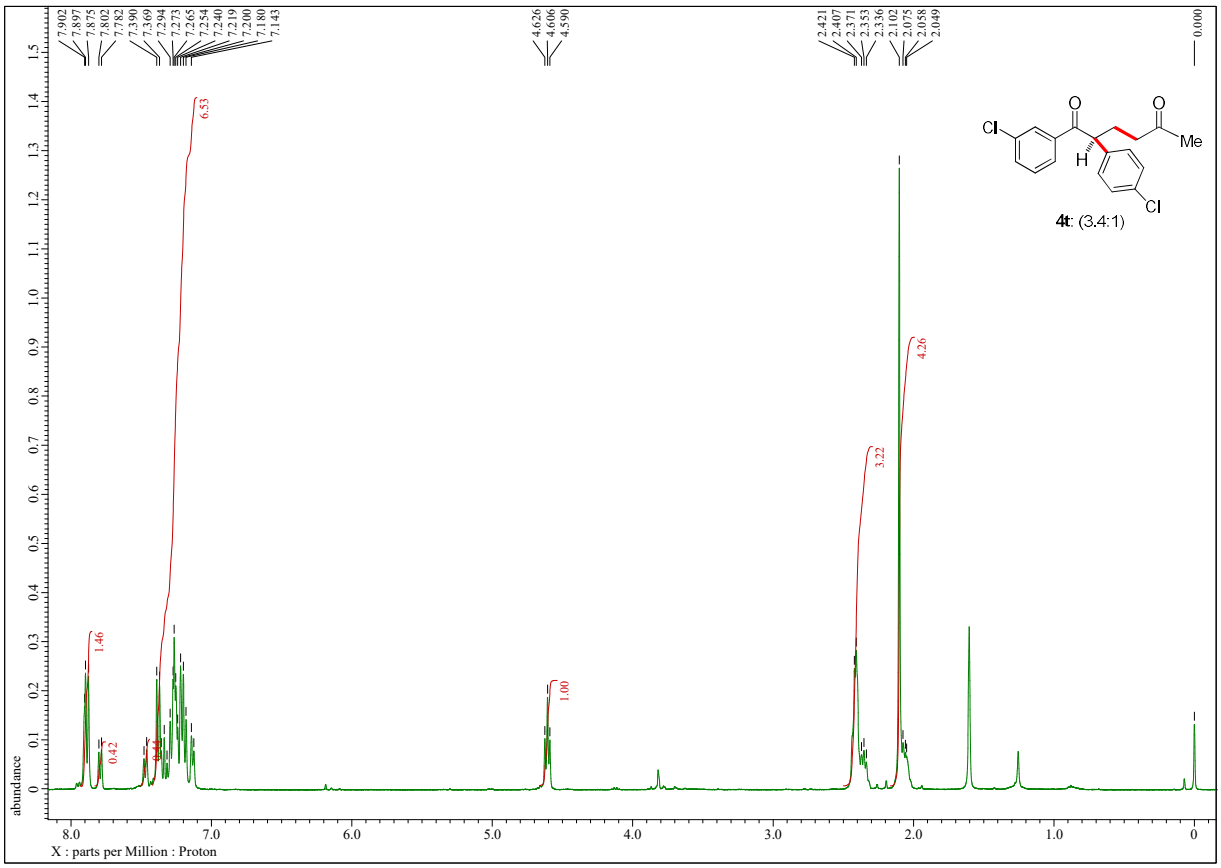
133.281
131.865
131.276
129.821
129.179
128.077
125.653
77.433
77.116
76.800
54.396
40.865
30.132
26.970
20.962
Me
O
O
Me
H
Cl
4s
(thousandths)
X : parts per Million : Carbon13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7.390
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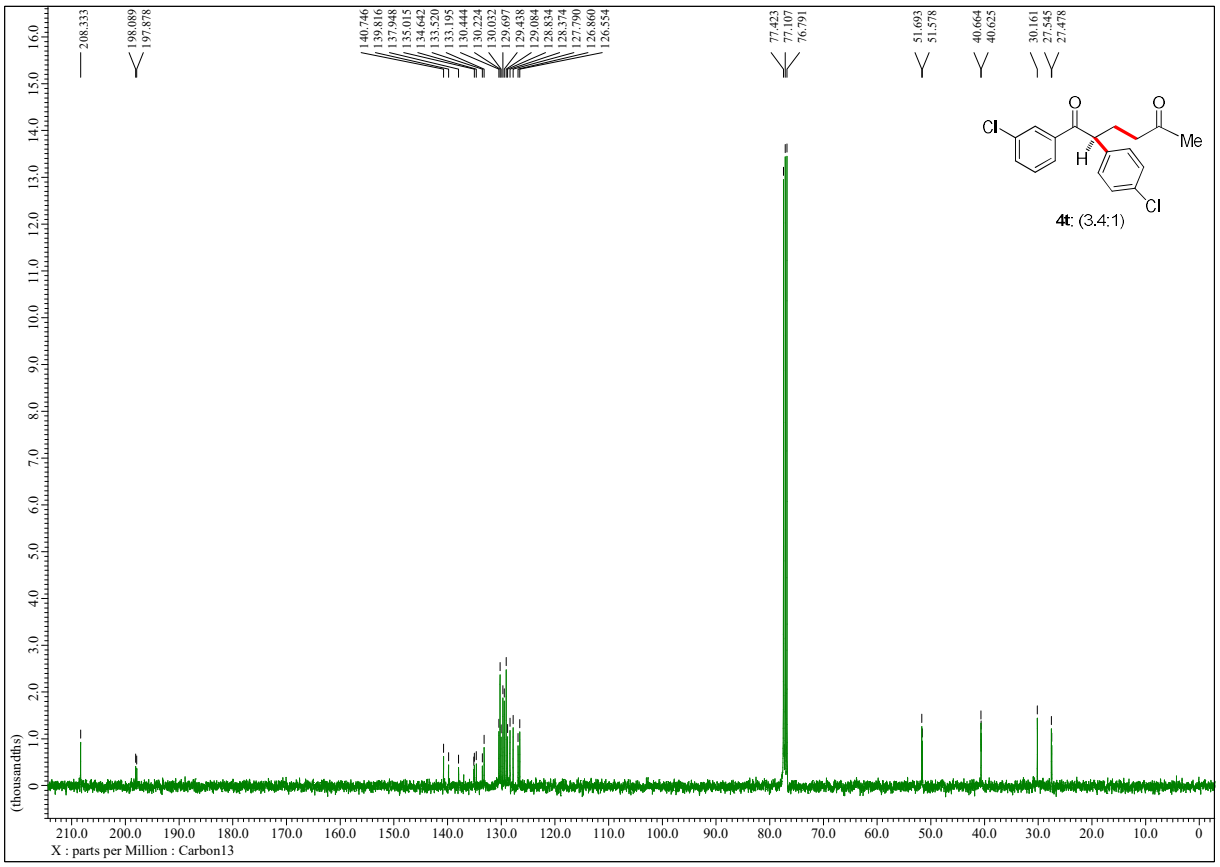
7.294
7.273
7.265
7.254
7.240
7.219
7.200
7.180
7.143
4.626
4.606
4.590
2.421
2.407
2.371
2.353
2.336
2.102
2.075
2.058
2.049
0.000
6.53
4.26
3.22
1.46
0.42
1.00
abundance
X : parts per Million : Proton
Cl
O
O
Me
H
Cl
4t: (3.4:1)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137.948
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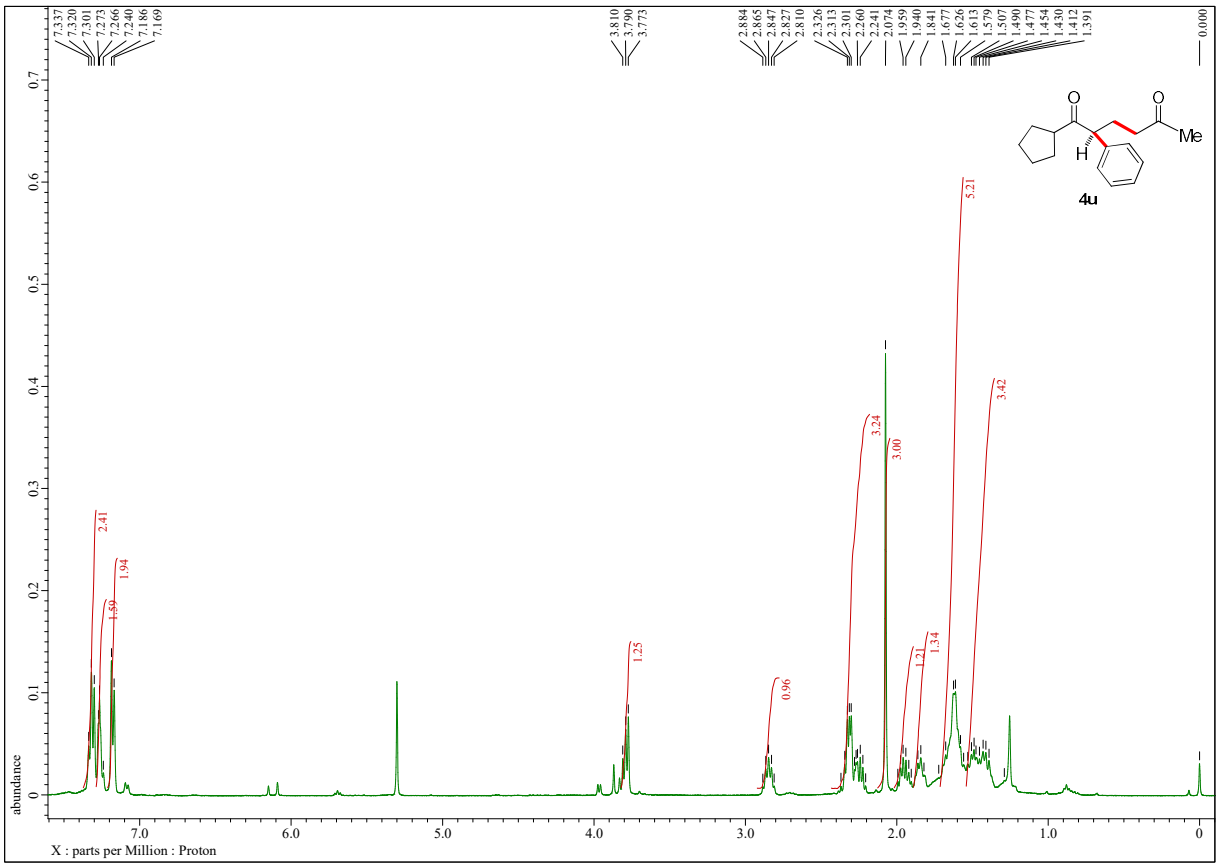
134.642
133.520
133.195
130.444
130.224
130.032
129.697
129.438
129.084
128.834
128.374
127.790
126.860
126.554
77.423
77.107
76.791
51.693
51.578
40.664
40.625
30.161
27.545
27.478
(thousandths)
X : parts per Million : Carbon13
Cl
O
O
Me
H
Cl
4t: (3.4:1)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3.790
3.773
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2.865
2.847
2.827
2.810
2.326
2.313
2.301
2.260
2.241
2.074
1.959
1.940
1.841
1.677
1.626
1.613
1.579
1.507
1.490
1.477
1.454
1.430
1.412
1.391
0.000
O
O
Me
H
4u
5.21
3.42
3.24
3.00
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1.94
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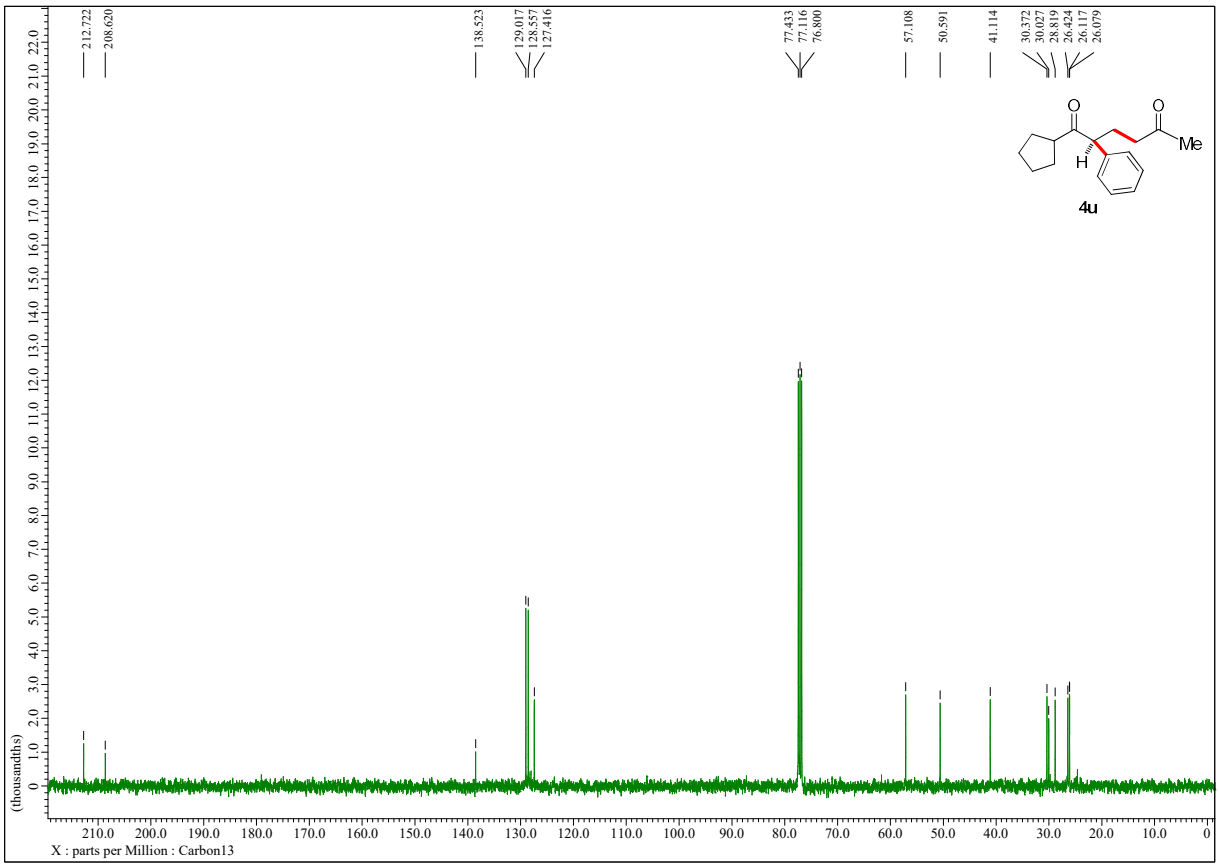
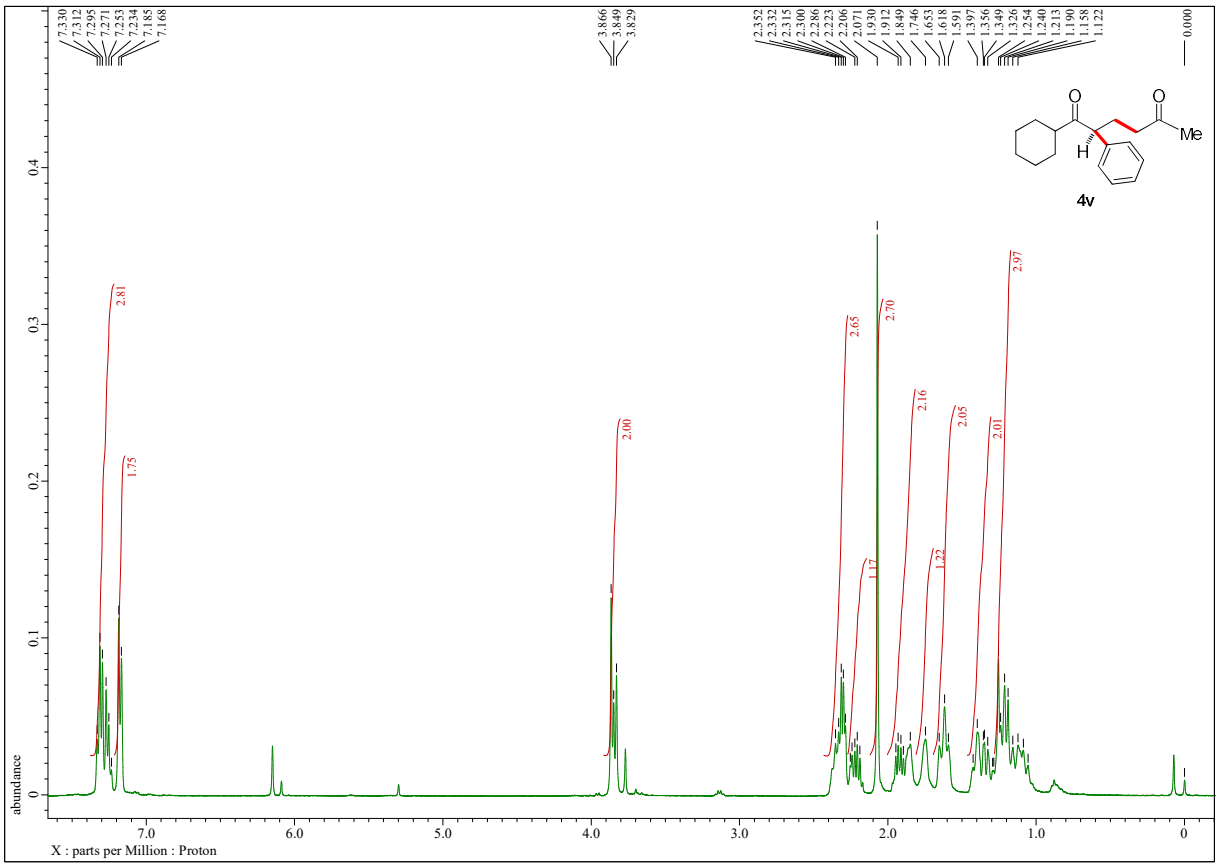
1.25
1.21
1.34
0.96
abundance
X : parts per Million : Proton


212.722
208.620
138.523
129.017
128.557
127.416
77.433
77.116
76.800
57.108
50.591
41.114
30.372
30.027
28.819
26.424
26.117
26.079
O
O
Me
H
4u
(thousandths)
X : parts per Million : Carbon13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7.234
7.185
7.168
3.866
3.849
3.829
2.352
2.332
2.315
2.300
2.286
2.223
2.206
2.071
1.930
1.912
1.849
1.746
1.653
1.618
1.591
1.397
1.356
1.349
1.326
1.254
1.240
1.213
1.190
1.158
1.122
0.000
O
O
Me
H
4v
2.81
1.75
2.00
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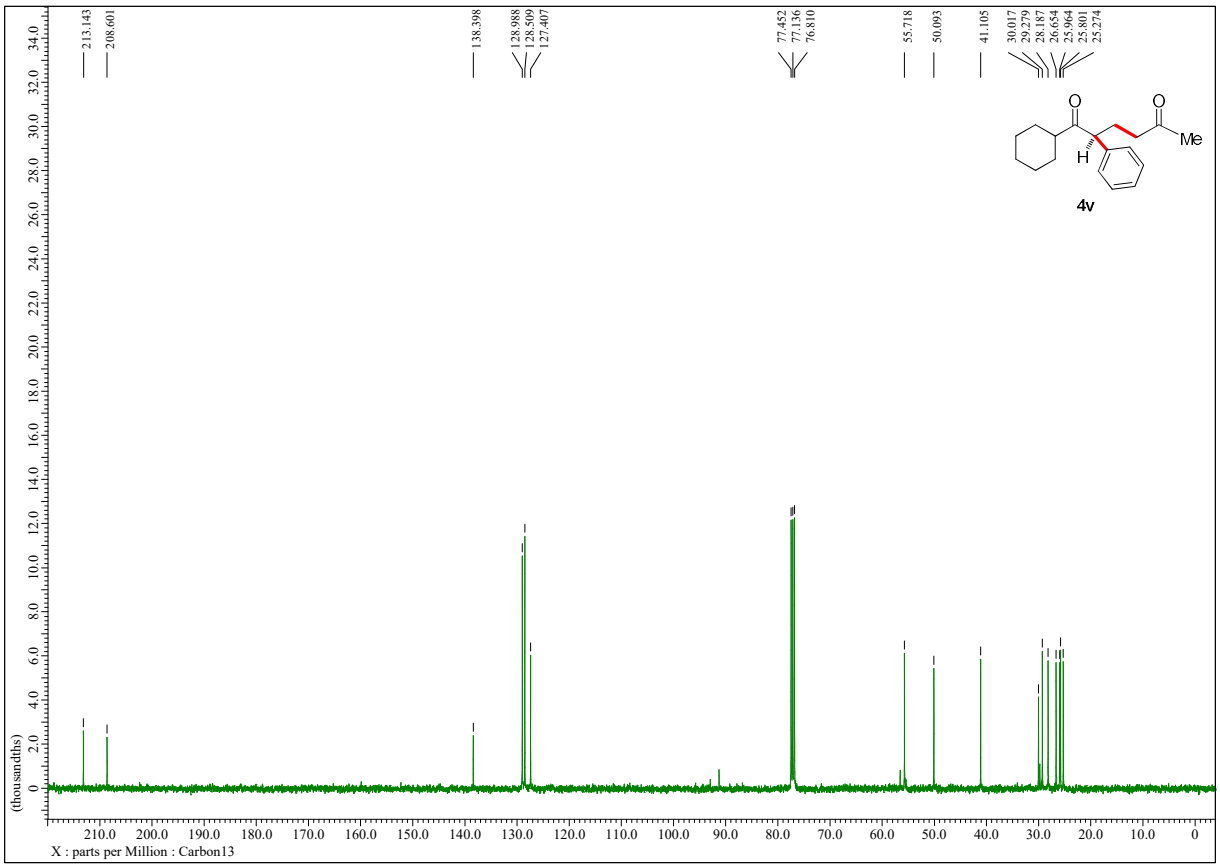
2.70
2.16
1.22
2.05
2.01
2.97
abundance
X : parts per Million : Proton


213.143
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128.988
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127.407
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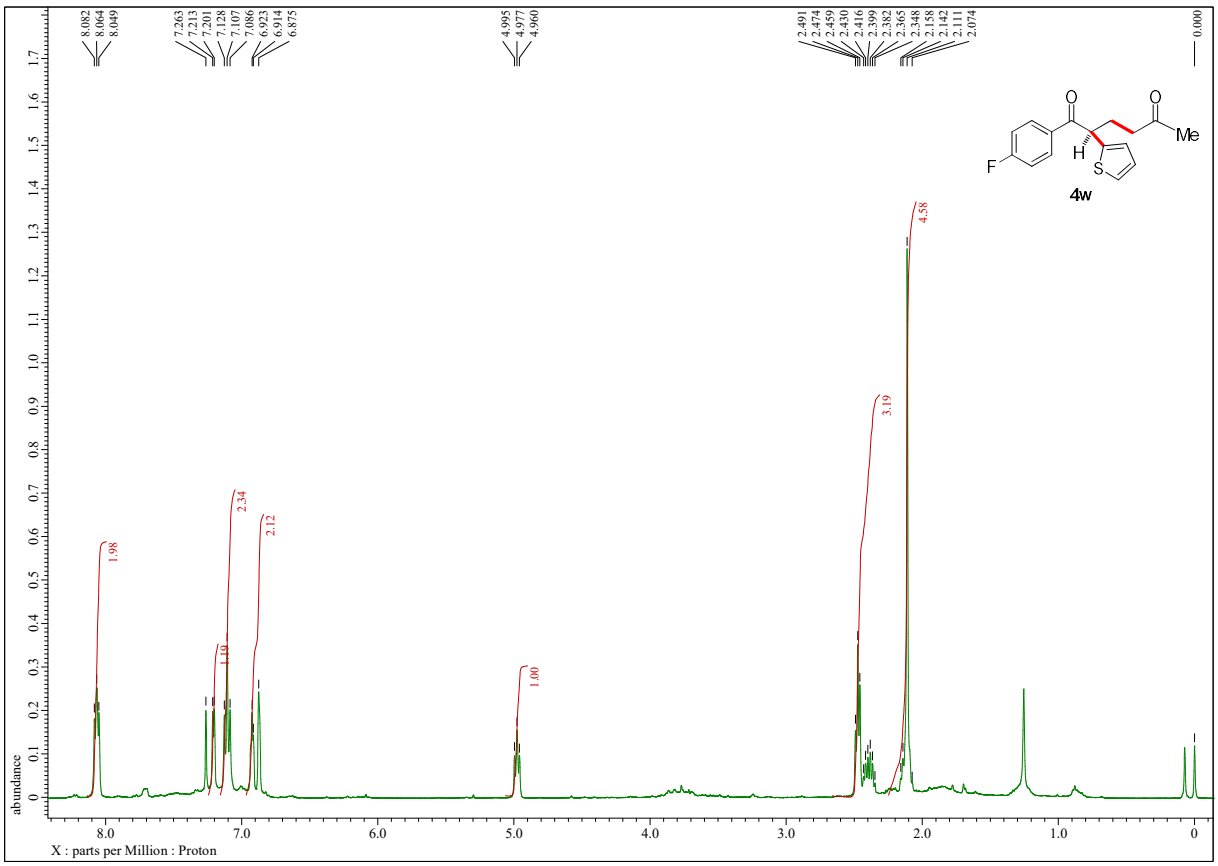
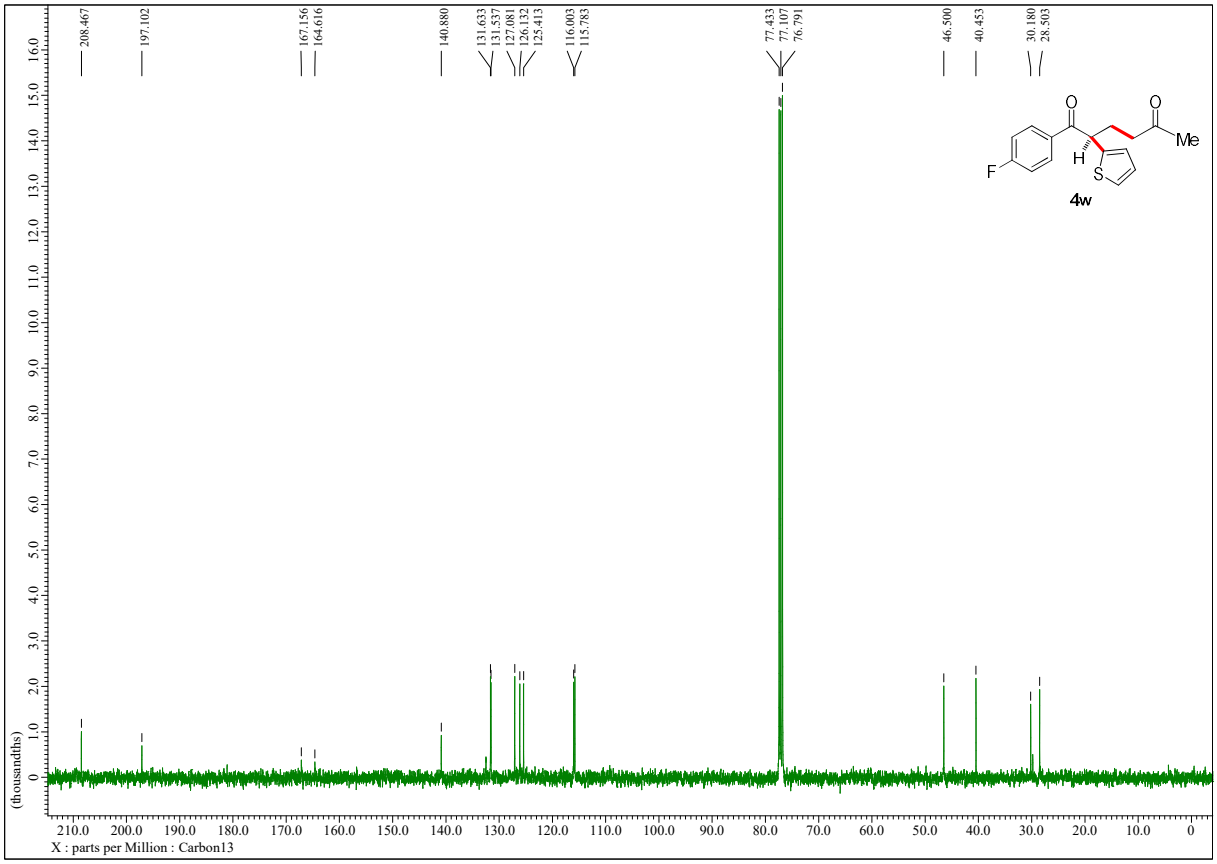
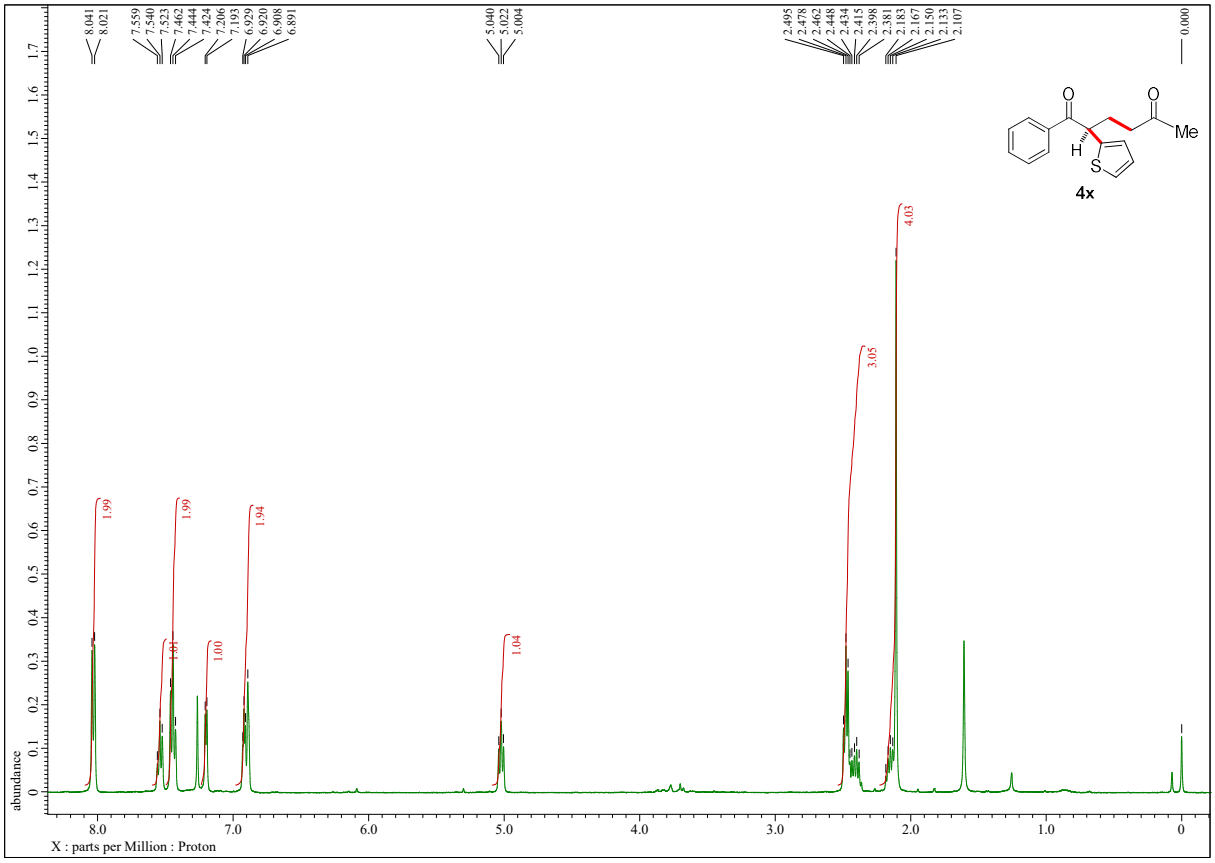
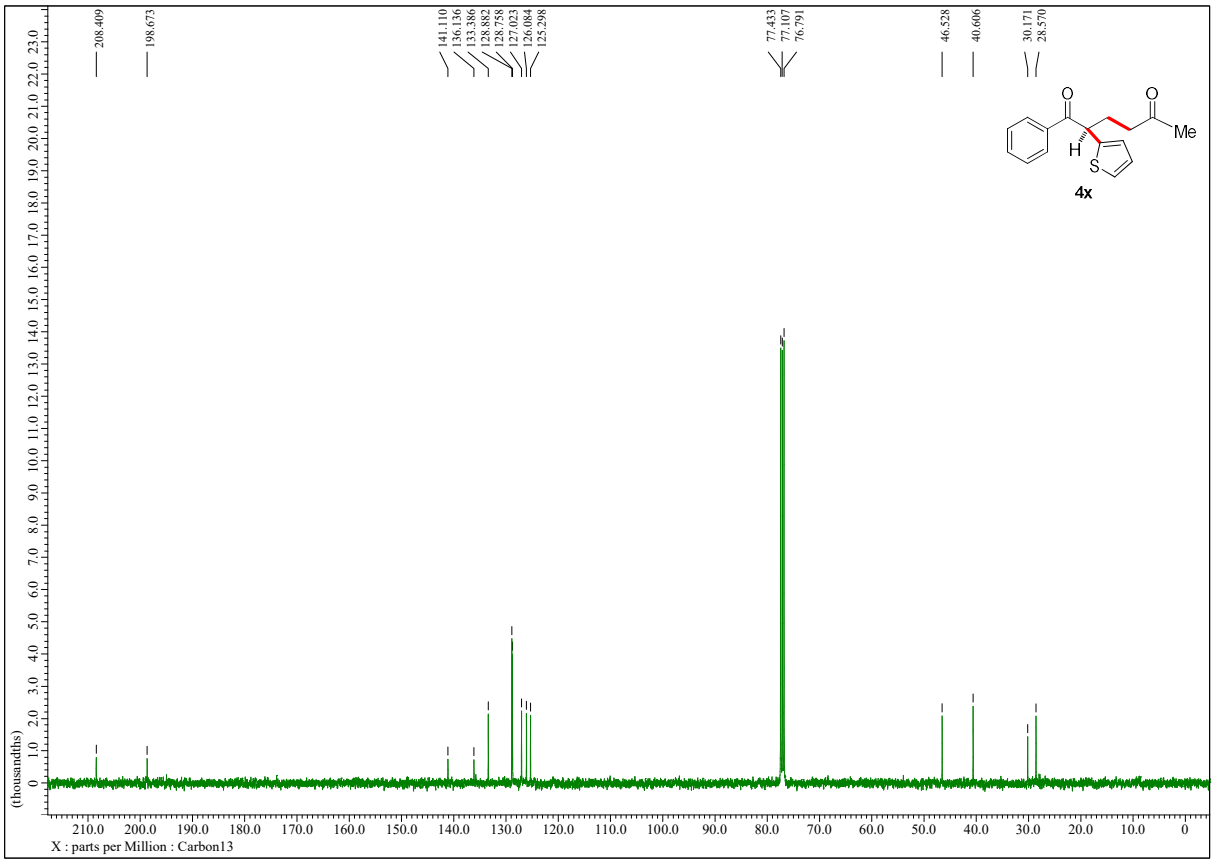
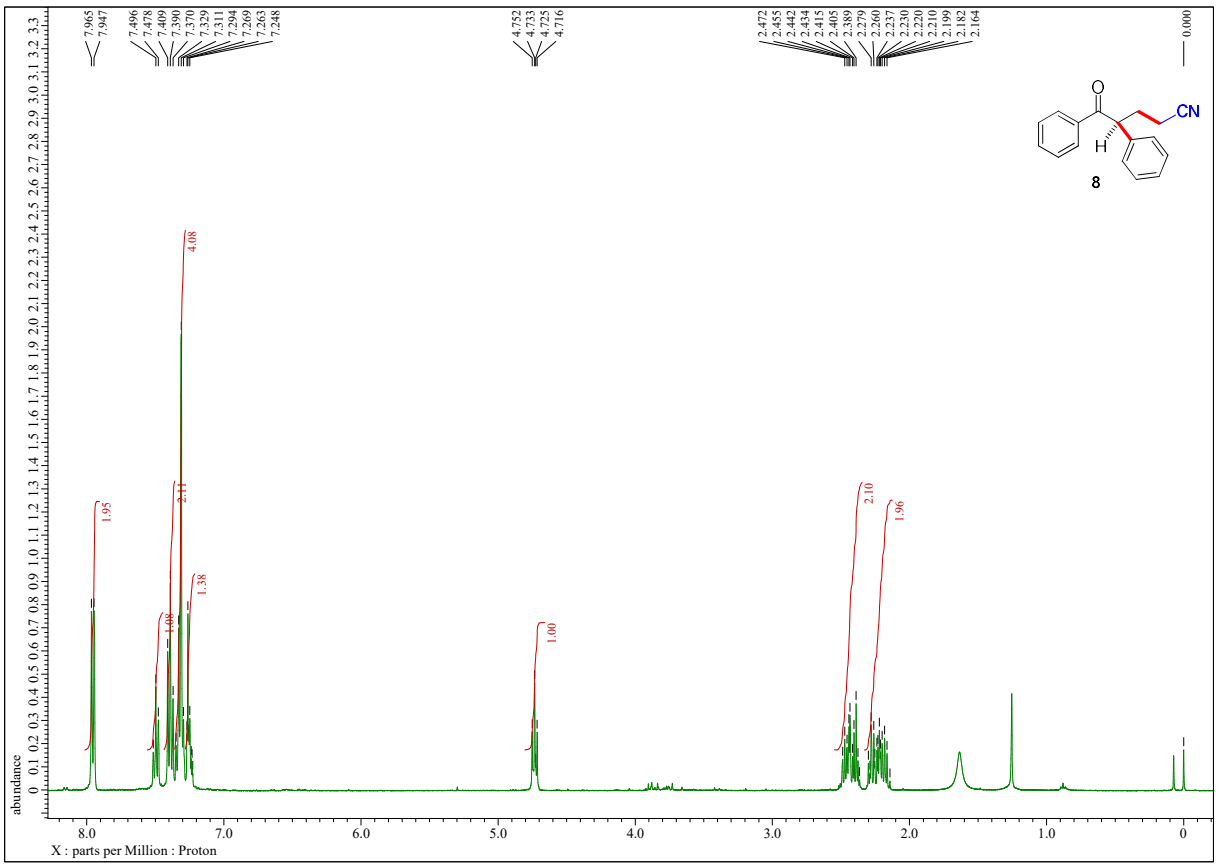
77.136
76.810
55.718
50.093
41.105
30.017
29.279
28.187
26.654
25.964
25.801
25.274
O
O
Me
H
4v
(thousandths)
X : parts per Million : Carbon13

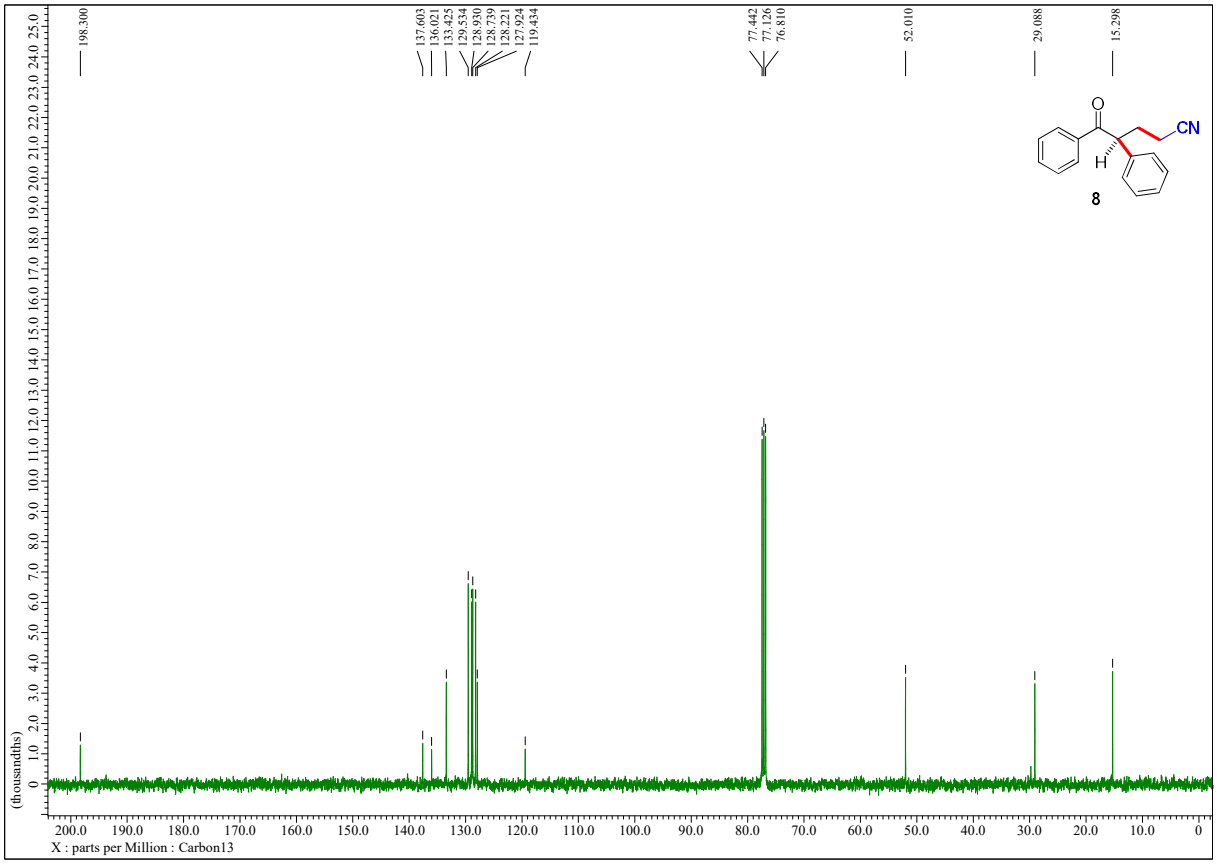

8.082
8.064
8.049
7.263
7.213
7.201
7.128
7.107
7.086
6.923
6.914
6.875
4.995
4.977
4.960
2.491
2.474
2.459
2.430
2.416
2.399
2.382
2.365
2.348
2.158
2.142
2.111
2.074
0.000
1.98
2.34
2.12
1.10
1.00
3.19
4.58
abundance
X : parts per Million : Proton
O
O
Me
H
S
F
4w

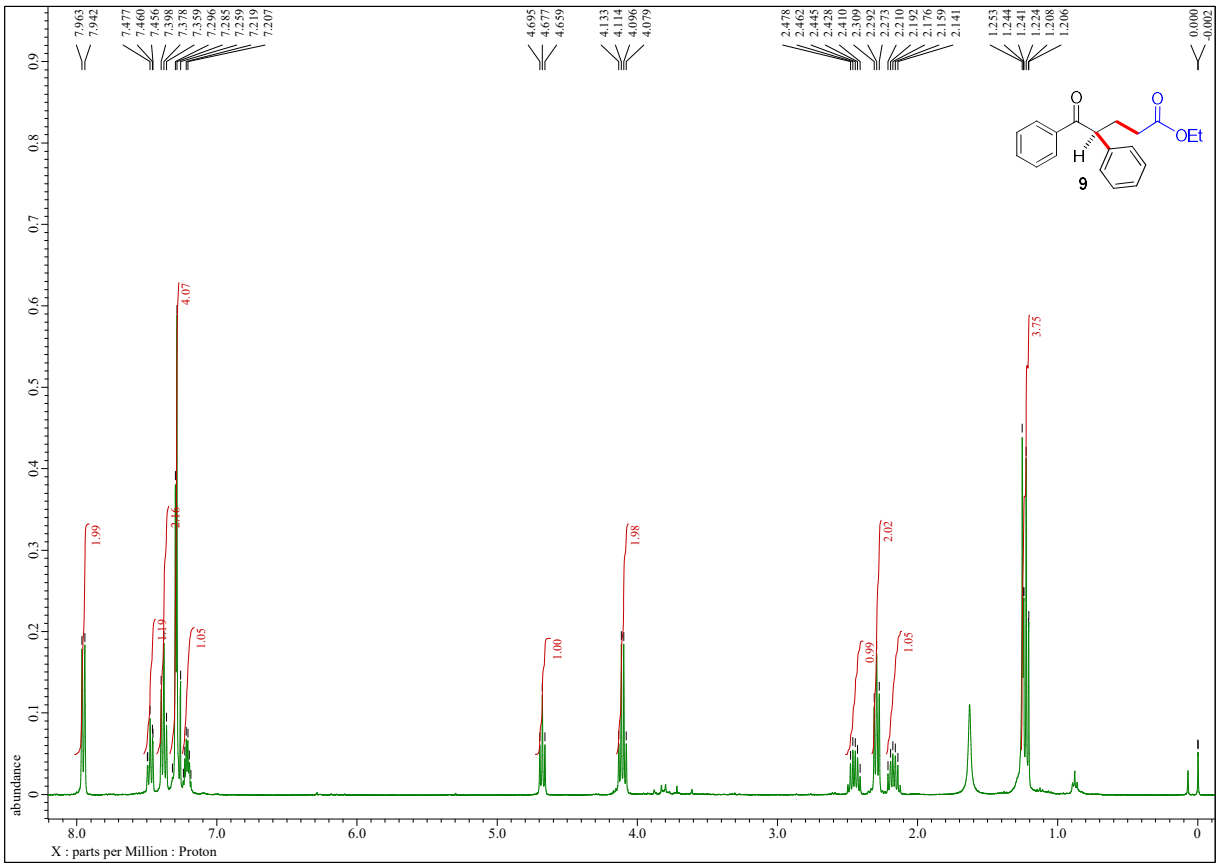

208.467
197.102
167.156
164.616
140.880
131.633
131.537
127.081
126.132
125.413
116.903
115.783
77.433
77.107
76.791
46.500
40.453
30.180
28.503
(thousandths)
X : parts per Million : Carbon13
O
O
Me
H
S
F
4w

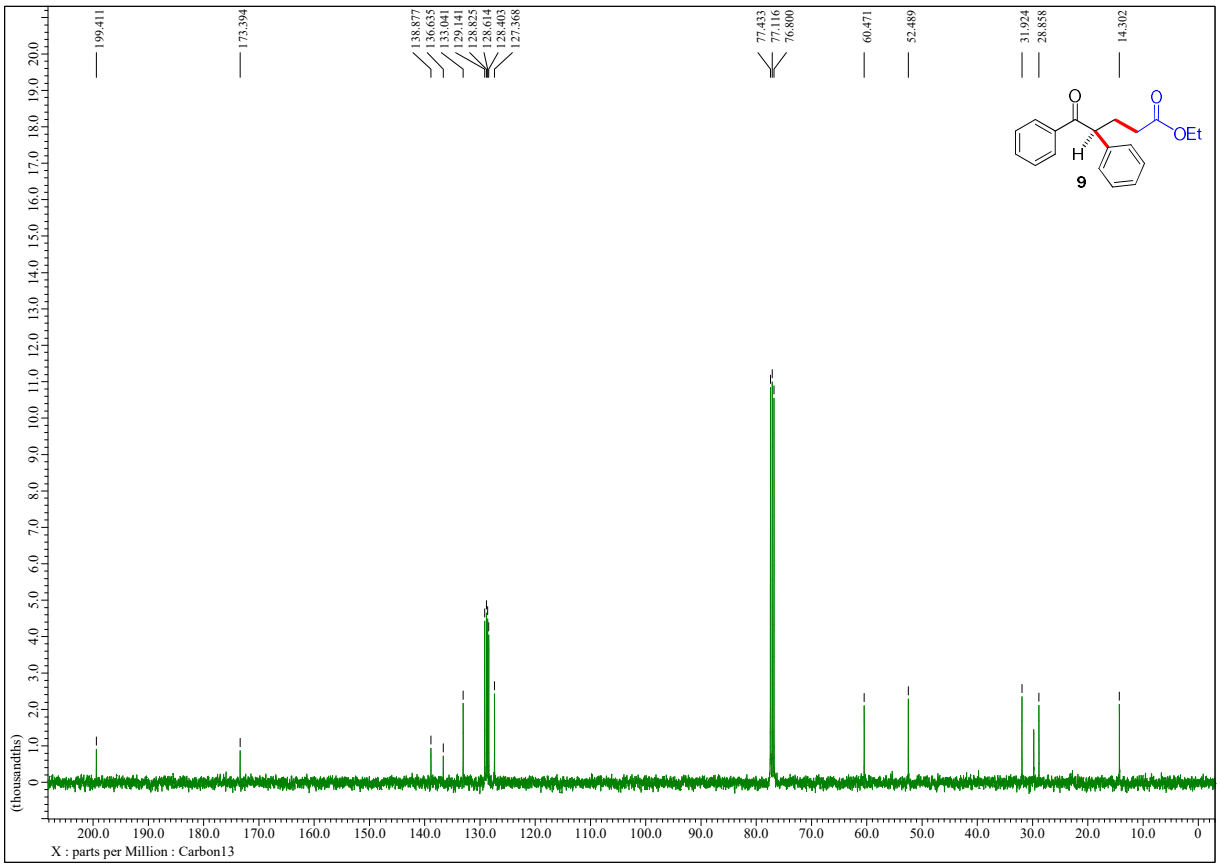

8.041
8.021
7.559
7.540
7.523
7.462
7.444
7.424
7.206
7.193
6.929
6.920
6.908
6.891
5.040
5.022
5.004
2.495
2.478
2.462
2.448
2.434
2.415
2.398
2.381
2.183
2.167
2.150
2.133
2.107
0.000
1.99
1.99
1.94
1.81
1.00
1.04
3.05
4.03
abundance
X : parts per Million : Proton
O
O
Me
H
S
4x

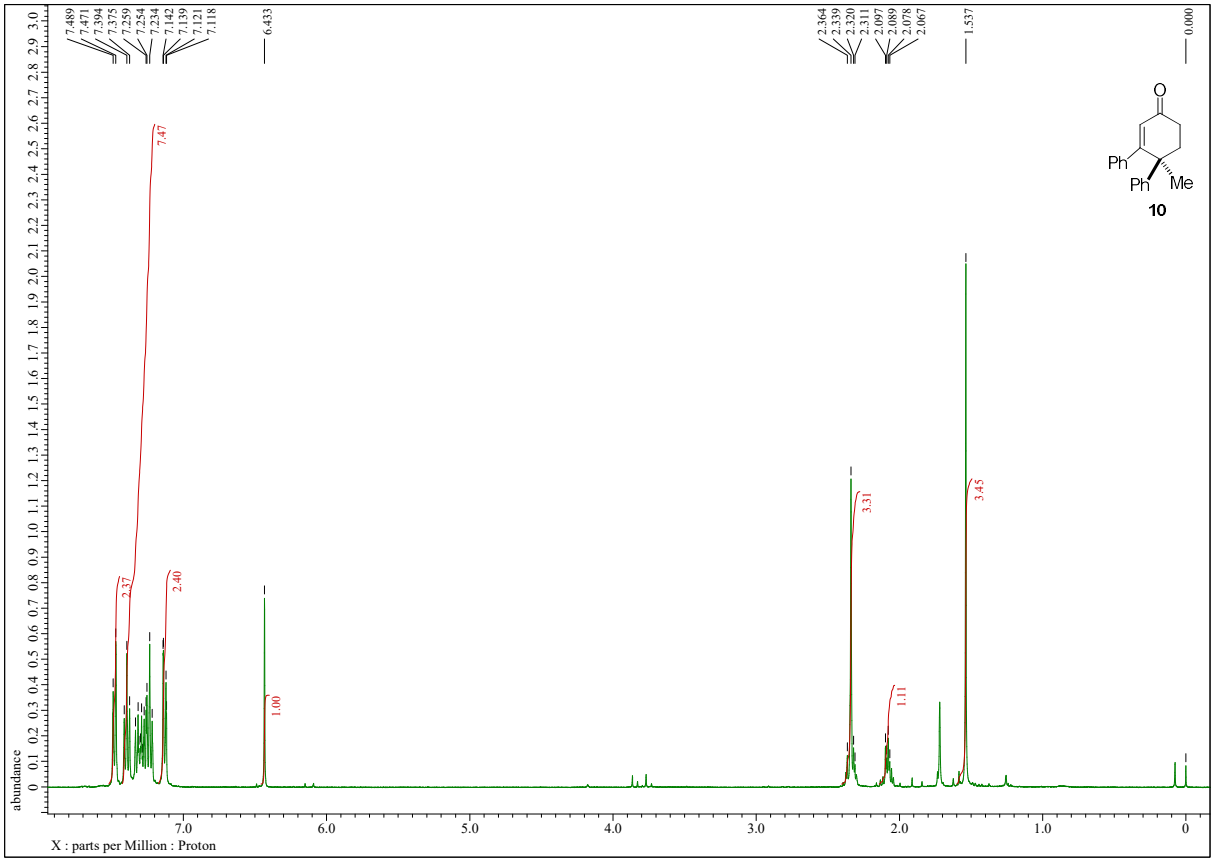

208.409
198.673
141.110
136.136
133.386
128.882
128.758
127.023
126.084
125.298
77.433
77.107
76.791
46.528
40.606
30.171
28.570
(thousandths)
X : parts per Million : Carbon13
O
O
Me
H
S
4x

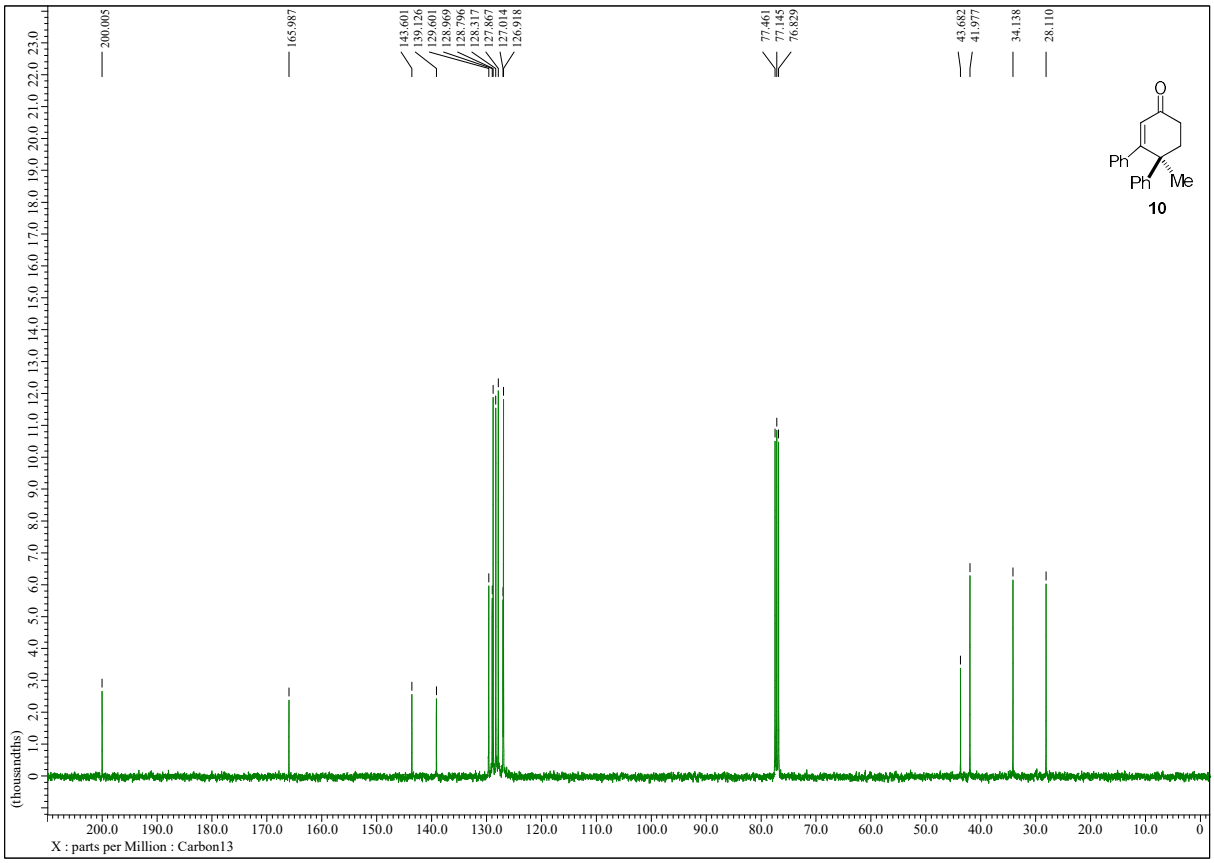

7.965
7.947
7.496
7.478
7.409
7.390
7.370
7.329
7.311
7.294
7.269
7.263
7.248
4.752
4.733
4.725
4.716
2.472
2.455
2.442
2.434
2.415
2.405
2.389
2.279
2.260
2.237
2.230
2.220
2.210
2.199
2.182
2.164
0.000
1.95
4.08
2.11
1.38
1.08
1.00
2.10
1.96
abundance
X : parts per Million : Proton
O
CN
H
8

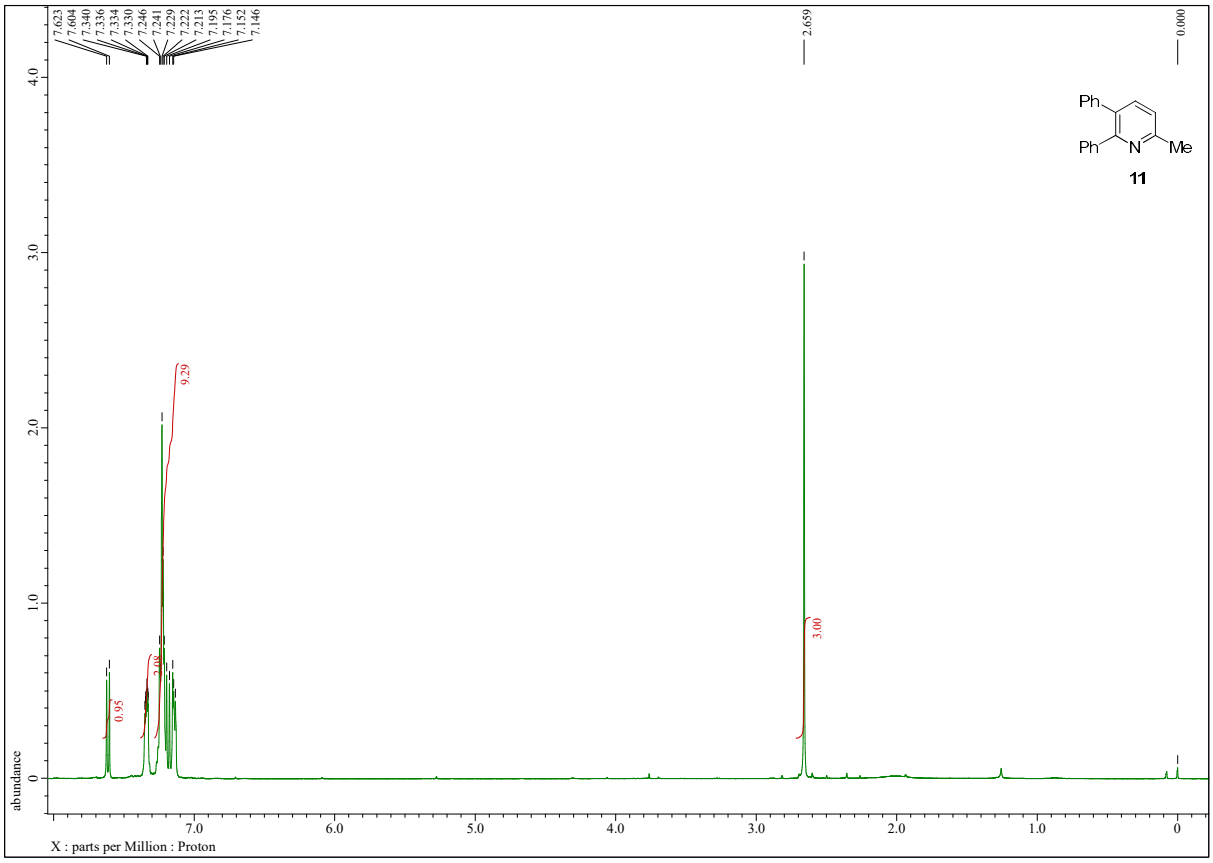

198.300
137.603
136.021
133.425
129.534
128.930
128.739
128.221
127.924
119.434
77.442
77.126
76.810
52.010
29.088
15.298
(thousandths)
X : parts per Million : Carbon13
O
CN
H
8

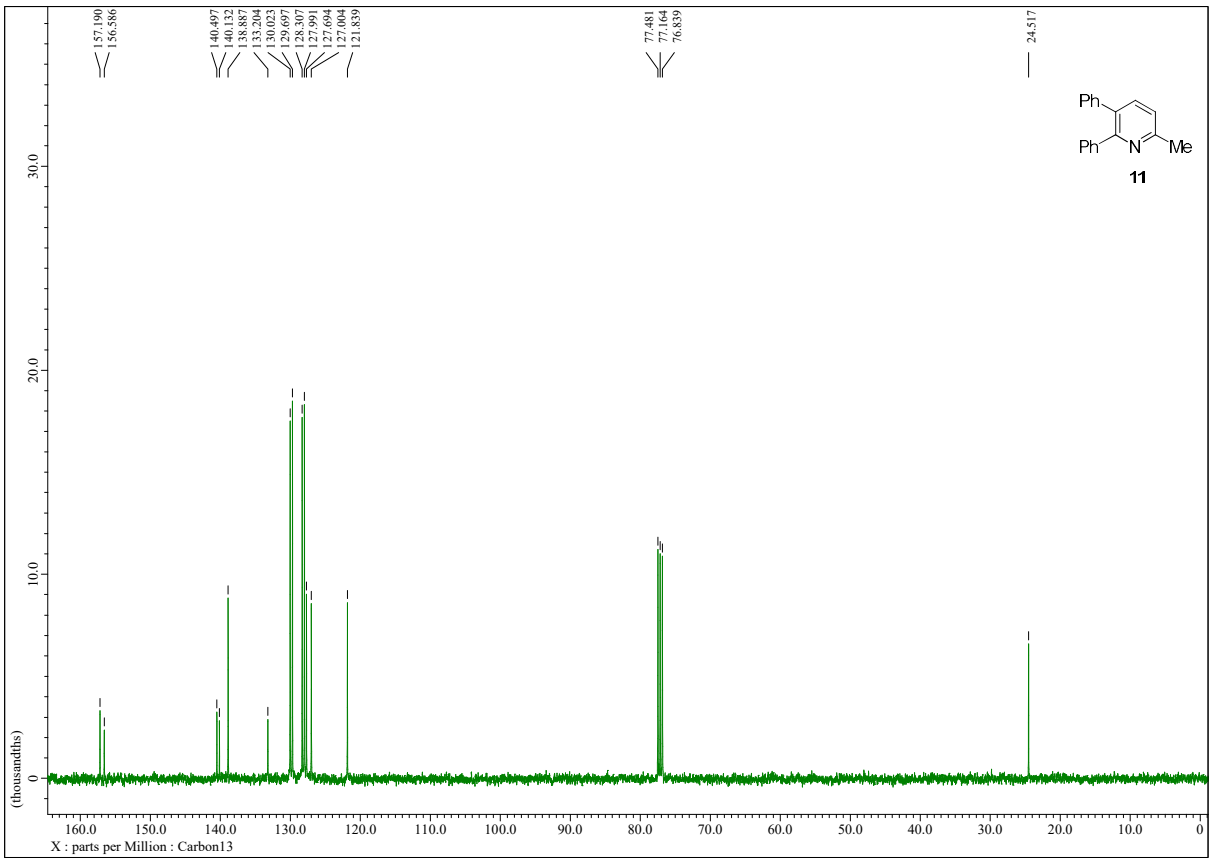

7.963
7.942
7.477
7.460
7.456
7.398
7.378
7.359
7.296
7.285
7.259
7.219
7.207
4.695
4.677
4.659
4.133
4.114
4.096
4.079
2.478
2.462
2.445
2.428
2.410
2.309
2.292
2.273
2.210
2.192
2.176
2.159
2.141
1.253
1.244
1.241
1.224
1.208
1.206
0.000
-0.002
1.99
3.16
4.19
4.07
1.05
1.00
1.98
0.99
2.02
1.05
3.75
O
OEt
H
9
abundance
X : parts per Million : Proton

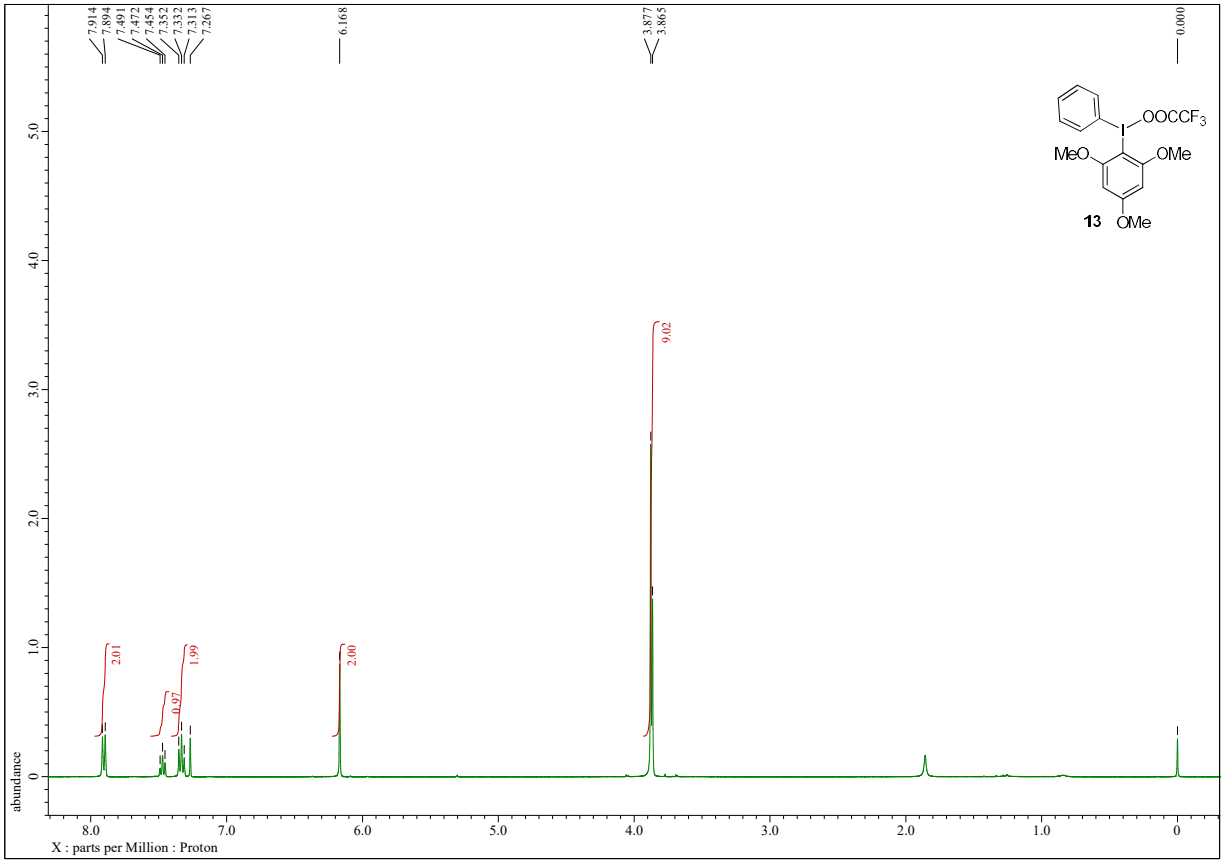

199.411
173.394
138.877
136.635
133.041
129.141
128.825
128.614
128.403
127.568
77.433
77.116
76.800
60.471
52.489
31.924
28.858
14.302
O
OEt
H
9
(thousandths)
X : parts per Million : Carbon13

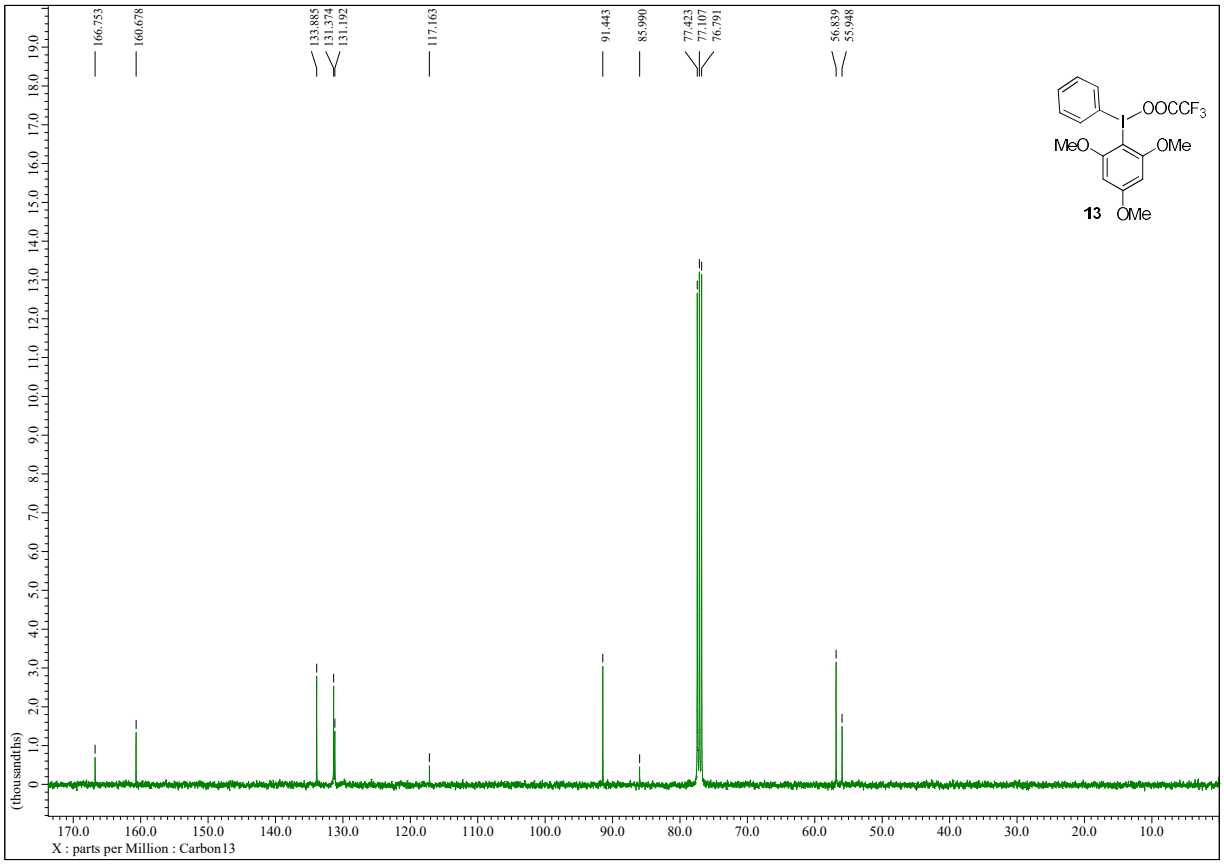

7.489
7.471
7.394
7.375
7.259
7.254
7.234
7.142
7.139
7.121
7.118
6.433
2.364
2.339
2.320
2.311
2.097
2.089
2.078
2.067
1.537
0.000
7.47
2.37
2.40
1.00
3.31
1.11
3.45
abundance
X : parts per Million : Proton
Ph
Ph
Me
10


200.005
165.987
143.601
139.126
129.601
128.969
128.796
128.317
127.867
127.014
126.918
77.461
77.145
76.829
43.682
41.977
34.138
28.110
(thousandths)
X : parts per Million : Carbon13
Ph
Ph
Me
10


7.623
7.604
7.340
7.336
7.334
7.330
7.246
7.241
7.229
7.222
7.213
7.195
7.176
7.152
7.146
2.659
0.000
9.29
3.00
2.08
0.95
abundance
X : parts per Million : Proton
Ph
Ph
N
Me
11


157.190
156.586
140.497
140.132
138.887
133.204
130.023
129.697
128.307
127.991
127.694
127.004
121.839
77.481
77.164
76.839
24.517
(thousandths)
X : parts per Million : Carbon13
Ph
Ph
N
Me
11


7.914
7.894
7.491
7.472
7.454
7.352
7.332
7.313
7.267
6.168
3.877
3.865
0.000
OOCCF3
MeO
OMe
13
OMe
9.02
2.01
1.99
0.97
2.00
abundance
X : parts per Million : Proton


166.753
160.678
133.885
131.374
131.192
117.163
91.443
85.990
77.423
77.107
76.791
56.839
55.948
OOCCF3
MeO
OMe
13
OMe
(thousandths)
X : parts per Million : Carbon13