

Photochemical ring expansion reactions: synthesis of tetrahydrofuran derivatives and mechanism studies

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General Information

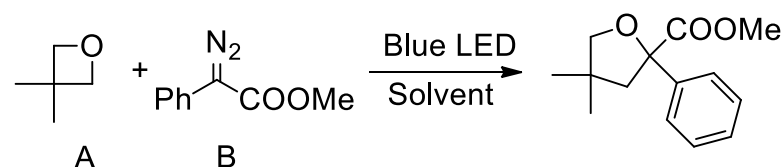
Unless otherwise noted, all commercially available compounds were used as provided without further purification. Chemicals used in this manuscript were purchased from Sigma Aldrich, Alfa Aesar, Chempur, Fluorochem and Carl Roth. Solvents used in reactions were p.A. grade. Solvents for chromatography were technical grade and distilled prior to use. Analytical thin-layer chromatography (TLC) was performed on Macherey-Nagel silica gel aluminium plates with F-254 indicator, visualized by irradiation with UV light. Column chromatography was performed using silica gel Merck 60 (particle size 0.063 – 0.2 mm). Solvent mixtures are understood as volume/volume. ¹H-NMR, ¹⁹F-NMR and ¹³C-NMR were recorded on a Varian AV600/AV400 or an Agilent DD2 400 NMR spectrometer in CDCl₃. Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated br (broadened singlet), s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet); coupling constants (J) are in Hertz (Hz). HRMS data were recorded on a ThermoFisher Scientific LTQ Orbitrap XL using ESI ionization or on a Finnigan MAT 95 using EI ionization at 70 eV. IR spectra were recorded on a Perkin Elmer-100 spectrometer and are reported in terms of frequency of absorption (cm⁻¹). LEDs used in this manuscript were purchased from Conrad Electronics: High Power LED-Module, 3 W, 30 lm, 30 °, 470 nm, art.nr. 180745 – 62. Used for batch and flow (1 to 8 modules) reactions. Reactions were irradiated from 1.5 cm, temperature was set to ambient and cooling was realized with a fan.

Important Safety Note

Handling of diazo compounds should only be done in a well-ventilated fume cupboard using an additional blast shield. No incidents occurred handling of diazoalkanes during the preparation of this manuscript, yet the reader should be aware of carcinogenicity and explosiveness of the herein described diazo compounds. General safety precautions when working with diazomethane and its derivatives should be followed. Any reactions described in this manuscript should not be performed without strict risk assessment and proper safety precautions.

Reaction Optimization

Table S1. Solvent Screen.

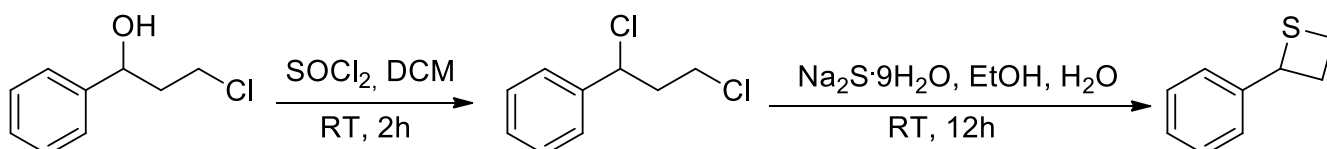


Entry ^[a]	Ratio (A : B)	Solvent	Time	Yield ^[b]
1.	5:1	DCM	Overnight	51%
2.	2:1	DCM	180 min	71%
3.	2:1	MeCN	180 min	62%
4.	2:1	Hexane	180 min	65%
5.	2:1	Chloroform	180 min	93%
6.	2:1	EtOAc	180 min	83%
7.	2:1	THF	180 min	11%
8.	2:1	Toluene	180 min	59%

[a] All reactions were done on 0.2 mmol scale using 2 mL of solvent. [b] Isolated yield.

Experimental Procedures

Synthesis of 2-phenylthietane^[1]



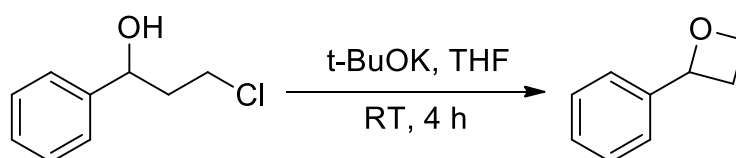
Step-I: To a solution of 3-chloro-1-phenylpropan-1-ol (5 mmol, 0.85 g, 1.0 equiv.) in 3 mL dichloromethane, thionyl chloride (SOCl₂, 15 mmol, 1.0 mol/L in dichloromethane, 15.0 mL, 3.0 equiv.) was added dropwise at room temperature. The mixture was kept stirring for 2 h, then poured into 15% sodium hydroxide solution slowly, extracted with dichloromethane (DCM, 3×30 mL), dried over sodium sulfate, filtered and concentrated in vacuo. The crude product was used directly without further purification.

Step-II: To a mixture of the crude product in 40 mL ethanol and 10 mL water, Na₂S·9H₂O (5.5 mmol, 1.32 g, 1.1 equiv.) was added at room temperature, stirred at 70 °C for 12 h. The reaction was concentrated in vacuo, water (30 mL) was added, extracted with diethyl ether (3×20 mL), dried over sodium sulfate, filtered and concentrated in vacuo. The crude product was further purified by silica gel flash chromatography (pentane : diethyl ether – 80:1) to give the product (15% yield) as a pale-yellow liquid.

¹H NMR (600 MHz, Chloroform-*d*): δ = 7.53 – 7.47 (m, 2H), 7.35 (t, *J* = 7.7 Hz, 2H), 7.28 – 7.24 (m, 1H), 4.95 (t, *J* = 8.4 Hz, 1H), 3.40 (q, *J* = 8.6 Hz, 1H), 3.22 – 3.09 (m, 2H), 2.98 (td, *J* = 9.0, 3.6 Hz, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 143.7, 128.4, 127.3, 127.1, 44.5, 36.3, 21.0 ppm.

Synthesis of 2-phenyloxetane^[2]

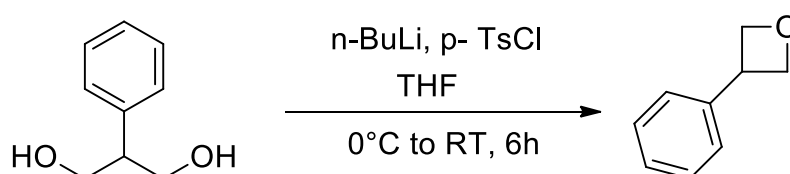


To a 100 mL round bottom flask equipped with a stir bar was added 3-chloro-1-phenylpropanol (5.0 mmol, 0.85 g, 1.0 equiv.) and THF 40 ml. Potassium tert-butoxide (1.68 g, 15 mmol, 3.0 equiv.) was added and the solution was allowed to stir at room temperature for four hours. Color change to orange was observed. After this time, the crude mixture was concentrated in vacuo by rotary evaporation, then diluted with Et₂O (30 ml) and deionized water (30 ml). The phases were separated and the aqueous layer was extracted with Et₂O (3 × 30 mL). The combined organic layers were washed with deionized water (≈ 25 mL), brine (≈ 25 mL), and dried with Na₂SO₄. The solvent was removed in vacuo by rotary evaporation to give the pure product (476 mg, 71%) as a colorless oil.

¹H NMR (600 MHz, Chloroform-*d*): δ = 7.48 – 7.43 (m, 2H), 7.43 – 7.37 (m, 1H), 7.33 – 7.29 (m, 1H), 5.82 (t, *J* = 7.5 Hz, 1H), 4.84 (td, *J* = 8.0, 5.9 Hz, 1H), 4.67 (dt, *J* = 9.2, 5.8 Hz, 1H), 3.06 – 3.00 (m, 1H), 2.71 – 2.64 (m, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 143.5, 128.4, 127.7, 125.2, 82.9, 68.2, 30.7 ppm.

Synthesis of 3-phenyloxetane^[3]



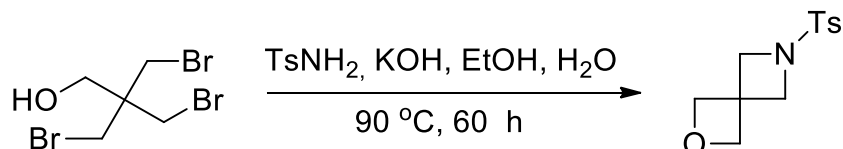
To a solution of 2-phenylpropane-1,3-diol (1.5g, 10 mmol, 1.0 equiv.) in THF (75 mL) was added *n*-BuLi (4.0 mL, 2.5 M in hexanes, 1.0 equiv.) at 0 °C. The reaction mixture was stirred for 30 min at 0 °C, at which point a solution

of *p*-toluenesulfonyl chloride (2.0 g, 11.0 mmol, 1.1 equiv.) in the THF (12 mL) was added via cannula. The reaction mixture was stirred for 1 h at 0 °C and *n*-BuLi (4.0 mL, 2.5 M in hexanes, 1.0 equiv.) was added. The reaction mixture was stirred at 60 °C for 6 h and cooled. The solution was diluted with Et₂O (100 mL) and extracted with H₂O (100 mL). The aqueous layer was extracted with Et₂O (2 x 500 mL). The combined organic layers were dried over MgSO₄, filtered and concentrated. The residue obtained was purified via column chromatography (pentane : diethyl ether – 20:1) to yield the product as a colorless oil (0.84g, 63%).

¹H NMR (600 MHz, Chloroform-*d*): δ = 7.45 – 7.35 (m, 4H), 7.30 – 7.24 (m, 1H), 5.08 (dd, *J* = 8.4, 6.0 Hz, 2H), 4.84 – 4.75 (m, 2H), 4.34 – 4.19 (m, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 141.5, 128.7, 127.0, 126.7, 78.9, 40.3 ppm.

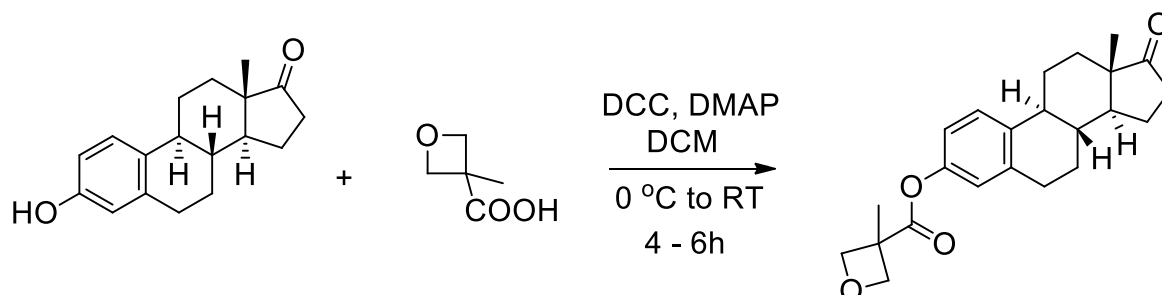
6-tosyl-2-oxa-6-azaspiro[3.3]heptane^[1]



To a mixture of potassium hydroxide (2.87 g, 51.2 mmol, 3.2 equiv.) and *p*-tosylamide (3.40 g, 19.2 mmol, 1.2 equiv.) in 260 mL ethanol, 3-bromo-2,2-bis(bromomethyl)propan-1-ol (5.23 g, 16 mmol, 1.0 equiv.) was added at room temperature and the reaction mixture was heated to 90 °C for 60 h. After completion of the reaction, the solvent was evaporated, then 50 mL 1.0 M potassium hydroxide aqueous solution was added and the white suspension was stirred for additional 2 h at room temperature. The mixture was filtered and the white filter was rinsed with water until the washing water was neutral. The filter was dried under vacuum to give the crude product (51% yield) as a white solid.

¹H NMR (400 MHz, Chloroform-*d*): δ = 7.69 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 4.57 (s, 4H), 3.89 (s, 4H), 2.44 (s, 3H) ppm.

(8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl 3-methyloxetane-3-carboxylate



To a stirred, ice cooled solution of the 3-methyloxetane-3-carboxylic acid (580 mg, 5.0 mmol, 1.0 equiv.), and estrone (1.6 g, 6.0 mmol, 1.2 equiv.) in 10 mL DCM was added a solution of DCC (1.34 g, 6.5 mmol, 1.3 equiv.) and DMAP (61 mg, 0.5 mmol, 0.1 equiv.) in 5 mL DCM at once. The solution was stirred 6 h while slowly warming up to room temperature. After finishing the reaction, the solid was filtered off and washed with Et₂O. The solvent was evaporated, and the residue was purified by silica gel column chromatography. (hexane : ethyl acetate - 9:1 – 4:1) provided the product as a white solid (76%, 1.4 g).

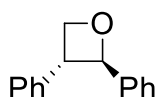
¹H NMR (300 MHz, Chloroform-*d*): δ = 7.37 – 7.24 (m, 1H), 6.95 – 6.80 (m, 2H), 5.10 (d, *J* = 6.1 Hz, 2H), 4.51 (d, *J* = 6.1 Hz, 2H), 2.92 (dd, *J* = 8.5, 3.9 Hz, 2H), 2.51 (dd, *J* = 18.3, 8.4 Hz, 1H), 2.45 – 2.37 (m, 1H), 2.36 – 2.24 (m, 1H), 2.22 – 2.11 (m, 1H), 2.11 – 1.91 (m, 3H), 1.76 (s, 3H), 1.68 – 1.40 (m, 6H), 0.91 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 220.6, 173.2, 148.3, 138.1, 137.6, 126.4, 121.2, 118.4, 79.4, 50.4, 47.9, 44.7, 44.1, 37.9, 35.8, 31.5, 29.3, 26.3, 25.7, 21.8, 21.5, 13.8 ppm.

HRMS (ESI): Mass found: 391.18799, calculated mass for C₂₃H₂₈NaO₄⁺: 391.18798.

IR (KBr): 3453, 3058, 2931, 2879, 2164, 1959, 1732, 1605, 1493, 1454, 1374, 1296, 1214, 1149, 1116, 1052, 977, 914, 832, 778, 704 cm⁻¹.

trans-2,3-diphenyloxetane



Anhydrous benzaldehyde (424 mg, 4 mmol) and styrene (2.0 g, 20 mmol, 5.0 equiv.) in degassed Benzene (20 mL) were taken in Pyrex tube (argon atmosphere) and irradiate with a 150 W mercury lamp at room temperature for 48 h. The solvent was removed in vacuo and chromatography on silica gel (pentane : diethyl ether – 20 : 1) yielded the 2,3-diphenyloxetane as a colorless oil, (65%, d.r. > 20:1, 546 mg).

¹H NMR (600 MHz, Chloroform-*d*): δ = 7.48 – 7.44 (m, 2H), 7.43 – 7.37 (m, 6H), 7.35 – 7.28 (m, 2H), 5.77 (d, *J* = 7.0 Hz, 1H), 4.99 (dd, *J* = 8.7, 6.0 Hz, 1H), 4.91 (dd, *J* = 7.7, 6.0 Hz, 1H), 4.06 – 4.12 (m, 1H) ppm.

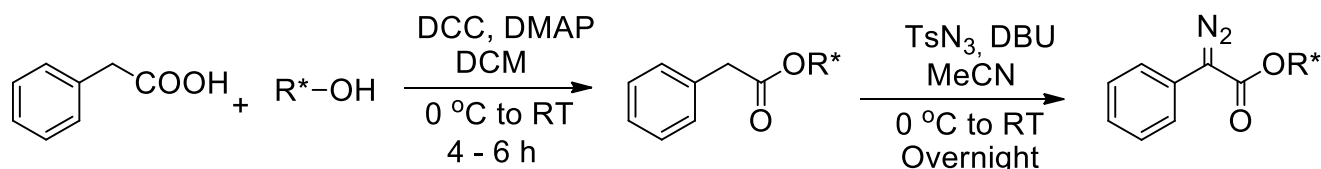
¹³C NMR (151 MHz, Chloroform-*d*): δ = 142.4, 140.0, 128.7, 128.5, 128.0, 127.2, 127.0, 125.2, 90.1, 74.1, 49.7 ppm.

HRMS (ESI): Mass found: 233.09331, calculated mass for C₁₅H₁₄NaO⁺: 233.09369.

IR (KBr): 3463, 3060, 3029, 2953, 2879, 2330, 2078, 1989, 1955, 1882, 1809, 1741, 1684, 1602, 1493, 1451, 1372, 1282, 1212, 1184, 1154, 1076, 1027, 977, 935, 869, 816 cm⁻¹.

General Procedures

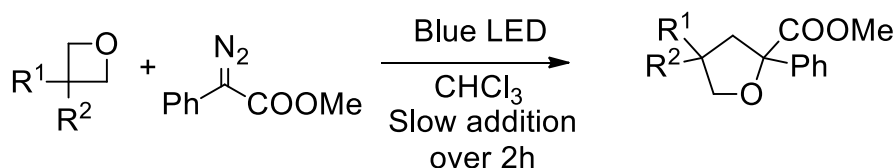
General Procedure for the synthesis of chiral diazoacetates – (GP-I):



Step-I: To a stirred, ice cooled solution of the phenylacetic acid (1.3 g, 10 mmol, 1 equiv.), and chiral alcohol (12 mmol, 1.2 equiv.) in 20 mL DCM was added a solution of DCC (13 mmol, 1.3 equiv.) and DMAP (1 mmol, 0.1 equiv.) in 10 mL DCM at once. The solution was stirred 6 h while slowly warming up to room temperature. After finishing the reaction, the solid was filtered off and washed with Et₂O. The solvent was evaporated, and the residue was purified by silica gel column chromatography (pentane : Et₂O 40:1 – 20:1) provided the desired ester.

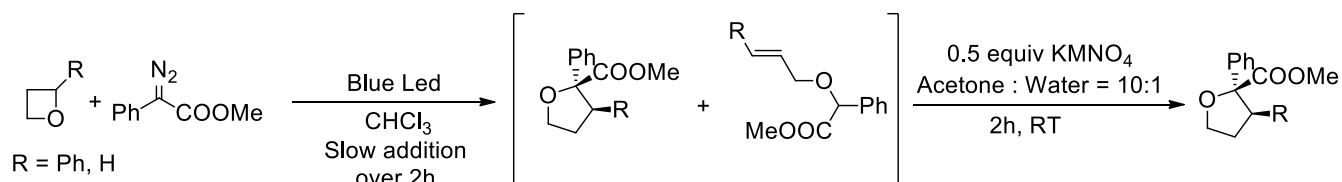
Step-II: To a stirred, ice cooled solution of the ester (5 mmol, 1 equiv.) and p-Tosyl azide (5.5 mmol, 1.1 equiv.) in 10 mL MeCN were added DBU (7 mmol, 1.4 equiv.) dropwise. The solution was stirred over night while slowly warming up to room temperature. DCM was added, and the organic layer was washed two times with sat. aq. NH₄Cl solution. The organic layer was dried over MgSO₄ and the solvent was removed in vacuum. The crude product was purified by silica gel column chromatography using (pentane : Et₂O - 80:1 to 40:1) provided the desired diazo compound.

General procedure for the photochemical ring expansion of 3,3 & 3- substituted oxetane (GP- 2) :



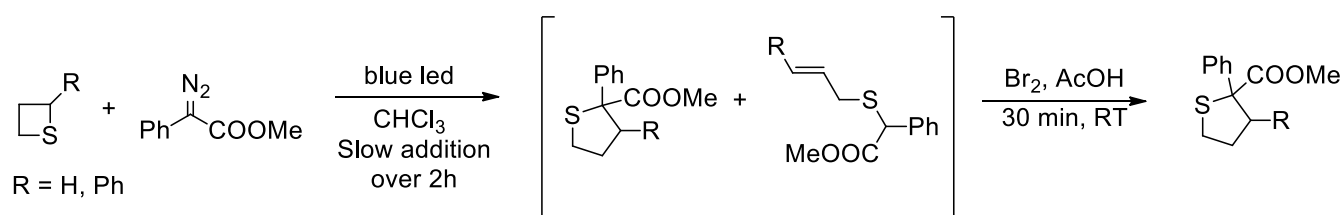
In a test tube 3,3 or 3- substituted oxetane (0.4 mmol, 2 equiv.) was dissolved in 1.0 mL chloroform and irradiated with one 3 W LED (distance 1.5 cm, cooling of the setup from the outside with a fan, reaction temperature: 25 °C). The diazoalkane (0.2 mmol, 1.0 equiv.) was dissolved in 1 mL chloroform and added to the reaction mixture over a period of 2 h and then stirred for another 1 h. The crude reaction mixture was purified by silica gel column chromatography (pentane : diethyl ether – 20:1 → 4:1) to afford the desired product.

General procedure for the photochemical ring expansion of oxetane & 2-phenyl oxetane (GP-3):



In a test tube oxetane or 2-phenyl oxetane (0.4 mmol, 2 equiv.) was dissolved in 1.0 mL chloroform and irradiated with one 3 W LED (distance 1.5 cm, cooling of the setup from the outside with a fan, reaction temperature: 25 °C). The diazoalkane (0.2 mmol, 1.0 equiv.) was dissolved in 1 mL chloroform and added to the reaction mixture over a period of 2 h and then stirred for another 1 h. Solvent was evaporated from the reaction mixture then 15.8 mg of KMnO_4 (0.1 mmol, 0.5 equiv.) was added followed by 2 mL of acetone and 0.2 mL of water were added to the mixture and stirred for another 2 h. Reaction mixture was passed through Na_2SO_4 bed and the filtrate were dried in reduced pressure and crude product was purified by silica gel column chromatography (pentane : diethyl ether – 20:1 \rightarrow 4:1) to afford the desired product.

General procedure for the photochemical ring expansion of thietane (GP-4):



In a test tube thietane or 2-phenyl thietane (0.4 mmol, 2 equiv.) was dissolved in 1.0 mL Chloroform and irradiated with one 3 W LED (distance 1.5 cm, cooling of the setup from the outside with a fan, reaction temperature: 25 °C). The diazoalkane (0.2 mmol, 1.0 equiv.) was dissolved in 1 mL Chloroform and added to the reaction mixture over a period of 2 h and then stirred for another 1 h. Solvent was evaporated from the reaction mixture then 15.9 mg of Br_2 (0.1 mmol, 0.5 equiv.) was added followed by 2 ml of acetic acid was added to the mixture and stirred for another 1 h. Reaction mixture was purified by silica gel column chromatography (pentane : diethyl ether – 20:1 \rightarrow 4:1) to afford the desired product.

DFT Calculations

Computational Details and Discussion

All of the calculations were performed with the Gaussian 09 program.⁴ The hybrid (U)B3LYP functional⁵ and the 6-31G(d) basis set⁶ were applied for the optimization of all stationary points in the chloroform in which the solvent effects ($\epsilon = 4.7113$) were evaluated by IEFPCM calculations with radii and non-electrostatic terms for SMD solvation model.⁷ Previous studies have shown that (U)B3LYP functional is a good method for studying the [1,2]-Stevens rearrangement reactions.⁸ For closed-shell species, B3LYP/6-31G(d) method was used. Singlet diradical intermediates and transition states were located with UB3LYP/6-31G(d), where the keyword guess=mix was used. Frequency calculations were performed to confirm that each stationary point is either a minimum or a transition structure. Key transition-state structures were confirmed to connect corresponding reactants and products by intrinsic reaction coordinate (IRC) calculations.⁹ To improve the calculation accuracy, single-point energies calculations in the chloroform were computed at the (U)B3LYP level of theory with the 6-311+G(d,p) basis set¹⁰ for all the atoms, and the Gibbs free energies in solution were used to discuss the rearrangements in the paper. The CYL View software was employed to show the 3D structures of the studied species.¹¹

In the paper, we have considered the heterolytic cleavage of the C-O bond of the oxonium ylide **INT1**. While all attempts in locating a suitable transition state led to other interesting transition states, such as hydrogen transfer via **TS4** and two [2,3]-sigmatropic rearrangements via **TS5** and **TS6**, respectively (Figure S1). All of these competitive pathways could not account for product formation and be less favorable than the [1,2]-Stevens rearrangement.

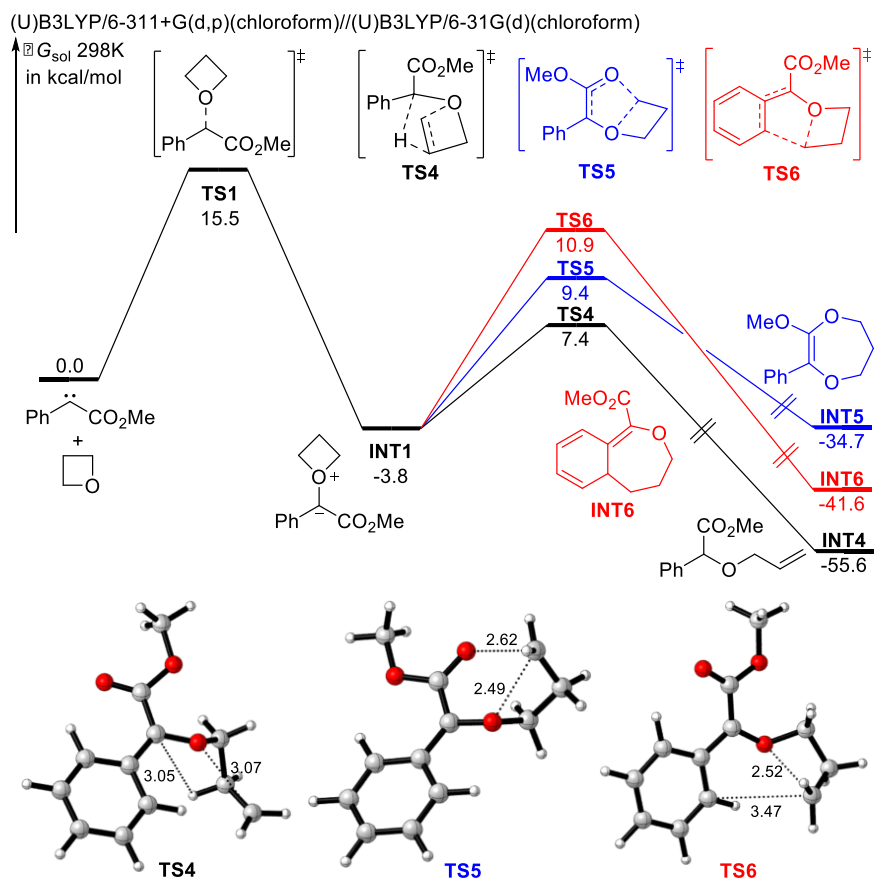


Figure S1. Free energy profiles for the concerted rearrangement process. The bond lengths in the structures at the bottom are given in Å.

We have considered the selectivity of the [1,2]-Stevens rearrangement of diazoacetate with 2-phenyloxetane and 2-phenylthietane and the corresponding DFT calculation results are shown in Figure S2 and Figure S3, respectively. These similar ring expansion processes involve the ylide formation, homolytic cleavage of C-O bond and intramolecular radical-radical coupling. Of note, we just got the optimized structure of ylide intermediate **INT_{Ph}1** in chloroform, which could not be located in the gas phase at this computational level.

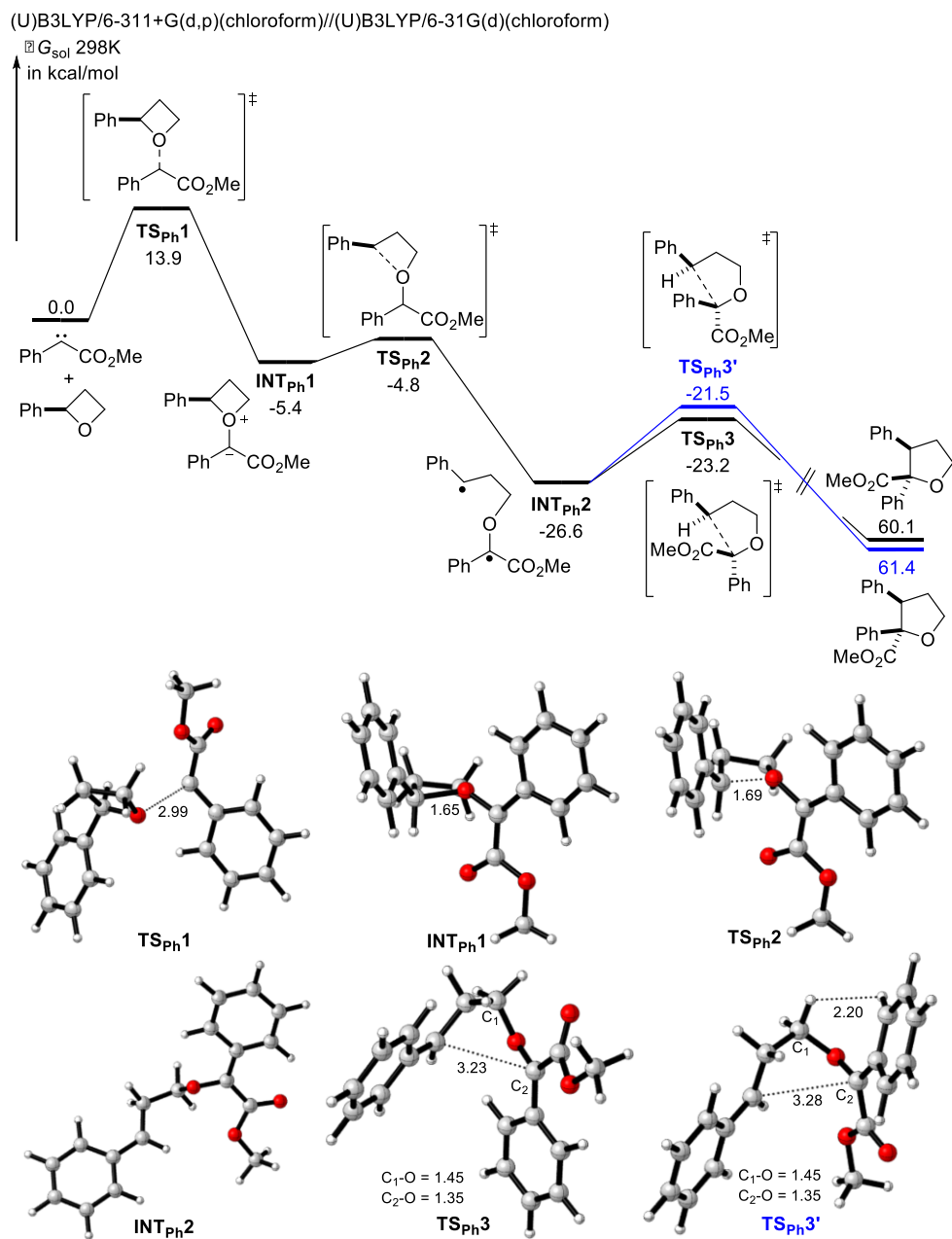


Figure S2. Potential energy surface and 3D structures of key species of ring expansion reaction of 2-phenyl oxetane and methyl phenyldiazoacetate. The bond lengths in the structures at the bottom are given in Å.

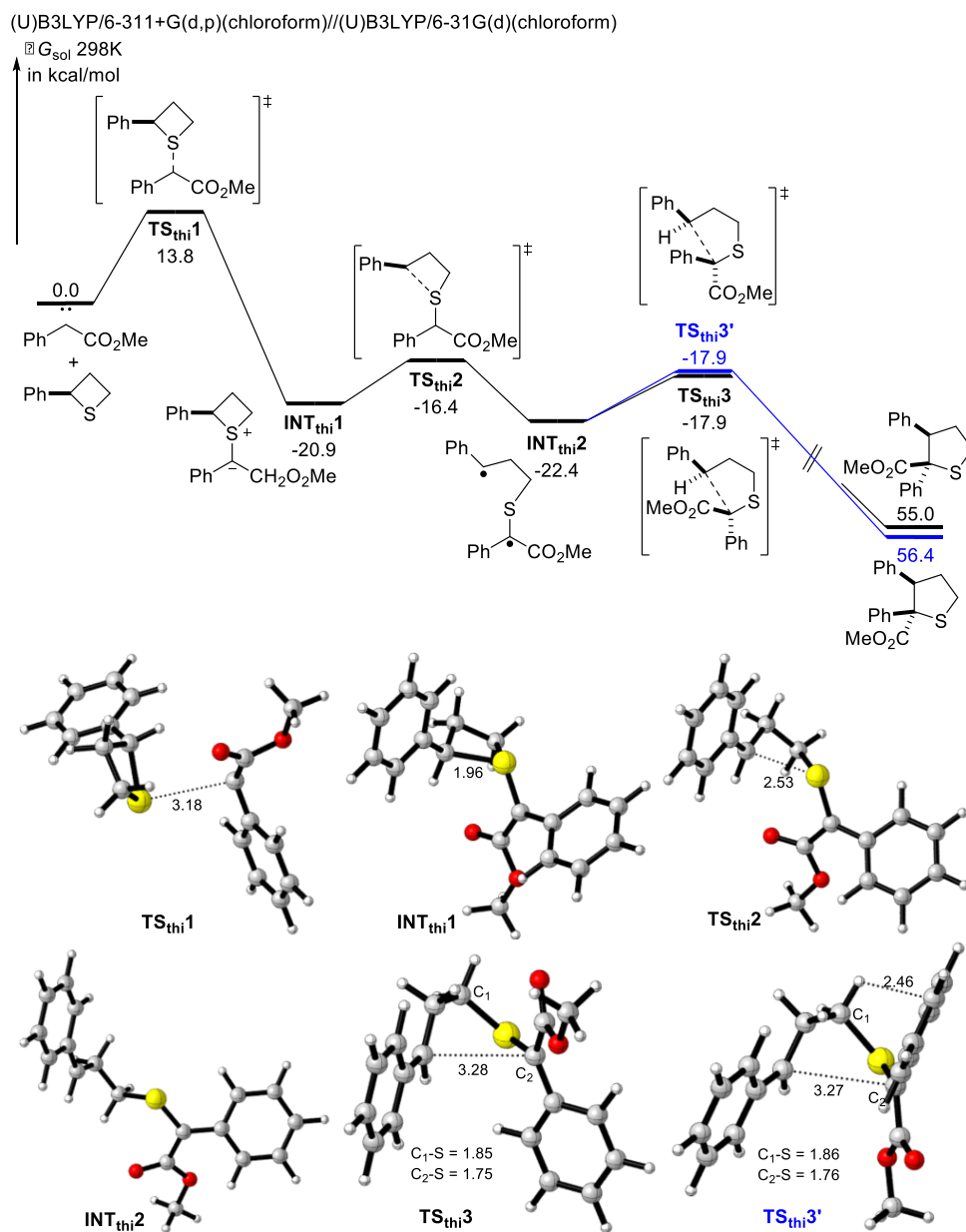
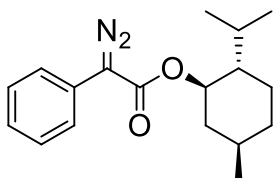


Figure S3. Potential energy surface and 3D structures of key species of ring expansion reaction of 2-phenylthietane and methyl phenyldiazoacetate. The bond lengths in the structures at the bottom are given in Å.

Characterization of compounds

(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 2-diazo-2-phenylacetate



The title compound was synthesized according to the **GP-I** and was obtained after silica gel column chromatography (pentane : Et₂O – 80:1 → 40:1) as an orange oil (53%, 795 mg).

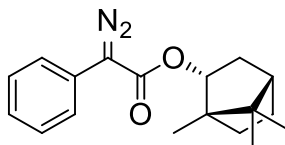
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.51 – 7.48 (m, 2H), 7.41 – 7.34 (m, 2H), 7.21 – 7.14 (m, 1H), 4.88 (td, *J* = 10.9, 4.4 Hz, 1H), 2.15 – 2.08 (m, 1H), 1.96 – 1.86 (m, 1H), 1.75 – 1.67 (m, 2H), 1.58 – 1.48 (m, 1H), 1.47 – 1.40 (m, 1H), 1.17 – 1.01 (m, 2H), 0.95 – 0.84 (m, 7H), 0.81 (d, *J* = 7.0 Hz, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 164.7, 128.8, 125.8, 125.6, 123.8, 75.0, 47.1, 41.3, 34.2, 31.4, 26.5, 23.6, 22.0, 20.7, 16.5 ppm.

HRMS (ESI): Mass found: 323.17313, calculated mass for C₁₈H₂₄N₂NaO₂⁺: 323.17300.

IR (KBr): 3385, 3062, 2953, 2868, 2664, 2480, 2329, 2225, 2183, 2082, 1951, 1866, 1788, 1697, 1597, 1497, 1454, 1354, 1285, 1096, 1038, 908, 842 cm⁻¹.

(1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl 2-diazo-2-phenylacetate



The titled compound was synthesized according to the general procedure-I. And was obtained after silica gel column chromatography (pentane : Et₂O – 80:1 → 40:1) as an orange gel (65%, 969 mg).

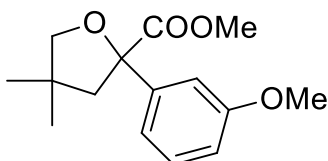
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.52 – 7.46 (m, 2H), 7.41 – 7.34 (m, 2H), 7.20 – 7.16 (m, 1H), 5.10 – 5.06 (m, 1H), 2.51 – 2.37 (m, 1H), 1.91 – 1.84 (m, 1H), 1.81 – 1.74 (m, 1H), 1.72 (t, *J* = 4.5 Hz, 1H), 1.38 – 1.31 (m, 1H), 1.29 – 1.23 (m, 1H), 1.13 – 1.09 (dd, *J* = 13.9, 3.5 Hz, 1H), 0.94 (s, 3H), 0.90 (s, 3H), 0.89 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 165.4, 128.8, 125.6, 123.8, 80.8, 48.9, 47.8, 44.9, 37.0, 28.0, 27.0, 19.7, 18.8, 13.5 ppm.

HRMS (ESI): Mass found: 321.15762, calculated mass for C₁₈H₂₂N₂NaO₂⁺: 321.15735.

IR (KBr): 3869, 3369, 3058, 2954, 2880, 2727, 2484, 2401, 2089, 1787, 1689, 1596, 1496, 1453, 1383, 1342, 1241, 1158, 1116, 1022, 891, 825, 749 cm⁻¹.

Methyl 4,4-dimethyl-2-phenyltetrahydrofuran-2-carboxylate (6a)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (93%, 44 mg).

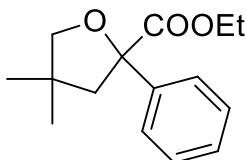
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.57 – 7.51 (m, 2H), 7.41 – 7.31 (m, 2H), 7.30 – 7.22 (m, 1H), 3.76 (d, *J* = 8.3 Hz, 1H), 3.71 (d, *J* = 8.3 Hz, 1H), 3.69 (s, 3H), 2.82 (d, *J* = 12.9 Hz, 1H), 2.11 (d, *J* = 12.9 Hz, 1H), 1.11 (s, 3H), 1.00 (s, 3H).

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.2, 142.3, 128.2, 127.5, 125.0, 87.7, 80.7, 52.8, 51.8, 39.9, 26.3, 26.0 ppm.

HRMS (ESI): Mass found: 257.11484, calculated mass for C₁₄H₁₈O₃Na⁺: 257.11536.

IR (KBr): 3452, 3061, 3028, 2956, 2868, 2318, 2070, 1990, 1886, 1828, 1731, 1599, 1491, 1448, 1369, 1248, 1197, 1148, 1098, 1058, 950, 915, 855, 785, 728, 700 cm^{-1} .

Ethyl 4,4-dimethyl-2-phenyltetrahydrofuran-2-carboxylate (6b)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (72%, 36 mg).

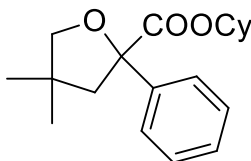
$^1\text{H NMR}$ (600 MHz, Chloroform-*d*): δ = 7.56 – 7.52 (m, 2H), 7.38 – 7.30 (t, *J* = 7.6 Hz, 2H), 7.28 – 7.24 (m, 1H), 4.18 – 4.11 (m, 2H), 3.76 (d, *J* = 8.2 Hz, 1H), 3.70 (d, *J* = 8.2 Hz, 1H), 2.81 (d, *J* = 12.8 Hz, 1H), 2.10 (d, *J* = 12.8 Hz, 1H), 1.20 (t, *J* = 7.1 Hz, 3H), 1.12 (s, 3H), 1.00 (s, 3H) ppm.

$^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*): δ = 173.7, 142.4, 128.1, 127.4, 125.1, 87.6, 80.6, 61.5, 51.8, 39.9, 26.4, 26.1, 14.0 ppm.

HRMS (ESI): Mass found: 271.13113, calculated mass for $\text{C}_{15}\text{H}_{20}\text{O}_3\text{Na}^+$: 271.13101.

IR (KBr): 3339, 3063, 2961, 2869, 2688, 2323, 2091, 1824, 1727, 1600, 1450, 1368, 1246, 1186, 1148, 1096, 1058, 916, 728, 700 cm^{-1} .

Cyclohexyl 4,4-dimethyl-2-phenyltetrahydrofuran-2-carboxylate (6c)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (87%, 53 mg).

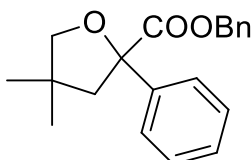
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*): δ = 7.58 – 7.46 (m, 2H), 7.36 – 7.27 (m, 2H), 7.26 – 7.16 (m, 1H), 4.78 – 4.68 (m, 1H), 3.75 (d, *J* = 8.2 Hz, 1H), 3.67 (d, *J* = 8.2 Hz, 1H), 2.77 (d, *J* = 12.9 Hz, 1H), 2.10 (d, *J* = 12.9 Hz, 1H), 1.78 – 1.67 (m, 2H), 1.67 – 1.58 (m, 2H), 1.52 – 1.42 (m, 1H), 1.43 – 1.18 (m, 5H), 1.10 (s, 3H), 0.99 (s, 3H) ppm.

$^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*): δ = 173.0, 142.6, 128.7, 128.0, 127.3, 125.2, 87.6, 80.5, 73.5, 51.7, 39.8, 31.2, 31.1, 26.5, 26.1, 25.2, 23.5, 23.5 ppm.

HRMS (ESI): Mass found: 325.17740, calculated mass for $\text{C}_{19}\text{H}_{26}\text{O}_3\text{Na}^+$: 325.17796.

IR (KBr): 3853, 3627, 3451, 3062, 3031, 2935, 2860, 2667, 2496, 2324, 2159, 1893, 1818, 1725, 1600, 1491, 1450, 1248, 1189, 1152, 1122, 1060, 917, 802, 700 cm^{-1} .

Benzyl 4,4-dimethyl-2-phenyltetrahydrofuran-2-carboxylate (6d)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (82%, 51 mg).

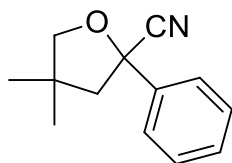
$^1\text{H NMR}$ (400 MHz, Chloroform-*d*): δ = 7.56 – 7.47 (m, 2H), 7.36 – 7.21 (m, 6H), 7.17 (dd, *J* = 6.8, 2.9 Hz, 2H), 5.20 – 5.01 (m, 2H), 3.74 (d, *J* = 8.3 Hz, 1H), 3.68 (d, *J* = 8.3 Hz, 1H), 2.78 (d, *J* = 12.9 Hz, 1H), 2.11 (d, *J* = 12.9 Hz, 1H), 1.04 (s, 3H), 0.98 (s, 3H) ppm.

$^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*): δ = 173.4, 142.2, 135.6, 128.3, 128.1, 128.0, 127.8, 127.5, 125.2, 87.7, 80.6, 67.0, 51.5, 39.9, 26.5, 26.0 ppm.

HRMS (ESI): Mass found: 333.14618, calculated mass for $\text{C}_{20}\text{H}_{22}\text{O}_3\text{Na}^+$: 333.14666.

IR (KBr): 3452, 3064, 3033, 2958, 2868, 2690, 2523, 2338, 2193, 2114, 2025, 1990, 1811, 1730, 1599, 1493, 1452, 1371, 1243, 1146, 1058, 730, 697 cm^{-1} .

4,4-dimethyl-2-phenyltetrahydrofuran-2-carbonitrile (6e)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as yellow oil (83%, 33 mg).

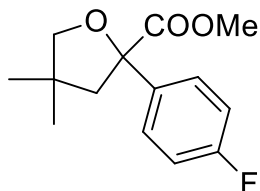
¹H NMR (300 MHz, Chloroform-*d*): δ = 7.61 – 7.48 (m, 2H), 7.44 – 7.32 (m, 3H), 3.97 (d, *J* = 8.7 Hz, 1H), 3.89 (d, *J* = 8.7 Hz, 1H), 2.66 (d, *J* = 13.3 Hz, 1H), 2.12 (d, *J* = 13.3 Hz, 1H), 1.35 (s, 3H), 1.14 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 139.6, 128.8, 128.7, 124.6, 81.6, 76.8, 55.7, 27.6, 26.2 ppm.

HRMS (ESI): Mass found: 224.10455, calculated mass for C₁₃H₁₅NNaO⁺: 224.10459.

IR (KBr): 3859, 3401, 3064, 3032, 2961, 2930, 2868, 2327, 2230, 2167, 2122, 2078, 1951, 1896, 1810, 1728, 1678, 1595, 1557, 1492, 1449, 1371, 1277, 1180, 1049, 916, 856, 748, 697 cm⁻¹.

Methyl 2-(4-fluorophenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6g)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (91%, 46 mg).

¹H NMR (600 MHz, Chloroform-*d*): δ = 7.55 – 7.46 (m, 2H), 7.05 – 6.98 (m, 2H), 3.76 (d, *J* = 8.3 Hz, 1H), 3.70 (m, 4H), 2.78 (d, *J* = 12.9 Hz, 1H), 2.08 (d, *J* = 12.9 Hz, 1H), 1.11 (s, 3H), 0.99 (s, 3H) ppm.

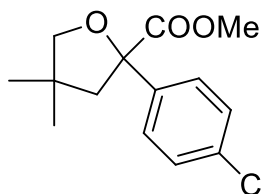
¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.1, 162.2 (d, *J* = 246.1 Hz), 138.1 (d, *J* = 3.0 Hz), 126.9 (d, *J* = 7.9 Hz), 115.0 (d, *J* = 21.0 Hz), 87.2, 80.7, 52.8, 51.9, 40.0, 26.4, 26.0 ppm.

¹⁹F NMR (564 MHz, Chloroform-*d*): δ = -115.2 ppm.

HRMS (ESI): Mass found: 275.10538, calculated mass for C₁₄H₁₇FO₃Na⁺: 275.10594.

IR (KBr): 3857, 3747, 3451, 2957, 2869, 2692, 2326, 2096, 2011, 1905, 1732, 1602, 1506, 1457, 1409, 1370, 1227, 1153, 1056, 1010, 973, 949, 914, 838, 749, 701 cm⁻¹.

Methyl 2-(4-chlorophenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6h)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (89%, 48 mg).

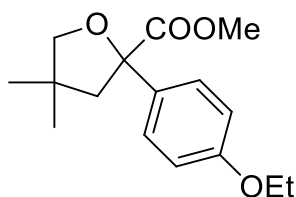
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.51 – 7.44 (m, 2H), 7.34 – 7.27 (m, 2H), 3.76 (d, *J* = 8.3 Hz, 1H), 3.72 – 3.68 (m, 4H), 2.78 (d, *J* = 12.9 Hz, 1H), 2.06 (dd, *J* = 12.9, 2.4 Hz, 1H), 1.10 (d, *J* = 2.4 Hz, 3H), 0.99 (d, *J* = 2.3 Hz, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.9, 140.9, 133.4, 128.3, 126.6, 80.7, 52.9, 51.8, 40.0, 26.3, 25.9 ppm.

HRMS (ESI): Mass found: 291.07599, calculated mass for C₁₄H₁₇ClO₃Na⁺: 291.07584.

IR (KBr): 3453, 2957, 2868, 2690, 2321, 2161, 2026, 1909, 1732, 1594, 1488, 1457, 1398, 1369, 1248, 1148, 1056, 1010, 832, 763, 725 cm⁻¹.

Methyl 2-(4-ethoxyphenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6i)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (81%, 45 mg).

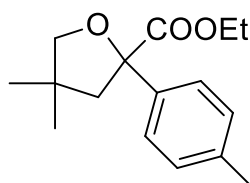
¹H NMR (400 MHz, Chloroform-*d*): δ = 7.43 – 7.39 (m, 2H), 6.85 – 6.81 (m, 2H), 4.00 (q, *J* = 7.0 Hz, 2H), 3.72 (d, *J* = 8.3 Hz, 1H), 3.70 – 3.64 (m, 4H), 2.74 (d, *J* = 12.9 Hz, 1H), 2.08 (d, *J* = 12.9 Hz, 1H), 1.38 (t, *J* = 7.0 Hz, 3H), 1.08 (s, 3H), 0.98 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.5, 158.3, 134.2, 126.3, 114.1, 87.4, 80.6, 63.3, 52.7, 51.7, 39.9, 26.4, 26.1, 14.8 ppm.

HRMS (ESI): Mass found: 301.14117, calculated mass for C₁₆H₂₂O₄Na⁺: 301.14158.

IR (KBr): 3453, 2957, 2870, 2320, 2161, 2071, 1988, 1894, 1731, 1608, 1509, 1456, 1392, 1240, 1175, 1150, 1114, 1049, 1010, 951, 921, 833, 751, 703 cm⁻¹.

Ethyl 4,4-dimethyl-2-(*p*-tolyl)tetrahydrofuran-2-carboxylate (6j)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (86%, 45 mg).

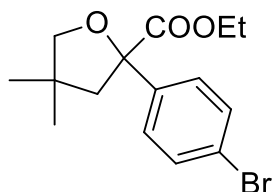
¹H NMR (400 MHz, Chloroform-*d*): δ = 7.45 – 7.36 (m, 2H), 7.16 – 7.02 (m, 2H), 4.13 (q, *J* = 7.1 Hz, 2H), 3.73 (d, *J* = 8.2 Hz, 1H), 3.67 (d, *J* = 8.2 Hz, 1H), 2.76 (d, *J* = 12.9 Hz, 1H), 2.31 (s, 3H), 2.07 (d, *J* = 12.9 Hz, 1H), 1.19 (t, *J* = 7.1 Hz, 3H), 1.09 (s, 3H), 0.98 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.8, 139.5, 137.1, 128.8, 125.0, 87.5, 80.6, 61.5, 51.7, 39.8, 26.4, 26.1, 21.0, 14.0 ppm.

HRMS (ESI): Mass found: 285.14606, calculated mass for C₁₆H₂₂O₃Na⁺: 285.14666.

IR (KBr): 3469, 2961, 2869, 2733, 1908, 1728, 1615, 1511, 11459, 1368, 1249, 1185, 1149, 1023, 917, 858, 822, 740, 507 cm⁻¹.

Ethyl 2-(4-bromophenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6k)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (96%, 63 mg).

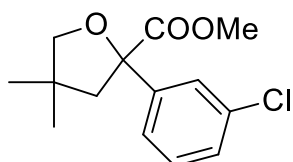
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.53 – 7.37 (m, 4H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.76 (d, *J* = 8.3 Hz, 1H), 3.69 (d, *J* = 8.3 Hz, 1H), 2.77 (d, *J* = 12.9 Hz, 1H), 2.05 (d, *J* = 12.9 Hz, 1H), 1.20 (t, *J* = 7.1 Hz, 3H), 1.11 (s, 3H), 0.99 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.2, 141.6, 131.2, 127.0, 121.5, 87.2, 80.7, 61.7, 51.8, 40.0, 26.4, 25.9, 14.0 ppm.

HRMS (ESI): Mass found: 349.04141, calculated mass for C₁₅H₁₉BrO₃Na⁺: 349.04098.

IR (KBr): 3449, 3075, 2961, 2869, 2689, 2324, 2156, 2021, 1992, 1907, 1826, 1728, 1588, 1483, 1392, 1368, 1244, 1187, 1148, 1058, 1009, 829, 756, 719, 660 cm⁻¹.

Methyl 2-(3-chlorophenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6l)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (76%, 41 mg).

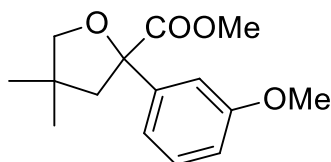
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.55 (t, *J* = 1.9 Hz, 1H), 7.43 – 7.38 (m, 1H), 7.28 – 7.23 (m, 2H), 3.76 (d, *J* = 8.3 Hz, 1H), 3.74 – 3.68 (m, 4H), 2.80 (d, *J* = 12.9 Hz, 1H), 2.07 (d, *J* = 12.9 Hz, 1H), 1.11 (s, 3H), 1.00 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.7, 144.4, 134.2, 129.5, 127.7, 125.4, 123.4, 87.2, 80.8, 52.9, 51.8, 40.0, 26.3, 25.9 ppm.

HRMS (ESI): Mass found: 291.07584, calculated mass for C₁₄H₁₇ClO₃Na⁺: 291.07639.

IR (KBr): 3857, 3747, 3453, 3071, 2957, 2868, 2330, 2072, 2007, 1943, 1723, 1594, 1573, 1466, 1370, 1241, 1198, 1150, 1057, 997, 950, 889, 795, 772, 689 cm⁻¹.

Methyl 2-(3-methoxyphenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6m)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (81%, 43 mg).

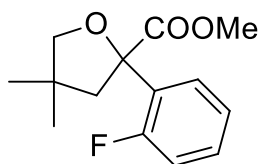
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.29 – 7.21 (m, 1H), 7.15 – 7.06 (m, 2H), 6.83 – 6.73 (m, 1H), 3.80 (s, 3H), 3.75 (d, *J* = 8.2 Hz, 1H), 3.71 – 3.68 (m, 4H), 2.81 (d, *J* = 12.9 Hz, 1H), 2.10 (d, *J* = 12.9 Hz, 1H), 1.10 (s, 3H), 1.00 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.1, 159.5, 144.0, 129.3, 117.5, 113.1, 110.5, 87.6, 80.7, 55.2, 52.8, 51.7, 39.9, 26.3, 26.0 ppm.

HRMS (ESI): Mass found: 287.12531, calculated mass for C₁₅H₂₀NaO₄⁺: 287.12538.

IR (KBr): 3454, 2956, 2869, 2317, 2161, 1933, 1732, 1597, 1484, 1458, 1434, 1258, 1150, 1047, 950, 876, 833, 782, 733, 696 cm⁻¹.

Methyl 2-(2-fluorophenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6n)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (81%, 41 mg).

¹H NMR (600 MHz, Chloroform-*d*): δ = 7.75 – 7.66 (m, 1H), 7.31 – 7.23 (m, 1H), 7.19 – 7.12 (m, 1H), 7.07 – 6.97 (m, 1H), 3.77 (d, *J* = 8.2 Hz, 1H), 3.73 – 3.68 (m, 4H), 2.98 (dd, *J* = 13.3, 2.1 Hz, 1H), 2.02 (dd, *J* = 13.3, 2.1 Hz, 1H), 1.17 (s, 3H), 1.01 (s, 3H) ppm.

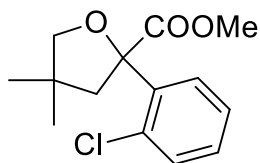
¹³C NMR (151 MHz, Chloroform-*d*): δ = 172.2, 159.4 (d, *J* = 246.4 Hz), 130.3 (d, *J* = 13.8 Hz), 129.2 (d, *J* = 8.0 Hz), 126.3 (d, *J* = 3.9 Hz), 123.9 (d, *J* = 3.3 Hz), 115.5 (d, *J* = 21.6 Hz), 85.2, 80.6, 52.8, 49.7, 40.1, 26.9, 25.7 ppm.

¹⁹F NMR (564 MHz, Chloroform-*d*): δ = -113.6 ppm.

HRMS (ESI): Mass found: 275.10556, calculated mass for C₁₄H₁₇FO₃Na⁺: 275.10594.

IR (KBr): 3474, 2958, 2870, 2316, 2168, 2071, 1991, 1922, 1740, 1696, 1612, 1584, 1483, 1453, 1369, 1251, 1204, 1147, 1088, 1048, 1003, 951, 914, 859, 818, 757, 707 cm⁻¹.

Methyl 2-(2-chlorophenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6o)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (76%, 41 mg).

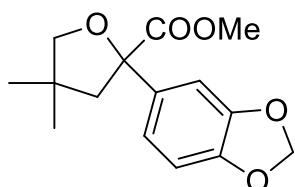
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.84 – 7.82 (m, 1H), 7.36 – 7.28 (m, 2H), 7.28 – 7.20 (m, 1H), 3.78 – 3.73 (m, 2H), 3.68 (s, 3H), 3.17 (d, *J* = 13.1 Hz, 1H), 1.87 (d, *J* = 13.1 Hz, 1H), 1.20 (s, 3H), 0.99 (s, 3H) ppm.

¹³C NMR (151 MHz, CDCl₃): δ = 171.3, 141.4, 131.1, 129.7, 128.5, 126.6, 126.0, 87.2, 80.6, 52.9, 49.2, 40.6, 27.4, 25.4 ppm.

HRMS (ESI): Mass found: 291.07626, calculated mass for C₁₄H₁₇ClO₃Na⁺: 291.07584.

IR (KBr): 2956, 2871, 2490, 2318, 2161, 2037, 1896, 1731, 1609, 1582, 1509, 1456, 1392, 1296, 1240, 1175, 1150, 1114, 1049, 1010, 921, 834, 752, 705 cm⁻¹.

Methyl 2-(benzo[d][1,3]dioxol-5-yl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6p)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (90%, 50 mg).

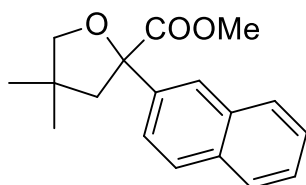
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.04 (d, *J* = 1.9 Hz, 1H), 7.00 (dd, *J* = 8.2, 1.8 Hz, 1H), 6.76 (d, *J* = 8.1 Hz, 1H), 5.94 (s, 2H), 3.73 (d, *J* = 8.3 Hz, 1H), 3.70 (s, 3H), 3.68 (d, *J* = 8.3 Hz, 1H), 2.76 (d, *J* = 12.9 Hz, 1H), 2.07 (d, *J* = 12.9 Hz, 1H), 1.09 (s, 3H), 1.01 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.2, 147.5, 146.9, 136.3, 118.4, 107.9, 106.1, 101.0, 87.4, 82.1, 80.7, 52.8, 51.8, 39.9, 26.4, 26.0 ppm.

HRMS (ESI): Mass found: 301.10461, calculated mass for C₁₅H₁₈O₅Na⁺: 301.10519.

IR (KBr): 3451, 2957, 2872, 2323, 2163, 2050, 1856, 1731, 1681, 1609, 1486, 1438, 1363, 1242, 1153, 1086, 1038, 933, 812, 750, 714 cm⁻¹.

Methyl 4,4-dimethyl-2-(naphthalen-2-yl)tetrahydrofuran-2-carboxylate (6q)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (86%, 49 mg).

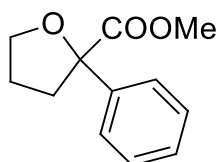
¹H NMR (600 MHz, Chloroform-*d*): δ = 8.07 – 8.03 (m, 1H), 7.91 – 7.76 (m, 3H), 7.66 – 7.57 (m, 1H), 7.50 – 7.44 (m, 2H), 3.82 (d, *J* = 8.3 Hz, 1H), 3.78 (d, *J* = 8.3 Hz, 1H), 3.70 (s, 3H), 2.91 (d, *J* = 12.9 Hz, 1H), 2.21 (d, *J* = 12.9 Hz, 1H), 1.15 (s, 3H), 1.01 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.2, 132.9, 132.7, 128.2, 128.0, 127.5, 126.1, 126.0, 123.7, 123.4, 87.8, 80.8, 52.9, 51.7, 40.0, 26.4, 26.0 ppm.

HRMS (ESI): Mass found: 307.13037, calculated mass for C₁₈H₂₀O₃Na⁺: 307.13101.

IR (KBr): 3438, 3058, 2957, 2868, 2322, 2166, 1922, 1723, 1630, 1596, 1505, 1441, 1356, 1260, 1101, 1059, 951, 864, 825, 783, 749, 694 cm⁻¹.

Methyl 2-phenyltetrahydrofuran-2-carboxylate (7a)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (70%, 29 mg).

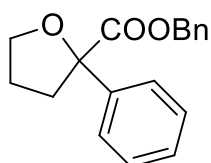
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.56 – 7.49 (m, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.31 – 7.27 (m, 1H), 4.15 – 4.04 (m, 2H), 3.70 (s, 3H), 2.88 – 2.80 (m, 1H), 2.20 (m, 1H), 2.03 – 1.89 (m, 2H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.7, 141.1, 128.2, 127.6, 125.3, 87.5, 68.9, 52.7, 37.2, 25.28 ppm.

HRMS (ESI): Mass found: 229.08379, calculated mass for C₁₂H₁₄NaO₃⁺: 229.08352.

IR (KBr): 3452, 2953, 2880, 2160, 2022, 1948, 1897, 1731, 1600, 1491, 1444, 1261, 1182, 1060, 774, 732, 698 cm⁻¹.

Benzyl 2-phenyltetrahydrofuran-2-carboxylate (7b)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (63%, 36 mg).

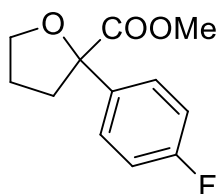
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.55 – 7.50 (m, 2H), 7.36 – 7.24 (m, 6H), 7.22 – 7.17 (m, 2H), 5.14 (q, *J* = 12.5 Hz, 2H), 4.12 – 4.04 (m, 2H), 2.83 (ddd, *J* = 12.8, 7.6, 5.8 Hz, 1H), 2.21 (dt, *J* = 12.6, 8.0 Hz, 1H), 2.03 – 1.88 (m, 2H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.0, 140.9, 135.7, 128.4, 128.2, 128.0, 127.6, 125.5, 87.5, 68.8, 66.9, 36.9, 25.2 ppm.

HRMS (ESI): Mass found: 305.11438, calculated mass for C₁₈H₁₈NaO₃⁺: 305.11482.

IR (KBr): 3856, 3450, 3062, 3032, 2952, 2879, 2687, 2328, 2089, 1999, 1881, 1810, 1730, 1601, 1493, 1450, 1374, 1257, 1223, 1104, 1029, 965, 916, 733 cm⁻¹.

Methyl 2-(4-fluorophenyl)tetrahydrofuran-2-carboxylate (7c)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (73%, 33 mg).

¹H NMR (600 MHz, Chloroform-*d*): δ = 7.57 – 7.45 (m, 2H), 7.11 – 6.97 (m, 2H), 4.12 – 4.03 (m, 2H), 3.70 (s, 3H), 2.82 (ddd, *J* = 13.0, 7.8, 5.7 Hz, 1H), 2.16 (dt, *J* = 12.6, 7.8 Hz, 1H), 2.03 – 1.88 (m, 2H) ppm.

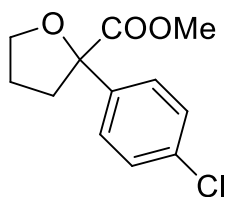
¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.6, 162.3 (d, *J* = 246.0 Hz), 136.9 (d, *J* = 3.3 Hz), 127.1 (d, *J* = 8.1 Hz), 115.0 (d, *J* = 21.1 Hz), 87.1, 68.9, 52.8, 37.3, 25.2 ppm.

¹⁹F NMR (564 MHz, Chloroform-*d*): δ = -115.0 ppm.

HRMS (ESI): Mass found: 247.07428, calculated mass for C₁₂H₁₃FNao₃⁺: 247.07409.

IR (KBr): 3326, 2953, 2884, 2160, 2040, 1901, 1733, 1603, 1506, 1440, 1225, 1187, 1110, 1081, 1056, 1012, 837, 751, 683 cm⁻¹.

Methyl 2-(4-chlorophenyl)tetrahydrofuran-2-carboxylate (7d)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (76%, 36 mg).

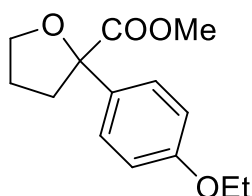
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.49 – 7.45 (m, 2H), 7.33 – 7.29 (m, 2H), 4.13 – 4.02 (m, 2H), 3.70 (s, 3H), 2.82 (ddd, *J* = 12.9, 7.8, 5.8 Hz, 1H), 2.19 – 2.11 (m, 1H), 2.03 – 1.88 (m, 2H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.4, 139.7, 133.6, 128.3, 126.8, 87.1, 69.0, 52.8, 37.3, 25.2 ppm.

HRMS (ESI): Mass found: 263.04456, calculated mass for C₁₂H₁₃ClNaO₃⁺: 263.04454.

IR (KBr): 3454, 2953, 2882, 2689, 2162, 2032, 1909, 1733, 1596, 1489, 1440, 1400, 1260, 1182, 1085, 1012, 829, 793, 760, 723 cm⁻¹.

Methyl 2-(4-ethoxyphenyl)tetrahydrofuran-2-carboxylate (7e)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (61%, 31 mg).

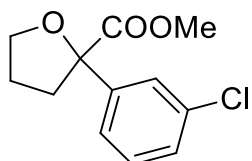
¹H NMR (400 MHz, Chloroform-*d*): δ = 7.43 – 7.39 (m, 2H), 6.91 – 6.79 (m, 2H), 4.10 – 3.95 (m, 4H), 3.68 (s, 3H), 2.77 (ddd, *J* = 13.0, 7.6, 6.0 Hz, 1H), 2.17 (dt, *J* = 12.6, 7.8 Hz, 1H), 2.01 – 1.85 (m, 2H), 1.38 (t, *J* = 7.0 Hz, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.0, 158.5, 132.9, 126.6, 114.1, 87.2, 68.7, 63.4, 52.6, 37.0, 25.2, 14.8 ppm.

HRMS (ESI): Mass found: 273.10986, calculated mass for C₁₄H₁₈NaO₄⁺: 273.10973.

IR (KBr): 3856, 3452, 3324, 2979, 2881, 2323, 2158, 2092, 1992, 1901, 1731, 1609, 1580, 1509, 1477, 1441, 1393, 1298, 1241, 1177, 1112, 1086, 1048, 1010, 922, 832, 755, 685 cm⁻¹.

Methyl 2-(3-chlorophenyl)tetrahydrofuran-2-carboxylate (7f)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (66%, 32 mg).

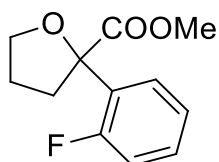
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.55 (m, 1H), 7.41 – 7.39 (m, 1H), 7.29 – 7.25 (m, 2H), 4.14 – 4.03 (m, 2H), 3.71 (s, 3H), 2.82 (ddd, *J* = 12.6, 7.8, 5.8 Hz, 1H), 2.16 (dt, *J* = 12.6, 7.8 Hz, 1H), 2.04 – 1.89 (m, 2H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.2, 143.2, 134.2, 129.5, 127.8, 125.6, 123.5, 87.1, 69.1, 52.9, 37.3, 25.3 ppm.

HRMS (ESI): Mass found: 263.04453, calculated mass for C₁₂H₁₃ClNaO₃⁺: 263.04454.

IR (KBr): 3855, 3455, 3070, 2952, 2882, 2691, 2328, 2181, 2075, 1998, 1733, 1594, 1573, 1433, 1257, 1186, 1109, 966, 884, 784, 690 cm⁻¹.

Methyl 2-(2-fluorophenyl)tetrahydrofuran-2-carboxylate (7g)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (71%, 32 mg).

¹H NMR (600 MHz, Chloroform-*d*): δ = 7.64 – 7.59 (m, 1H), 7.33 – 7.23 (m, 1H), 7.18 – 7.13 (m, 1H), 7.07 – 6.98 (m, 1H), 4.13 – 4.04 (m, 2H), 3.71 (s, 3H), 3.05 – 2.95 (m, 1H), 2.17 – 2.07 (m, 2H), 2.00 – 1.91 (m, 1H) ppm.

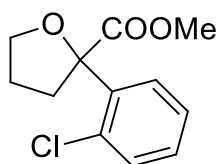
¹³C NMR (151 MHz, Chloroform-*d*): δ = 172.1, 159.4 (d, *J* = 246.0 Hz), 129.6 (d, *J* = 13.6 Hz), 129.3 (d, *J* = 8.1 Hz), 126.6 (d, *J* = 4.2 Hz), 123.9 (d, *J* = 3.5 Hz), 115.4 (d, *J* = 21.4 Hz), 84.7, 69.4, 52.8 (d, *J* = 4.5 Hz), 35.9 (d, *J* = 2.8 Hz), 25.9 ppm.

¹⁹F NMR (564 MHz, Chloroform-*d*): δ = -114.0 ppm.

HRMS (ESI): Mass found: 247.07407, calculated mass for C₁₂H₁₃FN₃⁺: 247.07409.

IR (KBr): 3472, 2954, 2880, 2161, 2033, 1829, 1740, 1615, 1584, 1485, 1450, 1259, 1199, 1108, 1052, 1008, 953, 816, 757, 704 cm⁻¹.

Methyl 2-(2-chlorophenyl)tetrahydrofuran-2-carboxylate (7h)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (67%, 32 mg).

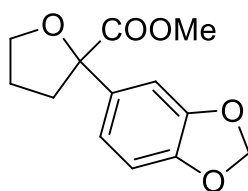
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.71 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.35 – 7.28 (m, 2H), 7.26 – 7.22 (m, 1H), 4.15 – 4.10 (m, 1H), 4.09 – 4.04 (m, 1H), 3.70 (s, 3H), 3.23 – 3.17 (m, 1H), 2.21 – 2.14 (m, 1H), 2.04 – 1.98 (m, 1H), 1.94 – 1.86 (m, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 171.5, 131.1, 129.8, 128.7, 126.6, 126.2, 86.6, 69.8, 52.8, 35.4, 26.3 ppm.

HRMS (ESI): Mass found: 263.04422, calculated mass for C₁₂H₁₃ClNaO₃⁺: 263.04454.

IR (KBr): 3468, 3067, 2952, 2876, 2325, 2167, 2073, 1930, 1739, 1572, 1464, 1436, 1254, 1189, 1113, 1039, 1009, 952, 874, 790, 752, 706 cm⁻¹.

Methyl 2-(benzo[d][1,3]dioxol-5-yl)tetrahydrofuran-2-carboxylate (7i)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (74%, 37 mg).

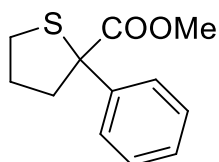
¹H NMR (400 MHz, Chloroform-*d*): δ = 7.04 – 6.94 (m, 2H), 6.75 (d, *J* = 8.1 Hz, 1H), 5.93 (s, 2H), 4.10 – 3.98 (m, 2H), 3.69 (s, 3H), 2.76 (ddd, *J* = 12.5, 7.6, 6.0 Hz, 1H), 2.14 (ddd, *J* = 12.5, 8.2, 7.2 Hz, 1H), 2.03 – 1.83 (m, 2H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.7, 147.5, 147.0, 135.1, 118.7, 107.9, 106.3, 101.0, 87.3, 68.8, 52.7, 37.2, 25.2 ppm.

HRMS (ESI): Mass found: 273.07321, calculated mass for C₁₃H₁₄NaO₅⁺: 273.07334.

IR (KBr): 3866, 3453, 2952, 2882, 2840, 2688, 2326, 2160, 2088, 1968, 1921, 1732, 1597, 1485, 1434, 1262, 1173, 1106, 1044, 989, 875, 833, 785, 696 cm⁻¹.

Methyl 2-phenyltetrahydrothiophene-2-carboxylate (8a)



The titled compound was synthesized according to the general procedure-4. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (73%, 32 mg).

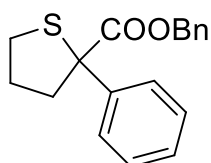
¹H NMR (400 MHz, Chloroform-*d*): δ = 7.55 – 7.50 (m, 2H), 7.36 – 7.28 (m, 2H), 7.27 – 7.21 (m, 1H), 3.66 (s, 3H), 3.08 – 2.90 (m, 3H), 2.25 – 2.04 (m, 2H), 1.99 – 1.90 (m, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.3, 141.8, 128.2, 127.3, 126.7, 66.5, 52.8, 42.8, 33.6, 30.4 ppm.

HRMS (ESI): Mass found: 245.06067, calculated mass for C₁₂H₁₄NaO₂S⁺: 245.06067.

IR (KBr): 3446, 3058, 3023, 2948, 2863, 2340, 2158, 1956, 1727, 1596, 1491, 1438, 1325, 1224, 1163, 1130, 1075, 1026, 978, 900, 828, 747, 698 cm⁻¹.

Benzyl 2-phenyltetrahydrothiophene-2-carboxylate (8b)



The titled compound was synthesized according to the general procedure-4. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (70%, 42 mg).

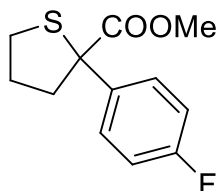
¹H NMR (300 MHz, Chloroform-*d*): δ = 7.57 – 7.46 (m, 2H), 7.37 – 7.13 (m, 8H), 5.13 (s, 2H), 3.17 – 2.89 (m, 3H), 2.25 – 2.06 (m, 2H), 2.05 – 1.94 (m, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.4, 141.7, 135.8, 128.2, 128.1, 127.8, 127.4, 127.2, 126.9, 66.9, 66.6, 42.5, 33.6, 30.4 ppm.

HRMS (ESI): Mass found: 321.09198, calculated mass for C₁₈H₁₈NaO₂S⁺: 321.09197.

IR (KBr): 3446, 3060, 2930, 2863, 2326, 2127, 1954, 1879, 1726, 1596, 1493, 1445, 1373, 1310, 1249, 1070, 1009, 968, 909, 824 cm⁻¹.

Methyl 2-(4-fluorophenyl)tetrahydrothiophene-2-carboxylate (8c)



The titled compound was synthesized according to the general procedure-4. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (72%, 35 mg).

¹H NMR (300 MHz, Chloroform-*d*): δ = 7.56 – 7.45 (m, 2H), 7.08 – 6.92 (m, 2H), 3.68 (s, 3H), 3.17 – 2.81 (m, 3H), 2.26 – 2.03 (m, 2H), 2.01 – 1.89 (m, 1H) ppm.

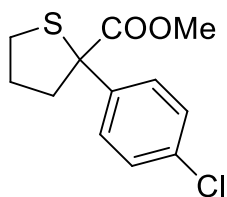
¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.0, 161.9 (d, *J* = 246.7 Hz), 137.6 (d, *J* = 2.7 Hz), 128.5 (d, *J* = 7.9 Hz), 115.0 (d, *J* = 21.4 Hz), 65.9, 52.8, 42.8, 33.7, 30.4 ppm.

¹⁹F NMR (564 MHz, Chloroform-*d*): δ = -115.53 ppm.

HRMS (ESI): Mass found: 263.05127, calculated mass for C₁₂H₁₃FNaO₂S⁺: 263.05125.

IR (KBr): 3858, 3446, 3072, 2948, 2864, 2664, 2329, 2085, 1994, 1893, 1800, 1728, 1600, 1505, 1437, 1331, 1224, 1161, 1130, 1076, 979, 901, 755, 708 cm⁻¹.

Methyl 2-(4-chlorophenyl)tetrahydrothiophene-2-carboxylate (8d)



The titled compound was synthesized according to the general procedure-4. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (73%, 37 mg).

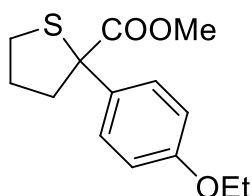
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.50 – 7.44 (m, 2H), 7.32 – 7.27 (m, 2H), 3.67 (s, 3H), 3.12 – 2.92 (m, 3H), 2.24 – 2.04 (m, 2H), 1.99 – 1.88 (m, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.8, 140.4, 133.2, 128.3, 128.2, 65.9, 52.9, 42.7, 33.7, 30.4 ppm.

HRMS (ESI): Mass found: 279.02182, calculated mass for C₁₂H₁₃ClNaO₂S⁺: 279.02170.

IR (KBr): 3859, 3444, 2947, 2862, 2326, 2232, 2074, 1990, 1908, 1728, 1591, 1487, 1437, 1397, 1307, 1225, 1130, 1091, 1012, 1036, 978, 925, 827, 767, 661 cm⁻¹.

Methyl 2-(4-ethoxyphenyl)tetrahydrothiophene-2-carboxylate (8e)



The titled compound was synthesized according to the general procedure-4. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (64%, 34 mg).

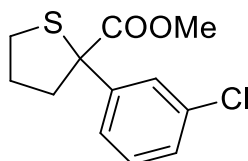
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.46 – 7.40 (m, 2H), 6.88 – 6.81 (m, 2H), 4.02 (q, *J* = 7.0 Hz, 2H), 3.67 (s, 3H), 3.02 (dd, *J* = 7.4, 5.7 Hz, 2H), 2.96 (dt, *J* = 12.7, 5.4 Hz, 1H), 2.19 – 2.06 (m, 2H), 2.02 – 1.93 (m, 1H), 1.40 (t, *J* = 7.0 Hz, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.4, 158.1, 133.7, 127.9, 114.0, 65.9, 63.4, 52.7, 42.7, 33.6, 30.3, 14.8 ppm.

HRMS (ESI): Mass found: 289.08694, calculated mass for C₁₄H₁₈NaO₃S⁺: 289.08689.

IR (KBr): 3444, 2943, 2869, 2322, 2163, 2035, 1889, 1727, 1607, 1579, 1507, 1477, 1438, 1392, 1297, 1227, 1179, 1119, 1078, 1044, 980, 921, 830, 757 cm⁻¹.

Methyl 2-(3-chlorophenyl)tetrahydrothiophene-2-carboxylate (8f)



The titled compound was synthesized according to the general procedure-4. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (66%, 34 mg).

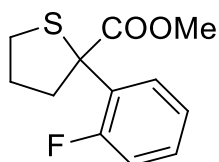
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.59 (t, *J* = 1.9 Hz, 1H), 7.40 – 7.36 (m, 1H), 7.30 – 7.21 (m, 2H), 3.68 (s, 2H), 3.06 – 3.02 (m, 2H), 3.00 – 2.94 (m, 1H), 2.23 – 2.05 (m, 2H), 1.97 – 1.91 (m, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.7, 143.9, 134.2, 129.4, 127.5, 127.1, 125.0, 66.1, 52.9, 42.7, 33.7, 30.4 ppm.

HRMS (ESI): Mass found: 279.02173, calculated mass for C₁₂H₁₃ClNaO₂S⁺: 279.02170.

IR (KBr): 3857, 3447, 3060, 2947, 2862, 2329, 2164, 2097, 1990, 1904, 1729, 1591, 1570, 1470, 1435, 1306, 1224, 1130, 1080, 1037, 1013, 978, 906, 830, 779, 692 cm⁻¹.

Methyl 2-(2-fluorophenyl)tetrahydrothiophene-2-carboxylate (8g)



The titled compound was synthesized according to the general procedure-4. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (66%, 32 mg).

¹H NMR (300 MHz, Chloroform-*d*): δ = 7.97 (td, *J* = 8.0, 1.8 Hz, 1H), 7.33 – 7.24 (m, 1H), 7.15 (td, *J* = 7.5, 1.3 Hz, 1H), 7.08 – 6.97 (m, 1H), 3.70 (s, 3H), 3.11 – 2.98 (m, 3H), 2.45 – 2.22 (m, 1H), 2.10 – 1.97 (m, 1H), 1.95 – 1.84 (m, 1H) ppm.

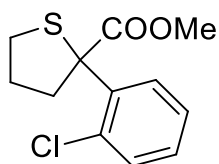
¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.7, 160.0 (d, *J* = 246.3 Hz), 129.7 (d, *J* = 12.9 Hz), 129.4 (d, *J* = 3.2 Hz), 129.2 (d, *J* = 8.4 Hz), 123.8 (d, *J* = 3.6 Hz), 115.3 (d, *J* = 21.8 Hz), 62.7, 52.8, 41.4, 33.6, 30.8 ppm.

¹⁹F NMR (564 MHz, Chloroform-*d*): δ = -113.40 ppm.

HRMS (ESI): Mass found: 263.05121, calculated mass for C₁₂H₁₃FN₂O₂S⁺: 263.05125.

IR (KBr): 3809, 3747, 3678, 3467, 3217, 2949, 2862, 2665, 2511, 2332, 2186, 2121, 1993, 1946, 1842, 1805, 1736, 1612, 1579, 1480, 1442, 1367, 1326, 1222, 1129, 1074, 1027, 976, 917, 831, 705 cm⁻¹.

Methyl 2-(2-chlorophenyl)tetrahydrothiophene-2-carboxylate (8h)



The titled compound was synthesized according to the general procedure-4. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (69%, 35 mg).

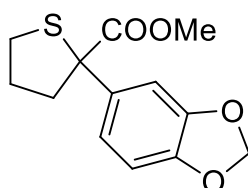
¹H NMR (300 MHz, Chloroform-*d*): δ = 8.21 – 8.14 (m, 1H), 7.38 – 7.20 (m, 3H), 3.70 (s, 3H), 3.20 – 3.11 (m, 1H), 3.10 – 3.02 (m, 2H), 2.44 – 2.26 (m, 1H), 2.08 – 1.87 (m, 2H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.8, 139.6, 133.0, 130.3, 129.8, 128.8, 126.5, 77.2, 76.9, 76.7, 66.2, 52.9, 40.5, 33.9, 30.9 ppm.

HRMS (ESI): Mass found: 279.02164, calculated mass for C₁₂H₁₃ClNaO₂S⁺: 279.02170.

IR (KBr): 3457, 3062, 2946, 2861, 2661, 2329, 2149, 2080, 1992, 1934, 1812, 1734, 1567, 1460, 1433, 1312, 1220, 1162, 1130, 1079, 1041, 972, 912, 823 cm⁻¹.

Methyl 2-(benzo[d][1,3]dioxol-5-yl)tetrahydrothiophene-2-carboxylate (8i)



The titled compound was synthesized according to the general procedure-4. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (71%, 38 mg).

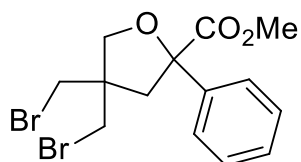
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.06 (d, *J* = 2.0 Hz, 1H), 7.02 – 6.98 (m, 1H), 6.74 (d, *J* = 8.1 Hz, 1H), 5.95 (s, 2H), 3.68 (s, 3H), 3.03 – 2.99 (m, 2H), 2.96 – 2.91 (m, 1H), 2.18 – 2.04 (m, 2H), 1.91 – 1.98 (m, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.2, 147.6, 146.8, 135.7, 120.0, 107.8, 107.7, 101.1, 77.1, 76.9, 76.7, 66.3, 52.8, 42.8, 33.6, 30.3 ppm.

HRMS (ESI): Mass found: 289.05051, calculated mass for C₁₃H₁₄NaO₄S⁺: 289.05050.

IR (KBr): 3445, 2949, 2897, 2779, 2064, 1856, 1726, 1610, 1484, 1435, 1343, 1228, 1161, 1127, 1069, 982, 930, 865, 811 cm⁻¹.

Methyl 4,4-bis(bromomethyl)-2-phenyltetrahydrofuran-2-carboxylate (9)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1) as colorless oil (79%, 62 mg).

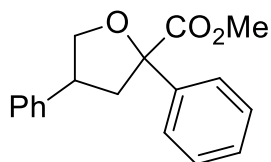
¹H NMR (400 MHz, Chloroform-*d*): δ = 7.52 – 7.44 (m, 2H), 7.41 – 7.28 (m, 3H), 4.01 (d, *J* = 9.9 Hz, 1H), 3.96 (d, *J* = 9.9 Hz, 1H), 3.71 (s, 3H), 3.69 – 3.62 (m, 2H), 3.55 (d, *J* = 10.4 Hz, 1H), 3.46 (d, *J* = 10.4 Hz, 1H), 3.06 (d, *J* = 14.0 Hz, 1H), 2.40 (d, *J* = 14.0 Hz, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 172.9, 140.2, 128.5, 128.2, 124.9, 87.8, 75.0, 53.1, 49.9, 46.5, 38.7, 37.9 ppm.

HRMS (ESI): Mass found: 412.93539, calculated mass for C₁₄H₁₆Br₂NaO₃⁺: 412.93584.

IR (KBr): 3877, 3648, 3452, 3196, 3060, 3027, 2861, 2666, 2326, 2113, 1989, 1941, 1809, 1733, 1597, 1491, 1432, 1359, 1253, 1074, 1028, 956, 878, 732, 699 cm⁻¹.

Methyl 2,4-diphenyltetrahydrofuran-2-carboxylate (10)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (88%, d.r- 3:2, 50 mg).

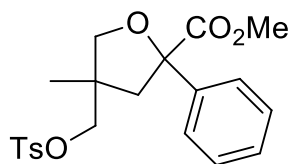
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.62 – 7.53 (m, 2H), 7.44 – 7.35 (m, 2H), 7.35 – 7.25 (m, 3H), 7.25 – 7.17 (m, 3H), 4.54 – 4.51 (m, 1H), 4.07 – 3.92 (m, 1H), 3.77 – 3.70 (m, 3H), 3.64 – 3.53 (m, 0.58H), 3.51 – 3.32 (m, 1H), 2.96 – 2.73 (m, 1H), 2.34 – 2.21 (m, 0.59H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.7, 173.4, 141.2, 141.0, 140.2, 139.7, 128.6, 128.4, 128.3, 127.88, 127.86, 127.3, 127.2, 126.94, 126.90, 125.3, 125.1, 88.3, 87.7, 75.2, 75.0, 52.9, 52.8, 45.4, 45.0, 44.9, 43.8 ppm.

HRMS (ESI): Mass found: 305.11490, calculated mass for C₁₈H₁₈NaO₃⁺: 305.11482.

IR (KBr): 3453, 3060, 029, 2950, 2877, 2665, 2329, 2083, 1995, 1951, 1882, 1825, 1731, 1601, 1493, 1446, 1256, 1169, 1100, 1067, 1042, 934, 911, 847, 735 cm⁻¹.

Methyl 4-methyl-2-phenyl-4-((tosyloxy)methyl)tetrahydrofuran-2-carboxylate (11)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (73%, d.r. = 1:1, 59 mg).

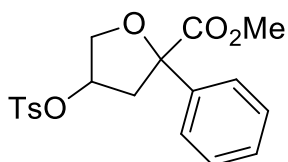
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.85 – 7.76 (m, 2H), 7.69 – 7.62 (m, 2H), 7.52 – 7.45 (m, 2H), 7.41 – 7.21 (m, 12H), 3.92 – 3.80 (m, 4H), 3.74 – 3.57 (m, 10H), 2.91 (d, *J* = 13.5 Hz, 1H), 2.74 (d, *J* = 13.5 Hz, 1H), 2.44 (d, *J* = 10.2 Hz, 6H), 2.07 (dd, *J* = 13.5, 2.6 Hz, 2H), 1.14 (s, 3H), 1.02 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.5, 173.1, 144.9, 144.8, 141.2, 140.8, 132.5, 132.3, 129.9, 129.8, 128.4, 128.3, 127.9, 127.8, 125.0, 124.8, 87.6, 87.3, 75.9, 75.6, 74.5, 74.4, 52.9, 46.9, 46.7, 43.86, 43.83, 22.2, 21.6, 21.0 ppm.

HRMS (ESI): Mass found: 427.11862, calculated mass for C₂₁H₂₄NaO₆S⁺: 427.11858.

IR (KBr): 3819, 3738, 3322, 3089, 2956, 2885, 2702, 2507, 2321, 2046, 1969, 1894, 1730, 1596, 1490, 1449, 1353, 1290, 1255, 1214, 1173, 1098, 1065, 965, 734, 665 cm⁻¹.

Methyl 2-phenyl-4-((tosyloxy)methyl)tetrahydrofuran-2-carboxylate (12)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (77%, d.r > 20:1, 58 mg).

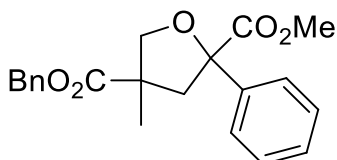
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.64 – 7.60 (m, 2H), 7.44 – 7.40 (m, 2H), 7.36 – 7.25 (m, 5H), 5.22 – 5.16 (m, 1H), 4.24 – 4.18 (m, 1H), 4.11 – 4.01 (m, 1H), 3.68 (s, 3H), 3.15 (dd, *J* = 14.6, 6.9 Hz, 1H), 2.49 – 2.41 (m, 4H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 172.7, 144.9, 139.6, 133.4, 129.8, 128.3, 128.0, 127.6, 125.0, 87.2, 80.3, 72.9, 53.4, 53.0, 43.1, 21.6 ppm.

HRMS (ESI): Mass found: 399.08801, calculated mass for C₁₉H₂₀NaO₆S⁺: 399.08728.

IR (KBr): 3653, 2954, 2874, 2685, 2322, 2162, 2044, 2001, 1917, 1734, 1597, 1494, 1442, 1361, 1252, 1177, 1086, 963, 890, 815, 736 cm⁻¹.

4-benzyl 2-methyl 4-methyl-2-phenyltetrahydrofuran-2,4-dicarboxylate (13)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (75%, d.r = 1:1, 53 mg).

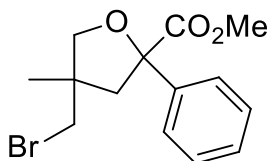
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.56 – 7.46 (m, 4H), 7.44 – 7.21 (m, 14H), 7.21 – 7.15 (m, 2H), 5.15 (s, 2H), 4.98 (d, *J* = 12.5 Hz, 1H), 4.89 (d, *J* = 12.4 Hz, 1H), 4.48 (t, *J* = 9.2 Hz, 2H), 3.81 (dd, *J* = 8.9, 3.3 Hz, 2H), 3.71 (s, 3H), 3.63 – 3.53 (m, 4H), 2.94 (d, *J* = 13.3 Hz, 1H), 2.86 (d, *J* = 13.3 Hz, 1H), 2.19 (d, *J* = 13.3 Hz, 1H), 1.40 (s, 3H), 1.31 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.8, 174.7, 173.4, 173.1, 141.3, 140.6, 135.6, 135.5, 128.5, 128.3, 128.2, 128.1, 128.0, 127.8, 125.1, 87.8, 87.6, 76.8, 76.6, 66.9, 66.7, 52.9, 52.7, 50.4, 50.2, 48.0, 47.3, 22.8, 22.5 ppm.

HRMS (ESI): Mass found: 377.13641, calculated mass for C₂₁H₂₂NaO₅⁺: 377.13594.

IR (KBr): 3450, 3032, 2952, 2879, 2668, 2326, 2085, 1993, 1954, 1888, 1730, 1598, 1449, 1256, 1130, 1168, 1061, 734, 698 cm⁻¹.

Methyl 4-(bromomethyl)-4-methyl-2-phenyltetrahydrofuran-2-carboxylate (14)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (89%, d.r 3:2, 56 mg).

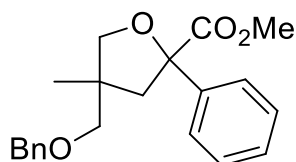
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.55 – 7.47 (m, 2H), 7.38 – 7.32 (m, 2H), 7.31 – 7.27 (m, 1H), 4.04 – 3.97 (m, 1H), 3.82 – 3.74 (m, 1H), 3.71 (s, 3H), 3.48 – 3.42 (m, 1H), 3.33 – 3.22 (m, 1H), 3.06 (d, *J* = 13.5 Hz, 0.60 H), 2.88 (d, *J* = 13.4 Hz, 0.40 H), 2.34 (d, *J* = 13.4 Hz, 0.40 H), 2.22 (d, *J* = 13.5 Hz, 0.60 H), 1.27 (s, 1.30 H), 1.16 (s, 1.70 H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.6, 173.4, 141.4, 141.1, 128.4, 127.9, 127.8, 125.04, 125.01, 87.6, 77.5, 77.4, 53.0, 52.9, 48.9, 48.8, 45.1, 45.0, 42.3, 41.7, 23.6, 22.9 ppm.

HRMS (ESI): Mass found: 335.02593, calculated mass for C₁₄H₁₇BrNaO₃⁺: 335.02533.

IR (KBr): 3867, 3454, 3060, 2955, 2865, 2670, 2329, 2192, 2112, 1991, 1938, 1825, 1732, 1598, 1490, 1446, 1381, 1248, 1145, 1058, 951, 857, 791, 729, 699, 657 cm⁻¹.

Methyl 4-((benzyloxy)methyl)-4-methyl-2-phenyltetrahydrofuran-2-carboxylate (15)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (69%, d.r. 1:1, 47 mg).

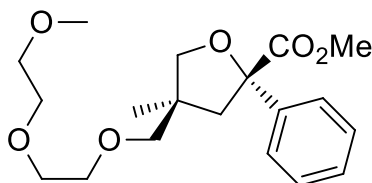
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.53 (d, *J* = 7.9 Hz, 2H), 7.49 (d, *J* = 7.8 Hz, 2H), 7.38 – 7.25 (m, 14H), 7.24 – 7.21 (m, 2H), 4.52 (s, 2H), 4.39 (s, 2H), 4.01 (t, *J* = 9.0 Hz, 2H), 3.73 – 3.67 (m, 5H), 3.61 (s, 3H), 3.32 (d, *J* = 8.8 Hz, 1H), 3.29 (d, *J* = 8.8 Hz, 1H), 3.19 (d, *J* = 8.7 Hz, 1H), 3.13 (d, *J* = 8.7 Hz, 1H), 2.99 (d, *J* = 13.1 Hz, 1H), 2.72 (d, *J* = 13.1 Hz, 1H), 2.23 (d, *J* = 13.1 Hz, 1H), 2.06 (d, *J* = 13.1 Hz, 1H), 1.18 (s, 3H), 1.06 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.2, 173.8, 142.0, 141.7, 138.33, 138.30, 128.34, 128.30, 128.28, 128.24, 127.6, 127.5, 127.4, 127.3, 125.18, 125.14, 87.7, 87.4, 75.8, 75.7, 73.3, 73.1, 52.8, 52.7, 47.7, 47.3, 44.5, 44.4, 30.3, 29.7, 22.8, 22.0 ppm.

HRMS (ESI): Mass found: 363.15668, calculated mass for C₂₁H₂₄NaO₄⁺: 363,15668.

IR (KBr): 3445, 3187, 3063, 3030, 2952, 2857, 2664, 2330, 2215, 2154, 2056, 1990, 1941, 1887, 1732, 1599, 1491, 1449, 1362, 1254, 1208, 1148, 1096, 1028, 910, 856, 806, 733, 698 cm⁻¹.

Methyl 4-((2-(2-methoxyethoxy)ethoxy)methyl)-4-methyl-2-phenyltetrahydrofuran-2-carboxylate (16)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (73%, d.r. > 20:1, 51 mg).

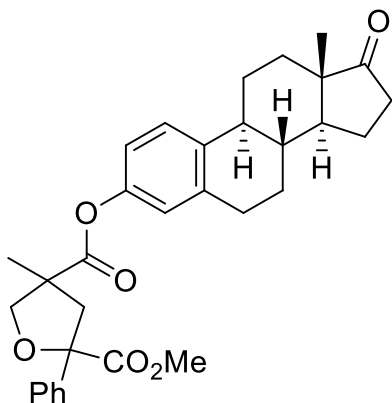
¹H NMR (300 MHz, Chloroform-*d*): δ = 7.57 – 7.46 (m, 2H), 7.41 – 7.25 (m, 3H), 4.00 (d, *J* = 8.8 Hz, 1H), 3.79 – 3.64 (m, 4H), 3.61 – 3.53 (m, 4H), 3.53 – 3.45 (m, 4H), 3.37 (s, 3H), 3.22 (d, *J* = 8.8 Hz, 1H), 3.15 (d, *J* = 8.8 Hz, 1H), 2.72 (d, *J* = 13.2 Hz, 1H), 2.22 (d, *J* = 13.2 Hz, 1H), 1.16 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.2, 141.7, 128.2, 127.6, 125.1, 87.4, 71.9, 70.8, 70.5, 70.3, 59.0, 52.8, 47.2, 44.4, 22.0 ppm.

HRMS (ESI): Mass found: 375.17780, calculated mass for C₁₉H₂₈NaO₆⁺: 375.17781.

IR (KBr): 3857, 3633, 3329, 3062, 2869, 2703, 2509, 2325, 2099, 1994, 1951, 1811, 1732, 1599, 1541, 1449, 1354, 1248, 1204, 1107, 1060, 851, 778, 730, 700 cm⁻¹.

(2*S*,4*S*)-2-methyl 4-((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclpenta[a]phenanthren-3-yl) 4-methyl-2-phenyltetrahydrofuran-2,4-dicarboxylate (17)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (hexane:ethyl acetate – 9:1 → 4:1) as colorless oil (76%, d.r. > 20:1, 78 mg).

¹H NMR (600 MHz, Chloroform-*d*): δ = 7.61 – 7.52 (m, 2H), 7.38 – 7.33 (m, 2H), 7.32 – 7.28 (m, 1H), 7.18 (d, *J* = 8.6 Hz, 1H), 6.54 – 6.47 (m, 1H), 6.40 – 6.35 (m, 1H), 4.65 (d, *J* = 9.0 Hz, 1H), 3.89 (d, *J* = 9.0 Hz, 1H), 3.74 (s, 3H), 3.12 (d, *J* = 13.4 Hz, 1H), 2.94 (d, *J* = 13.4 Hz, 1H), 2.87 – 2.79 (m, 2H), 2.53 – 2.46 (m, 1H), 2.39 – 2.33

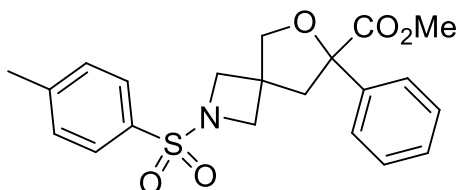
(m, 1H), 2.27 – 2.19 (m, 1H), 2.18 – 2.09 (m, 1H), 2.07 – 2.01 (m, 1H), 2.01 – 1.92 (m, 2H), 1.66 – 1.58 (m, 2H), 1.54 (s, 3H), 1.52 – 1.36 (m, 4H), 0.89 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 220.6, 173.7, 173.3, 148.3, 140.6, 137.9, 137.4, 128.3, 127.9, 126.2, 125.3, 121.1, 118.2, 87.6, 76.5, 52.9, 50.5, 50.3, 47.9, 47.4, 44.0, 37.9, 35.8, 31.5, 29.2, 26.2, 25.7, 22.4, 21.5, 13.7 ppm.

HRMS (ESI): Mass found: 539.23920, calculated mass for C₃₂H₃₆NaO₆⁺: 539.24041.

IR (KBr): 3853, 3456, 2929, 2871, 2697, 2505, 2219, 2175, 2087, 2036, 1996, 1949, 1907, 1735, 1605, 1492, 1450, 1377, 1253, 1211, 1150, 1112, 1057, 910, 814, 782, 731, 698, 658 cm⁻¹.

Methyl 7-phenyl-2-tosyl-6-oxa-2-azaspiro[3.4]octane-7-carboxylate (18)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (92%, 73 mg).

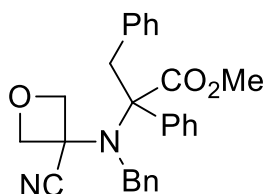
¹H NMR (300 MHz, Chloroform-*d*): δ = 7.74 – 7.62 (m, 2H), 7.47 – 7.24 (m, 7H), 4.02 – 3.92 (m, 2H), 3.79 (d, *J* = 8.2 Hz, 1H), 3.70 (d, *J* = 8.2 Hz, 1H), 3.66 (s, 3H), 3.60 – 3.47 (m, 2H), 2.91 (d, *J* = 13.2 Hz, 1H), 2.47 (s, 3H), 2.29 (d, *J* = 13.2 Hz, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 172.6, 144.3, 139.9, 131.2, 129.8, 128.4, 128.3, 128.1, 124.9, 87.3, 77.2, 59.7, 59.5, 52.9, 47.5, 40.2, 21.6 ppm.

HRMS (ESI): Mass found: 424.11798, calculated mass for C₂₁H₂₃NNaO₅S⁺: 424.11891.

IR (KBr): 3638, 3285, 3031, 2953, 2874, 2290, 2161, 2016, 1946, 1887, 1733, 1597, 1491, 1446, 1342, 1266, 1158, 1090, 1056, 941, 874, 815, 675 cm⁻¹.

Methyl 2-(benzyl(3-cyanooxetan-3-yl)amino)-2,3-diphenylpropanoate (21)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (62%, 52 mg).

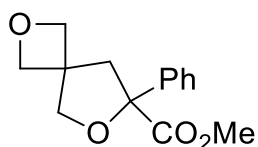
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.53 – 7.48 (m, 2H), 7.42 – 7.16 (m, 13H), 4.11 (d, *J* = 9.4 Hz, 1H), 3.88 (d, *J* = 14.1 Hz, 2H), 3.71 (s, 3H), 3.66 – 3.57 (m, 3H), 3.32 (d, *J* = 13.4 Hz, 1H), 2.88 (d, *J* = 13.4 Hz, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 172.6, 139.4, 137.8, 128.7, 128.5, 128.46, 128.41, 127.7, 124.8, 118.5, 86.4, 76.5, 68.2, 57.3, 53.1, 49.3 ppm.

HRMS (ESI): Mass found: 449.18359, calculated mass for C₂₇H₂₆N₂NaO₃⁺: 449.18356.

IR (KBr): 3063, 3030, 2952, 2847, 2254, 2160, 1959, 1886, 1825, 1733, 1601, 1448, 1245, 1208, 1126, 1031, 911, 734, 698 cm⁻¹.

Methyl 7-phenyl-2,6-dioxaspiro[3.4]octane-7-carboxylate (24)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (74%, 37 mg).

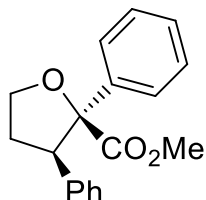
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.52 – 7.46 (m, 2H), 7.38 – 7.32 (m, 2H), 7.32 – 7.28 (m, 1H), 4.01 (d, *J* = 9.7 Hz, 1H), 3.86 (d, *J* = 9.7 Hz, 1H), 3.72 (s, 3H), 3.64 – 3.56 (m, 4H), 2.95 (d, *J* = 13.8 Hz, 1H), 2.25 (d, *J* = 13.8 Hz, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.3, 140.7, 128.4, 127.9, 125.0, 87.6, 73.8, 65.0, 53.0, 50.1, 44.5, 37.1, 29.7 ppm.

HRMS (ESI): Mass found: 271.09404, calculated mass for C₁₄H₁₆NaO₄⁺: 271.09408.

IR (KBr): 3477, 2951, 2874, 2161, 2047, 1890, 1731, 1600, 1445, 1367, 1254, 1029, 852, 786, 730, 698 cm⁻¹.

***cis*-methyl 2,3-diphenyltetrahydrofuran-2-carboxylate (25a)**



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (79%, 45 mg).

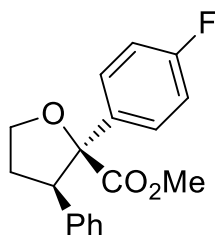
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.21 – 7.18 (m, 2H), 7.11 – 7.00 (m, 6H), 6.98 – 6.94 (m, 2H), 4.45 – 4.39 (m, 1H), 4.30 (dd, *J* = 7.7, 5.2 Hz, 1H), 4.23 – 4.7 (m, 1H), 3.75 (s, 3H), 2.49 – 2.42 (m, 1H), 2.24 – 2.17 (m, 1H) ppm.

¹³C NMR (151 MHz, CDCl₃): δ = 174.1, 140.2, 137.4, 128.8, 127.7, 127.4, 127.1, 126.3, 126.1, 91.0, 67.4, 52.9, 51.8, 33.3 ppm.

HRMS (ESI): Mass found: 305.11484, calculated mass for C₁₈H₁₈O₃Na⁺: 305.11536.

IR (KBr): 3452, 3062, 3030, 2951, 2890, 2162, 2043, 1955, 1884, 1728, 1602, 1493, 1449, 1212, 1030, 731, 700 cm⁻¹.

***cis*-methyl 2-(4-fluorophenyl)-3-phenyltetrahydrofuran-2-carboxylate (25b)**



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (81%, 49 mg).

¹H NMR (300 MHz, Chloroform-*d*): δ = 7.22 – 7.12 (m, 2H), 7.10 – 7.03 (m, 3H), 6.98 – 6.91 (m, 2H), 6.82 – 6.73 (m, 2H), 4.45 – 4.39 (m, 1H), 4.30 – 4.23 (m, 1H), 4.23 – 4.14 (m, 1H), 3.76 (s, 3H), 2.53 – 2.38 (m, 1H), 2.26 – 2.13 (m, 1H) ppm.

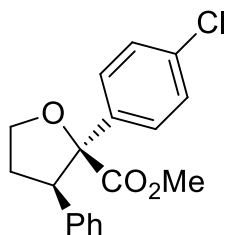
¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.0, 161.8 (d, *J* = 245.9 Hz), 140.0, 133.2, 128.8, 128.0 (d, *J* = 8.2 Hz), 127.9, 126.5, 114.3 (d, *J* = 21.5 Hz), 90.6, 67.5, 53.0, 52.0, 33.2 ppm.

¹⁹F NMR (564 MHz, Chloroform-*d*): δ = -115.2 ppm.

HRMS (ESI): Mass found: 323.10547, calculated mass for C₁₈H₁₇FO₃Na⁺: 323.10594.

IR (KBr): 3452, 3031, 2955, 2891, 2322, 2162, 2036, 1896, 1730, 1603, 1506, 1453, 1225, 1159, 1022, 835, 787, 701 cm⁻¹.

***cis*-methyl 2-(4-chlorophenyl)-3-phenyltetrahydrofuran-2-carboxylate (25c)**



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (78%, 49 mg).

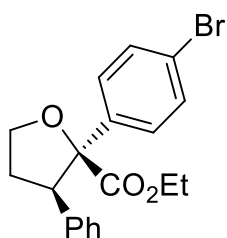
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.17 – 7.12 (m, 2H), 7.11 – 7.03 (m, 5H), 6.97 – 6.93 (m, 2H), 4.45 – 4.38 (m, 1H), 4.30 – 4.25 (m, 1H), 4.24 – 4.17 (m, 1H), 3.75 (s, 3H), 2.49 – 2.42 (m, 1H), 2.22 – 2.15 (m, 1H) ppm.

¹³C NMR (151 MHz, CDCl₃): δ = 173.8, 139.8, 136.0, 133.1, 129.2, 128.7, 127.9, 127.7, 127.6, 126.5, 90.6, 67.51, 53.0, 51.9, 33.3 ppm.

HRMS (ESI): Mass found: 339.07587, calculated mass for C₁₈H₁₇ClNaO₃⁺ = 339.07584.

IR (KBr): 3450, 3063, 3031, 2951, 2889, 2320, 2160, 2038, 1909, 1729, 1598, 1490, 1452, 1400, 1355, 1246, 1087, 1052, 827, 781, 702 cm⁻¹.

***cis*-ethyl 2-(4-bromophenyl)-3-phenyltetrahydrofuran-2-carboxylate (25d)**



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (78%, 58 mg).

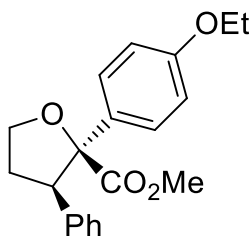
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.62 – 7.57 (m, 2H), 7.53 – 7.48 (m, 2H), 7.36 – 7.29 (m, 4H), 7.26 – 7.22 (m, 1H), 4.43 (q, *J* = 8.1 Hz, 1H), 4.14 – 4.06 (m, 1H), 3.84 (dd, *J* = 7.9, 3.2 Hz, 1H), 3.81 – 3.71 (m, 2H), 2.29 – 2.20 (m, 1H), 2.15 – 2.07 (m, 1H), 0.82 (t, *J* = 7.1 Hz, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 169.9, 141.4, 139.9, 131.3, 128.4, 128.0, 127.9, 127.0, 122.1, 90.9, 67.1, 61.2, 55.3, 33.0, 13.5 ppm.

HRMS (ESI): Mass found: 397.04095, calculated mass for C₁₉H₁₉BrNaO₃⁺ = 397.04098.

IR (KBr): 3902, 3633, 3449, 3065, 3031, 2977, 2893, 2329, 2084, 1999, 1945, 1822, 1726, 1591, 1487, 1452, 1392, 1365, 1246, 1122, 1074, 1013, 970, 828, 760 cm⁻¹.

***cis*-methyl 2-(4-ethoxyphenyl)-3-phenyltetrahydrofuran-2-carboxylate (25e)**



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (84%, 55 mg).

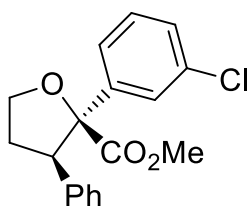
¹H NMR (400 MHz, Chloroform-*d*): δ = 7.09 – 7.00 (m, 5H), 6.98 – 6.92 (m, 2H), 6.62 – 6.54 (m, 2H), 4.42 – 4.31 (m, 1H), 4.26 – 4.20 (m, 1H), 4.20 – 4.11 (m, 1H), 3.88 (q, *J* = 7.0 Hz, 2H), 3.73 (s, 3H), 2.46 – 2.35 (m, 1H), 2.22 – 2.10 (m, 1H), 1.31 (t, *J* = 7.0 Hz, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.3, 157.9, 140.2, 129.4, 128.9, 127.7, 127.4, 126.3, 113.3, 90.6, 67.3, 63.1, 52.8, 51.8, 33.3, 14.7 ppm.

HRMS (ESI): Mass found: 365.11508, calculated mass for C₂₀H₂₂KO₄⁺ = 365.11497.

IR (KBr): 3434, 3027, 2978, 2932, 2682, 2329, 2241, 2154, 2046, 1948, 1825, 1727, 1609, 1513, 1480, 1453, 1394, 1295, 1245, 1179, 1109, 839, 702 cm⁻¹.

***cis*-methyl 2-(3-chlorophenyl)-3-phenyltetrahydrofuran-2-carboxylate (25f)**



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (83%, 52 mg).

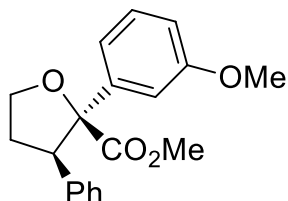
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.28 – 7.24 (m, 2H), 7.12 – 6.93 (m, 7H), 4.46 – 4.40 (m, 1H), 4.30 – 4.25 (m, 1H), 4.23 – 4.16 (m, 1H), 3.77 (s, 3H), 2.49 – 2.42 (m, 1H), 2.25 – 2.15 (m, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.6, 139.7, 139.5, 133.5, 128.7, 128.6, 127.9, 127.3, 126.6, 126.4, 124.5, 90.5, 67.6, 53.1, 52.0, 33.2 ppm.

HRMS (ESI): Mass found: 339.07584, calculated mass for C₁₈H₁₇ClNaO₃⁺ = 339.07584.

IR (KBr): 3860, 3449, 3065, 3030, 2950, 2890, 2329, 2086, 1991, 1882, 1730, 1596, 1573, 1475, 1452, 1428, 1348, 1111, 1077, 1055, 1030, 976, 939, 888, 747 cm⁻¹.

cis-methyl 2-(3-methoxyphenyl)-3-phenyltetrahydrofuran-2-carboxylate (25g)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (69%, 43 mg).

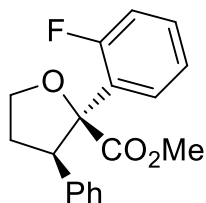
¹H NMR (400 MHz, Chloroform-*d*): δ = 7.38 – 7.13 (m, 1H), 6.88 -6.81 (m, 8H), 4.45 -4.36 (m, 1H), 4.10 (td, *J* = 9.0, 5.0 Hz, 1H), 3.91 (dd, *J* = 7.9, 3.2 Hz, 1H), 3.82 (s, 3H), 3.28 (s, 3H), 2.31 – 2.20 (m, 1H), 2.04 – 2.03 (m, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 170.8, 159.5, 142.2, 141.8, 129.2, 128.4, 127.9, 126.9, 118.5, 113.2, 111.9, 91.4, 67.0, 55.3, 55.3, 55.1, 52.0, 33.0 ppm.

HRMS (ESI): Mass found: 335.12534, calculated mass for C₁₉H₂₀NaO₄⁺ = 335.12538.

IR (KBr): 3458, 3062, 3028, 2949, 2889, 2837, 2328, 2161, 2102, 1992, 1937, 1737, 1597, 1487, 1432, 1354, 1255, 1085, 1045, 972, 934, 874, 827, 774 cm⁻¹.

cis-methyl 2-(2-fluorophenyl)-3-phenyltetrahydrofuran-2-carboxylate (25h)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (64%, 38 mg).

¹H NMR (600 MHz, Chloroform-*d*): δ = 7.70 (td, *J* = 7.8, 1.8 Hz, 1H), 7.39 – 7.28 (m, 5H), 7.25 – 7.22 (m, 1H), 7.18 (td, *J* = 7.6, 1.3 Hz, 1H), 7.13 – 7.06 (m, 1H), 4.49 – 4.43 (m, 1H), 4.27 (dd, *J* = 7.8, 5.4 Hz, 1H), 4.04 – 3.98 (m, 1H), 3.27 (s, 3H), 2.45 – 2.32 (m, 2H) ppm.

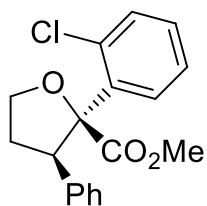
¹³C NMR (151 MHz, Chloroform-*d*): δ = 170.5, 160.6 (d, *J* = 249.2 Hz), 140.5, 130.1 (d, *J* = 8.7 Hz), 128.4, 128.2, 127.7 (d, *J* = 3.3 Hz), 127.5 (d, *J* = 12.0 Hz), 127.0, 123.9 (d, *J* = 3.5 Hz), 116.7 (d, *J* = 23.4 Hz), 89.3 (d, *J* = 3.3 Hz), 67.3, 52.0 (d, *J* = 4.3 Hz), 51.9, 33.2 ppm.

¹⁹F NMR (564 MHz, Chloroform-*d*): δ = -109.0 (ddd, *J* = 12.1, 8.0, 4.9 Hz).

HRMS (ESI): Mass found: 323.10538, calculated mass for C₁₈H₁₇FNaO₃⁺ = 323.10539.

IR (KBr): 3452, 3032, 2951, 2890, 2161, 2041, 1981, 1737, 1610, 1582, 1487, 1450, 1231, 1079, 941, 757, 701 cm⁻¹.

cis-methyl 2-(2-chlorophenyl)-3-phenyltetrahydrofuran-2-carboxylate (25i)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (66%, 42 mg).

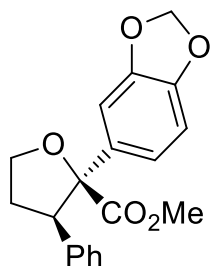
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.85 – 7.87 (m, 1H), 7.41 – 7.38 (m, 1H), 7.36 – 7.23 (m, 7H), 4.48 (td, *J* = 8.7, 4.1 Hz, 1H), 4.23 (t, *J* = 7.6 Hz, 1H), 4.01 – 3.94 (m, 1H), 3.32 (s, 3H), 2.64 – 2.55 (m, 1H), 2.52 – 2.42 (m, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 171.2, 138.8, 137.5, 134.4, 131.4, 129.4, 128.8, 128.1, 127.4, 127.3, 126.5, 89.9, 67.5, 51.9, 51.4, 32.9 ppm.

HRMS (ESI): Mass found: 339.07584, calculated mass for C₁₈H₁₇ClNaO₃⁺ = 339.07584.

IR (KBr): 3063, 3030, 2949, 2888, 2164, 2038, 1980, 1737, 1599, 1494, 1434, 1226, 1085, 1047, 975, 938, 797, 750, 700 cm⁻¹.

cis-methyl 2-(benzo[d][1,3]dioxol-5-yl)-3-phenyltetrahydrofuran-2-carboxylate (25j)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 20:1 → 9:1) as colorless oil (81%, 53 mg).

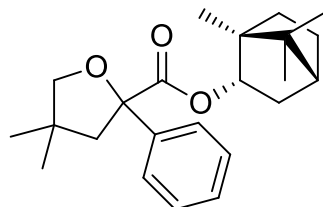
¹H NMR (400 MHz, Chloroform-*d*): δ = 7.12 – 7.02 (m, 3H), 7.01 – 6.93 (m, 2H), 6.75 – 6.61 (m, 2H), 6.51 (d, *J* = 8.2 Hz, 1H), 5.81 (s, 2H), 4.41 – 4.32 (m, 1H), 4.22 (dd, *J* = 7.6, 5.1 Hz, 1H), 4.18 – 4.10 (m, 1H), 3.74 (s, 3H), 2.47 – 2.35 (m, 1H), 2.22 – 2.11 (m, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.1, 146.9, 146.5, 140.2, 131.4, 128.8, 127.8, 126.3, 119.8, 107.3, 107.1, 100.7, 90.7, 67.3, 52.9, 51.8, 33.3 ppm.

HRMS (ESI): Mass found: 349.10471, calculated mass for C₁₉H₁₈NaO₅⁺ = 349.10464.

IR (KBr): 3450, 2952, 2890, 2780, 2322, 2163, 2039, 1956, 1870, 1728, 1606, 1489, 1439, 1350, 1243, 1100, 1034, 932, 872, 813, 779, 752, 703 cm⁻¹.

1-(4,4-dimethyl-2-phenyltetrahydrofuran-2-yl)-2-((1R,2S,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)ethenone (29)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (53%, d.r. = 1:1, 38 mg).

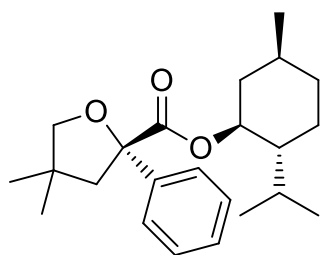
¹H NMR (300 MHz, Chloroform-*d*): δ = 7.76 – 7.43 (m, 2H), 7.40 – 7.17 (m, 3H), 4.90 – 4.76 (m, 1H), 3.91 – 3.54 (m, 1H), 2.76 (dd, *J* = 12.8, 1.9 Hz, 1H), 2.45 – 2.07 (m, 2H), 1.93 – 1.82 (m, 1H), 1.78 – 1.57 (m, 2H), 1.33 – 1.20 (m, 1H), 1.18 – 0.99 (m, 7H), 0.89 – 0.80 (m, 7H), 0.75 (s, 1.5H), 0.69 (s, 1.5H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.7, 173.6, 142.5, 128.0, 127.3, 125.4, 87.7, 87.6, 80.9, 80.7, 80.5, 80.4, 51.3, 51.2, 48.9, 48.8, 47.80, 44.7, 39.8, 36.5, 36.1, 27.9, 27.8, 27.1, 27.0, 26.8, 26.7, 26.2, 19.6, 18.8, 13.4, 13.3 ppm.

HRMS (ESI): Mass found: 379.22427, calculated mass for C₂₃H₃₂NaO₃⁺: 379.22437.

IR (KBr): 3452, 3062, 3029, 2954, 2874, 2727, 2331, 2112, 1811, 1726, 1452, 1370, 1248, 1149, 1113, 980, 826, 788, 725, 699 cm⁻¹.

(S)-(1S,2R,5S)-2-isopropyl-5-methylcyclohexyl 4,4-dimethyl-2-phenyltetrahydrofuran-2-carboxylate (30)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (62%, d.r. > 20:1, 44 mg).

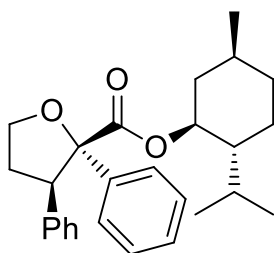
¹H NMR (300 MHz, Chloroform-*d*): δ = 7.56 – 7.48 (m, 2H), 7.36 – 7.19 (m, 3H), 4.64 (td, J = 10.9, 4.4 Hz, 1H), 3.76 (d, J = 8.2 Hz, 1H), 3.70 (d, J = 8.3 Hz, 1H), 2.73 (d, J = 12.9 Hz, 1H), 2.15 (d, J = 12.9 Hz, 1H), 1.86 – 1.76 (m, 1H), 1.70 – 1.56 (m, 2H), 1.53 – 1.29 (m, 3H), 1.12 (s, 3H), 1.02 (s, 3H), 1.00 – 0.77 (m, 7H), 0.74 (d, J = 7.0 Hz, 3H), 0.55 (d, J = 7.0 Hz, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 173.2, 142.3, 127.9, 127.3, 125.3, 87.7, 80.6, 75.2, 51.3, 46.9, 40.2, 39.7, 34.1, 31.3, 26.8, 26.2, 25.5, 22.9, 21.9, 20.7, 15.5 ppm.

HRMS (ESI): Mass found: 381.24005, calculated mass for $C_{23}H_{34}NaO_3^+$: 381.24002.

IR (KBr): 3870, 3445, 3175, 3031, 3063, 2953, 2868, 2663, 2326, 2109, 1989, 1808, 1723, 1600, 1453, 1370, 1247, 1185, 1150, 1098, 1008, 959, 915, 787, 699 cm^{-1} .

(2S,3R)-(1S,2R,5S)-2-isopropyl-5-methylcyclohexyl 2,3-diphenyltetrahydrofuran-2-carboxylate (31)



The titled compound was synthesized according to the general procedure-3. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (56%, d.r. > 20:1, 45 mg).

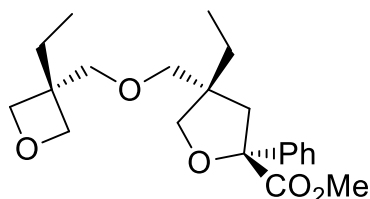
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.74 – 7.66 (m, 2H), 7.42 – 7.34 (m, 4H), 7.32 – 7.27 (m, 3H), 7.24 – 7.20 (m, 1H), 4.43 – 4.26 (m, 2H), 4.04 (ddd, J = 9.6, 8.7, 4.6 Hz, 1H), 3.98 (dd, J = 8.0, 2.3 Hz, 1H), 2.32 – 2.20 (m, 1H), 2.06 – 2.00 (m, 1H), 1.54 – 1.44 (m, J = 23.0, 13.4, 3.1 Hz, 2H), 1.30 – 0.72 (m, 7H), 0.68 (d, J = 6.6 Hz, 3H), 0.60 (d, J = 7.0 Hz, 3H), 0.30 (d, J = 7.0 Hz, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 169.6, 142.5, 140.7, 128.4, 128.1, 128.1, 127.8, 126.7, 126.0, 91.3, 74.6, 66.3, 53.6, 46.8, 39.3, 33.9, 33.4, 30.9, 25.1, 22.5, 21.8, 20.7, 15.3 ppm.

HRMS (ESI): Mass found: 429.24002, calculated mass for $C_{27}H_{34}NaO_3^+$: 429.24002.

IR (KBr): 3455, 3063, 3035, 2947, 2865, 2725, 2181, 2037, 1975, 1908, 1730, 1602, 1492, 1450, 1370, 1265, 1230, 1181, 1091, 994, 953, 916, 844, 700 cm^{-1} .

methyl 4-ethyl-4-(((3-ethyloxetan-3-yl)methoxy)methyl)-2-phenyltetrahydrofuran-2-carboxylate (35)



In a test tube 3,3'-(oxybis(methylene))bis(3-ethyloxetane) (0.2 mmol, 1 equiv.) was dissolved in 1.0 mL chloroform and irradiated with one 3 W LED (distance 1.5 cm, cooling of the setup from the outside with a fan, reaction temperature: 25 °C). The diazoalkane (0.2 mmol, 1.0 equiv.) was dissolved in 1 mL chloroform and added to the reaction mixture over a period of 2 h and then stirred for another 1 h. The crude reaction mixture was purified by silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (57%, d.r. > 20:1, 41 mg).

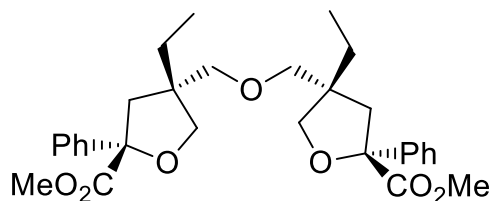
¹H NMR (300 MHz, Chloroform-*d*): δ = 7.56 – 7.50 (m, 2H), 7.38 – 7.27 (m, 3H), 4.39 – 4.26 (m, 4H), 3.97 (d, *J* = 8.9 Hz, 1H), 3.77 – 3.62 (m, 4H), 3.42 (d, *J* = 9.2 Hz, 1H), 3.33 (d, *J* = 9.2 Hz, 1H), 3.24 – 3.10 (m, 2H), 2.75 (d, *J* = 13.4 Hz, 1H), 2.13 (d, *J* = 13.3 Hz, 1H), 1.66 (q, *J* = 7.5 Hz, 2H), 1.56 – 1.43 (m, 2H), 0.89 (t, *J* = 7.5 Hz, 3H), 0.81 (t, *J* = 7.5 Hz, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.1, 141.7, 128.2, 127.6, 125.1, 87.3, 78.4, 78.4, 75.7, 73.8, 73.7, 52.8, 48.2, 45.1, 43.4, 27.2, 26.7, 9.1, 8.1 ppm.

HRMS (ESI): Mass found: 385.19852, calculated mass for C₂₁H₃₀NaO₅⁺: 385.19855.

IR (KBr): 3856, 3454, 3060, 2959, 2865, 2329, 2086, 2000, 1921, 1732, 1599, 1452, 1373, 1237, 1144, 1107, 1063, 822, 782, 729, 699 cm⁻¹.

Dimethyl 4,4'-(oxybis(methylene))bis(4-ethyl-2-phenyltetrahydrofuran-2-carboxylate (36)



In a test tube 3,3'-(oxybis(methylene))bis(3-ethyloxetane) (0.2 mmol, 1 equiv.) was dissolved in 1.0 mL chloroform and irradiated with one 3 W LED (distance 1.5 cm, cooling of the setup from the outside with a fan, reaction temperature: 25 °C). The diazoalkane (0.6 mmol, 3.0 equiv.) was dissolved in 1 mL chloroform and added to the reaction mixture over a period of 2 h and then stirred for another 1 h. The crude reaction mixture was purified by silica gel column chromatography (pentane : diethyl ether – 9:1 → 4:1) as colorless oil (46%, d.r. > 20:1, 47 mg).

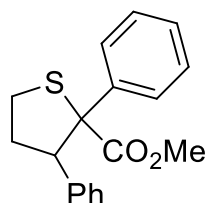
¹H NMR (300 MHz, Chloroform-*d*): δ = 7.51 – 7.45 (m, 4H), 7.36 – 7.26 (m, 6H), 3.86 (d, *J* = 9.0 Hz, 2H), 3.69 (s, 6H), 3.62 (dd, *J* = 8.9, 1.8 Hz, 2H), 3.07 – 2.89 (m, 4H), 2.68 (dd, *J* = 13.4, 1.9 Hz, 2H), 2.03 (d, *J* = 13.3, 2H), 1.53 – 1.34 (m, 4H), 0.81 (td, *J* = 7.4, 2.6 Hz, 6H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.1, 141.6, 128.2, 127.5, 125.1, 87.3, 75.6, 73.5, 52.7, 48.0, 45.1, 45.0, 27.2, 9.1 ppm.

HRMS (ESI): Mass found: 533.25024, calculated mass for C₂₁H₃₀NaO₅⁺: 533.25097.

IR (KBr): 3851, 3644, 3454, 3062, 3028, 2959, 2662, 1985, 1886, 1731, 1599, 1448, 1377, 1237, 1145, 1106, 1064, 963, 854, 813, 782, 729, 699 cm⁻¹.

Methyl 2,3-diphenyltetrahydrothiophene-2-carboxylate (37)



The titled compound was synthesized according to the general procedure-4. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (61%, 36 mg).

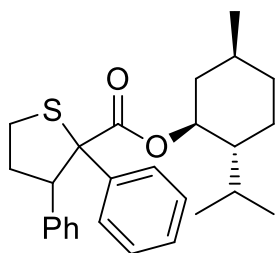
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.45 – 7.40 (m, 1H), 7.32 – 7.24 (m, 2H), 7.21 – 7.17 (m, 1H), 7.16 – 6.98 (m, 5H), 6.85 – 6.81 (m, 1H), 4.35 (dd, *J* = 10.8, 6.0 Hz, 0.55H), 3.70 (s, 1.61H), 3.56 (s, 1.20H), 3.48 – 3.43 (m, 0.44H), 3.24 – 3.12 (m, 2H), 3.03 – 2.94 (m, 0.48H), 2.47 (dddd, *J* = 12.4, 6.9, 5.5, 3.6 Hz, 0.48H), 2.42 – 2.32 (m, 1H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 174.2, 172.6, 140.1, 138.3, 138.1, 137.6, 129.7, 129.2, 128.7, 127.9, 127.8, 127.5, 127.5, 127.4, 127.1, 127.1, 126.9, 126.6, 68.9, 68.2, 60.9, 55.3, 52.8, 52.1, 35.3, 35.2, 30.3, 30.1 ppm.

HRMS (ESI): Mass found: 321.09161, calculated mass for C₁₈H₁₈NaO₂S⁺: 321.09197.

IR (KBr): 3448, 3057, 3029, 2948, 2865, 2319, 2034, 1811, 1728, 1597, 1492, 1440, 1320, 1225, 1065, 1027, 974, 910, 764, 729, 698 cm⁻¹.

((1S,2R,5S)-2-isopropyl-5-methylcyclohexyl 2,3-diphenyltetrahydrothiophene-2-carboxylate (38)



The titled compound was synthesized according to the general procedure-4. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (64%, d.r. = 3:1, 54 mg).

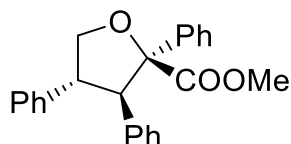
¹H NMR (600 MHz, Chloroform-*d*): δ = 7.55 – 7.48 (m, 2H), 7.32 – 7.26 (m, 3H), 7.25 – 7.18 (m, 4H), 7.13 – 6.99 (m, 1H), 4.55 – 4.46 (m, 1H), 3.66 (dd, *J* = 8.2, 5.6 Hz, 0.66H), 3.56 (dd, *J* = 8.9, 5.5 Hz, 0.33H), 3.18 – 3.06 (m, 2H), 2.80 – 2.68 (m, 1H), 2.48 – 2.31 (m, 1H), 1.66 – 1.58 (m, 1H), 1.54 – 1.48 (m, 1H), 1.42 – 1.13 (m, 4H), 1.00 – 0.65 (m, 8H), 0.63 – 0.45 (m, 4H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 171.5, 171.4, 141.3, 140.7, 139.1, 138.6, 129.9, 129.5, 129.4, 128.8, 127.8, 127.8, 127.6, 127.6, 127.6, 127.3, 127.3, 126.7, 126.7, 75.4, 75.0, 70.4, 70.0, 60.1, 59.3, 46.8, 46.5, 39.6, 39.6, 35.6, 35.6, 34.1, 34.0, 31.5, 31.3, 31.2, 30.1, 29.9, 25.2, 25.1, 22.7, 21.9, 21.9, 20.7, 20.7, 15.6, 15.5 ppm.

HRMS (ESI): Mass found: 445.21716, calculated mass for C₂₇H₃₄NaO₂S⁺: 445.21717.

IR (KBr): 3854, 3460, 3061, 1959, 2331, 1895, 1733, 1599, 1454, 1373, 1262, 1207, 1146, 1108, 1067, 978, 824, 784, 730, 699 cm⁻¹.

(2*S*,3*S*,4*S*)-methyl 2,3,4-triphenyltetrahydrofuran-2-carboxylate (42)



The titled compound was synthesized according to the general procedure-2. And was obtained after silica gel column chromatography (pentane:diethyl ether – 9:1 → 4:1) as colorless oil (61%, d.r. > 20:1, 44 mg).

¹H NMR (600 MHz, Chloroform-*d*): δ = 7.70 – 7.63 (m, 2H), 7.43 – 7.35 (m, 2H), 7.36 – 7.24 (m, 5H), 7.27 – 7.19 (m, 1H), 7.19 – 7.08 (m, 3H), 7.00 – 6.94 (m, 2H), 4.78 – 4.69 (m, 1H), 4.09 – 3.94 (m, 2H), 3.89 (d, *J* = 9.3 Hz, 1H), 3.33 (s, 3H) ppm.

¹³C NMR (151 MHz, Chloroform-*d*): δ = 171.2, 141.3, 138.9, 128.6, 128.5, 128.4, 128.1, 127.7, 127.5, 127.3, 126.9, 126.6, 91.2, 74.0, 65.3, 53.8, 52.0 ppm.

HRMS (ESI): Mass found: 381.14615, calculated mass for C₂₄H₂₂NaO₃⁺: 381.14612.

IR (KBr): 3462, 3061, 3030, 2949, 2162, 2018, 1887, 1737, 1603, 1493, 1447, 1282, 1215, 1092, 1029, 950, 872, 823, 783, 745, 695 cm⁻¹.

Computed Energies of All Stationary Points

Table S2. Thermal correction to Gibbs free energies (*TCG*, in Hartree), thermal correction to enthalpies (*TCH*, in Hartree), sum of electronic and thermal enthalpies (*H*, in Hartree), sum of electronic and thermal free energies (*G*, in Hartree), single point energies in chloroform computed at the (U)B3LYP/6-311+G(d,p) level (*E_{sof}*, in Hartree), and total spin-squared operator of singlet diradical *S*².

Name	<i>TCG</i> /a.u.	<i>TCH</i> /a.u.	<i>H</i> /a.u.	<i>G</i> /a.u.	<i>E_{sof}</i> /a.u.	<i>S</i> ²
4b	0.059183	0.092270	-193.018282	-193.051368	-193.170750	
43	0.109893	0.158087	-497.969019	-498.017213	-498.270989	
TS1	0.190134	0.251714	-690.988130	-691.049710	-691.438060	
INT1	0.197406	0.254403	-691.026864	-691.083861	-691.476101	
TS _{rad} 2	0.194916	0.251332	-691.016013	-691.072428	-691.462754	0.1403
TS _{con} 2	0.194629	0.250945	-690.970157	-691.026473	-691.419174	
INT2	0.189206	0.250655	-691.041309	-691.102758	-691.487453	0.9982
TS3	0.192095	0.249734	-691.038577	-691.096216	-691.483751	1.0176
7a	0.199805	0.255791	-691.133735	-691.189722	-691.582162	
TS4	0.193735	0.250149	-691.006042	-691.062456	-691.454672	
INT4	0.193960	0.254207	-691.101412	-691.161658	-691.555224	
TS5	0.194526	0.250740	-691.005033	-691.061248	-691.452152	
INT5	0.200632	0.255823	-691.082278	-691.137469	-691.528657	
TS6	0.194507	0.250322	-691.002713	-691.058527	-691.449814	
INT6	0.201308	0.255541	-691.092144	-691.146377	-691.540299	
2-phenyl oxetane	0.134467	0.177914	-423.997325	-424.040772	-424.290459	
TS _{Ph} 1	0.264077	0.337351	-921.967255	-922.040529	-922.559092	
INT _{Ph} 1	0.270395	0.339703	-922.006348	-922.075657	-922.596168	
TS _{Ph} 2	0.271494	0.338722	-922.007312	-922.074540	-922.596182	
INT _{Ph} 2	0.266005	0.337664	-922.037741	-922.109400	-922.625513	1.0390
TS _{Ph} 3	0.268284	0.337014	-922.035038	-922.103769	-922.622402	0.9984
<i>cis</i> - 25a	0.274336	0.341569	-922.098463	-922.165696	-922.687241	
TS _{Ph} 3'	0.269042	0.336789	-922.033168	-922.100915	-922.620343	1.0159
<i>trans</i> - 25a	0.273279	0.341404	-922.098992	-922.167116	-922.688226	
2-phenyl thietane	0.132250	0.176093	-746.988446	-747.032289	-747.281653	
TS _{thi} 1	0.260809	0.335156	-1244.957085	-1245.031432	-1245.5492907	
INT _{thi} 1	0.267416	0.337103	-1245.019601	-1245.089288	-1245.611267	
TS _{thi} 2	0.265771	0.335110	-1245.012960	-1245.082300	-1245.602398	0.3196
INT _{thi} 2	0.262038	0.335264	-1245.018343	-1245.091569	-1245.608236	0.9784
TS _{thi} 3	0.264509	0.334335	-1245.015146	-1245.084972	-1245.603555	0.9550
<i>cis</i> - 37	0.272044	0.339043	-1245.080282	-1245.147281	-1245.670222	
TS _{thi} 3'	0.264766	0.334291	-1245.015147	-1245.084671	-1245.603820	0.9562
<i>trans</i> - 37	0.271452	0.338945	-1245.081658	-1245.149151	-1245.671902	

Coordinates of All Stationary Points

4b

C -0.00036000 1.07670300 0.00000000
C -0.00036000 -0.06198100 1.03711800
C -0.00036000 -0.06198100 -1.03711800
H -0.89395100 -0.13139700 1.67141200
H 0.89198500 -0.13019300 1.67326500
H -0.89395100 -0.13139700 -1.67141200
H 0.89198500 -0.13019300 -1.67326500
O 0.00134500 -1.07609100 0.00000000
H -0.89213200 1.70800000 0.00000000
H 0.89179000 1.70746400 0.00000000

43

C 2.18551800 1.49075300 0.10678100
C 0.91610300 0.94035200 0.17072400
C 0.72277200 -0.46705700 0.03142900
C 1.87087300 -1.28389500 -0.17517800
C 3.13999200 -0.72784400 -0.25289600
C 3.29351500 0.65655800 -0.10924400
H 2.32775700 2.56172000 0.21718400
H 0.05232600 1.57701600 0.33976900
H 1.71849500 -2.35398100 -0.27559800
H 4.00951600 -1.35671700 -0.41838800
H 4.28711500 1.09361900 -0.16420200
C -0.54337500 -1.10594100 0.05831900
C -1.74752200 -0.35916600 0.28986600
O -2.15223500 -0.17447900 1.43800100
O -2.43814000 -0.02855600 -0.82311400
C -3.74659900 0.53554100 -0.60466800
H -4.16500700 0.68975000 -1.60034400
H -4.37666800 -0.15243700 -0.03418100
H -3.67820000 1.48950900 -0.07412600

TS1

C -3.05223300 0.21453300 1.24812400
C -1.78998000 0.60527300 0.82621300
C -1.25896100 0.14199200 -0.41179100
C -2.05651700 -0.73571800 -1.19580300
C -3.31803500 -1.12810000 -0.77072400
C -3.81287500 -0.65146300 0.44981700
H -3.45203500 0.57353700 2.19213400
H -1.19281400 1.27284600 1.44140100
H -1.64483000 -1.09035500 -2.13548300
H -3.91985500 -1.79941500 -1.37613400

H -4.80115400 -0.95721600 0.78381600
C 0.01148200 0.52566700 -0.92594400
C 0.87127300 1.42107200 -0.19342900
O 1.80804600 1.06907400 0.52103700
O 0.61838700 2.72126200 -0.50401200
C 1.56205200 3.68107900 0.00662900
H 1.22517400 4.64799700 -0.37065400
H 1.56412900 3.68675900 1.10065400
H 2.57194600 3.46747400 -0.35502600
C 1.67462500 -2.08985400 1.08147900
C 3.10756900 -2.06428400 0.52114200
C 2.41940200 -1.95565200 -0.85114200
H 1.36259100 -3.03045600 1.55466400
H 1.40292200 -1.24625500 1.72355700
H 3.69548600 -2.97111000 0.68422600
H 3.69047200 -1.18689800 0.80742400
H 2.54875800 -2.81866200 -1.51775900
H 2.60295900 -1.03405200 -1.41219500
O 1.09849800 -1.95301800 -0.24553200

INT1

C -3.41152500 0.85283400 -0.00010000
C -2.02967300 1.02246900 -0.00009100
C -1.15000400 -0.09227100 -0.00011300
C -1.75744400 -1.37542100 -0.00014600
C -3.14162200 -1.52953900 -0.00015300
C -3.99005600 -0.41984500 -0.00013000
H -4.04613400 1.73690800 -0.00008000
H -1.61569000 2.02217900 -0.00006300
H -1.13217700 -2.26274100 -0.00016400
H -3.55921600 -2.53439800 -0.00017600
H -5.06970100 -0.54250800 -0.00013400
C 0.29006400 0.05069300 -0.00008300
C 1.18259900 1.14547600 0.00004800
O 2.42584900 1.05354900 0.00021500
O 0.56974800 2.37513900 0.00000100
C 1.45331200 3.50024700 0.00017800
H 0.80563500 4.37982100 -0.00040700
H 2.08878400 3.50982200 0.89146700
H 2.08978400 3.50933600 -0.89038900
C 1.94325400 -1.68258100 1.07470100
C 2.75683700 -2.41489600 0.00012800
C 1.94359400 -1.68238500 -1.07457000
H 1.38020400 -2.26768700 1.80102500

H 2.42184700 -0.80856000 1.50863900
H 2.60541800 -3.49522900 0.00000700
H 3.82165600 -2.18101000 0.00031600
H 1.38078400 -2.26735200 -1.80119200
H 2.42233700 -0.80828500 -1.50818500
O 0.98820900 -1.20856100 -0.00005100

TS_{rad}2

C -3.51470400 1.08987100 0.07645200
C -2.13097900 1.21206200 -0.02007100
C -1.30004800 0.06516500 -0.07275900
C -1.93878300 -1.19921000 -0.02249000
C -3.32252700 -1.30760100 0.08118400
C -4.12743200 -0.16563200 0.12980600
H -4.12193200 1.99179500 0.11169600
H -1.67333600 2.19192100 -0.06290500
H -1.33516700 -2.09986900 -0.06344800
H -3.77637800 -2.29551200 0.11977500
H -5.20816100 -0.25262500 0.20452600
C 0.14858800 0.14569100 -0.18412300
C 0.92593300 1.35379500 -0.08773500
O 0.51487300 2.50620000 -0.22691600
O 2.25509700 1.10500000 0.18275200
C 3.08898600 2.26915600 0.24384100
H 4.09671500 1.89830000 0.44204800
H 3.07176400 2.81832300 -0.70249200
H 2.77337300 2.94011000 1.04854700
C 1.98358500 -1.98175800 1.14987100
C 2.45707000 -2.54139000 -0.15914500
C 1.79657200 -1.49004900 -1.06915800
H 1.32881400 -2.55098400 1.80141600
H 2.52835500 -1.16083700 1.60379500
H 2.06192600 -3.54404200 -0.33917000
H 3.54626500 -2.55984600 -0.26283200
H 1.28397100 -1.84889000 -1.96610500
H 2.45831000 -0.65883600 -1.30831500
O 0.80101900 -1.05740000 -0.08340600

TS_{con}2

C -1.72433500 2.46968800 1.04826500
C -0.62003200 2.46473500 -0.00952600
C -2.57406300 1.42024800 0.43653500
H 0.39084700 2.56477000 0.38723700
H -0.78605900 3.21089100 -0.78963000
H -2.86007900 0.52777800 0.97546300
H -3.14726900 1.64555400 -0.45690300

O -0.81825800 1.17607700 -0.67955100
C 3.24235600 -1.18718900 0.69833900
C 1.85435900 -1.09837600 0.72816000
C 1.16436200 -0.09561900 -0.00526400
C 1.96332800 0.80639800 -0.75701100
C 3.35152600 0.69879700 -0.78728900
C 4.01040700 -0.29251500 -0.05505800
H 3.73215300 -1.96807100 1.27655200
H 1.27655700 -1.80569800 1.30845900
H 1.48474200 1.57422300 -1.35659000
H 3.92339400 1.40062600 -1.39095000
H 5.09478900 -0.36351400 -0.06671700
C -0.28439200 0.01200500 0.00988600
C -1.11683000 -1.14696300 0.04571900
O -0.83213700 -2.22845500 0.57460000
O -2.32689300 -1.00418400 -0.62316800
C -3.17583300 -2.15462300 -0.59022700
H -4.08881500 -1.86099500 -1.11431700
H -2.71502300 -3.00437800 -1.10392800
H -3.41572100 -2.45303900 0.43565200
H -2.24829600 3.43271500 1.11008000
H -1.36804600 2.17212700 2.03537700

INT2

C -3.58509500 -0.85981400 0.00680400
C -2.22040800 -1.12509800 0.01969800
C -1.27769400 -0.06455700 -0.01967800
C -1.77893400 1.26222600 -0.08264000
C -3.14529800 1.51192900 -0.09826400
C -4.06067300 0.45466900 -0.05118900
H -4.28697600 -1.68926500 0.03989100
H -1.86828600 -2.14682200 0.06626900
H -1.07766700 2.08710800 -0.12211900
H -3.50043900 2.53826800 -0.14529900
H -5.12908200 0.65270300 -0.06060500
C 0.15452300 -0.27371000 -0.02071300
C 0.78763200 -1.59470200 0.06420000
O 0.24873600 -2.61796800 0.47298400
O 2.07082300 -1.57904000 -0.37891900
C 2.76770000 -2.83360400 -0.30060700
H 3.77136800 -2.63201700 -0.67759400
H 2.81501500 -3.18999000 0.73251300
H 2.27659800 -3.58951400 -0.91988800
C 2.37690500 3.33426400 -0.60187300
C 2.28480100 2.57521900 0.67612400
C 2.13703200 1.06607900 0.48023400

H 1.83464500 4.26229100 -0.75051100
H 3.05078600 3.00601900 -1.38915500
H 1.45902600 2.94701100 1.29428400
H 3.20422400 2.70770700 1.27678000
H 2.10603400 0.54574600 1.44371500
H 2.96585100 0.66763900 -0.10993200
O 0.89743600 0.83647200 -0.23293200

TS3

C 3.33023500 0.04585400 0.82441000
C 2.01669100 0.48487100 0.69836800
C 1.08631400 -0.23686500 -0.08905300
C 1.53965000 -1.41132000 -0.74061700
C 2.85698800 -1.83725200 -0.61424300
C 3.76059700 -1.11425100 0.17158900
H 4.02407500 0.61053900 1.44171800
H 1.69699600 1.37964400 1.21790400
H 0.85352500 -1.96106900 -1.37676800
H 3.18374100 -2.73201900 -1.13752000
H 4.78940600 -1.44904100 0.27171600
C -0.30087300 0.16034400 -0.23954000
C -0.84412300 1.52429000 -0.19625100
O -2.04067200 1.78390500 -0.21704300
O 0.11398900 2.48320200 -0.15279100
C -0.36873900 3.83542300 -0.09145200
H 0.52338900 4.45992600 -0.02569600
H -0.93778500 4.08444000 -0.99177800
H -1.00202900 3.98453000 0.78789600
C -3.89961900 -1.30037300 0.56363800
C -2.90314500 -2.33573000 0.16603600
C -1.45352300 -1.88902500 0.33011200
H -3.69044100 -0.24980800 0.38747700
H -4.90417200 -1.58887600 0.85914800
H -3.04350400 -2.63235700 -0.89020400
H -3.03851100 -3.25718900 0.74992400
H -0.76645100 -2.70002200 0.06898300
H -1.25007300 -1.57260200 1.35874800
O -1.24342900 -0.75859100 -0.55760900

7a

C 3.06077100 0.73179000 0.97011500
C 1.67981900 0.54239200 1.03180600
C 1.01887100 -0.19591700 0.03873600
C 1.76171900 -0.73154600 -1.01923000
C 3.14420600 -0.53960600 -1.07856900
C 3.79893700 0.19089300 -0.08553800
H 3.55910000 1.30420300 1.74834600

H 1.11335000 0.97485100 1.85147600
H 1.25072400 -1.29481300 -1.79168400
H 3.70838900 -0.96139700 -1.90669800
H 4.87439900 0.34050900 -0.13415900
C -0.49135700 -0.43372800 0.13107000
C -1.18581400 0.94573900 0.25932200
O -1.39635300 1.50355400 1.32060200
O -1.48900200 1.47323900 -0.93216200
C -2.07737100 2.78907100 -0.90350800
H -2.27819300 3.03947700 -1.94577700
H -3.00691900 2.78441600 -0.32810900
H -1.38127000 3.51025100 -0.46639300
C -0.90641300 -1.34345700 1.30858200
C -2.22176300 -1.94288900 0.79748300
C -1.93318400 -2.10854300 -0.69733700
H -1.00589700 -0.78698500 2.24187000
H -0.14776700 -2.12212600 1.43874800
H -3.04913300 -1.24164100 0.95824900
H -2.47998300 -2.88965800 1.28055200
H -2.81609000 -1.96223600 -1.32904000
H -1.50759900 -3.09569600 -0.92151600
O -0.95510000 -1.10483700 -1.04012100

TS4

C -3.14971500 1.62959600 -0.27338700
C -1.76160400 1.56453500 -0.25238300
C -1.09524800 0.35207300 0.07280500
C -1.90514600 -0.77634900 0.37634300
C -3.29135400 -0.69200000 0.36431600
C -3.92933900 0.50908600 0.03512100
H -3.63103400 2.57044000 -0.52921600
H -1.17298600 2.44141300 -0.48700500
H -1.42441600 -1.71514500 0.62748300
H -3.88135900 -1.57336400 0.60410300
H -5.01405900 0.56860400 0.01253100
C 0.34105300 0.22946400 0.14035400
C 1.27439700 1.32782400 -0.09354300
O 1.01657800 2.37336000 -0.68611300
O 2.50164100 1.10017200 0.45902400
C 3.46709500 2.14198700 0.26110500
H 4.37791400 1.79173200 0.75000500
H 3.65257300 2.31093200 -0.80425500
H 3.13284800 3.07832800 0.71765400
C 0.58806700 -3.90350400 -0.08768500
C 1.17657900 -2.84139300 -0.86088200
C 1.82498300 -1.63953800 -0.00328500

H -0.44483800 -3.86324700 0.24359400
H 1.18116600 -4.75284600 0.23831300
H 0.46454500 -2.32961500 -1.52225700
H 2.03287700 -3.20008500 -1.44774600
H 2.35822100 -1.00667100 -0.71887100
H 2.50868600 -2.04540900 0.74361500
O 0.80943900 -0.93424900 0.66443600

INT4

C -3.33198800 0.94195400 0.99130100
C -2.00461600 0.58153200 1.22840700
C -1.10002200 0.47456000 0.16512200
C -1.54029600 0.72221300 -1.14048100
C -2.86676300 1.08918200 -1.37453000
C -3.76610200 1.19863100 -0.31133500
H -4.02448900 1.02695700 1.82471600
H -1.66923700 0.38325700 2.24333500
H -0.84037100 0.63877200 -1.96508300
H -3.19756000 1.28823300 -2.39069500
H -4.79836400 1.48436300 -0.49622000
C 0.33669300 0.04373100 0.43114500
C 0.37036400 -1.49698500 0.50225100
O 0.12724700 -2.11712800 1.51822000
O 0.64361400 -2.05758600 -0.68302900
C 0.61182200 -3.49946700 -0.71642800
H 0.85280400 -3.77156400 -1.74453000
H 1.35189700 -3.91676700 -0.02843900
H -0.38298100 -3.86466600 -0.44800200
C 4.11229600 2.43010700 0.01595500
C 3.09265700 1.67777000 0.43089700
C 2.58052400 0.47342100 -0.30802300
H 4.63739400 2.22081800 -0.91497300
H 4.46725000 3.28163300 0.59173000
H 0.63823300 0.38813400 1.42965700
H 2.58866900 1.91720300 1.36780200
H 2.79310500 -0.44770600 0.25526800
H 3.07084400 0.38211300 -1.28239800
O 1.17231300 0.57087800 -0.57617300

TSS

C 3.04607400 -2.09026800 -0.15950100
C 1.86068600 -1.55790700 -0.98260900
C 3.18663100 -1.20677600 1.02412000
H 1.42056800 -2.29572000 -1.66719600
H 2.14708300 -0.66734000 -1.53908900
H 2.74839600 -1.48921400 1.97449300

H 3.88784300 -0.38347700 1.02795900
O 0.89517700 -1.21870200 0.05048300
C -3.53633000 0.71326300 -0.04021100
C -2.16071700 0.90690500 -0.12956600
C -1.26318800 -0.18852900 -0.04379900
C -1.83179800 -1.47842000 0.12456100
C -3.20696900 -1.65799600 0.21601900
C -4.07555100 -0.56444500 0.13568400
H -4.19614500 1.57483500 -0.11193100
H -1.77148000 1.90604300 -0.27031600
H -1.17103400 -2.33582100 0.18471100
H -3.60560700 -2.66124300 0.34801900
H -5.15084000 -0.70651300 0.20199400
C 0.17913200 -0.06812200 -0.14606800
C 1.01021000 1.09677600 -0.05740000
O 2.25246400 1.02651800 0.02536700
O 0.36838400 2.29993800 -0.02060700
C 1.21712300 3.45379300 0.03708500
H 0.54490800 4.31254300 -0.01202400
H 1.78539400 3.48010900 0.97186400
H 1.91426800 3.47324000 -0.80645400
H 3.95041200 -2.10643200 -0.77975200
H 2.81620800 -3.11269300 0.16588000

INT5

C -3.12963600 -1.59887300 -0.20088500
C -1.84753600 -1.97727900 0.54530600
C -2.99558100 -0.20393200 -0.80409900
H -1.77458100 -3.06177800 0.67391900
H -1.81830900 -1.51327800 1.53859300
H -2.37888500 -0.21887500 -1.70898100
H -3.97060400 0.22090300 -1.05654500
O -0.68446400 -1.58698100 -0.19596600
C 3.37420500 0.95675900 -0.37413300
C 1.98206600 0.95360500 -0.33097800
C 1.26876600 -0.22369000 -0.02442100
C 2.01298000 -1.39624100 0.21438000
C 3.40666700 -1.38838400 0.16830400
C 4.09898500 -0.21196700 -0.12280000
H 3.89681700 1.87987300 -0.61361200
H 1.44393300 1.87047100 -0.53916800
H 1.48612100 -2.31788100 0.43427400
H 3.95228900 -2.30893600 0.36214700
H 5.18524800 -0.20514100 -0.15936000
C -0.20569800 -0.29460500 0.00745300
C -1.05126700 0.74532100 0.23338400

O -2.41198700 0.71796000 0.13921900
O -0.59685800 1.92973100 0.70943000
C -1.14318900 3.11408600 0.10243900
H -0.56554500 3.94556300 0.51135700
H -1.02857400 3.08731800 -0.98782800
H -2.19891900 3.23988000 0.35695700
H -3.97612400 -1.64334700 0.49516700
H -3.33097300 -2.30924200 -1.01207400

TS6

C 3.21228300 -1.52054500 0.24030900
C 1.82968500 -1.51729700 0.14785300
C 1.12631800 -0.32169400 -0.17551700
C 1.89904100 0.84997900 -0.42534900
C 3.28878600 0.82629400 -0.31749800
C 3.95670800 -0.35160400 0.01363800
H 3.72408600 -2.44586800 0.49365100
H 1.26823400 -2.42041300 0.34459400
H 1.39957400 1.76037100 -0.72878900
H 3.85223700 1.73562800 -0.51295800
H 5.04115700 -0.37014200 0.08164100
C -0.30843300 -0.22534700 -0.21856200
C -1.22391600 -1.32308400 0.06017400
O -0.91334100 -2.41841000 0.52451700
O -2.50684700 -1.04253600 -0.31068100
C -3.46200100 -2.08361600 -0.05730000
H -4.42351600 -1.68183300 -0.38132600
H -3.21827800 -2.98291700 -0.63031200
H -3.49654600 -2.33471500 1.00693200
C -0.40985700 3.04428200 0.93932900
C -1.59277400 3.06299100 0.04167200
C -1.99569900 1.61052300 -0.12703000
H 0.33646600 3.83266200 0.91037500
H -0.37916400 2.36240200 1.78338400
H -1.32210700 3.48278900 -0.93771900
H -2.43251000 3.68033100 0.41455300
H -2.75469400 1.41568900 -0.88735400
H -2.31954400 1.18354400 0.82635700
O -0.72934300 1.02059400 -0.52800200

INT6

C 2.13764000 -2.34423200 0.31180000
C 0.87798400 -1.84154300 0.29607500
C 0.61128800 -0.47844500 -0.12599000
C 1.80097700 0.44353200 -0.41366800
C 3.12890300 -0.26667500 -0.44730900

C 3.28563900 -1.55478400 -0.09893000
H 2.29856900 -3.37197900 0.62786700
H 0.03732000 -2.45844000 0.58329000
H 1.63340200 0.88450000 -1.40972400
H 3.98412300 0.33782400 -0.74274400
H 4.26674100 -2.02256300 -0.11601400
C -0.65020000 0.03306500 -0.27567800
C -1.91389200 -0.71727200 -0.06489900
O -2.02179000 -1.91882300 0.13932600
O -2.98716300 0.10391800 -0.11668100
C -4.25977600 -0.53509900 0.07314300
H -4.99746700 0.26789400 0.03196600
H -4.45138700 -1.26380200 -0.72013200
H -4.30389200 -1.03991200 1.04254900
C 1.88930000 1.65260600 0.57463200
C 0.89992500 2.78284700 0.26967100
C -0.56091800 2.35599300 0.29058900
H 2.90576700 2.06180200 0.52043200
H 1.75549500 1.28378100 1.59944100
H 1.12383600 3.20105100 -0.72119600
H 1.03459600 3.59646700 0.99554000
H -1.21089900 3.19582700 0.02379000
H -0.85984700 1.99469400 1.28271900
O -0.82824500 1.33401700 -0.68944600

2-phenyl oxetane

C -1.24797900 -0.53537100 -0.37374500
C -2.12926800 -0.66891700 0.89875500
C -3.01512300 0.38868000 0.22362500
H -1.37302000 -1.39033700 -1.05349500
H -3.20603300 1.31170000 0.78342300
H -3.96440100 0.00693500 -0.17511900
O -2.04070900 0.59408400 -0.83356800
H -1.63321000 -0.32231000 1.80842700
H -2.57660500 -1.65043800 1.07247600
C 0.21826900 -0.22675500 -0.21051900
C 1.15722300 -1.26743000 -0.22018300
C 0.66155300 1.08611100 -0.00794800
C 2.51220900 -1.00331600 -0.01534400
H 0.82461900 -2.28967400 -0.38997900
C 2.01845000 1.35294800 0.18465700
H -0.06328700 1.89436200 -0.02011300
C 2.94700900 0.30931600 0.18679500
H 3.22983300 -1.81995800 -0.02331600
H 2.35061100 2.37770800 0.33202400
H 4.00311200 0.51773400 0.33765400

TS_{ph1}

C -3.35341500 2.69109500 0.77719200
C -3.11506400 1.42428800 0.26793000
C -1.90857600 1.13571600 -0.43346900
C -0.95653600 2.18043900 -0.58778200
C -1.18962000 3.44338800 -0.06065400
C -2.38829900 3.69661400 0.61672900
H -4.27808000 2.90687700 1.30479700
H -3.85737500 0.64009300 0.38546400
H -0.03836700 1.95657200 -1.12145800
H -0.45270400 4.23269000 -0.17584700
H -2.57574000 4.68722800 1.02322200
C -1.59008800 -0.13751400 -0.98056000
C -2.51927500 -1.22800300 -0.92542900
O -3.38914100 -1.31717600 -1.79481100
O -2.28395100 -2.18046000 0.00448200
C -3.11696800 -3.35326400 -0.08546300
H -2.77014700 -4.01680200 0.70799400
H -4.16923400 -3.10024600 0.07307400
H -3.00359500 -3.83942600 -1.05847500
C 1.44890900 -1.29560300 0.26083500
C 1.63244600 -2.44458000 1.29040200
C 0.46860900 -1.77633300 2.03747200
H 0.65835300 -1.46230000 3.07084700
H -0.48390700 -2.31490900 1.98870300
O 0.47570500 -0.64398600 1.12669000
H 2.58716500 -2.41043400 1.82082300
H 1.45675300 -3.45442700 0.91194700
H 0.96233500 -1.63187700 -0.66217600
C 2.63871200 -0.43320000 -0.07393700
C 3.37048600 -0.67854200 -1.24389700
C 3.05846200 0.59002700 0.78611900
C 4.51020700 0.07065300 -1.54052500
H 3.04295100 -1.45990700 -1.92651300
C 4.19213300 1.34737800 0.48530100
H 2.48128600 0.79555800 1.68279000
C 4.92439300 1.08706600 -0.67592200
H 5.06830800 -0.13226800 -2.45119500
H 4.50417400 2.14268100 1.15797600
H 5.80782400 1.67610200 -0.90892800

INT_{ph1}

C 2.75067900 -2.99100300 -0.36795100
C 2.53440500 -1.61510600 -0.36981700
C 1.42050100 -1.04165600 0.29784200

C 0.54916600 -1.94679500 0.95815400
C 0.77578600 -3.32037400 0.94998600
C 1.87981100 -3.86458500 0.28896900
H 3.61928400 -3.38406000 -0.89292200
H 3.22992900 -0.96950200 -0.88924000
H -0.32201200 -1.56324400 1.47805300
H 0.07612000 -3.97224900 1.46952200
H 2.05590600 -4.93692100 0.28516100
C 1.17023700 0.38740300 0.33316500
C 1.81331000 1.50374600 -0.25388300
O 1.40661000 2.68079800 -0.18778700
O 2.97539400 1.20744600 -0.92475800
C 3.63383300 2.32389100 -1.52987800
H 4.52549000 1.91320000 -2.00887800
H 2.99793400 2.80427700 -2.28031000
H 3.92400300 3.06916200 -0.78265600
C -1.31709000 1.56513400 0.44515300
C -1.42586700 2.16267900 1.85047000
C -0.02398600 1.66710100 2.21082500
H 0.10210200 1.07656400 3.11882100
H 0.76599500 2.40271200 2.07936900
O -0.01623200 0.74598800 1.03355700
H -2.20905300 1.71040300 2.45978600
H -1.54339500 3.24760700 1.84995400
H -0.84448900 2.24003200 -0.26373100
C -2.31196400 0.66546800 -0.16573100
C -2.33689200 0.55276900 -1.56710200
C -3.21330900 -0.10067000 0.59570700
C -3.24061600 -0.30288400 -2.19462300
H -1.64248700 1.14203600 -2.16016300
C -4.11739900 -0.95242900 -0.03314800
H -3.20886000 -0.03446200 1.67961000
C -4.13253500 -1.05580600 -1.42820800
H -3.24971400 -0.38057000 -3.27812000
H -4.81151200 -1.53820500 0.56305200
H -4.83982200 -1.72191900 -1.91498000

TS_{ph2}

C 2.78061200 2.96401400 0.39026700
C 2.54951400 1.59041700 0.38630700
C 1.44549700 1.02935800 -0.30724100
C 0.59949900 1.94387200 -0.98722900
C 0.83957400 3.31498300 -0.97222100
C 1.93372100 3.84693100 -0.28502200
H 3.64082900 3.34762900 0.93560400
H 3.22620200 0.93741200 0.92100100

H -0.26214800 1.56886400 -1.52879500
H 0.15926200 3.97464100 -1.50735400
H 2.12097900 4.91736100 -0.27625500
C 1.17848600 -0.39756500 -0.35180400
C 1.79975700 -1.51728000 0.25677600
O 1.36647700 -2.68530700 0.21475100
O 2.97204500 -1.23543500 0.91493100
C 3.61217300 -2.35606800 1.53213100
H 4.51460100 -1.95630200 1.99998400
H 2.97154100 -2.81361700 2.29269400
H 3.88283400 -3.11714800 0.79355700
C -1.36311300 -1.56109400 -0.45010700
C -1.45318800 -2.13180400 -1.86368300
C -0.03329700 -1.67199500 -2.20128400
H -0.88442900 -2.23886100 0.25154100
H 0.12220700 -1.10008500 -3.11707300
H 0.73225600 -2.43019200 -2.05286200
H -2.21314300 -1.65145600 -2.48121700
H -1.60020000 -3.21339400 -1.88119400
C -2.34025000 -0.65358600 0.16329400
C -2.34048600 -0.52456300 1.56494300
C -3.25184700 0.10982200 -0.59064500
C -3.22709700 0.34390100 2.19798100
H -1.63979700 -1.11206400 2.15233700
C -4.13985300 0.97288200 0.04466000
H -3.26788100 0.03034200 -1.67336600
C -4.12870300 1.09300000 1.43864600
H -3.21659300 0.43435900 3.28045200
H -4.84210100 1.55510900 -0.54543700
H -4.82337000 1.76879300 1.93017900
O -0.01190300 -0.73835200 -1.04073300

INT_{Ph2}

C 5.34675300 -0.89487100 -0.69155000
C 4.29961100 -0.01406700 -0.44980200
C 3.00631400 -0.50265600 -0.12052500
C 2.82644600 -1.91123700 -0.06108500
C 3.88228200 -2.77849400 -0.30718100
C 5.15148600 -2.27917600 -0.62250100
H 6.32780500 -0.49784100 -0.93935200
H 4.46378500 1.05366300 -0.50342900
H 1.84473300 -2.30425100 0.17596800
H 3.71697900 -3.85147600 -0.25424300
H 5.97654300 -2.95971600 -0.81419000
C 1.87543100 0.35220500 0.14359400
C 1.91847300 1.82110300 0.10758200

O 2.93403100 2.50749600 0.11734500
O 0.67633900 2.36661300 0.04676100
C 0.63690200 3.80351300 0.00088000
H -0.42169600 4.06372100 -0.03862800
H 1.09959400 4.23473400 0.89315300
H 1.15223800 4.17558300 -0.88893800
C -2.24040600 0.06025600 0.31531600
C -1.44055200 -0.65293000 1.36388400
C -0.04781700 -0.07279700 1.54756500
H 0.49424600 -0.59733400 2.34335500
H -0.09357800 0.99197700 1.79058700
O 0.67512500 -0.26377100 0.30516800
H -1.34993900 -1.72552600 1.12858200
H -1.94358900 -0.60935000 2.34317300
H -1.74408200 0.85426900 -0.23726800
C -3.58419200 -0.23596100 -0.01811100
C -4.25037900 0.50961300 -1.03631100
C -4.33141400 -1.26565000 0.62697700
C -5.56688500 0.24389300 -1.38085700
H -3.70322400 1.29981000 -1.54553200
C -5.64953400 -1.52271800 0.27334200
H -3.86161100 -1.85951600 1.40562600
C -6.28027200 -0.77417700 -0.72982300
H -6.04811500 0.82863400 -2.16112400
H -6.19578500 -2.31407300 0.78112800
H -7.31174000 -0.98109200 -1.00142500

TS_{Ph3}

C 3.51720800 1.79969100 -1.42688900
C 2.82934900 0.62915900 -1.12470600
C 2.18124000 0.46952000 0.12627700
C 2.27724000 1.54018300 1.05300600
C 2.96613800 2.70533500 0.73901400
C 3.59170300 2.84751800 -0.50403800
H 4.00577400 1.89164400 -2.39357100
H 2.79399000 -0.16867300 -1.85379800
H 1.80137400 1.44127800 2.02123400
H 3.01559600 3.50914700 1.46929400
H 4.13077900 3.75879300 -0.74823400
C 1.47248900 -0.73548000 0.52256800
C 1.19839000 -1.91886000 -0.29784100
O 0.95553900 -3.02857800 0.16828200
O 1.20185700 -1.67828600 -1.63135100
C 0.94554400 -2.82055900 -2.46705400
H 0.98639000 -2.44466900 -3.49020200
H 1.70511800 -3.59308500 -2.31676300

H -0.04280300 -3.23855200 -2.25709400
 C -1.54930800 0.07106800 1.34656300
 C -1.24037600 -1.34816700 1.70623300
 C 0.10176400 -1.54055700 2.41743500
 H -0.95266200 0.85191900 1.81257600
 H -1.29335300 -1.99680800 0.82383800
 H -1.99622200 -1.75081300 2.40341000
 H 0.35559400 -2.60059400 2.46293100
 H 0.05444600 -1.14051700 3.43401700
 O 1.21443000 -0.80680800 1.84813400
 C -2.59712700 0.48447200 0.48562400
 C -2.79872600 1.87294900 0.22702700
 C -3.48648200 -0.43063100 -0.15096900
 C -3.81341600 2.31128900 -0.61026400
 H -2.13432800 2.59311200 0.69912600
 C -4.49879400 0.02005700 -0.98814200
 H -3.37374500 -1.49653300 0.02315800
 C -4.67326900 1.39003900 -1.22676500
 H -3.94116100 3.37599900 -0.78979000
 H -5.16293800 -0.69973800 -1.46067300
 H -5.46784900 1.73530900 -1.88247200

cis-25a

C -2.56013200 -2.28692500 -1.04170100
 C -1.53096900 -1.37376900 -0.80730400
 C -1.77178300 -0.20145400 -0.07238100
 C -3.06481100 0.03265200 0.41278200
 C -4.09389900 -0.88141100 0.17357900
 C -3.84636500 -2.04592900 -0.55356000
 H -2.35305300 -3.18899900 -1.61213000
 H -0.54347300 -1.57280500 -1.20387300
 H -3.26082300 0.93713300 0.97662800
 H -5.09088200 -0.67760400 0.55660300
 H -4.64627800 -2.75811300 -0.73972100
 C -0.64620100 0.78586400 0.25240900
 C 0.03230200 1.29665400 -1.04590600
 O 0.10948800 0.68081100 -2.08844900
 O 0.55992100 2.52258400 -0.87575800
 C 1.20675200 3.08874800 -2.03338000
 H 1.58801300 4.05721900 -1.70758900
 H 2.02588100 2.45018000 -2.37424500
 H 0.48673400 3.21892100 -2.84571000
 C 0.41404800 0.16926600 1.26244800
 C 0.85591800 1.41091900 2.05857400
 C -0.42890300 2.22835600 2.13030900
 H -0.18982500 -0.45458500 1.93065100

H 1.63959000 1.96211100 1.53254900
 H 1.23582700 1.13890400 3.04806900
 H -0.25471200 3.30927800 2.13957500
 H -1.02934900 1.96607300 3.01224000
 O -1.18414000 1.90722800 0.94798100
 C 1.52978600 -0.69921900 0.71496100
 C 1.50293500 -2.08302700 0.94653900
 C 2.61784800 -0.16991100 0.00195600
 C 2.52201600 -2.91452900 0.47773800
 H 0.67269000 -2.51207700 1.50234400
 C 3.63767900 -0.99785600 -0.46872600
 H 2.67902200 0.89819400 -0.18599000
 C 3.59395900 -2.37403700 -0.23403600
 H 2.47786700 -3.98303700 0.67253000
 H 4.46940400 -0.56476200 -1.01852300
 H 4.39014000 -3.01737200 -0.59939400

TS_{Ph3'}

C 3.25805300 -1.60131100 -1.85655600
 C 2.34222600 -0.63533100 -1.45252400
 C 2.37810500 -0.11557600 -0.13551900
 C 3.37661900 -0.60066000 0.74485800
 C 4.29035300 -1.56276700 0.32824400
 C 4.23431600 -2.07333600 -0.97267000
 H 3.20766300 -1.99232400 -2.86941400
 H 1.58953500 -0.27728800 -2.14301900
 H 3.45515700 -0.18147600 1.74267800
 H 5.05686500 -1.90824000 1.01708200
 H 4.94719600 -2.82691500 -1.29613000
 C 1.43610800 0.88408700 0.33441900
 C 0.84769100 1.90036400 -0.54228700
 O 1.04641200 1.98041900 -1.75082900
 O 0.05678600 2.77412900 0.12735900
 C -0.53875400 3.79915800 -0.68302800
 H -1.11467600 4.41779500 0.00727200
 H 0.22832900 4.40097700 -1.17903500
 H -1.19904400 3.36414800 -1.43936200
 C -1.55591400 -0.07366700 1.27795400
 C -0.41564400 -0.91418200 1.76472700
 C 0.70449000 -0.11768200 2.43170700
 H -1.55294400 0.98106400 1.53980500
 H -0.00322600 -1.52065200 0.94625800
 H -0.75442600 -1.64393800 2.52026800
 H 1.54457500 -0.77756500 2.66666900
 H 0.35770300 0.34190400 3.36078800
 O 1.16007600 1.02274100 1.65369800

C	-2.64390900	-0.55426000	0.50801800
C	-3.67671200	0.34036700	0.09756100
C	-2.76913900	-1.91790500	0.10963800
C	-4.75247000	-0.09774600	-0.65967800
H	-3.60612500	1.38597500	0.38858700
C	-3.85095200	-2.34512400	-0.64924200
H	-2.00717900	-2.63346000	0.40444100
C	-4.85059200	-1.44438300	-1.04132700
H	-5.52346600	0.60794400	-0.95923100
H	-3.92143000	-3.39049800	-0.94019600
H	-5.69394900	-1.78604300	-1.63506300

trans-25a

C	0.46088900	2.83608900	-1.18310900
C	0.01992500	1.52298900	-1.01875100
C	-0.52118200	1.10016600	0.20459700
C	-0.61536400	2.01996700	1.25579100
C	-0.17121800	3.33390200	1.08968600
C	0.36733300	3.74804200	-0.12931500
H	0.87746400	3.14529900	-2.13823300
H	0.09888800	0.82469800	-1.84562200
H	-1.04604800	1.70416300	2.19879200
H	-0.25325300	4.03537500	1.91626500
H	0.70884400	4.77184100	-0.25840300
C	-1.00532800	-0.34295200	0.39546400
C	-1.87613600	-0.70810500	-0.83084000
O	-1.44476400	-1.23314700	-1.84078800
O	-3.15207300	-0.34065200	-0.67004500
C	-4.02447800	-0.59356100	-1.79022800
H	-5.00593300	-0.23369700	-1.47975100
H	-3.68091800	-0.05031300	-2.67462500
H	-4.06392500	-1.66332500	-2.01206300
C	0.12875700	-1.45373200	0.57459000
C	-0.02748200	-1.84298500	2.05816400
C	-1.51448900	-1.62158800	2.28243300
H	-0.20088500	-2.30665700	-0.02464100
H	0.54789300	-1.17783100	2.71012700
H	0.29240300	-2.87266500	2.24549600
H	-1.79945100	-1.46897000	3.32708000
H	-2.11429000	-2.44874000	1.87150600
O	-1.79625100	-0.40359200	1.58327200
C	1.53798300	-1.12060400	0.12336300
C	2.02176100	-1.66140300	-1.07729100
C	2.39731300	-0.30339600	0.87395000
C	3.32113600	-1.39915700	-1.51620800
H	1.36755500	-2.28966800	-1.67645700

C	3.69658000	-0.03901100	0.43891300
H	2.05239500	0.13824600	1.80416200
C	4.16549300	-0.58670700	-0.75748100
H	3.67250300	-1.83194500	-2.44962800
H	4.34365500	0.59741600	1.03743200
H	5.17884100	-0.38182000	-1.09331100

2-phenyl thietane

C	0.93204400	0.62289400	0.19277300
C	1.80112700	0.00693900	1.31976400
C	3.07947400	-0.19070600	0.48543100
H	1.04319000	1.71058500	0.17280300
H	3.60873200	-1.13646600	0.62107700
H	3.78816200	0.63841800	0.56333900
H	1.39459300	-0.95977000	1.63076500
H	1.90654700	0.64045300	2.20803900
C	-0.52478500	0.26775000	0.09320700
C	-1.48342200	1.28737300	0.00086400
C	-0.96587800	-1.06540500	0.09924300
C	-2.84588500	0.98825900	-0.07143100
H	-1.15822800	2.32542300	-0.01100400
C	-2.32497400	-1.36707200	0.02759900
H	-0.23890800	-1.87166200	0.14776000
C	-3.27092400	-0.34074900	-0.05740500
H	-3.57268800	1.79374600	-0.13973500
H	-2.64714300	-2.40530900	0.03356300
H	-4.33020900	-0.57756100	-0.11460700
S	2.11408100	-0.08834700	-1.10326700

TS_{thi}1

C	4.74245200	-1.30221200	0.39401600
C	3.75074900	-0.34766300	0.22280800
C	2.52415400	-0.67705000	-0.42214500
C	2.34717400	-2.01166800	-0.87996600
C	3.34123300	-2.96480700	-0.70960900
C	4.53623300	-2.60851900	-0.07150500
H	5.67525300	-1.04329600	0.88669700
H	3.90163900	0.66642300	0.58225800
H	1.41079400	-2.25966200	-1.37016600
H	3.19730600	-3.98064000	-1.06565800
H	5.31538100	-3.35429900	0.06376500
C	1.48327000	0.26117100	-0.68099800
C	1.64163700	1.65842300	-0.35326400
O	1.12626400	2.24537100	0.59574300
O	2.32275700	2.30592900	-1.34105000
C	2.29989600	3.74376700	-1.27697000

H 2.83850300 4.08212800 -2.16371900
H 1.27263600 4.11959500 -1.29579000
H 2.80024400 4.10525200 -0.37405900
C -1.85348000 0.54941600 0.73481300
C -2.12348400 1.17686500 2.12565600
C -0.84163600 0.66519200 2.80864000
H -1.26174400 1.22871300 0.11855300
H -0.94607900 0.27868100 3.82507800
H -0.01236700 1.37310300 2.75142400
H -3.01074900 0.73311200 2.58668200
H -2.24815500 2.26574600 2.10989300
C -2.98457700 -0.02425400 -0.06964400
C -3.08912000 0.28796300 -1.43309600
C -3.95313500 -0.86721800 0.49915400
C -4.13669300 -0.21546700 -2.20725900
H -2.33900700 0.92981300 -1.88910400
C -5.00046100 -1.37103500 -0.27105700
H -3.88102500 -1.13906700 1.54903600
C -5.09730000 -1.04563600 -1.62757400
H -4.19976500 0.04047600 -3.26190600
H -5.74181700 -2.02135600 0.18656300
H -5.91418000 -1.43961200 -2.22679900
S -0.62315700 -0.65244500 1.51610600

INT_{thi}1

C -3.37748200 2.39003200 -1.07539000
C -2.59911600 1.23544800 -1.01757000
C -2.08735600 0.76029200 0.20777100
C -2.39077700 1.50207800 1.36695300
C -3.14893000 2.67169400 1.30549900
C -3.65252100 3.12154400 0.08374700
H -3.75816100 2.72964000 -2.03586500
H -2.38100700 0.68949100 -1.92932600
H -2.03418900 1.14989200 2.33182100
H -3.36048000 3.22122200 2.21974800
H -4.25261400 4.02642100 0.03436200
C -1.24275200 -0.45789500 0.27287200
C -1.49178900 -1.69196000 -0.42675100
O -0.74393800 -2.67693500 -0.44812000
O -2.69370800 -1.71033100 -1.07522500
C -2.99863400 -2.92274200 -1.77484200
H -3.96789500 -2.75137700 -2.24768300
H -2.24431900 -3.14240500 -2.53660500
H -3.06588900 -3.77023400 -1.08559200
C 1.84058000 -1.05635600 0.41926700
C 2.07045800 -1.77637300 1.76427400

C 0.60534400 -1.83671600 2.22924500
H 1.47751800 -1.75727500 -0.33277700
H 0.39569300 -1.69178200 3.29069100
H 0.06372600 -2.69150300 1.82545500
H 2.67576300 -1.17387300 2.44713600
H 2.54677800 -2.75463500 1.65229900
C 2.80844600 -0.07749700 -0.14763400
C 2.99080000 -0.02166800 -1.53980900
C 3.52921700 0.82069900 0.65866900
C 3.87128800 0.89721000 -2.11070700
H 2.43832600 -0.70943300 -2.17560000
C 4.41018800 1.73852200 0.08884800
H 3.39908300 0.80803700 1.73758400
C 4.58501700 1.78000600 -1.29745400
H 4.00085200 0.92213700 -3.18950300
H 4.95987200 2.42492000 0.72757400
H 5.27255000 2.49622100 -1.73947400
S 0.18772900 -0.33657800 1.19691100

TS_{thi}2

C 4.04746600 -1.96017100 -1.28330200
C 3.16020700 -0.90291800 -1.10376400
C 2.43921600 -0.74989700 0.10298500
C 2.64716500 -1.71934900 1.10986000
C 3.52801800 -2.78226500 0.92244800
C 4.23624100 -2.91029700 -0.27462900
H 4.58515500 -2.05119500 -2.22397900
H 3.01429900 -0.18576300 -1.90367300
H 2.12260600 -1.62090200 2.05558700
H 3.66972900 -3.50680400 1.72061300
H 4.92763300 -3.73609100 -0.41973900
C 1.47994900 0.34880100 0.30059300
C 1.62243800 1.67756500 -0.27521100
O 0.72300900 2.51175400 -0.39295200
O 2.90022100 1.95835200 -0.65584000
C 3.10091300 3.25199100 -1.24259600
H 4.16163500 3.29446200 -1.49653000
H 2.49262000 3.37429000 -2.14389100
H 2.85219100 4.04716400 -0.53340900
C -2.26999800 0.95254800 0.49238600
C -2.06825600 1.23708400 1.95596100
C -0.55153100 1.35060700 2.13695200
H -1.79175800 1.66259800 -0.17803400
H -0.18747500 1.23001000 3.16097800
H -0.16723200 2.27304300 1.70231200
H -2.46778700 0.43342900 2.58302400

H -2.56859100 2.16735000 2.26310400
 C -3.29298900 0.12825600 -0.08350100
 C -3.48064400 0.14965500 -1.49082900
 C -4.13333600 -0.72278400 0.67932000
 C -4.45121400 -0.63463100 -2.09950500
 H -2.84586100 0.79537200 -2.09266500
 C -5.10599300 -1.50187300 0.06328800
 H -4.02167800 -0.76745300 1.75825600
 C -5.27159400 -1.46589500 -1.32642300
 H -4.57509300 -0.59951900 -3.17875300
 H -5.74143400 -2.14399100 0.66783000
 H -6.03267900 -2.07836700 -1.80204300
 S -0.01427900 -0.05169000 1.05919600

INT_{thi2}

C 4.67576200 2.02452000 0.94775200
 C 3.86695600 0.89673600 0.86855400
 C 2.71991700 0.87661100 0.03595100
 C 2.42846200 2.05028600 -0.70095400
 C 3.24486300 3.17419500 -0.61918100
 C 4.37285100 3.17124200 0.20568600
 H 5.54414500 2.01325800 1.60141800
 H 4.11000000 0.02412500 1.46296400
 H 1.56655500 2.06233900 -1.35967400
 H 3.00225800 4.05452800 -1.20865800
 H 5.00878000 4.05000400 0.26943400
 C 1.84275300 -0.28996900 -0.02811500
 C 2.29726300 -1.66738800 0.21027700
 O 1.58338900 -2.60014700 0.55984300
 O 3.62034300 -1.82919000 -0.04550800
 C 4.13168100 -3.15772700 0.15243300
 H 5.19494800 -3.09800900 -0.08503200
 H 3.99245900 -3.48046500 1.18816400
 H 3.63453700 -3.86746500 -0.51515500
 C -2.84056700 -1.10291000 -0.20019900
 C -2.02705700 -1.13099000 -1.45539000
 C -0.54071000 -1.40182300 -1.19132900
 H -2.55084200 -1.80871300 0.57692400
 H 0.02214100 -1.47208100 -2.12676800
 H -0.40045000 -2.32002100 -0.62052700
 H -2.14299700 -0.20708200 -2.03332400
 H -2.37376500 -1.94598500 -2.11469000
 C -3.98862700 -0.30932500 0.04859100
 C -4.66401000 -0.42675200 1.30075500
 C -4.52673600 0.61717300 -0.89300100
 C -5.79028600 0.32855800 1.58874500

H -4.27463700 -1.12527300 2.03785400
 C -5.65586900 1.36771600 -0.59361200
 H -4.05140400 0.73733400 -1.86164100
 C -6.29795900 1.23390900 0.64507300
 H -6.28157800 0.21671600 2.55218900
 H -6.04483400 2.06592700 -1.33085500
 H -7.18095900 1.82503700 0.87169500
 S 0.13147900 0.01163400 -0.20945100

TS_{thi3}

C -3.68783700 1.95750900 1.08250600
 C -2.94690300 0.78119600 1.05454500
 C -2.18323800 0.42502400 -0.08516500
 C -2.21667500 1.30786600 -1.19212800
 C -2.95744100 2.48489400 -1.15536000
 C -3.69873300 2.81933200 -0.01886500
 H -4.26958400 2.19929200 1.96823900
 H -2.96535600 0.12099800 1.91275300
 H -1.63504900 1.07112800 -2.07650100
 H -2.94973100 3.14807100 -2.01647100
 H -4.27683600 3.73895300 0.00882600
 C -1.43149000 -0.82783400 -0.14500400
 C -0.90842200 -1.53390700 1.02944500
 O -0.60085000 -2.72130700 1.05130300
 O -0.74052100 -0.72442200 2.10465500
 C -0.20491500 -1.35424200 3.28007300
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 C 0.23233800 -2.54053000 -1.81602500
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 H 1.47737900 -2.16813800 -0.09710400
 H 2.33320600 -2.41739700 -1.59852400
 H 0.09238700 -3.54721100 -1.42003300
 H 0.36421800 -2.61371200 -2.90117700
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 C 3.55331300 2.58898700 -0.26203600
 H 1.94620400 2.20719000 -1.63544000
 C 4.38988500 0.67258600 0.95888700
 H 3.45407300 -1.21000100 0.54641900
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H 5.07626800 0.24386600 1.68510100
H 5.16221000 2.68092200 1.18317000
S -1.38277600 -1.63942800 -1.69585500

cis-37

C -0.77509600 3.15440400 0.97772900
C -0.56941800 1.77621700 0.91024500
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C -1.52539000 3.80337900 -0.00483400
H -0.34612100 3.71932600 1.80124200
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trans-37

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TS_{thi3}[?]

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H	3.73630700	0.10905700	3.14443000	H	-2.08006500	0.64693000	-1.66074800
H	2.22932100	-0.71021800	3.66487900	C	-4.24013500	-0.56699900	0.66451100
H	3.45120900	-1.60967900	2.72093000	H	-3.80353600	-2.17724200	2.03360200
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C	1.38838000	-1.52860300	-2.66200800	S	2.39569900	-0.66120700	-1.37778700

References

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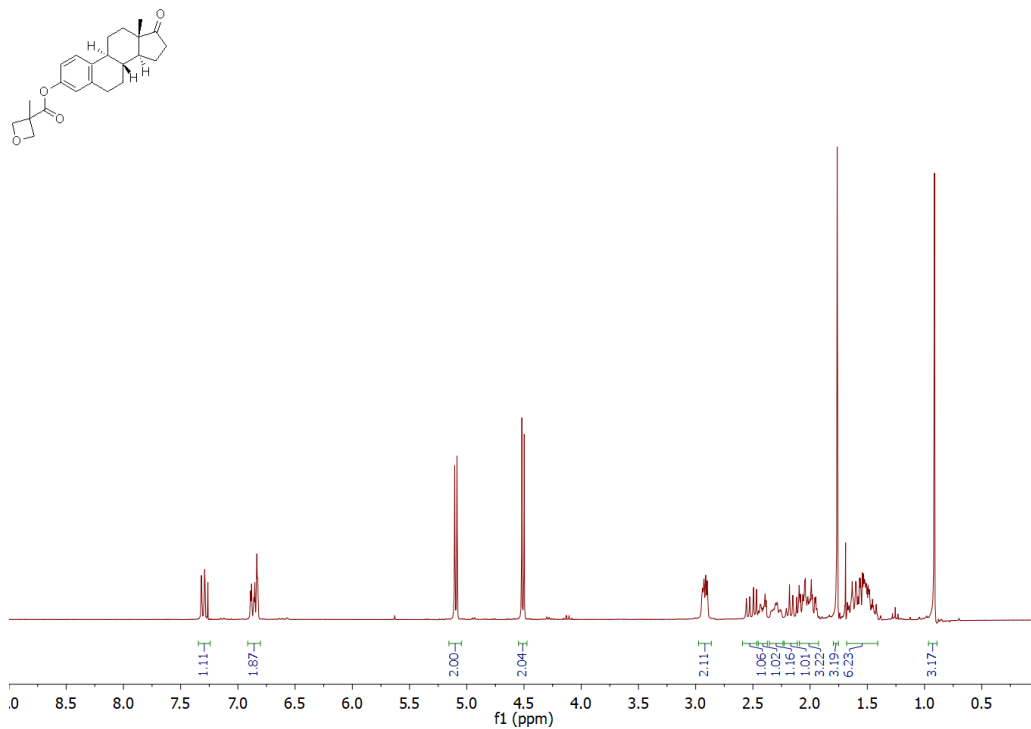
Author Contributions

S.J. discovered the photochemical ring expansion reaction. S.J. and R.M.K. designed the experiments and analyzed the data. S.J. and Z.Y. performed the experiments. C.P., performed the theoretical calculations. R.M.K. directed and supported the research. X.X. and R.M.K. wrote the manuscript.

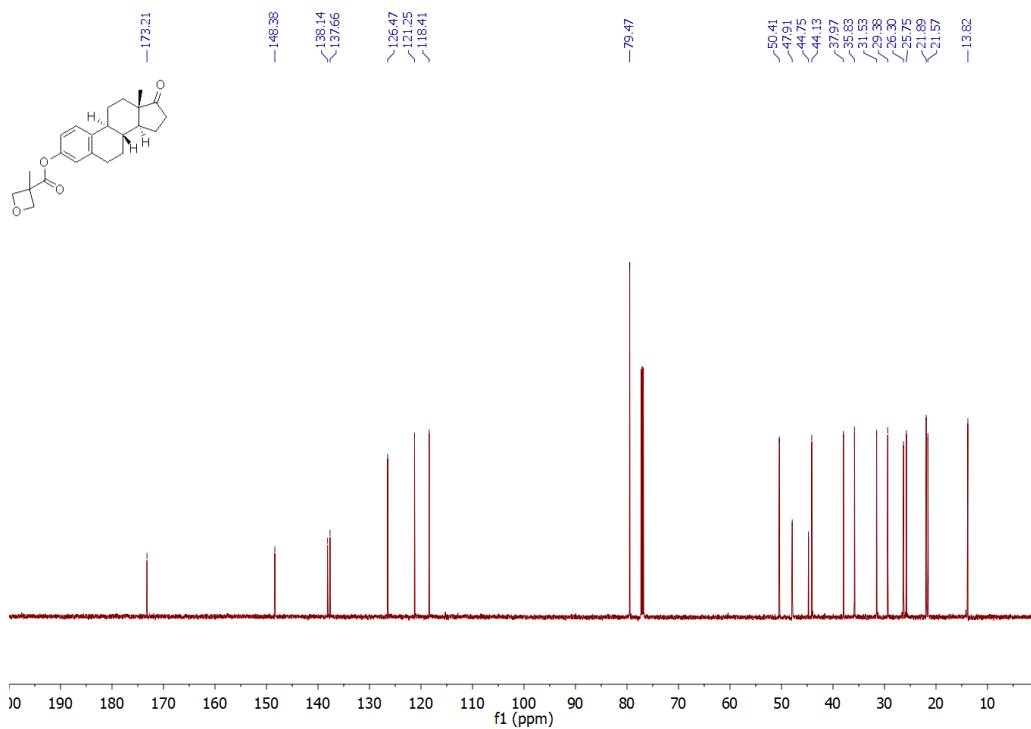
Copies of NMR spectra

(8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[*a*]phenanthren-3-yl 3-methyloxetane-3-carboxylate

¹H NMR (300 MHz, Chloroform-*d*):

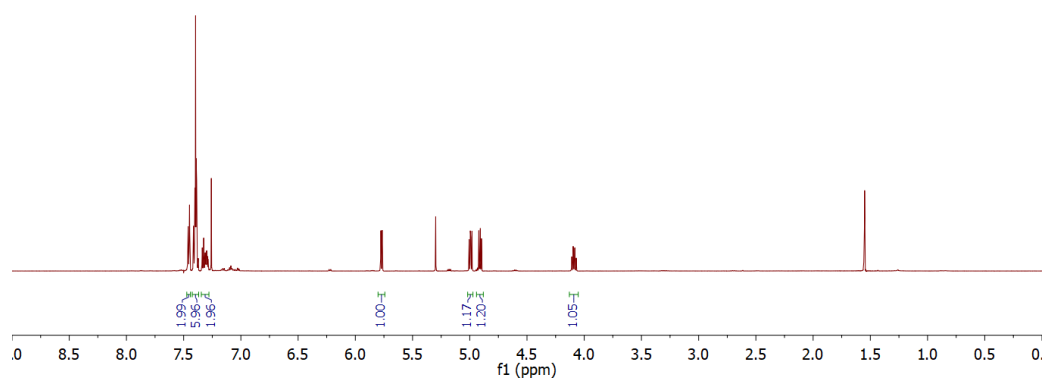
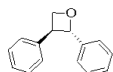


¹³C NMR (151 MHz, Chloroform-*d*):

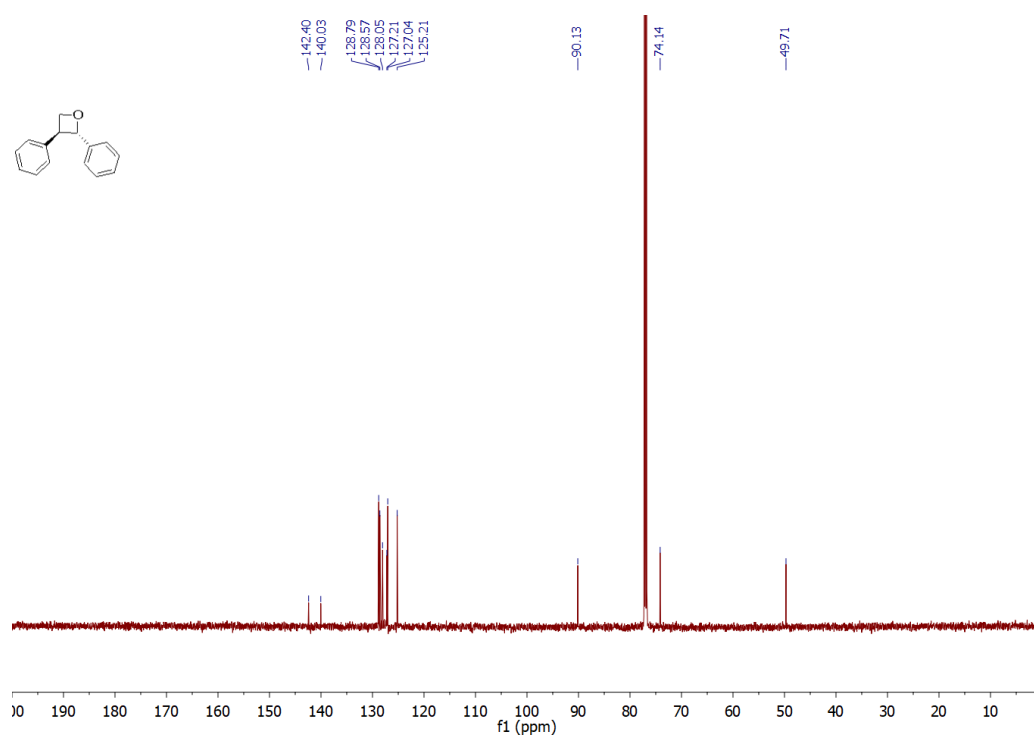
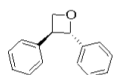


trans-2,3-diphenyloxetane (41)

¹H NMR (600 MHz, Chloroform-*d*):

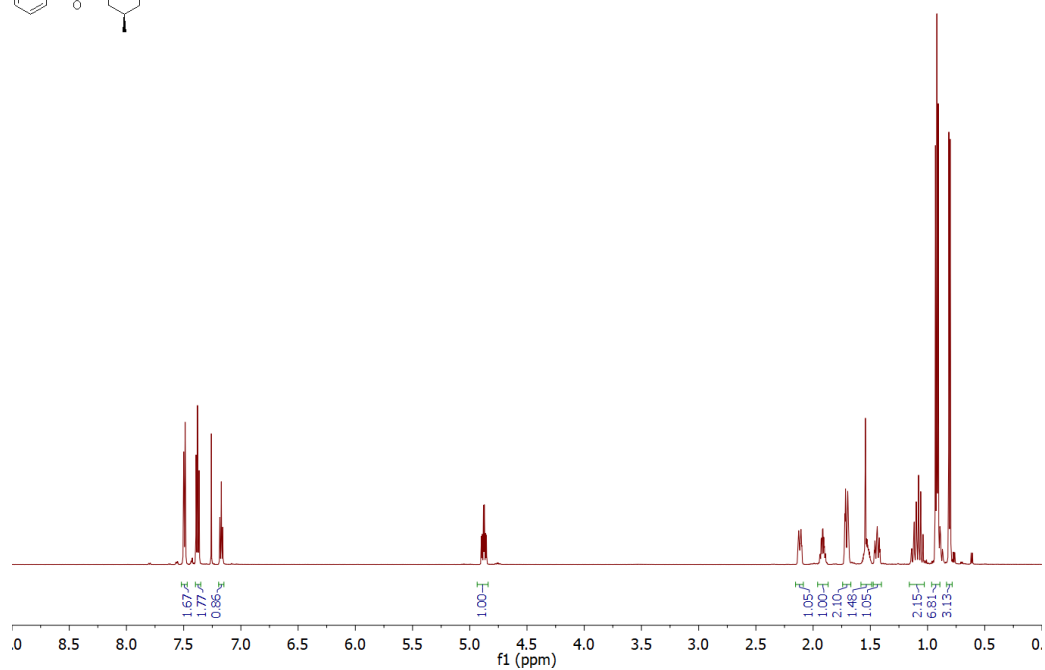
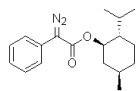


¹³C NMR (151 MHz, Chloroform-*d*):

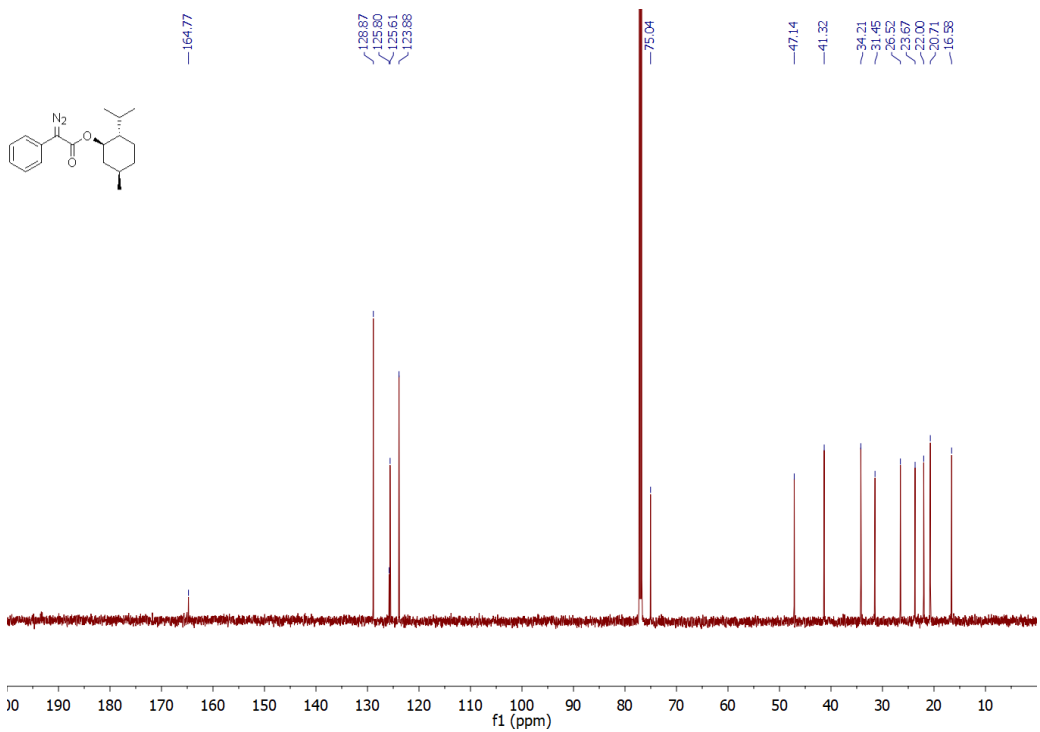


(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 2-diazo-2-phenylacetate

^1H NMR (600 MHz, Chloroform-*d*):

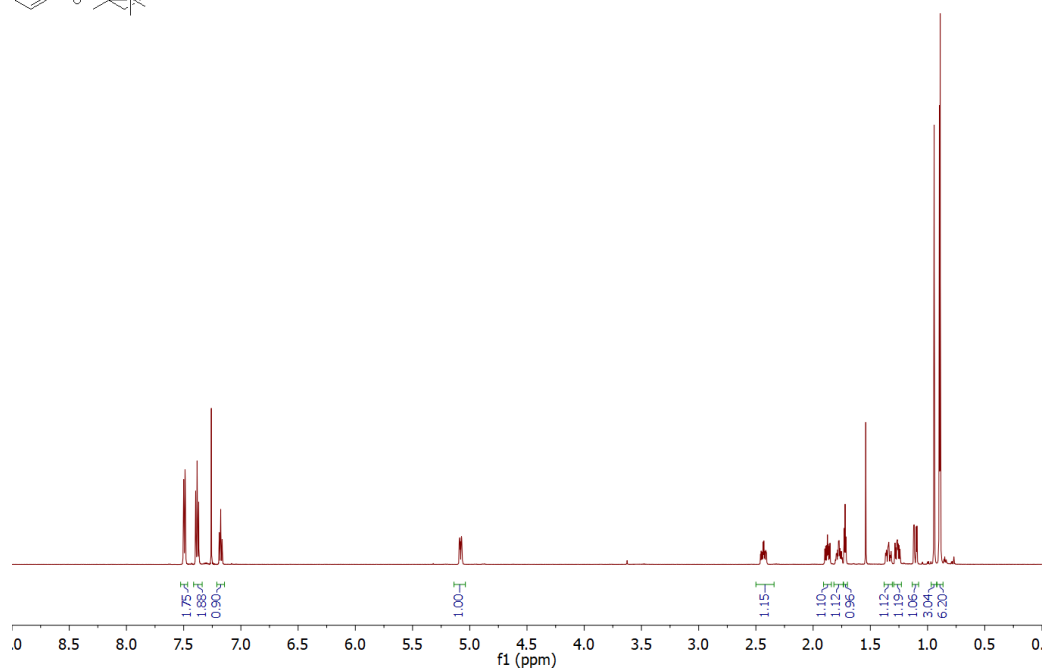
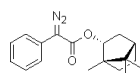


^{13}C NMR (151 MHz, Chloroform-*d*):

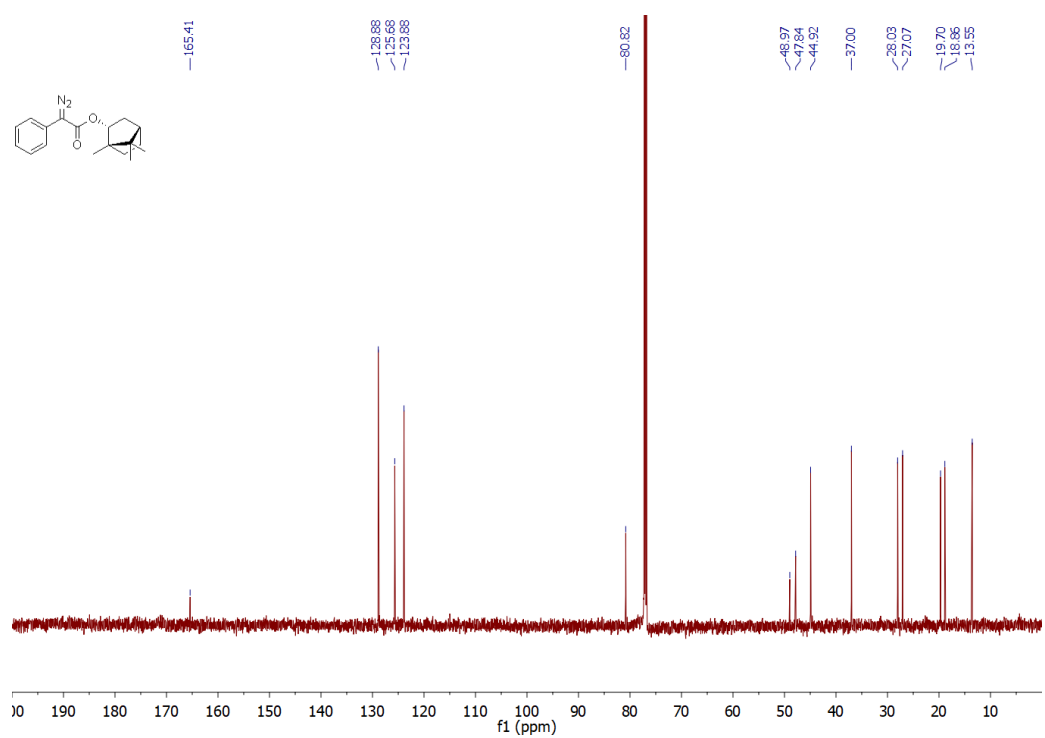
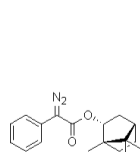


(1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl 2-diazo-2-phenylacetate

¹H NMR (600 MHz, Chloroform-d):

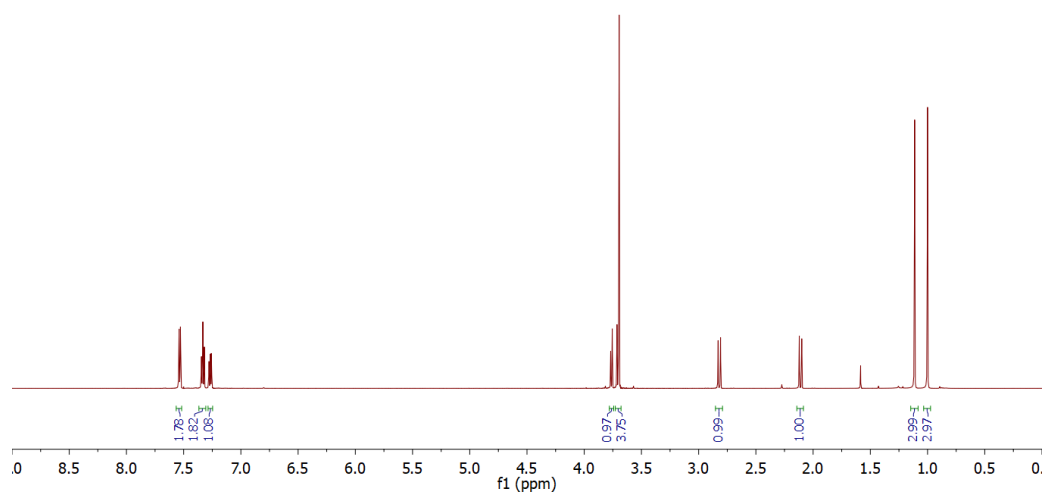
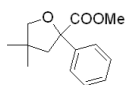


¹³C NMR (151 MHz, Chloroform-d):

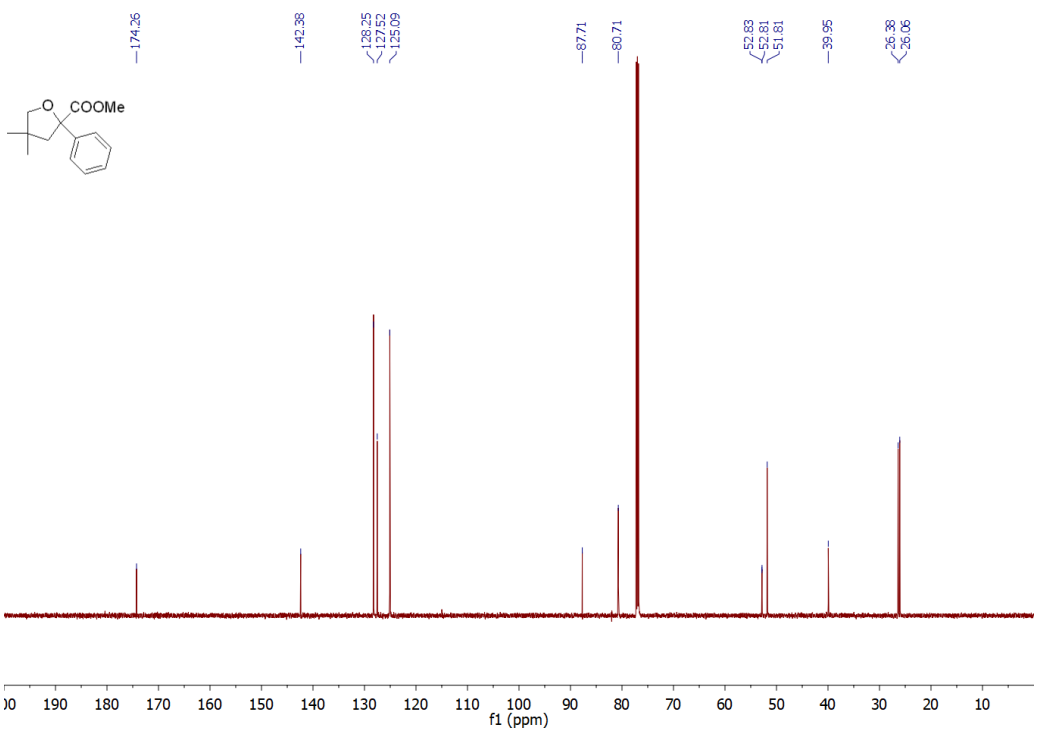


Methyl 4,4-dimethyl-2-phenyltetrahydrofuran-2-carboxylate (6a)

¹H NMR (300 MHz, Chloroform-*d*):

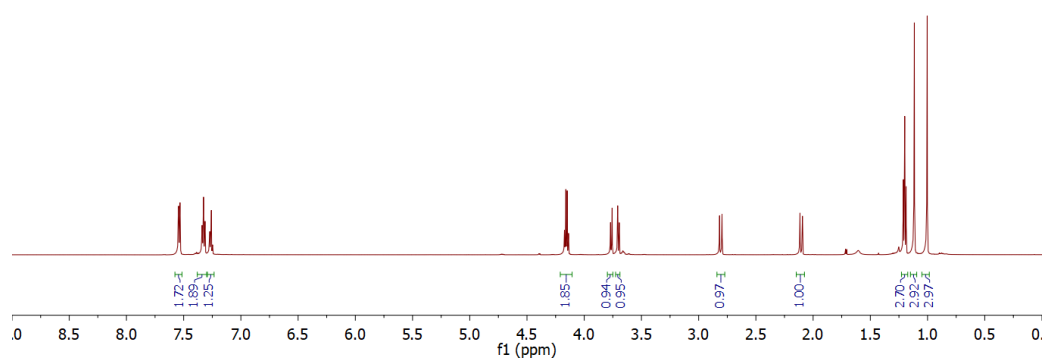
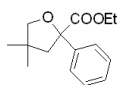


¹³C NMR (151 MHz, Chloroform-*d*):

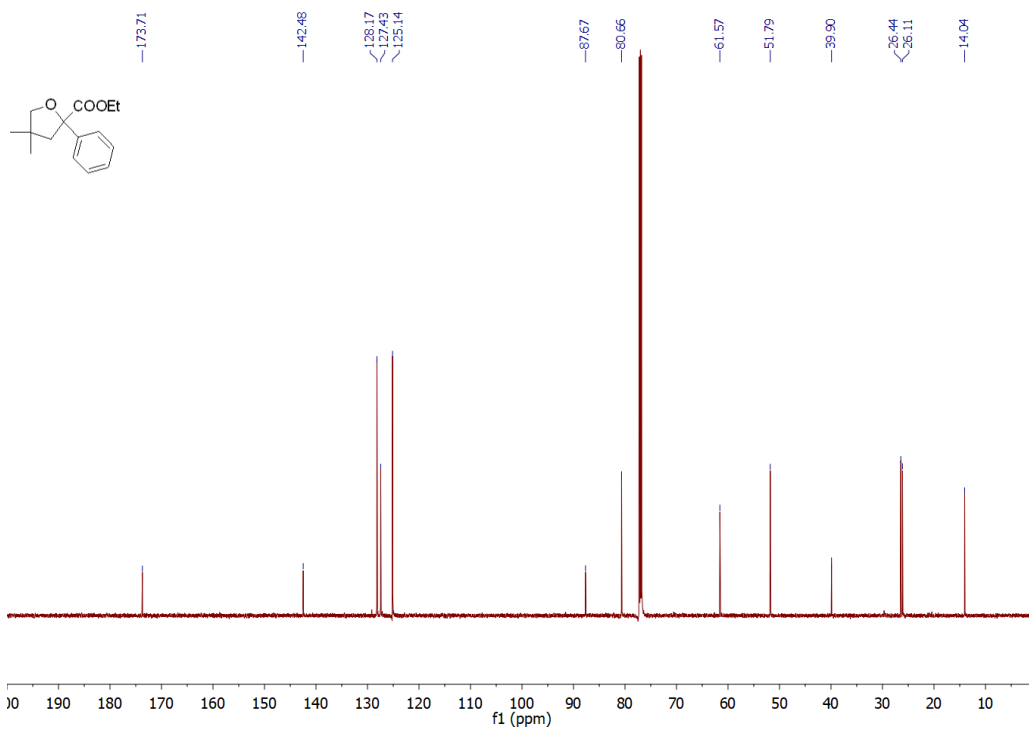


Ethyl 4,4-dimethyl-2-phenyltetrahydrofuran-2-carboxylate (6b)

^1H NMR (600 MHz, Chloroform-*d*):

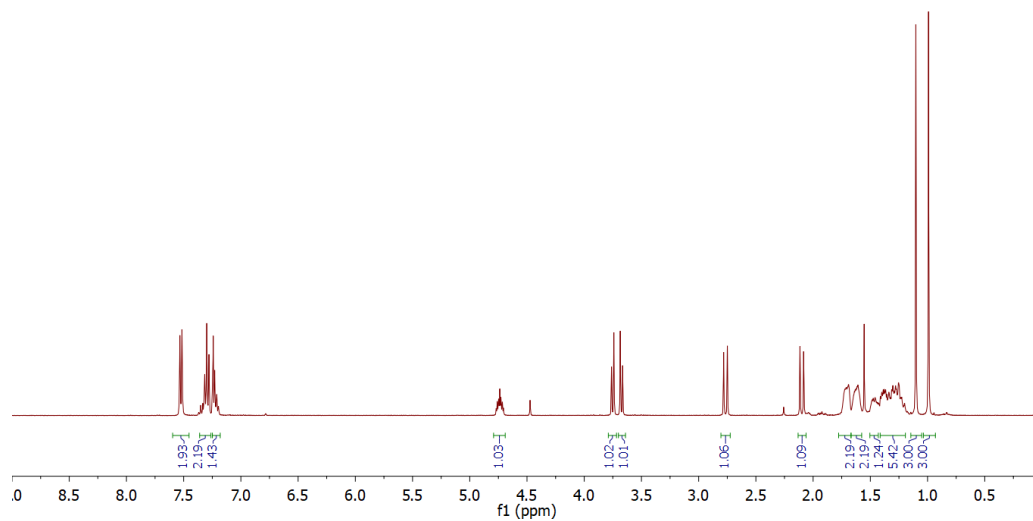
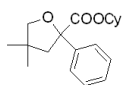


^{13}C NMR (151 MHz, Chloroform-*d*):

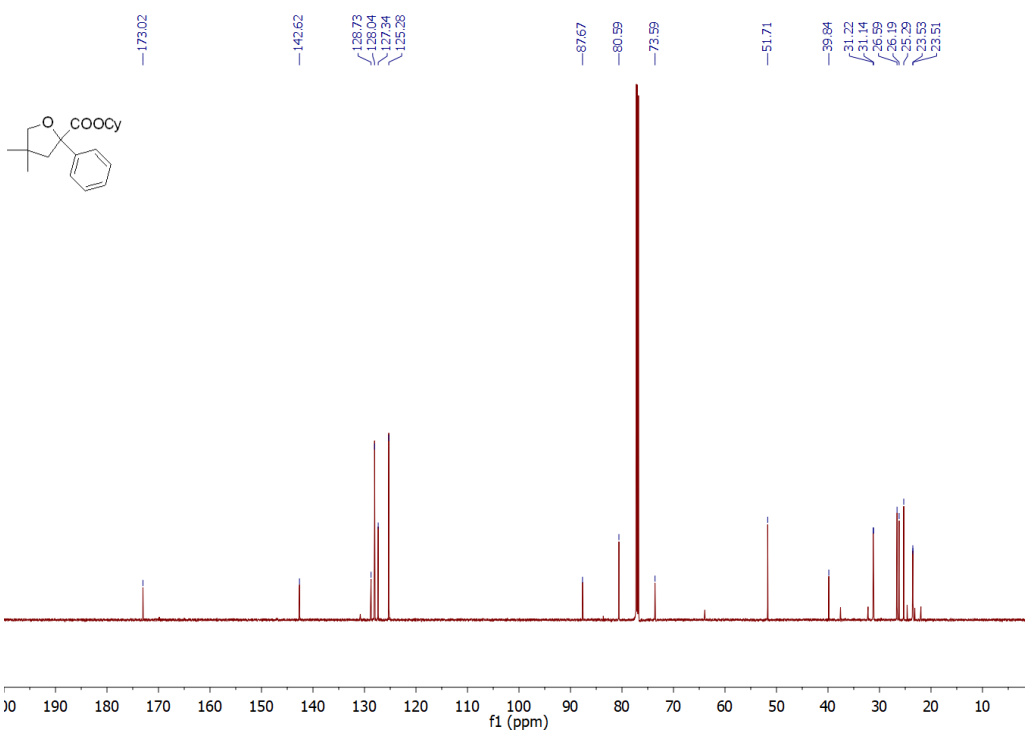


Cyclohexyl 4,4-dimethyl-2-phenyltetrahydrofuran-2-carboxylate (6c)

^1H NMR (400 MHz, Chloroform-*d*):

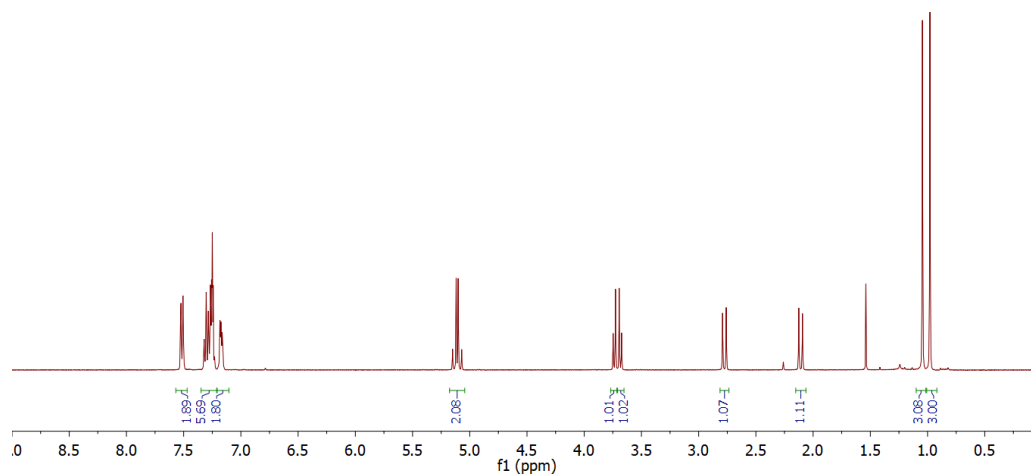
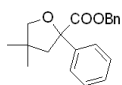


^{13}C NMR (151 MHz, Chloroform-*d*):

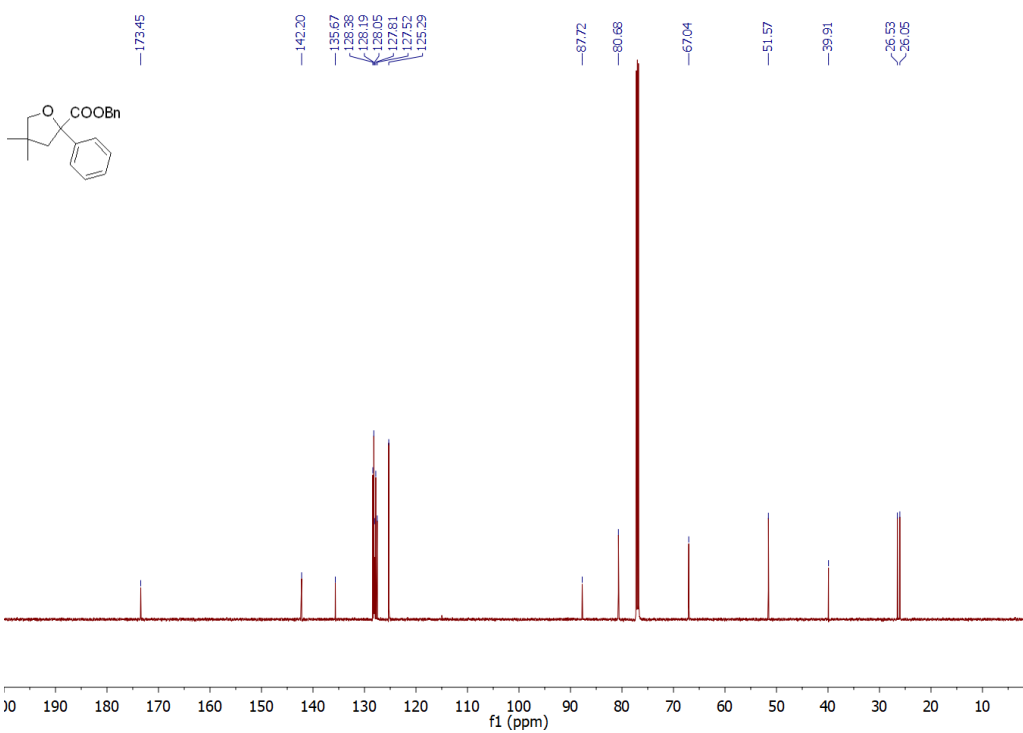


Benzyl 4,4-dimethyl-2-phenyltetrahydrofuran-2-carboxylate (6d)

^1H NMR (400 MHz, Chloroform-*d*):

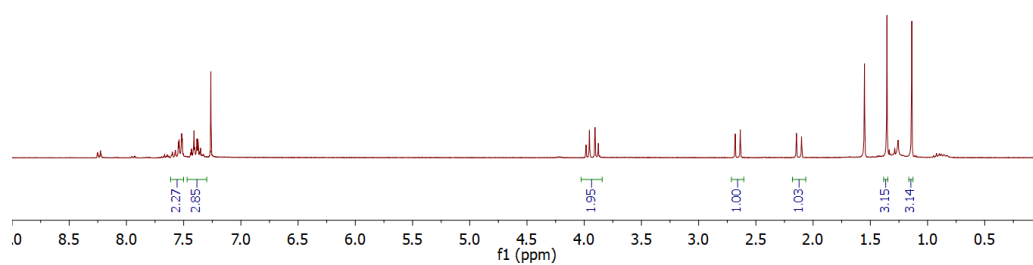
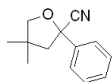


^{13}C NMR (151 MHz, Chloroform-*d*):

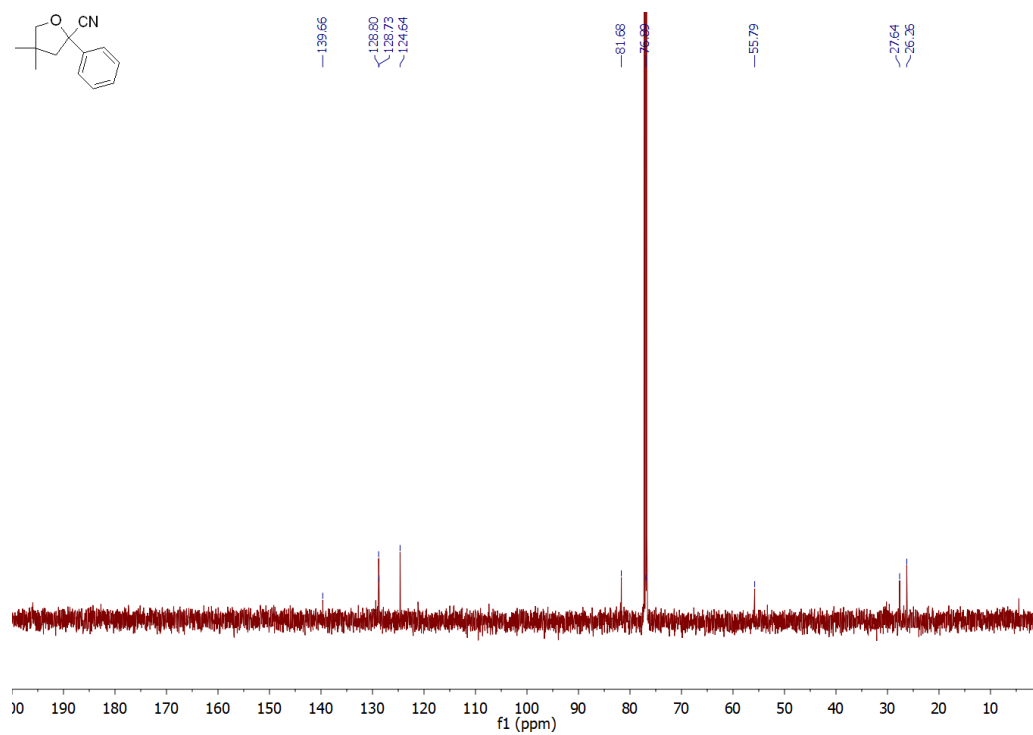
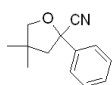


dimethyl-2-phenyltetrahydrofuran-2-carbonitrile (6e)

^1H NMR (300 MHz, Chloroform-*d*):

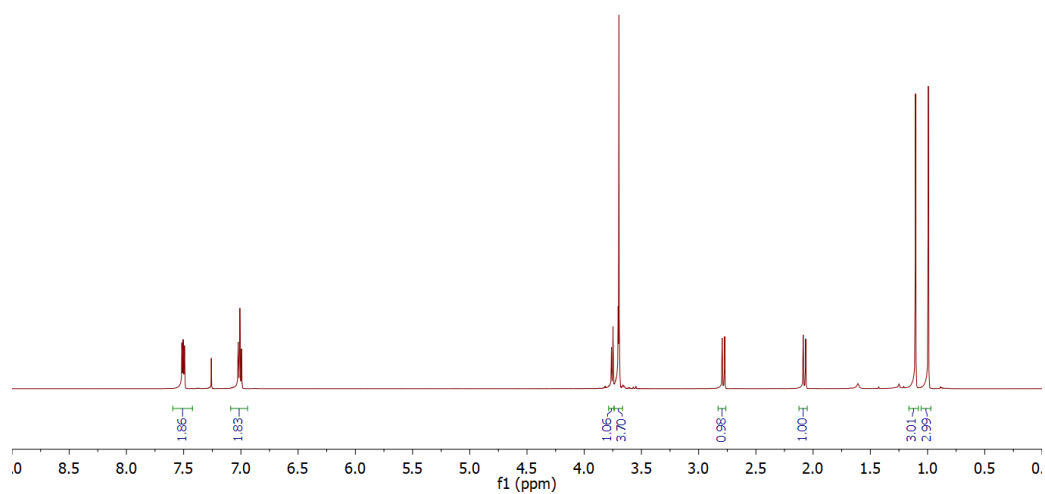
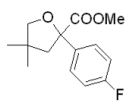


^{13}C NMR (151 MHz, Chloroform-*d*):

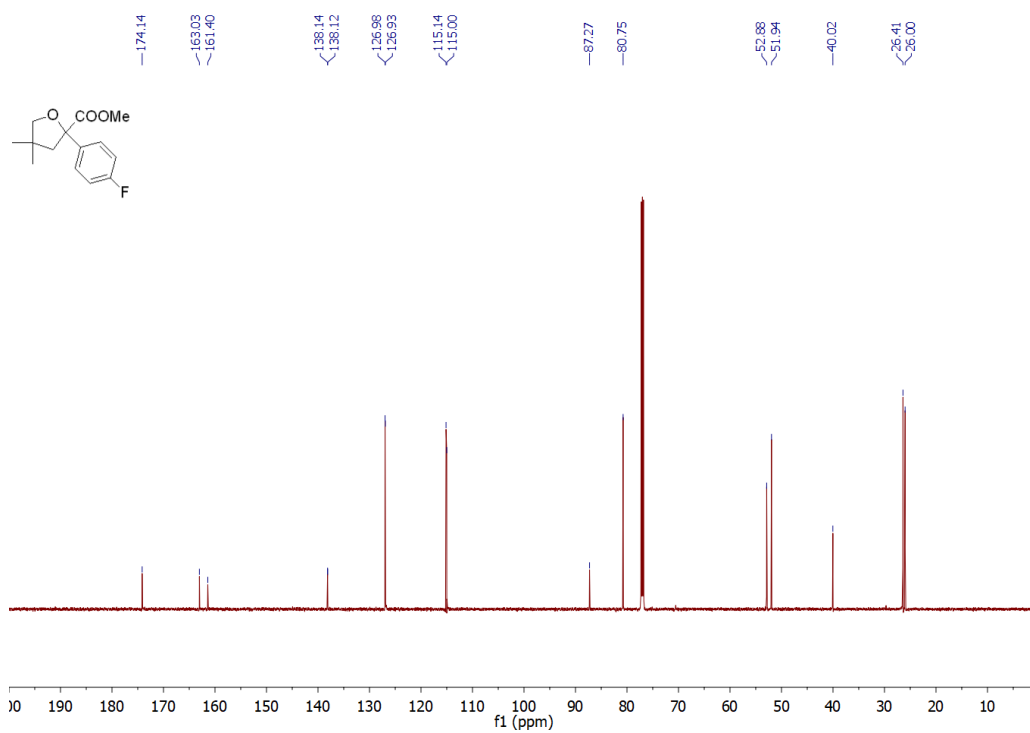


Methyl 2-(4-fluorophenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6g)

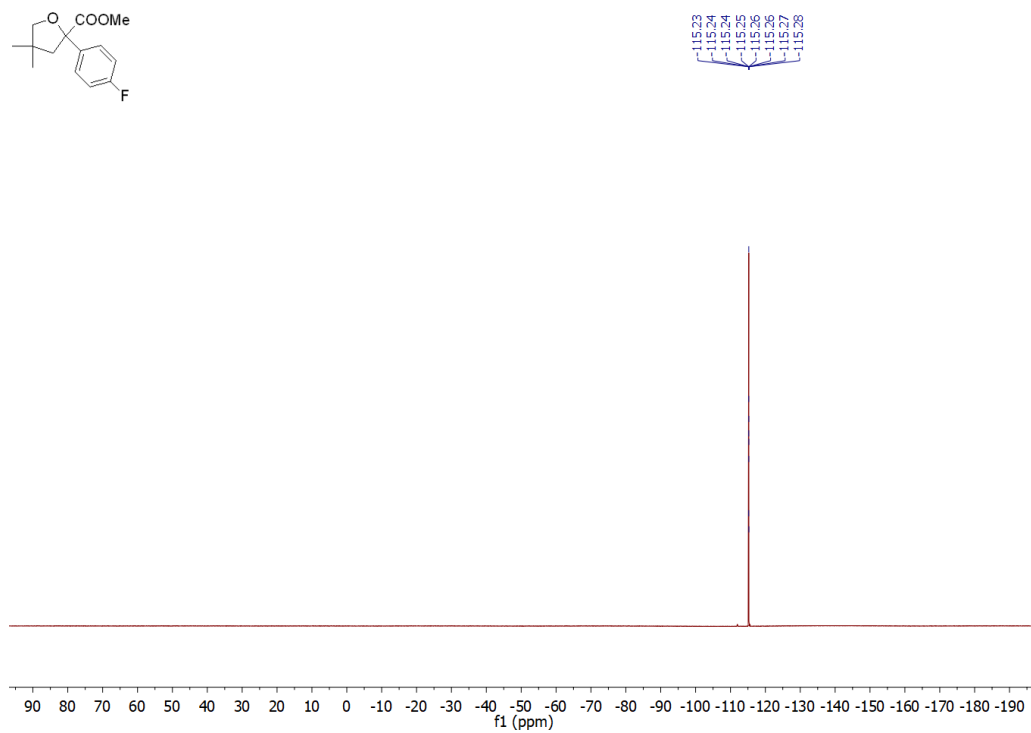
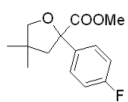
^1H NMR (600 MHz, Chloroform-*d*):



^{13}C NMR (151 MHz, Chloroform-*d*):

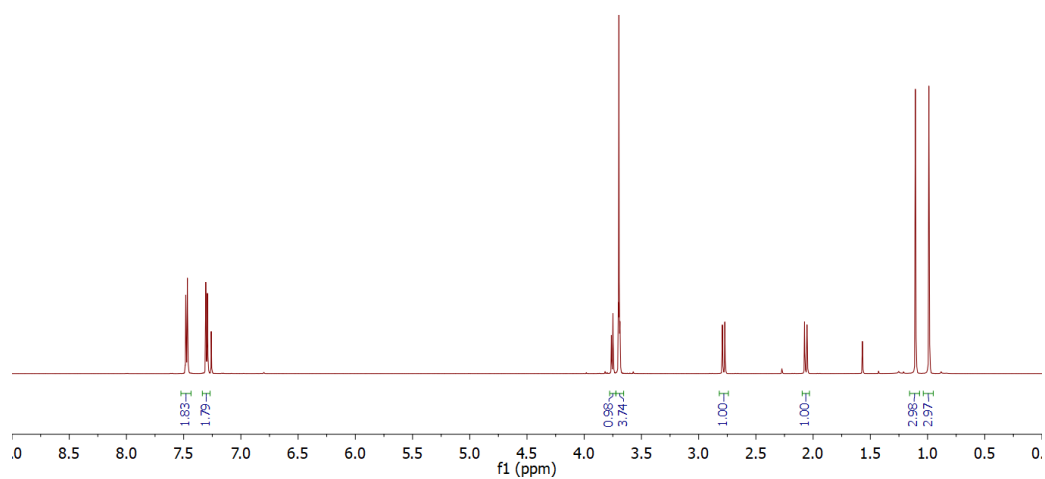
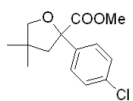


^{19}F NMR (564 MHz, Chloroform-*d*):

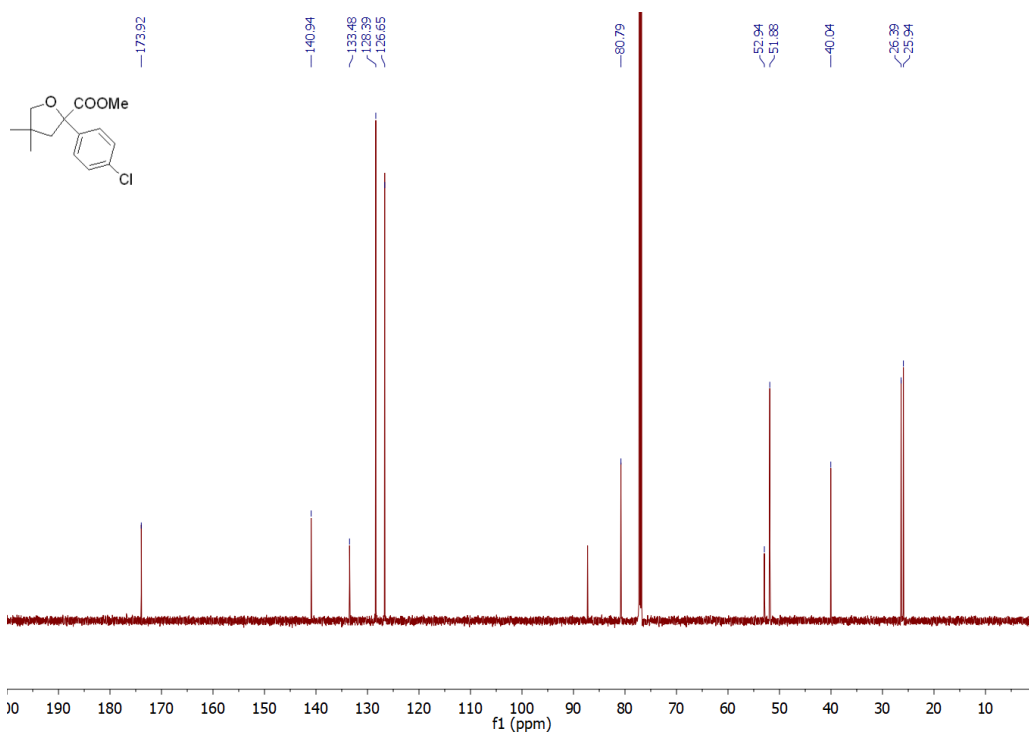


Methyl 2-(4-chlorophenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6h)

^1H NMR (600 MHz, Chloroform-*d*):

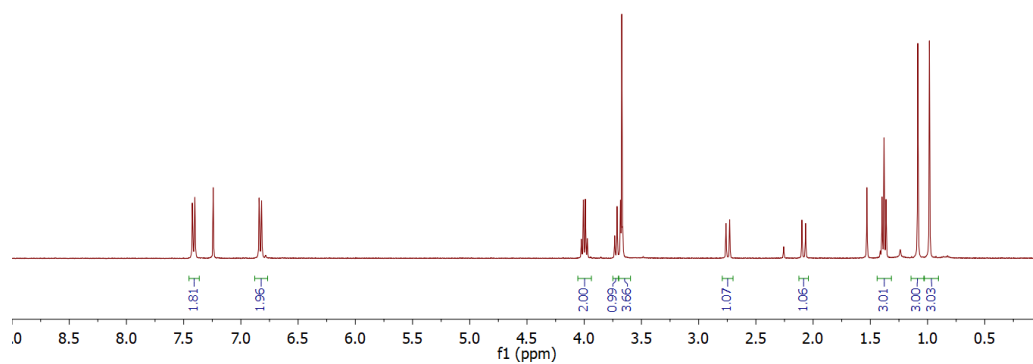
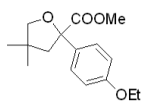


^{13}C NMR (151 MHz, Chloroform-*d*):

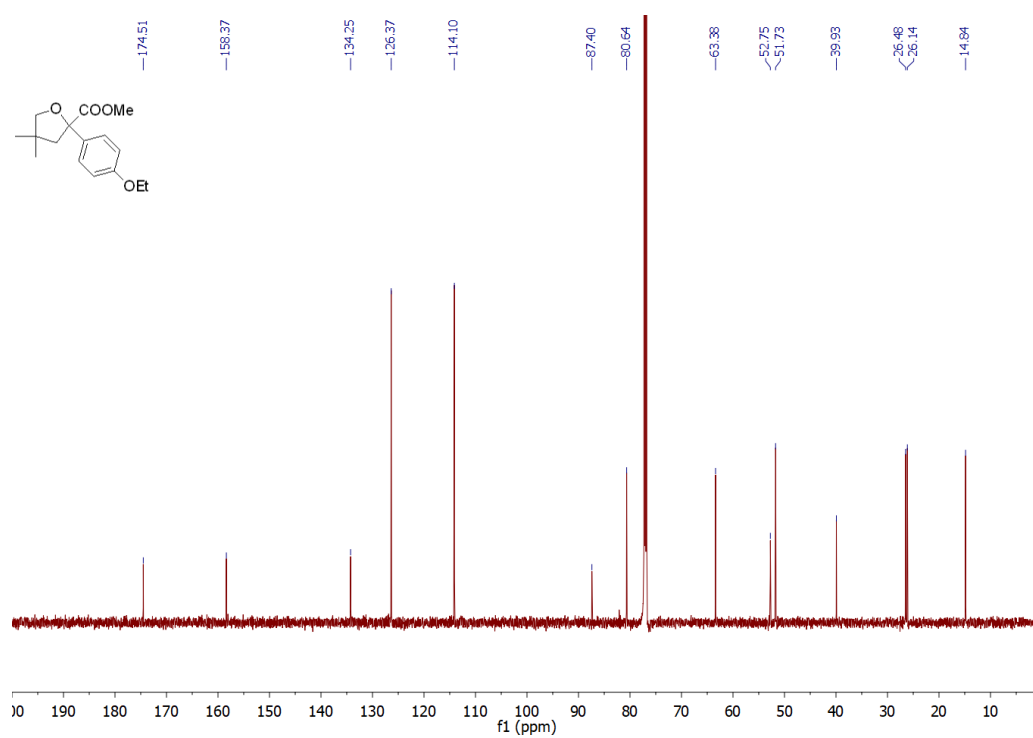
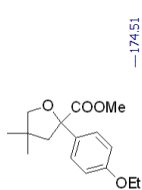


Methyl 2-(4-ethoxyphenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6i)

¹H NMR (400 MHz, Chloroform-*d*):

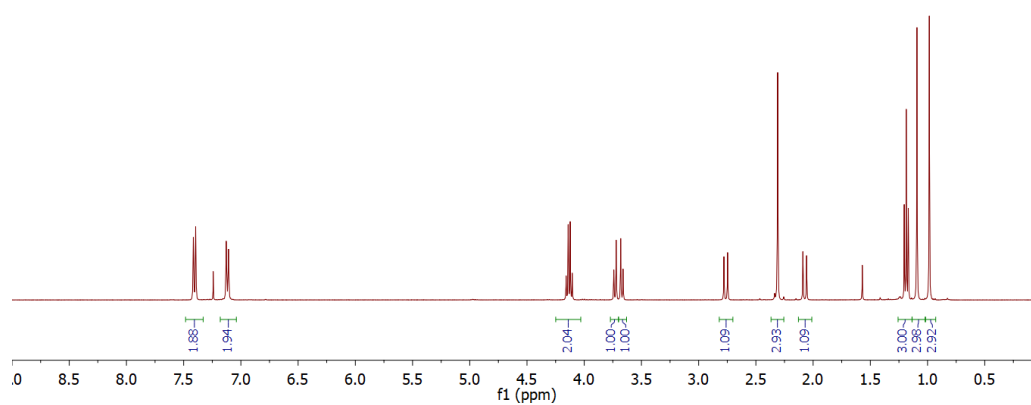
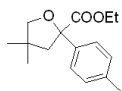


¹³C NMR (151 MHz, Chloroform-*d*):

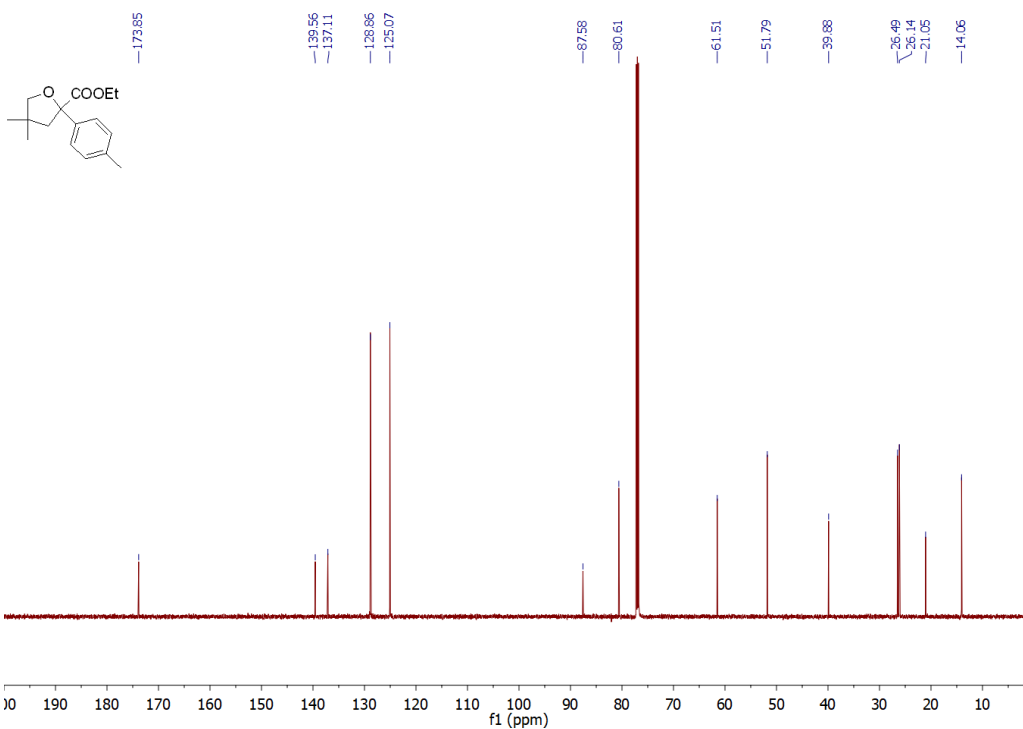


Ethyl 4,4-dimethyl-2-(p-tolyl)tetrahydrofuran-2-carboxylate (6j)

^1H NMR (400 MHz, Chloroform-*d*):

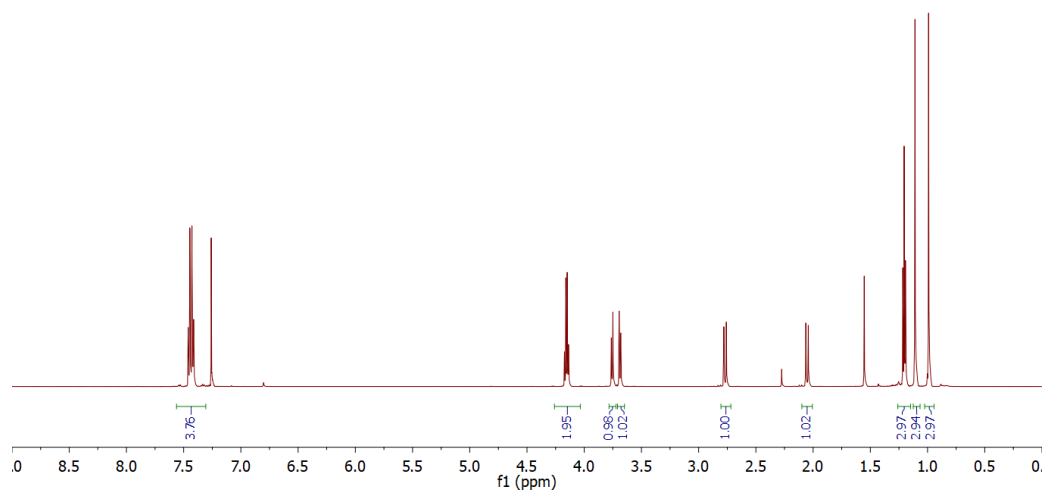
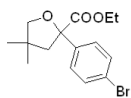


^{13}C NMR (151 MHz, Chloroform-*d*):

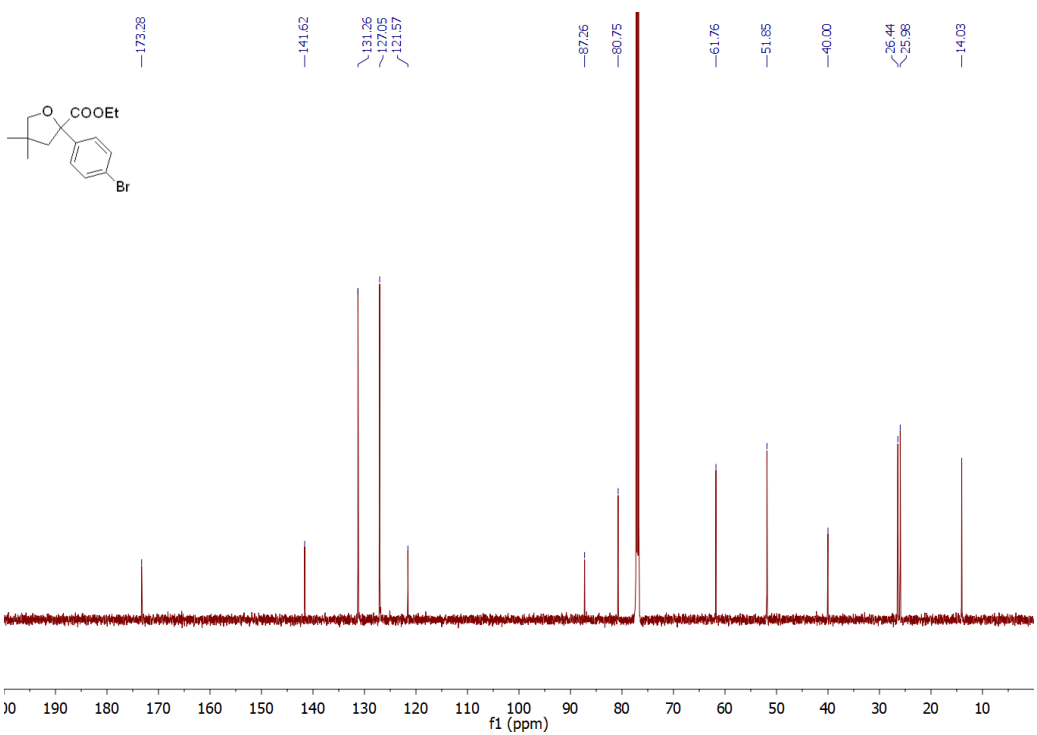


Ethyl 2-(4-bromophenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6k)

^1H NMR (600 MHz, Chloroform-*d*):

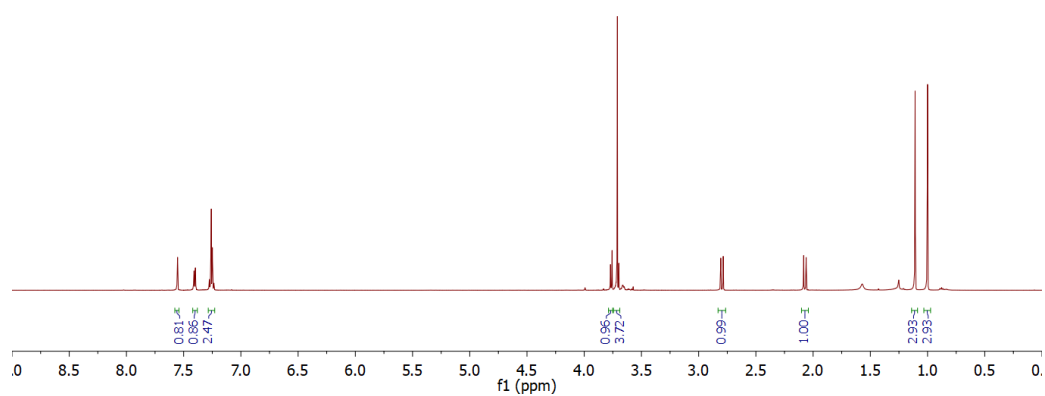
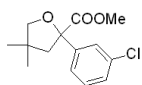


^{13}C NMR (151 MHz, Chloroform-*d*):

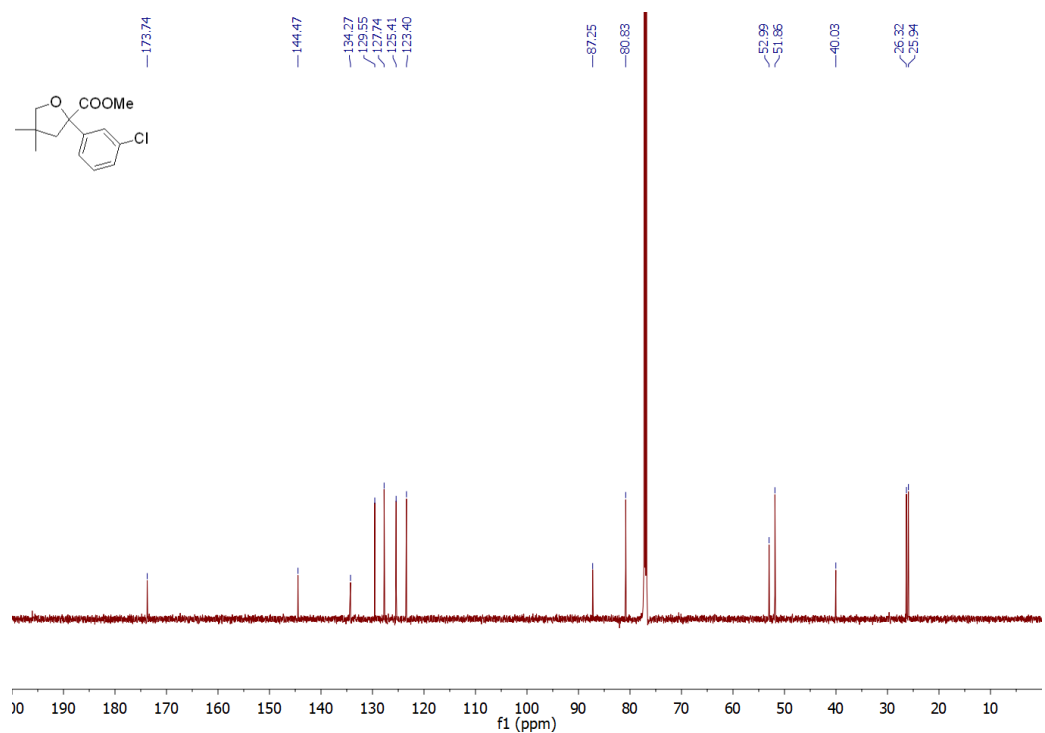
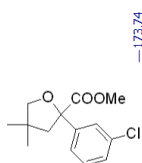


Methyl 2-(3-chlorophenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6I)

¹H NMR (600 MHz, Chloroform-d):

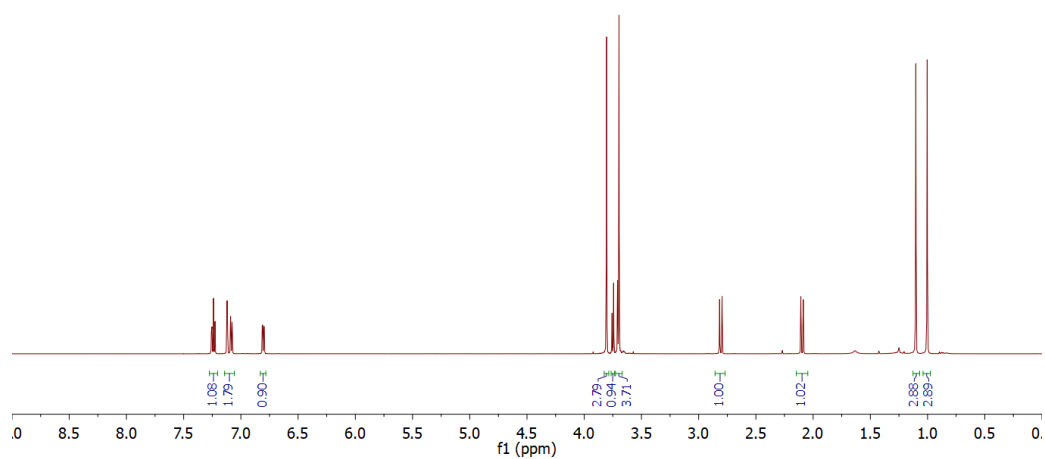
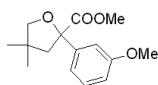


¹³C NMR (151 MHz, Chloroform-d):

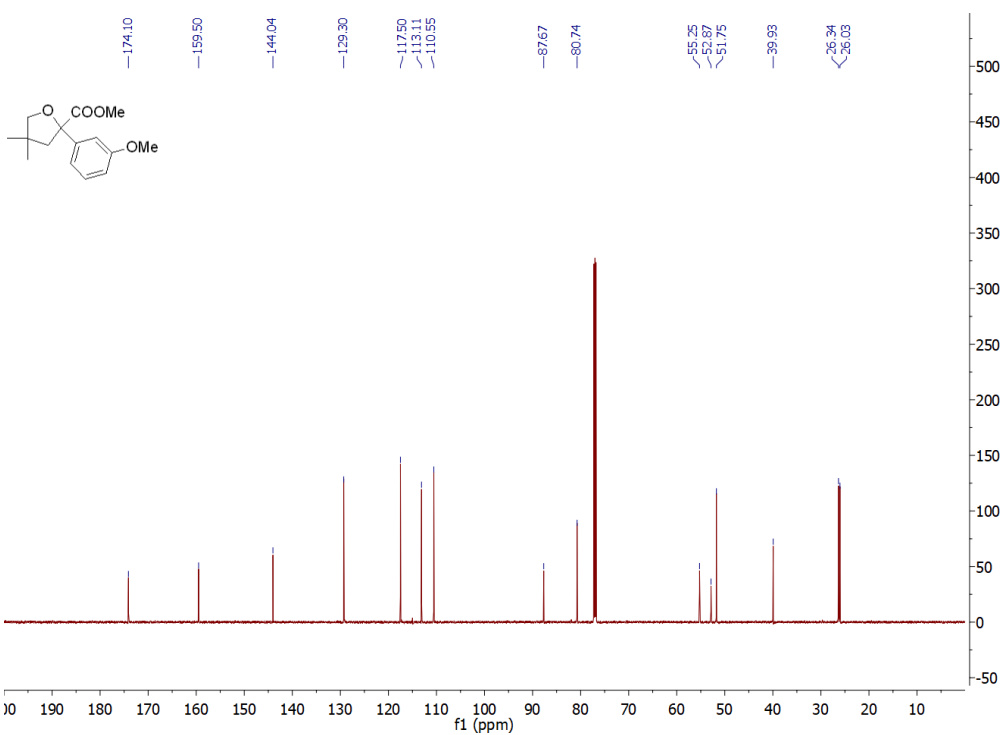


methyl 2-(3-methoxyphenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6m)

¹H NMR (600 MHz, Chloroform-d):

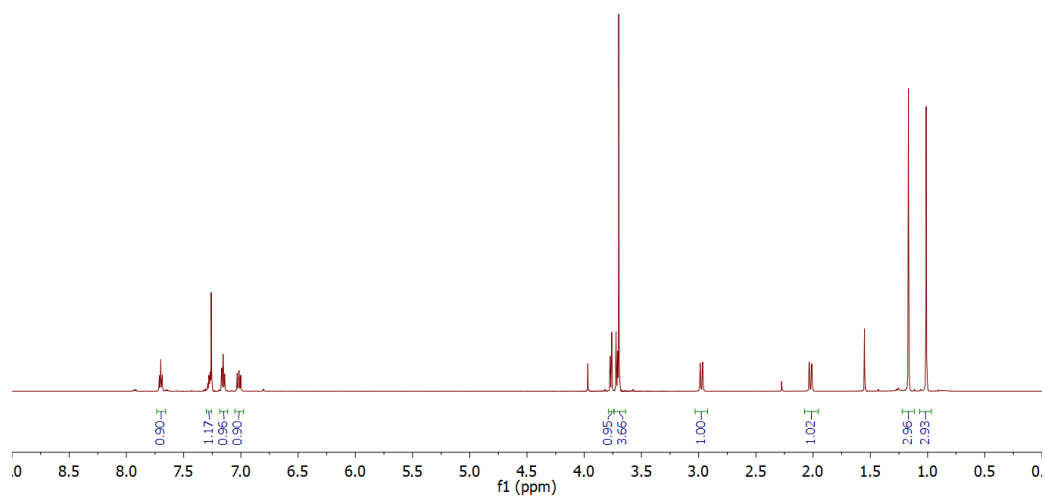
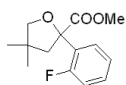


¹³C NMR (151 MHz, Chloroform-d):

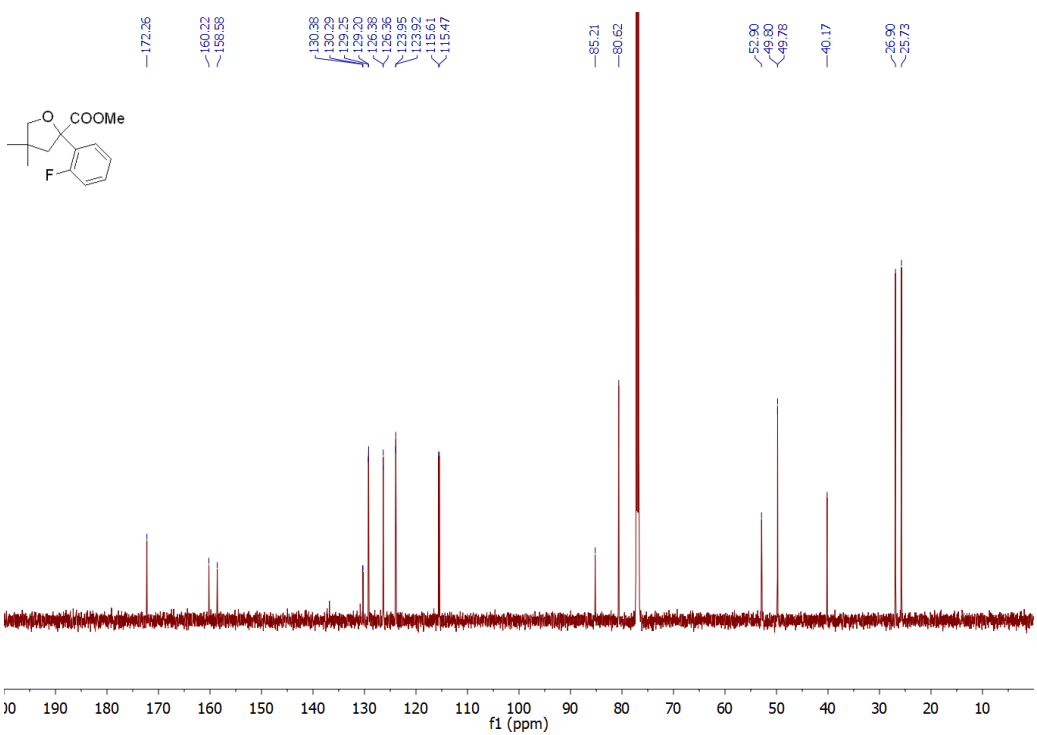


Methyl 2-(2-fluorophenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6n)

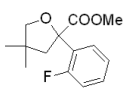
¹H NMR (600 MHz, Chloroform-*d*):



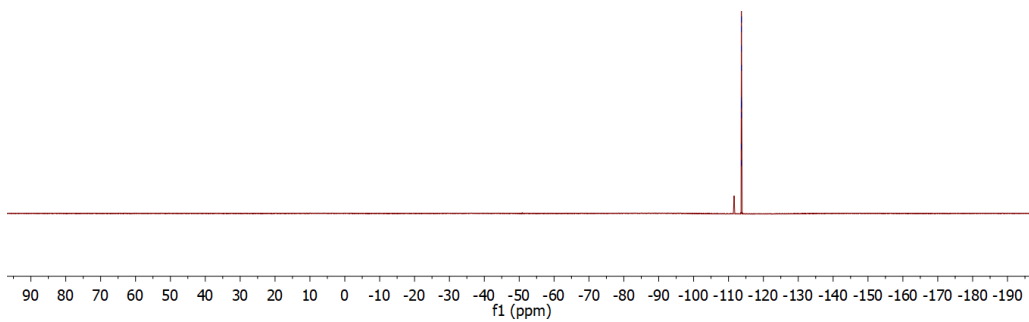
¹³C NMR (151 MHz, Chloroform-*d*):



^{19}F NMR (564 MHz, Chloroform-*d*):

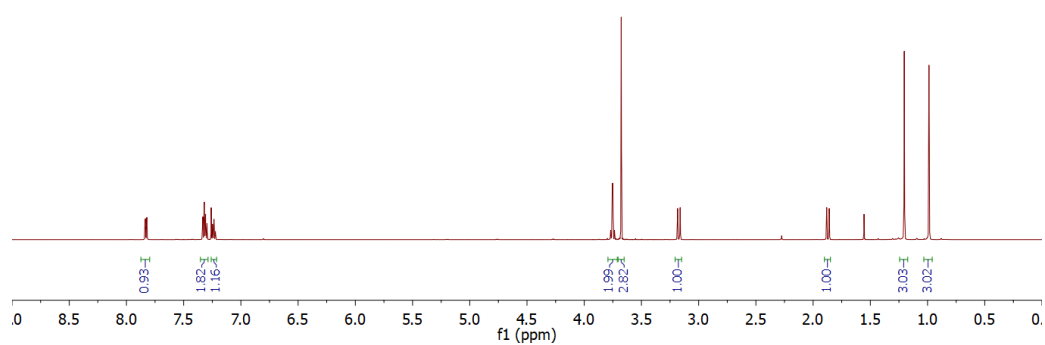
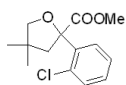


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113.71
113.72

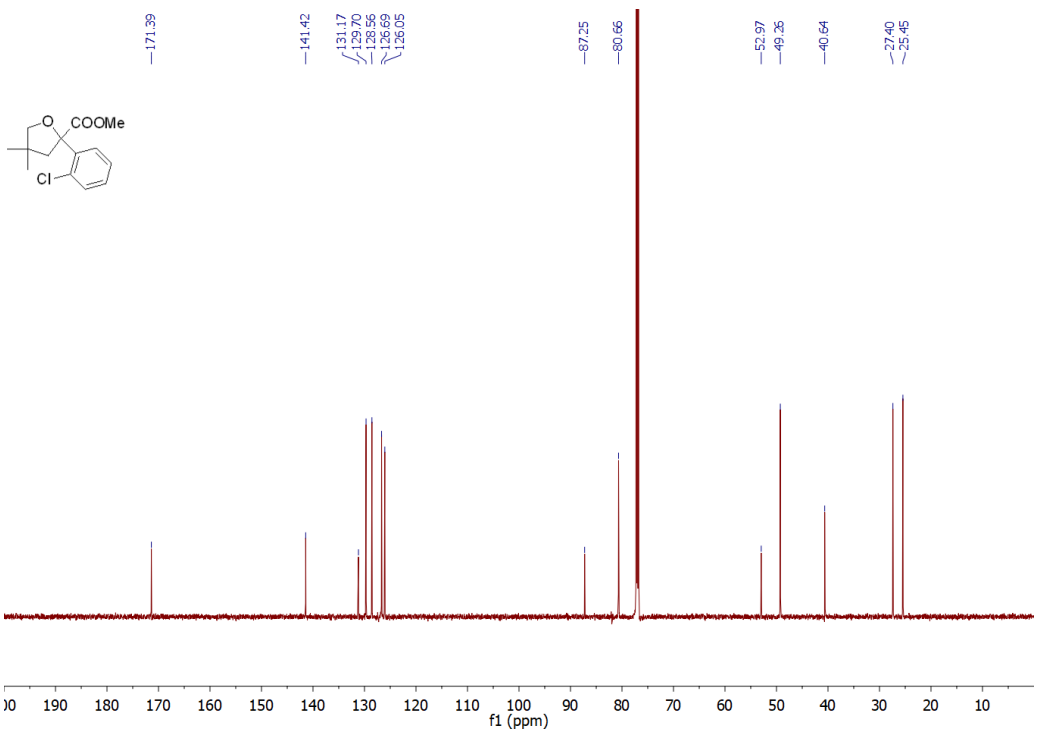


Methyl 2-(2-chlorophenyl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6o)

^1H NMR (600 MHz, Chloroform-*d*):

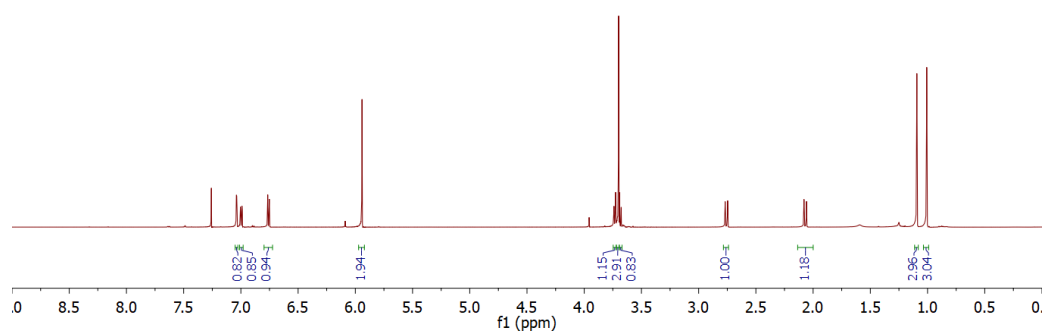
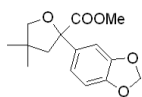


^{13}C NMR (151 MHz, CDCl_3):

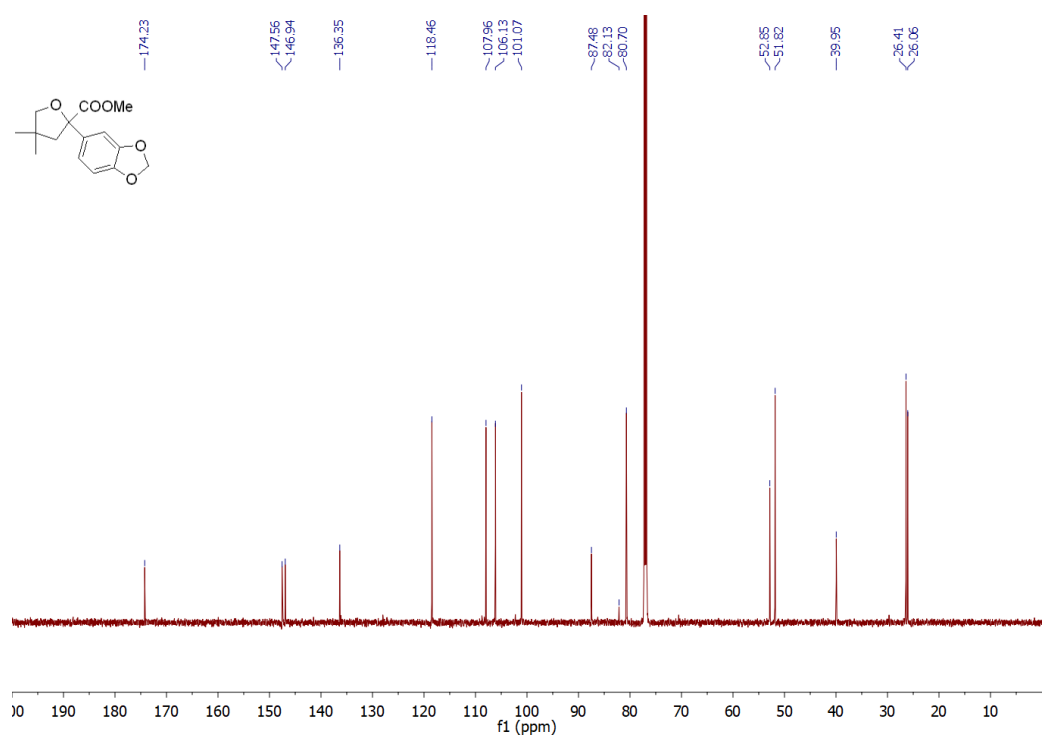
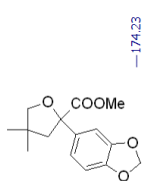


Methyl 2-(benzo[d][1,3]dioxol-5-yl)-4,4-dimethyltetrahydrofuran-2-carboxylate (6p)

¹H NMR (600 MHz, Chloroform-d):

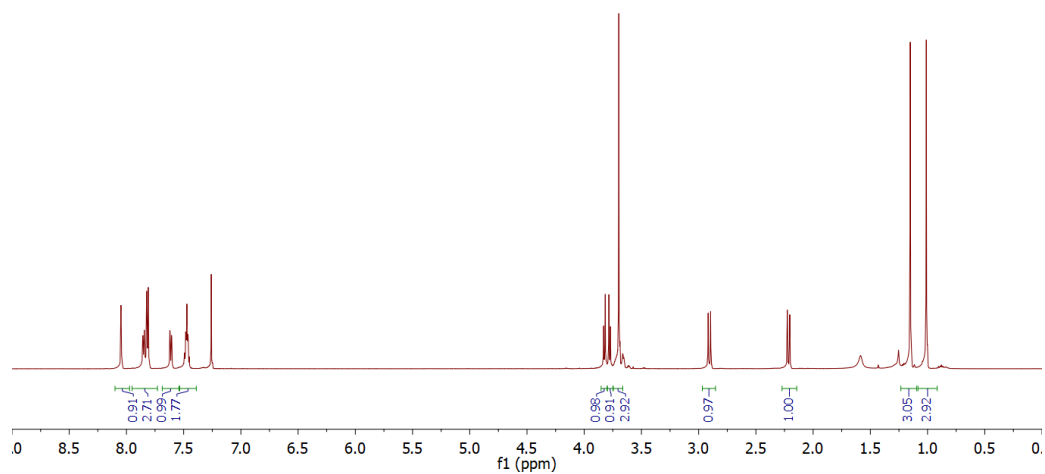
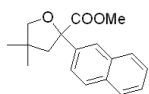


¹³C NMR (151 MHz, Chloroform-d):

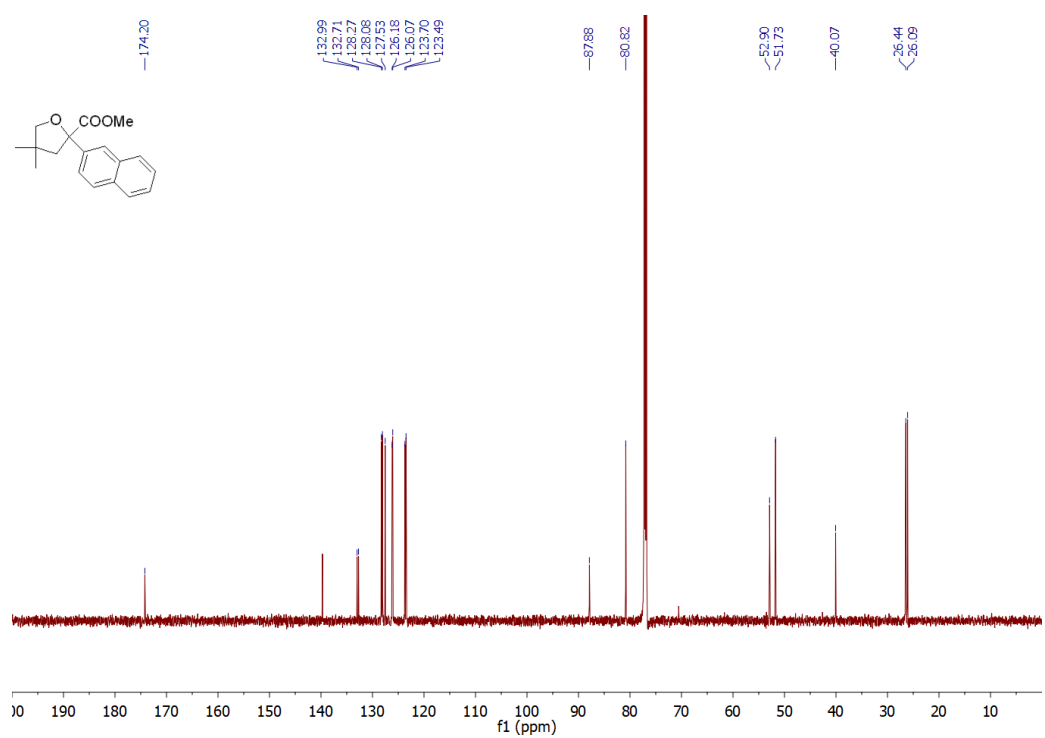
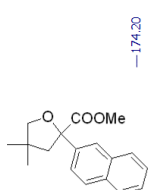


Methyl 4,4-dimethyl-2-(naphthalen-2-yl)tetrahydrofuran-2-carboxylate (6q)

^1H NMR (600 MHz, Chloroform- d):

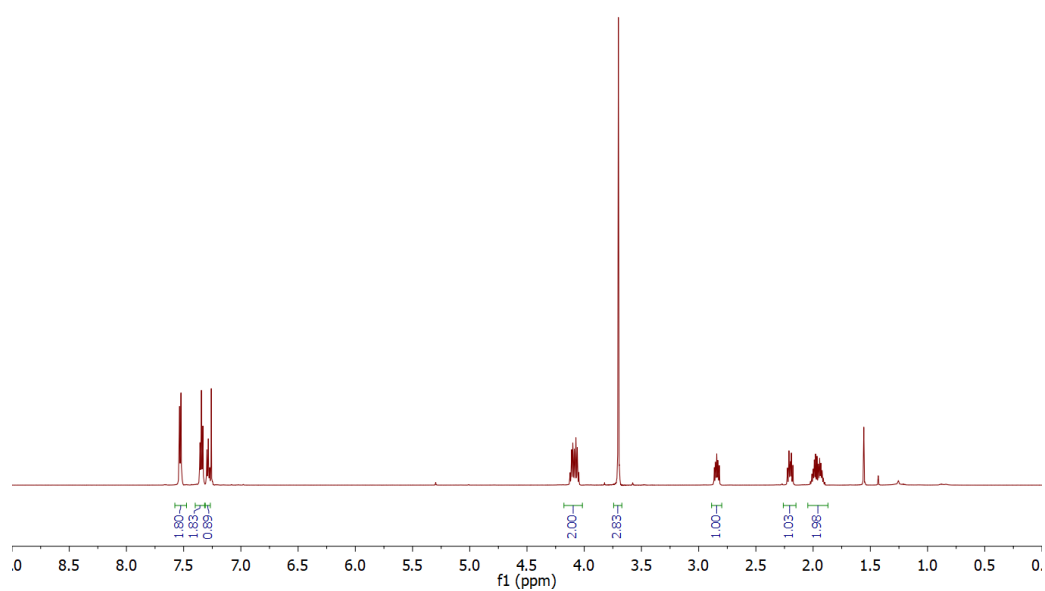
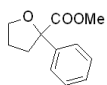


^{13}C NMR (151 MHz, Chloroform- d):

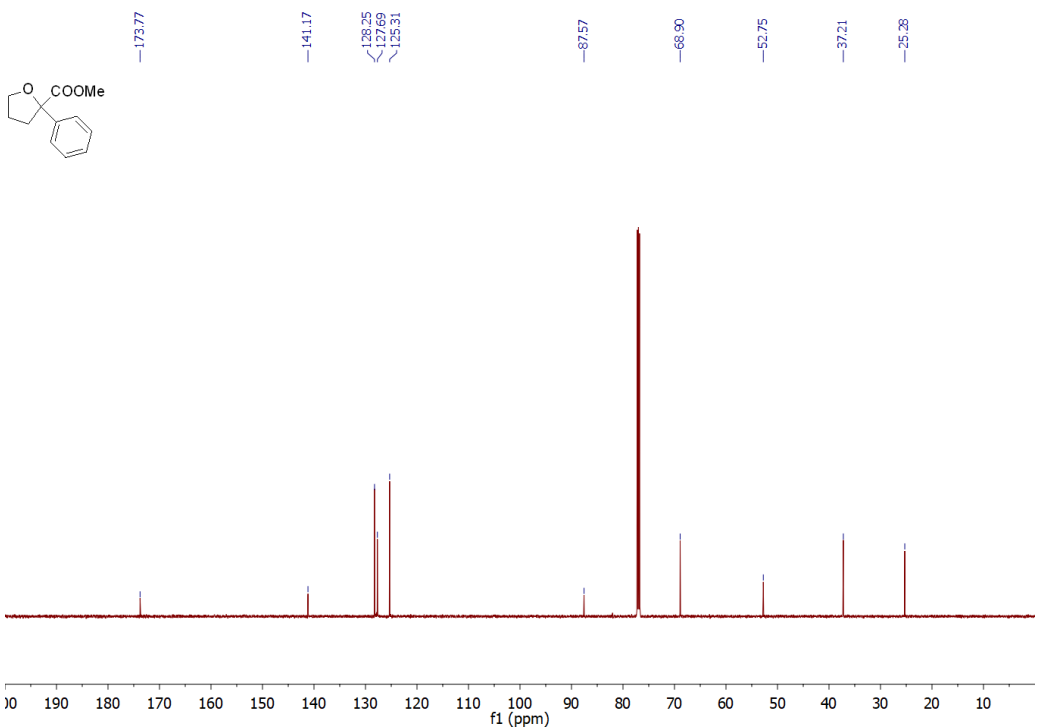


Methyl 2-phenyltetrahydrofuran-2-carboxylate (7a)

^1H NMR (600 MHz, Chloroform-*d*):

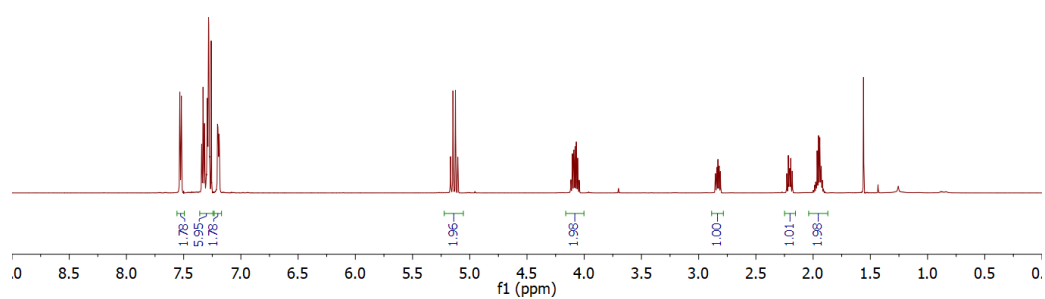
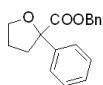


^{13}C NMR (151 MHz, Chloroform-*d*):

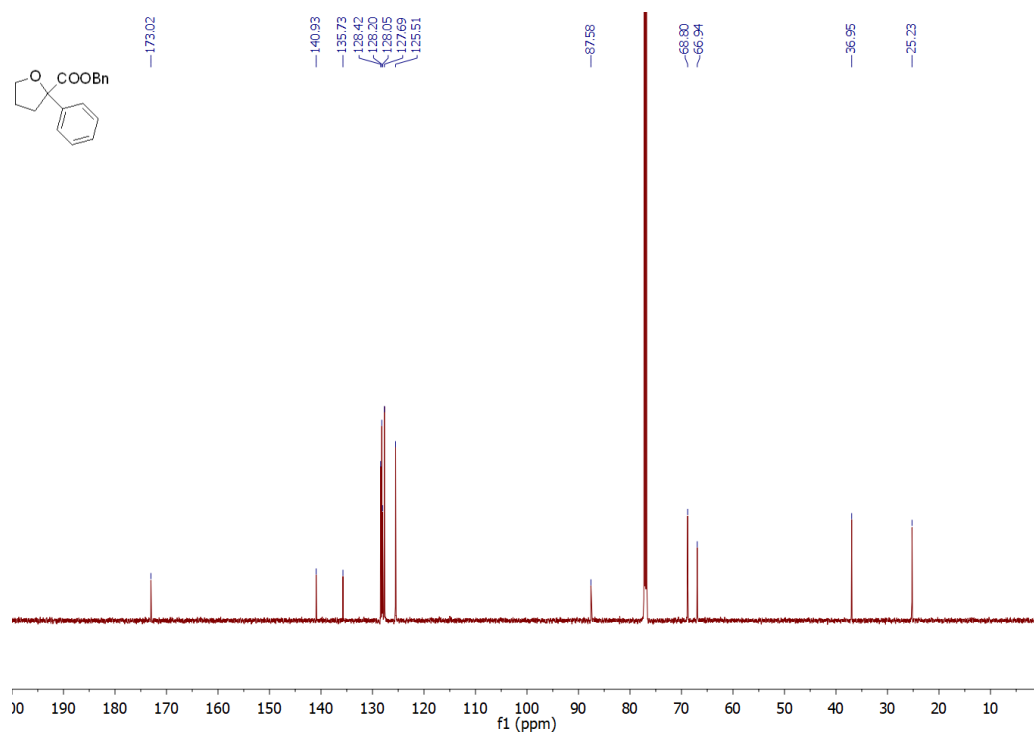
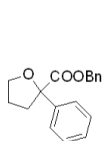


Benzyl 2-phenyltetrahydrofuran-2-carboxylate (7b)

^1H NMR (600 MHz, Chloroform-*d*):

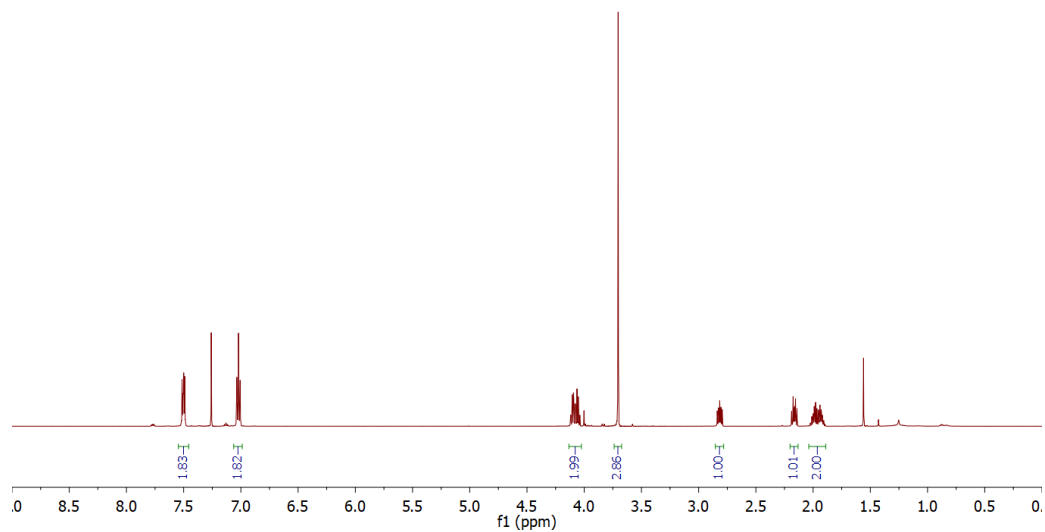
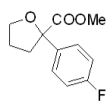


^{13}C NMR (151 MHz, Chloroform-*d*):

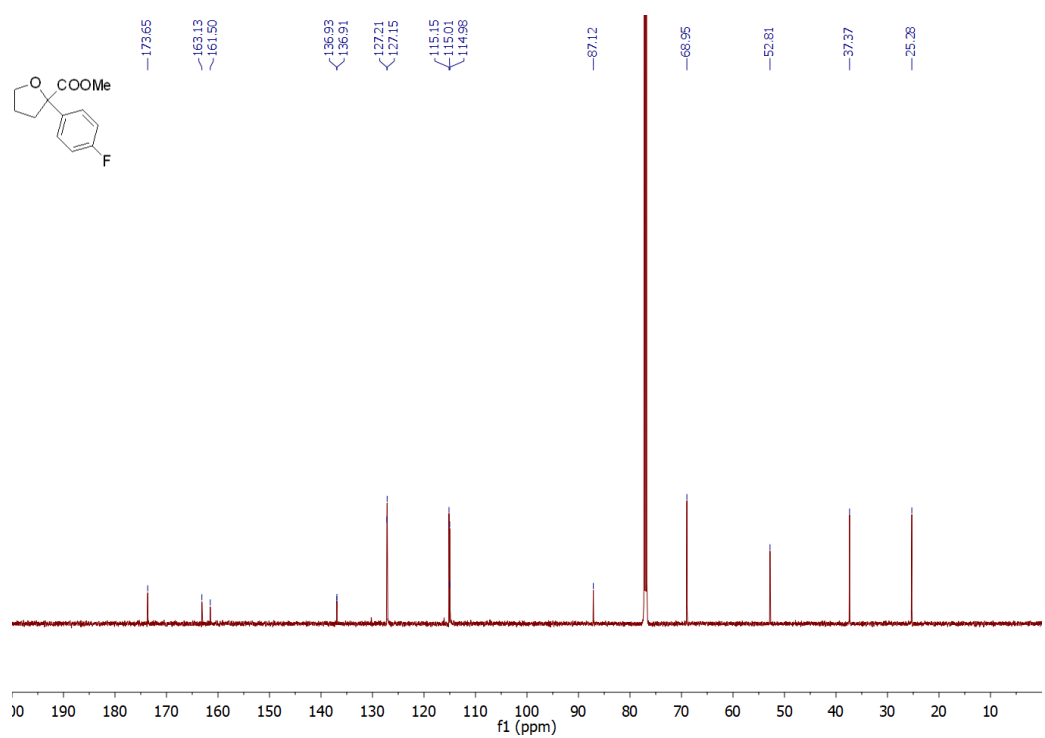
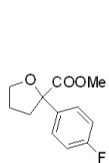


Methyl 2-(4-fluorophenyl)tetrahydrofuran-2-carboxylate (7c)

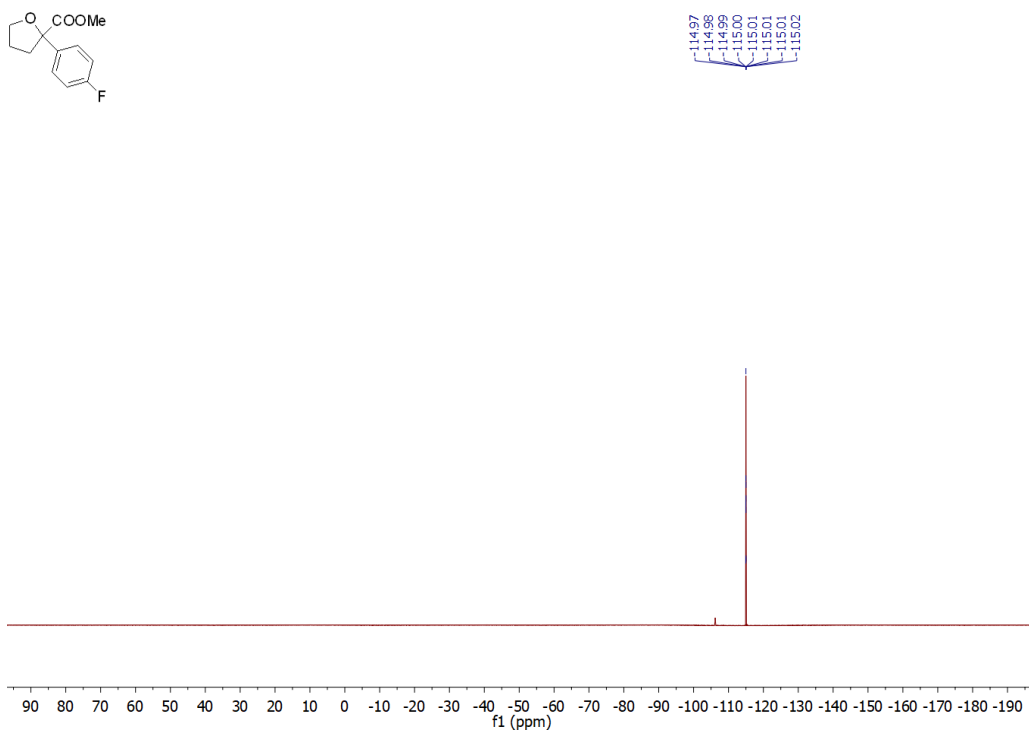
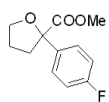
¹H NMR (600 MHz, Chloroform-*d*):



¹³C NMR (151 MHz, Chloroform-*d*):

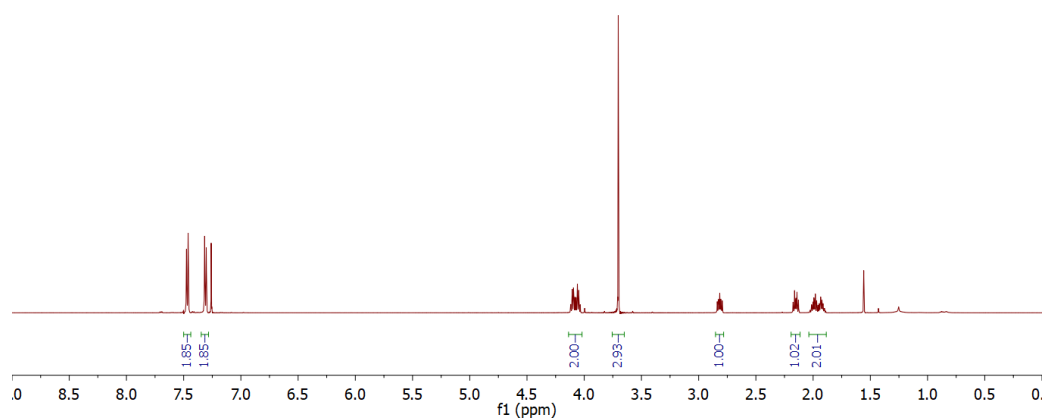
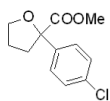


^{19}F NMR (564 MHz, Chloroform-*d*):

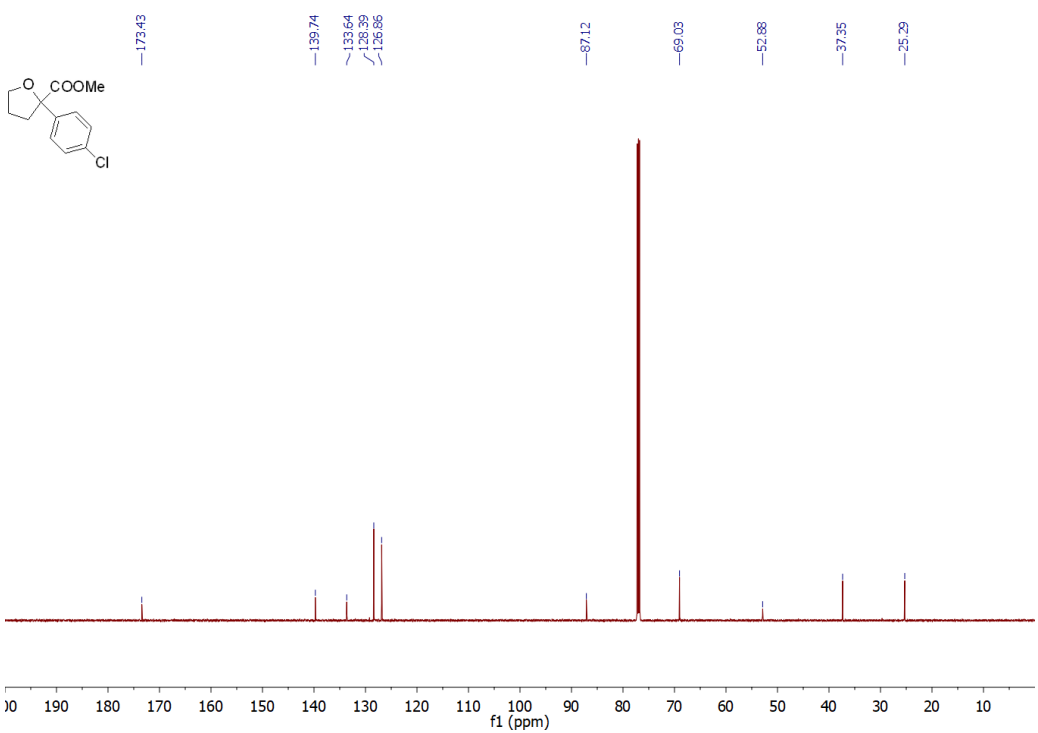


Methyl 2-(4-chlorophenyl)tetrahydrofuran-2-carboxylate (7d)

^1H NMR (600 MHz, Chloroform-*d*):

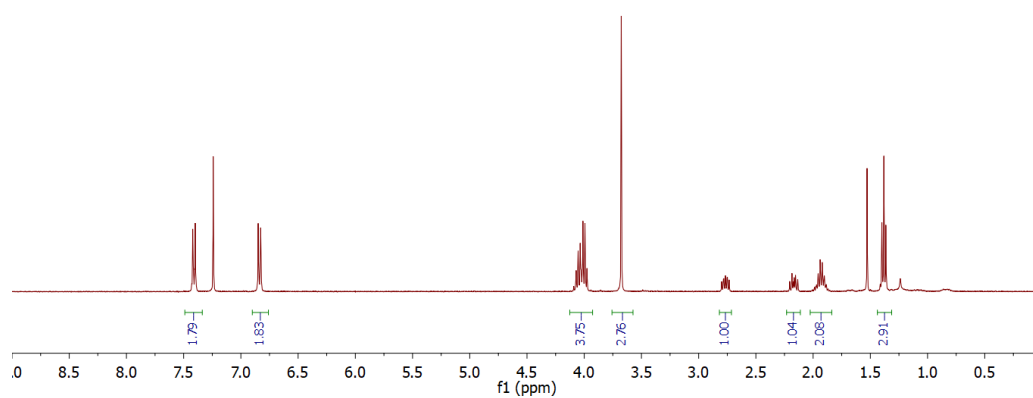
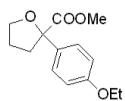


^{13}C NMR (151 MHz, Chloroform-*d*):

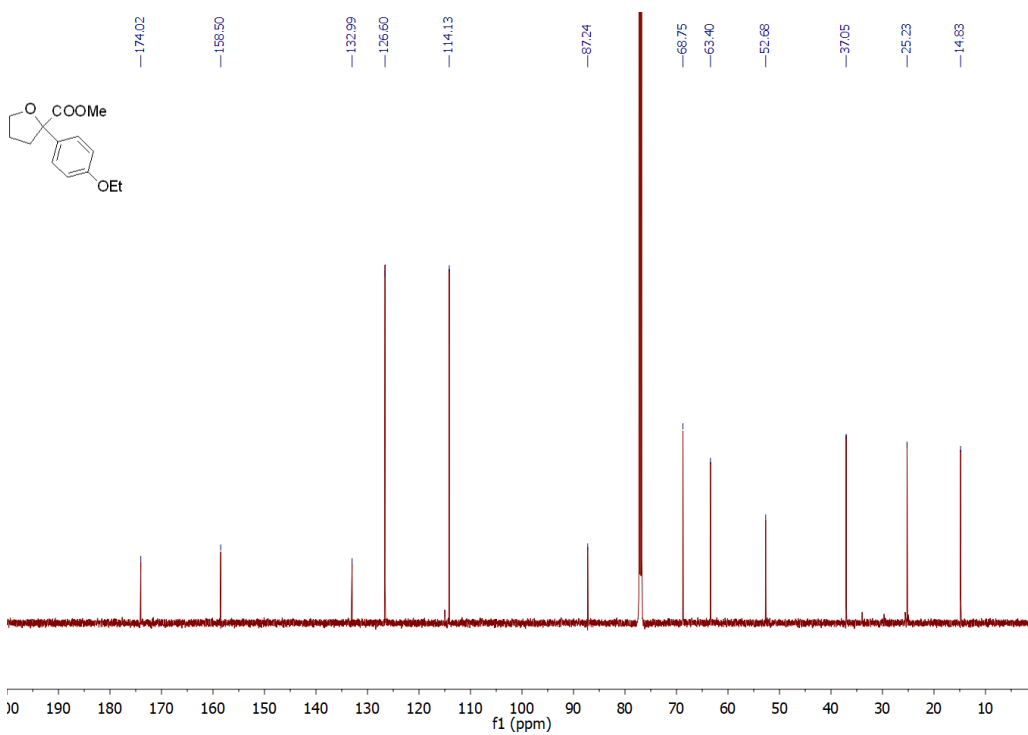


Methyl 2-(4-ethoxyphenyl)tetrahydrofuran-2-carboxylate (7e)

¹H NMR (400 MHz, Chloroform-*d*):

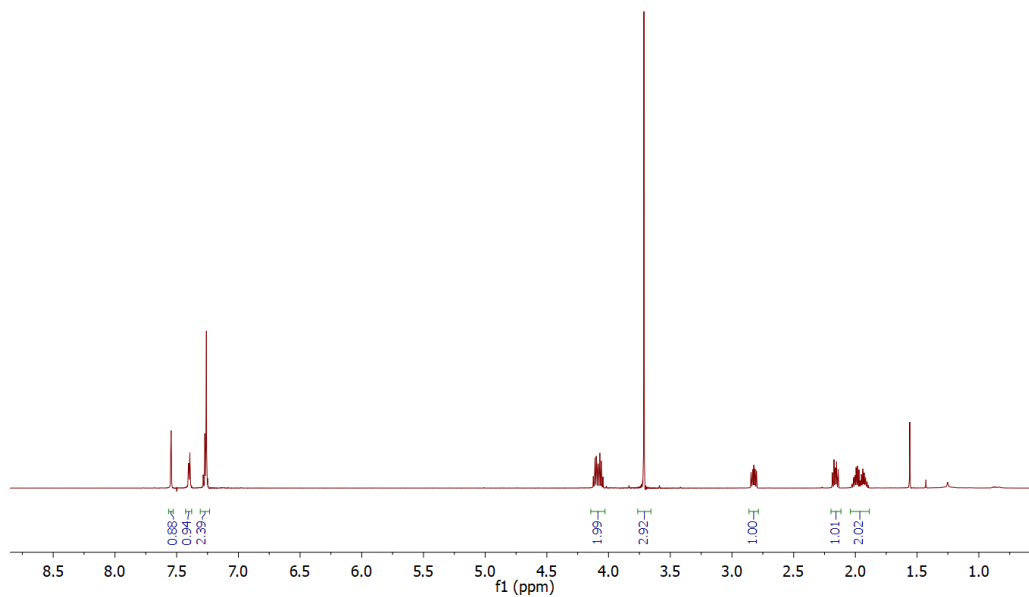
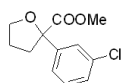


¹³C NMR (151 MHz, Chloroform-*d*):

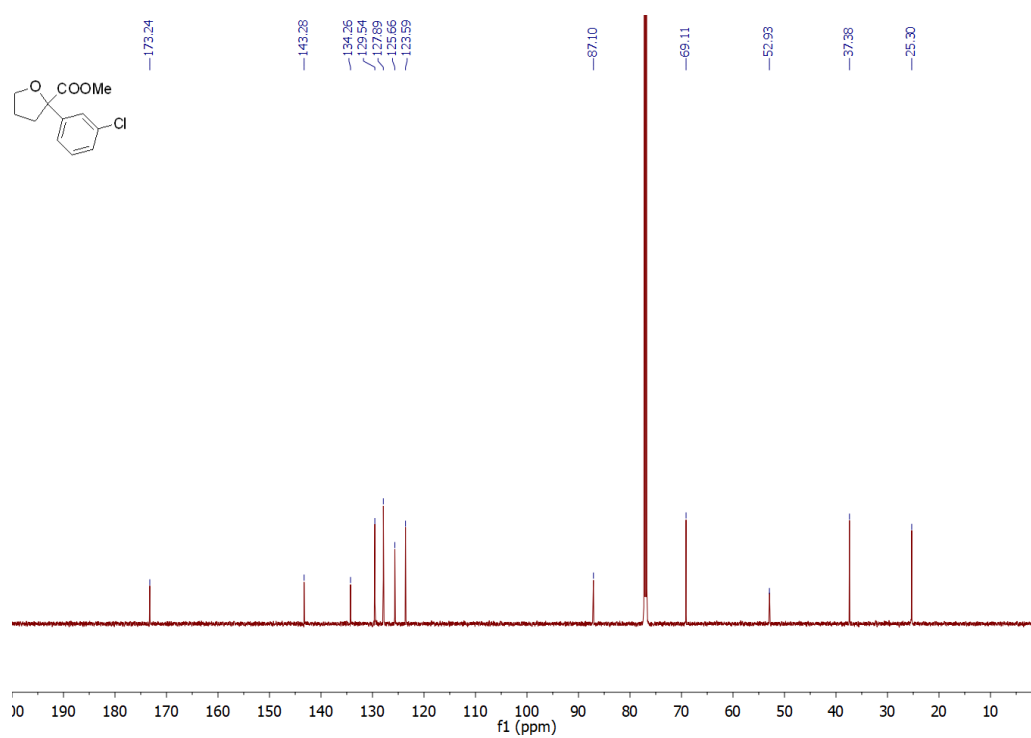
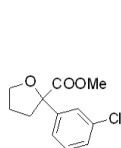


Methyl 2-(3-chlorophenyl)tetrahydrofuran-2-carboxylate (7f)

^1H NMR (600 MHz, Chloroform- d):

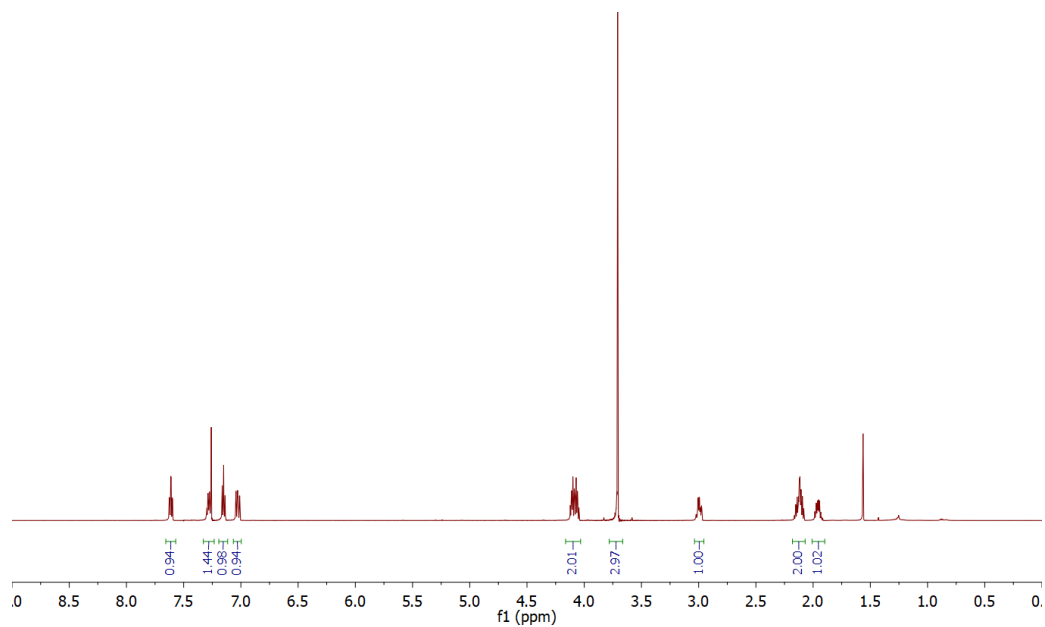
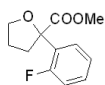


^{13}C NMR (151 MHz, Chloroform- d):

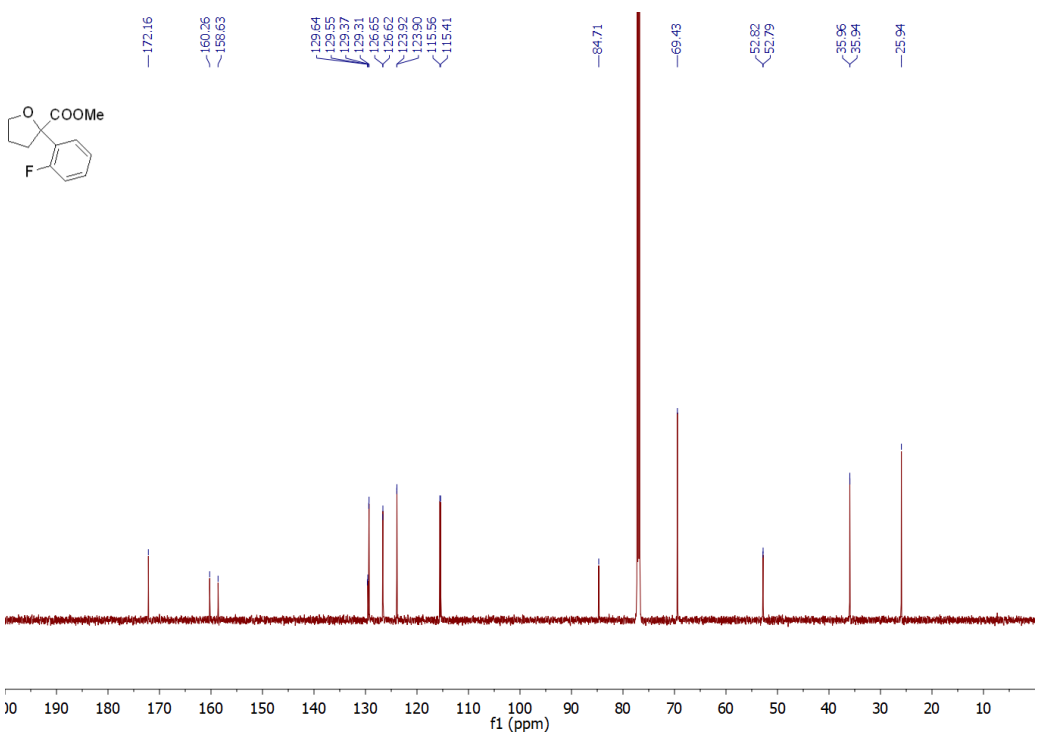


Methyl 2-(2-fluorophenyl)tetrahydrofuran-2-carboxylate (7g)

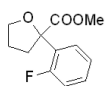
^1H NMR (600 MHz, Chloroform-*d*):



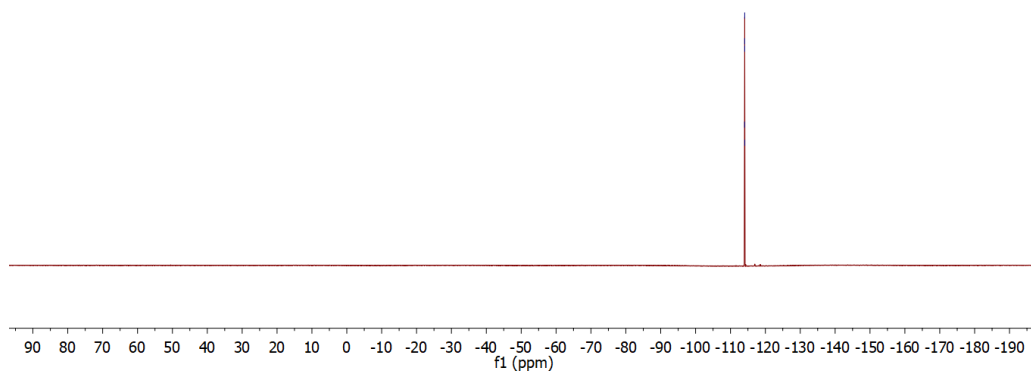
^{13}C NMR (151 MHz, Chloroform-*d*):



^{19}F NMR (564 MHz, Chloroform-*d*):

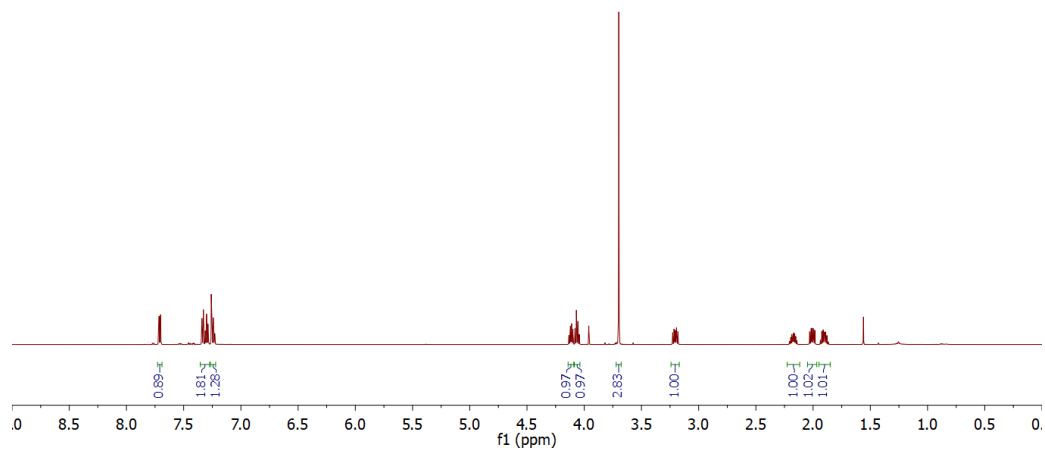
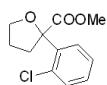


-114.06
-114.07
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-114.10

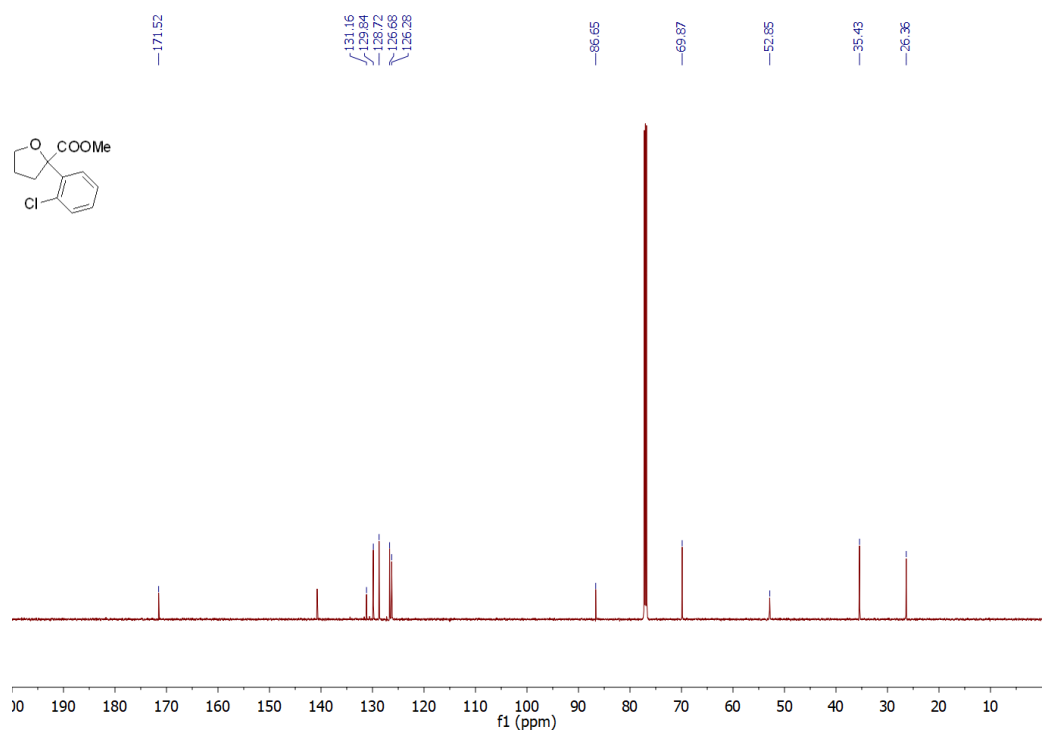


Methyl 2-(2-chlorophenyl)tetrahydrofuran-2-carboxylate (7h)

^1H NMR (600 MHz, Chloroform-*d*):

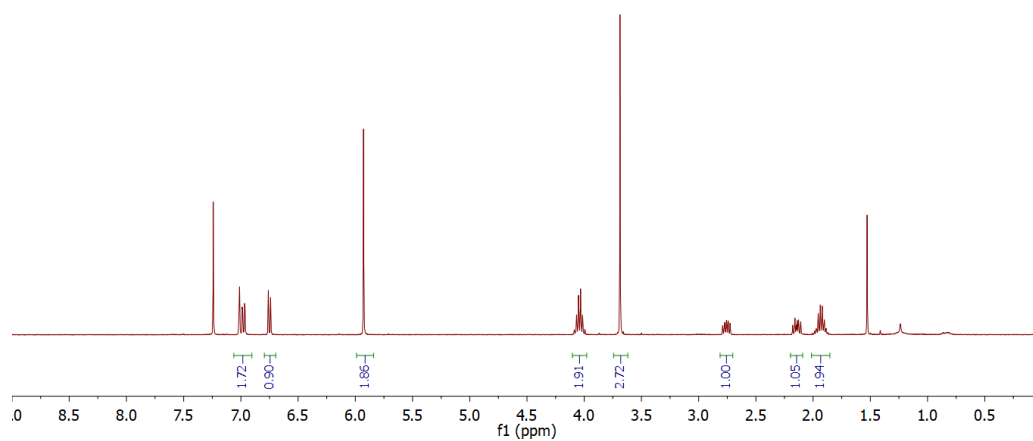
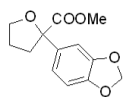


^{13}C NMR (151 MHz, Chloroform-*d*):

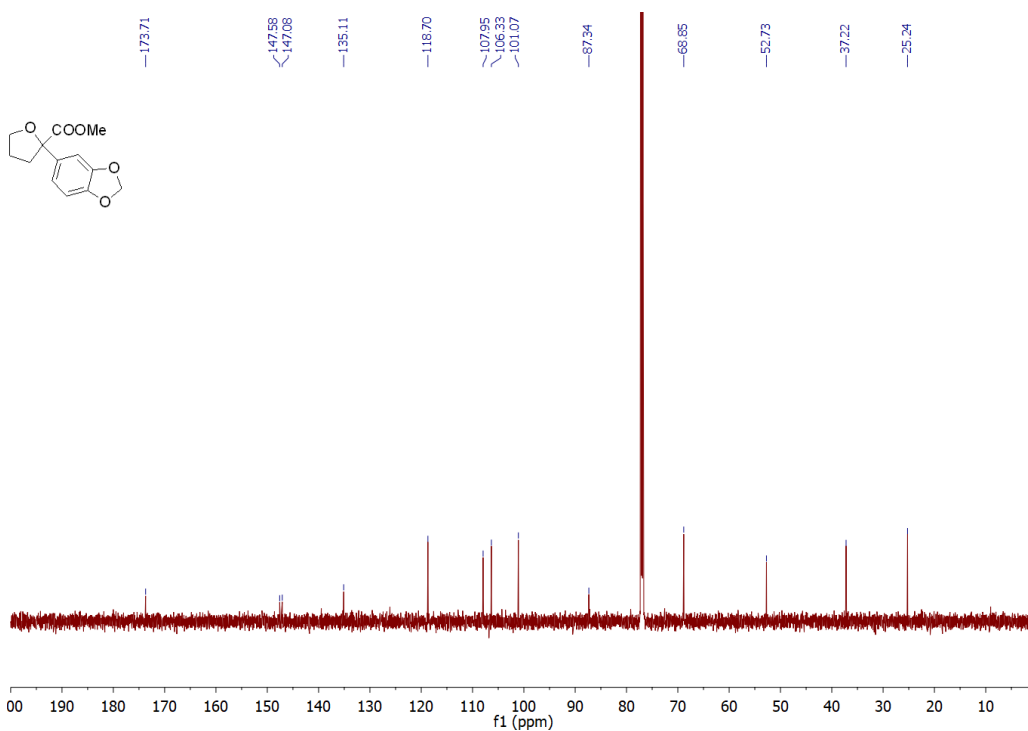


Methyl 2-(benzo[d][1,3]dioxol-5-yl)tetrahydrofuran-2-carboxylate (7i)

^1H NMR (400 MHz, Chloroform-*d*):

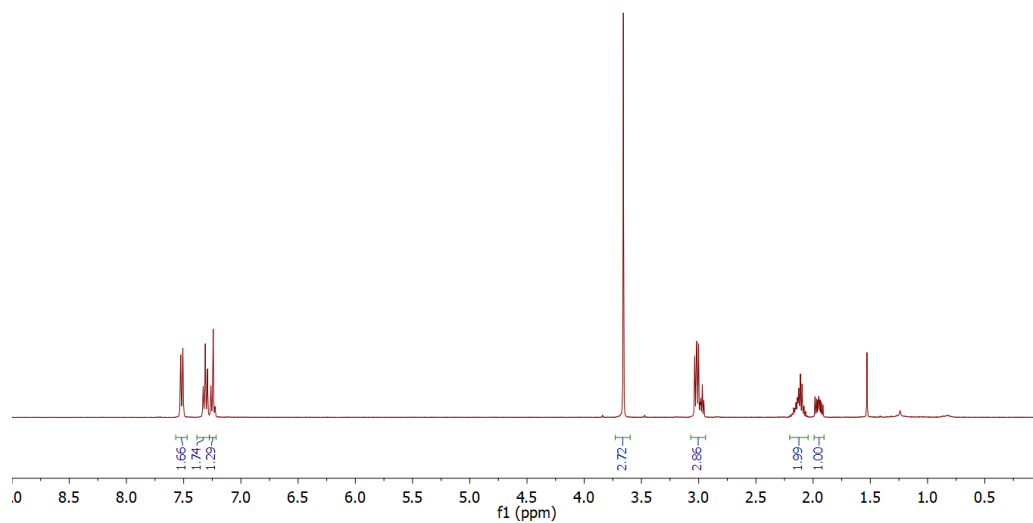
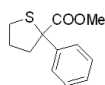


^{13}C NMR (151 MHz, Chloroform-*d*):

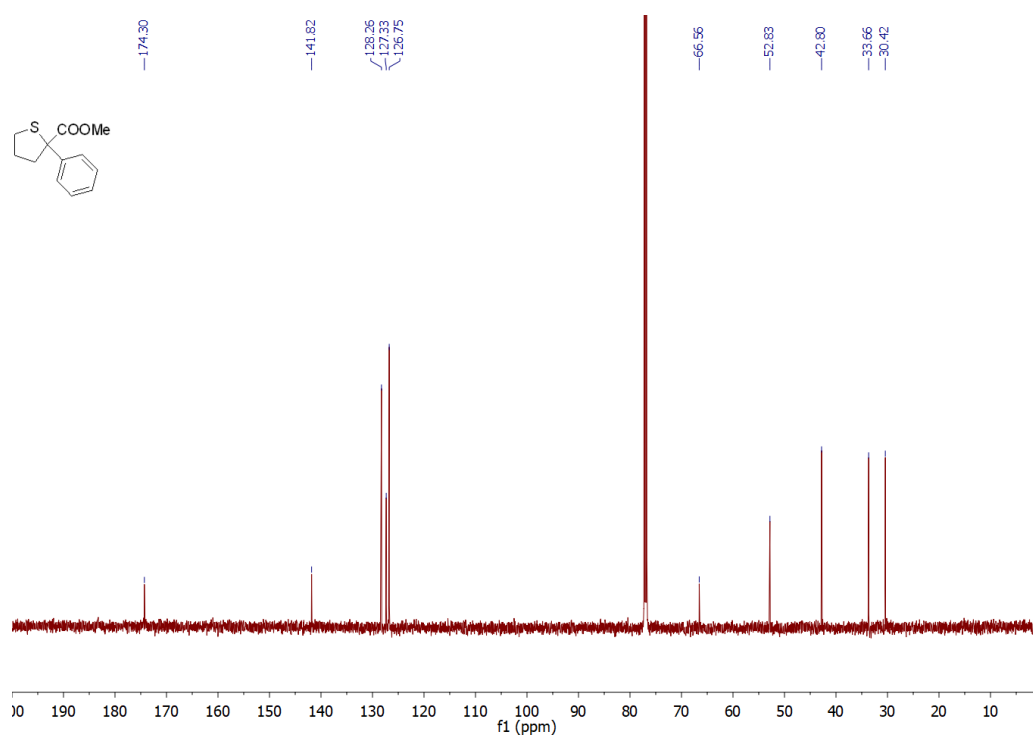
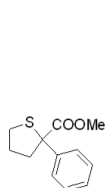


Methyl 2-phenyltetrahydrothiophene-2-carboxylate (8a)

^1H NMR (400 MHz, Chloroform-*d*):

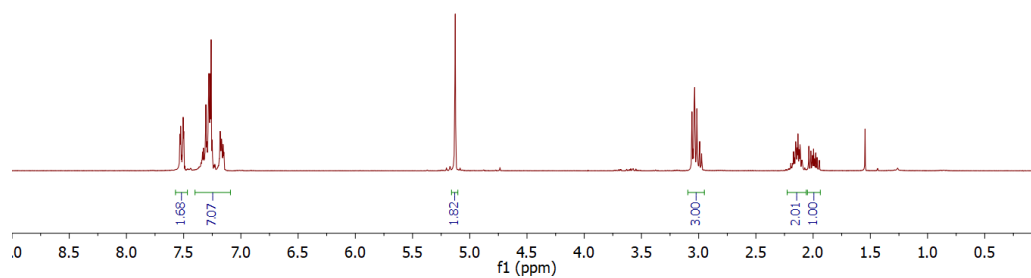
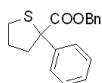


^{13}C NMR (151 MHz, Chloroform-*d*):

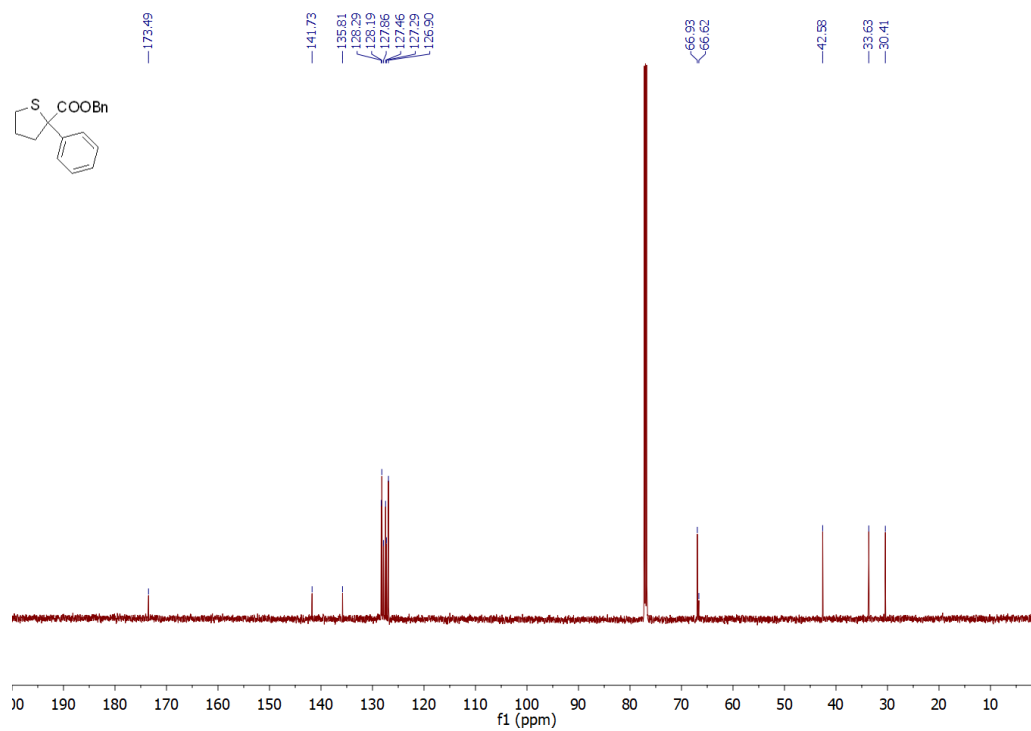
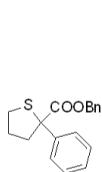


Benzyl 2-phenyltetrahydrothiophene-2-carboxylate (8b)

^1H NMR (300 MHz, Chloroform-*d*):

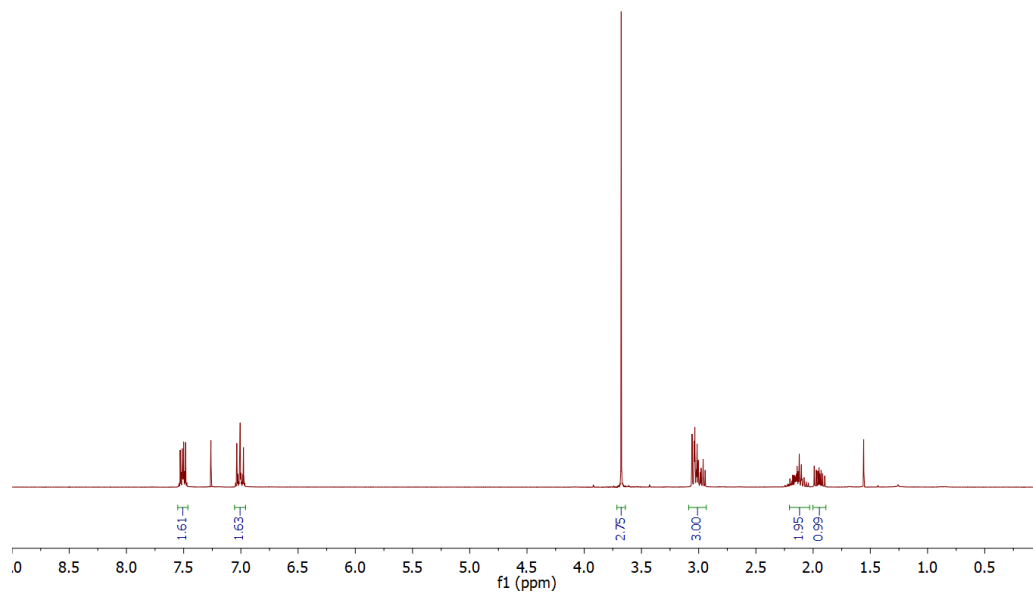
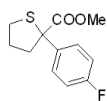


^{13}C NMR (151 MHz, Chloroform-*d*):

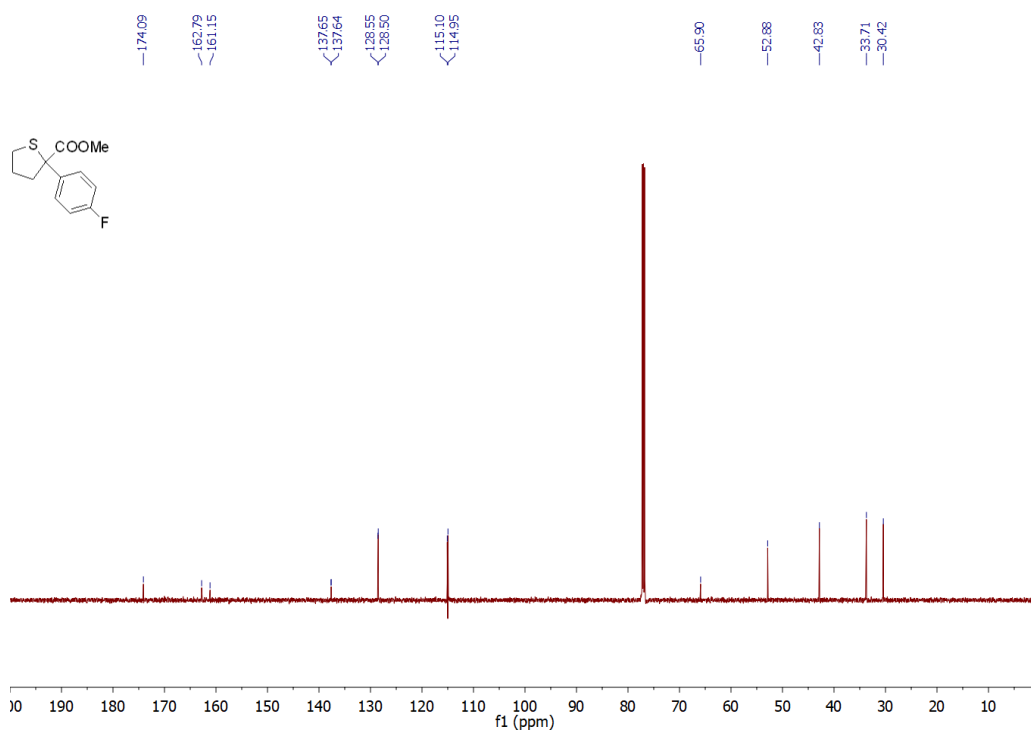


Methyl 2-(4-fluorophenyl)tetrahydrothiophene-2-carboxylate (8c)

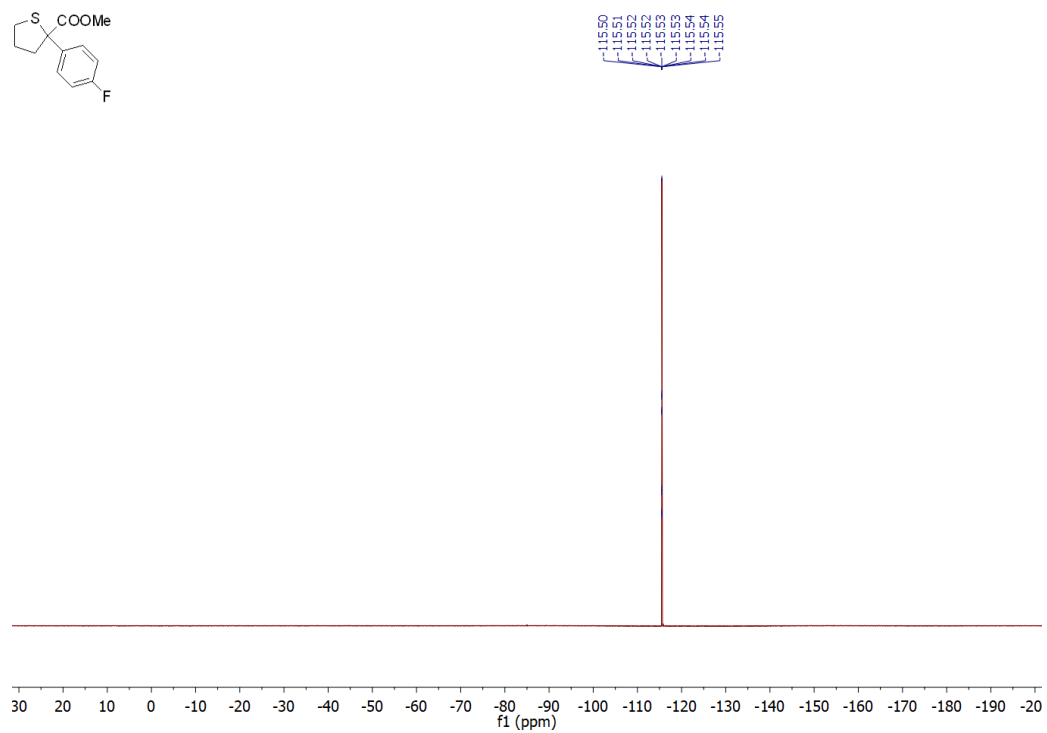
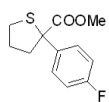
¹H NMR (300 MHz, Chloroform-*d*):



¹³C NMR (151 MHz, Chloroform-*d*):

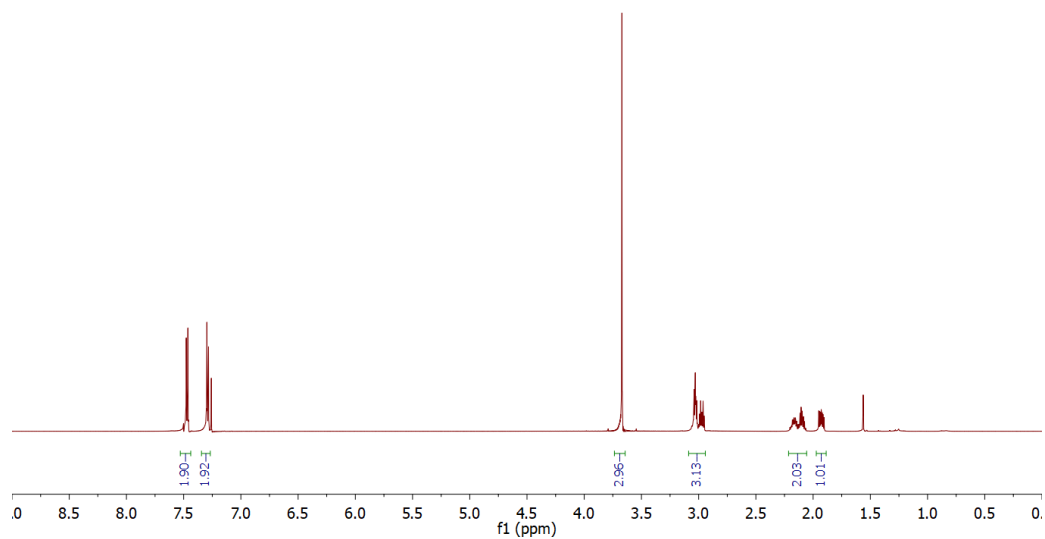
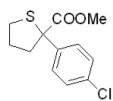


^{19}F NMR (564 MHz, Chloroform-*d*):

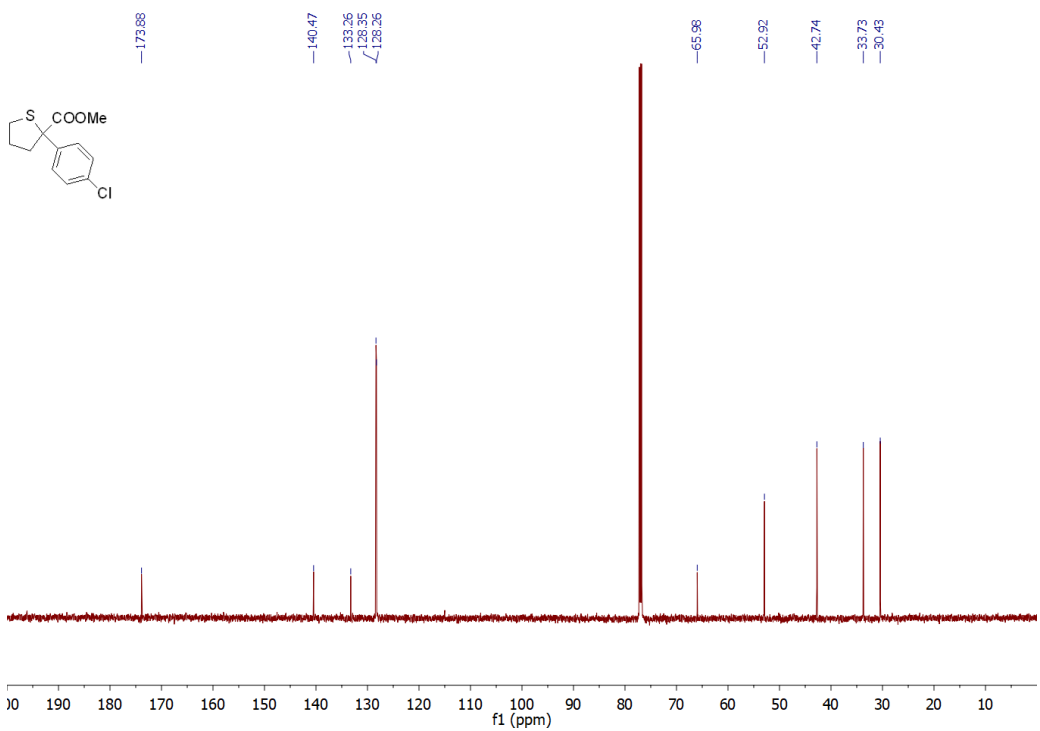


Methyl 2-(4-chlorophenyl)tetrahydrothiophene-2-carboxylate (8d)

¹H NMR (600 MHz, Chloroform-*d*):

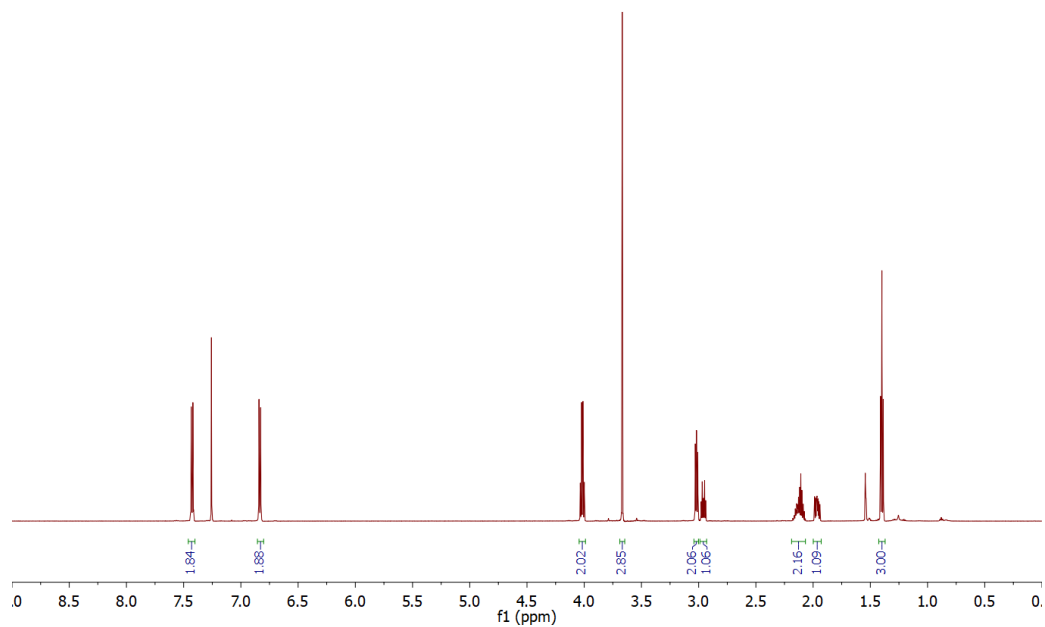
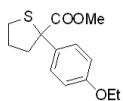


¹³C NMR (151 MHz, Chloroform-*d*):

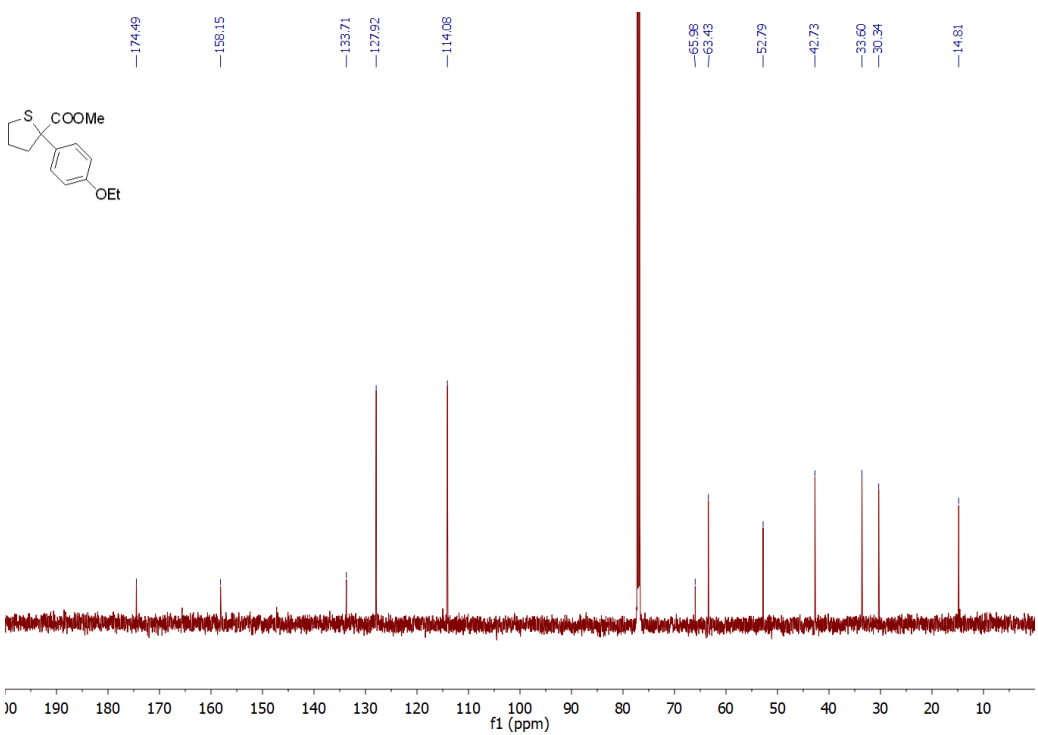


Methyl 2-(4-ethoxyphenyl)tetrahydrothiophene-2-carboxylate (8e)

^1H NMR (600 MHz, Chloroform-*d*):

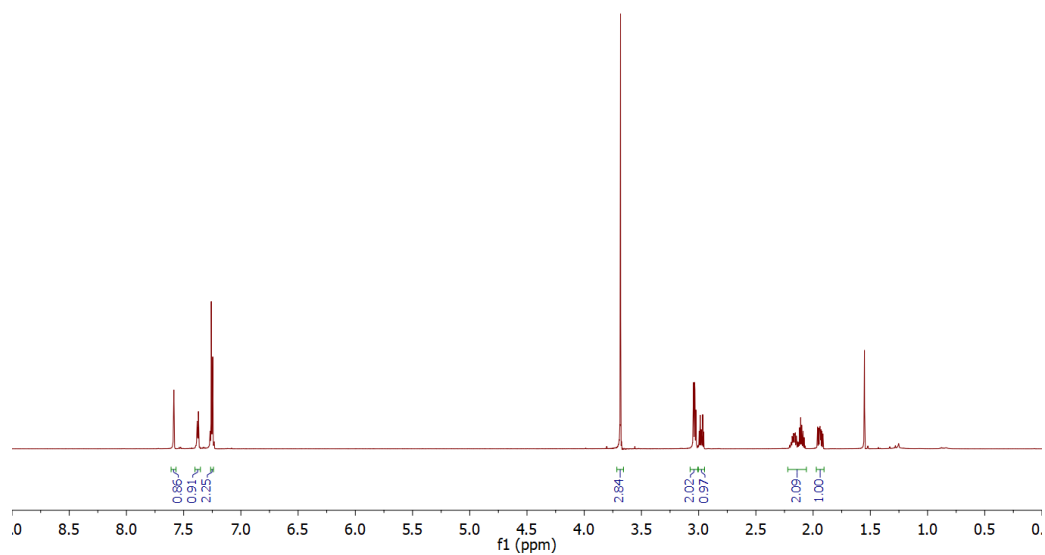
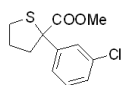


^{13}C NMR (151 MHz, Chloroform-*d*):

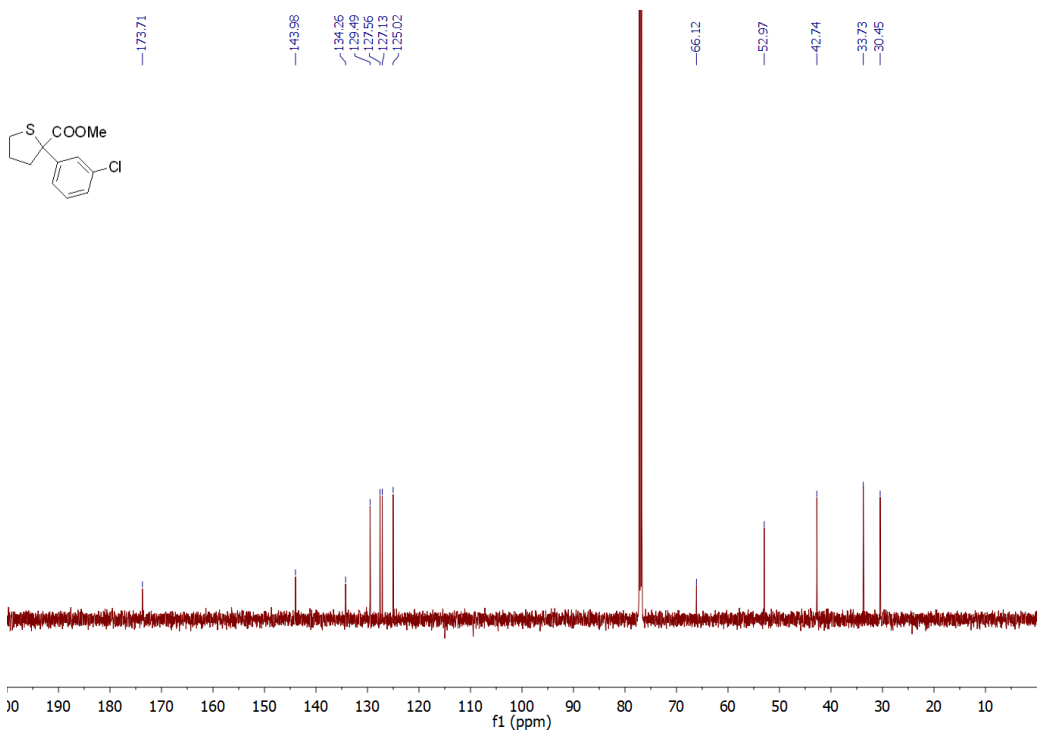


Methyl 2-(3-chlorophenyl)tetrahydrothiophene-2-carboxylate (8f)

^1H NMR (600 MHz, Chloroform-*d*):

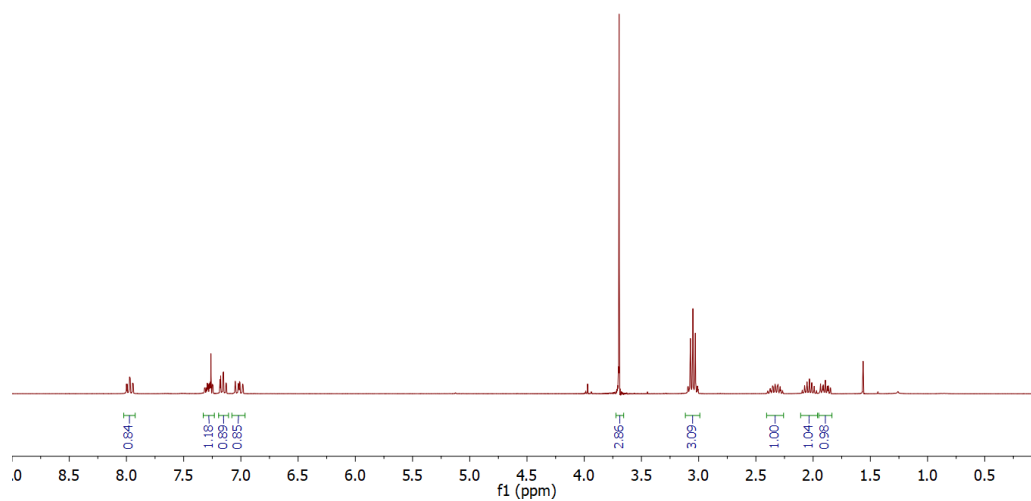
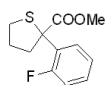


^{13}C NMR (151 MHz, Chloroform-*d*):

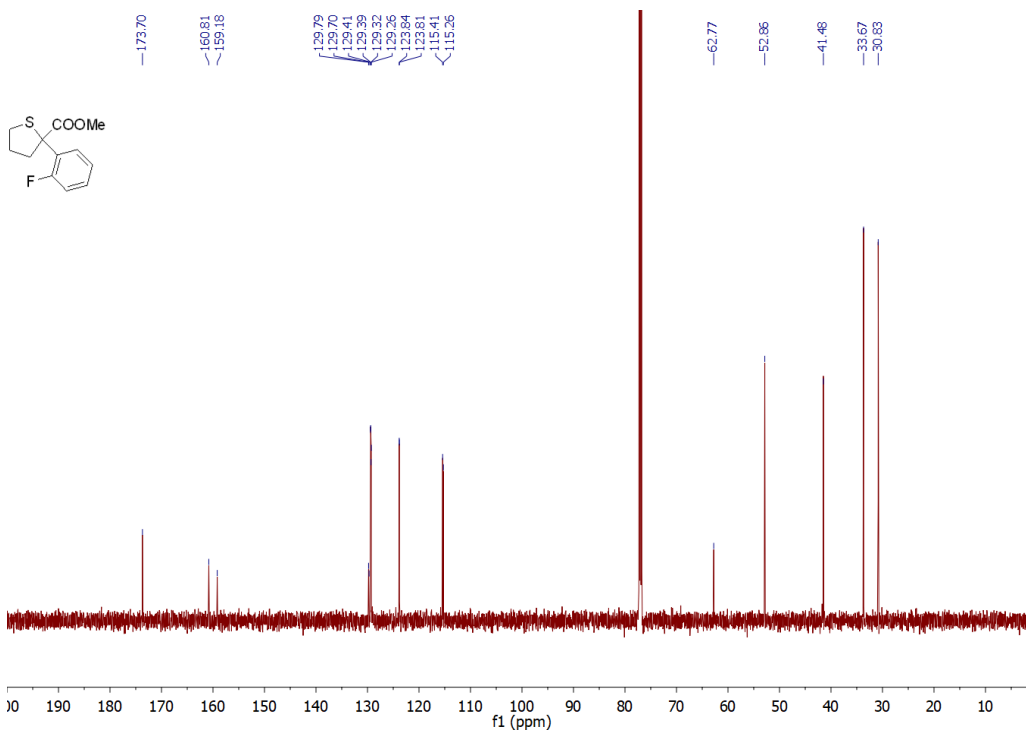


Methyl 2-(2-fluorophenyl)tetrahydrothiophene-2-carboxylate (8g)

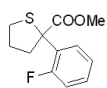
^1H NMR (300 MHz, Chloroform-*d*):



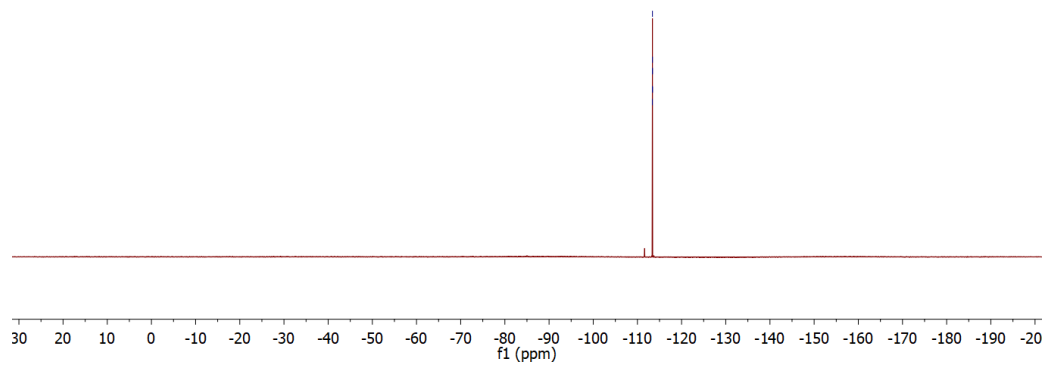
^{13}C NMR (151 MHz, Chloroform-*d*):



^{19}F NMR (564 MHz, Chloroform-*d*):

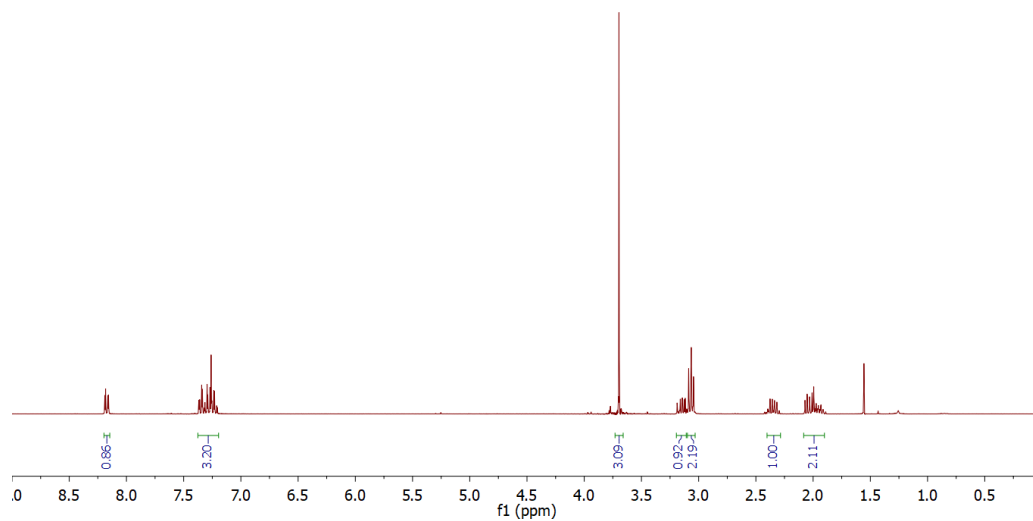
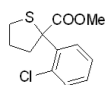


113.28
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113.42

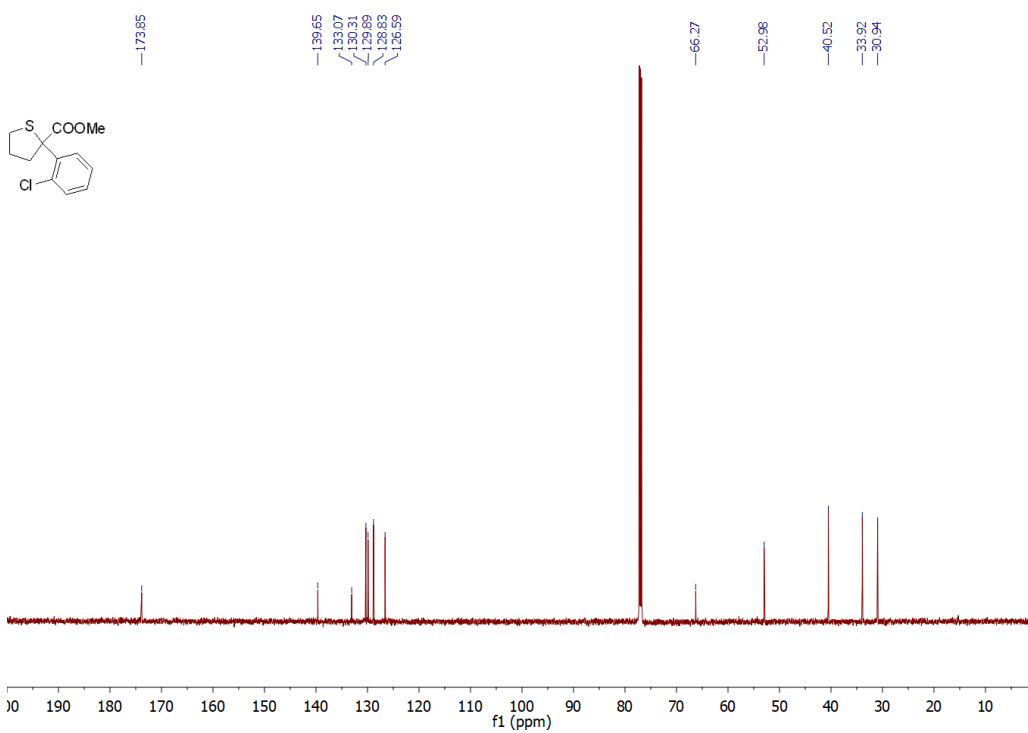


Methyl 2-(2-chlorophenyl)tetrahydrothiophene-2-carboxylate (8h)

¹H NMR (600 MHz, Chloroform-*d*):

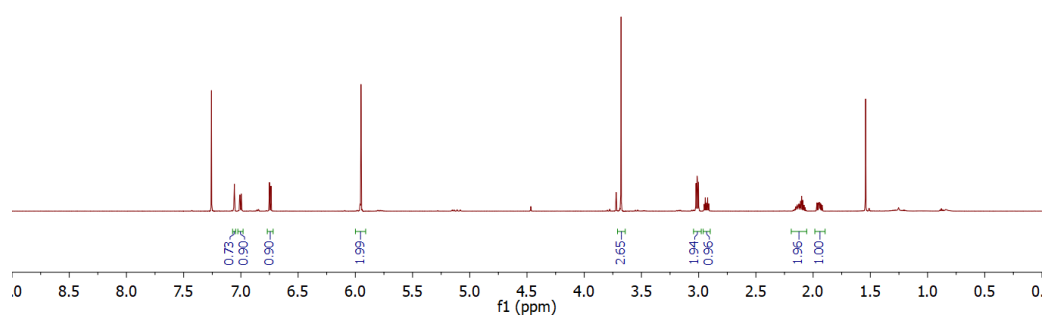
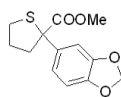


¹³C NMR (151 MHz, Chloroform-*d*):

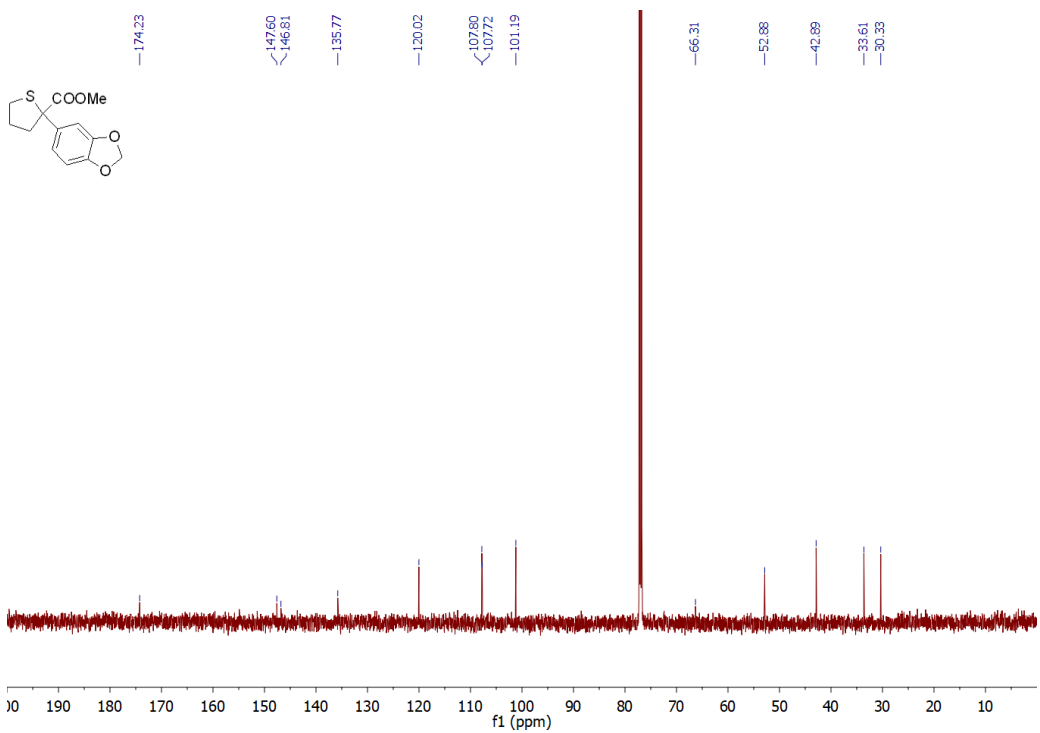


Methyl 2-(benzo[d][1,3]dioxol-5-yl)tetrahydrothiophene-2-carboxylate (8i)

^1H NMR (600 MHz, Chloroform-*d*):

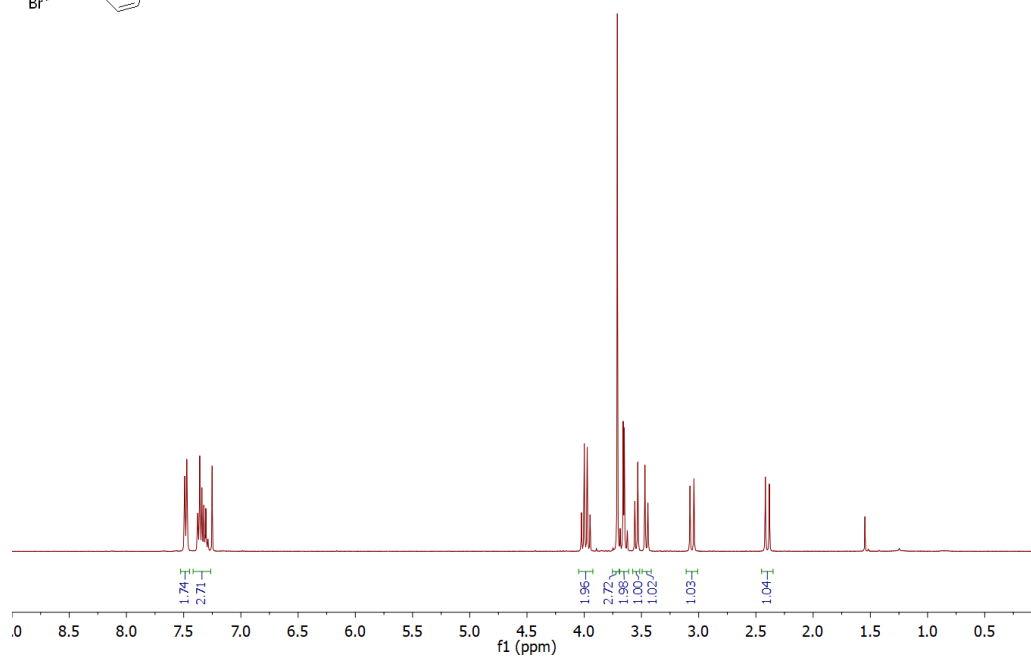
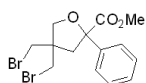


^{13}C NMR (151 MHz, Chloroform-*d*):

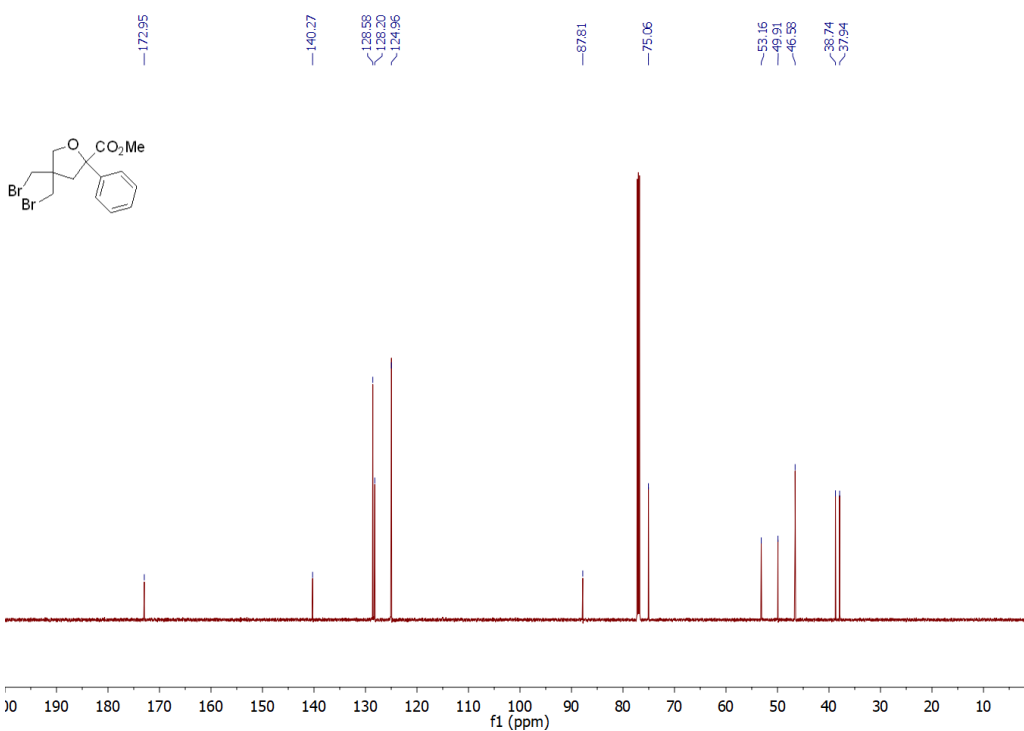


Methyl 4,4-bis(bromomethyl)-2-phenyltetrahydrofuran-2-carboxylate (9)

^1H NMR (400 MHz, Chloroform-*d*):

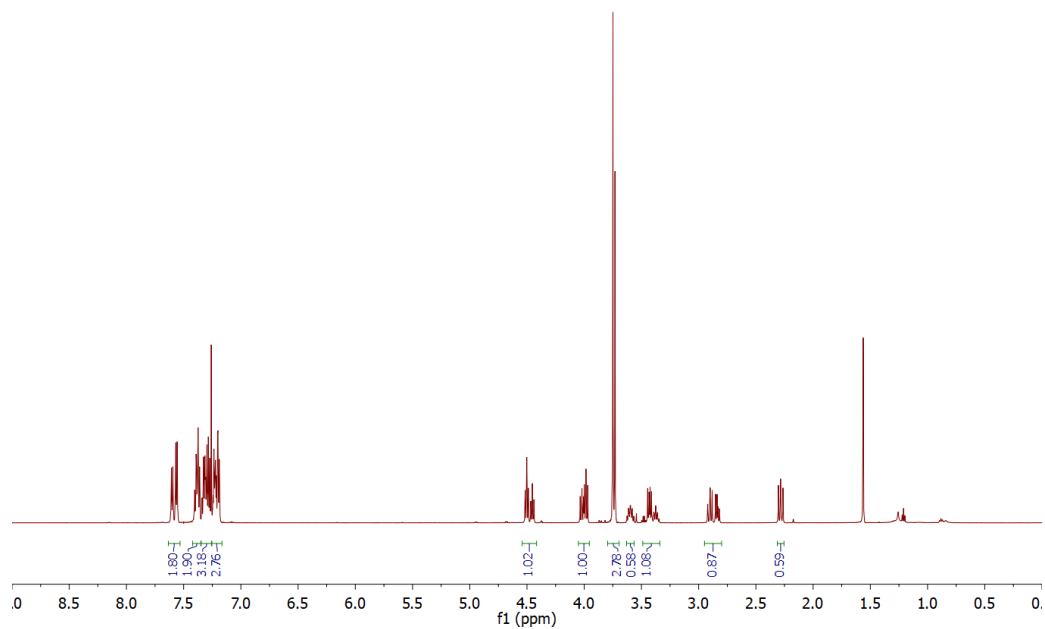
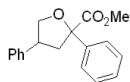


^{13}C NMR (151 MHz, Chloroform-*d*):

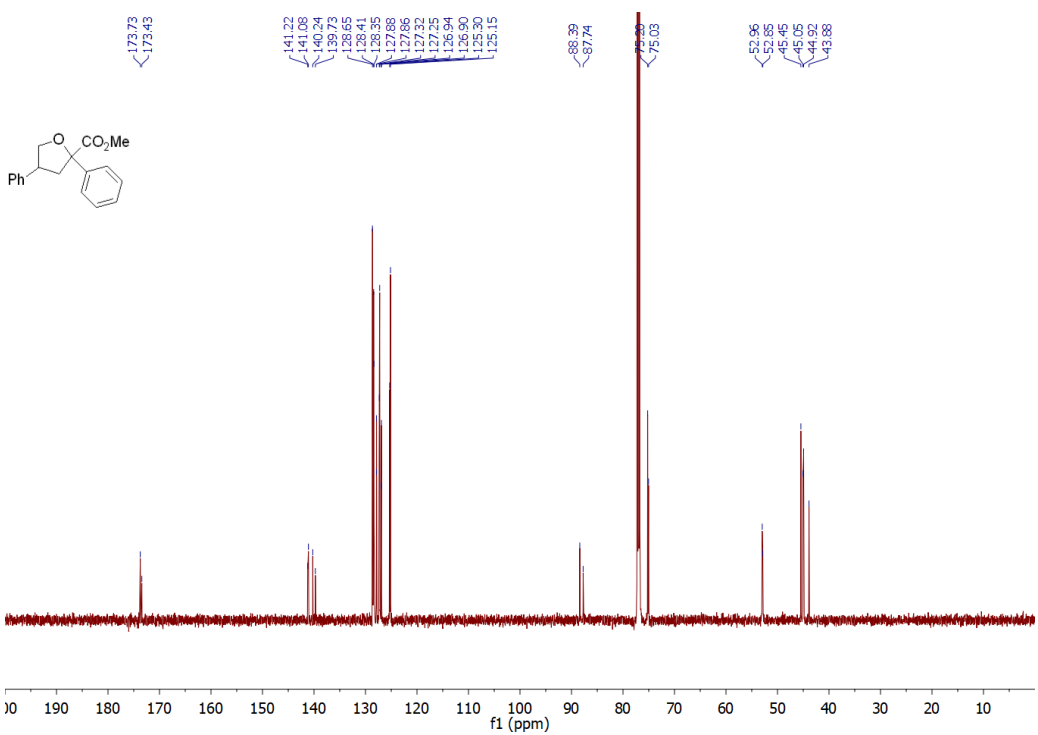


Methyl 2,4-diphenyltetrahydrofuran-2-carboxylate (10)

^1H NMR (600 MHz, Chloroform- d):

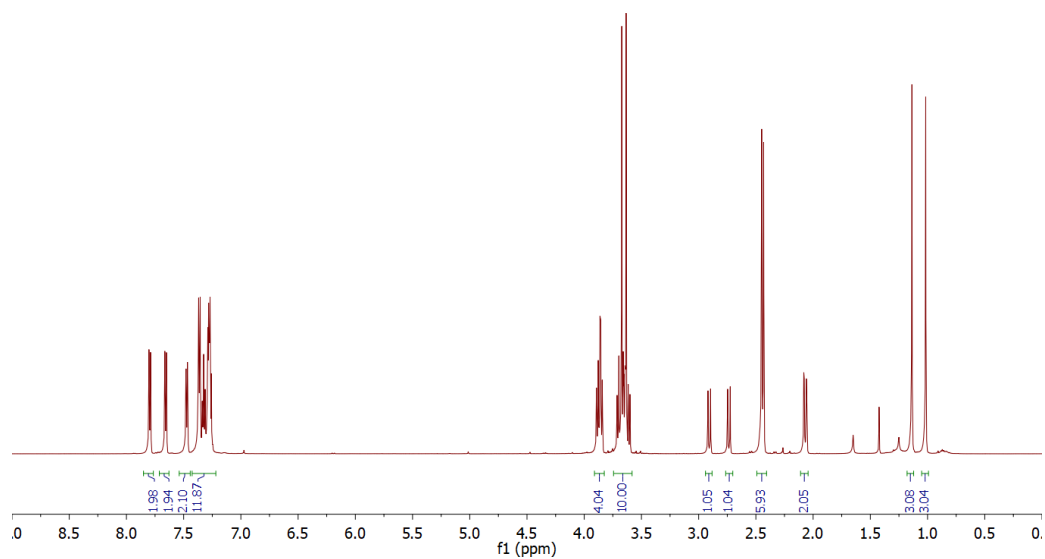
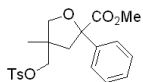


^{13}C NMR (151 MHz, Chloroform- d):

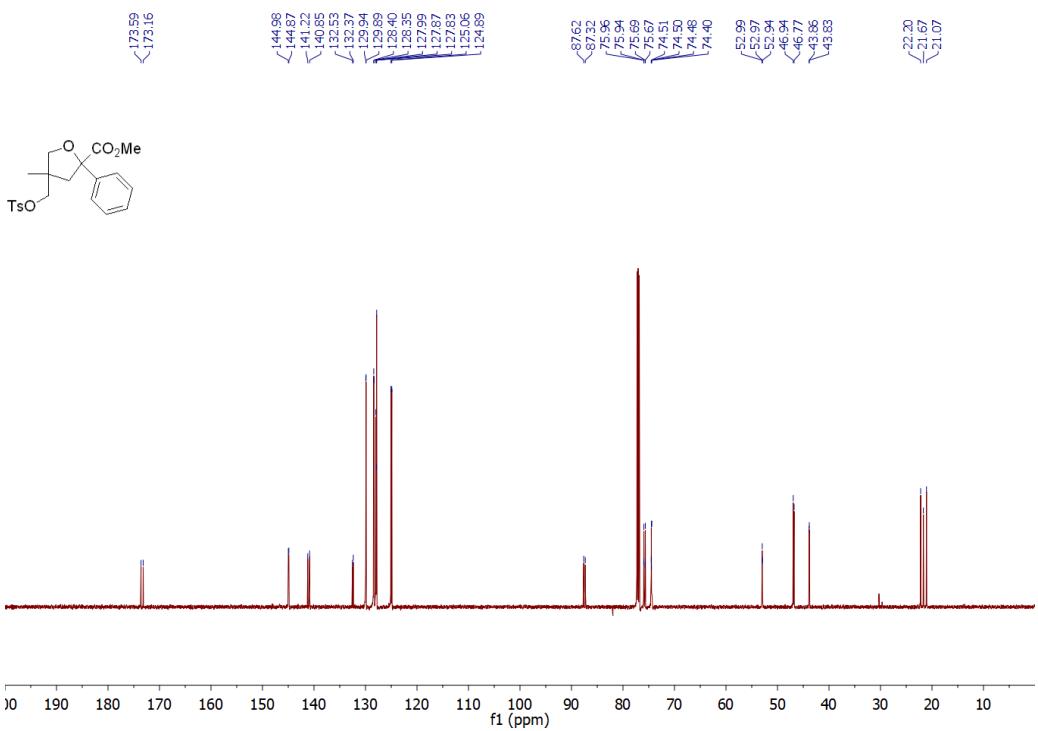


Methyl 4-methyl-2-phenyl-4-((tosyloxy)methyl)tetrahydrofuran-2-carboxylate (11)

¹H NMR (600 MHz, Chloroform-*d*):

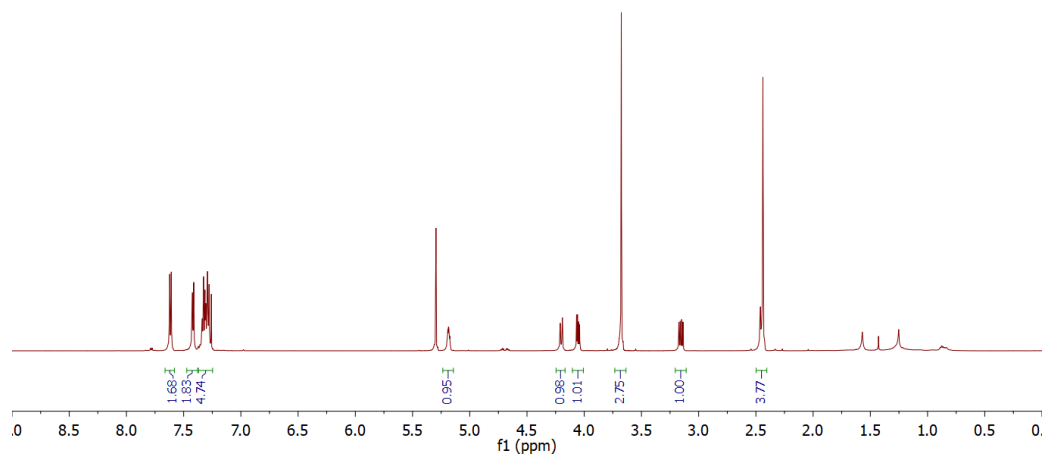
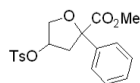


¹³C NMR (151 MHz, Chloroform-*d*):

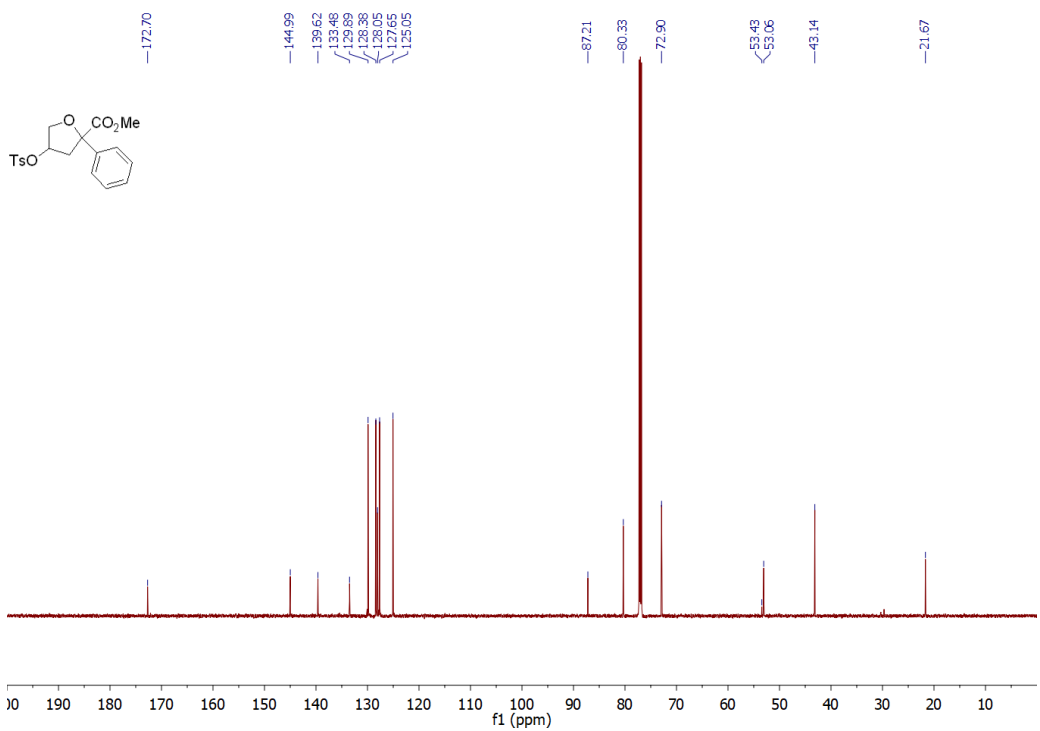


Methyl 2-phenyl-4-(tosyloxy)tetrahydrofuran-2-carboxylate (12)

^1H NMR (600 MHz, Chloroform-*d*):

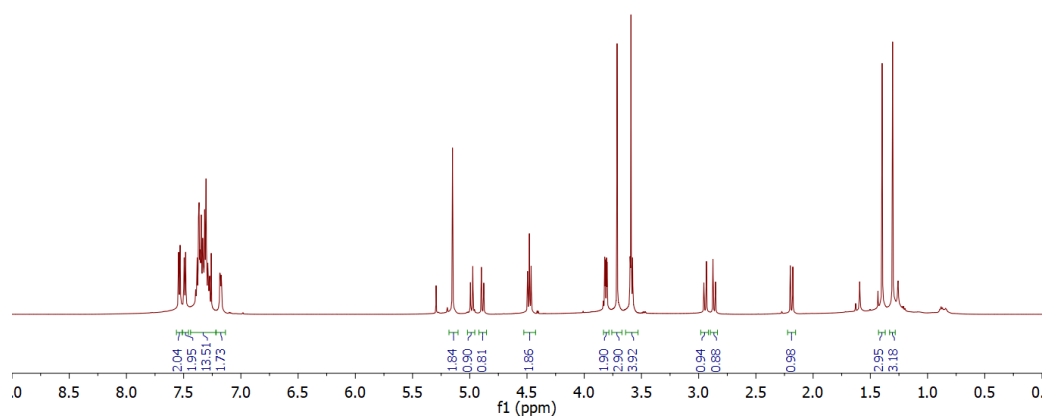
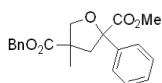


^{13}C NMR (151 MHz, Chloroform-*d*):



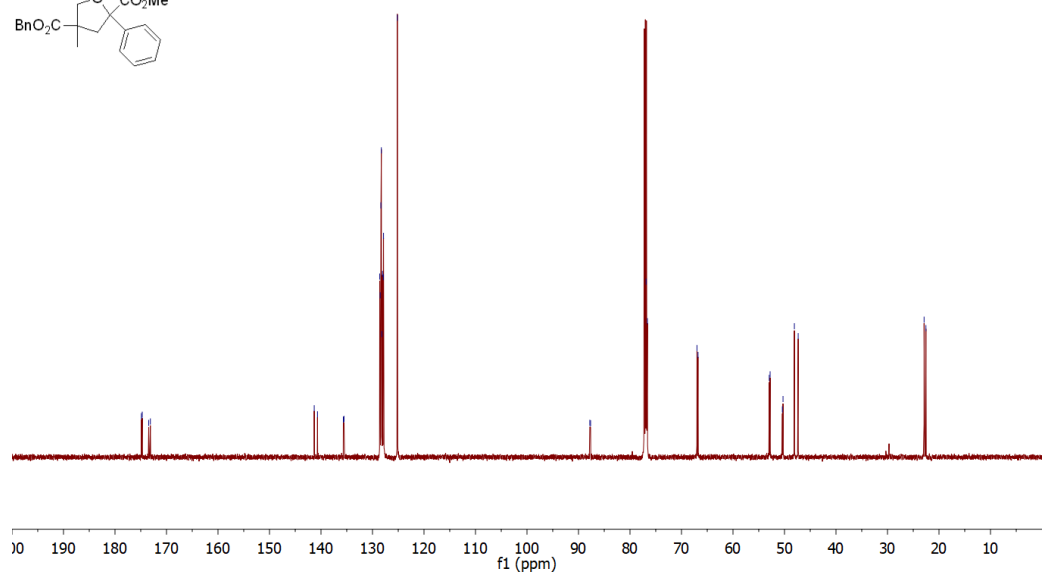
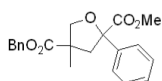
4-benzyl 2-methyl 4-methyl-2-phenyltetrahydrofuran-2,4-dicarboxylate (13)

^1H NMR (600 MHz, Chloroform- d):



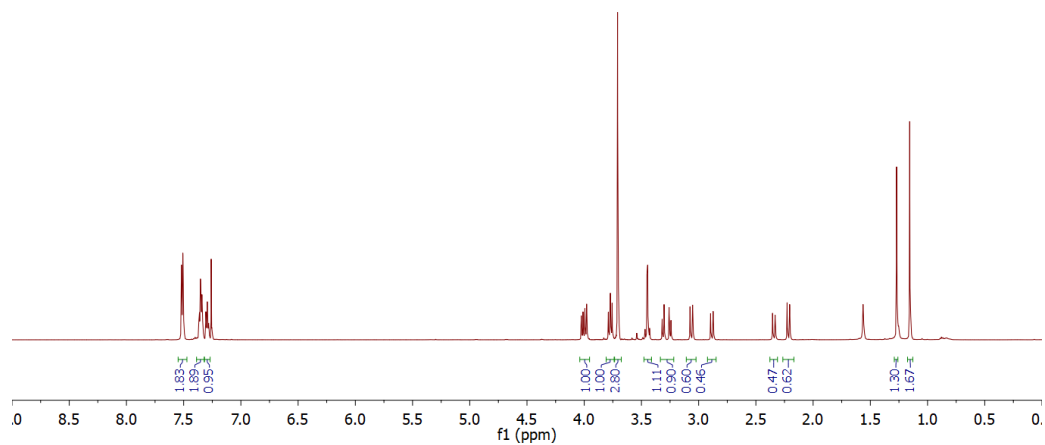
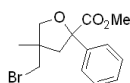
^{13}C NMR (151 MHz, Chloroform- d):

174.88, 174.71, 173.45, 173.13, 141.31, 136.28, 135.66, 135.53, 135.53, 128.59, 128.51, 128.36, 128.28, 128.19, 128.06, 127.89, 127.86, 125.17, 87.80, 87.65, 76.87, 76.61, 66.79, 52.96, 52.79, 50.41, 50.29, 48.08, 47.34, 22.89, 22.54

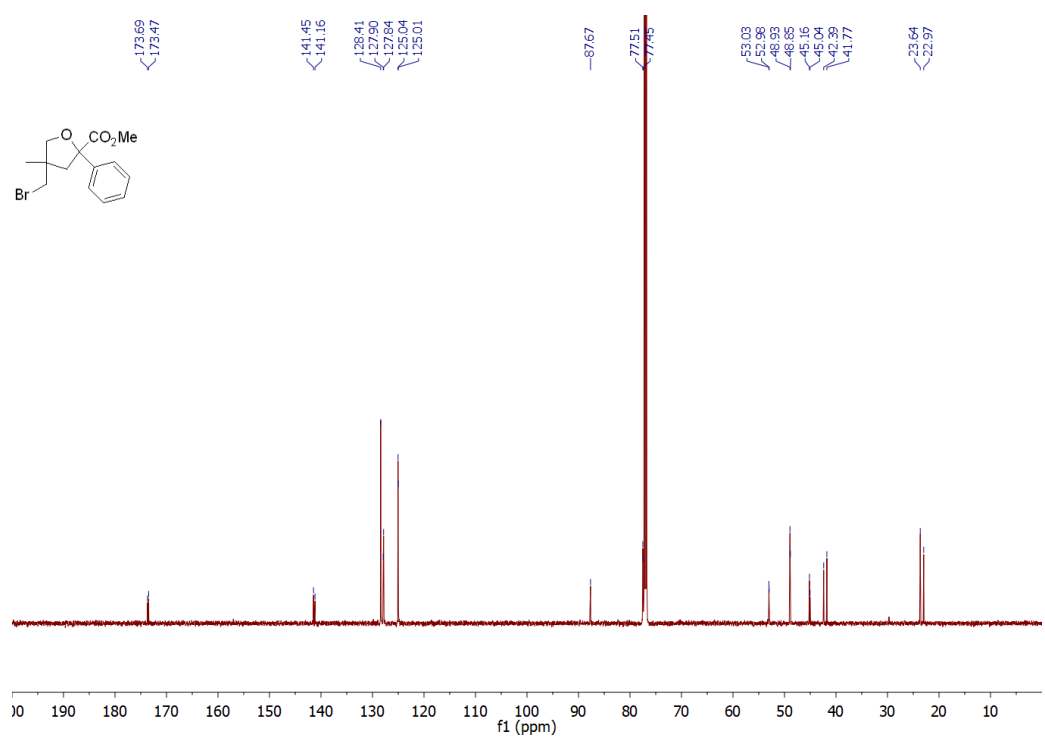
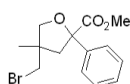


Methyl 4-(bromomethyl)-4-methyl-2-phenyltetrahydrofuran-2-carboxylate (14)

^1H NMR (600 MHz, Chloroform-*d*):

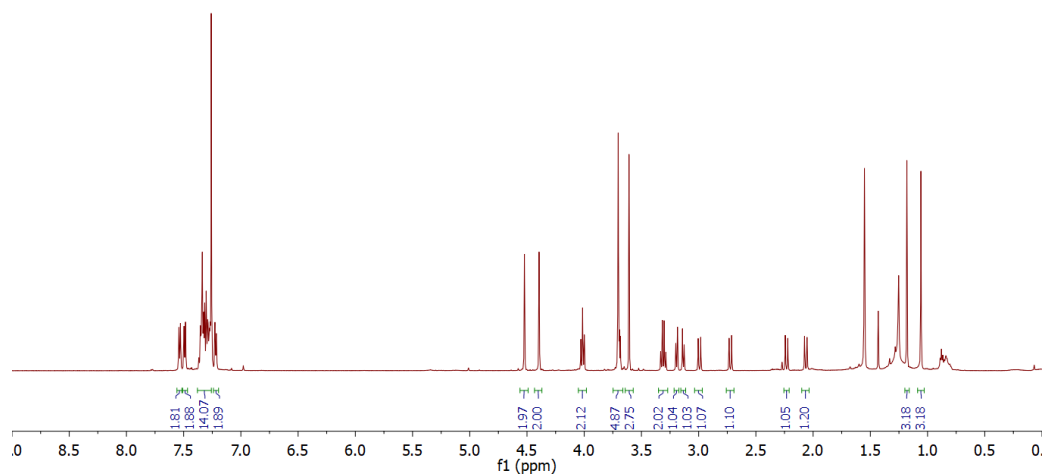
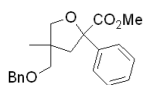


^{13}C NMR (151 MHz, CDCl_3):

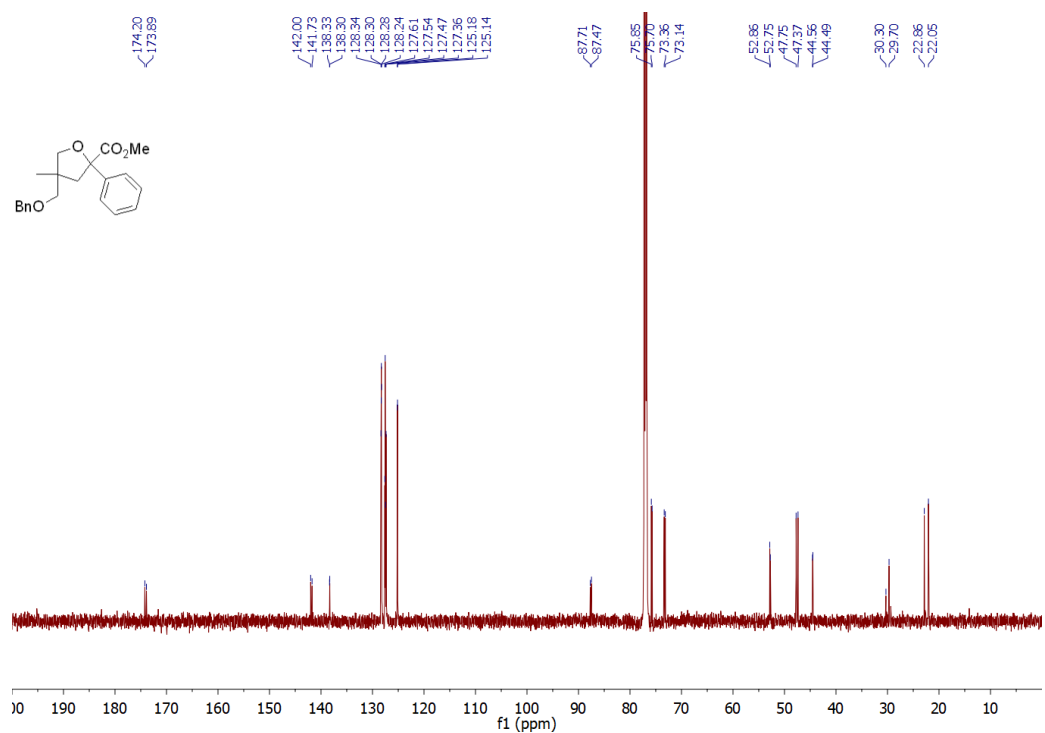
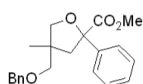


Methyl 4-((benzyloxy)methyl)-4-methyl-2-phenyltetrahydrofuran-2-carboxylate (15)

^1H NMR (600 MHz, Chloroform-*d*):

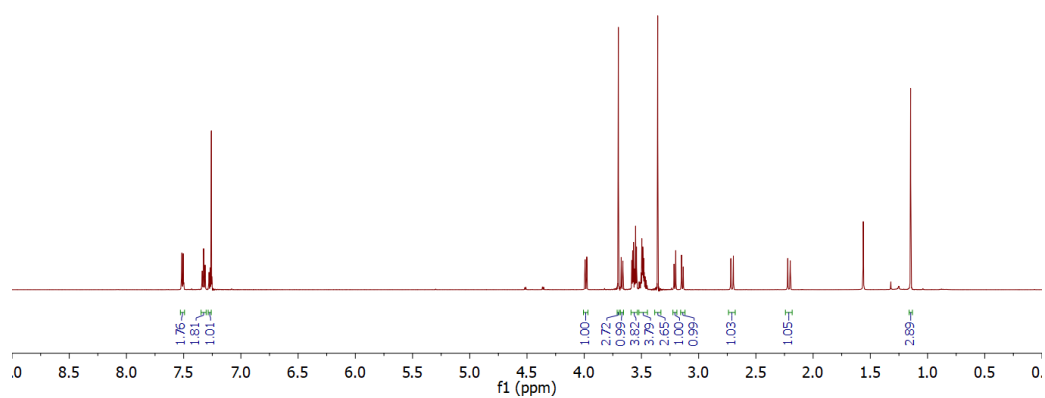
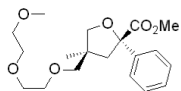


^{13}C NMR (151 MHz, Chloroform-*d*):

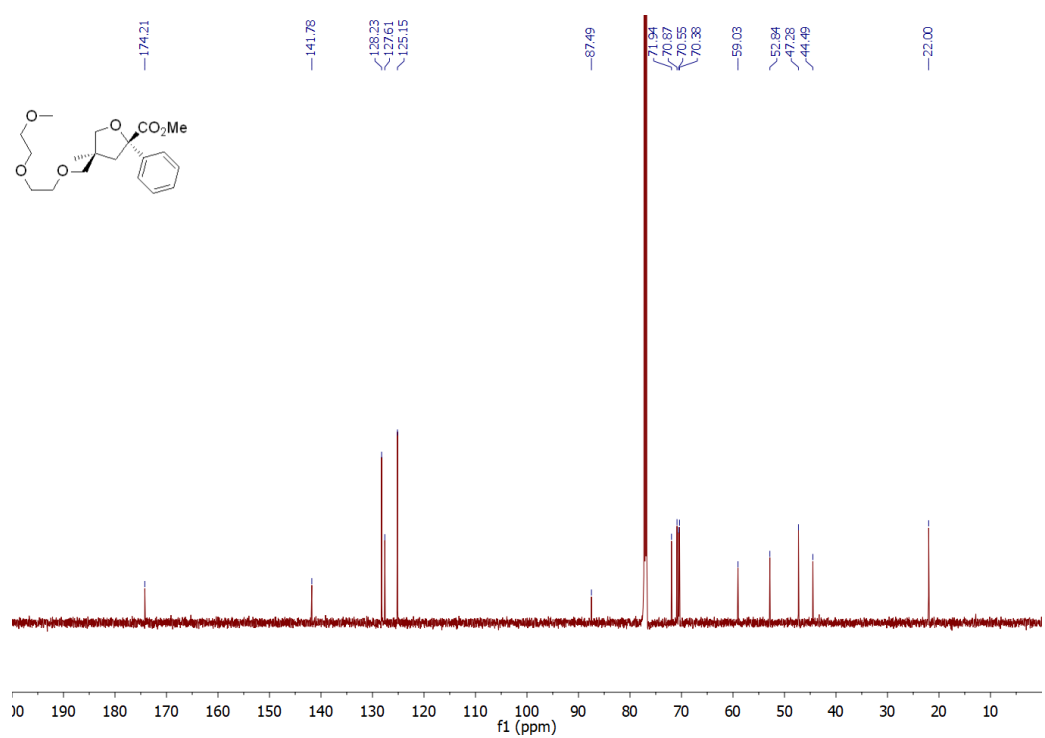
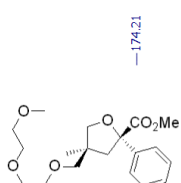


Methyl 4-((2-(2-methoxyethoxy)ethoxy)methyl)-4-methyl-2-phenyltetrahydrofuran-2-carboxylate (16)

¹H NMR (300 MHz, Chloroform-*d*):

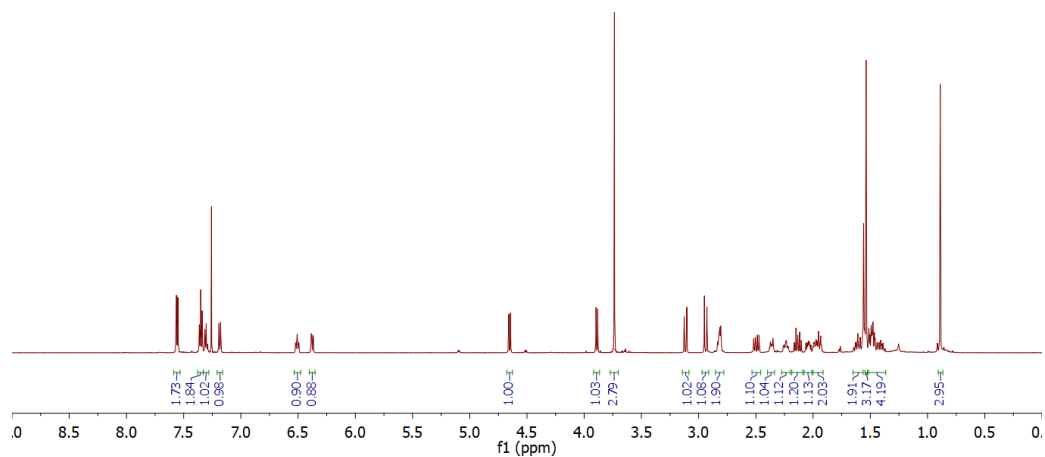
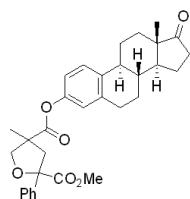


¹³C NMR (151 MHz, Chloroform-*d*):

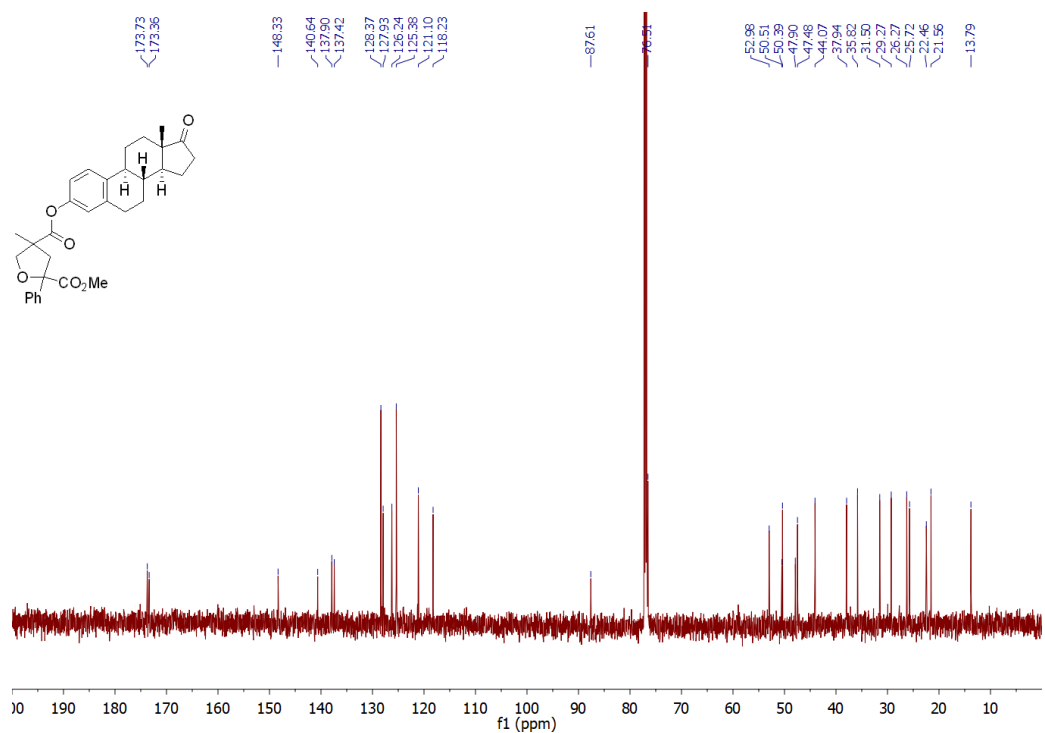
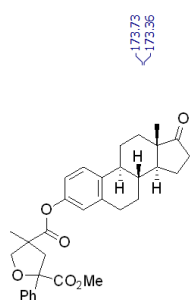


2S,4S)-2-methyl 4-((8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cycl penta[a]phenanthren-3-yl) 4-methyl-2-phenyltetrahydrofuran-2,4-dicarboxylate (17)

¹H NMR (600 MHz, Chloroform-d):

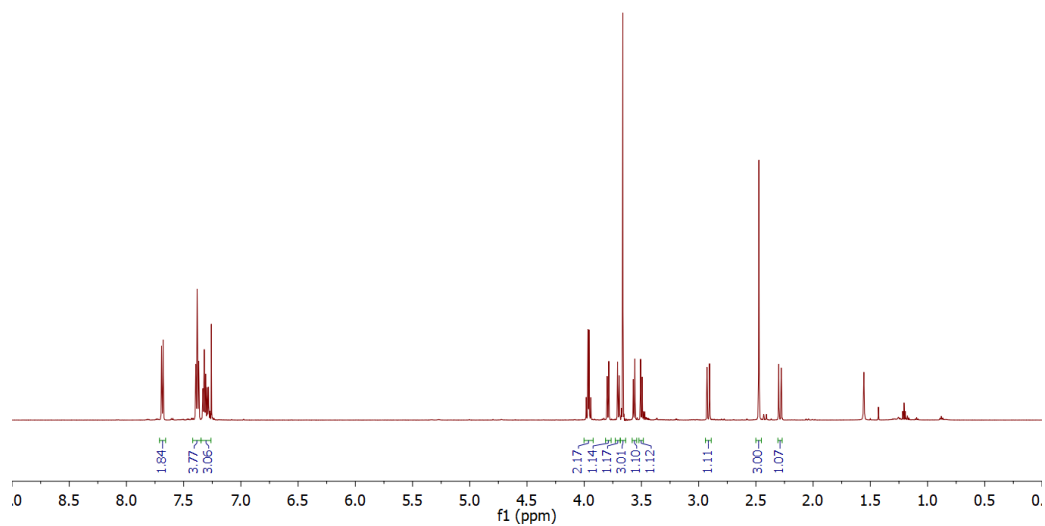
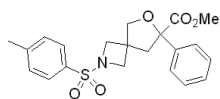


¹³C NMR (151 MHz, Chloroform-d):

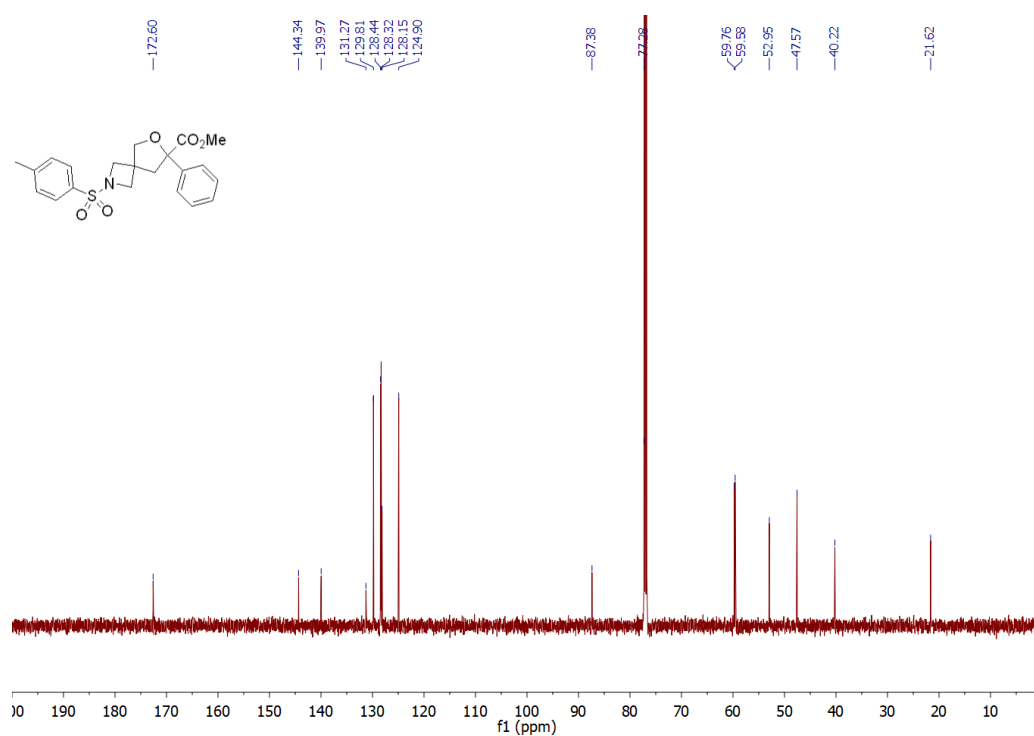
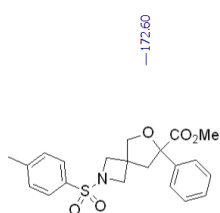


Methyl 7-phenyl-2-tosyl-6-oxa-2-azaspiro[3.4]octane-7-carboxylate (18)

^1H NMR (300 MHz, Chloroform- d):

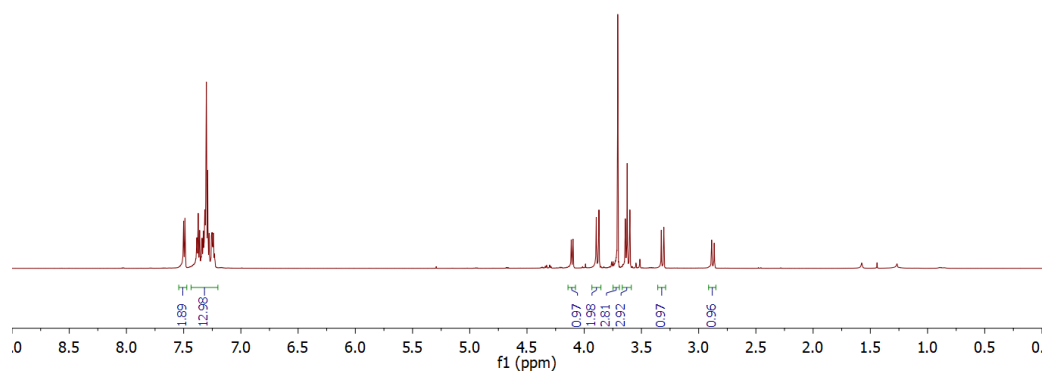
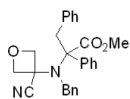


^{13}C NMR (151 MHz, Chloroform- d):

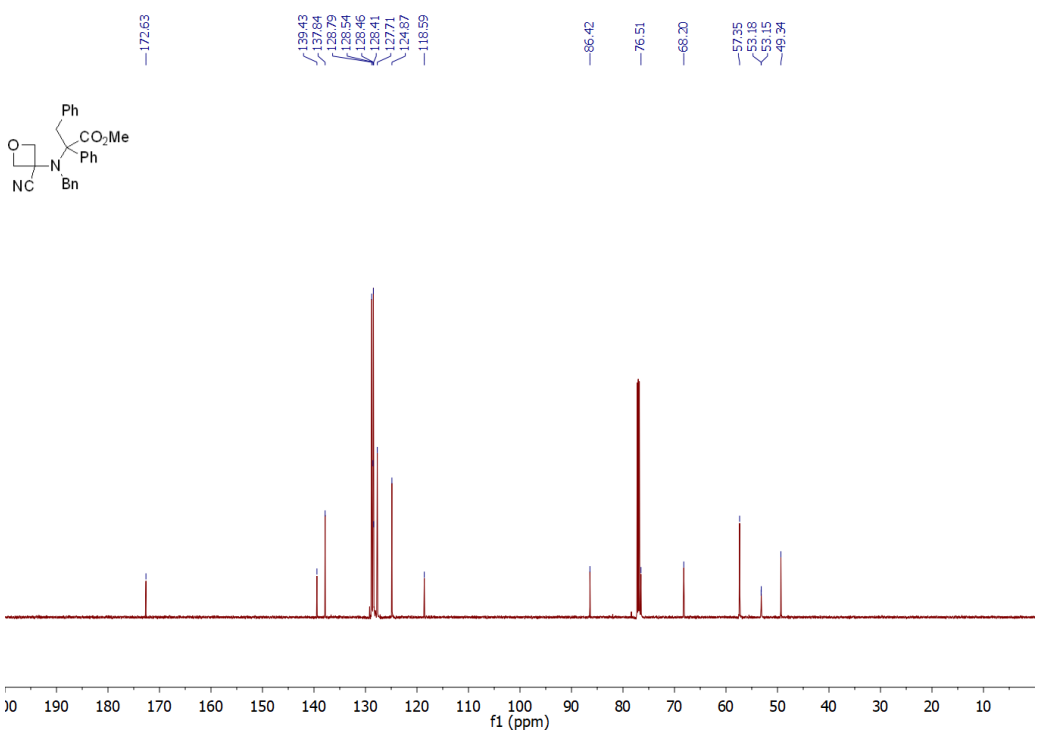


Methyl 2-(benzyl(3-cyanooxetan-3-yl)amino)-2,3-diphenylpropanoate (21)

^1H NMR (600 MHz, Chloroform-*d*):

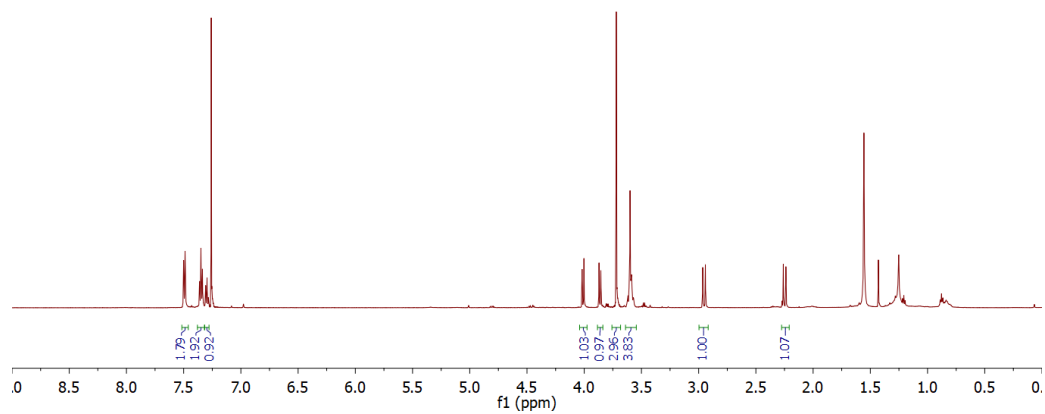
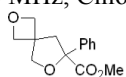


^{13}C NMR (151 MHz, Chloroform-*d*):

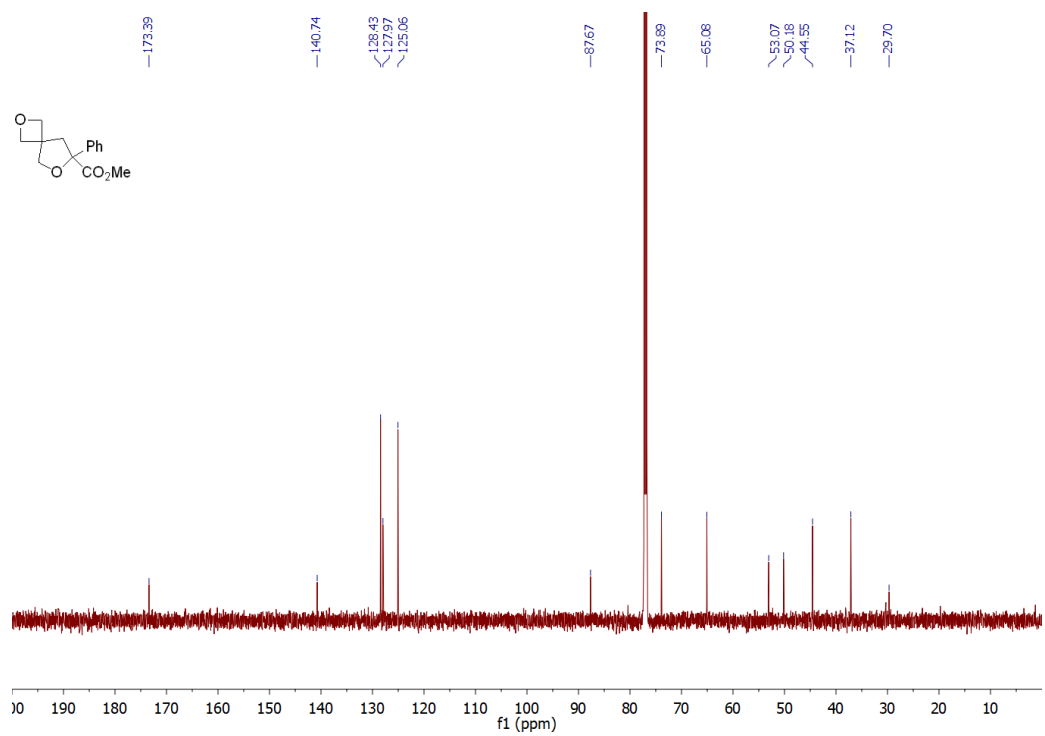
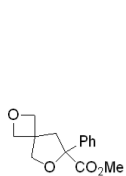


Methyl 7-phenyl-2,6-dioxaspiro[3.4]octane-7-carboxylate (24)

^1H NMR (600 MHz, Chloroform-*d*):

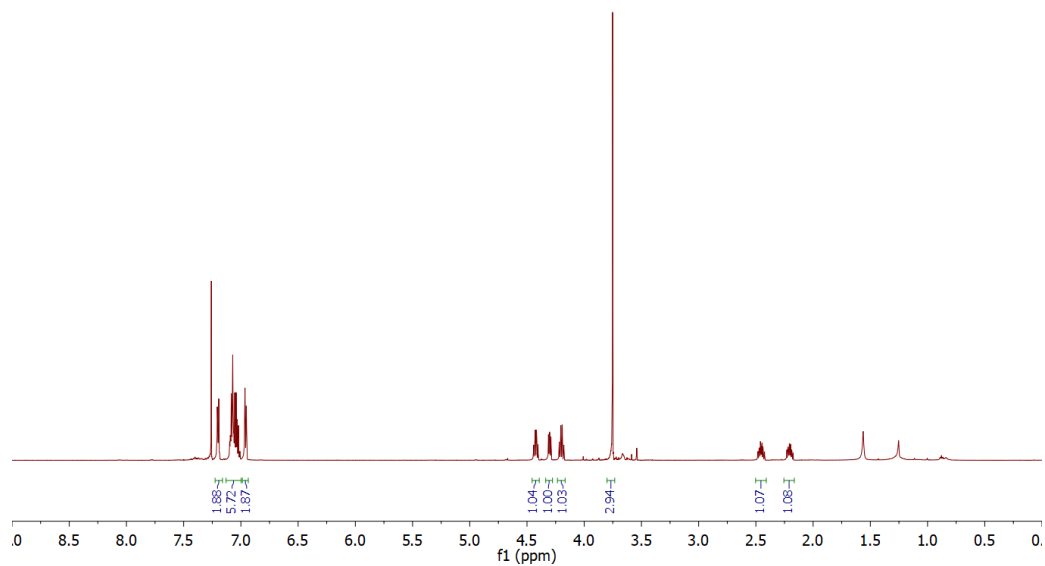
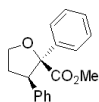


^{13}C NMR (151 MHz, Chloroform-*d*):

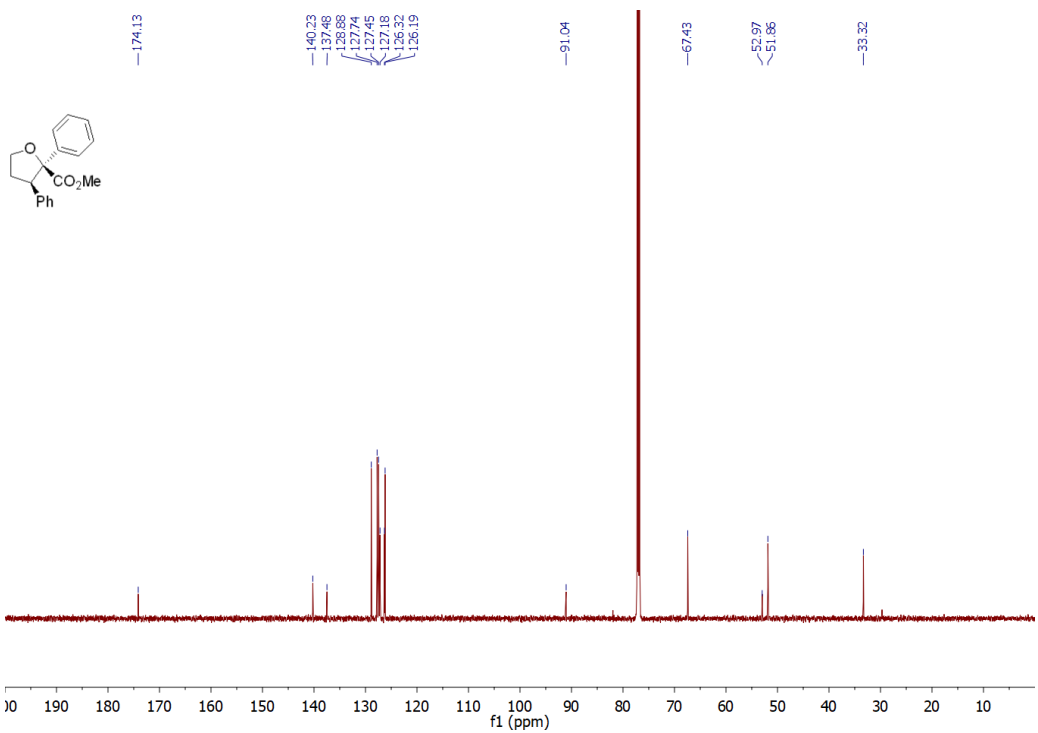


cis-methyl 2,3-diphenyltetrahydrofuran-2-carboxylate (25a)

^1H NMR (600 MHz, Chloroform-*d*):

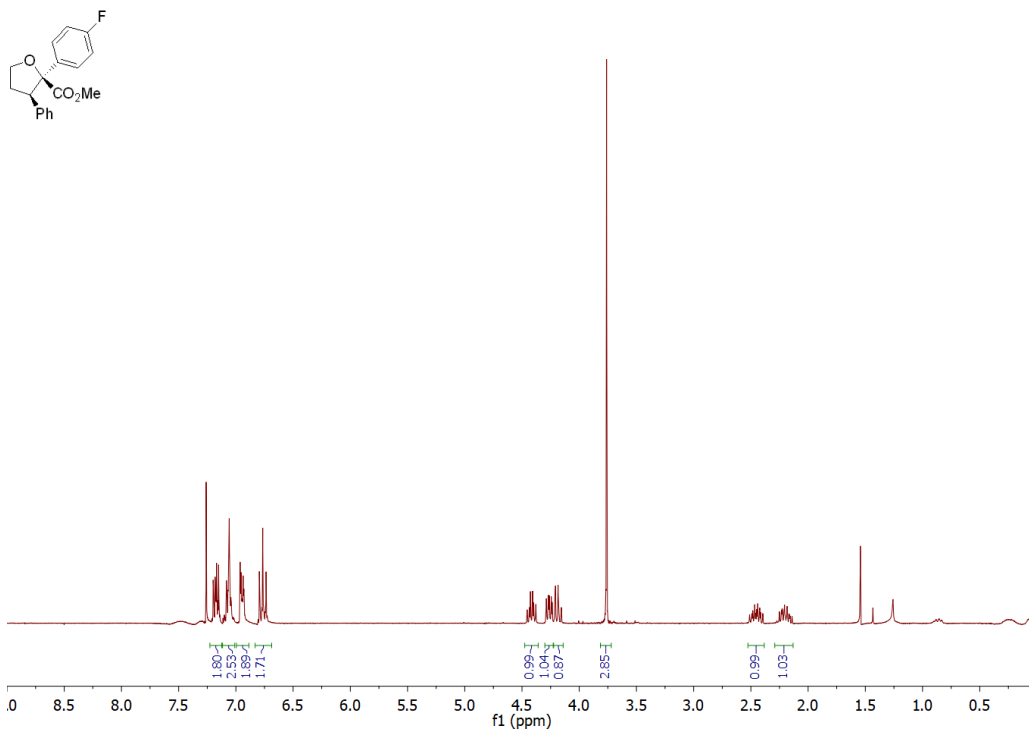


^{13}C NMR (151 MHz, CDCl_3):

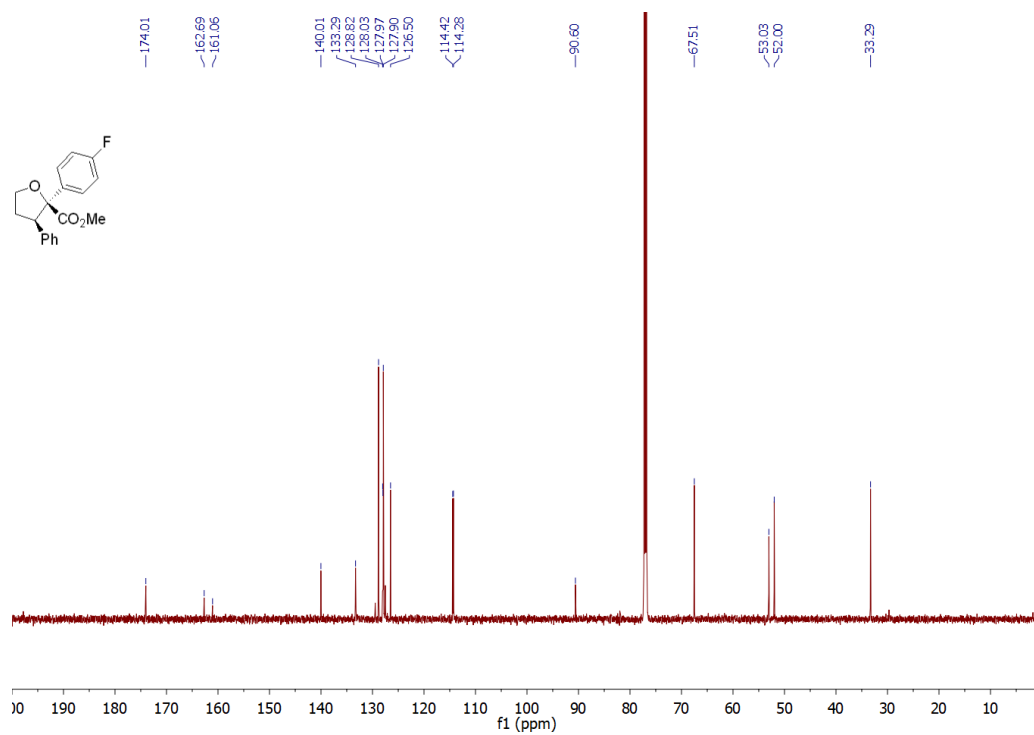


***cis*-methyl 2-(4-fluorophenyl)-3-phenyltetrahydrofuran-2-carboxylate (25b)**

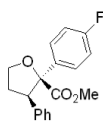
¹H NMR (300 MHz, Chloroform-*d*):



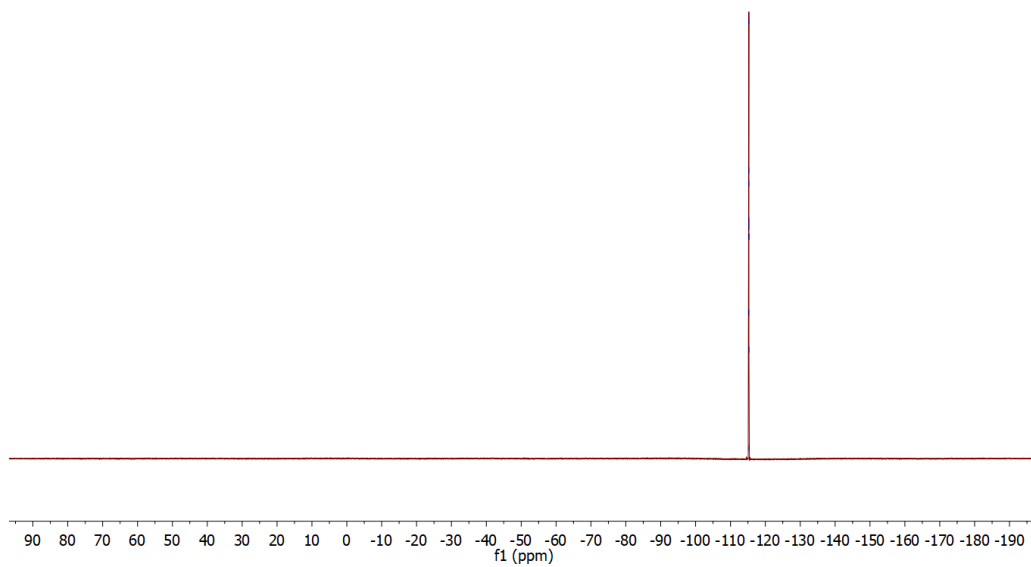
¹³C NMR (151 MHz, Chloroform-*d*):



^{19}F NMR (564 MHz, Chloroform-*d*):

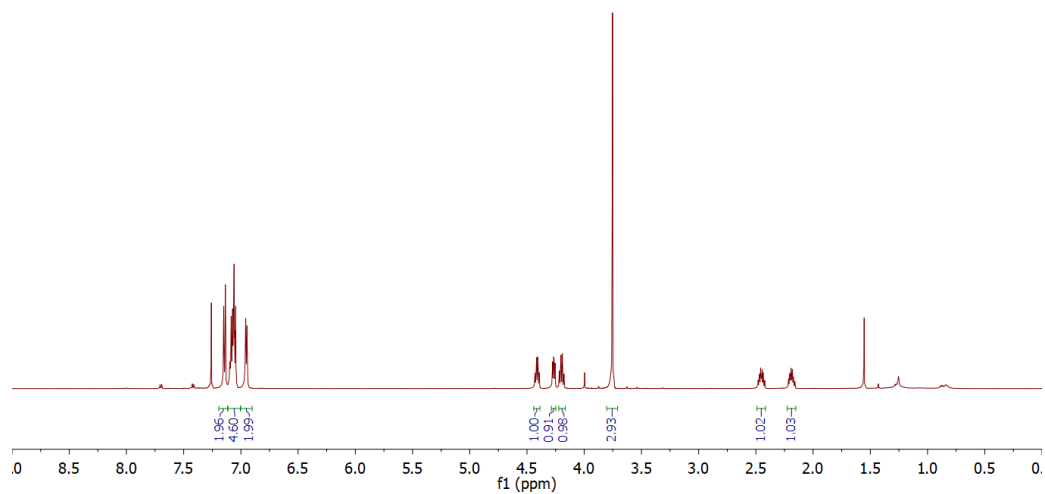
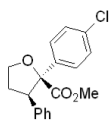


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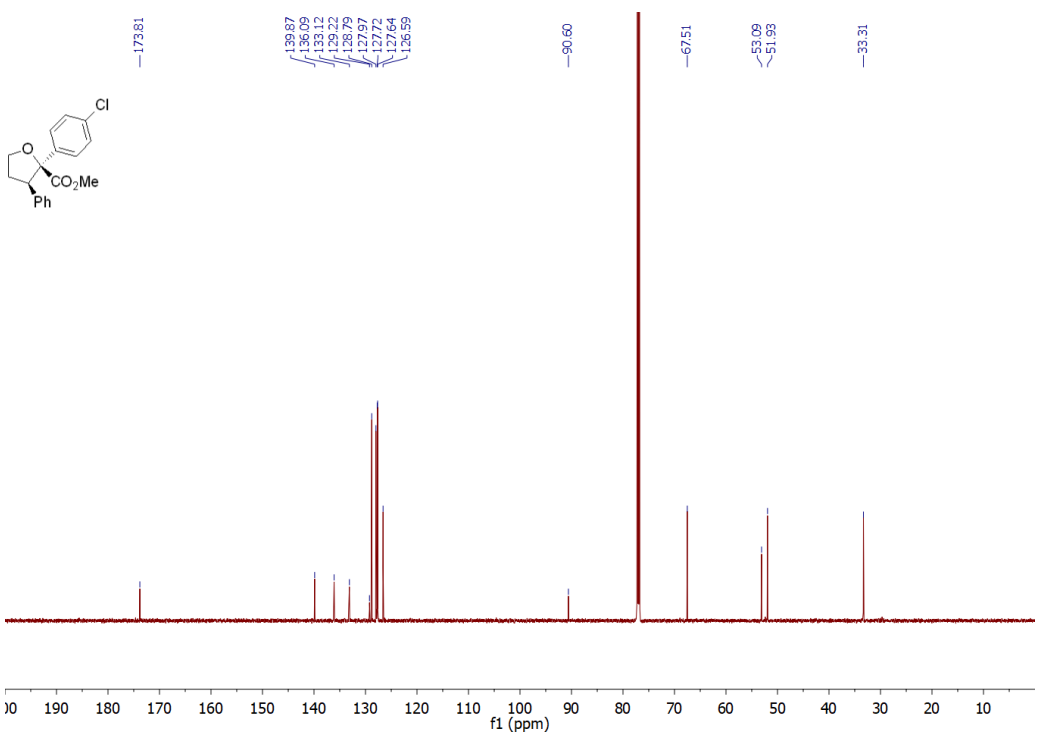


***cis*-methyl 2-(4-chlorophenyl)-3-phenyltetrahydrofuran-2-carboxylate (25c)**

¹H NMR (600 MHz, Chloroform-*d*):

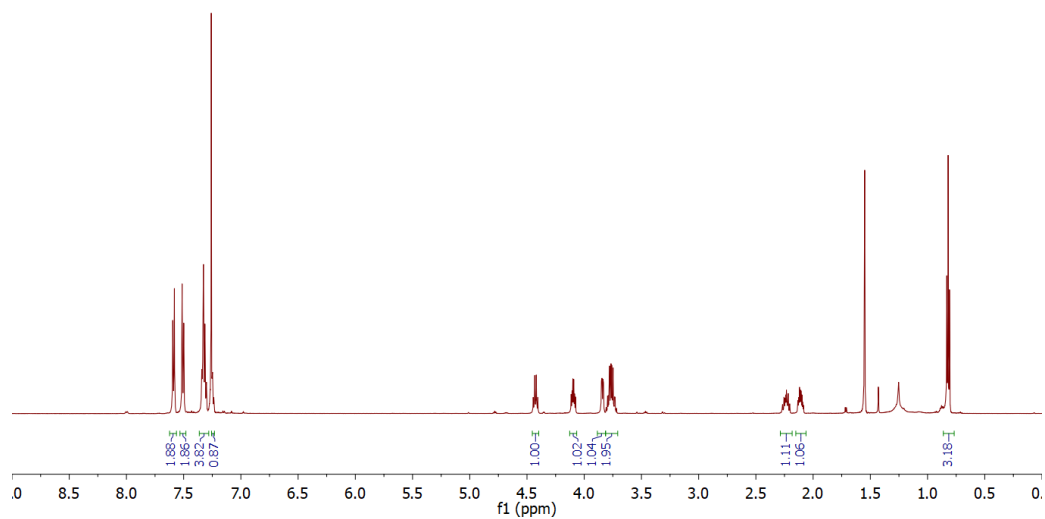
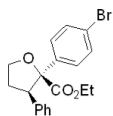


¹³C NMR (151 MHz, CDCl₃):

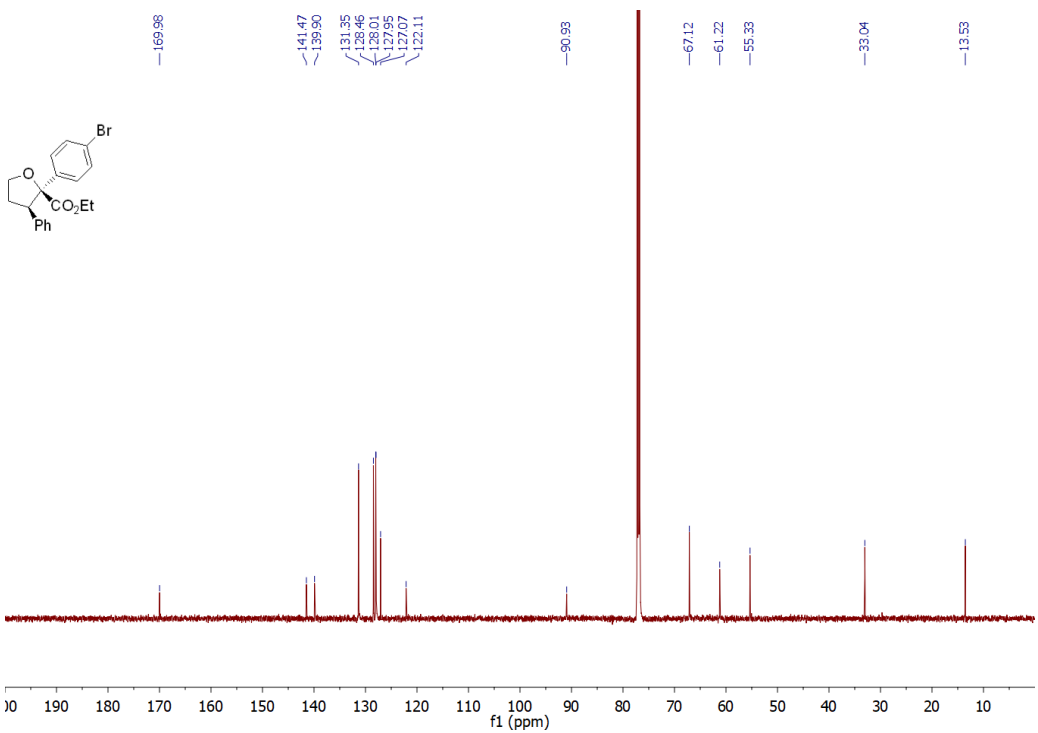


***cis*-ethyl 2-(4-bromophenyl)-3-phenyltetrahydrofuran-2-carboxylate (25d)**

¹H NMR (600 MHz, Chloroform-*d*):

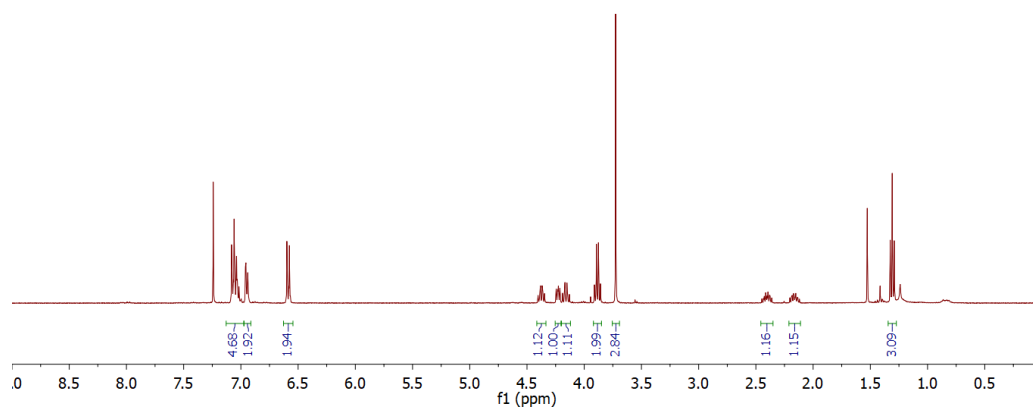
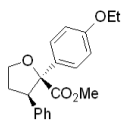


¹³C NMR (151 MHz, Chloroform-*d*):

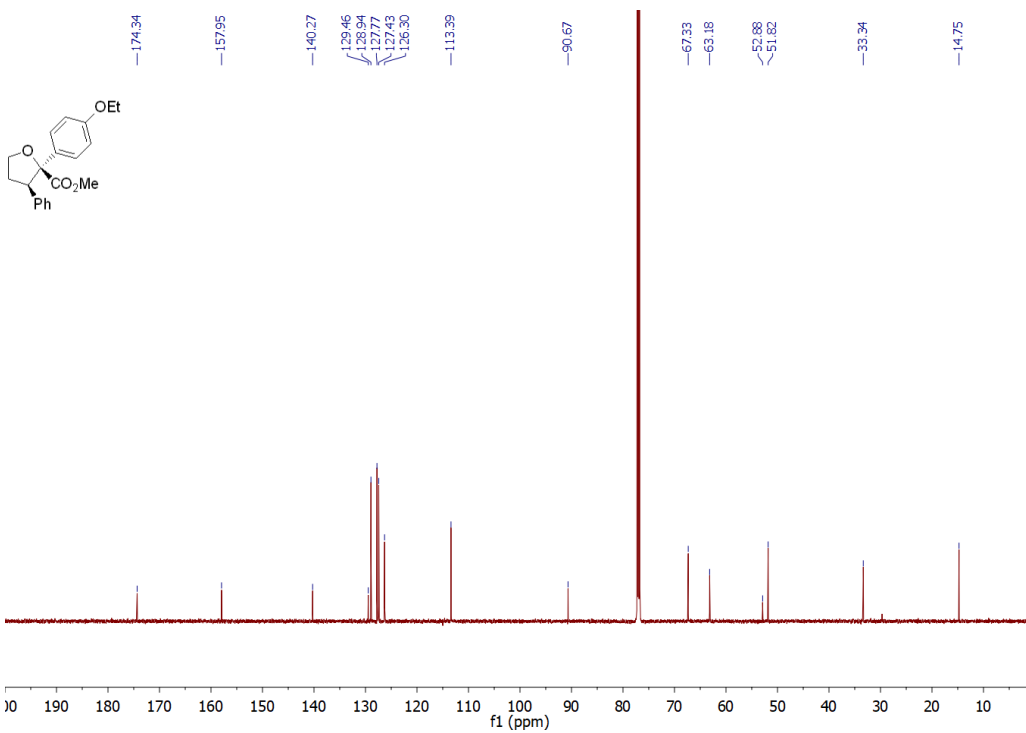


***cis*-methyl 2-(4-ethoxyphenyl)-3-phenyltetrahydrofuran-2-carboxylate (25e)**

¹H NMR (400 MHz, Chloroform-*d*):

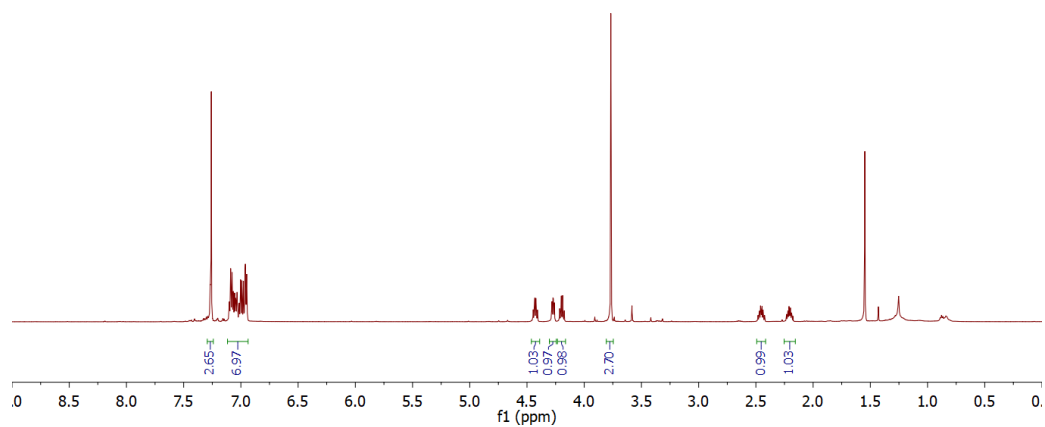
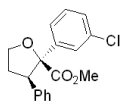


¹³C NMR (151 MHz, Chloroform-*d*):

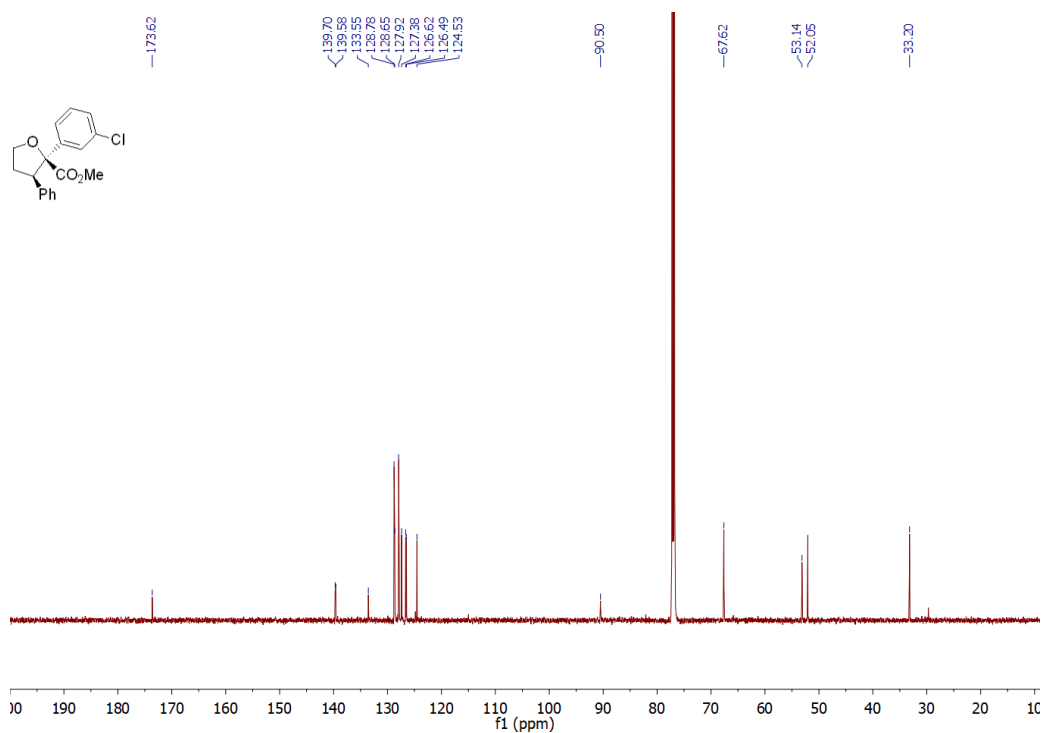


***cis*-methyl 2-(3-chlorophenyl)-3-phenyltetrahydrofuran-2-carboxylate (25e)**

¹H NMR (600 MHz, Chloroform-*d*):

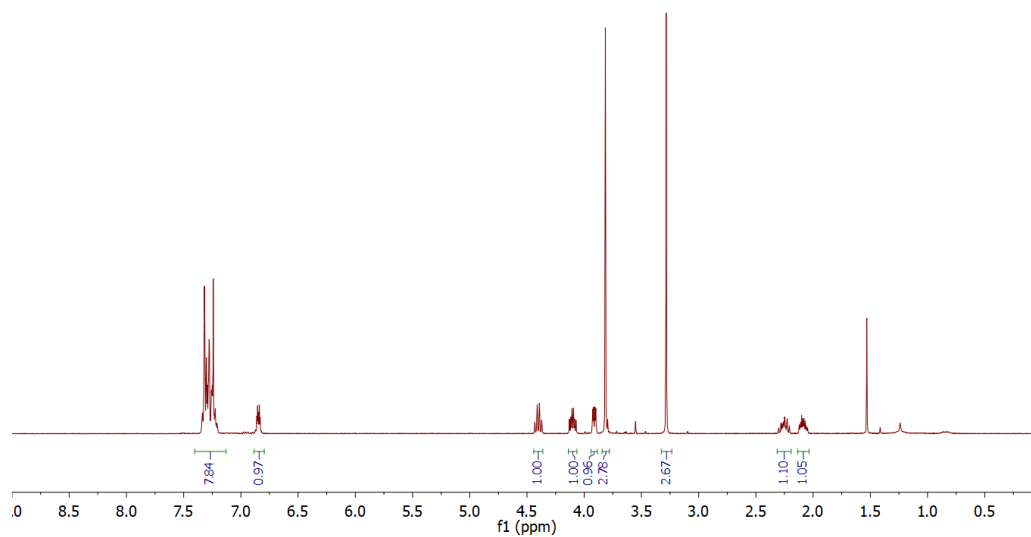
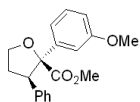


¹³C NMR (151 MHz, , Chloroform-*d*):

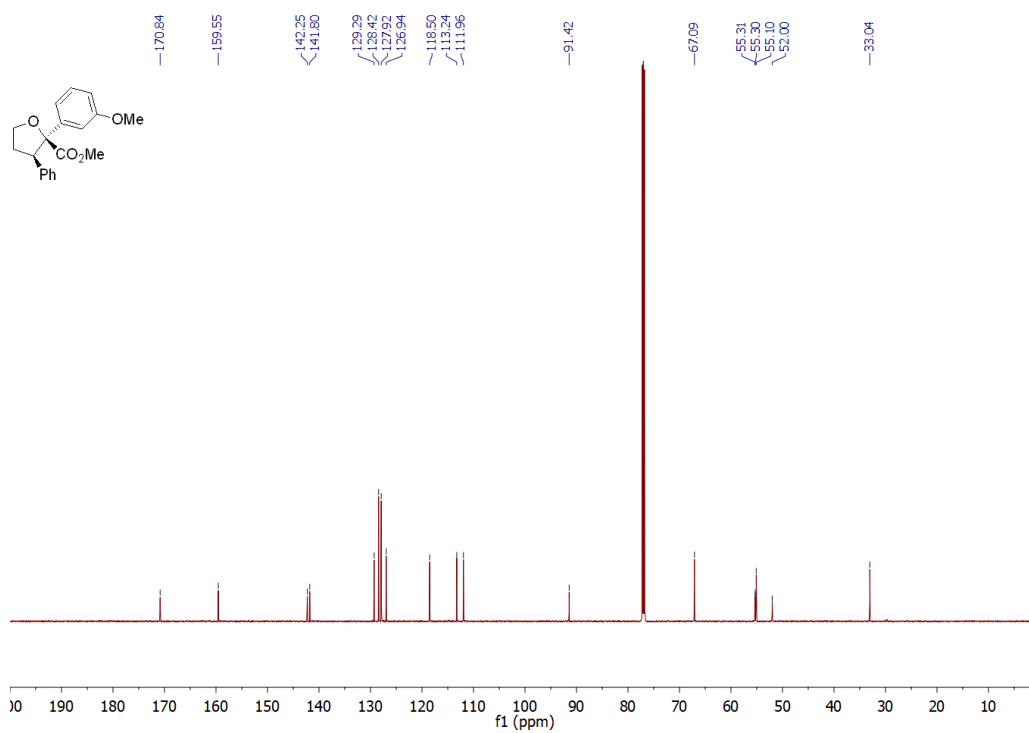


***cis*-methyl 2-(3-methoxyphenyl)-3-phenyltetrahydrofuran-2-carboxylate (25f)**

¹H NMR (400 MHz, Chloroform-*d*):

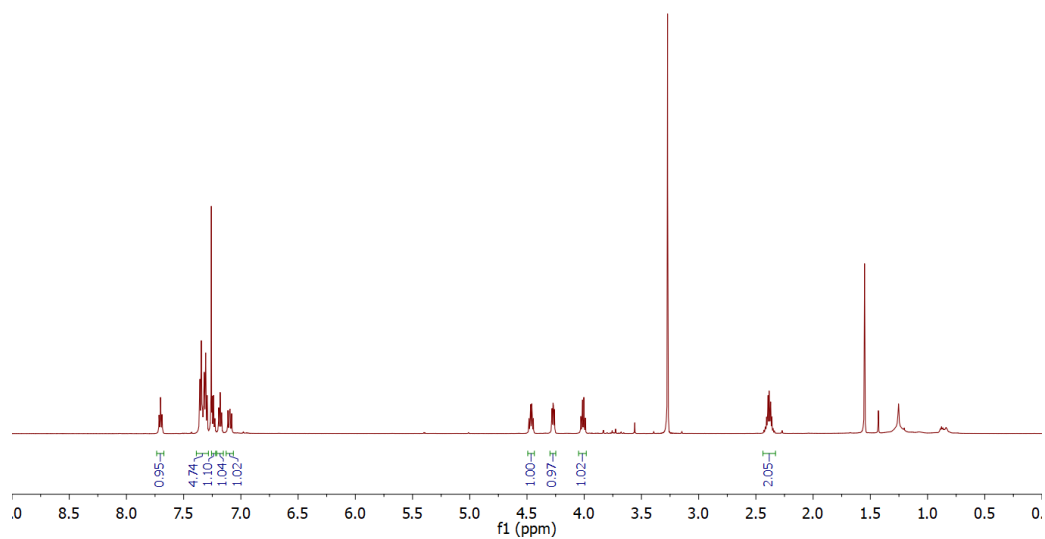
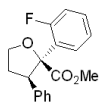


¹³C NMR (151 MHz, Chloroform-*d*):

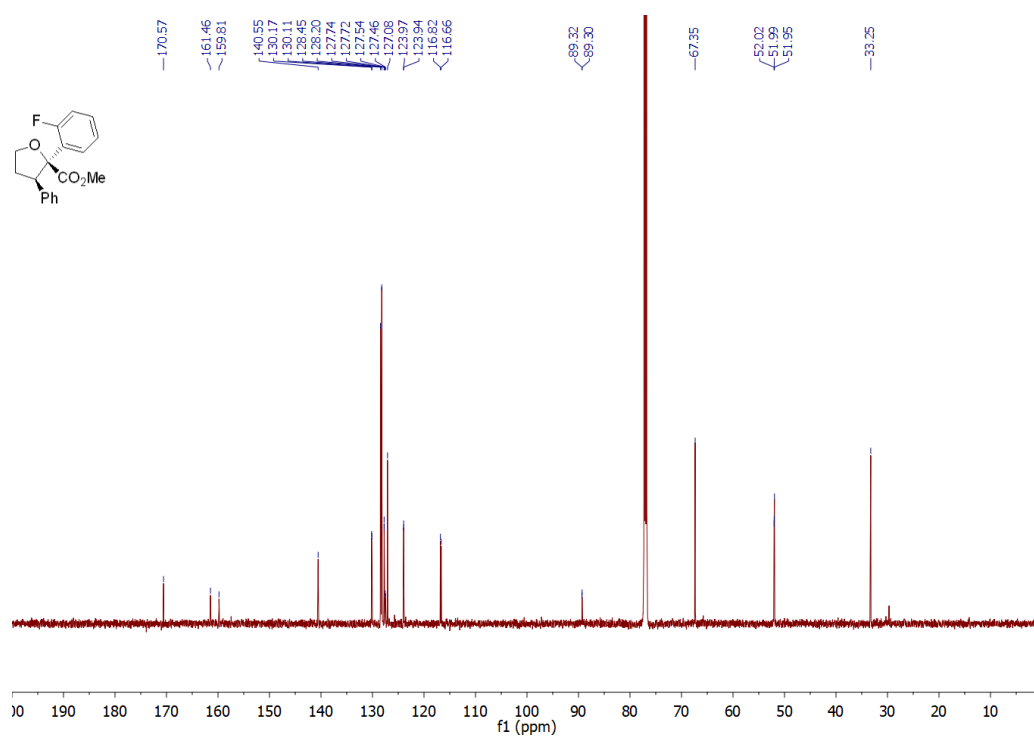
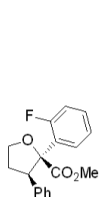


***cis*-methyl 2-(2-fluorophenyl)-3-phenyltetrahydrofuran-2-carboxylate (25g)**

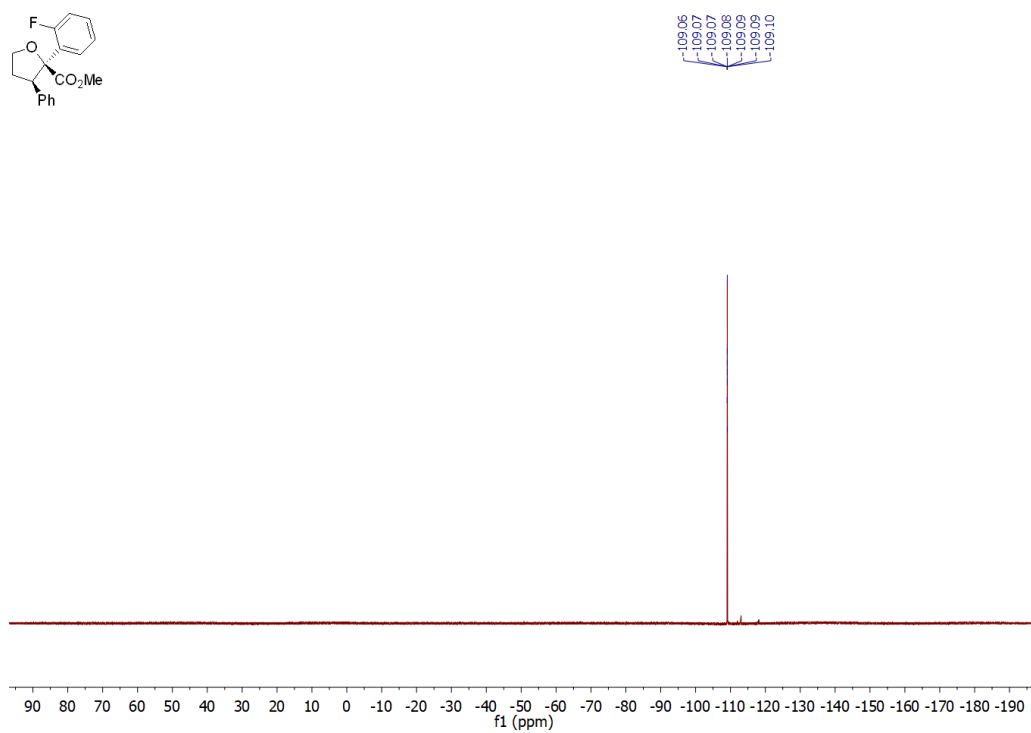
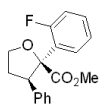
¹H NMR (600 MHz, Chloroform-*d*):



¹³C NMR (151 MHz, Chloroform-*d*):

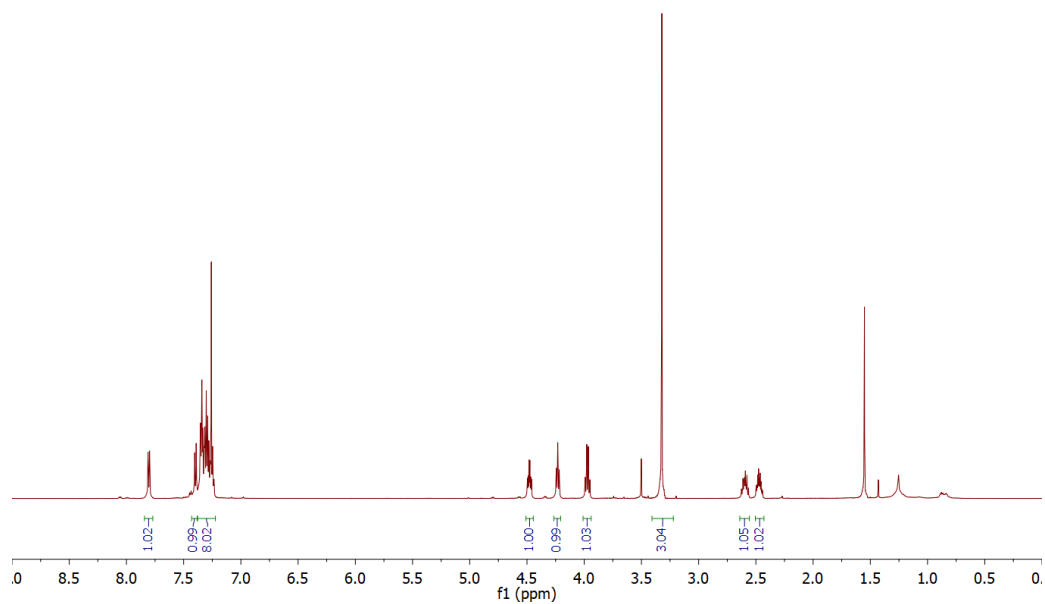
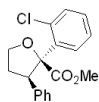


^{19}F NMR (564 MHz, Chloroform-*d*):

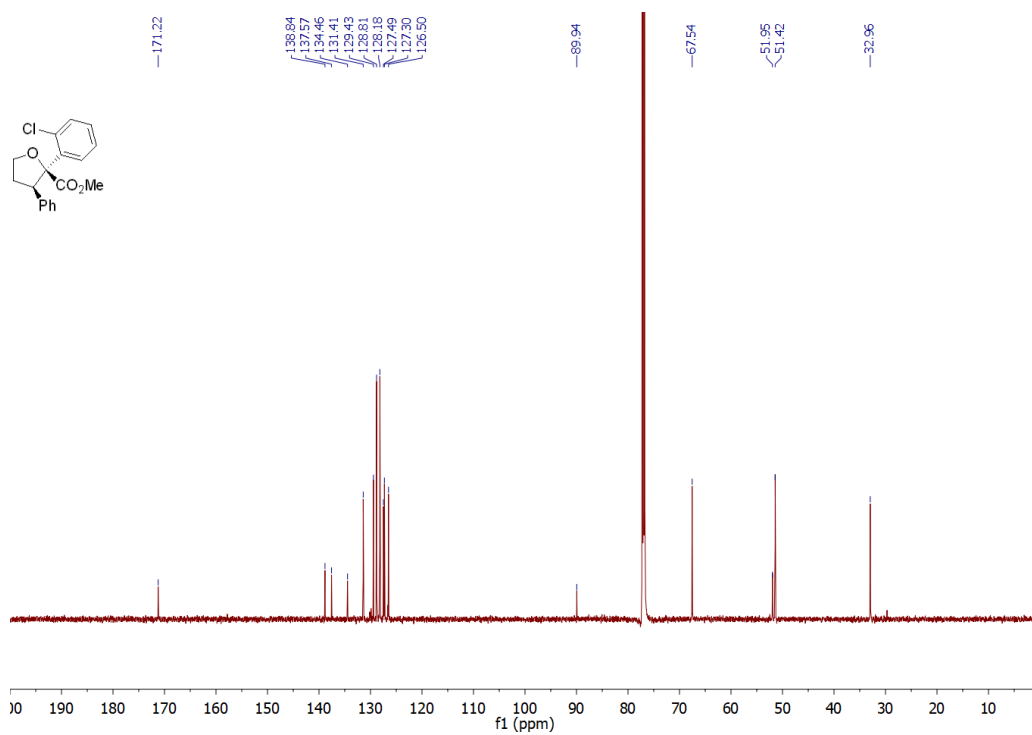


***cis*-methyl 2-(2-chlorophenyl)-3-phenyltetrahydrofuran-2-carboxylate (25h)**

¹H NMR (600 MHz, Chloroform-*d*):

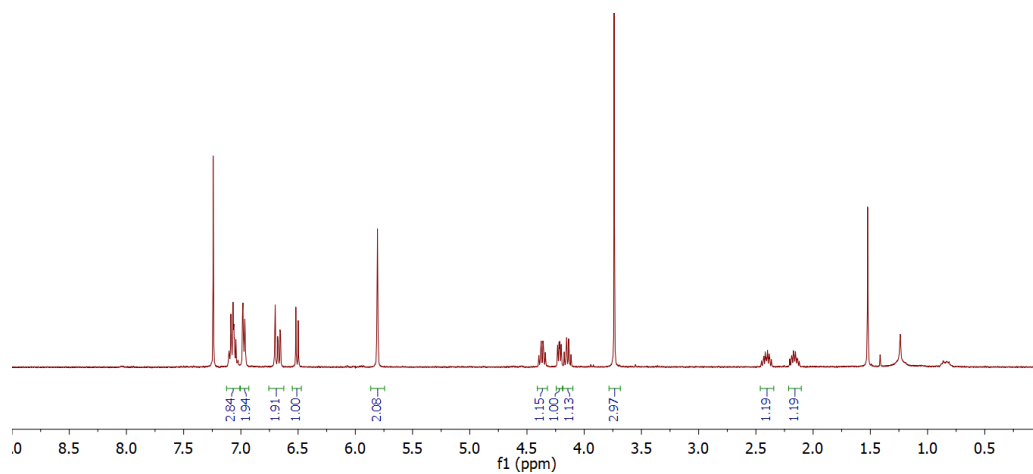
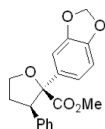


¹³C NMR (151 MHz, Chloroform-*d*):

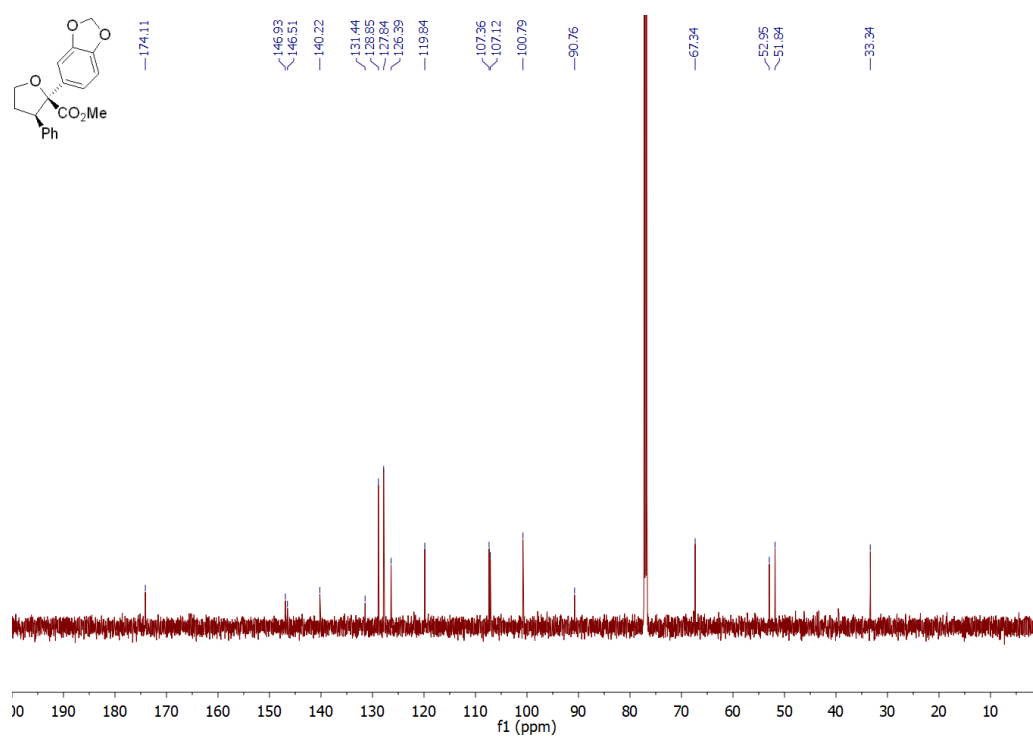
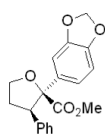


***cis*-methyl 2-(benzo[d][1,3]dioxol-5-yl)-3-phenyltetrahydrofuran-2-carboxylate (25j)**

¹H NMR (400 MHz, Chloroform-*d*):

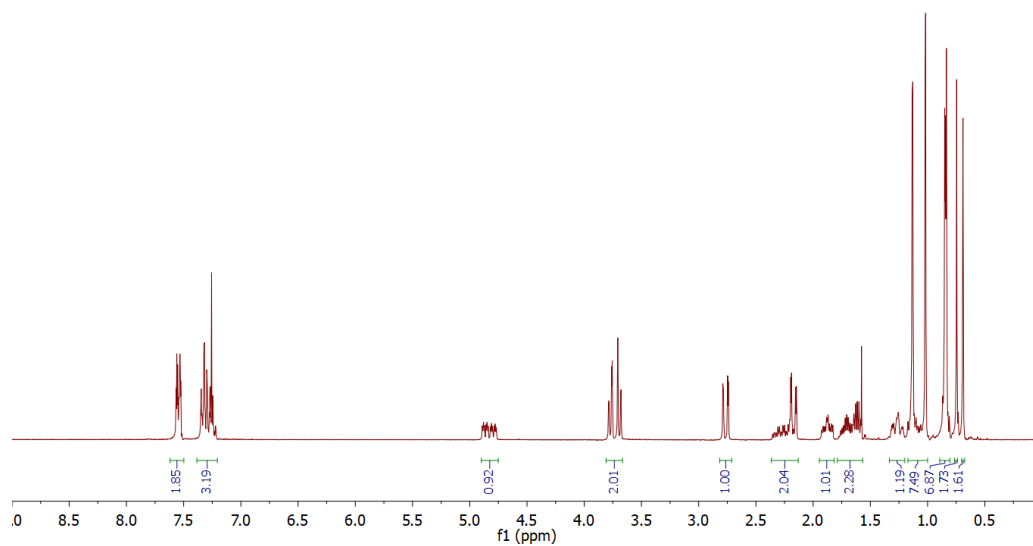
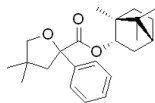


¹³C NMR (151 MHz, Chloroform-*d*):

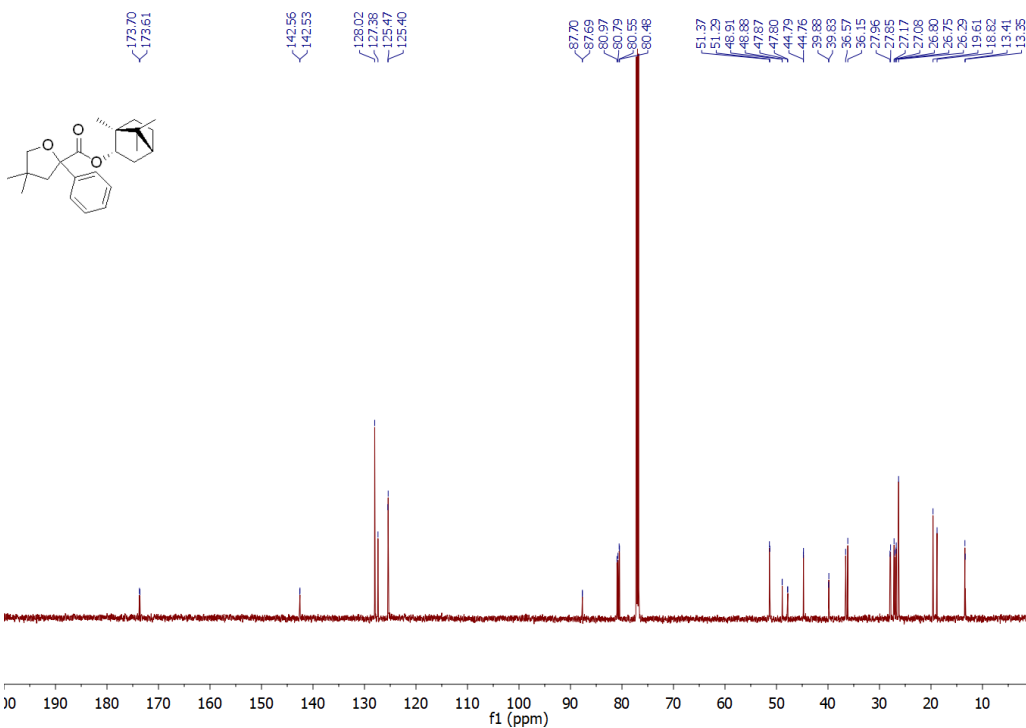


1-(4,4-dimethyl-2-phenyltetrahydrofuran-2-yl)-2-((1R,2S,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)ethanone (29)

^1H NMR (300 MHz, Chloroform-*d*):

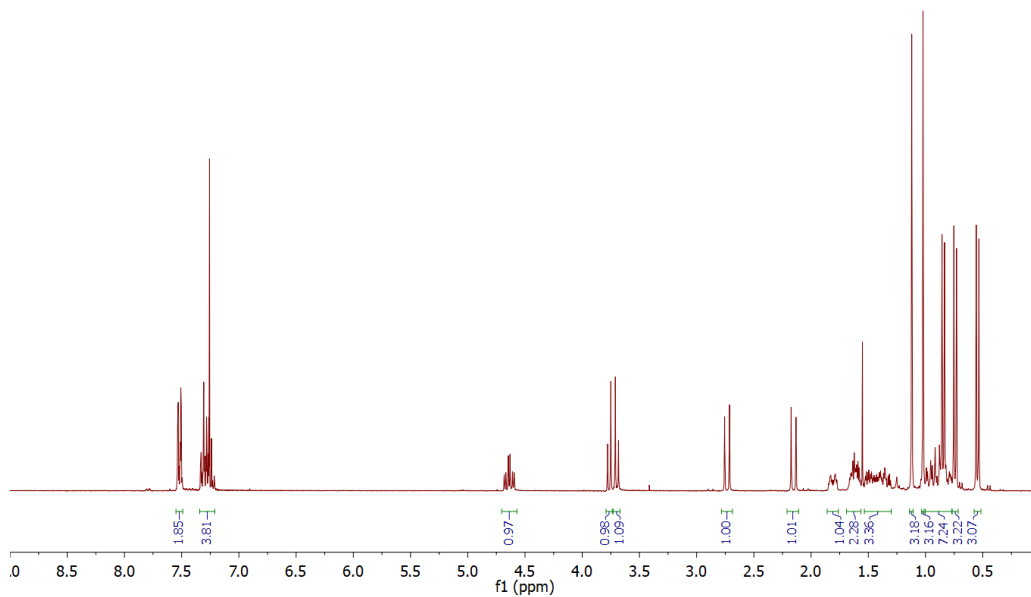
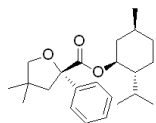


^{13}C NMR (151 MHz, Chloroform-*d*):

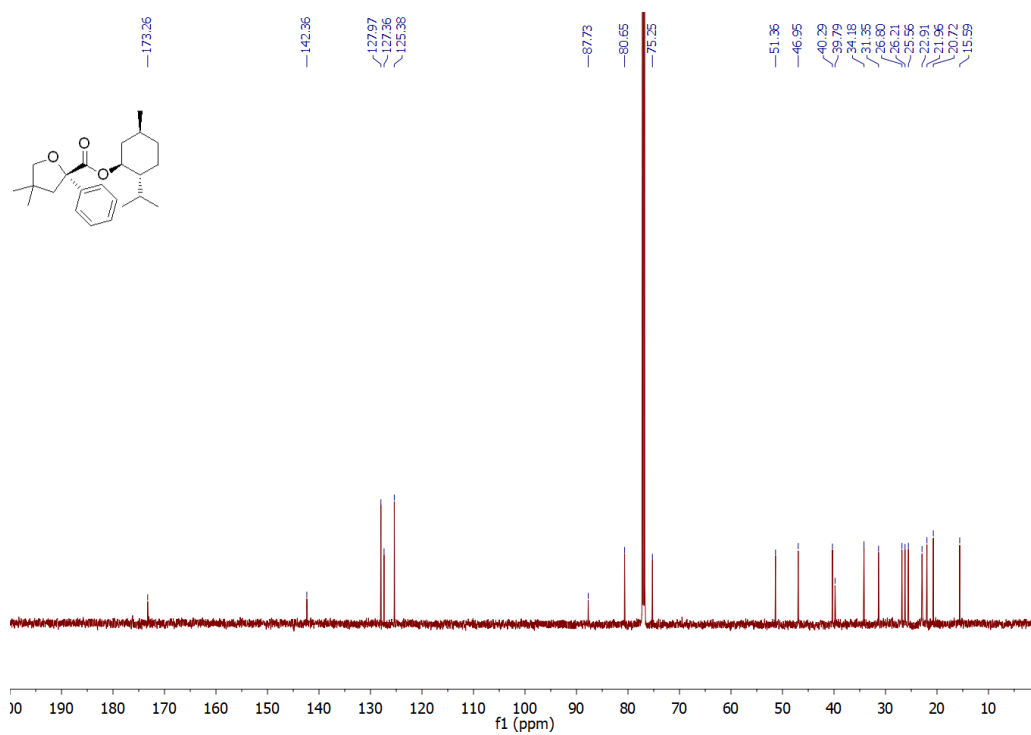
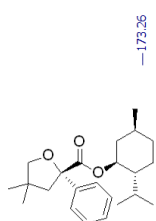


(S)-(1S,2R,5S)-2-isopropyl-5-methylcyclohexyl 4,4-dimethyl-2-phenyltetrahydrofuran-2-carboxylate (30)

^1H NMR (300 MHz, Chloroform-*d*):

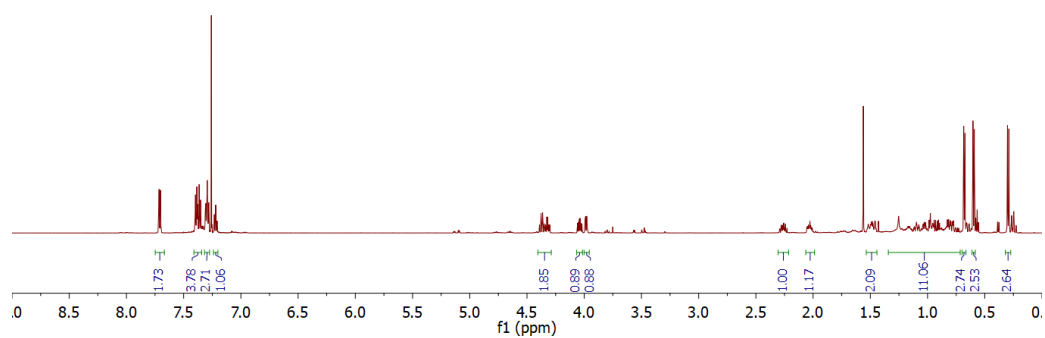
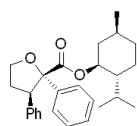


^{13}C NMR (151 MHz, Chloroform-*d*):

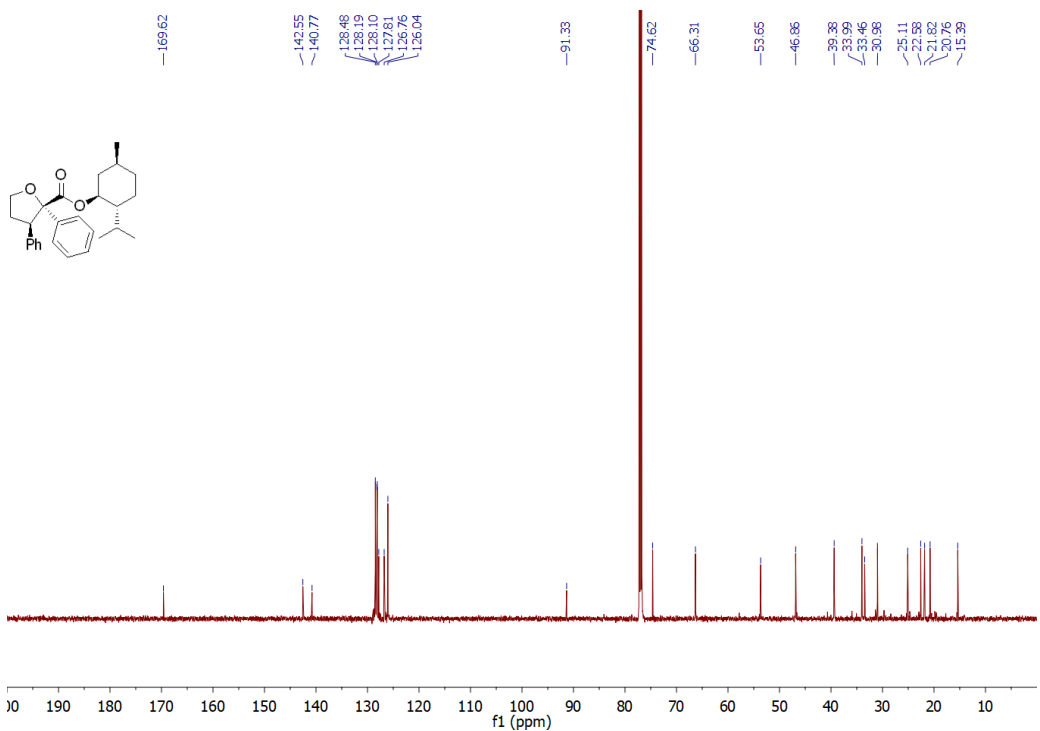


(2S,3R)-(1S,2R,5S)-2-isopropyl-5-methylcyclohexyl 2,3-diphenyltetrahydrofuran-2-carboxylate (31)

¹H NMR (600 MHz, Chloroform-*d*):

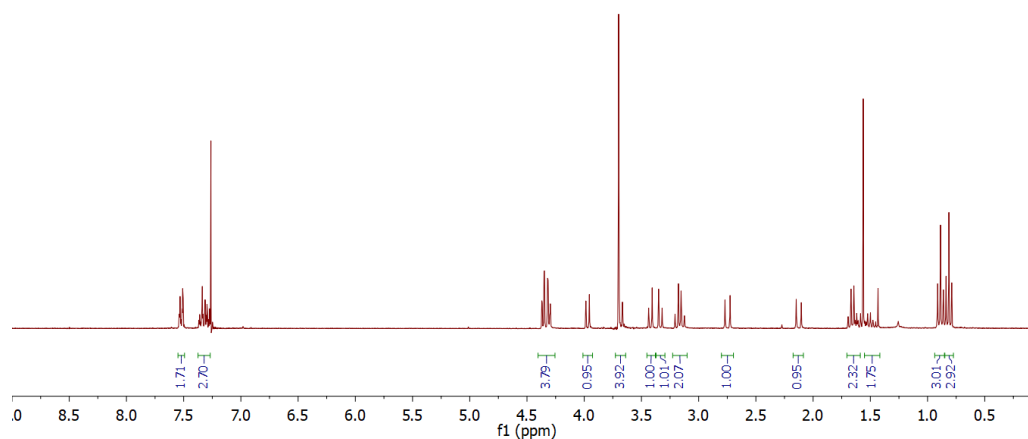
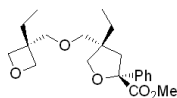


¹³C NMR (151 MHz, Chloroform-*d*):

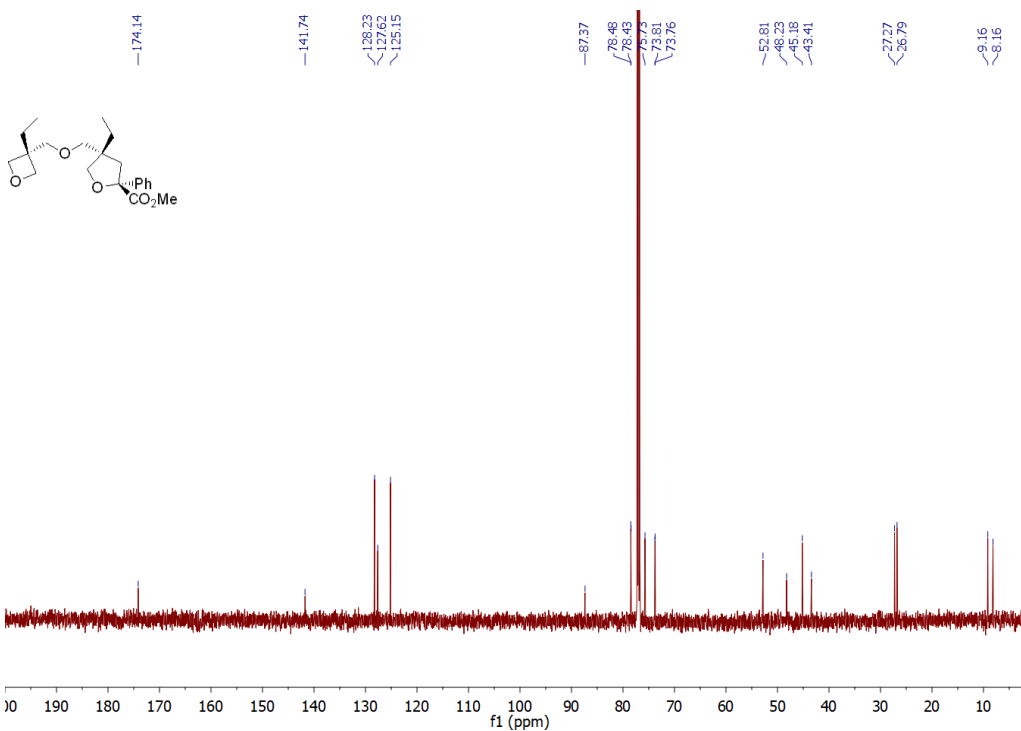


methyl 4-ethyl-4-(((3-ethyloxetan-3-yl)methoxy)methyl)-2-phenyltetrahydrofuran-2-carboxylate (35)

^1H NMR (300 MHz, Chloroform- d):

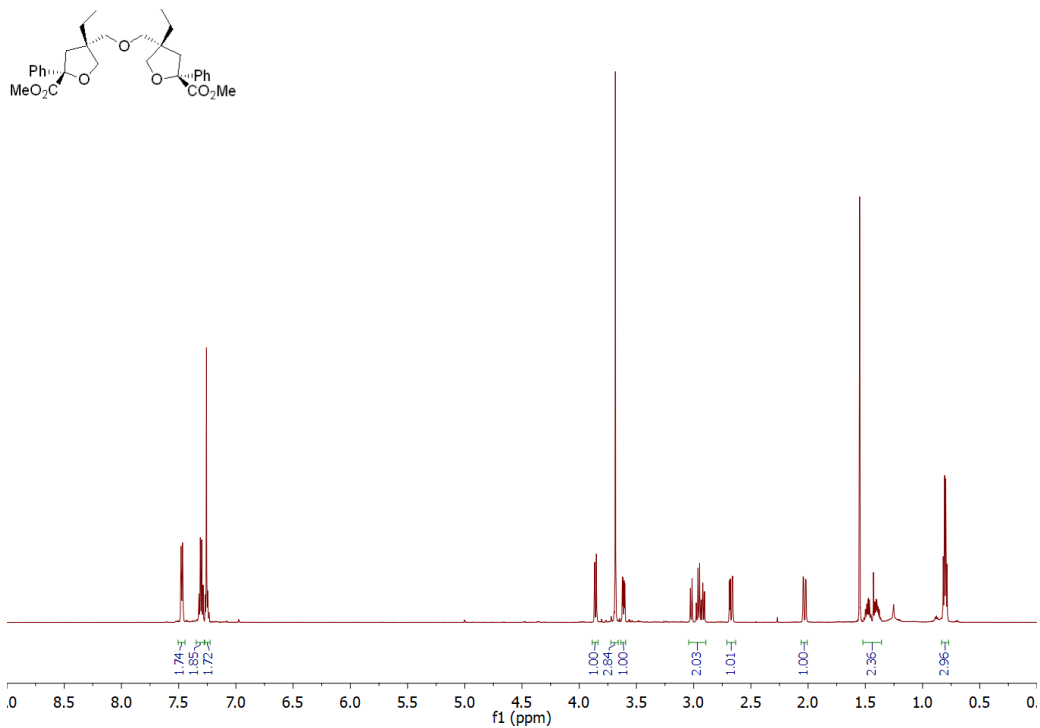


^{13}C NMR (151 MHz, Chloroform- d):

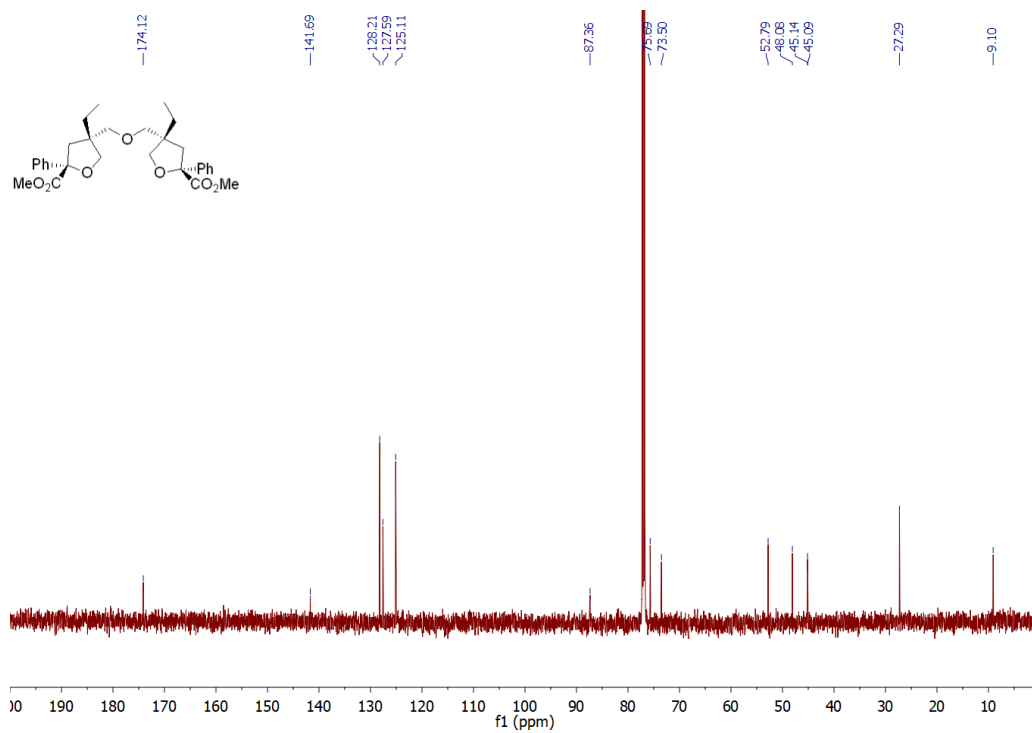


Dimethyl 4,4'-(oxybis(methylene))bis(4-ethyl-2-phenyltetrahydrofuran-2-carboxylate (36)

^1H NMR (300 MHz, Chloroform- d):

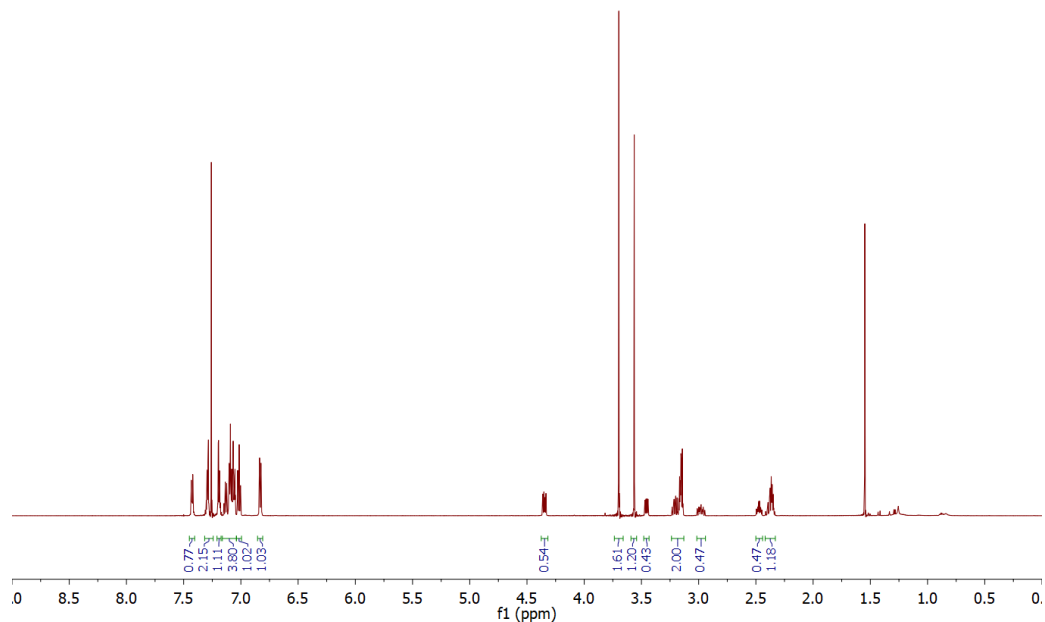
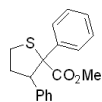


^{13}C NMR (151 MHz, Chloroform- d):

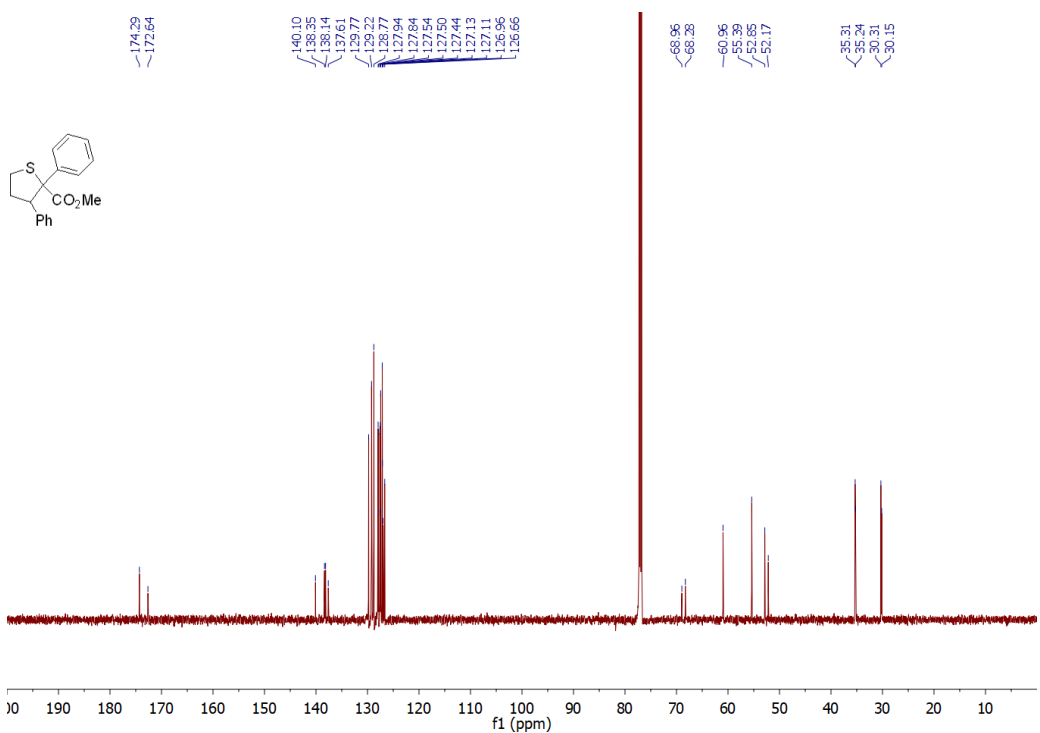


Methyl 2,3-diphenyltetrahydrothiophene-2-carboxylate (37)

¹H NMR (600 MHz, Chloroform-d):

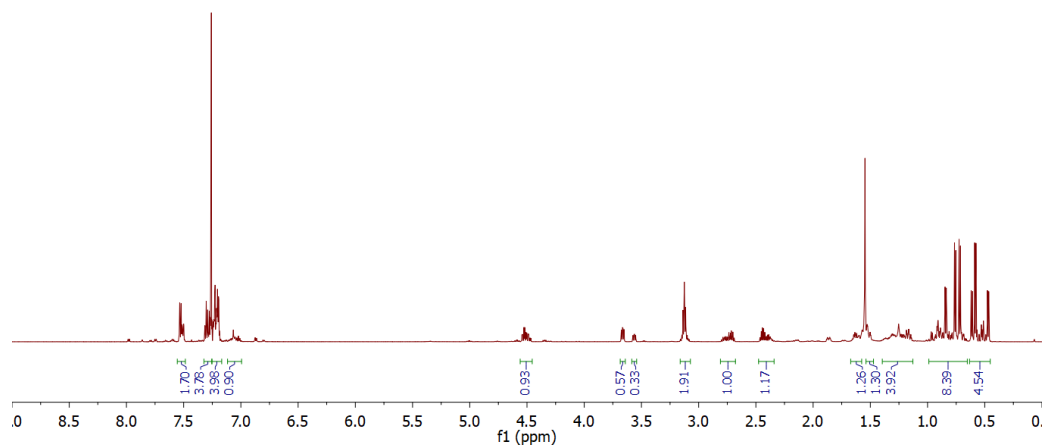
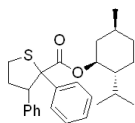


¹³C NMR (151 MHz, Chloroform-d):

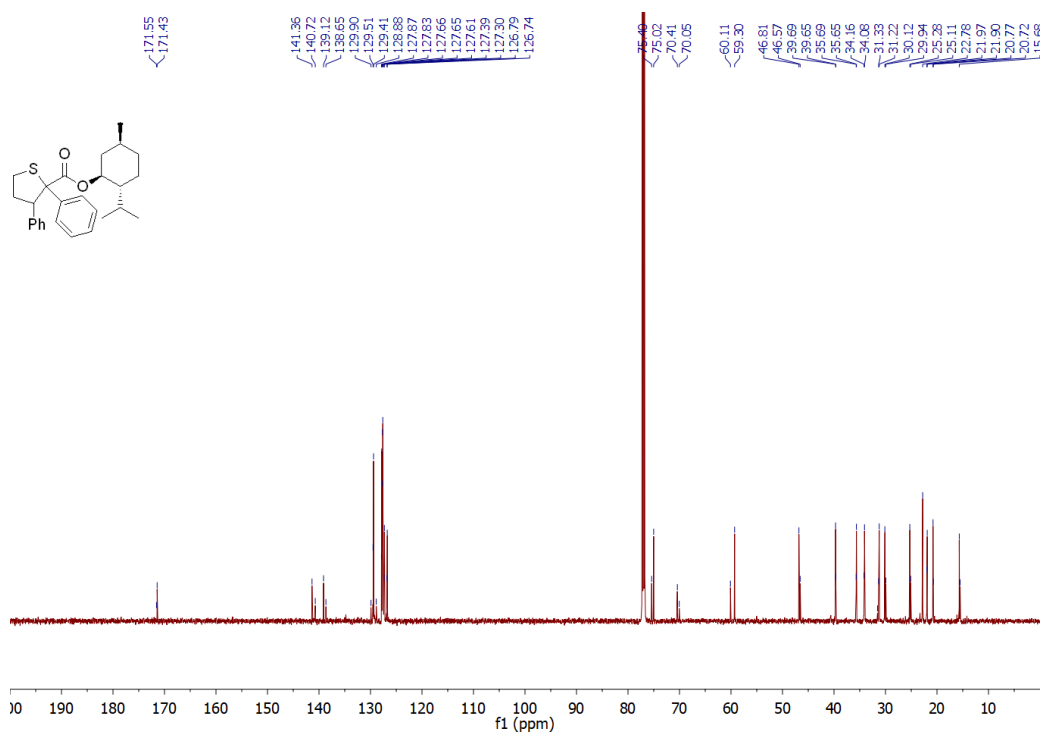


(1S*,2R*,5S*)-2-isopropyl-5-methylcyclohexyl 2,3-diphenyltetrahydrothiophene-2-carboxylate (38)

¹H NMR (600 MHz, Chloroform-*d*):

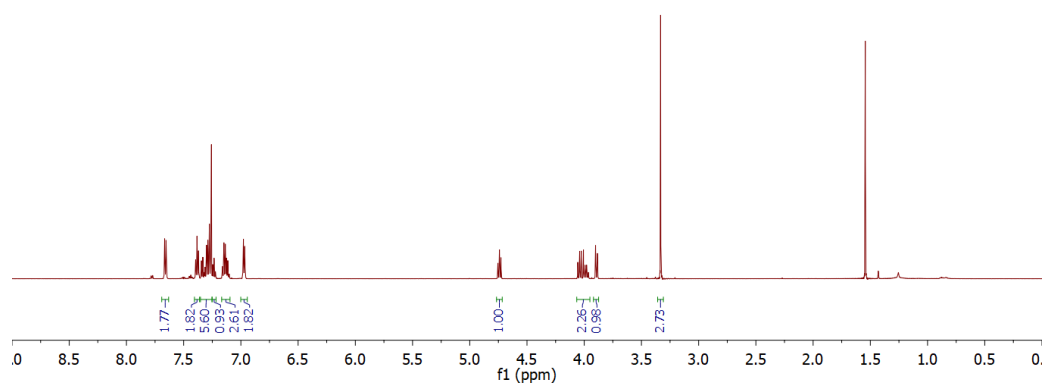
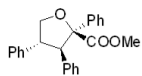


¹³C NMR (151 MHz, Chloroform-*d*):



(2S*,3S*,4S*)-methyl 2,3,4-triphenyltetrahydrofuran-2-carboxylate (42)

¹H NMR (600 MHz, Chloroform-*d*):



¹³C NMR (151 MHz, Chloroform-*d*):

