Supporting Information

A simple and efficient approach to realize difunctionalization of arylketones with malonate esters via an electrochemical oxidation

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Experimental Section

General Information

NMR spectra were recorded on a Bruker AV-400(1H:400 MHz, 13C:100Hz) spectrometer using TMS as internal reference. Chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz, respectively. HRMS was recorded on a Micromass UK LTD GCT spectrometer. GC-MS was Shimadzu QP-5050 GC-MS system.

Instruments

The instrument for electrolysis is dual display potentiostat (CJS-292) (made in China). The anode electrode and cathode electrode all are Pt (1.5×1.5 cm^2).

Experimental procedure

A mixture of acetophenone derivatives (0.5mmol), dimethyl malonate (2mmol), KI (1mmol), KOH (1mmol), MeOH (8mL), was added to an undivided cell. The cell was equipped with platinum electrodes (1.5×1.5 cm^2) as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 20 mA under room temperature for 3 h. When the reaction was finished, the solution was extracted with EtOAc (3×10mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel to afford the desired product.

Characterization data for the products

3aa tetramethyl 2-benzoylpropane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 8.01 (d, J = 8 Hz, 2 H), 7.58 (t, J = 7.2 Hz, 1 H), 7.49-7.44 (m, 2 H), 4.87 (t, J = 8 Hz, 1 H), 4.11 (d, J = 8 Hz, 2 H), 3.72 (s, 6 H), 3.53 (s, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 198.7, 168.1, 167.9, 136.2, 133.4, 128.8, 128.5, 77.3, 77.0, 76.7, 52.9, 52.7, 52.2, 43.9. HRMS calc. $C_{18}H_{20}O_9$: 380.1107, found: 380.1106.

3ab tetramethyl 2-(4-methylbenzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.91 (d, J = 8.4 Hz, 2 H),7.28 (d, J = 2.4 Hz, 2 H), 4.85 (t, J = 8.2 Hz,1 H), 4.11 (d, J = 8Hz, 2 H), 3.72 (s, 6 H), 3.53 (s, 6 H), 2.40 (s, 3 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ =198.2, 168.1, 167.9, 144.4, 133.6, 129.2, 129.0, 77.3, 77.0, 76.7, 52.8, 52.7, 52.2, 43.7, 21.6. HRMS calc. $C_{19}H_{22}O_9$: 394.1264, found: 394.1261.

3ac tetramethyl 2-(4-methoxybenzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 8.01 (d, J = 8.4 Hz, 2 H), 6.95 (d, J = 8.8 Hz, 2 H), 4.83 (t, J = 8 Hz, 1 H), 4.11 (d, J = 8 Hz, 2 H), 3.86 (s, 3 H), 3.72 (s, 6 H), 3.54 (s, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 196.9, 168.2, 168.0, 163.9, 131.3, 129.1, 113.7, 77.3, 77.0, 76.7, 55.5, 52.8, 52.7, 52.3, 43.6. HRMS calc. $C_{19}H_{22}O_{10}$: 410.1213, found: 410.1212

3ad tetramethyl 2-(4-fluorobenzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.99 (t, J = 6.8 Hz, 2 H), 7.07 (t, J = 8.4 Hz, 2 H), 4.75 (t, J = 7.8 Hz, 1 H), 4.02 (d, J = 8 Hz, 2 H), 3.66 (s, 6 H), 3.48 (s, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 196.3, 167.0, 166.8, 166.2, 163.6, 131.8, 131.7, 130.7, 130.6, 114.7, 114.5, 76.3, 76.0, 75.6, 51.9, 51.8, 51.3, 42.7. HRMS calc. $C_{18}H_{19}FO_9$: 398.1013, found: 398.1014.

3ae tetramethyl 2-(4-chlorobenzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.97 (d, J = 8.8 Hz, 2 H), 7.42 (d, J = 8.4 Hz, 2 H), 4.80 (t, J = 8 Hz, 1 H), 4.09 (d, J = 8 Hz, 2 H), 3.72 (s, 6 H), 3.56 (s, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 197.8, 168.0, 167.8, 140.0, 134.8, 130.3, 128.8, 77.3, 77.0, 76.7, 52.9, 52.8, 52.3, 43.7. HRMS calc. $C_{18}H_{19}ClO_9$: 414.0718, found: 414.0715.

3af tetramethyl 2-(4-bromobenzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.89 (d, J = 8.8 Hz, 2 H), 7.62 (d, J = 8.4 Hz, 2 H), 4.80 (t, J = 8 Hz, 1 H), 4.09 (d, J = 8 Hz, 2 H), 3.73 (s, 6 H), 3.56 (s, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 198.0, 168.0, 167.8, 135.2, 131.8, 130.4, 128.7, 77.3, 77.0, 76.7, 52.9, 52.8, 52.3, 43.7. HRMS calc. $C_{18}H_{19}BrO_9$: 458.0212, found: 458.0210.

3ag tetramethyl 2-([1,1'-biphenyl]-4-carbonyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 8.09 (d, J = 8.4 Hz, 2 H), 7.71 (d, J = 8.4 Hz, 2 H), 7.63 (d, J = 7.2 Hz, 2 H), 7.47 (t, J = 7.4 Hz, 2 H), 7.40 (t, J = 7.4 Hz, 1 H), 4.91 (t, J = 8 Hz, 1 H), 4.14 (d, J = 8 Hz, 2 H), 3.74 (s, 6 H), 3.56 (s, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 198.2, 168.1, 167.9, 146.1, 139.7, 134.9, 129.5, 128.9, 128.3, 127.2, 127.1, 77.3, 77.0, 76.7, 52.9, 52.8, 52.3, 43.9. HRMS calc. $C_{24}H_{24}O_9$: 456.1420, found: 456.1423.

3ah tetramethyl 2-(4-(trifluoromethyl)benzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 8.13 (d, J = 8 Hz, 2 H), 7.75 (d, J = 8.4 Hz, 2 H), 4.85 (t, J = 8 Hz, 1 H), 4.11 (d, J = 8 Hz, 2 H), 3.73 (s, 6 H), 3.57 (s, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 198.3, 167.9, 167.7, 139.4, 134.6, 134.3, 129.2, 127.7, 125.5, 125.5, 125.2, 125.1, 77.3, 77.0, 76.7, 53.0, 52.9, 52.4, 43.9. HRMS calc. $C_{19}H_{19}F_3O_9$: 448.0981, found 448.0980.

3ai tetramethyl 2-(benzo[*d*][1,3]dioxole-5-carbonyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.67 (dd, J_1 = 8.4 Hz, J_2 = 2 Hz, 1 H), 7.47 (d, J = 1.6 Hz, 1 H), 6.87 (d, J = 8 Hz, 1 H), 6.04 (s, 2 H), 4.77 (t, J = 8 Hz, 1 H), 4.09 (d, J = 8 Hz, 2 H), 3.73 (s, 6 H), 3.57 (s, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 196.5, 168.1, 168.0, 152.2, 148.2, 130.9, 125.5, 108.6, 107.9, 101.9, 77.3, 77.0, 76.7, 52.9, 52.8, 52.3, 43.7. HRMS calc. $C_{19}H_{20}O_{11}$: 424.1006, found: 424.1007.

3aj tetramethyl 2-(2-naphthoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 8.58 (s, 1 H), 8.05-7.99 (m, 2 H), 7.91-7.85 (m, 2 H), 7.62-7.53 (m, 2 H), 5.04 (t, J = 8 Hz, 1 H), 4.17 (d, J = 8 Hz, 2 H), 3.73 (s, 6 H), 3.51 (s, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 198.6, 168.2, 167.9, 135.7, 133.5, 132.4, 130.8, 129.9, 128.7, 128.4, 127.7, 126.8, 124.3, 77.3, 77.0, 76.7, 52.9, 52.8, 52.3, 44.0. HRMS calc. $C_{22}H_{22}O_9$: 430.1264, found: 430.1261.

3ak tetramethyl 2-(4-butylbenzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.92 (d, J = 8.4 Hz, 2 H), 7.27 (d, J = 7.2 Hz, 2 H), 4.85 (t, J = 8 Hz, 1 H), 4.11 (d, J = 8 Hz, 2 H), 3.72 (s, 6 H), 3.52 (s, 6 H), 2.65 (t, J = 7.6 Hz, 2 H), 1.64-1.56 (m, 2 H), 1.39-1.30 (m, 2 H), 0.92 (t, J = 7.4 Hz, 3 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 198.2, 168.1, 168.0, 149.3, 133.8, 129.0, 128.6, 77.3, 77.0, 76.7, 52.8, 52.7, 52.1, 43.9, 35.7, 33.1, 22.3, 13.8. HRMS calc. $C_{22}H_{28}O_9$: 436.1733, found: 436.1732.

3al tetramethyl 2-(4-isobutylbenzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.92 (d, J = 8.4 Hz, 2 H), 7.24 (d, J = 8.4 Hz, 2 H), 4.85 (t, J = 8 Hz, 1 H), 4.11 (d, J = 8 Hz, 2 H), 3.72 (s, 6 H), 3.52 (s, 6 H), 2.52 (d, J = 6.8 Hz, 2 H), 1.94-1.84 (m, 1 H), 0.90 (d, J = 6.8 Hz, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 198.2, 168.1, 168.0, 148.1, 133.8, 129.3, 128.9, 77.3, 77.0, 76.7, 52.8, 52.7, 52.1, 45.4, 43.9, 30.0, 22.3. HRMS calc. $C_{21}H_{25}O_9$: 421.1499, found: 421.1497.

3am tetramethyl 2-(4-(tert-butyl)benzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.94 (d, J = 8.4 Hz, 2 H), 7.48 (d, J = 8.4 Hz, 2 H), 4.87 (t, J = 8 Hz, 1 H), 4.11 (d, J = 8 Hz, 2 H), 3.72 (s, 6 H), 3.53 (s, 6 H), 1.32 (s, 9 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 198.1, 168.1, 168.0, 157.3, 133.4, 128.8, 125.5, 77.3, 77.0, 76.7, 52.8, 52.7, 52.1, 43.9, 35.1, 31.0. HRMS calc. $C_{22}H_{28}O_9$: 436.1733, found: 436.1735.

3an tetramethyl 2-(2-methylbenzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.86 (dd, J_1= 7.6 Hz, J_2 = 0.8 Hz, 1 H), 7.39-7.35 (m, 1 H), 7.28 (t, J = 7.2 Hz, 1 H), 7.23 (d, J = 7.6 Hz, 1 H), 4.77 (t, J = 7.8 Hz, 1 H), 4.04 (d, J = 8 Hz, 2 H), 3.65 (s, 6 H), 3.60 (s, 6 H), 2.44 (s, 3 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 200.8, 168.0, 167.9, 139.3, 136.4, 131.7, 131.7, 129.4, 125.5, 77.3, 77.0, 76.7, 52.7, 52.7, 51.5, 47.1, 20.6. HRMS calc. $C_{19}H_{22}O_9$: 394.1264, found: 394.1263.

3ao tetramethyl 2-(2-fluorobenzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.87-7.82 (m, 1 H), 7.55-7.49 (m, 1 H), 7.25-7.21 (m, 1 H), 7.17-7.12 (m, 1 H), 4.84-4.80(m, 1 H), 4.11 (d, J = 7.6 Hz, 2 H), 3.70 (s, 6 H), 3.63 (s, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 196.6, 196.6, 167.9, 167.9, 162.5, 160.0, 134.8, 134.7, 131.2, 131.2, 125.5, 125.4, 124.3, 124.3, 116.8, 116.5, 77.3, 77.0, 76.7, 52.8, 52.8, 52.0, 47.9, 47.8. HRMS calc. $C_{18}H_{19}FO_9$: 398.1013, found: 398.1012.

3ap tetramethyl 2-(2-bromobenzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.79 (dd, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1 H), 6.62 (dd, J_1 = 8 Hz, J_2 = 0.8 Hz, 1 H), 7.42-7.38 (m, 1 H), 7.33-7.28 (m, 1 H), 4.85 (t, J = 7.2 Hz , 1 H), 4.07 (d, J = 7.2 Hz, 2 H), 3.69 (s, 6 H), 3.65 (s, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 199.3, 167.8, 167.7, 138.6, 134.0, 132.2, 130.6, 127.2, 120.2, 77.3, 77.0, 76.7, 52.9, 52.8, 51.0, 48.1. HRMS calc. $C_{18}H_{19}BrO_9$: 458.0212, found: 458.0210.

3aq tetramethyl 2-(3-methylbenzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.82-7.78 (m, 2 H), 7.39-7.31 (m, 2 H), 4.86 (t, J = 8 Hz, 1 H), 4.11 (d, J = 8 Hz, 2 H), 3.72 (s, 6 H), 3.54 (s, 6 H), 2.41 (s, 3 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 199.8, 168.1, 167.9, 138.3, 136.1, 134.3, 129.2, 128.4, 126.1, 77.3, 77.0, 76.7, 52.8, 52.7, 52.1, 44.0, 21.3. HRMS calc. $C_{19}H_{22}O_9$: 394.1264, found: 394.1265.

3ar tetramethyl 2-(3-methoxybenzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.61 (d, J = 7.6 Hz, 1 H), 7.51 (s, 1 H), 7.38 (t, J = 8 Hz, 1 H), 7.12 (dd, J_1 = 8 Hz, J_2 = 2.4 Hz, 1 H), 4.84 (t, J = 8 Hz, 1 H), 4.12 (d, J = 8 Hz, 2 H), 3.85 (s, 3 H), 3.72 (s, 6 H), 3.55 (s, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 198.3, 168.1, 167.9, 159.7, 137.4, 129.5, 121.5, 120.3, 112.7, 77.3, 77.0, 76.7, 55.4, 52.9, 52.7, 52.1, 44.1. HRMS calc. $C_{19}H_{22}O_{10}$: 410.1213, found: 410.1211.

3as tetramethyl 2-(3,4-difluorobenzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.88-7.82 (m, 2 H), 7.30-7.23 (m, 1 H), 4.76 (t, J = 8 Hz, 1

H), 4.08 (d, J = 8 Hz, 2 H), 3.74 (s, 6 H), 3.59 (s, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 196.7, 167.9, 167.7, 155.1, 154.9, 152.5, 152.4, 151.5, 151.4, 149.0, 148.9, 133.7, 133.7, 133.6, 126.1, 126.1, 126.0, 126.0, 118.3, 118.1, 117.4, 117.2, 77.3, 77.0, 76.7, 53.0, 52.9, 52.4, 43.6. HRMS calc. $C_{18}H_{18}F_2O_9$: 416.0919, found: 416.0918.

3at tetramethyl 2-(2-fluoro-4-methoxybenzoyl)propane-1,1,3,3-tetracarboxylate

^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.85 (t, J = 8.8 Hz, 1 H), 6.75 (dd, J_1 = 8.8 Hz, J_2 = 2 Hz, 1 H), 6.64 (dd, J_1 = 13.6 Hz, J_2 = 2.4 Hz, 1 H), 4.81-4.77 (m, 1 H), 4.12 (d, J = 7.6 Hz, 2 H), 3.85 (s, 3 H), 3.72 (s, 6 H), 3.62 (s, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 195.1, 195.0, 168.1, 168.0, 164.4, 161.8, 132.8, 132.7, 118.1, 118.0, 110.7, 110.6, 102.0, 101.7, 77.3, 77.0, 76.7, 55.8, 52.8, 52.8, 52.1, 47.4, 47.3. HRMS calc. $C_{19}H_{21}FO_{10}$: 428.1119, found: 428.1116.

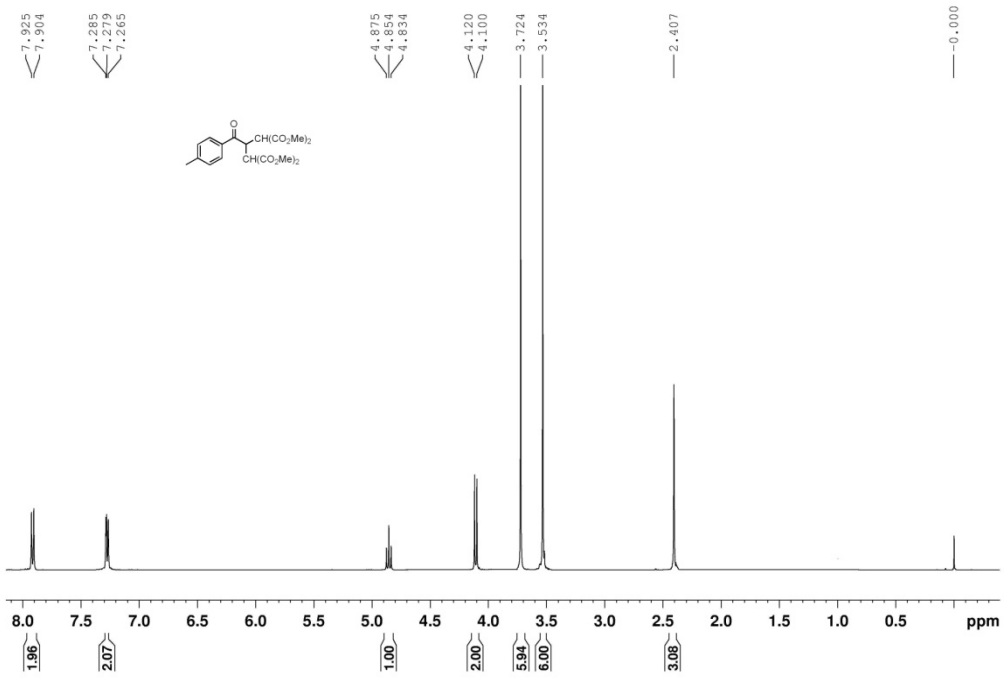
3ba tetraethyl 2-benzoylpropane-1,1,3,3-tetracarboxylate

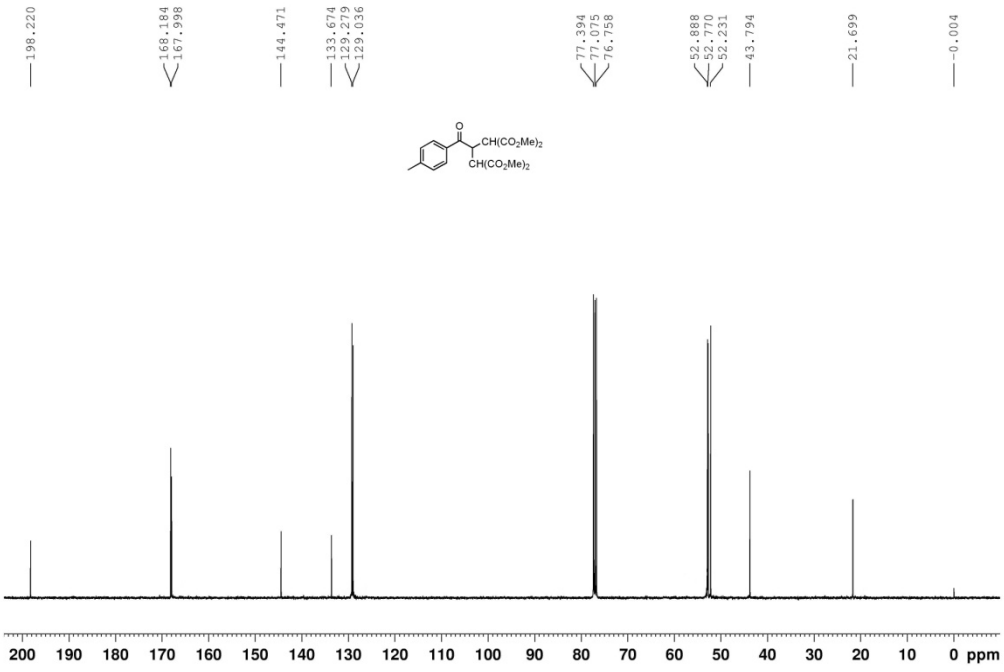
^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 8.02 (d, J = 7.2 Hz, 2 H), 7.56 (t, J = 7.4 Hz, 1 H), 7.46 (t, J = 7.6 Hz, 2 H), 4.86 (t, J = 8 Hz, 1 H), 4.19-4.13 (m, 4 H), 4.07 (d, J = 8 Hz, 2 H), 4.03-3.91 (m, 4 H), 1.23 (t, J = 7.2 Hz, 6 H), 1.11 (t, J = 7 Hz, 6 H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 198.8, 167.8, 167.6, 136.7, 133.2, 128.9, 128.4, 77.3, 77.0, 76.7, 61.9, 61.8, 52.7, 43.6, 13.8, 13.7. HRMS calc. $C_{22}H_{28}O_9$: 436.1733, found: 436.1732.

8 3-Benzoylpropanoic acid

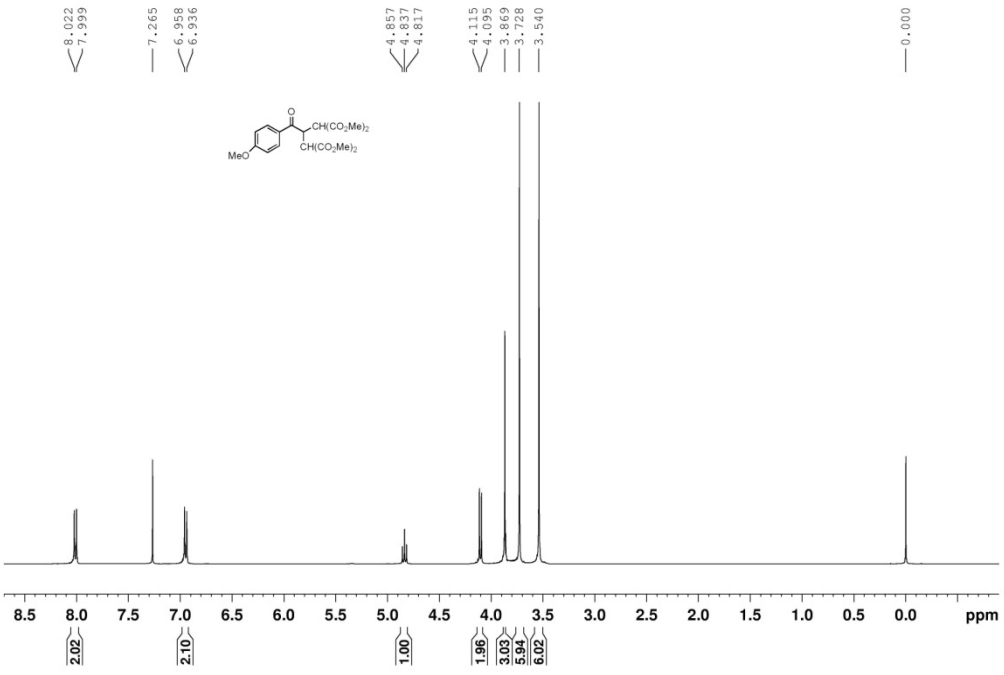
^{1}HNMR ($CDCl_3$, 400 MHz, ppm): δ = 7.99 (d, J = 7.2 Hz, 2 H), 7.58 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.4 Hz, 2H), 3.33 (t, J = 6.6 Hz, 2H), 2.82 (t, J = 6.6 Hz, 2H); ^{13}CNMR ($CDCl_3$, 100 MHz, ppm): δ = 197.8, 178.6, 136.3, 133.3, 128.6, 128.0, 77.3, 77.0, 76.7, 33.1, 27.9.

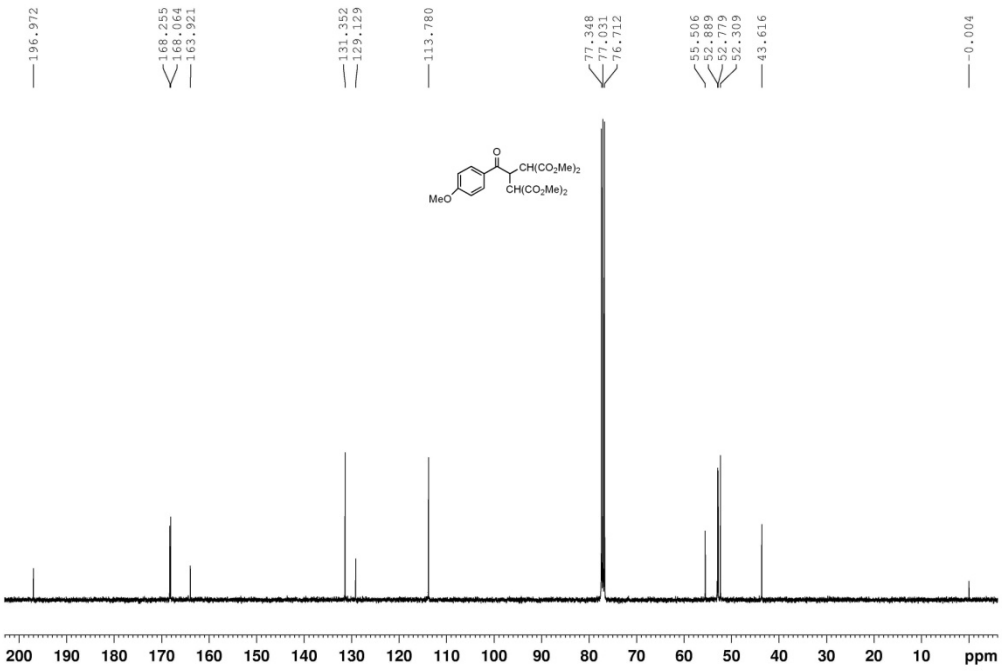
3ab tetramethyl 2-(4-methylbenzoyl)propane-1,1,3,3-tetracarboxylate





3ac tetramethyl 2-(4-methoxybenzoyl)propane-1,1,3,3-tetracarboxylate





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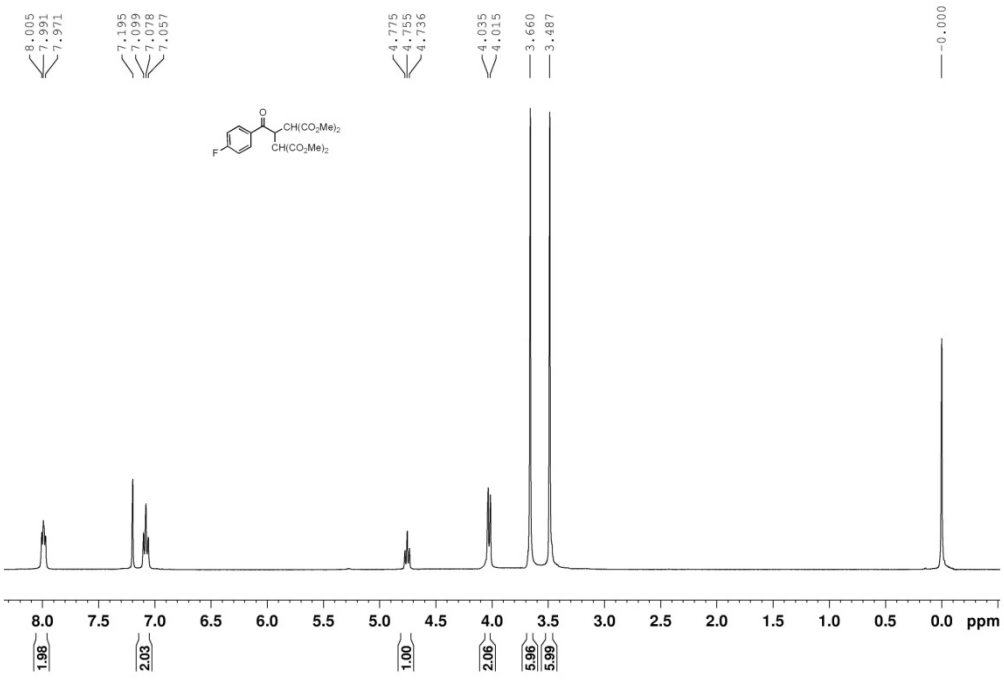
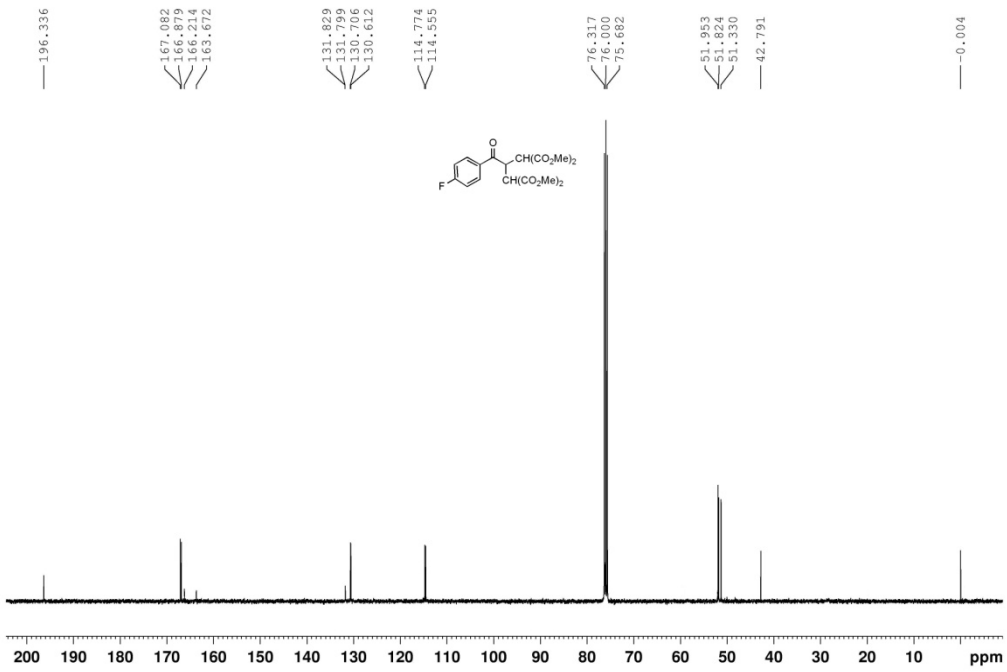
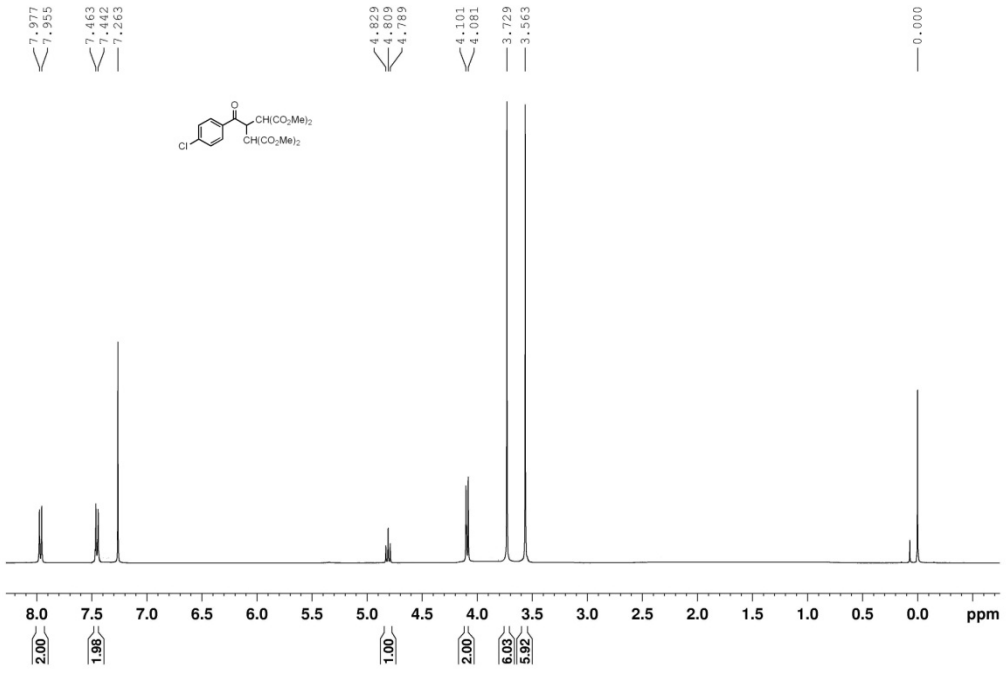
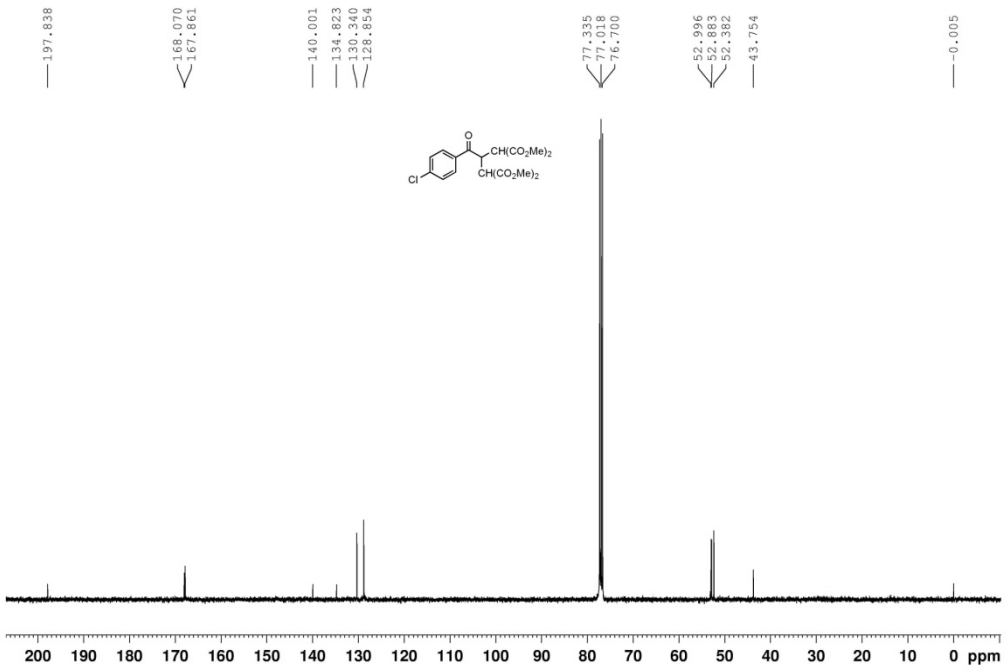


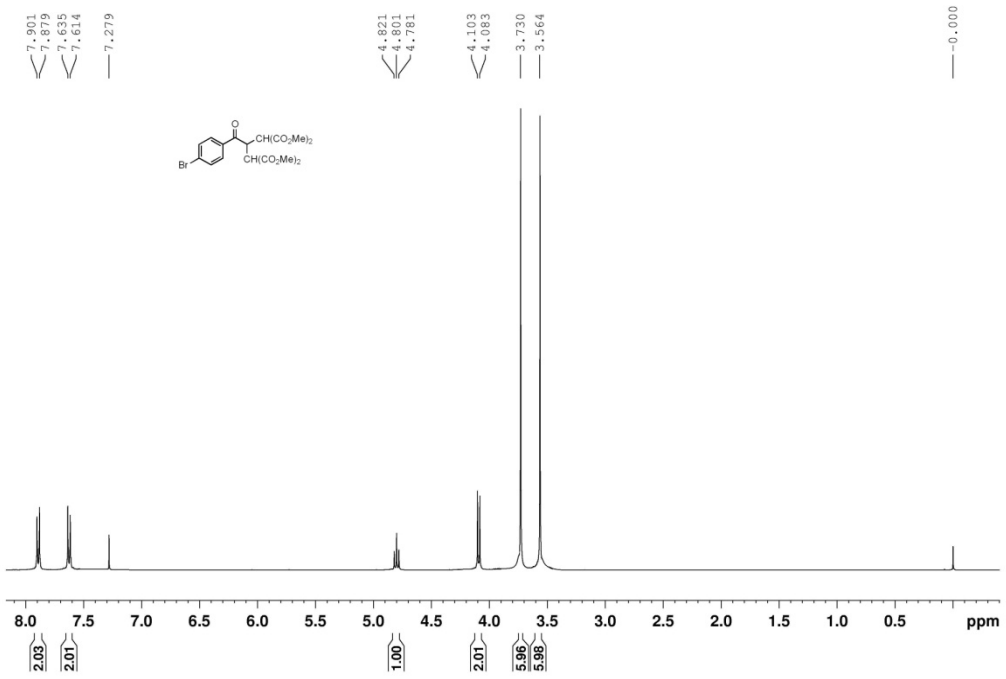


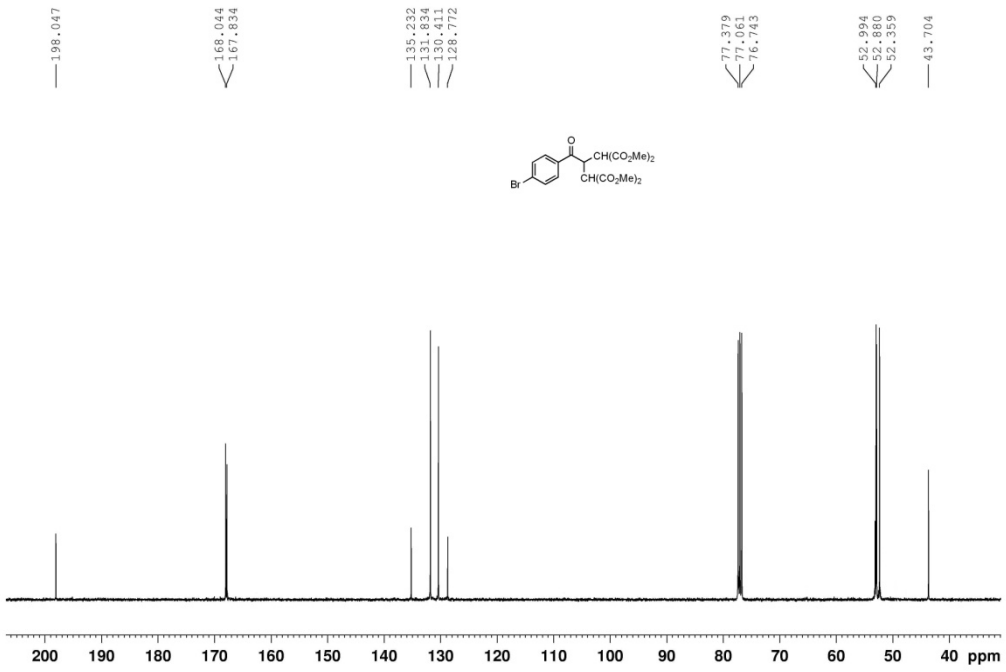
3ae tetramethyl 2-(4-chlorobenzoyl)propane-1,1,3,3-tetracarboxylate





3af tetramethyl 2-(4-bromobenzoyl)propane-1,1,3,3-tetracarboxylate





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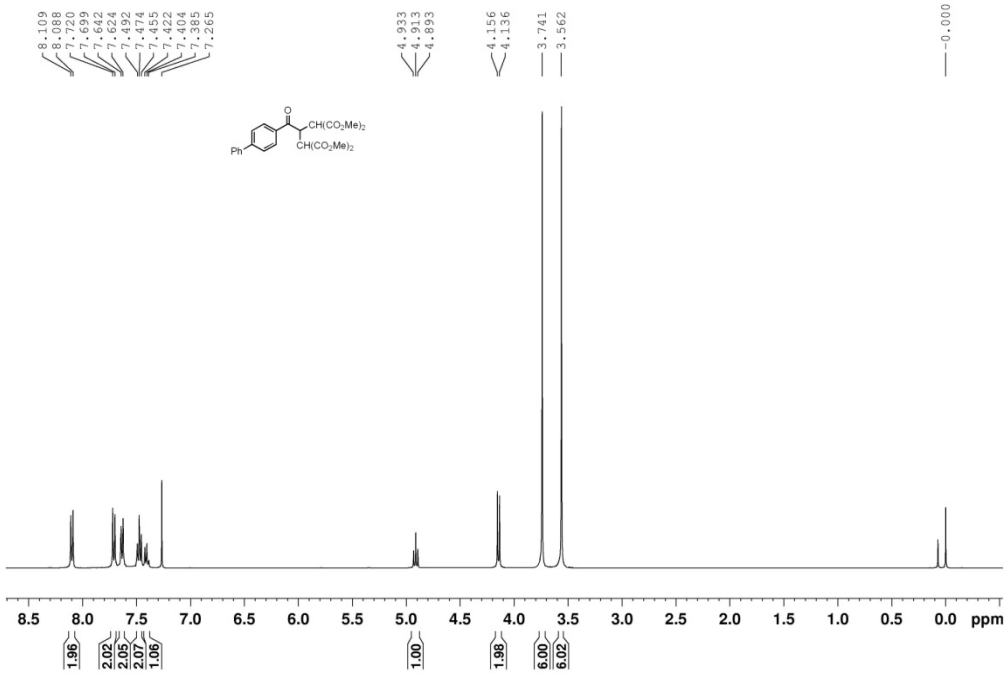
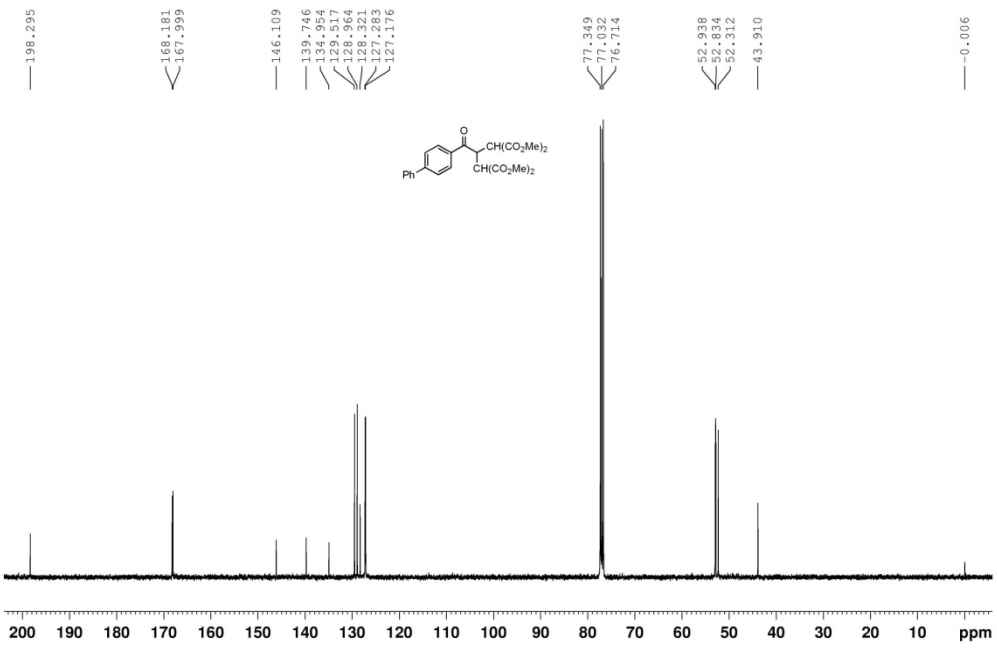
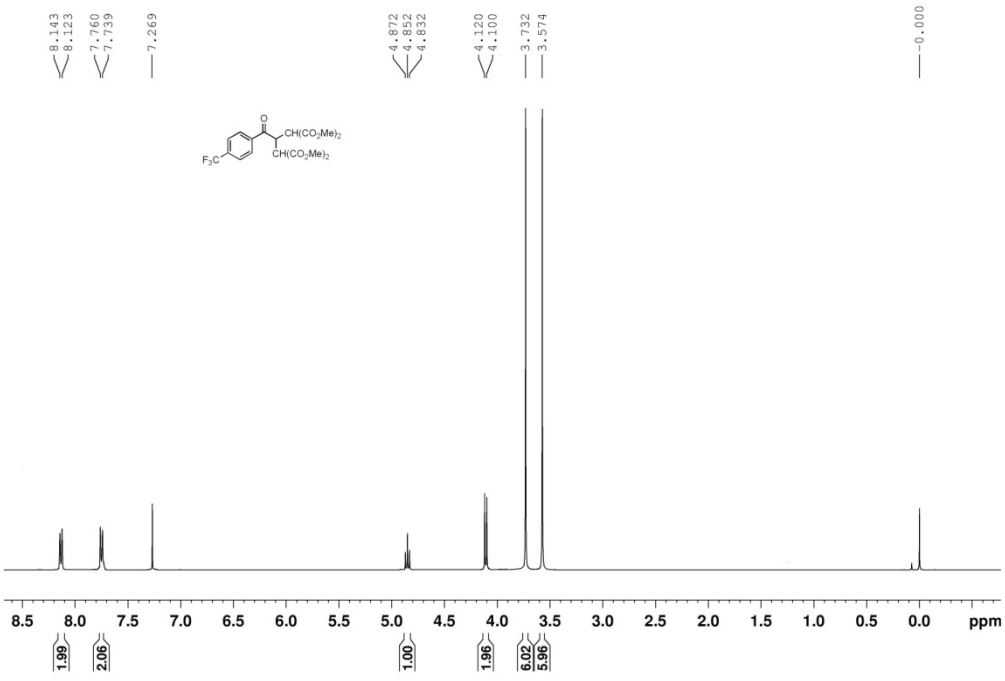
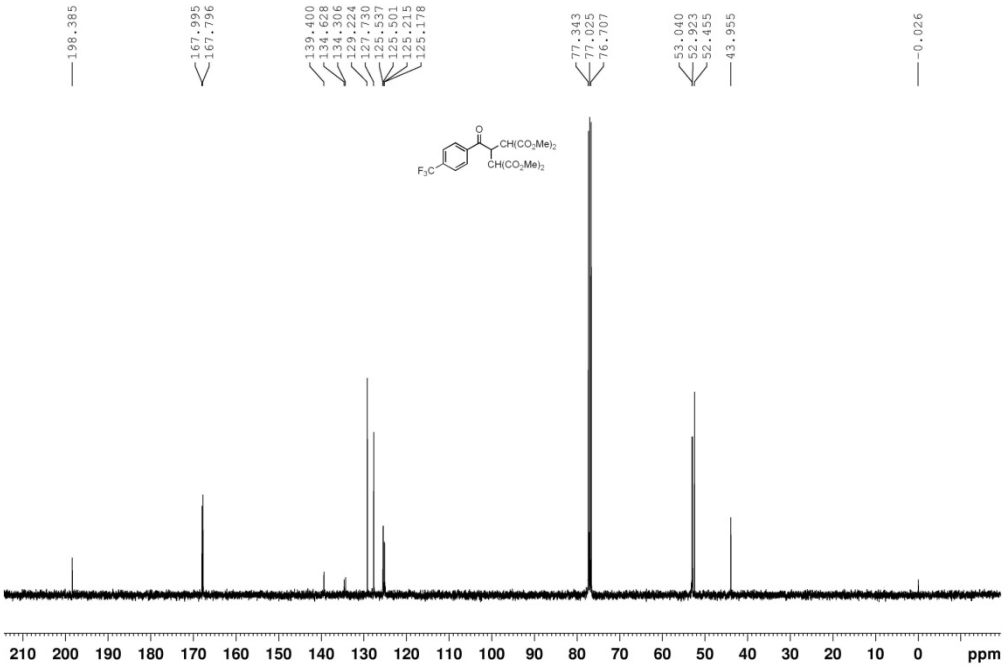




3ah tetramethyl 2-(4-(trifluoromethyl)benzoyl)propane-1,1,3,3-tetracarboxylate





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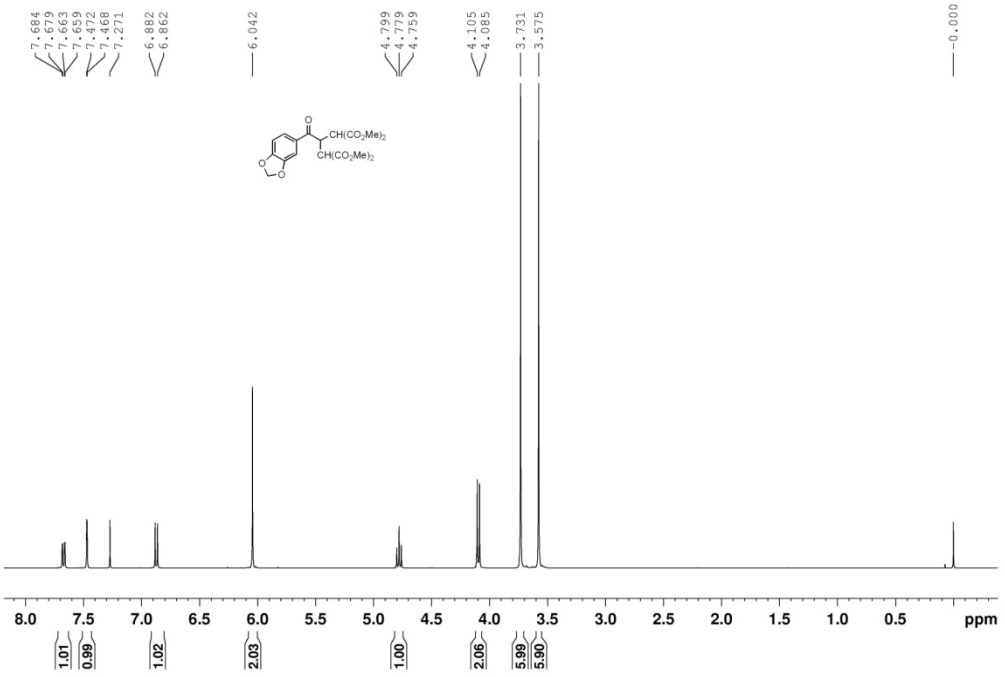

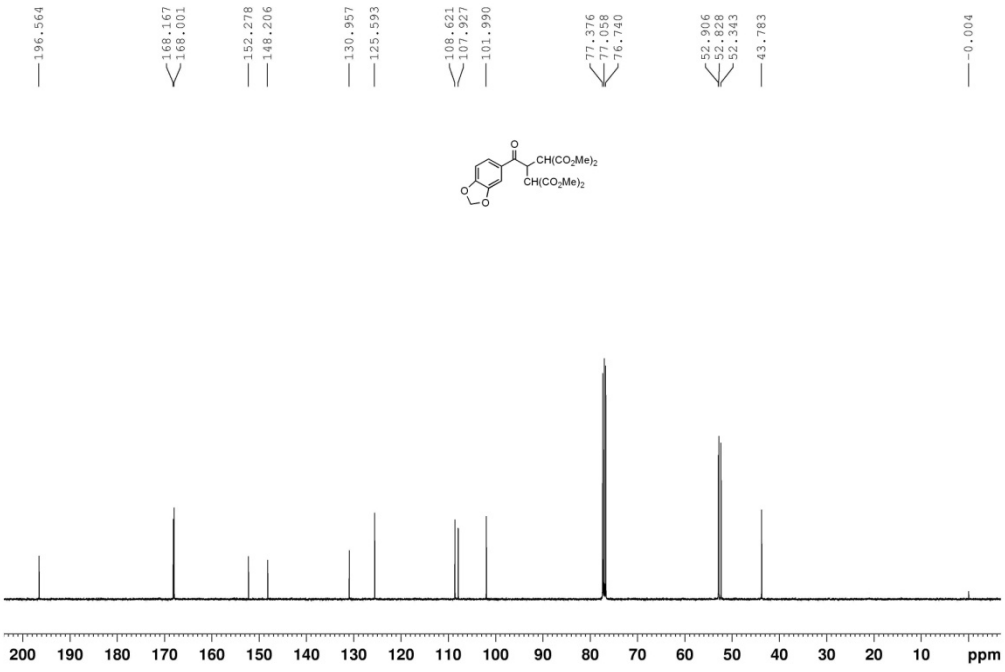

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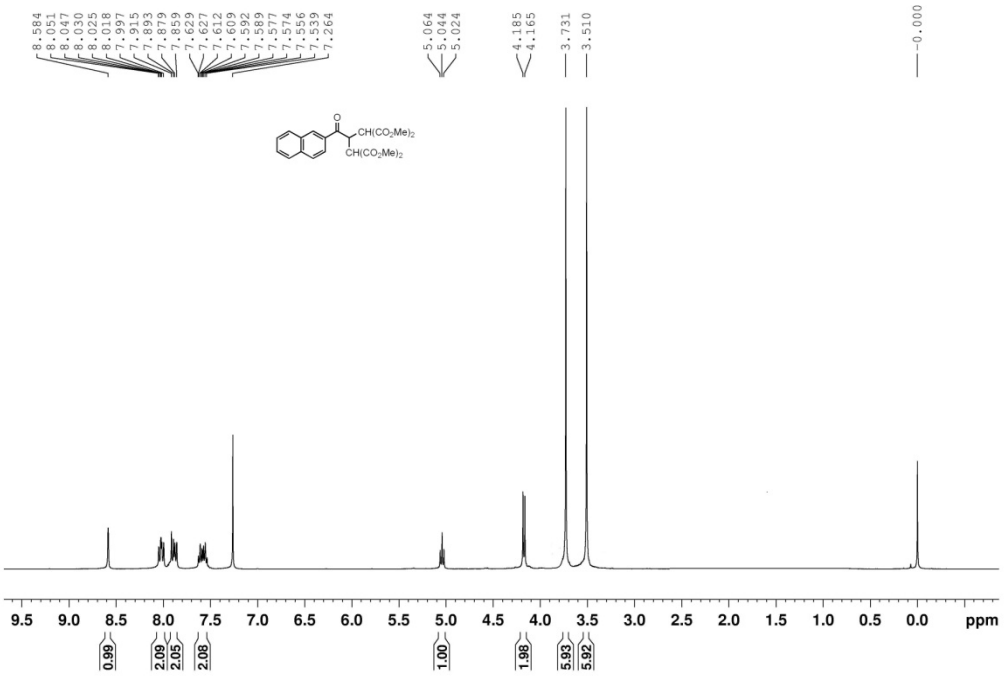
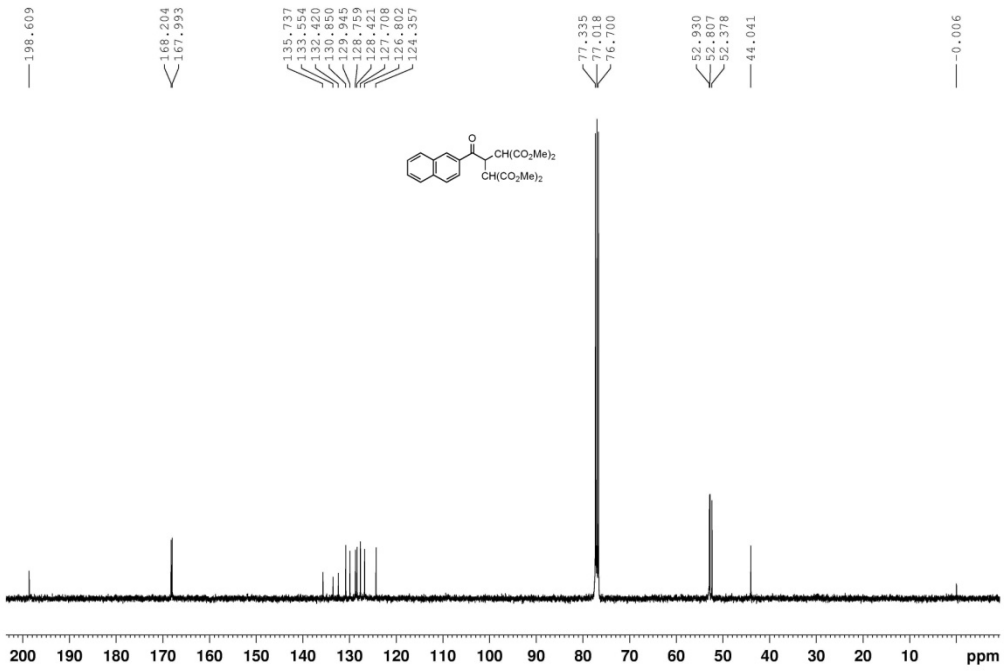
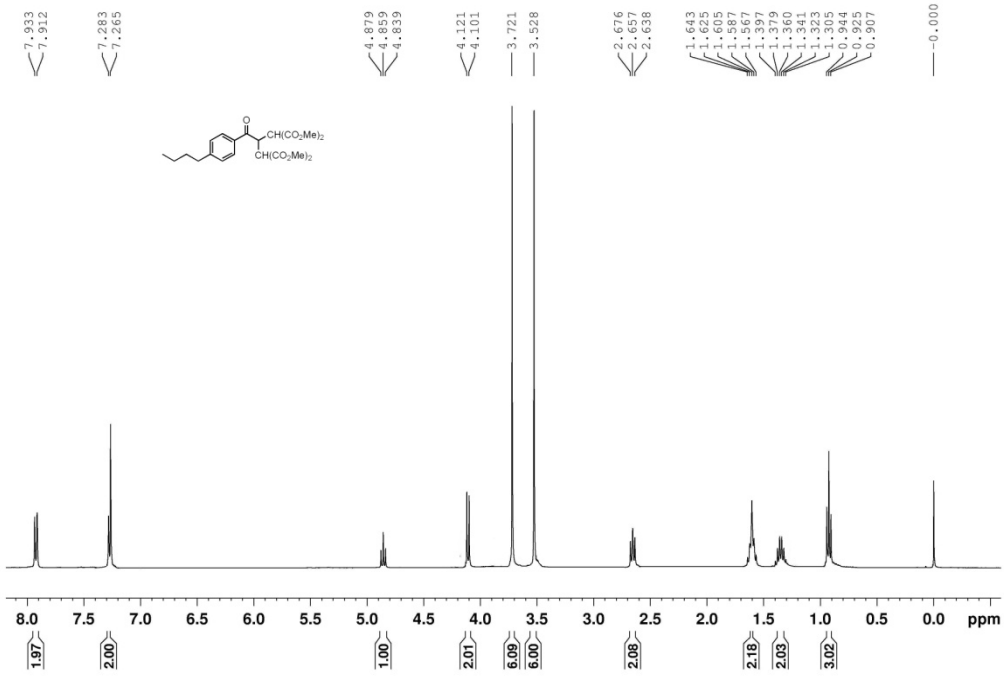
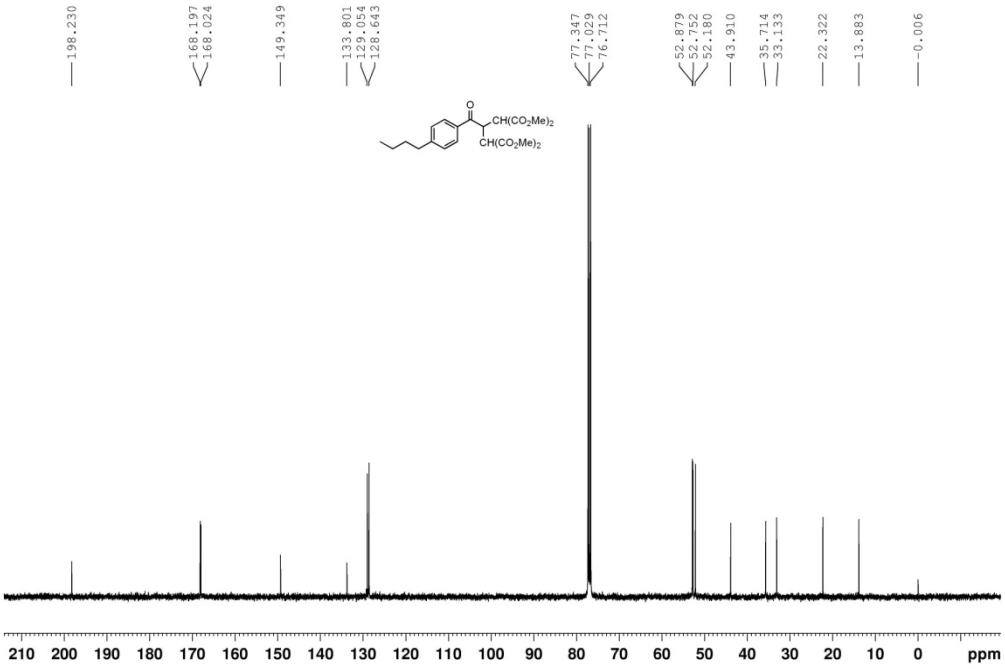


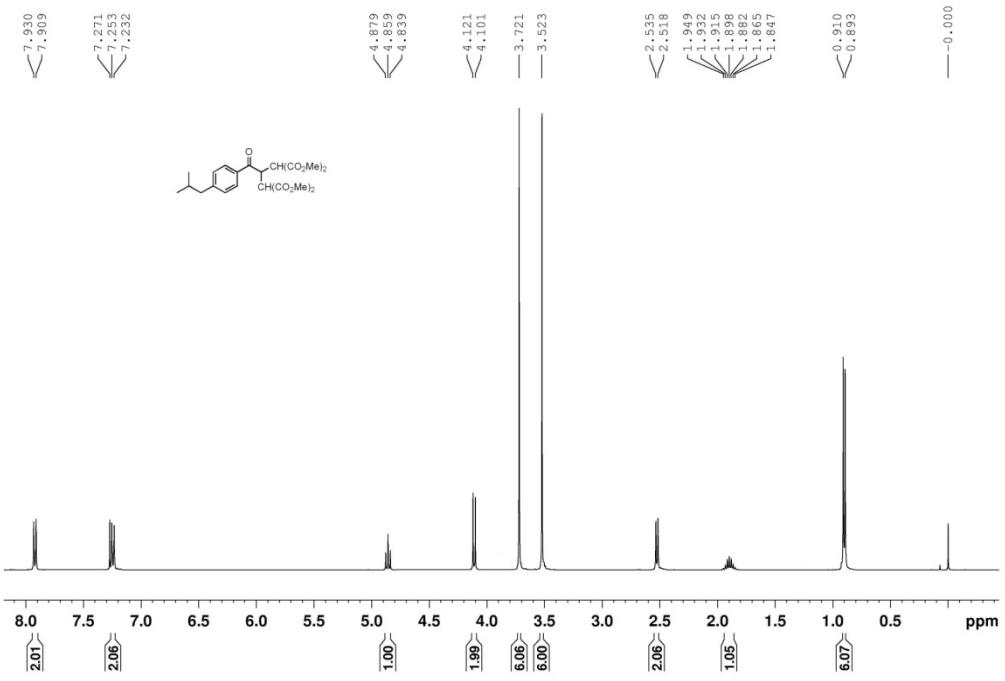


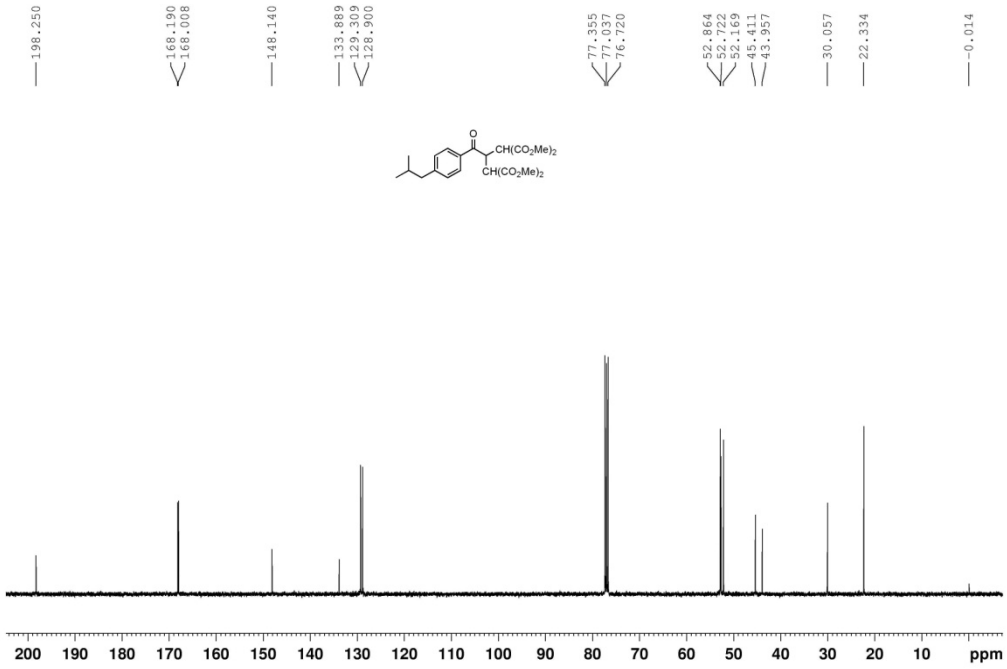
3ak tetramethyl 2-(4-butylbenzoyl)propane-1,1,3,3-tetracarboxylate





3al tetramethyl 2-(4-isobutylbenzoyl)propane-1,1,3,3-tetracarboxylate





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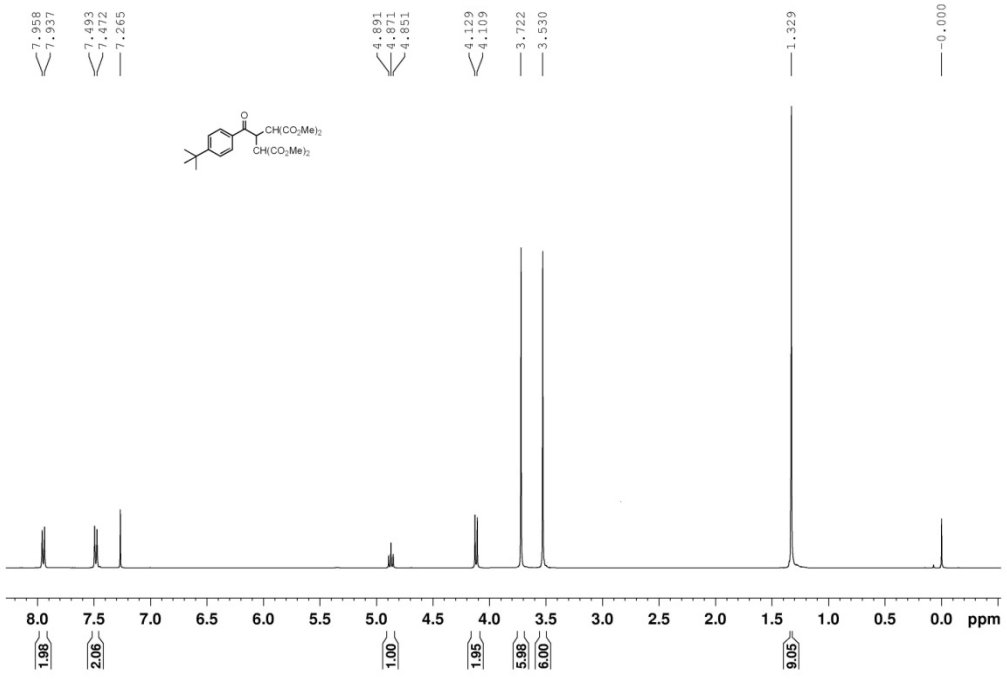
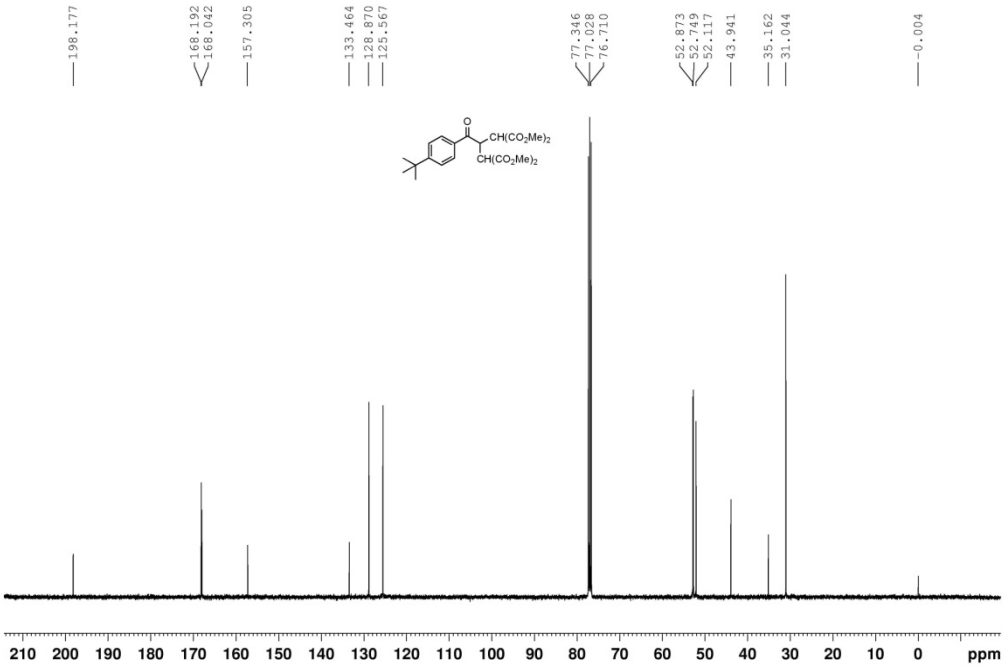
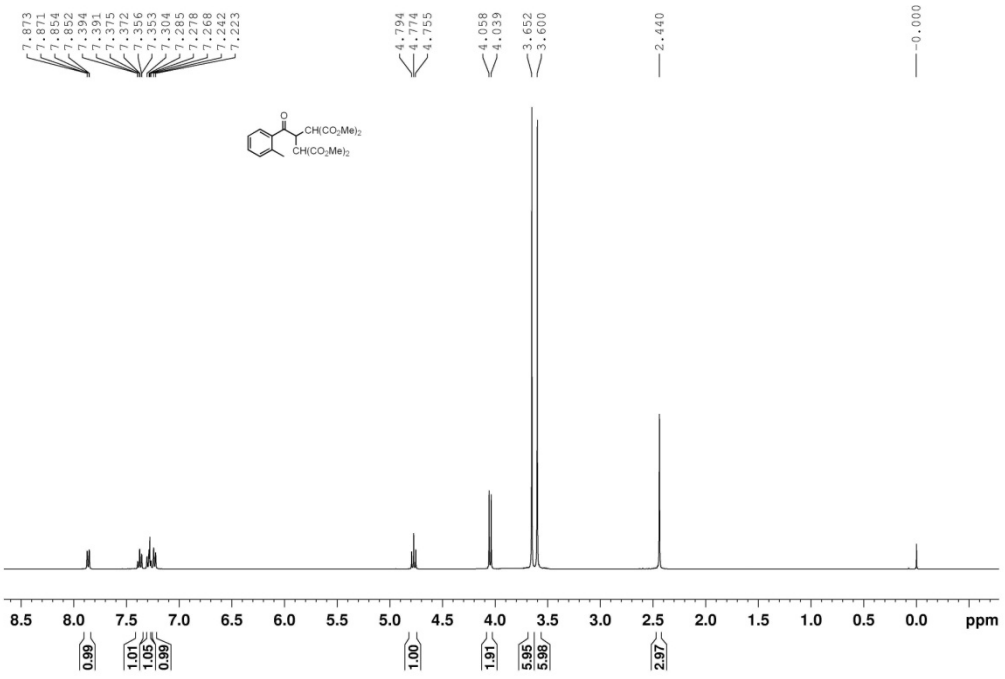
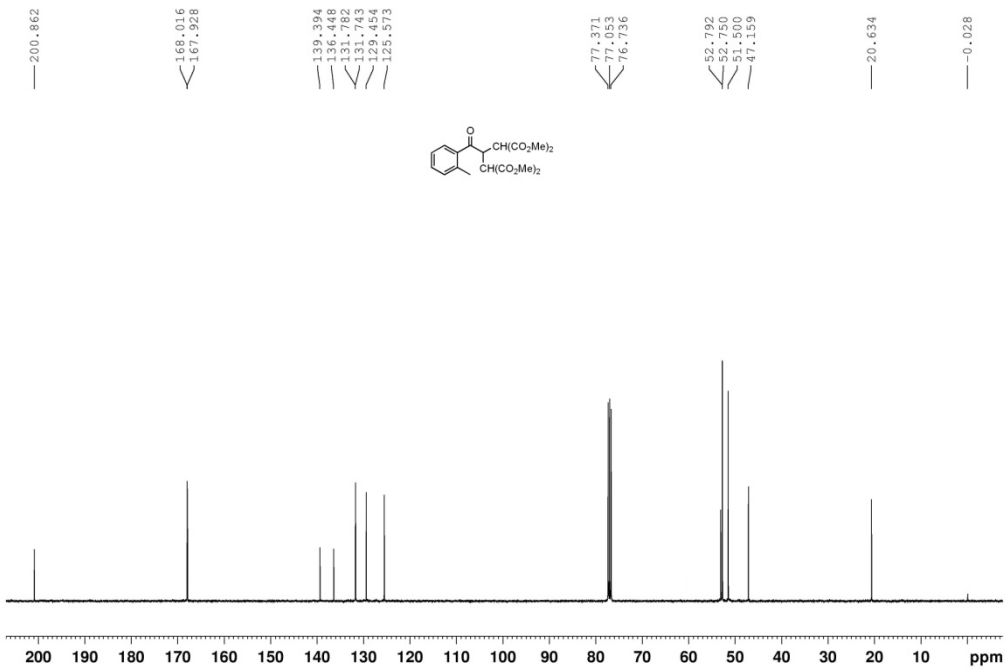




3an tetramethyl 2-(2-methylbenzoyl)propane-1,1,3,3-tetracarboxylate





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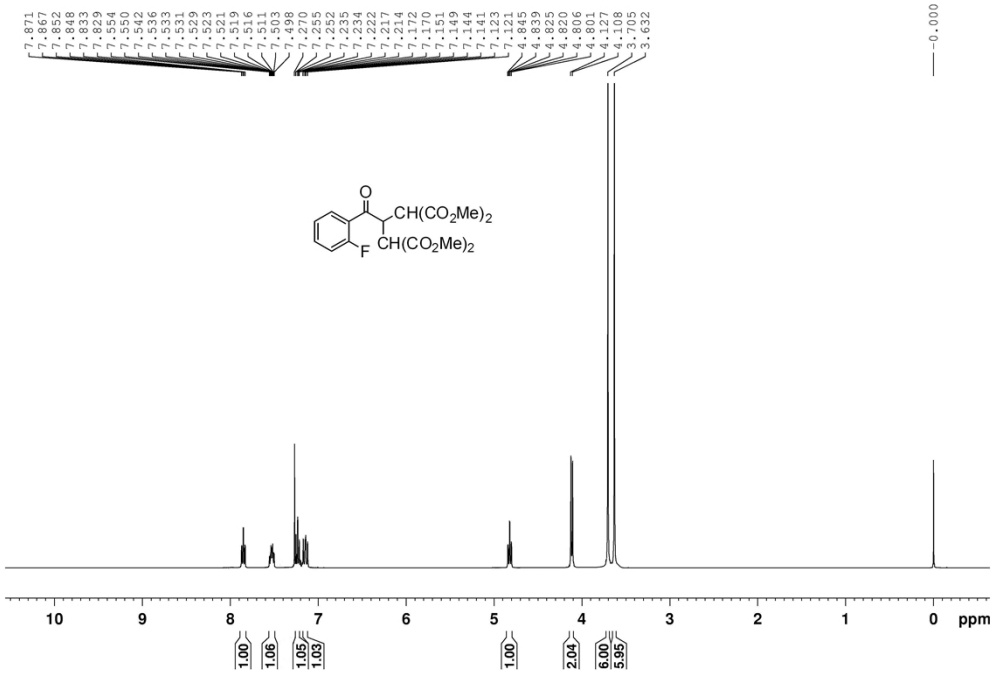

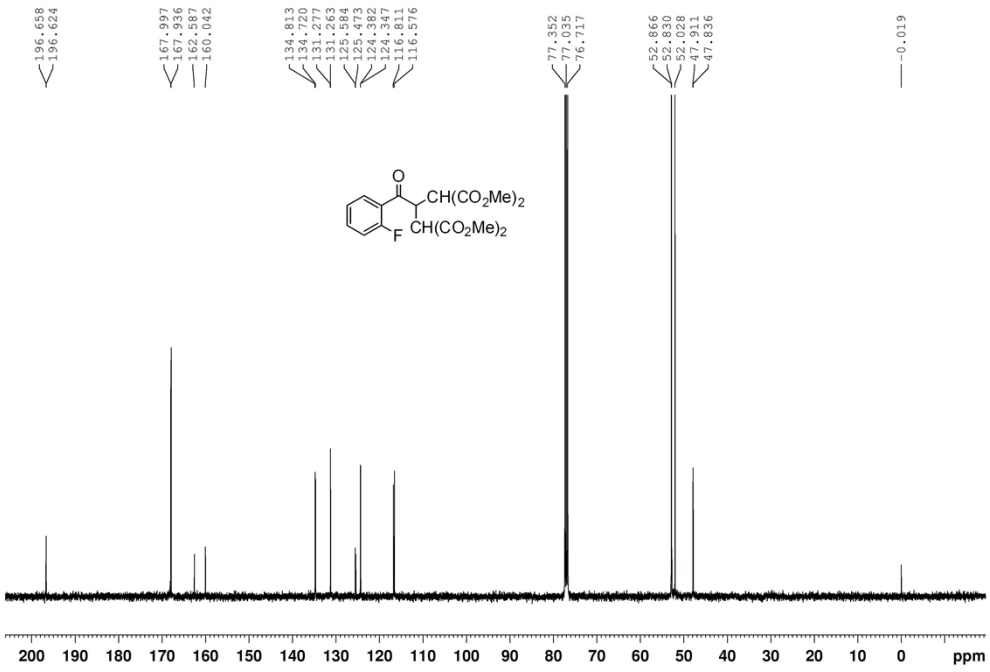

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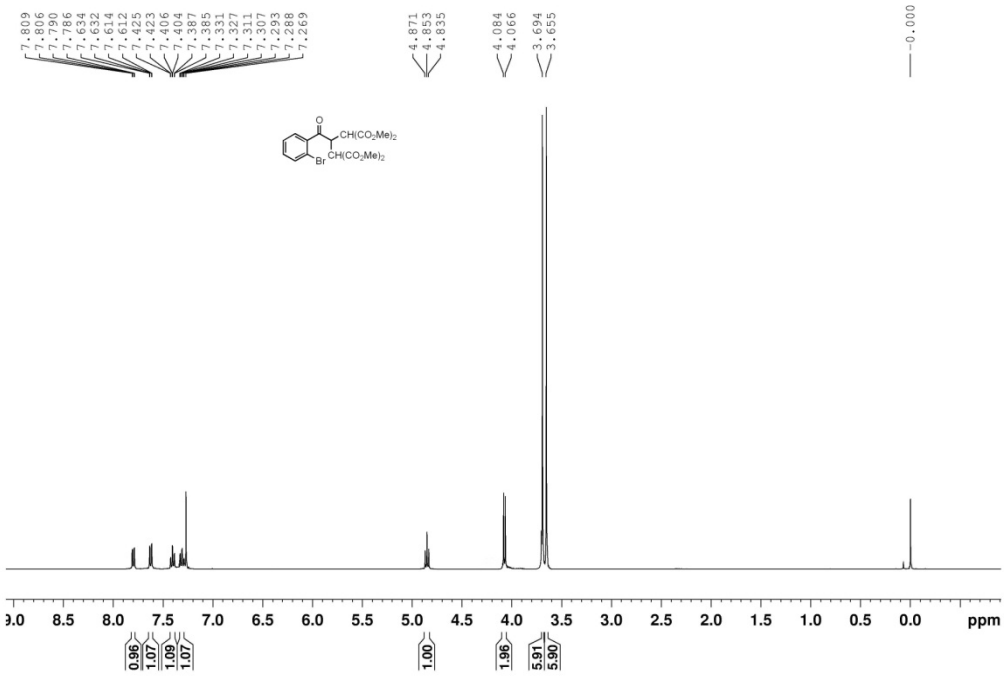

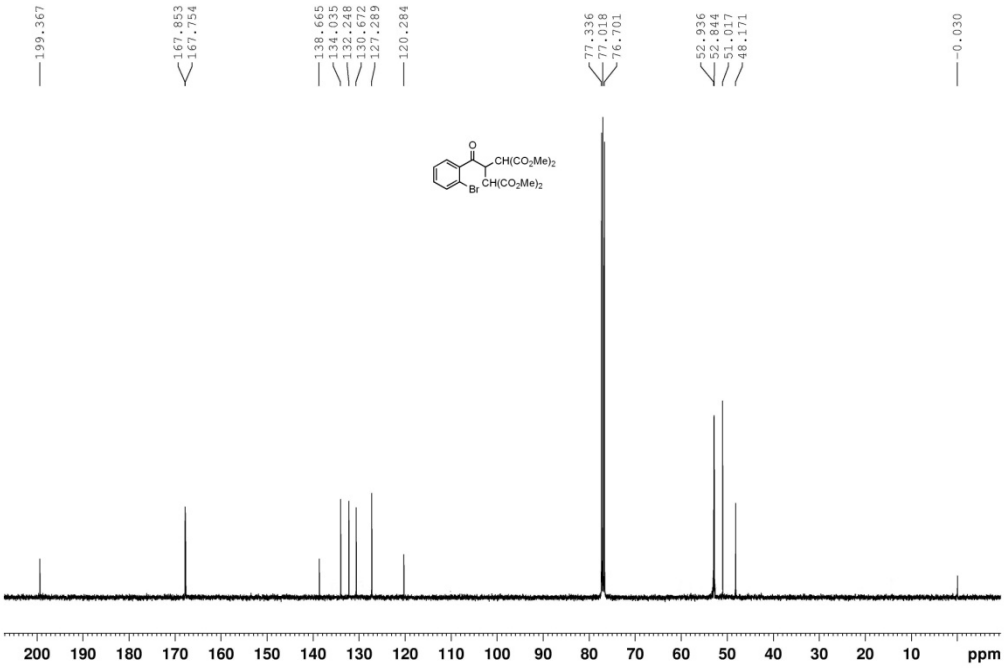

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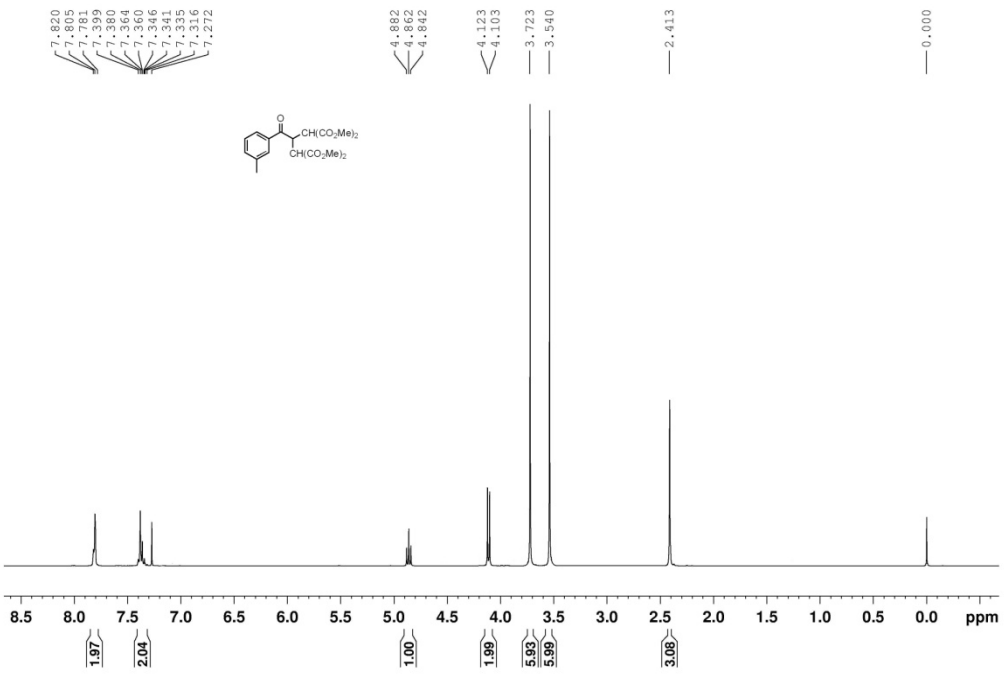
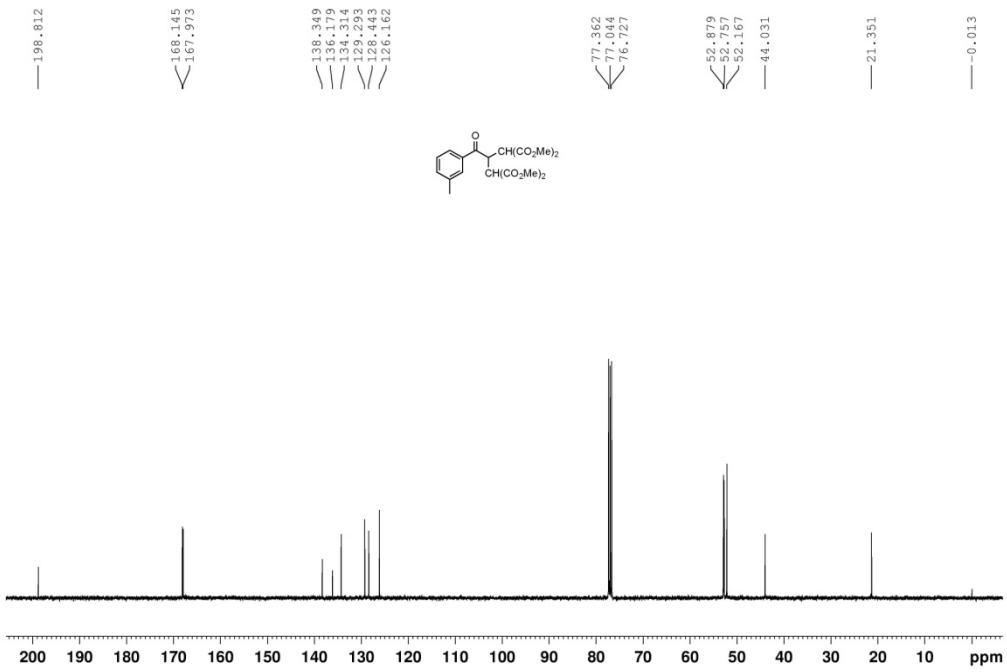
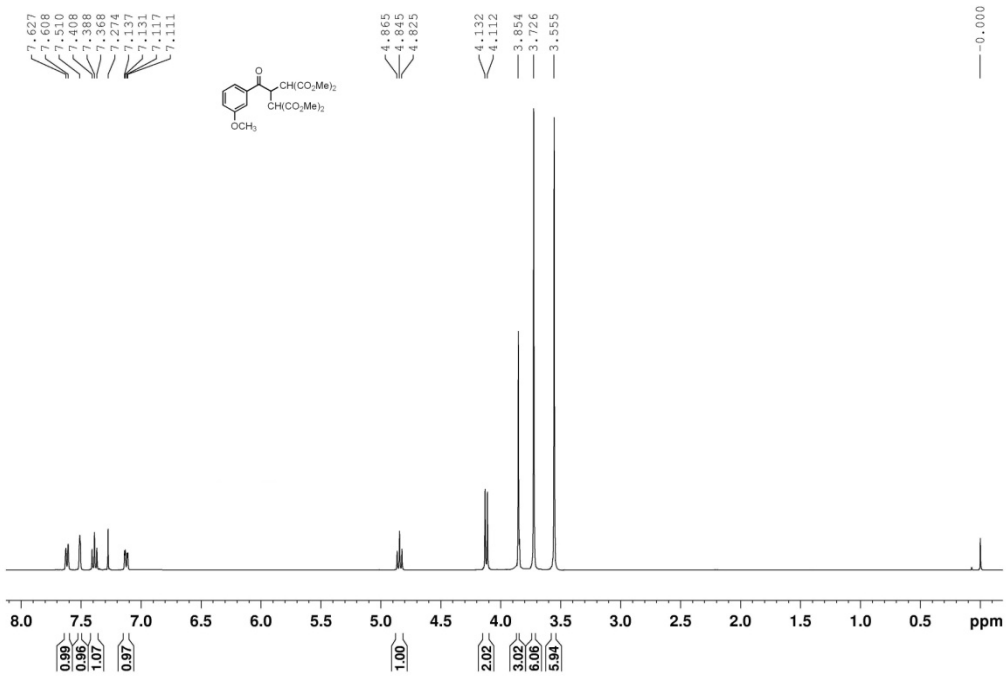
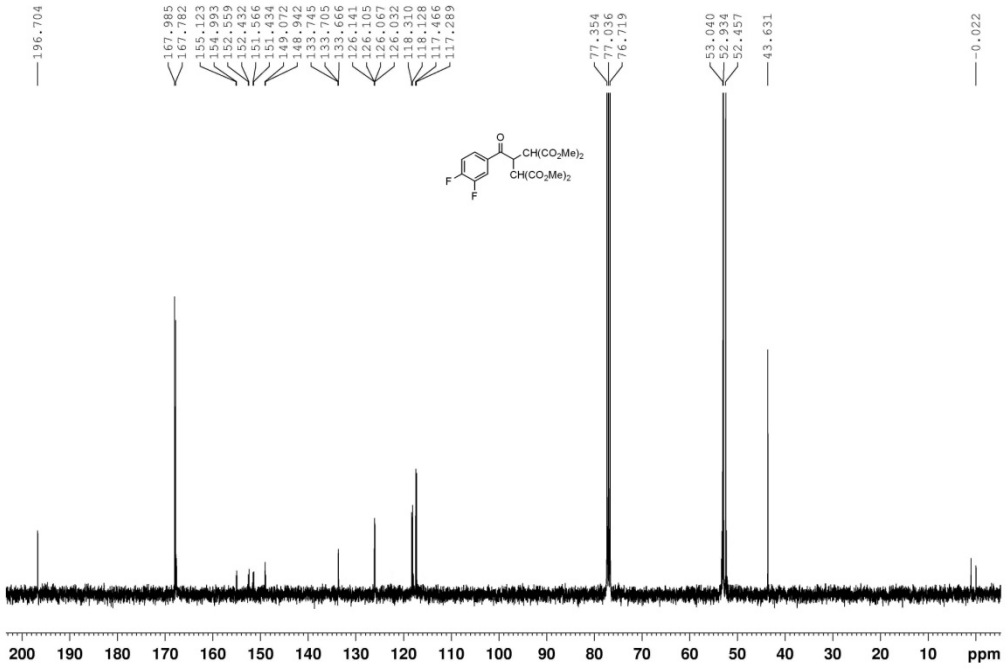




3ar tetramethyl 2-(3-methoxybenzoyl)propane-1,1,3,3-tetracarboxylate





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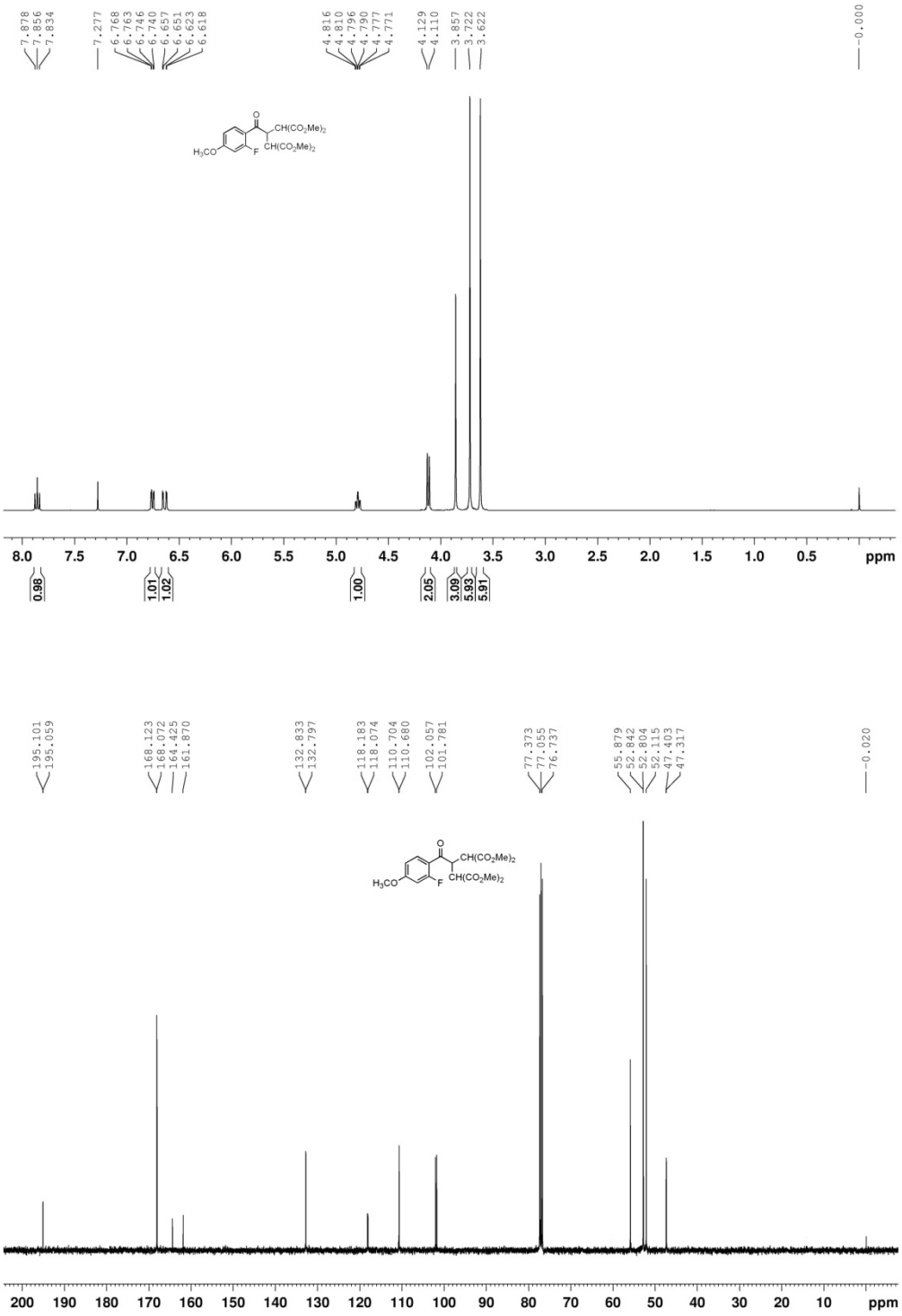

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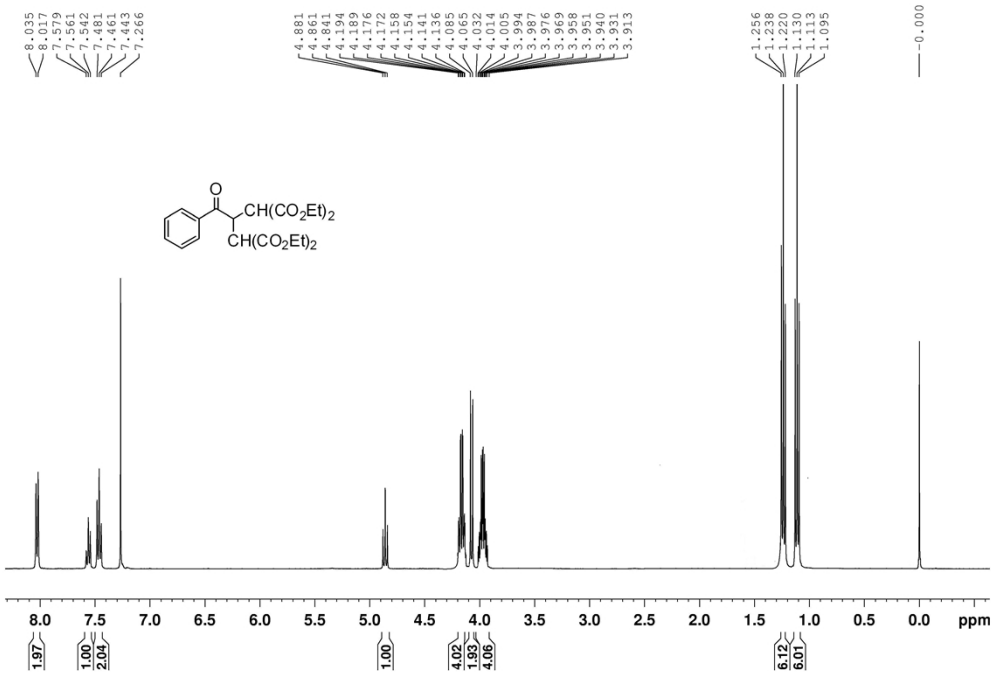
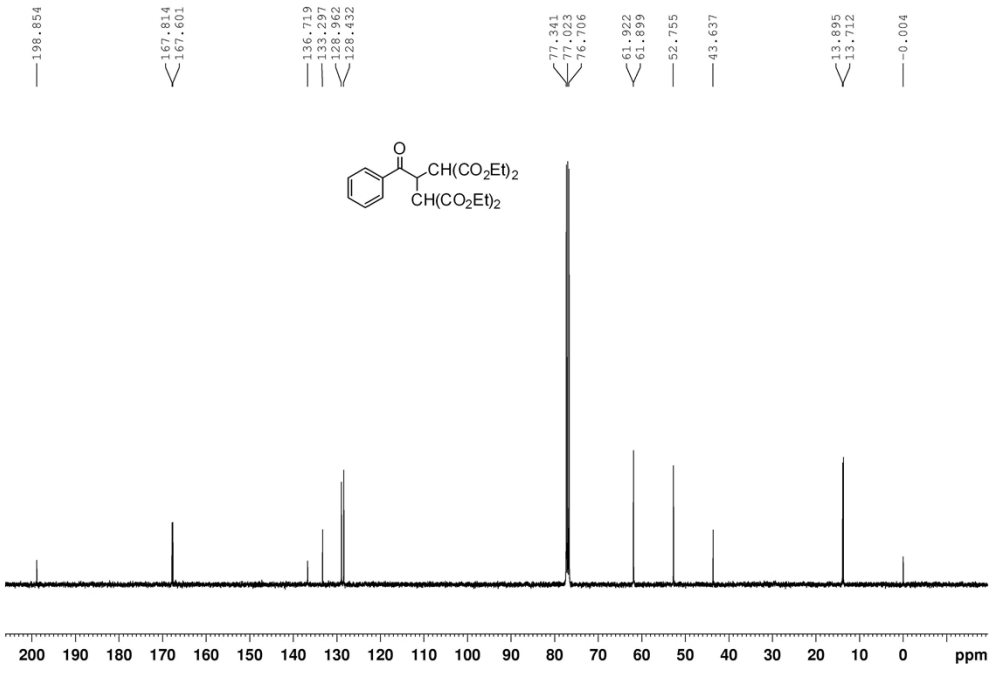
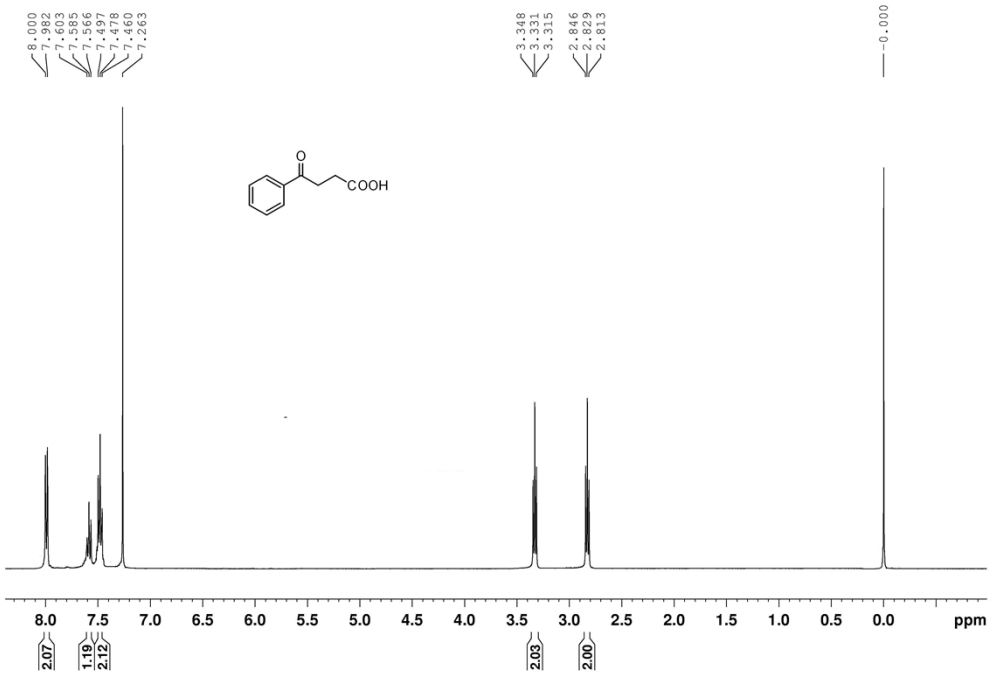




8 3-Benzoylpropanoic acid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7.460
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3.348
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2.846
2.829
2.813
0.000
O
COOH
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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1.0
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2.07
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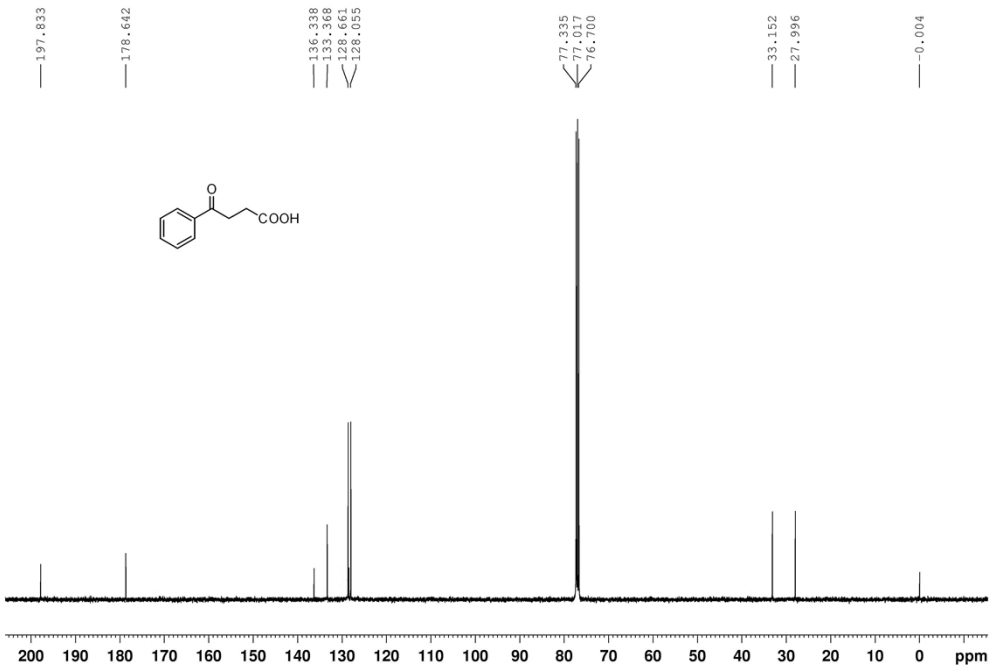
2.12
2.03
2.00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180
170
160
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140
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120
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100
90
80
70
60
50
40
30
20
10
0
ppm