Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

A Combined Computational and Experimental Investigation of the Oxidative Ring-Opening of Cyclic Ethers by Oxoammonium Cations

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Supporting Information: Experimental Studies

Key to Abbreviated Terms **S2**

General Considerations **S2**
Comments regarding origins of commercial starting materials, purification of solvents, and our spectroscopic techniques.

Synthesis of Substrates **S3**
Procedures for the preparations of starting materials and spectral characterization information

Reactions of Substrates with the Oxoammonium Salt **S7**
Procedures for oxidation of various species with the oxoammonium salt, isolation procedures, and spectral characterization of products

^{1}H-NMR Spectra of Synthesized Compounds **S9**

^{13}C-NMR Spectra of Synthesized Compounds **S24**

^{19}F-NMR Spectra of Synthesized Compounds **S39**

Key to Abbreviated Terms:

$CDCl_3$: deuterated chloroform
CH_2Cl_2: dichloromethane
EtOAc: ethyl acetate
Et_2O: diethyl ether
Hex: hexanes
MeCN: acetonitrile
THF: tetrahydrofuran
MeOH: methanol

General Considerations:

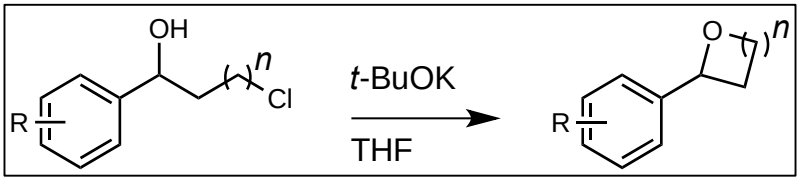
General:
NMR Spectra (^1H, ^{13}C, ^{19}F) were performed at 298 K on either a Brüker Avance Ultra Shield 300 MHz NMR, Brüker DRX-400 400 MHz NMR, or Brüker Avance 500 MHz NMR. ^1H-NMR Spectra obtained in $CDCl_3$ were referenced to residual non-deuterated chloroform (7.26 ppm) in the deuterated solvent. ^{13}C NMR Spectra obtained in $CDCl_3$ were referenced to chloroform (77.3 ppm). ^{19}F NMR spectra were referenced to hexafluorobenzene (-164.9 ppm).[1] Reactions were monitored by an Agilent Technologies 7820A Gas Chromatograph attached to a 5975 Mass Spectrometer, ^1H NMR, and/or by TLC on silica gel plates (60Å porosity, 250 μm thickness). TLC analysis was performed using hexanes/ethyl acetate as the eluent and visualized using permanganate stain, *p*-anisaldehyde stain, Seebach's Stain, and/or UV light. Flash chromatography and silica plugs utilized Dynamic Adsorbents Inc. Flash Silica Gel (60Å porosity, 32-63 μm).

Chemicals:
Deuterated NMR solvents ($CDCl_3$, DMSO-d_6) were purchased from Cambridge Isotope Laboratories. $CDCl_3$ stored over 4Å molecular sieves. Na_2SO_4, CH_2Cl_2, MeCN, MeOH, Et_2O (ACS Grade and reagent grade), THF, $NaBH_4$, *t*-BuOK, and $AlCl_3$ were purchased from Sigma-Aldrich. Alcohol starting materials were either prepared *via* Friedel-Crafts acylation or purchased from commercial suppliers. The oxoammonium salt 4-acetamido-2,2,6,6-tetramethyl-1-oxopiperidin-1-ium tetrafluoroborate was prepared according to established protocol.[2]

[1] I. Ravikumar, S. Saha, and P. Ghosh, *Chem. Commun.* 2011, **47**, 4721-4723.
[2] M. A. Mercadante, C. B. Kelly, J. M. Bobbitt, L. J. Tilley and N. E. Leadbeater, *Nat. Protoc.* 2013, **8**, 666-676.

Synthesis of Substrates

Synthesis of cyclic ethers



2-phenyloxetane (2a)[3]

The following is a modification of the cyclization procedure outlined by Pineschi.[3] To a 1000 mL round bottom flask equipped with a stir bar was added 3-chloro-1-phenylpropanol (8.2 g, 0.048 mol, 1.0 equiv.) and THF (410 mL, 0.117 M in the alcohol). Potassium *tert*-butoxide (16.16 g, 144 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 Et_2O (100 mL) and deionized water (100 mL). The phases were separated and the aqueous layer was extracted with Et_2O (3 × 100 mL). The combined organic layers were washed with deionized water (≈ 200 mL), brine (≈ 200 mL), and dried with Na_2SO_4. The solvent was removed *in vacuo* by rotary evaporation to give the pure product (6.44g, 77%) as a clear yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 2.62 - 2.73 (m, 1 H) 2.97 - 3.08 (m, 1 H) 4.62 - 4.70 (m, 1 H) 4.80 - 4.87 (m, 1 H) 5.81 (t, *J*=7.57 Hz, 1 H) 7.27 - 7.34 (m, 1 H) 7.35 - 7.47 (m, 4 H)
^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 30.75 (CH_2), 68.18 (CH_2), 82.88 (CH), 125.24 (CH), 127.80 (CH), 128.50 (CH), 143.66 (C)

2-(4'-fluorophenyl)oxetane (2b)

2-(4'-fluorophenyl)oxetane was obtained *via* the same protocol as **2a** with the following modification: the reaction was conducted using 3-chloro-1-(4'-fluorophenyl)-1-propanol (2.26 g, 0.012 mol). The product (1.40 g, 77%) was obtained as a clear yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 2.13 (s, 3 H) 2.38 (s, 3 H) 2.54 (m, 1 H) 3.01 - 3.12 (m, 1 H) 4.59 - 4.69 (m, 1 H) 4.80 - 4.89 (m, 1 H) 5.97 (t, *J*=7.52 Hz, 1 H) 6.97 - 7.05 (m, 2 H) 7.51 (s, 1 H)
^{13}C NMR ($CDCl_3$, 100 MHz) 31.16 (CH_2) 68.37 (CH_2) 82.61 (CH) 115.62 (d, $J_{C\text{-}C\text{-}F}$ = 21.46 Hz, CH) 127.38 (d, $J_{C\text{-}C\text{-}C\text{-}F}$ = 8.25 Hz, CH) 139.63 (d, $J_{C\text{-}C\text{-}C\text{-}C\text{-}F}$ = 2.93 Hz, C) 162.69 (d, $J_{C\text{-}F}$ = 245.75 Hz, CF)
^{19}F NMR (377 MHz, $CDCl_3$) δ ppm -117.77 (s, 1 F)

[3] F. Bertolini, S. Crotti, V. Di Bussolo, F. Macchia, and M. Pineschi, *J. Org. Chem.* **2008**, 73, 8998-9007.

2-(4'-*tert*-butylphenyl)oxetane (2c)

2-(4'-*tert*-butylphenyl)oxetane was obtained *via* the same protocol as **2a** with the following modification: the reaction was conducted using 3-chloro-1-(4'-*tert*-butylphenyl)-1-propanol (6.0 g, 0.026 mol). The product (4.54 g, 90%) was obtained as a clear yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 1.37 (s, 9 H) 2.73 (d, *J*=1.61 Hz, 1 H) 3.01 (d, *J*=5.64 Hz, 1 H) 4.64 - 4.72 (m, 1 H) 4.80 - 4.88 (m, 1 H) 5.83 (t, *J*=7.49 Hz, 1 H) 7.40 - 7.48 (m, 4 H)
^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 30.82 (CH_2), 31.58 (CH_3), 34.78 (C), 68.33 (CH_2), 83.03 (CH), 125.34 (CH), 125.58 (CH), 140.73 (C), 151.04 (C)

2-(2',5'-dimethylphenyl)oxetane (2d)

2-(2',5'-dimethylphenyl)oxetane was obtained *via* the same protocol as **2a** with the following modification: the reaction was conducted using 3-chloro-1-(2',5'-dimethylphenyl)-1-propanol (4.50 g, 0.0226 mol). The product (3.38 g, 92%) was obtained as a clear yellow-orange oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 2.13 (s, 3 H) 2.38 (s, 3 H) 2.54 (m, 1 H) 3.01 - 3.12 (m, 1 H) 4.59 - 4.69 (m, 1 H) 4.80 - 4.89 (m, 1 H) 5.97 (t, *J*=7.52 Hz, 1 H) 6.97 - 7.05 (m, 2 H) 7.51 (s, 1 H)
^{13}C NMR ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 18.10 (CH_3), 23.35 (CH_3), 30.03 (CH_2), 68.24 (CH_2), 80.89 (CH), 124.83 (CH), 127.95 (CH), 130.12 (CH), 130.22 (C), 135.74 (C), 141.61 (C)

2-phenyltetrahydrofuran (2e)

2-phenyltetrahydrofuran was obtained *via* the same protocol as **2a** with the following modification: the reaction was conducted using 4-chloro-1-phenylbutanol (6.79 g, 0.037 mol). The product (5.04 g, 92%) was obtained as a clear yellow-orange oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 1.76 - 1.87 (m, 1 H) 1.97 - 2.06 (m, 2 H) 2.33 (m, 1 H) 3.94 (m, 1 H) 4.06 - 4.15 (m, 1 H) 4.90 (t, *J*=7.15 Hz, 1 H) 7.22 - 7.29 (m, 1 H) 7.30 - 7.37 (m, 4 H)
^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 26.15 (CH_2), 34.75 (CH_2), 68.77 (CH_2), 80.80 (CH), 125.75 (CH), 127.24 (CH), 128.40 (CH), 143.56 (C)

2-(4'-fluorophenyl)tetrahydrofuran (2f)

2-(4'-fluorophenyl)tetrahydrofuran was obtained *via* the same protocol as **2a** with the following modification: the reaction was conducted using 4-chloro-1-**(**4'-fluorophenyl)-1-butanol (1.71 g, 0.0084 mol). The product (1.15 g, 67%) was obtained as a clear yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm 1.69 - 1.83 (m, 1 H) 2.01 (m, 2 H) 2.31 (m, 1 H) 3.92 (q, *J*=7.41 Hz, 1 H) 4.09 (q, *J*=7.14 Hz, 1 H) 4.85 (t, *J*=7.14 Hz, 1 H) 7.01 (t, *J*=8.64 Hz, 2 H) 7.25 - 7.33 (m, 2 H)
^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 26.23 (CH_2), 34.91 (CH_2), 68.85 (CH_2), 80.35 (CH), 115.28 (d, $J_{C\text{-}C\text{-}F}$ = 21.3 Hz, CH), 127.49 (d, $J_{C\text{-}C\text{-}C\text{-}F}$ = 8.0 Hz, CH), 139.32 (d, $J_{C\text{-}C\text{-}C\text{-}C\text{-}F}$ = 3.1 Hz, C), 162.23 (d, $J_{C\text{-}F}$ = 244.6 Hz, C)

^{19}F NMR (377 MHz, $CDCl_3$) δ ppm -119.11 (s, 1 F)

2-(4'-*tert*-butylphenyl)tetrahydrofuran (2g)

2-(4'-*tert*-butylphenyl)tetrahydrofuran was obtained *via* the same protocol as **2a** with the following modification: the reaction was conducted using 4-chloro-1-**(**4'-*tert*-butylphenyl)-1-butanol (3.28 g, 0.0136 mol). The product (2.53 g, 91%) was obtained as a clear yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 1.33 (s, 9 H) 1.80 - 1.89 (m, 1 H) 2.01 (dd, *J*=7.54, 6.57 Hz, 2 H) 2.26 - 2.36 (m, 1 H) 3.89 - 3.97 (m, 1 H) 4.09 (d, *J*=7.93 Hz, 1 H) 4.88 (t, *J*=7.15 Hz, 1 H) 7.26 - 7.31 (m, 2 H) 7.34 - 7.40 (m, 2 H)
^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 26.37 (CH_2), 31.65 (CH_3), 34.56 (CH_2), 34.72 (C), 68.80 (CH_2), 80.77 (CH), 125.44 (CH), 125.71 (CH), 140.53 (C), 150.27 (C)

2-(2',5'-dimethylphenyl)tetrahydrofuran (2h)

2-(2',5'-dimethylphenyl)tetrahydrofuran was obtained *via* the same protocol as **2a** with the following modification: the reaction was conducted using 4-chloro-1-**(**2',5'-dimethylphenyl)-1-butanol (6.79 g, 0.037 mol). The product (5.04 g, 92%) was obtained as a clear yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 1.61 - 1.74 (m, 1 H) 1.97 - 2.08 (m, 2 H) 2.26 (s, 3 H) 2.32 (s, 3 H) 2.33 - 2.43 (m, 1 H) 3.93 (q, *J*=7.41 Hz, 1 H) 4.16 (q, *J*=7.04 Hz, 1 H) 5.03 (t, *J*=7.20 Hz, 1 H) 6.92 - 7.06 (m, 2 H)
^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 18.80 (CH_3), 21.22 (CH_3), 26.14 (CH_2), 32.27 (CH_2), 68.60 (CH_2), 78.08 (CH), 125.24 (CH), 127.47 (CH), 130.14 (CH), 131.03 (C), 135.37 (C), 141.57 (C)

2-(4'-bromophenyl)tetrahydrofuran (2i)

2-(4'-bromophenyl)tetrahydrofuran was obtained *via* the same protocol as **2a** with the following modification: the reaction was conducted using 4-chloro-1-**(**4'-bromophenyl)-1-butanol (5.32 g, 0.020 mol). The product (4.23 g, 92%) was obtained as a clear orange oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm 1.67 - 1.81 (m, 1 H) 2.00 (m, 2 H) 2.25 - 2.38 (m, 1 H) 3.87 - 3.98 (m, 1 H) 4.03 - 4.13 (m, 1 H) 4.84 (t, *J*=7.14 Hz, 1 H) 7.21 (d, *J*=8.32 Hz, 2 H) 7.40 - 7.50 (m, 2 H)
^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 26.10 (CH_2), 34.78 (CH_2), 68.82 (CH_2), 80.10 (CH), 120.90 (C), 127.49 (CH), 131.44 (CH), 142.77 (C)

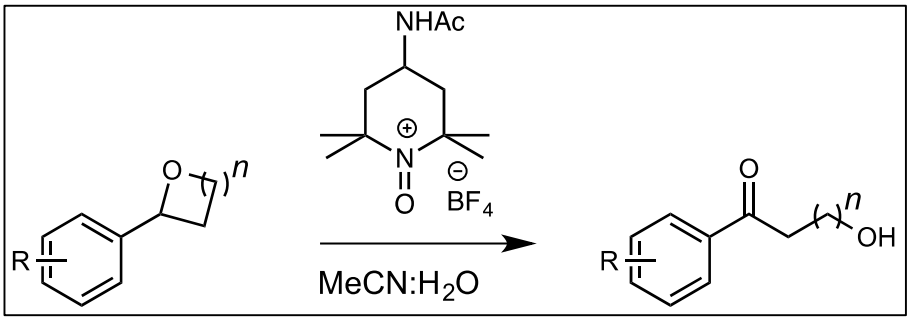
2-phenyltetrahydropyran (2j)

2-phenyltetrahydropyran was obtained *via* the same protocol as **2a** with the following modification: the reaction was conducted using 5-chloro-1-phenylpentanol (10.00 g, 0.0503 mol). The product (8.07 g, 99%) was obtained as a clear yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 1.56 - 1.74 (m, 4 H) 1.81 - 1.87 (m, 1 H) 1.91 - 2.00 (m, 1 H) 3.58 - 3.66 (m, 1 H) 4.15 (m, 1 H) 4.30 - 4.36 (m, 1 H) 7.23 - 7.28 (m, 1 H) 7.30 - 7.38 (m, 4 H)
^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 24.18 (CH_2), 26.07 (CH_2), 34.23 (CH_2), 69.11 (CH_2), 80.25 (CH), 125.96 (CH), 127.38 (CH), 128.39 (CH), 143.52 (C)

Reactions of Substrates with the Oxoammonium Salt (1)

Oxidative Ring-Opening of Cyclic Ethers



3-hydroxy-1-phenyl-1-propanone (3a)

To a 50 mL round bottom flask equipped with stirbar was added the oxoammonium salt **1** (3.36 g, 0.0112 mol, 1.12 equiv.) and 8:2 by volume MeCN:H_2O (25 mL, 0.4 M in the ether). The salt was allowed to dissolve in solution. After this time, the 2-phenyloxetane was added slowly to the stirred solution (1.34 g, 0.01 mol, 1.0 equiv.). The mixture was allowed to stir overnight. After this time, the crude mixture was diluted with Et_2O (200 mL) and deionized water (200 mL). The phases were separated and the aqueous layer was extracted with Et_2O (3 × 50 mL). The combined organic layers were washed with 2M HCl (≈ 100 mL) deionized water (≈ 100 mL), brine (≈ 100 mL), and dried with Na_2SO_4. The solvent was removed *in vacuo* by rotary evaporation to give the an orange oil which was then adhered to silica gel using 1.5 weight equivalents of SiO_2 (relative to the theoretical yield). The dry-packed material was gently added atop a silica gel plug. The plug was washed with a 9:1 by volume mixture of Hex:EtOAc (3 column volumes) followed by an 8:2 mixture of Hex:EtOAc (1.5 column volumes). The desired product was eluted off the plug *via* a 6:4 by volume mixture of Hex:EtOAc (2-3 column volumes). The solvent was removed *in vacuo* by rotary evaporation affording the pure **3a** (0.92 g, 61%) as a clear yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 2.67 (br. s., 1 H) 3.24 (t, *J*=5.33 Hz, 2 H) 4.04 (t, *J*=5.30 Hz, 2 H) 7.45 - 7.52 (m, 2 H) 7.56 - 7.63 (m, 1 H) 7.95 - 8.00 (m, 2 H)
^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 40.66 (CH_2), 57.81 (CH_2), 128.05 (CH), 128.59 (CH), 133.36 (CH), 136.66 (C), 200.18 (C)

3-hydroxy-1-(4'-fluorophenyl)-1-propanone (3b)

3-hydroxy-1-(4'-fluorophenyl)-1-propanone was obtained *via* the same protocol as **3a** with the following modification: the reaction was conducted using 2-(4'-fluorophenyl)oxetane (1.43 g, 0.0094 mol). The product (0.89 g, 56%) was obtained as a clear yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 2.73 (br. s, 1 H) 3.20 (t, *J*=5.30 Hz, 2 H) 4.03 (t, *J*=5.33 Hz, 2 H) 7.11 - 7.18 (m, 2 H) 7.95 - 8.03 (m, 2 H)
^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 40.62 (CH_2), 58.02 (CH_2), 115.89 (d, $J_{C\text{-}C\text{-}F}$ = 21.8, CH), 130.89 (d, $J_{C\text{-}C\text{-}C\text{-}F}$ = 9.4 Hz, CH), 133.32 (d, $J_{C\text{-}C\text{-}C\text{-}C\text{-}F}$ = 3.0 Hz, C), 166.05 (d, $J_{C\text{-}F}$ = 255.2 Hz, C), 198.75 (C)
^{19}F NMR (377 MHz, $CDCl_3$) δ ppm -107.66 (s, 1 F)

4-hydroxy-1-phenyl-1-butanone (3e)

To a 100 mL round bottom flask equipped with stirbar was added the oxoammonium salt **1** (3.83 g, 0.01275 mol, 1.25 equiv.) and 8:2 by volume MeCN:H_2O (50 mL, 0.2 M in the ether). The salt was allowed to dissolve in solution. After this time, the 2-phenyltetrahydrofuran was added slowly to the stirred solution (1.512 g, 0.0102 mol, 1.0 equiv.). The flask was then fitted with a reflux condenser and the mixture was heated to 50 °C. The mixture was allowed to stir overnight. After this time, pure product was obtained *via* the same protocol as **3a,** yielding **3e** (0.748 g, 45%) as a clear orange oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 1.84 (br. s., 1 H) 2.03 (m, 2 H) 3.14 (t, *J*=6.94 Hz, 2 H) 3.75 (t, *J*=6.05 Hz, 2 H) 7.42 - 7.51 (m, 2 H) 7.53 - 7.61 (m, 1 H) 7.93 - 8.04 (m, 2 H)
^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 27.18 (CH_2), 35.49 (CH_2), 62.42 (CH_2), 128.31 (CH), 128.82 (CH), 133.35 (CH), 137.07 (C), 200.84 (C)

4-hydroxy-1-(4'-fluorophenyl)-1-butanone (3f)

4-hydroxy-1-(4'-fluorophenyl)-1-butanone was obtained *via* the same protocol as **3e** with the following modification: the reaction was conducted using 2-(4'-fluorophenyl)tetrahydrofuran (0.673 g, 0.00405 mol). The product (0.166 g, 23%) was obtained as a clear yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 1.68 (br. s., 1 H) 1.97 - 2.06 (m, 2 H) 3.11 (t, *J*=6.91 Hz, 2 H) 3.75 (d, *J*=3.79 Hz, 2 H) 7.09 - 7.17 (m, 2 H) 7.98 - 8.07 (m, 2 H)
^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 27.14 (CH_2), 35.43 (CH_2), 62.44 (CH_2), 115.94 (d, $J_{C\text{-}C\text{-}F}$ = 21.9 Hz, CH), 130.98 (d, $J_{C\text{-}C\text{-}C\text{-}F}$ = 9.4 Hz, CH), 133.55 (d, $J_{C\text{-}C\text{-}C\text{-}C\text{-}F}$ = 3.2, C), 166.03 (d, $J_{C\text{-}F}$ = 254.60, C), 199.15 (C)

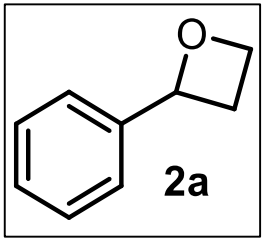
4-hydroxy-1-(4'-*tert*-butylphenyl)-1-butanone (3g)

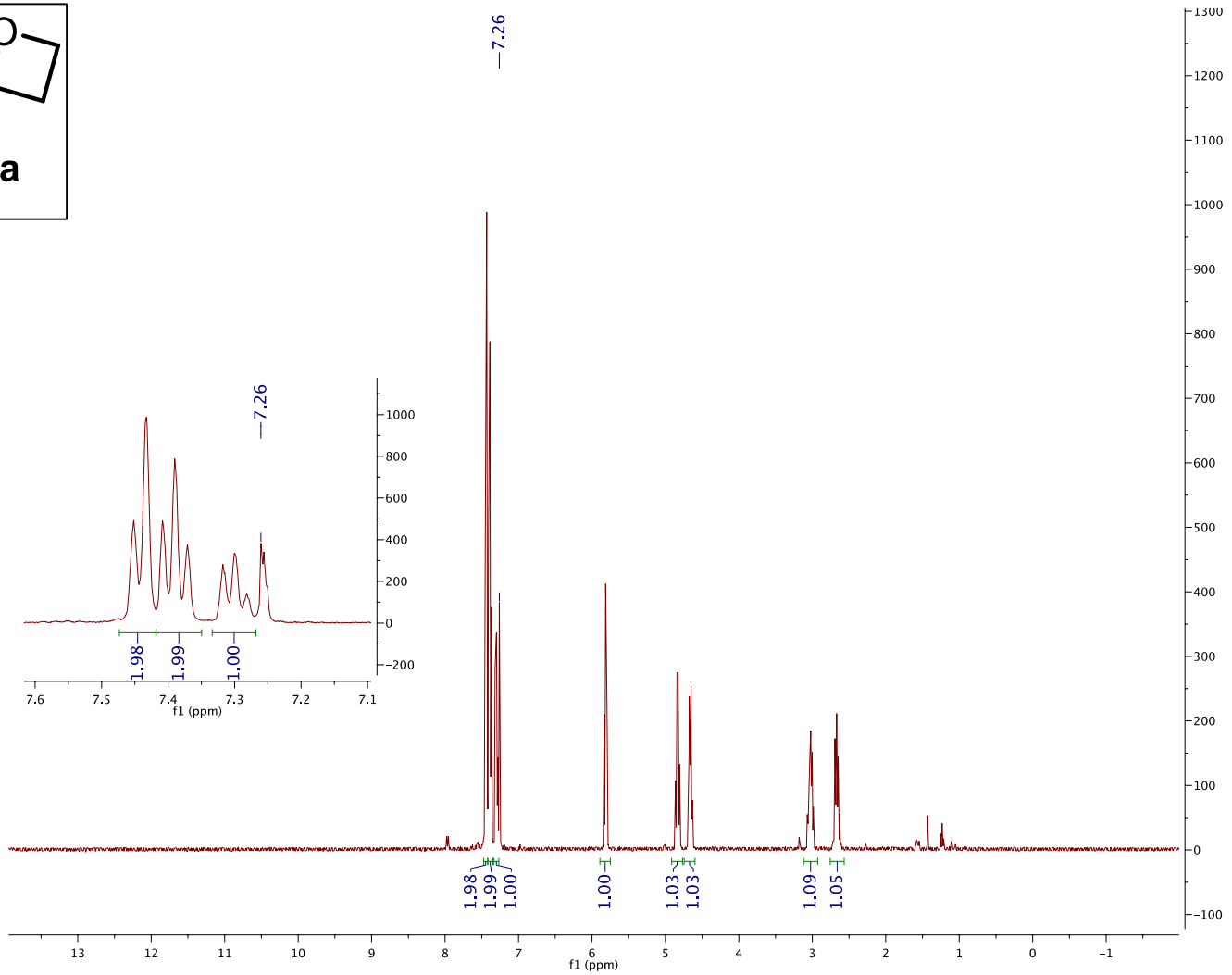
4-hydroxy-1-(4'-tert-butylphenyl)-1-butanone was obtained *via* the same protocol as **3e** with the following modification: the reaction was conducted using 2-(4'-*tert*-butylphenyl)tetrahydrofuran (1.57 g, 0.00768 mol). The product (0.602 g, 36%) was obtained as a clear yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm 1.34 (s, 9 H) 2.02 (t, *J*=6.27 Hz, 2 H) 3.12 (t, *J*=6.91 Hz, 2 H) 3.74 (t, *J*=6.05 Hz, 2 H) 7.44 - 7.51 (m, 2 H) 7.87 - 7.97 (m, 2 H)
^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 27.28 (CH_2), 31.34 (CH_3), 31.64 (C), 35.50 (CH_2), 62.61 (CH_2), 125.80 (CH), 128.35 (CH), 134.53 (C), 157.14 (C), 200.56 (C)

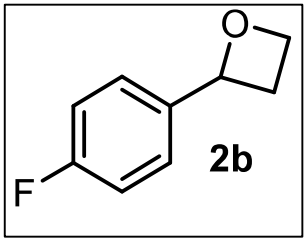
^{1}H-NMR Spectra of Synthesized Compounds

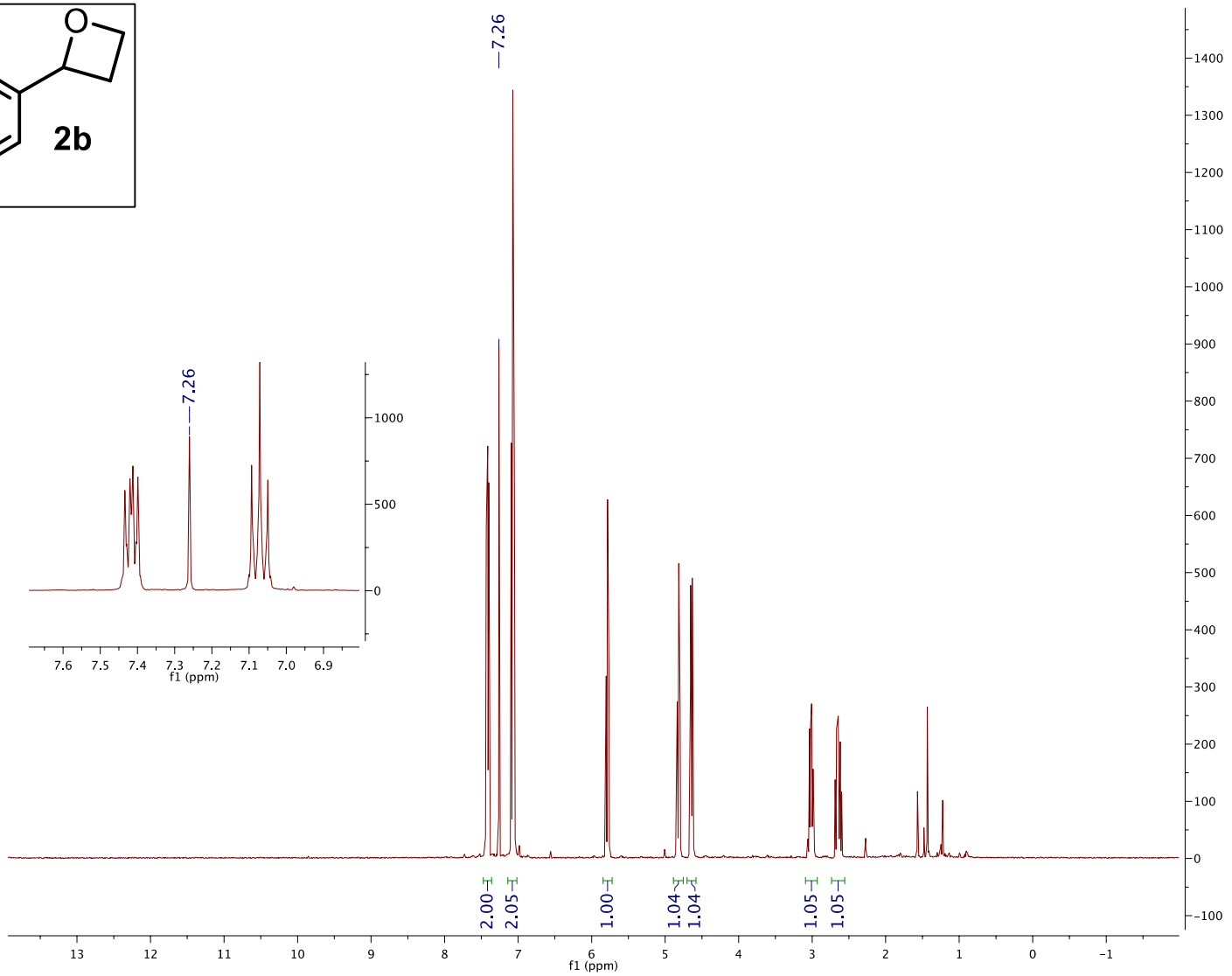
2-phenyloxetane (2a)
400 MHz, $CDCl_3$



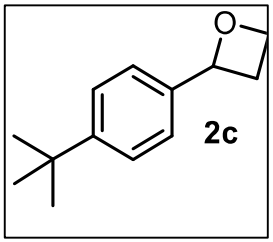


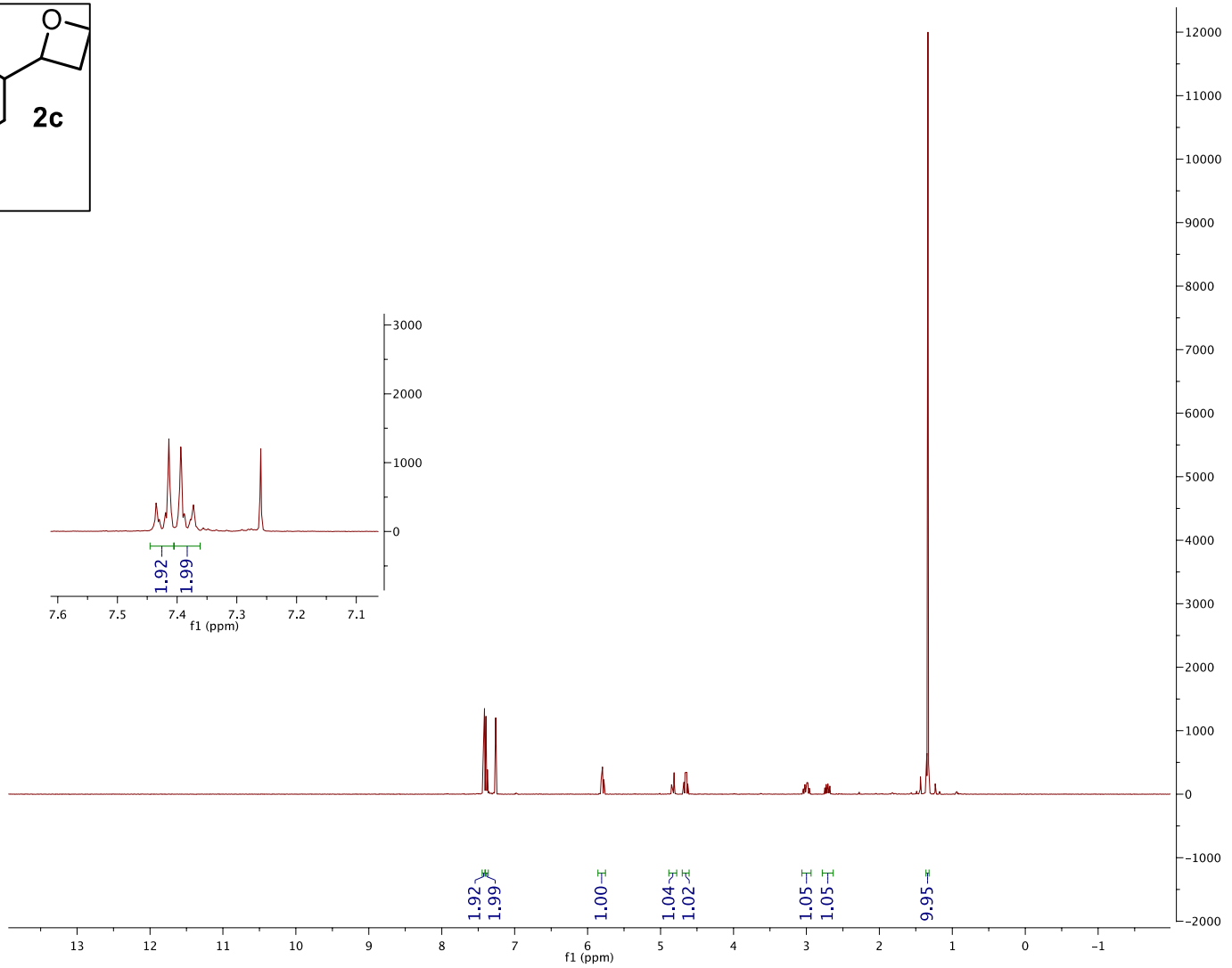
2-(4'-fluorophenyl)oxetane (2b)
400 MHz, $CDCl_3$



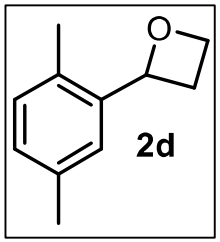


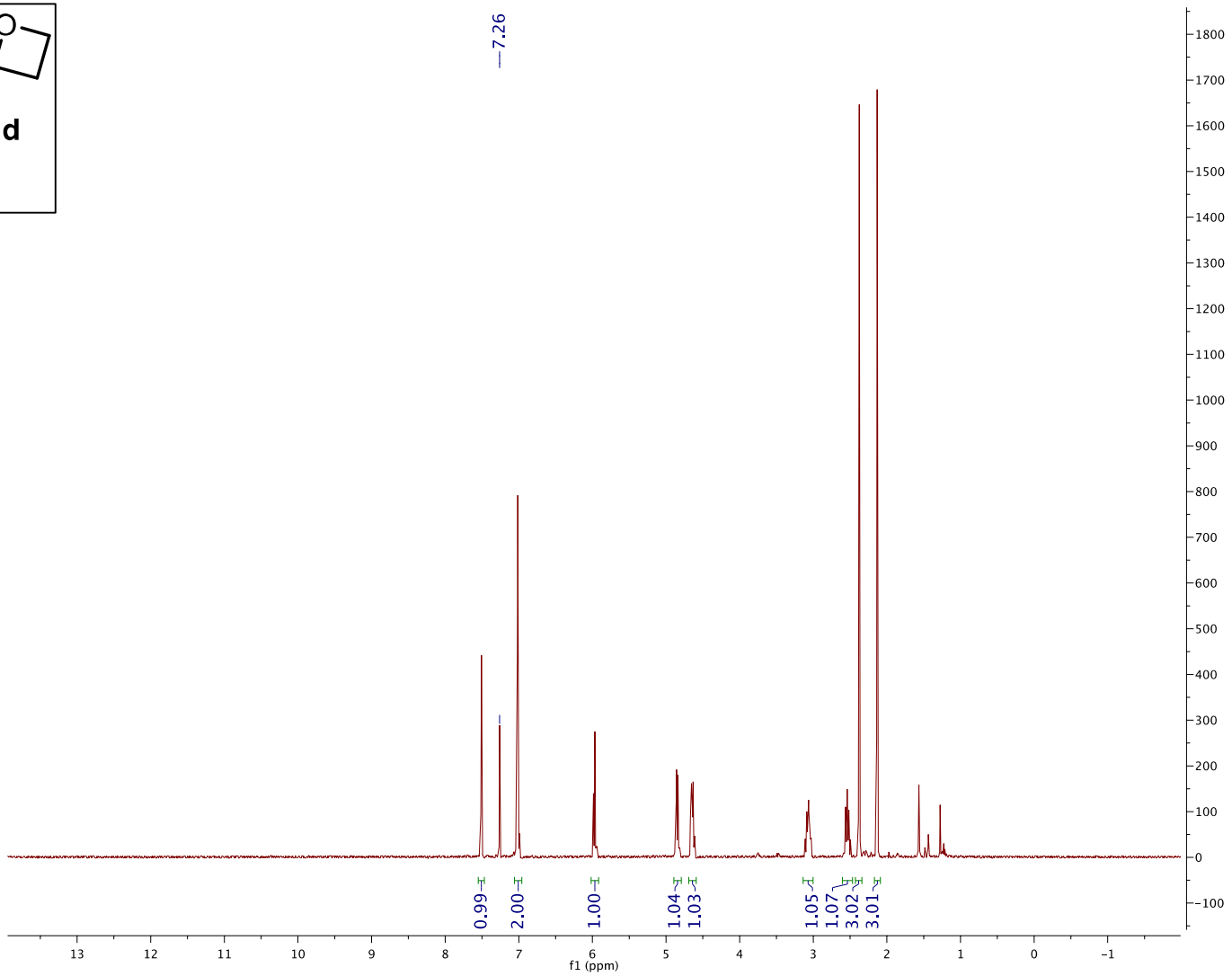
2-(4'-*tert*-butylphenyl)oxetane (2c)
400 MHz, $CDCl_3$



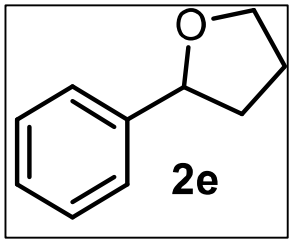


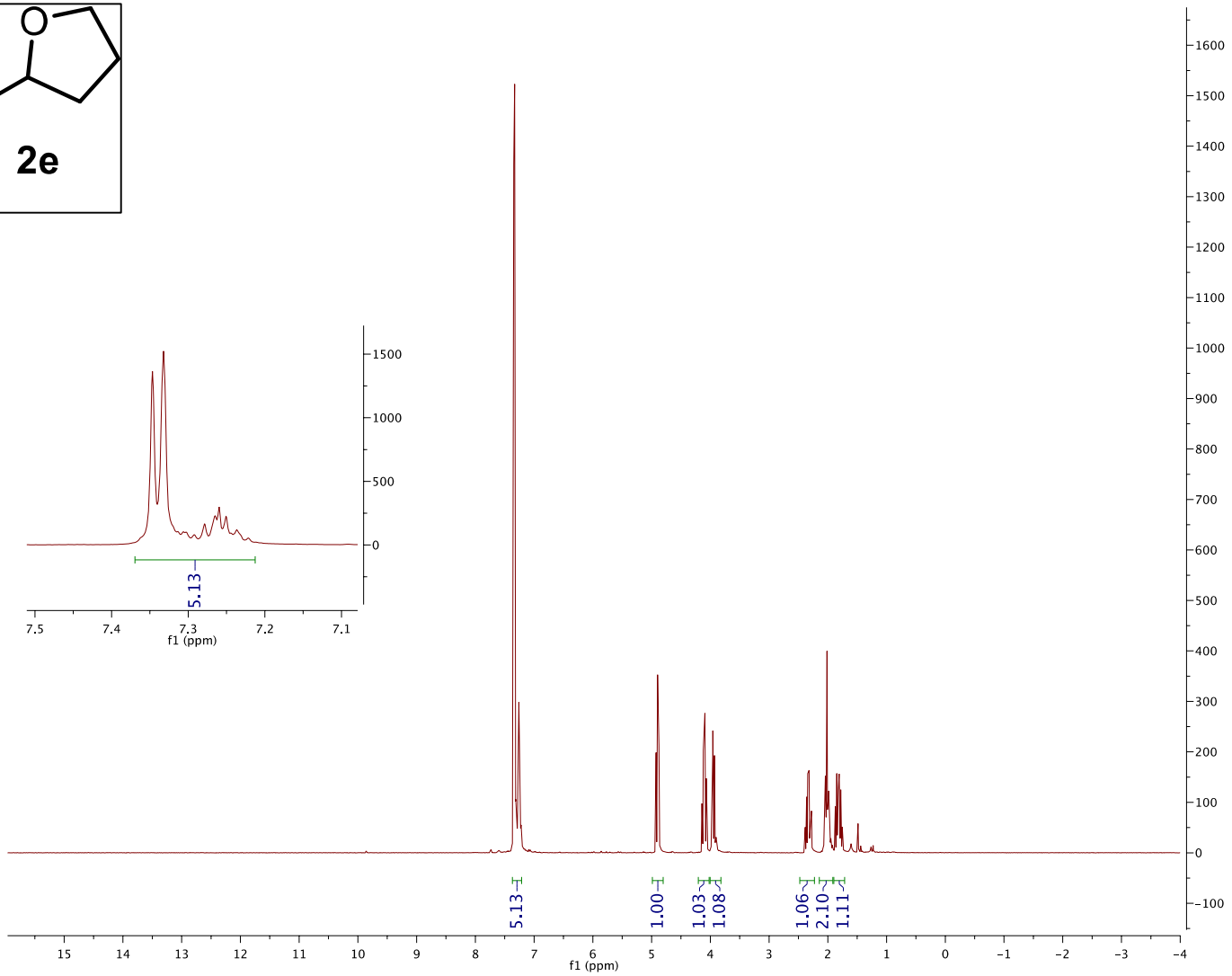
2-(2',5'-dimethylphenyl)oxetane (2d)
400 MHz, $CDCl_3$



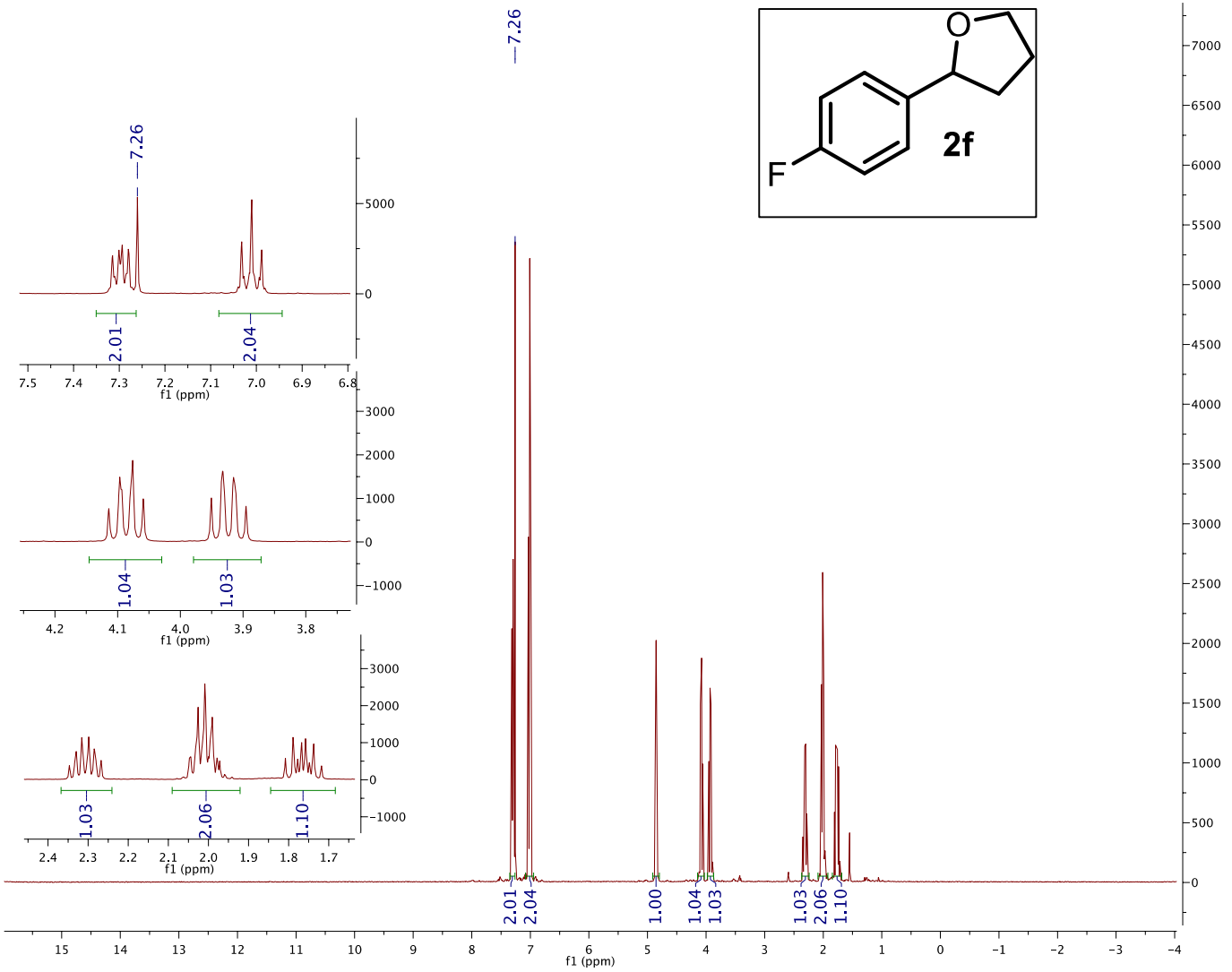


2-phenyltetrahydrofuran (2e)
400 MHz, $CDCl_3$

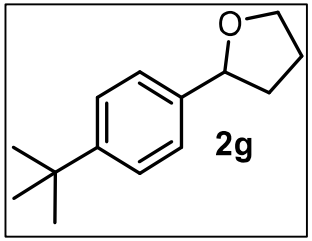


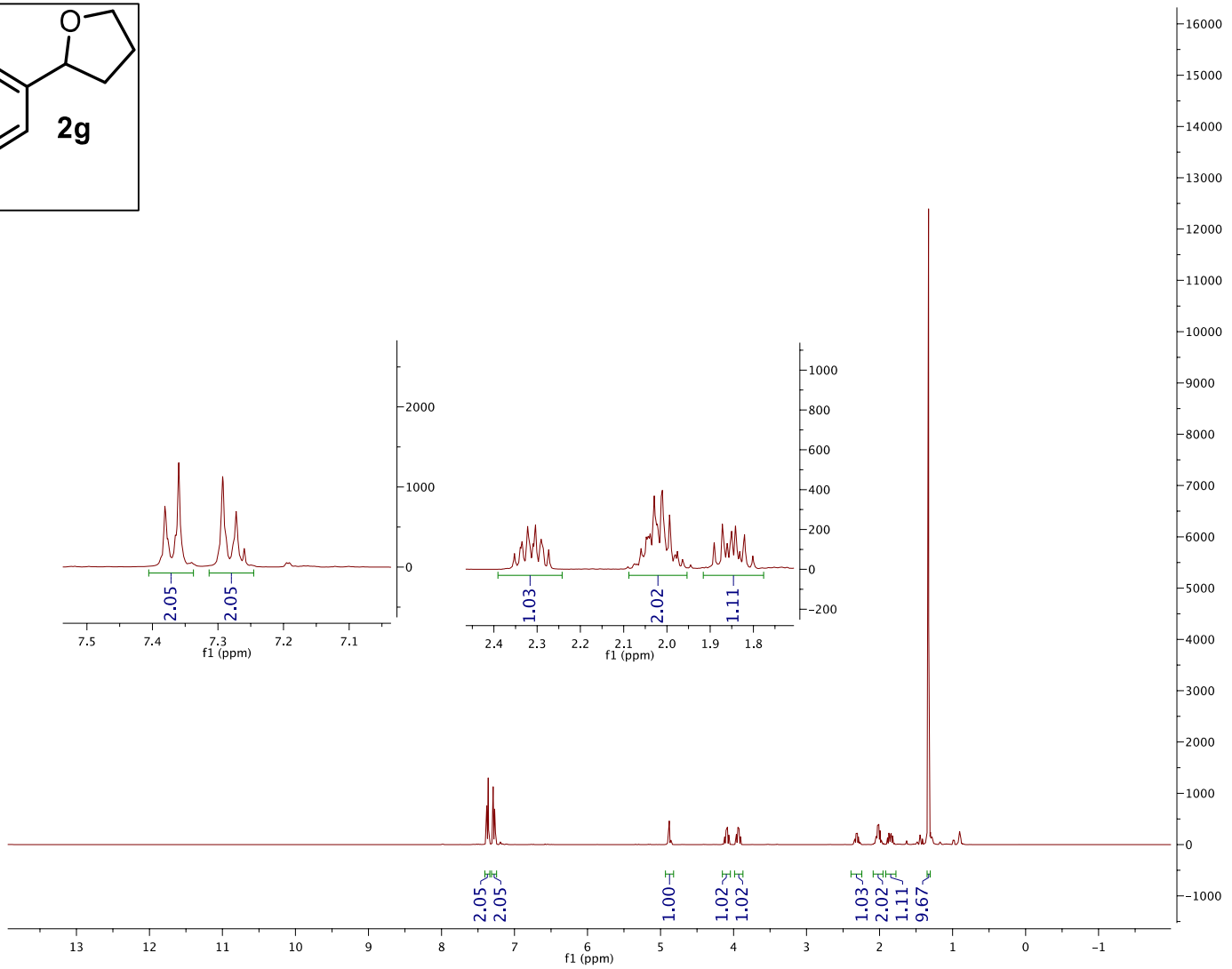


2-(4'-fluorophenyl)tetrahydrofuran (2f)
400 MHz, $CDCl_3$

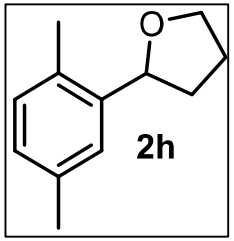


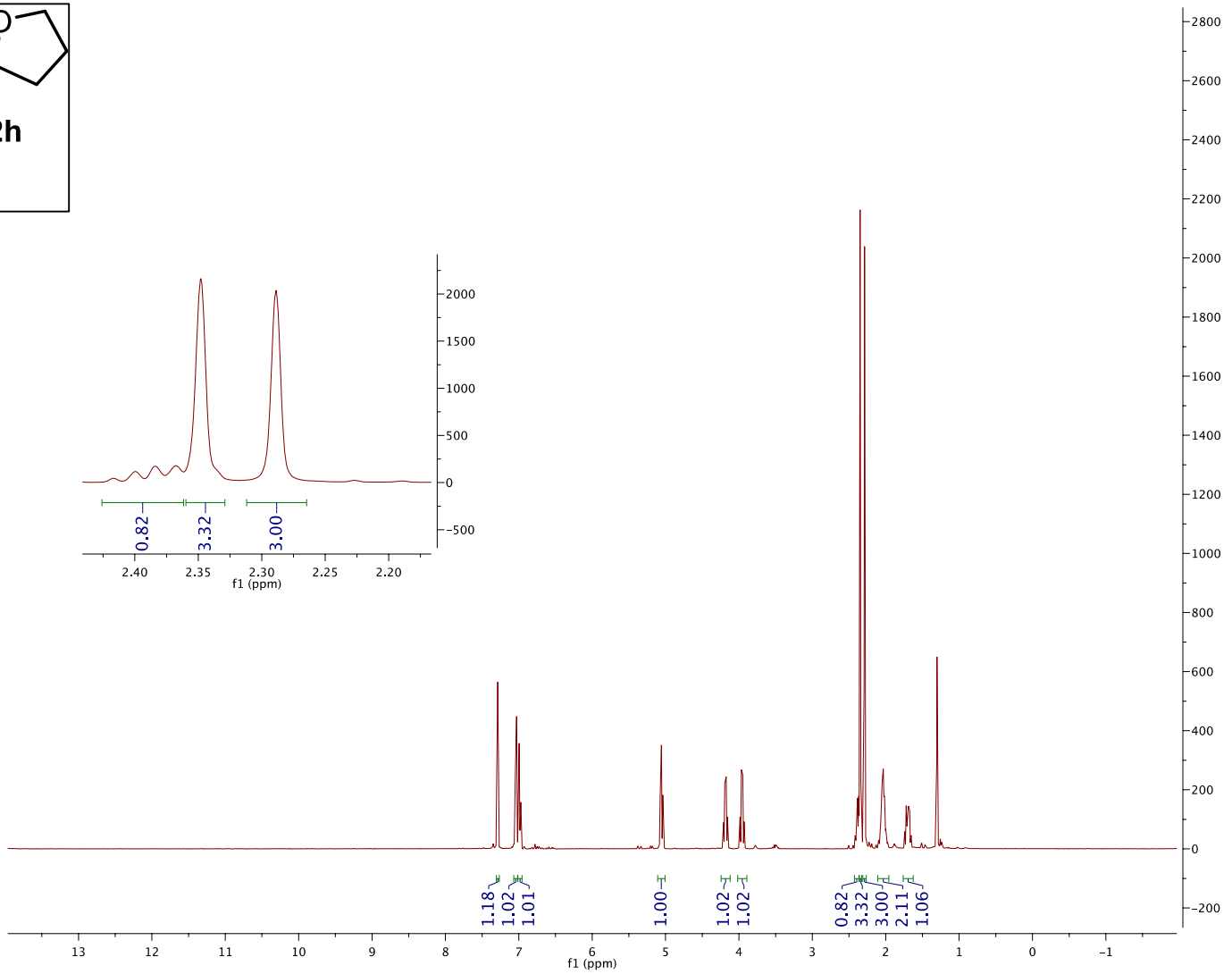
2-(4'-*tert*-butylphenyl)tetrahydrofuran (2g)
400 MHz, $CDCl_3$



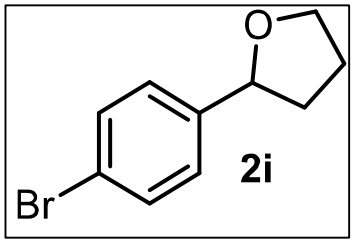


2-(2',5'-dimethylphenyl)tetrahydrofuran (2h)
400 MHz, $CDCl_3$

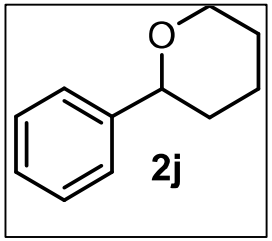


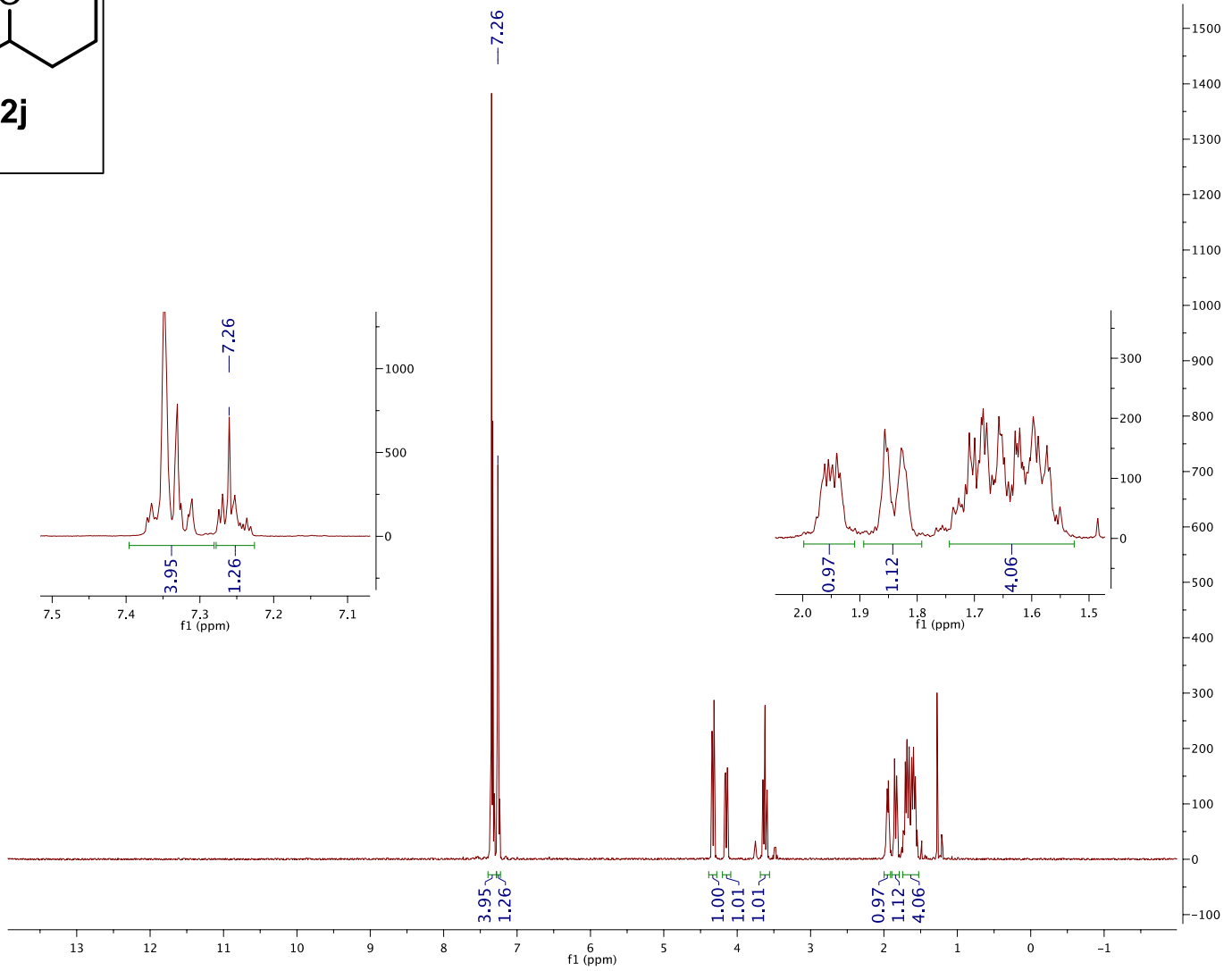


2-(4'-bromophenyl)tetrahydrofuran (2i)
400 MHz, $CDCl_3$

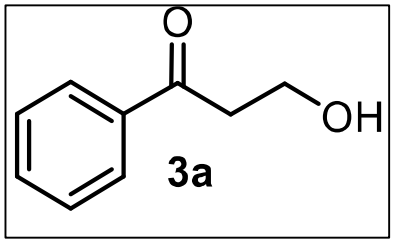


2-phenyltetrahydropyran (2j)
400 MHz, $CDCl_3$

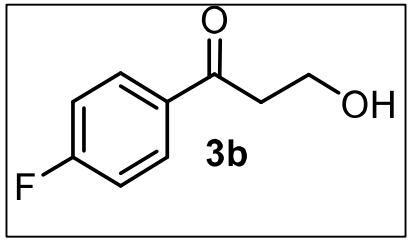




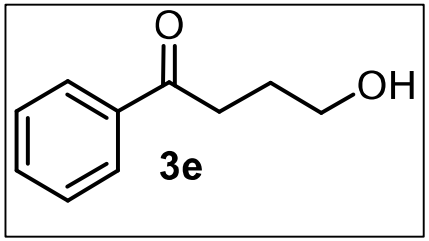
3-hydroxy-1-phenyl-1-propanone (3a)
400 MHz, $CDCl_3$



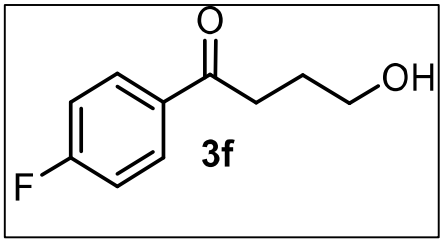
3-hydroxy-1-(4'-fluorophenyl)-1-propanone (3b)
400 MHz, $CDCl_3$



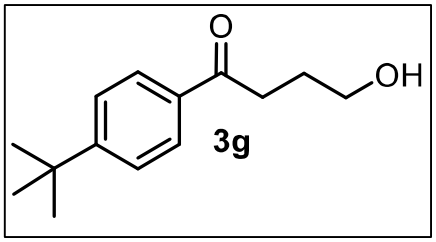
4-hydroxy-1-phenyl-1-butanone (3e)
400 MHz, $CDCl_3$



4-hydroxy-1-(4'-fluorophenyl)-1-butanone (3f)
400 MHz, $CDCl_3$

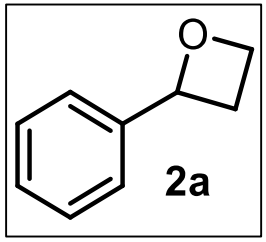


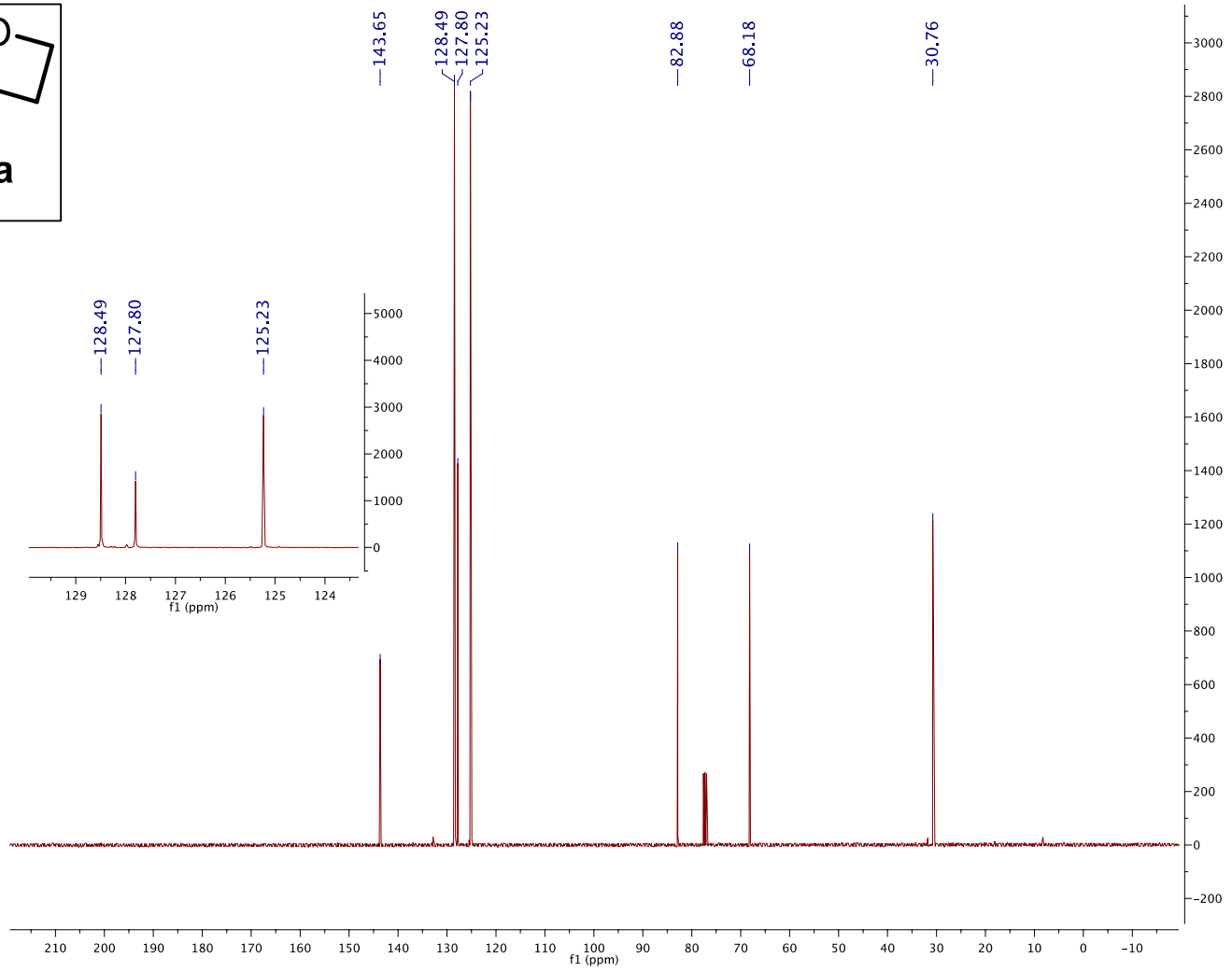
4-hydroxy-1-(4'-*tert*-butylphenyl)-1-butanone (3g)
400 MHz, $CDCl_3$



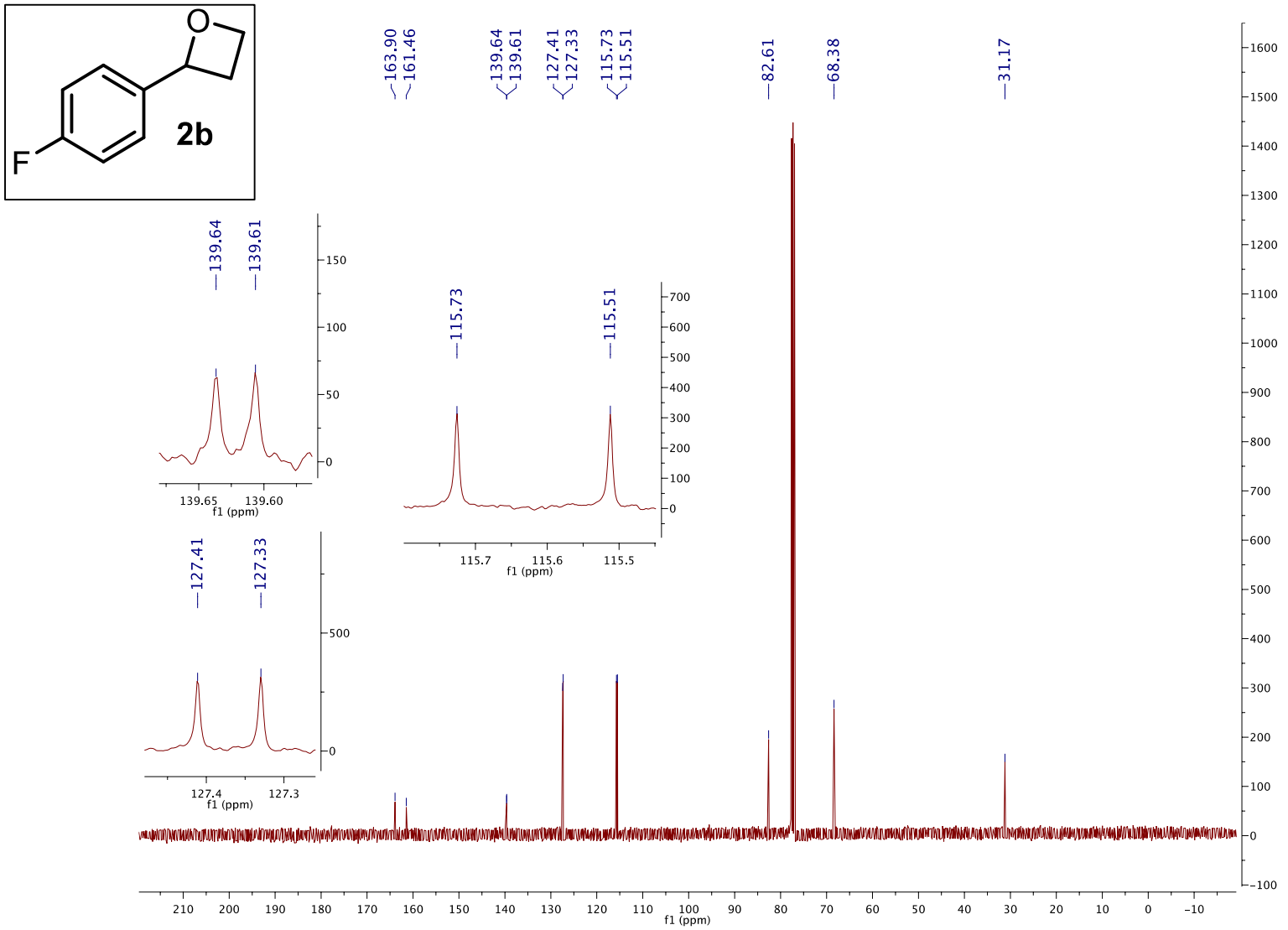
^{13}C-NMR Spectra of Synthesized Compounds

2-phenyloxetane (2a)
100 MHz, $CDCl_3$

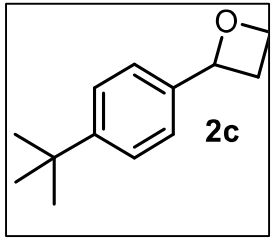


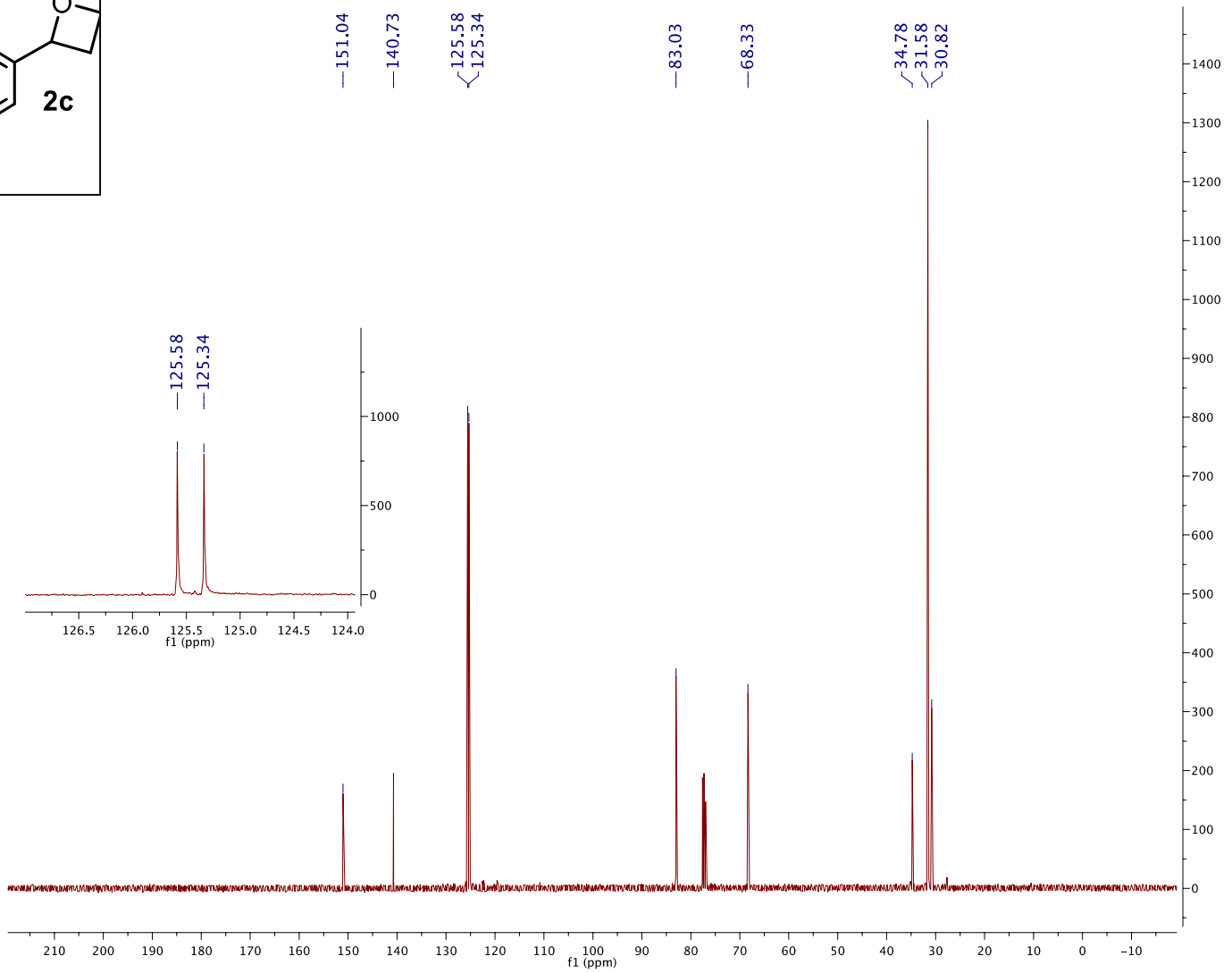


2-(4'-fluorophenyl)oxetane (2b)
100 MHz, $CDCl_3$

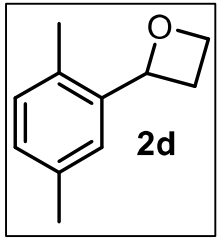


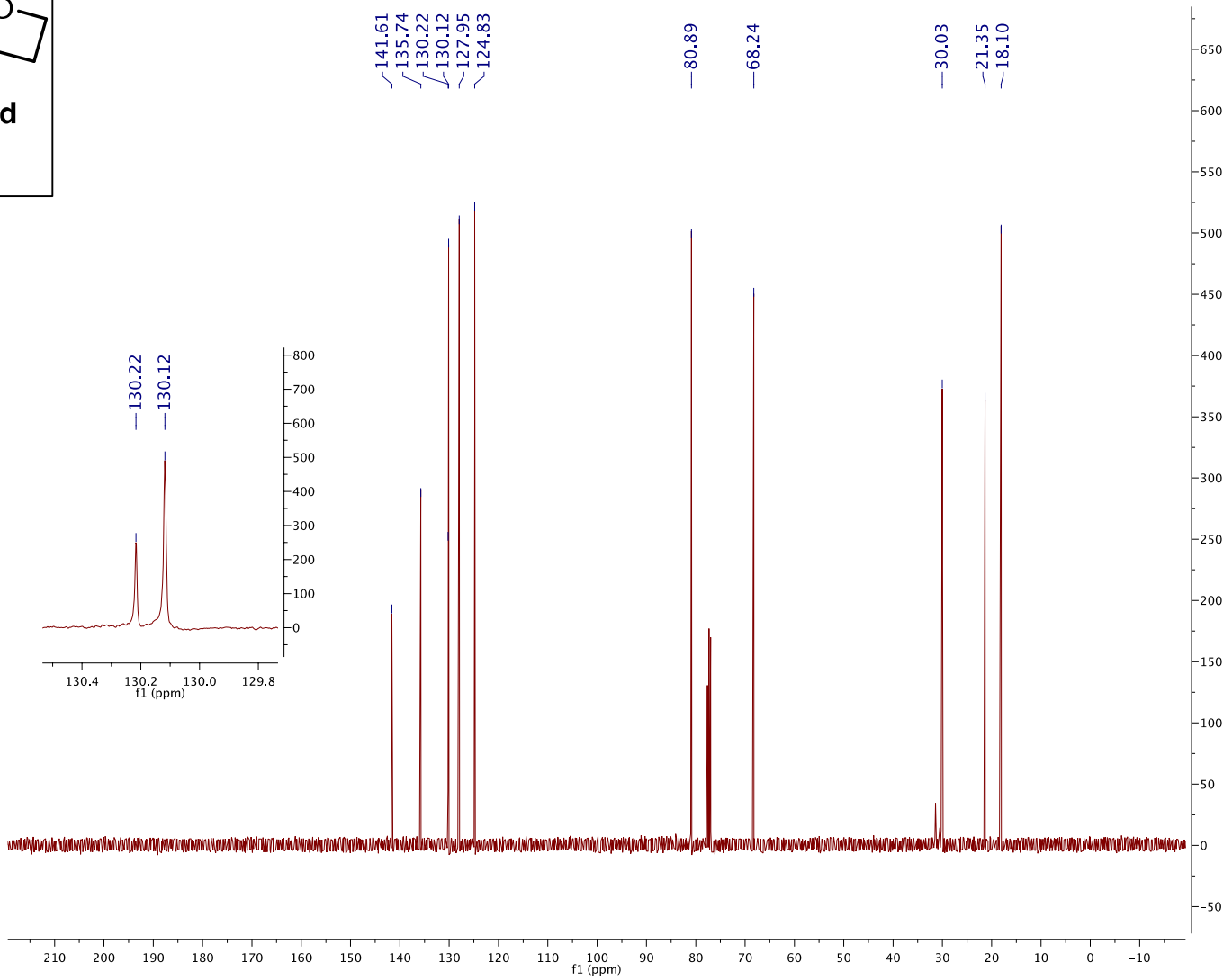
2-(4'-*tert*-butylphenyl)oxetane (2c)
100 MHz, $CDCl_3$



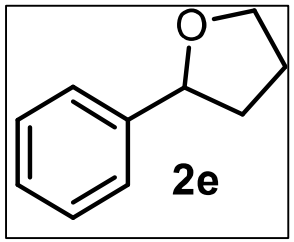


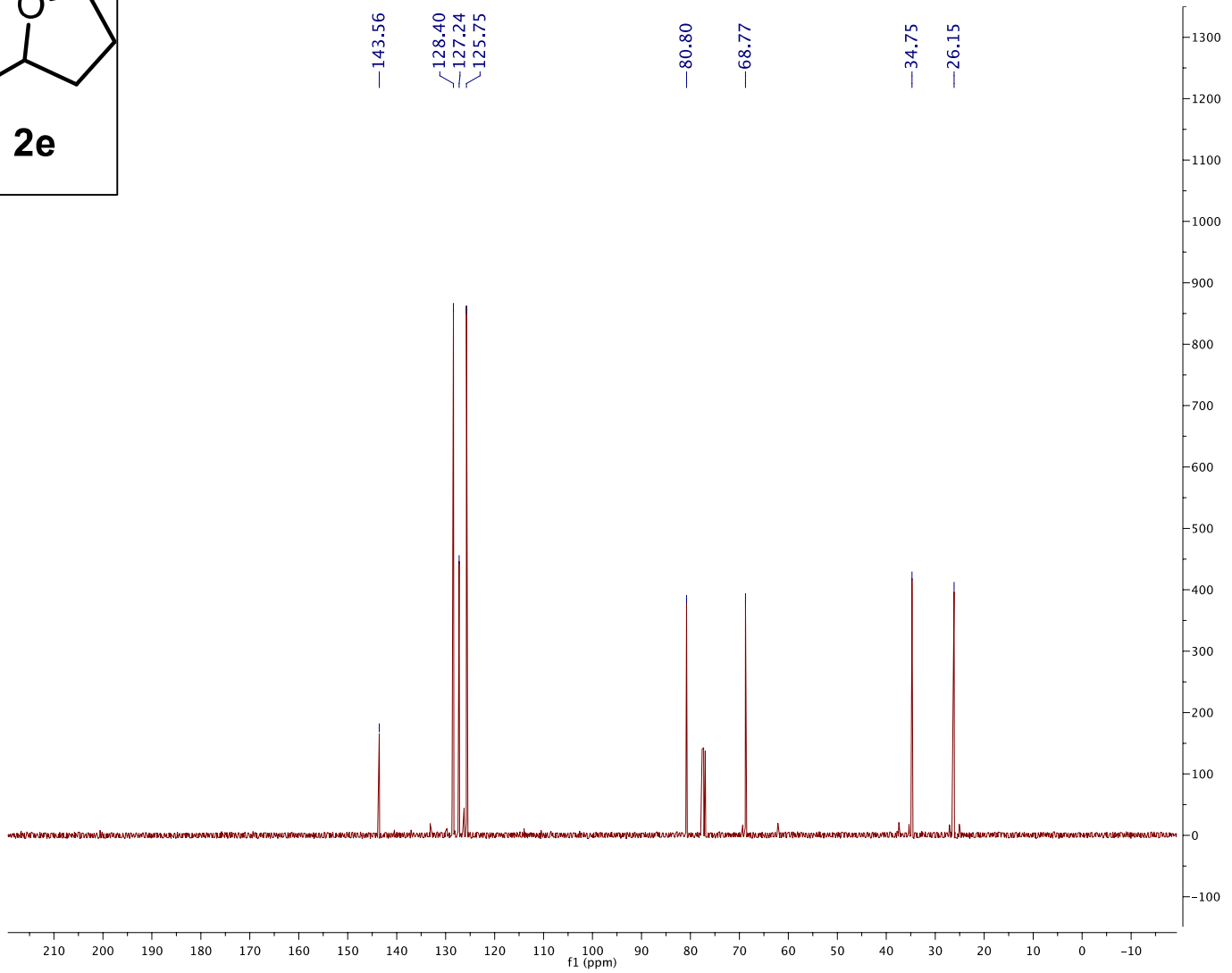
2-(2',5'-dimethylphenyl)oxetane (2d)
100 MHz, $CDCl_3$



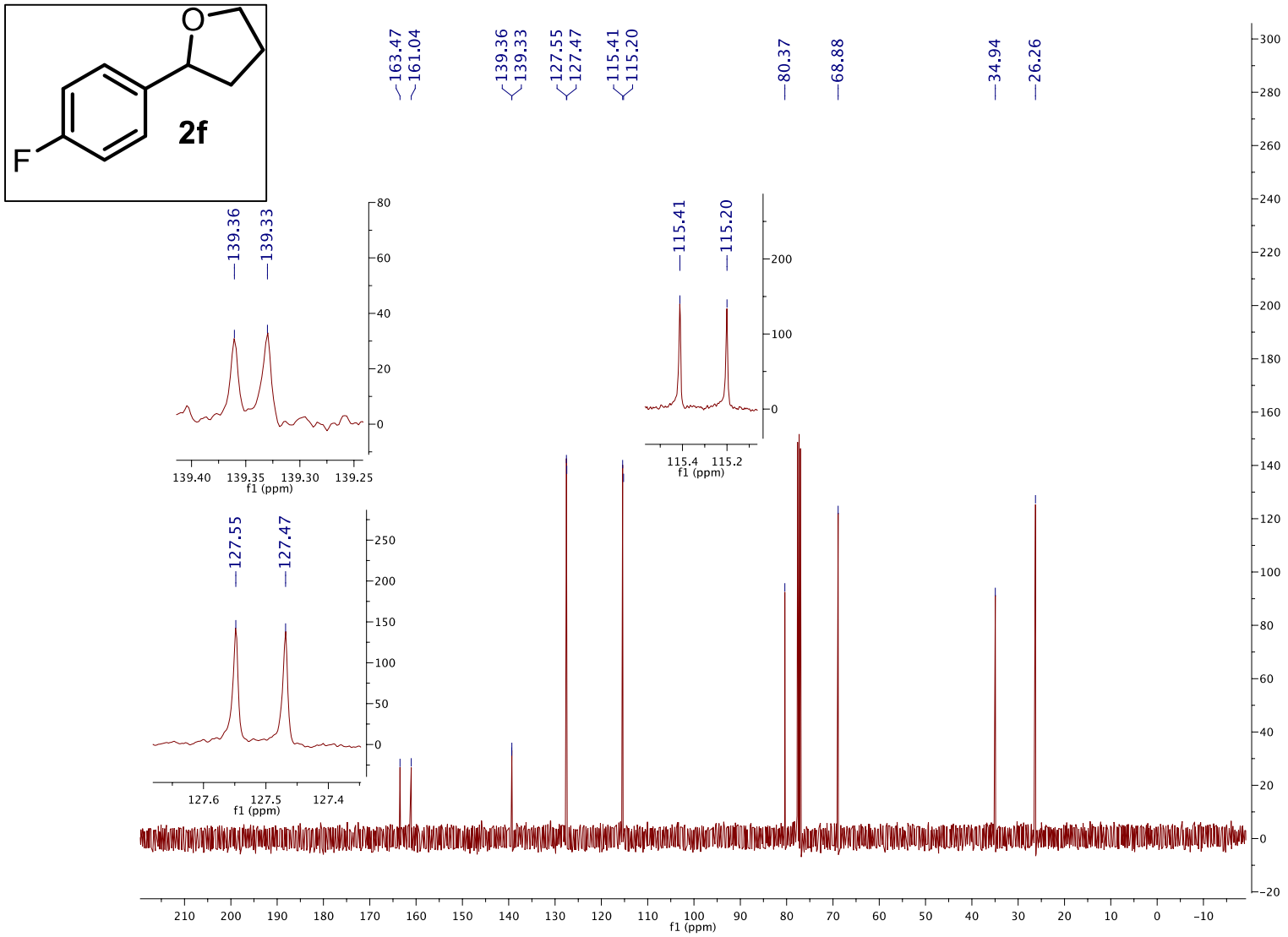


2-phenyltetrahydrofuran (2e)
100 MHz, $CDCl_3$

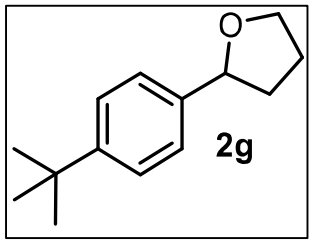


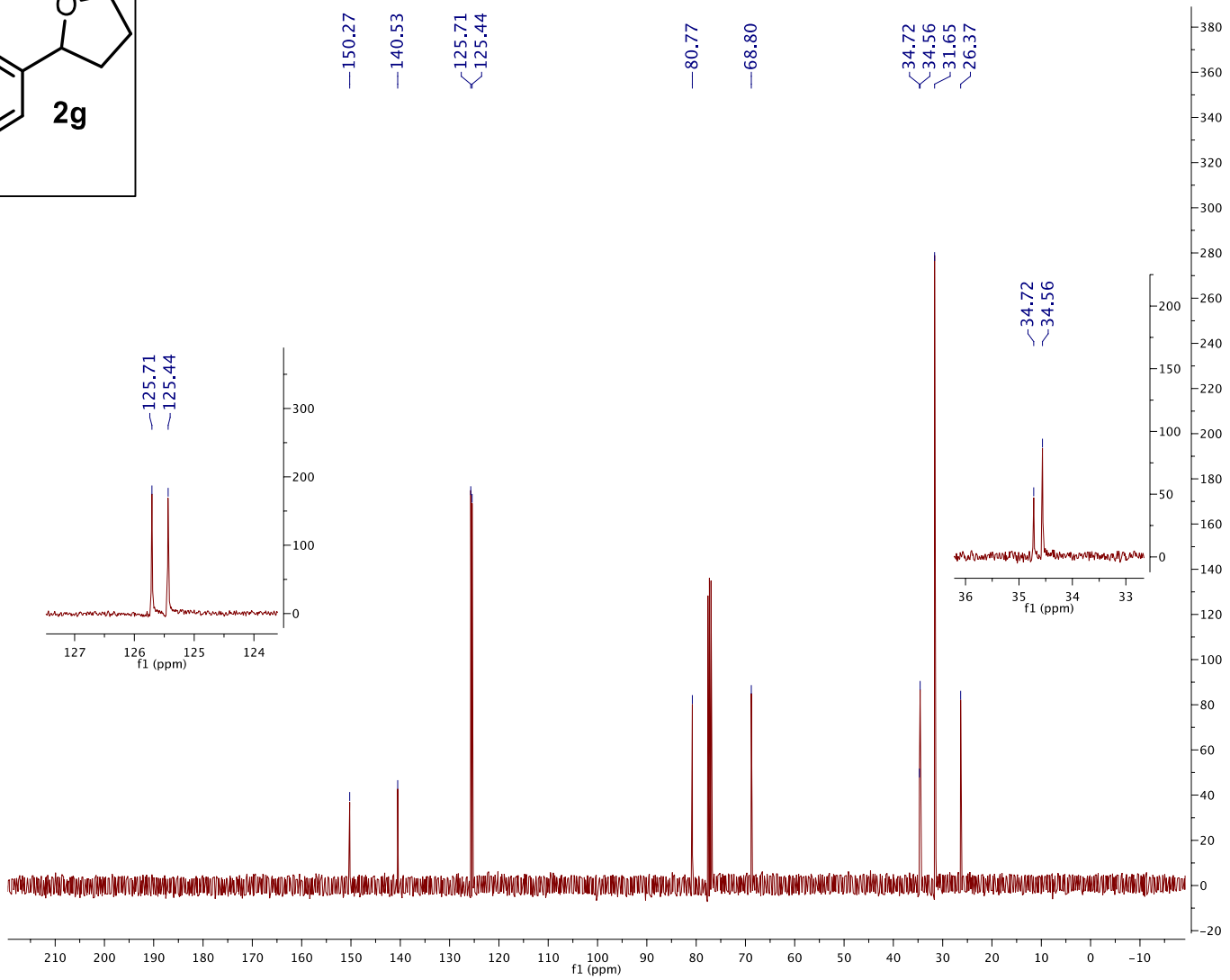


2-(4'-fluorophenyl)tetrahydrofuran (2f)
100 MHz, $CDCl_3$

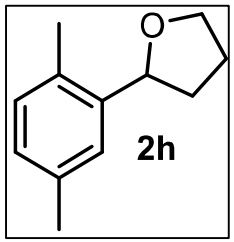


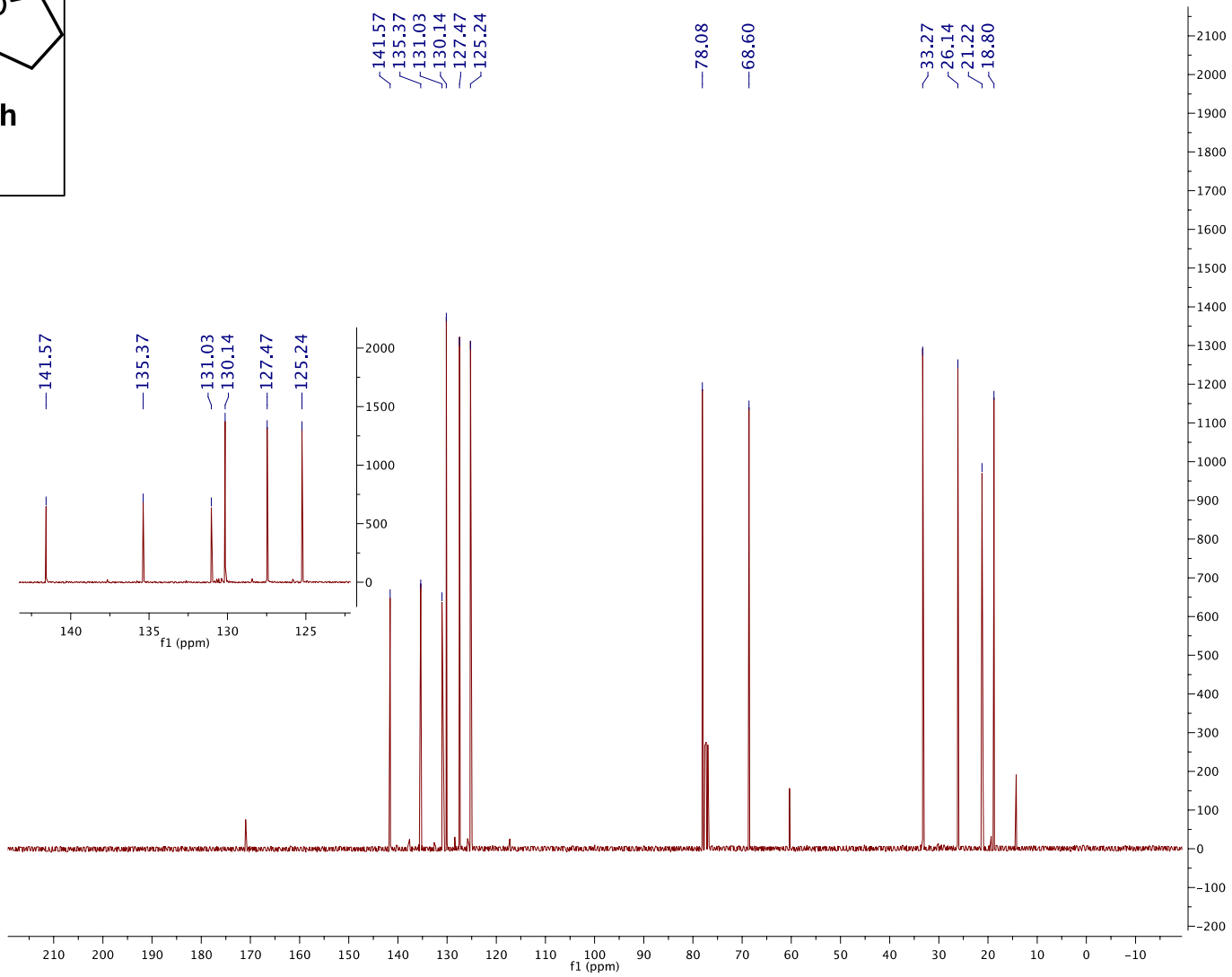
2-(4'-*tert*-butylphenyl)tetrahydrofuran (2g)
100 MHz, $CDCl_3$



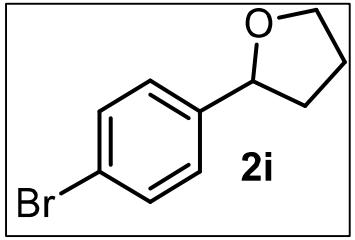


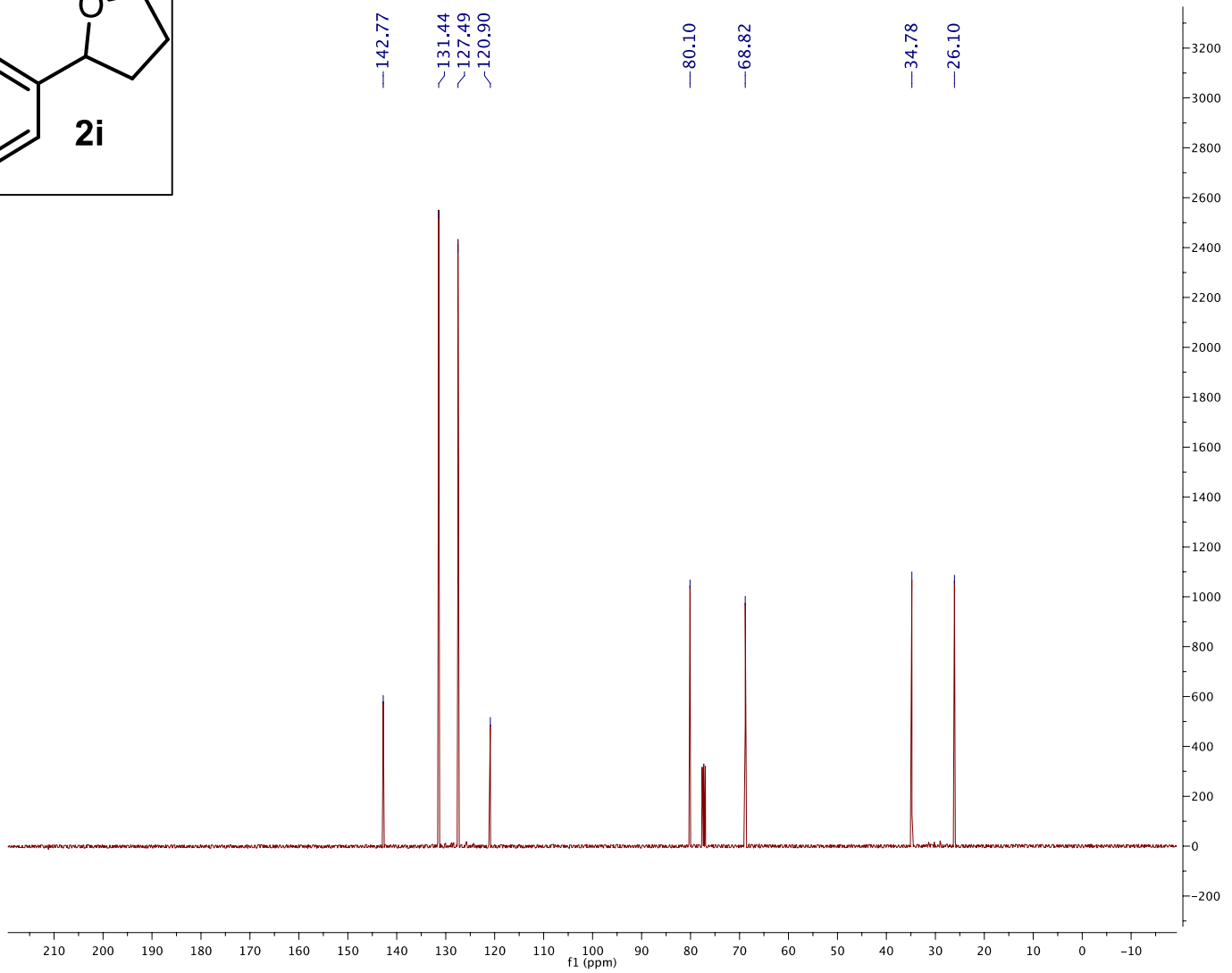
2-(2',5'-dimethylphenyl)tetrahydrofuran (2h)
100 MHz, $CDCl_3$



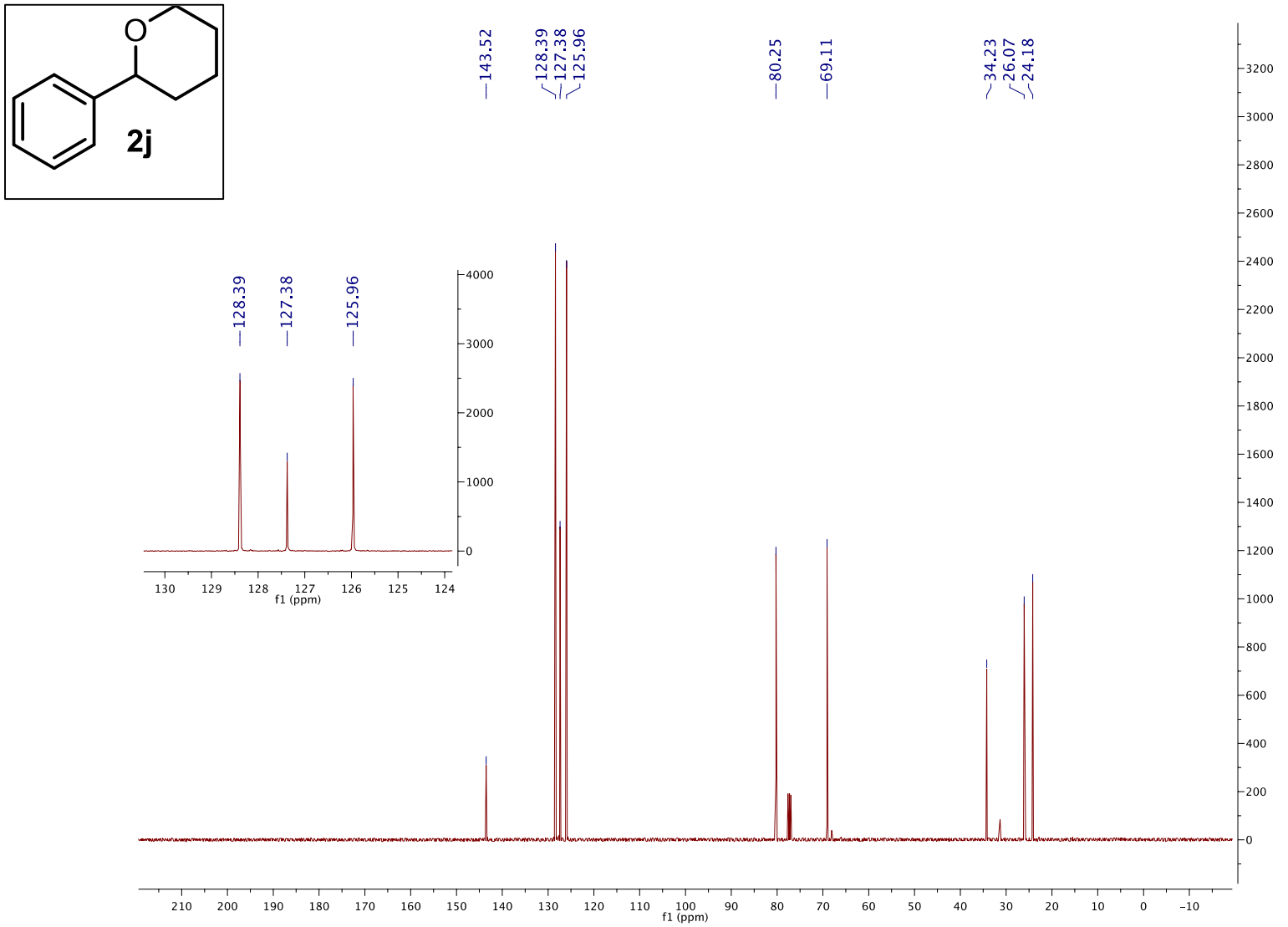


2-(4'-bromophenyl)tetrahydrofuran (2i)
100 MHz, $CDCl_3$

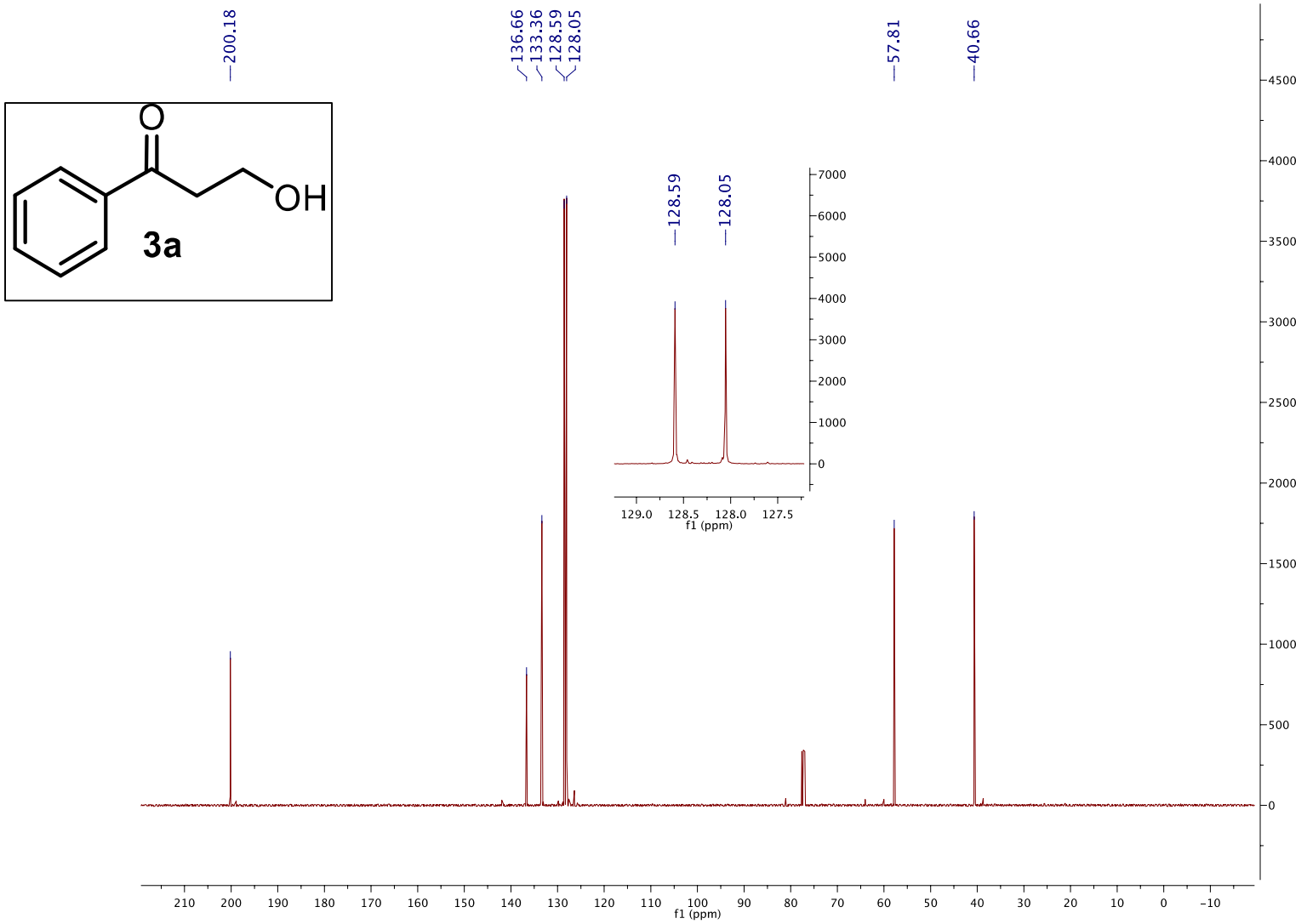




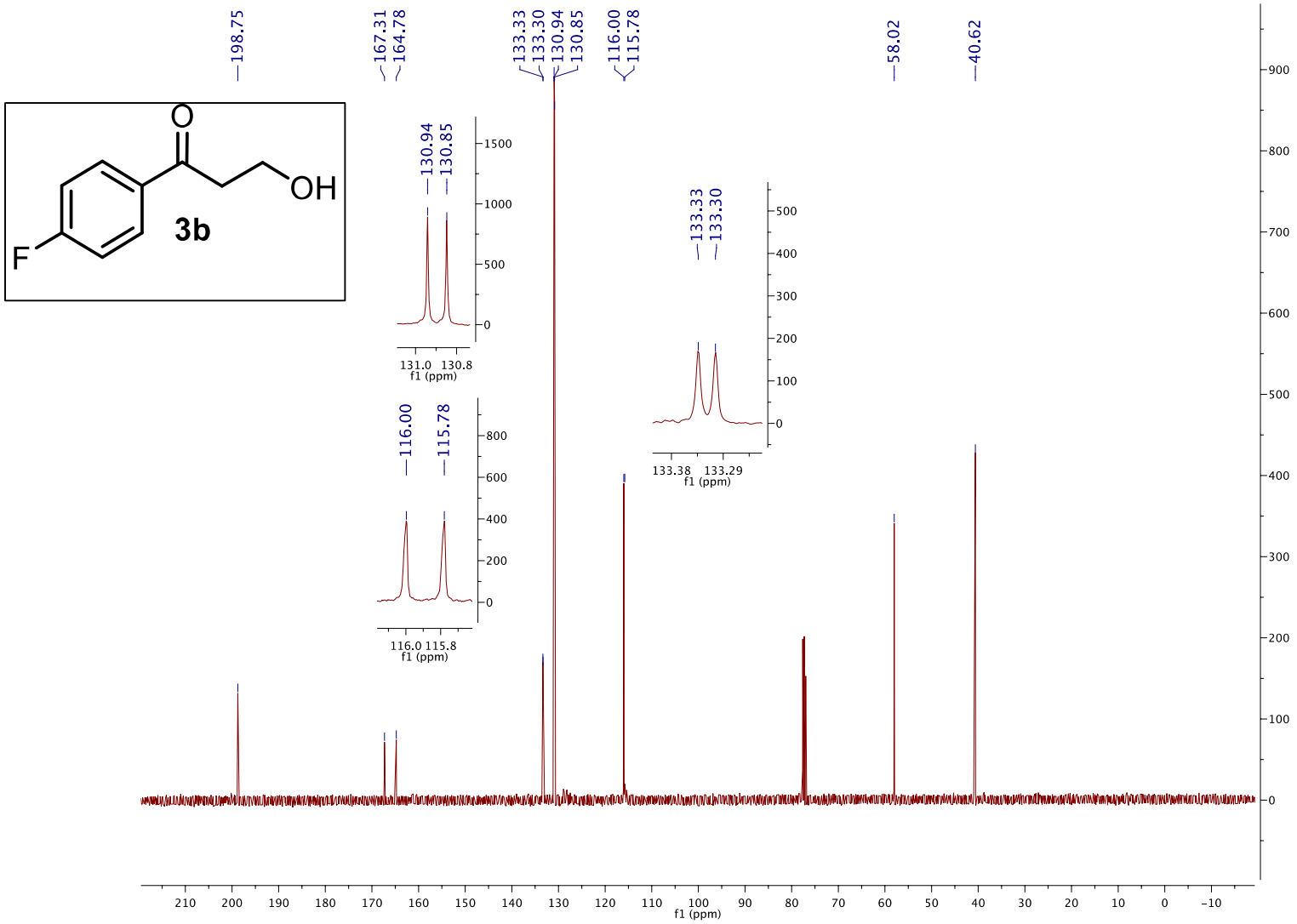
2-phenyltetrahydropyran (2j)
100 MHz, $CDCl_3$



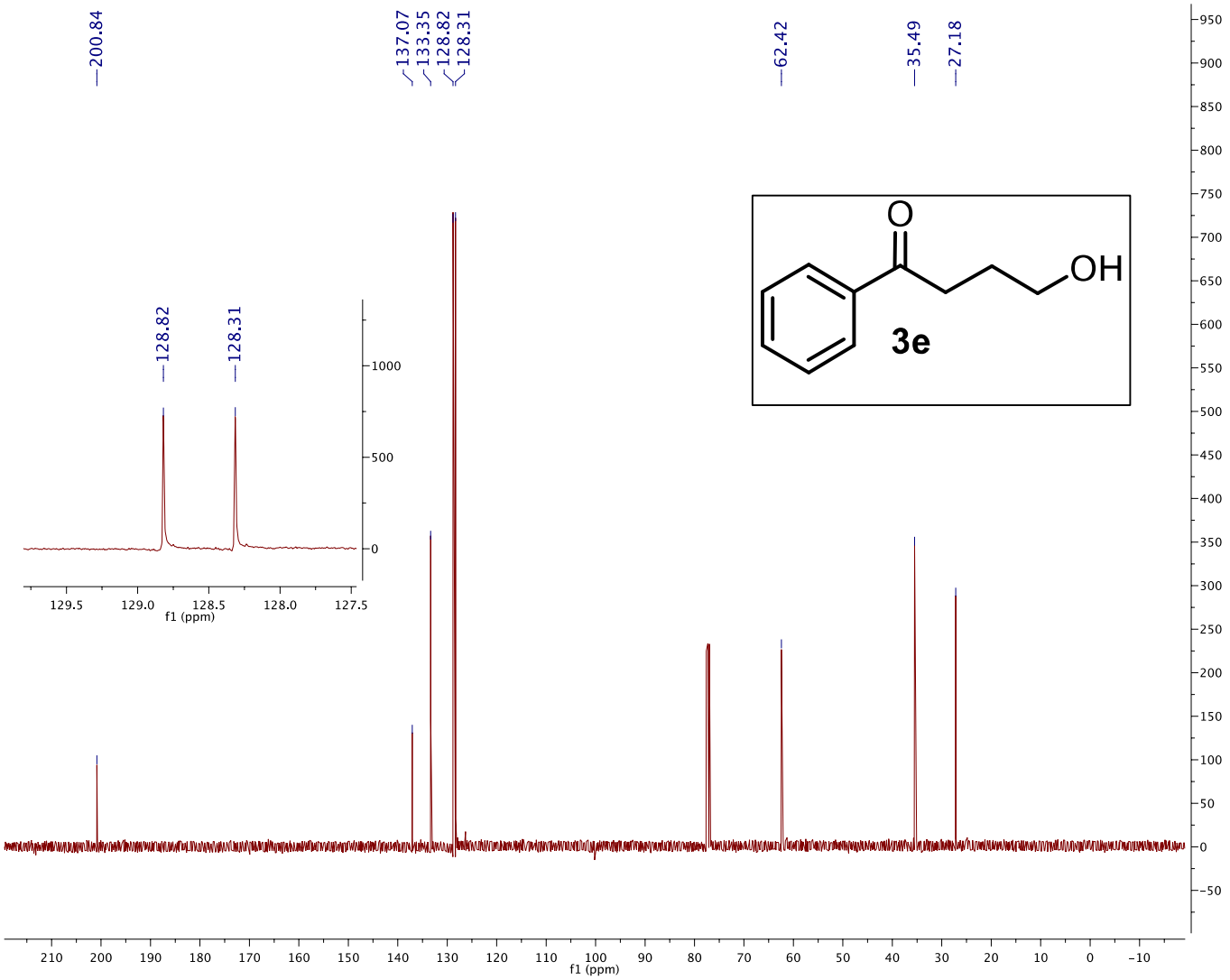
3-hydroxy-1-phenyl-1-propanone (3a)
100 MHz, $CDCl_3$



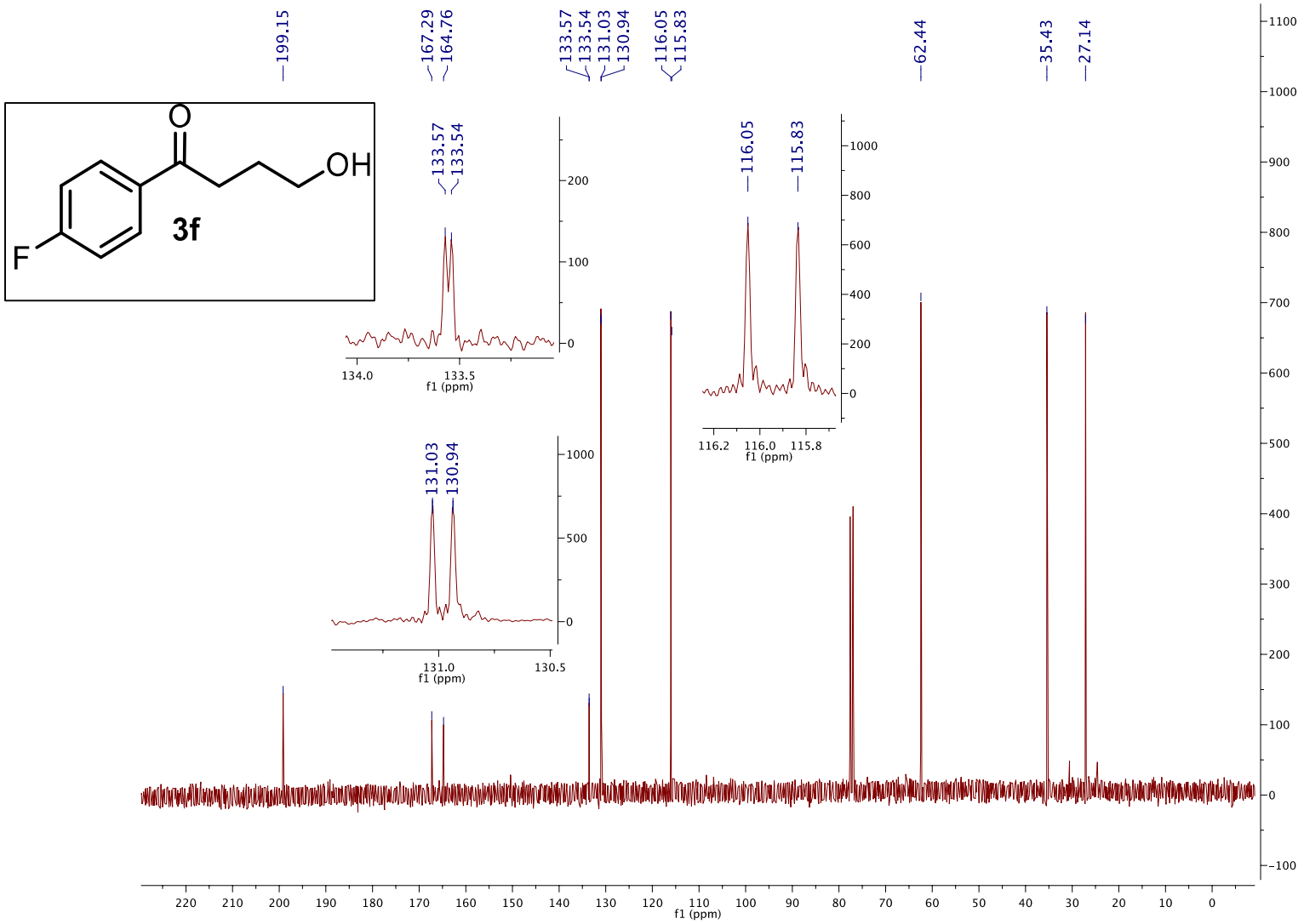
3-hydroxy-1-(4'-fluorophenyl)-1-propanone (3b)
100 MHz, $CDCl_3$



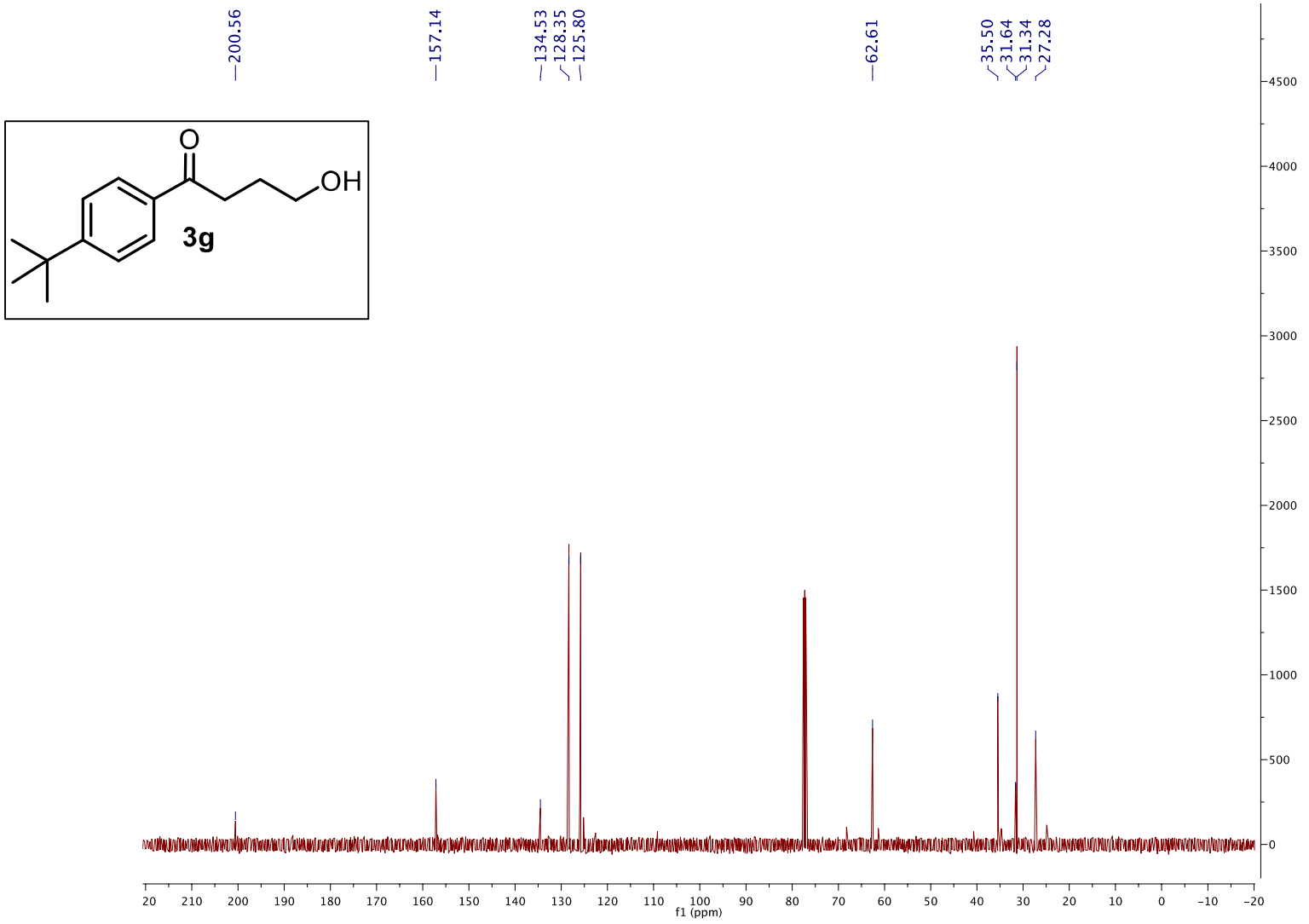
4-hydroxy-1-phenyl-1-butanone (3e)
100 MHz, $CDCl_3$



4-hydroxy-1-(4'-fluorophenyl)-1-butanone (3f)
100 MHz, $CDCl_3$

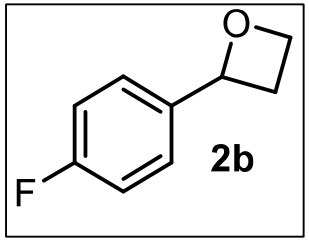


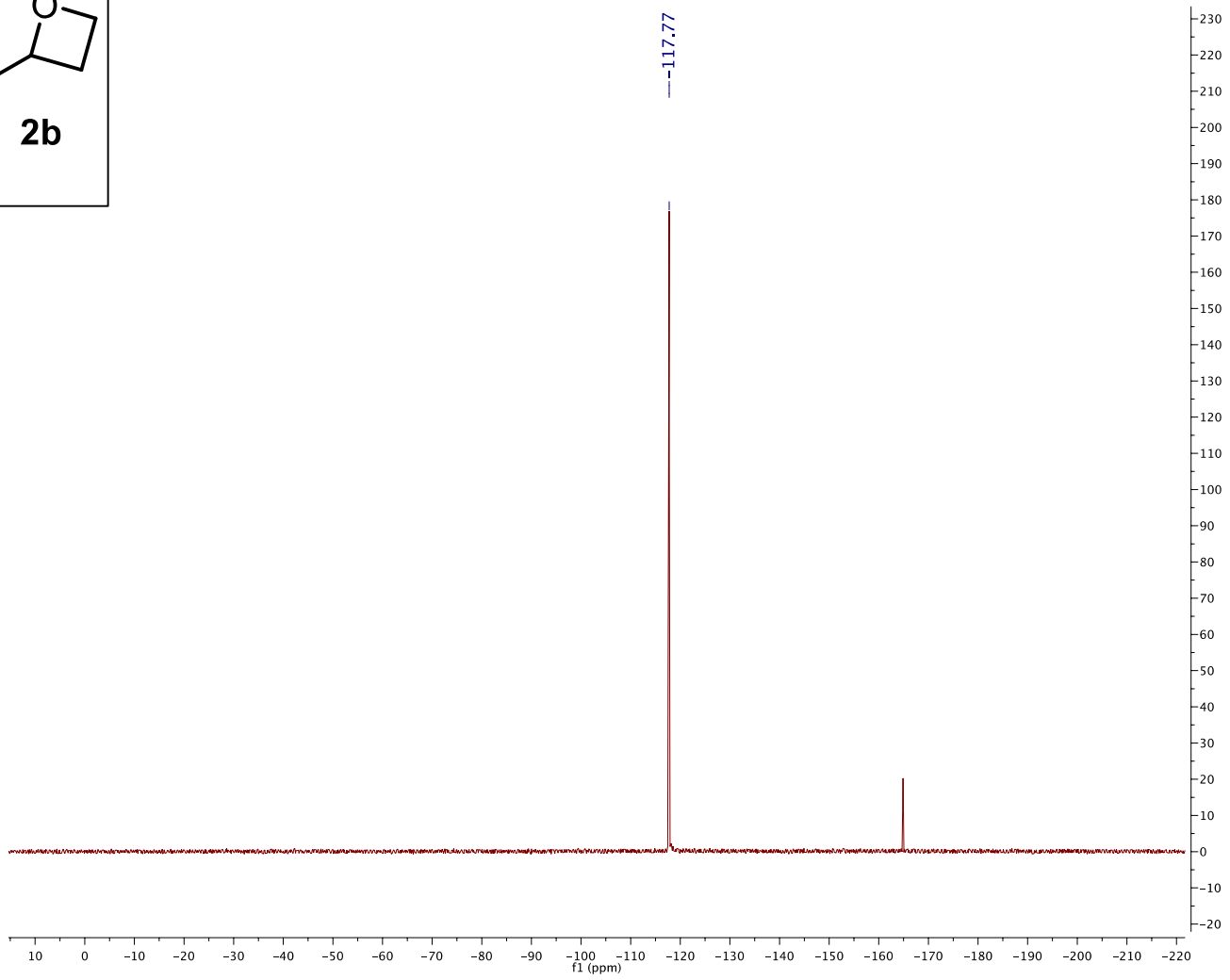
4-hydroxy-1-(4'-*tert*-butylphenyl)-1-butanone (3g)
100 MHz, $CDCl_3$



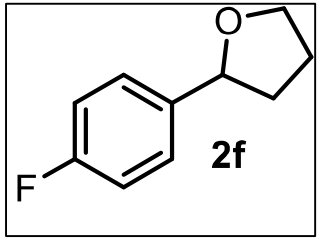
^{19}F-NMR Spectra of Synthesized Compounds

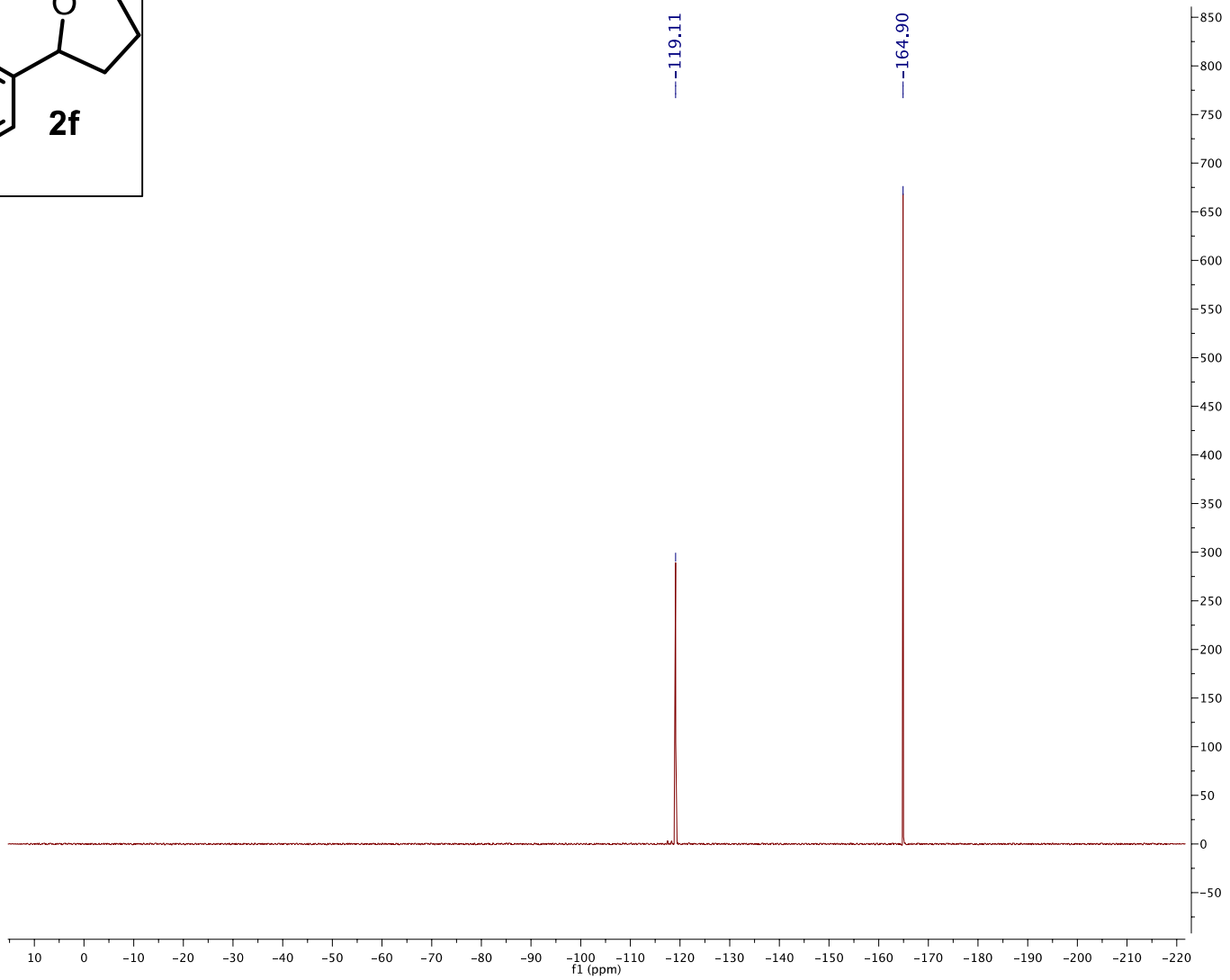
2-(4'-fluorophenyl)oxetane (2b)
377 MHz, $CDCl_3$





2-(4'-fluorophenyl)tetrahydrofuran (2f)
377 MHz, $CDCl_3$





3-hydroxy-1-(4'-fluorophenyl)-1-propanone (3b)
377 MHz, $CDCl_3$