

Supporting Information

Organic Dye-Catalyzed Radical Ring Expansion Reaction

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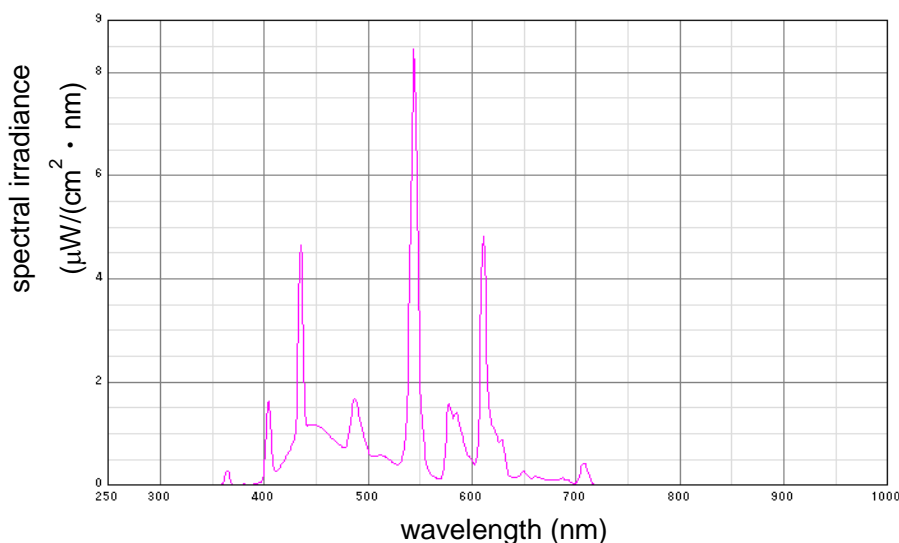
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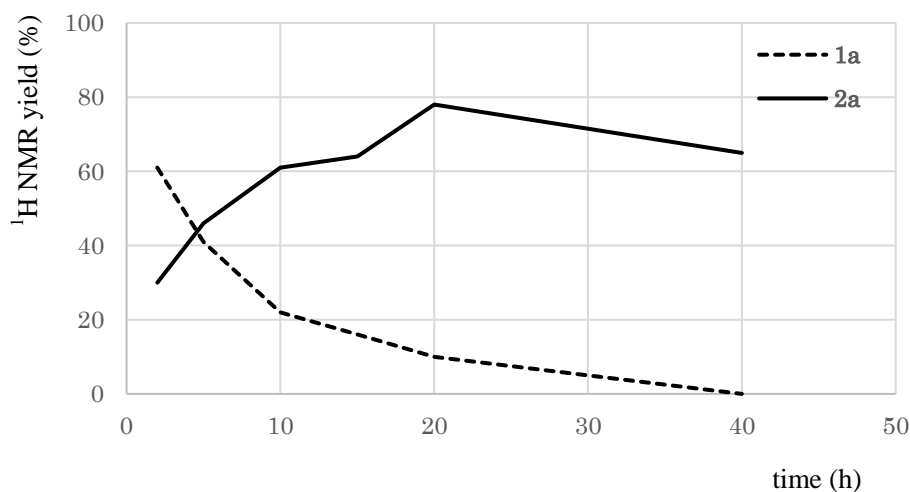
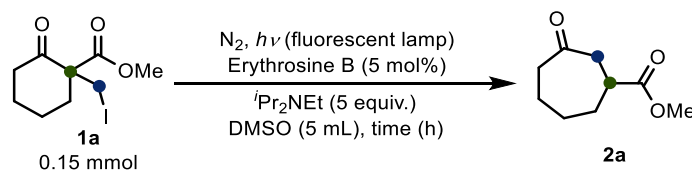
1. General Information

Unless otherwise noted, all reactants or reagents including dry solvents were obtained from commercial suppliers and used as received. Flash column chromatography was performed with Kanto silica gel 60N (Spherical, Neutral, 40–50 mm). Analytical thin-layer chromatography (TLC) was carried out using 0.25 mm commercial silica gel plates (Merck silica gel 60 F₂₅₄). The developed chromatogram was analyzed by UV lamp (254 nm). ¹H NMR and ¹³C NMR spectra were obtained on a JEOL ECA 500 (500 MHz for ¹H NMR and 125 MHz for ¹³C NMR). Chemical shifts (δ) are expressed in parts per million and are internally referenced [0.00 ppm (tetramethylsilane) for ¹H NMR and 77.0 ppm (CDCl₃) for ¹³C NMR]. Infrared spectra were taken on a Perkin Elmer Spectrum 100 FTIR and are reported in reciprocal centimeters (cm⁻¹). High-resolution mass spectra (HRMS) were obtained on a JEOL JMS-T100TD is reported as m/z (relative intensity). Melting points were measured on a Yanaco Micro Melting Point Apparatus and are uncorrected.

2. The wavelength and spectral irradiance of fluorescent lamp (EFR25ED/22-SP F)



3. Time course of 1a and 2a



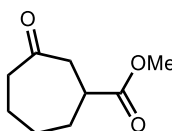
4. General Procedure

General Procedure for Ring Expansion. Methyl 3-oxocycloheptane-1-carboxylate (2a) (Table 1): A mixture of methyl 1-(iodomethyl)-2-oxocyclohexane-1-carboxylate^{S1} (**1a**, 0.15 mmol), erythrosine B (5 mol%), ⁱPr₂NEt (0.75 mmol, 5 equiv.), in DMSO (5 mL) as stirred under N₂ with irradiation of 22 W × 4 fluorescent lamps (EFR25ED/22-SP F from Panasonic) for 20 h. The reaction mixture was diluted with EtOAc (30 mL) and washed with brine (5 mL × 3), dried over magnesium sulfate, filtered and concentrated *in vacuo*. Purification of the residue by flash column chromatography (hexane : ethyl acetate = 4 : 1) on silica gel provided desired material. Other products were also provided in the same way in which the eluent of flash column chromatography depend on products.

Methyl 3-oxocycloheptane-1-carboxylate^{S1} (2a)

The product was isolated as a light brown oil.

TLC: *R_f* = 0.27 (hexane : ethyl acetate = 4 : 1).



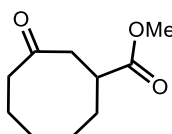
¹H NMR (500 MHz, CDCl₃): δ 3.70 (s, 3H), 2.84–2.67 (m, 3H), 2.58–2.45 (m, 2H), 2.15–2.05 (m, 1H), 1.96–1.53 (m, 5H).

¹³C NMR (125 MHz, CDCl₃): δ 212.1, 175.0, 52.0, 45.5, 43.9, 41.1, 33.2, 28.2, 23.9.

Methyl 3-oxocyclooctane-1-carboxylate^{S1} (2b)

The product was isolated as a light brown oil.

TLC: *R_f* = 0.34 (hexane : ethyl acetate = 4 : 1).



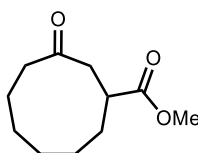
¹H NMR (500 MHz, CDCl₃): δ 3.70 (s, 3H), 2.96–2.91 (m, 1H), 2.80 (t, *J* = 12.6 Hz, 1H), 2.58–2.38 (m, 3H), 2.03–1.37 (m, 8H).

¹³C NMR (125 MHz, CDCl₃): δ 214.8, 175.0, 52.0, 42.9 (2C), 42.7, 29.7, 27.2, 24.7, 23.3 (the peak of 42.9 seems to be overlapped).

Methyl 3-oxocyclononane-1-carboxylate^{S1} (2c)

The product was isolated as a light brown oil.

TLC: *R_f* = 0.34 (hexane : ethyl acetate = 7 : 1).



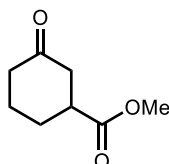
¹H NMR (500 MHz, CDCl₃): δ 3.70 (s, 3H), 3.05–2.99 (m, 1H), 2.87–2.82 (m, 1H), 2.65–2.62 (m, 1H), 2.54–2.43 (m, 2H), 1.93–1.20 (m, 10H).

¹³C NMR (125 MHz, CDCl₃): δ 215.1, 175.8, 52.0, 44.3, 43.8, 41.3, 29.7, 25.6, 25.5, 24.1, 22.9.

Methyl 3-oxocyclohexane-1-carboxylate^{S2} (2d)

The product was isolated as a light brown oil.

TLC: *R_f* = 0.29 (hexane : ethyl acetate = 4 : 1).



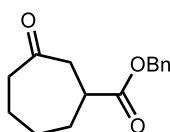
¹H NMR (500 MHz, CDCl₃): δ 3.71 (s, 3H), 2.85–2.79 (m, 1H), 2.56 (d, *J* = 8.6 Hz, 2H), 2.42–2.30 (m, 2H), 2.16–2.04 (m, 2H), 1.89–1.69 (m, 2H).

¹³C NMR (125 MHz, CDCl₃): δ 209.3, 174.2, 52.1, 43.10, 43.07, 40.9, 27.7, 24.5.

Benzyl 3-oxocycloheptane-1-carboxylate (2e)

The product was isolated as a light brown oil.

TLC: *R_f* = 0.36 (hexane : ethyl acetate = 4 : 1).



¹H NMR (500 MHz, CDCl₃): δ 7.39–7.32 (m, 5H), 5.13 (s, 2H), 2.85–2.69 (m, 3H), 2.55–2.44 (m, 2H), 2.15–2.10 (m, 1H), 1.94–1.76 (m, 3H), 1.69–1.61 (m, 1H), 1.56–1.49 (m, 1H).

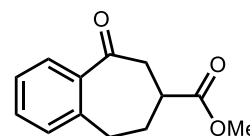
^{13}C NMR (125 MHz, CDCl_3): δ 212.3, 174.4, 135.8, 128.7, 128.5, 128.4, 66.8, 45.6, 44.0, 41.4, 33.3, 28.4, 24.0.

IR ν/cm^{-1} (ATR): 2929, 1731, 1700, 1456, 1276, 1155, 1011, 751, 698.

HRMS (DART): Found 247.1344, Calcd. for $\text{C}_{15}\text{H}_{19}\text{O}_3$, $[\text{M} + \text{H}]^+$: 247.1329.

Methyl 6,7,8,9-tetrahydro-5-oxo-5H-benzocycloheptene-7-carboxylate (2f)

The product was isolated as a colorless oil.



TLC: R_f = 0.42 (hexane : ethyl acetate = 3 : 1).

^1H NMR (500 MHz, CDCl_3): δ 7.73 (d, J = 6.9 Hz, 1H), 7.44 (t, J = 7.5 Hz, 1H), 7.32 (t, J = 7.5 Hz, 1H), 7.22 (d, J = 7.5 Hz, 1H), 3.65 (s, 3H), 3.10–2.85 (m, 5H), 2.32–2.25 (m, 1H), 2.18–2.10 (m, 1H).

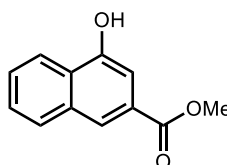
^{13}C NMR (125 MHz, CDCl_3): δ 203.0, 175.0, 141.0, 138.4, 132.8, 130.0, 129.0, 127.3, 52.4, 43.0, 38.4, 31.3, 28.8.

IR ν/cm^{-1} (ATR): 2952, 1731, 1676, 1599, 1449, 1435, 1294, 1254, 1198, 1171, 1092, 1065, 1028, 956, 922, 888, 830, 771.

HRMS (DART): Found 219.1018, Calcd. for $\text{C}_{13}\text{H}_{15}\text{O}_3$ $[\text{M} + \text{H}]^+$: 219.1016.

Methyl 4-hydroxy-2-naphthoate^{S3} (3g)

The product was isolated as a light brown solid.



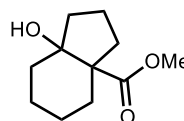
TLC: R_f = 0.38 (hexane : ethyl acetate = 3 : 1).

^1H NMR (500 MHz, CDCl_3): δ 8.26 (d, J = 8.0 Hz, 1H), 8.21 (s, 1H), 7.92 (d, J = 8.0 Hz, 1H), 7.63–7.54 (m, 3H), 6.44 (s, 1H), 4.00 (s, 3H).

^{13}C NMR (125 MHz, CDCl_3): δ 167.6, 152.0, 133.8, 129.1, 127.6, 127.3, 127.2, 126.9, 123.6, 122.0, 107.5, 52.4.

Methyl 7a-hydroxy-octahydro-1H-indene-3a-carboxylate (3i)

The product was isolated as a colorless oil.



TLC: R_f = 0.59 (hexane : ethyl acetate = 3 : 1).

^1H NMR (500 MHz, CDCl_3): δ 3.77 (s, 1H), 3.72 (s, 3H), 2.27–2.20 (m, 1H), 2.04–1.95 (m, 2H), 1.92–1.82 (m, 2H), 1.80–1.71 (m, 3H), 1.68–1.65 (m, 1H), 1.62–1.51 (m, 2H), 1.42–1.33 (m, 2H), 1.20–1.12 (m, 1H).

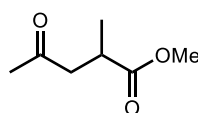
^{13}C NMR (125 MHz, CDCl_3): δ 178.1, 81.4, 56.1, 51.8, 34.5, 34.2, 34.1, 33.2, 23.8, 22.8, 19.0.

IR ν/cm^{-1} (ATR): 2936, 2862, 1710, 1453, 1326, 1293, 1233, 1194, 1164, 1142, 1084, 1046, 1026, 985, 888, 851.

HRMS (DART): Found 199.1324, Calcd. for $\text{C}_{11}\text{H}_{19}\text{O}_3$ $[\text{M} + \text{H}]^+$: 199.1329.

Methyl 2-methyl-4-oxopentanoate^{S1} (2j)

The product was isolated as a colorless oil.



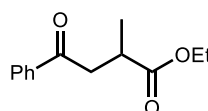
TLC: R_f = 0.27 (hexane : ethyl acetate = 3 : 1).

^1H NMR (500 MHz, CDCl_3): δ 3.68 (s, 3H), 2.99–2.89 (m, 2H), 2.51–2.45 (m, 1H), 2.16 (s, 3H), 1.19 (d, J = 6.9 Hz, 3H).

^{13}C NMR (125 MHz, CDCl_3): δ 206.7, 176.3, 51.9, 46.6, 34.6, 30.0, 17.1.

Ethyl 2-methyl-4-oxo-4-phenylbutanoate^{S4} (2k)

The product was isolated as a light brown oil.



TLC: R_f = 0.27 (hexane : ethyl acetate = 3 : 1).

^1H NMR (500 MHz, CDCl_3): δ 7.99–7.96 (m, 2H), 7.59–7.55 (m, 1H), 7.47 (m, 2H), 4.15 (q, J = 6.9 Hz, 2H), 3.49 (dd, J = 17.8, 8.0 Hz, 1H), 3.16–3.08 (m, 1H), 3.02 (dd, J = 17.8, 5.7 Hz, 1H), 1.29 (d, J = 6.9 Hz, 3H), 1.26 (t, J = 6.9 Hz, 3H).

^{13}C NMR (125 MHz, CDCl_3): δ 198.3, 176.2, 136.9, 133.4, 128.8, 128.2, 60.8, 42.1, 35.2, 17.5, 14.3.

Methyl 1-[(2,2,6,6-tetramethyl-1-piperidinyl)oxy]methyl]-2-oxocyclopentanoate

The product was isolated as a colorless oil.

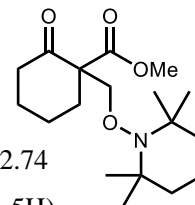
TLC: $R_f = 0.39$ (hexane : ethyl acetate = 9 : 1).

$^1\text{H NMR}$ (500 MHz, CDCl_3): δ 4.23 (d, $J = 8.6$ Hz, 1H), 3.85 (d, $J = 8.6$ Hz, 1H), 3.76 (s, 3H), 2.80–2.74 (m, 1H), 2.42–2.35 (m, 2H), 2.06–1.98 (m, 1H), 1.84–1.75 (m, 2H), 1.71–1.59 (m, 2H), 1.55–1.35 (m, 5H), 1.33–1.25 (m, 1H), 1.15–1.00 (m, 12H).

$^{13}\text{C NMR}$ (125 MHz, CDCl_3): δ 206.2, 170.5, 77.6, 61.3, 60.0, 52.3, 41.1, 39.7, 34.3, 32.8, 32.6, 27.4, 22.1, 20.1, 20.0, 16.9.

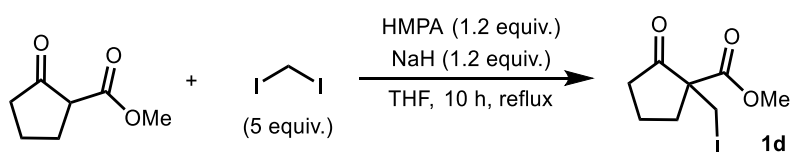
IR ν/cm^{-1} (ATR): 2931, 1714, 1452, 1375, 1360, 1266, 1200, 1147, 1133, 1103, 1083, 1046, 960, 847, 808, 713.

HRMS (DART): Found 326.2345, Calcd. for $\text{C}_{18}\text{H}_{32}\text{O}_4\text{N}$ $[\text{M} + \text{H}]^+$: 326.2326.



Syntheses of substrates

Methyl 1-iodomethyl-2-oxocyclopentanoate (**1d**)



A solution of 1.42 g (10.0 mmols) of methyl 2-oxocyclopentanoate^{S5} in 8 mL of dry THF was added slowly to a suspension of 0.48 g (12.0 mmols, 60% dispersion in mineral oil, washed with hexane 50 mL, two times) of NaH in 12 mL of dry THF containing 2.15 g (12.0 mmols) of hexamethylphosphoramide (HMPA) at room temperature under argon. The reaction mixture was stirred at room temperature for 1 h, then treated with 13.4 g (50.0 mmols) of diiodomethane. The reaction mixture was refluxed at 80 °C for 10 h, then washed with water (100 mL), extracted with Et_2O (100 mL \times 3), dried over K_2CO_3 , filtered and concentrated *in vacuo*. Purification of the residue by flash column chromatography (hexane : ethyl acetate = 9 : 1) on silica gel provided 0.90 g (32% yield) of **1d** as a colorless oil.

TLC: $R_f = 0.35$ (hexane : ethyl acetate = 9 : 1).

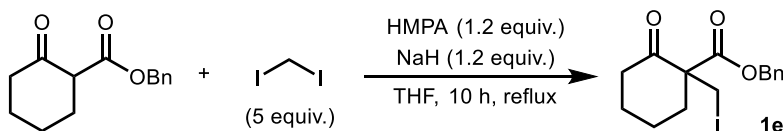
$^1\text{H NMR}$ (500 MHz, CDCl_3): δ 3.76 (s, 3H), 3.62 (d, $J = 10.3$ Hz, 1H), 3.36 (d, $J = 10.3$ Hz, 1H), 2.70–2.60 (m, 1H), 2.53–2.45 (m, 1H), 2.43–2.34 (m, 1H), 2.16–1.97 (m, 3H).

$^{13}\text{C NMR}$ (125 MHz, CDCl_3): δ 211.0, 168.8, 61.0, 53.1, 38.1, 34.6, 19.1, 7.0.

IR ν/cm^{-1} (ATR): 2955, 1753, 1726, 1435, 1277, 1205, 1168, 1123, 968, 919, 826.

HRMS (DART): Found 282.9831, Calcd. for $\text{C}_8\text{H}_{12}\text{IO}_3$ $[\text{M} + \text{H}]^+$: 282.9826.

Benzyl 1-iodomethyl-2-oxocyclohexanecarboxylate (**1e**)



A solution of 2.32 g (10.0 mmols) of benzyl 2-oxocyclohexanecarboxylate^{S6} in 8 mL of dry THF was added slowly to a suspension of 0.48 g (12.0 mmols, 60% dispersion in mineral oil, washed with hexane 50 mL, two times) of NaH in 12 mL of dry THF containing 2.15 g (12.0 mmols) of hexamethylphosphoramide (HMPA) at room temperature under argon. The reaction mixture was stirred at room temperature for 1 h, then treated with 13.4 g (50.0 mmols) of diiodomethane. The reaction mixture was refluxed at 80 °C for 10 h, then washed with water (100 mL), extracted with Et_2O (100 mL \times 3), dried over K_2CO_3 , filtered and concentrated *in vacuo*. Purification of the residue by flash column chromatography (CHCl_3) on silica gel provided 1.19 g (32% yield) of **1e** as a colorless oil.

TLC: R_f = 0.28 (CHCl₃).

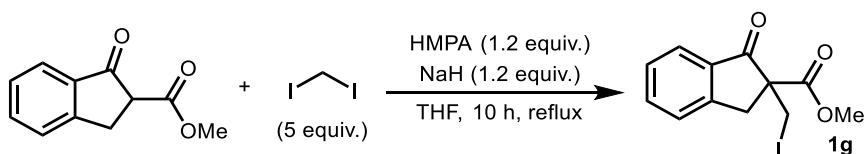
¹H NMR (500 MHz, CDCl₃): δ 7.40–7.33 (m, 5H), 5.24–5.18 (m, 2H), 3.64 (d, J = 10.3 Hz, 1H), 3.36 (d, J = 10.3 Hz, 1H), 2.70–2.65 (m, 1H), 2.46–2.33 (m, 2H), 2.03–1.95 (m, 1H), 1.88–1.75 (m, 2H), 1.71–1.55 (m, 2H).

¹³C NMR (125 MHz, CDCl₃): δ 205.0, 168.8, 135.0, 128.7, 128.6, 128.5, 67.7, 60.9, 40.8, 37.3, 27.4, 22.2, 8.4.

IR ν/cm^{-1} (ATR): 2945, 1710, 1455, 1263, 1212, 1155, 1101, 975, 750, 697.

HRMS (DART): Found 373.0301, Calcd. for C₁₅H₁₈IO₃ [M + H]⁺ : 373.0295.

Methyl 2,3-dihydro-2-(iodomethyl)-1-oxo-1H-indene-2-carboxylate (**1g**)



A solution of 1.90 g (10.0 mmols) of methyl 2,3-dihydro-1-oxo-1H-indene-2-carboxylate^{S7} in 8 mL of dry THF was added slowly to a suspension of 0.48 g (12.0 mmols, 60% dispersion in mineral oil, washed with hexane 50 mL, two times) of NaH in 12 mL of dry THF containing 2.15 g (12.0 mmols) of hexamethylphosphoramide (HMPA) at room temperature under argon. The reaction mixture was stirred at room temperature for 1 h, then treated with 14.8 g (50.0 mmols) of diiodomethane. The reaction mixture was refluxed at 80 °C for 10 h, then washed with water (100 mL), extracted with Et₂O (100 mL \times 3), dried over K₂CO₃, filtered and concentrated *in vacuo*. Purification of the residue by flash column chromatography (hexane : ethyl acetate = 5 : 1) on silica gel provided 2.05 g (62% yield) of **1g** as a light brown solid.

TLC: R_f = 0.35 (hexane : ethyl acetate = 5 : 1).

m.p.: 64–65 °C.

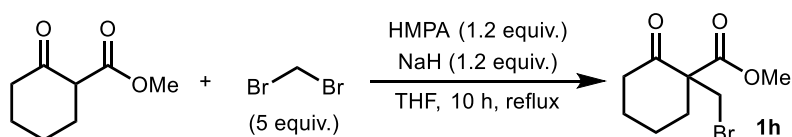
¹H NMR (500 MHz, CDCl₃): δ 7.78 (d, J = 8.0 Hz, 1H), 7.67 (t, J = 7.5 Hz, 1H), 7.53 (d, J = 7.5 Hz, 1H), 7.42 (t, J = 7.5 Hz, 1H), 3.84–3.78 (m, 2H), 3.73 (s, 3H), 3.55 (d, J = 9.7 Hz, 1H), 3.28 (d, J = 17.8 Hz, 1H).

¹³C NMR (125 MHz, CDCl₃): δ 199.1, 169.1, 153.0, 136.2, 134.7, 128.3, 126.7, 125.5, 61.4, 53.5, 39.2, 7.7.

IR ν/cm^{-1} (ATR): 2953, 1736, 1710, 1607, 1589, 1465, 1435, 1253, 1209, 1172, 1043, 1004, 954, 921, 891, 865, 824, 801, 752, 693.

HRMS (DART): Found 330.9834, Calcd. for C₁₂H₁₂O₃I, [M + H]⁺ : 330.9826.

Methyl 1-bromomethyl-2-oxocyclohexane-1-carboxylate (**1h**)



A solution of 1.56 g (10.0 mmols) of methyl 2-oxocyclohexanecarboxylate^{S5} in 8 mL of dry THF was added slowly to a suspension of 0.48 g (12.0 mmols, 60 % dispersion in mineral oil, washed with hexane 50 mL, two times) of NaH in 12 mL of dry THF containing 2.15 g (12.0 mmols) of hexamethylphosphoramide (HMPA) at room temperature under argon. The reaction mixture was stirred at room temperature for 1 h, then treated with 13.4 g (50.0 mmols) of dibromomethane. The reaction mixture was refluxed at 80 °C for 10 h, then washed with water (100 mL), extracted with Et₂O (100 mL \times 3), dried over K₂CO₃, filtered and concentrated *in vacuo*. Purification of the residue by flash column chromatography (hexane : ethyl acetate = 9 : 1) on silica gel provided 1.06 g (45% yield) of **1h** as a colorless oil.

TLC: R_f = 0.28 (hexane : ethyl acetate = 9 : 1).

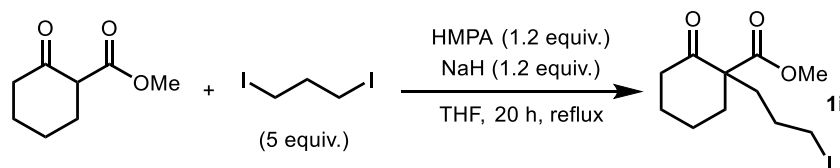
¹H NMR (500 MHz, CDCl₃): δ 3.85 (d, J = 10.3 Hz, 1H), 3.78 (s, 3H), 3.52 (d, J = 10.3 Hz, 1H), 2.75–2.69 (m, 1H), 2.51–2.40 (m, 2H), 2.10–2.01 (m, 1H), 1.91–1.78 (m, 2H), 1.74–1.55 (m, 2H).

¹³C NMR (125 MHz, CDCl₃): δ 205.5, 169.5, 61.5, 52.9, 40.9, 35.4, 35.3, 27.3, 22.2.

IR ν/cm⁻¹ (ATR): 2952, 1711, 1437, 1267, 1196, 1174, 1126, 1108, 1059, 996, 817.

HRMS (DART): Found 249.0130, Calcd. for C₉H₁₄O₃Br, [M + H]⁺ : 249.0121.

Methyl 1-(3-iodopropyl)-2-oxocyclohexanoate (**1i**)



A solution of 0.31 g (2.0 mmols) of methyl 2-oxocyclohexanoate^{S5} in 6 mL of dry THF was added slowly to a suspension of 96.0 mg (2.4 mmols, 60% dispersion in mineral oil, washed with hexane 10 mL, two times) of NaH in 9 mL of dry THF containing 430 mg (2.4 mmols) of hexamethylphosphoramide (HMPA) at room temperature under argon. The reaction mixture was stirred at room temperature for 1 h, then treated with 2.96 g (10.0 mmols) of 1,3-diiodopropane^{S8}. The reaction mixture was refluxed at 80 °C for 20 h, then washed with water (50 mL), extracted with Et₂O (50 mL × 3), dried over K₂CO₃, filtered and concentrated *in vacuo*. Purification of the residue by flash column chromatography (hexane : ethyl acetate = 7 : 1) on silica gel provided 317.7 mg (49%) of **1i** as a colorless oil.

TLC: *R_f* = 0.40 (hexane : ethyl acetate = 7 : 1).

¹H NMR (500 MHz, CDCl₃): δ 3.75 (s, 3H), 3.21–3.11 (m, 2H), 2.52–2.42 (m, 3H), 2.05–1.64 (m, 8H), 1.50–1.44 (m, 1H).

¹³C NMR (125 MHz, CDCl₃): δ 207.6, 172.3, 60.3, 52.4, 41.0, 36.2, 35.7, 28.6, 27.5, 22.5, 6.3.

IR ν/cm⁻¹ (ATR): 2946, 1712, 1449, 1209, 1164.

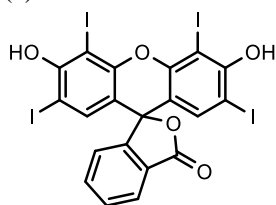
HRMS (DART): Found 325.0311, Calcd. for C₁₁H₁₈O₃I, [M + H]⁺ : 325.0295.

5. Computational details

Quantum chemical calculation were performed at the DFT levels as implemented in the Gaussian 09 program.^{S9} The M06-2X functional^{S10} combined with the 6-31G (d) basis set for hydrogen, carbon, nitrogen, oxygen, sulfur, and MIDI! basis set for iodine were adopted in the present calculations. The full-electron basis MIDI! was selected for iodine since it is superior to commonly used pseudopotential basis LANL2DZ and SDDALL in reproducing experimental bond length of iodine–iodine and carbon–iodine bonds. Numerical integrations were done using ultrafine grid. Geometry optimization and frequency analysis were performed in the solution environment (solvent = DMSO, ε = 46.826) simulated by the integral equation formalism variant of polarizable continuum model (IEF-PCM).^{S11} The obtained equilibrium and transition-state structures have been confirmed to be characterized by all positive vibrational frequencies and one imaginary vibrational mode, respectively. The adequacy of the transition states can be distinctly identified by visualizing the imaginary modes, which clearly display a nuclear motion along the ring-closure coordinate. Free energy corrections are made at the standard conditions of 1 atm and 298.15 K.

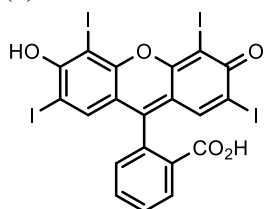
Table S1 The optimized geometries of erythrosine B (EB) (a and b), EB⁻ (c), and EB²⁻ (d) and their oxidized forms, calculated with the M06-2X functional combined with the 6-31G (d) basis sets for hydrogen, carbon, and oxygen and the MIDI! basis set for iodine in the solution environment (solvent = DMSO, $\epsilon = 46.826$) simulated by the IEF-PCM model. Coordinates are given in Å.

(a) EB

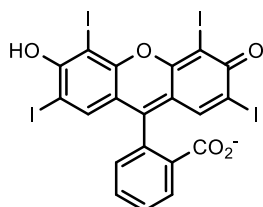


Atom type	Reduced form			Oxidized form		
	x	y	z	x	y	z
C	3.671401	-0.440662	0.074769	3.663110	-0.581662	-0.081382
C	2.478699	0.242002	0.225091	2.503398	-1.344327	-0.114534
C	1.249722	-0.408841	0.139711	1.250134	-0.743511	-0.132432
C	1.245407	-1.778106	-0.104129	1.196708	0.644480	-0.113146
C	2.435842	-2.491721	-0.267769	2.333317	1.444668	-0.070651
C	3.659822	-1.825365	-0.178095	3.583734	0.820558	-0.057488
C	-0.029565	0.365521	0.342045	-0.001350	-1.578661	-0.222298
C	-1.107668	-1.884316	-0.077254	-1.202308	0.671674	-0.111898
C	-1.235435	-0.524448	0.171155	-1.262663	-0.749604	-0.121172
C	-2.520425	0.006921	0.290287	-2.496920	-1.345479	-0.095142
H	-2.634606	1.068911	0.487438	-2.575664	-2.425077	-0.094214
C	-3.645805	-0.782764	0.165284	-3.676246	-0.574473	-0.067659
C	-3.510909	-2.158487	-0.098877	-3.590601	0.856867	-0.058150
C	-2.231645	-2.706351	-0.218574	-2.352347	1.475963	-0.079138
H	2.495971	1.311145	0.415148	2.573368	-2.424730	-0.123549
O	0.097503	-2.501315	-0.205268	-0.024950	1.311447	-0.124130
O	4.774542	-2.555759	-0.344381	4.671835	1.635062	-0.015980
H	5.563995	-1.992854	-0.257768	5.525242	1.154279	-0.006322
C	-0.099245	1.616222	-0.512939	-0.000416	-2.762904	0.731055
C	-0.141262	2.726371	0.311222	-0.014769	-3.945291	0.000638
C	-0.123124	1.748783	-1.894709	0.018806	-2.775080	2.116515
C	-0.208860	4.021510	-0.191877	-0.011572	-5.188828	0.620944
C	-0.190772	3.041190	-2.412256	0.020622	-4.020304	2.749739
H	-0.090579	0.882294	-2.548352	0.033220	-1.856807	2.689992
C	-0.233223	4.165241	-1.574743	0.005548	-5.212741	2.013708
H	-0.240872	4.876948	0.475001	-0.021374	-6.100037	0.036494
H	-0.211197	3.182407	-3.488138	0.035099	-4.065030	3.830967
H	-0.285647	5.155194	-2.015143	0.008565	-6.160008	2.535693
C	-0.101516	2.259997	1.712976	-0.028044	-3.627932	-1.433787
O	-0.037253	0.898670	1.700187	-0.023388	-2.232394	-1.556866
O	-0.118292	2.890153	2.737373	-0.041186	-4.348361	-2.413309
O	-4.637493	-2.878292	-0.224777	-4.761212	1.511699	-0.023317
H	-4.424691	-3.810994	-0.407423	-4.686338	2.491217	-0.021653
I	-1.981799	-4.738555	-0.607152	-2.179116	3.549276	-0.052830
I	2.395574	-4.536216	-0.644730	2.193953	3.519335	-0.018821
I	-5.544544	0.052774	0.366470	-5.495909	-1.480189	-0.043064
I	5.485591	0.587509	0.220885	5.531056	-1.528875	-0.065341

(b) EB

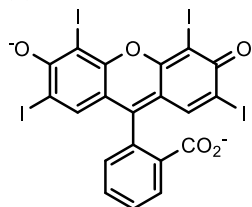


Atom type	Reduced form			Oxidized form		
	x	y	z	x	y	z
C	-2.421144	1.290698	-0.203129	-2.504014	1.272738	-0.365362
C	-1.168222	0.661901	-0.180116	-1.228659	0.656254	-0.258530
C	-1.133023	0.661901	-0.077755	-1.182117	-0.761705	-0.145464
C	-2.295529	-1.497904	0.005942	-2.327769	-1.545383	-0.145591
C	-3.534532	-0.849780	-0.011881	-3.566193	-0.905387	-0.260308
C	-3.586044	0.559076	-0.121136	-3.645032	0.525099	-0.370147
C	-2.468219	2.370710	-0.289224	-2.555069	2.352626	-0.441956
C	0.041563	-1.404617	-0.056373	-0.007772	-1.389228	-0.029967
C	0.079595	1.377627	-0.249050	-0.028439	1.381966	-0.237129
C	1.232807	-0.763976	-0.130311	1.160900	-0.723086	-0.017517
H	1.258464	0.676536	-0.241183	1.194971	0.681563	-0.131888
C	2.552238	1.308056	-0.307710	2.465442	1.354227	-0.122956
C	2.584954	2.389486	-0.382608	2.469016	2.433452	-0.225871
C	2.368578	-1.513469	-0.093908	2.318906	-1.481203	0.115551
H	3.689284	0.585337	-0.277775	3.624161	0.671573	0.003435
O	3.690138	-0.893636	-0.164964	3.630084	-0.804254	0.139547
O	4.730444	-1.540289	-0.131347	4.665923	-1.442151	0.265503
H	0.068966	2.858440	-0.421420	-0.045650	2.858509	-0.425272
C	-0.141810	3.756765	0.638973	0.112619	3.759379	0.640917
C	0.269828	3.358197	-1.709222	-0.220639	3.343761	-1.721465
C	-0.147868	5.131457	0.391845	0.101363	5.131657	0.393235
C	0.260893	4.730655	-1.945780	-0.227232	4.717153	-1.957203
C	0.433232	2.663132	-2.527302	-0.344744	2.646110	-2.543998
H	0.051256	5.618603	-0.894993	-0.065259	5.610004	-0.902586
C	-0.304591	5.815159	1.218009	0.218306	5.819071	1.223105
H	0.419421	5.102382	-2.952750	-0.360716	5.084555	-2.969057
H	0.045842	6.688173	-1.074835	-0.073068	6.678721	-1.086219
H	-0.332549	3.240886	2.025534	0.261757	3.227854	2.025464
C	-0.308795	2.069706	2.332289	0.237404	2.046641	2.298474
O	-2.197644	-3.566862	0.159953	-2.216506	-3.608774	0.025726
O	2.297887	-3.581221	0.071003	2.262642	-3.511553	0.288109
O	-5.431937	1.537837	-0.160963	-5.505949	1.445013	-0.528944
H	5.553488	1.505831	-0.383909	5.458026	1.628687	0.015946
I	-0.536697	4.218282	2.917163	0.424538	4.186723	2.937277
I	-0.647075	3.799991	3.790193	0.510351	3.760410	3.809680
I	-4.626178	-1.617226	0.076090	-4.638489	-1.672797	-0.257660
I	-5.432826	-1.071443	0.055274	-5.458899	-1.149614	-0.344259

(c) EB⁻

Atom type	Reduced form			Oxidized form		
	x	y	z	x	y	z
C	-2.417077	1.304654	-0.131537	2.515051	1.274090	0.370665
C	-1.167775	0.670115	-0.129155	1.253995	0.705040	0.207583
C	-1.141004	-0.728117	-0.071620	1.174926	-0.631179	-0.166144
C	-2.309754	-1.486763	-0.018690	2.324067	-1.395648	-0.380504
C	-3.544772	-0.833942	-0.020093	3.582272	-0.811919	-0.213678
C	-3.586229	0.577633	-0.078925	3.669093	0.540045	0.169926
H	-2.452730	2.387456	-0.171834	2.588979	2.317844	0.661344
O	0.028400	-1.407596	-0.066807	-0.012131	-1.272108	-0.354732
C	0.082317	1.391227	-0.172320	0.018588	1.536737	0.440889
C	1.221560	-0.767886	-0.131930	-1.186390	-0.623171	-0.141745
C	1.256084	0.669388	-0.206236	-1.240525	0.724247	0.245723
C	2.551867	1.288437	-0.269650	-2.488353	1.341027	0.469358
H	2.591296	2.371462	-0.310424	-2.503547	2.383026	0.773617
C	2.355371	-1.527390	-0.130254	-2.344983	-1.356138	-0.327203
C	3.685403	0.555585	-0.273941	-3.660571	0.659600	0.305584
C	3.679962	-0.921630	-0.204589	-3.656235	-0.746347	-0.116276
O	4.717094	-1.580194	-0.207594	-4.702664	-1.381506	-0.284119
C	0.075752	2.864149	-0.392745	0.003883	2.811524	-0.384898
C	-0.223543	3.777911	0.626364	0.008861	3.898672	0.471083
C	0.347193	3.321611	-1.687636	-0.006812	2.980813	-1.762373
C	-0.251388	5.138549	0.323517	0.004539	5.208615	0.003225
C	0.317626	4.683679	-1.972251	-0.013529	4.289325	-2.243627
H	0.577724	2.605081	-2.471775	-0.007312	2.132939	-2.440852
C	0.015260	5.596079	-0.963102	-0.007812	5.390209	-1.375535
H	-0.481095	5.824650	1.132206	0.010373	6.046573	0.692744
H	0.531362	5.027892	-2.979267	-0.022130	4.460757	-3.315140
H	-0.006125	6.659843	-1.179976	-0.011871	6.393218	-1.788288
C	-0.483555	3.301503	2.062725	0.022581	3.394206	1.859479
O	-0.328015	2.070410	2.252623	0.024979	2.026583	1.806862
O	-0.817739	4.176750	2.887506	0.030602	3.989030	2.902440
I	-2.222335	-3.561129	0.065505	2.174633	-3.392012	-0.940445
I	2.269483	-3.600075	-0.016635	-2.276050	-3.333768	-0.898664
I	-5.426699	1.569756	-0.082758	5.536538	1.442281	0.429445
I	5.556056	1.470247	-0.372265	-5.491926	1.563978	0.633784
O	-4.643738	-1.597735	0.033944	4.655114	-1.587352	-0.435433
H	-5.444594	-1.043464	0.027480	5.474691	-1.084069	-0.284589

(d) EB²⁻



Atom type	Reduced form			Oxidized form		
	x	y	z	x	y	z
C	2.393307	1.606150	-0.311608	2.438654	1.600760	-0.189662
C	1.138549	0.956599	-0.150297	1.166879	0.945444	-0.085795
C	1.146808	-0.461953	-0.043534	1.159436	-0.489054	0.000873
C	2.312456	-1.189900	-0.089254	2.307764	-1.223446	0.003034
C	3.609100	-0.559302	-0.255016	3.618420	-0.575733	-0.084269
C	3.554761	0.903102	-0.357895	3.596019	0.901744	-0.186822
H	2.399001	2.687746	-0.399811	2.443890	2.681555	-0.273873
O	4.671623	-1.193053	-0.305045	4.667569	-1.209555	-0.077857
O	-0.021761	-1.138009	0.113554	-0.018088	-1.153395	0.083986
C	-0.084146	1.642629	-0.122507	-0.037031	1.648594	-0.100613
C	-1.219280	-0.497288	0.165531	-1.206632	-0.502083	0.093285
C	-1.271910	0.920599	0.062609	-1.246579	0.920953	0.015026
C	-2.554221	1.532248	0.125293	-2.517983	1.566366	0.038287
H	-2.607343	2.612955	0.042146	-2.538117	2.648467	-0.021628
C	-2.352799	-1.259559	0.323033	-2.344255	-1.257337	0.181077
C	-3.684455	0.794975	0.281479	-3.668936	0.855489	0.128667
C	-3.676538	-0.668106	0.388692	-3.663521	-0.621317	0.200163
O	-4.712120	-1.333191	0.524085	-4.702875	-1.271436	0.272415
C	-0.104068	3.135355	-0.095722	-0.045815	3.138970	-0.079765
C	-0.217071	3.927197	-1.245785	-0.409747	3.902440	-1.197650
C	-0.002223	3.739743	1.162874	0.307964	3.769816	1.118556
C	-0.225132	5.316379	-1.104361	-0.414193	5.292571	-1.086004
C	-0.011945	5.125826	1.285418	0.301393	5.158501	1.210121
H	0.084966	3.114953	2.048233	0.586143	3.167877	1.979856
C	-0.124065	5.918983	0.144760	-0.062162	5.923018	0.103148
H	-0.313672	5.905779	-2.011088	-0.697194	5.861218	-1.965615
H	0.067765	5.581643	2.267538	0.579048	5.638264	2.143345
H	-0.132392	7.001484	0.232003	-0.067283	7.006836	0.168778
C	-0.331579	3.306246	-2.648149	-0.778058	3.241554	-2.536233
O	-0.317407	2.054211	-2.690261	-0.652749	1.992729	-2.573459
O	-0.426822	4.112167	-3.600090	-1.160472	4.008027	-3.443637
I	2.296958	-3.265021	0.070873	2.271481	-3.290538	0.120502
I	-2.247972	-3.332861	0.472826	-2.264616	-3.318941	0.285646
I	5.384102	1.887353	-0.586011	5.434507	1.855388	-0.335065
I	-5.553840	1.723951	0.379803	-5.516228	1.796284	0.165501

Table S2 The optimized geometries of the substrate **1a** and the corresponding radical **4a**, calculated with the M06-2X functional combined with the 6-31G (d) basis sets for hydrogen, carbon, and oxygen and the MIDI! basis set for iodine in the solution environment (solvent = DMSO, $\epsilon = 46.826$) simulated by the IEF-PCM model. Coordinates are given in Å.

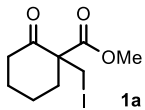
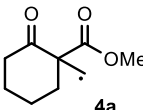
Atom type	 1a			 4a		
	x	y	z	x	y	z
C	1.211390	-0.947218	-0.854989	1.278994	-0.936637	-0.826396
C	0.823671	-0.306742	0.487699	0.915051	-0.333121	0.543580
C	1.963980	-0.611028	1.491465	2.057234	-0.622576	1.545583
C	3.327611	-0.159586	0.965016	3.424510	-0.187306	1.016800
C	3.653231	-0.820642	-0.374807	3.733313	-0.848506	-0.326691
C	2.555698	-0.529009	-1.413756	2.638524	-0.532552	-1.359862
H	1.726728	-0.108414	2.433872	1.823458	-0.109346	2.483316
H	3.327448	0.933002	0.852247	3.437667	0.904092	0.908379
H	4.099686	-0.398321	1.703660	4.196959	-0.443049	1.749557
H	4.619284	-0.473210	-0.753931	4.704176	-0.518423	-0.709631
H	3.735358	-1.906165	-0.235259	3.795233	-1.936376	-0.194703
H	2.534480	0.544478	-1.632371	2.625055	0.548662	-1.555619
H	2.719999	-1.074626	-2.345564	2.800507	-1.051497	-2.307341
H	1.977444	-1.693070	1.676979	2.057479	-1.701544	1.744333
O	0.539345	-1.822731	-1.346342	0.554345	-1.715489	-1.397077
C	0.656463	1.208987	0.406008	0.756513	1.186563	0.402261
O	0.662956	1.930579	1.371535	1.068479	1.997865	1.237565
O	0.449293	1.635269	-0.843773	0.164724	1.507084	-0.759046
C	0.108541	3.019305	-0.962562	-0.100668	2.899332	-0.938320
H	-0.045022	3.194174	-2.025686	-0.566609	2.987683	-1.918129
H	-0.805151	3.223244	-0.400018	-0.773199	3.258320	-0.156325
H	0.917333	3.643424	-0.576935	0.828991	3.471214	-0.897079
C	-0.472618	-0.899735	1.038240	-0.396146	-0.850654	1.033355
H	-0.432209	-1.986337	0.975134	-1.064001	-1.358389	0.351876
H	-0.614746	-0.578447	2.070033	-0.720395	-0.598169	2.035507
I	-2.263041	-0.320579	0.002125	-	-	-

Table S3 The SCF and thermal energies for the redox states of EB, EB⁻, and EB²⁻, calculated with the M06-2X functional combined with the 6-31G (d) basis sets for hydrogen, carbon, and oxygen and the MIDI! basis set for iodine in the solution environment (solvent = DMSO, $\epsilon = 46.826$) simulated by the IEF-PCM model. Free energy corrections are made at the standard conditions of 1 atm and 298.15 K. Energies are given in hartree/particle.

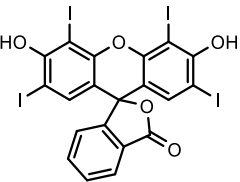
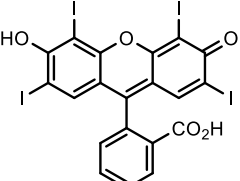
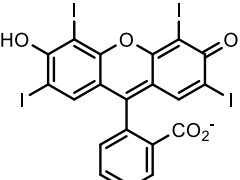
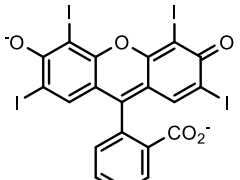
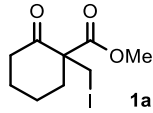
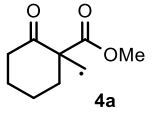
Erythrosine B		Reduced form	Oxidized form
	E(RM062X) or E(UM062X)	-28707.043805	-28705.412000
	Zero-point correction	0.236923	0.237148
	Thermal correction to Energy	0.260969	0.261850
	Thermal correction to Enthalpy	0.261914	0.262795
	Thermal correction to Gibbs Free Energy	0.179042	0.175792
	Sum of electronic and zero-point Energies	-28706.806882	-28705.174852
	Sum of electronic and thermal Energies	-28706.782835	-28705.150150
	Sum of electronic and thermal Enthalpies	-28706.781891	-28705.149205
	Sum of electronic and thermal Free Energies	-28706.864763	-28705.236208
	E(RM062X) or E(UM062X)	-28707.027536	-28706.806598
	Zero-point correction	0.235625	0.234662
	Thermal correction to Energy	0.261556	0.260636
	Thermal correction to Enthalpy	0.262501	0.261580
	Thermal correction to Gibbs Free Energy	0.172387	0.170314
	Sum of electronic and zero-point Energies	-28706.791911	-28706.571936
	Sum of electronic and thermal Energies	-28706.765980	-28706.545962
	Sum of electronic and thermal Enthalpies	-28706.765035	-28706.545018
	Sum of electronic and thermal Free Energies	-28706.855149	-28706.636284
	E(RM062X) or E(UM062X)	-28706.559161	-28706.398292
	Zero-point correction	0.222266	0.223619
	Thermal correction to Energy	0.247995	0.248428
	Thermal correction to Enthalpy	0.248939	0.249372
	Thermal correction to Gibbs Free Energy	0.159350	0.161832
	Sum of electronic and zero-point Energies	-28706.336895	-28706.174674
	Sum of electronic and thermal Energies	-28706.311166	-28706.149864
	Sum of electronic and thermal Enthalpies	-28706.310222	-28706.148920
	Sum of electronic and thermal Free Energies	-28706.399811	-28706.236461
	E(RM062X) or E(UM062X)	-28706.103184	-28705.920287
	Zero-point correction	0.209279	0.208586
	Thermal correction to Energy	0.233940	0.234238
	Thermal correction to Enthalpy	0.234884	0.235182
	Thermal correction to Gibbs Free Energy	0.147355	0.144212
	Sum of electronic and zero-point Energies	-28705.893905	-28705.711701
	Sum of electronic and thermal Energies	-28705.869244	-28705.686049
	Sum of electronic and thermal Enthalpies	-28705.868300	-28705.685105
	Sum of electronic and thermal Free Energies	-28705.955829	-28705.776075

Table S4 The SCF and thermal energies of the substrate **1a**, the corresponding radical **4a**, and iodide ion, calculated with the M06-2X functional combined with the 6-31G (d) basis sets for hydrogen, carbon, and oxygen and the MIDI! basis set for iodine in the solution environment (solvent = DMSO, $\epsilon = 46.826$) simulated by the IEF-PCM model. Free energy corrections are made at the standard conditions of 1 atm and 298.15 K. Energies are given in hartree/particle.

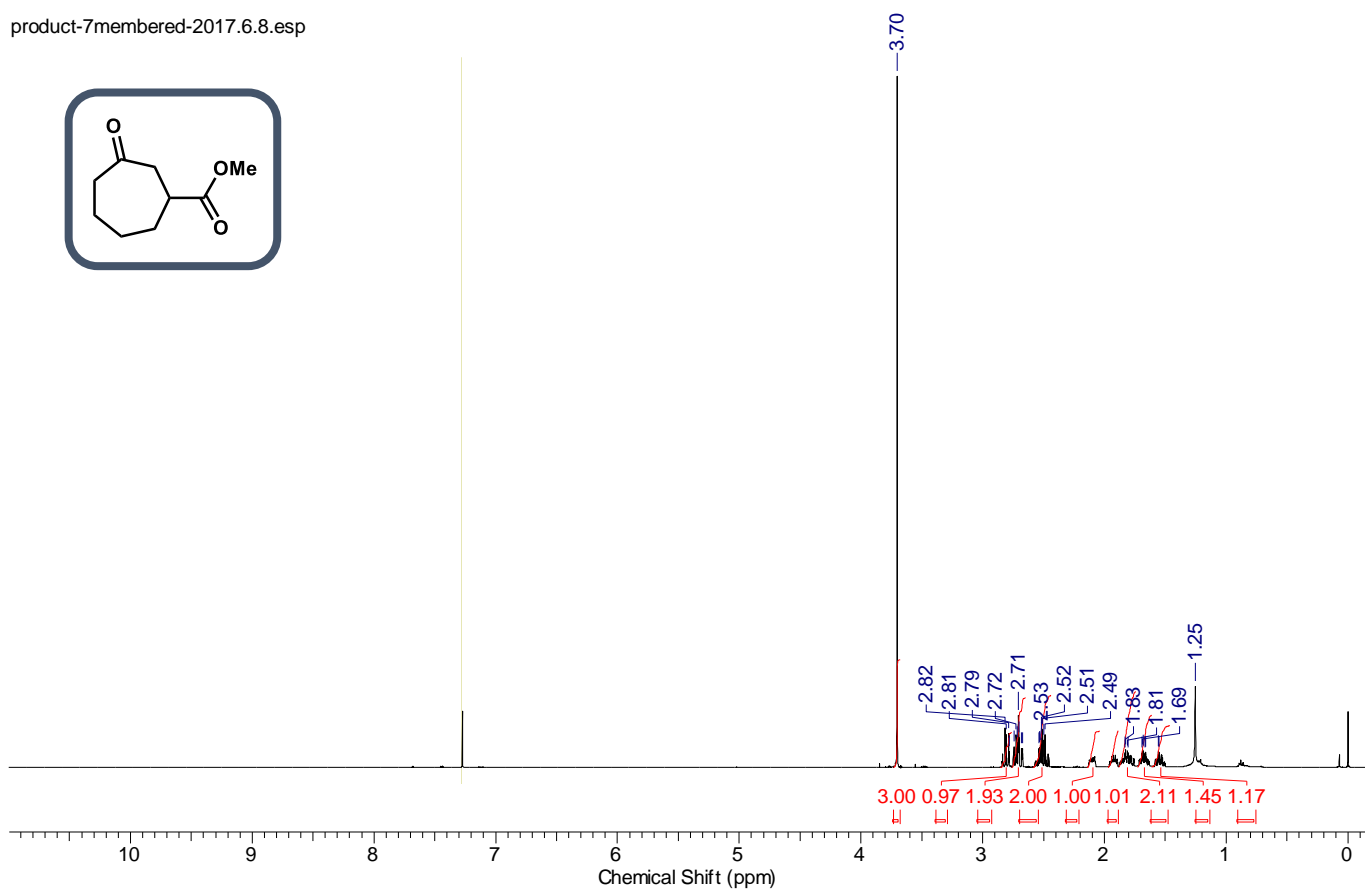
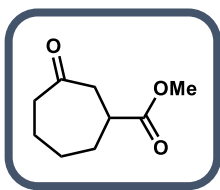
	 1a	 4a	I ⁻
E(RM062X) or E(UM062X)	-7467.320124	-576.157986	-6891.259474
Zero-point correction	0.215947	0.210626	0.000000
Thermal correction to Energy	0.229242	0.222928	0.001416
Thermal correction to Enthalpy	0.230187	0.223872	0.002360
Thermal correction to Gibbs Free Energy	0.174538	0.172012	-0.016848
Sum of electronic and zero-point Energies	-7467.104177	-575.947360	-6891.258058
Sum of electronic and thermal Energies	-7467.090882	-575.935058	-6891.259474
Sum of electronic and thermal Enthalpies	-7467.089938	-575.934114	-6891.257113
Sum of electronic and thermal Free Energies	-7467.145586	-575.985974	-6891.276322

6. References

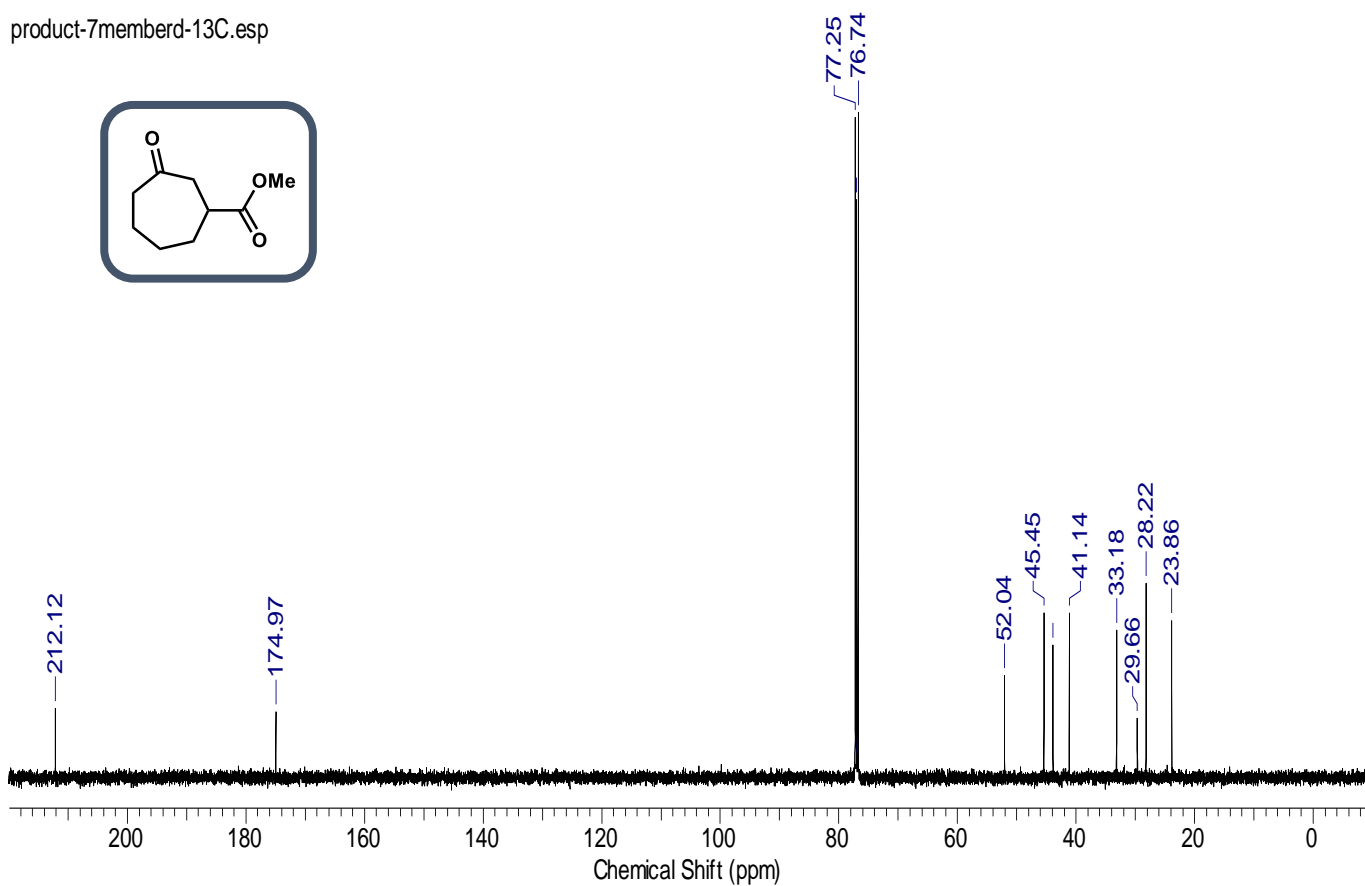
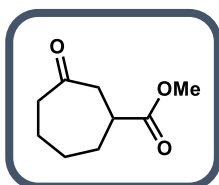
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7. ^1H and ^{13}C spectra

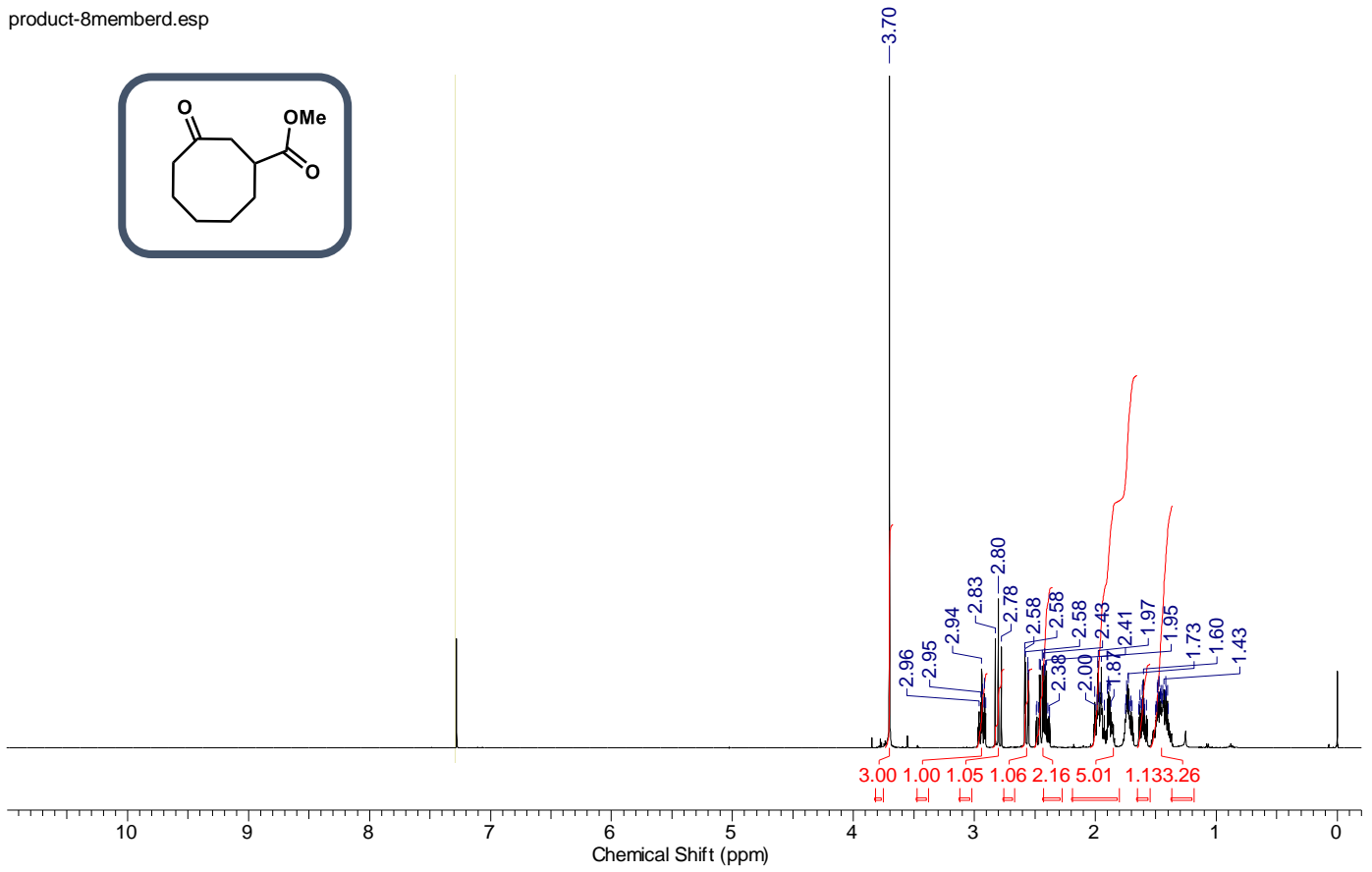
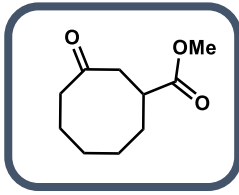
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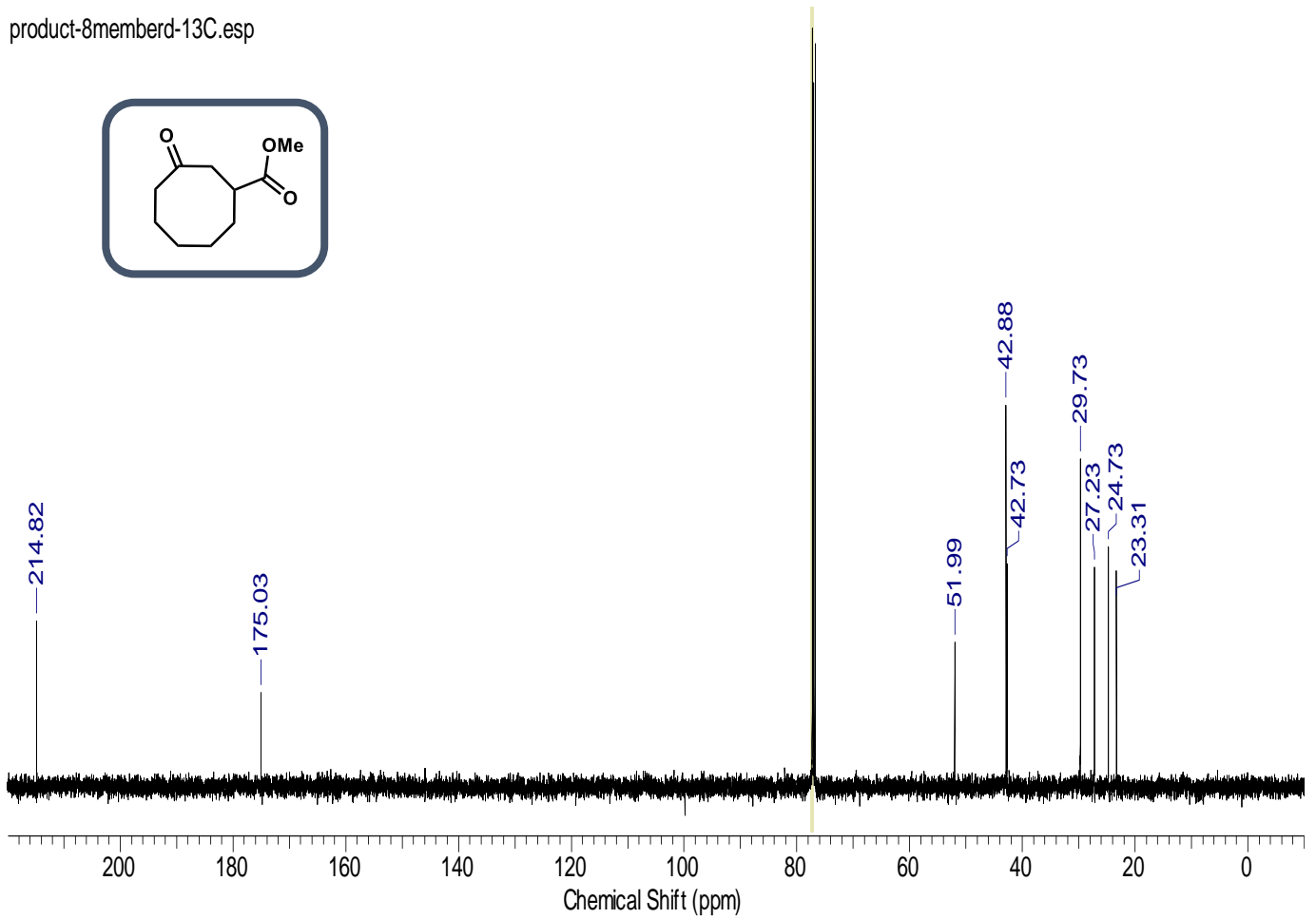
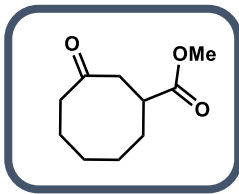
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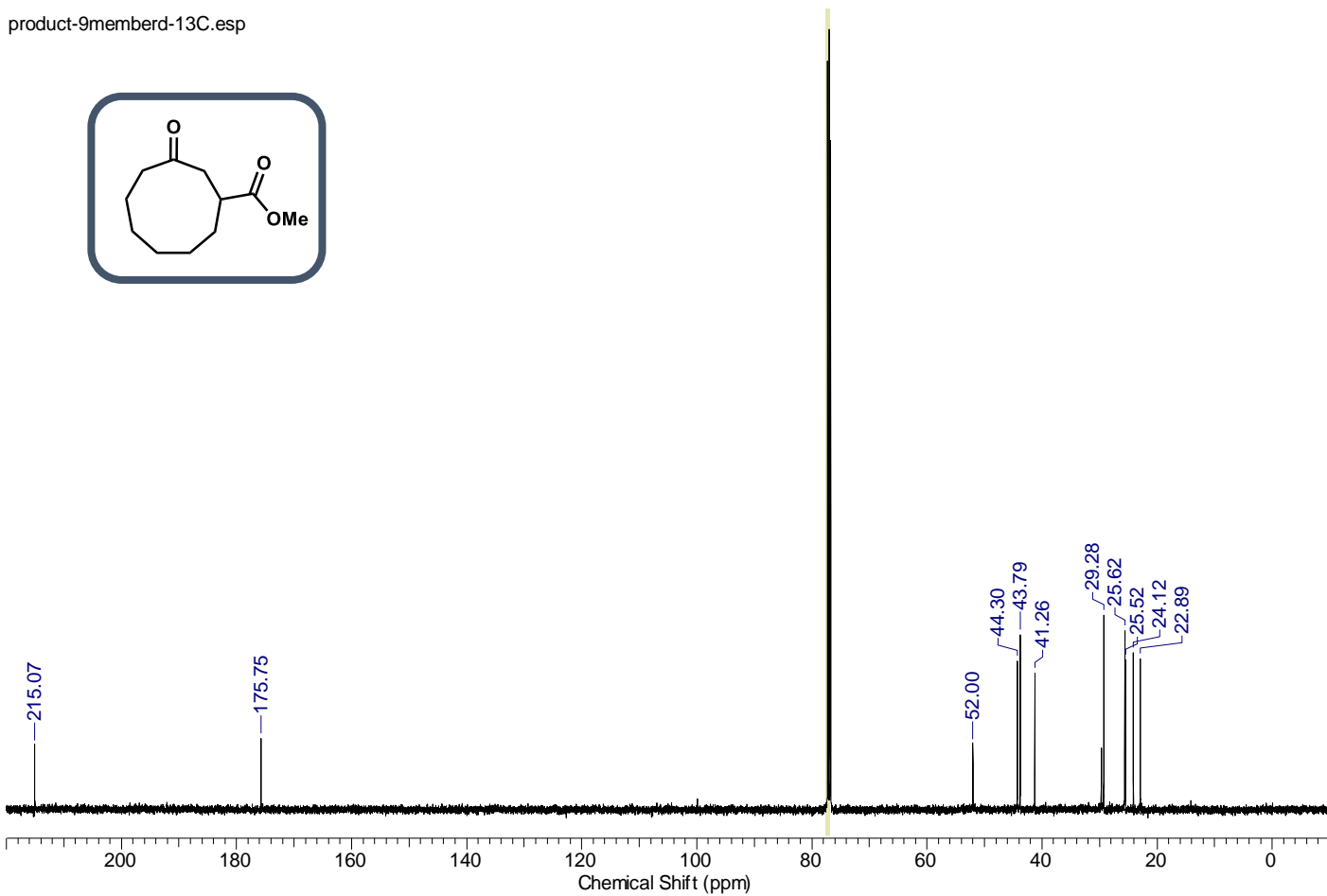
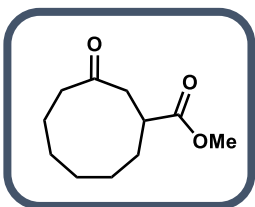
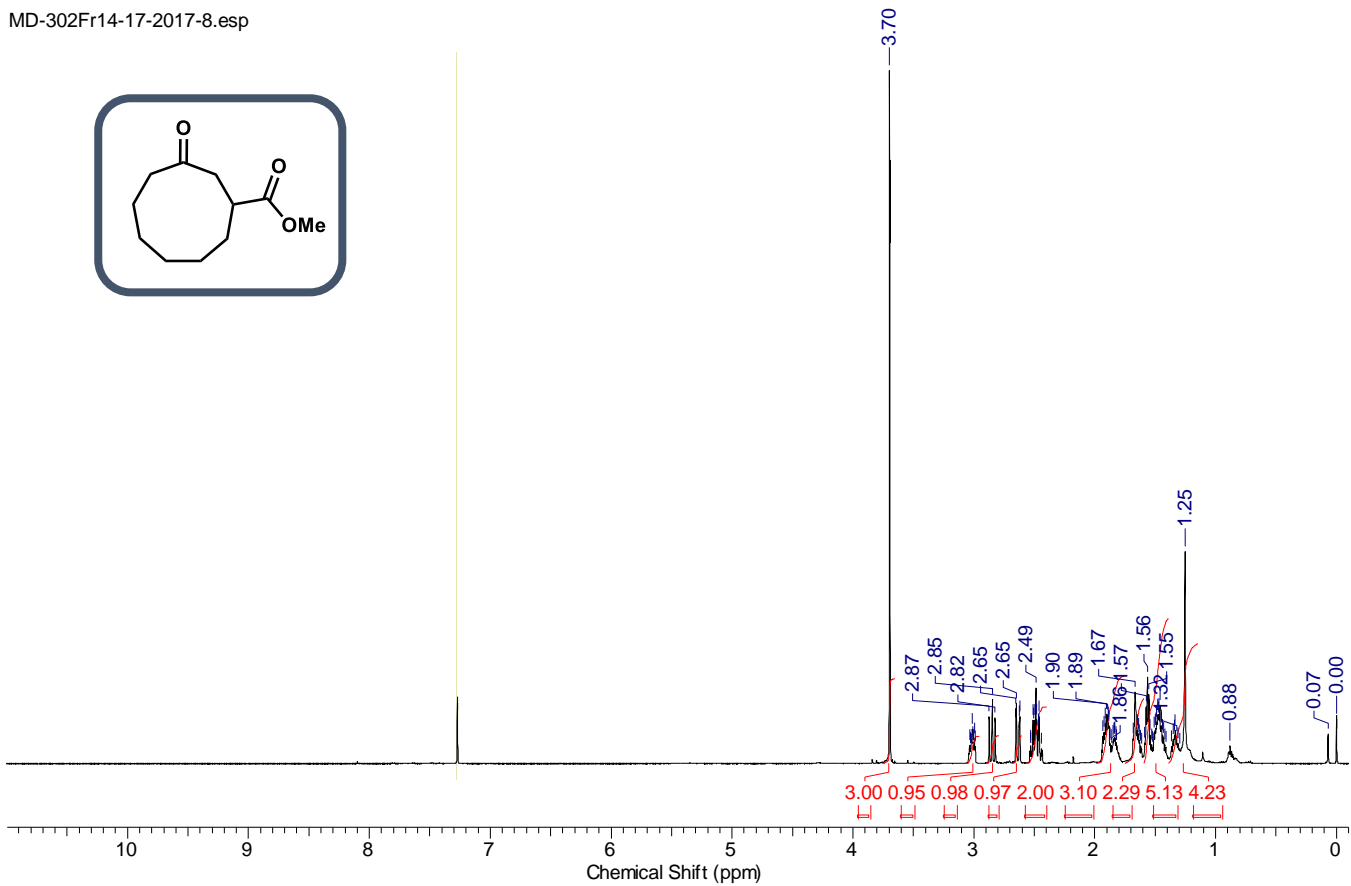
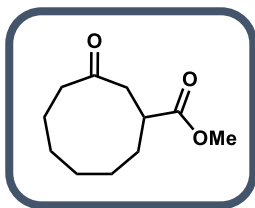


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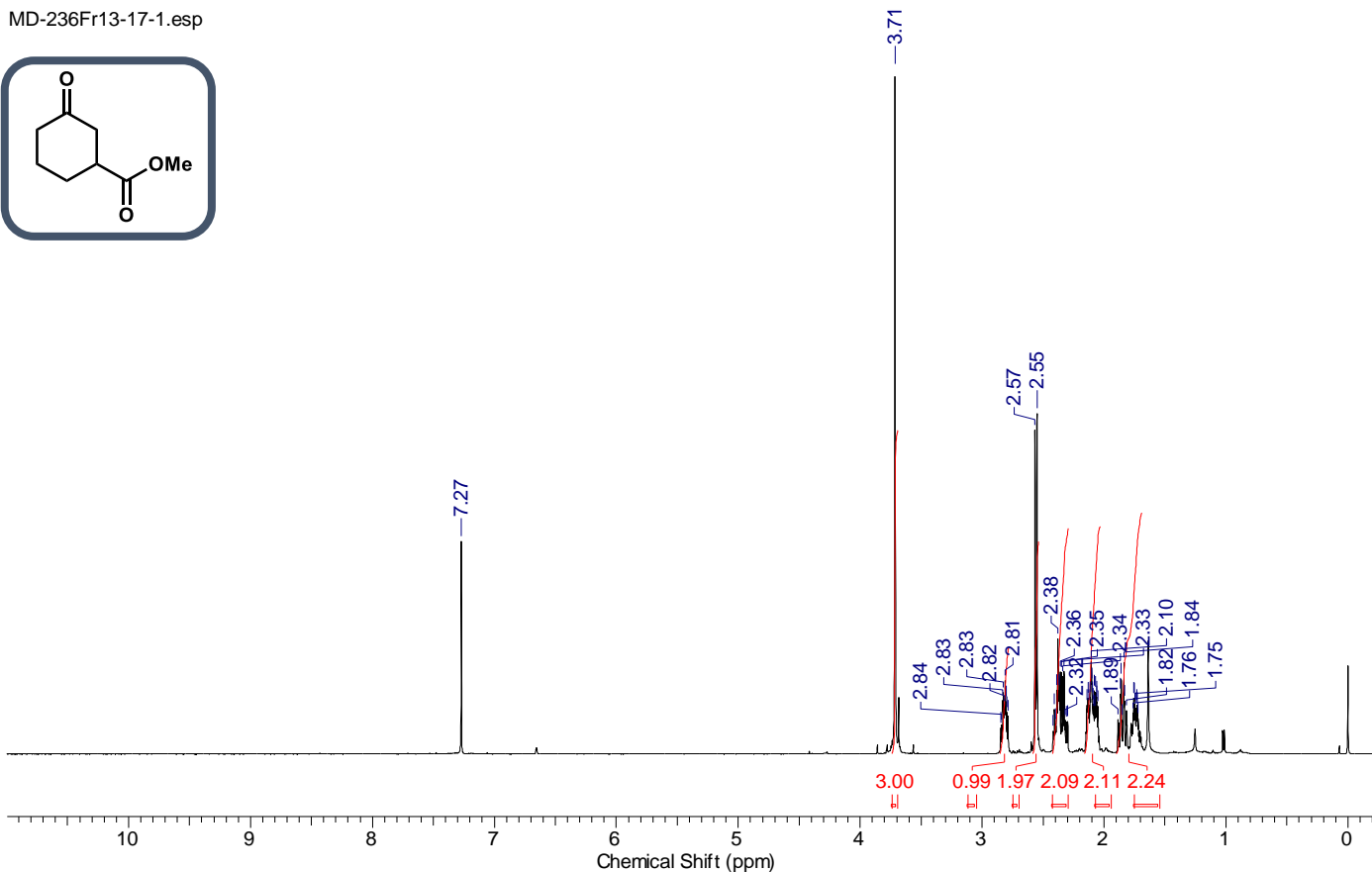
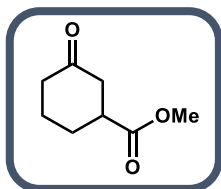


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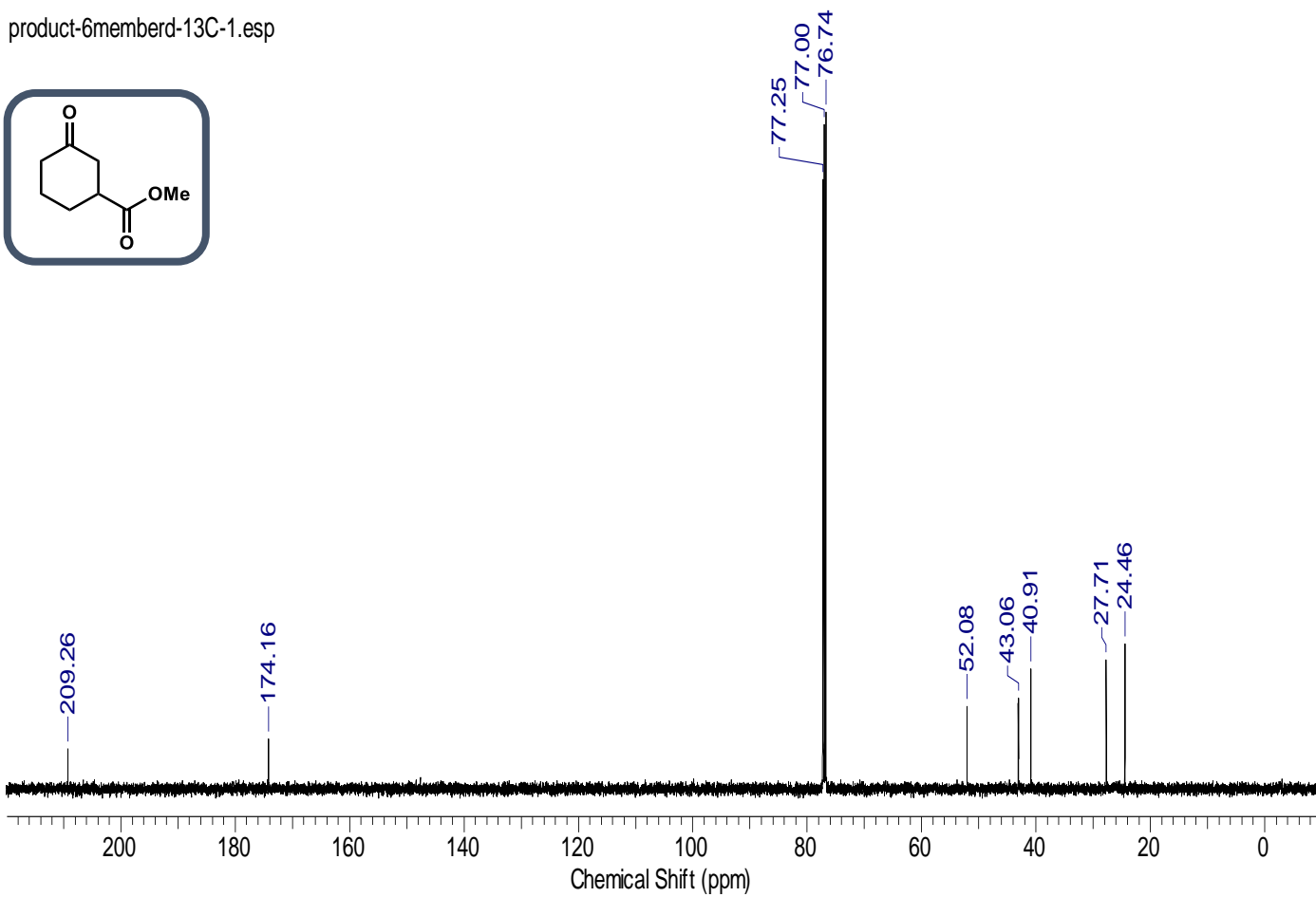
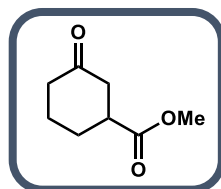




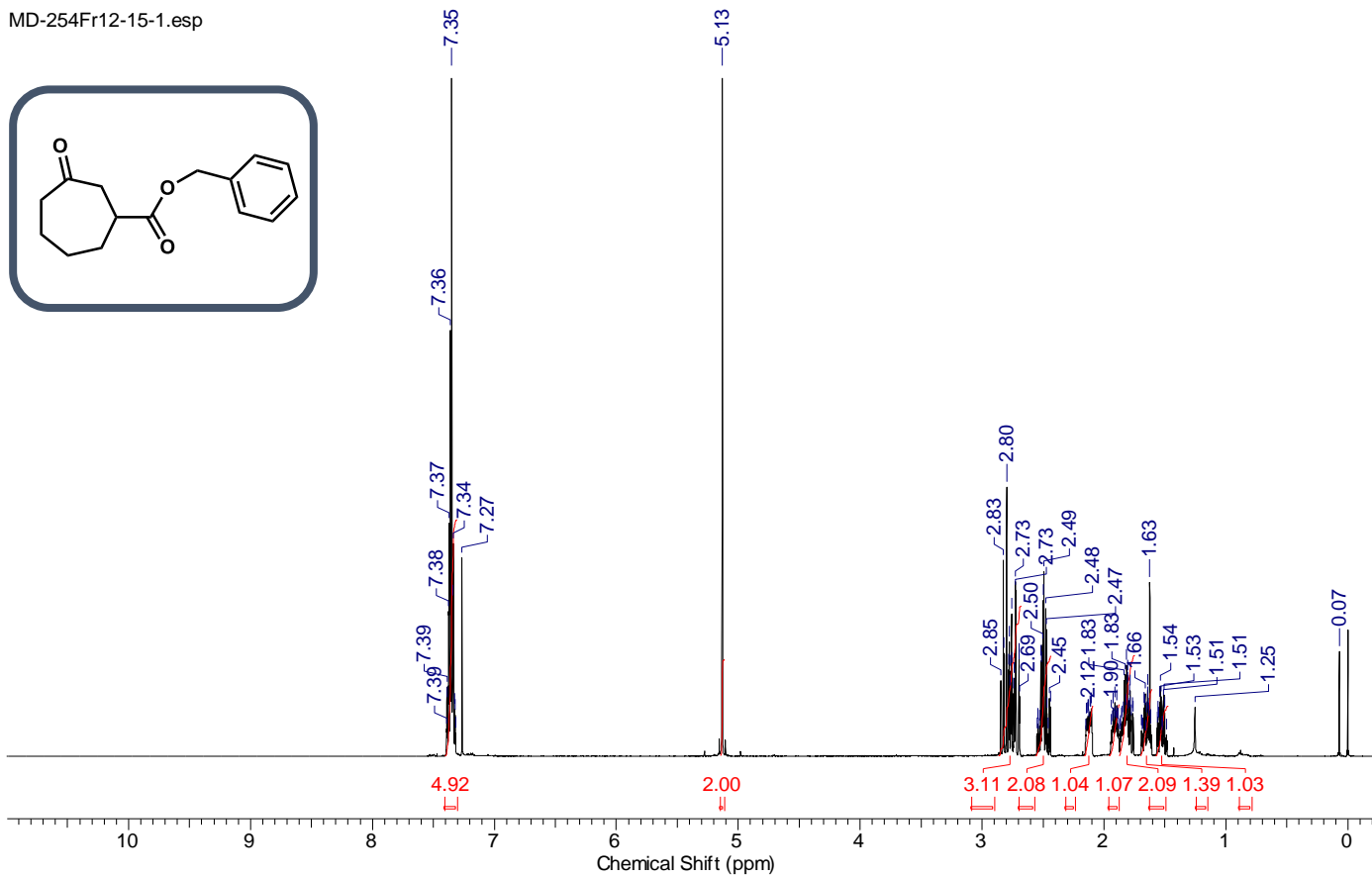
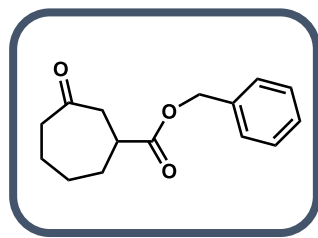
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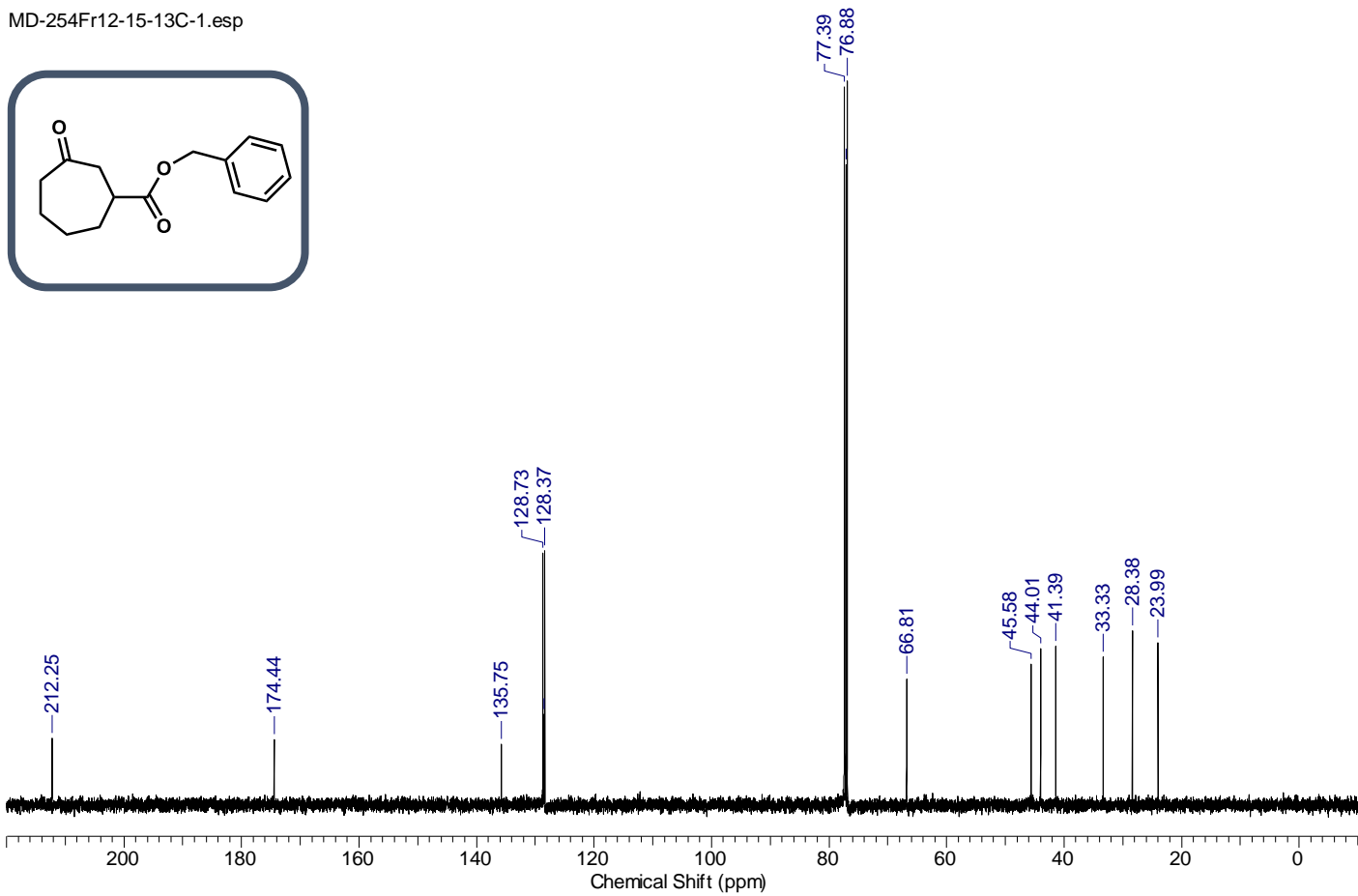
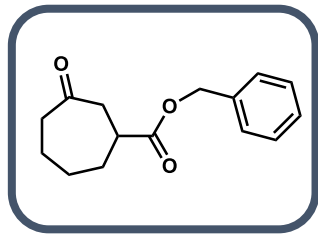
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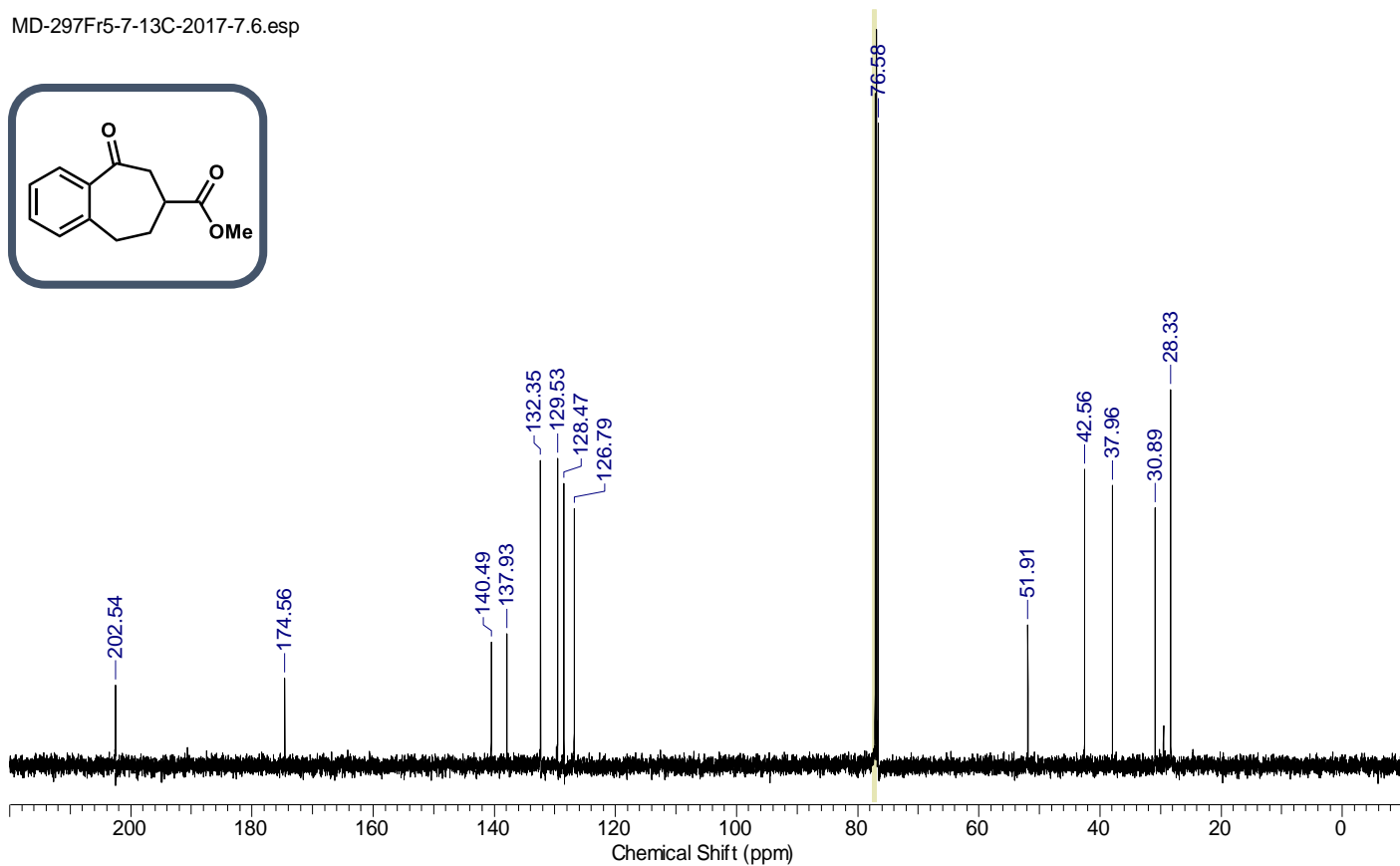
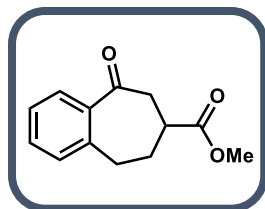
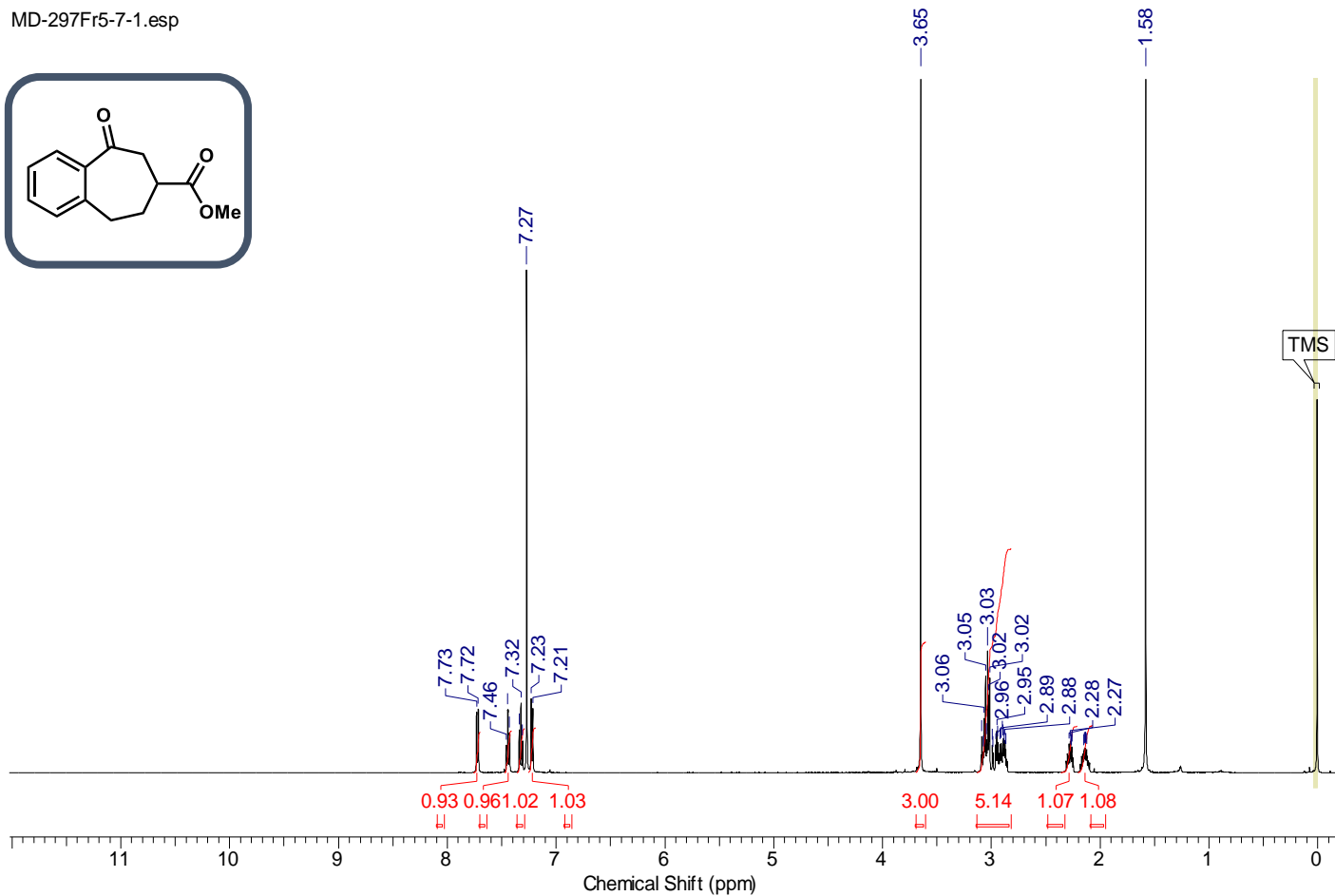
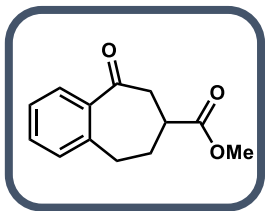


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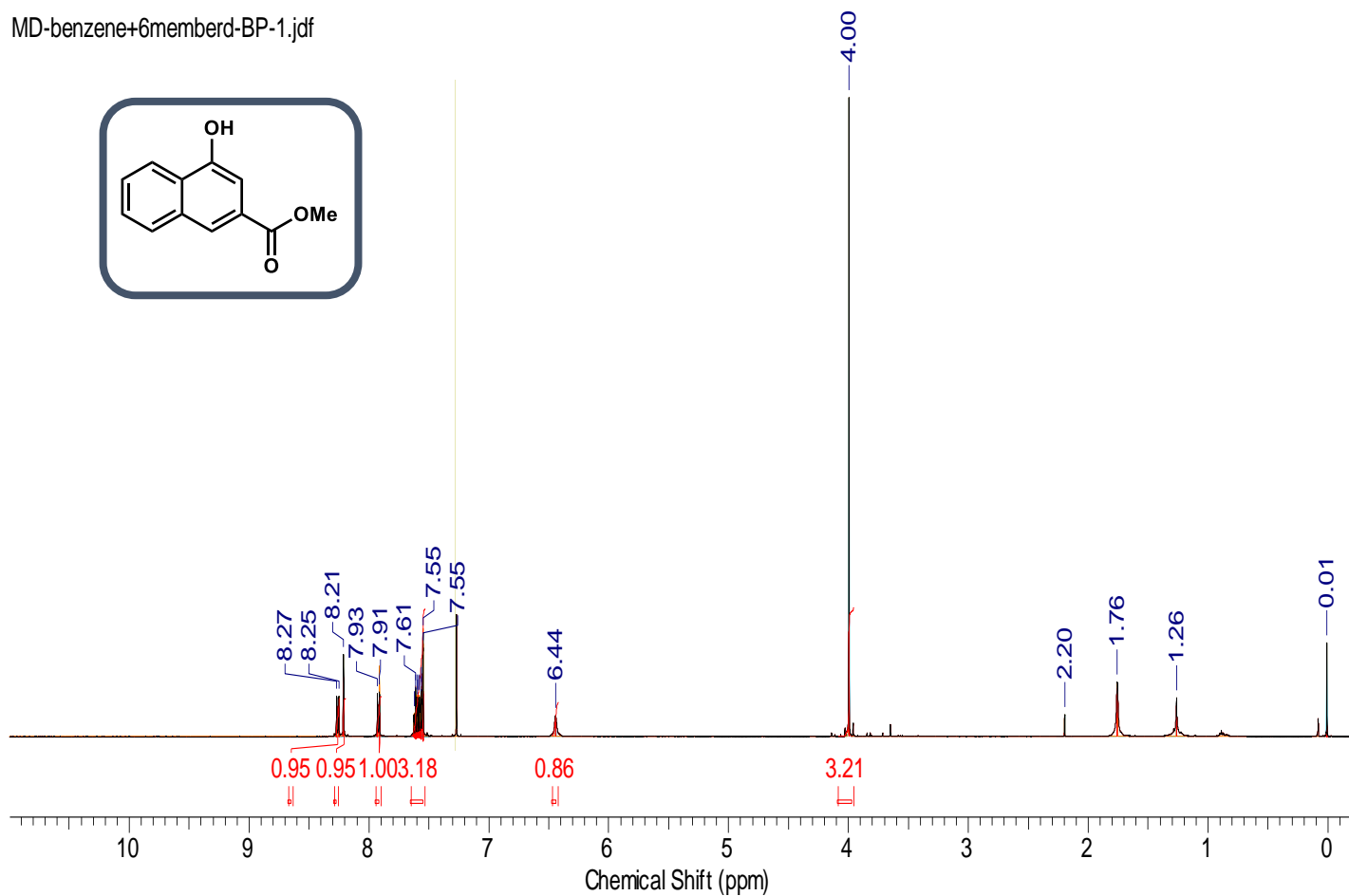
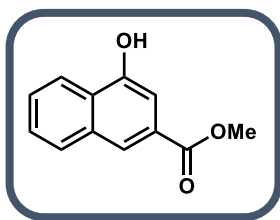


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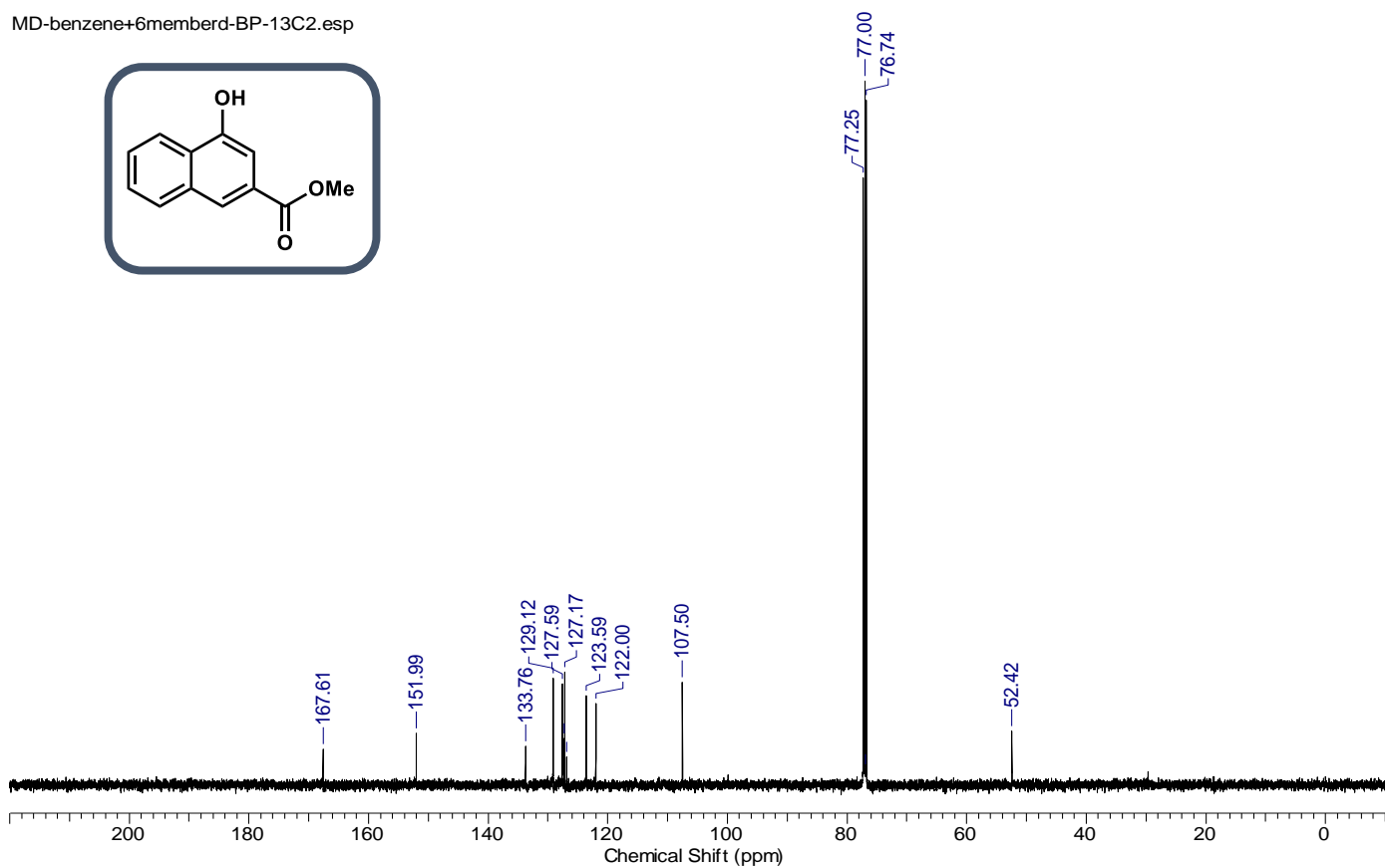
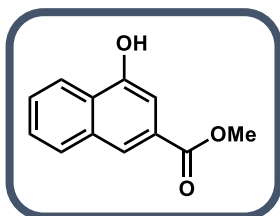




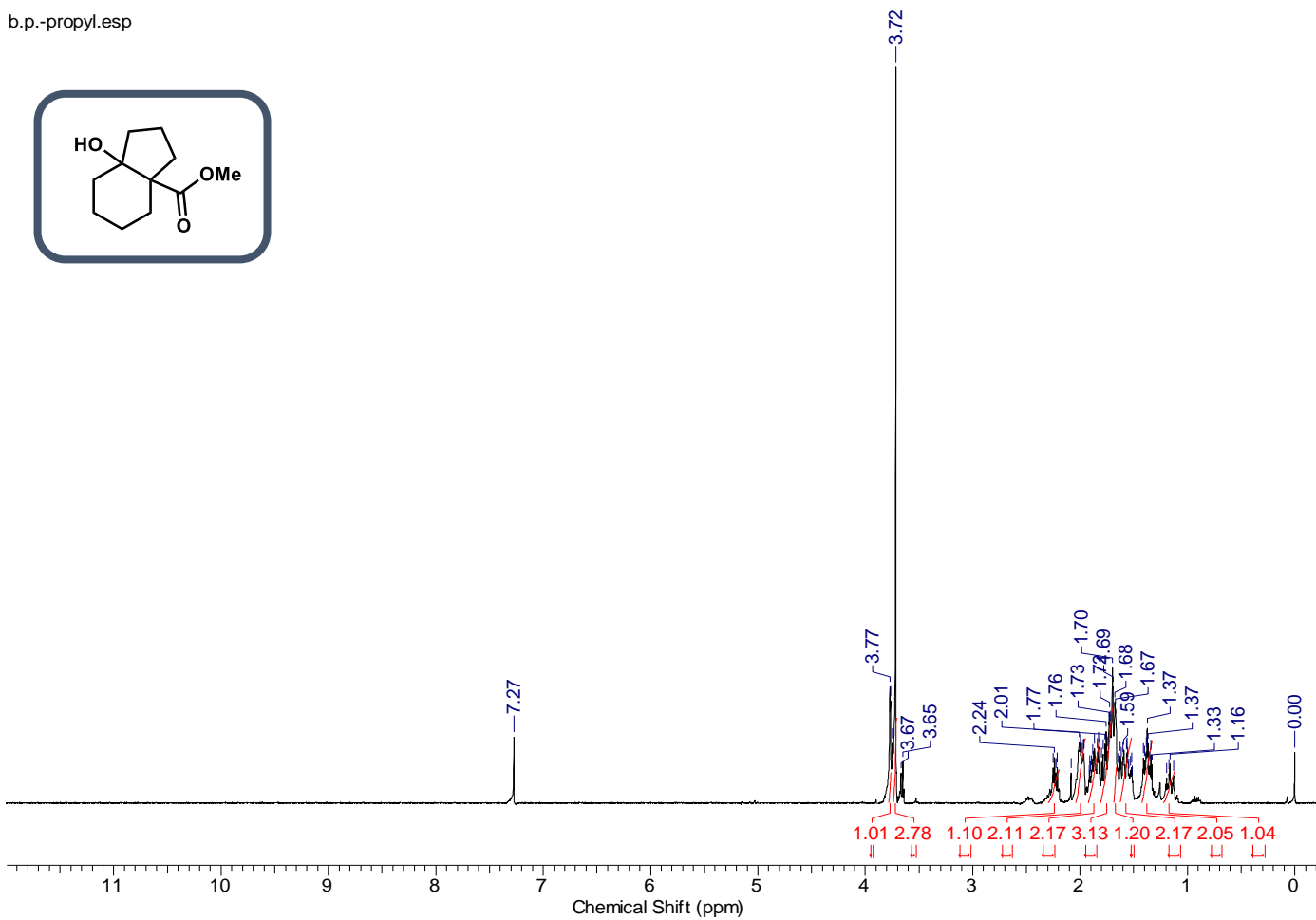
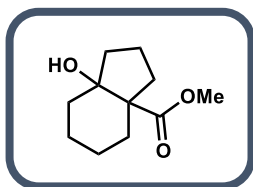
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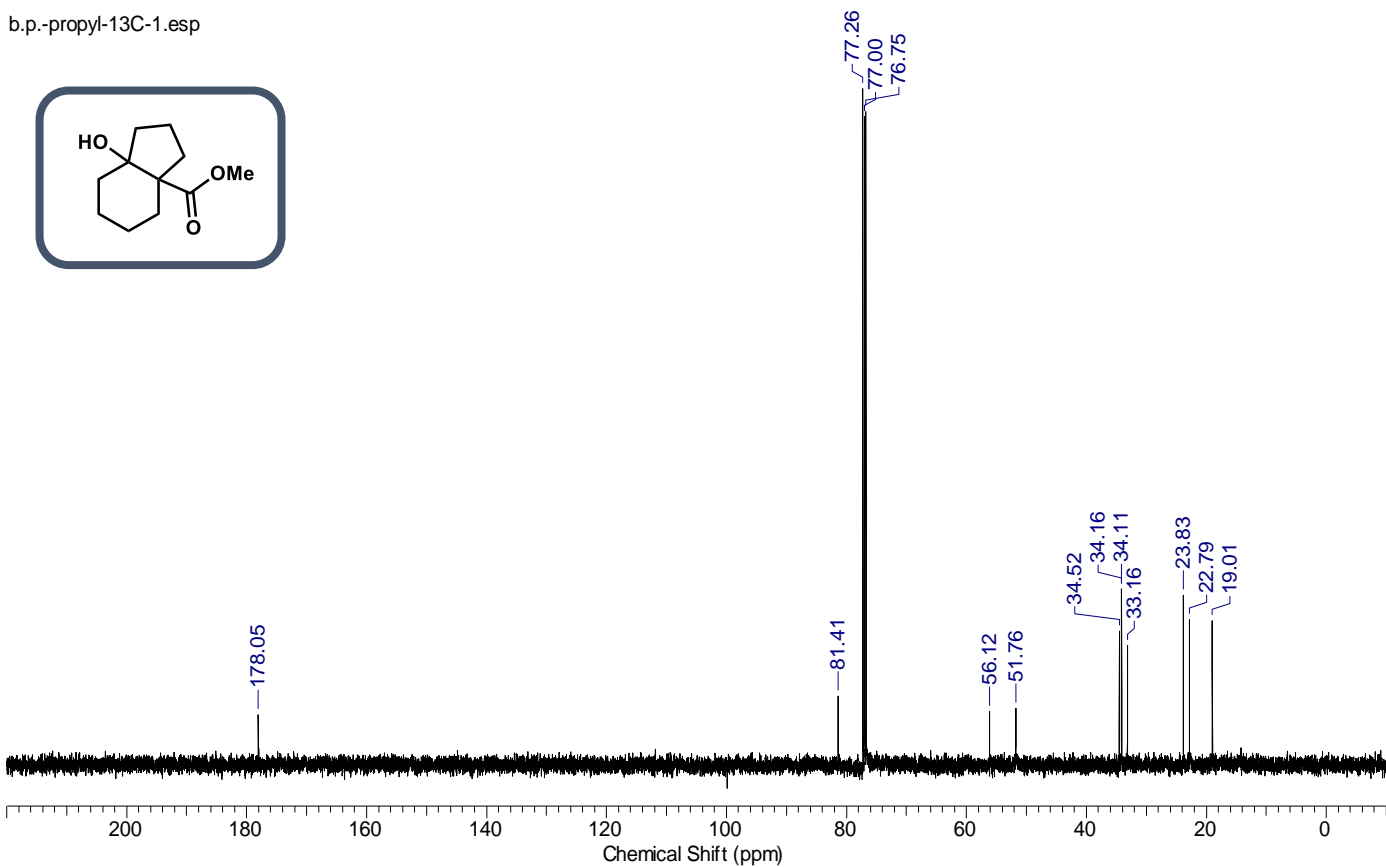
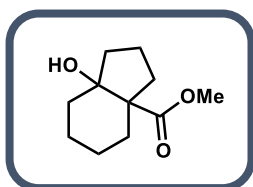
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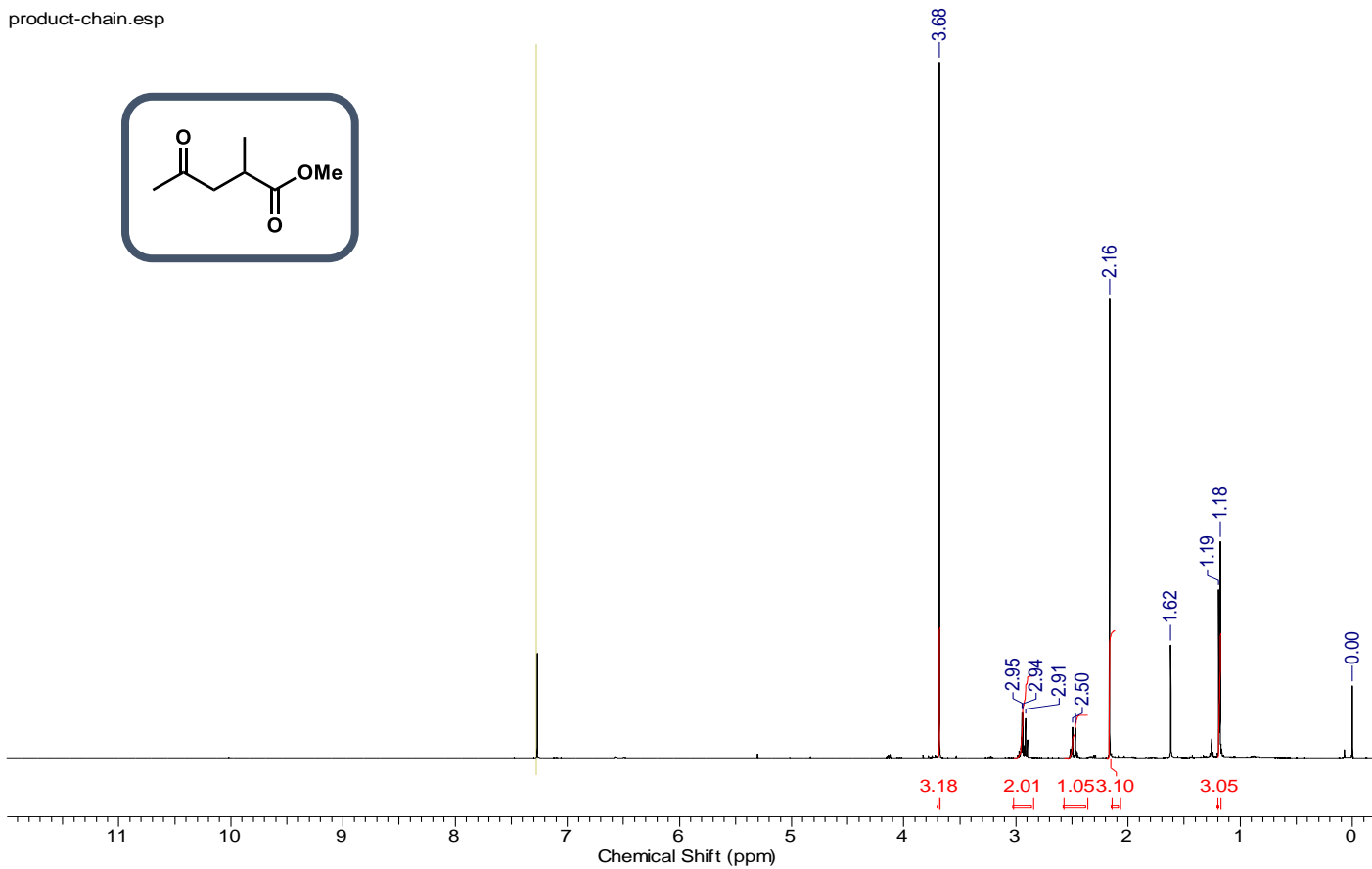
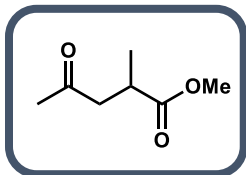
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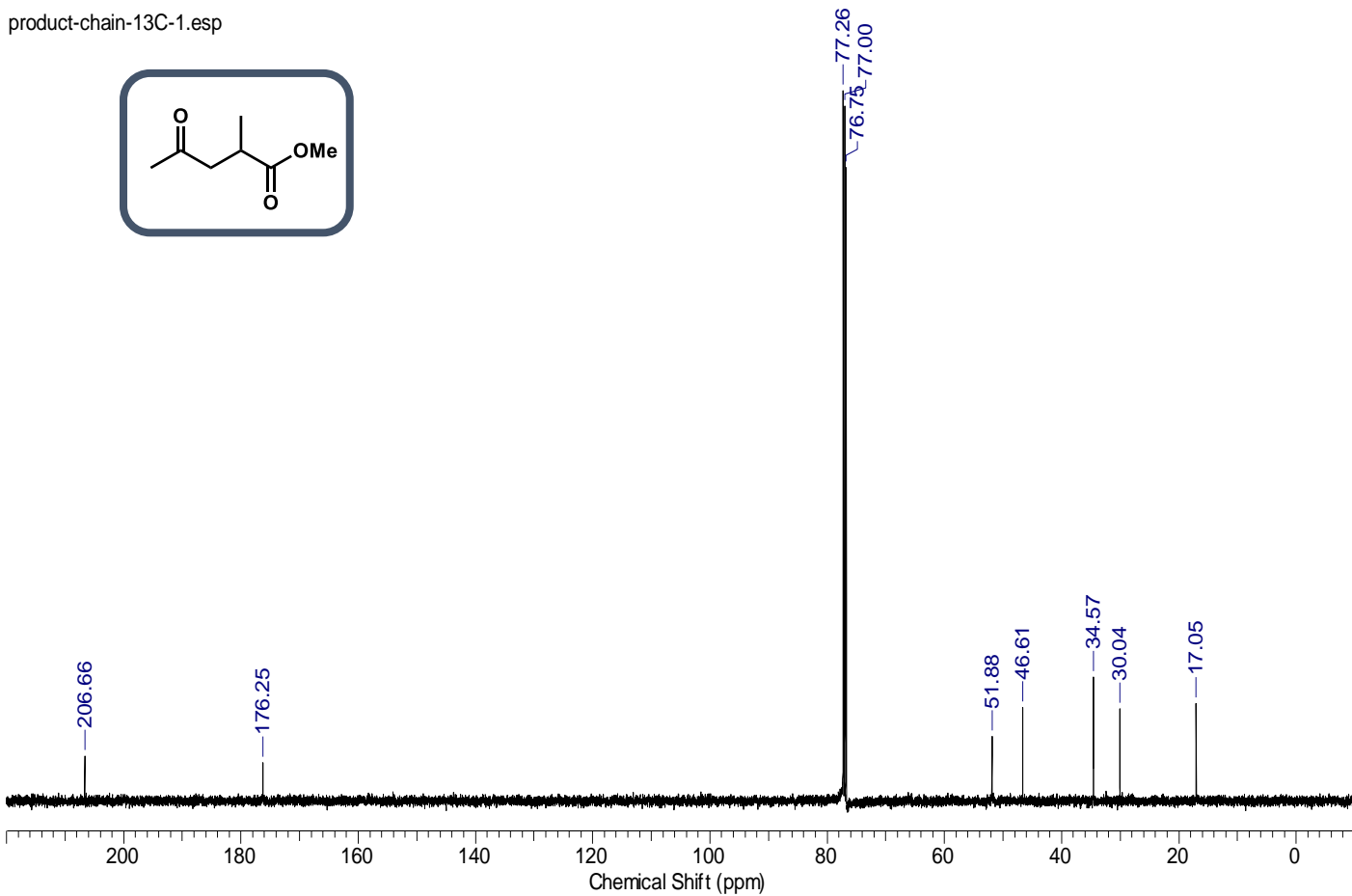
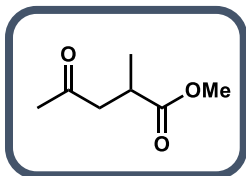
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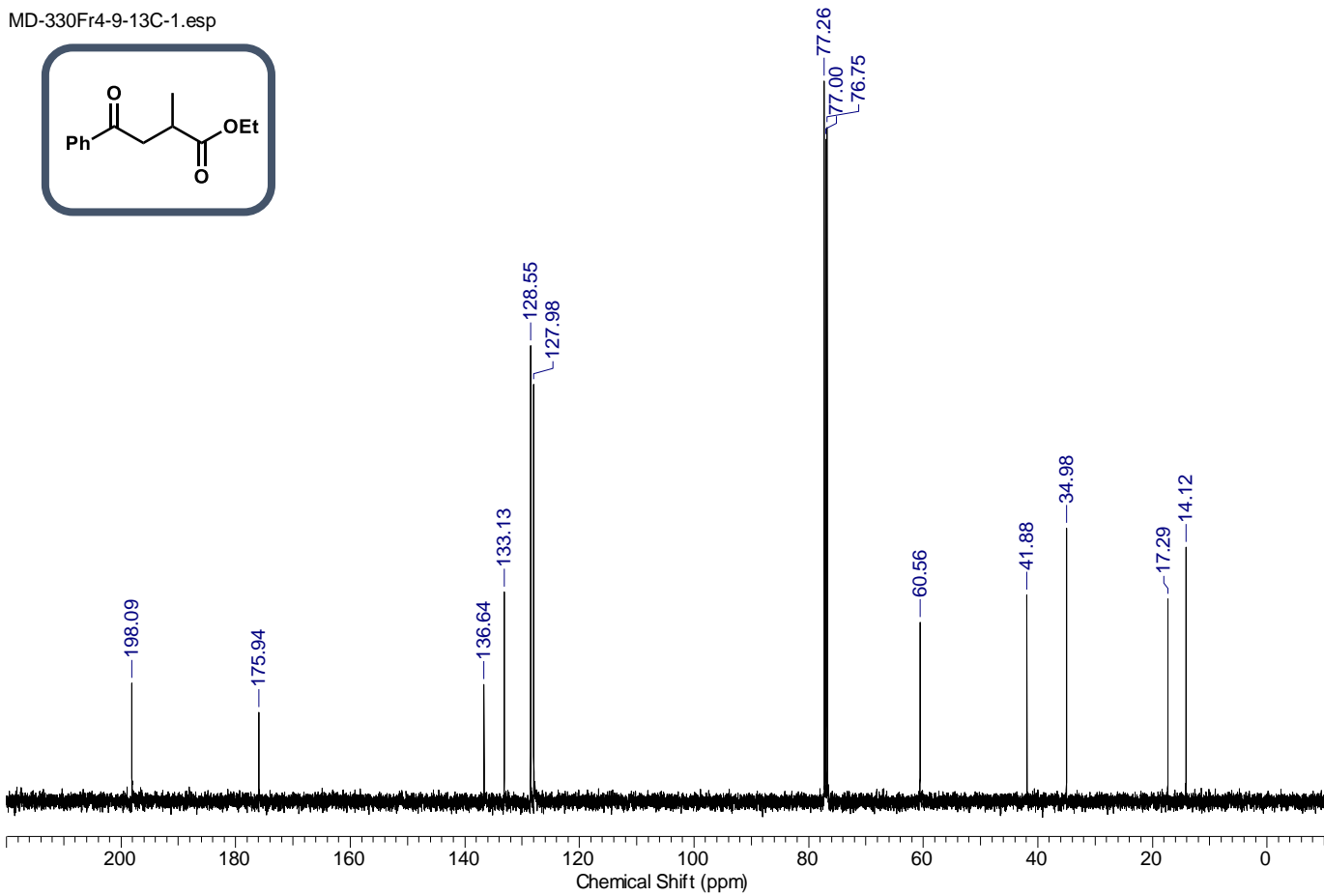
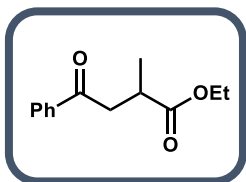
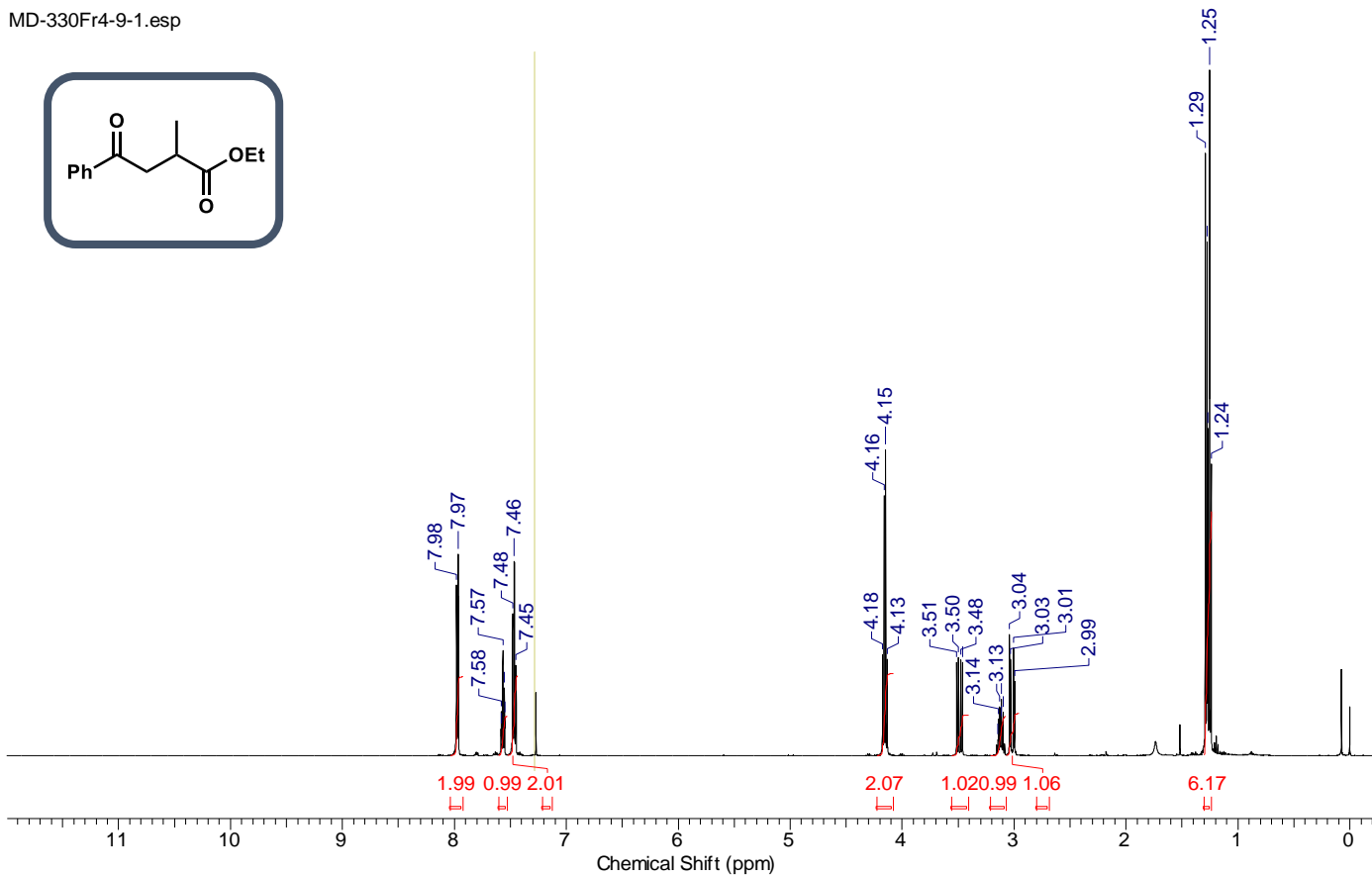
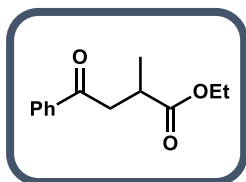


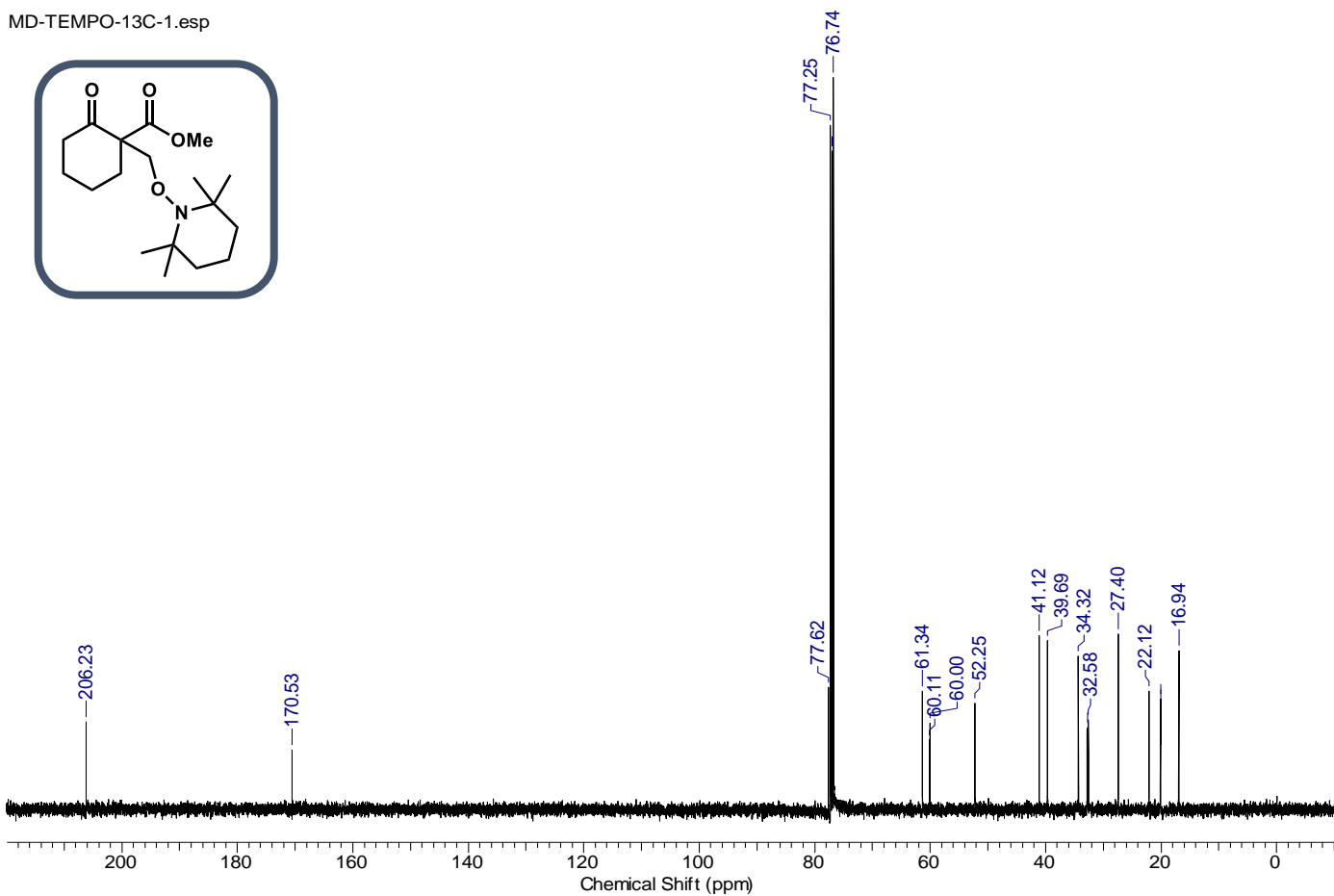
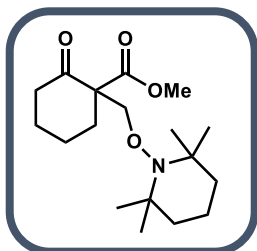
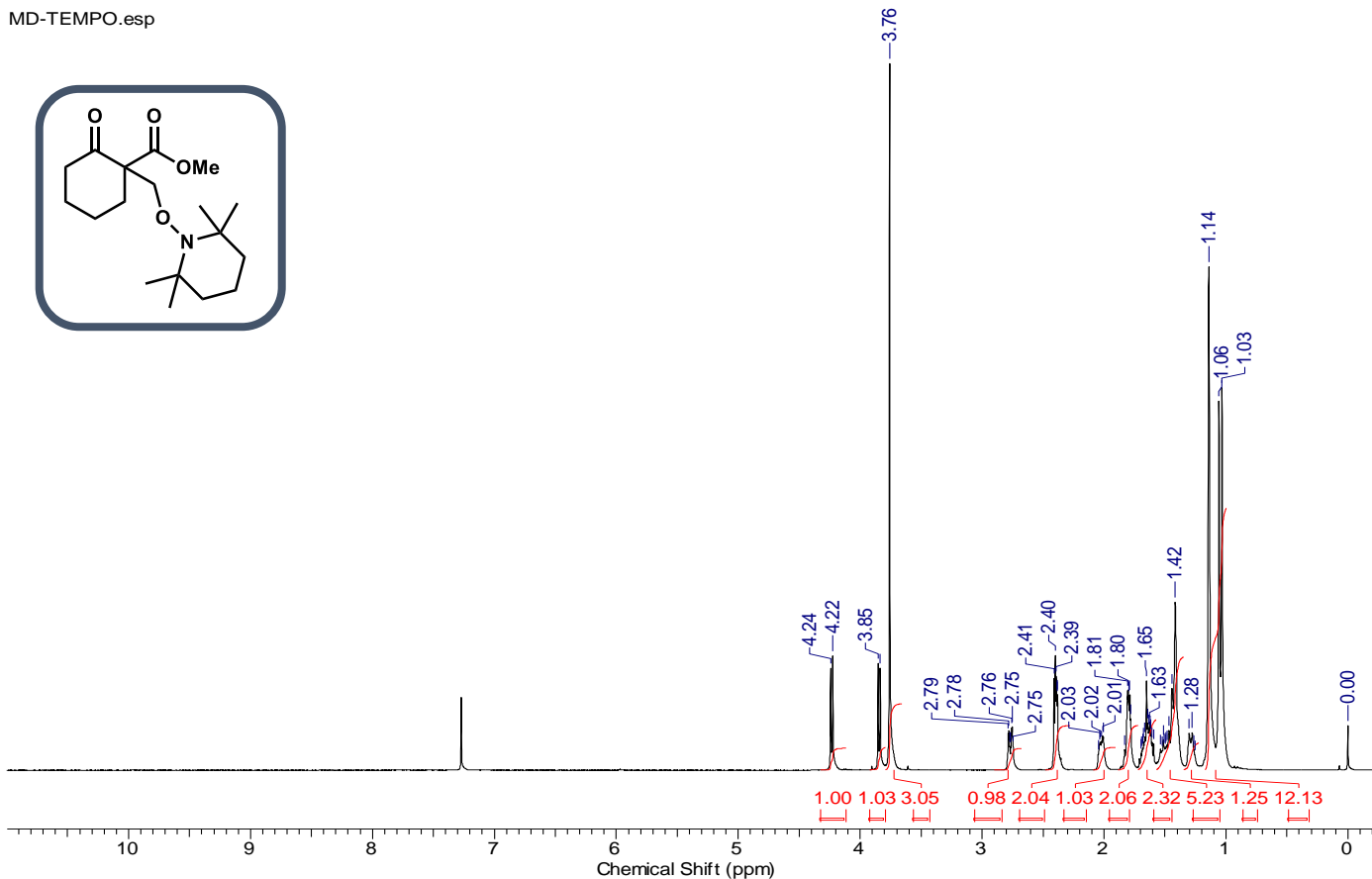
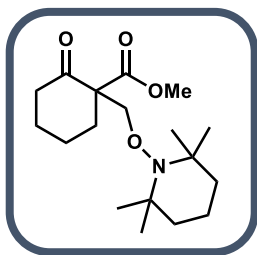
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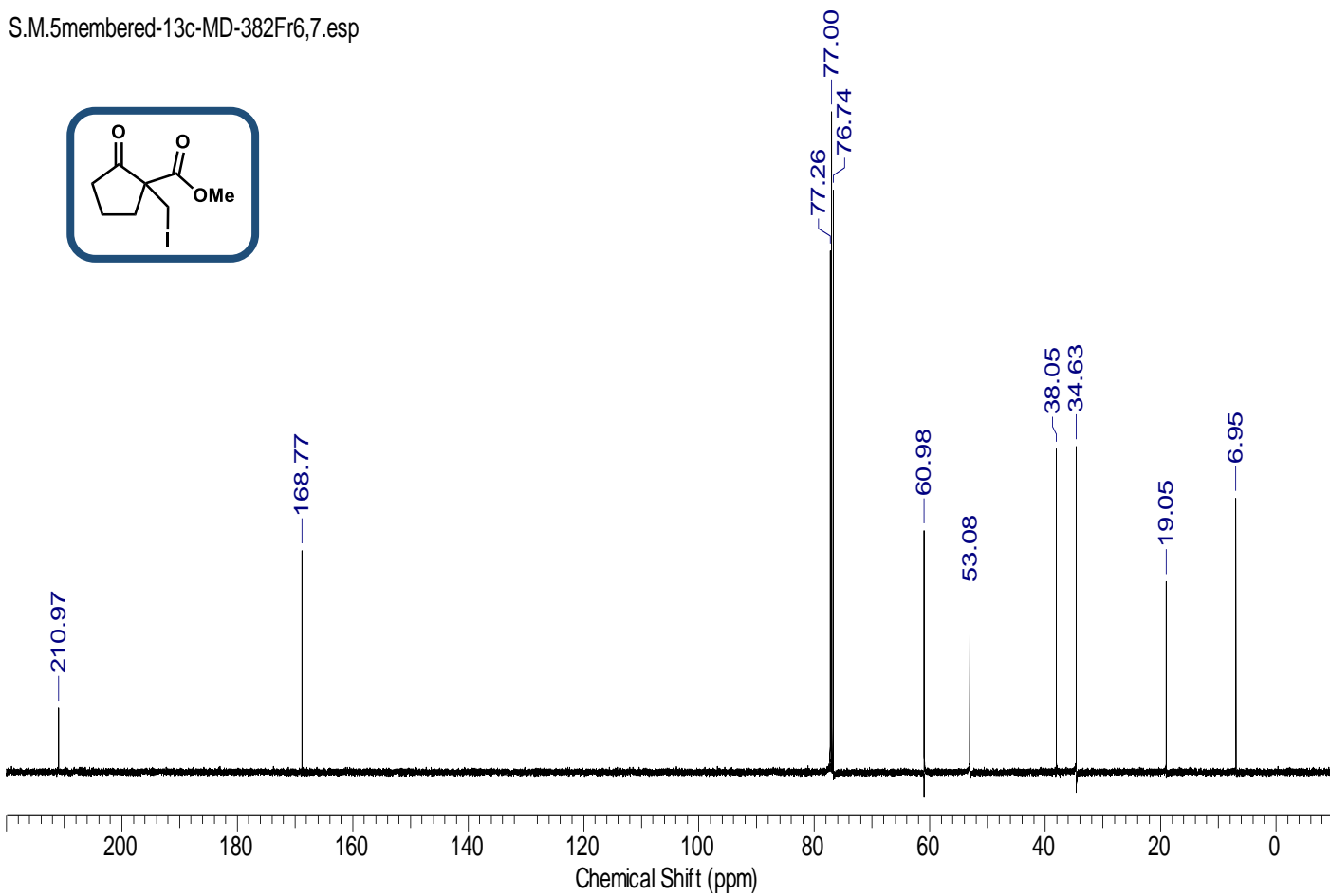
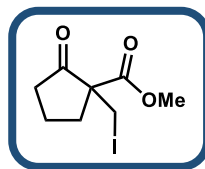
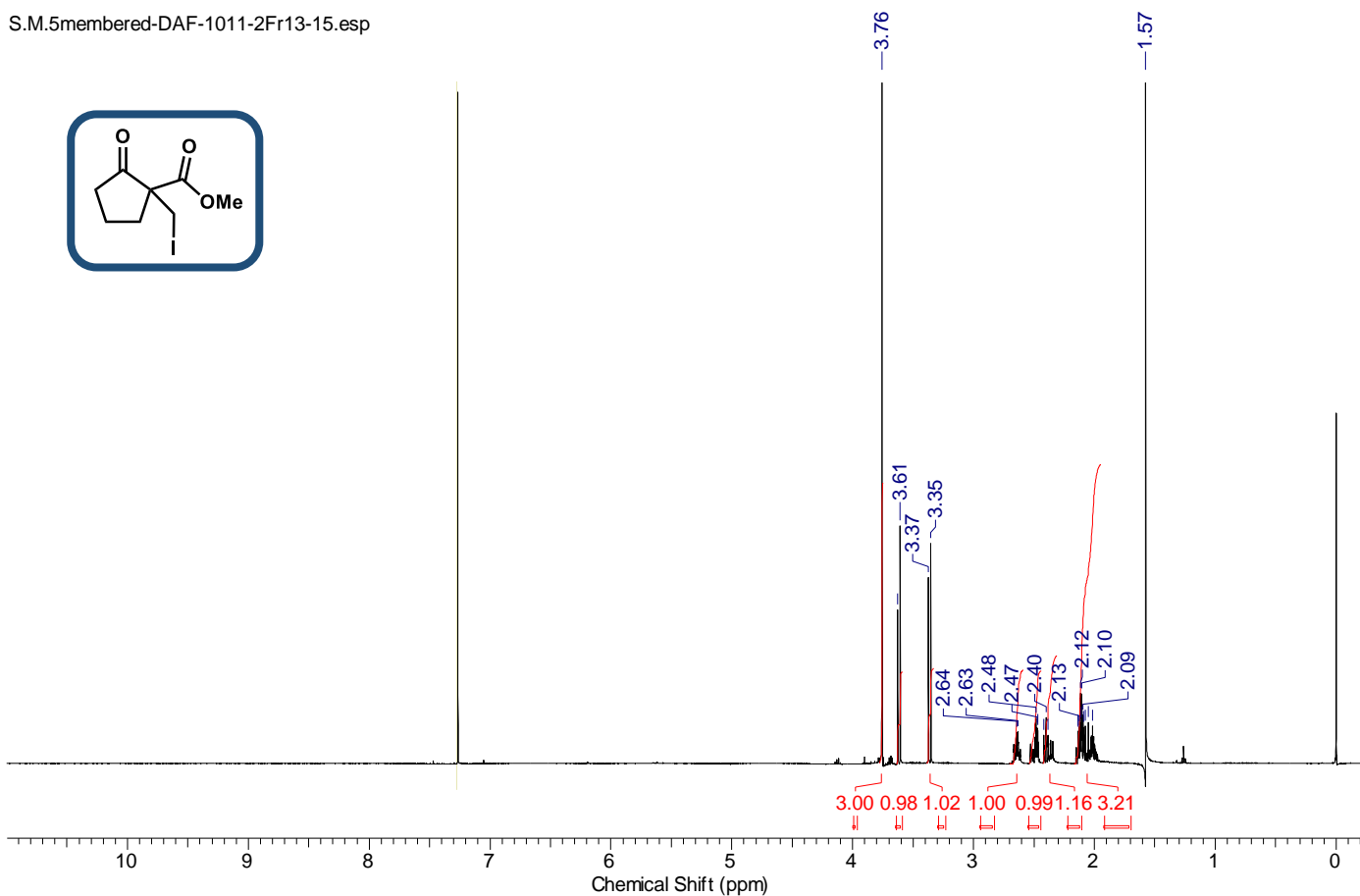
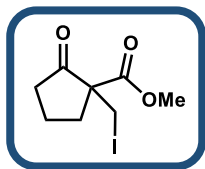


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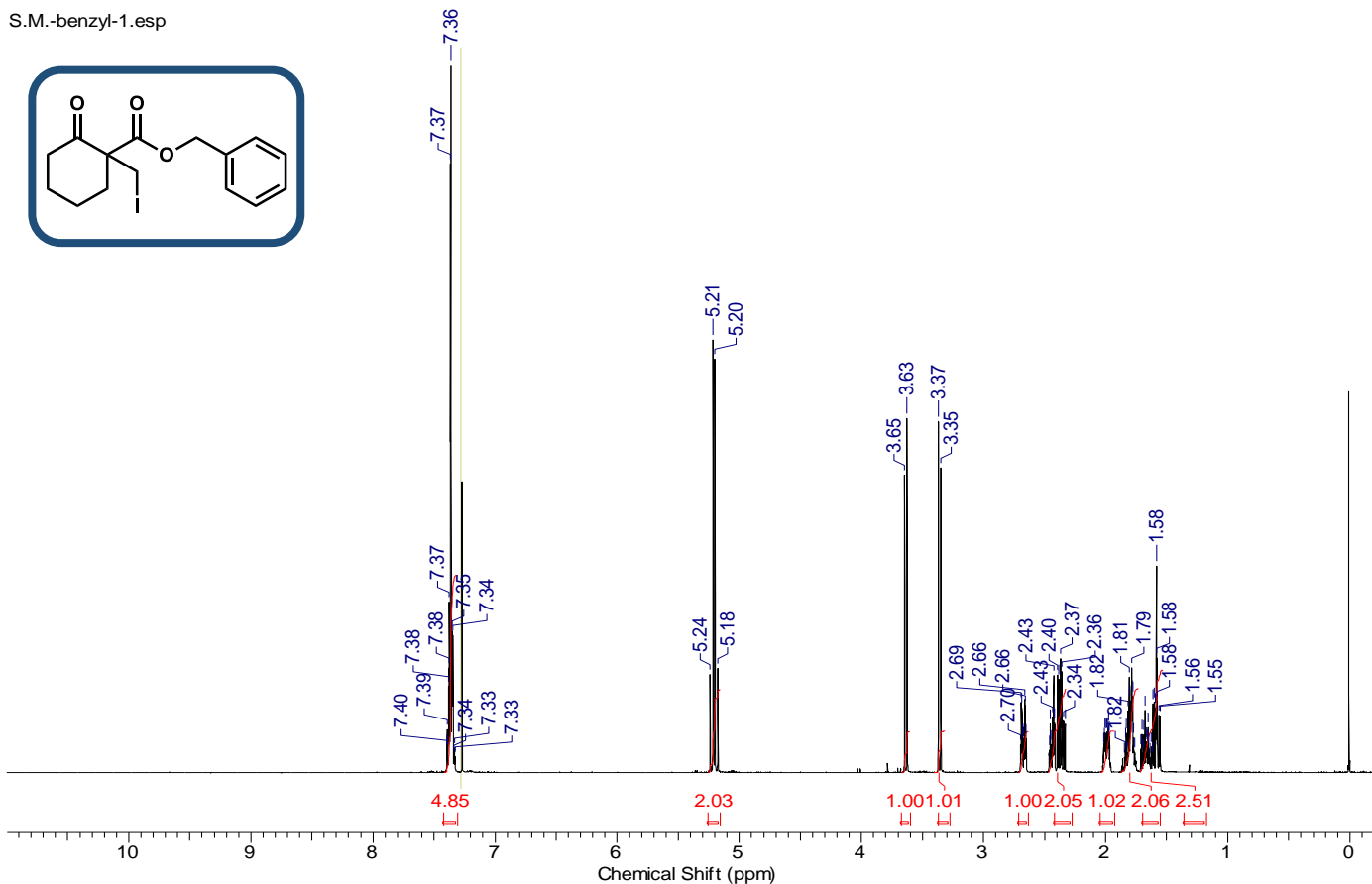
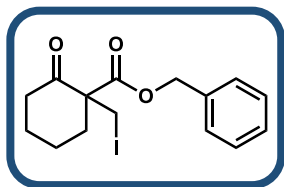




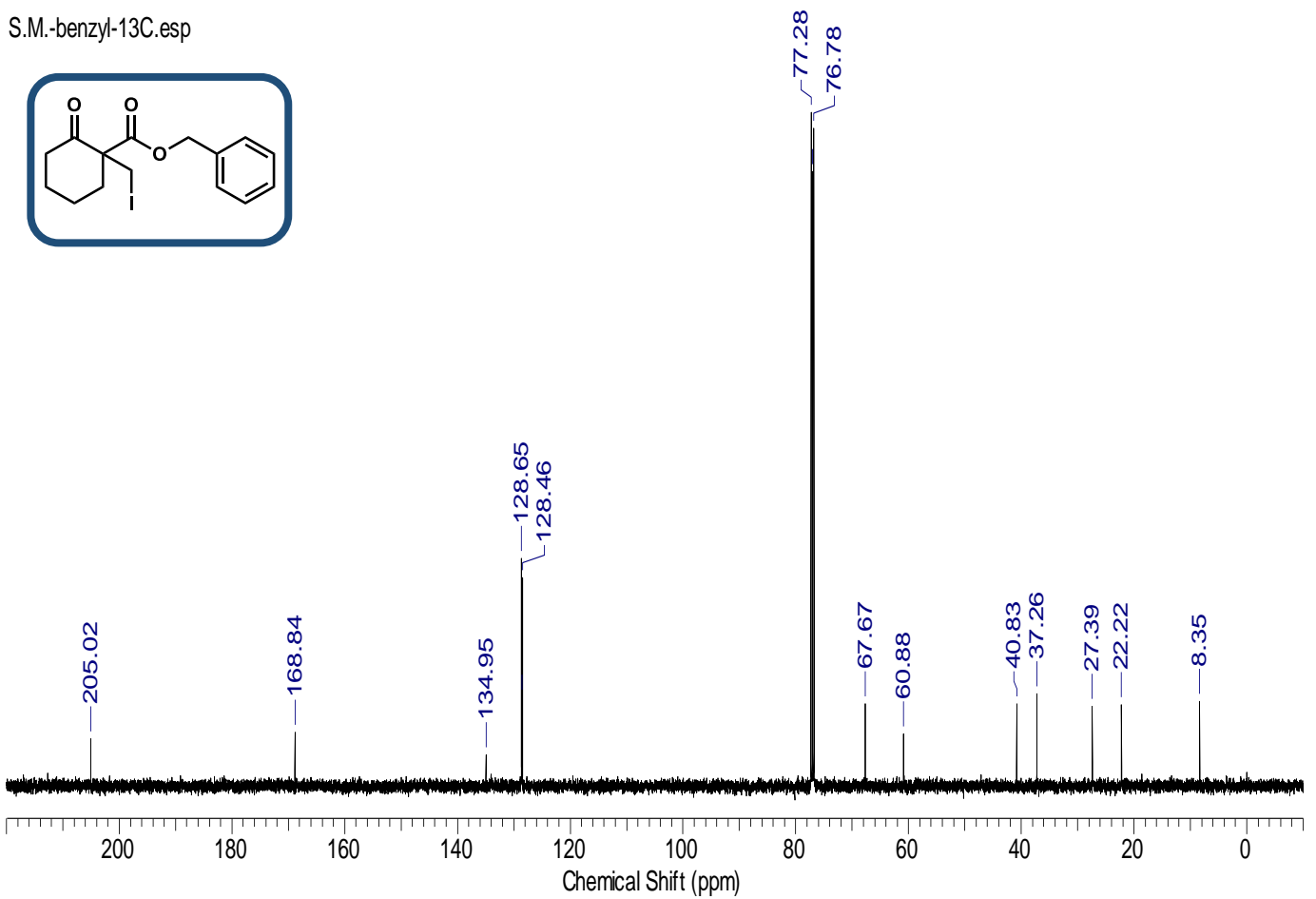
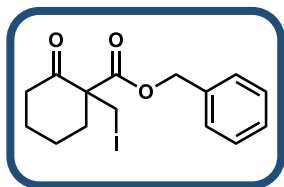




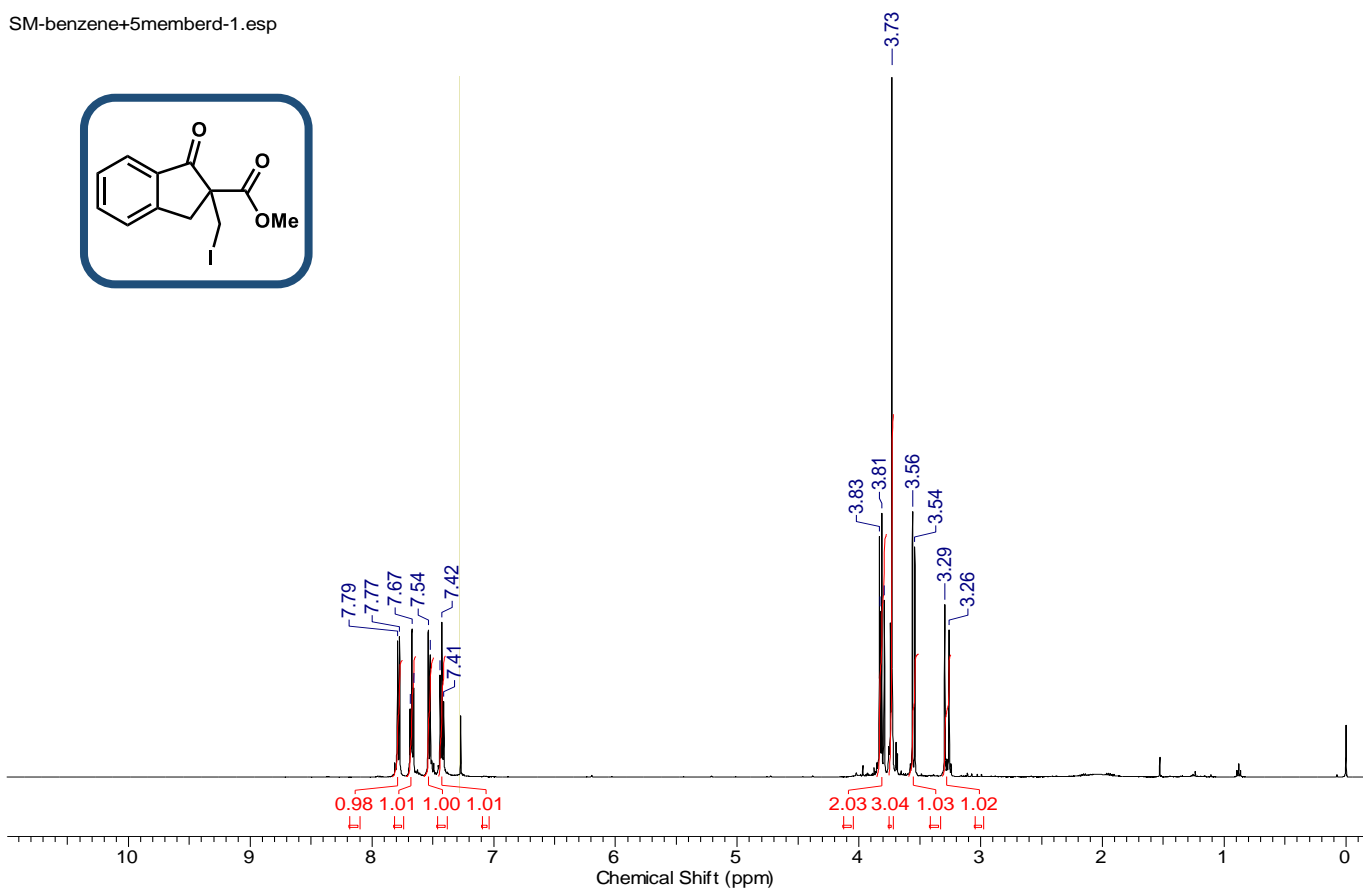
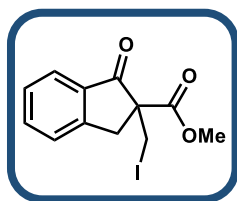
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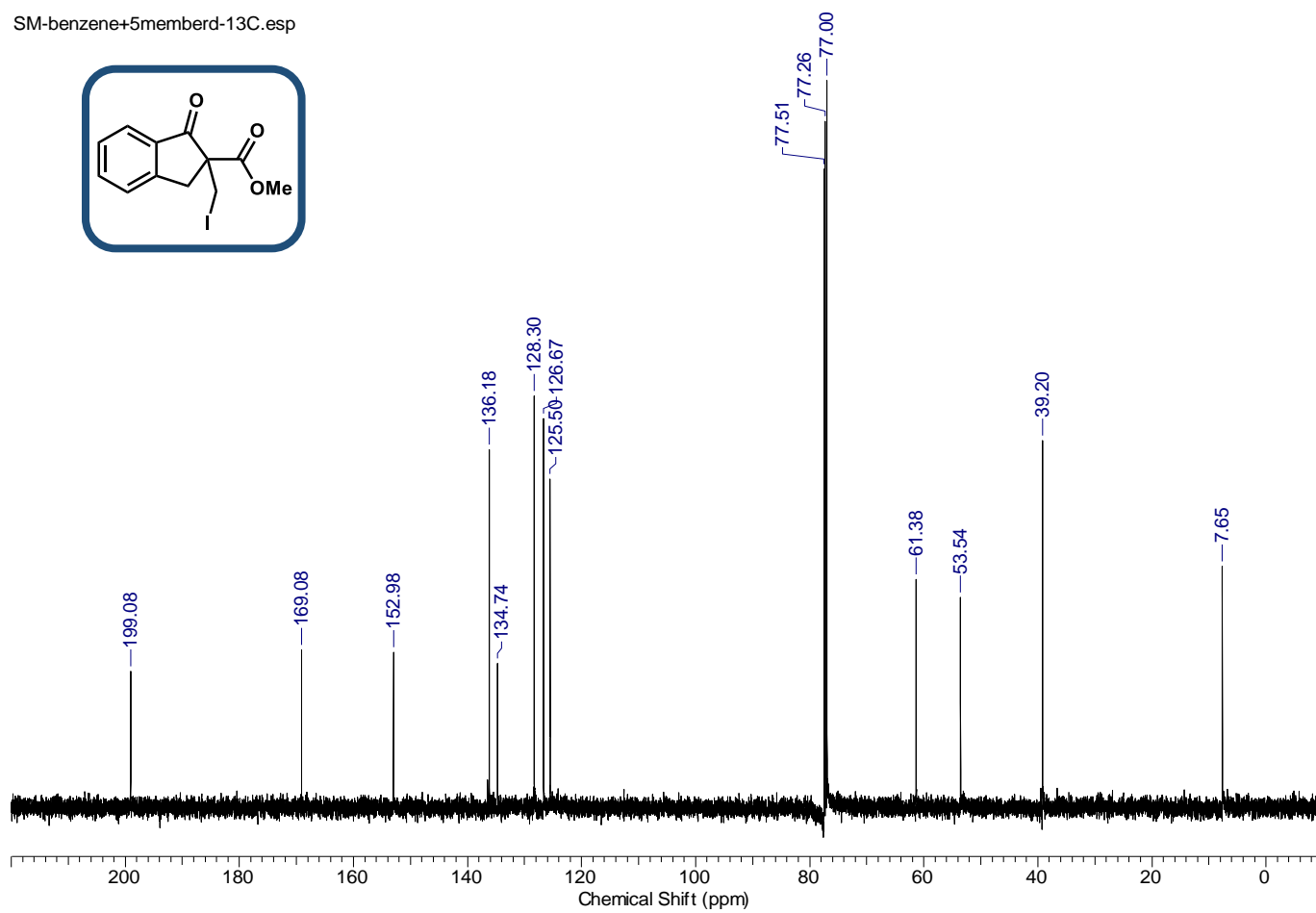
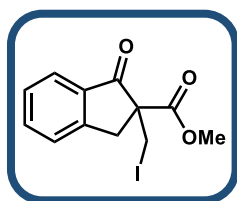
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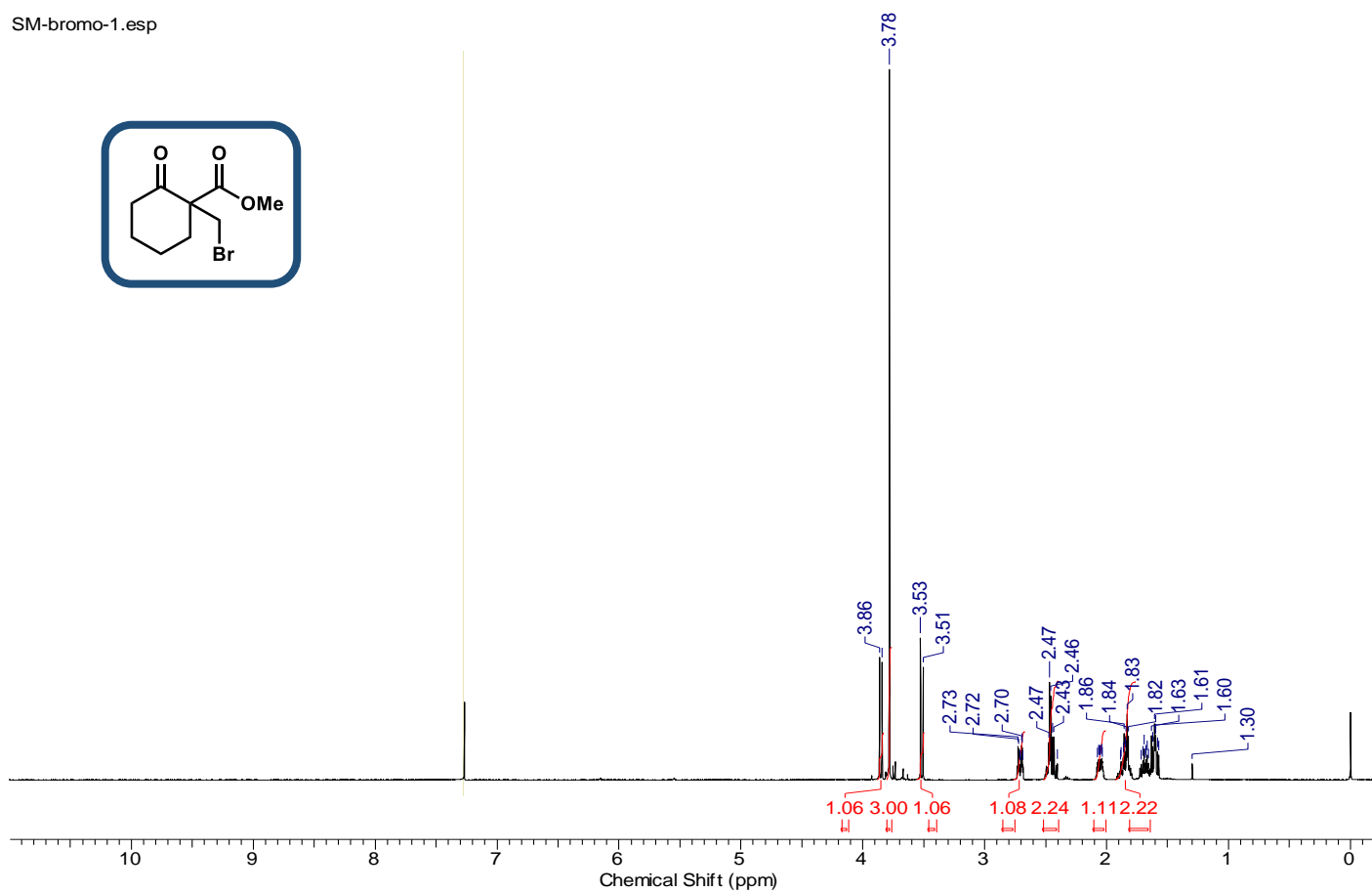
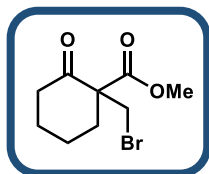
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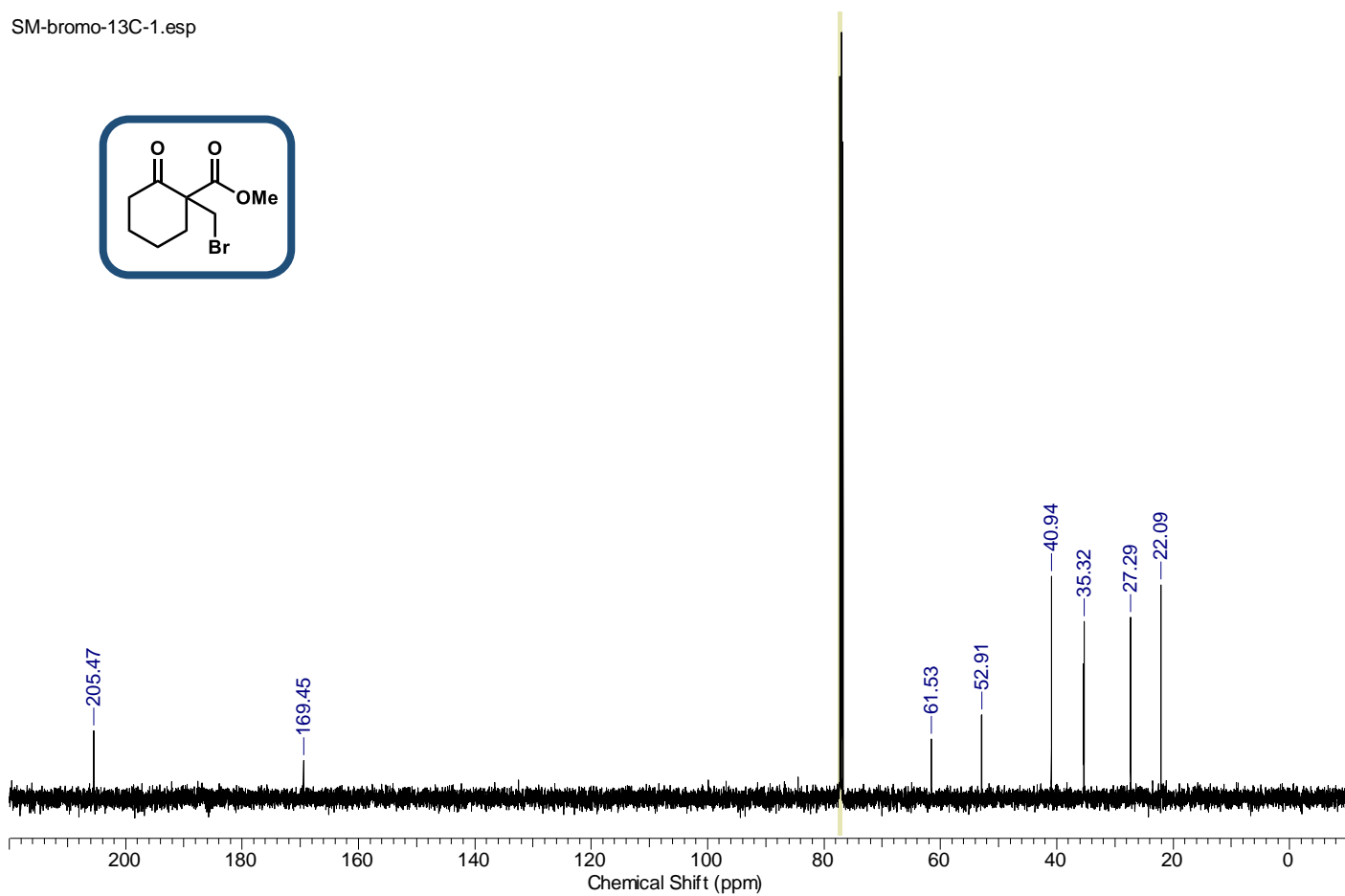
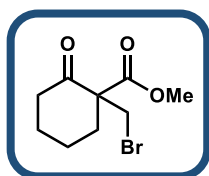
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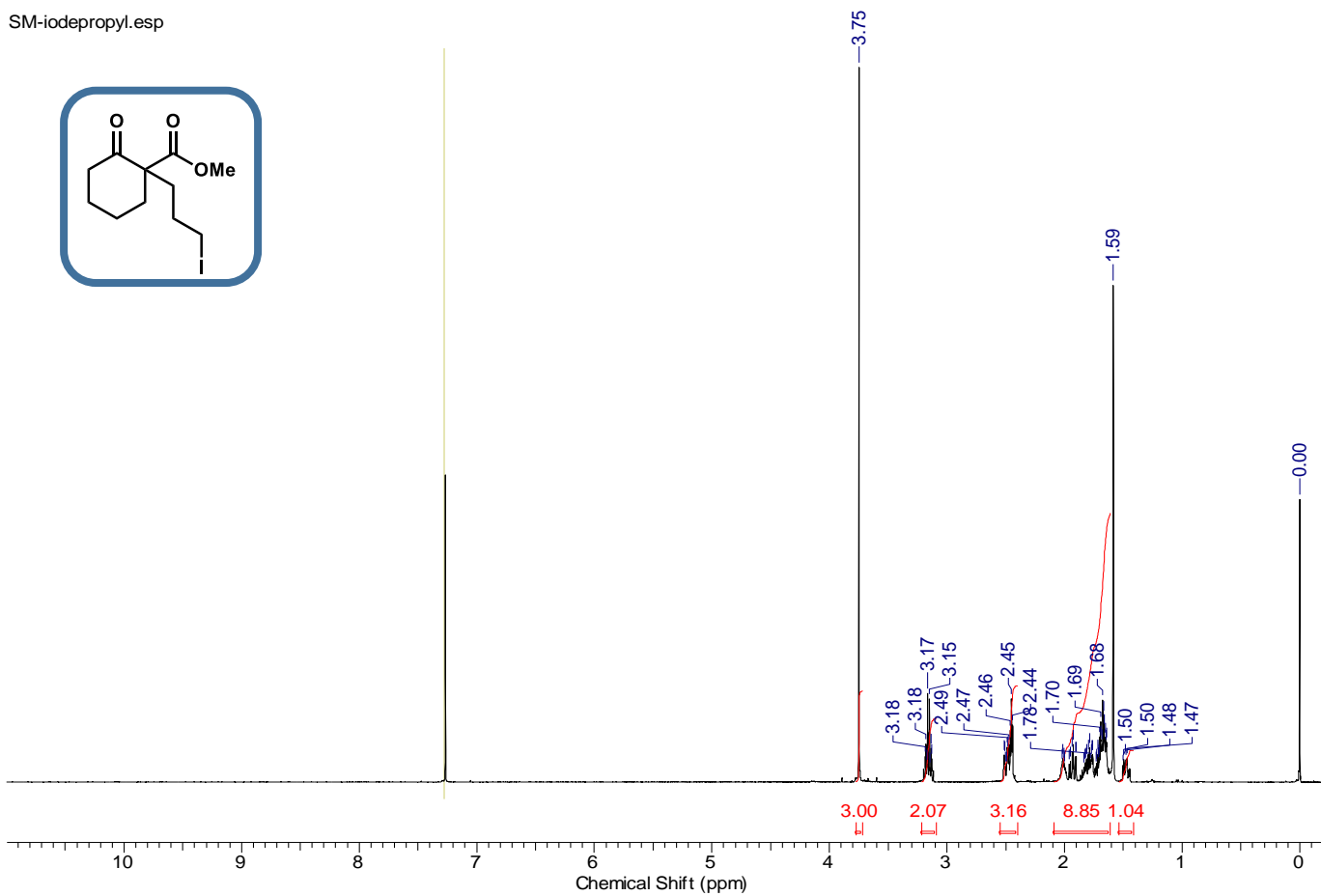
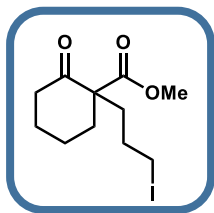
SM-bromo-1.esp



SM-bromo-13C-1.esp



SM-iodopropyl.esp



S.M.iodopropyl-13C-2017-1.esp

