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Supporting Information

[3+2] Regioselective Annulation Reaction of 2-Arylidene-1,3-Indandiones Towards Synthesis of Spirocyclopentenes: Understanding the Mechanism of γ-attack vs. α-attack using DFT Studies

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Supporting Information

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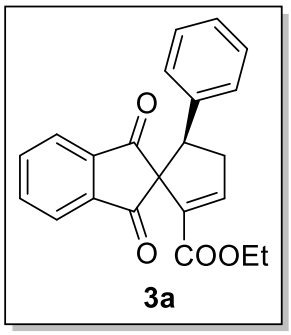
General remarks: All reagents were used as purchased from commercial suppliers without further purification. IR spectra were recorded on a Perkin Elmer 500 spectrometer. NMR spectra were recorded on a Bruker Avance 400 NMR spectrometer (400 MHz for ^{1}H and 100 MHz for ^{13}C). Chemical shifts are reported in δ ppm referenced to an internal TMS standard for ^{1}H NMR and chloroform-*d* (77.0 ppm) for ^{13}C NMR. HRMS spectra were recorded on JEOL SX-102A. The X-ray diffraction measurements were carried out at 298 K on a KAPPA APEX II CCD area detector system equipped with a graphite monochromator and a Mo-Kα fine-focus sealed tube (k = 0.71073 Å). Routine monitoring of reactions was performed using silica gel, glass-backed TLC plates (Merck Kieselgel 60 F254) and visualized by UV light (254 nm). Solutions were evaporated to dryness under reduced pressure on a rotary evaporator and the residues purified by flash column chromatography on silica gel (230–400 mesh) with the indicated eluents. Air and / or moisture sensitive reactions were performed under the usual inert atmosphere conditions.

General procedure for the synthesis of spirocyclopentenes: To a dried 2 neck RB flask was taken 2-benzylidene-1H-indene-1,3(2H)-dione **1a** (0.1 mmol) and PPh3 (5.24 mg, 20 mol%) followed by dry toluene (6 mL). It was stirred for 2-3 min so as to dissolve. To it was added ethyl 2,3-butadienoate **2** (23.2 µL, 0.2 mmol) and the reaction mixture was stirred for 24h at room temperature under nitrogen atmosphere until the full consumption of **1a**. The reaction mixture was concentrated under reduced pressure (crude H^{1}NMR was taken). It was column purified by (Hexane/EtOAc, 4:1).

Compound Characterization:

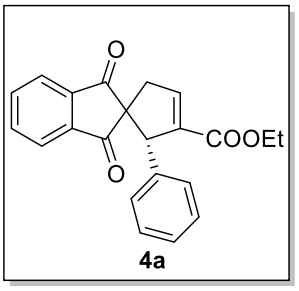
Ethyl 1',3'-dioxo-5-phenyl-1',3'-dihydrospiro[cyclopent[2]ene-1,2'-indene]-2-carboxylate（3a）:



3a

R_f = 0.37 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 7.95 (d, 1H, *J* = 7.56 Hz), 7.74-7.70 (m, 1H), 7.67-7.59 (m, 2H), 7.40 (t, 1H, *J* = 2.4 Hz), 7.10-7.00 (m, 5H), 4.23-4.18 (m, 1H), 3.97 (qd, 2H, *J* = 7.56, 2.0 Hz), 3.35 (ddd, 1H, *J* = 18.0, 10.6, 2.0 Hz), 2.96 (ddd, 1H, *J* = 18.0, 8.1, 2.8 Hz), 0.98 (t, 3H, *J* = 7.1 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 202.0, 199.9, 162.8, 149.4, 142.8, 141.7, 136.1, 135.6, 135.3, 135.2, 128.4, 128.2, 127.4, 123.0, 122.7, 70.6, 60.8, 54.7, 37.4, 13.6; **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{22}H_{18}NaO_4$ 369.1103, found 369.1105; **IR** (ν/cm^{-1})(CH_2Cl_2): 2982, 2919, 1706, 1245, 1103.

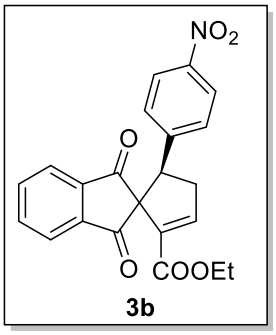
Ethyl 1',3'-dioxo-2-phenyl-1',3'-dihydrospiro[cyclopent[3]ene-1,2'-indene]-3-carboxylate（4a）:



4a

R_f = 0.30 (4:1 Hex/EtOAc); **^{1}H-NMR** (500 MHz, $CDCl_3$): δ (ppm) = 8.04 (d, 1H, *J* = 7.6 Hz), 7.82 (t, 1H, *J* = 7.5 Hz), 7.73 (t, 1H, *J* = 7.5 Hz), 7.59 (d, 1H, *J* = 7.5 Hz), 7.19-7.08 (m, 4H), 6.87-6.78 (m, 2H), 4.55 (s, 1H), 4.12 -3.99 (m, 2H), 3.11 (dt, 1H, *J* = 18.6, 2.6 Hz), 2.95 (dt, 1H, *J* = 18.6, 2.0 Hz), 1.08 (t, 3H, *J* = 7.1 Hz) ; **^{13}C-NMR** (125 MHz, $CDCl_3$): δ (ppm) = 201.4, 199.2, 163.4, 142.9, 142.8, 141.3, 136.7, 135.8, 135.7, 135.4, 128.2, 128.1, 127.4, 123.5, 123.1,64.3, 61.0, 60.3, 36.4, 13.9; **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{22}H_{18}NaO_4$ 369.1103, found 369.1107;; **IR** (ν/cm^{-1})(CH_2Cl_2): 2919, 2850, 1710, 1263,1100.

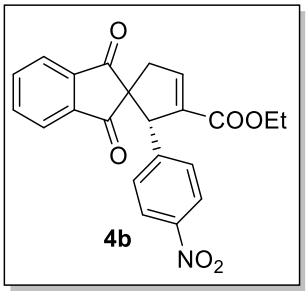
Ethyl 5-(4-nitrophenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[2]ene-1,2'-indene]-2-carboxylate（3b）:



3b

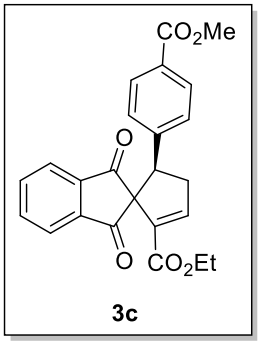
R_f = 0.23 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.01-7.92 (m, 3H), 7.78 (t, 1H, *J* = 8.0 Hz), 7.73-7.64 (m, 2H), 7.39 (s, 1H), 7.24-7.22 (m, 1H), 4.33-4.26 (m, 1H), 3.98 (q, 2H, *J* = 7.13 Hz), 3.42-3,32 (m, 1H), 3.03 (ddd, 1H, *J* = 18.0, 8.1, 2.7 Hz), 0.98 (t, 3H, *J* = 7.1 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.2, 199.5, 162.5, 148.6, 147.2, 144.0, 142.7, 141.4, 135.8, 135.8, 129.4, 123.4, 123.2, 123.0, 70.3, 61.0, 53.5, 37.4, 13.6; **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd for $C_{22}H_{18}NO_6$ 392.1134, found 392.1136; **IR** (ν/cm^{-1})(CH_2Cl_2): 3081, 2983, 2927, 1742, 1706, 1523, 1105.

Ethyl 2-(4-nitrophenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[3]ene-1,2'-indene]-3-carboxylate（4b）:



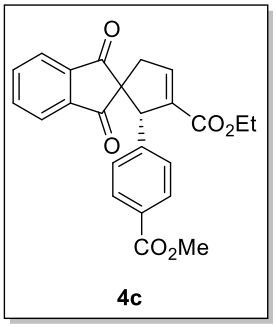
Rf = 0.18 (4:1 Hex/EtOAc); 1H-NMR (500 MHz, CDCl3): δ (ppm) = 8.05 (d, 1H, J = 7.6 Hz), 8.0 (d, 1H, J = 8.7 Hz), 7.86 (t, 1H, J = 7.4 Hz), 7.80 -7.74 (m, 1H), 7.62 (d, 1H, J = 7.6 Hz), 7.17-7.14 (m, 1H), 7.03 (d, 2H, J = 8.1 Hz) 4.64 (s, 1H), 4.12 -4.01 (m, 2H), 3.11 (dt, 1H, J = 18.8, 2.5 Hz), 2.98 (dt, 1H, J = 18.8, 2.0 Hz), 1.11 (t, 3H, J = 7.1 Hz) ; 13C-NMR (125 MHz, CDCl3): δ (ppm) = 200.9, 199.0, 162.9, 147.2, 144.7, 143.8, 142.2, 141.1, 136.3, 136.0, 135.1, 129.2, 123.8, 123.3, 63.4, 60.7, 59.7, 37.6, 13.9; HRMS (ESI) m/z: [M+H]+ calcd for C22H18NO6 392.1134, found 392.1139; IR (ν/cm-1)(CH2Cl2): 3078, 2920, 2851, 1743, 1709, 1521, 1100; **m.p.** = 185-188 ℃.

Ethyl 5-(4-(methoxycarbonyl)phenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[2]ene-1,2'-indene]-2-carboxylate（3c）:



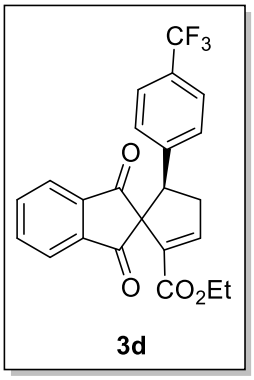
R_f = 0.16 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 7.98-7.94 (d, 1H, J = 7.2 Hz), 7.78-7.60(m, 6H), 7.41-7.38 (s, 1H), 7.16-7.10 (m, 2H), 4.29-4.22 (t, 1H), 4.43-3.94 (m, 2H), 3.85-3.79 (s, 3H), 3.42-3.33 (dd, 1H, J = 18.0, 10.8 Hz), 3.03-2.95 (dd, 1H, J = 18.0, 8 Hz), 1.01-0.94 (t, 3H, J = 6.8 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.6, 199.6, 166.6, 162.7, 149.1, 142.7, 141.6, 135.6, 135.5, 129.4, 129.3, 128.5.2, 123.1, 122.8, 70.4, 60.4, 54.1, 52.0, 37.3, 13.6; **HRMS** (EI) *m/z*: $[M+H]^+$ calcd for $C_{24}H_{20}O_6$ 405.1338, found 405.1337; **IR** (ν/cm^{-1})(CH_2Cl_2): 3061, 2954, 1710, 1611, 1436, 1333, 1283, 1257, 1104.

Ethyl2-(4-(methoxycarbonyl)phenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[3]ene-1,2'-indene]-3-carboxylate（4c）:



R_f = 0.14 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.01-7.92 (m, 3H), 7.78 (t, 1H, J = 8.0 Hz), 7.73-7.64 (m, 2H), 7.39 (s, 1H), 7.24-7.22 (m, 1H), 4.33-4.26 (m, 1H), 3.98 (q, 2H, J = 7.13 Hz), 3.42-3,32 (m, 1H), 3.03 (ddd, 1H, J = 18.0, 8.1, 2.7 Hz), 0.98 (t, 3H, J = 7.1 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.2, 199.0, 166.7, 163.2, 143.4, 142.5, 142.3, 141.2, 136.0, 135.6, 129.4, 129.2, 128.3, 123.6, 123.2, 63.9, 60.4, 60.4, 52.0, 37.0, 13.9; **HRMS** (EI) *m/z*: $[M+H]^+$ calcd for $C_{24}H_{20}O_6$ 405.1338, found 405.1337; **IR** (ν/cm^{-1})(CH_2Cl_2): 3061, 2946, 1706, 1607, 1436, 1333, 1280, 1257, 1104; **m.p.** = 147-148 ℃.

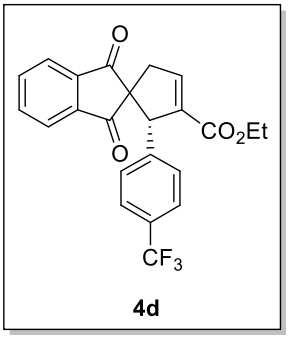
Ethyl 5-(4-(trifluoromethyl)phenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[2]ene-1,2'-indene]-2-carboxylate（3d）:



3d

R_f = 0.42 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.00-7.97 (d, 1H, *J* = 7.6 Hz), 7.80-7.74 (td, 1H, *J* = 6.8, 1.2 Hz), 7.72-7.64 (m, 2H), 7.41-7.39 (t, 1H, *J* = 2.0Hz), 7.36-7.32 (d, 2H, *J* = 8.4 Hz), 7.21-7.17 (d, 2H, *J* = 8.0 Hz), 4.29-4.25 (m, 1H), 4.01-3.94 (m, 2H), 3.41-3.32 (ddd, 1H, *J* = 18.0, 10.4, 2.0 Hz), 3.05-2.96 (ddd, 1H, *J* = 18.0, 8.0, 2.8 Hz), 1.01-0.96 (t, 3H, *J* = 7.2 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.5, 199.7, 162.7, 149.0, 142.8, 141.6, 140.5, 135.8, 135.6, 128.9, 125.2, 125.2, 125.1, 125.1, 123.2, 122.9, 70.3, 61.0, 53.8, 37.5, 13.6; **HRMS** (EI) *m/z*: $[M+H]^+$ calcd for $C_{23}H_{18}O_4F_3$ 415.1157, found 415.1159; **IR** (ν/cm^{-1})(CH_2Cl_2): 3076, 2984, 1706, 1619, 1325, 1253, 1165, 1120, 1066.

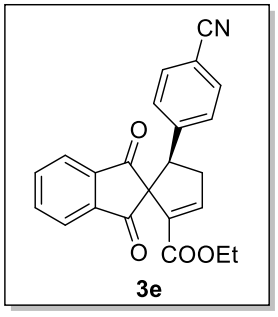
Ethyl 2-(4-(trifluoromethyl)phenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[3]ene-1,2'-indene]-3-carboxylate（4d）:



4d

R_f = 0.30 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.06-8.02 (d, 1H, *J* = 7.6 Hz), 7.80-7.74 (t, 1H, *J* = 7.2 Hz), 7.78-7.73 (t, 1H, *J* = 7.6 Hz), 7.62-7.58 (d, 1H, *J* = 7.6 Hz), 7.40-7.36 (d, 2H, *J* = 8.0 Hz), 7.15-7.12 (m, 1H), 6.98-6.94 (d, 2H, *J* = 8.0 Hz), 4.62-4.59 (s, 1H), 4.13-3.98 (m, 2H), 3.14-3.07 (dt,1H, *J* = 18.8, 5.2, 2.4 Hz), 3.01-2.94 (dt, 1H, *J* = 18.8, 4.4, 2.0 Hz), 1.12-1.07 (t, 3H, *J* = 6.8 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.1, 199.1, 163.1, 143.5, 142.5, 141.2, 141.1, 136.1, 135.7, 135.3, 128.6, 125.1, 125.1, 125.0, 125.0, 123.7, 123.2, 63.8, 60.5, 60.2, 37.1, 13.9; **HRMS** (EI) *m/z*: $[M+H]^+$ calcd for $C_{23}H_{18}O_4F_3$ 415.1157, found 415.1159; **IR** (ν/cm^{-1})(CH_2Cl_2): 3068, 2977, 1744, 1714, 1596, 1325, 1257, 1161, 1116, 1066; **m.p.** = 163-165 °C

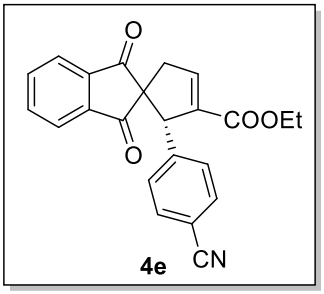
Ethyl 5-(4-cyanophenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[2]ene-1,2'-indene]-2-carboxylate（3e）:



3e

R_f = 0.36 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 7.97 (d, 1H, *J* = 7.64 Hz), 7.78 (td, 1H, *J* = 7.33, 1.1 Hz), 7.74-7.63 (m, 2H), 7.41-7.35 (m, 2H), 7.21-7.15 (m, 2H), 4.28-4.20 (m, 1H), 4.02-3.93 (m, 2H), 3.33 (ddd, 1H, *J* = 18.0, 10.4, 2.0 Hz), 3.00 (ddd, 1H, *J* = 18.0, 8.1, 2.9 Hz), 0.98 (t, 3H, *J* = 7.1 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.2, 199.5, 162.5, 148.7, 142.7, 141.9, 141.4, 135.8, 135.7, 132.0, 129.2, 123.1,122.9, 118.3, 111.5, 70.3, 61.0, 53.8, 37.2, 13.6; **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{23}H_{17}NaNO_4$ 394.1055, found 394.1056; **IR** (ν/cm^{-1})(CH_2Cl_2): 2919, 2815, 2228, 1710, 1245, 1034.

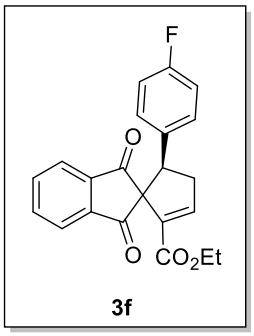
Ethyl 2-(4-cyanophenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[3]ene-1,2'-indene]-3-carboxylate（ **4e** ）:



4e

R_f = 0,14 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.03 (d, 1H, *J* = 8.0 Hz), 7.85 (t, 1H, *J* = 7.4 Hz), 7.77 (t, 1H, *J* = 7.4 Hz), 7.61 (d, 1H, *J* = 7.5 Hz), 7.42 (d, 2H, *J* = 8.0 Hz), 7.17-7.11 (m, 1H), 6.96 (d, 2H, *J* = 7.8 Hz), 4.58 (s, 1H), 4.11-4.00 (m, 2H), 3.14-3.04 (m,1H), 3.02-2.93 (m, 1H), 1.10 (t, 3H, *J* = 7.1 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 200.9, 199.0, 163.0, 143.8, 142.6, 142.3, 141.1, 136.2, 135.9, 135.0, 131.9, 129.0, 123.7, 123.3, 118.6, 111.4, 63.5, 60.6, 60.1, 37.4, 13.9; **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd for $C_{23}H_{17}NaNO_4$ 394.1055, found 394.1058; **IR** (ν/cm^{-1})(CH_2Cl_2): 3055, 2925, 2853, 2229, 1744, 1709, 1245, 1101. **m.p.**=166 ºC

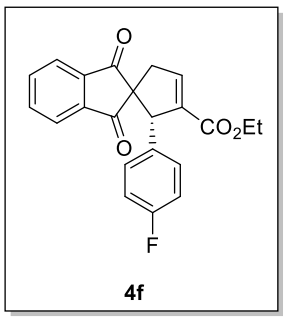
Ethyl5-(4-fluorophenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[2]ene-1,2'-indene]-2-carboxylate（ **3f** ）:



3f

R_f = 0.30 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 7.97-7.93 (d, 1H, *J* = 7.2 Hz), 7.77-7.64 (m, 1H), 7.41-7.37 (s, 1H), 7.06-7.00 (m, 2H), 6.80-6.73 (t, 2H, *J* = 8.8 Hz), 4.22-4.15 (m, 1H), 4.02-3.93 (m, 2H), 3.34-3.25 (m, 1H), 3.01-2.92 (ddd, 1H, *J* = 18.0, 8.0, 2.4 Hz), 1.01-0.95 (t, 3H, *J* = 7.2 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.9, 200.0, 163.2, 162.8, 160.7, 149.2, 142.8, 141.8, 135.6, 135.5, 131.9, 131.9, 130.1, 130.0, 123.0, 122.8, 115.2, 114.9, 70.5, 60.9, 53.8, 37.8, 13.6; **HRMS** (EI) *m/z*: $[M]^+$ calcd for $C_{22}H_{17}O_3F$ 364.1111, found 364.1114; **IR** (ν/cm^{-1})(CH_2Cl_2): 3068, 2977, 1702, 1600, 1512, 1337, 1280, 1241, 1100.

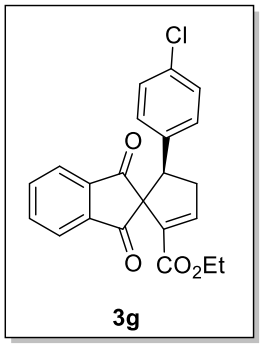
Ethyl 2-(4-fluorophenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[3]ene-1,2'-indene]-3-carboxylate（**4f**）:



4f

R_f = 0.26 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.05-8.01 (d, 1H, *J* = 7.6 Hz), 7.85-7.80 (t, 1H, *J* = 7.2 Hz), 7.77-7.72 (t, 1H, *J* = 7.6 Hz), 7.63-7.59 (d, 1H, *J* = 7.6 Hz), 7.11-7.08 (m, 1H), 6.83-6.78 (m, 4H), 4.55-4.52 (s, 1H), 4.13-3.97 (m, 2H), 3.12-3.05 (dt,1H, *J* = 18.8, 5.2, 2.4 Hz), 2.98-2.91 (dt, 1H, *J* = 18.8, 4.4, 2.0 Hz), 1.12-1.07 (t, 3H, *J* = 7.2 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.2, 199.2, 163.3, 163.2, 160.7, 143.0, 142.6, 141.3, 135.9, 135.6, 135.5, 132.7, 132.6, 129.8, 129.7, 123.6, 123.1, 115.1, 114.9, 64.0, 60.4, 60.1, 36.5, 13.9; **HRMS** (EI) *m/z*: $[M]^+$ calcd for $C_{22}H_{17}O_4F$ 364.1111, found 364.1107; **IR** (ν/cm^{-1})(CH_2Cl_2): 3068, 2977, 2937, 1744, 1714, 1600, 1508, 1337, 1257, 1097; **m.p.** = 167-168 ℃.

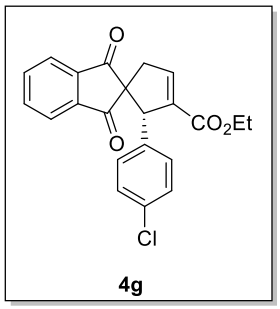
Ethyl 5-(4-chlorophenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[2]ene-1,2'-indene]-2-carboxylate（3g）:



3g

$\mathbf{R_f}$ = 0.35 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 7.98-7.94 (d, 1H, J = 7.6 Hz), 7.78-7.65 (m, 4H), 7.40-7.36 (s, 1H), 7.07-7.03 (d, 2H, J = 8.4 Hz), 7.03-6.97 (d, 2H, J = 8.4 Hz), 4.21-4.13 (m, 1H), 4.01-3.93 (m, 2H), 3.34-3.24 (m, 1H), 3.00-2.91 (ddd, 1H, J = 18.0, 8.4, 2.8 Hz), 1.00-0.94 (t, 3H, J = 7.2 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.7, 199.8, 162.7, 149.1, 142.8, 141.6, 135.7, 135.6, 135.5, 134.8, 133.3, 129.8, 128.4, 123.1, 122.8, 70.3, 60.9, 53.7, 37.6, 13.6; **HRMS** (EI) *m/z*: $[M]^+$ calcd for $C_{22}H_{17}O_4Cl$ 380.0815, found 380.0817; **IR** (ν/cm^{-1})(CH_2Cl_2): 3068, 2977, 2931, 1725, 1702, 1596, 1493, 1333, 1257, 1093.

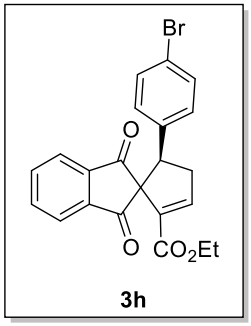
Ethyl 2-(4-chlorophenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[3]ene-1,2'-indene]-3-carboxylate（4g）:



4g

$\mathbf{R_f}$ = 0.26 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.05-8.01 (d, 1H, J = 7.6 Hz), 7.86-7.80 (t, 1H, J = 7.2 Hz), 7.78-7.73 (t, 1H, J = 7.6 Hz), 7.63-7.59 (d, 1H, J = 7.6 Hz), 7.12-7.07 (d, 1H, J = 7.6 Hz), 6.80-6.74 (d, 2H, J = 8.0 Hz), 4.53-4.50 (s, 1H), 4.13-3.98 (m, 2H), 3.12-3.05 (d,1H, J = 18.4 Hz), 2.98-2.90 (d, 1H, J = 18.4 Hz), 1.13-1.07 (t, 3H, J = 6.8 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.2, 199.1, 163.2, 144.2, 142.5, 141.2, 136.0, 135.6, 135.5, 135.5, 133.2, 129.5, 128.3, 123.6, 123.2, 63.9, 60.4, 60.1, 36.8, 13.9; **HRMS** (EI) *m/z*: $[M+H]^+$ calcd for $C_{22}H_{17}O_4Cl$ 380.0815, found 380.0818; **IR** (ν/cm^{-1})(CH_2Cl_2): 3068, 2977, 2923, 1744, 1710, 1596, 1489, 1333, 1257, 1097; **m.p.** = 187-189 °C.

Ethyl 5-(4-bromophenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[2]ene-1,2'-indene]-2-carboxylate（3h）:

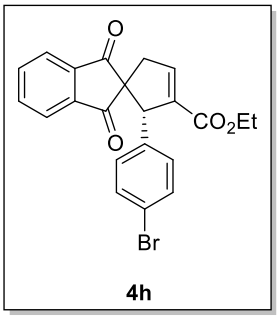


3h

$\mathbf{R_f}$ = 0.33 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 7.98-7.94 (d, 1H, J = 7.6 Hz), 7.78-7.66 (m, 4H), 7.39-7.36 (s, 1H), 7.22-7.18 (d, 2H, J = 8.4 Hz), 6.96-6.92 (d, 2H, J = 8.4 Hz), 4.19-4.13 (m, 1H), 4.00-3.94 (m, 2H), 3.33-3.25 (ddd, 1H, J = 18.0, 10.4, 1.6 Hz), 3.00-2.92 (ddd, 1H, J = 18.0, 8.4, 2.8 Hz), 1.00-0.94 (t, 3H, J = 7.2 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.7, 199.8, 162.7, 149.1, 142.8, 141.6, 135.7, 135.6, 135.5, 135.3, 131.3,

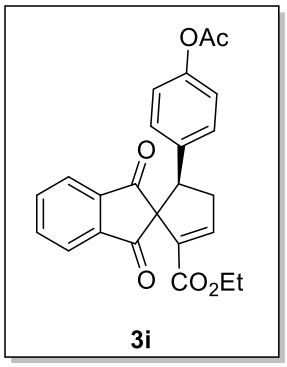
130.1, 123.2, 122.8, 121.4, 70.2, 60.8, 53.7, 37.6, 13.6; **HRMS** (EI) *m/z*: $[M]^+$ calcd for $C_{22}H_{17}O_4Br$ 424.0310, found 424.0316; **IR** (ν/cm^{-1})(CH_2Cl_2): 3068, 2977, 2931, 1702, 1596, 1485, 1333, 1253, 1100.

Ethyl 2-(4-bromophenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[3]ene-1,2'-indene]-3-carboxylate（4h）:



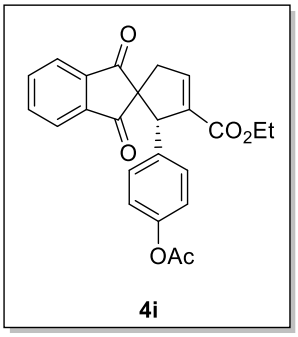
R$_f$ = 0.23 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.05-8.01 (d, 1H, *J* = 7.6 Hz), 7.86-7.81 (t, 1H, *J* = 7.2 Hz), 7.78-7.74 (t, 1H, *J* = 7.2 Hz), 7.65-7.62 (d, 1H, *J* = 7.6 Hz), 7.28-7.23 (m, 2H), 7.12-7.09 (d, 1H, *J* = 2.0 Hz), 6.74-6.69 (d, 2H, *J* = 8.0 Hz), 4.52-4.49 (s, 1H), 4.11-3.98 (m, 2H), 3.12-3.05 (dt,1H, *J* = 18.4, 4.8, 2.4 Hz), 2.97-2.91 (d, 1H, *J* = 18.4 Hz), 1.13-1.08 (t, 3H, *J* = 7.2 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.2, 199.1, 163.2, 143.2, 142.5, 141.2, 136.0, 135.6, 135.4, 131.2, 129.9, 123.6, 123.2, 121.4, 63.8, 60.4, 60.1, 36.8, 13.9; **HRMS** (EI) *m/z*: $[M+H]^+$ calcd for $C_{22}H_{17}O_4Br$ 424.0310, found 424.0300; **IR** (ν/cm^{-1})(CH_2Cl_2): 3068, 2977, 2931, 1744, 1714, 1596, 1485, 1337, 1253, 1097; **m.p.** = 192-193 ℃.

Ethyl 5-(4-acetoxyphenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[2]ene-1,2'-indene]-2-carboxylate（3i）:



R$_f$ = 0.14 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 7.97-7.93 (d, 1H, *J* = 7.6 Hz), 7.76-7.71(m, 1H), 7.68-7.64 (d, 2H), 7.40-7.38 (s, 1H), 7.10-7.05 (d, 2H, *J* = 8.4 Hz), 6.83-6.78 (d, 2H, *J* = 8.4 Hz), 4.23-4.17 (m, 1H), 4.02-3.94 (m, 2H), 3.36-3.26 (ddd, 1H, *J* = 18.1, 10.8, 1.6 Hz), 3.01-2.92 (ddd, 1H, *J* = 18.0, 8, 2.8 Hz), 2.21-2.18 (s, 3H), 1.01-0.95 (t, 3H, *J* = 7.2 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.9, 199.9, 169.0, 162.8, 149.8, 149.2, 142.8, 141.7, 135.6, 135.5, 135.3, 133.7, 129.5, 123.1, 122.8, 121,3, 70.5, 60.8, 54.0, 37.8, 21.0, 13.6; **HRMS** (EI) *m/z*: $[M+H]^+$ calcd for $C_{24}H_{21}O_6$ 405.1338, found 405.1328; **IR** (ν/cm^{-1})(CH_2Cl_2): 3068, 2977, 2923, 1763, 1702, 1596, 1337, 1245, 1200, 1100; **m.p.** = 166-168 ℃

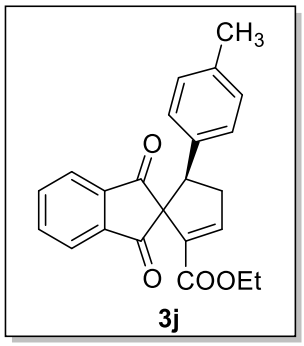
Ethyl 2-(4-acetoxyphenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[3]ene-1,2'-indene]-3-carboxylate（4i）:



R$_f$ = 0.09 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.04-7.99 (d, 1H, *J* = 7.6 Hz), 7.83-7.78 (t, 1H, *J* = 7.2 Hz), 7.76-7.70 (t, 1H, *J* = 7.2 Hz), 7.62-7.58 (d, 1H, *J* = 7.6 Hz), 7.11-7.08 (m, 1H), 6.88-6.79 (m, 4H), 4.56-4.53 (s, 1H), 4.13-3.95 (m, 2H), 3.12-3,04 (dt, 1H, J = 18.8, 4.8, 2.4), 2.98-2.91 (m, 1H), 2.25-2.20 (s, 3H), 1.10-1.04 (t, 3H, *J* = 7.2 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.3, 199.2, 168.9, 163.3, 149.9, 143.0, 141.3, 135.9, 135.7,

135.4, 129.2, 123.5, 123.3, 121.0, 64.3, 60.4, 60.4, 36.5, 21.1, 13.9; **HRMS** (EI) *m/z*: $[M+H]^+$ calcd for $C_{24}H_{21}O_6$ 405.1338, found 405.1343; **IR** (ν/cm^{-1})(CH_2Cl_2): 3061, 2977, 2923, 1744, 1714, 1596, 1333, 1257, 1200, 1097; **m.p.** = 130-134 °C.

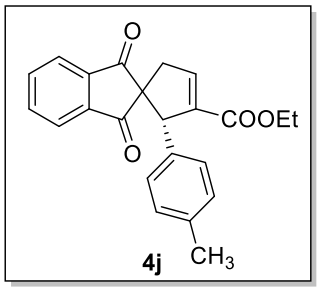
Ethyl 1',3'-dioxo-5-p-tolyl-1',3'-dihydrospiro[cyclopent[2]ene-1,2'-indene]-2-carboxylate（3j）:



3j

R$_f$ = 0.36 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 7.95 (d, 1H, *J* = 7.56 Hz), 7.76-7.68 (m, 1H), 7.65 (d, 2H, *J* = 3.8 Hz), 7.41-7.36 (m, 1H), 6.98-6.81 (m, 4H), 4.22-4.14 (m, 1H), 4.02-3.89 (m, 2H), 3.38-3.26 (m, 1H), 3.00-2.85 (m, 1H), 2.15 (s, 3H), 0.97 (t, 3H, *J* = 7.1 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 202.1, 200.0, 162.9, 149.5, 142.9, 141.8, 137.0, 135.6, 135.2, 135.1, 133.0, 128.8, 128.2, 123.0, 122.7, 70.5, 60.7, 54.3, 37.6, 20.8, 13.6; **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{20}H_{22}NaO_4$ 333.1259, found 383.1257; **IR** (ν/cm^{-1})(CH_2Cl_2): 2920, 1707, 1244, 1102; **m.p.** = 133-135 °C.

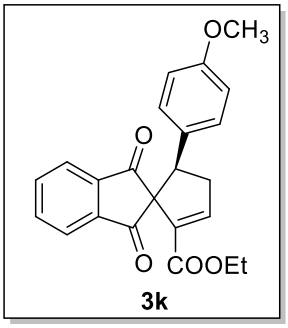
Ethyl 1',3'-dioxo-2-p-tolyl-1',3'-dihydrospiro[cyclopent[3]ene-1,2'-indene]-3-carboxylate（4j）:



4j

R$_f$=0.34 (4:1 Hex/EtOAc); **^{1}H-NMR** (500 MHz, $CDCl_3$): δ (ppm) = 8.02 (d, 1H, *J* = 7.6 Hz), 7.82 (t, 1H, *J* = 7.4 Hz), 7.73 (t, 1H, *J* = 7.4,Hz), 7.60 (d, 1H, *J* = 7.5 Hz), 7.09-7.06 (m, 1H), 6.91 (d, 2H, *J* = 7.7 Hz), 6.68 (d, 2H, *J* = 7.7 Hz), 4.49 (s, 1H), 3.14 -3.05 (m, 1H), 2.96-2.87 (m, 1H), 2.22 (s, 3H), 1.09 (t, 3H, *J* = 7.1 Hz) ; **^{13}C-NMR** (125 MHz, $CDCl_3$): δ (ppm) = 201.4, 199.2, 163.4, 142.8, 142.6, 141.3, 137.0, 135.9, 135.7, 135.3, 133.7, 128.8, 128.0, 123.5, 123.1, 64.3, 60.7, 60.3, 36.3, 21.1, 13.9; **HRMS** (ESI) *m/z*: $[M+Na]^+$ $C_{22}H_{18}NaO_4$ calcd for 383.1259, found 383.1154; **IR** (ν/cm^{-1}) (CH_2Cl_2): 2982, 2924, 1743, 1710, 1259, 1242, 1100.

Ethyl 5-(4-methoxyphenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[2]ene-1,2'-indene]-2-carboxylate（3k）:

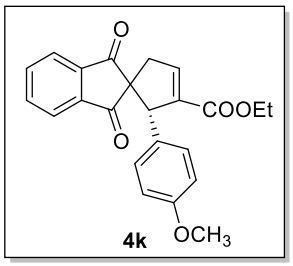


3k

R$_f$ = 0.27 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 7.94 (d, 1H, *J* = 7.52 Hz), 7.77-7.69 (m, 1H), 7.65 (d, 2H, *J* = 3.8 Hz), 7.42-7.36 (m, 1H), 6.97 (d, 2H, *J* = 8.64 Hz), 6.59 (d, 2H, *J* = 8.68 Hz), 4.20-4.13 (m, 1H), 3.97 (qd, 2H, *J* = 7.11, 1.93 Hz), 3.67 (s, 3H), 3.29 (ddd, 1H, *J* = 18.0, 10.7, 1.9 Hz), 2.93 (ddd, 1H, *J* = 18.1, 8.1, 2.8 Hz), 0.97 (t, 3H, *J* = 7.14 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 202.4, 200.4, 163.1, 158.9, 149.7, 143.1, 142.0, 135.8, 135.5, 135.4, 129.7, 128.3, 123.2, 122.9, 113.7, 70.8, 61.0, 55.3, 54.3, 38.0, 13.8; **HRMS** (ESI) *m/z*: $[M]^+$ calcd for $C_{22}H_{17}ClO_3$ 364.0866,

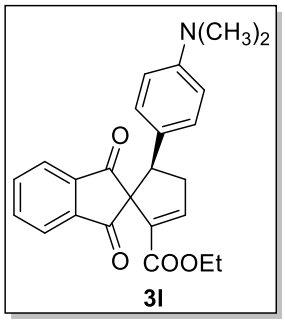
found 364.0875; **IR** (ν/cm^{-1})(CH_2Cl_2): 2851, 2821, 1709, 1244, 1029. **m.p.**= 106-107 °C

Ethyl 2-(4-methoxyphenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[3]ene-1,2'-indene]-3-carboxylate（4k）:



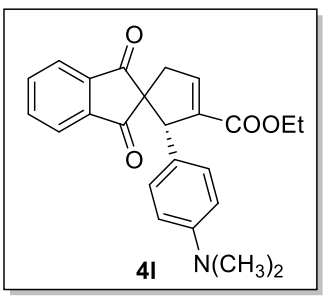
R_f = 0.18 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.02 (d, 1H, J = 7.5 Hz), 7.80 (t, 1H, J = 7.5 Hz), 7.72 (t, 1H, J = 7.4 Hz), 7.60 (d, 1H, J = 7.5 Hz), 7.09-7.04 (m, 1H), 6.72 (d, 1H, J = 8.0 Hz), 6.64 (d, 1H, J = 8.6 Hz), 4.49 (s,1H), 4.08-3.98 (m, 2H), 3.71 (s, 3H), 3.13-3.05 (m, 1H), 2.96-2.88 (m, 1H), 1.09 (t, 3H, J = 7.1 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.5, 199.3, 163.4, 158.7, 142.8, 142.5, 141.4, 135.9, 135.7, 135.3, 129.3, 128.8, 123.5, 123.1, 113.5, 64.4, 60.5, 60.3, 55.0, 36.2, 13.9; **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{22}H_{17}BrNaO_3$ 431.0259, found 431.0272; **IR** (ν/cm^{-1})(CH_2Cl_2): 2982, 2935, 1740, 1706, 1515, 1253, 1102, 1032. **m.p.** =123-124 °C

Ethyl 5-(4-(dimethylamino)phenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[2]ene-1,2'-indene]-2-carboxylate（3l）:



R_f = 0.23 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 7.97-7.92 (m, 1H), 7.74-7.64 (m, 3H), 7.39 (t, 1H, J = 2.5 Hz), 6.91 (d, 2H, J = 8.7 Hz), 6.42 (d, 2H, J = 8.8 Hz), 4.18-4.10 (m, 1H), 4.02-3.90 (m, 2H), 3.29 (ddd, 1H, J = 18.1, 10.7, 2.1 Hz), 2.90 (ddd, 1H, J = 18.1, 8.1, 2.9 Hz), 2.79 (s, 6H), 0.97 (t, 3H, J = 7.1 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 202.5, 200.3, 163.0, 149.7, 143.0, 141.9, 135.6, 135.2, 135.0, 129.1, 123.6, 123.0, 122.7, 112.1, 70.7, 60.7, 54.4, 40.3, 37.9, 13.6; **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{23}H_{20}NaO_4$ 383.1259, found 383.1255; **IR** (ν/cm^{-1})(CH_2Cl_2): 2920, 1706, 1521, 1245, 1189. **m.p.**=118-120 °C

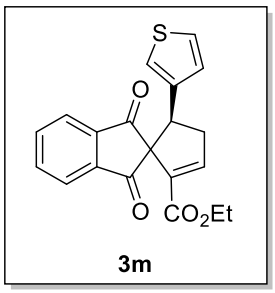
Ethyl 2-(4-(dimethylamino)phenyl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[3]ene-1,2'-indene]-3-carboxylate（4l）:



R_f = 0.16 (4:1 Hex/EtOAc);**^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.04 (d, 1H, J = 7.4 Hz), 7.81 (t, 1H, J = 7.3 Hz), 7.74 (t, 1H, J = 7.5 Hz), 7.63 (d, 1H, J = 7.7), 7.09-7.03 (m, 1H), 6.67 (d, 2H, J = 7.9 Hz), 6.48 (d, 2H, J = 8.3Hz), 4.47 (s, 1H), 4.13-3.99 (m, 2H), 3.16-3.08 (m,1H), 2.95-2.88 (m, 1H), 2.87 (s, 6H), 1.13 (t, 3H, J = 7.1 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm)= 201.6, 199.2, 163.6, 149.7, 143.0, 142.0, 141.4, 136.1, 135.5, 135.1, 128.9, 124.2,

123.5, 123.1, 112.0, 64.7, 60.9, 60.2, 40.3, 35.8, 14.4; **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd for $C_{20}H_{16}NaO_3S$ 359.0718, found 359.0729; **IR** (ν/cm^{-1})(CH_2Cl_2): 2921, 2851, 1742, 1709, 1261; **m.p.** = 150-151 ℃.

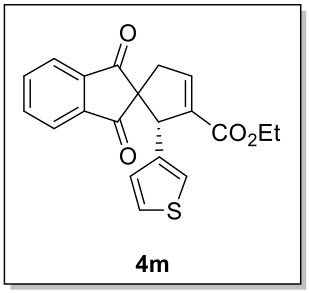
Ethyl 5-(thiophen-3-yl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[2]ene-1,2'-indene]-2-carboxylate (3m):



3m

R_f = 0.33 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.00-7.96 (d, 1H, J = 7.6 Hz), 7.80-7.68 (m, 3H), 7.02-6.99 (m, 1H), 6.92-6.90 (m, 1H), 6.69-6.66 (dd, 1H, J = 4.8, 0.8 Hz), 4.31-4.24 (m, 1H), 4.03-3.93 (m, 2H), 3.31-3.21 (m, 1H), 3.04-2.96 (m, 1H), 1.01-0.95 (t, 3H, J = 6.8 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.9, 199.9, 162.8, 149.2, 142.9, 141.7, 137.3, 135.8, 135.4, 135.3, 127.4, 125.8, 123.6, 123.1, 122.8, 122.8, 70.0, 60.8, 49.8, 38.4, 13.6; **HRMS** (EI) *m/z*: $[M+H]^+$ calcd for $C_{20}H_{16}O_4S$ 352.0769, found 352.0774; **IR** (ν/cm^{-1})(CH_2Cl_2): 3099, 2977, 1702, 1596, 1371, 1337, 1249, 1100.

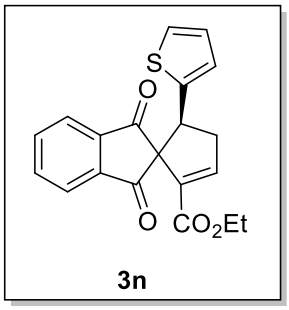
Ethyl 2-(thiophen-3-yl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[3]ene-1,2'-indene]-3-carboxylate（4m）:



4m

R_f = 0.28 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.04-8.00 (d, 1H, J = 7.2 Hz), 7.85-7.79 (m, 1H), 7.79-7.73 (m, 1H), 7.68-7.65 (m, 1H), 7.12-7.08 (m, 1H), 7.06-7.03 (m, 1H), 6.69-6.66 (m, 1H), 6.61-6.58 (m, 1H), 4.66-4.63 (s, 1H), 4.15-3.98 (m, 2H), 3.12-3.05 (dt,1H, J = 18.8, 5.2, 2.8 Hz), 2.96-2.89 (m, 1H), 1.13-1.08 (t, 3H, J = 6.8 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.3, 199.1, 163.4, 142.7, 142.4, 141.3, 137.6, 135.9, 135.8, 135.4, 127.4, 125.3, 123.5, 123.1, 122.7, 64.0, 60.3, 55.7, 36.3, 13.9; **HRMS** (EI) *m/z*: $[M+H]^+$ calcd for $C_{20}H_{16}O_4S$ 352.0769, found 352.0764; **IR** (ν/cm^{-1})(CH_2Cl_2): 3099, 2977, 1740, 1710, 1596, 1367, 1333, 1260, 1097; **m.p.** = 126-127 °C.

Ethyl 5-(thiophen-2-yl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[2]ene-1,2'-indene]-2-carboxylate（3n):

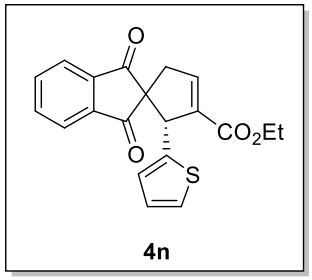


3n

R_f = 0.30 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.02-7.99 (d, 1H, J = 6.4 Hz), 7.81-7.69 (m, 3H), 7.37-7.34 (t, 1H), 6.97-6.94 (dd, 1H, J = 4.8, 1.2 Hz), 6.74-6.68 (m, 2H), 4.49-4.42 (m, 1H), 4.02-3.93 (m, 2H), 3.35-3.26 (ddd, 1H, J = 18.0, 10.8, 2.0 Hz), 3.13-3.04 (ddd, 1H, J = 18.0, 8.0, 2.8 Hz), 1.01-0.95 (t, 3H, J = 7.2 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 201.5, 199.4, 162.7, 148.8, 143.2, 141.9, 139.2, 136.0, 135.5, 135.4, 126.6,

126.2, 124.4, 123.2, 122.9, 70.0, 60.9, 49.2, 39.4, 13.6; **HRMS** (EI) *m/z*: $[M+H]^+$ calcd for $C_{20}H_{16}O_4S$ 352.0769, found 352.0774; **IR** (ν/cm^{-1})(CH_2Cl_2): 3068, 2977, 2923, 1702, 1596, 1371, 1337, 1249, 1100; **m.p.** = 110-111 °C.

Ethyl 2-(thiophen-2-yl)-1',3'-dioxo-1',3'-dihydrospiro[cyclopent[3]ene-1,2'-indene]-3-carboxylate（4n）:



4n

R_f = 0.21 (4:1 Hex/EtOAc); **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 8.06-8.02 (d, 1H, *J* = 7.2 Hz), 7.87-7.71 (m, 3H), 7.11-7.06 (d, 2H, *J* = 5.2 Hz), 6.85-6.81 (t, 1H, *J* = 4.0 Hz), 6.55-6.52 (d, 1H), 4.78-4.75 (s, 1H), 4.17-4.00 (m, 2H), 3.18-3.11 (d,1H, *J* = 18.4 Hz), 2.92-2.85 (d, 1H, *J* = 18.8 Hz), 1.16-1.10 (t, 3H, *J* = 6.8 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$): δ (ppm) = 200.8, 198.3, 163.1, 142.9, 142.7, 141.2, 140.1, 135.9, 135.5, 129.4, 126.9, 124.9, 123.7, 123.2, 64.0, 60.4, 55.0, 36.0, 13.9; **HRMS** (EI) *m/z*: $[M+H]^+$ calcd for $C_{20}H_{16}O_4S$ 352.0769, found 352.0774; **IR** (ν/cm^{-1})(CH_2Cl_2): 3068, 2977, 2923, 1744, 1714, 1596, 1371, 1333, 1264, 1097.

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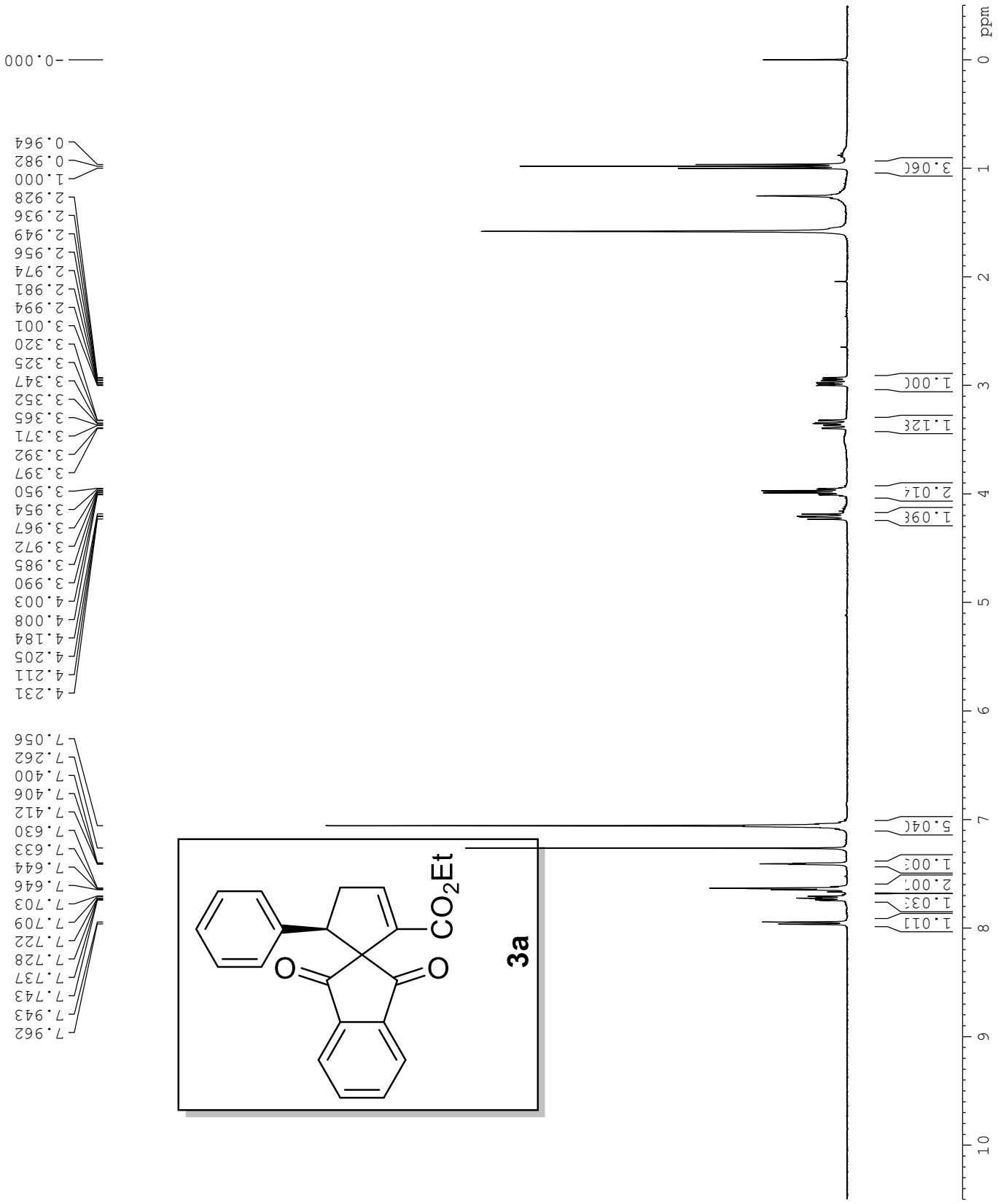
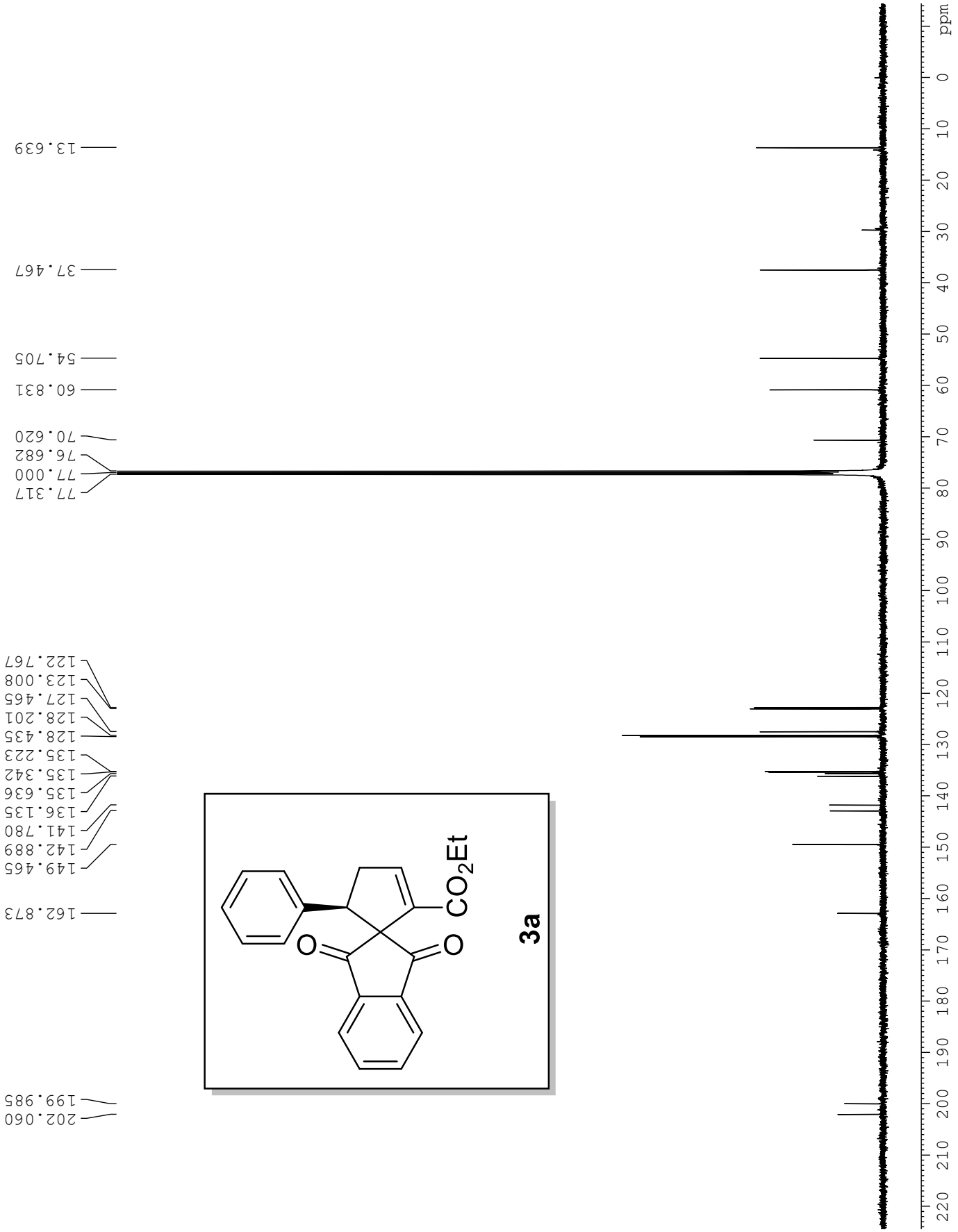
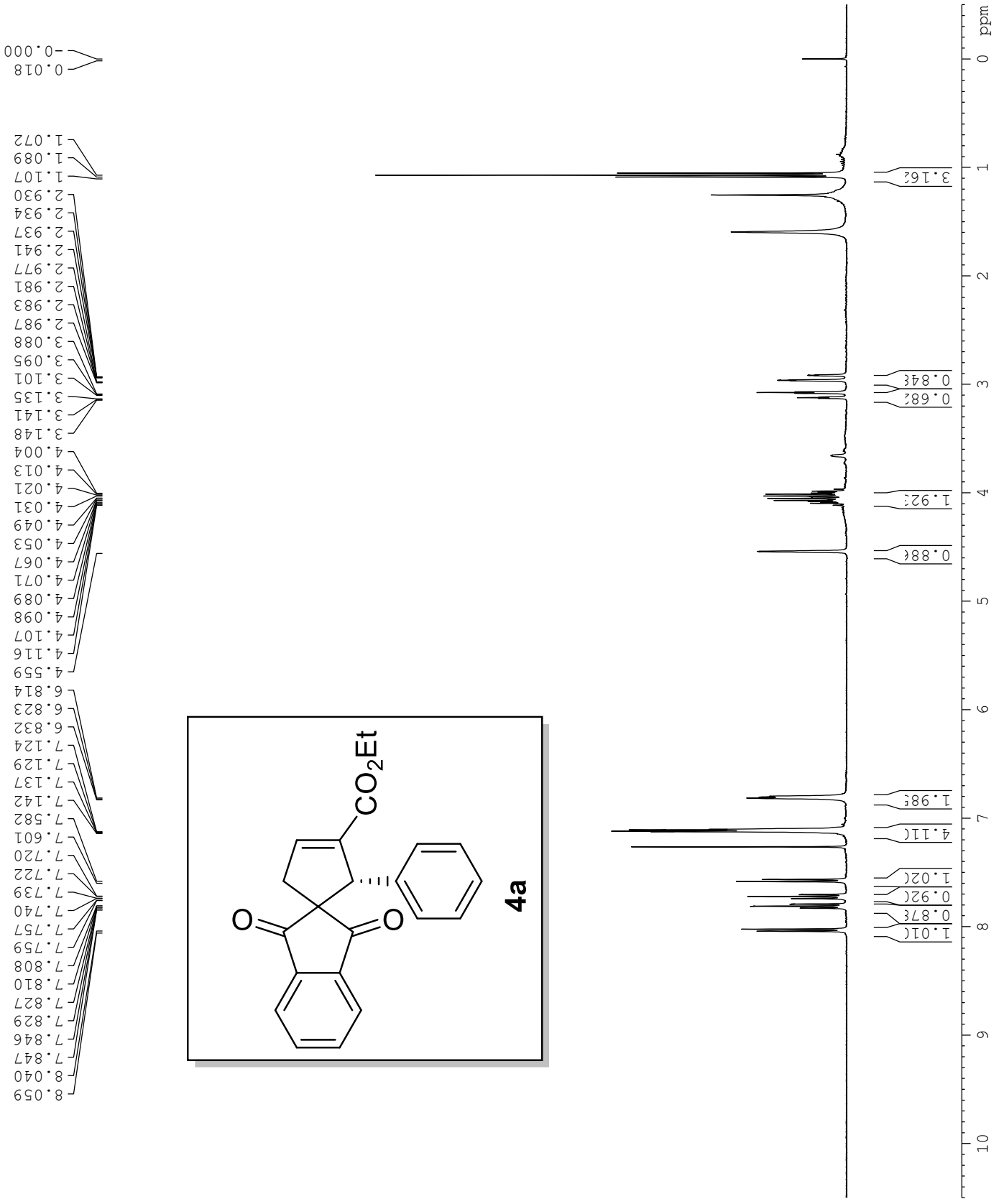


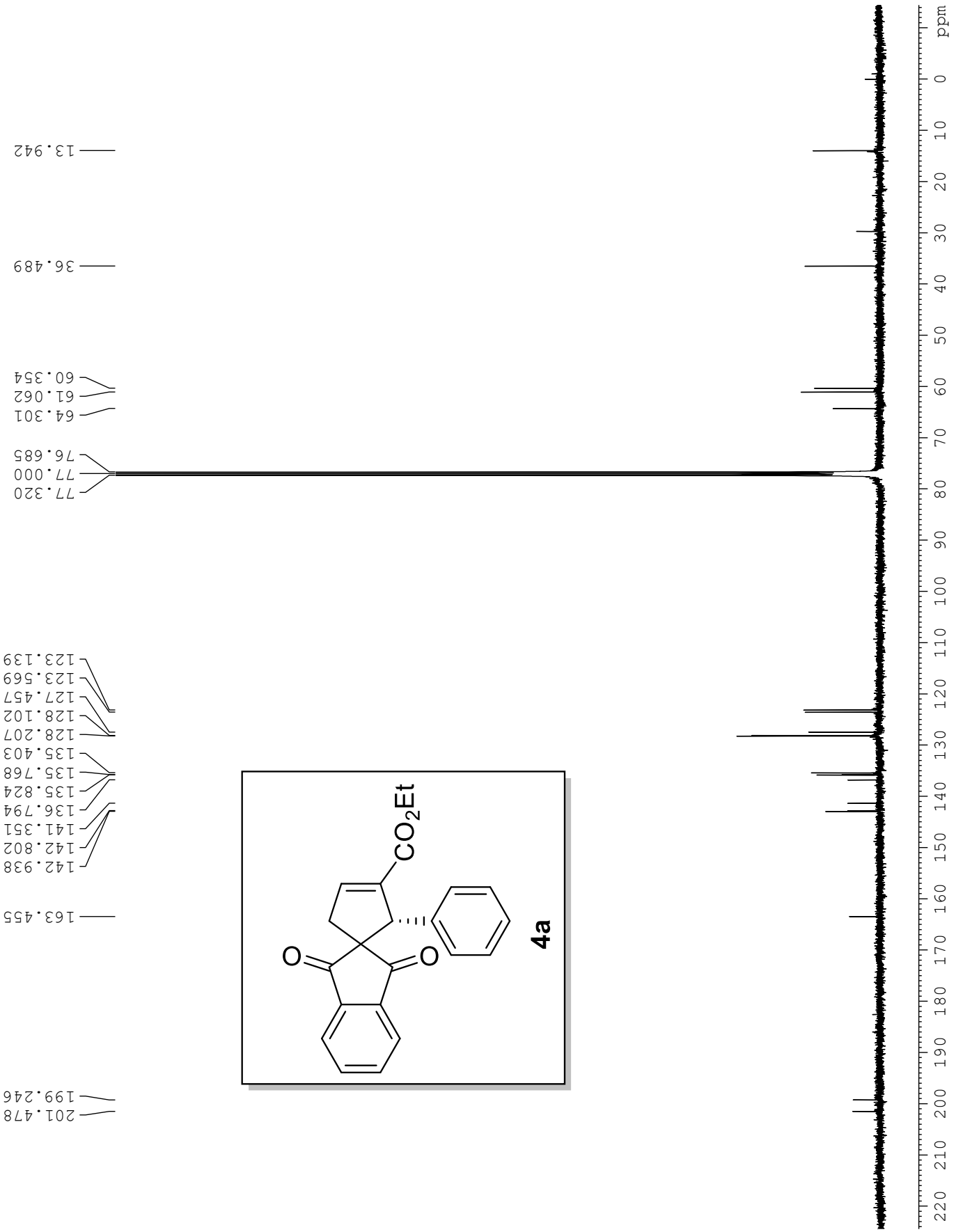
^{1}H NMR for compound 3a



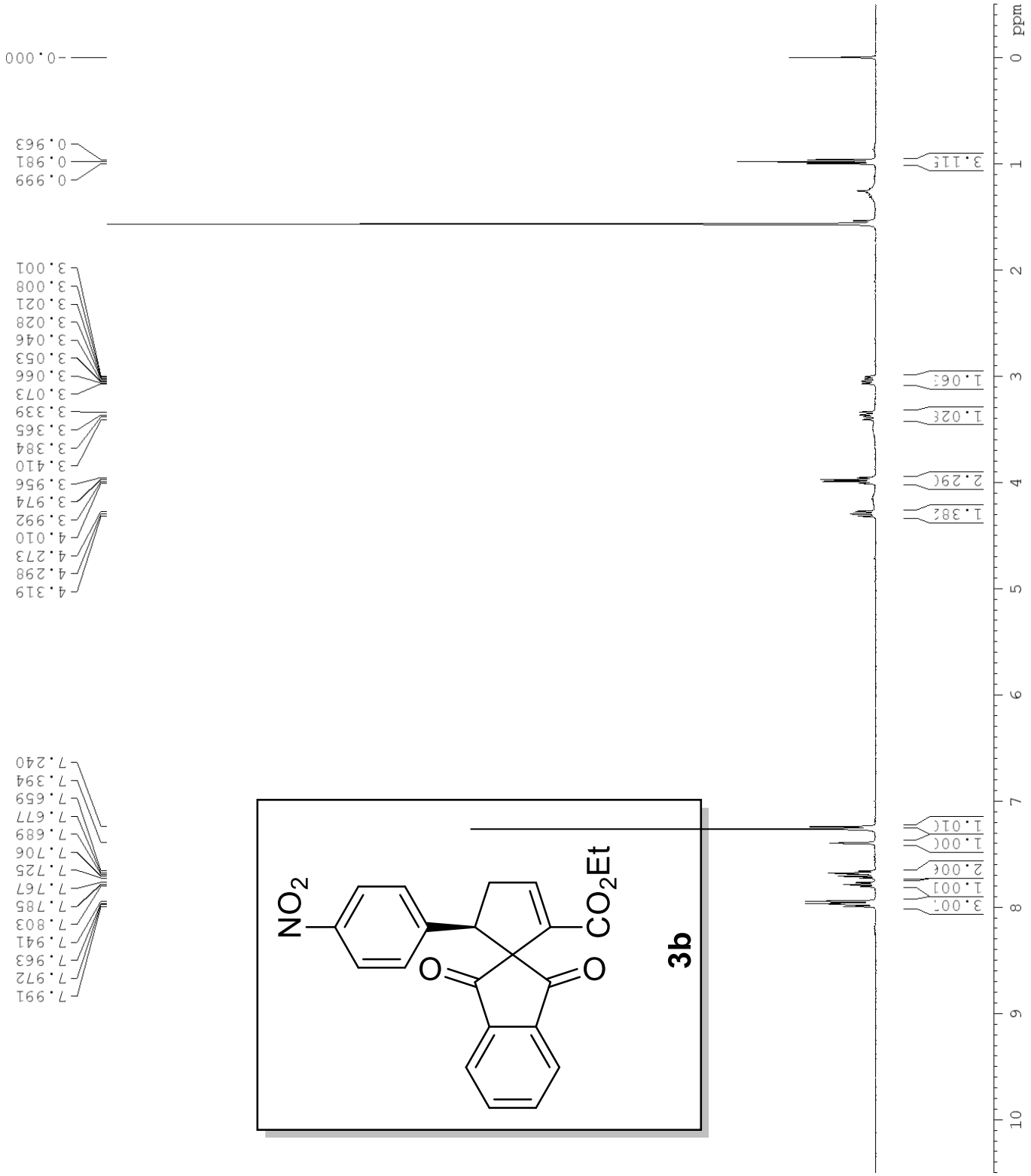
^{13}C NMR for compound 3a



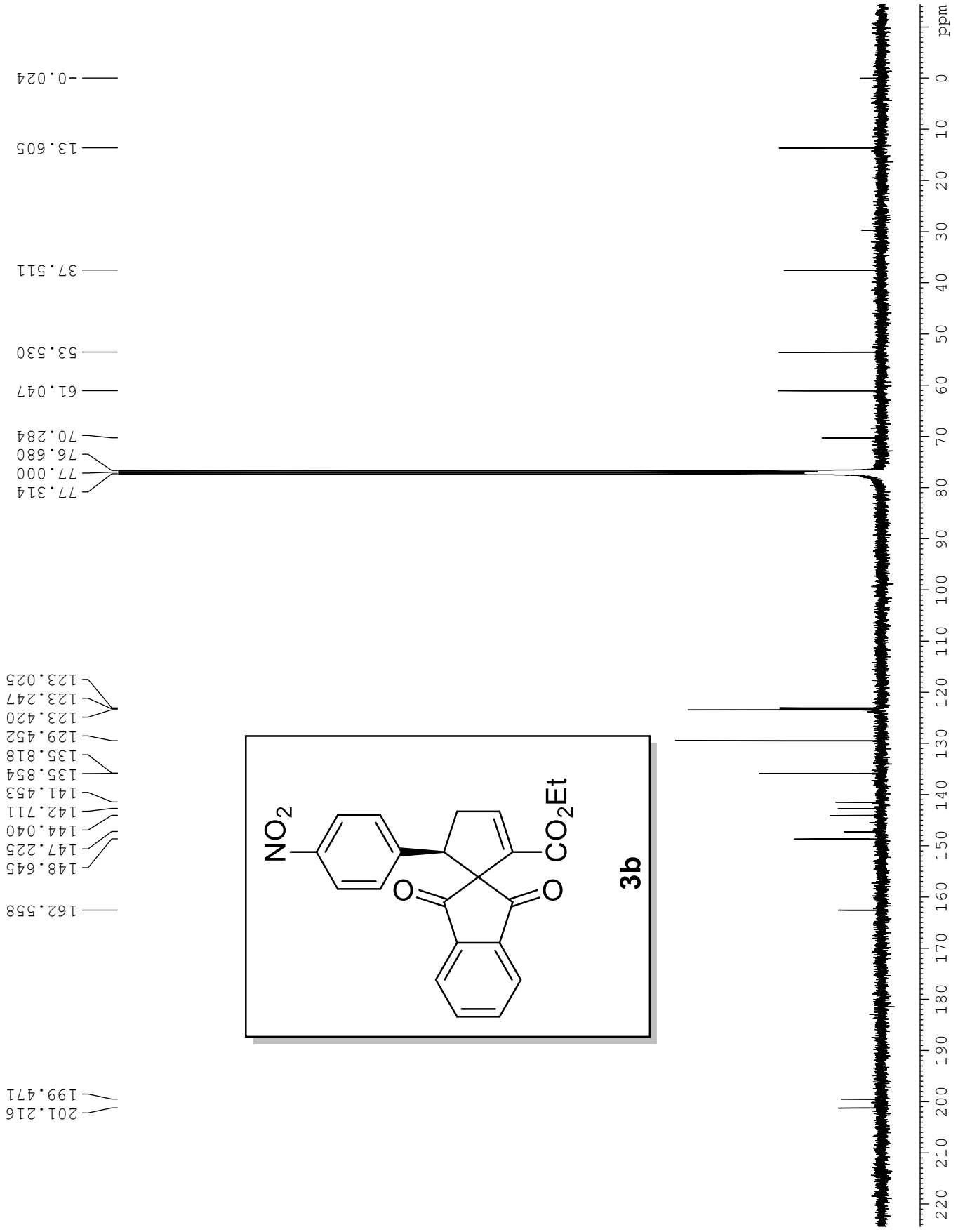
^{1}H NMR for compound 4a



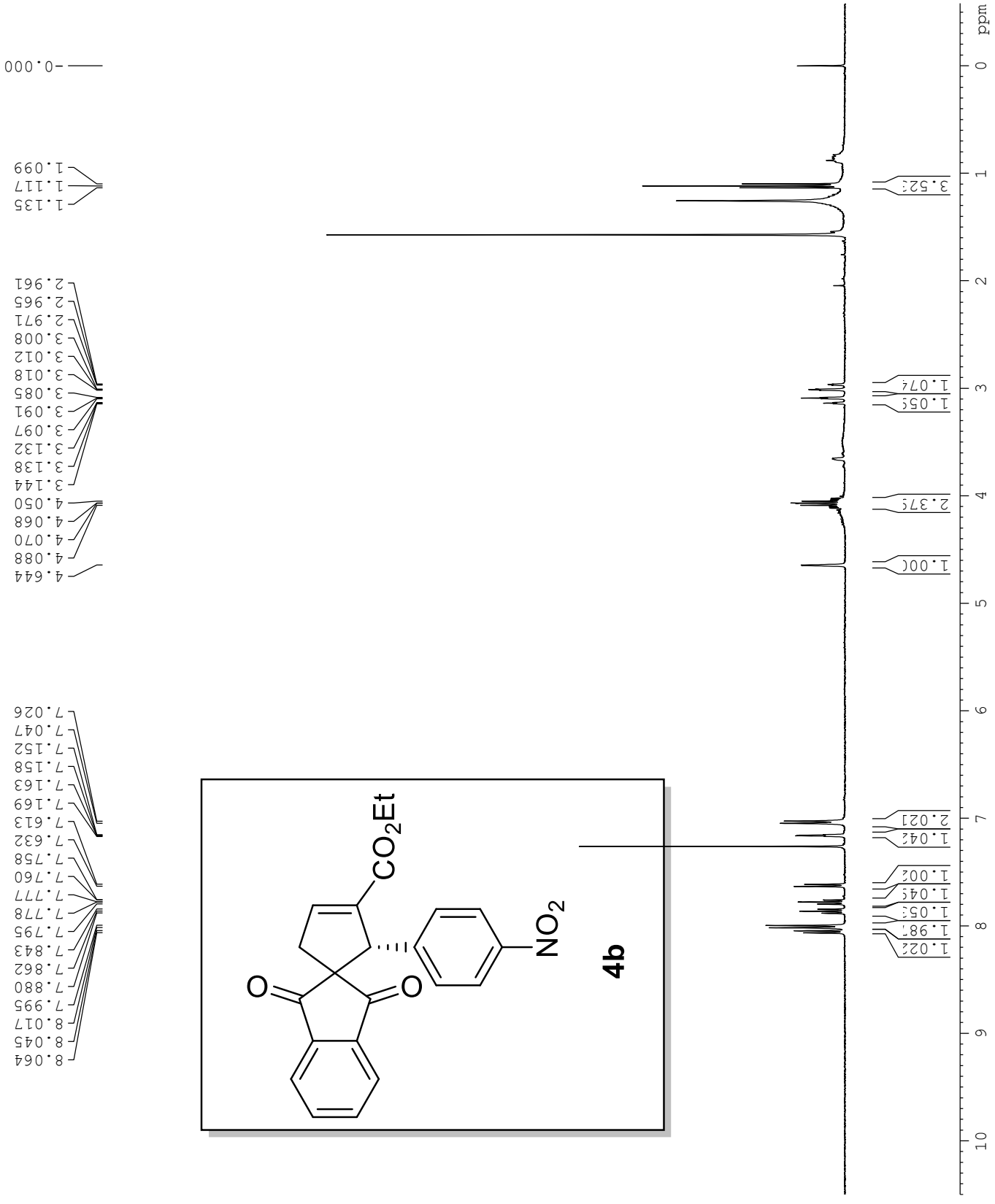
^{13}C NMR for compound 4a



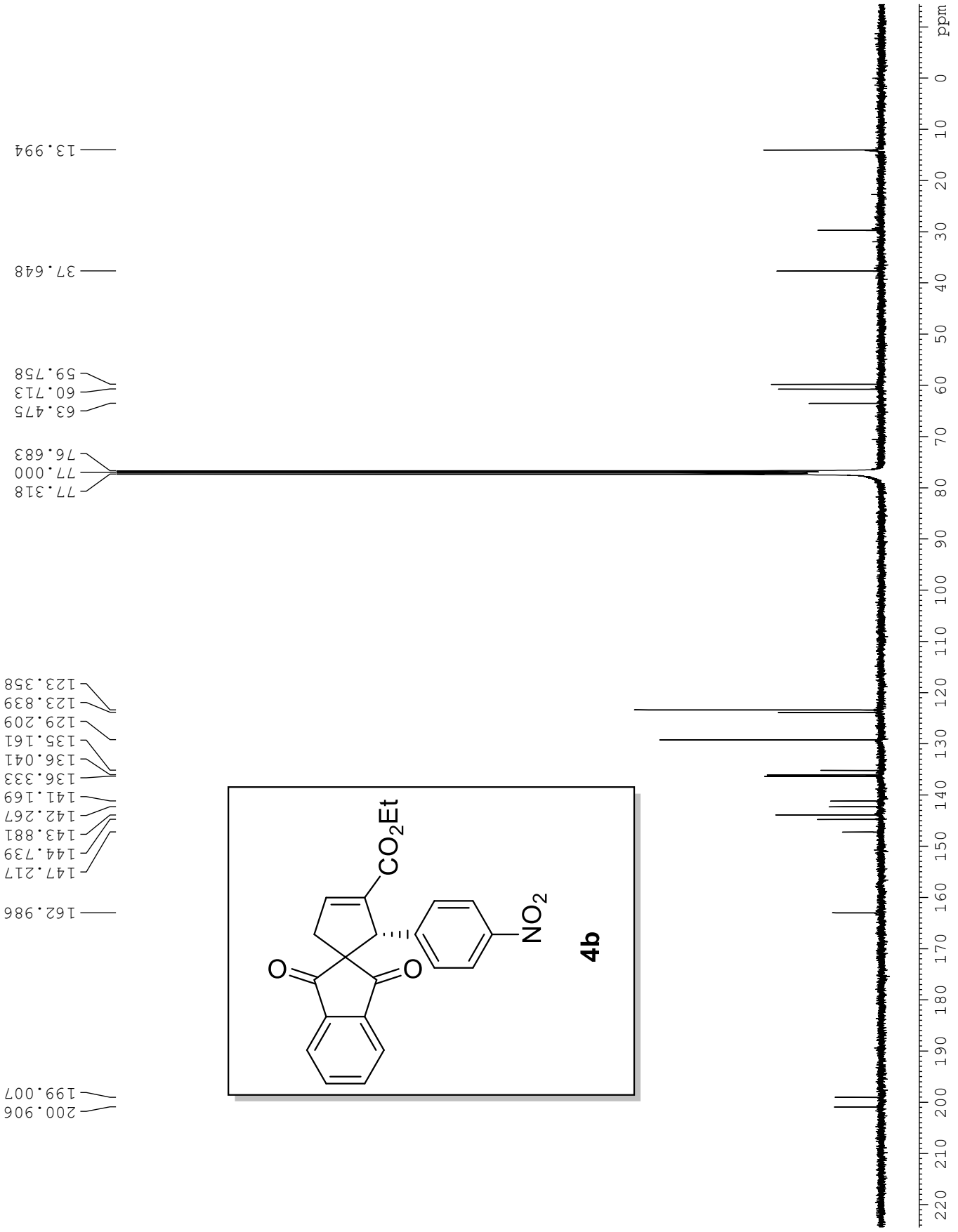
^{1}H NMR for compound 3b



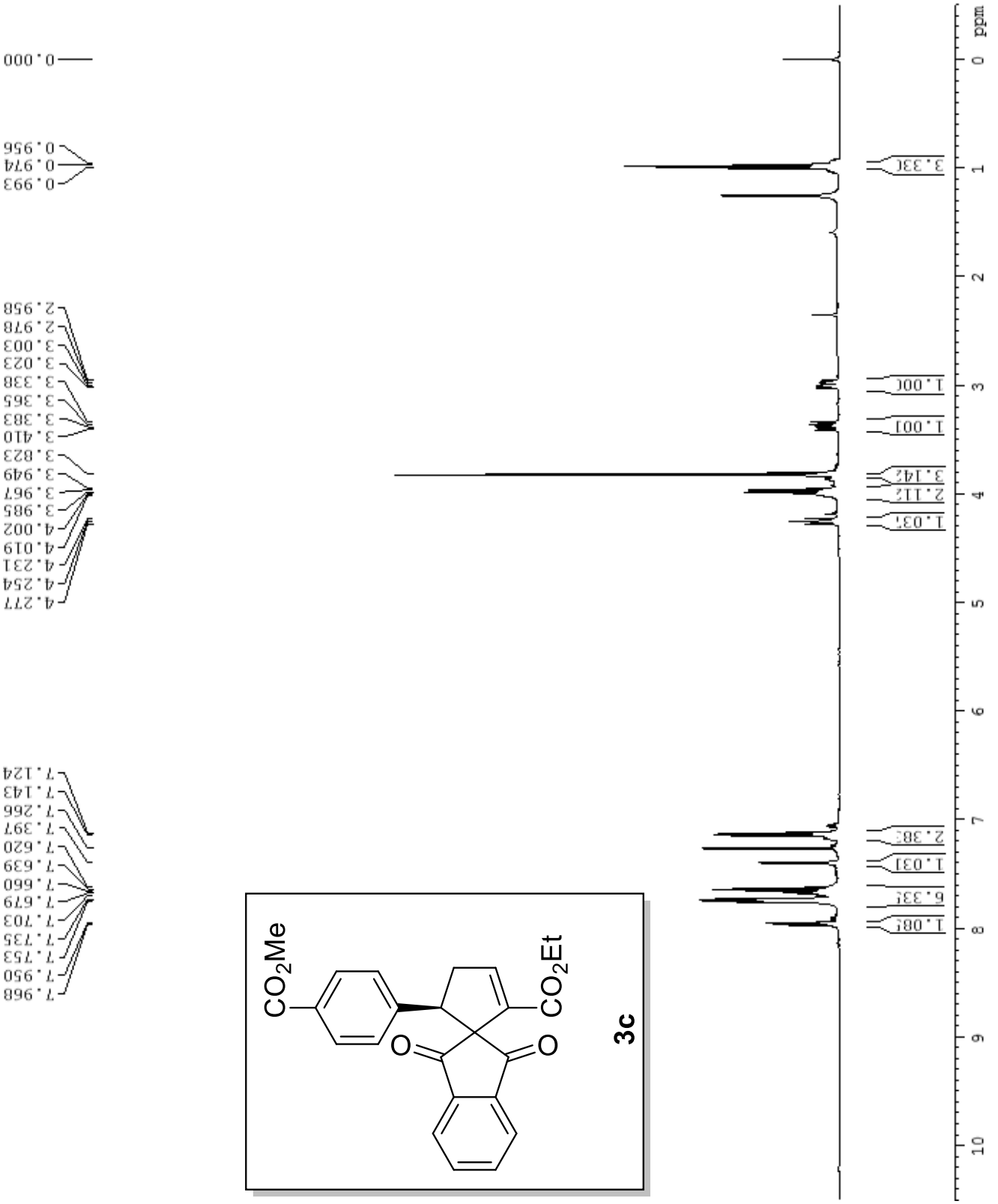
^{13}C NMR for compound 3b



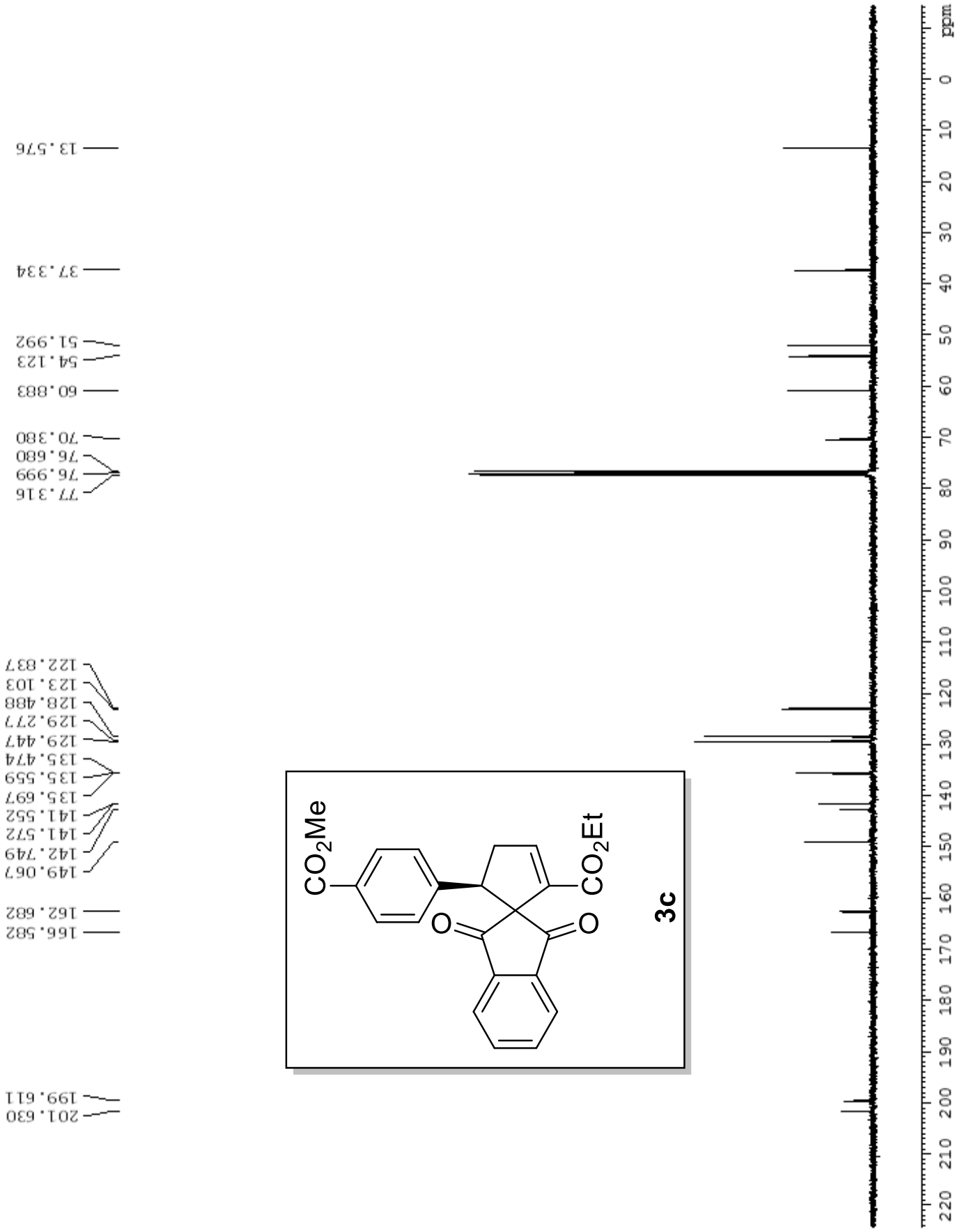
^{1}H NMR for compound 4b



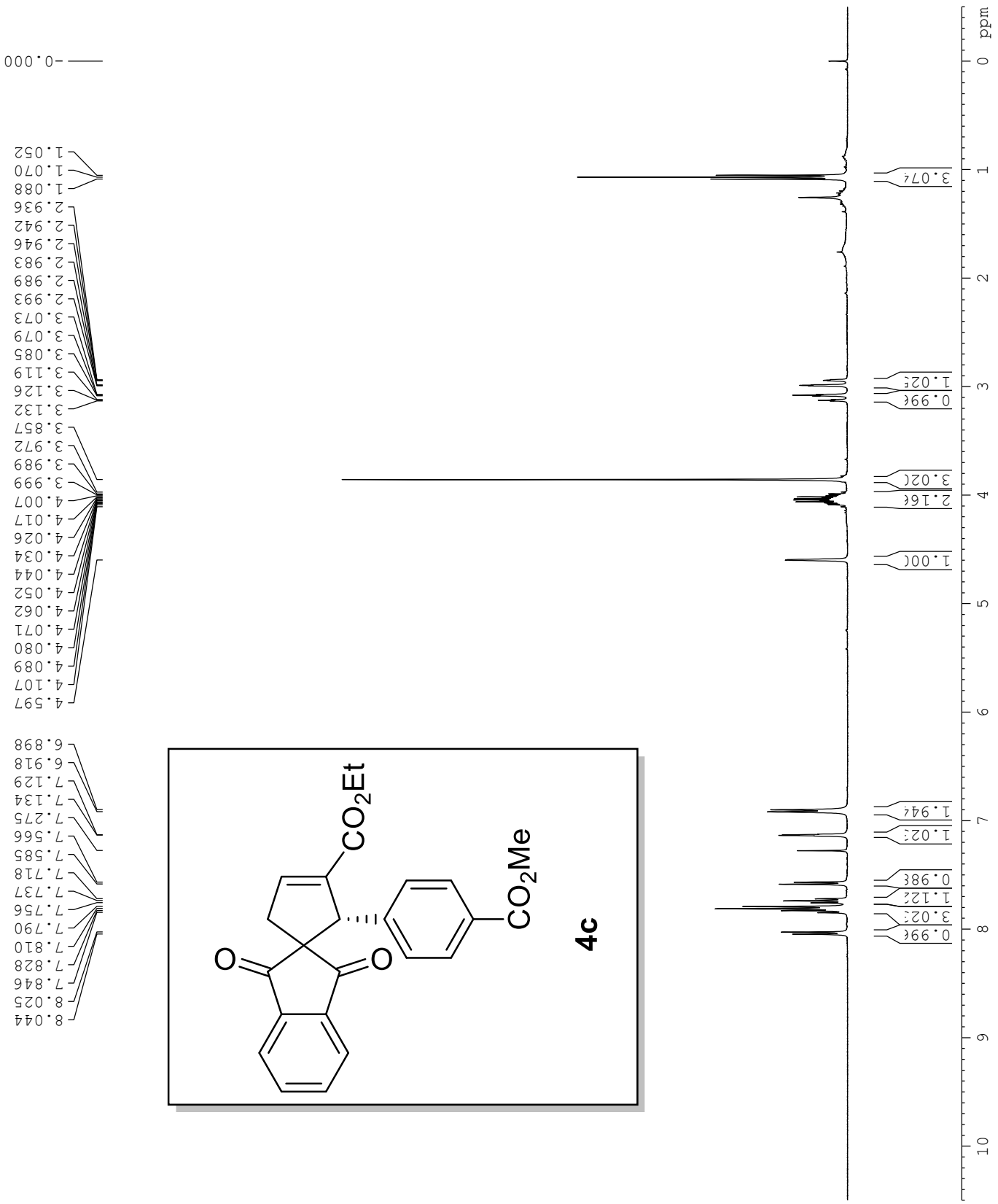
^{13}C NMR for compound 4b



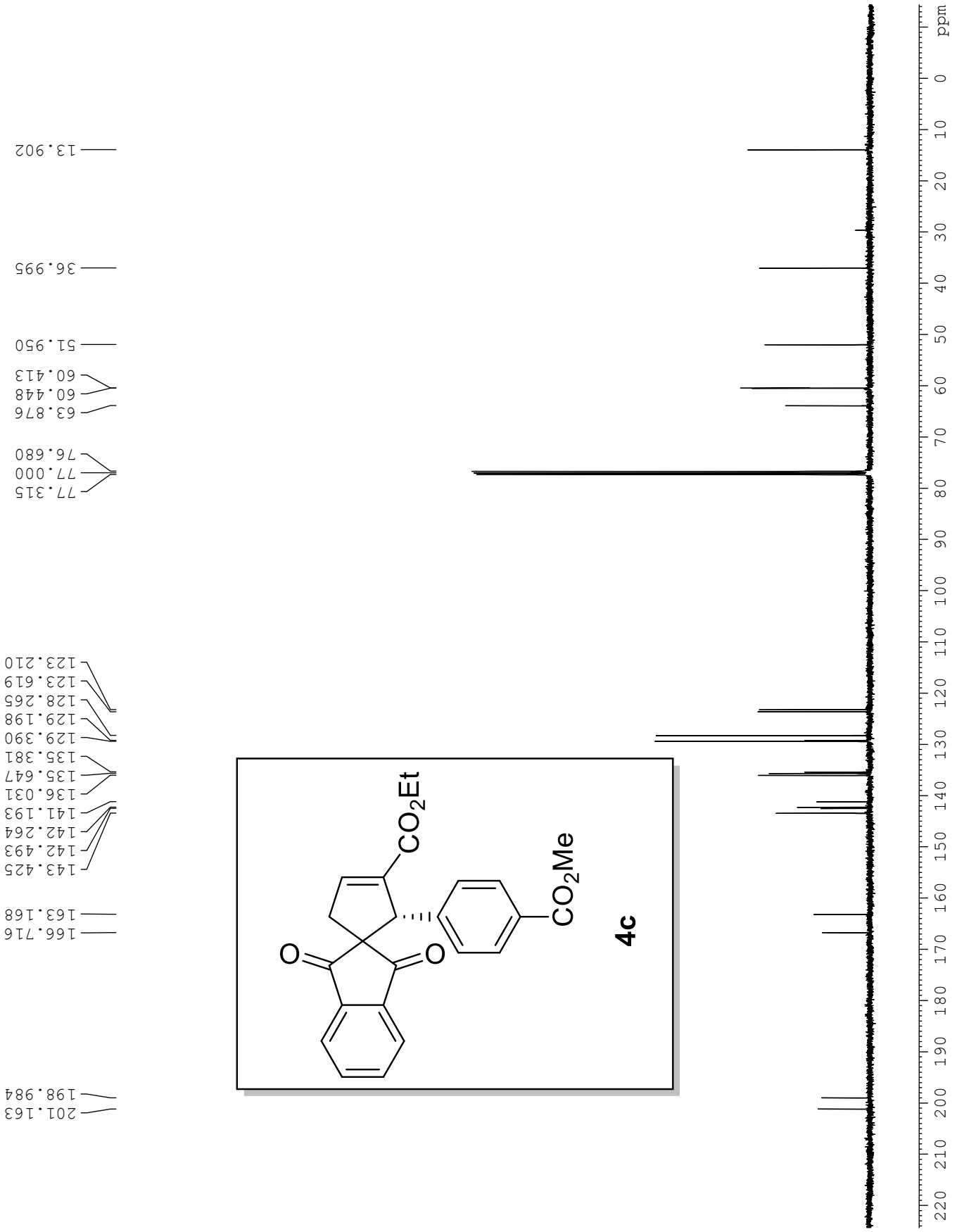
^{1}H NMR for compound 3c



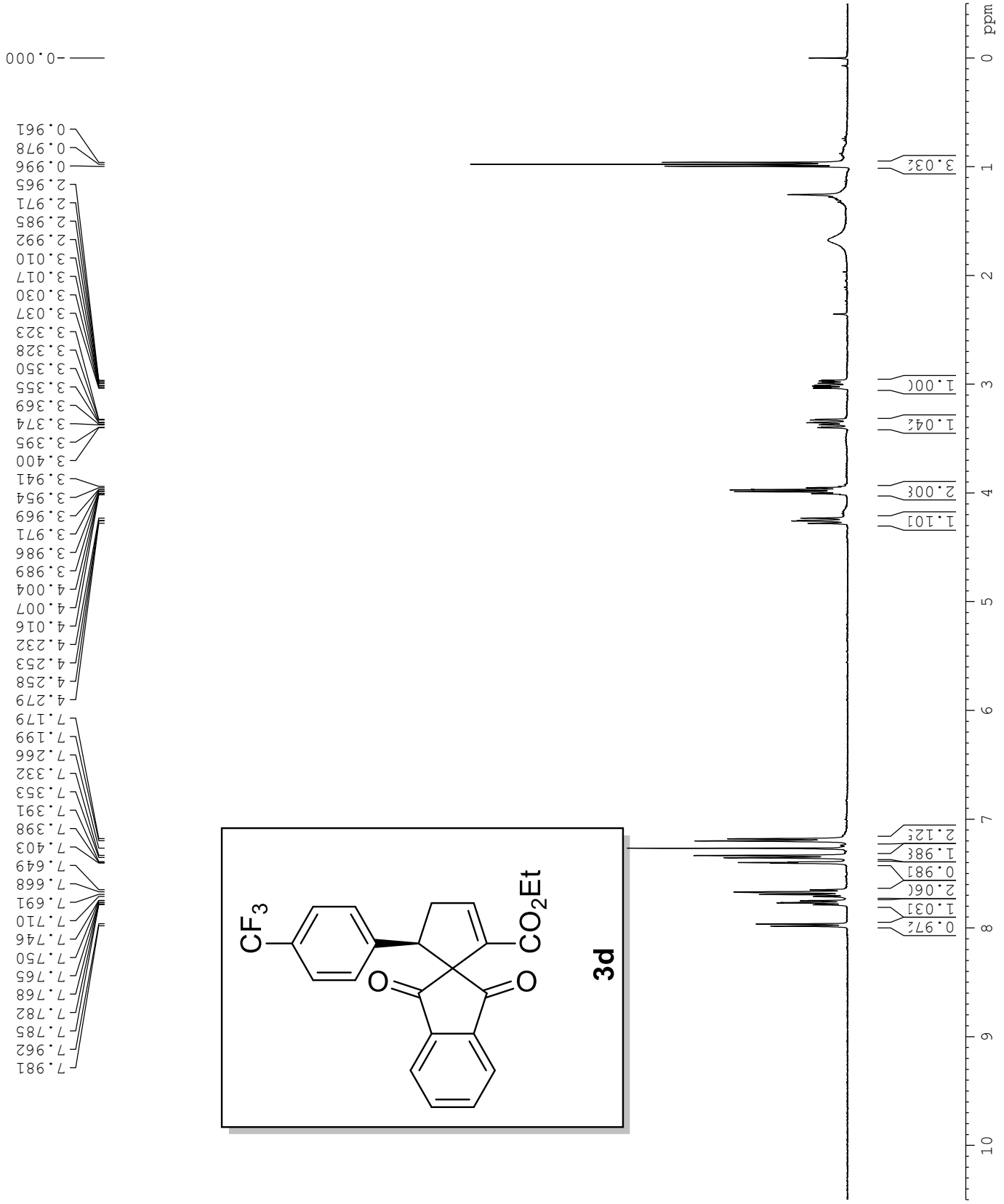
^{13}C NMR for compound 3c



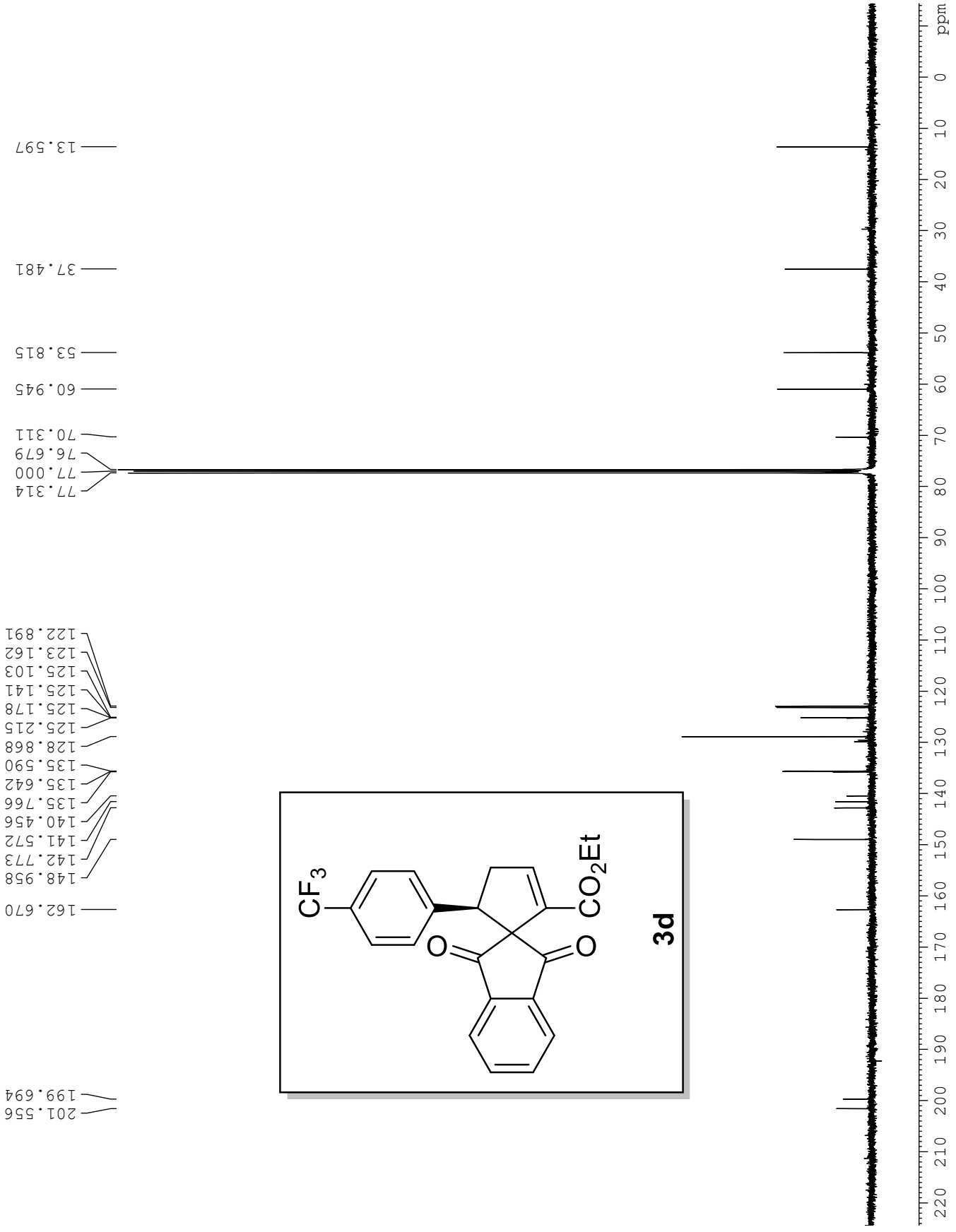
^{1}H NMR for compound 4c



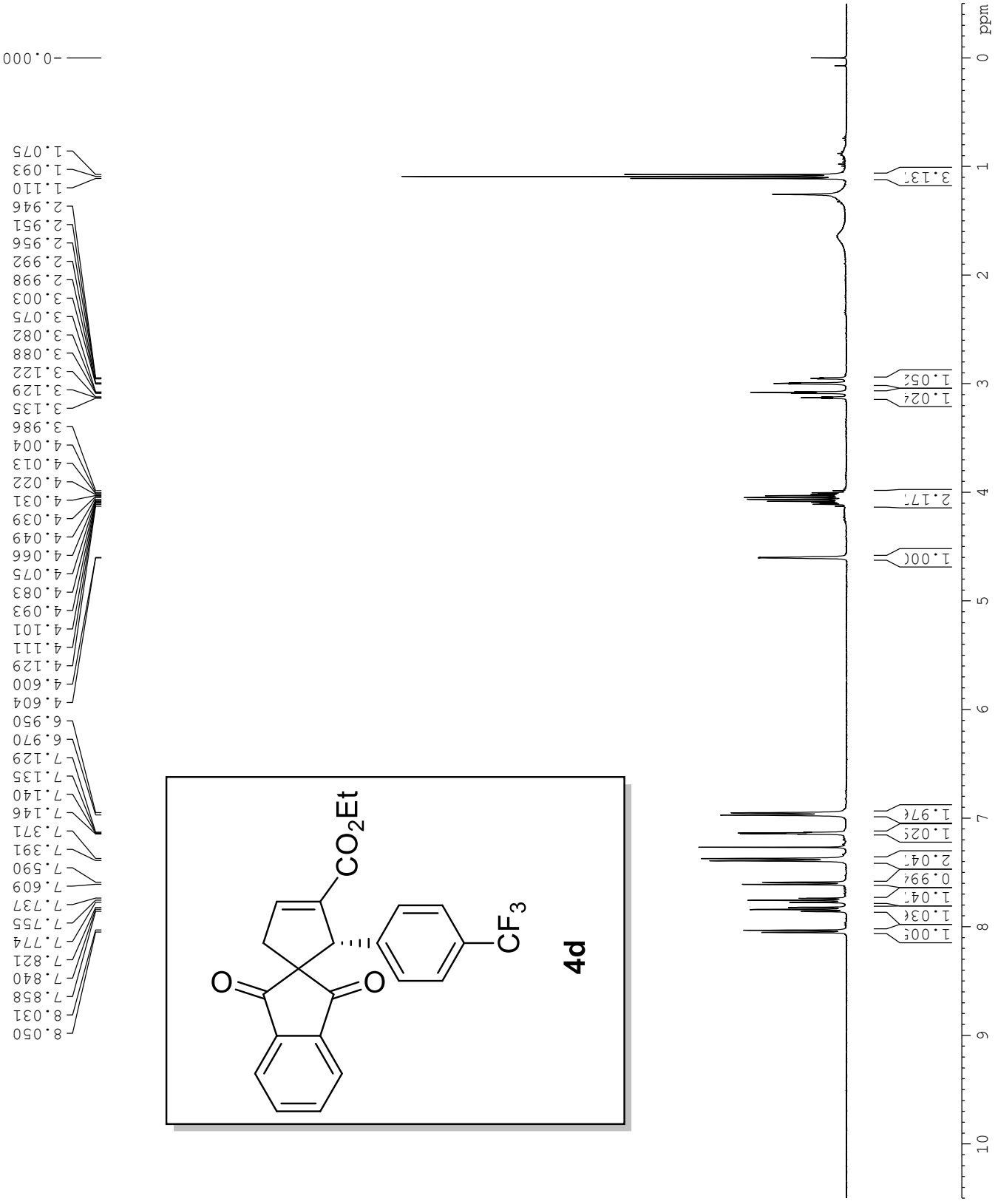
^{13}C NMR for compound 4c



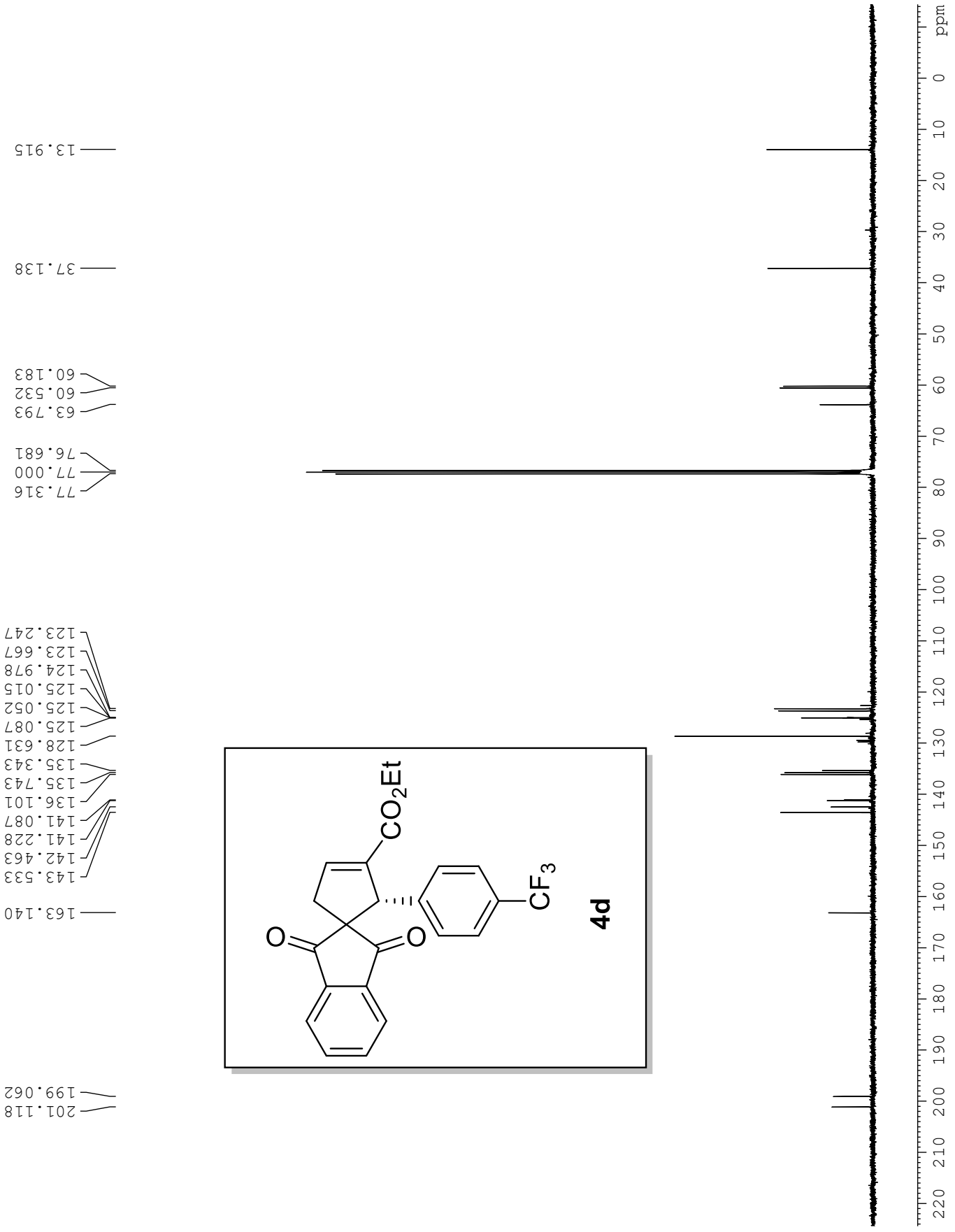
^{1}H NMR for compound 3d



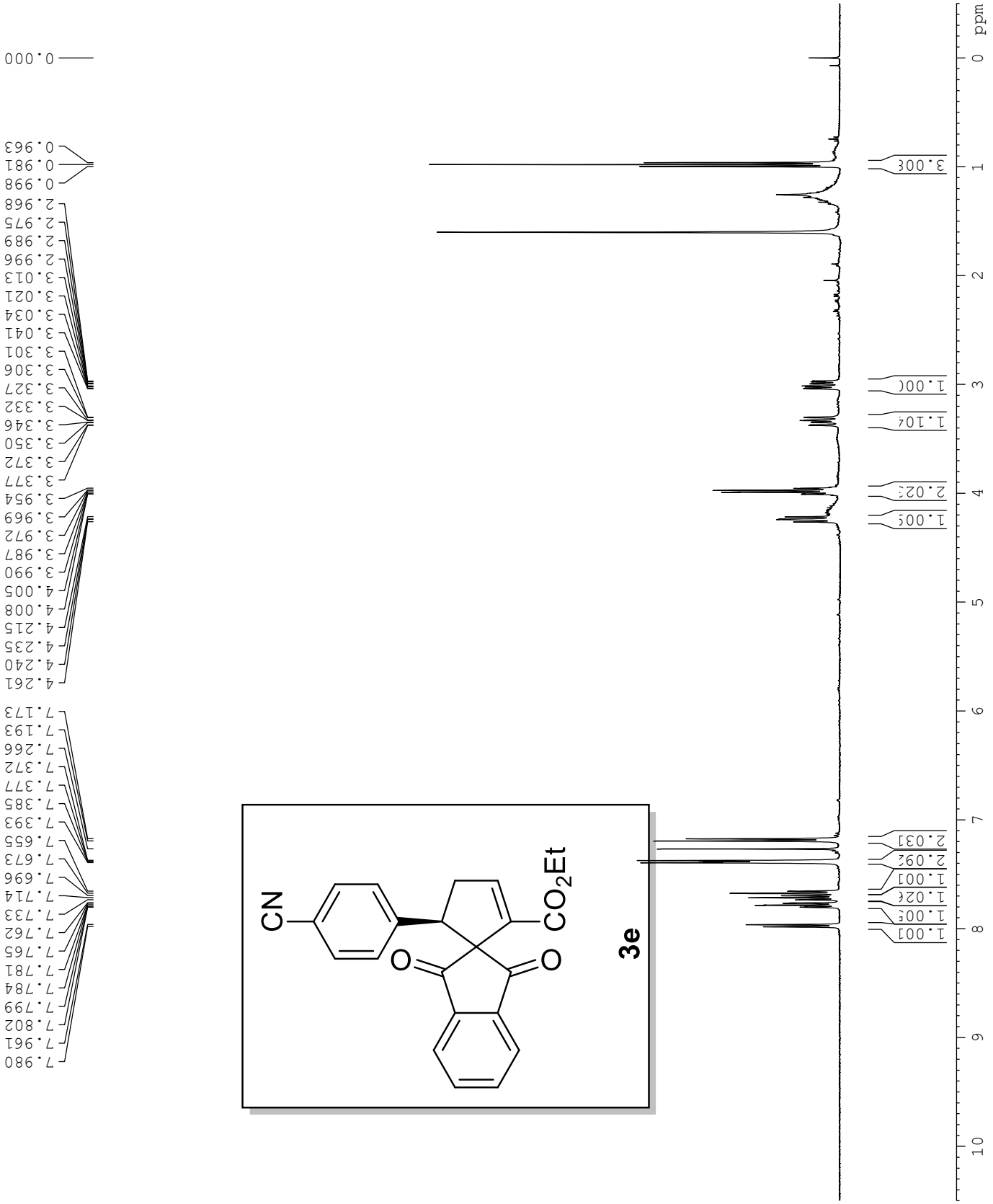
^{13}C NMR for compound 3d



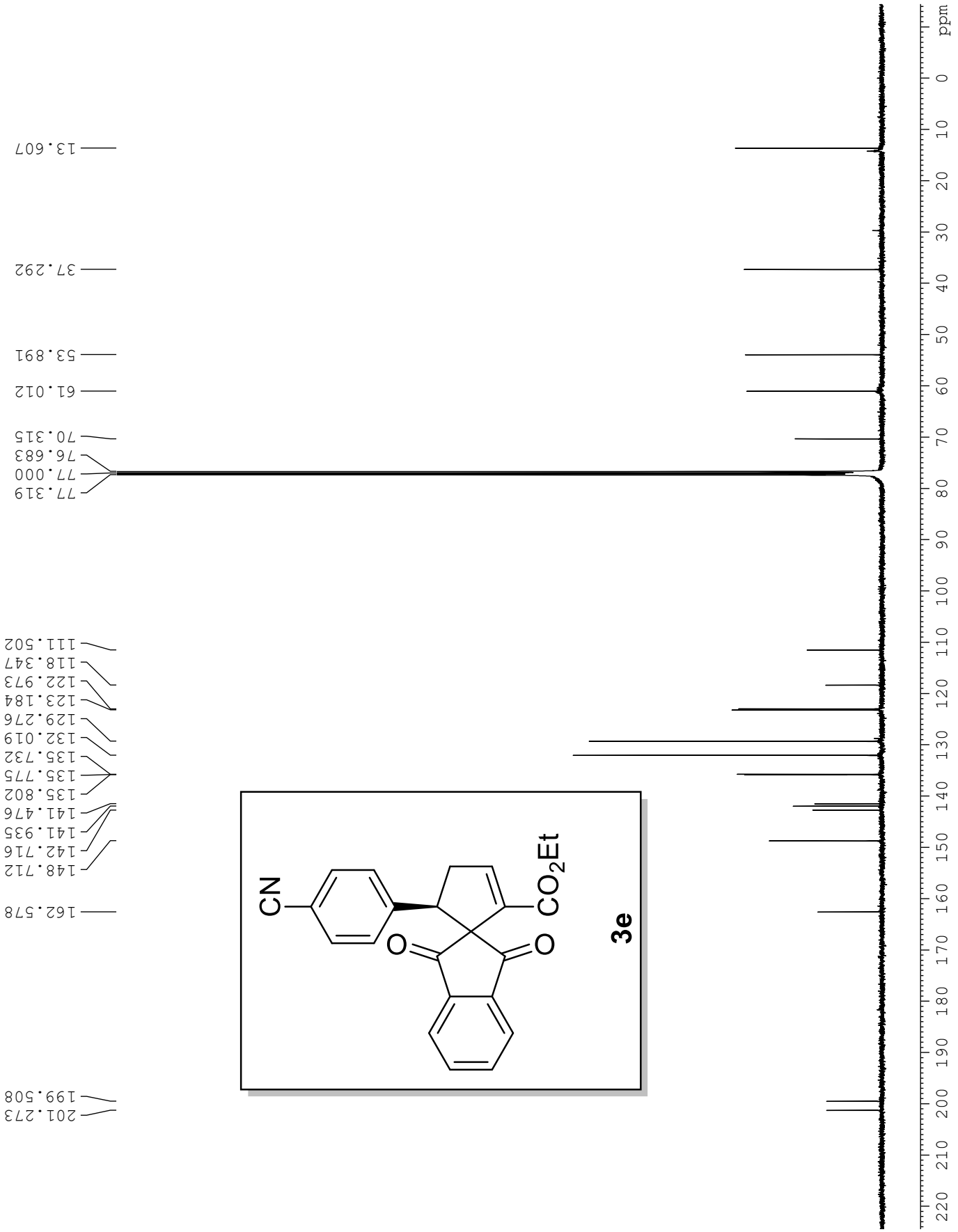
^{1}H NMR for compound 4d



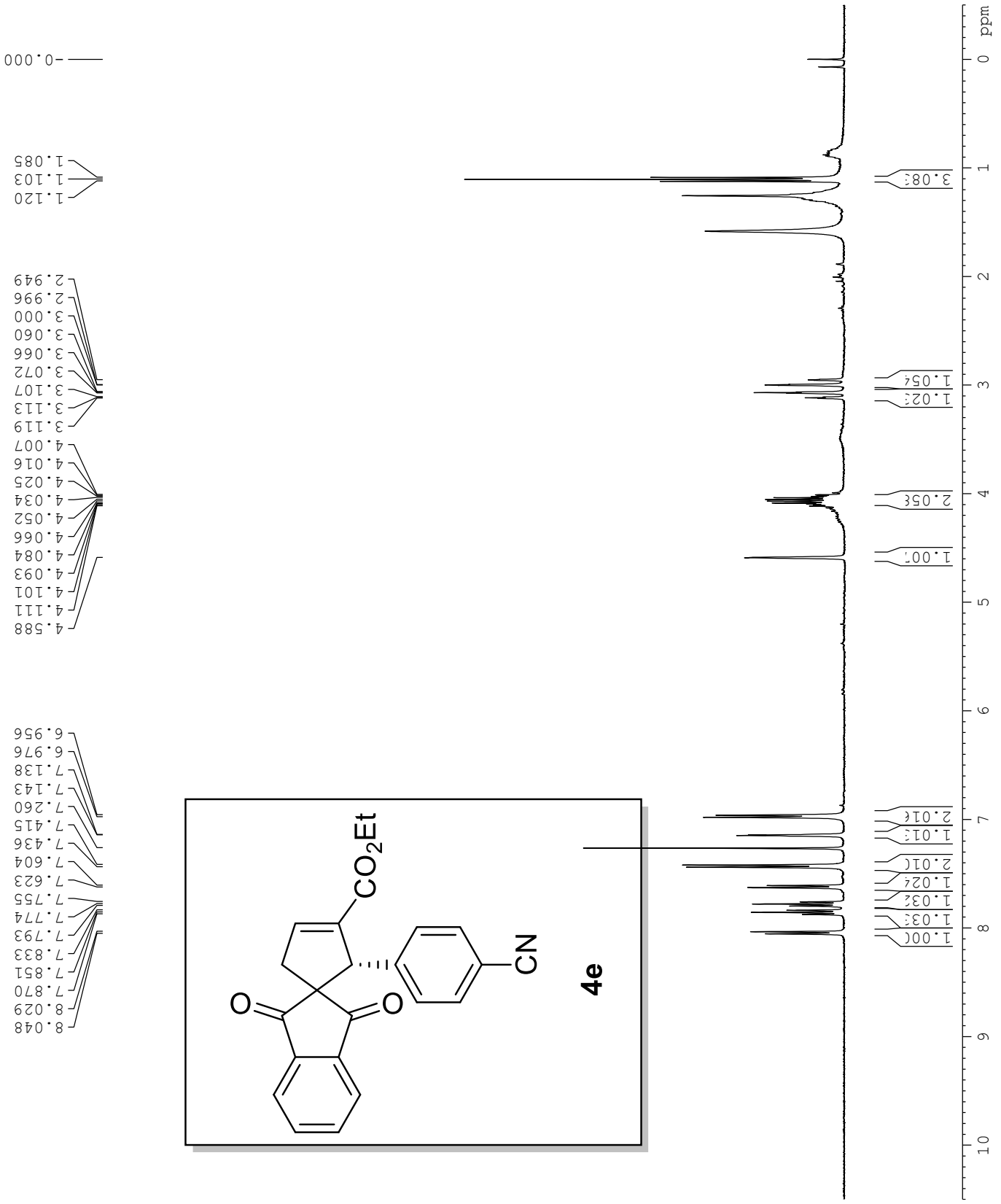
^{13}C NMR for compound 4d



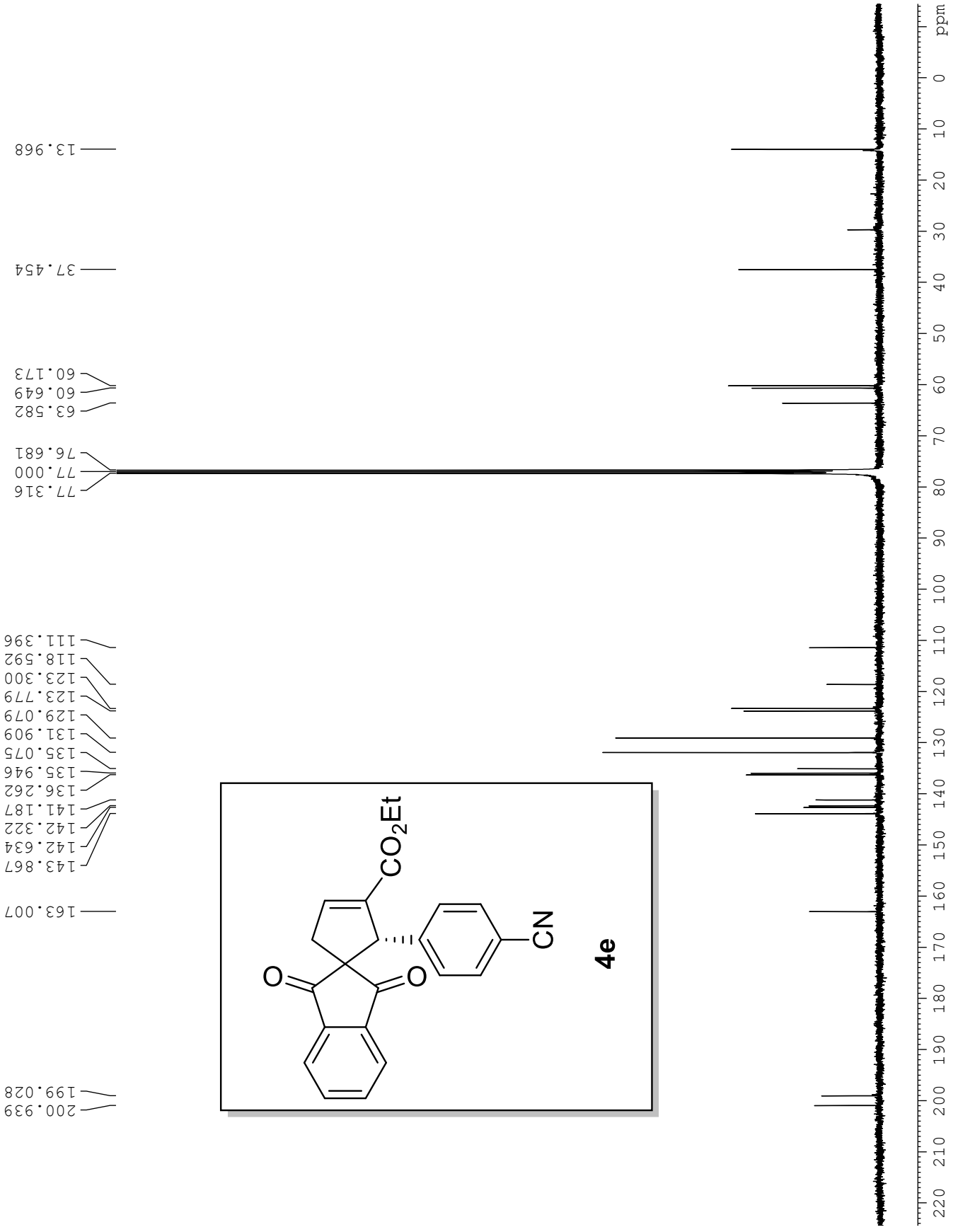
^{1}H NMR for compound 3e



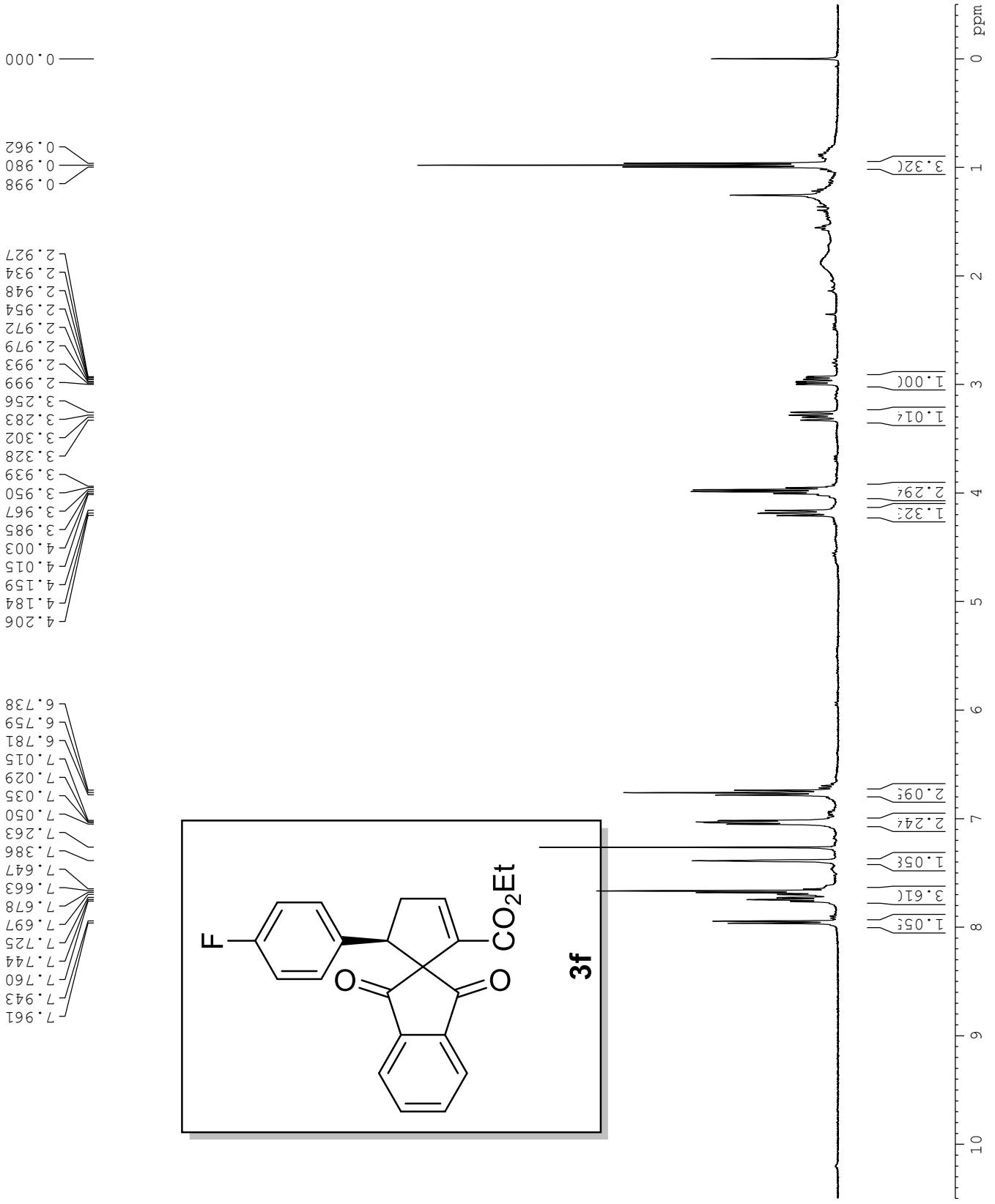
^{13}C NMR for compound 3e



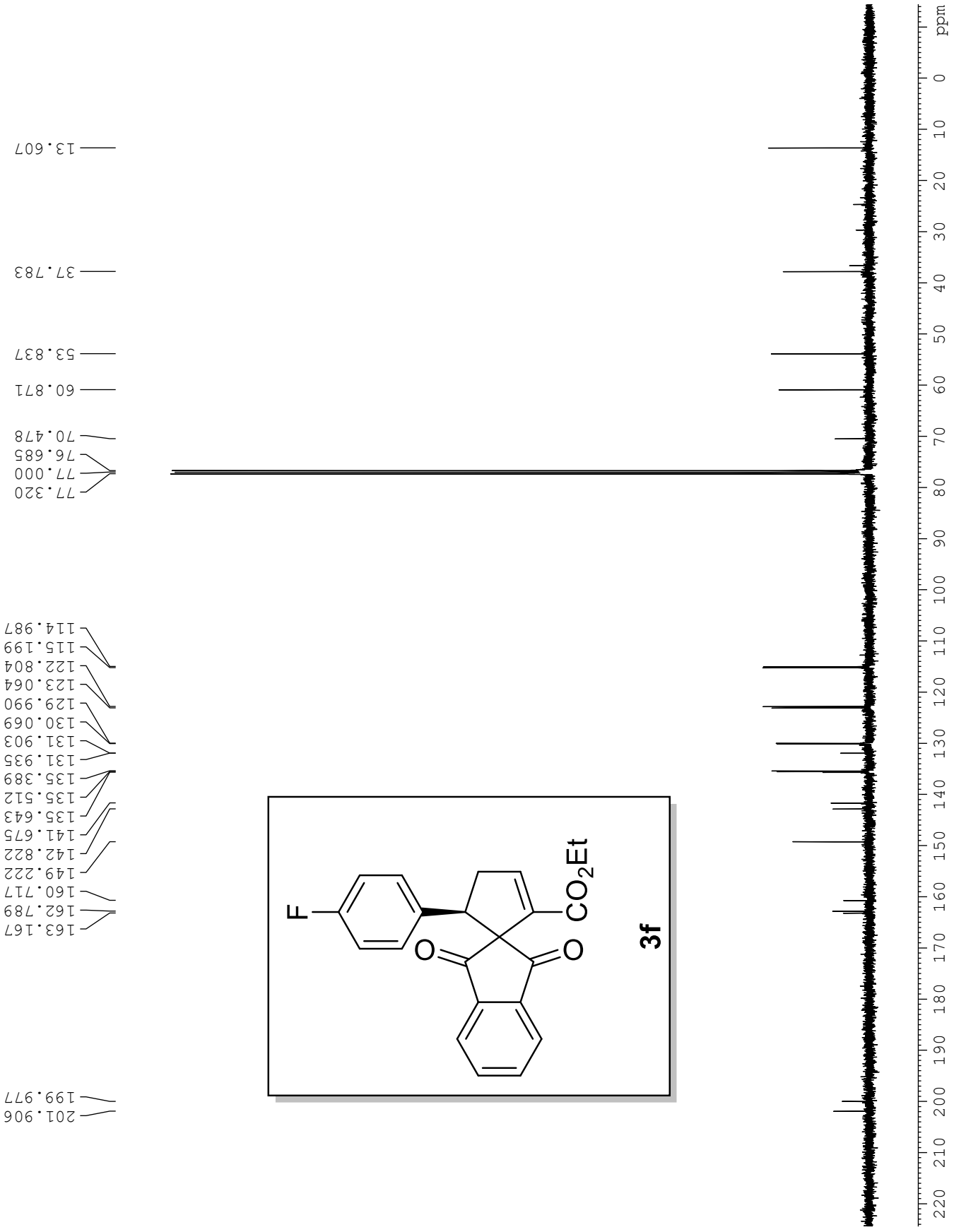
^{1}H NMR for compound 4e



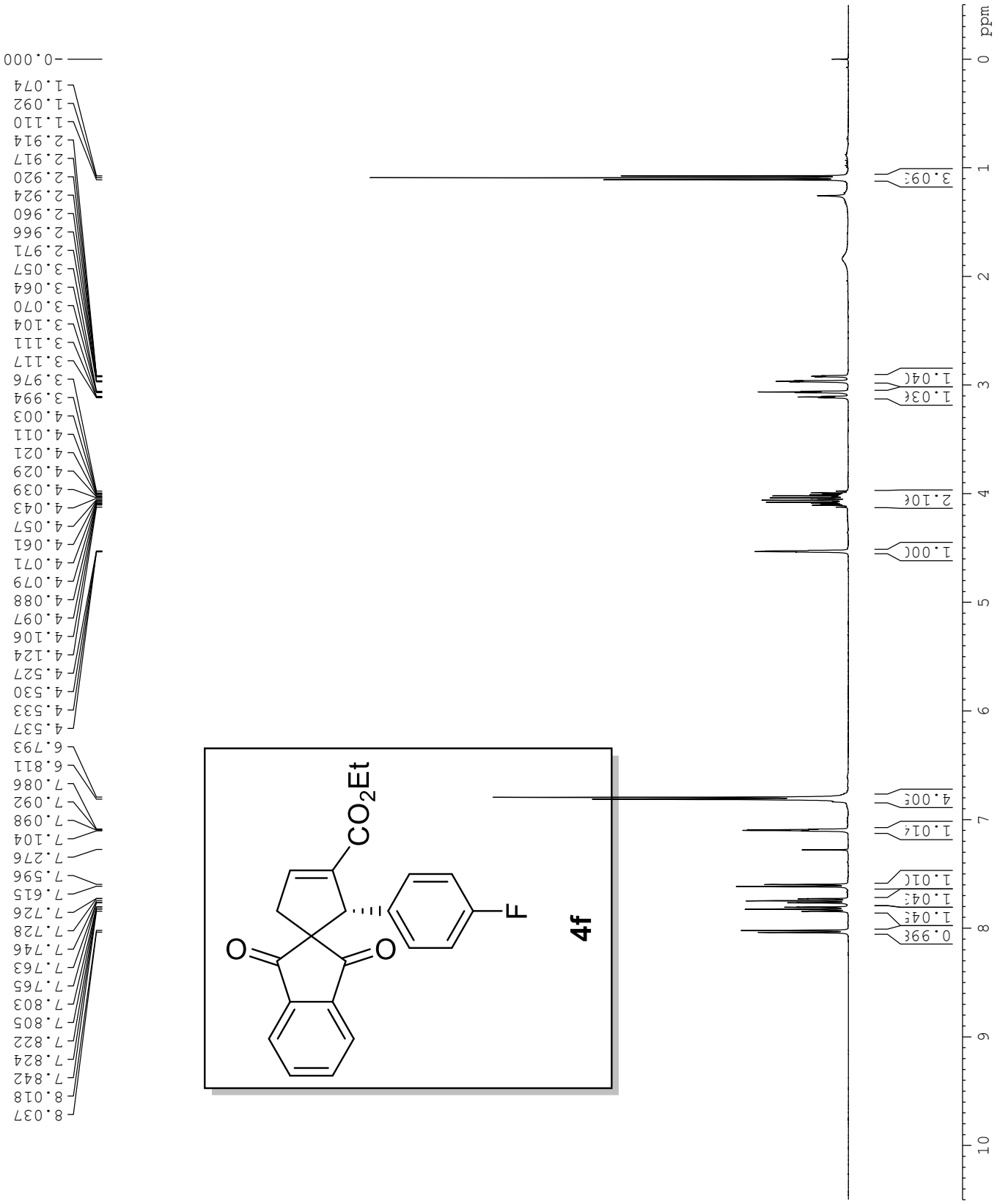
^{13}C NMR for compound 4e



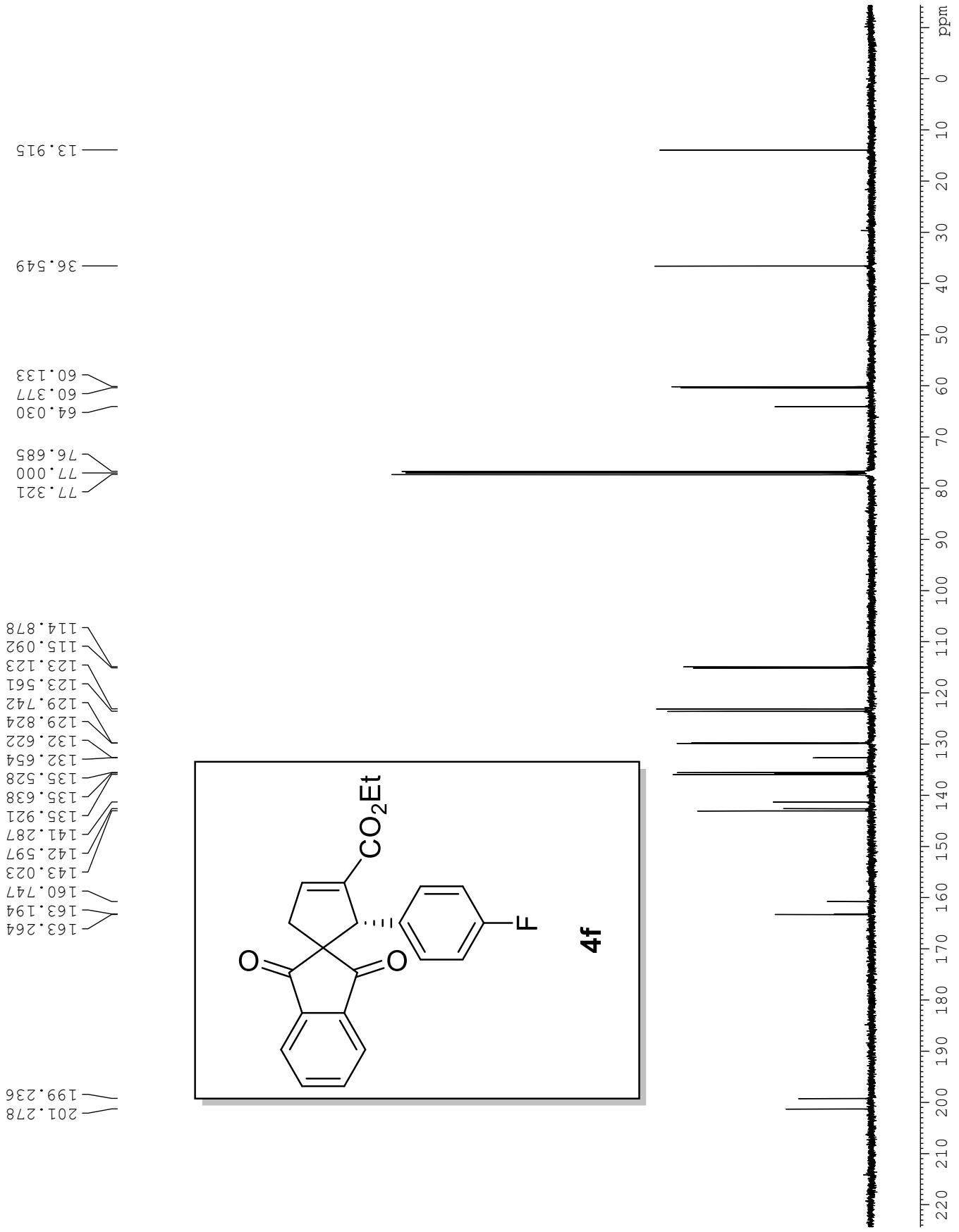
[1]H NMR for compound 3f



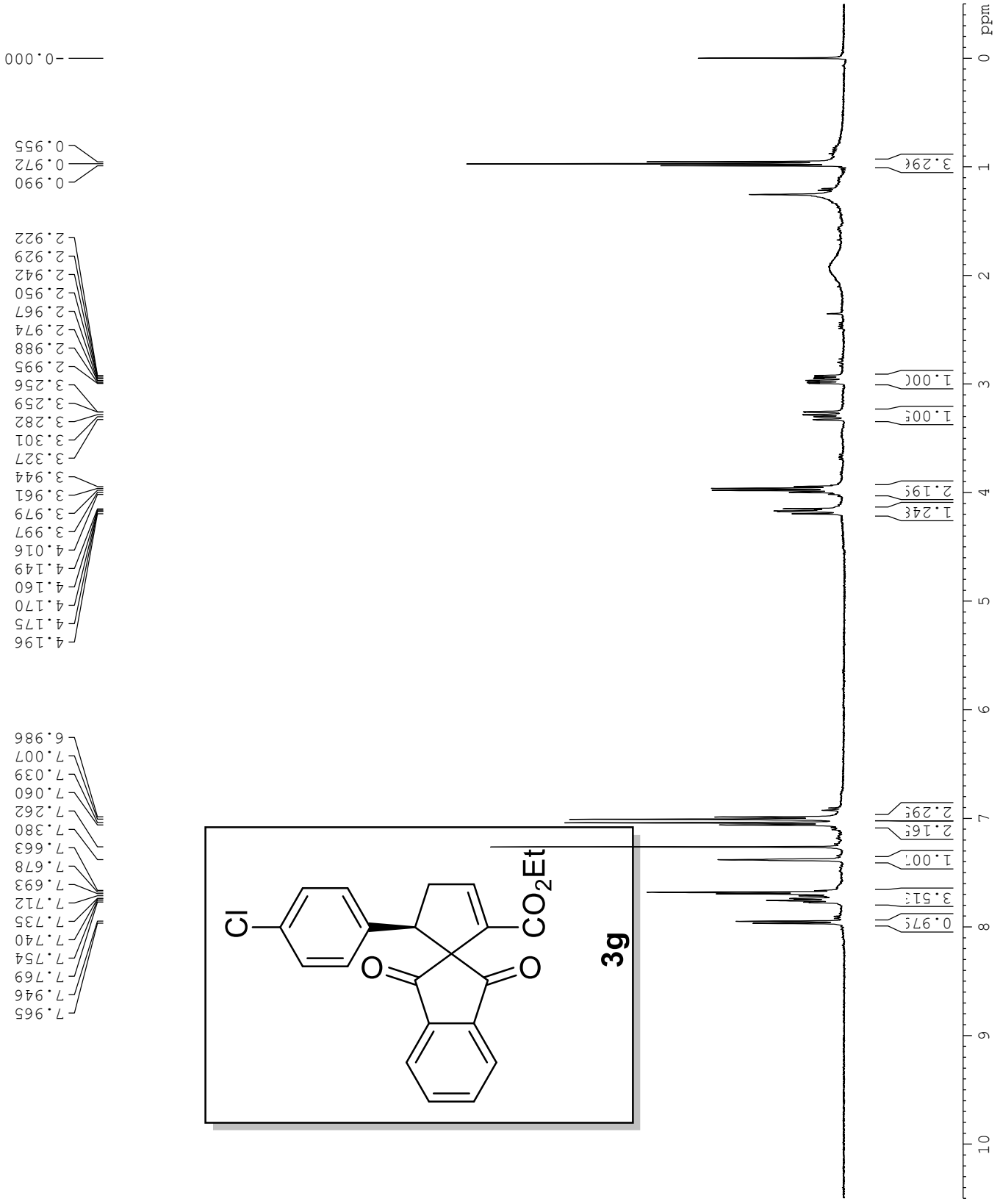
^{13}C NMR for compound 3f



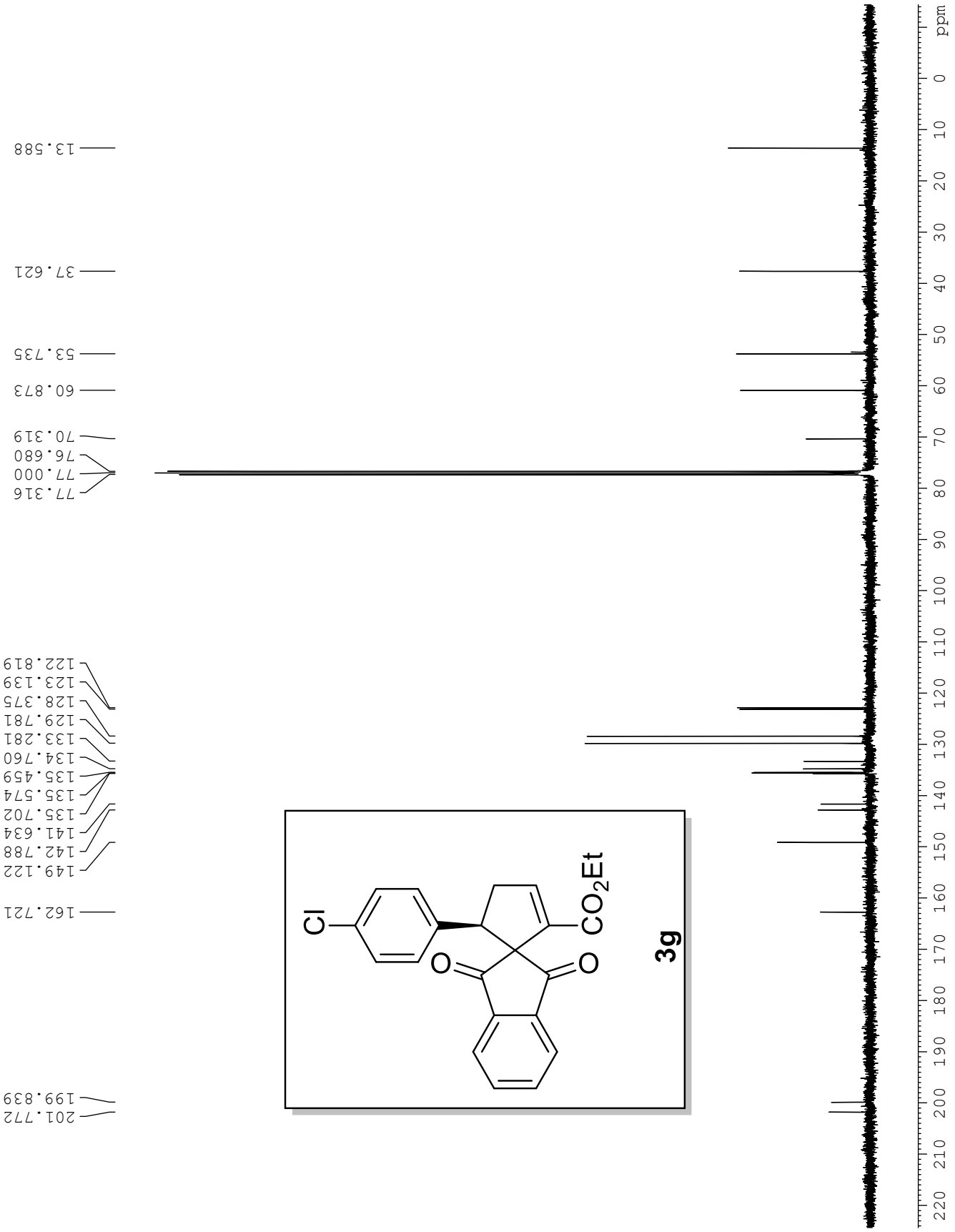
^{1}H NMR for compound 4f



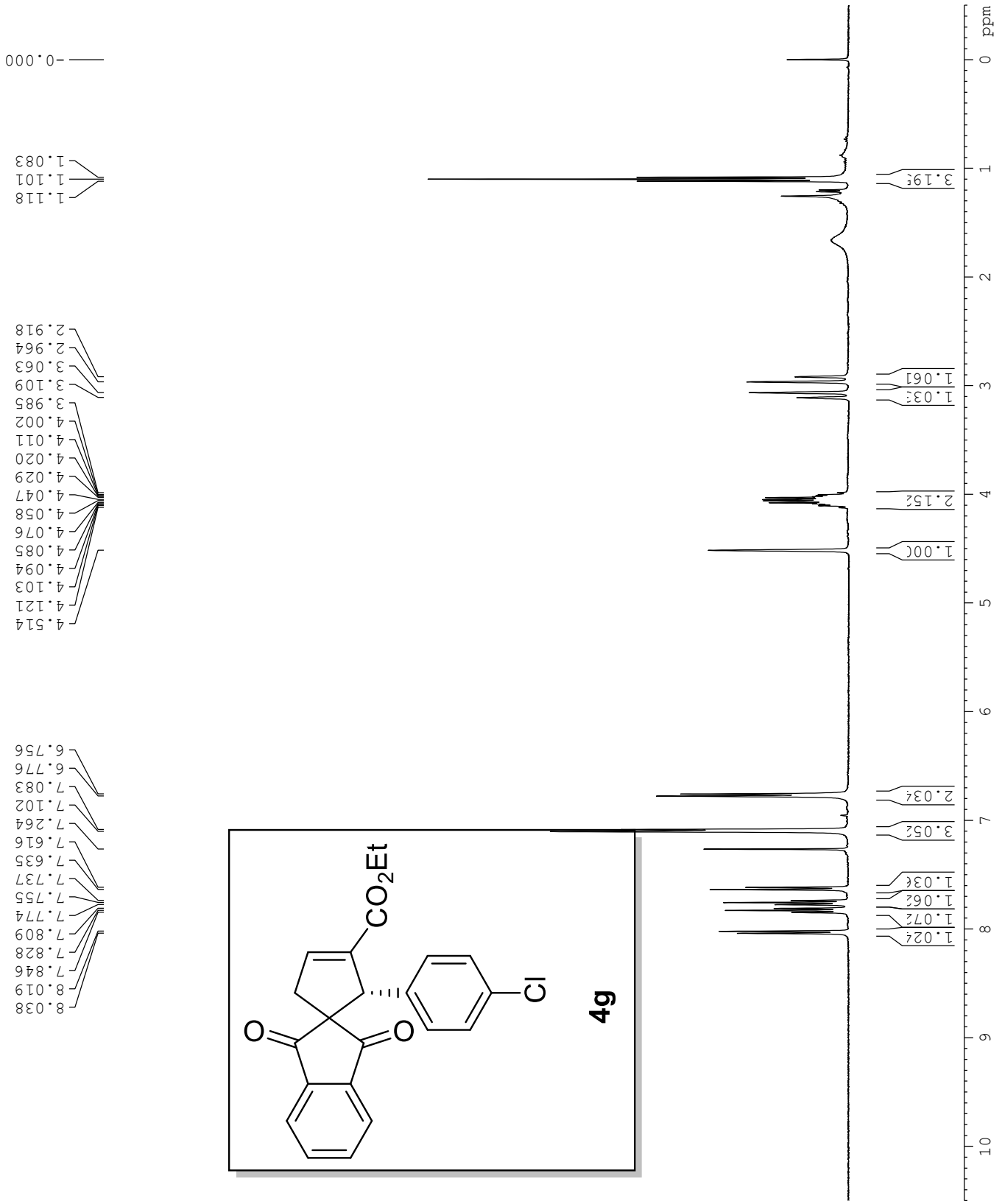
^{13}C NMR for compound 4f



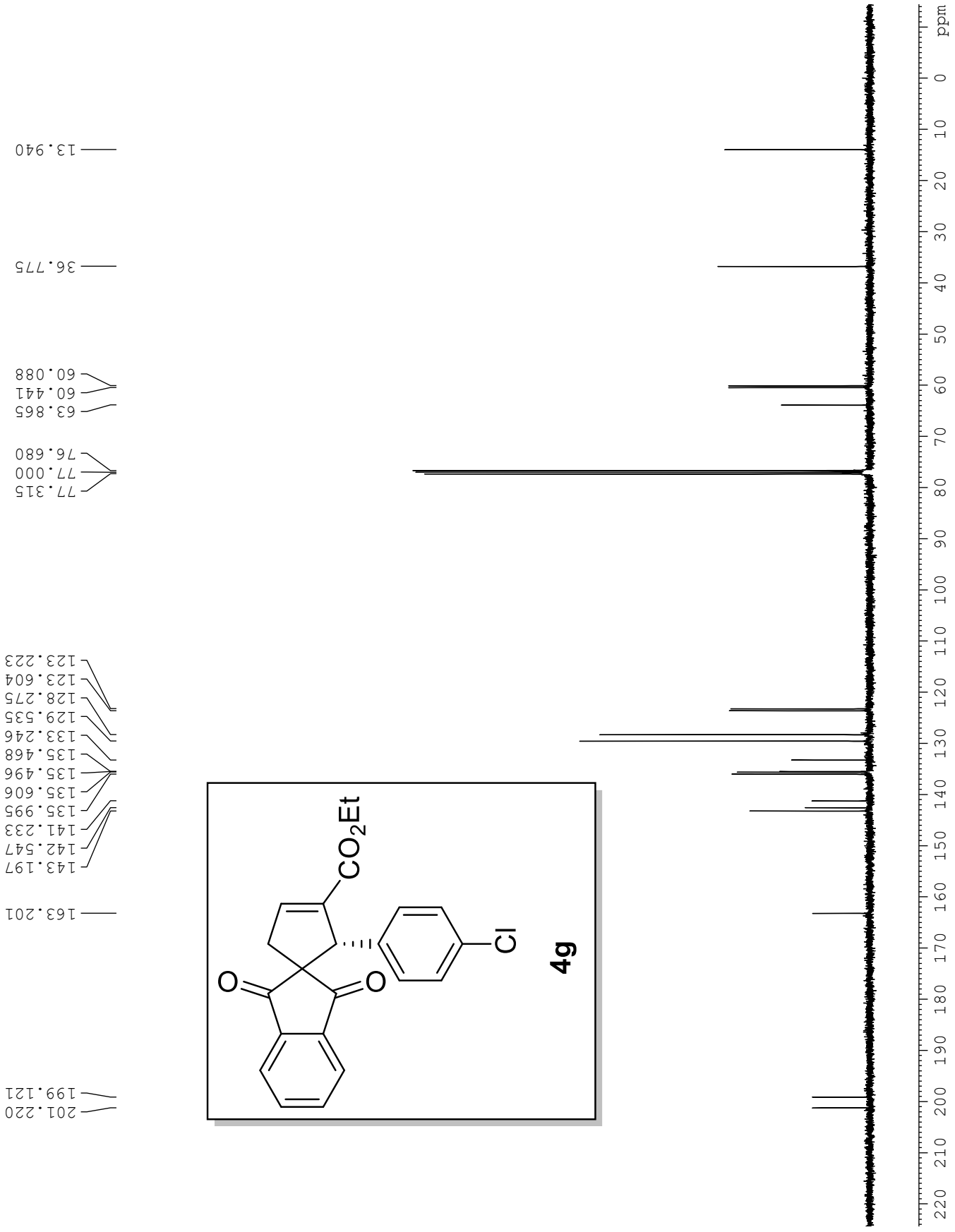
^{1}H NMR for compound 3g



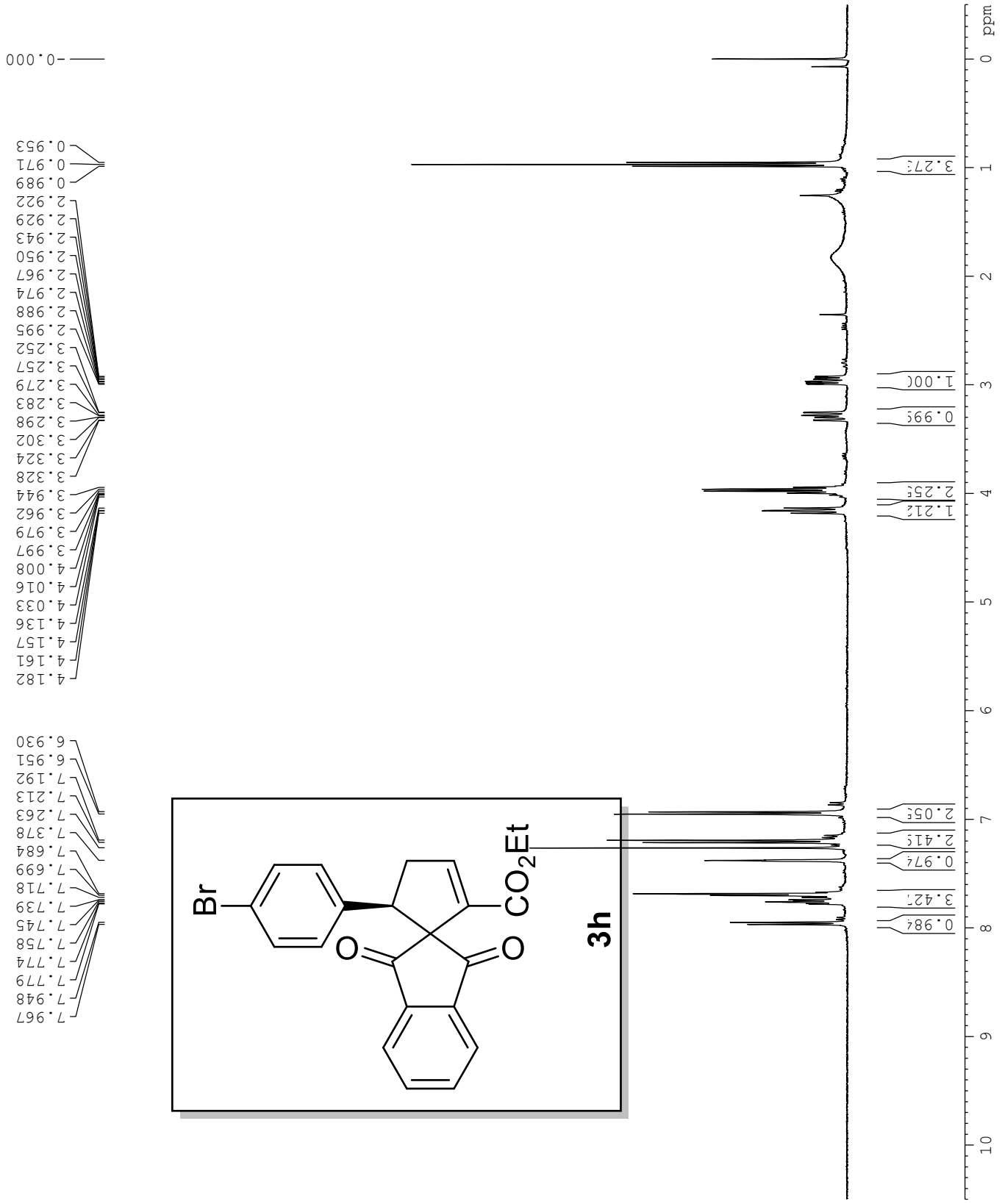
^{13}C NMR for compound 3g



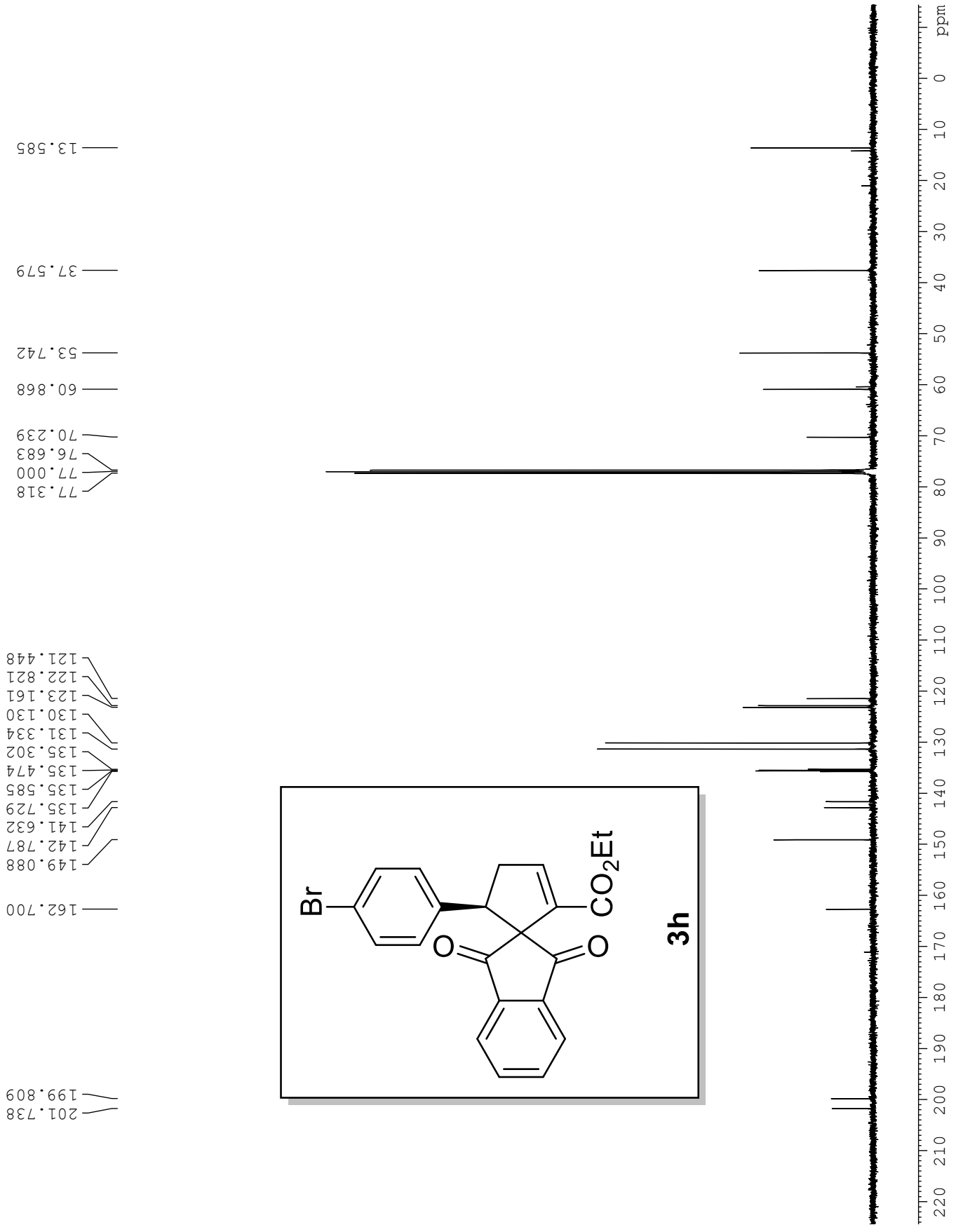
^{1}H NMR for compound 4g



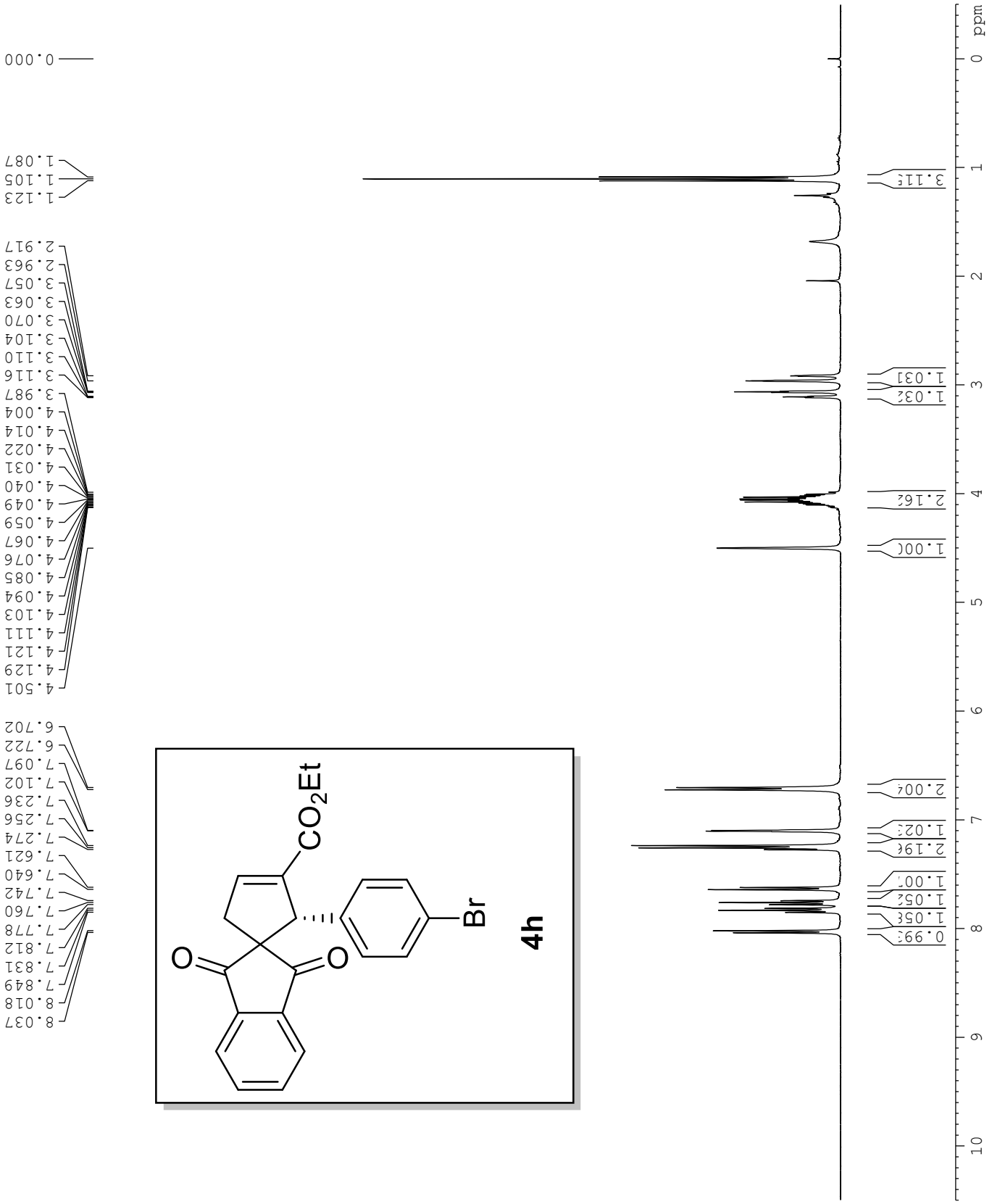
^{13}C NMR for compound 4g



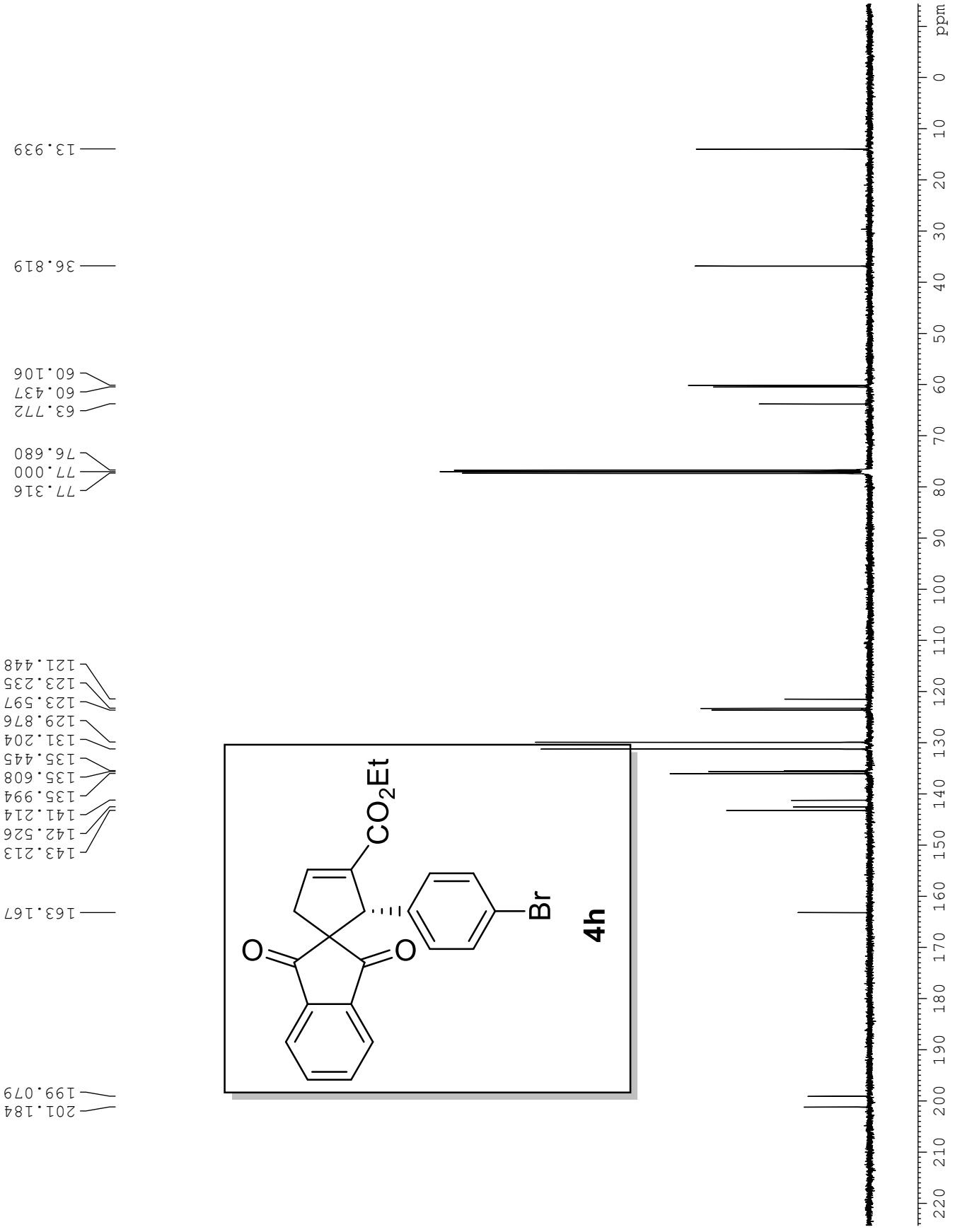
^{1}H NMR for compound 3h



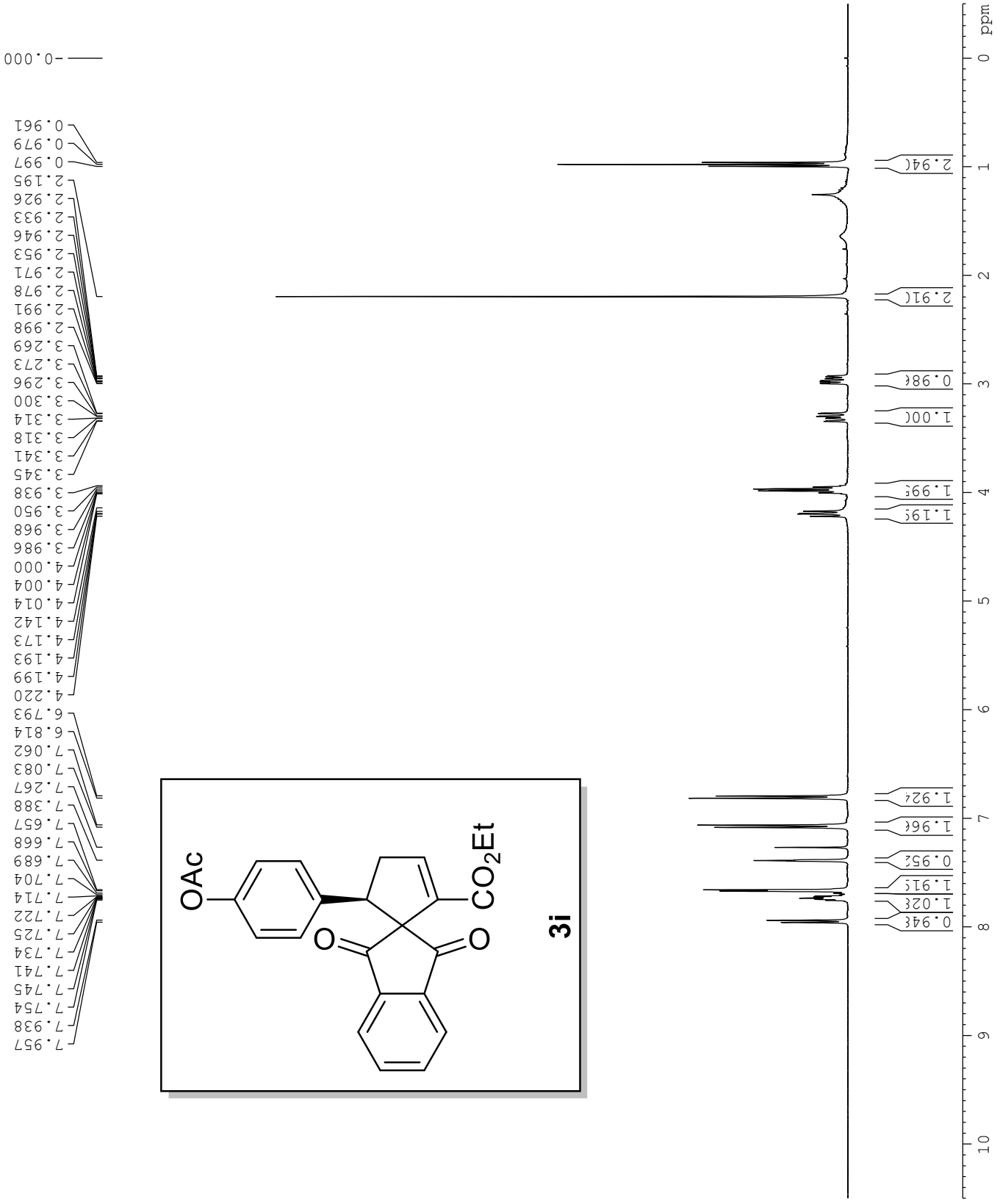
^{13}C NMR for compound 3h



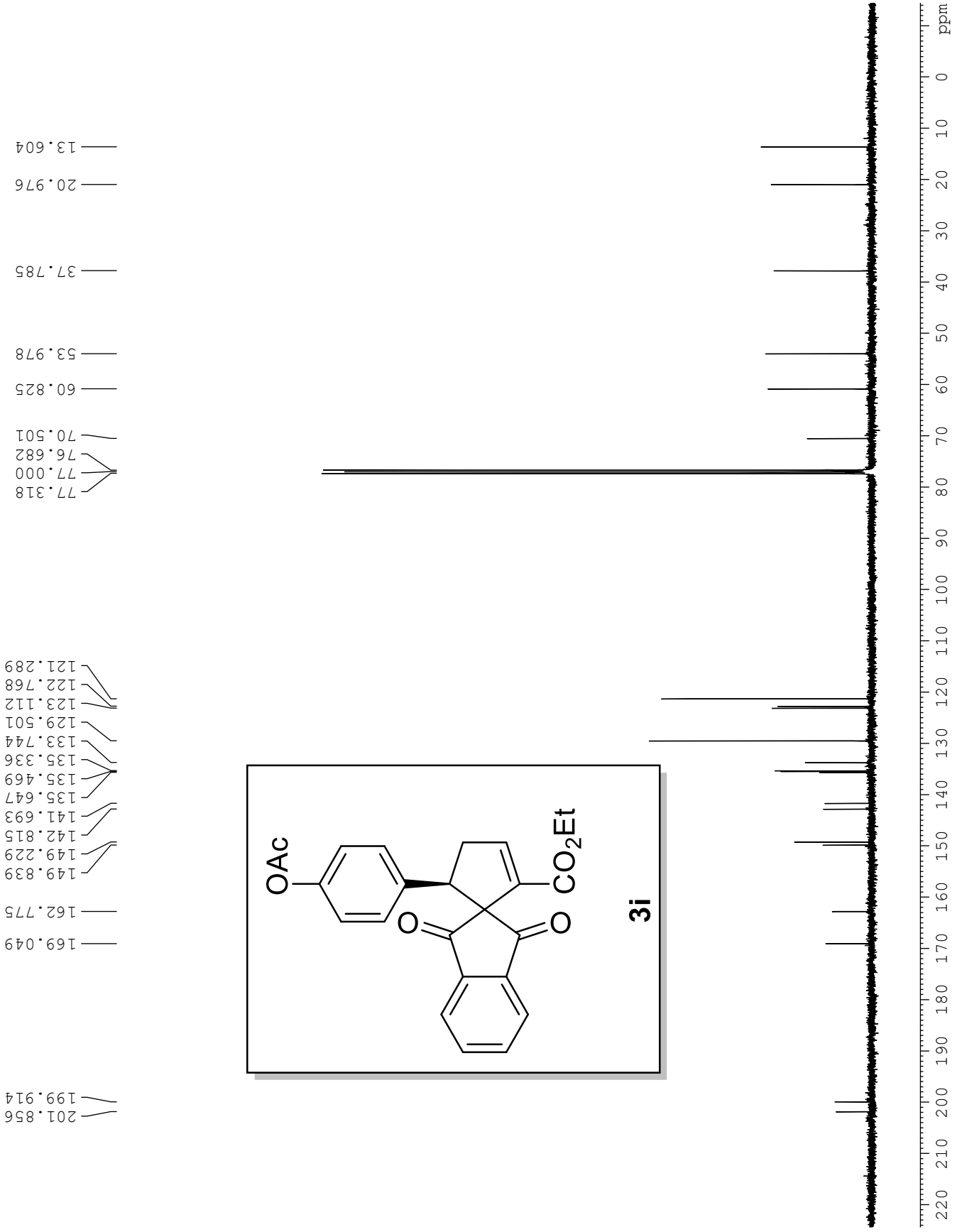
^{1}H NMR for compound 4h



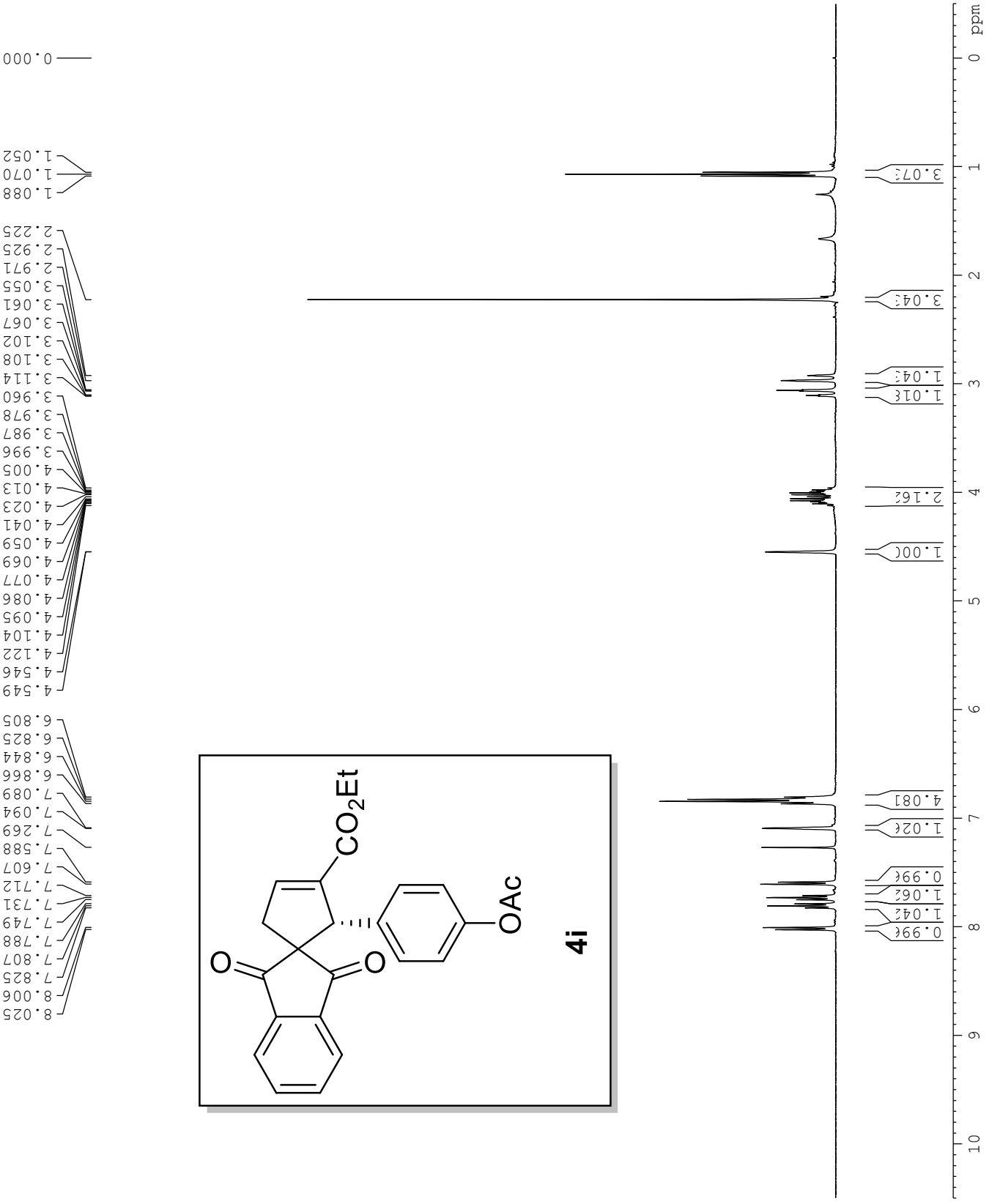
^{13}C NMR for compound 4h



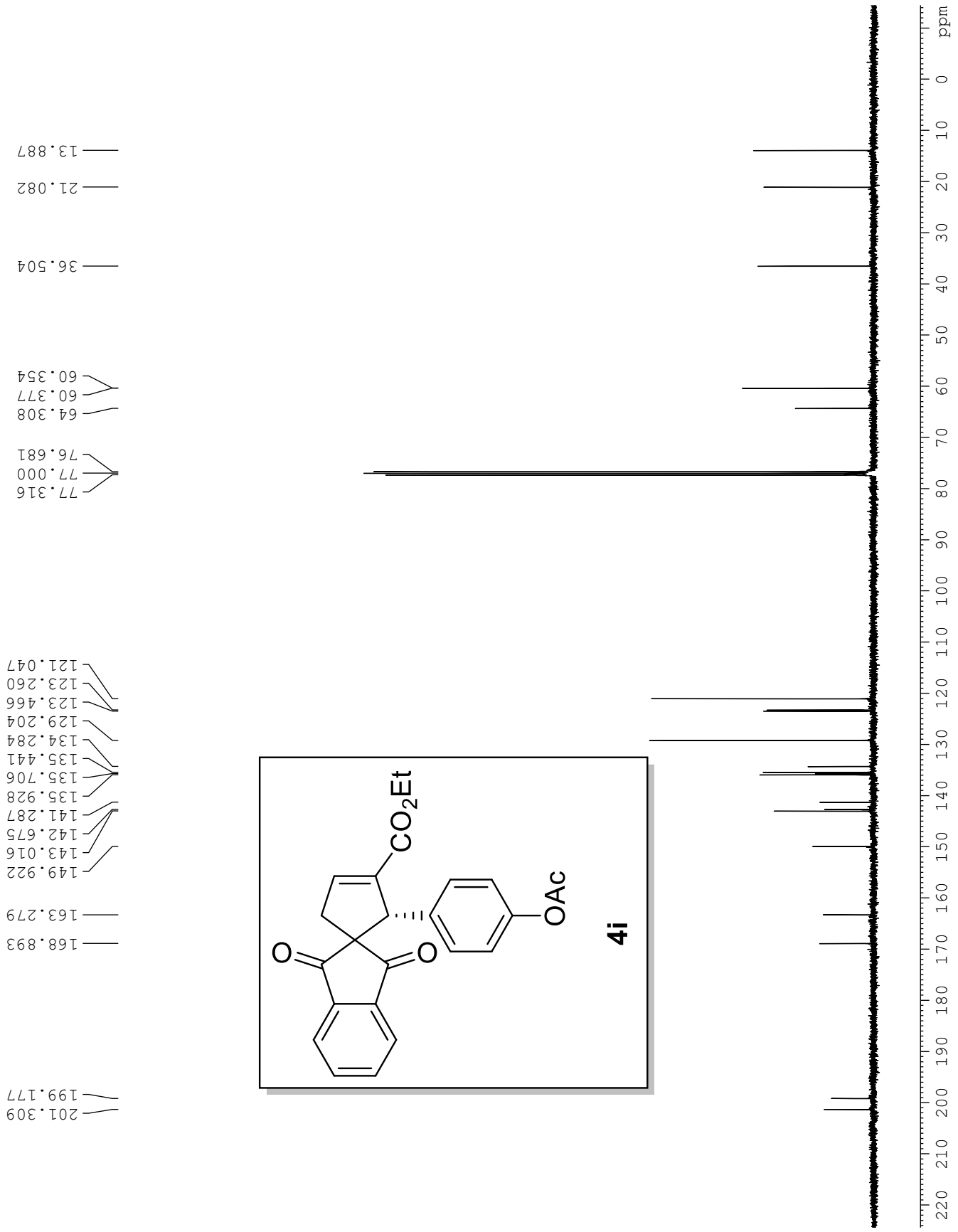
^{1}H NMR for compound 3i



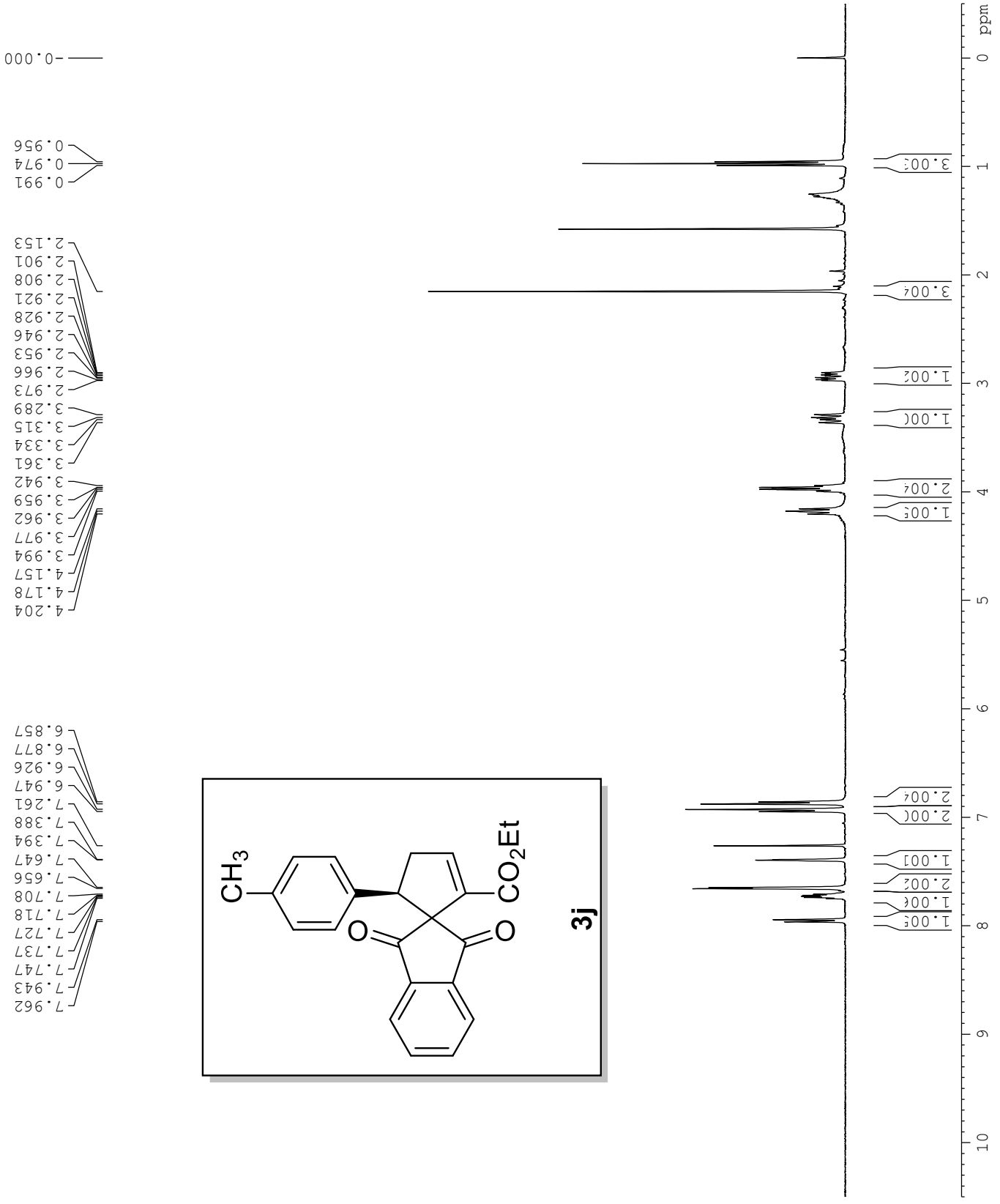
^{13}C NMR for compound 3i



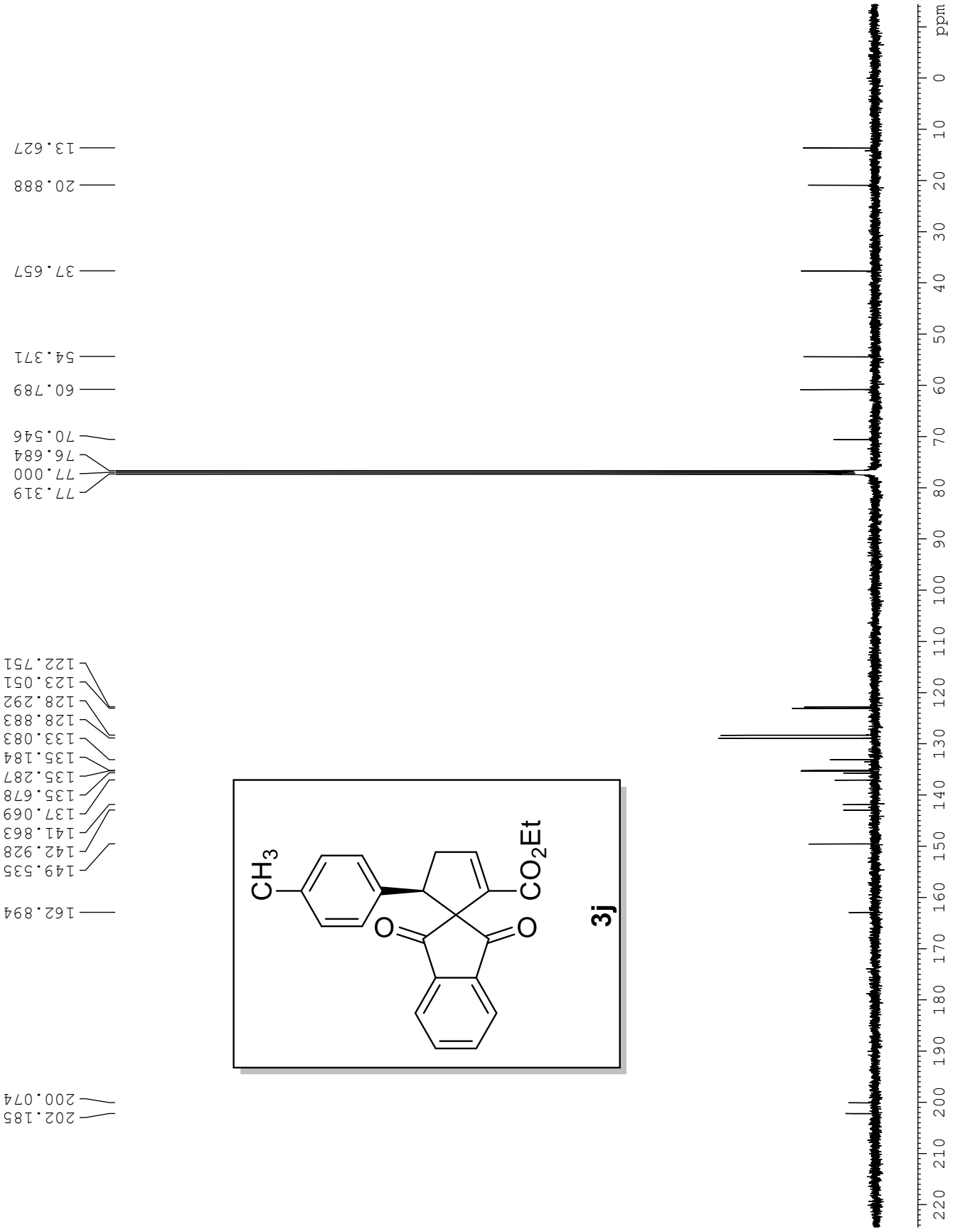
[1]H NMR for compound 4i



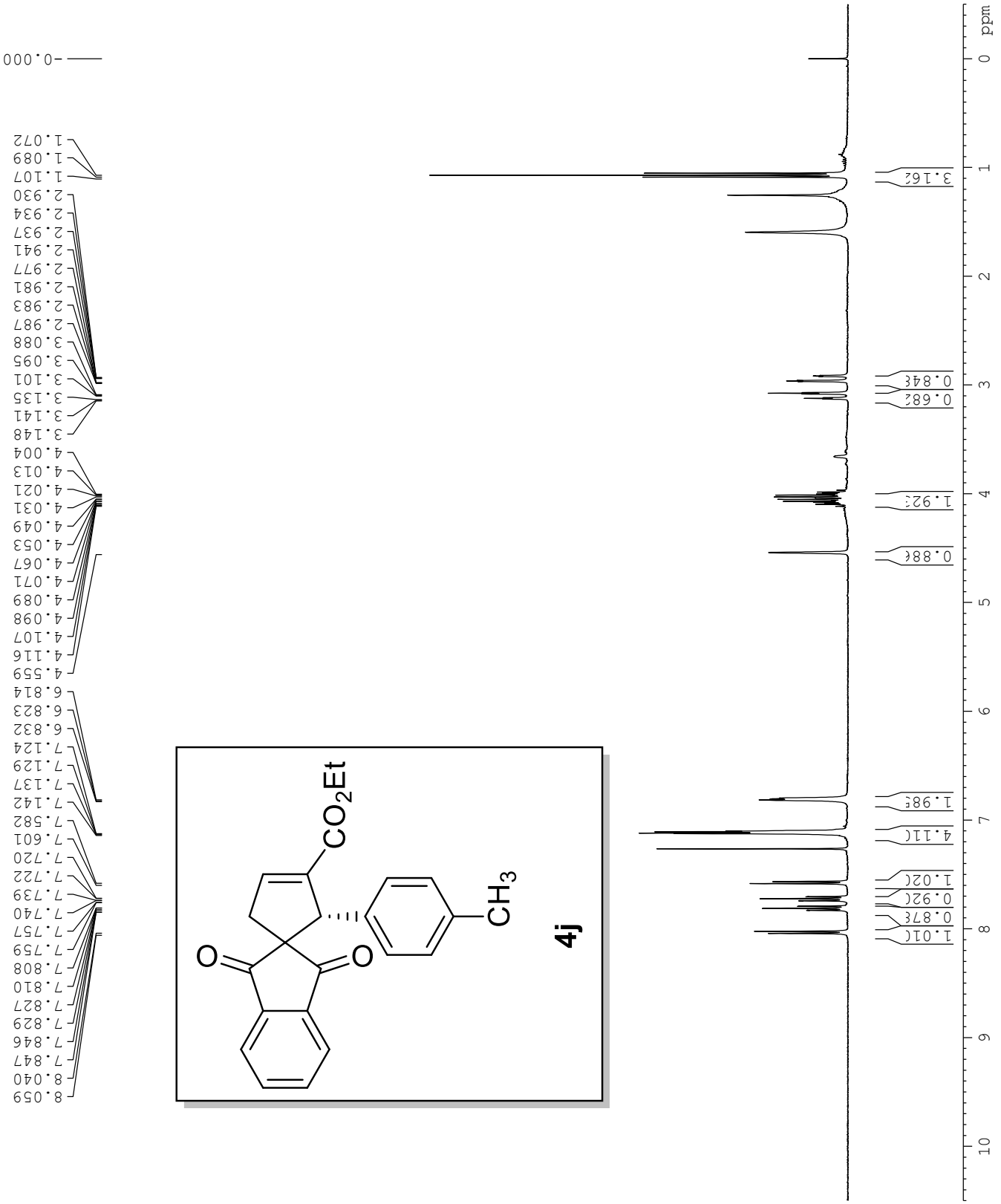
^{13}C NMR for compound 4i



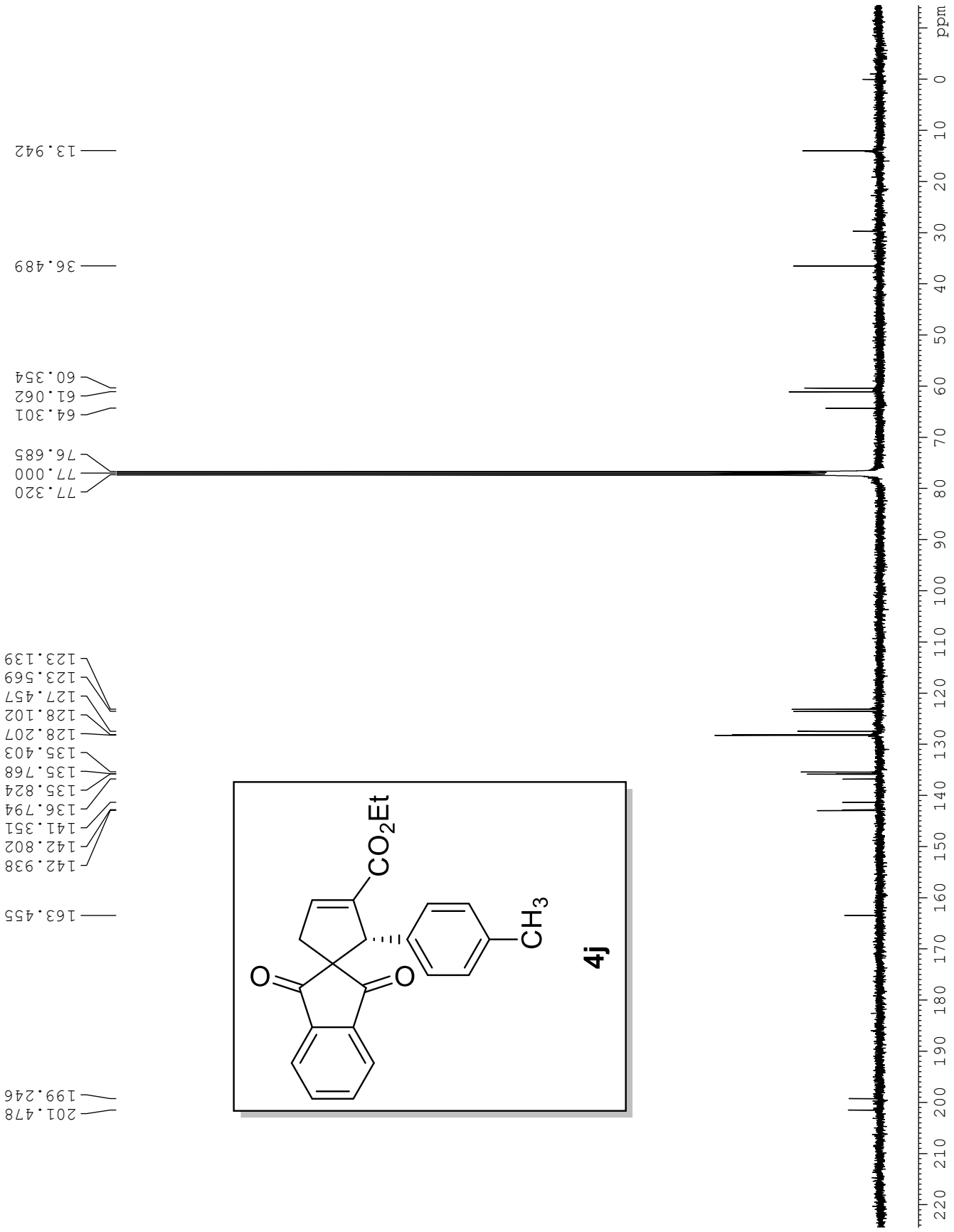
^{1}H NMR for compound 3j



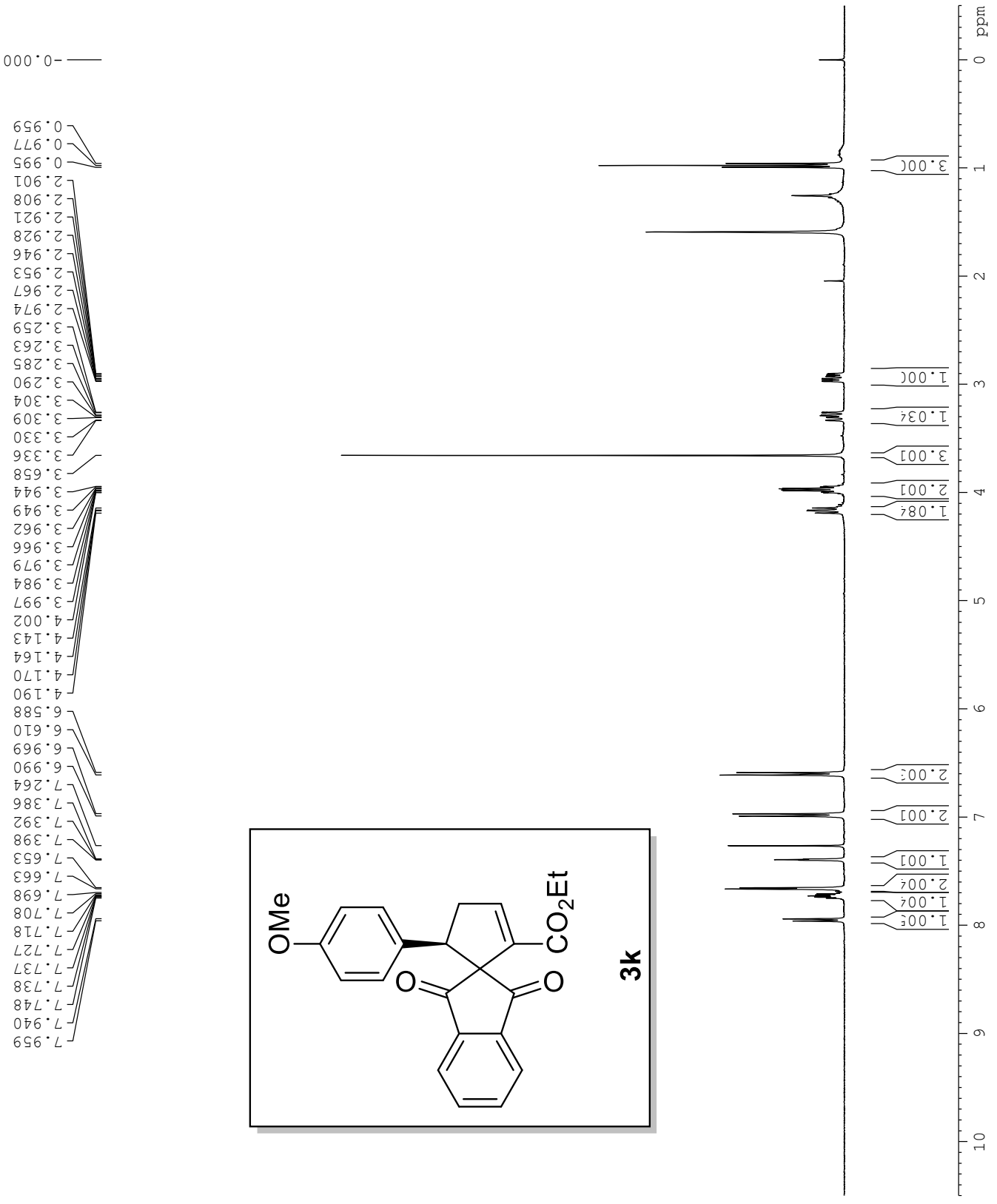
^{13}C NMR for compound 3j



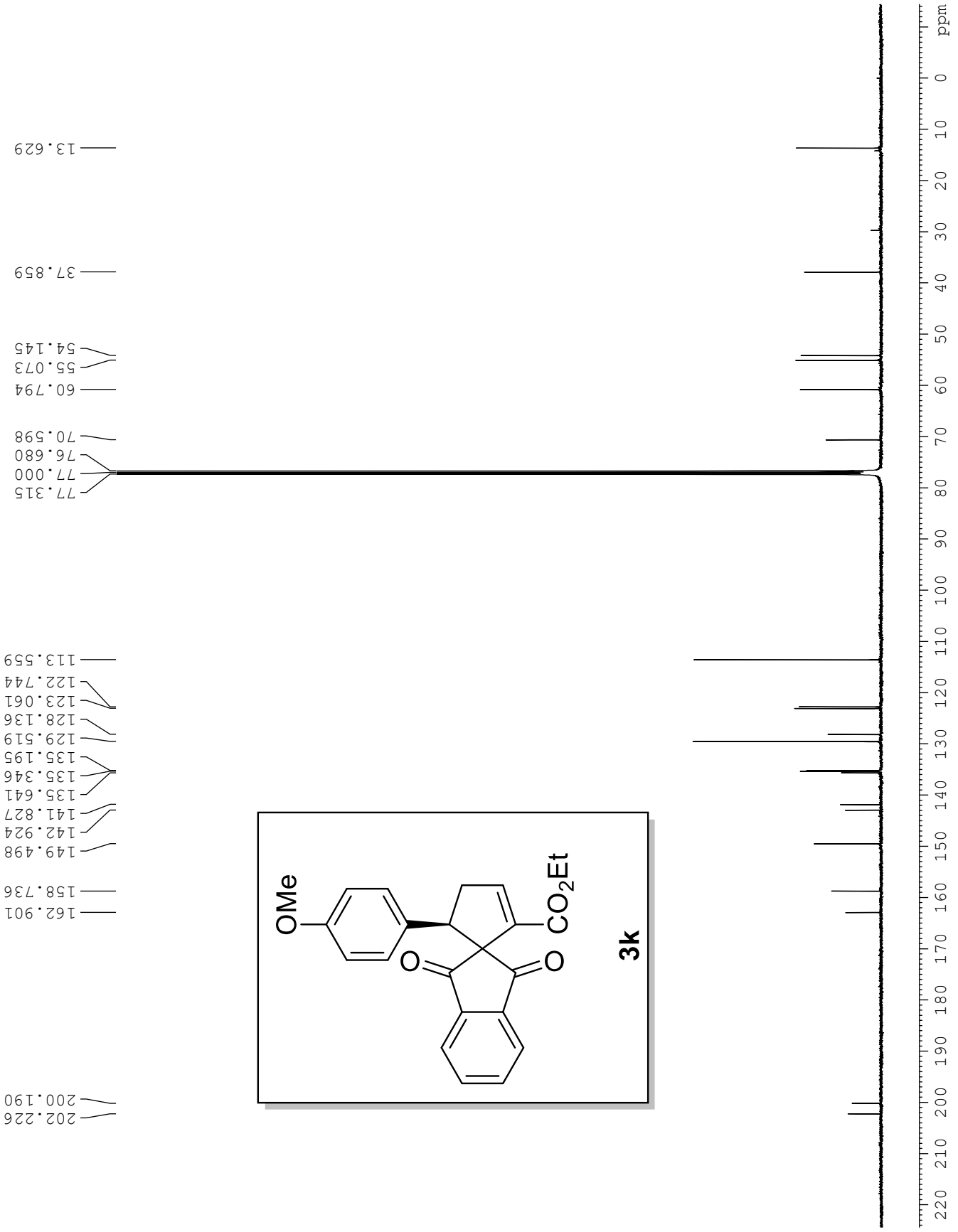
^{1}H NMR for compound 4j



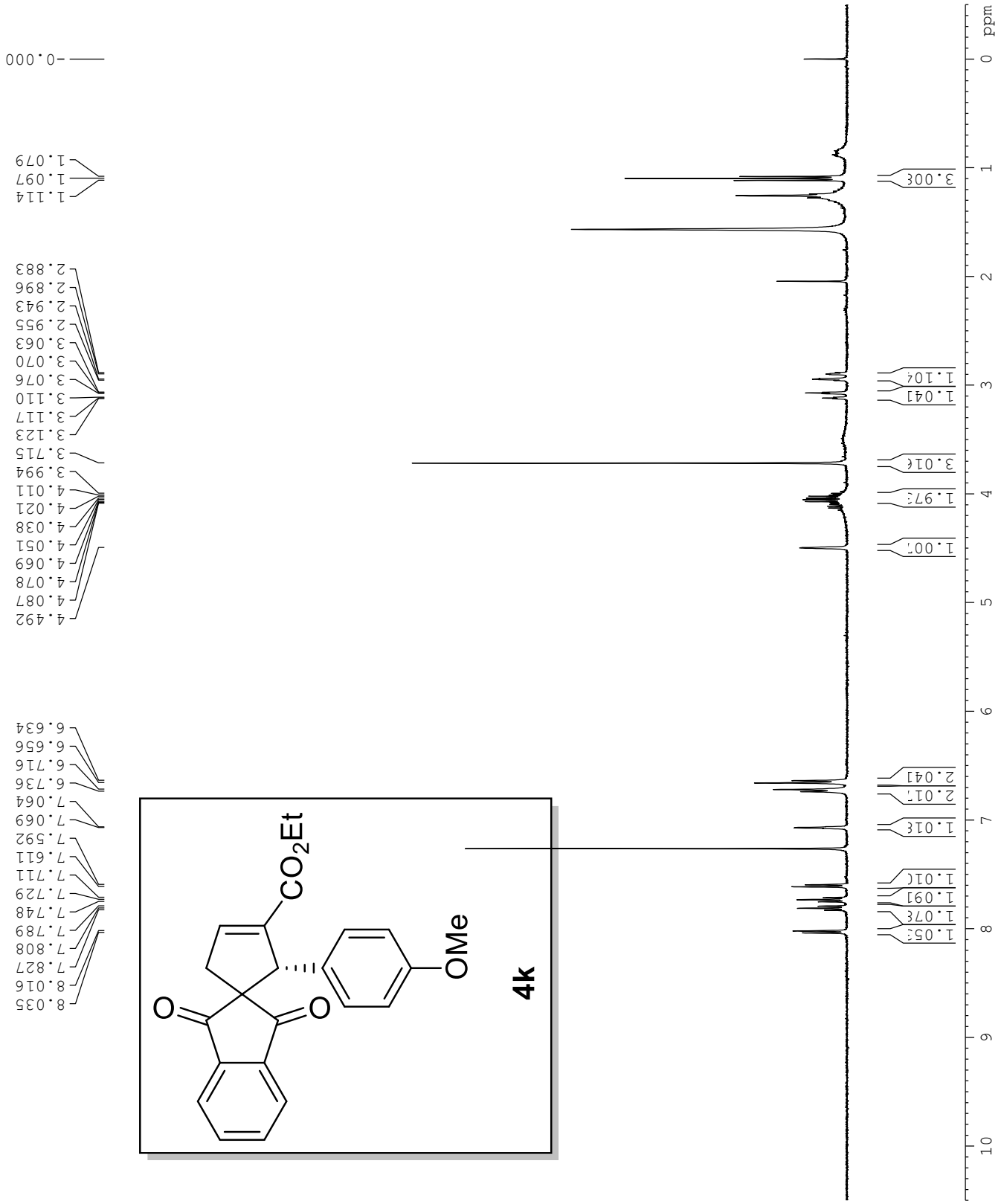
^{13}C NMR for compound 4j



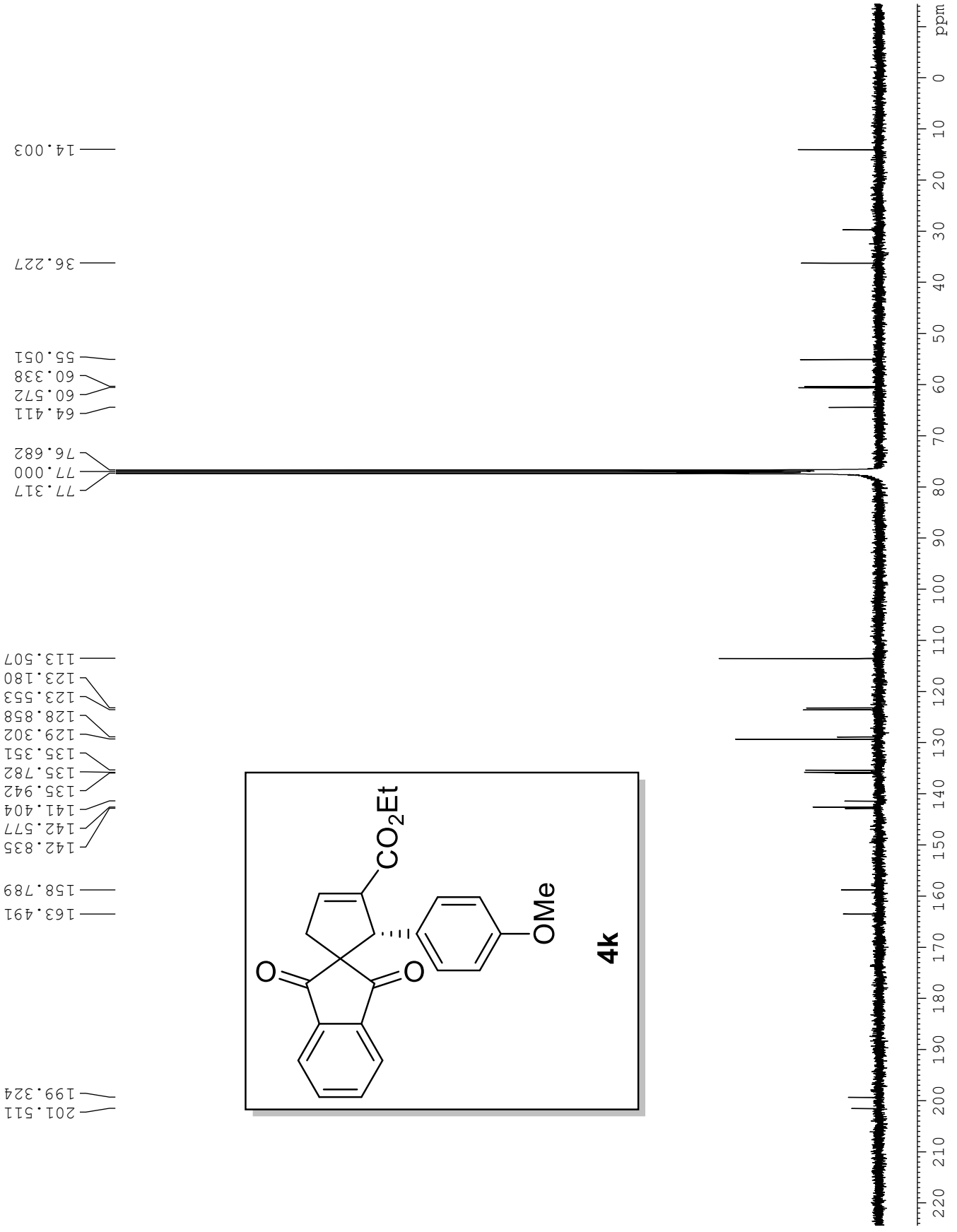
^{1}H NMR for compound 3k



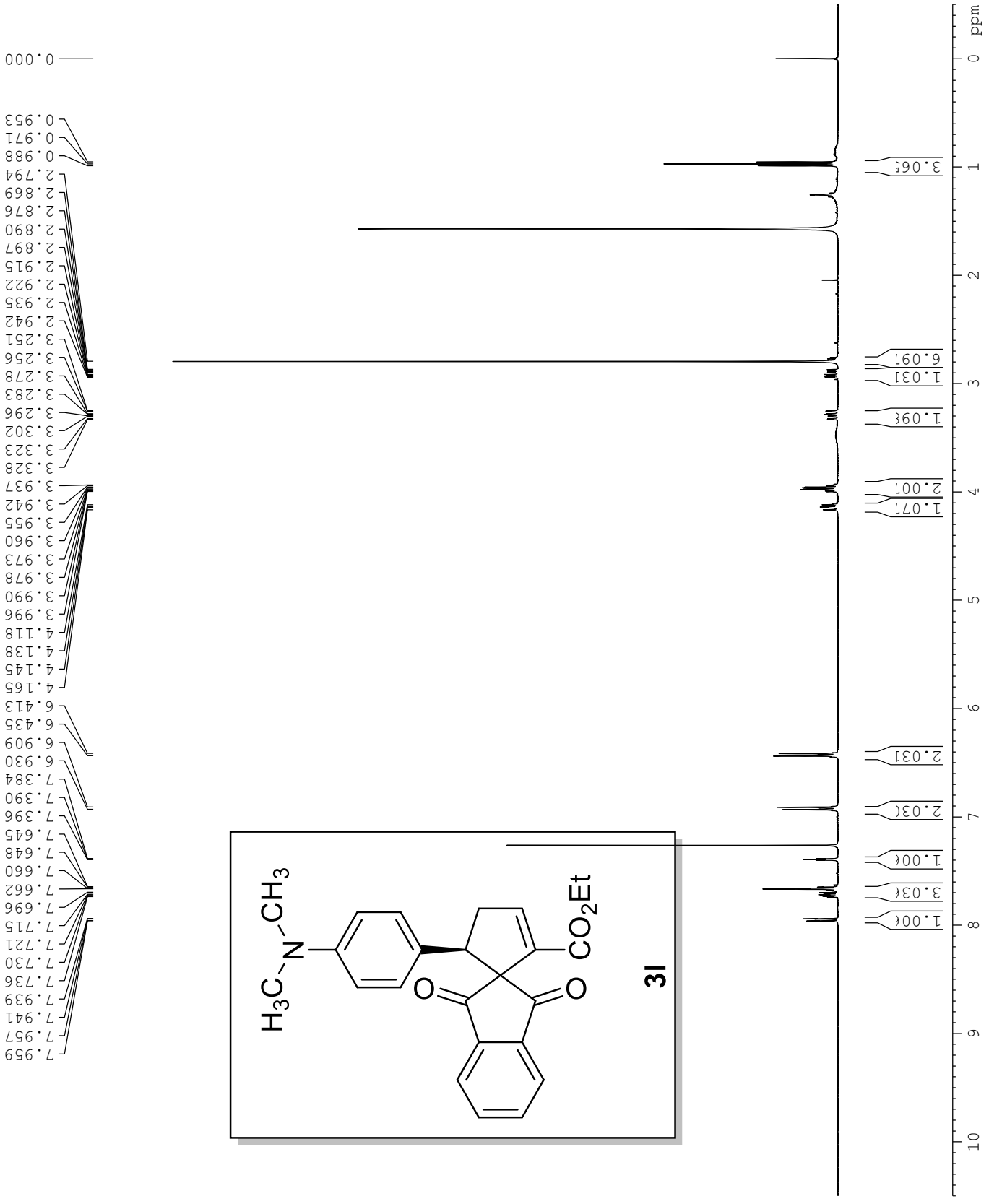
^{13}C NMR for compound 3k



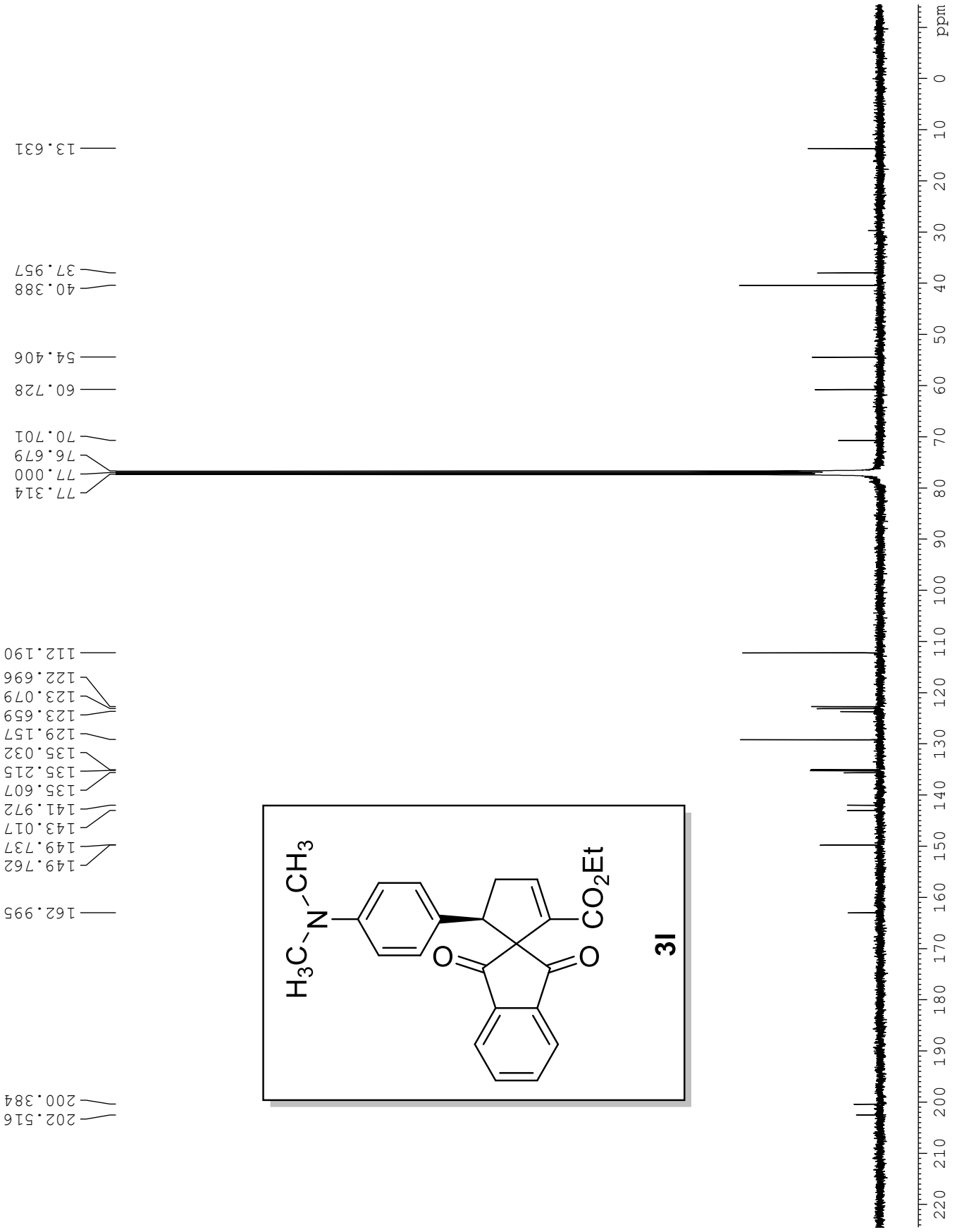
^{1}H NMR for compound 4k



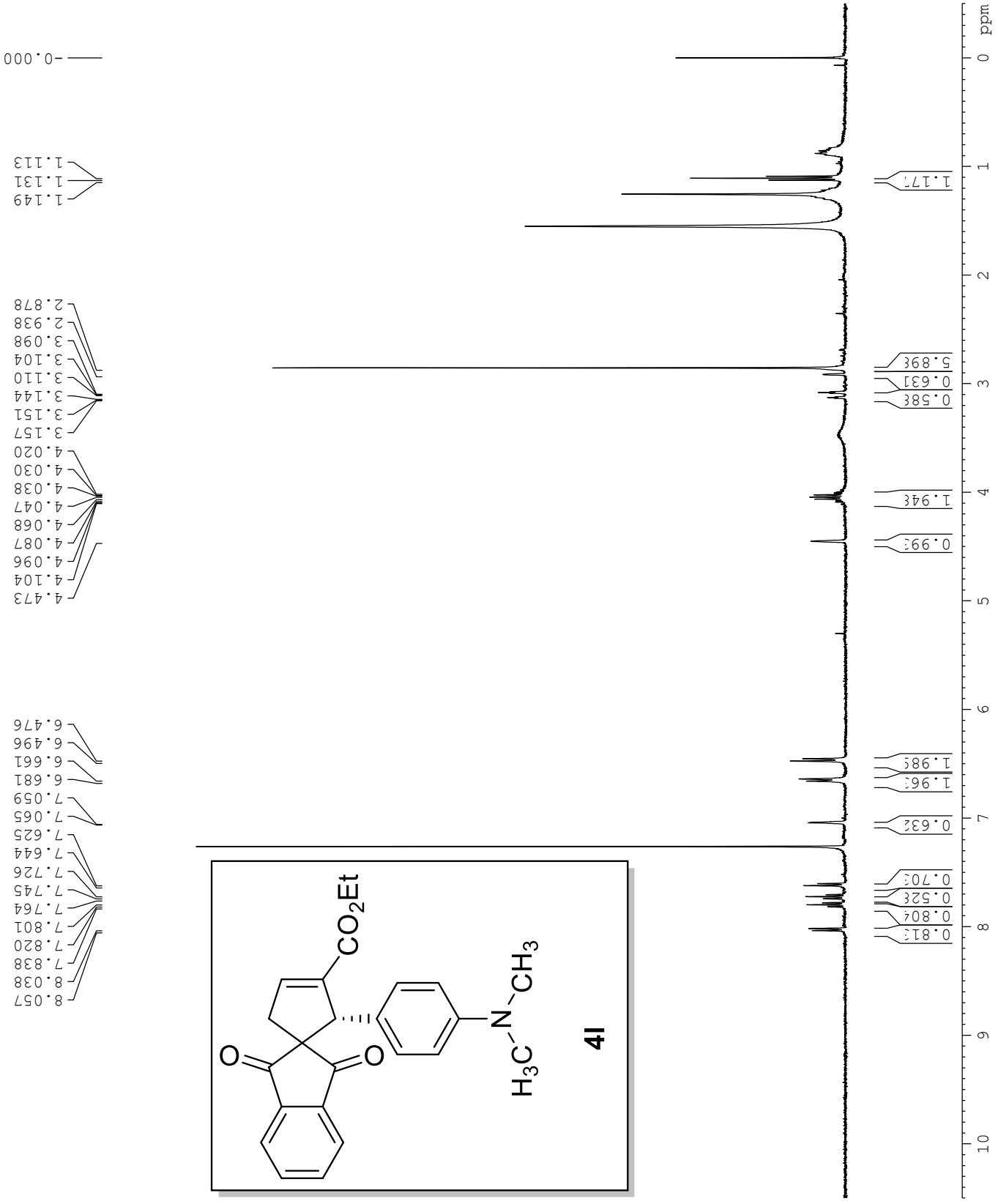
^{13}C NMR for compound 4k



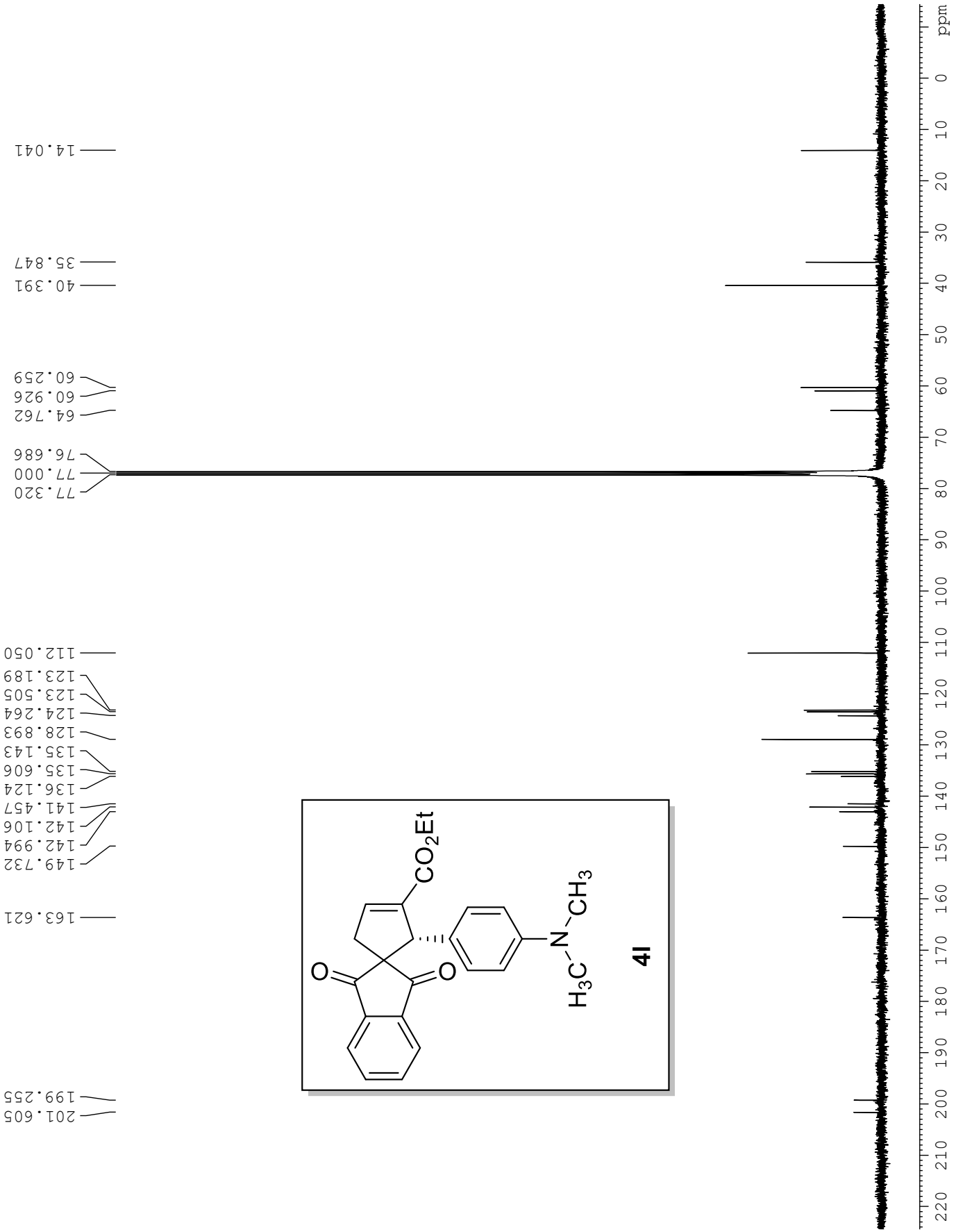
[1]H NMR for compound 3l



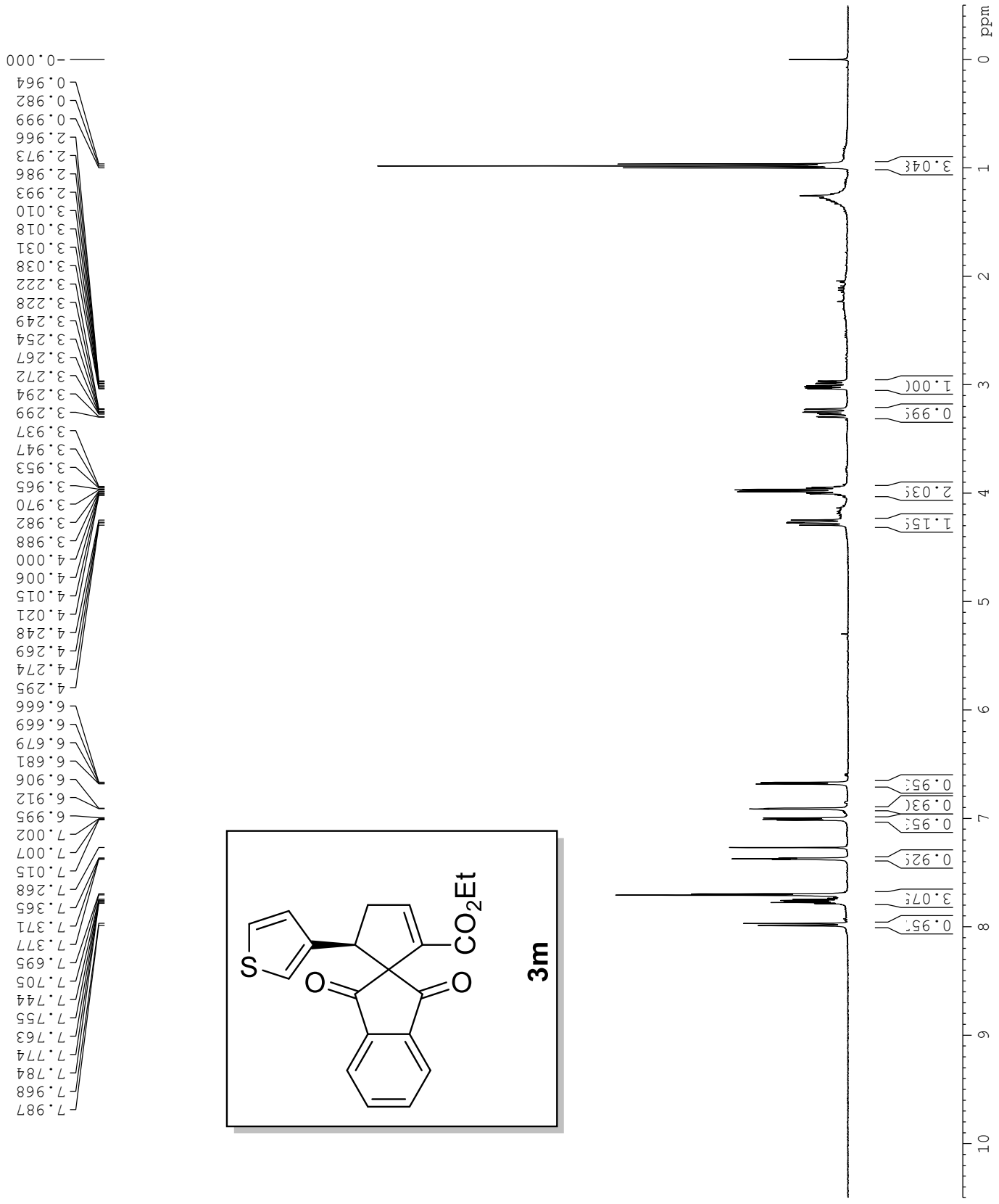
^{13}C NMR for compound 3l



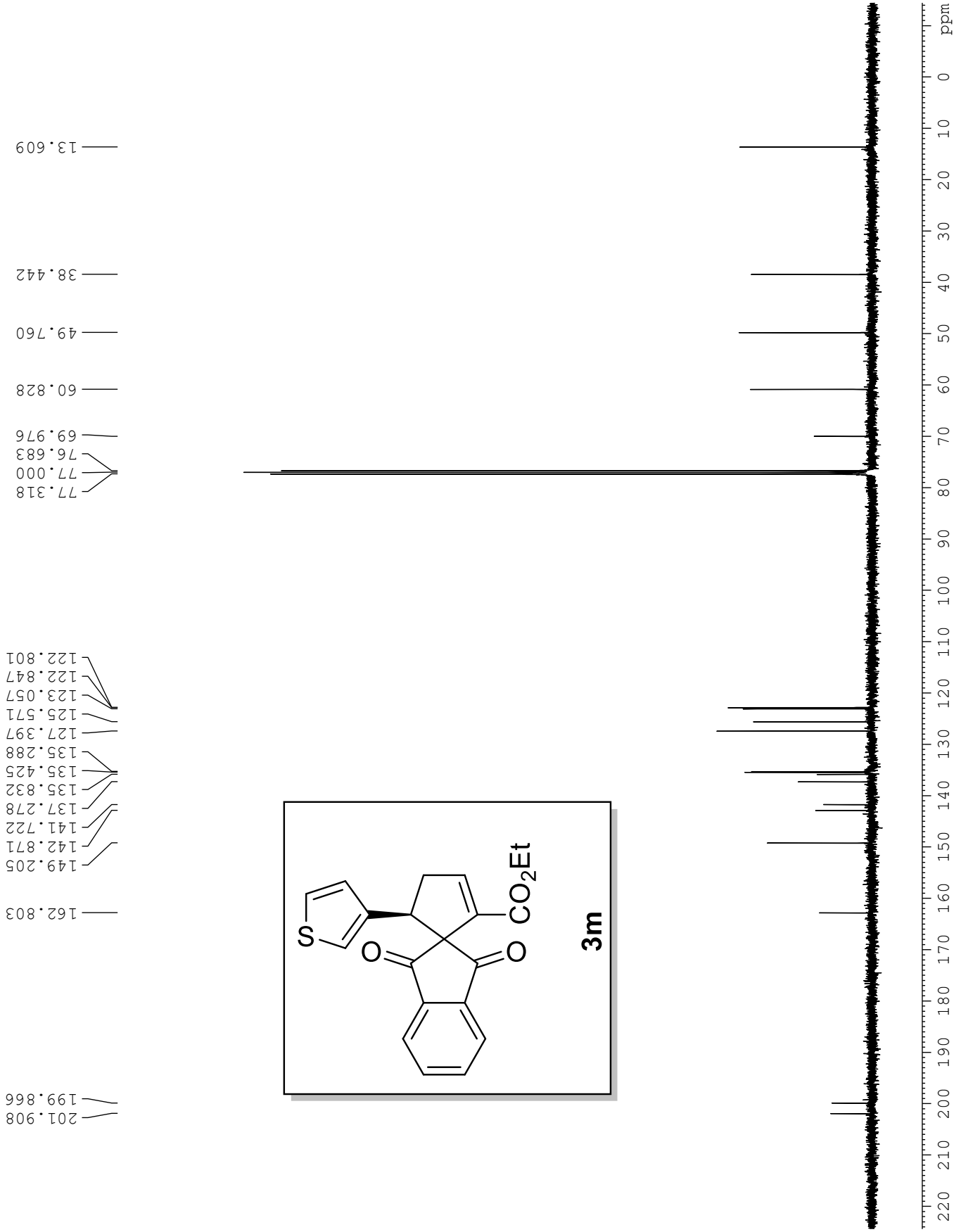
^{1}H NMR for compound 4l



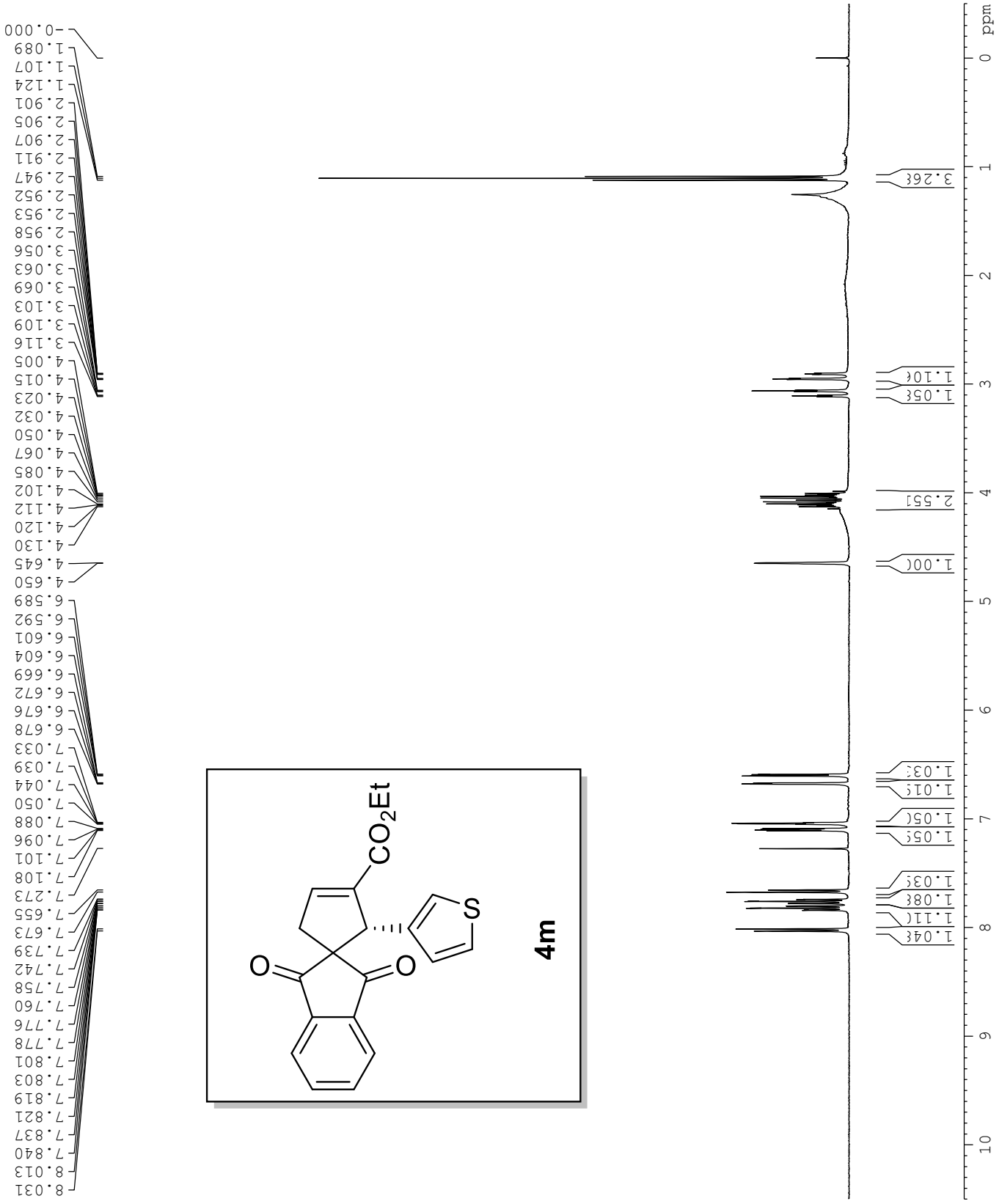
^{13}C NMR for compound 4l



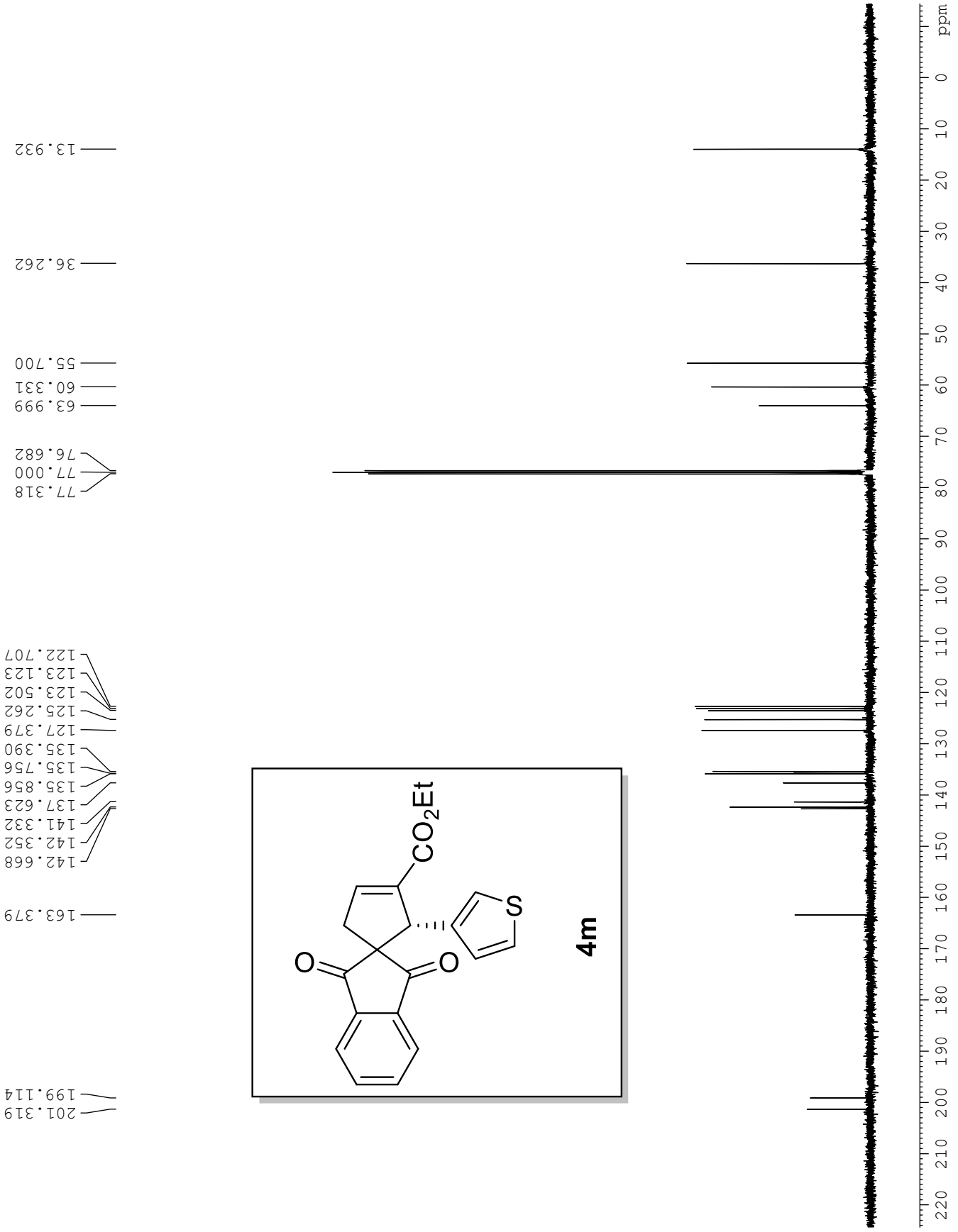
^{1}H NMR for compound 3m



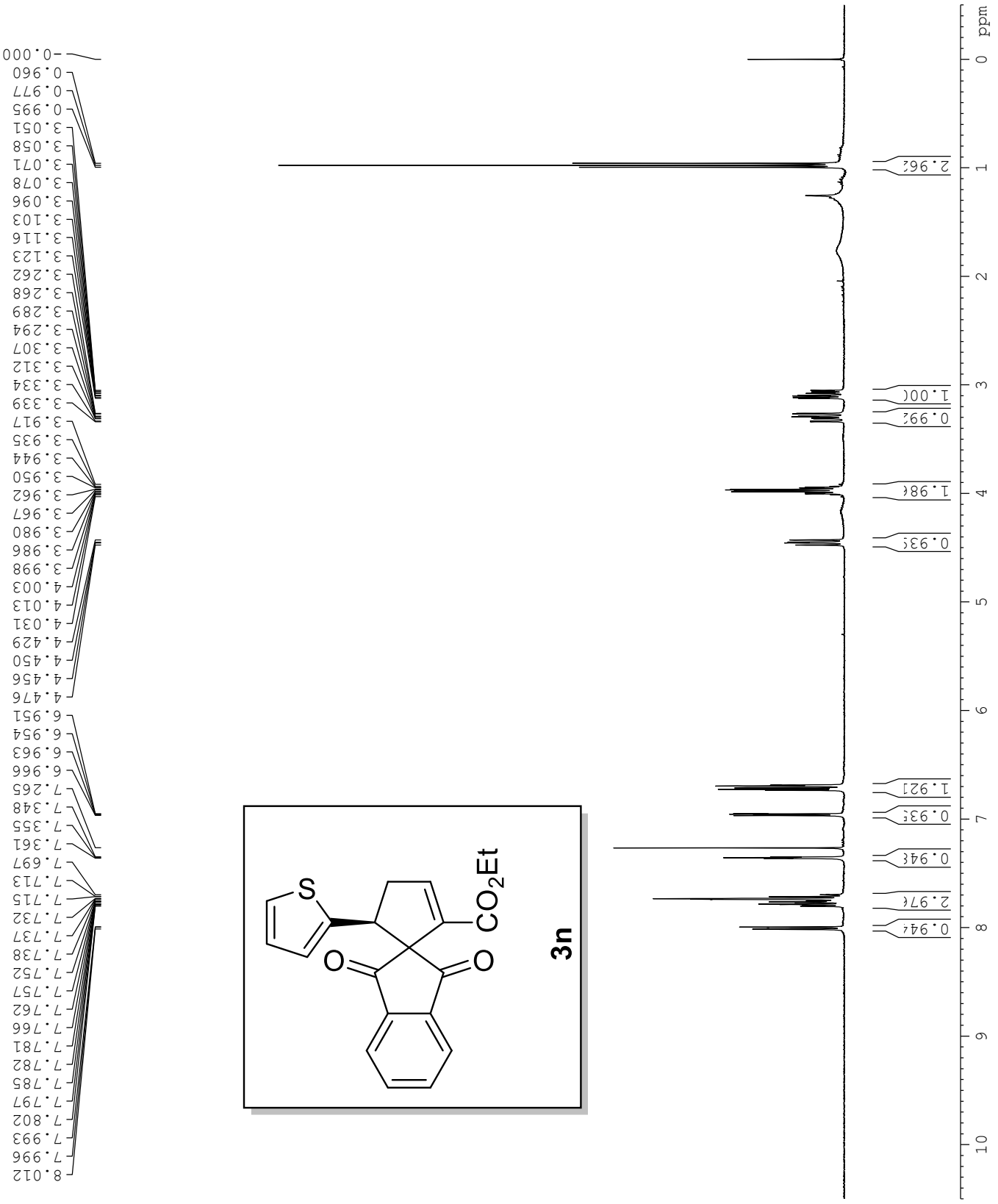
^{13}C NMR for compound 3m



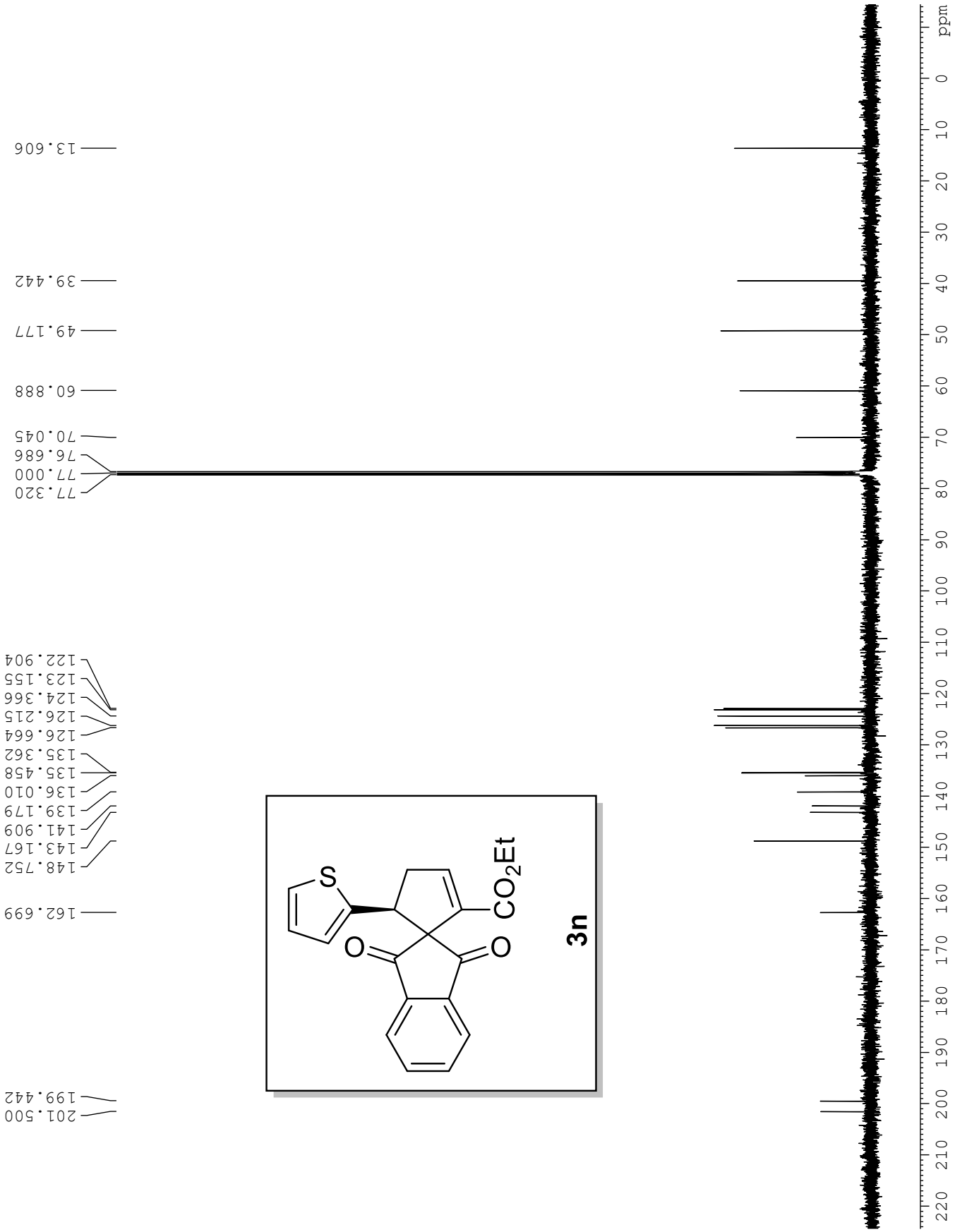
^{1}H NMR for compound 4m



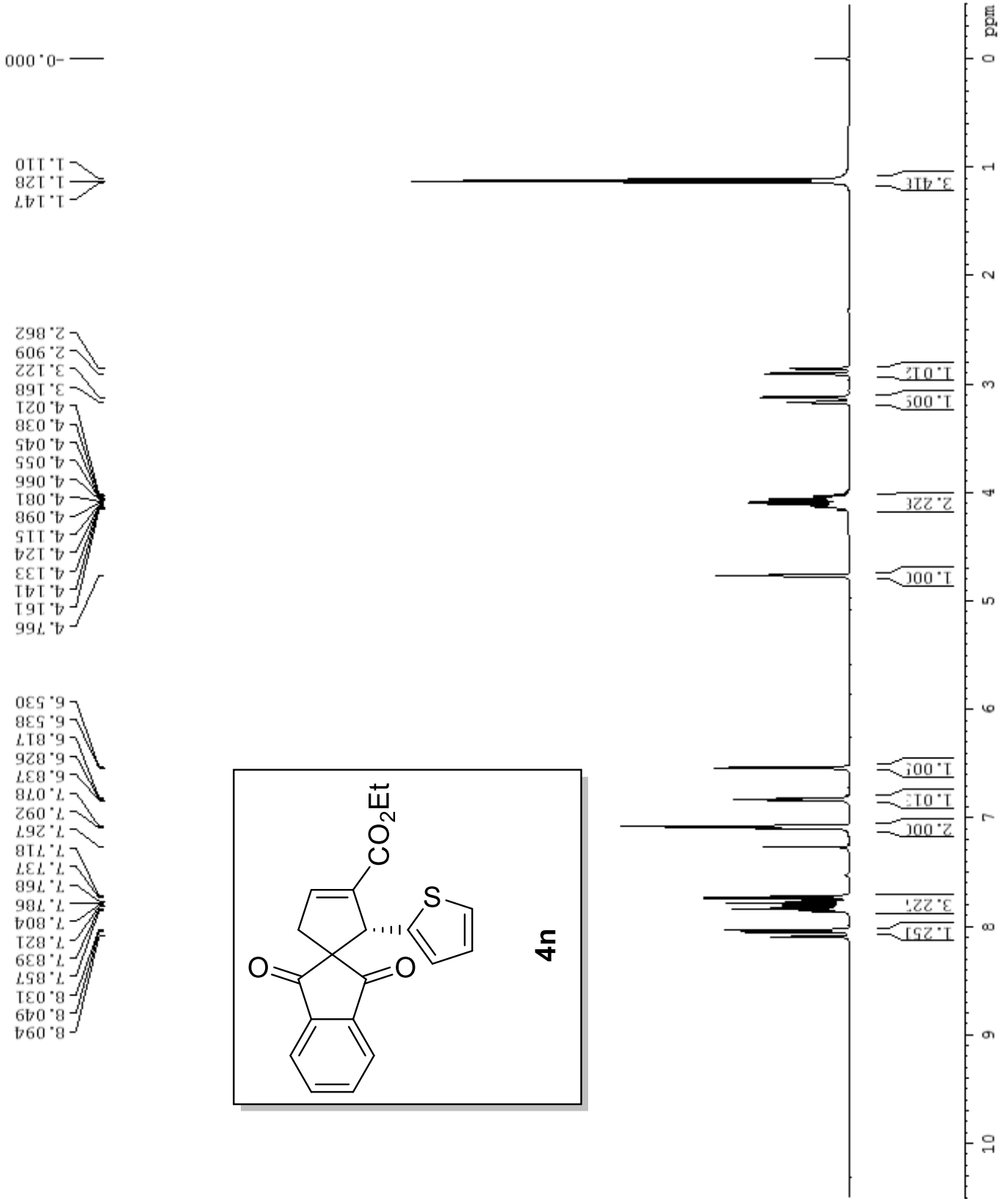
^{13}C NMR for compound 4m



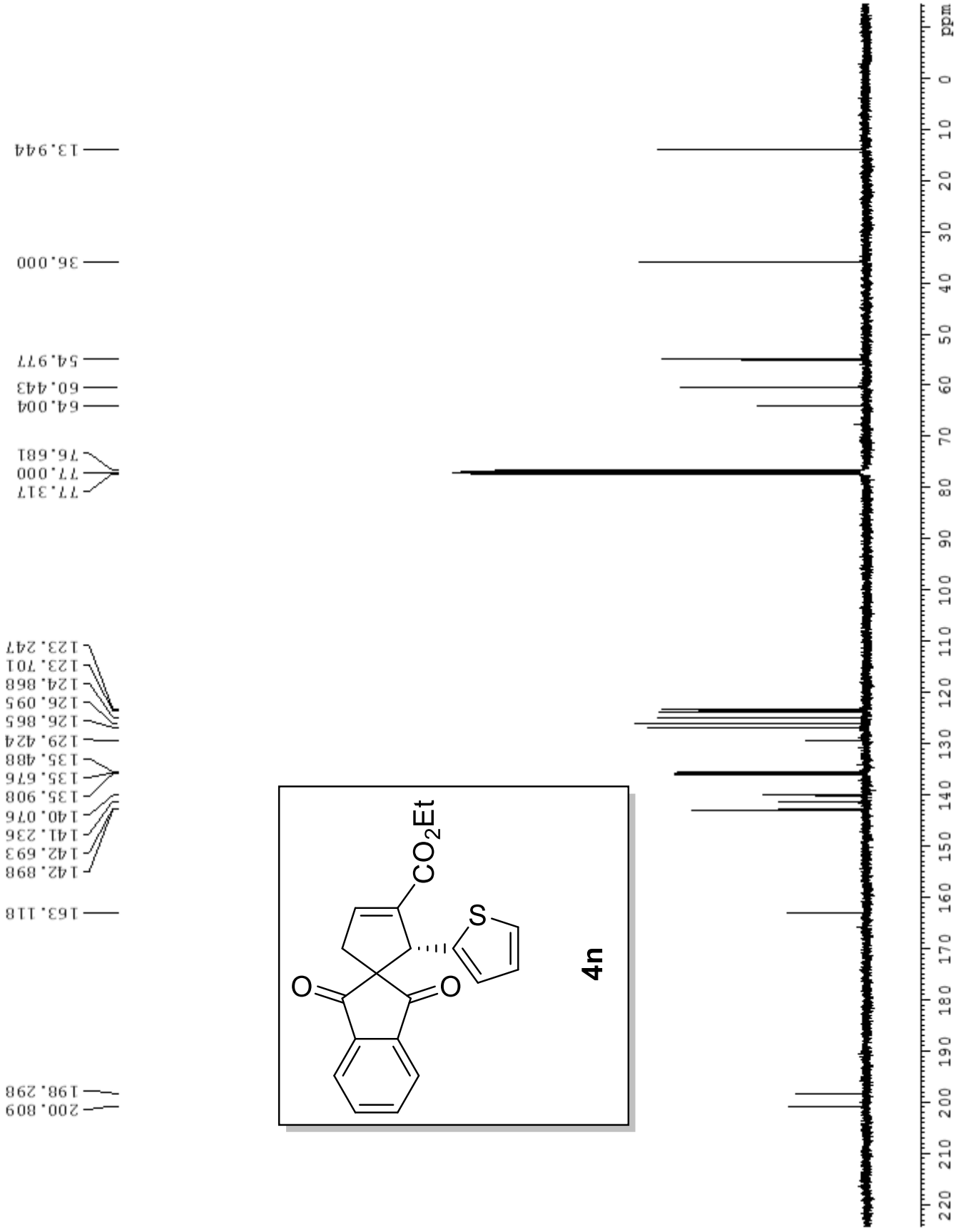
^{1}H NMR for compound 3n



^{13}C NMR for compound 3n

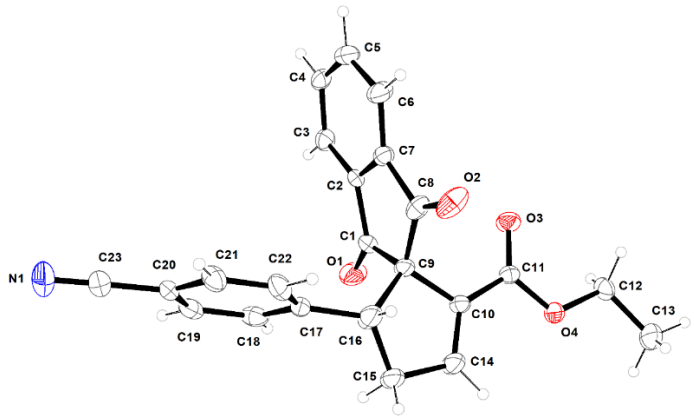


^{1}H NMR for compound 4n



^{13}C NMR for compound 4n

X-Ray analysis Data



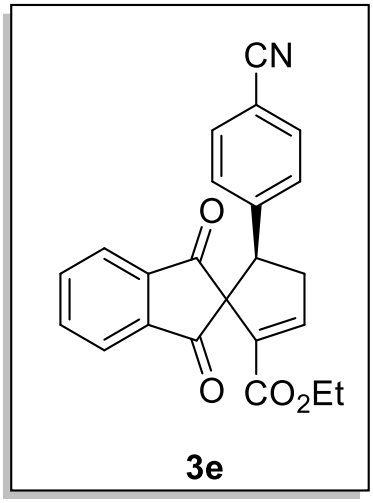


Table S1. Crystal data and structure refinement for **3e** (**CCDC 921839**).

Empirical formula	C23 H17 N O4	
Formula weight	371.38	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 31.098(4) Å	α= 90°.
	b = 8.4741(11) Å	β= 97.962(4)°.
	c = 14.651(2) Å	γ = 90°.
Volume	3823.7(9) $Å^3$	
Z	8	

Density (calculated)	1.290 Mg/m^3
Absorption coefficient	0.089 mm^{-1}
F(000)	1552
Crystal size	0.32 x 0.30 x 0.19 mm^3
Theta range for data collection	2.49 to 25.03°.
Index ranges	-34<=h<=36, -9<=k<=10, -17<=l<=13
Reflections collected	11967
Independent reflections	3276 [R(int) = 0.0471]
Completeness to theta = 25.03°	97.3 %
Absorption correction	multi-scan1
Max. and min. transmission	0.9833 and 0.9721
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3276 / 0 / 253
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0741, wR2 = 0.1662
R indices (all data)	R1 = 0.1196, wR2 = 0.1901
Largest diff. peak and hole	0.706 and -0.478 $e.Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for a14321. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3688(1)	4663(5)	2286(3)	38(1)
C(2)	3302(1)	5441(4)	2564(2)	31(1)
C(3)	3136(1)	5348(5)	3398(2)	39(1)
C(4)	2761(1)	6174(5)	3473(3)	44(1)
C(5)	2555(1)	7053(5)	2749(3)	51(1)
C(6)	2712(1)	7122(5)	1920(3)	50(1)
C(7)	3091(1)	6303(4)	1839(2)	34(1)
C(8)	3323(1)	6152(4)	1026(3)	40(1)
C(9)	3733(1)	5182(4)	1304(3)	37(1)
C(10)	3800(1)	3826(4)	682(2)	31(1)
C(11)	3460(1)	2639(4)	449(2)	31(1)
C(12)	3254(1)	340(4)	-443(3)	42(1)
C(13)	3427(2)	-542(6)	-1193(3)	62(1)
C(14)	4195(1)	3824(5)	465(3)	57(1)
C(15)	4458(1)	5186(5)	879(4)	63(1)
C(16)	4138(2)	6225(6)	1181(4)	68(2)
C(17)	4273(1)	7467(5)	1896(3)	40(1)
C(18)	4479(1)	7154(5)	2775(3)	46(1)
C(19)	4610(1)	8343(5)	3392(3)	44(1)
C(20)	4536(1)	9893(5)	3132(3)	39(1)
C(21)	4325(1)	10236(5)	2257(3)	46(1)
C(22)	4199(1)	9037(5)	1660(3)	46(1)
C(23)	4684(1)	11127(6)	3765(3)	61(1)
N(1)	4809(2)	12076(6)	4290(4)	93(2)
O(1)	3932(1)	3782(4)	2743(2)	61(1)
O(2)	3205(1)	6704(3)	267(2)	62(1)
O(3)	3119(1)	2655(3)	753(2)	48(1)
O(4)	3569(1)	1564(3)	-143(2)	39(1)

Table S3. Bond lengths [Å] and angles [°] for **3e**.

C(1)-O(1)	1.200(5)
C(1)-C(2)	1.475(5)
C(1)-C(9)	1.530(5)
C(2)-C(7)	1.378(5)
C(2)-C(3)	1.393(5)
C(3)-C(4)	1.378(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.379(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.372(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.386(5)
C(6)-H(6)	0.9500
C(7)-C(8)	1.482(5)
C(8)-O(2)	1.215(5)
C(8)-C(9)	1.524(5)
C(9)-C(10)	1.499(5)
C(9)-C(16)	1.570(5)
C(10)-C(14)	1.309(5)
C(10)-C(11)	1.466(5)
C(11)-O(3)	1.206(4)
C(11)-O(4)	1.333(4)
C(12)-O(4)	1.451(4)
C(12)-C(13)	1.491(6)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(15)	1.495(6)
C(14)-H(14)	0.9500
C(15)-C(16)	1.443(6)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.503(6)
C(16)-H(16)	1.0000
C(17)-C(18)	1.382(6)

C(17)-C(22)	1.386(6)
C(18)-C(19)	1.377(6)
C(18)-H(18)	0.9500
C(19)-C(20)	1.378(6)
C(19)-H(19)	0.9500
C(20)-C(21)	1.388(6)
C(20)-C(23)	1.431(6)
C(21)-C(22)	1.362(6)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500
C(23)-N(1)	1.142(6)

O(1)-C(1)-C(2)	126.9(4)
O(1)-C(1)-C(9)	124.8(3)
C(2)-C(1)-C(9)	108.3(3)
C(7)-C(2)-C(3)	120.7(3)
C(7)-C(2)-C(1)	110.1(3)
C(3)-C(2)-C(1)	129.1(4)
C(4)-C(3)-C(2)	117.5(4)
C(4)-C(3)-H(3)	121.3
C(2)-C(3)-H(3)	121.3
C(3)-C(4)-C(5)	121.4(3)
C(3)-C(4)-H(4)	119.3
C(5)-C(4)-H(4)	119.3
C(6)-C(5)-C(4)	121.3(4)
C(6)-C(5)-H(5)	119.4
C(4)-C(5)-H(5)	119.4
C(5)-C(6)-C(7)	117.7(4)
C(5)-C(6)-H(6)	121.1
C(7)-C(6)-H(6)	121.1
C(2)-C(7)-C(6)	121.3(3)
C(2)-C(7)-C(8)	109.9(3)
C(6)-C(7)-C(8)	128.8(4)
O(2)-C(8)-C(7)	125.7(4)
O(2)-C(8)-C(9)	125.9(3)
C(7)-C(8)-C(9)	108.3(3)
C(10)-C(9)-C(8)	115.7(3)
C(10)-C(9)-C(1)	113.0(3)
C(8)-C(9)-C(1)	103.0(3)

C(10)-C(9)-C(16)	100.3(3)
C(8)-C(9)-C(16)	108.7(3)
C(1)-C(9)-C(16)	116.7(3)
C(14)-C(10)-C(11)	127.8(3)
C(14)-C(10)-C(9)	111.3(3)
C(11)-C(10)-C(9)	120.7(3)
O(3)-C(11)-O(4)	124.3(3)
O(3)-C(11)-C(10)	123.4(3)
O(4)-C(11)-C(10)	112.3(3)
O(4)-C(12)-C(13)	106.5(3)
O(4)-C(12)-H(12A)	110.4
C(13)-C(12)-H(12A)	110.4
O(4)-C(12)-H(12B)	110.4
C(13)-C(12)-H(12B)	110.4
H(12A)-C(12)-H(12B)	108.6
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(10)-C(14)-C(15)	112.4(4)
C(10)-C(14)-H(14)	123.8
C(15)-C(14)-H(14)	123.8
C(16)-C(15)-C(14)	103.4(3)
C(16)-C(15)-H(15A)	111.1
C(14)-C(15)-H(15A)	111.1
C(16)-C(15)-H(15B)	111.1
C(14)-C(15)-H(15B)	111.1
H(15A)-C(15)-H(15B)	109.0
C(15)-C(16)-C(17)	120.2(4)
C(15)-C(16)-C(9)	106.9(4)
C(17)-C(16)-C(9)	117.6(3)
C(15)-C(16)-H(16)	103.2
C(17)-C(16)-H(16)	103.2
C(9)-C(16)-H(16)	103.2
C(18)-C(17)-C(22)	117.1(4)
C(18)-C(17)-C(16)	124.3(4)
C(22)-C(17)-C(16)	118.5(4)

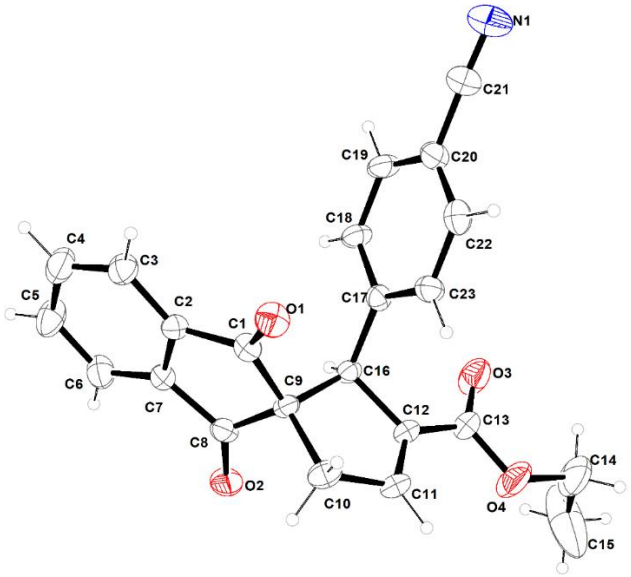
C(19)-C(18)-C(17)	121.9(4)
C(19)-C(18)-H(18)	119.1
C(17)-C(18)-H(18)	119.1
C(18)-C(19)-C(20)	119.6(4)
C(18)-C(19)-H(19)	120.2
C(20)-C(19)-H(19)	120.2
C(19)-C(20)-C(21)	119.6(4)
C(19)-C(20)-C(23)	119.4(4)
C(21)-C(20)-C(23)	121.0(4)
C(22)-C(21)-C(20)	119.6(4)
C(22)-C(21)-H(21)	120.2
C(20)-C(21)-H(21)	120.2
C(21)-C(22)-C(17)	122.2(4)
C(21)-C(22)-H(22)	118.9
C(17)-C(22)-H(22)	118.9
N(1)-C(23)-C(20)	177.8(6)
C(11)-O(4)-C(12)	117.6(3)

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **3e**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	25(2)	45(2)	42(2)	-8(2)	-1(2)	2(2)
C(2)	22(2)	35(2)	35(2)	-9(2)	3(2)	-6(2)
C(3)	41(2)	46(2)	29(2)	-2(2)	5(2)	-2(2)
C(4)	40(2)	57(3)	37(2)	-14(2)	16(2)	-8(2)
C(5)	38(2)	68(3)	49(3)	-9(2)	11(2)	13(2)
C(6)	50(3)	56(3)	44(2)	-2(2)	8(2)	21(2)
C(7)	34(2)	34(2)	34(2)	-2(2)	8(2)	0(2)
C(8)	56(3)	27(2)	41(2)	-2(2)	17(2)	-1(2)
C(9)	30(2)	36(2)	48(2)	-12(2)	15(2)	-8(2)
C(10)	29(2)	32(2)	35(2)	0(2)	10(2)	0(2)
C(11)	31(2)	31(2)	32(2)	3(2)	7(2)	3(2)
C(12)	38(2)	33(2)	54(2)	-7(2)	1(2)	-7(2)
C(13)	60(3)	63(3)	65(3)	-24(3)	12(2)	-16(2)
C(14)	47(3)	54(3)	73(3)	-32(2)	27(2)	-16(2)
C(15)	42(2)	65(3)	87(3)	-40(3)	33(2)	-20(2)
C(16)	55(3)	74(3)	83(3)	-42(3)	39(3)	-31(3)
C(17)	29(2)	51(3)	42(2)	-14(2)	12(2)	-10(2)
C(18)	33(2)	33(2)	74(3)	4(2)	15(2)	0(2)
C(19)	27(2)	63(3)	41(2)	5(2)	3(2)	-1(2)
C(20)	25(2)	44(2)	47(2)	-13(2)	3(2)	-4(2)
C(21)	40(2)	37(2)	57(3)	2(2)	-4(2)	0(2)
C(22)	39(2)	59(3)	38(2)	4(2)	-4(2)	-7(2)
C(23)	44(3)	68(3)	69(3)	-28(3)	0(2)	-2(2)
N(1)	77(3)	87(3)	110(4)	-56(3)	-8(3)	-9(3)
O(1)	54(2)	74(2)	53(2)	0(2)	1(2)	29(2)
O(2)	100(3)	47(2)	44(2)	11(2)	30(2)	19(2)
O(3)	39(2)	50(2)	60(2)	-11(1)	21(1)	-11(1)
O(4)	36(2)	33(1)	49(2)	-12(1)	9(1)	-7(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3e**.

	x	y	z	U(eq)
H(3)	3276	4737	3896	47
H(4)	2642	6138	4035	52
H(5)	2299	7621	2826	61
H(6)	2567	7712	1419	60
H(12A)	2969	814	-674	50
H(12B)	3218	-375	76	50
H(13A)	3224	-1384	-1420	94
H(13B)	3709	-1005	-953	94
H(13C)	3463	181	-1699	94
H(14)	4301	3044	88	68
H(15A)	4673	4841	1405	75
H(15B)	4614	5708	416	75
H(16)	4036	6857	616	82
H(18)	4531	6088	2958	55
H(19)	4750	8096	3992	52
H(21)	4270	11301	2074	55
H(22)	4054	9286	1063	55



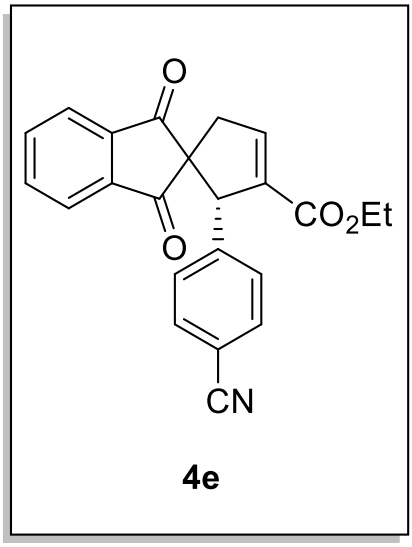


Table S6. Crystal data and structure refinement for **4e** (**CCDC 921702**) .

Empirical formula	C23 H17 N O4	
Formula weight	371.38	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 11.4044(13) Å	α= 90°.
	b = 5.5305(7) Å	β= 95.178(7)°.
	c = 15.6417(18) Å	γ = 90°.
Volume	982.5(2) $Å^3$	
Z	2	
Density (calculated)	1.255 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	388	
Crystal size	0.73 x 0.06 x 0.02 mm^3	

Theta range for data collection	2.61 to 25.10°.
Index ranges	-11<=h<=13, -4<=k<=6, -18<=l<=18
Reflections collected	7031
Independent reflections	2840 [R(int) = 0.0912]
Completeness to theta = 25.10°	97.7 %
Absorption correction	multi-scan
Max. and min. transmission	0.9983 and 0.9396
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2840 / 1 / 253
Goodness-of-fit on F^2	1.087
Final R indices [I>2sigma(I)]	R1 = 0.0882, wR2 = 0.1266
R indices (all data)	R1 = 0.1724, wR2 = 0.1488
Absolute structure parameter	0(3)
Largest diff. peak and hole	0.136 and -0.193 e.$Å^{-3}$

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4e**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9862(4)	2833(12)	7831(3)	44(1)
C(2)	10645(4)	1430(12)	8468(3)	49(2)
C(3)	10912(4)	1890(12)	9337(3)	61(2)
C(4)	11708(5)	356(16)	9780(4)	80(2)
C(5)	12228(5)	-1562(14)	9359(4)	79(2)
C(6)	11962(4)	-1952(14)	8505(4)	67(2)
C(7)	11158(4)	-421(12)	8056(3)	51(2)
C(8)	10721(4)	-477(12)	7137(3)	53(2)
C(9)	9733(4)	1386(11)	7002(3)	43(2)
C(10)	9787(4)	2888(12)	6168(3)	58(2)
C(11)	8865(4)	1736(12)	5551(3)	61(2)
C(12)	8205(4)	218(12)	5921(3)	45(2)
C(13)	7213(5)	-1223(14)	5512(4)	65(2)
C(14)	5993(6)	-2010(20)	4208(4)	126(4)
C(15)	6348(7)	-3730(30)	3708(8)	259(10)
C(16)	8530(3)	-78(11)	6877(2)	42(1)
C(17)	7585(4)	824(10)	7409(3)	44(2)
C(18)	7323(4)	-498(11)	8124(3)	53(2)
C(19)	6454(5)	312(14)	8622(3)	65(2)
C(20)	5839(4)	2393(13)	8408(4)	58(2)
C(21)	4938(5)	3205(15)	8920(4)	80(2)
C(22)	6103(4)	3718(12)	7705(3)	61(2)
C(23)	6967(4)	2904(13)	7205(3)	55(2)
N(1)	4197(5)	3849(14)	9307(3)	117(3)
O(1)	9406(3)	4750(9)	7956(2)	65(1)
O(2)	11072(3)	-1772(9)	6588(2)	67(1)
O(3)	6612(4)	-2506(10)	5886(3)	88(2)
O(4)	7003(3)	-743(11)	4679(2)	109(2)

Table S8. Bond lengths [Å] and angles [°] for **4e**.

C(1)-O(1)	1.205(6)
C(1)-C(2)	1.493(8)
C(1)-C(9)	1.521(7)
C(2)-C(7)	1.369(7)
C(2)-C(3)	1.391(6)
C(3)-C(4)	1.382(8)
C(3)-H(3)	0.9300
C(4)-C(5)	1.407(10)
C(4)-H(4)	0.9300
C(5)-C(6)	1.359(7)
C(5)-H(5)	0.9300
C(6)-C(7)	1.392(7)
C(6)-H(6)	0.9300
C(7)-C(8)	1.479(6)
C(8)-O(2)	1.214(6)
C(8)-C(9)	1.527(7)
C(9)-C(10)	1.552(7)
C(9)-C(16)	1.590(7)
C(10)-C(11)	1.503(7)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-C(12)	1.299(7)
C(11)-H(11)	0.9300
C(12)-C(13)	1.481(8)
C(12)-C(16)	1.517(5)
C(13)-O(3)	1.178(7)
C(13)-O(4)	1.330(6)
C(14)-C(15)	1.317(12)
C(14)-O(4)	1.487(8)
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-C(17)	1.505(6)
C(16)-H(16)	0.9800
C(17)-C(23)	1.372(7)

C(17)-C(18)	1.391(6)
C(18)-C(19)	1.388(6)
C(18)-H(18)	0.9300
C(19)-C(20)	1.374(8)
C(19)-H(19)	0.9300
C(20)-C(22)	1.377(7)
C(20)-C(21)	1.430(8)
C(21)-N(1)	1.140(6)
C(22)-C(23)	1.387(6)
C(22)-H(22)	0.9300
C(23)-H(23)	0.9300

O(1)-C(1)-C(2)	126.2(5)
O(1)-C(1)-C(9)	126.3(5)
C(2)-C(1)-C(9)	107.5(5)
C(7)-C(2)-C(3)	122.1(5)
C(7)-C(2)-C(1)	109.3(5)
C(3)-C(2)-C(1)	128.5(6)
C(4)-C(3)-C(2)	117.0(6)
C(4)-C(3)-H(3)	121.5
C(2)-C(3)-H(3)	121.5
C(3)-C(4)-C(5)	120.9(6)
C(3)-C(4)-H(4)	119.6
C(5)-C(4)-H(4)	119.6
C(6)-C(5)-C(4)	120.9(6)
C(6)-C(5)-H(5)	119.5
C(4)-C(5)-H(5)	119.5
C(5)-C(6)-C(7)	118.6(6)
C(5)-C(6)-H(6)	120.7
C(7)-C(6)-H(6)	120.7
C(2)-C(7)-C(6)	120.5(5)
C(2)-C(7)-C(8)	110.6(5)
C(6)-C(7)-C(8)	128.9(6)
O(2)-C(8)-C(7)	126.6(5)
O(2)-C(8)-C(9)	125.9(5)
C(7)-C(8)-C(9)	107.5(4)
C(1)-C(9)-C(8)	102.9(4)
C(1)-C(9)-C(10)	115.3(5)
C(8)-C(9)-C(10)	113.1(4)

C(1)-C(9)-C(16)	112.9(3)
C(8)-C(9)-C(16)	107.0(5)
C(10)-C(9)-C(16)	105.6(4)
C(11)-C(10)-C(9)	103.5(5)
C(11)-C(10)-H(10A)	111.1
C(9)-C(10)-H(10A)	111.1
C(11)-C(10)-H(10B)	111.1
C(9)-C(10)-H(10B)	111.1
H(10A)-C(10)-H(10B)	109.0
C(12)-C(11)-C(10)	112.8(5)
C(12)-C(11)-H(11)	123.6
C(10)-C(11)-H(11)	123.6
C(11)-C(12)-C(13)	127.3(5)
C(11)-C(12)-C(16)	114.2(5)
C(13)-C(12)-C(16)	118.5(5)
O(3)-C(13)-O(4)	123.1(6)
O(3)-C(13)-C(12)	124.4(5)
O(4)-C(13)-C(12)	112.3(6)
C(15)-C(14)-O(4)	111.7(8)
C(15)-C(14)-H(14A)	109.3
O(4)-C(14)-H(14A)	109.3
C(15)-C(14)-H(14B)	109.3
O(4)-C(14)-H(14B)	109.3
H(14A)-C(14)-H(14B)	107.9
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-C(12)	112.7(4)
C(17)-C(16)-C(9)	114.6(4)
C(12)-C(16)-C(9)	101.4(4)
C(17)-C(16)-H(16)	109.3
C(12)-C(16)-H(16)	109.3
C(9)-C(16)-H(16)	109.3
C(23)-C(17)-C(18)	119.0(5)
C(23)-C(17)-C(16)	121.8(5)
C(18)-C(17)-C(16)	119.1(5)

C(19)-C(18)-C(17)	119.8(5)
C(19)-C(18)-H(18)	120.1
C(17)-C(18)-H(18)	120.1
C(20)-C(19)-C(18)	120.6(5)
C(20)-C(19)-H(19)	119.7
C(18)-C(19)-H(19)	119.7
C(19)-C(20)-C(22)	119.8(5)
C(19)-C(20)-C(21)	120.2(6)
C(22)-C(20)-C(21)	120.0(6)
N(1)-C(21)-C(20)	178.0(6)
C(20)-C(22)-C(23)	119.7(6)
C(20)-C(22)-H(22)	120.2
C(23)-C(22)-H(22)	120.2
C(17)-C(23)-C(22)	121.1(5)
C(17)-C(23)-H(23)	119.4
C(22)-C(23)-H(23)	119.4
C(13)-O(4)-C(14)	117.0(6)

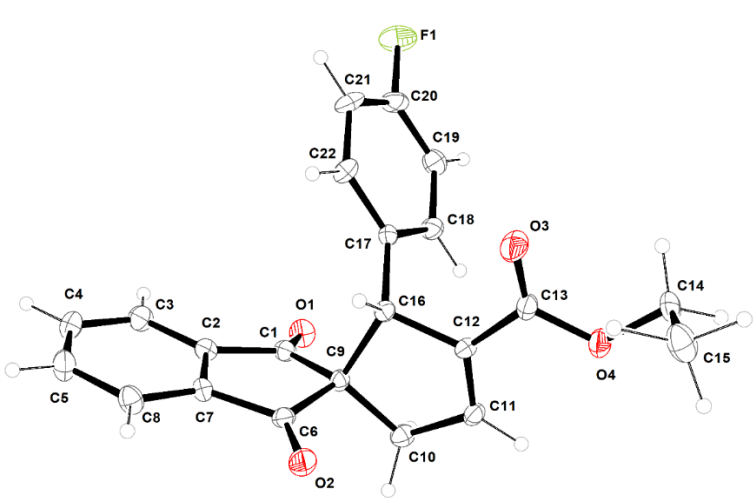
Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4e**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	44(3)	34(5)	54(3)	-5(3)	5(2)	-8(3)
C(2)	46(3)	58(5)	43(4)	-5(3)	7(3)	-1(3)
C(3)	63(4)	62(6)	56(4)	-12(3)	0(3)	1(3)
C(4)	79(4)	98(8)	60(4)	-9(4)	-16(3)	5(5)
C(5)	89(4)	74(7)	69(5)	-9(4)	-21(4)	29(4)
C(6)	55(3)	71(6)	74(4)	-11(4)	-4(3)	7(4)
C(7)	42(3)	64(6)	46(3)	-5(3)	4(3)	4(3)
C(8)	44(3)	67(6)	50(4)	-4(3)	13(2)	-7(3)
C(9)	49(3)	47(5)	31(3)	2(3)	6(2)	-3(3)
C(10)	77(4)	48(5)	50(3)	8(3)	12(3)	-5(4)
C(11)	68(3)	82(6)	34(3)	10(3)	9(3)	0(4)
C(12)	53(3)	50(5)	32(3)	3(3)	5(2)	0(3)
C(13)	64(4)	86(7)	43(4)	11(3)	-2(3)	5(4)
C(14)	106(6)	192(12)	73(5)	10(6)	-34(4)	-39(7)
C(15)	119(7)	310(20)	330(15)	-242(15)	-78(8)	87(9)
C(16)	48(3)	44(4)	34(3)	4(2)	5(2)	8(3)
C(17)	42(3)	43(5)	46(3)	6(2)	3(2)	1(3)
C(18)	67(3)	54(5)	39(3)	8(3)	14(3)	5(3)
C(19)	71(4)	84(7)	41(3)	6(3)	19(3)	-7(4)
C(20)	48(3)	70(7)	57(4)	-9(3)	8(3)	3(4)
C(21)	68(4)	103(7)	71(4)	-9(4)	19(3)	16(4)
C(22)	55(3)	55(6)	72(4)	1(3)	-6(3)	7(3)
C(23)	52(3)	61(5)	53(3)	9(3)	13(3)	6(3)
N(1)	104(4)	152(9)	101(4)	-16(4)	44(3)	29(5)
O(1)	71(2)	50(4)	74(3)	-3(2)	7(2)	10(2)
O(2)	67(2)	78(4)	59(2)	-27(2)	16(2)	10(2)
O(3)	92(3)	100(5)	68(3)	14(2)	-16(2)	-32(3)
O(4)	107(3)	166(7)	49(3)	12(3)	-21(2)	-51(4)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4e**.

	x	y	z	U(eq)
H(3)	10571	3172	9609	73
H(4)	11903	593	10364	97
H(5)	12760	-2577	9668	95
H(6)	12310	-3216	8228	80
H(10A)	9605	4574	6264	69
H(10B)	10560	2780	5957	69
H(11)	8777	2074	4966	74
H(14A)	5501	-2715	4617	151
H(14B)	5522	-855	3861	151
H(15A)	5676	-4472	3398	388
H(15B)	6778	-4930	4052	388
H(15C)	6848	-3049	3309	388
H(16)	8683	-1789	7006	50
H(18)	7728	-1921	8268	63
H(19)	6287	-562	9104	78
H(22)	5704	5152	7566	73
H(23)	7130	3784	6723	66



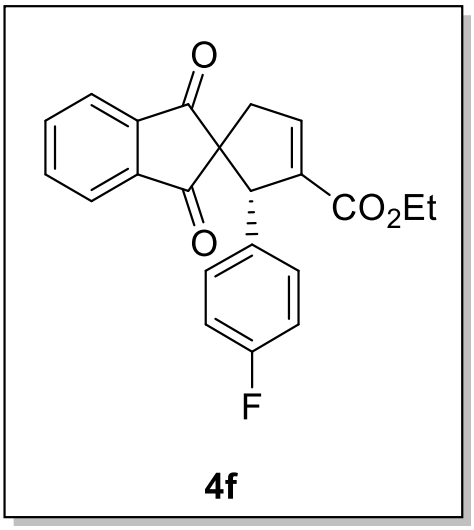


Table S11. Crystal data and structure refinement for **4f** (**CCDC 2110327**).

Empirical formula	C22 H17 F O4	
Formula weight	364.36	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 18.116(7) Å	α= 90°.
	b = 5.561(2) Å	β= 112.394(10)°.
	c = 18.910(7) Å	γ = 90°.
Volume	1761.2(12) $Å^3$	
Z	4	
Density (calculated)	1.374 Mg/m^3	

Absorption coefficient	0.101 mm^{-1}
F(000)	760
Crystal size	0.42 x 0.11 x 0.01 mm^3
Theta range for data collection	1.98 to 25.02°.
Index ranges	-21<=h<=21, -6<=k<=6, -22<=l<=22
Reflections collected	11711
Independent reflections	3101 [R(int) = 0.0672]
Completeness to theta = 25.02°	99.2 %
Absorption correction	multi-scan
Max. and min. transmission	0.9990 and 0.9588
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3101 / 0 / 244
Goodness-of-fit on F^2	0.959
Final R indices [I>2sigma(I)]	R1 = 0.0561, wR2 = 0.0946
R indices (all data)	R1 = 0.1469, wR2 = 0.1191
Largest diff. peak and hole	0.253 and -0.281 e.$Å^{-3}$

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4f**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1457(2)	12446(6)	3509(2)	26(1)
C(2)	2184(2)	11001(6)	3638(2)	24(1)
C(3)	2766(2)	11227(6)	3333(2)	34(1)
C(4)	3384(2)	9579(7)	3560(2)	39(1)
C(5)	3432(2)	7786(6)	4085(2)	39(1)
C(6)	2863(2)	7591(6)	4398(2)	34(1)
C(7)	2235(2)	9190(6)	4161(2)	25(1)
C(8)	1536(2)	9307(6)	4384(2)	26(1)
C(9)	952(2)	11154(6)	3871(2)	23(1)
C(10)	555(2)	12722(6)	4295(2)	29(1)
C(11)	-244(2)	11594(6)	4111(2)	27(1)
C(12)	-404(2)	9938(6)	3573(2)	23(1)
C(13)	-1129(2)	8434(6)	3254(2)	28(1)
C(14)	-2434(2)	7772(6)	3247(2)	39(1)
C(15)	-2394(2)	5639(7)	3740(2)	49(1)
C(16)	249(2)	9633(5)	3265(1)	22(1)
C(17)	-5(2)	10384(6)	2439(2)	23(1)
C(18)	-422(2)	12488(6)	2165(2)	28(1)
C(19)	-664(2)	13107(6)	1402(2)	34(1)
C(20)	-483(2)	11609(7)	926(2)	35(1)
C(21)	-72(2)	9505(7)	1169(2)	38(1)
C(22)	169(2)	8905(6)	1934(2)	30(1)
F(1)	-725(1)	12194(3)	172(1)	58(1)
O(1)	1303(1)	14375(4)	3179(1)	36(1)
O(2)	1431(1)	8098(4)	4872(1)	38(1)
O(3)	-1213(1)	6845(4)	2807(1)	48(1)
O(4)	-1686(1)	9107(4)	3521(1)	36(1)

Table S13. Bond lengths [Å] and angles [°] for **4f**.

C(1)-O(1)	1.219(3)
C(1)-C(2)	1.481(4)
C(1)-C(9)	1.516(4)
C(2)-C(7)	1.389(4)
C(2)-C(3)	1.387(4)
C(3)-C(4)	1.383(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.386(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.375(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.378(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.480(4)
C(8)-O(2)	1.213(3)
C(8)-C(9)	1.528(4)
C(9)-C(10)	1.536(4)
C(9)-C(16)	1.593(4)
C(10)-C(11)	1.491(4)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.320(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.479(4)
C(12)-C(16)	1.514(3)
C(13)-O(3)	1.192(3)
C(13)-O(4)	1.341(3)
C(14)-O(4)	1.456(3)
C(14)-C(15)	1.494(4)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	1.0776
C(15)-H(15B)	1.0777
C(15)-H(15C)	1.2232
C(16)-C(17)	1.509(3)
C(16)-H(16)	1.0000
C(17)-C(18)	1.383(4)

C(17)-C(22)	1.385(4)
C(18)-C(19)	1.383(4)
C(18)-H(18)	0.9500
C(19)-C(20)	1.355(4)
C(19)-H(19)	0.9500
C(20)-F(1)	1.362(3)
C(20)-C(21)	1.368(4)
C(21)-C(22)	1.383(4)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500
O(1)-C(1)-C(2)	125.3(3)
O(1)-C(1)-C(9)	126.1(3)
C(2)-C(1)-C(9)	108.6(3)
C(7)-C(2)-C(3)	120.4(3)
C(7)-C(2)-C(1)	109.0(3)
C(3)-C(2)-C(1)	130.6(3)
C(4)-C(3)-C(2)	117.8(3)
C(4)-C(3)-H(3)	121.1
C(2)-C(3)-H(3)	121.1
C(3)-C(4)-C(5)	121.4(3)
C(3)-C(4)-H(4)	119.3
C(5)-C(4)-H(4)	119.3
C(6)-C(5)-C(4)	120.8(3)
C(6)-C(5)-H(5)	119.6
C(4)-C(5)-H(5)	119.6
C(5)-C(6)-C(7)	118.1(3)
C(5)-C(6)-H(6)	121.0
C(7)-C(6)-H(6)	121.0
C(6)-C(7)-C(2)	121.5(3)
C(6)-C(7)-C(8)	128.7(3)
C(2)-C(7)-C(8)	109.8(3)
O(2)-C(8)-C(7)	126.3(3)
O(2)-C(8)-C(9)	125.7(3)
C(7)-C(8)-C(9)	108.0(3)
C(1)-C(9)-C(8)	102.4(2)
C(1)-C(9)-C(10)	116.7(2)
C(8)-C(9)-C(10)	113.5(2)
C(1)-C(9)-C(16)	112.4(2)
C(8)-C(9)-C(16)	105.7(2)

C(10)-C(9)-C(16)	105.8(2)
C(11)-C(10)-C(9)	104.2(2)
C(11)-C(10)-H(10A)	110.9
C(9)-C(10)-H(10A)	110.9
C(11)-C(10)-H(10B)	110.9
C(9)-C(10)-H(10B)	110.9
H(10A)-C(10)-H(10B)	108.9
C(12)-C(11)-C(10)	112.5(3)
C(12)-C(11)-H(11)	123.8
C(10)-C(11)-H(11)	123.8
C(11)-C(12)-C(13)	127.5(3)
C(11)-C(12)-C(16)	113.6(3)
C(13)-C(12)-C(16)	118.9(3)
O(3)-C(13)-O(4)	124.3(3)
O(3)-C(13)-C(12)	124.1(3)
O(4)-C(13)-C(12)	111.6(3)
O(4)-C(14)-C(15)	111.4(2)
O(4)-C(14)-H(14A)	109.3
C(15)-C(14)-H(14A)	109.3
O(4)-C(14)-H(14B)	109.3
C(15)-C(14)-H(14B)	109.3
H(14A)-C(14)-H(14B)	108.0
C(14)-C(15)-H(15A)	98.7
C(14)-C(15)-H(15B)	106.8
H(15A)-C(15)-H(15B)	97.0
C(14)-C(15)-H(15C)	106.4
H(15A)-C(15)-H(15C)	124.6
H(15B)-C(15)-H(15C)	120.5
C(17)-C(16)-C(12)	113.1(2)
C(17)-C(16)-C(9)	116.3(2)
C(12)-C(16)-C(9)	101.0(2)
C(17)-C(16)-H(16)	108.7
C(12)-C(16)-H(16)	108.7
C(9)-C(16)-H(16)	108.7
C(18)-C(17)-C(22)	118.6(3)
C(18)-C(17)-C(16)	122.0(3)
C(22)-C(17)-C(16)	119.3(3)
C(19)-C(18)-C(17)	120.8(3)
C(19)-C(18)-H(18)	119.6

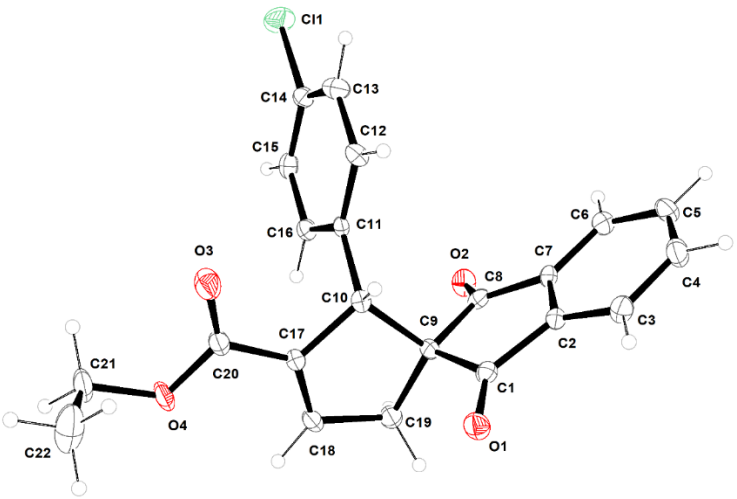
C(17)-C(18)-H(18)	119.6
C(20)-C(19)-C(18)	118.7(3)
C(20)-C(19)-H(19)	120.7
C(18)-C(19)-H(19)	120.7
C(19)-C(20)-F(1)	119.1(3)
C(19)-C(20)-C(21)	122.7(3)
F(1)-C(20)-C(21)	118.2(3)
C(20)-C(21)-C(22)	118.2(3)
C(20)-C(21)-H(21)	120.9
C(22)-C(21)-H(21)	120.9
C(21)-C(22)-C(17)	120.9(3)
C(21)-C(22)-H(22)	119.5
C(17)-C(22)-H(22)	119.5
C(13)-O(4)-C(14)	117.0(2)

Table S14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4f**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	26(2)	27(2)	24(2)	0(2)	8(2)	1(2)
C(2)	25(2)	23(2)	25(2)	2(2)	9(2)	-4(2)
C(3)	32(2)	39(2)	34(2)	3(2)	15(2)	-5(2)
C(4)	31(2)	51(3)	42(2)	-1(2)	21(2)	2(2)
C(5)	29(2)	43(3)	47(2)	6(2)	17(2)	8(2)
C(6)	30(2)	33(2)	37(2)	8(2)	10(2)	2(2)
C(7)	20(2)	26(2)	28(2)	1(2)	8(1)	1(2)
C(8)	26(2)	30(2)	22(2)	-4(2)	10(2)	-4(2)
C(9)	22(2)	26(2)	23(2)	4(2)	11(1)	1(2)
C(10)	33(2)	28(2)	28(2)	-3(2)	13(2)	-2(2)
C(11)	28(2)	32(2)	25(2)	2(2)	15(1)	4(2)
C(12)	26(2)	24(2)	22(2)	-2(2)	12(1)	0(2)
C(13)	25(2)	32(2)	30(2)	6(2)	14(2)	4(2)
C(14)	20(2)	54(3)	42(2)	-1(2)	13(2)	-9(2)
C(15)	35(2)	49(3)	58(2)	16(2)	12(2)	-6(2)
C(16)	23(2)	17(2)	25(2)	-3(2)	10(1)	2(2)
C(17)	19(2)	27(2)	23(2)	0(2)	8(1)	-1(2)
C(18)	30(2)	26(2)	29(2)	-2(2)	12(1)	3(2)
C(19)	31(2)	33(2)	34(2)	5(2)	8(2)	3(2)
C(20)	41(2)	45(3)	19(2)	4(2)	12(2)	-5(2)
C(21)	53(2)	39(3)	29(2)	-12(2)	24(2)	-1(2)
C(22)	37(2)	25(2)	33(2)	-2(2)	21(2)	3(2)
F(1)	80(1)	65(2)	26(1)	9(1)	19(1)	1(1)
O(1)	38(1)	30(2)	42(1)	7(1)	16(1)	-1(1)
O(2)	38(1)	49(2)	32(1)	12(1)	18(1)	3(1)
O(3)	41(1)	47(2)	62(2)	-30(1)	26(1)	-10(1)
O(4)	27(1)	43(2)	44(1)	-9(1)	18(1)	-6(1)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4f**.

	x	y	z	U(eq)
H(3)	2740	12472	2981	41
H(4)	3784	9678	3352	47
H(5)	3863	6678	4230	47
H(6)	2902	6388	4768	41
H(10A)	869	12704	4853	35
H(10B)	500	14405	4111	35
H(11)	-598	12020	4353	32
H(14A)	-2553	7229	2716	46
H(14B)	-2872	8843	3241	46
H(15A)	-2398	6568	4238	59
H(15B)	-2990	4917	3555	59
H(15C)	-1843	4393	3726	59
H(16)	412	7903	3311	26
H(18)	-545	13523	2505	34
H(19)	-951	14553	1215	40
H(21)	44	8485	822	46
H(22)	458	7459	2115	36



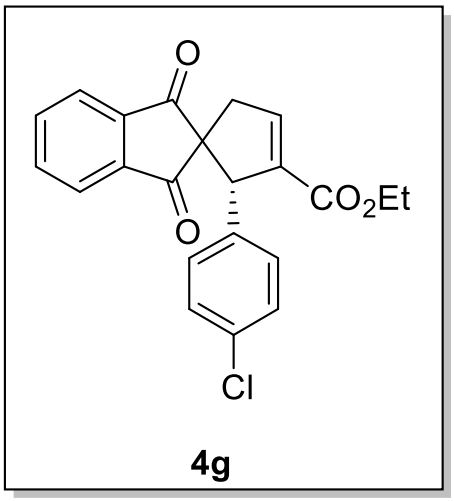


Table S16. Crystal data and structure refinement for **4g** (**CCDC 2110328**).

Empirical formula	C22 H17 Cl O4	
Formula weight	380.81	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 18.038(4) Å	α= 90°.
	b = 5.5757(14) Å	β= 111.044(6)°.
	c = 19.590(5) Å	γ = 90°.
Volume	1838.9(8) $Å^3$	
Z	4	
Density (calculated)	1.376 Mg/m^3	
Absorption coefficient	0.233 mm^{-1}	
F(000)	792	

Crystal size	0.62 x 0.06 x 0.01 mm^3
Theta range for data collection	1.32 to 25.09°.
Index ranges	-21<=h<=20, -6<=k<=6, -23<=l<=23
Reflections collected	11954
Independent reflections	3221 [R(int) = 0.0684]
Completeness to theta = 25.09°	98.1 %
Absorption correction	multi-scan
Max. and min. transmission	0.9977 and 0.8690
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3221 / 0 / 244
Goodness-of-fit on F^2	0.978
Final R indices [I>2sigma(I)]	R1 = 0.0587, wR2 = 0.1182
R indices (all data)	R1 = 0.1282, wR2 = 0.1409
Largest diff. peak and hole	0.243 and -0.264 e.$Å^{-3}$

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4g**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6542(2)	5857(6)	4361(2)	25(1)
C(2)	7224(2)	5975(6)	4110(2)	23(1)
C(3)	7843(2)	7593(7)	4300(2)	31(1)
C(4)	8396(2)	7358(7)	3971(2)	37(1)
C(5)	8347(2)	5513(7)	3478(2)	37(1)
C(6)	7736(2)	3852(7)	3302(2)	32(1)
C(7)	7172(2)	4114(6)	3623(2)	23(1)
C(8)	6458(2)	2644(7)	3532(2)	25(1)
C(9)	5960(2)	3981(6)	3895(2)	23(1)
C(10)	5255(2)	5475(6)	3318(2)	22(1)
C(11)	5016(2)	4644(6)	2532(2)	21(1)
C(12)	5177(2)	6062(6)	2024(2)	27(1)
C(13)	4933(2)	5400(7)	1297(2)	35(1)
C(14)	4547(2)	3235(7)	1090(2)	30(1)
C(15)	4379(2)	1791(7)	1583(2)	29(1)
C(16)	4614(2)	2498(6)	2306(2)	27(1)
C(17)	4604(2)	5171(6)	3622(2)	23(1)
C(18)	4767(2)	3556(6)	4147(2)	27(1)
C(19)	5566(2)	2466(6)	4324(2)	29(1)
C(20)	3868(2)	6600(7)	3306(2)	28(1)
C(21)	2560(2)	7233(7)	3292(2)	42(1)
C(22)	2564(2)	9380(9)	3733(2)	71(2)
O(1)	6449(1)	7058(5)	4839(1)	36(1)
O(2)	6304(1)	712(5)	3233(1)	34(1)
O(3)	3782(1)	8117(5)	2847(1)	48(1)
O(4)	3314(1)	5966(5)	3570(1)	42(1)
Cl(1)	4236(1)	2318(2)	178(1)	48(1)

Table S18. Bond lengths [Å] and angles [°] for **4g**.

C(1)-O(1)	1.209(4)
C(1)-C(2)	1.483(4)
C(1)-C(9)	1.530(4)
C(2)-C(3)	1.378(4)
C(2)-C(7)	1.390(4)
C(3)-C(4)	1.375(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.393(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.385(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.382(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.482(4)
C(8)-O(2)	1.210(4)
C(8)-C(9)	1.526(4)
C(9)-C(19)	1.534(4)
C(9)-C(10)	1.599(4)
C(10)-C(17)	1.506(4)
C(10)-C(11)	1.516(4)
C(10)-H(10)	1.0000
C(11)-C(12)	1.380(4)
C(11)-C(16)	1.387(4)
C(12)-C(13)	1.383(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.379(5)
C(13)-H(13)	0.9500
C(14)-C(15)	1.373(5)
C(14)-Cl(1)	1.745(3)
C(15)-C(16)	1.381(4)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(17)-C(18)	1.318(4)
C(17)-C(20)	1.479(4)
C(18)-C(19)	1.486(4)
C(18)-H(18)	0.9500
C(19)-H(19A)	0.9900

C(19)-H(19B)	0.9900
C(20)-O(3)	1.203(4)
C(20)-O(4)	1.329(4)
C(21)-O(4)	1.453(4)
C(21)-C(22)	1.476(5)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
O(1)-C(1)-C(2)	126.4(3)
O(1)-C(1)-C(9)	125.8(3)
C(2)-C(1)-C(9)	107.8(3)
C(3)-C(2)-C(7)	121.5(3)
C(3)-C(2)-C(1)	128.9(3)
C(7)-C(2)-C(1)	109.6(3)
C(4)-C(3)-C(2)	117.7(3)
C(4)-C(3)-H(3)	121.1
C(2)-C(3)-H(3)	121.1
C(3)-C(4)-C(5)	121.3(3)
C(3)-C(4)-H(4)	119.4
C(5)-C(4)-H(4)	119.4
C(6)-C(5)-C(4)	120.9(3)
C(6)-C(5)-H(5)	119.6
C(4)-C(5)-H(5)	119.6
C(7)-C(6)-C(5)	117.8(3)
C(7)-C(6)-H(6)	121.1
C(5)-C(6)-H(6)	121.1
C(6)-C(7)-C(2)	120.7(3)
C(6)-C(7)-C(8)	129.5(3)
C(2)-C(7)-C(8)	109.7(3)
O(2)-C(8)-C(7)	126.1(3)
O(2)-C(8)-C(9)	126.1(3)
C(7)-C(8)-C(9)	107.8(3)
C(8)-C(9)-C(1)	102.7(3)
C(8)-C(9)-C(19)	116.9(3)
C(1)-C(9)-C(19)	113.8(2)
C(8)-C(9)-C(10)	112.1(2)
C(1)-C(9)-C(10)	105.4(3)

C(19)-C(9)-C(10)	105.5(2)
C(17)-C(10)-C(11)	112.9(2)
C(17)-C(10)-C(9)	101.4(2)
C(11)-C(10)-C(9)	115.1(3)
C(17)-C(10)-H(10)	109.1
C(11)-C(10)-H(10)	109.1
C(9)-C(10)-H(10)	109.1
C(12)-C(11)-C(16)	119.0(3)
C(12)-C(11)-C(10)	120.0(3)
C(16)-C(11)-C(10)	120.9(3)
C(11)-C(12)-C(13)	121.2(3)
C(11)-C(12)-H(12)	119.4
C(13)-C(12)-H(12)	119.4
C(14)-C(13)-C(12)	118.5(3)
C(14)-C(13)-H(13)	120.7
C(12)-C(13)-H(13)	120.7
C(15)-C(14)-C(13)	121.4(3)
C(15)-C(14)-Cl(1)	118.5(3)
C(13)-C(14)-Cl(1)	120.0(3)
C(14)-C(15)-C(16)	119.4(3)
C(14)-C(15)-H(15)	120.3
C(16)-C(15)-H(15)	120.3
C(15)-C(16)-C(11)	120.4(3)
C(15)-C(16)-H(16)	119.8
C(11)-C(16)-H(16)	119.8
C(18)-C(17)-C(20)	127.6(3)
C(18)-C(17)-C(10)	113.5(3)
C(20)-C(17)-C(10)	118.9(3)
C(17)-C(18)-C(19)	112.8(3)
C(17)-C(18)-H(18)	123.6
C(19)-C(18)-H(18)	123.6
C(18)-C(19)-C(9)	104.4(3)
C(18)-C(19)-H(19A)	110.9
C(9)-C(19)-H(19A)	110.9
C(18)-C(19)-H(19B)	110.9
C(9)-C(19)-H(19B)	110.9
H(19A)-C(19)-H(19B)	108.9
O(3)-C(20)-O(4)	124.3(3)
O(3)-C(20)-C(17)	123.2(3)

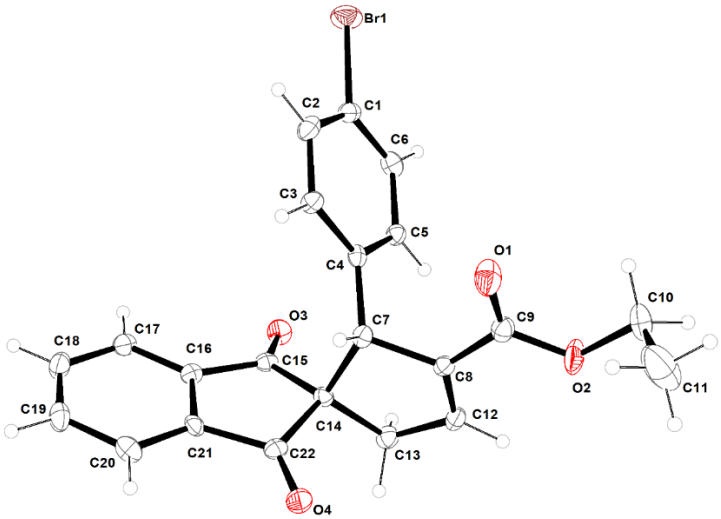
O(4)-C(20)-C(17)	112.4(3)
O(4)-C(21)-C(22)	111.6(3)
O(4)-C(21)-H(21A)	109.3
C(22)-C(21)-H(21A)	109.3
O(4)-C(21)-H(21B)	109.3
C(22)-C(21)-H(21B)	109.3
H(21A)-C(21)-H(21B)	108.0
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(20)-O(4)-C(21)	117.3(3)

Table S19. Anisotropic displacement parameters ($Å^2$x 10^3) for**4g**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	23(2)	26(2)	24(2)	2(2)	7(2)	3(2)
C(2)	20(2)	27(2)	22(2)	-1(2)	7(1)	0(2)
C(3)	27(2)	33(2)	32(2)	-4(2)	7(2)	0(2)
C(4)	25(2)	42(3)	45(2)	6(2)	13(2)	-4(2)
C(5)	28(2)	53(3)	37(2)	7(2)	19(2)	7(2)
C(6)	27(2)	42(3)	28(2)	0(2)	11(2)	3(2)
C(7)	16(2)	27(2)	24(2)	2(2)	5(1)	5(2)
C(8)	25(2)	26(2)	19(2)	2(2)	3(1)	4(2)
C(9)	21(2)	29(2)	23(2)	-2(2)	10(1)	1(2)
C(10)	20(2)	19(2)	26(2)	-2(2)	9(1)	-1(2)
C(11)	14(2)	26(2)	24(2)	3(2)	8(1)	2(2)
C(12)	28(2)	28(2)	30(2)	-2(2)	16(2)	-2(2)
C(13)	43(2)	36(2)	31(2)	4(2)	19(2)	3(2)
C(14)	26(2)	43(3)	23(2)	-3(2)	13(2)	9(2)
C(15)	21(2)	28(2)	35(2)	-5(2)	6(2)	-3(2)
C(16)	22(2)	30(2)	29(2)	4(2)	9(2)	-4(2)
C(17)	19(2)	27(2)	24(2)	0(2)	9(1)	-1(2)
C(18)	24(2)	31(2)	30(2)	-4(2)	15(2)	-4(2)
C(19)	28(2)	30(2)	30(2)	4(2)	11(2)	2(2)
C(20)	22(2)	33(2)	31(2)	-5(2)	12(2)	-2(2)
C(21)	20(2)	54(3)	54(2)	-3(2)	16(2)	6(2)
C(22)	41(3)	74(4)	82(3)	-39(3)	2(2)	11(3)
O(1)	33(1)	43(2)	35(1)	-12(1)	15(1)	-3(1)
O(2)	32(1)	29(2)	40(1)	-8(1)	12(1)	-1(1)
O(3)	36(2)	49(2)	62(2)	27(2)	23(1)	14(1)
O(4)	24(1)	56(2)	53(2)	15(1)	25(1)	9(1)
Cl(1)	56(1)	60(1)	27(1)	-10(1)	14(1)	1(1)

Table S20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4g**.

	x	y	z	U(eq)
H(3)	7885	8828	4646	38
H(4)	8821	8476	4083	45
H(5)	8737	5391	3258	45
H(6)	7705	2575	2972	39
H(10)	5410	7205	3349	26
H(12)	5461	7519	2178	33
H(13)	5028	6413	947	42
H(15)	4105	319	1429	35
H(16)	4498	1509	2650	32
H(18)	4411	3135	4387	32
H(19A)	5522	768	4167	35
H(19B)	5873	2548	4856	35
H(21A)	2129	6143	3296	51
H(21B)	2452	7718	2779	51
H(22A)	2049	10192	3530	107
H(22B)	2985	10474	3723	107
H(22C)	2660	8901	4239	107



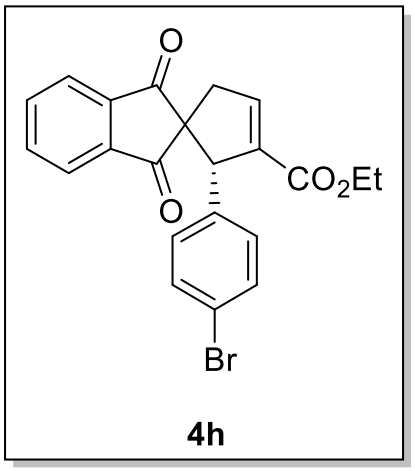


Table S21. Crystal data and structure refinement for **4h** (**CCDC 2110329**).

Empirical formula	C22 H17 Br O4	
Formula weight	425.27	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 18.073(5) Å	α= 90°.
	b = 5.5804(17) Å	β= 109.898(8)°.
	c = 19.888(6) Å	γ = 90°.
Volume	1886.1(10) $Å^3$	
Z	4	
Density (calculated)	1.498 Mg/m^3	
Absorption coefficient	2.204 mm^{-1}	
F(000)	864	

Crystal size	0.19 x 0.12 x 0.05 mm^3
Theta range for data collection	1.87 to 25.07°.
Index ranges	-20<=h<=21, -6<=k<=6, -23<=l<=23
Reflections collected	9089
Independent reflections	3338 [R(int) = 0.0750]
Completeness to theta = 25.07°	99.3 %
Absorption correction	multi-scan
Max. and min. transmission	0.8978 and 0.6795
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3338 / 0 / 244
Goodness-of-fit on F^2	0.971
Final R indices [I>2sigma(I)]	R1 = 0.0502, wR2 = 0.0878
R indices (all data)	R1 = 0.1029, wR2 = 0.1052
Largest diff. peak and hole	0.390 and -0.527 e.$Å^{-3}$

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4h**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4551(2)	11785(9)	1153(2)	29(1)
C(2)	4936(3)	9637(9)	1341(2)	33(1)
C(3)	5176(2)	8931(8)	2052(2)	25(1)
C(4)	5015(2)	10313(7)	2562(2)	22(1)
C(5)	4622(2)	12483(8)	2351(2)	25(1)
C(6)	4386(2)	13230(8)	1644(2)	31(1)
C(7)	5255(2)	9482(8)	3326(2)	23(1)
C(8)	4605(2)	9749(7)	3643(2)	23(1)
C(9)	3871(3)	8363(8)	3330(2)	31(1)
C(10)	2573(3)	7716(9)	3331(3)	54(2)
C(11)	2561(3)	5526(11)	3733(3)	89(2)
C(12)	4763(2)	11359(8)	4159(2)	28(1)
C(13)	5552(2)	12456(7)	4319(2)	30(1)
C(14)	5946(2)	10942(7)	3883(2)	22(1)
C(15)	6444(2)	12314(8)	3526(2)	24(1)
C(16)	7155(2)	10839(8)	3600(2)	24(1)
C(17)	7726(2)	11108(8)	3283(2)	30(1)
C(18)	8332(3)	9464(9)	3451(2)	37(1)
C(19)	8378(3)	7596(8)	3925(2)	36(1)
C(20)	7818(2)	7339(7)	4253(2)	32(1)
C(21)	7208(2)	8966(8)	4078(2)	25(1)
C(22)	6522(2)	9075(8)	4335(2)	25(1)
O(1)	3774(2)	6903(6)	2861(2)	49(1)
O(2)	3327(2)	8926(6)	3615(2)	51(1)
O(3)	6289(2)	14241(6)	3237(2)	34(1)
O(4)	6431(2)	7856(5)	4804(2)	36(1)
Br(1)	4211(1)	12838(1)	184(1)	48(1)

Table S23. Bond lengths [Å] and angles [°] for **4h**.

C(1)-C(6)	1.374(5)
C(1)-C(2)	1.373(6)
C(1)-Br(1)	1.905(4)
C(2)-C(3)	1.388(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.382(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.395(5)
C(4)-C(7)	1.504(5)
C(5)-C(6)	1.388(5)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(8)	1.517(5)
C(7)-C(14)	1.584(5)
C(7)-H(7)	1.0000
C(8)-C(12)	1.319(5)
C(8)-C(9)	1.479(6)
C(9)-O(1)	1.206(5)
C(9)-O(2)	1.329(4)
C(10)-O(2)	1.452(5)
C(10)-C(11)	1.465(7)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(13)	1.483(5)
C(12)-H(12)	0.9500
C(13)-C(14)	1.548(5)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.528(5)
C(14)-C(22)	1.530(6)
C(15)-O(3)	1.206(4)
C(15)-C(16)	1.491(6)
C(16)-C(17)	1.389(5)
C(16)-C(21)	1.394(5)

C(17)-C(18)	1.379(6)
C(17)-H(17)	0.9500
C(18)-C(19)	1.389(6)
C(18)-H(18)	0.9500
C(19)-C(20)	1.384(5)
C(19)-H(19)	0.9500
C(20)-C(21)	1.379(5)
C(20)-H(20)	0.9500
C(21)-C(22)	1.494(5)
C(22)-O(4)	1.211(4)

C(6)-C(1)-C(2)	122.2(4)
C(6)-C(1)-Br(1)	117.6(4)
C(2)-C(1)-Br(1)	120.2(3)
C(1)-C(2)-C(3)	118.6(4)
C(1)-C(2)-H(2)	120.7
C(3)-C(2)-H(2)	120.7
C(4)-C(3)-C(2)	121.3(4)
C(4)-C(3)-H(3)	119.4
C(2)-C(3)-H(3)	119.4
C(3)-C(4)-C(5)	118.4(4)
C(3)-C(4)-C(7)	120.6(4)
C(5)-C(4)-C(7)	121.0(4)
C(6)-C(5)-C(4)	121.0(4)
C(6)-C(5)-H(5)	119.5
C(4)-C(5)-H(5)	119.5
C(1)-C(6)-C(5)	118.5(4)
C(1)-C(6)-H(6)	120.7
C(5)-C(6)-H(6)	120.7
C(4)-C(7)-C(8)	113.1(3)
C(4)-C(7)-C(14)	115.8(3)
C(8)-C(7)-C(14)	101.3(3)
C(4)-C(7)-H(7)	108.8
C(8)-C(7)-H(7)	108.8
C(14)-C(7)-H(7)	108.8
C(12)-C(8)-C(9)	127.5(4)
C(12)-C(8)-C(7)	113.4(4)
C(9)-C(8)-C(7)	119.0(4)
O(1)-C(9)-O(2)	123.8(4)

O(1)-C(9)-C(8)	123.5(4)
O(2)-C(9)-C(8)	112.6(4)
O(2)-C(10)-C(11)	111.2(4)
O(2)-C(10)-H(10A)	109.4
C(11)-C(10)-H(10A)	109.4
O(2)-C(10)-H(10B)	109.4
C(11)-C(10)-H(10B)	109.4
H(10A)-C(10)-H(10B)	108.0
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(8)-C(12)-C(13)	112.7(4)
C(8)-C(12)-H(12)	123.7
C(13)-C(12)-H(12)	123.7
C(12)-C(13)-C(14)	104.2(3)
C(12)-C(13)-H(13A)	110.9
C(14)-C(13)-H(13A)	110.9
C(12)-C(13)-H(13B)	110.9
C(14)-C(13)-H(13B)	110.9
H(13A)-C(13)-H(13B)	108.9
C(15)-C(14)-C(22)	102.9(3)
C(15)-C(14)-C(13)	116.3(3)
C(22)-C(14)-C(13)	113.1(3)
C(15)-C(14)-C(7)	112.5(3)
C(22)-C(14)-C(7)	106.1(3)
C(13)-C(14)-C(7)	105.6(3)
O(3)-C(15)-C(16)	126.3(4)
O(3)-C(15)-C(14)	126.2(4)
C(16)-C(15)-C(14)	107.5(4)
C(17)-C(16)-C(21)	120.2(4)
C(17)-C(16)-C(15)	130.1(4)
C(21)-C(16)-C(15)	109.7(3)
C(18)-C(17)-C(16)	117.9(4)
C(18)-C(17)-H(17)	121.0
C(16)-C(17)-H(17)	121.0
C(17)-C(18)-C(19)	121.5(4)

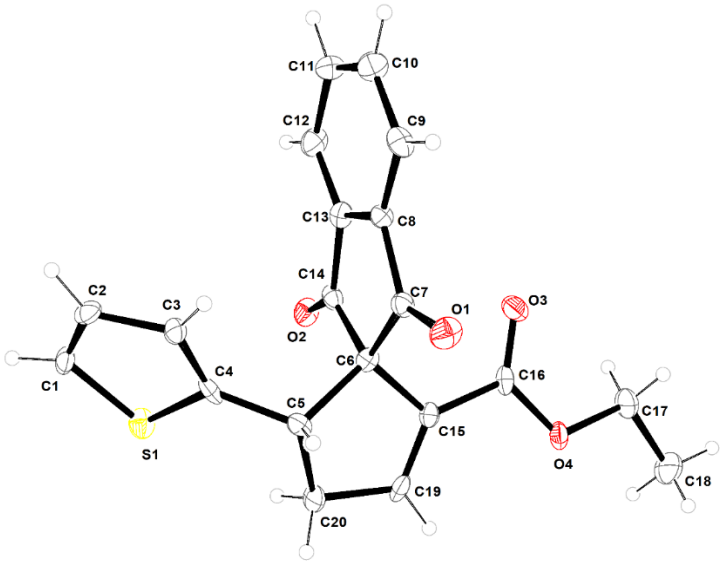
C(17)-C(18)-H(18)	119.2
C(19)-C(18)-H(18)	119.2
C(20)-C(19)-C(18)	120.8(4)
C(20)-C(19)-H(19)	119.6
C(18)-C(19)-H(19)	119.6
C(21)-C(20)-C(19)	117.6(4)
C(21)-C(20)-H(20)	121.2
C(19)-C(20)-H(20)	121.2
C(20)-C(21)-C(16)	121.9(4)
C(20)-C(21)-C(22)	128.8(4)
C(16)-C(21)-C(22)	109.3(4)
O(4)-C(22)-C(21)	125.9(4)
O(4)-C(22)-C(14)	126.3(4)
C(21)-C(22)-C(14)	107.7(3)
C(9)-O(2)-C(10)	117.1(4)

Table S24. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4h**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	28(3)	35(3)	23(2)	-1(2)	9(2)	-10(2)
C(2)	36(3)	33(3)	34(3)	-8(3)	19(2)	-4(3)
C(3)	31(3)	22(3)	25(2)	4(2)	12(2)	4(2)
C(4)	19(2)	19(3)	30(2)	-5(2)	9(2)	-3(2)
C(5)	24(2)	26(3)	27(2)	-5(2)	10(2)	1(2)
C(6)	27(3)	24(3)	39(3)	5(2)	8(2)	2(2)
C(7)	26(3)	18(3)	28(2)	2(2)	12(2)	3(2)
C(8)	26(3)	22(3)	22(2)	3(2)	9(2)	4(2)
C(9)	31(3)	31(3)	33(3)	4(2)	14(2)	2(2)
C(10)	25(3)	70(4)	68(4)	-1(3)	18(3)	-7(3)
C(11)	49(4)	96(5)	103(5)	50(5)	1(4)	-7(4)
C(12)	30(3)	29(3)	30(3)	6(2)	17(2)	7(2)
C(13)	33(3)	28(3)	30(2)	-1(2)	13(2)	4(2)
C(14)	22(2)	22(3)	22(2)	4(2)	6(2)	2(2)
C(15)	29(3)	22(3)	20(2)	-4(2)	7(2)	-5(2)
C(16)	26(3)	21(3)	24(2)	-3(2)	8(2)	-6(2)
C(17)	28(3)	35(3)	27(3)	-2(2)	10(2)	-10(2)
C(18)	29(3)	47(3)	40(3)	-5(3)	18(2)	-1(3)
C(19)	28(3)	35(3)	47(3)	-7(3)	15(2)	6(2)
C(20)	32(3)	23(3)	37(3)	3(2)	5(2)	1(2)
C(21)	17(2)	29(3)	25(2)	-4(2)	2(2)	-1(2)
C(22)	30(3)	24(3)	22(2)	-6(2)	8(2)	-4(2)
O(1)	38(2)	47(2)	68(2)	-26(2)	24(2)	-14(2)
O(2)	30(2)	69(3)	63(2)	-24(2)	29(2)	-18(2)
O(3)	36(2)	28(2)	39(2)	7(2)	14(2)	0(2)
O(4)	36(2)	42(2)	33(2)	14(2)	15(2)	3(2)
Br(1)	54(1)	60(1)	29(1)	11(1)	10(1)	-7(1)

Table S25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4h**.

	x	y	z	U(eq)
H(2)	5037	8655	991	39
H(3)	5455	7469	2190	30
H(5)	4514	13466	2697	30
H(6)	4117	14707	1502	37
H(7)	5410	7756	3348	28
H(10A)	2469	7305	2823	64
H(10B)	2151	8807	3355	64
H(11A)	2046	4749	3531	134
H(11B)	2655	5933	4235	134
H(11C)	2972	4432	3703	134
H(12)	4409	11771	4401	34
H(13A)	5857	12366	4837	35
H(13B)	5507	14155	4167	35
H(17)	7700	12385	2960	36
H(18)	8726	9611	3237	44
H(19)	8799	6481	4026	44
H(20)	7853	6087	4586	39



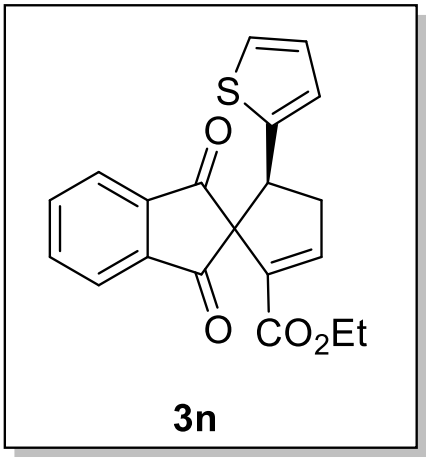


Table S26. Crystal data and structure refinement for **3n** (**CCDC 2110330**).

Empirical formula	C20 H16 O4 S	
Formula weight	352.39	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 8.833(13) Å	α= 90°.
	b = 6.042(11) Å	β= 103.32(3)°.
	c = 16.23(3) Å	γ = 90°.
Volume	843(2) $Å^3$	
Z	2	
Density (calculated)	1.388 Mg/m^3	
Absorption coefficient	0.214 mm^{-1}	
F(000)	368	
Crystal size	0.62 x 0.10 x 0.01 mm^3	

Theta range for data collection	2.37 to 25.02°.
Index ranges	-10<=h<=10, -7<=k<=5, -19<=l<=18
Reflections collected	6003
Independent reflections	2445 [R(int) = 0.1321]
Completeness to theta = 25.02°	98.7 %
Absorption correction	multi-scan
Max. and min. transmission	0.9979 and 0.8787
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2445 / 1 / 226
Goodness-of-fit on F^2	0.983
Final R indices [I>2sigma(I)]	R1 = 0.0822, wR2 = 0.1383
R indices (all data)	R1 = 0.1624, wR2 = 0.1726
Absolute structure parameter	-0.5(2)
Largest diff. peak and hole	0.301 and -0.353 e.$Å^{-3}$

Table S27. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3n**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3777(9)	1565(15)	5725(5)	30(2)
C(2)	3906(9)	-302(15)	5299(5)	30(2)
C(3)	2702(9)	-495(15)	4521(4)	29(2)
C(4)	1761(10)	1311(15)	4393(4)	28(2)
C(5)	390(9)	1722(15)	3648(4)	28(2)
C(6)	879(9)	2199(12)	2779(4)	23(2)
C(7)	1031(9)	57(14)	2294(4)	26(2)
C(8)	2648(9)	-168(14)	2211(4)	23(2)
C(9)	3309(9)	-1836(16)	1833(4)	32(2)
C(10)	4873(9)	-1695(17)	1840(5)	37(2)
C(11)	5763(10)	93(17)	2209(5)	39(2)
C(12)	5077(10)	1791(14)	2585(5)	36(2)
C(13)	3496(9)	1673(14)	2564(5)	27(2)
C(14)	2505(9)	3267(16)	2908(4)	26(2)
C(15)	-416(9)	3702(13)	2334(4)	24(2)
C(16)	-512(10)	4275(12)	1448(5)	24(2)
C(17)	-1900(10)	6152(16)	230(5)	47(3)
C(18)	-3290(10)	7561(18)	-24(5)	59(3)
C(19)	-1220(9)	4549(16)	2858(5)	31(2)
C(20)	-649(9)	3701(14)	3743(4)	34(2)
O(1)	-65(6)	-1166(9)	2010(3)	40(2)
O(2)	2886(6)	5016(10)	3212(3)	33(2)
O(3)	553(6)	3912(9)	1107(3)	39(2)
O(4)	-1864(6)	5258(9)	1072(3)	31(2)
S(1)	2278(3)	3187(4)	5208(1)	36(1)

Table S28. Bond lengths [Å] and angles [°] for **3n**.

C(1)-C(2)	1.341(11)
C(1)-S(1)	1.704(8)
C(1)-H(1)	0.9500
C(2)-C(3)	1.456(10)
C(2)-H(2)	0.9500
C(3)-C(4)	1.359(10)
C(3)-H(3)	0.9500
C(4)-C(5)	1.522(10)
C(4)-S(1)	1.722(8)
C(5)-C(20)	1.536(10)
C(5)-C(6)	1.593(10)
C(5)-H(5)	1.0000
C(6)-C(15)	1.508(10)
C(6)-C(7)	1.537(11)
C(6)-C(14)	1.544(11)
C(7)-O(1)	1.220(9)
C(7)-C(8)	1.472(10)
C(8)-C(9)	1.378(11)
C(8)-C(13)	1.389(11)
C(9)-C(10)	1.382(10)
C(9)-H(9)	0.9500
C(10)-C(11)	1.388(12)
C(10)-H(10)	0.9500
C(11)-C(12)	1.401(11)
C(11)-H(11)	0.9500
C(12)-C(13)	1.390(11)
C(12)-H(12)	0.9500
C(13)-C(14)	1.494(11)
C(14)-O(2)	1.182(10)
C(15)-C(19)	1.329(10)
C(15)-C(16)	1.463(10)
C(16)-O(3)	1.217(9)
C(16)-O(4)	1.347(8)
C(17)-O(4)	1.463(8)
C(17)-C(18)	1.473(11)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900

C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(20)	1.498(9)
C(19)-H(19)	0.9500
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900

C(2)-C(1)-S(1)	112.3(6)
C(2)-C(1)-H(1)	123.9
S(1)-C(1)-H(1)	123.9
C(1)-C(2)-C(3)	112.5(8)
C(1)-C(2)-H(2)	123.8
C(3)-C(2)-H(2)	123.8
C(4)-C(3)-C(2)	111.5(7)
C(4)-C(3)-H(3)	124.2
C(2)-C(3)-H(3)	124.2
C(3)-C(4)-C(5)	126.9(7)
C(3)-C(4)-S(1)	111.5(6)
C(5)-C(4)-S(1)	121.7(7)
C(4)-C(5)-C(20)	115.6(7)
C(4)-C(5)-C(6)	113.8(6)
C(20)-C(5)-C(6)	103.8(6)
C(4)-C(5)-H(5)	107.8
C(20)-C(5)-H(5)	107.8
C(6)-C(5)-H(5)	107.8
C(15)-C(6)-C(7)	114.0(6)
C(15)-C(6)-C(14)	113.1(6)
C(7)-C(6)-C(14)	103.5(6)
C(15)-C(6)-C(5)	101.7(6)
C(7)-C(6)-C(5)	112.0(6)
C(14)-C(6)-C(5)	113.0(6)
O(1)-C(7)-C(8)	127.7(8)
O(1)-C(7)-C(6)	123.2(7)
C(8)-C(7)-C(6)	109.0(7)
C(9)-C(8)-C(13)	121.7(7)
C(9)-C(8)-C(7)	128.9(8)
C(13)-C(8)-C(7)	109.3(7)
C(8)-C(9)-C(10)	118.5(8)

C(8)-C(9)-H(9)	120.8
C(10)-C(9)-H(9)	120.8
C(9)-C(10)-C(11)	121.2(9)
C(9)-C(10)-H(10)	119.4
C(11)-C(10)-H(10)	119.4
C(10)-C(11)-C(12)	119.9(8)
C(10)-C(11)-H(11)	120.1
C(12)-C(11)-H(11)	120.1
C(13)-C(12)-C(11)	119.0(8)
C(13)-C(12)-H(12)	120.5
C(11)-C(12)-H(12)	120.5
C(8)-C(13)-C(12)	119.6(8)
C(8)-C(13)-C(14)	111.3(7)
C(12)-C(13)-C(14)	129.0(8)
O(2)-C(14)-C(13)	126.7(8)
O(2)-C(14)-C(6)	126.6(7)
C(13)-C(14)-C(6)	106.7(7)
C(19)-C(15)-C(16)	128.2(7)
C(19)-C(15)-C(6)	112.6(7)
C(16)-C(15)-C(6)	118.7(7)
O(3)-C(16)-O(4)	124.8(7)
O(3)-C(16)-C(15)	121.9(7)
O(4)-C(16)-C(15)	113.3(7)
O(4)-C(17)-C(18)	108.2(7)
O(4)-C(17)-H(17A)	110.1
C(18)-C(17)-H(17A)	110.1
O(4)-C(17)-H(17B)	110.1
C(18)-C(17)-H(17B)	110.1
H(17A)-C(17)-H(17B)	108.4
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(15)-C(19)-C(20)	111.7(7)
C(15)-C(19)-H(19)	124.2
C(20)-C(19)-H(19)	124.2
C(19)-C(20)-C(5)	104.3(6)

C(19)-C(20)-H(20A)	110.9
C(5)-C(20)-H(20A)	110.9
C(19)-C(20)-H(20B)	110.9
C(5)-C(20)-H(20B)	110.9
H(20A)-C(20)-H(20B)	108.9
C(16)-O(4)-C(17)	114.4(6)
C(1)-S(1)-C(4)	92.2(4)

Cartesian Coordinates of Reactants, Complexes, Intermediates, Transition states and Products

1a:

C	2.48802000	0.34842700	0.00006500
C	-3.82254500	1.09091300	0.00001100
C	-4.82683100	0.11991700	0.00004400
C	-4.50896500	-1.24860200	0.00006600
C	-3.17974700	-1.67802000	0.00003400
C	-2.18272200	-0.70630300	-0.00001500
C	-2.49988400	0.65700100	-0.00001900
C	-0.69902200	-0.89664400	-0.00001500
C	-0.10459500	0.47053200	0.00003600
C	-1.24002200	1.45315900	-0.00009000
O	-1.15303200	2.67094400	-0.00013500
O	-0.14876500	-1.99087500	-0.00008800
C	1.16757100	0.95365400	0.00005100
C	2.73986900	-1.04133900	0.00000500
C	4.04846900	-1.51373300	-0.00006100
C	5.12776400	-0.62482900	-0.00001200
C	4.89589200	0.75314600	0.00002000
C	3.59103100	1.23219400	0.00010500
H	-4.05304900	2.15201800	0.00000300
H	-5.87020800	0.42340100	0.00006800
H	-5.31192200	-1.98071300	0.00011800
H	-2.91916400	-2.73213100	0.00007400
H	1.18627200	2.04616700	0.00015500
H	1.90266200	-1.72955800	-0.00008700

H	4.22915200	-2.58517200	-0.00009600
H	6.14612600	-1.00452600	-0.00007900
H	5.73001600	1.44913800	0.00006500
H	3.40879700	2.30397500	0.00020900

A:

C	0.44883300	-0.28770300	-2.57557900
C	0.74484500	-0.06026500	-1.25540100
C	1.98922400	0.03204400	-0.56474700
C	3.23702700	-0.14210600	-1.22948700
P	-0.67543400	-0.00311000	-0.14272400
O	4.30232500	0.01117700	-0.34718400
O	3.43778800	-0.39507100	-2.41968200
C	-2.25697100	0.22449000	-1.02632500
C	-0.49971800	1.39720700	1.01408000
C	-0.84107600	-1.54762800	0.81624300
C	-2.86345500	1.48638600	-1.10395500
C	-4.04736500	1.65106900	-1.82348700
C	-4.63299100	0.56112100	-2.46880000
C	-4.03434900	-0.69834800	-2.39439500
C	-2.85224700	-0.87041600	-1.67564600
C	-1.06210200	1.36721600	2.29846900
C	-0.94816400	2.47528100	3.13741500
C	-0.27123900	3.61629000	2.70153600
C	0.29744800	3.64798600	1.42715900
C	0.18942900	2.54295200	0.58190500

C	0.26596900	-2.39809200	0.96443400
C	0.14235300	-3.57504100	1.70269500
C	-1.07349700	-3.90866800	2.30237300
C	-2.17788400	-3.06707400	2.15535000
C	-2.06734100	-1.89221700	1.41178900
C	5.59748400	-0.14125300	-0.92871600
C	6.62185900	0.05588500	0.17750000
H	-0.56680500	-0.31287100	-2.94765100
H	1.26351100	-0.43337500	-3.27382100
H	2.01836200	0.29863100	0.48477100
H	-2.41490100	2.33883600	-0.60463100
H	-4.50997100	2.63231300	-1.87877000
H	-5.55490100	0.69185200	-3.02870700
H	-4.48644800	-1.54888900	-2.89648500
H	-2.39099900	-1.85157700	-1.62434700
H	-1.57541600	0.47815200	2.65082200
H	-1.38131600	2.44341900	4.13313300
H	-0.17923800	4.47676100	3.35867500
H	0.83789900	4.52831000	1.09148700
H	0.66034800	2.55419500	-0.39530300
H	1.21131500	-2.12543300	0.50260400
H	1.00138300	-4.23149400	1.80756700
H	-1.16273500	-4.82476000	2.87994700
H	-3.12872400	-3.32675100	2.61238000
H	-2.93924500	-1.25759100	1.28279500
H	5.73421200	0.59021000	-1.73483500

H	5.68829500	-1.13461000	-1.38535700
H	7.63800700	-0.05058800	-0.22020400
H	6.52796100	1.05273700	0.62204900
H	6.48357700	-0.68435200	0.97322800

B:

C	0.64130400	0.63350300	-2.53206100
C	0.76723200	0.01065500	-1.14929100
C	2.02113400	-0.16146900	-0.53342600
C	3.29374300	0.08914100	-1.15864900
P	-0.66175100	0.04803200	-0.12609800
O	4.32374400	-0.21764600	-0.28742800
O	3.52027200	0.50585900	-2.29431100
C	-2.13603300	-0.51929200	-1.05225800
C	-1.07552000	1.69312400	0.58883700
C	-0.49259600	-1.10857200	1.28942200
C	-3.43282700	-0.24651100	-0.58520700
C	-4.54357500	-0.79200100	-1.22792900
C	-4.37553900	-1.62192300	-2.33803300
C	-3.08910900	-1.91471900	-2.79585000
C	-1.97545100	-1.37848100	-2.15128500
C	-0.32140900	2.17512000	1.67962900
C	-0.42282000	3.50466100	2.08146800
C	-1.26198100	4.38798900	1.39730900
C	-1.99187300	3.93050100	0.29701400
C	-1.89361700	2.60225100	-0.11152100

C	0.19213700	-2.32214900	1.10831300
C	0.21787700	-3.27467200	2.12528200
C	-0.45330000	-3.03923200	3.32735500
C	-1.15429600	-1.84645700	3.50679800
C	-1.17939300	-0.88741700	2.49347200
C	5.64241700	-0.00824500	-0.80350800
C	6.62748400	-0.39957900	0.28534000
H	1.20518600	0.04840900	-3.26442600
H	-0.39882700	0.70177100	-2.86542900
H	1.07121300	1.64159400	-2.55610800
H	2.08072200	-0.52285000	0.48696500
H	-3.57735300	0.39433700	0.27906400
H	-5.54089000	-0.56845700	-0.85905600
H	-5.24212200	-2.04632100	-2.83754000
H	-2.94998400	-2.56752000	-3.65315100
H	-0.97649300	-1.62697400	-2.49499300
H	0.34660000	1.50799500	2.21656800
H	0.15768400	3.85247000	2.93189500
H	-1.33796800	5.42504500	1.71169700
H	-2.64036600	4.61136000	-0.24811500
H	-2.45711700	2.27069600	-0.97826700
H	0.71260900	-2.51181200	0.17553700
H	0.76272600	-4.20271400	1.97642500
H	-0.43383600	-3.78451500	4.11782300
H	-1.68432400	-1.65849500	4.43654700
H	-1.72988500	0.03509700	2.64602300

H	5.76114700	1.04194200	-1.09596200
H	5.78329100	-0.60918300	-1.70988200
H	7.65601600	-0.25351300	-0.06414900
H	6.47837000	0.20982300	1.18311500
H	6.50380300	-1.45173100	0.56347700

1a...A complex:

C	-1.78155000	-0.39291100	2.24227100
C	-2.37394000	-0.25288200	1.01479800
C	-3.17956300	-1.14796200	0.24616700
C	-3.40747100	-2.49266400	0.63843500
P	-1.98427700	1.27555600	0.12739100
O	-4.25965500	-3.14355300	-0.24455900
O	-2.94051100	-3.09519100	1.61629600
C	-1.24850200	2.55263800	1.20375200
C	-3.52300100	1.97576900	-0.56380900
C	-0.80238700	0.99026200	-1.23216800
C	-2.02918600	3.60418700	1.70564600
C	-1.46448700	4.54423500	2.56812200
C	-0.12259200	4.43891100	2.93620200
C	0.65711900	3.39247300	2.43885200
C	0.10475100	2.44960400	1.57143600
C	-3.52069600	2.73042400	-1.74555400
C	-4.70603100	3.29319200	-2.21829700
C	-5.89848100	3.10557500	-1.51683800
C	-5.90743100	2.34939400	-0.34330500

C	-4.72641100	1.78101000	0.13474600
C	-0.62835500	-0.30099300	-1.75291200
C	0.26815800	-0.51036300	-2.80065200
C	0.98705900	0.55789900	-3.33948300
C	0.82008000	1.84360200	-2.82083700
C	-0.06659400	2.06189400	-1.76712900
C	-4.53211600	-4.51137400	0.06071500
C	-5.52729800	-5.02005600	-0.97008400
H	-1.92425300	-1.31530700	2.79123400
H	-1.18108700	0.38691400	2.69131600
H	-3.68636700	-0.79996600	-0.64551900
H	-3.07373800	3.69134000	1.42558800
H	-2.07542100	5.35613600	2.95240400
H	0.31437400	5.17002200	3.61110200
H	1.70007700	3.30109800	2.72951200
H	0.72743100	1.64292500	1.19531100
H	-2.60070900	2.86845200	-2.30472200
H	-4.69775700	3.87146100	-3.13789500
H	-6.82172800	3.54093000	-1.88934900
H	-6.83618100	2.18935700	0.19670400
H	-4.73929600	1.16724100	1.02946400
H	-1.19590000	-1.12677100	-1.33341300
H	0.40489900	-1.51404700	-3.19251100
H	1.68122600	0.38915700	-4.15832000
H	1.38559300	2.67635800	-3.22964100
H	-0.17001300	3.06053700	-1.35292700

H	-4.93022600	-4.59574400	1.07882100
H	-3.60159000	-5.09348400	0.03494100
H	-5.76675500	-6.07315400	-0.78149000
H	-6.45695900	-4.44213100	-0.93058100
H	-5.11780600	-4.93501700	-1.98255800
C	2.61400600	-3.36637800	0.38602600
C	4.33499800	2.41035500	0.16171900
C	5.43075300	3.22628000	-0.13249900
C	6.66136000	2.67185400	-0.51975500
C	6.82335600	1.28777800	-0.62408100
C	5.72827800	0.48145200	-0.33000700
C	4.50225300	1.03207800	0.05910100
C	5.60786500	-1.00598400	-0.36003700
C	4.20419200	-1.33695400	0.04473700
C	3.50649100	-0.05649900	0.31951400
O	2.35508500	0.14371000	0.69362500
O	6.49189800	-1.79210800	-0.66383000
C	3.83351400	-2.65092600	0.07728600
C	1.39929100	-2.76991400	0.79831700
C	0.28152300	-3.55718000	1.05671100
C	0.35179600	-4.94706800	0.91216300
C	1.54421700	-5.55779700	0.51137000
C	2.66212300	-4.77527400	0.25206600
H	3.37814500	2.83014400	0.45807700
H	5.33331200	4.30633300	-0.06127700
H	7.49622500	3.33130500	-0.74090900

H	7.76787300	0.84351200	-0.92360900
H	4.66202700	-3.30435900	-0.20706900
H	1.34727600	-1.69406600	0.91257100
H	-0.65573700	-3.10381400	1.36831200
H	-0.53171400	-5.54617200	1.11568200
H	1.59971600	-6.63753000	0.40223600
H	3.59214800	-5.24397700	-0.06086700

1a...B complex:

C	1.72873600	1.78063400	1.39898200
C	2.07015100	1.22145200	0.19645300
C	1.51248100	1.36006300	-1.11049900
C	0.31649000	2.08014000	-1.35387900
P	3.30486000	-0.09339800	0.27684200
O	-0.01889800	2.07591100	-2.69801500
O	-0.39747400	2.66756200	-0.52589200
C	4.31857200	-0.02427100	1.79644200
C	4.45304700	0.05337200	-1.13486700
C	2.51069600	-1.73197700	0.25748300
C	5.57816800	0.59217600	1.79509000
C	6.31500900	0.68233700	2.97623200
C	5.80243800	0.15928500	4.16412800
C	4.54974600	-0.45761000	4.17172700
C	3.80887500	-0.55242300	2.99431400
C	5.03652000	-1.07131000	-1.73505300
C	5.94448600	-0.91346400	-2.78200800

C	6.27414300	0.36454900	-3.23699000
C	5.68887400	1.48760400	-2.64959000
C	4.77773900	1.33793200	-1.60383500
C	1.16472800	-1.84752700	-0.12222900
C	0.55187800	-3.10089600	-0.12826300
C	1.27395300	-4.23963700	0.23171100
C	2.61298900	-4.12880000	0.61524900
C	3.23138800	-2.87940700	0.63641700
C	-1.22655800	2.75555700	-3.04129800
C	-1.36518500	2.70262500	-4.55435200
H	0.89635200	2.47148000	1.44012800
H	2.25957000	1.55554100	2.31509100
H	1.99680400	0.90572800	-1.96529900
H	5.98587600	0.99842300	0.87533400
H	7.29006400	1.16105900	2.96576000
H	6.37845400	0.23047100	5.08265600
H	4.14722900	-0.86640800	5.09410000
H	2.83614100	-1.03376700	3.00671900
H	4.77337000	-2.06917400	-1.39970200
H	6.38748400	-1.79004100	-3.24617200
H	6.97843700	0.48464400	-4.05564300
H	5.92973800	2.48259000	-3.01263300
H	4.29620200	2.20938200	-1.17229900
H	0.59869000	-0.96754800	-0.41120100
H	-0.49397500	-3.15870800	-0.41151200
H	0.79399300	-5.21482600	0.22248300

H	3.17441500	-5.01186900	0.90793700
H	4.26351800	-2.79873200	0.96587400
H	-1.19055000	3.78968700	-2.67821300
H	-2.08110500	2.27253300	-2.55022500
H	-2.28421500	3.20991500	-4.87025100
H	-0.51472100	3.19352500	-5.03975900
H	-1.40477600	1.66565600	-4.90462800
C	-4.09901800	2.27750000	0.91830800
C	-6.55865400	-3.13417400	0.07772300
C	-6.29667000	-4.41011900	-0.42781800
C	-5.02881600	-4.73906000	-0.93390400
C	-3.99350400	-3.80054300	-0.94262700
C	-4.25952800	-2.53218600	-0.43455800
C	-5.52352600	-2.20428600	0.06384200
C	-3.36514000	-1.34225800	-0.31462800
C	-4.18333200	-0.23369600	0.26848100
C	-5.54261500	-0.78224800	0.53296800
O	-6.52936800	-0.25169700	1.02917800
O	-2.18428000	-1.30673000	-0.63534700
C	-3.61683800	1.00189500	0.41983500
C	-5.37386000	2.49475700	1.49062600
C	-5.72840900	3.76037200	1.94317500
C	-4.83342200	4.83055300	1.83532700
C	-3.57252300	4.63096900	1.26912500
C	-3.20203000	3.36831000	0.81612000
H	-7.53422500	-2.86269300	0.46980300

H	-7.08286400	-5.16036000	-0.43344400
H	-4.85487400	-5.73790400	-1.32518900
H	-3.01176600	-4.04319800	-1.33877700
H	-2.57779800	1.03638100	0.08326300
H	-6.06849700	1.66758000	1.56895300
H	-6.71000100	3.91589800	2.38316500
H	-5.12084400	5.81684600	2.19179900
H	-2.87450000	5.45902400	1.18113900
H	-2.22321300	3.21233800	0.36857100

TS1:

C	1.60546100	-1.28315100	-1.69733900
C	1.11856200	-0.80022700	-0.52530800
C	0.33540900	-1.51404700	0.46332100
C	0.69345600	-2.88795300	0.77997900
P	1.75426600	0.82842600	-0.03821000
O	0.06258800	-3.30698100	1.92134000
O	1.43112500	-3.62995600	0.13864800
C	0.65560800	1.73240100	1.09995000
C	2.07974600	1.84969900	-1.50868300
C	3.31087300	0.56249700	0.88062600
C	-0.16641900	2.77357800	0.64521100
C	-1.01298600	3.43181100	1.53722200
C	-1.04968100	3.05546900	2.87965400
C	-0.23391500	2.01888900	3.33776100
C	0.61947900	1.35995200	2.45595900

C	1.06429900	1.97536300	-2.47484300
C	1.29043900	2.75781800	-3.60787900
C	2.51528900	3.40229300	-3.79092300
C	3.52584900	3.26705500	-2.83710900
C	3.31277900	2.49266200	-1.69717200
C	3.93214400	-0.69551500	0.86553500
C	5.13179300	-0.88315500	1.55453700
C	5.71731000	0.17352700	2.25241100
C	5.09727100	1.42545300	2.27588000
C	3.89385200	1.62041200	1.60024400
C	0.30938800	-4.66710400	2.31299800
C	-0.50635000	-4.93303800	3.56592500
H	1.41171900	-2.30852200	-1.98374700
H	2.21578000	-0.68447000	-2.36443900
H	-0.07472400	-0.95648500	1.29508800
H	-0.16237600	3.06252200	-0.39935500
H	-1.65908600	4.22456300	1.17433200
H	-1.71923100	3.56405000	3.56718500
H	-0.26463200	1.71722000	4.38048600
H	1.25322700	0.55911000	2.82303800
H	0.10495100	1.47660100	-2.34977200
H	0.50249700	2.85598000	-4.34887000
H	2.68499700	4.00547800	-4.67872900
H	4.48334700	3.75980800	-2.98023400
H	4.10713800	2.38409800	-0.96660600
H	3.47600600	-1.52481800	0.33328000

H	5.60382700	-1.86122300	1.54613400
H	6.65197200	0.02184700	2.78530300
H	5.54496400	2.24771300	2.82681000
H	3.40590400	2.59009200	1.64217600
H	1.38277200	-4.80555100	2.48766800
H	0.02779000	-5.33863900	1.49410800
H	-0.35857400	-5.96679100	3.89860100
H	-0.20522400	-4.26217500	4.37726700
H	-1.57274500	-4.77684100	3.37496600
C	-1.47189300	-2.42818000	-1.66276000
C	-4.04220800	2.82769800	-0.59439200
C	-4.95529800	3.44674300	0.27264400
C	-5.34825100	2.82470900	1.46409700
C	-4.84164900	1.56498900	1.81747400
C	-3.94411600	0.95918100	0.95041400
C	-3.54885500	1.58036300	-0.23688000
C	-3.24177400	-0.36694700	1.04236600
C	-2.45938100	-0.52564400	-0.19569700
C	-2.55838800	0.70229000	-0.95639300
O	-1.95447200	1.09020300	-1.97441800
O	-3.33375200	-1.14894300	1.98594200
C	-1.77789000	-1.74744200	-0.39830900
C	-1.36839400	-1.77753000	-2.90917100
C	-1.13012300	-2.51011500	-4.07276100
C	-0.97684200	-3.89601700	-4.02348200
C	-1.06839100	-4.55548000	-2.79400600

C	-1.31154300	-3.83024300	-1.63281300
H	-3.72960400	3.29796400	-1.52284000
H	-5.36852500	4.41940100	0.01642400
H	-6.05814800	3.32436700	2.11875600
H	-5.13847300	1.06874300	2.73735400
H	-1.97427200	-2.43499800	0.42314300
H	-1.49543000	-0.70235100	-2.95227300
H	-1.06413600	-1.99023100	-5.02554800
H	-0.79045300	-4.46051900	-4.93370900
H	-0.95369600	-5.63491000	-2.74200600
H	-1.39341200	-4.35040500	-0.68266400

Ts1a:

C	0.28149300	1.47884000	1.02400400
C	1.25534700	0.83580000	0.22647300
C	2.02666200	1.36591500	-0.80544400
C	1.95065600	2.74586100	-1.24029800
P	1.59653700	-0.93242500	0.53448700
O	2.82901500	2.97695700	-2.26441700
O	1.22560300	3.63015000	-0.79450300
C	0.84668700	-1.51531200	2.08313400
C	3.40642600	-1.12753700	0.67316200
C	0.98580900	-2.00976900	-0.79896900
C	1.62231200	-1.88135700	3.19340700
C	0.99305700	-2.30392000	4.36486000
C	-0.40089900	-2.35182400	4.43738200

C	-1.17536800	-1.98294500	3.33501600
C	-0.55401300	-1.57533800	2.15699900
C	4.06438700	-2.24517100	0.14172300
C	5.44336500	-2.38600500	0.30575900
C	6.16906500	-1.41814300	1.00039000
C	5.51744000	-0.30113800	1.52962900
C	4.14199800	-0.15012600	1.36537900
C	0.66318600	-1.48027400	-2.05577700
C	0.22395700	-2.33242400	-3.07040500
C	0.11518500	-3.70319300	-2.84205900
C	0.42821000	-4.23279000	-1.58645700
C	0.85356400	-3.39106800	-0.56205500
C	2.81511400	4.30973500	-2.80352300
C	3.81067000	4.34933600	-3.94930100
H	0.37842500	2.55437200	1.07476000
H	-0.06694700	0.99342400	1.92716100
H	2.75117200	0.75272700	-1.32951400
H	2.70537400	-1.83792000	3.14774800
H	1.59494400	-2.59048200	5.22263500
H	-0.88358300	-2.67251800	5.35655400
H	-2.25976500	-1.99109400	3.37503100
H	-1.16511600	-1.28652300	1.31072700
H	3.50868500	-2.99687200	-0.40902600
H	5.94843800	-3.25016100	-0.11603000
H	7.24277000	-1.52883000	1.12387000
H	6.08113400	0.45933800	2.06208000

H	3.64330400	0.73058300	1.75769500
H	0.70636800	-0.41249800	-2.23553800
H	-0.05239100	-1.90726900	-4.02978400
H	-0.23086000	-4.36073400	-3.63472100
H	0.32485200	-5.29791900	-1.40007400
H	1.06614900	-3.80361500	0.42006900
H	3.07641100	5.02236700	-2.01294200
H	1.80036900	4.55274600	-3.13693700
H	3.83375900	5.35174500	-4.39122000
H	4.81915900	4.10309300	-3.60043700
H	3.53387800	3.63430200	-4.73094800
C	-2.15313800	2.78168000	1.02682300
C	-4.81140400	-2.22652800	-0.57711500
C	-5.17278000	-2.94358300	-1.72697200
C	-4.58321600	-2.65953400	-2.96466700
C	-3.61467900	-1.65216200	-3.08436700
C	-3.26550700	-0.94687100	-1.94152000
C	-3.85824400	-1.22656000	-0.70786400
C	-2.27723000	0.16793900	-1.74934200
C	-2.37152900	0.59416900	-0.34609200
C	-3.29030000	-0.30506100	0.33997900
O	-3.56583000	-0.42065200	1.54426200
O	-1.54146400	0.60947300	-2.63542800
C	-1.68002900	1.76757800	0.05503500
C	-2.94733200	2.49404800	2.15211600
C	-3.37928100	3.52133000	2.99066000

C	-3.02920400	4.84818400	2.73269500
C	-2.22970200	5.14481300	1.62602500
C	-1.79079000	4.12359000	0.78780100
H	-5.26191000	-2.43369800	0.38952800
H	-5.92250900	-3.72813600	-1.66007400
H	-4.88353000	-3.22690800	-3.84221400
H	-3.15144300	-1.41892000	-4.03912100
H	-1.15944500	2.21115500	-0.79111900
H	-3.22532500	1.46564700	2.35384400
H	-3.99696600	3.28083900	3.85275400
H	-3.37124000	5.64358300	3.39038800
H	-1.94439800	6.17280600	1.41693900
H	-1.14607600	4.35321200	-0.05603600

Int1:

C	1.07607200	1.28047500	1.92874300
C	0.78883000	0.80243900	0.70863400
C	-0.15951600	1.47101400	-0.26721500
C	0.28838600	2.90357600	-0.57733700
P	1.80147300	-0.59245600	0.12350300
O	-0.28976500	3.32785800	-1.71844200
O	1.03964600	3.59413500	0.08222000
C	1.02929900	-1.66273900	-1.13070600
C	2.42521700	-1.57105400	1.53297100
C	3.25881800	0.13286500	-0.72455500
C	0.58224000	-2.95105600	-0.80610600

C	0.01098700	-3.75435900	-1.79159300
C	-0.12855900	-3.27931600	-3.09609400
C	0.31411800	-1.99722900	-3.42422800
C	0.89808600	-1.19135600	-2.44871500
C	3.80338300	-1.80620400	1.67038400
C	4.27841800	-2.56064300	2.74275400
C	3.38740200	-3.07997500	3.68269400
C	2.01801800	-2.84214800	3.55064600
C	1.52615100	-2.08936200	2.48404400
C	3.63638600	1.46421600	-0.49249600
C	4.77360400	1.98433800	-1.11463800
C	5.54237300	1.18587500	-1.96075300
C	5.17094700	-0.14067000	-2.19556900
C	4.03298700	-0.66559000	-1.58654300
C	-0.02704000	4.69826600	-2.10275100
C	-0.80418700	4.96800700	-3.37706200
H	0.60596800	2.18449900	2.29363400
H	1.77147100	0.78676400	2.60013300
H	-0.15637500	0.94364600	-1.22341600
H	0.65613800	-3.31562100	0.21000000
H	-0.34323700	-4.74708100	-1.53211700
H	-0.58678100	-3.90617300	-3.85568800
H	0.20415400	-1.62052500	-4.43672600
H	1.25920100	-0.20475100	-2.72196100
H	4.50714200	-1.40087300	0.95227500
H	5.34564400	-2.73649500	2.84327000

H	3.76027500	-3.66600600	4.51840600
H	1.32176500	-3.24225200	4.28221500
H	0.46155700	-1.90723200	2.37180800
H	3.03864200	2.10137700	0.15027400
H	5.05100400	3.01922300	-0.93659500
H	6.42625800	1.59523100	-2.44214600
H	5.76280100	-0.76562100	-2.85829200
H	3.74413100	-1.69259600	-1.78767500
H	1.05215000	4.82350200	-2.24007700
H	-0.33483900	5.35621500	-1.28388000
H	-0.63978300	6.00212300	-3.69934900
H	-0.48124100	4.29994600	-4.18187500
H	-1.87657600	4.81957700	-3.21812400
C	-1.97741000	2.11422400	1.49550200
C	-3.20638800	-3.47124000	0.18202700
C	-4.27196500	-4.14650000	-0.44289900
C	-5.15252200	-3.46593800	-1.28499600
C	-4.99574500	-2.08719800	-1.52360700
C	-3.94861400	-1.43379300	-0.90045600
C	-3.06068000	-2.11627600	-0.06073400
C	-3.51939000	0.01793900	-0.94234200
C	-2.36525000	0.13023100	-0.07293800
C	-2.03366600	-1.13243300	0.45221000
O	-1.06682400	-1.48094700	1.19084100
O	-4.06941100	0.89626700	-1.61422000
C	-1.71433800	1.46284500	0.14036900

C	-2.05069500	1.36823100	2.68285400
C	-2.30741500	1.99528700	3.90296900
C	-2.49967500	3.37748500	3.96362600
C	-2.43731600	4.12959800	2.79007600
C	-2.18080600	3.49990600	1.57084100
H	-2.51845400	-3.99122300	0.84429200
H	-4.41470700	-5.21015900	-0.26473500
H	-5.96992400	-4.00627100	-1.75686500
H	-5.67506200	-1.54254700	-2.17420900
H	-2.17608500	2.10979800	-0.61518600
H	-1.90008500	0.29474800	2.64162000
H	-2.36371700	1.39898200	4.81071500
H	-2.70564500	3.86197900	4.91480300
H	-2.60047200	5.20413900	2.81956400
H	-2.15984500	4.09160100	0.65807100

Int1a:

C	3.83844500	0.81154400	-0.82408200
C	4.97348300	1.55440500	-1.09036700
C	5.03109900	2.26617900	-2.30427900
C	3.96892500	2.21763900	-3.20698800
C	2.81567700	1.46065800	-2.92313900
C	2.76708600	0.76794900	-1.72534400
C	1.69590300	-0.11923100	-1.13797300
C	2.17759300	-0.61985500	0.08694100
C	3.47890400	-0.05004400	0.36956200

O	4.17996200	-0.16686200	1.38143900
O	0.55705200	-0.28433300	-1.66908700
C	1.48176000	-1.57243200	1.01182600
C	-0.07773700	-1.33345600	1.15631300
C	-0.54918000	0.08105300	0.92119500
C	0.02161100	1.19625800	1.42325400
C	1.06406900	1.17960200	2.48775800
O	1.10565200	0.36256100	3.38957600
O	1.89535200	2.22476700	2.36387400
C	3.95355600	3.34995800	2.82039100
C	3.00873800	2.26601100	3.29957200
P	-2.04917200	0.32436900	-0.07374500
C	-3.45308500	0.27951800	1.10931600
C	-4.76858900	0.13219000	0.63349400
C	-5.84010800	0.12663400	1.52420700
C	-5.61122300	0.25790800	2.89653600
C	-4.30871700	0.39647000	3.37516400
C	-3.23042700	0.41030600	2.48813200
C	-2.41342700	-1.00040000	-1.27047500
C	-2.94647000	-2.21460500	-0.80478000
C	-3.22673500	-3.24481400	-1.70094400
C	-2.99176900	-3.06666300	-3.06500900
C	-2.46830300	-1.85967300	-3.53106800
C	-2.17182100	-0.82986300	-2.64048600
C	-2.06945300	1.96503200	-0.87540800
C	-1.02480500	2.32312200	-1.74693300

C	-1.03254500	3.57977400	-2.35101700
C	-2.06664000	4.48227400	-2.09500200
C	-3.10129300	4.12919000	-1.22753200
C	-3.10620000	2.87619200	-0.61464000
C	1.69539500	-3.04431400	0.65204600
C	1.37622800	-3.53545400	-0.62420200
C	1.56463800	-4.88094800	-0.93554400
C	2.07710300	-5.76282900	0.02088600
C	2.39975100	-5.28483400	1.29035100
C	2.20793000	-3.93568200	1.60105000
H	5.79612500	1.57607200	-0.38017100
H	5.91362400	2.85433600	-2.54417600
H	4.03582400	2.76595300	-4.14393600
H	1.99116800	1.40802500	-3.63060600
H	1.92863500	-1.42117400	1.99812500
H	-0.35944500	-1.64740700	2.16881800
H	-0.58985400	-1.99831900	0.45953100
H	-0.29179000	2.18631400	1.10332700
H	4.80434600	3.42482000	3.50668000
H	4.33432700	3.10446500	1.82470800
H	3.45601900	4.32497600	2.77868000
H	2.60977100	2.47101500	4.29929300
H	3.48490300	1.28397300	3.30016000
H	-4.95547900	0.01480600	-0.42975000
H	-6.85254600	0.01370800	1.14707100
H	-6.44759800	0.24683300	3.58985400

H	-4.12463700	0.49049700	4.44137200
H	-2.22042200	0.51331500	2.87067200
H	-3.14630600	-2.36008600	0.25205500
H	-3.62834900	-4.18351200	-1.33087800
H	-3.21424800	-3.86856900	-3.76348400
H	-2.27750300	-1.71997200	-4.59098600
H	-1.73668000	0.08959400	-3.00932700
H	-0.22366100	1.61198100	-1.93969500
H	-0.21903100	3.85227100	-3.01714200
H	-2.06382300	5.46155100	-2.56593300
H	-3.90451900	4.83023600	-1.01927400
H	-3.91031600	2.61960300	0.06567700
H	0.98658200	-2.84949000	-1.37203000
H	1.31745600	-5.24298400	-1.93101800
H	2.22802300	-6.81108600	-0.22516500
H	2.80615800	-5.95873700	2.04086400
H	2.47047300	-3.56621300	2.58977800

TS2:

C	0.30558200	-0.68954000	-1.35195600
C	-0.47599400	0.12913000	-0.53511700
C	0.26189000	1.33721300	-0.02910700
C	0.45570900	2.41511500	-1.08984800
P	-2.01147800	-0.38230500	0.10585200
O	0.44604600	3.63930700	-0.51572100
O	0.58375100	2.23637800	-2.28542500

C	-2.23713000	0.12080600	1.85897600
C	-2.24992600	-2.19271300	-0.08830200
C	-3.40749300	0.37196500	-0.82853400
C	-1.25458700	-0.25887900	2.79188900
C	-1.38767200	0.10970000	4.13071800
C	-2.48296100	0.86593000	4.55153400
C	-3.44737800	1.26381300	3.62550800
C	-3.32688700	0.89670000	2.28473600
C	-3.01938600	-2.69787400	-1.14916800
C	-3.16147000	-4.07501100	-1.32284100
C	-2.53992600	-4.95955700	-0.44154300
C	-1.76258900	-4.46322000	0.60633000
C	-1.60989700	-3.08873000	0.78349300
C	-3.11874500	1.27215200	-1.86251900
C	-4.15607400	1.85589200	-2.59435700
C	-5.48315800	1.54091400	-2.30512400
C	-5.77838600	0.63194100	-1.28453900
C	-4.74780200	0.04779000	-0.55044800
C	0.72565100	4.76868200	-1.37502600
C	-0.54591500	5.30456900	-2.01620600
H	0.92883100	-0.22231500	-2.10746400
H	-0.00020600	-1.70943800	-1.57972800
H	-0.24749800	1.82918200	0.80408100
H	-0.37676200	-0.81806200	2.47480800
H	-0.62424700	-0.19135900	4.84262200
H	-2.57889600	1.15378300	5.59505600

H	-4.29371000	1.86736300	3.94172100
H	-4.07648600	1.22888500	1.57635600
H	-3.50671700	-2.02246000	-1.84320700
H	-3.75611300	-4.45235700	-2.15007300
H	-2.65257400	-6.03190500	-0.57632900
H	-1.26203600	-5.14572100	1.28706600
H	-0.96041200	-2.72800700	1.57170100
H	-2.08470900	1.50007700	-2.10484200
H	-3.92143900	2.55229200	-3.39438700
H	-6.28825800	1.99442700	-2.87687600
H	-6.81078900	0.37487500	-1.06387300
H	-4.98735400	-0.66817700	0.23117300
H	1.45317900	4.46470300	-2.13072600
H	1.18200000	5.50619900	-0.71046300
H	-1.29029700	5.55851600	-1.25396600
H	-0.32091400	6.21011100	-2.59184800
H	-0.97446900	4.56382200	-2.69747700
C	2.73744600	1.81894400	0.76217000
C	4.39846400	-3.00020400	-1.74599100
C	4.60016400	-4.34314600	-1.39465700
C	3.91899300	-4.91167300	-0.31203200
C	3.01729800	-4.15306400	0.44858300
C	2.82942100	-2.82366500	0.09707700
C	3.51246900	-2.25552100	-0.98165500
C	1.95934300	-1.77011500	0.71244400
C	2.08200000	-0.55527200	-0.08961800

C	3.10189000	-0.81236600	-1.12225700
O	3.50511400	-0.07707600	-2.02127600
O	1.25369400	-1.94465100	1.71876600
C	1.66813500	0.75359500	0.56192000
C	3.46757500	2.39075800	-0.29282800
C	4.41268000	3.38702100	-0.04355200
C	4.64816800	3.83704400	1.25705100
C	3.92941600	3.27750500	2.31350700
C	2.98570200	2.28060800	2.06353600
H	4.91896500	-2.54499200	-2.58382900
H	5.29561200	-4.95172100	-1.96717900
H	4.09457700	-5.95415400	-0.05836800
H	2.48313900	-4.58286800	1.29142600
H	1.36213600	0.44664000	1.56672500
H	3.31509100	2.02971100	-1.30316800
H	4.97393000	3.80792900	-0.87441200
H	5.38767600	4.61144700	1.44543700
H	4.10311400	3.61302600	3.33313900
H	2.43123000	1.85001900	2.89491100

TS2a:

C	3.80682400	-0.81476600	0.68418300
C	4.96661000	-1.52356000	0.96311700
C	5.23636000	-1.84235700	2.30159800
C	4.35993000	-1.45282100	3.32158600
C	3.19003800	-0.73701800	3.03068500

C	2.92737500	-0.42938400	1.70217300
C	1.78756900	0.33857400	1.09786700
C	1.94751900	0.29834600	-0.35461200
C	3.27136400	-0.31391400	-0.62593200
O	3.84166500	-0.41304100	-1.70840400
O	0.86125400	0.84639600	1.74575600
C	1.38362100	1.31381800	-1.33652600
C	-0.18828700	1.19500600	-1.47038500
C	-0.62297100	-0.08301900	-0.79199800
C	0.36321500	-1.08661400	-0.74641700
C	0.97244700	-1.61728200	-2.00855700
O	0.75300500	-1.20159900	-3.13119300
O	1.77568000	-2.66892400	-1.74330700
C	3.38432700	-4.32541300	-2.35072900
C	2.50674000	-3.20354500	-2.87225800
P	-2.09562700	-0.16707500	0.12437400
C	-2.58450000	1.41855600	0.91216100
C	-2.25569900	1.70321700	2.24556900
C	-2.57691400	2.94208600	2.79852800
C	-3.21249200	3.91563500	2.02576100
C	-3.53057100	3.64616800	0.69439900
C	-3.22307000	2.40364400	0.13971300
C	-2.09237400	-1.52246100	1.36081000
C	-1.11936700	-1.54780700	2.37717000
C	-1.11858500	-2.57829300	3.31729800
C	-2.07504700	-3.59309600	3.25625200

C	-3.03530600	-3.57872000	2.24490200
C	-3.04553300	-2.55178000	1.30027200
C	-3.50572100	-0.53043700	-1.00997500
C	-3.22290300	-0.98275000	-2.30575600
C	-4.26532900	-1.28659600	-3.18476100
C	-5.59128100	-1.14179800	-2.77705400
C	-5.88007800	-0.68830300	-1.48639600
C	-4.84373300	-0.38026000	-0.60661000
C	1.84929700	2.74518300	-1.08656700
C	1.38451700	3.51316400	-0.00625100
C	1.83357600	4.81986200	0.18321200
C	2.75370700	5.38890800	-0.70085200
C	3.22555300	4.63497200	-1.77498500
C	2.77626000	3.32616400	-1.96262200
H	5.64305200	-1.80971000	0.16258400
H	6.13996000	-2.39112900	2.55423000
H	4.59621900	-1.70320900	4.35275700
H	2.51115100	-0.41730600	3.81662700
H	1.80490000	1.01633000	-2.30135200
H	-0.41926900	1.21560900	-2.54223000
H	-0.68407500	2.06109200	-1.02130900
H	0.31333600	-1.85430300	0.02499900
H	3.95767400	-4.76237700	-3.17591400
H	4.08846400	-3.94700800	-1.60326600
H	2.78274500	-5.11704400	-1.89142200
H	1.78927600	-3.55506200	-3.62123600

H	3.09392100	-2.39336100	-3.31115500
H	-1.74391800	0.96770500	2.85342300
H	-2.32273200	3.14702600	3.83457800
H	-3.45605300	4.88189200	2.45899400
H	-4.01919000	4.40057200	0.08418600
H	-3.48728900	2.20255400	-0.89361700
H	-0.35903200	-0.77327000	2.42287900
H	-0.36035500	-2.58807300	4.09528200
H	-2.06770400	-4.39476400	3.98983000
H	-3.77761400	-4.36969700	2.18378900
H	-3.79389700	-2.56169800	0.51641800
H	-2.18833500	-1.08546100	-2.62312700
H	-4.03696300	-1.63215800	-4.18909300
H	-6.40086200	-1.37660000	-3.46293100
H	-6.91216000	-0.57004000	-1.16756100
H	-5.07667100	-0.01899300	0.39140900
H	0.68310700	3.07544100	0.69687800
H	1.46293800	5.39657400	1.02751400
H	3.09955300	6.40876300	-0.55169300
H	3.94399900	5.06280600	-2.47005800
H	3.15485300	2.74049700	-2.79692400

Int2:

C	-0.45621800	0.78750100	-1.12182900
C	0.50507200	-0.04649300	-0.33459600
C	-0.22768100	-1.26752700	0.15255700

C	-0.27454800	-2.41887000	-0.85353500
P	2.09768500	0.35577600	0.03747600
O	-0.30591900	-3.61024200	-0.21386500
O	-0.26632800	-2.32399800	-2.06656200
C	2.52117200	-0.19206000	1.74757600
C	2.36176200	2.17068200	-0.12035600
C	3.47099800	-0.32010000	-1.02694200
C	3.67713600	-0.91640100	2.07113200
C	3.92352100	-1.30077400	3.39063800
C	3.01938000	-0.96787400	4.39952300
C	1.85910500	-0.25733500	4.08451300
C	1.60394000	0.12333600	2.76698300
C	2.72303500	2.71844100	-1.36150200
C	2.84535600	4.10027200	-1.51568300
C	2.62322100	4.94765800	-0.42958900
C	2.26854700	4.41010700	0.80912800
C	2.13032300	3.03055800	0.96292500
C	3.12976700	-1.24158600	-2.02488000
C	4.11503600	-1.76661700	-2.86636400
C	5.44424300	-1.36996000	-2.72252500
C	5.79134100	-0.43807100	-1.73926600
C	4.81039500	0.08708700	-0.89894400
C	-0.41447500	-4.78208600	-1.05002200
C	-0.45058300	-5.99177100	-0.13465100
H	-0.68010900	0.37593900	-2.11545900
H	-0.14795900	1.83142300	-1.25310200

H	0.19449100	-1.69549700	1.06804100
H	4.38254400	-1.19386300	1.29595500
H	4.82098700	-1.86649300	3.62659000
H	3.21337700	-1.26836200	5.42588400
H	1.14528200	-0.00426300	4.86386700
H	0.68847300	0.65583800	2.52018800
H	2.91246400	2.06666000	-2.20867400
H	3.11734400	4.51162300	-2.48402200
H	2.72567500	6.02319400	-0.54773800
H	2.09488900	5.06448200	1.65900000
H	1.84133800	2.62820400	1.92731200
H	2.08958100	-1.53116100	-2.15300700
H	3.83875600	-2.48009600	-3.63823300
H	6.20927800	-1.77616300	-3.37922200
H	6.82439300	-0.11666000	-1.63303800
H	5.08779000	0.82276300	-0.14768700
H	0.43838900	-4.80845100	-1.73650900
H	-1.32404300	-4.69882800	-1.65325100
H	-0.53509900	-6.90819600	-0.72945700
H	0.46153600	-6.05451500	0.46792300
H	-1.30863000	-5.93845000	0.54283300
C	-2.83888200	-1.67000300	0.49041400
C	-4.74956700	2.80695800	-1.45680900
C	-5.18430800	4.01575300	-0.91067600
C	-4.53983600	4.57834100	0.20477800
C	-3.44820900	3.94338700	0.79899200

C	-3.02055800	2.73435800	0.25120900
C	-3.66277300	2.17452300	-0.85578500
C	-1.91840400	1.83845800	0.69438500
C	-1.80801900	0.66722500	-0.29122200
C	-2.99207500	0.89955500	-1.24324200
O	-3.28724200	0.23495200	-2.21938000
O	-1.23742400	2.01130800	1.69410200
C	-1.67406600	-0.69329900	0.50306000
C	-3.31575100	-2.29869600	-0.67268500
C	-4.36704200	-3.21383500	-0.60746900
C	-4.96609300	-3.52363400	0.61521300
C	-4.50489200	-2.90661200	1.77788200
C	-3.45342600	-1.99163300	1.71028100
H	-5.23526600	2.36032300	-2.31923500
H	-6.03346000	4.53239000	-1.35006100
H	-4.90090700	5.52093100	0.60759800
H	-2.94072800	4.36585400	1.66108900
H	-1.55936300	-0.37745100	1.54338700
H	-2.87773600	-2.05628600	-1.63296600
H	-4.72337900	-3.68155400	-1.52197700
H	-5.78628900	-4.23573000	0.65985700
H	-4.96097100	-3.13500400	2.73800200
H	-3.09827400	-1.51917600	2.62391400

Int2a:

C	3.89912600	-1.03278300	0.48446800
C	5.11639700	-1.70195600	0.60455100
C	5.78133500	-1.63045000	1.82920200
C	5.24070300	-0.90227300	2.90380700
C	4.02426400	-0.23089200	2.77659200
C	3.36171500	-0.30873800	1.55194300
C	2.07105900	0.31681300	1.15003600
C	1.75783600	-0.10950100	-0.29235100
C	2.99761800	-0.93011900	-0.69322700
O	3.22343600	-1.39016900	-1.79861100
O	1.38800500	1.02284400	1.87474400
C	1.47233500	1.04518200	-1.31359400
C	0.00166500	1.45726600	-1.05579300
C	-0.62399300	0.22453800	-0.41880300
C	0.37499200	-0.89420500	-0.30548700
C	0.38181800	-1.91514200	-1.45638700
O	-0.01115200	-1.72601200	-2.58907300
O	0.88506900	-3.09710100	-1.03536500
C	1.67319900	-5.32506500	-1.38654800
C	1.06856900	-4.10480100	-2.05537700
P	-2.20942800	0.18983800	0.15456800
C	-3.58452300	-0.27136600	-1.01768700
C	-4.94075400	-0.05438500	-0.71942500
C	-5.92971400	-0.40864600	-1.63624600
C	-5.57320600	-0.97452800	-2.86451200

C	-4.22849900	-1.18128300	-3.17156600
C	-3.23440100	-0.82942900	-2.25356000
C	-2.74686000	1.87234300	0.68836900
C	-3.16720600	2.80091700	-0.27693000
C	-3.48384300	4.10957400	0.08974600
C	-3.39905300	4.50203100	1.42621400
C	-2.98871800	3.58294100	2.39362700
C	-2.65749000	2.27824000	2.02717900
C	-2.38216000	-0.98280900	1.56189200
C	-1.44360800	-0.90033000	2.60660900
C	-1.53196600	-1.75921000	3.70209100
C	-2.54843500	-2.71483400	3.76546900
C	-3.47508600	-2.81102700	2.72715600
C	-3.39414400	-1.95108900	1.63003100
C	2.50180400	2.16109300	-1.34783500
C	2.54417700	3.18278900	-0.38556800
C	3.51619000	4.18207900	-0.44690900
C	4.46637600	4.18258000	-1.46999000
C	4.43755000	3.17240000	-2.43184800
C	3.46430000	2.17413700	-2.36853700
H	5.52341000	-2.25618700	-0.23586900
H	6.73236300	-2.14024100	1.95788800
H	5.78379200	-0.86191200	3.84426800
H	3.59780700	0.34093900	3.59530400
H	1.50601100	0.53933300	-2.28459300
H	-0.43608700	1.76368700	-2.01778900

H	-0.05553500	2.33238900	-0.39578400
H	0.27963000	-1.48687600	0.61277900
H	1.82766700	-6.11803600	-2.12679200
H	2.64069400	-5.08128800	-0.93605000
H	1.01392600	-5.71000800	-0.60148000
H	0.09854500	-4.32468900	-2.51299600
H	1.72185200	-3.69343200	-2.83039600
H	-5.22518100	0.39865900	0.22733300
H	-6.97651500	-0.23788500	-1.39759000
H	-6.34457900	-1.24572000	-3.58088000
H	-3.94746800	-1.61240900	-4.12888600
H	-2.18436100	-0.97728600	-2.49520000
H	-3.25404100	2.50157100	-1.31734200
H	-3.80022500	4.81967700	-0.66963200
H	-3.65218600	5.51929500	1.71292700
H	-2.92410400	3.88054900	3.43679500
H	-2.33335100	1.57707000	2.78866900
H	-0.64027800	-0.17089000	2.54787500
H	-0.80170400	-1.68459400	4.50339700
H	-2.61409400	-3.38547900	4.61825100
H	-4.26249700	-3.55902800	2.76592200
H	-4.11650200	-2.04198200	0.82637100
H	1.81703700	3.19320400	0.42005200
H	3.52871500	4.96458200	0.30787700
H	5.22020000	4.96434900	-1.51749300
H	5.17003100	3.16097800	-3.23513900

H	3.44937600	1.38721000	-3.11869900

TS3:

C	-0.09515600	0.67005600	-1.58596700
C	0.80924100	-0.37698500	-0.91415400
C	-0.17390100	-1.39532400	-0.33192700
C	-0.56783000	-2.43550600	-1.29423700
P	2.24656700	0.11168200	-0.00648200
O	-1.79719900	-2.96378700	-1.06494300
O	0.15824900	-2.88487000	-2.18320900
C	2.17286400	0.17659600	1.83374500
C	2.84517500	1.72686000	-0.63038200
C	3.65268300	-1.02177900	-0.38499600
C	2.75103300	-0.83210100	2.62127400
C	2.60023300	-0.81817900	4.00841600
C	1.86995900	0.19784100	4.62587500
C	1.27294500	1.19266500	3.84860900
C	1.41018200	1.17998400	2.46007200
C	3.00705000	1.86395000	-2.02059300
C	3.50615500	3.04855200	-2.55699600
C	3.86039300	4.10552600	-1.71481100
C	3.71782600	3.96978600	-0.33474500
C	3.21507000	2.78550800	0.20884500
C	3.51087300	-2.08128800	-1.29287200
C	4.61300500	-2.88400000	-1.60239300
C	5.85787200	-2.62898500	-1.02998100

C	6.00870800	-1.56197800	-0.13943600
C	4.91405700	-0.76293200	0.18060700
C	-2.18761300	-4.02390600	-1.95627400
C	-3.52627700	-4.56197600	-1.48188000
H	-0.36906600	0.32252300	-2.58765700
H	0.33821100	1.67094200	-1.67676800
H	1.07540900	-1.63677000	-0.69822100
H	3.31785300	-1.63129000	2.15704600
H	3.05324000	-1.60568900	4.60434900
H	1.75655000	0.20805900	5.70660600
H	0.68698300	1.97737500	4.31911200
H	0.89592600	1.92868300	1.86565700
H	2.74210700	1.04316300	-2.68036600
H	3.62128500	3.14420400	-3.63299500
H	4.25050300	5.02880000	-2.13438000
H	3.99584200	4.78567300	0.32658000
H	3.11318200	2.69562700	1.28435300
H	2.55286000	-2.28466500	-1.76552600
H	4.48998900	-3.70706900	-2.30060500
H	6.71182100	-3.25314600	-1.27963600
H	6.97851100	-1.35094300	0.30293900
H	5.04279400	0.06643500	0.87086700
H	-1.41496900	-4.79937200	-1.95038300
H	-2.24842800	-3.62785200	-2.97529300
H	-3.83611500	-5.39909600	-2.11830200
H	-3.46062000	-4.91736200	-0.44843800

H	-4.30209700	-3.79115200	-1.52943400
C	-2.37074700	-0.99505600	1.19314800
C	-4.90300700	1.83128900	-1.71533900
C	-5.59208200	2.95030000	-1.24504600
C	-4.99967000	3.82994100	-0.32229400
C	-3.70511300	3.60948500	0.14987700
C	-3.02471800	2.48546800	-0.31677800
C	-3.61481800	1.60960400	-1.23238100
C	-1.64808800	2.01894600	0.00002800
C	-1.40348700	0.68957000	-0.70730100
C	-2.65048100	0.52583900	-1.58150900
O	-2.81471400	-0.29886800	-2.46387300
O	-0.85717800	2.61148200	0.72163200
C	-1.16868700	-0.48766400	0.40469700
C	-3.58804800	-1.42972100	0.64630800
C	-4.63750500	-1.84280400	1.46771400
C	-4.49732200	-1.84647400	2.85628300
C	-3.29198800	-1.42643600	3.41745200
C	-2.25035900	-1.00046300	2.59294600
H	-5.34536000	1.14741300	-2.43358300
H	-6.60088700	3.14996800	-1.59647300
H	-5.56062400	4.69419700	0.02323900
H	-3.23251600	4.28410000	0.85751100
H	-0.57242600	0.04560300	1.14726100
H	-3.71405300	-1.46994500	-0.42654200
H	-5.57024300	-2.17092500	1.01508700

H	-5.31707300	-2.17292900	3.49133500
H	-3.16161900	-1.42145100	4.49696100
H	-1.31930300	-0.66524200	3.04444500

TS3a:

C	-3.31702300	-1.56323500	1.34251900
C	-3.58482000	-2.15772900	2.57388000
C	-4.66147800	-3.04177700	2.65020800
C	-5.45169100	-3.32197100	1.52136600
C	-5.18073100	-2.72488700	0.29057100
C	-4.10474500	-1.83986300	0.21957800
C	-3.58887100	-1.09904700	-0.95425700
C	-2.41130800	-0.21581000	-0.49248900
C	-2.25984800	-0.57563100	0.99934400
O	-1.49091700	-0.05032600	1.78131700
O	-3.97086000	-1.19982600	-2.10737100
C	-2.57947400	1.33789900	-0.67389500
C	-1.86835000	1.63297600	-2.02920000
C	-0.81703900	0.56900400	-2.25895300
C	-1.19332200	-0.48506400	-1.40782700
C	-0.41132200	-1.76550000	-1.17661000
O	-0.65005200	-2.49081400	-0.23111700
O	0.51301700	-1.99215800	-2.10705100
C	2.30875800	-3.24150900	-3.07375500
C	1.31220600	-3.19354300	-1.93317400
P	2.60099000	0.22745400	0.26266900

C	2.96846600	1.83686900	-0.58417300
C	2.32976800	2.06622200	-1.81475200
C	2.55817700	3.24886000	-2.52276400
C	3.41338400	4.22287700	-2.00634500
C	4.04079600	4.01100900	-0.77626300
C	3.82226200	2.82667600	-0.07183400
C	4.08533800	-0.80156900	-0.16471000
C	4.98276100	-0.47664700	-1.19291100
C	6.01499300	-1.35172800	-1.54372600
C	6.17220600	-2.56383100	-0.87206500
C	5.28524500	-2.90014900	0.15437500
C	4.24949400	-2.03258200	0.49811800
C	2.88929400	0.60419300	2.05284200
C	1.74781600	0.84178400	2.83619200
C	1.87010300	1.14743200	4.19323600
C	3.13063600	1.20559700	4.78925800
C	4.27167900	0.95450000	4.02363500
C	4.15256800	0.65614000	2.66559400
C	-3.96459100	1.92204200	-0.47805300
C	-4.97220800	1.81274600	-1.44981200
C	-6.23091600	2.37597600	-1.23885100
C	-6.50867600	3.06085000	-0.05426700
C	-5.51725000	3.17629800	0.92051900
C	-4.25904500	2.61178300	0.70738700
H	-2.96535900	-1.93460300	3.43695600
H	-4.89626200	-3.52441600	3.59500000

H	-6.28396200	-4.01425400	1.61375000
H	-5.78116000	-2.93233200	-0.58986200
H	-1.93506300	1.75115600	0.11180400
H	-1.40532900	2.62658500	-2.02889100
H	-2.56071700	1.63326100	-2.88119800
H	-1.47802000	-0.57588100	-2.62129000
H	2.92016800	-4.14613700	-2.98621000
H	1.79816000	-3.26010700	-4.04195000
H	2.97491400	-2.37446300	-3.04301700
H	1.80619700	-3.13858800	-0.95984400
H	0.63916700	-4.05712600	-1.92875900
H	1.63267300	1.33117000	-2.21365200
H	2.05705000	3.40961000	-3.47401900
H	3.58488700	5.14629500	-2.55390000
H	4.70187800	4.76934800	-0.36386200
H	4.31129100	2.67718700	0.88598600
H	4.87995300	0.46615800	-1.72091800
H	6.70110300	-1.07801200	-2.34155300
H	6.97747600	-3.24125100	-1.14381600
H	5.39907800	-3.84081700	0.68760000
H	3.56615000	-2.30840900	1.29836000
H	0.76089500	0.76984400	2.38618800
H	0.97702000	1.32792700	4.78600300
H	3.22480700	1.43649200	5.84739400
H	5.25600100	0.99046600	4.48411300
H	5.04546900	0.45176900	2.08140800

H	-4.77861400	1.27448300	-2.37244100
H	-6.99598000	2.28052400	-2.00503000
H	-7.48867700	3.50260100	0.10571000
H	-5.71954100	3.70900900	1.84610800
H	-3.48945200	2.70773400	1.46996400

3a:

C	-1.42810800	3.95422400	-0.99312900
C	-1.26786100	4.16661000	0.38785300
C	-0.78434200	3.15622700	1.21873000
C	-0.46334300	1.93096700	0.63592700
C	-0.62347000	1.71925100	-0.73758200
C	-1.10714700	2.72689400	-1.57192100
C	0.04901700	0.69889700	1.28771100
C	0.20346400	-0.39139700	0.20470100
C	-0.20853900	0.34008500	-1.09679700
C	1.58917200	-1.00049500	0.07541200
C	1.54190900	-2.33070500	-0.08410400
C	0.13284400	-2.84966000	-0.05542200
C	-0.65832800	-1.66748600	0.56385900
C	2.77958600	-0.13025400	0.01939900
O	-0.18336800	-0.13790700	-2.21531200
O	0.25019300	0.53930800	2.47605300
C	-2.14529600	-1.60442700	0.27525000
C	-3.03527500	-1.35404400	1.33018200
C	-4.41197600	-1.28905000	1.11236300

C	-4.92538000	-1.47754400	-0.17112900
C	-4.05139000	-1.72621200	-1.23107700
C	-2.67507000	-1.78853700	-1.01135500
O	3.93578000	-0.82092900	-0.04901800
C	5.14152700	-0.02455100	-0.11812800
O	2.71528300	1.08706100	0.03133600
C	6.31700600	-0.98215000	-0.16170500
H	-1.80724500	4.76131800	-1.61412400
H	-1.52534100	5.13457100	0.80927200
H	-0.65475700	3.30657600	2.28614000
H	-1.22513800	2.54805400	-2.63630700
H	2.41388200	-2.95451700	-0.25076500
H	0.01742900	-3.76765000	0.53377900
H	-0.19909400	-3.08556100	-1.07515800
H	-0.53392200	-1.74879900	1.65049600
H	-2.64143200	-1.21002900	2.33380900
H	-5.08145600	-1.09620300	1.94663500
H	-5.99733500	-1.43262100	-0.34453200
H	-4.44082300	-1.87275100	-2.23522100
H	-2.00910800	-1.96492200	-1.84999300
H	5.09315000	0.60960600	-1.00929100
H	5.17765600	0.63399700	0.75543300
H	6.25821600	-1.63541900	-1.03827500
H	7.25367500	-0.41671600	-0.21593000
H	6.34453000	-1.60904500	0.73531500

4a:

C	0.19848400	-1.65246400	1.74297100
C	1.60974800	-1.50790700	1.25714300
C	1.70801400	-0.72084000	0.17947800
C	2.93595900	-0.42811900	-0.59309700
O	4.05512400	-0.87843300	0.02048100
O	2.93904700	0.13804900	-1.66938800
C	5.29091600	-0.66429900	-0.69729300
C	6.41496400	-1.22404300	0.15414700
H	0.05998000	-1.18648600	2.72828000
H	-0.08755200	-2.70781200	1.83724700
H	2.44964300	-2.00529100	1.73065700
H	5.40946100	0.40813600	-0.88267100
H	5.22531300	-1.16149500	-1.67069200
H	7.37398300	-1.08031100	-0.35549300
H	6.46092000	-0.71748600	1.12361400
H	6.27628300	-2.29556500	0.33089700
C	0.31511300	1.37304800	-0.22454300
C	-4.21686200	0.43445300	0.53631500
C	-5.25090800	0.00293100	-0.29446800
C	-5.07603400	-1.09071100	-1.16158600
C	-3.86237500	-1.77583600	-1.21741200
C	-2.82624000	-1.33272300	-0.39514400
C	-3.00035700	-0.24433700	0.46772600
C	-1.45594300	-1.89231500	-0.23108300
C	-0.66144300	-0.93135700	0.67274500

C	-1.76010200	-0.03098400	1.26353700
O	-1.65365600	0.67816900	2.24484000
O	-1.03472900	-2.92027500	-0.72517800
C	0.37816200	-0.14746100	-0.27245100
C	0.79998100	2.09644600	0.87353400
C	0.72765800	3.48838000	0.89584700
C	0.16812200	4.18129500	-0.17975100
C	-0.31760500	3.47168700	-1.27832300
C	-0.24216200	2.07844800	-1.29790800
H	-4.34158200	1.27086500	1.21724500
H	-6.20981000	0.51348200	-0.27139500
H	-5.90303800	-1.40578400	-1.79202600
H	-3.71648100	-2.62810600	-1.87423100
H	0.19483800	-0.44204900	-1.31201100
H	1.23269800	1.56655800	1.71681900
H	1.10789000	4.03270200	1.75626300
H	0.11449500	5.26666100	-0.16230600
H	-0.74767500	4.00079500	-2.12474400
H	-0.60818400	1.53134900	-2.16379300