

Domino construction of a bullataketal core *via* double bond cleavage in activated dihydrofurans

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General information

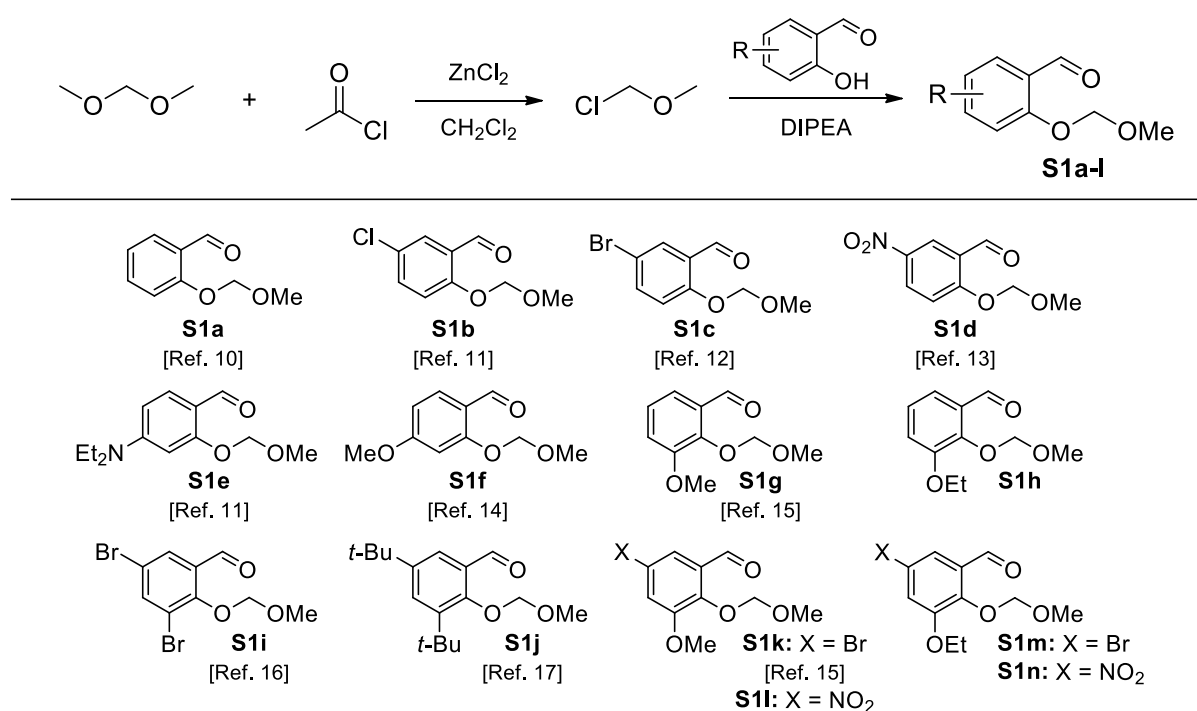
NMR spectra were acquired either on Bruker Avance 400 MHz or on Bruker Avance 600 MHz spectrometers at room temperature. The structures of compounds were elucidated with the aid of 1D NMR (^1H , ^{13}C) and 2D NMR (^1H – ^1H COSY, ^1H – ^1H NOESY, ^1H – ^{13}C HSQC, ^1H – ^{13}C HMBC) spectroscopy. The chemical shifts δ were measured in ppm with respect to solvent (^1H : CDCl_3 , δ = 7.27 ppm; ^{13}C : CDCl_3 , δ = 77.0 ppm). High resolution mass spectra (HRMS) were obtained using Thermo ScientificTM LTQ Orbitrap and AB Sciex TripleTOF 5600+ mass spectrometers with a TurboV ESI source. Single crystal X-ray analysis was performed with Enraf-Nonius CAD-4 and Bruker SMART APEX II diffractometers. Crystallographic data were collected at 298 and 150 K, respectively, using graphite monochromatized Cu K α (λ = 1.5418 Å) or Mo K α radiation (λ = 0.71073 Å) using a ω -scan mode. Absorption corrections based on measurements of equivalent reflections were applied (APEX II). The data were corrected for Lorentz and polarization effects (CAD 4). The structures were solved by direct methods and refined by full matrix least-squares on F² with anisotropic thermal parameters for all non-hydrogen atoms. Elemental analyses were performed with Fisons EA-1108 CHNS elemental analyser instrument. Melting points (mp) were determined using Electrothermal IA 9100 capillary melting point apparatus. Analytical thin layer chromatography (TLC) was carried out with silica gel plates (silica gel 60, F₂₅₄, supported on aluminium) visualized with UV lamp (254 nm). Column chromatography was performed on silica gel 60 (230-400 mesh).

All the calculations reported in this paper have been performed within density functional theory (DFT),¹ using the hybrid functional B3LYP.^{2,3} The standard def2-SVP basis set,⁴ as implemented in the ORCA 3.0 suite of programs,⁵ have been used in all cases together with the RIJCOSX approximation.⁶ The solvent effects were estimated using the continuous solvation model COSMO⁷ with ethanol as a solvent. Frequency analysis was carried out to check whether optimized structures were local minima or transition states. No imaginary frequencies were found for local minima, and only one imaginary frequency was found for each transition state. Computed structures were visualized using CYLview 1.0b.⁸

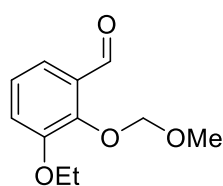
General procedure for the synthesis of protected salicylaldehydes **S1**

Following the described procedure,⁹ to a solution of dimethoxymethane (2.28 g, 2.65 mL, 30 mmol) and anhydrous ZnCl₂ (5 mg) in CH₂Cl₂ (8 mL) acetyl chloride (2.36 g, 2.13 mL, 30 mmol) was added dropwise. Reaction temperature (gentle reflux) was maintained by an ambient temperature external water bath. Then, the reaction was allowed to cool to ambient temperature (*ca.* 30 min). To the resulting solution the corresponding salicylaldehyde (15 mmol) and diisopropylethylamine (3.87 g, 5.22 mL, 30 mmol) were sequentially added and the resulting slurry was stirred for 24 h. The reaction mixture was quenched with saturated aqueous NaHCO₃ solution (15 mL), organic layer was separated, water layer was extracted with CH₂Cl₂ (15 mL). Combined organic fractions were washed twice with water, dried with Na₂SO₄ and concentrated under reduced pressure. Obtained MOM-aldehydes **S1** (Scheme S1) were used in the next step without purification.

Scheme S1. Synthesis of MOM-aldehydes **S1**^{10–17}



3-Ethoxy-2-(methoxymethoxy)benzaldehyde (S1h)



S1h was synthesized from 3-ethoxy-2-hydroxybenzaldehyde (2.49 g, 15 mmol).

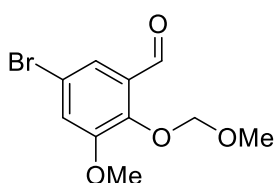
Yield 2.84 g (90%); yellowish oil; R_f = 0.31 (diethyl ether : petroleum ether; 1:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.41 (t, 3J = 7.0 Hz, 3H, CH_3), 3.52 (s, 3H, CH_3O), 4.04 (q, 3J = 7.0 Hz, 2H, CH_2O), 5.22 (s, 2H, OCH_2O), 7.07 (dd, 3J = 8.0, 3J = 6.9 Hz, 1H, Ar), 7.09 (dd, 3J = 8.0, 4J = 2.5 Hz, 1H, Ar), 7.37 (dd, 3J = 6.9, 4J = 2.5 Hz, 1H, Ar), 10.44 (s, 1H, CHO).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.6 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 57.6 ($^1J_{\text{CH}}$ = 143 Hz, CH_3O), 64.5 ($^1J_{\text{CH}}$ = 144 Hz, CH_2O), 99.2 ($^1J_{\text{CH}}$ = 168 Hz, OCH_2O), 118.8 (CH, Ar), 118.9 (CH, Ar), 124.2 (CH, Ar), 130.2 (C, Ar), 149.3 (C, Ar), 151.6 (C, Ar), 190.2 (CHO).

HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{11}\text{H}_{14}\text{NaO}_4^+$ 233.0784; Found 233.0785.

5-Brom-3-methoxy-2-(methoxymethoxy)benzaldehyde (S1k)



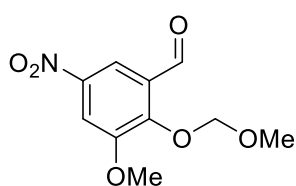
S1k was synthesized from 5-bromo-2-hydroxy-3-methoxybenzaldehyde (5.47 g, 23.7 mmol). Yield 5.93 g (91%); yellowish solid, mp 68–69 °C; R_f = 0.63 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 3.50 (s, 3H, CH_3O), 3.84 (s, 3H, CH_3O), 5.16 (s, 2H, OCH_2O), 7.18 (d, 4J = 2.3 Hz, 1H, Ar), 7.47 (d, 4J = 2.3 Hz, 1H, Ar), 10.32 (s, 1H, CHO).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 56.2 ($^1J_{\text{CH}}$ = 145 Hz, CH_3O), 57.8 ($^1J_{\text{CH}}$ = 143 Hz, CH_3O), 99.2 ($^1J_{\text{CH}}$ = 169 Hz, OCH_2O), 117.1 (C, Ar), 120.5 (CH, Ar), 121.5 (CH, Ar), 131.0 (C, Ar), 148.4 (C, Ar), 153.2 (C, Ar), 188.7 (CHO).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{10}\text{H}_{12}\text{BrO}_4^+$ 274.9913; Found 274.9919.

3-Methoxy-2-(methoxymethoxy)-5-nitrobenzaldehyde (S1l)



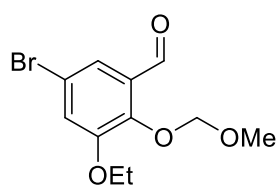
S1l was synthesized from 2-hydroxy-3-methoxy-5-nitrobenzaldehyde (12.5 g, 63.4 mmol). Yield 13.6 g (89%); white solid, mp 96–97 °C; R_f = 0.71 (petroleum ether : ethyl acetate, 1:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 3.55 (s, 3H, CH_3O), 3.98 (s, 3H, CH_3O), 5.36 (s, 2H, OCH_2O), 7.92 (d, 4J = 2.6 Hz, 1H, Ar), 8.25 (d, 4J = 2.6 Hz, 1H, Ar), 10.42 (s, 1H, CHO).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 56.6 (CH_3O), 58.0 (CH_3O), 99.4 (OCH_2O), 111.3 (CH, Ar), 115.0 (CH, Ar), 129.4 (C, Ar), 143.8 (C, Ar), 152.8 (C, Ar), 154.0 (C, Ar), 188.0 (CHO).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{10}\text{H}_{12}\text{NO}_6^+$ 242.0659; Found 242.0661.

5-Brom-3-ethoxy-2-(methoxymethoxy)benzaldehyde (S1m)



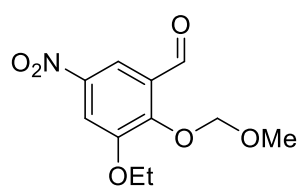
S1m was synthesized from 5-bromo-3-ethoxy-2-hydroxybenzaldehyde (5.53 g, 22.6 mmol). Yield 6.14 g (94%); colorless solid, mp 69–70 °C; R_f = 0.66 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.46 (t, 3J = 7.0 Hz, 3H, CH_3), 3.54 (s, 3H, CH_3O), 4.07 (q, 3J = 7.0 Hz, 2H, CH_2O), 5.22 (s, 2H, OCH_2O), 7.20 (d, 4J = 2.4 Hz, 1H, Ar), 7.51 (d, 4J = 2.4 Hz, 1H, Ar), 10.37 (s, 1H, CHO).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.6 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 57.9 ($^1J_{\text{CH}}$ = 143 Hz, CH_3O), 65.0 ($^1J_{\text{CH}}$ = 145 Hz, CH_2O), 99.2 ($^1J_{\text{CH}}$ = 168 Hz, OCH_2O), 117.2 (C, Ar), 121.5 (CH, Ar), 121.6 (CH, Ar), 131.1 (C, Ar), 148.6 (C, Ar), 152.6 (C, Ar), 188.9 (CHO).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{11}\text{H}_{14}\text{BrO}_4^+$ 289.0070; Found 289.0074.

3-Ethoxy-2-(methoxymethoxy)-5-nitrobenzaldehyde (S1n)



S1n was synthesized from 3-ethoxy-2-hydroxy-5-nitrobenzaldehyde (6.30 g, 29.9 mmol). In this case, product was isolated by filtration from the quenched reaction mixture. Yield 6.28 g (83%); yellowish solid, mp 84–85 °C; R_f = 0.83 (petroleum ether : ethyl acetate, 1:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.53 (t, 3J = 7.0 Hz, 3H, CH_3), 3.58 (s, 3H, CH_3O), 4.21 (q, 3J = 7.0 Hz, 2H, CH_2O), 5.41 (s, 2H, OCH_2O), 7.94 (d, 4J = 2.7 Hz, 1H, Ar), 8.31 (d, 4J = 2.7 Hz, 1H, Ar), 10.47 (s, 1H, CHO).

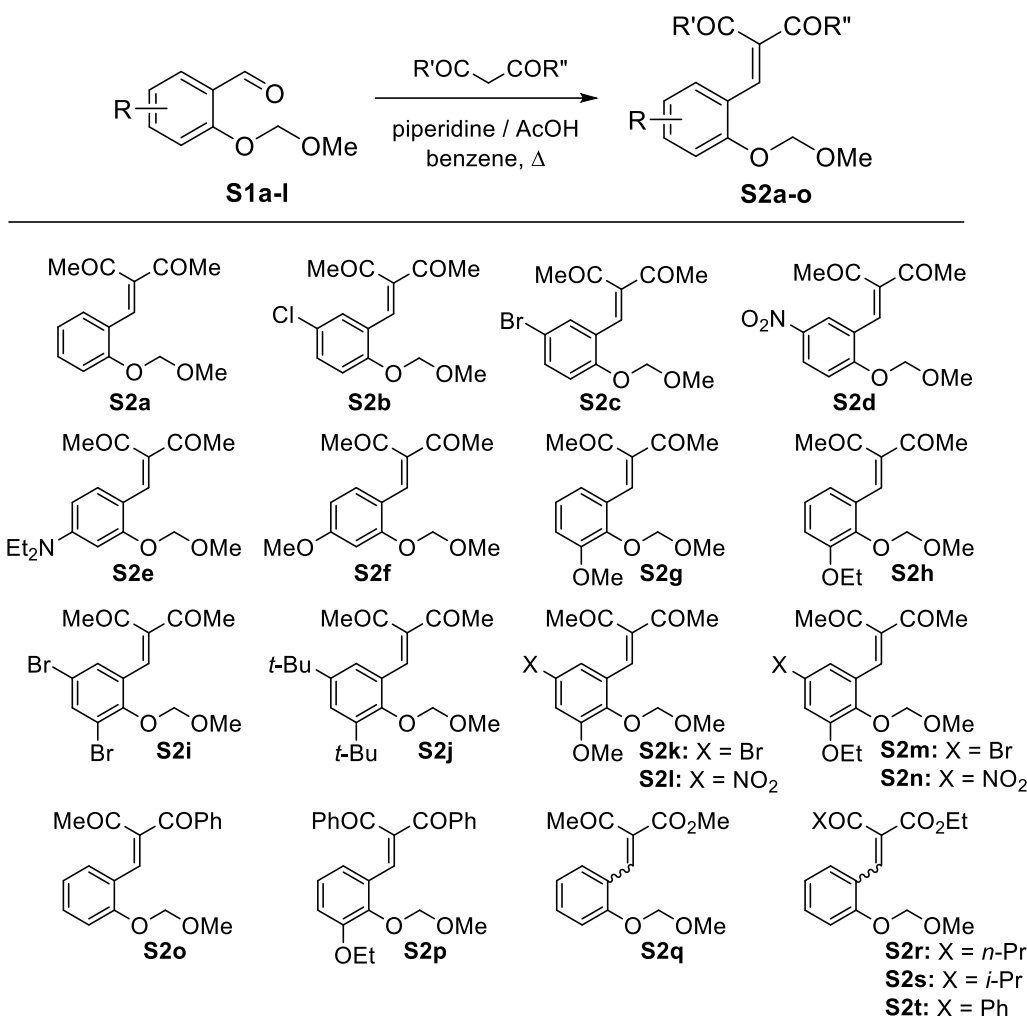
^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.5 (CH_3), 58.1 (CH_3O), 65.6 (CH_2O), 99.4 (OCH_2O), 112.1 (CH, Ar), 115.1 (CH, Ar), 129.5 (C, Ar), 143.9 (C, Ar), 152.2 (C, Ar), 154.1 (C, Ar), 188.2 (CHO).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{11}\text{H}_{14}\text{NO}_6^+$ 256.0816; Found 256.0816.

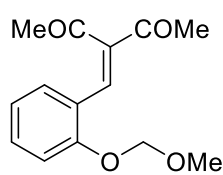
General procedure for the synthesis of alkenes **S2**

Alkenes **S2** were synthesized *via* Knoevenagel condensation under piperidinium acetate catalysis. Mixture of corresponding *o*-methoxymethylbenzaldehyde **S1** (1 equiv), methylene compound (1 equiv), piperidine (0.05 equiv) and acetic acid (0.2 equiv) in benzene (1.0–1.5 M) was heated under reflux with 20-mL Dean-Stark trap for specified time. After cooling to the ambient temperature, reaction mixture was diluted with ethyl acetate and washed twice with brine, dried with Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether – ethyl acetate) yielding alkene **S2** (Scheme S2). It should be noted that partial decomposition of the target alkenes **S2** was detected during purification, leading to the initial aldehydes **S1**. In most cases parent aldehydes **S1** were isolated in 3–7% yield, while for **S2e,f**, containing electron-abundant groups, these values reached 12–15%. Taking this into account, one needs to know that the crude reaction product can be used in the next step without purification.

Scheme S2. Synthesis of Knoevenagel alkenes S2



3-[[2-(Methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2a)



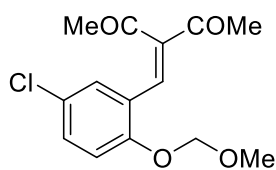
S2a was synthesized from aldehyde **S1a** (16.6 g, 0.1 mol) and acetylacetone (10.8 mL, 0.105 mol). Reaction time 2 h. Yield 20.1 g (81%); yellow oil; R_f = 0.30 (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 2.19 (s, 3H, CH_3), 2.38 (s, 3H, CH_3), 3.46 (s, 3H, CH_3O), 5.21 (s, 2H, OCH_2O), 6.91–6.94 (m, 1H, Ar), 7.13 (d, 3J = 8.4 Hz, 1H, Ar), 7.21–7.24 (m, 1H, Ar), 7.30–7.33 (m, 1H, Ar), 7.82 (s, 1H, CH=).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 26.5 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 31.3 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 56.2 ($^1J_{\text{CH}}$ = 143 Hz, CH_3O), 94.6 ($^1J_{\text{CH}}$ = 166 Hz, OCH_2O), 114.5 (CH, Ar), 121.8 (CH, Ar), 122.7 (C, Ar), 129.7 (CH, Ar), 132.0 (CH, Ar), 135.6 (CH=), 142.4 (C=), 155.5 (C, Ar), 196.5 (CO), 205.0 (CO).

HRMS (ESI) m/z : $[M + Na]^+$ Calcd for $C_{14}H_{16}NaO_4^+$ 271.0941; Found 271.0942.

3-[[5-Chloro-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2b)



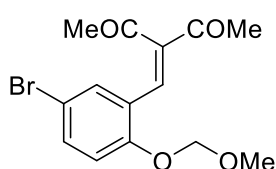
S2b was synthesized from aldehyde **S1b** (2.20 g, 11.0 mmol) and acetylacetone (1.13 mL, 11.0 mmol). Reaction time 2 h. Yield 2.39 g (77%); yellow oil; R_f = 0.30 (petroleum ether : ethyl acetate, 3:1).

1H NMR ($CDCl_3$, 600 MHz) δ = 2.24 (s, 3H, CH_3), 2.41 (s, 3H, CH_3), 3.48 (s, 3H, CH_3O), 5.21 (s, 2H, OCH_2O), 7.12 (d, 3J = 8.9 Hz, 1H, Ar), 7.21 (d, 4J = 2.4 Hz, 1H, Ar), 7.28 (dd, 3J = 8.9 Hz, 4J = 2.4 Hz, 1H, Ar), 7.68 (s, 1H, $CH=$).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 26.7 (CH_3), 31.4 (CH_3), 56.4 (CH_3O), 94.9 (OCH_2O), 115.9 (CH, Ar), 124.3 (C, Ar), 127.0 (C, Ar), 129.3 (CH, Ar), 131.5 (CH, Ar), 134.2 ($CH=$), 143.4 ($C=$), 154.0 (C, Ar), 196.4 (CO), 204.2 (CO).

HRMS (ESI) m/z : $[M + Na]^+$ Calcd for $C_{14}H_{15}ClNaO_4^+$ 305.0551; Found 305.0553.

3-[[5-Bromo-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2c)



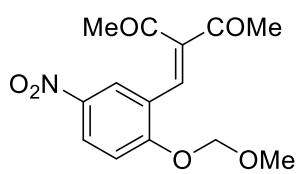
S2c was synthesized from aldehyde **S1c** (2.69 g, 11.0 mmol) and acetylacetone (1.13 mL, 11.0 mmol). Reaction time 2 h. Yield 2.91 g (81%); yellow oil; R_f = 0.36 (petroleum ether : ethyl acetate, 3:1).

1H NMR ($CDCl_3$, 600 MHz) δ = 2.26 (s, 3H, CH_3), 2.42 (s, 3H, CH_3), 3.49 (s, 3H, CH_3O), 5.22 (s, 2H, OCH_2O), 7.08 (d, 3J = 8.8 Hz, 1H, Ar), 7.36 (d, 4J = 2.4 Hz, 1H, Ar), 7.44 (dd, 3J = 8.8 Hz, 4J = 2.4 Hz, 1H, Ar), 7.68 (s, 1H, $CH=$).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 26.8 ($^1J_{CH}$ = 128 Hz, CH_3), 31.4 ($^1J_{CH}$ = 129 Hz, CH_3), 56.4 ($^1J_{CH}$ = 143 Hz, CH_3O), 94.9 ($^1J_{CH}$ = 166 Hz, OCH_2O), 114.3 (C, Ar), 116.3 (CH, Ar), 124.9 (C, Ar), 132.3 (CH, Ar), 134.2 ($CH=$), 134.5 (CH, Ar), 143.5 ($C=$), 154.5 (C, Ar), 196.4 (CO), 204.1 (CO).

HRMS (ESI) m/z : $[M + Na]^+$ Calcd for $C_{14}H_{15}BrNaO_4^+$ 349.0046; Found 349.0048.

3-{{2-(Methoxymethoxy)-5-nitrophenyl}methylidene}pentane-2,4-dione (S2d)



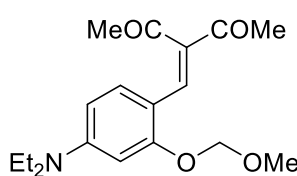
S2d was synthesized from aldehyde **S1d** (1.82 g, 8.6 mmol) and acetylacetone (0.89 mL, 8.6 mmol). Reaction time 2 h. Yield 1.94 g (77%); yellow solid, mp 74–75 °C; R_f = 0.54 (petroleum ether : ethyl acetate, 1:1).

^1H NMR (CDCl_3 , 400 MHz) δ = 2.23 (s, 3H, CH_3), 2.40 (s, 3H, CH_3), 3.46 (s, 3H, CH_3O), 5.31 (s, 2H, OCH_2O), 7.24 (d, 3J = 9.2 Hz, 1H, Ar), 7.62 (s, 1H, CH=), 8.06 (d, 4J = 2.7 Hz, 1H, Ar), 8.13 (dd, 3J = 9.2 Hz, 4J = 2.7 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 100 MHz) δ = 26.4 (CH_3), 31.2 (CH_3), 56.7 (CH_3O), 94.8 (OCH_2O), 114.2 (CH, Ar), 123.2 (C, Ar), 125.2 (CH, Ar), 126.8 (CH, Ar), 133.3 (CH=), 141.5 (C, Ar), 144.5 (C=), 159.7 (C, Ar), 196.5 (CO), 203.5 (CO).

HRMS (ESI) m/z : $[\text{M} + \text{K}]^+$ Calcd for $\text{C}_{14}\text{H}_{15}\text{KNO}_6^+$ 332.0531; Found 332.0533.

3-{{4-(Diethylamino)-2-(methoxymethoxy)phenyl}methylidene}pentane-2,4-dione (S2e)



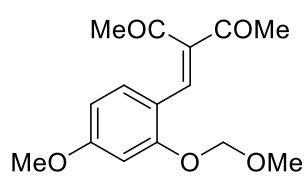
S2e was synthesized from aldehyde **S1e** (2.44 g, 10.3 mmol) and acetylacetone (1.06 mL, 10.3 mmol). Reaction time 5 h; conversion 90%. Yield 2.42 g (74%); yellow oil; R_f = 0.33 (petroleum ether : ethyl acetate, 2:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.15 (t, 3J = 7.1 Hz, 6H, $2\times\text{CH}_3$), 2.30 (s, 3H, CH_3), 2.34 (s, 3H, CH_3), 3.35 (q, 3J = 7.1 Hz, 4H, $2\times\text{CH}_2\text{N}$), 3.49 (s, 3H, CH_3O), 5.20 (s, 2H, OCH_2O), 6.23 (dd, 3J = 8.9 Hz, 4J = 2.5 Hz, 1H, Ar), 6.40 (d, 4J = 2.5 Hz, 1H, Ar), 7.12 (d, 3J = 8.9 Hz, 1H, Ar), 7.85 (s, 1H, CH=).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 12.4 ($^1J_{\text{CH}}$ = 126 Hz, $2\times\text{CH}_3$), 26.2 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 31.4 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 44.5 ($^1J_{\text{CH}}$ = 135 Hz, $2\times\text{CH}_2\text{N}$), 56.1 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 94.8 ($^1J_{\text{CH}}$ = 166 Hz, OCH_2O), 96.9 (CH, Ar), 105.4 (CH, Ar), 109.4 (C, Ar), 131.3 (CH, Ar), 135.9 (CH=), 136.5 (C=), 151.3 (C, Ar), 158.4 (C, Ar), 196.3 (CO), 207.0 (CO).

HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{18}\text{H}_{25}\text{NNaO}_4^+$ 342.1676; Found 342.1676.

3-[[4-Methoxy-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2f)



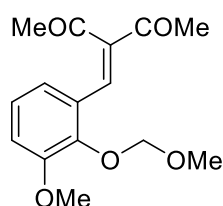
S2f was synthesized from aldehyde **S1f** (4.96 g, 25.3 mmol) and acetylacetone (2.60 mL, 25.3 mmol). Reaction time 4 h. Yield 5.28 g (75%); yellow oil; R_f = 0.44 (petroleum ether : ethyl acetate, 2:1).

^1H NMR (CDCl_3 , 400 MHz) δ = 2.27 (s, 3H, CH_3), 2.40 (s, 3H, CH_3), 3.51 (s, 3H, CH_3O), 3.81 (s, 3H, CH_3O), 5.23 (s, 2H, OCH_2O), 6.51 (dd, 3J = 8.7 Hz, 4J = 2.4 Hz, 1H, Ar), 6.74 (d, 4J = 2.4 Hz, 1H, Ar), 7.22 (d, 3J = 8.7 Hz, 1H, Ar), 7.82 (s, 1H, $\text{CH}=\text{C}$).

^{13}C NMR (CDCl_3 , 100 MHz) δ = 26.6 (CH_3), 31.5 (CH_3), 55.5 (CH_3O), 56.4 (CH_3O), 94.8 (OCH_2O), 101.3 (CH, Ar), 107.2 (CH, Ar), 115.3 (C, Ar), 131.1 (CH, Ar), 135.4 ($\text{CH}=\text{C}$), 140.3 ($\text{C}=\text{C}$), 157.4 (C, Ar), 163.2 (C, Ar), 196.7 (CO), 206.1 (CO).

HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{15}\text{H}_{18}\text{NaO}_5^+$ 301.1046; Found 301.1048.

3-[[3-Methoxy-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2g)



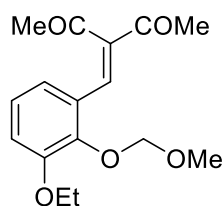
S2g was synthesized from aldehyde **S1g** (7.85 g, 40 mmol) and acetylacetone (4.11 mL, 40 mmol). Reaction time 4 h. Yield 9.03 g (81%); yellow oil; R_f = 0.45 (petroleum ether : ethyl acetate, 2:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 2.20 (s, 3H, CH_3), 2.41 (s, 3H, CH_3), 3.56 (s, 3H, CH_3O), 3.85 (s, 3H, CH_3O), 5.14 (s, 2H, OCH_2O), 6.86 (ddd, 3J = 7.9, 4J = 1.5, 4J = 0.8 Hz, 1H, Ar), 6.97 (dd, 3J = 8.3, 4J = 1.5 Hz, 1H, Ar), 7.01–7.04 (m, 1H, Ar), 7.92 (br.s, 1H, $\text{CH}=\text{C}$).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 26.6 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 31.4 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 55.8 ($^1J_{\text{CH}}$ = 145 Hz, CH_3O), 57.6 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 99.2 ($^1J_{\text{CH}}$ = 168 Hz, OCH_2O), 114.5 (CH, Ar), 121.2 (CH, Ar), 124.6 (CH, Ar), 128.1 (C, Ar), 136.4 ($\text{CH}=\text{C}$), 143.1 ($\text{C}=\text{C}$), 144.9 (C, Ar), 152.2 (C, Ar), 196.4 (CO), 205.0 (CO).

HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{15}\text{H}_{18}\text{NaO}_5^+$ 301.1046; Found 301.1049.

3-[[3-Ethoxy-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2h)



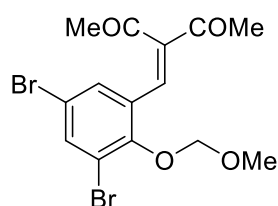
S2h was synthesized from aldehyde **S1h** (4.10 g, 19.5 mmol) and acetylacetone (2.00 mL, 19.5 mmol). Reaction time 4 h. Yield 3.42 g (60%); yellow oil; R_f = 0.30 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 400 MHz) δ = 1.35 (t, 3J = 7.0 Hz, 3H, CH_3), 2.13 (s, 3H, CH_3), 2.33 (s, 3H, CH_3), 3.49 (s, 3H, CH_3O), 3.98 (q, 3J = 7.0 Hz, 2H, CH_2O), 5.10 (s, 2H, OCH_2O), 6.76 (dd, 3J = 7.3, 4J = 2.0 Hz, 1H, Ar), 6.87–6.94 (m, 2H, Ar), 7.85 (s, 1H, CH=).

^{13}C NMR (CDCl_3 , 100 MHz) δ = 14.5 (CH_3), 26.3 (CH_3), 31.1 (CH_3), 57.3 (CH_3O), 64.0 (CH_2O), 98.8 (OCH_2O), 115.2 (CH, Ar), 120.7 (CH, Ar), 124.3 (CH, Ar), 127.8 (C, Ar), 136.1 (CH=), 142.8 (C=), 144.8 (C, Ar), 151.3 (C, Ar), 196.2 (CO), 204.7 (CO).

HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{16}\text{H}_{20}\text{NaO}_5^+$ 315.1203; Found 315.1205.

3-[[3,5-Dibromo-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2i)



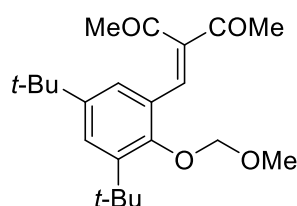
S2i was synthesized from aldehyde **S1i** (3.25 g, 10.0 mmol) and acetylacetone (1.03 mL, 10.0 mmol). Reaction time 1.5 h. Yield 3.36 g (83%); yellow oil; R_f = 0.47 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 400 MHz) δ = 2.23 (s, 3H, CH_3), 2.41 (s, 3H, CH_3), 3.58 (s, 3H, CH_3O), 5.08 (s, 2H, OCH_2O), 7.32 (d, 4J = 2.3 Hz, 1H, Ar), 7.70 (s, 1H, CH=), 7.73 (d, 4J = 2.3 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 100 MHz) δ = 26.8 (CH_3), 31.3 (CH_3), 58.1 (CH_3O), 100.5 (OCH_2O), 117.7 (C, Ar), 118.8 (C, Ar), 131.2 (C, Ar), 131.4 (CH, Ar), 134.5 (CH=), 137.3 (CH, Ar), 144.5 (C=), 152.6 (C, Ar), 196.0 (CO), 203.6 (CO).

HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{14}\text{H}_{14}\text{Br}_2\text{NaO}_4^+$ 426.9151; Found 426.9152.

3-[[3,5-Bis(*tert*-butyl)-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2j)



S2j was synthesized from aldehyde **S1j** (2.38 g, 8.5 mmol, from 3.24 g of 70:30 mixture of **S1j** with unprotected aldehyde) and acetylacetone (1.29 mL,

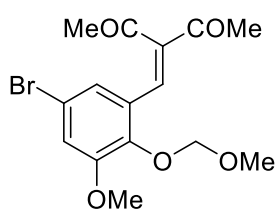
12.5 mmol). Reaction time 3 h. Yield 2.53 g (82%); yellow solid, mp 79–80 °C; R_f = 0.63 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.26 (s, 9H, $3\times\text{CH}_3$), 1.42 (s, 9H, $3\times\text{CH}_3$), 2.27 (s, 3H, CH_3), 2.45 (s, 3H, CH_3), 3.65 (s, 3H, CH_3O), 4.98 (s, 2H, OCH_2O), 7.15 (d, 4J = 1.9 Hz, 1H, Ar), 7.42 (d, 4J = 1.9 Hz, 1H, Ar), 7.91 (s, 1H, $\text{CH}=\text{}$).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 26.7 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 30.8 ($^1J_{\text{CH}}$ = 125 Hz, $3\times\text{CH}_3$), 31.2 ($^1J_{\text{CH}}$ = 125 Hz, $3\times\text{CH}_3$), 31.4 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 34.7 (C), 35.2 (C), 57.4 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 101.1 ($^1J_{\text{CH}}$ = 166 Hz, OCH_2O), 125.4 (CH, Ar), 126.6 (C, Ar), 126.8 (CH, Ar), 139.4 ($\text{CH}=\text{}$), 142.0 ($\text{C}=\text{}$), 142.4 (C, Ar), 146.3 (C, Ar), 154.0 (C, Ar), 197.0 (CO), 204.9 (CO).

HRMS (ESI) m/z : $[\text{M} - \text{OCH}_2\text{OCH}_3]^+$ Calcd for $\text{C}_{20}\text{H}_{27}\text{O}_2^+$ 299.2006; Found 299.2010.

3-[[5-Bromo-3-methoxy-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2k)



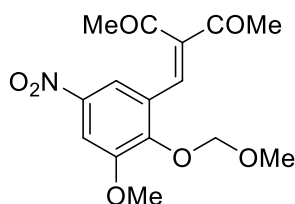
S2k was synthesized from aldehyde **S1k** (2.75 g, 10.0 mmol) and acetylacetone (1.03 mL, 10.0 mmol). Reaction time 1.5 h. Yield 2.85 g (80%); yellow oil; R_f = 0.52 (petroleum ether : ethyl acetate, 2:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 2.23 (s, 3H, CH_3), 2.40 (s, 3H, CH_3), 3.53 (s, 3H, CH_3O), 3.84 (s, 3H, CH_3O), 5.10 (s, 2H, OCH_2O), 6.97 (dd, 4J = 2.2, 4J = 0.6 Hz, 1H, Ar), 7.07 (d, 4J = 2.2 Hz, 1H, Ar), 7.76 (br.s, 1H, $\text{CH}=\text{}$).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 26.7 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 31.3 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 56.1 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 57.7 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 99.1 ($^1J_{\text{CH}}$ = 166 Hz, OCH_2O), 117.0 (C, Ar), 117.5 (CH, Ar), 123.5 (CH, Ar), 129.6 (C, Ar), 134.9 ($\text{CH}=\text{}$), 143.91 (C), 143.92 (C), 152.8 (C, Ar), 196.2 (CO), 204.1 (CO).

HRMS (ESI) m/z : $[\text{M} - \text{OCH}_2\text{OCH}_3]^+$ Calcd for $\text{C}_{13}\text{H}_{12}\text{BrO}_3^+$ 294.9964; Found 294.9968.

3-[[3-Methoxy-2-(methoxymethoxy)-5-nitrophenyl]methylidene]pentane-2,4-dione (S2l)



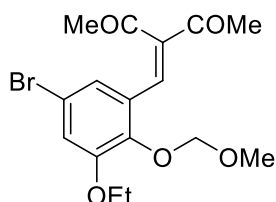
S2l was synthesized from aldehyde **S1l** (2.41 g, 10.0 mmol) and acetylacetone (1.03 mL, 10.0 mmol). Reaction time 1.5 h. Yield 2.72 g (84%); yellow oil; $R_f = 0.55$ (petroleum ether : ethyl acetate, 1:1).

^1H NMR (CDCl_3 , 600 MHz) $\delta = 2.29$ (s, 3H, CH_3), 2.45 (s, 3H, CH_3), 3.55 (s, 3H, CH_3O), 3.97 (s, 3H, CH_3O), 5.28 (s, 2H, OCH_2O), 7.76 (br.s, 1H, $\text{CH}=\text{}$), 7.81 (dd, $^4J = 2.6$, $^4J = 0.6$ Hz, 1H, Ar), 7.82 (d, $^4J = 2.6$ Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) $\delta = 26.8$ ($^1J_{\text{CH}} = 128$ Hz, CH_3), 31.4 ($^1J_{\text{CH}} = 128$ Hz, CH_3), 56.5 ($^1J_{\text{CH}} = 145$ Hz, CH_3O), 57.9 ($^1J_{\text{CH}} = 143$ Hz, CH_3O), 99.2 ($^1J_{\text{CH}} = 169$ Hz, OCH_2O), 108.7 (CH, Ar), 116.9 (CH, Ar), 128.3 (C, Ar), 134.2 ($\text{CH}=\text{}$), 143.7 (C=), 145.2 (C, Ar), 149.8 (C, Ar), 152.3 (C, Ar), 196.1 (CO), 203.3 (CO).

HRMS (ESI) m/z : $[\text{M} - \text{OCH}_2\text{OCH}_3]^+$ Calcd for $\text{C}_{13}\text{H}_{12}\text{NO}_5^+$ 262.0710; Found 262.0713.

3-[[5-Bromo-3-ethoxy-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2m)



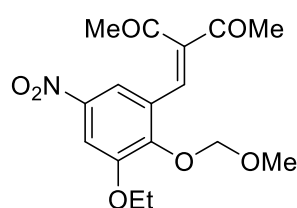
S2m was synthesized from aldehyde **S1m** (2.81 g, 9.7 mmol) and acetylacetone (1.00 mL, 9.7 mmol). Reaction time 1.5 h. Yield 2.64 g (73%); yellow oil; $R_f = 0.51$ (petroleum ether : ethyl acetate, 2:1).

^1H NMR (CDCl_3 , 400 MHz) $\delta = 1.44$ (t, $^3J = 7.0$ Hz, 3H, CH_3), 2.23 (s, 3H, CH_3), 2.40 (s, 3H, CH_3), 3.54 (s, 3H, CH_3O), 4.04 (q, $^3J = 7.0$ Hz, 2H, CH_2O), 5.13 (s, 2H, OCH_2O), 6.95 (d, $^4J = 2.2$ Hz, 1H, Ar), 7.05 (d, $^4J = 2.2$ Hz, 1H, Ar), 7.77 (br.s, 1H, $\text{CH}=\text{}$).

^{13}C NMR (CDCl_3 , 100 MHz) $\delta = 14.6$ ($^1J_{\text{CH}} = 127$ Hz, CH_3), 26.7 ($^1J_{\text{CH}} = 128$ Hz, CH_3), 31.3 ($^1J_{\text{CH}} = 128$ Hz, CH_3), 57.7 ($^1J_{\text{CH}} = 143$ Hz, CH_3O), 64.7 ($^1J_{\text{CH}} = 145$ Hz, CH_2O), 99.0 ($^1J_{\text{CH}} = 168$ Hz, OCH_2O), 116.9 (C, Ar), 118.3 (CH, Ar), 123.3 (CH, Ar), 129.5 (C, Ar), 135.0 ($\text{CH}=\text{}$), 143.8 (C), 144.0 (C), 152.2 (C, Ar), 196.3 (CO), 204.1 (CO).

HRMS (ESI) m/z : $[\text{M} - \text{OCH}_2\text{OCH}_3]^+$ Calcd for $\text{C}_{14}\text{H}_{14}\text{BrO}_3^+$ 309.0121; Found 309.0121.

3-[[3-Ethoxy-2-(methoxymethoxy)-5-nitrophenyl]methylidene]pentane-2,4-dione (S2n)



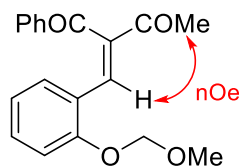
S2n was synthesized from aldehyde **S1n** (2.55 g, 10.0 mmol) and acetylacetone (1.03 mL, 10.0 mmol). Reaction time 1.5 h. Yield 2.61 g (77%); yellow oil; R_f = 0.69 (petroleum ether : ethyl acetate, 1:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.50 (t, 3J = 7.0 Hz, 3H, CH_3), 2.28 (s, 3H, CH_3), 2.44 (s, 3H, CH_3), 3.55 (s, 3H, CH_3O), 4.17 (q, 3J = 7.0 Hz, 2H, CH_2O), 5.29 (s, 2H, OCH_2O), 7.75 (br.s, 1H, CH=), 7.77–7.79 (m, 2H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.5 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 26.7 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 31.3 ($^1J_{\text{CH}}$ = 129 Hz, CH_3), 57.9 ($^1J_{\text{CH}}$ = 143 Hz, CH_3O), 65.2 ($^1J_{\text{CH}}$ = 145 Hz, CH_2O), 99.1 ($^1J_{\text{CH}}$ = 169 Hz, OCH_2O), 109.4 (CH, Ar), 116.6 (CH, Ar), 128.1 (C, Ar), 134.3 (CH=), 143.6 (C), 145.1 (C), 149.8 (C, Ar), 151.5 (C, Ar), 196.2 (CO), 203.3 (CO).

HRMS (ESI) m/z : $[\text{M} - \text{OCH}_2\text{OCH}_3]^+$ Calcd for $\text{C}_{14}\text{H}_{14}\text{NO}_5^+$ 276.0866; Found 276.0868.

(2Z)-2-[[2-(Methoxymethoxy)phenyl]methylidene]-1-phenylbutane-1,3-dione (S2o)



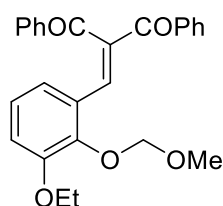
S2o was synthesized from aldehyde **S1a** (5.00 g, 30.1 mmol) and benzoylacetone (4.88 g, 30.1 mmol). Reaction time 4 h. Yield 8.12 g (87%); yellow solid, mp 87–88 °C; R_f = 0.45 (petroleum ether : ethyl acetate, 2:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 2.41 (s, 3H, CH_3), 3.45 (s, 3H, CH_3O), 5.15 (s, 2H, OCH_2O), 6.74–6.77 (m, 1H, Ar), 7.05–7.07 (m, 1H, Ar), 7.18–7.21 (m, 2H, Ar), 7.35–7.38 (m, 2H, Ar), 7.47–7.50 (m, 1H, Ar), 7.88–7.90 (m, 2H, Ar), 8.17 (br.s, 1H, CH=).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 27.1 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 56.1 ($^1J_{\text{CH}}$ = 143 Hz, CH_3O), 94.4 ($^1J_{\text{CH}}$ = 166 Hz, OCH_2O), 114.2 (CH, Ar), 121.6 (CH, Ar), 122.7 (C, Ar), 128.6 (2 $\times$ CH, Ar), 128.9 (2 $\times$ CH, Ar), 130.3 (CH, Ar), 131.9 (CH, Ar), 133.6 (CH, Ar), 136.2 (C, Ar), 137.0 (CH=), 139.4 (C=), 155.7 (C, Ar), 196.3 (CO), 197.6 (CO).

HRMS (ESI) m/z : $[\text{M} - \text{OCH}_2\text{OCH}_3]^+$ Calcd for $\text{C}_{17}\text{H}_{13}\text{O}_2^+$ 249.0910; Found 249.0910.

2-(3-Ethoxy-2-(methoxymethoxy)benzylidene)-1,3-diphenylpropane-1,3-dione (S2p)



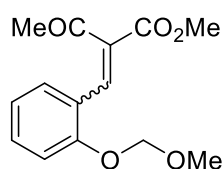
S2p was synthesized from aldehyde **S1h** (5.00 g, 23.8 mmol) and dibenzoylmethane (5.33 g, 23.8 mmol). Yield 8.61 g (87%); yellow oil; R_f = 0.29 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 400 MHz) δ = 1.39 (t, 3J = 7.0 Hz, 3H, CH_3), 3.28 (s, 3H, CH_3O), 3.98 (q, 3J = 7.0 Hz, 2H, CH_2O), 5.08 (s, 2H, OCH_2O), 6.78–6.83 (m, 2H, Ar), 6.87–6.92 (m, 1H, Ar), 7.36–7.40 (m, 2H, Ar), 7.46–7.51 (m, 3H, Ar), 7.55–7.59 (m, 1H, Ar), 7.88–7.91 (m, 2H, Ar), 7.96–7.99 (m, 2H, Ar), 8.00 (s, 1H, CH=).

^{13}C NMR (CDCl_3 , 100 MHz) δ = 14.7 (CH_3), 57.2 (CH_3O), 64.2 (CH_2O), 99.2 (OCH_2O), 115.3 (CH, Ar), 121.4 (CH, Ar), 124.2 (CH, Ar), 128.1 (C), 128.4 (2 $\times$ CH, Ar), 128.6 (2 $\times$ CH, Ar), 129.3 (2 $\times$ CH, Ar), 129.5 (2 $\times$ CH, Ar), 132.4 (CH, Ar), 133.5 (CH, Ar), 136.3 (C), 137.5 (C), 139.5 (C), 140.1 (CH=), 145.4 (C), 151.3 (C), 195.2 (CO), 196.9 (CO).

HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{26}\text{H}_{24}\text{NaO}_5^+$ 439.1516; Found 439.1517.

Methyl 2-[2-(methoxymethoxy)benzylidene]-3-oxobutanoate (S2q)



S2q was synthesized from aldehyde **S1a** (8.3 g, 50 mmol) and methyl acetoacetate (5.4 mL, 50 mmol). Reaction time 2 h. Yield 10.5 g (80%); yellow oil; R_f = 0.48, 0.39 (petroleum ether : ethyl acetate, 3:1). $E:Z$ = 60:40.

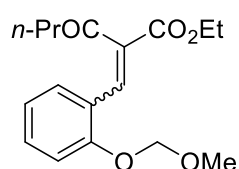
^1H NMR (CDCl_3 , 600 MHz) δ = 2.30 (s, 3H, CH_3 , **Z**), 2.44 (s, 3H, CH_3 , **E**), 3.496 (s, 3H, CH_3O , **Z**), 3.500 (s, 3H, CH_3O , **E**), 3.79 (s, 3H, CH_3O , **E**), 3.84 (s, 3H, CH_3O , **Z**), 5.23 (s, 2H, OCH_2O , **Z**), 5.24 (s, 2H, OCH_2O , **E**), 6.95–6.98 (m, 1H, Ar, **Z**), 6.97–7.00 (m, 1H, Ar, **E**), 6.16–6.18 (m, 1H + 1H, Ar, **E**, **Z**), 7.26–7.28 (m, 1H, Ar, **Z**), 7.33–7.37 (m, 2H + 1H, Ar, **E**, **Z**), 7.97 (br.s, 1H, CH= , **E**), 8.02 (br.s, 1H, CH= , **Z**).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 26.6 (CH_3 , **E**), 31.1 (CH_3 , **Z**), 52.3 (CH_3O , **E**), 52.4 (CH_3O , **Z**), 56.31 (CH_3O , **Z**), 56.34 (CH_3O , **E**), 94.6 (OCH_2O , **Z**), 94.7 (OCH_2O , **E**), 114.59 (CH, Ar, **Z**), 114.63 (CH, Ar, **E**), 121.9 (CH + CH, Ar, **E**, **Z**), 122.8 (C, Ar, **Z**), 123.0 (C, Ar, **E**), 128.8 (CH, Ar, **E**), 130.0

(CH, Ar, **Z**), 131.9 (CH, Ar, **Z**), 132.2 (CH, Ar, **E**), 133.6 (C, **E**), 134.4 (C, **Z**), 137.0 (CH=, **Z**), 137.4 (CH=, **E**), 155.7 (C, **Z**), 155.9 (C, **E**), 165.1 (CO₂Me, **Z**), 168.3 (CO₂Me, **E**), 194.9 (COMe, **E**), 202.9 (COMe, **Z**).

HRMS (ESI) *m/z*: [M + Na]⁺ Calcd for C₁₄H₁₆NaO₅⁺ 287.0890; Found 287.0892.

Ethyl 2-[2-(methoxymethoxy)benzylidene]-3-oxohexanoate (**S2r**)



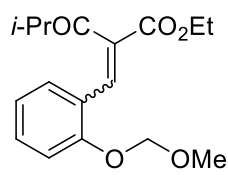
S2r was synthesized from aldehyde **S1a** (4.98 g, 30 mmol) and ethyl 3-oxohexanoate (4.79 mL, 30 mmol). Reaction time 3 h. Yield 7.28 g (79%); yellow oil; *R_f* = 0.73 (petroleum ether : ethyl acetate, 3:1). *Z:E* = 54:46.

¹H NMR (CDCl₃, 600 MHz) δ = 0.85 (t, ³*J* = 7.4 Hz, 3H, CH₃, **E**), 0.97 (t, ³*J* = 7.4 Hz, 3H, CH₃, **Z**), 1.21 (t, ³*J* = 7.1 Hz, 3H, CH₃, **Z**), 1.31 (t, ³*J* = 7.1 Hz, 3H, CH₃, **E**), 1.57–1.63 (m, 2H, CH₂), 1.68–1.74 (m, 2H, CH₂), 2.47 (t, ³*J* = 7.2 Hz, 2H, CH₂, **E**), 2.72 (t, ³*J* = 7.3 Hz, 2H, CH₂, **Z**), 3.48 (s, 3H, CH₃O, **Z**), 3.49 (s, 3H, CH₃O, **E**), 4.26 (q, ³*J* = 7.1 Hz, 2H, CH₂, **Z**), 4.28 (q, ³*J* = 7.1 Hz, 2H, CH₂, **E**), 5.22 (s, 2H, OCH₂O, **Z**), 5.23 (s, 2H, OCH₂O, **E**), 6.92–6.97 (m, 1H + 1H, Ar, **E**, **Z**), 7.13–7.15 (m, 1H + 1H, Ar, **E**, **Z**), 7.23–7.25 (m, 1H, Ar, **E**), 7.30–7.34 (m, 1H + 1H, Ar, **E**, **Z**), 7.37–7.38 (m, 1H, Ar, **Z**), 7.95 (br.s, 1H, CH=, **Z**), 8.03 (br.s, 1H, CH=, **E**).

¹³C NMR (CDCl₃, 150 MHz) δ = 13.4 (CH₃, **E**), 13.7 (CH₃, **Z**), 13.8 (CH₃, **Z**), 14.1 (CH₃, **E**), 16.8 (CH₂, **E**), 17.5 (CH₂, **Z**), 40.7 (CH₂, **Z**), 45.5 (CH₂, **E**), 56.24 (CH₃O, **E**), 56.25 (CH₃O, **Z**), 61.29 (CH₂O, **E**), 61.34 (CH₂O, **Z**), 94.6 (OCH₂O, **E**), 94.7 (OCH₂O, **Z**), 114.50 (CH, Ar, **E**), 114.51 (CH, Ar, **Z**), 121.66 (CH, Ar, **Z**), 121.73 (CH, Ar, **E**), 123.0 (C, Ar, **E**), 123.2 (C, Ar, **Z**), 128.9 (CH, Ar, **Z**), 129.8 (CH, Ar, **E**), 131.7 (CH, Ar, **E**), 131.9 (CH, Ar, **Z**), 134.0 (C=, **E**), 134.5 (C=, **Z**), 136.20 (CH=, **E**), 136.22 (CH=, **Z**), 155.7 (C, Ar, **E**), 155.8 (C, Ar, **Z**), 164.8 (CO₂Et, **E**), 167.9 (CO₂Et, **Z**), 197.1 (COPrⁿ, **Z**), 205.5 (COPrⁿ, **E**).

HRMS (ESI) *m/z*: [M – OCH₂OCH₃]⁺ Calcd for C₁₅H₁₇O₃⁺ 245.1172; Found 245.1176.

Ethyl 2-[2-(methoxymethoxy)benzylidene]-4-methyl-3-oxopentanoate (S2s)



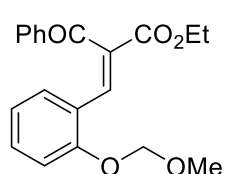
S2s was synthesized from aldehyde **S1a** (4.98 g, 30 mmol) and ethyl isobutyrylacetate (4.84 mL, 30 mmol). Reaction time 2 h. Yield 7.15 g (78%); yellow oil; $R_f = 0.47$ (petroleum ether : ethyl acetate, 4:1). $E:Z = 59:41$.

^1H NMR (CDCl_3 , 600 MHz) $\delta = 1.02$ (d, $^3J = 7.0$ Hz, 6H, $2\times\text{CH}_3$, E), 1.19 (d, $^3J = 6.8$ Hz, 6H, $2\times\text{CH}_3$, Z), 1.21 (t, $^3J = 7.2$ Hz, 3H, CH_3 , Z), 1.31 (t, $^3J = 7.2$ Hz, 3H, CH_3 , E), 2.61 (spt, $^3J = 7.0$ Hz, 1H, CH, E), 3.23 (spt, $^3J = 6.8$ Hz, 1H, CH, Z), 3.48 (s, 3H, CH_3O , Z), 3.49 (s, 3H, CH_3O , E), 4.25 (q, $^3J = 7.2$ Hz, 2H, CH_2O , Z), 4.28 (q, $^3J = 7.2$ Hz, 2H, CH_2O , E), 5.22 (s, 2H, OCH_2O , Z), 5.23 (s, 2H, OCH_2O , E), 6.92–6.94 (m, 1H, Ar, E), 6.95–6.97 (m, 1H, Ar, Z), 7.13–7.14 (m, 1H+1H, Ar, Z , E), 7.23 (dd, $^3J = 7.7$, $^4J = 1.5$ Hz, 1H, Ar, E), 7.30–7.34 (m, 1H+1H, Ar, Z , E), 7.39 (dd, $^3J = 7.7$, $^4J = 1.6$ Hz, 1H, Ar, Z), 7.95 (br.s, 1H, $\text{CH}=\text{}$, Z), 8.10 (br.s, 1H, $\text{CH}=\text{}$, E).

^{13}C NMR (CDCl_3 , 150 MHz) $\delta = 13.8$ ($^1J_{\text{CH}} = 127$ Hz, CH_3 , Z), 14.1 ($^1J_{\text{CH}} = 127$ Hz, CH_3 , E), 17.8 ($^1J_{\text{CH}} = 128$ Hz, $2\times\text{CH}_3$, E), 18.9 ($^1J_{\text{CH}} = 128$ Hz, $2\times\text{CH}_3$, Z), 36.1 ($^1J_{\text{CH}} = 128$ Hz, CH, E), 41.5 ($^1J_{\text{CH}} = 128$ Hz, CH, Z), 56.2 ($^1J_{\text{CH}} = 143$ Hz, CH_3O , E), 56.3 ($^1J_{\text{CH}} = 143$ Hz, CH_3O , Z), 61.27 ($^1J_{\text{CH}} = 148$ Hz, CH_2O , E), 61.31 ($^1J_{\text{CH}} = 148$ Hz, CH_2O , Z), 94.6 ($^1J_{\text{CH}} = 166$ Hz, OCH_2O , Z), 94.7 ($^1J_{\text{CH}} = 166$ Hz, OCH_2O , E), 114.46 (CH, Ar, E), 114.54 (CH, Ar, Z), 121.65 (CH, Ar, Z), 121.68 (CH, Ar, E), 123.4 (C, Ar, Z), 123.5 (C, Ar, E), 129.0 (CH, Ar, Z), 129.9 (CH, Ar, E), 131.7 (CH, Ar, E), 131.8 (CH, Ar, Z), 133.6 ($\text{C}=\text{}$, E), 133.8 ($\text{C}=\text{}$, Z), 136.5 ($\text{CH}=\text{}$, Z), 136.8 ($\text{CH}=\text{}$, E), 155.7 (C, Ar, E), 155.8 (C, Ar, Z), 164.9 (CO_2Et , E), 167.9 (CO_2Et , Z), 201.4 (COPr^i , Z), 209.1 (COPr^i , E).

HRMS (ESI) m/z : $[\text{M} - \text{OCH}_2\text{OCH}_3]^+$ Calcd for $\text{C}_{15}\text{H}_{17}\text{O}_3^+$ 245.1172; Found 245.1170.

Ethyl (2E)-2-benzoyl-3-[2-(methoxymethoxy)phenyl]prop-2-enoate (S2t)



S2t was synthesized from aldehyde **S1a** (4.98 g, 30 mmol) and ethyl benzoylacetate (5.19 mL, 30 mmol). Reaction time 2.5 h. Yield 9.44 g (92%); yellow oil; $R_f = 0.50$ (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.15 (t, 3J = 7.2 Hz, 3H, CH_3), 3.40 (s, 3H, CH_3O), 4.21 (q, 3J = 7.2 Hz, 2H, CH_2O), 5.09 (s, 2H, OCH_2O), 6.76–6.79 (m, 1H, Ar), 7.06 (dd, 3J = 8.4, 4J = 1.0 Hz, 1H, Ar), 7.18–7.21 (m, 1H, Ar), 7.22–7.24 (m, 1H, Ar), 7.38–7.41 (m, 2H, Ar), 7.49–7.52 (m, 1H, Ar), 7.92–7.94 (m, 2H, Ar), 8.28 (br.s, 1H, CH=).

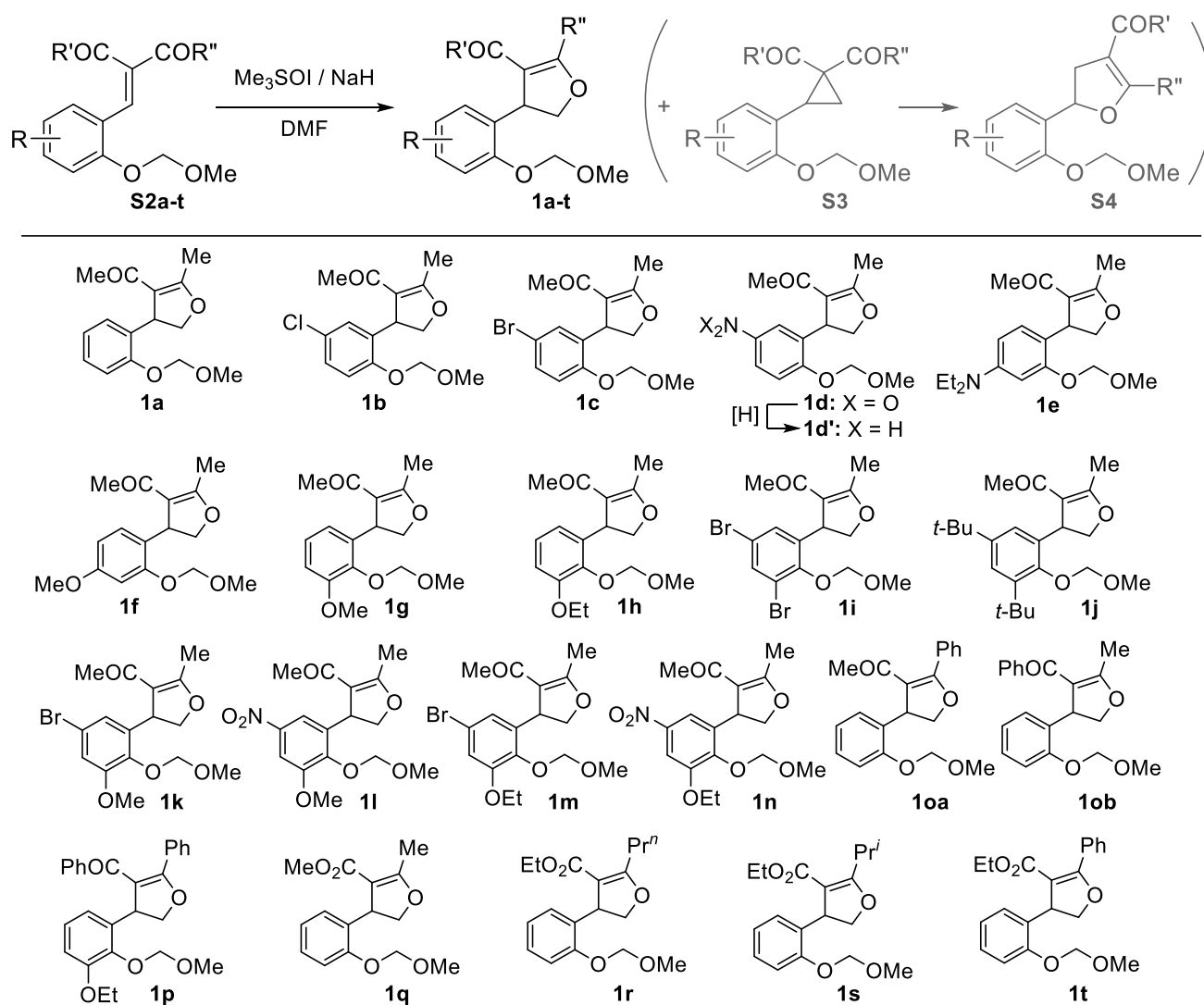
^{13}C NMR (CDCl_3 , 150 MHz) δ = 13.9 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 56.1 ($^1J_{\text{CH}}$ = 143 Hz, CH_3O), 61.3 ($^1J_{\text{CH}}$ = 148 Hz, CH_2O), 94.2 ($^1J_{\text{CH}}$ = 166 Hz, OCH_2O), 114.3 (CH, Ar), 121.6 (CH, Ar), 122.8 (C, Ar), 128.5 (2 $\times$ CH, Ar), 128.9 (2 $\times$ CH, Ar), 130.4 (CH, Ar), 131.2 (C, Ar), 131.7 (CH, Ar), 133.4 (CH, Ar), 136.5 (C=), 138.5 (CH=), 155.6 (C, Ar), 165.2 (CO_2Et), 195.1 (COPh).

HRMS (ESI) m/z : $[\text{M} - \text{OCH}_2\text{OCH}_3]^+$ Calcd for $\text{C}_{18}\text{H}_{15}\text{O}_3^+$ 279.1016; Found 279.1017.

General procedure for the synthesis of dihydrofurans **1**

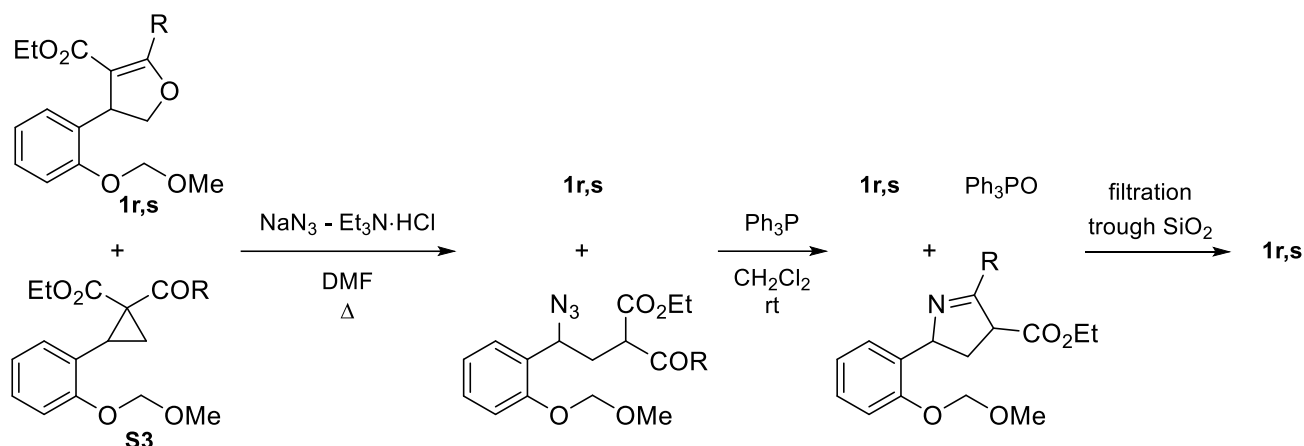
Dihydrofurans **1** were synthesized under Corey-Chaykovsky reaction conditions.¹⁸ To a suspension of NaH (0.30 g, 7.5 mmol, 60% suspension in mineral oil) in dry DMF (8 mL) Me_3SOI (1.65 g, 7.5 mmol) was added in one portion under inert atmosphere. After stirring for 20 min at ambient temperature, reaction mixture was cooled in ice-water bath and then a solution of an alkene **S2** (6.8 mmol) in dry DMF (7 mL) was added dropwise under vigorous stirring. Cooling bath was taken away and the mixture was stirred for additional 30 min, quenched with ice water (15 mL) and extracted with EtOAc (3 $\times$ 30 mL). Combined organic fractions were washed with water (5 $\times$ 15 mL), dried with Na_2SO_4 and concentrated under reduced pressure. Residue was purified by column chromatography on silica gel yielding dihydrofurans **1** (Scheme S3).

Scheme S3. Synthesis of dihydrofurans **1** under Corey-Chaykovsky conditions



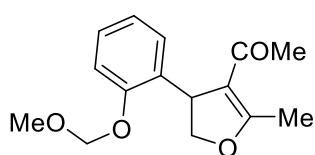
Cyclopropanes **S3** or regioisomeric dihydrofurans **S4** were formed in specified cases as side products. Dihydrofurans **1** and cyclopropanes **S3** formed mixtures which were difficult to separate due to identical chromatographic mobility. Therefore, for isomers **10a-10b-S3o**, **1p-S3p**, **1q-S3q**, **1t-S3t**, yields are given for the fractions, containing individual compounds, which have been separated by column chromatography among mixed fractions. For dihydrofurans **1r** and **1s**, which were also formed as mixtures with the corresponding cyclopropanes **S3**, the separating procedure based on our previous study of donor-acceptor cyclopropane reactivity¹⁹ was used (Scheme S4).

Scheme S4. Reaction sequence for the separation of dihydrofurans **1** from isomeric cyclopropanes **S3**



Donor-acceptor cyclopropanes rather than dihydrofurans readily undergo nucleophilic ring opening with the azide ion. Obtained azide derivatives can be easily transformed into the corresponding pyrrolines upon treatment with triphenylphosphine. We used this described sequence¹⁹ for the crude reaction mixtures of the desired dihydrofurans **1r** and **1s** which were separated from the corresponding pyrrolines and triphenylphosphine oxide by filtration through silica gel.

1-{4-[2-(Methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1a**)**



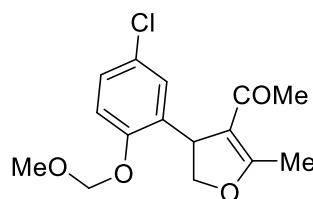
1a was synthesized from alkene **S2a** (3.37 g, 13.6 mmol). Yield 1.71 g (48%); yellow oil; R_f = 0.33 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.95 (s, 3H, CH_3), 2.35 (d, 5J = 1.2 Hz, 3H, CH_3), 3.48 (s, 3H, CH_3O), 4.19 (dd, 2J = 8.9, 3J = 4.7 Hz, 1H, CH_2O), 4.74 (dd, 2J = 8.9, 3J = 10.5 Hz, 1H, CH_2O), 4.81 (ddq, 3J = 10.5, 3J = 4.7, 5J = 1.2 Hz, 1H, CH), 5.22 (s, 2H, OCH_2O), 6.94–6.98 (m, 1H, Ar), 7.06–7.11 (m, 2H, Ar), 7.17–7.21 (m, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 15.0 ($^1J_{\text{CH}}$ = 130 Hz, CH_3), 29.1 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 41.7 ($^1J_{\text{CH}}$ = 138 Hz, CH), 56.0 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 78.3 ($^1J_{\text{CH}}$ = 152 Hz, CH_2O), 94.4 ($^1J_{\text{CH}}$ = 165 Hz, OCH_2O), 113.9 (CH, Ar), 114.3 (C=), 122.0 (CH, Ar), 127.5 (CH, Ar), 128.0 (CH, Ar), 132.1 (C, Ar), 154.2 (C, Ar), 170.2 (C=), 195.2 (COMe).

Anal. calcd for $\text{C}_{15}\text{H}_{18}\text{O}_4$: C, 68.68; H, 6.92. Found: C, 68.57; H, 6.93.

1-{4-[5-Chloro-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1b)



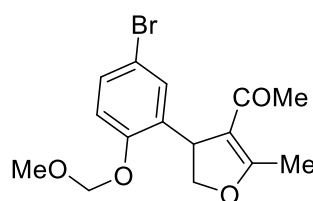
1b was synthesized from alkene **S2b** (2.10 g, 7.4 mmol). Yield 1.22 g (55%); yellow oil; R_f = 0.30 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 400 MHz) δ = 2.01 (s, 3H, CH_3), 2.38 (d, 5J = 0.9 Hz, 3H, CH_3), 3.47 (s, 3H, CH_3O), 4.16 (dd, 2J = 8.1, 3J = 3.5 Hz, 1H, CH_2O), 4.72 (dd, 2J = 8.1, 3J = 10.5 Hz, 1H, CH_2O), 4.77 (ddq, 3J = 10.5, 3J = 3.5, 5J = 0.9 Hz, 1H, CH), 5.20 (s, 2H, OCH_2O), 7.01 (d, 4J = 2.6 Hz, 1H, Ar), 7.04 (d, 3J = 8.8 Hz, 1H, Ar), 7.15 (dd, 3J = 8.8, 4J = 2.6 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 100 MHz) δ = 15.2 (CH_3), 29.2 (CH_3), 41.6 (CH), 56.1 (CH_3O), 78.0 (CH_2O), 94.6 (OCH_2O), 114.3 (C=), 115.3 (CH, Ar), 127.2 (C, Ar), 127.4 (CH, Ar), 127.9 (CH, Ar), 134.1 (C, Ar), 152.8 (C, Ar), 170.7 (C=), 194.7 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{15}\text{H}_{18}\text{ClO}_4^+$ 297.0888; Found 297.0891.

1-{4-[5-Bromo-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1c)



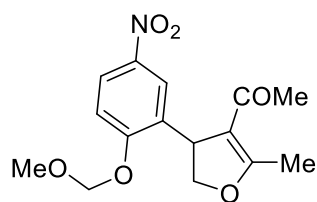
1c was synthesized from alkene **S2c** (2.80 g, 8.6 mmol). Yield 1.51 g (52%); yellow oil; R_f = 0.45 (petroleum ether : ethyl acetate, 2:1).

^1H NMR (CDCl_3 , 400 MHz) δ = 1.96 (s, 3H, CH_3), 2.32 (d, 5J = 0.9 Hz, 3H, CH_3), 3.42 (s, 3H, CH_3O), 4.11 (dd, 2J = 8.4, 3J = 3.8 Hz, 1H, CH_2O), 4.67 (dd, 2J = 8.4, 3J = 10.5 Hz, 1H, CH_2O), 4.73 (ddq, 3J = 10.5, 3J = 3.8, 5J = 0.9 Hz, 1H, CH), 5.16 (s, 2H, OCH_2O), 6.95 (d, 3J = 8.8 Hz, 1H, Ar), 7.09 (d, 4J = 2.5 Hz, 1H, Ar), 7.23 (dd, 3J = 8.8, 4J = 2.5 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 100 MHz) δ = 15.0 (CH_3), 29.0 (CH_3), 41.3 (CH), 55.9 (CH_3O), 77.8 (CH_2O), 94.3 (OCH_2O), 114.0 (C), 114.4 (C), 115.6 (CH, Ar), 130.1 (CH, Ar), 130.6 (CH, Ar), 134.4 (C, Ar), 153.1 (C, Ar), 170.4 (C=), 194.3 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{15}\text{H}_{18}\text{BrO}_4^+$ 341.0383; Found 341.0390.

1-{4-[5-Nitro-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1d)



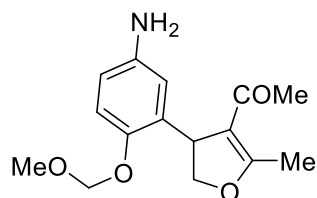
1d was synthesized from alkene **S2d** (1.90 g, 6.5 mmol). Yield 0.96 g (48%); yellow solid, mp 68–69 °C; R_f = 0.33 (petroleum ether : ethyl acetate, 1:1).

^1H NMR (CDCl_3 , 400 MHz) δ = 1.99 (s, 3H, CH_3), 2.28 (d, 5J = 1.1 Hz, 3H, CH_3), 3.38 (s, 3H, CH_3O), 4.05 (dd, 2J = 9.0, 3J = 4.2 Hz, 1H, CH_2O), 4.64 (dd, 2J = 9.0, 3J = 10.4 Hz, 1H, CH_2O), 4.71 (ddq, 3J = 10.4, 3J = 4.2, 5J = 1.1 Hz, 1H, CH), 5.23 (s, 2H, OCH_2O), 7.09 (d, 3J = 9.1 Hz, 1H, Ar), 7.77 (d, 4J = 2.8 Hz, 1H, Ar), 7.95 (dd, 3J = 9.1, 4J = 2.8 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 100 MHz) δ = 14.9 (CH_3), 28.8 (CH_3), 41.6 (CH), 56.1 (CH_3O), 77.1 (CH_2O), 94.1 (OCH_2O), 113.2 (CH, Ar), 114.1 ($\text{C}=\text{C}$), 122.9 (CH, Ar), 123.8 (CH, Ar), 133.1 (C, Ar), 141.8 (C, Ar), 158.9 (C, Ar), 170.4 ($\text{C}=\text{O}$), 193.2 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{15}\text{H}_{18}\text{NO}_6^+$ 308.1129; Found 308.1132.

1-{4-[5-Amino-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1d')



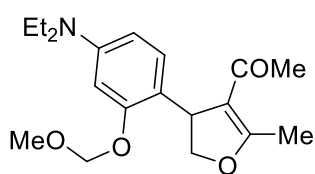
To the 0.1 M solution of nitro derivative **1d** (480 mg, 1.56 mmol) in ethanol zinc powder (610 mg, 9.4 mmol) and acetic acid (0.54 mL, 9.4 mmol) were sequentially added. The mixture was heated under reflux for 30 min. After cooling to the ambient temperature, remaining zinc was filtered off and washed with ethyl acetate (5 mL). Filtrate was diluted with water (10 mL) and extracted with ethyl acetate (2×20 mL); combined organic fractions were dried with Na_2SO_4 and concentrated under reduced pressure. Product **1d'** was purified by column chromatography on silica gel. Yield 295 mg (68%); yellowish viscous oil; R_f = 0.79 (ethyl acetate).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.96 (s, 3H, CH_3), 2.35 (d, 5J = 1.2 Hz, 3H, CH_3), 3.47 (s, 3H, CH_3O), 3.48 (br.s, 2H, NH_2), 4.18 (dd, 2J = 8.5, 3J = 4.3 Hz, 1H, CH_2O), 4.72 (dd, 2J = 8.5, 3J = 10.6 Hz, 1H, CH_2O), 4.76 (ddq, 3J = 10.6, 3J = 4.3, 5J = 1.2 Hz, 1H, CH), 5.11 (s, 2H, OCH_2O), 6.42 (d, 4J = 2.8 Hz, 1H, Ar), 6.52 (dd, 3J = 8.6, 4J = 2.8 Hz, 1H, Ar), 6.91 (d, 3J = 8.6 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 15.0 ($^1J_{\text{CH}}$ = 130 Hz, CH_3), 29.3 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 41.5 ($^1J_{\text{CH}}$ = 138 Hz, CH), 56.0 ($^1J_{\text{CH}}$ = 143 Hz, CH_3O), 78.5 ($^1J_{\text{CH}}$ = 153 Hz, CH_2O), 95.5 ($^1J_{\text{CH}}$ = 165 Hz, OCH_2O), 114.35 (CH, Ar), 114.41 (C=), 114.6 (CH, Ar), 116.1 (CH, Ar), 133.6 (C, Ar), 141.5 (C, Ar), 147.3 (C, Ar), 170.2 (C=), 195.6 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{15}\text{H}_{20}\text{NO}_4^+$ 278.1387; Found 278.1391.

1-{4-[4-Diethylamino-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (**1e**)



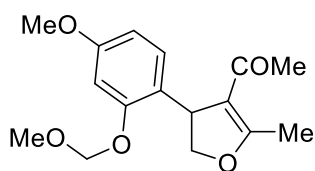
1e was synthesized from alkene **S2e** (2.40 g, 7.5 mmol). Yield 1.37 g (55%); yellow oil; R_f = 0.38 (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.15 (t, 3J = 7.1 Hz, 6H, $2\times\text{CH}_3$), 1.96 (s, 3H, CH_3), 2.34 (d, 5J = 0.9 Hz, 3H, CH_3), 3.32 (q, 3J = 7.1 Hz, 4H, $2\times\text{CH}_2\text{N}$), 3.48 (s, 3H, CH_3O), 4.16–4.21 (m, 1H, CH_2O), 4.66–4.71 (m, 2H, CH_2O , CH), 5.19 (s, 2H, OCH_2O), 6.29 (dd, 3J = 8.5, 4J = 2.6 Hz, 1H, Ar), 6.45 (d, 4J = 2.6 Hz, 1H, Ar), 6.87 (d, 3J = 8.5 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 12.5 ($^1J_{\text{CH}}$ = 126 Hz, $2\times\text{CH}_3$), 14.9 ($^1J_{\text{CH}}$ = 129 Hz, CH_3), 29.2 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 41.0 ($^1J_{\text{CH}}$ = 137 Hz, CH), 44.3 ($^1J_{\text{CH}}$ = 134 Hz, $2\times\text{CH}_2\text{N}$), 55.8 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 78.8 ($^1J_{\text{CH}}$ = 152 Hz, CH_2O), 94.6 ($^1J_{\text{CH}}$ = 166 Hz, OCH_2O), 98.2 (CH, Ar), 105.5 (CH, Ar), 114.6 (C=), 118.8 (C, Ar), 128.1 (CH, Ar), 148.1 (C, Ar), 155.5 (C, Ar), 169.6 (C=), 195.9 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{19}\text{H}_{28}\text{NO}_4^+$ 334.2013; Found 334.2015.

1-{4-[4-Methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (**1f**)



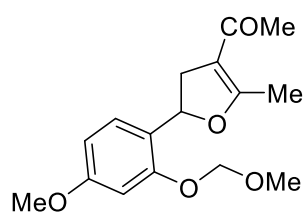
1f was synthesized from alkene **S2f** (4.80 g, 17.3 mmol). Yield 3.69 g (73%); yellow oil; R_f = 0.39 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 400 MHz) δ = 1.95 (s, 3H, CH_3), 2.34 (d, 5J = 0.6 Hz, 3H, CH_3), 3.47 (s, 3H, CH_3O), 3.77 (s, 3H, CH_3O), 4.12–4.19 (m, 1H, CH_2O), 4.68–4.74 (m, 2H, CH_2O , CH), 5.20 (s, 2H, OCH_2O), 6.50 (dd, 3J = 8.5, 4J = 2.5 Hz, 1H, Ar), 6.69 (d, 4J = 2.5 Hz, 1H, Ar), 6.96 (d, 3J = 8.5 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 100 MHz) δ = 15.0 (CH_3), 29.1 (CH_3), 41.2 (CH), 55.3 (CH_3O), 56.0 (CH_3O), 78.5 (CH_2O), 94.4 (OCH_2O), 101.2 (CH , Ar), 106.3 (CH , Ar), 114.4 ($\text{C}=\text{C}$), 124.4 (C , Ar), 128.1 (CH , Ar), 155.0 (C , Ar), 159.6 (C , Ar), 170.0 ($\text{C}=\text{O}$), 195.4 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{21}\text{O}_5^+$ 293.1384; Found 293.1387.

1-{5-[4-Methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (S4f)



S4f was synthesized from alkene **S2f** (4.80 g, 17.3 mmol) as a side product.

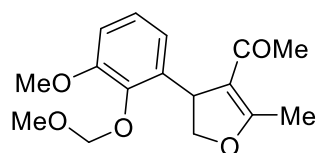
Yield 0.47 g (9%); yellow oil; R_f = 0.23 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 400 MHz) δ = 2.20 (s, 3H, CH_3), 2.31 (t, 5J = 1.5 Hz, 3H, CH_3), 2.86 (ddq, 2J = 14.2, 3J = 8.2, 5J = 1.5 Hz, 1H, CH_2), 3.37 (ddq, 2J = 14.2, 3J = 10.8, 5J = 1.5 Hz, 1H, CH_2), 3.48 (s, 3H, CH_3O), 3.79 (s, 3H, CH_3O), 5.19 (s, 2H, OCH_2O), 5.84 (dd, 3J = 10.8, 3J = 8.2 Hz, 1H, CHO), 6.55 (dd, 3J = 8.5, 4J = 2.4 Hz, 1H, Ar), 6.71 (d, 4J = 2.4 Hz, 1H, Ar), 7.21 (d, 3J = 8.5 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 100 MHz) δ = 15.0 (CH_3), 29.5 (CH_3), 37.9 (CH_2), 55.4 (CH_3O), 56.1 (CH_3O), 78.8 (CHO), 94.3 (OCH_2O), 101.2 (CH , Ar), 106.1 (CH , Ar), 112.0 ($\text{C}=\text{C}$), 122.5 (C , Ar), 126.6 (CH , Ar), 154.8 (C , Ar), 160.5 (C , Ar), 167.5 ($\text{C}=\text{O}$), 194.6 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{21}\text{O}_5^+$ 293.1384; Found 293.1386.

1-{4-[3-Methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1g)



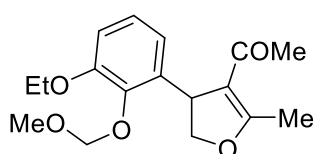
1g was synthesized from alkene **S2g** (8.66 g, 31.2 mmol). Yield 6.83 g (75%); yellow oil; R_f = 0.35 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.87 (s, 3H, CH_3), 2.31 (d, 5J = 1.2 Hz, 3H, CH_3), 3.53 (s, 3H, CH_3O), 3.79 (s, 3H, CH_3O), 4.14 (dd, 2J = 9.3, 3J = 5.3 Hz, 1H, CH_2O), 4.69 (dd, 2J = 9.3, 3J = 10.6 Hz, 1H, CH_2O), 4.90 (ddq, 3J = 10.6, 3J = 5.3, 5J = 1.2 Hz, 1H, CH), 5.04 (d, 2J = 6.0 Hz, 1H, OCH_2O), 5.09 (d, 2J = 6.0 Hz, 1H, OCH_2O), 6.66 (dd, 3J = 7.8, 4J = 1.4 Hz, 1H, Ar), 6.78 (dd, 3J = 8.1, 4J = 1.4 Hz, 1H, Ar), 6.99 (dd, 3J = 8.1, 3J = 7.8 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.7 ($^1J_{\text{CH}}$ = 129 Hz, CH_3), 29.1 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 41.4 ($^1J_{\text{CH}}$ = 137 Hz, CH), 55.5 ($^1J_{\text{CH}}$ = 144 Hz, CH_3O), 57.2 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 78.4 ($^1J_{\text{CH}}$ = 152 Hz, CH_2O), 99.0 ($^1J_{\text{CH}}$ = 166 Hz, OCH_2O), 110.7 (CH, Ar), 114.6 ($\text{C}=\text{C}$), 118.9 (CH, Ar), 124.8 (CH, Ar), 137.5 (C, Ar), 143.5 (C, Ar), 151.8 (C, Ar), 169.9 ($\text{C}=\text{C}$), 195.2 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{21}\text{O}_5^+$ 293.1384; Found 293.1384.

1-{4-[3-Ethoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1h)



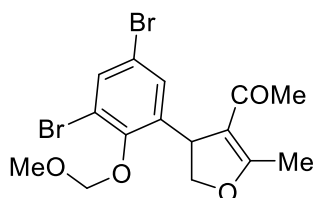
1h was synthesized from alkene **S2h** (3.36 g, 11.5 mmol). Yield 2.36 g (67%); yellow oil; R_f = 0.34 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.35 (t, 3J = 7.0 Hz, 3H, CH_3), 1.84 (s, 3H, CH_3), 2.27 (d, 5J = 1.2 Hz, 3H, CH_3), 3.50 (s, 3H, CH_3O), 3.93–4.00 (m, 2H, CH_2O), 4.10 (dd, 2J = 9.2, 3J = 5.3 Hz, 1H, CH_2O), 4.66 (dd, 2J = 9.2, 3J = 10.6 Hz, 1H, CH_2O), 4.87 (ddq, 3J = 10.6, 3J = 5.3, 5J = 1.2 Hz, 1H, CH), 5.04 (d, 2J = 5.9 Hz, 1H, OCH_2O), 5.08 (d, 2J = 5.9 Hz, 1H, OCH_2O), 6.62 (dd, 3J = 7.8, 4J = 1.5 Hz, 1H, Ar), 6.73 (dd, 3J = 8.2, 4J = 1.5 Hz, 1H, Ar), 6.92–6.94 (m, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.5 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 14.6 ($^1J_{\text{CH}}$ = 130 Hz, CH_3), 29.0 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 41.4 ($^1J_{\text{CH}}$ = 137 Hz, CH), 57.0 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 63.7 ($^1J_{\text{CH}}$ = 145 Hz, CH_2O), 78.3 ($^1J_{\text{CH}}$ = 152 Hz, CH_2O), 98.8 ($^1J_{\text{CH}}$ = 167 Hz, OCH_2O), 111.5 (CH, Ar), 114.4 ($\text{C}=\text{C}$), 118.6 (CH, Ar), 124.5 (CH, Ar), 137.4 (C, Ar), 143.5 (C, Ar), 151.0 (C, Ar), 169.7 ($\text{C}=\text{C}$), 195.0 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{17}\text{H}_{23}\text{O}_5^+$ 307.1540; Found 307.1542.

1-{4-[3,5-Dibromo-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1i)



1i was synthesized from alkene **S2i** (3.34 g, 8.2 mmol). Yield 1.55 g (45%); yellow oil; R_f = 0.29 (petroleum ether : ethyl acetate, 4:1).

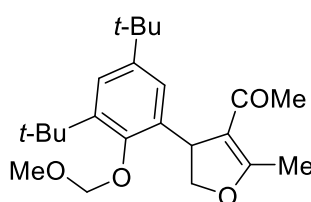
^1H NMR (CDCl_3 , 400 MHz) δ = 1.96 (s, 3H, CH_3), 2.33 (d, 5J = 1.0 Hz, 3H, CH_3), 3.57 (s, 3H, CH_3O), 4.10 (dd, 2J = 9.6, 3J = 4.9 Hz, 1H, CH_2O), 4.66 (dd, 2J = 9.6, 3J = 10.5 Hz, 1H, CH_2O), 4.85 (ddq, 3J = 10.5, 3J = 4.9, 5J = 1.0 Hz, 1H, CH), 5.02 (d, 2J = 6.0 Hz, 1H, OCH_2O), 5.12 (d, 2J = 6.0, 1H, OCH_2O), 7.09 (d, 4J = 2.4 Hz, 1H, Ar), 7.56 (d, 4J = 2.4 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 100 MHz) δ = 15.0 (CH_3), 29.2 (CH_3), 42.1 (CH), 57.5 (CH_3O), 78.1 (CH_2O), 100.1 (OCH_2O), 114.8 ($\text{C}=\text{C}$), 118.25 (C , Ar), 118.26 (C , Ar), 129.5 (CH , Ar), 134.3 (CH , Ar), 141.1 (C , Ar), 151.6 (C , Ar), 170.5 ($\text{C}=\text{O}$), 193.9 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{15}\text{H}_{17}\text{Br}_2\text{O}_4^+$ 420.9468; Found 420.9475.

1-{4-[3,5-Di-*tert*-butyl-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone

(1j)



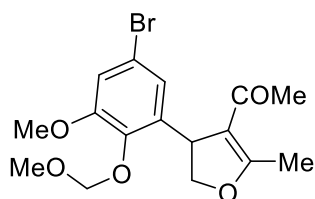
1j was synthesized from alkene **S2j** (2.50 g, 6.9 mmol). Yield 1.40 g (54%); yellowish solid, mp 71–72 °C; R_f = 0.45 (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.25 (s, 9H, $3\times\text{CH}_3$), 1.40 (s, 9H, $3\times\text{CH}_3$), 1.78 (s, 3H, CH_3), 2.36 (d, 5J = 1.3 Hz, 3H, CH_3), 3.63 (s, 3H, CH_3O), 4.26 (dd, 2J = 9.2, 3J = 5.5 Hz, 1H, CH_2O), 4.78 (dd, 2J = 9.2, 3J = 10.6 Hz, 1H, CH_2O), 4.80 (d, 2J = 5.8 Hz, 1H, OCH_2O), 4.97 (ddq, 3J = 10.6, 3J = 5.5, 5J = 1.3 Hz, 1H, CH), 5.09 (d, 2J = 5.8 Hz, 1H, OCH_2O), 6.99 (d, 4J = 2.5 Hz, 1H, Ar), 7.25 (d, 4J = 2.5 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.8 ($^1J_{\text{CH}}$ = 129 Hz, CH_3), 28.9 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 31.2 ($^1J_{\text{CH}}$ = 125 Hz, $3\times\text{CH}_3$), 31.4 ($^1J_{\text{CH}}$ = 125 Hz, $3\times\text{CH}_3$), 34.5 (C), 35.2 (C), 42.3 ($^1J_{\text{CH}}$ = 137 Hz, CH), 56.9 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 79.2 ($^1J_{\text{CH}}$ = 152 Hz, CH_2O), 100.9 ($^1J_{\text{CH}}$ = 163 Hz, OCH_2O), 116.4 ($\text{C}=\text{C}$), 122.8 (CH, Ar), 123.0 (CH, Ar), 136.7 (C, Ar), 142.0 (C, Ar), 147.0 (C, Ar), 152.6 (C, Ar), 169.3 ($\text{C}=\text{O}$), 195.7 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{23}\text{H}_{35}\text{O}_4^+$ 375.2530; Found 375.2533.

1-{4-[5-Bromo-3-methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1k)



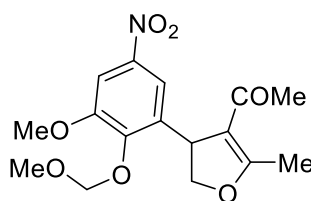
1k was synthesized from alkene **S2k** (2.65 g, 7.4 mmol). Yield 1.78 g (65%); yellow oil; R_f = 0.28 (petroleum ether : ethyl acetate, 2:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.92 (s, 3H, CH_3), 2.32 (d, 5J = 1.3 Hz, 3H, CH_3), 3.52 (s, 3H, CH_3O), 3.79 (s, 3H, CH_3O), 4.11 (dd, 2J = 9.4, 3J = 5.1 Hz, 1H, CH_2O), 4.67 (dd, 2J = 9.4, 3J = 10.6 Hz, 1H, CH_2O), 4.85 (ddq, 3J = 10.6, 3J = 5.1, 5J = 1.3 Hz, 1H, CH), 5.02 (d, 2J = 6.0 Hz, 1H, OCH_2O), 5.06 (d, 2J = 6.0 Hz, 1H, OCH_2O), 6.76 (d, 4J = 2.3 Hz, 1H, Ar), 6.90 (d, 4J = 2.3 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.9 (CH_3), 29.2 (CH_3), 41.4 (CH), 55.9 (CH_3O), 57.3 (CH_3O), 78.1 (CH_2O), 99.0 (OCH_2O), 114.3 (CH, Ar), 114.5 (C=), 117.3 (C, Ar), 121.7 (CH, Ar), 139.3 (C, Ar), 142.7 (C, Ar), 152.6 (C, Ar), 170.4 (C=), 194.6 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{20}\text{BrO}_5^+$ 371.0489; Found 371.0490.

**1-{4-[3-Methoxy-2-(methoxymethoxy)-5-nitrophenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone
(11)**



11 was synthesized from alkene **S2I** (2.71 g, 8.4 mmol). Yield 1.23 g (43%);

yellow oil; R_f = 0.34 (petroleum ether : ethyl acetate, 2:1).

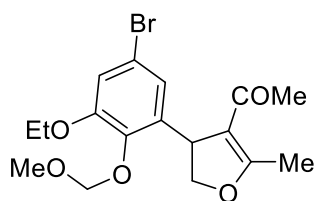
^1H NMR (CDCl_3 , 600 MHz) δ = 2.05 (s, 3H, CH_3), 2.38 (d, 5J = 1.1 Hz, 3H, CH_3), 3.57 (s, 3H, CH_3O), 3.92 (s, 3H, CH_3O), 4.14 (dd, 2J = 9.6, 3J = 5.0 Hz, 1H, CH_2O), 4.72 (dd, 2J = 9.6, 3J = 10.6 Hz, 1H, CH_2O), 4.94 (ddq, 3J = 10.6, 3J = 5.0, 5J = 1.1 Hz, 1H, CH), 5.23 (d, 2J = 5.8 Hz, 1H, OCH_2O), 5.25 (d, 2J = 5.8 Hz, 1H, OCH_2O), 7.58 (d, 4J = 2.6 Hz, 1H, Ar), 7.67 (d, 4J = 2.6 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 15.2 ($^1J_{\text{CH}}$ = 130 Hz, CH_3), 29.2 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 41.9 ($^1J_{\text{CH}}$ = 139 Hz, CH), 56.2 ($^1J_{\text{CH}}$ = 145 Hz, CH_3O), 57.7 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 77.7 ($^1J_{\text{CH}}$ = 153 Hz, CH_2O), 99.1 ($^1J_{\text{CH}}$ = 169 Hz, OCH_2O), 106.2 (CH, Ar), 115.0 (CH, Ar), 115.1 (C=), 138.3 (C, Ar), 144.2 (C, Ar), 148.9 (C, Ar), 152.0 (C, Ar), 170.7 (C=), 193.7 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{20}\text{NO}_7^+$ 338.1234; Found 338.1241.

1-{4-[5-Bromo-3-ethoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone

(1m)



1m was synthesized from alkene **S2m** (2.57 g, 6.9 mmol). Yield 1.75 g (66%); yellowish solid, mp 87–88 °C; R_f = 0.38 (petroleum ether : ethyl acetate, 3:1).

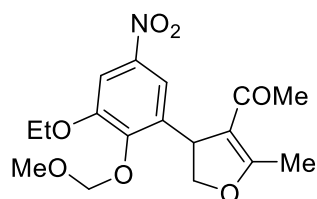
^1H NMR (CDCl_3 , 600 MHz) δ = 1.42 (t, 3J = 7.0 Hz, 3H, CH_3), 1.94 (s, 3H, CH_3), 2.34 (d, 5J = 1.2 Hz, 3H, CH_3), 3.55 (s, 3H, CH_3O), 4.01 (q, 3J = 7.0 Hz, 3H, CH_2O), 4.13 (dd, 2J = 9.5, 3J = 5.1 Hz, 1H, CH_2O), 4.69 (dd, 2J = 9.5, 3J = 10.5 Hz, 1H, CH_2O), 4.87 (ddq, 3J = 10.5, 3J = 5.1, 5J = 1.2 Hz, 1H, CH), 5.07 (d, 2J = 5.9 Hz, 1H, OCH_2O), 5.10 (d, 2J = 5.9 Hz, 1H, OCH_2O), 6.76 (d, 4J = 2.3 Hz, 1H, Ar), 6.90 (d, 4J = 2.3 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.6 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 15.0 ($^1J_{\text{CH}}$ = 129 Hz, CH_3), 29.2 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 41.5 ($^1J_{\text{CH}}$ = 139 Hz, CH), 57.4 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 64.4 ($^1J_{\text{CH}}$ = 144 Hz, CH_2O), 78.2 ($^1J_{\text{CH}}$ = 152 Hz, CH_2O), 99.0 ($^1J_{\text{CH}}$ = 169 Hz, OCH_2O), 114.5 (C=), 115.2 (CH, Ar), 117.3 (C, Ar), 121.6 (CH, Ar), 139.3 (C, Ar), 142.8 (C, Ar), 152.0 (C, Ar), 170.5 (C=), 194.7 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{17}\text{H}_{22}\text{BrO}_5^+$ 385.0645; Found 385.0643.

1-{4-[3-Ethoxy-2-(methoxymethoxy)-5-nitrophenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone

(1n)



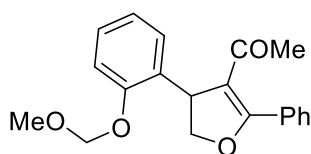
1n was synthesized from alkene **S2n** (2.50 g, 7.4 mmol). Yield 0.78 g (30%); yellow solid, mp 79–80 °C; R_f = 0.36 (petroleum ether : ethyl acetate, 1:1).

^1H NMR (CDCl_3 , 400 MHz) δ = 1.49 (t, 3J = 7.0 Hz, 3H, CH_3), 2.07 (s, 3H, CH_3), 2.40 (d, 5J = 1.1 Hz, 3H, CH_3), 3.59 (s, 3H, CH_3O), 4.12–4.18 (m, 3H), 4.73 (dd, 2J = 9.6, 3J = 10.5 Hz, 1H, CH_2O), 4.95 (ddq, 3J = 10.5, 3J = 5.0, 5J = 1.1 Hz, 1H, CH), 5.27 (d, 2J = 5.8 Hz, 1H, OCH_2O), 5.29 (d, 2J = 5.8 Hz, 1H, OCH_2O), 7.58 (d, 4J = 2.6 Hz, 1H, Ar), 7.67 (d, 4J = 2.6 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 100 MHz) δ = 14.6 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 15.3 ($^1J_{\text{CH}}$ = 129 Hz, CH_3), 29.3 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 41.9 ($^1J_{\text{CH}}$ = 139 Hz, CH), 57.8 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 65.0 ($^1J_{\text{CH}}$ = 144 Hz, CH_2O), 77.8 ($^1J_{\text{CH}}$ = 152 Hz, CH_2O), 99.1 ($^1J_{\text{CH}}$ = 169 Hz, OCH_2O), 106.9 (CH, Ar), 114.9 (CH, Ar), 115.1 (C=), 138.3 (C, Ar), 144.2 (C, Ar), 149.0 (C, Ar), 151.2 (C, Ar), 170.7 (C=), 193.8 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{17}\text{H}_{22}\text{NO}_7^+$ 352.1391; Found 352.1397.

1-{4-[2-(Methoxymethoxy)phenyl]-2-phenyl-4,5-dihydrofuran-3-yl}ethanone (**10a**)



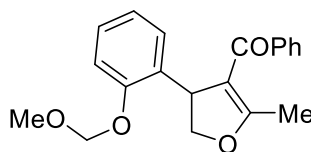
10a was synthesized from alkene **S2o** (18.0 g, 58.1 mmol). Yield 4.14 g (22%); yellowish oil; R_f = 0.32 (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.98 (s, 3H, CH_3), 3.52 (s, 3H, CH_3O), 4.38 (dd, 2J = 9.1, 3J = 4.8 Hz, 1H, CH_2O), 4.90 (dd, 2J = 9.1, 3J = 10.3 Hz, 1H, CH_2O), 5.02 (dd, 3J = 10.3, 3J = 4.8 Hz, 1H, CH), 5.27 (s, 2H, OCH_2O), 7.00–7.03 (m, 1H, Ar), 7.15 (dd, 3J = 8.1, 4J = 0.9 Hz, 1H, Ar), 7.21–7.26 (m, 2H, Ar), 7.46–7.52 (m, 3H, Ar), 7.75–7.77 (m, 2H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 29.0 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 43.0 ($^1J_{\text{CH}}$ = 136 Hz, CH), 55.9 ($^1J_{\text{CH}}$ = 143 Hz, CH_3O), 77.8 ($^1J_{\text{CH}}$ = 154, $^1J_{\text{CH}}$ = 148 Hz, CH_2O), 94.3 ($^1J_{\text{CH}}$ = 165 Hz, OCH_2O), 113.9 (CH, Ar), 116.4 (C=), 121.8 (CH, Ar), 127.3 (CH, Ar), 130.9 (CH, Ar), 128.0 (2 $\times$ CH, Ar), 129.2 (2 $\times$ CH, Ar), 130.5 (C, Ar), 130.6 (CH, Ar), 131.8 (C, Ar), 154.1 (C, Ar), 167.4 (C=), 193.9 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{20}\text{H}_{21}\text{O}_4^+$ 325.1434; Found 325.1437.

{4-[2-(Methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}(phenyl)methanone (**10b**)



10b was synthesized from alkene **S2o** (18.0 g, 58.1 mmol). Yield 2.82 g (15%); yellowish oil; R_f = 0.39 (petroleum ether : ethyl acetate, 4:1).

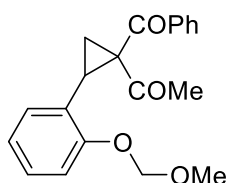
^1H NMR (CDCl_3 , 600 MHz) δ = 1.95 (d, 5J = 1.3 Hz, 3H, CH_3), 3.46 (s, 3H, CH_3O), 4.24 (dd, 2J = 9.1, 3J = 6.8 Hz, 1H, CH_2O), 4.85 (dd, 2J = 9.1, 3J = 10.7 Hz, 1H, CH_2O), 5.11 (ddq, 3J = 10.7, 3J = 6.8, 5J = 1.3 Hz, 1H, CH), 5.15 (d, 2J = 6.6 Hz, 1H, OCH_2O), 5.17 (d, 2J = 6.6 Hz, 1H, OCH_2O), 6.90–6.93 (m, 1H, Ar), 7.04 (dd, 3J = 8.2, 4J = 1.1 Hz, 1H, Ar), 7.12 (ddd, 3J = 8.2, 3J =

7.5, $^4J = 1.8$ Hz, 1H, Ar), 7.16 (dd, $^3J = 7.6$, $^4J = 1.8$ Hz, 1H, Ar), 7.33–7.37 (m, 2H, Ar), 7.39–7.42 (m, 1H, Ar), 7.59–7.61 (m, 2H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) $\delta = 15.2$ ($^1J_{\text{CH}} = 130$ Hz, CH_3), 43.0 ($^1J_{\text{CH}} = 138$ Hz, CH), 55.7 ($^1J_{\text{CH}} = 143$ Hz, CH_3O), 77.5 ($^1J_{\text{CH}} = 151$ Hz, CH_2O), 94.2 ($^1J_{\text{CH}} = 166$ Hz, OCH_2O), 113.8 (CH, Ar), 115.2 (C=), 121.6 (CH, Ar), 127.3 (CH, Ar), 127.5 (3 $\times$ CH, Ar), 127.9 (2 $\times$ CH, Ar), 130.7 (CH, Ar), 131.4 (C, Ar), 140.6 (C, Ar), 154.3 (C, Ar), 169.4 (C=), 192.4 (COPh).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{20}\text{H}_{21}\text{O}_4^+$ 325.1434; Found 325.1440.

1-{1-Benzoyl-2-[2-(methoxymethoxy)phenyl]cyclopropyl}ethanone (S3o)



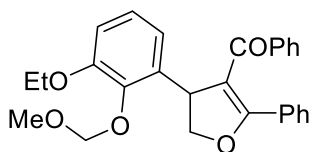
S3o was synthesized from alkene **S2o** (18.0 g, 58.1 mmol). Yield 3.76 g (20%); yellowish oil; $R_f = 0.42$ (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) $\delta = 1.67$ (dd, $^2J = 4.6$, $^3J = 9.1$ Hz, 1H, CH_2), 2.07 (s, 3H, CH_3), 2.47 (dd, $^2J = 4.6$, $^3J = 8.2$ Hz, 1H, CH_2), 3.55 (s, 3H, CH_3O), 3.94–3.97 (m, 1H, CH), 5.20 (d, $^2J = 6.5$ Hz, 1H, OCH_2O), 5.22 (d, $^2J = 6.5$ Hz, 1H, OCH_2O), 6.75–6.78 (m, 1H, Ar), 6.80 (dd, $^3J = 7.7$, $^4J = 1.8$ Hz, 1H, Ar), 6.92 (dd, $^3J = 8.3$, $^4J = 1.1$ Hz, 1H, Ar), 6.97–7.00 (m, 1H, Ar), 7.27–7.30 (m, 2H, Ar), 7.40–7.43 (m, 1H, Ar), 7.79–7.81 (m, 2H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) $\delta = 19.7$ (CH_2), 29.3 (CH_3), 39.5 (CH), 50.2 (C), 56.0 (CH_3O), 94.7 (OCH_2O), 113.4 (CH, Ar), 121.1 (CH, Ar), 122.9 (C, Ar), 126.8 (CH, Ar), 128.16 (CH, Ar), 128.21 (2 $\times$ CH, Ar), 128.6 (2 $\times$ CH, Ar), 133.0 (CH, Ar), 137.1 (C, Ar), 156.4 (C, Ar), 194.4 (CO), 202.9 (CO).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{20}\text{H}_{21}\text{O}_4^+$ 325.1434; Found 325.1438.

{4-[3-Ethoxy-2-(methoxymethoxy)phenyl]-2-phenyl-4,5-dihydrofuran-3-yl}(phenyl)methanone (1p)



1p was synthesized from alkene **S2p** (6.15 g, 14.8 mmol). Yield 3.05 g (48%); white solid, mp 90–91 °C; $R_f = 0.23$ (petroleum ether : ethyl acetate, 2:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.43 (t, 3J = 7.0 Hz, 3H, CH_3), 3.68 (s, 3H, CH_3O), 4.01–4.05 (m, 2H, CH_2O), 4.42 (dd, 3J = 9.1, 3J = 7.1 Hz, 1H, CH_2O), 5.01 (dd, 2J = 9.1, 3J = 10.3 Hz, 1H, CH_2O), 5.25 (d, 2J = 5.4 Hz, 1H, OCH_2O), 5.27 (d, 2J = 5.4 Hz, 1H, OCH_2O), 5.42 (dd, 3J = 10.3, 3J = 7.1 Hz, 1H, CH), 6.78 (dd, 3J = 7.9, 4J = 1.6 Hz, 1H, Ar), 6.95 (dd, 3J = 7.9, 4J = 1.6 Hz, 1H, Ar), 6.98–7.00 (m, 1H, Ar), 7.07–7.12 (m, 4H, Ar), 7.19–7.23 (m, 2H, Ar), 7.33–7.35 (m, 2H, Ar), 7.53–7.56 (m, 2H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.7 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 44.7 ($^1J_{\text{CH}}$ = 139 Hz, CH), 57.5 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 63.9 ($^1J_{\text{CH}}$ = 144 Hz, CH_2O), 77.9 ($^1J_{\text{CH}}$ = 152 Hz, CH_2O), 98.7 ($^1J_{\text{CH}}$ = 167 Hz, OCH_2O), 111.7 (CH, Ar), 115.0 (C=), 118.6 (CH, Ar), 124.4 (CH, Ar), 127.4 (2 $\times$ CH, Ar), 127.5 (2 $\times$ CH, Ar), 128.8 (2 $\times$ CH, Ar), 129.2 (2 $\times$ CH, Ar), 129.8 (C, Ar), 139.9 (CH, Ar), 131.0 (CH, Ar), 136.7 (C, Ar), 138.8 (C, Ar), 143.4 (C, Ar), 151.3 (C, Ar), 166.6 (C=), 192.3 (COPh).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{27}\text{H}_{27}\text{O}_5^+$ 431.1853; Found 431.1856.

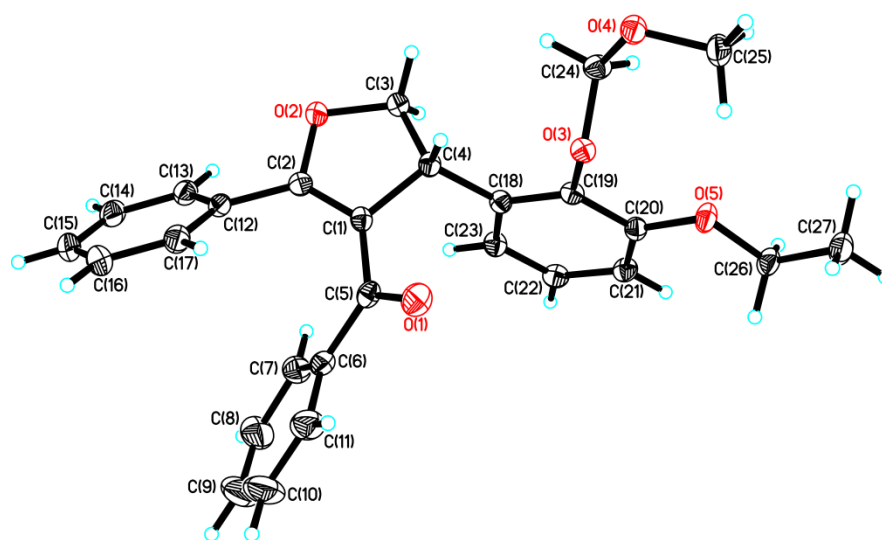
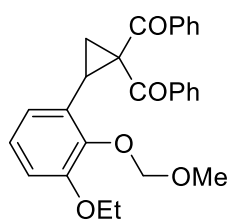


Figure S1. Molecular structure (ORTEP-3) from single crystal X-ray study of **1p** (thermal ellipsoids are set at a 50% probability level); CCDC 1580258.

{2-[3-Ethoxy-2-(methoxymethoxy)phenyl]cyclopropane-1,1-diyl}bis(phenylmethanone) (S3p)



S3p was synthesized from alkene **S2p** (6.15 g, 14.8 mmol) as a side product. Yield 1.39 g (22%); white solid, mp 132–133 °C; R_f = 0.34 (petroleum ether : ethyl acetate, 2:1).

^1H NMR (CDCl_3 , 400 MHz) δ = 1.27 (t, 3J = 7.0 Hz, 3H, CH_3), 1.75 (dd, 2J = 4.6, 3J = 9.0 Hz, 1H, CH_2), 2.80 (dd, 2J = 4.6, 3J = 8.3 Hz, 1H, CH_2), 3.78–3.90 (m, 2H, CH_2O), 3.88 (s, 3H, CH_3O), 4.41 (dd, 3J = 9.0, 3J = 8.3 Hz, 1H, CH), 5.28 (d, 2J = 6.0 Hz, 1H, OCH_2O), 5.32 (d, 2J = 6.0 Hz, 1H, OCH_2O), 6.62–6.66 (m, 2H, Ar), 6.83–6.87 (m, 1H, Ar), 7.08–7.12 (m, 2H, Ar), 7.16–7.23 (m, 3H, Ar), 7.28–7.32 (m, 1H, Ar), 7.67–7.71 (m, 2H, Ar), 7.72–7.75 (m, 2H, Ar).

^{13}C NMR (CDCl_3 , 100 MHz) δ = 14.6 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 19.9 ($^1J_{\text{CH}}$ = 165 Hz, CH_2), 28.0 ($^1J_{\text{CH}}$ = 167 Hz, CH), 49.6 (C), 57.8 ($^1J_{\text{CH}}$ = 142 Hz, CH_3O), 64.1 ($^1J_{\text{CH}}$ = 144 Hz, CH_2O), 99.0 ($^1J_{\text{CH}}$ = 167 Hz, OCH_2O), 113.0 (CH, Ar), 119.8 (CH, Ar), 123.1 (CH, Ar), 127.9 (2 $\times$ CH, Ar), 128.1 (C, Ar), 128.2 (4 $\times$ CH, Ar), 128.5 (2 $\times$ CH, Ar), 132.3 (CH, Ar), 132.4 (CH, Ar), 137.9 (C, Ar), 138.0 (C, Ar), 146.5 (C, Ar), 150.7 (C, Ar), 195.0 (COPh), 196.9 (COPh).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{27}\text{H}_{27}\text{O}_5^+$ 431.1853; Found 431.1857.

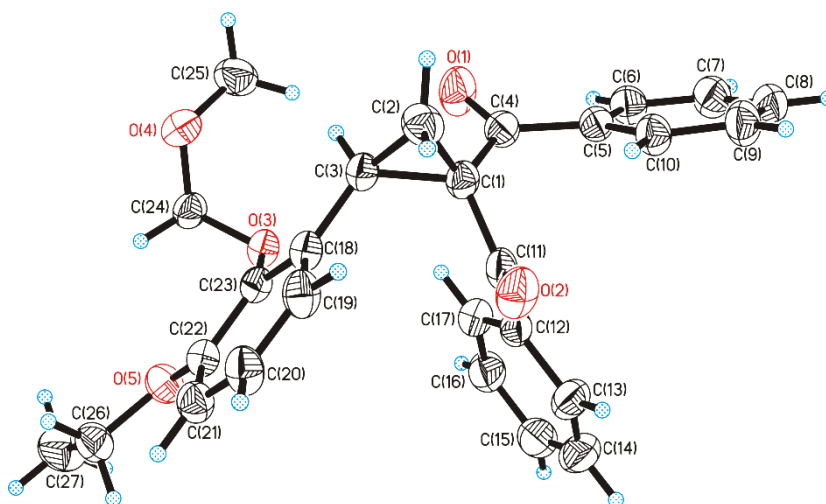
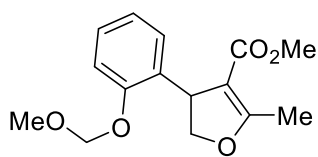


Figure S2. Molecular structure (ORTEP-3) from single crystal X-ray study of **S3p** (thermal ellipsoids are set at a 30% probability level); CCDC 1576709.

Methyl 4-[2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-carboxylate (1q)



1q was synthesized from alkene **S2q** (9.55 g, 36.2 mmol). Yield 5.19 g (52%); white solid, mp 56–57 °C; R_f = 0.39 (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 2.34 (d, 5J = 0.9 Hz, 3H, CH_3), 3.49 (s, 3H, CH_3O), 3.58 (s, 3H, CH_3O), 4.18–4.23 (m, 1H, CH_2O), 4.72–4.76 (m, 2H, CH, CH_2O), 5.21 (s, 2H, OCH_2O), 6.94–6.96 (m, 1H, Ar), 7.06–7.09 (m, 2H, Ar), 7.16–7.19 (m, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.2 ($^1J_{\text{CH}}$ = 129 Hz, CH_3), 41.4 ($^1J_{\text{CH}}$ = 140 Hz, CH), 50.6 ($^1J_{\text{CH}}$ = 146 Hz, CH_3O), 55.8 ($^1J_{\text{CH}}$ = 143 Hz, CH_3O), 78.0 ($^1J_{\text{CH}}$ = 152 Hz, CH_2O), 94.3 ($^1J_{\text{CH}}$ = 166 Hz, OCH_2O), 104.5 (C=), 113.8 (CH, Ar), 121.7 (CH, Ar), 127.3 (CH, Ar), 127.6 (CH, Ar), 132.4 (C, Ar), 154.2 (C, Ar), 166.2 (CO_2Me), 170.3 (C=).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{15}\text{H}_{19}\text{O}_5^+$ 279.1227; Found 279.1228.

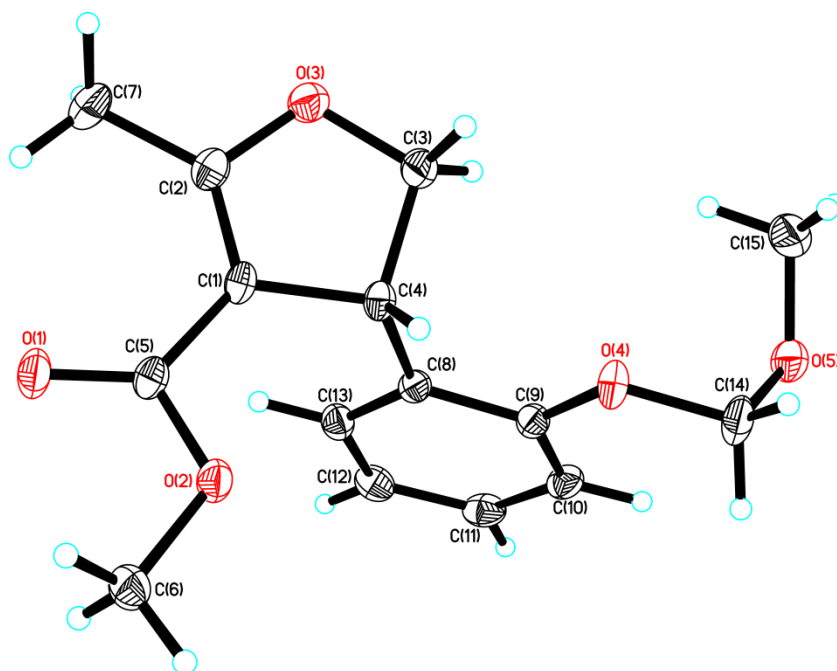
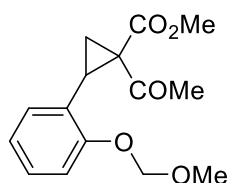


Figure S3. Molecular structure (ORTEP-3) from single crystal X-ray study of **1q** (thermal ellipsoids are set at a 50% probability level); CCDC 1580257.

Methyl 1-acetyl-2-[2-(methoxymethoxy)phenyl]cyclopropane-1-carboxylate (S3q)



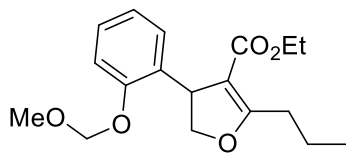
S3q was synthesized from alkene **S2q** (9.55 g, 36.2 mmol) as a side product. Yield 2.42 g (23%); yellowish oil; R_f = 0.35 (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.83 (dd, 2J = 4.6, 3J = 9.1 Hz, 1H, CH_2), 2.19 (dd, 2J = 4.6, 3J = 8.5 Hz, 1H, CH_2), 2.47 (s, 3H, CH_3), 3.14–3.16 (m, 1H, CH), 3.25 (s, 3H, CH_3O), 3.43 (s, 3H, CH_3O), 5.11 (d, 2J = 6.8 Hz, 1H, OCH_2O), 5.14 (d, 2J = 6.8 Hz, 1H, OCH_2O), 6.86–6.89 (m, 1H, Ar), 7.01–7.03 (m, 2H, Ar), 7.14–7.17 (m, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 20.2 ($^1J_{\text{CH}}$ = 165 Hz, CH_2), 29.4 ($^1J_{\text{CH}}$ = 129 Hz, CH_3), 32.5 ($^1J_{\text{CH}}$ = 167 Hz, CH), 43.2 (C), 51.3 ($^1J_{\text{CH}}$ = 147 Hz, CH_3O), 55.7 ($^1J_{\text{CH}}$ = 143 Hz, CH_3O), 94.2 ($^1J_{\text{CH}}$ = 166 Hz, OCH_2O), 113.2 (CH, Ar), 120.8 (CH, Ar), 123.8 (C, Ar), 128.5 (2 $\times$ CH, Ar), 156.6 (C, Ar), 168.6 (CO_2Me), 202.2 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{15}\text{H}_{19}\text{O}_5^+$ 279.1227; Found 279.1228.

Ethyl 4-[2-(methoxymethoxy)phenyl]-2-(1-propyl)-4,5-dihydrofuran-3-carboxylate (1r)



1r was synthesized from alkene **S2r** (6.45 g, 21.1 mmol). Yield 2.03 g (30%); yellowish oil; R_f = 0.63 (petroleum ether : ethyl acetate, 3:1).

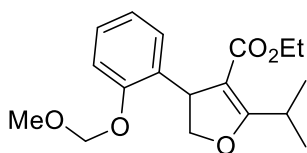
^1H NMR (CDCl_3 , 600 MHz) δ = 1.03 (t, 3J = 7.5 Hz, 3H, CH_3), 1.08 (t, 3J = 7.2 Hz, 3H, CH_3), 1.67–1.73 (m, 2H, CH_2), 2.72–2.82 (m, 2H, CH_2), 3.48 (s, 3H, CH_3O), 4.02 (dq, 2J = 10.9, 3J = 7.5 Hz, 1H, CH_2O), 4.08 (dq, 2J = 10.9, 3J = 7.5 Hz, 1H, CH_2O), 4.21 (dd, 2J = 8.0, 3J = 4.1 Hz, 1H, CH_2O), 4.72 (dd, 2J = 8.0, 3J = 10.7 Hz, 1H, CH_2O), 4.76 (br.dd, 3J = 10.7, 3J = 4.1 Hz, 1H, CH), 5.21 (s, 2H, OCH_2O), 6.93–6.96 (m, 1H, Ar), 7.07–7.10 (m, 2H, Ar), 7.16 (ddd, 3J = 8.2, 3J = 7.4, 4J = 1.8 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 13.8 ($^1J_{\text{CH}}$ = 125 Hz, CH_3), 14.1 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 20.3 ($^1J_{\text{CH}}$ = 129 Hz, CH_2), 29.8 ($^1J_{\text{CH}}$ = 130 Hz, CH_2), 41.6 ($^1J_{\text{CH}}$ = 141 Hz, CH), 55.9 ($^1J_{\text{CH}}$ = 143 Hz, CH_3O), 59.0 ($^1J_{\text{CH}}$ = 147 Hz, CH_2O), 77.8 ($^1J_{\text{CH}}$ = 151 Hz, CH_2O), 94.4 ($^1J_{\text{CH}}$ = 165 Hz, OCH_2O), 104.6 (C=), 113.9

(CH, Ar), 121.7 (CH, Ar), 127.46 (CH, Ar), 127.51 (CH, Ar), 132.7 (C, Ar), 154.4 (C, Ar), 165.7 (C), 173.5 (C).

HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{18}H_{25}O_5^+$ 321.1697; Found 321.1704.

Ethyl 4-[2-(methoxymethoxy)phenyl]-2-(propan-2-yl)-4,5-dihydrofuran-3-carboxylate (**1s**)



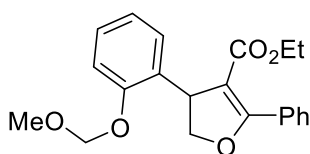
1s was synthesized from alkene **S2s** (8.00 g, 26.3 mmol). Yield 3.21 g (38%); colorless oil; R_f = 0.45 (petroleum ether : ethyl acetate, 4:1).

1H NMR ($CDCl_3$, 600 MHz) δ = 1.06 (t, 3J = 7.2 Hz, 3H, CH_3), 1.19 (d, 3J = 6.9 Hz, 3H, CH_3), 1.24 (d, 3J = 6.9 Hz, 3H, CH_3), 3.49 (s, 3H, CH_3O), 3.79 (spt, 3J = 6.9 Hz, 1H, CH), 4.01 (dq, 2J = 10.9, 3J = 7.2 Hz, 1H, CH_2O), 4.07 (dq, 2J = 10.9, 3J = 7.2 Hz, 1H, CH_2O), 4.22 (dd, 2J = 7.9, 3J = 4.0 Hz, 1H, CH_2O), 4.69 (dd, 2J = 7.9, 3J = 10.7 Hz, 1H, CH_2O), 4.73 (br.dd, 3J = 10.7, 3J = 4.0 Hz, 1H, CH), 5.21 (s, 2H, OCH_2O), 6.93–6.96 (m, 1H, Ar), 7.07–7.08 (m, 2H, Ar), 7.15–7.18 (m, 1H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 14.1 ($^1J_{CH}$ = 127 Hz, CH_3), 19.5 ($^1J_{CH}$ = 127 Hz, CH_3), 19.7 ($^1J_{CH}$ = 127 Hz, CH_3), 27.0 ($^1J_{CH}$ = 134 Hz, CH), 41.6 ($^1J_{CH}$ = 141 Hz, CH), 55.9 ($^1J_{CH}$ = 143 Hz, CH_3O), 59.0 ($^1J_{CH}$ = 147 Hz, CH_2O), 77.8 ($^1J_{CH}$ = 151 Hz, CH_2O), 94.4 ($^1J_{CH}$ = 165 Hz, OCH_2O), 102.8 (C=), 114.0 (CH, Ar), 121.7 (CH, Ar), 127.50 (CH, Ar), 127.51 (CH, Ar), 132.8 (C, Ar), 154.4 (C, Ar), 165.6 (C), 177.7 (C).

HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{18}H_{25}O_5^+$ 321.1697; Found 321.1708.

Ethyl 4-[2-(methoxymethoxy)phenyl]-2-phenyl-4,5-dihydrofuran-3-carboxylate (**1t**)



1t was synthesized from alkene **S2t** (6.54 g, 19.2 mmol). Yield 2.12 g (31%); yellowish oil; R_f = 0.54 (petroleum ether : diethyl ether, 1:1).

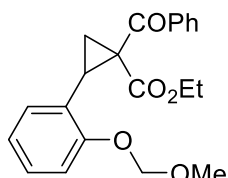
1H NMR ($CDCl_3$, 600 MHz) δ = 1.04 (t, 3J = 7.1 Hz, 3H, CH_3), 3.53 (s, 3H, CH_3O), 4.03 (dq, 2J = 10.9, 3J = 7.1 Hz, 1H, CH_2O), 4.07 (dq, 2J = 10.9, 3J = 7.1 Hz, 1H, CH_2O), 4.41 (dd, 2J = 9.0, 3J = 5.2 Hz, 1H, CH_2O), 4.91 (dd, 2J = 9.0, 3J = 10.7 Hz, 1H, CH_2O), 5.01 (dd, 3J = 10.7, 3J = 5.2 Hz, 1H, CH), 5.26 (s, 2H, OCH_2O), 7.00–7.03 (m, 1H, Ar), 7.15 (dd, 3J = 8.3, 4J = 1.2 Hz, 1H,

Ar), 7.22–7.25 (m, 1H, Ar), 7.29 (dd, $^3J = 7.6$, $^4J = 1.7$ Hz, 1H, Ar), 7.44–7.48 (m, 3H, Ar), 7.92–7.94 (m, 2H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) $\delta = 13.8$ ($^1J_{\text{CH}} = 127$ Hz, CH_3), 43.4 ($^1J_{\text{CH}} = 140$ Hz, CH), 55.9 ($^1J_{\text{CH}} = 142$ Hz, CH_3O), 59.4 ($^1J_{\text{CH}} = 147$ Hz, CH_2O), 77.2 ($^1J_{\text{CH}} = 152$ Hz, CH_2O), 94.5 ($^1J_{\text{CH}} = 165$ Hz, OCH_2O), 105.5 (C=), 114.0 (CH, Ar), 121.8 (CH, Ar), 127.5 (2 $\times$ CH, Ar), 127.71 (CH, Ar), 127.73 (CH, Ar), 129.4 (2 $\times$ CH, Ar), 130.0 (C, Ar), 130.3 (CH, Ar), 132.4 (C, Ar), 154.4 (C, Ar), 164.9 (C), 166.8 (C).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{21}\text{H}_{23}\text{O}_5^+$ 355.1540; Found 355.1537.

Ethyl 1-benzoyl-2-[2-(methoxymethoxy)phenyl]cyclopropanecarboxylate (S3t)



S3t was synthesized from alkene **S2t** (6.54 g, 19.2 mmol) as a side product. Yield 1.29 g (19%); yellowish oil; $R_f = 0.47$ (petroleum ether : diethyl ether, 1:1).

^1H NMR (CDCl_3 , 600 MHz) $\delta = 0.94$ (t, $^3J = 7.2$ Hz, 3H, CH_3), 1.76 (dd, $^2J = 4.9$, $^3J = 9.3$ Hz, 1H, CH_2), 2.51 (dd, $^2J = 4.9$, $^3J = 8.4$ Hz, 1H, CH_2), 3.58 (s, 3H, CH_3O), 3.88–3.91 (m, 1H, CH), 4.02 (dq, $^2J = 10.8$, $^3J = 7.2$ Hz, 1H, CH_2O), 4.13 (dq, $^2J = 10.9$, $^3J = 7.2$ Hz, 1H, CH_2O), 5.24 (d, $^2J = 6.5$ Hz, 1H, OCH_2O), 5.26 (d, $^2J = 6.5$ Hz, 1H, OCH_2O), 6.78–6.81 (m, 1H, Ar), 6.84 (dd, $^3J = 7.8$, $^4J = 1.8$ Hz, 1H, Ar), 6.94 (dd, $^3J = 8.3$, $^4J = 1.1$ Hz, 1H, Ar), 7.00–7.03 (m, 1H, Ar), 7.25–7.28 (m, 2H, Ar), 7.38–7.41 (m, 1H, Ar), 7.77–7.79 (m, 2H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) $\delta = 13.6$ ($^1J_{\text{CH}} = 127$ Hz, CH_3), 17.4 ($^1J_{\text{CH}} = 166$ Hz, CH_2), 28.9 ($^1J_{\text{CH}} = 167$ Hz, CH), 41.6 (C), 56.1 ($^1J_{\text{CH}} = 143$ Hz, CH_3O), 61.3 ($^1J_{\text{CH}} = 148$ Hz, CH_2O), 94.8 ($^1J_{\text{CH}} = 165$ Hz, OCH_2O), 113.5 (CH, Ar), 121.2 (CH, Ar), 122.6 (C, Ar), 126.9 (CH, Ar), 127.7 (2 $\times$ CH, Ar), 128.3 (2 $\times$ CH, Ar), 128.4 (CH, Ar), 132.3 (CH, Ar), 137.5 (C, Ar), 156.6 (C, Ar), 171.2 (CO_2Et), 192.9 (COPh).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{21}\text{H}_{23}\text{O}_5^+$ 355.1540; Found 355.1541.

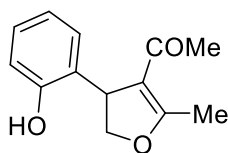
Deprotection of the 1a

To solution of dihydrofuran **1a** (2.62 g, 10 mmol) in ethanol (100 mL) 10 M solution of HCl (5 mL) was added dropwise. Resulting mixture was heated under reflux for 15 min, then cooled off and slowly poured into ice-water mixture with NaHCO₃. Resulting mixture was extracted with ethyl acetate. Combined organic fractions were washed once with brine, dried with Na₂SO₄ and concentrated under reduced pressure, yielding a mixture of **2a**, **3a** and **4a**. From this mixture, the minor diastereomer of **3a** and the final product **4a** were isolated by column chromatography on silica gel; therefore the isolated yield values could be obtained (Table S1). Meanwhile, the major diastereomer of **3a** and DHF **2a** have close *R_f* values and both products were isolated as fractions. Their yields were defined on the basis of the ratios in the reaction mixture.

Table S1. Yields of the major components of the reaction mixture after **1a** deprotection

2a	3a (71:29)		4a
	major	minor	
34%	23%	9%	9%

1-[4-(2-Hydroxyphenyl)-2-methyl-4,5-dihydrofuran-3-yl]ethanone (**2a**)



Phenol **2a** was isolated in its pure form as a fraction; calc. yield 0.74 g (34%); white crystals, mp 89–90 °C; *R_f* = 0.32 (petroleum ether : ethyl acetate, 3:1).

¹H NMR (CDCl₃, 600 MHz) δ = 2.26 (s, 3H, CH₃), 2.35 (d, ⁵*J* = 0.9 Hz, 3H, CH₃), 4.59 (ddq, ³*J* = 9.6, ³*J* = 3.2, ⁵*J* = 0.9 Hz, 1H, CH), 4.66 (dd, ²*J* = 9.7, ³*J* = 3.2 Hz, 1H, CH₂O), 4.69 (dd, ²*J* = 9.7, ³*J* = 9.6 Hz, 1H, CH₂O), 6.90–6.93 (m, 2H, Ar), 7.12–7.15 (m, 1H, Ar), 7.18 (dd, ³*J* = 7.7, ⁴*J* = 1.6 Hz, 1H, Ar), 8.63 (br.s, 1H, OH).

¹³C NMR (CDCl₃, 150 MHz) δ = 15.9 (¹*J*_{CH} = 130 Hz, CH₃), 28.6 (¹*J*_{CH} = 128 Hz, CH₃), 40.6 (¹*J*_{CH} = 139 Hz, CH), 78.0 (¹*J*_{CH} = 152 Hz, CH₂O), 118.0 (CH, Ar), 119.2 (C=), 121.3 (CH, Ar), 126.4 (CH, Ar), 128.2 (CH, Ar), 131.1 (C, Ar), 153.6 (C, Ar), 170.4 (C=), 195.6 (COMe).

HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₃H₁₅O₃⁺ 219.1016; Found 219.1019.

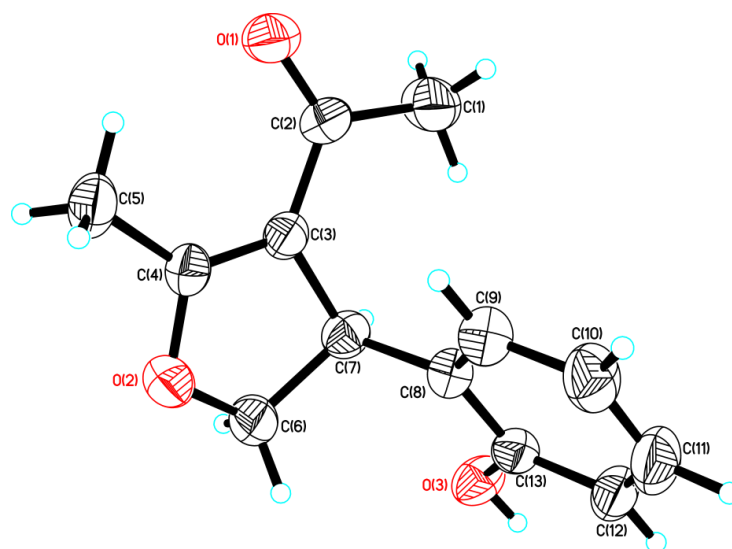
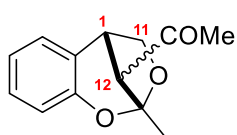


Figure S4. Molecular structure (ORTEP-3) from single crystal X-ray study of **2a** (thermal ellipsoids are set at a 30% probability level); CCDC 1576712.

1-(9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-12-yl)ethanone (3a)



dr 71:29

Major isomer was isolated as a fraction (80:20 mixture with **2a**); calc. yield 0.50 g (23%); yellowish oil. R_f = 0.34 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.82 (s, 3H, CH_3), 2.04 (s, 3H, CH_3), 3.00 (br.d, 3J = 3.8 Hz, 1H, CH), 3.54–3.56 (m, 1H, CH), 4.10 (dd, 2J = 7.4, 3J = 3.5 Hz, 1H, CH_2O), 4.13 (d, 2J = 7.4 Hz, 1H, CH_2O), 6.78 (br.d, 3J = 8.1 Hz, 1H, Ar), 6.82–6.86 (m, 1H, Ar), 7.03 (dd, 3J = 7.5, 4J = 1.5 Hz, 1H, Ar), 7.09–7.13 (m, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 22.8 (CH_3), 29.2 (CH_3), 41.7 (CH), 55.8 (CH), 77.4 (CH_2O), 104.4 (C), 116.1 (CH, Ar), 120.8 (CH, Ar), 124.8 (C, Ar), 126.8 (CH, Ar), 128.8 (CH, Ar), 152.1 (C, Ar), 202.7 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_{15}\text{O}_3^+$ 219.1016; Found 219.1023.

Minor isomer was isolated in its pure form; yield 192 mg (9%); colorless oil. R_f = 0.61 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.76 (s, 3H, CH_3), 2.36 (s, 3H, CH_3), 3.35 (br.d, 3J = 3.9 Hz, 1H, C(1)H), 3.40 (br.s, 1H, C(12)H), 4.21 (d, 2J = 7.3 Hz, 1H, CH_2O), 4.55 (dd, 2J = 7.3, 3J = 3.9 Hz, 1H, CH_2O), 6.81–6.84 (m, 1H, Ar), 6.85 (ddd, 3J = 7.4, 3J = 7.4, 4J = 1.2 Hz, 1H, Ar), 7.01 (dd, 3J = 7.4, 4J = 1.7 Hz, 1H, Ar), 7.16 (ddd, 3J = 8.1, 3J = 7.4, 4J = 1.7 Hz, 1H, Ar).

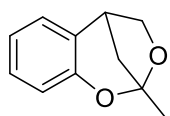
^{13}C NMR (CDCl_3 , 150 MHz) δ = 21.0 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 31.9 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 42.2 ($^1J_{\text{CH}}$ = 142 Hz, C(1)H), 58.3 ($^1J_{\text{CH}}$ = 136 Hz, C(12)H), 79.5 ($^1J_{\text{CH}}$ = 151 Hz, CH_2O), 107.2 (C), 116.2 (CH, Ar), 120.6 (CH, Ar), 125.8 (CH, Ar), 128.7 (CH, Ar), 129.0 (C, Ar), 152.1 (C, Ar), 206.0 (COMe).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_{15}\text{O}_3^+$ 219.1016; Found 219.1017.

General procedure for the synthesis of methanobenzodioxepines **4**

To solution of dihydrofuran **1** (1 mmol) in ethanol (10 mL) 10 M solution of HCl (1 mL) was added dropwise. Resulting solution was heated under reflux for specified time, then cooled off and slowly poured into ice-water mixture with NaHCO_3 . Resulting mixture was extracted with ethyl acetate. Combined organic fractions were washed once with brine, dried with Na_2SO_4 and concentrated under reduced pressure. Residue was purified by column chromatography on silica gel yielding pure methanobenzodioxepines **4**.

9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (**4a**)



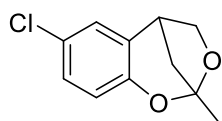
Reaction time and yield from **1a**: 2 h, 123 mg (70%); from **1q**: 4 h, 143 mg (81%); colorless oil; R_f = 0.57 (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.75 (s, 3H, CH_3), 2.12 (dd, 2J = 11.4, 3J = 3.9 Hz, 1H, CH_2), 2.20 (br.d, 2J = 11.4 Hz, 1H, CH_2), 3.22–3.26 (m, 1H, CH), 4.12 (dd, 2J = 7.4, 3J = 3.5 Hz, 1H, CH_2O), 4.22 (dd, 2J = 7.4, 4J = 0.9 Hz, 1H, CH_2O), 6.80–6.82 (m, 1H, Ar), 6.83–6.86 (m, 1H, Ar), 7.03 (dd, 3J = 7.4, 4J = 1.7 Hz, 1H, Ar), 7.14 (ddd, 3J = 8.1, 3J = 7.4, 4J = 1.7 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 23.1 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 36.9 ($^1J_{\text{CH}}$ = 136 Hz, CH_2), 39.1 ($^1J_{\text{CH}}$ = 142 Hz, CH), 79.6 ($^1J_{\text{CH}}$ = 149 Hz, CH_2O), 106.1 (C), 116.0 (CH, Ar), 120.2 (CH, Ar), 126.4 (CH, Ar), 128.2 (CH, Ar), 128.3 (C, Ar), 152.6 (C, Ar).

HRMS ESI m/z: $[M + H]^+$ Calcd for $C_{11}H_{13}O_2^+$ 177.0910; Found 177.0910.

4-Chloro-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4b)



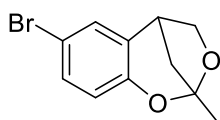
Reaction time 3 h. Yield 132 mg (63%); colorless oil; R_f = 0.62 (petroleum ether : ethyl acetate, 4:1).

1H NMR ($CDCl_3$, 600 MHz) δ = 1.72 (s, 3H, CH_3), 2.11 (dd, 2J = 11.6, 3J = 3.8 Hz, 1H, CH_2), 2.15 (br.d, 2J = 11.6 Hz, 1H, CH_2), 3.18–3.20 (m, 1H, CH), 4.09 (dd, 2J = 7.6, 3J = 3.4 Hz, 1H, CH_2O), 4.19 (br.d, 2J = 7.6 Hz, 1H, CH_2O), 6.71 (d, 3J = 8.7 Hz, 1H, Ar), 7.00 (d, 4J = 2.6 Hz, 1H, Ar), 7.07 (dd, 3J = 8.7, 4J = 2.6 Hz, 1H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.9 ($^1J_{CH}$ = 128 Hz, CH_3), 36.6 ($^1J_{CH}$ = 136 Hz, CH_2), 38.9 ($^1J_{CH}$ = 143 Hz, CH), 79.4 ($^1J_{CH}$ = 150 Hz, CH_2O), 106.3 (C), 117.3 (CH, Ar), 124.8 (C, Ar), 126.2 (CH, Ar), 128.0 (CH, Ar), 129.8 (C, Ar), 151.3 (C, Ar).

HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{11}H_{12}ClO_2^+$ 211.0520; Found 211.0521.

4-Bromo-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4c)



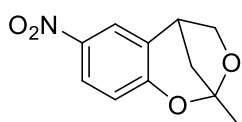
Reaction time 4 h. Yield 169 mg (66%); yellow oil; R_f = 0.61 (petroleum ether : ethyl acetate, 4:1).

1H NMR ($CDCl_3$, 600 MHz) δ = 1.72 (s, 3H, CH_3), 2.11 (dd, 2J = 11.6, 3J = 3.9 Hz, 1H, CH_2), 2.15 (br.d, 2J = 11.6 Hz, 1H, CH_2), 3.19–3.21 (m, 1H, CH), 4.09 (dd, 2J = 7.6, 3J = 3.6 Hz, 1H, CH_2O), 4.20 (br.d, 2J = 7.6 Hz, 1H, CH_2O), 6.67 (d, 3J = 8.6 Hz, 1H, Ar), 7.15 (d, 4J = 2.4 Hz, 1H, Ar), 7.22 (dd, 3J = 8.6, 4J = 2.4 Hz, 1H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.9 ($^1J_{CH}$ = 128 Hz, CH_3), 36.6 ($^1J_{CH}$ = 136 Hz, CH_2), 38.9 ($^1J_{CH}$ = 143 Hz, CH), 79.4 ($^1J_{CH}$ = 150 Hz, CH_2O), 106.4 (C), 112.1 (C, Ar), 117.9 (CH, Ar), 129.1 (CH, Ar), 130.4 (C, Ar), 131.0 (CH, Ar), 151.9 (C, Ar).

HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{11}H_{12}BrO_2^+$ 255.0015; Found 255.0013.

9-Methyl-4-nitro-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (**4d**)



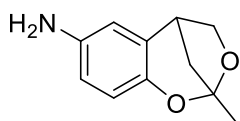
Reaction time 4 h. Yield 171 mg (77%); yellowish solid, mp 104–105 °C; R_f = 0.39 (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.74 (s, 3H, CH_3), 2.18 (br.d, 2J = 11.8 Hz, 1H, CH_2), 2.22 (dd, 2J = 11.8, 3J = 3.8 Hz, 1H, CH_2), 3.36–3.39 (m, 1H, CH), 4.14 (dd, 2J = 7.8, 3J = 3.6 Hz, 1H, CH_2O), 4.20 (br.d, 2J = 7.8 Hz, 1H, CH_2O), 6.82 (d, 3J = 8.9 Hz, 1H, Ar), 7.96 (d, 4J = 2.7 Hz, 1H, Ar), 8.02 (dd, 3J = 8.9, 4J = 2.7 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 22.6 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 36.6 ($^1J_{\text{CH}}$ = 136 Hz, CH_2), 38.9 ($^1J_{\text{CH}}$ = 143 Hz, CH), 79.3 ($^1J_{\text{CH}}$ = 150 Hz, CH_2O), 107.5 (C), 116.5 (CH, Ar), 122.5 (CH, Ar), 124.6 (CH, Ar), 128.9 (C, Ar), 140.9 (C, Ar), 158.6 (C, Ar).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{11}\text{H}_{12}\text{NO}_4^+$ 222.0761; Found 222.0762.

9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-4-amine (**4d'**)



4d' was synthesized from **1d'** (277 mg, 1 mmol) by the treatment of its solution in EtOH (10 mL) with saturated HCl solution in Et₂O (1 mL) at room

temperature. Yield 146 mg (76%); colorless solid, mp 150–151 °C; R_f = 0.70 (ethyl acetate).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.70 (s, 3H, CH_3), 2.06 (dd, 2J = 11.3, 3J = 3.9 Hz, 1H, CH_2), 2.16 (br.d, 2J = 11.3 Hz, 1H, CH_2), 3.09–3.11 (m, 1H, CH), 3.39 (br.s, 2H, NH_2), 4.08 (dd, 2J = 7.4, 3J = 3.6 Hz, 1H, CH_2O), 4.18 (dd, 2J = 7.4, 4J = 0.9 Hz, 1H, CH_2O), 6.39 (d, 4J = 2.8 Hz, 1H, Ar), 6.48 (dd, 3J = 8.5, 4J = 2.8 Hz, 1H, Ar), 6.61 (d, 3J = 8.5 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 23.2 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 37.0 ($^1J_{\text{CH}}$ = 136 Hz, CH_2), 39.2 ($^1J_{\text{CH}}$ = 142 Hz, CH), 79.4 ($^1J_{\text{CH}}$ = 149 Hz, CH_2O), 105.8 (C), 113.6 (CH, Ar), 115.1 (CH, Ar), 116.4 (CH, Ar), 128.9 (C, Ar), 139.4 (C, Ar), 145.2 (C, Ar).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{11}\text{H}_{14}\text{NO}_2^+$ 192.1019; Found 192.1022.

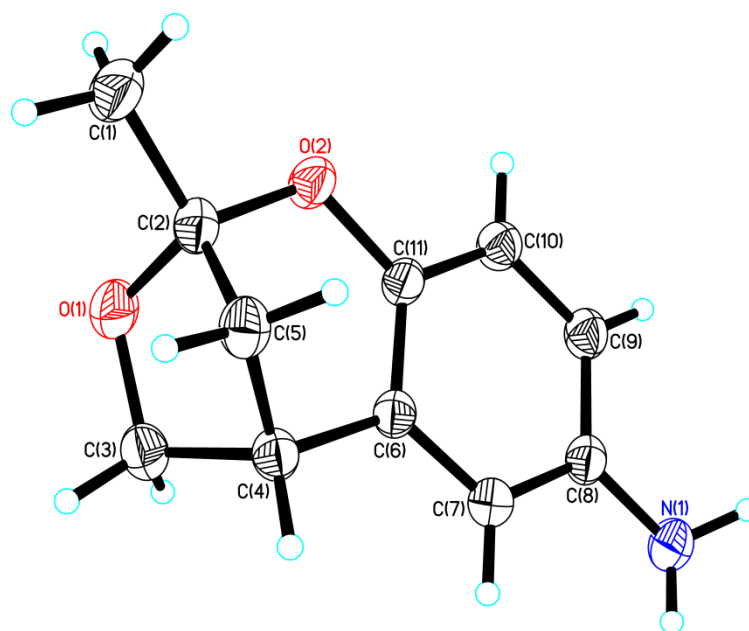
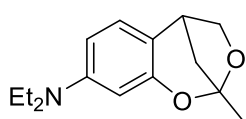


Figure S5. Molecular structure (ORTEP-3) from single crystal X-ray study of **4d'** (thermal ellipsoids are set at a 30% probability level); CCDC 1576718.

***N,N*-Diethyl-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-5-amine (**4e**)**



Reaction time 4 h. Yield 177 mg (72%); colorless crystals, mp 90–91 °C; R_f = 0.64 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.14 (t, 3J = 7.1 Hz, 6H, $2\times\text{CH}_3$), 1.74 (s, 3H, CH_3), 2.06 (dd, 2J = 11.2, 3J = 4.0 Hz, 1H, CH_2), 2.16 (br.d, 2J = 11.2 Hz, 1H, CH_2), 3.13–3.16 (m, 1H, CH), 3.30 (q, 3J = 7.1 Hz, 4H, $2\times\text{CH}_2\text{N}$), 4.08 (dd, 2J = 7.1, 3J = 3.3 Hz, 1H, CH_2O), 4.16 (dd, 2J = 7.1, 4J = 0.9 Hz, 1H, CH_2O), 6.17 (d, 4J = 2.6 Hz, 1H, Ar), 6.20 (dd, 3J = 8.3, 4J = 2.6 Hz, 1H, Ar), 6.85 (d, 3J = 8.3 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 12.6 ($^1J_{\text{CH}}$ = 126 Hz, $2\times\text{CH}_3$), 23.3 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 37.7 ($^1J_{\text{CH}}$ = 136 Hz, CH_2), 38.3 ($^1J_{\text{CH}}$ = 143 Hz, CH), 44.3 ($^1J_{\text{CH}}$ = 134 Hz, $2\times\text{CH}_2\text{N}$), 80.0 ($^1J_{\text{CH}}$ = 149 Hz, CH_2O), 99.4 (CH, Ar), 104.0 (CH, Ar), 106.0 (C), 115.6 (C, Ar), 126.7 (CH, Ar), 148.4 (C, Ar), 153.5 (C, Ar).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{15}\text{H}_{22}\text{NO}_2^+$ 248.1645; Found 248.1646.

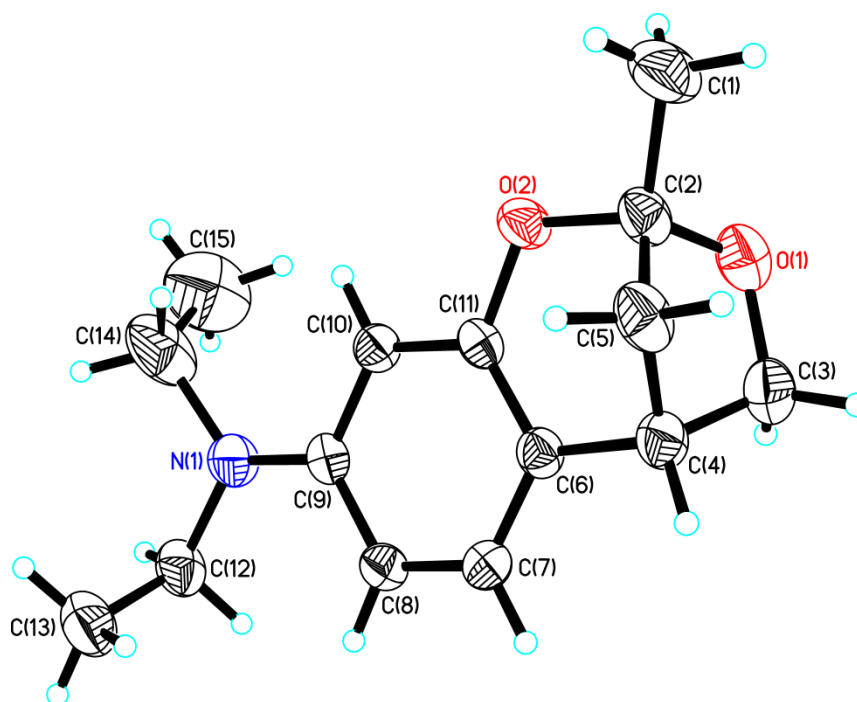
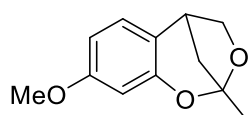


Figure S6. Molecular structure (ORTEP-3) from single crystal X-ray study of **4e** (thermal ellipsoids are set at a 30% probability level); CCDC 1576717.

5-Methoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4f**)**



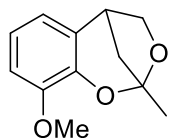
Reaction time 1.5 h. Yield 140 mg (68%); colorless oil; $R_f = 0.58$ (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) $\delta = 1.73$ (s, 3H, CH_3), 2.08 (dd, $^2J = 11.4$, $^3J = 4.0$ Hz, 1H, CH_2), 2.14 (br.d, $^2J = 11.4$ Hz, 1H, CH_2), 3.17–3.20 (m, 1H, CH), 3.74 (s, 3H, CH_3O), 4.08 (dd, $^2J = 7.3$, $^3J = 3.4$ Hz, 1H, CH_2O), 4.22 (br.d, $^2J = 7.3$ Hz, 1H, CH_2O), 6.39 (d, $^4J = 2.4$ Hz, 1H, Ar), 6.41 (dd, $^3J = 8.1$, $^4J = 2.4$ Hz, 1H, Ar), 6.91 (d, $^3J = 8.1$ Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) $\delta = 23.0$ ($^1J_{\text{CH}} = 128$ Hz, CH_3), 37.2 ($^1J_{\text{CH}} = 135$ Hz, CH_2), 38.4 ($^1J_{\text{CH}} = 142$ Hz, CH), 55.2 ($^1J_{\text{CH}} = 144$ Hz, CH_3O), 79.8 ($^1J_{\text{CH}} = 149$ Hz, CH_2O), 101.5 (CH, Ar), 106.1 (C), 106.3 (CH, Ar), 120.7 (C, Ar), 126.7 (CH, Ar), 153.5 (C, Ar), 159.8 (C, Ar).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{12}\text{H}_{15}\text{O}_3^+$ 207.1016; Found 207.1017.

6-Methoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4g)



Reaction time 2.5 h. Yield 635 mg (77%, 4 mmol run); colorless crystals, mp 126–127 °C; R_f = 0.53 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.81 (s, 3H, CH_3), 2.11 (dd, 2J = 11.4, 3J = 3.9 Hz, 1H, CH_2), 2.22 (br.d, 2J = 11.4 Hz, 1H, CH_2), 3.21–3.24 (m, 1H, CH), 3.84 (s, 3H, CH_3O), 4.10 (dd, 2J = 7.4, 3J = 3.5 Hz, 1H, CH_2O), 4.22 (br.d, 2J = 7.4 Hz, 1H, CH_2O), 6.64 (dd, 3J = 7.3, 4J = 1.7 Hz, 1H, Ar), 6.76 (dd, 3J = 8.1, 4J = 1.7 Hz, 1H, Ar), 6.80 (dd, 3J = 8.1, 3J = 7.3 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 23.2 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 36.8 ($^1J_{\text{CH}}$ = 136 Hz, CH_2), 39.0 ($^1J_{\text{CH}}$ = 143 Hz, CH), 55.7 ($^1J_{\text{CH}}$ = 144 Hz, CH_3O), 79.7 ($^1J_{\text{CH}}$ = 149 Hz, CH_2O), 106.3 (C), 110.6 (CH, Ar), 118.5 (CH, Ar), 120.2 (CH, Ar), 129.1 (C, Ar), 141.7 (C, Ar), 147.8 (C, Ar).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{12}\text{H}_{15}\text{O}_3^+$ 207.1016; Found 207.1017.

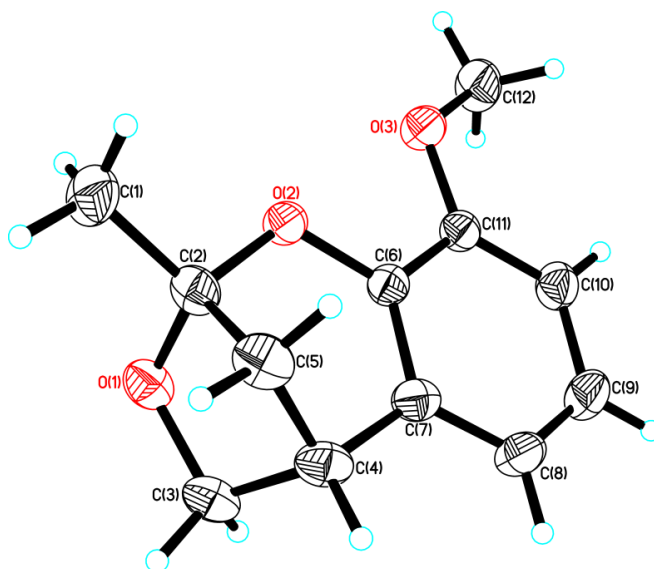
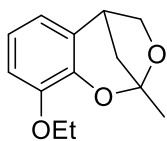


Figure S7. Molecular structure (ORTEP-3) from single crystal X-ray study of **4g** (thermal ellipsoids are set at a 30% probability level); CCDC 1576714.

6-Ethoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4h)



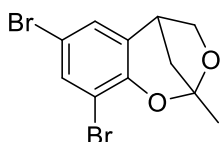
Reaction time 2.5 h. Yield 175 mg (79%); colorless oil; R_f = 0.56 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.43 (t, 3J = 7.1 Hz, 3H, CH_3), 1.80 (s, 3H, CH_3), 2.09 (dd, 2J = 11.4, 3J = 3.9 Hz, 1H, CH_2), 2.21 (br.d, 2J = 11.4 Hz, 1H, CH_2), 3.20–3.22 (m, 1H, CH), 4.04–4.11 (m, 3H), 4.21 (br.d, 2J = 7.4 Hz, 1H, CH_2O), 6.61–6.65 (m, 1H, Ar), 6.75–6.77 (m, 2H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.7 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 23.1 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 36.7 ($^1J_{\text{CH}}$ = 136 Hz, CH_2), 39.1 ($^1J_{\text{CH}}$ = 143 Hz, CH), 64.4 ($^1J_{\text{CH}}$ = 144 Hz, CH_2O), 79.6 ($^1J_{\text{CH}}$ = 150 Hz, CH_2O), 106.2 (C), 112.6 (CH, Ar), 118.5 (CH, Ar), 120.0 (CH, Ar), 129.3 (C, Ar), 142.1 (C, Ar), 147.1 (C, Ar).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_{17}\text{O}_3^+$ 221.1172; Found 221.1173.

4,6-Dibromo-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4i)



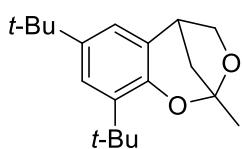
Reaction time 8 h. Yield 245 mg (73%); yellow oil; R_f = 0.52 (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.78 (s, 3H, CH_3), 2.14 (dd, 2J = 11.6, 3J = 3.6 Hz, 1H, CH_2), 2.17 (br.d, 2J = 11.6 Hz, 1H, CH_2), 3.21–3.23 (m, 1H, CH), 4.11 (dd, 2J = 7.7, 3J = 3.5 Hz, 1H, CH_2O), 4.19 (br.d, 2J = 7.7 Hz, 1H, CH_2O), 7.10 (d, 4J = 2.3 Hz, 1H, Ar), 7.49 (d, 4J = 2.3 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 22.7 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 36.6 ($^1J_{\text{CH}}$ = 136 Hz, CH_2), 39.1 ($^1J_{\text{CH}}$ = 144 Hz, CH), 79.3 ($^1J_{\text{CH}}$ = 151 Hz, CH_2O), 107.3 (C), 110.9 (C, Ar), 112.0 (C, Ar), 128.3 (CH, Ar), 131.2 (C, Ar), 133.9 (CH, Ar), 149.2 (C, Ar).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{11}\text{H}_{11}\text{Br}_2\text{O}_2^+$ 332.9120; Found 332.9119.

4,6-Di-*tert*-butyl-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4j)



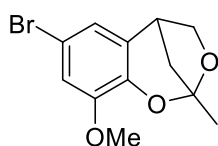
Reaction time 1 h. Yield 245 mg (85%); yellowish crystals, mp 97–98 °C; R_f = 0.76 (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.34 (s, 9H, $3 \times \text{CH}_3$), 1.42 (s, 9H, $3 \times \text{CH}_3$), 1.79 (s, 3H, CH_3), 2.10 (dd, 2J = 11.1, 3J = 3.9 Hz, 1H, CH_2), 2.18 (br.d, 2J = 11.1 Hz, 1H, CH_2), 3.22–3.24 (m, 1H, CH), 4.13 (dd, 2J = 7.3, 3J = 3.5 Hz, 1H, CH_2O), 4.25 (br.d, 2J = 7.3 Hz, 1H, CH_2O), 6.91 (br.d, 4J = 2.4 Hz, 1H, Ar), 7.22 (br.d, 4J = 2.4 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 23.3 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 29.7 ($^1J_{\text{CH}}$ = 126 Hz, $3\times\text{CH}_3$), 31.7 ($^1J_{\text{CH}}$ = 125 Hz, $3\times\text{CH}_3$), 34.2 (C), 34.8 (C), 37.0 ($^1J_{\text{CH}}$ = 135 Hz, CH_2), 40.0 ($^1J_{\text{CH}}$ = 140 Hz, CH), 79.4 ($^1J_{\text{CH}}$ = 150 Hz, CH_2O), 105.4 (C), 121.4 (CH, Ar), 122.5 (CH, Ar), 127.7 (C, Ar), 136.0 (C, Ar), 141.8 (C, Ar), 148.6 (C, Ar).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{19}\text{H}_{29}\text{O}_2^+$ 289.2162; Found 289.2169.

4-Bromo-6-methoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4k)



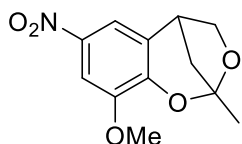
Reaction time 3 h. Yield 215 mg (75%); yellowish crystals, mp 79–80 °C; R_f = 0.51 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.77 (s, 3H, CH_3), 2.09 (dd, 2J = 11.6, 3J = 4.0 Hz, 1H, CH_2), 2.17 (br.d, 2J = 11.6 Hz, 1H, CH_2), 3.16–3.18 (m, 1H, CH), 3.81 (s, 3H, CH_3O), 4.07 (dd, 2J = 7.5, 3J = 3.5 Hz, 1H, CH_2O), 4.23 (dd, 2J = 7.5, 4J = 0.8 Hz, 1H, CH_2O), 6.78 (br.d, 4J = 2.2 Hz, 1H, Ar), 6.85 (d, 4J = 2.2 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 23.0 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 36.6 ($^1J_{\text{CH}}$ = 136 Hz, CH_2), 38.9 ($^1J_{\text{CH}}$ = 142 Hz, CH), 56.0 ($^1J_{\text{CH}}$ = 144 Hz, CH_3O), 79.5 ($^1J_{\text{CH}}$ = 150 Hz, CH_2O), 106.5 (C), 111.8 (C, Ar), 114.0 (CH, Ar), 121.1 (CH, Ar), 130.4 (C, Ar), 141.0 (C, Ar), 148.6 (C, Ar).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{12}\text{H}_{14}\text{BrO}_3^+$ 285.0121; Found 285.0126.

6-Methoxy-9-methyl-4-nitro-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4l)



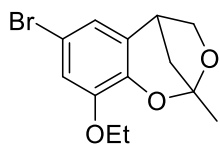
Reaction time 4 h. Yield 198 mg (79%); yellowish solid, mp 108–109 °C; R_f = 0.36 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.80 (s, 3H, CH_3), 2.18–2.23 (m, 2H, CH_2), 3.33–3.36 (m, 1H, CH), 3.89 (s, 3H, CH_3O), 4.12 (dd, 2J = 7.7, 3J = 3.4 Hz, 1H, CH_2O), 4.20 (d, 2J = 7.7 Hz, 1H, CH_2O), 7.61 (br.d, 4J = 2.5 Hz, 1H, Ar), 7.64 (d, 4J = 2.5 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 22.6 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 36.5 ($^1J_{\text{CH}}$ = 138 Hz, CH_2), 38.9 ($^1J_{\text{CH}}$ = 144 Hz, CH), 56.1 ($^1J_{\text{CH}}$ = 145 Hz, CH_3O), 79.4 ($^1J_{\text{CH}}$ = 150 Hz, CH_2O), 106.1 (CH, Ar), 107.6 (C), 115.0 (CH, Ar), 128.6 (C, Ar), 140.6 (C, Ar), 147.8 (C, Ar), 148.1 (C, Ar).

HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{12}H_{14}NO_5^+$ 252.0866; Found 252.0868.

4-Bromo-6-ethoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4m)



Reaction time 3 h. Yield 214 mg (72%); colorless crystals, mp 109–110 °C; R_f = 0.55 (petroleum ether : ethyl acetate, 3:1).

1H NMR ($CDCl_3$, 600 MHz) δ = 1.41 (t, 3J = 7.1 Hz, 3H, CH_3), 1.77 (s, 3H, CH_3), 2.09 (dd, 2J = 11.6, 3J = 4.0 Hz, 1H, CH_2), 2.18 (br.d, 2J = 11.6 Hz, 1H, CH_2), 3.15–3.18 (m, 1H, CH), 3.99–4.05 (m, 2H, CH_2O), 4.07 (dd, 2J = 7.6, 3J = 3.5 Hz, 1H, CH_2O), 4.19 (dd, 2J = 7.6, 4J = 0.8 Hz, 1H, CH_2O), 6.77 (br.d, 4J = 2.3 Hz, 1H, Ar), 6.85 (d, 4J = 2.3 Hz, 1H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 14.5 ($^1J_{CH}$ = 127 Hz, CH_3), 23.0 ($^1J_{CH}$ = 128 Hz, CH_3), 36.5 ($^1J_{CH}$ = 136 Hz, CH_2), 38.9 ($^1J_{CH}$ = 143 Hz, CH), 64.7 ($^1J_{CH}$ = 144 Hz, CH_2O), 79.4 ($^1J_{CH}$ = 150 Hz, CH_2O), 106.4 (CH, Ar), 111.7 (C), 115.5 (CH, Ar), 121.1 (C, Ar), 130.5 (C, Ar), 141.4 (C, Ar), 147.9 (C, Ar).

HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{13}H_{16}BrO_3^+$ 299.0277; Found 299.0281.

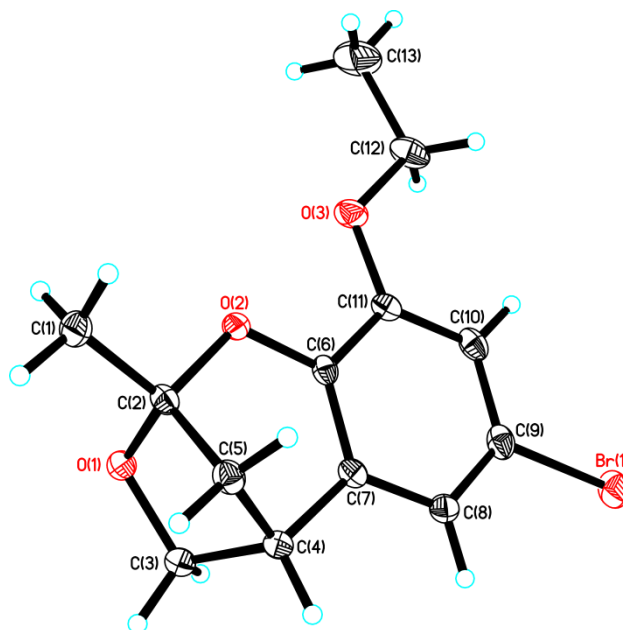
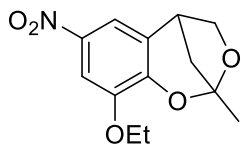


Figure S8. Molecular structure (ORTEP-3) from single crystal X-ray study of **4m** (thermal ellipsoids are set at a 50% probability level); CCDC 1580281.

6-Ethoxy-9-methyl-4-nitro-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4n)



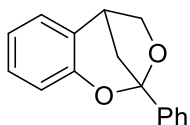
Reaction time 3.5 h. Yield 182 mg (69%); yellowish solid, mp 94–95 °C; R_f = 0.41 (petroleum ether : ethyl acetate, 3:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.48 (t, 3J = 7.0 Hz, 3H, CH_3), 1.83 (s, 3H, CH_3), 2.21 (dd, 2J = 11.8, 3J = 3.6 Hz, 1H, CH_2), 2.23 (br.d, 2J = 11.8 Hz, 1H, CH_2), 3.34–3.36 (m, 1H, CH), 4.11–4.18 (m, 3H), 4.24 (d, 2J = 7.8 Hz, 1H, CH_2O), 6.78 (d, 4J = 2.6 Hz, 1H, Ar), 6.85 (br.d, 4J = 2.6 Hz, 1H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.5 ($^1J_{\text{CH}}$ = 126 Hz, CH_3), 22.8 ($^1J_{\text{CH}}$ = 128 Hz, CH_3), 36.6 ($^1J_{\text{CH}}$ = 137 Hz, CH_2), 39.2 ($^1J_{\text{CH}}$ = 142 Hz, CH), 65.0 ($^1J_{\text{CH}}$ = 145 Hz, CH_2O), 79.6 ($^1J_{\text{CH}}$ = 150 Hz, CH_2O), 107.6 (C), 107.7 (CH, Ar), 115.0 (CH, Ar), 128.8 (C, Ar), 140.8 (C, Ar), 147.3 (C, Ar), 148.6 (C, Ar).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_{16}\text{NO}_5^+$ 266.1023; Found 266.1029.

9-Phenyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4o)



4o was synthesized from **10a**: reaction time 0.5 h, yield 155 mg (65%); from **10b**: reaction time 0.5 h, yield 164 mg (69%); from **1t**: reaction time 2 h, yield 143 mg

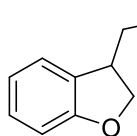
(60%); colorless oil; R_f = 0.68 (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 2.38 (dd, 2J = 11.6, 3J = 4.0 Hz, 1H, CH_2), 2.51 (br.d, 2J = 11.6 Hz, 1H, CH_2), 3.39–3.41 (m, 1H, CH), 4.34 (dd, 2J = 7.4, 3J = 3.4 Hz, 1H, CH_2O), 4.47 (br.d, 2J = 7.4 Hz, 1H, CH_2O), 6.90–6.92 (m, 1H, Ar), 6.95 (d, 3J = 8.1 Hz, 1H, Ar), 7.11 (dd, 3J = 7.4, 4J = 1.4 Hz, 1H, Ar), 7.18–7.21 (m, 1H, Ar), 7.39–7.42 (m, 1H, Ar), 7.43–7.46 (m, 2H, Ar), 7.71–7.73 (m, 2H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 38.7 ($^1J_{\text{CH}}$ = 137 Hz, CH_2), 39.4 ($^1J_{\text{CH}}$ = 144 Hz, CH), 80.3 ($^1J_{\text{CH}}$ = 150 Hz, CH_2O), 107.0 (C), 116.5 (CH, Ar), 120.6 (CH, Ar), 125.9 (2 $\times$ CH, Ar), 126.5 (CH, Ar), 128.30 (2 $\times$ CH, Ar), 128.32 (C, Ar), 128.4 (CH, Ar), 128.7 (CH, Ar), 139.3 (C, Ar), 152.8 (C, Ar).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{15}\text{O}_2^+$ 239.1067; Found 239.1068.

2-(2,3-Dihydro-1-benzofuran-3-yl)-1-phenylethanone²⁰ (5o)

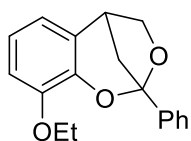


Reaction time 18 h. Conversion 66%. Yield 77 mg (49%); white solid, mp 105–106 °C; R_f = 0.43 (petroleum ether : diethyl ether, 6:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 3.29 (dd, 2J = 18.1, 3J = 9.5 Hz, 1H, CH_2), 3.55 (dd, 2J = 18.1, 3J = 4.5 Hz, 1H, CH_2), 4.07–4.12 (m, 1H, CH), 4.22 (dd, 2J = 9.2, 3J = 6.2 Hz, 1H, CH_2O), 4.90 (dd, 2J = 9.2, 3J = 9.0 Hz, 1H, CH_2O), 6.83–6.84 (m, 1H, Ar), 6.88–6.90 (m, 1H, Ar), 7.15–7.18 (m, 1H, Ar), 7.21–7.23 (m, 1H, Ar), 7.47–7.50 (m, 2H, Ar), 7.58–7.61 (m, 1H, Ar), 7.97–7.99 (m, 2H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 37.4 ($^1J_{\text{CH}}$ = 136 Hz, CH), 44.5 ($^1J_{\text{CH}}$ = 126 Hz, CH_2), 77.3 ($^1J_{\text{CH}}$ = 151 Hz, CH_2O), 109.7 (CH, Ar), 120.5 (CH, Ar), 124.3 (CH, Ar), 128.0 (2 $\times$ CH, Ar), 128.5 (CH, Ar), 128.7 (2 $\times$ CH, Ar), 129.7 (C, Ar), 133.4 (CH, Ar), 136.6 (C, Ar), 159.9 (C, Ar), 198.3 (COPh).

6-Ethoxy-9-phenyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4p)



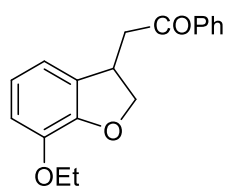
Reaction time 2 h. Yield 102 mg (36%); yellowish oil; R_f = 0.74 (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.44 (t, 3J = 7.0 Hz, 3H, CH_3), 2.40 (dd, 2J = 11.6, 3J = 3.9 Hz, 1H, CH_2), 2.49 (br.d, 2J = 11.6 Hz, 1H, CH_2), 3.38–3.39 (m, 1H, CH), 4.12 (q, 3J = 7.0 Hz, 2H, CH_2O), 4.34 (dd, 2J = 7.4, 3J = 3.5 Hz, 1H, CH_2O), 4.48 (br.d, 2J = 7.4 Hz, 1H, CH_2O), 6.72–6.75 (m, 1H, Ar), 6.85–6.86 (m, 2H, Ar), 7.39–7.42 (m, 1H, Ar), 7.44–7.47 (m, 2H, Ar), 7.77–7.79 (m, 2H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.9 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 38.8 ($^1J_{\text{CH}}$ = 139 Hz, CH_2), 39.4 ($^1J_{\text{CH}}$ = 142 Hz, CH), 64.8 ($^1J_{\text{CH}}$ = 142 Hz, CH_2O), 80.3 ($^1J_{\text{CH}}$ = 150 Hz, CH_2O), 106.8 (C), 113.6 (CH, Ar), 118.8 (CH, Ar), 120.4 (CH, Ar), 126.0 (2 $\times$ CH, Ar), 128.1 (2 $\times$ CH, Ar), 128.5 (CH, Ar), 129.3 (C, Ar), 139.4 (C, Ar), 142.5 (C, Ar), 147.6 (C, Ar).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{18}\text{H}_{19}\text{O}_3^+$ 283.1329; Found 283.1324.

2-(7-Ethoxy-2,3-dihydro-1-benzofuran-3-yl)-1-phenylethanone (5p)



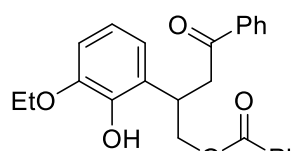
Yield 34 mg (40%); yellowish oil; R_f = 0.36 (petroleum ether : diethyl ether, 5:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.46 (t, 3J = 7.0 Hz, 3H, CH_3), 3.29 (dd, 2J = 18.1, 3J = 9.7 Hz, 1H, CH_2), 3.54 (dd, 2J = 18.1, 3J = 4.4 Hz, 1H, CH_2), 4.07–4.12 (m, 1H, CH), 4.13 (q, 3J = 7.0 Hz, 2H, CH_2O), 4.28 (dd, 2J = 9.3, 3J = 6.3 Hz, 1H, CH_2O), 4.96 (dd, 2J = 9.3, 3J = 9.1 Hz, 1H, CH_2O), 6.77–6.80 (m, 1H, Ar), 6.83–6.84 (m, 2H, Ar), 7.47–7.50 (m, 2H, Ar), 7.58–7.61 (m, 1H, Ar), 7.96–7.98 (m, 2H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.9 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 38.0 ($^1J_{\text{CH}}$ = 135 Hz, CH), 44.5 ($^1J_{\text{CH}}$ = 125 Hz, CH_2), 64.3 ($^1J_{\text{CH}}$ = 144 Hz, CH_2O), 77.9 ($^1J_{\text{CH}}$ = 153 Hz, CH_2O), 112.7 (CH, Ar), 116.3 (CH, Ar), 121.1 (CH, Ar), 128.0 (2 $\times$ CH, Ar), 128.7 (2 $\times$ CH, Ar), 131.0 (C, Ar), 133.4 (CH, Ar), 136.5 (C, Ar), 144.0 (C, Ar), 148.3 (C, Ar), 198.3 (COPh).

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{18}\text{H}_{19}\text{O}_3^+$ 283.1329; Found 283.1321.

2-(3-Ethoxy-2-hydroxyphenyl)-4-oxo-4-phenylbutyl benzoate (6p)



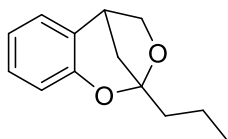
Yield 121 mg (30%); yellowish oil; R_f = 0.51 (petroleum ether : ethyl acetate, 4:1).

^1H NMR (CDCl_3 , 600 MHz) δ = 1.44 (t, 3J = 7.0 Hz, 3H, CH_3), 3.55 (dd, 2J = 17.1, 3J = 6.8 Hz, 1H, CH_2), 3.64 (dd, 2J = 17.1, 3J = 7.1 Hz, 1H, CH_2), 4.10 (q, 3J = 7.0 Hz, 2H, CH_2O), 4.23–4.28 (m, 1H, CH), 4.64–4.69 (m, 2H, CH_2O), 6.06 (s, 1H, OH), 6.76 (dd, 3J = 8.1, 4J = 1.5 Hz, 1H, Ar), 6.79–6.81 (m, 1H, Ar), 6.91 (dd, 3J = 7.8, 4J = 1.5 Hz, 1H, Ar), 7.38–7.41 (m, 2H, Ar), 7.41–7.44 (m, 2H, Ar), 7.51–7.55 (m, 2H, Ar), 7.95–7.97 (m, 2H, Ar), 7.97–7.99 (m, 2H, Ar).

^{13}C NMR (CDCl_3 , 150 MHz) δ = 14.8 ($^1J_{\text{CH}}$ = 127 Hz, CH_3), 35.6 ($^1J_{\text{CH}}$ = 131 Hz, CH), 40.1 ($^1J_{\text{CH}}$ = 127 Hz, CH_2), 64.5 ($^1J_{\text{CH}}$ = 144 Hz, CH_2O), 66.7 ($^1J_{\text{CH}}$ = 150 Hz, CH_2O), 110.1 (CH, Ar), 119.5 (CH, Ar), 121.0 (CH, Ar), 126.3 (C, Ar), 128.1 (2 $\times$ CH, Ar), 128.2 (2 $\times$ CH, Ar), 128.4 (2 $\times$ CH, Ar), 129.5 (2 $\times$ CH, Ar), 130.2 (C, Ar), 132.7 (CH, Ar), 132.9 (CH, Ar), 136.9 (C, Ar), 143.8 (C, Ar), 145.8 (C, Ar), 166.4 (CO_2Ph), 198.4 (COPh).

HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{25}H_{25}O_5^+$ 405.1697; Found 405.1700.

9-Propyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4q)



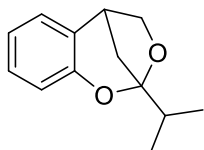
Reaction time 4 h. Yield 133 mg (65%); colorless oil; R_f = 0.66 (petroleum ether : ethyl acetate, 4:1).

1H NMR ($CDCl_3$, 600 MHz) δ = 1.04 (t, 3J = 7.5 Hz, 3H, CH_3), 1.58–1.65 (m, 2H, CH_2), 1.94 (ddd, 2J = 13.9, 3J = 10.2, 3J = 6.2 Hz, 1H, CH_2), 2.02 (ddd, 2J = 13.9, 3J = 10.5, 3J = 6.2 Hz, 1H, CH_2), 2.09 (dd, 2J = 11.4, 3J = 4.0 Hz, 1H, CH_2), 2.15 (br.d, 2J = 11.4 Hz, 1H, CH_2), 3.22–3.23 (m, 1H, CH), 4.09 (dd, 2J = 7.4, 3J = 3.5 Hz, 1H, CH_2O), 4.24 (dd, 2J = 7.4, 4J = 0.8 Hz, 1H, CH_2O), 6.82 (d, 3J = 7.9 Hz, 1H, Ar), 6.83–6.85 (m, 1H, Ar), 7.02 (dd, 3J = 7.5, 4J = 1.6 Hz, 1H, Ar), 7.13–7.15 (m, 1H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 14.3 ($^1J_{CH}$ = 125 Hz, CH_3), 17.5 ($^1J_{CH}$ = 127 Hz, CH_2), 35.1 ($^1J_{CH}$ = 136 Hz, CH_2), 38.7 ($^1J_{CH}$ = 126 Hz, CH_2), 38.8 ($^1J_{CH}$ = 141 Hz, CH), 79.5 ($^1J_{CH}$ = 149 Hz, CH_2O), 108.1 (C), 116.1 (CH, Ar), 120.1 (CH, Ar), 126.3 (CH, Ar), 128.2 (CH, Ar), 128.6 (C, Ar), 152.8 (C, Ar).

HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{13}H_{17}O_2^+$ 205.1223; Found 205.1226.

9-(Propan-2-yl)-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4r)



Reaction time 4 h. Yield 218 mg (66%); colorless oil; R_f = 0.69 (petroleum ether : ethyl acetate, 4:1).

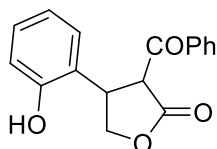
1H NMR ($CDCl_3$, 600 MHz) δ = 1.15 (d, 3J = 6.9 Hz, 3H, CH_3), 1.19 (d, 3J = 6.9 Hz, 3H, CH_3), 2.09 (dd, 2J = 11.4, 3J = 3.5 Hz, 1H, CH_2), 2.10–2.13 (m, 1H, CH_2), 2.25 (spt, 3J = 6.9 Hz, 1H, CH), 3.22–3.24 (m, 1H, CH), 4.08 (dd, 2J = 7.4, 3J = 3.5 Hz, 1H, CH_2O), 4.47 (dd, 2J = 7.4, 4J = 0.8 Hz, 1H, CH_2O), 6.85 (dd, 3J = 7.5, 4J = 1.1 Hz, 1H, Ar), 6.85–6.87 (m, 1H, Ar), 7.03–7.05 (m, 1H, Ar), 7.15–7.17 (m, 1H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 17.2 ($^1J_{CH}$ = 126 Hz, CH_3), 17.3 ($^1J_{CH}$ = 126 Hz, CH_3), 32.7 ($^1J_{CH}$ = 137 Hz, CH_2), 34.1 ($^1J_{CH}$ = 128 Hz, CH), 38.6 ($^1J_{CH}$ = 141 Hz, CH), 79.6 ($^1J_{CH}$ = 149 Hz, CH_2O),

110.3 (C), 116.1 (CH, Ar), 119.9 (CH, Ar), 126.3 (CH, Ar), 128.1 (CH, Ar), 128.6 (C, Ar), 152.9 (C, Ar).

HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{13}H_{17}O_2^+$ 205.1223; Found 205.1222.

3-Benzoyl-4-(2-hydroxyphenyl)dihydrofuran-2(3H)-one (7)



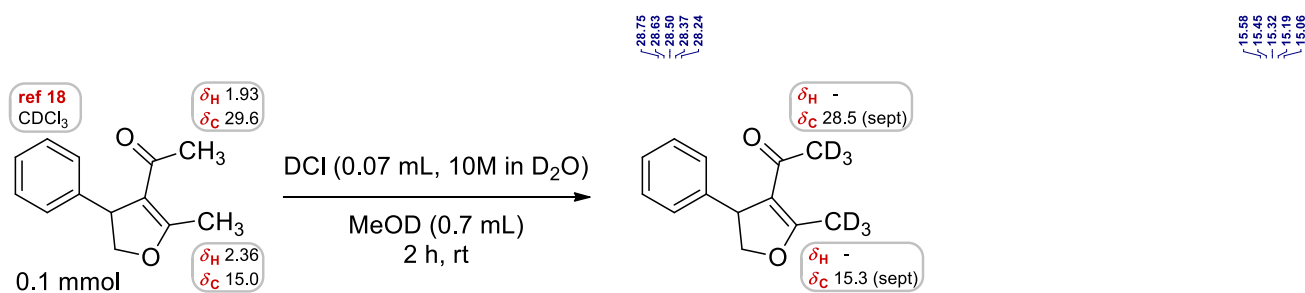
Reaction time 15 min. Yield 123 mg (44%); colorless oil; R_f = 0.43 (petroleum ether : ethyl acetate, 2:1).

1H NMR ($CDCl_3$, 600 MHz) δ = 4.44 (ddd, 3J = 8.3, 3J = 7.7, 3J = 7.4 Hz, 1H, CH), 4.59 (dd, 2J = 8.8, 3J = 7.4 Hz, 1H, CH_2O), 4.74 (dd, 2J = 8.8, 3J = 8.3 Hz, 1H, CH_2O), 5.05 (d, 3J = 7.7 Hz, 1H, CH), 6.82–6.89 (m, 3H, OH, Ar), 7.11–7.16 (m, 2H, Ar), 7.42–7.46 (m, 2H, Ph), 7.56–7.59 (m, 1H, Ph), 7.99–8.02 (m, 2H, Ph).

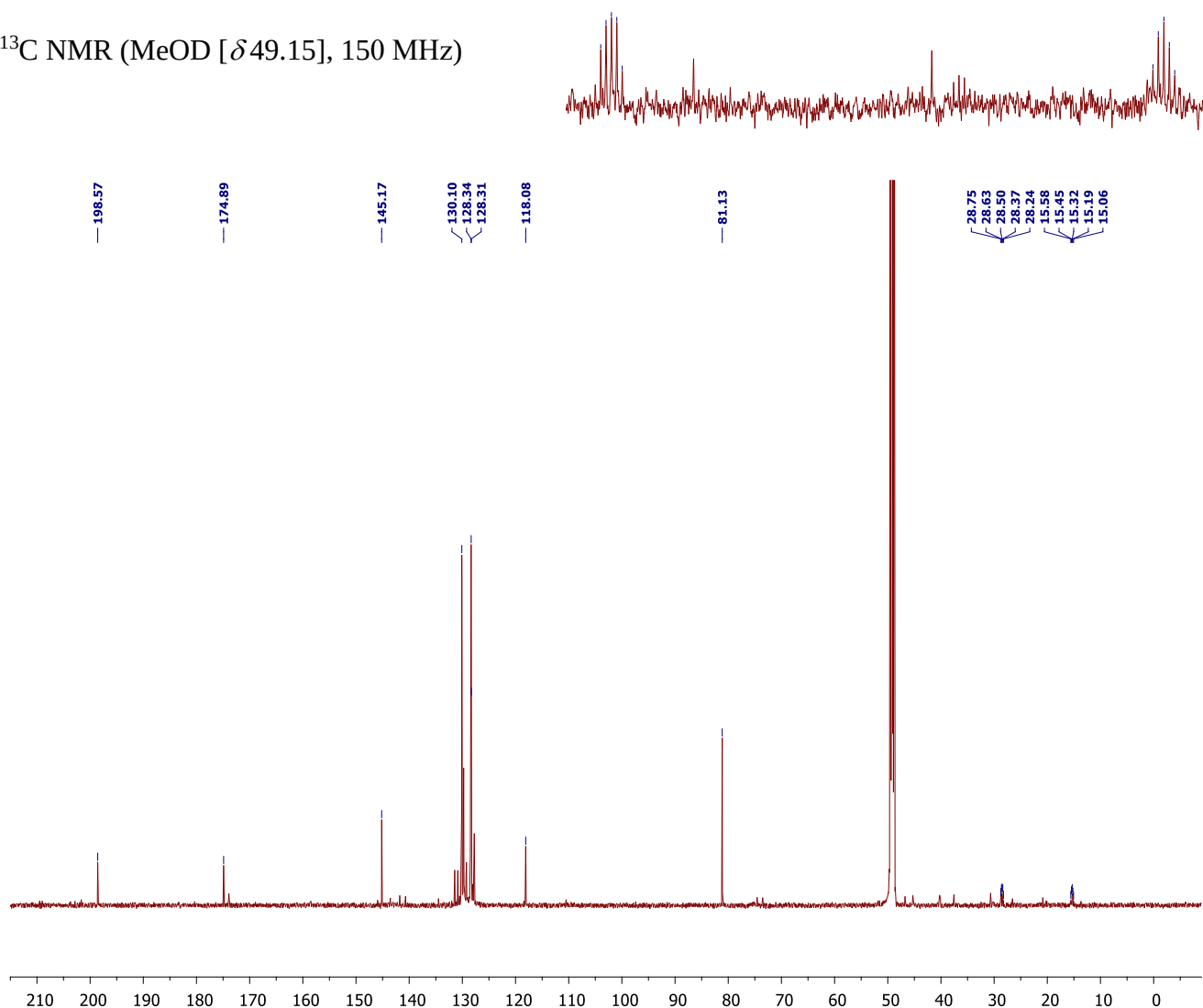
^{13}C NMR ($CDCl_3$, 150 MHz) δ = 41.6 ($^1J_{CH}$ = 134 Hz, CH), 54.1 ($^1J_{CH}$ = 135 Hz, CH), 71.7 ($^1J_{CH}$ = 154 Hz, CH_2O), 116.4 (CH, Ar), 120.8 (CH, Ar), 124.2 (C, Ar), 128.7 (2 $\times$ CH, Ph), 129.2 (CH, Ar), 129.4 (CH, Ar), 129.5 (2 $\times$ CH, Ph), 134.1 (CH, Ph), 135.5 (C, Ph), 154.2 (C, Ar), 173.7 (CO), 194.0 (COPh).

HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{17}H_{15}O_4^+$ 283.0965; Found 283.0972.

Deuterium exchange in 1-(2-methyl-4-phenyl-4,5-dihydrofuran-3-yl)ethanone¹⁸



¹³C NMR (MeOD [δ 49.15], 150 MHz)



Results of DFT calculations

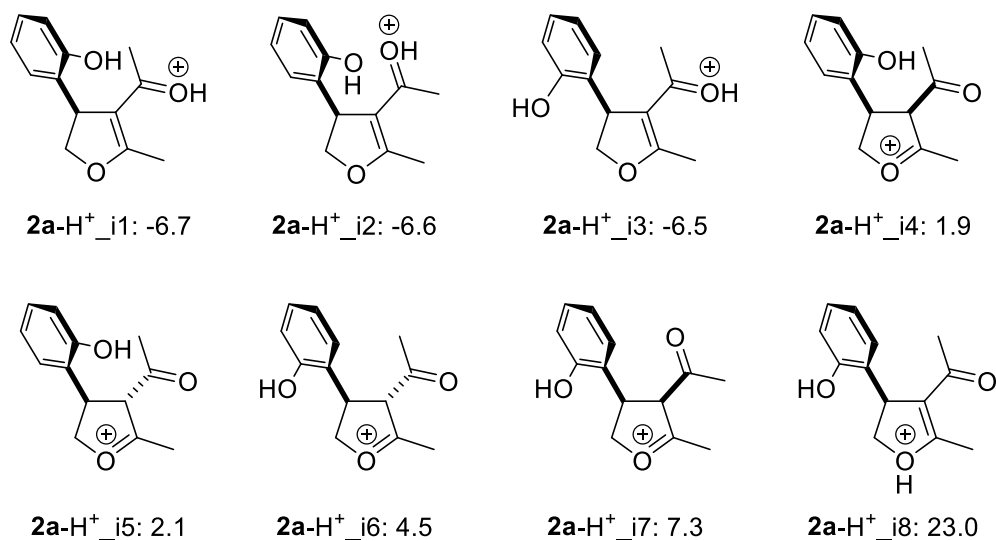


Figure S9. Selected isomers of protonated DHF **2a**. Enthalpies ΔH_{298} are given in kcal/mol relative to **II1**

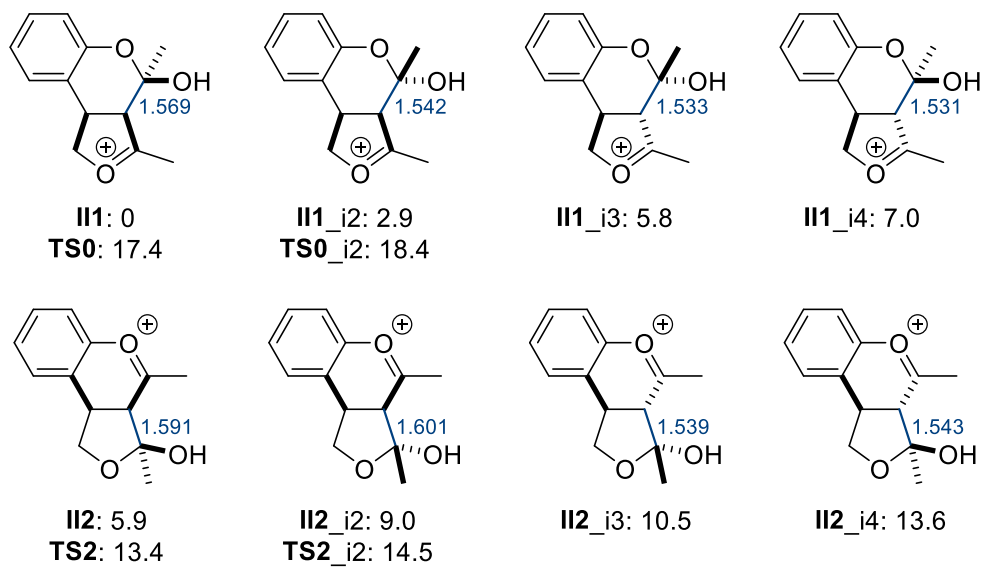


Figure S10. Selected isomers of protonated hemiketals **II1** and **II2** and corresponding transition states **TS0** and **TS2** for cleavage of C–C bond (length in Å). Enthalpies ΔH_{298} are given in kcal/mol relative to **II1**

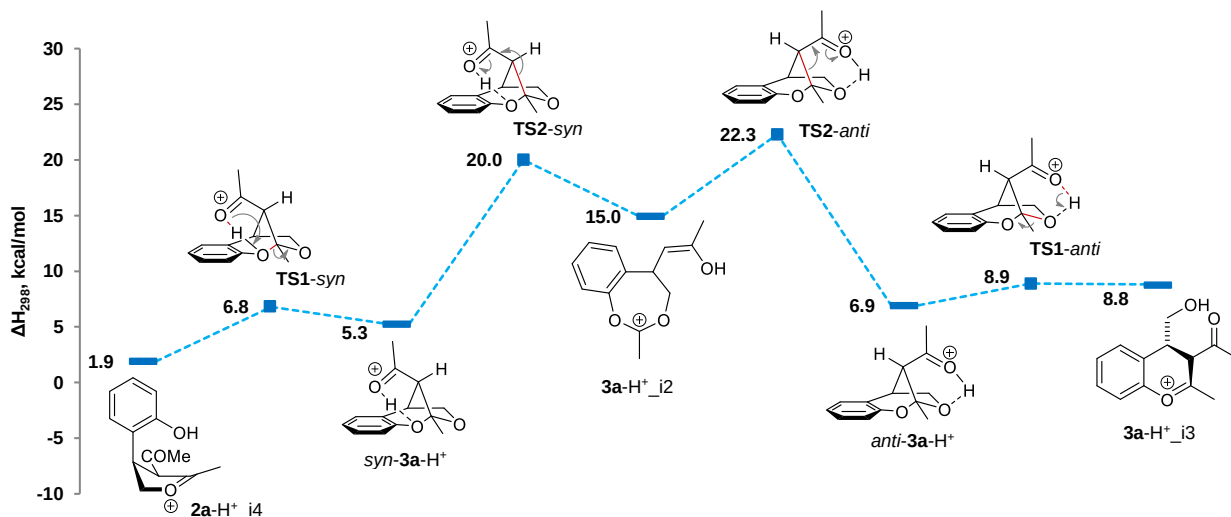


Figure S11. Energy profile for ring opening in diastereomeric ketals **3a-H⁺** (relative to **II1**)

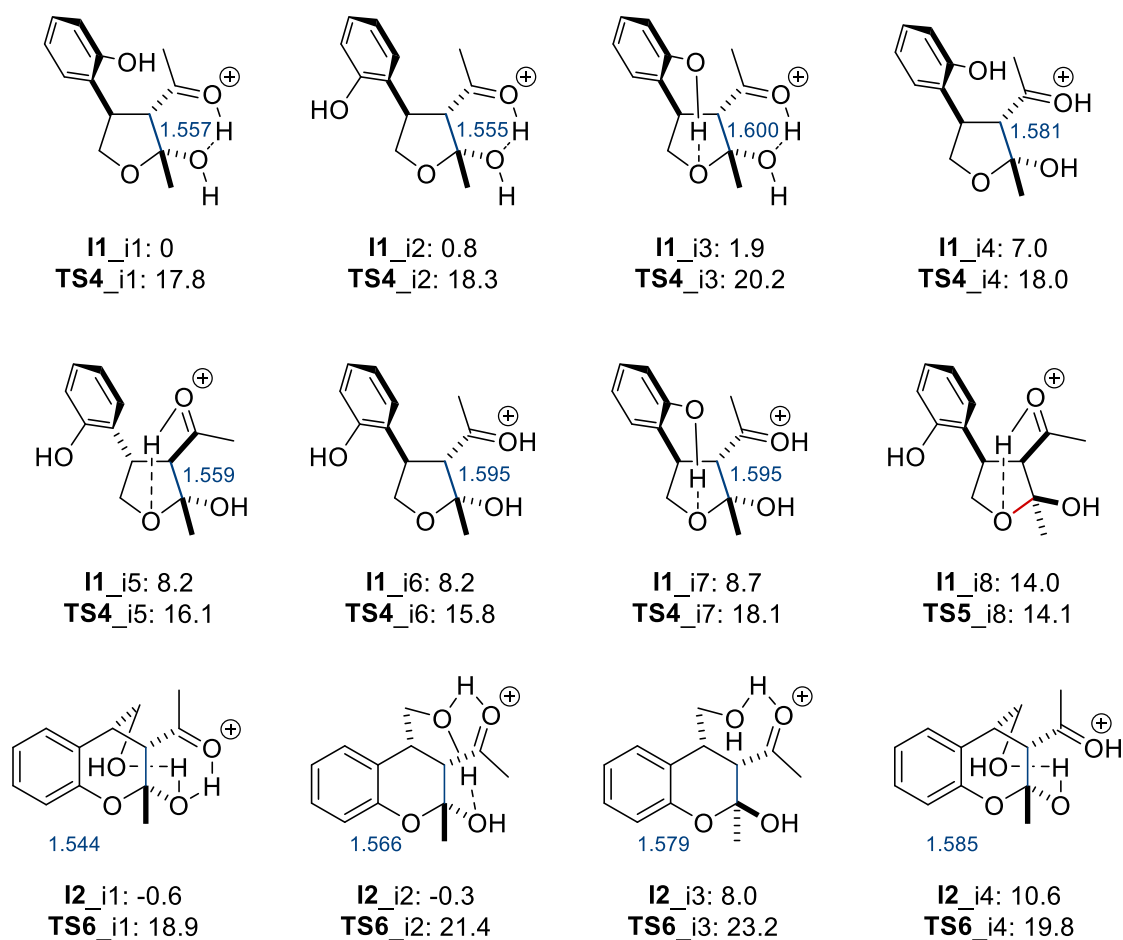


Figure S12. Selected isomers of protonated hemiketals **I1**, **I2** and corresponding transition states **TS4**, **TS6** for cleavage of C–C bond (length in Å) and **TS5** for cleavage of C–O bond. Enthalpies ΔH_{298} are given in kcal/mol relative to **I1_i1**

Table S2. Comparison of transition states with the lowest free energies for C–C bond cleavage in corresponding hemiketals **II1**, **I1** and **I2**

Transition state	ΔG_{298} [kcal/mol]
TS2	0
TS4_i5	6.1
TS6_i1	9.5

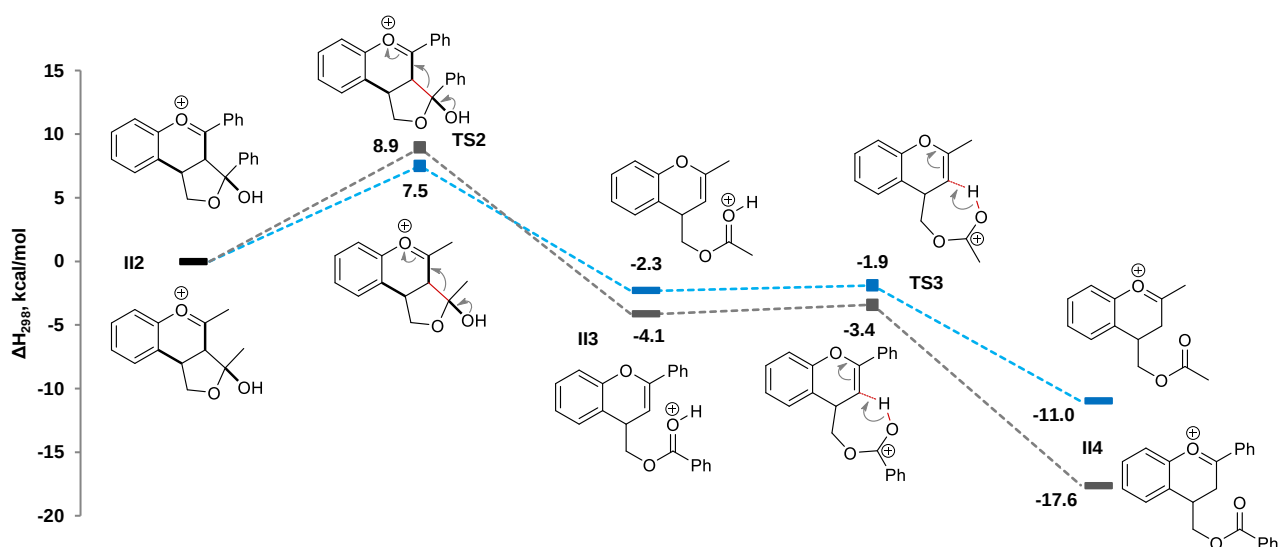
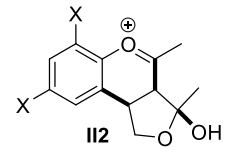


Figure S13. Energy profiles for ring opening in hemiketals **II2** and **II2_PhPh**

To compare the relevant fragments of energy profiles for the fastest (**1j**→**4j**) and the slowest (**1i**→**4i**) reactions within 2-methyl-3-acetyl series (Scheme 2), we optimized the geometries of the corresponding intermediates **II2** as well as protonated DHF **2-H⁺** and **TS2**. As seen in Table S3, the trend of variation of effective activation energy (defined as ΔH_{298} between **TS2** and **2-H⁺**) agrees with the changes in the experimental reaction time. The splitting of this ΔH_{298} into two components, the energy barrier of C–C bond cleavage in **II2** as well as ΔH_{298} between this intermediate and **2-H⁺**, shows different effects of substituents X in the aryl fragment. Electron-donating *t*-Bu groups stabilize cationic **II2**. This decreases the enthalpy difference between **II2** and **2-H⁺**, whereas the C–C bond becomes less activated. Oppositely, electron-withdrawing Br atoms destabilize **II2**. This increases the

enthalpy difference between **II2** and 2-H^+ , while the energy barrier of C–C bond cleavage in **II2** becomes lower. In total, the gain *via* stabilizing electron-donating substituents exceeds the destabilizing influence of electron-withdrawing groups.

Table S3. Enthalpy differences of the key stationary points for ring opening in X-substituted hemiketals **II2** and experimental reaction times (**1**→**4**)

 II2 X	ΔH_{298} [kcal/mol]			t [h]
	II2 vs. 2-H^+	TS2 vs. II2	TS2 vs. 2-H^+	
<i>t</i> -Bu	9.2	9.4	18.6	1 (1j)
H	12.6	7.5	20.1	2 (1a)
Br	17.0	5.5	22.5	9 (1i)

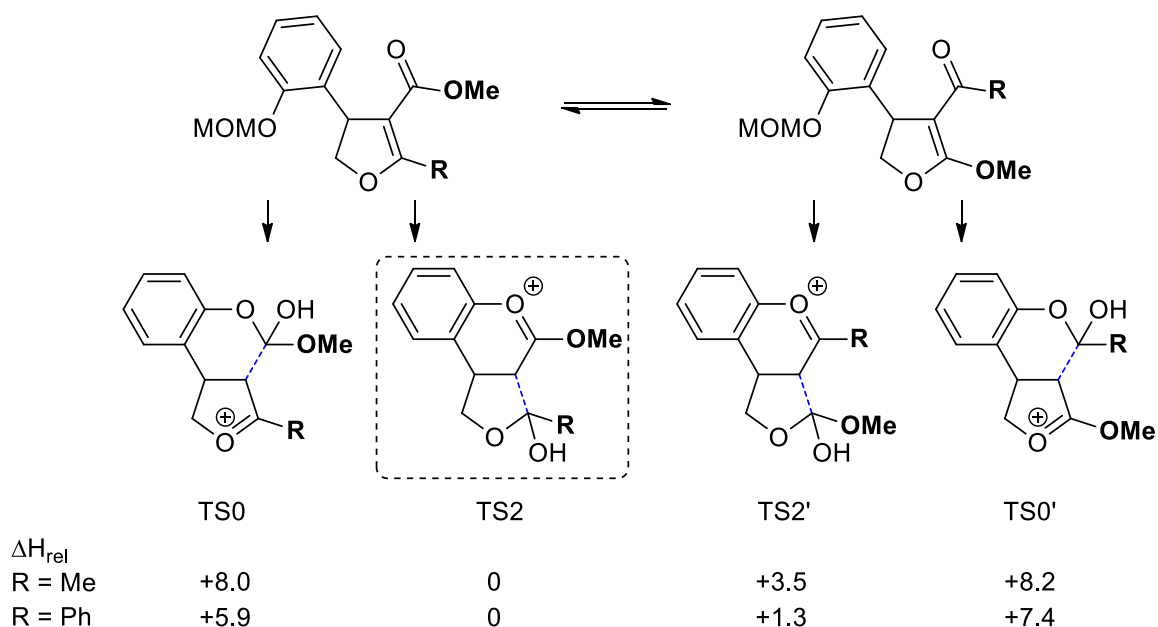


Figure S14. Isomeric transition states of retro-aldol cleavage in protonated hemiketals, derived from dimethyl derivative **1q** or the methyl analogue of **1t**. Enthalpies ΔH_{298} are given in kcal/mol relative to **TS2**

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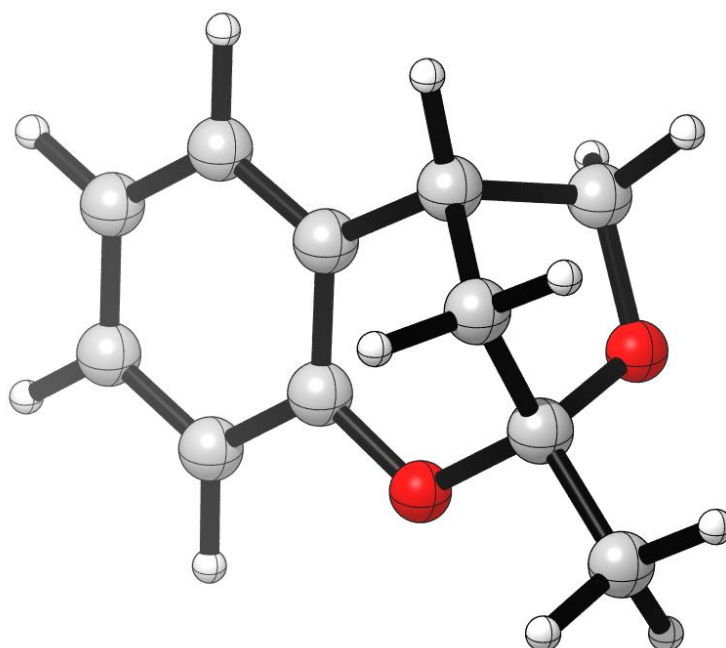
Cartesian coordinates of stationary points

To Table 2

H₂O

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4a

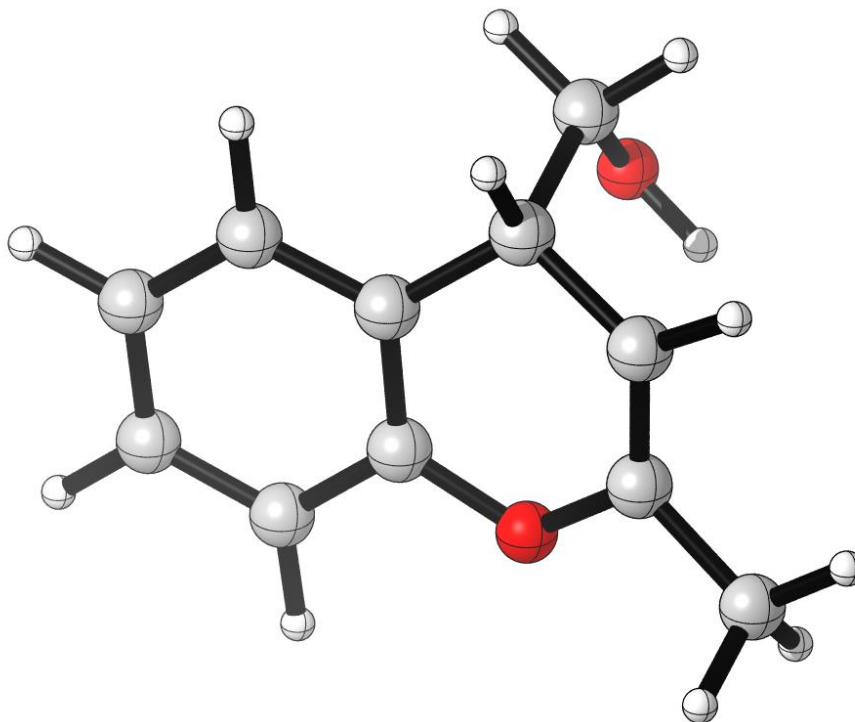


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1	-0.813857000	4.628529000	9.247435000

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4a_i1

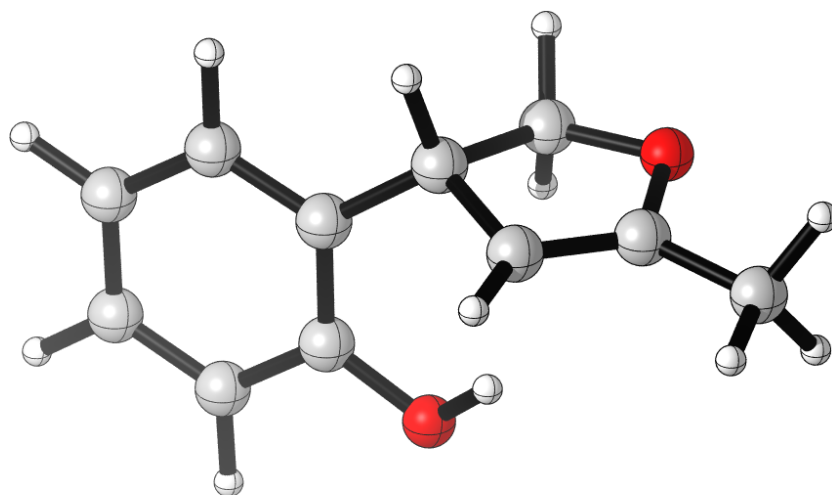


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4a_i2

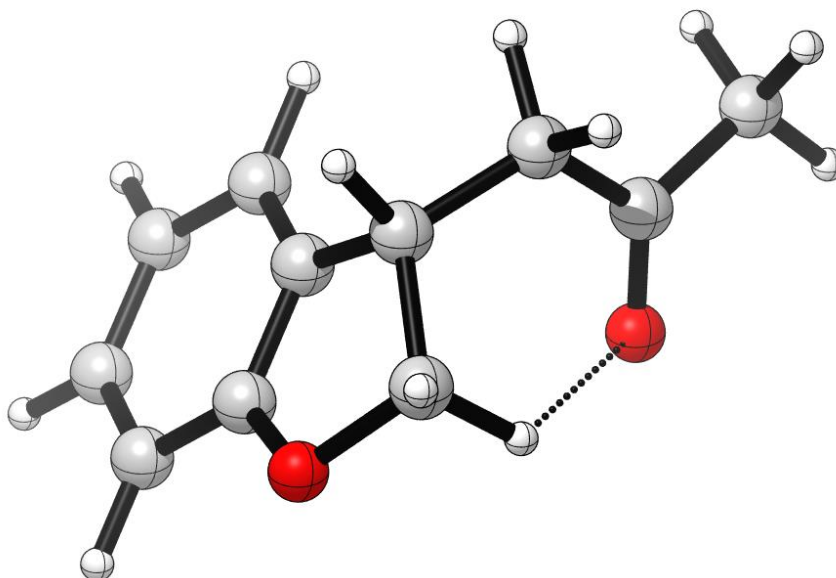


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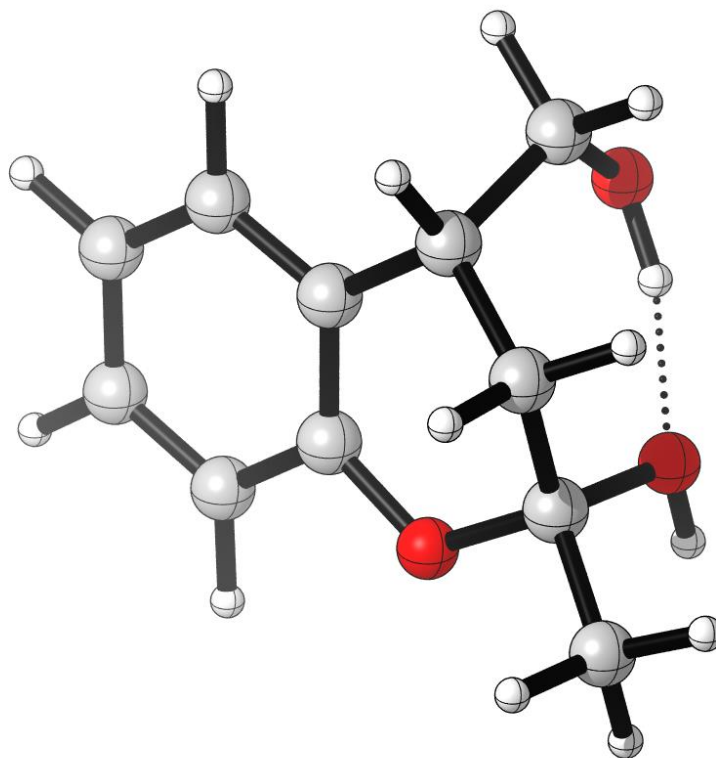
5a



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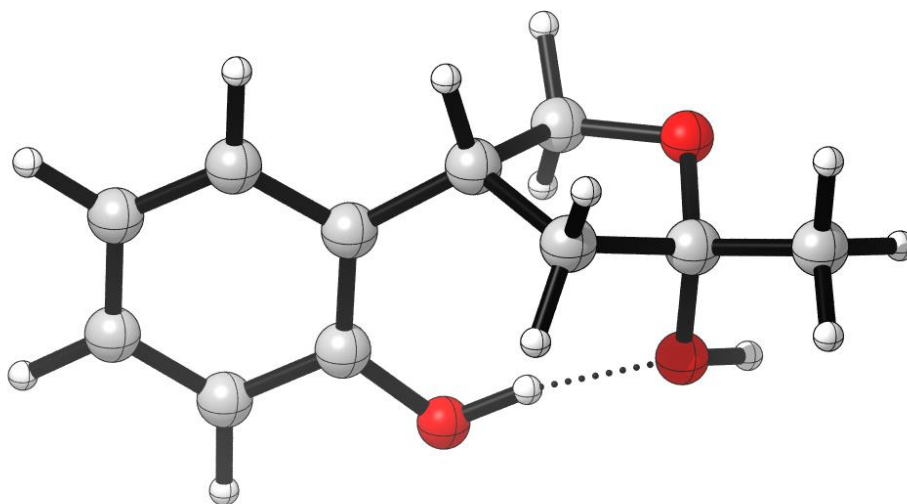


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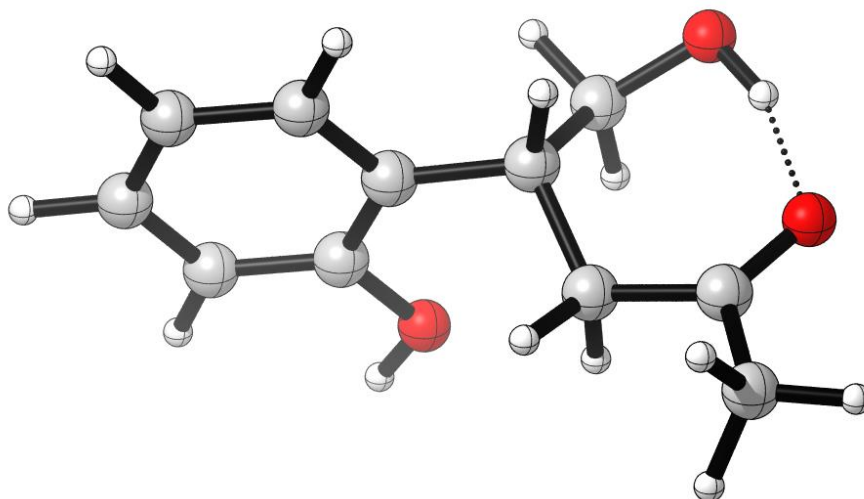
4a-H₂O_i2



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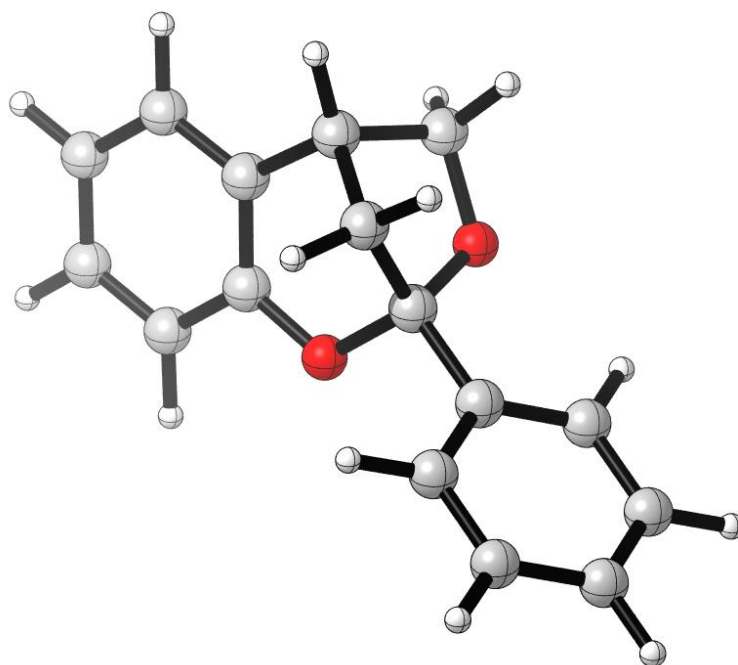
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6	2.373812000	4.202417000	4.906583000
8	1.642287000	3.927982000	6.107881000
6	2.859353000	5.640050000	4.894437000
1	3.545172000	5.816753000	5.738535000
1	3.398204000	5.857613000	3.960171000
1	2.004431000	6.326107000	4.985574000
8	-0.093803000	1.882005000	5.911624000
1	0.597542000	2.584374000	5.906880000
1	1.690670000	4.341852000	2.856316000
1	0.395194000	3.948248000	4.006859000
8	3.485604000	3.337515000	4.826019000
1	2.236646000	4.015510000	6.871579000



SPE = -652.4281; H₂₉₈ = -652.1817; G₂₉₈ = -652.2380

6	1.501146000	2.500128000	4.916388000
1	2.316546000	2.035643000	4.337454000
6	0.312267000	1.552528000	4.822167000
6	-0.923307000	1.823130000	5.454555000
6	-1.995010000	0.924920000	5.342349000
1	-2.939090000	1.160749000	5.843202000
6	-1.857665000	-0.254589000	4.604180000
1	-2.702865000	-0.943996000	4.523046000
6	-0.642856000	-0.544540000	3.975766000
1	-0.518150000	-1.465008000	3.399895000
6	0.419951000	0.358421000	4.092099000
1	1.371044000	0.132988000	3.599739000

6	1.162074000	3.857911000	4.245543000
6	2.040847000	2.597308000	6.366005000
1	1.416658000	3.304293000	6.947346000
1	1.928702000	1.609624000	6.843287000
6	2.297869000	4.807938000	3.919152000
8	3.294175000	4.927447000	4.621908000
6	2.144078000	5.632200000	2.666665000
1	2.304449000	4.965000000	1.800558000
1	1.123927000	6.037641000	2.575717000
1	2.884590000	6.442798000	2.641214000
8	-1.039789000	2.977775000	6.169751000
1	-1.934960000	3.051664000	6.534480000
1	0.593510000	3.673734000	3.320353000
1	0.475930000	4.433996000	4.894601000
8	3.410822000	2.924447000	6.428274000
1	3.523742000	3.739939000	5.897212000

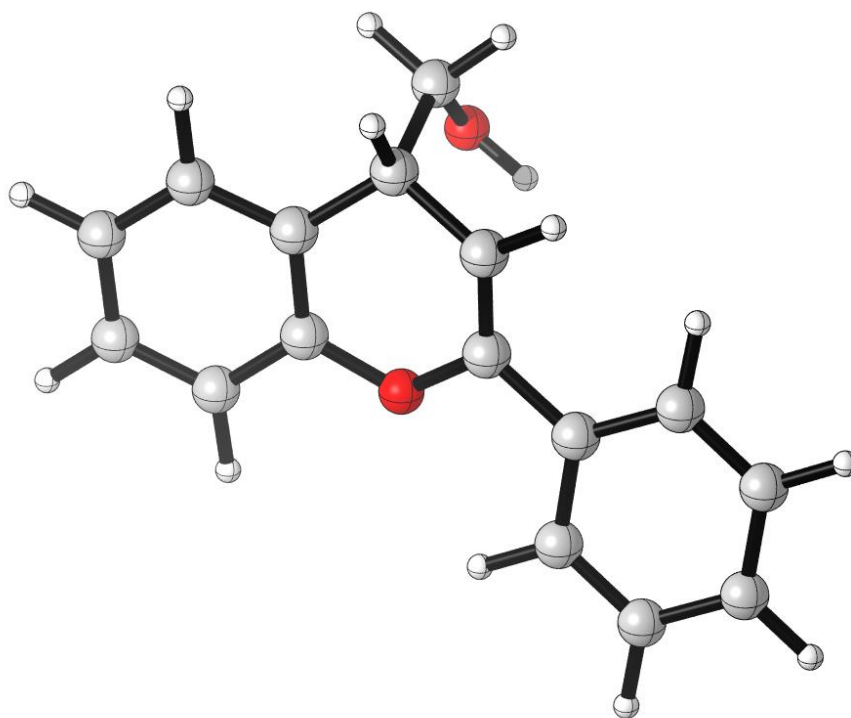


SPE = -767.5707; H₂₉₈ = -767.2968; G₂₉₈ = -767.3481

6	0.791871000	2.562033000	4.953825000
1	0.889511000	3.518438000	4.421061000
6	-0.191410000	2.651797000	6.107329000
6	-0.125597000	1.649145000	7.099708000
6	-1.006648000	1.663165000	8.189527000
1	-0.933237000	0.872307000	8.941015000
6	-1.959109000	2.681748000	8.298284000
1	-2.641286000	2.691135000	9.153375000
6	-2.036557000	3.685152000	7.323950000
1	-2.777795000	4.483981000	7.413058000
6	-1.154244000	3.660863000	6.235955000
1	-1.207653000	4.444418000	5.472895000

6	2.112275000	2.004067000	5.507659000
6	0.415877000	1.404818000	4.017805000
1	-0.659090000	1.339636000	3.794591000
1	0.978022000	1.453414000	3.068483000
6	1.623099000	0.585014000	5.845477000
8	0.807302000	0.225359000	4.752984000
8	0.804489000	0.642162000	7.042782000
1	2.501005000	2.542129000	6.382898000
1	2.893411000	1.960234000	4.734230000
6	2.687999000	-0.463987000	6.110214000
6	3.668081000	-0.232563000	7.090402000
6	2.713466000	-1.667201000	5.390918000
6	4.660267000	-1.185442000	7.341420000
6	3.703768000	-2.624242000	5.646828000
6	4.680950000	-2.385981000	6.619277000
1	3.661515000	0.698730000	7.661956000
1	1.955077000	-1.851283000	4.628351000
1	5.419424000	-0.987716000	8.103486000
1	3.707610000	-3.561057000	5.082788000
1	5.454682000	-3.133382000	6.817406000

4o_i1

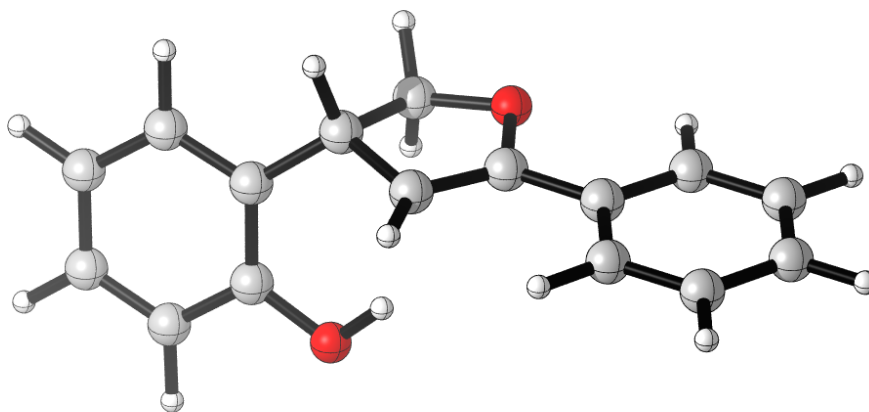


SPE = -767.5588; H₂₉₈ = -767.2851; G₂₉₈ = -767.3399

6	1.286355000	0.353034000	2.817419000
1	1.350062000	1.167110000	2.072400000
6	0.009311000	0.503197000	3.619103000
6	0.019061000	0.269907000	5.001789000
6	-1.153294000	0.341794000	5.764792000
1	-1.096519000	0.151094000	6.839166000
6	-2.363451000	0.650446000	5.141532000
1	-3.279473000	0.705953000	5.735598000
6	-2.396270000	0.904434000	3.763356000
1	-3.336441000	1.165242000	3.270892000
6	-1.216106000	0.831548000	3.019239000
1	-1.238070000	1.034704000	1.944126000

6	2.477651000	0.411971000	3.736195000
6	1.309076000	-0.966532000	1.999946000
1	0.430489000	-0.998091000	1.334716000
1	2.212815000	-0.967906000	1.357613000
6	2.392758000	0.171146000	5.060041000
8	1.248907000	-2.117697000	2.812275000
8	1.178482000	-0.019303000	5.681720000
1	3.456738000	0.606123000	3.296244000
1	2.024131000	-2.109392000	3.394801000
6	3.524858000	0.108485000	6.014896000
6	3.286632000	0.116377000	7.402642000
6	4.859590000	0.040432000	5.565115000
6	4.348740000	0.074410000	8.310451000
6	5.917559000	0.001318000	6.473070000
6	5.668423000	0.019687000	7.851731000
1	2.260593000	0.161777000	7.769149000
1	5.078307000	0.005518000	4.495670000
1	4.139225000	0.085787000	9.384089000
1	6.943932000	-0.054880000	6.099902000
1	6.499354000	-0.015607000	8.561076000

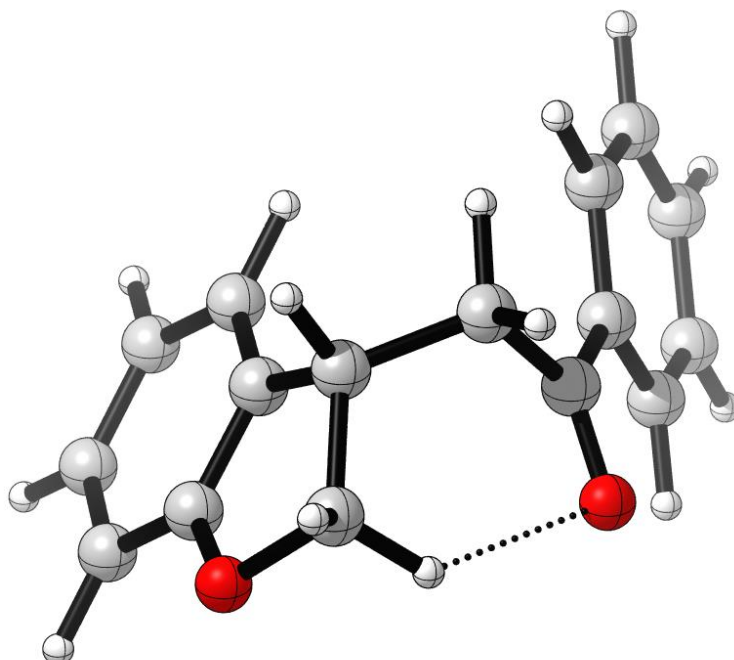
4o_i2



SPE = -767.5563; H₂₉₈ = -767.2827; G₂₉₈ = -767.3378

6	1.043398000	0.987829000	3.858784000
1	0.937622000	1.976429000	3.374375000
6	-0.359723000	0.422452000	4.015236000
6	-0.679498000	-0.570320000	4.972904000
6	-1.979640000	-1.099547000	5.037566000
1	-2.193417000	-1.857737000	5.795545000
6	-2.965985000	-0.663999000	4.151976000
1	-3.971138000	-1.090130000	4.215935000
6	-2.667864000	0.313543000	3.193801000
1	-3.435093000	0.662719000	2.498290000
6	-1.376005000	0.844122000	3.140520000
1	-1.136674000	1.612488000	2.398910000

6	1.906798000	1.139517000	5.104272000
6	1.974511000	0.090089000	3.000113000
1	1.688843000	-0.973343000	3.089084000
1	2.004484000	0.368459000	1.937941000
6	3.169591000	0.742591000	4.814726000
8	3.299816000	0.246215000	3.548686000
8	0.226950000	-1.053189000	5.862070000
1	1.059512000	-0.543964000	5.795034000
1	1.596357000	1.650189000	6.015027000
6	4.400451000	0.770795000	5.619834000
6	4.420154000	1.345976000	6.906252000
6	5.586880000	0.214137000	5.105939000
6	5.599488000	1.369097000	7.651216000
6	6.765625000	0.237430000	5.856686000
6	6.777816000	0.818701000	7.128521000
1	3.511392000	1.781786000	7.327752000
1	5.577664000	-0.238910000	4.114035000
1	5.600327000	1.822430000	8.645581000
1	7.676805000	-0.203194000	5.443431000
1	7.700368000	0.844008000	7.714677000

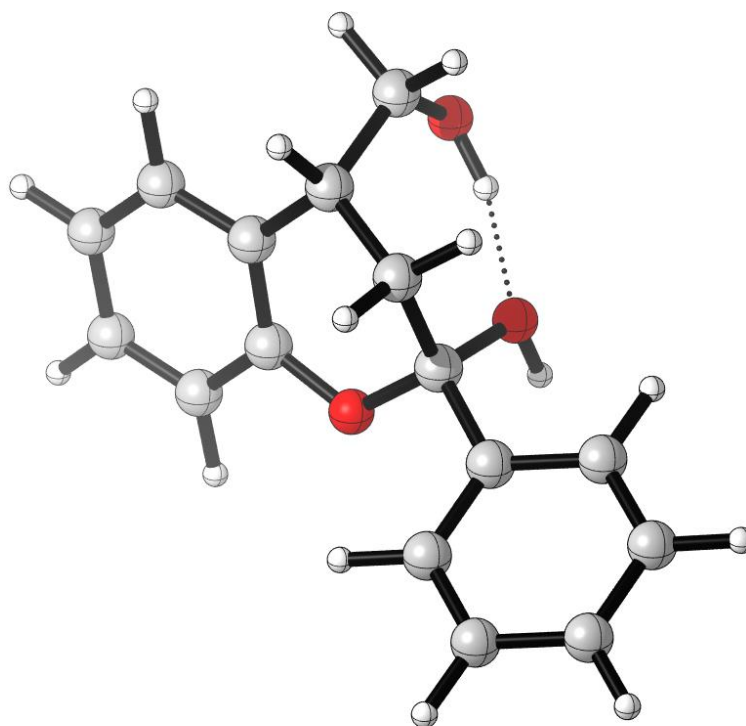


SPE = -767.5688; H_{298} = -767.2938; G_{298} = -767.3508

6	0.075082000	2.102180000	3.907200000
1	0.776675000	2.283384000	3.073165000
6	-0.781525000	3.344539000	4.088688000
6	-0.299157000	4.037319000	5.209177000
6	-0.836581000	5.257540000	5.617921000
1	-0.439374000	5.776268000	6.493171000
6	-1.897131000	5.783702000	4.863776000
1	-2.345924000	6.733712000	5.167423000
6	-2.391160000	5.109704000	3.739064000
1	-3.217338000	5.538704000	3.166258000
6	-1.827330000	3.884379000	3.342414000
1	-2.214854000	3.363680000	2.462814000

6	-0.643895000	0.767829000	3.577704000
6	0.863484000	2.084495000	5.243273000
1	0.434067000	1.352820000	5.943382000
1	1.934324000	1.872327000	5.111452000
6	-1.781273000	0.421520000	4.527855000
8	-1.529792000	0.117386000	5.687504000
8	0.732249000	3.403356000	5.829096000
1	0.099828000	-0.043121000	3.656760000
1	-0.978879000	0.794864000	2.533255000
6	-3.206139000	0.470658000	4.063332000
6	-3.581927000	0.532735000	2.708297000
6	-4.214919000	0.429238000	5.046211000
6	-4.933068000	0.555147000	2.347913000
6	-5.560864000	0.468655000	4.687384000
6	-5.923357000	0.530306000	3.334608000
1	-2.828076000	0.545598000	1.919270000
1	-3.915955000	0.370553000	6.094911000
1	-5.214050000	0.593897000	1.292088000
1	-6.332540000	0.449031000	5.461387000
1	-6.978896000	0.557093000	3.049343000

4o-H₂O_i1

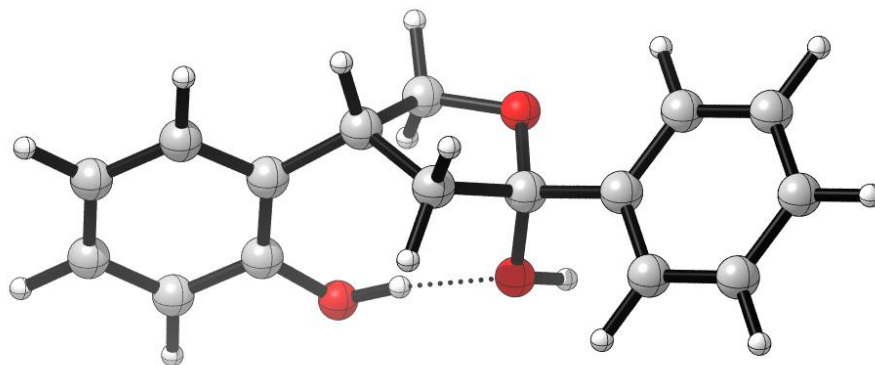


SPE = -843.9161; H₂₉₈ = -843.6141; G₂₉₈ = -843.6682

6	1.151649000	1.061413000	3.011661000
6	-0.073711000	0.446867000	3.661842000
6	0.041331000	-0.293123000	4.852106000
6	-1.086019000	-0.867238000	5.459599000
1	-0.946388000	-1.434918000	6.382568000
6	-2.349087000	-0.692147000	4.895257000
1	-3.222766000	-1.137200000	5.378783000
6	-2.490383000	0.056653000	3.718610000
1	-3.476878000	0.212615000	3.274144000
6	-1.358885000	0.610758000	3.117057000
1	-1.468298000	1.196289000	2.199056000
6	2.299353000	1.140977000	4.037399000

6	1.520378000	0.406070000	1.657490000
1	0.732684000	0.657064000	0.926461000
1	2.450157000	0.895419000	1.295242000
6	2.460973000	-0.112854000	4.908627000
8	2.889777000	-1.168857000	4.071854000
8	1.228312000	-0.470949000	5.521829000
1	3.259530000	1.352492000	3.542477000
1	2.161019000	-1.241280000	2.451249000
1	2.104279000	1.976053000	4.726786000
8	1.635336000	-0.996589000	1.665283000
1	0.902296000	2.104187000	2.747468000
1	2.978769000	-1.978317000	4.602120000
6	3.467186000	0.116928000	6.034663000
6	3.058628000	0.593340000	7.289895000
6	4.834076000	-0.084978000	5.789998000
6	4.004547000	0.864087000	8.283965000
6	5.779219000	0.188788000	6.783479000
6	5.366895000	0.665017000	8.033037000
1	1.996947000	0.753840000	7.488206000
1	5.157482000	-0.466477000	4.819224000
1	3.672492000	1.240077000	9.255685000
1	6.840863000	0.025050000	6.577296000
1	6.105007000	0.884108000	8.809011000

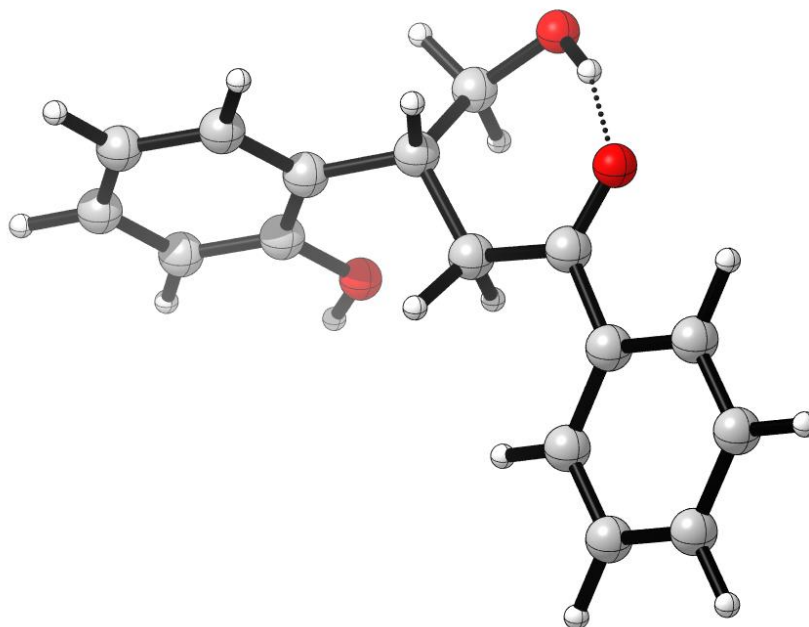
4o-H₂O_i2



SPE = -843.9164; H₂₉₈ = -843.6127; G₂₉₈ = -843.6714

6	1.051490000	2.491659000	3.765340000
1	0.822931000	2.571613000	2.694579000
6	0.106378000	1.441904000	4.324663000
6	0.175777000	0.940326000	5.650648000
6	-0.716314000	-0.066917000	6.062916000
1	-0.623301000	-0.440424000	7.085906000
6	-1.686836000	-0.573893000	5.199155000
1	-2.367331000	-1.356354000	5.547198000
6	-1.785669000	-0.073783000	3.895900000
1	-2.540377000	-0.455894000	3.203923000
6	-0.892009000	0.917360000	3.482275000
1	-0.959652000	1.305407000	2.460852000

6	0.948052000	3.926616000	4.368112000
6	2.564874000	2.159626000	3.893510000
1	2.764404000	1.444218000	4.707318000
1	2.990254000	1.750116000	2.966938000
6	2.358563000	4.207314000	4.923971000
8	2.329259000	3.746119000	6.281036000
8	1.078977000	1.346676000	6.579392000
1	1.509515000	2.211437000	6.388288000
1	0.709045000	4.651904000	3.579214000
1	0.187351000	4.023403000	5.155709000
8	3.219089000	3.403242000	4.159517000
1	3.226094000	3.801952000	6.652248000
6	2.816314000	5.656251000	4.863240000
6	2.223114000	6.601661000	5.716621000
6	3.792673000	6.075944000	3.947234000
6	2.597129000	7.947378000	5.647326000
6	4.172899000	7.422087000	3.885249000
6	3.573388000	8.360750000	4.731213000
1	1.468970000	6.280875000	6.439982000
1	4.256435000	5.341836000	3.287567000
1	2.124533000	8.676235000	6.310976000
1	4.941373000	7.737668000	3.173689000
1	3.871727000	9.411799000	4.680462000



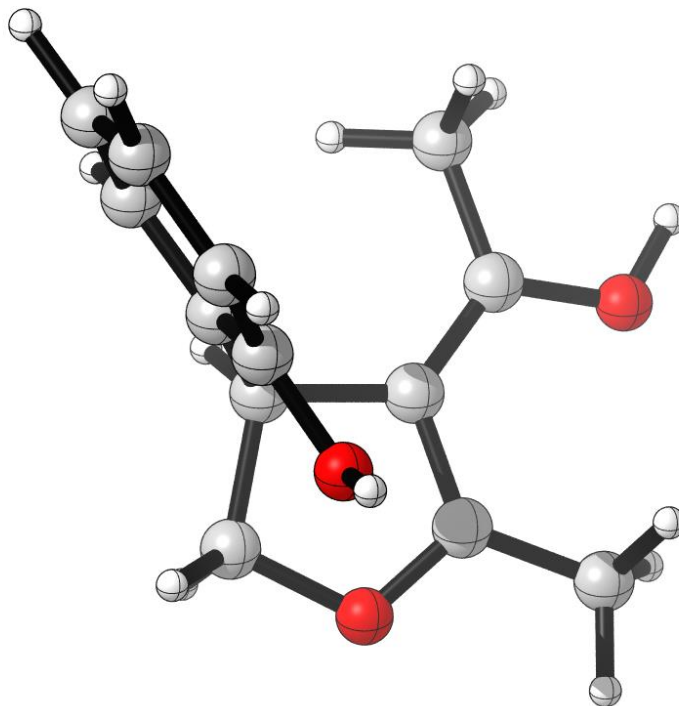
SPE = -843.9141; H₂₉₈ = -843.6117; G₂₉₈ = -843.6725

6	1.532600000	2.537201000	4.949844000
1	2.356823000	2.053606000	4.399419000
6	0.328852000	1.609044000	4.827479000
6	-0.930206000	1.921287000	5.391564000
6	-2.014596000	1.042581000	5.248871000
1	-2.975582000	1.310299000	5.699037000
6	-1.868462000	-0.156822000	4.545982000
1	-2.724411000	-0.829062000	4.438403000
6	-0.631799000	-0.487317000	3.984173000
1	-0.501662000	-1.422027000	3.432990000
6	0.444406000	0.395083000	4.132011000
1	1.411382000	0.138120000	3.688513000

6	1.239019000	3.895858000	4.264019000
6	2.017563000	2.646514000	6.416307000
1	1.366765000	3.356263000	6.963883000
1	1.886991000	1.662638000	6.899416000
6	2.427240000	4.745779000	3.861906000
8	3.560063000	4.527308000	4.286503000
8	-1.059473000	3.096473000	6.069392000
1	-1.967374000	3.191941000	6.395412000
1	0.638628000	3.717059000	3.357679000
1	0.594023000	4.515090000	4.911794000
8	3.382833000	2.990387000	6.538563000
1	3.602656000	3.588534000	5.796892000
6	2.202481000	5.885843000	2.916235000
6	3.327329000	6.583114000	2.433551000
6	0.918054000	6.293350000	2.507156000
6	3.173575000	7.651496000	1.550203000
6	0.765265000	7.373047000	1.633164000
6	1.891157000	8.048981000	1.148981000
1	4.318627000	6.266923000	2.764066000
1	0.028757000	5.777491000	2.872935000
1	4.051854000	8.181250000	1.172925000
1	-0.234478000	7.689411000	1.324296000
1	1.766638000	8.890674000	0.462190000

To Figure S9

2a-H⁺_i1

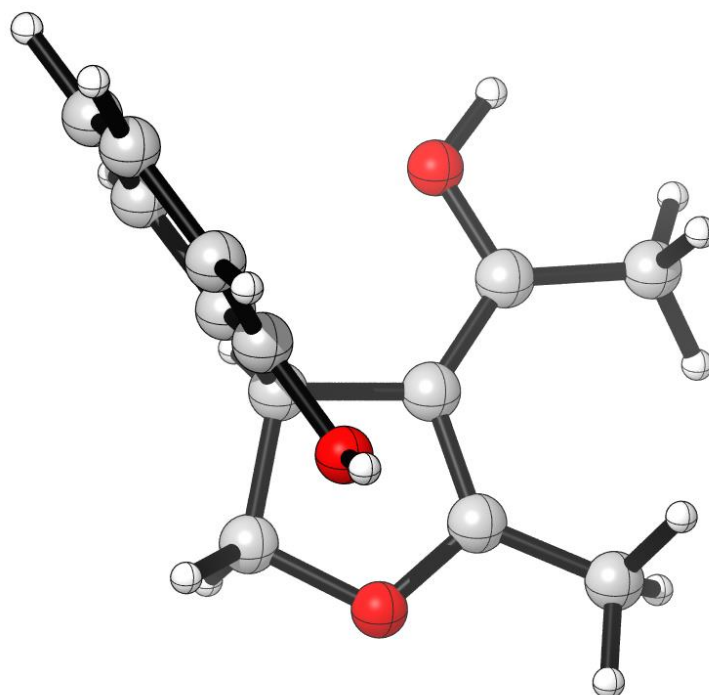


SPE = -728.9690; H₂₉₈ = -728.6970

6	0.597151000	0.883642000	3.514648000
1	0.875902000	1.336100000	2.552269000
6	-0.878593000	1.172292000	3.753452000
6	-1.561767000	0.638266000	4.869846000
6	-2.908083000	0.955115000	5.098006000
1	-3.414581000	0.531695000	5.970659000
6	-3.590129000	1.799413000	4.217848000
1	-4.635131000	2.052280000	4.416831000
6	-2.937659000	2.319997000	3.095352000
1	-3.468093000	2.970729000	2.395998000
6	-1.594202000	1.999298000	2.874747000

1	-1.079966000	2.408558000	2.000169000
6	1.524382000	1.390980000	4.624994000
6	0.978375000	-0.617519000	3.486849000
1	0.125284000	-1.302895000	3.542850000
1	1.614686000	-0.880871000	2.631360000
6	2.082107000	0.270653000	5.272801000
8	1.789168000	-0.851844000	4.683007000
6	2.912746000	0.191957000	6.496271000
1	3.073799000	-0.854881000	6.781672000
1	3.881883000	0.686312000	6.319256000
1	2.425282000	0.743696000	7.314499000
8	-0.865964000	-0.184771000	5.697684000
1	-1.429999000	-0.491853000	6.424417000
6	1.787692000	2.713484000	4.955242000
8	2.637114000	2.959783000	5.934079000
6	1.168883000	3.888157000	4.278510000
1	1.914893000	4.690463000	4.165875000
1	0.751559000	3.638202000	3.297223000
1	0.352676000	4.278031000	4.911642000
1	2.758012000	3.914758000	6.078160000

2a-H⁺_i2

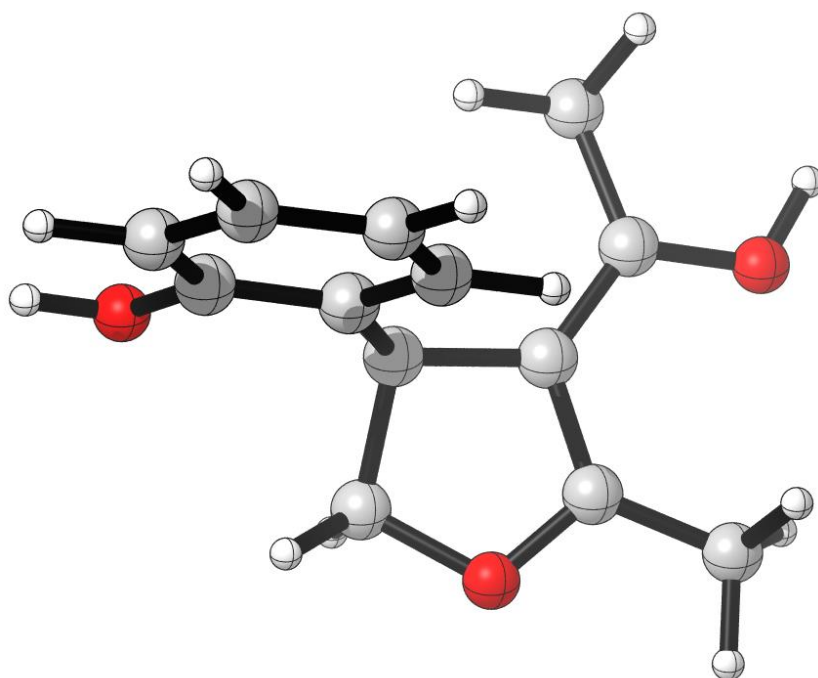


SPE = -728.9677; H₂₉₈ = -728.6969

6	2.268316000	0.505271000	3.610656000
1	3.340617000	0.513962000	3.853527000
6	2.124255000	0.965933000	2.167748000
6	0.860901000	1.035035000	1.541304000
6	0.741585000	1.505083000	0.226631000
1	-0.250116000	1.559024000	-0.233458000
6	1.878357000	1.901529000	-0.481021000
1	1.771727000	2.275963000	-1.502358000
6	3.140064000	1.826589000	0.117727000
1	4.031963000	2.138945000	-0.430061000
6	3.249082000	1.363025000	1.432407000
1	4.231355000	1.314912000	1.911203000

6	1.510760000	1.372423000	4.620056000
6	1.679917000	-0.889861000	3.922292000
1	1.288977000	-1.426335000	3.049949000
1	2.375266000	-1.533539000	4.479193000
6	0.481872000	0.594480000	5.178961000
8	0.541107000	-0.652967000	4.807064000
6	-0.643199000	0.930636000	6.086194000
1	-1.387324000	0.123823000	6.053142000
1	-0.271152000	1.017448000	7.121792000
1	-1.114740000	1.881553000	5.805972000
8	-0.219330000	0.627838000	2.257578000
1	-1.028470000	0.723164000	1.732237000
6	1.841460000	2.692160000	4.899376000
8	2.855207000	3.177287000	4.212889000
6	1.176886000	3.605627000	5.873383000
1	0.451846000	4.240838000	5.333147000
1	0.652269000	3.073801000	6.672014000
1	1.928247000	4.270374000	6.329189000
1	3.060015000	4.095744000	4.461914000

2a-H⁺_i3

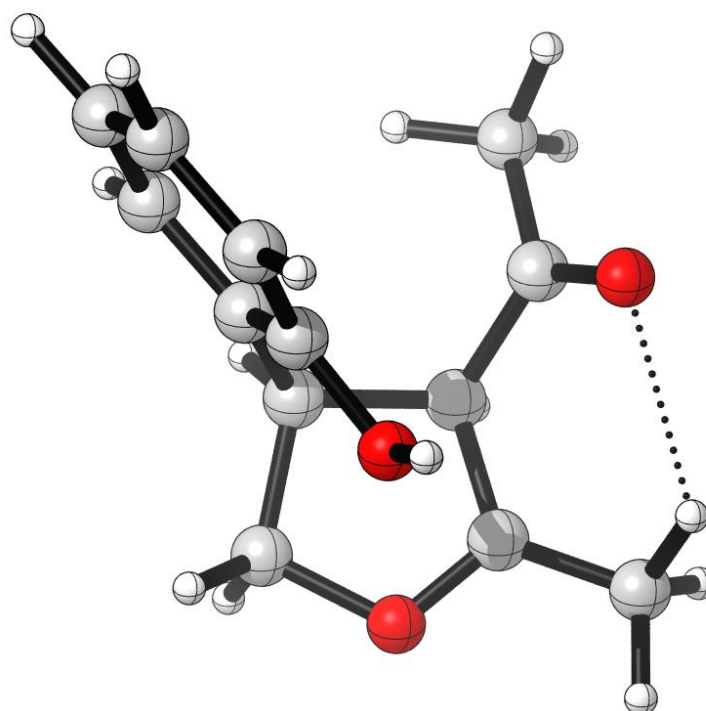


SPE = -728.9674; H₂₉₈ = -728.6967

6	1.432912000	1.085638000	3.139742000
1	1.856052000	0.668811000	2.214981000
6	0.474302000	2.220640000	2.785062000
6	-0.473396000	1.986024000	1.763068000
6	-1.415517000	2.964901000	1.420272000
1	-2.141329000	2.755984000	0.628857000
6	-1.420683000	4.191438000	2.092103000
1	-2.158482000	4.950866000	1.819751000
6	-0.485107000	4.444655000	3.099637000
1	-0.479672000	5.402484000	3.624642000
6	0.449972000	3.458444000	3.439673000
1	1.172581000	3.663948000	4.233415000

6	2.514969000	1.471881000	4.138607000
6	0.738402000	-0.054045000	3.915461000
1	-0.355151000	-0.057572000	3.860288000
1	1.134085000	-1.046958000	3.658434000
6	2.140132000	0.959108000	5.396459000
8	1.098386000	0.176621000	5.319517000
6	2.730977000	1.157057000	6.739337000
1	2.135531000	0.630284000	7.494694000
1	3.762735000	0.768820000	6.743008000
1	2.797839000	2.229511000	6.977471000
8	-0.421849000	0.775171000	1.153403000
1	-1.123458000	0.698366000	0.488526000
6	3.666812000	2.199834000	3.867725000
8	4.461645000	2.511089000	4.868025000
6	4.079112000	2.599241000	2.493559000
1	4.877321000	1.913525000	2.156661000
1	3.251820000	2.548051000	1.777120000
1	4.501779000	3.616554000	2.498866000
1	5.253710000	2.993600000	4.570570000

2a-H⁺_i4

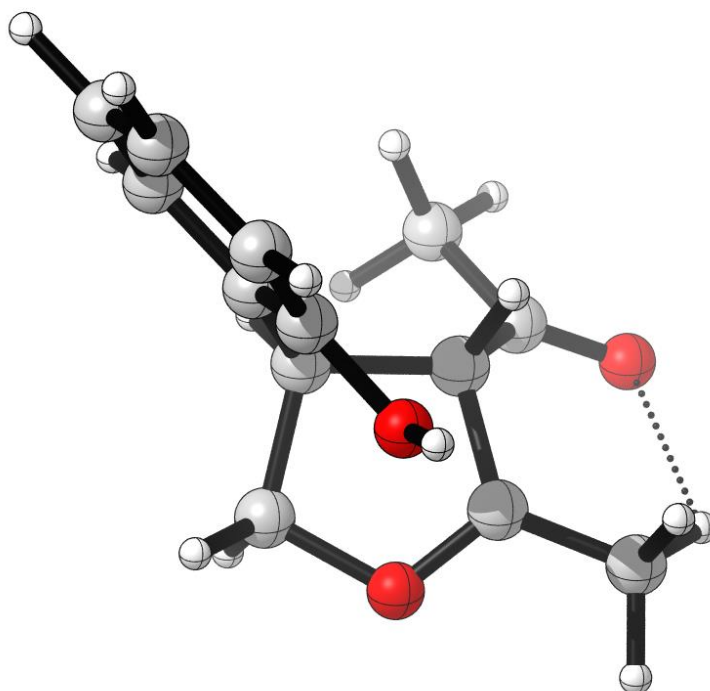


SPE = -728.9539; H₂₉₈ = -728.6832

6	1.432912000	1.085638000	3.139742000
1	1.856052000	0.668811000	2.214981000
6	0.474302000	2.220640000	2.785062000
6	-0.473396000	1.986024000	1.763068000
6	-1.415517000	2.964901000	1.420272000
1	-2.141329000	2.755984000	0.628857000
6	-1.420683000	4.191438000	2.092103000
1	-2.158482000	4.950866000	1.819751000
6	-0.485107000	4.444655000	3.099637000
1	-0.479672000	5.402484000	3.624642000
6	0.449972000	3.458444000	3.439673000
1	1.172581000	3.663948000	4.233415000

6	2.514969000	1.471881000	4.138607000
6	0.738402000	-0.054045000	3.915461000
1	-0.355151000	-0.057572000	3.860288000
1	1.134085000	-1.046958000	3.658434000
6	2.140132000	0.959108000	5.396459000
8	1.098386000	0.176621000	5.319517000
6	2.730977000	1.157057000	6.739337000
1	2.135531000	0.630284000	7.494694000
1	3.762735000	0.768820000	6.743008000
1	2.797839000	2.229511000	6.977471000
8	-0.421849000	0.775171000	1.153403000
1	-1.123458000	0.698366000	0.488526000
6	3.666812000	2.199834000	3.867725000
8	4.461645000	2.511089000	4.868025000
6	4.079112000	2.599241000	2.493559000
1	4.877321000	1.913525000	2.156661000
1	3.251820000	2.548051000	1.777120000
1	4.501779000	3.616554000	2.498866000
1	5.253710000	2.993600000	4.570570000

2a-H⁺_i5

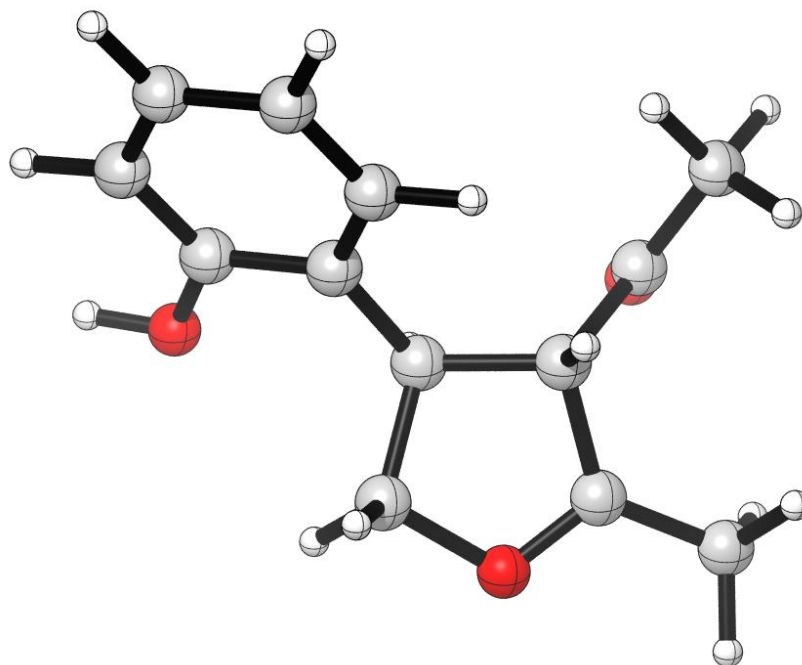


SPE = -728.9526; H₂₉₈ = -728.6830

6	1.667351000	0.279216000	2.979773000
1	1.933113000	0.942306000	2.148827000
6	0.214775000	-0.124818000	2.795763000
6	-0.445434000	-0.925769000	3.752888000
6	-1.781191000	-1.305246000	3.573740000
1	-2.271646000	-1.919469000	4.335661000
6	-2.467971000	-0.903841000	2.423915000
1	-3.505373000	-1.217880000	2.281441000
6	-1.831428000	-0.113282000	1.461432000
1	-2.367212000	0.206069000	0.564643000
6	-0.499830000	0.269253000	1.655571000
1	0.001136000	0.884401000	0.902639000

6	1.970952000	0.968562000	4.345416000
6	2.658722000	-0.904129000	2.983241000
1	2.229366000	-1.871711000	2.699149000
1	3.575060000	-0.715606000	2.409302000
6	2.684882000	-0.090292000	5.112636000
8	3.089612000	-1.047279000	4.385109000
6	2.987405000	-0.100424000	6.543962000
1	3.653911000	-0.928667000	6.810491000
1	3.410150000	0.881961000	6.813308000
1	2.031249000	-0.186527000	7.089677000
8	0.278657000	-1.310854000	4.840682000
1	-0.264097000	-1.834526000	5.450820000
6	2.775239000	2.323828000	4.345228000
8	3.361486000	2.664790000	5.344451000
6	2.707529000	3.166215000	3.103012000
1	3.287002000	2.691368000	2.294221000
1	1.670611000	3.269235000	2.746967000
1	3.137443000	4.152443000	3.319274000
1	1.048365000	1.247450000	4.882839000

2a-H⁺_i6

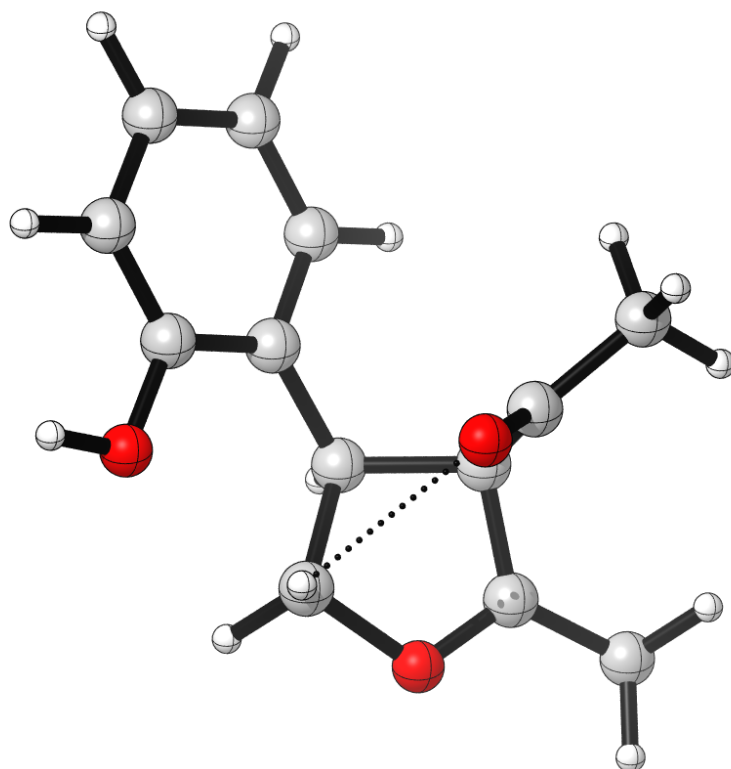


SPE = -728.9487; H₂₉₈ = -728.6792

6	2.637161000	0.056172000	3.207117000
1	3.604699000	-0.451799000	3.064144000
6	2.105842000	0.479788000	1.852031000
6	2.110872000	-0.488915000	0.821795000
6	1.628315000	-0.173739000	-0.454763000
1	1.638411000	-0.941730000	-1.234214000
6	1.134302000	1.106961000	-0.719239000
1	0.750019000	1.343813000	-1.714834000
6	1.119082000	2.075692000	0.287563000
1	0.724990000	3.074557000	0.087474000
6	1.601501000	1.754009000	1.562130000
1	1.573760000	2.522330000	2.338848000

6	2.867915000	1.152869000	4.278557000
6	1.718111000	-0.926604000	3.945256000
1	0.647371000	-0.698315000	3.852740000
1	1.913208000	-1.985169000	3.746127000
6	2.649062000	0.395298000	5.549423000
8	2.043997000	-0.702546000	5.374010000
6	3.058666000	0.798037000	6.897078000
1	2.580150000	0.181965000	7.666652000
1	4.157121000	0.668408000	6.952480000
1	2.857265000	1.870198000	7.049002000
8	2.593976000	-1.718554000	1.135072000
1	2.537734000	-2.310580000	0.369276000
6	4.272732000	1.816104000	4.208295000
8	5.248696000	1.105514000	4.294608000
6	4.318958000	3.301831000	4.029473000
1	3.808971000	3.579087000	3.090799000
1	3.763532000	3.799180000	4.842603000
1	5.357827000	3.653390000	4.009232000
1	2.075666000	1.924723000	4.270049000

2a-H⁺_i7

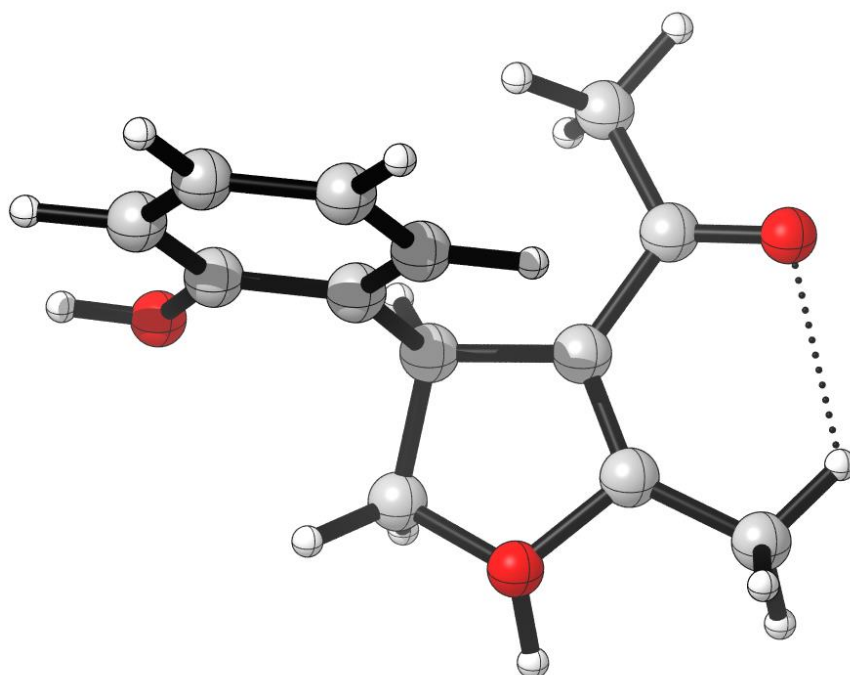


SPE = -728.9444; H₂₉₈ = -728.6746

6	3.896171000	0.759315000	3.315500000
1	4.521415000	0.030268000	3.859626000
6	4.811560000	1.891534000	2.872789000
6	5.139638000	2.152433000	1.525561000
6	6.041857000	3.179443000	1.201124000
1	6.278859000	3.363618000	0.148525000
6	6.634824000	3.947368000	2.203038000
1	7.337247000	4.739527000	1.930097000
6	6.330106000	3.694963000	3.545170000
1	6.792917000	4.283570000	4.339882000
6	5.430067000	2.674229000	3.862559000
1	5.213015000	2.466451000	4.914694000

6	2.763392000	1.145087000	4.319544000
6	3.113305000	-0.039171000	2.264899000
1	2.600129000	0.557999000	1.509673000
1	3.648778000	-0.877207000	1.810323000
6	1.851278000	-0.023519000	4.175788000
8	2.024084000	-0.649390000	3.087348000
6	0.848068000	-0.488976000	5.138336000
1	0.147199000	-1.199443000	4.682388000
1	1.403693000	-0.991129000	5.954634000
1	0.324866000	0.361080000	5.602369000
8	4.581155000	1.377195000	0.561278000
1	4.913487000	1.633667000	-0.312328000
6	1.976520000	2.448022000	3.902830000
8	1.650478000	2.593462000	2.749710000
6	1.696151000	3.433051000	4.996811000
1	1.156985000	2.940551000	5.823235000
1	2.648445000	3.797983000	5.418601000
1	1.109662000	4.273981000	4.604727000
1	3.096687000	1.243443000	5.360722000

2a-H⁺_i8



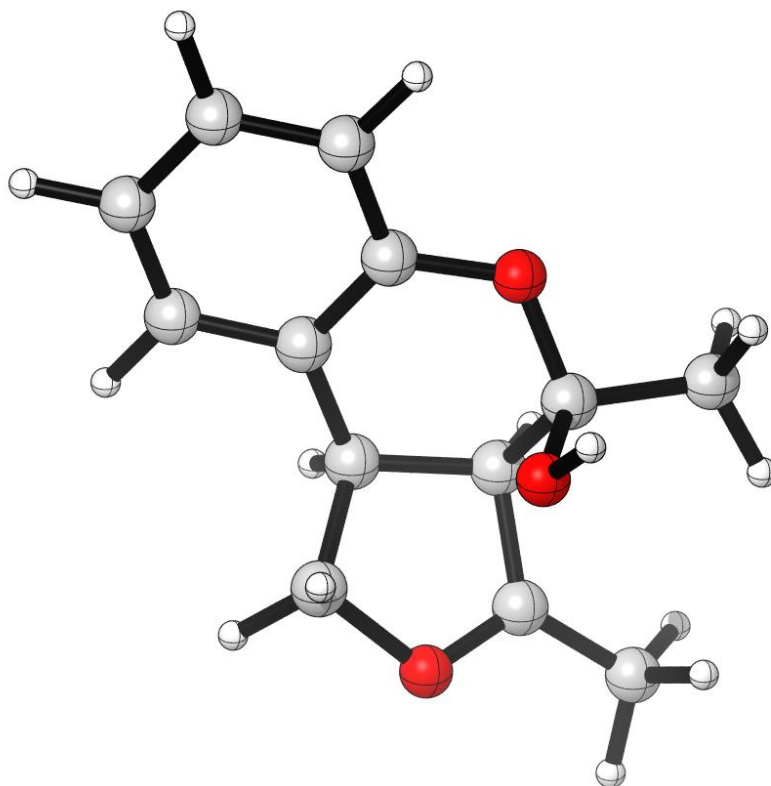
SPE = -728.9197; H₂₉₈ = -728.6497

6	1.413535000	1.104793000	3.202515000
1	1.875014000	0.709528000	2.285663000
6	0.466335000	2.241539000	2.820680000
6	-0.473857000	1.991313000	1.796556000
6	-1.377200000	2.983312000	1.393415000
1	-2.097120000	2.762908000	0.599631000
6	-1.346895000	4.238836000	2.007285000
1	-2.050217000	5.011389000	1.685430000
6	-0.420836000	4.505175000	3.020859000
1	-0.391201000	5.485296000	3.501767000
6	0.473457000	3.505237000	3.423769000
1	1.186423000	3.721542000	4.223714000

6	2.477954000	1.497037000	4.220231000
6	0.709885000	-0.066411000	3.898852000
1	-0.375826000	-0.118031000	3.783995000
1	1.191528000	-1.034890000	3.719673000
6	2.191031000	1.027128000	5.443558000
8	0.961321000	0.262888000	5.346447000
6	2.747718000	1.117649000	6.805416000
1	2.946042000	0.114764000	7.219423000
1	3.676191000	1.697817000	6.769246000
1	2.029316000	1.626405000	7.470837000
8	-0.451591000	0.751695000	1.247305000
1	-1.142377000	0.662123000	0.572480000
6	3.688806000	2.324600000	3.912229000
8	4.378968000	2.781753000	4.806898000
6	4.016975000	2.533315000	2.455889000
1	4.217458000	1.562057000	1.972005000
1	3.166662000	2.989284000	1.923939000
1	4.900650000	3.177507000	2.364446000
1	0.848713000	-0.472004000	5.987457000

To Figures 2 and S10

II1

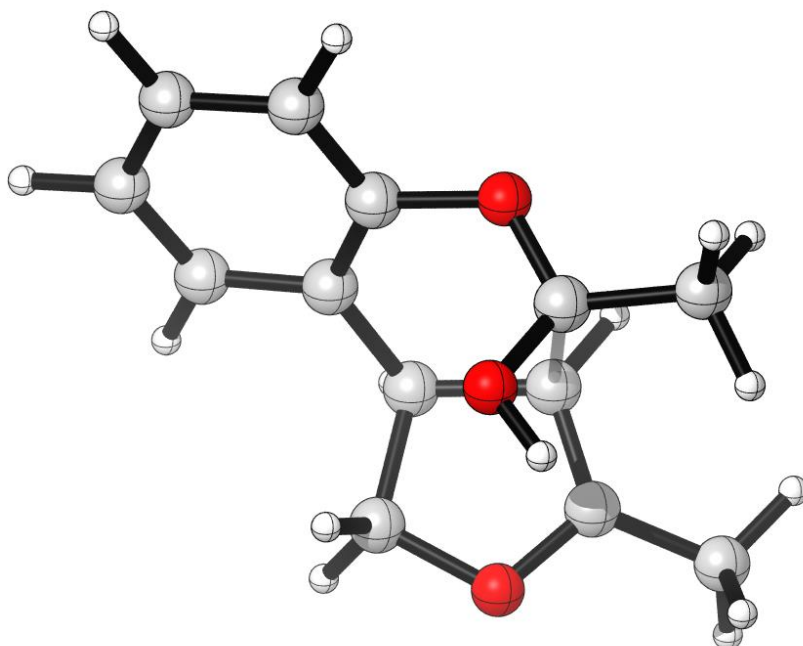


SPE = -728.9584; H₂₉₈ = -728.6863

6	-0.002552000	-2.705287000	-3.847560000
6	-1.082515000	-3.395935000	-3.278127000
6	0.933084000	-2.068575000	-3.032702000
1	-1.817219000	-3.893474000	-3.915294000
1	1.782355000	-1.525536000	-3.453549000
6	-1.208762000	-3.454324000	-1.888887000
6	0.792306000	-2.129049000	-1.640168000
1	-2.039452000	-4.006606000	-1.439433000
6	-0.274435000	-2.822937000	-1.051011000
1	0.113929000	-2.662223000	-4.934093000
6	-0.379832000	-2.914589000	0.449343000

6	0.836910000	-2.327002000	1.213198000
6	1.502438000	-1.133923000	0.441727000
6	-1.568161000	-2.162370000	1.066079000
1	-1.809850000	-1.213901000	0.571330000
1	-2.470608000	-2.759716000	1.235566000
6	0.196704000	-1.865908000	2.484611000
8	-1.067239000	-1.797454000	2.411985000
6	0.851877000	-1.521345000	3.751997000
1	0.138109000	-1.568885000	4.584882000
1	1.726289000	-2.163661000	3.922589000
1	1.221076000	-0.481079000	3.671184000
6	2.850795000	-0.693985000	0.994125000
1	2.766745000	-0.317287000	2.021552000
1	3.571007000	-1.523536000	0.963167000
1	3.233882000	0.119261000	0.358670000
1	-0.468566000	-3.974284000	0.734845000
8	1.773733000	-1.530525000	-0.890275000
8	0.538549000	-0.117220000	0.483265000
1	0.897301000	0.689713000	0.078003000
1	1.614039000	-3.073604000	1.426059000

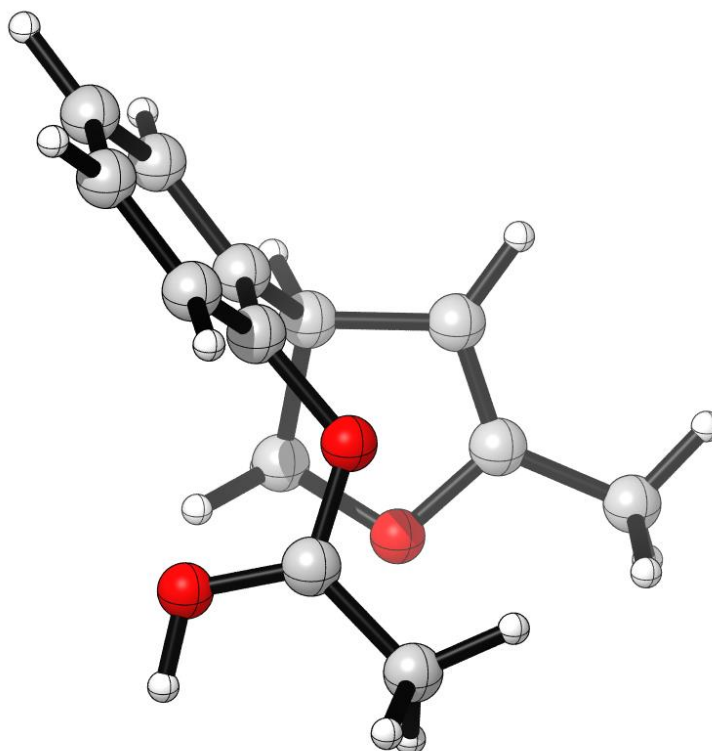
TS0



SPE = -728.9283; H₂₉₈ = -728.6586

6	-0.019193000	-2.671738000	-3.827687000
6	-1.121575000	-3.319103000	-3.254806000
6	0.977611000	-2.142834000	-3.006205000
1	-1.902993000	-3.739953000	-3.891872000
1	1.854597000	-1.639085000	-3.417979000
6	-1.223379000	-3.433260000	-1.866570000
6	0.839926000	-2.263229000	-1.624752000
1	-2.081524000	-3.949948000	-1.426910000
6	-0.243065000	-2.900159000	-1.010153000
1	0.069217000	-2.578041000	-4.913006000
6	-0.422143000	-3.018491000	0.494182000
6	0.735402000	-2.648653000	1.411634000

6	1.692913000	-0.949583000	0.149572000
6	-1.551256000	-2.097147000	1.044779000
1	-1.793854000	-1.266392000	0.369238000
1	-2.470596000	-2.640425000	1.300590000
6	0.228483000	-1.925824000	2.462764000
8	-1.029155000	-1.523906000	2.278055000
6	0.864247000	-1.520795000	3.741986000
1	0.298089000	-1.964807000	4.577142000
1	1.905005000	-1.863398000	3.796765000
1	0.819283000	-0.426452000	3.870072000
6	2.898595000	-0.551013000	0.927457000
1	2.626682000	-0.026236000	1.851328000
1	3.526451000	-1.421871000	1.147838000
1	3.473450000	0.143919000	0.288932000
1	-0.693803000	-4.070268000	0.691402000
8	1.908593000	-1.780314000	-0.839410000
8	0.670005000	-0.142815000	0.005907000
1	0.659913000	0.563212000	0.677319000
1	1.656009000	-3.226637000	1.485467000

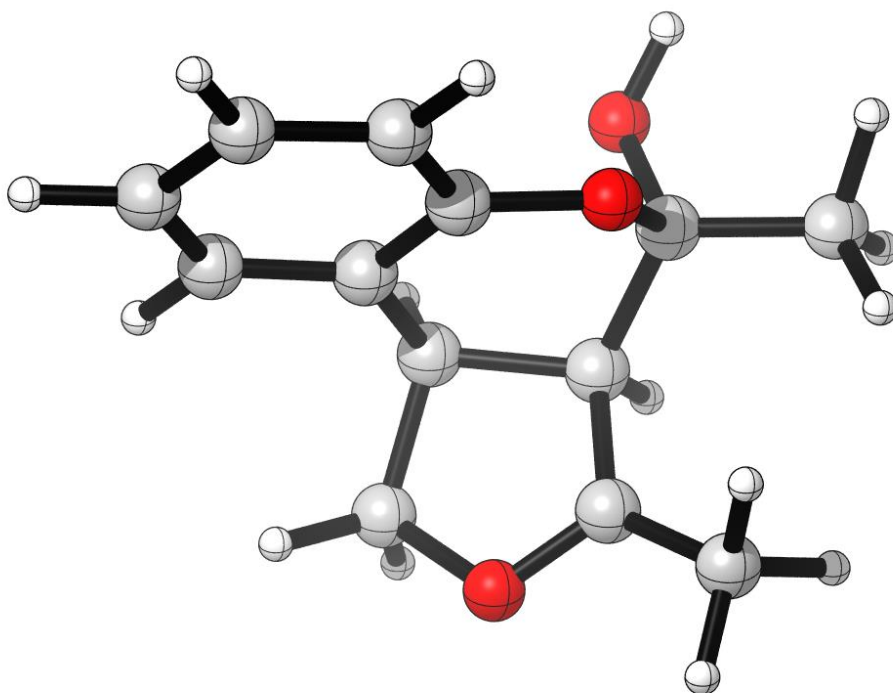


SPE = -728.9358; H₂₉₈ = -728.6642

6	0.448756000	-3.040388000	-3.530371000
6	-0.742225000	-3.670189000	-3.157171000
6	1.190363000	-2.346325000	-2.572065000
1	-1.327808000	-4.217787000	-3.899152000
1	2.130983000	-1.854507000	-2.827938000
6	-1.191750000	-3.598712000	-1.835709000
6	0.710009000	-2.300613000	-1.267007000
1	-2.127655000	-4.089487000	-1.556268000
6	-0.478724000	-2.906287000	-0.840304000
1	0.809952000	-3.090903000	-4.560327000
6	-1.021441000	-2.842965000	0.585365000
6	-0.095499000	-3.403820000	1.652142000

6	1.582673000	-0.377671000	-0.163750000
6	-1.257075000	-1.420012000	1.164574000
1	-1.269999000	-0.616803000	0.414724000
1	-2.202718000	-1.389385000	1.729390000
6	0.335006000	-2.407894000	2.442268000
8	-0.178251000	-1.175916000	2.094369000
6	1.268125000	-2.406343000	3.600982000
1	0.764356000	-2.010274000	4.498273000
1	1.633707000	-3.420770000	3.810171000
1	2.136817000	-1.756430000	3.403355000
6	2.534564000	0.208370000	0.799087000
1	1.966931000	0.782904000	1.548107000
1	3.126398000	-0.576018000	1.282508000
1	3.196131000	0.906271000	0.259349000
1	-1.978951000	-3.383790000	0.565923000
8	1.544023000	-1.649894000	-0.298717000
8	0.800746000	0.325315000	-0.897584000
1	0.882960000	1.288597000	-0.746993000
1	0.211095000	-4.446747000	1.725313000

III_i2

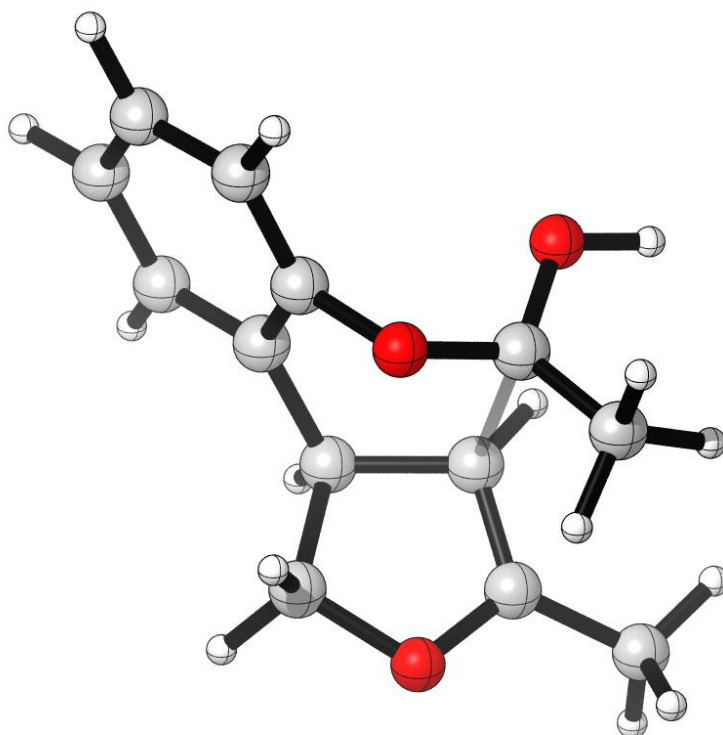


SPE = -728.9531; H₂₉₈ = -728.6816

6	1.268968000	-2.285877000	-3.680873000
6	0.131636000	-3.089600000	-3.516649000
6	1.943685000	-1.793746000	-2.565068000
1	-0.391887000	-3.495031000	-4.385278000
1	2.845650000	-1.185880000	-2.664409000
6	-0.335870000	-3.367229000	-2.231310000
6	1.473458000	-2.086913000	-1.277838000
1	-1.229849000	-3.985124000	-2.104322000
6	0.308213000	-2.855811000	-1.091864000
1	1.640237000	-2.046303000	-4.680893000
6	-0.253986000	-3.099508000	0.301989000
6	0.475805000	-2.201521000	1.325694000

6	1.993992000	-2.156567000	1.057658000
6	-1.689878000	-2.605980000	0.466597000
1	-2.323804000	-2.623426000	-0.426115000
1	-2.214939000	-3.049771000	1.322841000
6	-0.331103000	-0.940029000	1.231199000
8	-1.505022000	-1.168480000	0.807274000
6	0.039137000	0.438461000	1.561808000
1	-0.801924000	1.123050000	1.401215000
1	0.396986000	0.487417000	2.603576000
1	0.894291000	0.723324000	0.923441000
6	2.835069000	-1.366806000	2.047028000
1	2.704169000	-1.785343000	3.054949000
1	3.893008000	-1.466200000	1.756824000
1	2.592759000	-0.297228000	2.060470000
1	-0.180855000	-4.158916000	0.583948000
8	2.196038000	-1.565983000	-0.229339000
1	0.304763000	-2.573690000	2.354951000
8	2.362462000	-3.502175000	1.051101000
1	3.327827000	-3.566454000	0.974769000

TS0_i2

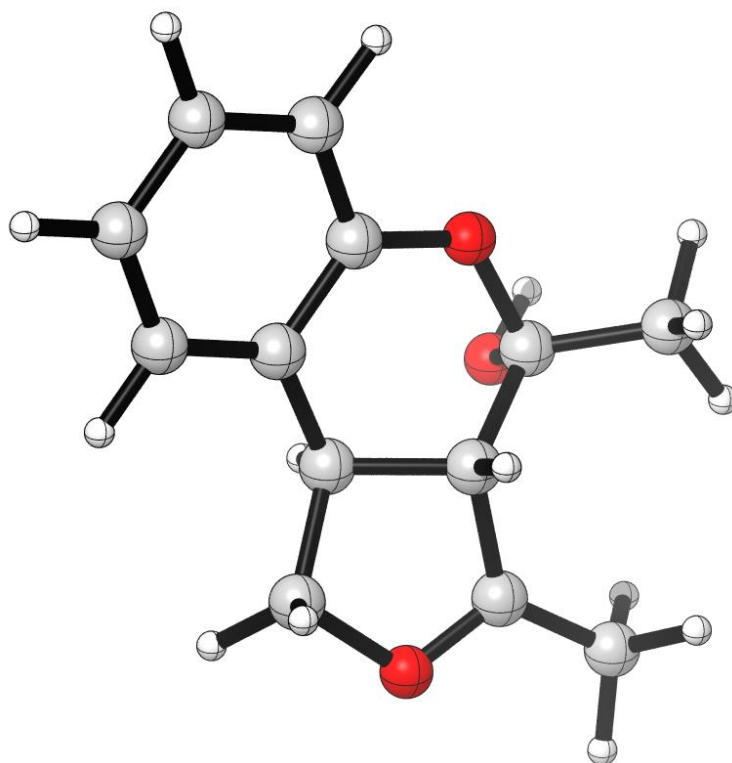


SPE = -728.9269; H₂₉₈ = -728.6570

6	1.533281000	-3.534432000	-3.658897000
6	0.325698000	-4.170791000	-3.351872000
6	2.050431000	-2.556270000	-2.800318000
1	-0.074044000	-4.936586000	-4.021096000
1	2.990304000	-2.042814000	-3.011447000
6	-0.377477000	-3.827522000	-2.191462000
6	1.329864000	-2.245453000	-1.654598000
1	-1.323221000	-4.322826000	-1.956631000
6	0.113932000	-2.846449000	-1.319979000
1	2.080432000	-3.801905000	-4.565790000
6	-0.618143000	-2.426553000	-0.064262000
6	0.225307000	-2.308856000	1.204869000

6	2.199062000	-1.542950000	0.429146000
6	-1.237204000	-1.003673000	-0.127316000
1	-0.690810000	-0.326245000	-0.798080000
1	-2.303274000	-0.985266000	-0.385569000
6	-0.298200000	-1.253825000	1.932131000
8	-1.104151000	-0.472890000	1.229512000
6	-0.094271000	-0.902194000	3.357246000
1	-1.046686000	-1.057341000	3.893672000
1	0.673167000	-1.535436000	3.818416000
1	0.171097000	0.161246000	3.467685000
6	2.574842000	-0.370461000	1.274619000
1	2.727077000	-0.665405000	2.320723000
1	3.528359000	0.020346000	0.878032000
1	1.821255000	0.423089000	1.201728000
1	-1.419958000	-3.162348000	0.115492000
8	1.793080000	-1.228979000	-0.792397000
1	0.654775000	-3.177898000	1.702959000
8	2.872357000	-2.670543000	0.517270000
1	3.292151000	-2.776109000	1.389588000

III_i3

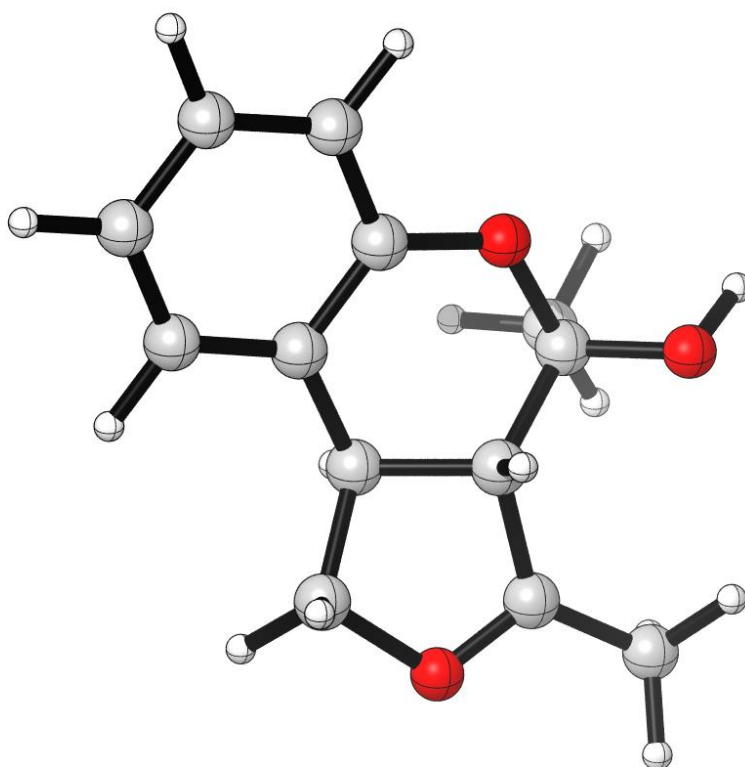


SPE = -728.9485; H₂₉₈ = -728.6771

6	-0.313119000	-2.151463000	-3.951478000
6	-1.248441000	-3.019431000	-3.371834000
6	0.584904000	-1.437946000	-3.155276000
1	-1.950965000	-3.573983000	-3.997888000
1	1.315192000	-0.754494000	-3.594221000
6	-1.276445000	-3.171741000	-1.982716000
6	0.553344000	-1.591892000	-1.762320000
1	-1.998902000	-3.850404000	-1.520381000
6	-0.384044000	-2.461495000	-1.169311000
1	-0.285485000	-2.020899000	-5.036991000
6	-0.306348000	-2.577112000	0.321336000
6	0.115875000	-1.219838000	0.914742000

6	1.502458000	-0.812345000	0.401866000
6	-1.519519000	-2.900821000	1.174223000
1	-2.436438000	-2.364525000	0.894273000
1	-1.727638000	-3.957728000	1.366680000
6	-0.189279000	-1.450583000	2.356357000
8	-1.096339000	-2.331201000	2.491331000
6	0.372476000	-0.806754000	3.544016000
1	-0.096946000	-1.176237000	4.462847000
1	1.458503000	-1.013467000	3.547356000
1	0.260657000	0.287355000	3.455000000
6	1.936943000	0.610269000	0.730379000
1	2.103746000	0.739681000	1.807954000
1	2.880892000	0.819944000	0.203559000
1	1.186231000	1.335542000	0.385790000
1	0.486460000	-3.299184000	0.586277000
8	1.454457000	-0.848970000	-1.041065000
8	2.383386000	-1.777565000	0.892215000
1	3.293473000	-1.529835000	0.660773000
1	-0.613223000	-0.441483000	0.607071000

III_i4

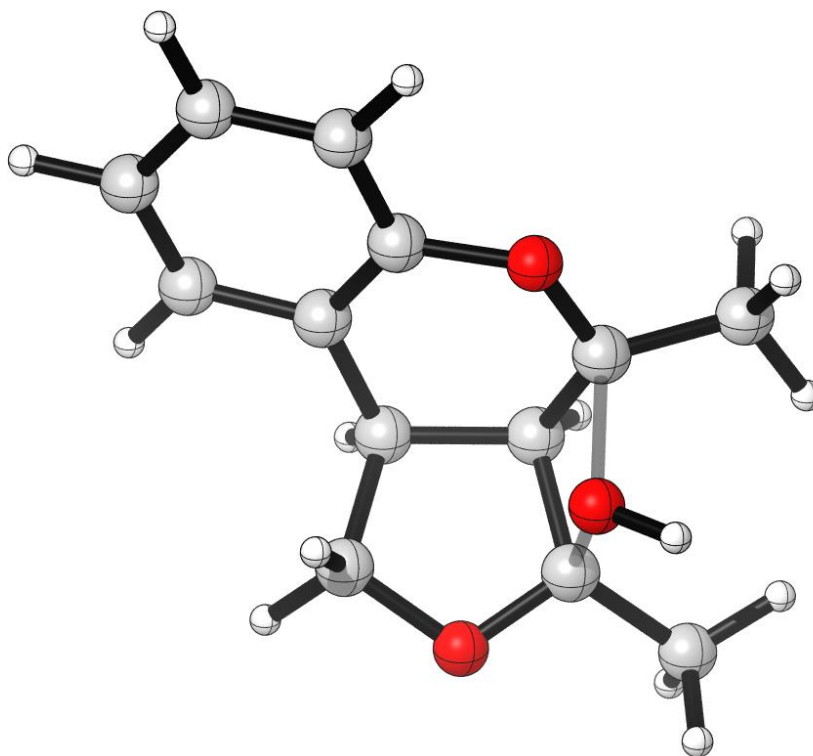


SPE = -728.9457; H₂₉₈ = -728.6752

6	-0.363292000	-2.183506000	-3.909980000
6	-1.136638000	-3.177607000	-3.294846000
6	0.449212000	-1.341777000	-3.149318000
1	-1.768340000	-3.838004000	-3.893130000
1	1.058638000	-0.565804000	-3.617512000
6	-1.095557000	-3.315132000	-1.905630000
6	0.491371000	-1.480960000	-1.753648000
1	-1.694277000	-4.088087000	-1.415377000
6	-0.295839000	-2.470338000	-1.123064000
1	-0.395743000	-2.056974000	-4.995816000
6	-0.203367000	-2.555053000	0.374477000
6	0.146826000	-1.167343000	0.920366000

6	1.462141000	-0.612415000	0.367204000
6	-1.424682000	-2.888107000	1.221103000
1	-2.357963000	-2.423420000	0.874589000
1	-1.583304000	-3.940373000	1.476168000
6	-0.214485000	-1.299212000	2.355346000
8	-1.090901000	-2.208457000	2.512843000
6	0.224098000	-0.501053000	3.499367000
1	-0.393293000	-0.688462000	4.385730000
1	1.275630000	-0.772063000	3.712152000
1	0.237382000	0.562173000	3.211106000
6	2.724152000	-1.394089000	0.711468000
1	2.679212000	-2.428581000	0.342510000
1	3.579613000	-0.902533000	0.222626000
1	2.896031000	-1.403869000	1.798109000
1	0.598393000	-3.258340000	0.664605000
8	1.309800000	-0.612549000	-1.078971000
8	1.543776000	0.708436000	0.775008000
1	2.441539000	1.042454000	0.619350000
1	-0.627268000	-0.444633000	0.573995000

TS1

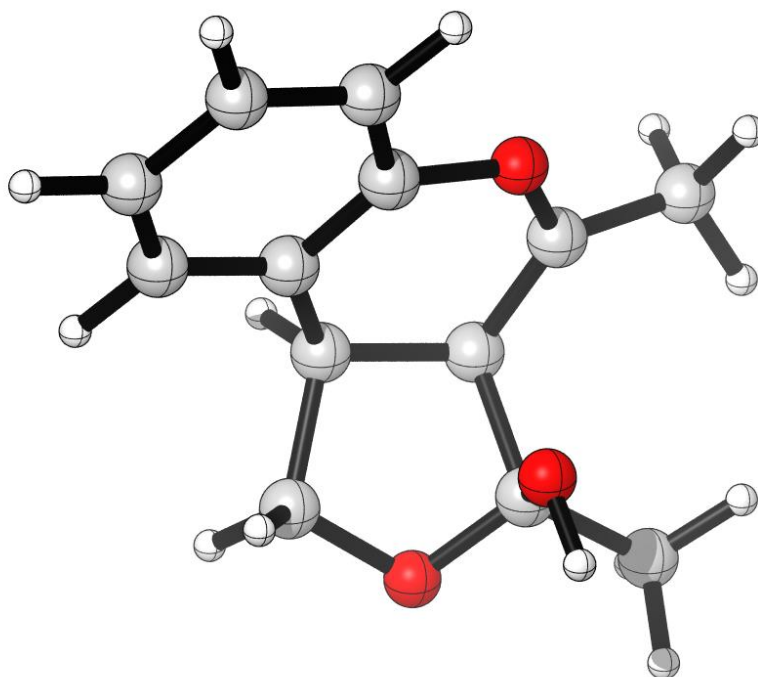


SPE = -728.9349; H₂₉₈ = -728.6644

6	-0.157911000	-2.546637000	-3.846179000
6	-1.014250000	-3.503276000	-3.284868000
6	0.690012000	-1.800813000	-3.025972000
1	-1.672314000	-4.093191000	-3.926821000
1	1.381931000	-1.060523000	-3.432703000
6	-1.029931000	-3.702719000	-1.901525000
6	0.649953000	-2.017533000	-1.648942000
1	-1.701947000	-4.445690000	-1.462725000
6	-0.198883000	-2.952289000	-1.054298000
1	-0.147170000	-2.379166000	-4.926358000
6	-0.289968000	-3.051743000	0.447360000
6	0.903148000	-2.412689000	1.202276000

6	1.678253000	-1.358382000	0.413367000
6	-1.532009000	-2.278756000	0.977183000
1	-1.861289000	-1.507948000	0.263417000
1	-2.378601000	-2.933313000	1.220839000
6	0.221410000	-1.410527000	2.163534000
8	-1.108409000	-1.641160000	2.190573000
6	0.741449000	-1.093529000	3.539898000
1	0.140580000	-0.282143000	3.976566000
1	0.623814000	-1.988090000	4.168826000
1	1.797993000	-0.798049000	3.535122000
6	3.049965000	-0.946298000	0.853344000
1	3.139596000	-0.836779000	1.939718000
1	3.737511000	-1.744745000	0.528458000
1	3.346128000	-0.016402000	0.348161000
1	-0.363760000	-4.105727000	0.747482000
8	1.557672000	-1.262790000	-0.896971000
8	0.537979000	-0.259210000	1.162128000
1	0.847268000	0.585334000	1.548436000
1	1.563718000	-3.150460000	1.673752000

II2

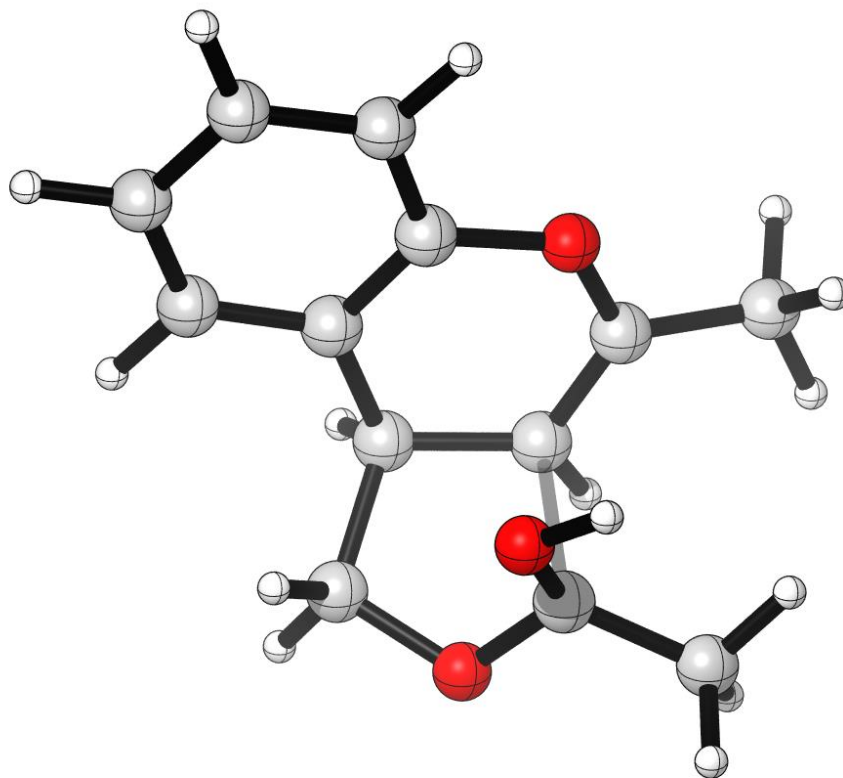


SPE = -728.9486; H₂₉₈ = -728.6769

6	-0.543905000	-1.762938000	-3.701658000
6	-1.351215000	-2.807065000	-3.232044000
6	0.394582000	-1.176997000	-2.851009000
1	-2.074882000	-3.277537000	-3.901603000
1	1.057108000	-0.373305000	-3.178326000
6	-1.237751000	-3.257263000	-1.911729000
6	0.475709000	-1.651996000	-1.544993000
1	-1.873353000	-4.075251000	-1.562860000
6	-0.319919000	-2.673130000	-1.027365000
1	-0.640685000	-1.406958000	-4.729650000
6	-0.182214000	-3.107400000	0.413131000
6	0.729938000	-2.172755000	1.247825000

6	1.666319000	-1.323526000	0.481285000
6	-1.538532000	-3.061532000	1.192226000
1	-2.328113000	-2.618932000	0.564481000
1	-1.864141000	-4.051641000	1.537399000
6	-0.321938000	-1.307793000	2.069992000
8	-1.308335000	-2.258889000	2.343327000
6	0.142670000	-0.717075000	3.388315000
1	-0.726282000	-0.258068000	3.886445000
1	0.547162000	-1.497960000	4.047617000
1	0.897031000	0.065667000	3.232688000
6	2.893015000	-0.756316000	1.067642000
1	2.755397000	-0.482271000	2.122427000
1	3.647159000	-1.569030000	1.045857000
1	3.271741000	0.084793000	0.473947000
1	0.225700000	-4.129061000	0.436657000
8	1.484386000	-1.067511000	-0.754683000
8	-0.760790000	-0.330667000	1.158853000
1	-1.416800000	0.238356000	1.593844000
1	1.314614000	-2.737372000	1.986292000

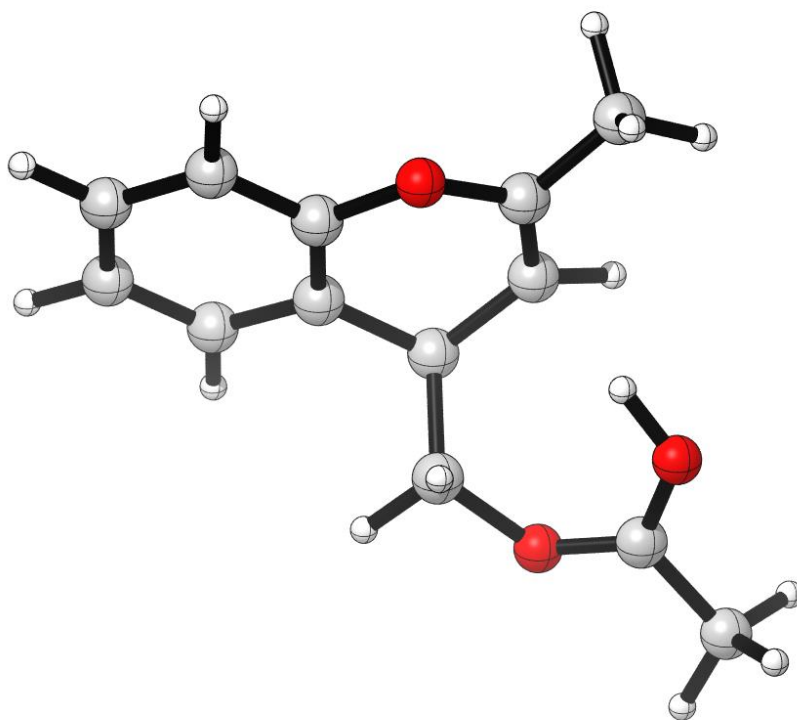
TS2



SPE = -728.9355; H₂₉₈ = -728.6650

6	-0.598887000	-1.665027000	-3.619048000
6	-1.357793000	-2.766476000	-3.203190000
6	0.328744000	-1.092277000	-2.748086000
1	-2.075776000	-3.224622000	-3.887268000
1	0.947579000	-0.240687000	-3.038980000
6	-1.200273000	-3.281918000	-1.913166000
6	0.464274000	-1.628758000	-1.468312000
1	-1.798742000	-4.140527000	-1.596533000
6	-0.290776000	-2.711738000	-1.009764000
1	-0.726529000	-1.252074000	-4.622334000
6	-0.145388000	-3.211322000	0.413619000
6	0.874807000	-2.394761000	1.185906000

6	1.708122000	-1.483434000	0.542514000
6	-1.495224000	-3.156589000	1.222326000
1	-2.311613000	-2.752209000	0.607559000
1	-1.786862000	-4.129471000	1.633119000
6	-0.555745000	-1.224209000	2.088772000
8	-1.266348000	-2.312345000	2.358862000
6	0.020273000	-0.520759000	3.277203000
1	-0.807540000	-0.019297000	3.807485000
1	0.496399000	-1.237011000	3.958119000
1	0.745097000	0.244933000	2.969035000
6	2.926229000	-0.881901000	1.145131000
1	3.034349000	-1.159489000	2.200690000
1	3.803848000	-1.257250000	0.590151000
1	2.917939000	0.213750000	1.029816000
1	0.181663000	-4.263371000	0.392901000
8	1.439508000	-1.031702000	-0.664850000
8	-1.064681000	-0.493387000	1.089408000
1	-0.691166000	0.403978000	1.070567000
1	1.298186000	-2.851471000	2.082675000

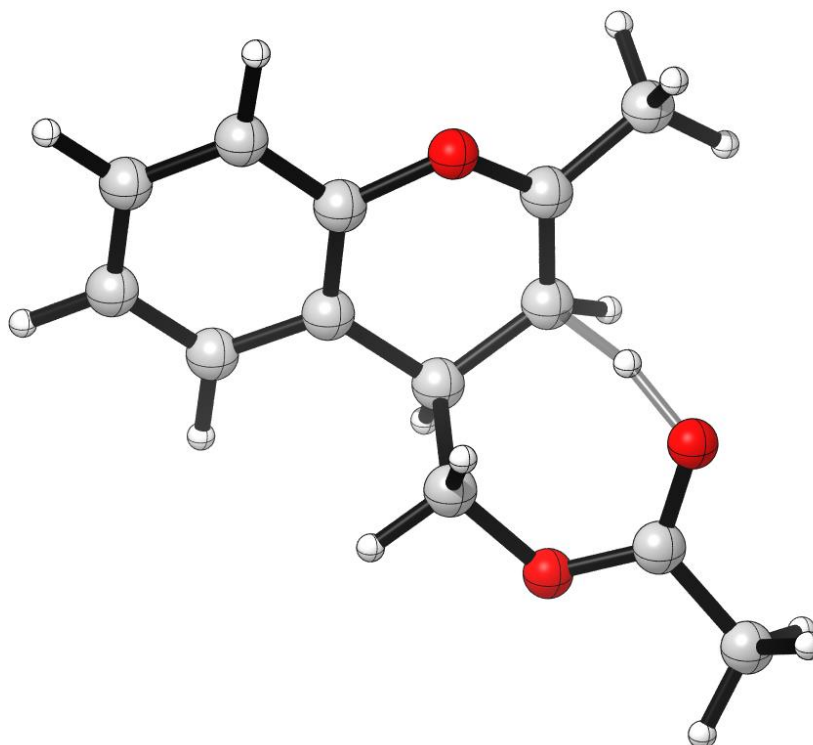


SPE = -728.9512; H₂₉₈ = -728.6805

6	-2.423213000	-3.300507000	-3.182084000
6	-1.320665000	-3.990711000	-2.659706000
6	-2.751246000	-2.033956000	-2.696254000
1	-1.049051000	-4.972624000	-3.053715000
1	-3.587480000	-1.462267000	-3.104698000
6	-0.564872000	-3.419836000	-1.632786000
6	-1.974911000	-1.472521000	-1.677315000
1	0.288614000	-3.961649000	-1.215727000
6	-0.885196000	-2.154856000	-1.117805000
1	-3.023403000	-3.744549000	-3.980355000
6	-0.123828000	-1.527844000	0.041833000
6	-0.331997000	-0.026942000	0.027921000

6	-1.390948000	0.545568000	-0.594216000
6	-0.628456000	-2.209771000	1.328197000
1	-1.696594000	-2.013490000	1.504897000
1	-0.452391000	-3.290560000	1.290704000
6	-0.128538000	-0.751126000	3.225003000
8	0.092626000	-1.822040000	2.561488000
6	0.451616000	-0.623343000	4.579178000
1	-0.319903000	-0.223857000	5.255005000
1	0.836353000	-1.585157000	4.933570000
1	1.265469000	0.120193000	4.536051000
6	-1.690498000	2.006431000	-0.652655000
1	-0.991226000	2.582650000	-0.034535000
1	-1.623990000	2.358996000	-1.695340000
1	-2.719485000	2.196009000	-0.304808000
1	0.949155000	-1.760583000	-0.051601000
8	-2.306836000	-0.191416000	-1.277803000
8	-0.822104000	0.228853000	2.779725000
1	-1.022718000	0.193367000	1.792437000
1	0.446966000	0.629423000	0.423170000

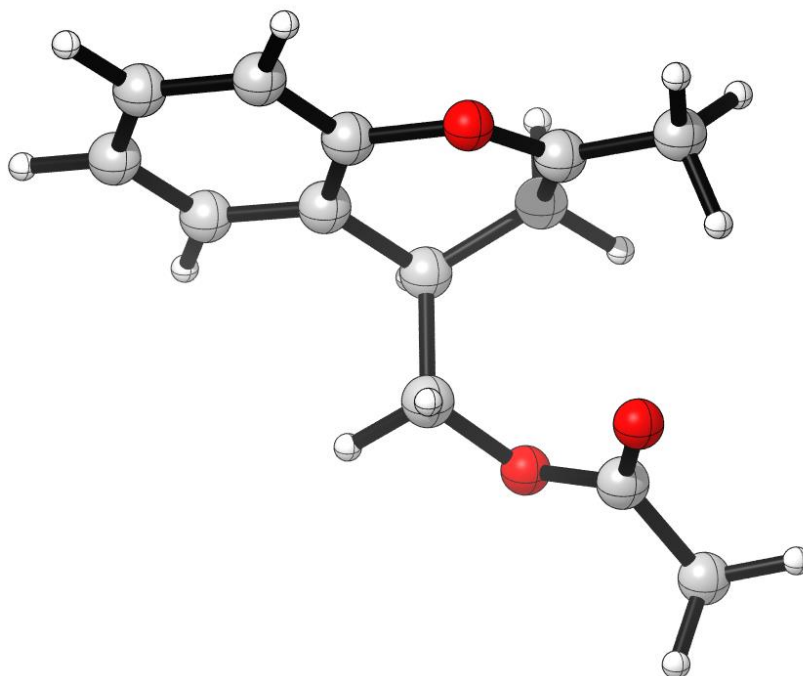
TS3



SPE = -728.9457; H₂₉₈ = -728.6799

6	-2.448501000	-3.281437000	-3.146076000
6	-1.341422000	-3.974025000	-2.639354000
6	-2.764156000	-2.013407000	-2.653081000
1	-1.079421000	-4.956765000	-3.037669000
1	-3.601577000	-1.434031000	-3.047368000
6	-0.567061000	-3.410908000	-1.620580000
6	-1.967463000	-1.470314000	-1.645213000
1	0.289156000	-3.958876000	-1.218168000
6	-0.874410000	-2.147637000	-1.094777000
1	-3.061759000	-3.722741000	-3.935567000
6	-0.107734000	-1.534815000	0.066906000
6	-0.353503000	-0.025708000	0.127145000

6	-1.402667000	0.555014000	-0.570793000
6	-0.567465000	-2.264931000	1.344770000
1	-1.646314000	-2.123766000	1.513181000
1	-0.346454000	-3.335714000	1.270311000
6	-0.169458000	-0.757295000	3.187035000
8	0.124170000	-1.868559000	2.573834000
6	0.371674000	-0.592108000	4.562794000
1	-0.424061000	-0.194024000	5.209948000
1	0.767332000	-1.535364000	4.954987000
1	1.172329000	0.165645000	4.526624000
6	-1.688336000	2.013433000	-0.597747000
1	-0.998943000	2.572213000	0.045462000
1	-1.596328000	2.376840000	-1.635272000
1	-2.727286000	2.196583000	-0.277247000
1	0.968840000	-1.727960000	-0.060629000
8	-2.281228000	-0.164756000	-1.251715000
8	-0.854057000	0.148604000	2.657150000
1	-0.825964000	0.153408000	1.432570000
1	0.503321000	0.635286000	0.306313000

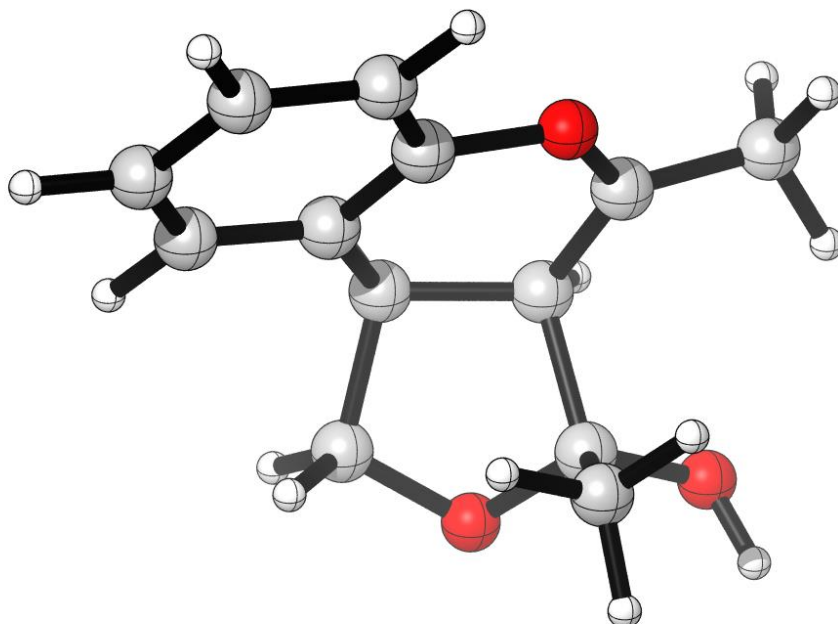


SPE = -728.9703; H₂₉₈ = -728.6991

6	-2.591154000	-3.268687000	-3.073470000
6	-1.503897000	-4.030561000	-2.627922000
6	-2.787986000	-1.977257000	-2.576252000
1	-1.347795000	-5.037076000	-3.022405000
1	-3.619128000	-1.348768000	-2.901490000
6	-0.612844000	-3.517946000	-1.677189000
6	-1.877662000	-1.499601000	-1.639679000
1	0.225429000	-4.125833000	-1.327021000
6	-0.783508000	-2.227377000	-1.163585000
1	-3.288639000	-3.676931000	-3.808292000
6	0.068891000	-1.629605000	-0.064657000
6	0.061351000	-0.099881000	-0.202323000

6	-1.271850000	0.479155000	-0.480789000
6	-0.468890000	-2.159477000	1.281997000
1	-1.554257000	-1.999365000	1.359261000
1	-0.259592000	-3.236646000	1.339034000
6	-0.449342000	-0.567368000	3.058893000
8	0.174090000	-1.583763000	2.425885000
6	0.165477000	-0.277997000	4.397715000
1	-0.333039000	-0.920126000	5.142697000
1	1.237351000	-0.519692000	4.408788000
1	-0.010349000	0.770201000	4.672205000
6	-1.665188000	1.834703000	-0.078518000
1	-1.832914000	1.807528000	1.015130000
1	-0.822413000	2.524722000	-0.249729000
1	-2.572930000	2.167905000	-0.594798000
1	1.109030000	-1.967827000	-0.176845000
8	-2.123785000	-0.190122000	-1.158577000
8	-1.414798000	0.000259000	2.589584000
1	0.535150000	0.420240000	0.638985000
1	0.656454000	0.186632000	-1.096430000

II2_i2

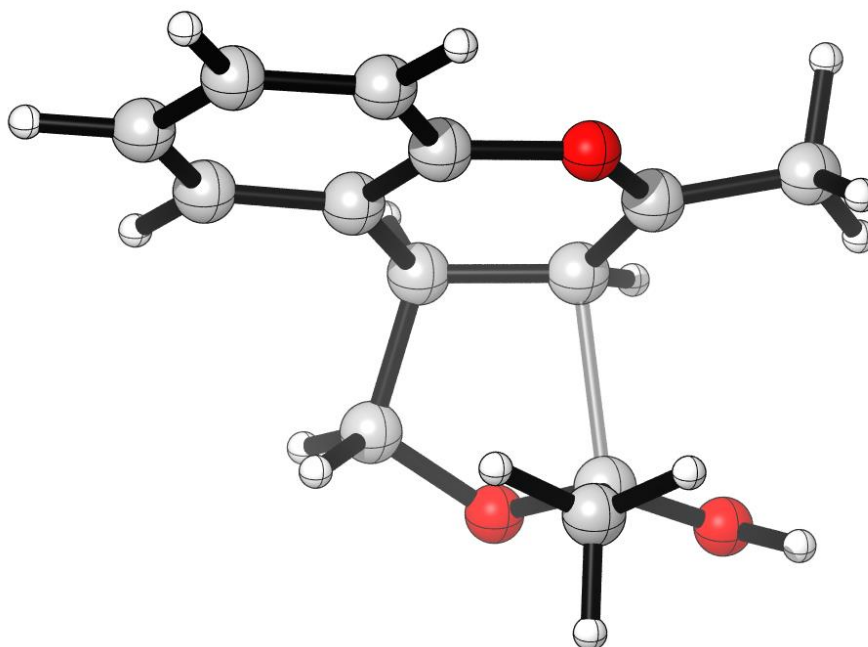


SPE = -728.9436; H₂₉₈ = -728.6720

6	-0.502876000	-1.582934000	-3.621503000
6	-1.388489000	-2.569874000	-3.169294000
6	0.498594000	-1.107855000	-2.773266000
1	-2.163475000	-2.951616000	-3.837815000
1	1.217626000	-0.348323000	-3.086359000
6	-1.288252000	-3.075244000	-1.868154000
6	0.565818000	-1.634041000	-1.486263000
1	-1.984703000	-3.848171000	-1.532760000
6	-0.305060000	-2.604779000	-0.985992000
1	-0.588170000	-1.184278000	-4.634487000
6	-0.159898000	-3.111928000	0.430341000
6	0.787907000	-2.241382000	1.273741000

6	1.773237000	-1.426152000	0.545841000
6	-1.488059000	-3.073060000	1.262616000
1	-2.298999000	-2.607629000	0.676619000
1	-1.814500000	-4.073061000	1.578387000
6	-0.193459000	-1.369407000	2.189349000
8	-1.209921000	-2.320838000	2.433111000
6	-0.748723000	-0.108813000	1.528332000
1	-1.464874000	0.362395000	2.220387000
1	0.051198000	0.615216000	1.310388000
1	-1.288311000	-0.333267000	0.597177000
6	2.968796000	-0.885978000	1.208698000
1	2.704019000	-0.547308000	2.223688000
1	3.673639000	-1.729961000	1.340803000
1	3.450032000	-0.098896000	0.616183000
1	0.223969000	-4.142647000	0.394801000
8	1.622687000	-1.137901000	-0.690713000
8	0.468860000	-1.090705000	3.369181000
1	0.047859000	-0.336432000	3.810929000
1	1.337327000	-2.842412000	2.011356000

TS2_i2

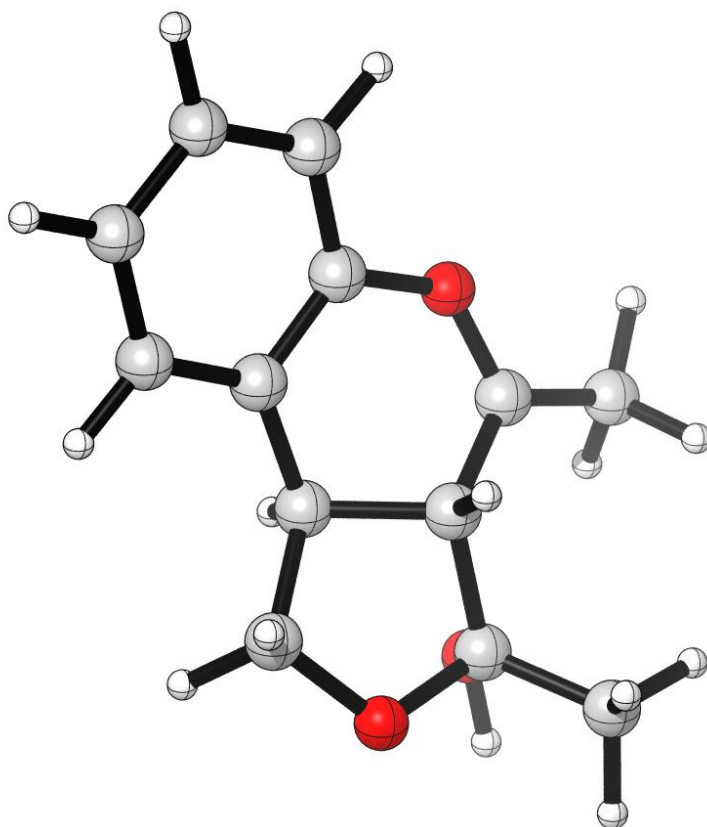


SPE = -728.9337; H₂₉₈ = -728.6633

6	-0.491715000	-1.632812000	-3.634248000
6	-1.311084000	-2.689817000	-3.215180000
6	0.448737000	-1.091360000	-2.757697000
1	-2.038696000	-3.123208000	-3.905173000
1	1.113376000	-0.276375000	-3.052197000
6	-1.199969000	-3.192778000	-1.916155000
6	0.540000000	-1.614949000	-1.467453000
1	-1.843757000	-4.017142000	-1.596790000
6	-0.275443000	-2.654051000	-1.007277000
1	-0.582381000	-1.230750000	-4.645922000
6	-0.179158000	-3.137492000	0.424197000
6	0.890812000	-2.393621000	1.195591000

6	1.753407000	-1.502001000	0.563042000
6	-1.530584000	-2.943932000	1.208239000
1	-2.234921000	-2.319762000	0.637635000
1	-2.016321000	-3.893475000	1.457766000
6	-0.376786000	-1.291562000	2.387583000
8	-1.218124000	-2.327150000	2.456486000
6	-0.775841000	-0.061621000	1.613683000
1	-1.581609000	0.433649000	2.182745000
1	0.067394000	0.636075000	1.518391000
1	-1.160825000	-0.299102000	0.615230000
6	2.968661000	-0.930508000	1.197457000
1	2.990095000	-1.134095000	2.275989000
1	3.855007000	-1.400312000	0.735796000
1	3.036121000	0.151255000	1.001652000
1	0.058604000	-4.213068000	0.430376000
8	1.530790000	-1.055388000	-0.656782000
8	0.216242000	-1.108519000	3.561292000
1	0.529958000	-0.194566000	3.665442000
1	1.321812000	-2.898838000	2.061609000

II2_i3

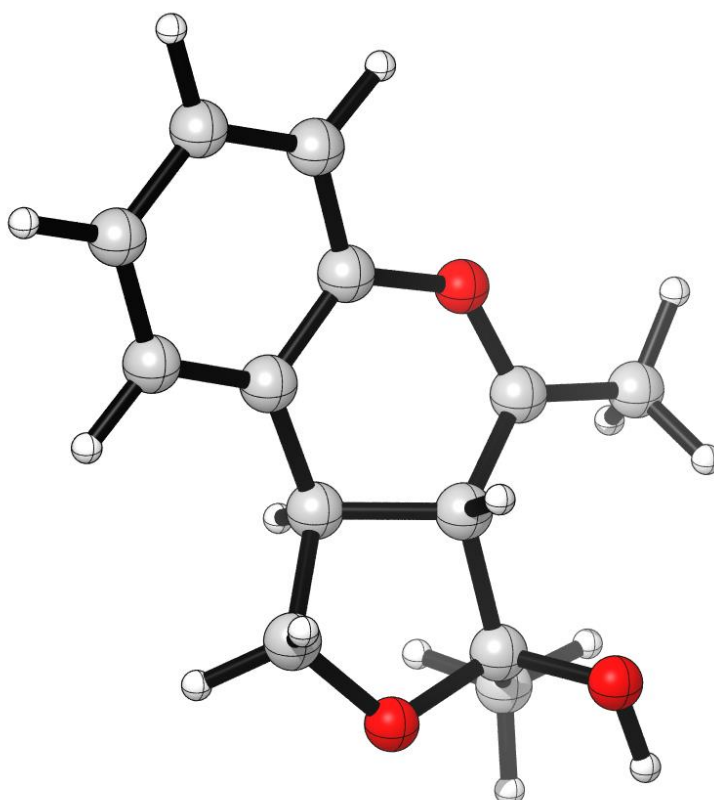


SPE = -728.9408; H₂₉₈ = -728.6696

6	-0.286801000	-2.060290000	-3.948021000
6	-1.241607000	-2.922541000	-3.394824000
6	0.642955000	-1.419013000	-3.124010000
1	-1.960616000	-3.424313000	-4.046083000
1	1.407567000	-0.748995000	-3.521660000
6	-1.287259000	-3.151495000	-2.012041000
6	0.561480000	-1.658822000	-1.758073000
1	-2.034400000	-3.829676000	-1.592583000
6	-0.384236000	-2.506698000	-1.162751000
1	-0.261894000	-1.882508000	-5.025695000
6	-0.291972000	-2.639551000	0.329611000
6	0.134341000	-1.278043000	0.910914000

6	1.418944000	-0.855464000	0.310871000
6	-1.521120000	-2.926272000	1.193663000
1	-2.430245000	-2.482919000	0.752775000
1	-1.692226000	-4.000183000	1.356809000
6	-0.072970000	-1.481209000	2.421831000
8	-1.247043000	-2.291092000	2.454032000
6	-0.345288000	-0.235224000	3.248756000
1	-0.649845000	-0.540382000	4.262489000
1	0.555429000	0.390650000	3.326440000
1	-1.161340000	0.353445000	2.805500000
6	2.542975000	-0.231432000	1.011206000
1	2.874489000	-0.928966000	1.800381000
1	3.358201000	0.028315000	0.326378000
1	2.172839000	0.662677000	1.543825000
1	0.491591000	-3.377270000	0.577539000
8	1.544493000	-1.028155000	-0.952541000
8	1.047640000	-2.192715000	2.880672000
1	0.958111000	-2.344347000	3.834894000
1	-0.590156000	-0.515002000	0.555518000

II2_i4



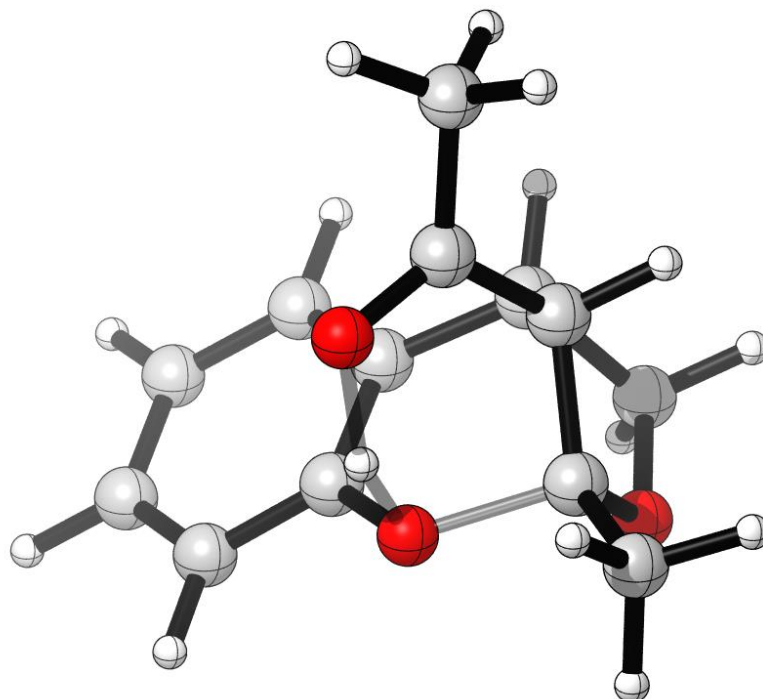
SPE = -728.9359; H₂₉₈ = -728.6646

6	1.282527000	0.878326000	-3.427500000
6	0.583288000	-0.322927000	-3.596181000
6	1.714096000	1.267383000	-2.155536000
1	0.247171000	-0.626451000	-4.590558000
1	2.263101000	2.195585000	-1.987838000
6	0.305433000	-1.148229000	-2.499193000
6	1.412377000	0.430967000	-1.087109000
1	-0.232142000	-2.087954000	-2.644204000
6	0.712876000	-0.776779000	-1.214925000
1	1.497908000	1.516589000	-4.286907000
6	0.511907000	-1.572856000	0.040517000
6	0.381034000	-0.616654000	1.227770000

6	1.467536000	0.376435000	1.296287000
6	-0.752523000	-2.402082000	0.265090000
1	-1.640357000	-1.879624000	-0.136206000
1	-0.703974000	-3.408973000	-0.172206000
6	-0.090573000	-1.516126000	2.389801000
8	-0.832267000	-2.530208000	1.688800000
6	0.980023000	-2.219062000	3.218083000
1	0.476270000	-2.966025000	3.852594000
1	1.697265000	-2.754238000	2.578573000
1	1.523863000	-1.520098000	3.869715000
6	2.051132000	0.936811000	2.521090000
1	2.800921000	0.216596000	2.900685000
1	2.550535000	1.893903000	2.325323000
1	1.270868000	1.024277000	3.292523000
1	1.393331000	-2.221893000	0.196642000
8	1.887666000	0.853281000	0.183355000
8	-0.936200000	-0.743129000	3.184968000
1	-1.163342000	-1.242811000	3.985243000
1	-0.491973000	0.047598000	1.021276000

To Figure S11

TS1-syn

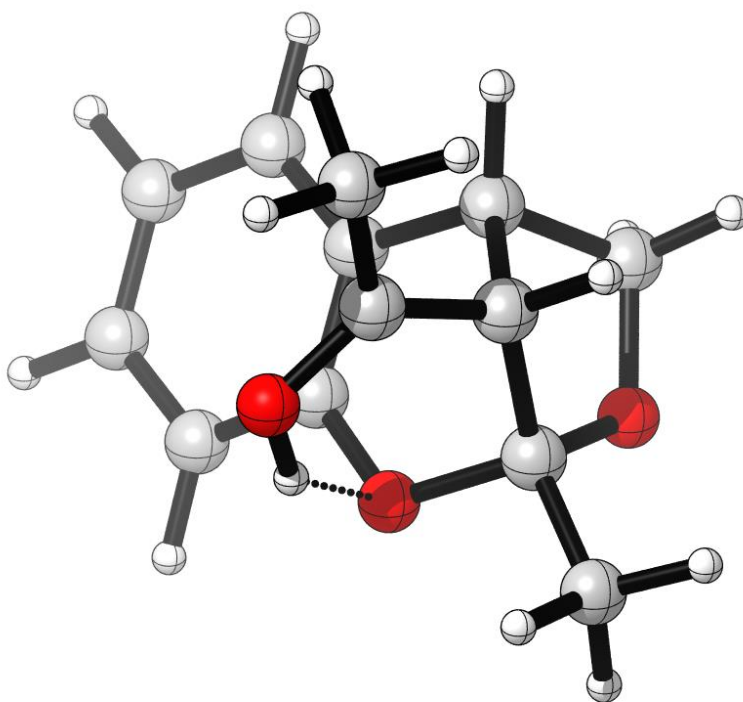


SPE = -728.9429; H₂₉₈ = -728.6754

6	0.405137000	2.155071000	5.495331000
1	-0.139577000	3.035088000	5.131760000
6	0.748361000	2.256036000	6.967656000
6	1.739823000	1.416388000	7.492817000
6	2.060742000	1.373264000	8.844094000
1	2.850694000	0.707175000	9.196628000
6	1.357465000	2.211561000	9.715976000
1	1.600949000	2.201938000	10.781263000
6	0.360625000	3.063467000	9.226357000
1	-0.182097000	3.718751000	9.911131000
6	0.052611000	3.080026000	7.861149000

1	-0.730804000	3.740840000	7.479540000
6	1.672781000	1.816521000	4.646759000
6	-0.369565000	0.849403000	5.265521000
1	-1.115679000	0.636014000	6.040233000
1	-0.838742000	0.805769000	4.270727000
6	1.889076000	0.379815000	5.155885000
8	0.667747000	-0.169210000	5.338642000
6	2.864518000	-0.545841000	4.486760000
1	2.499627000	-0.752079000	3.470025000
1	3.867519000	-0.102857000	4.422164000
1	2.916157000	-1.489982000	5.045756000
8	2.543321000	0.652409000	6.596974000
1	1.388858000	1.794480000	3.583524000
6	2.862902000	2.741920000	4.810559000
8	3.746914000	2.467754000	5.638063000
6	2.958842000	3.955525000	3.964808000
1	1.971600000	4.422824000	3.828626000
1	3.684744000	4.665226000	4.381333000
1	3.300163000	3.633748000	2.963156000
1	3.334532000	1.396365000	6.270653000

syn-**3a**-H⁺

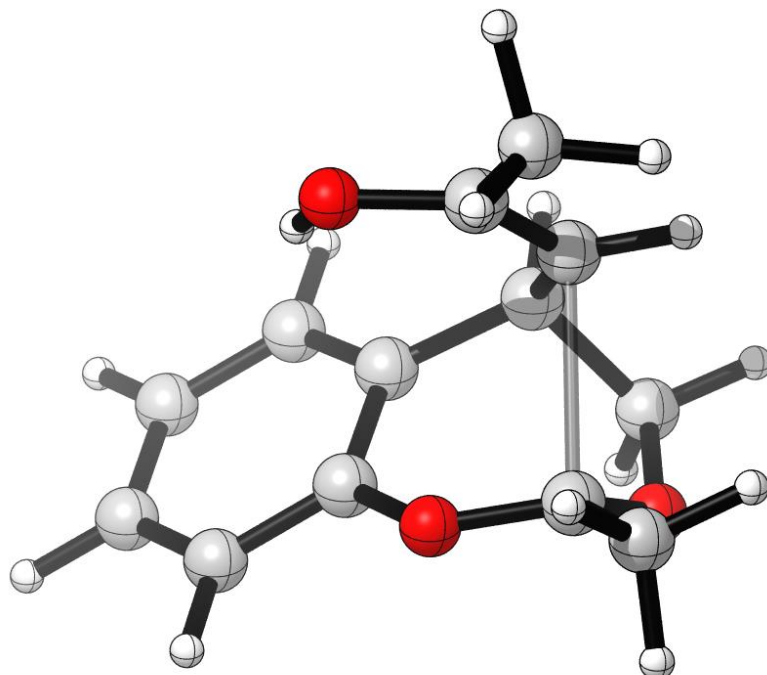


SPE = -728.9484; H₂₉₈ = -728.6779

6	0.402062000	2.111869000	5.453606000
1	-0.114782000	2.998304000	5.065649000
6	0.723844000	2.215685000	6.927514000
6	1.694552000	1.346347000	7.454485000
6	2.027277000	1.352580000	8.808652000
1	2.794395000	0.667832000	9.176650000
6	1.374548000	2.250562000	9.658326000
1	1.638539000	2.271354000	10.718782000
6	0.403574000	3.126631000	9.157100000
1	-0.098207000	3.829821000	9.825336000
6	0.078116000	3.103916000	7.796878000
1	-0.676237000	3.787775000	7.397033000

6	1.710802000	1.756994000	4.662072000
6	-0.364431000	0.809815000	5.180786000
1	-1.152289000	0.619344000	5.921504000
1	-0.798890000	0.790824000	4.167804000
6	1.916782000	0.332559000	5.243434000
8	0.644801000	-0.215747000	5.294888000
6	2.875762000	-0.600092000	4.540914000
1	2.509416000	-0.793702000	3.523290000
1	3.888877000	-0.177422000	4.483993000
1	2.916863000	-1.549658000	5.093080000
8	2.444665000	0.526809000	6.606152000
1	1.467320000	1.712779000	3.590468000
6	2.828366000	2.726321000	4.837999000
8	3.747720000	2.520540000	5.689371000
6	2.878167000	3.985482000	4.082838000
1	2.131415000	4.661834000	4.545848000
1	3.866395000	4.456786000	4.159167000
1	2.562592000	3.837655000	3.039676000
1	3.585950000	1.655038000	6.191803000

TS2-syn

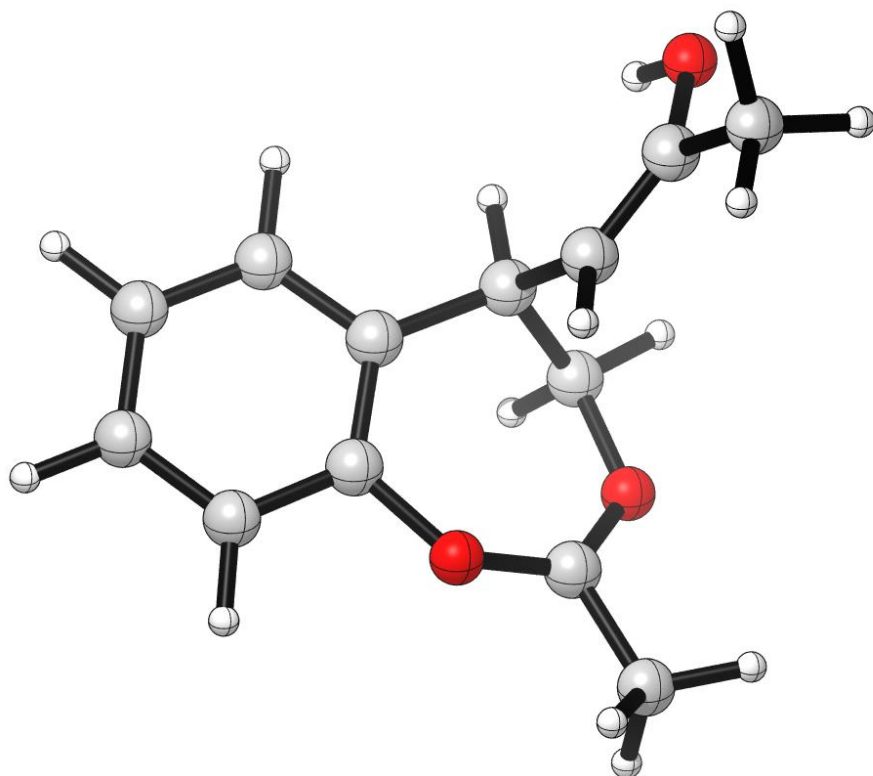


SPE = -728.9242; H₂₉₈ = -728.6544

6	0.937125000	1.395145000	6.000083000
1	0.271899000	2.062011000	6.573448000
6	1.932865000	0.733722000	6.937230000
6	2.915507000	-0.120337000	6.413890000
6	3.817918000	-0.819340000	7.212803000
1	4.577172000	-1.448761000	6.744160000
6	3.719716000	-0.686394000	8.600112000
1	4.411743000	-1.233403000	9.244186000
6	2.741975000	0.146966000	9.159219000
1	2.665555000	0.251396000	10.244373000
6	1.860076000	0.851051000	8.334446000
1	1.097432000	1.499586000	8.772992000

6	1.552564000	2.118665000	4.813186000
6	0.069139000	0.290559000	5.384855000
1	-0.258004000	-0.460298000	6.114454000
1	-0.797495000	0.690811000	4.839980000
6	2.130218000	-0.021479000	4.146574000
8	0.889452000	-0.373619000	4.376121000
6	2.584068000	-0.032574000	2.730862000
1	1.832092000	0.437889000	2.086039000
1	3.558701000	0.459377000	2.627539000
1	2.694739000	-1.087201000	2.421211000
8	3.092058000	-0.226805000	5.031335000
1	0.859841000	2.331196000	3.994987000
6	2.748158000	2.798025000	4.737612000
8	3.678454000	2.814507000	5.685955000
6	3.162589000	3.553487000	3.518466000
1	3.302713000	4.617120000	3.775398000
1	4.137493000	3.177685000	3.165926000
1	2.422756000	3.466805000	2.713538000
1	3.374968000	2.378256000	6.503326000

3a-H⁺_i2

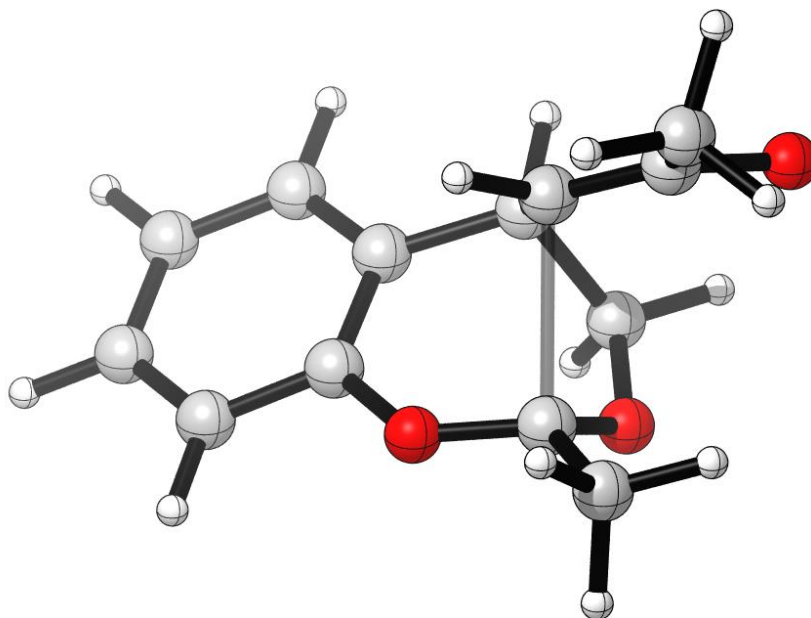


SPE = -728.9340; H₂₉₈ = -728.6624

6	0.262846000	1.829613000	4.573989000
1	-0.501195000	2.150730000	3.845612000
6	0.025067000	2.645668000	5.830341000
6	0.553964000	2.271177000	7.069570000
6	0.351131000	2.992616000	8.245345000
1	0.813357000	2.645197000	9.171101000
6	-0.439763000	4.140630000	8.197706000
1	-0.621879000	4.713120000	9.109950000
6	-0.991620000	4.550818000	6.978603000
1	-1.605515000	5.453082000	6.931084000
6	-0.757183000	3.811767000	5.815943000
1	-1.191299000	4.141109000	4.868273000

6	1.651091000	2.036513000	3.995374000
6	-0.067709000	0.353661000	4.827411000
1	-0.996042000	0.214120000	5.397955000
1	-0.119066000	-0.216857000	3.894646000
6	1.586268000	0.043292000	6.628769000
8	0.992659000	-0.340337000	5.569216000
6	2.565767000	-0.893024000	7.232338000
1	3.034919000	-1.506652000	6.452510000
1	3.309979000	-0.342391000	7.820639000
1	2.004071000	-1.562418000	7.909120000
8	1.405727000	1.151695000	7.251746000
1	2.482075000	2.129809000	4.699089000
6	1.957214000	2.119771000	2.681724000
8	1.064216000	2.047382000	1.662410000
6	3.351933000	2.300640000	2.163526000
1	4.082812000	2.344914000	2.981454000
1	3.612458000	1.464934000	1.492275000
1	3.420791000	3.225205000	1.565618000
1	0.156890000	1.940476000	1.985857000

TS2-*anti*

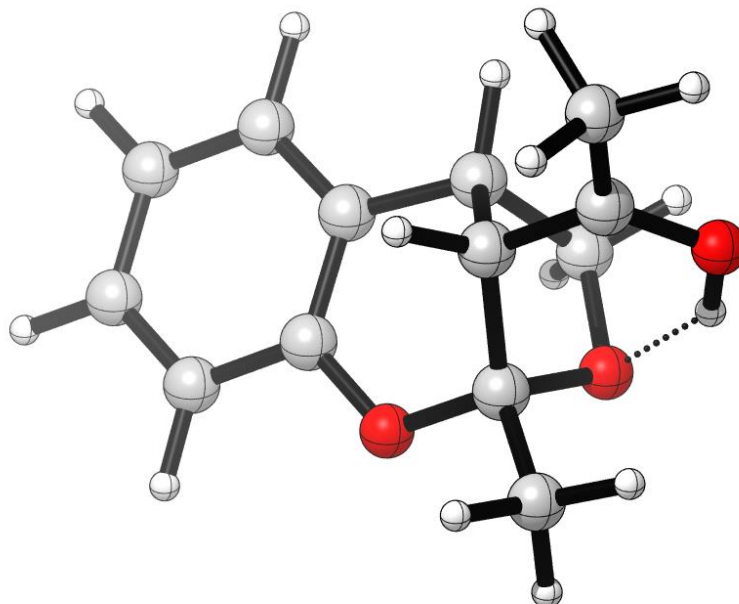


SPE = -728.9207; H₂₉₈ = -728.6508

6	0.075826000	2.155326000	4.557835000
1	-0.483251000	2.659751000	3.753985000
6	-0.143239000	2.875570000	5.872060000
6	0.541018000	2.413205000	7.003661000
6	0.373289000	2.972368000	8.269134000
1	0.946392000	2.578794000	9.111052000
6	-0.530902000	4.027455000	8.414693000
1	-0.685987000	4.475925000	9.398784000
6	-1.228479000	4.516560000	7.302726000
1	-1.922835000	5.351928000	7.419692000
6	-1.034344000	3.942973000	6.042112000
1	-1.578074000	4.325462000	5.174502000

6	1.573244000	2.091138000	4.275201000
6	-0.490126000	0.724801000	4.723807000
1	-1.404790000	0.715802000	5.329989000
1	-0.709424000	0.199362000	3.782646000
6	1.587481000	0.520134000	5.909453000
8	0.530142000	-0.061129000	5.385431000
6	2.834313000	-0.292728000	5.947498000
1	2.958509000	-0.852150000	5.012342000
1	3.702548000	0.347081000	6.149161000
1	2.740779000	-1.018537000	6.774778000
8	1.502467000	1.401817000	6.894787000
1	2.196146000	2.839524000	4.768919000
6	2.184204000	1.437399000	3.224108000
8	1.563621000	0.622028000	2.380893000
6	3.642784000	1.547288000	2.935078000
1	4.176227000	2.103190000	3.714781000
1	4.079322000	0.542320000	2.821647000
1	3.777173000	2.064384000	1.969438000
1	0.596748000	0.644469000	2.465495000

anti-**3a**-H⁺

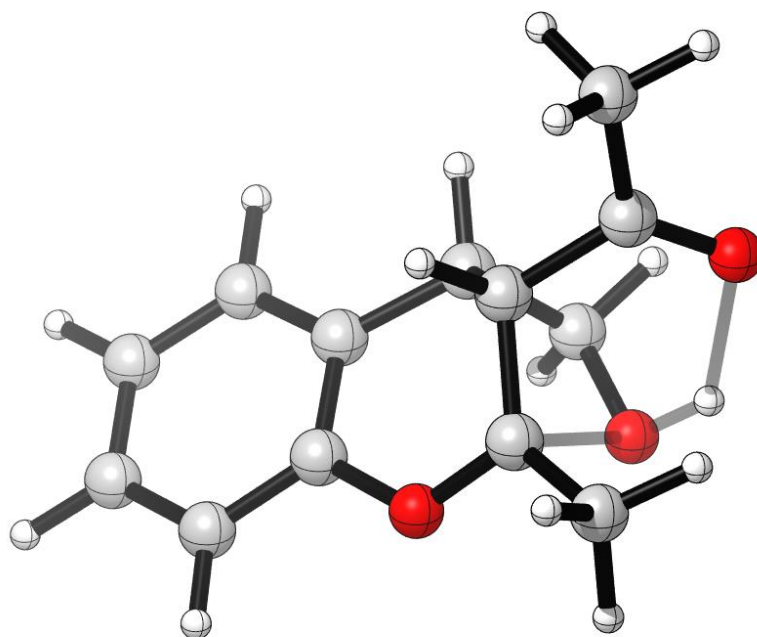


SPE = -728.9471; H₂₉₈ = -728.6752

6	0.259100000	2.152834000	4.573992000
1	0.036522000	2.756699000	3.685358000
6	-0.044471000	2.895139000	5.851379000
6	0.436722000	2.302902000	7.028581000
6	0.194841000	2.868681000	8.281859000
1	0.596385000	2.383257000	9.174043000
6	-0.561853000	4.042128000	8.354959000
1	-0.771107000	4.488956000	9.330471000
6	-1.050527000	4.649495000	7.190802000
1	-1.634448000	5.570263000	7.257622000
6	-0.782667000	4.080715000	5.940617000
1	-1.158871000	4.551921000	5.028743000

6	1.776516000	1.718160000	4.686952000
6	-0.451337000	0.777209000	4.553366000
1	-1.360530000	0.771674000	5.168528000
1	-0.707694000	0.430702000	3.542003000
6	1.576201000	0.593153000	5.743001000
8	0.519623000	-0.155826000	5.113353000
6	2.730720000	-0.335161000	6.055456000
1	3.108319000	-0.855195000	5.165335000
1	3.547056000	0.242466000	6.510236000
1	2.382105000	-1.086237000	6.778194000
8	1.166675000	1.135692000	6.975191000
1	2.403673000	2.551620000	5.023796000
6	2.302042000	1.183170000	3.402101000
8	1.959875000	0.024793000	3.000081000
6	3.208281000	1.968845000	2.557743000
1	4.124243000	2.179514000	3.139255000
1	3.452805000	1.449319000	1.624424000
1	2.751958000	2.954277000	2.358481000
1	1.360625000	-0.419655000	3.689765000

TS1-anti

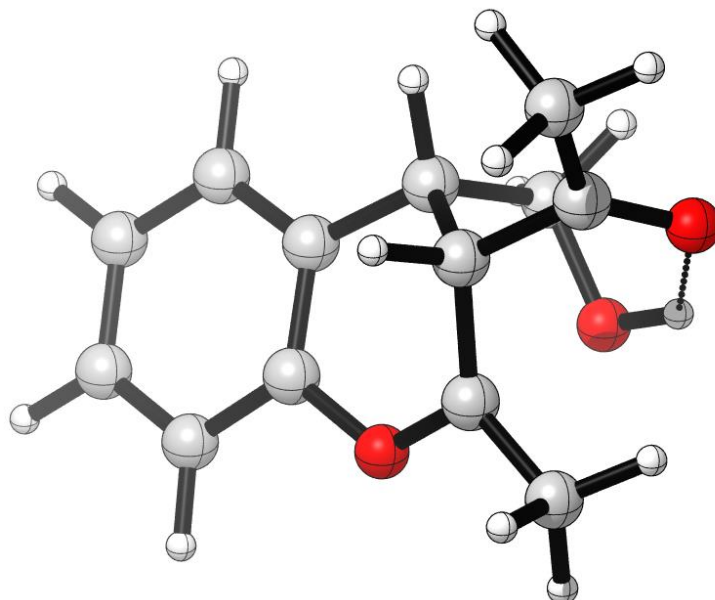


SPE = -728.9424; H₂₉₈ = -728.6721

6	0.327424000	2.166777000	4.565113000
1	0.184774000	2.845150000	3.712886000
6	-0.020938000	2.877044000	5.859501000
6	0.510136000	2.355721000	7.041200000
6	0.259409000	2.888625000	8.299311000
1	0.715150000	2.435997000	9.182178000
6	-0.579815000	4.005882000	8.379459000
1	-0.801440000	4.448203000	9.353488000
6	-1.131938000	4.556268000	7.217466000
1	-1.780904000	5.432306000	7.286392000
6	-0.851181000	3.997546000	5.963014000
1	-1.280794000	4.435310000	5.058531000

6	1.813713000	1.714051000	4.683549000
6	-0.489020000	0.865869000	4.376496000
1	-1.475794000	0.940634000	4.851688000
1	-0.618901000	0.622361000	3.313653000
6	1.839157000	0.780380000	5.870089000
8	0.231636000	-0.205466000	5.026863000
6	2.807193000	-0.326490000	6.061733000
1	3.009619000	-0.880704000	5.139682000
1	3.749992000	0.140516000	6.401438000
1	2.456276000	-0.997747000	6.856711000
8	1.329214000	1.212289000	6.986420000
1	2.428816000	2.588839000	4.956444000
6	2.345175000	1.099754000	3.376590000
8	2.005320000	-0.022439000	3.035780000
6	3.243788000	1.962028000	2.549035000
1	4.139591000	2.231412000	3.133260000
1	3.533144000	1.443773000	1.626445000
1	2.731187000	2.909208000	2.308732000
1	0.740791000	-0.651581000	4.312539000

3a-H⁺_i3



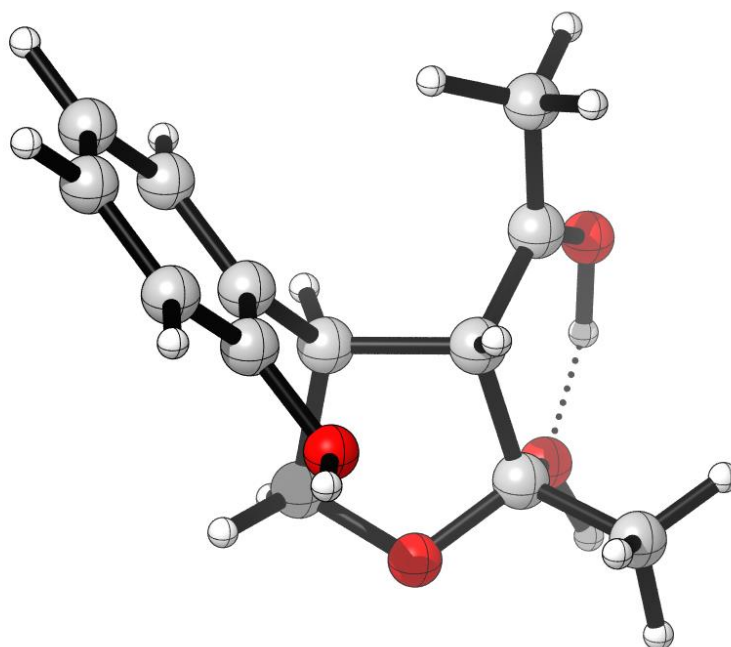
SPE = -728.9425; H₂₉₈ = -728.6723

6	0.414967000	2.121951000	4.417618000
1	0.301811000	2.832183000	3.586104000
6	0.167543000	2.837940000	5.732028000
6	0.755440000	2.321697000	6.887670000
6	0.563189000	2.845239000	8.160452000
1	1.058904000	2.387228000	9.018568000
6	-0.275131000	3.957854000	8.285361000
1	-0.454136000	4.394596000	9.270456000
6	-0.881066000	4.509762000	7.150805000
1	-1.528538000	5.383610000	7.252903000
6	-0.660565000	3.955172000	5.882737000
1	-1.137708000	4.392633000	5.002466000

6	1.867909000	1.562010000	4.448465000
6	-0.540282000	0.920604000	4.228612000
1	-1.528312000	1.157067000	4.650097000
1	-0.665114000	0.688596000	3.161159000
6	2.003134000	0.711654000	5.680149000
8	-0.011321000	-0.212433000	4.926158000
6	2.883165000	-0.465247000	5.815295000
1	2.905118000	-1.081912000	4.911247000
1	3.904424000	-0.067454000	5.980811000
1	2.603564000	-1.052121000	6.700086000
8	1.568646000	1.174610000	6.798175000
1	2.554332000	2.413196000	4.616233000
6	2.244022000	0.859784000	3.126600000
8	1.843464000	-0.265407000	2.885768000
6	3.065768000	1.657907000	2.163244000
1	4.026501000	1.934495000	2.629385000
1	3.239538000	1.086239000	1.243196000
1	2.548539000	2.603961000	1.929397000
1	0.439130000	-0.761003000	4.255692000

To Figure S12

I1_i1

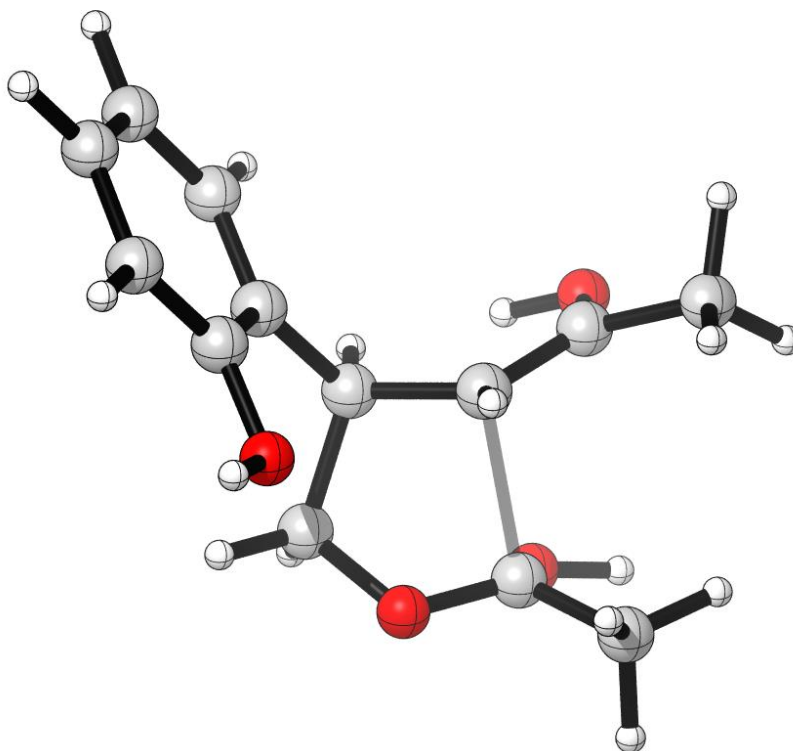


SPE = -805.3044; H₂₉₈ = -805.0051

6	2.853290000	0.327822000	3.181352000
1	3.829674000	0.830577000	3.206490000
6	2.085862000	0.881103000	2.001354000
6	0.796039000	0.398579000	1.677391000
6	0.109414000	0.891304000	0.559985000
1	-0.880193000	0.488892000	0.321824000
6	0.690408000	1.878280000	-0.241707000
1	0.143797000	2.257579000	-1.109155000
6	1.959409000	2.377610000	0.067471000
1	2.418279000	3.148539000	-0.555872000
6	2.642627000	1.874025000	1.180229000

1	3.639629000	2.254800000	1.418990000
6	2.130168000	0.524264000	4.583349000
6	3.098043000	-1.214403000	3.161693000
1	2.697738000	-1.688084000	2.256868000
1	4.176508000	-1.428161000	3.232045000
6	2.313906000	-0.844834000	5.300874000
8	2.411981000	-1.772960000	4.279244000
6	1.196721000	-1.246799000	6.243078000
1	1.420091000	-2.233128000	6.679441000
1	1.082460000	-0.514678000	7.054891000
1	0.254338000	-1.319512000	5.682899000
8	0.269988000	-0.550636000	2.492648000
1	-0.610633000	-0.815178000	2.184560000
6	2.656568000	1.744512000	5.265469000
8	3.541615000	1.662958000	6.163814000
6	2.186662000	3.087041000	4.877091000
1	2.235731000	3.192901000	3.779280000
1	1.119776000	3.173286000	5.148975000
1	2.769735000	3.869353000	5.376401000
1	1.058783000	0.669114000	4.395168000
8	3.574125000	-0.750194000	6.007722000
1	3.687336000	-1.485733000	6.633860000
1	3.757536000	0.649522000	6.325420000

TS4_i1

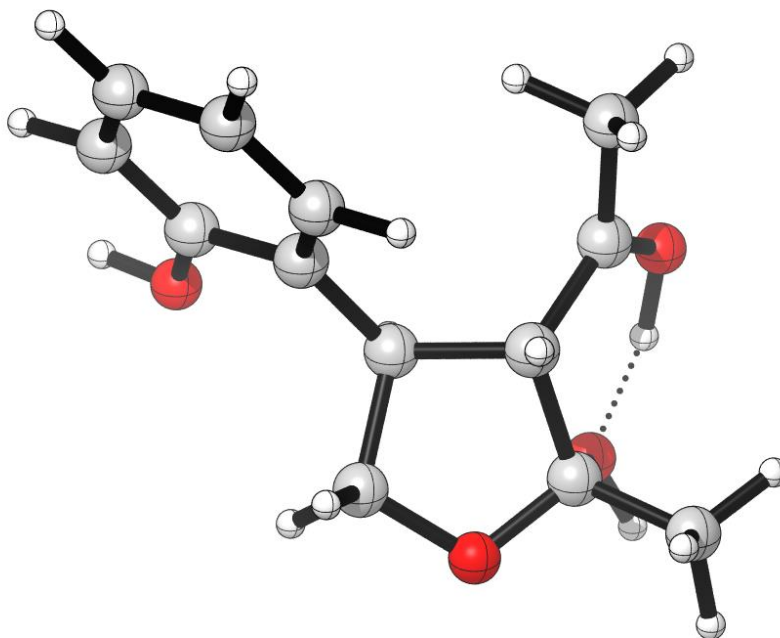


SPE = -805.2760; H₂₉₈ = -804.9768

6	2.729638000	0.263451000	3.061010000
1	3.777613000	0.600656000	3.035036000
6	2.102621000	0.756762000	1.764116000
6	0.803227000	0.358504000	1.379492000
6	0.236059000	0.833503000	0.188521000
1	-0.765192000	0.496405000	-0.096986000
6	0.949217000	1.718801000	-0.624826000
1	0.494890000	2.088493000	-1.547728000
6	2.233782000	2.130005000	-0.256051000
1	2.799462000	2.818398000	-0.888534000
6	2.797506000	1.642283000	0.927682000
1	3.803229000	1.961293000	1.215231000

6	2.038415000	0.846135000	4.288608000
6	2.761789000	-1.298157000	3.206026000
1	2.245761000	-1.817048000	2.394424000
1	3.793975000	-1.664809000	3.284839000
6	2.338421000	-0.892075000	5.452394000
8	2.034548000	-1.630510000	4.400016000
6	1.341698000	-0.911280000	6.566312000
1	1.385621000	-1.905505000	7.044108000
1	1.575656000	-0.154992000	7.328043000
1	0.328800000	-0.753855000	6.174684000
8	0.142801000	-0.493362000	2.208218000
1	-0.734251000	-0.700982000	1.850506000
6	2.609867000	1.816970000	5.103883000
8	3.904796000	2.056920000	5.147398000
6	1.832890000	2.619995000	6.085414000
1	1.902808000	3.684742000	5.801875000
1	0.776977000	2.325316000	6.107575000
1	2.278883000	2.527171000	7.089525000
1	0.946685000	0.845748000	4.266734000
8	3.641355000	-0.853542000	5.738545000
1	3.804525000	-0.528696000	6.640634000
1	4.403339000	1.531020000	4.496421000

I1_i2

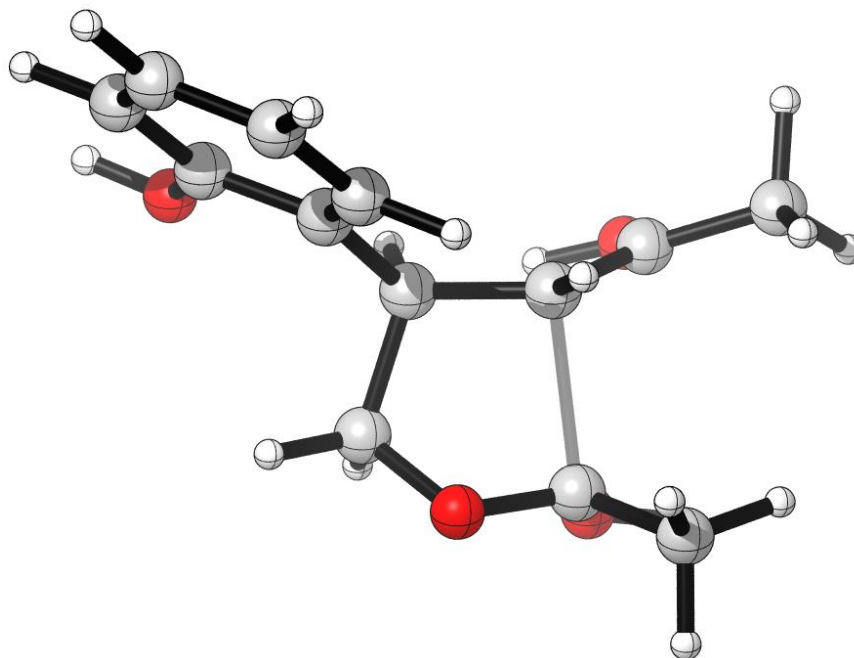


SPE = -805.3017; H₂₉₈ = -805.0038

6	2.383520000	0.205093000	3.390259000
1	3.245275000	-0.460355000	3.237894000
6	1.894215000	0.665970000	2.034219000
6	1.999798000	-0.235439000	0.948034000
6	1.563525000	0.138277000	-0.331241000
1	1.673714000	-0.570135000	-1.158261000
6	0.992953000	1.396108000	-0.540741000
1	0.650549000	1.677124000	-1.540345000
6	0.847927000	2.286153000	0.527491000
1	0.387248000	3.264479000	0.373736000
6	1.294989000	1.912861000	1.799766000
1	1.169787000	2.618534000	2.625006000

6	2.799271000	1.274287000	4.458723000
6	1.322898000	-0.568556000	4.203864000
1	0.321932000	-0.129480000	4.062929000
1	1.292386000	-1.631171000	3.922248000
6	2.760853000	0.416841000	5.755587000
8	1.683220000	-0.438794000	5.586734000
6	2.639977000	1.173529000	7.063999000
1	2.597353000	0.452546000	7.895925000
1	3.501671000	1.839654000	7.218081000
1	1.718146000	1.771977000	7.073327000
8	2.522959000	-1.463562000	1.197475000
1	2.571203000	-1.979529000	0.378135000
6	4.101058000	1.964777000	4.186706000
8	5.172637000	1.506561000	4.670854000
6	4.176826000	3.167257000	3.340374000
1	3.945605000	2.853775000	2.303807000
1	3.397491000	3.889184000	3.626401000
1	5.176420000	3.617399000	3.376371000
1	2.015747000	2.042867000	4.527619000
8	4.002158000	-0.342470000	5.731076000
1	4.166774000	-0.766844000	6.591233000
1	4.948583000	0.633716000	5.216700000

TS4_i2

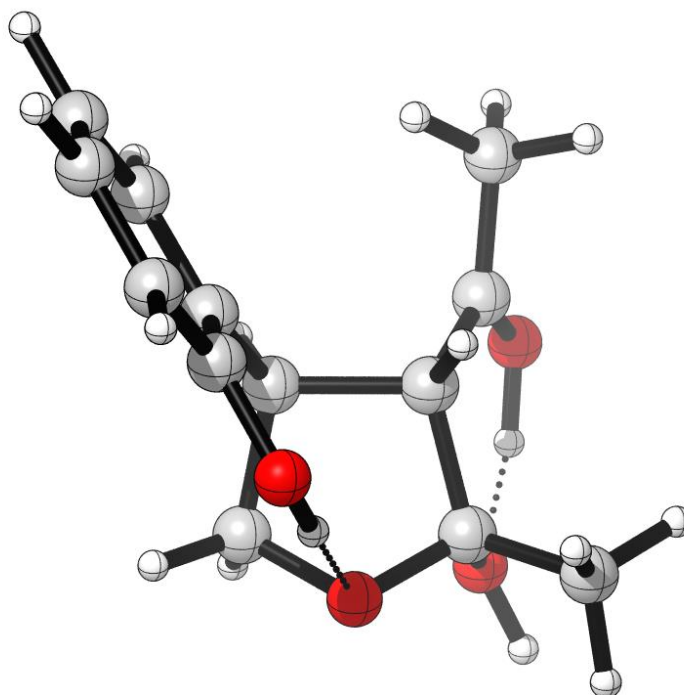


SPE = -805.2736; H₂₉₈ = -804.9760

6	2.718278000	0.238870000	3.076465000
1	3.604587000	-0.288515000	2.691059000
6	1.865055000	0.599279000	1.860527000
6	1.846445000	-0.313575000	0.779019000
6	1.066821000	-0.062608000	-0.359241000
1	1.085231000	-0.777404000	-1.188875000
6	0.276220000	1.088890000	-0.427118000
1	-0.325194000	1.282371000	-1.319599000
6	0.258781000	1.988009000	0.642839000
1	-0.358158000	2.888882000	0.600193000
6	1.048229000	1.735350000	1.772027000
1	1.010471000	2.450087000	2.597517000

6	3.142497000	1.436120000	3.918459000
6	1.967102000	-0.778850000	4.006108000
1	1.078126000	-1.210997000	3.535802000
1	2.630180000	-1.584153000	4.349512000
6	2.475605000	0.637422000	5.753110000
8	1.503912000	-0.012632000	5.126115000
6	2.033862000	1.761139000	6.635246000
1	1.542769000	1.318515000	7.518912000
1	2.889005000	2.359826000	6.978094000
1	1.312786000	2.401016000	6.113085000
8	2.601146000	-1.438878000	0.900061000
1	2.515163000	-1.984725000	0.103483000
6	4.470610000	1.743277000	4.222875000
8	5.436734000	0.854128000	4.224338000
6	4.914713000	3.094332000	4.665196000
1	5.496591000	3.544883000	3.840702000
1	4.067874000	3.753468000	4.889994000
1	5.590903000	3.020668000	5.530860000
1	2.504854000	2.319274000	3.869433000
8	3.471333000	-0.154573000	6.160373000
1	4.042803000	0.284800000	6.812588000
1	5.153337000	-0.011064000	3.874829000

I1_i3

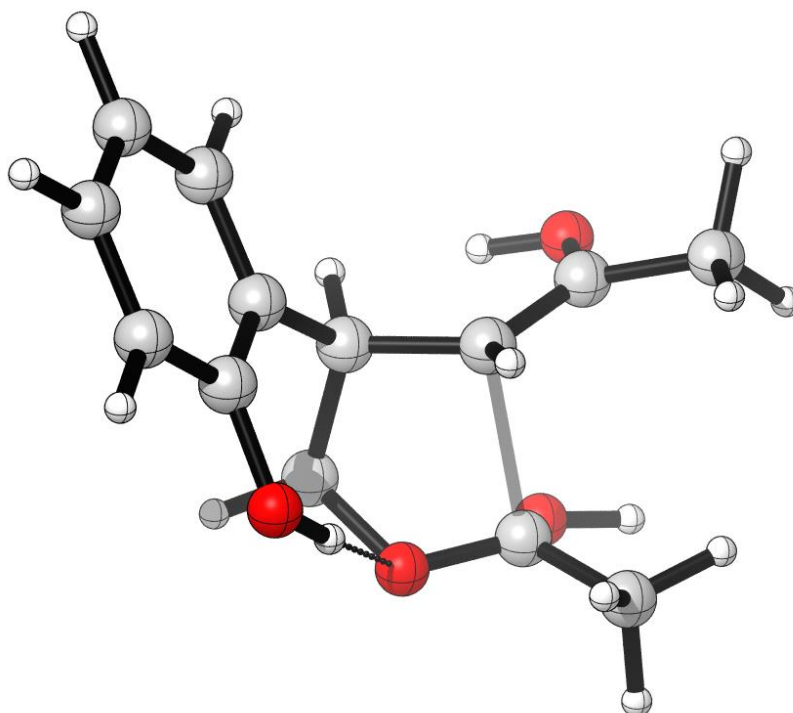


SPE = -805.3020; H₂₉₈ = -805.0021

6	2.914663000	0.408100000	3.162484000
1	3.851866000	0.978216000	3.118216000
6	2.056706000	0.830535000	1.989082000
6	0.858175000	0.162528000	1.628103000
6	0.117227000	0.618015000	0.524452000
1	-0.797846000	0.080372000	0.263744000
6	0.540511000	1.720266000	-0.218263000
1	-0.054829000	2.056589000	-1.071432000
6	1.722021000	2.388076000	0.124655000
1	2.066742000	3.247999000	-0.454201000
6	2.461057000	1.936100000	1.218991000
1	3.389528000	2.446560000	1.491376000

6	2.196402000	0.633009000	4.579065000
6	3.249453000	-1.103568000	3.233207000
1	3.143618000	-1.616773000	2.269422000
1	4.260787000	-1.270956000	3.628951000
6	2.199726000	-0.778969000	5.241880000
8	2.278571000	-1.653540000	4.137545000
6	0.975632000	-1.109870000	6.068456000
1	1.058666000	-2.133087000	6.466064000
1	0.879635000	-0.406744000	6.907507000
1	0.072793000	-1.048308000	5.444488000
8	0.351634000	-0.912328000	2.288774000
1	0.949273000	-1.274402000	2.972799000
6	2.849315000	1.755019000	5.312773000
8	3.740087000	1.540246000	6.184036000
6	2.481569000	3.153400000	5.034929000
1	2.201108000	3.297246000	3.981081000
1	1.571709000	3.359263000	5.631451000
1	3.272360000	3.843741000	5.355164000
1	1.156826000	0.929465000	4.387613000
8	3.402763000	-0.875336000	6.003832000
1	3.386618000	-1.630700000	6.616650000
1	3.834559000	0.520681000	6.328601000

TS4_i3

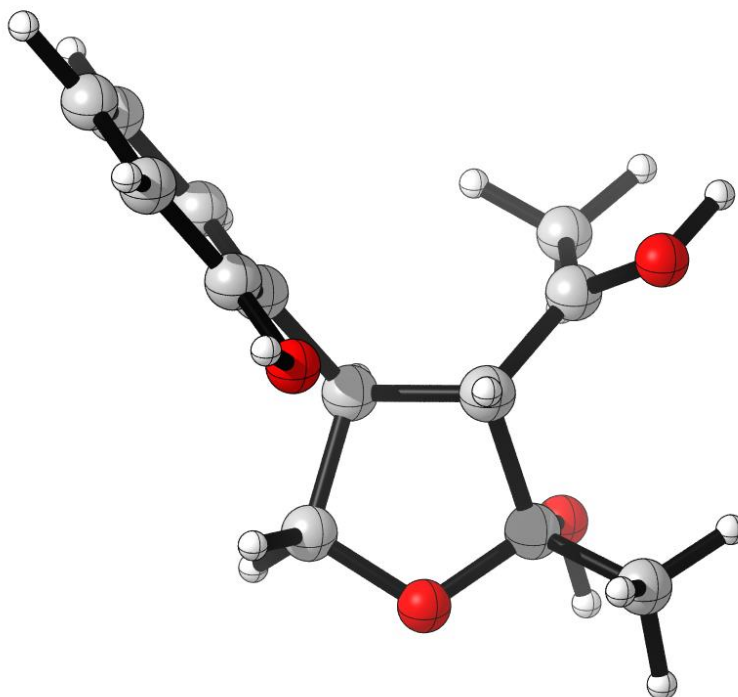


SPE = -805.2711; H₂₉₈ = -804.9729

6	2.848842000	0.405232000	3.019259000
1	3.853119000	0.836002000	2.879847000
6	2.066845000	0.750277000	1.756799000
6	0.828859000	0.149641000	1.431723000
6	0.159007000	0.517532000	0.253199000
1	-0.787055000	0.019817000	0.026280000
6	0.687797000	1.489770000	-0.593612000
1	0.147664000	1.766350000	-1.502788000
6	1.904568000	2.106676000	-0.278293000
1	2.329377000	2.869202000	-0.935196000
6	2.576041000	1.728692000	0.885086000
1	3.530482000	2.201508000	1.133058000

6	2.198262000	1.009139000	4.263629000
6	3.045598000	-1.128056000	3.252476000
1	2.838633000	-1.740303000	2.368862000
1	4.047699000	-1.359244000	3.632484000
6	2.206493000	-0.841604000	5.393564000
8	2.058567000	-1.499216000	4.245142000
6	1.030657000	-0.815471000	6.309706000
1	0.951463000	-1.808567000	6.785510000
1	1.168897000	-0.070600000	7.106161000
1	0.106652000	-0.608674000	5.756986000
8	0.209434000	-0.791478000	2.194213000
1	0.703555000	-1.048167000	2.988853000
6	2.867187000	1.831021000	5.162316000
8	4.179439000	1.890849000	5.247237000
6	2.172114000	2.641518000	6.197579000
1	2.457731000	3.700341000	6.072858000
1	1.081532000	2.549985000	6.124494000
1	2.513686000	2.339231000	7.202502000
1	1.118838000	1.175100000	4.217611000
8	3.431357000	-0.923189000	5.888678000
1	3.476371000	-0.637329000	6.817998000
1	4.629210000	1.384855000	4.547273000

I1_i4

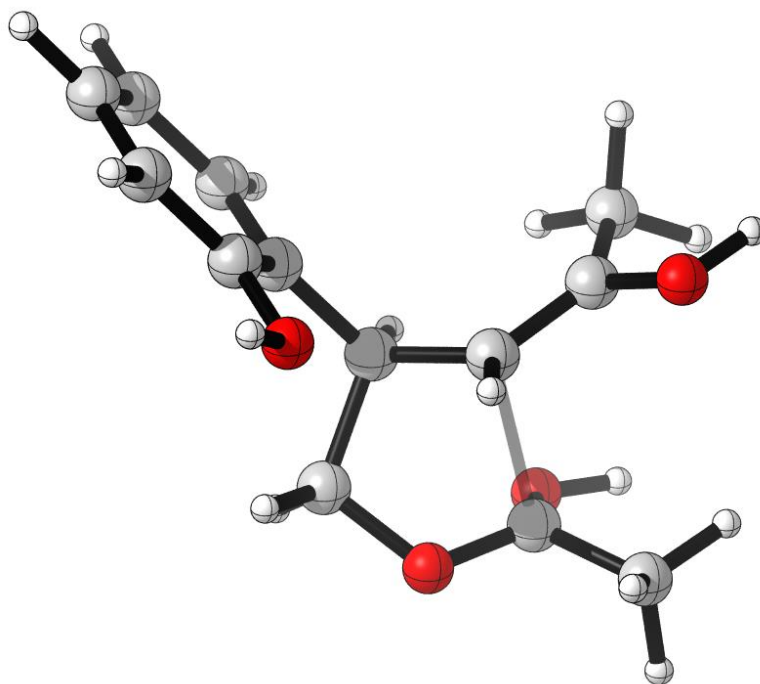


SPE = -805.2930; H₂₉₈ = -804.9939

6	1.005583000	0.395088000	3.297781000
1	1.253324000	1.209838000	2.605004000
6	-0.454370000	0.532483000	3.676710000
6	-1.071668000	-0.337760000	4.605960000
6	-2.424696000	-0.182084000	4.936134000
1	-2.879351000	-0.869079000	5.656901000
6	-3.179428000	0.835910000	4.346403000
1	-4.230682000	0.953468000	4.623171000
6	-2.592484000	1.699069000	3.416150000
1	-3.179969000	2.490206000	2.944987000
6	-1.241570000	1.536564000	3.090684000
1	-0.778127000	2.206262000	2.359893000

6	2.024108000	0.439930000	4.467157000
6	1.393103000	-0.938621000	2.609752000
1	0.753817000	-1.769439000	2.939784000
1	1.327621000	-0.852440000	1.513653000
6	3.295581000	-0.206456000	3.784782000
8	2.738295000	-1.231733000	3.007833000
6	4.310542000	-0.809710000	4.739808000
1	5.110540000	-1.287062000	4.151683000
1	4.761677000	-0.034826000	5.376438000
1	3.841102000	-1.575493000	5.372701000
8	-0.307655000	-1.314660000	5.163079000
1	-0.837988000	-1.856385000	5.767870000
6	2.309631000	1.763216000	5.060932000
8	2.646674000	1.732349000	6.292841000
6	2.241766000	3.035942000	4.330978000
1	2.843384000	2.935669000	3.413044000
1	1.199666000	3.201764000	4.002768000
1	2.581435000	3.884656000	4.939411000
1	1.722776000	-0.238797000	5.276044000
8	3.860245000	0.806363000	2.989058000
1	4.629262000	0.441420000	2.522360000
1	2.859346000	2.615243000	6.664115000

TS4_i4

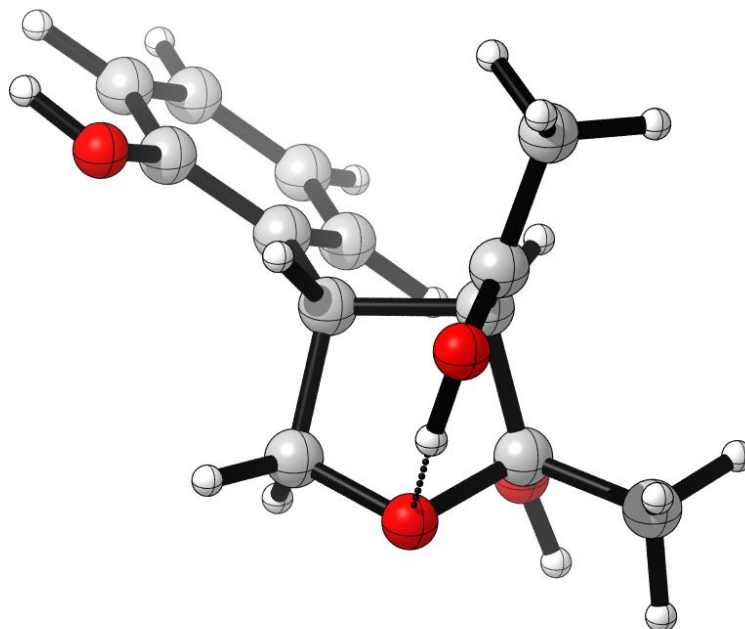


SPE = -805.2740; H₂₉₈ = -804.9765

6	0.942878000	0.368313000	3.474164000
1	1.220490000	1.171743000	2.780600000
6	-0.556005000	0.495066000	3.699823000
6	-1.245701000	-0.310432000	4.633458000
6	-2.628786000	-0.163188000	4.810130000
1	-3.143631000	-0.794569000	5.540740000
6	-3.339453000	0.776379000	4.057490000
1	-4.415924000	0.888345000	4.215457000
6	-2.676108000	1.573264000	3.119062000
1	-3.226615000	2.305002000	2.523185000
6	-1.295696000	1.422497000	2.950757000
1	-0.767259000	2.044029000	2.221760000

6	1.819921000	0.482744000	4.705616000
6	1.317984000	-0.976455000	2.792255000
1	0.706400000	-1.812407000	3.151066000
1	1.253941000	-0.913726000	1.696694000
6	3.456689000	-0.317160000	3.541557000
8	2.670128000	-1.315896000	3.193239000
6	4.566135000	-0.646633000	4.484856000
1	5.349599000	-1.178704000	3.916961000
1	5.008698000	0.261562000	4.917234000
1	4.201937000	-1.299864000	5.286871000
8	-0.522285000	-1.213534000	5.346825000
1	-1.104707000	-1.722695000	5.931713000
6	2.332003000	1.656698000	5.229114000
8	2.848629000	1.574229000	6.448071000
6	2.417699000	2.976950000	4.543612000
1	2.031789000	2.952730000	3.519053000
1	1.833165000	3.715571000	5.117923000
1	3.462072000	3.333795000	4.534773000
1	1.747562000	-0.332901000	5.429147000
8	3.637523000	0.600169000	2.596896000
1	4.378543000	1.195315000	2.805810000
1	3.249875000	2.414656000	6.729957000

I1_i5

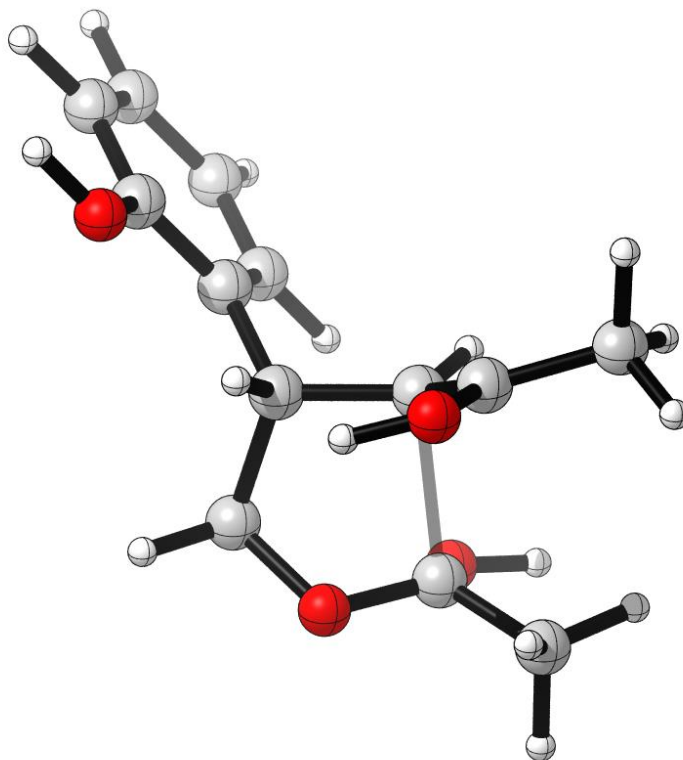


SPE = -805.2911; H₂₉₈ = -804.9921

6	0.959058000	0.418852000	3.451472000
6	2.147069000	0.542865000	4.507202000
6	1.448147000	-0.779023000	2.574207000
1	0.676679000	-1.541760000	2.416366000
1	1.826765000	-0.421891000	1.608026000
6	3.296051000	-0.285776000	3.856923000
8	2.522766000	-1.388835000	3.317430000
6	4.387395000	-0.837195000	4.759633000
1	5.084673000	-1.429203000	4.146023000
1	4.940301000	-0.002494000	5.213526000
1	4.009830000	-1.490869000	5.557178000
8	3.821554000	0.499888000	2.846929000

1	4.622253000	0.081505000	2.490125000
1	0.054162000	0.085168000	3.977695000
6	0.573953000	1.688982000	2.726312000
6	1.506012000	2.623010000	2.244234000
6	-0.801635000	1.950898000	2.521673000
6	1.098812000	3.796097000	1.602047000
6	-1.213345000	3.131350000	1.883248000
6	-0.266447000	4.050630000	1.428203000
1	2.570460000	2.420756000	2.377251000
1	1.843658000	4.508661000	1.240908000
1	-2.282341000	3.322511000	1.745739000
1	-0.602079000	4.966978000	0.934839000
1	2.429949000	1.577274000	4.727696000
6	1.614896000	-0.137308000	5.717063000
8	1.466529000	-1.403302000	5.698022000
6	1.187774000	0.598053000	6.912117000
1	0.517961000	1.420692000	6.607004000
1	0.707669000	-0.055414000	7.650116000
1	2.078267000	1.091265000	7.344492000
1	1.812659000	-1.774860000	4.816104000
8	-1.693520000	1.026492000	2.962773000
1	-2.599167000	1.328004000	2.792988000

TS4_i5

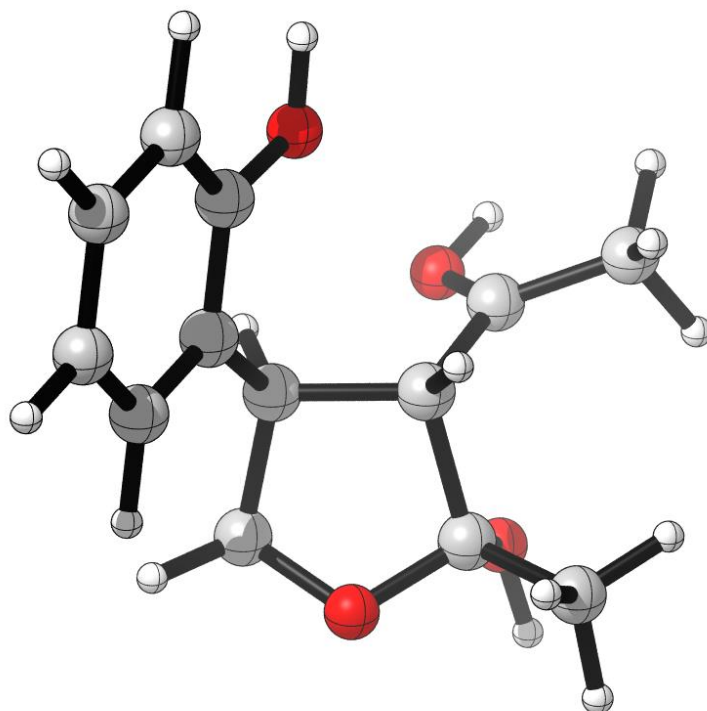


SPE = -805.2772; H₂₉₈ = -804.9795; G₂₉₈ = -805.0378

6	0.979726000	0.394989000	3.234252000
6	1.846645000	0.662072000	4.464324000
6	1.795979000	-0.483837000	2.239061000
1	1.165726000	-1.171992000	1.664863000
1	2.397996000	0.125501000	1.552176000
6	3.423130000	-0.560590000	3.866222000
8	2.649535000	-1.288418000	3.063436000
6	4.060860000	-1.322458000	4.985290000
1	4.834430000	-1.973531000	4.543241000
1	4.545212000	-0.643576000	5.701145000
1	3.326631000	-1.955438000	5.499364000
8	4.161672000	0.354319000	3.229563000

1	4.848521000	0.725746000	3.809301000
1	0.101460000	-0.197637000	3.532020000
6	0.459314000	1.662497000	2.575379000
6	1.335077000	2.659204000	2.116966000
6	-0.927504000	1.852520000	2.394332000
6	0.864453000	3.826079000	1.508003000
6	-1.405161000	3.021594000	1.779083000
6	-0.513960000	4.003365000	1.341333000
1	2.413238000	2.517272000	2.240416000
1	1.567956000	4.587826000	1.164723000
1	-2.483196000	3.153096000	1.642540000
1	-0.902995000	4.907528000	0.865010000
1	2.363376000	1.621918000	4.507489000
6	1.527668000	0.140624000	5.724129000
8	0.754297000	-0.907132000	5.894827000
6	2.075536000	0.678609000	6.998778000
1	1.244361000	1.149851000	7.554028000
1	2.457363000	-0.139698000	7.629494000
1	2.853940000	1.430929000	6.826682000
1	0.375652000	-1.235092000	5.057837000
8	-1.766370000	0.877251000	2.830659000
1	-2.683802000	1.108612000	2.619598000

I1_i6

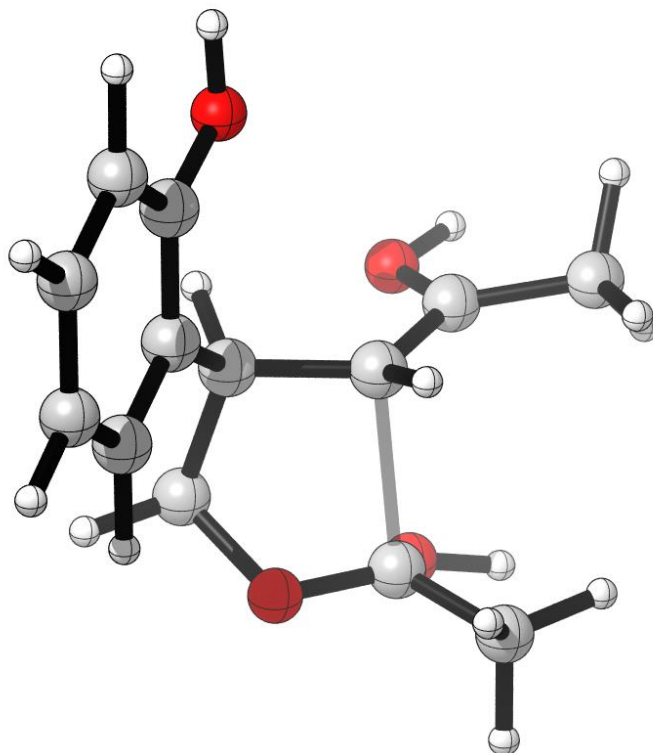


SPE = -805.2916; H₂₉₈ = -804.9920

6	0.050555000	-0.490828000	3.437679000
1	0.101918000	-0.517779000	4.534009000
6	-0.499812000	-1.822618000	2.964227000
6	0.097436000	-2.986596000	3.500637000
6	-0.329213000	-4.261379000	3.110714000
1	0.151185000	-5.142366000	3.547920000
6	-1.357453000	-4.390694000	2.171731000
1	-1.691776000	-5.386018000	1.866657000
6	-1.954039000	-3.251843000	1.621569000
1	-2.756372000	-3.351662000	0.886502000
6	-1.520261000	-1.980605000	2.018570000
1	-1.989036000	-1.099995000	1.575251000

6	1.488075000	-0.272713000	2.857788000
6	-0.688314000	0.787547000	2.992695000
1	-1.737122000	0.635399000	2.710378000
1	-0.639614000	1.542491000	3.794508000
6	1.384053000	1.112548000	2.074012000
8	0.013734000	1.252065000	1.840270000
6	2.100980000	1.150610000	0.737330000
1	1.971459000	2.149733000	0.290076000
1	3.176767000	0.955791000	0.854935000
1	1.670139000	0.406648000	0.053307000
8	1.107107000	-2.795533000	4.395293000
1	1.468364000	-3.646983000	4.687093000
6	2.590436000	-0.243634000	3.843150000
8	2.295945000	0.086993000	5.037254000
6	3.991239000	-0.512086000	3.466772000
1	4.061168000	-1.227210000	2.637889000
1	4.411458000	0.451565000	3.116518000
1	4.590333000	-0.841839000	4.328259000
1	1.731571000	-1.041110000	2.113030000
8	1.869430000	2.081818000	2.973755000
1	1.852037000	2.949891000	2.538875000
1	3.066851000	0.109149000	5.642458000

TS4_i6

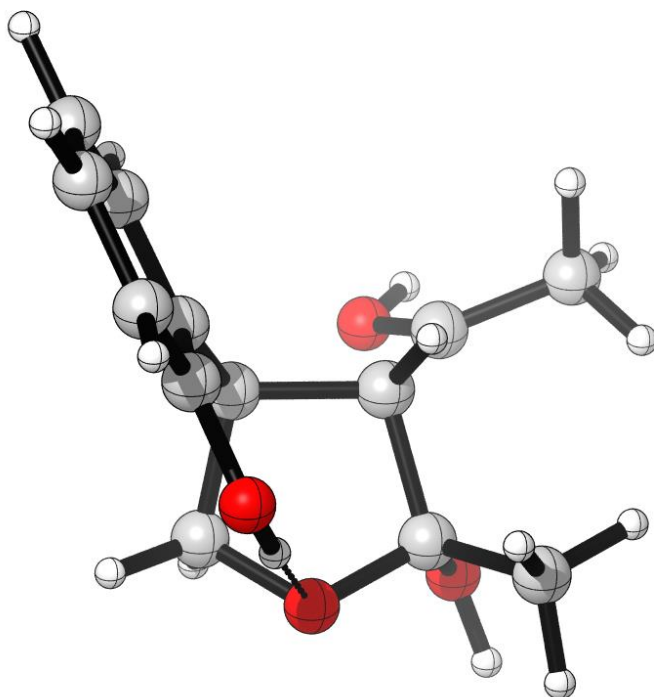


SPE = -805.2765; H₂₉₈ = -804.9799

6	0.188246000	-0.698318000	3.528699000
1	0.237913000	-0.782157000	4.623531000
6	-0.426227000	-1.980368000	2.988225000
6	-0.061748000	-3.202579000	3.598255000
6	-0.589102000	-4.415851000	3.134180000
1	-0.292805000	-5.346328000	3.628791000
6	-1.474250000	-4.428474000	2.051834000
1	-1.881187000	-5.378356000	1.694546000
6	-1.835441000	-3.230425000	1.427931000
1	-2.520512000	-3.233198000	0.576495000
6	-1.306960000	-2.022327000	1.898719000
1	-1.587453000	-1.093837000	1.396478000

6	1.609990000	-0.513187000	2.997321000
6	-0.602629000	0.588742000	3.200376000
1	-1.676737000	0.429494000	3.056428000
1	-0.444313000	1.358180000	3.968626000
6	1.211285000	1.332468000	1.962806000
8	-0.082655000	1.048399000	1.938567000
6	1.915588000	1.260148000	0.643935000
1	1.587572000	2.126112000	0.042058000
1	3.006008000	1.320983000	0.767855000
1	1.648975000	0.340606000	0.108565000
8	0.812645000	-3.143786000	4.637475000
1	0.983087000	-4.034105000	4.980947000
6	2.659625000	-0.143747000	3.831295000
8	2.365449000	0.369123000	5.007538000
6	4.094633000	-0.206691000	3.438967000
1	4.227035000	-0.631807000	2.437179000
1	4.546317000	0.800183000	3.478680000
1	4.643803000	-0.831198000	4.164119000
1	1.896723000	-1.109399000	2.128306000
8	1.541994000	2.300999000	2.817553000
1	2.429477000	2.652540000	2.633735000
1	3.159157000	0.642697000	5.501005000

I1_i7

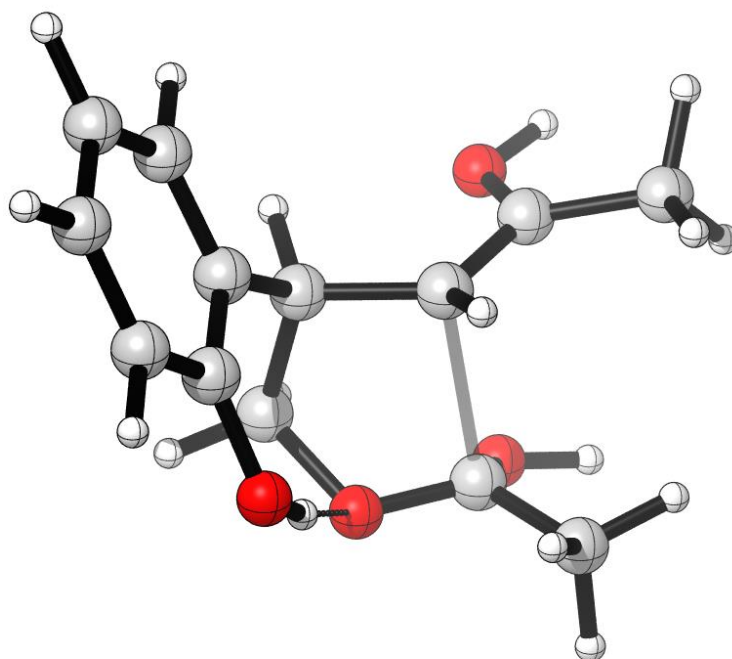


SPE = -805.2920; H₂₉₈ = -804.9912

6	2.975875000	0.506462000	3.030456000
1	3.904940000	1.076509000	2.910483000
6	2.120733000	0.781452000	1.799431000
6	0.954685000	0.048764000	1.458237000
6	0.207695000	0.414324000	0.323407000
1	-0.684989000	-0.172168000	0.091057000
6	0.594356000	1.487453000	-0.476850000
1	-0.005759000	1.754307000	-1.350929000
6	1.748026000	2.215119000	-0.160472000
1	2.068896000	3.053032000	-0.783818000
6	2.489768000	1.853620000	0.964785000
1	3.392020000	2.420125000	1.213019000

6	2.267000000	0.928710000	4.363531000
6	3.325930000	-0.971035000	3.309010000
1	3.339291000	-1.607966000	2.416064000
1	4.286841000	-1.059992000	3.836734000
6	2.045234000	-0.437170000	5.156980000
8	2.263466000	-1.426269000	4.164228000
6	0.655083000	-0.631762000	5.733098000
1	0.597579000	-1.619244000	6.217775000
1	0.436956000	0.136512000	6.487607000
1	-0.104988000	-0.583856000	4.940057000
8	0.480350000	-1.013932000	2.157279000
1	1.049808000	-1.266161000	2.914365000
6	3.023883000	1.867349000	5.234438000
8	4.283662000	1.922939000	5.071398000
6	2.341064000	2.736236000	6.203771000
1	1.842661000	3.528488000	5.611465000
1	1.538341000	2.191437000	6.722129000
1	3.034143000	3.199174000	6.919355000
1	1.282888000	1.378482000	4.174434000
8	3.051406000	-0.469866000	6.132971000
1	2.923883000	-1.243571000	6.706294000
1	4.737379000	2.540087000	5.684626000

TS4_i7

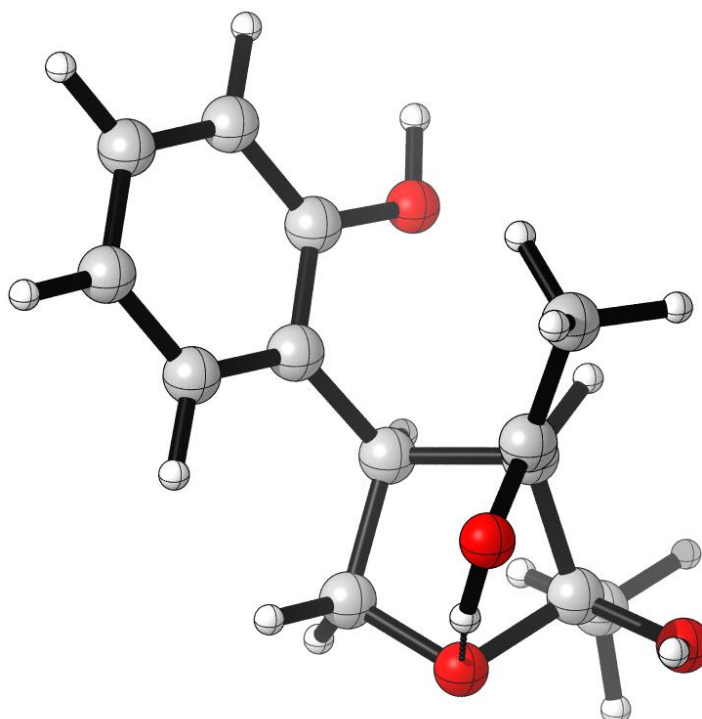


SPE = -805.2741; H₂₉₈ = -804.9763

6	2.910394000	0.588664000	2.977330000
1	3.866116000	1.114110000	2.842308000
6	2.092026000	0.826453000	1.709434000
6	0.894393000	0.138187000	1.397018000
6	0.182542000	0.459427000	0.228327000
1	-0.734545000	-0.097795000	0.020790000
6	0.633593000	1.456871000	-0.633703000
1	0.061319000	1.692750000	-1.534853000
6	1.816568000	2.147119000	-0.343517000
1	2.185934000	2.926580000	-1.014196000
6	2.524434000	1.824018000	0.815257000
1	3.448620000	2.362558000	1.043501000

6	2.224899000	1.155837000	4.218189000
6	3.277611000	-0.893162000	3.267541000
1	3.279294000	-1.536364000	2.380986000
1	4.237886000	-0.979408000	3.790951000
6	2.139532000	-0.764892000	5.304764000
8	2.221791000	-1.390204000	4.132089000
6	0.810517000	-0.780950000	5.984879000
1	0.670690000	-1.779794000	6.433963000
1	0.770606000	-0.038344000	6.794362000
1	0.003333000	-0.593261000	5.267335000
8	0.348938000	-0.843655000	2.164311000
1	0.915308000	-1.110382000	2.908058000
6	2.902936000	1.931776000	5.147996000
8	4.221076000	1.927517000	5.121048000
6	2.227941000	2.695755000	6.233417000
1	2.572022000	3.744256000	6.213747000
1	1.136167000	2.676213000	6.129985000
1	2.514213000	2.282944000	7.217336000
1	1.149488000	1.339955000	4.160822000
8	3.247209000	-0.843423000	6.020594000
1	3.108059000	-0.571086000	6.944565000
1	4.607200000	2.469320000	5.831783000

I1_i8

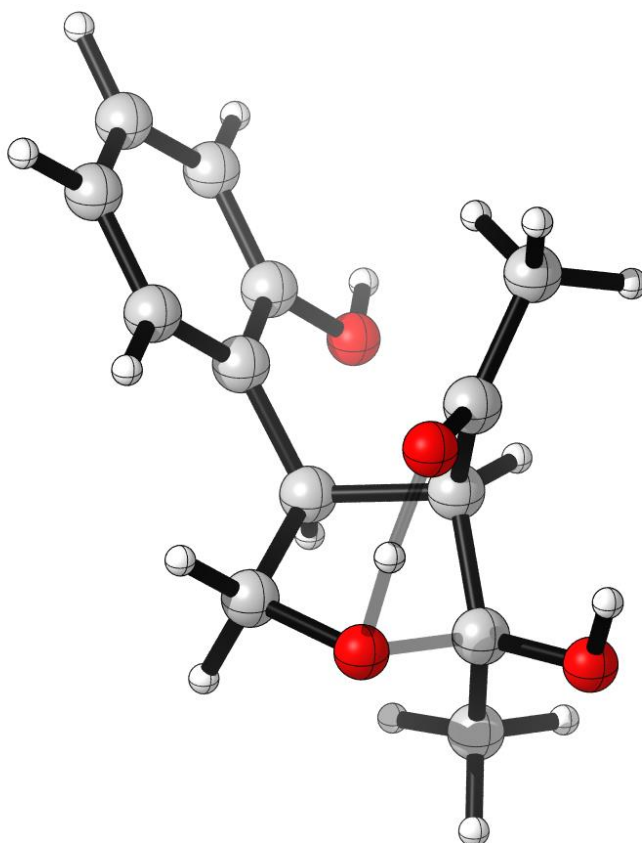


SPE = -805.2822; H₂₉₈ = -804.9828

6	0.749143000	0.353713000	3.248144000
6	1.716841000	-0.893622000	3.129082000
6	0.708022000	0.874759000	1.784394000
1	-0.263993000	0.772124000	1.287431000
1	1.009072000	1.931209000	1.734465000
6	2.664174000	-0.421458000	1.968120000
8	1.646496000	0.068893000	1.037016000
6	3.641769000	0.660438000	2.398051000
1	3.157054000	1.499338000	2.912514000
1	4.387375000	0.218927000	3.074712000
1	4.153209000	1.039380000	1.502122000
8	3.404752000	-1.395237000	1.338058000

1	2.859898000	-2.083022000	0.926212000
1	1.323614000	1.058670000	3.863139000
6	-0.565878000	0.134314000	3.971948000
6	-1.815058000	0.036534000	3.342703000
6	-0.523957000	0.042469000	5.384511000
6	-2.993212000	-0.133850000	4.079231000
6	-1.699573000	-0.126236000	6.126773000
6	-2.931717000	-0.211571000	5.473605000
1	-1.886329000	0.109240000	2.255111000
1	-3.952269000	-0.201967000	3.560581000
1	-1.637505000	-0.191438000	7.217818000
1	-3.843739000	-0.342993000	6.061569000
1	2.234263000	-1.088551000	4.074719000
6	0.950782000	-2.096847000	2.700654000
8	0.514969000	-2.154350000	1.504166000
6	0.674105000	-3.218712000	3.599966000
1	0.245121000	-2.830455000	4.540063000
1	0.025582000	-3.972201000	3.138263000
1	1.645635000	-3.662140000	3.888943000
1	0.821293000	-1.316183000	0.991083000
8	0.697601000	0.123326000	5.969748000
1	0.615933000	0.076281000	6.934906000

TS5_i8

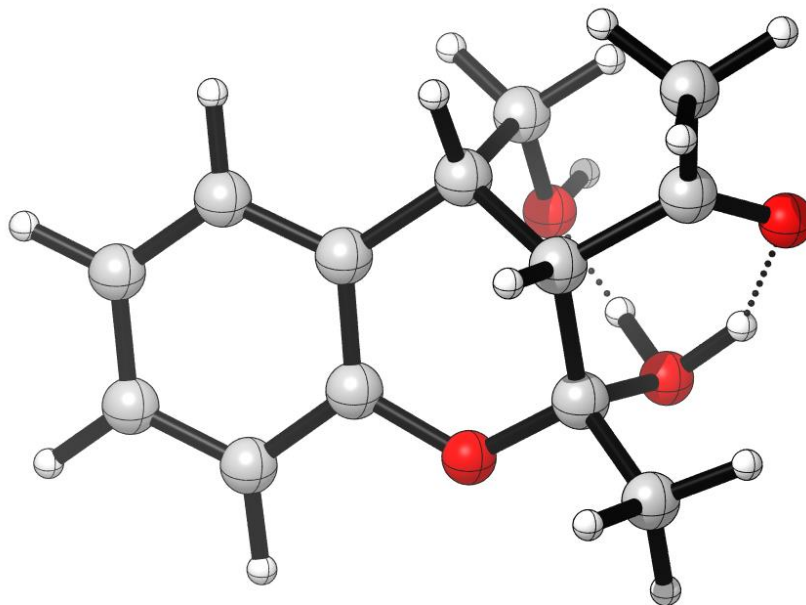


SPE = -805.2804; H₂₉₈ = -804.9842

6	0.761089000	0.359030000	3.249202000
6	1.711232000	-0.895208000	3.131472000
6	0.695639000	0.865364000	1.782576000
1	-0.281082000	0.762673000	1.297712000
1	1.024199000	1.907897000	1.690401000
6	2.686552000	-0.447452000	2.003956000
8	1.620125000	0.026051000	1.025900000
6	3.629224000	0.682506000	2.363378000
1	3.135754000	1.520714000	2.868650000
1	4.406789000	0.280744000	3.028642000
1	4.105538000	1.046823000	1.442338000
8	3.425150000	-1.408839000	1.383025000

1	2.926923000	-2.213333000	1.171890000
1	1.335683000	1.075640000	3.849889000
6	-0.546259000	0.133929000	3.984097000
6	-1.796440000	-0.003922000	3.364944000
6	-0.489330000	0.057006000	5.396510000
6	-2.963570000	-0.199945000	4.112518000
6	-1.653605000	-0.139784000	6.149468000
6	-2.888243000	-0.264615000	5.506837000
1	-1.878193000	0.051514000	2.276958000
1	-3.923950000	-0.301590000	3.601858000
1	-1.580754000	-0.196447000	7.240219000
1	-3.791171000	-0.419040000	6.103031000
1	2.210984000	-1.117565000	4.080950000
6	0.908044000	-2.076451000	2.639748000
8	0.540461000	-2.063435000	1.437342000
6	0.545042000	-3.193919000	3.527199000
1	-0.021406000	-2.787797000	4.384716000
1	-0.039624000	-3.958002000	3.000663000
1	1.466273000	-3.622839000	3.958754000
1	0.991600000	-1.070015000	0.972188000
8	0.734835000	0.176483000	5.969399000
1	0.663891000	0.132916000	6.935495000

I2_i1

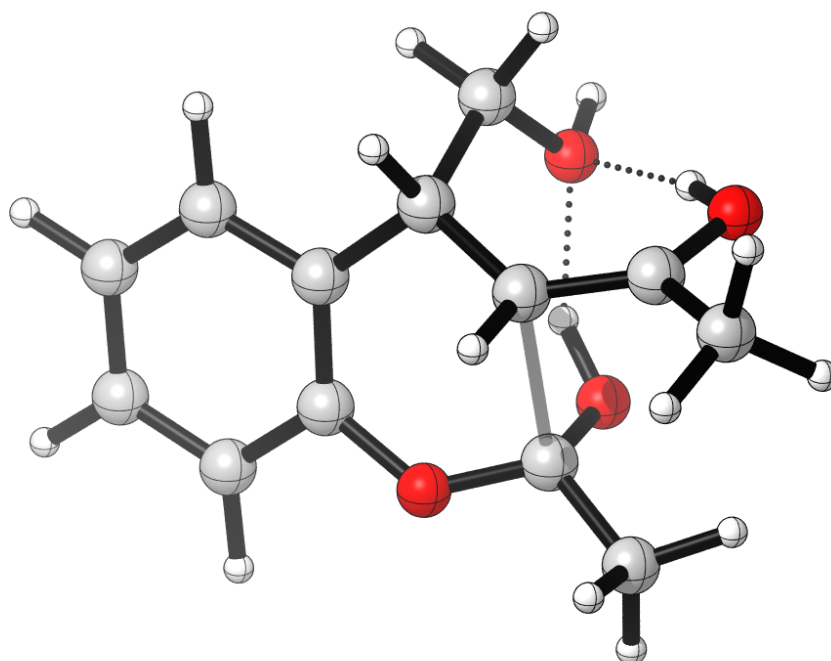


SPE = -805.3056; H₂₉₈ = -805.0061

6	0.594335000	2.251121000	4.370675000
1	0.682902000	3.073840000	3.644311000
6	0.245487000	2.838574000	5.722436000
6	0.742467000	2.238578000	6.884058000
6	0.408720000	2.714690000	8.156278000
1	0.830662000	2.215074000	9.031195000
6	-0.447331000	3.810439000	8.271575000
1	-0.718151000	4.185988000	9.261769000
6	-0.953008000	4.434113000	7.122581000
1	-1.610935000	5.301595000	7.212946000
6	-0.601351000	3.949720000	5.861213000
1	-0.988547000	4.437702000	4.962057000

6	2.004713000	1.579495000	4.470209000
6	-0.538369000	1.363350000	3.832350000
1	-1.433346000	1.986507000	3.689016000
1	-0.274012000	0.915940000	2.859015000
6	2.136484000	0.641155000	5.689616000
8	-0.842521000	0.328005000	4.784985000
6	3.551320000	0.178103000	5.988770000
1	4.010406000	-0.322689000	5.125671000
1	4.158665000	1.050958000	6.265889000
1	3.525886000	-0.520309000	6.836790000
8	1.599308000	1.152171000	6.855779000
1	2.720941000	2.400799000	4.625555000
6	2.381965000	0.876618000	3.161887000
8	2.294207000	-0.346166000	3.064732000
6	2.835516000	1.726043000	2.020268000
1	3.840517000	2.118978000	2.256007000
1	2.875970000	1.137182000	1.095180000
1	2.184165000	2.604207000	1.896151000
1	-1.564649000	-0.236974000	4.462150000
8	1.343929000	-0.605024000	5.377535000
1	0.321473000	-0.331882000	5.192496000
1	1.697981000	-0.869181000	4.456168000

TS6_i1

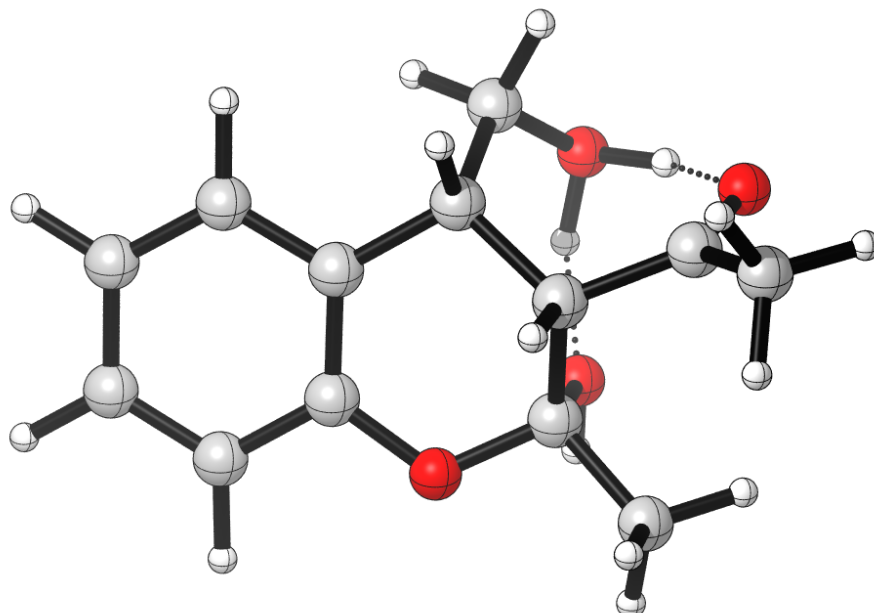


SPE = -805.2733; H₂₉₈ = -804.9749; G₂₉₈ = -805.0325

6	0.343710000	2.440171000	4.318281000
1	0.244098000	3.383531000	3.750864000
6	0.115901000	2.829896000	5.780380000
6	0.926449000	2.437866000	6.851487000
6	0.676328000	2.819835000	8.173320000
1	1.359932000	2.481865000	8.954871000
6	-0.416935000	3.636927000	8.452655000
1	-0.619797000	3.950021000	9.479680000
6	-1.239759000	4.071674000	7.404738000
1	-2.086132000	4.731671000	7.609559000
6	-0.970685000	3.669810000	6.097651000
1	-1.610257000	4.027281000	5.286068000

6	1.763560000	1.964873000	3.997300000
6	-0.804276000	1.574714000	3.788413000
1	-1.769169000	2.000553000	4.096685000
1	-0.782282000	1.534393000	2.687008000
6	2.297492000	0.715012000	5.848595000
8	-0.662279000	0.243275000	4.318025000
6	3.725722000	0.295576000	5.733596000
1	3.855376000	-0.442055000	4.933389000
1	4.378758000	1.162898000	5.583391000
1	4.000556000	-0.183737000	6.689638000
8	2.131471000	1.754201000	6.651594000
1	2.505806000	2.754472000	4.139384000
6	2.164740000	0.988287000	3.097329000
8	1.456950000	-0.072930000	2.752732000
6	3.506082000	1.032343000	2.438998000
1	4.179542000	1.747633000	2.926666000
1	3.960112000	0.030545000	2.411959000
1	3.365264000	1.357503000	1.392505000
1	-1.486276000	-0.263795000	4.225875000
8	1.418737000	-0.249018000	5.767091000
1	0.471816000	0.007003000	5.597227000
1	0.615246000	-0.153580000	3.270356000

I2_i2

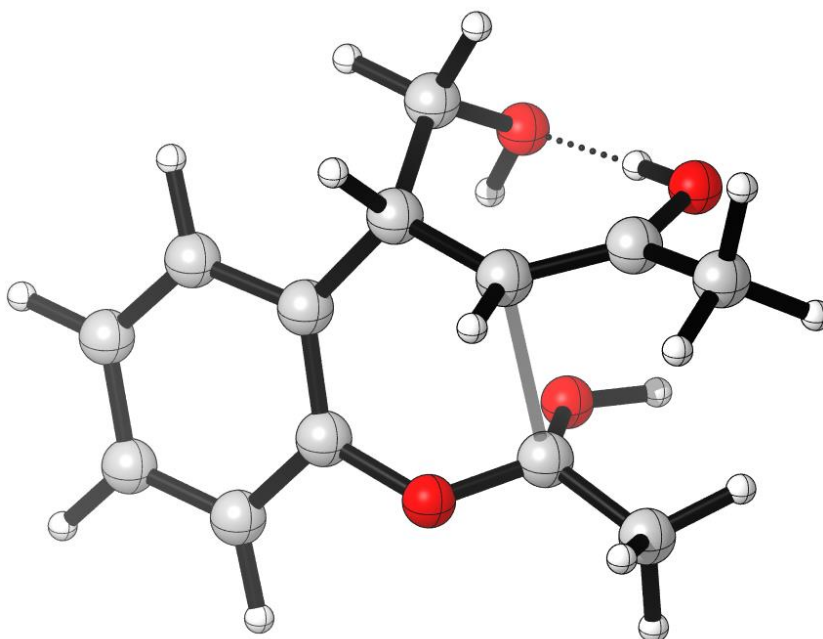


SPE = -805.3050; H₂₉₈ = -805.0056

6	0.293663000	2.464156000	4.407365000
1	0.240278000	3.353644000	3.759483000
6	0.054893000	2.946462000	5.832647000
6	0.933606000	2.624276000	6.875923000
6	0.711795000	3.082421000	8.182263000
1	1.423934000	2.798730000	8.960672000
6	-0.392570000	3.887648000	8.455340000
1	-0.563892000	4.251238000	9.471830000
6	-1.279191000	4.234647000	7.426199000
1	-2.141591000	4.872526000	7.633700000
6	-1.048446000	3.766342000	6.132610000
1	-1.733228000	4.049595000	5.327871000

6	1.756321000	1.924006000	4.269465000
6	-0.843081000	1.556763000	3.882973000
1	-1.779256000	1.738716000	4.422495000
1	-1.018286000	1.708102000	2.811309000
6	2.199327000	1.091889000	5.519525000
8	-0.556394000	0.125654000	4.009833000
6	3.653947000	0.645962000	5.481580000
1	4.322120000	1.513414000	5.389872000
1	3.892090000	0.128183000	6.422940000
1	3.833993000	-0.048644000	4.649422000
8	2.072525000	1.880687000	6.679446000
1	2.404266000	2.809171000	4.305518000
6	2.076765000	1.206106000	2.951702000
8	1.395885000	0.265981000	2.534102000
6	3.245321000	1.687769000	2.160071000
1	4.127905000	1.834789000	2.800675000
1	3.465222000	1.001183000	1.333172000
1	2.988492000	2.683160000	1.752845000
1	-0.055060000	-0.056401000	4.871775000
8	1.336774000	-0.035248000	5.620770000
1	1.571395000	-0.578649000	6.392398000
1	0.222107000	-0.027253000	3.309540000

TS6_i2

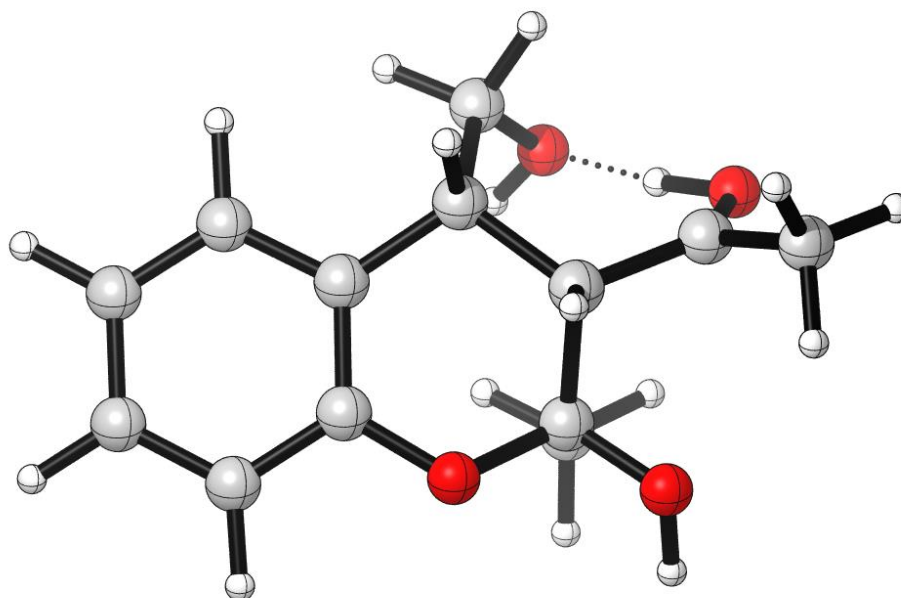


SPE = -805.2703; H₂₉₈ = -804.9710

6	0.225938000	2.675476000	4.328758000
1	0.087303000	3.665127000	3.853655000
6	0.034879000	2.954310000	5.828152000
6	0.989180000	2.716001000	6.823949000
6	0.804226000	3.046340000	8.167013000
1	1.608582000	2.838440000	8.875689000
6	-0.395672000	3.633594000	8.563169000
1	-0.556120000	3.902068000	9.610000000
6	-1.381113000	3.891675000	7.603033000
1	-2.320164000	4.366315000	7.896891000
6	-1.159263000	3.563345000	6.265461000
1	-1.930979000	3.804520000	5.530385000

6	1.634209000	2.272333000	3.886868000
6	-0.922993000	1.839396000	3.736295000
1	-1.893161000	2.265806000	4.032306000
1	-0.872109000	1.876368000	2.638479000
6	2.412312000	1.136845000	5.765907000
8	-0.875832000	0.452606000	4.077395000
6	3.827884000	0.743344000	5.515531000
1	4.429968000	1.611117000	5.223409000
1	4.222563000	0.349999000	6.469236000
1	3.903274000	-0.050624000	4.762294000
8	2.261146000	2.205977000	6.506230000
1	2.349533000	3.098346000	3.919772000
6	2.021818000	1.236908000	3.053871000
8	1.345607000	0.116762000	2.851451000
6	3.318910000	1.274021000	2.306690000
1	3.990474000	2.059947000	2.674113000
1	3.818420000	0.294165000	2.346765000
1	3.096653000	1.482236000	1.244831000
1	-0.927949000	0.341061000	5.040715000
8	1.464320000	0.229979000	5.855064000
1	1.736345000	-0.615095000	5.453642000
1	0.471777000	0.096122000	3.350477000

I2_i3

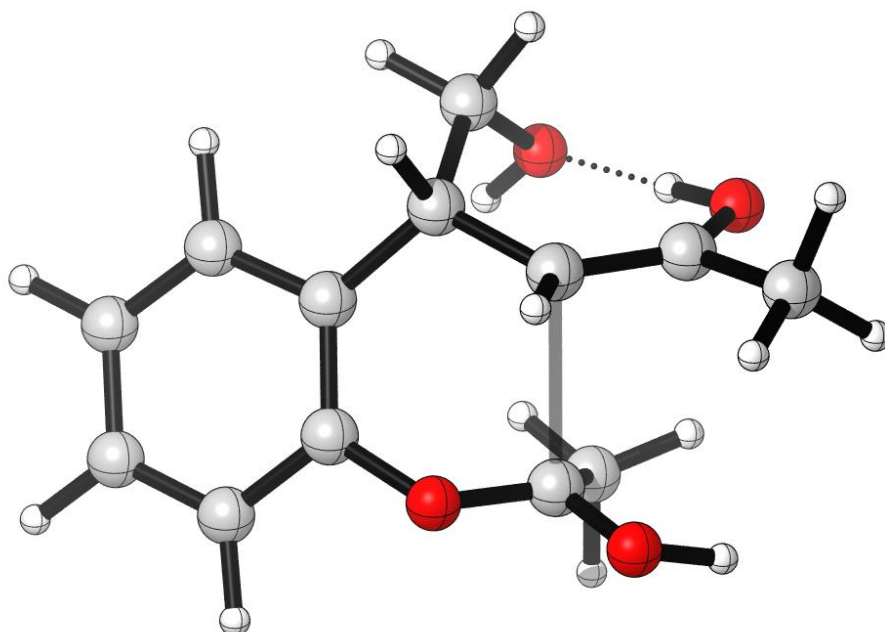


SPE = -805.2917; H₂₉₈ = -804.9924

6	0.319488000	2.511319000	4.404942000
1	0.363724000	3.473788000	3.869415000
6	0.068334000	2.862794000	5.870390000
6	1.022612000	2.603764000	6.870062000
6	0.819348000	3.019737000	8.194559000
1	1.592093000	2.795194000	8.933450000
6	-0.345033000	3.704255000	8.538367000
1	-0.499865000	4.034839000	9.568794000
6	-1.311743000	3.973400000	7.560397000
1	-2.224071000	4.514914000	7.821734000
6	-1.096036000	3.559952000	6.245324000
1	-1.843426000	3.803866000	5.485205000

6	1.750422000	1.891523000	4.229584000
6	-0.845394000	1.779678000	3.707322000
1	-1.811677000	2.131662000	4.090977000
1	-0.824733000	1.993332000	2.629880000
6	2.251270000	1.076995000	5.485938000
8	-0.791492000	0.345415000	3.797492000
6	1.504393000	-0.205445000	5.847192000
1	1.506301000	-0.929154000	5.020929000
1	2.032582000	-0.664202000	6.698006000
1	0.474858000	-0.011785000	6.175246000
8	2.208280000	1.970089000	6.596342000
1	2.450813000	2.736152000	4.213268000
6	2.044343000	1.095391000	2.982492000
8	1.315328000	0.138472000	2.606907000
6	3.251165000	1.391030000	2.189171000
1	4.120688000	1.359211000	2.866814000
1	3.366560000	0.691500000	1.353229000
1	3.183501000	2.430289000	1.820822000
1	-1.078362000	0.006484000	4.660656000
8	3.588639000	0.810679000	5.223349000
1	3.941991000	0.220078000	5.908018000
1	0.408382000	0.033259000	3.170220000

TS6_i3

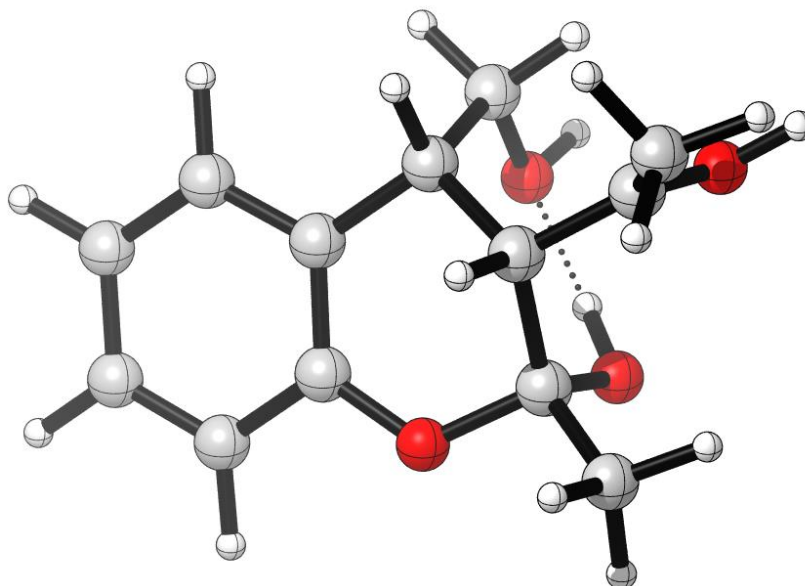


SPE = -805.2669; H₂₉₈ = -804.9682

6	0.242070000	2.682616000	4.314769000
1	0.207971000	3.705118000	3.892112000
6	0.050138000	2.888350000	5.825201000
6	1.023231000	2.643701000	6.805888000
6	0.833835000	2.923847000	8.161028000
1	1.649987000	2.717744000	8.856474000
6	-0.377264000	3.463076000	8.587785000
1	-0.535293000	3.690503000	9.644589000
6	-1.376253000	3.727519000	7.644301000
1	-2.324812000	4.168743000	7.959103000
6	-1.156033000	3.448741000	6.295932000
1	-1.941689000	3.695895000	5.579051000

6	1.616351000	2.167054000	3.887371000
6	-0.952308000	1.980900000	3.645851000
1	-1.896507000	2.470134000	3.922897000
1	-0.853203000	2.070322000	2.554077000
6	2.545725000	1.134831000	5.748013000
8	-1.027553000	0.579306000	3.918758000
6	1.735617000	-0.110407000	5.896687000
1	1.849990000	-0.773227000	5.029438000
1	2.129833000	-0.632625000	6.787346000
1	0.675919000	0.107632000	6.061766000
8	2.315852000	2.200568000	6.480660000
1	2.398894000	2.925728000	3.965100000
6	1.939543000	1.143601000	3.012562000
8	1.170698000	0.114606000	2.696215000
6	3.287245000	1.074354000	2.365205000
1	4.012003000	1.740021000	2.849417000
1	3.658975000	0.037567000	2.360218000
1	3.189348000	1.387963000	1.310595000
1	-1.366798000	0.413788000	4.811594000
8	3.822606000	1.057784000	5.463332000
1	4.068670000	0.181126000	5.118286000
1	0.296496000	0.121594000	3.184872000

I2_i4

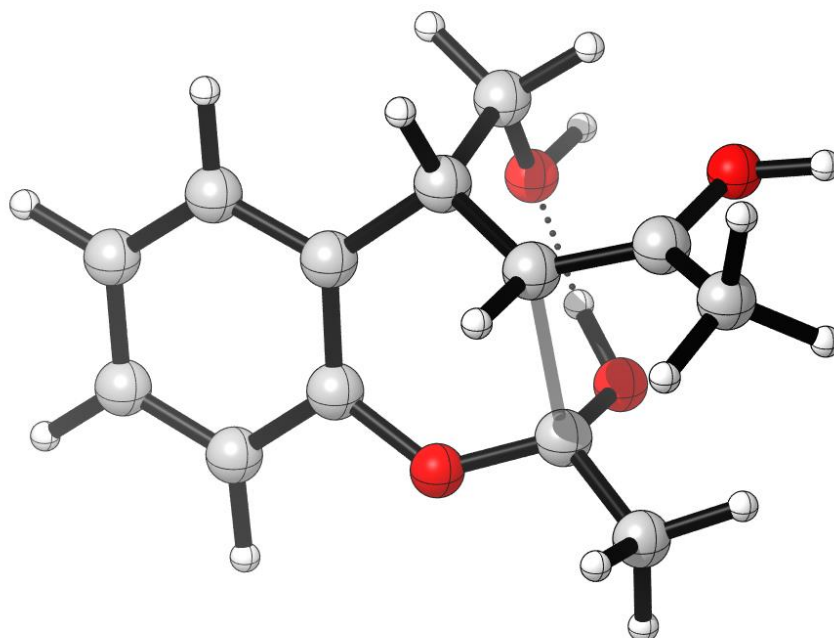


SPE = -805.2878; H₂₉₈ = -804.9882

6	0.490048000	2.258137000	4.365561000
1	0.567052000	3.098738000	3.656624000
6	0.202899000	2.821546000	5.745621000
6	0.864764000	2.331685000	6.882799000
6	0.535477000	2.803396000	8.163570000
1	1.071418000	2.386535000	9.019668000
6	-0.447809000	3.779258000	8.314896000
1	-0.706673000	4.141591000	9.313390000
6	-1.098969000	4.302319000	7.188186000
1	-1.859317000	5.078902000	7.301688000
6	-0.767919000	3.822585000	5.920886000
1	-1.272867000	4.228210000	5.039416000

6	1.921379000	1.603032000	4.402161000
6	-0.685777000	1.413976000	3.849407000
1	-1.547090000	2.095677000	3.741943000
1	-0.471827000	1.002668000	2.849183000
6	2.141479000	0.645358000	5.646037000
8	-0.994009000	0.377645000	4.772678000
6	3.600251000	0.218442000	5.762548000
1	3.893661000	-0.401122000	4.901677000
1	4.263546000	1.091844000	5.832975000
1	3.714244000	-0.390097000	6.671137000
8	1.887736000	1.424829000	6.820939000
1	2.621314000	2.437363000	4.540380000
6	2.294871000	0.942294000	3.128844000
8	1.666900000	-0.124410000	2.828144000
6	3.318504000	1.497195000	2.233822000
1	4.224953000	1.747807000	2.808611000
1	3.552342000	0.837726000	1.387202000
1	2.930709000	2.463421000	1.855659000
1	-1.646988000	-0.221494000	4.379588000
8	1.360387000	-0.486717000	5.607967000
1	0.427464000	-0.265990000	5.359403000
1	1.951169000	-0.521660000	1.976533000

TS6_i4



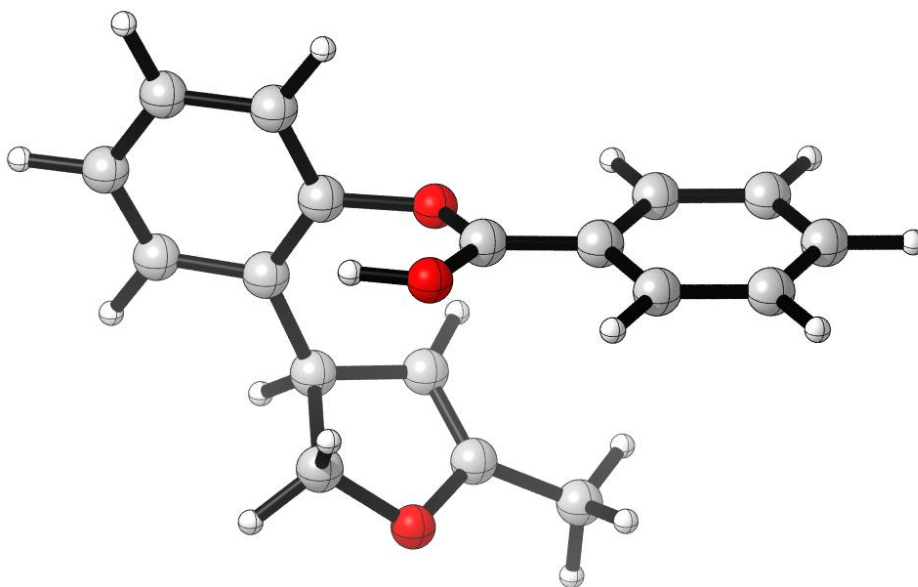
SPE = -805.2710; H₂₉₈ = -804.9735

6	0.341420000	2.379325000	4.288263000
1	0.198268000	3.260808000	3.637813000
6	0.130103000	2.859220000	5.718340000
6	0.870063000	2.379950000	6.806042000
6	0.602431000	2.768856000	8.122703000
1	1.222179000	2.363135000	8.925162000
6	-0.427876000	3.674441000	8.373937000
1	-0.644641000	3.986762000	9.398535000
6	-1.169995000	4.196007000	7.305840000
1	-1.964939000	4.922294000	7.492457000
6	-0.889119000	3.786476000	6.002531000
1	-1.469369000	4.195558000	5.171000000

6	1.790791000	1.952044000	4.028565000
6	-0.816551000	1.441343000	3.893346000
1	-1.742456000	2.038683000	3.884872000
1	-0.664246000	1.017013000	2.892598000
6	2.197190000	0.633045000	5.721241000
8	-0.954389000	0.398576000	4.869916000
6	3.637134000	0.220947000	5.661163000
1	3.813161000	-0.465626000	4.825103000
1	4.298213000	1.093399000	5.599561000
1	3.860303000	-0.316758000	6.598704000
8	2.011286000	1.596127000	6.639288000
1	2.504368000	2.734725000	4.299394000
6	2.245048000	1.138652000	3.001705000
8	1.438381000	0.232779000	2.474938000
6	3.634024000	1.212571000	2.459329000
1	4.285675000	1.839040000	3.079337000
1	4.072445000	0.207360000	2.350650000
1	3.588980000	1.662621000	1.451282000
1	-1.565535000	-0.284121000	4.550676000
8	1.332325000	-0.320651000	5.546099000
1	0.347330000	-0.054850000	5.393076000
1	1.891320000	-0.309062000	1.805677000

To Table 3

II0_PhMe

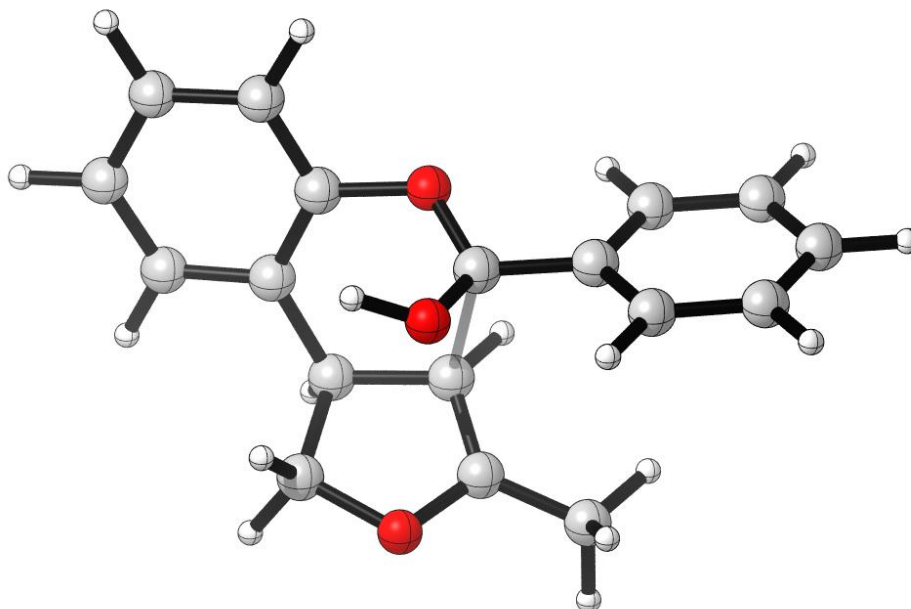


SPE = -920.4185; H₂₉₈ = -920.0917

6	-0.197313000	-5.007157000	-1.354466000
6	-1.540536000	-4.687206000	-1.134257000
6	0.798847000	-4.202972000	-0.797629000
1	-2.328041000	-5.316525000	-1.553980000
1	1.856839000	-4.445651000	-0.921749000
6	-1.882946000	-3.568370000	-0.371196000
6	0.420477000	-3.081201000	-0.057144000
1	-2.936371000	-3.334270000	-0.194235000
6	-0.913322000	-2.720112000	0.193529000
1	0.082171000	-5.886678000	-1.938436000
6	-1.366872000	-1.485776000	0.952372000

6	-0.529665000	-0.953029000	2.099439000
6	2.159020000	-1.457837000	-0.098513000
6	-1.433939000	-0.216323000	0.049907000
1	-0.700584000	-0.274266000	-0.775434000
1	-2.425684000	-0.035838000	-0.386687000
6	-0.463560000	0.386692000	2.010553000
8	-1.082113000	0.892809000	0.891230000
6	0.134346000	1.404410000	2.918969000
1	0.868048000	2.022977000	2.375020000
1	-0.644775000	2.086786000	3.298715000
1	0.630883000	0.924766000	3.773085000
1	-2.379909000	-1.725294000	1.324825000
8	1.471525000	-2.336875000	0.556434000
8	1.883310000	-1.163059000	-1.325169000
1	1.157107000	-1.706287000	-1.703150000
1	-0.150151000	-1.550463000	2.926794000
6	3.244480000	-0.784606000	0.574536000
6	3.611526000	-1.179184000	1.882198000
6	3.944575000	0.252837000	-0.084442000
6	4.673467000	-0.541572000	2.515075000
6	4.996384000	0.889038000	0.567081000
6	5.362817000	0.490247000	1.860503000
1	3.072090000	-1.983673000	2.383816000
1	3.654259000	0.558327000	-1.090476000
1	4.974930000	-0.852841000	3.517343000
1	5.538552000	1.693662000	0.066312000
1	6.193396000	0.990090000	2.365236000

TS0_PhMe

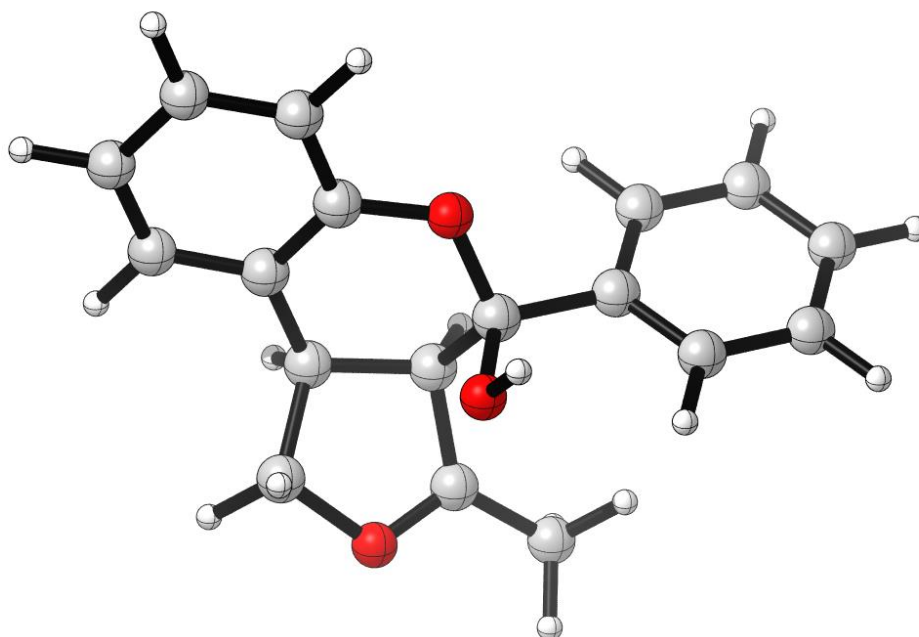


SPE = -920.4110; H₂₉₈ = -920.0847

6	-0.294958000	-5.102692000	-1.482518000
6	-1.600326000	-4.713881000	-1.155696000
6	0.787922000	-4.367353000	-1.000676000
1	-2.451218000	-5.291486000	-1.523594000
1	1.817967000	-4.651811000	-1.225364000
6	-1.816921000	-3.593210000	-0.352643000
6	0.543014000	-3.243740000	-0.208245000
1	-2.837659000	-3.305686000	-0.083940000
6	-0.748061000	-2.821461000	0.138289000
1	-0.116595000	-5.983458000	-2.103593000
6	-1.044094000	-1.600403000	0.990142000
6	0.121991000	-0.900517000	1.668338000

6	1.790198000	-1.266339000	0.221295000
6	-1.678144000	-0.425316000	0.187520000
1	-1.505488000	-0.496175000	-0.895625000
1	-2.752877000	-0.298334000	0.374726000
6	-0.065029000	0.461375000	1.529480000
8	-1.012489000	0.781090000	0.658623000
6	0.660350000	1.586450000	2.162508000
1	1.147709000	2.200651000	1.386793000
1	-0.059596000	2.238095000	2.685376000
1	1.413338000	1.227760000	2.873753000
1	-1.754101000	-1.927521000	1.769761000
8	1.677802000	-2.586224000	0.306986000
8	1.373113000	-0.650448000	-0.871515000
1	0.880761000	-1.244966000	-1.469438000
1	0.653014000	-1.327668000	2.517963000
6	2.949815000	-0.681466000	0.914893000
6	3.493412000	-1.318093000	2.047311000
6	3.533992000	0.499446000	0.421077000
6	4.604859000	-0.767117000	2.682743000
6	4.651759000	1.038439000	1.060086000
6	5.184874000	0.410856000	2.191502000
1	3.043712000	-2.236763000	2.428698000
1	3.122189000	0.981957000	-0.465797000
1	5.025712000	-1.260030000	3.561939000
1	5.111078000	1.948312000	0.667480000
1	6.054896000	0.840496000	2.693997000

III_PhMe

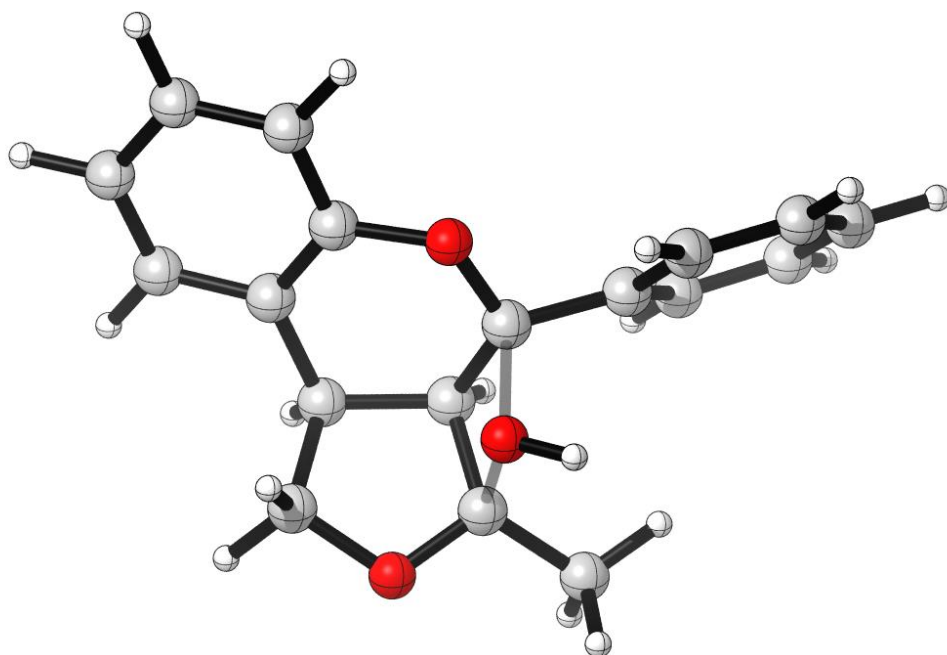


SPE = -920.4383; H₂₉₈ = -920.1099

6	-0.255027000	-5.175630000	-1.360515000
6	-1.561382000	-4.857215000	-0.963961000
6	0.806182000	-4.338352000	-1.017094000
1	-2.393309000	-5.512443000	-1.231706000
1	1.831730000	-4.570209000	-1.313157000
6	-1.793642000	-3.699509000	-0.219416000
6	0.557922000	-3.173647000	-0.279483000
1	-2.808082000	-3.454892000	0.109727000
6	-0.739235000	-2.839657000	0.129112000
1	-0.059337000	-6.081619000	-1.939673000
6	-0.988145000	-1.584628000	0.924481000
6	0.294981000	-0.837724000	1.370159000

6	1.509042000	-1.046034000	0.385959000
6	-1.770931000	-0.507897000	0.159727000
1	-1.557936000	-0.477112000	-0.916440000
1	-2.849837000	-0.487993000	0.351745000
6	-0.153912000	0.592397000	1.335867000
8	-1.242093000	0.757741000	0.706382000
6	0.483307000	1.754743000	1.959229000
1	0.032145000	2.690972000	1.608634000
1	0.340329000	1.656766000	3.052753000
1	1.570475000	1.736022000	1.785508000
1	-1.553448000	-1.840300000	1.833932000
8	1.652288000	-2.414731000	0.067464000
8	1.158523000	-0.295500000	-0.741582000
1	1.837805000	-0.393515000	-1.430266000
1	0.622228000	-1.120945000	2.379302000
6	2.844642000	-0.636706000	1.005175000
6	3.390545000	-1.405183000	2.047191000
6	3.534835000	0.494336000	0.549679000
6	4.601516000	-1.034926000	2.635647000
6	4.753868000	0.859182000	1.135448000
6	5.284912000	0.101201000	2.182391000
1	2.870284000	-2.299842000	2.397978000
1	3.122032000	1.099321000	-0.259734000
1	5.016188000	-1.637954000	3.447656000
1	5.286015000	1.740289000	0.768545000
1	6.230444000	0.393965000	2.645972000

TS1_PhMe

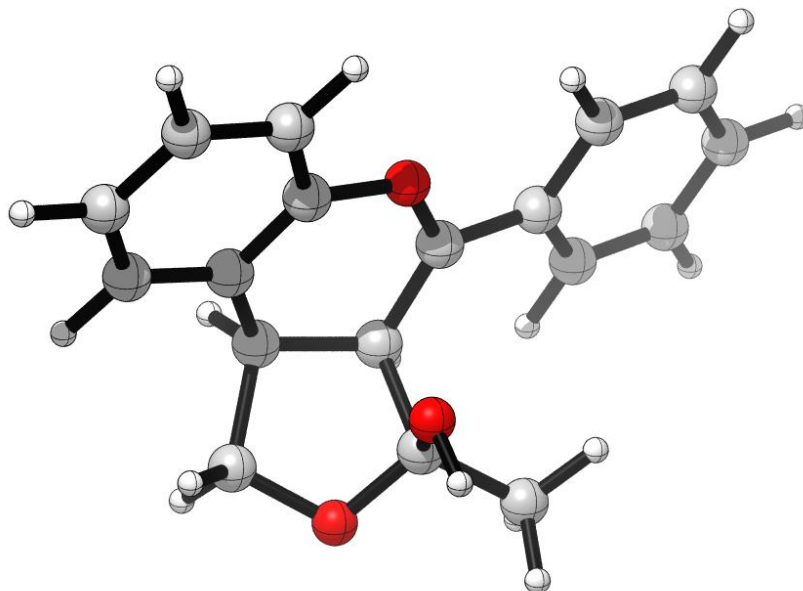


SPE = -920.4123; H₂₉₈ = -920.0868

6	0.211274000	-3.934744000	-2.783281000
6	-0.916862000	-4.404197000	-2.097439000
6	0.982144000	-2.906406000	-2.238753000
1	-1.520656000	-5.210806000	-2.519824000
1	1.872259000	-2.523218000	-2.741320000
6	-1.269153000	-3.842691000	-0.868007000
6	0.607670000	-2.362133000	-1.010282000
1	-2.145917000	-4.212672000	-0.329584000
6	-0.508558000	-2.807976000	-0.299930000
1	0.499761000	-4.375957000	-3.740136000
6	-0.902687000	-2.145980000	0.995472000
6	0.239687000	-1.337610000	1.659536000

6	1.321602000	-0.834790000	0.699991000
6	-2.042174000	-1.106742000	0.800275000
1	-2.089636000	-0.737772000	-0.235467000
1	-3.026883000	-1.485739000	1.101792000
6	-0.397643000	0.047261000	1.884819000
8	-1.717086000	-0.005228000	1.666322000
1	-1.237714000	-2.910333000	1.708647000
8	1.465851000	-1.381323000	-0.506204000
8	0.337645000	0.536386000	0.545283000
1	0.778070000	1.410275000	0.587211000
1	0.635396000	-1.825894000	2.554366000
6	2.644677000	-0.357137000	1.221812000
6	3.144504000	-0.783516000	2.461114000
6	3.421646000	0.491152000	0.409880000
6	4.402755000	-0.349601000	2.892552000
6	4.665735000	0.936237000	0.855810000
6	5.159501000	0.515555000	2.097875000
1	2.571625000	-1.461486000	3.095404000
1	3.047636000	0.811362000	-0.565627000
1	4.789142000	-0.696314000	3.853614000
1	5.258579000	1.605670000	0.227502000
1	6.134361000	0.866071000	2.445502000
6	-0.036940000	0.945854000	3.029366000
1	-0.460740000	0.511701000	3.947266000
1	1.048826000	1.045361000	3.151200000
1	-0.486714000	1.938011000	2.874745000

II2_PhMe

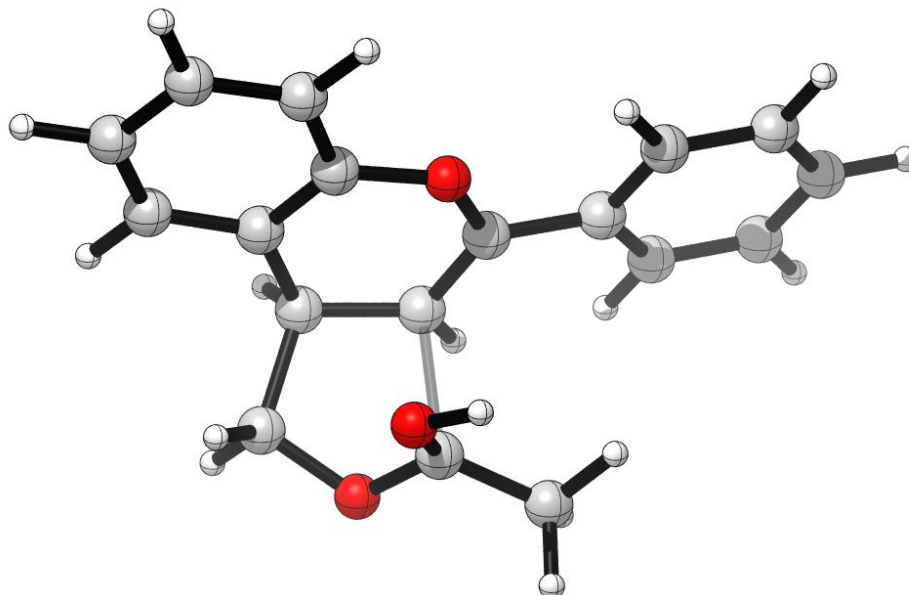


SPE = -920.4389; H₂₉₈ = -920.1097

6	-2.449335000	-1.353845000	-3.462199000
6	-2.144321000	-2.674259000	-3.109167000
6	-1.943374000	-0.298469000	-2.701417000
1	-2.527007000	-3.500835000	-3.711820000
1	-2.148168000	0.743232000	-2.957052000
6	-1.350261000	-2.944006000	-1.988246000
6	-1.159643000	-0.604008000	-1.589691000
1	-1.112587000	-3.978530000	-1.726965000
6	-0.853065000	-1.905880000	-1.189762000
1	-3.069154000	-1.141455000	-4.336176000
6	-0.007787000	-2.148509000	0.039635000
6	0.137516000	-0.885348000	0.920846000

6	0.035186000	0.411818000	0.204082000
6	-0.623235000	-3.179902000	1.034750000
1	-1.528583000	-3.643894000	0.613161000
1	0.088831000	-3.973507000	1.300898000
6	-1.018863000	-1.086663000	1.984736000
8	-0.938181000	-2.464298000	2.228839000
1	0.984813000	-2.498229000	-0.283670000
8	-0.627143000	0.493647000	-0.903051000
8	-2.197701000	-0.724006000	1.310325000
1	-2.951808000	-0.815424000	1.914829000
1	1.081695000	-0.923536000	1.472886000
6	0.607883000	1.645514000	0.680598000
6	1.484777000	1.660938000	1.795554000
6	0.300635000	2.867311000	0.023766000
6	2.028542000	2.859823000	2.241920000
6	0.843227000	4.059080000	0.483215000
6	1.706871000	4.058419000	1.590873000
1	1.758039000	0.738925000	2.306641000
1	-0.370200000	2.864258000	-0.835934000
1	2.706118000	2.863082000	3.098271000
1	0.594567000	4.995799000	-0.019904000
1	2.136240000	4.997485000	1.948974000
6	-0.885769000	-0.365446000	3.313947000
1	-1.697631000	-0.709516000	3.974835000
1	0.071471000	-0.597669000	3.802267000
1	-0.984718000	0.721227000	3.185037000

TS2_PhMe

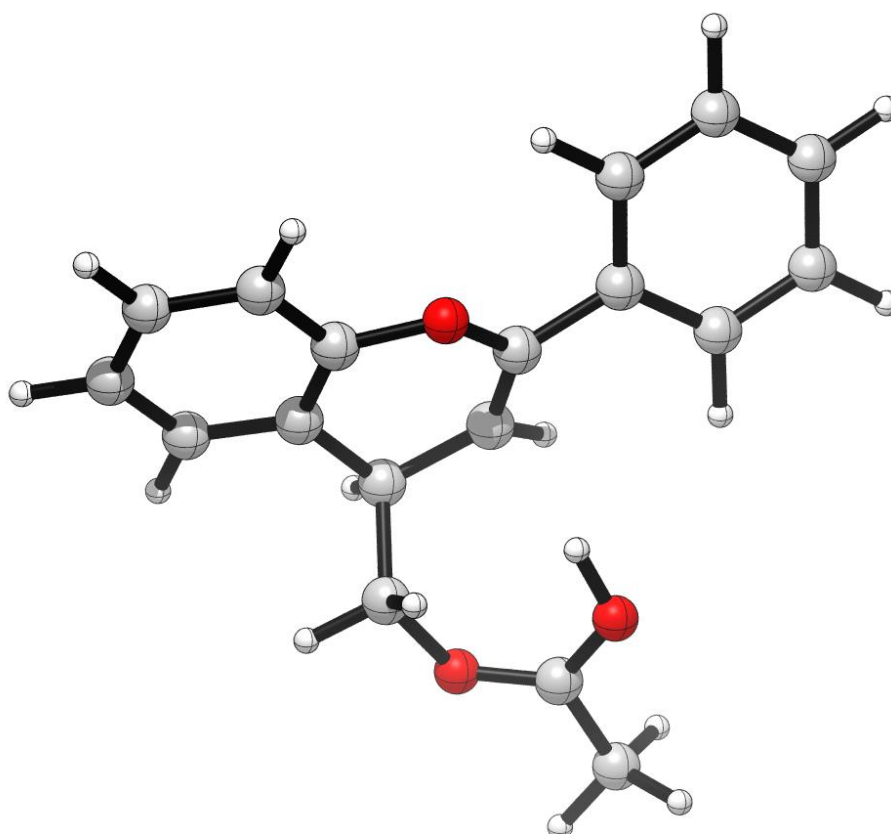


SPE = -920.4226; H₂₉₈ = -920.0963

6	-2.373658000	-1.375195000	-3.506568000
6	-1.995352000	-2.692378000	-3.214647000
6	-1.962150000	-0.333128000	-2.675115000
1	-2.307631000	-3.508539000	-3.869961000
1	-2.229651000	0.704847000	-2.884682000
6	-1.218227000	-2.965106000	-2.085039000
6	-1.187361000	-0.634047000	-1.552984000
1	-0.922034000	-3.994289000	-1.862762000
6	-0.808590000	-1.937665000	-1.221389000
1	-2.980994000	-1.154384000	-4.387540000
6	-0.014137000	-2.212822000	0.036673000
6	0.352227000	-0.930584000	0.760537000

6	0.093073000	0.321403000	0.206974000
6	-0.786129000	-3.140884000	1.051760000
1	-1.795130000	-3.378437000	0.687183000
1	-0.246250000	-4.066520000	1.276974000
6	-1.196620000	-1.156991000	2.185808000
8	-0.863869000	-2.432818000	2.296741000
1	0.911364000	-2.744292000	-0.237166000
8	-0.767889000	0.455392000	-0.795204000
8	-2.304832000	-0.939139000	1.476302000
1	-2.644130000	-0.036739000	1.604252000
1	1.190079000	-0.991396000	1.454331000
6	0.631540000	1.594425000	0.699277000
6	1.655420000	1.629850000	1.672329000
6	0.136442000	2.812327000	0.181731000
6	2.159767000	2.848763000	2.121095000
6	0.646235000	4.027670000	0.635016000
6	1.656009000	4.049896000	1.605715000
1	2.078080000	0.708290000	2.073852000
1	-0.647845000	2.798014000	-0.575858000
1	2.954792000	2.862794000	2.870605000
1	0.253912000	4.961476000	0.225308000
1	2.058129000	5.002379000	1.960722000
6	-0.923801000	-0.301861000	3.378547000
1	-1.681299000	-0.541413000	4.144796000
1	0.071068000	-0.510393000	3.790462000
1	-1.012681000	0.764816000	3.127759000

II3_PhMe

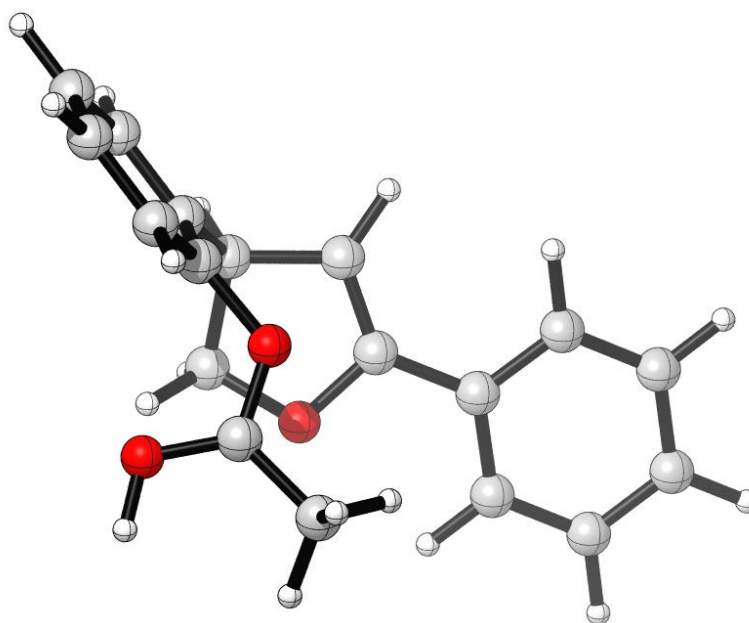


SPE = -920.4352; H₂₉₈ = -920.1068

6	-1.636767000	-3.045372000	-3.521601000
6	-0.780380000	-3.812596000	-2.720165000
6	-2.068869000	-1.792007000	-3.086041000
1	-0.422390000	-4.783703000	-3.069120000
1	-2.712351000	-1.161175000	-3.703715000
6	-0.385014000	-3.332133000	-1.469638000
6	-1.649993000	-1.319864000	-1.838426000
1	0.271826000	-3.935704000	-0.835838000
6	-0.828039000	-2.086027000	-1.000111000
1	-1.963955000	-3.420439000	-4.494317000
6	-0.485927000	-1.573751000	0.390047000
6	-0.689877000	-0.075035000	0.447980000

6	-1.443110000	0.594097000	-0.461571000
6	-1.350290000	-2.354646000	1.393714000
1	-2.426538000	-2.184014000	1.241546000
1	-1.140916000	-3.429328000	1.349366000
6	-1.565054000	-1.048907000	3.436600000
8	-1.040525000	-2.025490000	2.802244000
6	-1.351915000	-0.954619000	4.894045000
1	-2.276282000	-0.601382000	5.373434000
1	-1.018859000	-1.914042000	5.304048000
1	-0.578863000	-0.186545000	5.070806000
1	0.565694000	-1.809367000	0.622084000
8	-2.060220000	-0.046857000	-1.492053000
8	-2.259164000	-0.128019000	2.871440000
1	-2.179330000	-0.103193000	1.877920000
1	-0.093123000	0.510995000	1.149676000
6	-1.626880000	2.063538000	-0.504487000
6	-1.768229000	2.713890000	-1.745547000
6	-1.613475000	2.835534000	0.672794000
6	-1.862067000	4.106373000	-1.805674000
6	-1.719907000	4.226120000	0.608868000
6	-1.836469000	4.865815000	-0.630778000
1	-1.784082000	2.125200000	-2.664312000
1	-1.534305000	2.352036000	1.648939000
1	-1.955302000	4.602677000	-2.775208000
1	-1.717664000	4.811821000	1.531468000
1	-1.916375000	5.955277000	-0.680926000

II0_MePh

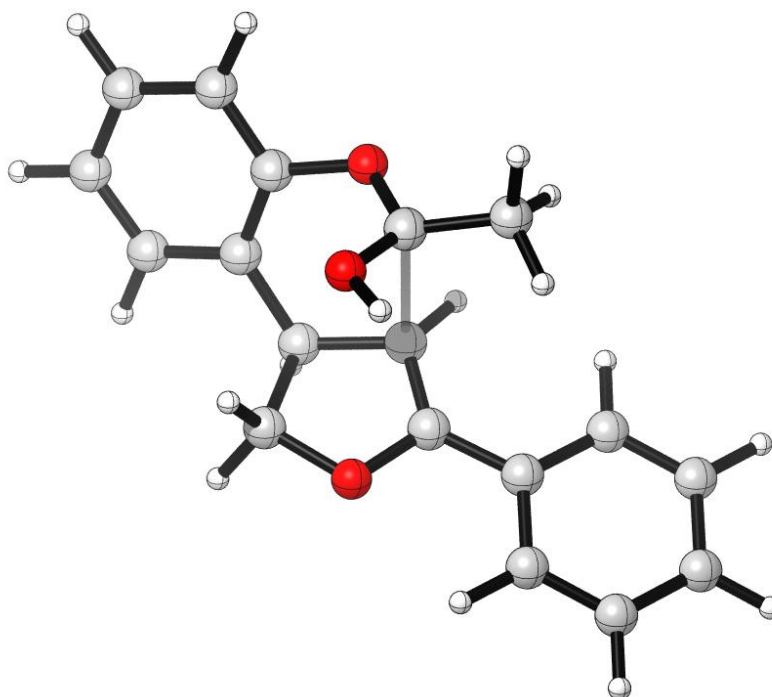


SPE = -920.4235; H₂₉₈ = -920.0971

6	0.229097000	-0.732286000	-2.944856000
6	-0.466395000	-1.920108000	-3.192329000
6	0.794152000	-0.516285000	-1.685611000
1	-0.911908000	-2.103308000	-4.172865000
1	1.355823000	0.393203000	-1.462916000
6	-0.594615000	-2.881767000	-2.187336000
6	0.638320000	-1.495089000	-0.708960000
1	-1.138056000	-3.807633000	-2.393271000
6	-0.045055000	-2.701474000	-0.905274000
1	0.340704000	0.024693000	-3.724641000
6	-0.214315000	-3.786820000	0.152576000
6	1.080612000	-4.363391000	0.692285000

6	0.845720000	-0.430632000	1.413386000
6	-0.894789000	-3.358396000	1.481802000
1	-1.392136000	-2.379038000	1.448405000
1	-1.634226000	-4.113446000	1.792342000
6	1.205348000	-4.051961000	1.997963000
8	0.146779000	-3.314015000	2.478303000
1	-0.822876000	-4.572177000	-0.320450000
8	1.292581000	-1.260067000	0.544720000
8	-0.302862000	0.095844000	1.202381000
1	-0.577561000	0.722735000	1.901480000
1	1.793873000	-4.923896000	0.091482000
6	2.262982000	-4.368864000	2.968845000
6	2.088688000	-4.059399000	4.331516000
6	3.453227000	-5.008657000	2.564454000
6	3.075896000	-4.387687000	5.265626000
6	4.434415000	-5.336204000	3.499912000
6	4.250359000	-5.027504000	4.855200000
1	1.169936000	-3.568776000	4.657084000
1	3.610809000	-5.261835000	1.513393000
1	2.921938000	-4.140376000	6.319790000
1	5.346971000	-5.839206000	3.168787000
1	5.019477000	-5.290362000	5.585985000
6	1.706245000	-0.096787000	2.564786000
1	1.115565000	0.300479000	3.400105000
1	2.289920000	-0.975285000	2.868224000
1	2.415073000	0.679499000	2.223687000

TS0_MePh

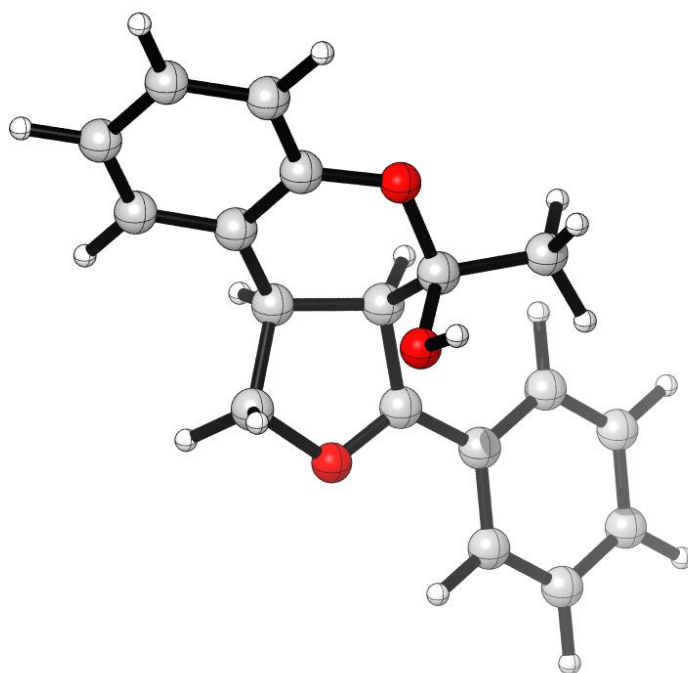


SPE = -920.4157; H₂₉₈ = -920.0890

6	-0.917489000	-1.240257000	-3.764319000
6	-1.584751000	-2.354205000	-3.239962000
6	-0.040272000	-0.514618000	-2.956573000
1	-2.264194000	-2.933329000	-3.869891000
1	0.511148000	0.347884000	-3.335854000
6	-1.372271000	-2.738095000	-1.914973000
6	0.133140000	-0.911153000	-1.631711000
1	-1.879571000	-3.622495000	-1.518958000
6	-0.508761000	-2.018647000	-1.068951000
1	-1.079879000	-0.933795000	-4.800371000
6	-0.337618000	-2.472401000	0.368633000
6	0.781986000	-1.889349000	1.217791000

6	0.822312000	0.292928000	0.299716000
6	-1.578474000	-2.160180000	1.248906000
1	-2.148761000	-1.295990000	0.880951000
1	-2.256541000	-3.014460000	1.375854000
6	0.286385000	-1.715163000	2.492375000
8	-1.048187000	-1.819598000	2.556856000
6	1.963992000	0.924378000	1.012742000
1	1.745228000	1.061896000	2.079599000
1	2.877818000	0.335080000	0.876731000
1	2.116869000	1.918654000	0.555572000
1	-0.190068000	-3.567068000	0.329696000
8	1.091370000	-0.196067000	-0.881515000
8	-0.413579000	0.672604000	0.503391000
1	-0.514212000	1.166899000	1.337212000
1	1.834830000	-2.071913000	1.006331000
6	0.974591000	-1.465257000	3.760519000
6	0.223515000	-1.344555000	4.948436000
6	2.382124000	-1.398291000	3.827319000
6	0.866567000	-1.177125000	6.174911000
6	3.018245000	-1.222686000	5.055946000
6	2.264245000	-1.118114000	6.232064000
1	-0.865243000	-1.399066000	4.900598000
1	2.983626000	-1.501535000	2.922412000
1	0.275009000	-1.093912000	7.089927000
1	4.109259000	-1.174414000	5.099919000
1	2.769409000	-0.989228000	7.192887000

III_MePh

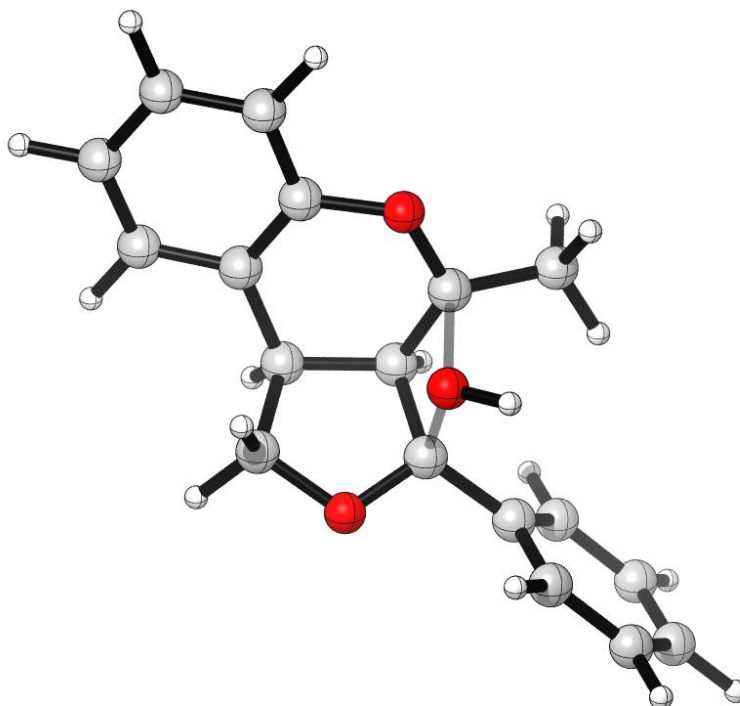


SPE = -920.4494; H₂₉₈ = -920.1199

6	-0.875875000	-1.235040000	-3.768317000
6	-1.536053000	-2.367183000	-3.270597000
6	-0.051841000	-0.477876000	-2.935082000
1	-2.178554000	-2.962773000	-3.923435000
1	0.475813000	0.405056000	-3.302614000
6	-1.359317000	-2.738146000	-1.936651000
6	0.105811000	-0.851387000	-1.593743000
1	-1.857280000	-3.631425000	-1.548422000
6	-0.540351000	-1.984344000	-1.080073000
1	-1.010475000	-0.934307000	-4.810826000
6	-0.342393000	-2.379251000	0.359588000
6	0.733008000	-1.553231000	1.111701000

6	0.790765000	-0.074640000	0.587457000
6	-1.586617000	-2.203247000	1.242753000
1	-2.188868000	-1.322383000	0.990553000
1	-2.217146000	-3.094460000	1.340374000
6	0.222365000	-1.630019000	2.524521000
8	-1.020232000	-1.957333000	2.576462000
6	1.967183000	0.745250000	1.095772000
1	1.889022000	0.927567000	2.175222000
1	2.921354000	0.247710000	0.869935000
1	1.958717000	1.715235000	0.575823000
1	-0.039723000	-3.437342000	0.404512000
8	0.948984000	-0.089189000	-0.824207000
8	-0.443913000	0.478787000	0.948576000
1	-0.463924000	1.416917000	0.697843000
1	1.735898000	-1.988852000	1.018623000
6	0.930965000	-1.420150000	3.753595000
6	0.209451000	-1.346175000	4.973855000
6	2.345813000	-1.336236000	3.767155000
6	0.891058000	-1.188679000	6.172440000
6	3.016795000	-1.186228000	4.975858000
6	2.293253000	-1.111542000	6.174108000
1	-0.880130000	-1.406362000	4.959235000
1	2.916401000	-1.417762000	2.841866000
1	0.336286000	-1.123324000	7.110724000
1	4.107402000	-1.129928000	4.990124000
1	2.828141000	-0.990356000	7.119508000

TS1_MePh

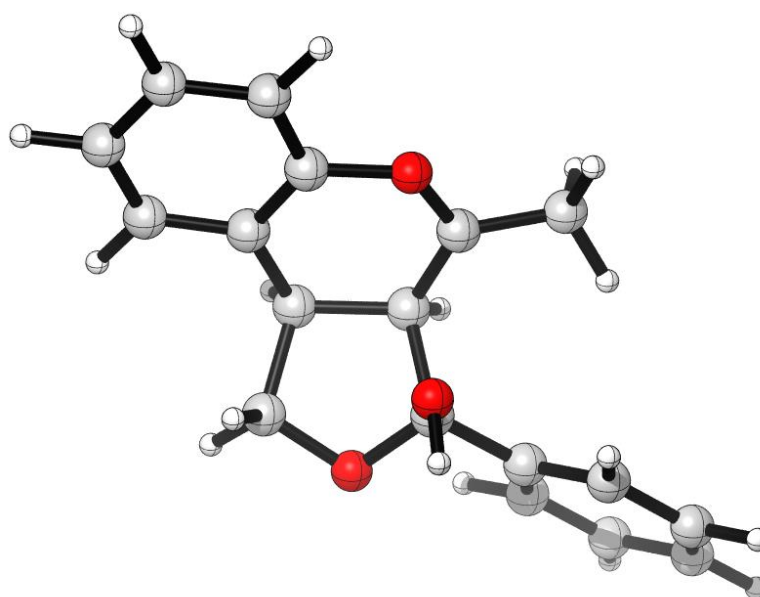


SPE = -920.4123; H₂₉₈ = -920.0850

6	-1.244526000	-0.948261000	-3.634796000
6	-1.553129000	-2.277503000	-3.317636000
6	-0.526755000	-0.165135000	-2.730085000
1	-2.108123000	-2.895013000	-4.027793000
1	-0.250439000	0.867546000	-2.952285000
6	-1.147078000	-2.819366000	-2.095745000
6	-0.144927000	-0.728440000	-1.512537000
1	-1.393137000	-3.855930000	-1.850035000
6	-0.433582000	-2.048126000	-1.164218000
1	-1.559717000	-0.520348000	-4.589295000
6	-0.080705000	-2.580557000	0.202715000
6	0.944828000	-1.711402000	0.976607000

6	1.032434000	-0.258969000	0.517023000
6	-1.329581000	-2.615802000	1.129812000
1	-2.101391000	-1.907914000	0.793710000
1	-1.771404000	-3.614599000	1.232734000
6	0.213871000	-1.410547000	2.304995000
8	-0.861786000	-2.212897000	2.427918000
6	2.178545000	0.596103000	0.953931000
1	2.471824000	0.409214000	1.993612000
1	3.029686000	0.348435000	0.298921000
1	1.927823000	1.657149000	0.807491000
1	0.329291000	-3.594503000	0.106448000
8	0.592158000	0.110211000	-0.668052000
8	-0.241843000	-0.023910000	1.710875000
1	-0.177032000	0.740947000	2.317743000
1	1.930835000	-2.183173000	1.056726000
6	0.898893000	-1.204103000	3.627206000
6	0.182451000	-0.559160000	4.651339000
6	2.192679000	-1.681530000	3.876955000
6	0.767689000	-0.370761000	5.904576000
6	2.769913000	-1.501015000	5.139894000
6	2.063797000	-0.840592000	6.149534000
1	-0.835392000	-0.202861000	4.471582000
1	2.756356000	-2.200698000	3.098667000
1	0.209732000	0.140199000	6.692953000
1	3.776561000	-1.879226000	5.332594000
1	2.522976000	-0.690107000	7.130136000

II2_MePh

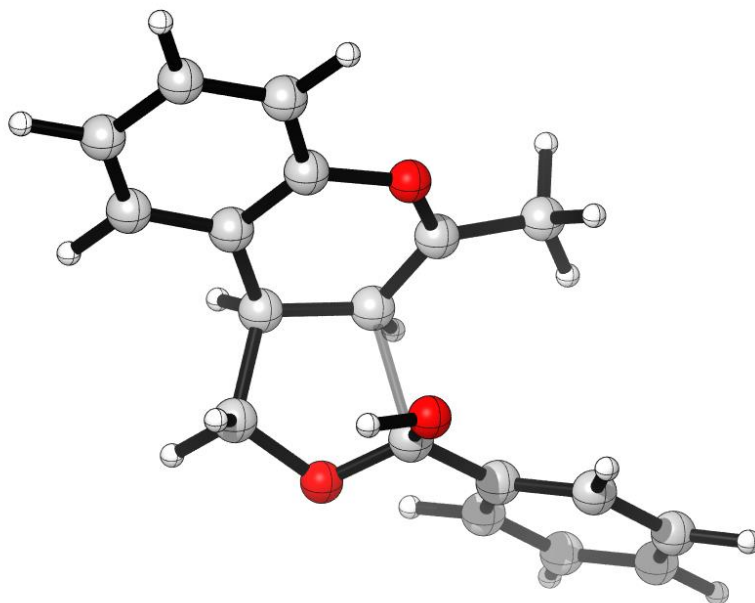


SPE = -920.4302; H_{298} = -920.1028

6	-1.798478000	-1.553384000	-3.851909000
6	-1.520445000	-2.849795000	-3.398571000
6	-1.583198000	-0.463835000	-3.008597000
1	-1.683523000	-3.703649000	-4.059926000
1	-1.774834000	0.562620000	-3.326752000
6	-1.039667000	-3.063542000	-2.102990000
6	-1.102510000	-0.716403000	-1.726432000
1	-0.819117000	-4.079263000	-1.764047000
6	-0.823050000	-1.987652000	-1.230100000
1	-2.180354000	-1.389197000	-4.861627000
6	-0.319190000	-2.174696000	0.177464000
6	-0.147696000	-0.854166000	0.972716000

6	-0.333266000	0.407102000	0.221958000
6	-1.298552000	-3.011972000	1.059211000
1	-2.301023000	-3.044421000	0.604078000
1	-0.946975000	-4.036362000	1.235995000
6	-1.261757000	-0.970078000	2.124831000
8	-1.341182000	-2.349073000	2.316351000
1	0.650606000	-2.690549000	0.134892000
8	-0.827411000	0.427468000	-0.953599000
8	-2.414305000	-0.439688000	1.526028000
1	-3.175526000	-0.565186000	2.117244000
1	0.824931000	-0.809092000	1.480942000
6	-0.904406000	-0.326081000	3.454196000
6	-1.586666000	0.802487000	3.929459000
6	0.131235000	-0.882085000	4.224360000
6	-1.236864000	1.368301000	5.162600000
6	0.485312000	-0.310999000	5.447037000
6	-0.196975000	0.818951000	5.917685000
1	-2.388835000	1.247497000	3.337349000
1	0.652944000	-1.772387000	3.866391000
1	-1.777797000	2.244667000	5.528364000
1	1.291801000	-0.751734000	6.038739000
1	0.085903000	1.268266000	6.873058000
6	0.050058000	1.722144000	0.760785000
1	-0.145305000	1.785230000	1.841014000
1	1.146333000	1.813202000	0.627037000
1	-0.442971000	2.531954000	0.209714000

TS2_MePh

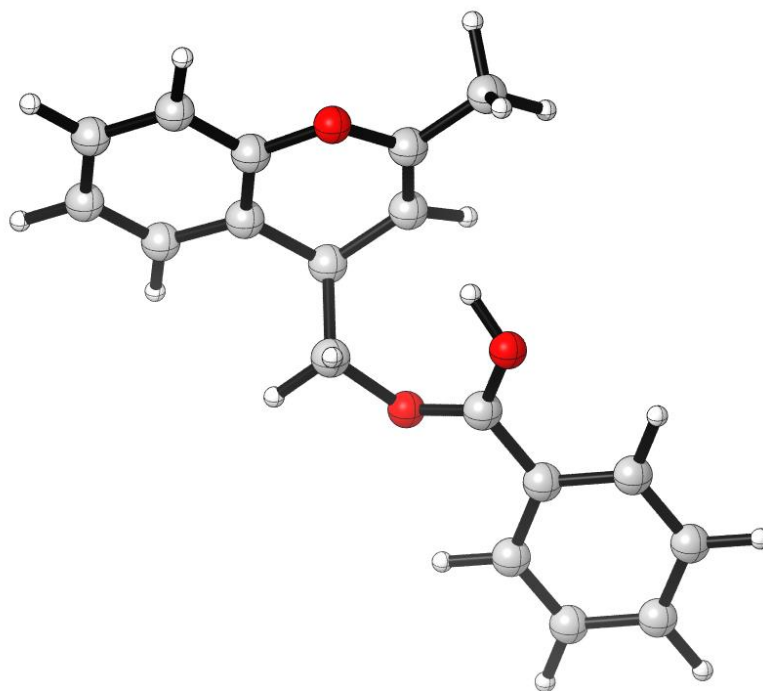


SPE = -920.4165; H₂₉₈ = -920.0909

6	-1.922768000	-1.468240000	-3.747044000
6	-1.561523000	-2.770911000	-3.377040000
6	-1.699410000	-0.407907000	-2.869189000
1	-1.730352000	-3.601288000	-4.066417000
1	-1.955544000	0.620365000	-3.132230000
6	-0.994570000	-3.014749000	-2.123725000
6	-1.127490000	-0.679638000	-1.626117000
1	-0.714983000	-4.033054000	-1.839044000
6	-0.774200000	-1.967888000	-1.215602000
1	-2.375713000	-1.275239000	-4.722029000
6	-0.239300000	-2.208685000	0.176936000
6	0.048441000	-0.907028000	0.908671000

6	-0.168287000	0.330200000	0.287603000
6	-1.262969000	-3.027824000	1.046869000
1	-2.252398000	-3.074599000	0.562943000
1	-0.928730000	-4.049596000	1.258138000
6	-1.458636000	-1.035701000	2.249271000
8	-1.354615000	-2.371811000	2.313335000
1	0.688161000	-2.798286000	0.120227000
8	-0.858561000	0.433502000	-0.823696000
8	-2.545064000	-0.520037000	1.643560000
1	-3.068415000	-1.201185000	1.187959000
1	0.872244000	-0.914827000	1.624223000
6	-1.030040000	-0.330349000	3.486298000
6	-1.683926000	0.838038000	3.912583000
6	0.032985000	-0.854906000	4.244604000
6	-1.269005000	1.476850000	5.084714000
6	0.443906000	-0.210581000	5.410112000
6	-0.203648000	0.959415000	5.829572000
1	-2.519867000	1.237023000	3.336254000
1	0.532096000	-1.769895000	3.919850000
1	-1.783044000	2.380904000	5.419689000
1	1.269157000	-0.622631000	5.995920000
1	0.124782000	1.465709000	6.740802000
6	0.265650000	1.637952000	0.837399000
1	0.644129000	1.547328000	1.862087000
1	1.073491000	2.033937000	0.196883000
1	-0.564738000	2.360230000	0.790574000

II3_MePh



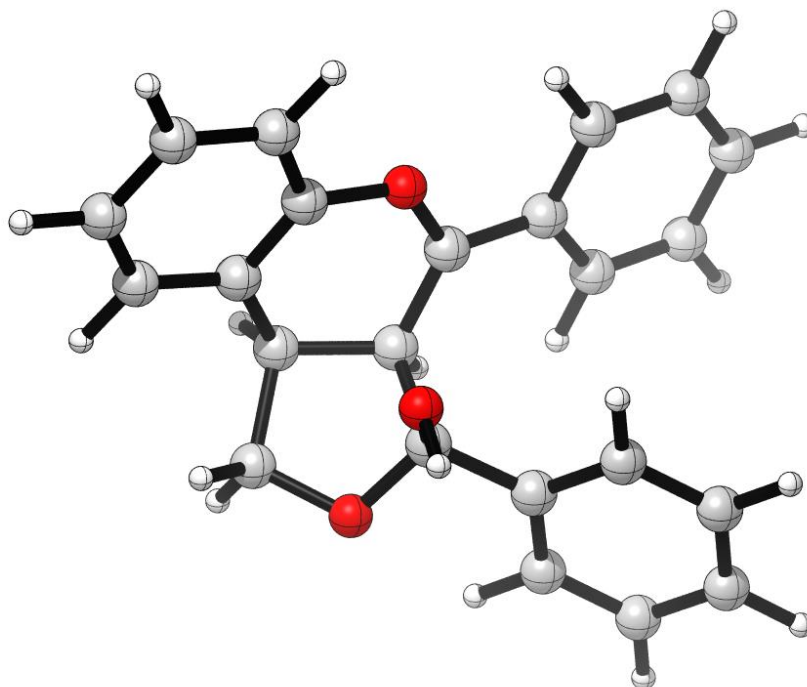
SPE = -920.4400; H₂₉₈ = -920.1132

6	-1.518112000	-2.763434000	-3.595736000
6	-0.181824000	-2.946019000	-3.216567000
6	-2.340773000	-1.906539000	-2.863233000
1	0.468625000	-3.608935000	-3.792030000
1	-3.378139000	-1.722736000	-3.151132000
6	0.322455000	-2.272594000	-2.101110000
6	-1.823547000	-1.250268000	-1.741936000
1	1.366583000	-2.417062000	-1.808827000
6	-0.490892000	-1.418465000	-1.339174000
1	-1.920302000	-3.282133000	-4.469528000
6	0.014430000	-0.716908000	-0.086835000
6	-0.927790000	0.406238000	0.294868000

6	-2.196786000	0.483557000	-0.172708000
6	0.133182000	-1.782192000	1.020042000
1	-0.835499000	-2.260060000	1.229146000
1	0.867203000	-2.552119000	0.758203000
6	-0.093779000	-0.751612000	3.215244000
8	0.653663000	-1.249365000	2.289851000
6	-3.215967000	1.504735000	0.215348000
1	-2.791585000	2.248864000	0.901892000
1	-3.606275000	2.012893000	-0.681033000
1	-4.070445000	1.007571000	0.705148000
1	1.023605000	-0.311848000	-0.268309000
8	-2.690421000	-0.409606000	-1.070558000
8	-1.301440000	-0.356089000	2.996787000
1	-1.511772000	-0.224387000	2.022736000
1	-0.548969000	1.238988000	0.893939000
6	0.446620000	-0.634040000	4.555926000
6	-0.229157000	0.160330000	5.508589000
6	1.634101000	-1.315210000	4.903432000
6	0.289172000	0.276108000	6.794779000
6	2.133880000	-1.201131000	6.197481000
6	1.466124000	-0.403929000	7.137852000
1	-1.143930000	0.685324000	5.230064000
1	2.146306000	-1.932307000	4.163653000
1	-0.221408000	0.895981000	7.534651000
1	3.047175000	-1.730091000	6.478063000
1	1.870249000	-0.309079000	8.149138000

To Figure S13

II2_PhPh



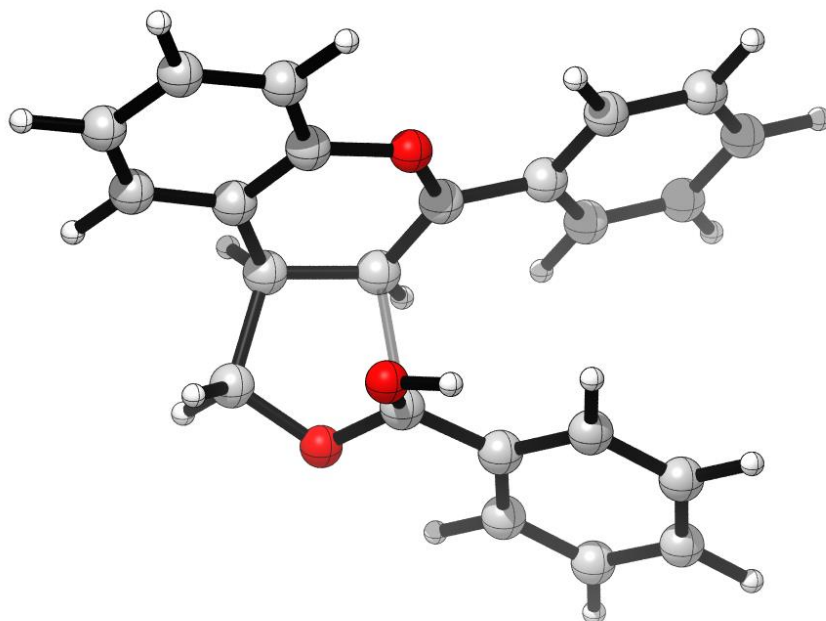
SPE = -1111.9204; H₂₉₈ = -1111.5354

6	-2.532026000	-1.348118000	-3.394726000
6	-2.202345000	-2.667103000	-3.059897000
6	-2.001751000	-0.291367000	-2.651988000
1	-2.605807000	-3.494889000	-3.647147000
1	-2.228007000	0.749344000	-2.892937000
6	-1.357679000	-2.934697000	-1.975431000
6	-1.170249000	-0.594750000	-1.575239000
1	-1.102623000	-3.968537000	-1.728400000
6	-0.837348000	-1.895920000	-1.193759000
1	-3.192139000	-1.137290000	-4.239172000
6	0.052100000	-2.131223000	0.007062000

6	0.165099000	-0.880131000	0.908726000
6	0.046626000	0.421210000	0.204694000
6	-0.493137000	-3.201075000	0.997158000
1	-1.365186000	-3.725698000	0.578156000
1	0.270599000	-3.943488000	1.267374000
6	-0.999989000	-1.137693000	1.966785000
8	-0.862028000	-2.509646000	2.192070000
1	1.050141000	-2.433611000	-0.346916000
8	-0.629607000	0.503151000	-0.895991000
8	-2.181034000	-0.819073000	1.280139000
1	-2.940807000	-0.983728000	1.862715000
1	1.103200000	-0.909265000	1.470495000
6	-0.905651000	-0.410083000	3.299415000
6	-1.555046000	0.822719000	3.473186000
6	-0.207519000	-0.975997000	4.378463000
6	-1.519106000	1.473936000	4.710301000
6	-0.172783000	-0.323296000	5.614031000
6	-0.833968000	0.898871000	5.785166000
1	-2.103246000	1.269444000	2.641552000
1	0.288487000	-1.939441000	4.253244000
1	-2.034479000	2.429616000	4.834285000
1	0.362816000	-0.778513000	6.451116000
1	-0.816677000	1.402519000	6.755411000
6	0.618920000	1.653062000	0.680818000
6	1.463527000	1.671697000	1.820743000
6	0.341743000	2.871362000	0.002949000
6	2.009593000	2.869569000	2.267031000
6	0.886813000	4.061482000	0.462125000

6	1.721850000	4.063287000	1.592153000
1	1.704860000	0.753061000	2.353050000
1	-0.305200000	2.865417000	-0.874774000
1	2.662225000	2.876569000	3.142380000
1	0.663987000	4.995239000	-0.058304000
1	2.154863000	5.001243000	1.948885000

TS2_PhPh



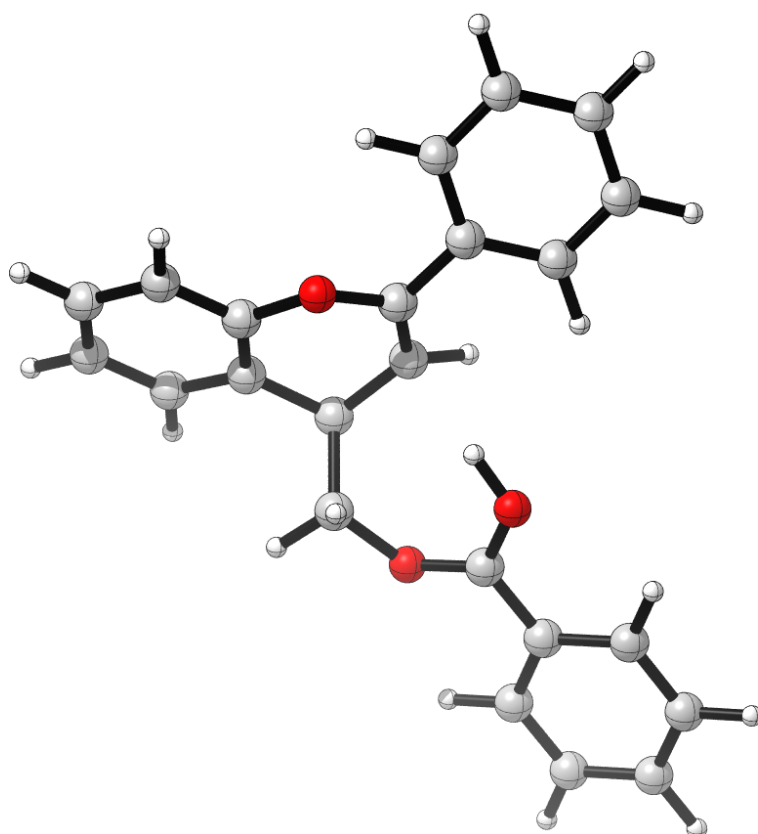
SPE = -1111.9049; H₂₉₈ = -1111.5212

6	-2.393242000	-1.375374000	-3.505093000
6	-2.000340000	-2.690626000	-3.224259000
6	-1.978880000	-0.333527000	-2.674451000
1	-2.316262000	-3.506963000	-3.877631000
1	-2.260211000	0.702684000	-2.873913000
6	-1.205143000	-2.961940000	-2.106764000
6	-1.187263000	-0.633831000	-1.564135000
1	-0.898905000	-3.989773000	-1.892263000
6	-0.793526000	-1.935164000	-1.243995000
1	-3.016123000	-1.156107000	-4.375492000
6	0.013651000	-2.209543000	0.005366000
6	0.315295000	-0.937113000	0.777878000

6	0.062202000	0.322584000	0.219499000
6	-0.717735000	-3.196459000	0.987867000
1	-1.705644000	-3.481585000	0.598983000
1	-0.132555000	-4.097356000	1.202330000
6	-1.204395000	-1.238405000	2.149537000
8	-0.861364000	-2.523256000	2.240942000
1	0.965088000	-2.686371000	-0.281010000
8	-0.770997000	0.453461000	-0.802126000
8	-2.310975000	-1.018409000	1.420616000
1	-2.769240000	-0.205813000	1.692417000
1	1.154535000	-0.992113000	1.470101000
6	-0.967920000	-0.433138000	3.372322000
6	-1.512517000	0.858305000	3.498817000
6	-0.222218000	-0.977125000	4.435452000
6	-1.340993000	1.580792000	4.681347000
6	-0.052977000	-0.249256000	5.613779000
6	-0.616676000	1.026376000	5.742334000
1	-2.072782000	1.320251000	2.681105000
1	0.203697000	-1.976440000	4.341370000
1	-1.776189000	2.578299000	4.772719000
1	0.514527000	-0.683387000	6.440417000
1	-0.487231000	1.592142000	6.668475000
6	0.578428000	1.591688000	0.730995000
6	1.534565000	1.628809000	1.771099000
6	0.130372000	2.809778000	0.168589000
6	2.023154000	2.847712000	2.235727000
6	0.621458000	4.024242000	0.640517000
6	1.567774000	4.047124000	1.674231000

1	1.912486000	0.708456000	2.215864000
1	-0.601208000	2.793658000	-0.639800000
1	2.764722000	2.863904000	3.037963000
1	0.265851000	4.957231000	0.196942000
1	1.957712000	4.999742000	2.042331000

II3_PhPh



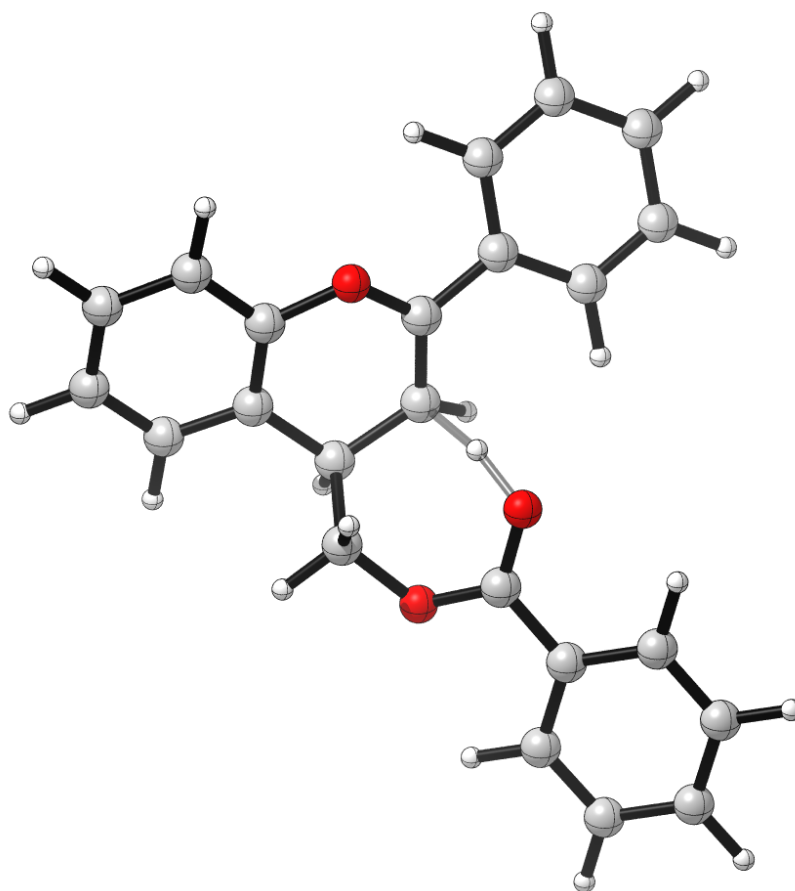
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6	-3.127567000	-3.247895000	-2.402142000
6	-1.852839000	-3.812815000	-2.547778000
6	-3.284408000	-2.031646000	-1.736373000
1	-1.727833000	-4.756932000	-3.082707000
1	-4.261901000	-1.555639000	-1.630098000
6	-0.740593000	-3.173107000	-1.996160000
6	-2.156591000	-1.397589000	-1.207457000
1	0.251828000	-3.621517000	-2.100019000
6	-0.878033000	-1.961137000	-1.302000000
1	-4.001719000	-3.749550000	-2.824170000
6	0.288579000	-1.265158000	-0.617383000
6	-0.014314000	0.217432000	-0.491941000

6	-1.291427000	0.683833000	-0.497357000
6	0.522526000	-1.973258000	0.731048000
1	-0.306526000	-1.807558000	1.435107000
1	0.665151000	-3.050231000	0.587448000
6	1.874071000	-0.545110000	2.174766000
8	1.770683000	-1.570259000	1.401719000
1	1.201327000	-1.407812000	-1.217279000
8	-2.352831000	-0.158822000	-0.626644000
8	0.990328000	0.394462000	2.205579000
1	0.327943000	0.363417000	1.457040000
1	0.802128000	0.938355000	-0.578843000
6	3.023539000	-0.450395000	3.056238000
6	3.159430000	0.669775000	3.908326000
6	3.986393000	-1.485088000	3.077144000
6	4.248173000	0.745645000	4.772815000
6	5.072178000	-1.393621000	3.943828000
6	5.202000000	-0.282560000	4.790492000
1	2.413280000	1.466417000	3.890779000
1	3.875159000	-2.348844000	2.419744000
1	4.360629000	1.608990000	5.432717000
1	5.819440000	-2.190625000	3.965698000
1	6.056582000	-0.214612000	5.469075000
6	-1.704479000	2.104657000	-0.451831000
6	-2.862762000	2.507983000	-1.144842000
6	-0.947658000	3.071266000	0.235698000
6	-3.240906000	3.852126000	-1.168824000
6	-1.337768000	4.412548000	0.221251000
6	-2.481904000	4.806781000	-0.483292000

1	-3.457433000	1.765910000	-1.679251000
1	-0.058209000	2.778184000	0.798569000
1	-4.133775000	4.154831000	-1.722235000
1	-0.748515000	5.152097000	0.768349000
1	-2.788539000	5.856454000	-0.492134000

TS3_PhPh



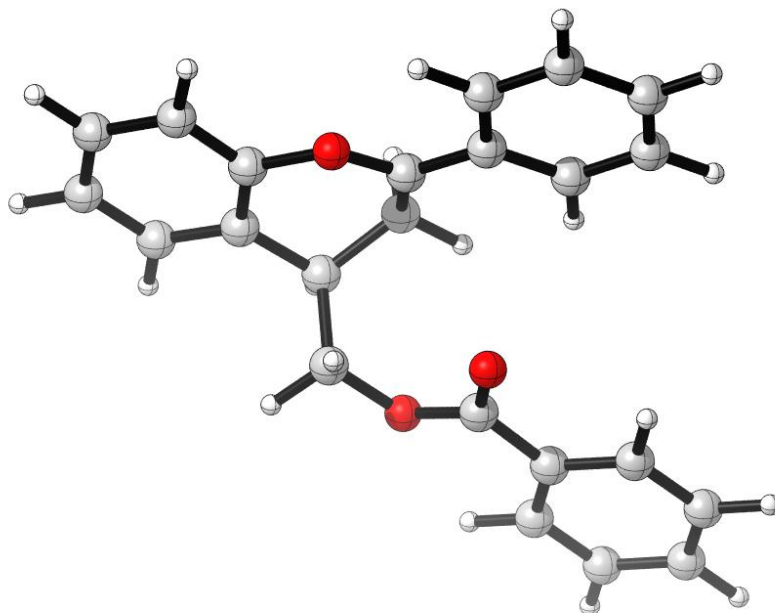
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6	-3.245483000	-3.292776000	-2.255513000
6	-2.000121000	-3.914941000	-2.408579000
6	-3.325800000	-2.024647000	-1.678206000
1	-1.932748000	-4.899387000	-2.876532000
1	-4.277307000	-1.500656000	-1.565099000
6	-0.840221000	-3.283006000	-1.953140000
6	-2.151565000	-1.409486000	-1.244662000
1	0.127596000	-3.779374000	-2.067860000
6	-0.898262000	-2.021635000	-1.342138000
1	-4.154965000	-3.789616000	-2.600847000
6	0.324170000	-1.352210000	-0.738745000
6	0.051302000	0.126133000	-0.445598000

6	-1.230481000	0.658119000	-0.551421000
6	0.705994000	-2.145313000	0.523583000
1	-0.125736000	-2.179004000	1.243301000
1	1.004831000	-3.167960000	0.266275000
6	1.754651000	-0.616176000	2.059145000
8	1.876485000	-1.608359000	1.216917000
1	1.168044000	-1.428126000	-1.443141000
8	-2.292711000	-0.112389000	-0.752661000
8	0.734519000	0.130950000	2.056871000
1	0.227282000	0.182079000	0.971425000
1	0.860714000	0.827766000	-0.667652000
6	2.858664000	-0.409606000	2.998083000
6	2.779339000	0.639730000	3.938030000
6	3.995955000	-1.245021000	2.963856000
6	3.825487000	0.846200000	4.835530000
6	5.041708000	-1.022070000	3.858006000
6	4.957227000	0.019499000	4.793340000
1	1.895042000	1.279164000	3.964241000
1	4.057620000	-2.056509000	2.236653000
1	3.763027000	1.657157000	5.565262000
1	5.928619000	-1.659518000	3.824550000
1	5.780988000	0.192139000	5.491638000
6	-1.556590000	2.086261000	-0.420755000
6	-2.736543000	2.588792000	-1.007063000
6	-0.691785000	2.969047000	0.259016000
6	-3.034287000	3.949712000	-0.928728000
6	-1.005827000	4.324333000	0.349695000
6	-2.174197000	4.817704000	-0.246138000

1	-3.408262000	1.911645000	-1.536195000
1	0.215589000	2.596481000	0.738670000
1	-3.942212000	4.335258000	-1.398940000
1	-0.336944000	4.998518000	0.889618000
1	-2.419970000	5.880483000	-0.171423000

II4_PhPh



SPE = -1111.9473; H₂₉₈ = -1111.5635

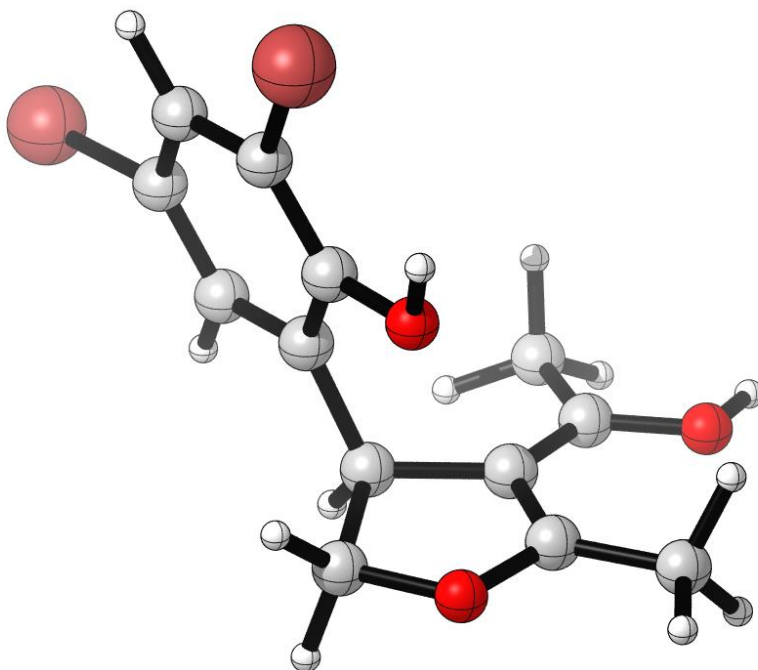
6	-2.170007000	-2.804169000	-3.411558000
6	-0.913537000	-3.294633000	-3.034187000
6	-2.774591000	-1.785943000	-2.670260000
1	-0.440809000	-4.088110000	-3.617383000
1	-3.749143000	-1.373674000	-2.938663000
6	-0.250470000	-2.766468000	-1.920174000
6	-2.088111000	-1.284951000	-1.567272000
1	0.733899000	-3.146134000	-1.635472000
6	-0.829008000	-1.740078000	-1.165037000
1	-2.682534000	-3.214566000	-4.284154000
6	-0.189588000	-1.112116000	0.053938000
6	-0.663086000	0.350300000	0.147631000

6	-2.133962000	0.513838000	-0.010268000
6	-0.480091000	-1.964937000	1.303702000
1	-1.559404000	-2.058568000	1.488996000
1	-0.051460000	-2.965261000	1.159720000
6	-0.566603000	-0.651873000	3.294005000
8	0.164773000	-1.429790000	2.470321000
1	0.901698000	-1.093657000	-0.083888000
8	-2.741787000	-0.276577000	-0.839617000
8	-1.720774000	-0.350274000	3.054934000
1	-0.292153000	0.858968000	1.041168000
1	-0.234027000	0.910711000	-0.708431000
6	0.186273000	-0.184474000	4.490270000
6	-0.436985000	0.756118000	5.330578000
6	1.478785000	-0.645684000	4.797569000
6	0.226712000	1.240188000	6.458339000
6	2.134157000	-0.167461000	5.935280000
6	1.513314000	0.777271000	6.762361000
1	-1.441556000	1.103979000	5.083205000
1	1.965534000	-1.375329000	4.148153000
1	-0.259570000	1.975593000	7.104476000
1	3.133601000	-0.534735000	6.181090000
1	2.034077000	1.156386000	7.645696000
6	-2.939914000	1.537048000	0.598995000
6	-4.277323000	1.747894000	0.165219000
6	-2.404142000	2.366444000	1.617150000
6	-5.036135000	2.766162000	0.726695000
6	-3.177171000	3.375867000	2.178947000
6	-4.490845000	3.578407000	1.734481000

1	-4.699041000	1.120564000	-0.621074000
1	-1.390564000	2.208743000	1.981120000
1	-6.056460000	2.940879000	0.378664000
1	-2.760189000	4.006897000	2.966720000
1	-5.097069000	4.372848000	2.177391000

To Table S3

2i-H⁺

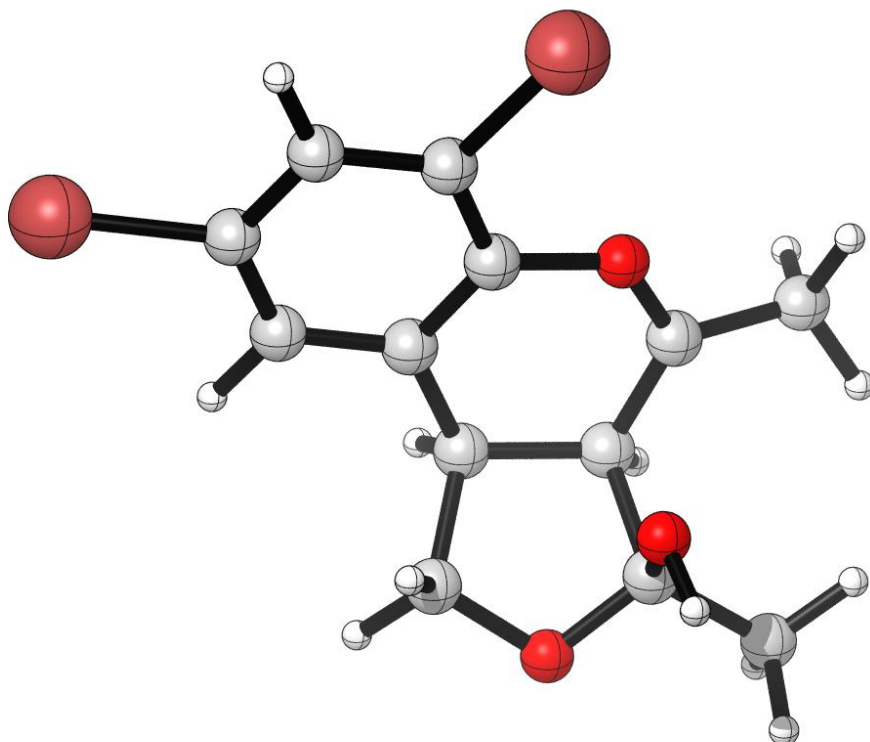


SPE = -5875.2275; H₂₉₈ = -5874.9741

6	0.390236000	2.225623000	4.874349000
1	0.685937000	3.119623000	4.307347000
6	-1.023039000	1.856952000	4.431783000
6	-1.658837000	0.703142000	4.944755000
6	-2.929068000	0.349832000	4.454615000
6	-3.585626000	1.111766000	3.487737000
1	-4.566728000	0.809107000	3.121487000
6	-2.947131000	2.250818000	2.996276000
6	-1.680492000	2.620548000	3.459044000
1	-1.187461000	3.501821000	3.045007000
6	0.590219000	2.461505000	6.373798000

6	1.429530000	1.105910000	4.617186000
1	1.024942000	0.220578000	4.114052000
1	2.318240000	1.465564000	4.081794000
6	1.430983000	1.446127000	6.872024000
8	1.890533000	0.671423000	5.933322000
6	1.868904000	1.153533000	8.256882000
1	2.531305000	0.279169000	8.270222000
1	2.388039000	2.029686000	8.676719000
1	0.990521000	0.976577000	8.896558000
8	-0.997828000	-0.025230000	5.863057000
1	-1.519437000	-0.806067000	6.123691000
6	0.110891000	3.530162000	7.118048000
8	0.363421000	3.556551000	8.410381000
6	-0.670336000	4.655888000	6.536234000
1	-0.440055000	5.589899000	7.071880000
1	-0.459926000	4.791325000	5.467802000
1	-1.750370000	4.455246000	6.657357000
1	0.017242000	4.364390000	8.829537000
35	-3.814167000	3.298790000	1.652290000
35	-3.743452000	-1.240921000	5.128823000

II2i

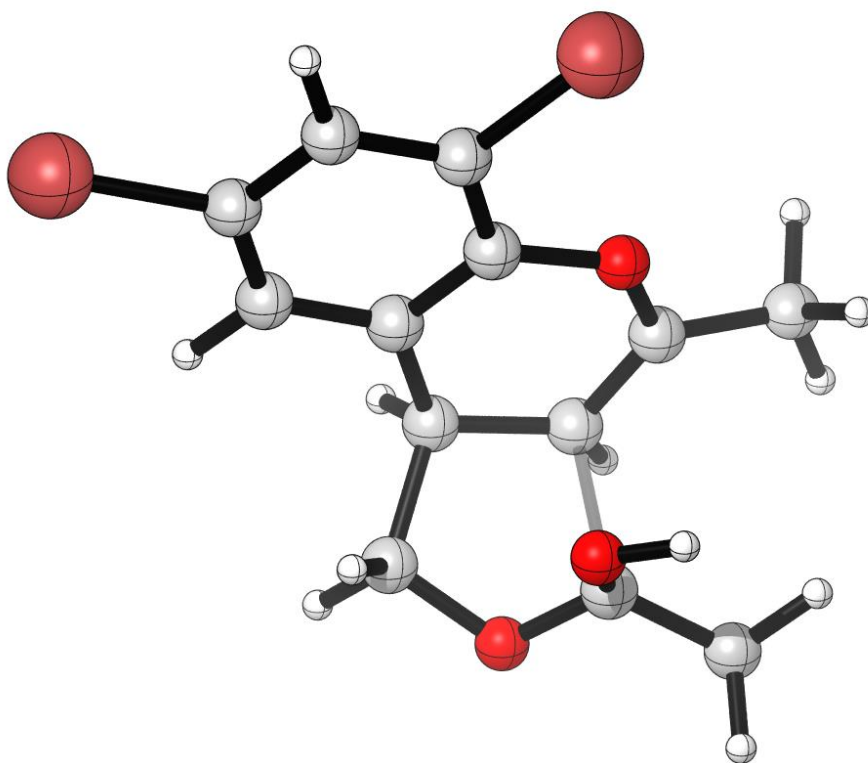


SPE = -5875.1993; H₂₉₈ = -5874.9470

6	-0.952620000	-1.538618000	-3.545440000
6	-1.283777000	-2.878865000	-3.317797000
6	-0.119483000	-0.888548000	-2.634184000
6	-0.835529000	-3.564005000	-2.185179000
6	0.353088000	-1.594743000	-1.519714000
1	-1.128849000	-4.601418000	-2.017505000
6	-0.009121000	-2.916713000	-1.260536000
1	-1.327826000	-1.007328000	-4.420136000
6	0.441496000	-3.599628000	0.004613000
6	1.366220000	-2.734208000	0.900981000
6	1.852409000	-1.473156000	0.311361000
6	-0.767281000	-3.924012000	0.945570000

1	-1.643992000	-3.319074000	0.666572000
1	-1.043451000	-4.985989000	0.939640000
6	0.458711000	-2.434486000	2.181749000
8	-0.324862000	-3.589322000	2.251603000
6	1.175153000	-2.260244000	3.506770000
1	0.418349000	-2.127438000	4.296287000
1	1.777641000	-3.147371000	3.747078000
1	1.818775000	-1.370413000	3.500574000
6	3.035189000	-0.760849000	0.817262000
1	3.156144000	-0.874009000	1.902180000
1	3.904129000	-1.267746000	0.349618000
1	3.042513000	0.290782000	0.503044000
1	0.963093000	-4.529396000	-0.260766000
8	1.299137000	-0.951131000	-0.718906000
8	-0.287633000	-1.300565000	1.810896000
1	-0.843598000	-1.020331000	2.556352000
1	2.236890000	-3.301185000	1.256123000
35	-2.372112000	-3.788665000	-4.582642000
35	0.357524000	0.920377000	-2.918167000

TS2i

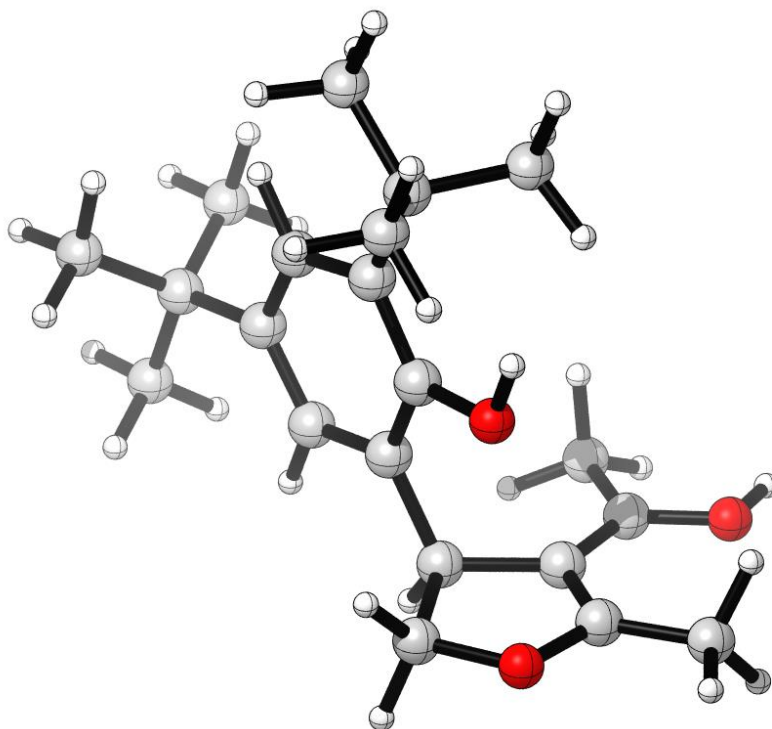


SPE = -5875.1890; H₂₉₈ = -5874.9382

6	-0.558667000	-1.760654000	-3.697607000
6	-1.283438000	-2.871375000	-3.253407000
6	0.310990000	-1.127884000	-2.808776000
6	-1.172865000	-3.337439000	-1.941935000
6	0.425146000	-1.598286000	-1.492618000
1	-1.750778000	-4.204439000	-1.617250000
6	-0.318391000	-2.692068000	-1.039109000
1	-0.656913000	-1.396075000	-4.720438000
6	-0.203886000	-3.151377000	0.399492000
6	0.829572000	-2.348026000	1.173142000
6	1.649677000	-1.426270000	0.522253000
6	-1.566921000	-3.032899000	1.180295000

1	-2.327169000	-2.513730000	0.579521000
1	-1.952613000	-4.003117000	1.510503000
6	-0.517004000	-1.223269000	2.165600000
8	-1.284996000	-2.292845000	2.372009000
6	0.098810000	-0.641782000	3.401527000
1	-0.705657000	-0.160814000	3.983693000
1	0.557296000	-1.428816000	4.013310000
1	0.845868000	0.123053000	3.150065000
6	2.867857000	-0.809638000	1.101724000
1	3.011453000	-1.100968000	2.148800000
1	3.736116000	-1.156581000	0.514007000
1	2.832746000	0.287225000	1.001297000
1	0.095432000	-4.210705000	0.406818000
8	1.355083000	-0.970382000	-0.678694000
8	-1.016803000	-0.385025000	1.243928000
1	-0.624303000	0.501523000	1.313905000
1	1.290421000	-2.840448000	2.031663000
35	-2.436336000	-3.773811000	-4.472171000
35	1.352224000	0.344509000	-3.399431000

2j-H⁺



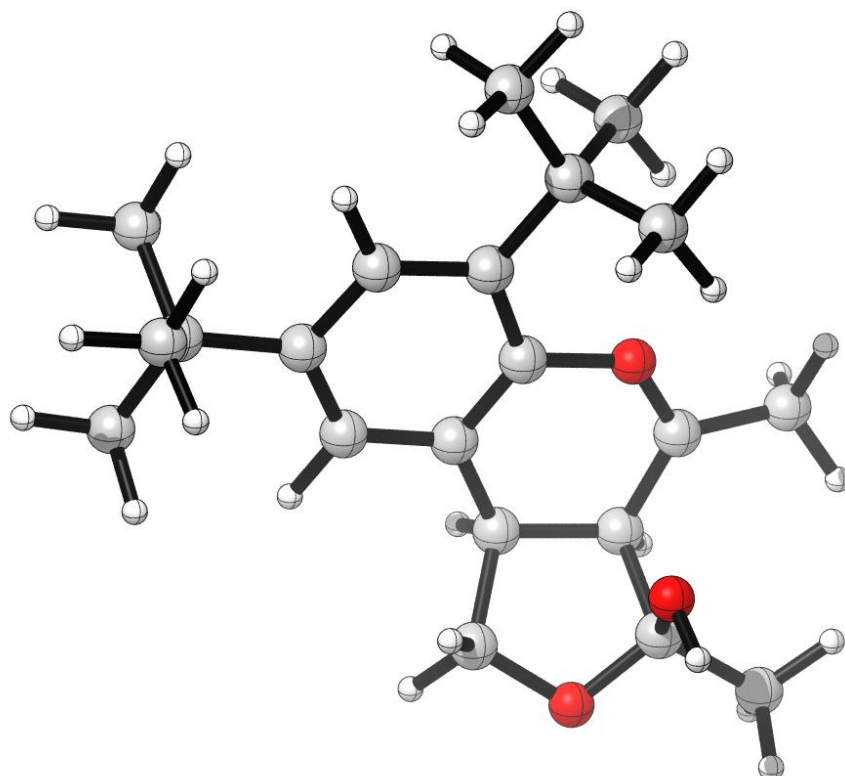
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6	-1.006324000	3.419371000	5.902032000
1	-1.023377000	4.422075000	5.450345000
6	-1.624639000	2.458544000	4.893676000
6	-1.834371000	1.105795000	5.222230000
6	-2.445703000	0.214233000	4.304998000
6	-2.783936000	0.740225000	3.048883000
1	-3.256850000	0.074424000	2.328700000
6	-2.551709000	2.073325000	2.662907000
6	-1.974260000	2.918187000	3.616654000
1	-1.776427000	3.965418000	3.382257000
6	-1.680149000	3.453413000	7.275855000
6	0.452930000	3.075965000	6.297279000

1	0.843911000	2.172171000	5.815225000
1	1.152430000	3.908508000	6.143520000
6	-0.746855000	3.021111000	8.237837000
8	0.434983000	2.808538000	7.735856000
6	-0.905830000	2.776559000	9.689159000
1	0.039410000	2.425559000	10.121187000
1	-1.236944000	3.698713000	10.191535000
1	-1.701296000	2.033769000	9.855227000
8	-1.401461000	0.738556000	6.465224000
1	-1.601248000	-0.186849000	6.652681000
6	-2.994081000	3.799711000	7.548168000
8	-3.429000000	3.683503000	8.789349000
6	-3.956916000	4.275187000	6.513950000
1	-4.666938000	4.991208000	6.957114000
1	-3.448100000	4.742207000	5.662205000
1	-4.539286000	3.417898000	6.131573000
1	-4.349348000	3.987944000	8.877135000
6	-2.956975000	2.546802000	1.252432000
6	-4.495198000	2.467470000	1.125040000
6	-2.301041000	1.639891000	0.186153000
1	-1.201856000	1.660140000	0.271517000
1	-2.628114000	0.592241000	0.274840000
1	-2.571228000	1.985395000	-0.825811000
1	-4.863927000	1.443102000	1.291690000
1	-4.821166000	2.786224000	0.120254000
1	-4.985286000	3.123112000	1.862061000
6	-2.523196000	3.998305000	0.971991000
1	-2.983812000	4.713133000	1.671019000

1	-1.429251000	4.120007000	1.027338000
1	-2.839384000	4.285679000	-0.043592000
6	-2.754175000	-1.258065000	4.675281000
6	-1.453180000	-2.022660000	5.032373000
6	-3.409882000	-2.021670000	3.505918000
1	-4.357640000	-1.563365000	3.185968000
1	-2.744718000	-2.083623000	2.630500000
1	-3.634321000	-3.050971000	3.826478000
1	-0.758754000	-2.025979000	4.177082000
1	-1.688637000	-3.068405000	5.289795000
1	-0.901362000	-1.604649000	5.888672000
6	-3.751587000	-1.296114000	5.861563000
1	-4.692741000	-0.793409000	5.587167000
1	-3.987151000	-2.337523000	6.133238000
1	-3.375609000	-0.801527000	6.771020000

II2j



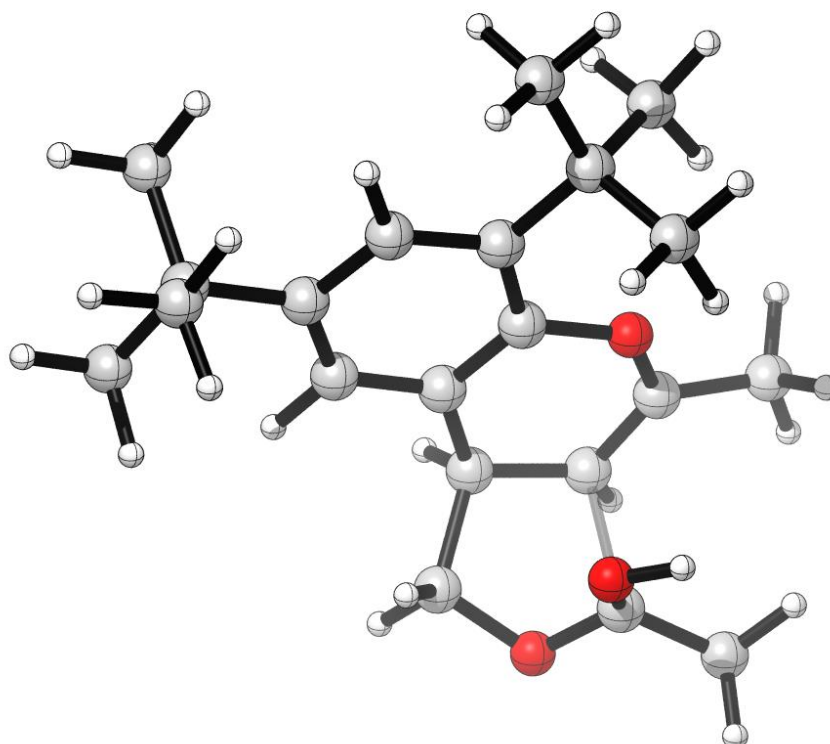
SPE = -1042.9922; H₂₉₈ = -1042.4897

6	-0.281357000	-1.861374000	-3.702126000
6	-1.085033000	-2.984404000	-3.416858000
6	0.338056000	-1.077339000	-2.720806000
6	-1.280600000	-3.326858000	-2.072828000
6	0.087994000	-1.490181000	-1.395177000
1	-1.889544000	-4.189566000	-1.803351000
6	-0.693955000	-2.585725000	-1.039369000
1	-0.126402000	-1.593763000	-4.745211000
6	-0.898350000	-2.970216000	0.408162000
6	-0.264892000	-1.991478000	1.428555000
6	0.665472000	-0.988836000	0.871158000
6	-2.405818000	-2.988466000	0.820362000

1	-3.017645000	-2.464828000	0.069173000
1	-2.796390000	-4.004164000	0.962639000
6	-1.523129000	-1.293501000	2.101552000
8	-2.473847000	-2.318689000	2.072484000
6	-1.367181000	-0.832546000	3.539739000
1	-2.348602000	-0.495341000	3.908522000
1	-1.018127000	-1.654110000	4.181586000
1	-0.671177000	0.013447000	3.616938000
6	1.606880000	-0.216511000	1.701872000
1	1.174388000	0.051040000	2.674012000
1	2.461423000	-0.888832000	1.912838000
1	1.977659000	0.669523000	1.171543000
1	-0.468578000	-3.970318000	0.563906000
8	0.746330000	-0.766728000	-0.380482000
8	-1.847404000	-0.243571000	1.221660000
1	-2.605965000	0.248405000	1.576629000
1	0.265361000	-2.528878000	2.227311000
6	-1.707149000	-3.786785000	-4.576210000
6	-2.507463000	-5.005298000	-4.078997000
6	-0.580311000	-4.299037000	-5.504547000
1	-0.000542000	-3.475053000	-5.947662000
1	0.118547000	-4.949686000	-4.953382000
1	-1.012463000	-4.885631000	-6.331826000
1	-1.873958000	-5.707865000	-3.514782000
1	-2.918991000	-5.550589000	-4.942932000
1	-3.353034000	-4.713365000	-3.436296000
6	1.232403000	0.131455000	-3.076780000
6	1.297736000	0.355027000	-4.601019000

6	2.683221000	-0.119502000	-2.588097000
1	2.749178000	-0.269202000	-1.502109000
1	3.113267000	-1.005576000	-3.081636000
1	3.315132000	0.746220000	-2.844111000
1	1.736358000	-0.504303000	-5.131922000
1	1.940271000	1.225320000	-4.806415000
1	0.307719000	0.566422000	-5.034145000
6	0.659535000	1.428592000	-2.448623000
1	-0.357570000	1.627381000	-2.823637000
1	0.616180000	1.392450000	-1.351560000
1	1.294082000	2.283981000	-2.731045000
6	-2.658296000	-2.865615000	-5.376480000
1	-2.121336000	-2.019925000	-5.833898000
1	-3.139817000	-3.434145000	-6.188967000
1	-3.451223000	-2.456621000	-4.729219000

TS2j



SPE = -1042.9782; H₂₉₈ = -1042.4747

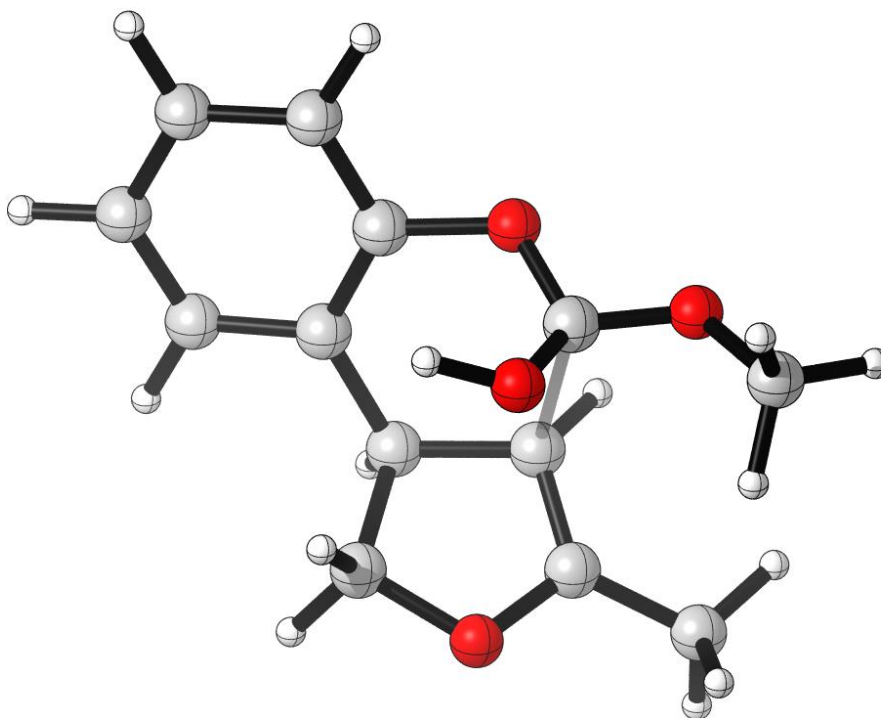
6	-0.157255000	-2.015363000	-3.656221000
6	-0.930807000	-3.124865000	-3.262303000
6	0.346294000	-1.054961000	-2.768741000
6	-1.193000000	-3.279171000	-1.898927000
6	0.013909000	-1.260956000	-1.410131000
1	-1.776687000	-4.125973000	-1.536809000
6	-0.730068000	-2.351990000	-0.956498000
1	0.064198000	-1.901392000	-4.715200000
6	-1.050035000	-2.540976000	0.513495000
6	-0.445949000	-1.445194000	1.365951000
6	0.404655000	-0.496311000	0.811809000
6	-2.598056000	-2.572238000	0.808137000

1	-3.182514000	-2.364762000	-0.099063000
1	-2.930029000	-3.515586000	1.255610000
6	-2.225230000	-0.417426000	1.568227000
8	-2.851110000	-1.565198000	1.798018000
6	-2.137981000	0.511124000	2.736616000
1	-3.142319000	0.929923000	2.918382000
1	-1.810979000	-0.030386000	3.632871000
1	-1.454441000	1.346302000	2.530922000
6	1.213770000	0.469271000	1.599753000
1	1.055603000	0.341833000	2.677654000
1	2.282390000	0.308707000	1.372460000
1	0.973259000	1.503588000	1.300307000
1	-0.641564000	-3.511071000	0.838096000
8	0.502028000	-0.324712000	-0.488103000
8	-2.465044000	0.086907000	0.350910000
1	-2.236136000	1.029955000	0.298244000
1	-0.276055000	-1.663376000	2.422327000
6	-1.448085000	-4.111359000	-4.324492000
6	-2.337275000	-5.206648000	-3.708073000
1	-2.704871000	-5.875050000	-4.502229000
1	-3.216128000	-4.781601000	-3.196340000
1	-1.782739000	-5.825755000	-2.984861000
1	-3.120682000	-2.806521000	-4.893359000
6	-2.279492000	-3.334775000	-5.371703000
1	-2.692319000	-4.028721000	-6.121736000
1	-1.671867000	-2.589465000	-5.908443000
1	-0.592807000	-5.506762000	-5.777677000
6	-0.242598000	-4.791167000	-5.015541000

1	0.369972000	-5.343783000	-4.283652000
1	0.409441000	-4.059372000	-5.518937000
6	1.198987000	0.137501000	-3.270745000
6	1.479509000	0.030382000	-4.784219000
1	2.112517000	0.876773000	-5.091895000
1	0.558642000	0.071201000	-5.385658000
1	2.023286000	-0.892675000	-5.041769000
1	-0.508979000	1.479799000	-3.585778000
6	0.442342000	1.467240000	-3.031129000
1	1.052534000	2.312646000	-3.390920000
1	0.222985000	1.637328000	-1.967138000
1	3.207898000	0.946698000	-3.028788000
6	2.577522000	0.173026000	-2.561967000
1	3.100544000	-0.791483000	-2.668543000
1	2.498997000	0.408015000	-1.492682000

To Figure S14

TS0_Me

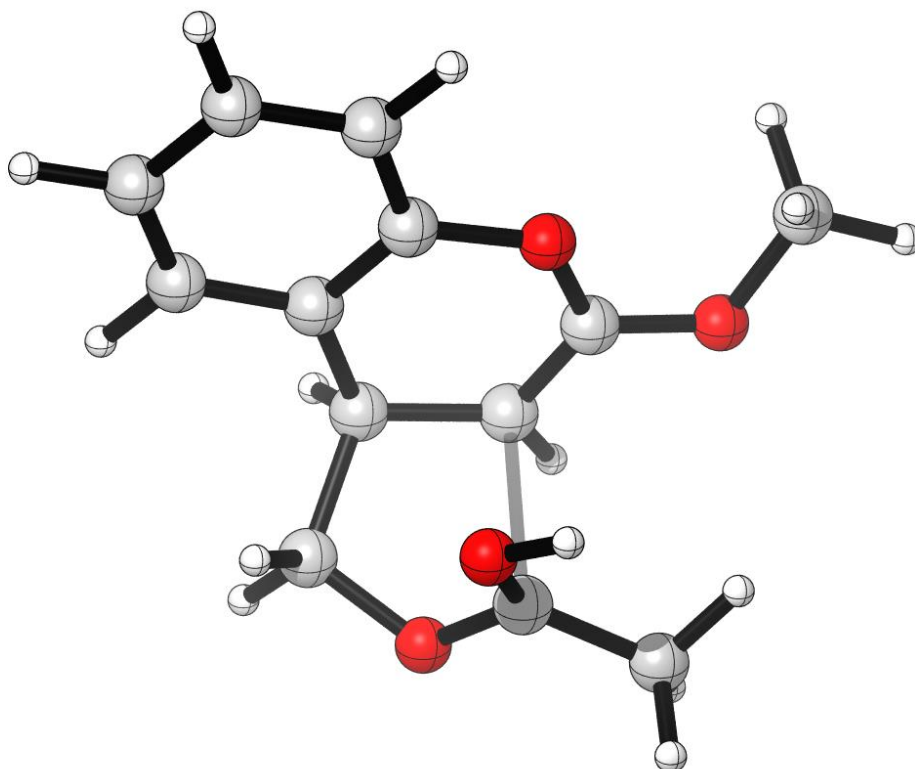


SPE = -804.0515; H₂₉₈ = -803.7758

6	1.667226000	1.431770000	3.991174000
1	1.196433000	0.494702000	4.336379000
6	0.541436000	2.370883000	3.609845000
6	0.477657000	3.048708000	2.384812000
6	-0.566450000	3.912239000	2.046799000
1	-0.560763000	4.399615000	1.070325000
6	-1.591841000	4.126528000	2.968025000
1	-2.411454000	4.803659000	2.716679000
6	-1.563642000	3.467222000	4.203974000
1	-2.364699000	3.626717000	4.929942000
6	-0.513734000	2.601167000	4.512528000

1	-0.507503000	2.081019000	5.474159000
6	2.702015000	1.090921000	2.925551000
6	2.577432000	1.985600000	5.123999000
1	2.577497000	3.084011000	5.181873000
1	2.353341000	1.576203000	6.116903000
6	3.931786000	1.042545000	3.555629000
8	3.926925000	1.566147000	4.772973000
6	5.225519000	0.481059000	3.092835000
1	6.047725000	1.187928000	3.283458000
1	5.442390000	-0.425902000	3.683189000
1	5.191400000	0.203818000	2.032104000
8	1.446892000	2.830583000	1.385282000
6	2.735818000	2.913999000	1.684239000
8	3.178999000	3.856006000	2.496111000
1	2.455826000	4.302615000	2.976581000
8	3.494703000	2.563076000	0.687338000
6	4.854064000	3.053813000	0.593127000
1	4.839395000	4.132917000	0.388555000
1	5.405626000	2.851492000	1.519604000
1	5.298244000	2.505845000	-0.243846000
1	2.479244000	0.452742000	2.070058000

TS2_Me

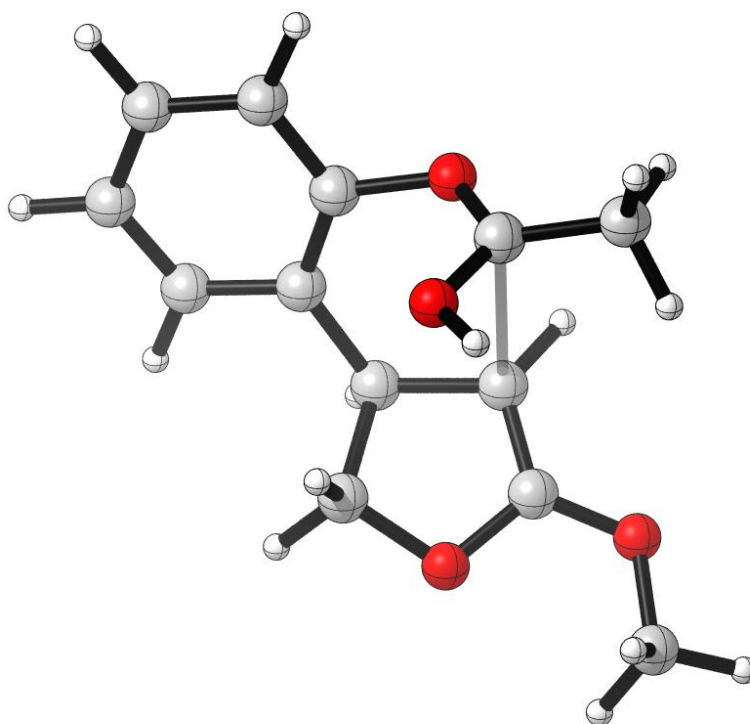


SPE = -804.0642; H₂₉₈ = -803.7885

6	-0.542794000	-1.629946000	-3.630726000
6	-1.264490000	-2.758314000	-3.220647000
6	0.342864000	-1.012870000	-2.747376000
1	-1.954412000	-3.247401000	-3.912275000
1	0.926777000	-0.136049000	-3.035453000
6	-1.100596000	-3.261175000	-1.927461000
6	0.481898000	-1.531509000	-1.459541000
1	-1.663740000	-4.145398000	-1.616459000
6	-0.226442000	-2.652131000	-1.011957000
1	-0.669155000	-1.227911000	-4.638885000
6	-0.063101000	-3.168250000	0.406772000
6	0.966804000	-2.370346000	1.166394000

6	1.657538000	-1.339202000	0.576221000
6	-1.430023000	-3.173042000	1.207972000
1	-2.239821000	-2.715979000	0.623682000
1	-1.725813000	-4.173165000	1.539771000
6	-0.717045000	-1.234810000	2.267168000
8	-1.223214000	-2.426012000	2.423578000
6	-0.084255000	-0.571994000	3.437043000
1	-0.863102000	-0.010023000	3.982828000
1	0.360735000	-1.319193000	4.104888000
1	0.683634000	0.141281000	3.103538000
1	0.260860000	-4.220980000	0.360777000
8	1.383618000	-0.861126000	-0.633143000
8	-1.229605000	-0.528140000	1.280790000
1	-0.936971000	0.400285000	1.299426000
1	1.409069000	-2.790963000	2.069501000
8	2.598883000	-0.687379000	1.226438000
6	3.468584000	0.233071000	0.531676000
1	4.128056000	0.644784000	1.303716000
1	4.058037000	-0.308759000	-0.222214000
1	2.892104000	1.036288000	0.055185000

TS0'_Me

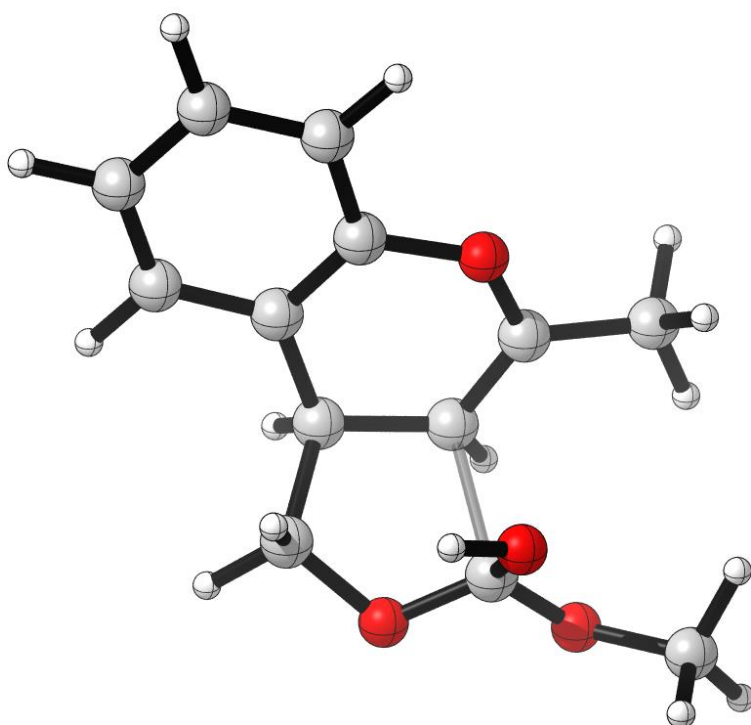


SPE = -804.0508; H₂₉₈ = -803.7755

6	1.788114000	1.817018000	3.852860000
1	0.979868000	1.184724000	3.436868000
6	1.149718000	3.183710000	4.072376000
6	1.663750000	4.420469000	3.669133000
6	1.032533000	5.643468000	3.886363000
1	1.492381000	6.559686000	3.510974000
6	-0.175642000	5.657537000	4.582973000
1	-0.682870000	6.604992000	4.778875000
6	-0.728543000	4.449503000	5.022583000
1	-1.677003000	4.446620000	5.564595000
6	-0.081068000	3.241938000	4.757106000
1	-0.540915000	2.306513000	5.087887000

6	3.043845000	1.644364000	3.012168000
6	2.273875000	1.193017000	5.193642000
1	2.668122000	1.969158000	5.870084000
1	1.514542000	0.599594000	5.719003000
6	3.803348000	0.700229000	3.624708000
8	3.366437000	0.314187000	4.842916000
8	2.876416000	4.479485000	2.917213000
6	4.017892000	4.262185000	3.458049000
8	4.068984000	4.160085000	4.738550000
1	4.979572000	4.066740000	5.080175000
1	3.171284000	1.937656000	1.971901000
6	5.217923000	4.286326000	2.595410000
1	5.843685000	3.403696000	2.796427000
1	4.923651000	4.322514000	1.540456000
1	5.805941000	5.185281000	2.851137000
8	4.885956000	0.096840000	3.157362000
6	5.686687000	-0.696562000	4.051027000
1	6.162149000	-0.059328000	4.813012000
1	5.081412000	-1.470324000	4.542798000
1	6.455365000	-1.164743000	3.424867000

TS2'_Me

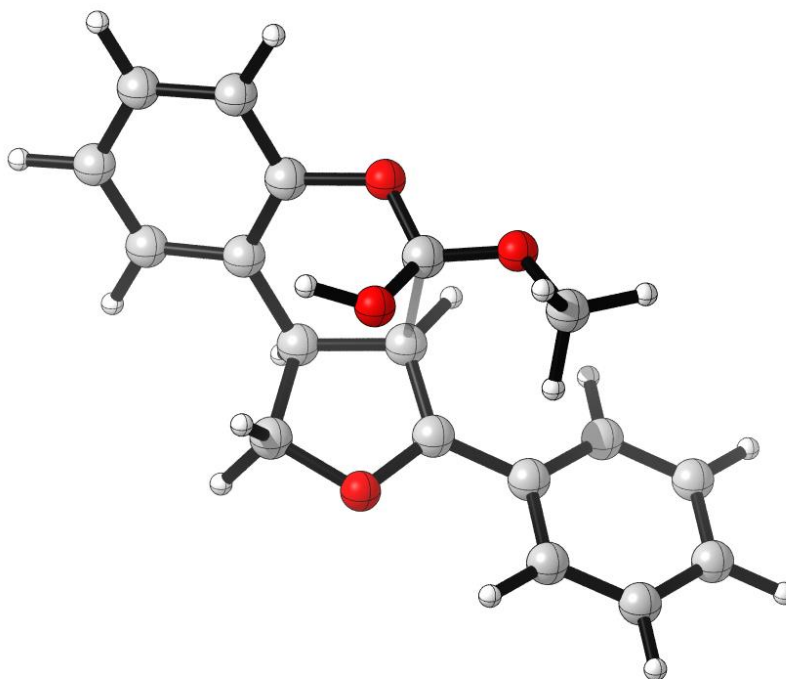


SPE = -804.0580; H₂₉₈ = -803.7830

6	1.614884000	1.878927000	3.683018000
1	0.922935000	1.390648000	2.981122000
6	1.077106000	3.237683000	4.065596000
6	1.909826000	4.359364000	4.033018000
6	1.489307000	5.632356000	4.418874000
1	2.187105000	6.470058000	4.357076000
6	0.174045000	5.796612000	4.855551000
1	-0.178855000	6.783029000	5.165479000
6	-0.690550000	4.694945000	4.895256000
1	-1.718750000	4.822060000	5.241768000
6	-0.241691000	3.430958000	4.503302000
1	-0.921779000	2.575677000	4.541896000

6	2.992743000	1.962746000	3.043894000
6	1.760029000	0.947280000	4.932697000
1	1.845362000	1.533076000	5.863511000
1	0.935498000	0.235074000	5.044892000
6	4.020470000	0.891376000	4.392588000
8	2.940904000	0.166045000	4.728457000
8	3.217782000	4.272081000	3.543006000
6	3.658481000	3.189355000	2.943429000
8	4.542005000	1.722322000	5.304521000
1	3.934911000	1.890619000	6.045647000
1	3.212668000	1.262499000	2.235546000
6	4.943506000	3.393581000	2.227933000
1	5.354638000	2.450143000	1.850964000
1	4.770898000	4.072358000	1.374542000
1	5.665317000	3.894259000	2.893061000
8	4.906039000	0.189138000	3.707790000
6	6.318451000	0.341218000	3.972235000
1	6.654332000	1.362474000	3.748534000
1	6.535378000	0.094789000	5.020456000
1	6.812937000	-0.368940000	3.302046000

TS0_Ph

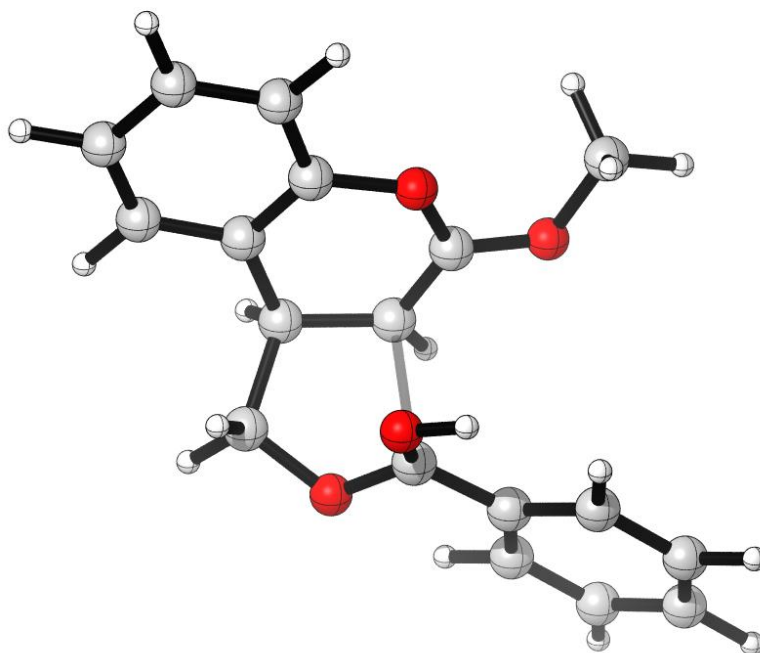


SPE = -995.5390; H₂₉₈ = -995.2073

6	1.804125000	1.787818000	3.968671000
1	1.141249000	0.904012000	3.957782000
6	0.905231000	2.996505000	3.780240000
6	1.143064000	4.001324000	2.829164000
6	0.284735000	5.085695000	2.634370000
1	0.524755000	5.823089000	1.865639000
6	-0.855671000	5.195775000	3.430308000
1	-1.534696000	6.040028000	3.289965000
6	-1.122943000	4.219693000	4.399596000
1	-2.017270000	4.297263000	5.022030000
6	-0.255514000	3.138023000	4.563924000
1	-0.486943000	2.367373000	5.304791000

6	2.911275000	1.572702000	2.949228000
6	2.619967000	1.794039000	5.293686000
1	2.793176000	2.803179000	5.693098000
1	2.186280000	1.171021000	6.085863000
6	4.012480000	1.084756000	3.631762000
8	3.916448000	1.227677000	4.953262000
8	2.248869000	3.931346000	1.958589000
6	3.450421000	3.681677000	2.455353000
8	3.819106000	4.192404000	3.614391000
1	3.073237000	4.598332000	4.097125000
8	4.361284000	3.543600000	1.537918000
6	5.755456000	3.750509000	1.881780000
1	5.902292000	4.789261000	2.205913000
1	6.058263000	3.059267000	2.676995000
1	6.309975000	3.542633000	0.961159000
1	2.707268000	1.317746000	1.910025000
6	5.240780000	0.478682000	3.115308000
6	6.404131000	0.438138000	3.913097000
6	5.274043000	-0.066899000	1.815951000
6	7.580364000	-0.115717000	3.408194000
6	6.450130000	-0.632832000	1.323705000
6	7.605941000	-0.652912000	2.114311000
1	6.382057000	0.862668000	4.917982000
1	4.374852000	-0.071224000	1.197093000
1	8.482195000	-0.129213000	4.025289000
1	6.465201000	-1.066631000	0.321393000
1	8.525694000	-1.094867000	1.722151000

TS2_Ph

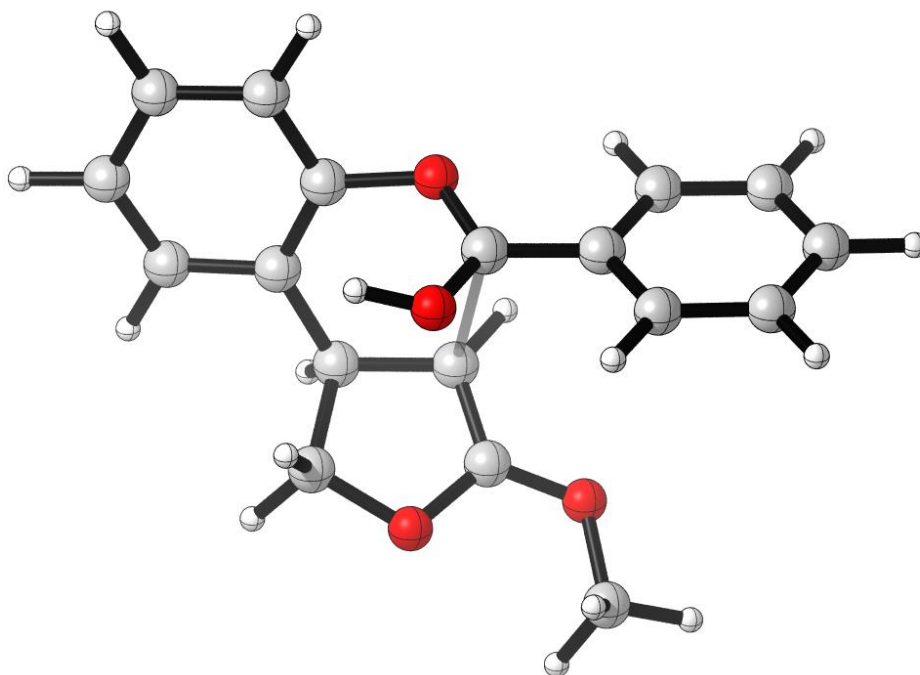


SPE = -995.5477; H₂₉₈ = -995.2168

6	0.064078000	-2.937253000	-3.403958000
6	-1.269389000	-3.262992000	-3.125738000
6	0.981155000	-2.812038000	-2.360230000
1	-1.988400000	-3.371970000	-3.940884000
1	2.028825000	-2.564579000	-2.542583000
6	-1.684062000	-3.455043000	-1.805485000
6	0.538364000	-3.005935000	-1.052138000
1	-2.724788000	-3.717573000	-1.595231000
6	-0.785028000	-3.323353000	-0.735238000
1	0.395641000	-2.783422000	-4.433858000
6	-1.228567000	-3.462503000	0.705980000
6	-0.064104000	-3.403037000	1.668299000

6	1.227877000	-3.239111000	1.192414000
6	-2.275446000	-2.340825000	1.083135000
1	-2.285332000	-1.540355000	0.330492000
1	-3.286493000	-2.737527000	1.222671000
6	-0.642876000	-1.391125000	2.438489000
8	-1.892153000	-1.805287000	2.352965000
1	-1.745205000	-4.427153000	0.831210000
8	1.512349000	-2.902689000	-0.054844000
8	-0.246650000	-0.597304000	1.447804000
1	0.566412000	-0.110041000	1.661762000
1	-0.150121000	-3.912108000	2.628077000
8	2.262912000	-3.333655000	1.988175000
6	3.605248000	-3.249293000	1.455246000
1	4.265389000	-3.428111000	2.310379000
1	3.755759000	-4.020770000	0.688153000
1	3.786958000	-2.254353000	1.025745000
6	-0.092123000	-1.255604000	3.797966000
6	-0.711741000	-1.937664000	4.864511000
6	1.016713000	-0.427917000	4.052900000
6	-0.238468000	-1.772325000	6.164734000
6	1.479960000	-0.258994000	5.358620000
6	0.850616000	-0.926060000	6.415397000
1	-1.569029000	-2.583310000	4.667389000
1	1.529712000	0.110295000	3.250719000
1	-0.725553000	-2.300239000	6.987617000
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1	1.215112000	-0.787765000	7.436644000

TS0'_Ph

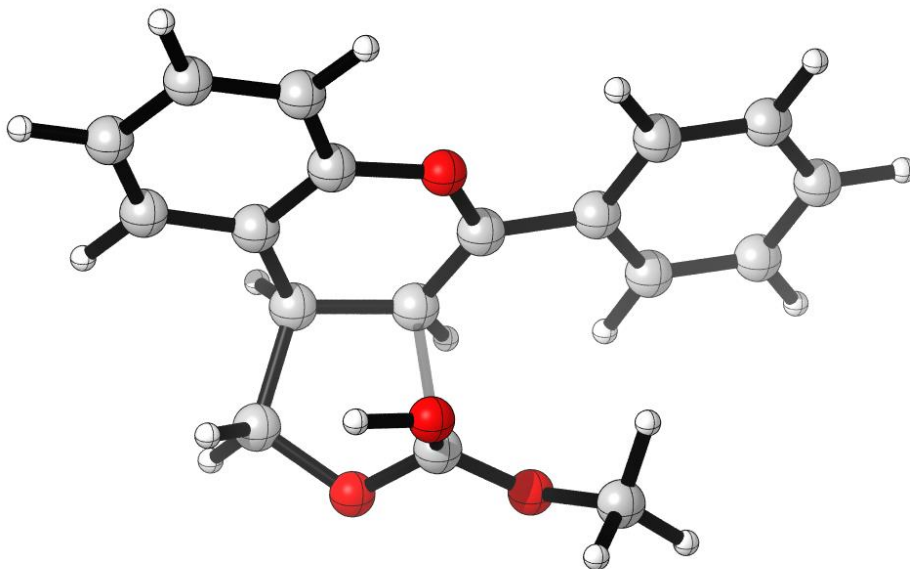


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6	1.813892000	1.909167000	3.819387000
1	1.041128000	1.272178000	3.350951000
6	1.133590000	3.251294000	4.064332000
6	1.645929000	4.508753000	3.706098000
6	0.969494000	5.709909000	3.927478000
1	1.424914000	6.645220000	3.596161000
6	-0.267860000	5.677823000	4.568390000
1	-0.805873000	6.608118000	4.763074000
6	-0.809091000	4.448012000	4.961964000
1	-1.776337000	4.411873000	5.468035000
6	-0.122204000	3.262274000	4.701428000
1	-0.568953000	2.308037000	4.994782000

6	3.082743000	1.862621000	2.996048000
6	2.293442000	1.227438000	5.142058000
1	2.476634000	1.954961000	5.946160000
1	1.610079000	0.453320000	5.513582000
6	3.945298000	1.009458000	3.617551000
8	3.560334000	0.589495000	4.831915000
8	2.889044000	4.620789000	3.033462000
6	3.983705000	4.202106000	3.614051000
8	4.056447000	4.091277000	4.909920000
1	3.211926000	4.310542000	5.354698000
1	3.170080000	2.138596000	1.948320000
8	5.095828000	0.574213000	3.153331000
6	5.946380000	-0.218476000	4.002012000
1	6.299915000	0.377832000	4.856047000
1	5.414111000	-1.107734000	4.367246000
1	6.793923000	-0.516828000	3.374740000
6	5.214693000	4.184255000	2.843935000
6	6.450005000	4.062999000	3.514092000
6	5.179247000	4.325542000	1.440386000
6	7.635912000	4.086497000	2.783932000
6	6.370729000	4.338725000	0.721790000
6	7.597994000	4.221706000	1.390158000
1	6.474770000	3.966654000	4.601048000
1	4.223233000	4.423627000	0.923499000
1	8.592892000	4.001701000	3.303668000
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1	8.529725000	4.239684000	0.819263000

TS2'_Ph



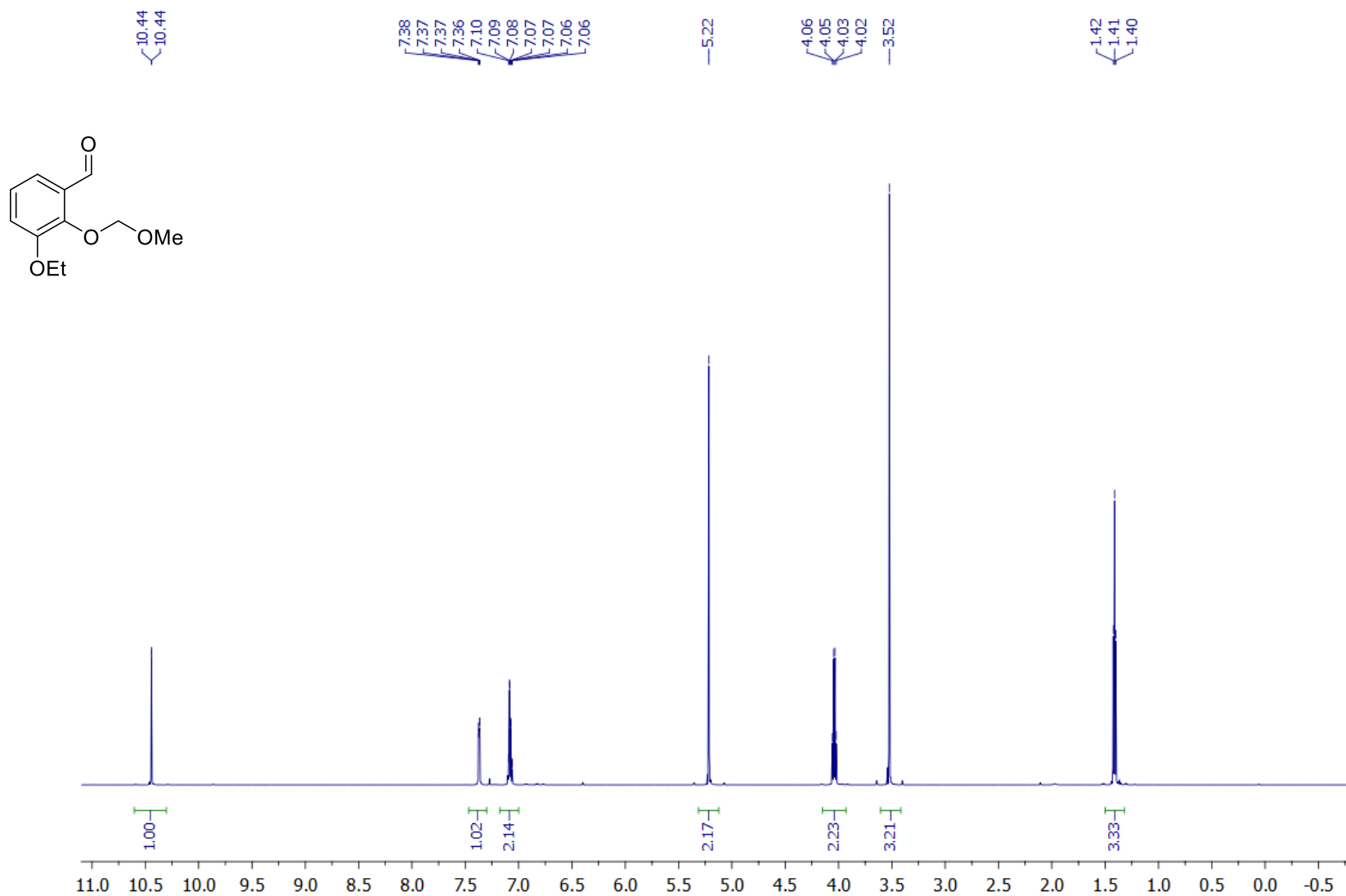
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6	2.520439000	3.797165000	4.763946000
6	2.642691000	4.406518000	6.014900000
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6	1.525743000	4.462375000	6.847857000
1	1.606083000	4.940873000	7.826564000
6	0.307603000	3.915746000	6.422551000
1	-0.572310000	3.973584000	7.067666000
6	0.216025000	3.295837000	5.173764000
1	-0.735406000	2.864675000	4.849600000

6	2.592575000	2.590228000	2.250836000
6	0.866931000	1.008032000	3.087787000
1	0.681972000	0.711402000	4.132668000
1	-0.015504000	0.752500000	2.491607000
6	3.166009000	0.658876000	2.786015000
8	1.935640000	0.214933000	2.542198000
8	3.653209000	3.836762000	3.960128000
6	3.648156000	3.369478000	2.717954000
8	3.604194000	0.761670000	4.042226000
1	2.894781000	0.648651000	4.698362000
1	2.563176000	2.412427000	1.176355000
8	4.046611000	0.245351000	1.904827000
6	5.403879000	-0.047024000	2.318041000
1	5.891616000	0.852716000	2.714877000
1	5.398055000	-0.839309000	3.078990000
1	5.910335000	-0.388933000	1.409474000
6	4.875723000	3.665018000	1.971934000
6	5.898343000	4.427156000	2.579857000
6	5.064001000	3.192477000	0.653957000
6	7.077300000	4.702060000	1.889718000
6	6.250961000	3.462645000	-0.025207000
6	7.258382000	4.218503000	0.587645000
1	5.760498000	4.803180000	3.593420000
1	4.290219000	2.609199000	0.153832000
1	7.860118000	5.295546000	2.368013000
1	6.390104000	3.082870000	-1.039918000
1	8.182869000	4.436631000	0.046992000

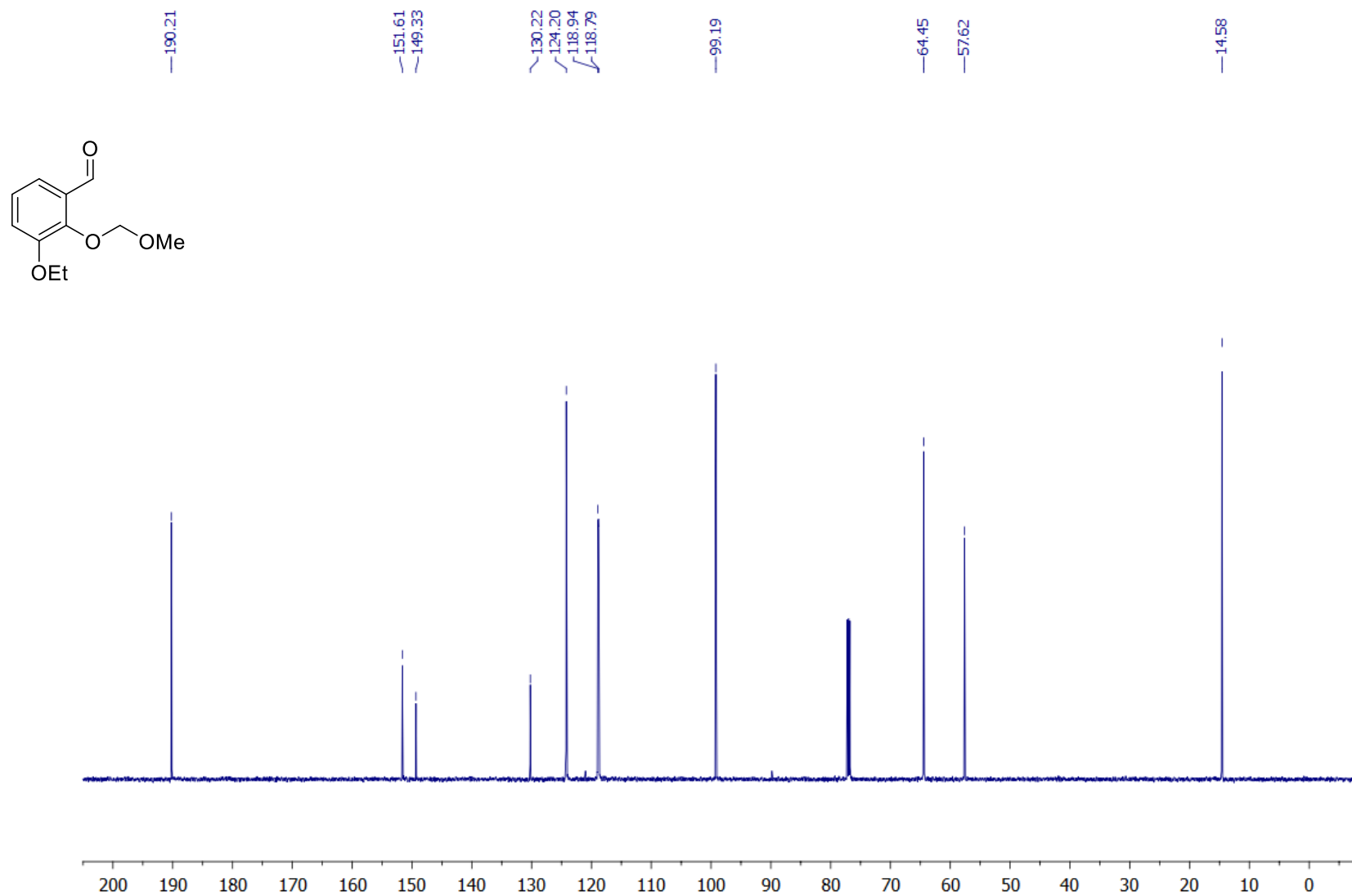
3-Ethoxy-2-(methoxymethoxy)benzaldehyde (S1h)

^1H NMR (CDCl_3 , 600 MHz)



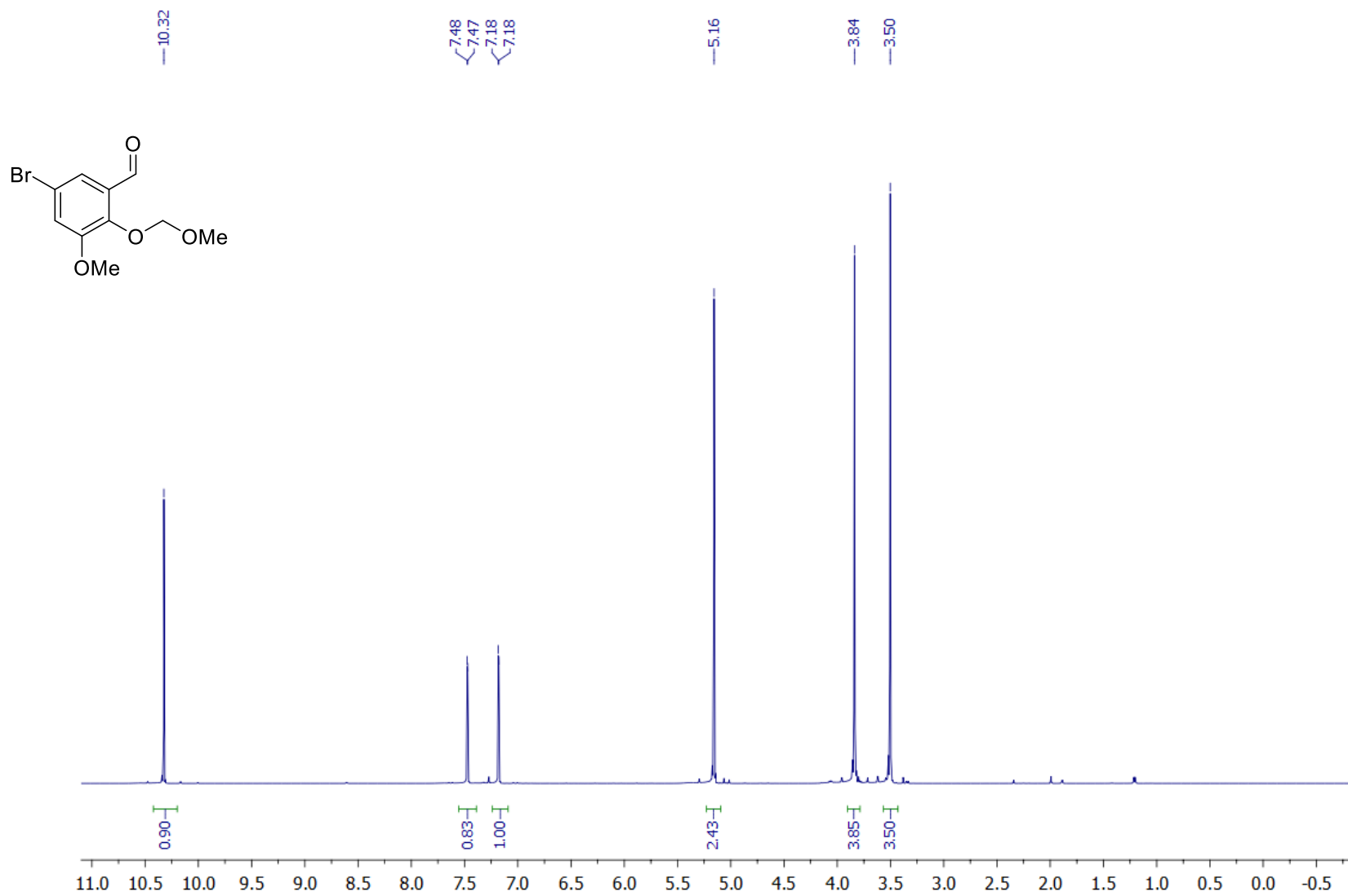
3-Ethoxy-2-(methoxymethoxy)benzaldehyde (S1h)

^{13}C NMR (CDCl_3 , 150 MHz)



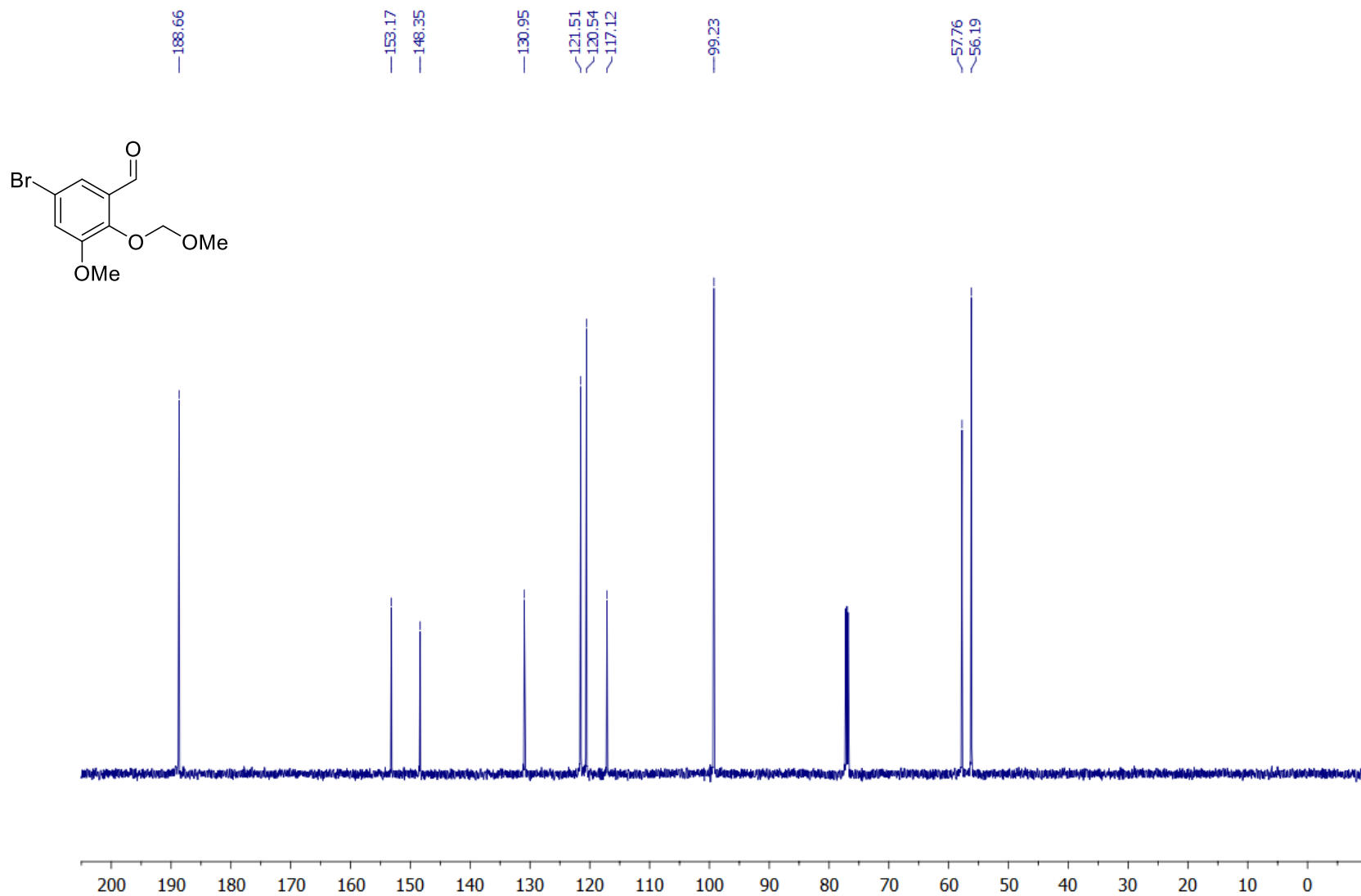
5-Brom-3-methoxy-2-(methoxymethoxy)benzaldehyde (S1k)

^1H NMR (CDCl_3 , 600 MHz)



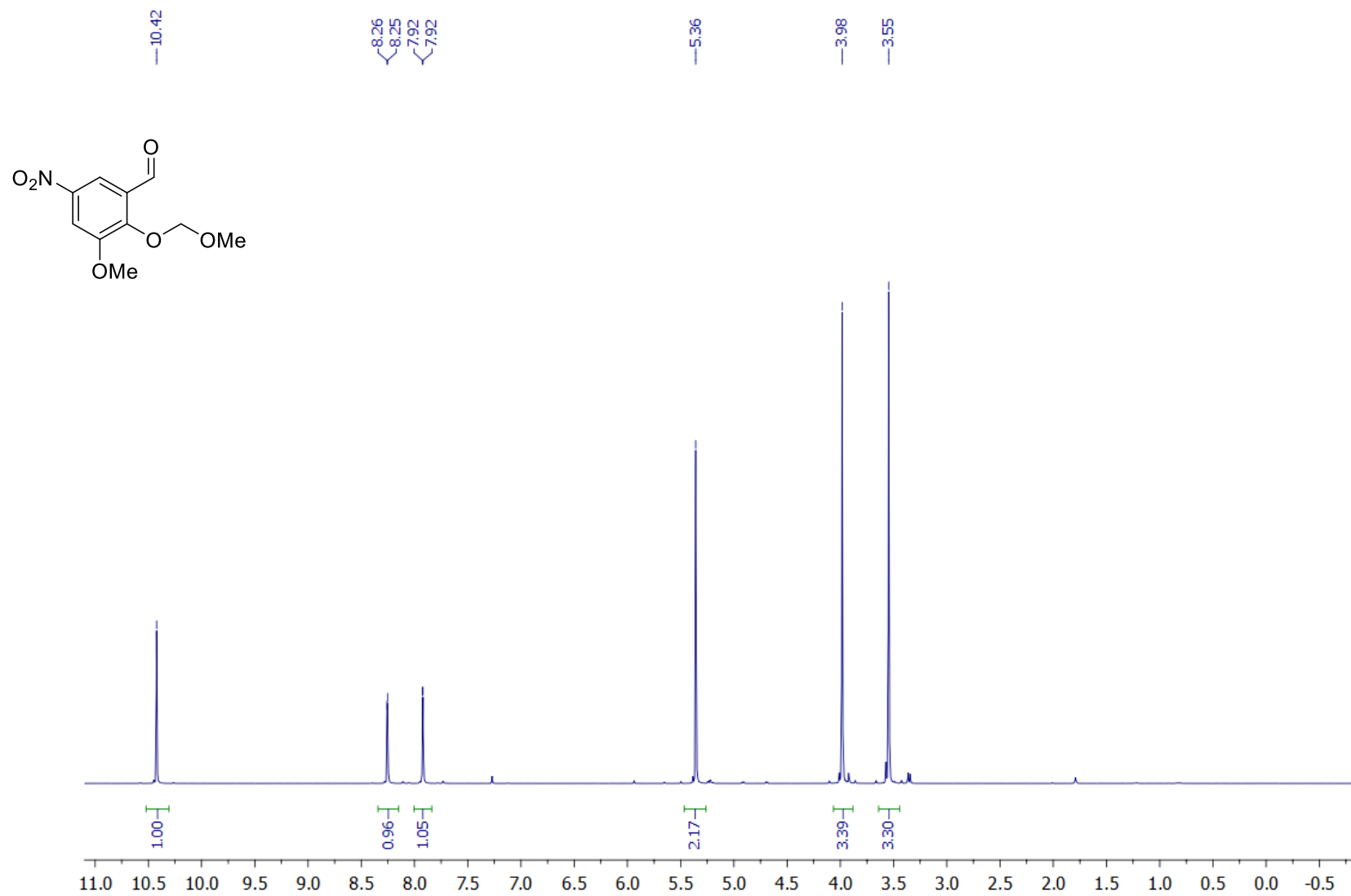
5-Brom-3-methoxy-2-(methoxymethoxy)benzaldehyde (S1k)

^{13}C NMR (CDCl_3 , 150 MHz)



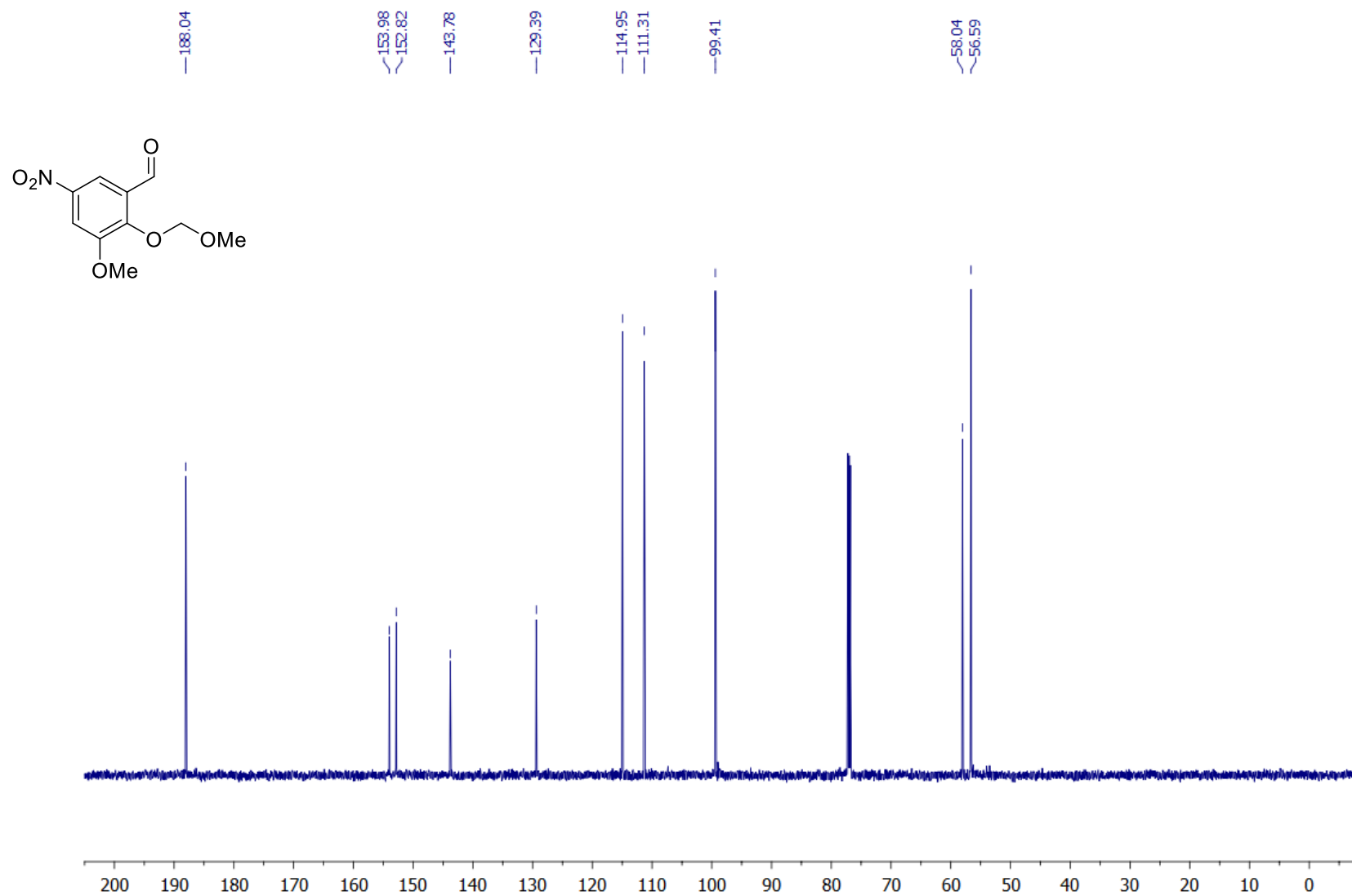
3-Methoxy-2-(methoxymethoxy)-5-nitrobenzaldehyde (S11)

^1H NMR (CDCl_3 , 600 MHz)



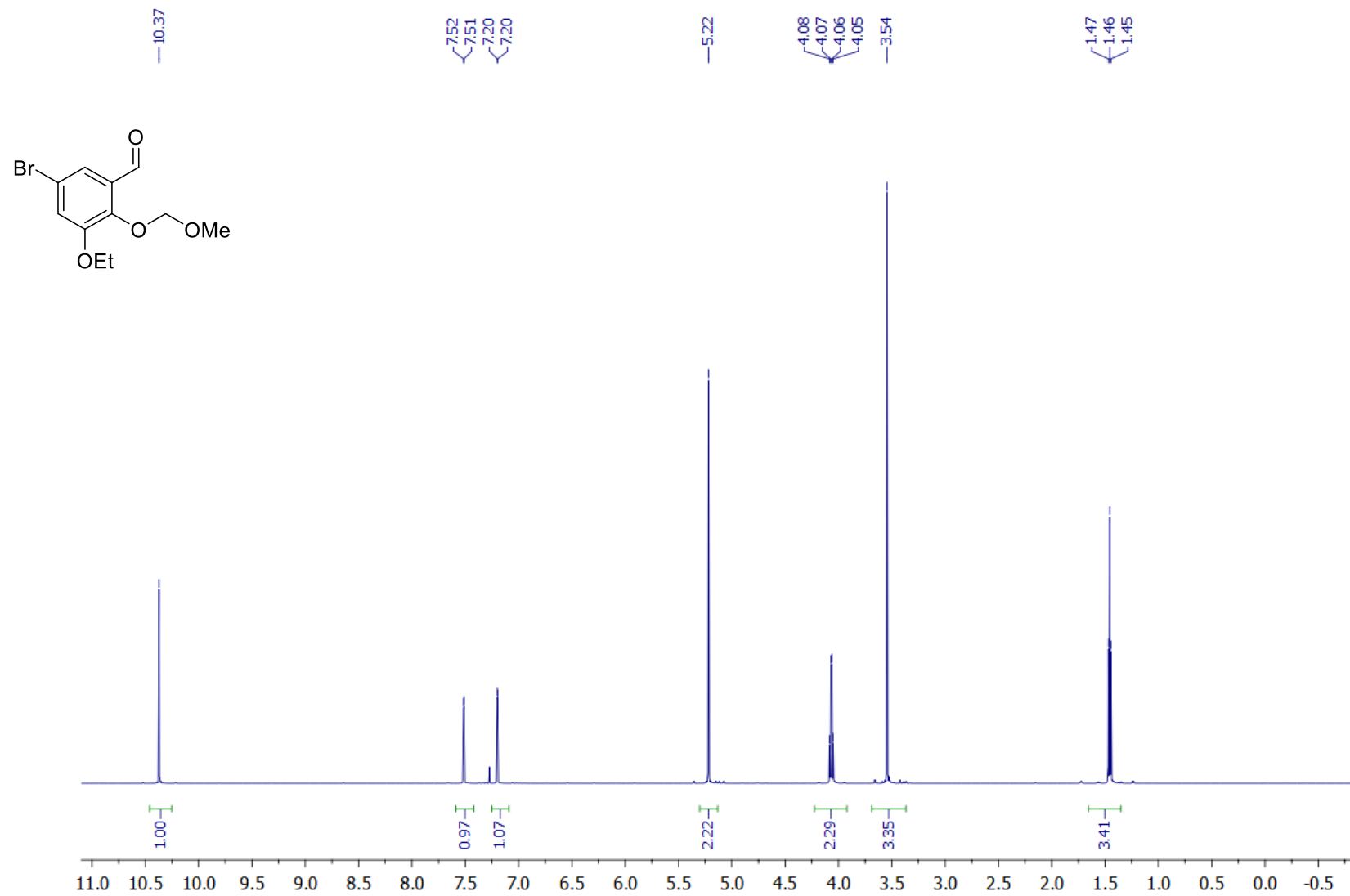
3-Methoxy-2-(methoxymethoxy)-5-nitrobenzaldehyde (S11)

^{13}C NMR (CDCl_3 , 150 MHz)



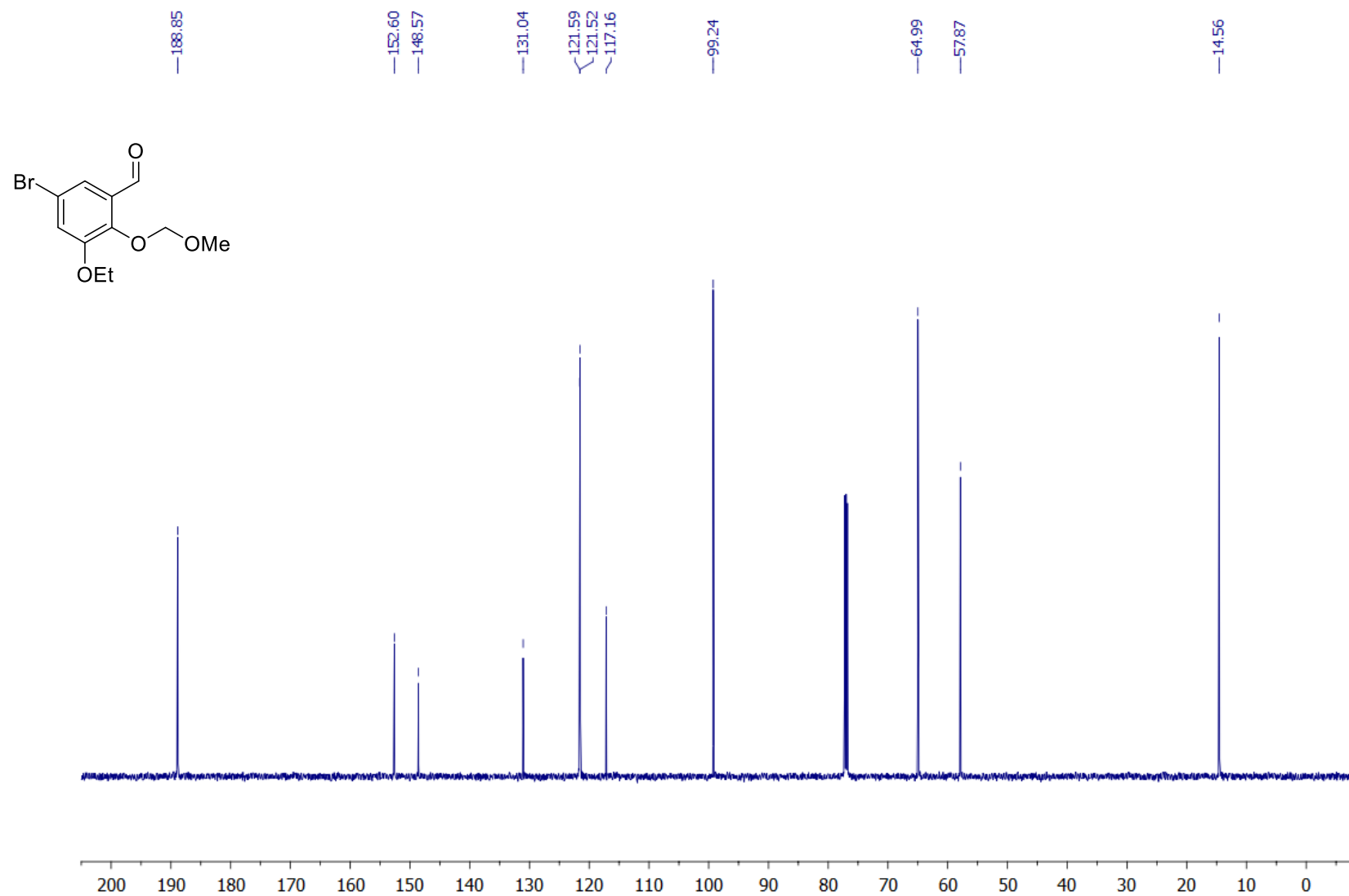
5-Brom-3-ethoxy-2-(methoxymethoxy)benzaldehyde (S1m)

^1H NMR (CDCl_3 , 600 MHz)



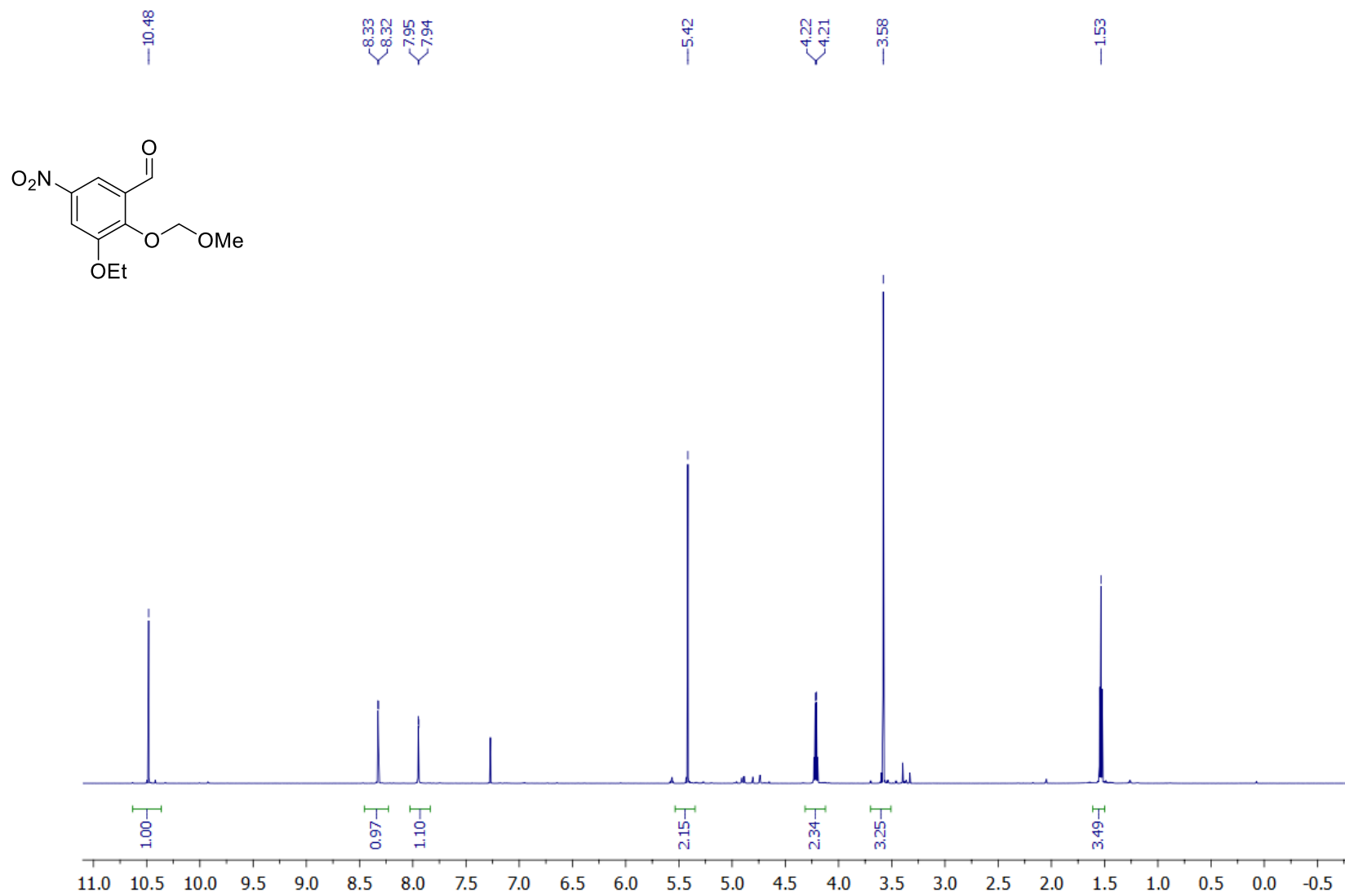
5-Brom-3-ethoxy-2-(methoxymethoxy)benzaldehyde (S1m)

^{13}C NMR (CDCl_3 , 150 MHz)



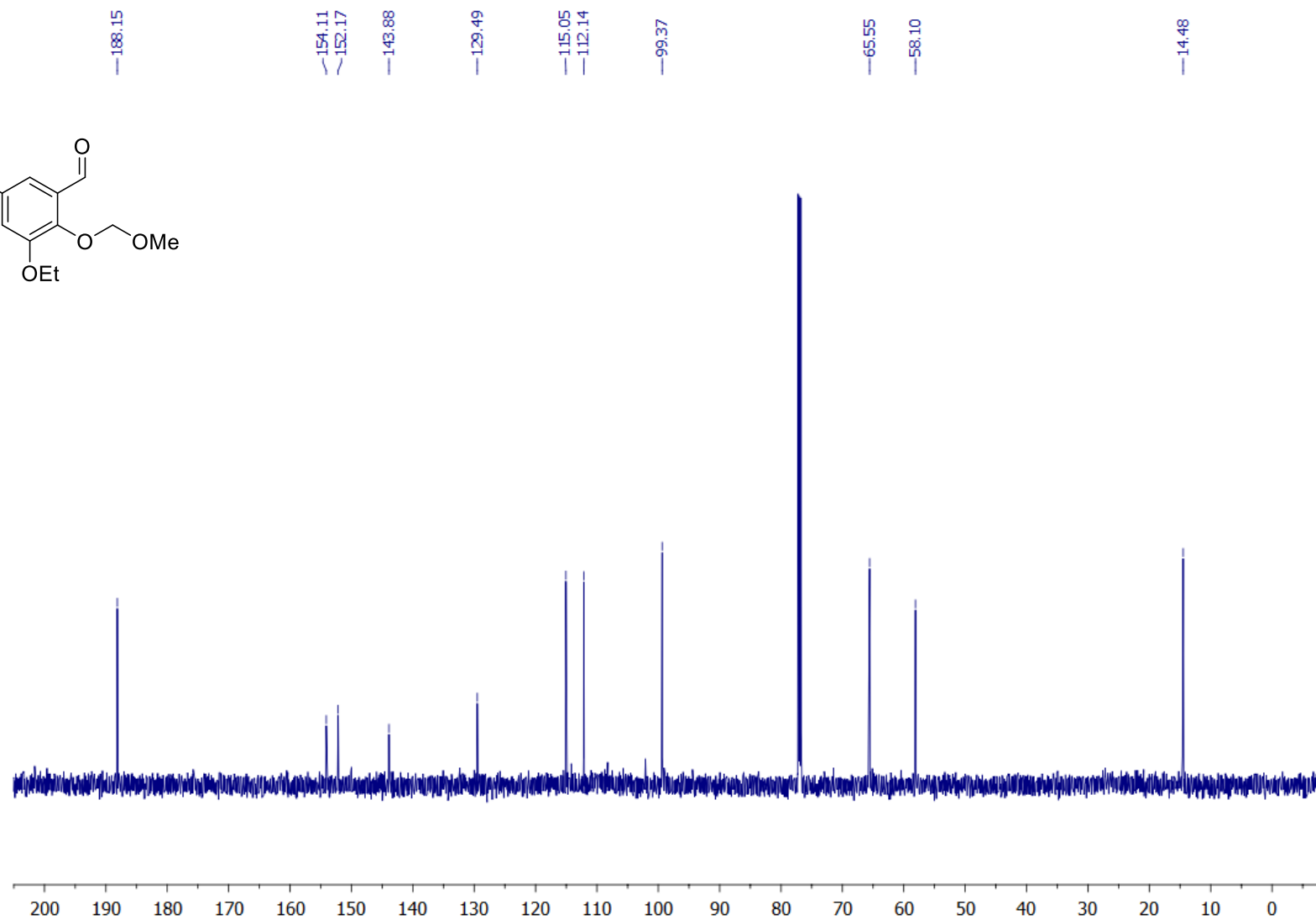
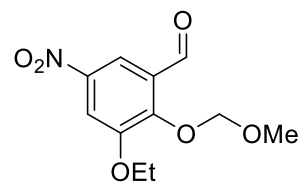
3-Ethoxy-2-(methoxymethoxy)-5-nitrobenzaldehyde (S1n)

^1H NMR (CDCl_3 , 600 MHz)



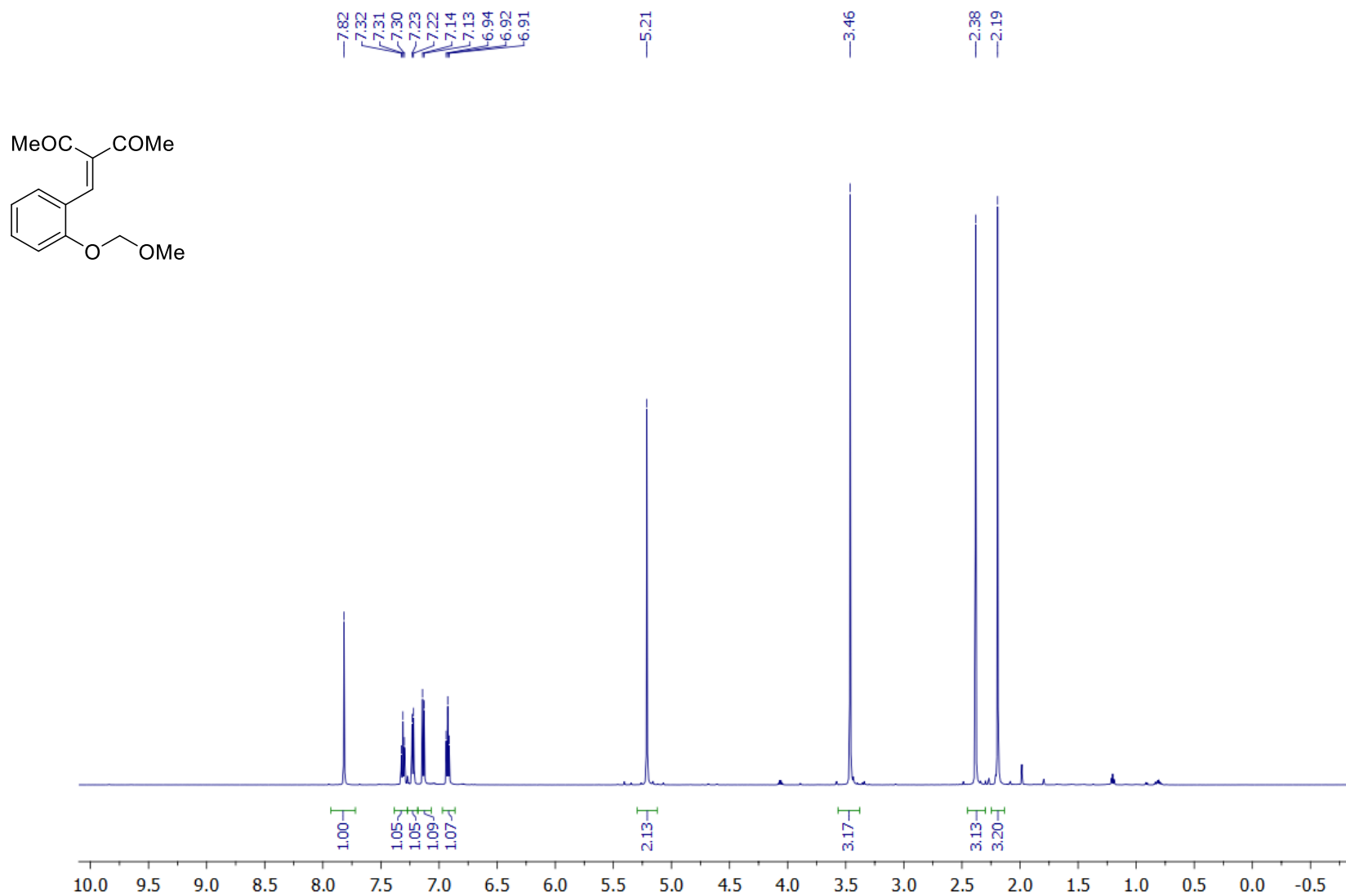
3-Ethoxy-2-(methoxymethoxy)-5-nitrobenzaldehyde (S1n)

^{13}C NMR (CDCl_3 , 150 MHz)



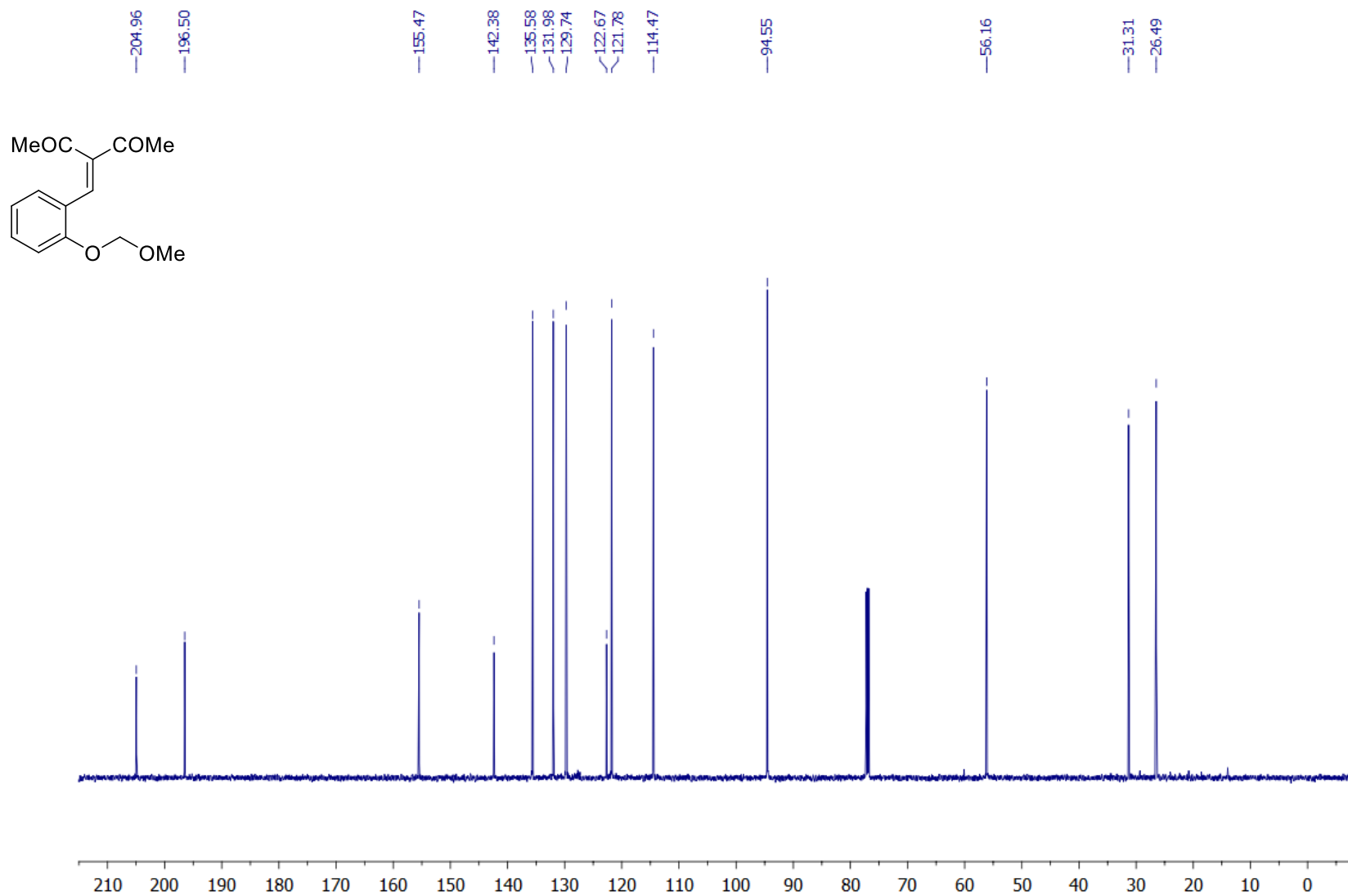
3-[[2-(Methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2a)

^1H NMR (CDCl_3 , 600 MHz)



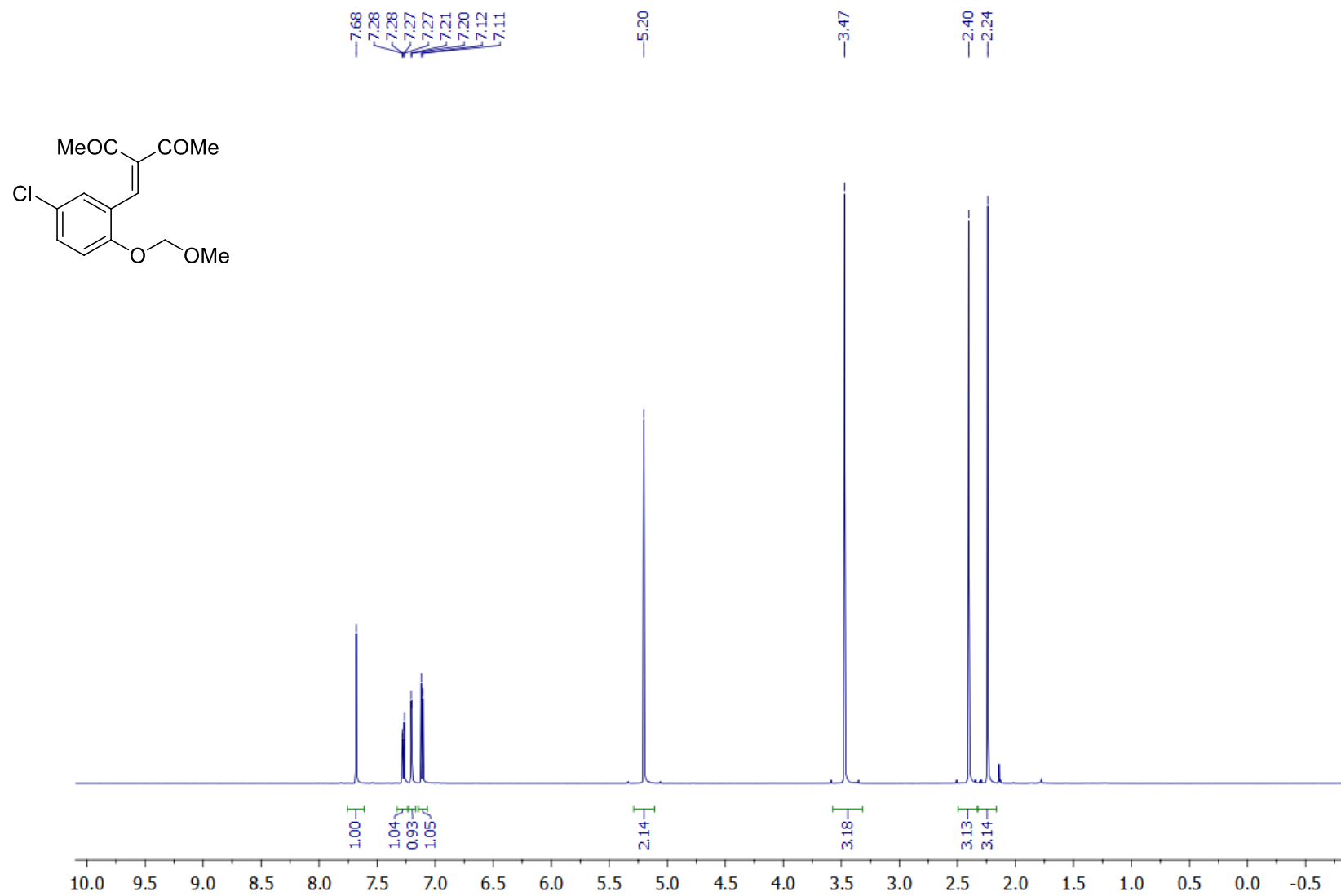
3-[[2-(Methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2a)

^{13}C NMR (CDCl_3 , 150 MHz)



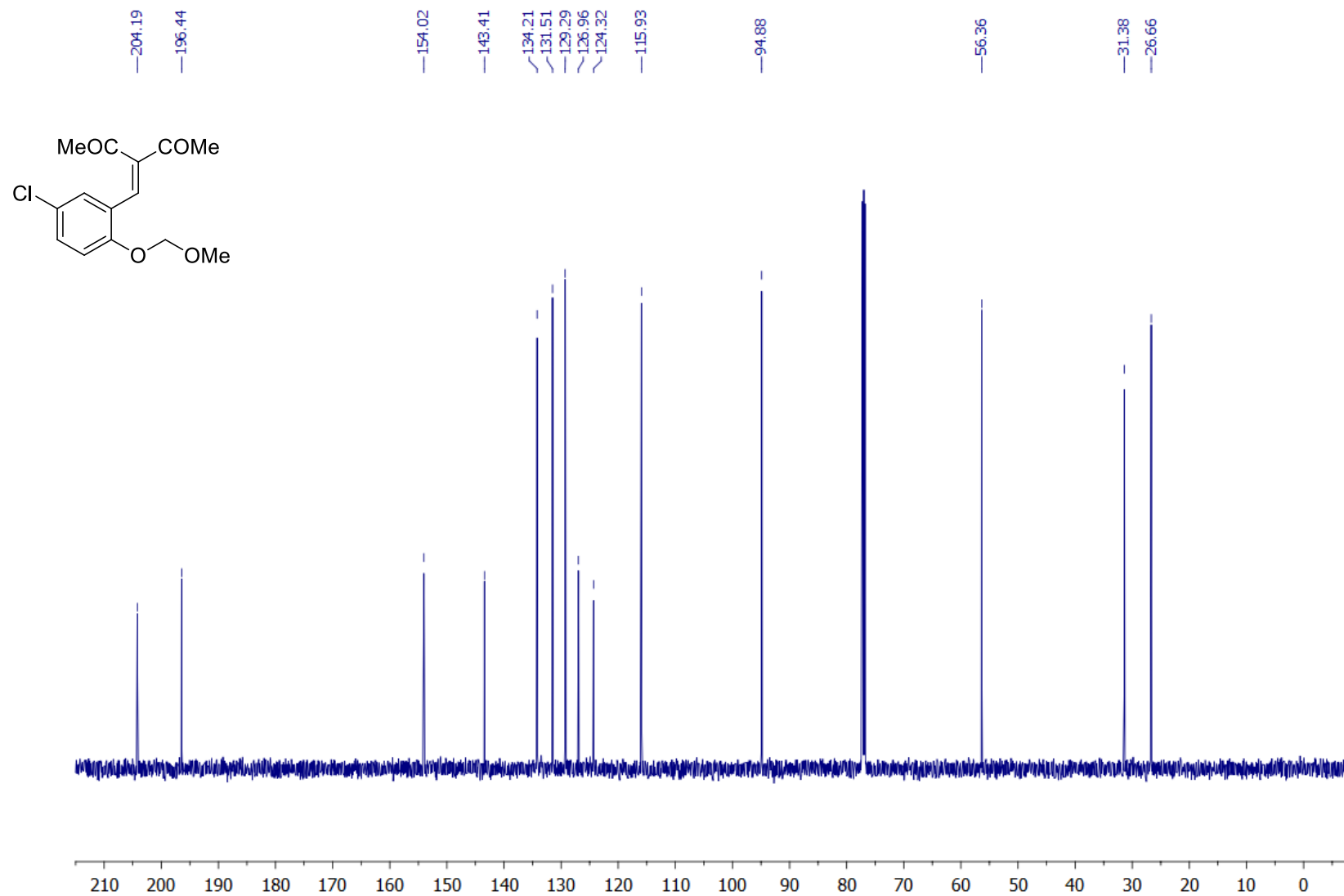
3-[[5-Chloro-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2b)

^1H NMR (CDCl_3 , 600 MHz)



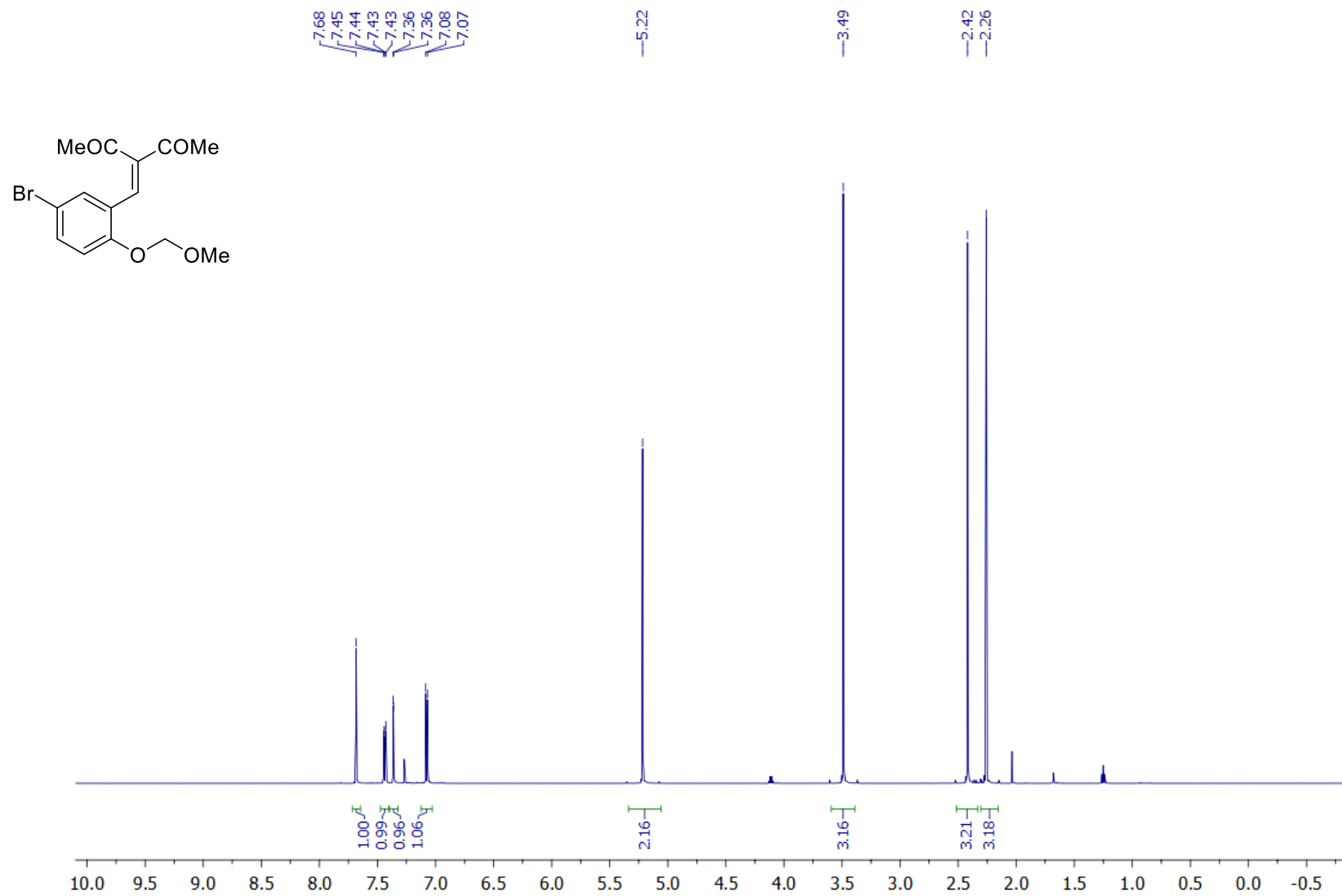
3-{{5-Chloro-2-(methoxymethoxy)phenyl}methylidene}pentane-2,4-dione (S2b)

^{13}C NMR (CDCl_3 , 150 MHz)



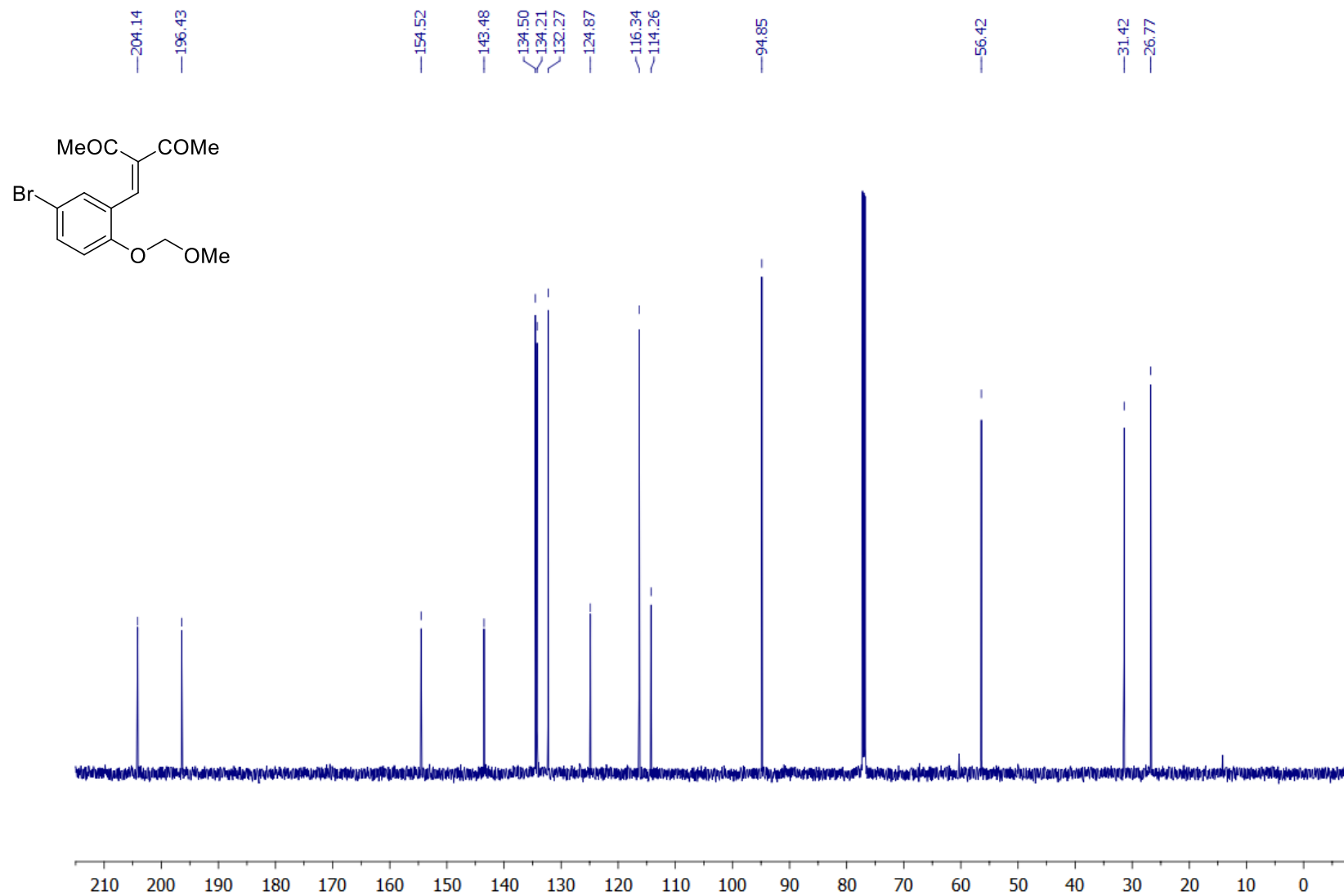
3-**{[5-Bromo-2-(methoxymethoxy)phenyl]methylidene}pentane-2,4-dione (S2c)**

^1H NMR (CDCl_3 , 600 MHz)



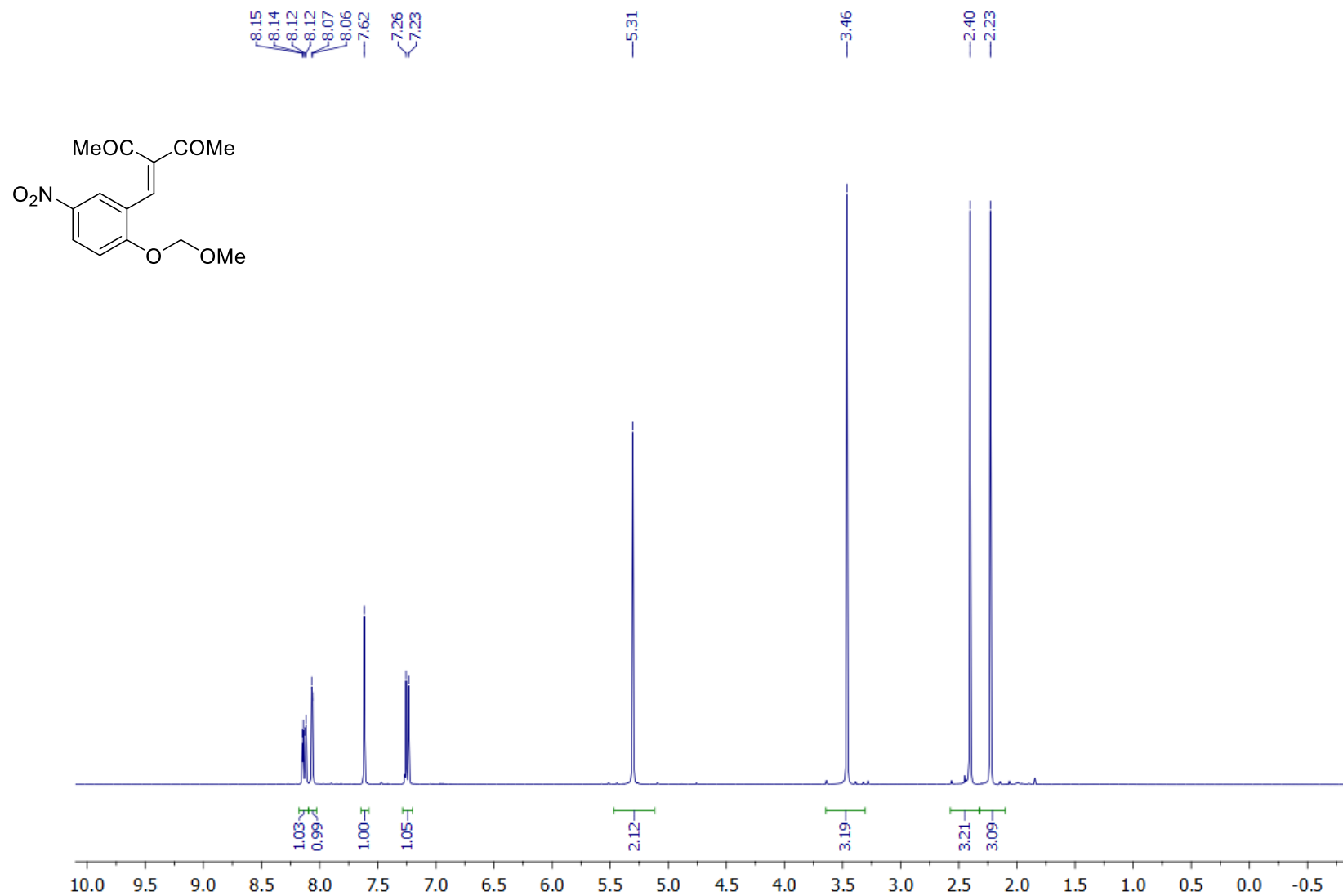
3-[[5-Bromo-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2c)

^{13}C NMR (CDCl_3 , 150 MHz)



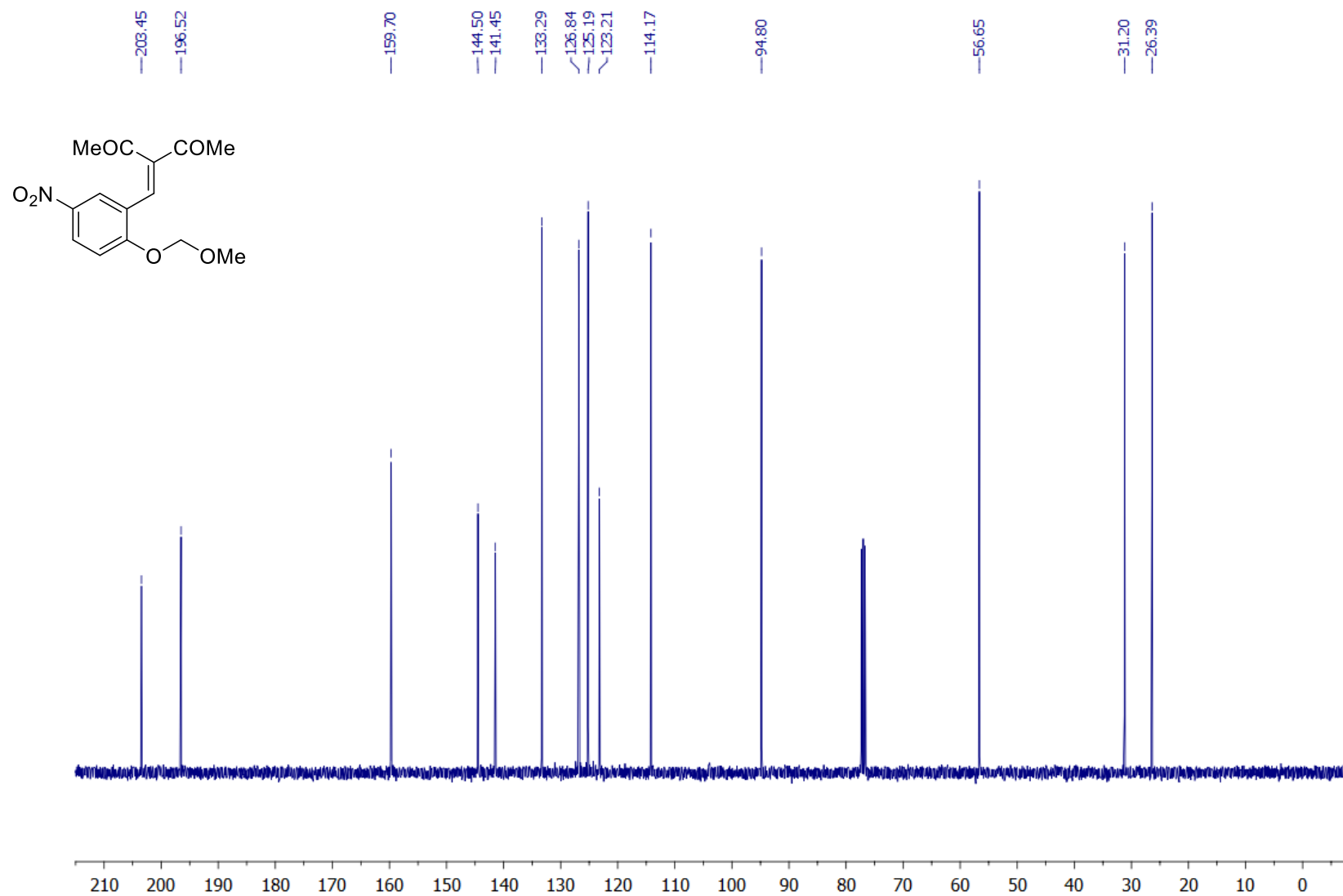
3-{[2-(Methoxymethoxy)-5-nitrophenyl]methylidene}pentane-2,4-dione (S2d)

^1H NMR (CDCl_3 , 400 MHz)



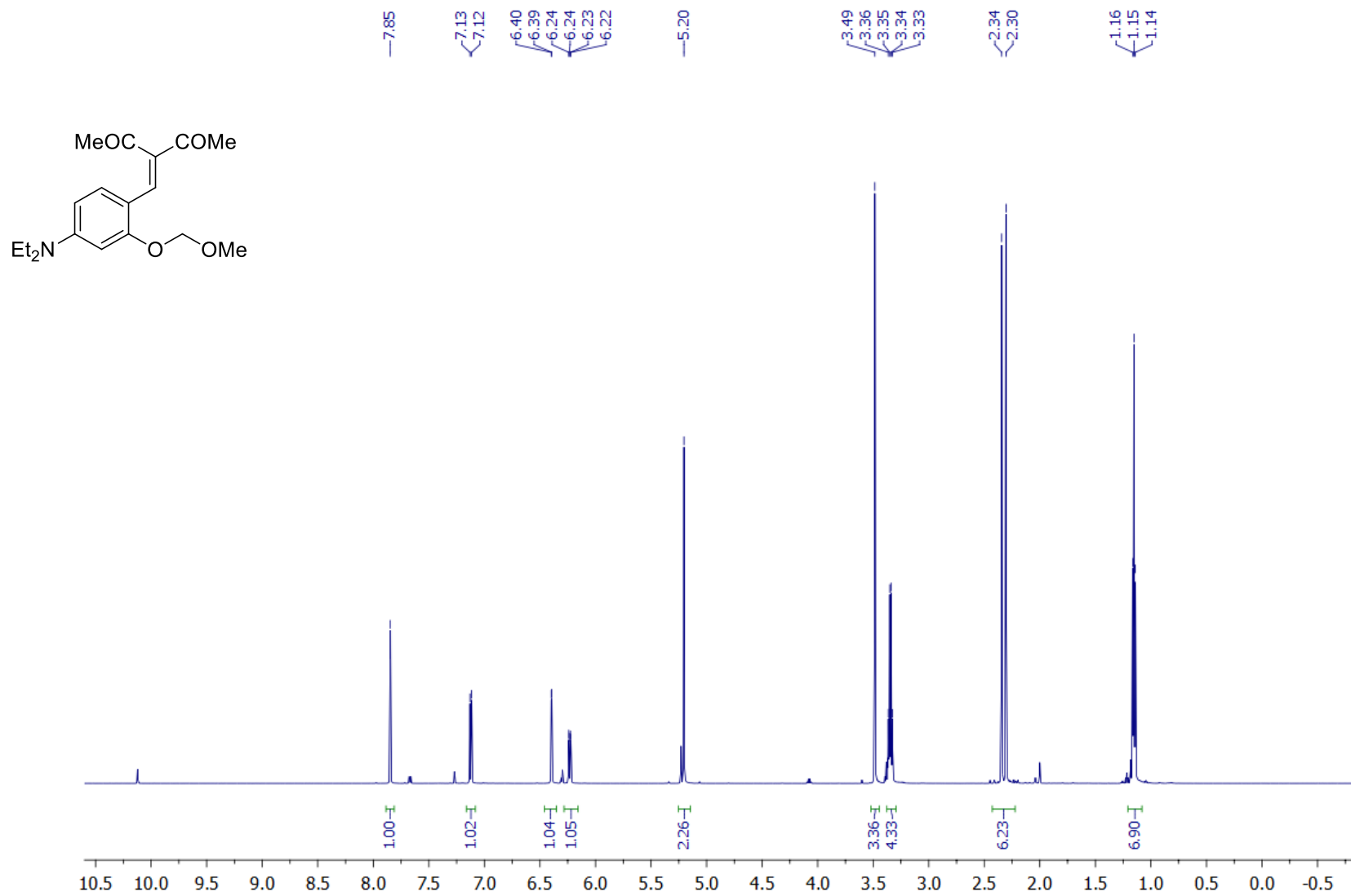
3-{[2-(Methoxymethoxy)-5-nitrophenyl]methylidene}pentane-2,4-dione (S2d)

^{13}C NMR (CDCl_3 , 100 MHz)



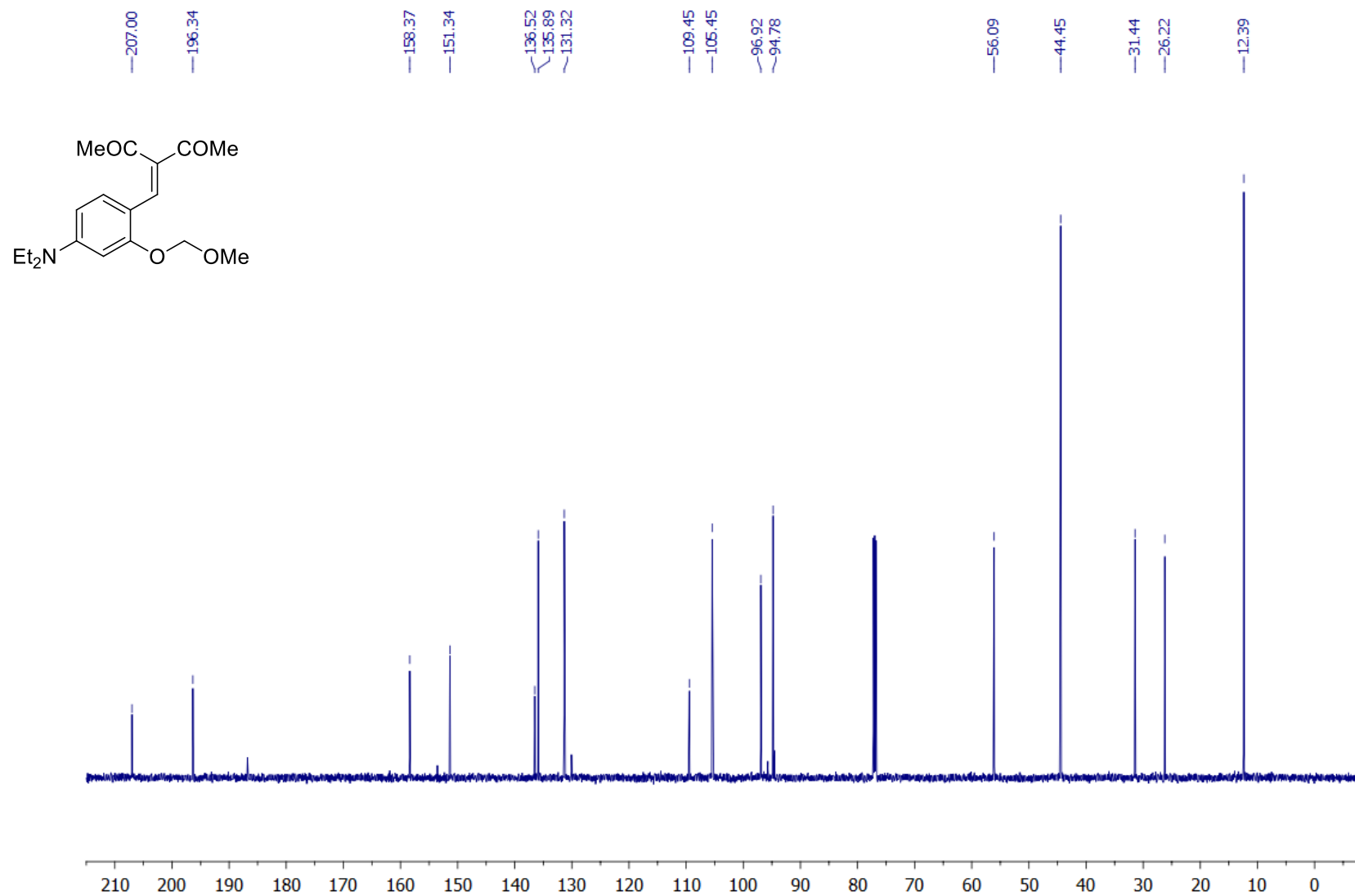
3-[[4-(Diethylamino)-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2e)

^1H NMR (CDCl_3 , 600 MHz)



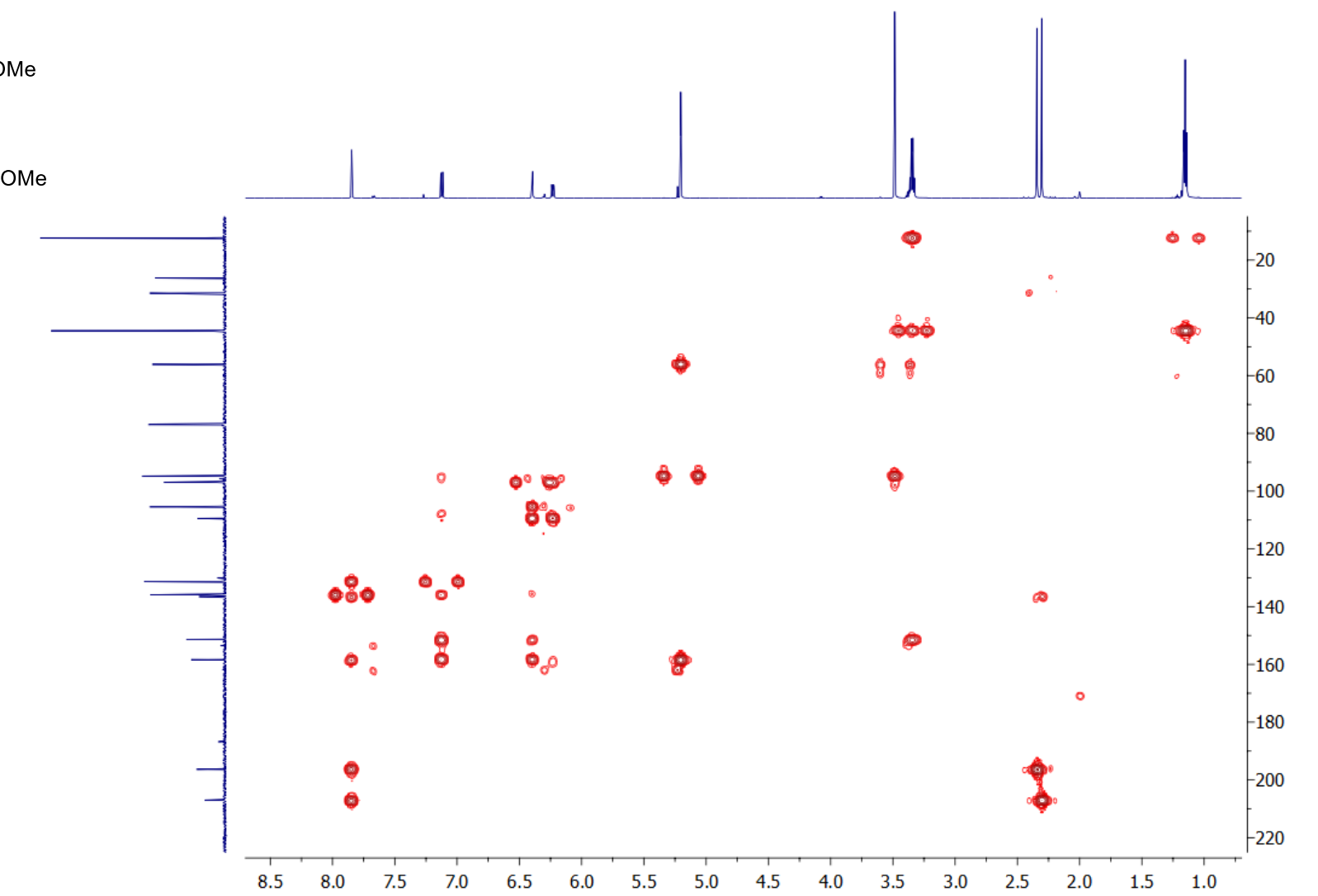
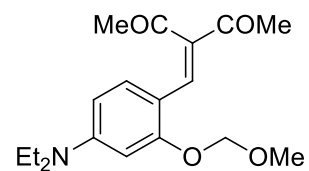
3-[[4-(Diethylamino)-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2e)

^{13}C NMR (CDCl_3 , 150 MHz)



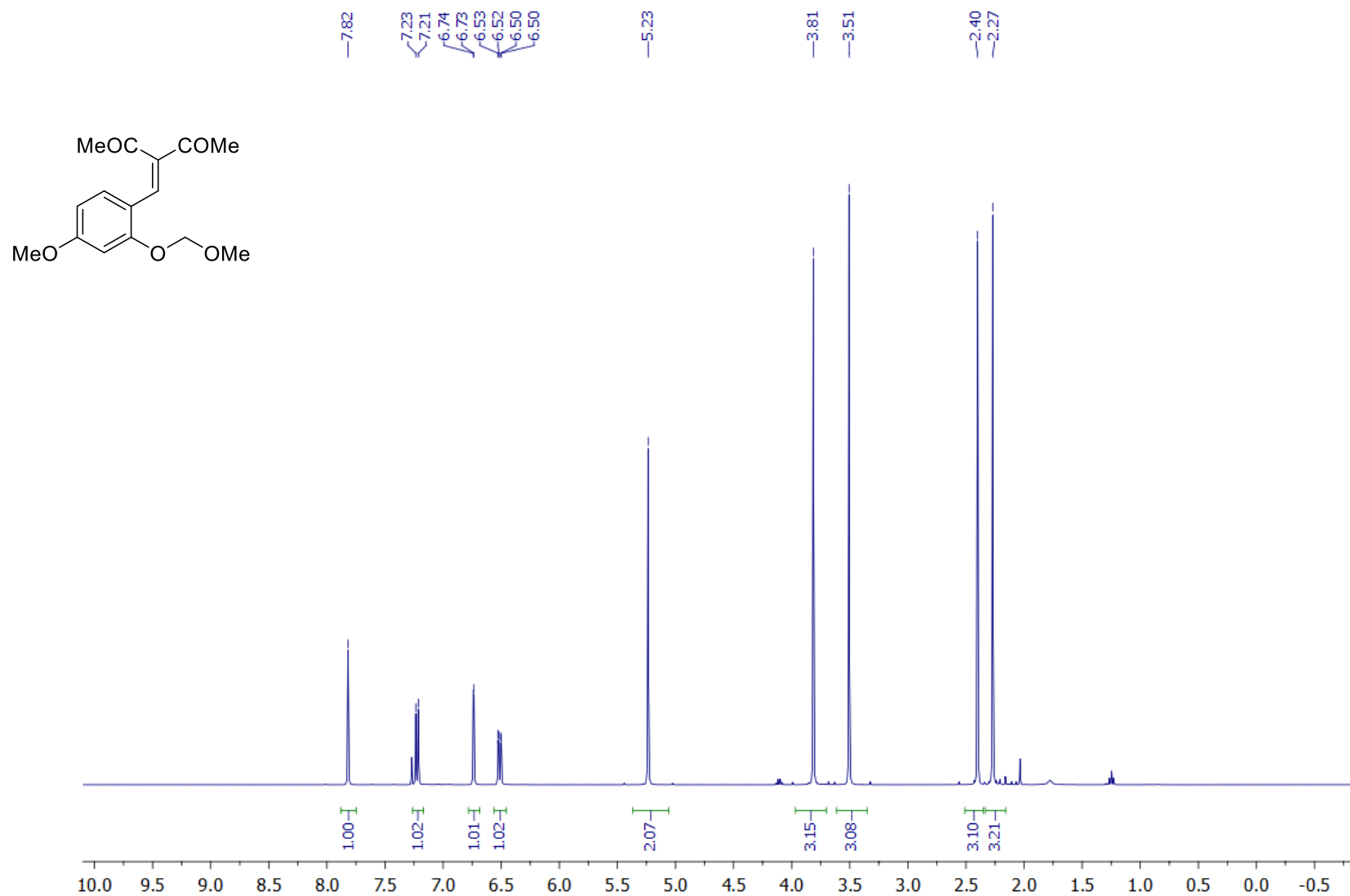
3-[[4-(Diethylamino)-2-(methoxymethoxy)phenyl]methylidene}pentane-2,4-dione (S2e)

^1H - ^{13}C HMBC (CDCl_3)



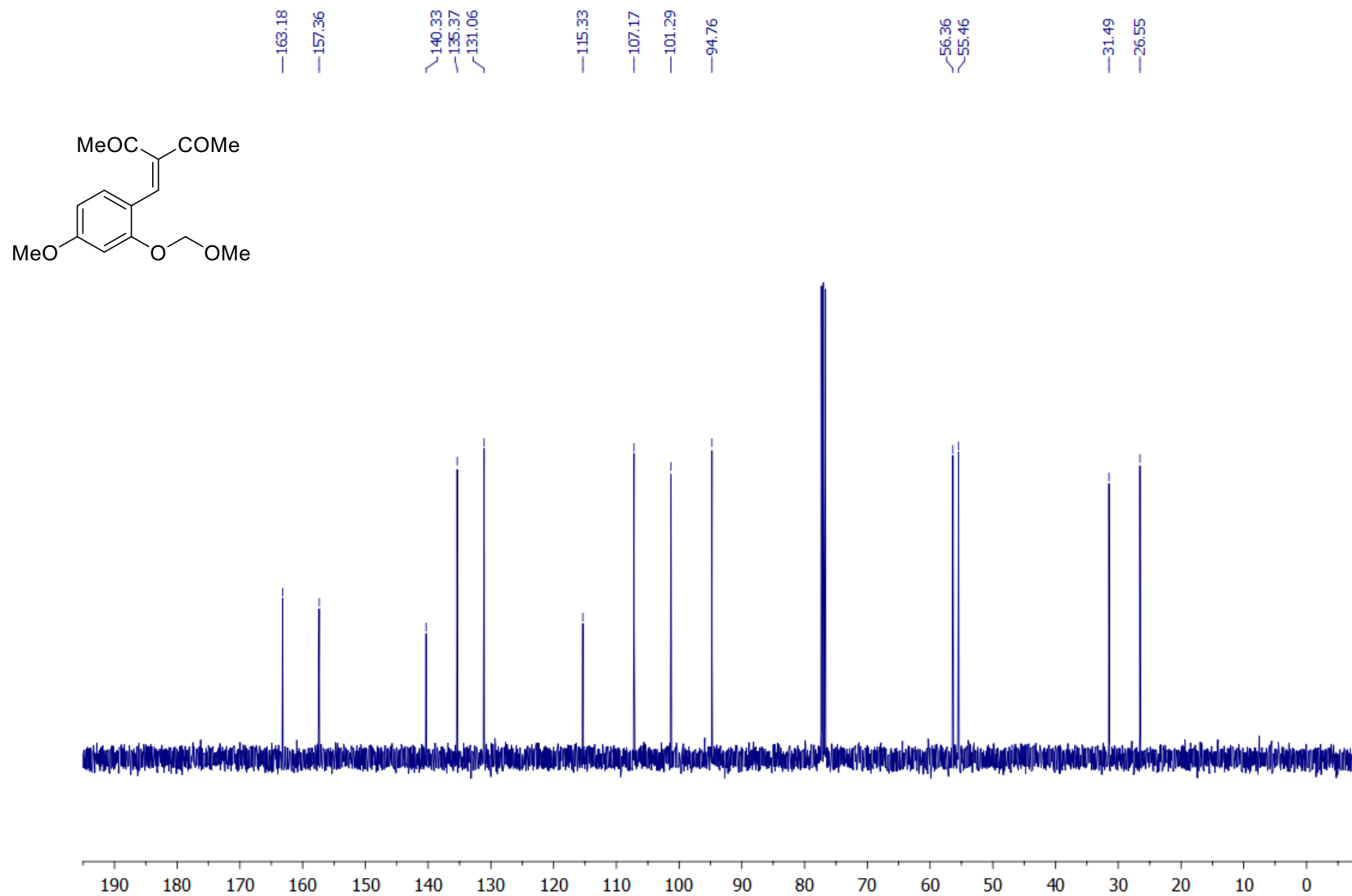
3-**{[4-Methoxy-2-(methoxymethoxy)phenyl]methylidene}pentane-2,4-dione (S2f)**

¹H NMR (CDCl₃, 400 MHz)



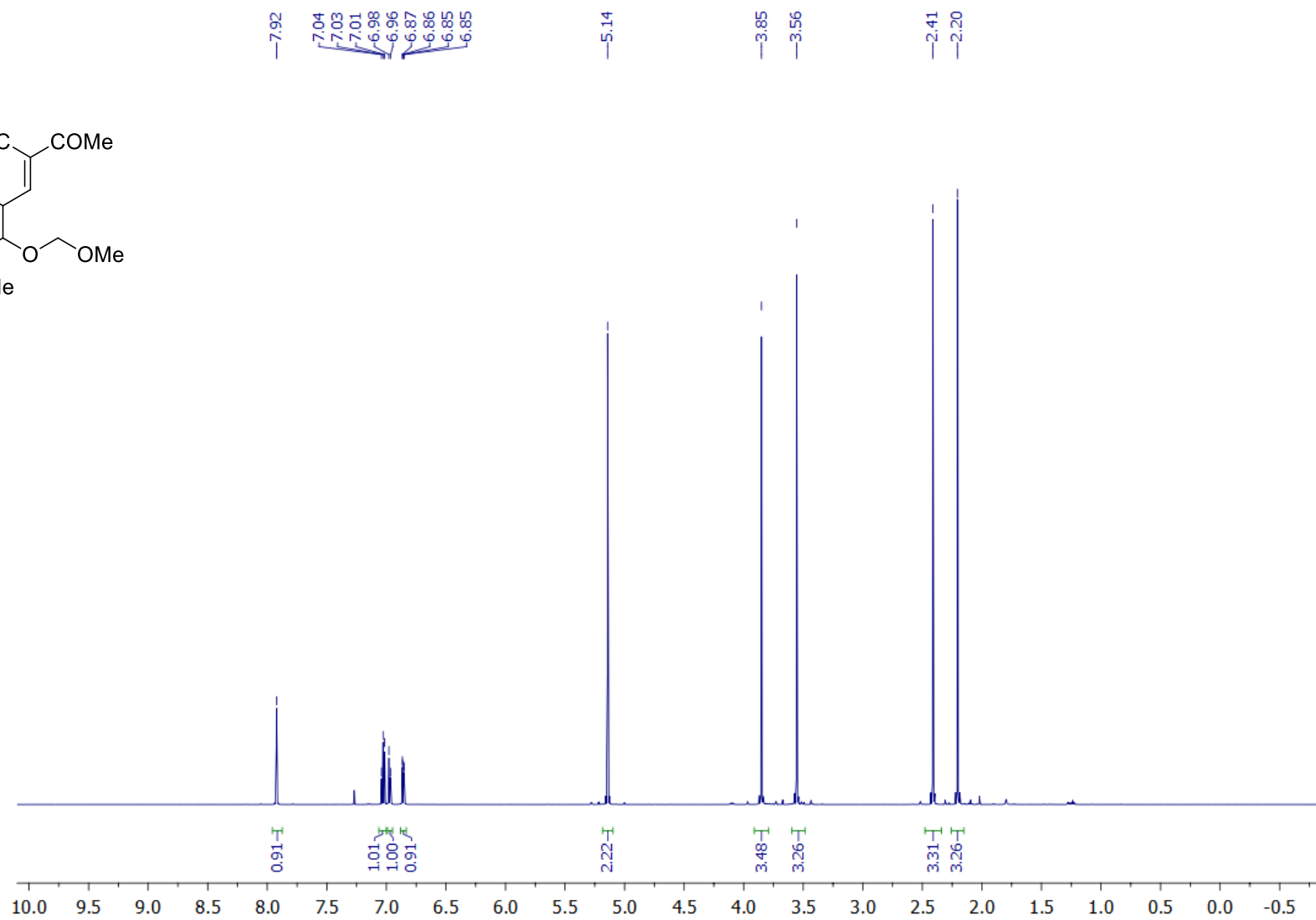
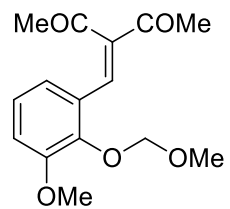
3-[[4-Methoxy-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2f)

^{13}C NMR (CDCl_3 , 100 MHz)



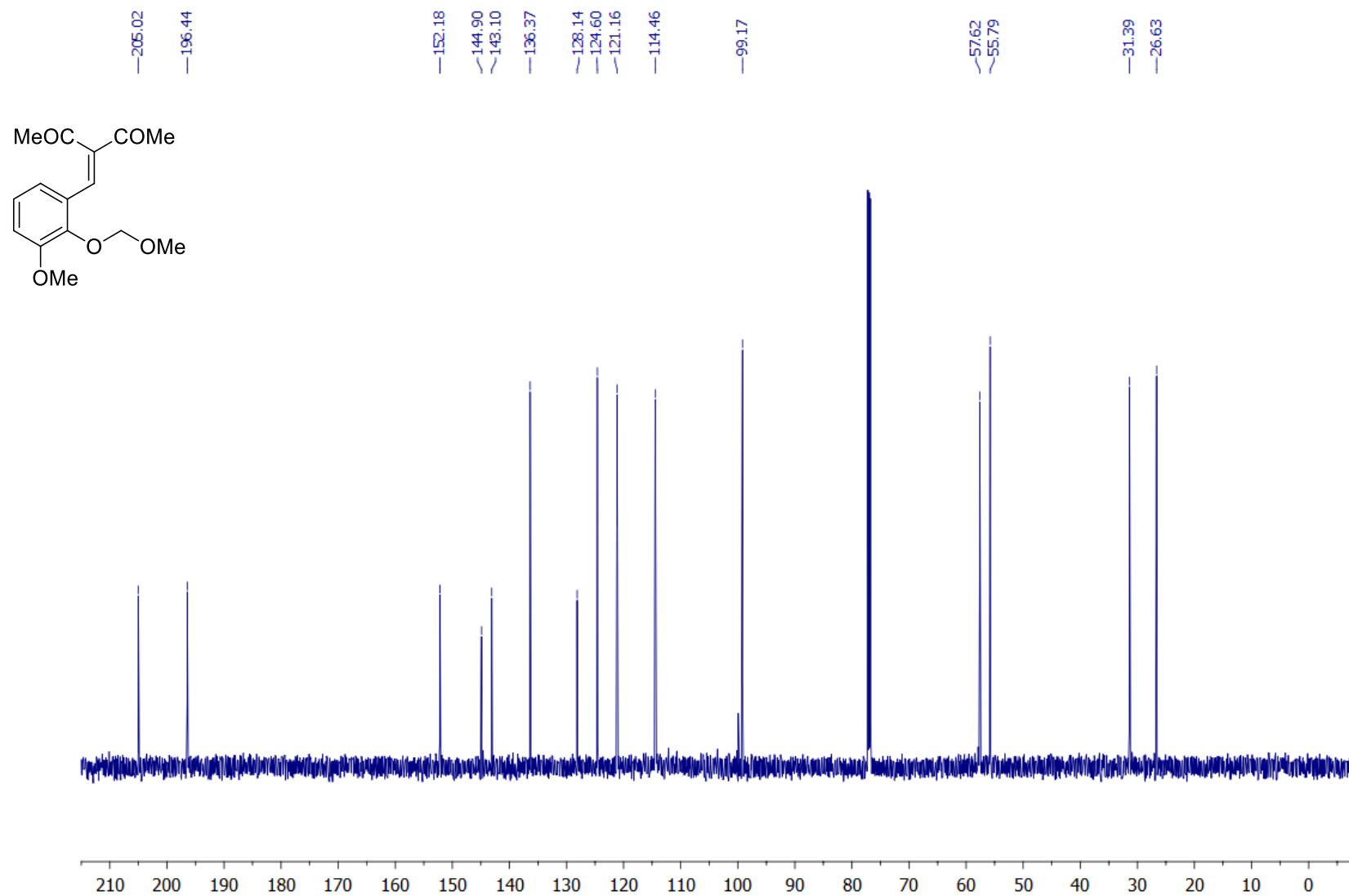
3-{[3-Methoxy-2-(methoxymethoxy)phenyl]methylidene}pentane-2,4-dione (S2g)

^1H NMR (CDCl_3 , 600 MHz)



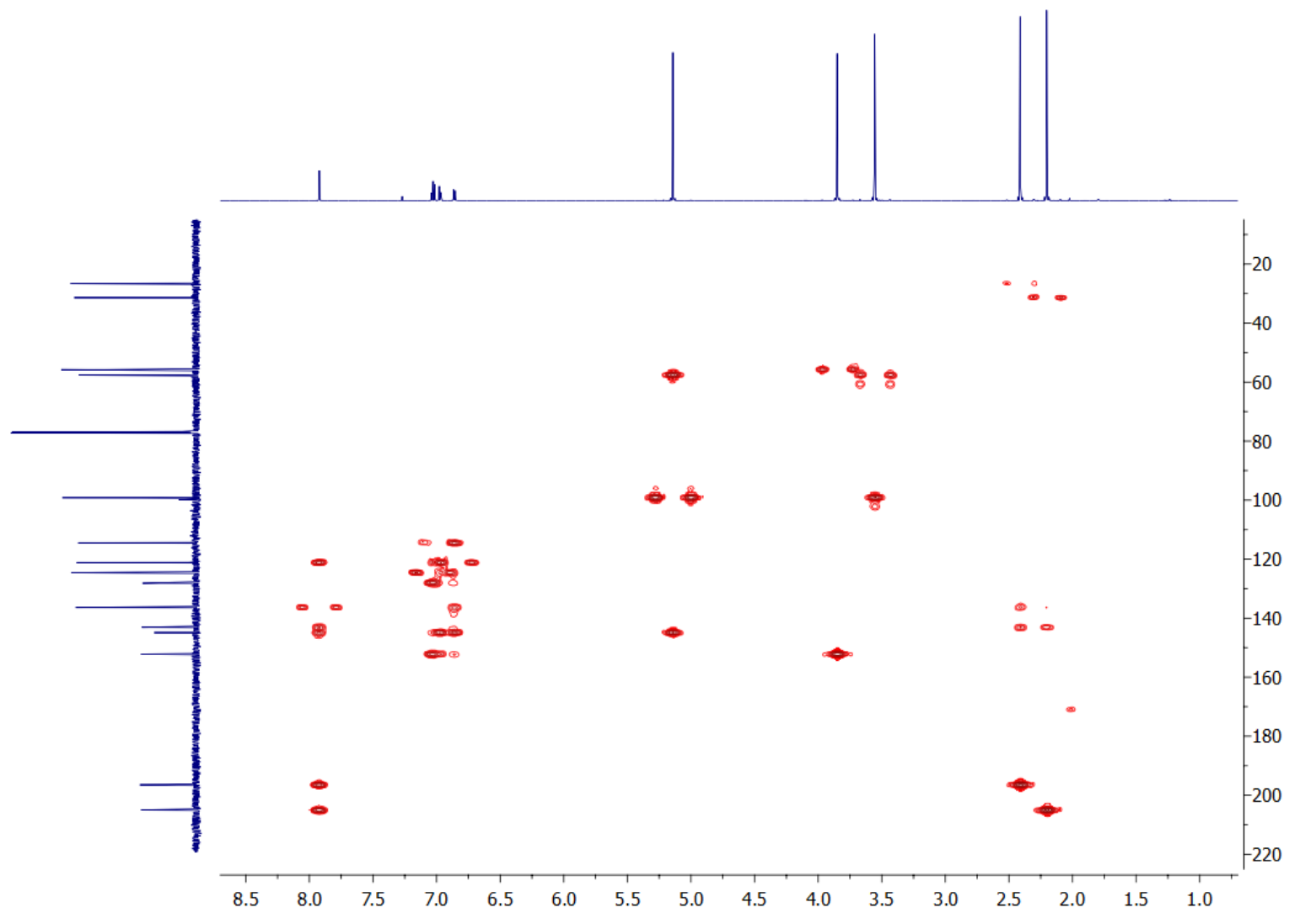
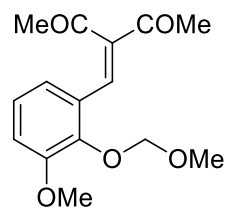
3-{[3-Methoxy-2-(methoxymethoxy)phenyl]methylidene}pentane-2,4-dione (S2g)

^{13}C NMR (CDCl_3 , 150 MHz)



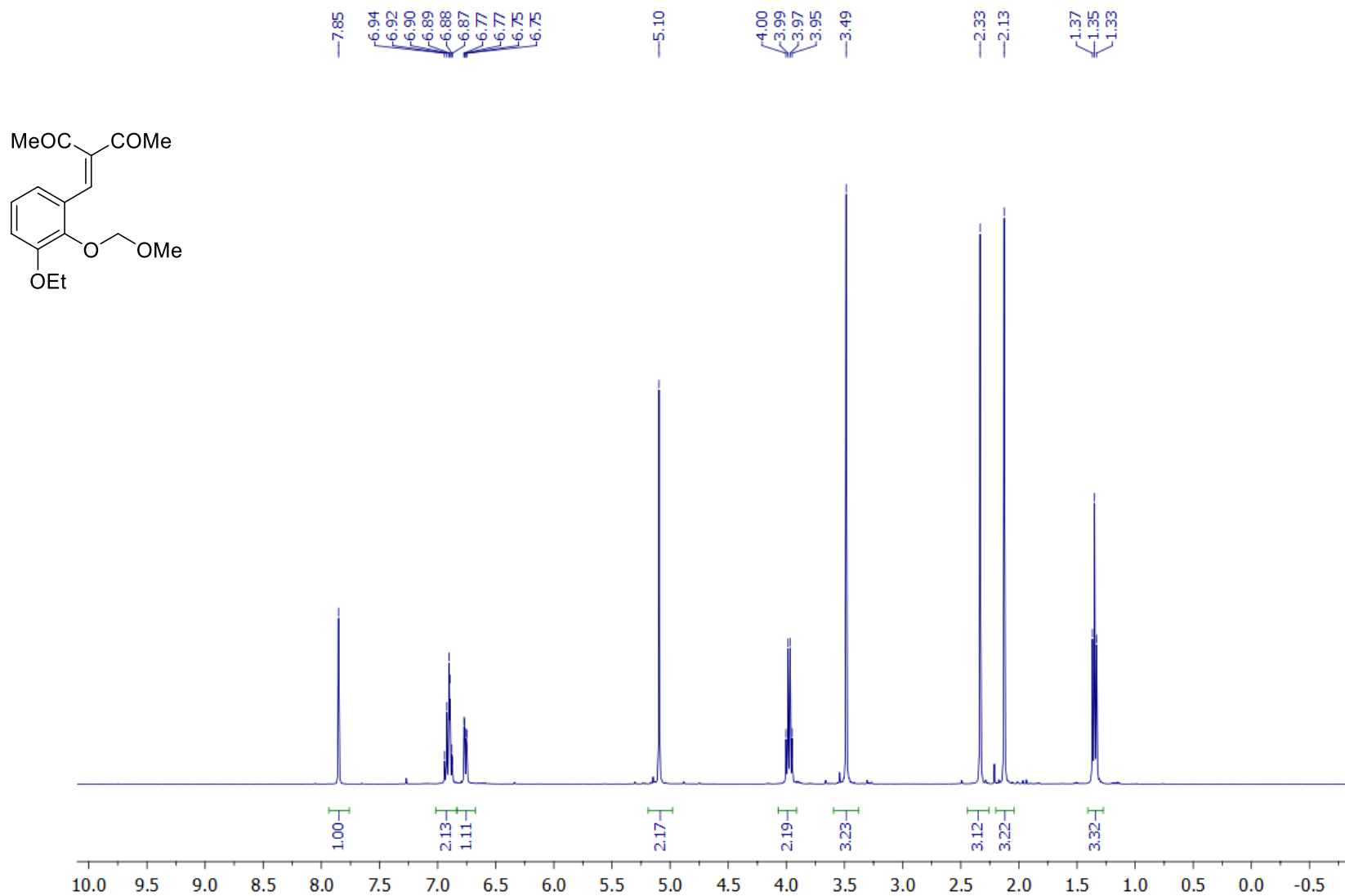
3-[[3-Methoxy-2-(methoxymethoxy)phenyl]methylidene}pentane-2,4-dione (S2g)

^1H - ^{13}C HMBC (CDCl_3)



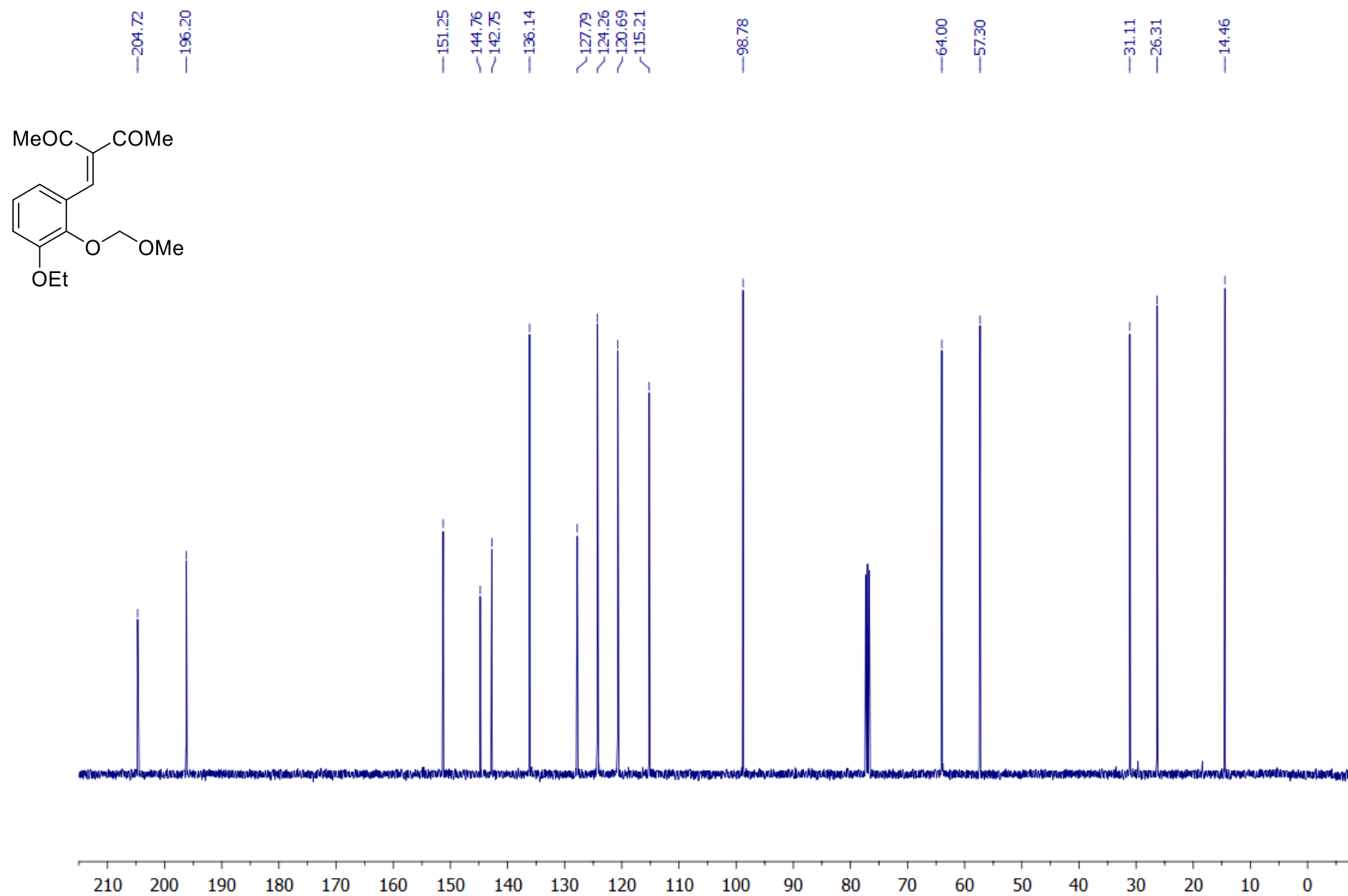
3-[[3-Ethoxy-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2h)

^1H NMR (CDCl_3 , 400 MHz)



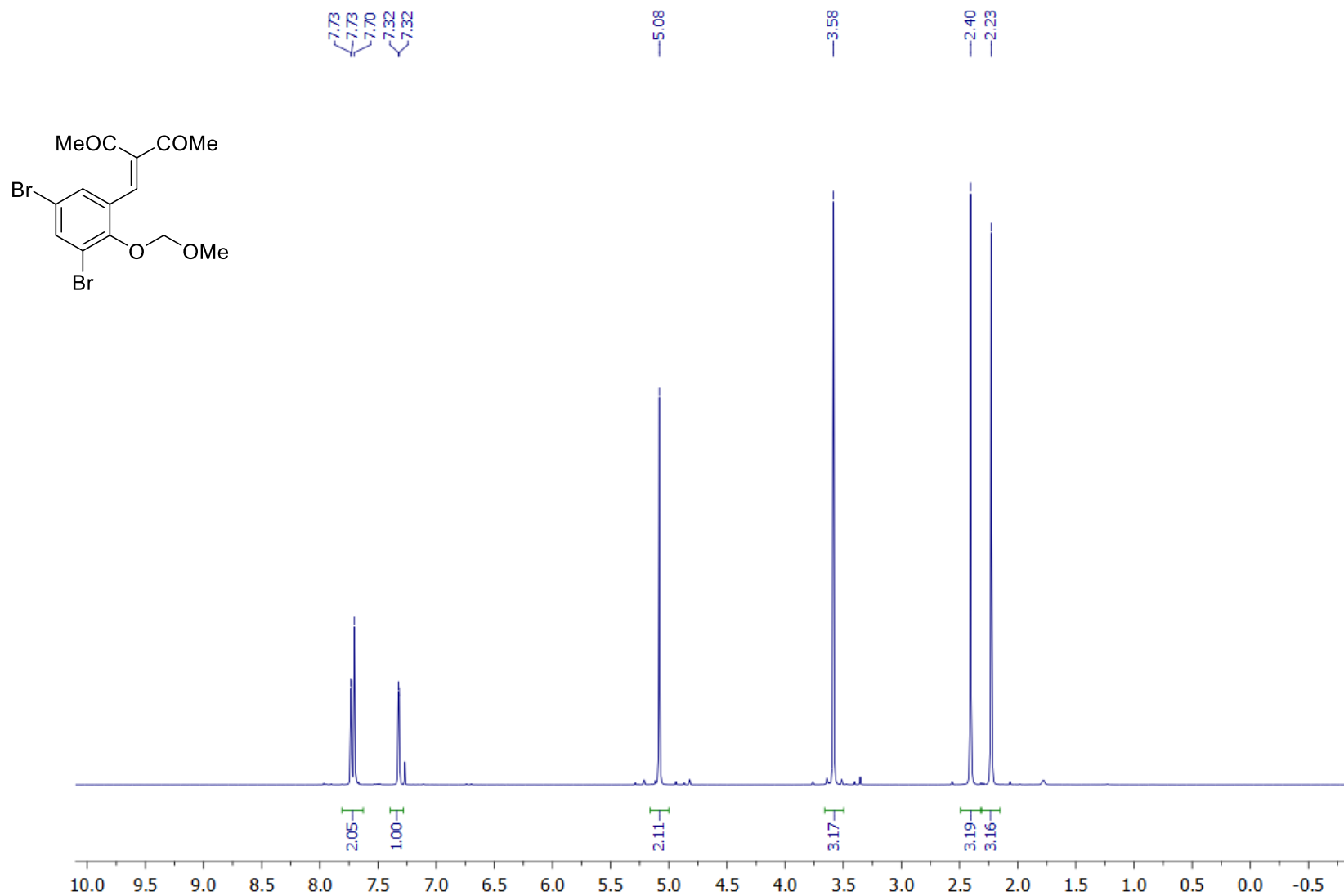
3-[[3-Ethoxy-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2h)

^{13}C NMR (CDCl_3 , 100 MHz)



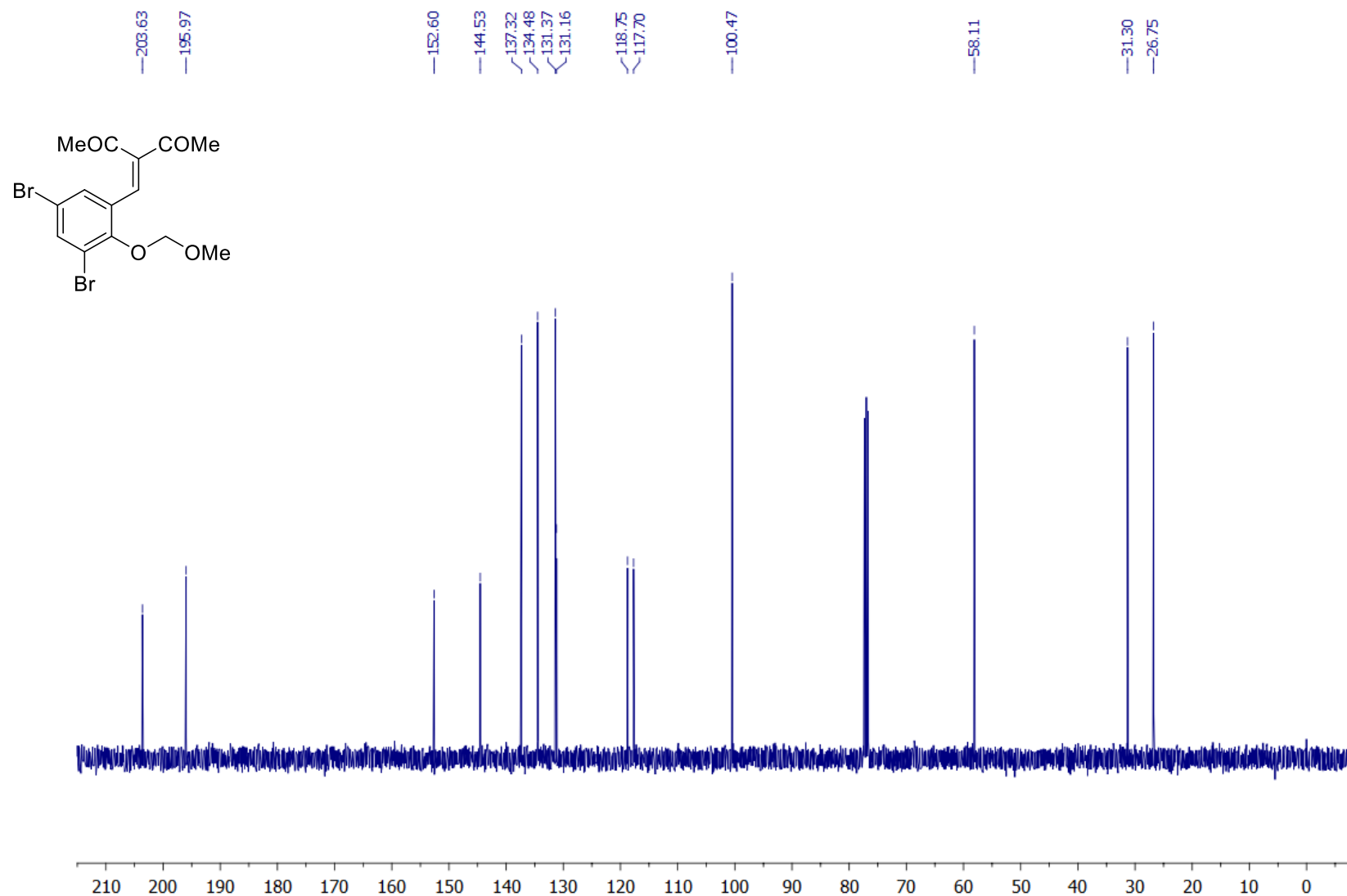
3-[[3,5-Dibromo-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2i)

^1H NMR (CDCl_3 , 400 MHz)



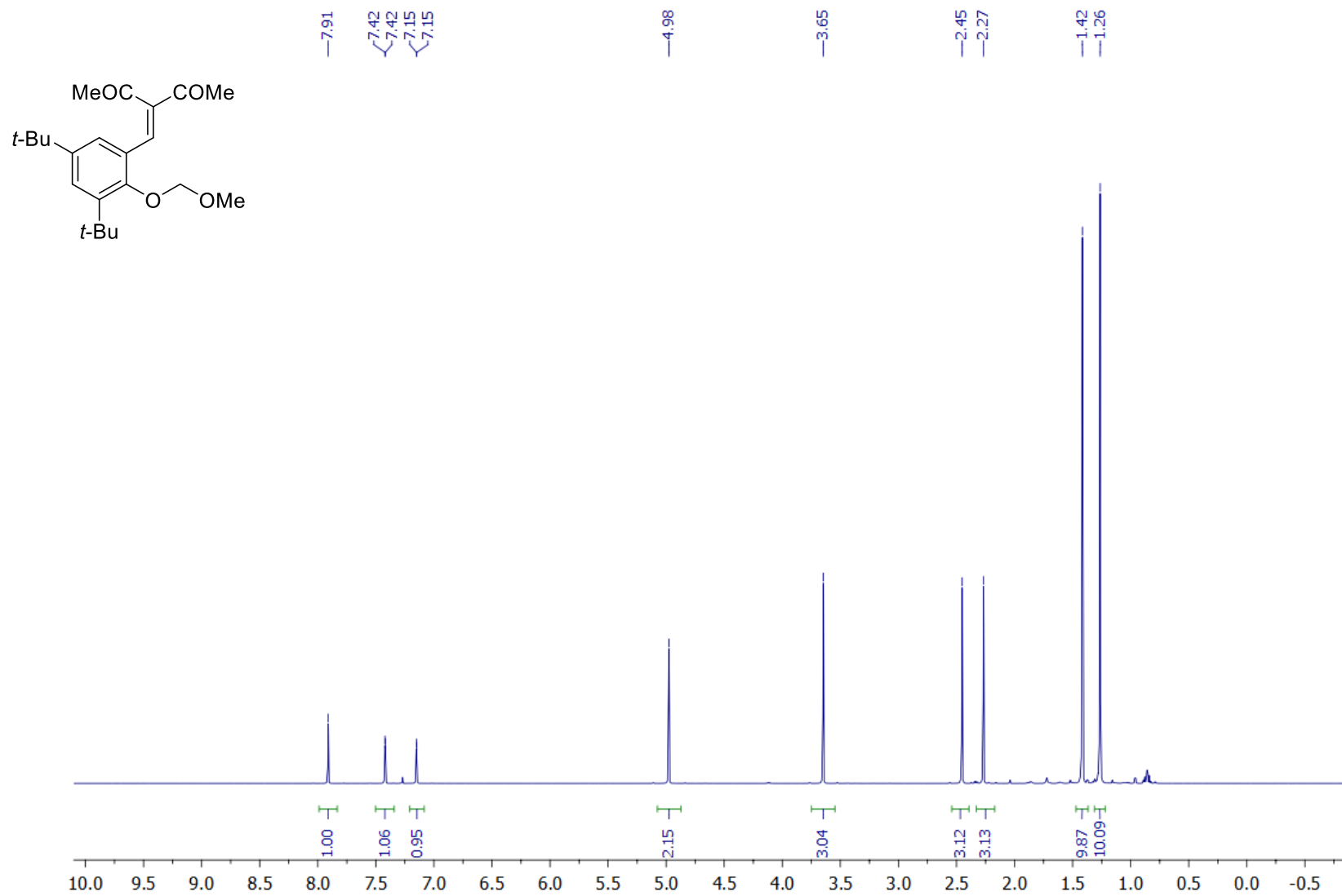
3-[[3,5-Dibromo-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2i)

^{13}C NMR (CDCl_3 , 100 MHz)



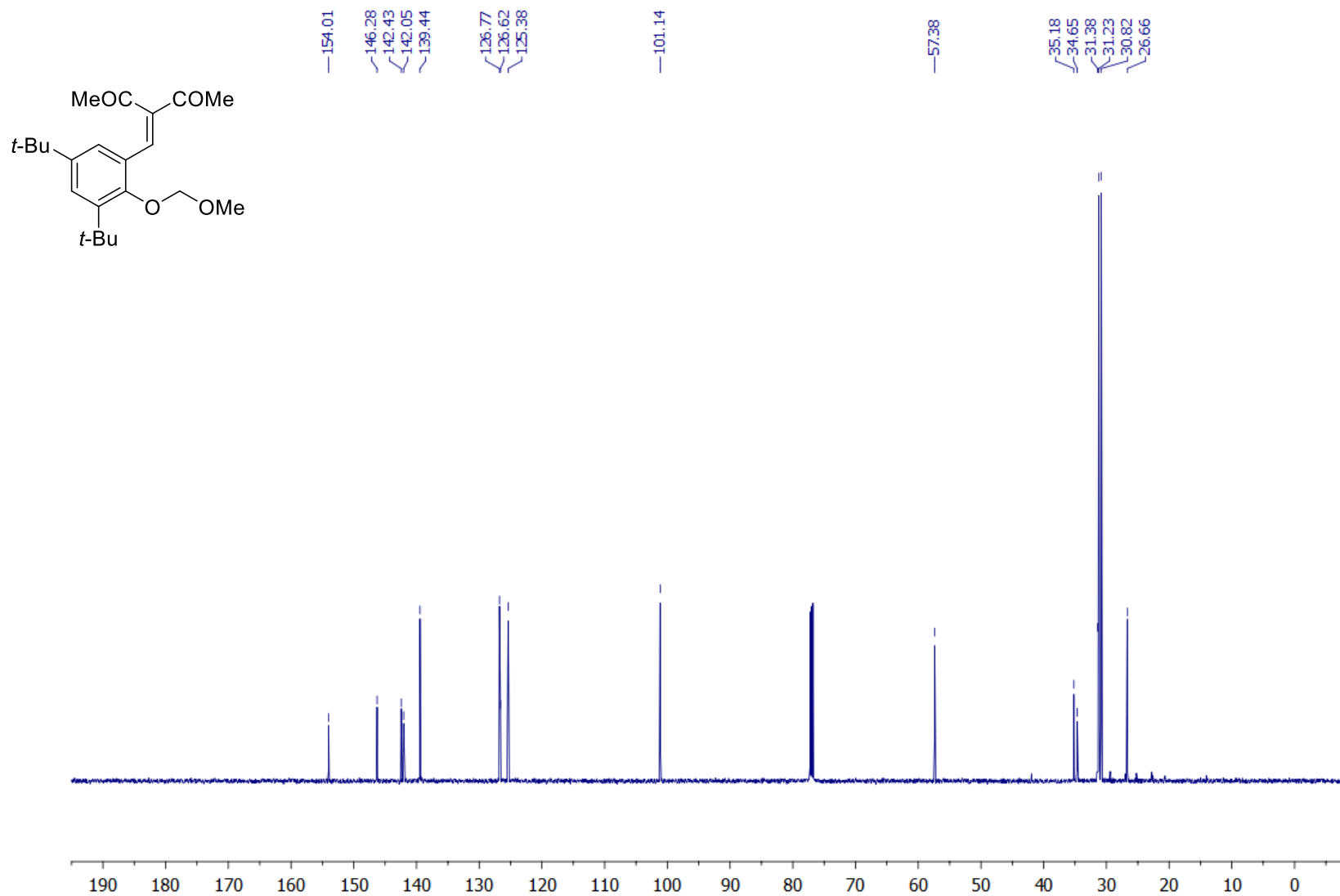
3- $\{[3,5\text{-Bis}(tert\text{-butyl})\text{-}2\text{-(methoxymethoxy)phenyl}]\text{methylidene}\}$ pentane-2,4-dione (S2j)

^1H NMR (CDCl_3 , 600 MHz)



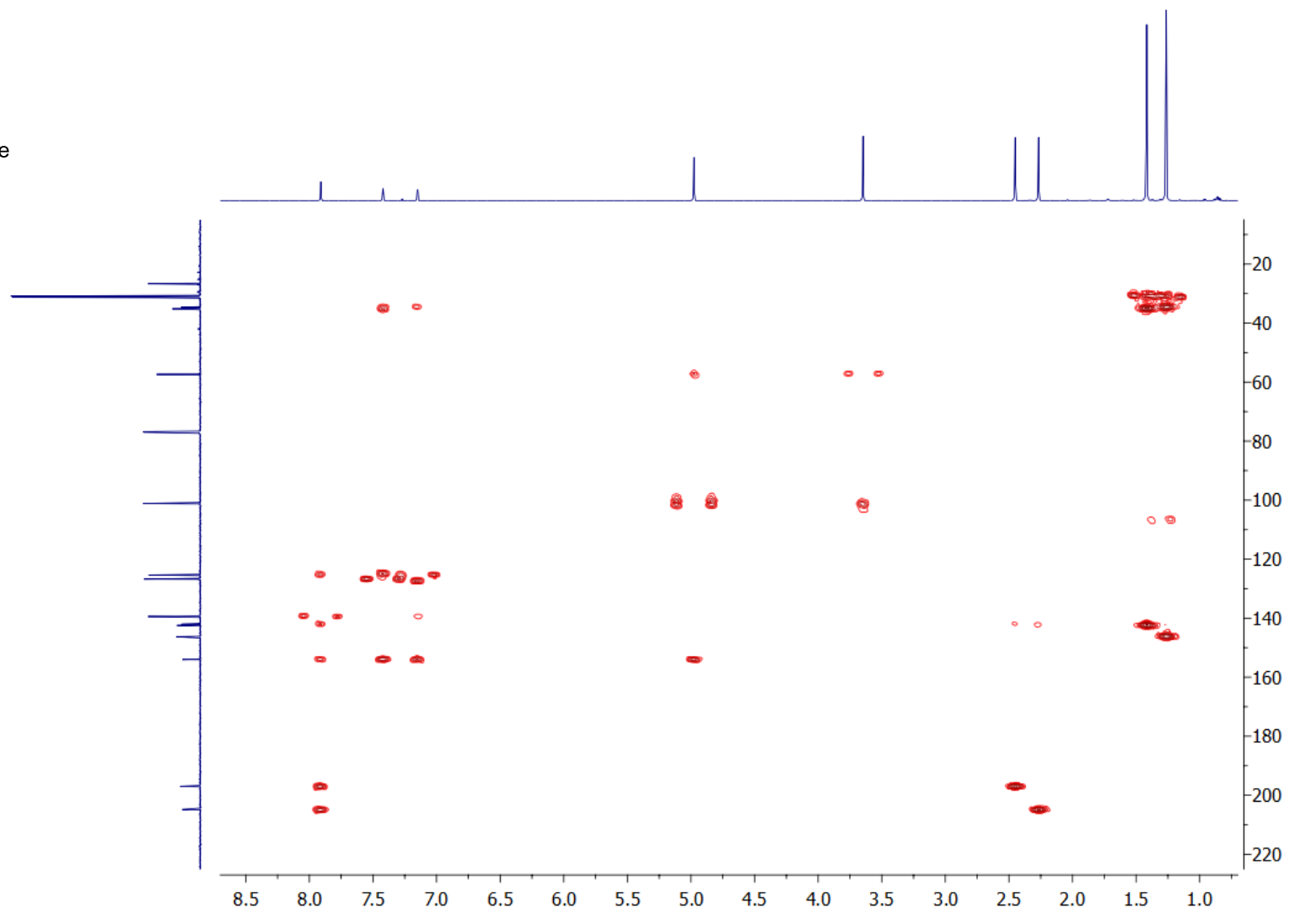
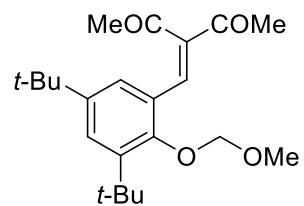
3- $\{[3,5\text{-Bis}(tert\text{-butyl})\text{-2-(methoxymethoxy)phenyl]methylidene}\}$ pentane-2,4-dione (S2j)

^{13}C NMR (CDCl_3 , 150 MHz)



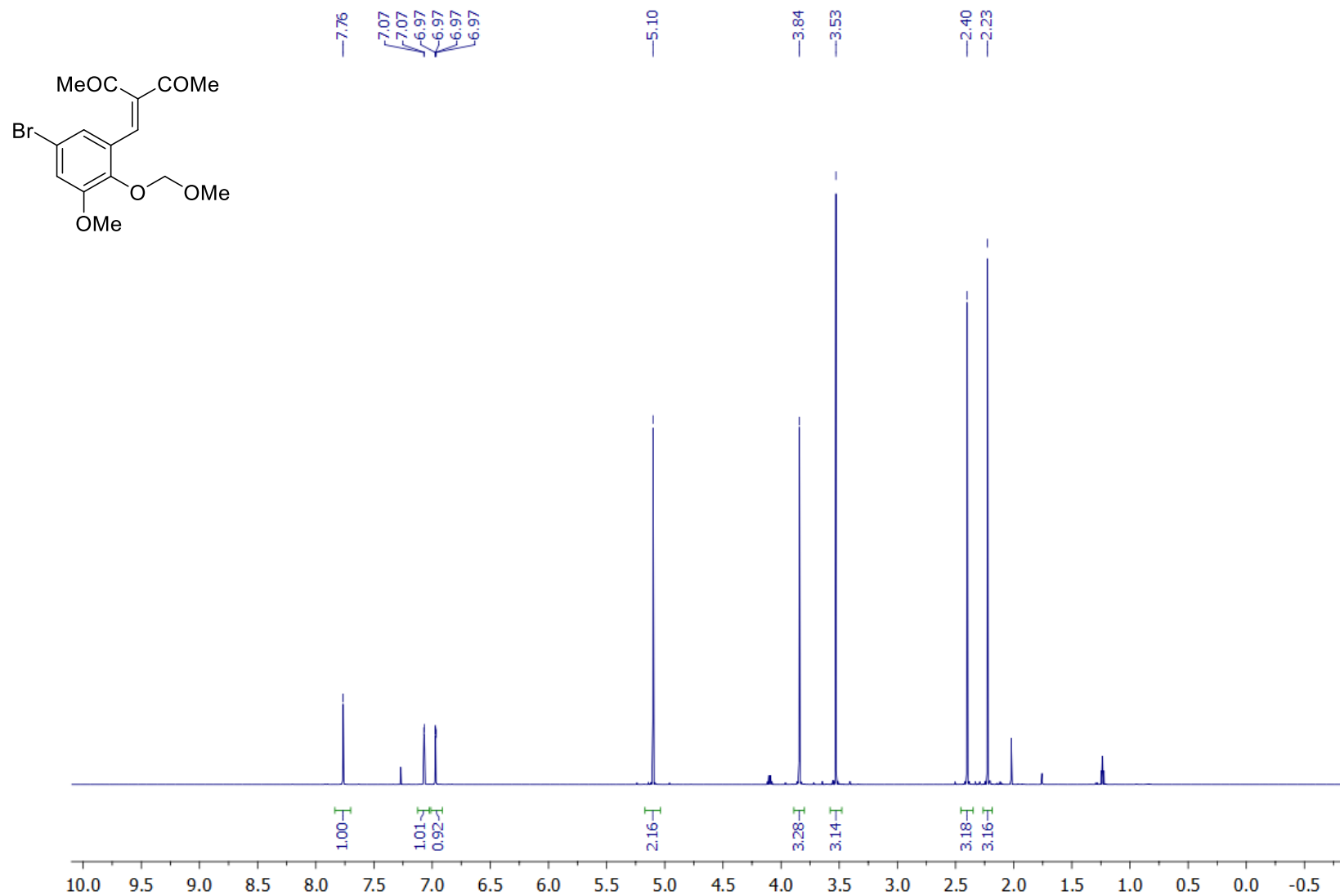
3-[[3,5-Bis(*tert*-butyl)-2-(methoxymethoxy)phenyl]methylidene}pentane-2,4-dione (S2j)

^1H - ^{13}C HMBC (CDCl_3)



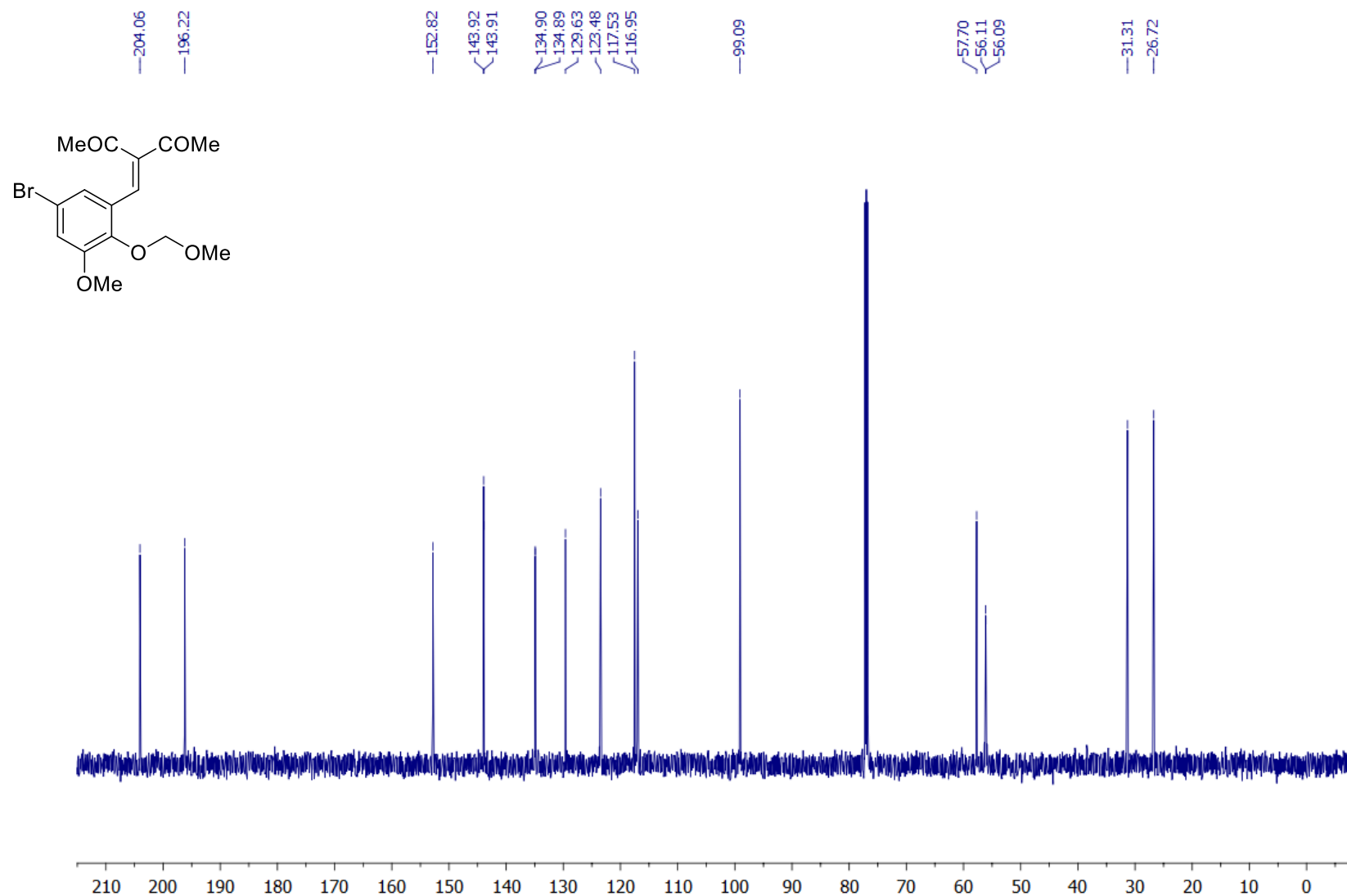
3-**{[5-Bromo-3-methoxy-2-(methoxymethoxy)phenyl]methylidene}pentane-2,4-dione (S2k)**

^1H NMR (CDCl_3 , 600 MHz)



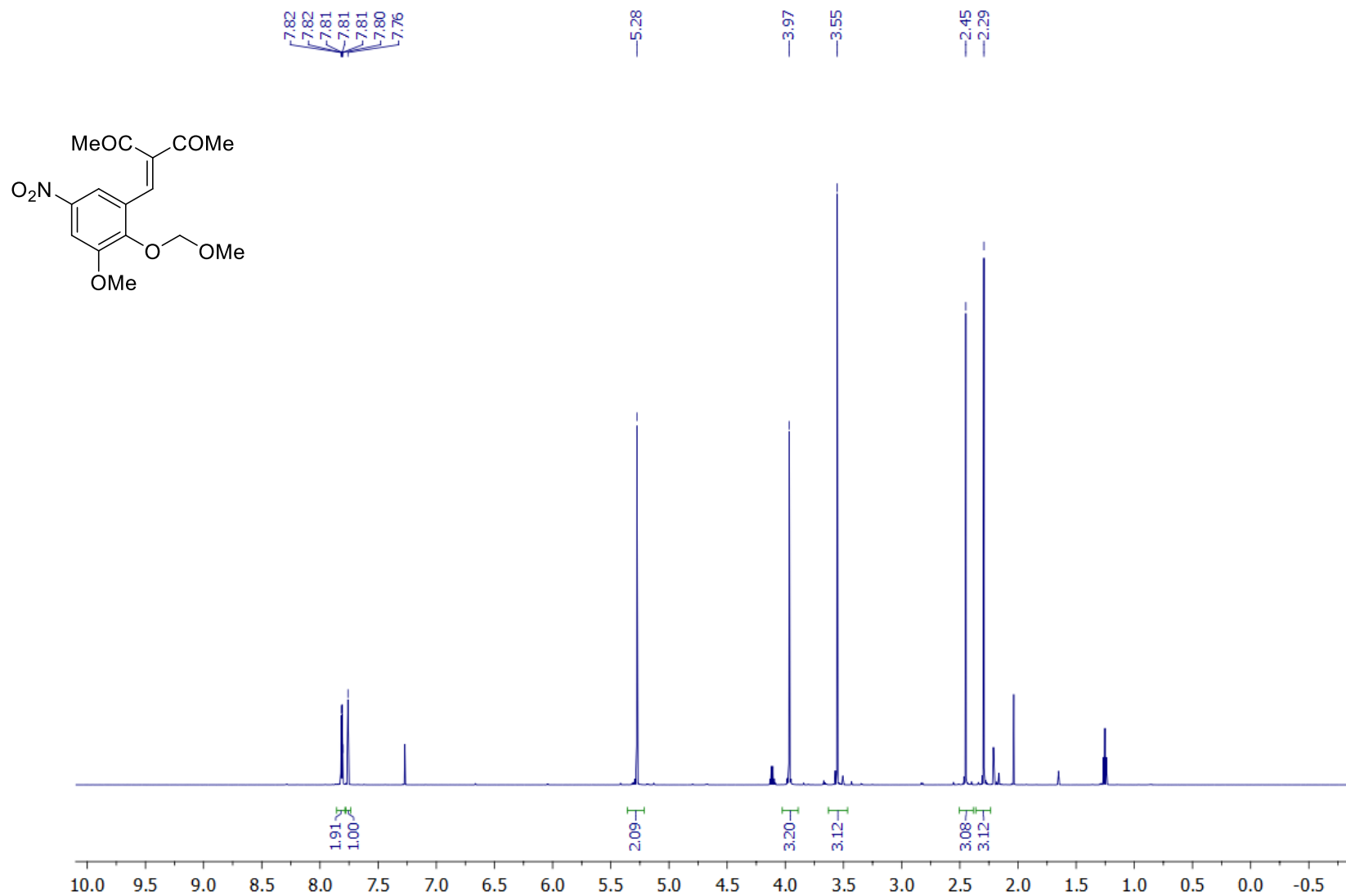
3-**{[5-Bromo-3-methoxy-2-(methoxymethoxy)phenyl]methylidene}pentane-2,4-dione (S2k)**

^{13}C NMR (CDCl_3 , 150 MHz)



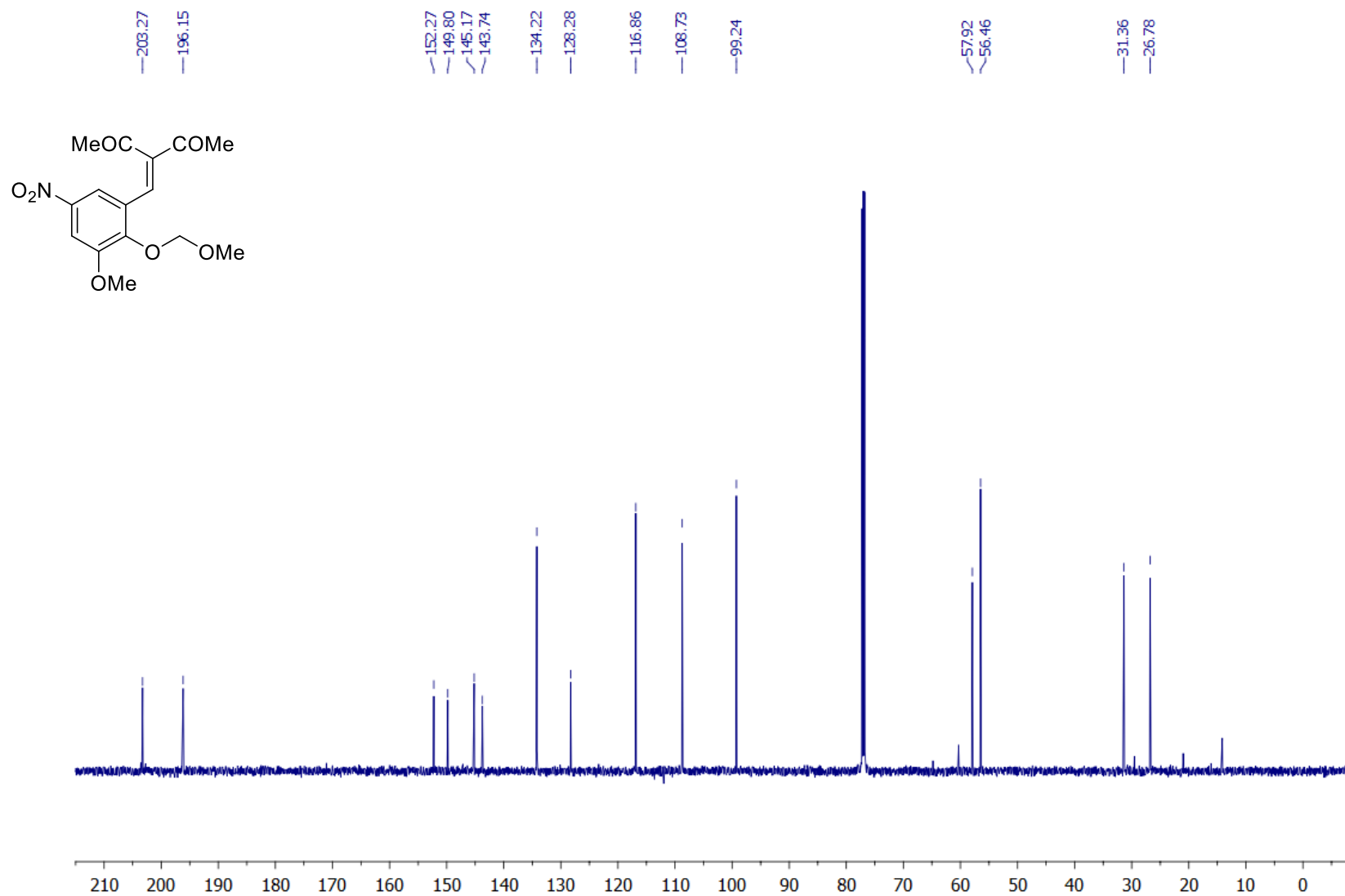
3-[[3-Methoxy-2-(methoxymethoxy)-5-nitrophenyl]methylidene]pentane-2,4-dione (S2l)

^1H NMR (CDCl_3 , 600 MHz)



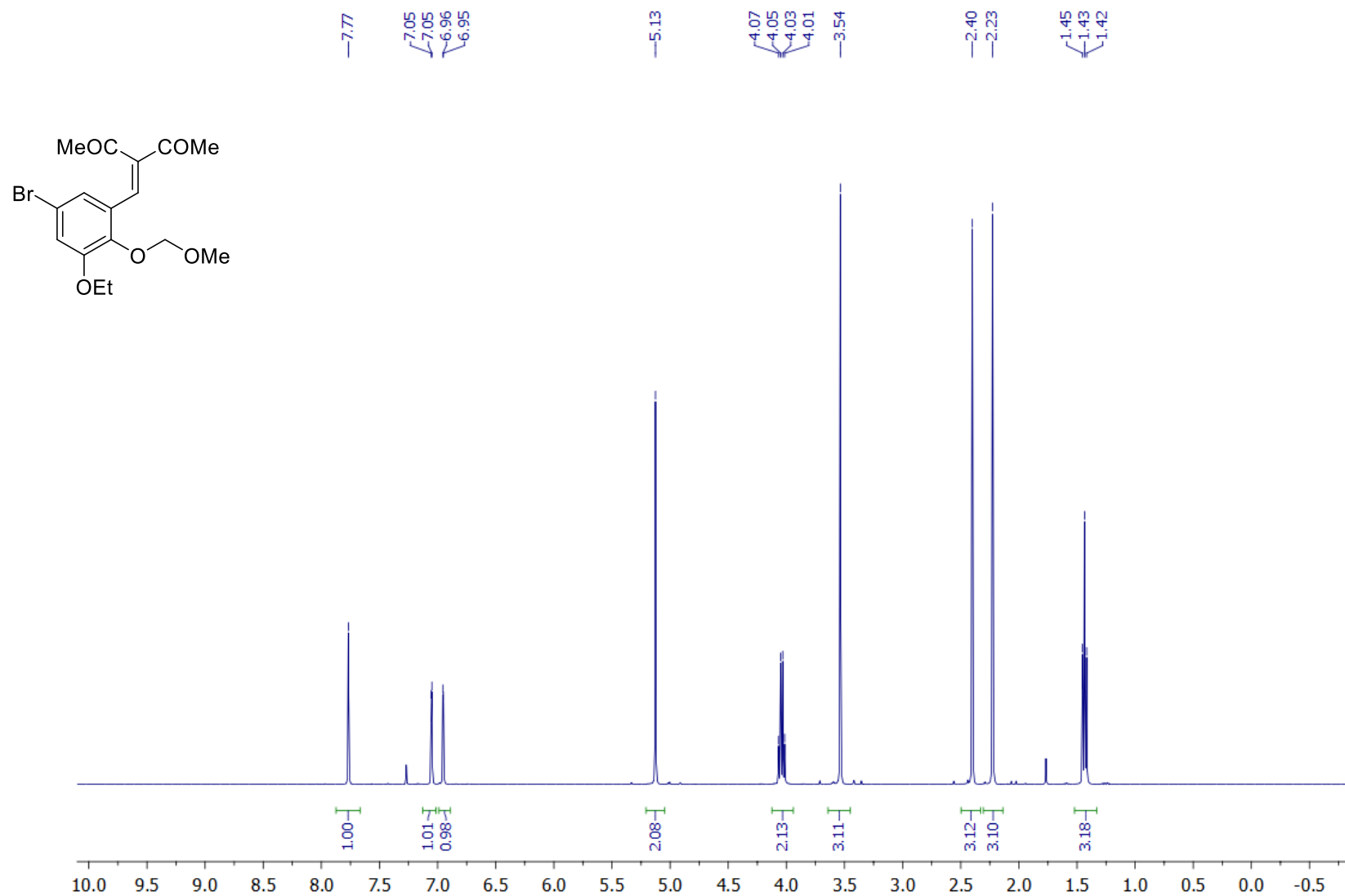
3-[[3-Methoxy-2-(methoxymethoxy)-5-nitrophenyl]methylidene]pentane-2,4-dione (S2l)

^{13}C NMR (CDCl_3 , 150 MHz)



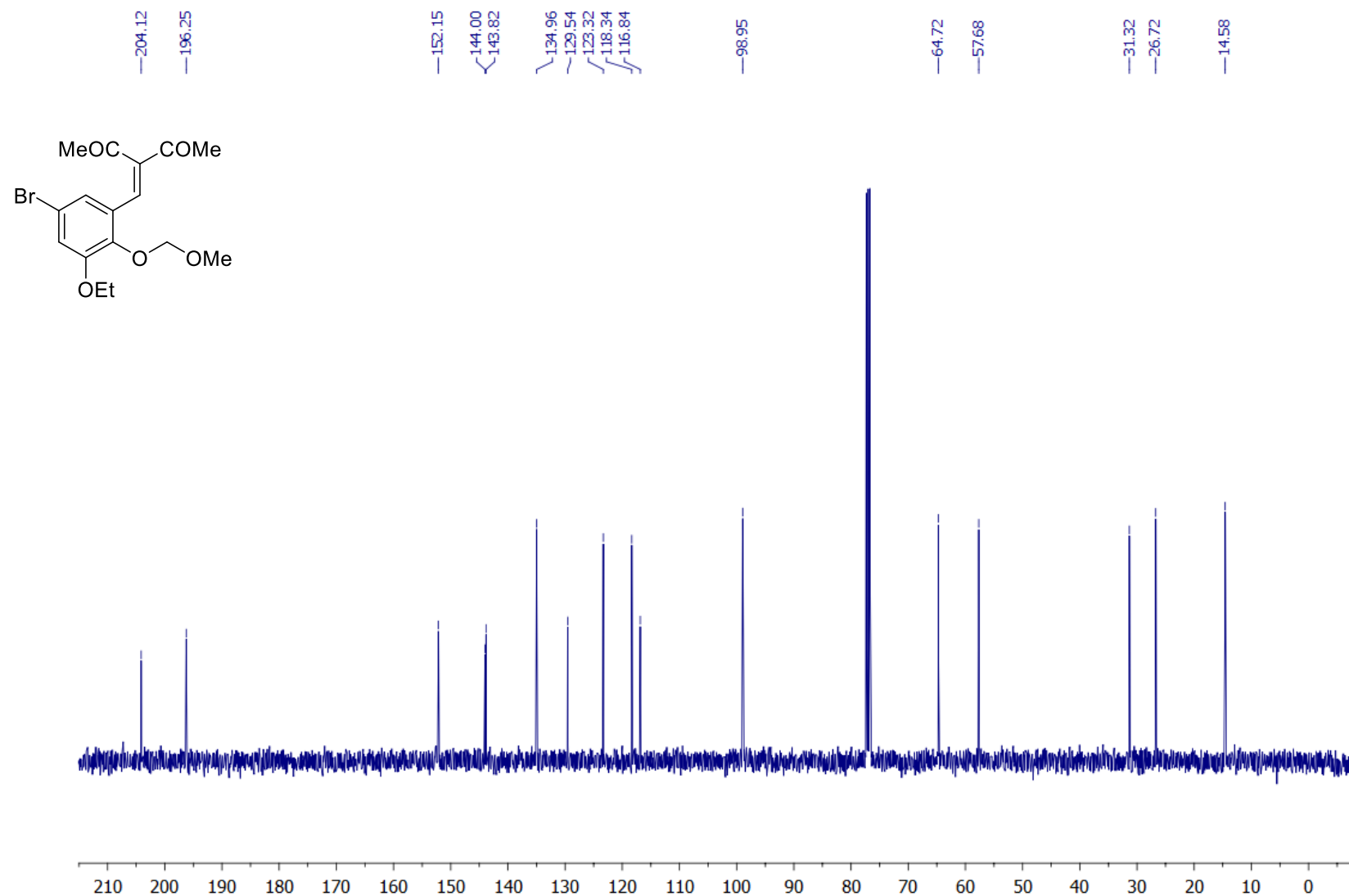
3-[[5-Bromo-3-ethoxy-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2m)

^1H NMR (CDCl_3 , 400 MHz)



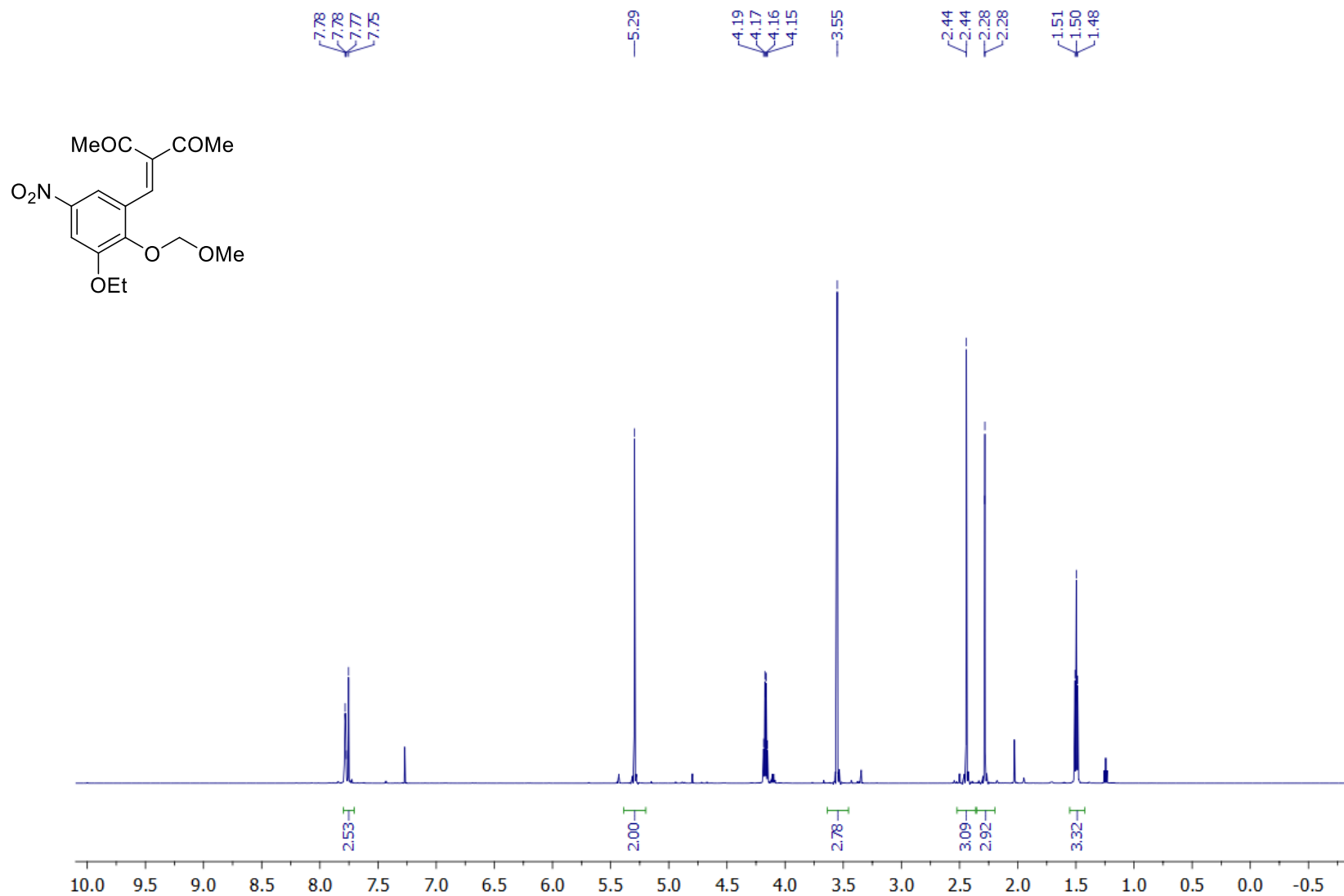
3-[[5-Bromo-3-ethoxy-2-(methoxymethoxy)phenyl]methylidene]pentane-2,4-dione (S2m)

¹³C NMR (CDCl₃, 100 MHz)



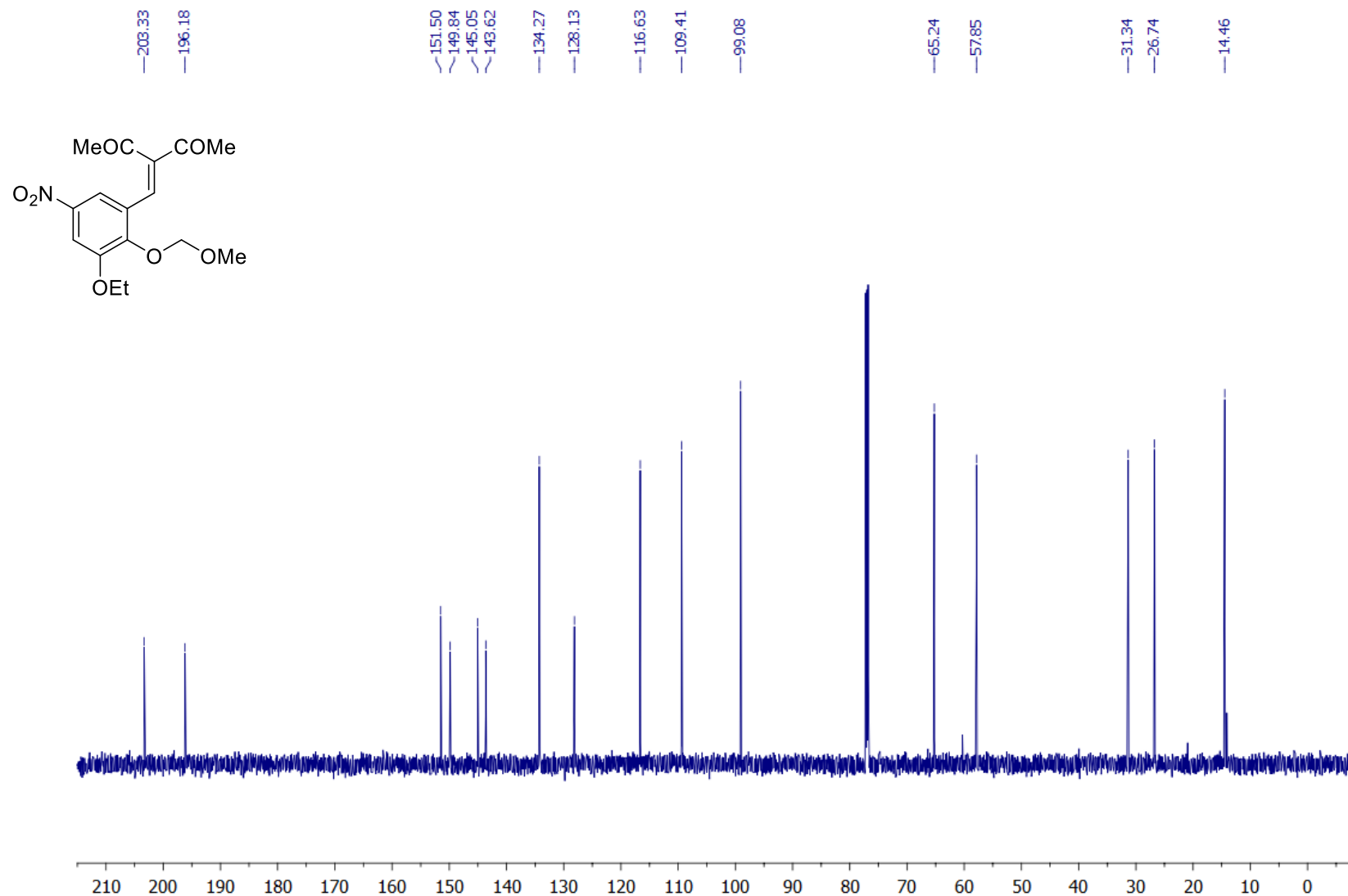
3-[[3-Ethoxy-2-(methoxymethoxy)-5-nitrophenyl]methylidene}pentane-2,4-dione (S2n)

^1H NMR (CDCl_3 , 600 MHz)

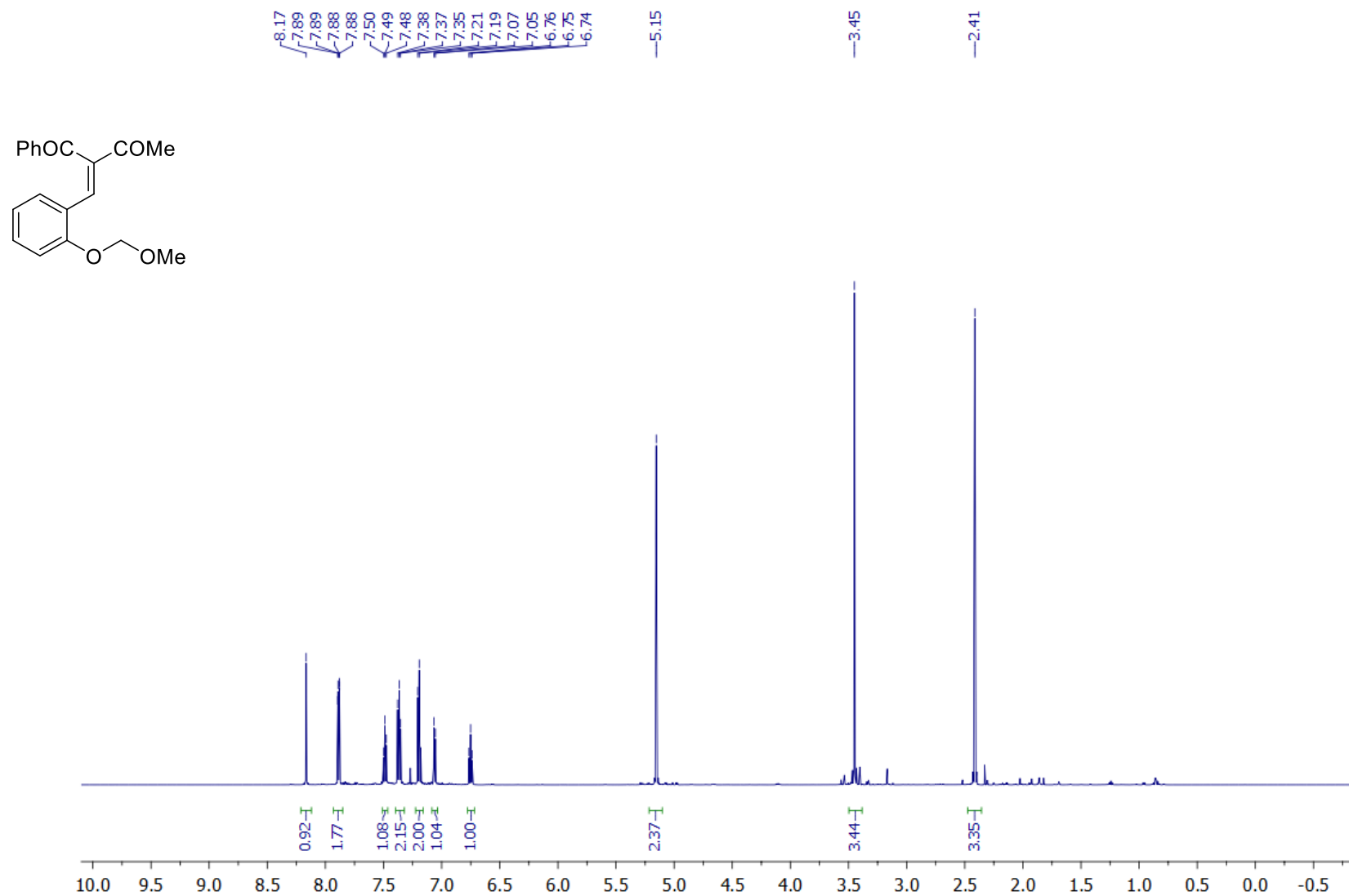


3-[[3-Ethoxy-2-(methoxymethoxy)-5-nitrophenyl]methylidene}pentane-2,4-dione (S2n)

^{13}C NMR (CDCl_3 , 150 MHz)

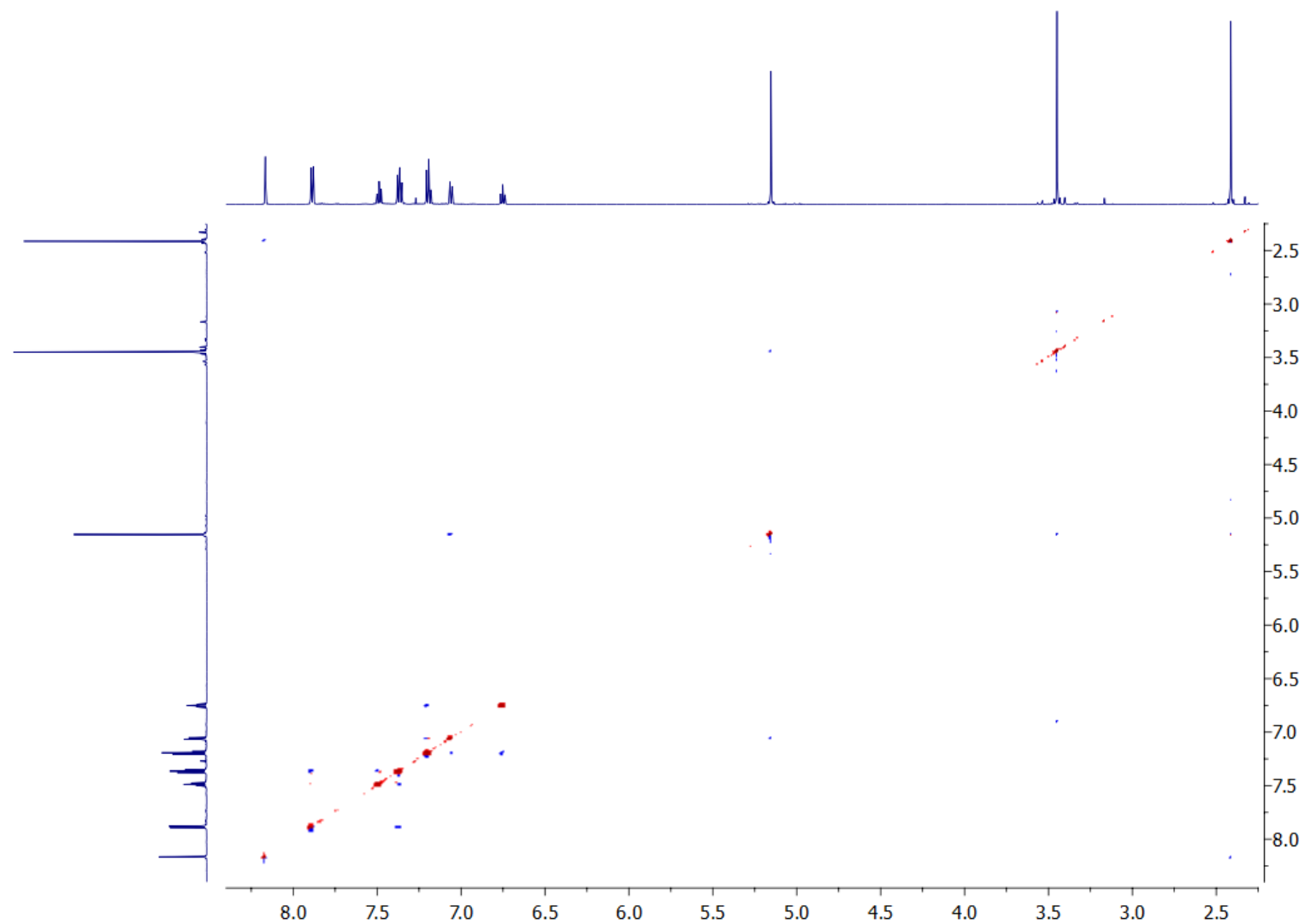
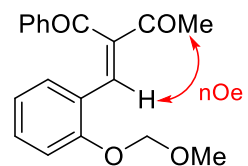


(2Z)-2-{[2-(Methoxymethoxy)phenyl]methylidene}-1-phenylbutane-1,3-dione (S2o)

¹H NMR (CDCl₃, 600 MHz)

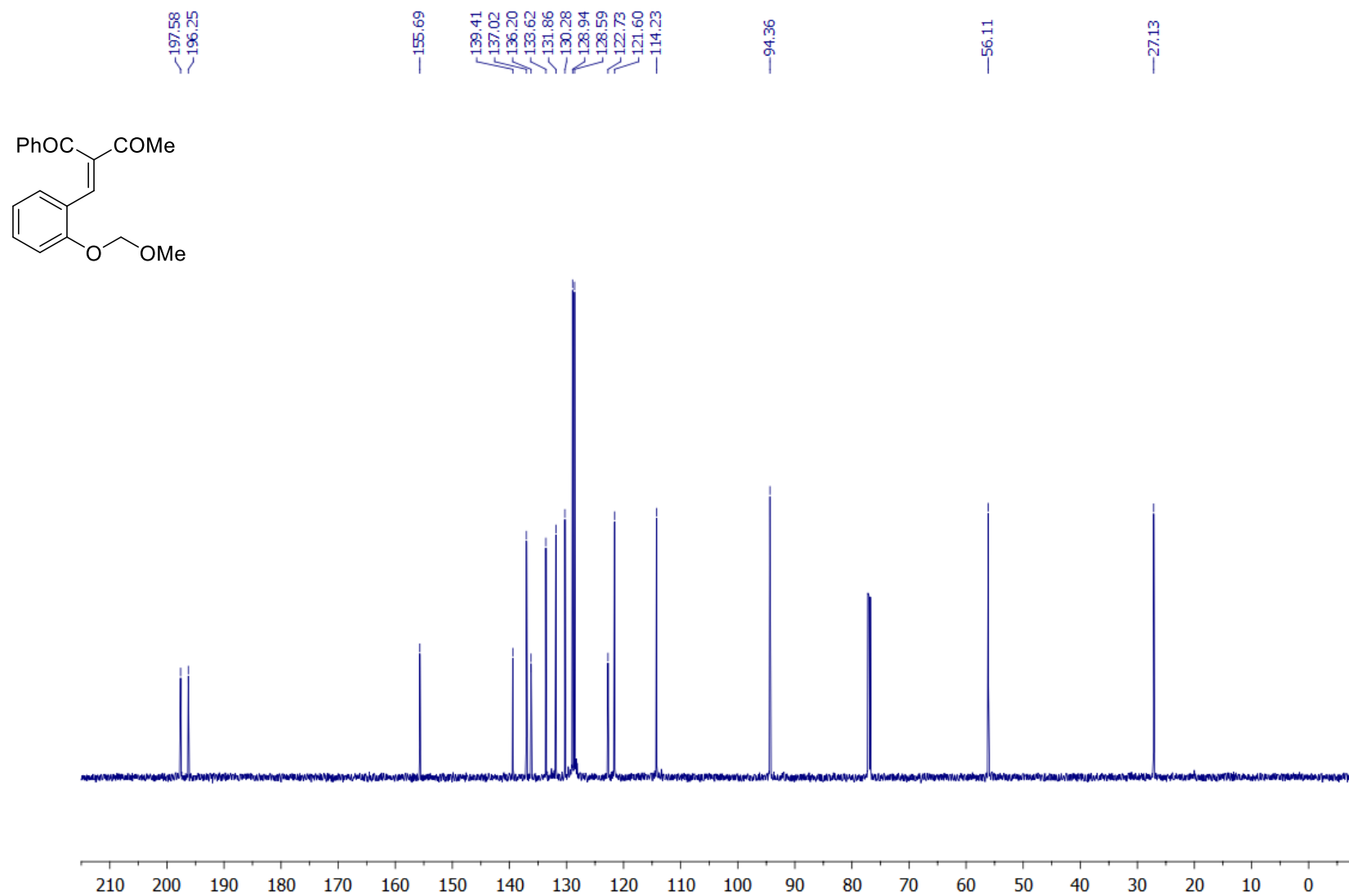
(2Z)-2-[[2-(Methoxymethoxy)phenyl]methylidene]-1-phenylbutane-1,3-dione (S2o)

^1H - ^1H NOESY (CDCl_3)



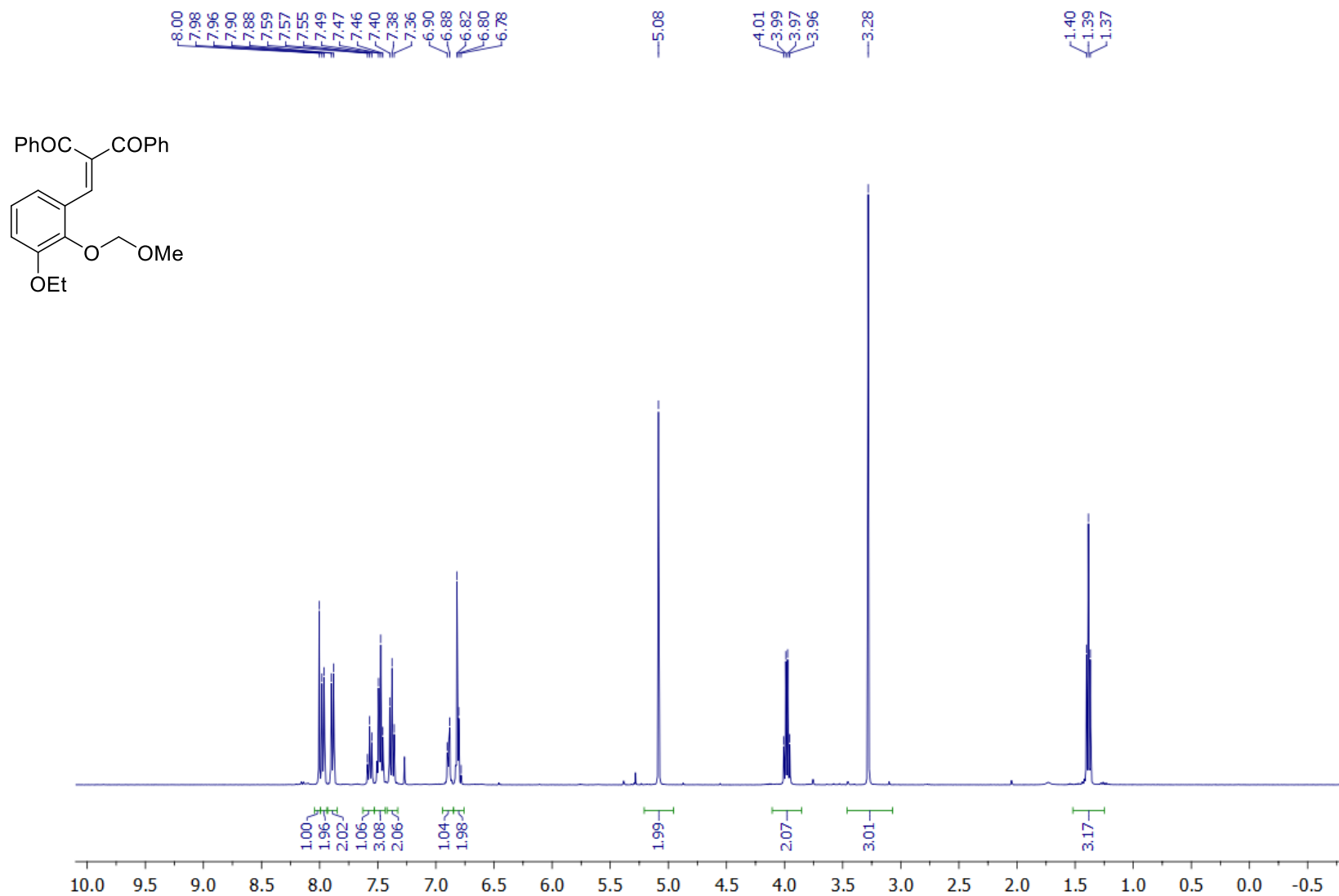
(2Z)-2-[[2-(Methoxymethoxy)phenyl]methylidene]-1-phenylbutane-1,3-dione (S2o)

^{13}C NMR (CDCl_3 , 150 MHz)



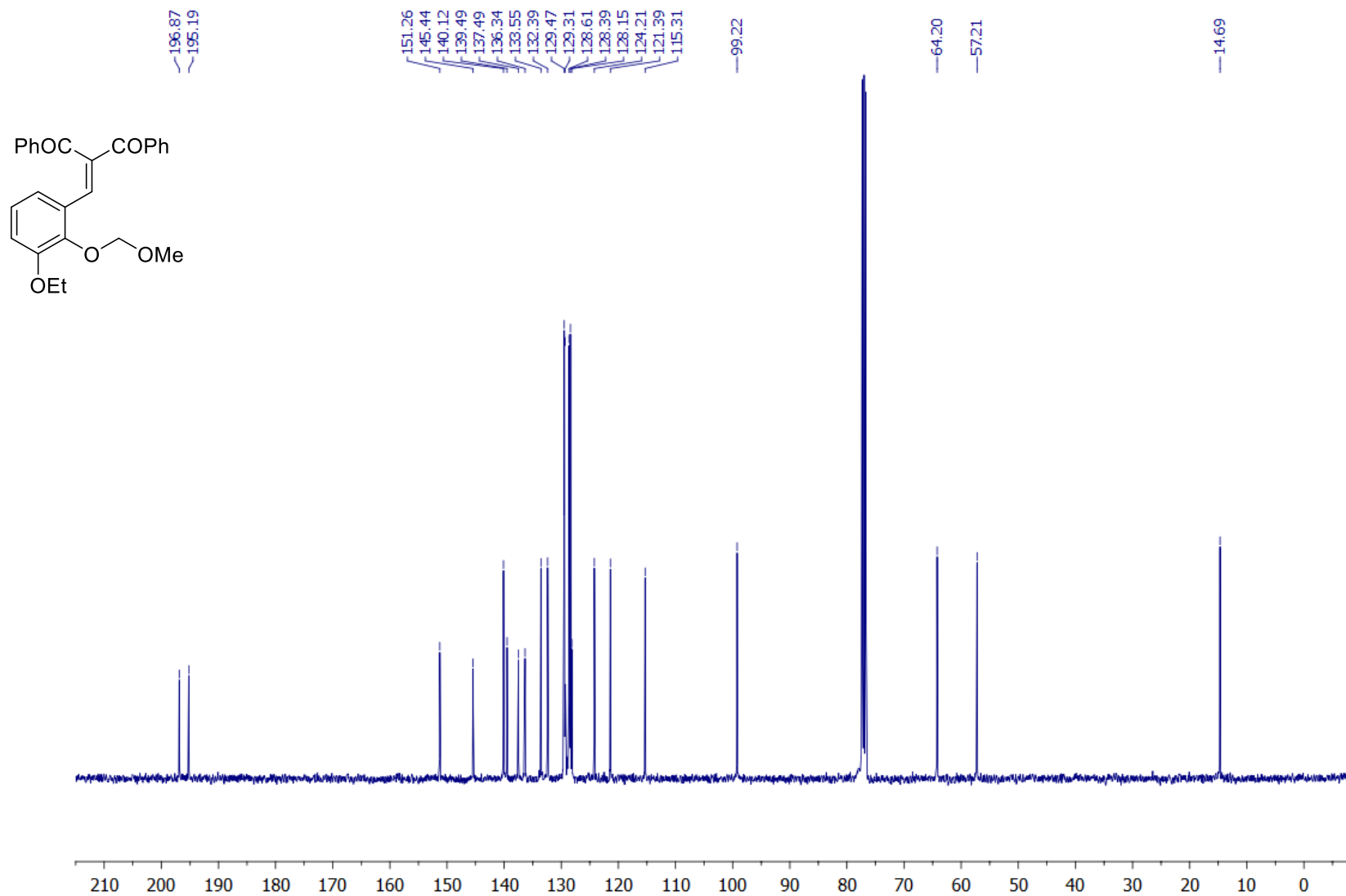
2-(3-Ethoxy-2-(methoxymethoxy)benzylidene)-1,3-diphenylpropane-1,3-dione (S2p)

^1H NMR (CDCl_3 , 400 MHz)



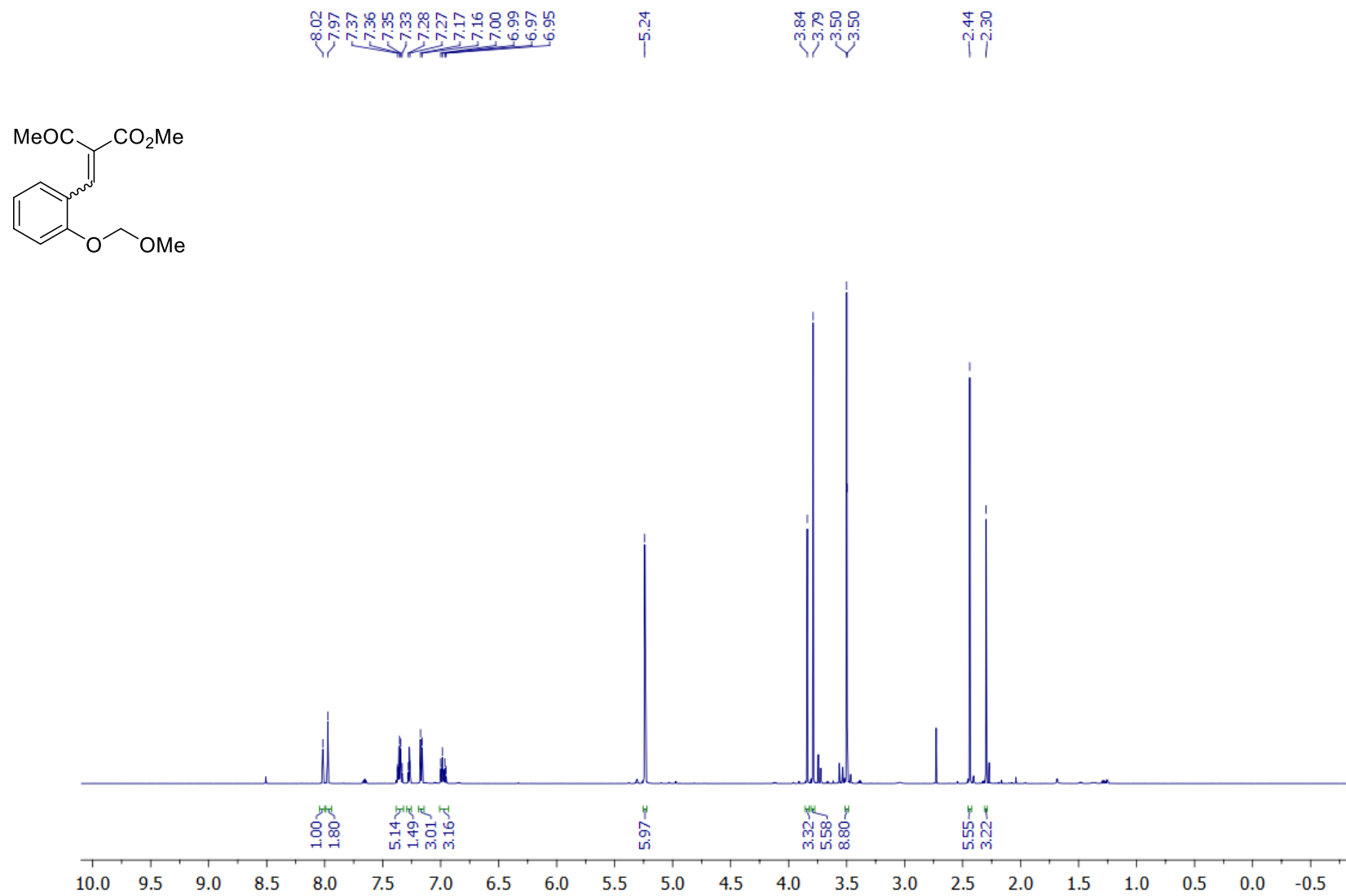
2-(3-Ethoxy-2-(methoxymethoxy)benzylidene)-1,3-diphenylpropane-1,3-dione (S2p)

^{13}C NMR (CDCl_3 , 100 MHz)



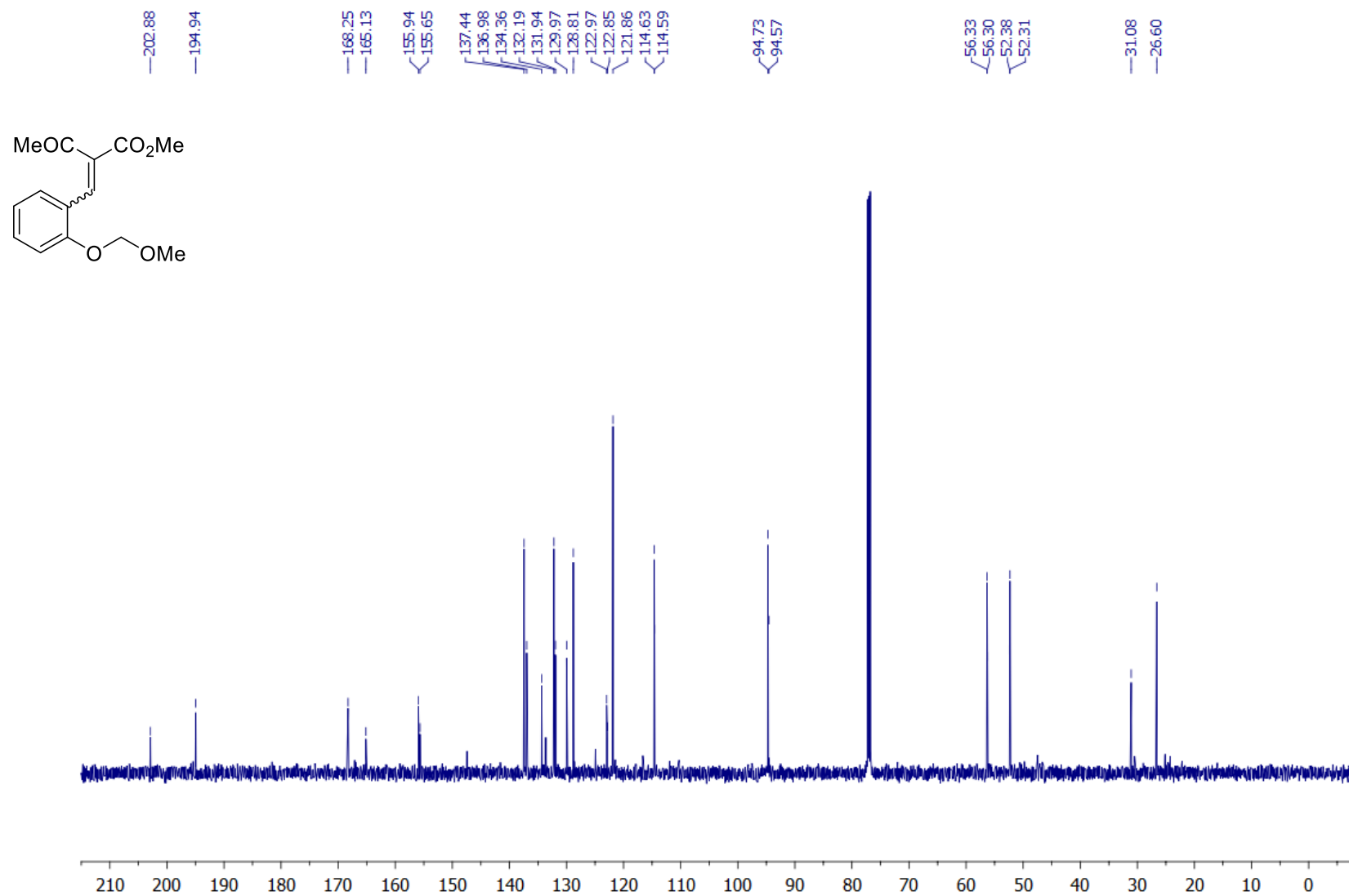
Methyl 2-[2-(methoxymethoxy)benzylidene]-3-oxobutanoate (S2q)

^1H NMR (CDCl_3 , 600 MHz)



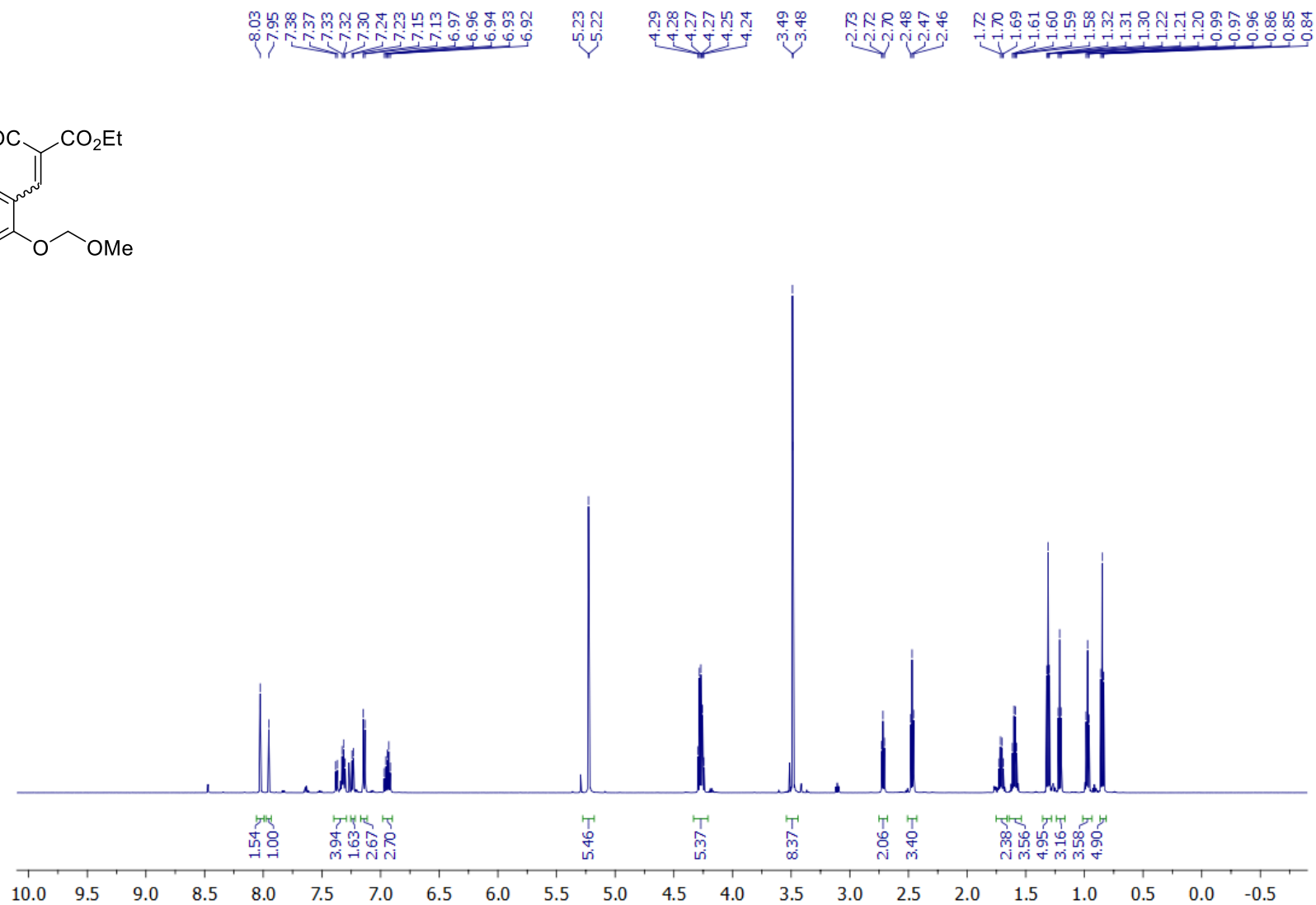
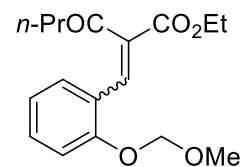
Methyl 2-[2-(methoxymethoxy)benzylidene]-3-oxobutanoate (S2q)

^{13}C NMR (CDCl_3 , 150 MHz)



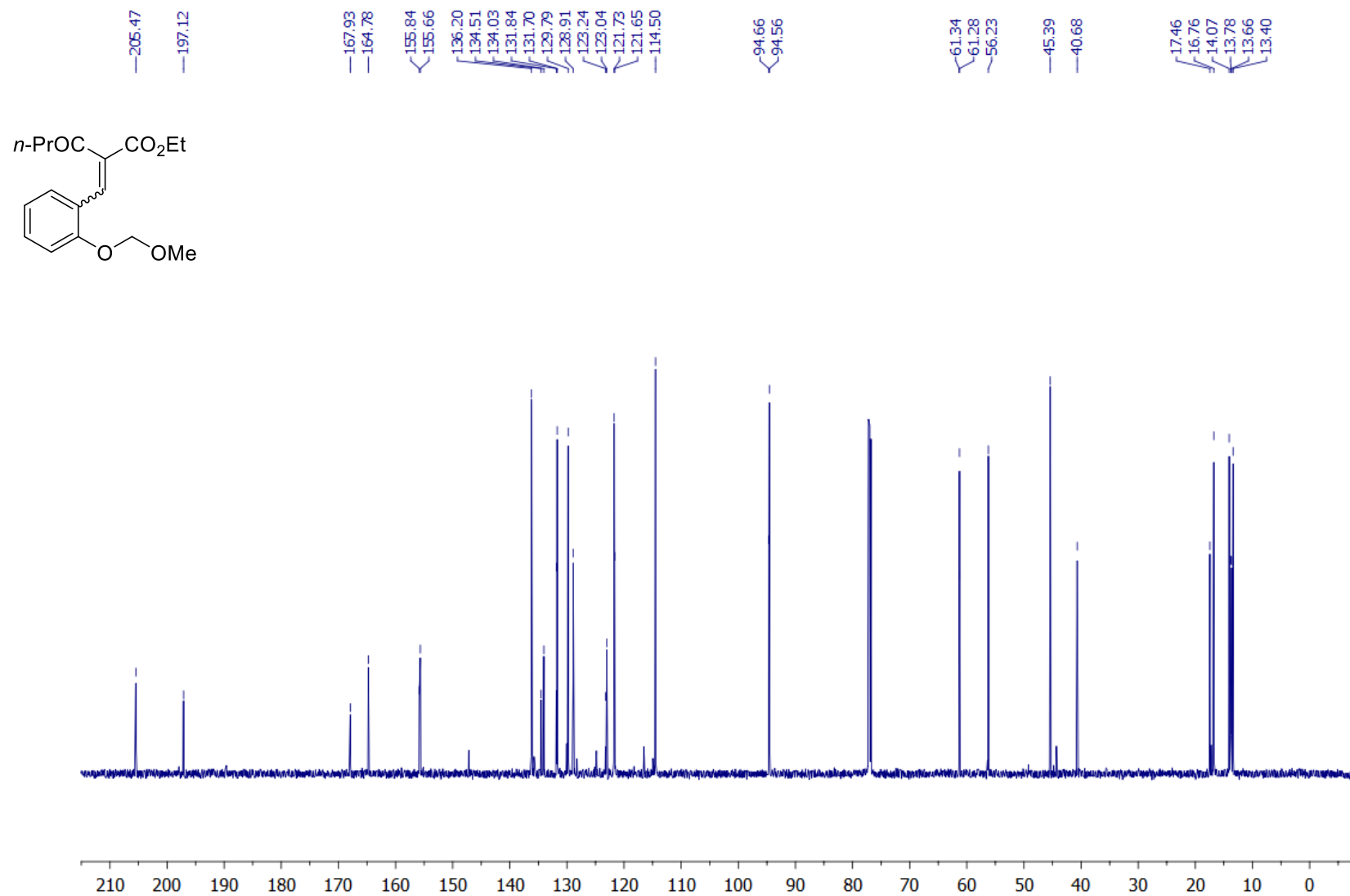
Ethyl 2-[2-(methoxymethoxy)benzylidene]-3-oxohexanoate (S2r)

^1H NMR (CDCl_3 , 600 MHz)



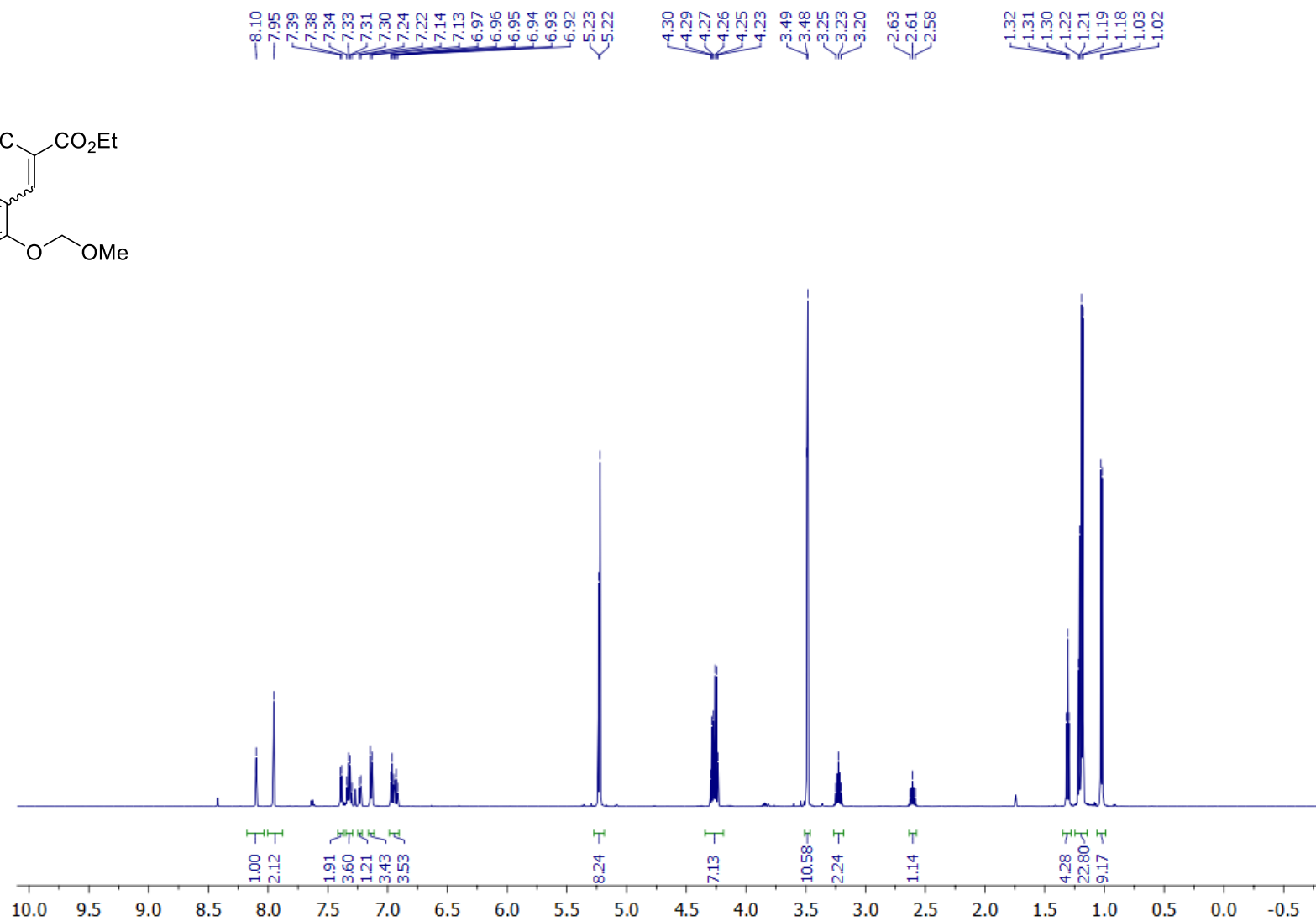
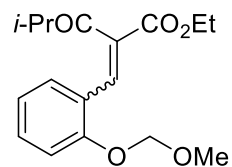
Ethyl 2-[2-(methoxymethoxy)benzylidene]-3-oxohexanoate (S2r)

¹³C NMR (CDCl₃, 150 MHz)



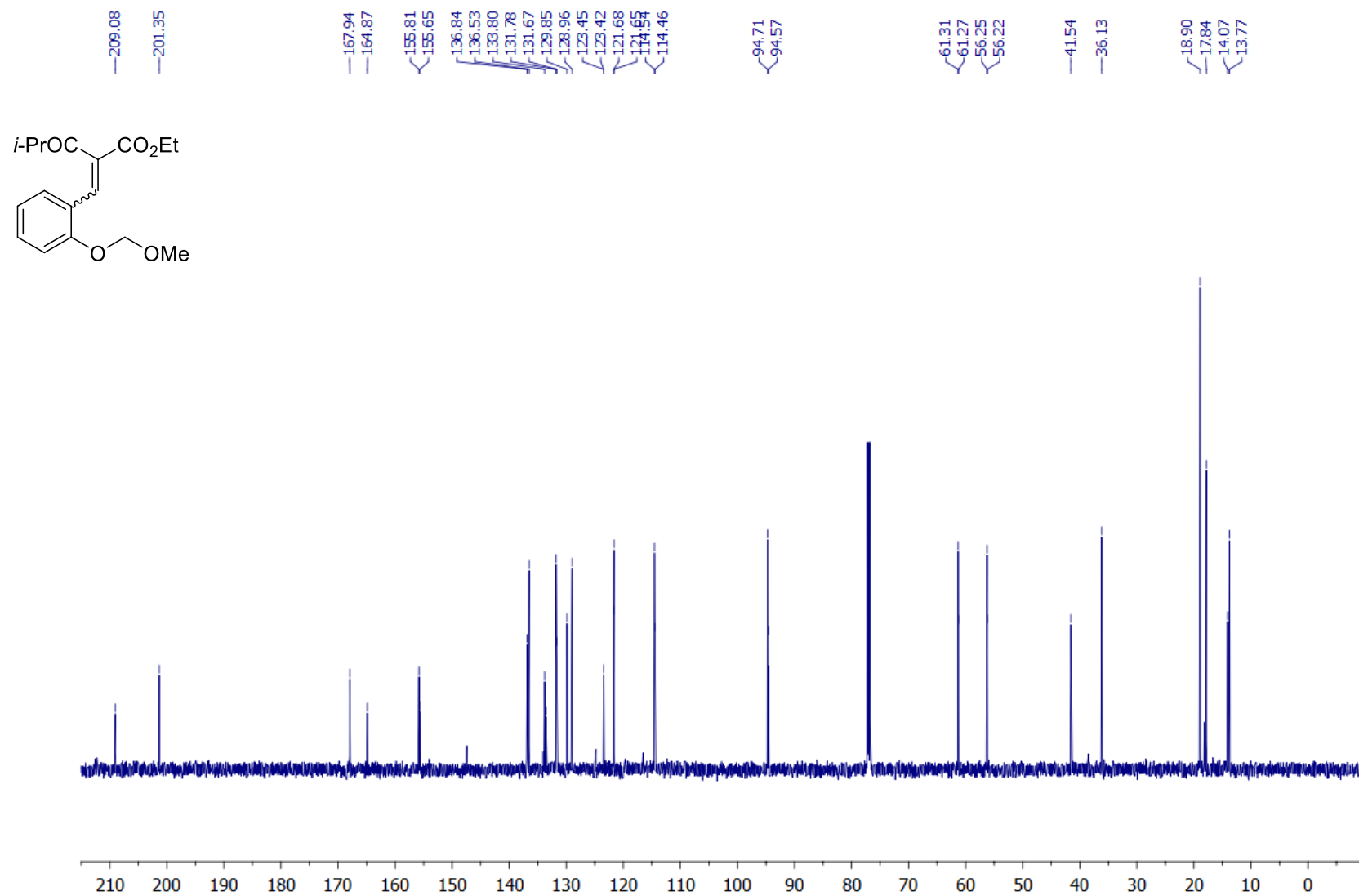
Ethyl 2-[2-(methoxymethoxy)benzylidene]-4-methyl-3-oxopentanoate (S2s)

^1H NMR (CDCl_3 , 600 MHz)



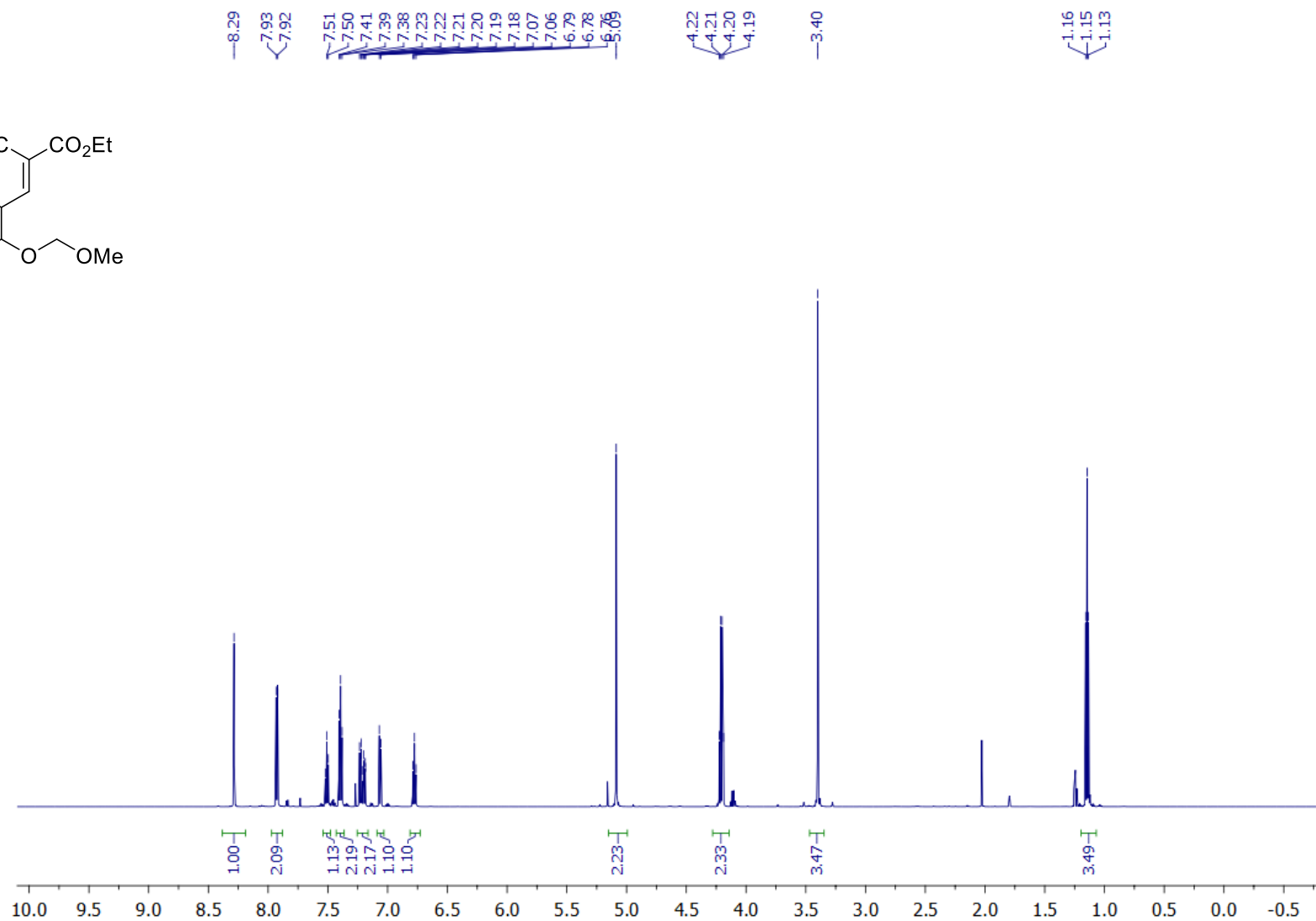
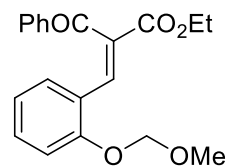
Ethyl 2-[2-(methoxymethoxy)benzylidene]-4-methyl-3-oxopentanoate (S2s)

^{13}C NMR (CDCl_3 , 150 MHz)



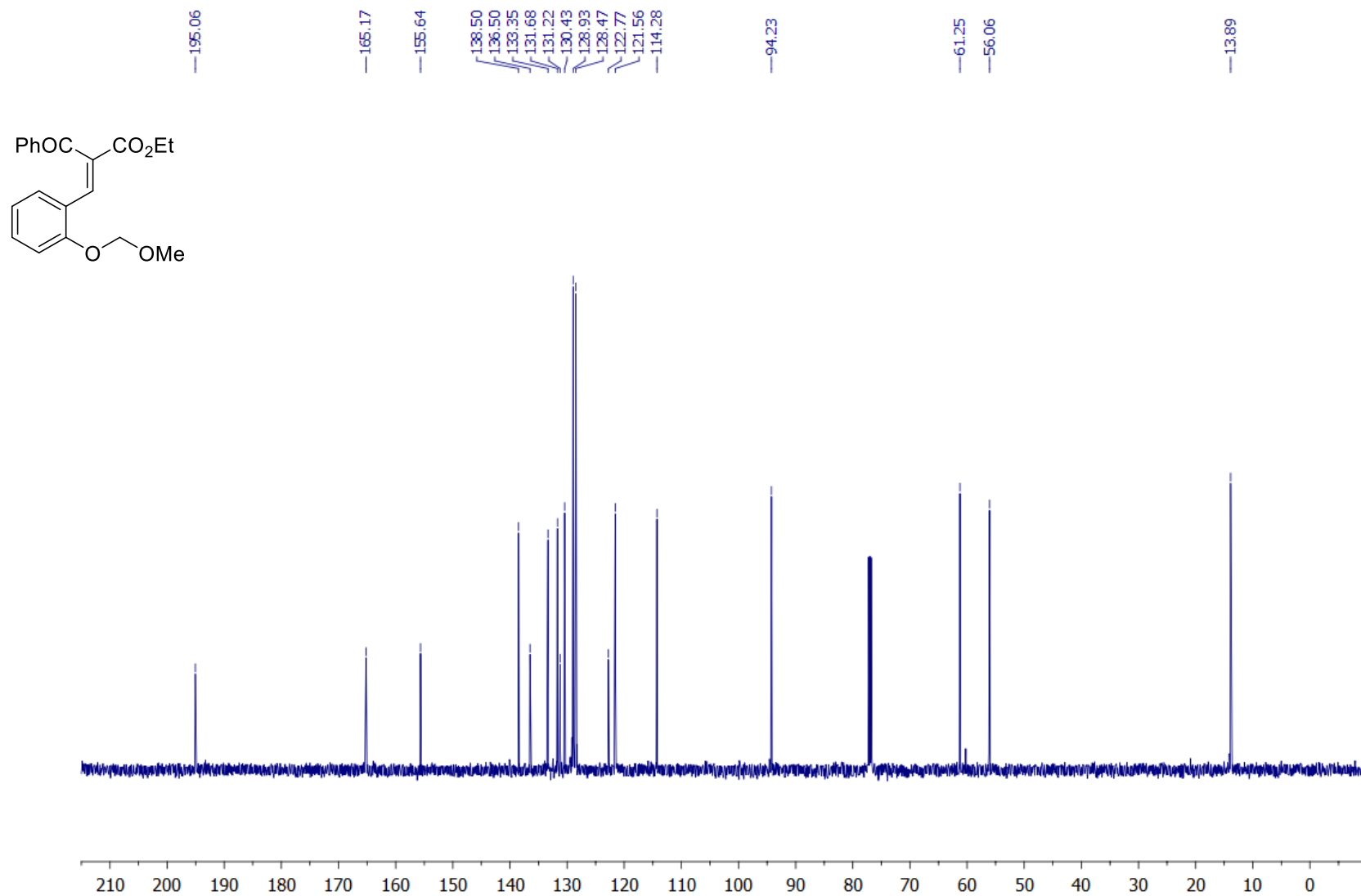
Ethyl (2*E*)-2-benzoyl-3-[2-(methoxymethoxy)phenyl]prop-2-enoate (S2t)

¹H NMR (CDCl₃, 600 MHz)



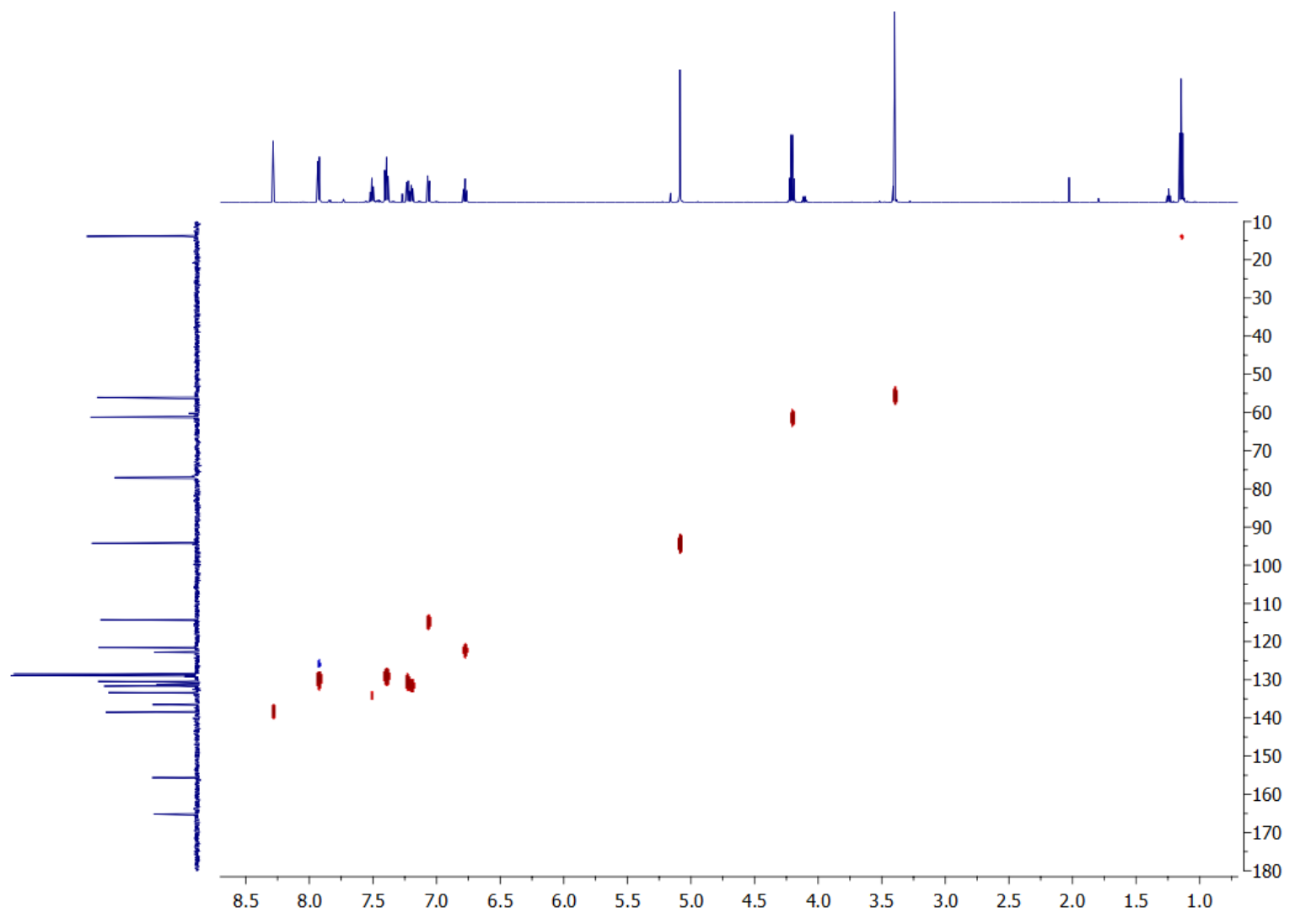
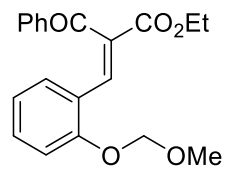
Ethyl (2*E*)-2-benzoyl-3-[2-(methoxymethoxy)phenyl]prop-2-enoate (S2t)

^{13}C NMR (CDCl_3 , 150 MHz)



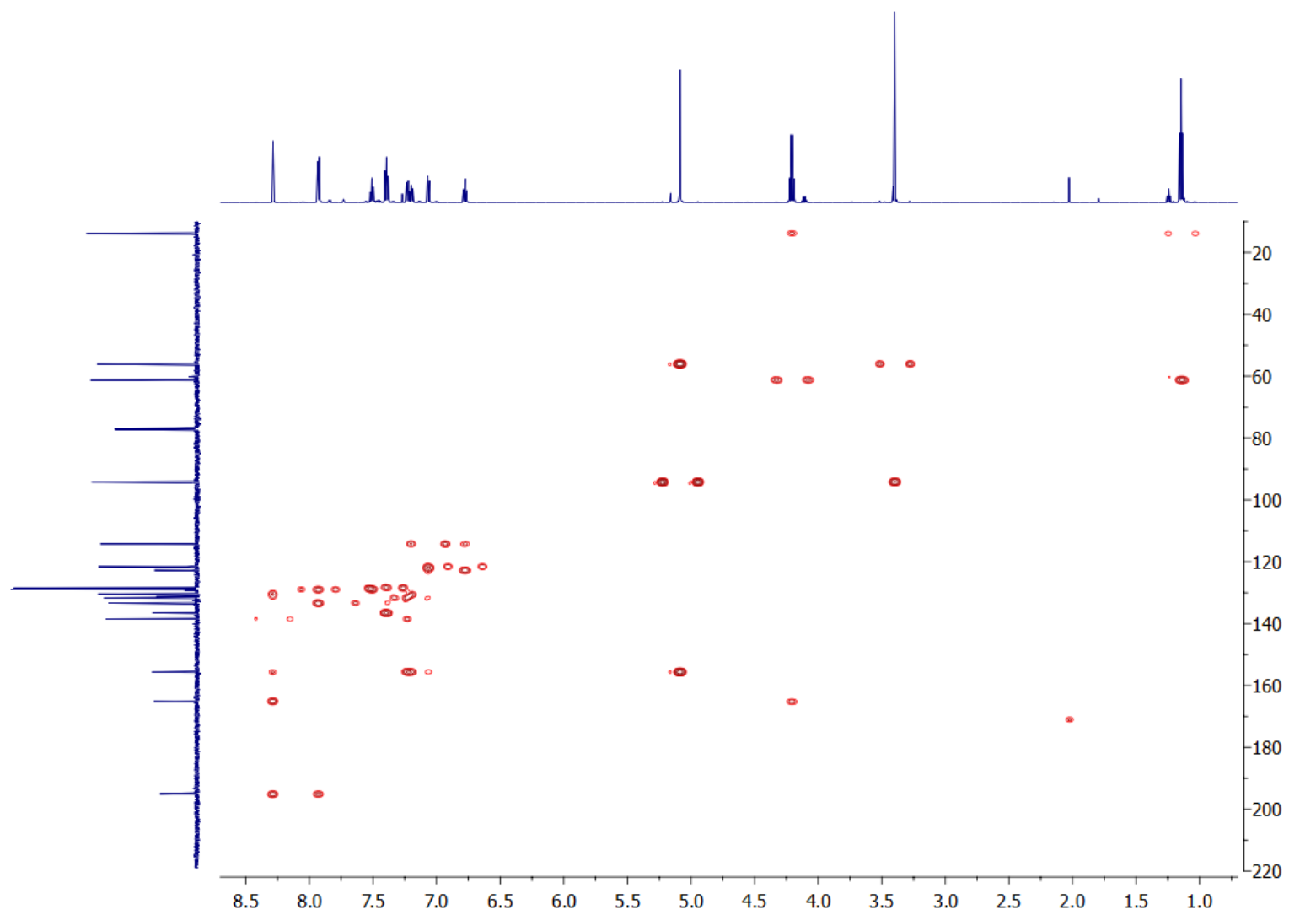
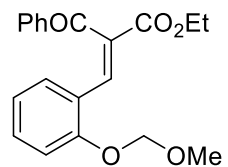
Ethyl (2*E*)-2-benzoyl-3-[2-(methoxymethoxy)phenyl]prop-2-enoate (S2t)

^1H - ^{13}C HSQC (CDCl_3)



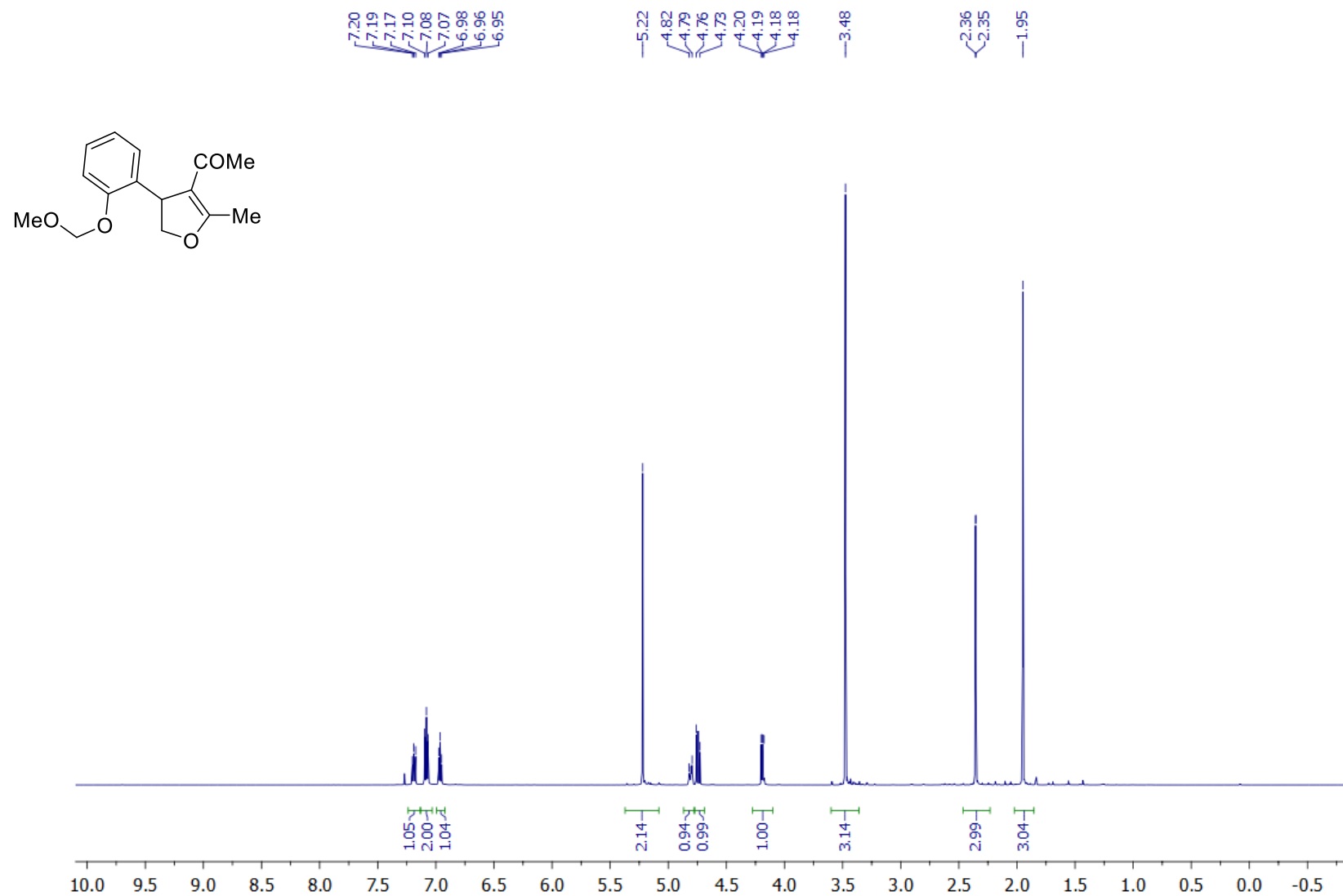
Ethyl (2*E*)-2-benzoyl-3-[2-(methoxymethoxy)phenyl]prop-2-enoate (S2t)

^1H - ^{13}C HMBC (CDCl_3)



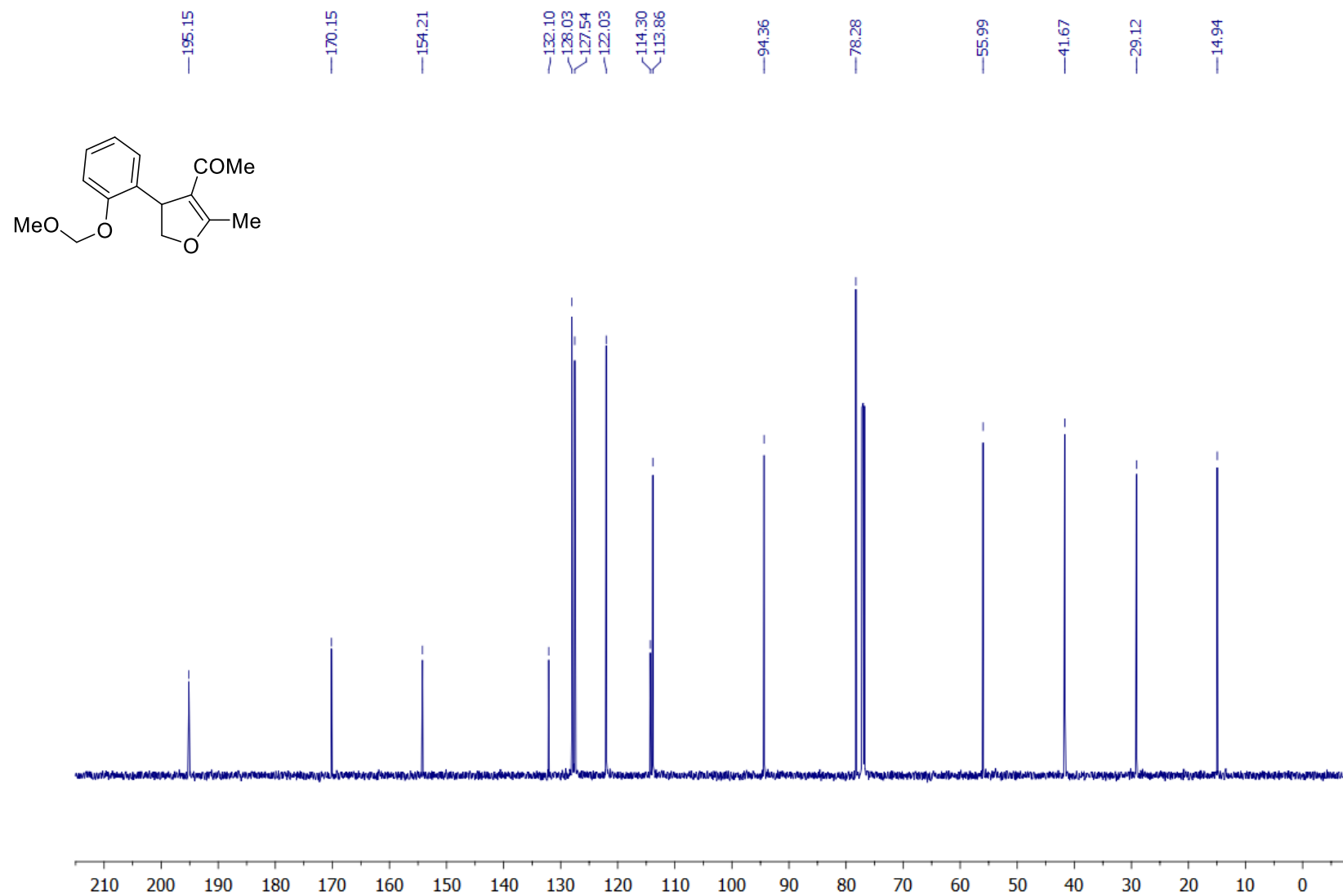
1-{4-[2-(Methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1a)

^1H NMR (CDCl_3 , 600 MHz)



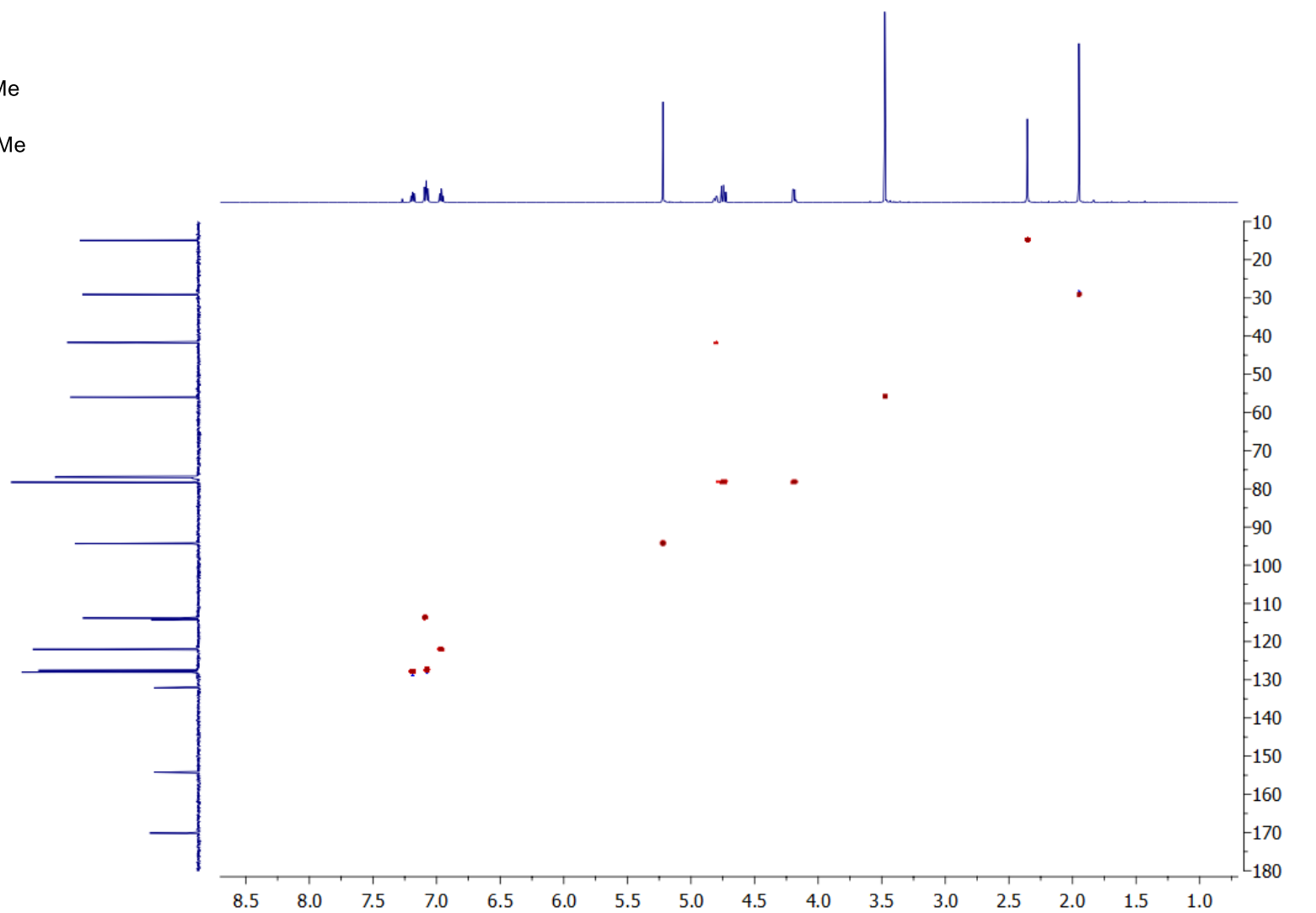
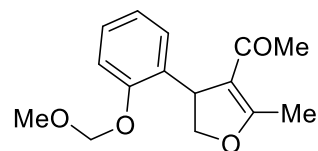
1-{4-[2-(Methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1a)

^{13}C NMR (CDCl_3 , 150 MHz)



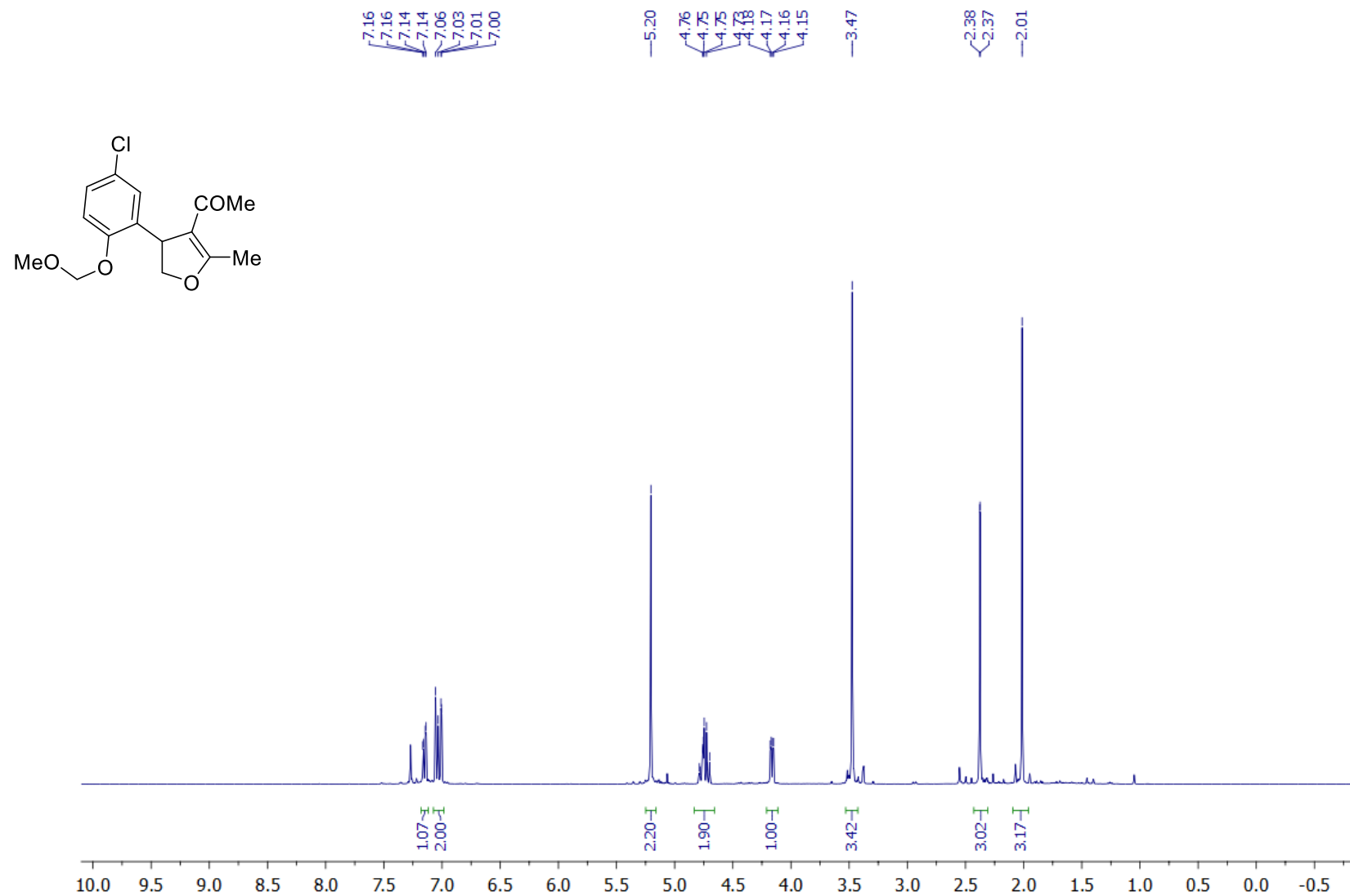
1-{4-[2-(Methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1a)

^1H - ^{13}C HSQC (CDCl_3)



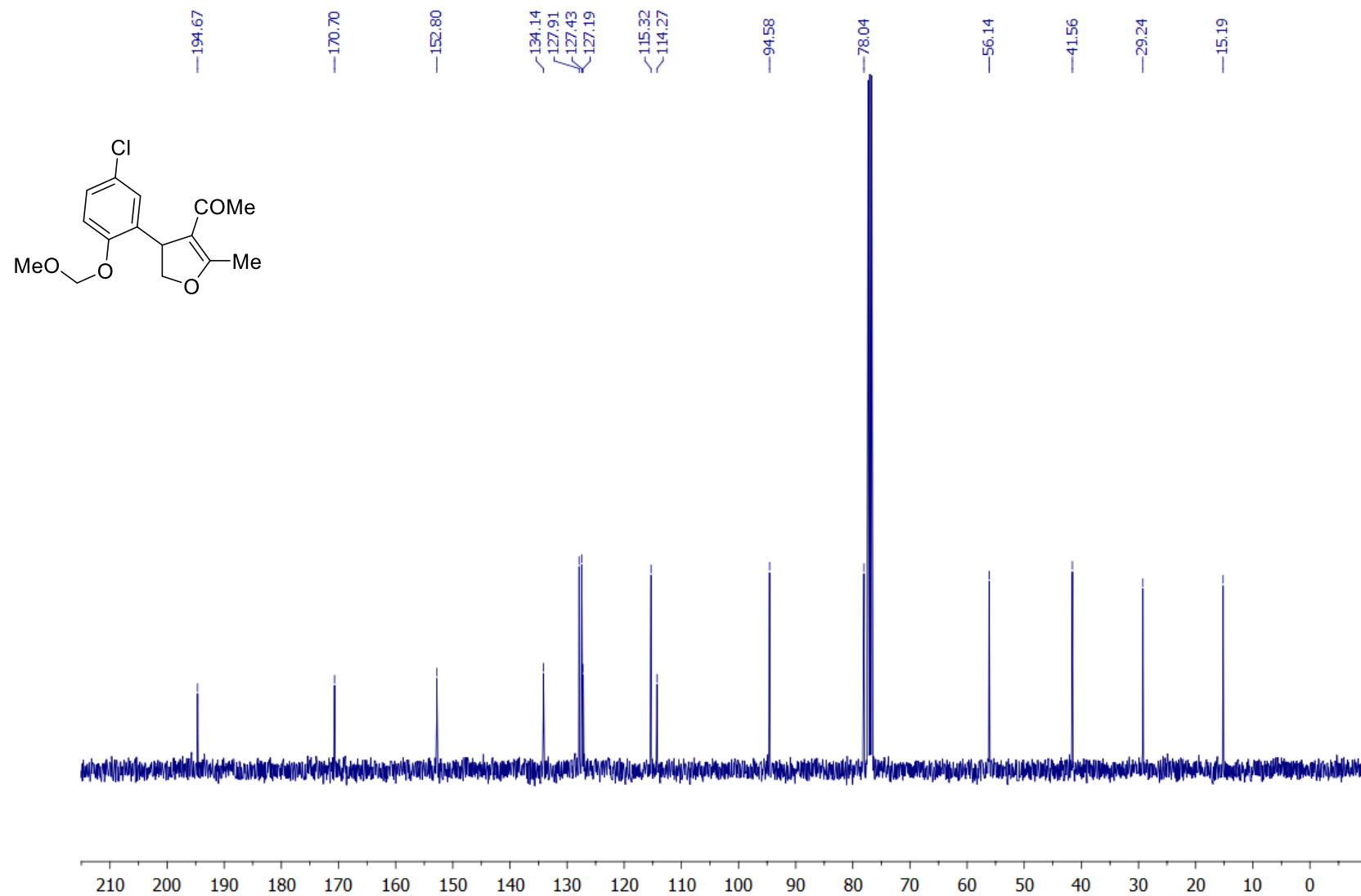
1-{4-[5-Chloro-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1b)

^1H NMR (CDCl_3 , 400 MHz)



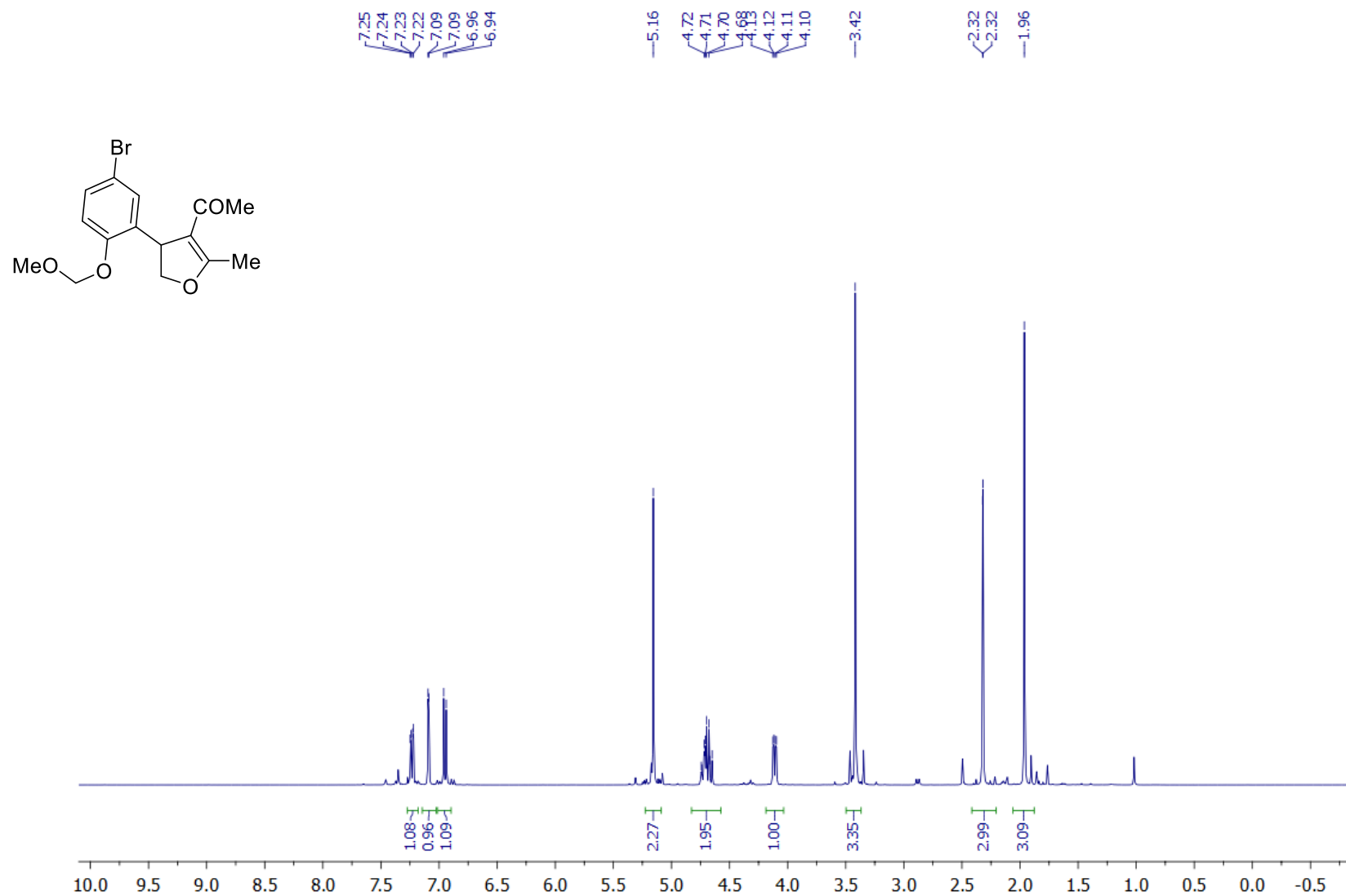
1-{4-[5-Chloro-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1b)

^{13}C NMR (CDCl_3 , 100 MHz)



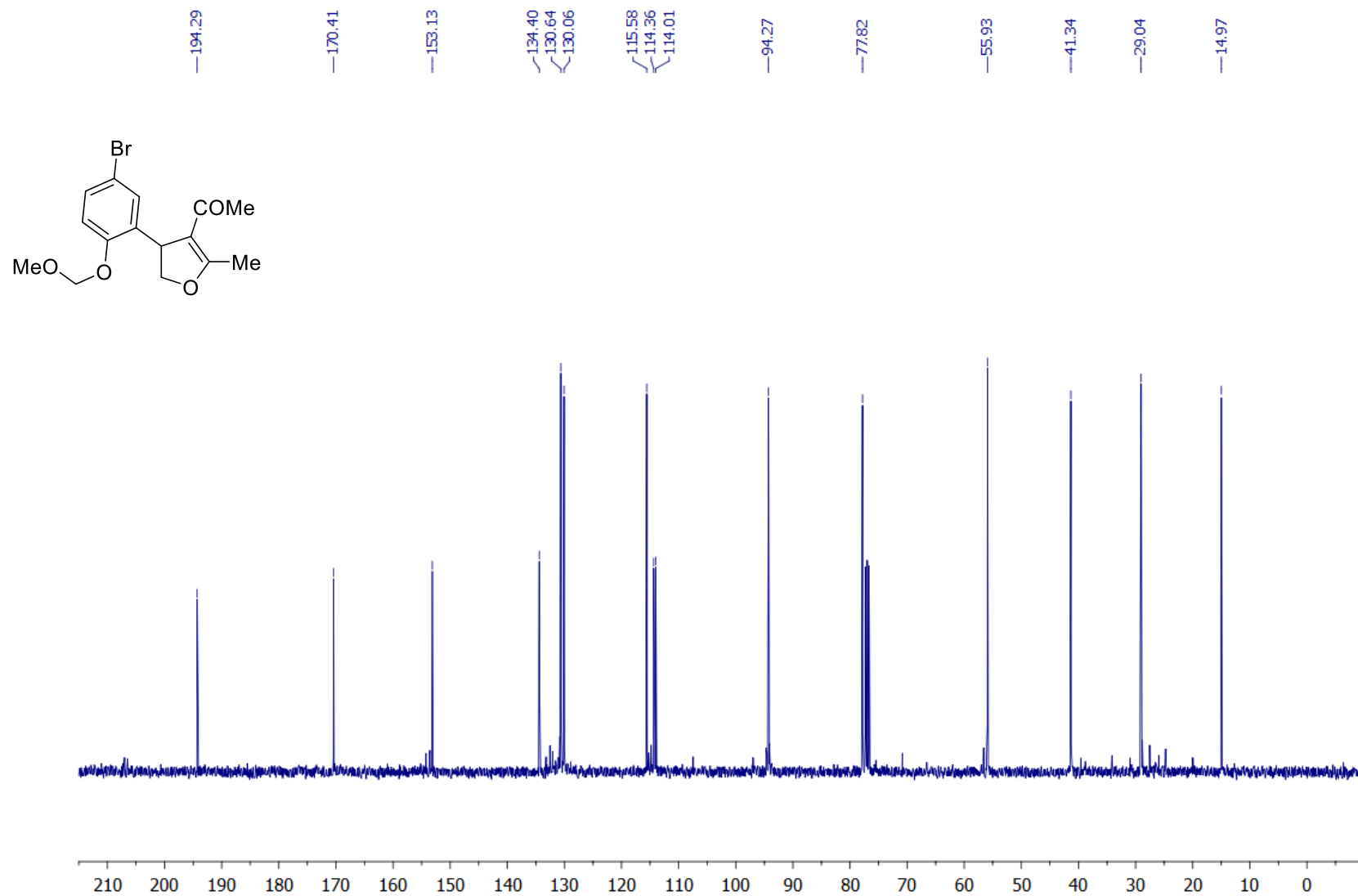
1-{4-[5-Bromo-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1c)

^1H NMR (CDCl_3 , 400 MHz)



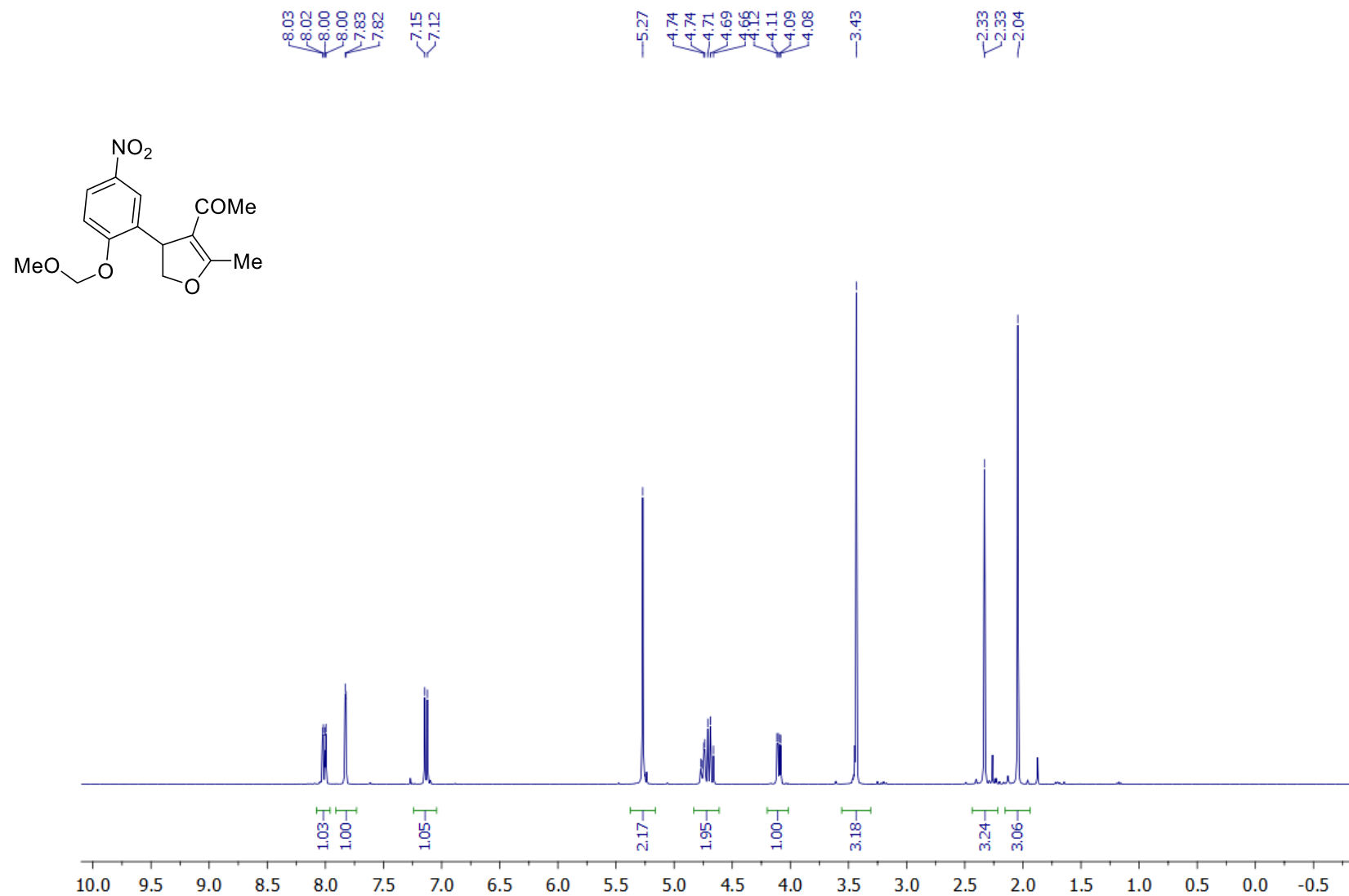
1-{4-[5-Bromo-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1c)

^{13}C NMR (CDCl_3 , 100 MHz)



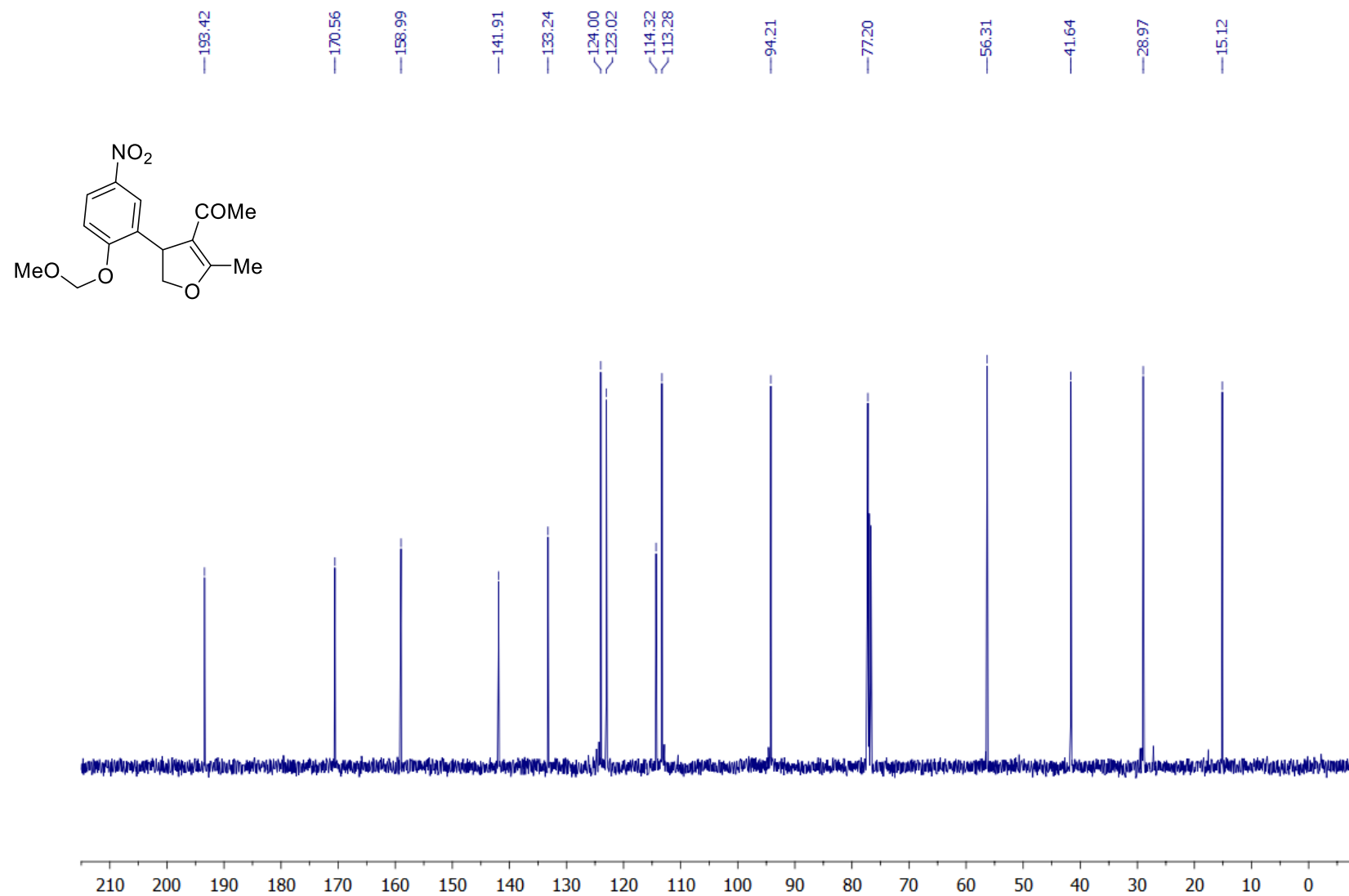
1-{4-[5-Nitro-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1d)

^1H NMR (CDCl_3 , 400 MHz)



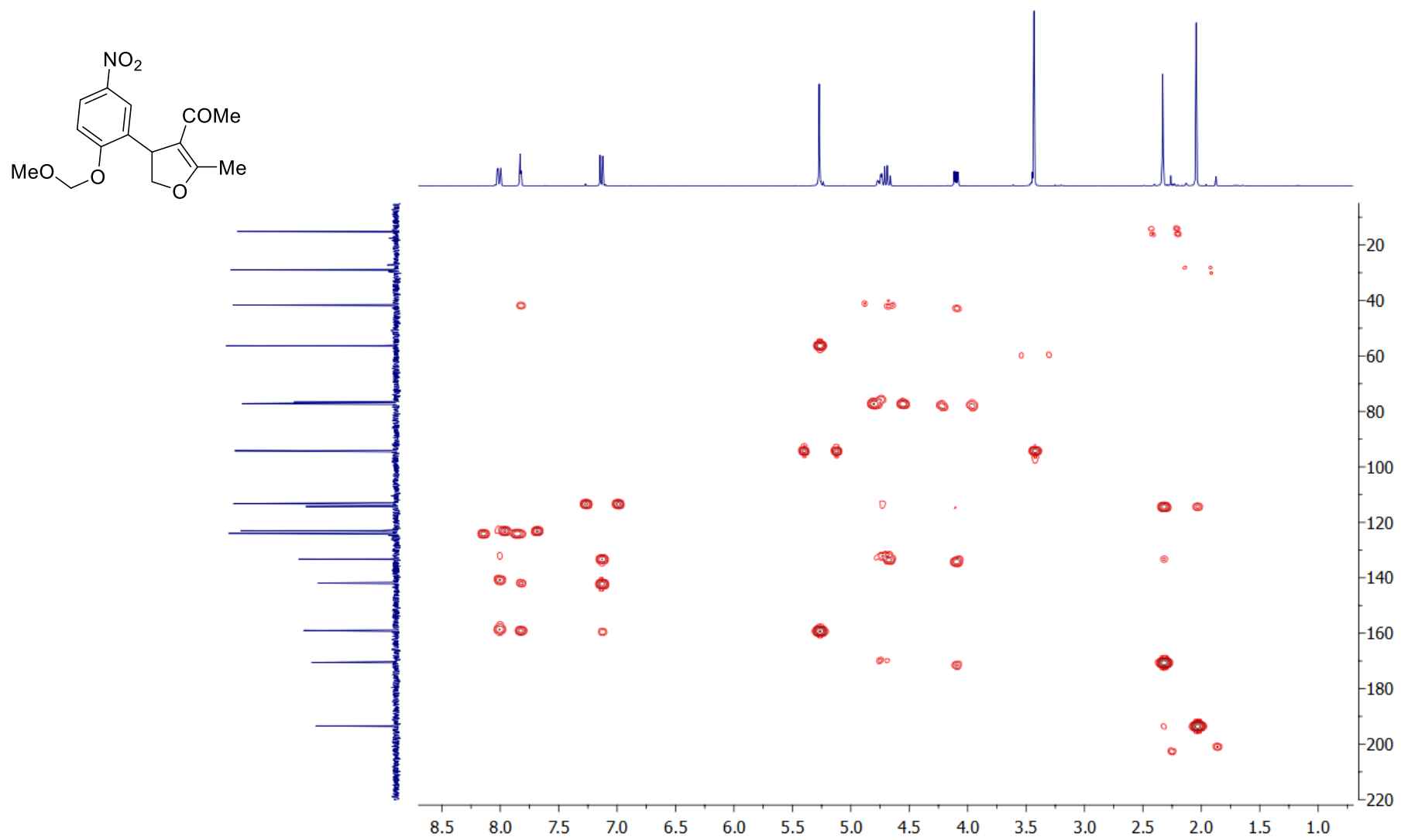
1-{4-[5-Nitro-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1d)

^{13}C NMR (CDCl_3 , 100 MHz)



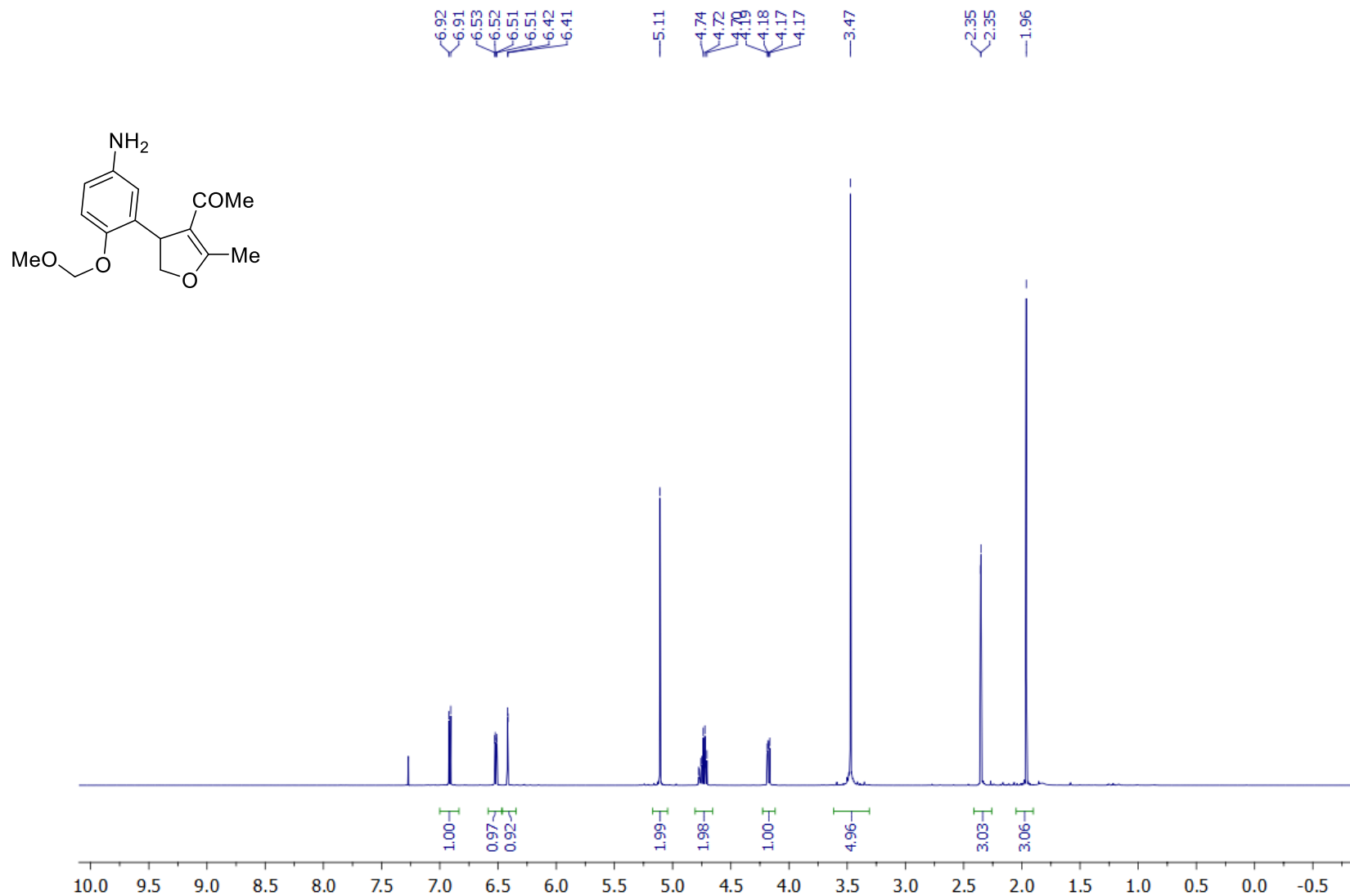
1-{4-[5-Nitro-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1d)

^1H - ^{13}C HMBC (CDCl_3)



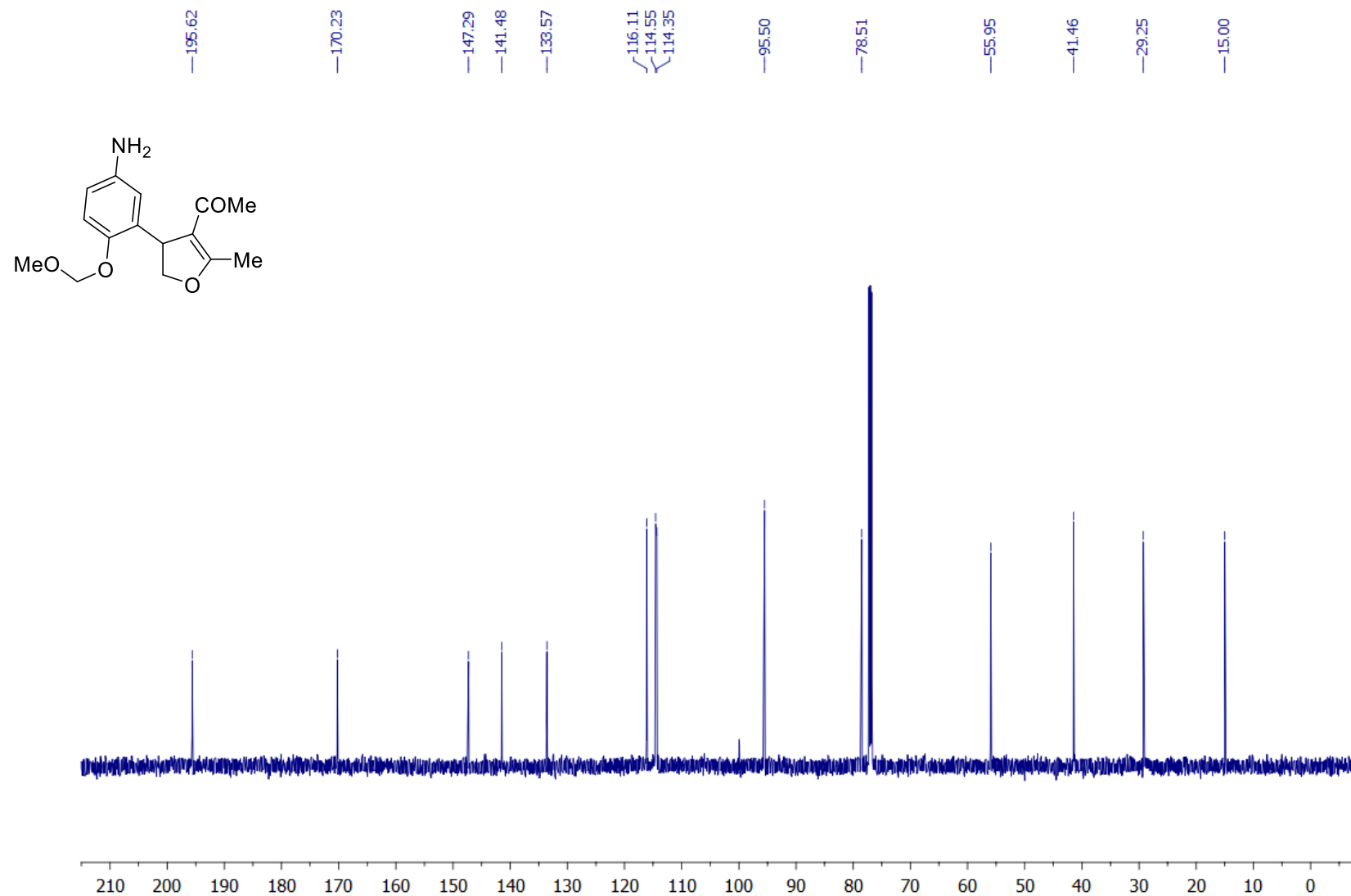
1-{4-[5-Amino-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1d')

^1H NMR (CDCl_3 , 600 MHz)



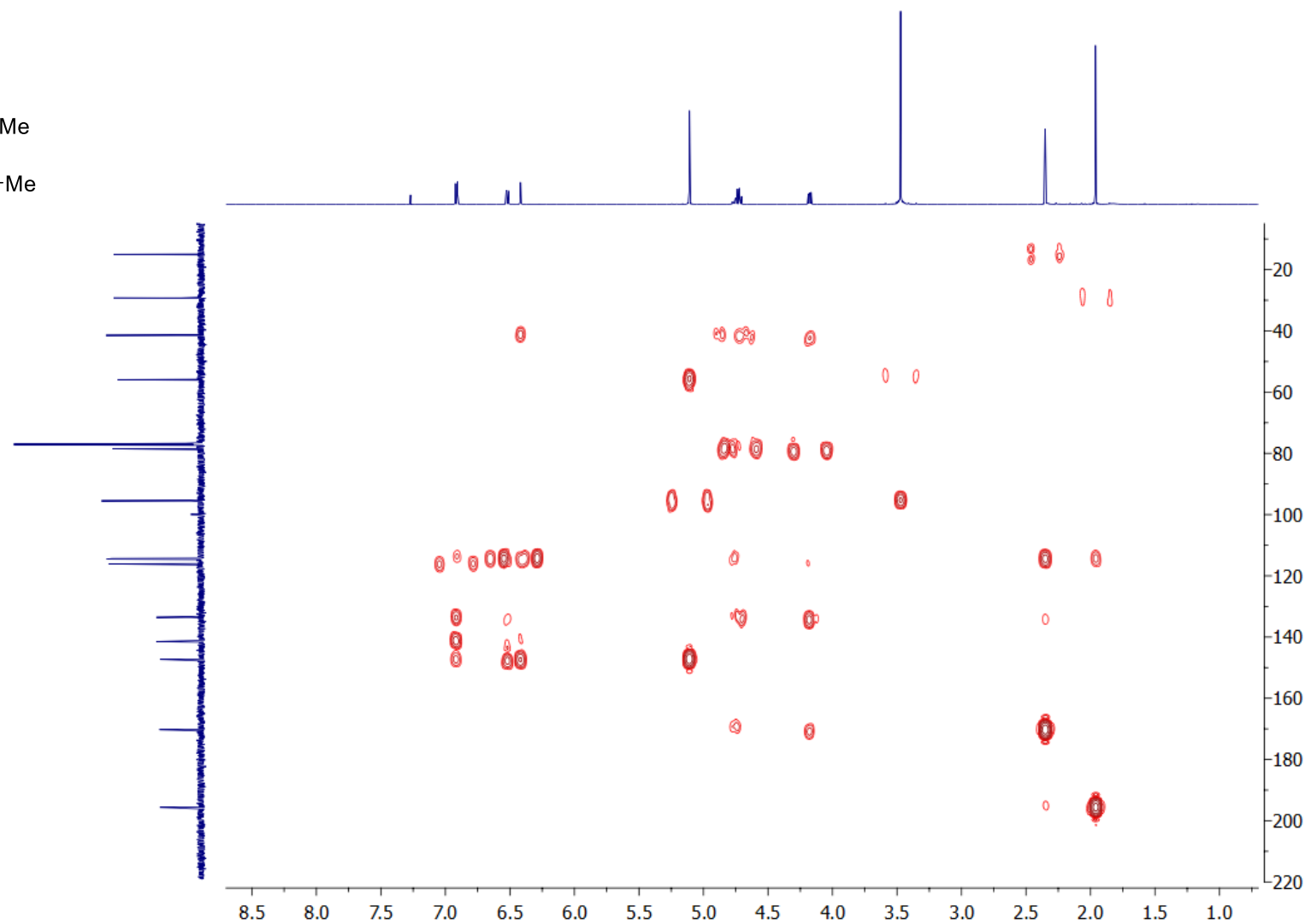
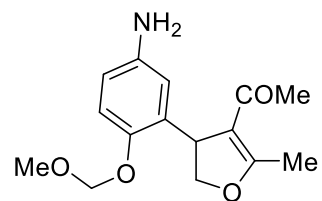
1-{4-[5-Amino-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1d')

^{13}C NMR (CDCl_3 , 150 MHz)



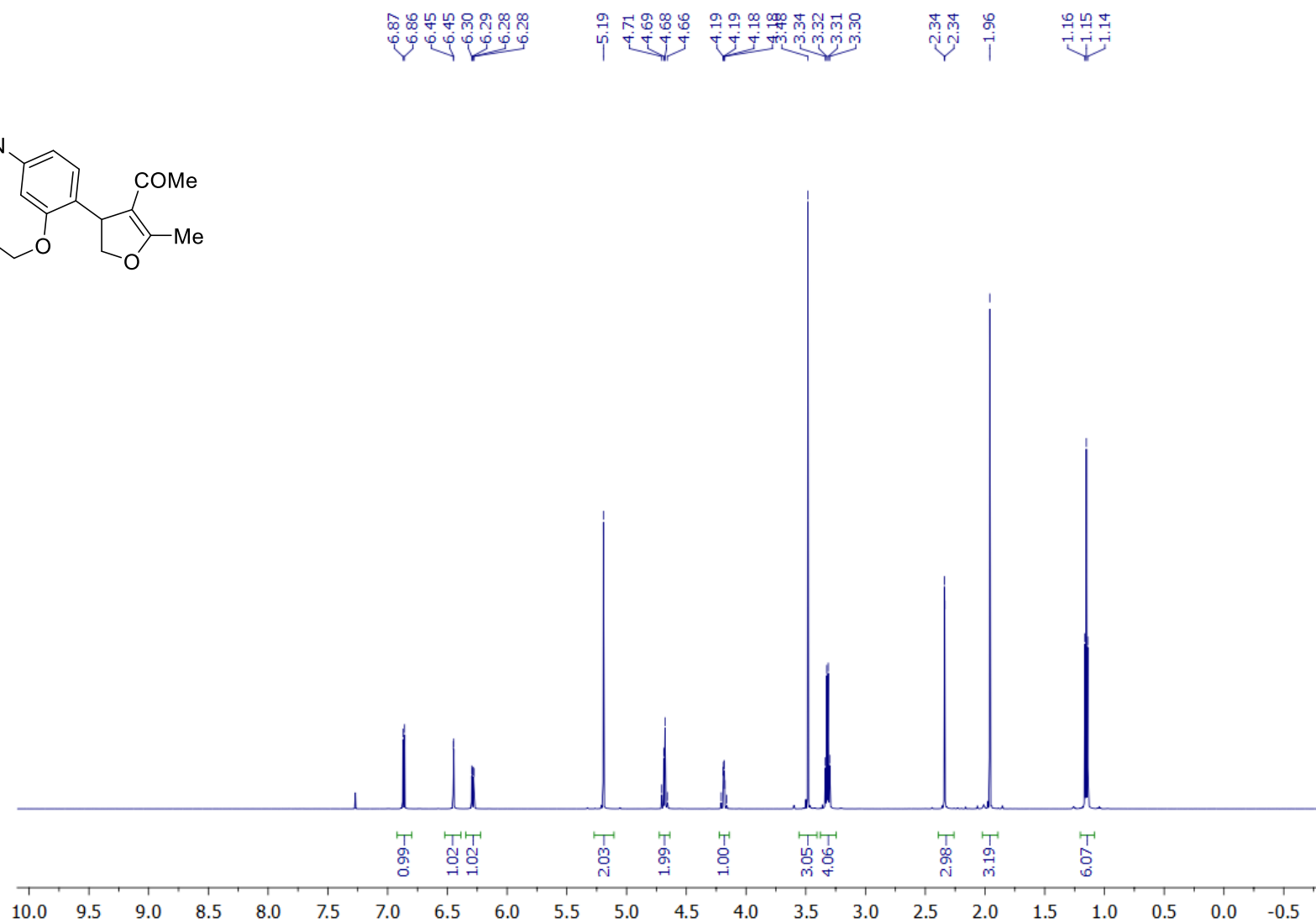
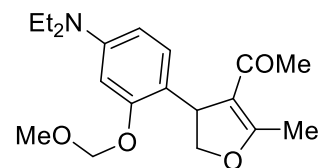
1-{4-[5-Amino-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1d')

^1H - ^{13}C HMBC (CDCl_3)



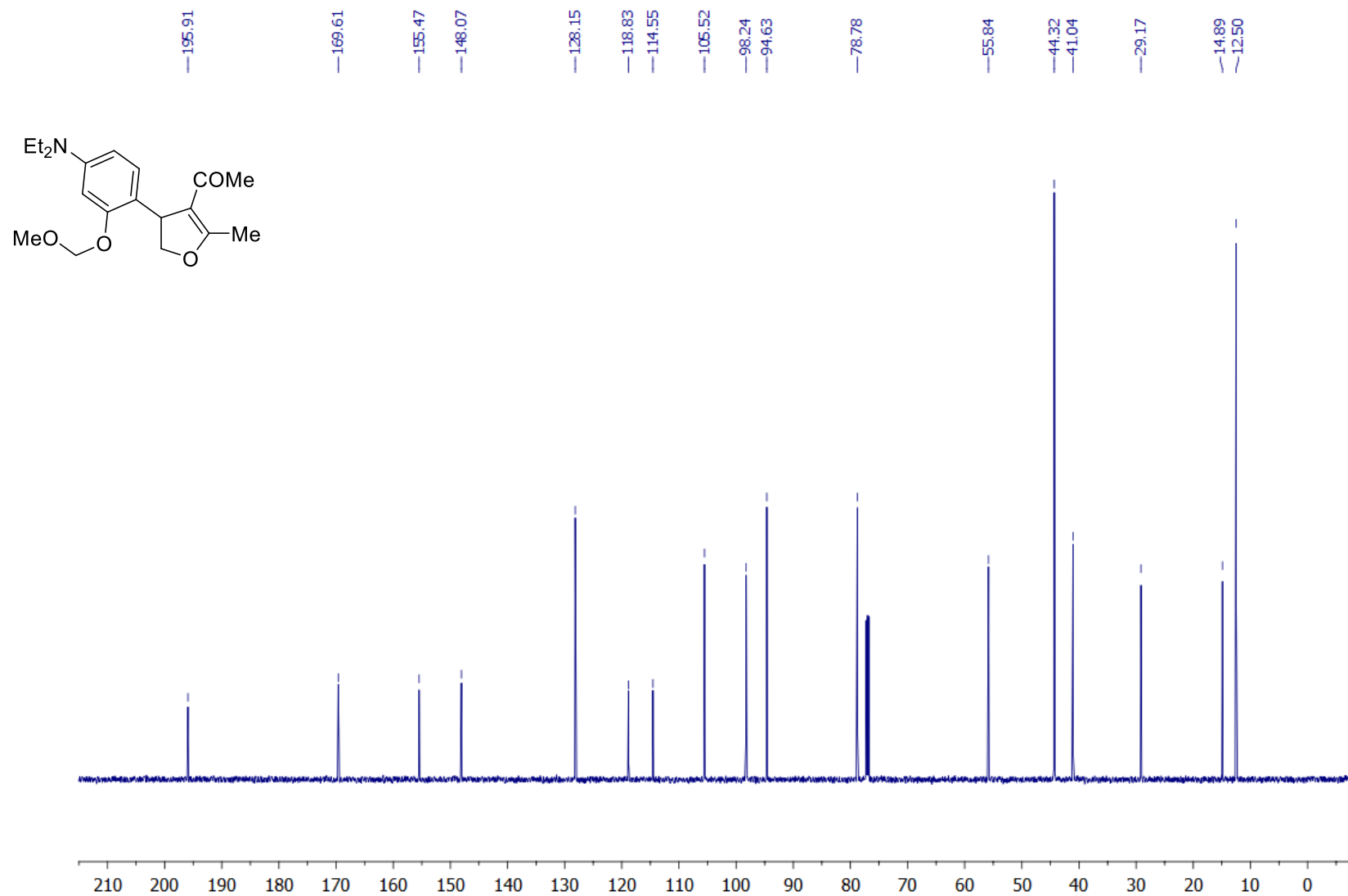
1-{4-[4-Diethylamino-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1e)

^1H NMR (CDCl_3 , 600 MHz)



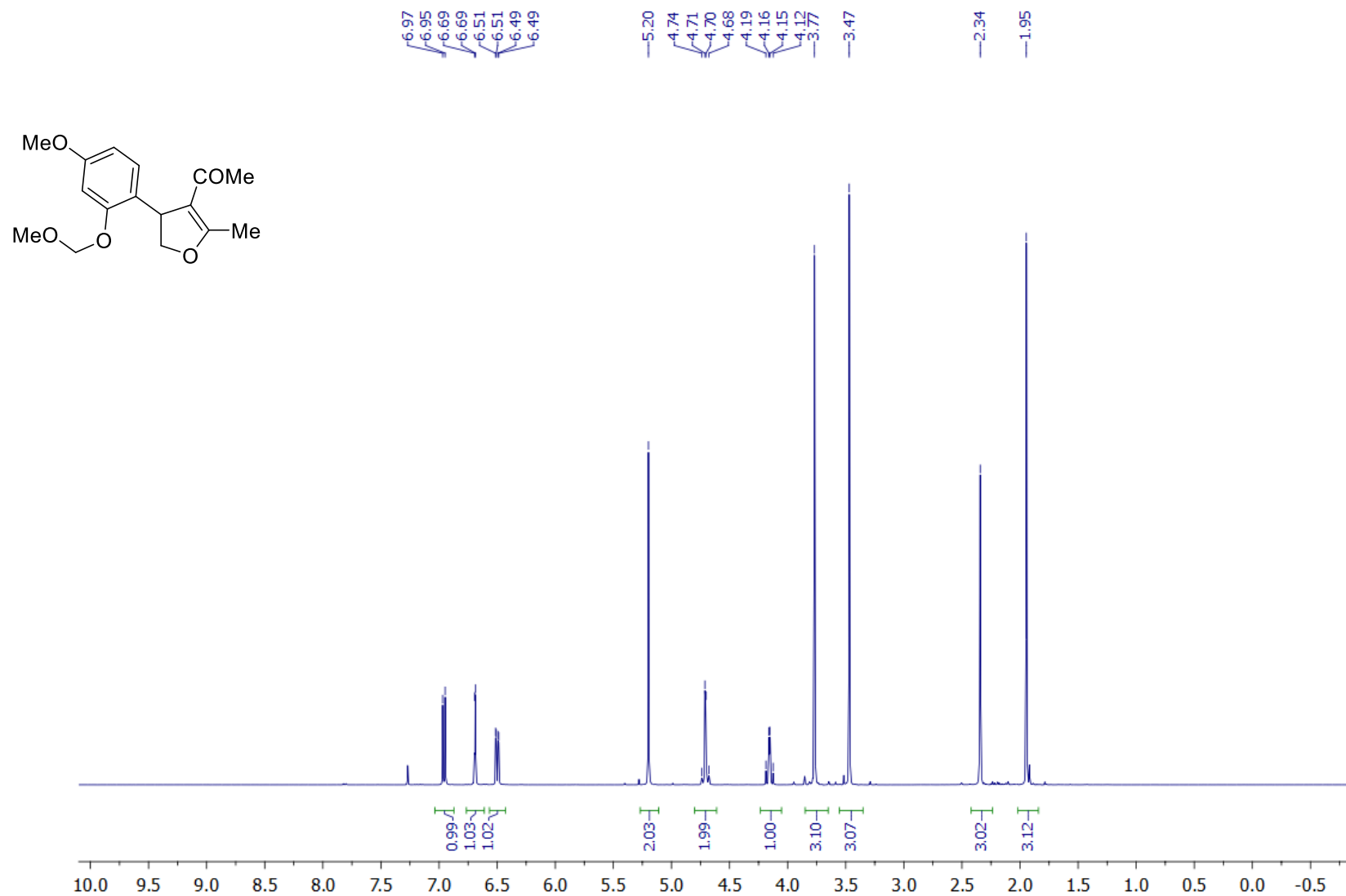
1-{4-[4-Diethylamino-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1e)

^{13}C NMR (CDCl_3 , 150 MHz)



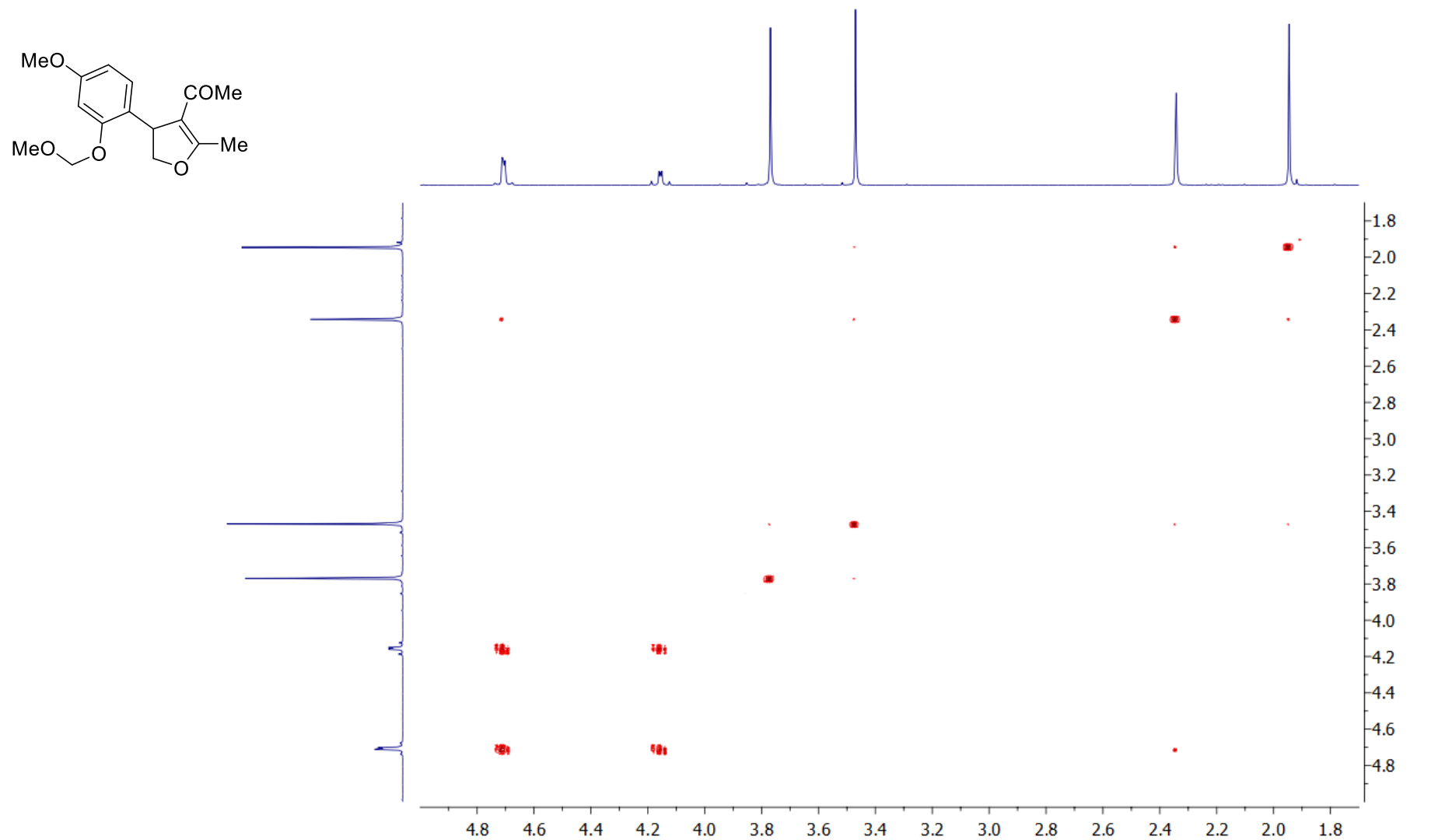
1-{4-[4-Methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1f)

^1H NMR (CDCl_3 , 400 MHz)



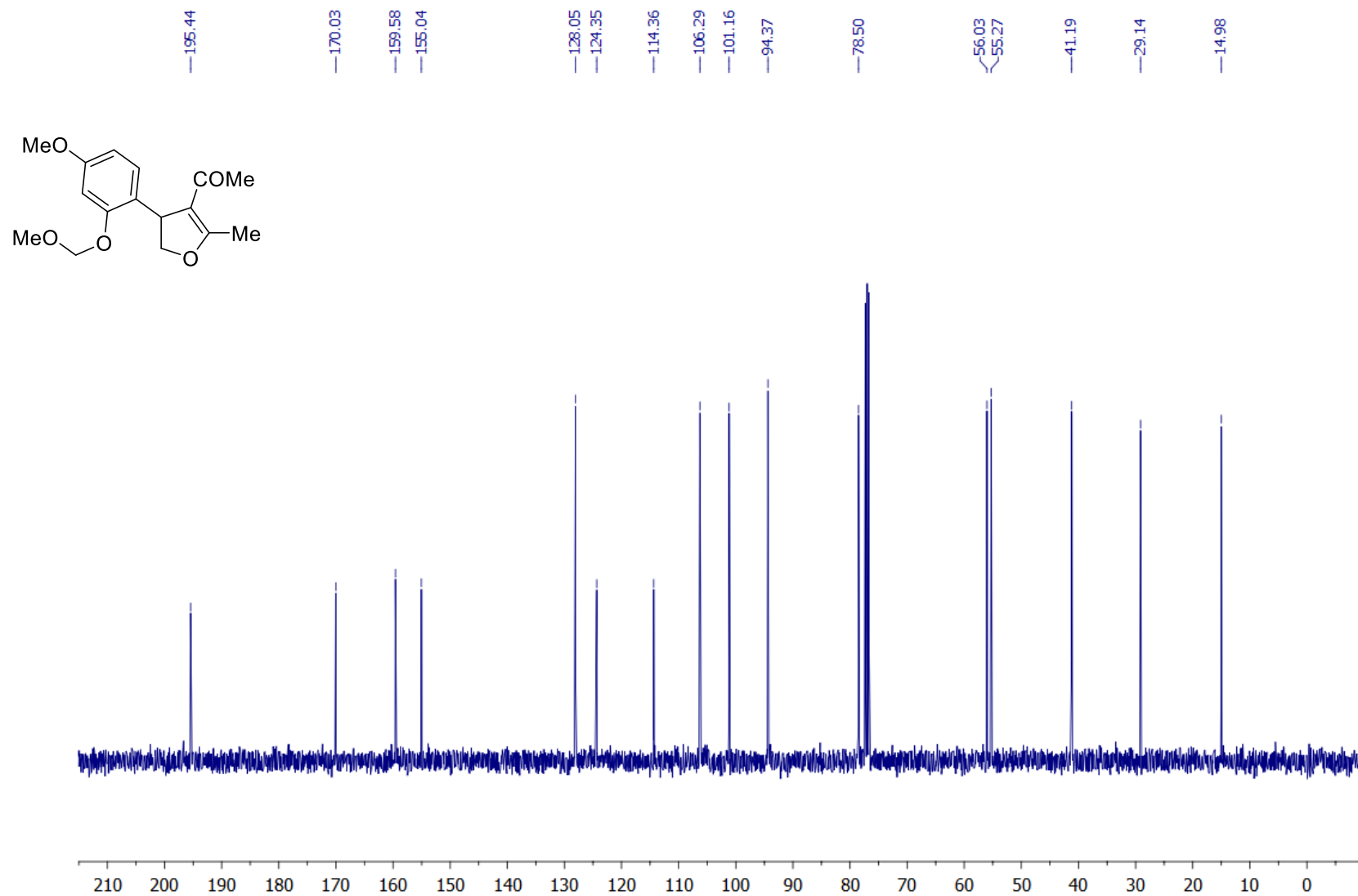
1-{4-[4-Methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1f)

^1H - ^1H COSY (CDCl_3)



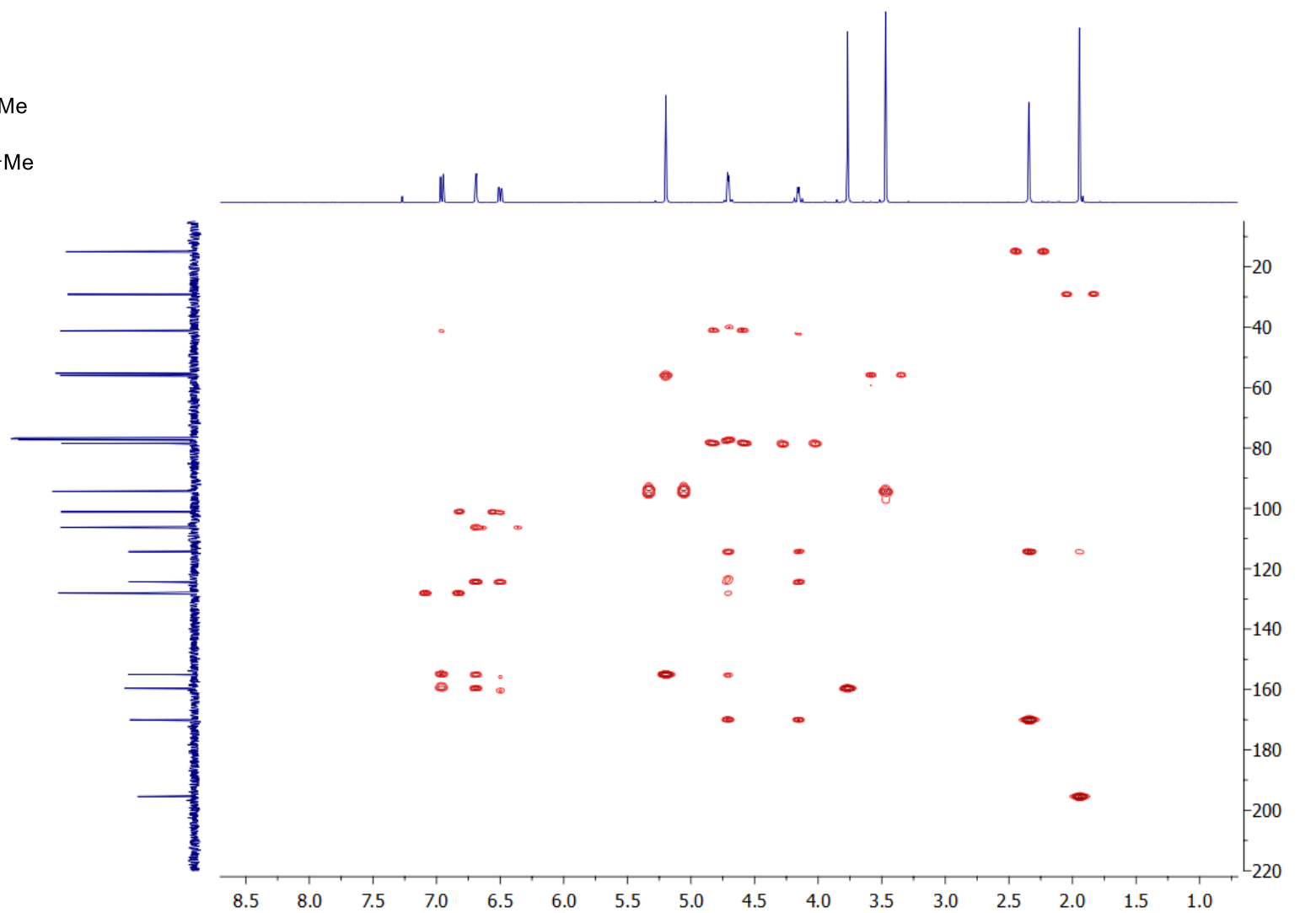
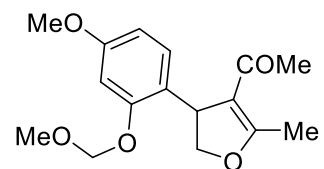
1-{4-[4-Methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1f)

^{13}C NMR (CDCl_3 , 100 MHz)



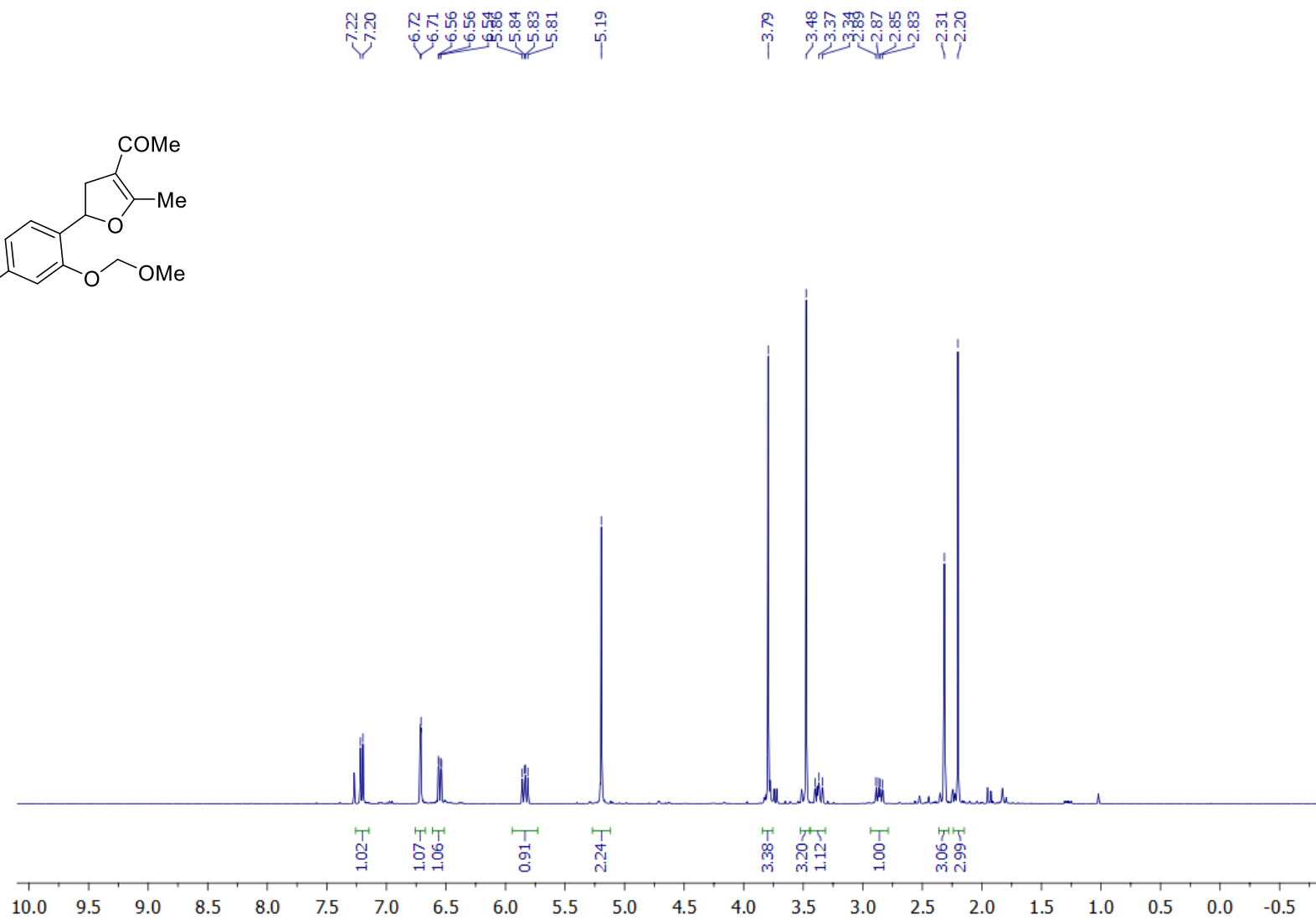
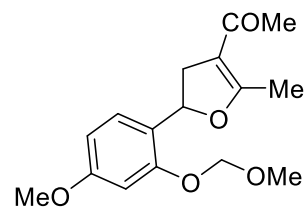
1-{4-[4-Methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1f)

^1H - ^{13}C HMBC (CDCl_3)



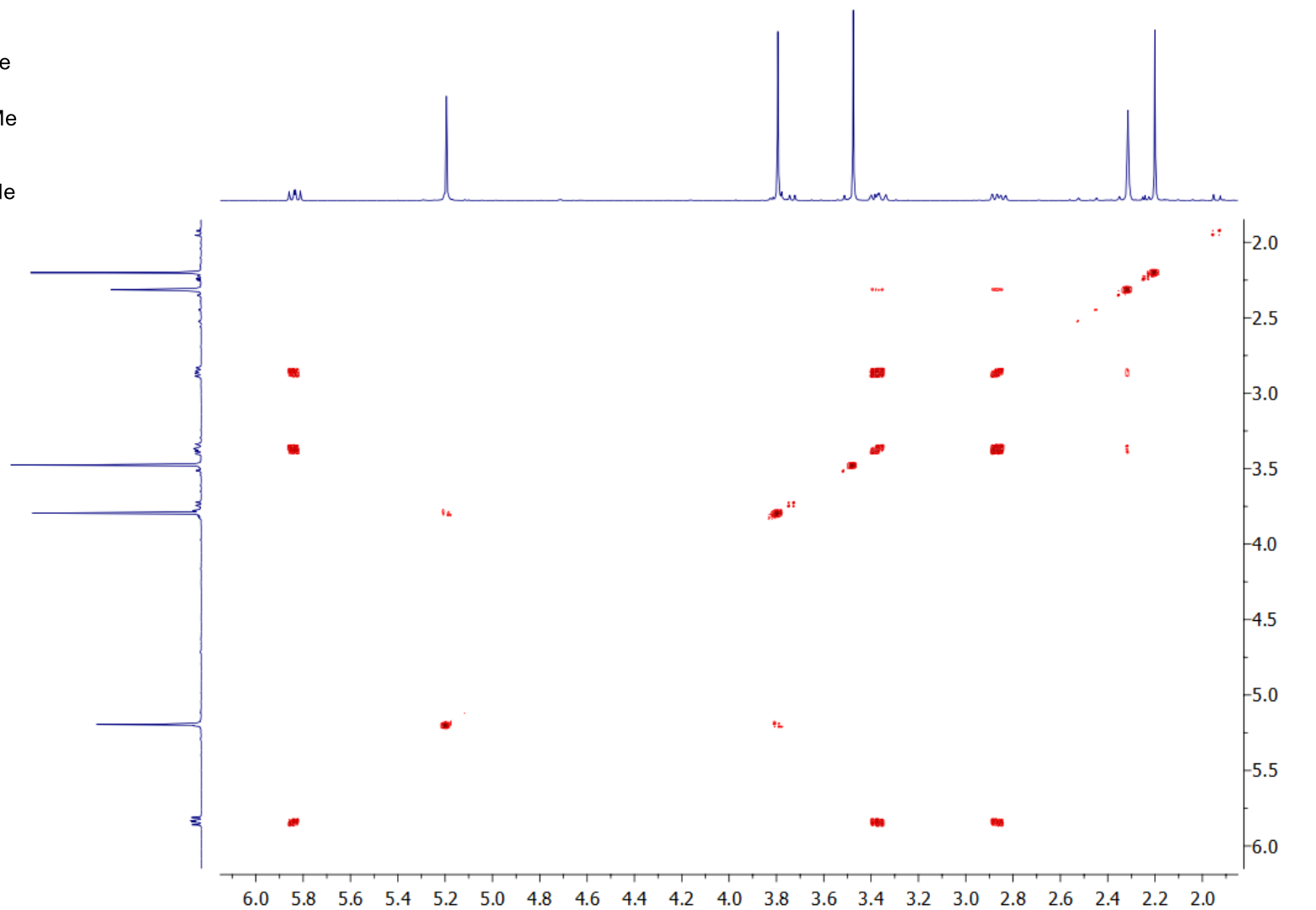
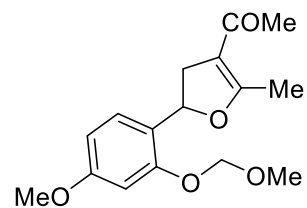
1-{5-[4-Methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (S4f)

^1H NMR (CDCl_3 , 400 MHz)



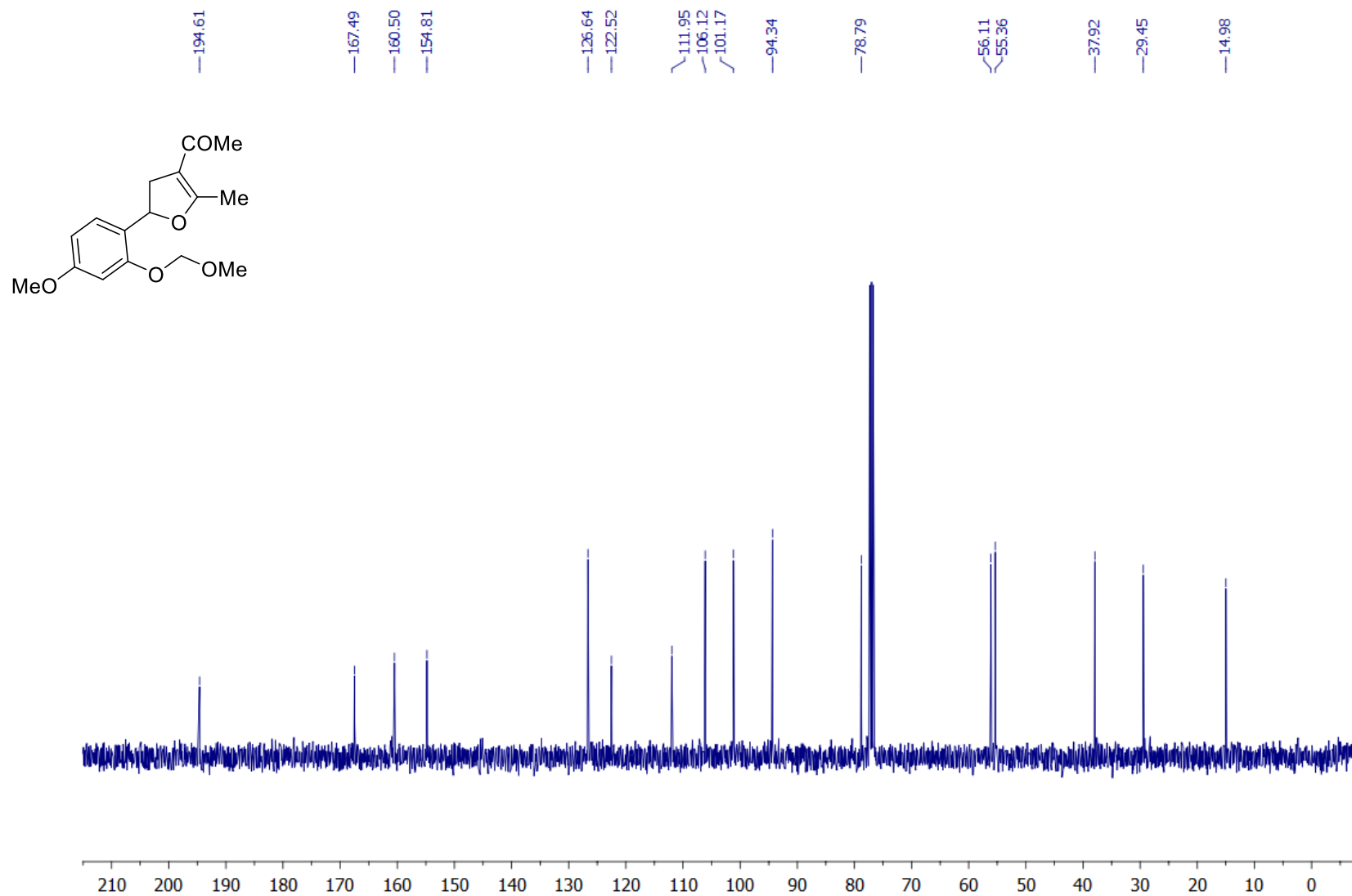
1-{5-[4-Methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (S4f)

^1H - ^1H COSY (CDCl_3)



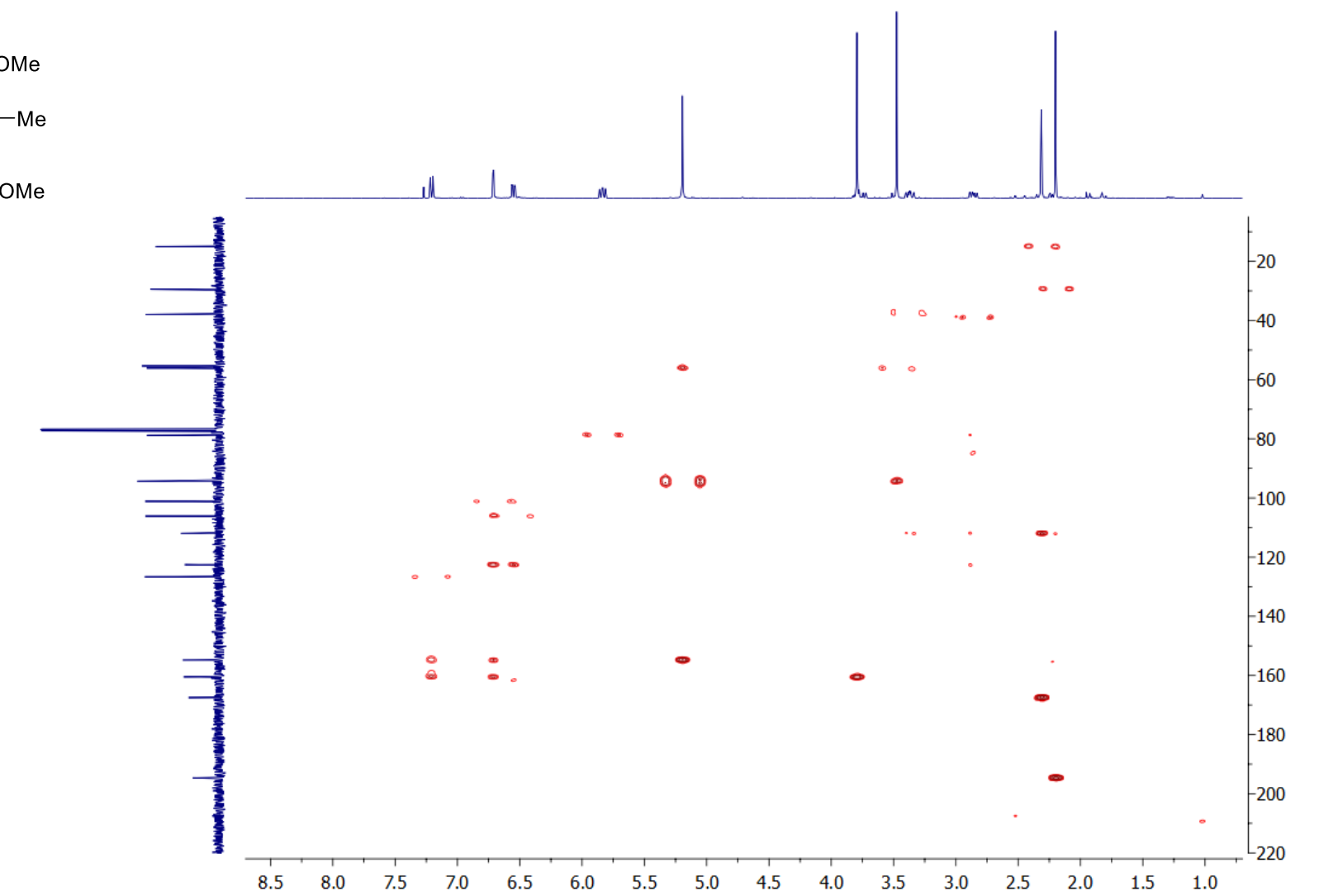
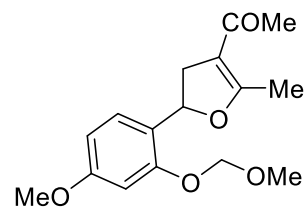
1-{5-[4-Methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (S4f)

^{13}C NMR (CDCl_3 , 100 MHz)



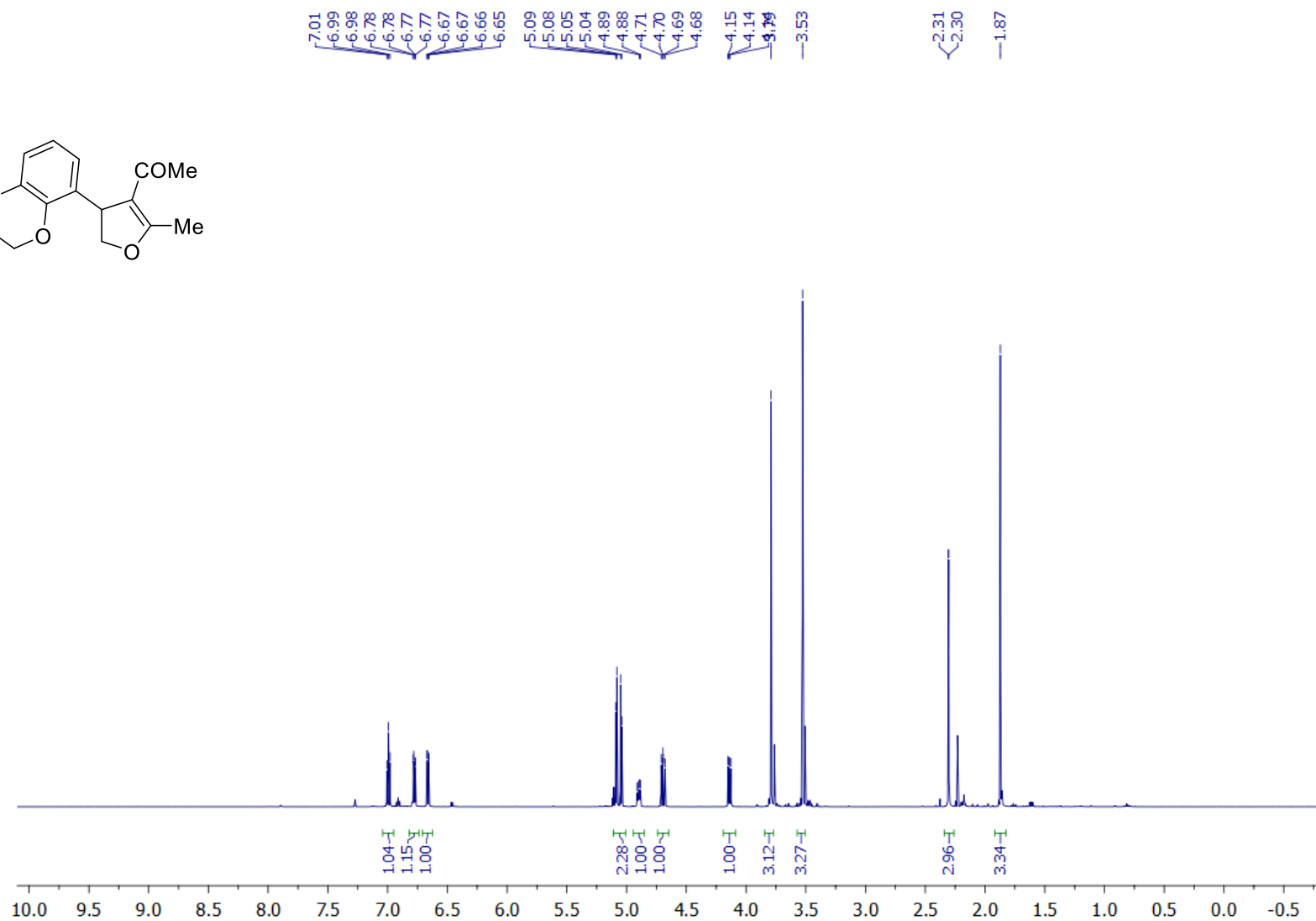
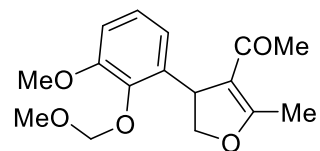
1-{5-[4-Methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (S4f)

^1H - ^{13}C HMBC (CDCl_3)



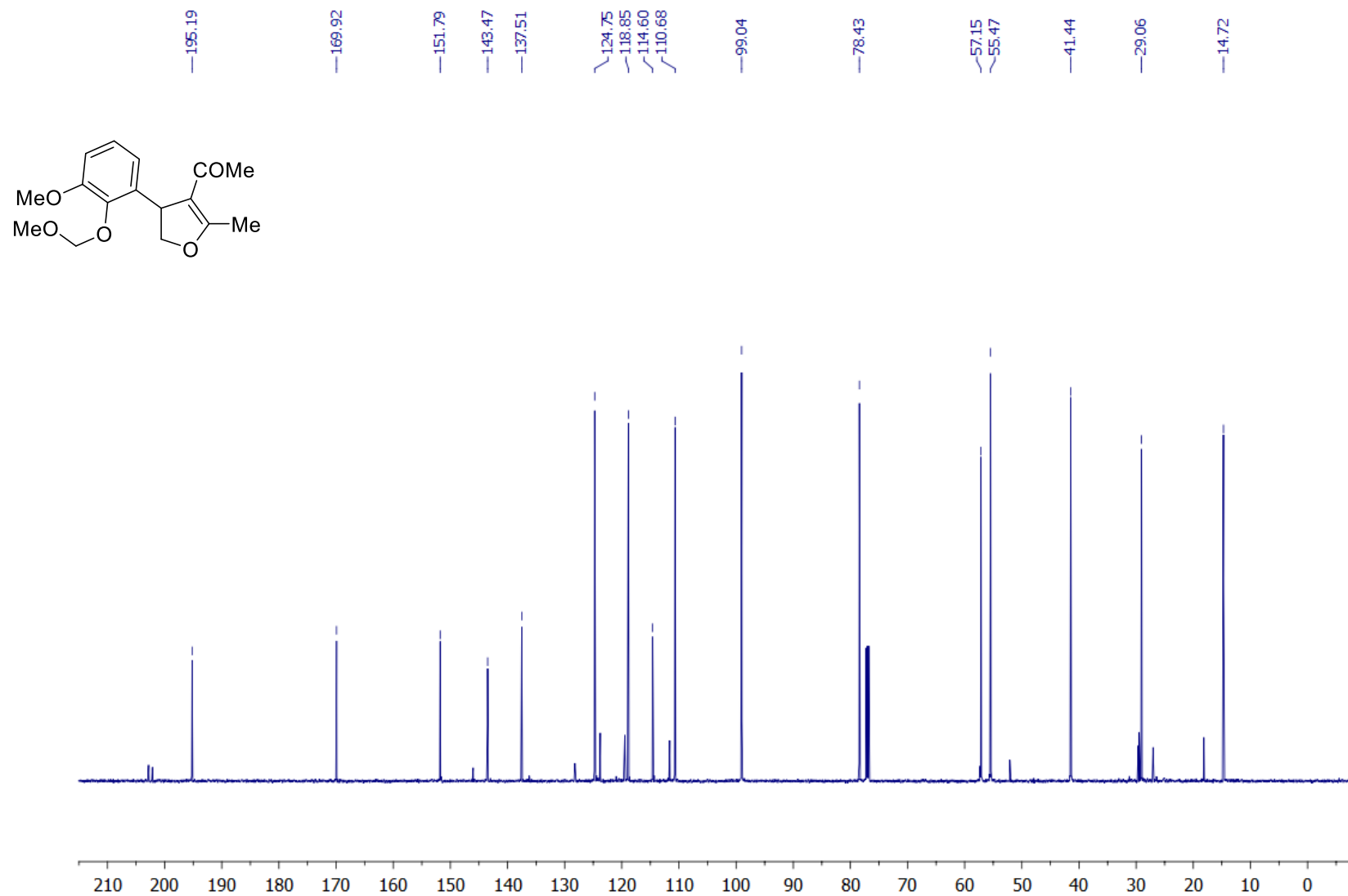
1-{4-[3-Methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1g)

^1H NMR (CDCl_3 , 600 MHz)



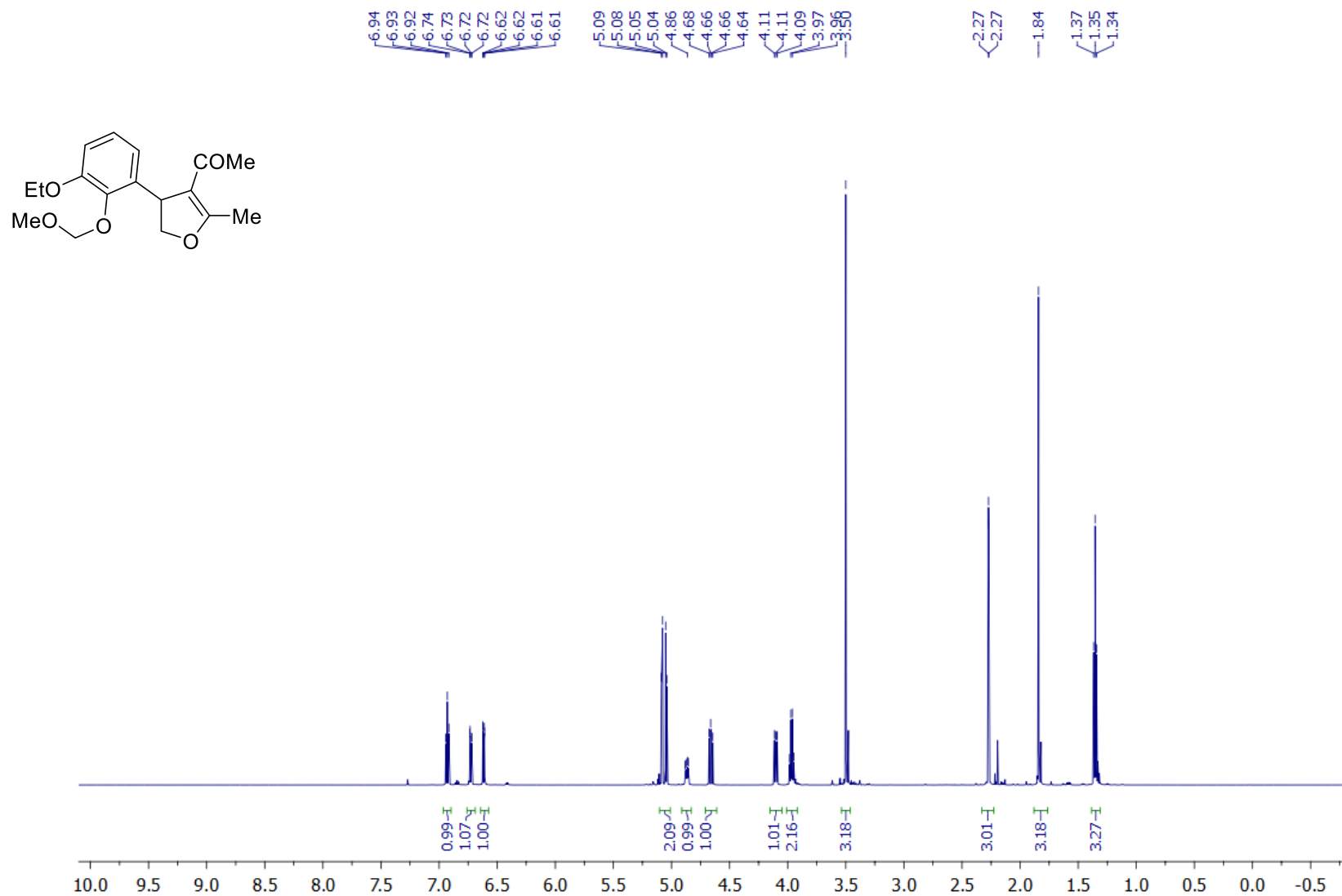
1-{4-[3-Methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1g)

^{13}C NMR (CDCl_3 , 150 MHz)



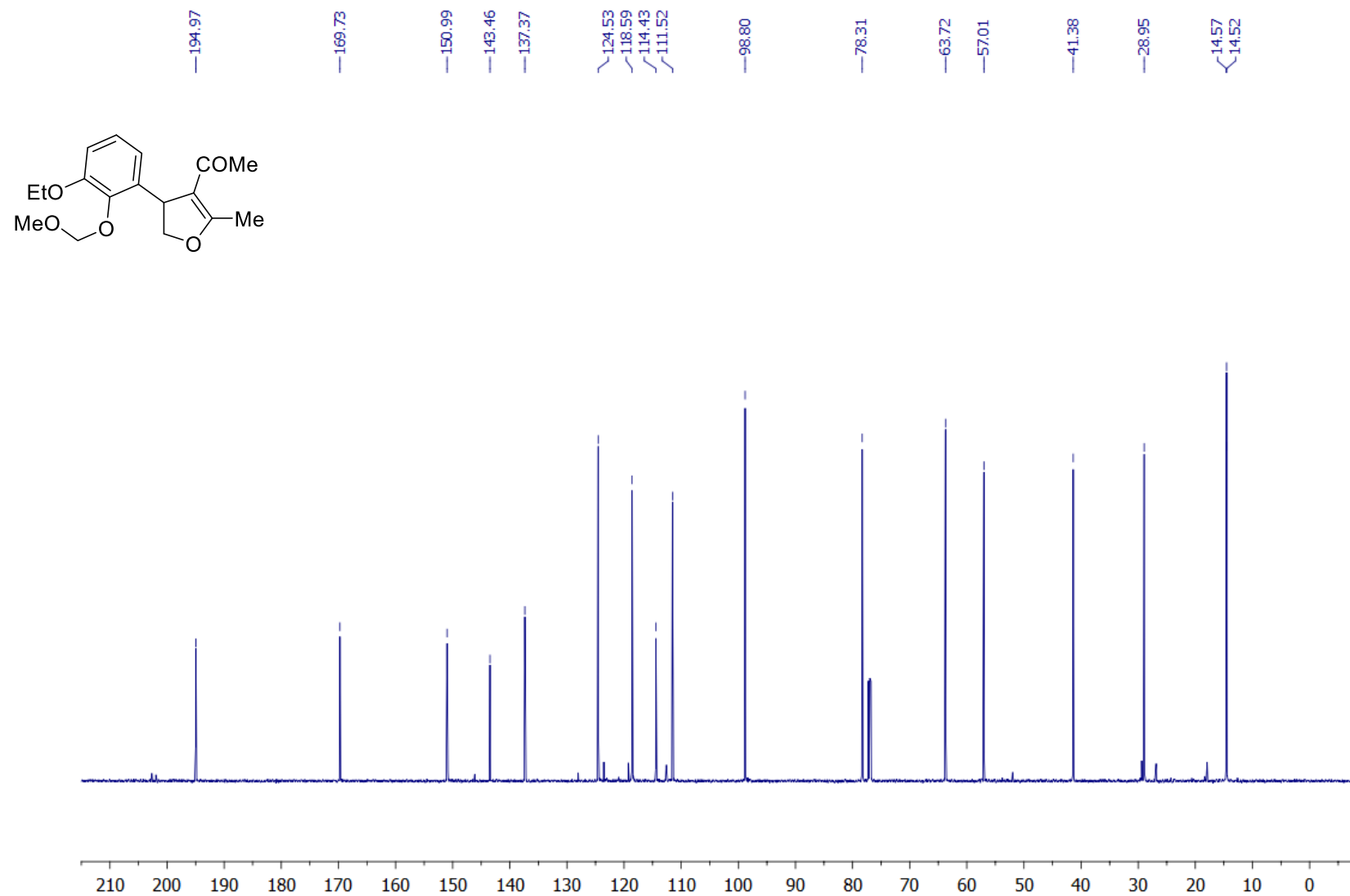
1-{4-[3-Ethoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1h)

^1H NMR (CDCl_3 , 600 MHz)



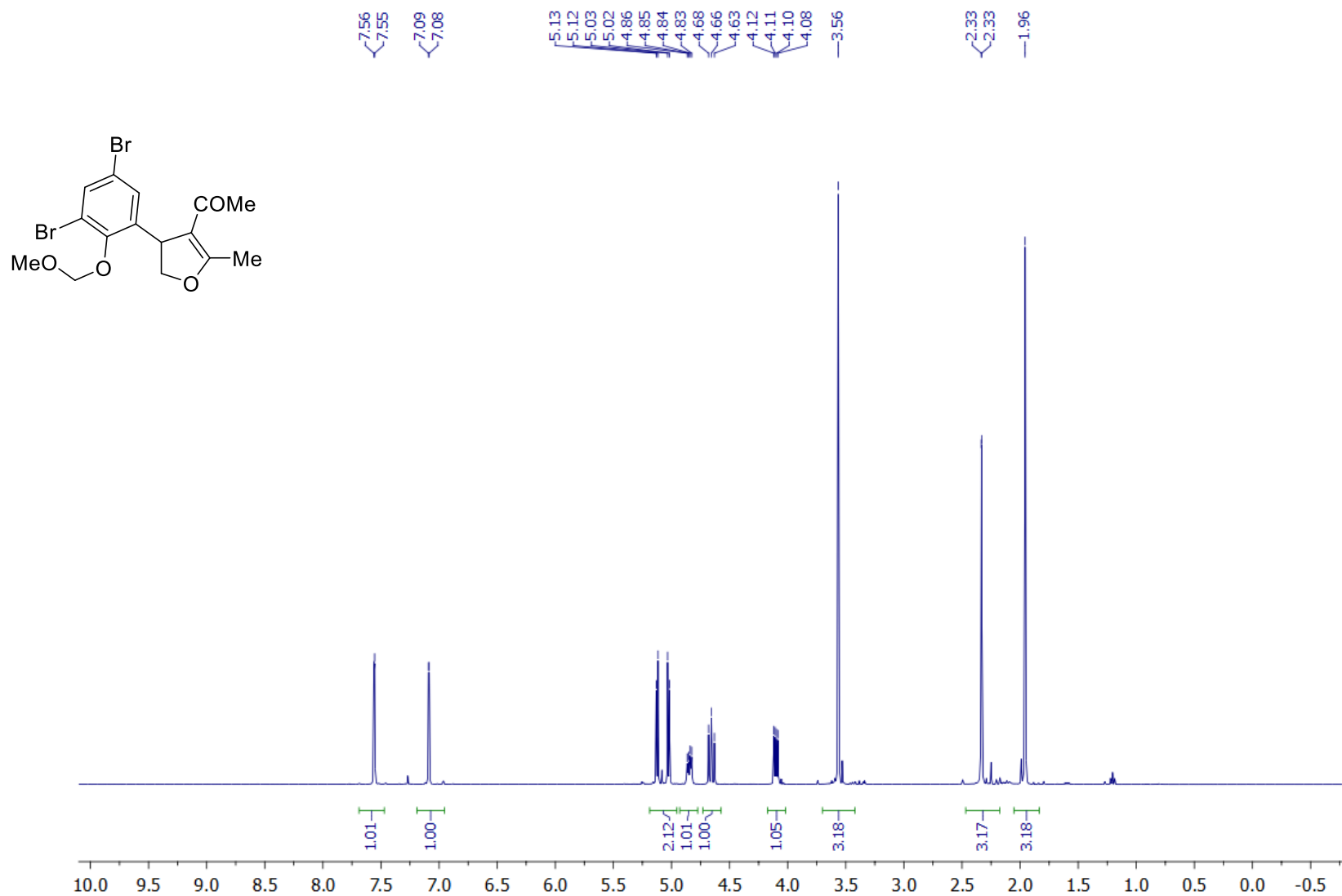
1-{4-[3-Ethoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1h)

^{13}C NMR (CDCl_3 , 150 MHz)



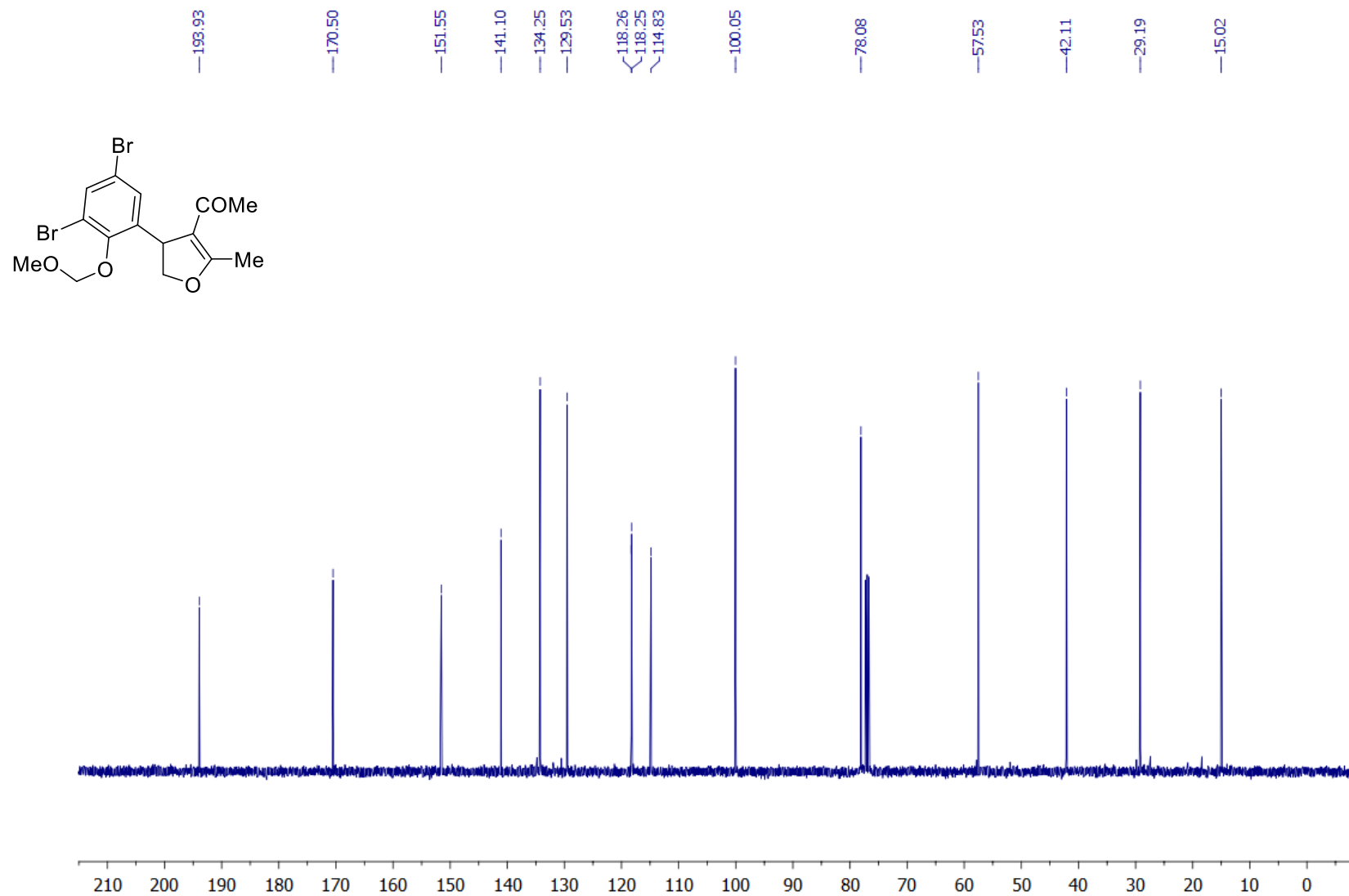
1-{4-[3,5-Dibromo-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1i)

^1H NMR (CDCl_3 , 400 MHz)



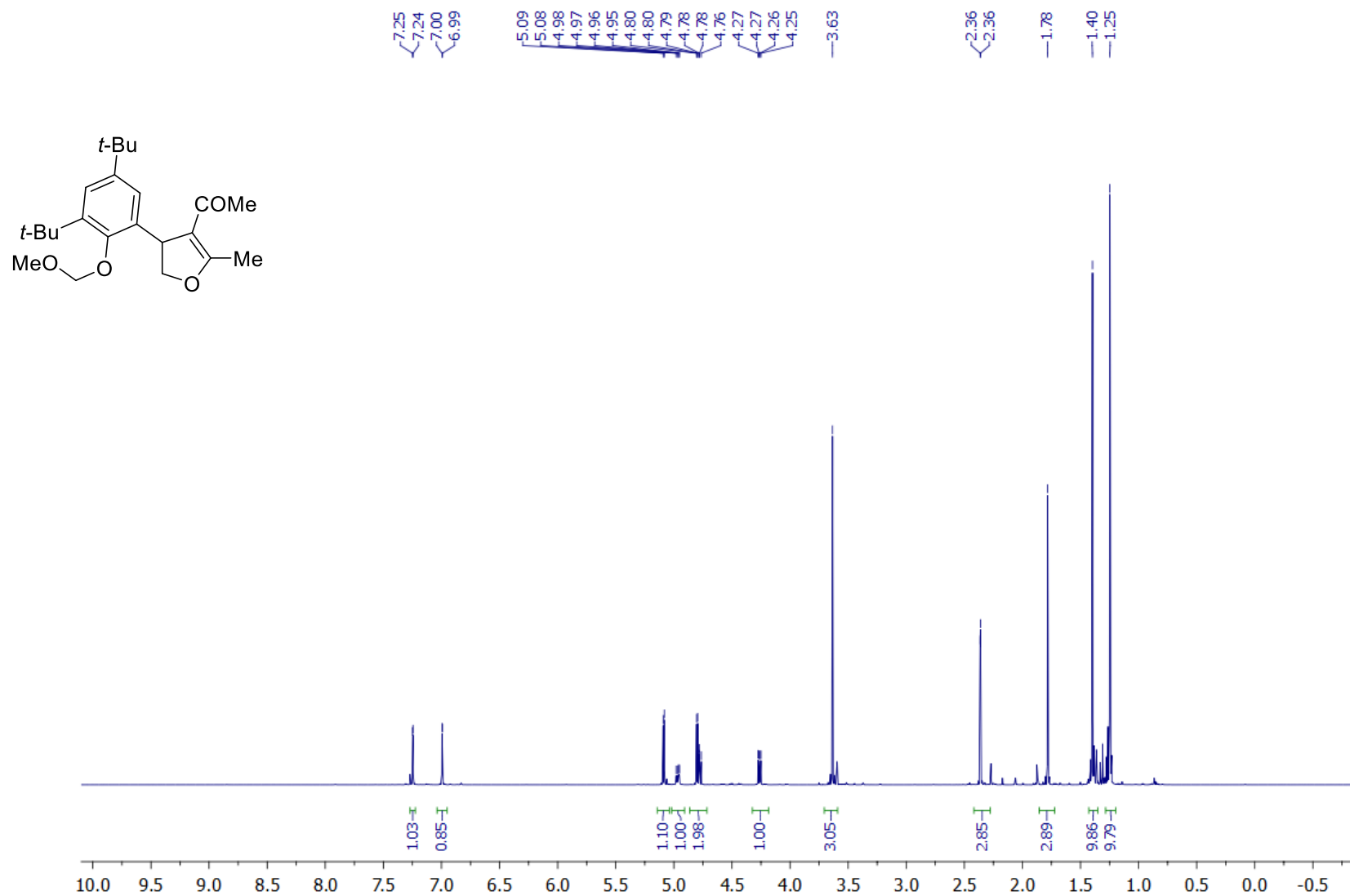
1-{4-[3,5-Dibromo-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1i)

^{13}C NMR (CDCl_3 , 100 MHz)



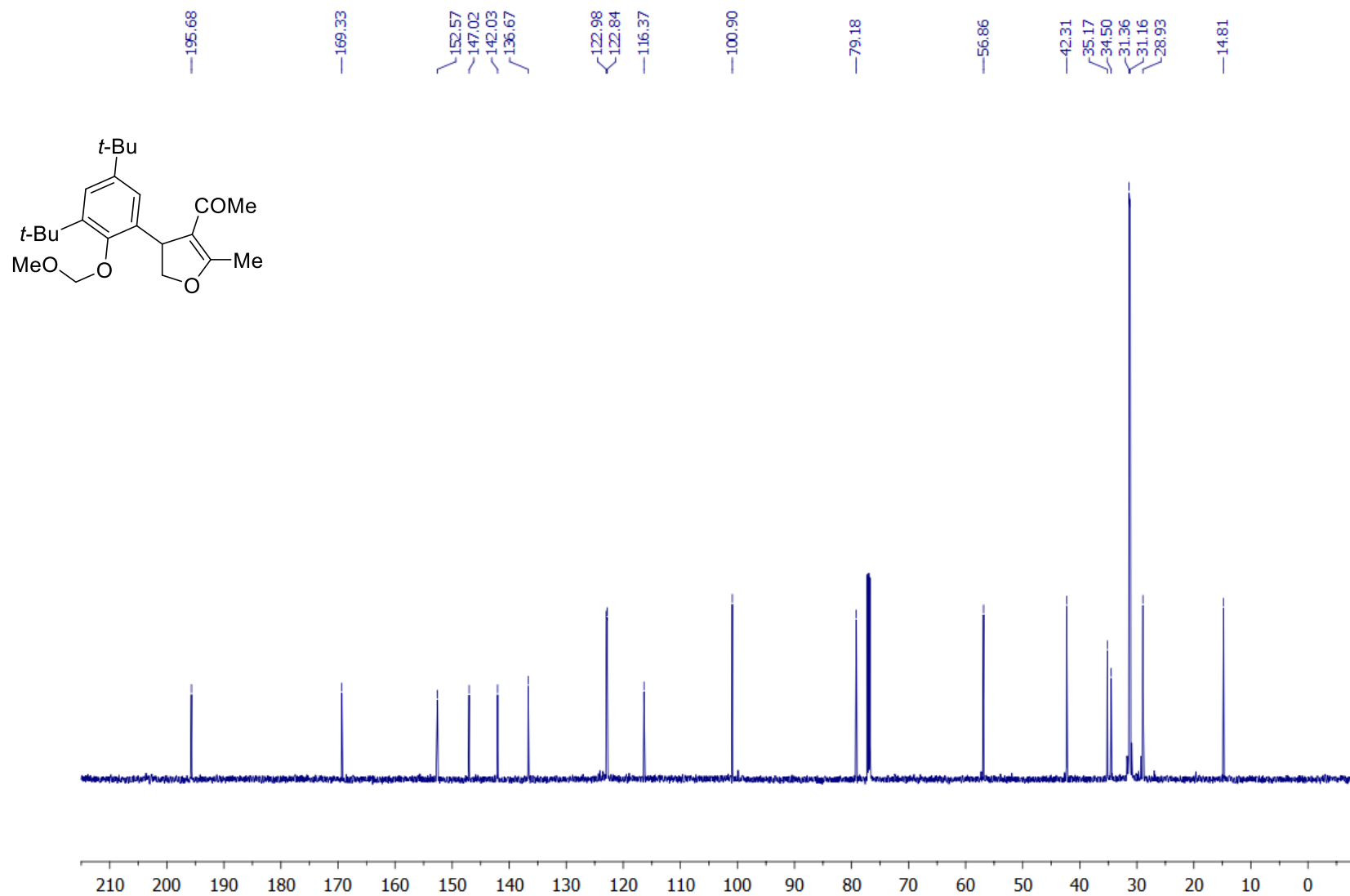
1-{4-[3,5-Di-*tert*-butyl-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1j)

¹H NMR (CDCl₃, 600 MHz)



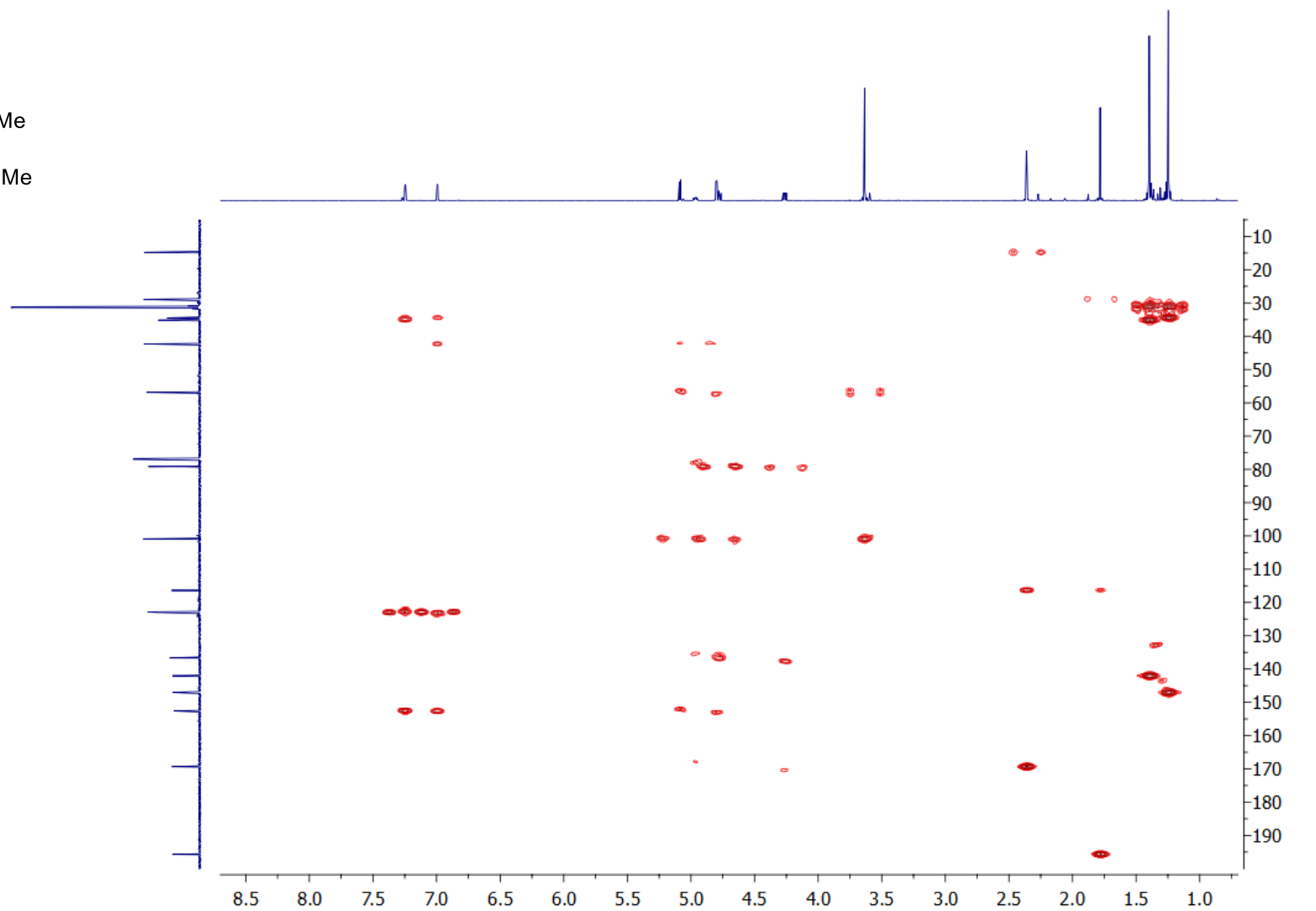
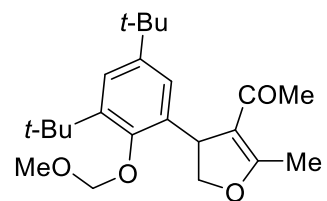
1-{4-[3,5-Di-*tert*-butyl-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1j)

^{13}C NMR (CDCl_3 , 150 MHz)



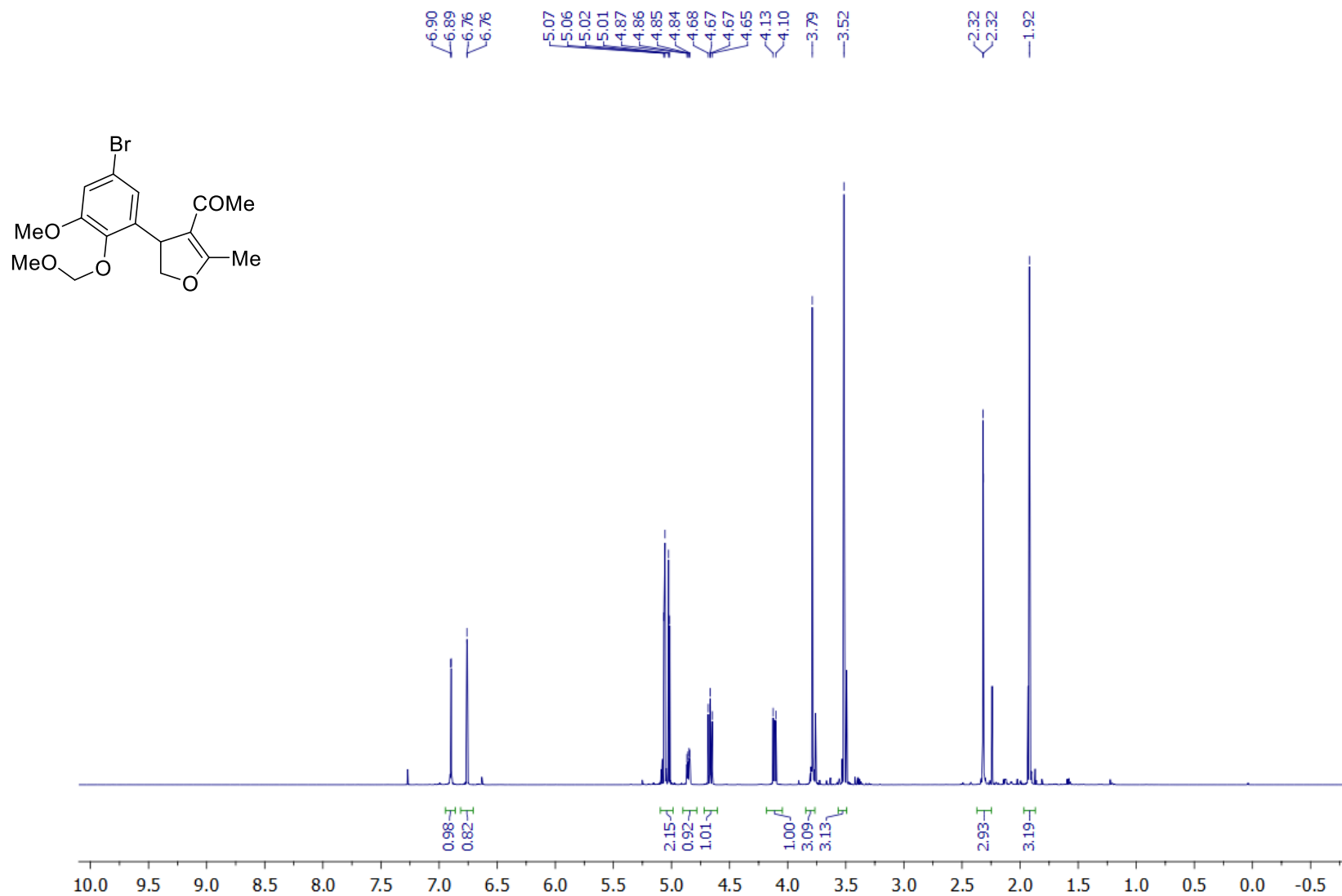
1-{4-[3,5-Di-*tert*-butyl-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1j)

^1H - ^{13}C HMBC (CDCl_3)



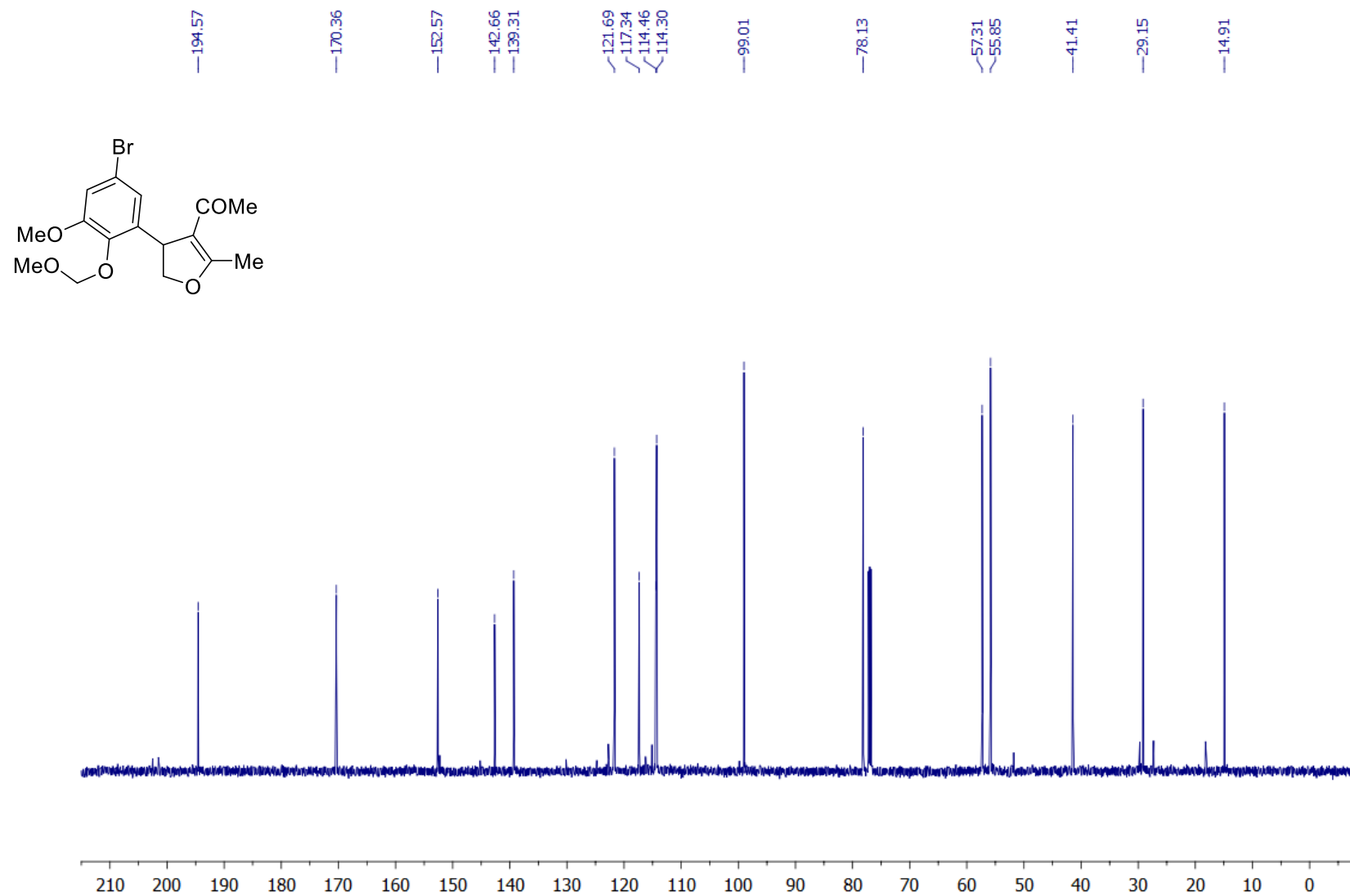
1-{4-[5-Bromo-3-methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1k)

^1H NMR (CDCl_3 , 600 MHz)



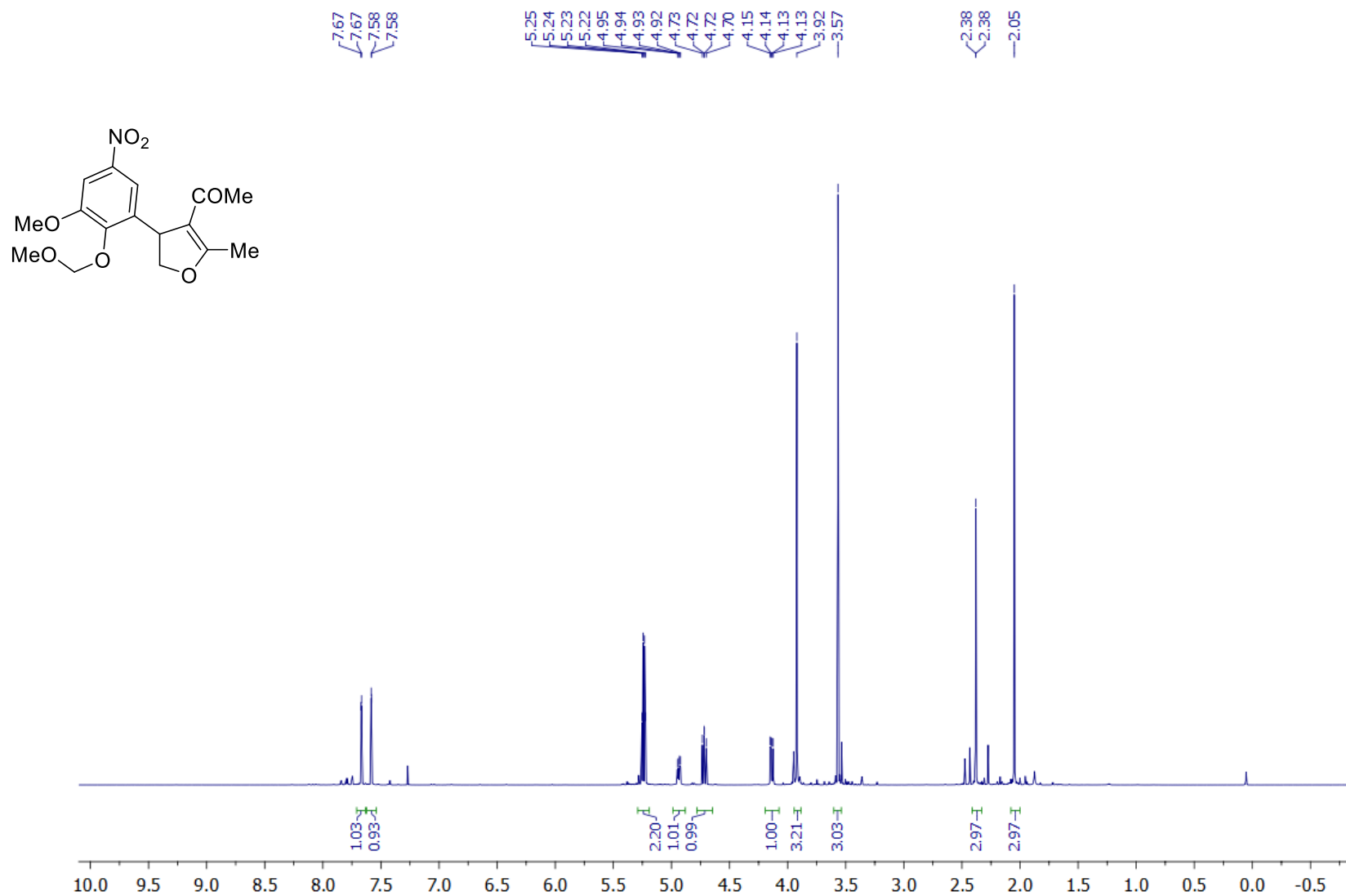
1-{4-[5-Bromo-3-methoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1k)

^{13}C NMR (CDCl_3 , 150 MHz)



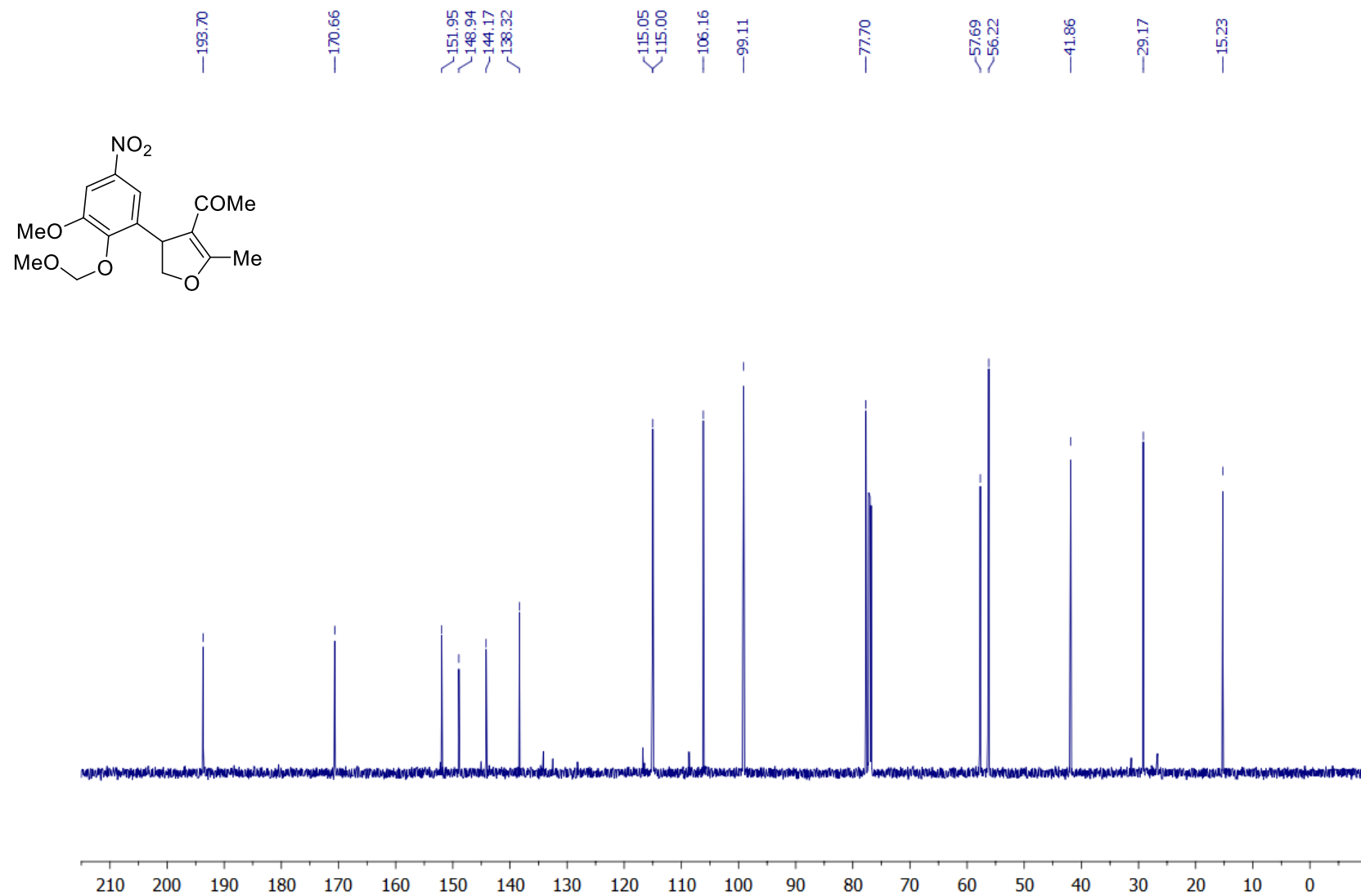
1-{4-[3-Methoxy-2-(methoxymethoxy)-5-nitrophenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1l)

^1H NMR (CDCl_3 , 600 MHz)



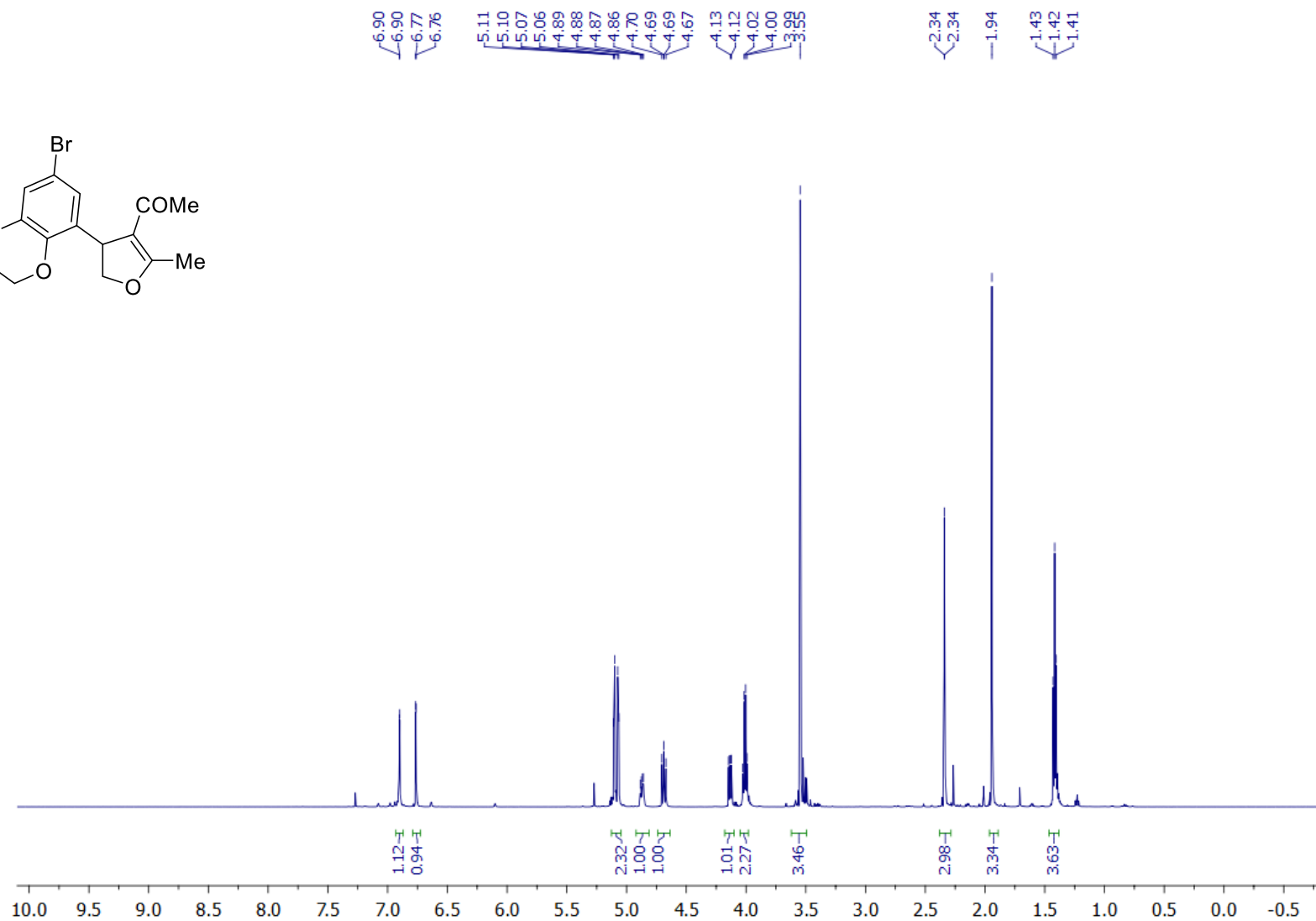
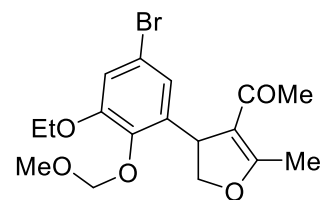
1-{4-[3-Methoxy-2-(methoxymethoxy)-5-nitrophenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1l)

^{13}C NMR (CDCl_3 , 150 MHz)



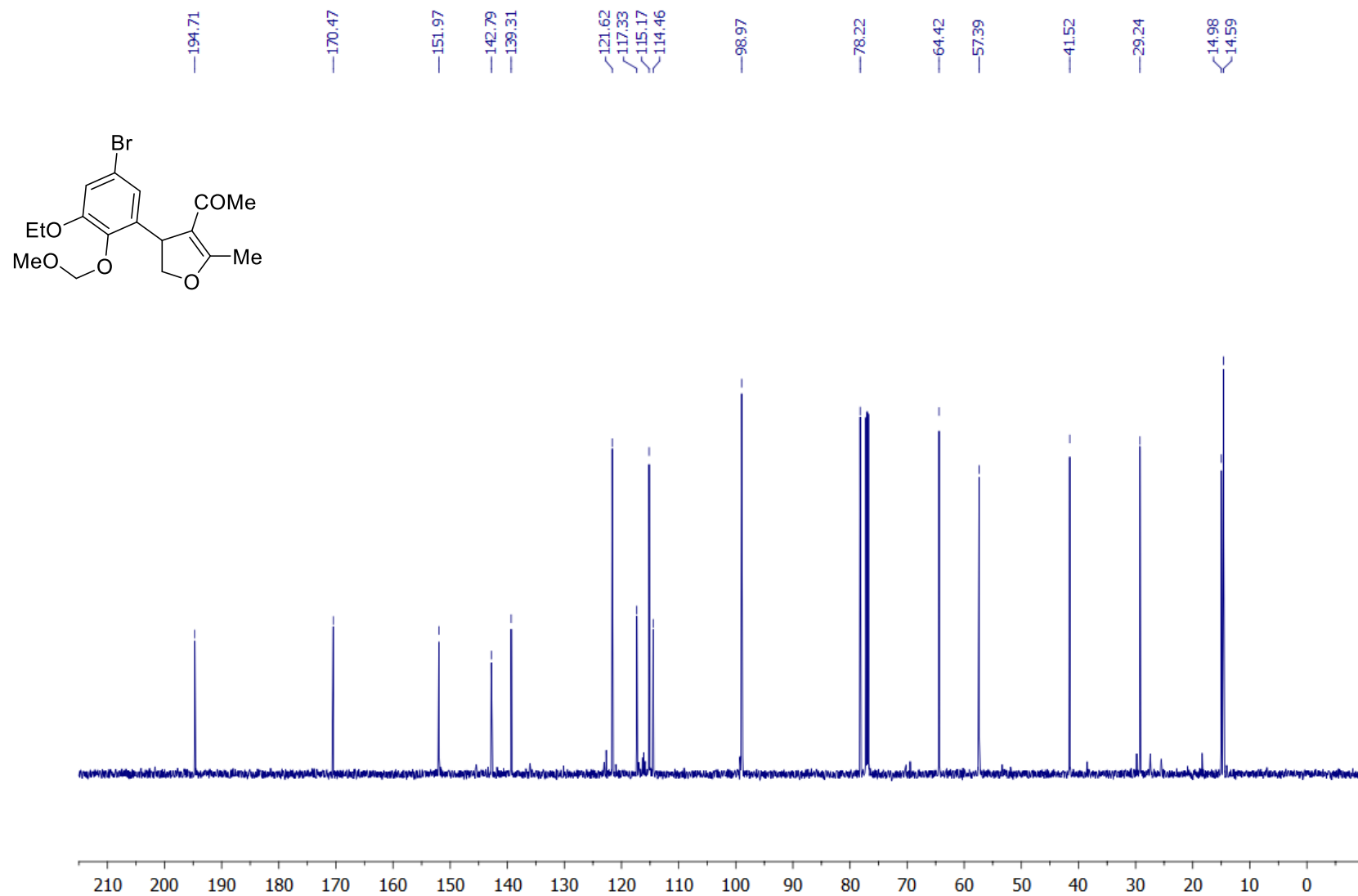
1-{4-[5-Bromo-3-ethoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1m)

^1H NMR (CDCl_3 , 600 MHz)



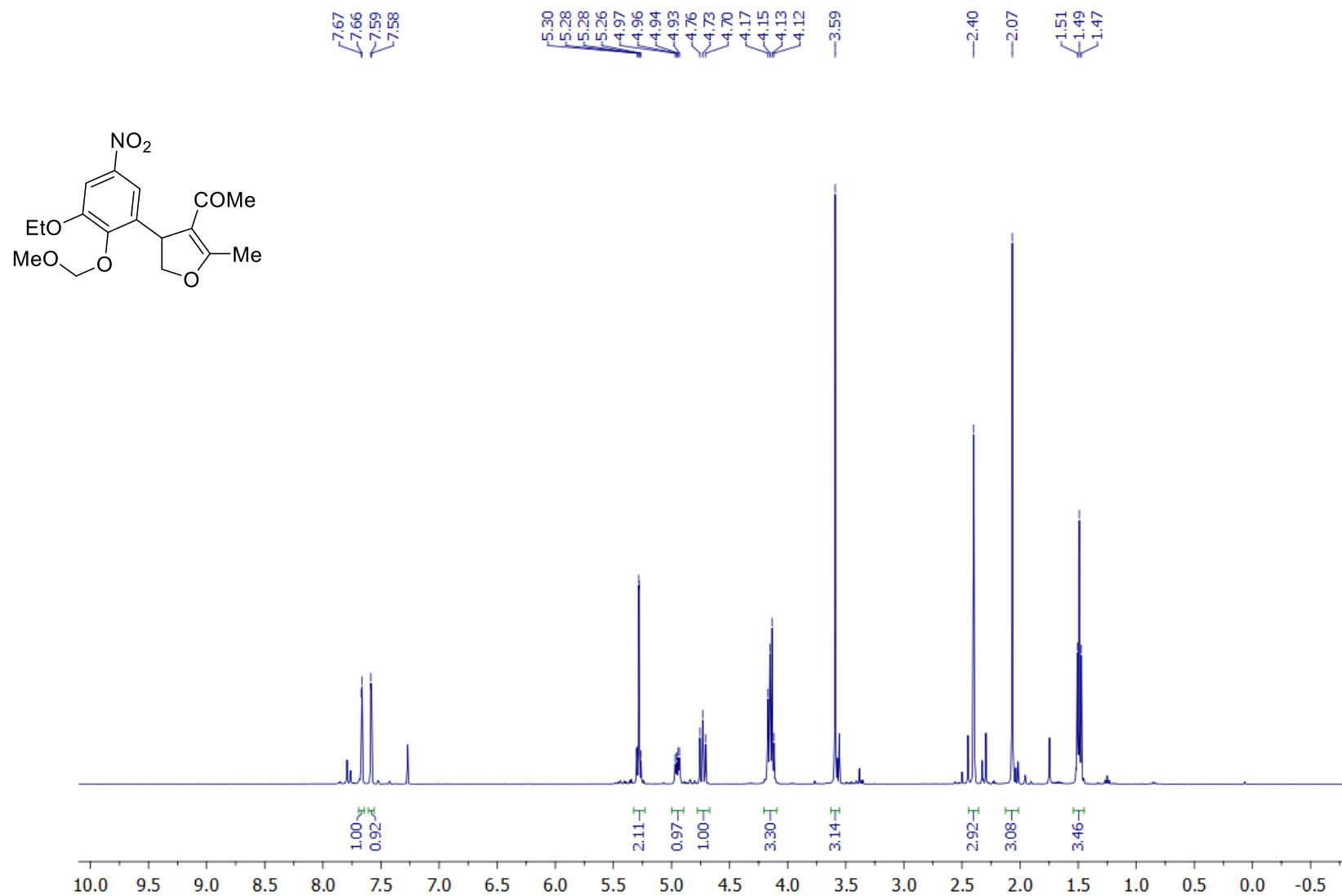
1-{4-[5-Bromo-3-ethoxy-2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1m)

^{13}C NMR (CDCl_3 , 150 MHz)



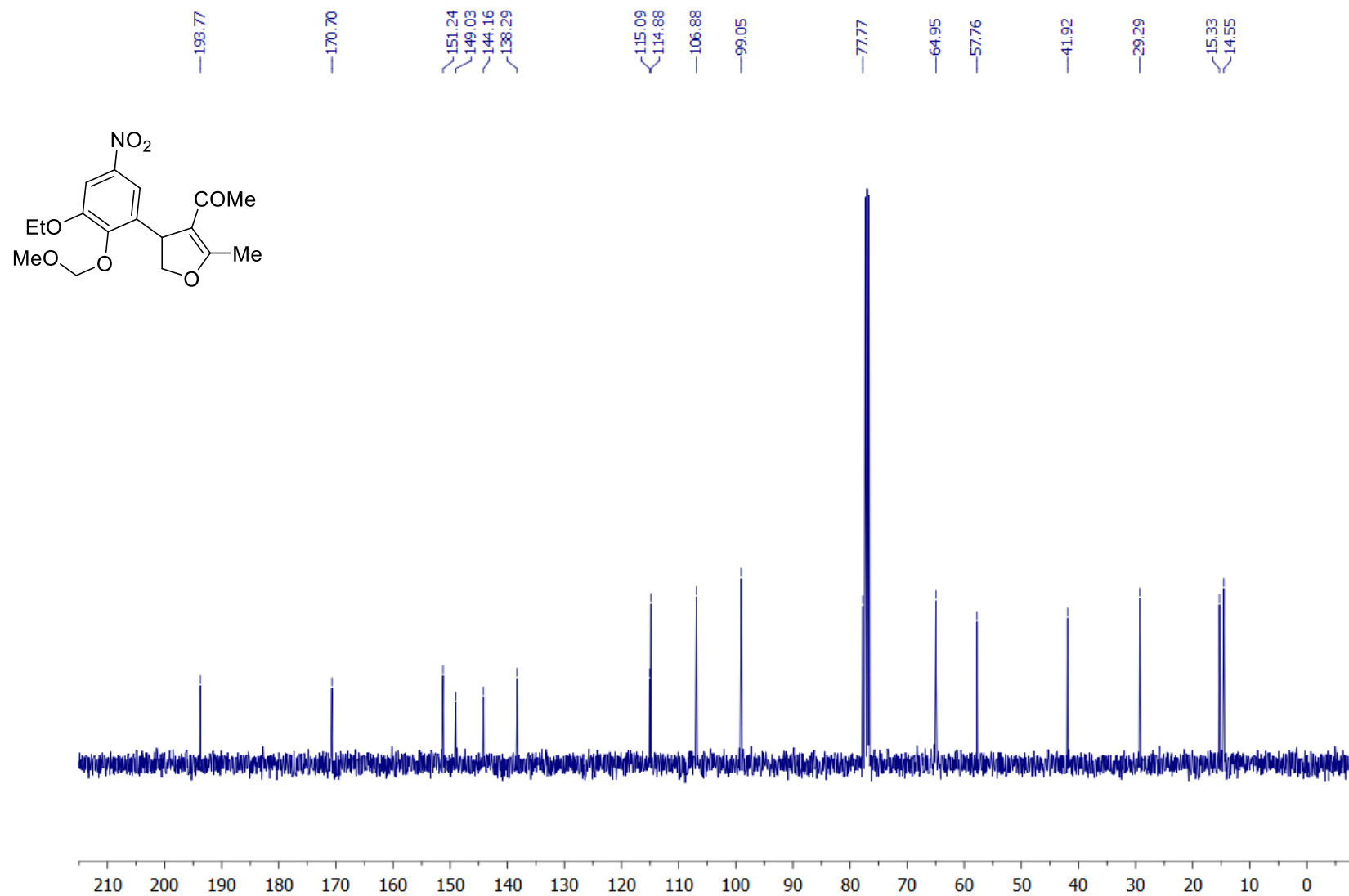
1-{4-[3-Ethoxy-2-(methoxymethoxy)-5-nitrophenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1n)

^1H NMR (CDCl_3 , 600 MHz)



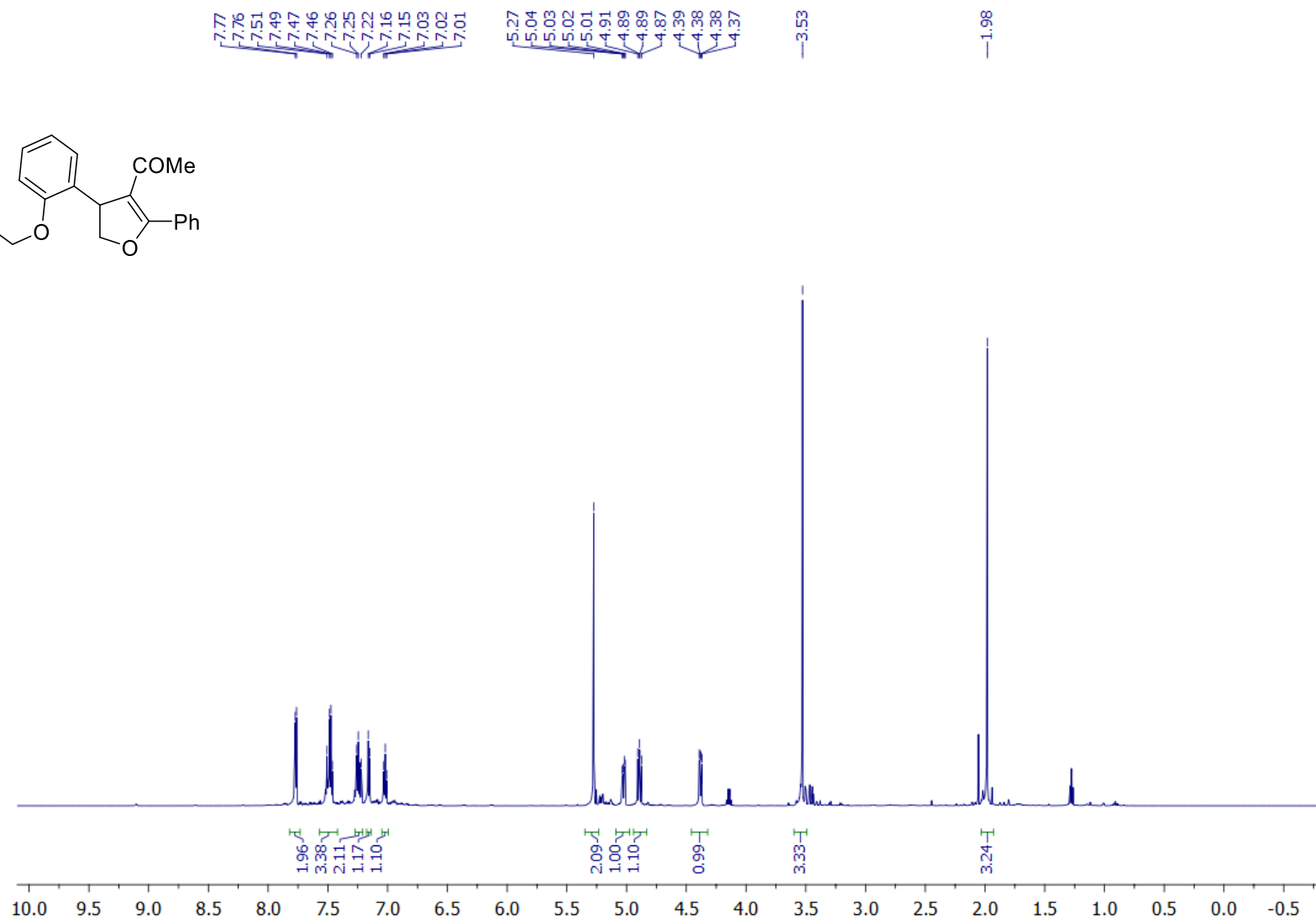
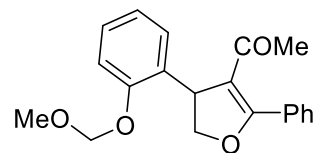
1-{4-[3-Ethoxy-2-(methoxymethoxy)-5-nitrophenyl]-2-methyl-4,5-dihydrofuran-3-yl}ethanone (1n)

¹³C NMR (CDCl₃, 150 MHz)



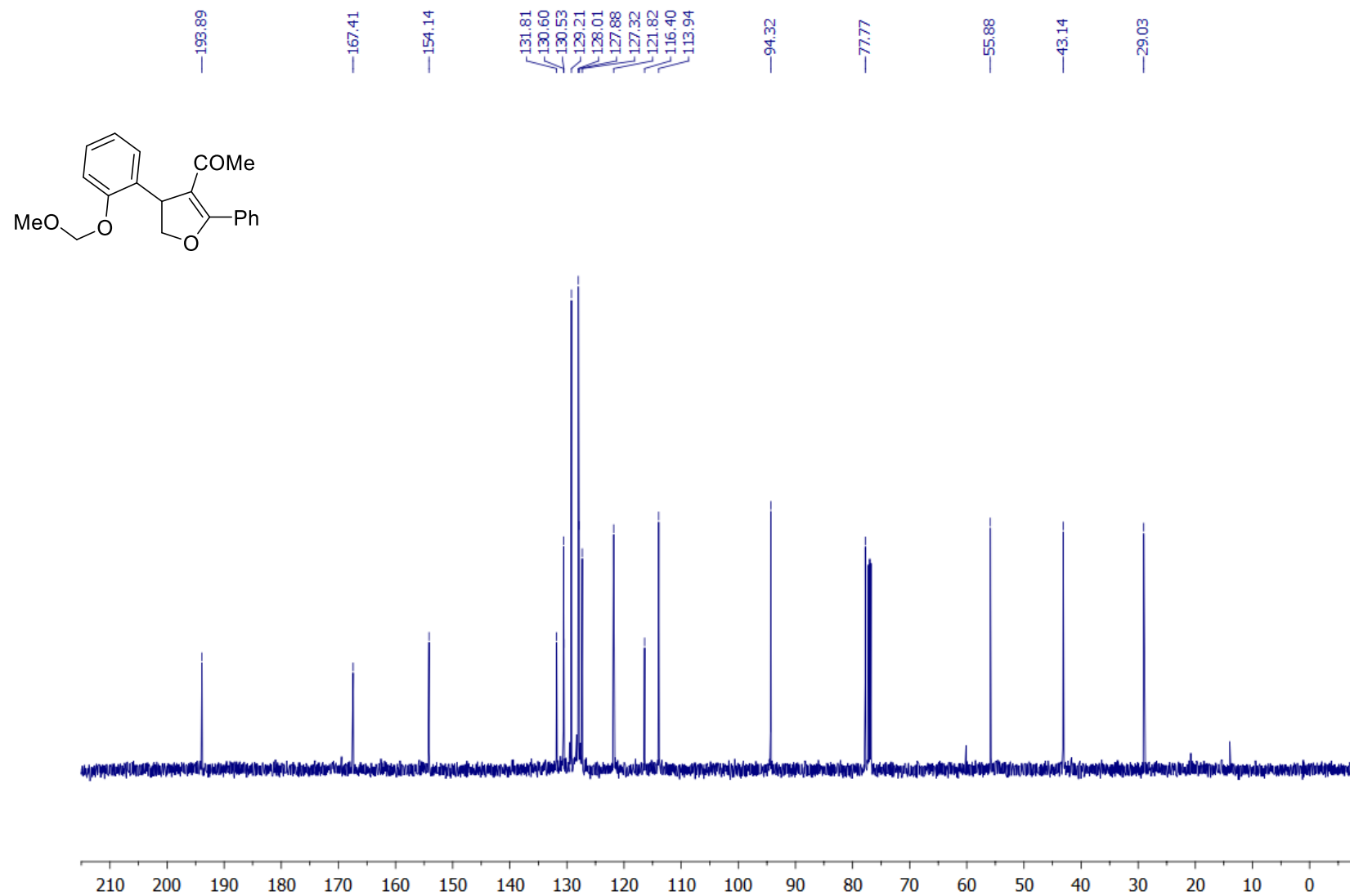
1-{4-[2-(Methoxymethoxy)phenyl]-2-phenyl-4,5-dihydrofuran-3-yl}ethanone (10a)

^1H NMR (CDCl_3 , 600 MHz)



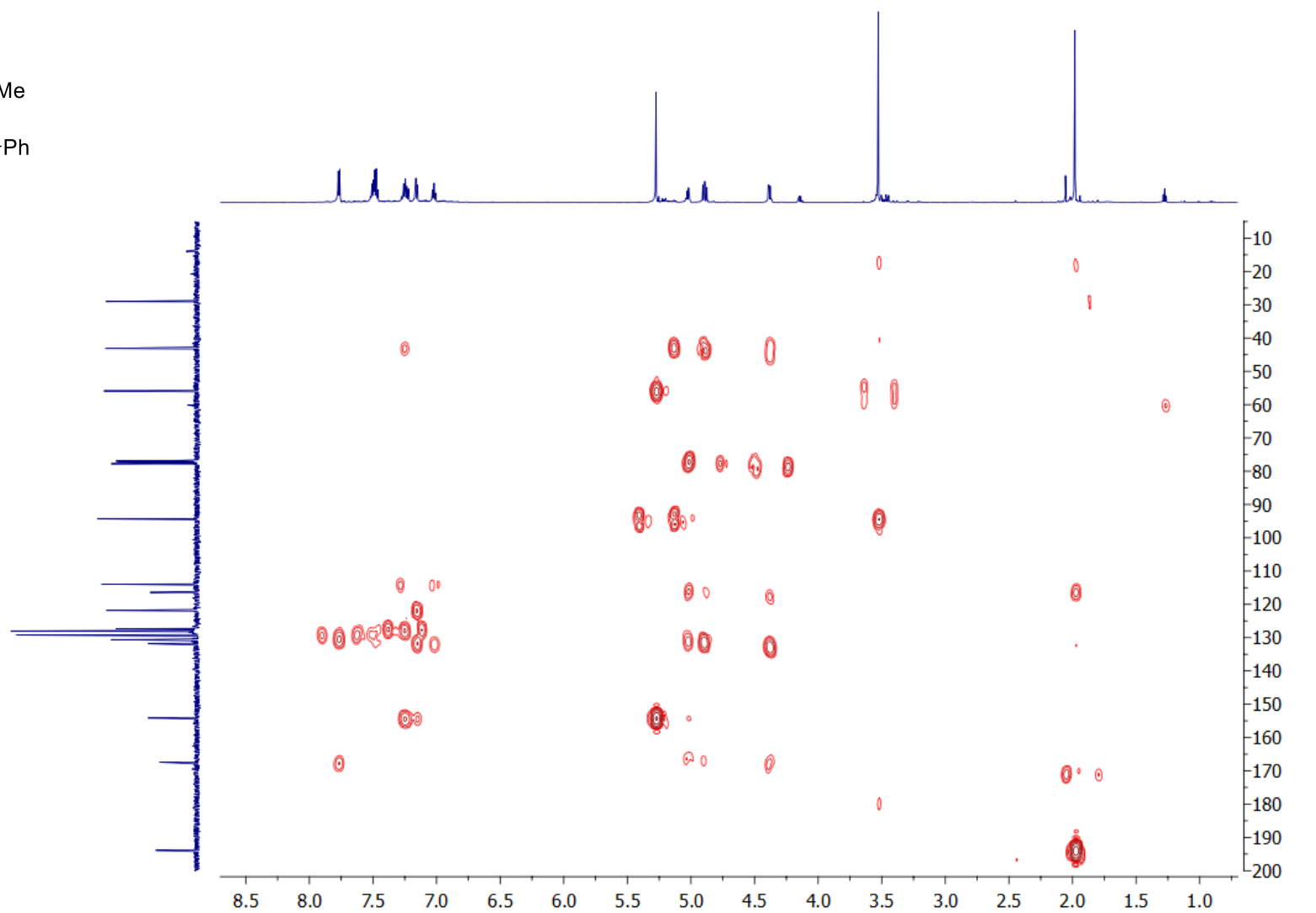
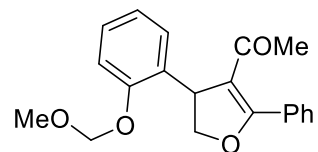
1-{4-[2-(Methoxymethoxy)phenyl]-2-phenyl-4,5-dihydrofuran-3-yl}ethanone (10a)

^{13}C NMR (CDCl_3 , 150 MHz)



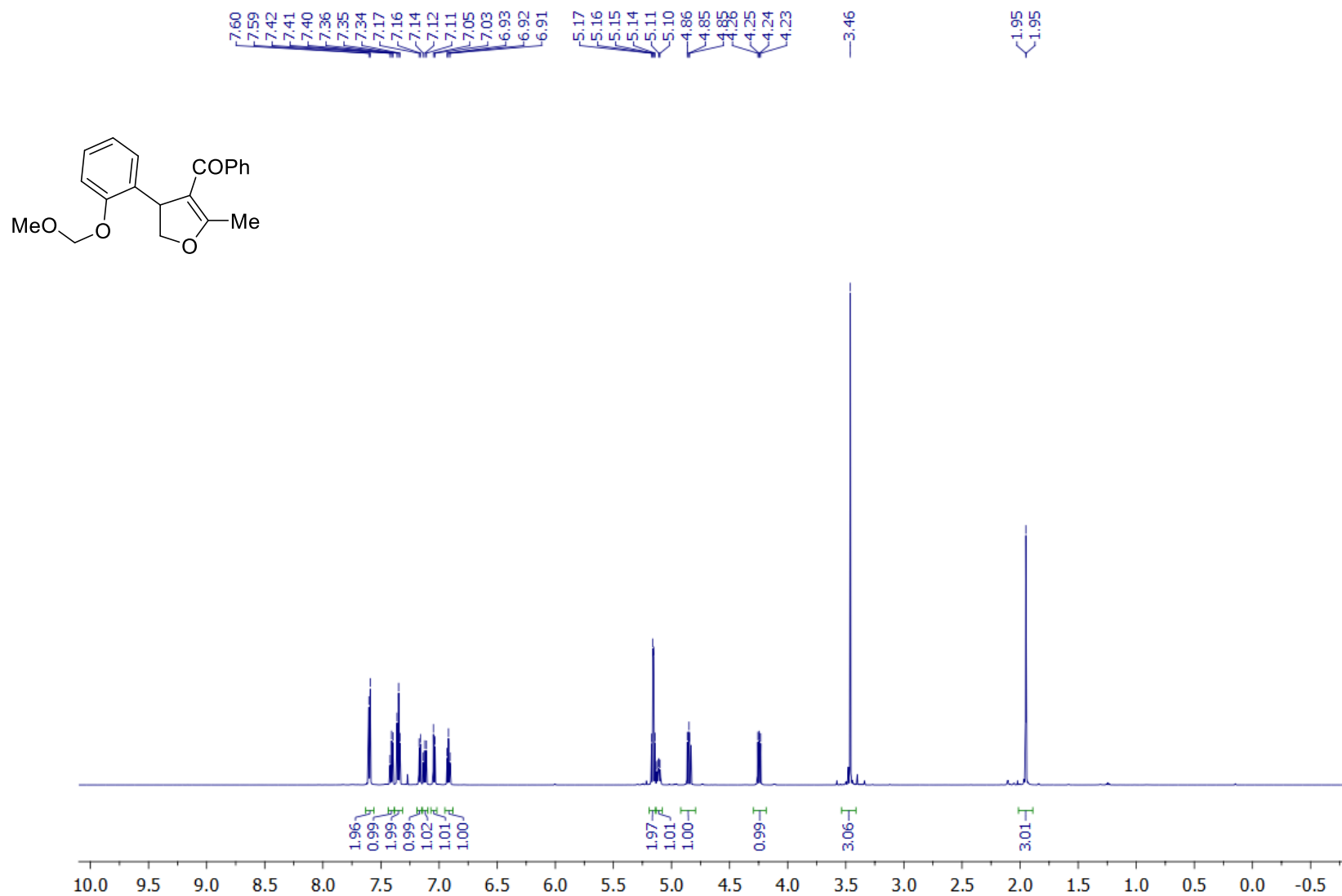
1-{4-[2-(Methoxymethoxy)phenyl]-2-phenyl-4,5-dihydrofuran-3-yl}ethanone (10a)

^1H - ^{13}C HMBC (CDCl_3)



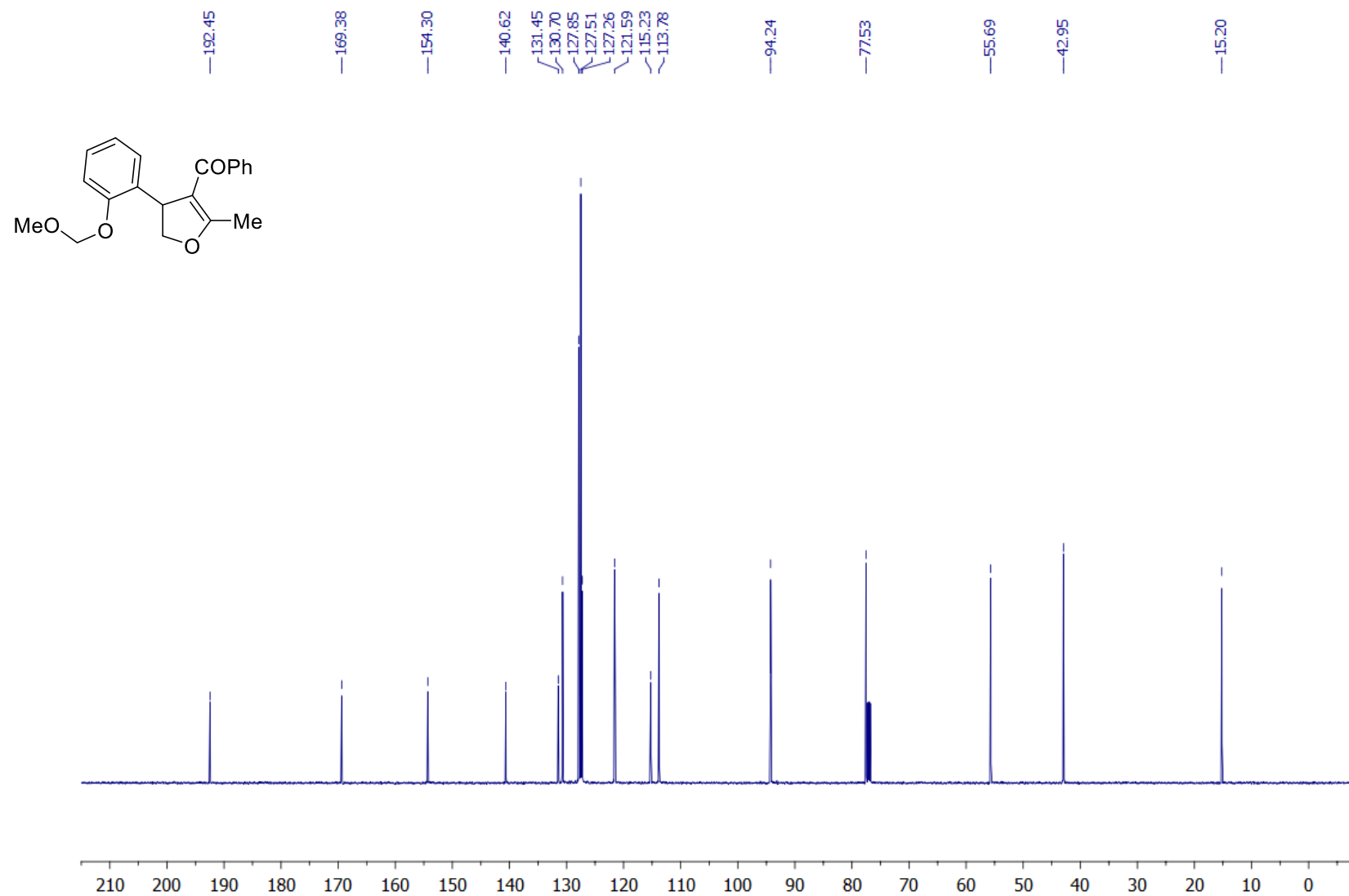
{4-[2-(Methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}(phenyl)methanone (1ob)

¹H NMR (CDCl₃, 600 MHz)



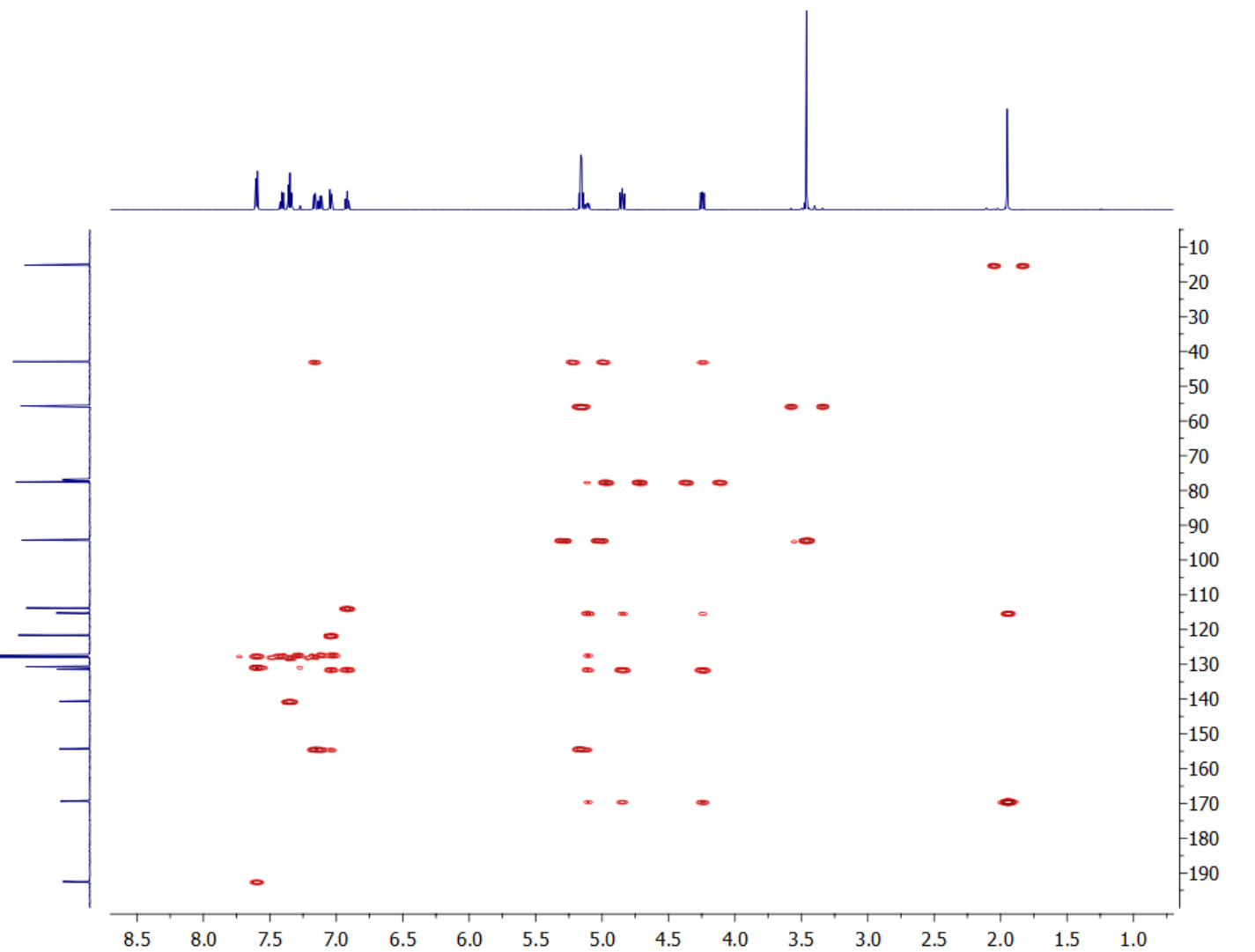
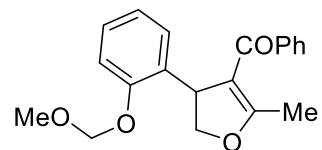
{4-[2-(Methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}(phenyl)methanone (1ob)

¹³C NMR (CDCl₃, 150 MHz)



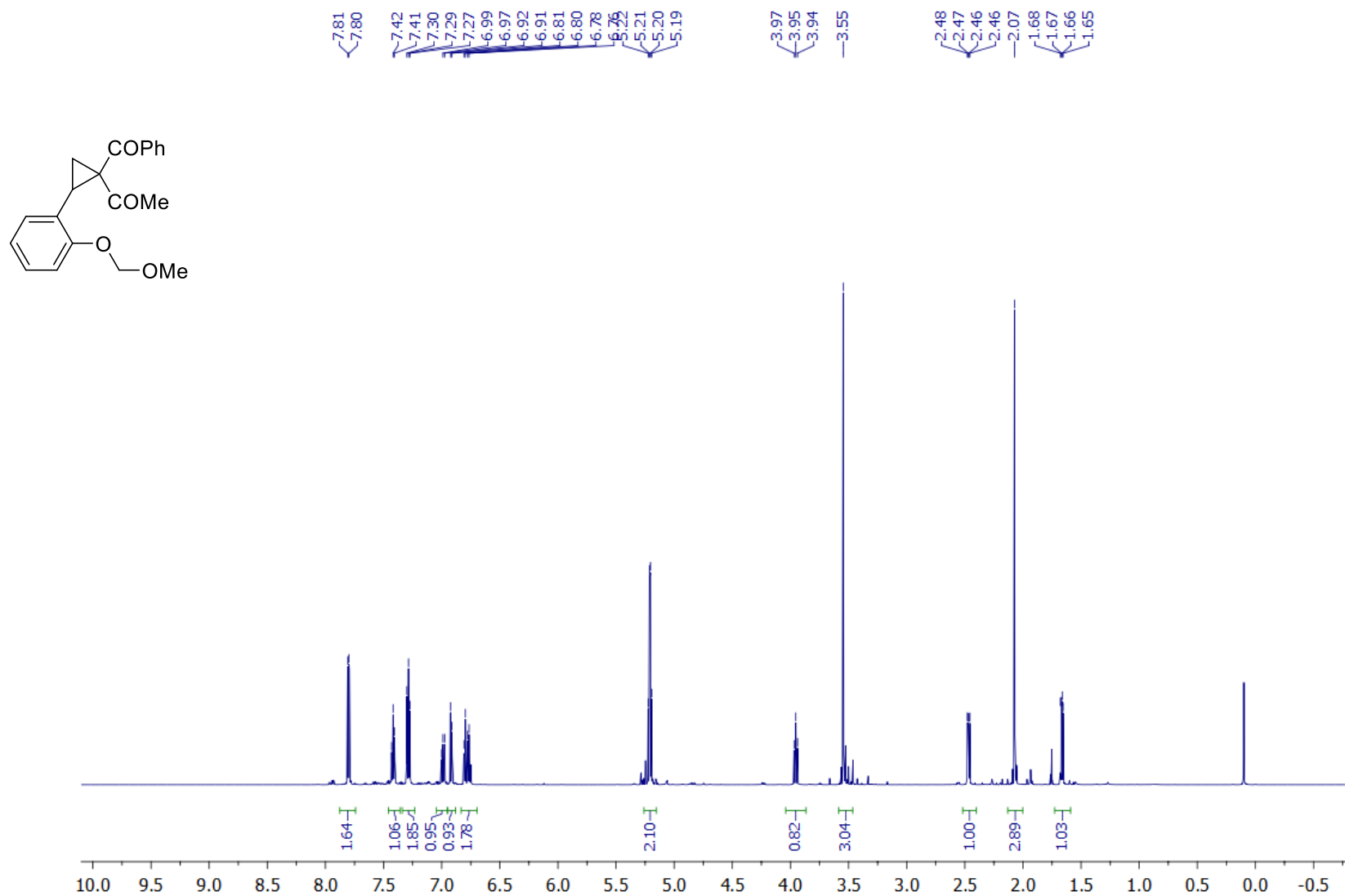
{4-[2-(Methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-yl}(phenyl)methanone (1ob)

^1H - ^{13}C HMBC (CDCl_3)



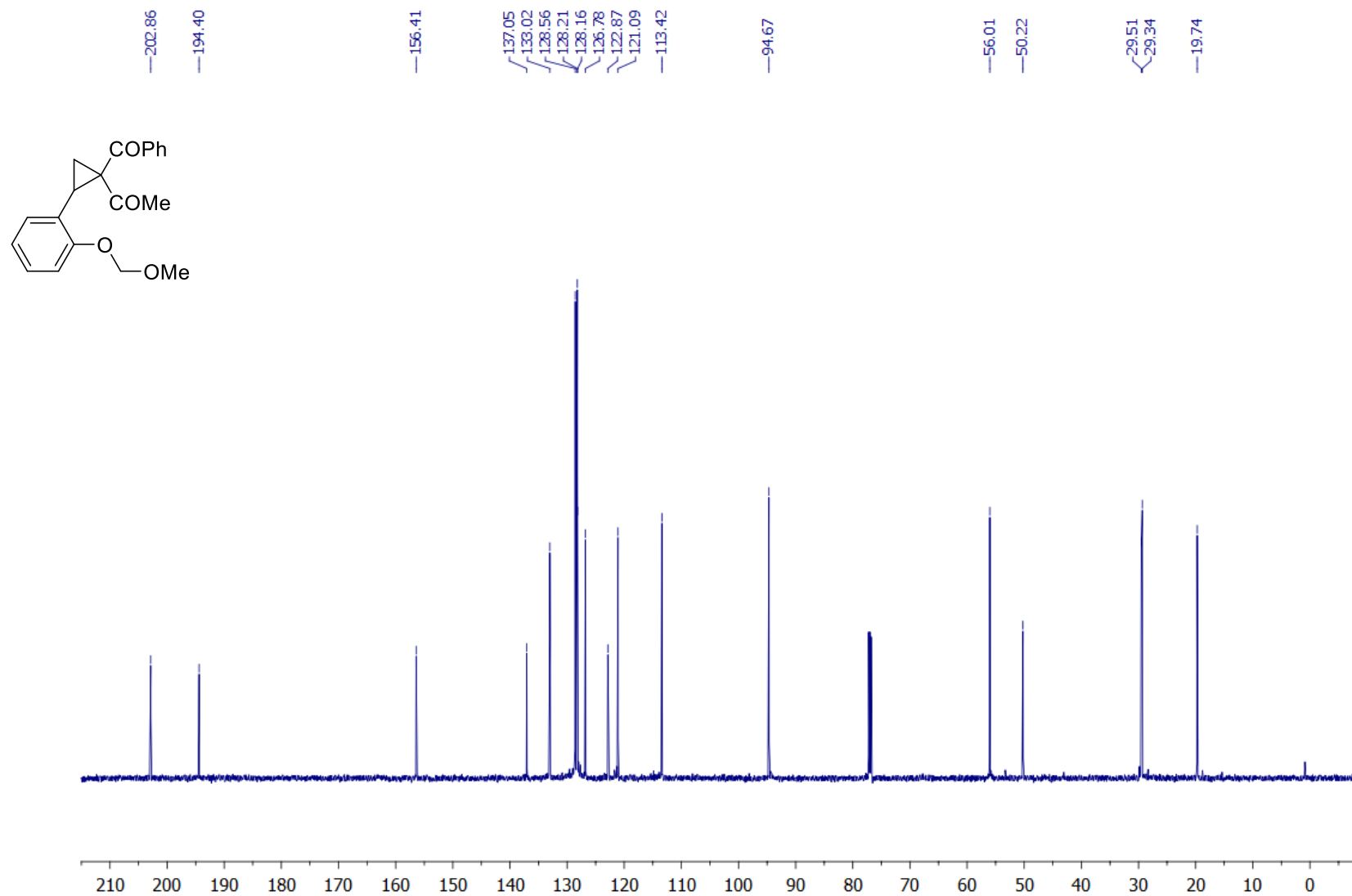
1-{1-Benzoyl-2-[2-(methoxymethoxy)phenyl]cyclopropyl}ethanone (S3o)

^1H NMR (CDCl_3 , 600 MHz)

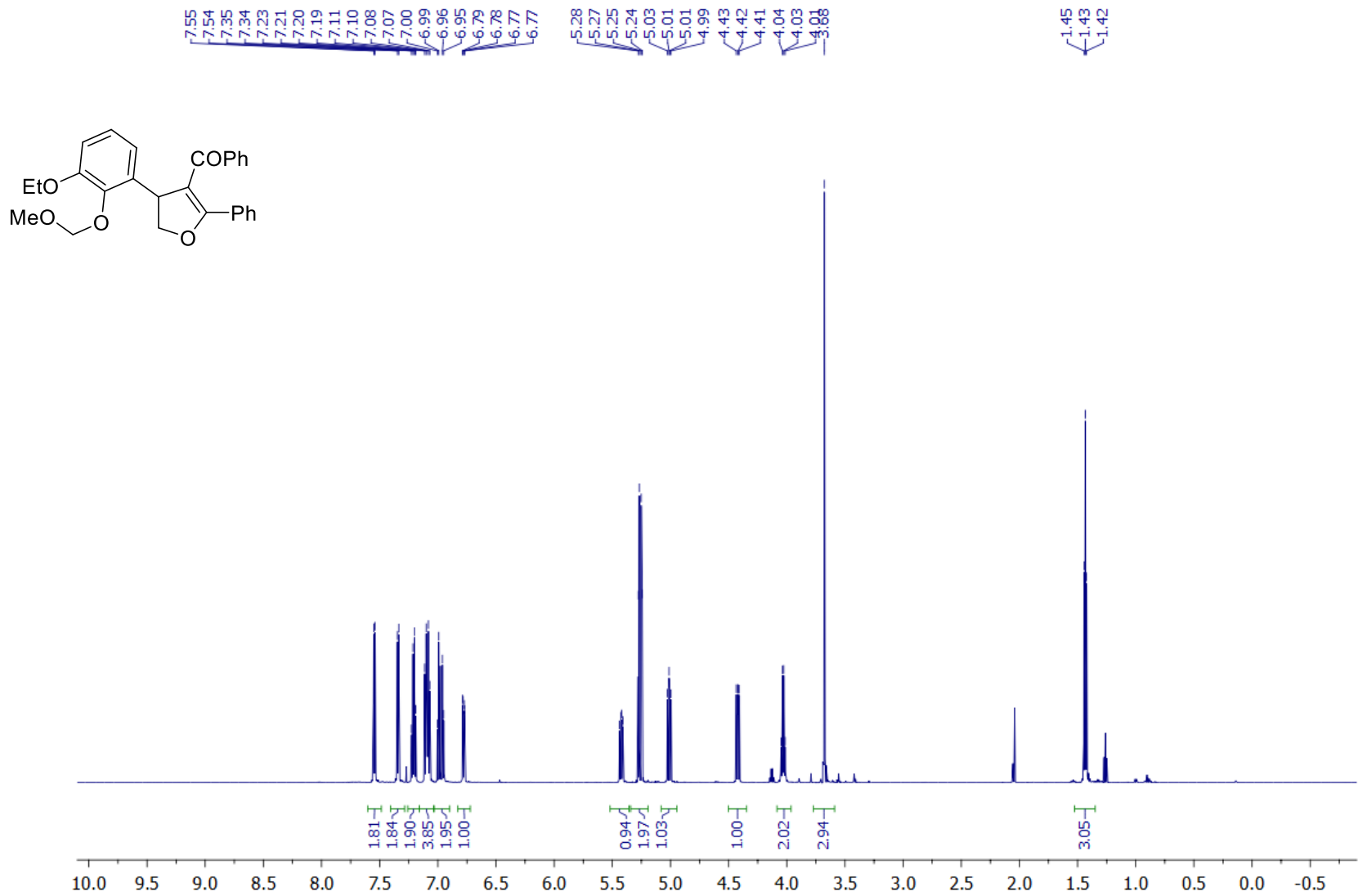


1-{1-Benzoyl-2-[2-(methoxymethoxy)phenyl]cyclopropyl}ethanone (S3o)

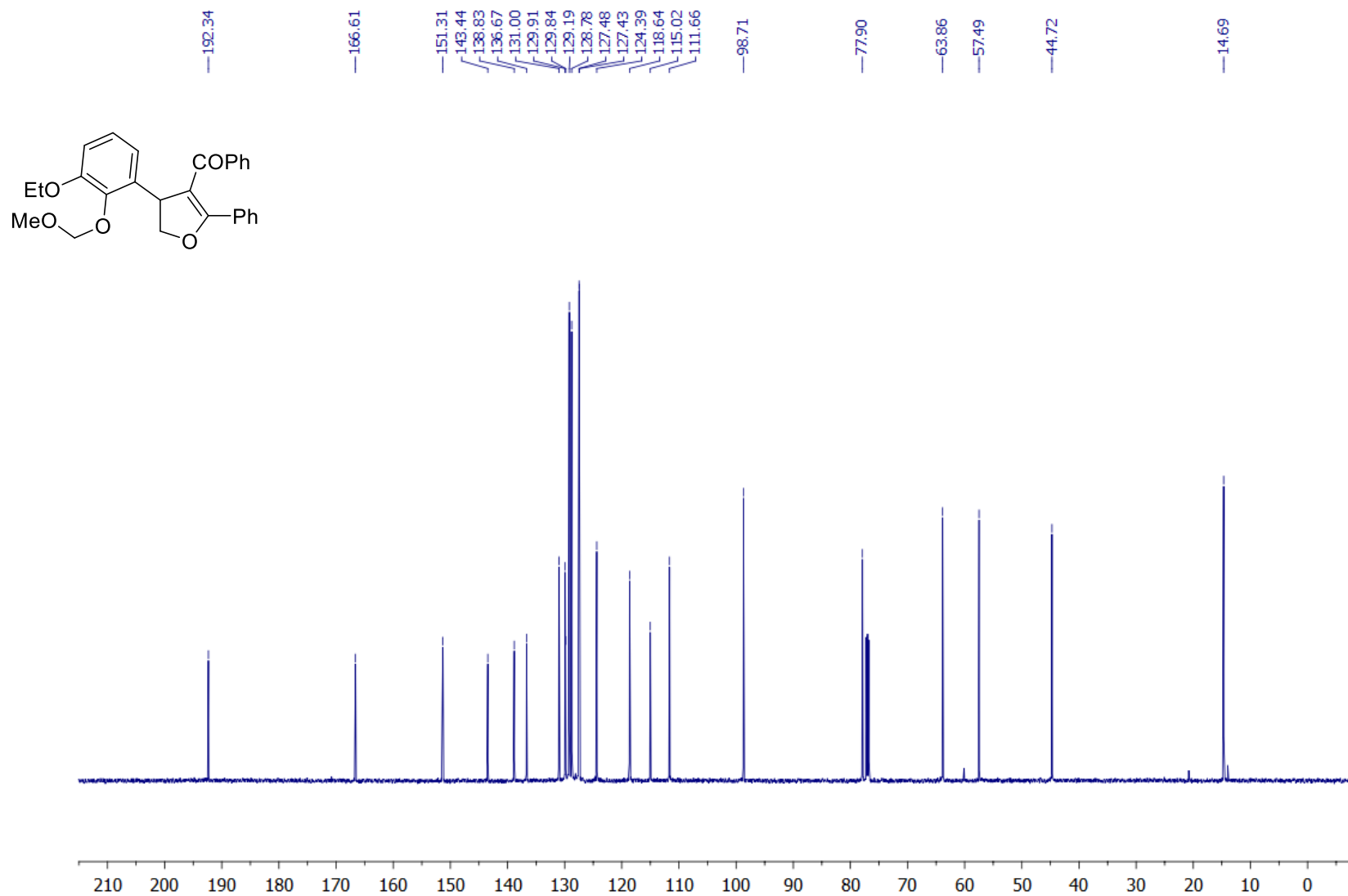
^{13}C NMR (CDCl_3 , 150 MHz)



{4-[3-Ethoxy-2-(methoxymethoxy)phenyl]-2-phenyl-4,5-dihydrofuran-3-yl}(phenyl)methanone (1p)

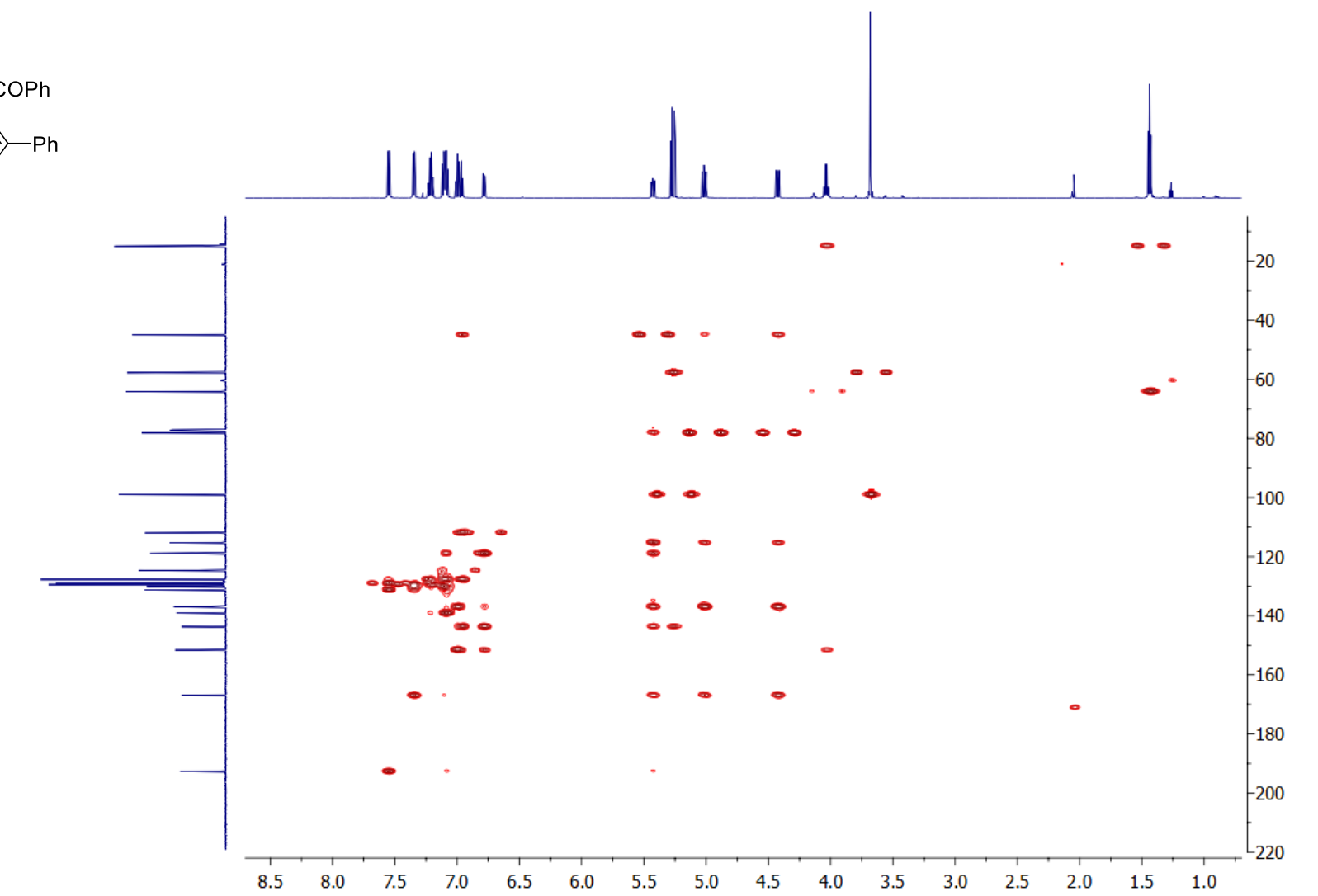
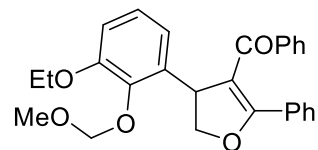
¹H NMR (CDCl₃, 600 MHz)

{4-[3-Ethoxy-2-(methoxymethoxy)phenyl]-2-phenyl-4,5-dihydrofuran-3-yl}(phenyl)methanone (1p)

 ^{13}C NMR (CDCl_3 , 150 MHz)

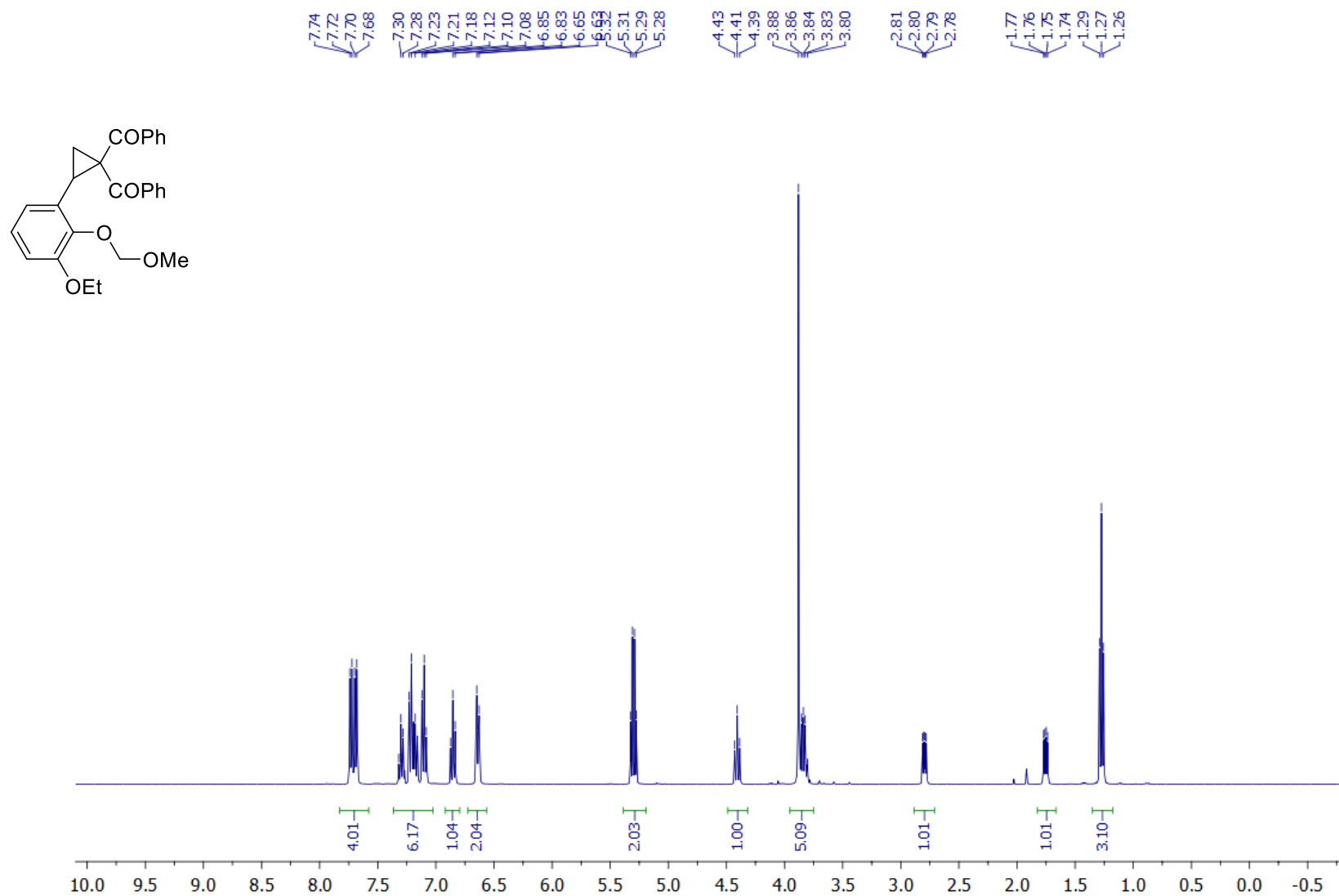
{4-[3-Ethoxy-2-(methoxymethoxy)phenyl]-2-phenyl-4,5-dihydrofuran-3-yl}(phenyl)methanone (1p)

^1H - ^{13}C HMBC (CDCl_3)



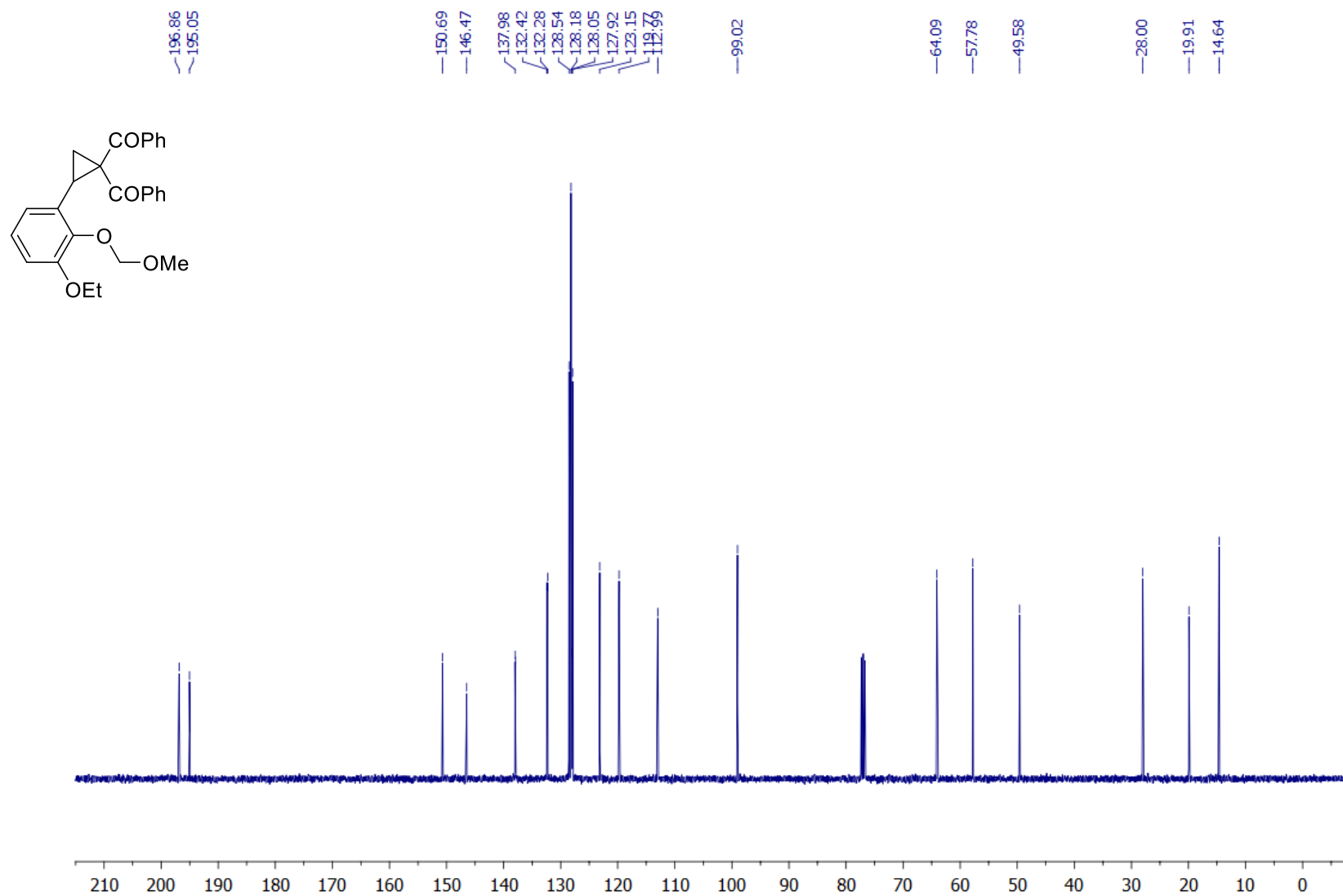
{2-[3-Ethoxy-2-(methoxymethoxy)phenyl]cyclopropane-1,1-diyl}bis(phenylmethanone) (S3p)

¹H NMR (CDCl₃, 400 MHz)



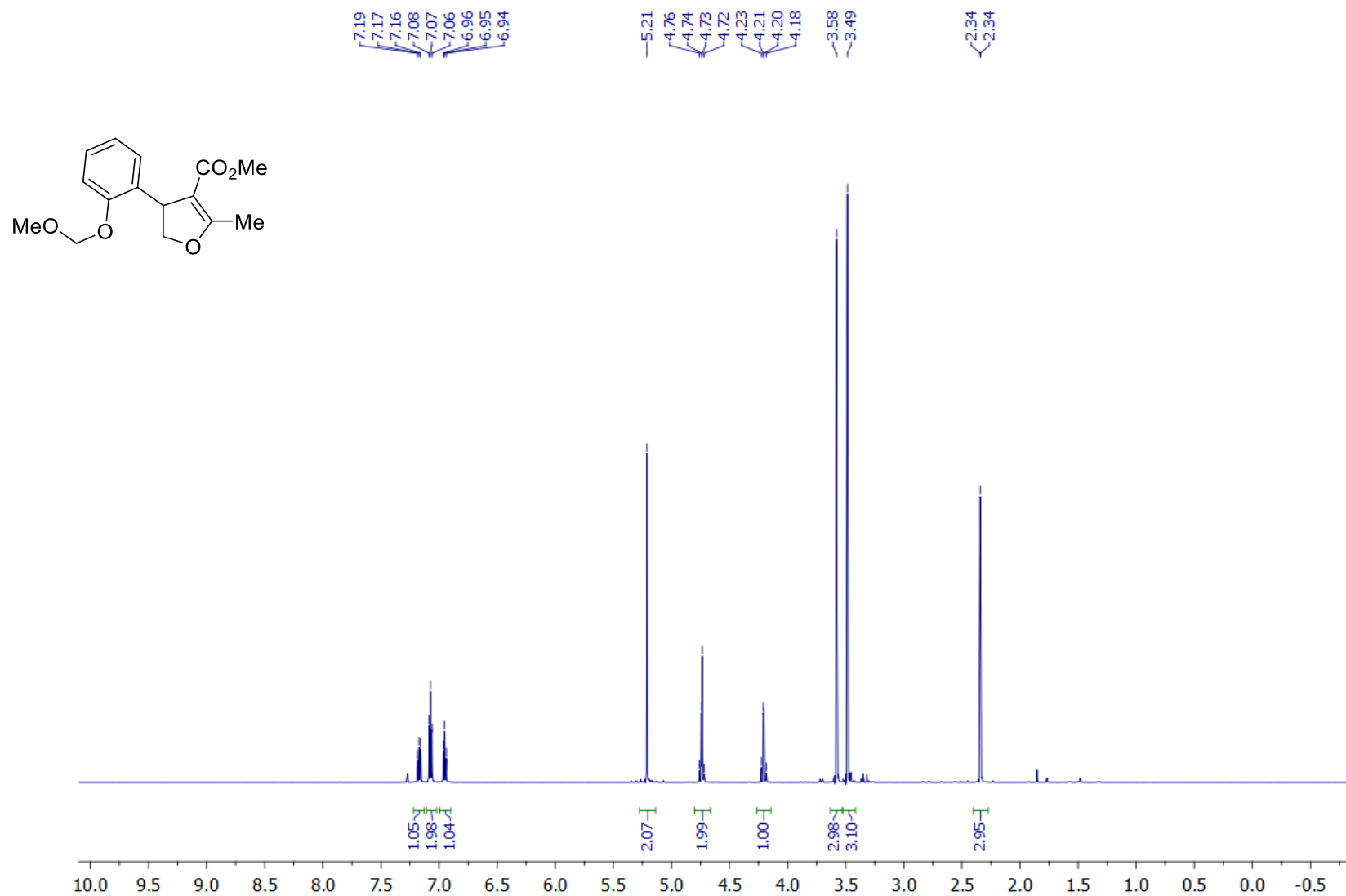
{2-[3-Ethoxy-2-(methoxymethoxy)phenyl]cyclopropane-1,1-diyl}bis(phenylmethanone) (S3p)

^{13}C NMR (CDCl_3 , 100 MHz)



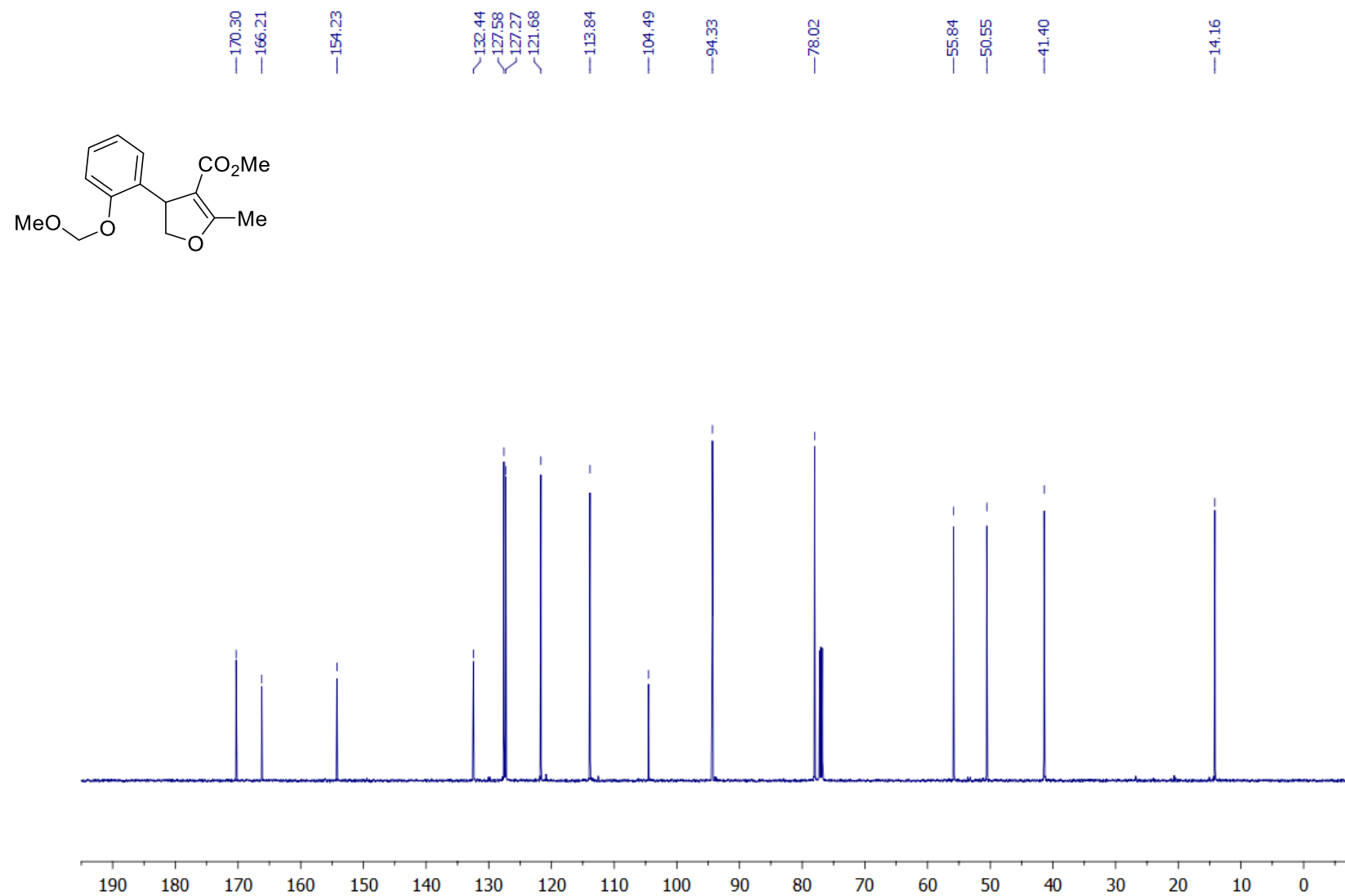
Methyl 4-[2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-carboxylate (1q)

^1H NMR (CDCl_3 , 600 MHz)



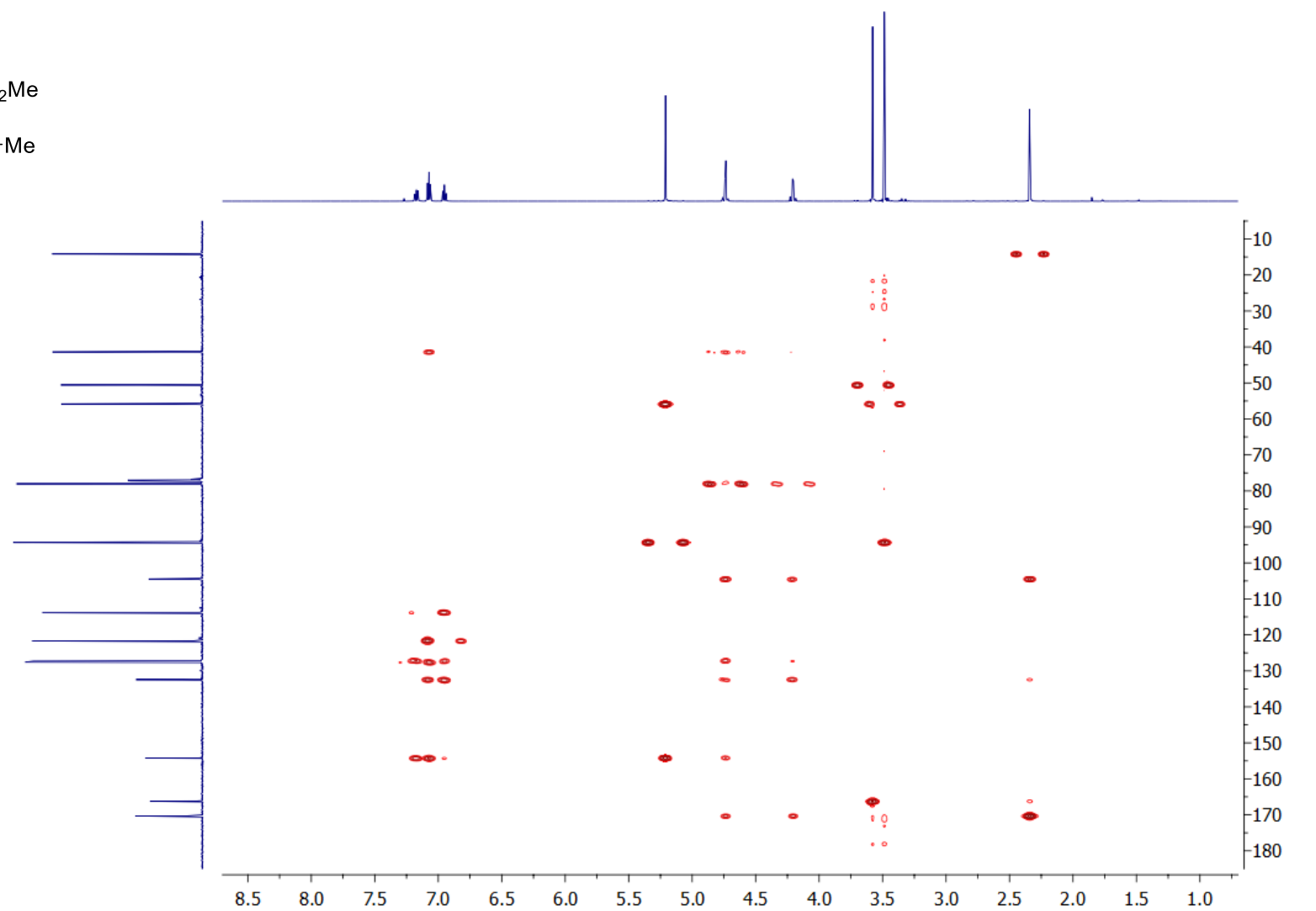
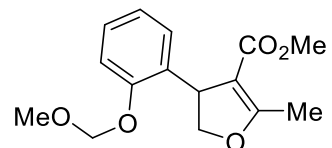
Methyl 4-[2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-carboxylate (1q)

^{13}C NMR (CDCl_3 , 150 MHz)



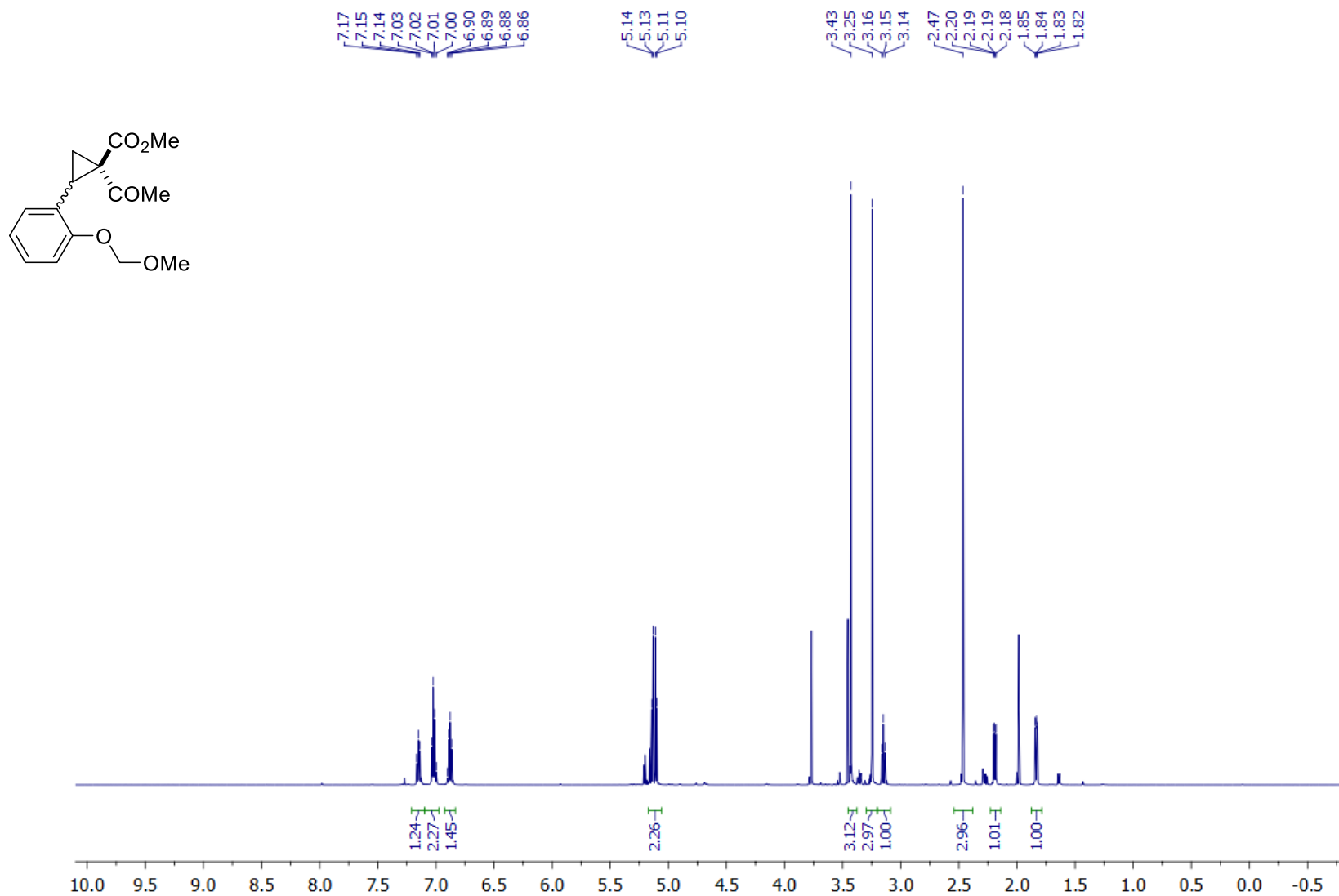
Methyl 4-[2-(methoxymethoxy)phenyl]-2-methyl-4,5-dihydrofuran-3-carboxylate (1q)

^1H - ^{13}C HMBC (CDCl_3)



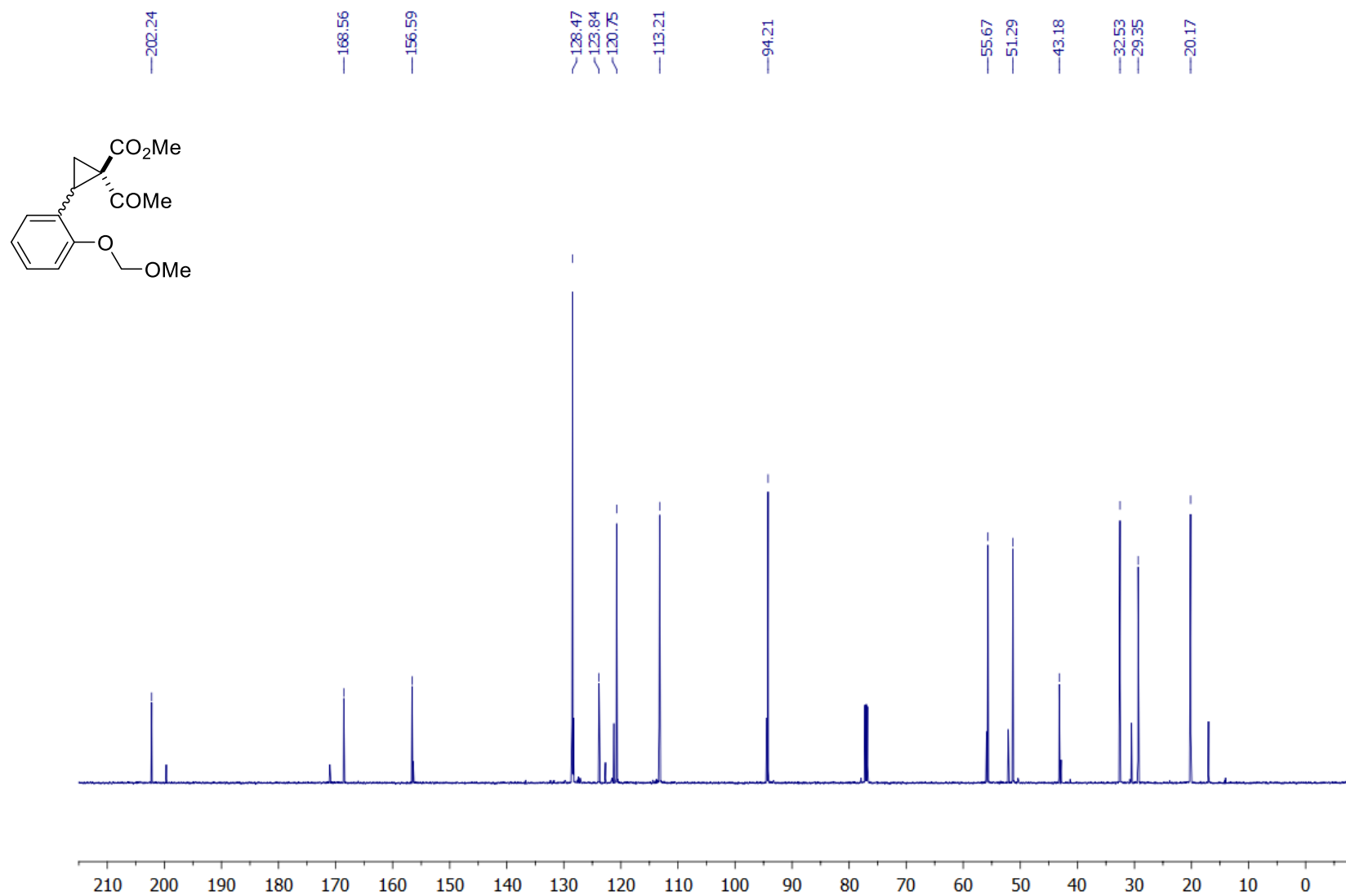
Methyl 1-acetyl-2-[2-(methoxymethoxy)phenyl]cyclopropane-1-carboxylate (S3q)

^1H NMR (CDCl_3 , 600 MHz)



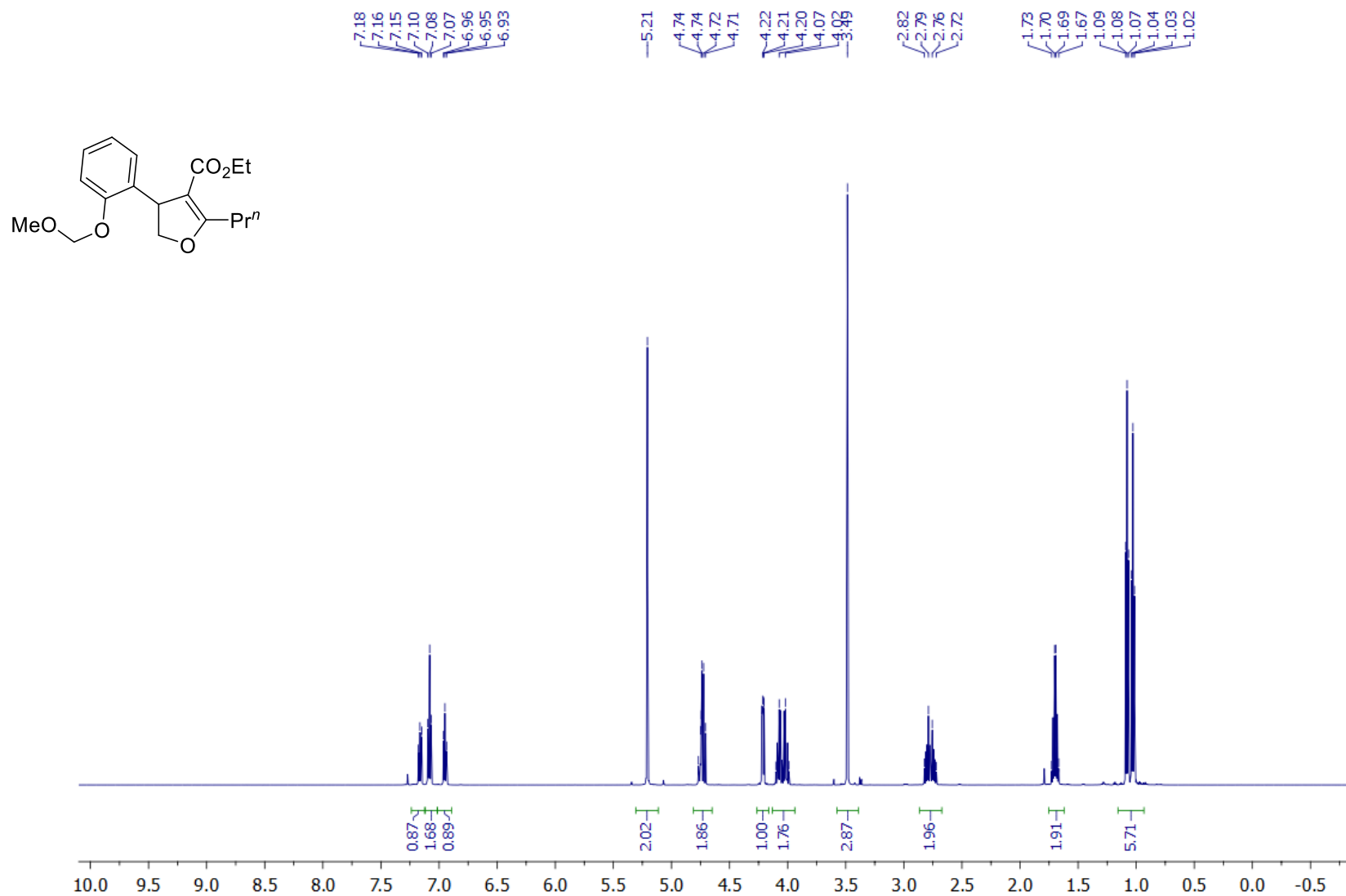
Methyl 1-acetyl-2-[2-(methoxymethoxy)phenyl]cyclopropane-1-carboxylate (S3q)

^{13}C NMR (CDCl_3 , 150 MHz)



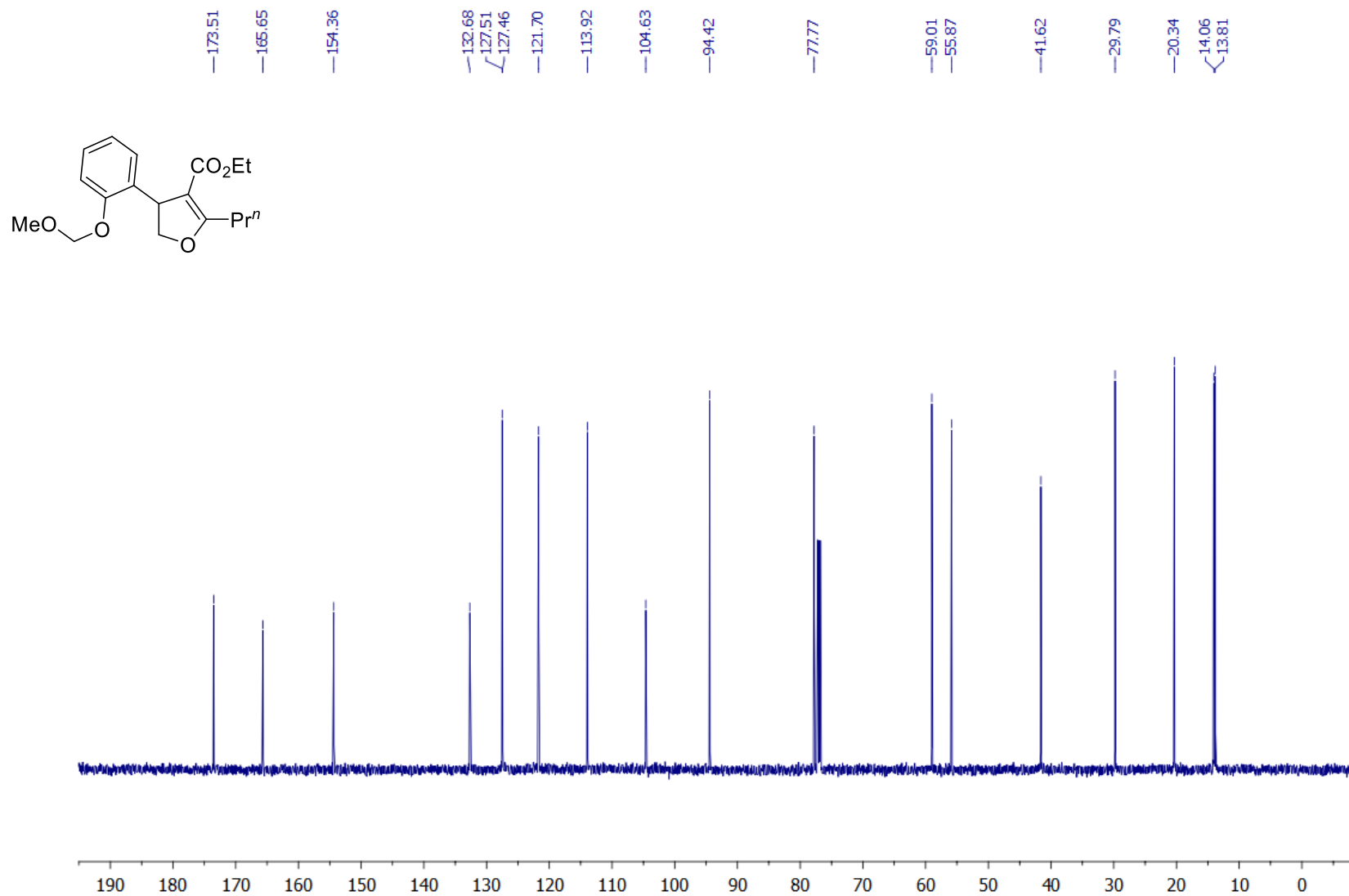
Ethyl 4-[2-(methoxymethoxy)phenyl]-2-(1-propyl)-4,5-dihydrofuran-3-carboxylate (1r)

^1H NMR (CDCl_3 , 600 MHz)



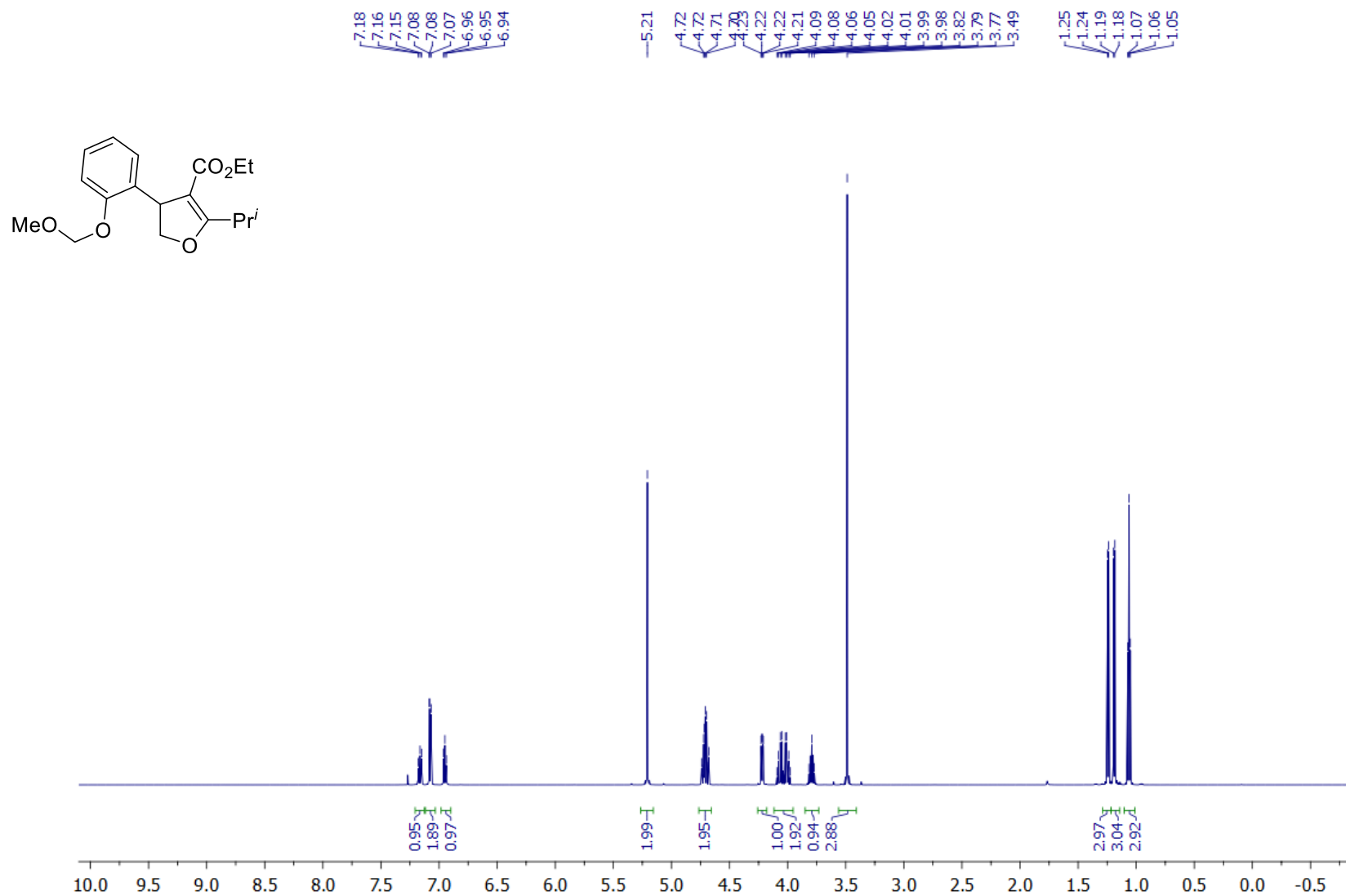
Ethyl 4-[2-(methoxymethoxy)phenyl]-2-(1-propyl)-4,5-dihydrofuran-3-carboxylate (1r)

^{13}C NMR (CDCl_3 , 150 MHz)



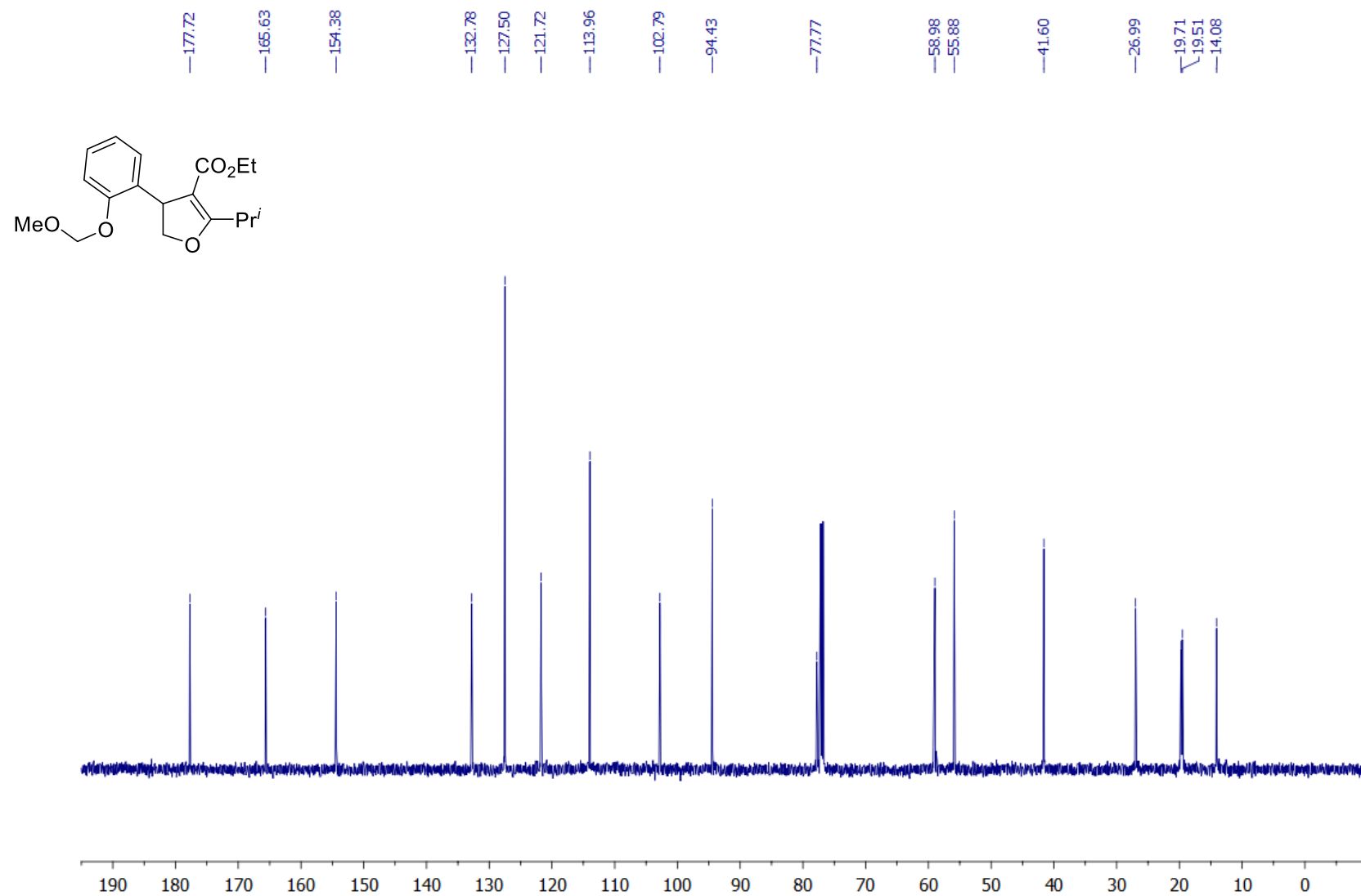
Ethyl 4-[2-(methoxymethoxy)phenyl]-2-(propan-2-yl)-4,5-dihydrofuran-3-carboxylate (1s)

^1H NMR (CDCl_3 , 600 MHz)



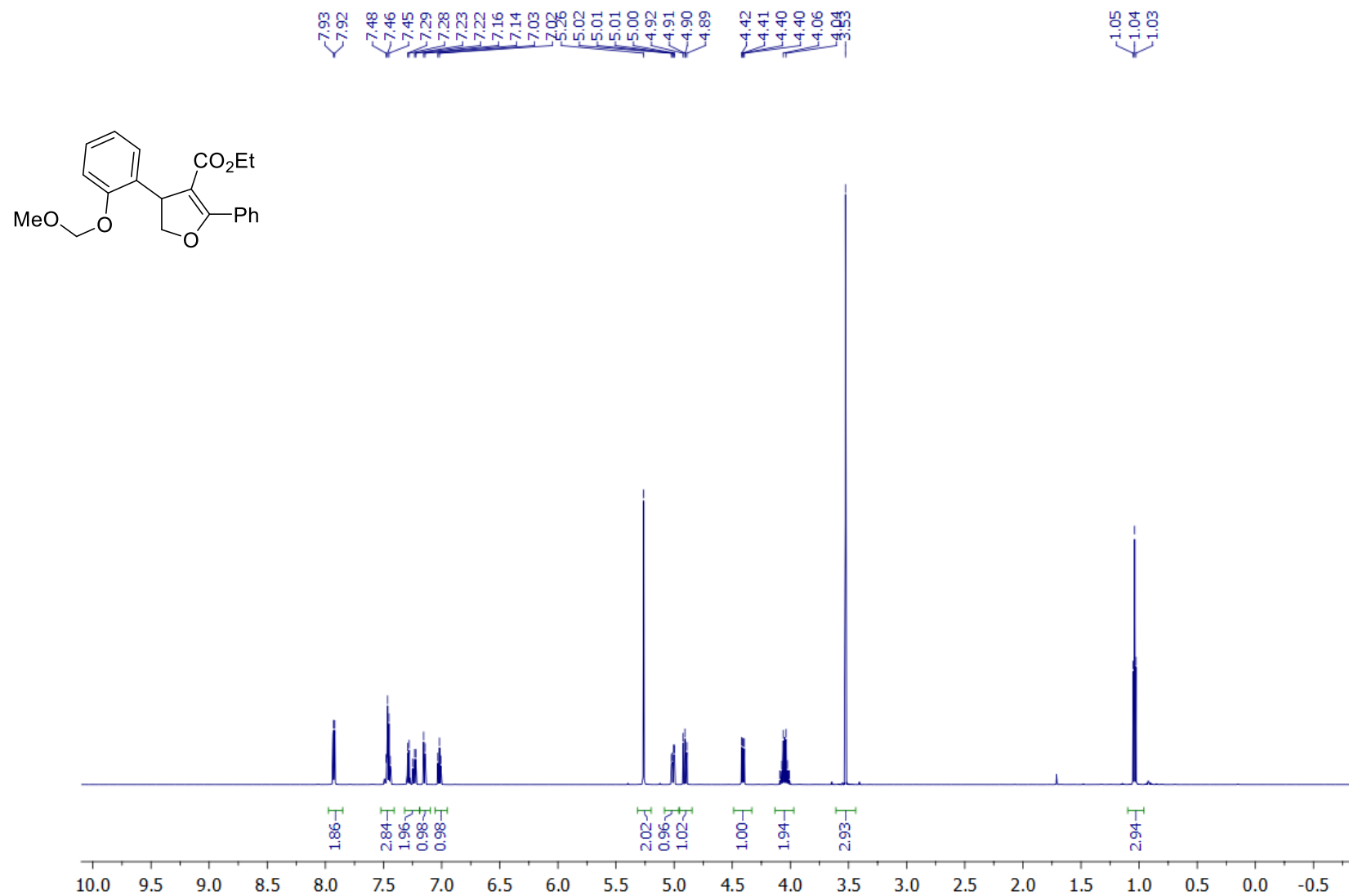
Ethyl 4-[2-(methoxymethoxy)phenyl]-2-(propan-2-yl)-4,5-dihydrofuran-3-carboxylate (1s)

^{13}C NMR (CDCl_3 , 150 MHz)



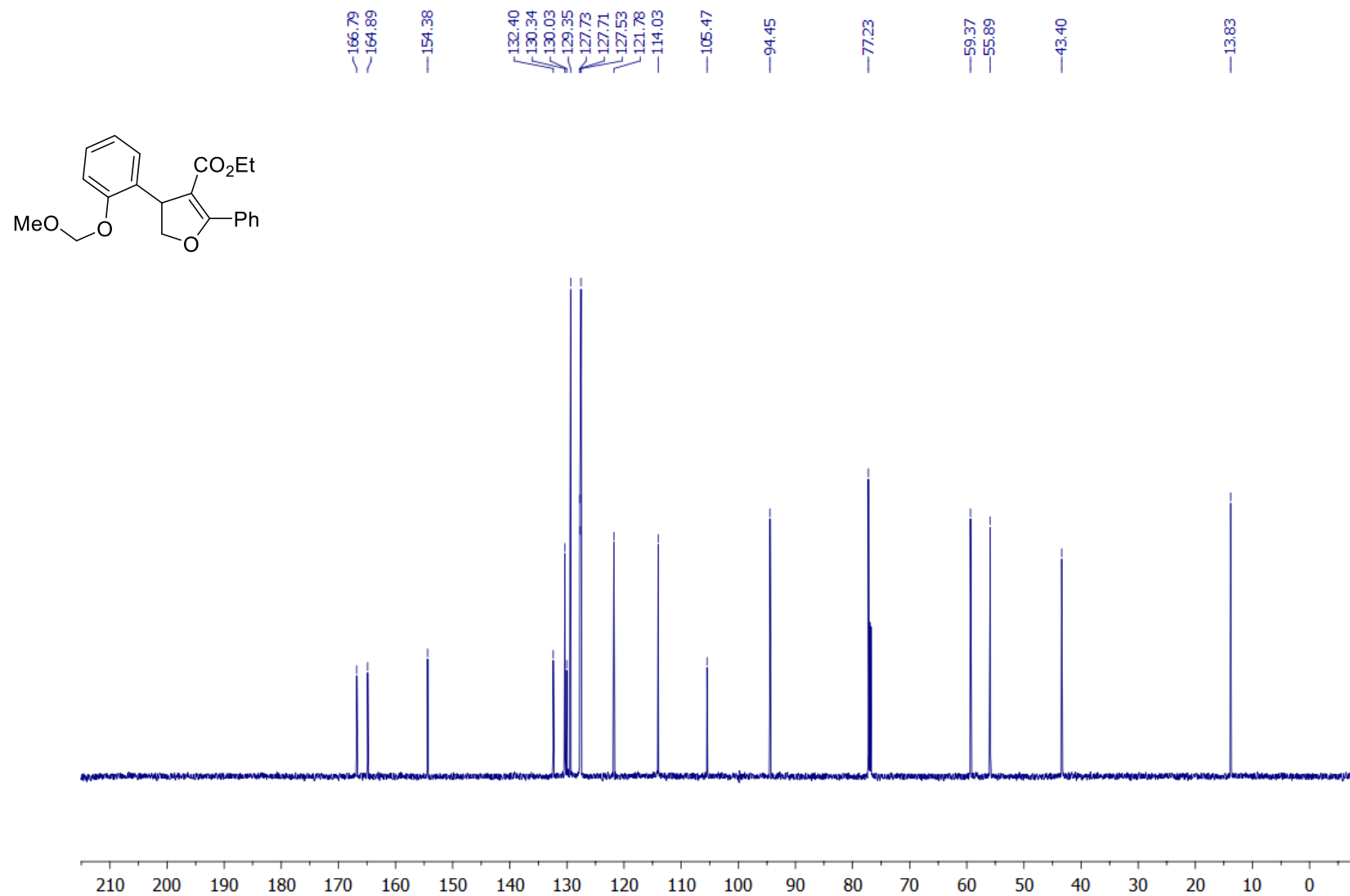
Ethyl 4-[2-(methoxymethoxy)phenyl]-2-phenyl-4,5-dihydrofuran-3-carboxylate (1t)

^1H NMR (CDCl_3 , 600 MHz)



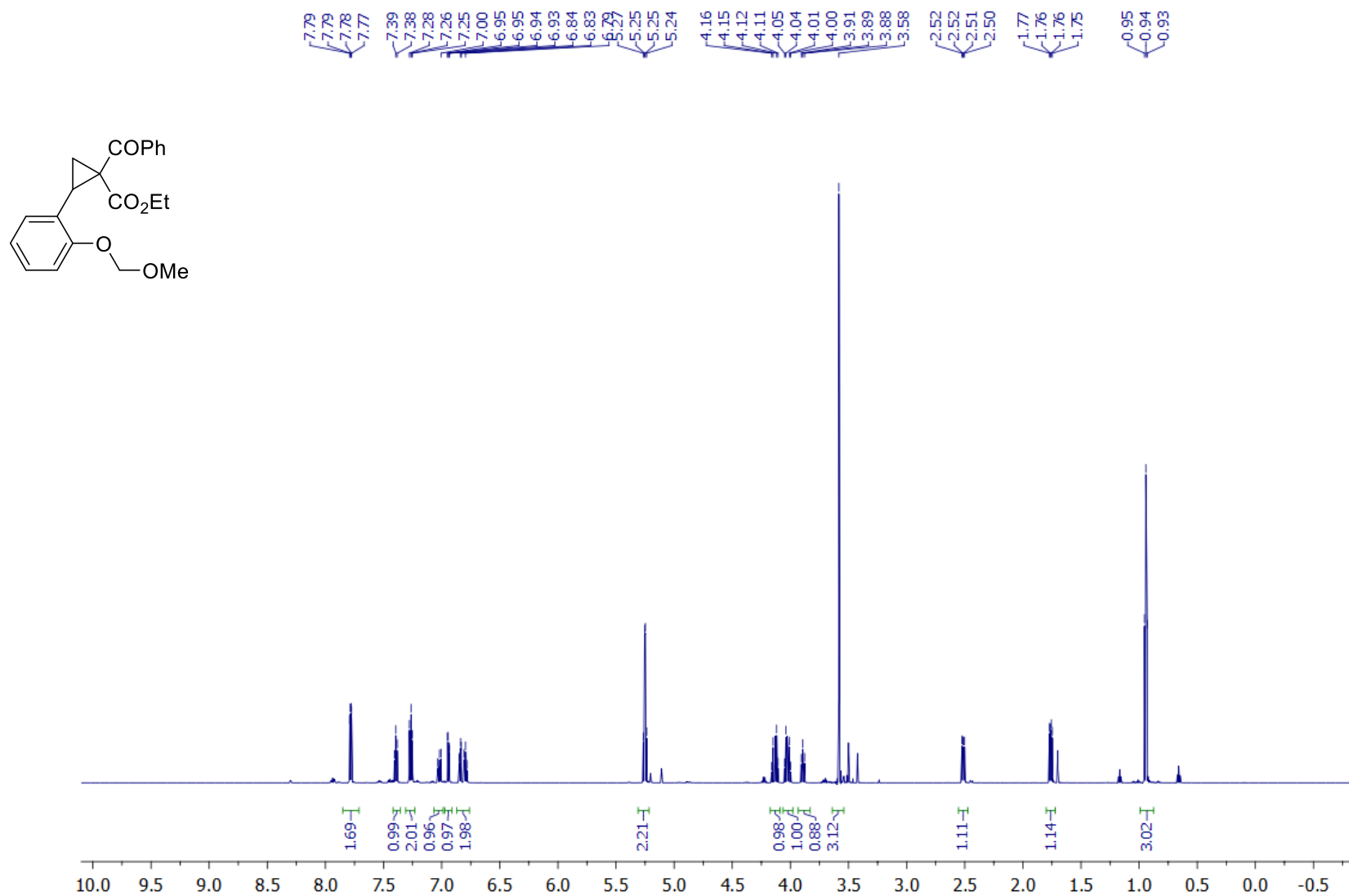
Ethyl 4-[2-(methoxymethoxy)phenyl]-2-phenyl-4,5-dihydrofuran-3-carboxylate (1t)

^{13}C NMR (CDCl_3 , 150 MHz)



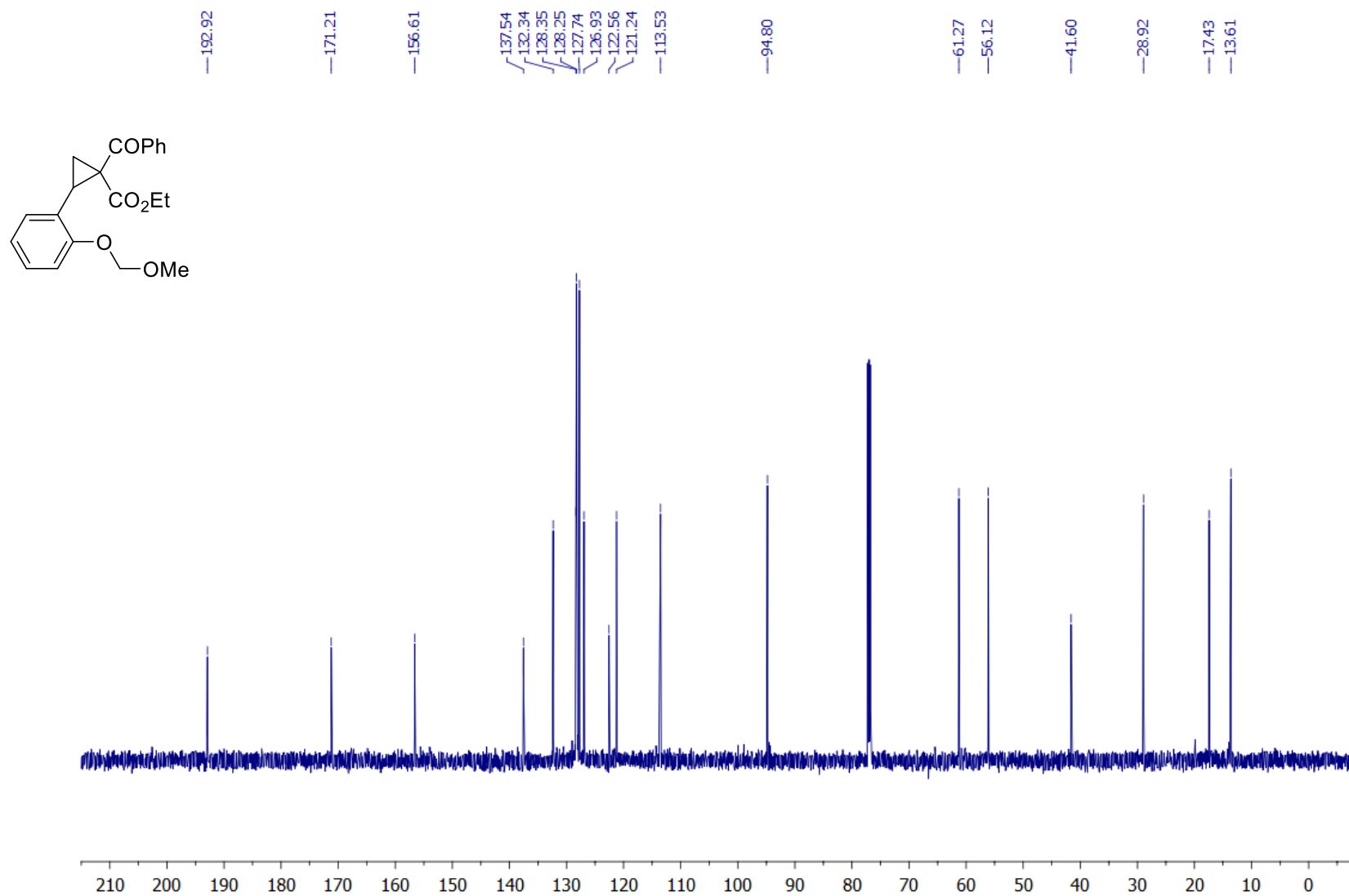
Ethyl 1-benzoyl-2-[2-(methoxymethoxy)phenyl]cyclopropanecarboxylate (S3t)

¹H NMR (CDCl₃, 600 MHz)



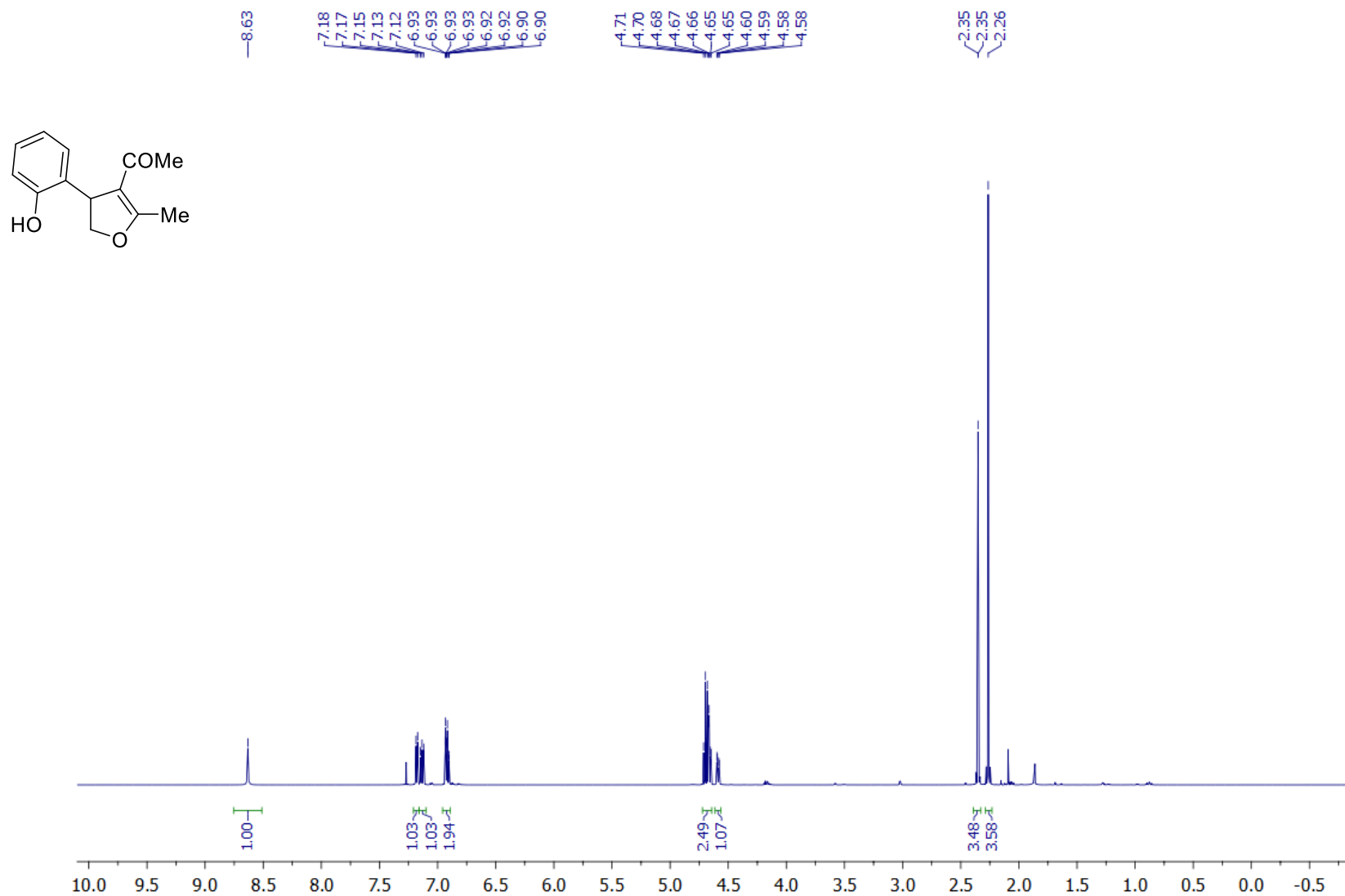
Ethyl 1-benzoyl-2-[2-(methoxymethoxy)phenyl]cyclopropanecarboxylate (S3t)

^{13}C NMR (CDCl_3 , 150 MHz)



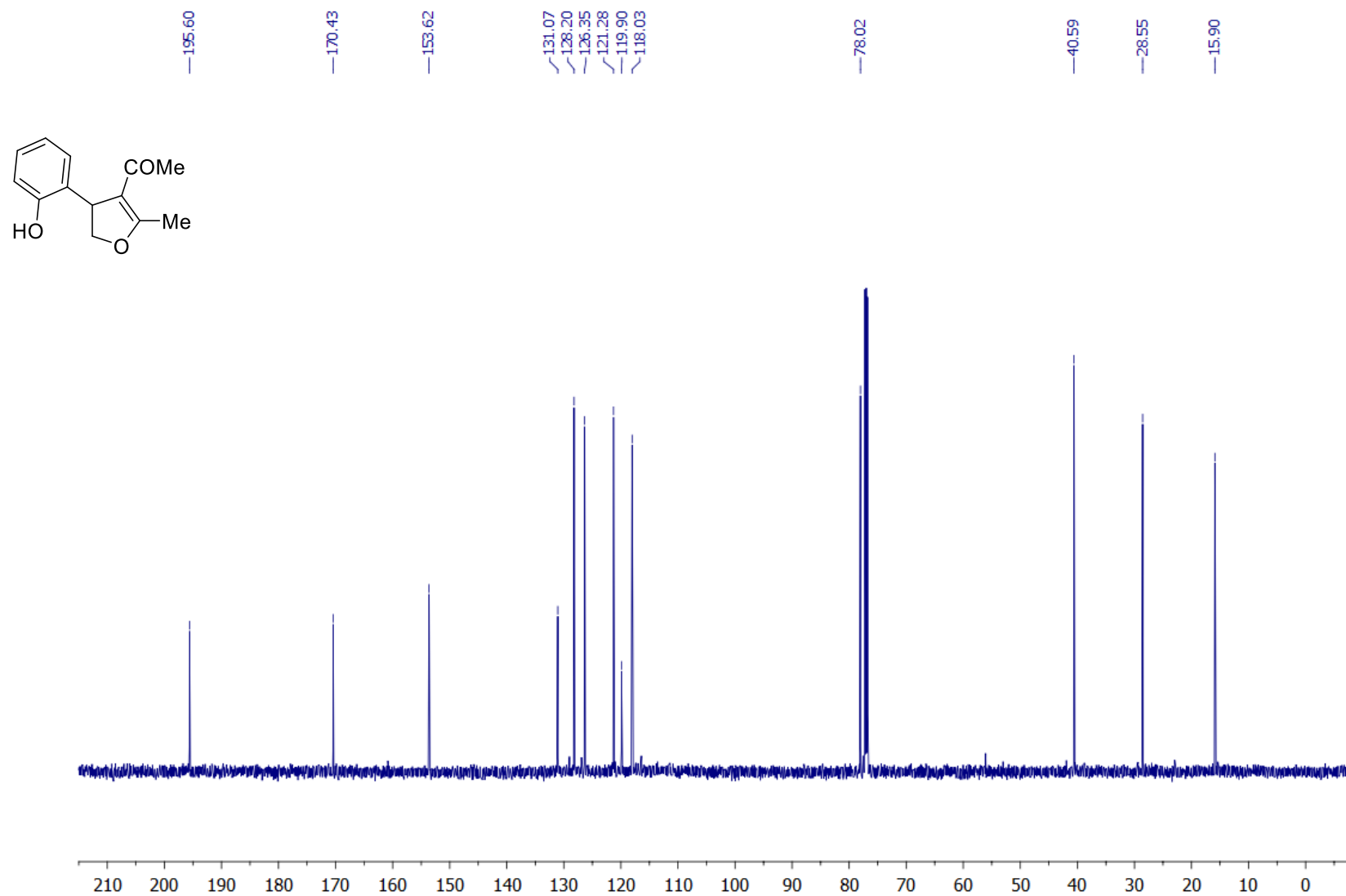
1-[4-(2-Hydroxyphenyl)-2-methyl-4,5-dihydrofuran-3-yl]ethanone (2a)

^1H NMR (CDCl_3 , 600 MHz)



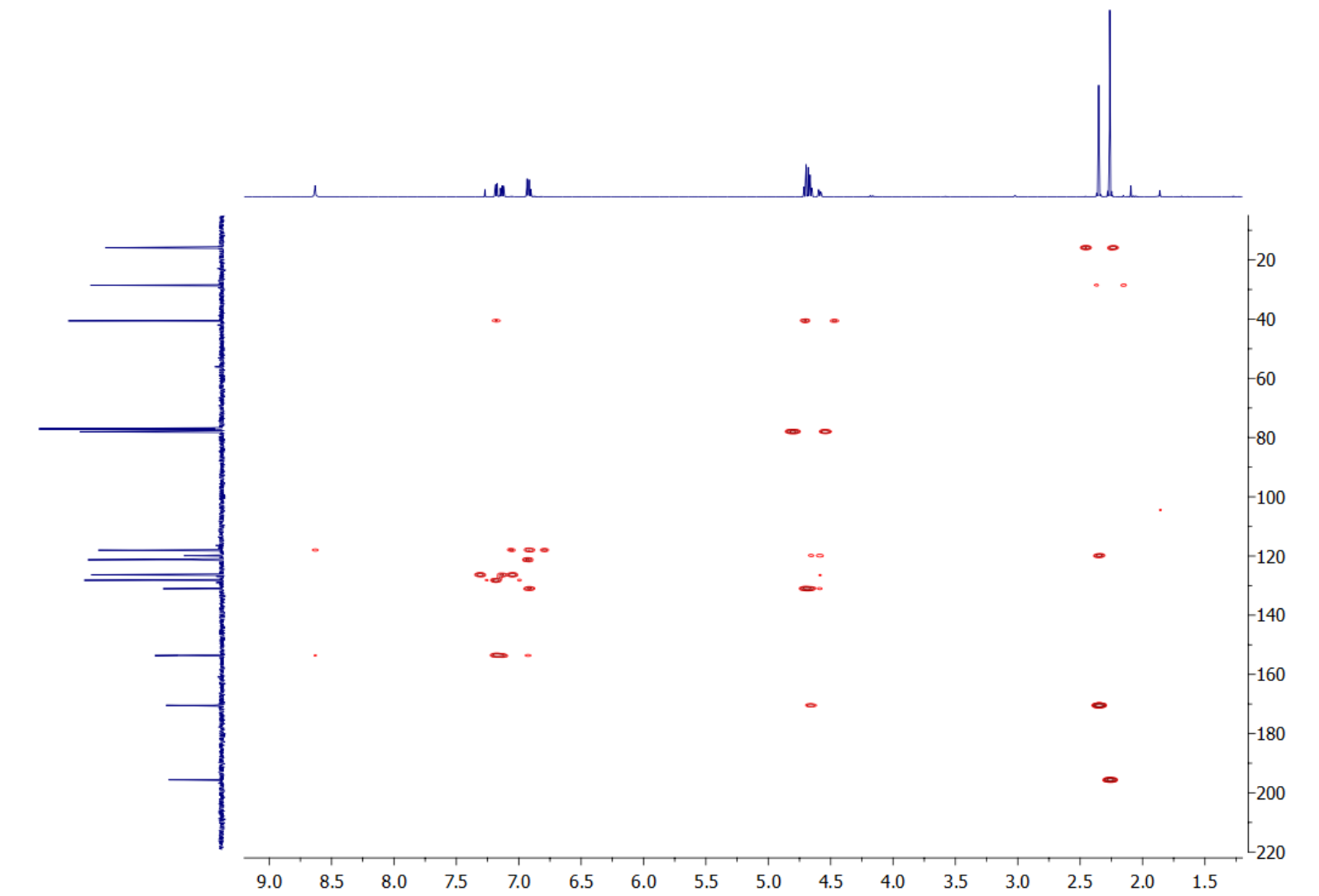
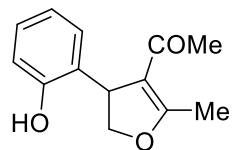
1-[4-(2-Hydroxyphenyl)-2-methyl-4,5-dihydrofuran-3-yl]ethanone (2a)

^{13}C NMR (CDCl_3 , 150 MHz)



1-[4-(2-Hydroxyphenyl)-2-methyl-4,5-dihydrofuran-3-yl]ethanone (2a)

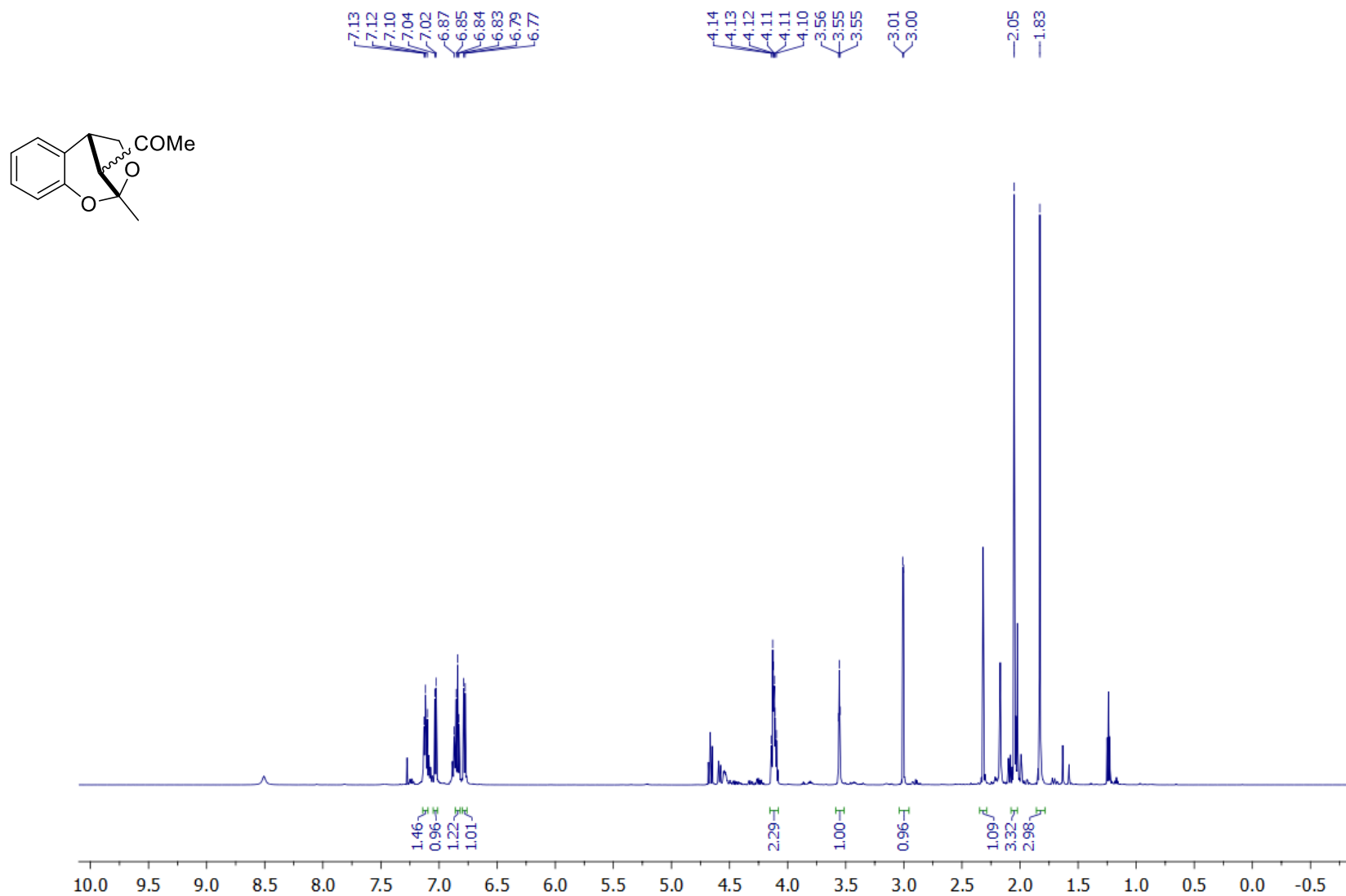
^1H - ^{13}C HMBC (CDCl_3)



S400

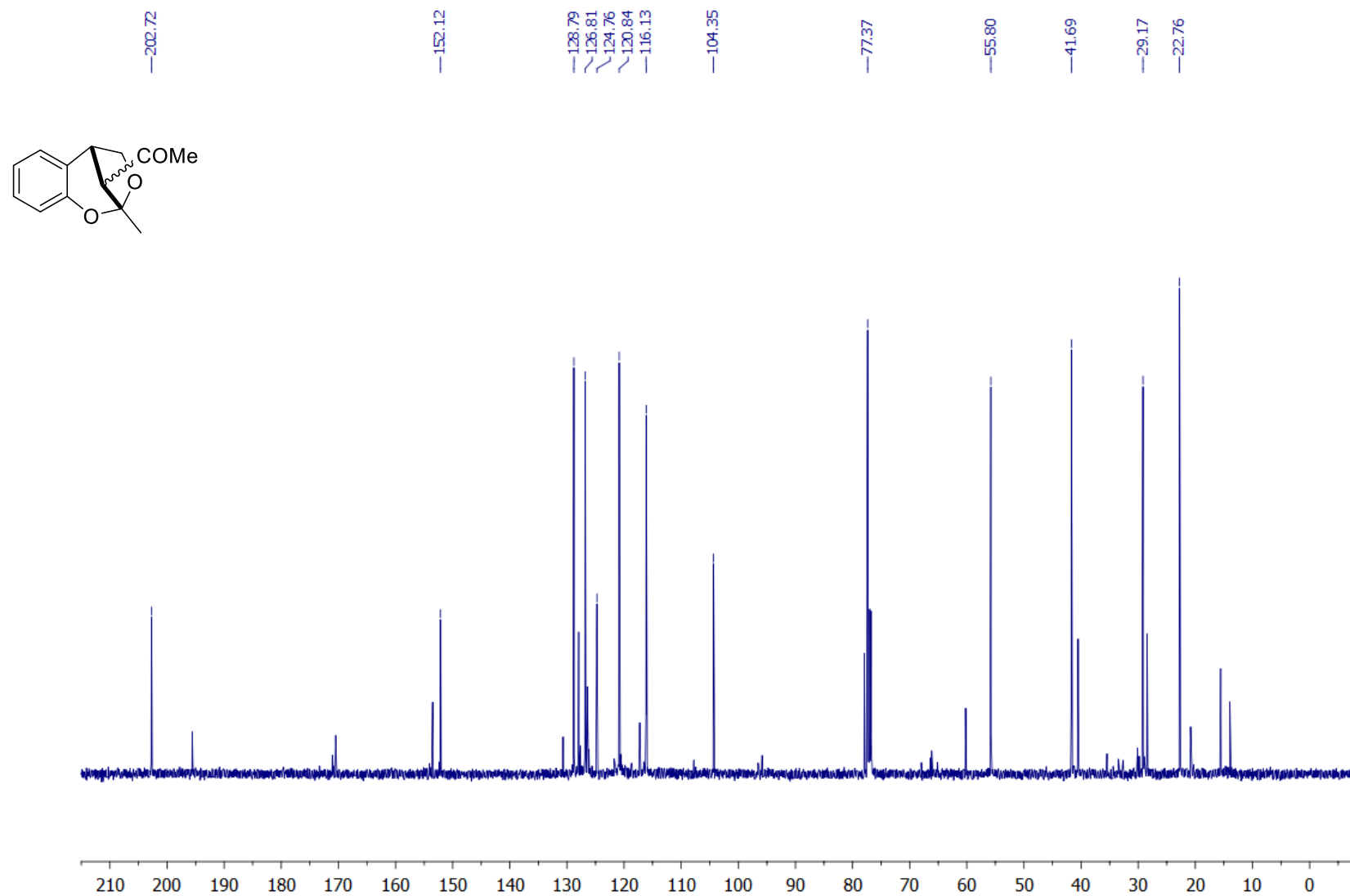
1-(9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-12-yl)ethanone (3a), major isomer

¹H NMR (CDCl₃, 600 MHz)



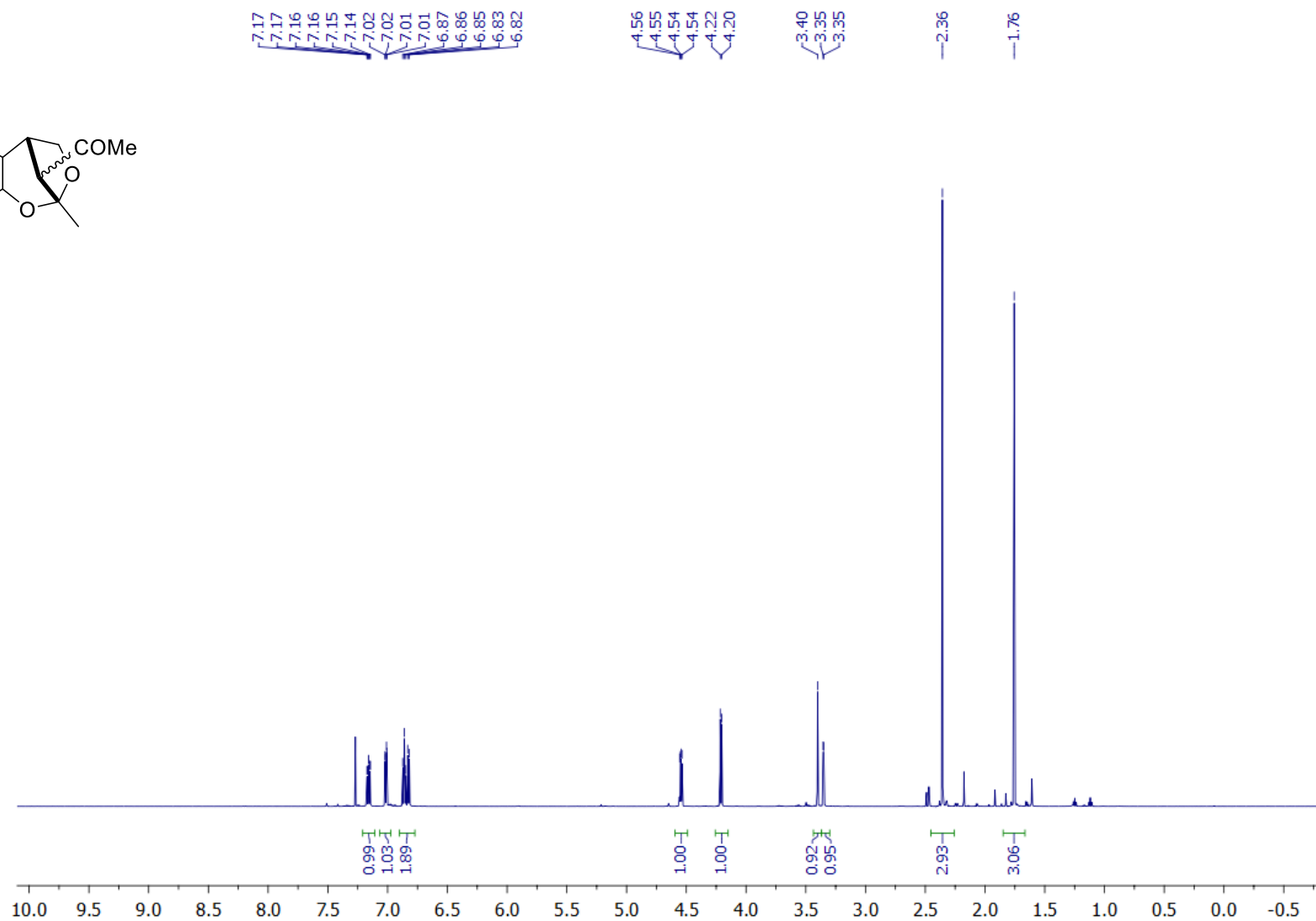
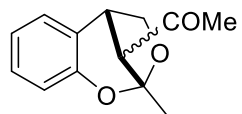
1-(9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-12-yl)ethanone (3a), major isomer

¹³C NMR (CDCl₃, 150 MHz)



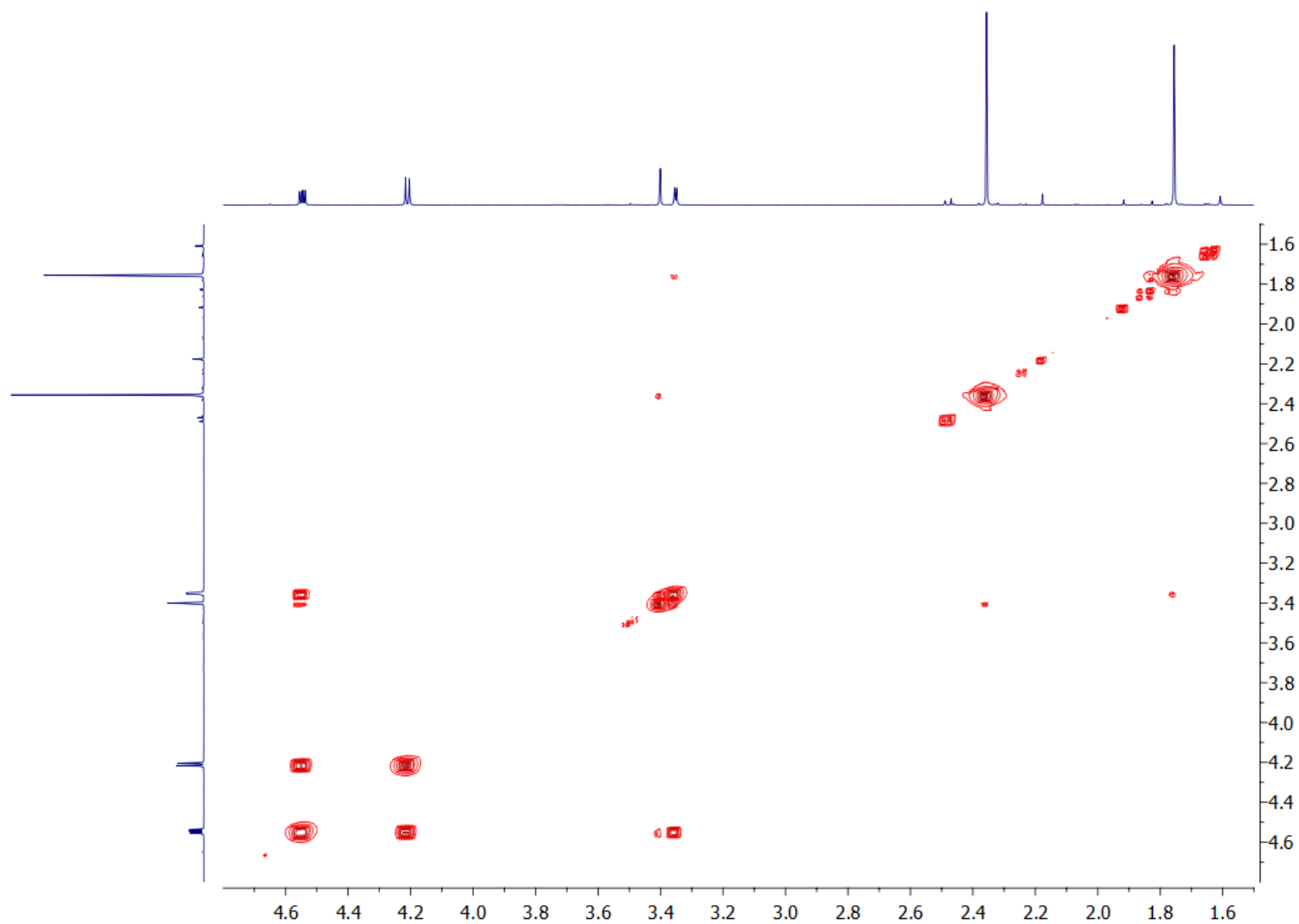
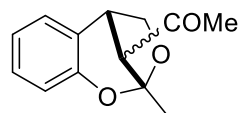
1-(9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-12-yl)ethanone (3a), minor isomer

¹H NMR (CDCl₃, 600 MHz)



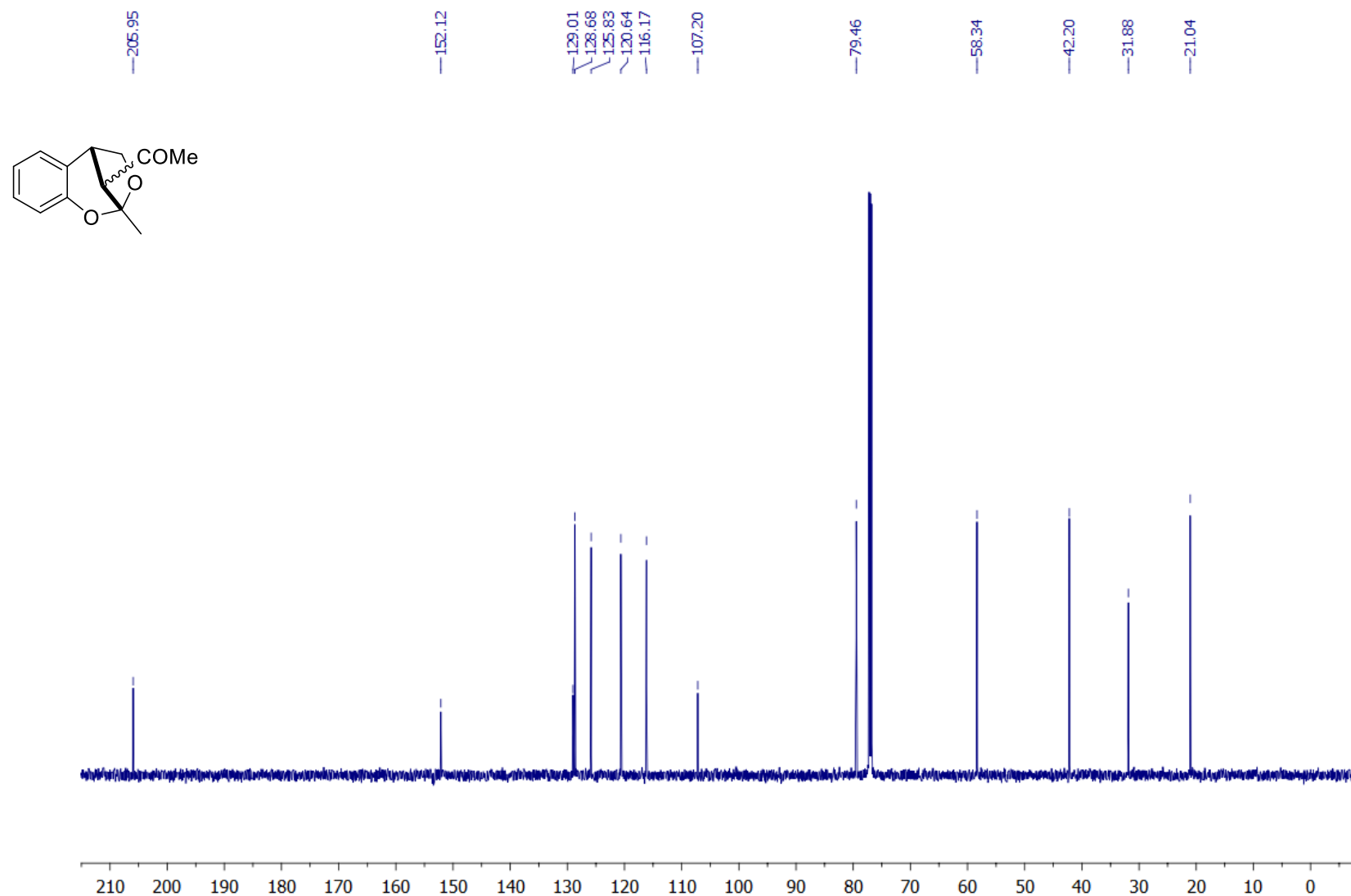
1-(9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-12-yl)ethanone (3a), minor isomer

¹H-¹H COSY (CDCl₃)



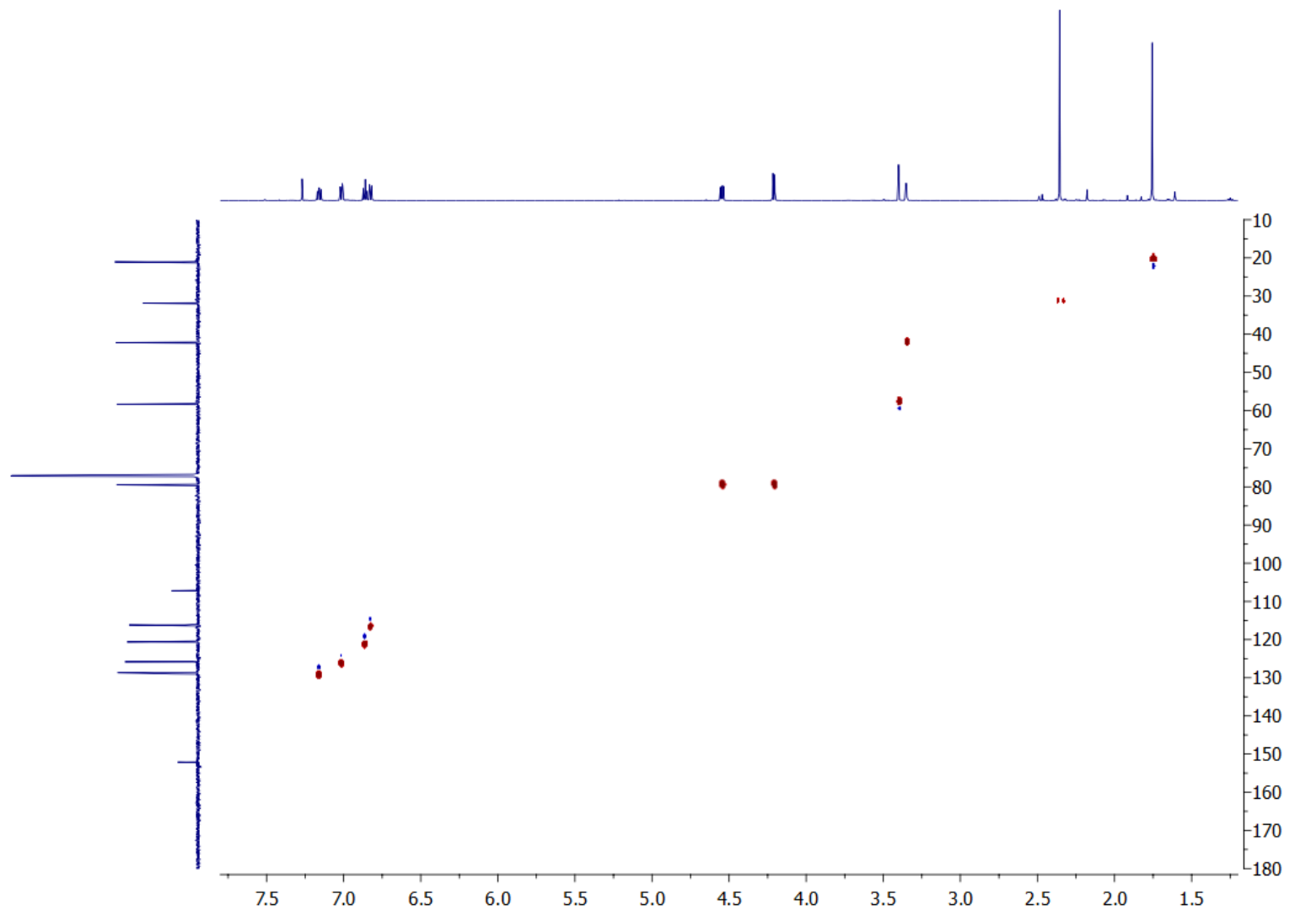
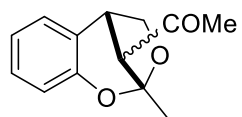
1-(9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-12-yl)ethanone (3a), minor isomer

¹³C NMR (CDCl₃, 150 MHz)



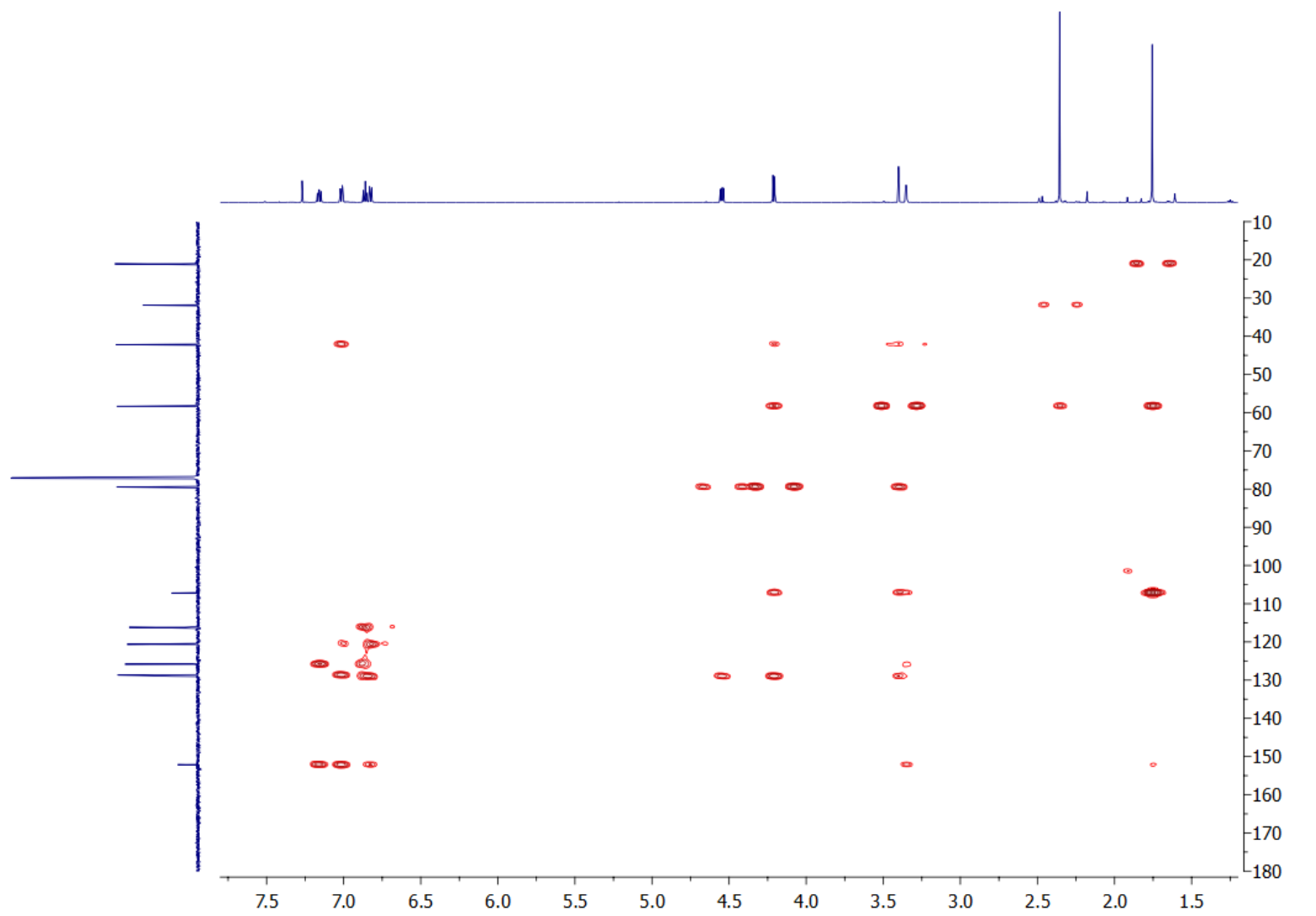
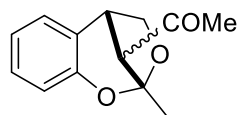
1-(9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-12-yl)ethanone (3a), minor isomer

¹H-¹³C HSQC (CDCl₃)



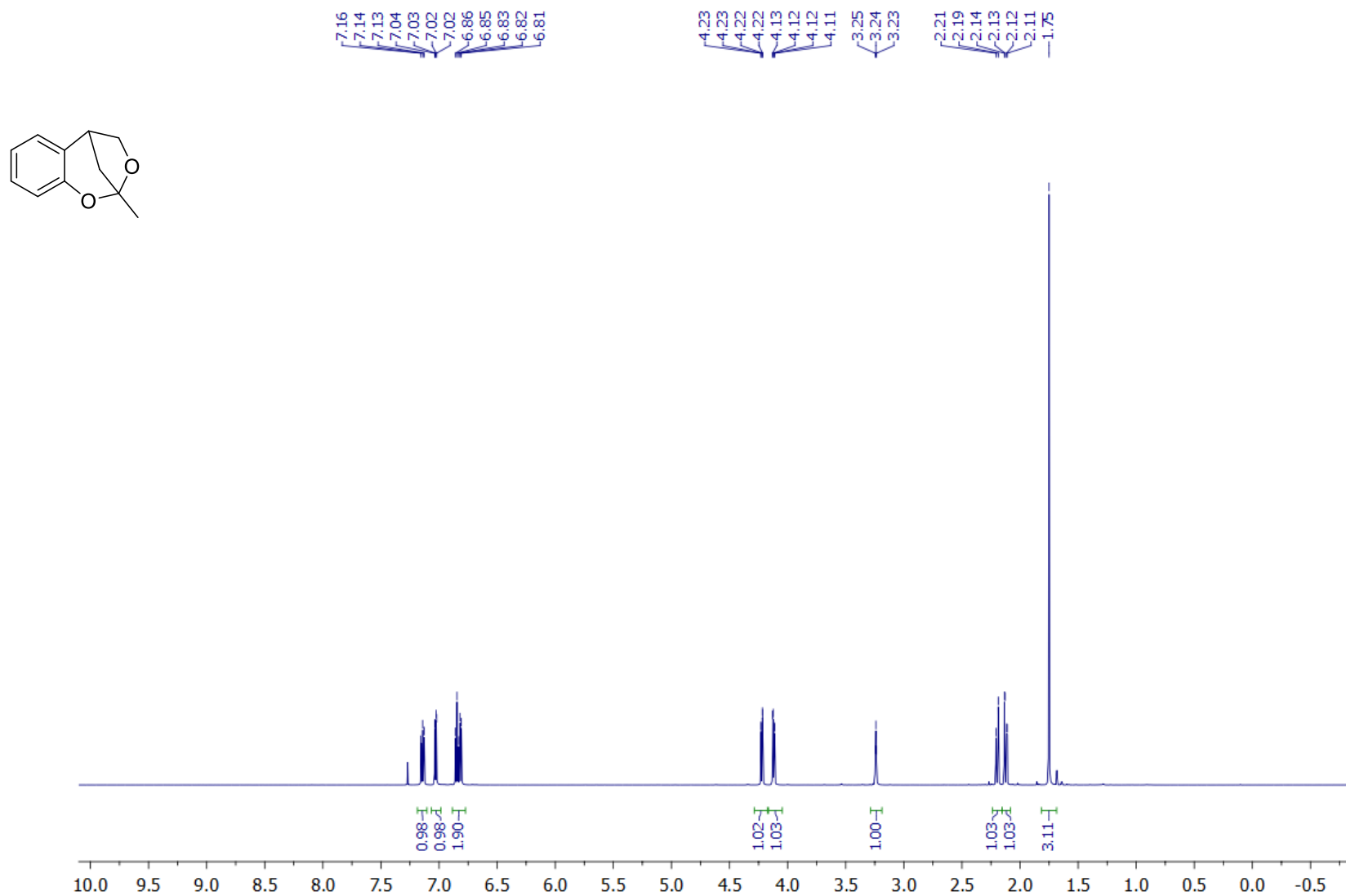
1-(9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-12-yl)ethanone (3a), minor isomer

¹H-¹³C HMBC (CDCl₃)



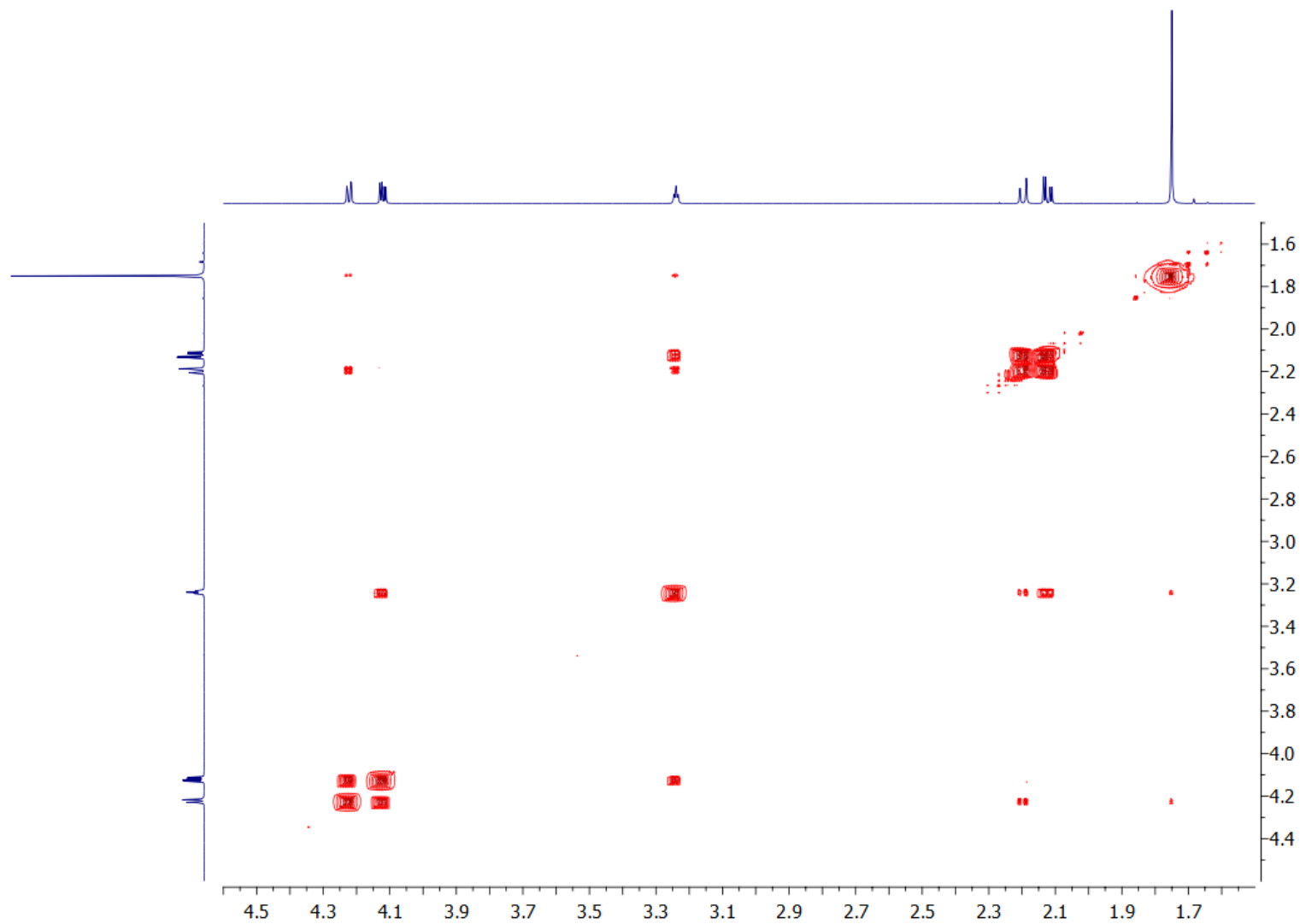
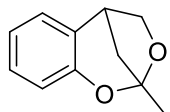
9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4a)

¹H NMR (CDCl₃, 600 MHz)



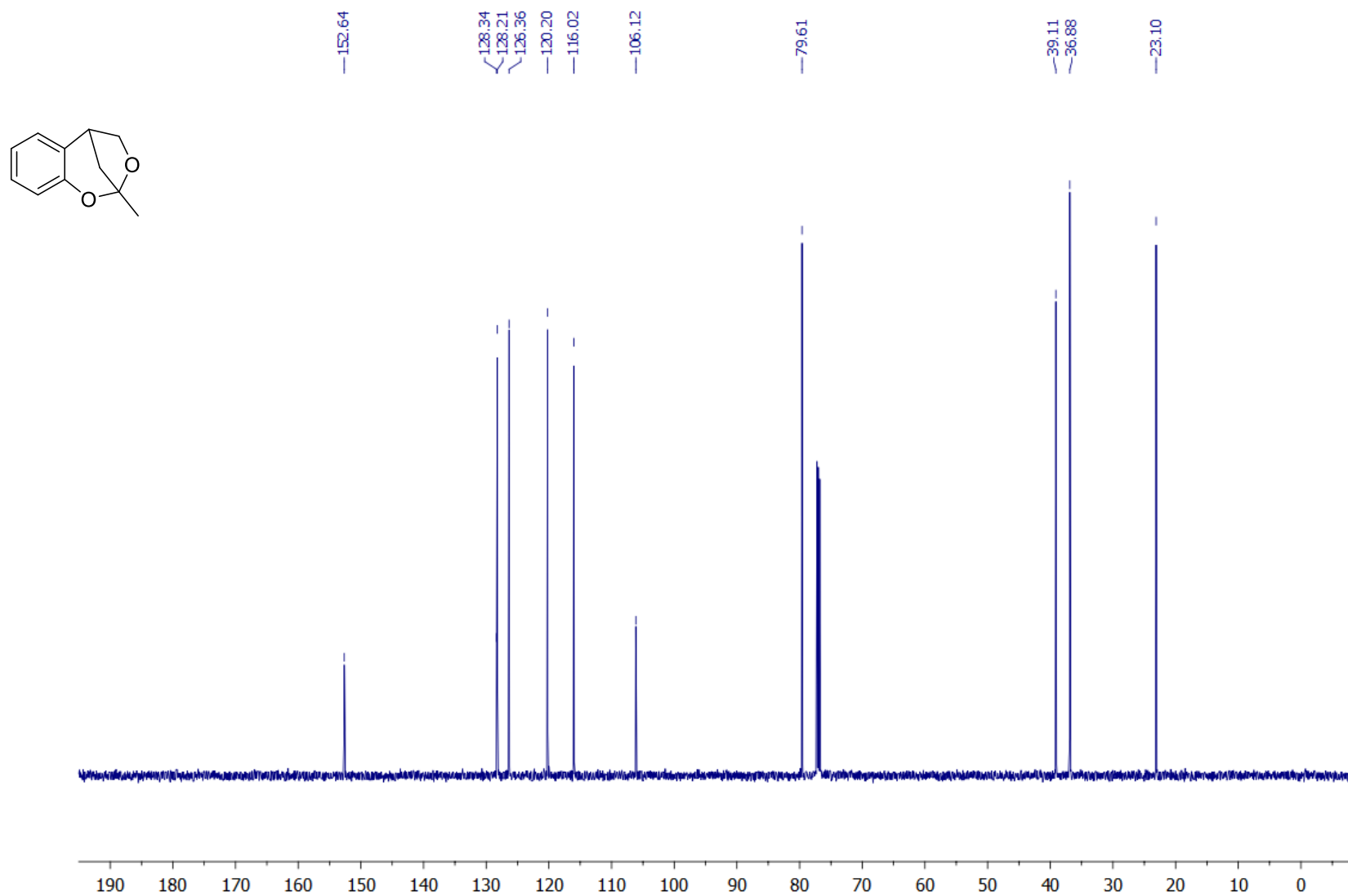
9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4a)

¹H-¹H COSY (CDCl₃)



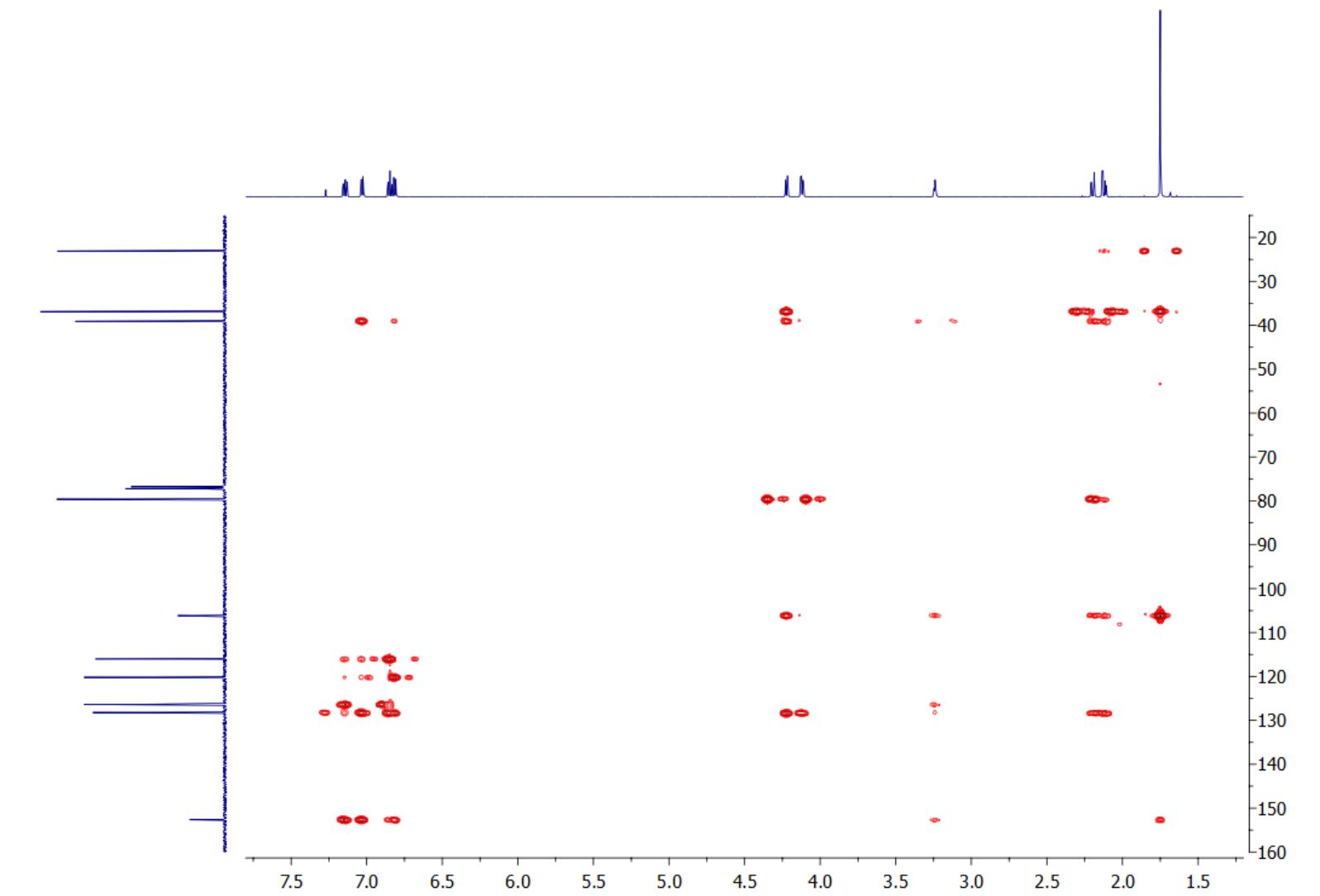
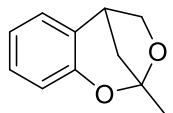
9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4a)

¹³C NMR (CDCl₃, 150 MHz)



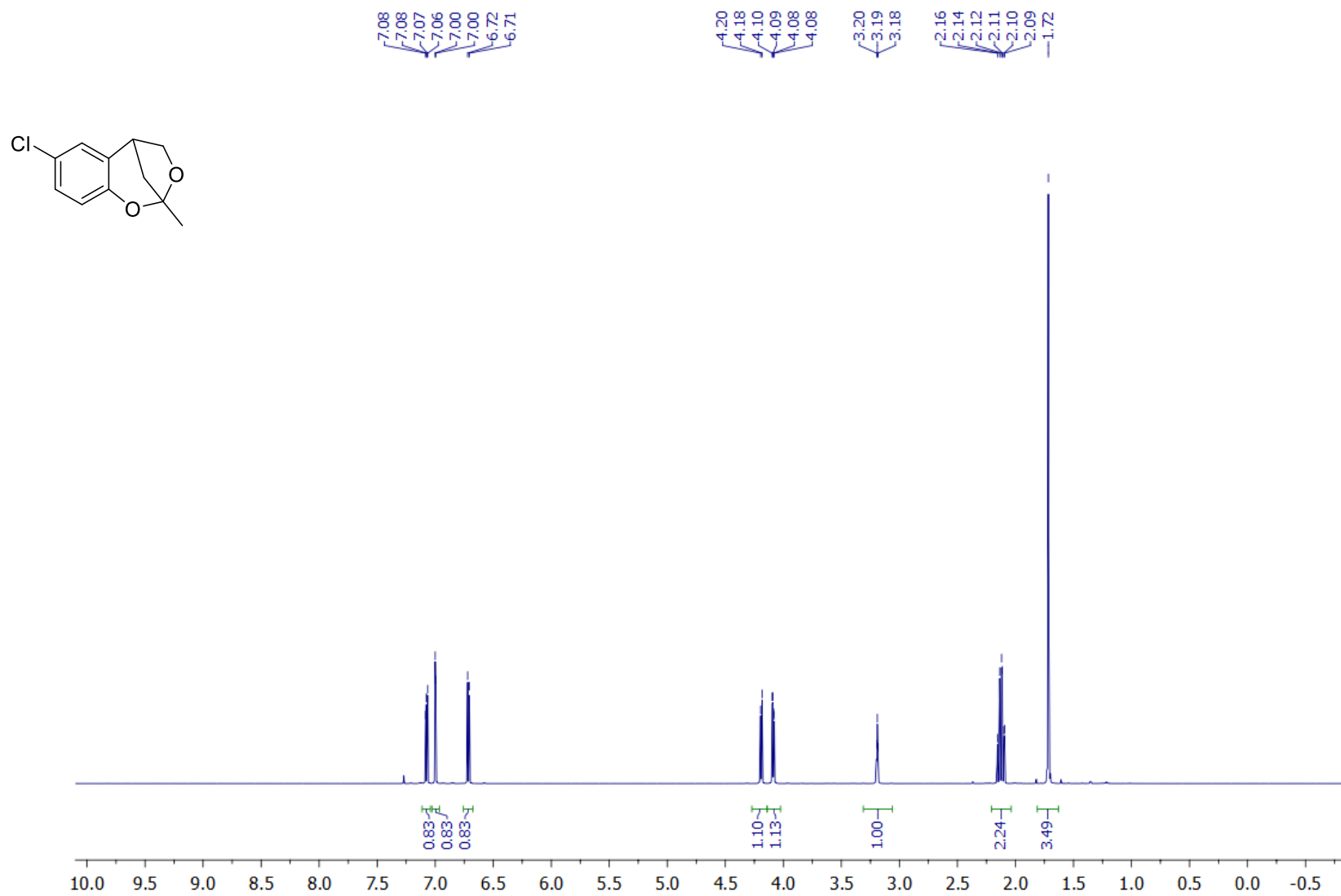
9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4a)

¹H-¹³C HMBC (CDCl₃)



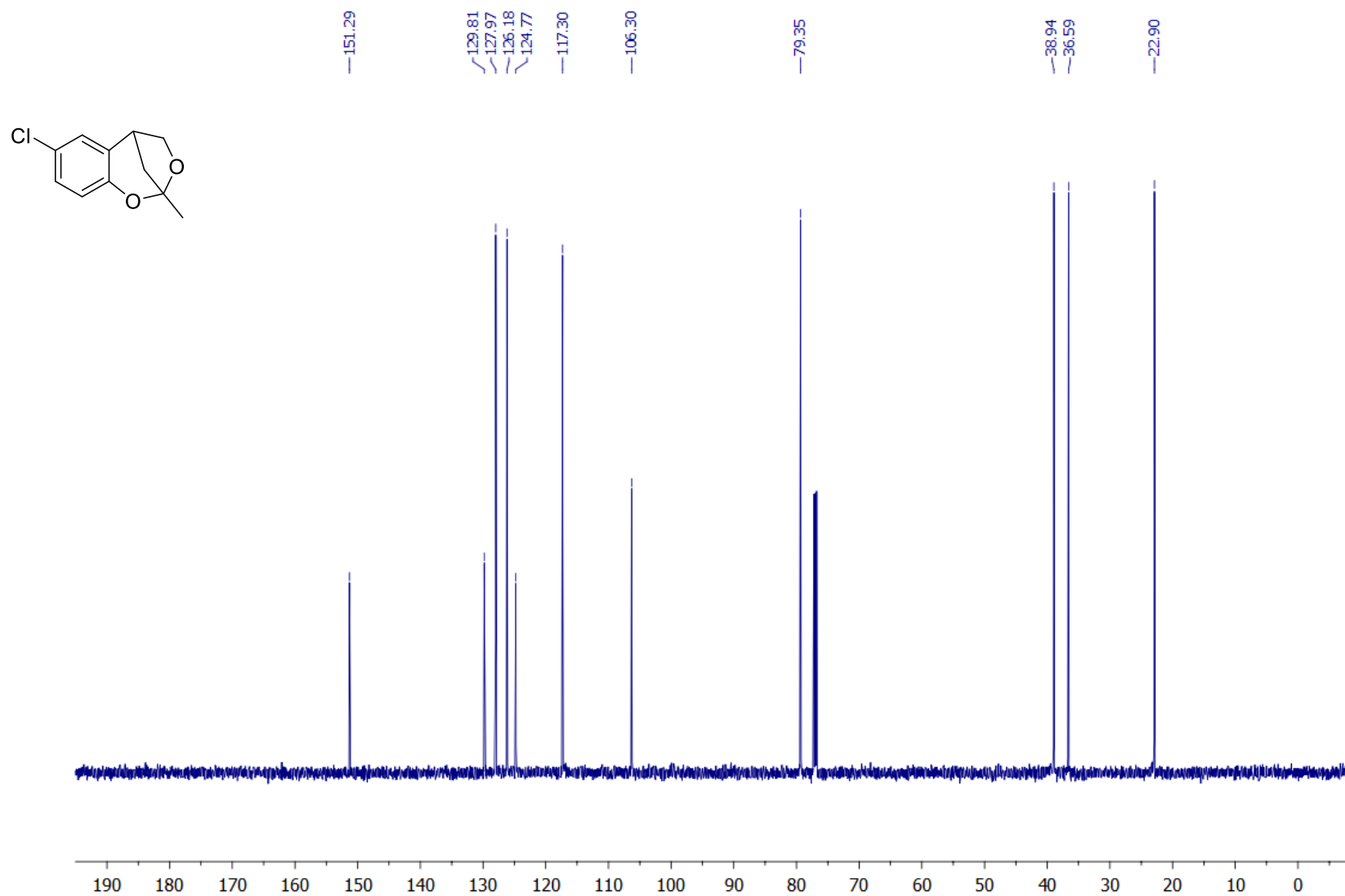
4-Chloro-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4b)

¹H NMR (CDCl₃, 600 MHz)



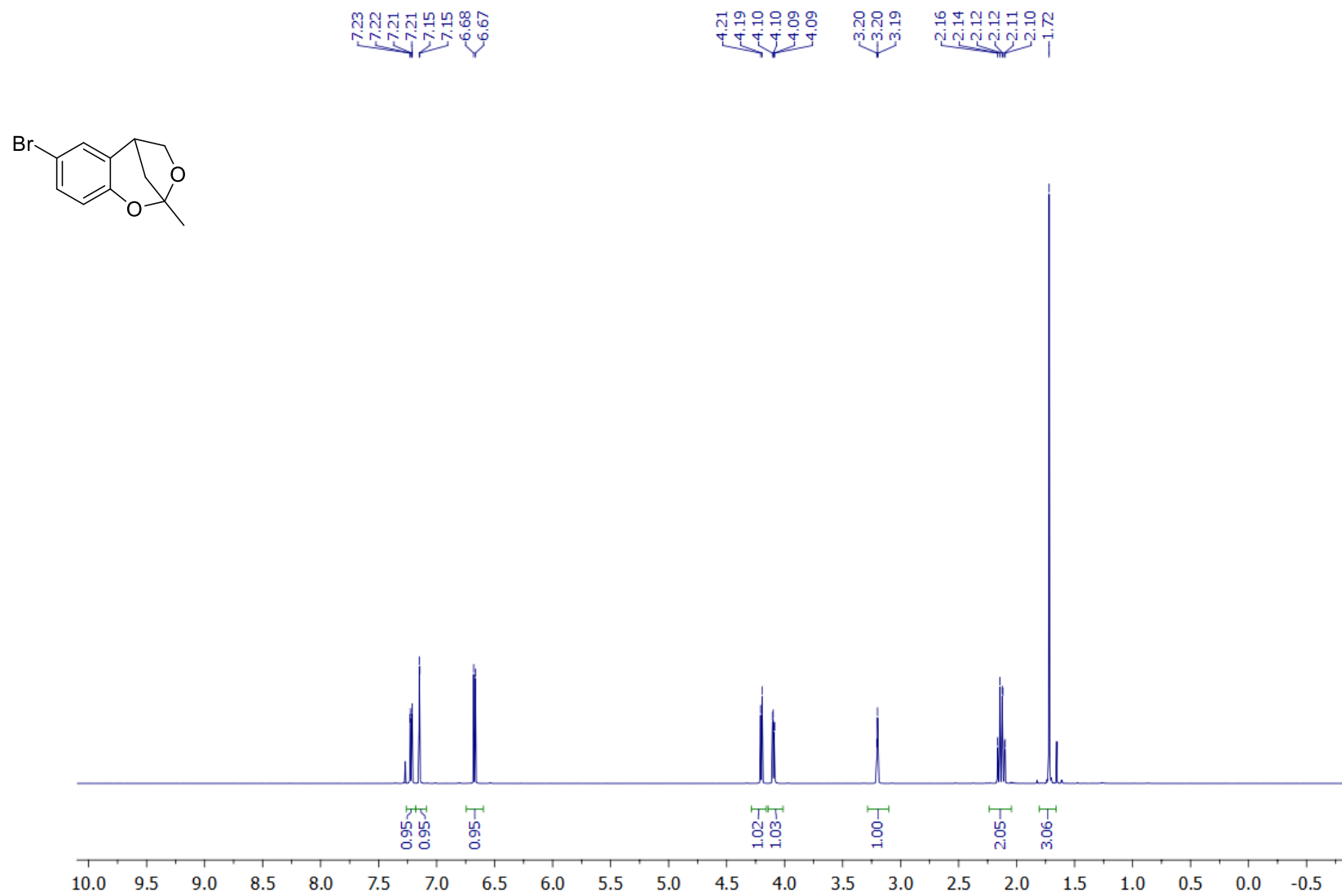
4-Chloro-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4b)

¹³C NMR (CDCl₃, 150 MHz)



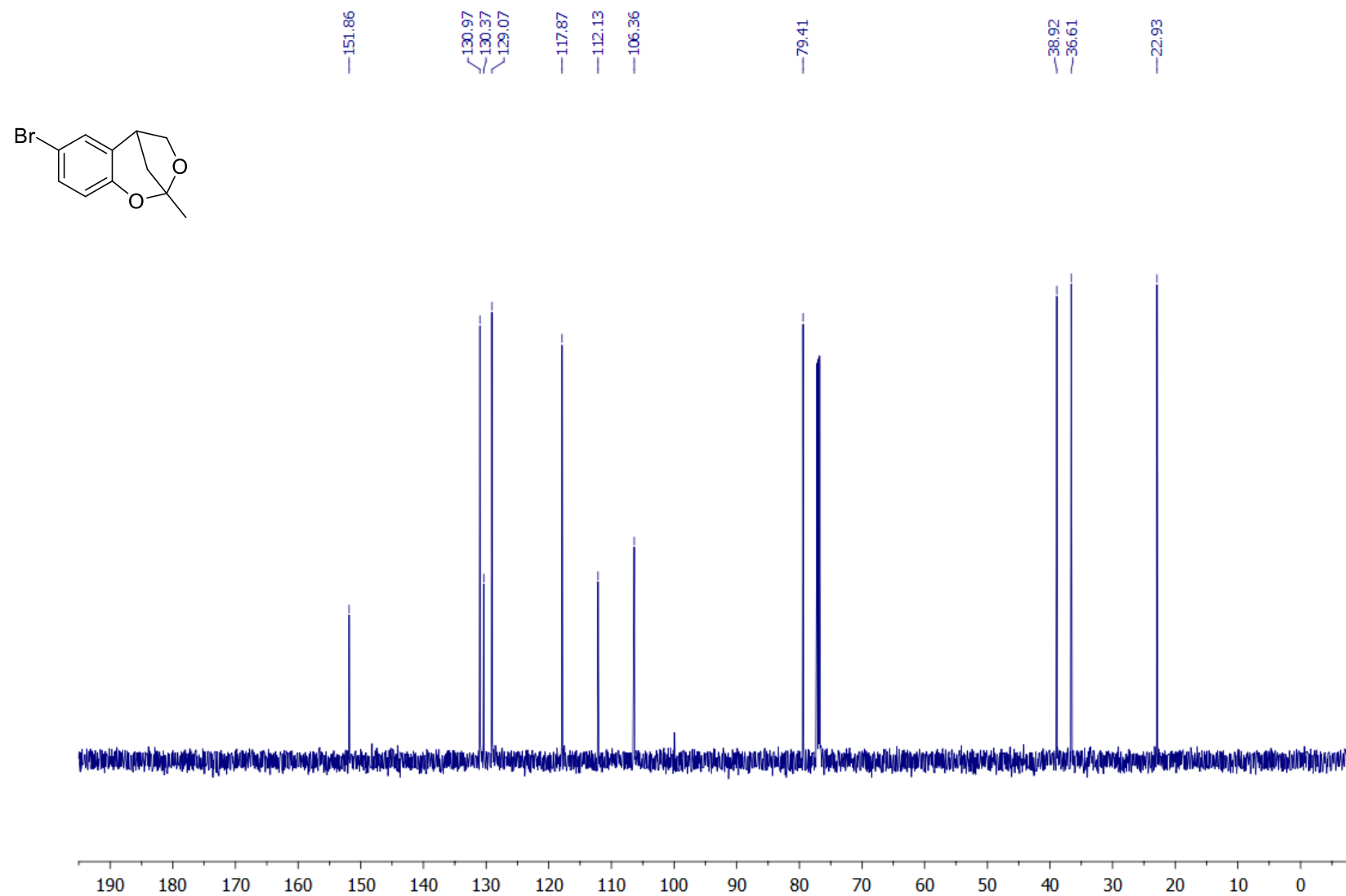
4-Bromo-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4c)

¹H NMR (CDCl₃, 600 MHz)



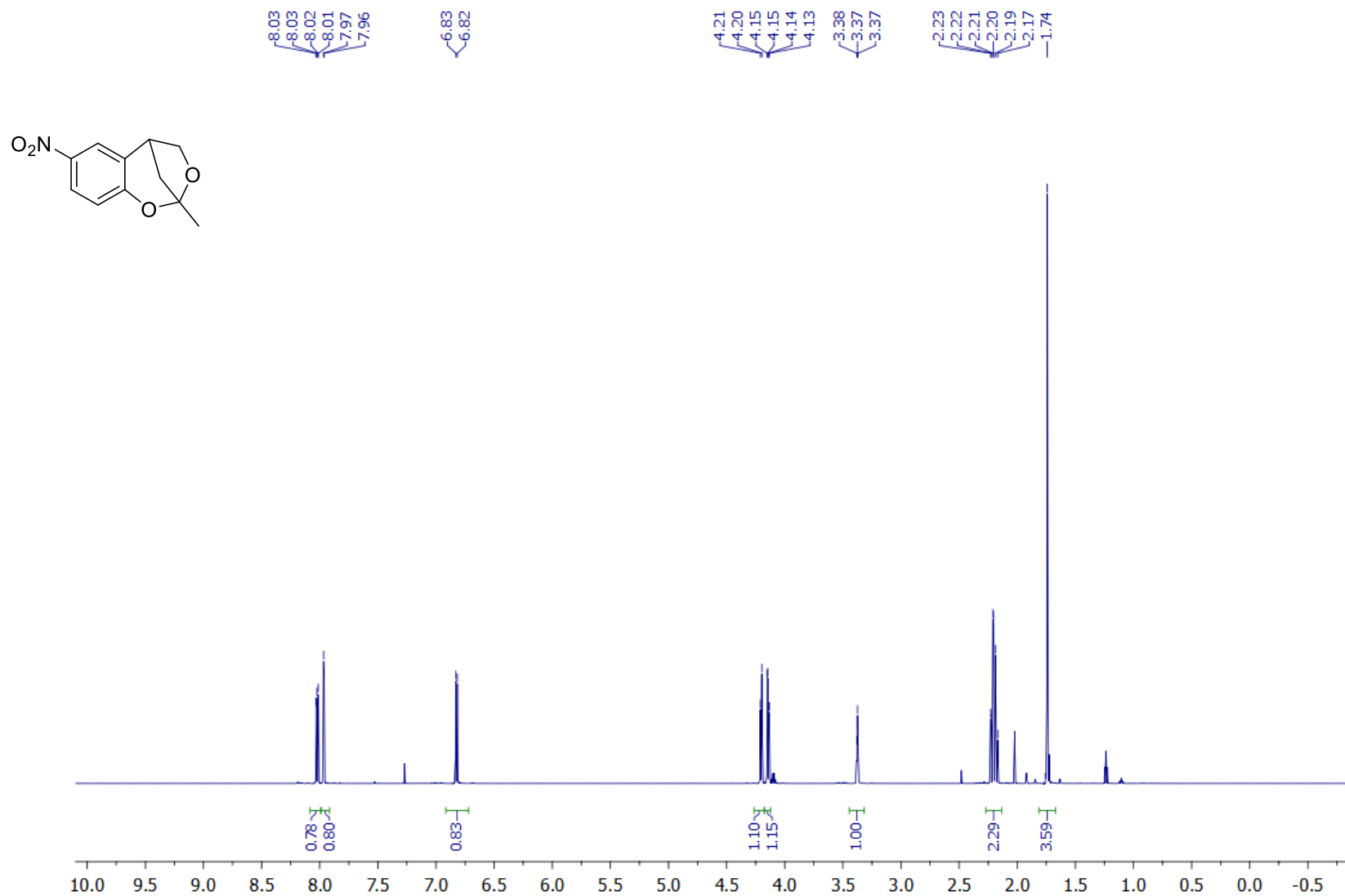
4-Bromo-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4c)

¹³C NMR (CDCl₃, 150 MHz)



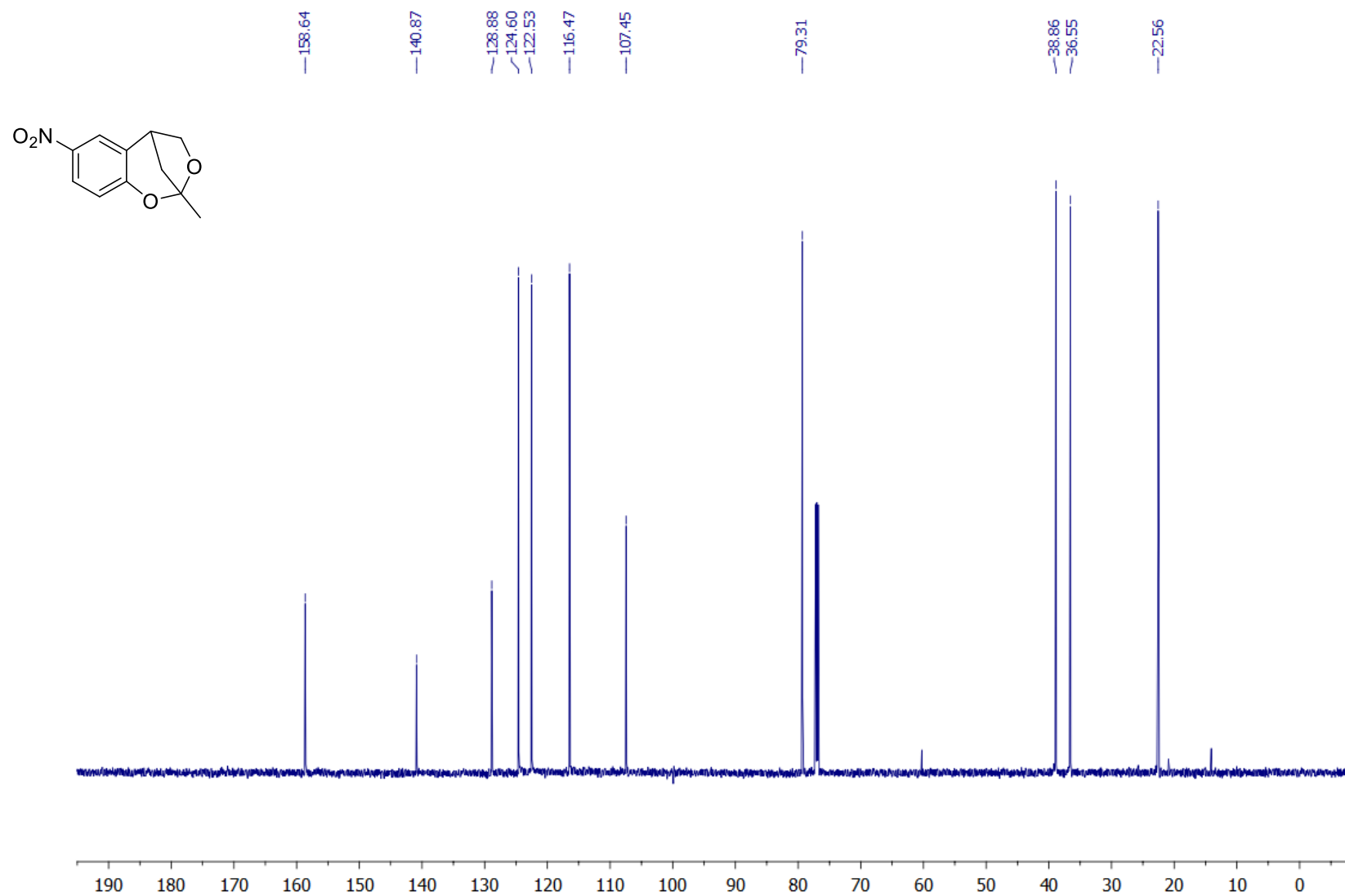
9-Methyl-4-nitro-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4d)

¹H NMR (CDCl₃, 600 MHz)



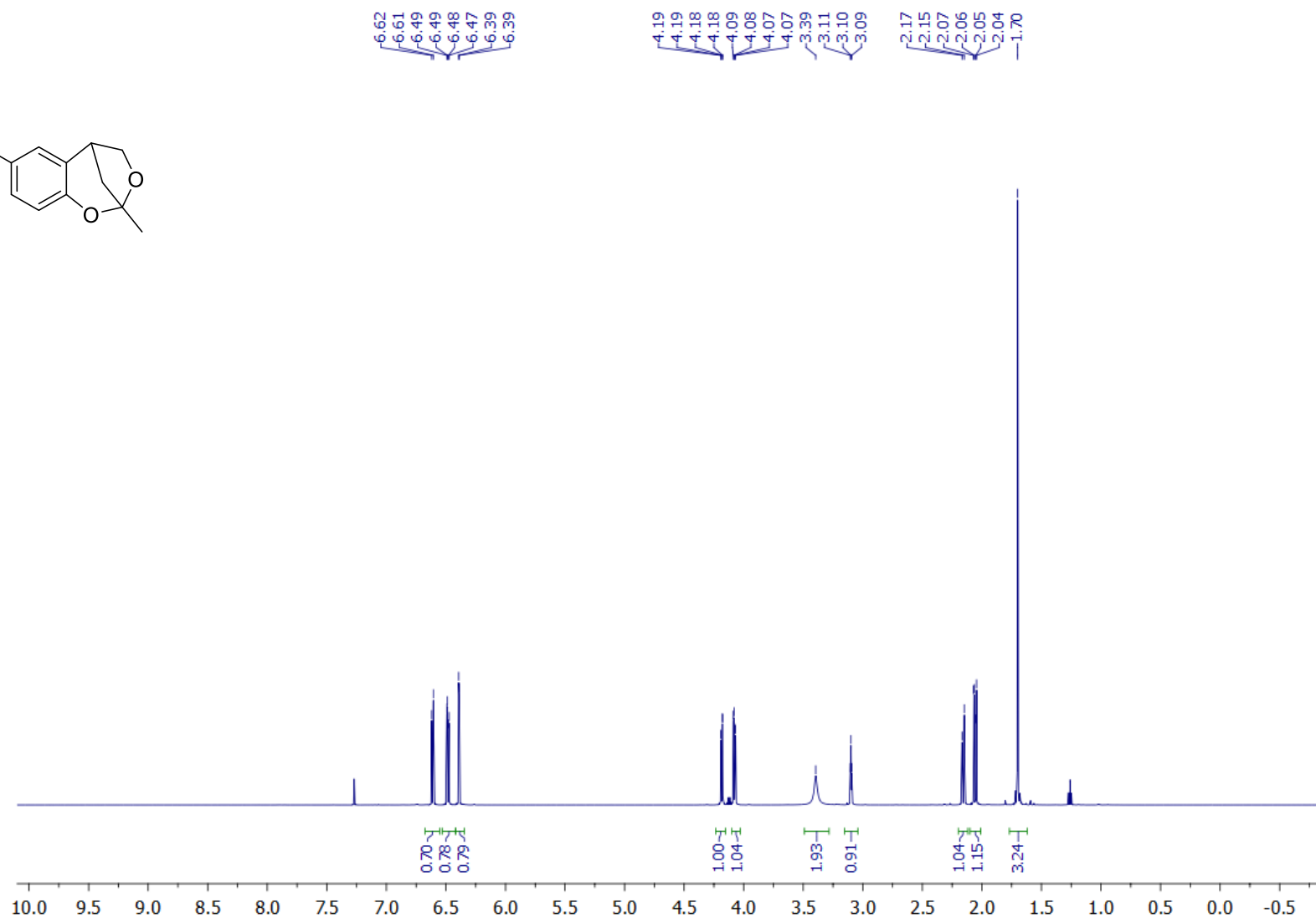
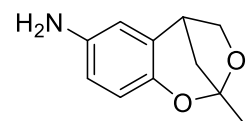
9-Methyl-4-nitro-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4d)

¹³C NMR (CDCl₃, 150 MHz)



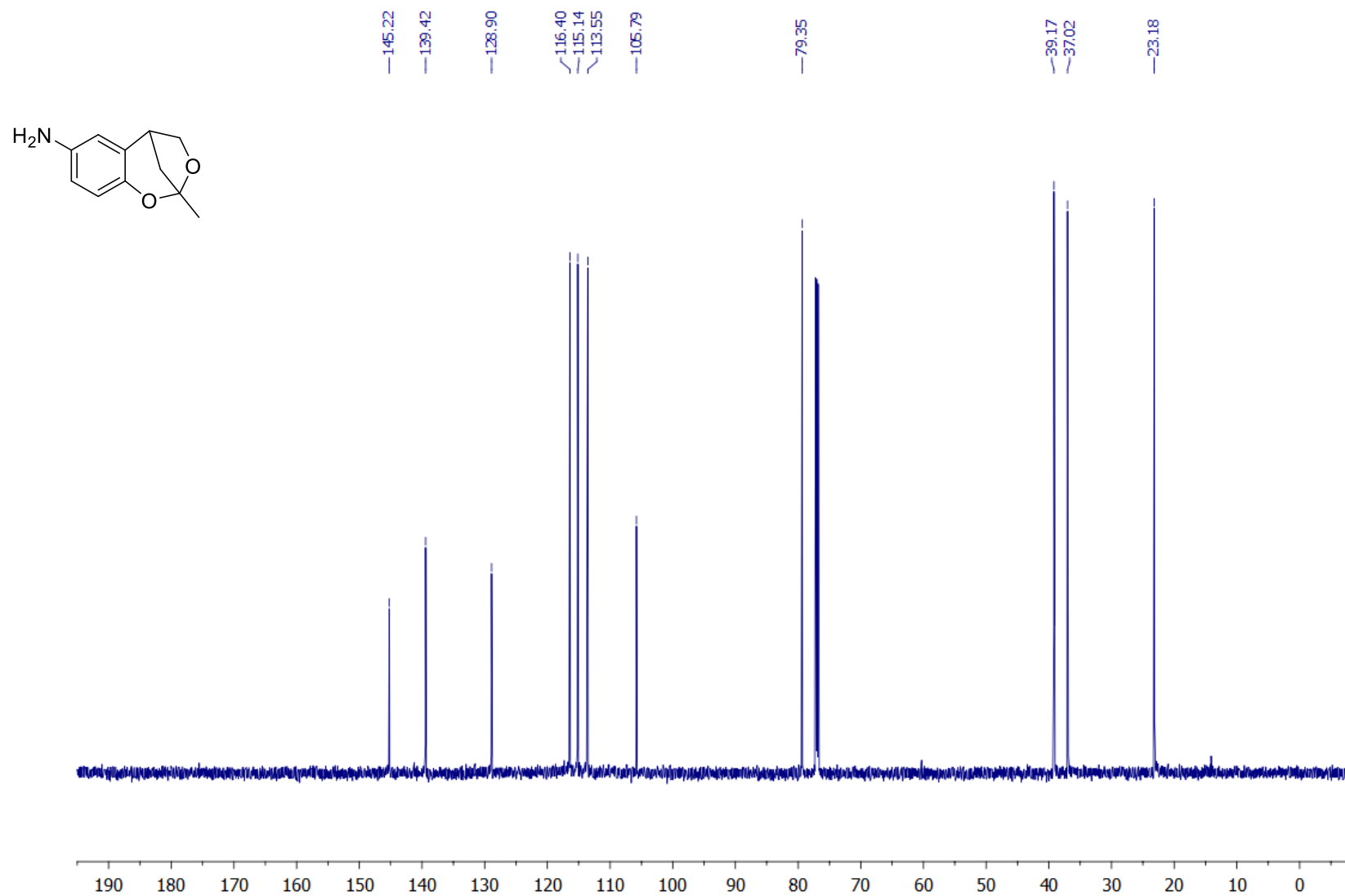
9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-4-amine (4d')

¹H NMR (CDCl₃, 600 MHz)



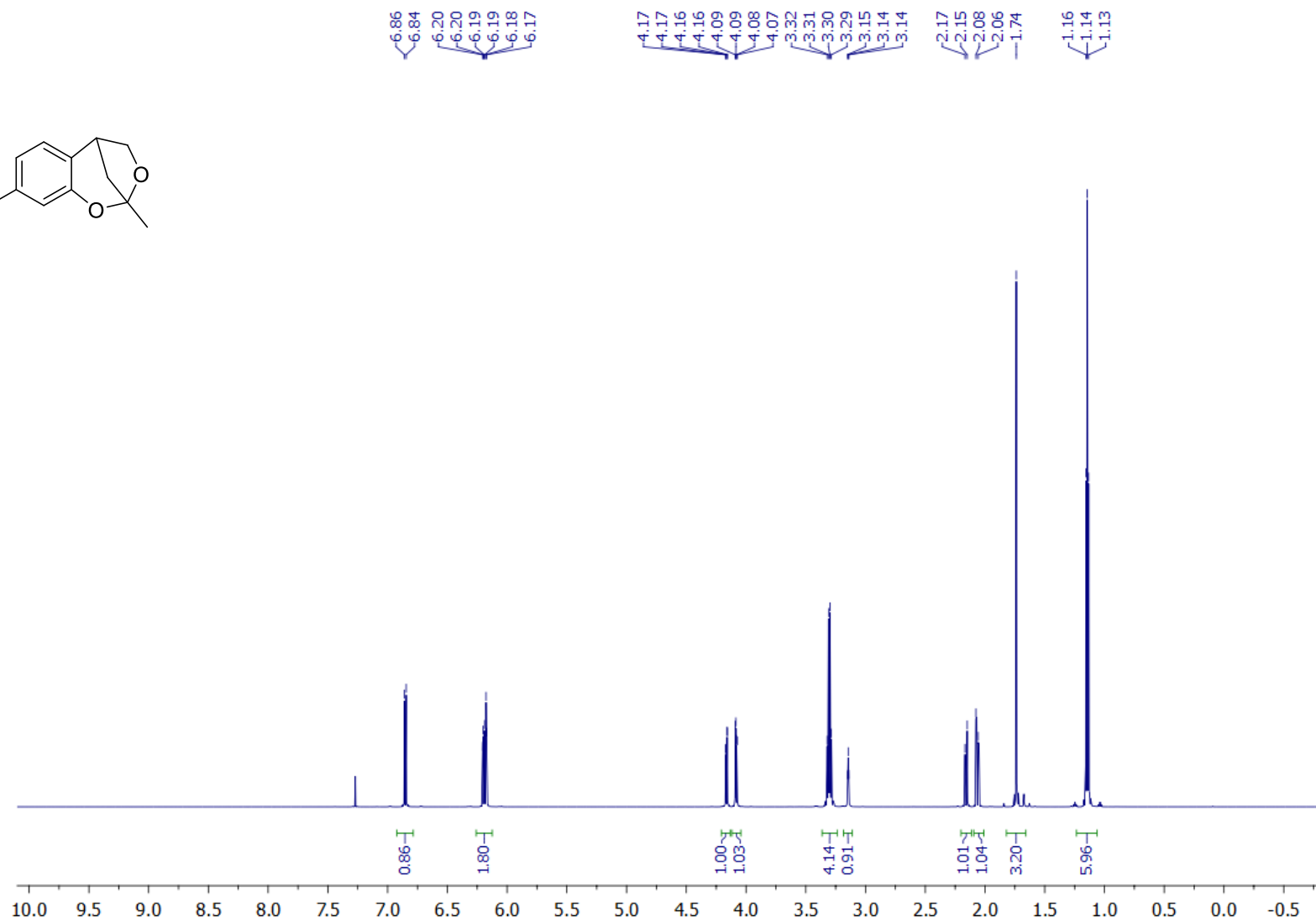
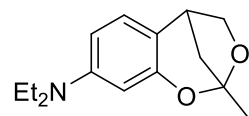
9-Methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-4-amine (4d')

¹³C NMR (CDCl₃, 150 MHz)



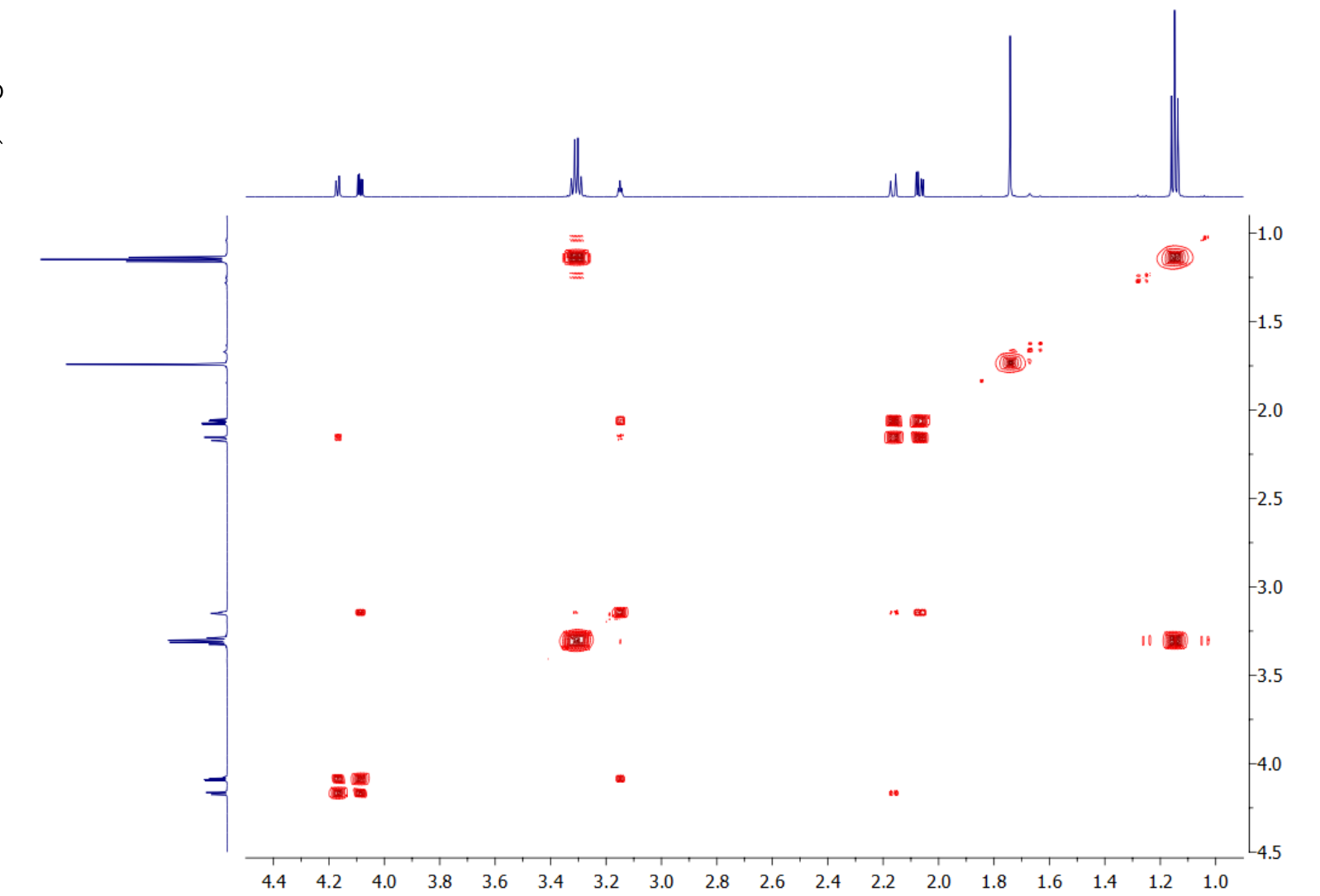
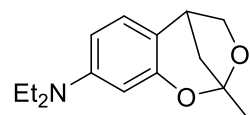
***N,N*-Diethyl-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-5-amine (4e)**

¹H NMR (CDCl₃, 600 MHz)



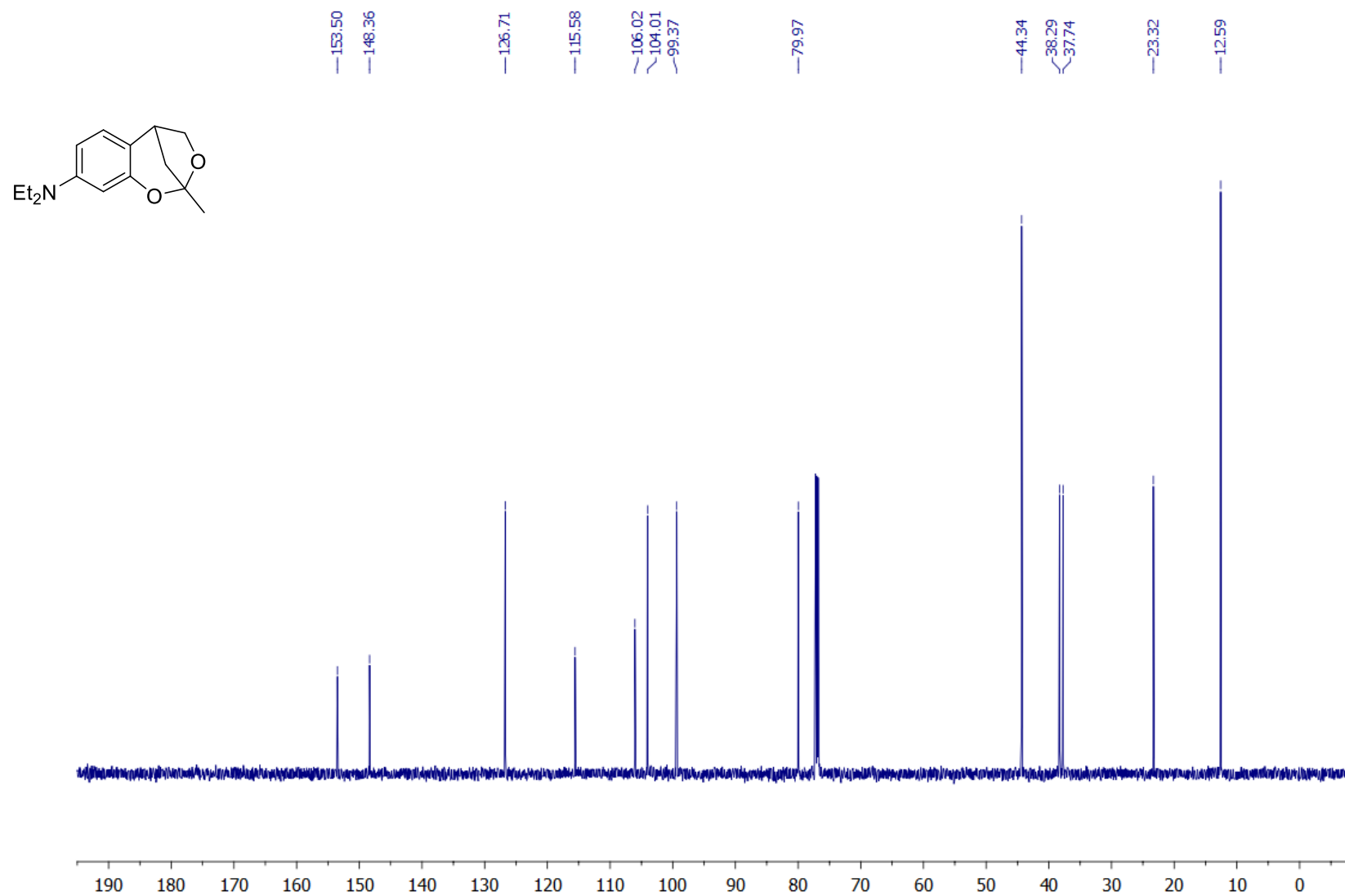
***N,N*-Diethyl-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-5-amine (4e)**

¹H-¹H COSY (CDCl₃)



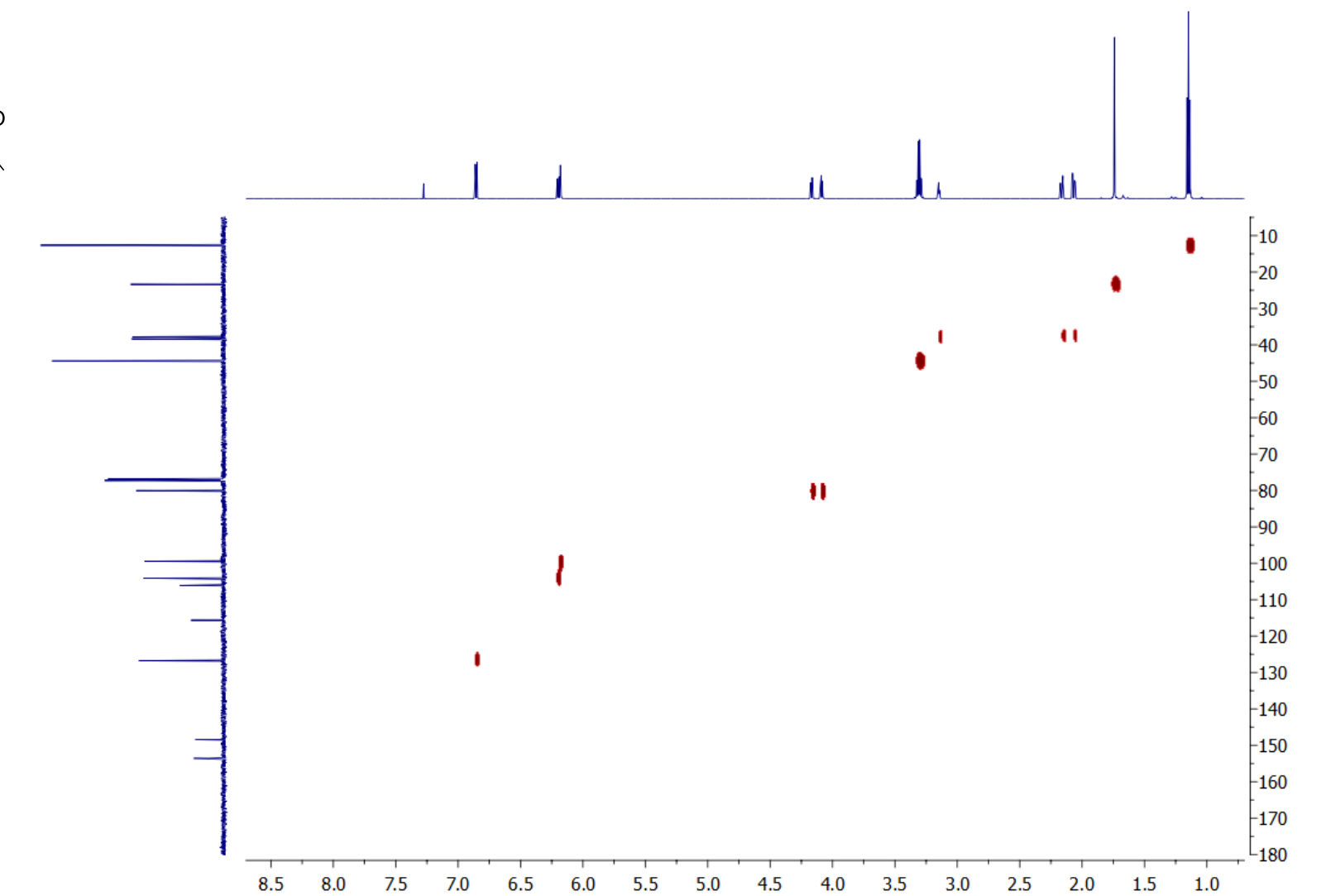
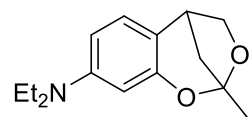
***N,N*-Diethyl-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-5-amine (4e)**

¹³C NMR (CDCl₃, 150 MHz)



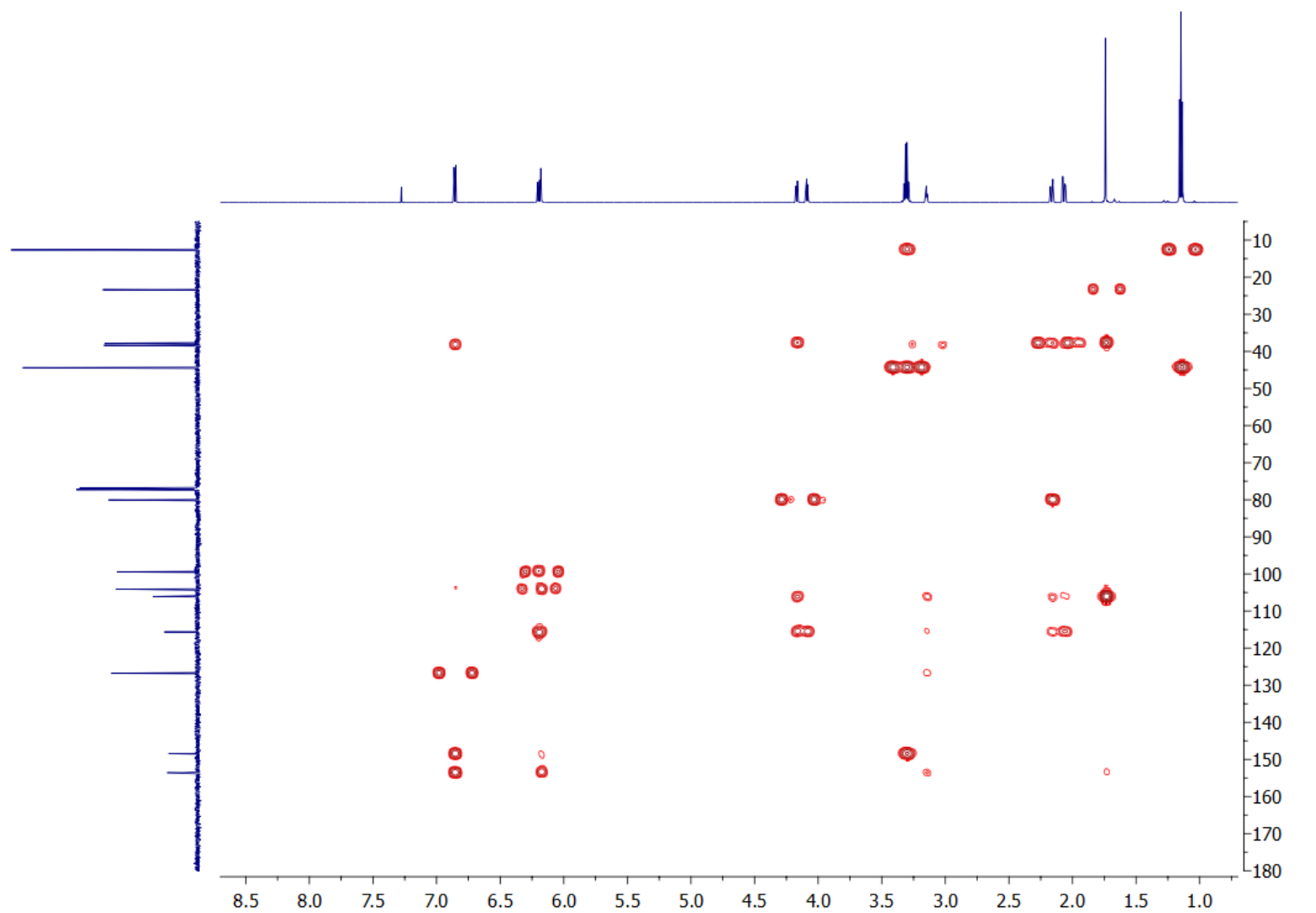
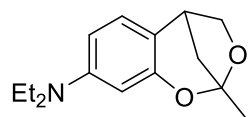
***N,N*-Diethyl-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-5-amine (4e)**

¹H-¹³C HSQC (CDCl₃)



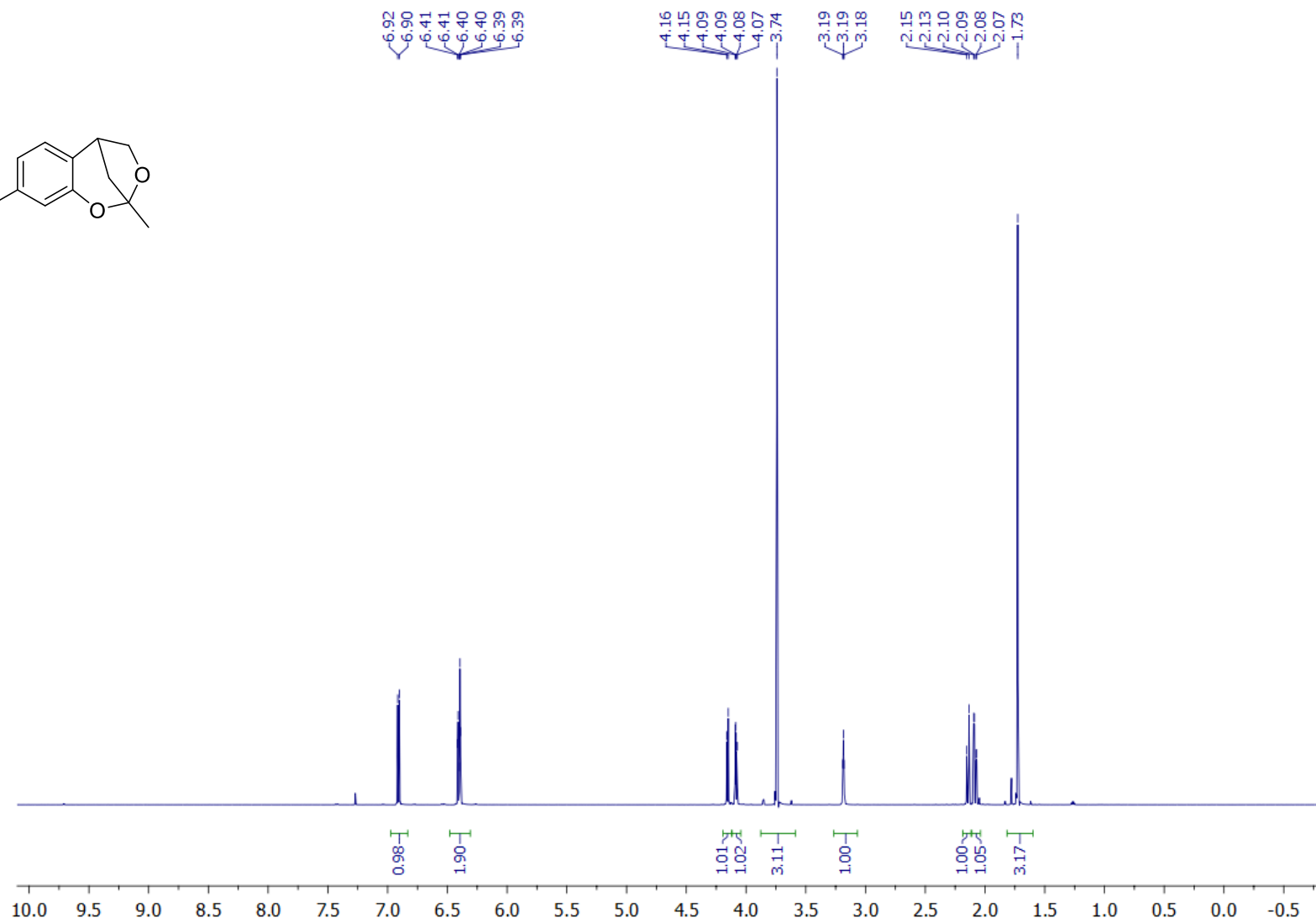
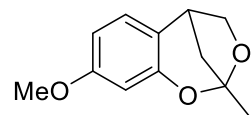
***N,N*-Diethyl-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-trien-5-amine (4e)**

¹H-¹³C HMBC (CDCl₃)



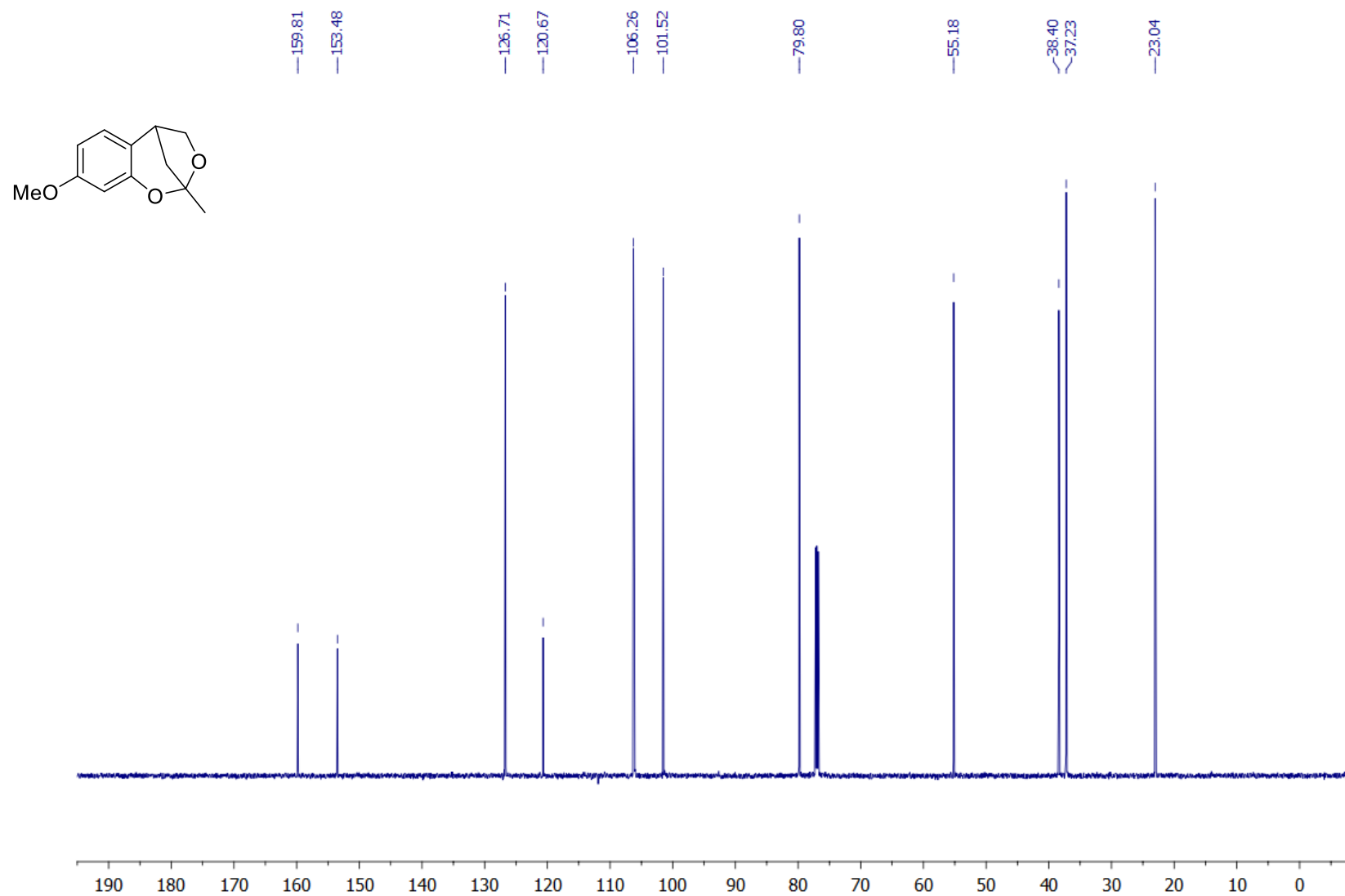
5-Methoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4f)

¹H NMR (CDCl₃, 600 MHz)



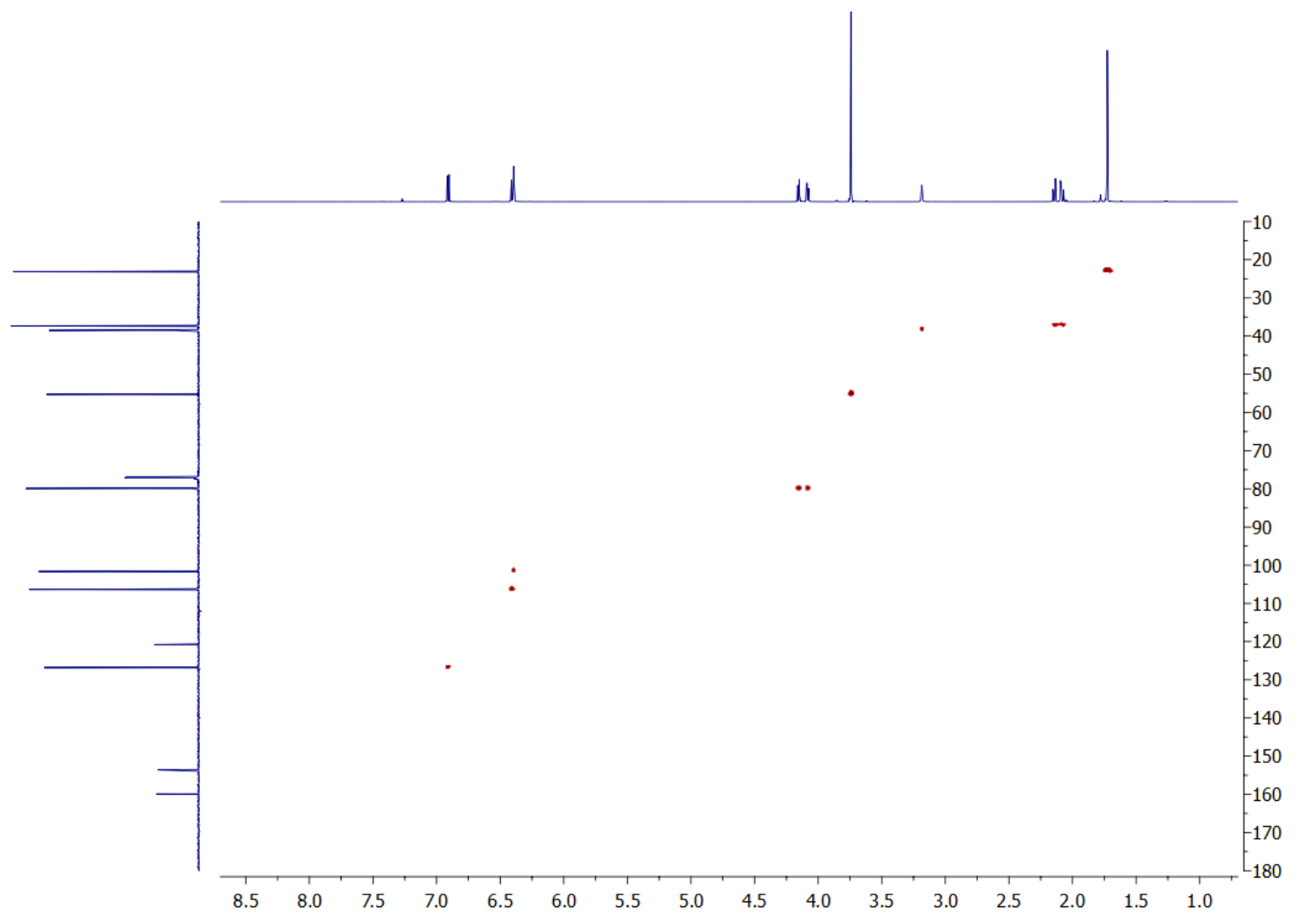
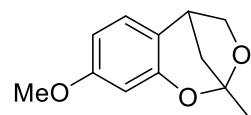
5-Methoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4f)

¹³C NMR (CDCl₃, 150 MHz)



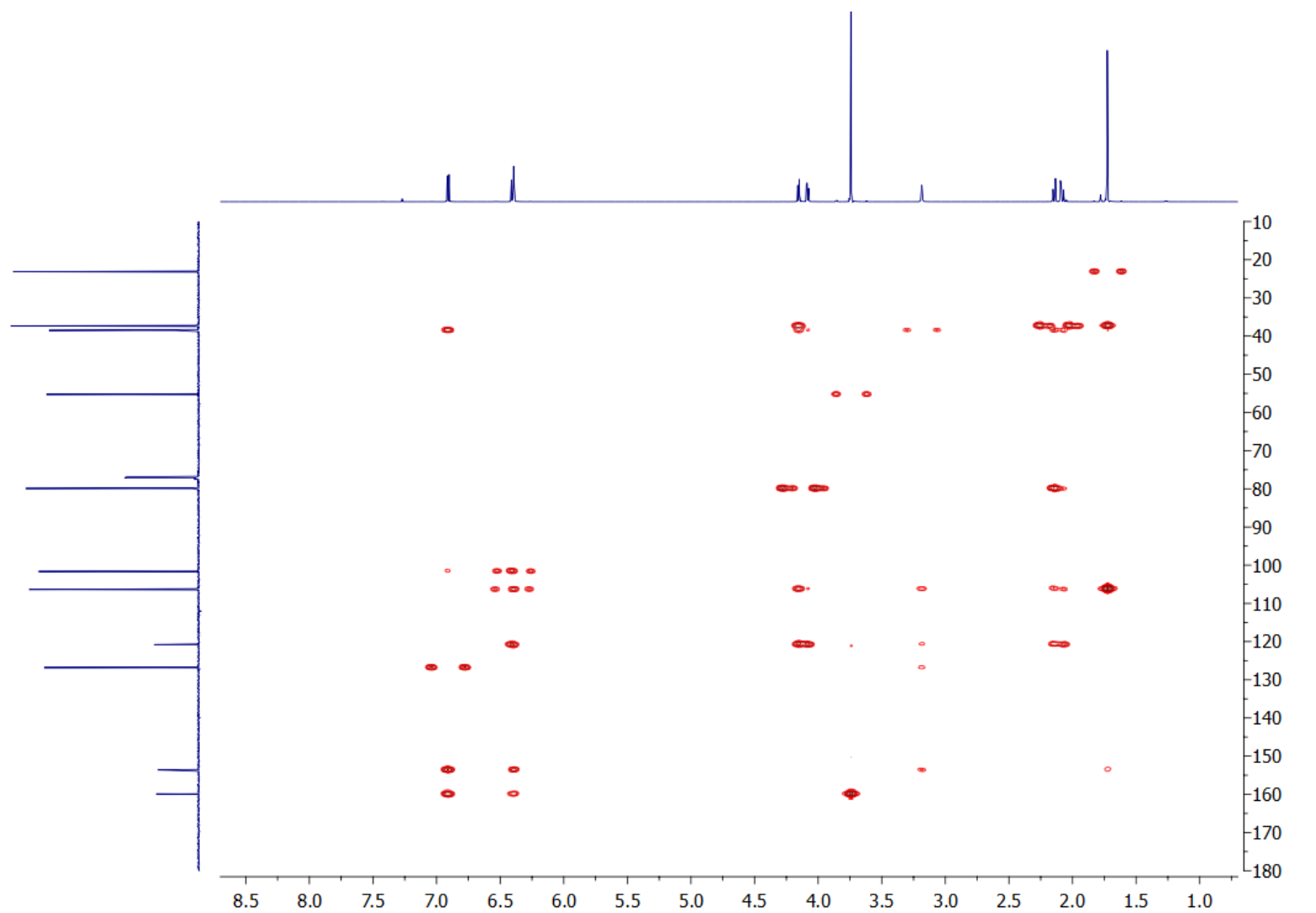
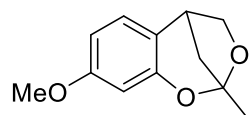
5-Methoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4f)

¹H-¹³C HSQC (CDCl₃)



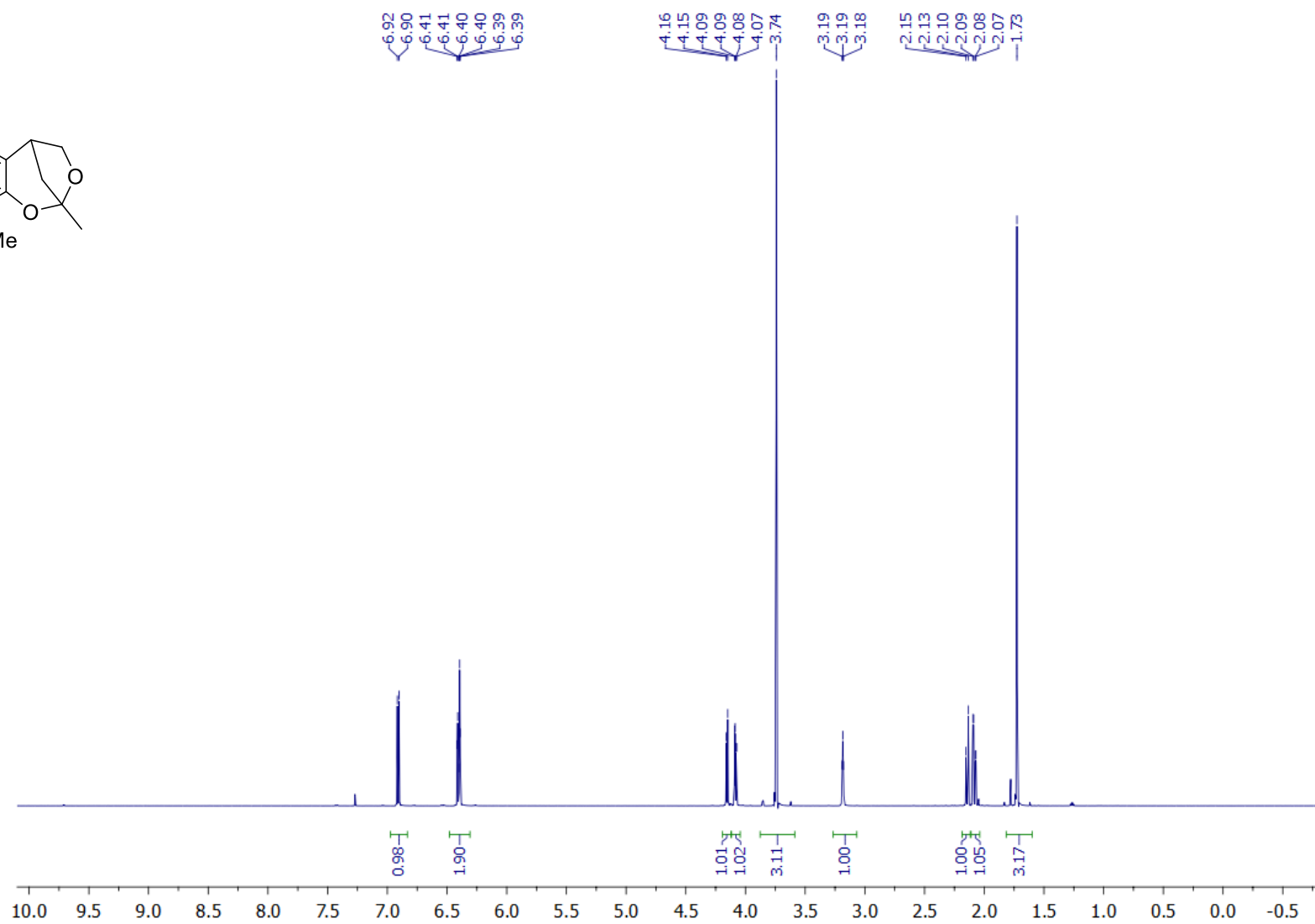
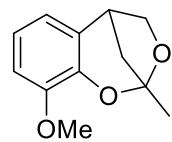
5-Methoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4f)

¹H-¹³C HMBC (CDCl₃)



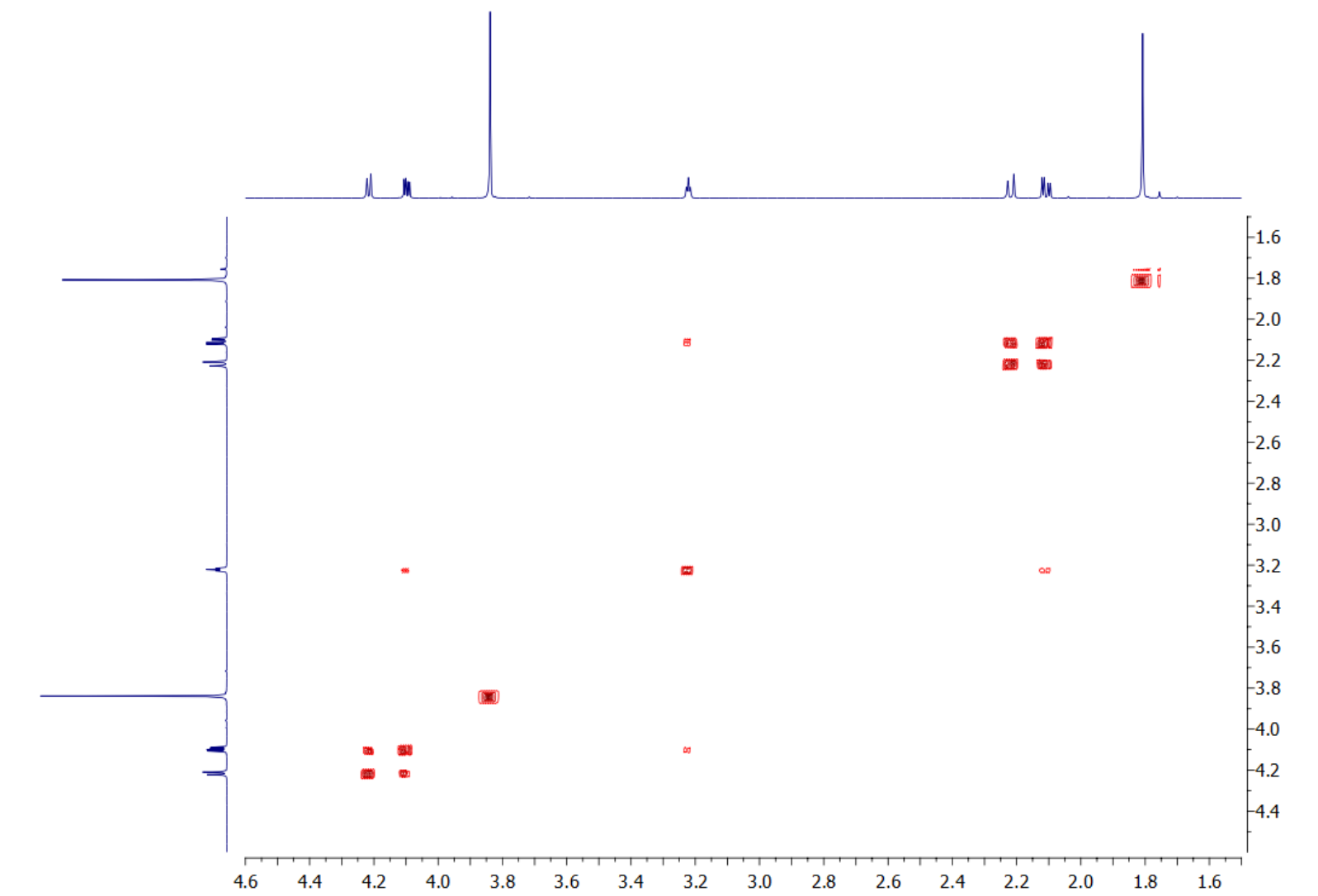
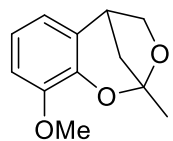
6-Methoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4g)

¹H NMR (CDCl₃, 600 MHz)



6-Methoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4g)

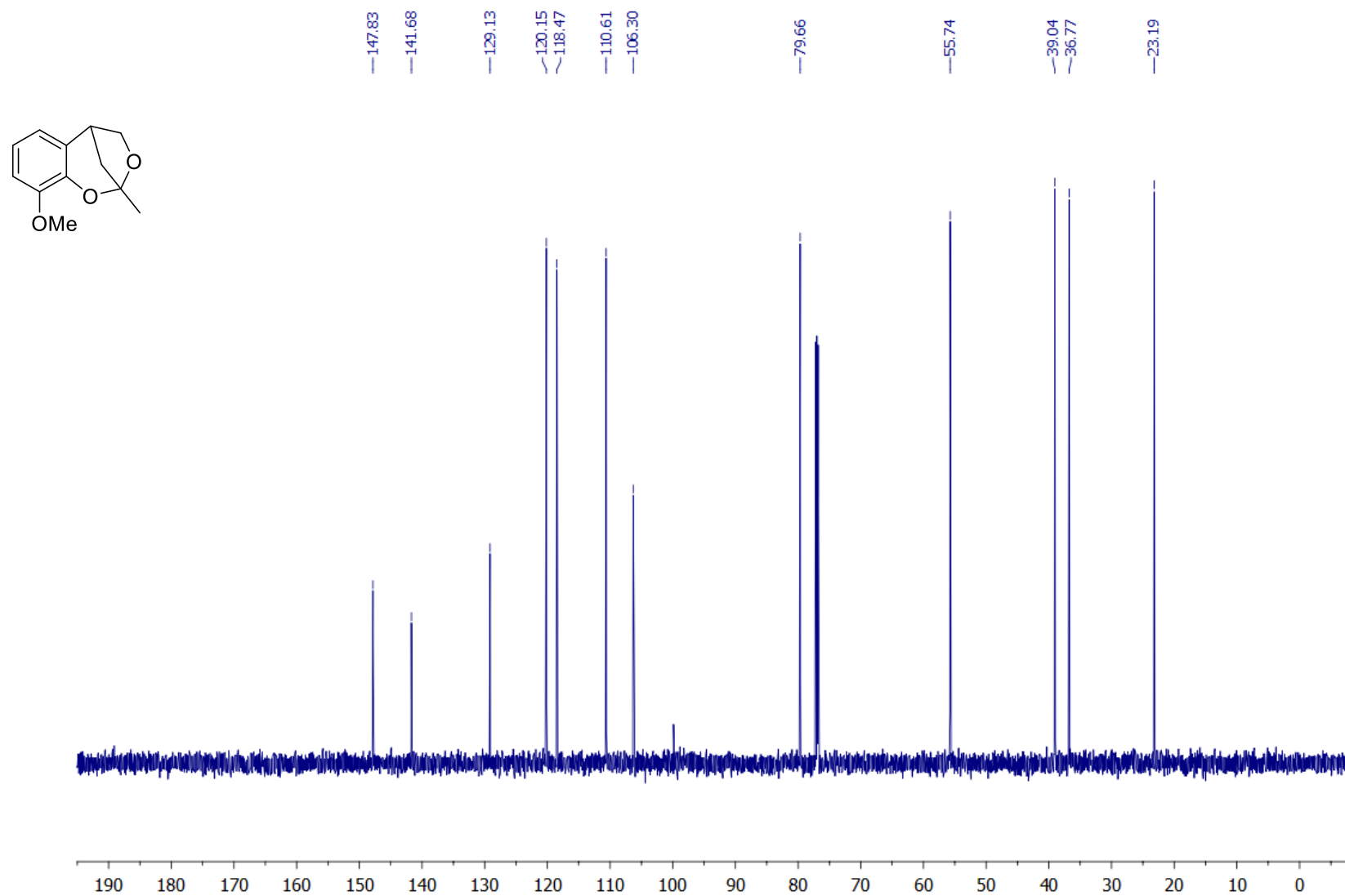
¹H-¹H COSY (CDCl₃)



S430

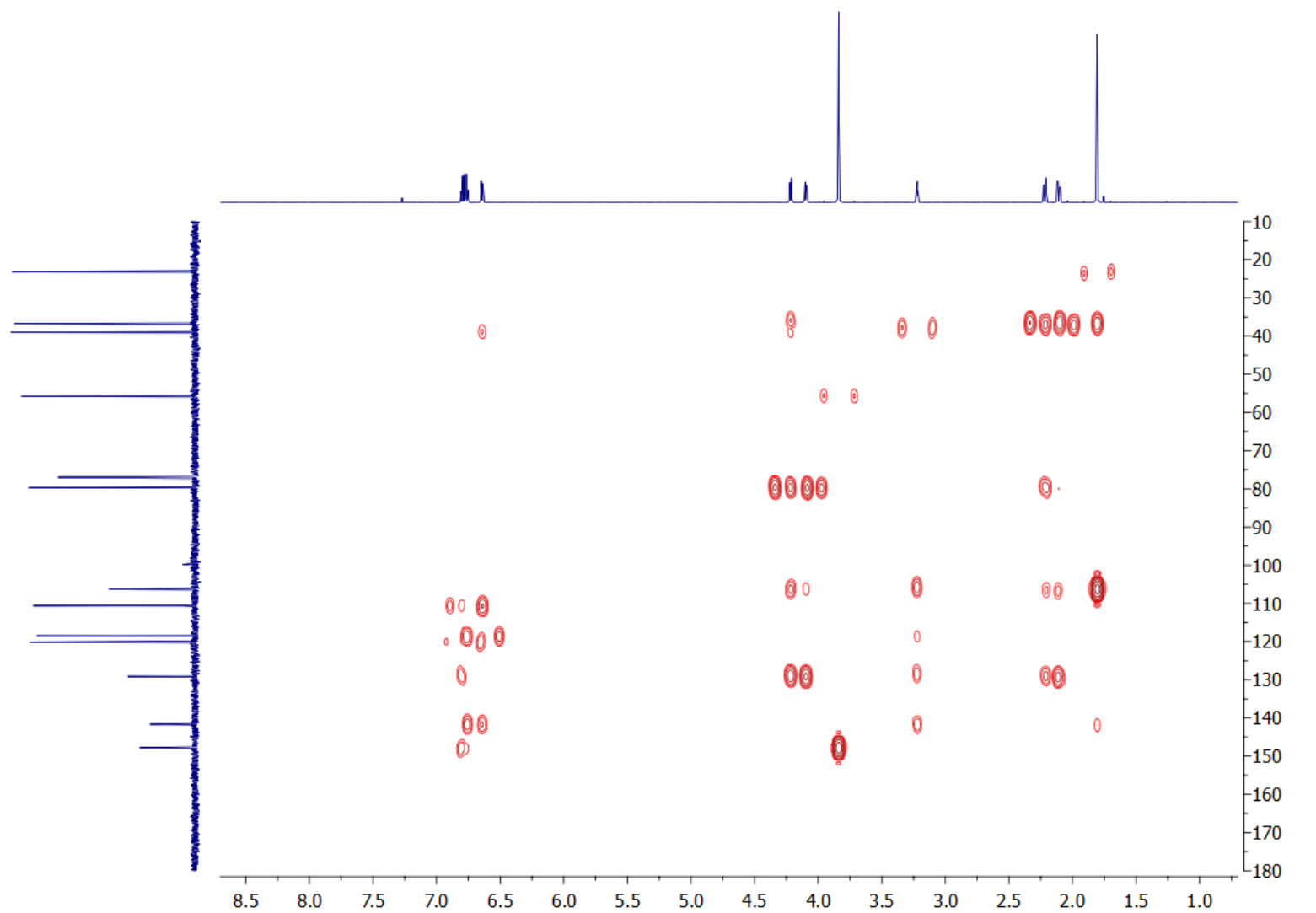
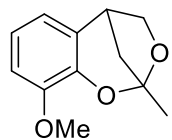
6-Methoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4g)

¹³C NMR (CDCl₃, 150 MHz)



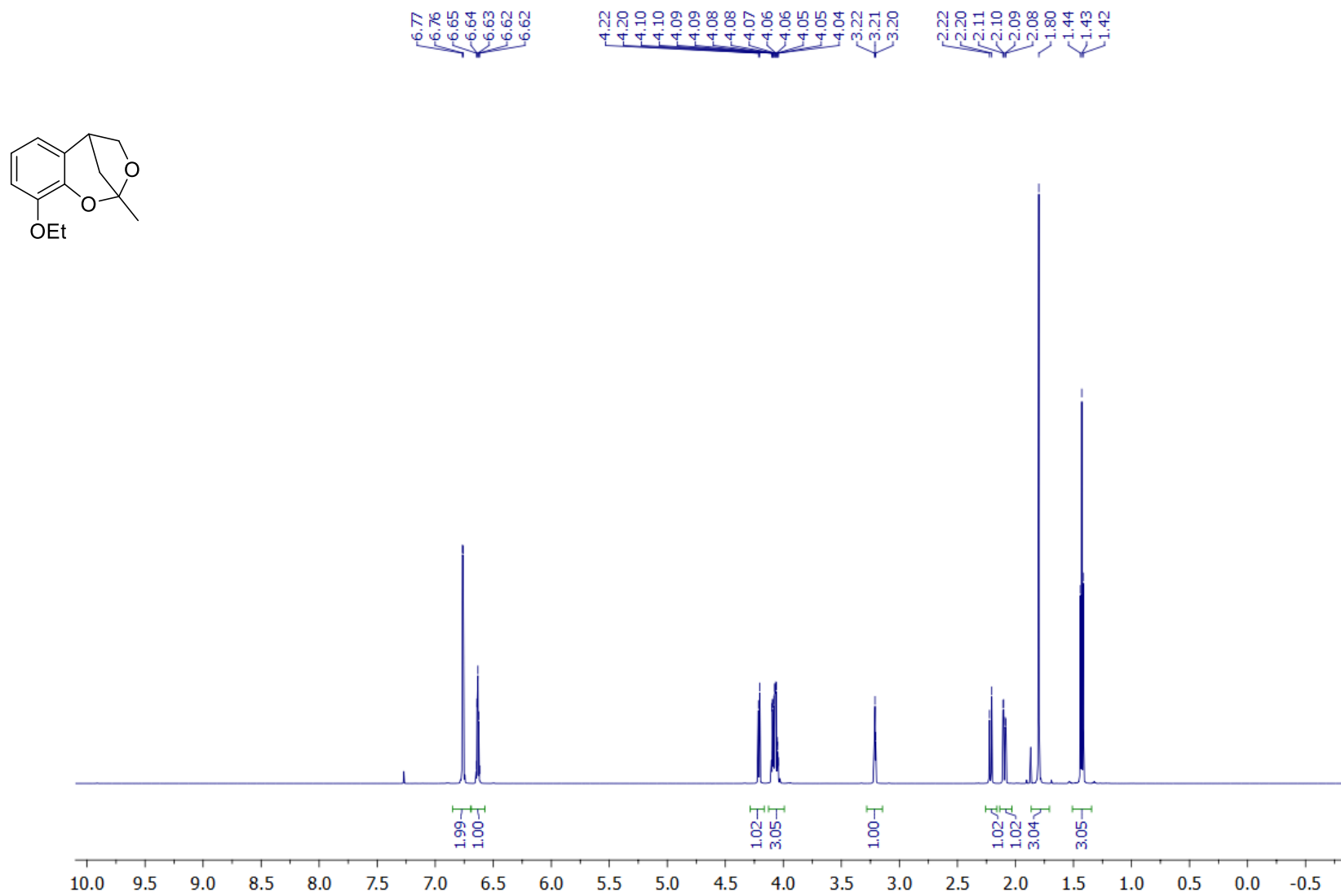
6-Methoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4g)

¹H-¹³C HMBC (CDCl₃)



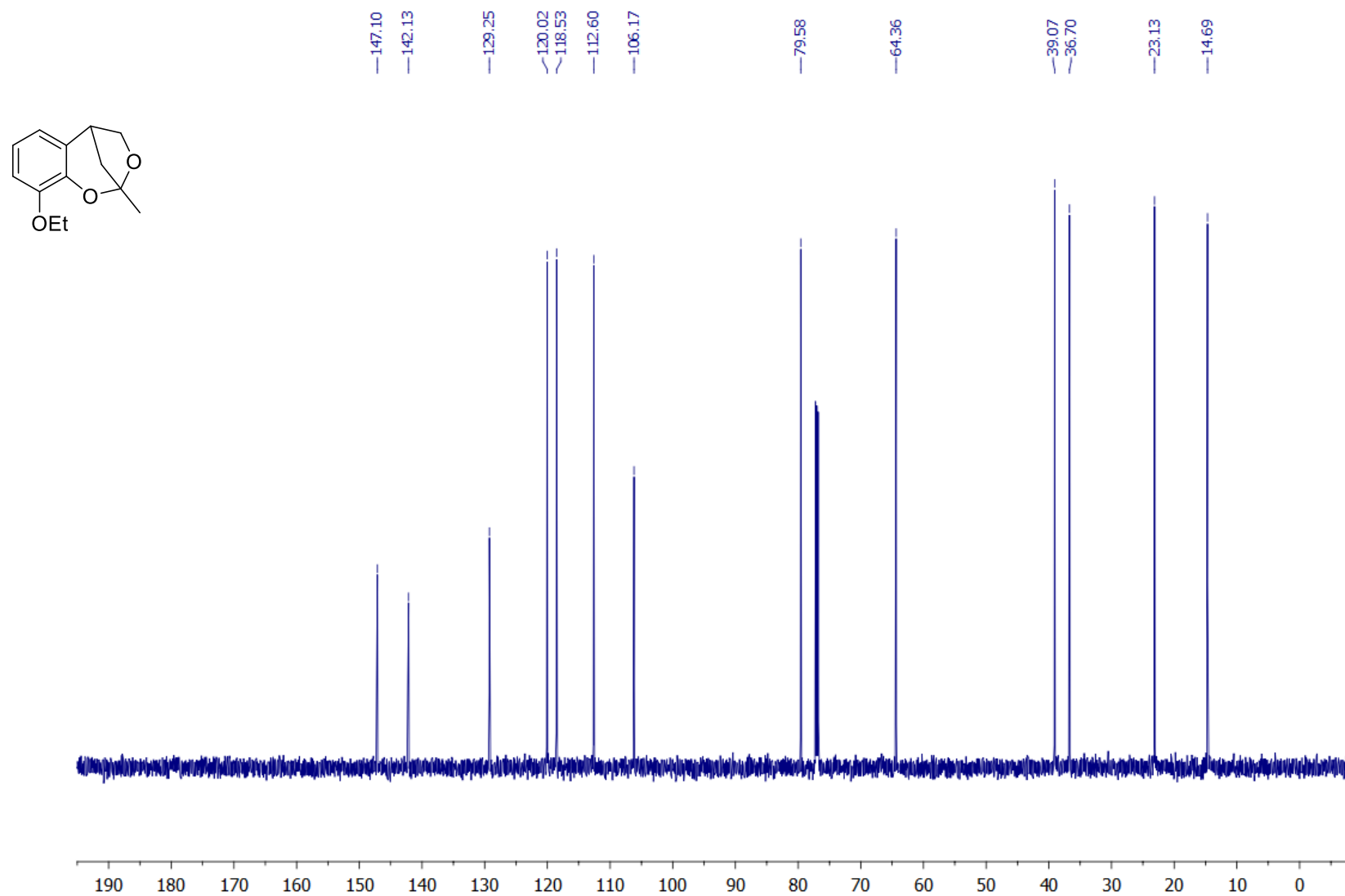
6-Ethoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4h)

¹H NMR (CDCl₃, 600 MHz)



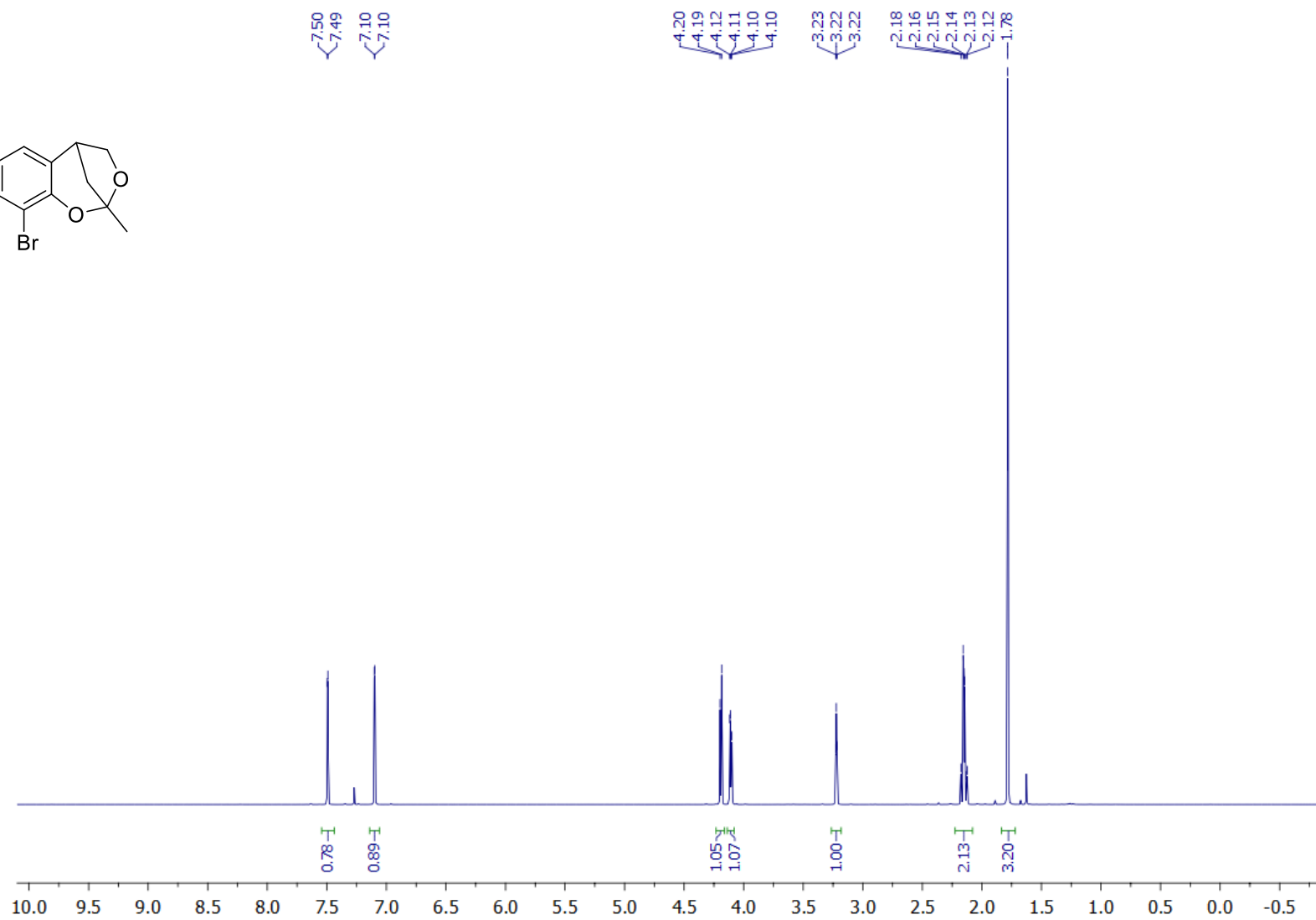
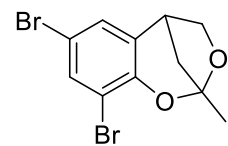
6-Ethoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4h)

¹³C NMR (CDCl₃, 150 MHz)



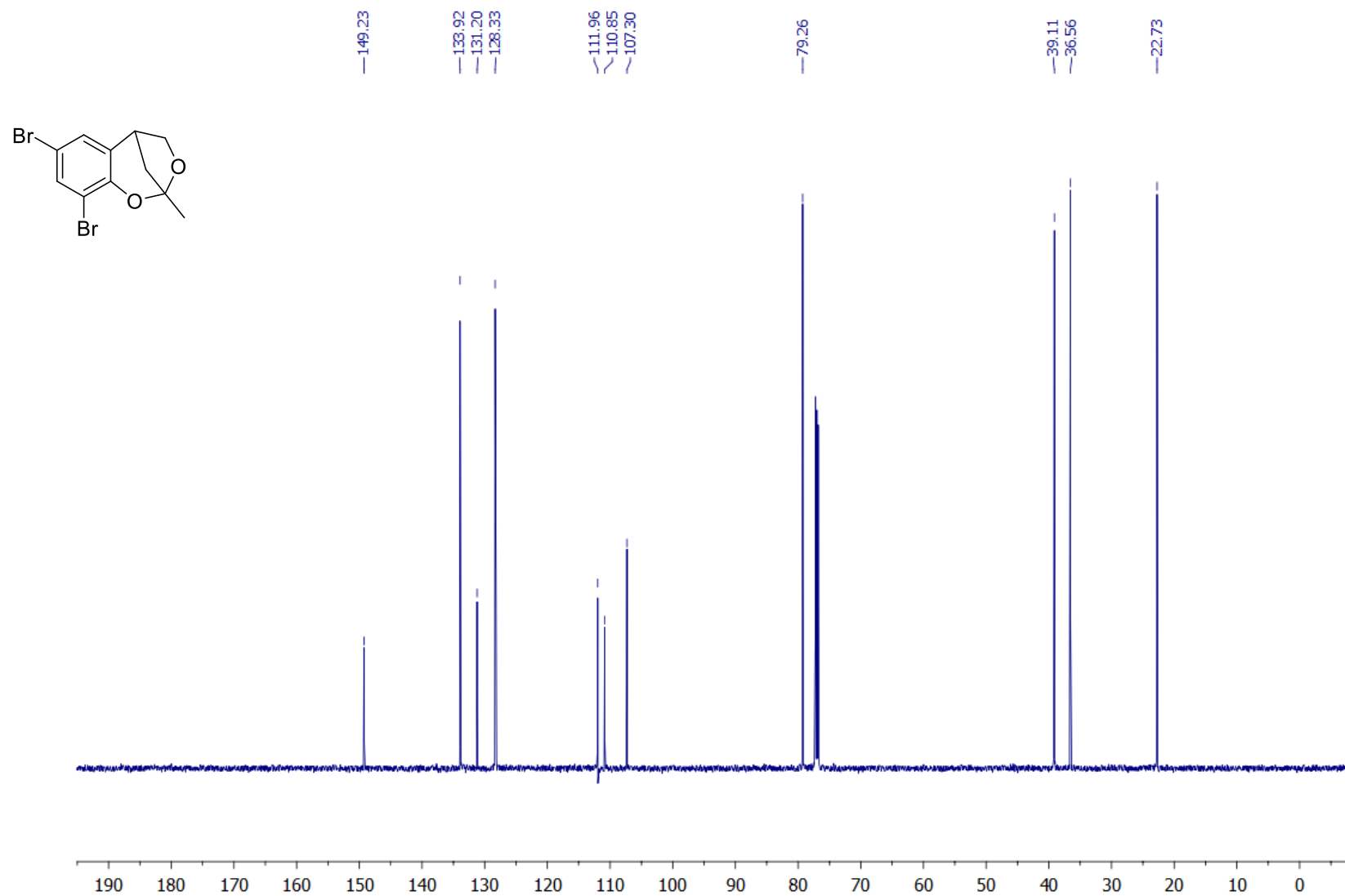
4,6-Dibromo-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4i)

¹H NMR (CDCl₃, 600 MHz)



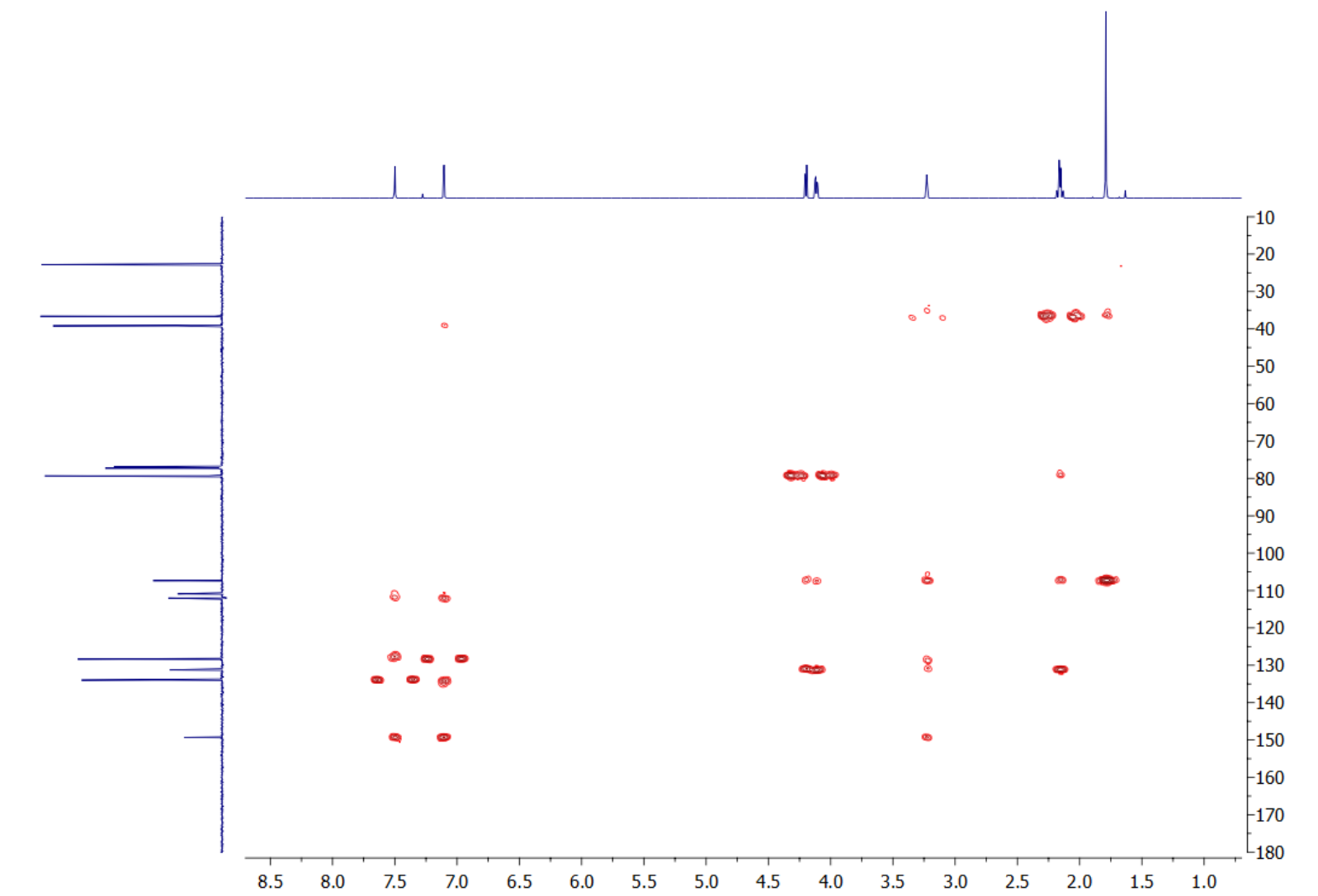
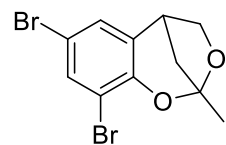
4,6-Dibromo-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4i)

¹³C NMR (CDCl₃, 150 MHz)



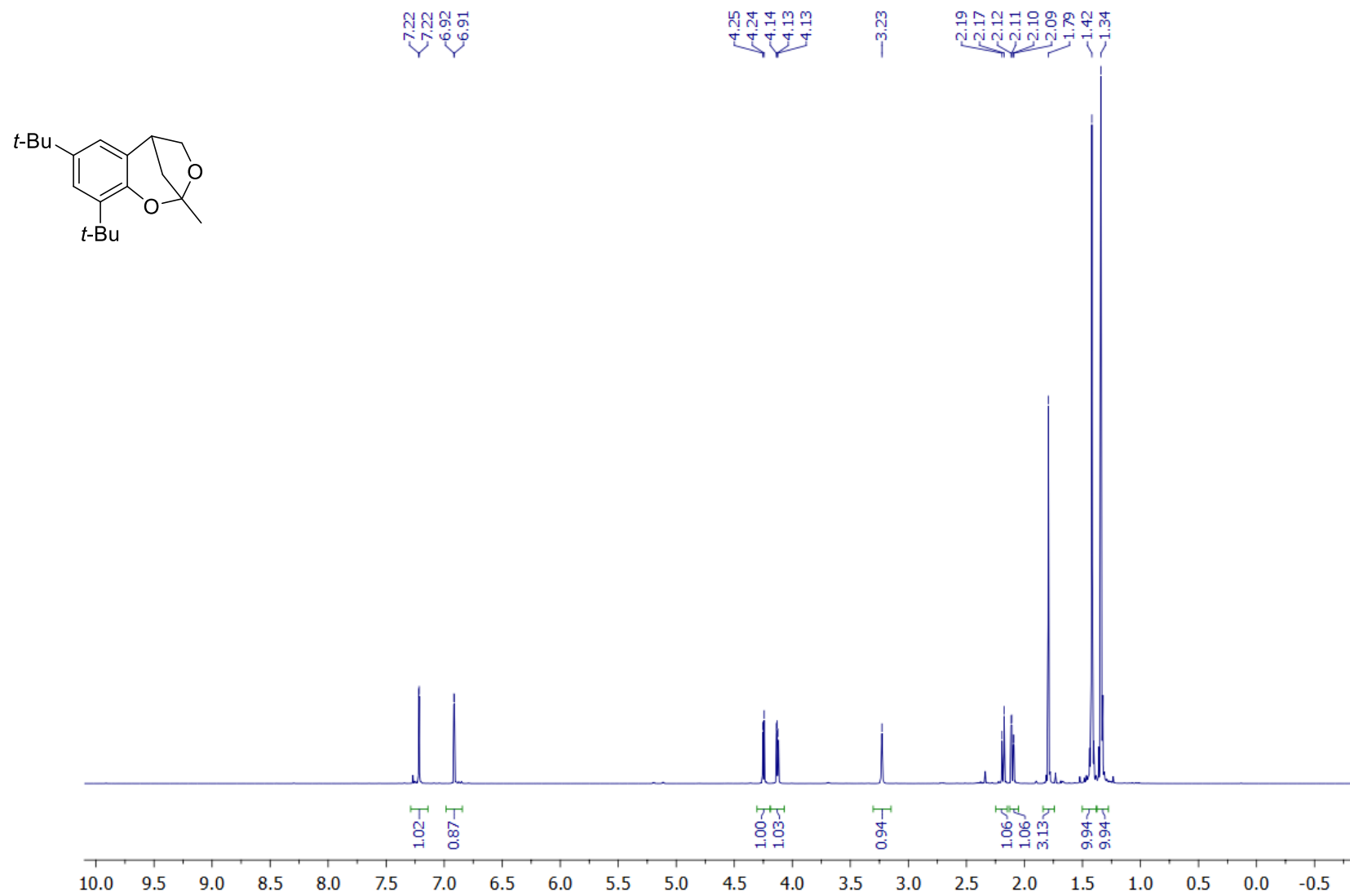
4,6-Dibromo-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4i)

¹H-¹³C HMBC (CDCl₃)



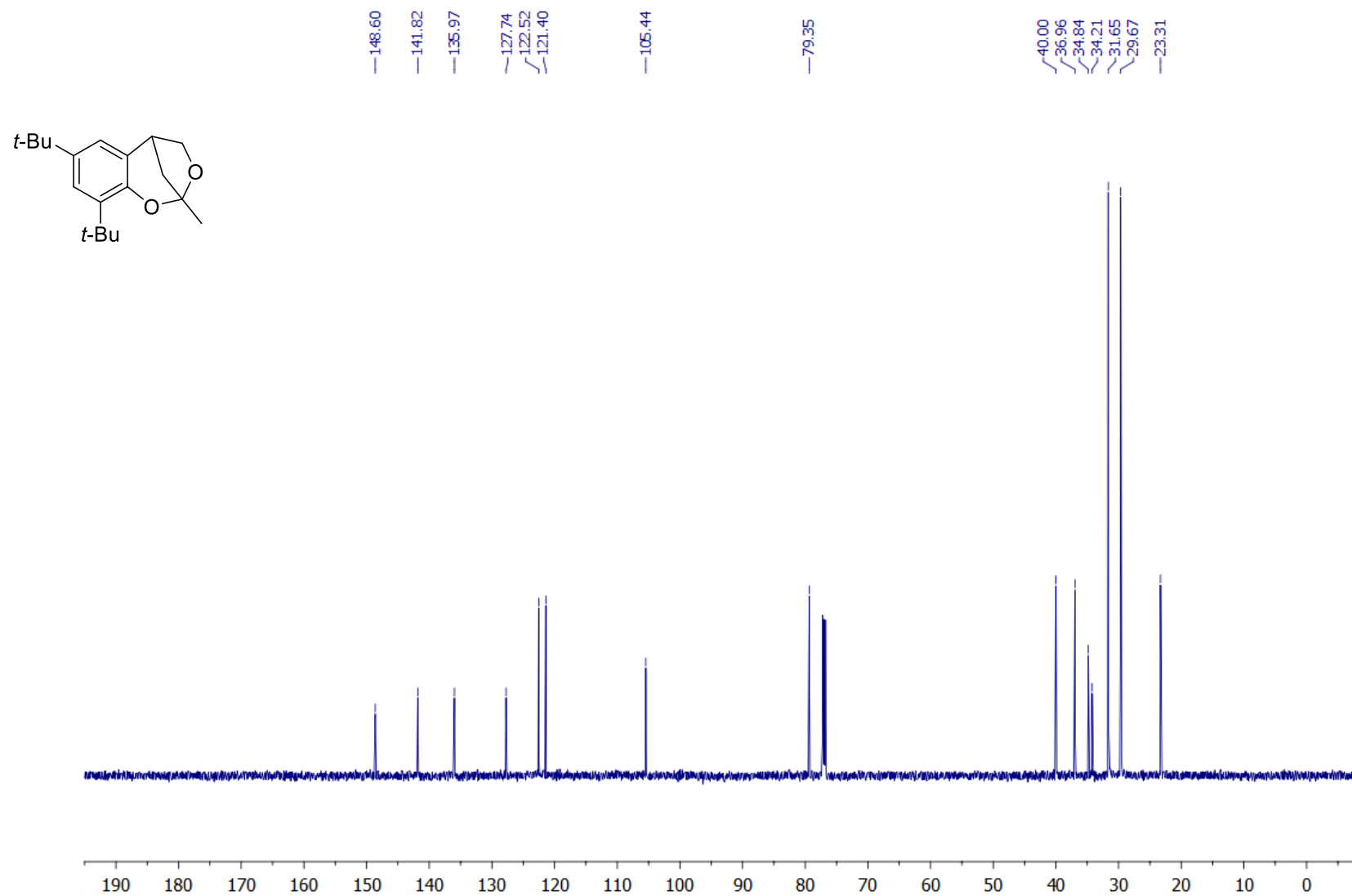
4,6-Di-*tert*-butyl-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4j)

¹H NMR (CDCl₃, 600 MHz)



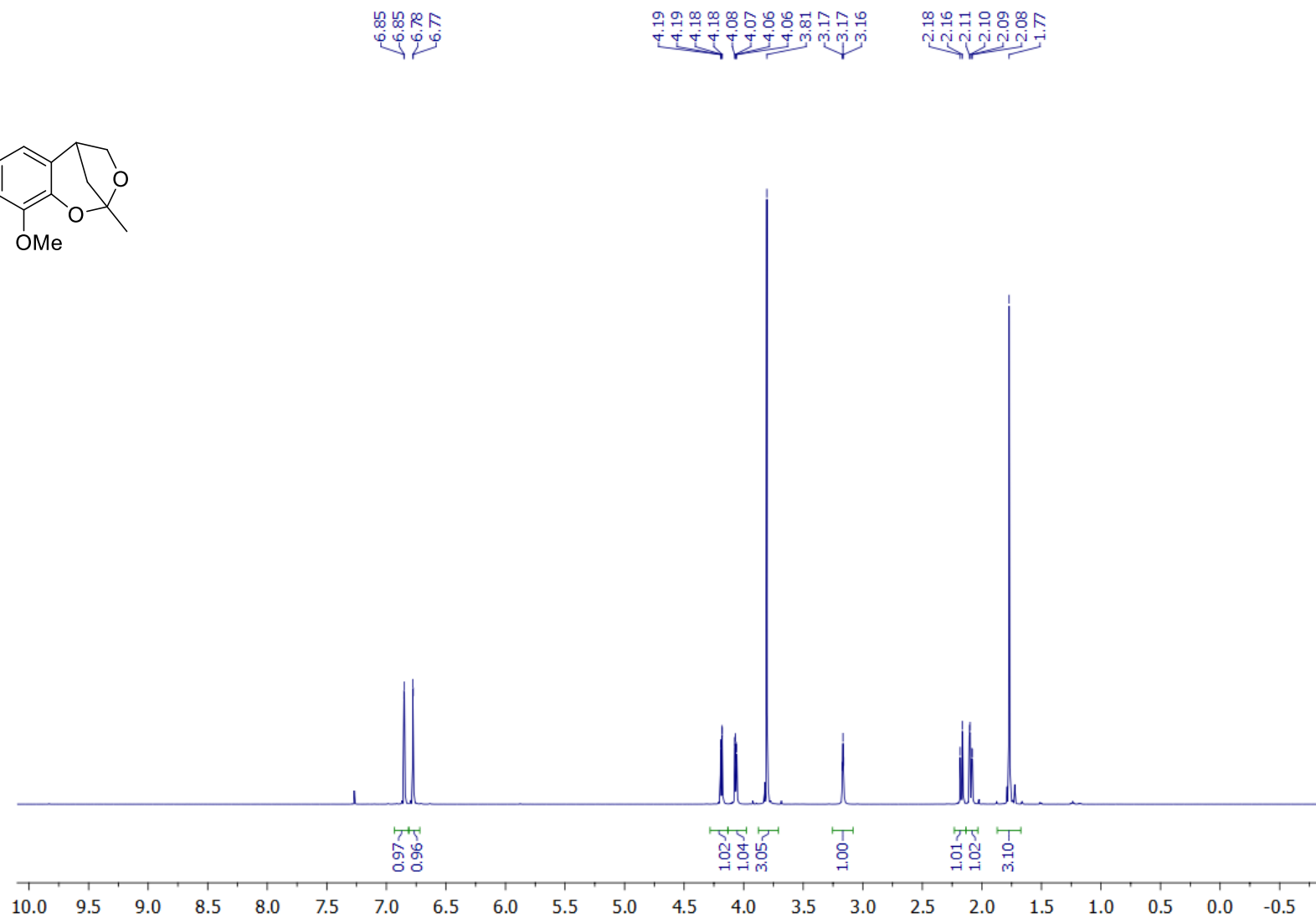
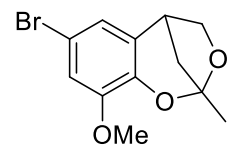
4,6-Di-*tert*-butyl-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4j)

¹³C NMR (CDCl₃, 150 MHz)



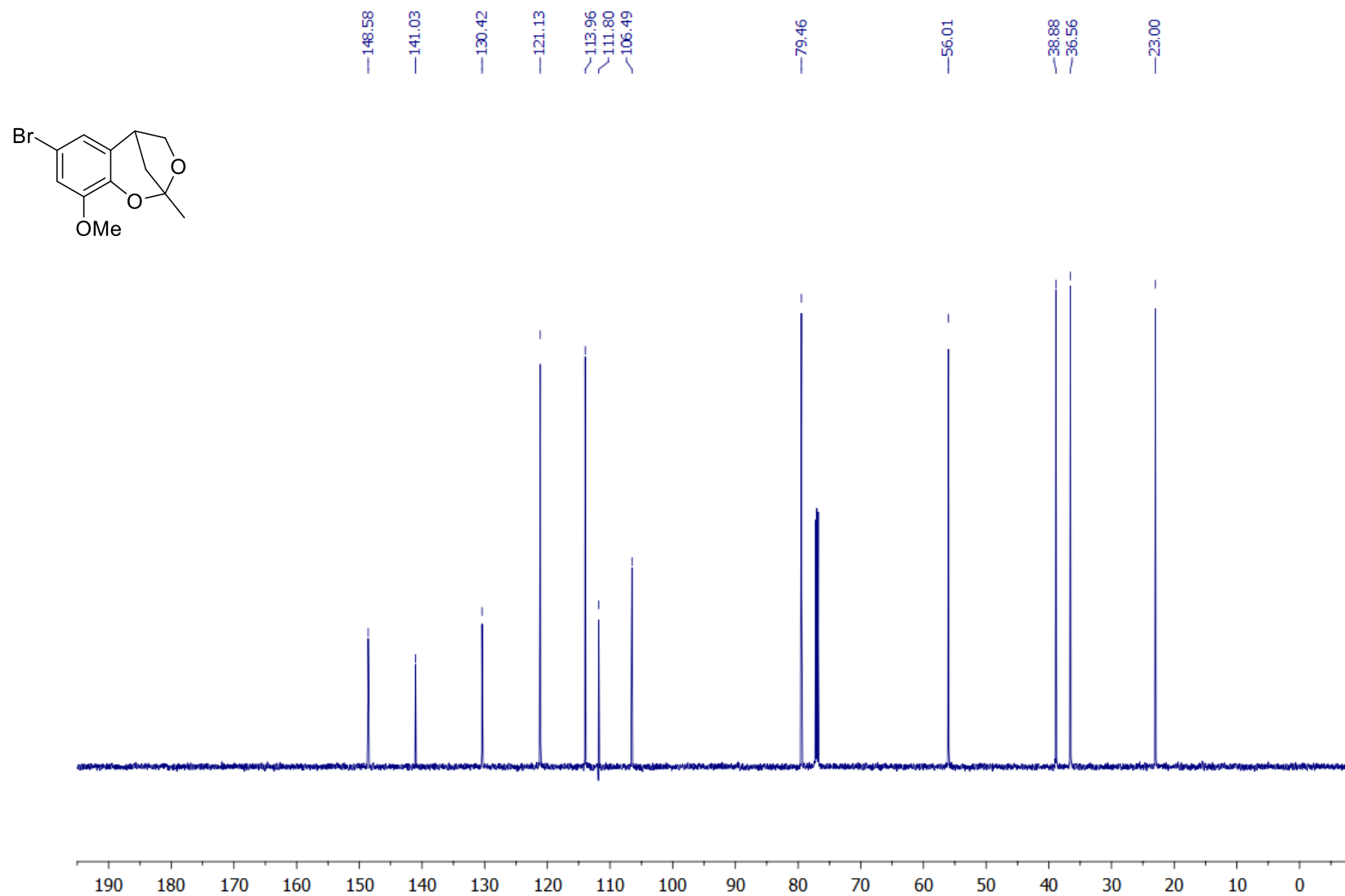
4-Bromo-6-methoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4k)

¹H NMR (CDCl₃, 600 MHz)



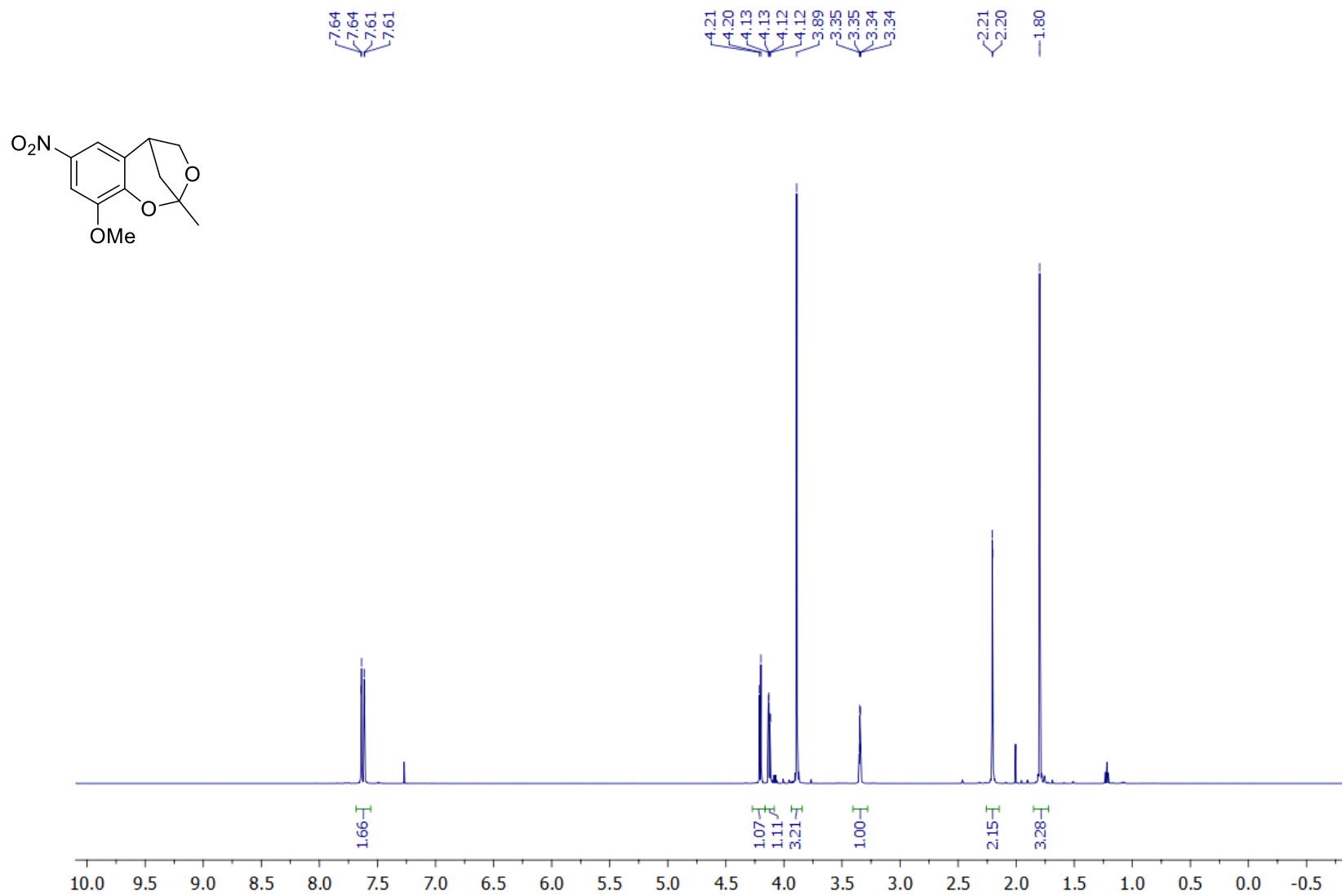
4-Bromo-6-methoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4k)

¹³C NMR (CDCl₃, 150 MHz)



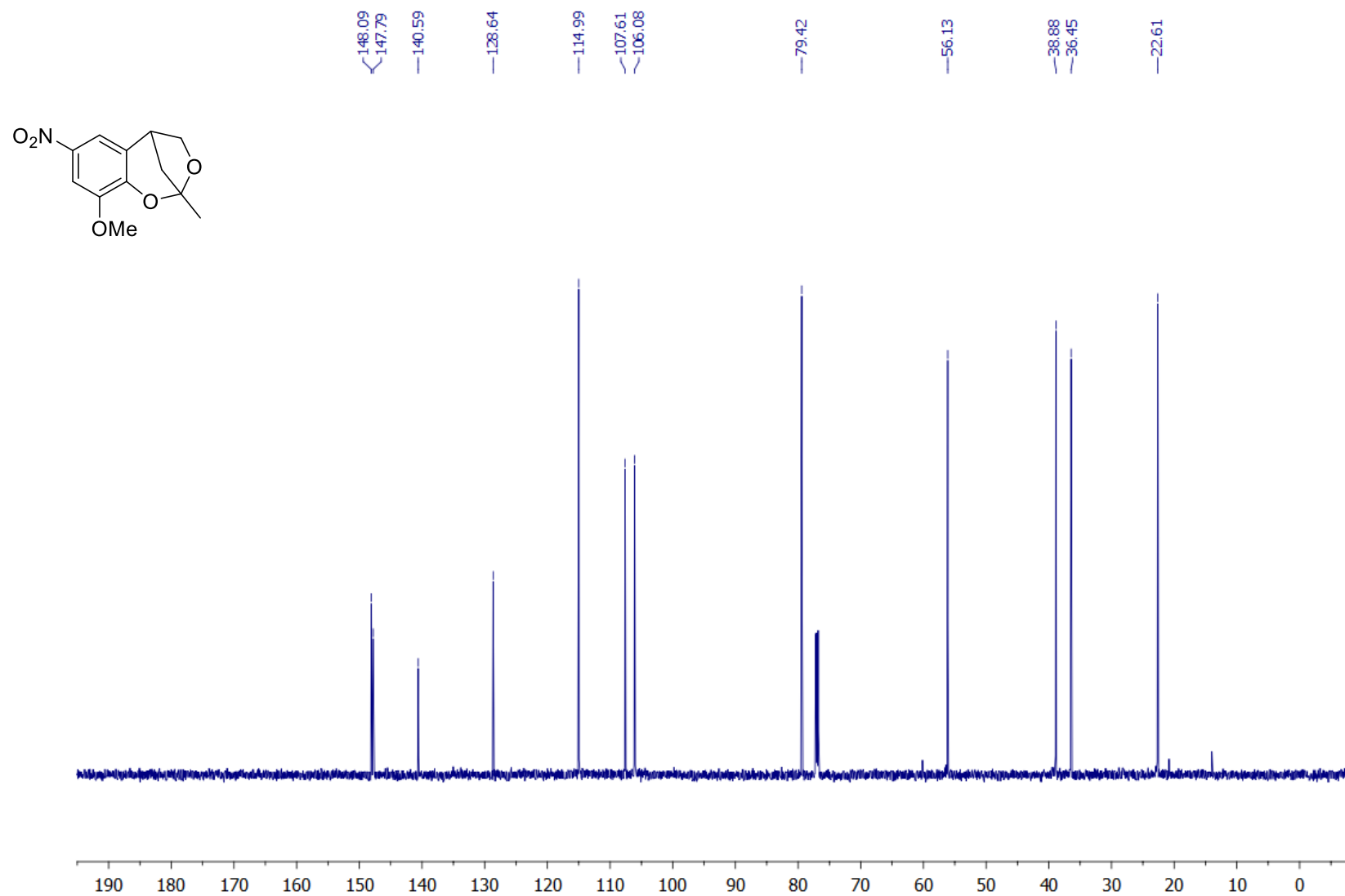
6-Methoxy-9-methyl-4-nitro-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4l)

¹H NMR (CDCl₃, 600 MHz)



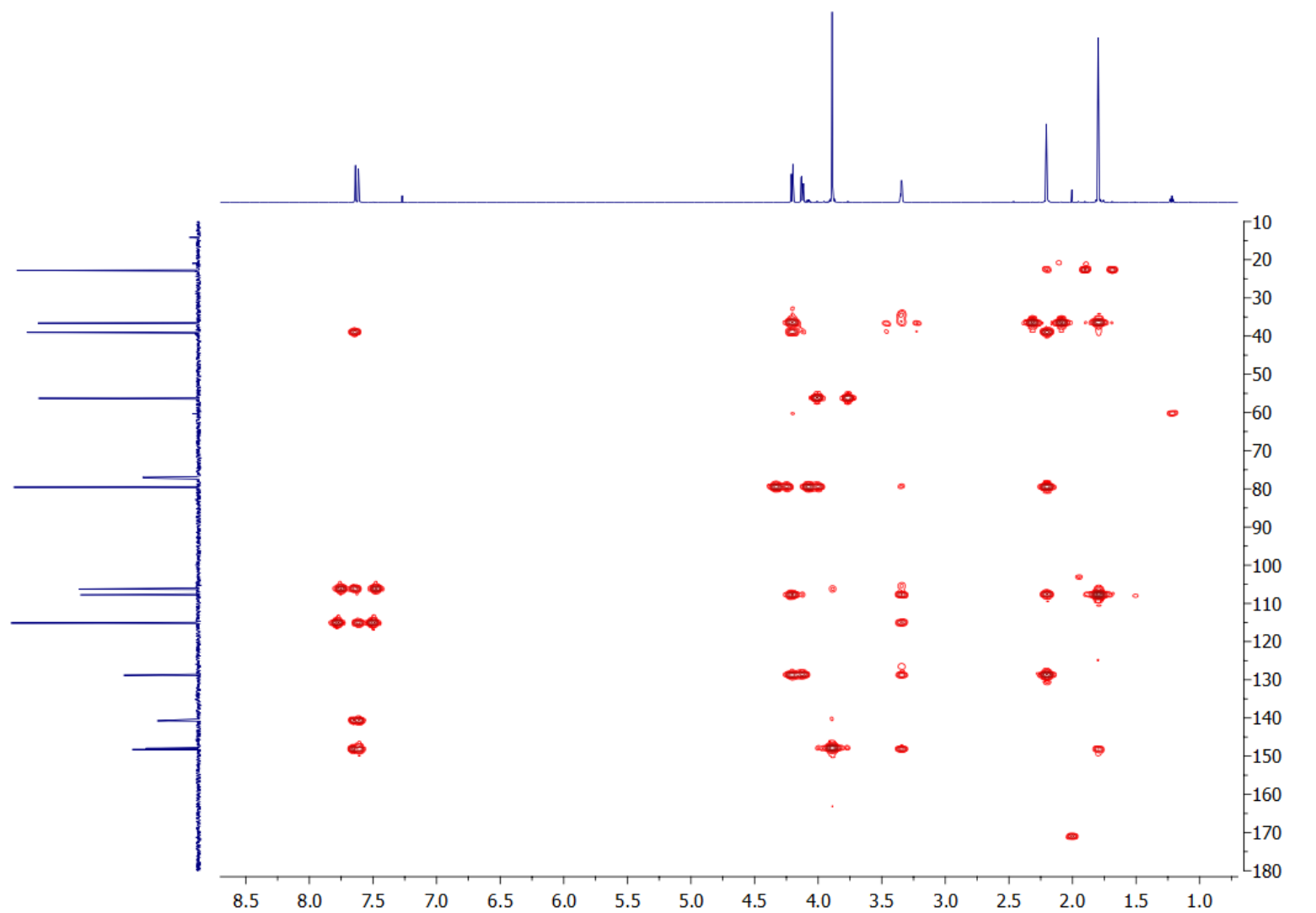
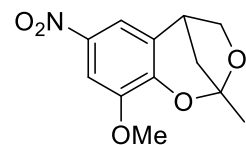
6-Methoxy-9-methyl-4-nitro-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4l)

¹³C NMR (CDCl₃, 150 MHz)



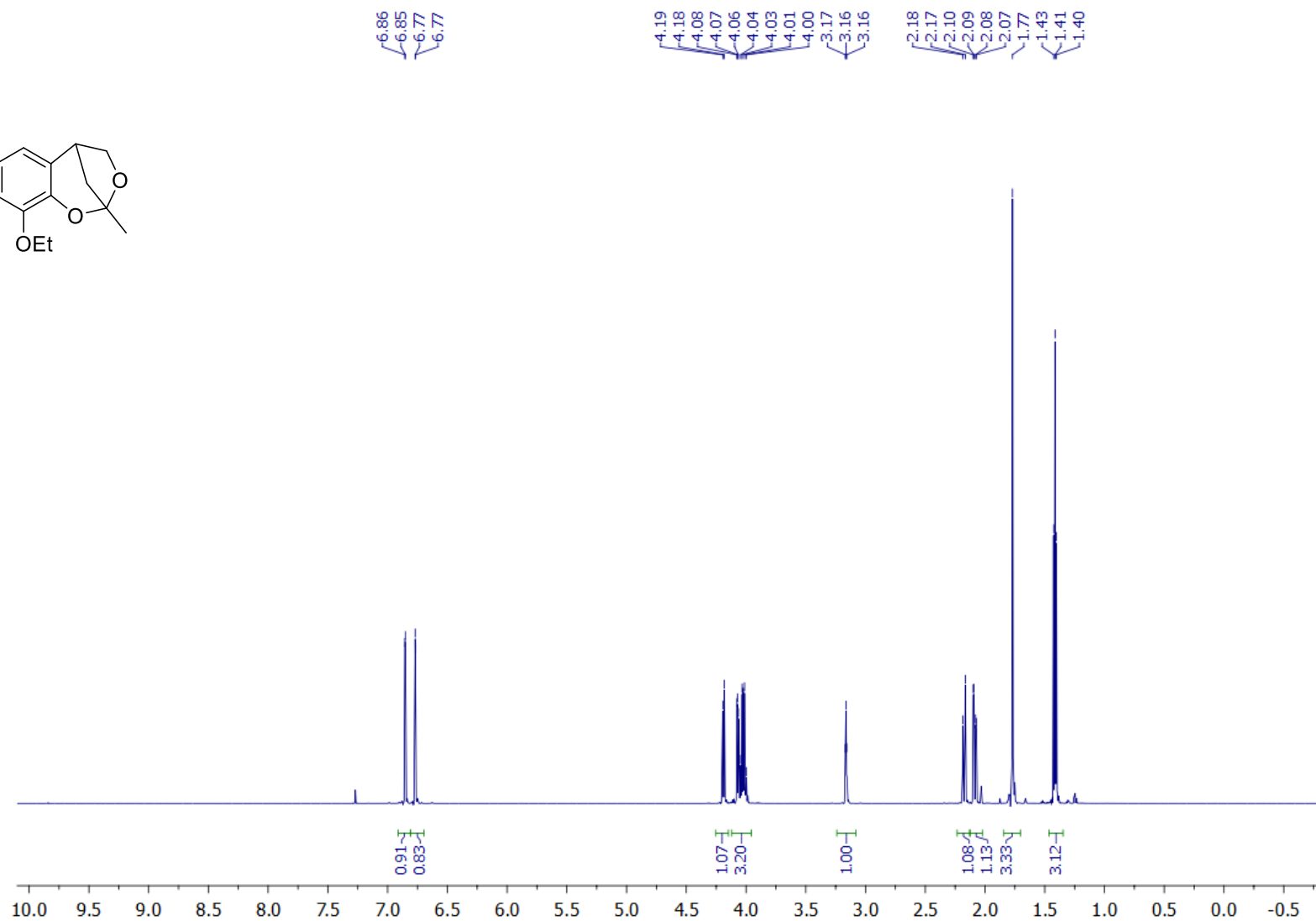
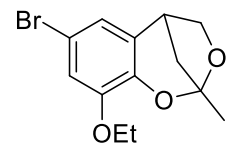
6-Methoxy-9-methyl-4-nitro-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4l)

¹H-¹³C HMBC (CDCl₃)



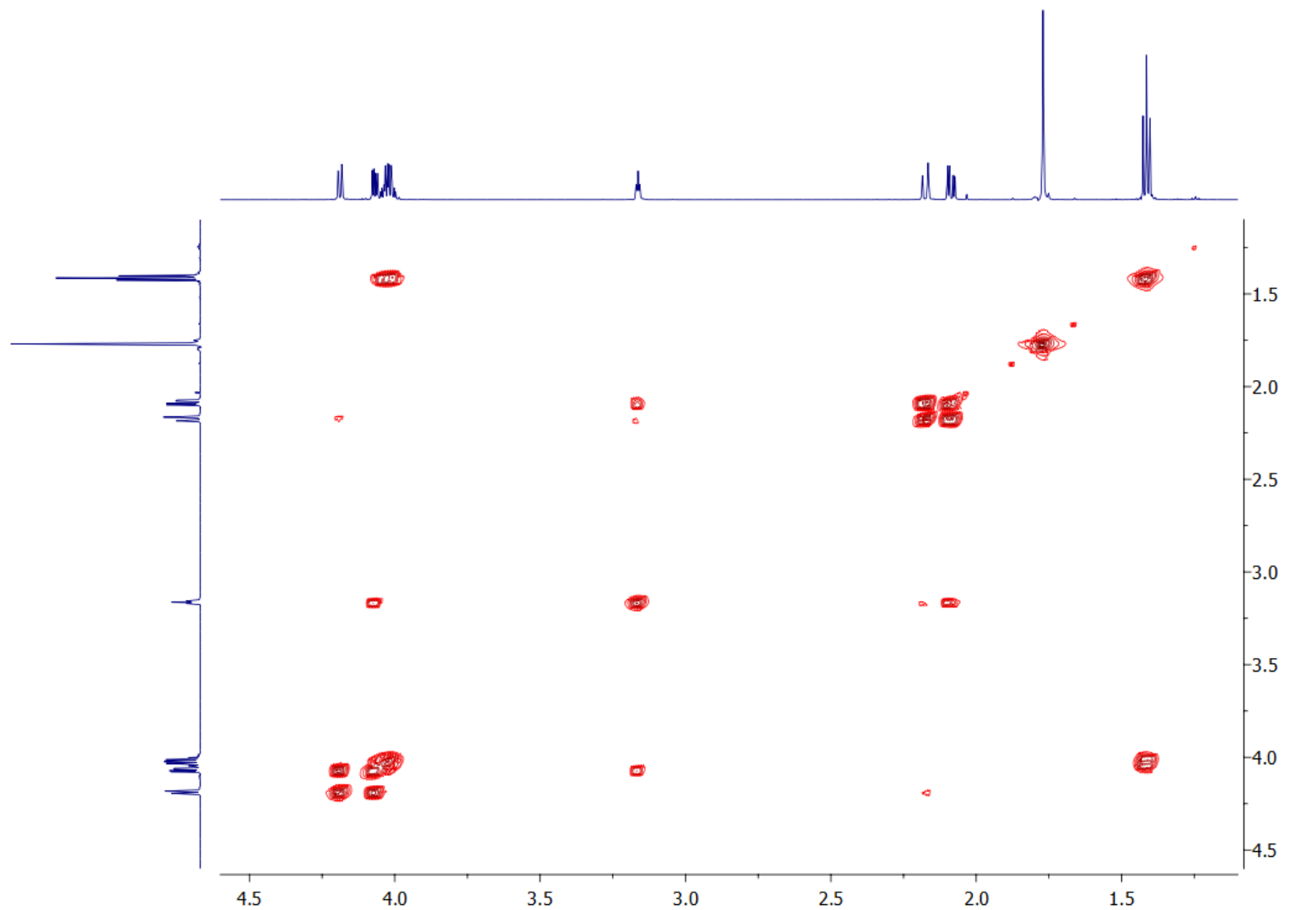
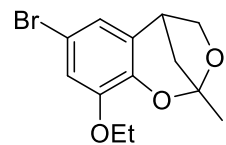
4-Bromo-6-ethoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4m)

¹H NMR (CDCl₃, 600 MHz)



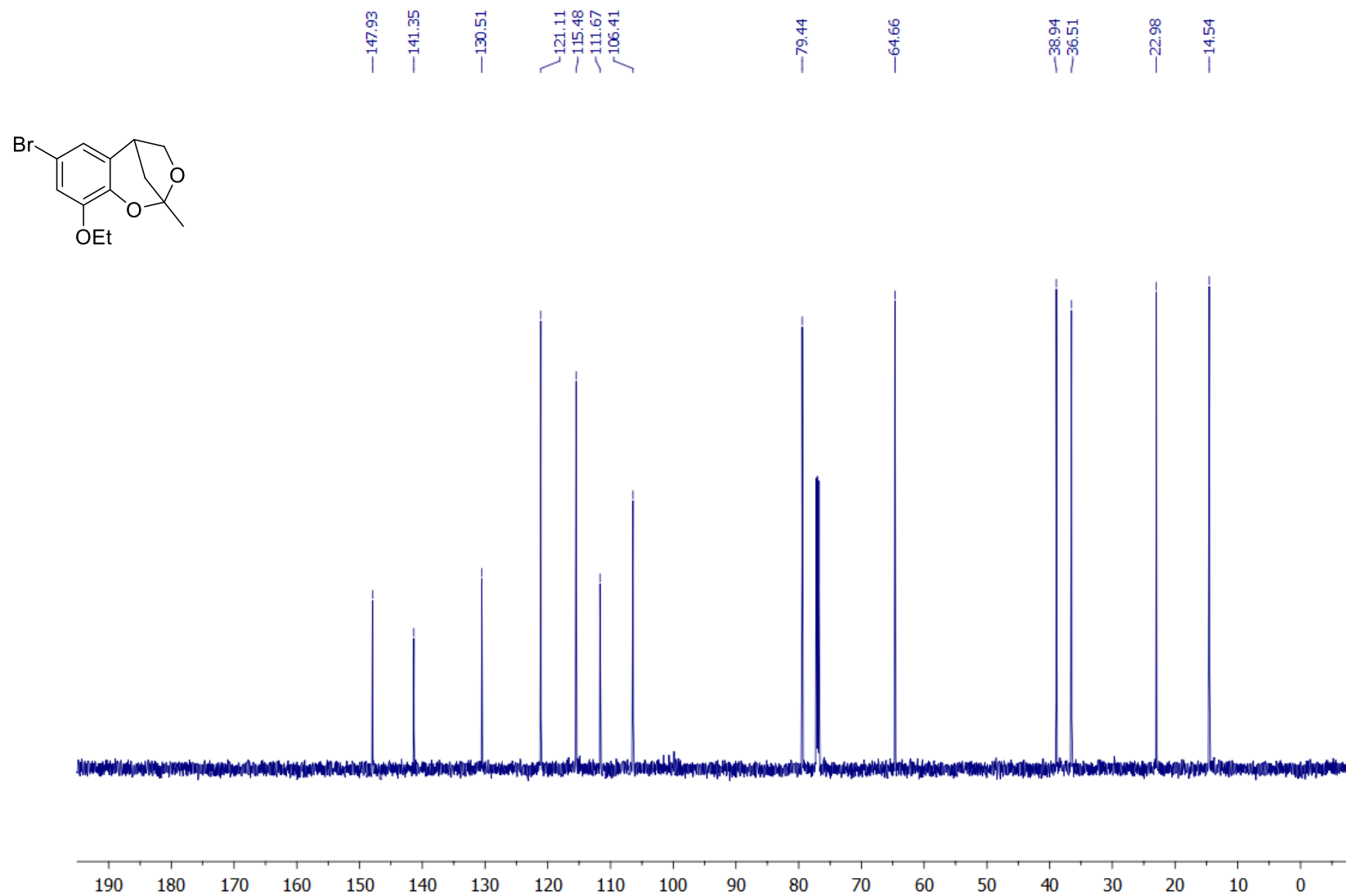
4-Bromo-6-ethoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4m)

¹H-¹H COSY (CDCl₃)



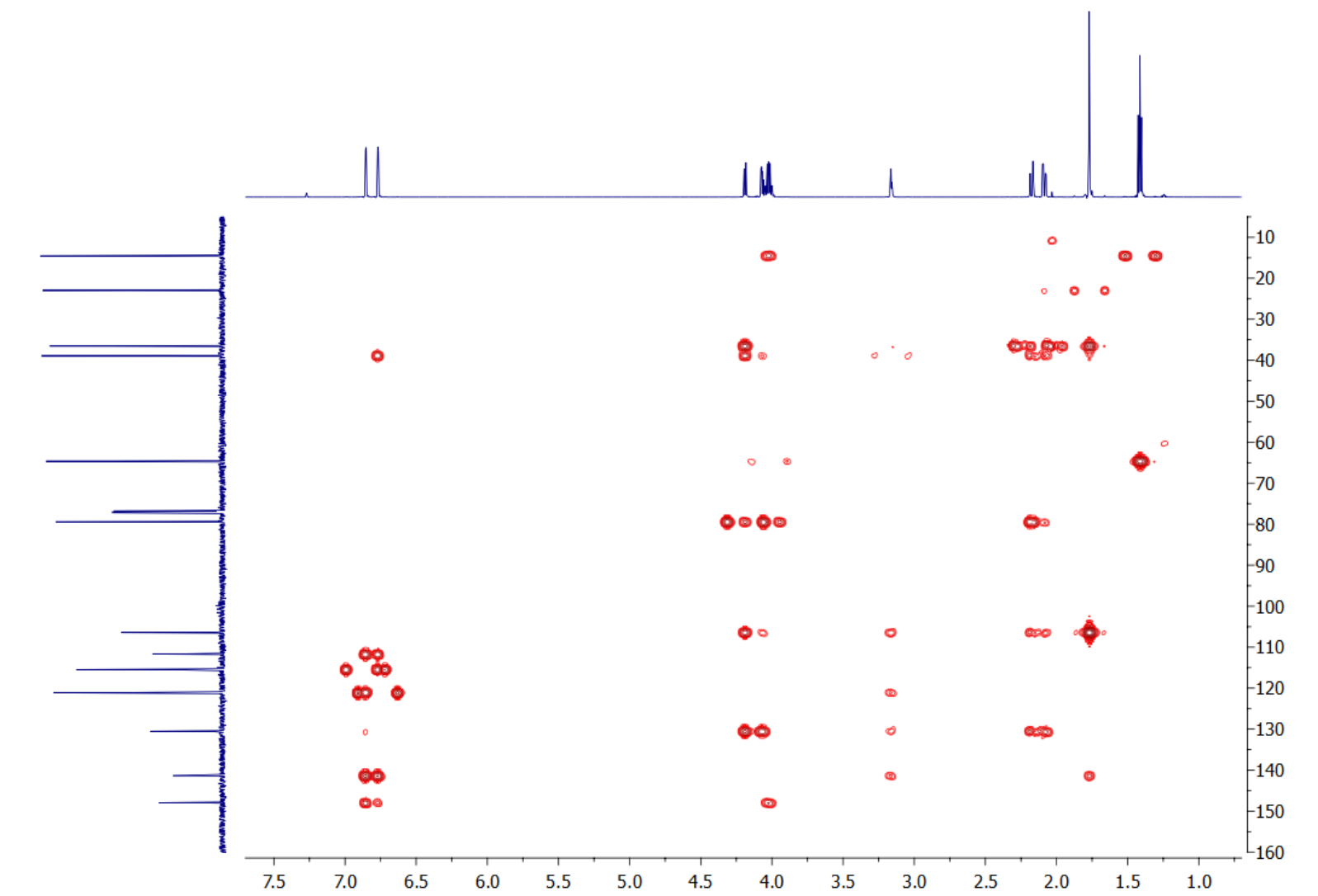
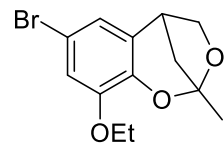
4-Bromo-6-ethoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4m)

¹³C NMR (CDCl₃, 150 MHz)



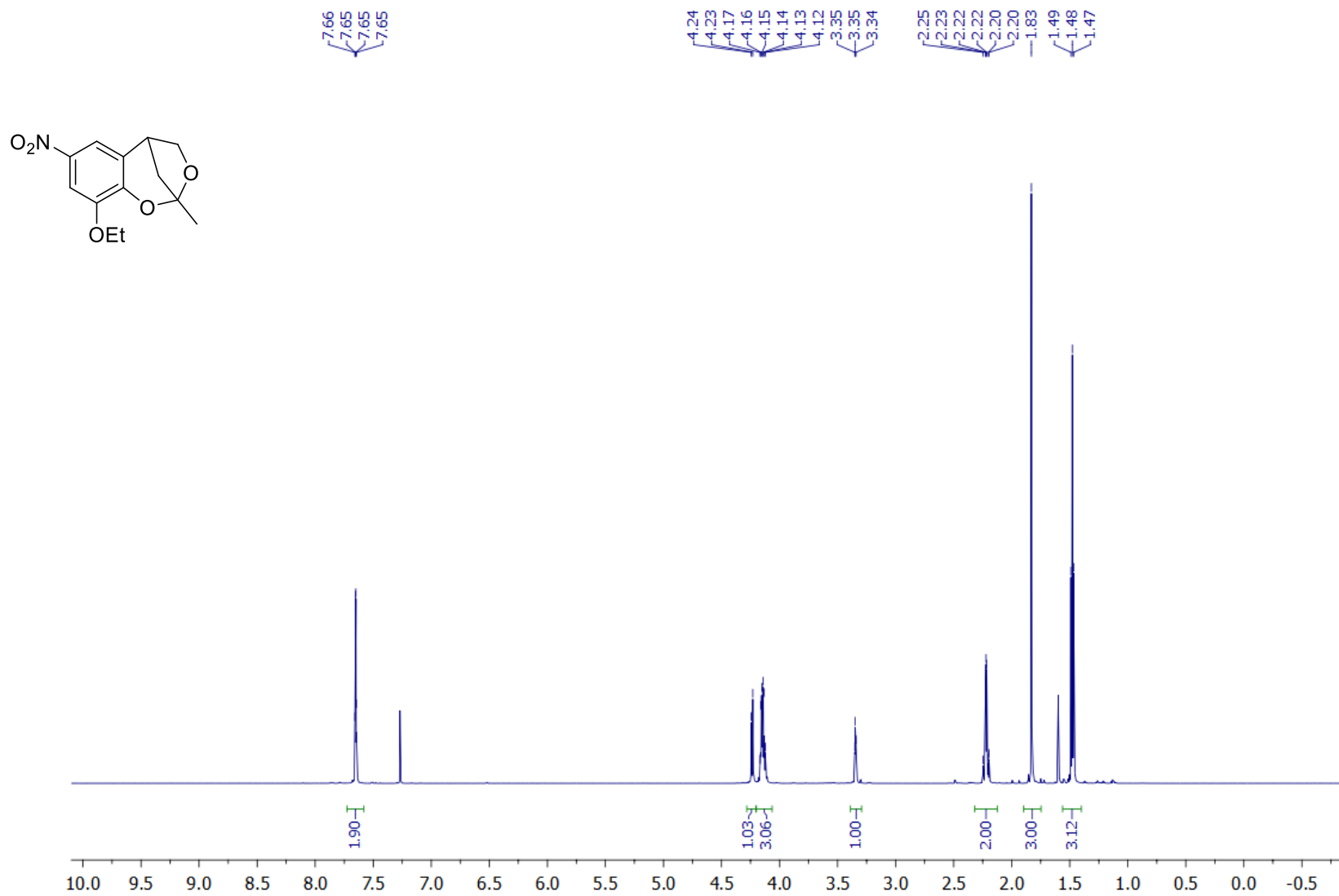
4-Bromo-6-ethoxy-9-methyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4m)

¹H-¹³C HMBC (CDCl₃)



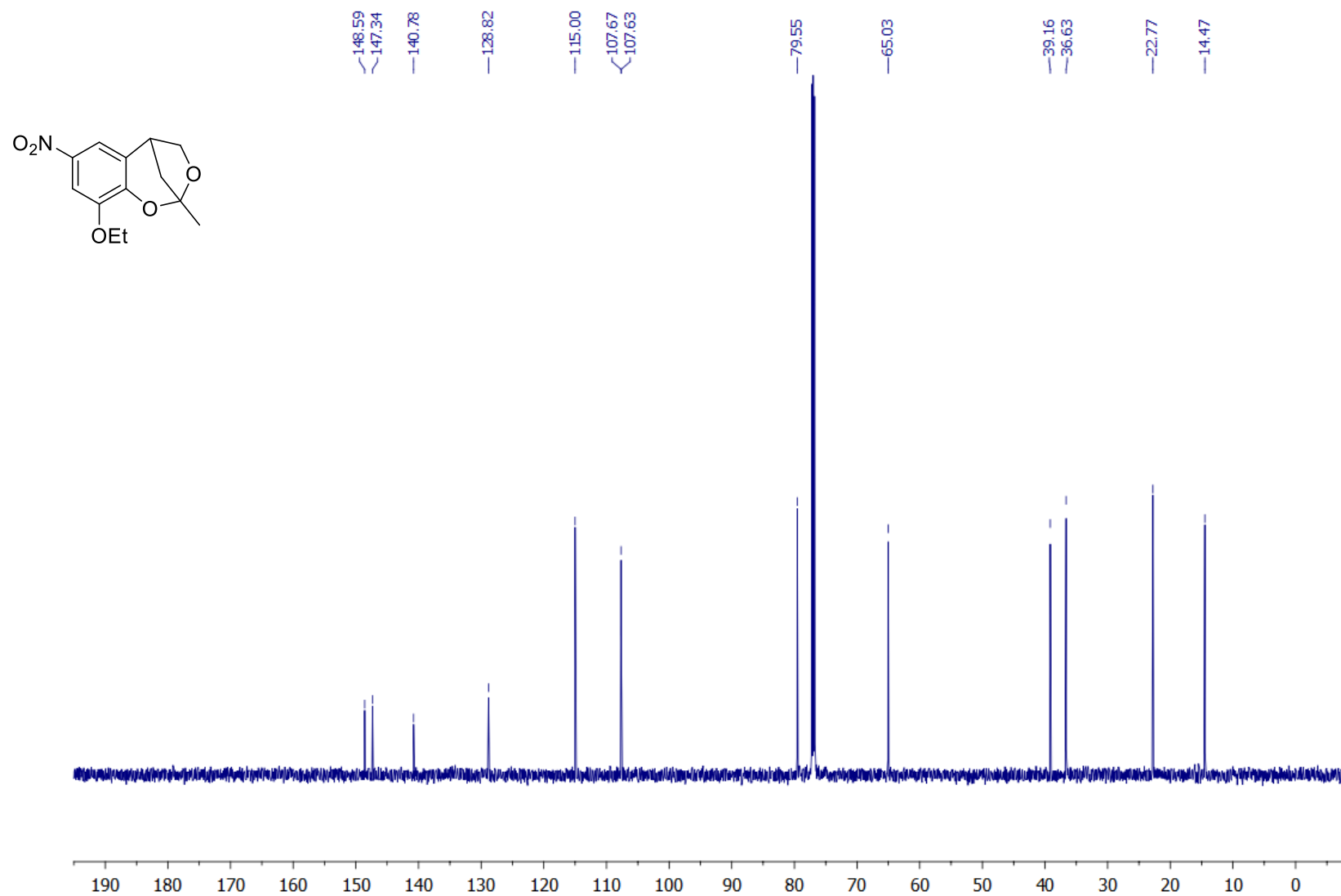
6-Ethoxy-9-methyl-4-nitro-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4n)

¹H NMR (CDCl₃, 600 MHz)



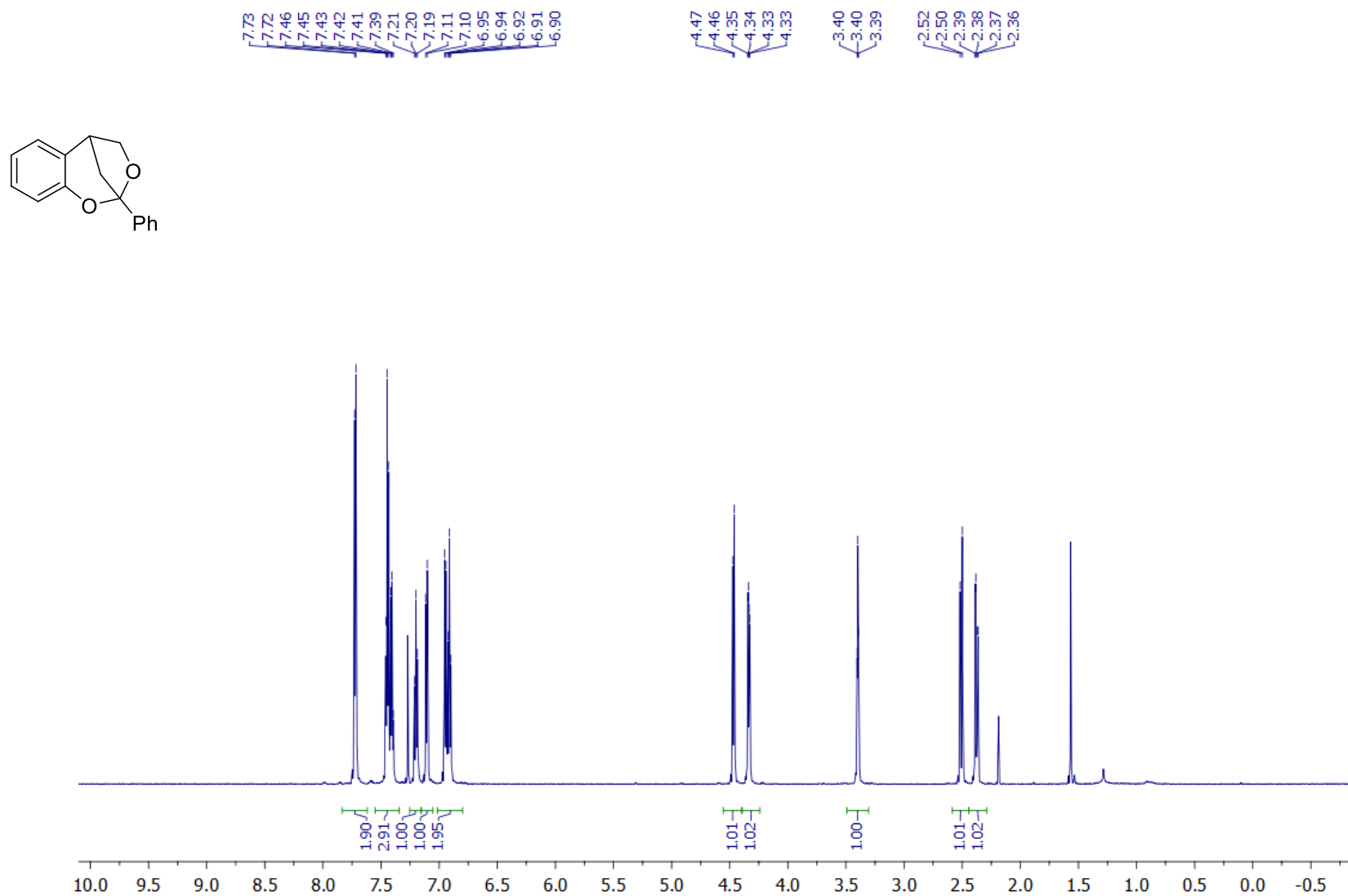
6-Ethoxy-9-methyl-4-nitro-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4n)

¹³C NMR (CDCl₃, 150 MHz)



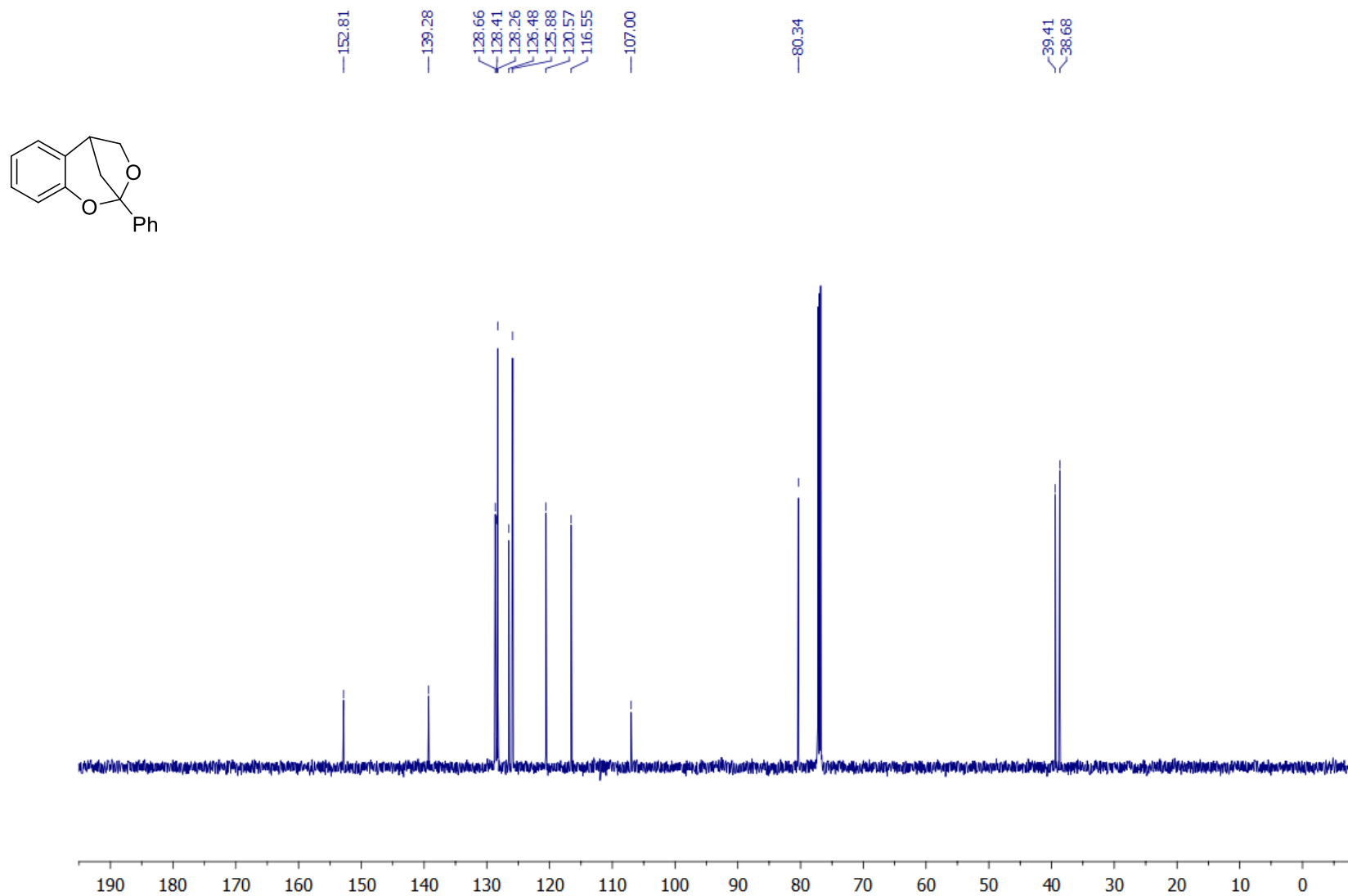
9-Phenyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4o)

¹H NMR (CDCl₃, 600 MHz)



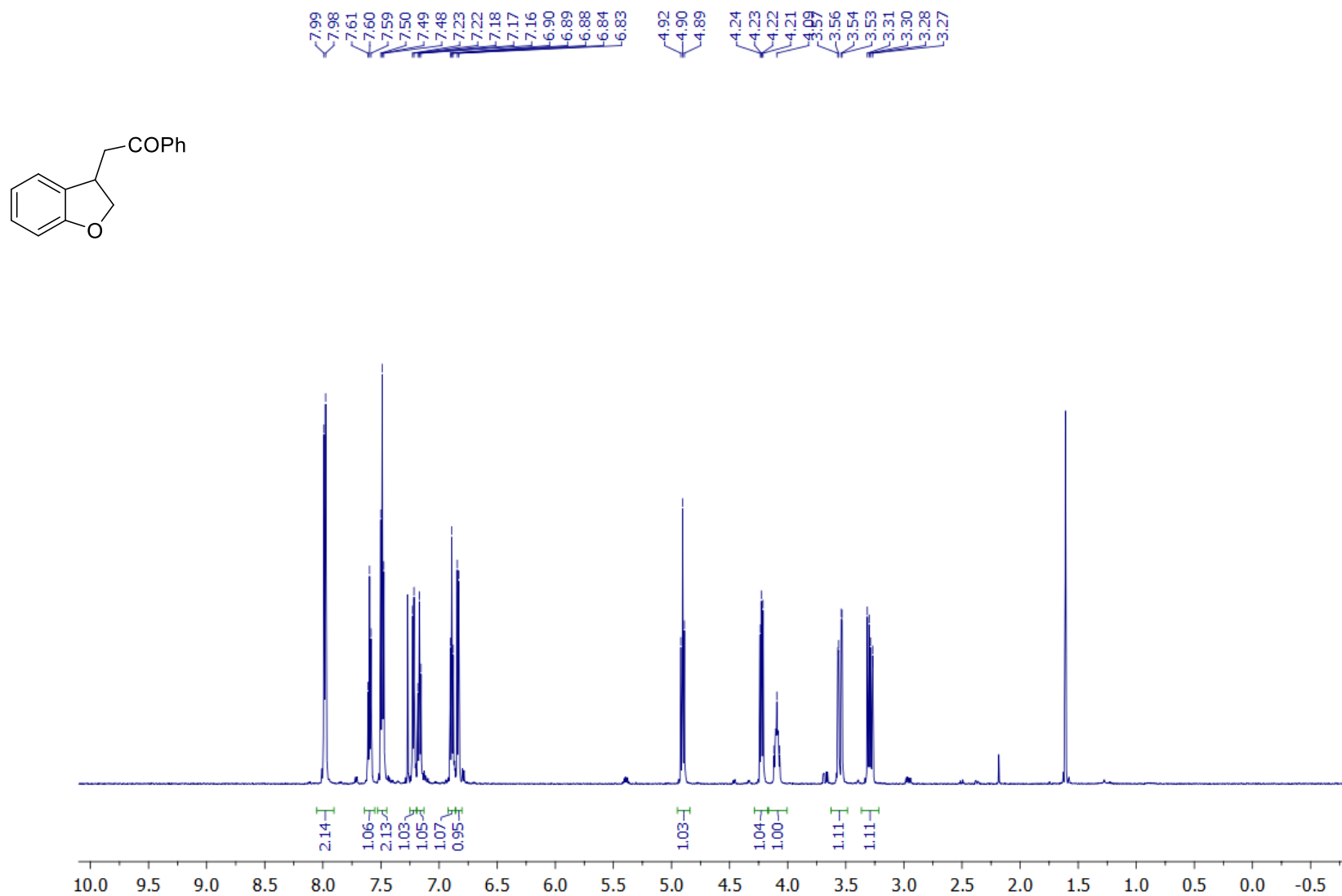
9-Phenyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4o)

¹³C NMR (CDCl₃, 150 MHz)



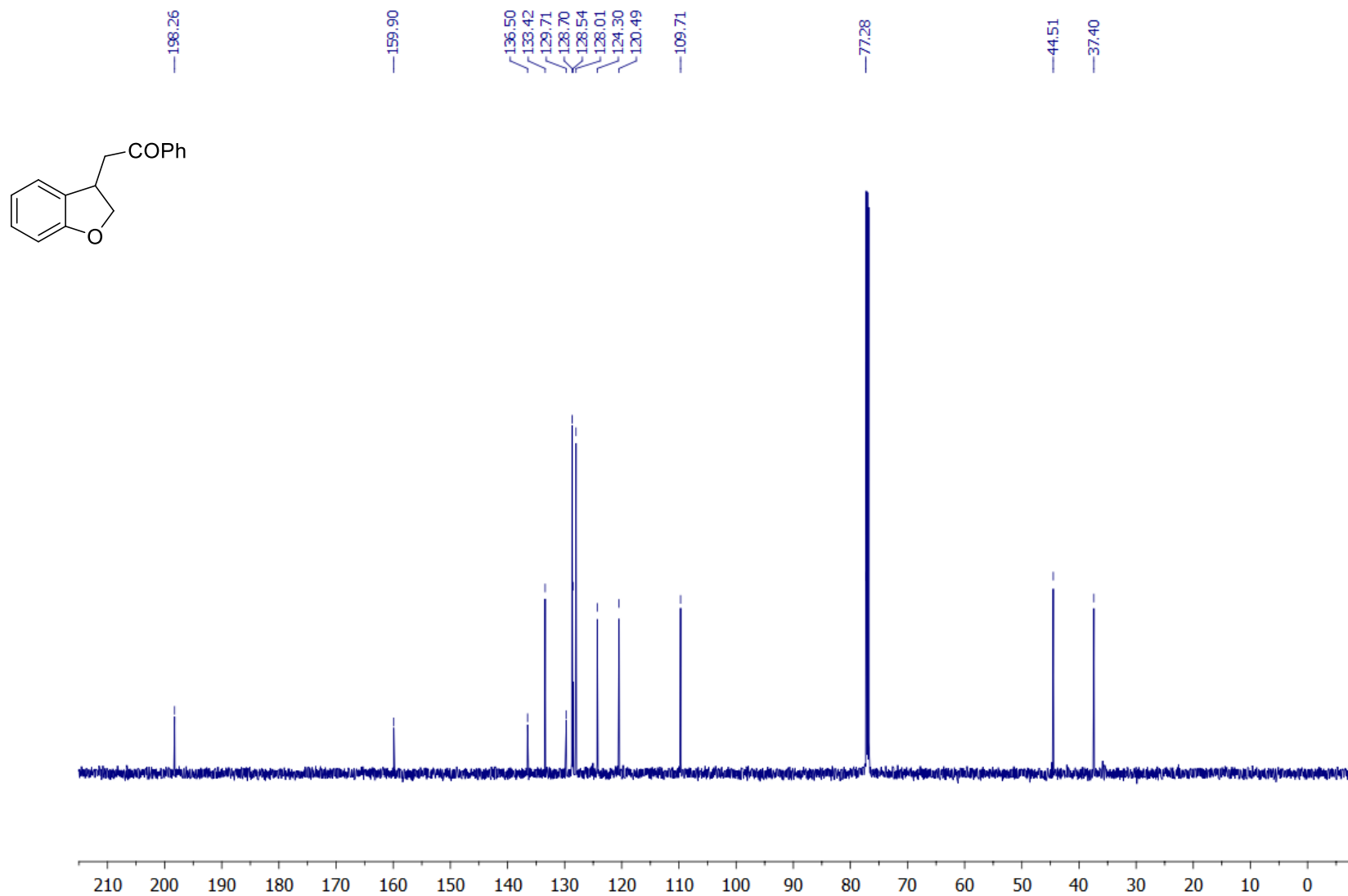
2-(2,3-Dihydro-1-benzofuran-3-yl)-1-phenylethanone (5o)

^1H NMR (CDCl_3 , 600 MHz)



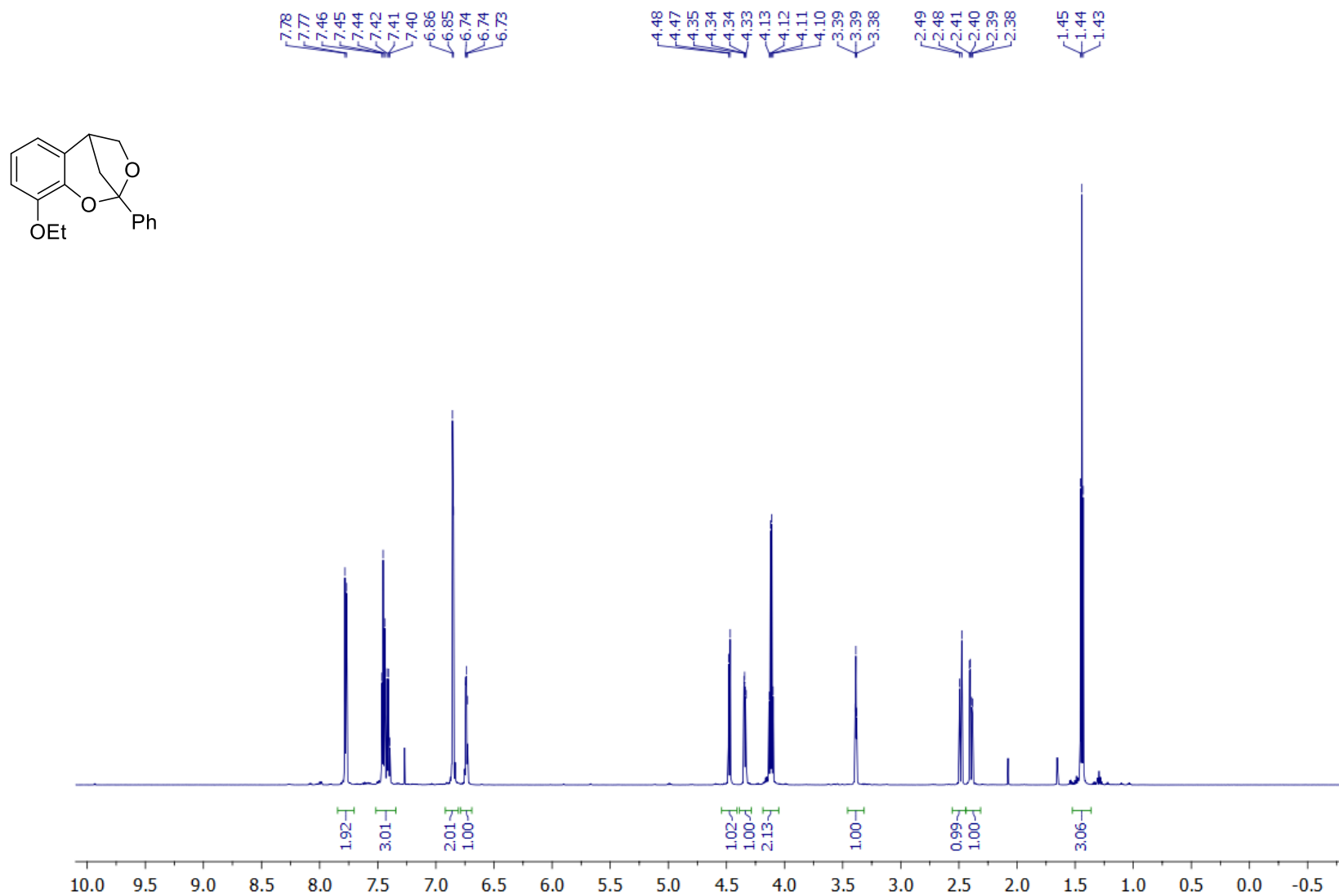
2-(2,3-Dihydro-1-benzofuran-3-yl)-1-phenylethanone (5o)

^{13}C NMR (CDCl_3 , 150 MHz)



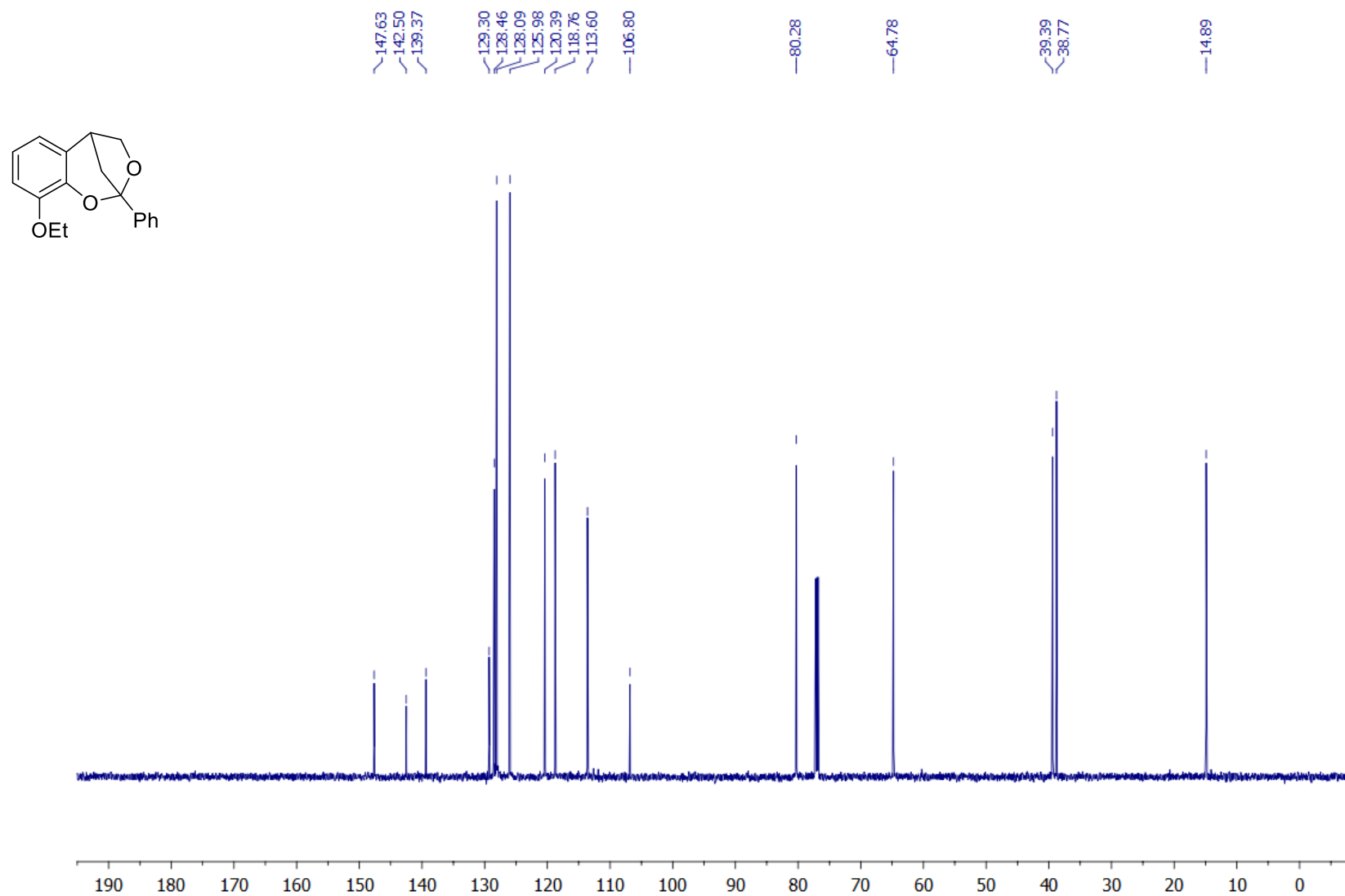
6-Ethoxy-9-phenyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4p)

¹H NMR (CDCl₃, 600 MHz)



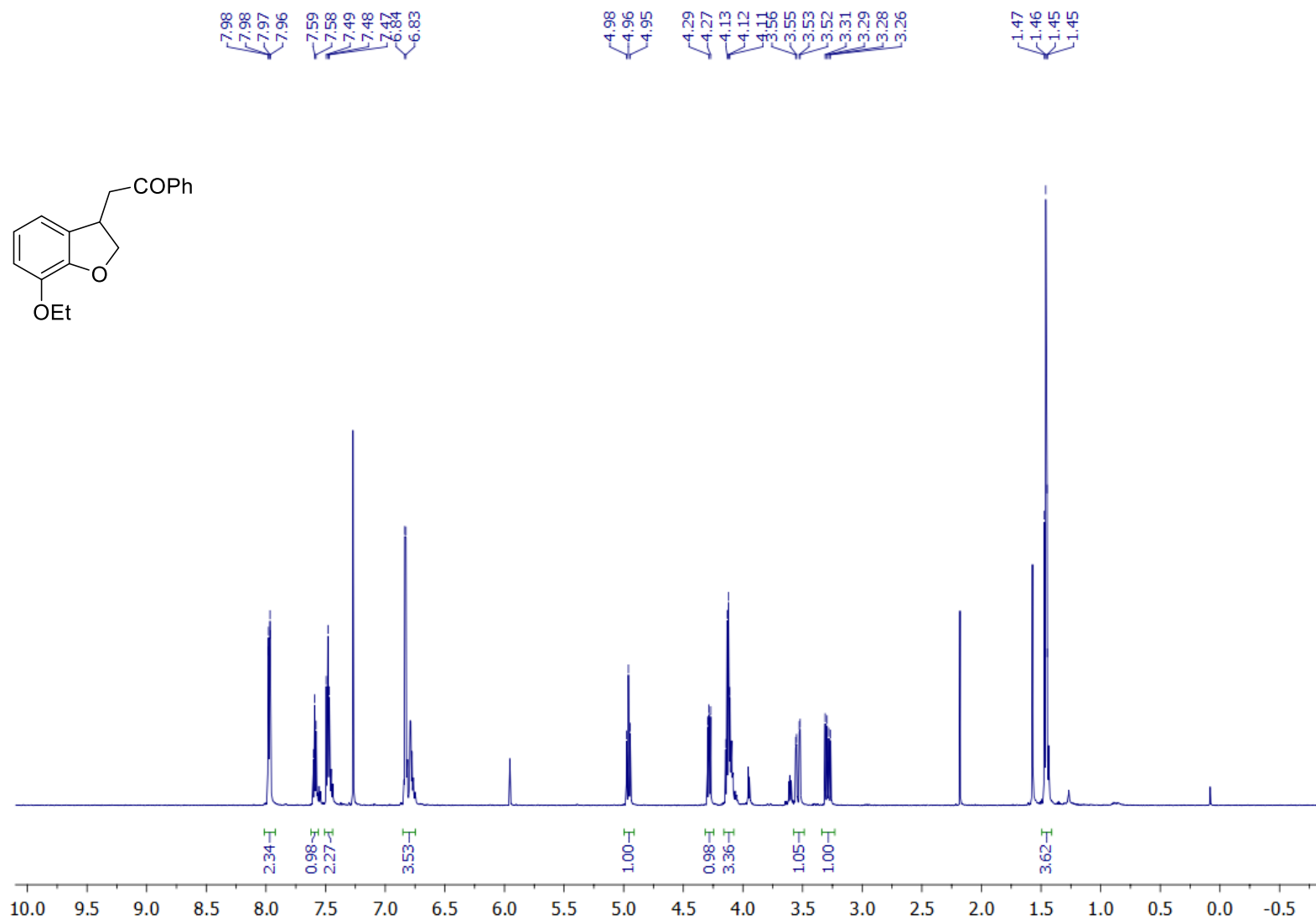
6-Ethoxy-9-phenyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4p)

¹³C NMR (CDCl₃, 150 MHz)



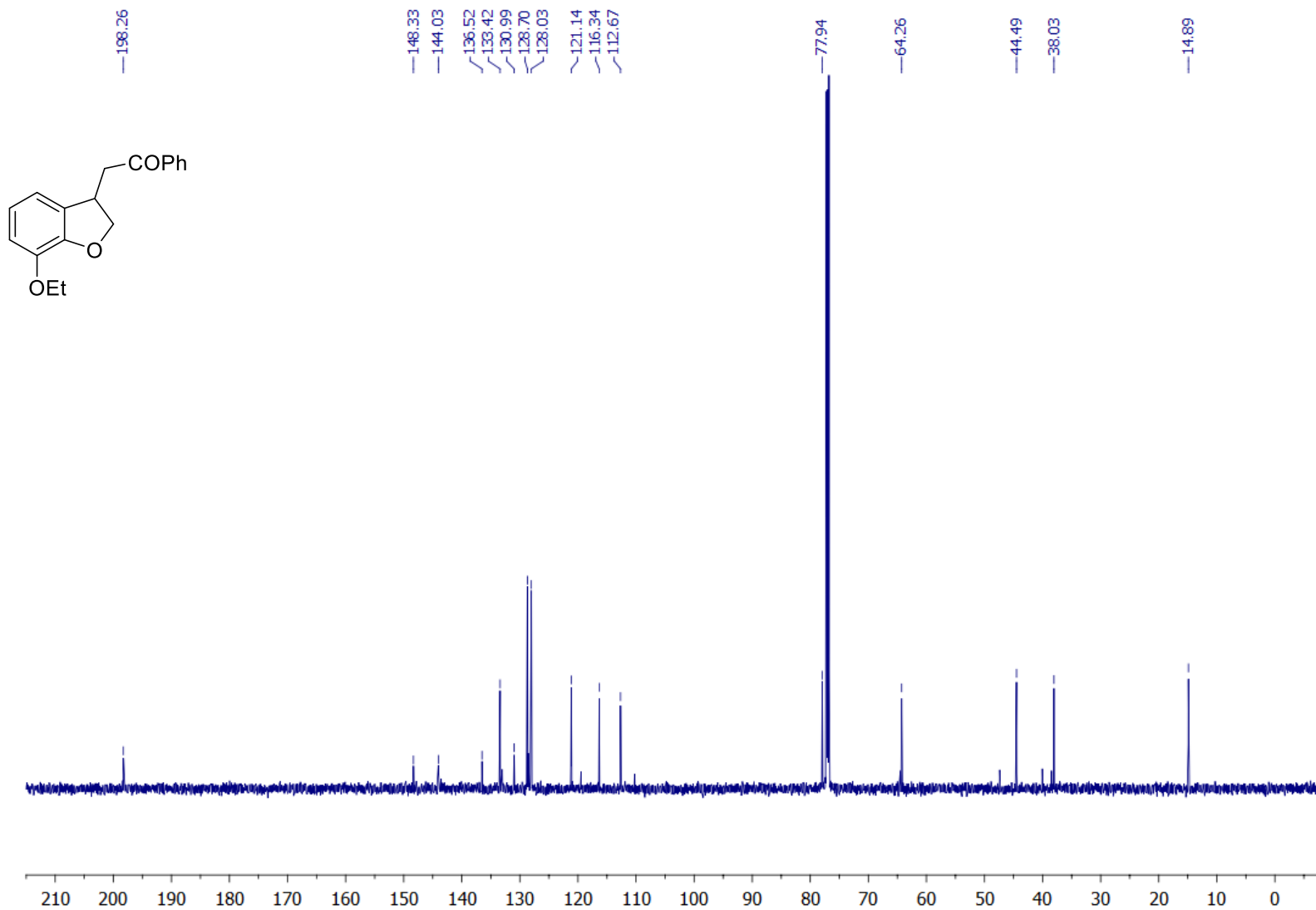
2-(7-Ethoxy-2,3-dihydro-1-benzofuran-3-yl)-1-phenylethanone (5p)

^1H NMR (CDCl_3 , 600 MHz)



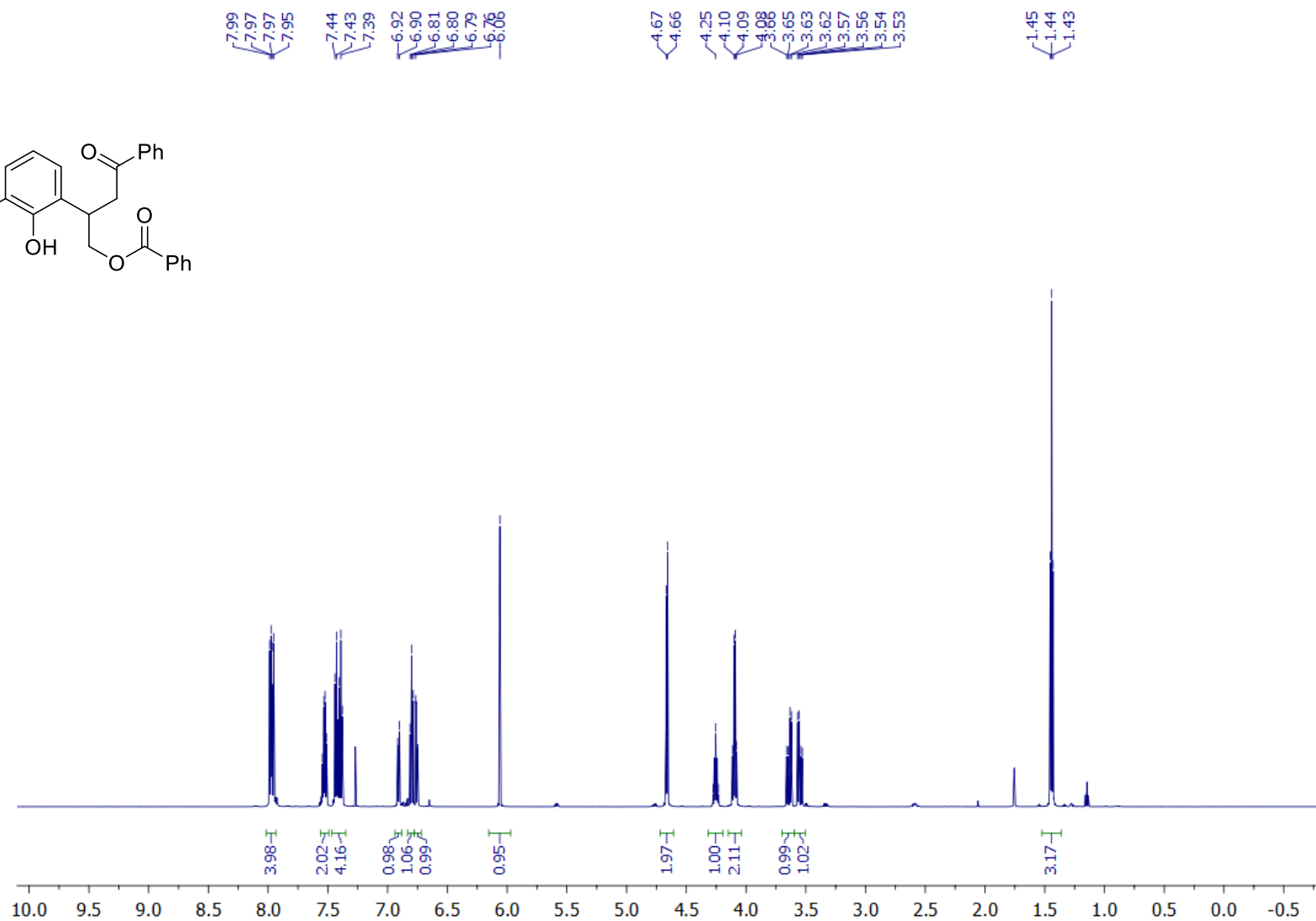
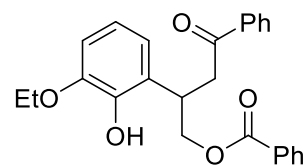
2-(7-Ethoxy-2,3-dihydro-1-benzofuran-3-yl)-1-phenylethanone (5p)

^{13}C NMR (CDCl_3 , 150 MHz)

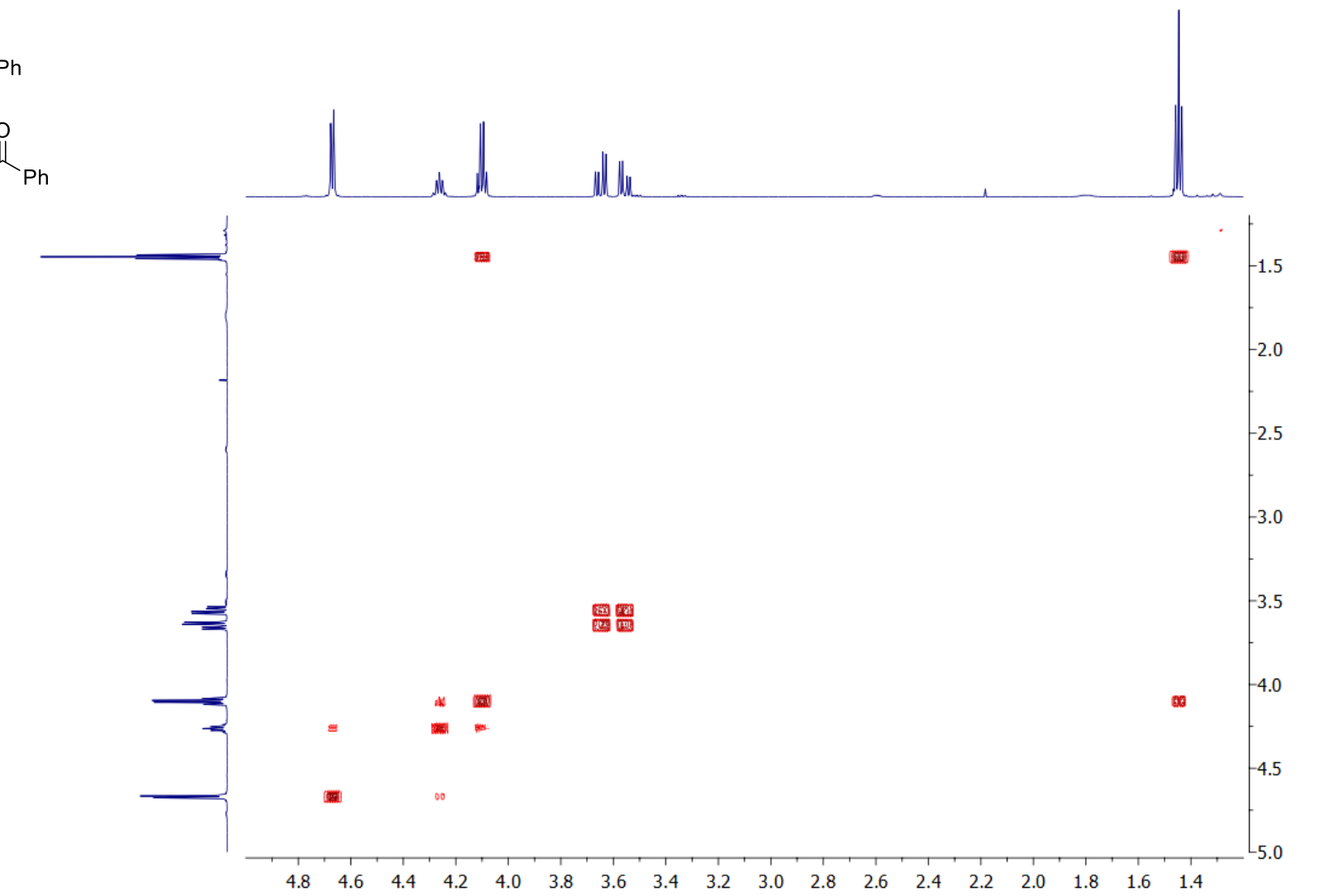
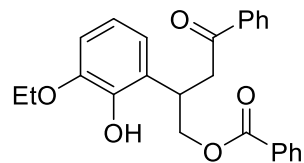


2-(3-Ethoxy-2-hydroxyphenyl)-4-oxo-4-phenylbutyl benzoate (6p)

^1H NMR (CDCl_3 , 600 MHz)



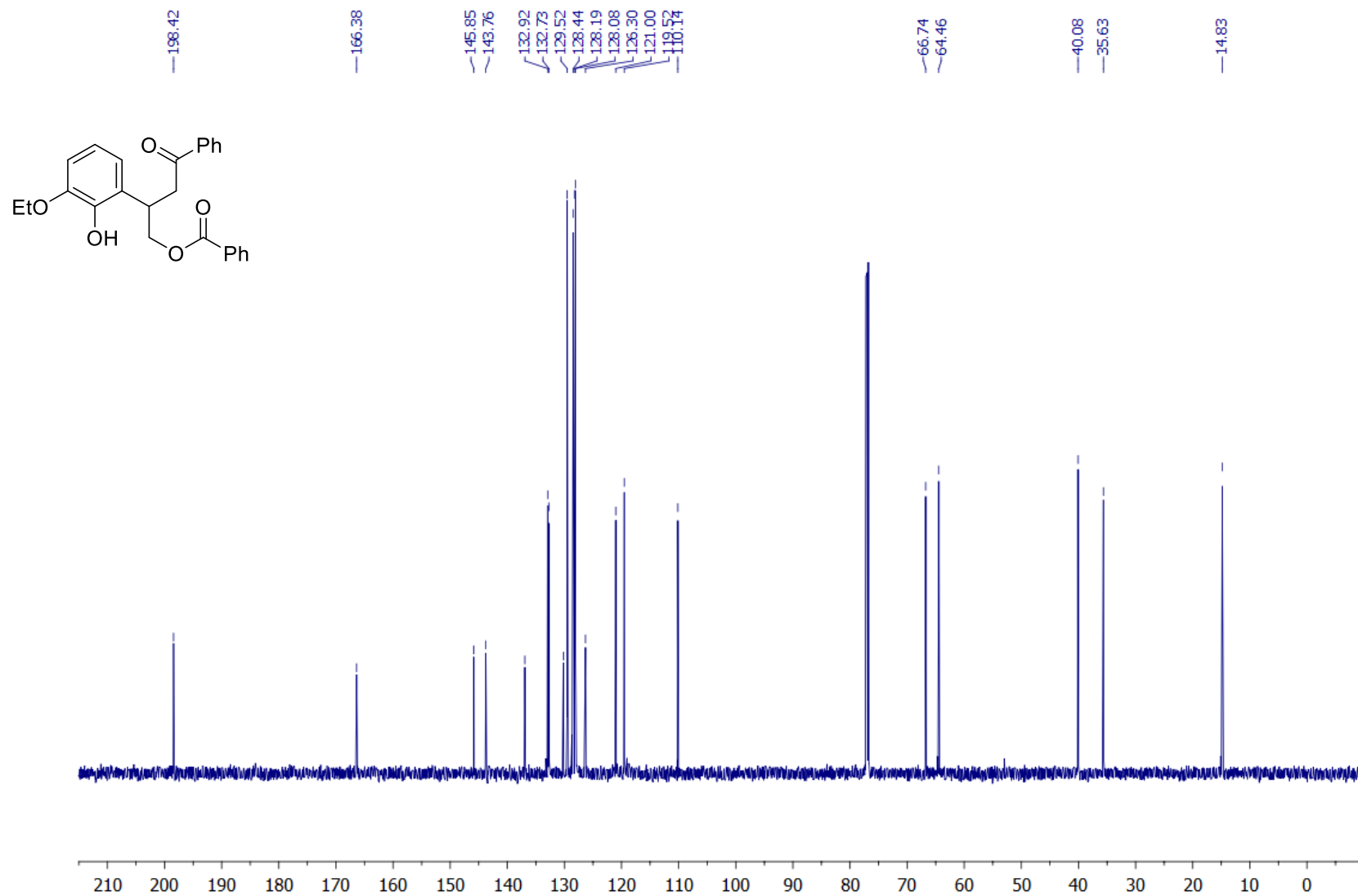
2-(3-Ethoxy-2-hydroxyphenyl)-4-oxo-4-phenylbutyl benzoate (6p)

¹H-¹H COSY (CDCl₃)

S460

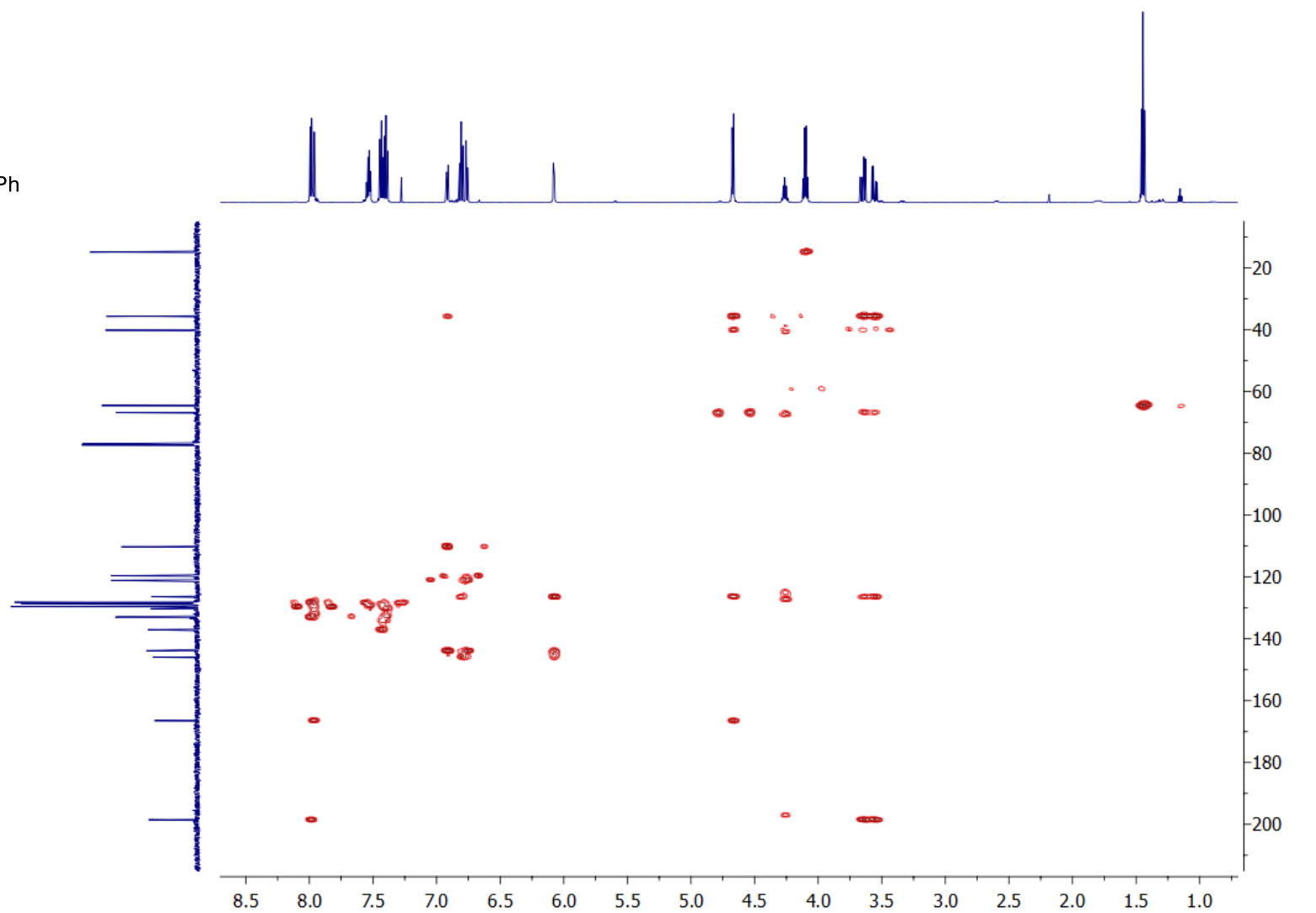
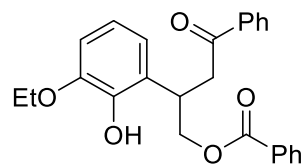
2-(3-Ethoxy-2-hydroxyphenyl)-4-oxo-4-phenylbutyl benzoate (6p)

^{13}C NMR (CDCl_3 , 150 MHz)



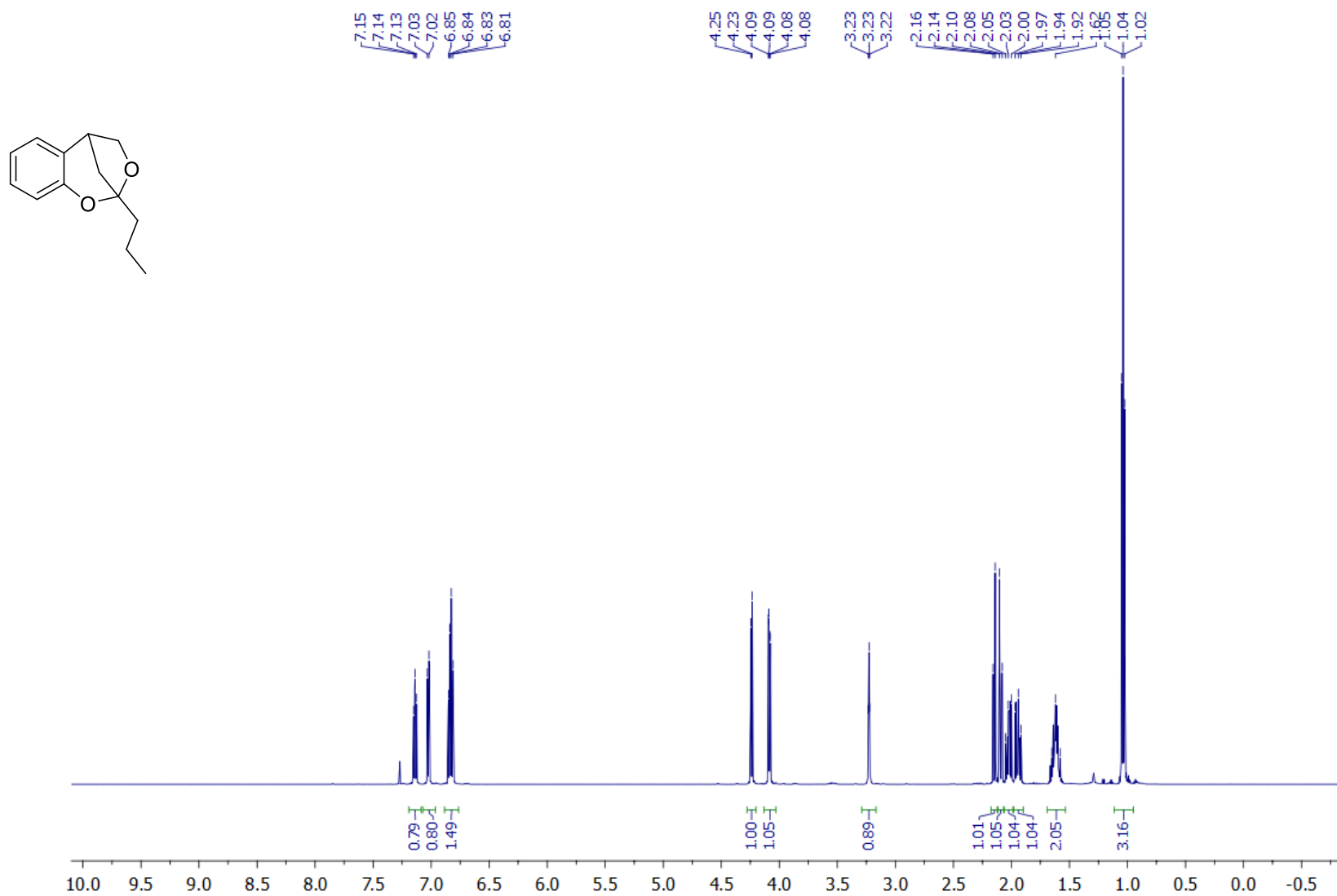
2-(3-Ethoxy-2-hydroxyphenyl)-4-oxo-4-phenylbutyl benzoate (6p)

^1H - ^{13}C HMBC (CDCl_3)



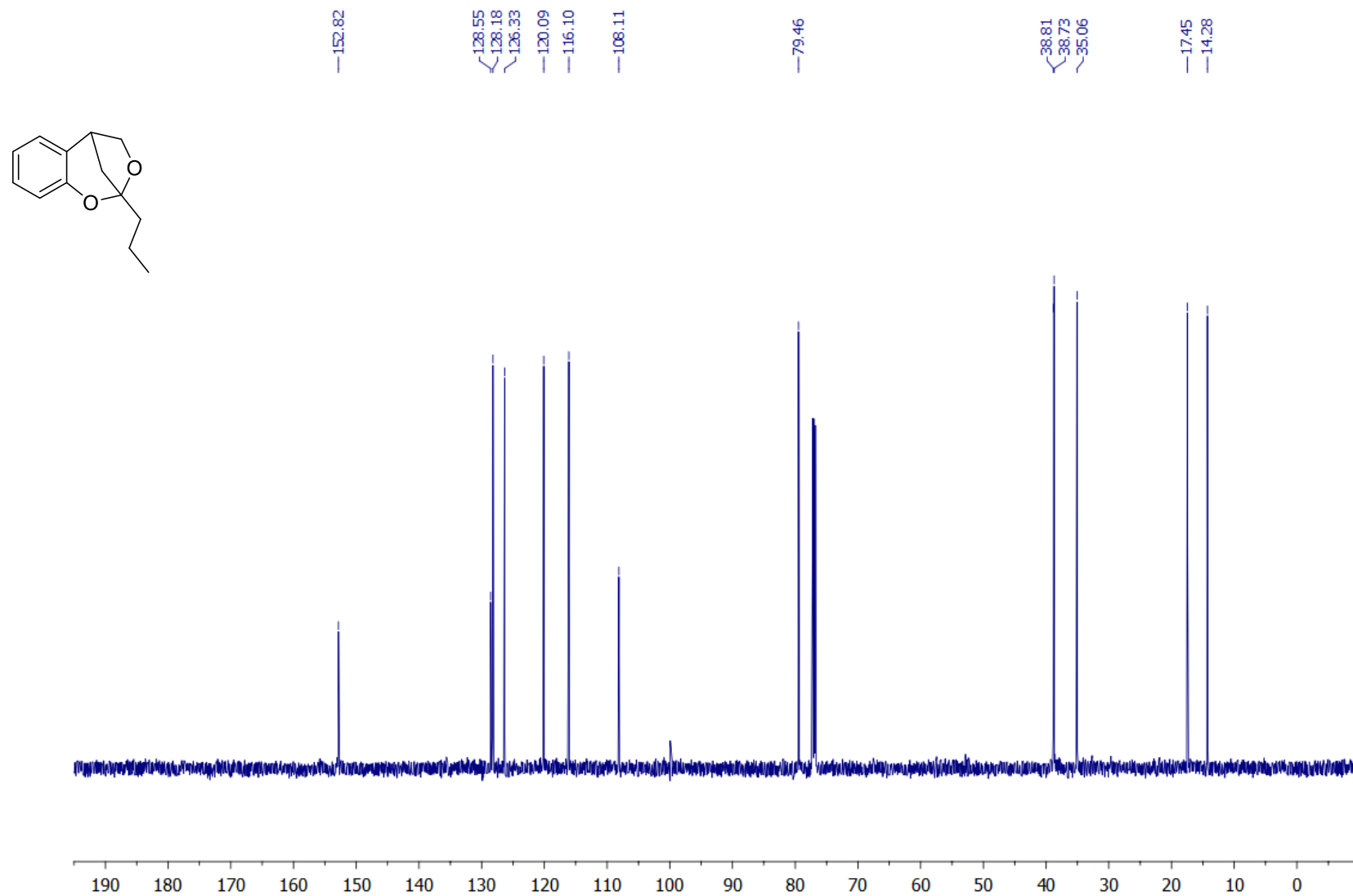
9-Propyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4q)

¹H NMR (CDCl₃, 600 MHz)



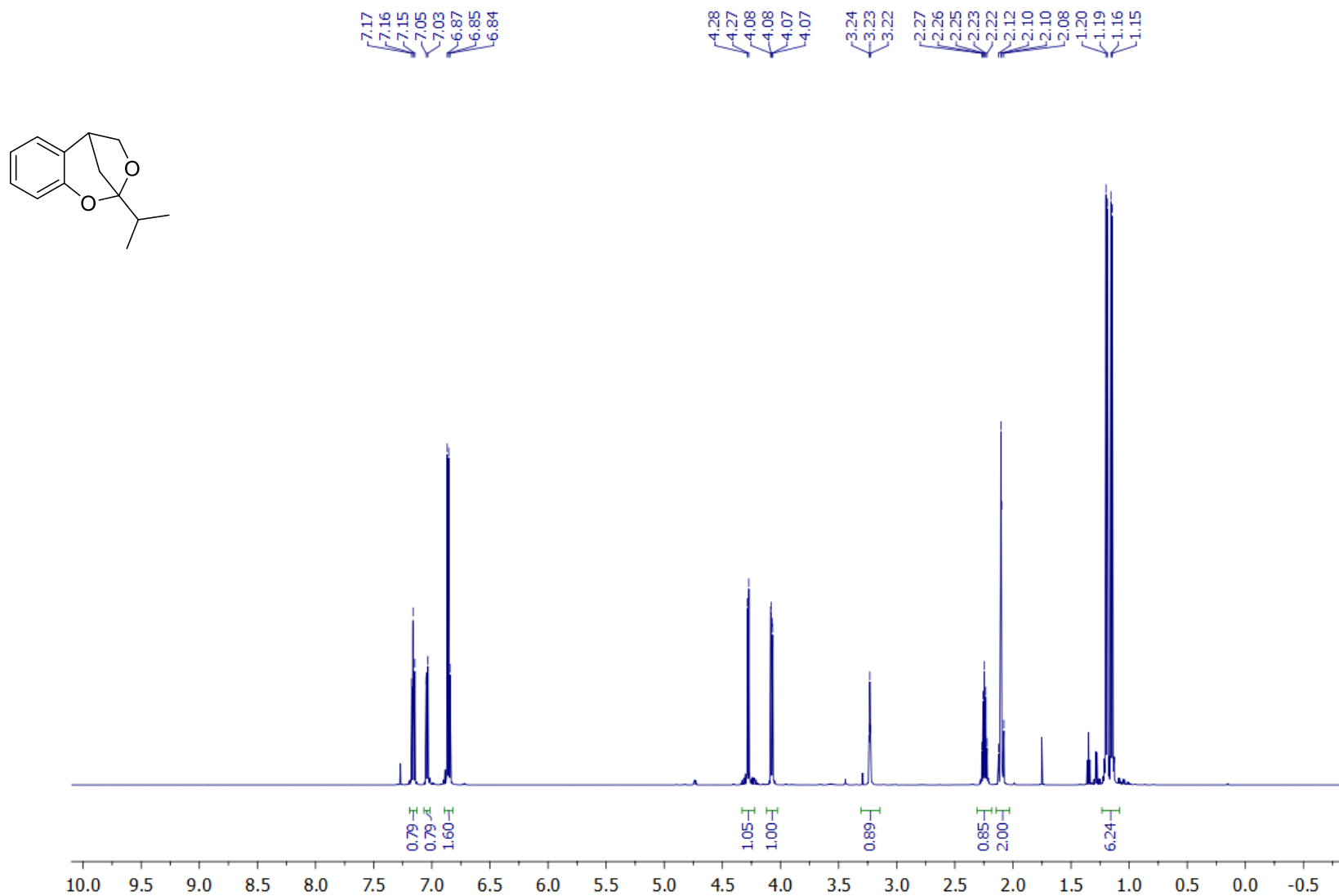
9-Propyl-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4q)

¹³C NMR (CDCl₃, 150 MHz)



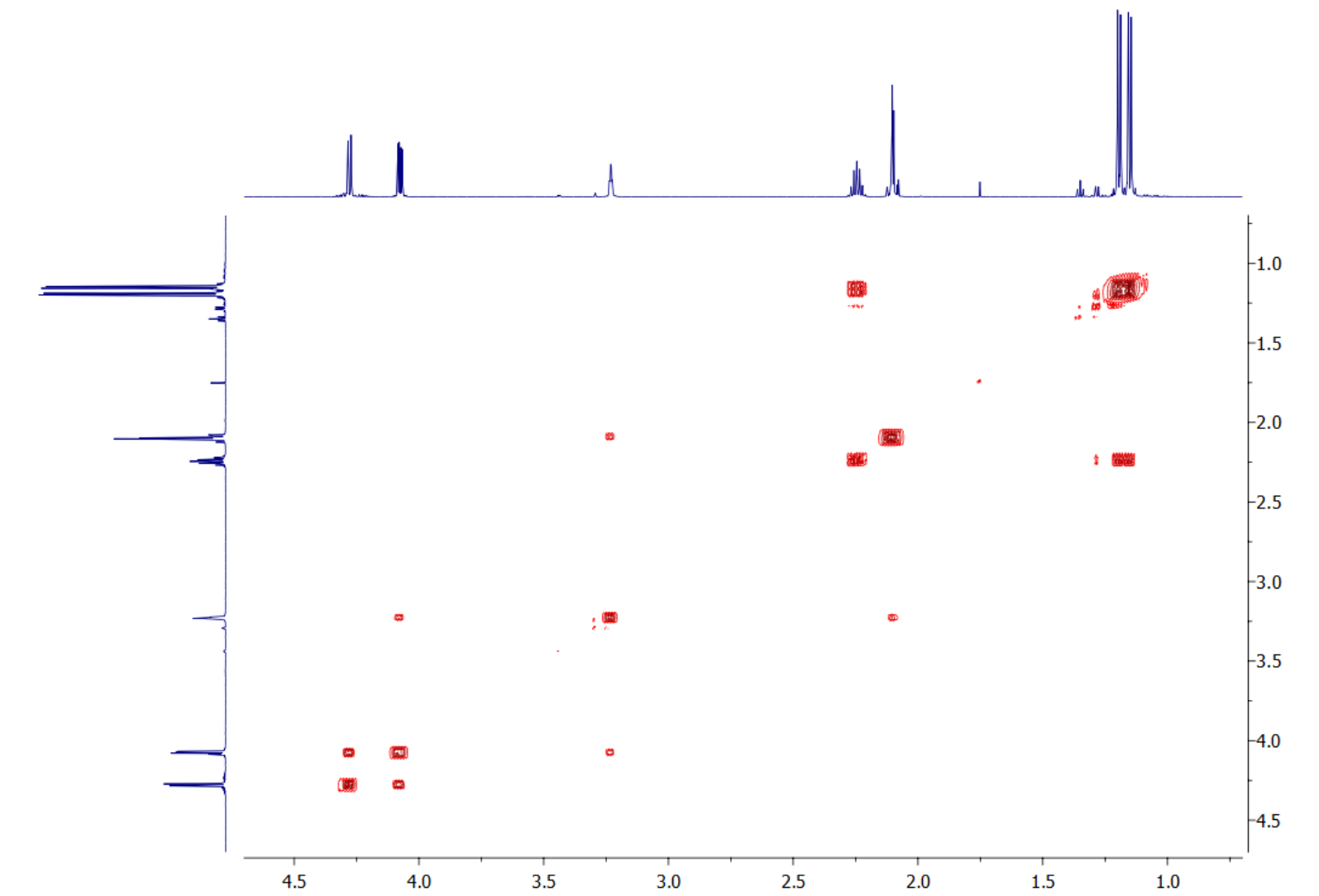
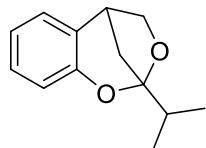
9-(Propan-2-yl)-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4r)

¹H NMR (CDCl₃, 600 MHz)



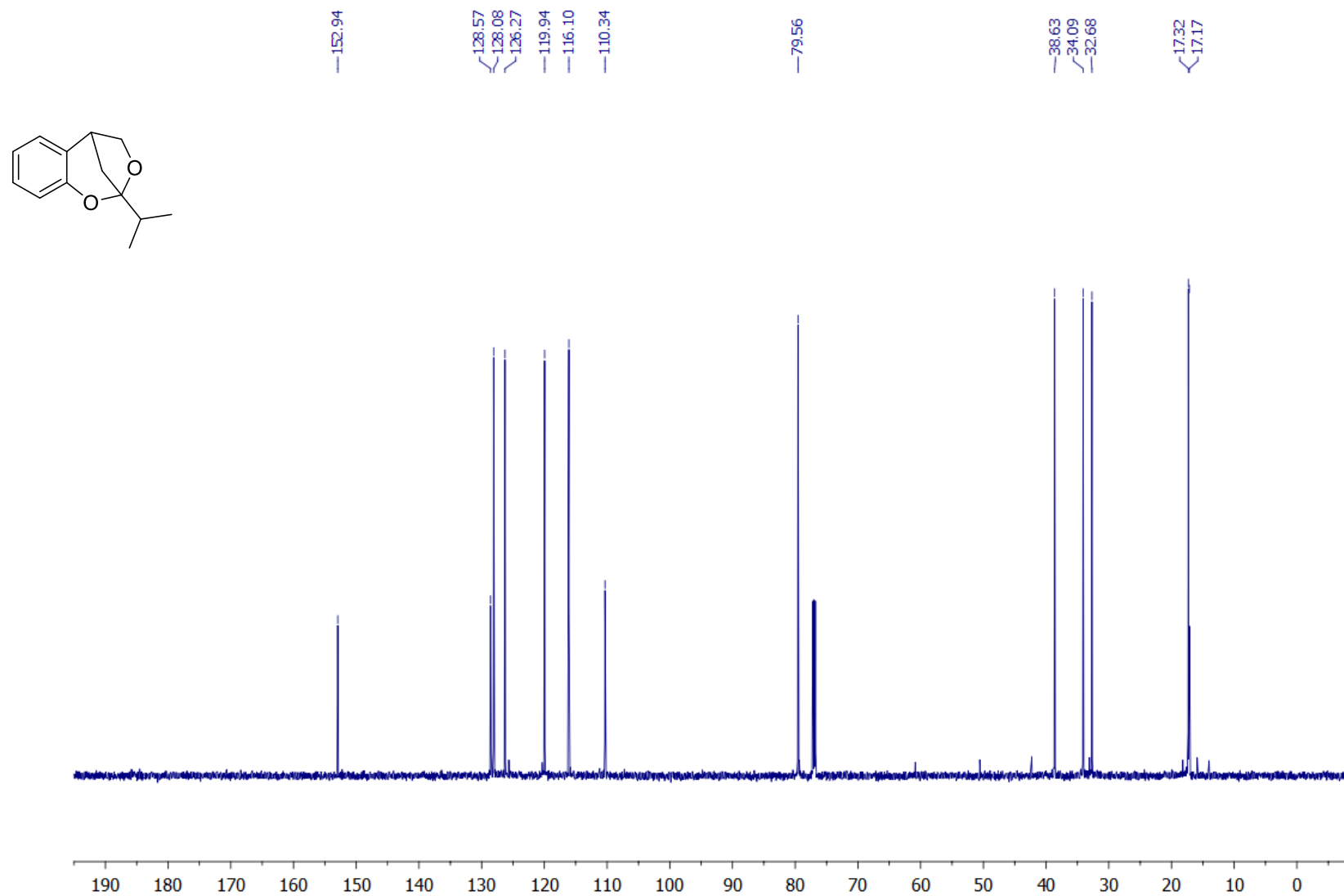
9-(Propan-2-yl)-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4r)

¹H-¹H COSY (CDCl₃)



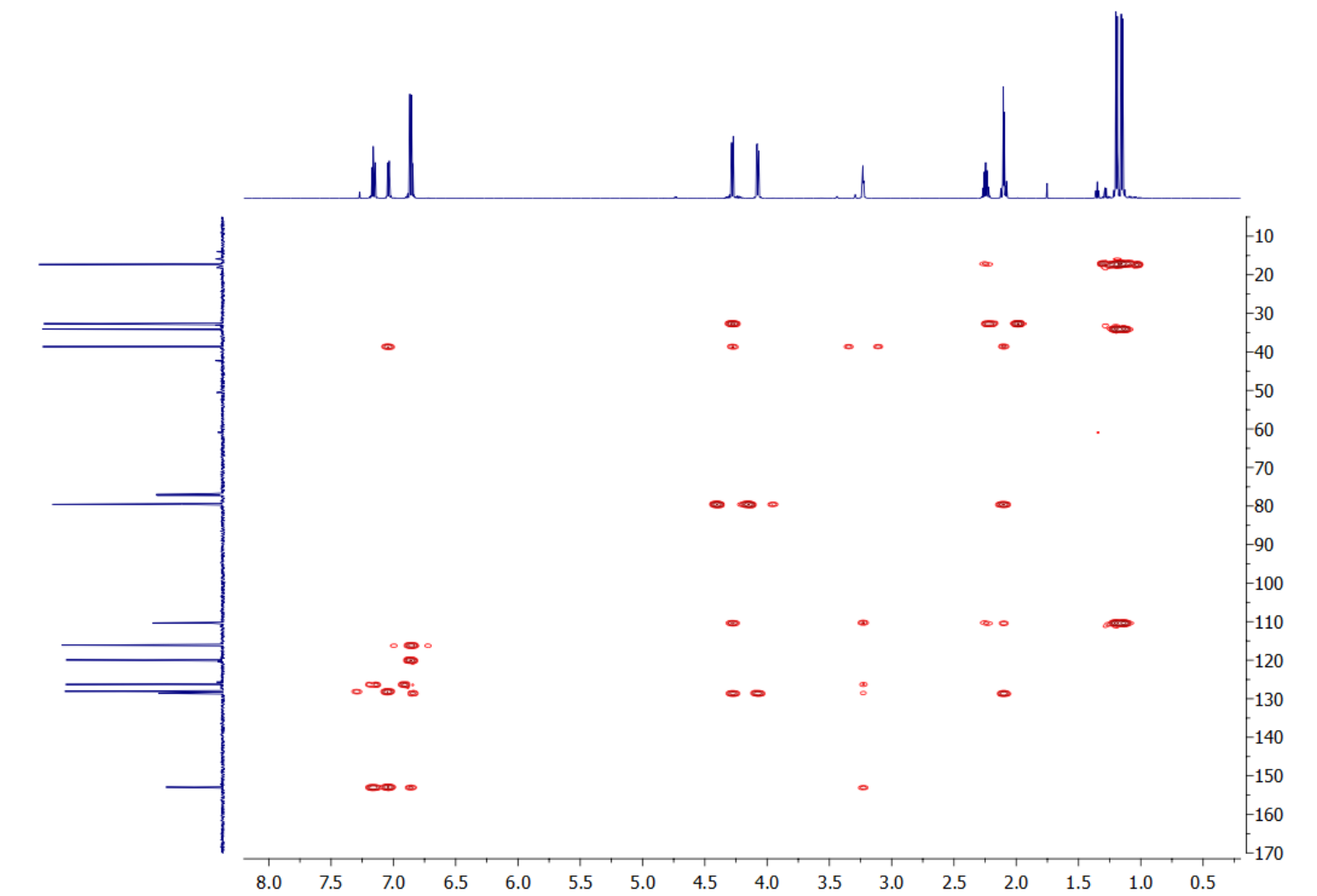
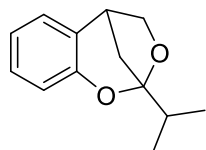
9-(Propan-2-yl)-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4r)

¹³C NMR (CDCl₃, 150 MHz)



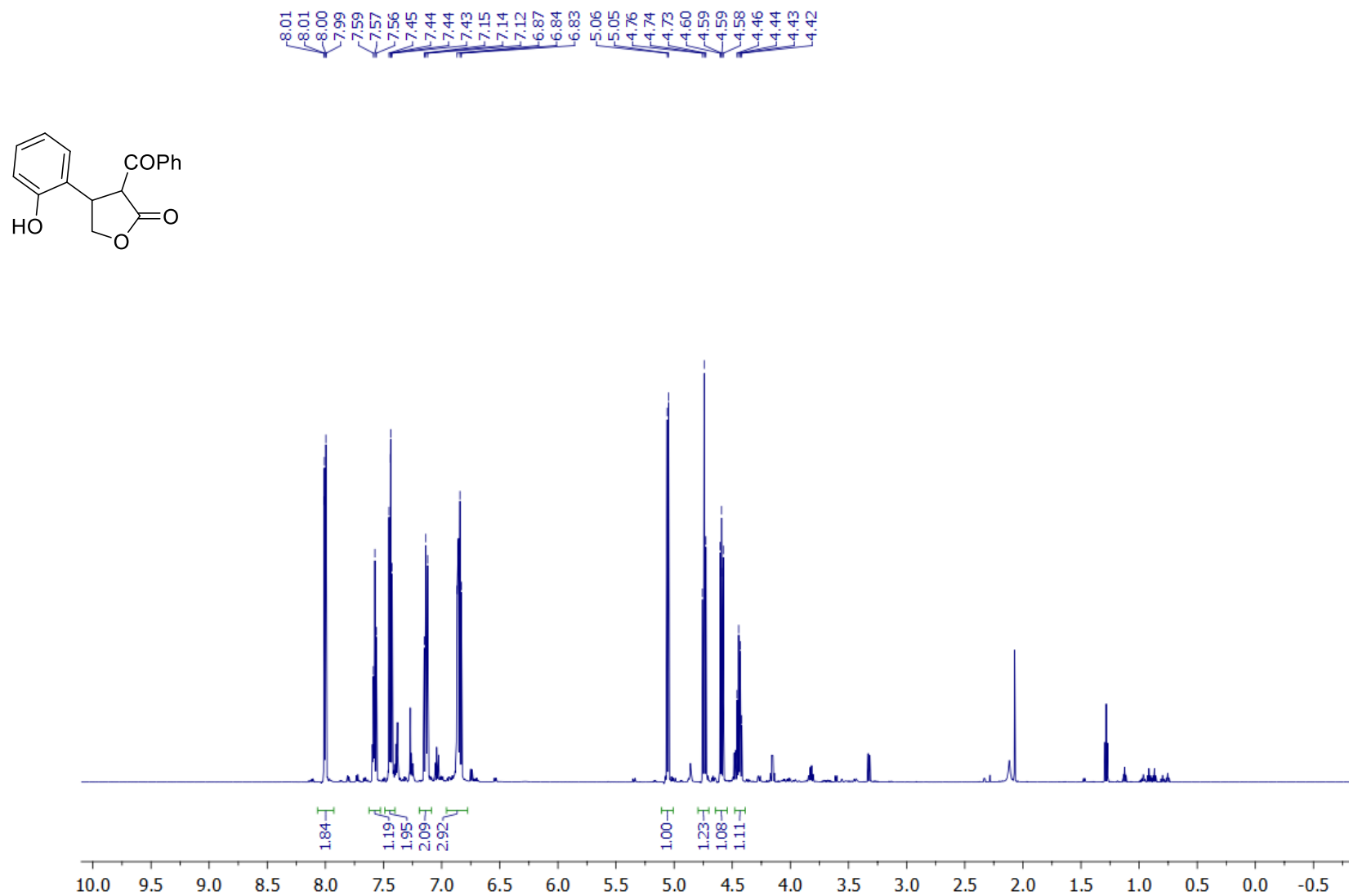
9-(Propan-2-yl)-8,10-dioxatricyclo[7.2.1.0^{2,7}]dodeca-2,4,6-triene (4r)

¹H-¹³C HMBC (CDCl₃)



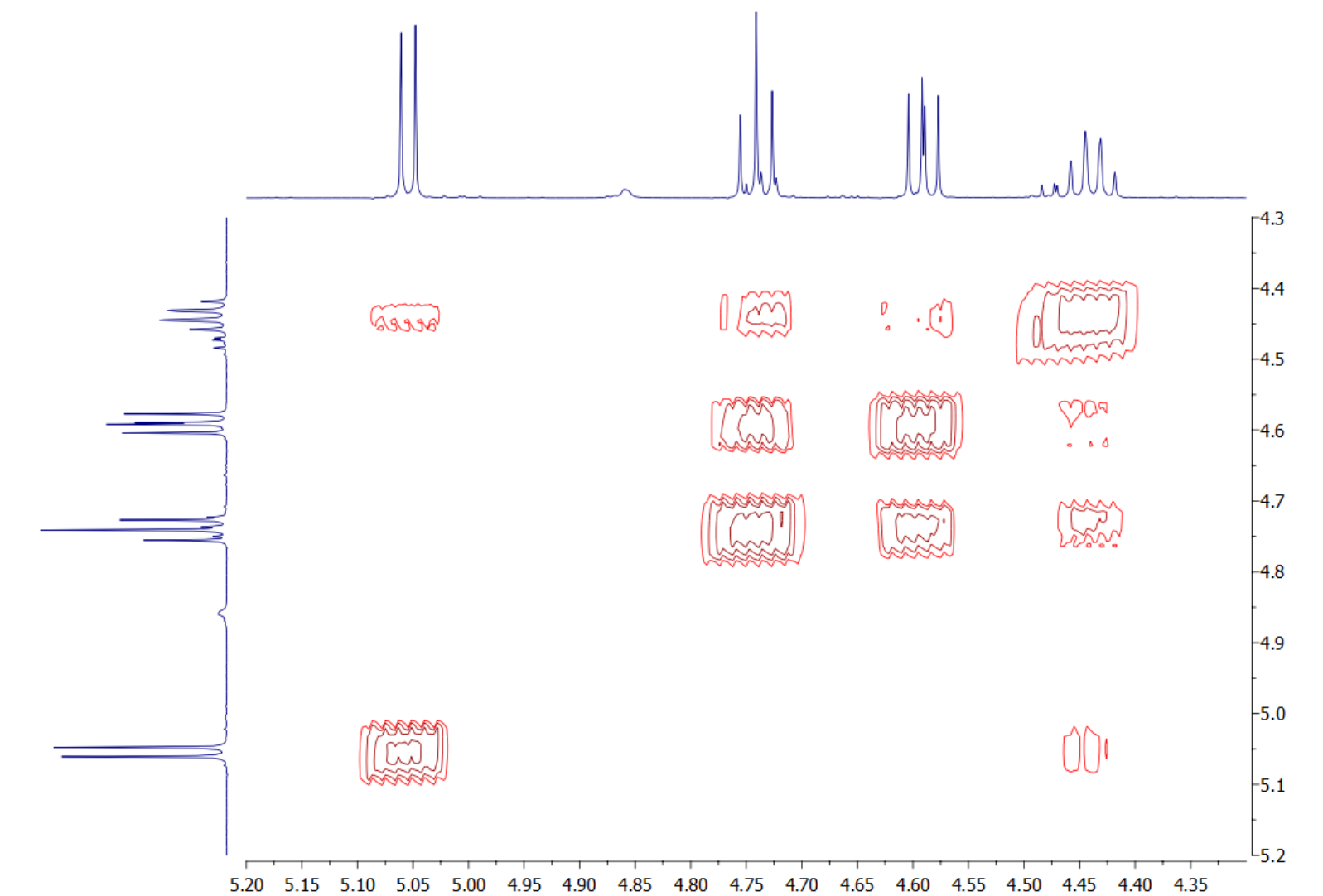
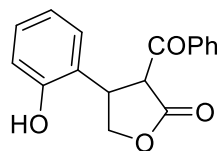
3-Benzoyl-4-(2-hydroxyphenyl)dihydrofuran-2(3H)-one (7)

^1H NMR (CDCl_3 , 600 MHz)



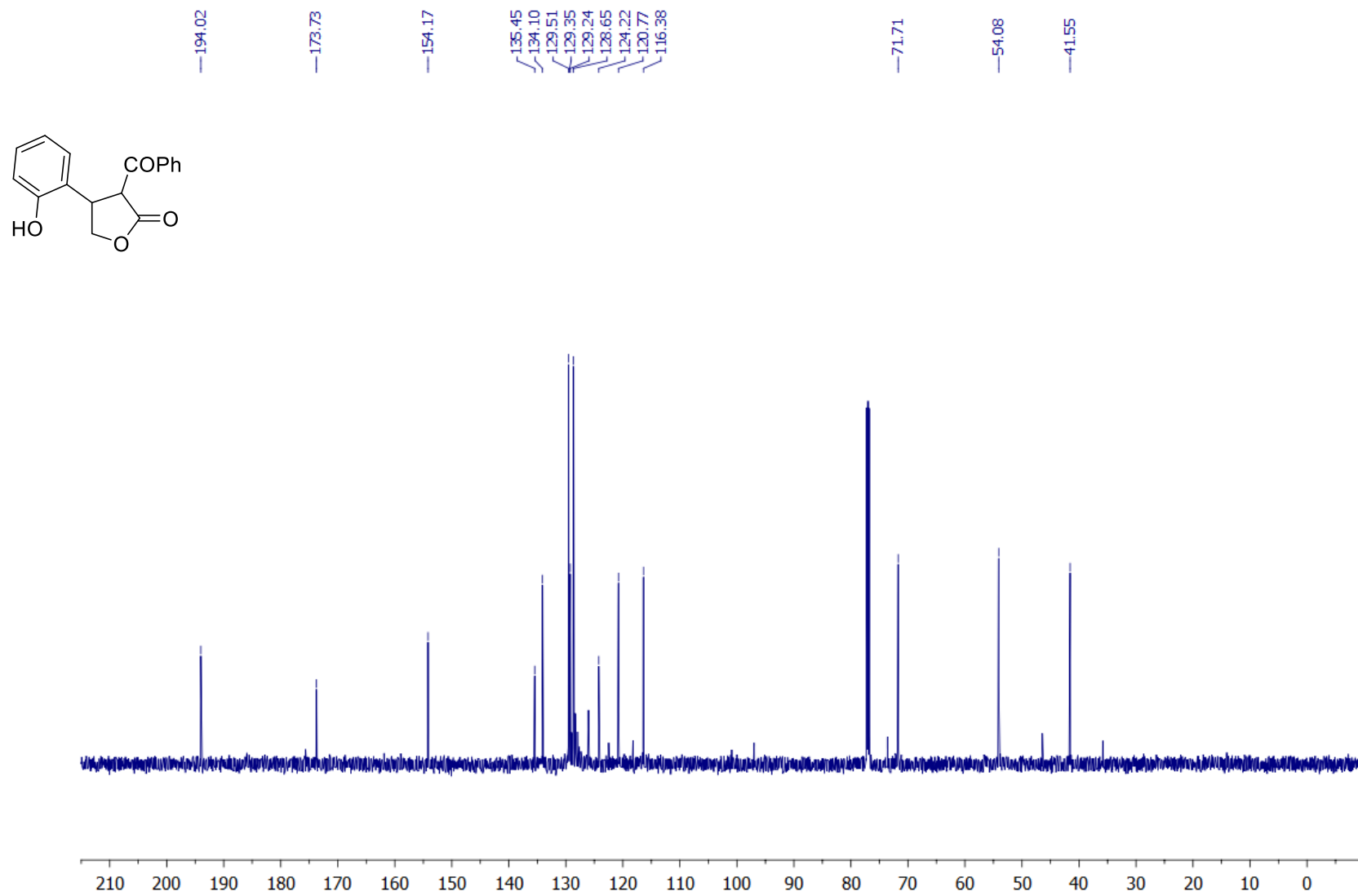
3-Benzoyl-4-(2-hydroxyphenyl)dihydrofuran-2(3H)-one (7)

^1H - ^1H COSY (CDCl_3)



3-Benzoyl-4-(2-hydroxyphenyl)dihydrofuran-2(3H)-one (7)

^{13}C NMR (CDCl_3 , 150 MHz)



3-Benzoyl-4-(2-hydroxyphenyl)dihydrofuran-2(3H)-one (7)

^1H - ^{13}C HMBC (CDCl_3)

