A Palladium-Catalyzed Regioselective Hydroesterification of Alkenylphenols to Lactones with Phenyl Formate as CO Source

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Supporting Information

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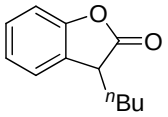
General Methods. All commercially available reagents were used without further purification. Mesitylene was purchased from commercial suppliers and purified by distillation prior to use. Other solvents were purified with solvent purification systems. Column chromatography was performed on silica gel (300-400 mesh). ^{1}H NMR spectra were recorded on a 400 MHz NMR spectrometer and ^{13}C NMR spectra were recorded on a 100 MHz NMR spectrometer. IR spectra were recorded on a FT-IR spectrometer. Melting points were uncorrected. Compounds **1n**, **4a**, **4b,** and all ligands were purchased from commercial suppliers. Compounds **4c**,[1] **4d**,[2] **4e**,[3] **1a-c**,[4] **1e**,[5] **1f-m**,[4] **1o**,[6] and **5a**[4] were prepared according to the reported procedures. Compound **1d** was prepared from the esterification of *trans*-2-hydroxycinnamic acid. Compound **1p** was prepared from the reduction of 2-vinylbenzoic acid.

(1) Ueda, T.; Konishi, H.; Manabe, K. *Org. Lett.* **2012**, *14*, 3100. (2) Katafuchi, Y.; Fujihara, T.; Iwai, T.; Terao, J.; Tsuji, Y. *Adv. Synth. Catal.* **2011**, *353*, 475. (3) Pasqua, A. E.; Matheson, M.; Sewell, A. L.; Marquez, R. *Org. Process Res. Dev.* **2011**, *15*, 467. (4) Konishi, H.; Ueda, T.; Muto, T.; Manabe, K. *Org. Lett.* **2012**, *14*, 4722. (5) Van, T. N.; Debenedetti, S.; Kimpe, N. D. *Tetrahedron Lett.* **2003**, *44*, 4199. (6) Karanewsky, D. S.; Kishi, Y. *J. Org. Chem.* **1976**, *41*, 3026.

Representative procedure for hydroesterification (Table 2, entry1). To a stirred mixture of $Pd(OAc)_2$ (0.0056 g, 0.025 mmol), PPh_3 (0.0262 g, 0.10 mmol), and mesitylene (0.5 mL) in a vial (1.5 mL) were added (*Z*)-2-(pent-1-enyl)phenol (**1a**) (0.0811 g, 0.50 mmol), HCO_2H (0.0230 g, 0.50 mmol), and phenyl formate (0.0733 g, 0.60 mmol) successively via syringe. Upon sealing by a septum cap and stirring at 90 ^{o}C for 16 h, the reaction mixture was purified by flash chromatography (silica gel, eluent: petroleum ether/ethyl acetate = 50/1) to give compound **2a** as a colorless oil (0.0951 g, 99% yield).

Table 2, entry 1

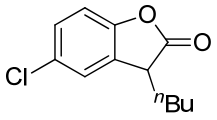


2a

Colorless oil; IR (film) 1808, 1479 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.37-7.21 (m, 2H), 7.14 (t, *J* = 7.6 Hz, 1H), 7.09 (d, *J* = 8.0 Hz, 1H), 3.71 (t, *J* = 6.4 Hz, 1H), 2.12-1.87 (m, 2H), 1.49-1.27 (m, 4H), 0.89 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.5, 154.0, 128.9, 127.8, 124.4, 124.2, 110.8, 43.6, 31.0, 28.2, 22.6, 13.9; HRMS (EI) Calcd for $C_{12}H_{14}O_2$ (M^+): 190.0994; Found: 190.0990.

Azzena, U.; Pisano, L.; Pittalis, M. *Appl. Organomet. Chem.* **2008**, *22*, 523.

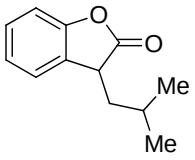
Table 2, entry 2



2b

Colorless oil; IR (film) 1812, 1472 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.35-7.19 (m, 2H), 7.03 (d, *J* = 8.0 Hz, 1H), 3.73 (t, *J* = 6.0 Hz, 1H), 2.11-1.84 (m, 2H), 1.45-1.28 (m, 4H), 0.90 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.6, 152.4, 129.5, 129.4, 129.0, 124.7, 112.0, 43.8, 30.9, 28.1, 22.6, 13.9; HRMS (EI) Calcd for $C_{12}H_{13}O_2Cl$ (M^+): 224.0604; Found: 224.0607.

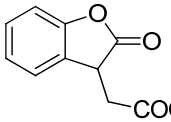
Table 2, entry 3



2c

Colorless oil; IR (film) 1808, 1479 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.40-7.20 (m, 2H), 7.19-7.02 (m, 2H), 3.72 (t, *J* = 7.2 Hz, 1H), 2.10-1.95 (m, 1H), 1.95-1.84 (m, 1H), 1.81-1.70 (m, 1H), 1.00 (d, *J* = 6.6 Hz, 3H), 0.97 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.8, 153.9, 128.9, 128.1, 124.6, 124.2, 111.0, 41.8, 40.6, 25.4, 22.7, 22.3; HRMS (EI) Calcd for $C_{12}H_{14}O_2$ (M^+): 190.0994; Found: 190.0991.

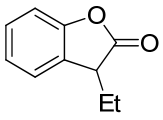
Table 2, entry 4



2d

White solid; mp. 70-72 °C; IR (film) 1808, 1732, 1479 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.45-7.23 (m, 2H), 7.22-7.04 (m, 2H), 4.27-4.07 (m, 2H), 4.07-3.99 (m, 1H), 3.11 (dd, *J* = 17.2, 4.4 Hz, 1H), 2.99 (dd, *J* = 17.2, 7.2 Hz, 1H), 1.18 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.5, 170.2, 154.2, 129.5, 126.7, 124.5, 124.3, 111.0, 61.6, 40.1, 35.4, 14.2; HRMS (EI) Calcd for $C_{12}H_{12}O_4$ (M^+): 220.0736; Found: 220.0727.

Table 2, entry 5

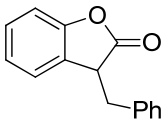


2e

Colorless oil; IR (film) 1804, 1479 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.33-7.24 (m, 2H), 7.15 (t, *J* = 7.6 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 3.70 (t, *J* = 6.0 Hz, 1H), 2.13-1.99 (m, 2H), 0.97 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.4, 154.2, 128.9, 127.4, 124.4, 124.3, 110.9, 44.8, 24.5, 10.4; HRMS (EI) Calcd for $C_{10}H_{10}O_2$ (M^+): 162.0681; Found: 162.0679.

Konishi, H.; Ueda, T.; Muto, T.; Manabe, K. *Org. Lett.* **2012**, *14*, 4722.

Table 2, entry 6



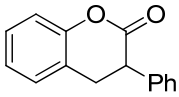
2f

White solid; mp. 54-55 °C (lit. 57 °C); IR (film) 1803, 1463 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.32-7.20 (m, 4H), 7.18-7.10 (m, 2H), 7.05-6.98 (m, 2H), 6.79 (d, *J* = 7.6 Hz, 1H), 4.00 (dd, *J* = 8.8, 4.8 Hz, 1H), 3.49 (dd, *J* = 14.0, 4.8 Hz, 1H), 3.02 (dd, *J* = 14.0, 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.7, 153.9, 136.8, 129.5, 129.1, 128.8, 127.3, 126.9, 125.0, 124.0, 110.9, 45.2, 37.4; HRMS (EI) Calcd for

$C_{15}H_{12}O_2$ (M^+): 224.0837; Found: 224.0839.

Yoneda, E.; Sugioka, T.; Hirao, K.; Zhang, S.-W.; Takahashi, S. *J. Chem. Soc., Perkin Trans. 1* **1998**, 477.

Table 2, entry 6

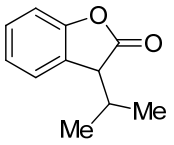


3f

White solid; mp. 123-125 °C (lit. 128.2 °C); IR (film) 1767, 1488 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.41-7.24 (m, 6H), 7.21 (d, *J* = 7.2 Hz, 1H), 7.15-7.07 (m, 2H), 3.98 (dd, *J* = 11.2, 6.0 Hz, 1H), 3.36 (dd, *J* = 15.8, 11.2 Hz, 1H), 3.23 (dd, *J* = 15.8, 6.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.5, 152.0, 136.7, 129.1, 128.7, 128.3, 128.2, 128.1, 124.7, 122.9, 117.0, 45.8, 31.9; HRMS (EI) Calcd for $C_{15}H_{12}O_2$ (M^+): 224.0837; Found: 224.0839.

Lee, J.; List, B. *J. Am. Chem. Soc.* **2012**, *134*, 18245.

Table 2, entry 7

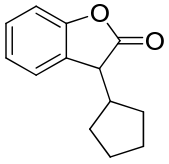


2g

Colorless oil; IR (film) 1808, 1462 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.36-7.23 (m, 2H), 7.20-7.11 (m, 1H), 7.09 (d, *J* = 7.9 Hz, 1H), 3.64 (d, *J* = 3.6 Hz, 1H), 2.60-2.40 (m, 1H), 1.08 (d, *J* = 6.8 Hz, 3H), 0.98 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.7, 154.3, 128.9, 126.4, 124.8, 124.1, 110.8, 49.9, 31.5, 19.5, 18.6; HRMS (EI) Calcd for $C_{11}H_{12}O_2$ (M^+): 176.0837; Found: 176.0834.

Konishi, H.; Ueda, T.; Muto, T.; Manabe, K. *Org. Lett.* **2012**, *14*, 4722.

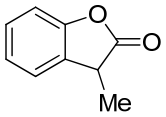
Table 2, entry 8



2h

Colorless oil; IR (film) 1807, 1478 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.34-7.22 (m, 2H), 7.19-7.04 (m, 2H), 3.74 (d, *J* = 6.0 Hz, 1H), 2.56-2.34 (m, 1H), 2.01-1.76 (m, 2H), 1.75-1.32 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.8, 154.1, 128.9, 127.3, 124.9, 124.1, 110.8, 47.0, 42.5, 30.0, 29.1, 25.24, 25.21; HRMS (EI) Calcd for $C_{13}H_{14}O_2$ (M^+): 202.0994; Found: 202.0992.

Table 2, entry 9

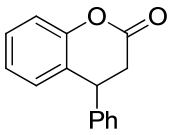


2i

Colorless oil; IR (film) 1807, 1479 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.33-7.21 (m, 2H), 7.15 (t, *J* = 7.6 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 3.73 (q, *J* = 7.6 Hz, 1H), 1.58 (d, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.1, 153.7, 129.0, 124.4, 124.1, 110.9, 38.6, 16.1; HRMS (EI) Calcd for $C_9H_8O_2$ (M^+): 148.0524; Found: 148.0522.

Konishi, H.; Ueda, T.; Muto, T.; Manabe, K. *Org. Lett.* **2012**, *14*, 4722.

Table 2, entry 10



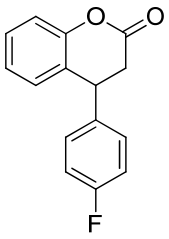
3j

White solid; mp. 79-80 °C (lit. 82 °C); IR (film) 1770, 1485 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.43-7.22 (m, 4H), 7.21-7.04 (m, 4H), 6.98 (d, *J* = 7.6 Hz, 1H), 4.35 (dd, *J* = 7.2, 6.4 Hz, 1H), 3.09 (dd, *J* = 16.0, 6.4 Hz, 1H), 3.02 (dd, *J* = 16.0, 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.8, 151.9, 140.5, 129.4, 129.0, 128.6, 127.9, 127.8, 126.0, 124.9, 117.4, 40.9, 37.2; HRMS (EI) Calcd for $C_{15}H_{12}O_2$ (M^+):

224.0837; Found: 224.0841.

Konishi, H.; Ueda, T.; Muto, T.; Manabe, K. *Org. Lett.* **2012**, *14*, 4722.

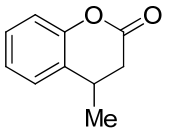
Table 2, entry 11



3k

Colorless oil; IR (film) 1766, 1487 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.42-7.28 (m, 1H), 7.22-6.84 (m, 7H), 4.34 (dd, *J* = 7.2, 6.4 Hz, 1H), 3.07 (dd, *J* = 16.0, 6.4 Hz, 1H), 2.98 (dd, *J* = 16.0, 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 163.5, 161.1, 151.8, 136.23, 136.20, 129.4, 129.3, 129.2, 128.4, 125.7, 124.9, 117.4, 116.3, 116.1, 40.2, 37.3; HRMS (EI) Calcd for $C_{15}H_{11}O_2F$ (M^+): 242.0743; Found: 242.0742.

Table 2, entry 12

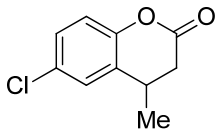


3l

Colorless oil; IR (film) 1770, 1488 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.36-7.19 (m, 2H), 7.12 (t, *J* = 7.6 Hz, 1H), 7.04 (d, *J* = 8.0 Hz, 1H), 3.25-3.10 (m, 1H), 2.83 (dd, *J* = 16.0, 5.6 Hz, 1H), 2.57 (dd, *J* = 16.0, 7.2 Hz, 1H), 1.33 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 151.3, 128.3, 128.0, 126.6, 124.7, 117.0, 36.8, 29.5, 20.0; HRMS (EI) Calcd for $C_{10}H_{10}O_2$ (M^+): 162.0681; Found: 162.0682.

Konishi, H.; Ueda, T.; Muto, T.; Manabe, K. *Org. Lett.* **2012**, *14*, 4722.

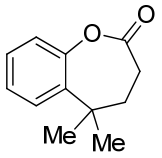
Table 2, entry 13



3m

White solid; mp. 57-59 ^{o}C; IR (film) 1804, 1416 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.19 (m, 2H), 7.05-6.92 (m, 1H), 3.25-3.09 (m, 1H), 2.84 (dd, *J* = 15.6, 5.2 Hz, 1H), 2.58 (dd, *J* = 15.6, 7.2 Hz, 1H), 1.34 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.7, 149.9, 129.8, 129.7, 128.4, 126.7, 118.5, 36.5, 29.6, 19.8; HRMS (EI) Calcd for $C_{10}H_9O_2Cl$ (M^+): 196.0291; Found: 196.0296.

Table 2, entry 15

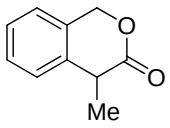


3o

Colorless oil; IR (film) 1766, 1204 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.34 (m, 1H), 7.32-7.24 (m, 1H), 7.24-7.17 (m, 1H), 7.13-7.07 (m, 1H), 2.44 (t, *J* = 7.2 Hz, 2H), 2.08 (t, *J* = 7.2 Hz, 2H), 1.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.2, 151.9, 136.4, 128.4, 126.8, 126.1, 121.1, 41.3, 36.3, 31.0, 29.7; HRMS (EI) Calcd for $C_{12}H_{14}O_2$ (M^+): 190.0994; Found: 190.0991.

Konishi, H.; Ueda, T.; Muto, T.; Manabe, K. *Org. Lett.* **2012**, *14*, 4722.

Table 2, entry 16



2p

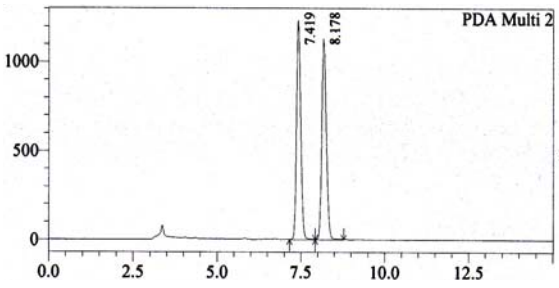
Colorless oil; IR (film) 1745, 1381 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.36 (m, 1H), 7.35-7.27 (m, 2H), 7.27-7.22 (m, 1H), 5.34 (d, *J* = 14.0 Hz, 1H), 5.28 (d, *J* = 14.0 Hz, 1H), 3.64 (q, *J* = 7.2 Hz, 1H), 1.65 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.7, 135.7, 132.1, 129.1, 127.3, 124.9, 124.8, 69.4, 39.6, 13.1; HRMS (EI) Calcd for $C_{10}H_{10}O_2$ (M^+): 162.0681; Found: 162.0679.

Konishi, H.; Ueda, T.; Muto, T.; Manabe, K. *Org. Lett.* **2012**, *14*, 4722.

Procedure for enantioselective hydroesterification (Scheme 4). To a stirred mixture of $Pd(OAc)_2$ (0.0028 g, 0.0125 mmol), (*R*)-(–)-DTBM- SEGPHOS (0.0295 g, 0.025 mmol), and THF (0.5 mL) in a vial (1.5 mL) were added isopropenylphenol (**1l**) (0.0671 g, 0.50 mmol), HCO_2H (0.0230 g, 0.50 mmol), and phenyl formate (0.0733 g, 0.60 mmol) successively with syringe. Upon sealing by a septum cap and stirring at 55 ^oC for 24 h, the reaction mixture was filtered through a plug of silica gel with CH_2Cl_2 (20 mL) as eluent, concentrated, and purified by flash chromatography (silica gel, eluent: petroleum ether/ethyl acetate = 50/1) to give compound **3l** as a colorless oil (0.073 g, 90% yield, 76 % ee), $[\alpha]^D_{20} = -16.8$ (*c* 1.0, $CHCl_3$).

HPLC Condition: **Column:** Chiralpak OJ-H, Daicel Corporation;
Eluent: Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV228 nm.

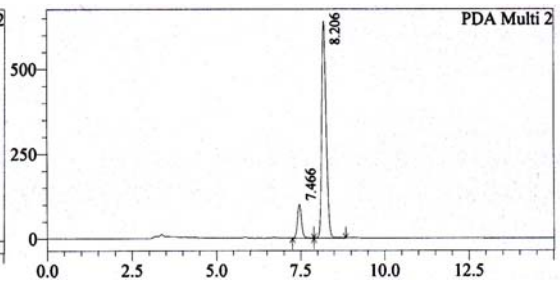
Racemic



PDA Ch2 228nm 4nm

Peak#	Ret. Time	Area %	Peak Start	Peak End
1	7.419	49.632	7.157	7.925
2	8.178	50.368	7.925	8.779
Total		100.000		

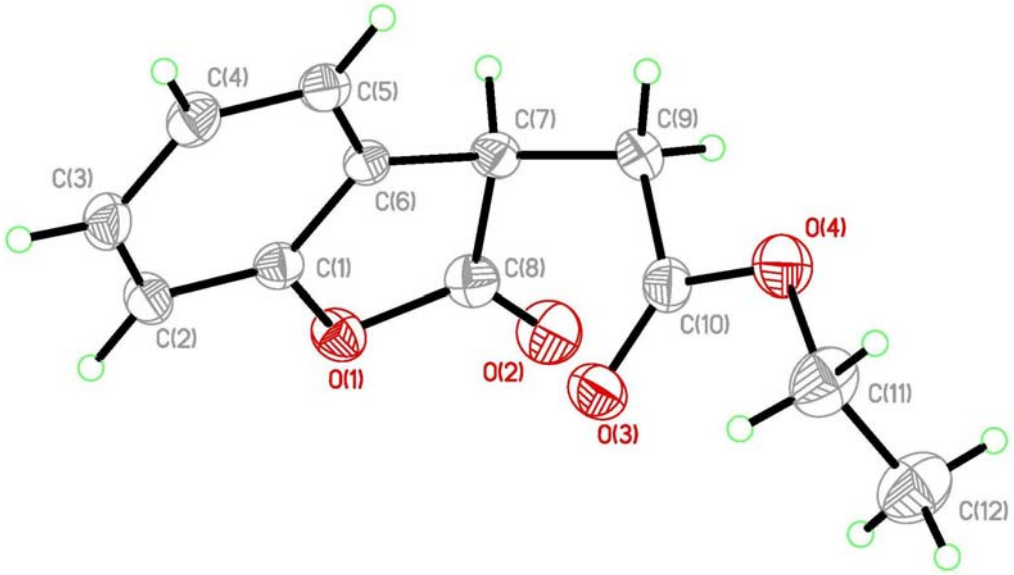
Chiral



PDA Ch2 228nm 4nm

Peak#	Ret. Time	Area %	Peak Start	Peak End
1	7.466	12.106	7.253	7.893
2	8.206	87.894	7.893	8.843
Total		100.000		

The X-ray structure of compound **2d**



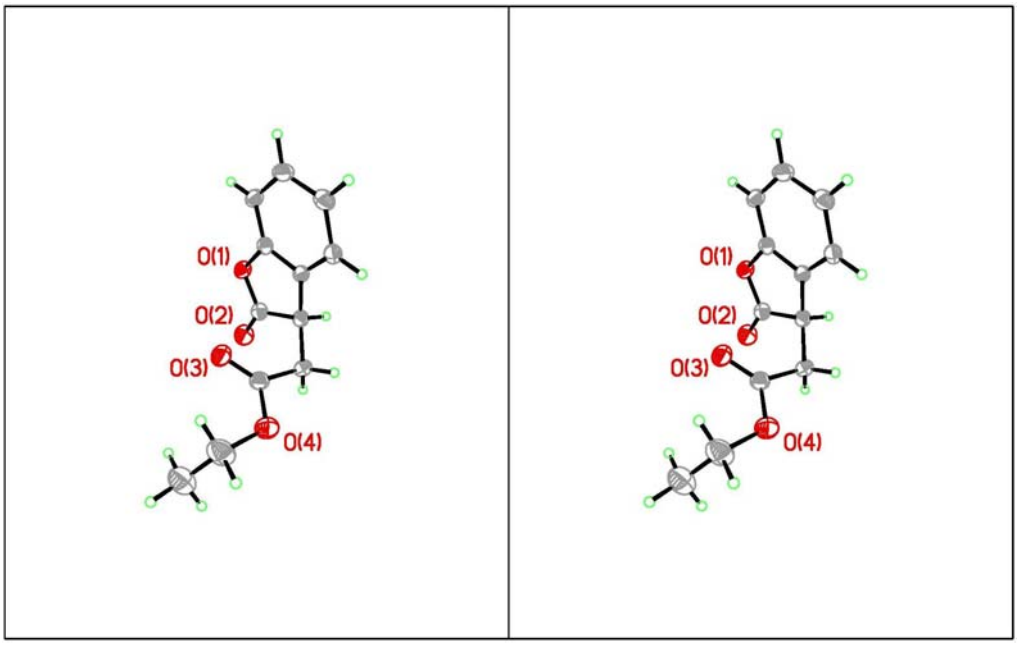


Table S1 - Crystal Data and Details of the Structure Determination for: **2d**

Formula	$C_{12}H_{12}O_4$
Formula Weight	220.22
Crystal System	Monoclinic
Space group	P21/c (No. 14)
a, b, c [Angstrom]	13.273(10) 5.392(4) 16.338(12)
alpha, beta, gamma [deg]	90 112.857(10) 90
V [Ang**3]	1077.5(14)
Z	4
D(calc) [g/cm**3]	1.357
Mu(MoKa) [/mm]	0.102
F(000)	464
Crystal Size [mm]	0.18 x 0.20 x 0.24
Data Collection	
Temperature (K)	296
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	1.7, 25.0
Dataset	-15: 15 ; -6: 6 ; -19: 17
Tot., Uniq. Data, R(int)	5624, 1905, 0.030
Observed data [I > 2.0 sigma(I)]	1700
Refinement	
Nref, Npar	1905, 147
R, wR2, S	0.0340, 0.0922, 1.04
w = 1/[\s^2^(Fo^2^)+(0.0470P)^2^+0.2210P]	where P=(Fo^2^+2Fc^2^)/3
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.14, 0.17

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms

for: **2d** R = 0.03

Atom	x	y	z	U(eq) [Ang^2]
O1	0.06549(7)	0.17099(16)	0.45065(6)	0.0433(3)
O2	0.04722(9)	0.1293(2)	0.30955(6)	0.0604(3)
O3	0.31180(8)	0.1812(2)	0.43698(7)	0.0593(4)
O4	0.39421(8)	0.4289(2)	0.37180(8)	0.0616(4)
C1	0.11864(9)	0.3380(2)	0.51942(8)	0.0356(3)
C2	0.12780(10)	0.3071(3)	0.60534(8)	0.0423(4)
C3	0.18601(11)	0.4890(3)	0.66565(9)	0.0467(4)
C4	0.23220(11)	0.6884(3)	0.63971(9)	0.0450(4)
C5	0.21987(10)	0.7163(2)	0.55151(8)	0.0388(4)
C6	0.16188(9)	0.5376(2)	0.49084(7)	0.0333(3)
C7	0.13019(10)	0.5097(2)	0.39245(8)	0.0373(4)
C8	0.07788(10)	0.2537(3)	0.37550(8)	0.0419(4)
C9	0.21856(11)	0.5421(3)	0.35584(8)	0.0433(4)
C10	0.31120(11)	0.3617(3)	0.39367(8)	0.0423(4)
C11	0.49231(13)	0.2753(4)	0.40417(13)	0.0685(6)
C12	0.48450(15)	0.0640(4)	0.34333(14)	0.0784(7)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters

for: **2d** R = 0.03

Atom	x	y	z	U(iso) [Ang^2]
H2	0.09690	0.17210	0.62240	0.0510
H3	0.19400	0.47620	0.72460	0.0560
H4	0.27200	0.80530	0.68170	0.0540
H5	0.24990	0.85190	0.53390	0.0470
H7	0.07250	0.63100	0.36280	0.0450
H9A	0.18600	0.52240	0.29180	0.0520
H9B	0.24730	0.70940	0.36840	0.0520
H11A	0.50330	0.21150	0.46250	0.0820
H11B	0.55520	0.37640	0.41000	0.0820
H12A	0.42760	-0.04680	0.34270	0.1180
H12B	0.55290	-0.02320	0.36360	0.1180
H12C	0.46790	0.12580	0.28440	0.1180

==========

The Temperature Factor has the Form of Exp(-T) Where

T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters
for: **2d** R = 0.03

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O1	0.0459(5)	0.0396(5)	0.0420(5)	-0.0011(4)	0.0146(4)	-0.0087(4)
O2	0.0729(7)	0.0564(6)	0.0427(5)	-0.0117(5)	0.0123(5)	-0.0099(5)
O3	0.0593(6)	0.0562(7)	0.0709(7)	0.0218(5)	0.0345(5)	0.0131(5)
O4	0.0526(6)	0.0613(7)	0.0824(8)	0.0074(6)	0.0388(6)	-0.0002(5)
C1	0.0319(6)	0.0348(6)	0.0387(6)	0.0005(5)	0.0123(5)	0.0020(5)
C2	0.0440(7)	0.0433(7)	0.0436(7)	0.0081(6)	0.0214(6)	0.0032(6)
C3	0.0529(8)	0.0543(8)	0.0353(6)	0.0026(6)	0.0197(6)	0.0075(7)
C4	0.0469(7)	0.0455(8)	0.0399(7)	-0.0080(6)	0.0140(6)	0.0004(6)
C5	0.0379(6)	0.0348(7)	0.0443(7)	-0.0002(5)	0.0166(5)	0.0006(5)
C6	0.0309(6)	0.0339(6)	0.0355(6)	0.0032(5)	0.0134(5)	0.0052(5)
C7	0.0387(6)	0.0367(7)	0.0345(6)	0.0040(5)	0.0122(5)	0.0047(5)
C8	0.0403(7)	0.0432(7)	0.0366(7)	0.0005(6)	0.0089(5)	0.0012(6)
C9	0.0526(7)	0.0427(7)	0.0386(6)	0.0064(6)	0.0222(6)	0.0016(6)
C10	0.0460(7)	0.0443(7)	0.0400(7)	-0.0021(6)	0.0203(6)	-0.0023(6)
C11	0.0446(8)	0.0747(11)	0.0881(12)	-0.0081(10)	0.0278(8)	-0.0016(8)
C12	0.0645(10)	0.0761(12)	0.0957(13)	-0.0144(11)	0.0323(10)	0.0004(9)

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)

for: **2d** R = 0.03

O1	-C1	1.3983(18)	C9	-C10	1.500(2)
O1	-C8	1.3749(19)	C11	-C12	1.489(3)
O2	-C8	1.1983(19)	C2	-H2	0.9300
O3	-C10	1.202(2)	C3	-H3	0.9300
O4	-C10	1.334(2)	C4	-H4	0.9300
O4	-C11	1.458(3)	C5	-H5	0.9300
C1	-C2	1.371(2)	C7	-H7	0.9800
C1	-C6	1.3834(19)	C9	-H9A	0.9700
C2	-C3	1.392(2)	C9	-H9B	0.9700
C3	-C4	1.383(2)	C11	-H11A	0.9700
C4	-C5	1.394(2)	C11	-H11B	0.9700
C5	-C6	1.3823(19)	C12	-H12A	0.9600
C6	-C7	1.503(2)	C12	-H12B	0.9600
C7	-C8	1.521(2)	C12	-H12C	0.9600
C7	-C9	1.520(2)			

Table S6 - Bond Angles (Degrees)
for: **2d** R = 0.03

C1	-O1	-C8	108.10(10)	C2	-C3	-H3	119.00
C10	-O4	-C11	117.57(13)	C4	-C3	-H3	119.00
O1	-C1	-C2	124.11(11)	C3	-C4	-H4	120.00
O1	-C1	-C6	112.07(10)	C5	-C4	-H4	120.00
C2	-C1	-C6	123.82(12)	C4	-C5	-H5	121.00
C1	-C2	-C3	116.30(13)	C6	-C5	-H5	121.00
C2	-C3	-C4	121.39(13)	C6	-C7	-H7	108.00
C3	-C4	-C5	120.84(13)	C8	-C7	-H7	108.00
C4	-C5	-C6	118.37(12)	C9	-C7	-H7	108.00
C1	-C6	-C5	119.26(10)	C7	-C9	-H9A	109.00
C1	-C6	-C7	107.62(10)	C7	-C9	-H9B	109.00
C5	-C6	-C7	133.11(11)	C10	-C9	-H9A	109.00
C6	-C7	-C8	101.76(9)	C10	-C9	-H9B	109.00
C6	-C7	-C9	118.13(11)	H9A	-C9	-H9B	108.00
C8	-C7	-C9	113.59(11)	O4	-C11	-H11A	109.00
O1	-C8	-O2	120.32(14)	O4	-C11	-H11B	109.00
O1	-C8	-C7	109.64(11)	C12	-C11	-H11A	109.00
O2	-C8	-C7	130.02(13)	C12	-C11	-H11B	109.00
C7	-C9	-C10	113.44(12)	H11A	-C11	-H11B	108.00
O3	-C10	-O4	124.10(14)	C11	-C12	-H12A	110.00
O3	-C10	-C9	125.79(14)	C11	-C12	-H12B	109.00
O4	-C10	-C9	110.11(13)	C11	-C12	-H12C	109.00
O4	-C11	-C12	111.82(16)	H12A	-C12	-H12B	109.00
C1	-C2	-H2	122.00	H12A	-C12	-H12C	109.00
C3	-C2	-H2	122.00	H12B	-C12	-H12C	110.00

Table S7 - Torsion Angles (Degrees)

for: **2d** R = 0.03

C8	-O1	-C1	-C2	-176.52(13)
C8	-O1	-C1	-C6	2.96(14)
C1	-O1	-C8	-C7	-7.71(14)
C1	-O1	-C8	-O2	173.55(13)
C11	-O4	-C10	-C9	179.23(13)
C10	-O4	-C11	-C12	86.41(19)
C11	-O4	-C10	-O3	-1.2(2)
C6	-C1	-C2	-C3	-1.0(2)
O1	-C1	-C6	-C5	-178.16(11)
O1	-C1	-C2	-C3	178.39(13)
C2	-C1	-C6	-C5	1.3(2)
C2	-C1	-C6	-C7	-177.45(13)
O1	-C1	-C6	-C7	3.07(14)
C1	-C2	-C3	-C4	-0.3(2)
C2	-C3	-C4	-C5	1.4(2)
C3	-C4	-C5	-C6	-1.1(2)
C4	-C5	-C6	-C1	-0.23(19)
C4	-C5	-C6	-C7	178.16(14)
C5	-C6	-C7	-C8	174.37(14)
C1	-C6	-C7	-C8	-7.10(14)
C1	-C6	-C7	-C9	-132.18(12)
C5	-C6	-C7	-C9	49.3(2)
C6	-C7	-C8	-O2	-172.33(15)
C9	-C7	-C8	-O1	137.14(11)
C6	-C7	-C8	-O1	9.09(14)
C6	-C7	-C9	-C10	59.76(15)
C8	-C7	-C9	-C10	-59.29(15)
C9	-C7	-C8	-O2	-44.3(2)
C7	-C9	-C10	-O3	12.0(2)
C7	-C9	-C10	-O4	-168.50(11)

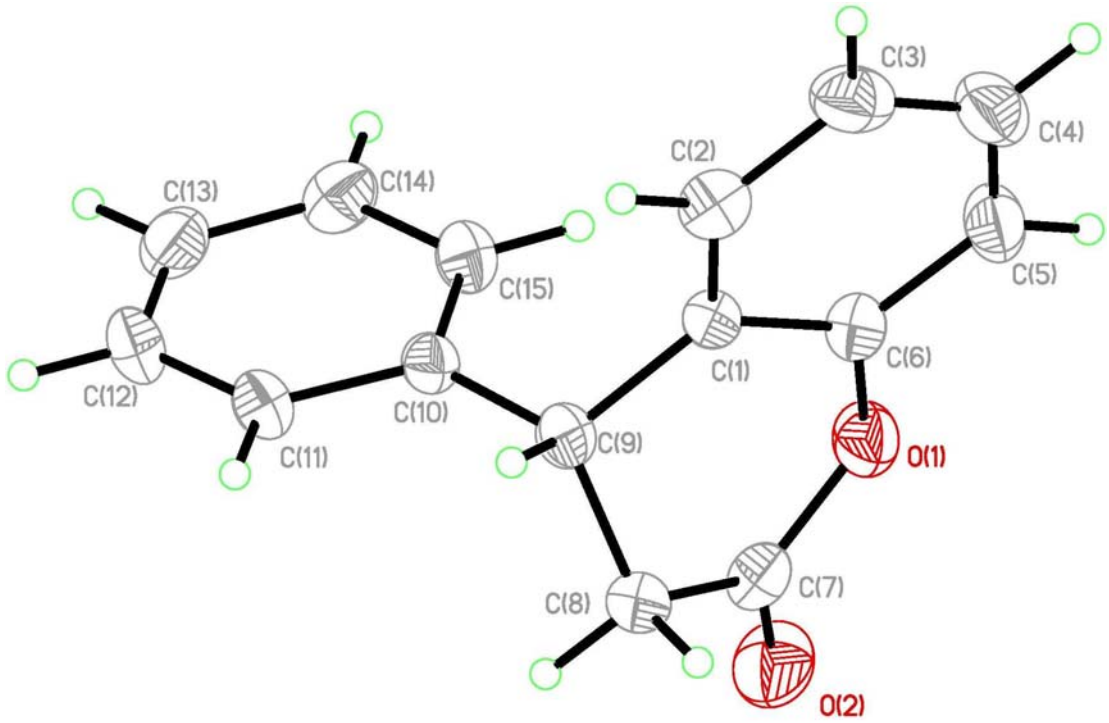
Table S8 - Contact Distances(Angstrom)
for: **2d** R = 0.03

O1	.C5_a	3.210(3)	C7	.C2_e	3.578(3)
O2	.C7_c	3.289(3)	C7	.O2_h	3.289(3)
O3	.C6	3.129(3)	C8	.C3_e	3.580(3)
O3	.C12	3.274(3)	C8	.O3	2.895(3)
O3	.C8	2.895(3)	C12	.O3	3.274(3)
O1	.H2_b	2.7400	C2	.H7_e	2.9200
O1	.H5_a	2.8700	C5	.H11B_g	2.8500
O2	.H9A	2.9000	C10	.H12A	2.9900
O2	.H3_d	2.8500	H2	.O1_b	2.7400
O2	.H7_c	2.6400	H2	.H7_e	2.5800
O2	.H7_a	2.8000	H3	.O2_i	2.8500
O3	.H5_a	2.7100	H5	.O1_f	2.8700
O3	.H9B_a	2.7800	H5	.O3_f	2.7100
O3	.H11A	2.4200	H7	.O2_f	2.8000
O3	.H12A	2.8400	H7	.O2_h	2.6400
C1	.C5_a	3.574(3)	H7	.C2_e	2.9200
C1	.C1_e	3.438(3)	H7	.H2_e	2.5800
C2	.C4_a	3.572(4)	H9A	.O2	2.9000
C2	.C7_e	3.578(3)	H9B	.O3_f	2.7800
C3	.C8_e	3.580(3)	H11A	.O3	2.4200
C4	.C2_f	3.572(4)	H11B	.C5_g	2.8500
C5	.O1_f	3.210(3)	H12A	.O3	2.8400
C5	.C1_f	3.574(3)	H12A	.C10	2.9900
C6	.O3	3.129(3)			

Translation of Symmetry Code to Equiv.Pos

a = [1545.00] = [1_545] = x,-1+y,z
b = [3556.00] = [3_556] = -x,-y,1-z
c = [2545.00] = [2_545] = -x,-1/2+y,1/2-z
d = [4554.00] = [4_565] = x,1/2-y,-1/2+z
e = [3566.00] = [3_566] = -x,1-y,1-z
f = [1565.00] = [1_565] = x,1+y,z
g = [3666.00] = [3_666] = 1-x,1-y,1-z
h = [2555.00] = [2_555] = -x,1/2+y,1/2-z
i = [4555.00] = [4_566] = x,1/2-y,1/2+z

The X-ray structure of compound **3j**



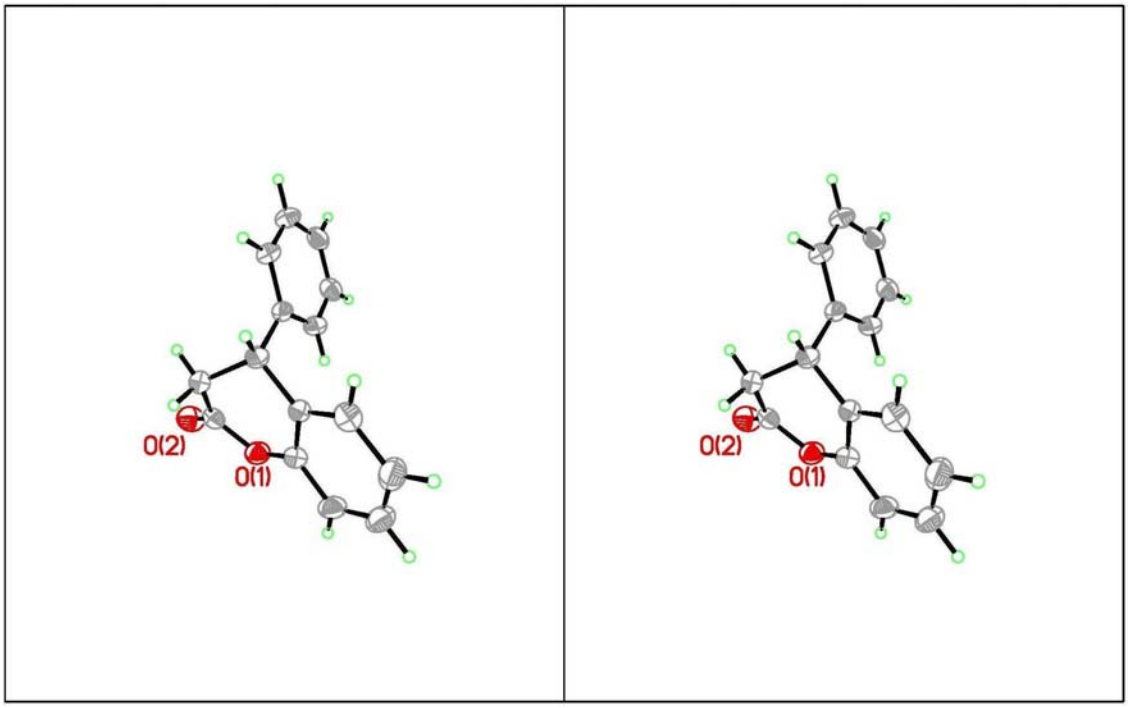


Table S1 - Crystal Data and Details of the Structure Determination for: **3j**

Formula	C_{15} H_{12} O_2
Formula Weight	224.25
Crystal System	monoclinic
Space group	P21 (No. 4)
a, b, c [Angstrom]	5.7170(11) 7.8120(16) 12.901(3)
alpha, beta, gamma [deg]	90 93.75(3) 90
V [Ang**3]	574.9(2)
Z	2
D(calc) [g/cm**3]	1.295
Mu(MoKa) [/mm]	0.085
F(000)	236
Crystal Size [mm]	0.10 x 0.10 x 0.20
Data Collection	
Temperature (K)	293
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	1.6, 25.4
Dataset	0: 6 ; 0: 9 ; -15: 15
Tot., Uniq. Data, R(int)	1255, 1136, 0.054
Observed data [I > 2.0 sigma(I)]	855
Refinement	
Nref, Npar	1136, 154
R, wR2, S	0.0471, 0.1150, 1.00
w = 1/[\s^2^(Fo^2^)+(0.0570P)^2^]	where P=(Fo^2^+2Fc^2^)/3
Max. and Av. Shift/Error	0.00, 0.00
Flack x	-1(3)
Min. and Max. Resd. Dens. [e/Ang^3]	-0.14, 0.12

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms

for: **3j** R = 0.05

Atom	x	y	z	U(eq) [Ang^2]
O1	0.4172(4)	0.3760(4)	0.1412(2)	0.0579(10)
O2	0.5187(6)	0.6362(5)	0.1879(2)	0.0762(12)
C1	0.0577(6)	0.2442(5)	0.1953(3)	0.0425(11)
C2	-0.0970(7)	0.1083(5)	0.1831(3)	0.0554(14)
C3	-0.0595(8)	-0.0248(6)	0.1155(3)	0.0675(16)
C4	0.1359(9)	-0.0209(6)	0.0577(3)	0.0691(17)
C5	0.2914(8)	0.1127(6)	0.0667(3)	0.0613(16)
C6	0.2498(7)	0.2442(5)	0.1345(3)	0.0490(11)
C7	0.3656(7)	0.5313(5)	0.1837(3)	0.0540(16)
C8	0.1219(7)	0.5527(5)	0.2179(3)	0.0531(14)
C9	0.0253(6)	0.3908(5)	0.2679(3)	0.0452(11)
C10	0.1318(6)	0.3652(5)	0.3770(3)	0.0428(11)
C11	0.0192(7)	0.4311(5)	0.4592(3)	0.0551(12)
C12	0.1119(8)	0.4151(6)	0.5594(3)	0.0675(17)
C13	0.3208(10)	0.3321(6)	0.5795(3)	0.0676(16)
C14	0.4387(7)	0.2631(6)	0.5000(3)	0.0591(16)
C15	0.3430(7)	0.2798(5)	0.3995(3)	0.0535(12)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters

for: **3j** R = 0.05

Atom	x	y	z	U(iso) [Ang^2]
H2A	-0.22940	0.10640	0.22130	0.0670
H3A	-0.16430	-0.11580	0.10890	0.0810
H4A	0.16210	-0.11010	0.01210	0.0830
H5A	0.42280	0.11460	0.02780	0.0740
H8A	0.01860	0.58410	0.15830	0.0640
H8B	0.12100	0.64600	0.26750	0.0640
H9A	-0.14370	0.40720	0.27240	0.0540
H11A	-0.12290	0.48770	0.44660	0.0660
H12A	0.03280	0.46060	0.61380	0.0810
H13A	0.38350	0.32240	0.64760	0.0810
H14A	0.58020	0.20620	0.51370	0.0710
H15A	0.42160	0.23270	0.34540	0.0640

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters
for: **3j** R = 0.05

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O1	0.0584(16)	0.0599(18)	0.0571(16)	-0.0038(15)	0.0173(12)	-0.0033(15)
O2	0.082(2)	0.074(2)	0.074(2)	-0.0020(18)	0.0151(16)	-0.0295(19)
C1	0.049(2)	0.039(2)	0.0400(18)	0.0020(16)	0.0071(15)	0.0058(19)
C2	0.056(2)	0.055(3)	0.055(2)	0.005(2)	0.0027(18)	-0.002(2)
C3	0.087(3)	0.047(2)	0.066(3)	-0.003(2)	-0.015(2)	0.000(2)
C4	0.094(3)	0.057(3)	0.055(3)	-0.013(2)	-0.004(2)	0.015(3)
C5	0.069(3)	0.069(3)	0.047(2)	-0.006(2)	0.0124(19)	0.015(3)
C6	0.057(2)	0.051(2)	0.0393(19)	-0.0001(19)	0.0055(17)	0.001(2)
C7	0.068(3)	0.052(3)	0.043(2)	0.0078(19)	0.0104(18)	-0.002(2)
C8	0.070(3)	0.042(2)	0.048(2)	0.0022(18)	0.0093(19)	0.009(2)
C9	0.0428(18)	0.047(2)	0.0471(19)	-0.0003(19)	0.0122(15)	0.0071(18)
C10	0.0466(19)	0.039(2)	0.0441(19)	-0.0010(17)	0.0141(15)	0.0002(18)
C11	0.063(2)	0.051(2)	0.053(2)	-0.0053(19)	0.0177(18)	0.011(2)
C12	0.096(3)	0.058(3)	0.051(3)	-0.015(2)	0.024(2)	0.005(3)
C13	0.105(3)	0.054(3)	0.044(2)	0.003(2)	0.007(2)	-0.015(3)
C14	0.060(3)	0.063(3)	0.054(2)	0.011(2)	0.001(2)	0.002(2)
C15	0.054(2)	0.057(2)	0.051(2)	-0.003(2)	0.0160(17)	0.007(2)

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)

for: **3j** R = 0.05

O1	-C6	1.405(5)	C12	-C13	1.369(7)
O1	-C7	1.371(5)	C13	-C14	1.374(6)
O2	-C7	1.198(5)	C14	-C15	1.380(6)
C1	-C2	1.384(5)	C2	-H2A	0.9300
C1	-C6	1.391(5)	C3	-H3A	0.9300
C1	-C9	1.499(5)	C4	-H4A	0.9300
C2	-C3	1.383(6)	C5	-H5A	0.9300
C3	-C4	1.383(7)	C8	-H8A	0.9700
C4	-C5	1.371(7)	C8	-H8B	0.9700
C5	-C6	1.380(6)	C9	-H9A	0.9800
C7	-C8	1.498(6)	C11	-H11A	0.9300
C8	-C9	1.539(5)	C12	-H12A	0.9300
C9	-C10	1.510(5)	C13	-H13A	0.9300
C10	-C11	1.376(5)	C14	-H14A	0.9300
C10	-C15	1.393(5)	C15	-H15A	0.9300
C11	-C12	1.370(6)			

Table S6 - Bond Angles (Degrees)

for: **3j** R = 0.05

C6	-O1	-C7	120.6(3)	C1	-C2	-H2A	119.00
C2	-C1	-C6	117.3(4)	C3	-C2	-H2A	119.00
C2	-C1	-C9	123.6(3)	C2	-C3	-H3A	120.00
C6	-C1	-C9	119.1(3)	C4	-C3	-H3A	120.00
C1	-C2	-C3	121.6(4)	C3	-C4	-H4A	120.00
C2	-C3	-C4	119.2(4)	C5	-C4	-H4A	120.00
C3	-C4	-C5	120.9(4)	C4	-C5	-H5A	121.00
C4	-C5	-C6	118.9(4)	C6	-C5	-H5A	121.00
O1	-C6	-C1	121.7(3)	C7	-C8	-H8A	109.00
O1	-C6	-C5	116.1(4)	C7	-C8	-H8B	109.00
C1	-C6	-C5	122.2(4)	C9	-C8	-H8A	109.00
O1	-C7	-O2	116.6(4)	C9	-C8	-H8B	109.00
O1	-C7	-C8	116.4(3)	H8A	-C8	-H8B	108.00
O2	-C7	-C8	127.0(4)	C1	-C9	-H9A	107.00
C7	-C8	-C9	113.5(3)	C8	-C9	-H9A	107.00
C1	-C9	-C8	107.7(3)	C10	-C9	-H9A	108.00
C1	-C9	-C10	115.0(3)	C10	-C11	-H11A	119.00
C8	-C9	-C10	111.5(3)	C12	-C11	-H11A	119.00
C9	-C10	-C11	119.2(3)	C11	-C12	-H12A	120.00
C9	-C10	-C15	123.3(3)	C13	-C12	-H12A	120.00
C11	-C10	-C15	117.5(4)	C12	-C13	-H13A	120.00
C10	-C11	-C12	121.4(4)	C14	-C13	-H13A	120.00
C11	-C12	-C13	120.1(4)	C13	-C14	-H14A	121.00
C12	-C13	-C14	120.6(4)	C15	-C14	-H14A	121.00
C13	-C14	-C15	118.7(4)	C10	-C15	-H15A	119.00
C10	-C15	-C14	121.7(4)	C14	-C15	-H15A	119.00

Table S7 - Torsion Angles (Degrees)

for: **3j** R = 0.05

C7	-O1	-C6	-C1	-19.1(5)
C7	-O1	-C6	-C5	162.9(4)
C6	-O1	-C7	-O2	179.0(3)
C6	-O1	-C7	-C8	-2.2(5)
C6	-C1	-C2	-C3	1.8(6)
C9	-C1	-C2	-C3	-179.7(4)
C2	-C1	-C6	-O1	-179.9(3)
C2	-C1	-C6	-C5	-2.0(6)
C9	-C1	-C6	-O1	1.6(6)
C9	-C1	-C6	-C5	179.4(4)
C2	-C1	-C9	-C8	-146.1(4)
C2	-C1	-C9	-C10	89.0(4)
C6	-C1	-C9	-C8	32.4(5)
C6	-C1	-C9	-C10	-92.5(4)
C1	-C2	-C3	-C4	-0.8(6)
C2	-C3	-C4	-C5	0.0(7)
C3	-C4	-C5	-C6	-0.1(6)
C4	-C5	-C6	-O1	179.2(4)
C4	-C5	-C6	-C1	1.2(6)
O1	-C7	-C8	-C9	38.4(5)
O2	-C7	-C8	-C9	-143.0(4)
C7	-C8	-C9	-C1	-51.4(4)
C7	-C8	-C9	-C10	75.6(4)
C1	-C9	-C10	-C11	-144.6(4)
C1	-C9	-C10	-C15	36.6(5)
C8	-C9	-C10	-C11	92.5(4)
C8	-C9	-C10	-C15	-86.3(5)
C9	-C10	-C11	-C12	-178.3(4)
C15	-C10	-C11	-C12	0.6(6)
C9	-C10	-C15	-C14	178.1(4)
C11	-C10	-C15	-C14	-0.8(6)
C10	-C11	-C12	-C13	0.0(7)
C11	-C12	-C13	-C14	-0.5(7)
C12	-C13	-C14	-C15	0.3(7)
C13	-C14	-C15	-C10	0.4(6)

Table S8 - Contact Distances(Angstrom)

for: **3j** R = 0.05

O1	.C9	2.861(4)	C9	.O1	2.861(4)
O1	.H5A	2.5100	C10	.C13	2.773(6)
O1	.H8A	2.8200	C10	.C2	3.401(6)
O1	.H15A	2.8600	C10	.C7	3.182(5)
O2	.H3A_a	2.8800	C10	.C6	3.378(6)
O2	.H8A	2.8900	C11	.C8	3.343(6)
O2	.H8B	2.5600	C11	.C14	2.754(6)
O2	.H9A_b	2.8000	C12	.C15	2.734(6)
O2	.H5A_c	2.8300	C13	.C10	2.773(6)
O2	.H13A_d	2.6000	C14	.C11	2.754(6)
C1	.C4	2.783(6)	C15	.C8	3.353(6)
C1	.C7	2.861(5)	C15	.C1	3.019(5)
C1	.C15	3.019(5)	C15	.C12	2.734(6)
C2	.C5	2.761(6)	C15	.C7	3.417(6)
C2	.C10	3.401(6)	C15	.C6	3.437(6)
C3	.C6	2.747(6)	C1	.H15A	2.7500
C4	.C1	2.783(6)	C1	.H4A_e	3.1000
C5	.C2	2.761(6)	C1	.H8A	2.7000
C6	.C8	2.757(6)	C2	.H12A_f	2.8600
C6	.C3	2.747(6)	C2	.H9A	2.6300
C6	.C10	3.378(6)	C4	.H8A_g	2.9800
C6	.C15	3.437(6)	C6	.H15A	2.8300
C7	.C1	2.861(5)	C6	.H8A	2.9900
C7	.C15	3.417(6)	C9	.H15A	2.7100
C7	.C10	3.182(5)	C9	.H2A	2.7000
C8	.C15	3.353(6)	C9	.H11A	2.6200
C8	.C11	3.343(6)	C10	.H8B	2.6100
C8	.C6	2.757(6)	C11	.H8B	3.0800

Table S8 - Contact Distances(Angstrom) (continued)

for: **3j** R = 0.05

C11	.H9A	2.5300	H9A	.O2_j	2.8000
C12	.H14A_d	3.0600	H9A	.C2	2.6300
C13	.H11A_f	2.9300	H9A	.C11	2.5300
C14	.H11A_f	2.9200	H9A	.H2A	2.4800
H2A	.C9	2.7000	H9A	.H8A	2.2600
H2A	.H3A	2.3100	H9A	.H8B	2.4100
H2A	.H9A	2.4800	H9A	.H11A	2.3300
H3A	.O2_h	2.8800	H11A	.C9	2.6200
H3A	.H2A	2.3100	H11A	.H9A	2.3300
H3A	.H4A	2.3100	H11A	.H12A	2.2900
H4A	.H3A	2.3100	H11A	.C13_k	2.9300
H4A	.H5A	2.3000	H11A	.C14_k	2.9200
H4A	.C1_g	3.1000	H12A	.H11A	2.2900
H5A	.O1	2.5100	H12A	.H13A	2.2900
H5A	.H4A	2.3000	H12A	.C2_k	2.8600
H5A	.O2_i	2.8300	H13A	.H12A	2.2900
H8A	.O1	2.8200	H13A	.H14A	2.3100
H8A	.O2	2.8900	H13A	.O2_l	2.6000
H8A	.C1	2.7000	H14A	.H13A	2.3100
H8A	.C6	2.9900	H14A	.H15A	2.3100
H8A	.H9A	2.2600	H14A	.C12_l	3.0600
H8A	.C4_e	2.9800	H15A	.O1	2.8600
H8B	.O2	2.5600	H15A	.C1	2.7500
H8B	.C10	2.6100	H15A	.C6	2.8300
H8B	.C11	3.0800	H15A	.C9	2.7100
H8B	.H9A	2.4100	H15A	.H14A	2.3100

Translation of Symmetry Code to Equiv.Pos

a = [1665.00] = [1_665] = 1+x,1+y,z
b = [1655.00] = [1_655] = 1+x,y,z
c = [2655.00] = [2_655] = 1-x,1/2+y,-z
d = [2656.00] = [2_656] = 1-x,1/2+y,1-z
e = [2555.00] = [2_555] = -x,1/2+y,-z
f = [2546.00] = [2_546] = -x,-1/2+y,1-z
g = [2545.00] = [2_545] = -x,-1/2+y,-z
h = [1445.00] = [1_445] = -1+x,-1+y,z
i = [2645.00] = [2_645] = 1-x,-1/2+y,-z
j = [1455.00] = [1_455] = -1+x,y,z
k = [2556.00] = [2_556] = -x,1/2+y,1-z
l = [2646.00] = [2_646] = 1-x,-1/2+y,1-z

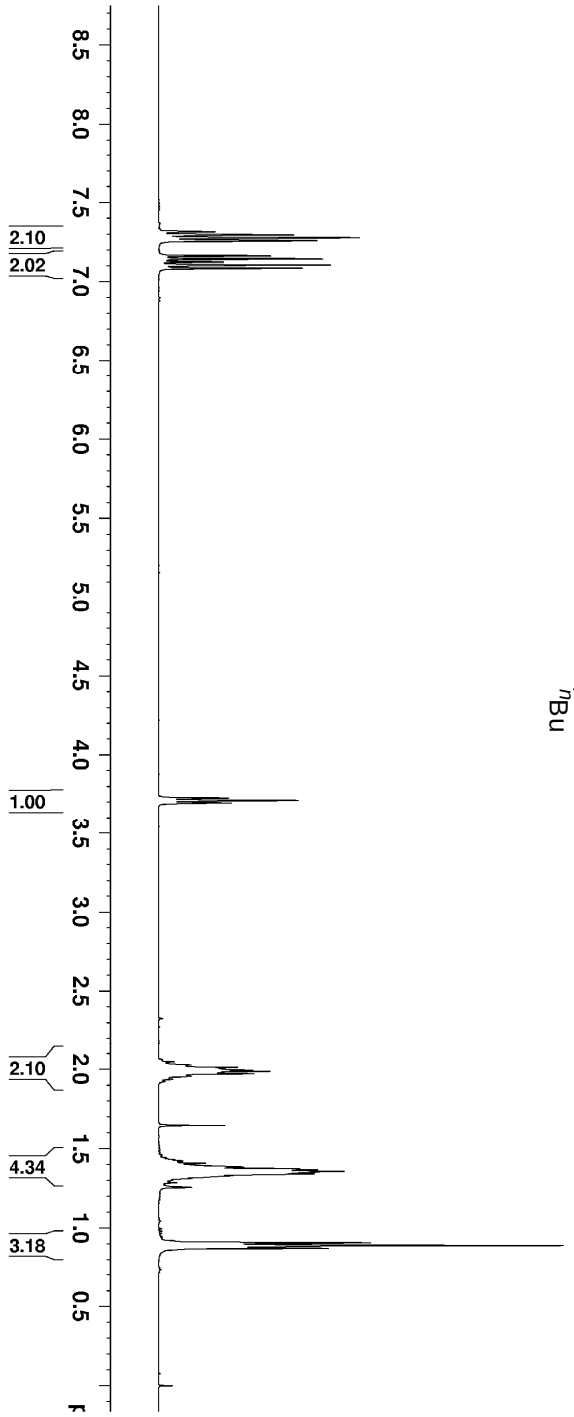


Table 2, Entry 1, **2a**

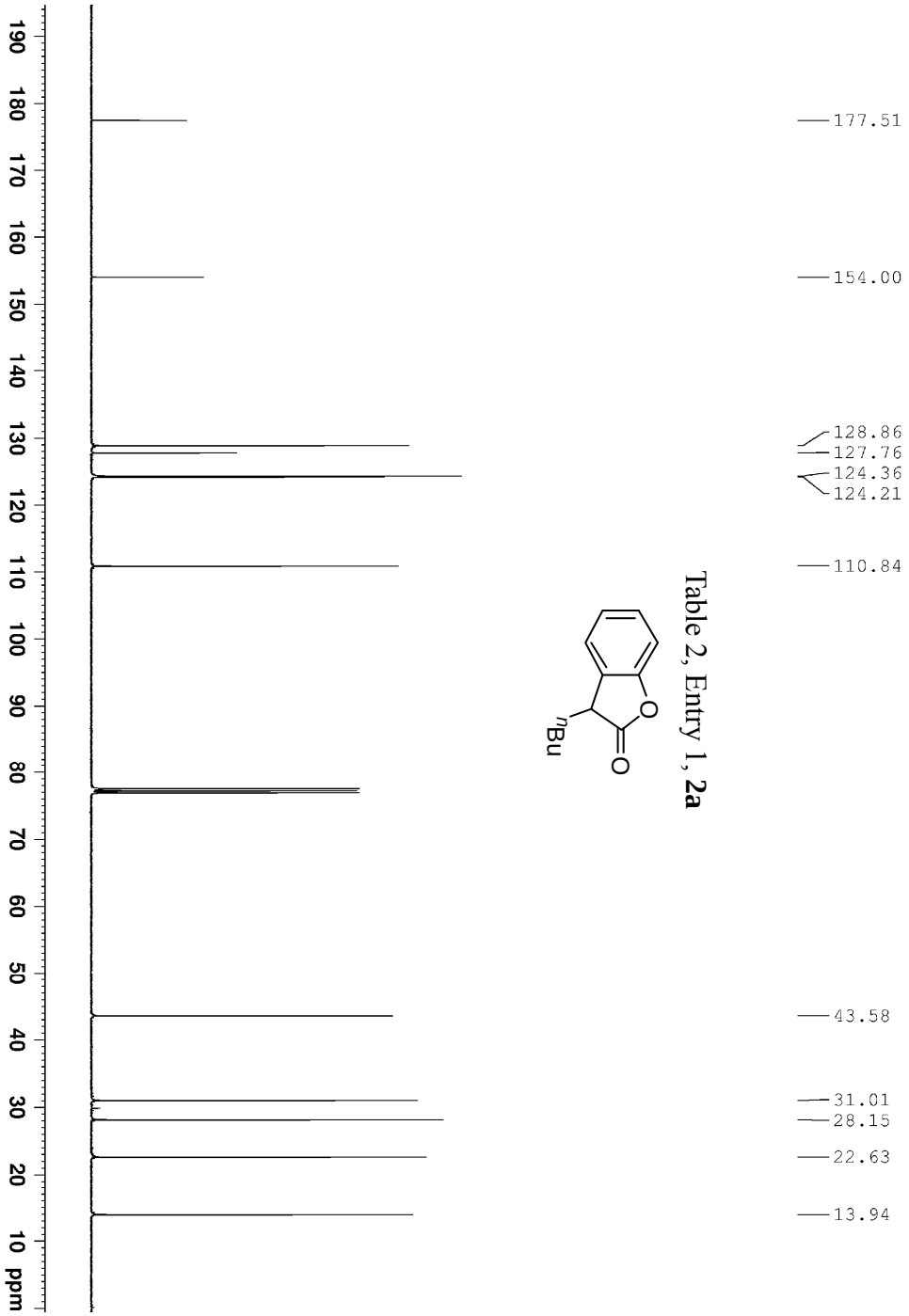
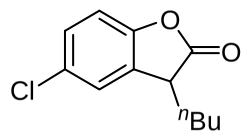
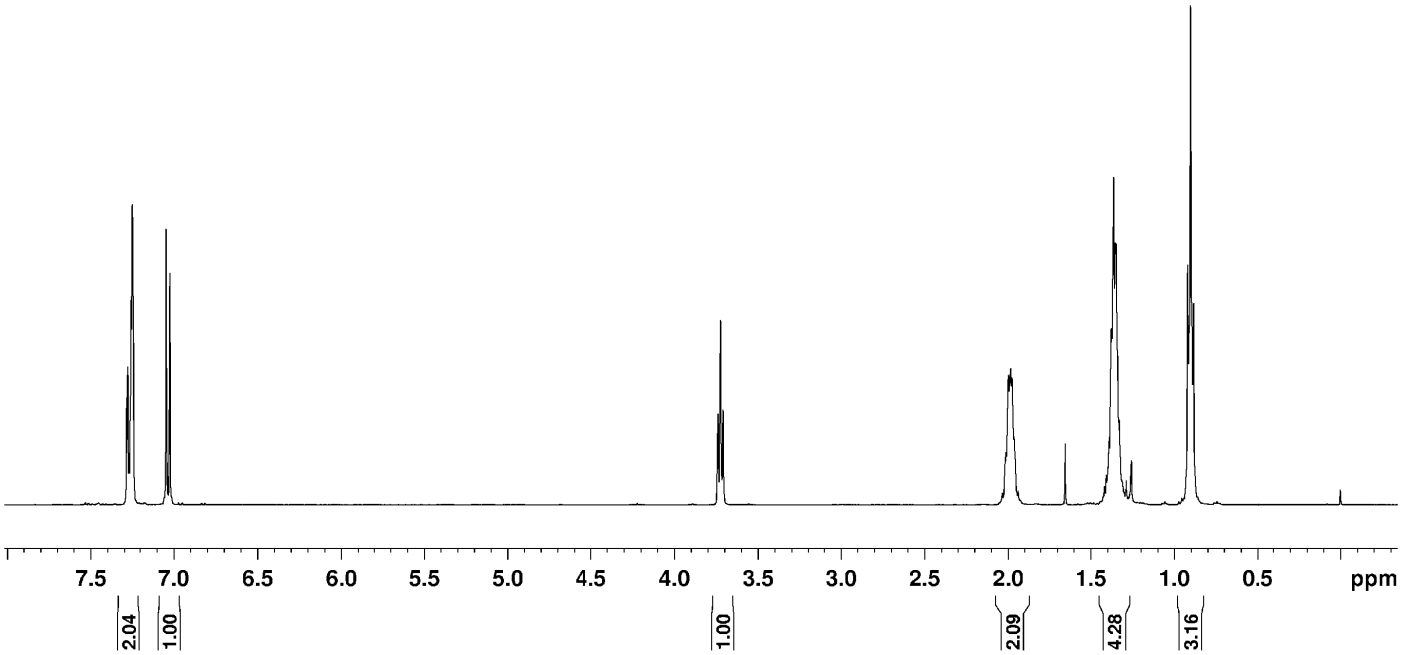


Table 2, Entry 1, **2a**

Table 2, Entry 2, **2b**





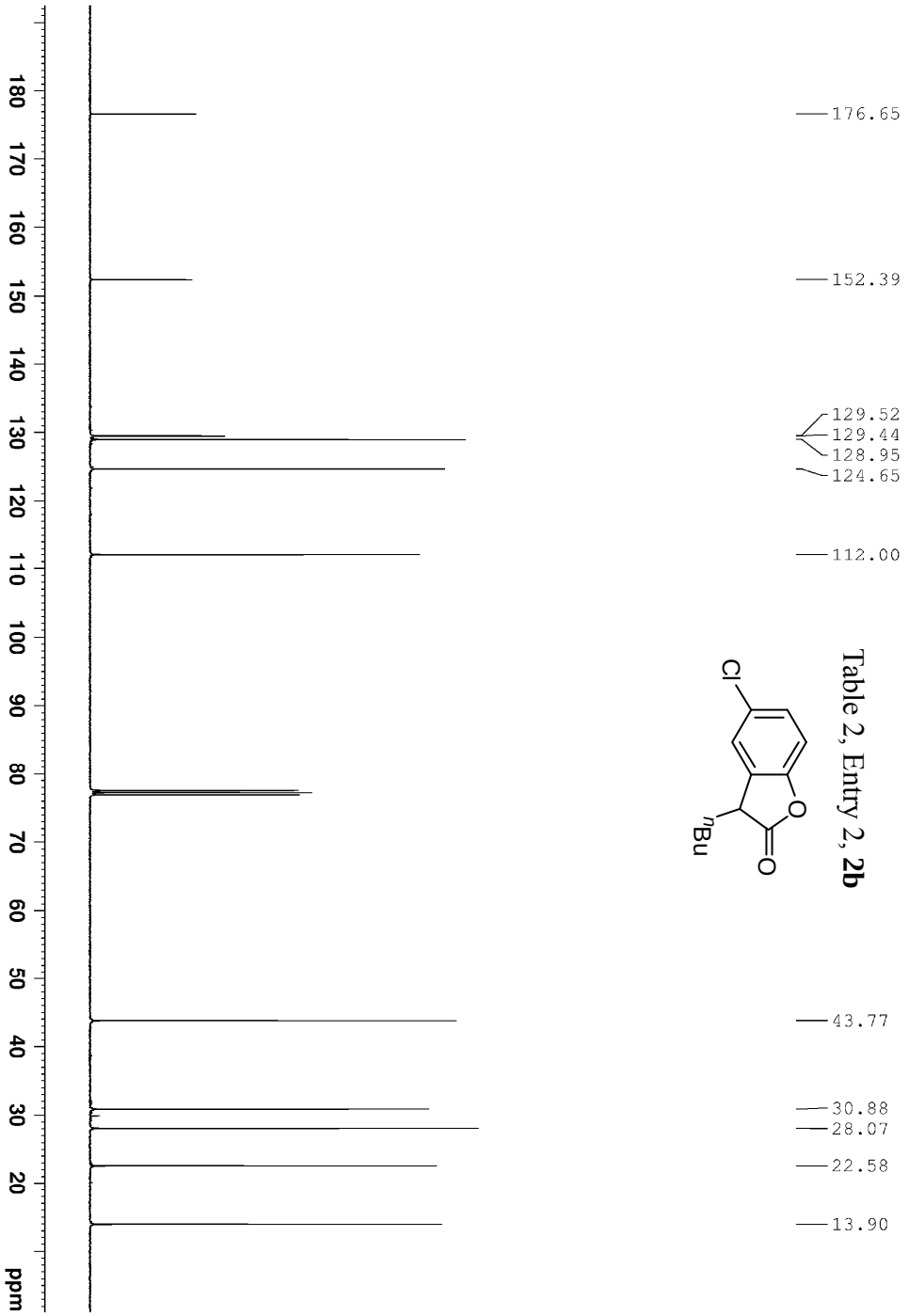
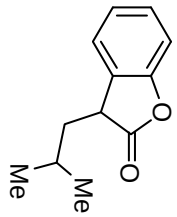
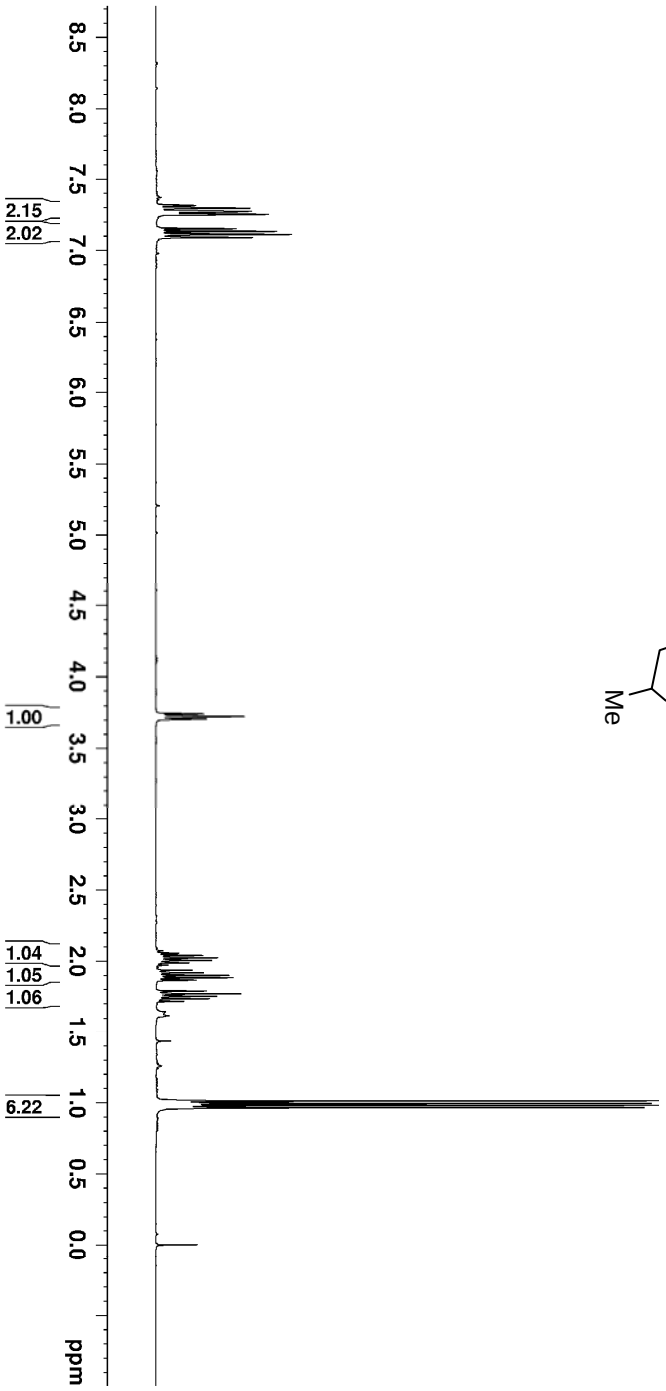


Table 2, Entry 2, **2b**

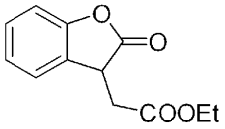
Table 2, Entry 3, **2c**

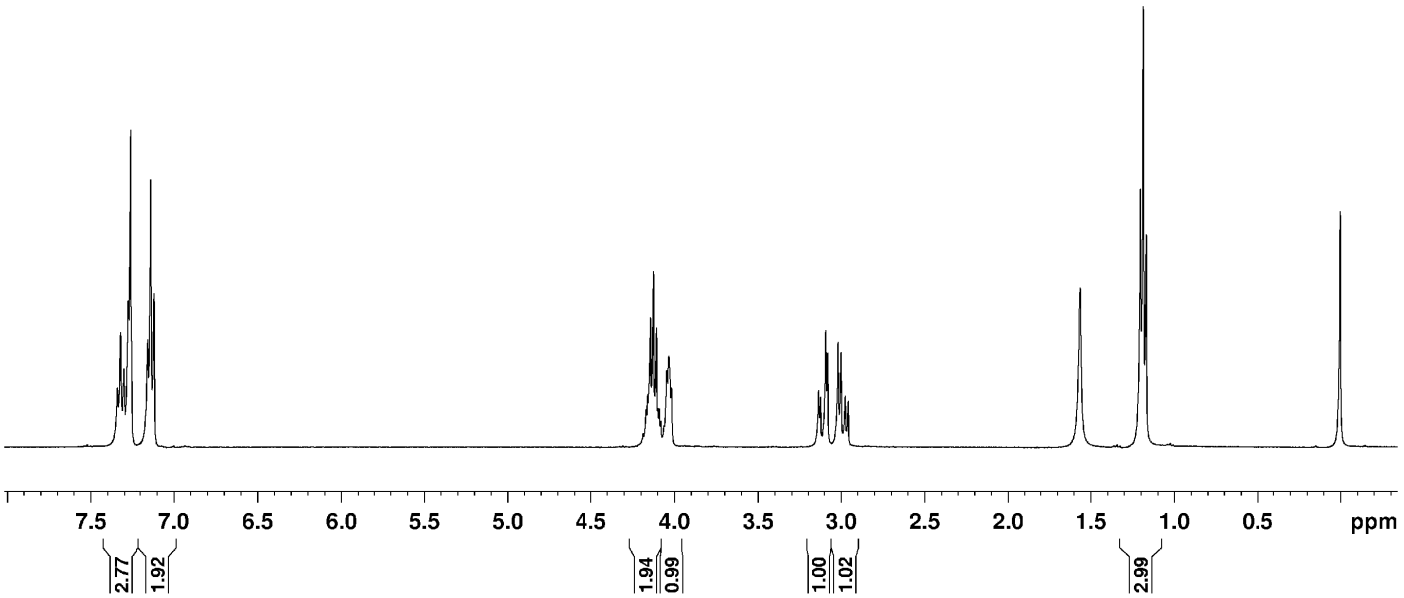





177.79
153.85
128.88
128.14
124.57
124.18
110.95
41.75
40.63
25.35
22.73
22.32
Me
Me
O
O
Table 2, Entry 3, 2c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Table 2, Entry 4, **2d**





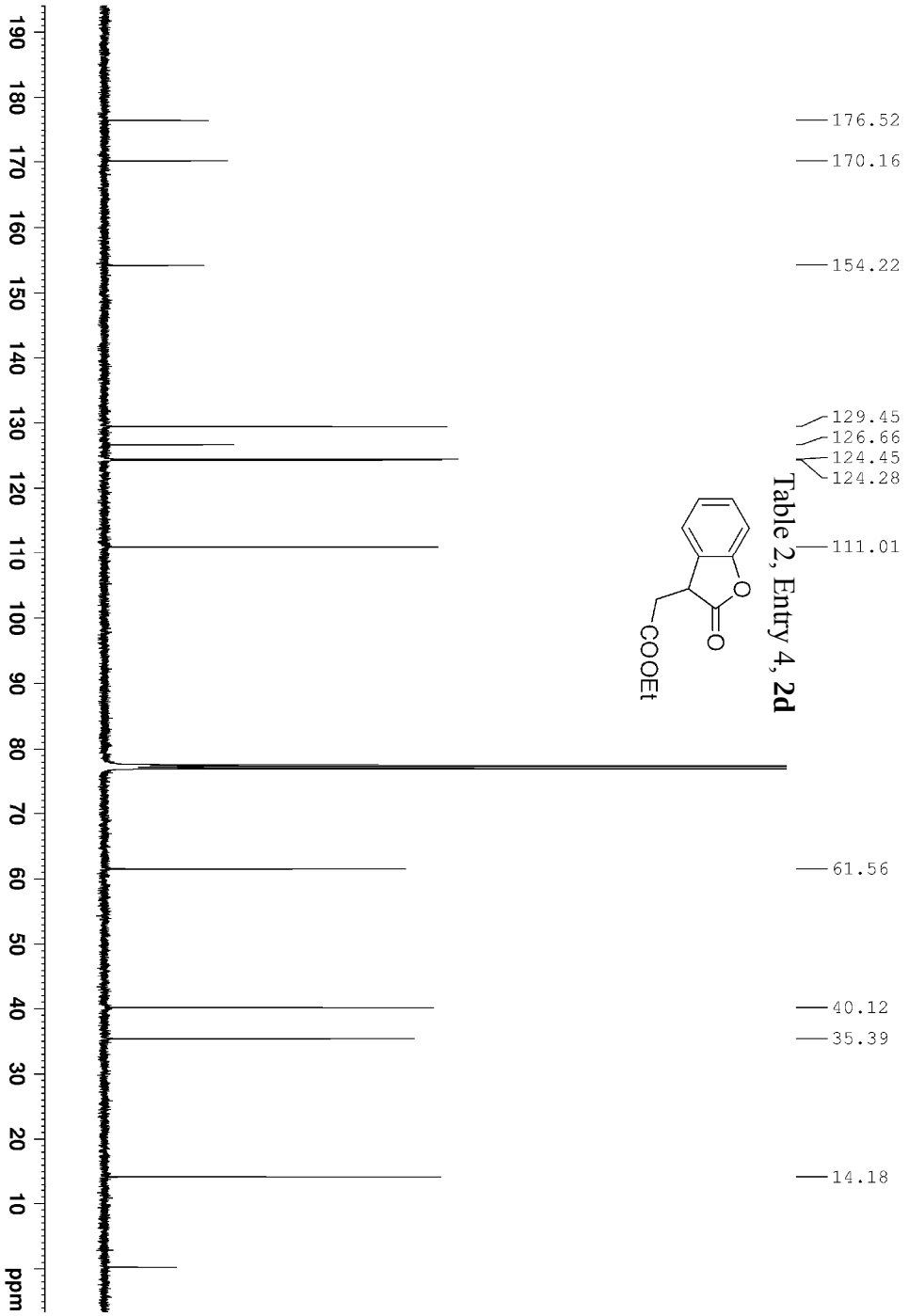
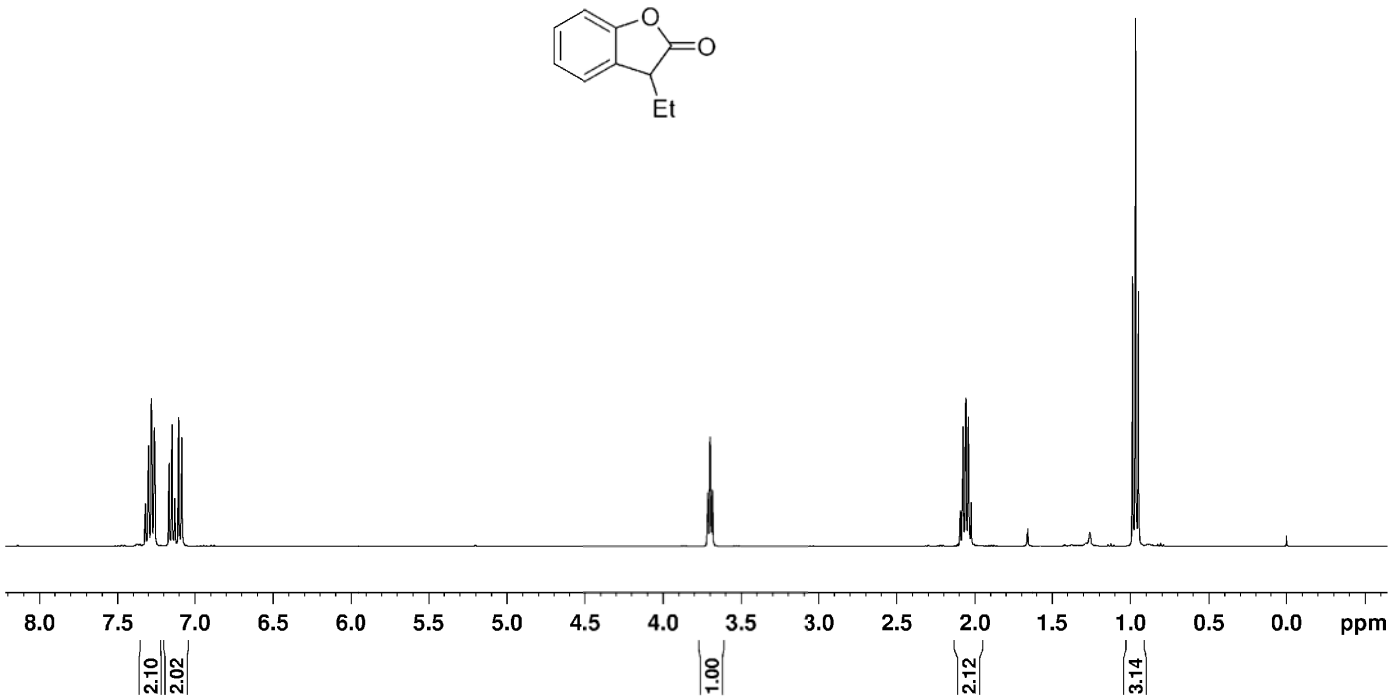


Table 2, Entry 4, **2d**

Table 2, Entry 5, **2e**



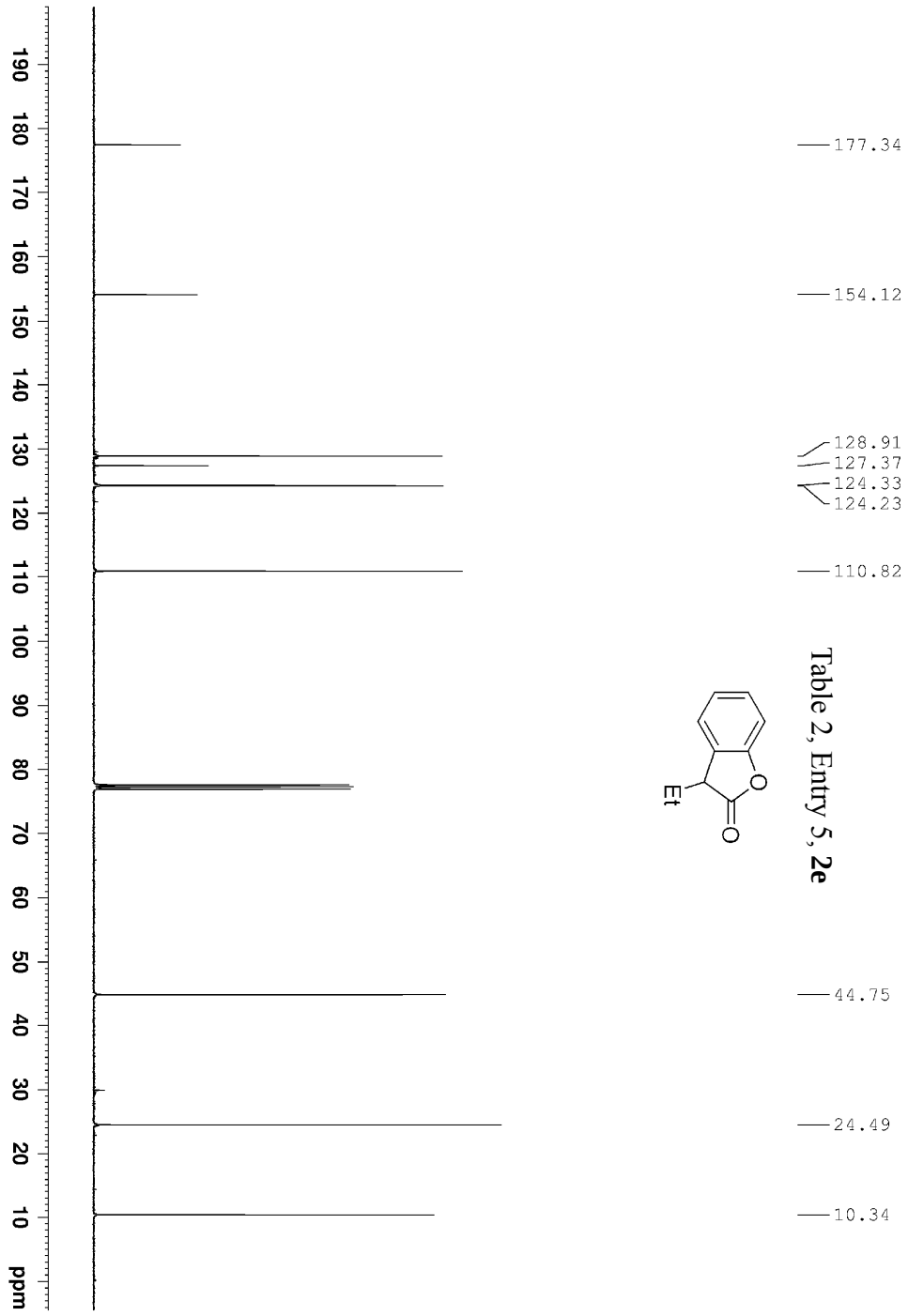
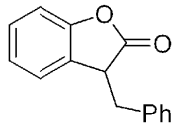
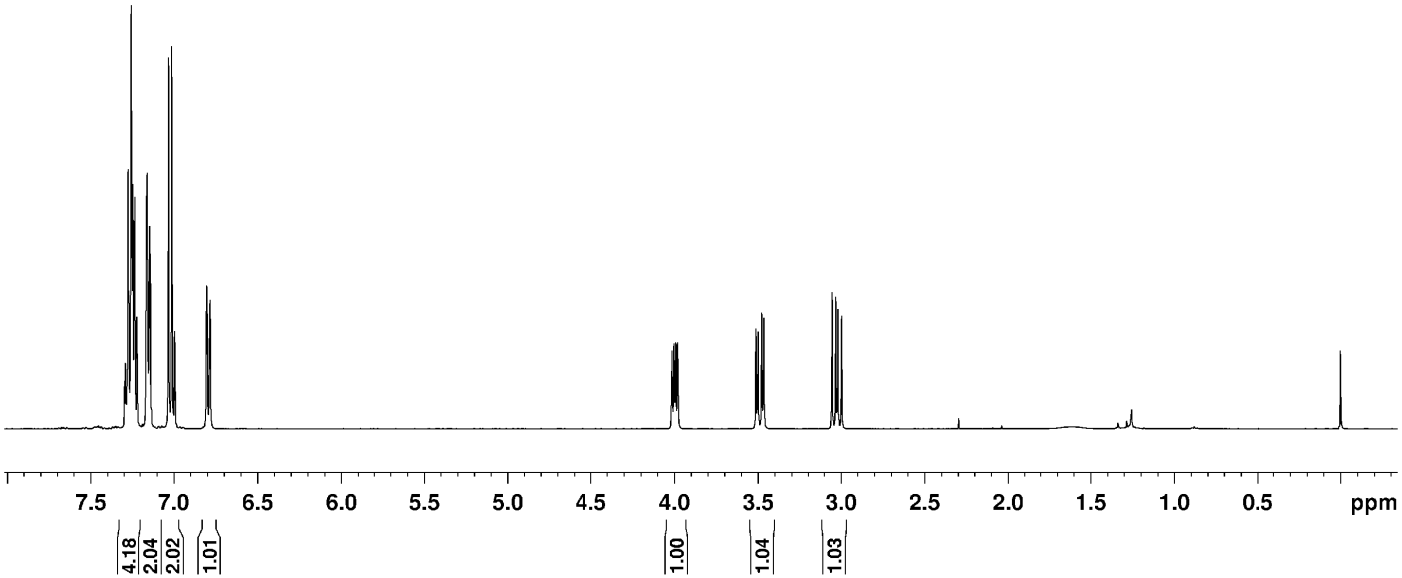


Table 2, Entry 5, **2e**

Table 2, Entry 6, **2f**





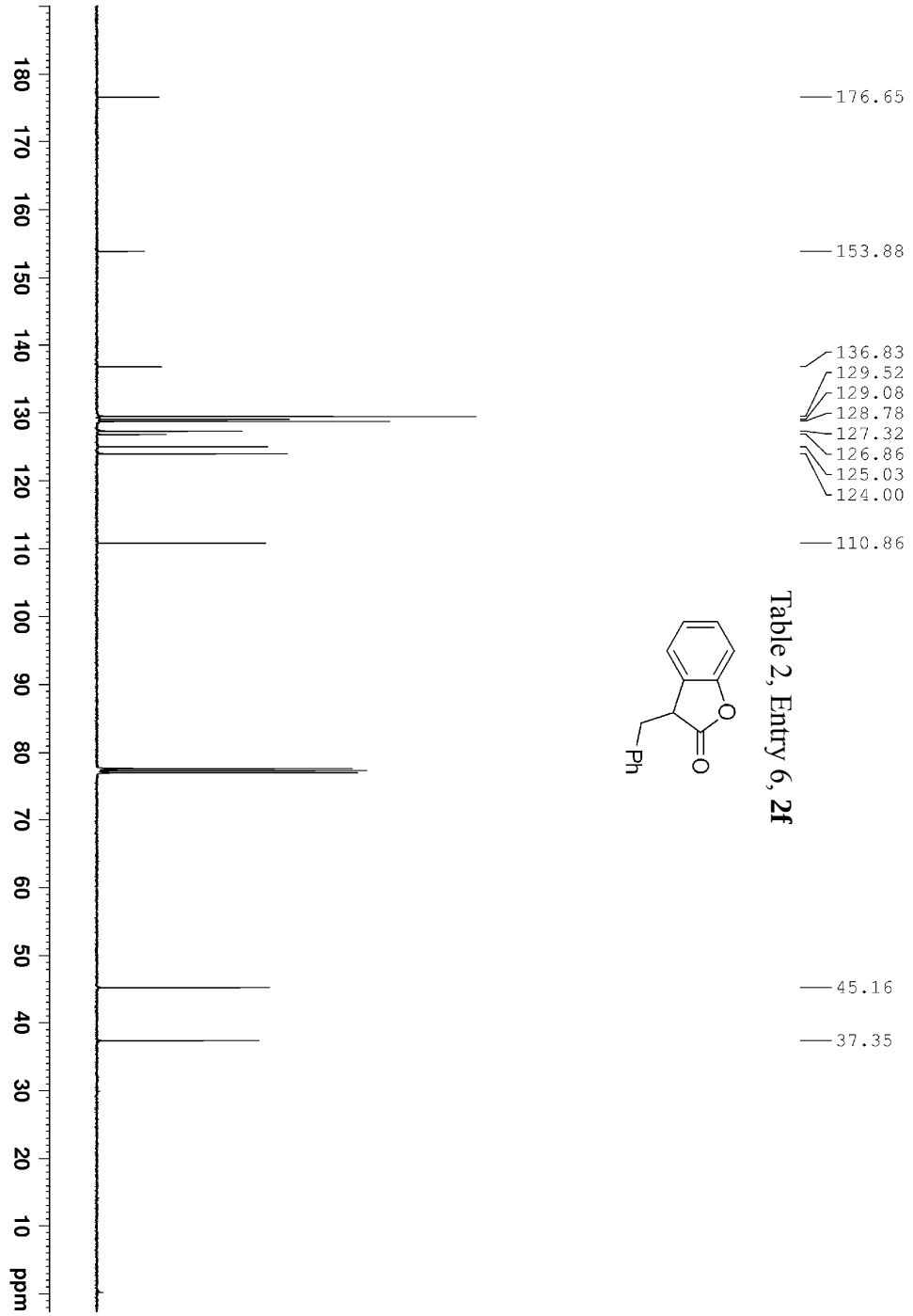
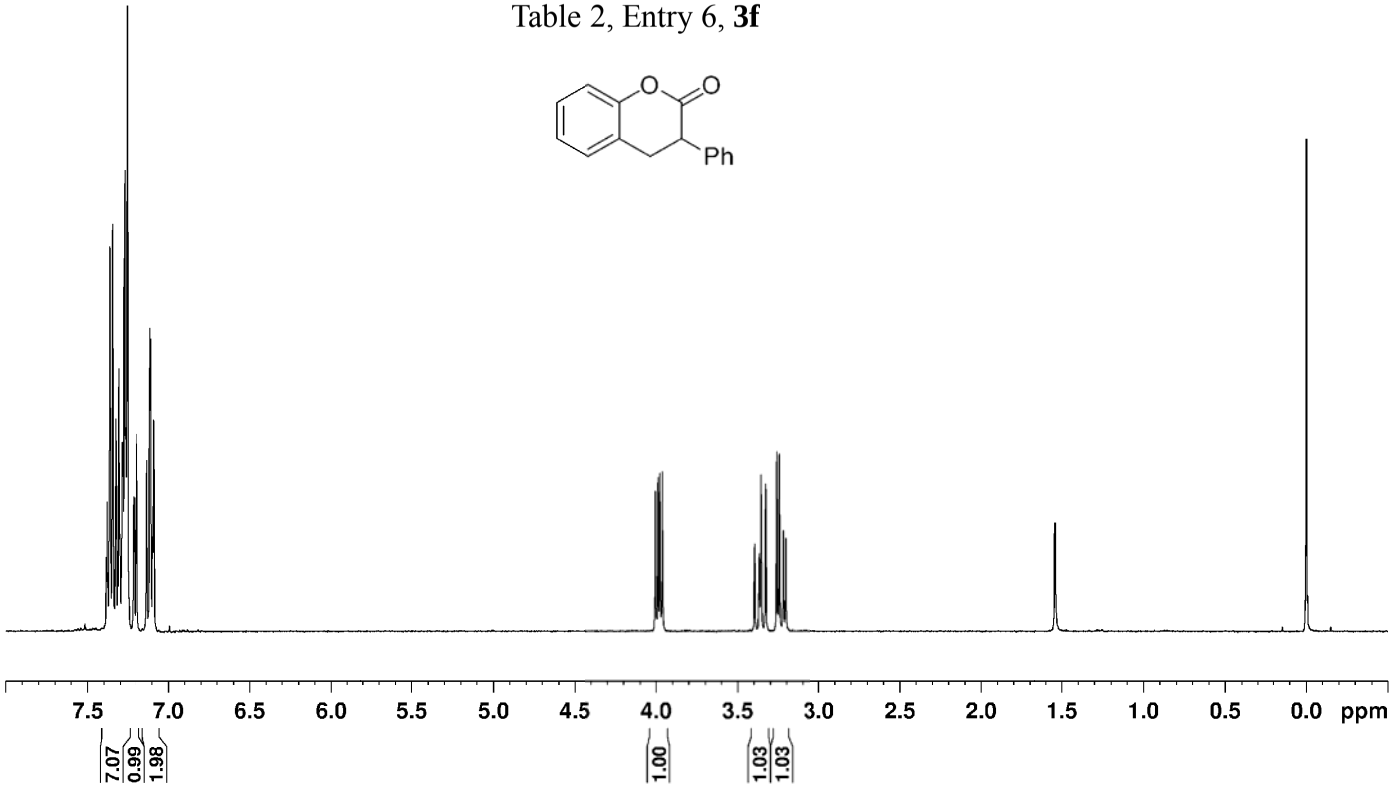


Table 2, Entry 6, **2f**

Table 2, Entry 6, **3f**



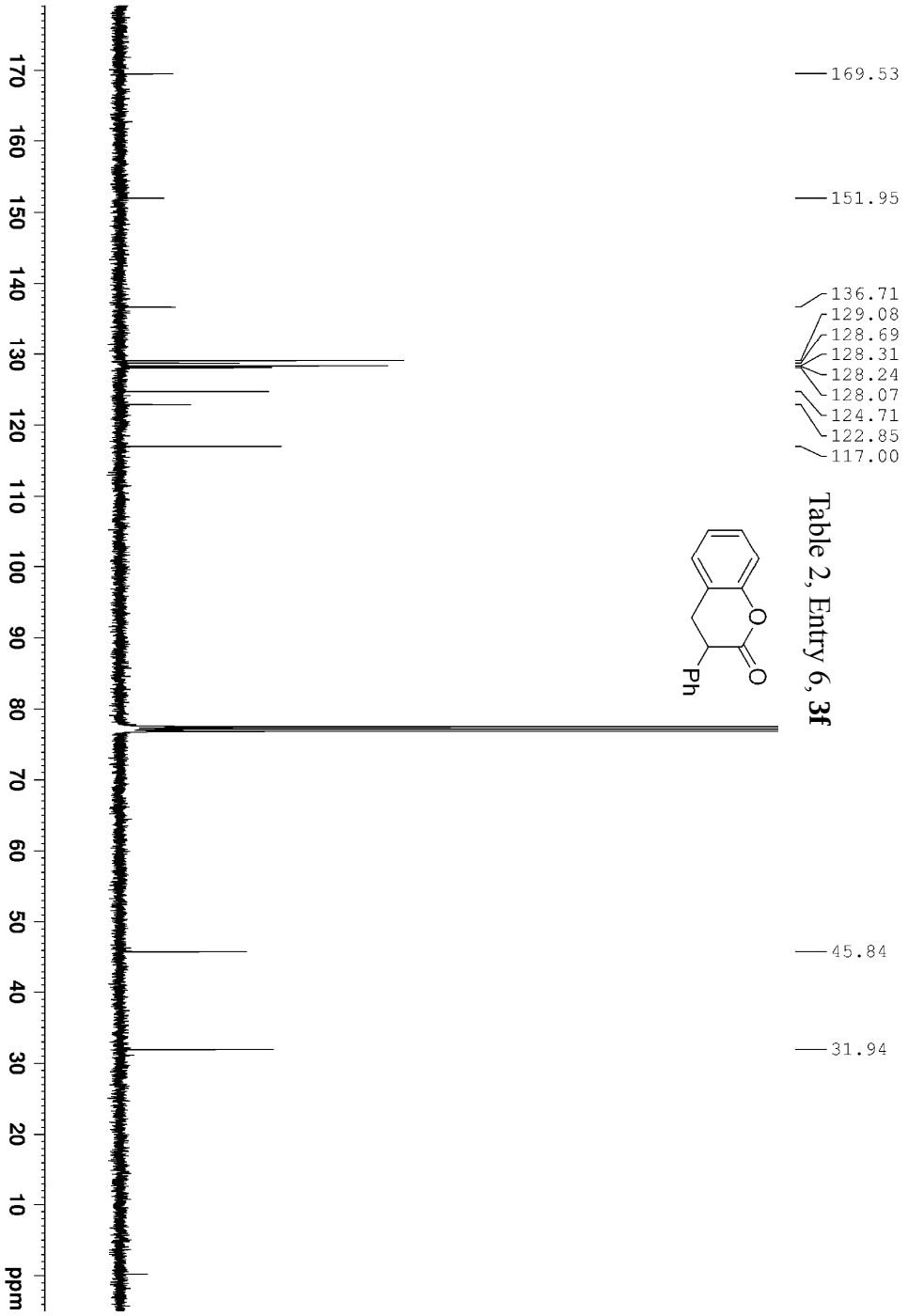
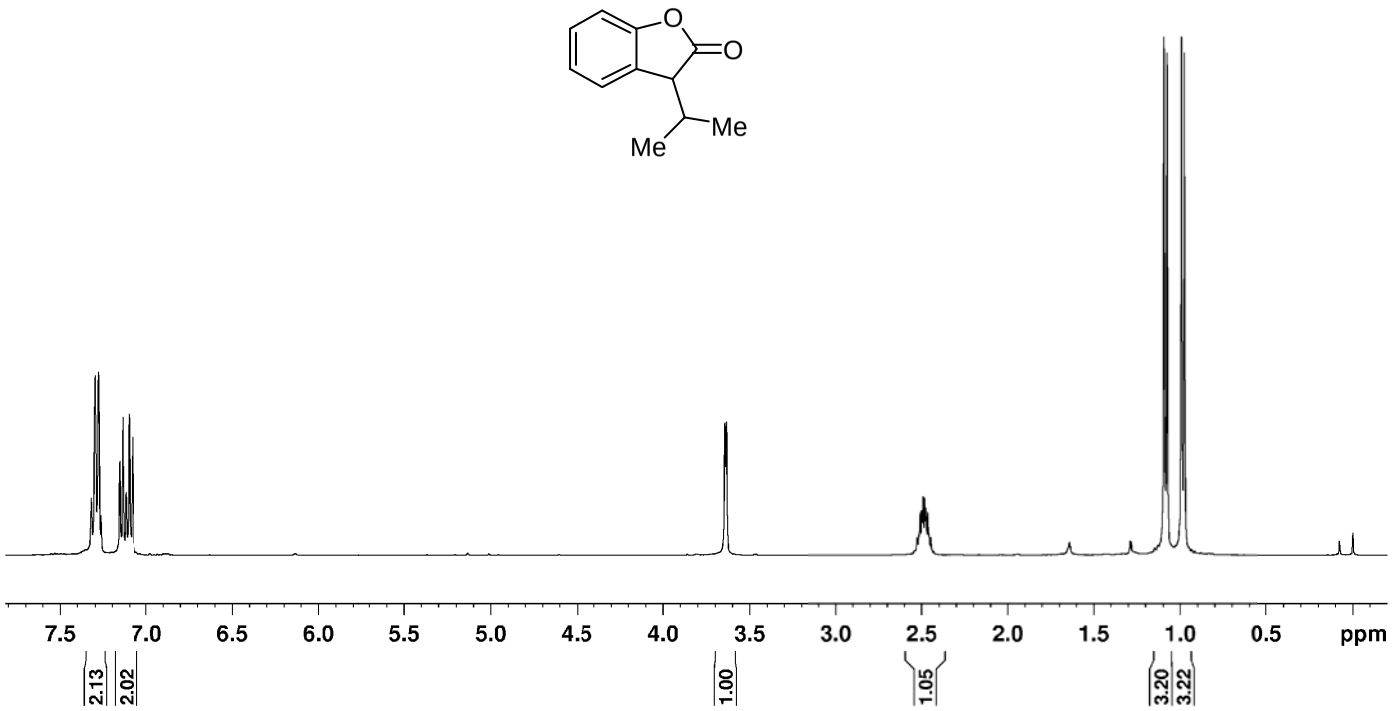


Table 2, Entry 6, **3f**

Table 2, Entry 7, **2g**



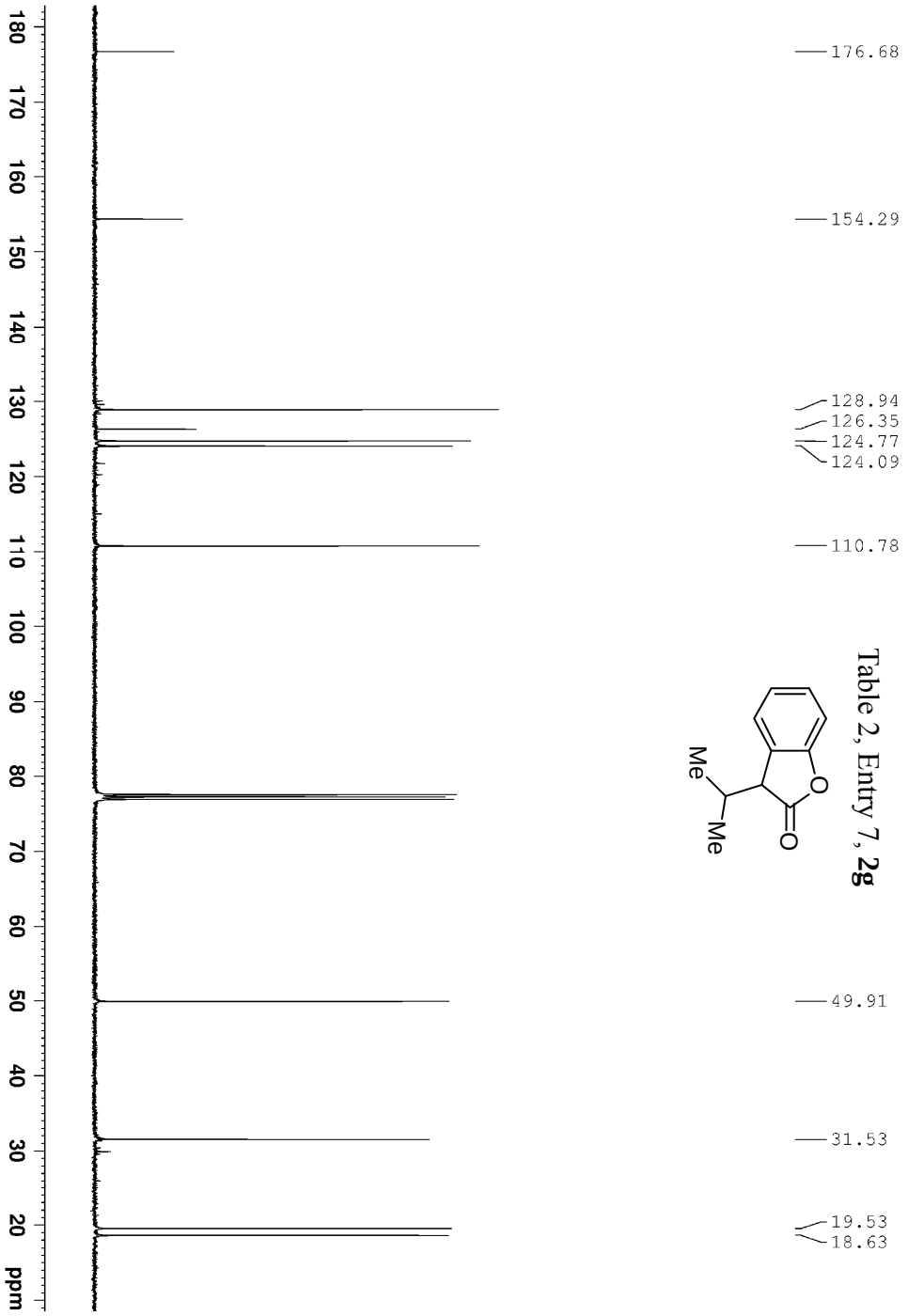
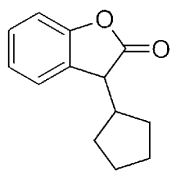
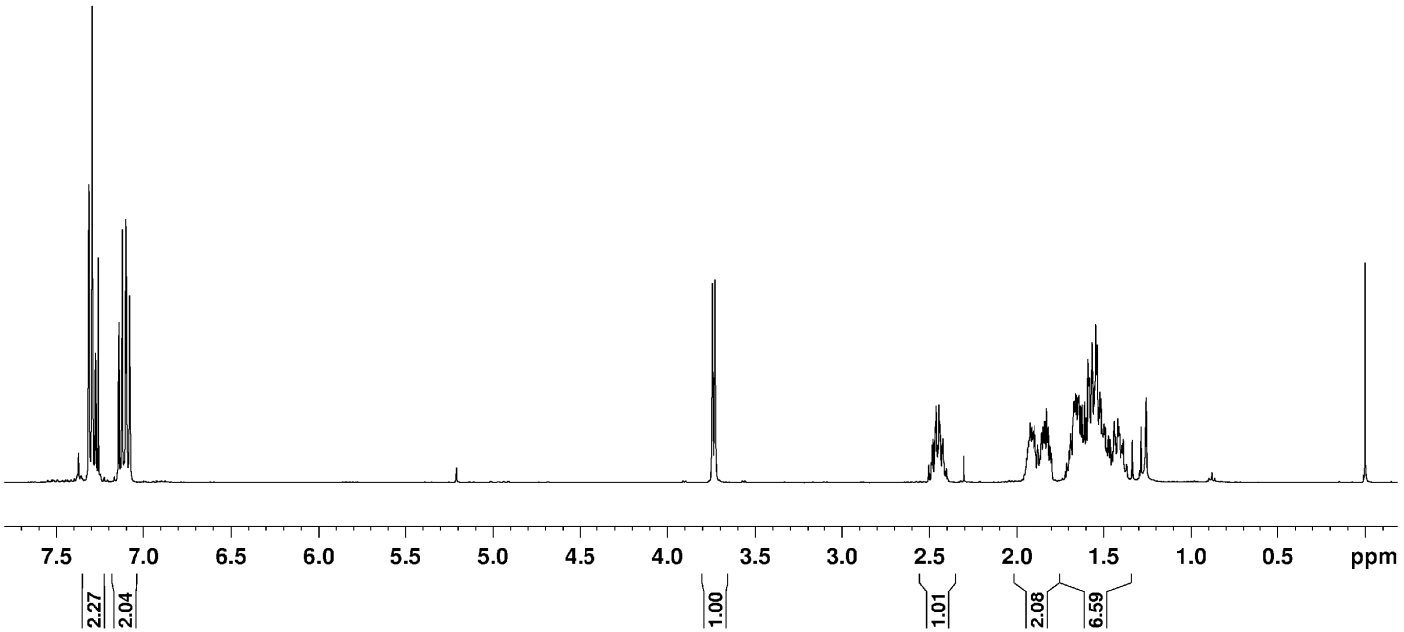


Table 2, Entry 7, **2g**

Table 2, Entry 8, **2h**





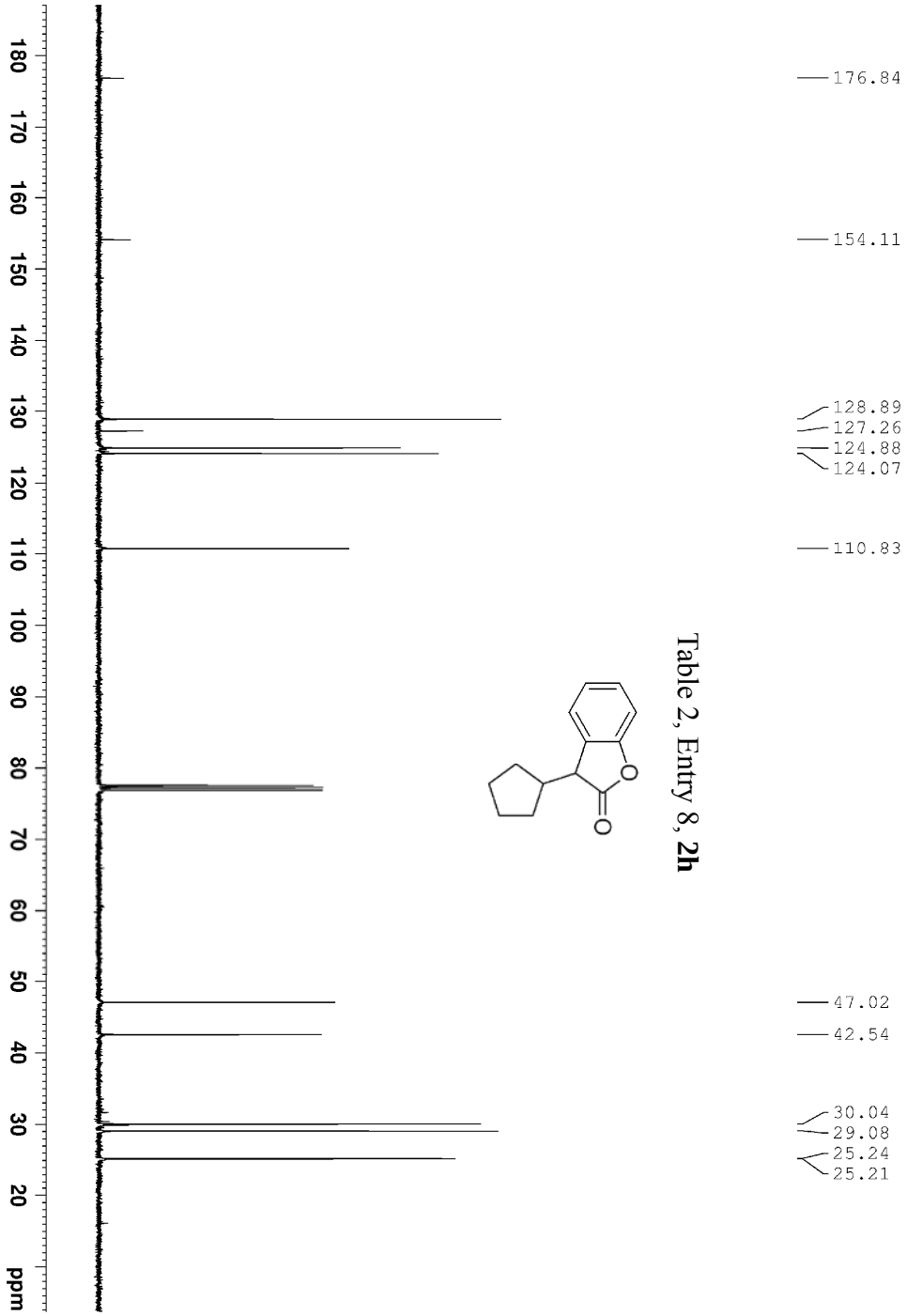
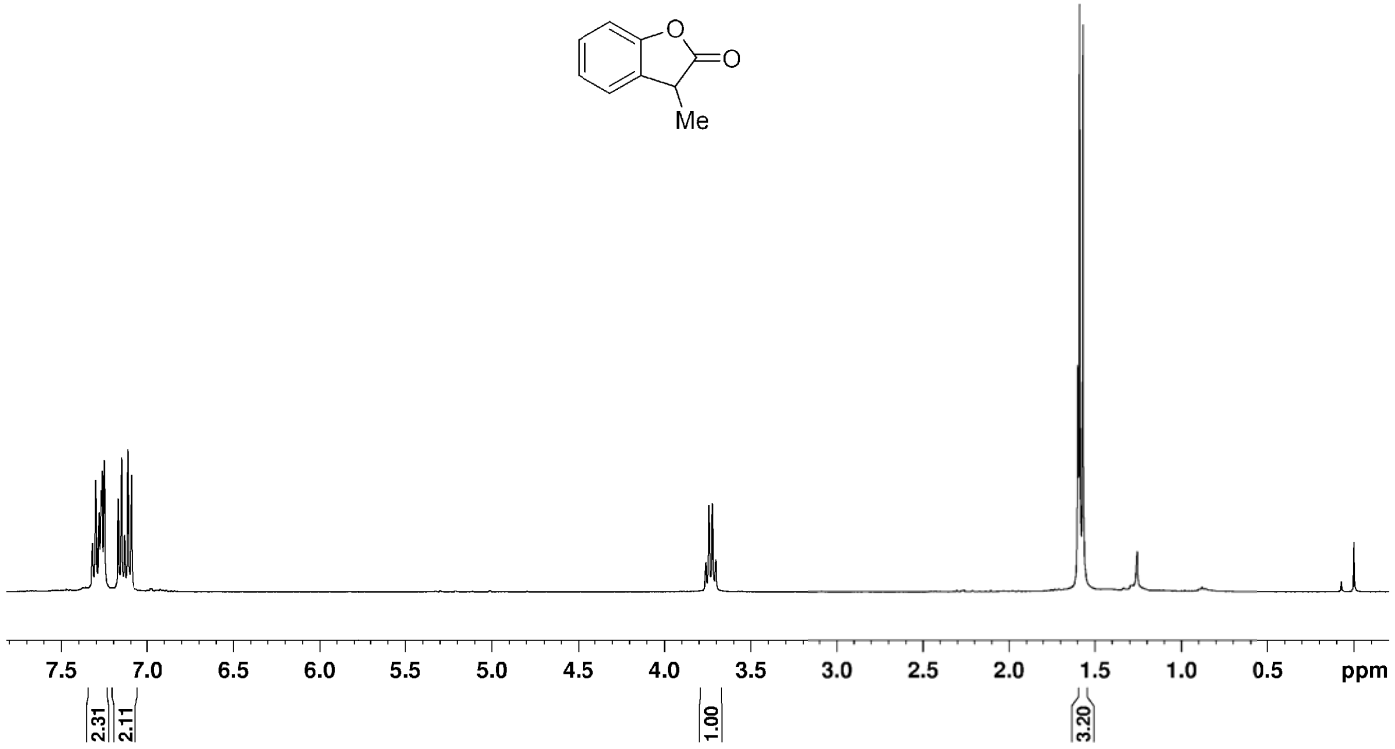


Table 2, Entry 8, **2h**

Table 2, Entry 9, **2i**



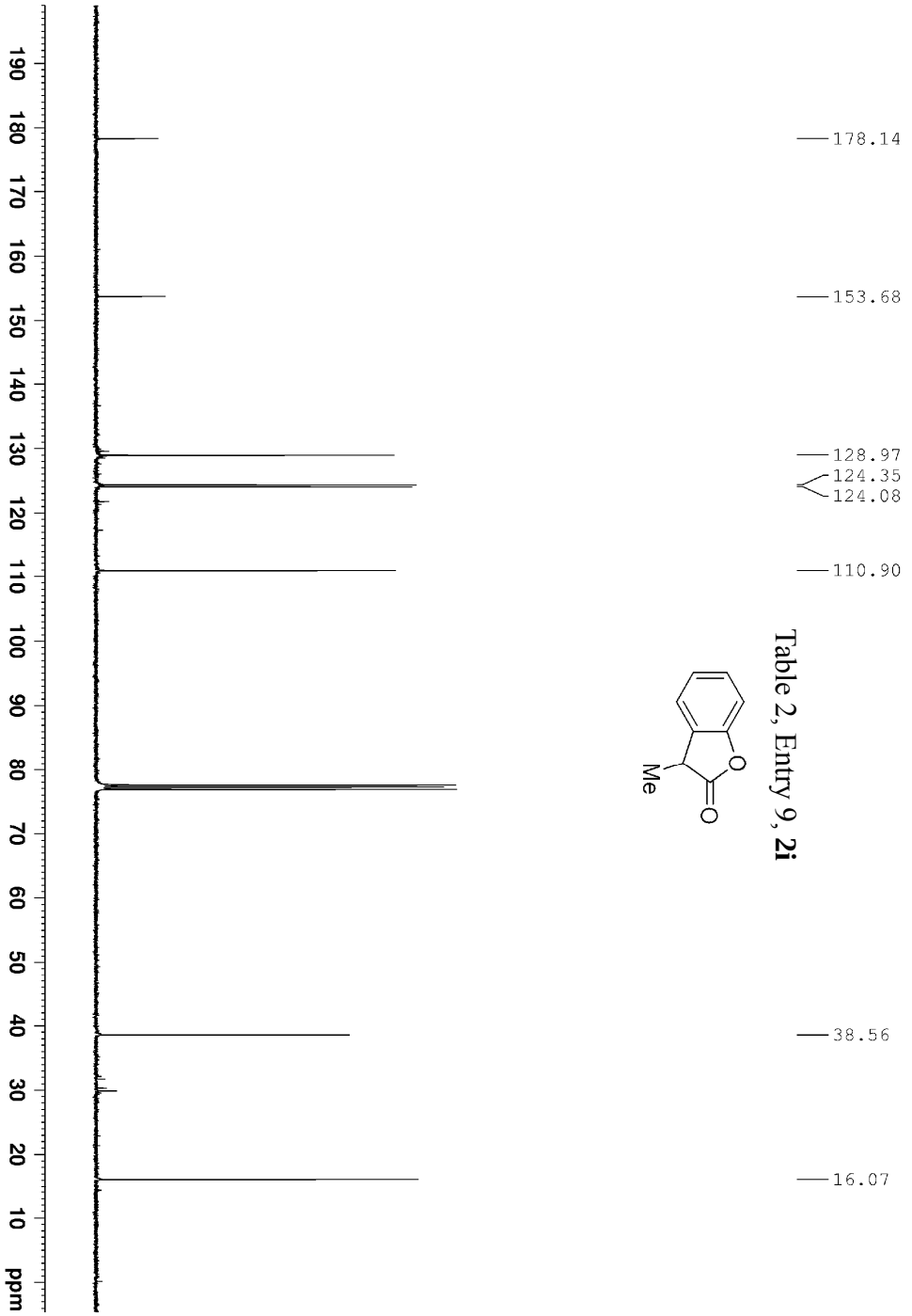
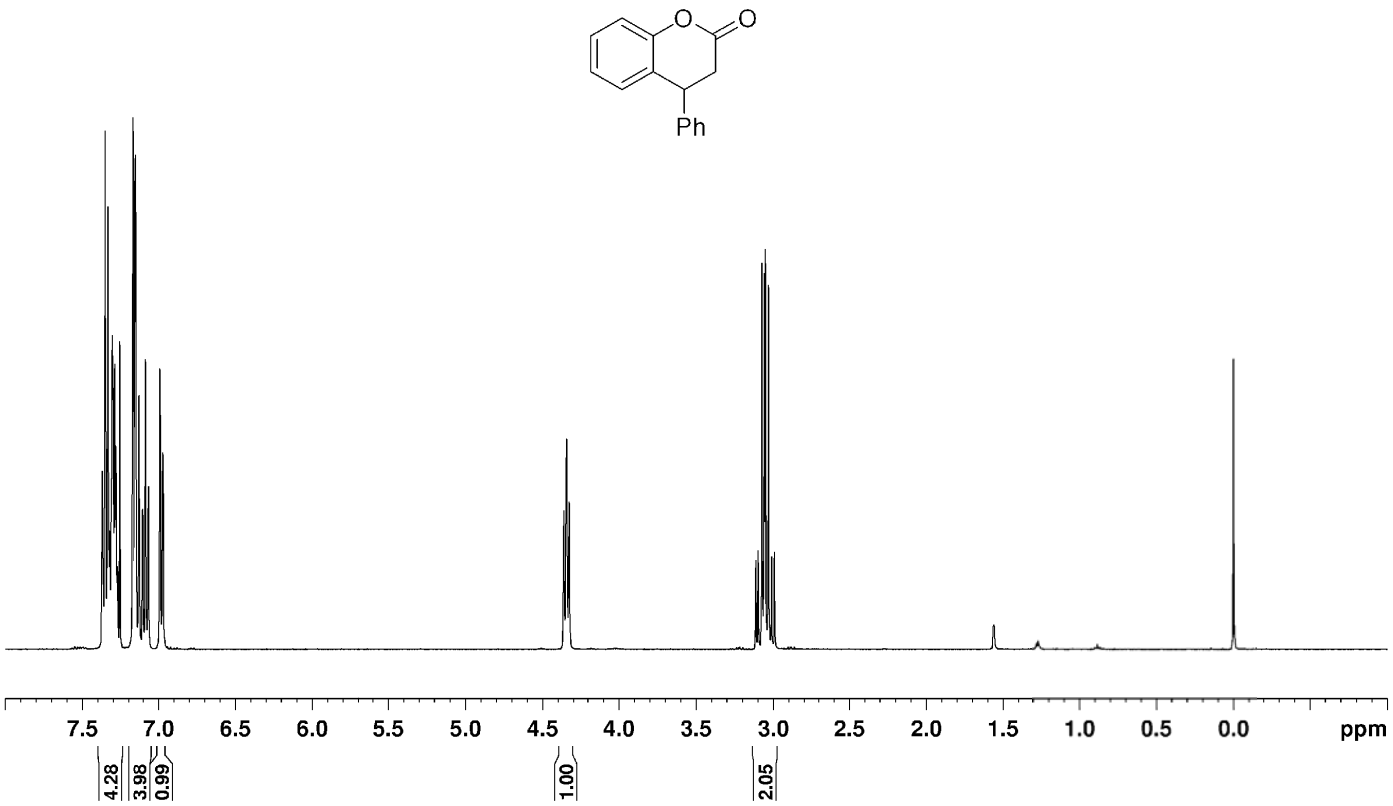


Table 2, Entry 9, **2i**

Table 2, Entry 10, **3j**



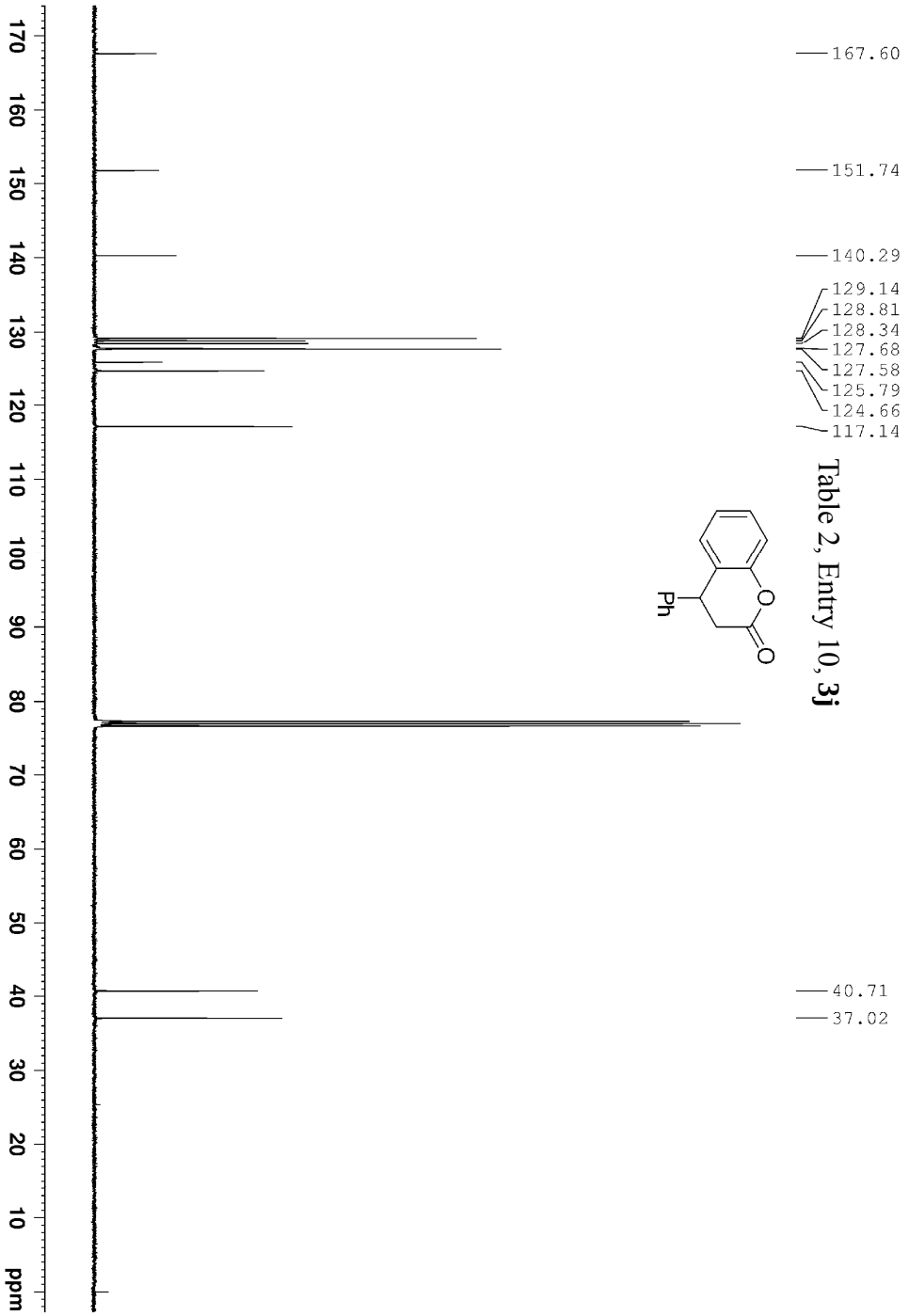


Table 2, Entry 10, **3j**

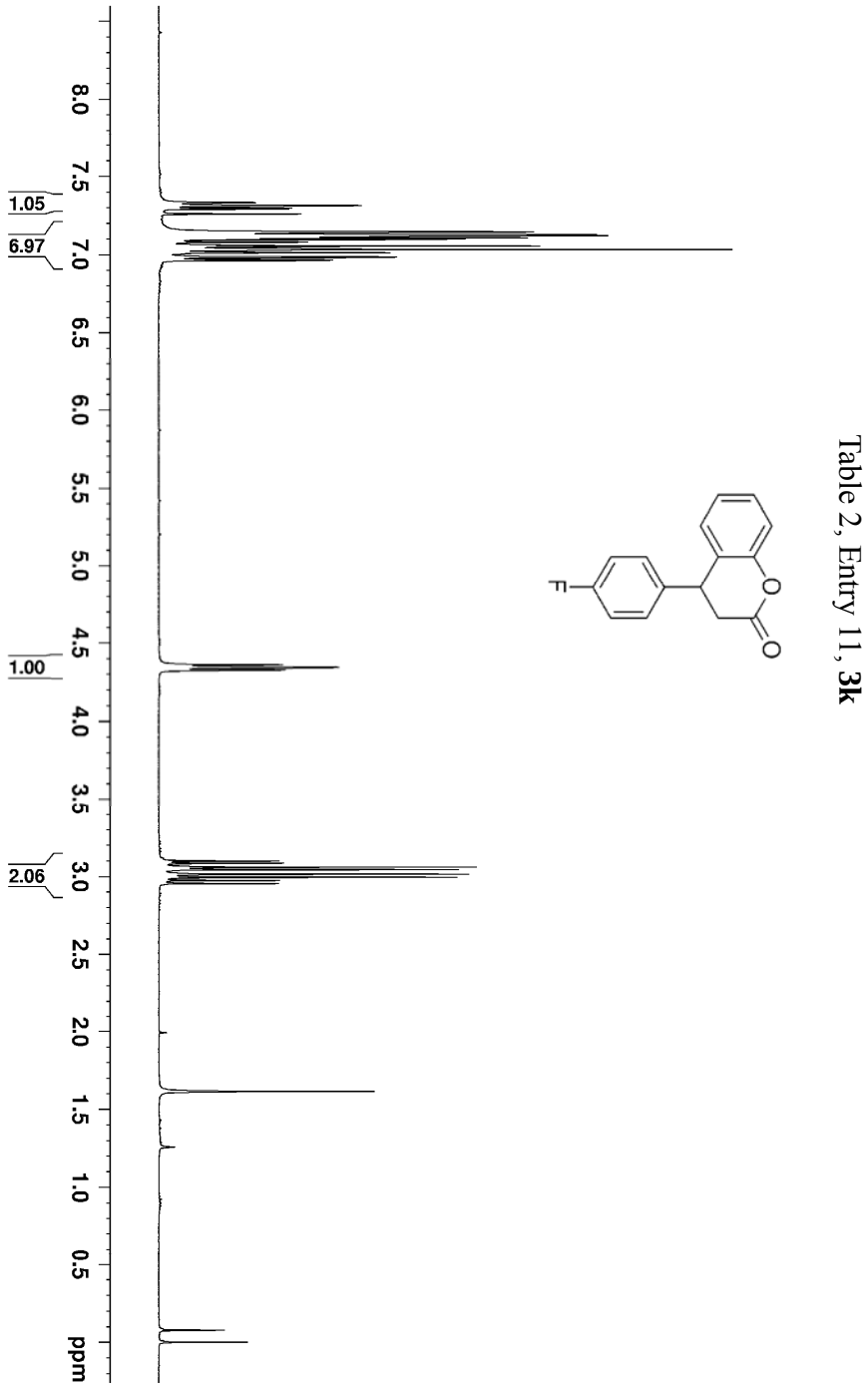


Table 2, Entry 11, **3k**

Table 2, Entry 11, **3k**

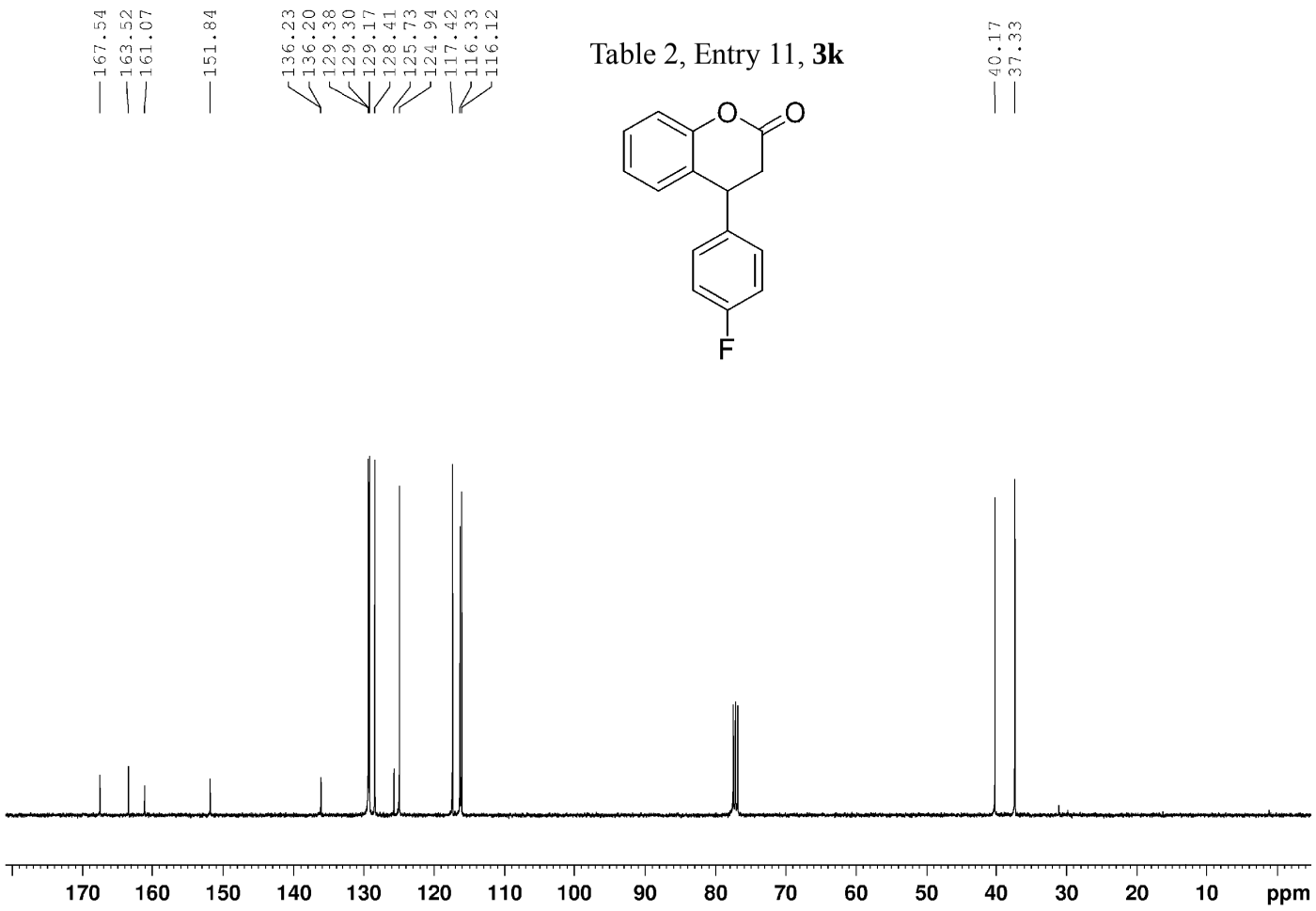
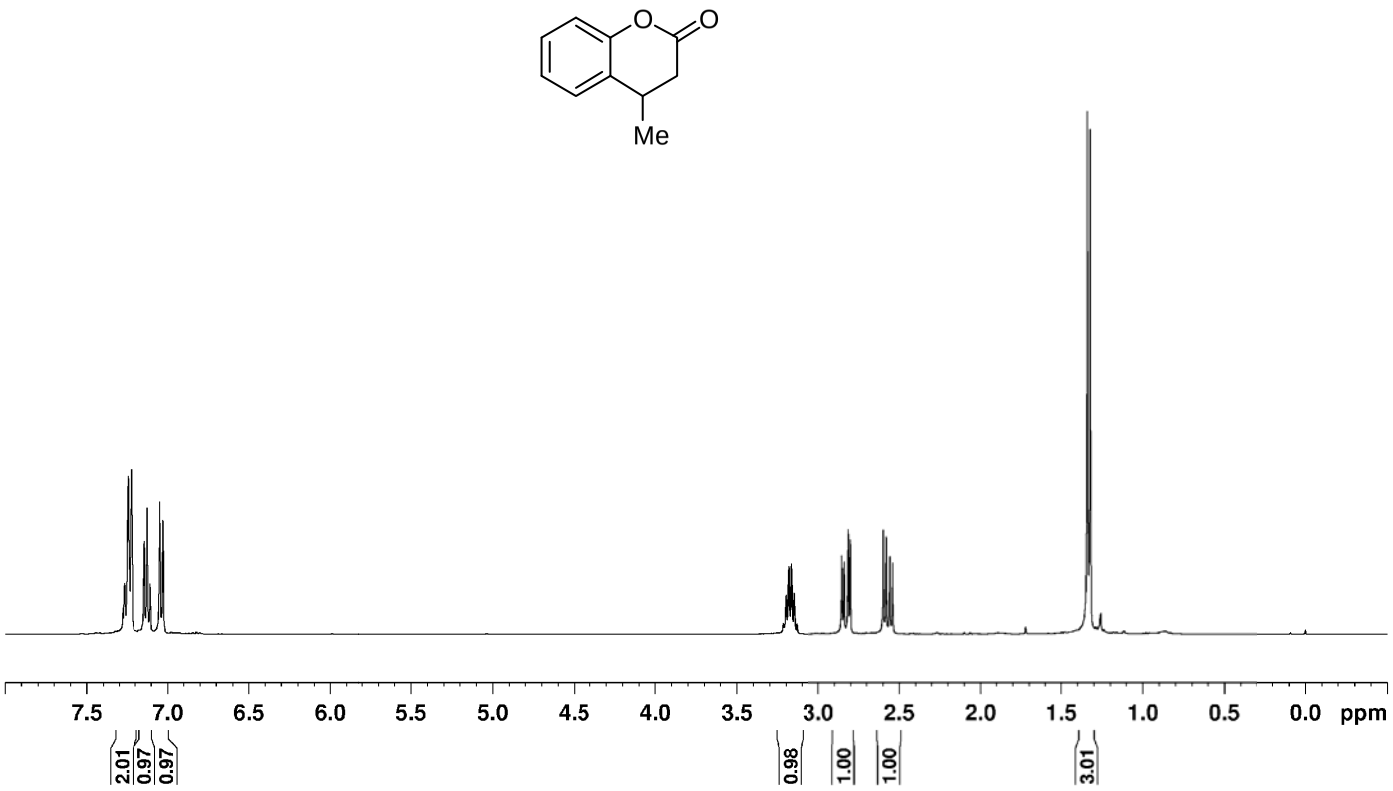


Table 2, Entry 12, **3l**



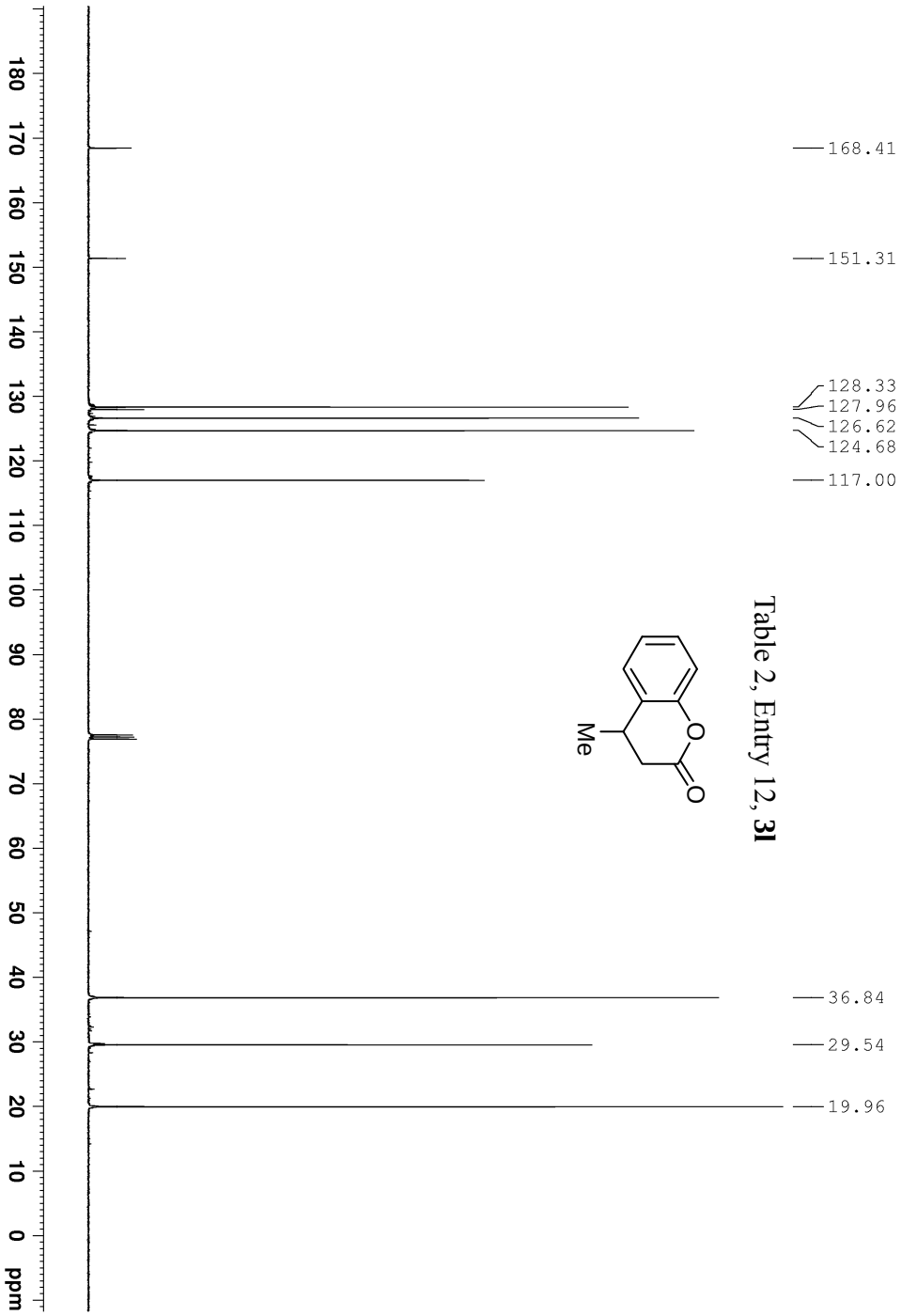
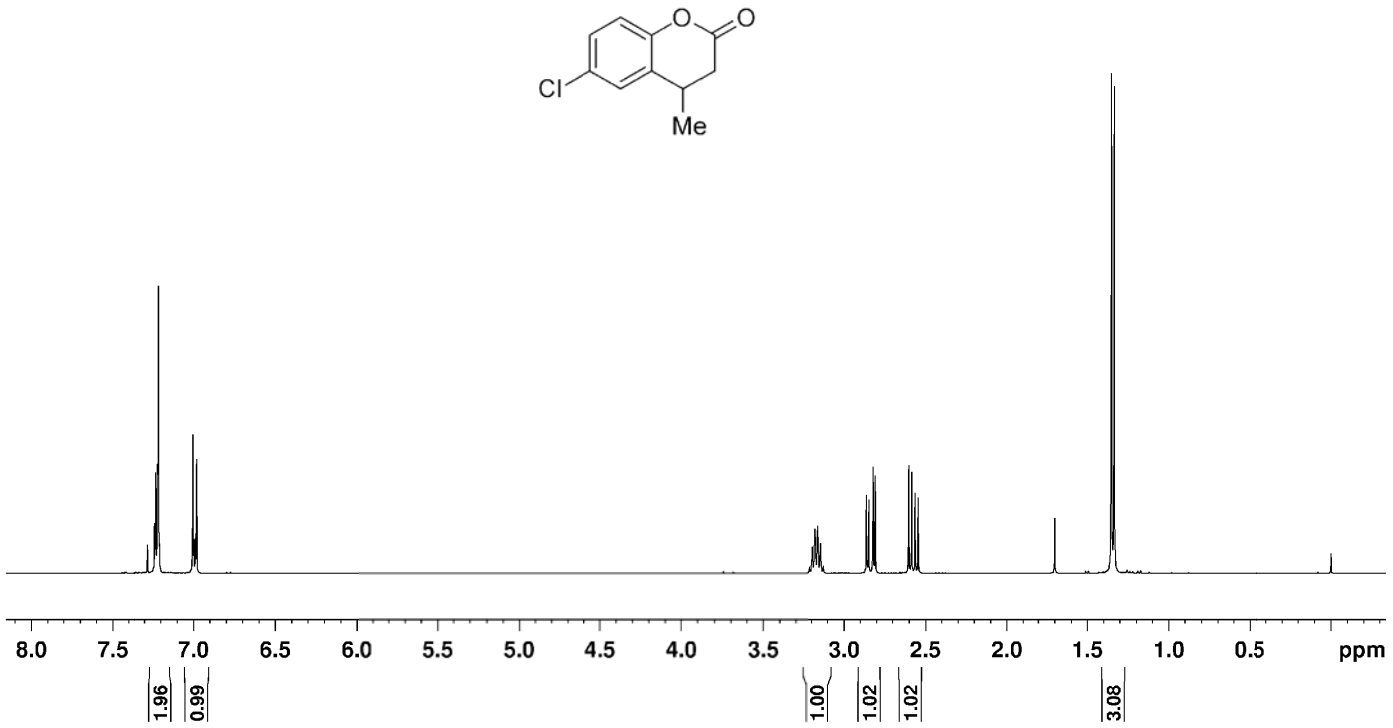


Table 2, Entry 12, **3l**

Table 2, Entry 13, **3m**



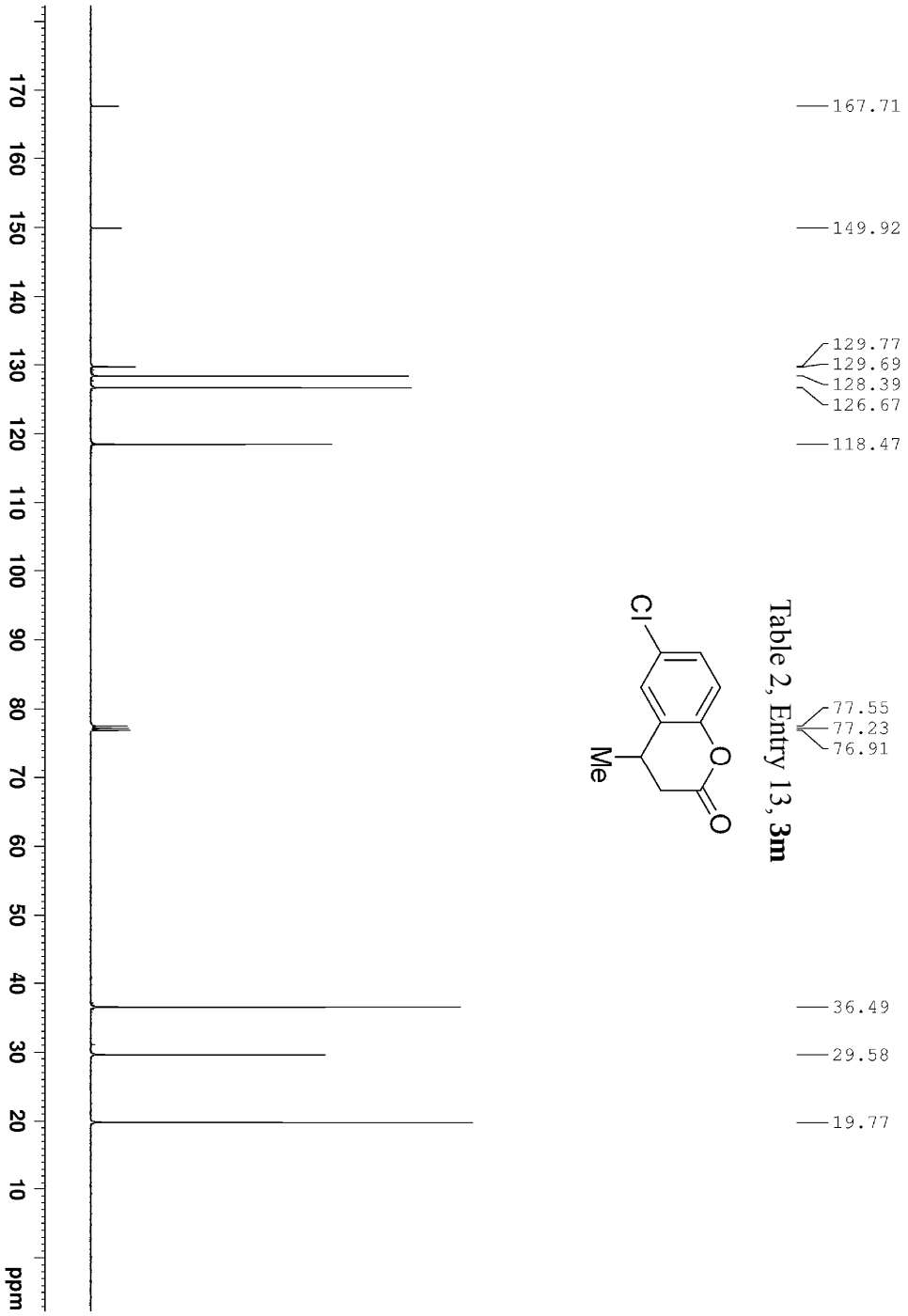
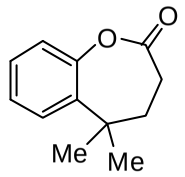
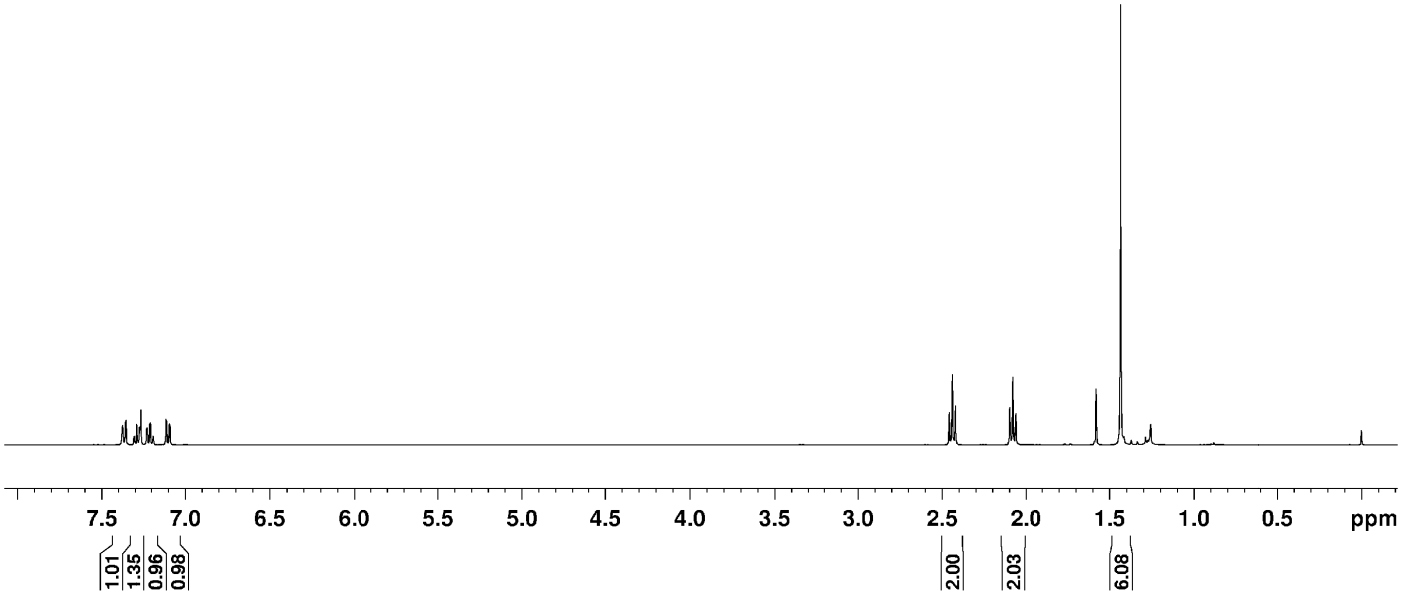


Table 2, Entry 13, **3m**

Table 2, Entry 15, **3o**





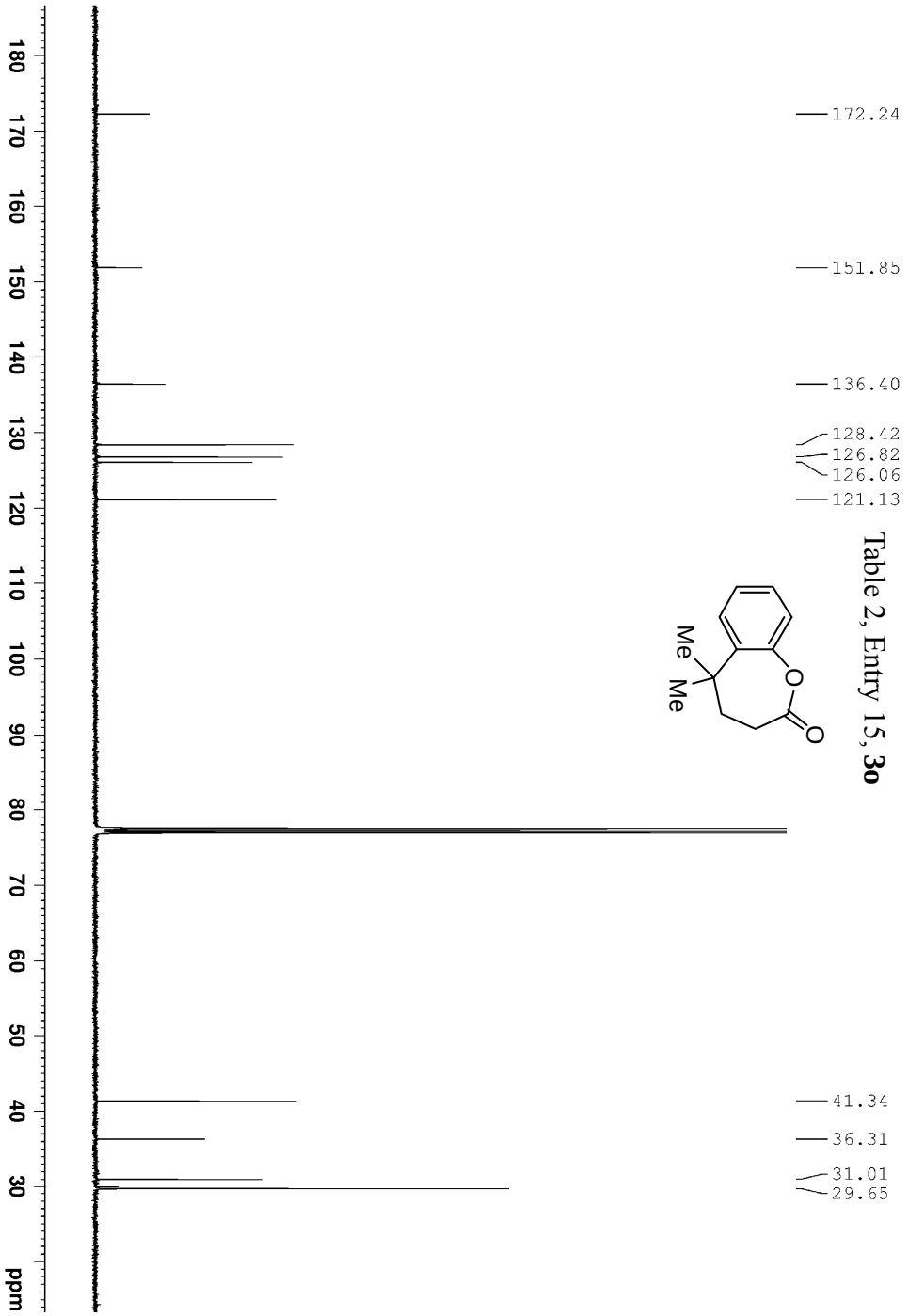
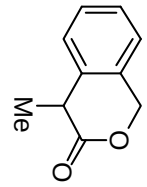
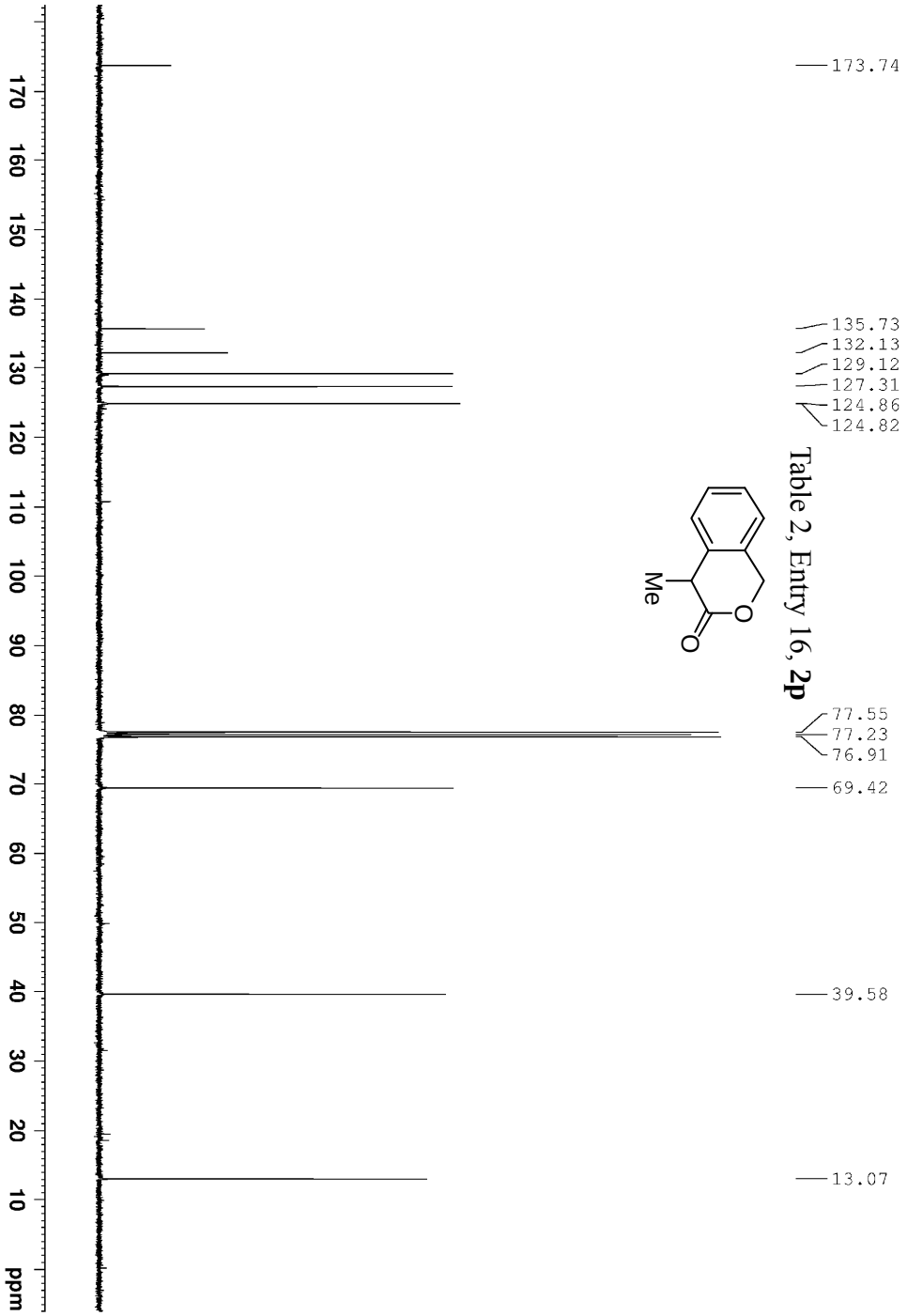


Table 2, Entry 15, **3o**

Table 2, Entry 16, **2p**

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135.73
132.13
129.12
127.31
124.86
124.82
77.55
77.23
76.91
69.42
39.58
13.07
Me
O
O
Table 2, Entry 16, 2p
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm