Supplementary Information (SI) for Organic Chemistry Frontiers.

A Visible Light-Mediated Three-Component Strategy Based on the Ring-Opening of Cyclic Ethers with Aryldiazoacetates and Nucleophiles

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ELECTRONIC SUPPLEMENTARY INFORMATION

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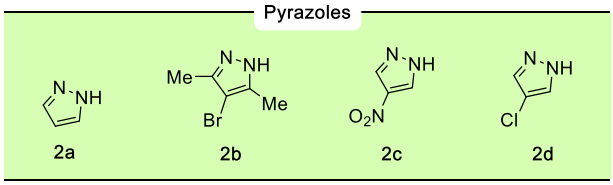
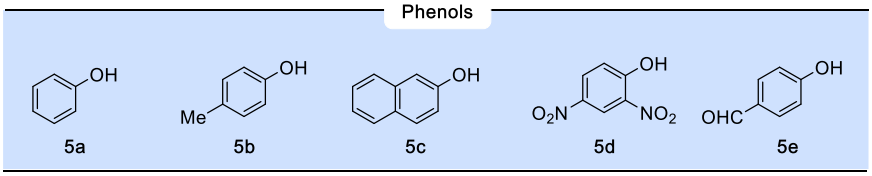
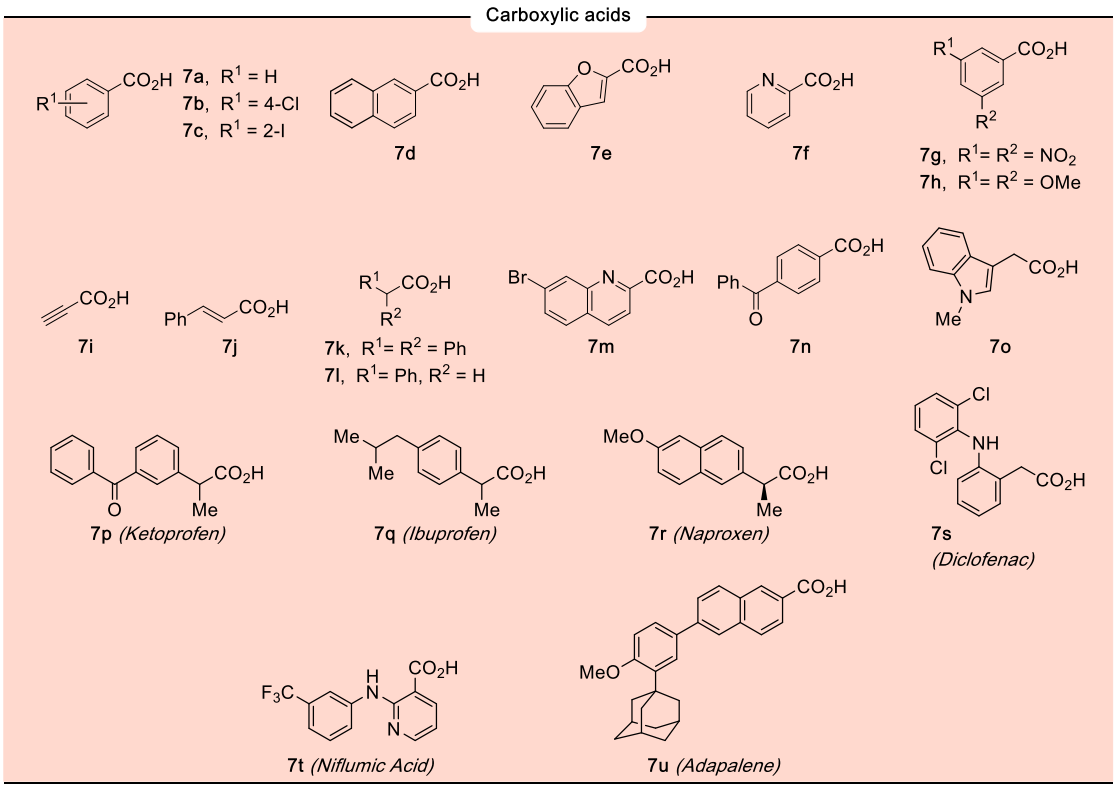
1. MATERIALS AND METHODS

All reactions were carried out under air, in oven dried glassware with magnetic stirring, unless otherwise noted. All reagents employed in this work were purchased from Sigma-Aldrich/Merck or Oakwood and used as such without further purification. All solvents employed in the reactions were distilled from appropriate drying agents prior to use. Organic solutions were concentrated under reduced pressure on a IKA rotary evaporator RV-10 Control. Reactions were monitored by thin-layer chromatography (TLC) on Silica gel 60 F_{254} aluminium plates (Merck). Chromatograms were visualized by fluorescence quenching with UV light at 254 nm or by staining using anisaldehyde or vanillin solution. Flash column chromatography was performed using Merck silica gel 60 (particle size 35-70µm). ^{1}H and ^{13}C NMR spectra were recorded on Bruker AV–250. Chemical shifts (δ) are given in parts per million, referenced to the residual peak of $CDCl_3$, δ = 7.26 (^{1}H NMR) and δ = 77.0 (^{13}C NMR) as internal references. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, quint. = quintuplet, sext. = sextuplet, sept. = septuplet, m = multiplet, br s = broad singlet. High-resolution mass spectra were recorded on Q Exactive Orbitrap spectrometer working with an electronspray ionization (ESI). Infrared spectra were performed on the Agilent Cary 630 FTIR spectrometer. Melting points was mesured on Metler Toledo MP50 Melting Point System and are uncorrected. Commercially available blue LED lamps (PAR38 Reflector Flood, Medium Base E26, from Westinghouse) emitting only in the blue region (maximum wavelength at 452 nm, no filters are used), 15W and intensity measured with an approximate value of 31 mW/ cm2 were employed.

1.1. MOLECULES COMMERCIALLY AVAILABLE EMPLOYED IN THIS WORK







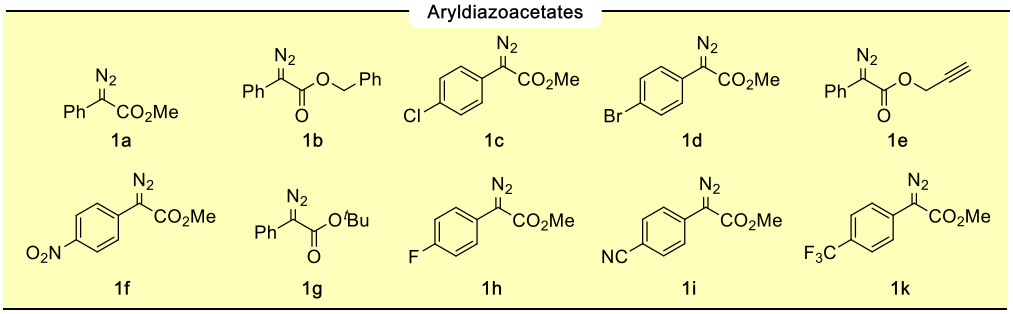
1.2. PREPARATION OF ARYLDIAZOACETATES 1

1.2.1 Known Aryldiazoacetates

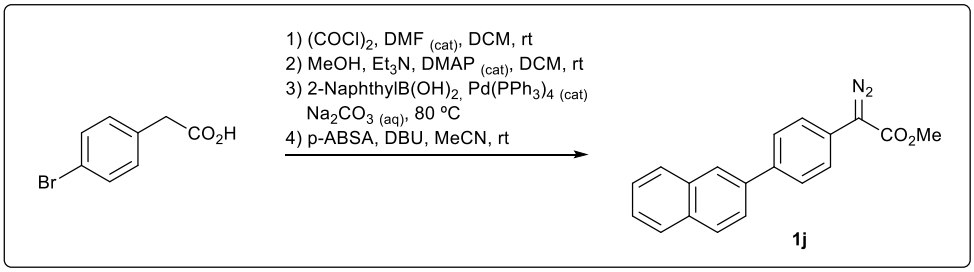
The following aryldiazoacetates have been prepared as previously described in the literature, being numbered following their order of appearance in the manuscript: *methyl 2-diazo-2-phenylacetate* (**1a**), [1] *benzyl 2-diazo-2-phenylacetate* (**1b**),[1] *methyl 2-(4-chlorophenyl)-2-diazoacetate* (**1c**),[1] *methyl 2-(4-bromophenyl)-2-diazoacetate* (**1d**),[1] *prop-2-yn-1-yl 2-diazo-2-phenylacetate*

[1] M. L. Stivanin, A. A. G. Fernandes, A. F. da Silva, C. Y. Okada Jr, I. D. Jurberg, *Adv. Synth. Catal.* 2020, ***362***, 1106 – 1111.

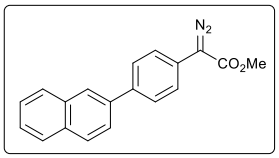
(**1e**), [2] *methyl 2-diazo-2-(4-nitrophenyl)acetate* (**1f**), [3] *tert-butyl 2-diazo-2-phenylacetate* (**1g**),[3] *methyl 2-diazo-2-(4-fluorophenyl)acetate* (**1h**),[4] *methyl 2-(4-cyanophenyl)-2-diazoacetate* (**1i**), [5] *methyl 2-diazo-2-(4-(trifluoromethyl)phenyl)acetate* (**1k**).[1]



1.2.2 New Aryldiazoacetates



Molecule 1j: *methyl 2-diazo-2-(4-(naphthalen-2-yl)phenyl)acetate*



Step 1: Under nitrogen, at room temperature, a round bottomed flask is charged with 2-(4-bromophenyl)acetic acid (1.07 g, 5 mmol, 1 equiv.), dry DCM (25 mL, 0.2 M), oxalyl chloride (847 µL, 10 mmol, 2 equiv.). Then, DMF (2 drops) is added and the reaction is allowed to stir overnight at room temperature. Then, the reaction mixture is concentrated under reduced pressure. The corresponding acyl chloride is obtained clean and is directly employed in the next step. *Step 2:* Under nitrogen, at room temperature, a round bottom flask is charged with dry DCM (25 mL, 0.2 M), MeOH (242 µL, 6 mmol, 1.2 equiv.), Et_3N (834 µL, 6 mmol, 1.2 equiv.)

[2] S. Thurow, A. A. G. Fernandes, Y. Quevedo-Acosta, M. F. Oliveira, M. G. Oliveira, I. D. Jurberg, *Org. Lett*. 2019, ***21***, 6909 - 6913.
[3] W. -W. Chan, S.-H. Yeung, Z. Zhou, A. S. C. Chan, W.-Y. Yu, *Org. Lett.* 2010, ***12***, 604 – 607.
[4] A. F. da Silva, M. A. S. Afonso, R. A. Cormanich, I. D. Jurberg, *Chem. Eur. J.* 2020, ***26***, 5648 - 5653.
[5] K. Orłowska, K. Rybicka-Jasińska, P. Krajewski, D. Gryko, *Org. Lett*. 2020, ***22***, 1018 – 1021.

and DMAP (61 mg, 0.5 mmol, 0.1 equiv.). Then, the temperature of the reaction mixture is cooled to 0 ºC and the previously prepared acyl chloride (5 mmol, 1 equiv., dissolved in a minimun amount of DCM) is added. The reaction is allowed to warm up to room temperature and to stir at this temperature overnight. Then, the reaction is quenched with a saturated aqueous solution of $NaHCO_3$, extracted with AcOEt (3x), dried ($MgSO_4$) and concentrated under reduced pressure. Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords methyl 2-(4-bromophenyl)acetate as a transparent oil: 664 mg, 58 %. *Step 3:* A round bottom flask is charged with the previously prepared ester (664 mg, 2.9 mmol, 1 equiv.), $Pd(PPh_3)_4$ (5 mg, 0.004 mmol, 1.5 mol%), a 2M aqueous solution of Na_2CO_3 (2.6 mL, 2 equiv.), naphthalen-2-ylboronic acid (598 mg, 3.5 mmol, 1.2 equiv) and dioxane (10.5 mL). The reaction mixture is heated at 80 ºC for 12 h. Upon completion (TLC), the reaction is filtered through a short pad of celite, while eluting with DCM. Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords methyl 2-(4-(naphthalen-2-yl)phenyl)acetate as a transparent oil: 641 mg, 80 %. *Step 4:* Under nitrogen, a round bottom flask is charged with the previously prepared ester (243 mg, 0.88 mmol, 1 equiv.), dry MeCN (9 mL, 0.1 M) and *p*-ABSA (274 mg, 1.14 mmol, 1.3 equiv.). The solution is cooled to 0 °C and DBU (170 µL, 1.14 mmol, 1.3 equiv.) is slowly added. The temperature is allowed to warm up to 25 ºC and the reaction mixture is stirred at this temperature overnight. Then, a saturated aqueous solution of NH_4Cl is added. The resulting mixture is extracted with AcOEt (3x). The combined organic extracts are dried ($MgSO_4$), filtered and concentrated under reduced pressure. The resulting residue is purified by flash column chromatography (SiO_2, gradient: Hex - 98:2 Hex:AcOEt - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) to afford the title compound as a yellow solid: 136 mg, 45%.

^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.05 – 8.04 (m, 1H), 7.94 – 7.85 (m, 3H), 7.79 – 7.73 (m, 3H), 7.63 – 7.48 (m, 4H), 3.90 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 165.6, 138.5, 137.6, 133.7, 132.6, 128.5, 128.2, 127.8, 127.6, 126.3, 126.0, 125.5, 125.2, 124.4, 124.3, 63.3, 52.1.

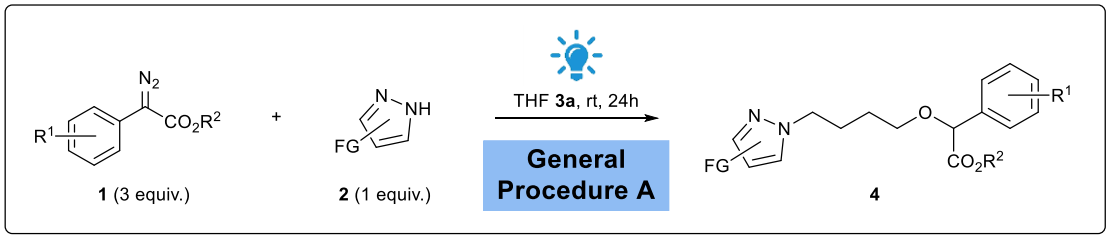
M.P.: 122 – 123 °C.

IR (ATR, cm^{-1}): 2089, 1702, 1438, 1361, 1287, 1273, 1252, 1162, 1058.

HRMS (ESI+): calcd. for $[C_{19}H_{15}N_2O_2 - N_2]^+$: 275.1067, found: 275.1065.

2. BLUE LIGHT-MEDIATED RING-OPENING OF THF WITH ARYLDIAZOACETATES AND NUCLEOPHILES

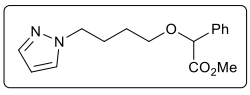
2.1 Using Pyrazoles as Nucleophiles



General Procedure A: *Photochemical Ring-Opening of THF Using Aryldiazoacetates and Pyrazoles*

A 4 mL vial is charged with aryldiazoacetate **1** (3 equiv.), pyrazole **2** (1 equiv.), and THF **3a** (0.1 M in relation to the pyrazole **2**). The reaction mixture is stirred under blue-light irradiation for 24h (using two lamps, 15 W each, displaced at approximate distances of 10 cm each from the reaction vessel). Then, the reaction mixture is concentrated under reduced pressure and the resulting residue is purified by flash column chromatography to afford the corresponding compound **4** in the stated yield.

Molecule 4a: *methyl 2-(4-(1H-pyrazol-1-yl)butoxy)-2-phenylacetate*



General Procedure A is employed with aryldiazoacetate **1a** (53 mg, 0.3 mmol), pyrazole **2a** (7 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 9:1 Hex:AcOEt – 8:2 Hex:AcOEt – 7:3 Hex:AcOEt) affords the title compound as a colorless oil: 22 mg, 76%.

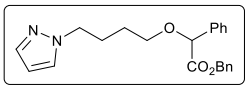
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.50 – 7.49 (m, 1H), 7.45 – 7.33 (m, 6H), 6.22 (t, *J* = 2.1 Hz, 1H), 4.84 (s, 1H), 4.18 (t, *J* = 7.0 Hz, 2H), 3.70 (s, 3H), 3.58 – 3.40 (m, 2H), 2.05 – 1.93 (m, 2H), 1.68 – 1.57 (m, 2H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 139.0, 136.4, 129.1, 128.7, 128.6, 127.1, 105.2, 81.1, 69.2, 52.2, 51.7, 27.3, 26.5.

IR (ATR, cm^{-1}): 2952, 2872, 1749, 1437, 1173, 1093.

HRMS (ESI+): calcd. for $[C_{16}H_{20}N_2O_3 + H]^+$: 289.1547, found: 289.1550.

Molecule 4b: *benzyl 2-(4-(1H-pyrazol-1-yl)butoxy)-2-phenylacetate*



General Procedure A is employed with aryldiazoacetate **1b** (76 mg, 0.3 mmol), pyrazole **2a** (10 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt - 7:3 Hex:AcOEt) affords the title compound as an yellow oil: 24 mg, 66%.

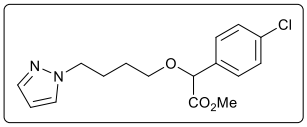
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.49 – 7.20 (m, 12H), 6.21 (t, *J* = 2.1 Hz, 1H), 5.18 (d, *J* = 12.4 Hz, 1H), 5.10 (d, *J* = 12.4 Hz, 1H), 4.88 (s, 1H), 4.16 (t, *J* = 7.0 Hz, 2H), 3.56 – 3.43 (m, 2H), 2.01 – 1.92 (m, 2H), 1.65 – 1.59 (m, 2H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 170.7, 139.0, 136.4, 135.4, 129.0, 128.6, 128.5, 128.4, 128.2, 127.9, 127.1, 105.1, 81.1, 69.2, 66.7, 51.6, 27.2, 26.5.

IR (ATR, cm^{-1}): 2935, 2872, 1749, 1456, 1167, 1121.

HRMS (ESI+): calcd. for $[C_{22}H_{24}N_2O_3 + H]^+$: 365.1860, found: 365.1861.

Molecule 4c: *methyl 2-(4-(1H-pyrazol-1-yl)butoxy)-2-(4-chlorophenyl)acetate*



General Procedure A is employed with aryldiazoacetate **1c** (63 mg, 0.3 mmol), pyrazole **2a** (10 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt - 1:1 Hex:AcOEt) affords the title compound as a colorless oil: 21 mg, 65%.

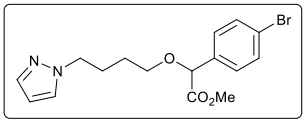
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.48 (s, 1H), 7.39 – 7.30 (m, 5H), 6.22 (t, *J* = 2.0 Hz, 1H), 4.80 (s, 1H), 4.17 (t, *J* = 7.0 Hz, 2H), 3.70 (s, 3H), 3.55 – 3.38 (m, 2H), 2.03 – 1.92 (m, 2H), 1.67 – 1.56 (m, 2H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.0, 139.2, 135.0, 134.6, 129.0, 128.9, 128.5, 105.2, 80.4, 69.4, 52.4, 51.7, 27.3, 26.6.

IR (ATR, cm^{-1}): 2952, 2872, 1752, 1491, 1173, 1089, 1016.

HRMS (ESI+): calcd. for $[C_{16}H_{19}ClN_2O_3 + H]^+$: 323.1157, found: 323.1163.

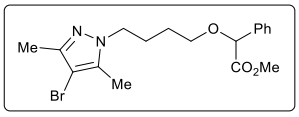
Molecule 4d: *methyl 2-(4-(1H-pyrazol-1-yl)butoxy)-2-(4-bromophenyl)acetate*



General Procedure A is employed with aryldiazoacetate **1d** (76 mg, 0.3 mmol), pyrazole **2a** (10 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 9:1 Hex:AcOEt - 8:2 Hex:AcOEt - 1:1 Hex:AcOEt) affords the title compound as a colorless oil: 23 mg, 63%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.50 – 7.47 (m, 3H), 7.37 (d, *J* = 2.3 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 2H) 6.22 (t, *J* = 2.0 Hz, 1H), 4.79 (s, 1H), 4.17 (t, *J* = 7.0 Hz, 2H), 3.70 (s, 3H), 3.56 – 3.40 (m, 2H), 2.04 – 1.92 (m, 2H), 1.68 – 1.56 (m, 2H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 170.9, 139.2, 135.5, 131.8, 129.0, 128.8, 122.8, 105.2, 80.4, 69.4, 52.4, 51.7, 27.3, 26.6.
IR (ATR, cm^{-1}): 2950, 2872, 1749, 1072, 1091, 1013.
HRMS (ESI+): calcd. for $[C_{16}H_{19}BrN_2O_3 + H]^+$: 367.0652, found: 367.0661.

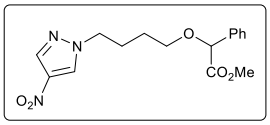
Molecule 4f: *methyl 2-(4-(4-bromo-3,5-dimethyl-1H-pyrazol-1-yl)butoxy)-2-phenylacetate*



General Procedure A is employed with aryldiazoacetate **1a** (53 mg, 0.3 mmol), pyrazole **2b** (18 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a colorless oil: 32 mg, 81%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.44 – 7.32 (m, 5H), 4.83 (s, 1H), 4.02 (t, *J* = 7.2 Hz, 2H), 3.69 (s, 3H), 3.58 – 3.41 (m, 2H), 2.19 (s, 3H), 2.18 (s, 3H), 1.94 – 1.82 (m, 2H), 1.69 – 1.58 (m, 2H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 145.6, 136.7, 136.4, 128.7, 128.6, 127.1, 93.6, 81.0, 69.2, 52.2, 49.5, 26.9, 26.5, 12.2, 10.2.
IR (ATR, cm^{-1}): 2950, 2872, 1752, 1436, 1210, 1119.
HRMS (ESI+): calcd. for $[C_{18}H_{23}BrN_2O_3 + H]^+$: 395.0965, found: 395.0968.

Molecule 4g: *methyl 2-(4-(4-nitro-1H-pyrazol-1-yl)butoxy)-2-phenylacetate*



General Procedure A is employed with aryldiazoacetate **1a** (53 mg, 0.3 mmol), pyrazole **2c** (11 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a yellow oil: 31 mg, 93%.

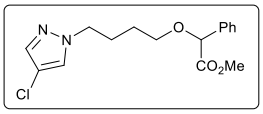
^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.23 (s, 1H), 8.04 (s, 1H), 7.42 – 7.33 (m, 5H), 4.84 (s, 1H), 4.26 (t, *J* = 7.0 Hz, 2H), 3.71 (s, 3H), 3.58 – 3.46 (m, 2H), 2.08 – 1.98 (m, 2H), 1.67 – 1.57 (m, 2H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.2, 136.2, 135.7, 135.5, 128.9, 128.8, 128.7, 127.1, 81.1, 69.0, 52.9, 52.2, 27.1, 25.9.

IR (ATR, cm^{-1}): 3129, 2954, 2874, 1745, 1510, 1408, 1301.

HRMS (ESI+): calcd. for $[C_{16}H_{19}N_3O_5 + H]^+$: 334.1397, found: 334.1402.

Molecule 4h: *methyl 2-(4-(4-chloro-1H-pyrazol-1-yl)butoxy)-2-phenylacetate*



General Procedure A is employed with aryldiazoacetate **1a** (53 mg, 0.3 mmol), pyrazole **2d** (10 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt - 7:3 Hex:AcOEt) affords the title compound as a pale yellow oil: 26 mg, 81%.

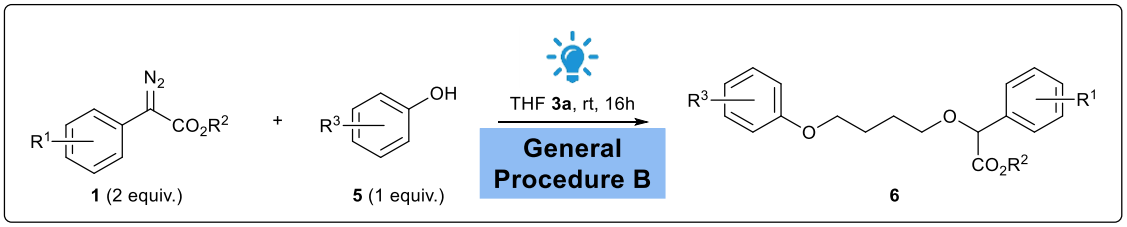
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.44 – 7.32 (m, 7H), 4.83 (s, 1H), 4.12 (t, *J* = 7.0 Hz, 2H), 3.70 (s, 3H), 3.56 – 3.43 (m, 2H), 2.00 – 1.93 (m, 2H), 1.64 – 1.58 (m, 2H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 137.4, 136.4, 128.7, 128.6, 127.2, 127.1, 109.4, 81.1, 69.1, 52.4, 52.2, 27.1, 26.3.

IR (ATR, cm^{-1}): 3129, 3055, 2950, 2872, 1749, 1437, 1119.

HRMS (ESI+): calcd. for $[C_{16}H_{19}ClN_2O_3 + H]^+$: 323.1157, found: 323.1161.

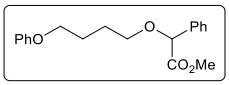
2.2 Using Phenols as Nucleophiles



General Procedure B: *Photochemical Ring-Opening of THF Using Aryldiazoacetates and Phenols*

A 4 mL vial is charged with aryldiazoacetate **1** (2 equiv.), phenol **5** (1 equiv.), and THF **3a** (0.1 M in relation to the phenol **5**). The reaction mixture is stirred under blue light irradiation for 16h (using two lamps, 15 W each, displaced at approximate distances of 10 cm each from the reaction vessel). Then, the reaction is concentrated under reduced pressure and the resulting residue is purified by flash column chromatography to afford the corresponding compound **6** in the stated yield.

Molecule 6a: *methyl 2-(4-phenoxybutoxy)-2-phenylacetate*



General Procedure B is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), phenol **5a** (9.4 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a colorless oil: 30 mg, 96%.

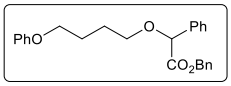
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.48 – 7.44 (m, 2H), 7.39 – 7.24 (m, 5H), 6.96 – 6.87 (m, 3H), 4.90 (s, 1H), 3.99 (t, *J* = 6.0 Hz, 2H), 3.71 (s, 3H), 3.68 – 3.51 (m, 2H), 1.94 – 1.83 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.4, 159.0, 136.6, 129.4, 128.6 (2x), 127.1, 120.5, 114.4, 81.0, 69.4, 67.3, 52.2, 26.2, 26.0.

IR (ATR, cm^{-1}): 2952, 2872, 1752, 1601, 1499, 1246.

HRMS (ESI+): calcd. for $[C_{19}H_{22}O_4 + H]^+$: 315.1591, found: 315.1591.

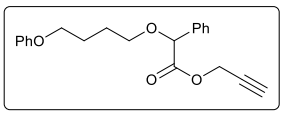
Molecule 6b: *benzyl 2-(4-phenoxybutoxy)-2-phenylacetate*



General Procedure B is employed with aryldiazoacetate **1b** (50 mg, 0.2 mmol), phenol **5a** (9.4 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt) affords the title compound as a colorless oil: 35 mg, 90%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.51 – 7.48 (m, 2H), 7.39 – 7.25 (m, 10H), 6.99 – 6.89 (m, 3H), 5.21 (d, *J* = 12.4 Hz, 1H), 5.14 (d, *J* = 12.4 Hz, 1H), 4.96 (s, 1H), 4.01 (t, *J* = 6.0 Hz, 2H), 3.70 – 3.51 (m, 2H), 1.96 – 1.85 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 170.8, 159.0, 136.5, 135.5, 129.4, 128.6, 128.5, 128.4, 128.2, 127.9, 127.1, 120.5, 114.4, 81.1, 69.5, 67.3, 66.7, 26.2, 26.0.
IR (ATR, cm^{-1}): 3034, 2950, 2874, 1749, 1499, 1246, 1169.
HRMS (ESI+): calcd. for $[C_{25}H_{26}O_4 + H]^+$: 391.1904, found: 391.1903.

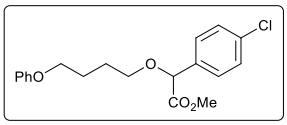
Molecule 6c: *prop-2-yn-1-yl 2-(4-phenoxybutoxy)-2-phenylacetate*



General Procedure B is employed with aryldiazoacetate **1e** (40 mg, 0.2 mmol), phenol **5a** (9.4 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt) affords the title compound as a colorless oil: 33 mg, 98%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.49 – 7.24 (m, 7H), 6.96 – 6.86 (m, 3H), 4.93 (s, 1H), 4.77 (dd, *J* = 15.5 Hz, *J* = 2.5 Hz, 1H), 4.65 (dd, *J* = 15.5 Hz, *J* = 2.5 Hz, 1H), 4.00 (t, *J* = 6.0 Hz, 2H), 3.67 – 3.54 (m, 2H), 2.44 (t, *J* = 2.5 Hz, 1H), 1.95 – 1.85 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 170.2, 159.0, 136.1, 129.4, 128.7, 128.6, 127.2, 120.5, 114.5, 80.9, 77.1, 75.3, 69.6, 67.3, 52.5, 26.2, 26.0.
IR (ATR, cm^{-1}): 3289, 2946, 2872, 1756, 1601, 1499, 1244.
HRMS (ESI+): calcd. for $[C_{21}H_{22}O_4 + H]^+$: 339.1591, found: 339.1590.

Molecule 6d: *methyl 2-(4-chlorophenyl)-2-(4-phenoxybutoxy)acetate*



General Procedure B is employed with aryldiazoacetate **1c** (42 mg, 0.2 mmol), phenol **5a** (9.4 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a pale yellow oil: 32 mg, 92%.

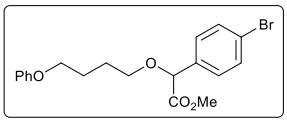
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.42 – 7.24 (m, 6H), 6.96 – 6.86 (m, 3H), 4.86 (s, 1H), 3.99 (t, *J* = 6.0 Hz, 2H), 3.71 (s, 3H), 3.65 – 3.49 (m, 2H), 1.92 – 1.82 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.0, 158.9, 135.1, 134.5, 129.4, 128.8, 128.4, 120.5, 114.4, 80.3, 69.6, 67.3, 52.3, 26.2, 26.0.

IR (ATR, cm^{-1}): 2952, 2874, 1737, 1493, 1246, 1091.

HRMS (ESI+): calcd. for $[C_{19}H_{21}ClO_4 + H]^+$: 349.1201, found: 349.1199.

Molecule 6e: *methyl 2-(4-bromophenyl)-2-(4-phenoxybutoxy)acetate*



General Procedure B is employed with aryldiazoacetate **1d** (51 mg, 0.2 mmol), phenol **5a** (9.4 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a pale yellow oil: 38 mg, 97%.

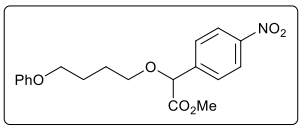
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.49 (d, *J* = 8.5 Hz, 2H), 7.35 – 7.24 (m, 4H), 6.97 – 6.86 (m, 3H), 4.84 (s, 1H), 3.99 (t, *J* = 6.0 Hz, 2H), 3.71 (s, 3H), 3.65 – 3.49 (m, 2H), 1.93 – 1.82 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 170.9, 158.9, 135.6, 131.7, 129.4, 128.7, 122.7, 120.5, 114.4, 80.3, 69.6, 67.3, 52.3, 26.2, 26.0.

IR (ATR, cm^{-1}): 2952, 2872, 1737, 1490, 1246, 1072, 1013, 753.

HRMS (ESI+): calcd. for $[C_{19}H_{21}BrO_4 + H]^+$: 393.0696, found: 393.0697.

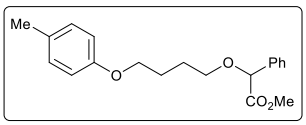
Molecule 6f: *methyl 2-(4-nitrophenyl)-2-(4-phenoxybutoxy)acetate*



General Procedure B is employed with aryldiazoacetate **1f** (44 mg, 0.2 mmol), phenol **5a** (9.4 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as an yellow oil: 13 mg, 36%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.23 (d, *J* = 8.6 Hz, 2H), 7.66 (d, *J* = 8.6 Hz, 2H), 7.33 – 7.26 (m, 2H), 6.99 – 6.88 (m, 3H), 5.01 (s, 1H), 4.03 (t, *J* = 6.0 Hz, 2H), 3.77 – 3.69 (m, 1H), 3.75 (s, 3H), 3.61 – 3.53 (m, 1H), 1.99 – 1.85 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 170.3, 158.9, 148.0, 143.6, 129.4, 127.8, 123.7, 120.6, 114.4, 80.1, 70.2, 67.2, 52.6, 26.2, 26.0.
IR (ATR, cm^{-1}): 2952, 2872, 1754, 1525, 1348, 1246.
HRMS (ESI+): calcd. for $[C_{19}H_{21}NO_6 + H]^+$: 360.1442, found: 360.1442.

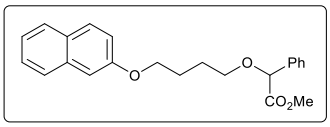
Molecule 6g: *methyl 2-phenyl-2-(4-(p-tolyloxy)butoxy)acetate*



General Procedure B is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), *p*-cresol **5b** (11 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt) affords the title compound as a colorless oil: 32 mg, 98%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.49 – 7.45 (m, 2H), 7.40 – 7.34 (m, 3H), 7.06 (d, *J* = 7.4 Hz, 2H), 6.78 (d, *J* = 7.4 Hz, 2H), 4.90 (s, 1H), 3.96 (t, *J* = 6.0 Hz, 2H), 3.72 (s, 3H), 3.64 – 3.50 (m, 2H), 2.29 (s, 3H), 1.92 – 1.83 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.4, 156.8, 136.6, 129.8, 129.7, 128.6 (2x), 127.1, 114.3, 81.0, 69.5, 67.5, 52.2, 26.2, 26.0, 20.4.
IR (ATR, cm^{-1}): 3032, 2950, 2872, 1752, 1512, 1242, 1106.
HRMS (ESI+): calcd. for $[C_{20}H_{24}O_4 + H]^+$: 329.1747, found: 329.1748.

Molecule 6h: *methyl 2-(4-(naphthalen-2-yloxy)butoxy)-2-phenylacetate*



General Procedure B is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), naphthalen-2-ol **5c** (14 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a colorless oil: 36 mg, 99%.

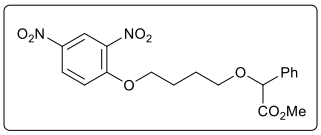
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.77 – 7.69 (m, 3H), 7.48 – 7.29 (m, 7H), 7.15 – 7.11 (m, 2H), 4.90 (s, 1H), 4.11 (t, *J* = 6.0 Hz, 2H), 3.71 (s, 3H), 3.67 – 3.51 (m, 2H), 2.04 – 1.83 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.4, 156.9, 136.6, 134.5, 129.3, 128.8, 128.6 (2x), 127.6, 127.1, 126.6, 126.2, 123.4, 118.9, 106.5, 81.0, 69.4, 67.5, 52.2, 26.2, 26.0.

IR (ATR, cm^{-1}): 3060, 3030, 2952, 2874, 1737, 1631, 1218.

HRMS (ESI+): calcd. for $[C_{23}H_{24}O_4 + H]^+$: 365.1747, found: 365.1750.

Molecule 6i: *methyl 2-(4-(2,4-dinitrophenoxy)butoxy)-2-phenylacetate*



General Procedure B is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), 2,4-dinitrophenol **5d** (18 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt - 7:3 Hex:AcOEt) affords the title compound as an yellow oil: 28 mg, 69%.

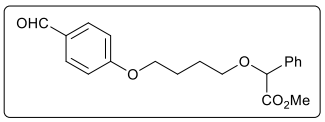
^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.71 (d, *J* = 2.8 Hz, 1H), 8.36 (dd, *J* = 9.3 Hz, *J* = 2.8 Hz, 1H), 7.43 – 7.32 (m, 5H), 7.19 (d, *J* = 9.3 Hz, 1H), 4.87 (s, 1H), 4.33 (t, *J* = 6.0 Hz, 2H), 3.70 (s, 3H), 3.66 – 3.52 (m, 2H), 2.10 – 1.99 (m, 2H), 1.92 – 1.81 (m, 2H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 156.8, 139.8, 138.8, 136.4, 129.0, 128.7, 128.6, 127.1, 121.8, 114.4, 80.9, 70.5, 69.1, 52.2, 25.8, 25.6.

IR (ATR, cm^{-1}): 3090, 2954, 2877, 1749, 1607, 1525, 1342, 1285.

HRMS (ESI+): calcd. for $[C_{19}H_{20}N_2O_8 + H]^+$: 405.1292, found: 405.1293.

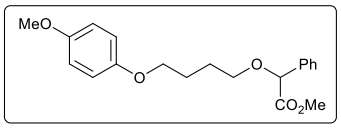
Molecule 6j: *methyl 2-(4-(4-formylphenoxy)butoxy)-2-phenylacetate*



General Procedure B is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), phenol **5e** (12 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a colorless oil: 33 mg, 97%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 9.87 (s, 1H), 7.81 (d, *J* = 8.7 Hz, 2H), 7.46 – 7.33 (m, 5H), 6.96 (d, *J* = 8.7 Hz, 2H), 4.88 (s, 1H), 4.08 (t, *J* = 6.0 Hz, 2H), 3.70 (s, 3H), 3.65 – 3.50 (m, 2H), 1.97 – 1.81 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 190.8, 171.3, 164.1, 136.5, 131.9, 129.7, 128.7, 128.6, 127.1, 114.7, 81.0, 69.3, 67.9, 52.2, 26.0, 25.9.
IR (ATR, cm^{-1}): 2954, 2875, 1749, 1637, 1599, 1255, 1160.
HRMS (ESI+): calcd. for $[C_{20}H_{22}O_5 + H]^+$: 343.1540, found: 343.1540.

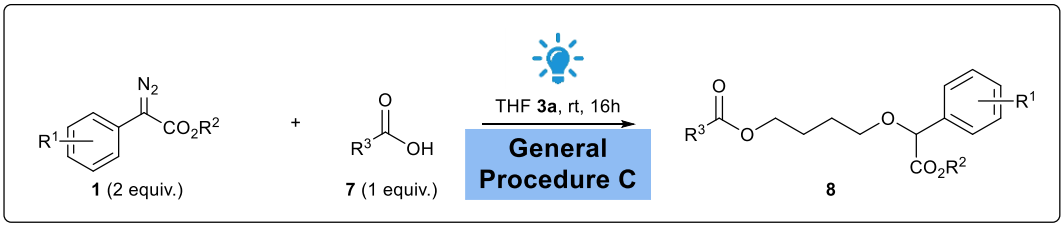
Molecule 6k: *methyl 2-(4-(4-methoxyphenoxy)butoxy)-2-phenylacetate*



General Procedure B is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), phenol **5f** (12 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a pale yellow oil: 26 mg, 76%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.48 - 7.44 (m, 2H), 7.37 - 7.33 (m, 3H), 6.82 (app s, 4H), 4.89 (s, 1H), 3.96 -3.91 (m, 2H), 3.76 (s, 3H), 3.71 (s, 3H), 3.67 – 3.60 (m, 1H), 3.55 - 3.49 (m, 1H), 1.90 – 1.81 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.4, 153.7, 153.2, 136.6, 128.6 (x2), 127.1, 115.4, 114.6, 81.1, 69.5, 68.1, 55.7, 52.2, 26.2, 26.1.
IR (ATR, cm^{-1}): 2951, 2873, 1739, 1508, 1459, 1440, 1229, 1172, 1106, 1036.
HRMS (ESI+): calcd. for $[C_{20}H_{24}O_5 + H]^+$: 345.1697, found: 345.1698.

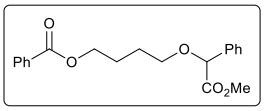
2.3 Using Carboxylic Acids as Nucleophiles



General Procedure C: *Photochemical Ring-Opening of THF Using Aryldiazoacetates and Carboxylic Acids*

A 4 mL vial is charged with aryldiazoacetate **1** (2 equiv.), carboxylic acid **7** (1 equiv.), and THF **3a** (0.1 M in relation to the carboxylic acid **7**). The reaction mixture is stirred under blue light irradiation for 16h (using two lamps, 15 W each, displaced at approximate distances of 10 cm each from the reaction vessel). Then, the reaction mixture is concentrated under reduced pressure and the resulting residue is purified by flash column chromatography to afford the corresponding compound **8** in the stated yield.

Molecule 8a: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl benzoate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7a** (12 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a colorless oil: 34 mg, 99%.

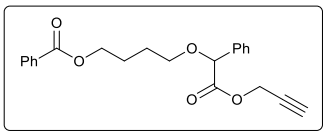
^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.05 – 8.01 (m, 2H), 7.55 – 7.52 (m, 1H), 7.47 – 7.34 (m, 7H), 4.88 (s, 1H), 4.35 (t, *J* = 6.1 Hz, 2H), 3.71 (s, 3H), 3.64 – 3.49 (m, 2H), 1.92 – 1.80 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 166.5, 136.5, 132.8, 130.3, 129.4, 128.6, 128.5, 128.2, 127.0, 81.0, 69.2, 64.6, 52.1, 26.2, 25.4.

IR (ATR, cm^{-1}): 2952, 2874, 1752, 1717, 1454, 1272, 1100, 1072.

HRMS (ESI+): calcd. for $[C_{20}H_{22}O_5 + H]^+$: 343.1540, found: 343.1546.

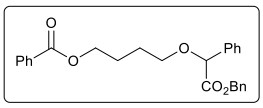
Molecule 8b: *4-(2-oxo-1-phenyl-2-(prop-2-yn-1-yloxy)ethoxy)butyl benzoate*



General Procedure C is employed with aryldiazoacetate **1e** (40 mg, 0.2 mmol), carboxylic acid **7a** (12 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a yellow oil: 35 mg, 96%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.05 – 8.01 (m, 2H), 7.58 – 7.52 (m, 1H), 7.49 – 7.33 (m, 7H), 4.93 (s, 1H), 4.75 (dd, *J* = 15.6 Hz, *J* = 2.5 Hz, 1H), 4.64 (dd, *J* = 15.6 Hz, *J* = 2.5 Hz, 1H), 4.35 (t, *J* = 6.1 Hz, 2H), 3.66 – 3.50 (m, 2H), 2.45 (t, *J* = 2.5 Hz, 1H), 1.96 – 1.77 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 170.1, 166.5, 136.0, 132.8, 130.3, 129.5, 128.8, 128.6, 128.3, 127.1, 80.9, 76.5, 75.3, 69.4, 64.6, 52.5, 26.2, 25.5.
IR (ATR, cm^{-1}): 3289, 2950, 2875, 1756, 1715, 1274, 1100.
HRMS (ESI+): calcd. for $[C_{22}H_{22}O_5 + H]^+$: 367.1540, found: 367.1546.

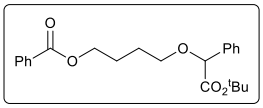
Molecule 8c: *4-(2-(benzyloxy)-2-oxo-1-phenylethoxy)butyl benzoate*



General Procedure C is employed with aryldiazoacetate **1b** (50 mg, 0.2 mmol), carboxylic acid **7a** (12 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt) affords the title compound as a colorless oil: 41 mg, 98%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.06 – 8.02 (m, 2H), 7.59 – 7.53 (m, 1H), 7.47 – 7.20 (m, 12H), 5.18 (d, *J* = 12.4 Hz, 1H), 5.12 (d, *J* = 12.4 Hz, 1H), 4.93 (s, 1H), 4.34 (t, *J* = 5.0 Hz, 2H), 3.67 – 3.51 (m, 2H), 1.92 – 1.80 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 170.7, 166.5, 136.4, 135.4, 132.8, 130.3, 129.5, 128.6, 128.5, 128.4, 128.3, 128.2, 127.9, 127.1, 81.1, 69.3, 66.7, 64.6, 26.2, 25.5.
IR (ATR, cm^{-1}): 3065, 3034, 2954, 2875, 1748, 1715, 1454, 1274, 1100.
HRMS (ESI+): calcd. for $[C_{26}H_{26}O_5 + H]^+$: 419.1853, found: 419.1858.

Molecule 8d: *4-(2-(tert-butoxy)-2-oxo-1-phenylethoxy)butyl benzoate*



General Procedure C is employed with aryldiazoacetate **1g** (44 mg, 0.2 mmol), carboxylic acid **7a** (12 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt) affords the title compound as a colorless oil: 34 mg, 89%.

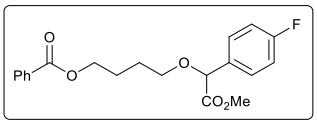
^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.05 – 8.01 (m, 2H), 7.58 – 7.51 (m, 1H), 7.46 – 7.31 (m, 7H), 4.74 (s, 1H), 4.35 (t, *J* = 6.1 Hz, 2H), 3.67 – 3.46 (m, 2H), 1.91 – 1.79 (m, 4H), 1.39 (s, 9H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 170.1, 166.6, 137.1, 132.8, 130.4, 129.5, 128.4, 128.3 (2x), 127.0, 81.7, 81.5, 69.0, 64.7, 27.9, 26.3, 25.6.

IR (ATR, cm^{-1}): 2978, 2874, 1743, 1719, 1274, 1100, 1072.

HRMS (ESI+): calcd. for $[C_{23}H_{28}O_5 + H]^+$: 385.2010, found: 385.2013.

Molecule 8e: *4-(1-(4-fluorophenyl)-2-methoxy-2-oxoethoxy)butyl benzoate*



General Procedure C is employed with aryldiazoacetate **1h** (39 mg, 0.2 mmol), carboxylic acid **7a** (12 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a colorless oil: 34 mg, 94%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.05 – 8.01 (m, 2H), 7.58 – 7.52 (m, 1H), 7.46 – 7.40 (m, 4H), 7.07 – 7.01 (m, 2H), 4.85 (s, 1H), 4.35 (t, *J* = 6.2 Hz, 2H), 3.71 (s, 3H), 3.63 – 3.48 (m, 2H), 1.92 – 1.79 (m, 4H).

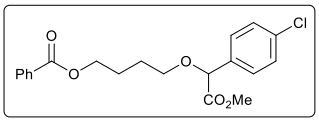
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.2, 166.6, 162.9 (d, *J* = 245.6 Hz), 132.8, 132.4 (d, *J* = 3.1 Hz), 130.3, 129.5, 128.9 (d, *J* = 8.8 Hz), 128.3, 115.6 (d, *J* = 21.9 Hz), 80.4, 69.3, 64.6, 52.3, 26.2, 25.5.

^{19}F NMR (235 MHz, $CDCl_3$) δ: -113.2

IR (ATR, cm^{-1}): 2954, 1737, 1715, 1510, 1274, 1110, 1095.

HRMS (ESI+): calcd. for $[C_{20}H_{21}FO_5 + H]^+$: 361.1446, found: 361.1451.

Molecule 8f: *4-(1-(4-chlorophenyl)-2-methoxy-2-oxoethoxy)butyl benzoate*



General Procedure C is employed with aryldiazoacetate **1c** (42 mg, 0.2 mmol), carboxylic acid **7a** (12 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 AcOEt - 9:1 Hex:AcOEt) affords the title compound as a yellow oil: 32 mg, 85%.

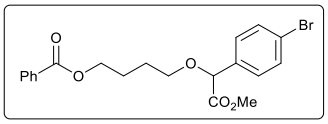
^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.04 – 8.00 (m, 2H), 7.58 – 7.52 (m, 1H), 7.46 – 7.29 (m, 6H), 4.85 (s, 1H), 4.35 (t, *J* = 6.0 Hz, 2H), 3.70 (s, 3H), 3.64 – 3.48 (m, 2H), 1.92 – 1.78 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.0, 166.5, 135.0, 134.5, 132.8, 130.3, 129.5, 128.8, 128.4, 128.3, 80.4, 69.4, 64.6, 52.3, 26.2, 25.5.

IR (ATR, cm^{-1}): 2954, 1737, 1715, 1272, 1072, 1111, 1091.

HRMS (ESI+): calcd. for $[C_{20}H_{21}ClO_5 + H]^+$: 377.1150, found: 377.1156.

Molecule 8g: *4-(1-(4-bromophenyl)-2-methoxy-2-oxoethoxy)butyl benzoate*



General Procedure C is employed with aryldiazoacetate **1d** (51 mg, 0.2 mmol), carboxylic acid **7a** (12 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 Hex:AcOEt - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a yellow oil: 42 mg, 100%.

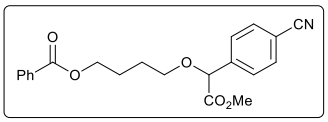
^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.02 (d, *J* = 7.0 Hz, 2H), 7.58 – 7.42 (m, 5H), 7.32 (d, *J* = 7.0 Hz, 2H), 4.83 (s, 1H), 4.35 (t, *J* = 6.0 Hz, 2H), 3.70 (s, 3H), 3.66 – 3.48 (m, 2H), 1.91 – 1.79 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 170.9, 166.5, 135.5, 132.8, 131.7, 130.3, 129.5, 128.7, 128.3, 122.7, 80.4, 69.4, 64.5, 52.3, 26.2, 25.4.

IR (ATR, cm^{-1}): 2954, 2872, 1737, 1715, 1272, 1110, 1072.

HRMS (ESI+): calcd. for $[C_{20}H_{21}BrO_5 + H]^+$: 421.0645, found: 421.0650.

Molecule 8h: *4-(1-(4-cyanophenyl)-2-methoxy-2-oxoethoxy)butyl benzoate*



General Procedure C is employed with aryldiazoacetate **1i** (40 mg, 0.2 mmol), carboxylic acid **7a** (12 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 Hex:AcOEt - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a pale yellow oil: 36 mg, 98%.

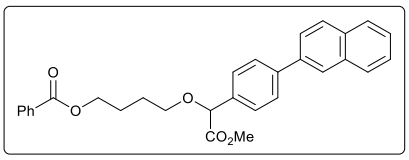
^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.04 – 8.00 (m, 2H), 7.66 – 7.52 (m, 5H), 7.46 – 7.39 (m, 2H), 4.92 (s, 1H), 4.35 (t, *J* = 6.2 Hz, 2H), 3.71 (s, 3H), 3.69 – 3.44 (m, 2H), 1.93 – 1.80 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 170.3, 166.5, 141.6, 132.9, 132.3, 130.2, 129.5, 128.3, 127.6, 118.4, 112.4, 80.3, 69.8, 64.5, 52.5, 26.2, 25.4.

IR (ATR, cm^{-1}): 2954, 2231, 1737, 1715, 1274, 1175, 1100.

HRMS (ESI+): calcd. for $[C_{21}H_{21}NO_5 + H]^+$: 368.1492, found: 368.1499.

Molecule 8i: *4-(2-methoxy-1-(4-(naphthalen-2-yl)phenyl)-2-oxoethoxy)butyl benzoate*



General Procedure C is employed with aryldiazoacetate **1j** (60 mg, 0.2 mmol), carboxylic acid **7a** (12 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as yellow oil: 45 mg, 96%.

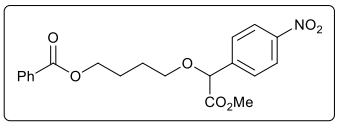
^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.06 – 8.02 (m, 3H), 7.93 – 7.85 (m, 3H), 7.75 – 7.71 (m, 3H), 7.59 – 7.43 (m, 7H), 4.96 (s, 1H), 4.38 (t, *J* = 6.2 Hz, 2H), 3.75 (s, 3H), 3.69 – 3.55 (m, 2H), 1.95 – 1.84 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) (1C cannot be unambiguously assigned) δ: 171.3, 166.6, 141.5, 137.9, 135.6, 133.6, 132.8, 132.7, 130.4, 129.5, 128.9, 128.5, 128.3, 128.2, 127.6, 126.3, 126.0, 125.9, 125.4, 80.9, 69.4, 64.7, 52.3, 26.3, 25.5.

IR (ATR, cm^{-1}): 3058, 2954, 1737, 1715, 1274, 1100.

HRMS (ESI+): calcd. for $[C_{30}H_{28}O_5 + H]^+$: 469.2010, found: 469.2016.

Molecule 8j: *4-(2-methoxy-1-(4-nitrophenyl)-2-oxoethoxy)butyl benzoate*



General Procedure C is employed with aryldiazoacetate **1f** (44 mg, 0.2 mmol), carboxylic acid **7a** (12 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a yellow oil: 38 mg, 98%.

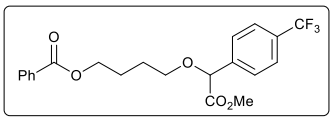
^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.20 (d, *J* = 8.8 Hz, 2H), 8.04 – 8.00 (m, 2H), 7.64 (d, *J* = 8.3 Hz, 2H), 7.58 – 7.52 (m, 1H), 7.46 – 7.39 (m, 2H), 4.98 (s, 1H), 4.36 (t, *J* = 6.1 Hz, 2H), 3.72 (s, 3H), 3.70 – 3.65 (m, 1H), 3.58 – 3.49 (m, 1H), 1.94 – 1.82 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 170.2, 166.5, 148.0, 143.5, 132.9, 130.2, 129.5, 128.3, 127.8, 123.7, 80.2, 69.9, 64.5, 52.6, 26.2, 25.5.

IR (ATR, cm^{-1}): 2955, 2874, 1737, 1715, 1521, 1272, 1100.

HRMS (ESI+): calcd. for $[C_{20}H_{21}NO_7 + H]^+$: 388.1391, found: 388.1396.

Molecule 8k: *4-(2-methoxy-2-oxo-1-(4-(trifluoromethyl)phenyl)ethoxy)butyl benzoate*



General Procedure C is employed with aryldiazoacetate **1k** (44 mg, 0.2 mmol), carboxylic acid **7a** (12 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a yellow oil: 41 mg, 100%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.05 – 8.01 (m, 2H), 7.64 – 7.52 (m, 5H), 7.46 – 7.39 (m, 2H), 4.94 (s, 1H), 4.36 (t, *J* = 6.1 Hz, 2H), 3.72 (s, 3H), 3.68 – 3.51 (m, 2H), 1.93 – 1.81 (m, 4H).

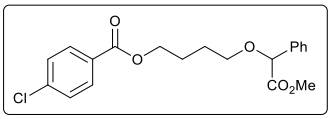
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 170.7, 166.6, 140.4, 132.9, 130.8 (q, *J* = 32.5 Hz), 130.3, 129.5, 128.3, 127.3, 125.5 (q, *J* = 3.8 Hz), 123.9 (q, *J* = 270.6 Hz), 80.5, 69.7, 64.6, 52.4, 26.2, 25.5.

^{19}F NMR (235 MHz, $CDCl_3$) δ: - 62.7.

IR (ATR, cm^{-1}): 2955, 1737, 1719, 1326, 1274, 1106, 1069.

HRMS (ESI+): calcd. for $[C_{21}H_{21}F_3O_5 + H]^+$: 411.1414, found: 411.1418.

Molecule 8l: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl 4-chlorobenzoate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7b** (16 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a pale yellow oil: 30 mg, 80%.

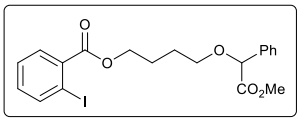
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.95 (d, *J* = 8.6 Hz, 2H), 7.47 – 7.33 (m, 7H), 4.88 (s, 1H), 4.34 (t, *J* = 6.1 Hz, 2H), 3.71 (s, 3H), 3.63 – 3.49 (m, 2H), 1.91 – 1.77 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 165.7, 139.2, 136.5, 130.9, 128.8, 128.7, 128.6 (2x), 127.1, 81.1, 69.2, 64.9, 52.2, 26.2, 25.4.

IR (ATR, cm^{-1}): 2952, 2874, 1752, 1719, 1596, 1272, 1093, 1016.

HRMS (ESI+): calcd. for $[C_{20}H_{21}ClO_5 + H]^+$: 377.1150, found: 377.1155.

Molecule 8m: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl 2-iodobenzoate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7c** (25 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a colorless oil: 44 mg, 94%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.98 (dd, *J* = 7.8 Hz, *J* = 1.2 Hz, 1H), 7.76 (dd, *J* = 7.8 Hz, *J* = 1.7 Hz, 1H), 7.47 – 7.33 (m, 6H), 7.14 (td, *J* = 7.8 Hz, *J* = 1.7 Hz, 1H),

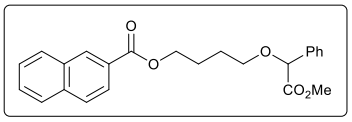
4.88 (s, 1H), 4.36 (t, *J* = 6.0 Hz, 2H), 3.71 (s, 3H), 3.65 – 3.46 (m, 2H), 1.97 – 1.76 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 166.6, 141.2, 136.5, 135.4, 132.5, 130.8, 128.6 (x2), 127.8, 127.1, 93.9, 81.1, 69.2, 65.4, 52.2, 26.2, 25.3.

IR (ATR, cm^{-1}): 2952, 2872, 1726 1456, 1288, 1251, 1098, 1016.

HRMS (ESI+): calcd. for $[C_{20}H_{21}IO_5 + H]^+$: 469.0506, found: 469.0514.

Molecule 8n: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl 2-naphthoate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7d** (16 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex) affords the title compound as a colorless oil: 39 mg, 100%.

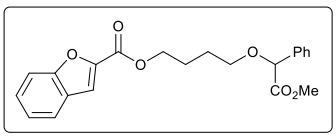
^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.61 – 8.60 (m, 1H), 8.08 – 8.04 (m, 1H), 7.98 – 7.94 (m, 1H), 7.89 – 7.85 (m, 2H), 7.62 – 7.45 (m, 4H), 7.39 – 7.33 (m, 3H), 4.91 (s, 1H), 4.42 (t, *J* = 6.1 Hz, 2H), 3.71 (s, 3H), 3.67 – 3.53 (m, 2H), 1.97 – 1.85 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 166.7, 136.5, 135.4, 132.4, 130.9, 129.3, 128.6 (2x), 128.1, 128.0, 127.7, 127.6, 127.1, 126.5, 125.2, 81.1, 69.3, 64.8, 52.2, 26.3, 25.5.

IR (ATR, cm^{-1}): 3062, 3032, 2952, 2875, 1752, 1715, 1279, 1197.

HRMS (ESI+): calcd. for $[C_{24}H_{24}O_5 + H]^+$: 393.1697, found: 393.1702.

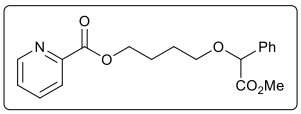
Molecule 8o: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl benzofuran-2-carboxylate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7e** (16 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a yellow oil: 38 mg, 100%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.67 (dq, *J* = 7.9 Hz, *J* = 1.0 Hz, 1H), 7.59 (dq, *J* = 7.4 Hz, *J* = 1.0 Hz, 1H), 7.50 – 7.29 (m, 8H), 4.89 (s, 1H), 4.41 (t, *J* = 6.2 Hz, 2H), 3.70 (s, 3H), 3.64 – 3.48 (m, 2H), 1.95 – 1.80 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 159.5, 155.6, 145.5, 136.4, 128.6 (2x), 127.5, 127.1, 126.9, 123.7, 122.7, 113.7, 112.3, 81.0, 69.1, 65.1, 52.2, 26.1, 25.4.
IR (ATR, cm^{-1}): 2954, 2920, 1722, 1563, 1298, 1177, 1097.
HRMS (ESI+): calcd. for $[C_{22}H_{22}O_6 + H]^+$: 383.1489, found: 383.1493.

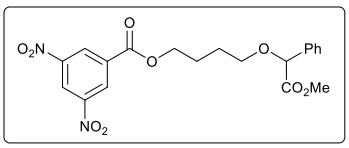
Molecule 8p: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl picolinate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7f** (12 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt - 1:1 Hex:AcOEt) affords the title compound as a yellow oil: 31 mg, 90%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.74 (dq, *J* = 4.8 Hz, *J* = 1.0 Hz, 1H), 8.09 (dt, *J* = 5.9 Hz, *J* = 1.0 Hz, 1H), 7.81 (td, *J* = 7.7 Hz, *J* = 1.8 Hz, 1H), 7.48 – 7.30 (m, 6H), 4.86 (s, 1H), 4.43 (t, *J* = 6.4 Hz, 2H), 3.69 (s, 3H), 3.68 – 3.45 (m, 2H), 1.95 – 1.77 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 165.1, 149.8, 148.1, 136.9, 136.5, 128.6, 128.5, 127.1, 126.8, 125.1, 81.1, 69.2, 65.6, 52.2, 26.1, 25.4.
IR (ATR, cm^{-1}): 2954, 1721, 1586, 1439, 1247, 1124, 1091.
HRMS (ESI+): calcd. for $[C_{19}H_{21}NO_5 + H]^+$: 344.1492, found: 344.1500.

Molecule 8q: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl 3,5-dinitrobenzoate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7g** (21 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a pale yellow oil: 24 mg, 56%.

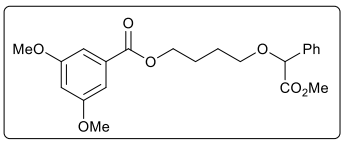
^{1}H NMR (250 MHz, $CDCl_3$) δ: 9.21 (t, *J* = 2.2 Hz, 1H), 9.13 (d, *J* = 2.2 Hz, 2H), 7.45 – 7.33 (m, 5H), 4.87 (s, 1H), 4.50 (t, *J* = 6.5 Hz, 2H), 3.71 (s, 3H), 3.70 – 3.51 (m, 2H), 2.04 – 1.93 (m, 2H), 1.87 – 1.80 (m, 2H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.2, 162.4, 148.6, 136.3, 134.0, 129.3, 128.7, 128.6, 127.1, 122.2, 81.1, 69.0, 66.7, 52.2, 26.0, 25.5.

IR (ATR, cm^{-1}): 3101, 2955, 2920, 1730, 1544, 1346, 1275, 1167, 1076.

HRMS (ESI+): calcd. for $[C_{20}H_{20}N_2O_9 + H]^+$: 433.1242, found: 433.1248.

Molecule 8r: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl 3,5-dimethoxybenzoate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7h** (18 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a colorless oil: 38 mg, 95%.

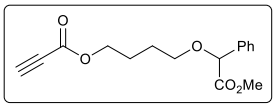
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.47 – 7.32 (m, 5H), 7.18 (d, *J* = 2.4 Hz, 2H), 6.64 (t, *J* = 2.4 Hz, 1H), 4.88 (s, 1H), 4.33 (t, *J* = 6.2 Hz, 2H), 3.71 (s, 6H), 3.63 (s, 3H), 3.61 – 3.48 (m, 2H), 1.91 – 1.80 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 166.3, 160.6, 136.5, 132.2, 128.6 (2x), 127.1, 107.1, 105.5, 81.1, 69.2, 64.8, 55.5, 52.2, 26.2, 25.5.

IR (ATR, cm^{-1}): 2954, 2842, 1752, 1715, 1596, 1206, 1156, 1050.

HRMS (ESI+): calcd. for $[C_{22}H_{26}O_7 + H]^+$: 403.1751, found: 407.1757.

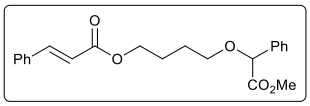
Molecule 8s: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl propiolate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7i** (7 mg, 6 μL, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a pale yellow oil: 26 mg, 90%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.46 – 7.32 (m, 5H), 4.86 (s, 1H), 4.22 (t, *J* = 6.1 Hz, 2H), 3.71 (s, 3H), 3.61 – 3.45 (m, 2H), 2.87 (s, 1H), 1.85 – 1.71 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 152.7, 136.5, 128.7, 128.6, 127.1, 81.1, 74.7, 74.5, 69.0, 66.0, 52.2, 25.9, 25.2.
IR (ATR, cm^{-1}): 3257, 2955, 2117, 1748, 1711, 1214, 1102.
HRMS (ESI+): calcd. for $[C_{16}H_{18}O_5 + H]^+$: 291.1227, found: 291.1230.

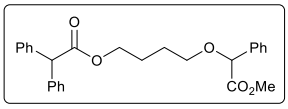
Molecule 8t: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl cinnamate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7j** (15 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt, 8:2 Hex:AcOEt) affords the title compound as a colorless oil: 36 mg, 98%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.68 (d, *J* = 16.0 Hz, 1H), 7.54 – 7.44 (m, 4H), 7.39 – 7.32 (m, 6H), 6.43 (d, *J* = 16.0 Hz, 1H), 4.89 (s, 1H), 4.23 (t, *J* = 6.2 Hz, 2H), 3.71 (s, 3H), 3.62 – 3.48 (m, 2H), 1.85 – 1.77 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 167.0, 144.6, 136.5, 134.4, 130.2, 128.8 128.6 (2x), 128.0, 127.1, 118.1, 81.1, 69.2, 64.2, 52.2, 26.1, 25.4.
IR (ATR, cm^{-1}): 3062, 2954, 1737, 1704, 1639, 1169.
HRMS (ESI+): calcd. for $[C_{22}H_{24}O_5 + H]^+$: 369.1697, found: 369.1704.

Molecule 8u: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl 2,2-diphenylacetate*

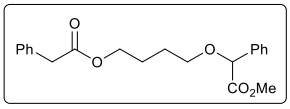


General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7k** (21 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt, 8:2 Hex:AcOEt) affords the title compound as a pale yellow oil: 43 mg, 100%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.44 – 7.25 (m, 15H), 5.01 (s, 1H), 4.83 (s, 1H), 4.18 (t, *J* = 6.1 Hz, 2H), 3.70 (s, 3H), 3.55 – 3.38 (m, 2H), 1.79 – 1.61 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 172.4, 171.3, 138.7, 136.5, 128.6 (2x), 128.5 (2x), 127.2, 127.1, 81.0, 69.1, 64.8, 57.1, 52.2, 25.9, 25.2.

IR (ATR, cm^{-1}): 2088, 3065, 3032, 2954, 1734, 1456, 1190, 1152.
HRMS (ESI+): calcd. for $[C_{27}H_{28}O_5 + H]^+$: 433.2010, found: 433.2017.

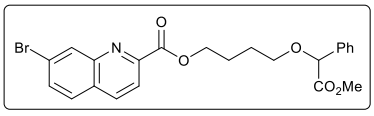
Molecule 8v: *methyl 2-phenyl-2-(4-(2-phenylacetoxy)butoxy)acetate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7l** (14 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a pale yellow oil: 33 mg, 93%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.46 – 7.25 (m, 10H), 4.85 (s, 1H), 4.11 (t, *J* = 6.2 Hz, 2H), 3.71 (s, 3H), 3.60 (s, 2H), 3.56 – 3.41 (m, 2H), 1.77 – 1.67 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.6, 171.3, 136.5, 134.1, 129.2, 128.6 (2x), 128.5, 127.1, 127.0, 81.0, 69.1, 64.5, 52.2, 41.4, 26.0, 25.3.
IR (ATR, cm^{-1}): 3065, 3032, 2954, 1734, 1499, 1456, 1128.
HRMS (ESI+): calcd. for $[C_{21}H_{24}O_5 + H]^+$: 357.1697, found: 357.1701.

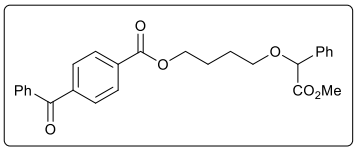
Molecule 8w: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl 7-bromoquinoline-2-carboxylate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7m** (25 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt - 1:1 Hex:AcOEt) affords the title compound as a yellow oil: 42 mg, 89%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.50 – 8.48 (m, 1H), 8.27 – 8.23 (m, 1H), 8.16 – 8.12 (m, 1H), 7.76 – 7.68 (m, 2H), 7.46 – 7.32 (m, 5H), 4.89 (s, 1H), 4.51 (t, *J* = 6.5 Hz, 2H), 3.70 (s, 3H), 3.65 – 3.51 (m, 2H), 2.02 – 1.78 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 164.9, 148.9, 148.1, 137.1, 136.5, 132.9, 132.0, 128.6 (3x), 127.8, 127.1, 124.4, 121.3, 81.1, 69.2, 66.0, 52.2, 26.1, 25.4.
IR (ATR, cm^{-1}): 2954, 1737, 1611, 1270, 1139, 1113.
HRMS (ESI+): calcd. for $[C_{23}H_{22}BrNO_5 + H]^+$: 472.0754, found: 472.0764.

Molecule 8x: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl 4-benzoylbenzoate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7n** (23 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt, 8:2 Hex:AcOEt) affords the title compound as as white solid: 44 mg, 99%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.13 (d, *J* = 8.2 Hz, 2H), 7.85 – 7.78 (m, 4H), 7.65 – 7.58 (m, 1H), 7.53 – 7.34 (m, 7H), 4.88 (s, 1H), 4.39 (t, *J* = 6.0 Hz, 2H), 3.71 (s, 3H), 3.64 – 3.50 (m, 2H), 1.95 – 1.80 (m, 4H).

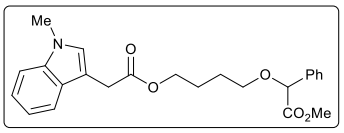
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 196.0, 171.3, 165.8, 141.2, 136.9, 136.5, 133.4, 132.9, 130.1, 129.7, 129.4, 128.7, 128.6, 128.4, 127.1, 81.1, 69.2, 65.1, 52.2, 26.2, 25.5.

M.P.: 77 – 78 ºC.

IR (ATR, cm^{-1}): 2967, 2875, 1737, 1721, 1661, 1268, 1100.

HRMS (ESI+): calcd. for $[C_{27}H_{26}O_6 + H]^+$: 447.1802, found: 447.1808.

Molecule 8y: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl 1-methyl-1H-indole-3-carboxylate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7o** (19 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt, 8:2 Hex:AcOEt) affords the title compound as an yellow oil: 38 mg, 96%.

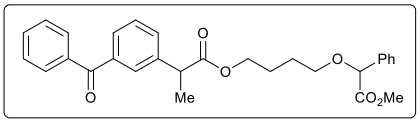
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.63 – 7.59 (m, 1H), 7.47 – 7.35 (m, 5H), 7.29 – 7.20 (m, 2H), 7.16 – 7.09 (m, 1H), 7.04 (s, 1H), 4.85 (s, 1H), 4.14 (t, *J* = 6.1 Hz, 2H), 3.75 (s, 2H), 3.75 (s, 3H), 3.72 (s, 3H), 3.58 – 3.39 (m, 2H), 1.78 – 1.67 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 172.1, 171.3, 136.8, 136.5, 128.6 (2x), 127.6 (2x), 127.1, 121.6, 119.0, 118.9, 109.2, 106.8, 81.0, 69.2, 64.4, 52.2, 32.6, 31.2, 26.0, 25.3.

IR (ATR, cm^{-1}): 3058, 2952, 1730, 1475, 1134, 1117.

HRMS (ESI+): calcd. for $[C_{24}H_{27}NO_5 + H]^+$: 410.1962, found: 410.1967.

Molecule 8z: 4-(2-methoxy-2-oxo-1-phenylethoxy)butyl 2-(3-benzoylphenyl)propanoate



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), Ketoprofen **7p** (25 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a pale yellow oil: 47 mg, 99%, > 20:1 dr.

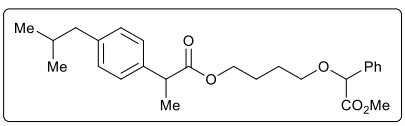
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.80 – 7.73 (m, 3H), 7.66 (dt, *J* = 7.5, 1.4 Hz, 1H), 7.61 – 7.32 (m, 10H), 4.83 (s, 1H), 4.10 (t, *J* = 6.0 Hz, 2H), 3.77 (q, *J* = 7.3 Hz, 1H), 3.68 (s, 3H), 3.55 – 3.36 (m, 2H), 1.74 – 1.60 (m, 4H), 1.52 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 196.4, 174.0, 171.3, 140.9, 137.8 137.4, 136.4, 132.4, 131.4, 130.0, 129.1, 128.9, 128.6, 128.5 (2x), 128.2, 127.1, 81.0, 69.1, 64.6, 52.2, 45.4, 25.9, 25.2, 18.4.

IR (ATR, cm^{-1}): 2952, 2877, 1732, 1657, 1283, 1171.

HRMS (ESI+): calcd. for $[C_{29}H_{30}O_6 + H]^+$: 475.2115, found: 475.2121.

Molecule 8aa: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl 2-(4-isobutylphenyl)propanoate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), Ibuprofen **7q** (21 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as an yellow oil: 42 mg, 99%, >20:1 dr.

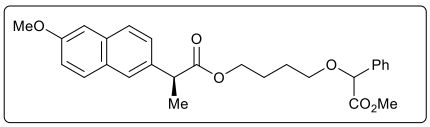
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.45 – 7.41 (m, 2H), 7.38 – 7.33 (m, 3H), 7.19 (d, *J* = 8.1 Hz, 2H), 7.08 (d, *J* = 8.1 Hz, 2H), 4.83 (s, 1H), 4.08 (t, *J* = 6.1 Hz, 2H), 3.70 (s, 3H), 3.69 - 3.62 (m, 1H), 3.51 – 3.37 (m, 2H), 2.44 (d, *J* = 7.0 Hz, 2H), 1.89 – 1.78 (m, 1H), 1.74 – 1.59 (m, 4H), 1.48 (d, *J* = 7.0 Hz, 3H), 0.89 (d, *J* = 7.0 Hz, 6H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 174.7, 171.3, 140.4, 137.8, 136.5,129.2, 128.6, 128.5, 127.1 (2x), 81.0, 69.1, 64.3, 52.1, 45.1, 45.0, 30.1, 25.9, 25.2, 22.3, 18.4.

IR (ATR, cm^{-1}): 2955, 2870, 1734, 1456, 1167, 1097.

HRMS (ESI+): calcd. for $[C_{26}H_{34}O_5 + H]^+$: 427.2479, found: 427.2486.

Molecule 8bb: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl (2S)-2-(6-methoxynaphthalen-2-yl)propanoate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), Naproxen **7r** (23 mg, 0.1 mmol), and THF (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a pale yellow oil: 32 mg, 71%, >20:1 dr.

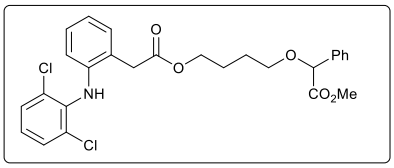
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.71 – 7.66 (m, 3H), 7.42 – 7.32 (m, 6H), 7.16 – 7.11 (m, 2H), 4.79 (s, 1H), 4.10 (t, *J* = 6.0 Hz, 2H), 3.91 (s, 3H), 3.83 (q, *J* = 7.2 Hz, 1H), 3.69 (s, 3H), 3.51 – 3.32 (m, 2H), 1.76 – 1.62 (m, 4H), 1.57 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (62.5 MHz, $CDCl_3$) (1C cannot be unambiguously assigned) δ: 174.7, 171.3, 157.6, 136.5, 135.7, 133.6, 129.2, 128.9, 128.6 (2x), 127.1, 126.2, 125.9, 118.9, 105.5, 81.0, 69.1, 64.4, 55.2, 52.2, 45.4, 26.0, 25.2, 18.5.

IR (ATR, cm^{-1}): 2954, 2851, 1730, 1607, 1456, 1175.

HRMS (ESI+): calcd. for $[C_{27}H_{30}O_6 + H]^+$: 451.2115, found: 451.2122.

Molecule 8cc: *methyl 2-(4-(2-(2-((2,6-dichlorophenyl)amino)phenyl)acetoxy) butoxy)-2-phenylacetate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), Diclofenac **7s** (25 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a pale yellow oil: 44 mg, 85%.

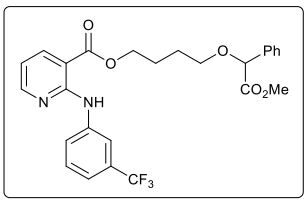
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.46 – 7.32 (m, 7H), 7.22 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.12 (td, *J* = 7.7, 1.4 Hz, 1H), 7.01 – 6.92 (m, 3H), 6.55 (d, *J* = 7.9 Hz, 1H), 4.85 (s, 1H), 4.17 (t, *J* = 6.3 Hz, 2H), 3.80 (s, 2H), 3.71 (s, 3H), 3.57 – 3.43 (m, 2H), 1.82 – 1.68 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 172.4, 171.3, 142.7, 137.8, 136.5, 130.8, 129.4, 128.8, 128.6 (2x), 127.9, 127.1, 124.4, 123.9, 121.9, 118.2, 81.0, 69.1, 65.0, 52.2, 38.6, 26.0, 25.3.

IR (ATR, cm^{-1}): 2954, 2918, 2851, 1737, 1721, 1452, 1210.

HRMS (ESI+): calcd. for $[C_{27}H_{27}Cl_2NO_5 + H]^+$: 516.1339, found: 516.1349.

Molecule 8dd: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl 2-((3-(trifluoromethyl) phenyl)amino)nicotinate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), Niflumic Acid **7t** (28 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a pale yellow oil: 40 mg, 80%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 10.39 (s, 1H), 8.41 (dd, *J* = 4.8, 2.0 Hz, 1H), 8.25 (dd, *J* = 7.8, 2.0 Hz, 1H), 8.10 (s, 1H), 7.88 (d, *J* = 8.2 Hz, 1H), 7.47 – 7.32 (m, 6H), 7.29 (s, 1H), 6.78 (dd, *J* = 7.8, 4.8 Hz, 1H), 4.89 (s, 1H), 4.38 (t, *J* = 6.0 Hz, 2H), 3.71 (s, 3H), 3.65 – 3.51 (m, 2H), 1.99 – 1.77 (m, 4H).

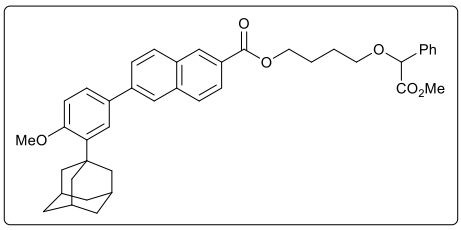
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 167.4, 155.7, 152.9, 140.3, 140.1, 136.4, 131.0 (q, *J* = 31.9 Hz), 129.1, 128.7, 128.6, 127.1, 124.2 (q, *J* = 270.6 Hz), 123.4,

118.9 (q, *J* = 3.8 Hz), 117.0 (q, *J* = 4.4 Hz), 114.0, 107.6, 81.1, 69.1, 65.1, 52.2, 26.2, 25.4.

IR (ATR, cm^{-1}): 3276, 3315, 2954, 1687, 1331, 1089, 1119.

HRMS (ESI+): calcd. for $[C_{26}H_{25}F_3N_2O_5 + H]^+$: 503.1788, found: 503.1797.

Molecule 8ee: *4-(2-methoxy-2-oxo-1-phenylethoxy)butyl 6-(3-((3r,5r,7r)-adamantan-1-yl)-4-methoxyphenyl)-2-naphthoate*



General Procedure C is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), Adapalene **7u** (41 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as an white solid: 58 mg, 92%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.64 (s, 1H), 8.12 – 7.93 (m, 4H), 7.83 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.66 – 7.49 (m, 4H), 7.44 – 7.36 (m, 3H), 7.02 (d, *J* = 8.5 Hz, 1H), 4.95 (s, 1H), 4.46 (t, *J* = 6.0 Hz, 2H), 3.93 (s, 3H), 3.75 (s, 3H), 3.71 – 3.55 (m, 2H), 2.23 (s, 6H), 2.15 (s, 3H), 2.02 – 1.89 (m, 4H), 1.85 (s, 6H).

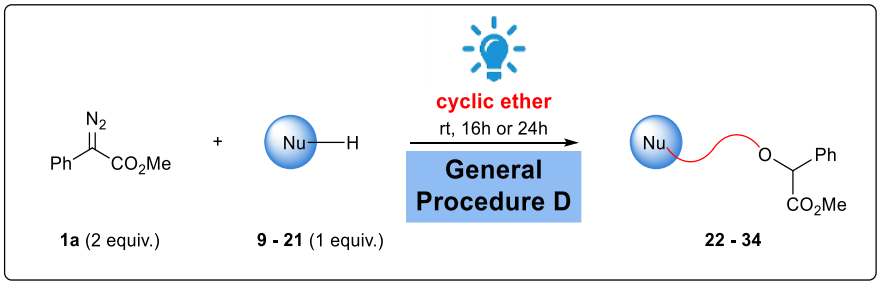
^{13}C NMR (62.5 MHz, $CDCl_3$) (1C cannot be unambiguously assigned) δ: 171.3, 166.7, 158.8, 141.3, 138.9, 136.5, 135.9, 132.5, 131.2, 130.7, 129.6, 128.6 (2x), 128.1, 127.1, 126.4, 125.9, 125.7, 125.5, 124.6, 112.0, 81.1, 69.3, 64.7, 55.1, 52.2, 40.5, 37.1 (2x), 29.0, 26.3, 25.5.

M.P.: 142 – 143 ^{o}C.

IR (ATR, cm^{-1}): 2903, 2879, 2851, 1711, 1275, 1218, 1098.

HRMS (ESI+): calcd. for $[C_{41}H_{44}O_6 + H]^+$: 633.3211, found: 633.3219.

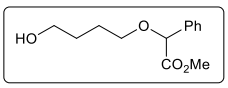
2.4 Using Other Nucleophiles and Cyclic Ethers



General Procedure D: *Photochemical Ring-Opening of Cyclic Ethers Using Aryldiazoacetates and Nucleophiles*

A 4 mL vial is charged with aryldiazoacetate **1a** (2 equiv.), a nucleophile **9** - **21** (1 equiv.), and the cyclic ether **3** (0.1 M in relation to the nucleophile). The reaction mixture is stirred under blue light irradiation (using two lamps, 15 W each, displaced at approximate distances of 10 cm each from the reaction vessel). Then, the reaction mixture is concentrated under reduced pressure and the resulting residue is purified by flash column chromatography to afford the corresponding compound **22** – **34** in the stated yield.

Molecule 22: *methyl 2-(4-hydroxybutoxy)-2-phenylacetate*



General Procedure D is employed with aryldiazoacetate **1a** (18 mg, 0.1 mmol), H_2O **9** (250 μL, 13.9 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a colorless oil: 22 mg, 92%.

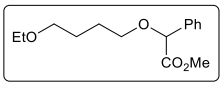
^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.44 – 7.42 (m, 2H), 7.38 – 7.33 (m, 3H), 4.87 (s, 1H), 3.70 (s, 3H), 3.67 (t, *J* = 6.0 Hz, 2H), 3.57 (dt, *J* = 9.0 Hz, *J* = 6.0 Hz, 1H), 3.48 (dt, *J* = 9.0 Hz, *J* = 6.0 Hz, 1H), 1.98 (br s, 1H), 1.78 – 1.72 (m, 2H), 1.71 – 1.65 (m, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ: 171.3, 136.4, 128.8, 128.7, 127.2, 81.2, 69.8, 62.6, 52.3, 29.8, 26.4.

IR (ATR, cm^{-1}): 3425, 2950, 2872, 1749, 1437, 1212, 1121.

HRMS (ESI+): calcd. for $[C_{13}H_{18}O_4 + H]^+$: 239.1278, found: 239.1277.

Molecule 23: *methyl 2-(4-ethoxybutoxy)-2-phenylacetate*



General Procedure D is employed with aryldiazoacetate **1a** (18 mg, 0.1 mmol), 1:4 EtOH **10**:THF **3a** (200 µL:800 µL, 0.1 M), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a colorless oil: 24 mg, 91%.

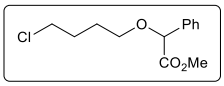
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.46 -7.42 (m, 2H), 7.39 – 7.29 (m, 3H), 4.87 (s, 1H), 3.70 (s, 3H), 3.60 – 3.39 (m, 6H), 1.76 – 1.62 (m, 4H), 1.18 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.4, 136.6, 128.5 (x2), 127.1, 81.0, 70.2, 69.6, 66.0, 52.2, 26.3 (x2), 15.2.

IR (ATR, cm^{-1}): 2952, 2864, 1752, 1737, 1171, 1108.

HRMS (ESI+): calcd. for $[C_{15}H_{22}O_4 + H]^+$: 267.1591, found: 267.1590.

Molecule 24: *methyl 2-(4-chlorobutoxy)-2-phenylacetate*



General Procedure D is employed with aryldiazoacetate **1a** (18 mg, 0.1 mmol), and 1:4 $HCl_{(aq)}$ 1M **11**:THF **3a** (200 µL:800 µL, 0.1 M). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a colorless oil: 21 mg, 83%.

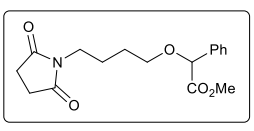
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.46 – 7.34 (m, 5H), 4.86 (s, 1H), 3.71 (s, 3H), 3.62 - 3.41 (m, 4H), 1.97 - 1.75 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 136.5, 128.7, 128.6, 127.1, 81.0, 68.9, 52.2, 44.8, 29.3, 26.9.

IR (ATR, cm^{-1}): 2954, 2875, 1748, 1210, 1117.

HRMS (ESI+): calcd. for $[C_{13}H_{17}ClO_3 + H]^+$: 257.0939, found: 257.0940.

Molecule 25: *methyl 2-(4-(2,5-dioxopyrrolidin-1-yl)butoxy)-2-phenylacetate*



General Procedure D is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), succinimide **12** (10 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a colorless oil: 23 mg, 72%.

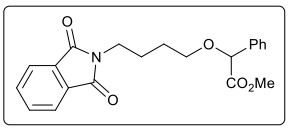
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.45 – 7.30 (m, 5H), 4.84 (s, 1H), 3.69 (s, 3H), 3.58 – 3.39 (m, 4H), 2.67 (s, 4H), 1.71 – 1.64 (m, 4H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 177.2, 171.3, 136.5, 128.6 (2x), 127.1, 81.0, 69.1, 52.2, 38.4, 28.1, 26.9, 24.4.

IR (ATR, cm^{-1}): 2950, 2872, 1750, 1694, 1402, 1171, 1125.

HRMS (ESI+): calcd. for $[C_{17}H_{21}NO_5 + H]^+$: 320.1492, found: 320.1494.

Molecule 26: *methyl 2-(4-(1,3-dioxoisoindolin-2-yl)butoxy)-2-phenylacetate*



General Procedure D is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), phthalimide **13** (15 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a colorless oil: 31 mg, 85%.

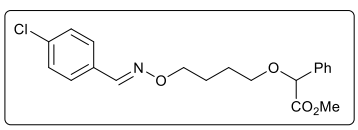
‘^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.82 (dd, *J* = 5.5 Hz, *J* = 3.0 Hz, 2H), 7.70 (dd, *J* = 5.5 Hz, *J* = 3.0 Hz, 2H), 7.43 (dd, *J* = 7.9 Hz, *J* = 1.5 Hz, 2H), 7.36 – 7.29 (m, 3H), 4.85 (s, 1H), 3.73 – 3.71 (m, 2H), 3.69 (s, 3H), 3.57 (dt, *J* = 9.0 Hz, *J* = 6.3 Hz, 1H), 3.47 (dt, *J* = 9.0 Hz, *J* = 6.3 Hz, 1H), 1.83 – 1.76 (m, 2H), 1.73 – 1.66 (m, 2H).

^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 168.4, 136.5, 133.8, 132.1, 128.6, 127.1, 123.1, 81.1, 69.1, 52.2, 37.6, 26.9, 25.3.

IR (ATR, cm^{-1}): 2950, 2872, 1752, 1704, 1396, 1210, 1048.

HRMS (ESI+): calcd. for $[C_{21}H_{21}NO_5 + H]^+$: 368.1492, found: 368.1494.

Molecule 27: [6] *methyl (E)-2-(4-(((4-chlorobenzylidene)amino)oxy)butoxy)-2-phenylacetate*



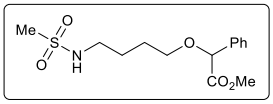
General Procedure D is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), (*E*)-4-chlorobenzaldehyde oxime **14** (15 mg, 0.1 mmol) and

[6] Spectroscopic data is in good agreement with the literature. See: Q. Li, B.-G. Cai, L. Li, J. Xuan, *Org. Lett.* 2021, **23**, 6951-6955.

THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt) affords the title compound as a pale yellow oil: 36 mg, 96%.

^{1}H NMR (250 MHz, $CDCl_3$): 8.01 (s, 1H), 7.52 – 7.43 (m, 4H), 7.38 – 7.31 (m, 5H), 4.88 (s, 1H), 4.18 (t, *J* = 6.1 Hz, 2H), 3.71 (s, 3H), 3.62 – 3.47 (m, 2H), 1.84 – 1.77 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.4, 147.1, 136.6, 135.4, 130.9, 128.9, 128.6 (2x), 128.1, 127.1, 81.0, 74.0, 69.5, 52.2, 26.0, 25.8.
IR (ATR, cm^{-1}): 2950, 2874, 1752, 1737, 1493, 1210, 1091, 1015.
HRMS (ESI+): calcd. for $[C_{20}H_{22}ClNO_4 + H]^+$: 376.1310, found: 376.1312.

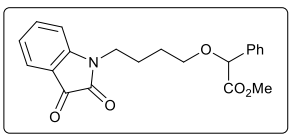
Molecule 28: *methyl 2-(4-(methylsulfonamido)butoxy)-2-phenylacetate*



General Procedure D is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), methanesulfonamide **15** (9.5 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a colorless oil: 28 mg, 89%.

^{1}H NMR (500 MHz, $CDCl_3$) (1H cannot be unambiguously assigned) δ: 7.44 – 7.32 (m, 5H), 4.85 (s, 1H), 3.70 (s, 3H), 3.59 – 3.40 (m, 2H), 3.18 (t, *J* = 6.5 Hz, 2H), 2.92 (s, 3H), 1.77 – 1.67 (m, 4H).
^{13}C NMR (125 MHz, $CDCl_3$) δ: 171.3, 136.2, 128.8, 128.7, 127.2, 81.1, 69.2, 52.3, 42.9, 40.0, 27.2, 26.7.
IR (ATR, cm^{-1}): 3303, 2954, 2872, 1745, 1316, 1212, 1149.
HRMS (ESI+): calcd. for $[C_{14}H_{21}NO_5S + H]^+$: 316.1213, found: 316.1214.

Molecule 29: *methyl 2-(4-(2,3-dioxoindolin-1-yl)butoxy)-2-phenylacetate*

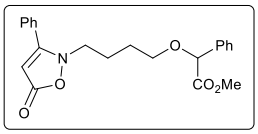


General Procedure D is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), isatin **16** (15 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column

chromatography (SiO_2, gradient: Hex – 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as a reddish oil: 29 mg, 79%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.60 – 7.50 (m, 2H), 7.43 – 7.33 (m, 5H), 7.09 (t, *J* = 7.7 Hz, 1H), 6.97 (d, *J* = 7.7 Hz, 1H), 4.86 (s, 1H), 3.78 (t, *J* = 7.3 Hz, 2H), 3.71 (s, 3H), 3.66 – 3.47 (m, 2H), 1.89 - 1.68 (m, 4H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 183.6, 171.3, 158.2, 151.0, 138.3, 136.4, 128.7 (x2), 127.1, 125.4, 123.6, 117.6, 110.4, 81.1, 69.0, 52.2, 39.9, 26.7, 24.0.
IR (ATR, cm^{-1}): 2952, 2874, 1737, 1613, 1471, 1359, 1097.
HRMS (ESI+): calcd. for $[C_{21}H_{21}NO_5 + H]^+$: 368.1492, found: 368.1492.

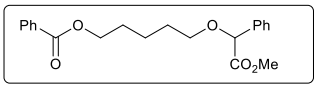
Molecule 30: *methyl 2-(4-(5-oxo-3-phenylisoxazol-2(5H)-yl)butoxy)-2-phenylacetate*



General Procedure D is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), 3-phenylisoxazol-5(4*H*)-one **17** (16 mg, 0.1 mmol), and THF **3a** (0.1 M, 1 mL). Purification by flash column chromatography (SiO_2, gradient: Hex – 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) affords the title compound as an brownish oil: 27 mg, 71%.

^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.74 (dd, *J* = 6.6 Hz, *J* = 3.0 Hz, 2H), 7.45 – 7.43 (m, 5H), 7.38 – 7.33 (m, 3H), 5.51 (s, 1H), 4.88 (s, 1H), 4.32 – 4.28 (m, 2H), 3.71 (s, 3H), 3.62 (dt, *J* = 9.0 Hz, *J* = 6.1 Hz, 1H), 3.53 (dt, *J* = 9.1 Hz, *J* = 6.0 Hz, 1H), 2.03 – 1.96 (m, 2H), 1.87 – 1.81 (m, 2H).
^{13}C NMR (125 MHz, $CDCl_3$) δ: 173.8, 171.3, 164.1, 136.4, 130.0, 129.6, 128.8, 128.7, 128.6, 127.1, 126.4, 81.1, 75.7, 72.1, 69.0, 52.2, 25.8, 25.7.
IR (ATR, cm^{-1}): 2359, 2345, 1750, 1655, 1613, 1475, 1138.
HRMS (ESI+): calcd. for $[C_{22}H_{23}NO_5 + H]^+$: 382.1649, found: 382.1649.

Molecule 8ff: *5-(2-methoxy-2-oxo-1-phenylethoxy)pentyl benzoate*

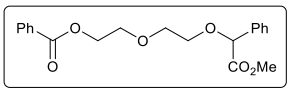


General Procedure D is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), benzoic acid **7a** (12 mg, 0.1 mmol), and tetrahydro-2*H*-pyran **3b** (0.1 M, 1 mL), while

simultaneously heating at 60 °C. Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt) affords the title compound as a colorless oil: 29 mg, 80%.

^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.06 – 8.02 (m, 2H), 7.58 – 7.52 (m, 1H), 7.47 – 7.26 (m, 7H), 4.87 (s, 1H), 4.32 (t, *J* = 6.0 Hz, 2H), 3.70 (s, 3H), 3.59 – 3.45 (m, 2H), 1.82 – 1.52 (m, 6H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.4, 166.6, 136.6, 132.8, 130.4, 129.5, 128.6 (2x), 128.3, 127.1, 81.1, 69.6, 64.9, 52.2, 29.2, 28.4, 22.6.
IR (ATR, cm^{-1}): 3065, 3032, 2950, 2868, 1752, 1715, 1274, 1100.
HRMS (ESI+): calcd. for $[C_{21}H_{24}O_5 + H]^+$: 357.1697, found: 357.1701.

Molecule 8gg: *2-(2-(2-methoxy-2-oxo-1-phenylethoxy)ethoxy)ethyl benzoate*

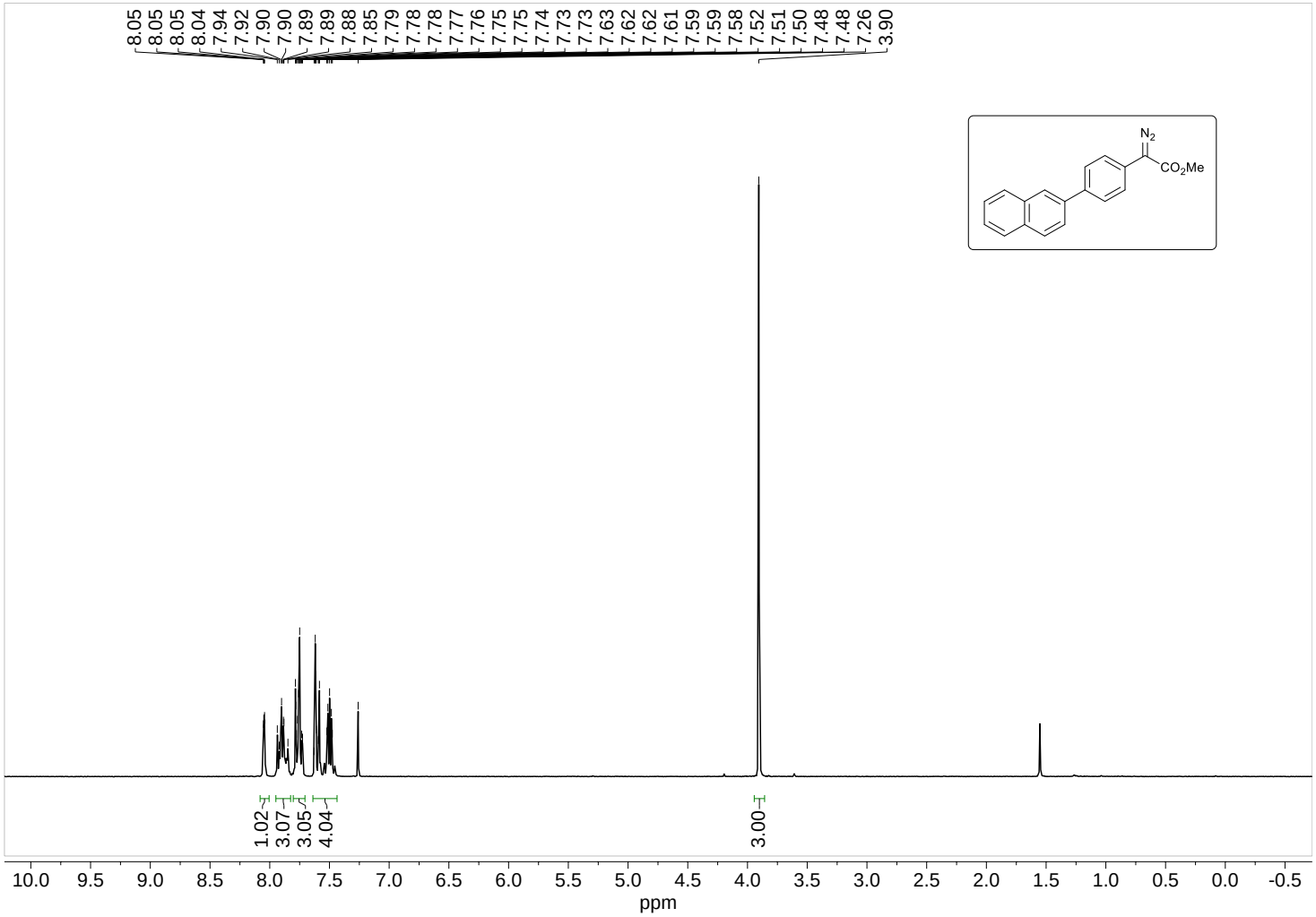


General Procedure D is employed with aryldiazoacetate **1a** (35 mg, 0.2 mmol), carboxylic acid **7a** (12 mg, 0.1 mmol), and 1,4-dioxane **3c** (0.1 M, 1 mL), while simultaneously heating at 60 °C. Purification by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt) affords the title compound as a colorless oil: 29 mg, 80%.

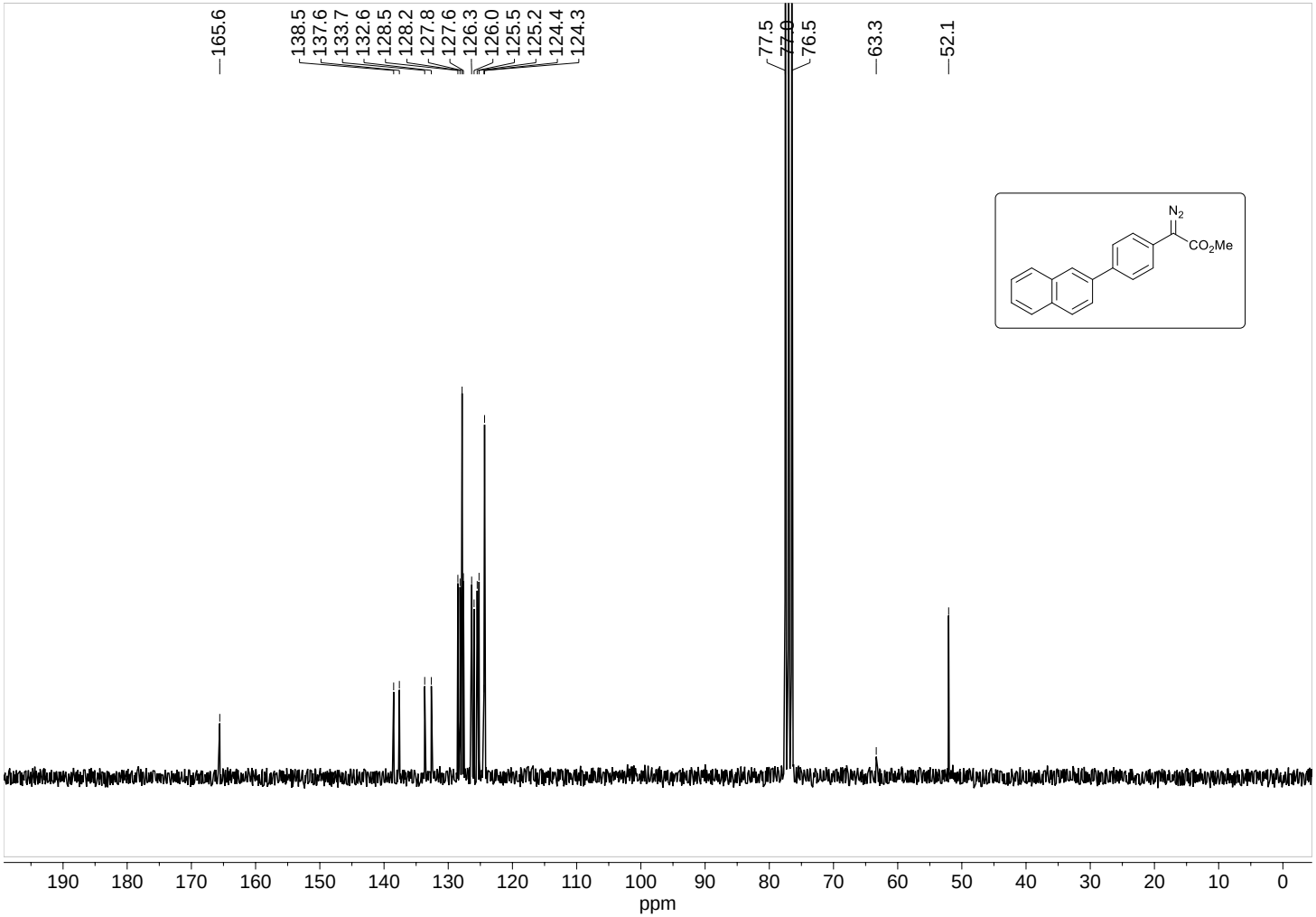
^{1}H NMR (250 MHz, $CDCl_3$): δ 8.07 – 8.04 (m, 2H), 7.59 – 7.52 (m, 1H), 7.46 – 7.40 (m, 4H), 7.37 – 7.31 (m, 3H), 5.02 (s, 1H), 4.49 – 4.45 (m, 2H), 3.85 – 3.81 (m, 2H), 3.79 – 3.70 (m, 4H), 3.68 (s, 3H).
^{13}C NMR (62.5 MHz, $CDCl_3$) δ: 171.3, 166.5, 136.3, 132.9, 130.1, 129.7, 128.7, 128.6, 128.3, 127.3, 81.3, 70.7, 69.3, 68.9, 64.1, 52.2.
IR (ATR, cm^{-1}): 3036, 3005, 2954, 1756, 1722, 1251, 1098, 1028.
HRMS (ESI+): calcd. for $[C_{20}H_{22}O_6 + H]^+$: 359.1489, found: 359.1491.

3. ^{1}H AND ^{13}C NMR SPECTRA OF COMPOUNDS

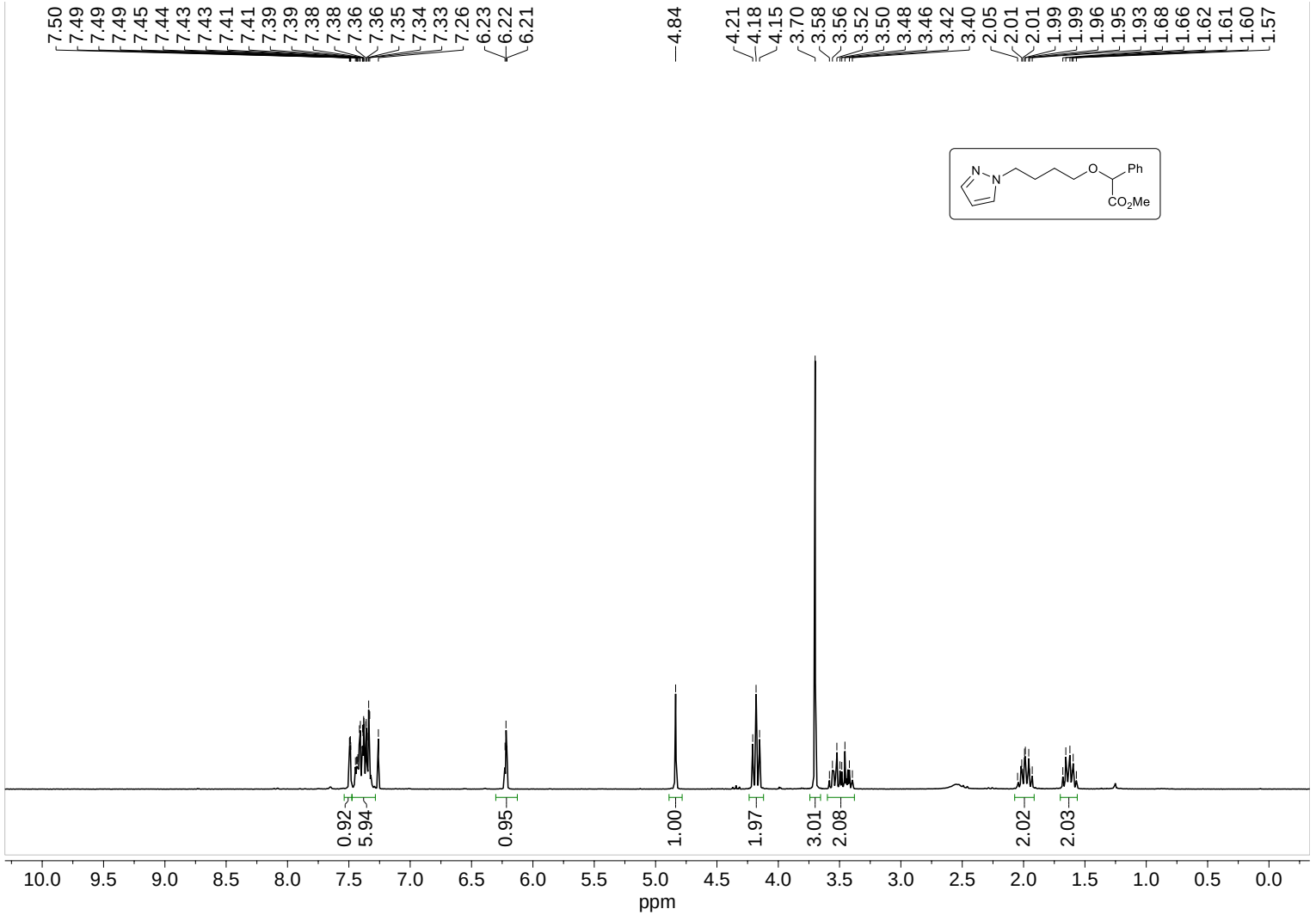
Molecule 1j - ^{1}H NMR (250 MHz, $CDCl_3$)



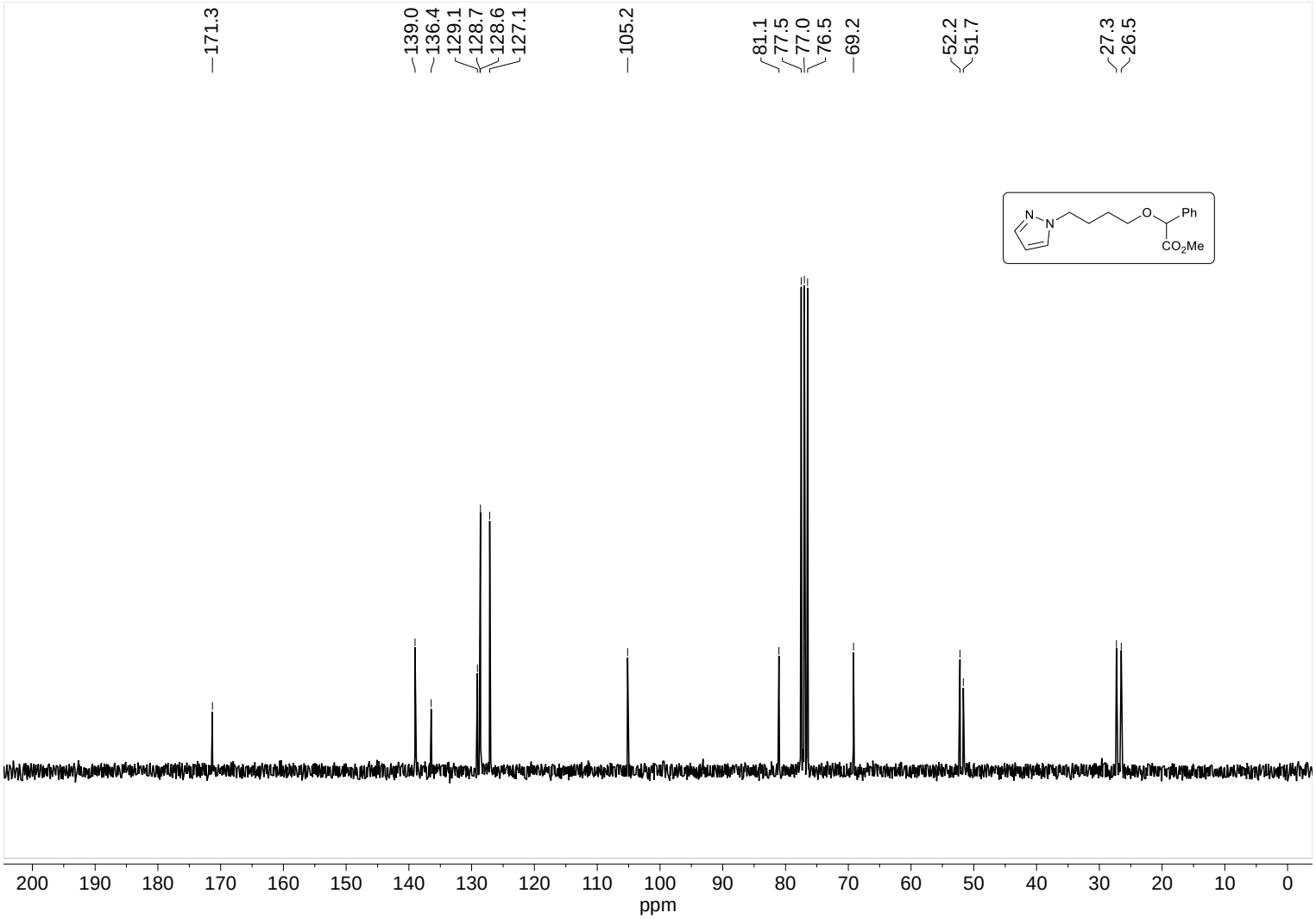
Molecule 1j - ^{13}C NMR (62.5 MHz, $CDCl_3$)



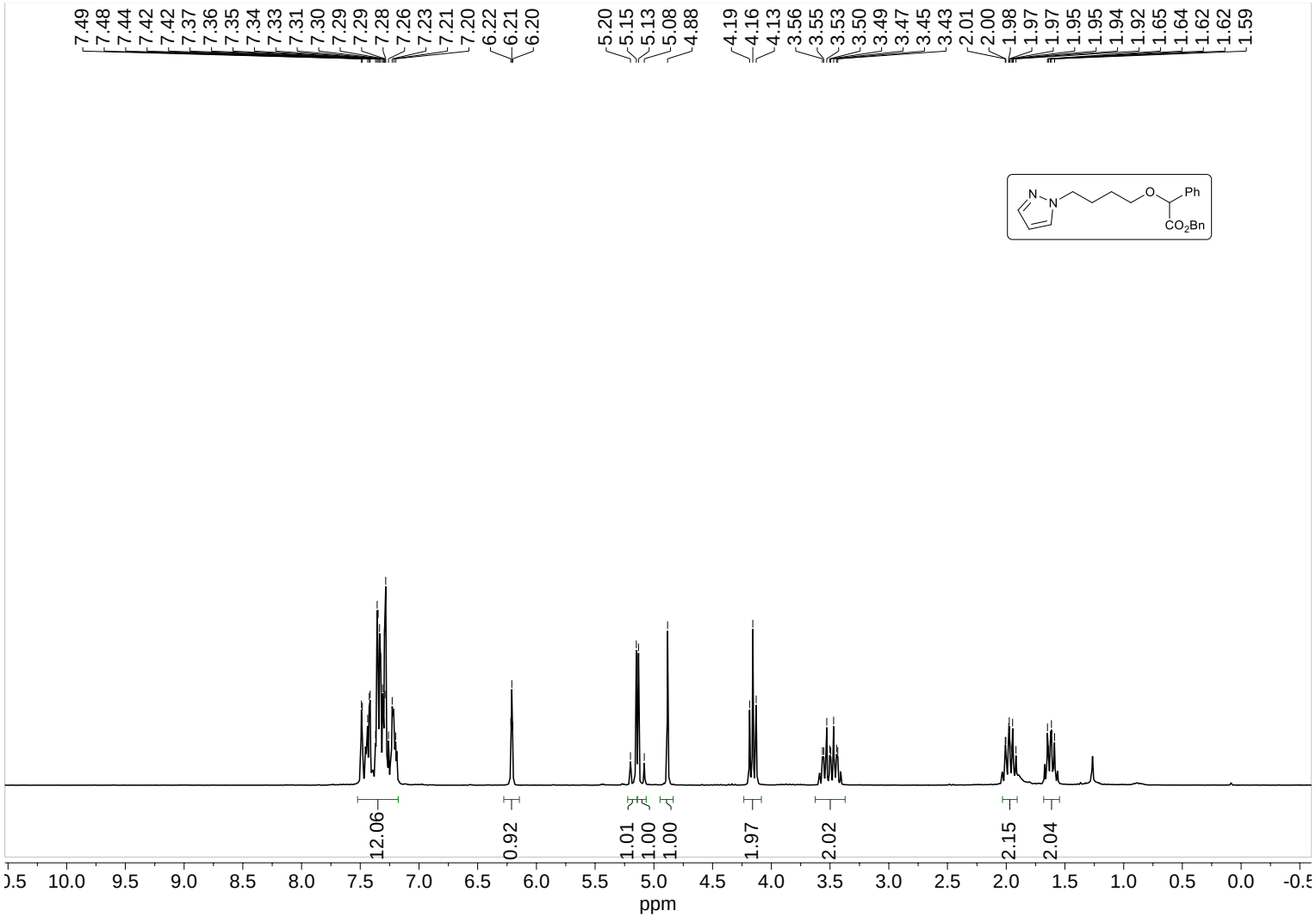
Molecule 4a - ^{1}H NMR (250 MHz, $CDCl_3$)



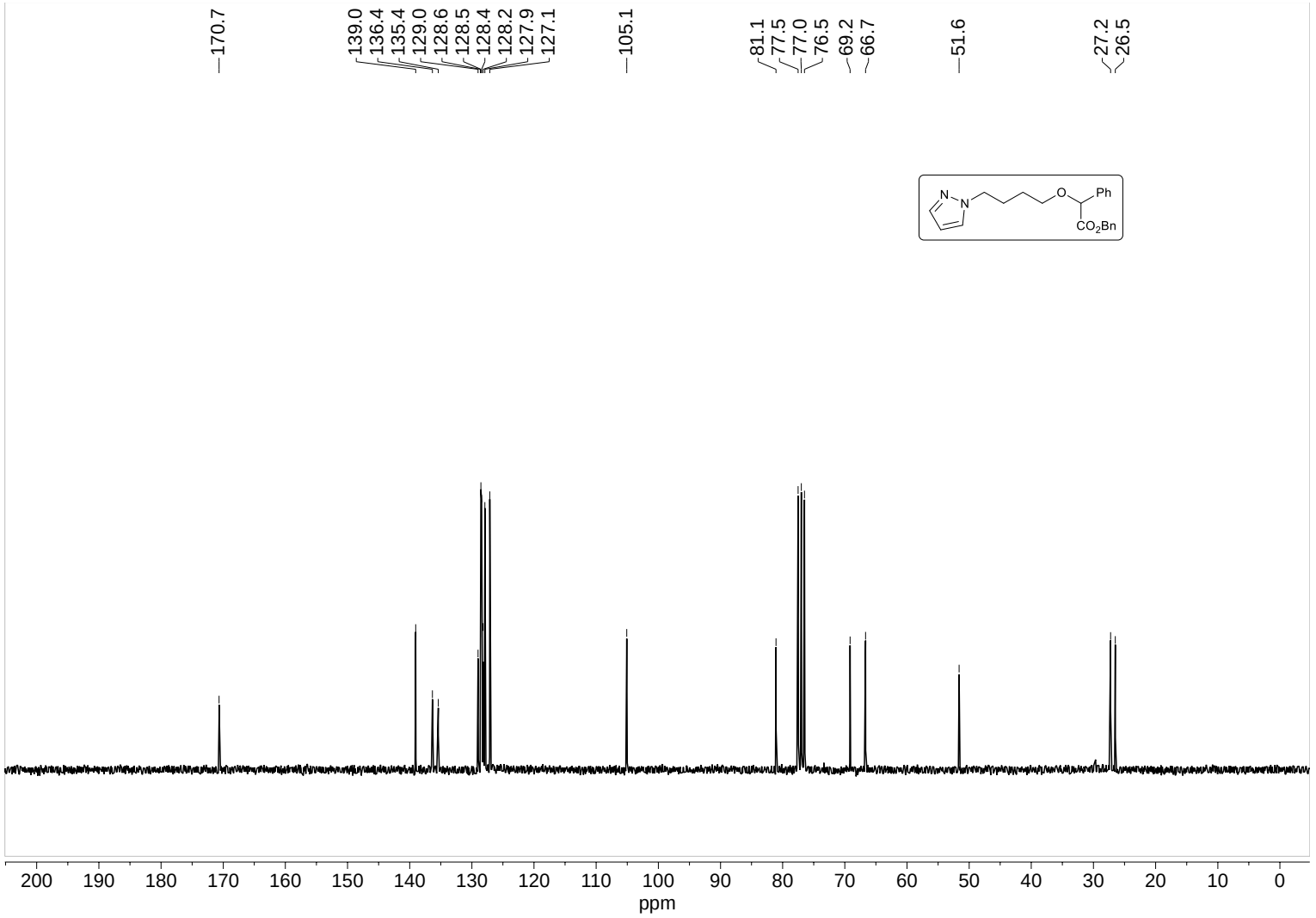
Molecule 4a - ^{13}C NMR (62.5 MHz, $CDCl_3$)



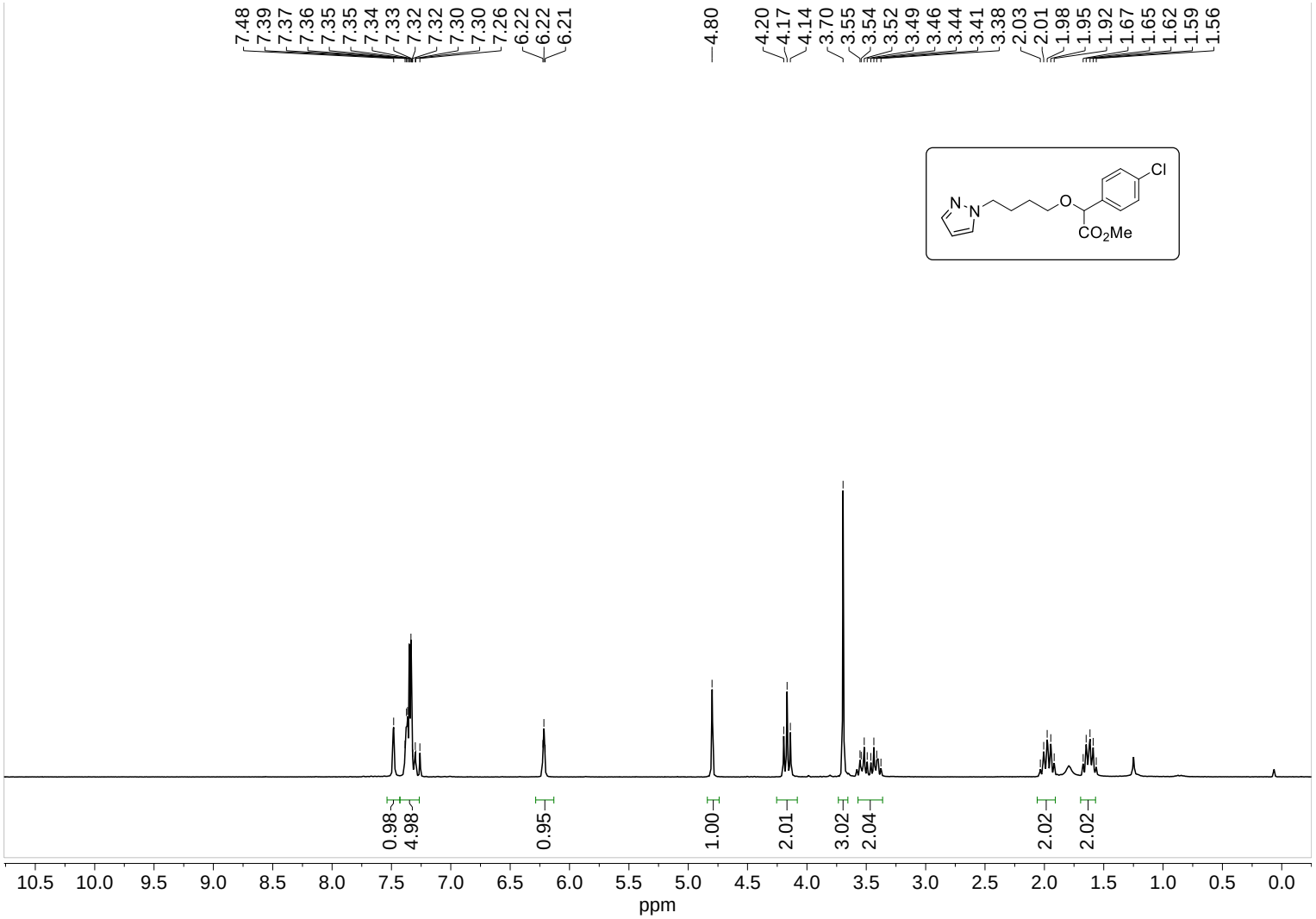
Molecule 4b - ^{1}H NMR (250 MHz, $CDCl_3$)



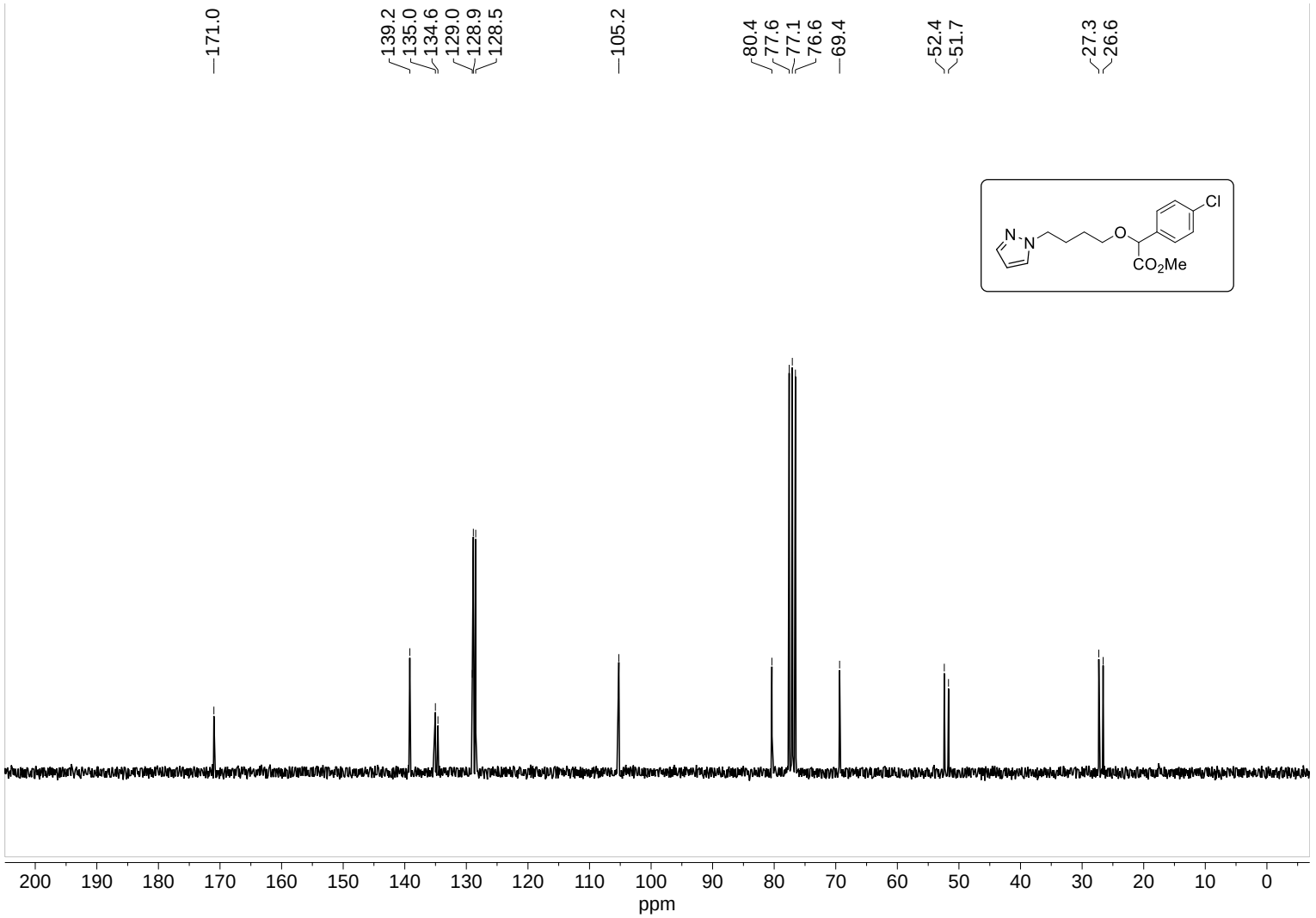
Molecule 4b - ^{13}C NMR (62.5 MHz, $CDCl_3$)



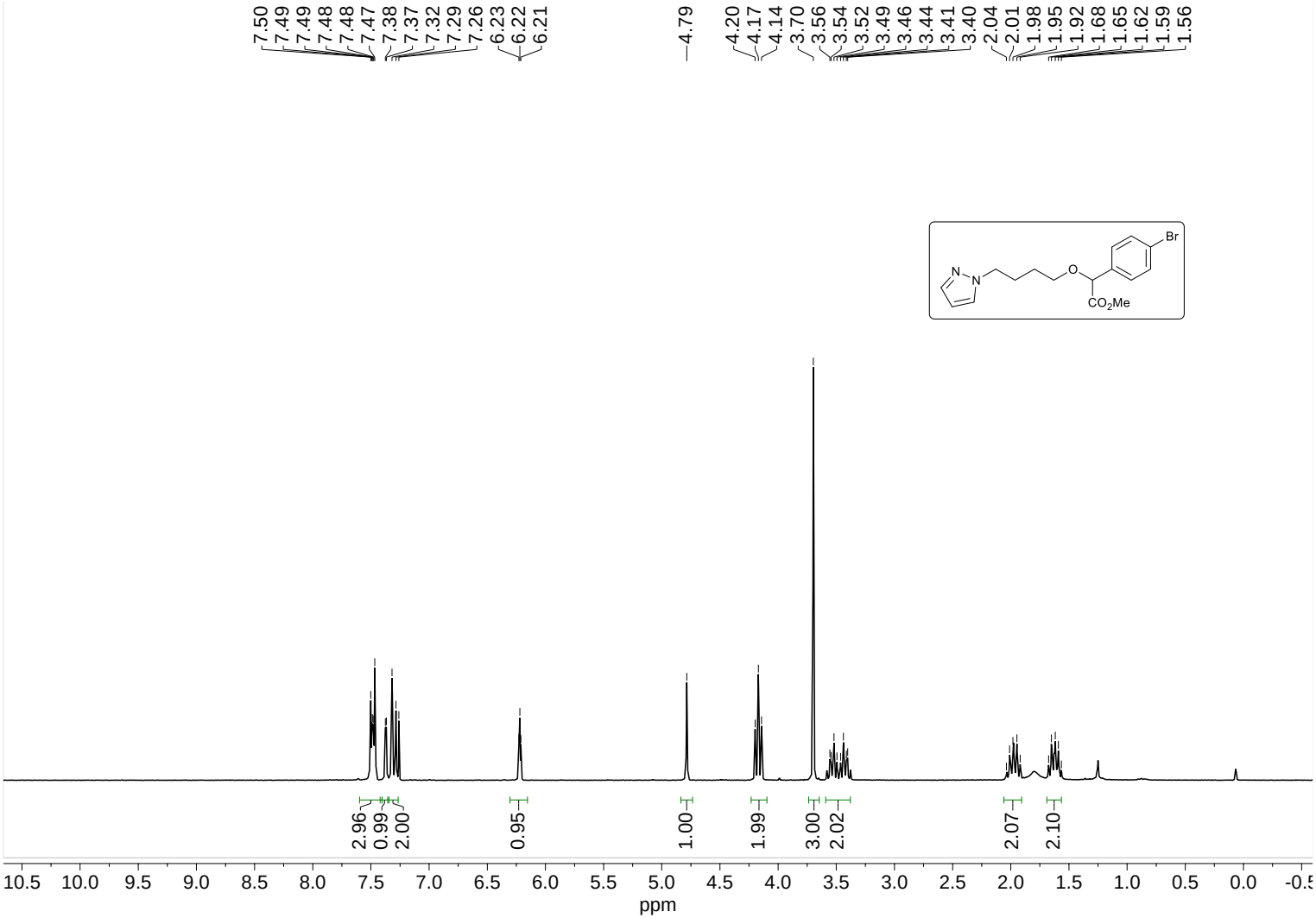
Molecule 4c - ^{1}H NMR (250 MHz, $CDCl_3$)



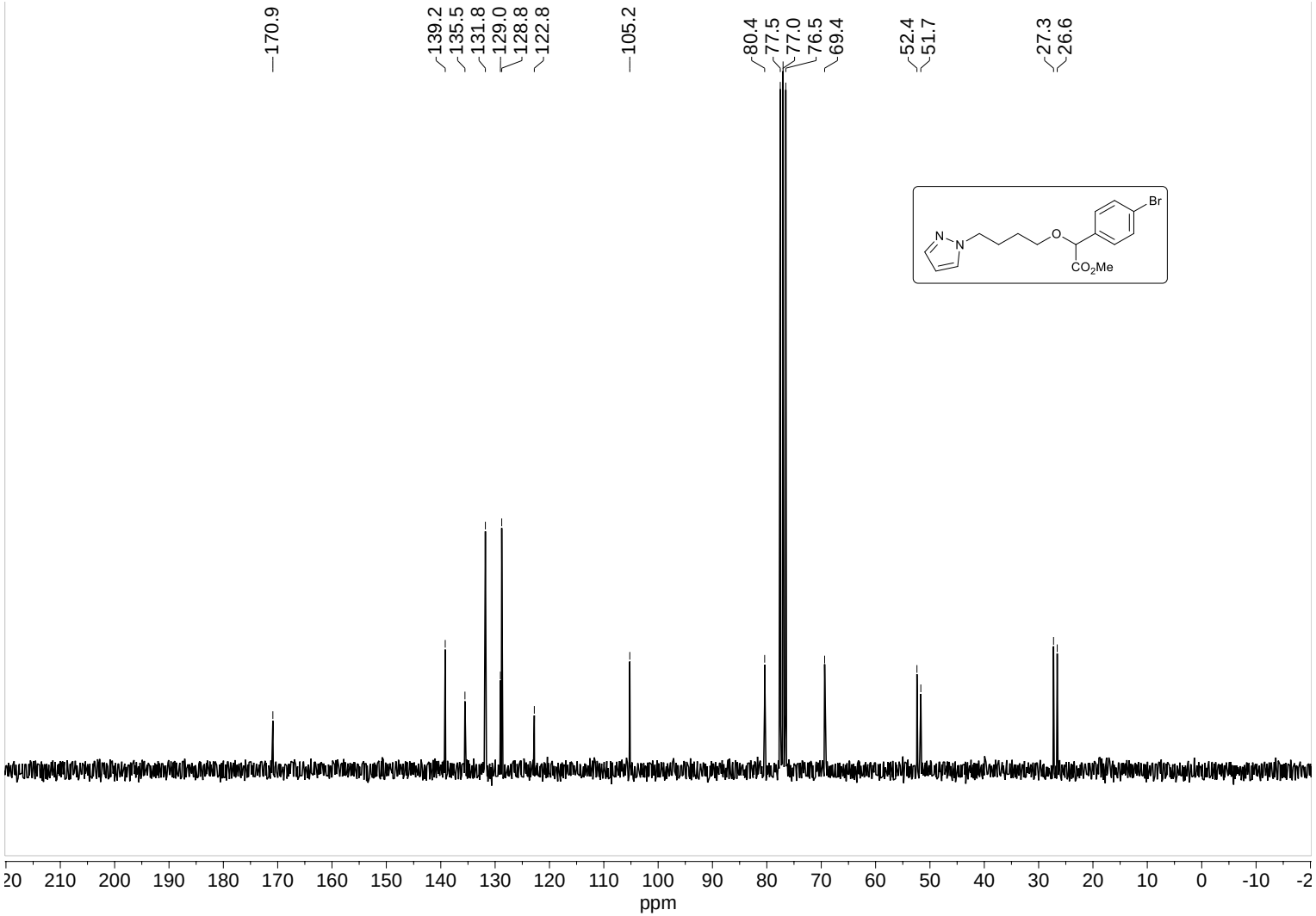
Molecule 4c - ^{13}C NMR (62.5 MHz, $CDCl_3$)



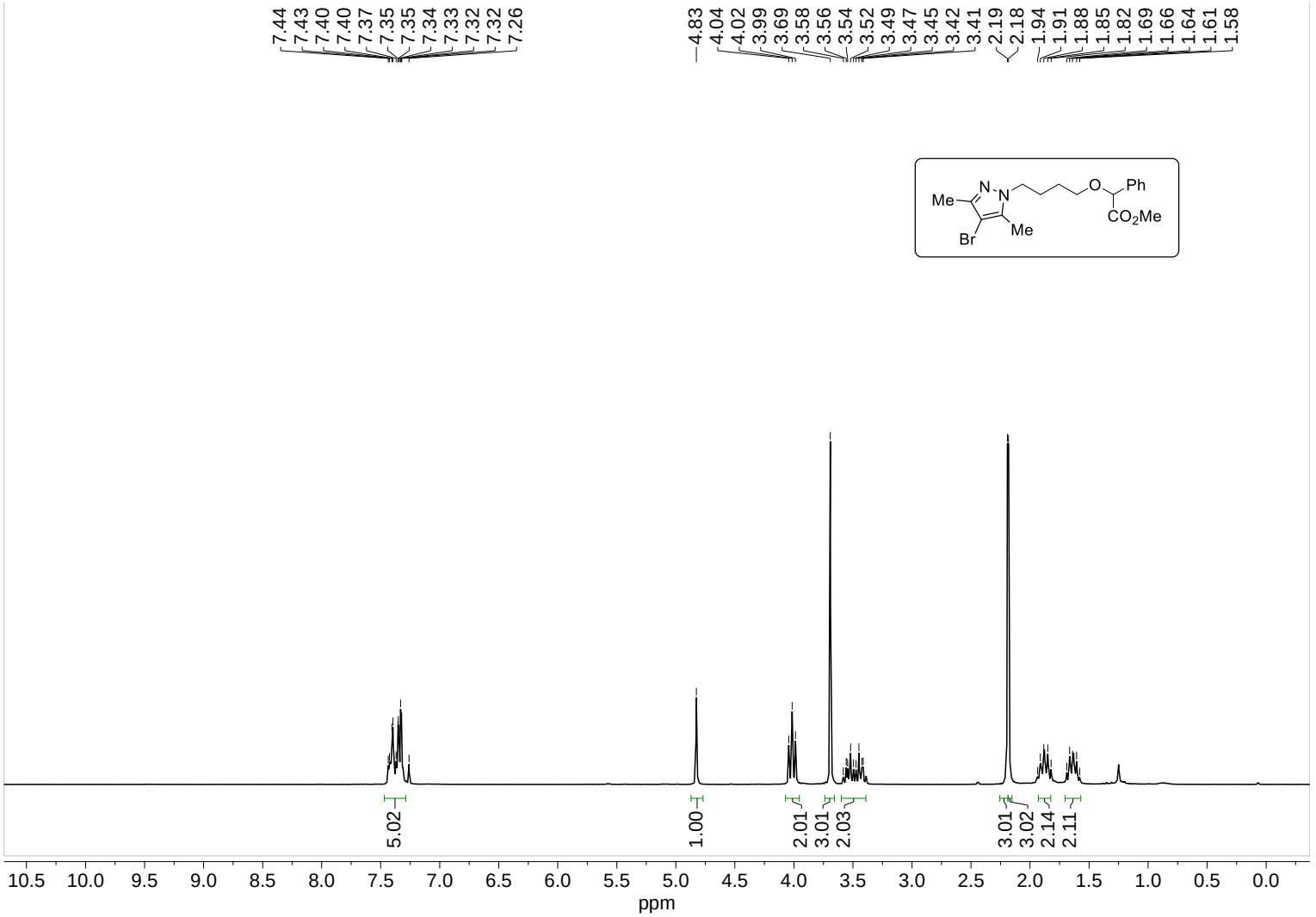
Molecule 4d - ^{1}H NMR (250 MHz, $CDCl_3$)



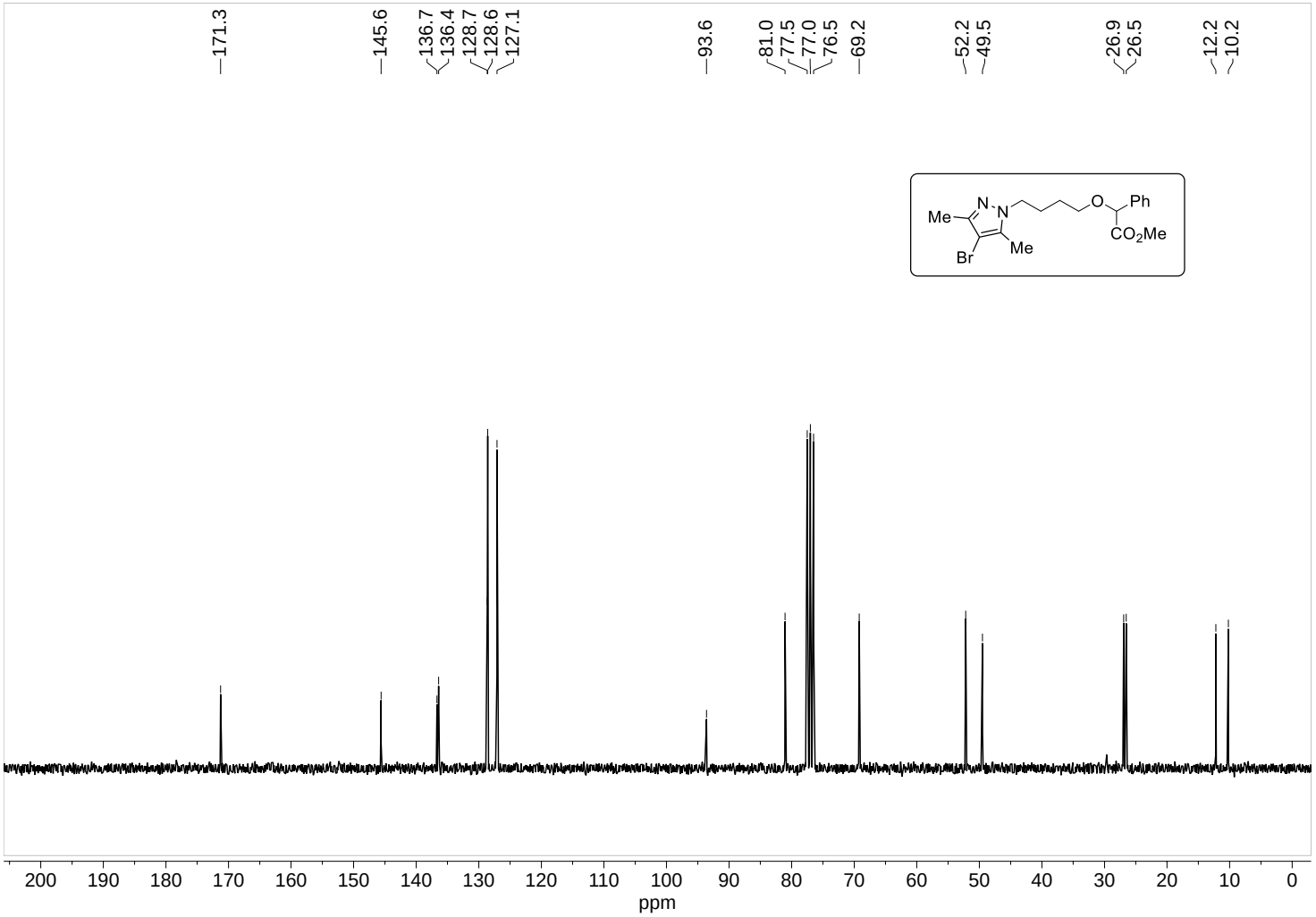
Molecule 4d - ^{13}C NMR (62.5 MHz, $CDCl_3$)



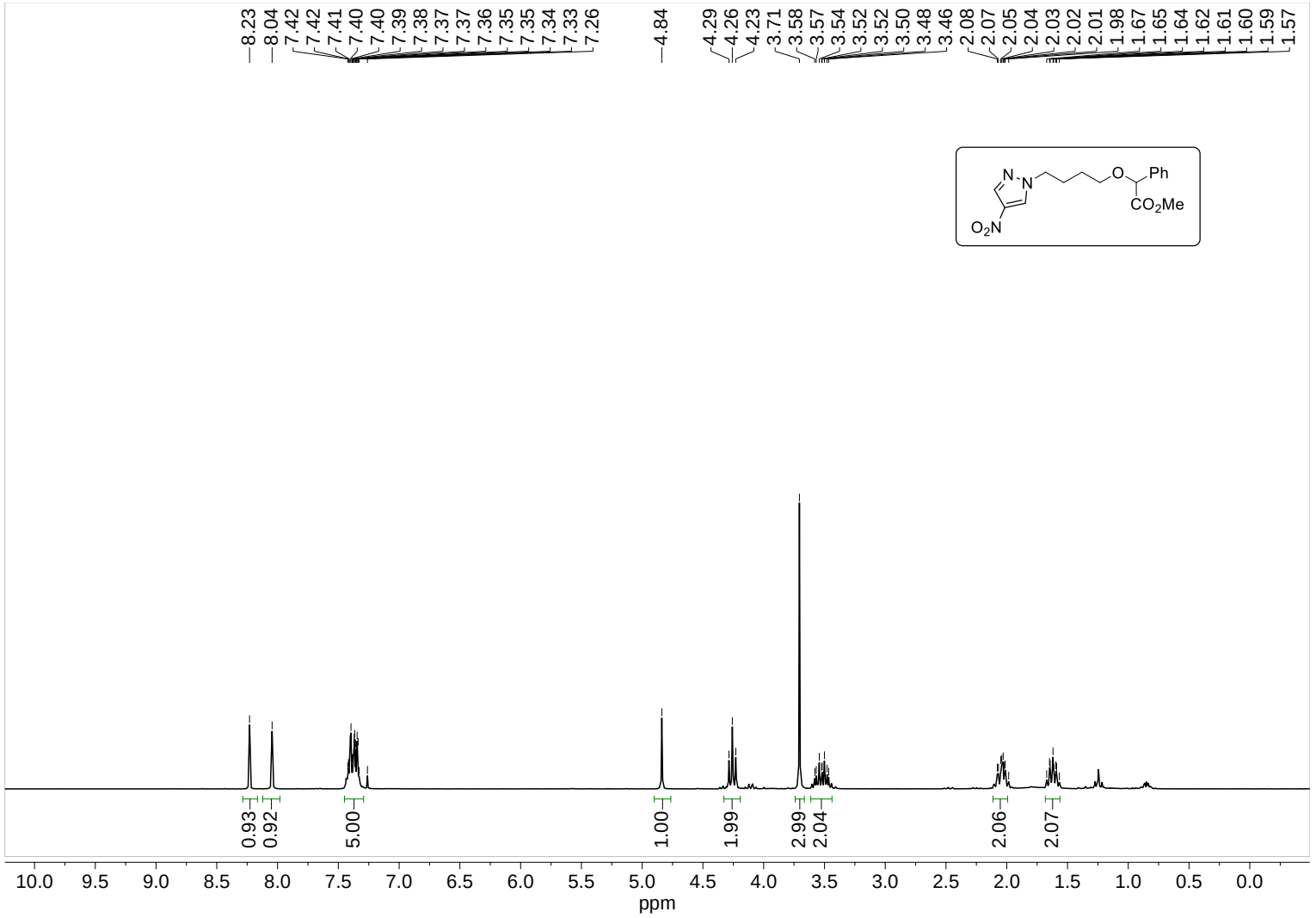
Molecule 4f - ^{1}H NMR (250 MHz, $CDCl_3$)



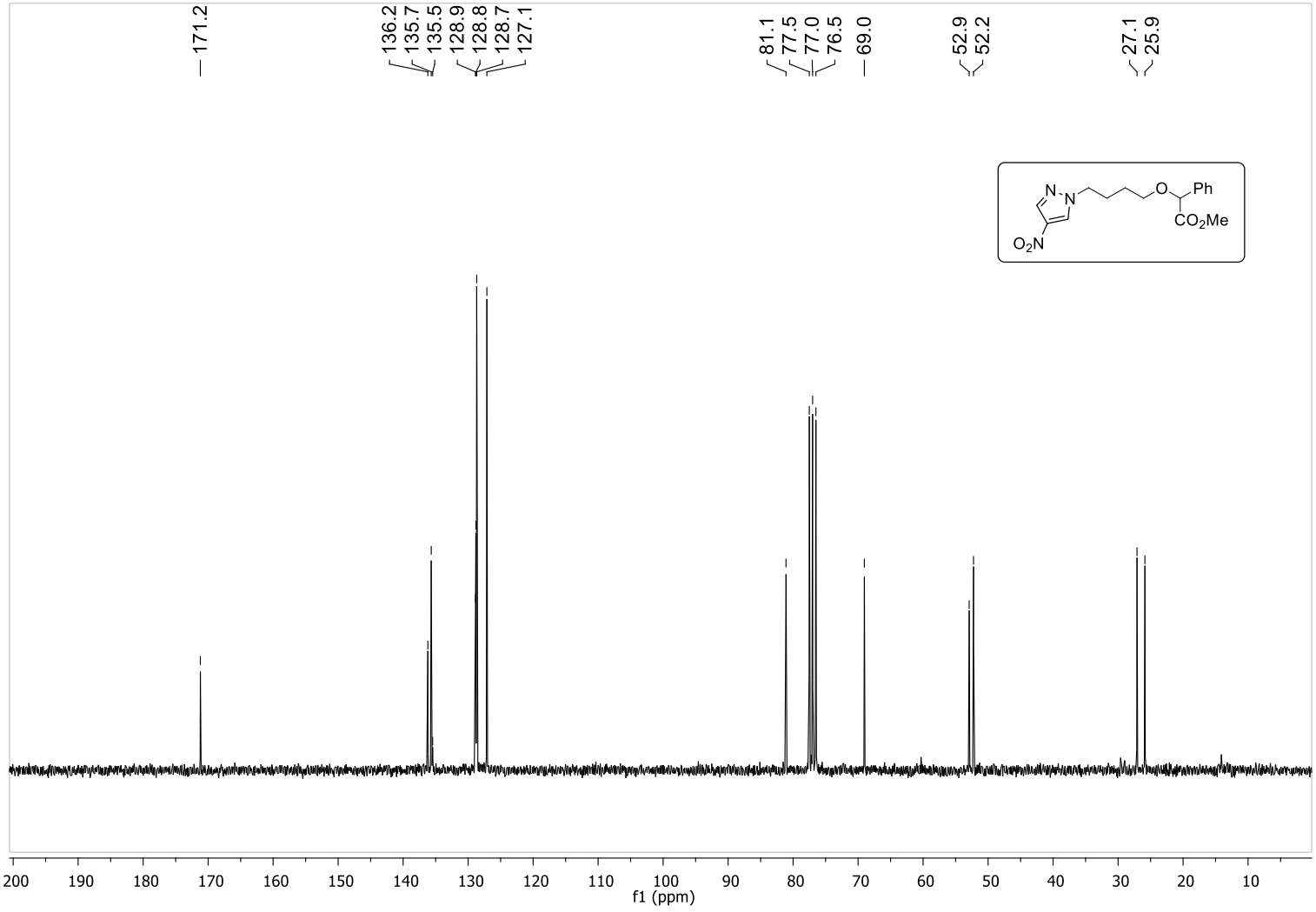
Molecule 4f - ^{13}C NMR (62.5 MHz, $CDCl_3$)



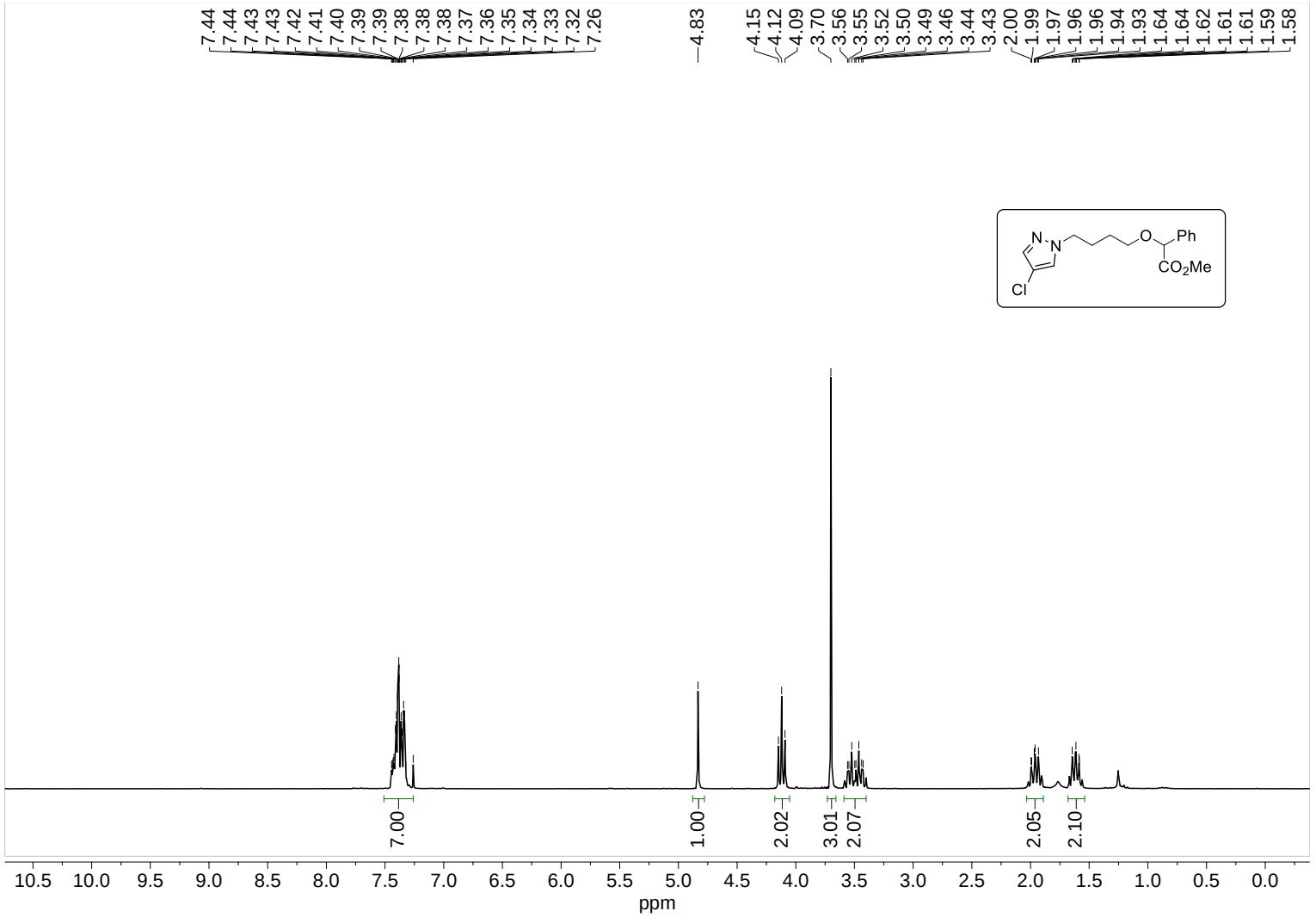
Molecule 4g - ^{1}H NMR (250 MHz, $CDCl_3$)



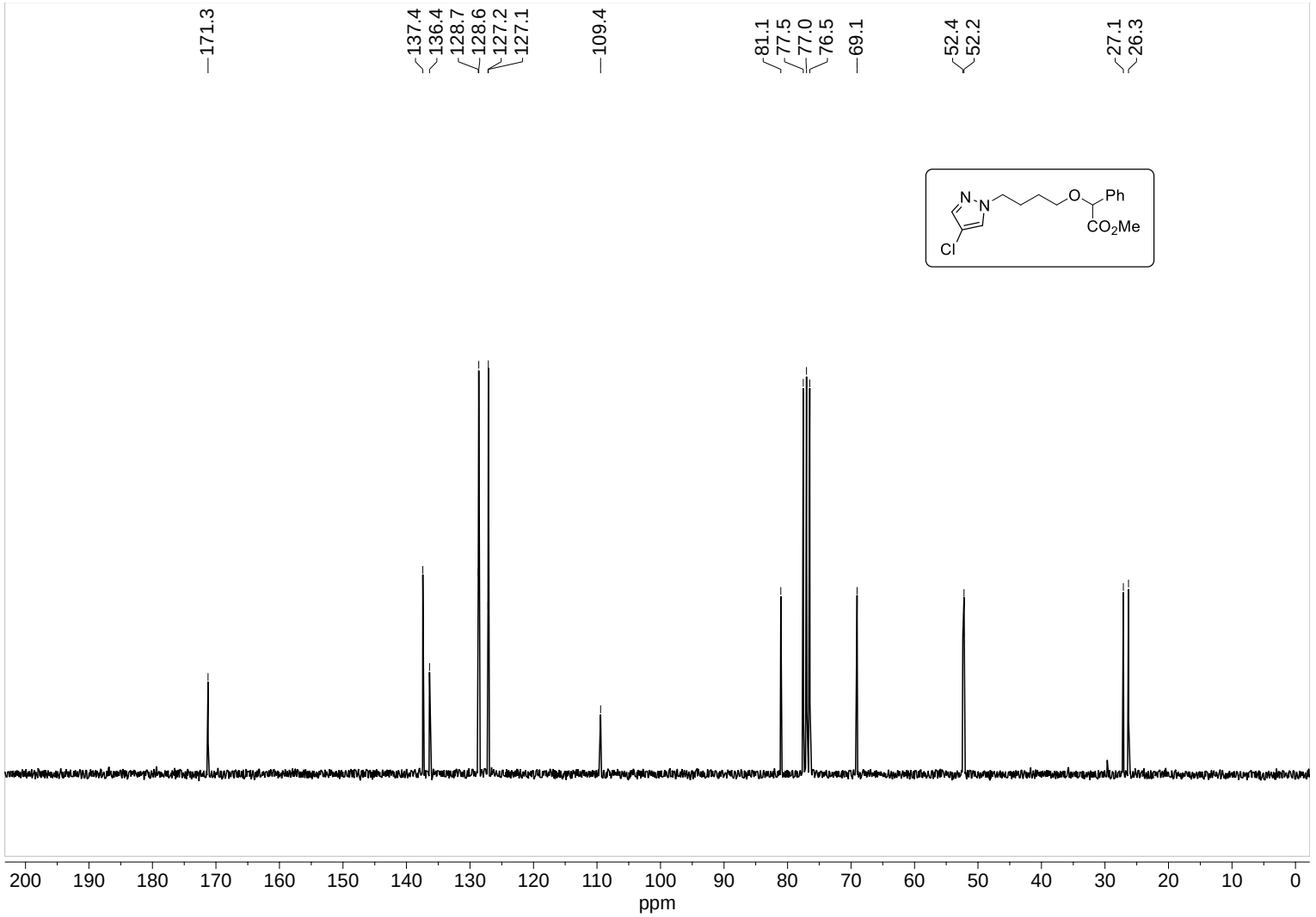
Molecule 4g - ^{13}C NMR (62.5 MHz, $CDCl_3$)



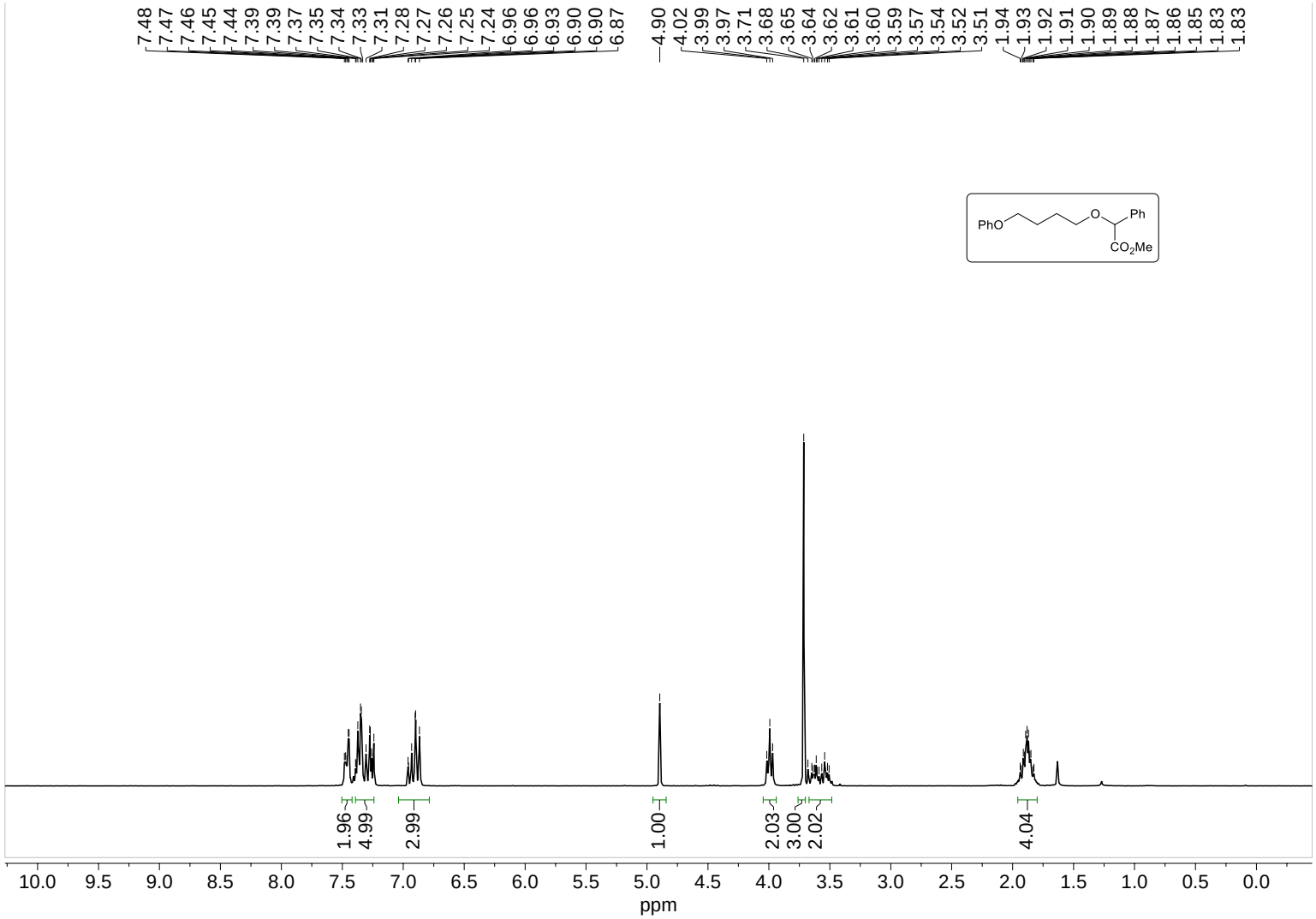
Molecule 4h - ^{1}H NMR (250 MHz, $CDCl_3$)



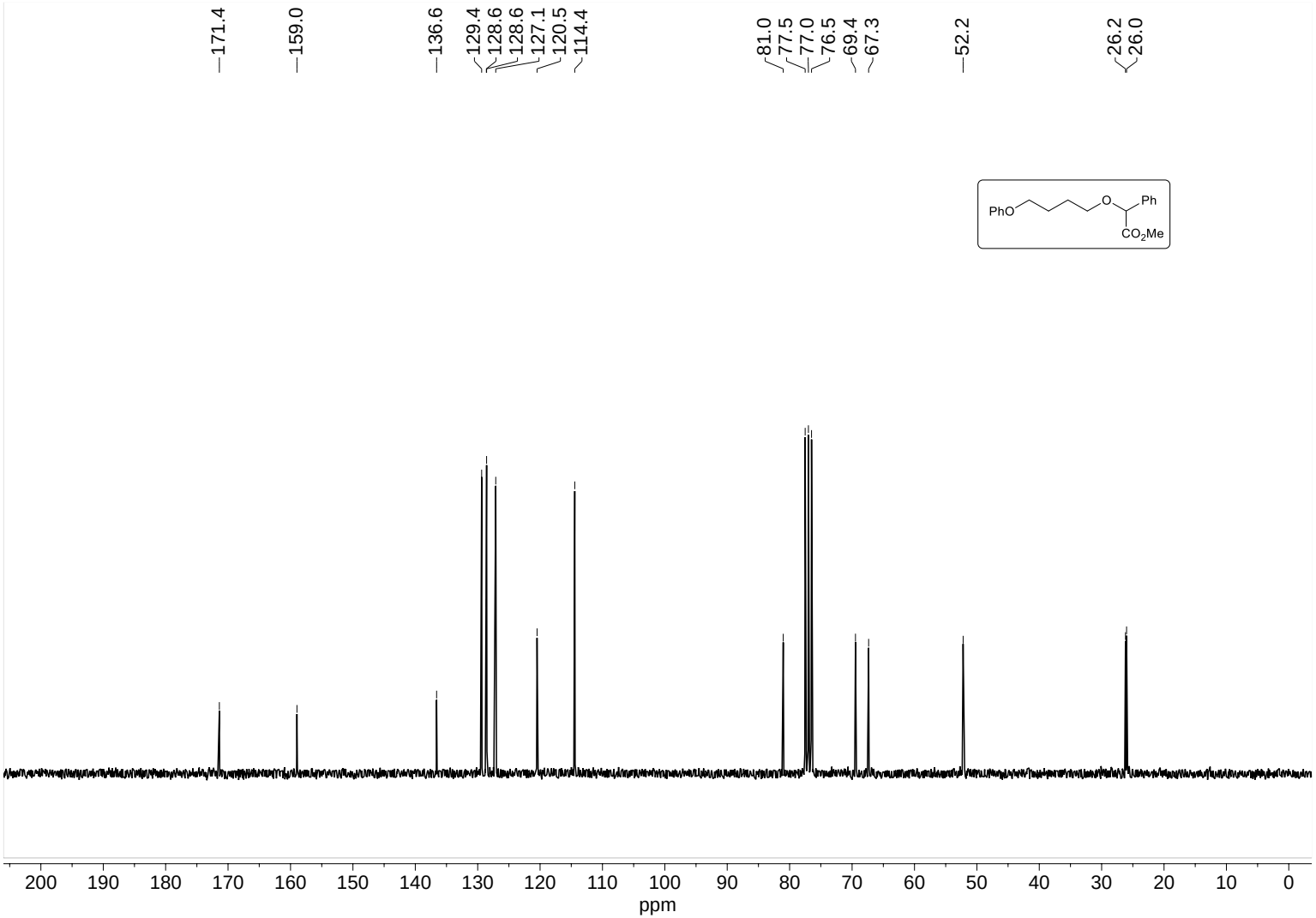
Molecule 4h - ^{13}C NMR (62.5 MHz, $CDCl_3$)



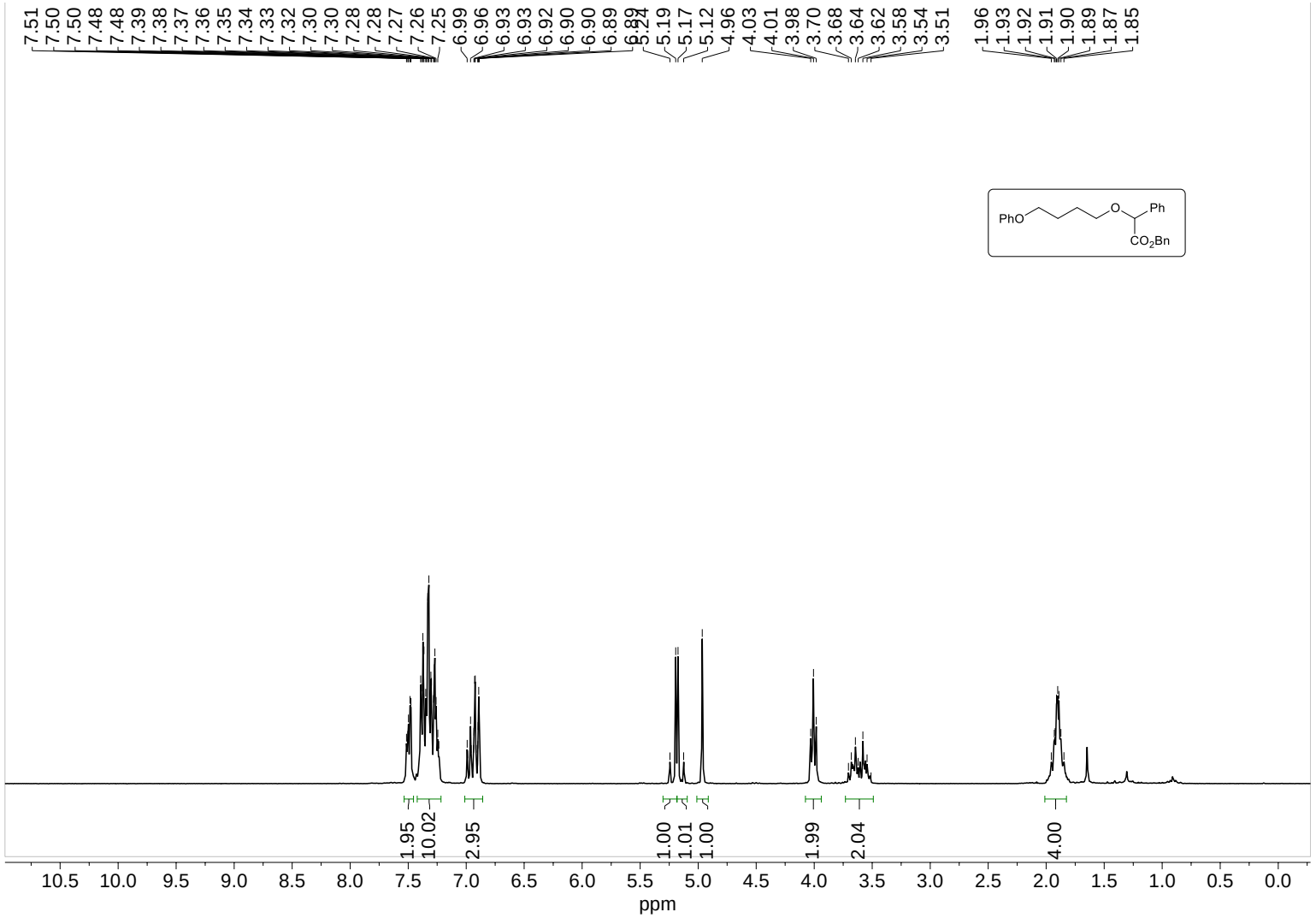
Molecule 6a - ^{1}H NMR (250 MHz, $CDCl_3$)



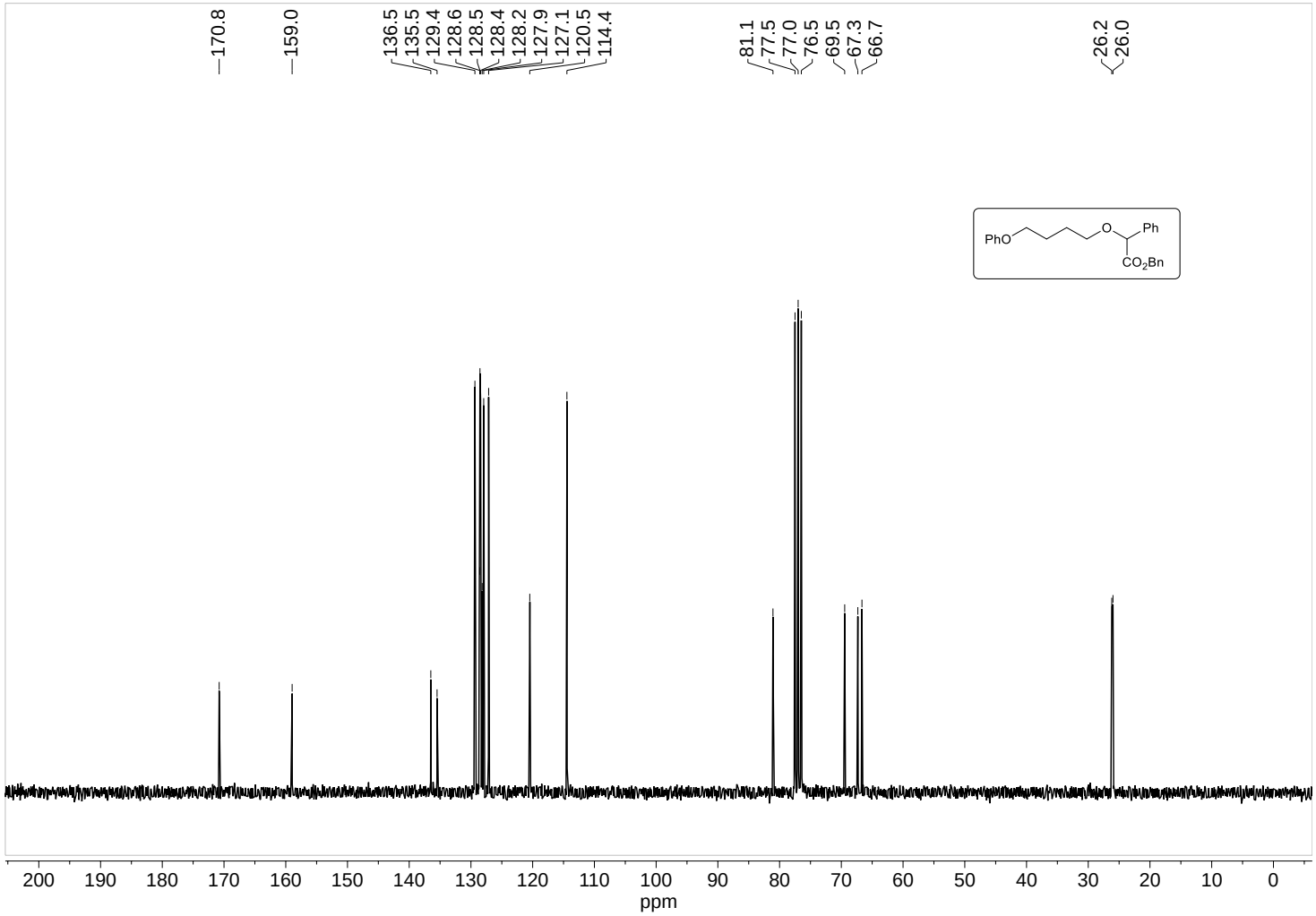
Molecule 6a - ^{13}C NMR (62.5 MHz, $CDCl_3$)



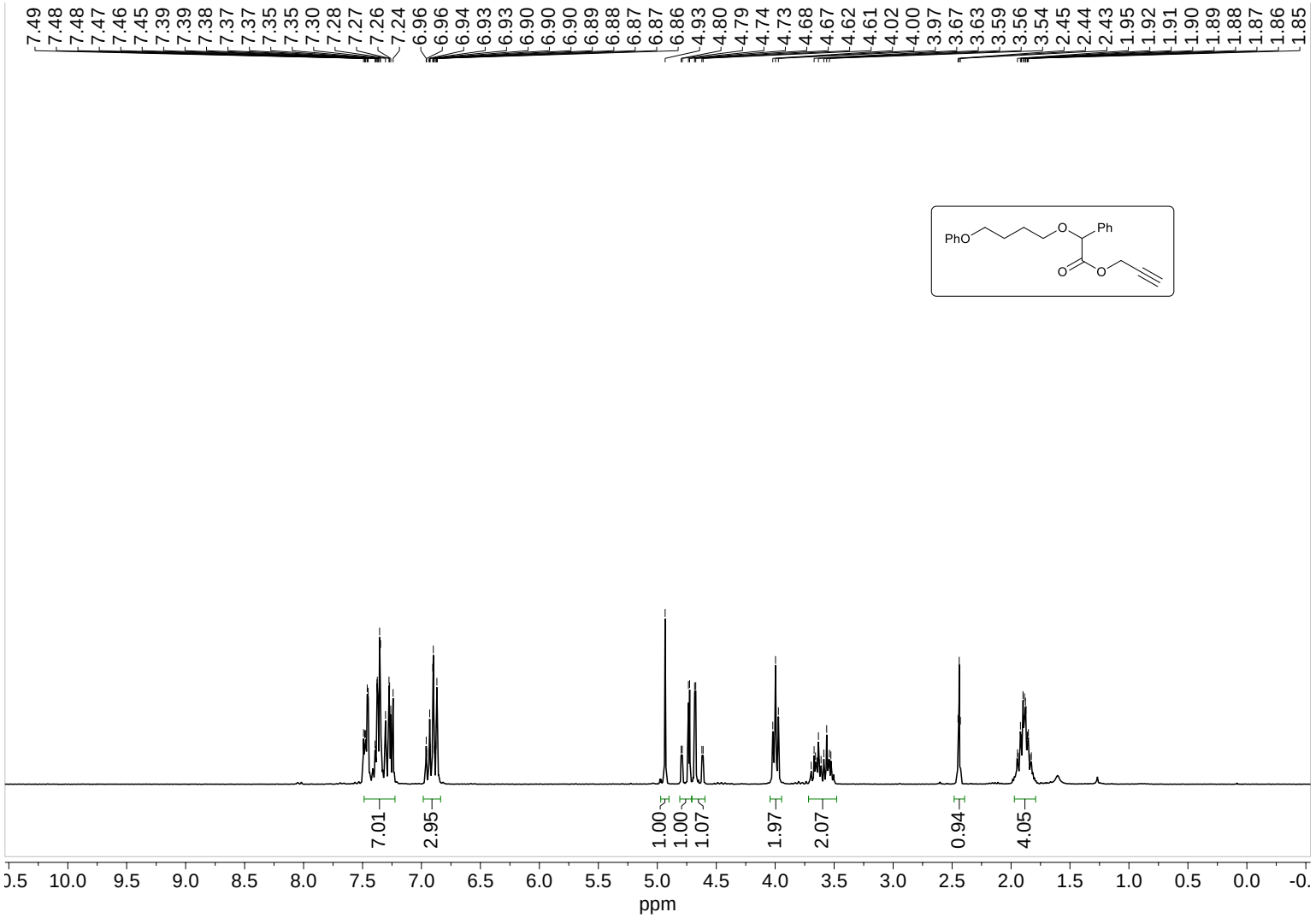
Molecule 6b - ^{1}H NMR (250 MHz, $CDCl_3$)



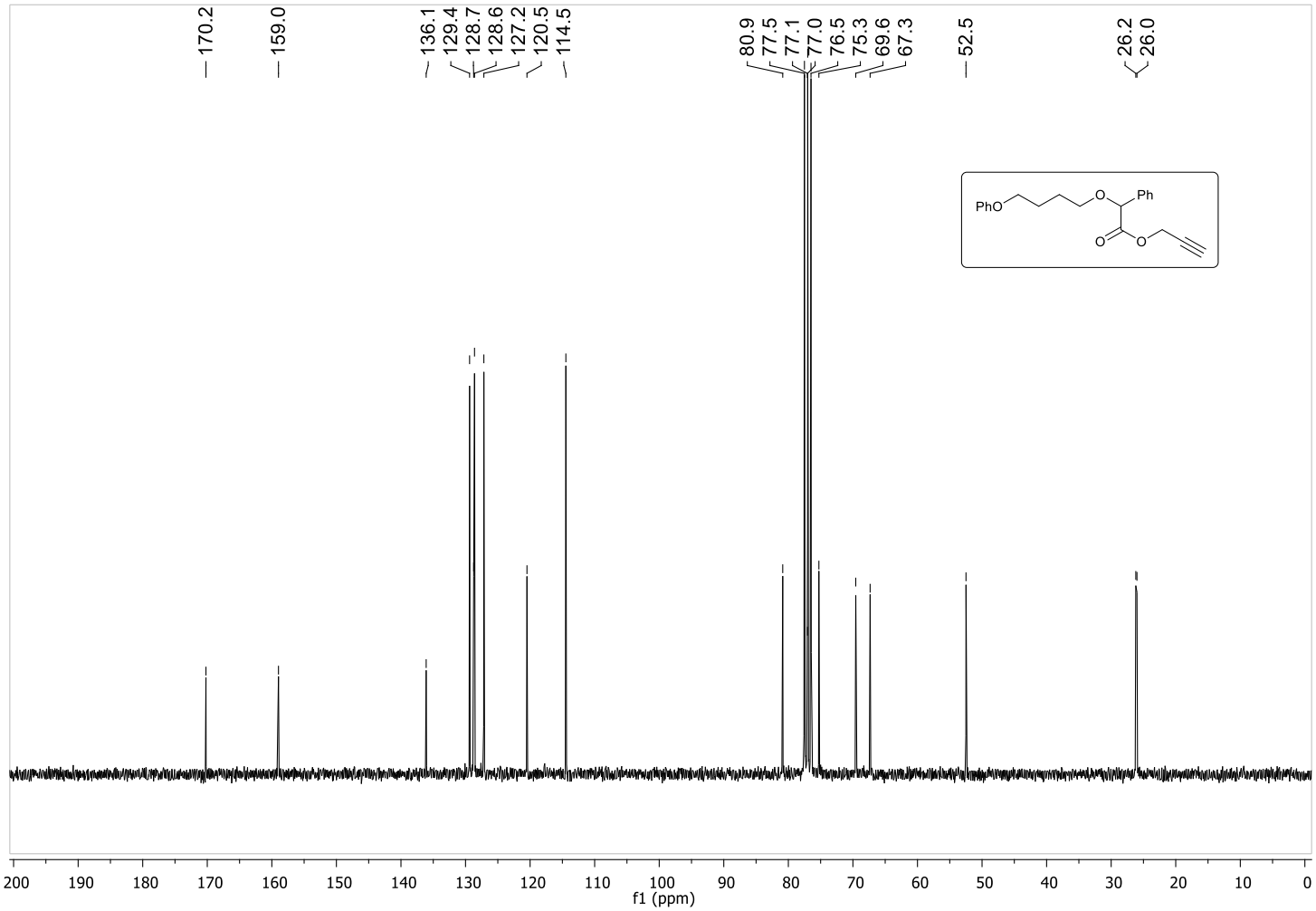
Molecule 6b - ^{13}C NMR (62.5 MHz, $CDCl_3$)



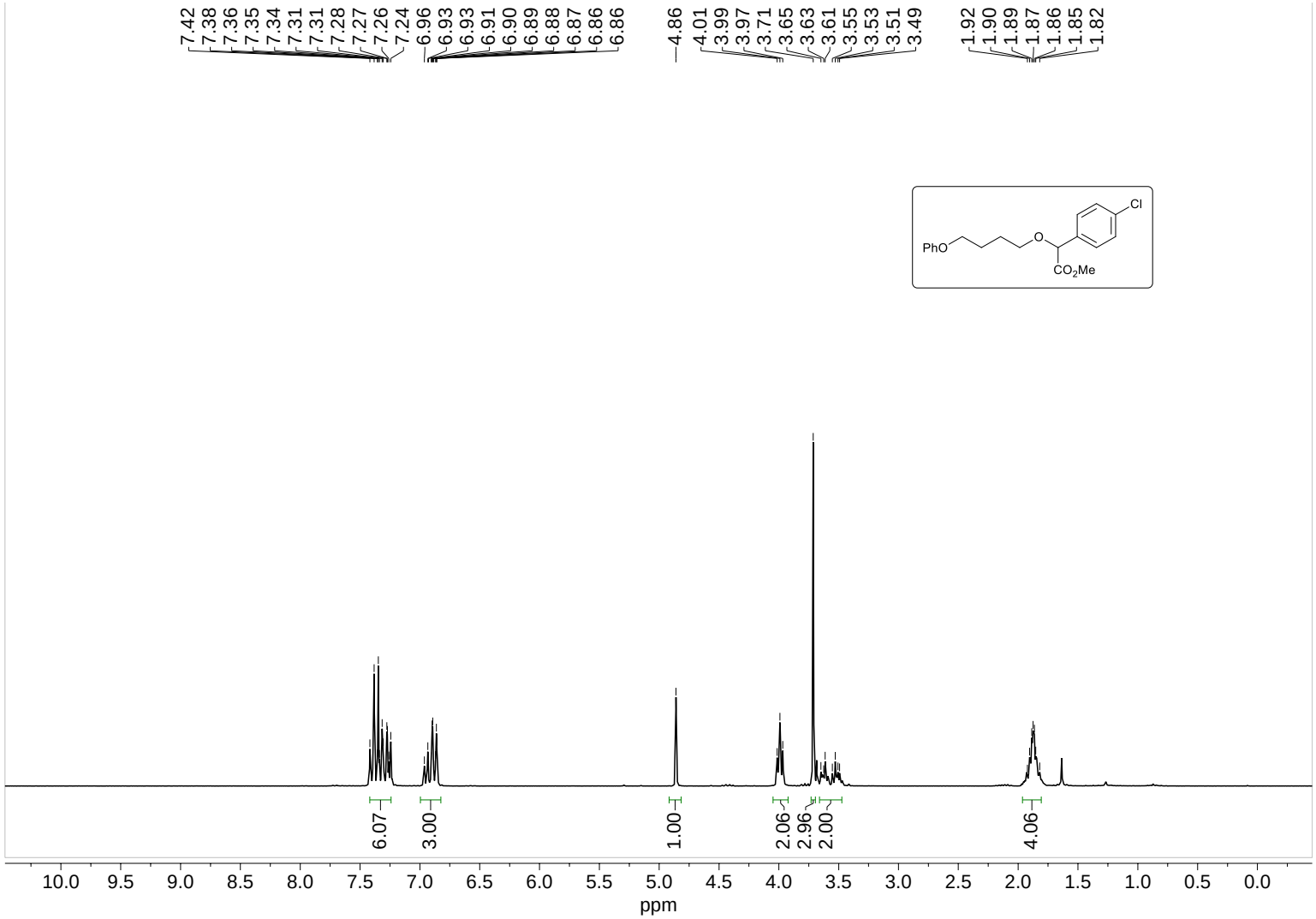
Molecule 6c - ^{1}H NMR (250 MHz, $CDCl_3$)



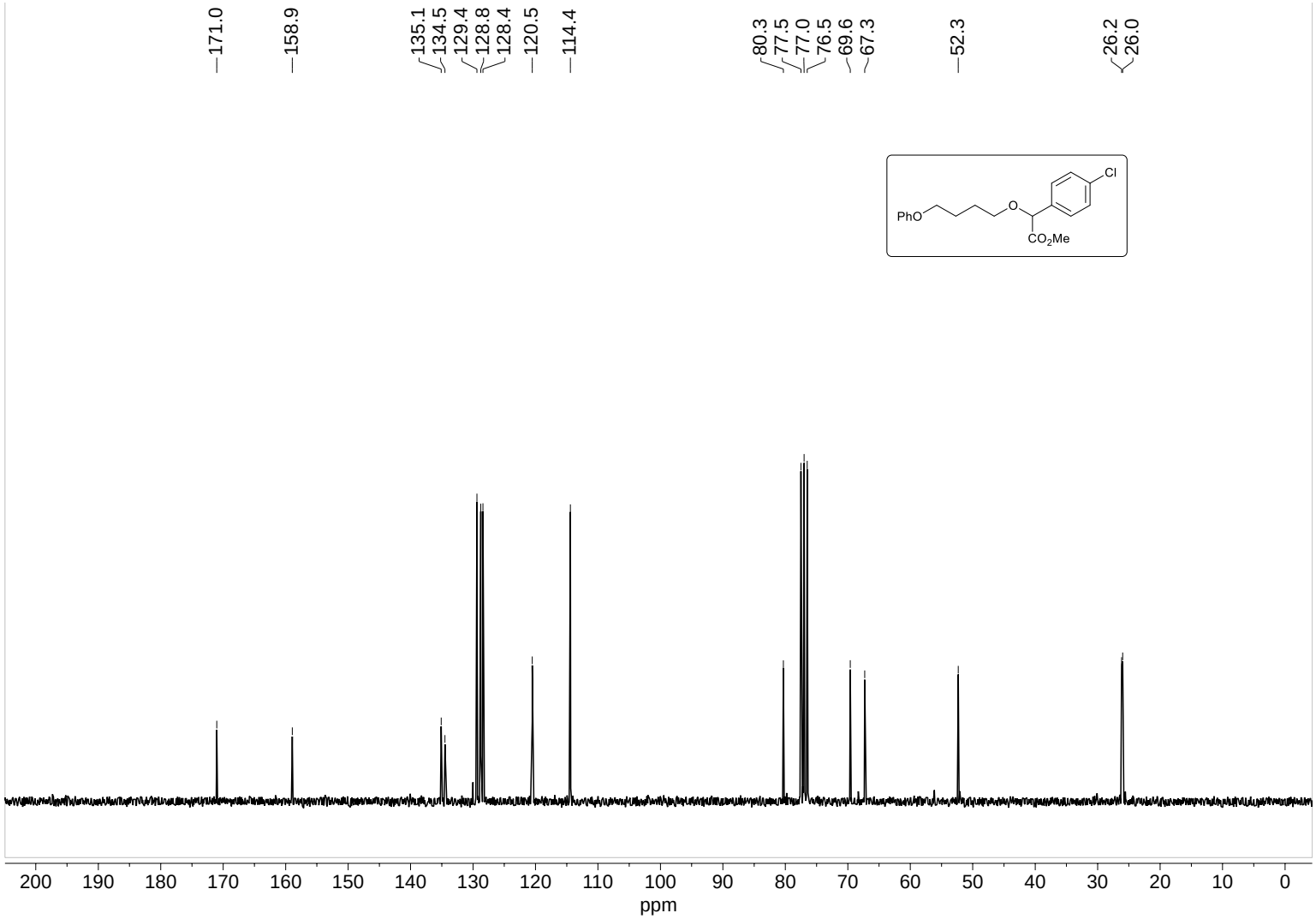
Molecule 6c - ^{13}C NMR (62.5 MHz, $CDCl_3$)



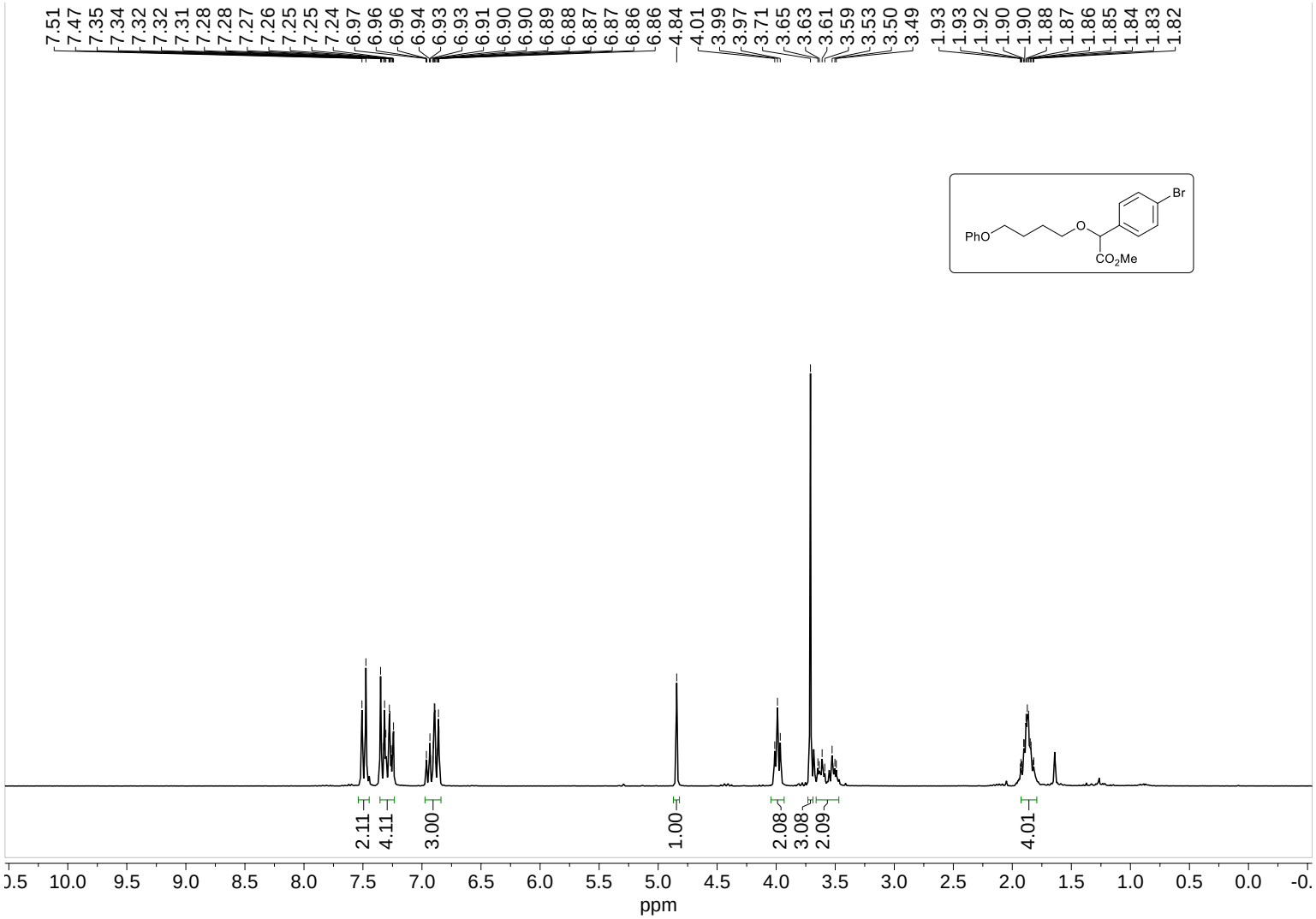
Molecule 6d - ^{1}H NMR (250 MHz, $CDCl_3$)



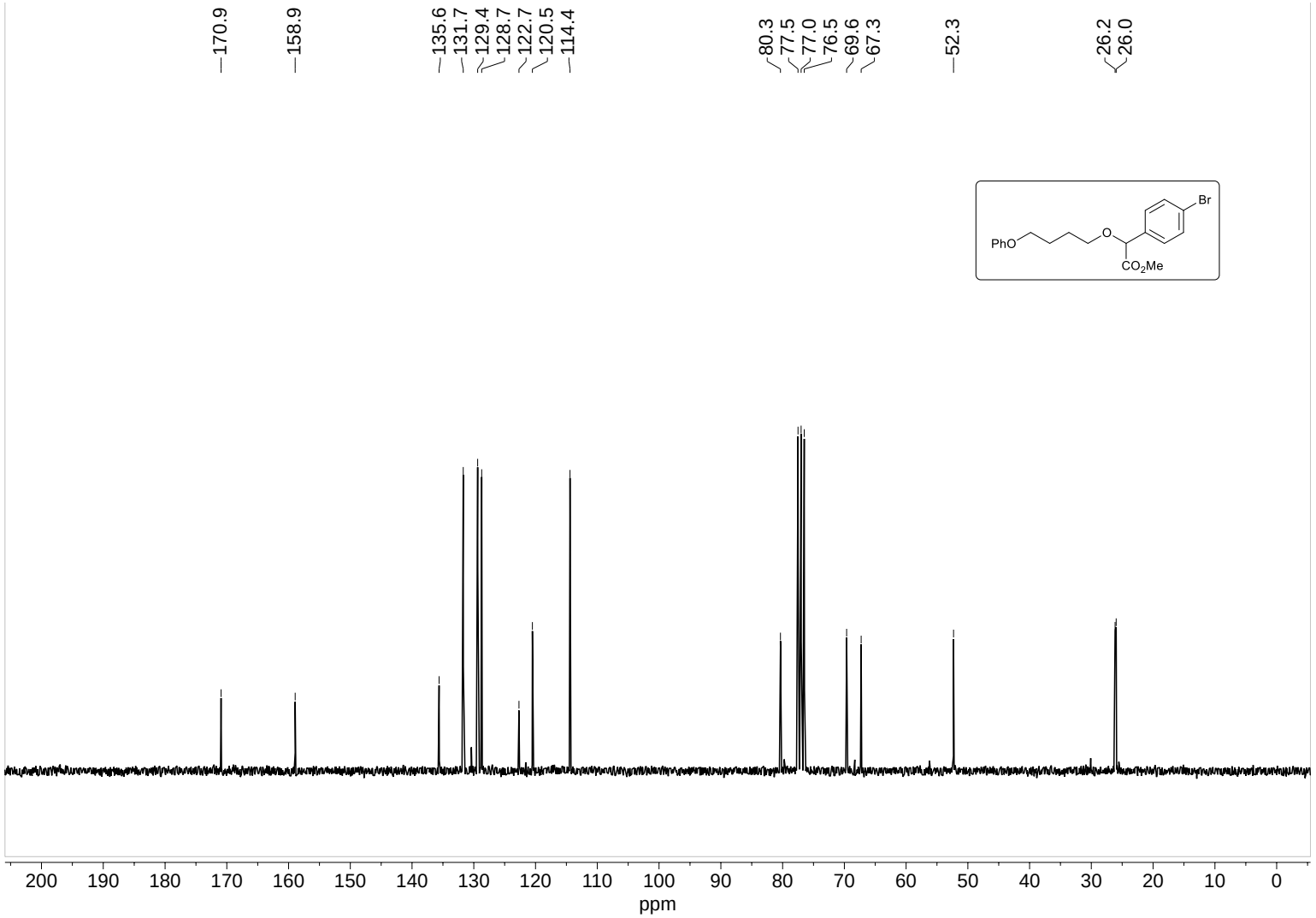
Molecule 6d - ^{13}C NMR (62.5 MHz, $CDCl_3$)



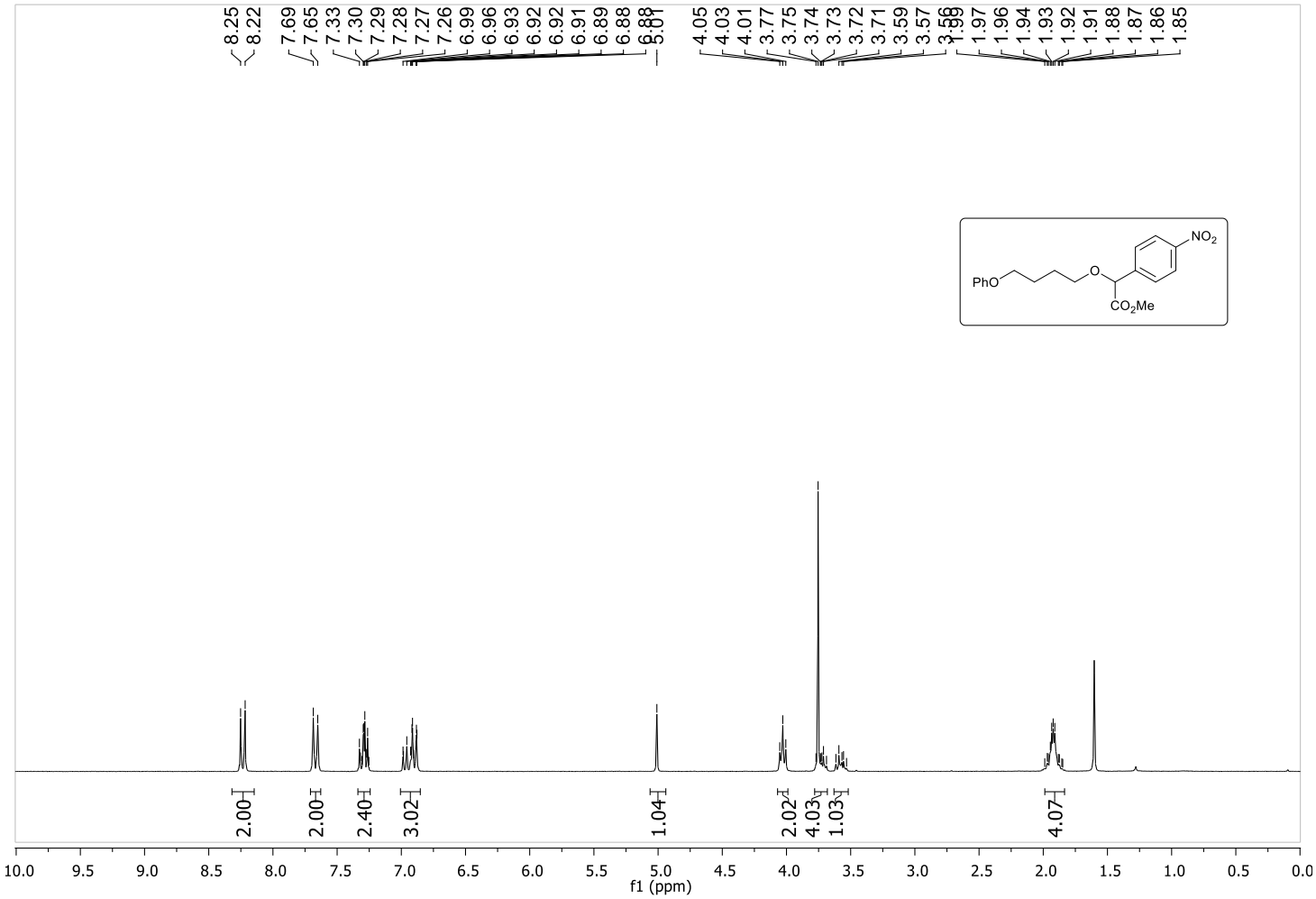
Molecule 6e - ^{1}H NMR (250 MHz, $CDCl_3$)



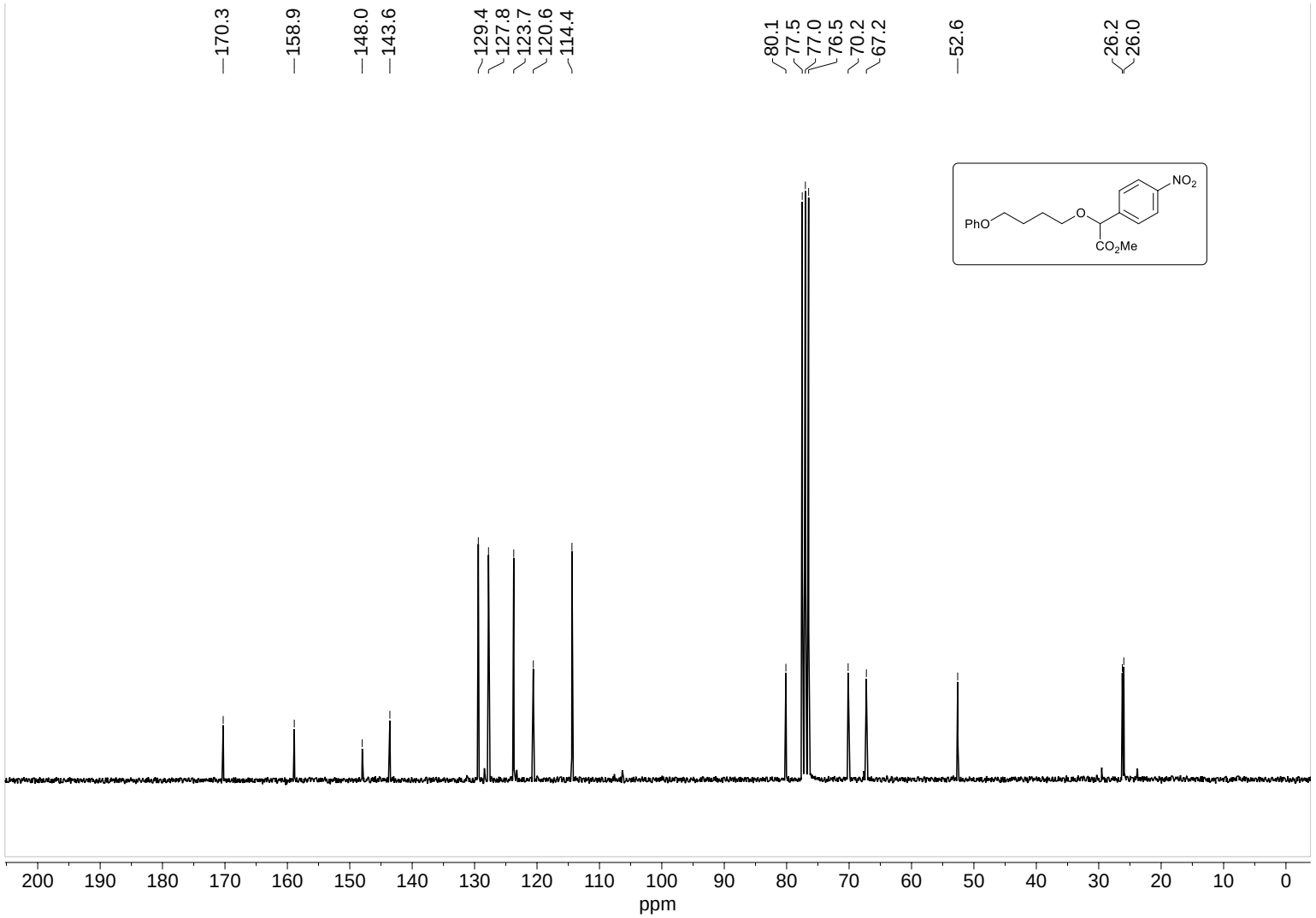
Molecule 6e - ^{13}C NMR (62.5 MHz, $CDCl_3$)



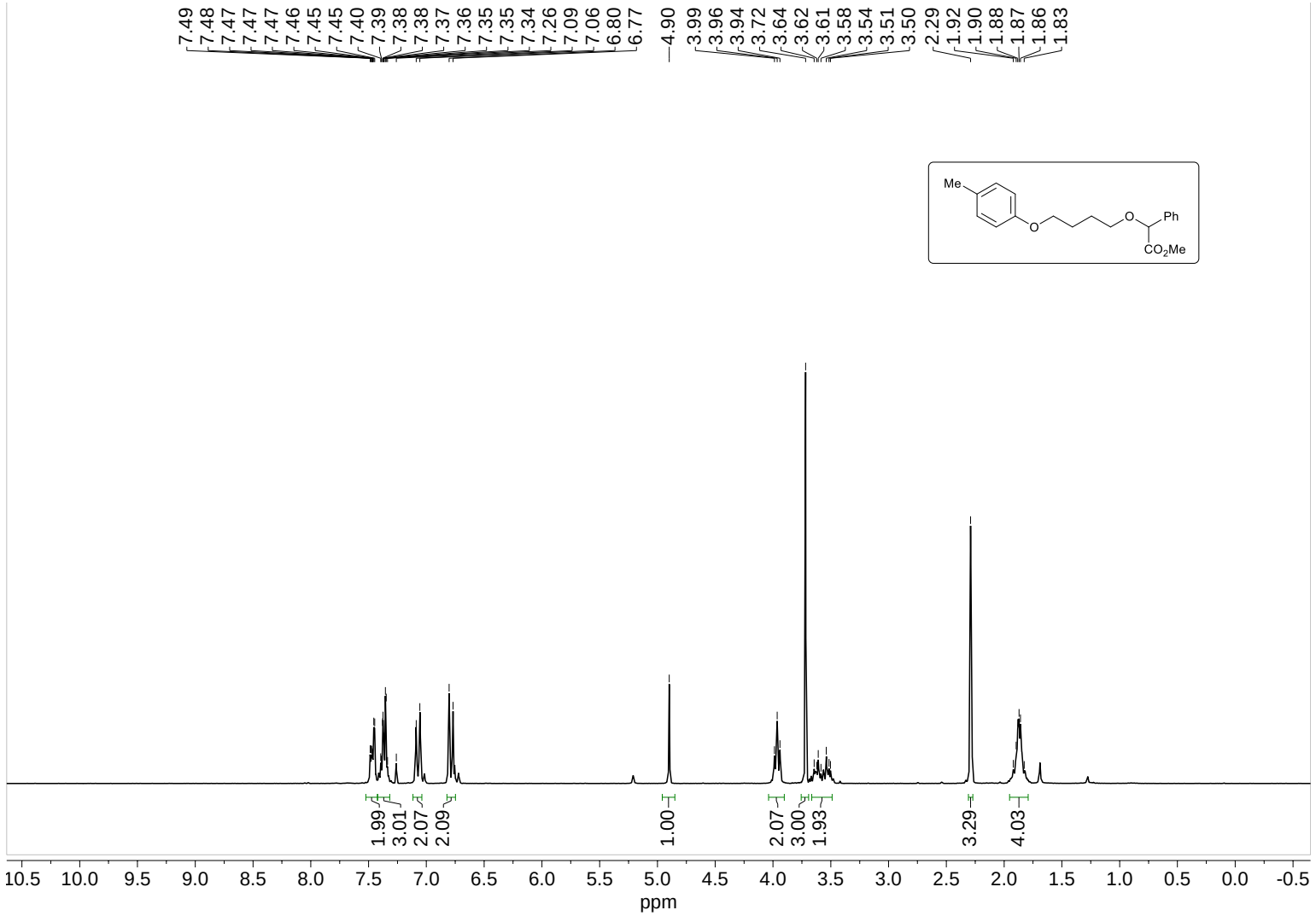
Molecule 6f - ^{1}H NMR (250 MHz, $CDCl_3$)



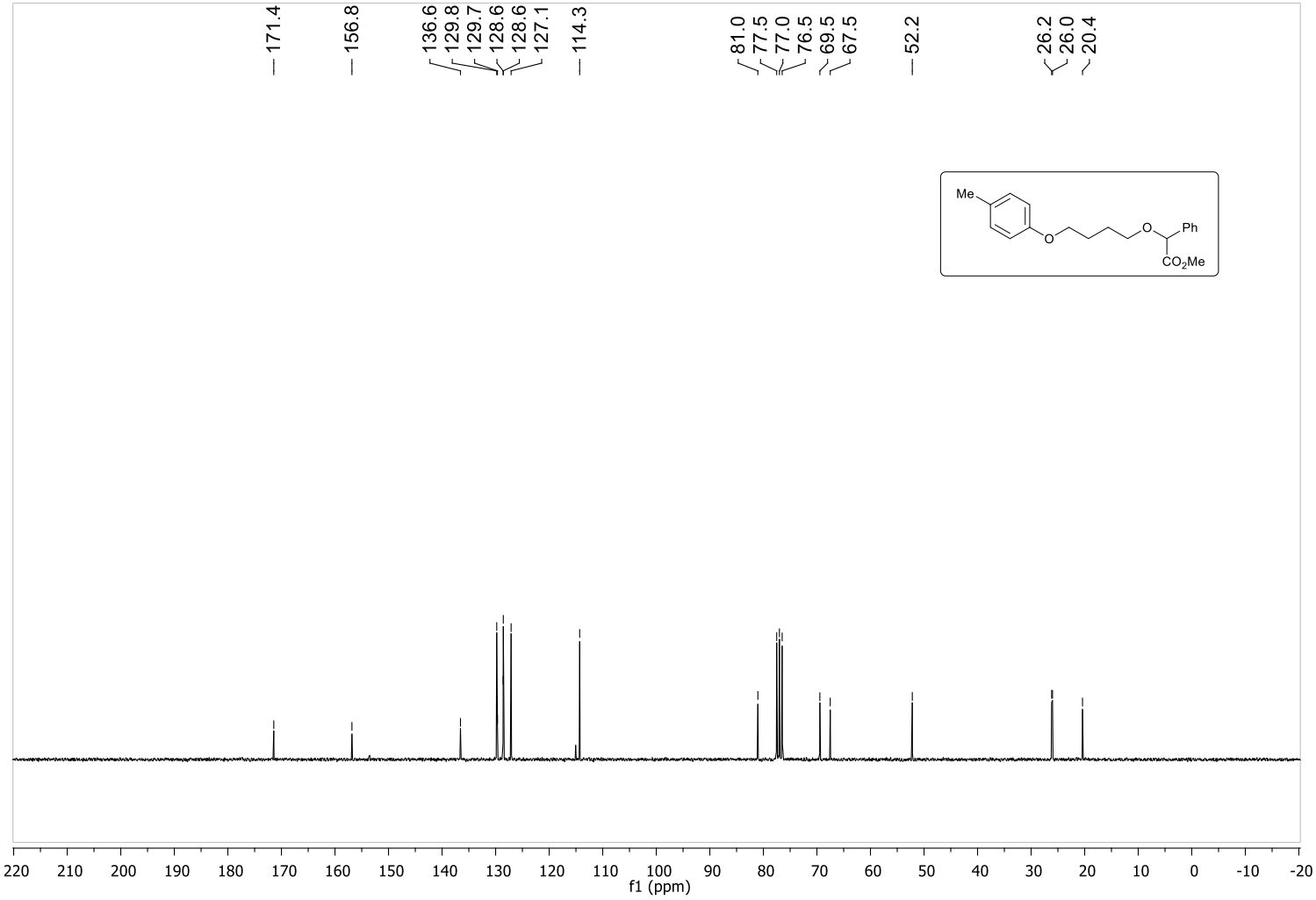
Molecule 6f ^{13}C NMR (62.5 MHz, $CDCl_3$)



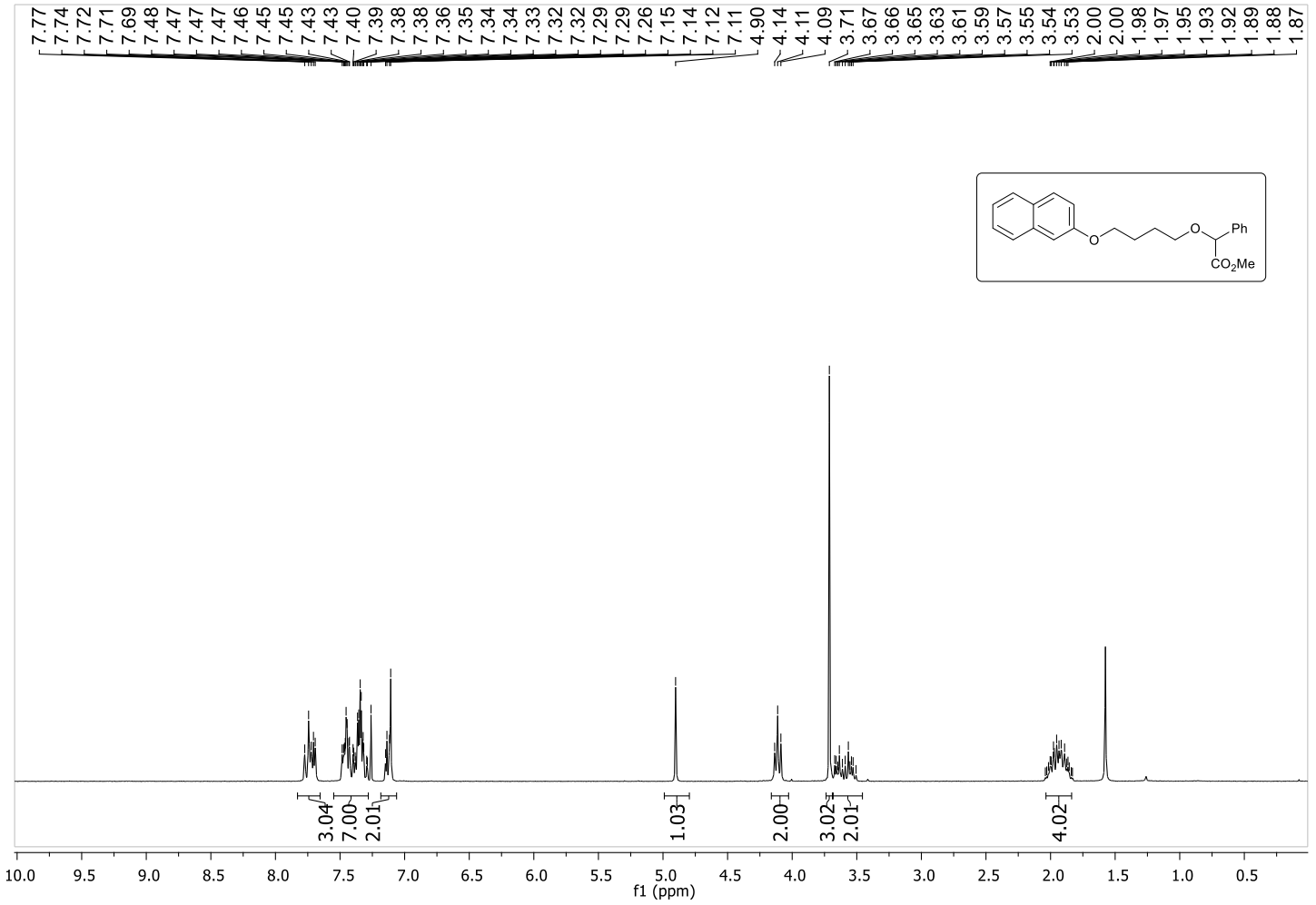
Molecule 6g - ^{1}H NMR (250 MHz, $CDCl_3$)



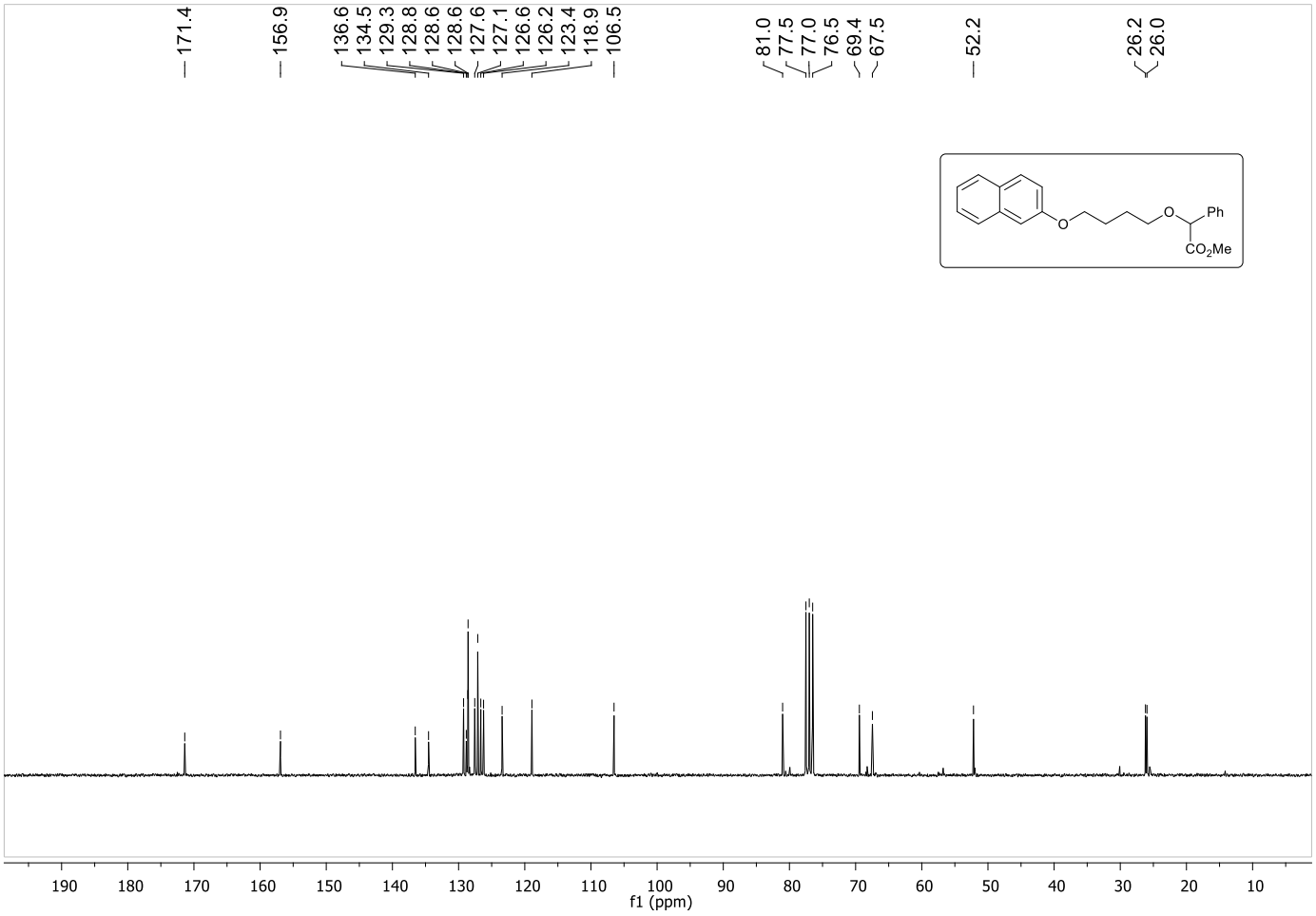
Molecule 6g - ^{13}C NMR (62.5 MHz, $CDCl_3$)



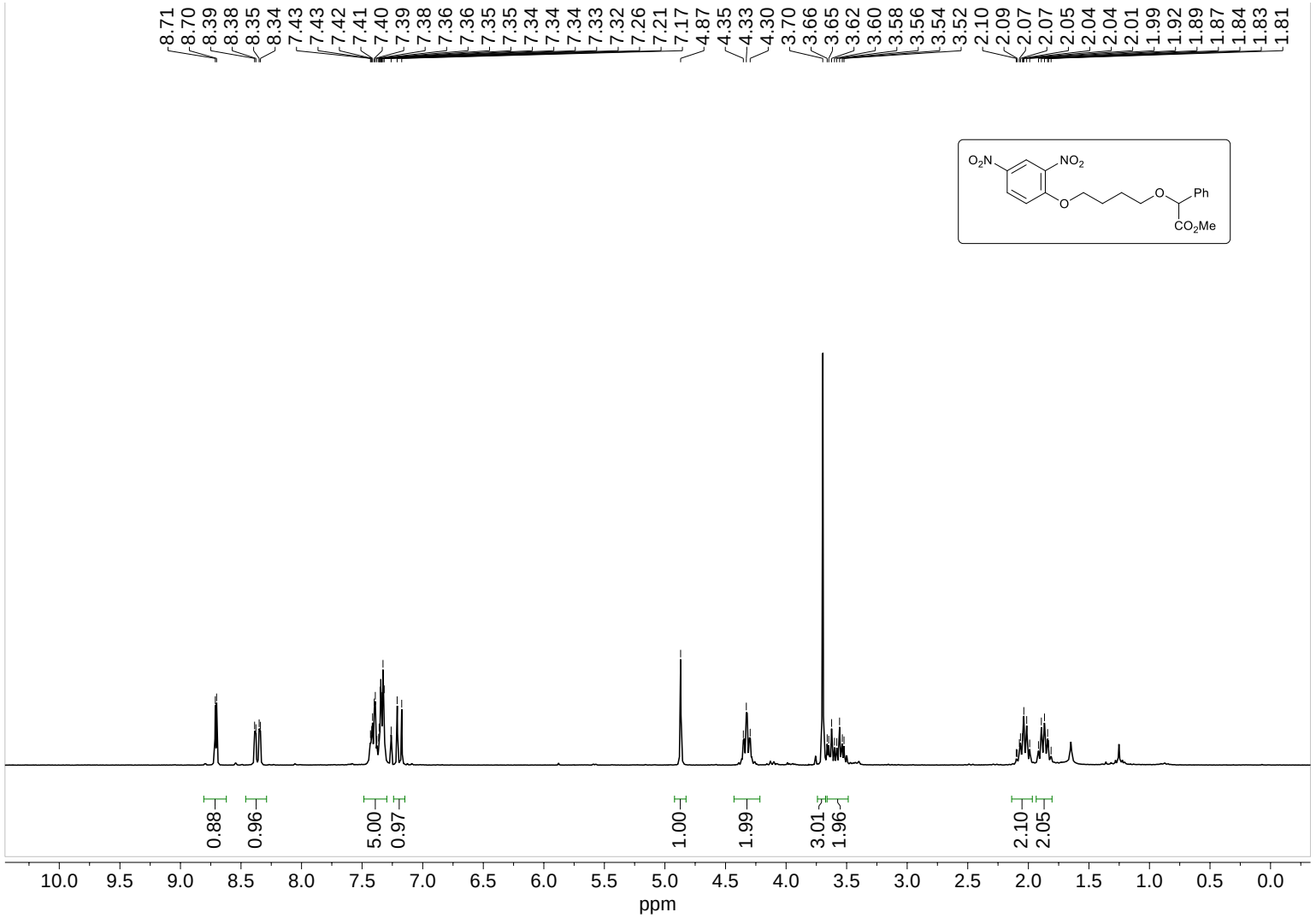
Molecule 6h - ^{1}H NMR (250 MHz, $CDCl_3$)



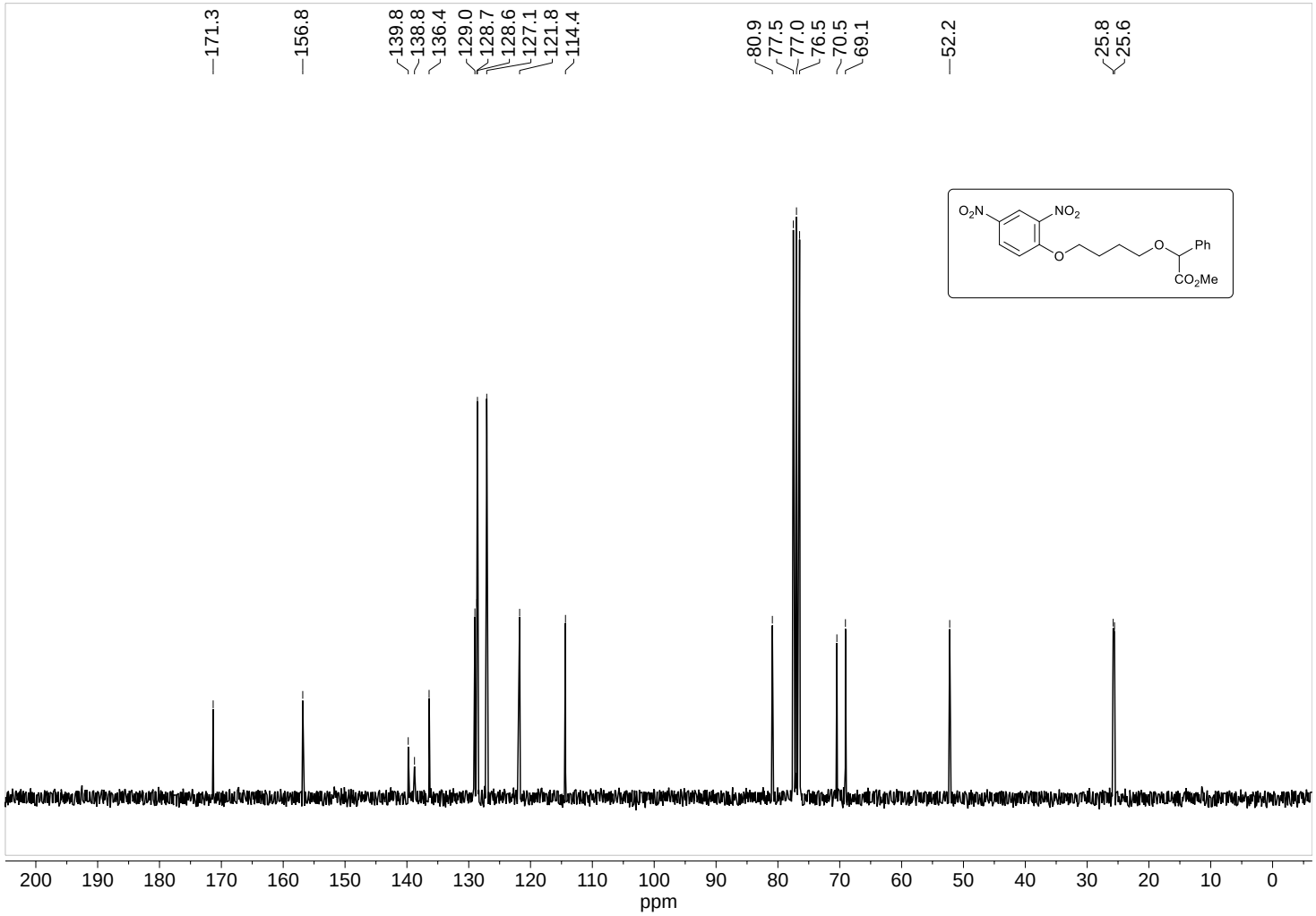
Molecule 6h - ^{13}C NMR (62.5 MHz, $CDCl_3$)



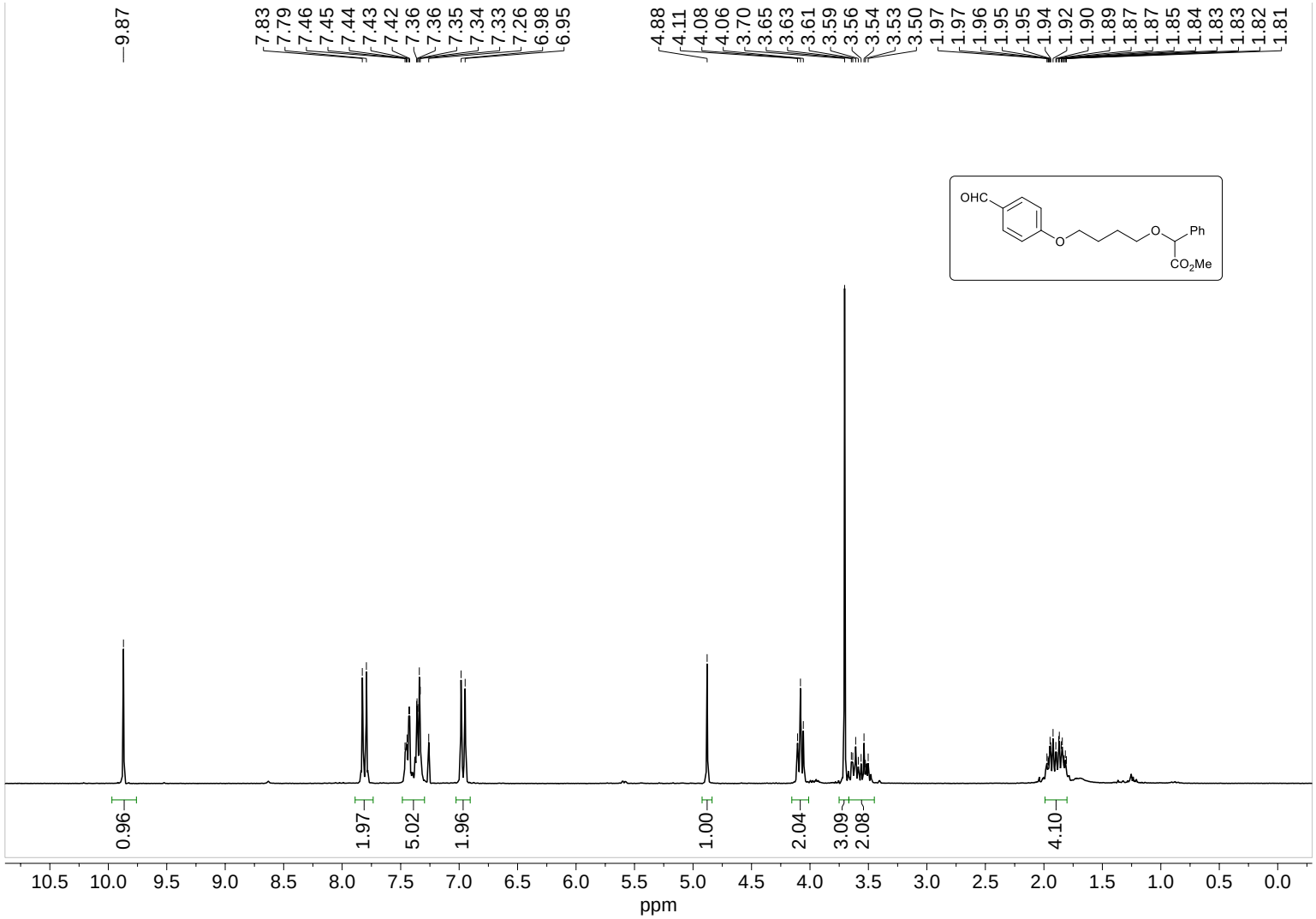
Molecule 6i - ^{1}H NMR (250 MHz, $CDCl_3$)



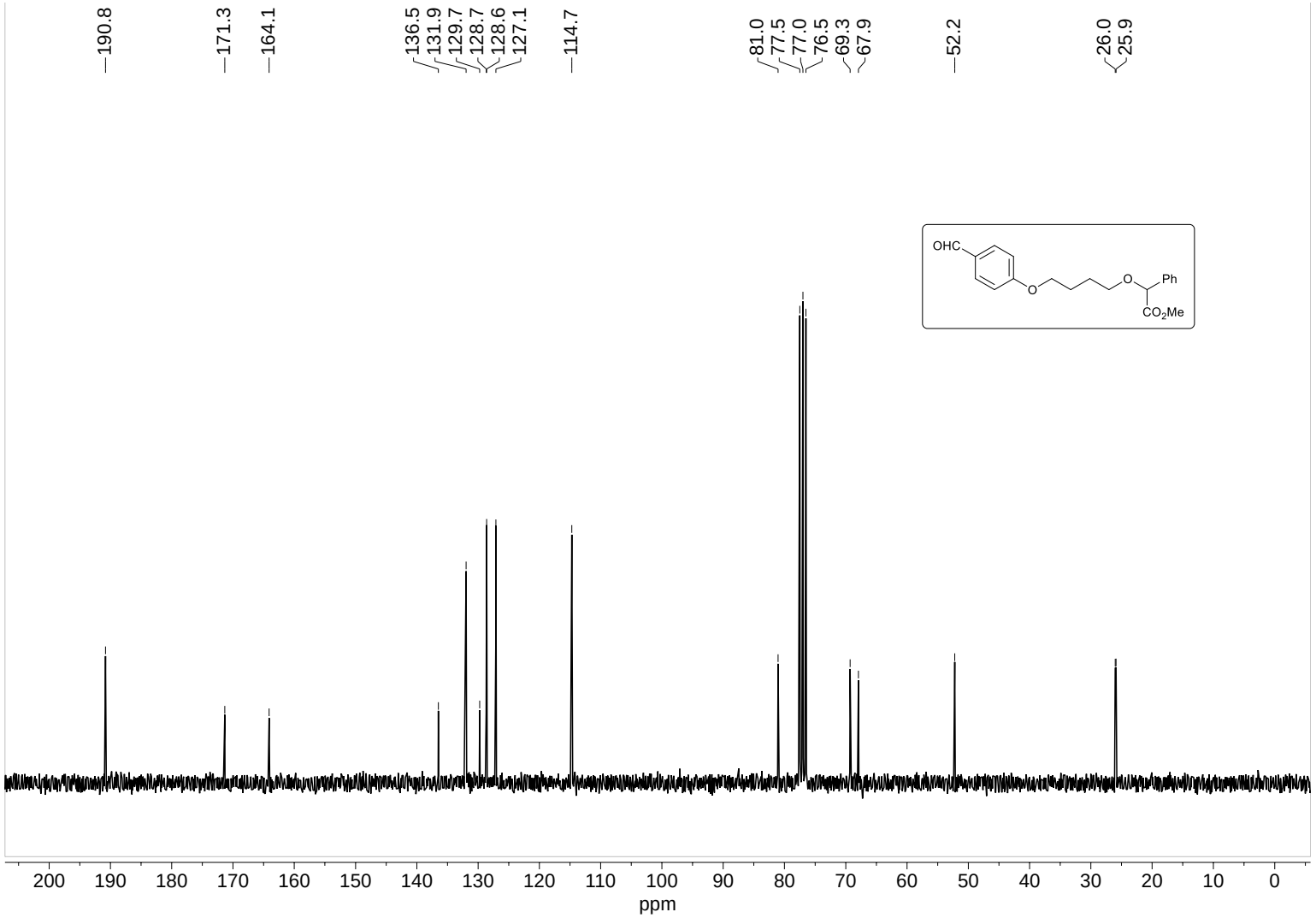
Molecule 6i - ^{13}C NMR (62.5 MHz, $CDCl_3$)



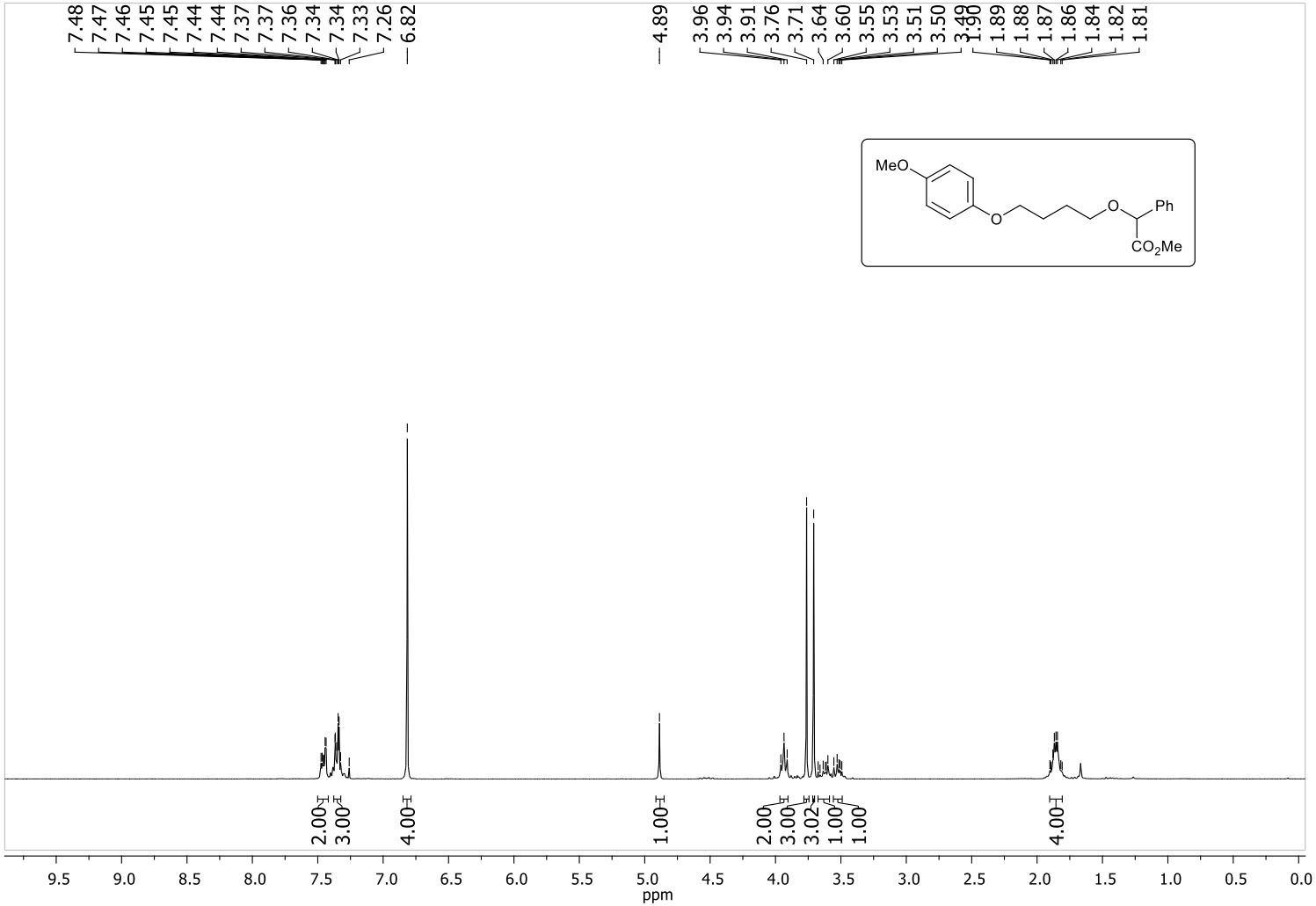
Molecule 6j - ^{1}H NMR (250 MHz, $CDCl_3$)



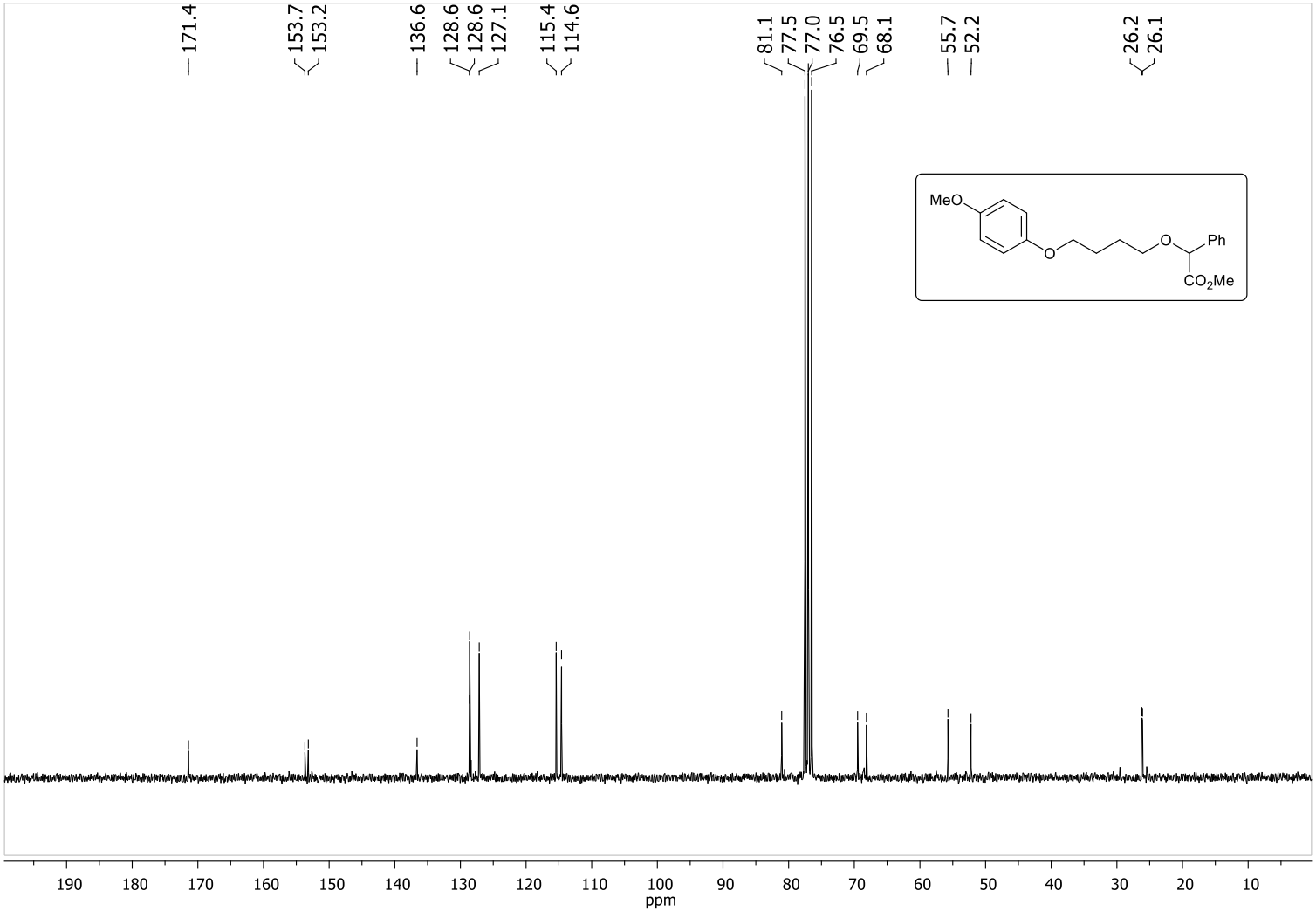
Molecule 6j - ^{13}C NMR (62.5 MHz, $CDCl_3$)



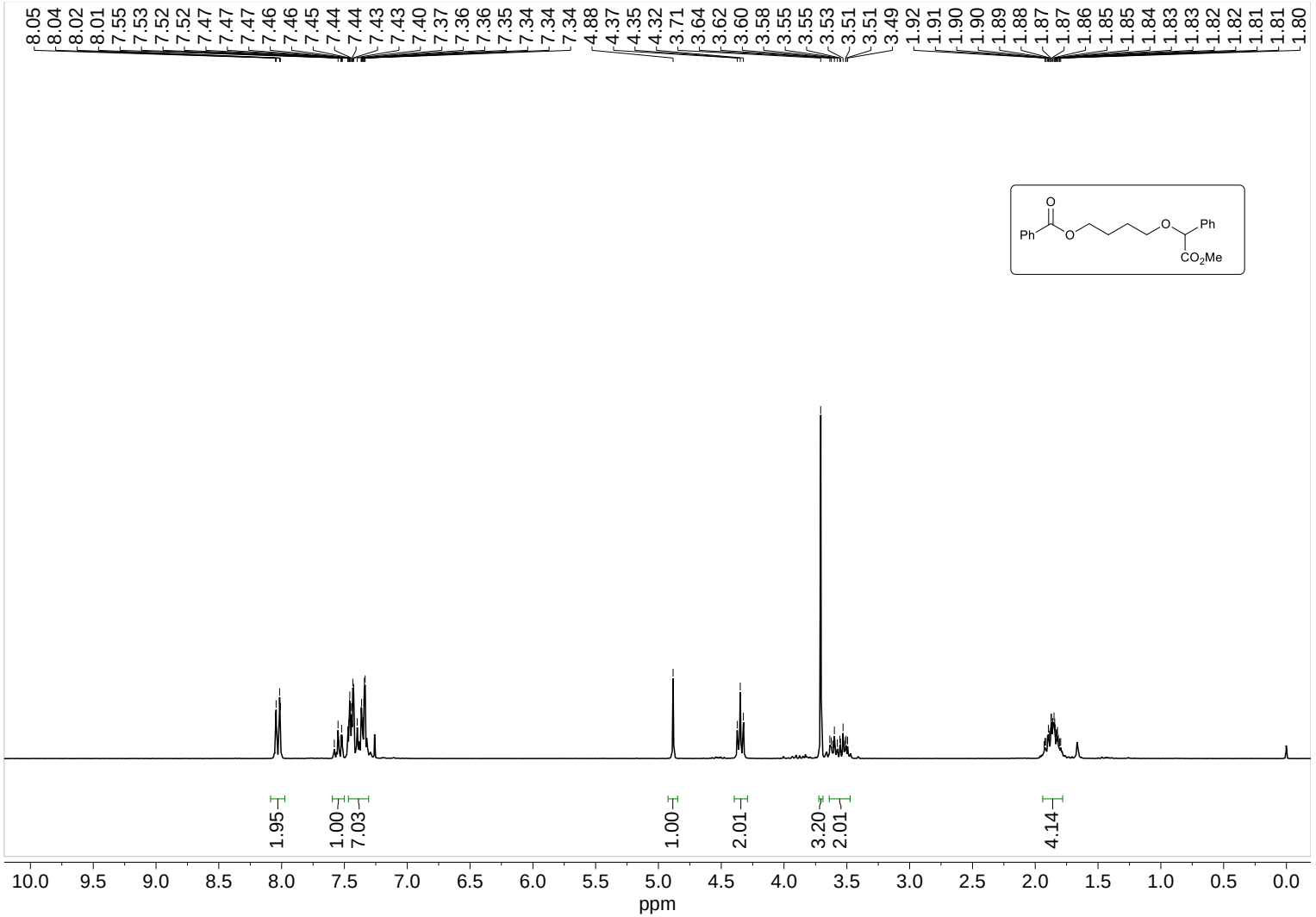
Molecule 6k – ^{1}H NMR (250 MHz, $CDCl_3$)



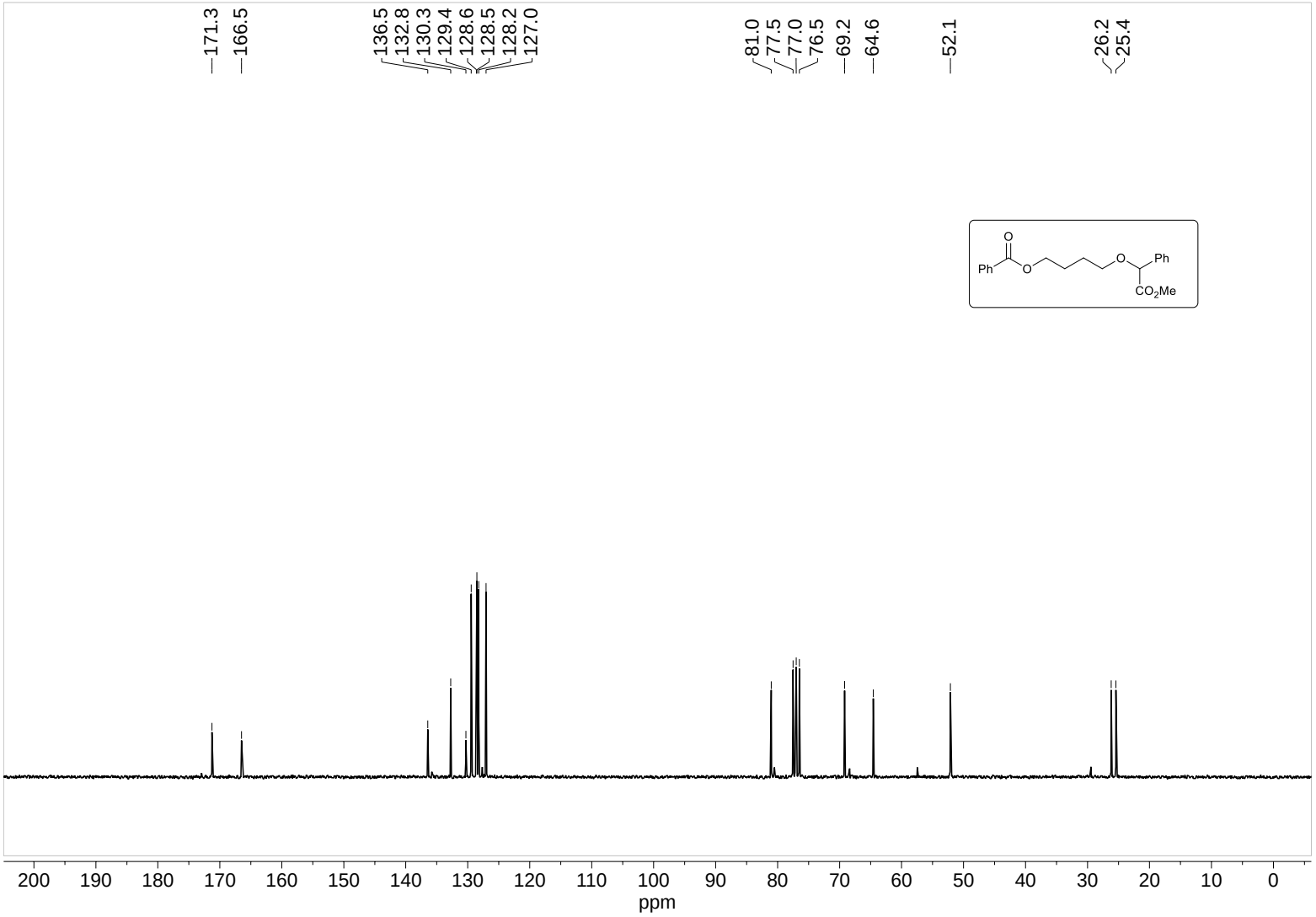
Molecule 6k – ^{13}C NMR (62.5 MHz, $CDCl_3$)



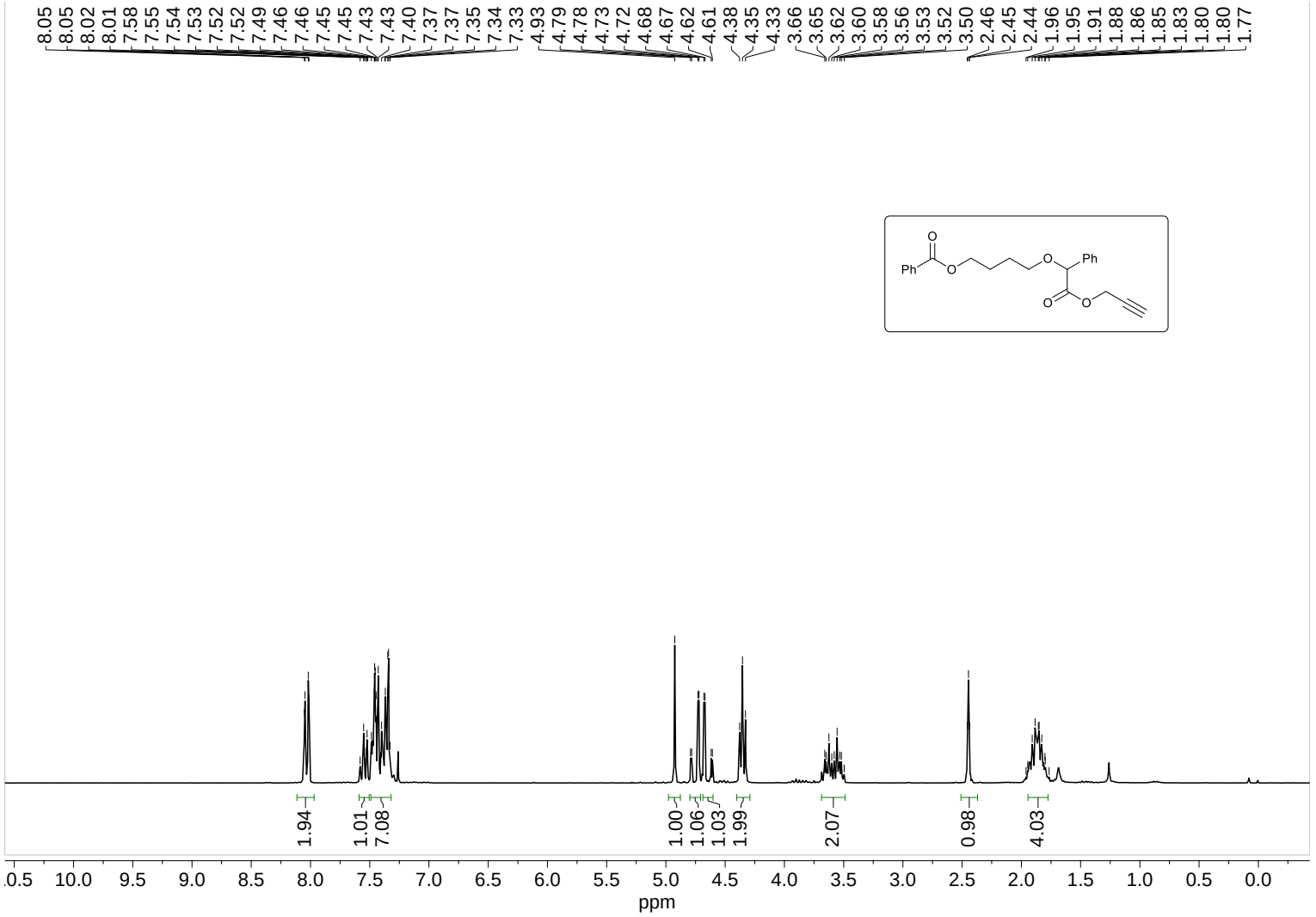
Molecule 8a - ^{1}H NMR (250 MHz, $CDCl_3$)



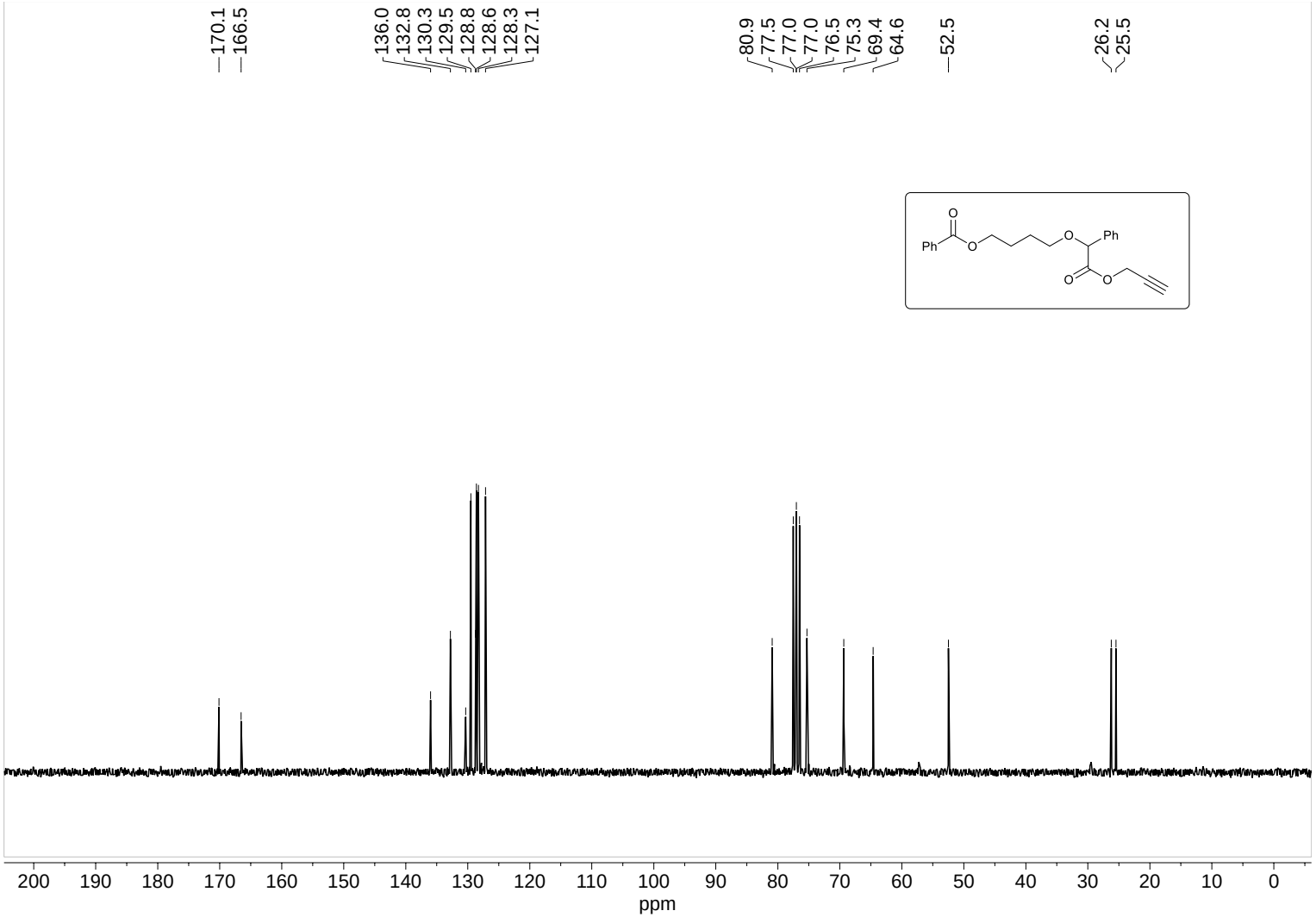
Molecule 8a - ^{13}C NMR (62.5 MHz, $CDCl_3$)



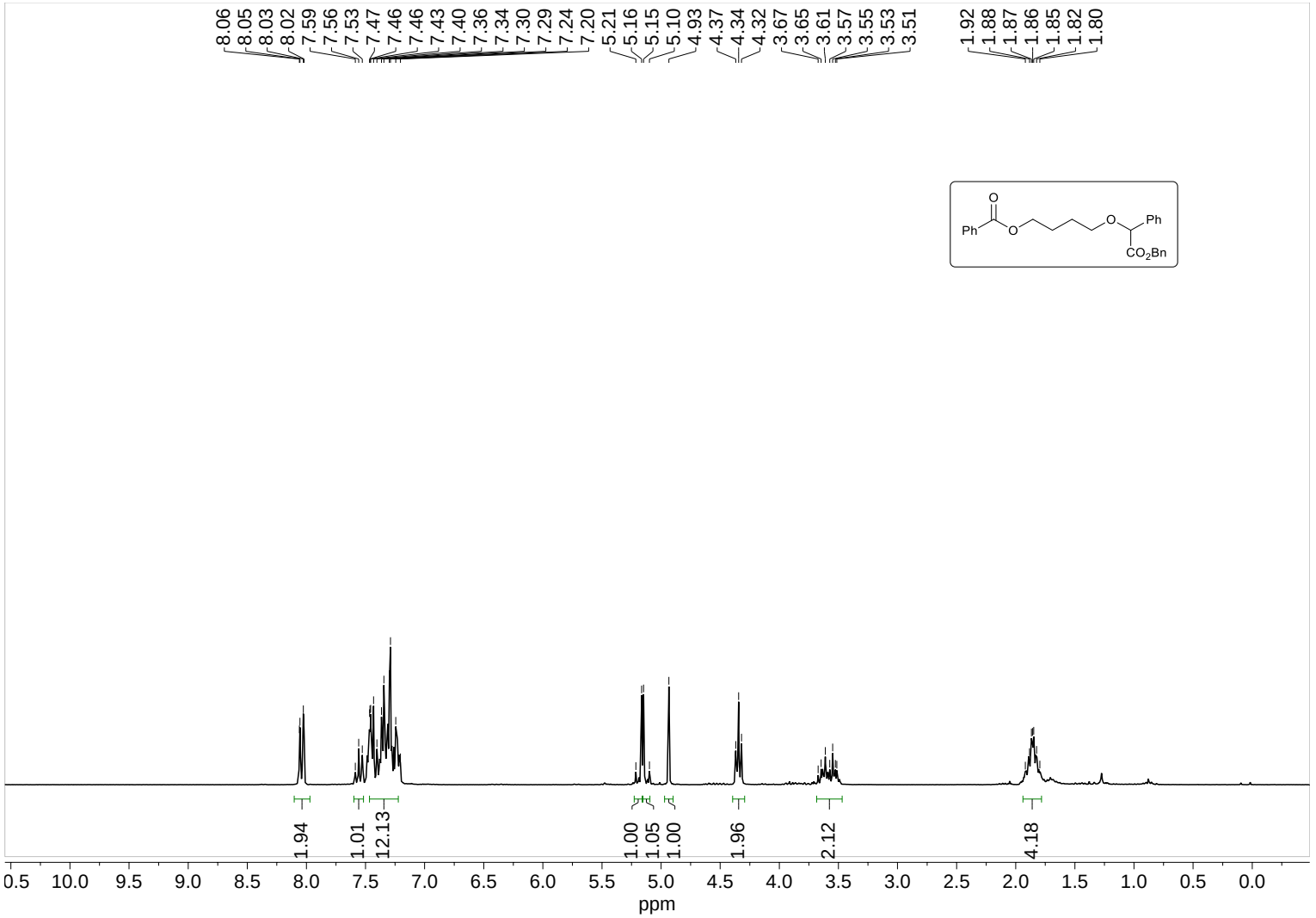
Molecule 8b - ^{1}H NMR (250 MHz, $CDCl_3$)



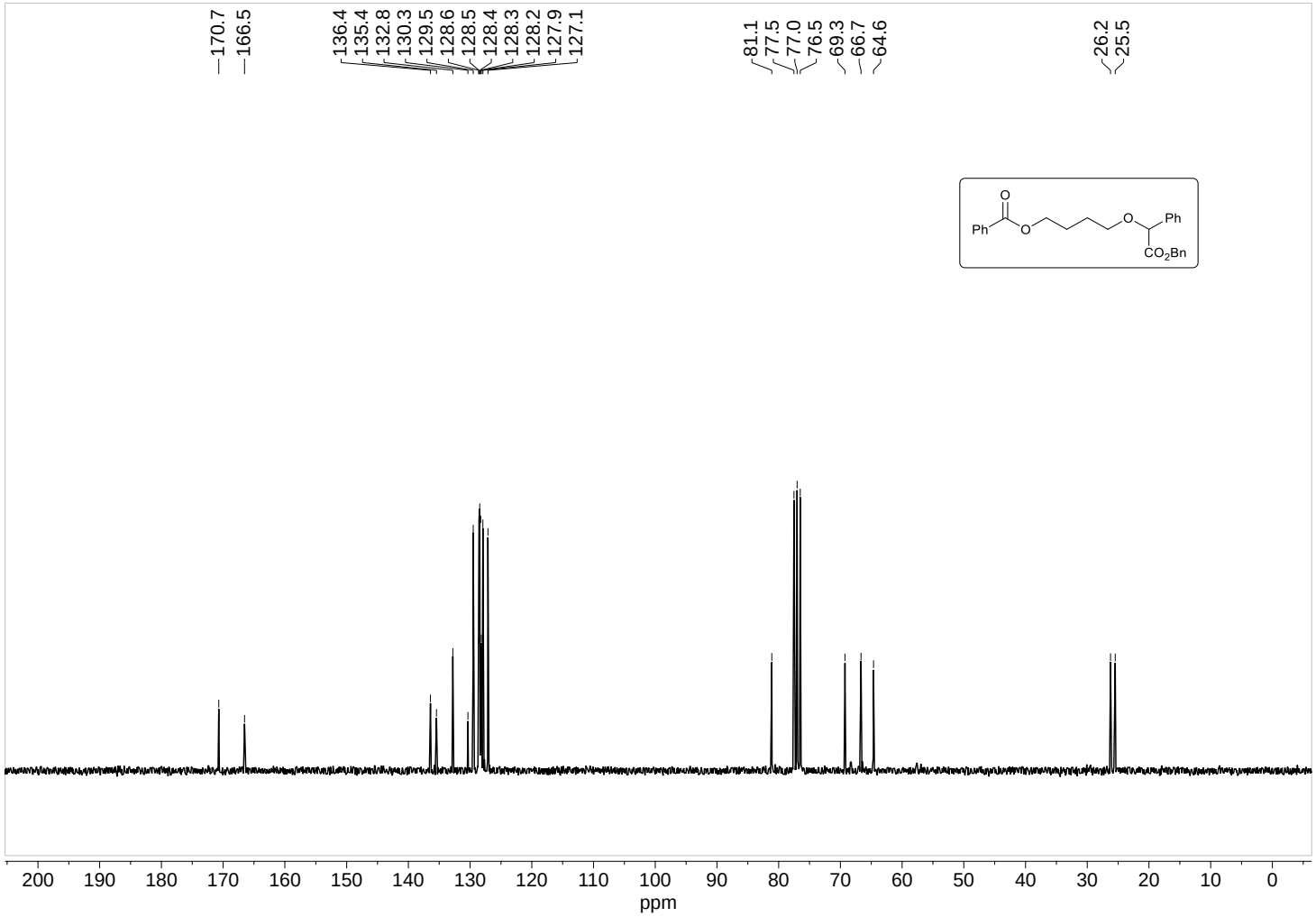
Molecule 8b - ^{13}C NMR (62.5 MHz, $CDCl_3$)



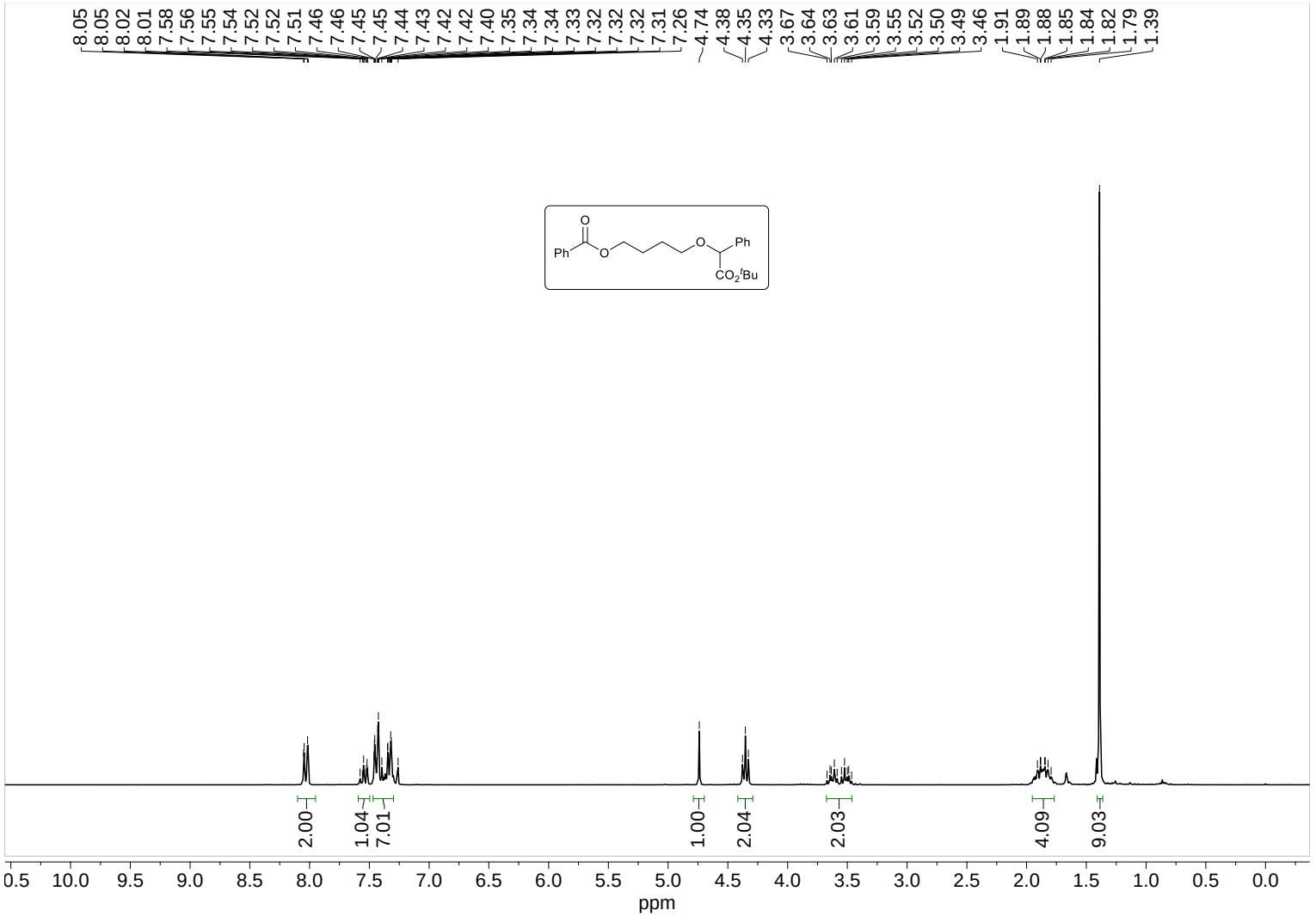
Molecule 8c - ^{1}H NMR (250 MHz, $CDCl_3$)



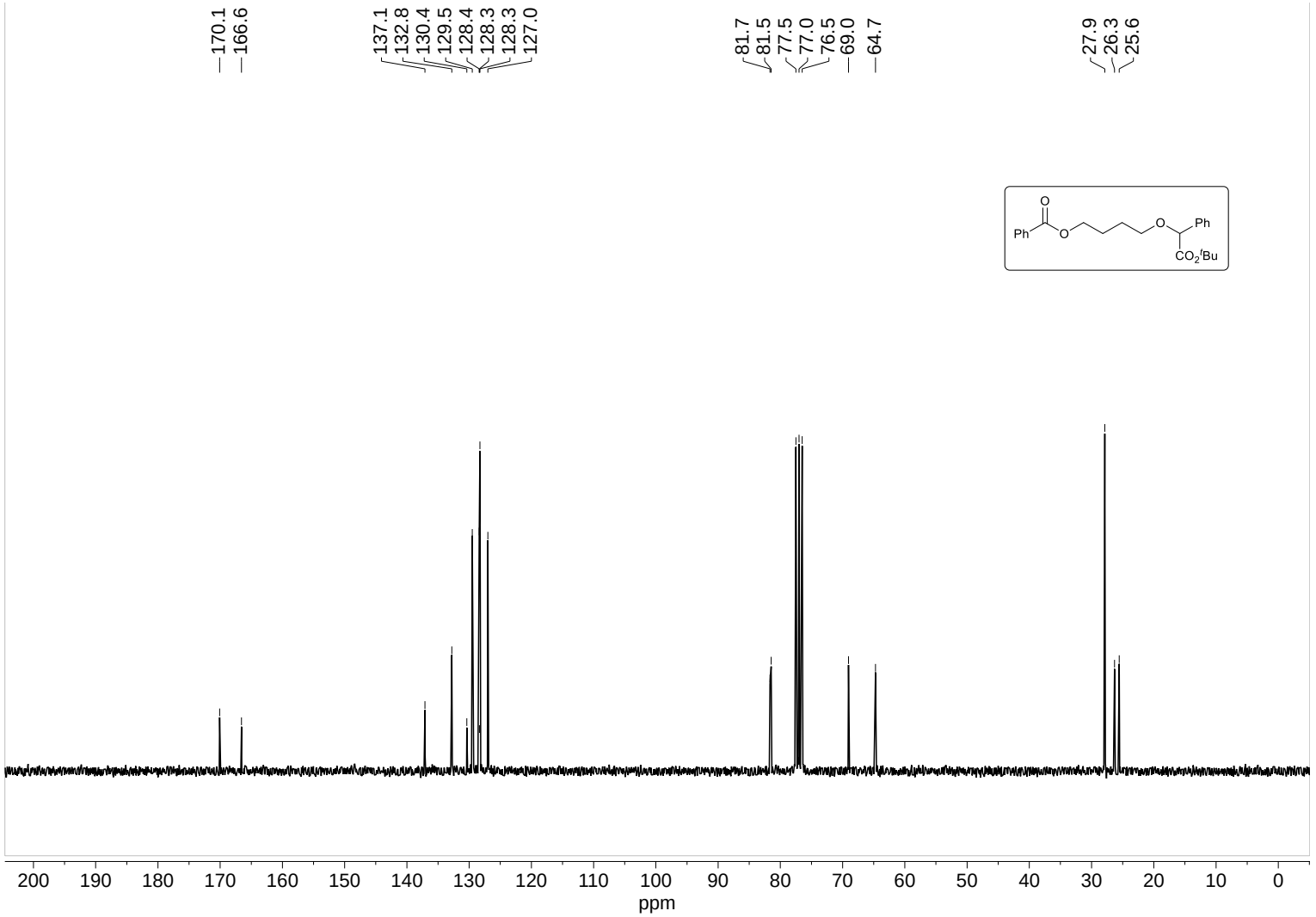
Molecule 8c - ^{13}C NMR (62.5 MHz, $CDCl_3$)



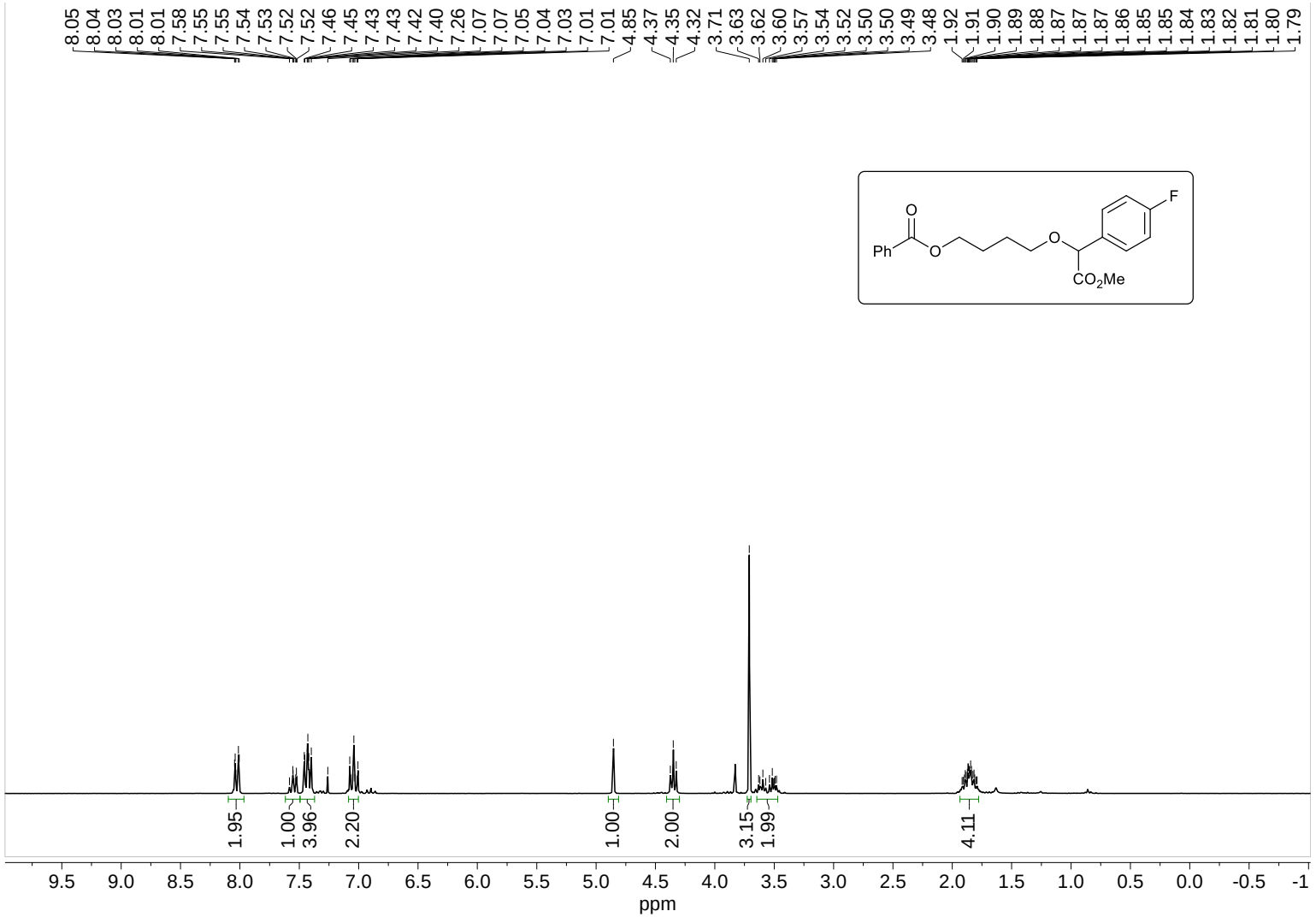
Molecule 8d - ^{1}H NMR (250 MHz, $CDCl_3$)



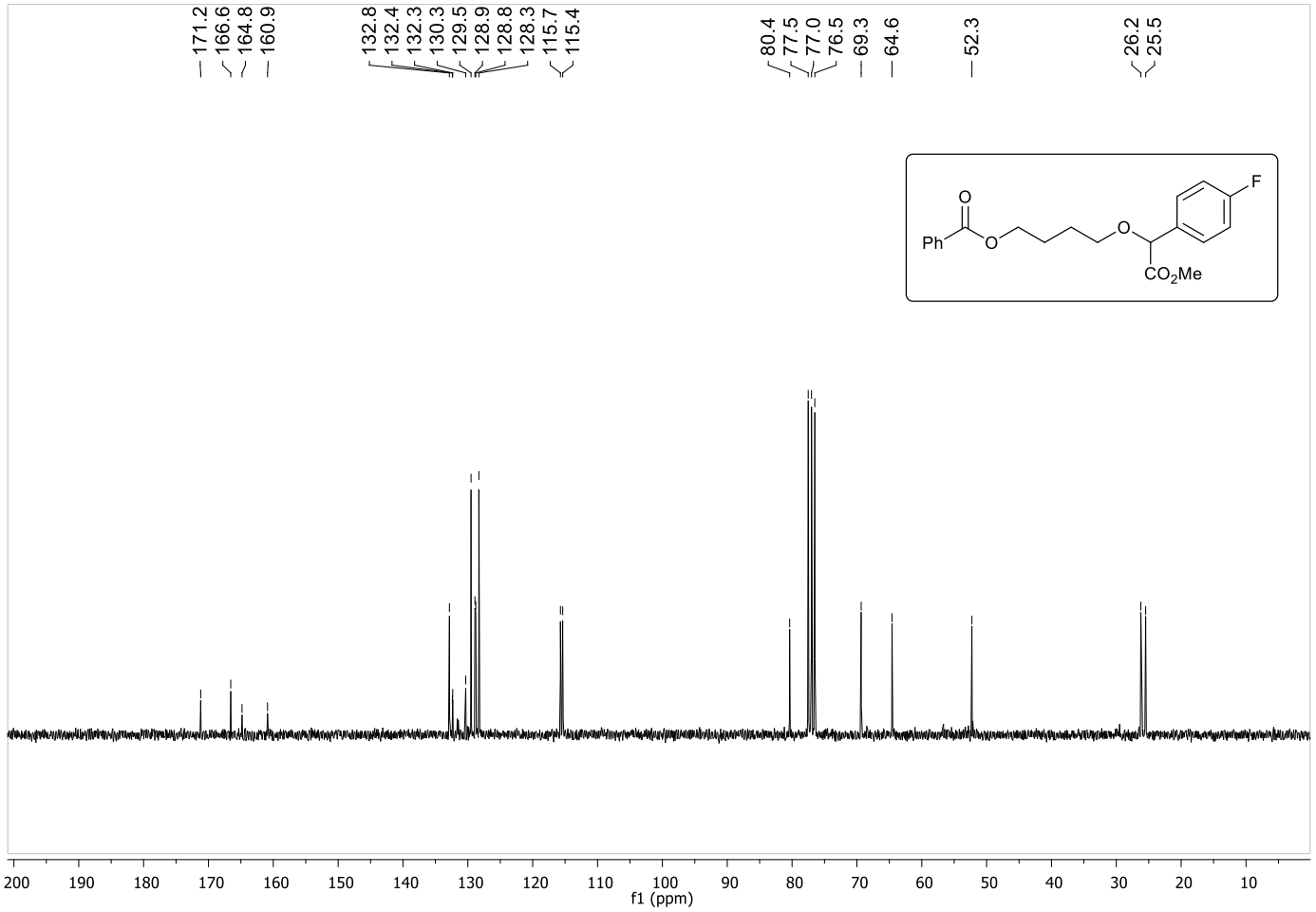
Molecule 8d - ^{13}C NMR (62.5 MHz, $CDCl_3$)



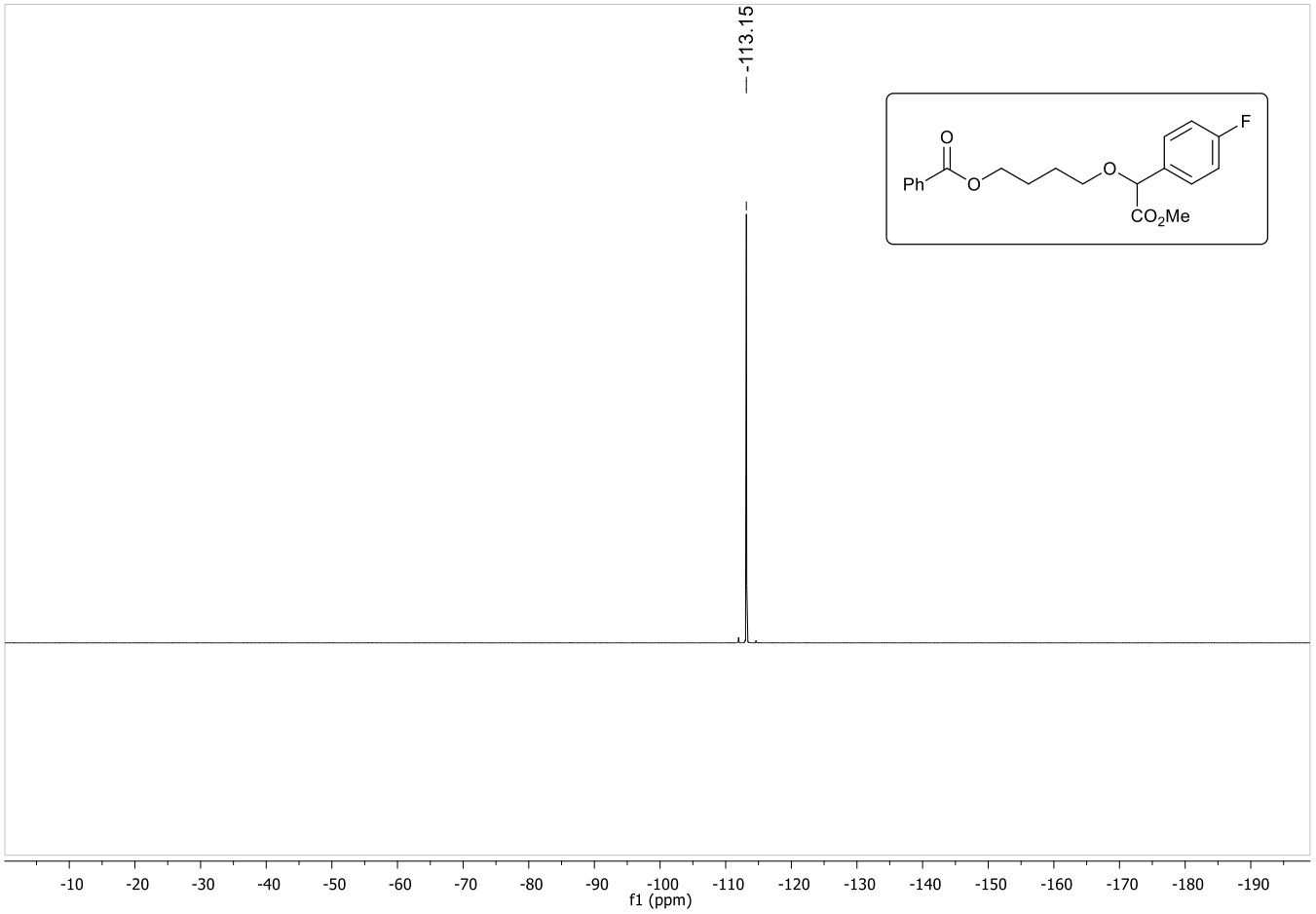
Molecule 8e - ^{1}H NMR (250 MHz, $CDCl_3$)



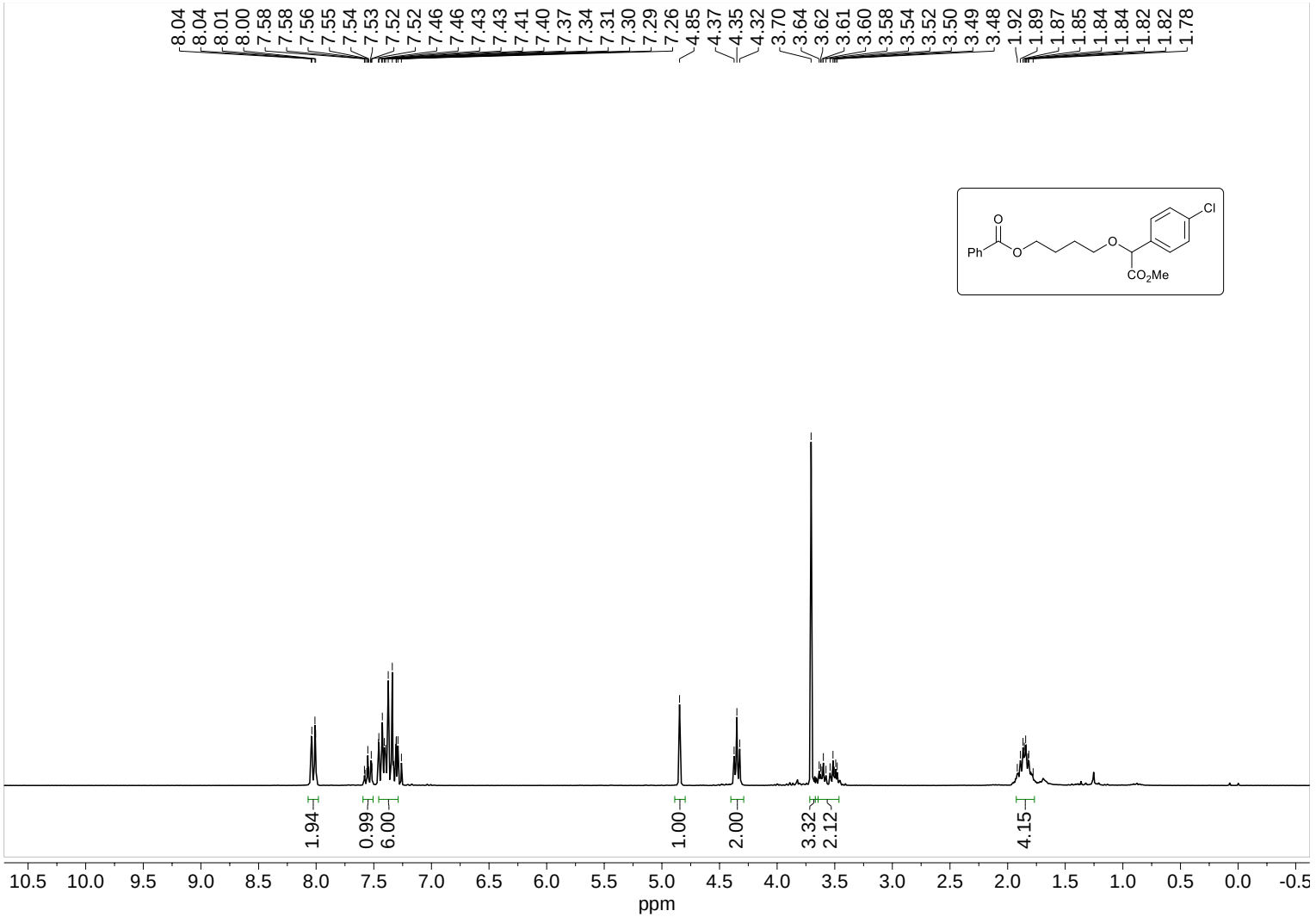
Molecule 8e - ^{13}C NMR (62.5 MHz, $CDCl_3$)



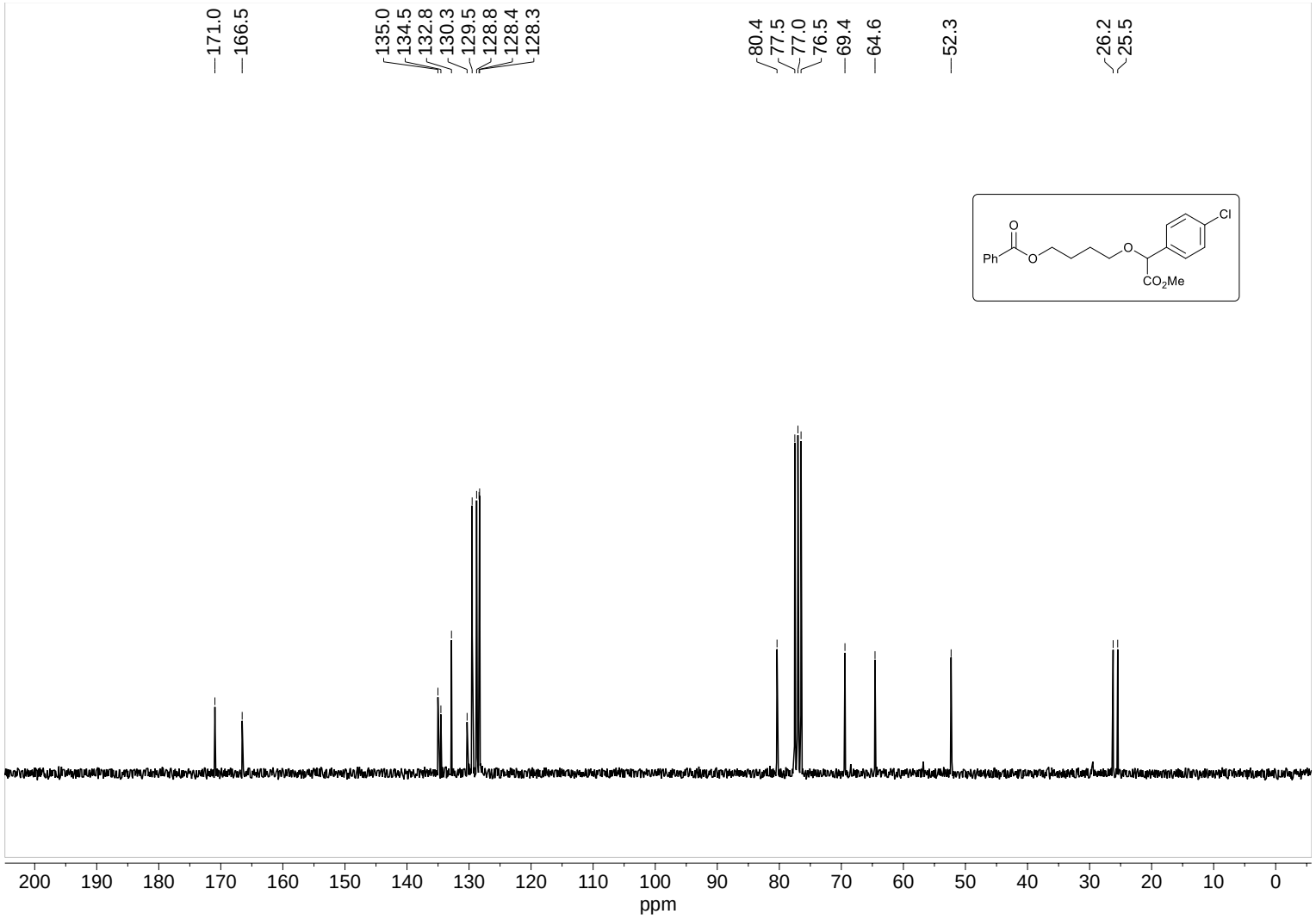
Molecule 8e - ^{19}F NMR (235 MHz, $CDCl_3$)



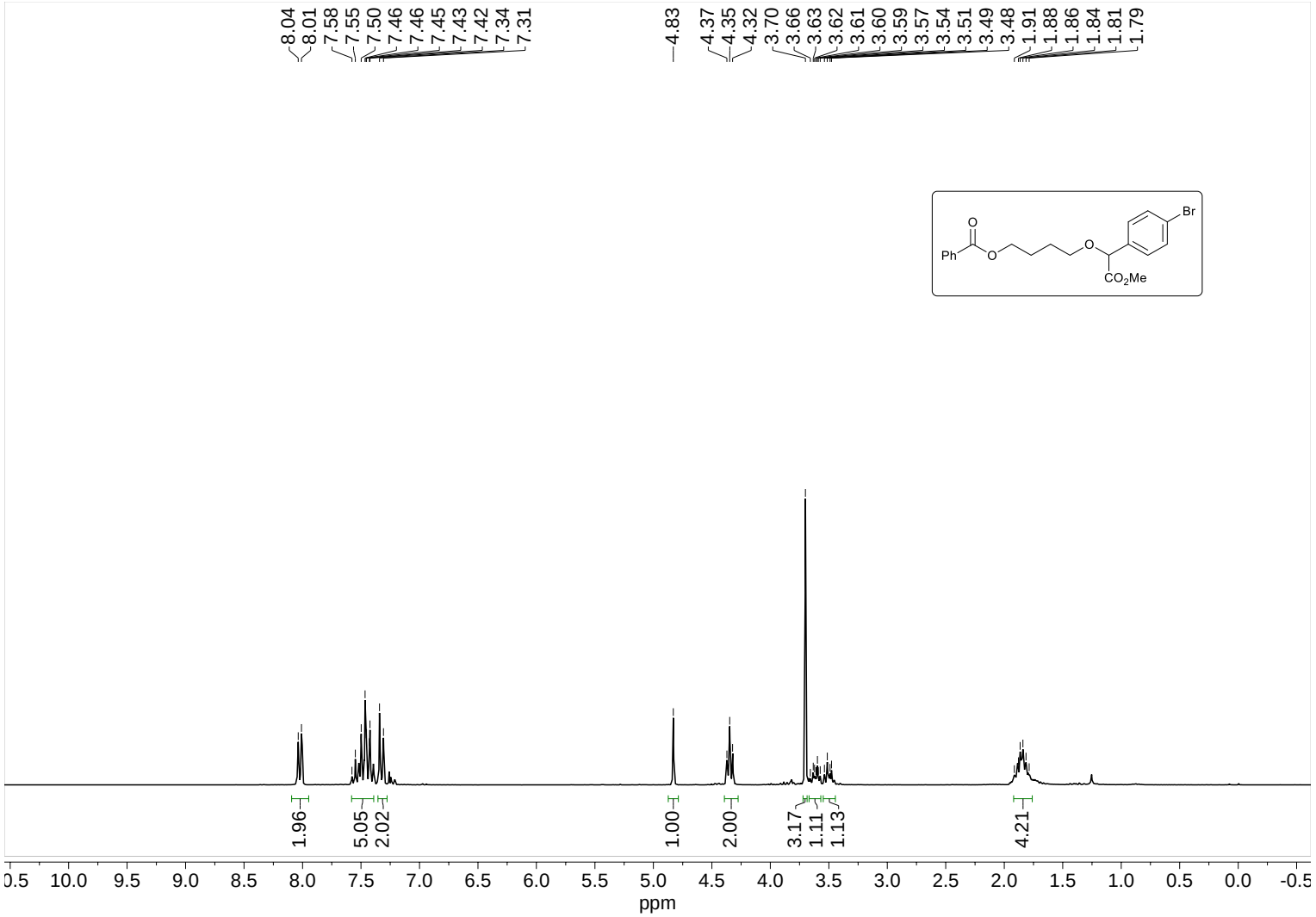
Molecule 8f - ^{1}H NMR (250 MHz, $CDCl_3$)



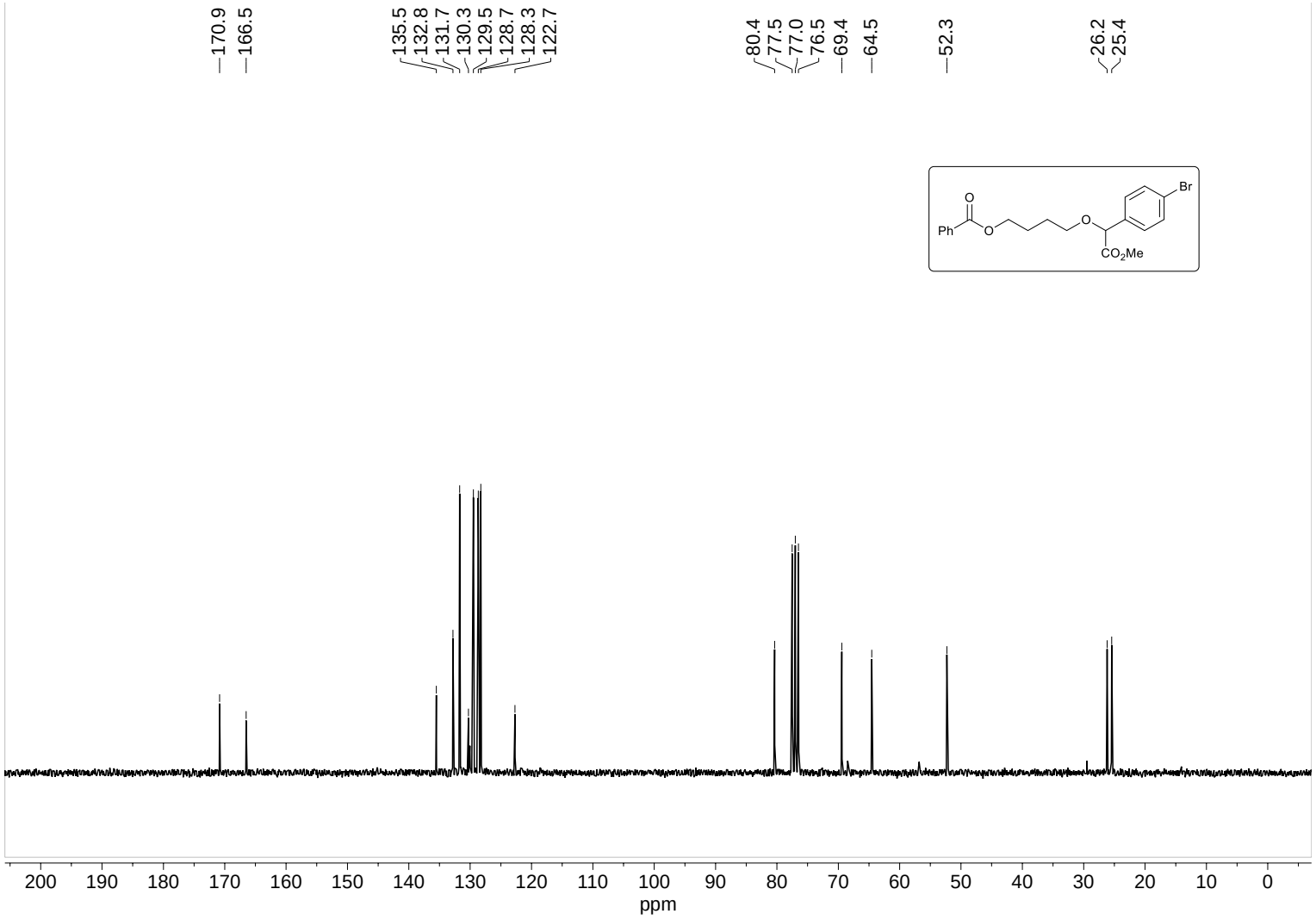
Molecule 8f - ^{13}C NMR (62.5 MHz, $CDCl_3$)



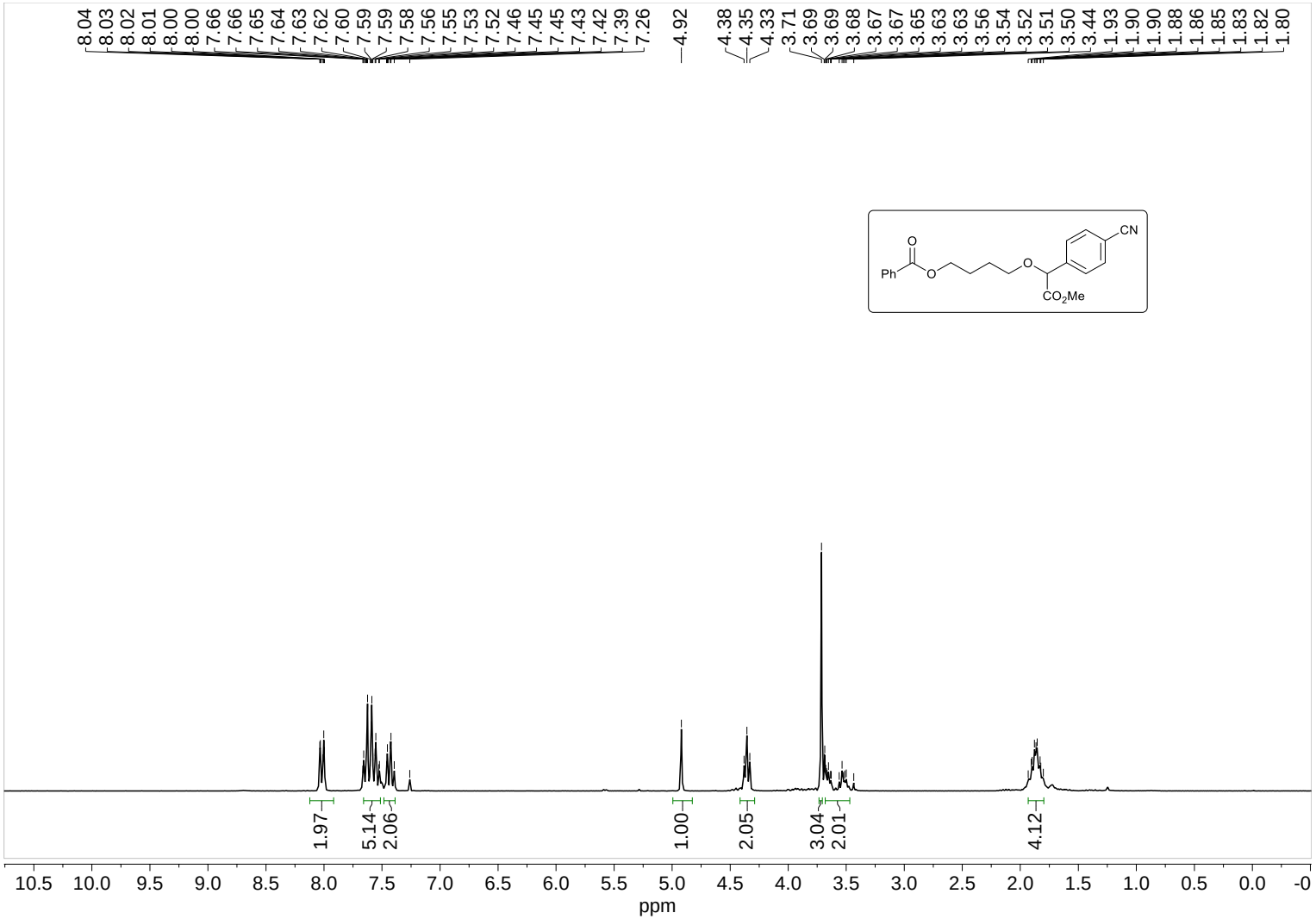
Molecule 8g - ^{1}H NMR (250 MHz, $CDCl_3$)



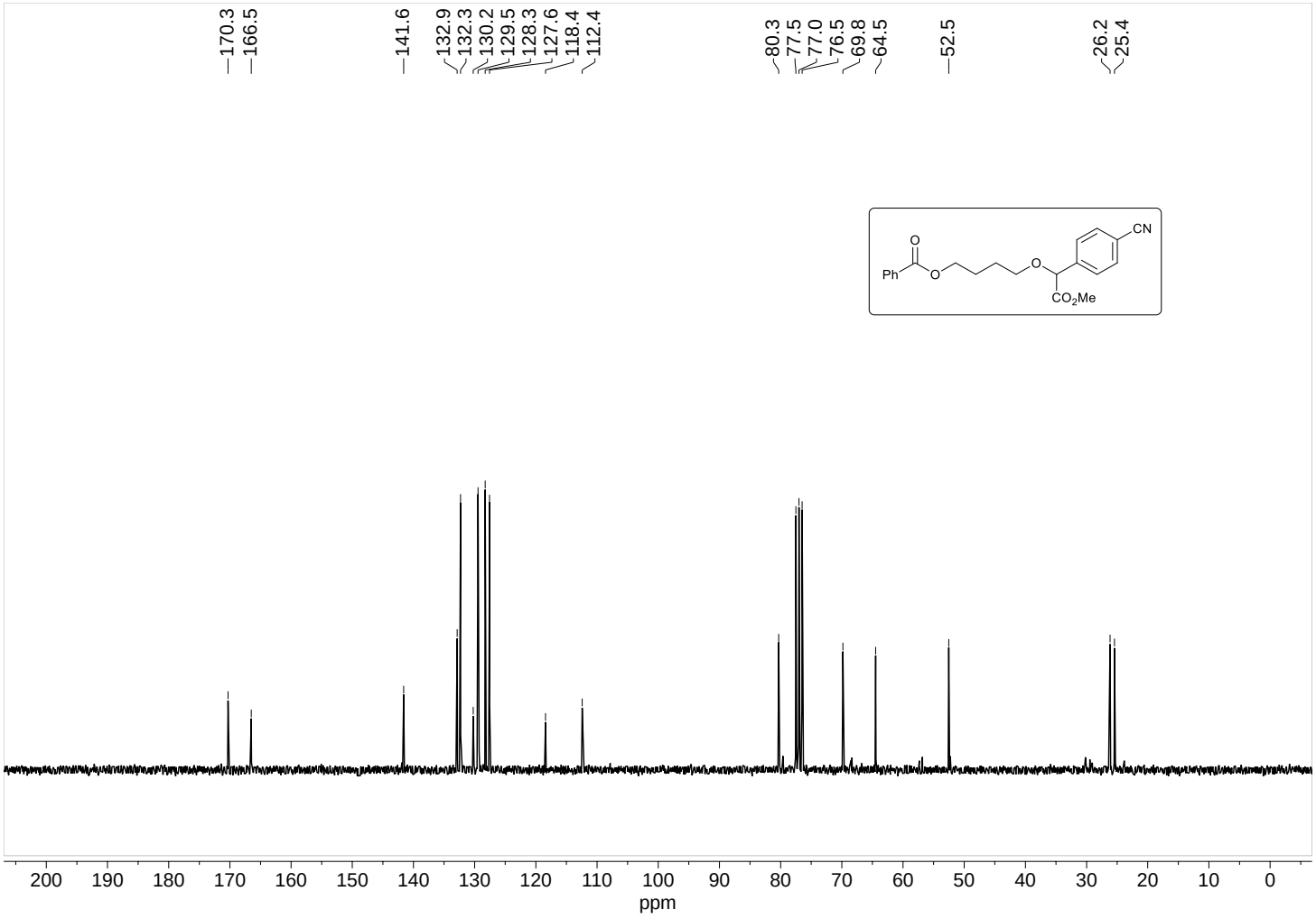
Molecule 8g - ^{13}C NMR (62.5 MHz, $CDCl_3$)



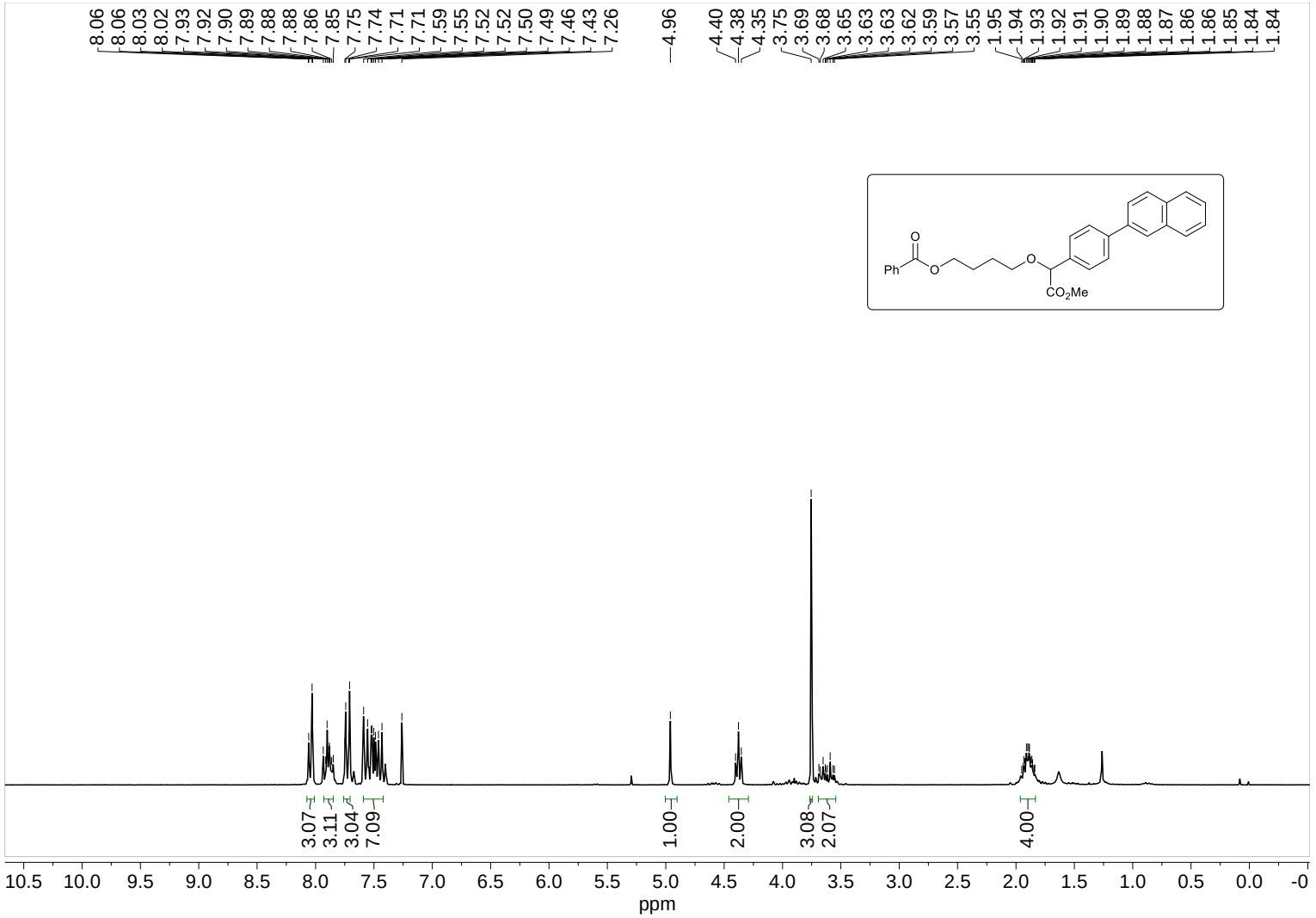
Molecule 8h - ^{1}H NMR (250 MHz, $CDCl_3$)



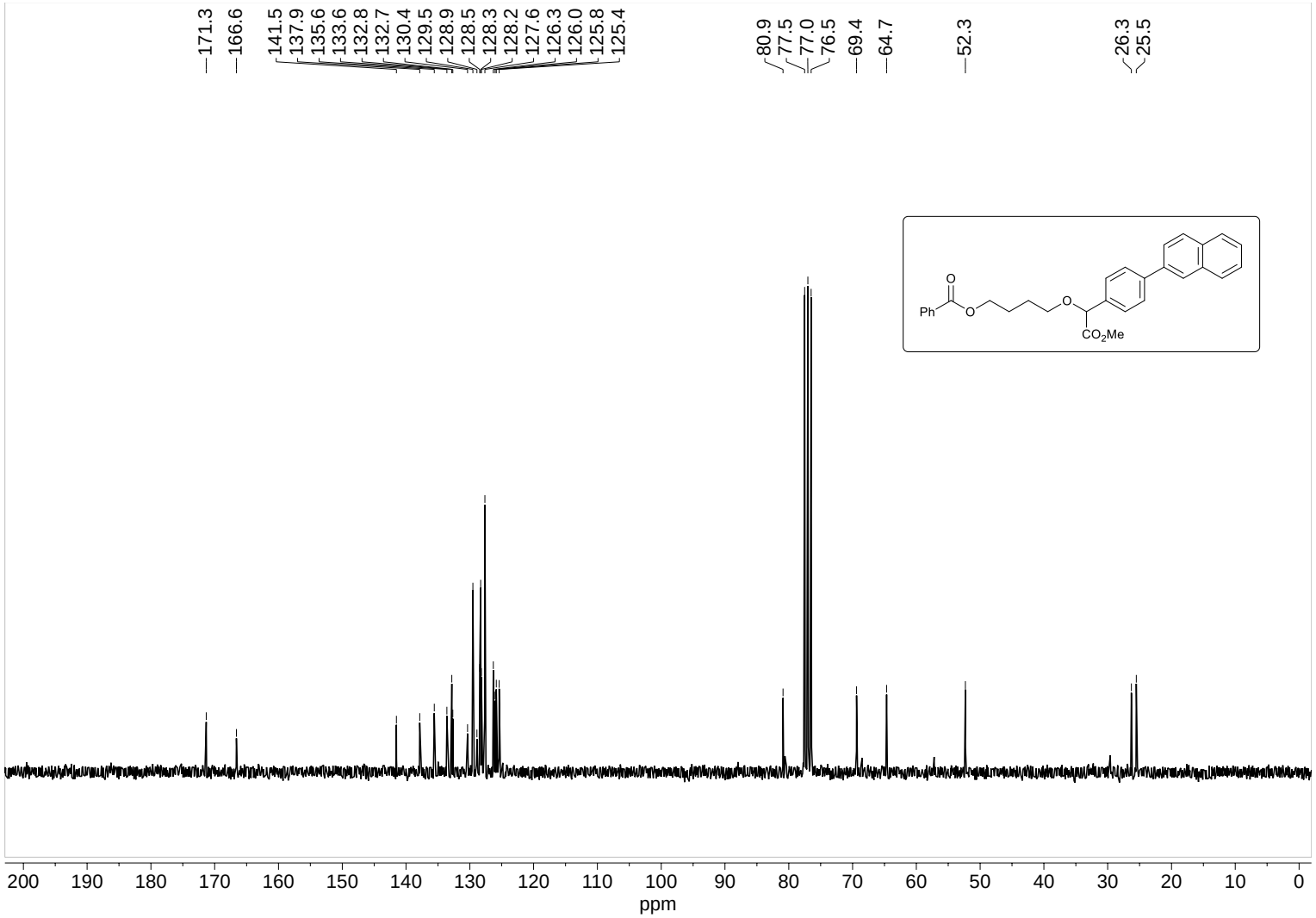
Molecule 8h - ^{13}C NMR (62.5 MHz, $CDCl_3$)



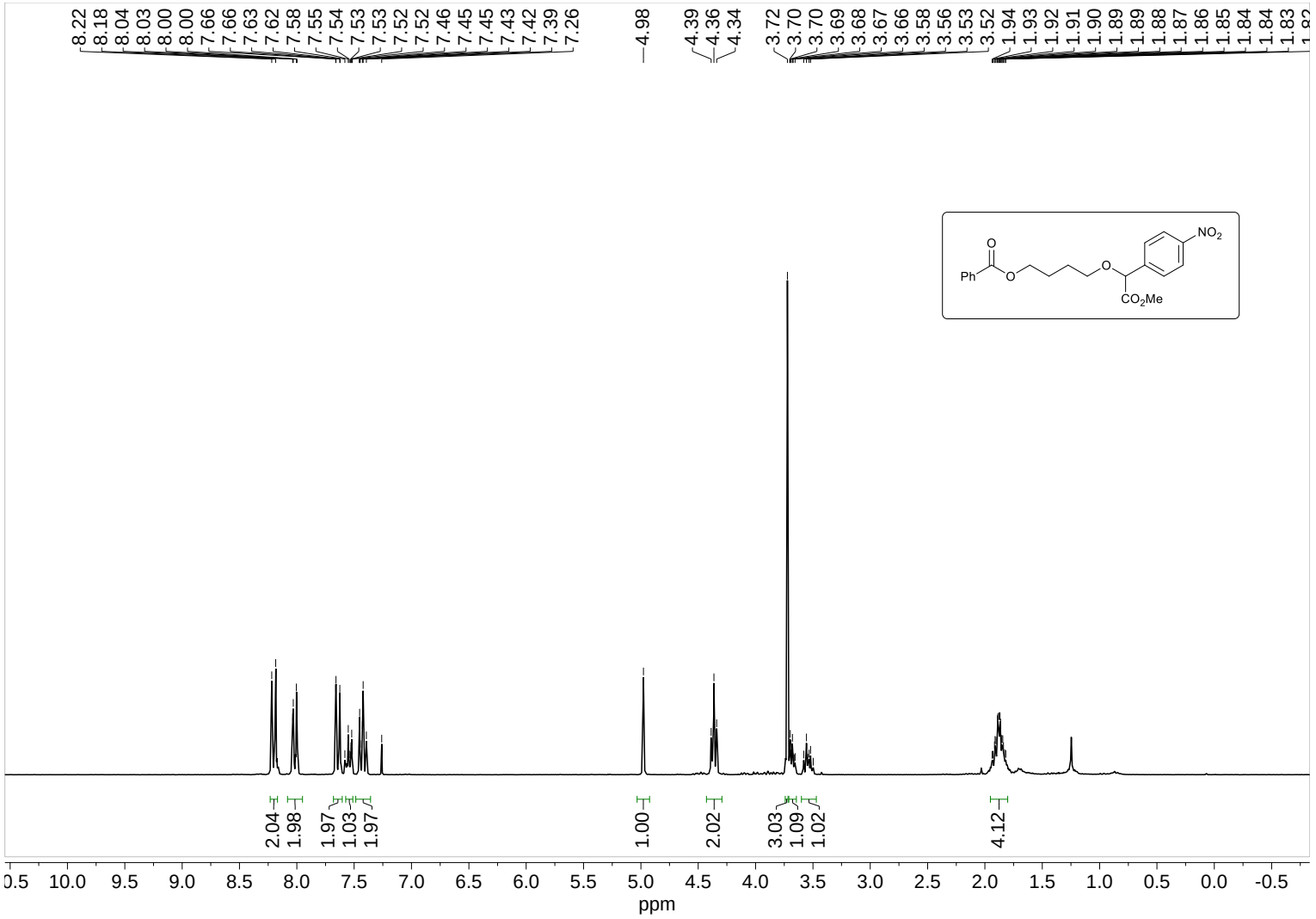
Molecule 8i - ^{1}H NMR (250 MHz, $CDCl_3$)



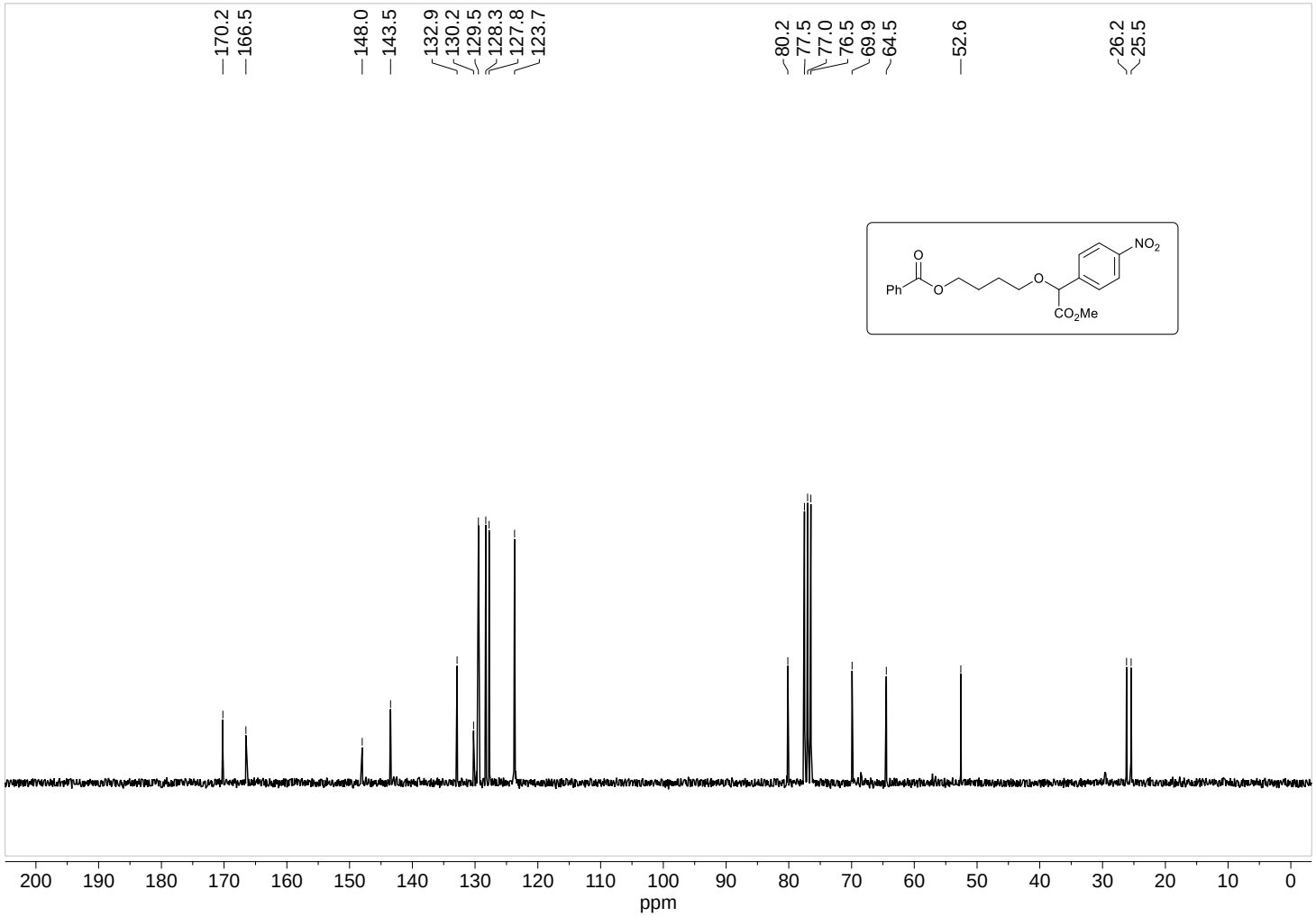
Molecule 8i - ^{13}C NMR (62.5 MHz, $CDCl_3$)



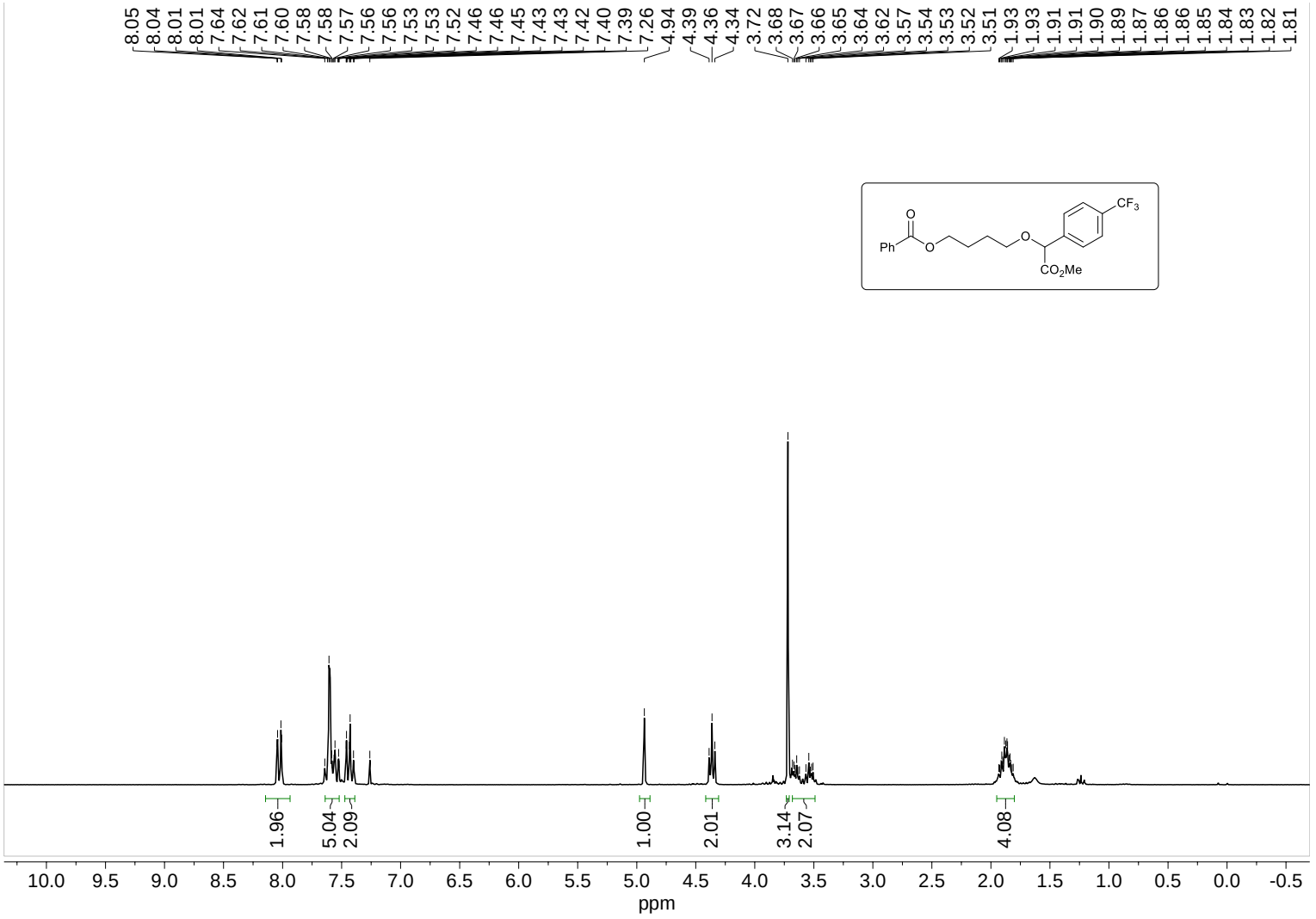
Molecule 8j - ^{1}H NMR (250 MHz, $CDCl_3$)



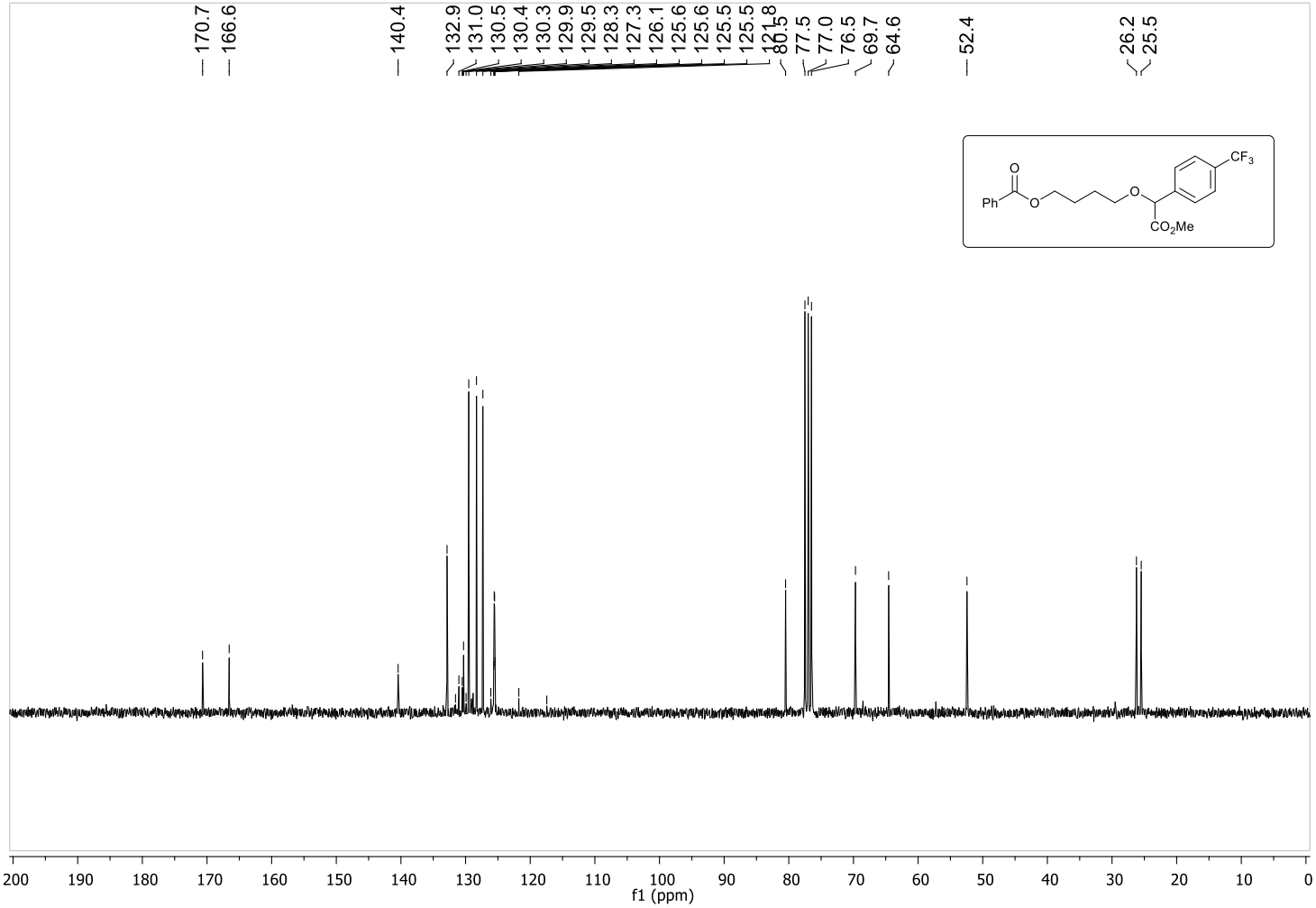
Molecule 8j - ^{13}C NMR (62.5 MHz, $CDCl_3$)



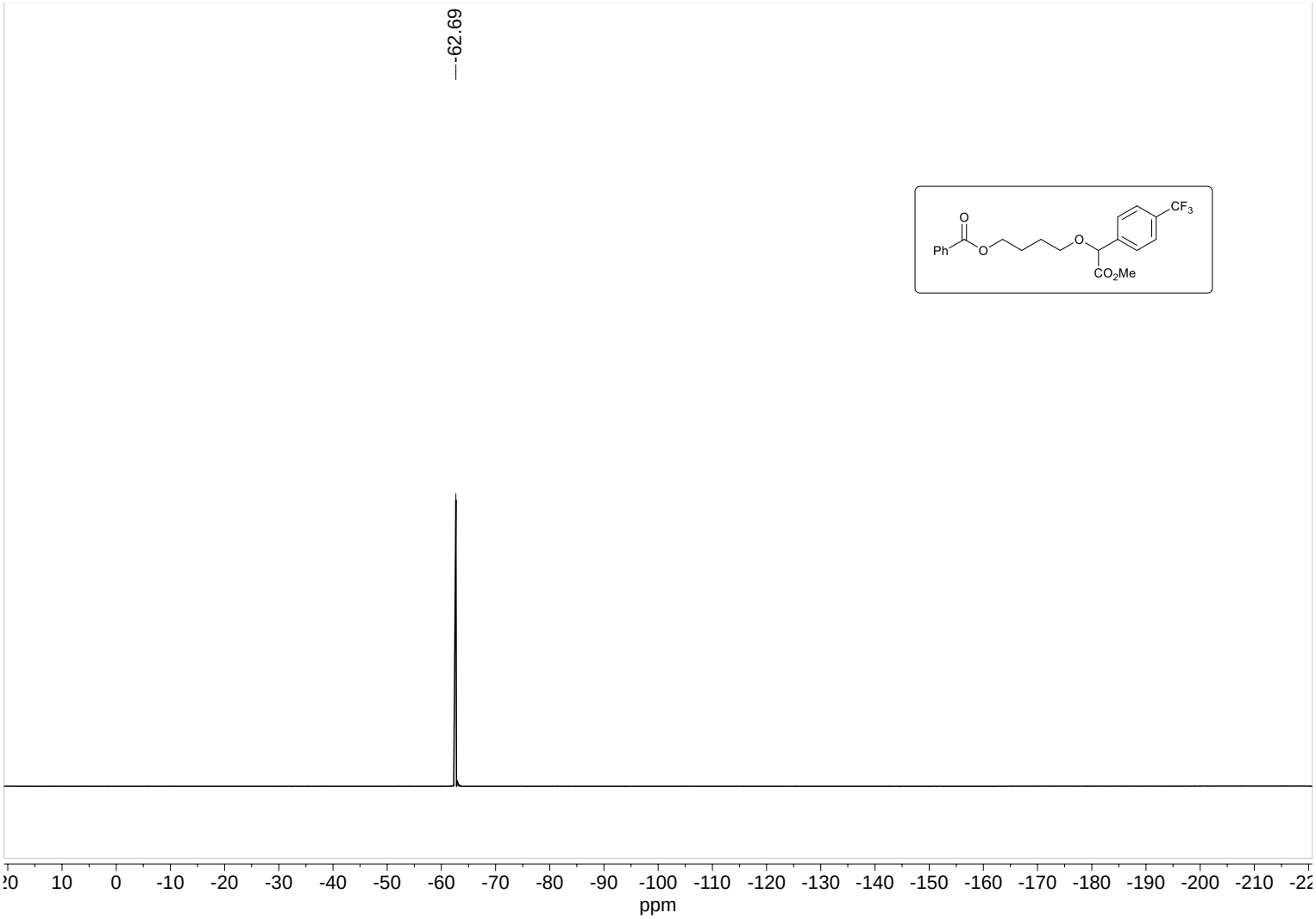
Molecule 8k - ^{1}H NMR (250 MHz, $CDCl_3$)



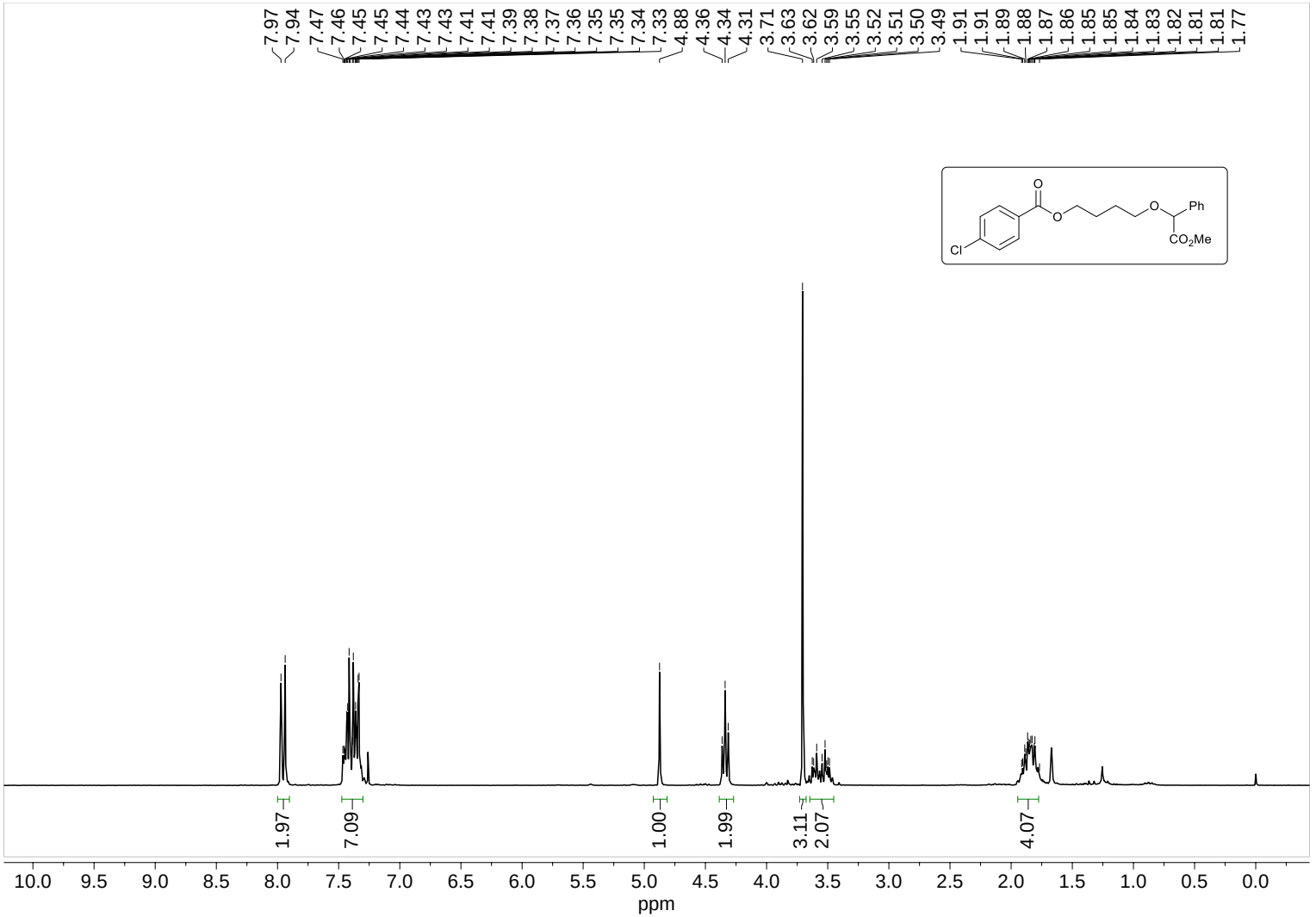
Molecule 8k - ^{13}C NMR (62.5 MHz, $CDCl_3$)



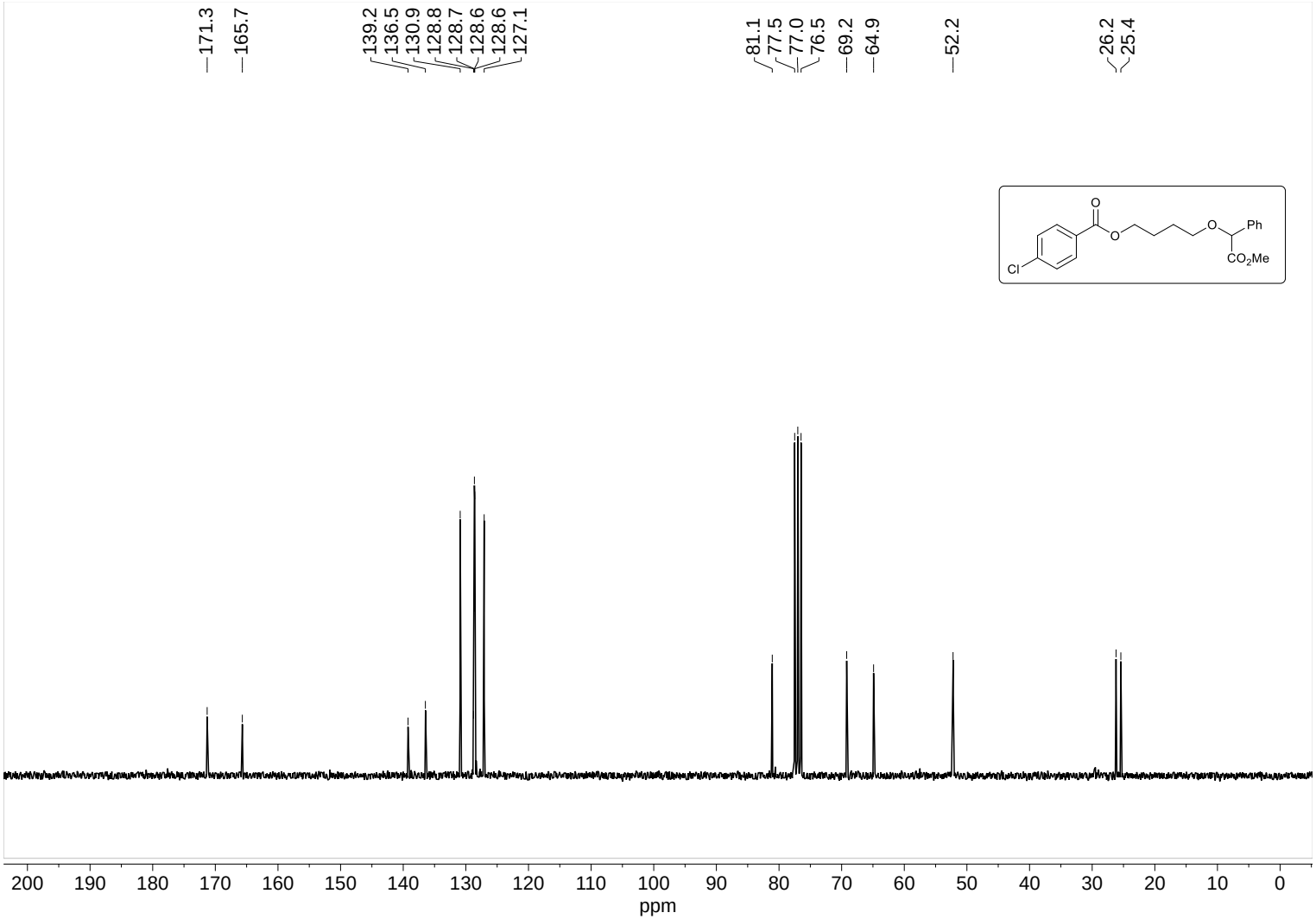
Molecule 8k - ^{19}F NMR (235 MHz, $CDCl_3$)



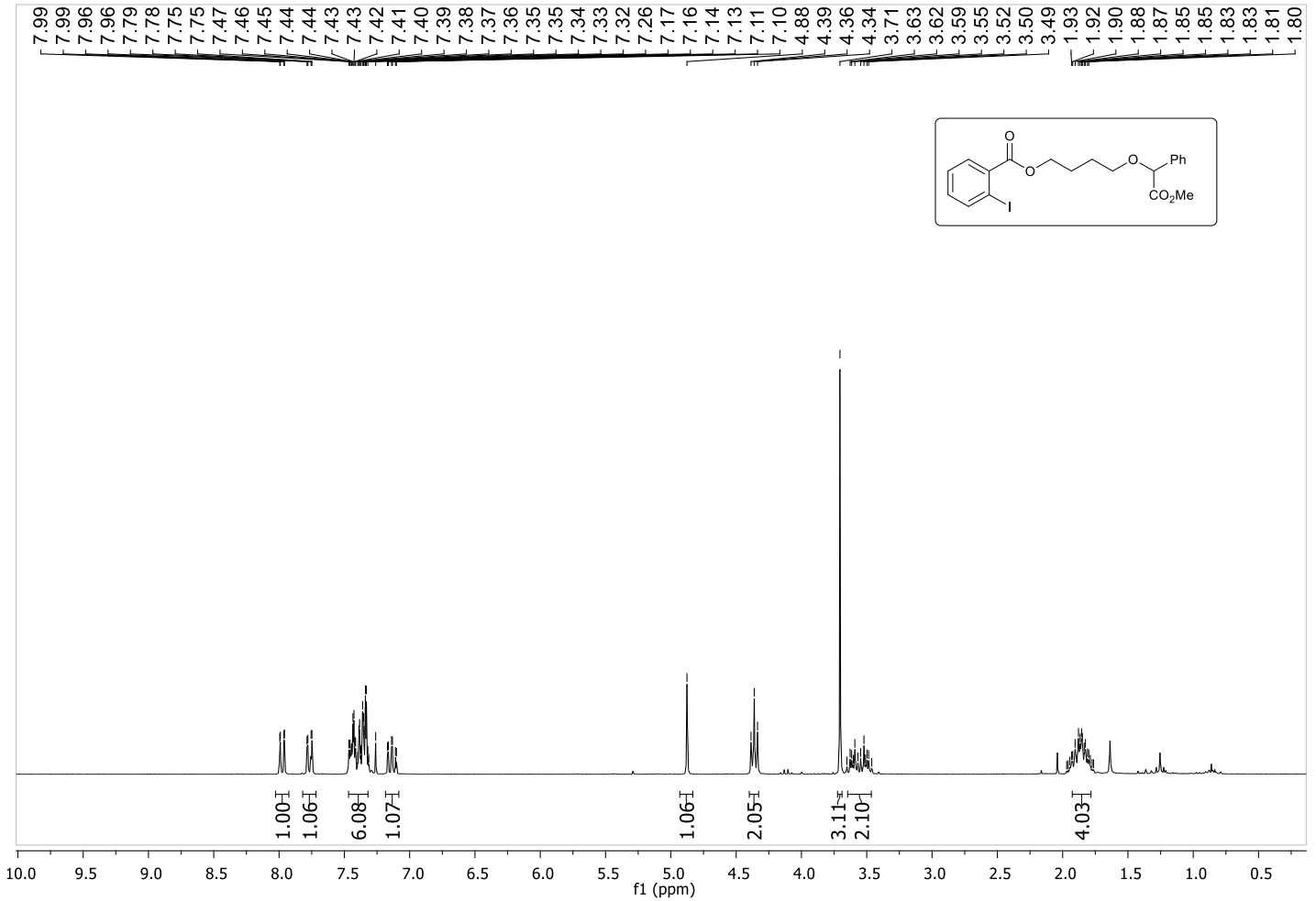
Molecule 8l - ^{1}H NMR (250 MHz, $CDCl_3$)



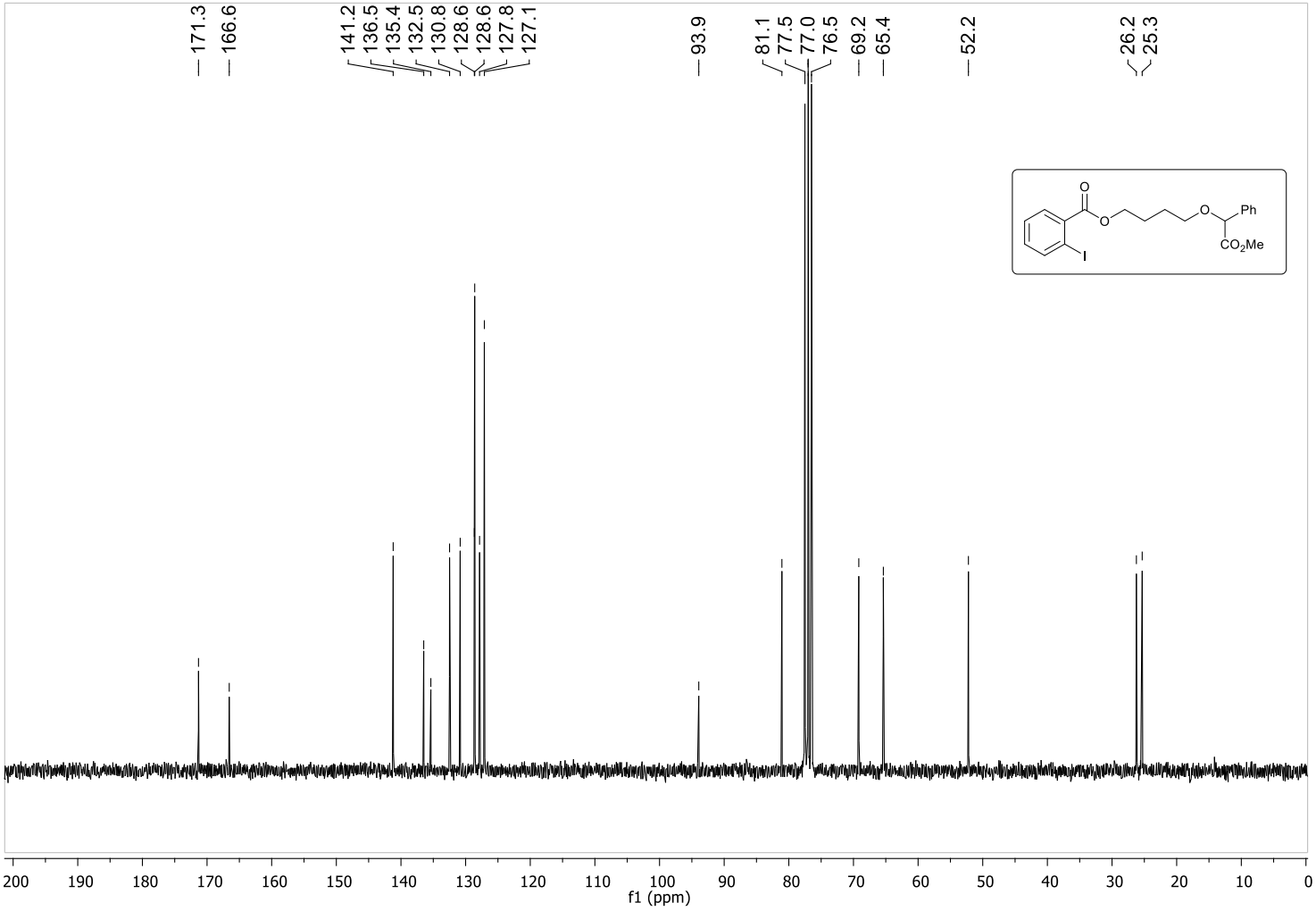
Molecule 8l - ^{13}C NMR (62.5 MHz, $CDCl_3$)



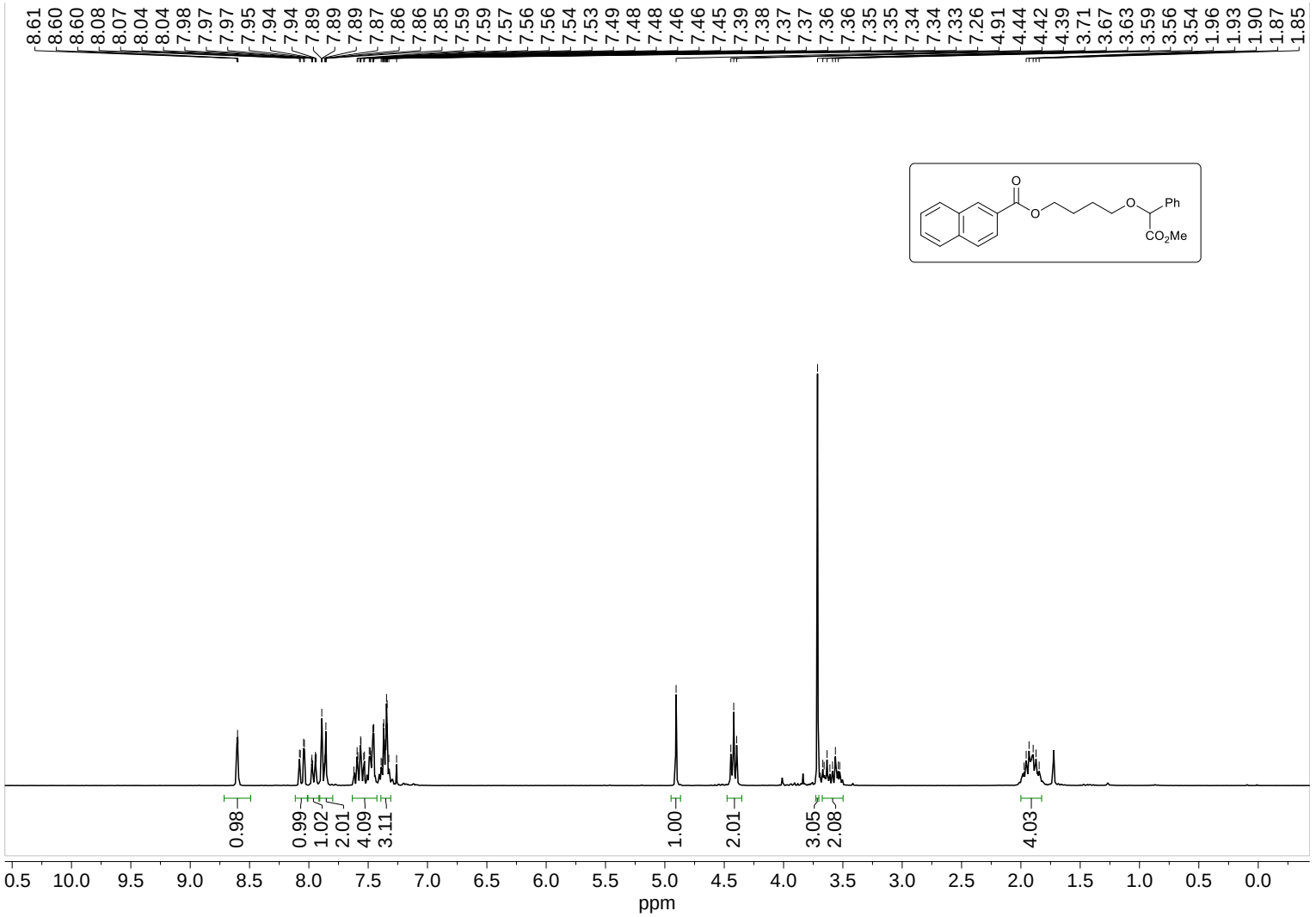
Molecule 8m - ^{1}H NMR (250 MHz, $CDCl_3$)



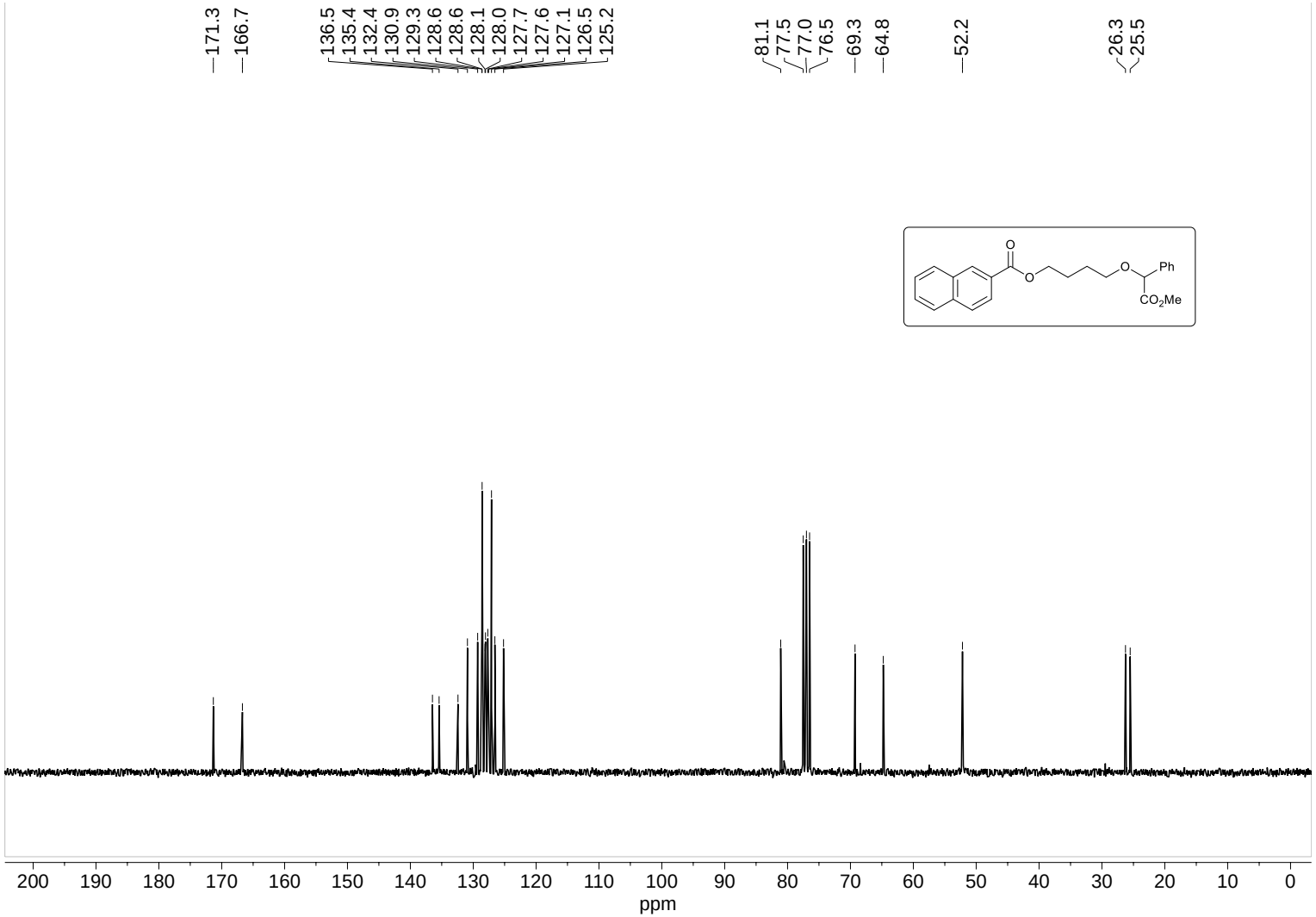
Molecule 8m - ^{13}C NMR (62.5 MHz, $CDCl_3$)



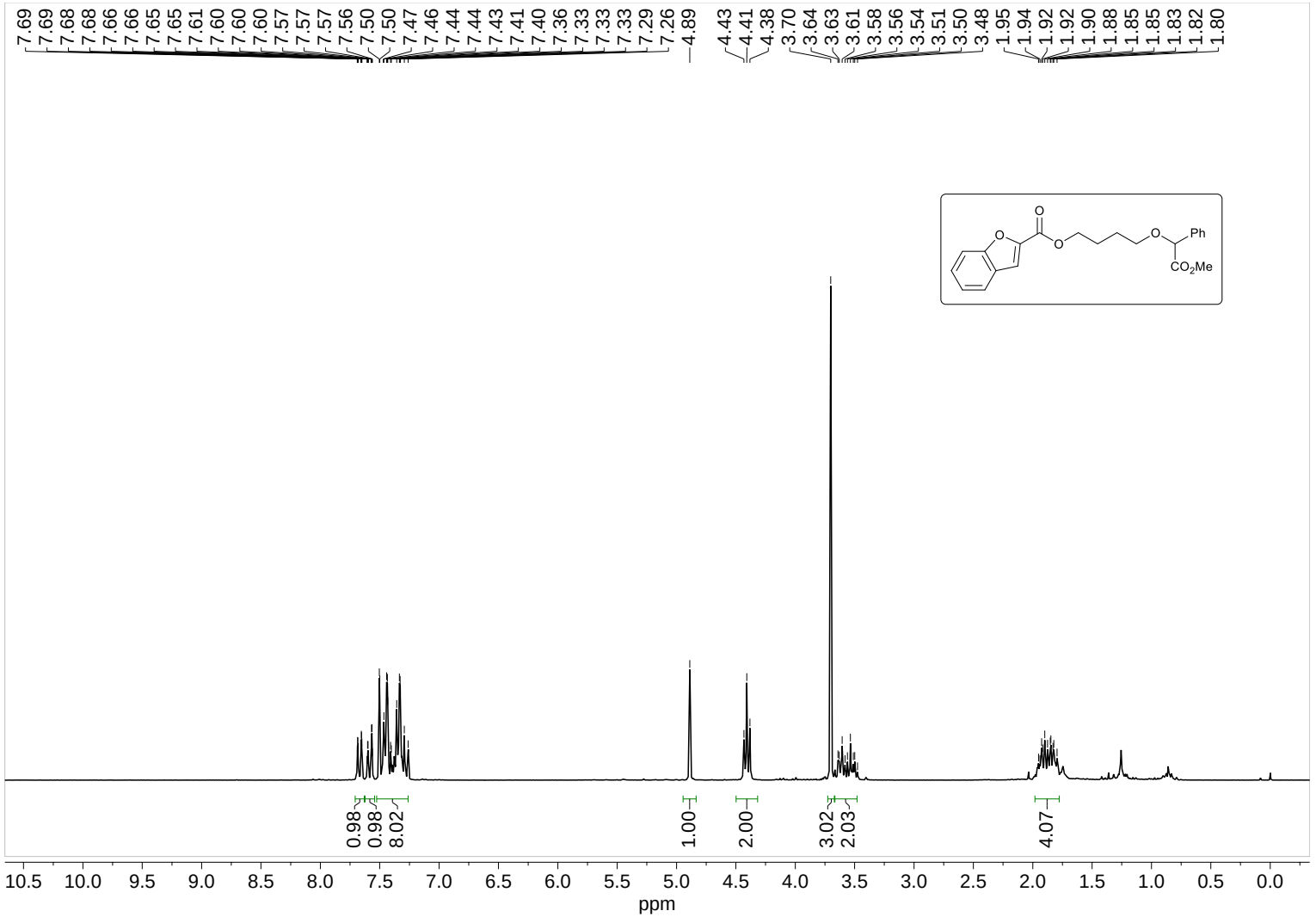
Molecule 8n - ^{1}H NMR (250 MHz, $CDCl_3$)



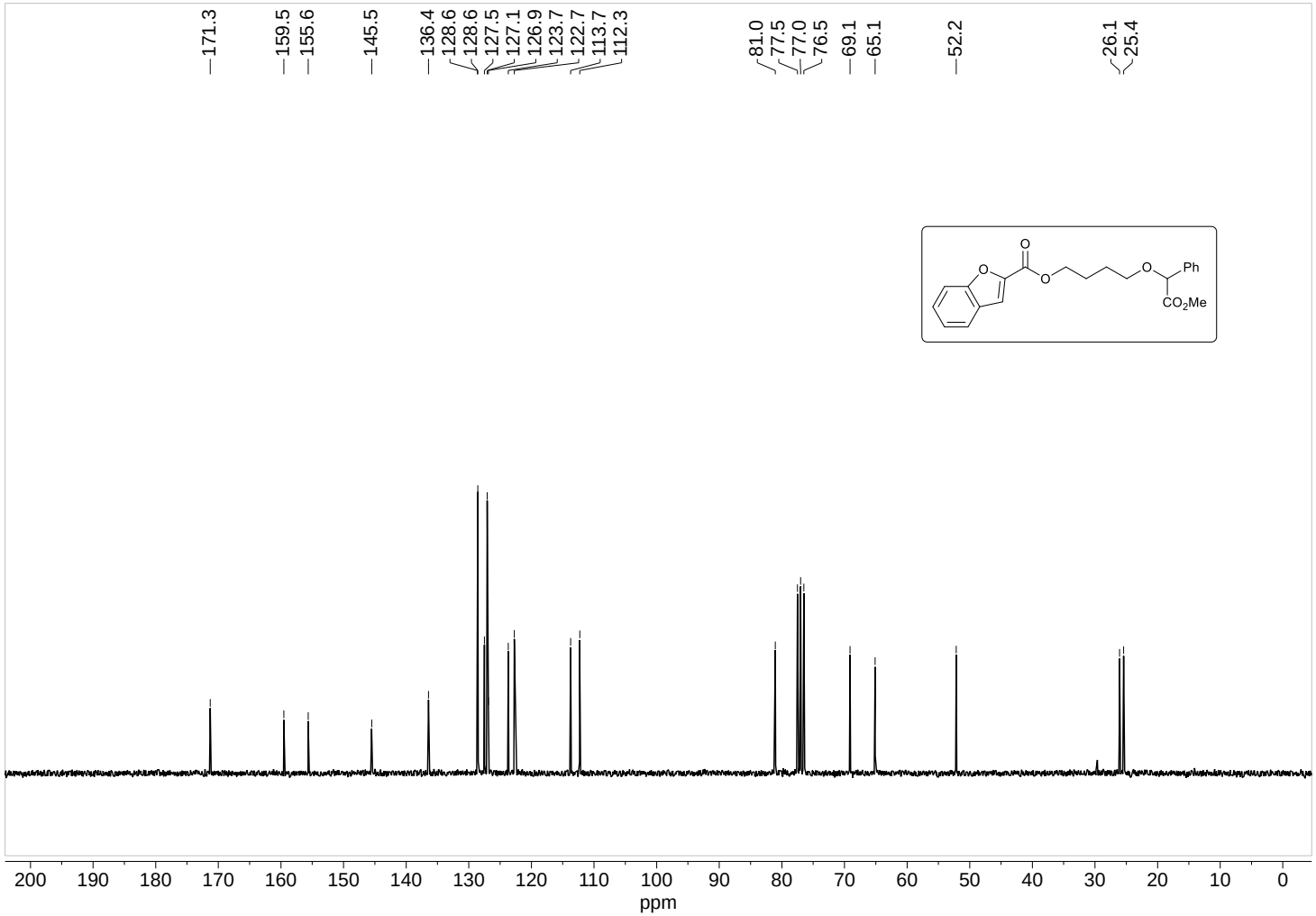
Molecule 8n - ^{13}C NMR (62.5 MHz, $CDCl_3$)



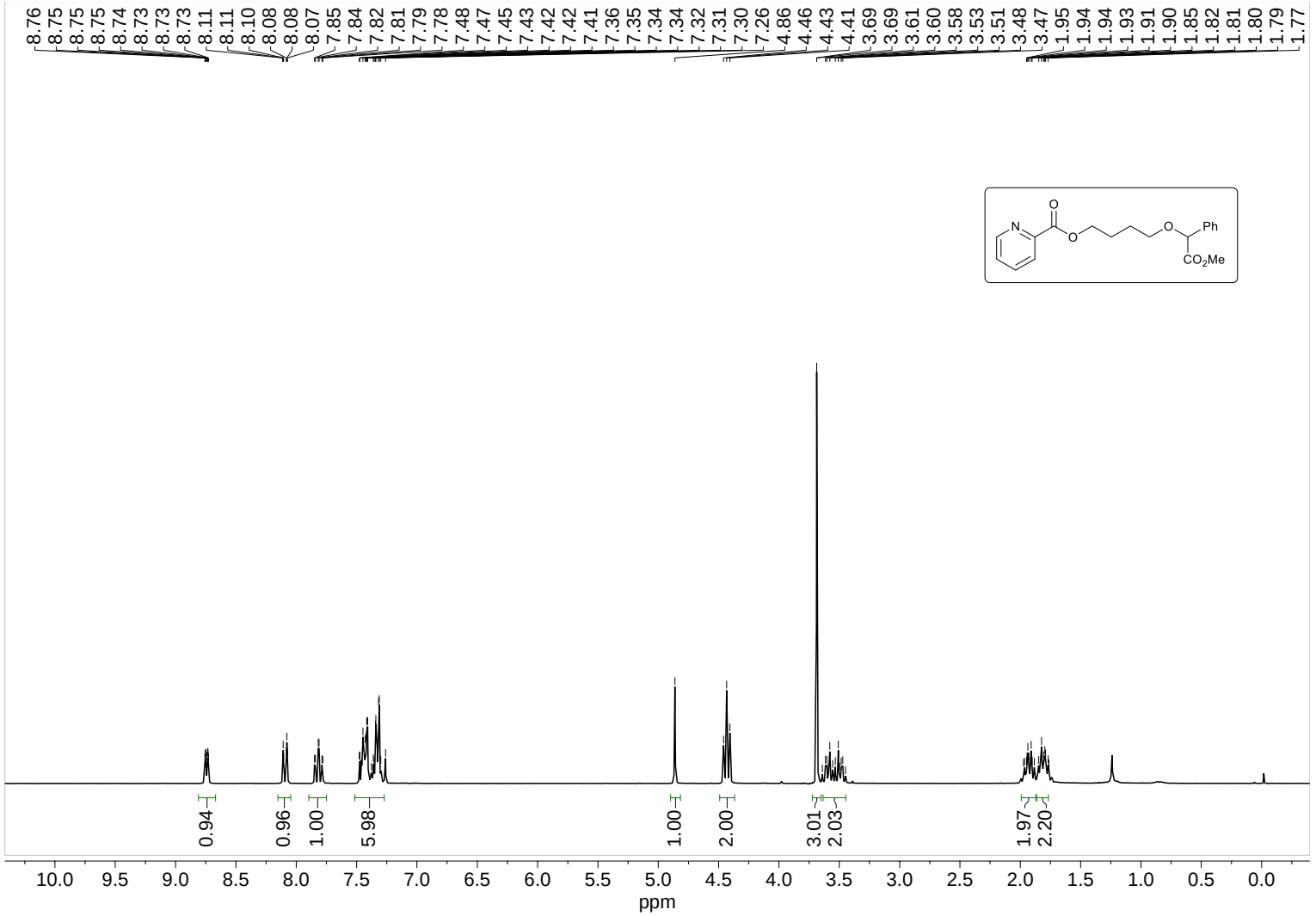
Molecule 8o - ^{1}H NMR (250 MHz, $CDCl_3$)



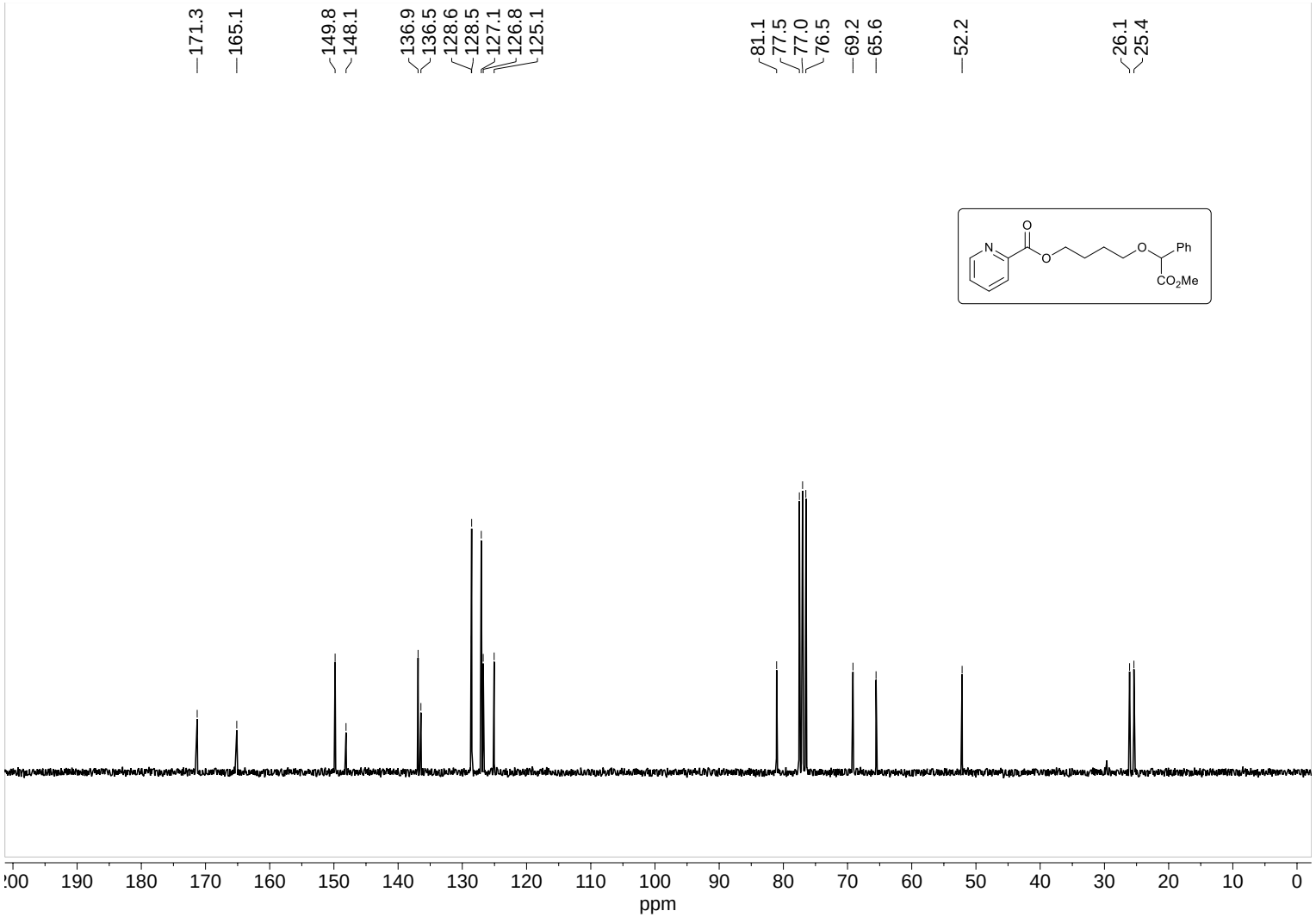
Molecule 8o - ^{13}C NMR (62.5 MHz, $CDCl_3$)



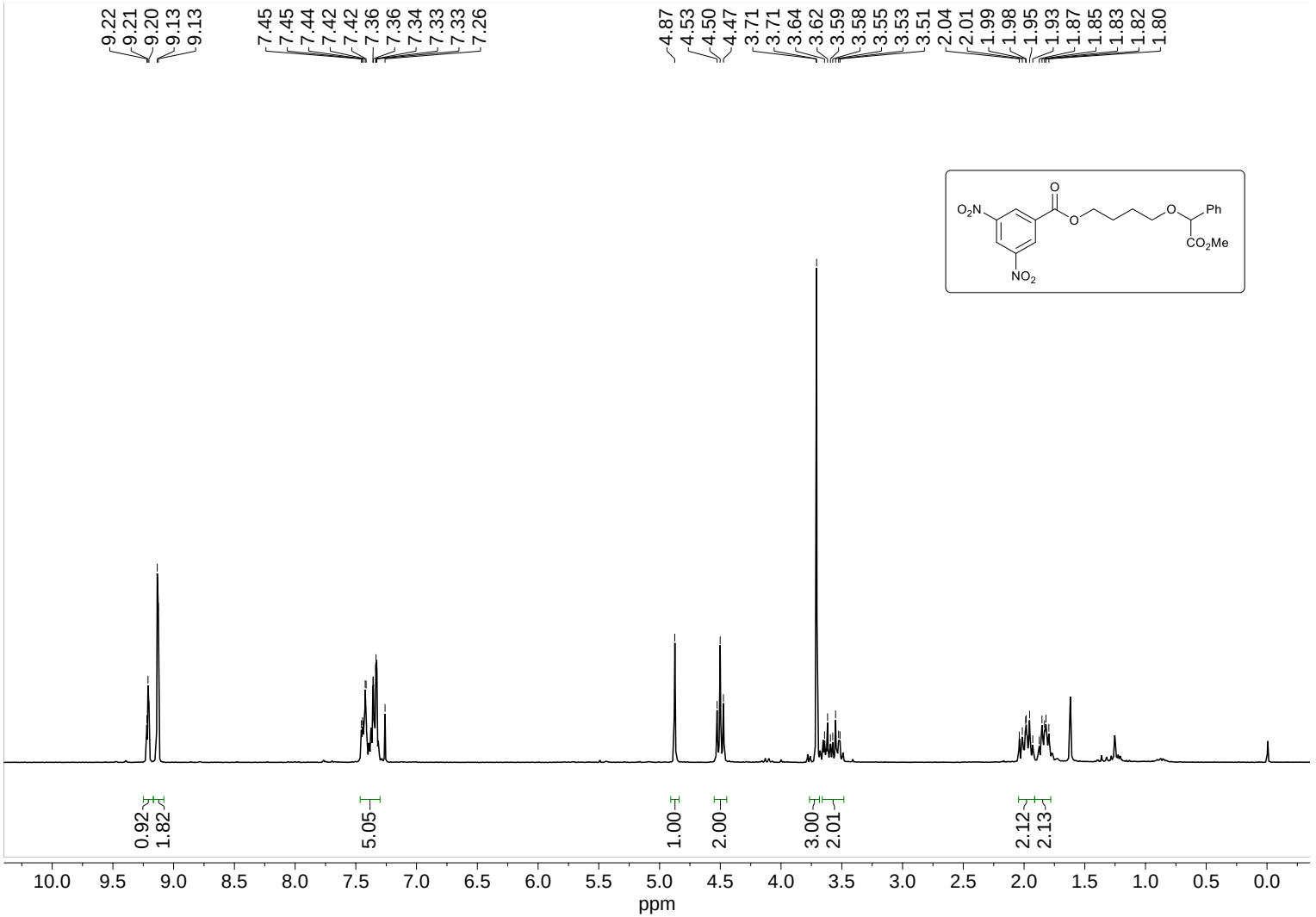
Molecule 8p - ^{1}H NMR (250 MHz, $CDCl_3$)



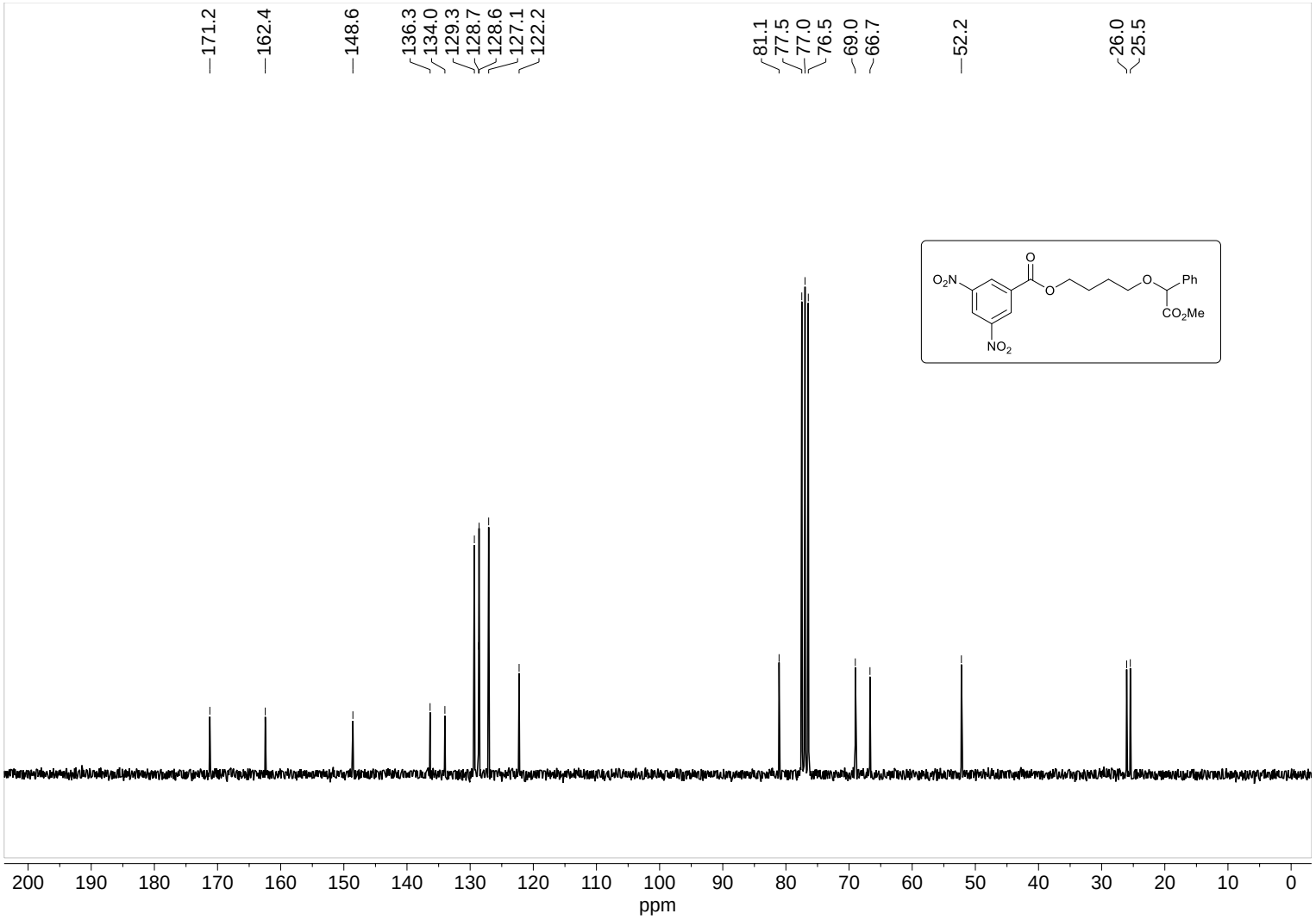
Molecule 8p - ^{13}C NMR (62.5 MHz, $CDCl_3$)



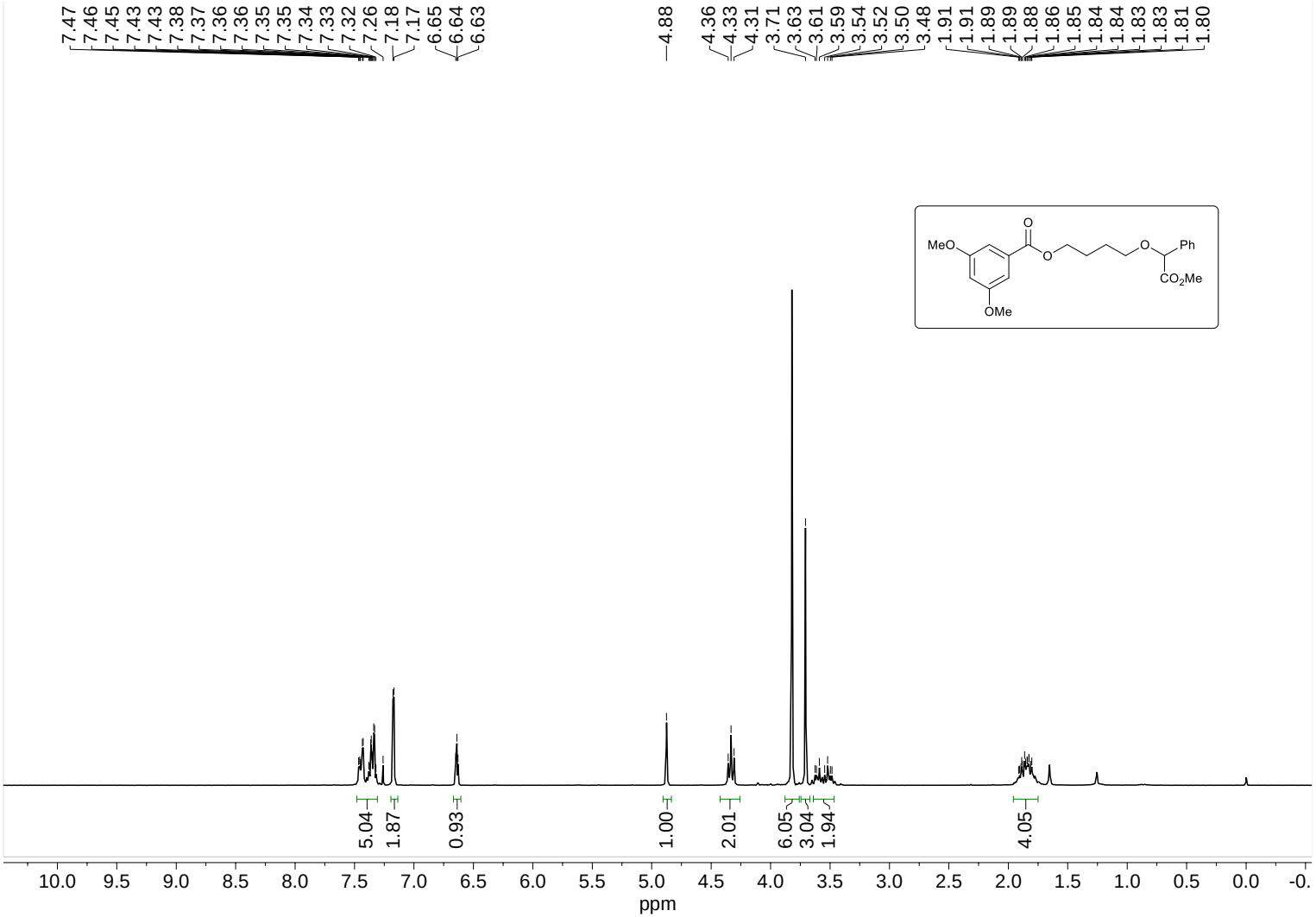
Molecule 8q - ^{1}H NMR (250 MHz, $CDCl_3$)



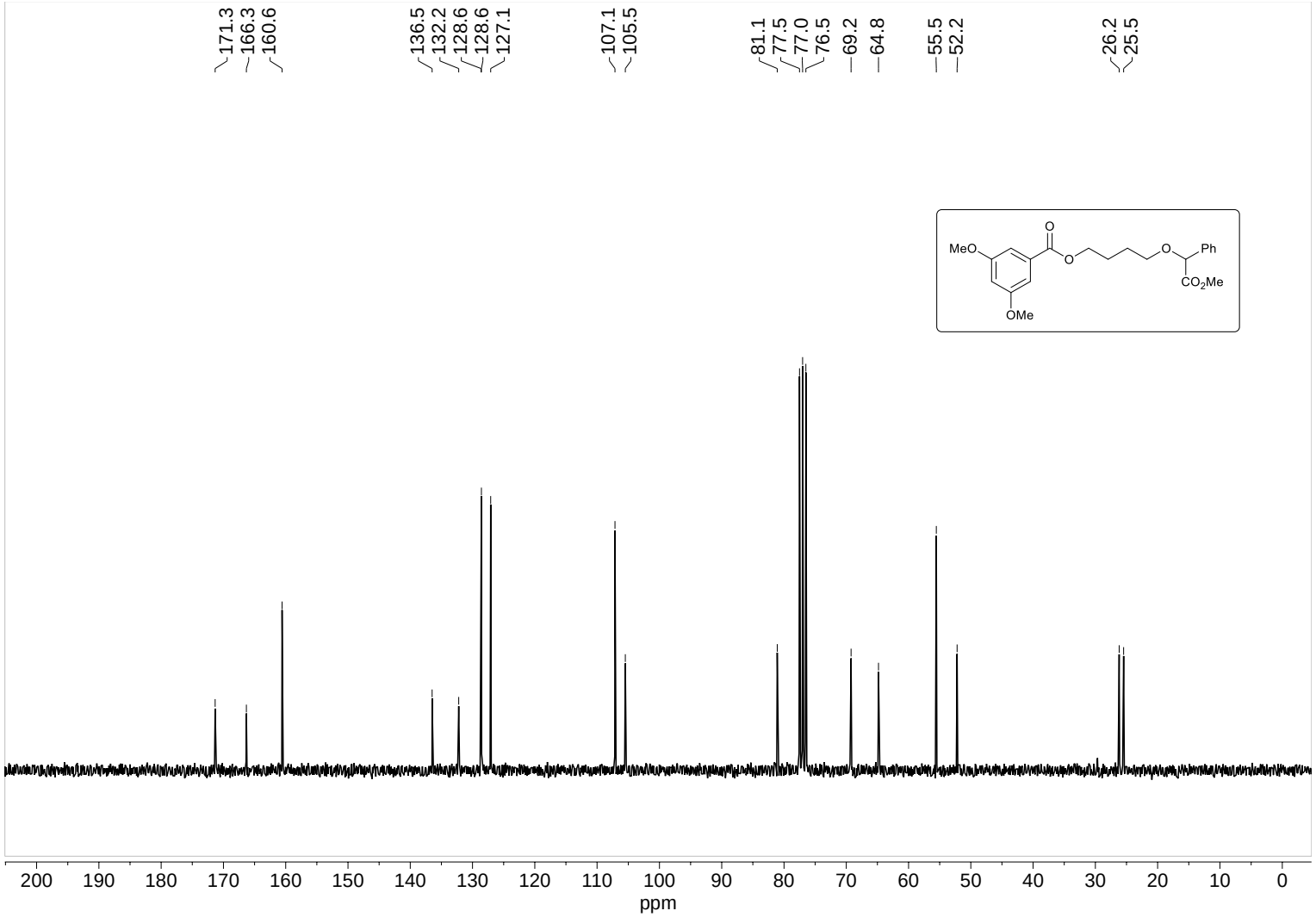
Molecule 8q - ^{13}C NMR (62.5 MHz, $CDCl_3$)



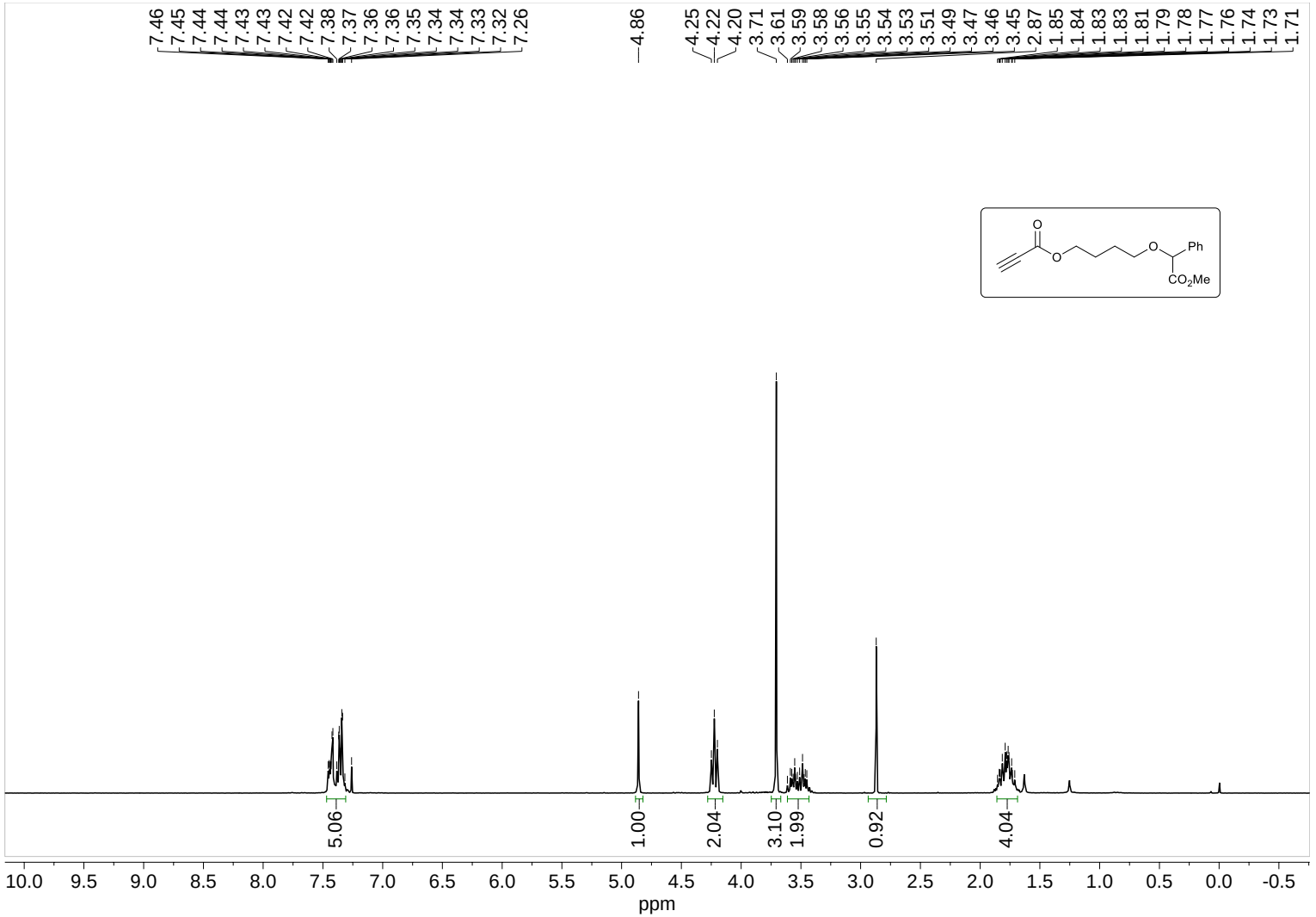
Molecule 8r - ^{1}H NMR (250 MHz, $CDCl_3$)



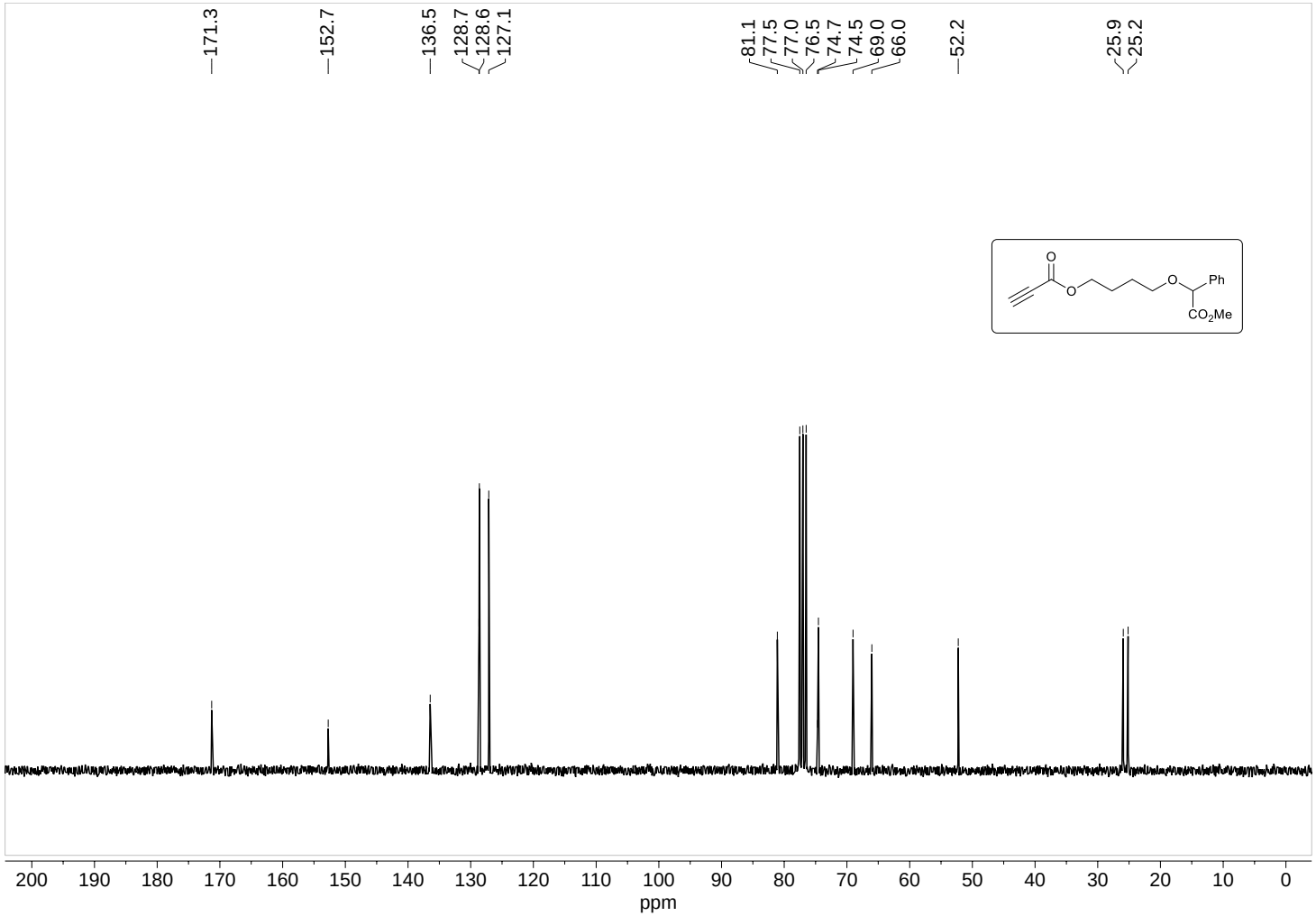
Molecule 8r - ^{13}C NMR (62.5 MHz, $CDCl_3$)



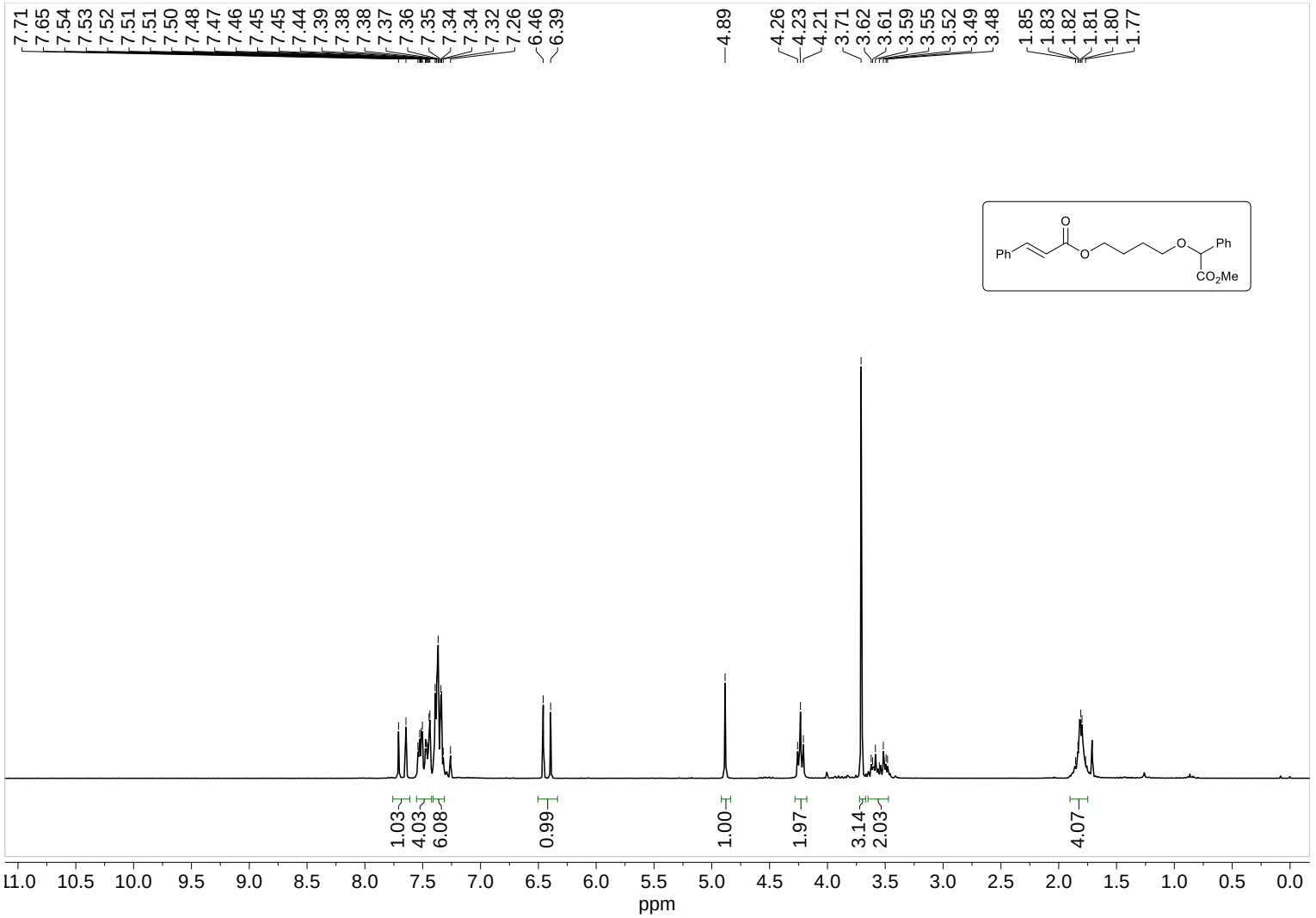
Molecule 8s - ^{1}H NMR (250 MHz, $CDCl_3$)



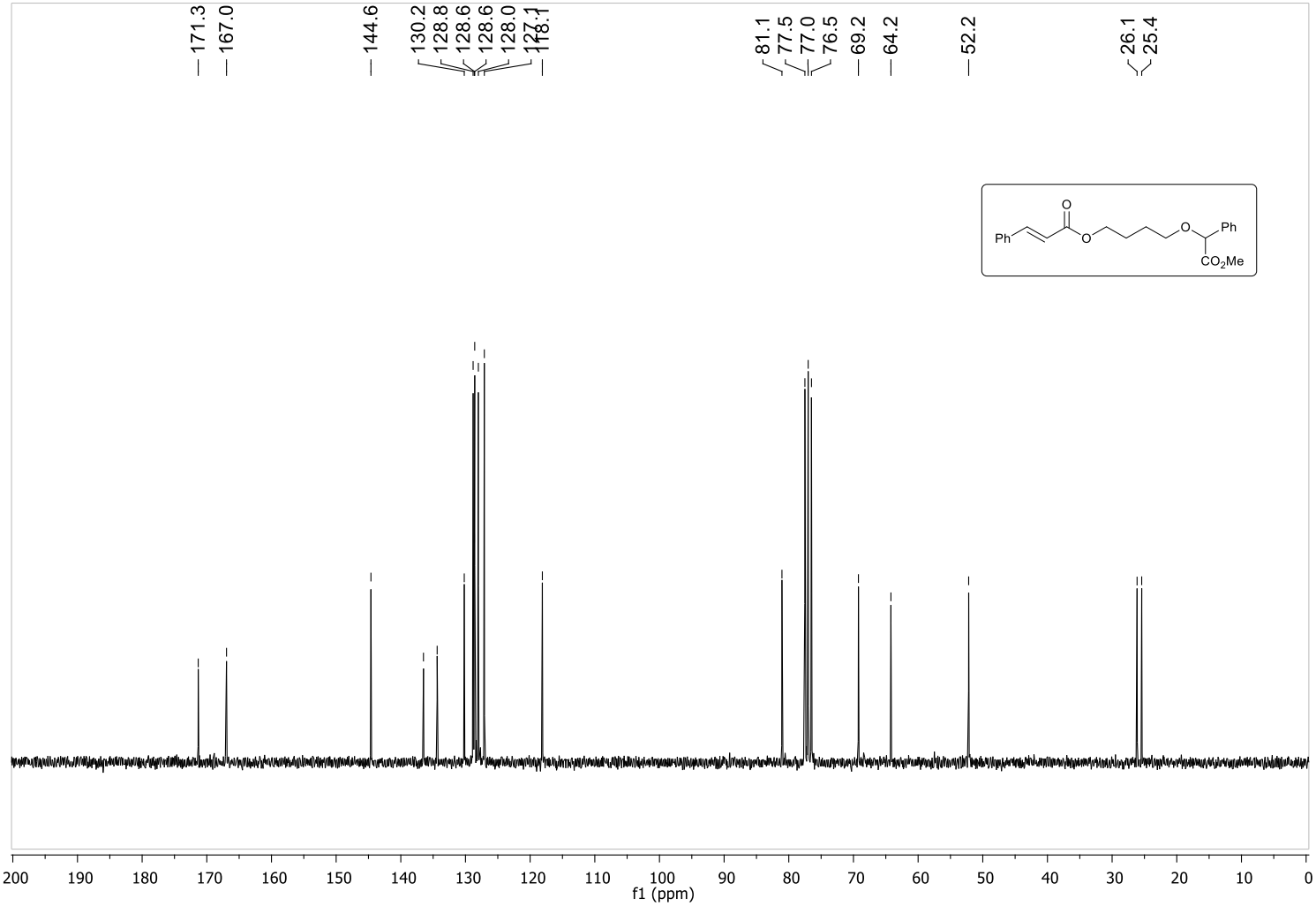
Molecule 8s - ^{13}C NMR (62.5 MHz, $CDCl_3$)



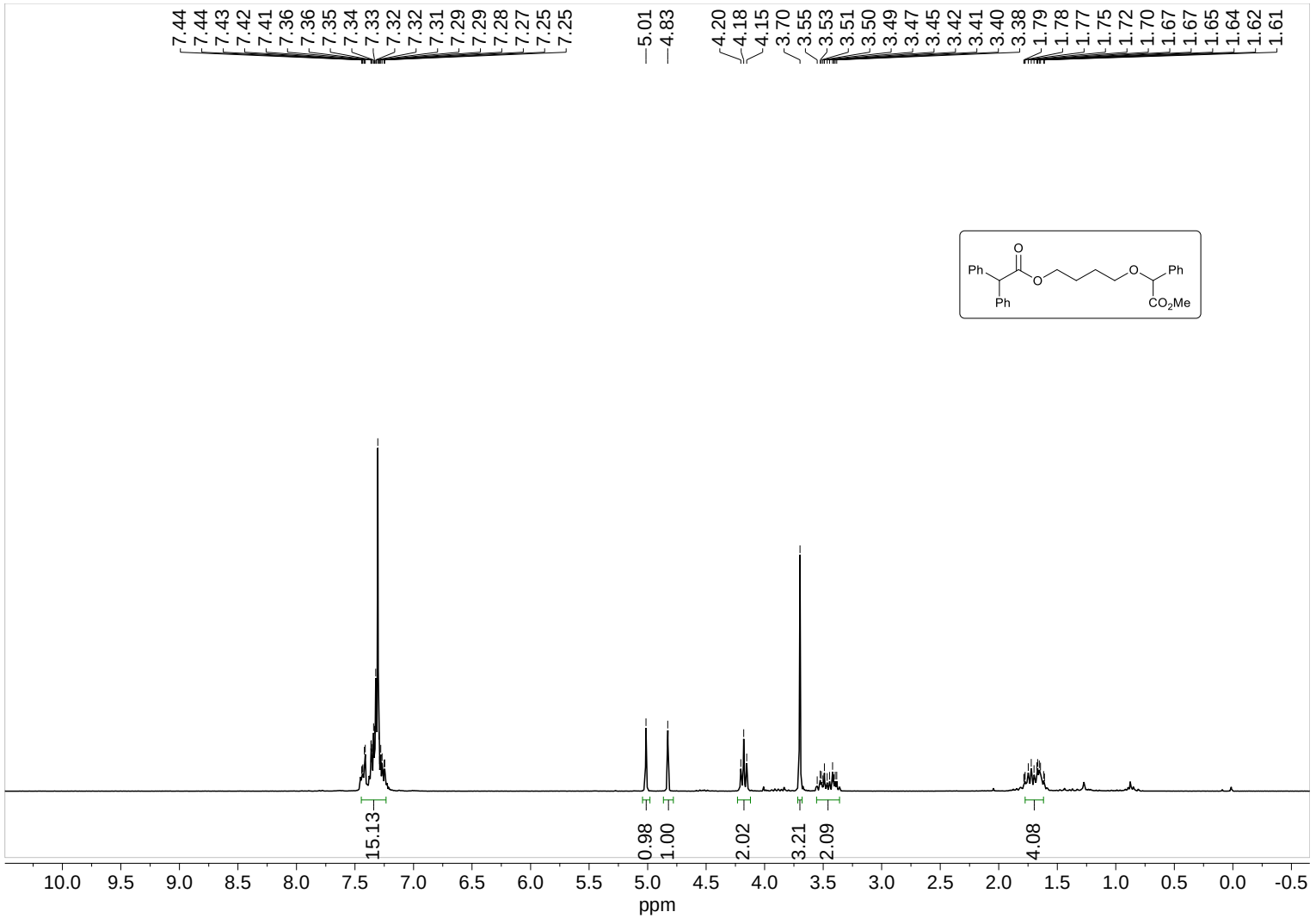
Molecule 8t - ^{1}H NMR (250 MHz, $CDCl_3$)



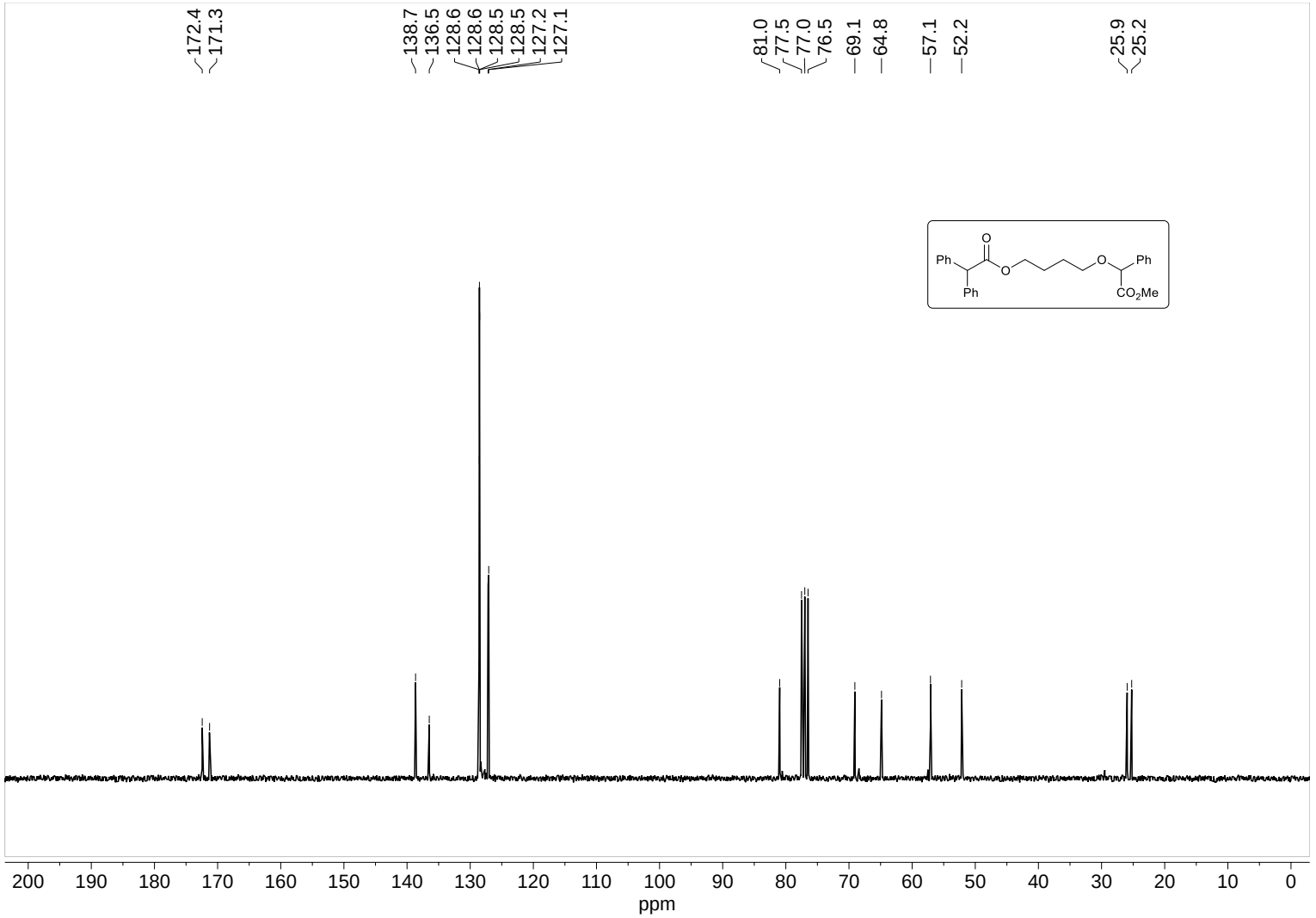
Molecule 8t - ^{13}C NMR (62.5 MHz, $CDCl_3$)



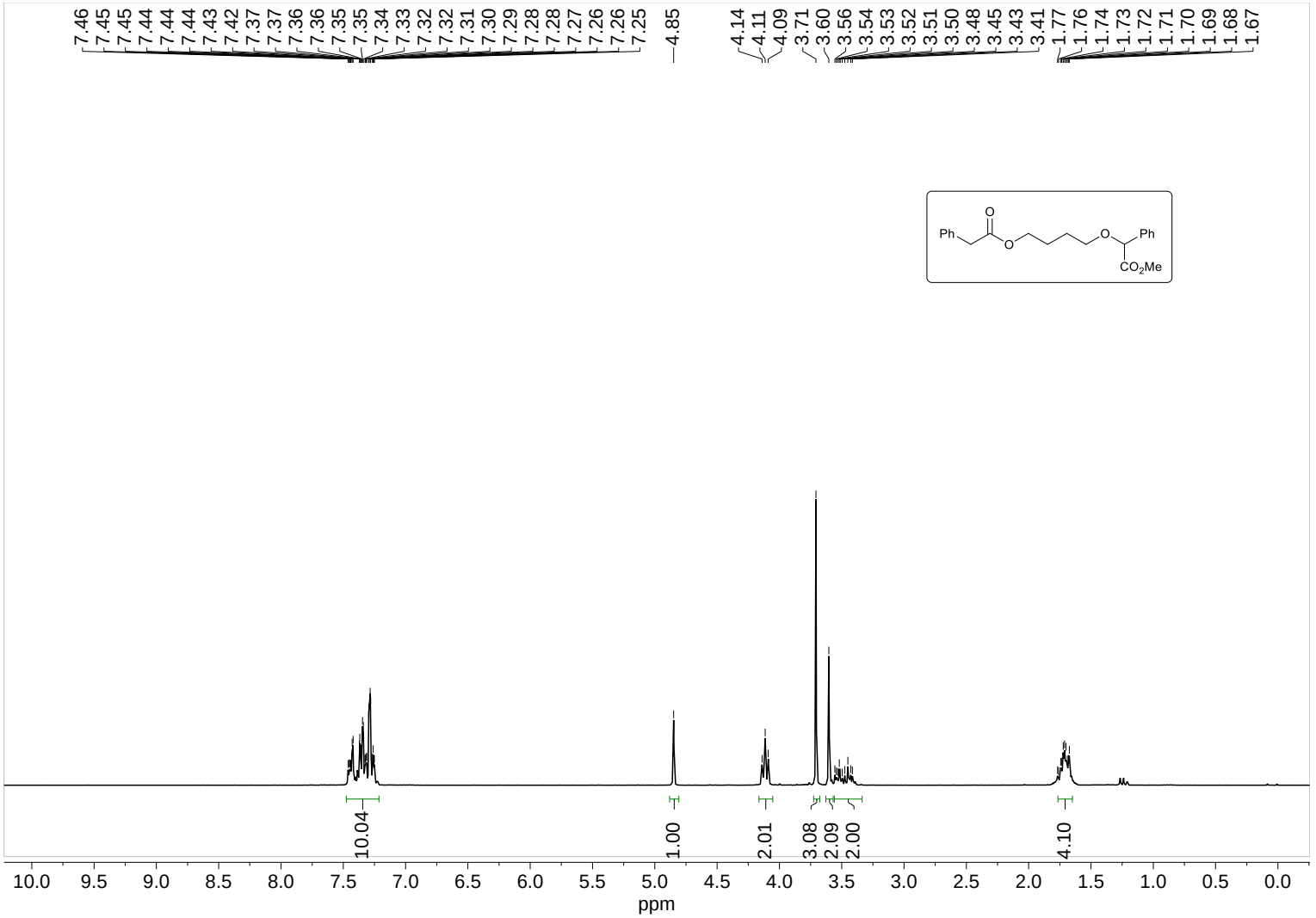
Molecule 8u - ^{1}H NMR (250 MHz, $CDCl_3$)



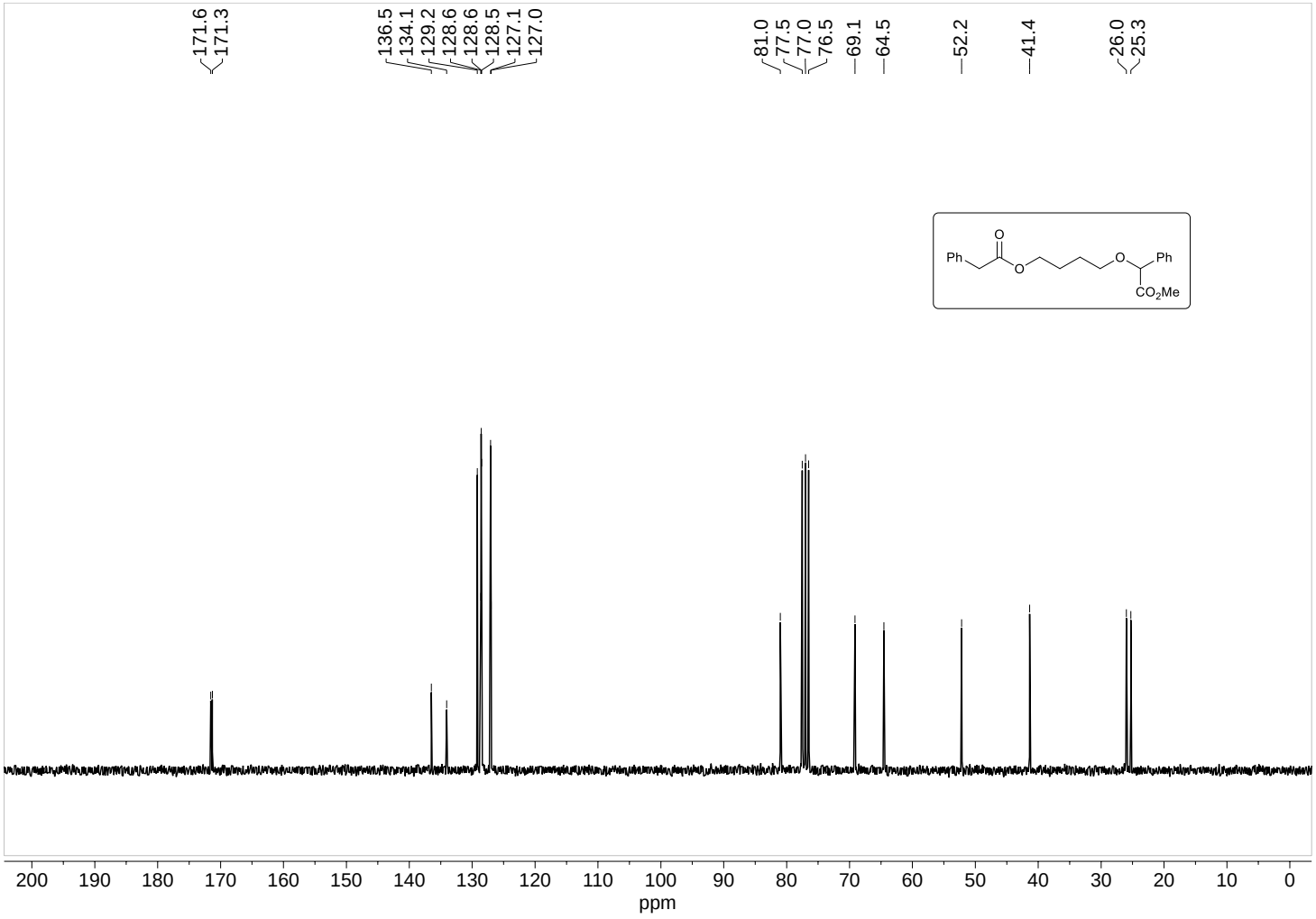
Molecule 8u - ^{13}C NMR (62.5 MHz, $CDCl_3$)



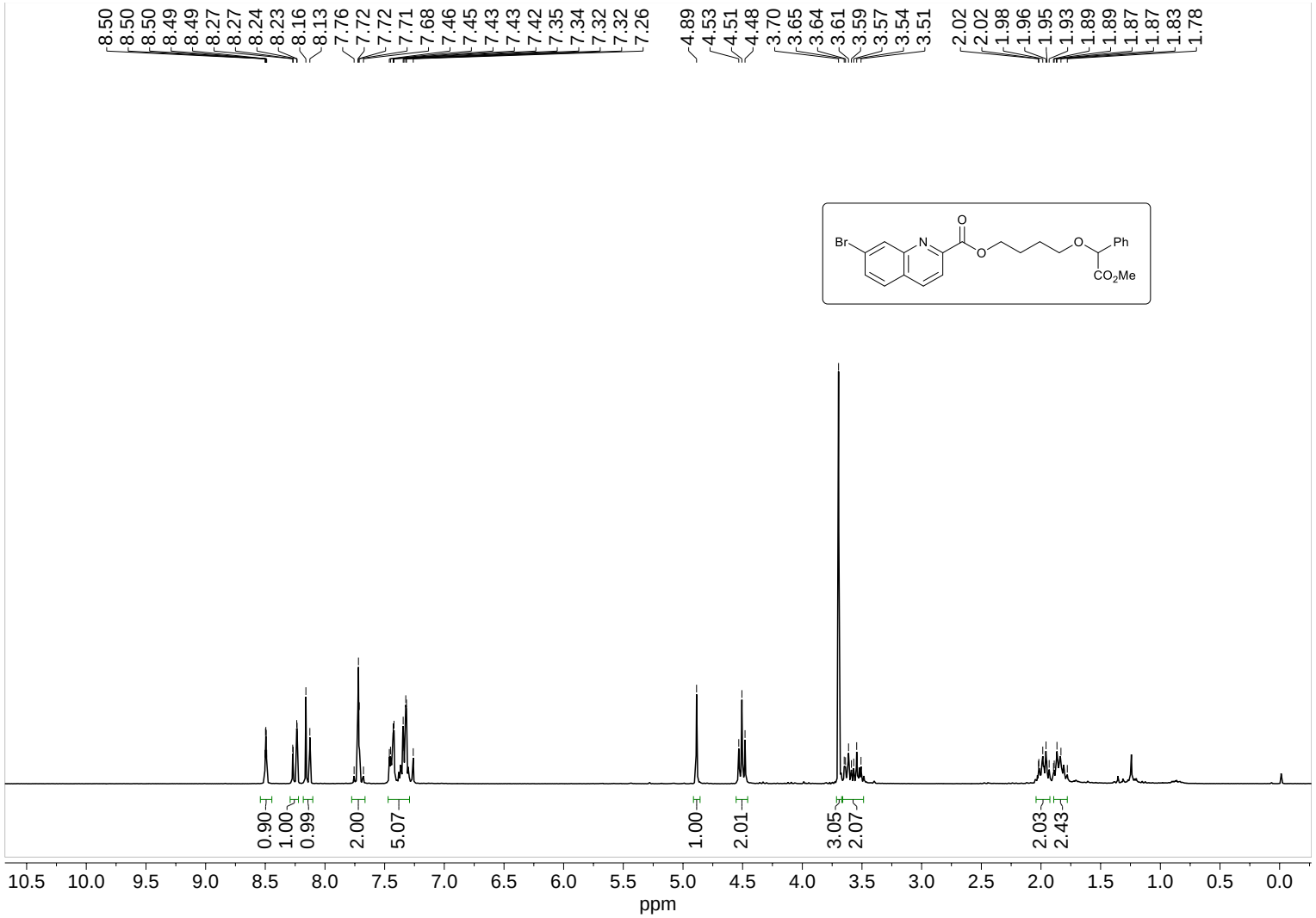
Molecule 8v - ^{1}H NMR (250 MHz, $CDCl_3$)



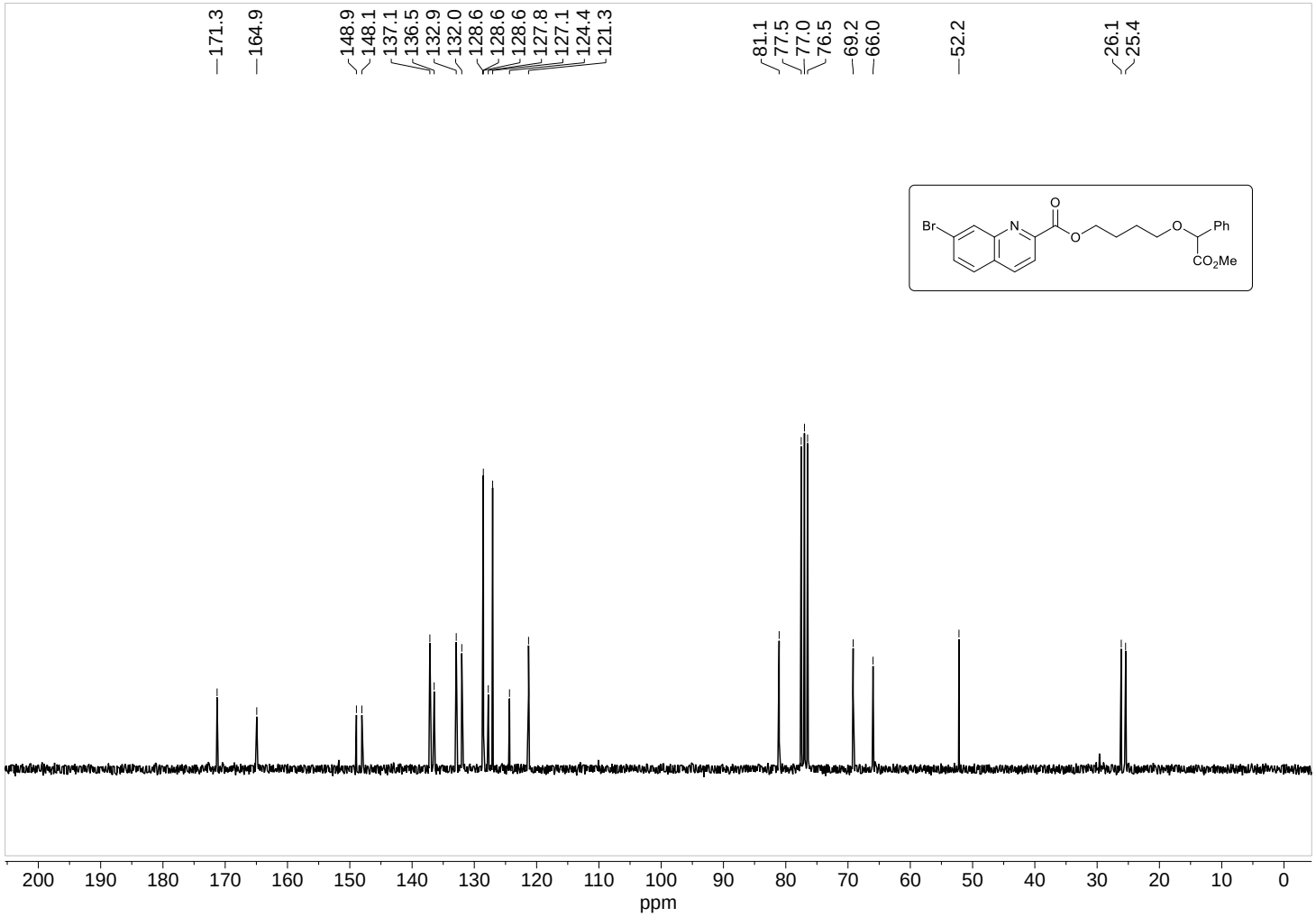
Molecule 8v - ^{13}C NMR (62.5 MHz, $CDCl_3$)



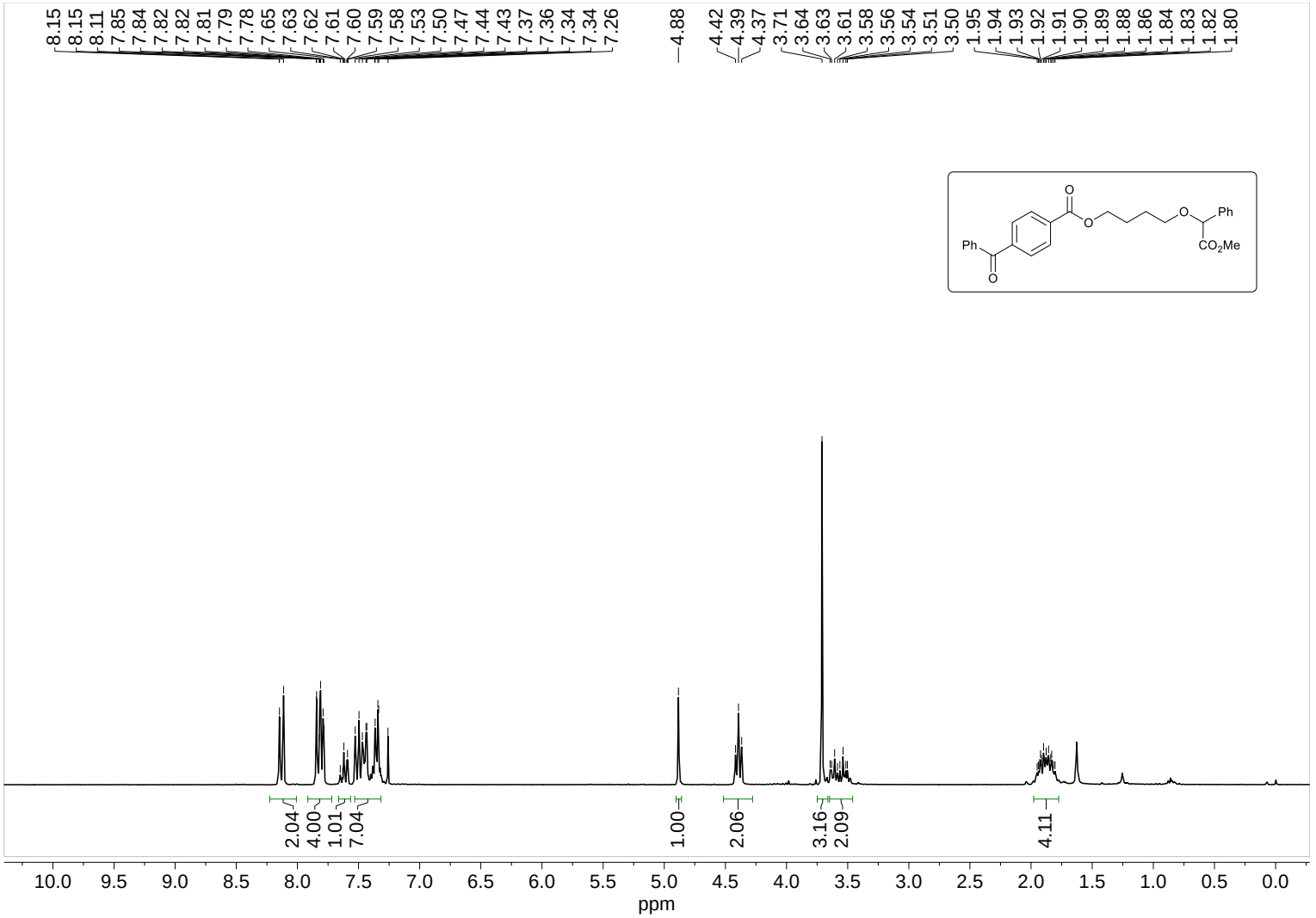
Molecule 8w - ^{1}H NMR (250 MHz, $CDCl_3$)



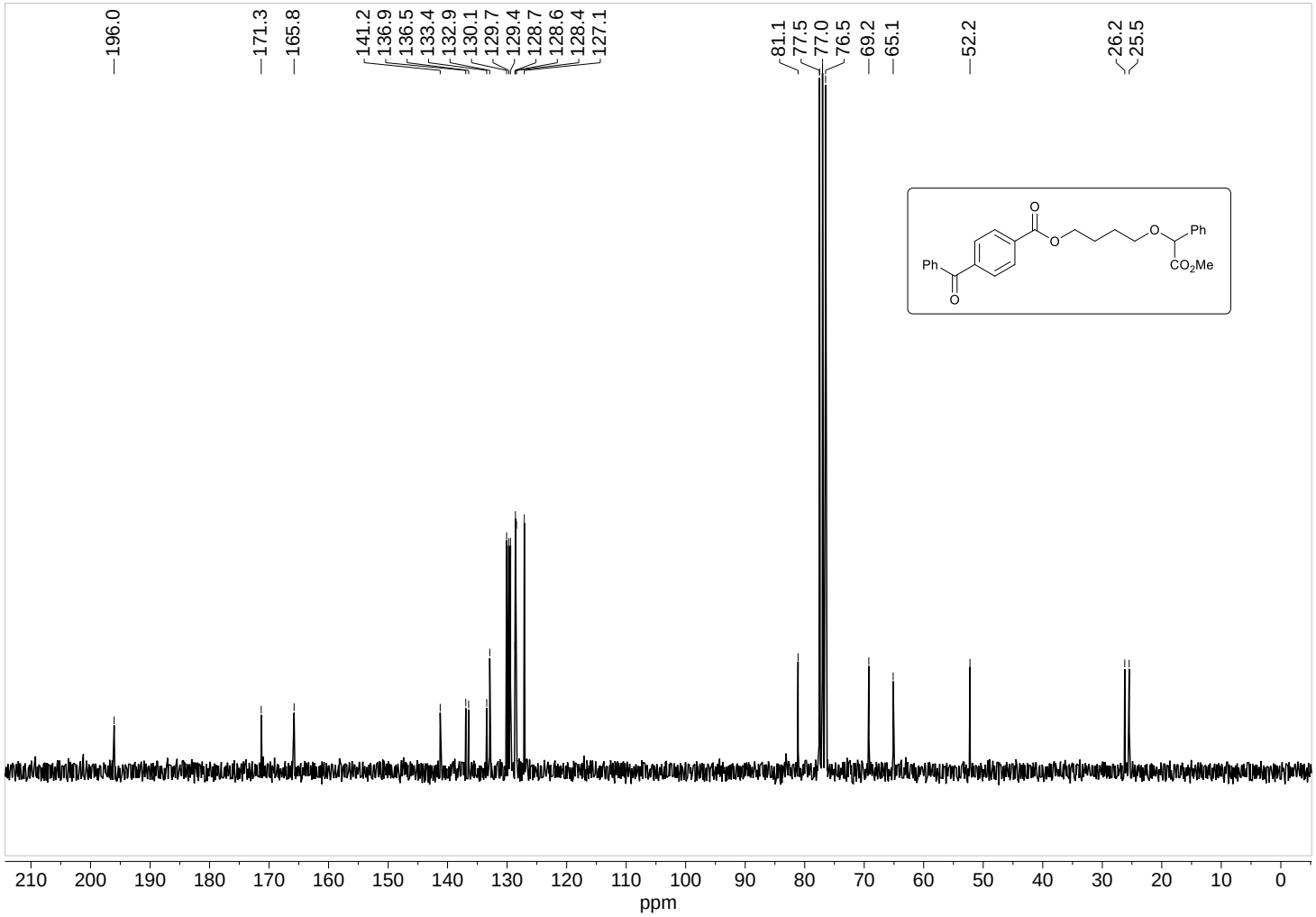
Molecule 8w - ^{13}C NMR (62.5 MHz, $CDCl_3$)



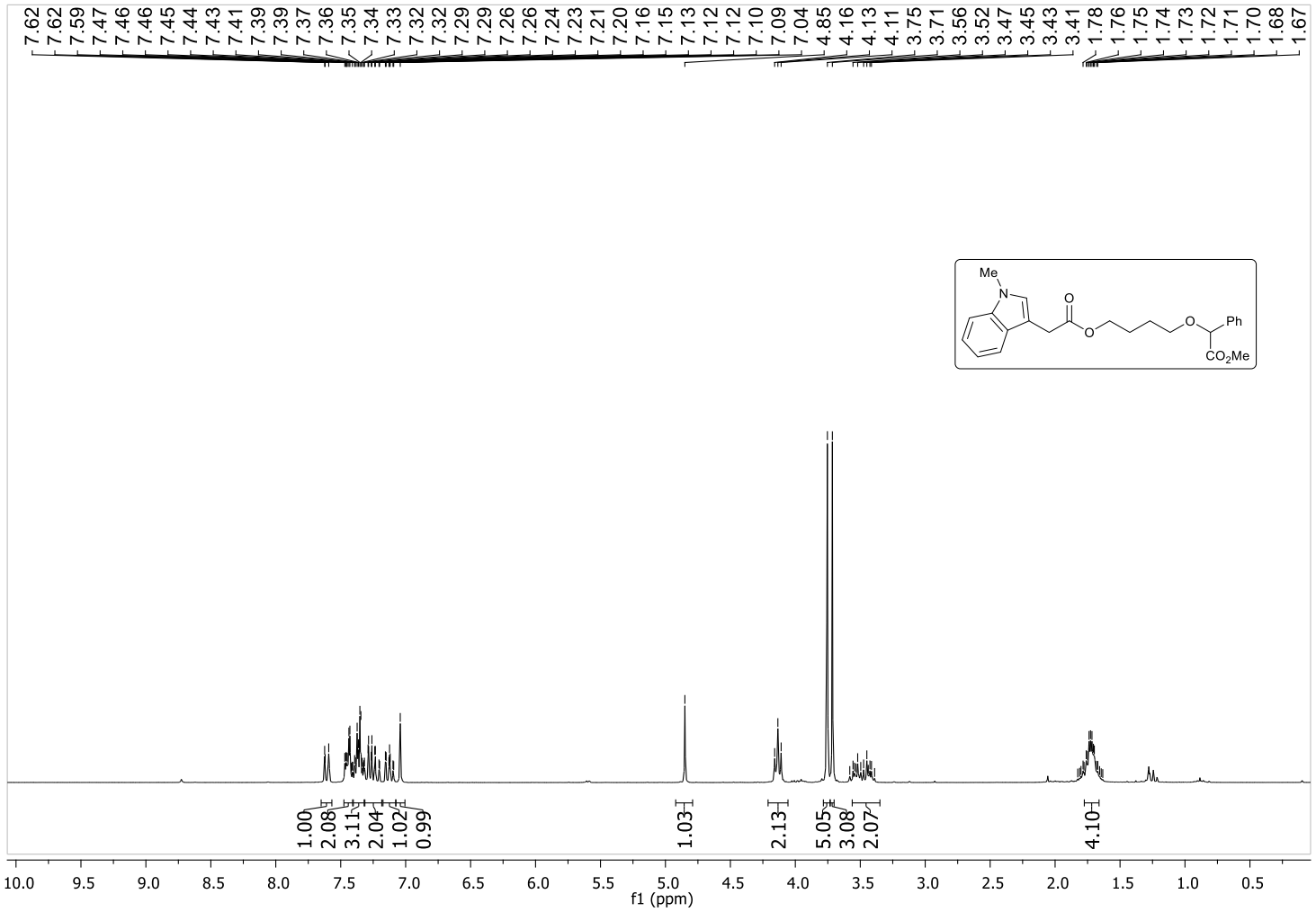
Molecule 8x - ^{1}H NMR (250 MHz, $CDCl_3$)



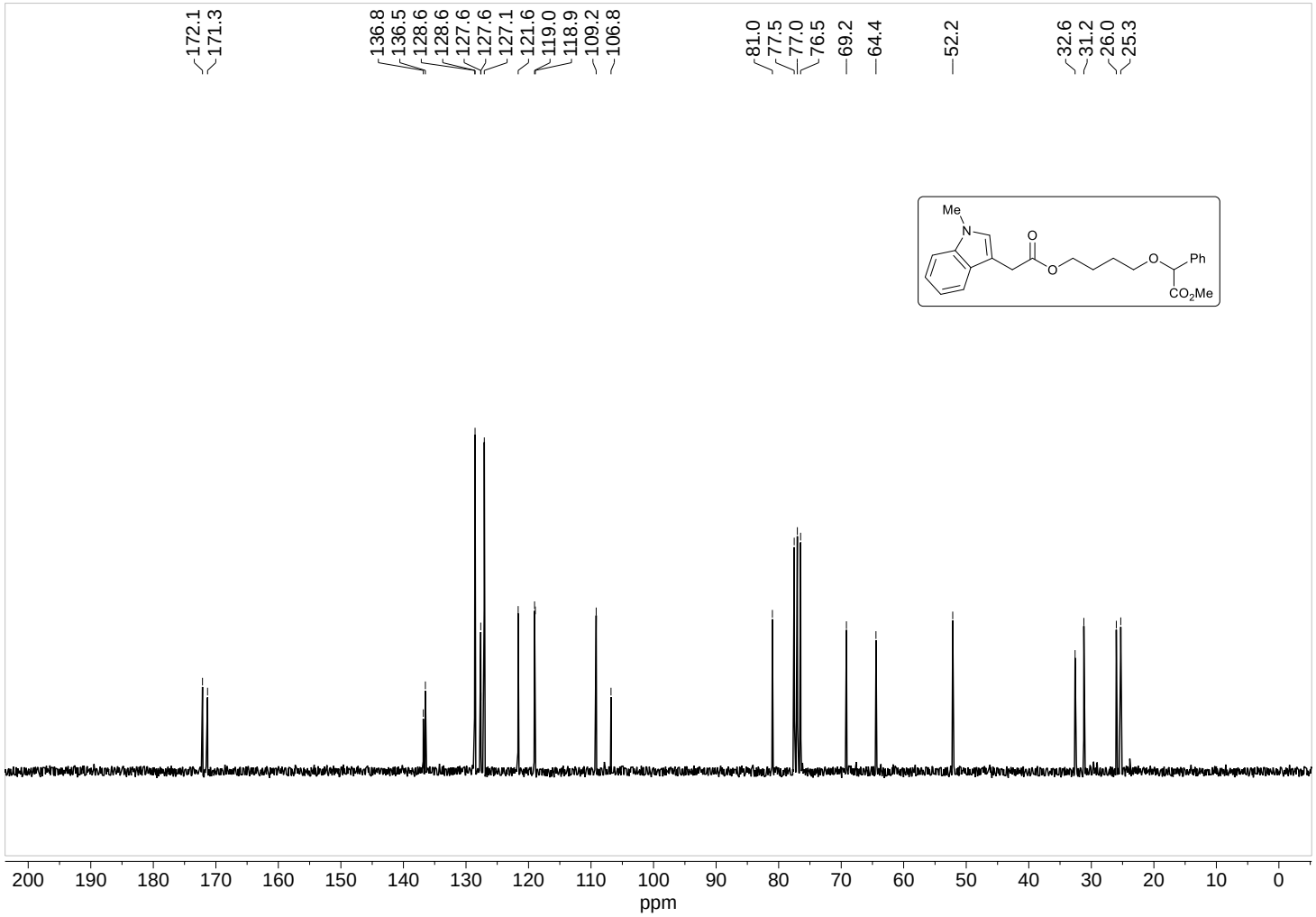
Molecule 8x - ^{13}C NMR (62.5 MHz, $CDCl_3$)



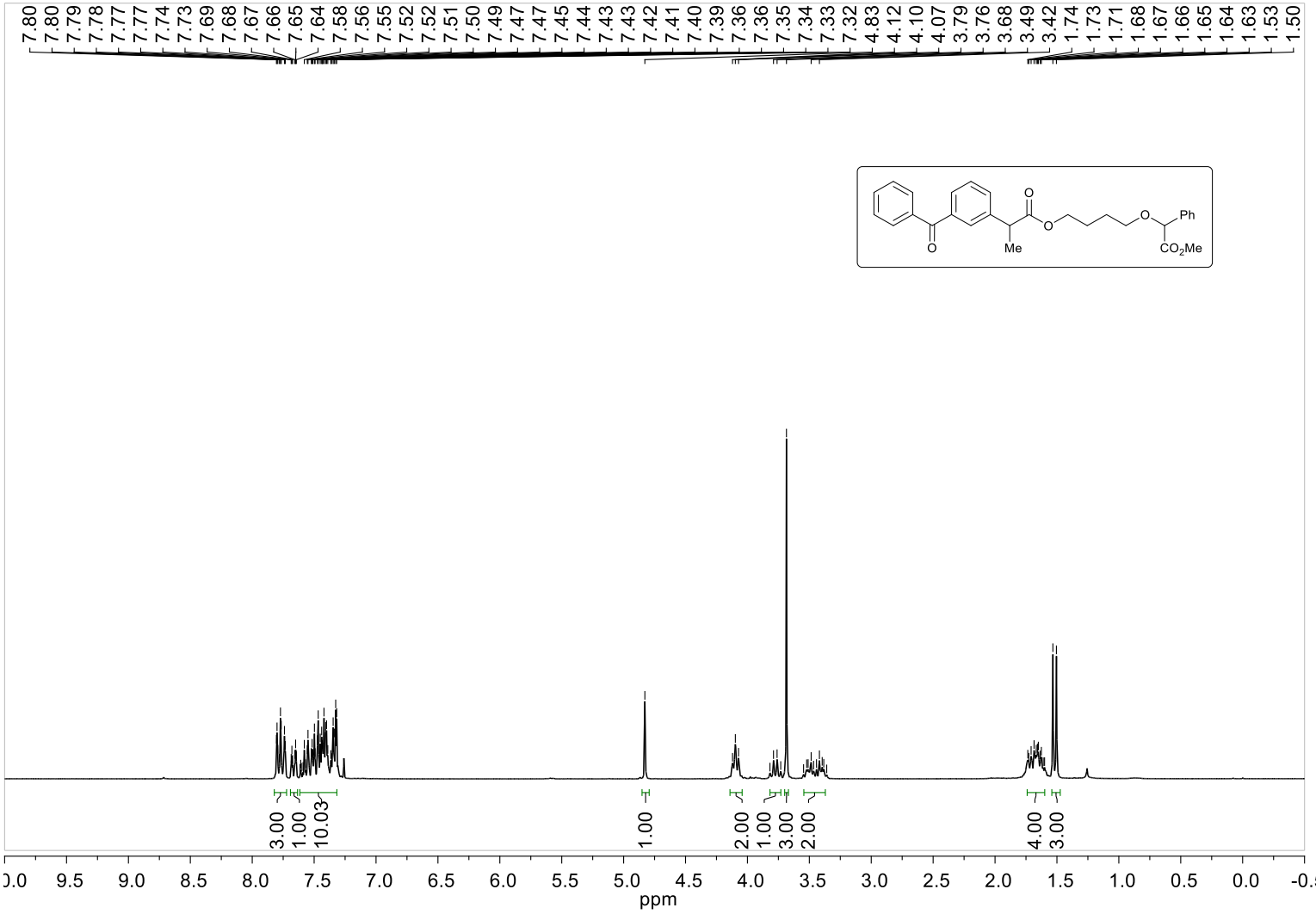
Molecule 8y - ^{1}H NMR (250 MHz, $CDCl_3$)



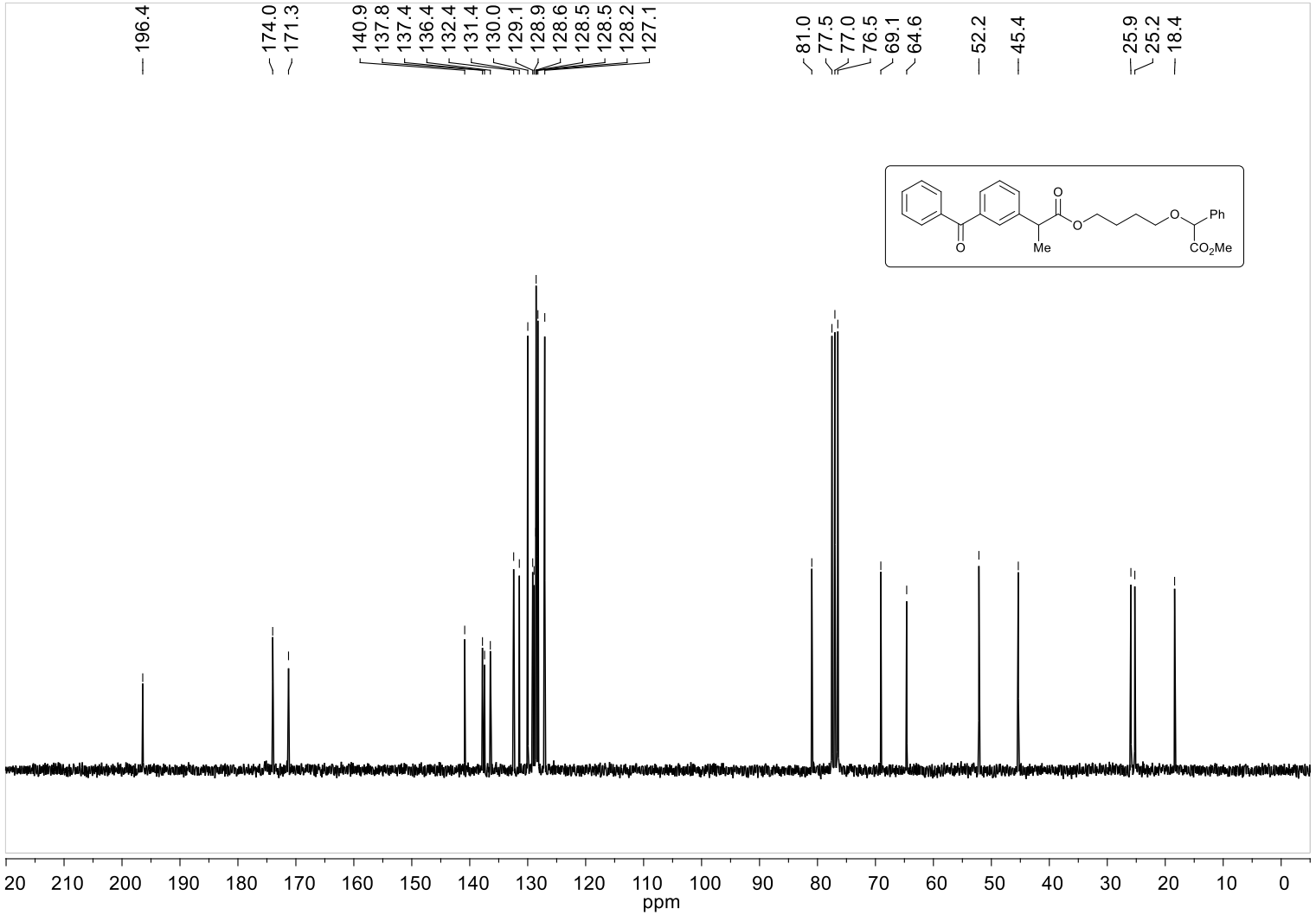
Molecule 8y - ^{13}C NMR (62.5 MHz, $CDCl_3$)



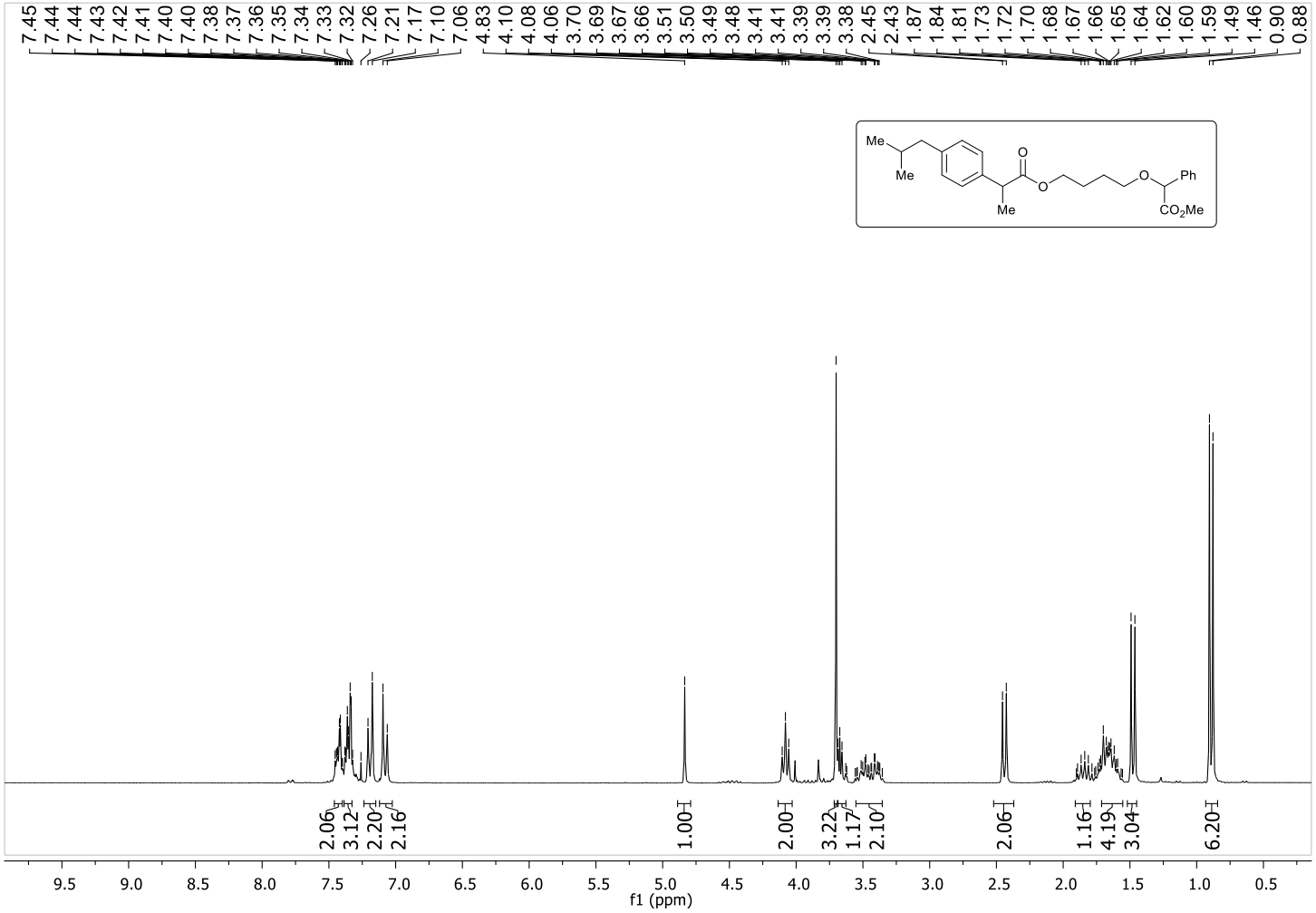
Molecule 8z - ^{1}H NMR (250 MHz, $CDCl_3$)



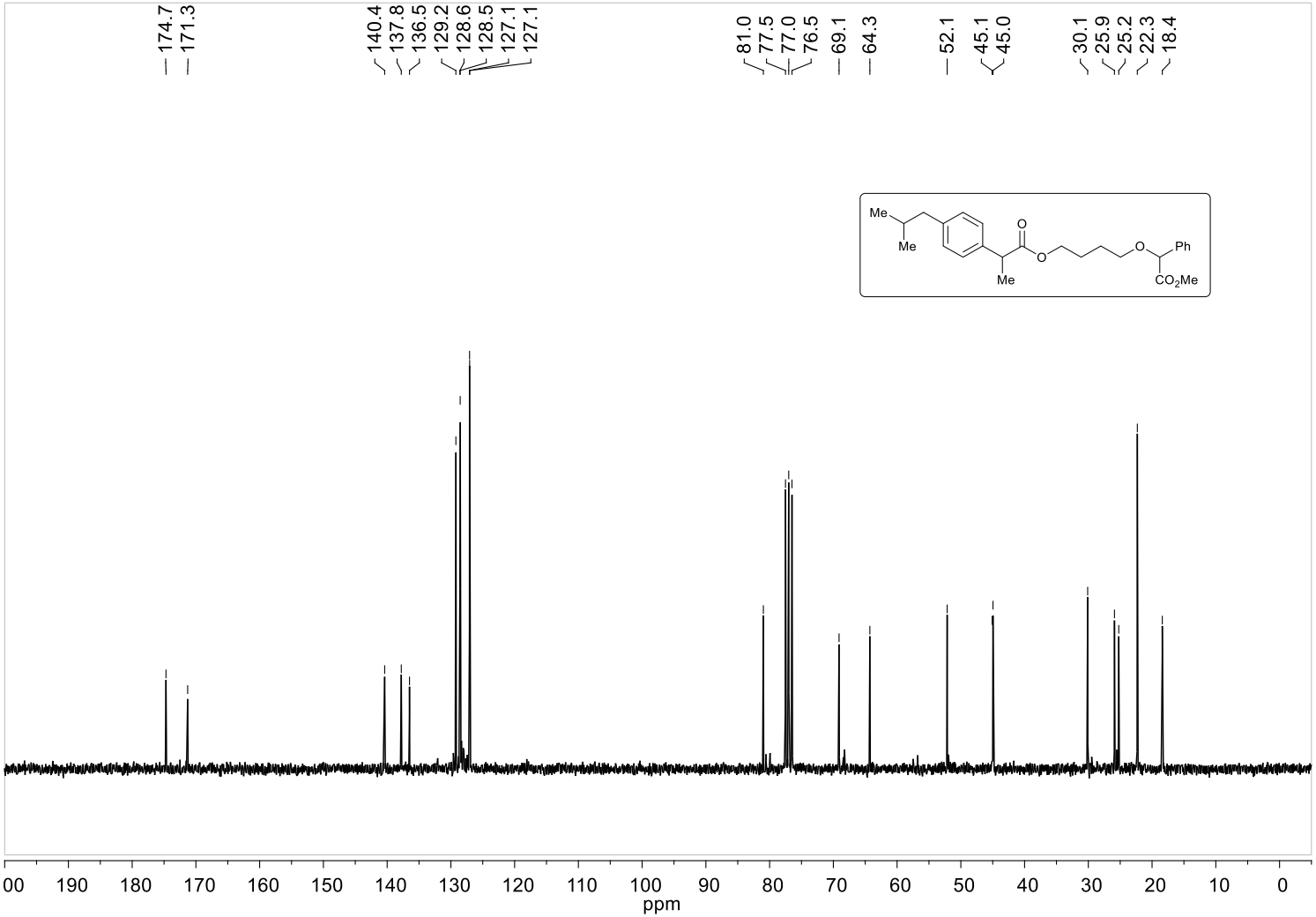
Molecule 8z - ^{13}C NMR (62.5 MHz, $CDCl_3$)



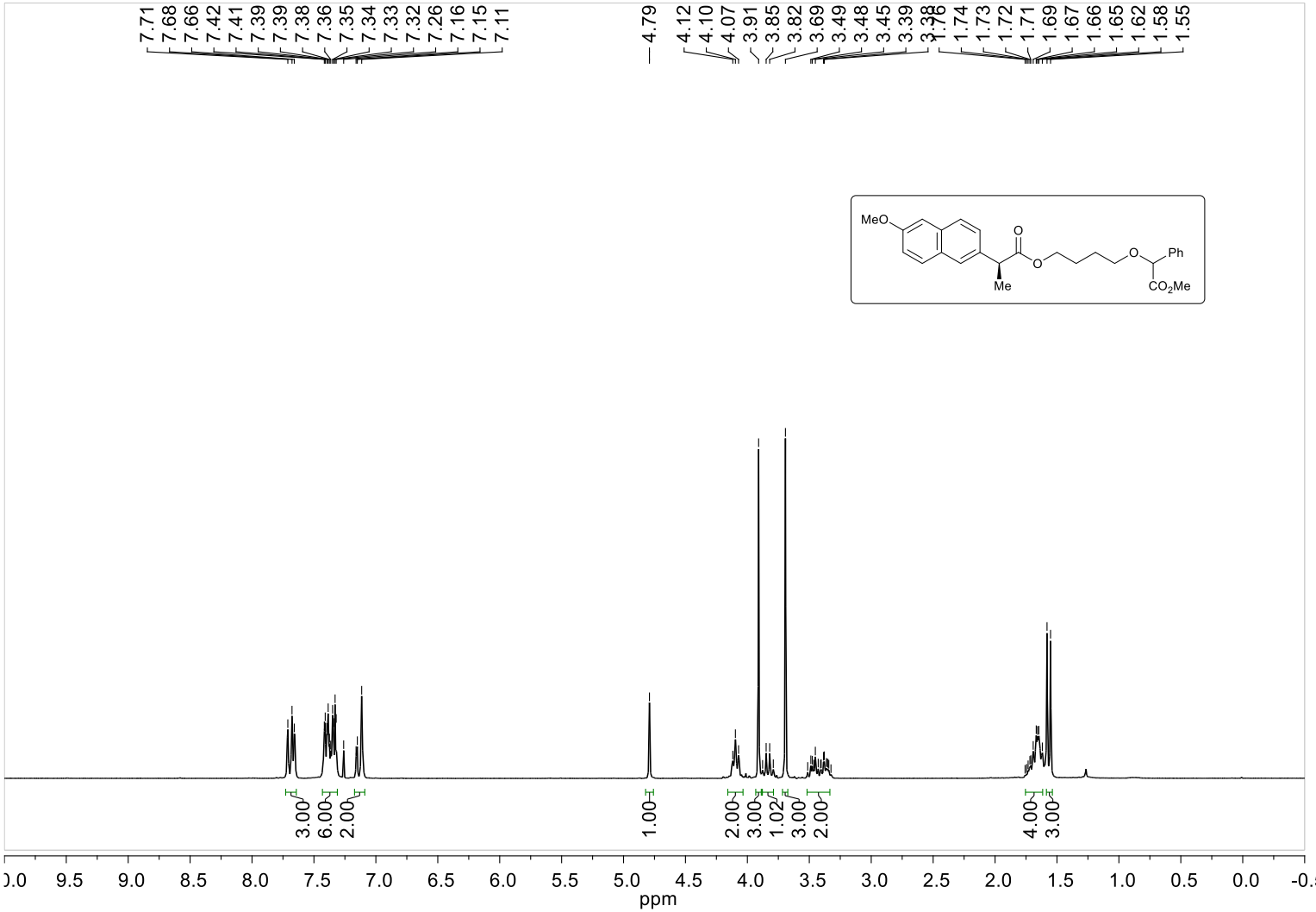
Molecule 8aa - ^{1}H NMR (250 MHz, $CDCl_3$)



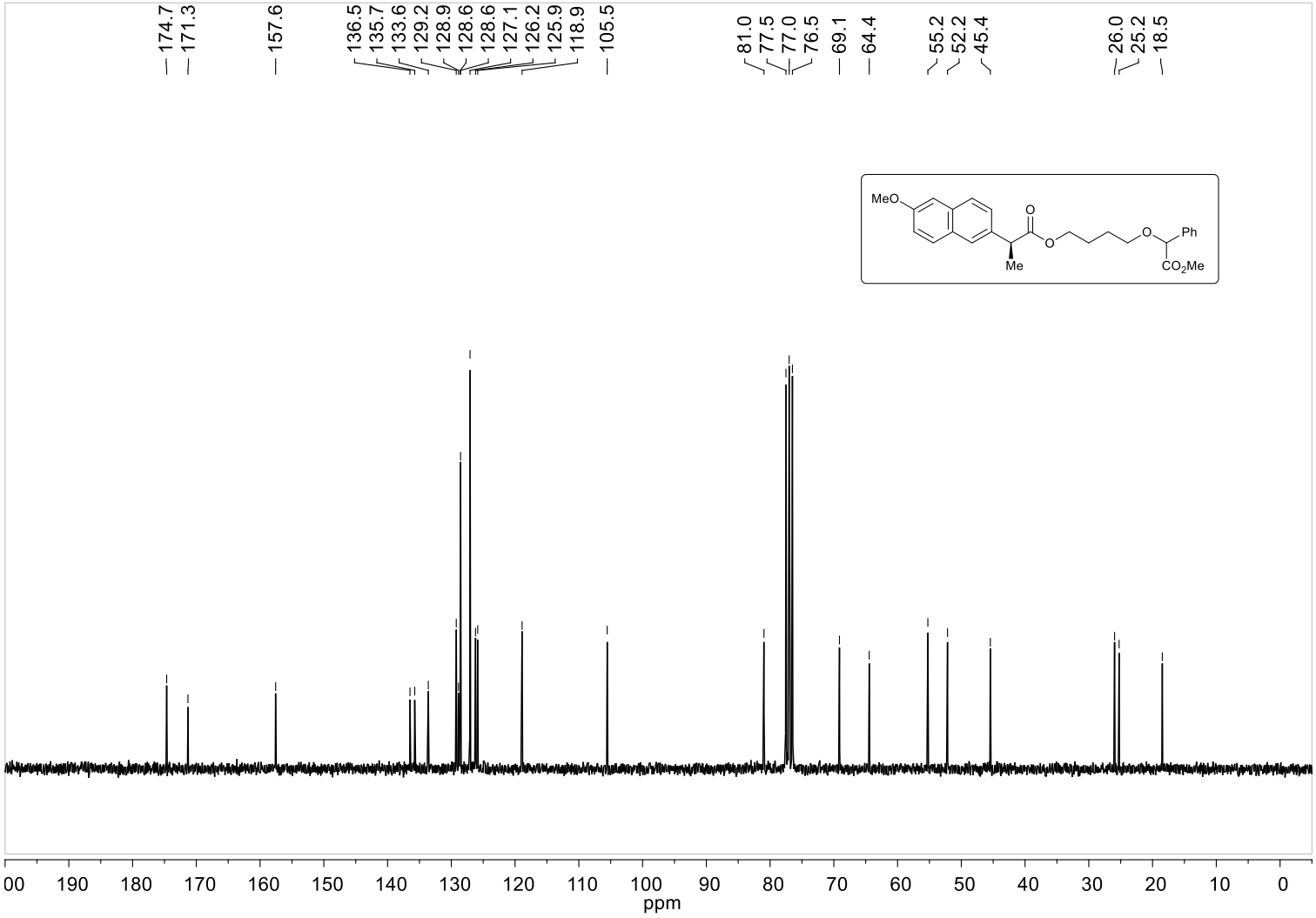
Molecule 8aa - ^{13}C NMR (62.5 MHz, $CDCl_3$)



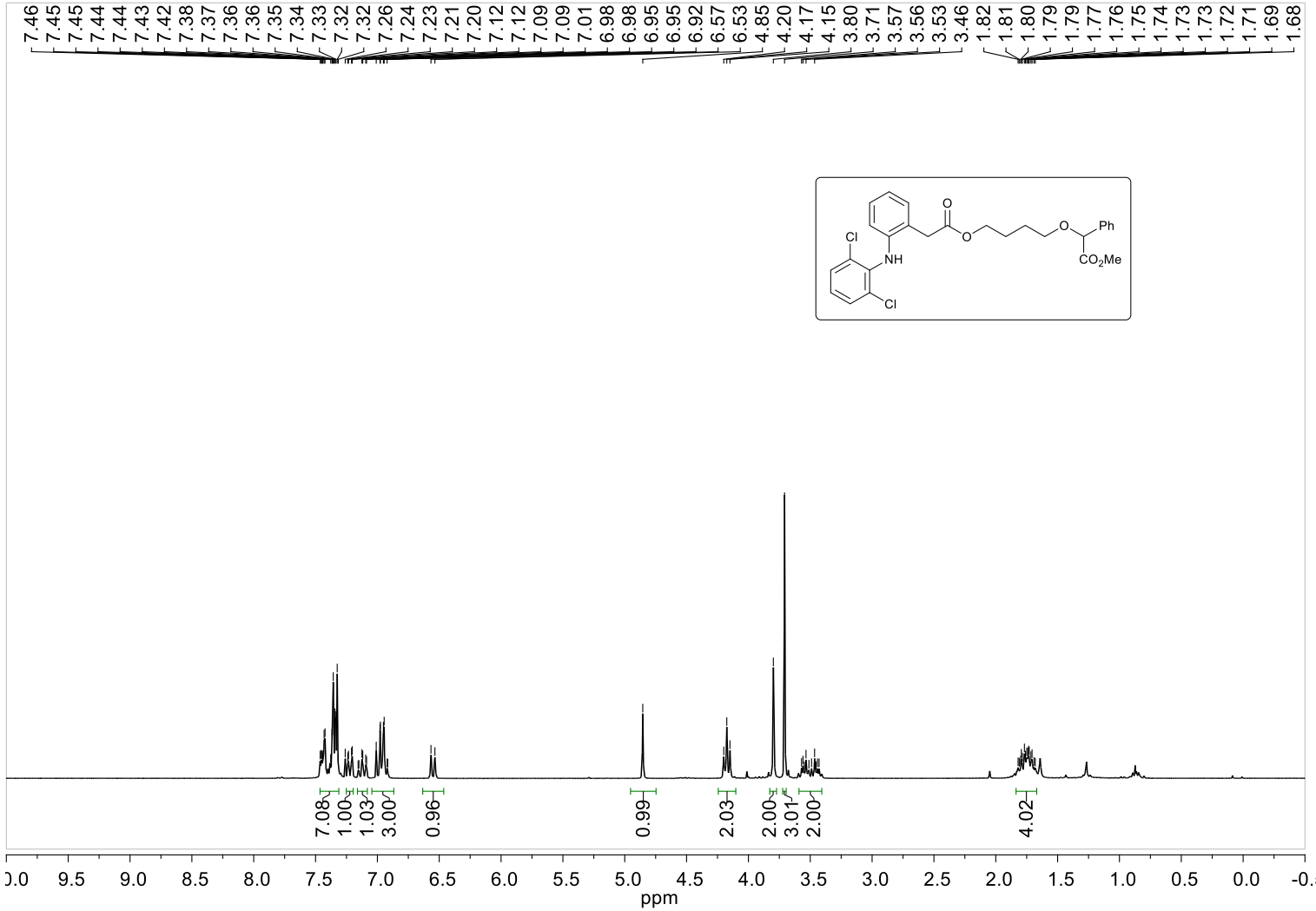
Molecule 8bb - ^{1}H NMR (250 MHz, $CDCl_3$)



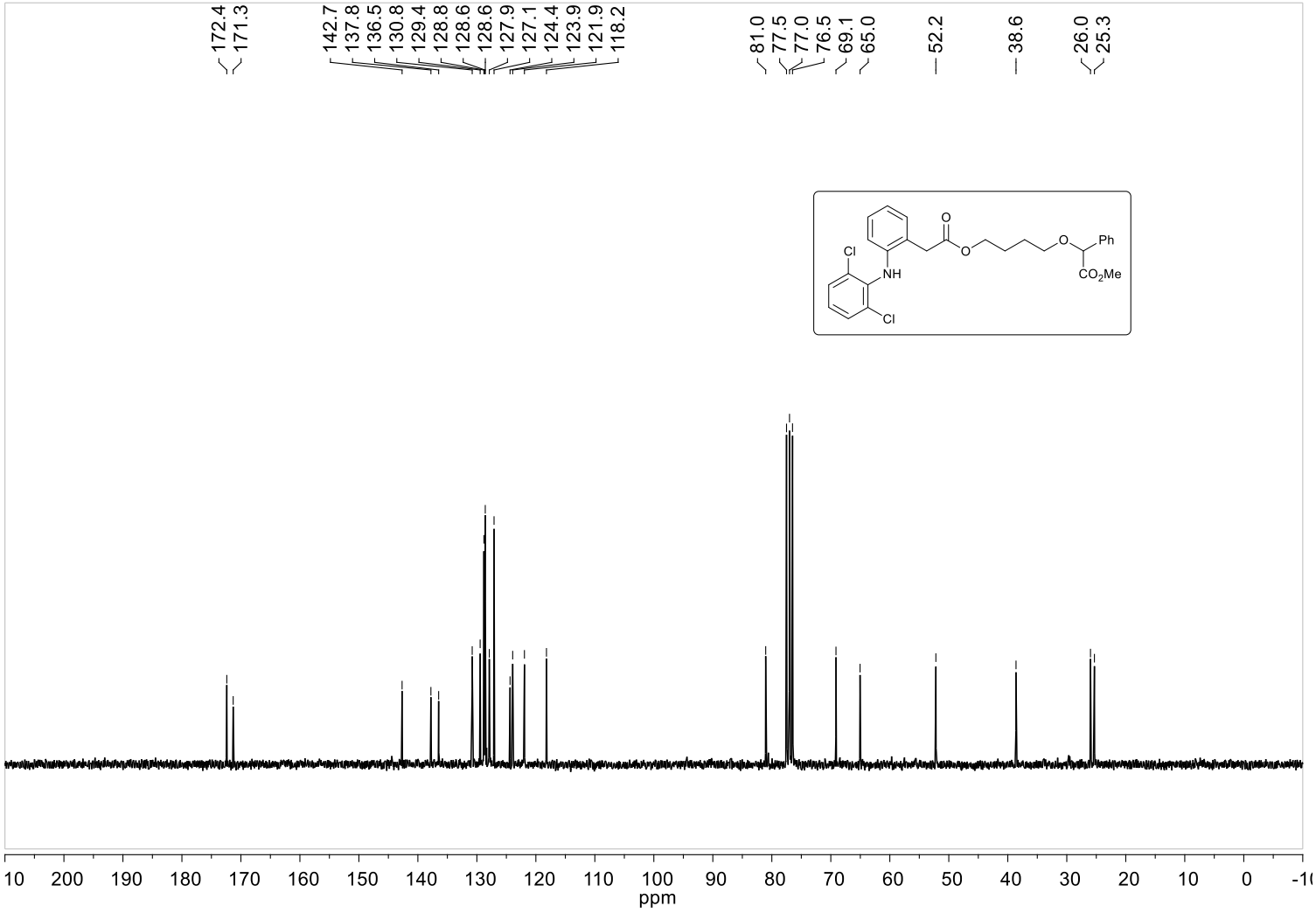
Molecule 8bb - ^{13}C NMR (62.5 MHz, $CDCl_3$)



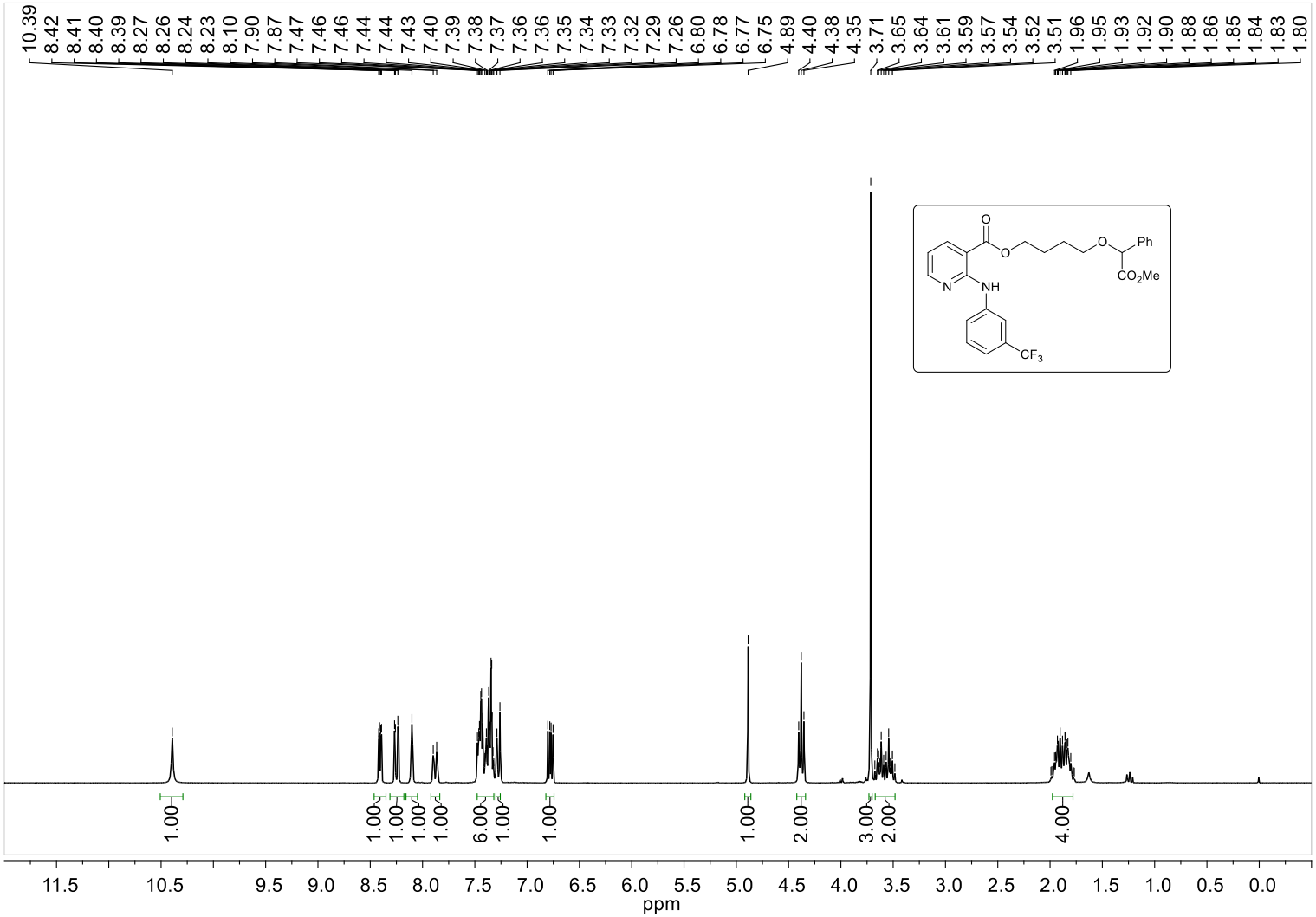
Molecule 8cc - ^{1}H NMR (250 MHz, $CDCl_3$)



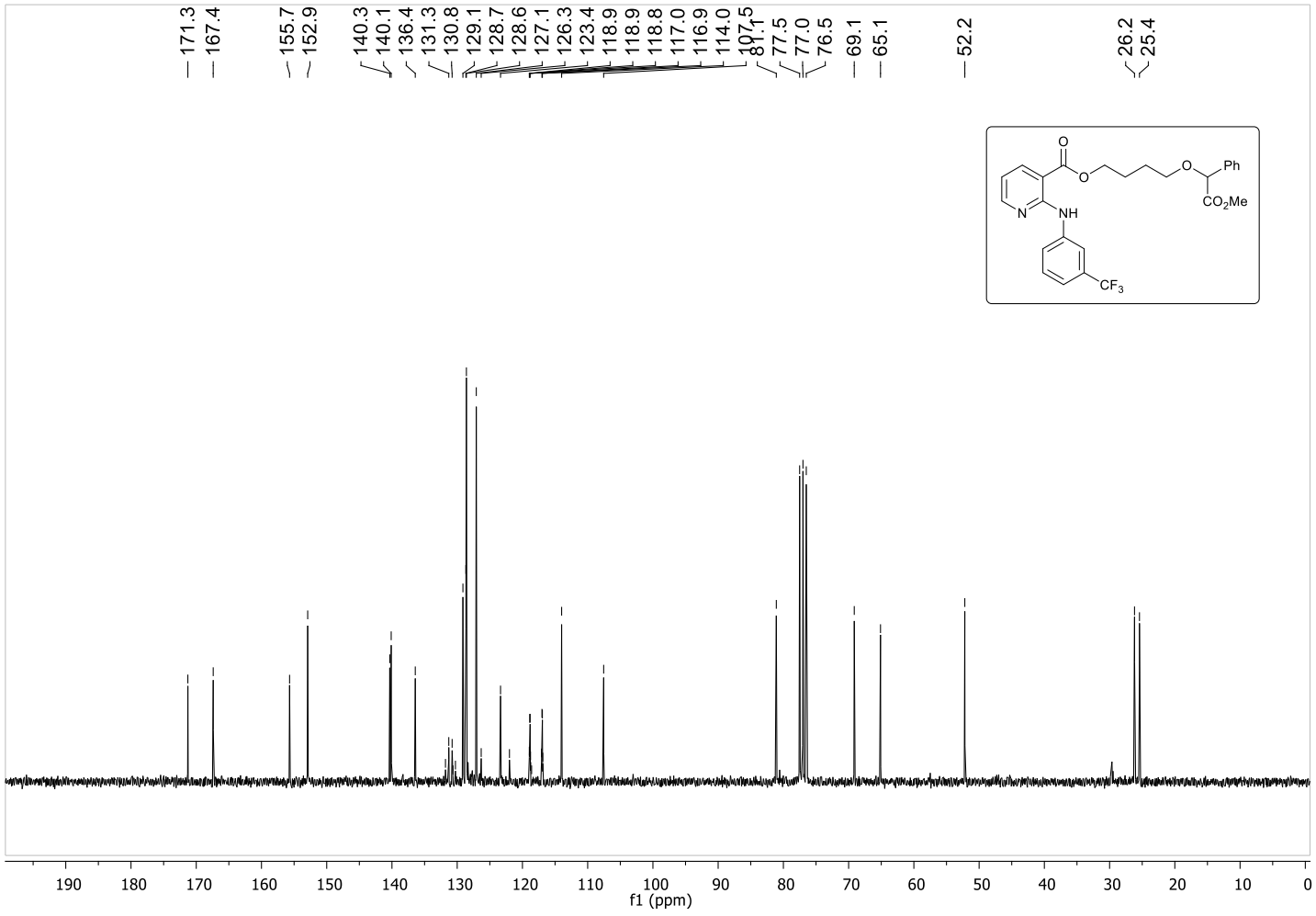
Molecule 8cc - ^{13}C NMR (62.5 MHz, $CDCl_3$)



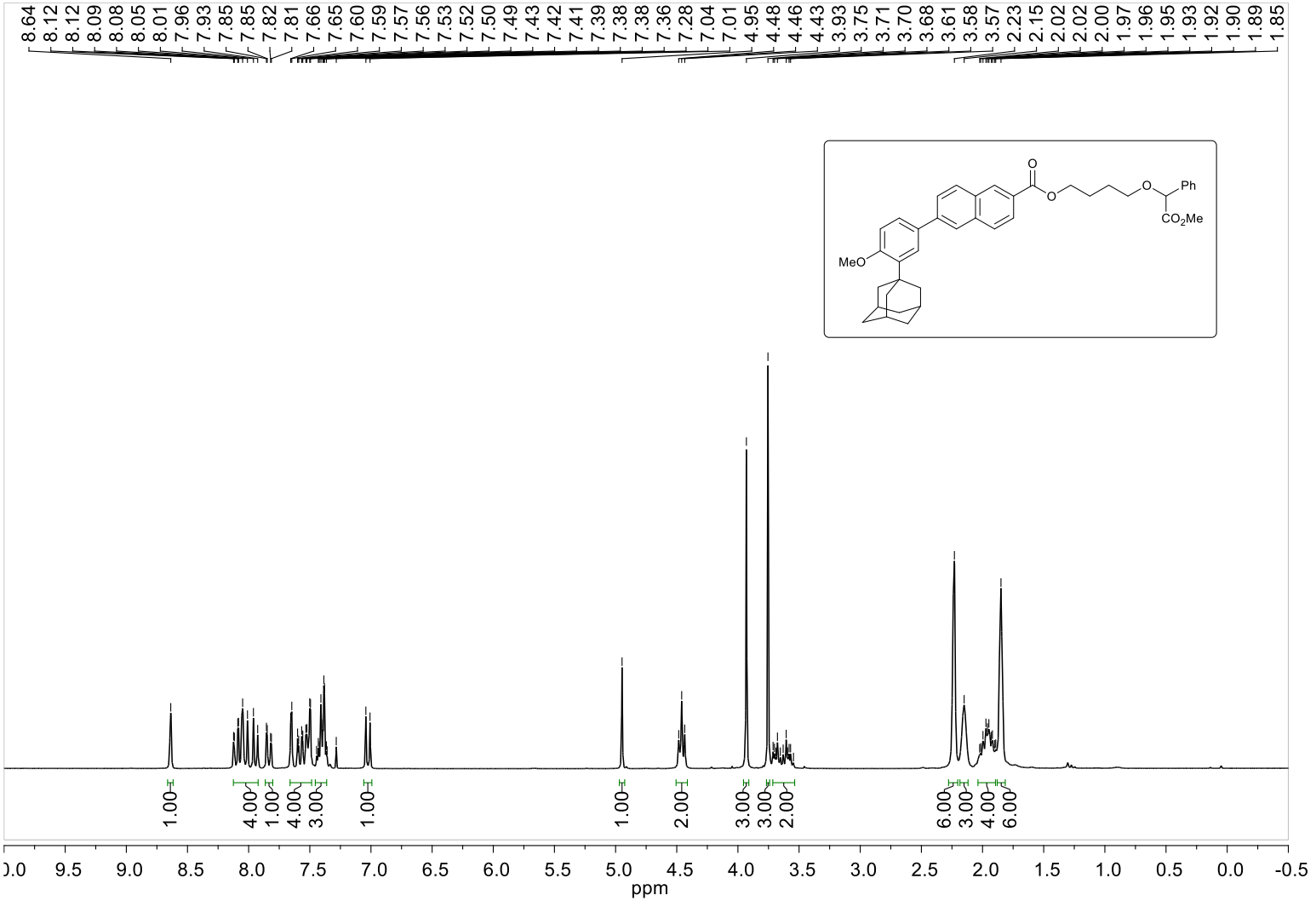
Molecule 8dd - ^{1}H NMR (250 MHz, $CDCl_3$)



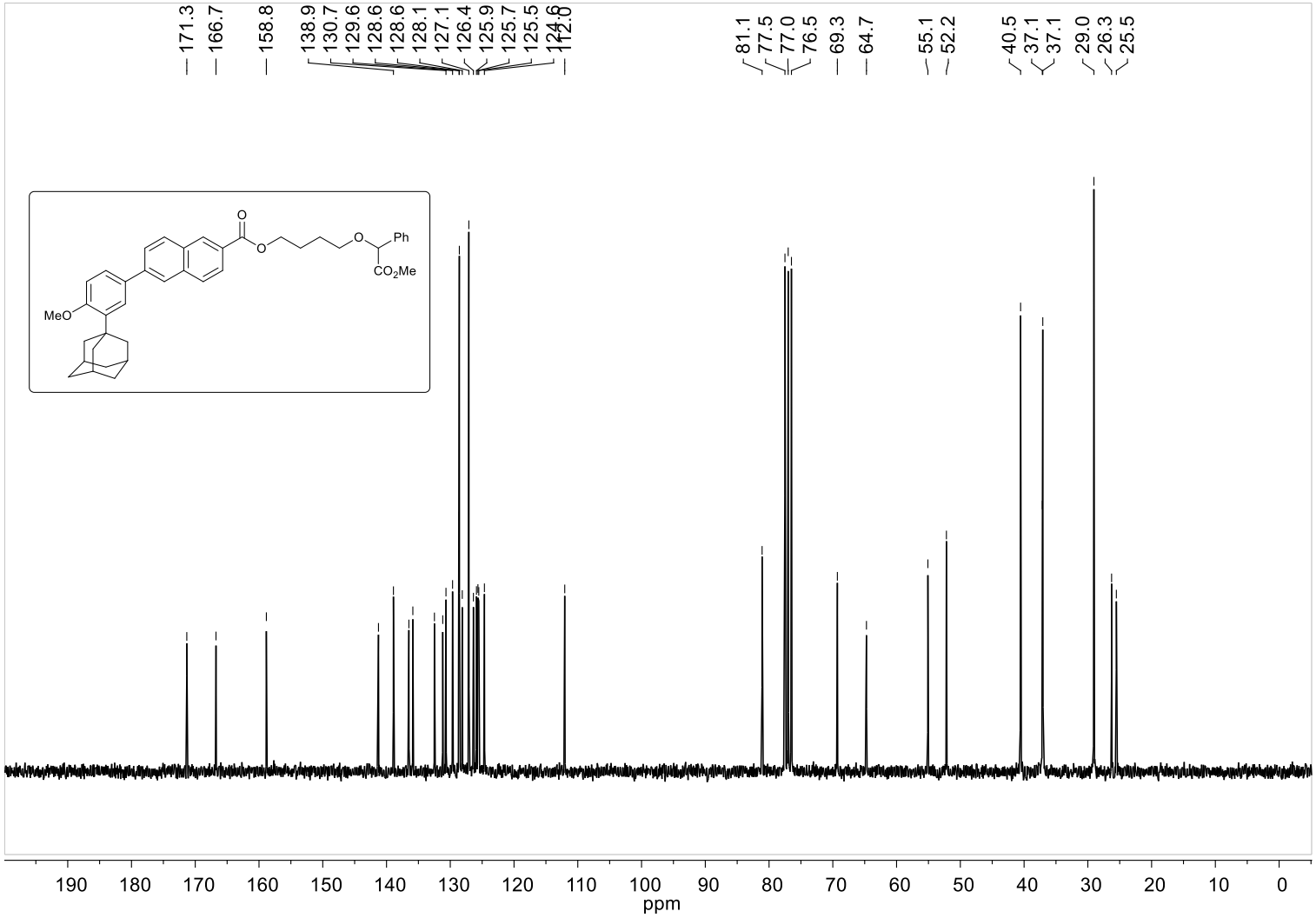
Molecule 8dd - ^{13}C NMR (62.5 MHz, $CDCl_3$)



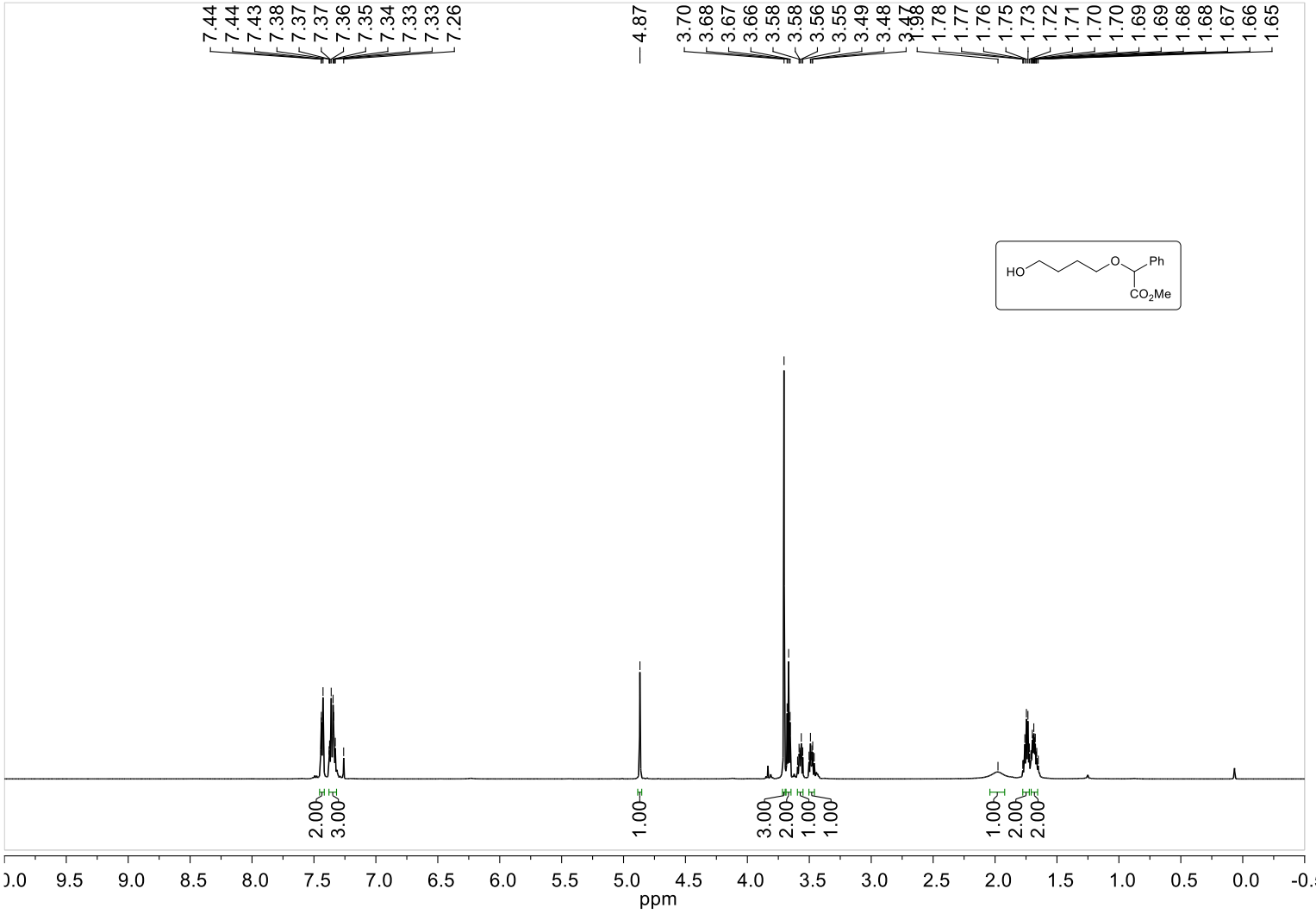
Molecule 8ee - ^{1}H NMR (250 MHz, $CDCl_3$)



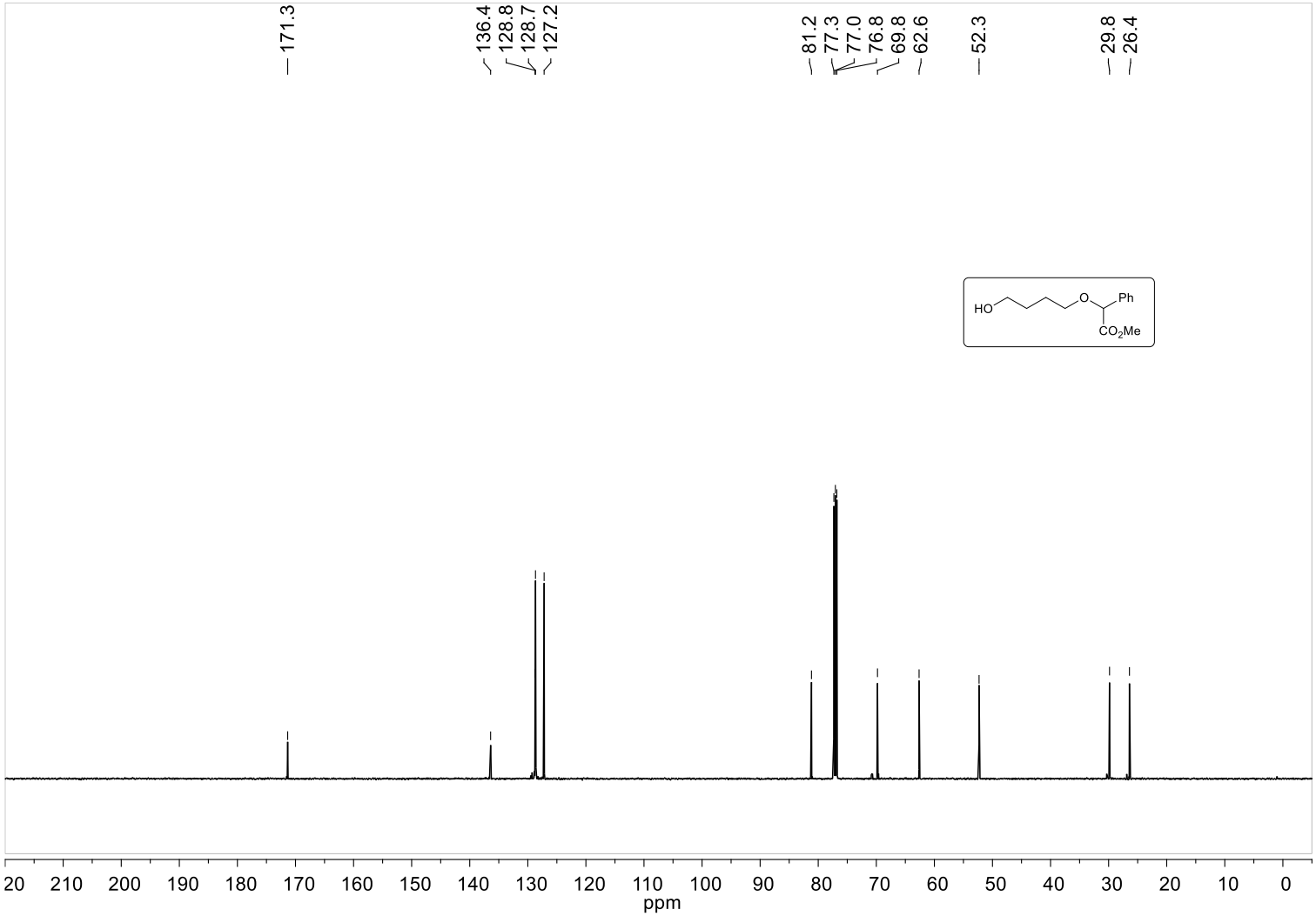
Molecule 8ee - ^{13}C NMR (62.5 MHz, $CDCl_3$)



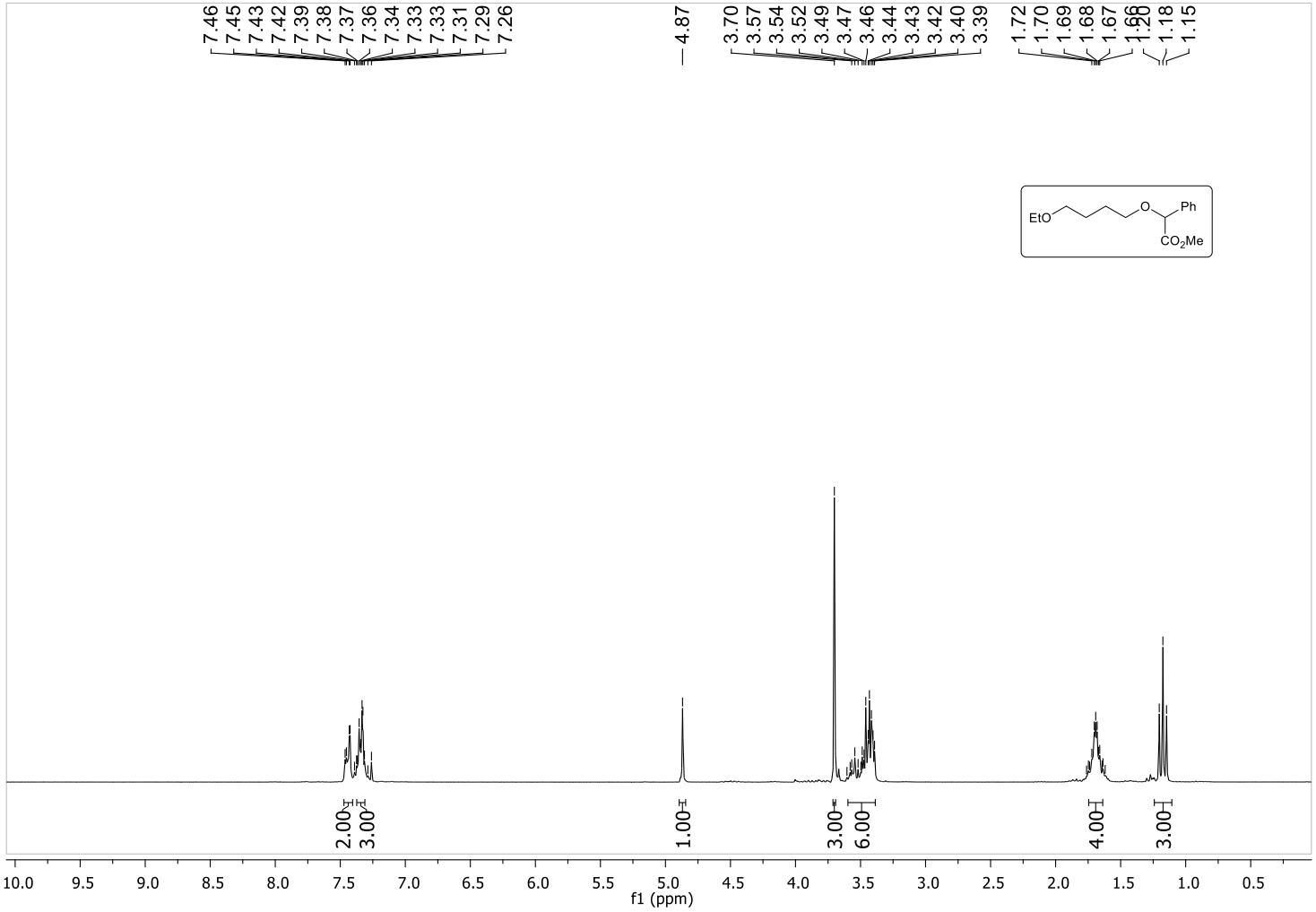
Molecule 22 - ^{1}H NMR (500 MHz, $CDCl_3$)



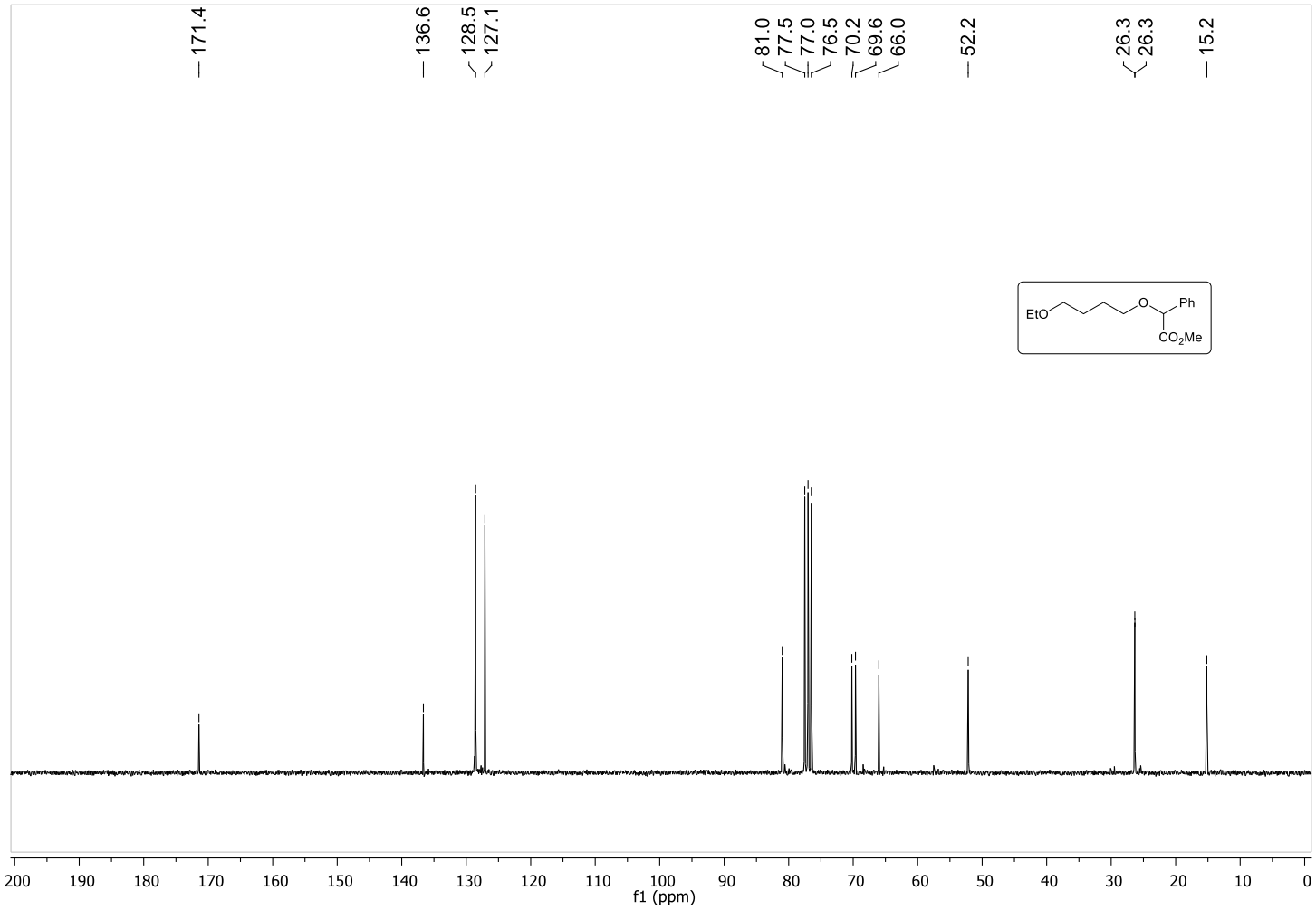
Molecule 22 - ^{13}C NMR (125 MHz, $CDCl_3$)



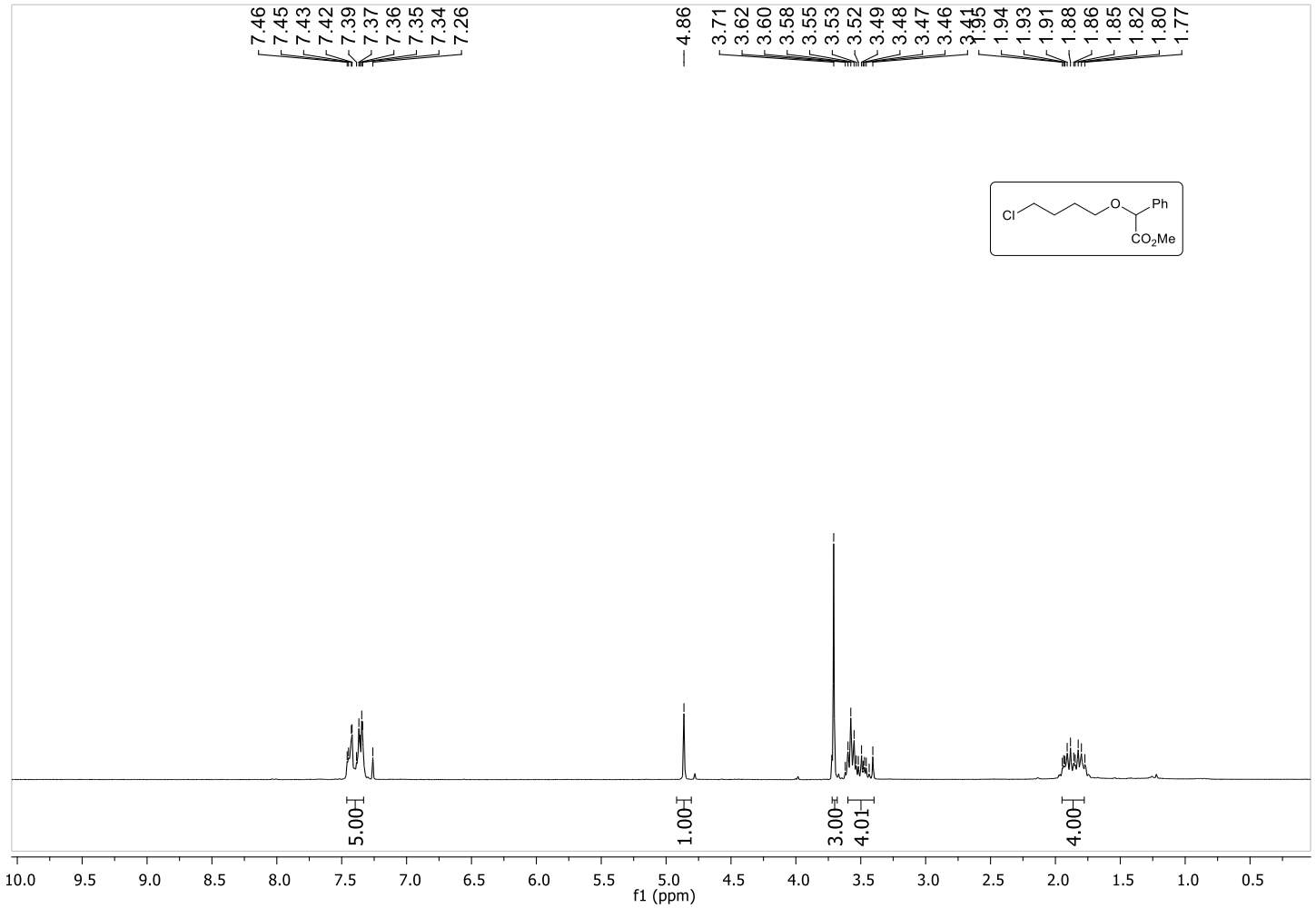
Molecule 23 - ^{1}H NMR (250 MHz, $CDCl_3$)



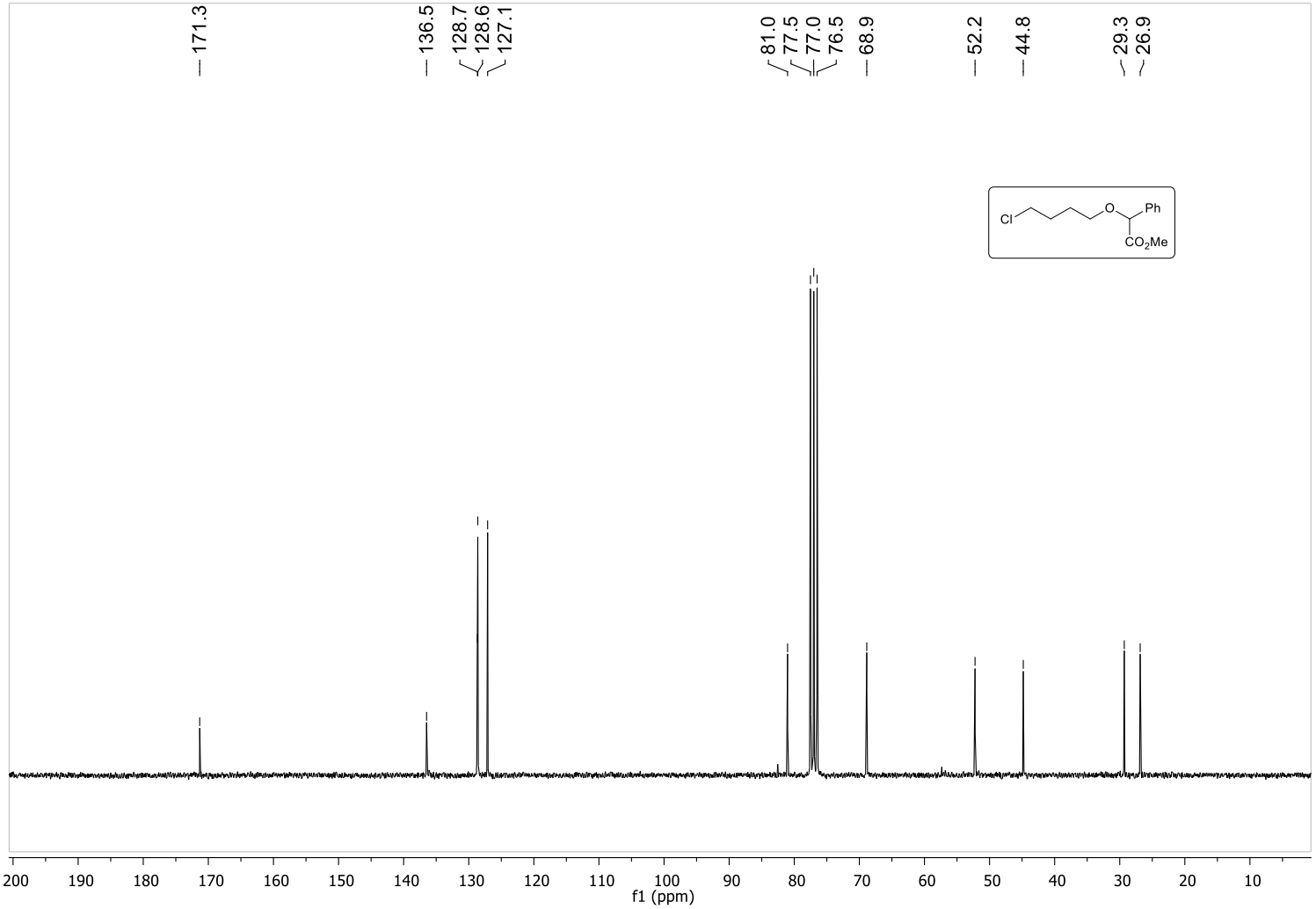
Molecule 23 – ^{13}C NMR (62.5 MHz, $CDCl_3$)



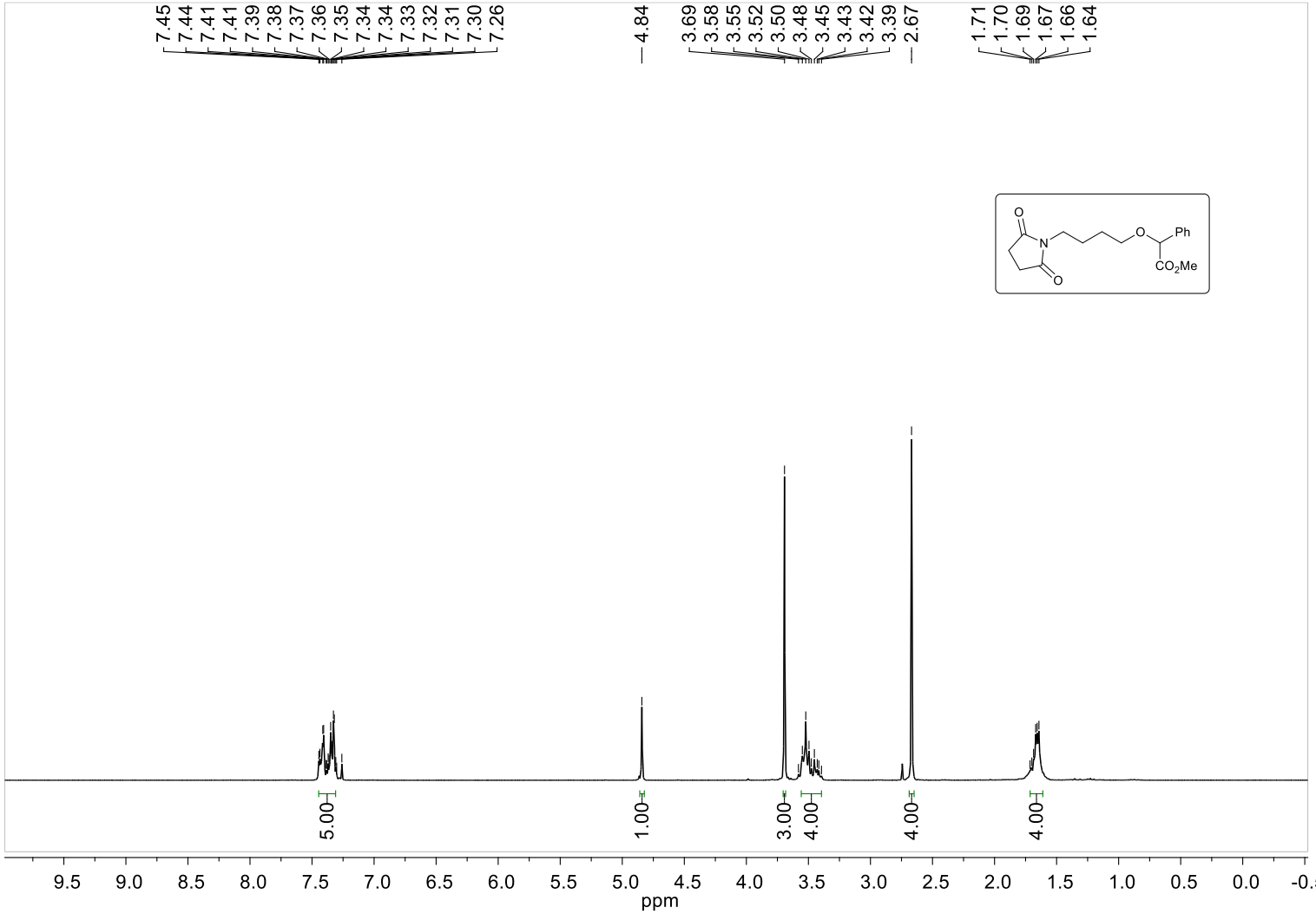
Molecule 24 - ^{1}H NMR (250 MHz, $CDCl_3$)



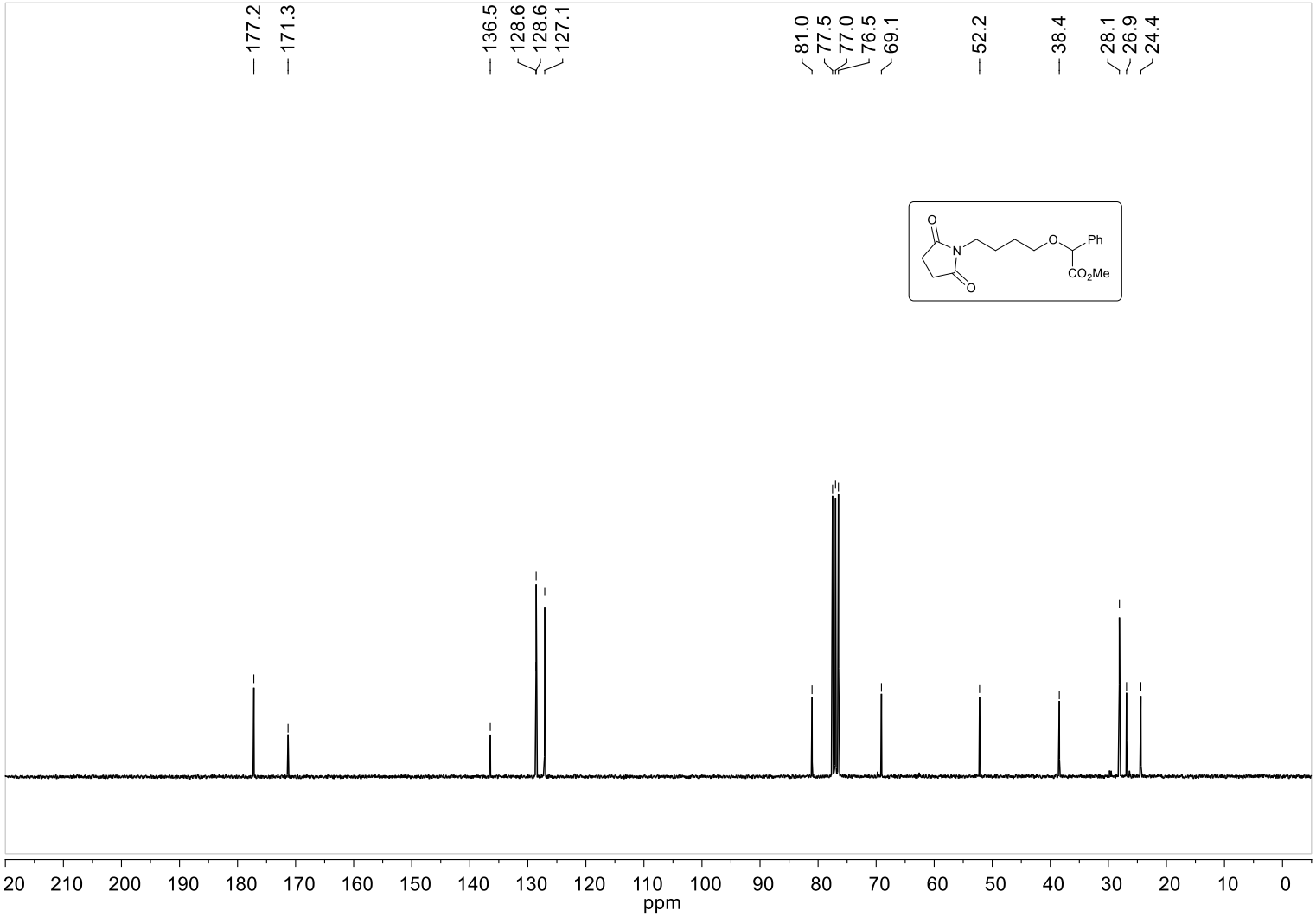
Molecule 24 – ^{13}C NMR (62.5 MHz, $CDCl_3$)



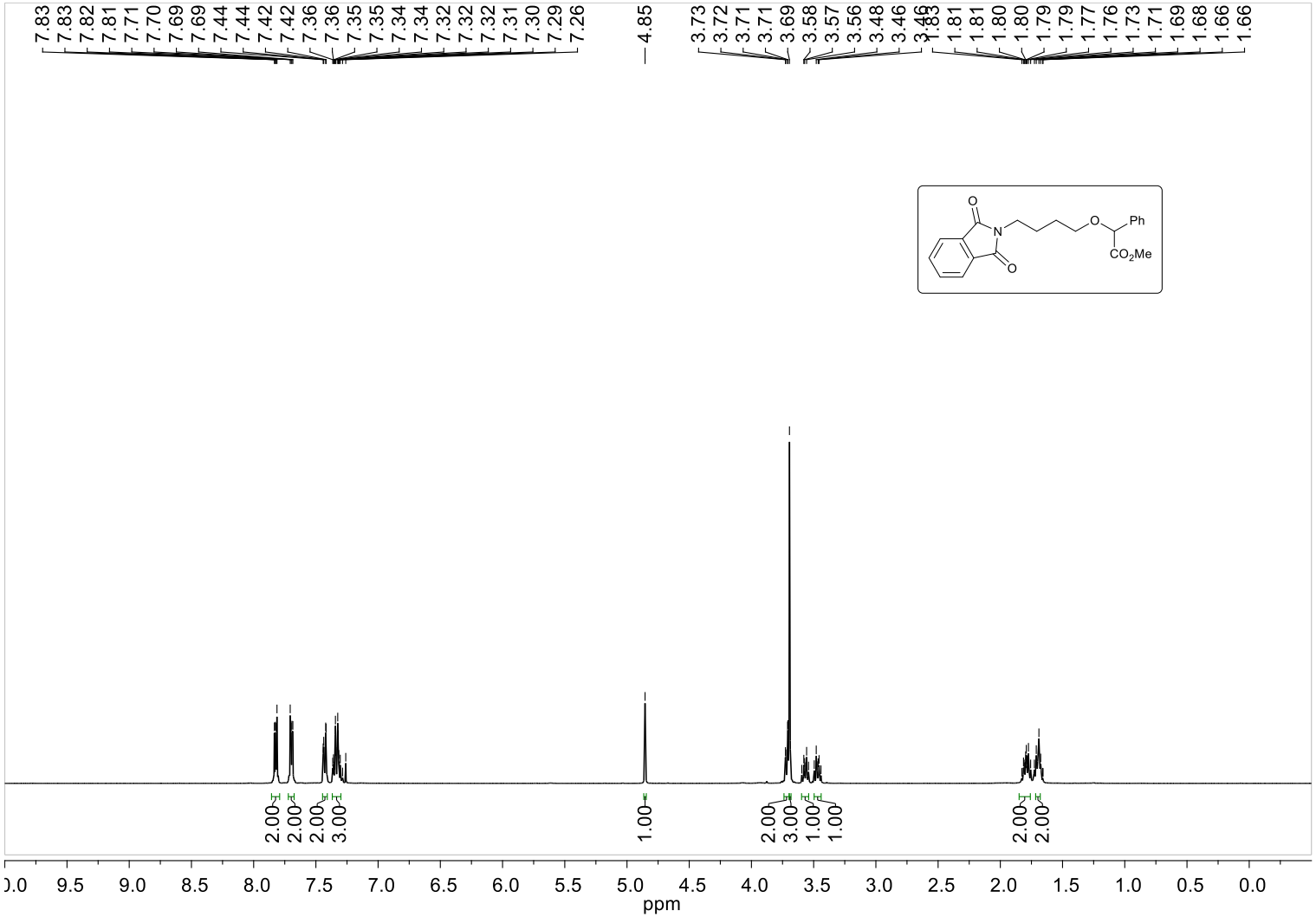
Molecule 25 ^{1}H NMR (250 MHz, $CDCl_3$)



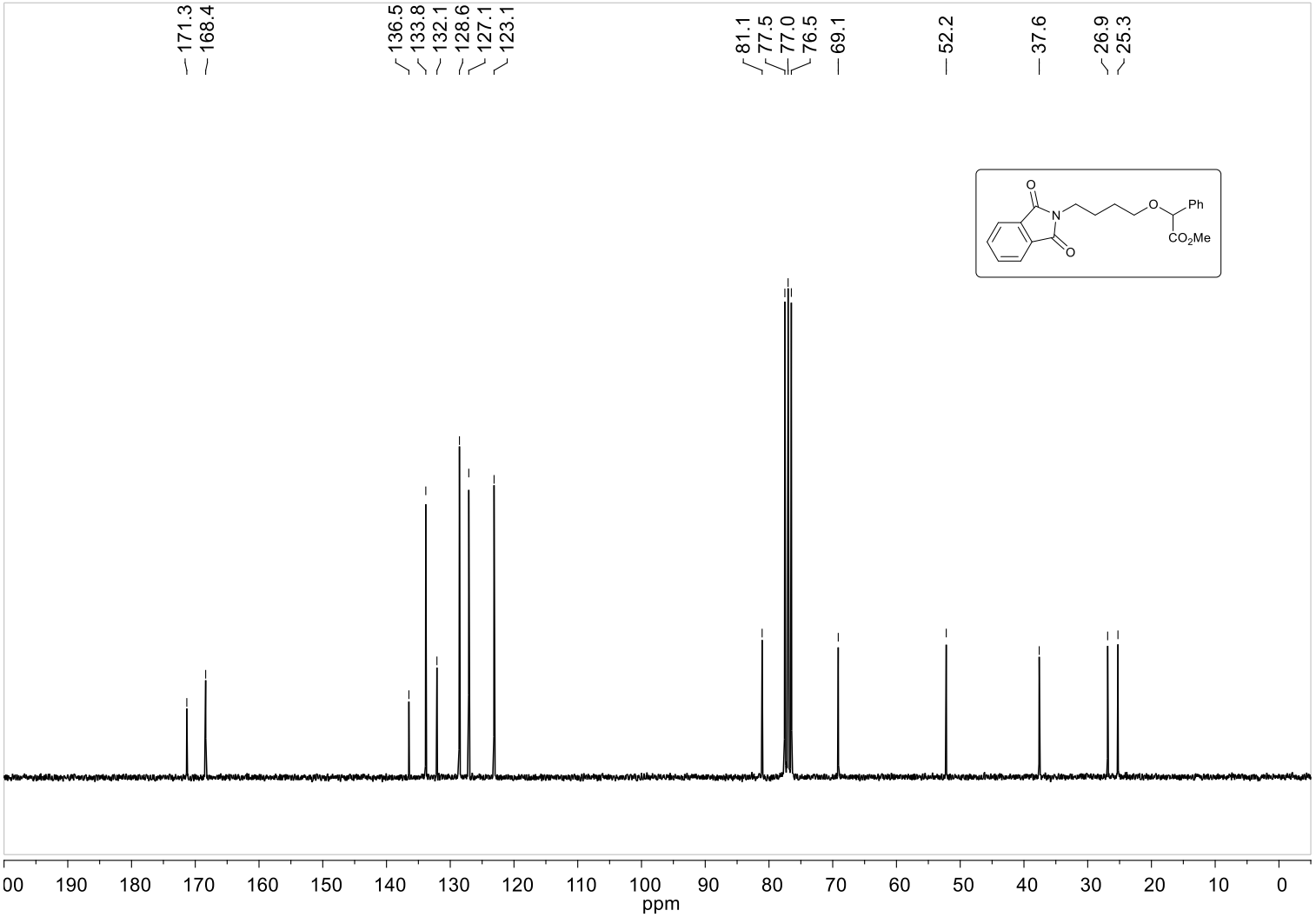
Molecule 25 - ^{13}C NMR (62.5 MHz, $CDCl_3$)



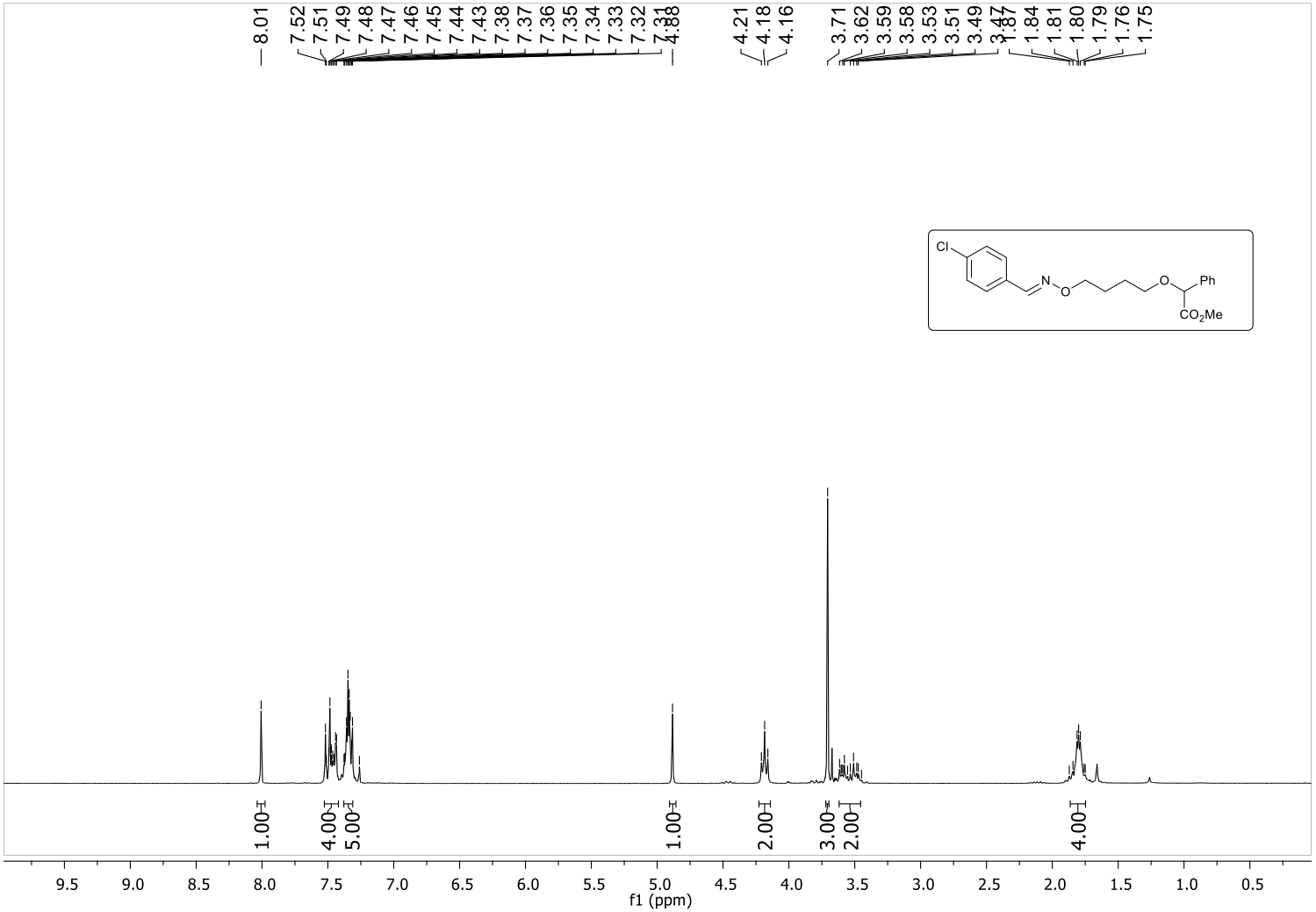
Molecule 26 - ^{1}H NMR (250 MHz, $CDCl_3$)



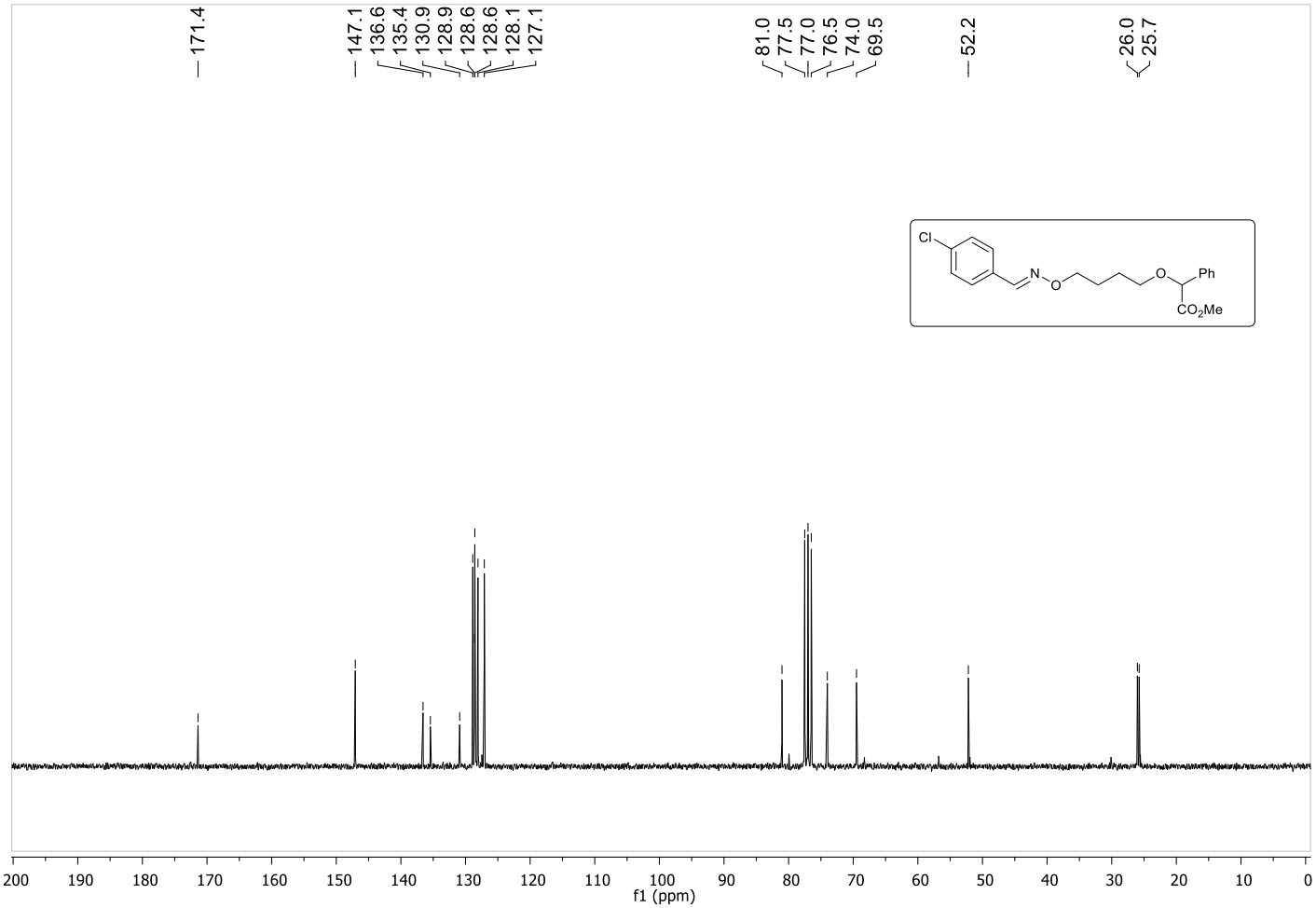
Molecule 26 - ^{13}C NMR (62.5 MHz, $CDCl_3$)



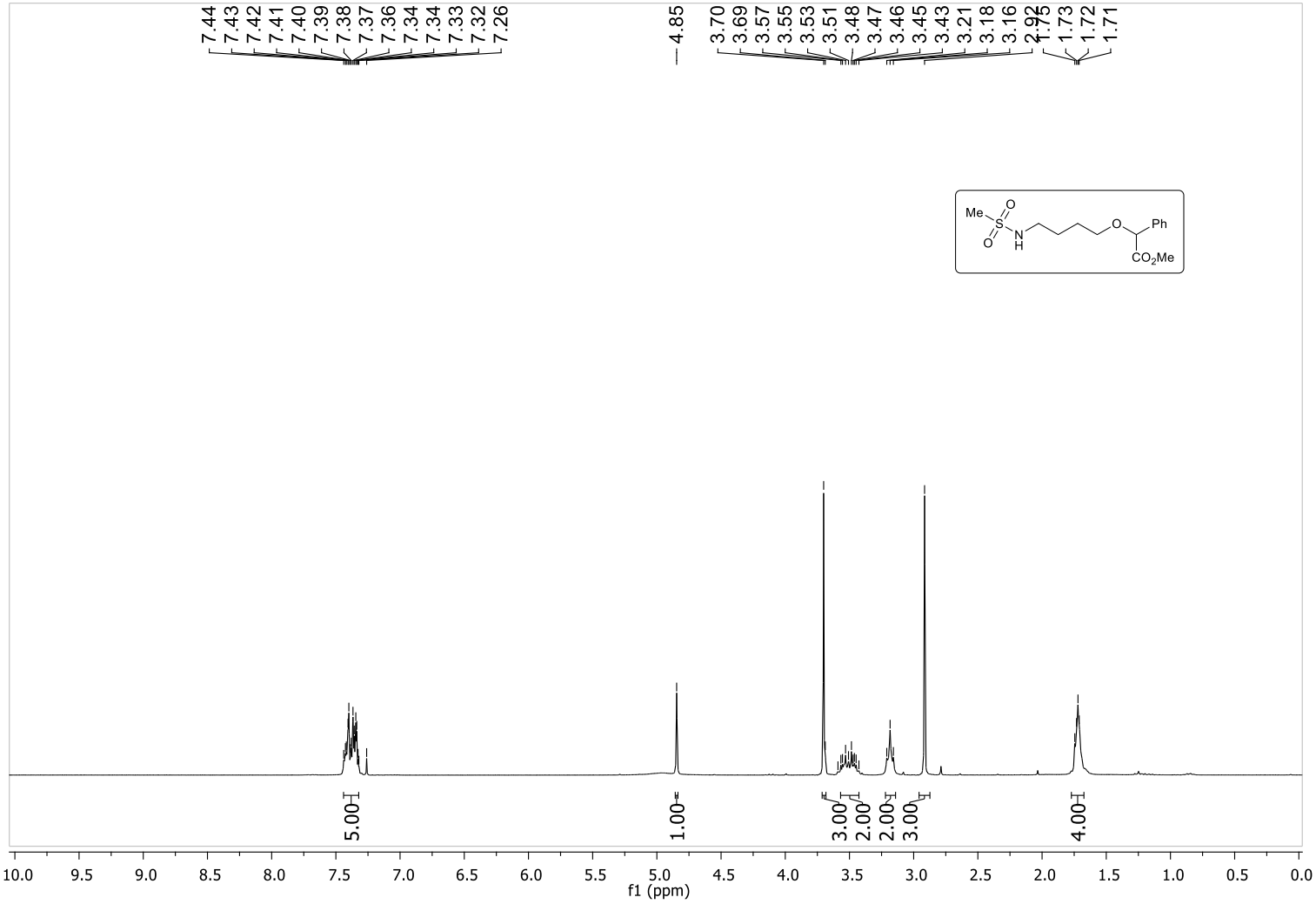
Molecule 27 - ^{1}H NMR (250 MHz, $CDCl_3$)



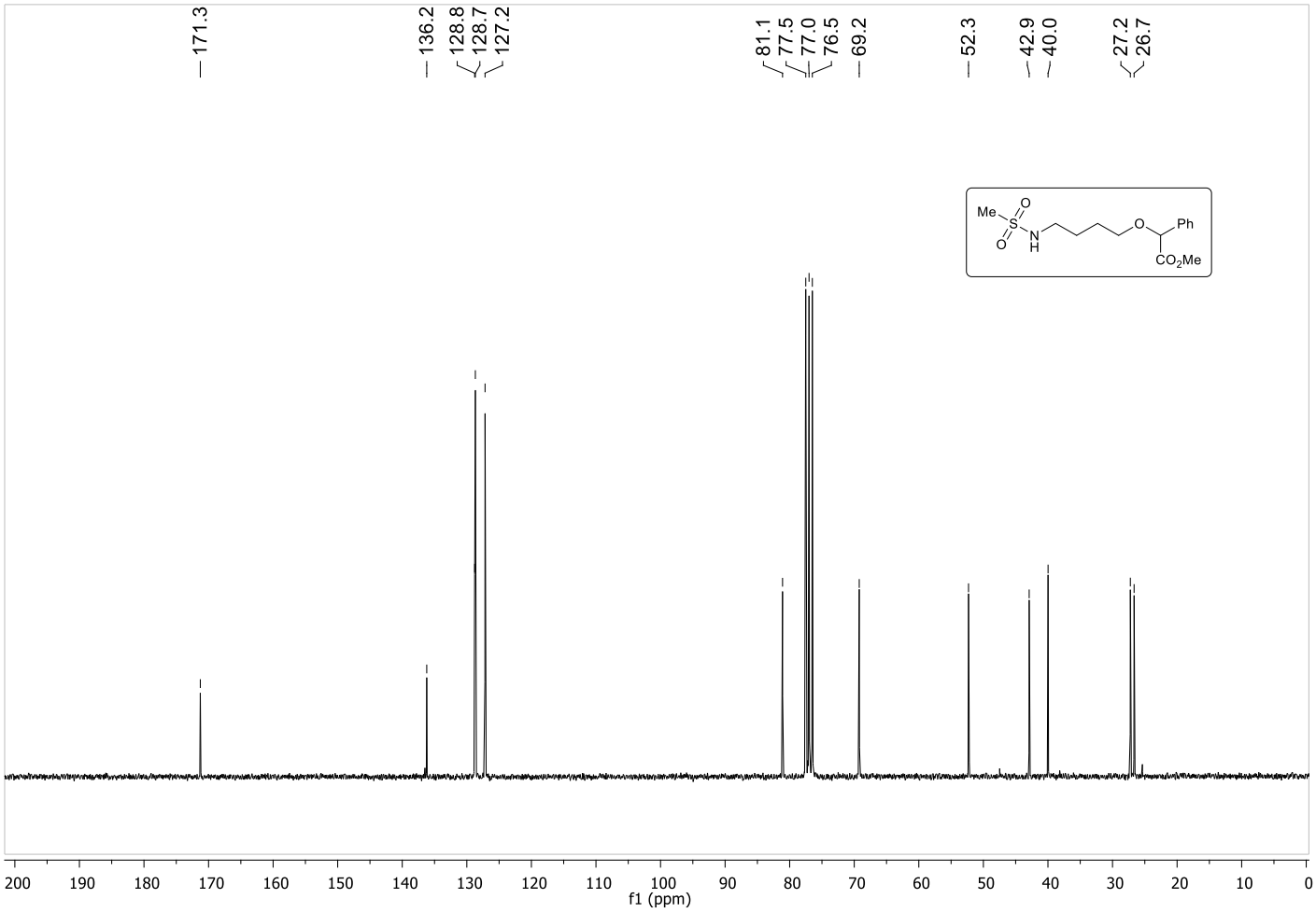
Molecule 27 - ^{13}C NMR (62.5 MHz, $CDCl_3$)



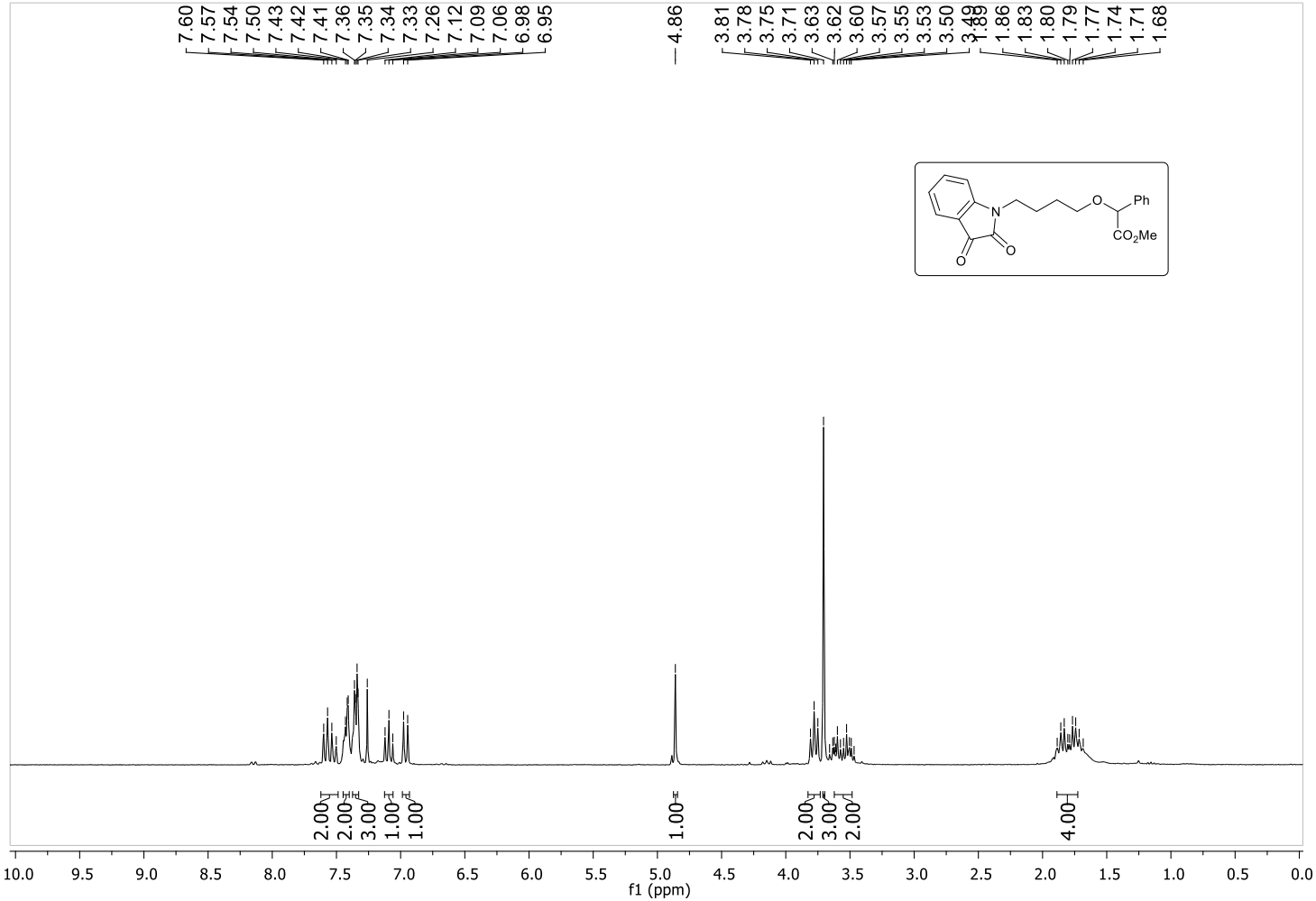
Molecule 28 - ^{1}H NMR (250 MHz, $CDCl_3$)



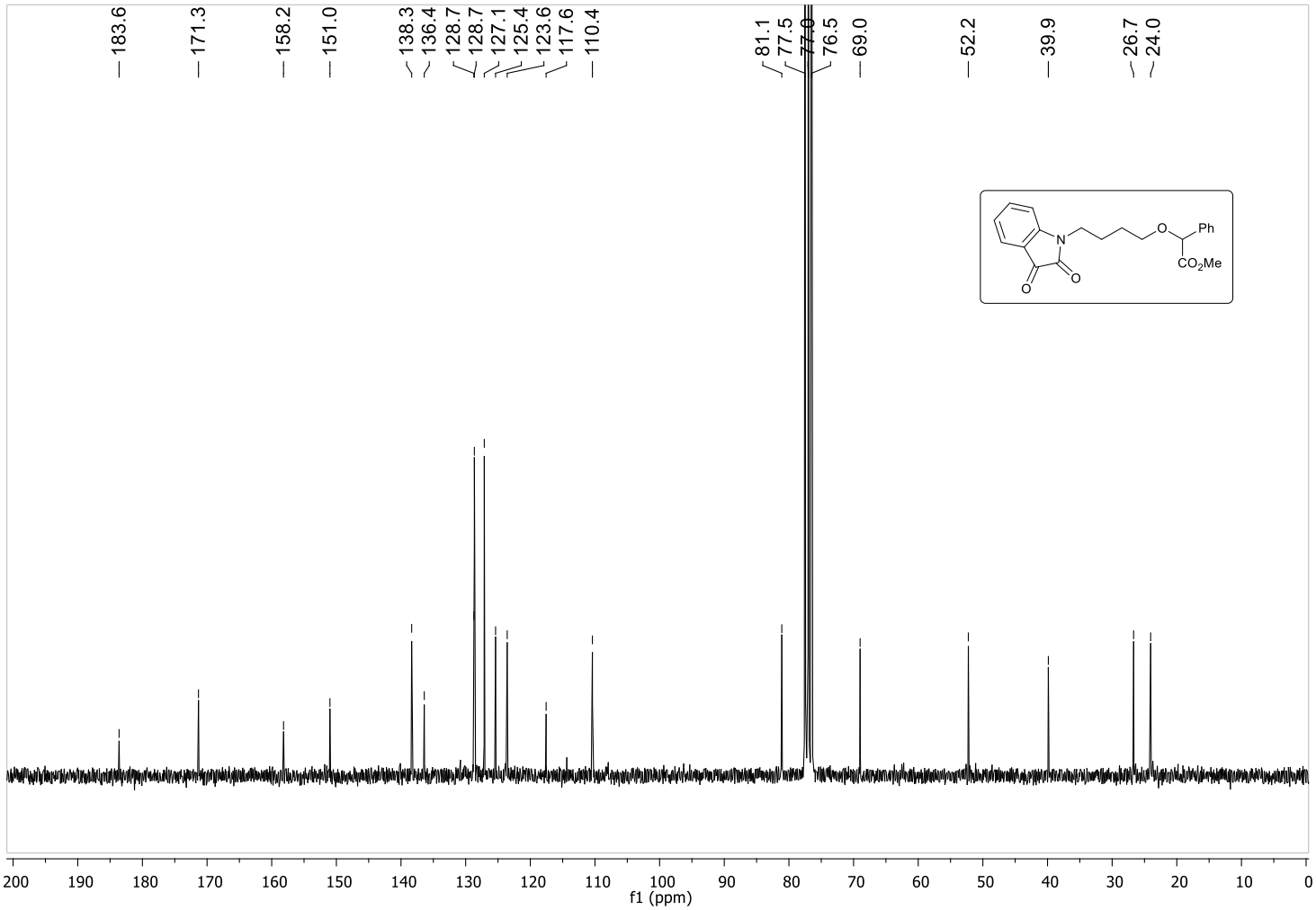
Molecule 28 - ^{13}C NMR (62.5 MHz, $CDCl_3$)



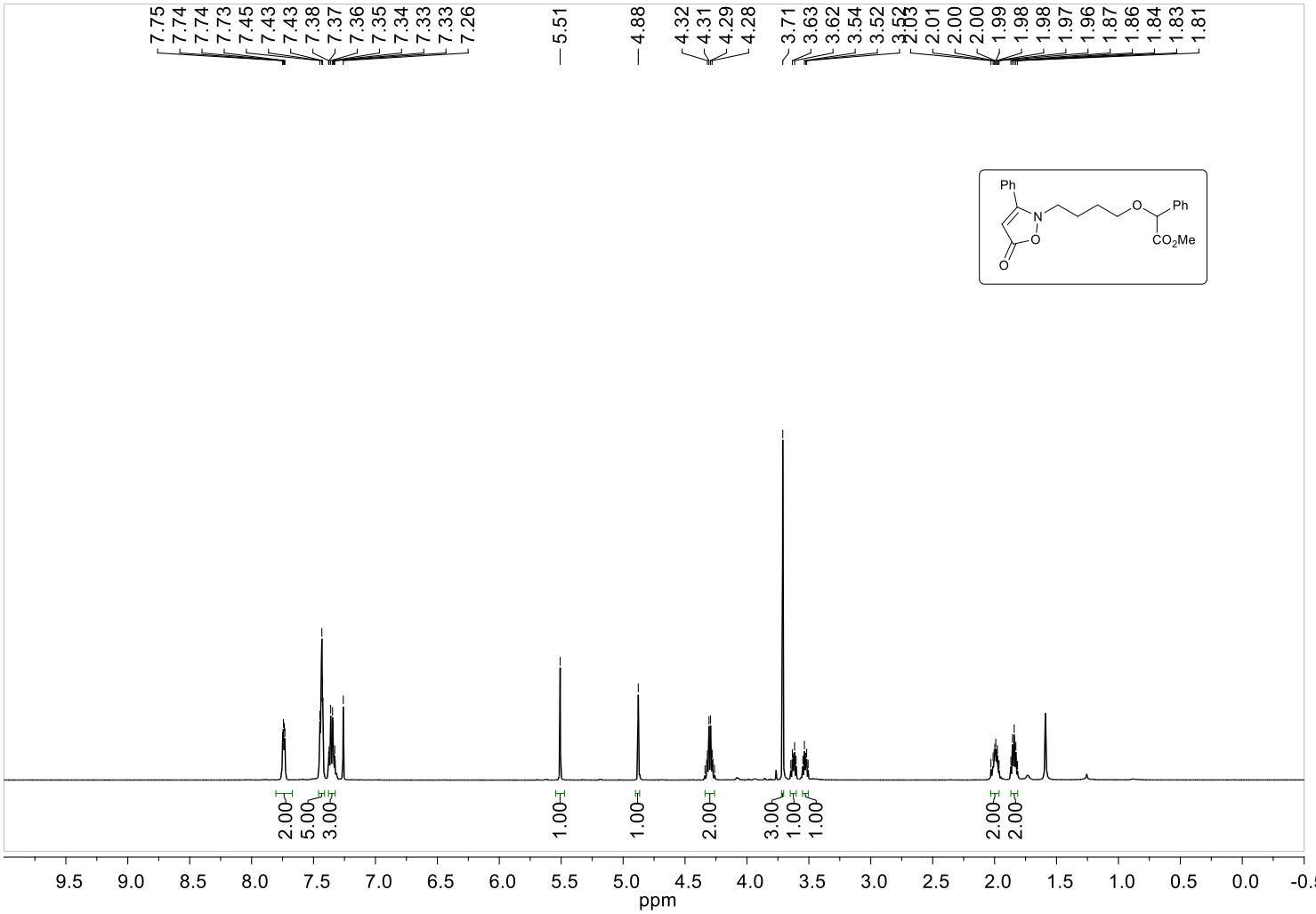
Molecule 29 - ^{1}H NMR (250 MHz, $CDCl_3$)



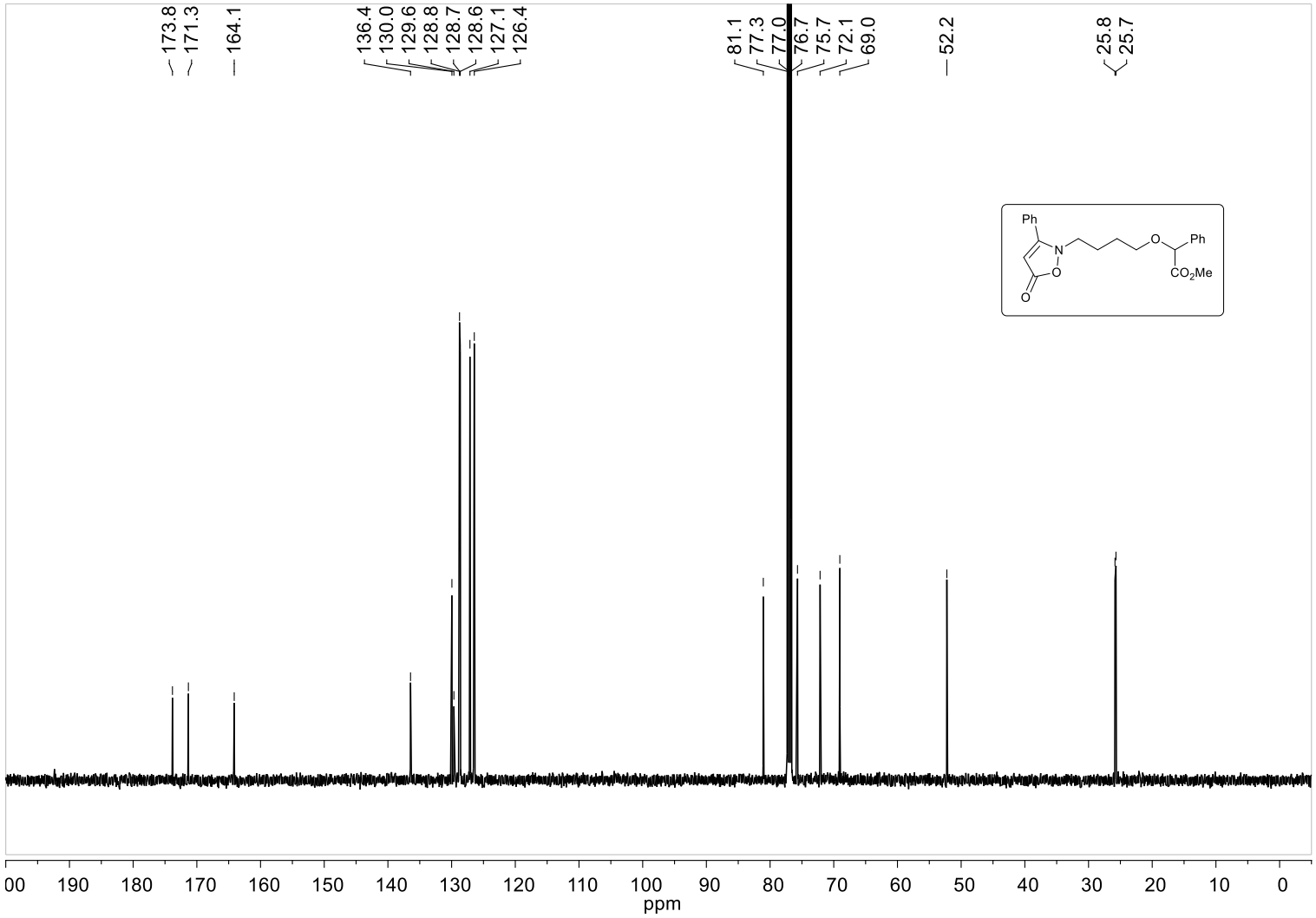
Molecule 29 - ^{13}C NMR (62.5 MHz, $CDCl_3$)



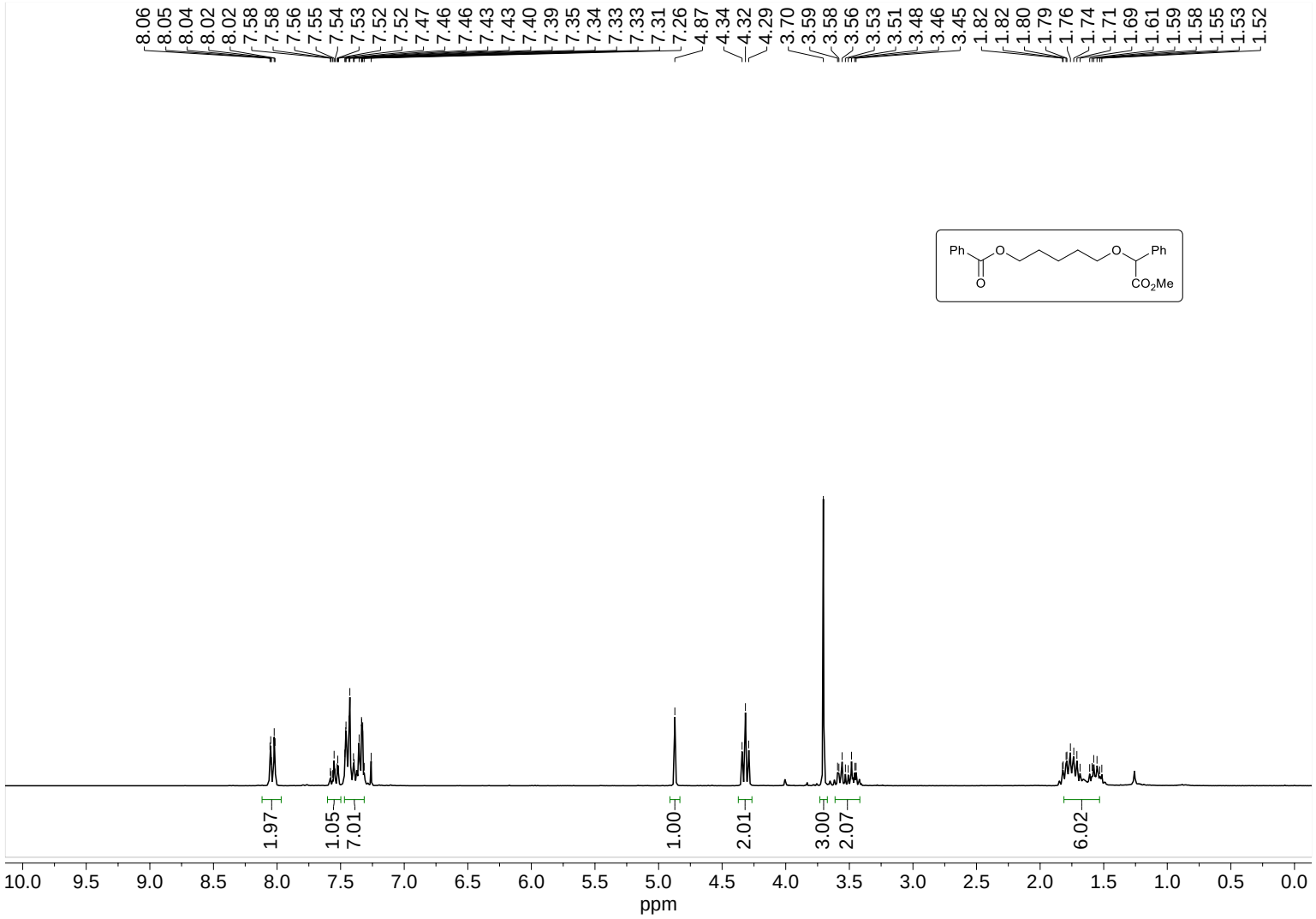
Molecule 30 - ^{1}H NMR (500 MHz, $CDCl_3$)



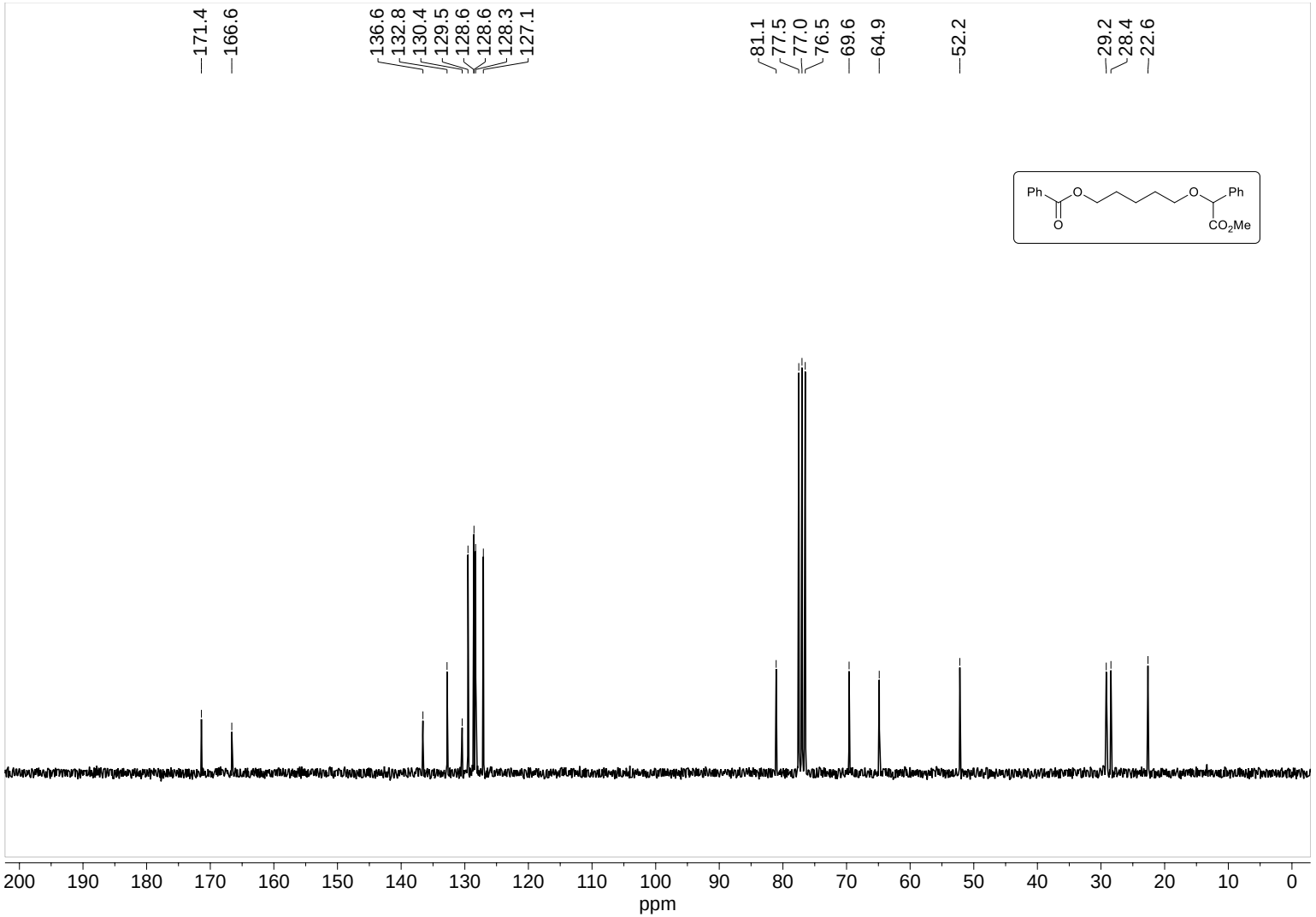
Molecule 30 - ^{13}C NMR (125 MHz, $CDCl_3$)



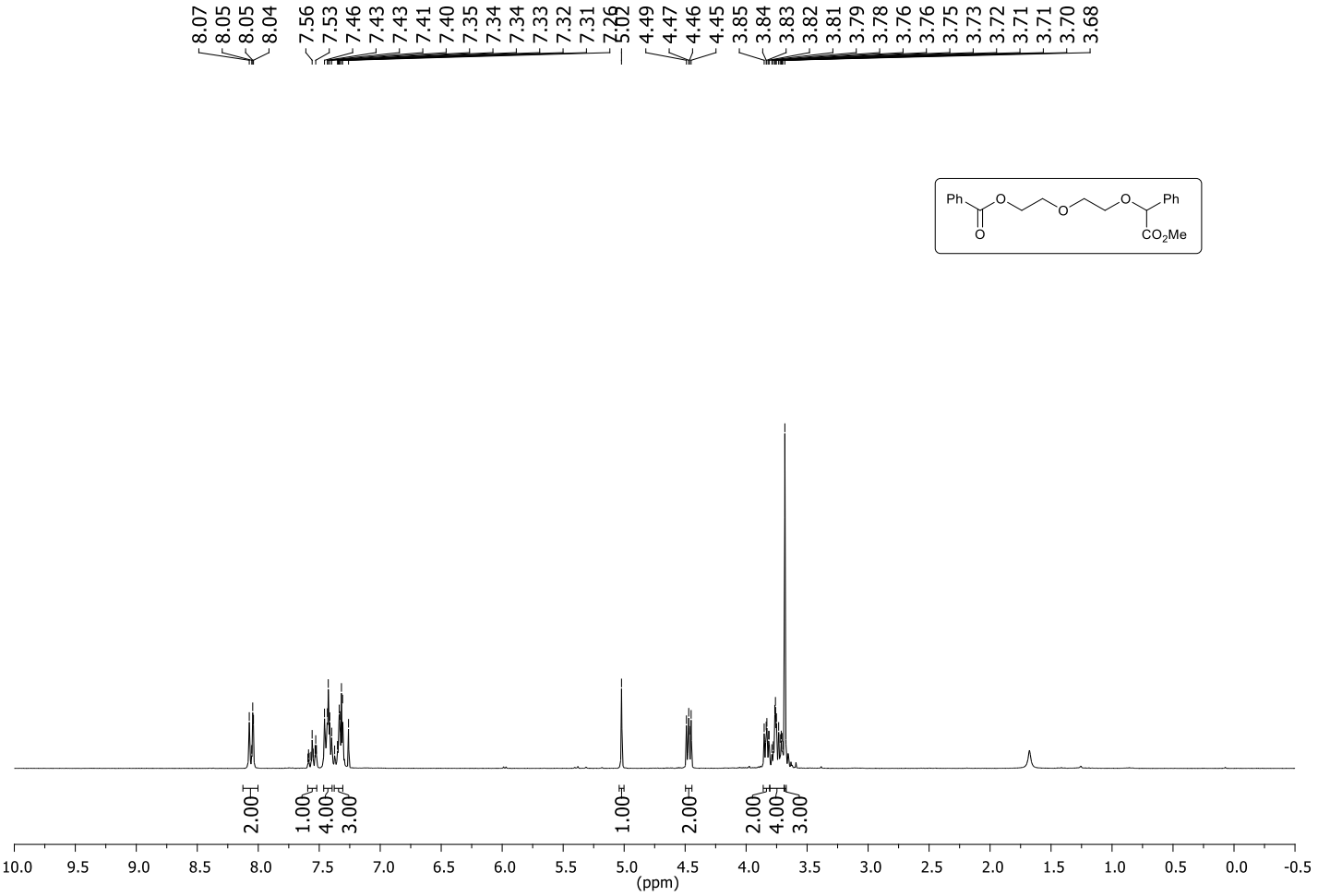
Molecule 8ff - ^{1}H NMR (250 MHz, $CDCl_3$)



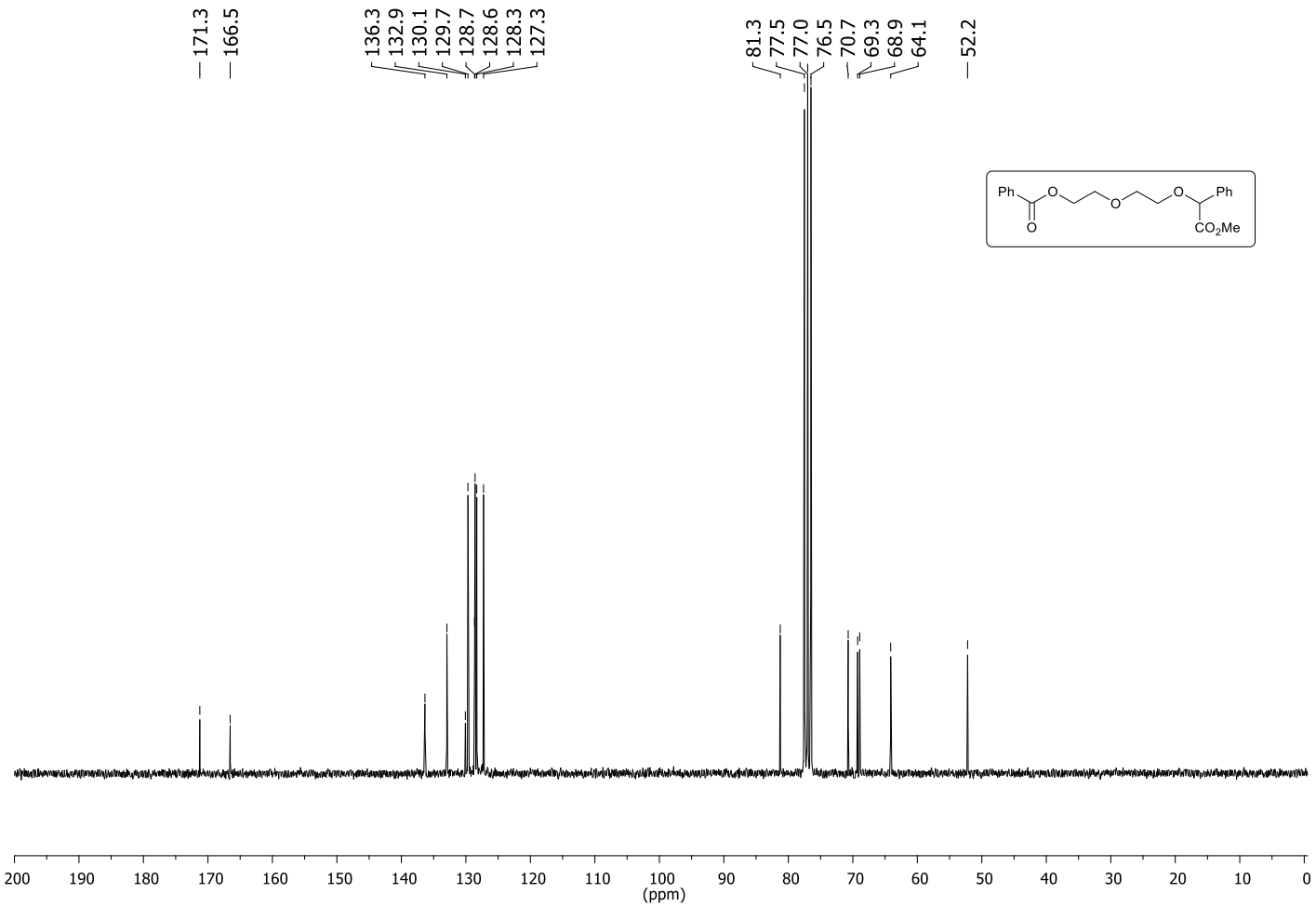
Molecule 8ff - ^{13}C NMR (62.5 MHz, $CDCl_3$)



Molecule 8gg - ^{1}H NMR (250 MHz, $CDCl_3$)



Molecule 8gg - ^{13}C NMR (62.5 MHz, $CDCl_3$)

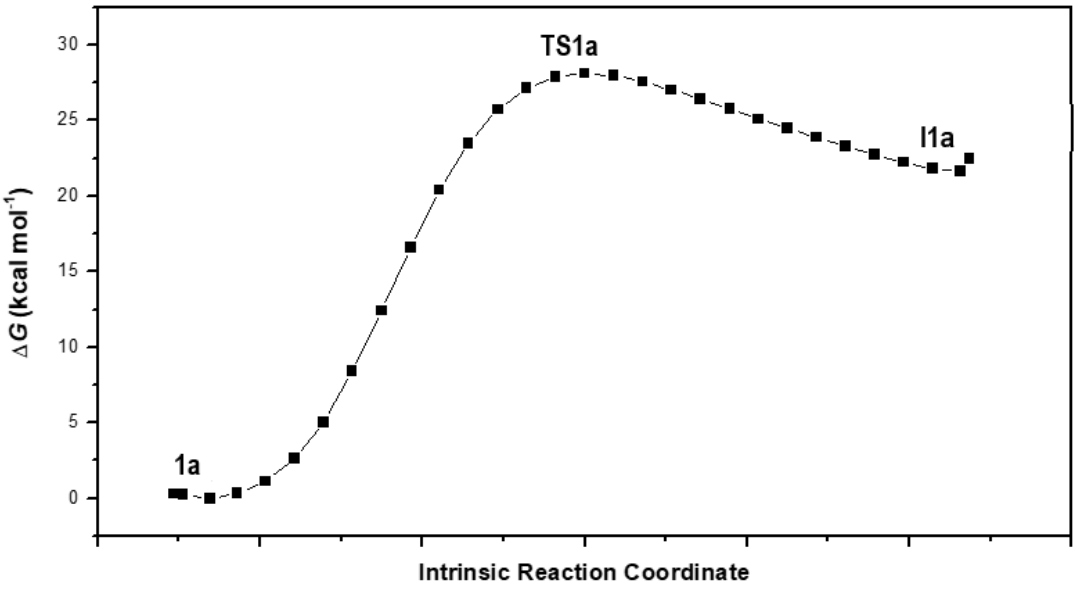


4. COMPUTATIONAL METHODS

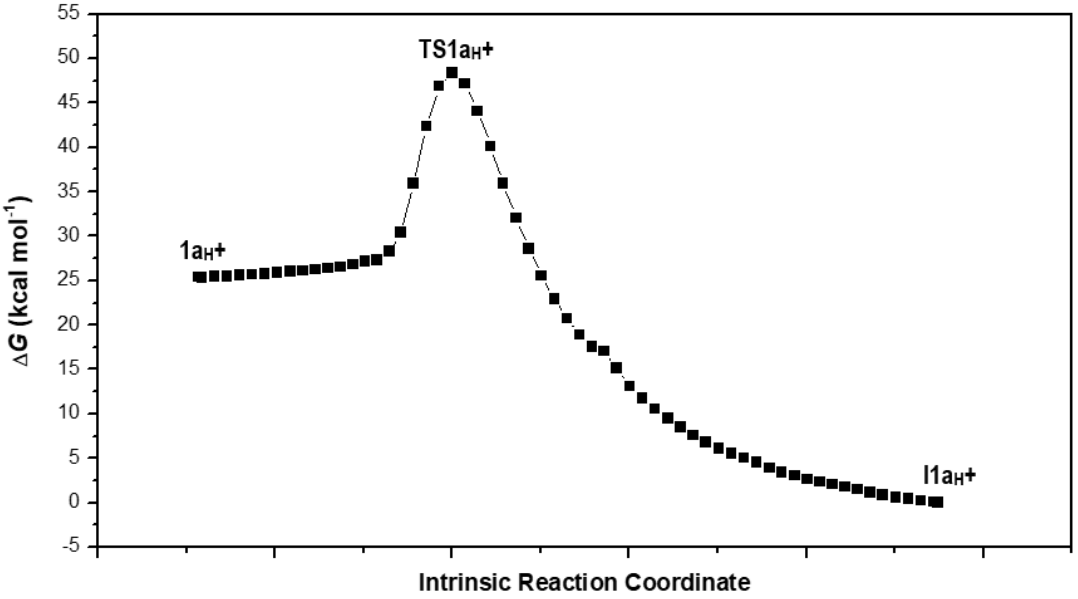
Initially, a conformational search was done for all starting materials using the Dreiding[7] force field in MarvinSketch 21.14.[8] The resulting conformers were reoptimized using Gaussian 16 Rev C.01[9] at the B3LYP/6-31+G* level for the ground (S_0) and CIS/6-31+G* level for the first excited (S_1) states, respectively, and using the IEFPCM[10] implicit solvent model with parameters of THF ($\varepsilon = 7.43$). Frequency calculations at the same level of the optimizations were carried out to confirm the converged geometries as either minima (without negative frequencies) or transition states (one negative frequency). IRC calculations[11] at the same level of optimization and frequency calculations carried out to confirm whether the obtained transition states are connected with two minima for each reaction step. The rate constants were calculated from the Eyring equation by using the calculated Gibbs free energies for the rate determining step of the mechanism.

[7] S. L. Mayo, B. D. Olafson, W. A. Goddard, *J. Phys. Chem.*, 1990, **94**, 8897–8909.
[8] ChemAxon (http://www.chemaxon.com), **2021**.
[9] Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
[10] B. Mennucci, *WIREs Comput. Mol. Sci.*, 2012, **2**, 386–404.
[11] K. Fukui, *J. Phys. Chem.*, 1970, **74**, 4161-4163.

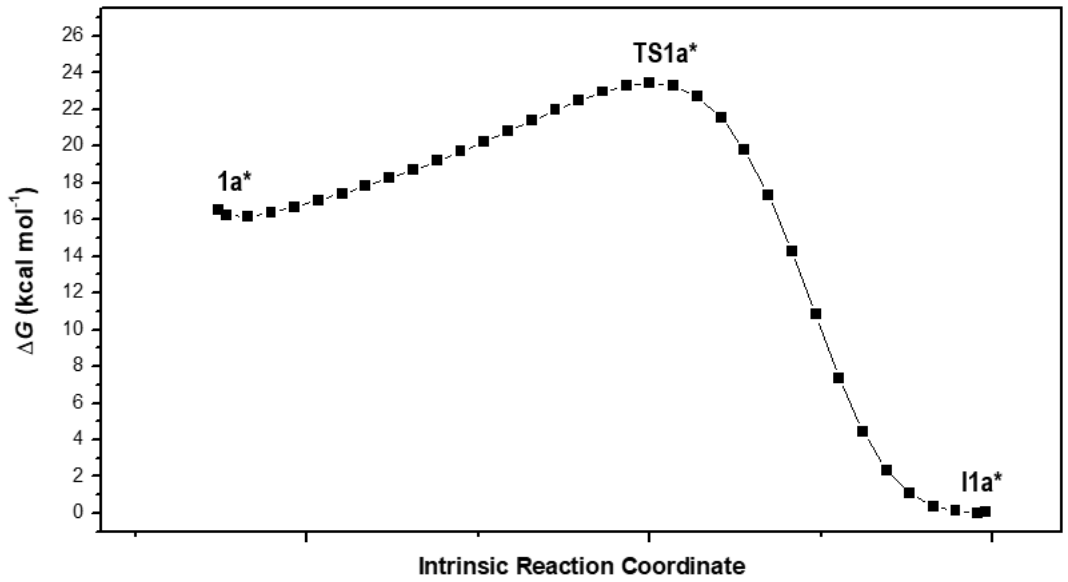
a)


TS1a
I1a
1a
ΔG (kcal mol-1)
Intrinsic Reaction Coordinate

b)


TS1aH+
1aH+
I1aH+
ΔG (kcal mol-1)
Intrinsic Reaction Coordinate

c)



d)

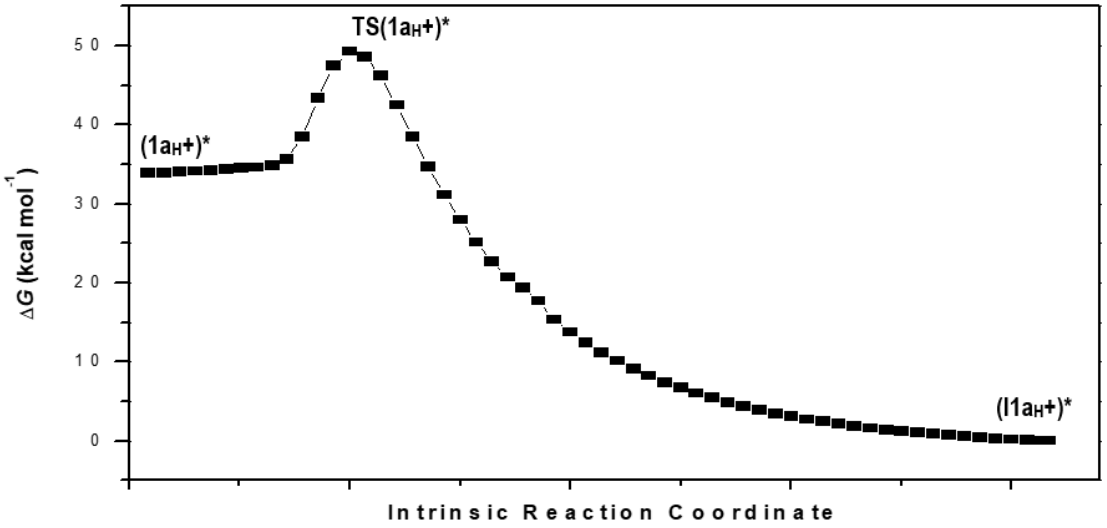


Figure S1: IRC calculation for the first reaction mechanism step (N_2 extrusion) for **a) 1a - TS1a - I1a** pathway (B3LYP/6-31+G* level) **b) $1a_H$+ - $TS1a_H$+ - $I1a_H$+** pathway (B3LYP/6-31+G* level) **c) 1a* - TS1a* - I1a*** pathway (CIS/6-31+G* level) **d) ($1a_H$+)* -$TS(1a_H+)$* - ($I1a_H$+)*** pathway (CIS/6-31+G* level).

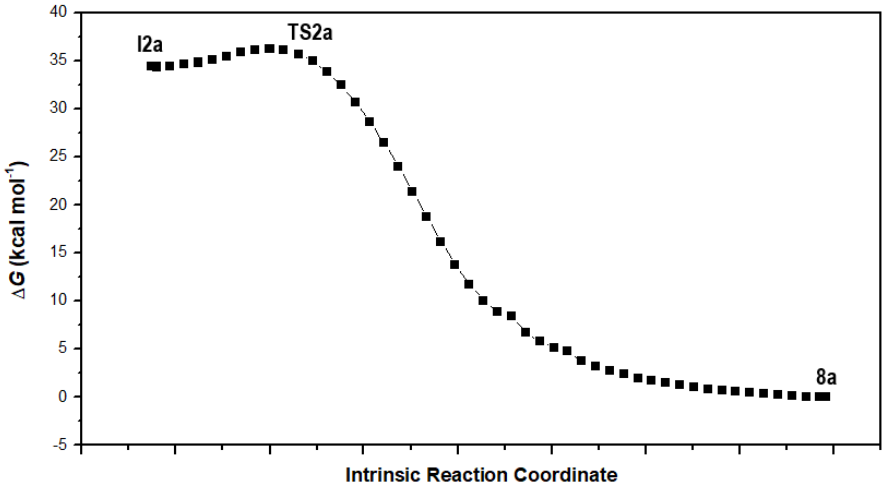


Figure S2: IRC calculation for the **I2a - TS2a - 8a** pathway calculated at the B3LYP/6-31+G* level.

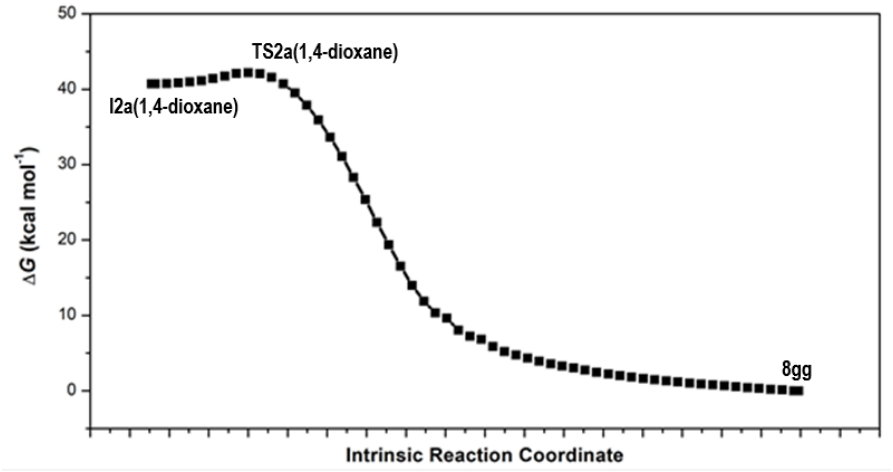
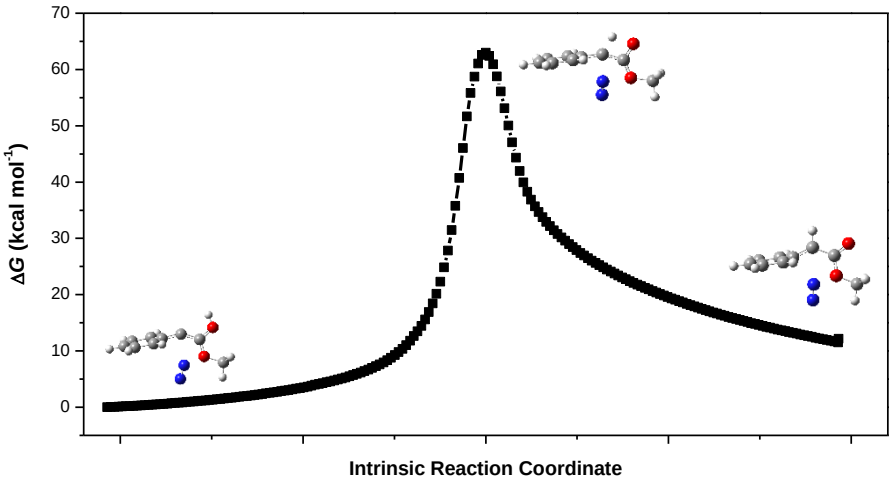


Figure S3: IRC calculation for the **I2a(1,4-dioxane) - TS2a(1,4-dioxane) – 8gg** pathway calculated at the B3LYP/6-31+G* level.

a)



b)

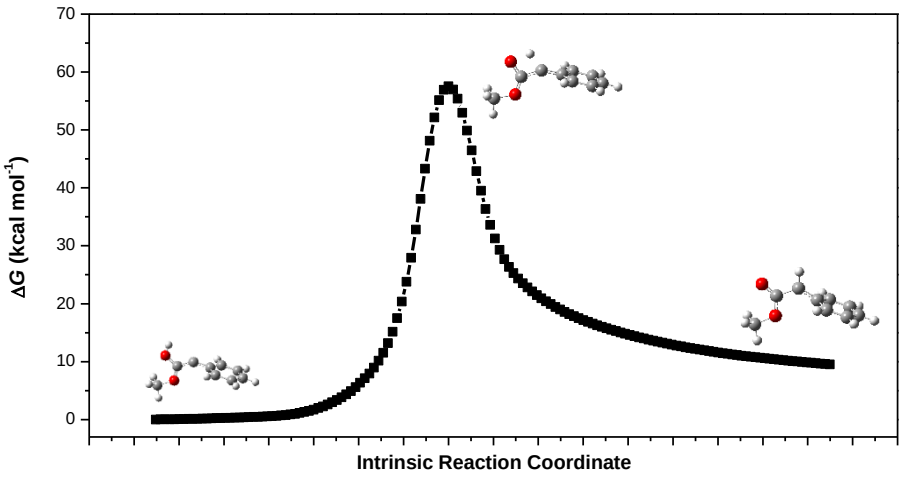


Figure S4: IRC calculation for intramolecular proton transfer event in the first excited state calculated at the CIS/6-31+G* level for **a) (1a$_H$+)*** and **b) (l1a$_H$+)***.

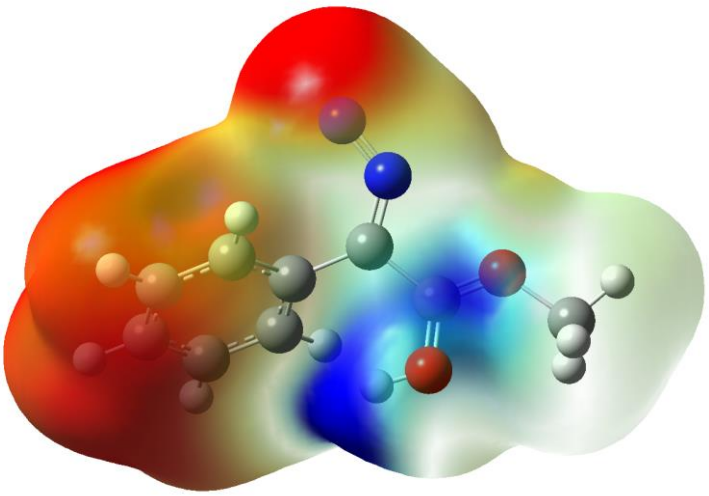


Figure S5: Calculated electrostatic profiles and dipole moments of **(1a$_H$+)***. Red–green–blue colour scales used, from 0.010 atomic units (au) to 0.020 au.

Cartesian coordinates obtained from B3LYP/6-31+G* (ground state) and CIS/6-31+G* (excited state) theoretical calculations for each species.

B3LYP/6-31+G*							
	1a				**TS1a**		
C	-1.619087	-0.007822	-1.218119	C	1.234111	-1.013191	-0.644441
C	-2.979688	-0.320071	-1.212407	C	2.563732	-1.315515	-0.922406
C	-3.657700	-0.471751	0.001666	C	3.588992	-0.562493	-0.333375
C	-2.979014	-0.314578	1.214701	C	3.284917	0.486607	0.542983
C	-1.618400	-0.002454	1.218353	C	1.954814	0.777915	0.835530
C	-0.933829	0.143293	-0.000425	C	0.903828	0.036908	0.246699
C	0.521144	0.482618	-0.001445	C	-0.460064	0.366418	0.611690
C	1.581524	-0.442477	-0.000028	C	-1.570798	-0.528650	0.404354
O	1.381348	-1.737248	-0.001483	O	-1.571258	-1.607885	1.006801
O	2.809577	-0.026177	0.003020	O	-2.622696	-0.081606	-0.315102
C	3.917052	-0.988475	0.002453	C	-3.808637	-0.904837	-0.284770
H	-1.088355	0.118276	-2.157545	H	0.438886	-1.591978	-1.105241
H	-3.509110	-0.439183	-2.152996	H	2.807175	-2.128189	-1.601072
H	-4.717439	-0.710475	0.002479	H	4.626587	-0.796346	-0.556987
H	-3.507956	-0.429494	2.156081	H	4.083485	1.063333	1.000836
H	-1.087097	0.127575	2.156925	H	1.703548	1.577736	1.526397
H	3.860746	-1.600791	0.902400	H	-4.182575	-0.996654	0.738035
H	4.806644	-0.363984	0.003264	H	-3.596959	-1.896327	-0.692074
H	3.861303	-1.599372	-0.898487	H	-4.531742	-0.382235	-0.910780
N	0.878381	1.773232	-0.002660	N	-0.922417	1.921969	-0.444534
N	1.126312	2.869816	-0.003974	N	-1.069318	3.021975	-0.508364
H	0.428994	-1.966188	-0.006468				
	$1a_H^+$				**$TS1a_H$+**		
C	-1.619087	-0.007822	-1.218119	C	-1.462591	-0.662431	-1.041322
C	-2.979688	-0.320071	-1.212407	C	-2.827698	-0.853619	-1.189555
C	-3.657700	-0.471751	0.001666	C	-3.705504	-0.409708	-0.187284
C	-2.979014	-0.314578	1.214701	C	-3.227222	0.223678	0.970449
C	-1.618400	-0.002454	1.218353	C	-1.863682	0.417403	1.132651
C	-0.933829	0.143293	-0.000425	C	-0.954425	-0.034579	0.134100
C	0.521144	0.482618	-0.001445	C	0.429494	0.135286	0.329729
C	1.581524	-0.442477	-0.000028	C	1.608465	-0.539328	0.177923
C	1.381348	-1.737248	-0.001483	O	1.728659	-1.792745	0.625400
O	2.809577	-0.026177	0.003020	O	2.702445	-0.000174	-0.304586
C	3.917052	-0.988475	0.002453	C	3.987059	-0.655996	-0.074319
H	-1.088355	0.118276	-2.157545	H	-0.769666	-0.987961	-1.811300
H	-3.509110	-0.439183	-2.152996	H	-3.218424	-1.338609	-2.078451
H	-4.717439	-0.710475	0.002479	H	-4.774551	-0.557679	-0.311538
H	-3.507956	-0.429494	2.156081	H	-3.922587	0.558363	1.733470
H	-1.087097	0.127575	2.156925	H	-1.469837	0.904033	2.019498
H	3.860746	-1.600791	0.902400	H	4.162879	-0.759073	0.997558
H	4.806644	-0.363984	0.003264	H	4.711026	0.019954	-0.524355
H	3.861303	-1.599372	-0.898487	H	4.000642	-1.626620	-0.570490
N	0.878381	1.773232	-0.002660	N	0.945765	1.914837	-0.304652
N	1.126312	2.869816	-0.003974	N	0.915332	3.020445	-0.344252
H	0.428994	-1.966188	-0.006468	H	0.900633	-2.140273	1.007182

		I1a				**I1a$_H$+**	
6	-0.990358	-1.054413	0.837051	C	1.611730	-0.986753	0.902776
6	-2.264501	-1.083547	1.382085	C	2.916384	-0.700633	1.244701
6	-3.354300	-0.618080	0.626528	C	3.689855	0.122426	0.401502
6	-3.177280	-0.125627	-0.674267	C	3.171998	0.667356	-0.788764
6	-1.903186	-0.100057	-1.225911	C	1.869138	0.389792	-1.149175
6	-0.773292	-0.558649	-0.486269	C	1.047674	-0.446248	-0.311265
6	0.498131	-0.477029	-1.103328	C	-0.243842	-0.703109	-0.685293
6	1.683414	-0.970658	-0.460566	C	-1.372706	-1.355745	-0.284881
8	2.052603	-2.137409	-0.629840	O	-1.756795	-2.536232	-0.769821
8	2.398578	-0.039812	0.206323	O	-2.220278	-0.750104	0.516410
6	3.707118	-0.439746	0.675275	C	-3.626652	-1.151891	0.509383
1	-0.143215	-1.413367	1.414595	H	0.991921	-1.615884	1.533459
1	-2.424631	-1.461476	2.387476	H	3.350408	-1.102143	2.154369
1	-4.351273	-0.641433	1.058736	H	4.717135	0.342069	0.678957
1	-4.031900	0.228352	-1.242772	H	3.797354	1.297226	-1.412408
1	-1.735337	0.272317	-2.231807	H	1.434569	0.790224	-2.059153
1	4.330342	-0.755597	-0.164942	H	-4.030637	-1.057619	-0.500031
1	3.622185	-1.252320	1.400653	H	-4.105907	-0.448717	1.187150
1	4.123392	0.450158	1.146691	H	-3.720125	-2.174075	0.876099
7	0.071833	3.665475	0.594135	N	-1.369591	3.750450	0.303941
7	0.563383	4.128522	-0.280432	N	-2.044166	4.559409	-0.029724
				H	-1.103304	-2.920573	-1.384568
		I2a				**TS2a**	
O	-1.154308	-0.790471	0.409436	O	1.527866	-1.069516	-0.068864
C	-2.527198	-0.703270	1.051054	C	-0.278919	-1.221088	-0.147236
C	-3.436367	-1.344028	0.015057	C	-0.316117	-2.124502	-1.349814
C	-2.510223	-2.286337	-0.777205	C	1.013820	-2.902431	-1.403544
C	-1.224897	-1.497163	-0.926971	C	2.110090	-1.882936	-1.146109
C	-0.146816	0.278226	0.698124	C	2.104558	0.213685	0.309019
C	1.230429	-0.199794	0.322125	C	3.577005	0.076700	0.642334
C	-0.601336	1.578375	0.018465	C	1.806654	1.282451	-0.752452
O	-1.477272	1.636895	-0.820929	O	1.493534	1.051049	-1.903569
O	0.094872	2.599912	0.498291	O	1.940738	2.497161	-0.220375
C	-0.196130	3.915410	-0.050246	C	1.700165	3.627314	-1.097224
C	3.062553	-0.394301	-1.254131	C	5.922662	0.127720	0.020699
C	1.788438	0.077845	-0.934994	C	4.576969	0.289970	-0.317465
C	1.962399	-0.948385	1.256920	C	3.941276	-0.296384	1.944423
C	3.235266	-1.420694	0.934361	C	5.286321	-0.460302	2.281381
C	3.785802	-1.144420	-0.321479	C	6.279256	-0.248458	1.319285
H	-0.225385	0.393118	1.780950	H	1.552929	0.479950	1.213386
H	-2.426080	-1.268668	1.977558	H	-0.371898	-1.659513	0.837284
H	-2.723815	0.349558	1.245614	H	-0.528554	-0.171324	-0.225447
H	-4.254762	-1.881795	0.500112	H	-1.162877	-2.807163	-1.256095
H	-3.860914	-0.579555	-0.641462	H	-0.452963	-1.529619	-2.257935
H	-2.327892	-3.215012	-0.227781	H	1.032995	-3.679740	-0.631224
H	-2.920802	-2.538005	-1.758500	H	1.155265	-3.386093	-2.374680
H	-0.314054	-2.087097	-0.993524	H	3.038497	-2.314213	-0.769239
H	-1.269791	-0.721890	-1.690767	H	2.297669	-1.242191	-2.008531
H	0.014926	3.921849	-1.121056	H	2.408947	3.610712	-1.927809

H	-1.242190	4.167034	0.132954	H	0.676079	3.591393	-1.473504
H	0.468122	4.593468	0.481863	H	1.854199	4.506221	-0.473473
H	3.489695	-0.173431	-2.227881	H	6.690066	0.298017	-0.729215
H	1.239126	0.662728	-1.668243	H	4.314308	0.584634	-1.330449
H	1.539257	-1.158018	2.236172	H	3.171131	-0.456856	2.694913
H	3.797881	-1.996009	1.663683	H	5.557765	-0.746284	3.293748
H	4.778817	-1.507746	-0.570549	H	7.326511	-0.371396	1.581668
				C	-7.350522	0.310156	0.602994
				C	-6.555072	1.459194	0.526333
				C	-5.169605	1.343748	0.383347
				C	-4.560108	0.082054	0.313871
				C	-5.365683	-1.064216	0.390752
				C	-6.751551	-0.952853	0.534862
				H	-8.428588	0.398286	0.714695
				H	-7.014451	2.443604	0.578191
				H	-4.543804	2.228819	0.323348
				H	-4.893103	-2.039910	0.336651
				H	-7.364142	-1.849553	0.593767
				C	-3.047821	-0.032273	0.157576
				O	-2.571996	-1.214866	0.079858
				O	-2.372172	1.029536	0.114419

8a

O	1.687085	-0.779091	0.602645
C	-1.318016	-1.238536	0.323562
C	-0.763304	-2.223181	-0.696498
C	0.661506	-2.717393	-0.388250
C	1.775225	-1.682503	-0.512516
C	2.549253	0.351823	0.617623
C	4.019208	0.032361	0.361406
C	2.018833	1.471667	-0.294437
O	1.181158	1.339254	-1.165623
O	2.595299	2.642191	0.022152
C	2.194075	3.797382	-0.749416
C	5.928749	-0.249303	-1.117706
C	4.586725	0.087632	-0.919578
C	4.820922	-0.365844	1.440869
C	6.162365	-0.704932	1.246110
C	6.719730	-0.646918	-0.035386
H	2.462085	0.735192	1.639533
H	-1.287780	-1.644705	1.339830
H	-0.787523	-0.286063	0.314352
H	-1.431729	-3.093291	-0.733177
H	-0.786265	-1.762407	-1.693061
H	0.701080	-3.161612	0.616001
H	0.897362	-3.525397	-1.093087
H	2.750480	-2.185595	-0.495604
H	1.685049	-1.129309	-1.455040
H	2.439370	3.649094	-1.803706
H	1.121092	3.969207	-0.637808
H	2.762689	4.629375	-0.335772

I2a(1,4-dioxane)

O	1.160911	-0.223091	-0.301493
O	3.695992	-1.199069	0.436031
C	2.513623	-1.835836	0.899385
C	1.375563	-0.845032	1.055324
C	-0.164363	0.480531	-0.633730
C	-1.312214	-0.432414	-0.330103
C	-0.189563	1.839269	0.076334
O	0.451277	2.096498	1.074700
O	-1.008000	2.656975	-0.570189
C	-1.201896	3.986900	-0.008543
C	-3.085588	-1.217818	1.126404
C	-2.025290	-0.345868	0.877648
C	-1.678281	-1.395663	-1.285833
C	-2.735871	-2.267839	-1.031288
C	-3.439080	-2.179701	0.174985
H	-0.056144	0.625738	-1.709369
H	2.222936	-2.649943	0.219860
H	2.736674	-2.258600	1.882521
H	0.435350	-1.332051	1.305349
H	1.596720	-0.023845	1.736868
H	-1.626041	3.903899	0.993576
H	-0.246330	4.513045	0.025282
H	-1.896336	4.476857	-0.688062
H	-3.635513	-1.144265	2.059865
H	-1.757401	0.397023	1.624293
H	-1.142446	-1.457201	-2.230218
H	-3.016995	-3.007753	-1.774628
H	-4.266499	-2.855842	0.370148

H	6.354738	-0.199825	-2.116364	C	3.493877	-0.622675	-0.844060
H	3.984949	0.395024	-1.771862	C	2.411599	0.441711	-0.796727
H	4.392334	-0.409351	2.439625	H	3.237828	-1.397130	-1.582021
H	6.771465	-1.007794	2.093789	H	4.433318	-0.148492	-1.140922
H	7.763994	-0.906139	-0.188922	H	2.167638	0.827042	-1.787144
C	-7.468144	0.449662	-0.506578	H	2.636699	1.247635	-0.096550
C	-6.964027	1.105440	0.622428				
C	-5.641066	0.901544	1.015053				
C	-4.811213	0.039520	0.281068				
C	-5.320363	-0.616781	-0.851295				
C	-6.644877	-0.410417	-1.241436				
H	-8.498905	0.608506	-0.812614				
H	-7.601089	1.774029	1.195021				
H	-5.238901	1.404700	1.888593				
H	-4.681378	-1.282662	-1.420767				
H	-7.034195	-0.920196	-2.118560				
C	-3.402433	-0.146067	0.739748				
O	-2.709886	-0.999483	-0.032860				
O	-2.923384	0.414414	1.716307				

TS2a(1,4-dioxane) **8gg**

O	-1.613217	1.071451	0.102800	O	1.888623	-0.936075	0.702992
O	-0.604972	3.559260	-0.758949	O	-0.478536	-2.712936	-0.002429
C	-1.995559	3.279246	-0.728633	C	0.907221	-2.903001	-0.264658
C	-2.287046	1.810068	-0.976699	C	1.697746	-1.631800	-0.537720
C	-1.923072	-0.358762	0.325078	C	2.661219	0.264184	0.704119
C	-3.409213	-0.575159	0.497850	C	4.023196	0.139508	0.027860
C	-1.280849	-1.222849	-0.768126	C	1.855674	1.452053	0.158864
O	-1.124391	-0.861576	-1.918008	O	1.011730	1.392063	-0.713280
O	-0.948337	-2.407758	-0.270406	O	2.214882	2.588123	0.780786
C	-0.209627	-3.296264	-1.148216	C	1.556184	3.797794	0.342126
C	-5.598110	-1.189231	-0.352542	C	5.489222	0.316108	-1.903266
C	-4.227570	-1.010164	-0.555414	C	4.229747	0.475197	-1.317909
C	-3.981164	-0.326291	1.755251	C	5.100798	-0.357338	0.775728
C	-5.350972	-0.501753	1.955503	C	6.359318	-0.519148	0.192504
C	-6.161655	-0.934182	0.900797	C	6.556327	-0.181380	-1.150330
H	-1.410769	-0.563776	1.266106	H	2.828273	0.461679	1.766488
H	-2.427442	3.593036	0.234397	H	1.378749	-3.464647	0.556149
H	-2.453535	3.868803	-1.528129	H	0.947855	-3.521753	-1.168130
H	-3.355371	1.600080	-0.901641	H	2.671022	-1.915602	-0.961874
H	-1.890726	1.458557	-1.930627	H	1.164725	-0.998977	-1.254617
H	-0.777757	-3.478884	-2.062767	H	0.477360	3.712112	0.490208
H	0.755577	-2.838634	-1.372162	H	1.971396	4.590608	0.963604
H	-0.083268	-4.214472	-0.576583	H	1.770852	3.981138	-0.713580
H	-6.222796	-1.530454	-1.173303	H	5.634776	0.581922	-2.947070
H	-3.800037	-1.210601	-1.534103	H	3.407615	0.860234	-1.915764
H	-3.350813	0.001619	2.578409	H	4.951400	-0.618398	1.821073
H	-5.782580	-0.310134	2.933941	H	7.185219	-0.901937	0.786457
H	-7.227390	-1.077219	1.057320	H	7.535981	-0.301998	-1.605418
C	7.063757	-0.673692	0.393778	C	-7.015770	0.272895	-1.388839
C	6.158296	-1.740297	0.366979	C	-6.626282	1.396763	-0.651599

C	4.785521	-1.491239	0.292258	C	-5.420381	1.387577	0.049023
C	4.299113	-0.176992	0.244522	C	-4.595730	0.252731	0.018313
C	5.213144	0.886289	0.274021	C	-4.988255	-0.873104	-0.722678
C	6.587066	0.640989	0.346830	C	-6.195409	-0.859548	-1.423635
H	8.132819	-0.865631	0.450914	H	-7.955337	0.280250	-1.935594
H	6.522856	-2.764532	0.404297	H	-7.261546	2.278107	-0.623806
H	4.070777	-2.308001	0.271296	H	-5.103162	2.251734	0.624119
H	4.831921	1.901998	0.238257	H	-4.347928	-1.747938	-0.749874
H	7.286146	1.474138	0.367158	H	-6.495079	-1.732160	-1.997956
C	2.799496	0.080007	0.163913	C	-3.315107	0.291549	0.783905
O	2.433347	1.305674	0.159705	O	-2.641712	-0.873167	0.727693
O	2.025412	-0.909932	0.112603	O	-2.916510	1.265627	1.403716
C	0.111190	2.900223	0.282713	C	-0.841367	-2.341909	1.326093
C	0.121550	1.403058	0.109410	C	-1.368636	-0.922751	1.414925
H	-0.310453	3.171270	1.261649	H	0.018124	-2.430846	2.001538
H	1.144038	3.243750	0.228341	H	-1.619230	-3.040498	1.660655
H	0.363112	0.776212	0.953196	H	-1.521589	-0.639703	2.462357
H	0.357200	0.997915	-0.863578	H	-0.685591	-0.210700	0.948253

CIS/6-31+G*

	1a*				**TS1a***		
C	-1.243423	-0.969119	-0.814412	C	1.406422	-1.202057	-0.243956
C	-2.554992	-1.412276	-0.790716	C	2.757159	-1.481623	-0.317657
C	-3.492825	-0.760357	-0.001179	C	3.694391	-0.472304	-0.124035
C	-3.124122	0.339006	0.762920	C	3.271396	0.821879	0.145775
C	-1.817444	0.794596	0.737563	C	1.920407	1.113143	0.220025
C	-0.870538	0.139598	-0.050786	C	0.962488	0.105665	0.023153
C	0.522309	0.637147	-0.093608	C	-0.440198	0.406845	0.072243
C	1.653699	-0.311873	0.162160	C	-1.566413	-0.527714	0.218927
O	1.471506	-1.416013	0.756188	O	-1.477498	-1.542382	0.851971
O	2.797217	0.002381	-0.203940	O	-2.655229	-0.133065	-0.390461
C	3.967134	-0.841685	0.063729	C	-3.827325	-0.932191	-0.246134
H	-0.531093	-1.468431	-1.447825	H	0.693644	-1.989252	-0.391843
H	-2.842992	-2.255810	-1.389799	H	3.080962	-2.484978	-0.526743
H	-4.509343	-1.107919	0.017895	H	4.744430	-0.695248	-0.180058
H	-3.850161	0.839882	1.375676	H	3.992178	1.603437	0.303387
H	-1.534432	1.641586	1.333797	H	1.607479	2.114470	0.441069
H	4.082007	-0.929847	1.130218	H	-4.100924	-1.004054	0.795570
H	4.779511	-0.301648	-0.383600	H	-3.657409	-1.917163	-0.653720
H	3.810689	-1.796461	-0.406936	H	-4.592805	-0.418887	-0.803543
N	0.919305	1.839914	-0.282311	N	-0.770869	1.986627	-0.164319
N	0.171954	2.814280	-0.508705	N	-1.768515	2.471286	-0.002289
H	0.568423	-1.581880	1.035673				

	(1a$_H$+)*				**TS(1a$_H$+)***		
C	-1.243423	-0.969119	-0.814412	C	-1.277118	-1.150467	-0.605158
C	-2.554992	-1.412276	-0.790716	C	-2.607079	-1.504858	-0.638879
C	-3.492825	-0.760357	-0.001179	C	-3.563889	-0.677259	-0.052860
C	-3.124122	0.339006	0.762920	C	-3.188197	0.508964	0.561707
C	-1.817444	0.794596	0.737563	C	-1.857775	0.884400	0.592179
C	-0.870538	0.139598	-0.050786	C	-0.880368	0.054224	0.015382
C	0.522309	0.637147	-0.093608	C	0.494661	0.444859	0.012125

C	1.653699	-0.311873	0.162160	C	1.660235	-0.370672	0.163550
O	1.471506	-1.416013	0.756188	O	1.629426	-1.525363	0.719723
O	2.797217	0.002381	-0.203940	O	2.768913	0.057723	-0.240265
C	3.967134	-0.841685	0.063729	C	4.005027	-0.689422	-0.041418
H	-0.531093	-1.468431	-1.447825	H	-0.550341	-1.778203	-1.088248
H	-2.842992	-2.255810	-1.389799	H	-2.905274	-2.414674	-1.125199
H	-4.509343	-1.107919	0.017895	H	-4.599643	-0.961384	-0.077637
H	-3.850161	0.839882	1.375676	H	-3.928408	1.137849	1.019559
H	-1.534432	1.641586	1.333797	H	-1.573402	1.788694	1.092763
H	4.082007	-0.929847	1.130218	H	4.147346	-0.850831	1.013433
H	4.779511	-0.301648	-0.383600	H	4.763707	-0.049035	-0.450403
H	3.810689	-1.796461	-0.406936	H	3.935805	-1.617995	-0.581934
N	0.919305	1.839914	-0.282311	N	0.931296	1.958204	-0.231656
N	0.171954	2.814280	-0.508705	N	0.215340	2.793444	-0.449932
H	0.568423	-1.581880	1.035673	H	0.784051	-1.773470	1.093348
		I1a*				**(I1a$_H$+)***	
C	-1.872248	-1.288501	-0.053334	C	-1.872970	-0.924277	-1.079543
C	-3.251603	-1.181895	-0.048823	C	-3.246445	-0.856559	-0.934388
C	-3.860783	0.067166	0.003125	C	-3.800824	-0.142378	0.120650
C	-3.084736	1.216834	0.051654	C	-2.986618	0.512365	1.036263
C	-1.702648	1.122534	0.047855	C	-1.611363	0.454413	0.904704
C	-1.078845	-0.129429	-0.004778	C	-1.046051	-0.279673	-0.148224
C	0.349124	-0.211504	-0.011754	C	0.368631	-0.340355	-0.289960
C	1.408425	-1.187769	0.005141	C	1.524775	-1.056411	0.060412
O	1.205365	-2.373551	0.029138	O	1.514036	-2.095936	0.817069
O	2.608759	-0.647770	-0.008520	O	2.640047	-0.667620	-0.380288
C	3.729595	-1.526132	0.010521	C	3.877461	-1.358096	-0.045792
H	-1.403311	-2.252595	-0.092517	H	-1.438849	-1.465917	-1.898838
H	-3.852660	-2.072522	-0.085768	H	-3.881565	-1.354673	-1.642890
H	-4.933252	0.141682	0.005779	H	-4.868770	-0.091349	0.226342
H	-3.553038	2.183554	0.092128	H	-3.421079	1.068872	1.845680
H	-1.099958	2.010657	0.086443	H	-0.976775	0.966668	1.603127
H	3.717193	-2.167866	-0.857675	H	4.021720	-1.313965	1.020453
H	3.722041	-2.122637	0.910506	H	4.634372	-0.804960	-0.569600
H	4.595775	-0.885452	-0.008043	H	3.815854	-2.374142	-0.396512
N	2.012145	3.323833	0.512388	N	1.751637	3.485641	0.134381
N	2.055932	3.540155	-0.542879	N	1.247572	4.196904	-0.499860
				H	0.648393	-2.354082	1.131618