catalysts

Supplementary Materials: Tin(IV)-Porphyrin Tetracarbonyl Cobaltate: An Efficient Catalyst for the Carbonylation of Epoxides

Ek Raj Baral [1], Dongwook Kim [2], Sunwoo Lee [3,*], Myung Hwan Park [4,*] and Jeung Gon Kim [1,*]

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1. Crystallographic Data for 2a

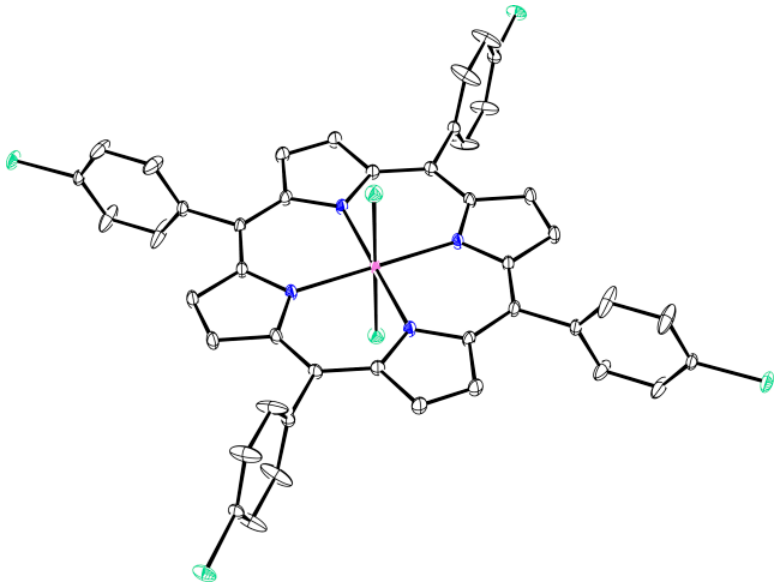


Figure S1. ORTEP of **2a** (Hydrogen atoms are omitted for clarity)

Table S1. Crystallographic data and parameters for **2a**

Compound	**2a**
Formula	$C_{60}H_{56}Cl_6N_4O_4Sn$
Formula weight	1228.47
Crystal system	Tetragonal
Space group	I 4/m
a (Å)	16.9599(5)
b (Å)	16.9599(5)
c (Å)	9.5082(4)
α (°)	90
β (°)	90
γ (°)	90
V (Å^3)	2734.9(2)

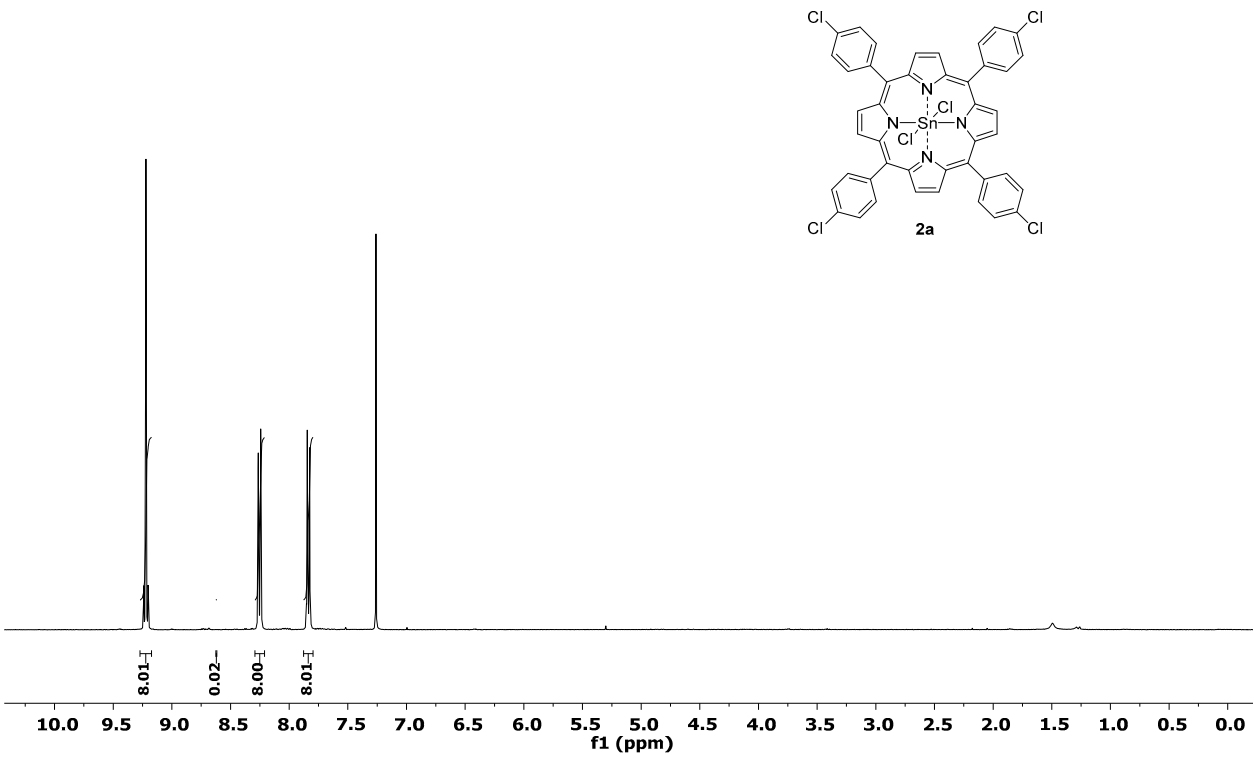
Z	2
ρ_{calc}(g cm^{-3})	1.492
μ (mm^{-1})	0.813
F(000)	1256
T (K)	173(2)
Scan mode	MULTI-SCAN
hkl range	–23 → +23, –20 → +23, –12 → +13
Measd reflns	24403
Unique reflns [R_{int}]	1957 [0.0260]
Reflns used for refinement	1957
Refined parameters	120
R_1[a] (I > 2σ(I))	0.0315
wR_2[b] all data	0.0774
GOF on F^2	1.053
ρ_{fin} (max/min) (e Å^{-3})	0.447, −0.539

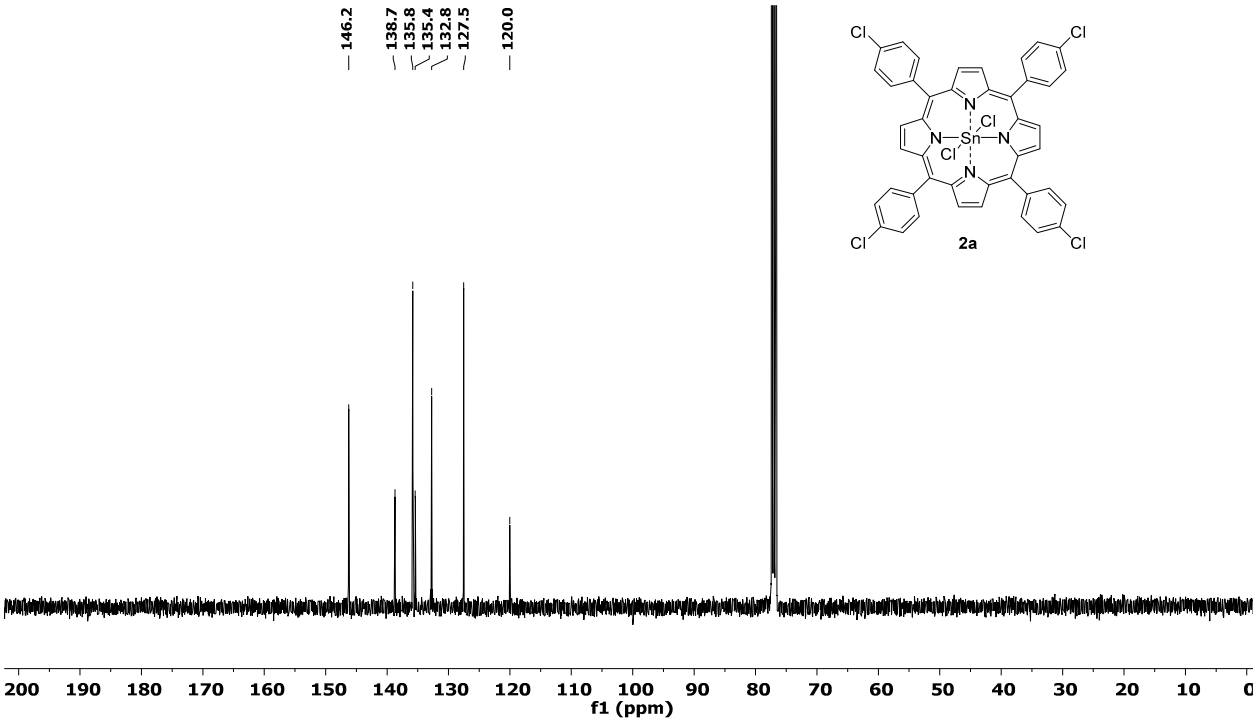
[a]$R_1 = \sum||Fo| - |Fc||/\sum|Fo|$. [b]$wR_2 = \{[\sum w(Fo^2 - Fc^2)^2]/[\sum w(Fo^2)^2]\}^{1/2}$.

Table S2. Selected bond lengths (Å) and angles (deg) for **2a**

Compound	**2a**
	lengths
Sn–N1	2.0966(18)
Sn–Cl2	2.4326(9)
Cl1–C9	1.744(2)
Nl–C1	1.371(3)
Nl–C4	1.376(3)
C1–C2	1.444(3)
C2–C3	1.363(3)
C3–C4	1.445(3)
C4–C5	1.403(3)
C5–C6	1.500(3)
C6–C7	1.370(2)
C7–C8	1.393(3)
C8–C9	1.360(2)
	angles
N1–Sn–N1a	90.0
N1–Sn–N1b	180.0
N1–Sn–Cl2	90.0
Cl–Sn–Cl2d	180.0
C1–N1–C4	108.99(18)
C1–N1–Sn	125.59(15)
C4–N1–Sn	125.42(15)
N1–C1–C2	108.09(19)
C3–C2–C1	107.5(2)
C2–C3–C4	107.7(2)
N1–C4–C5	126.1(2)
N1–C4–C3	107.75(19)
C5–C4–C3	126.1(2)
C4–C5–C6	116.42(19)
C7–C6–C5	120.85(11)
C6–C7–C8	121.10(18)
C8–C9–Cl1	119.65(11)

2. ^{1}H NMR and ^{13}C NMR Spectra of Synthesized Compounds


Cl
Cl
N
Cl
N—Sn—N
Cl
N
Cl
Cl
2a
8.01
0.02
8.00
8.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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138.7
135.8
135.4
132.8
127.5
120.0
Cl
Cl
N
Cl
N—Sn—N
Cl
N
Cl
Cl
2a
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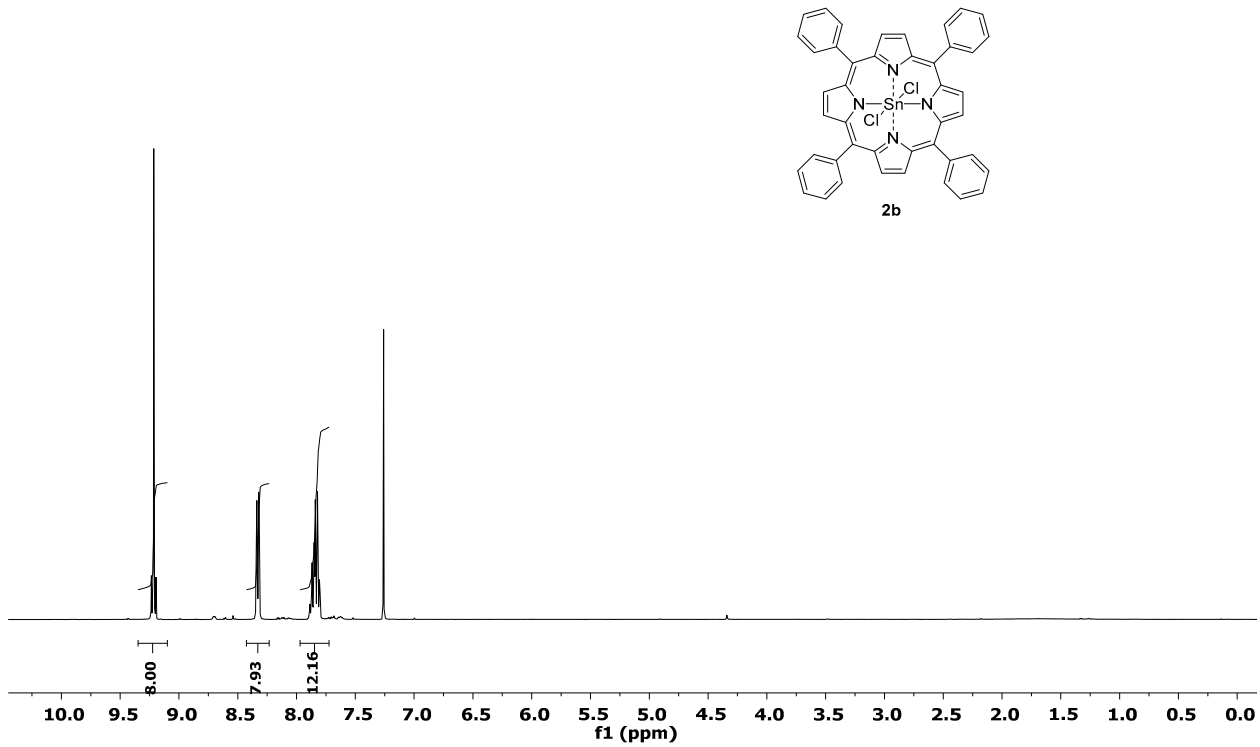
f1 (ppm)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Cl
N
Sn
N
Cl
N
2b
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7.93
12.16
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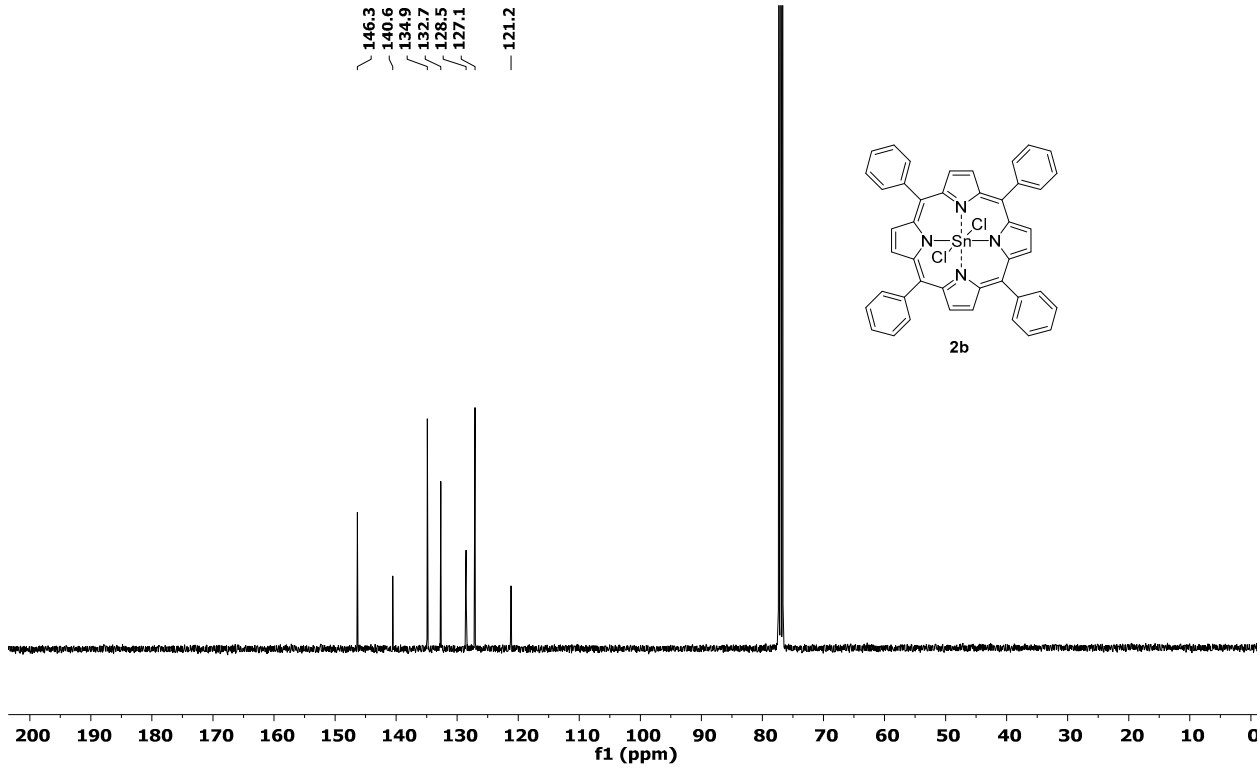
f1 (ppm)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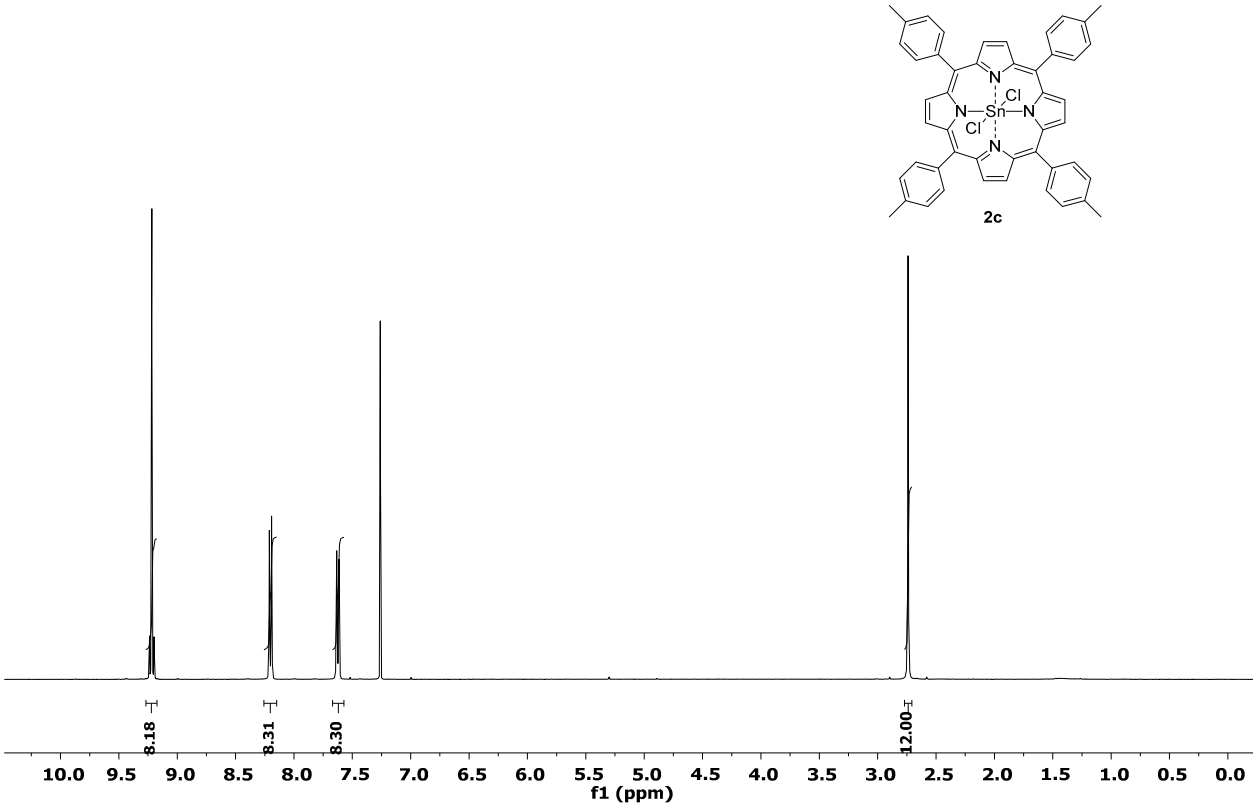
140.6
134.9
132.7
128.5
127.1
121.2
N
Cl
N
Sn
N
Cl
N
2b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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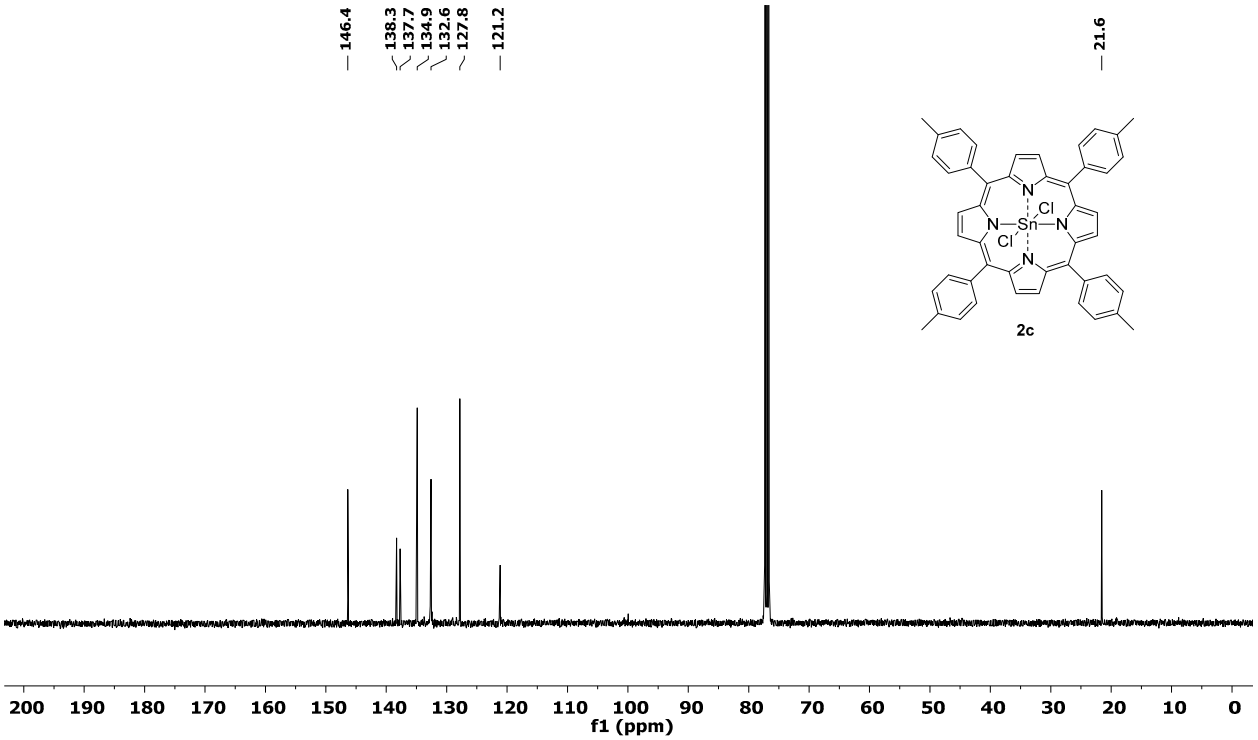
8.31
8.30
12.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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137.7
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132.6
127.8
121.2
21.6
2c
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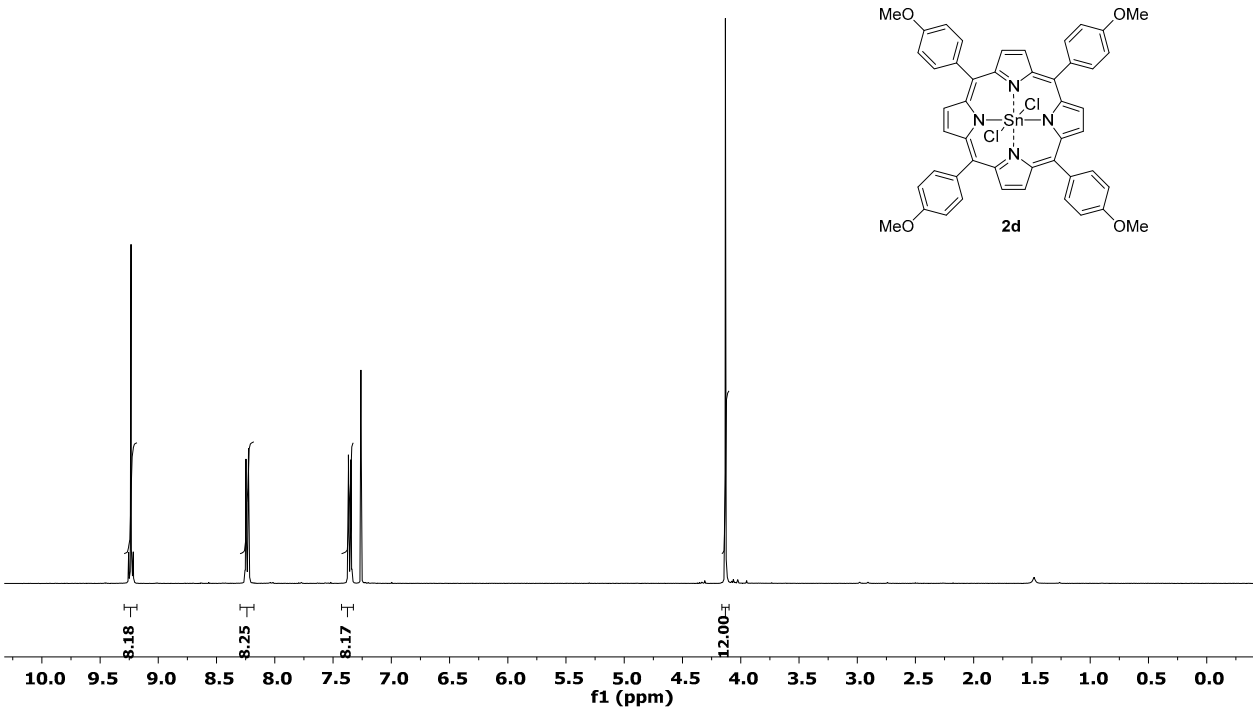
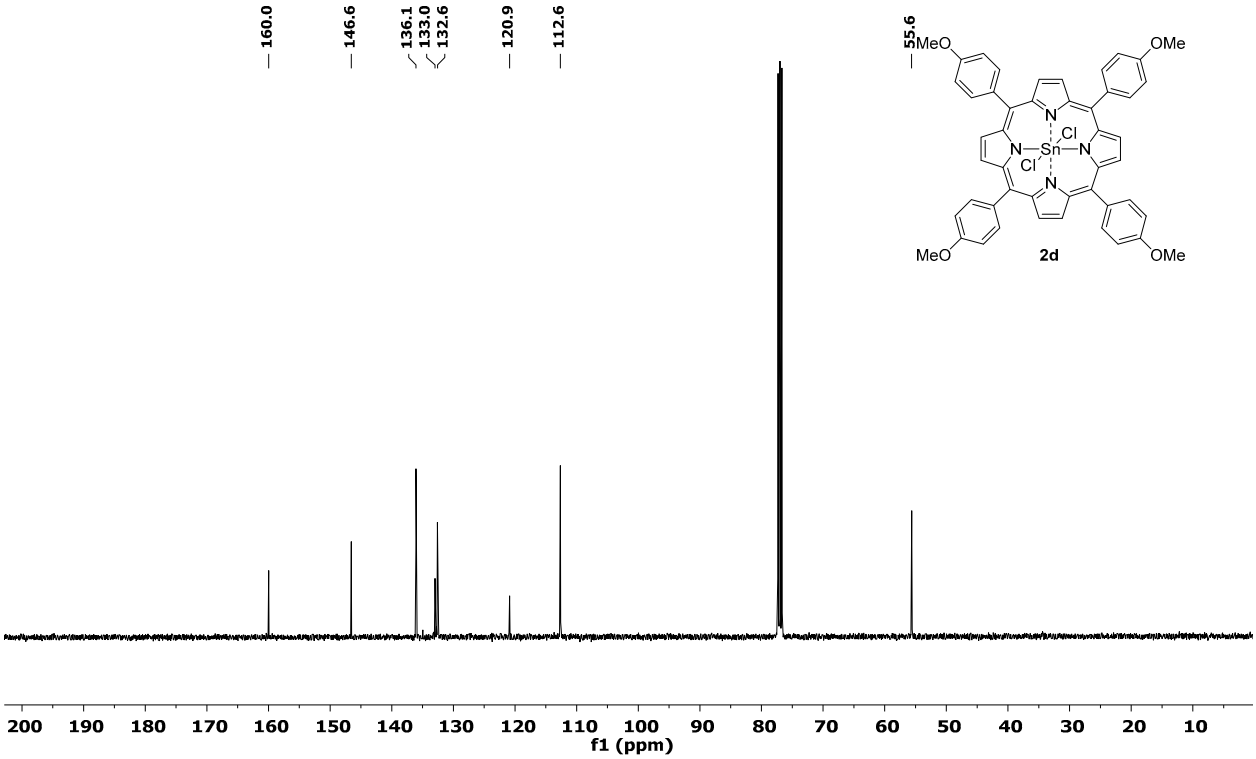
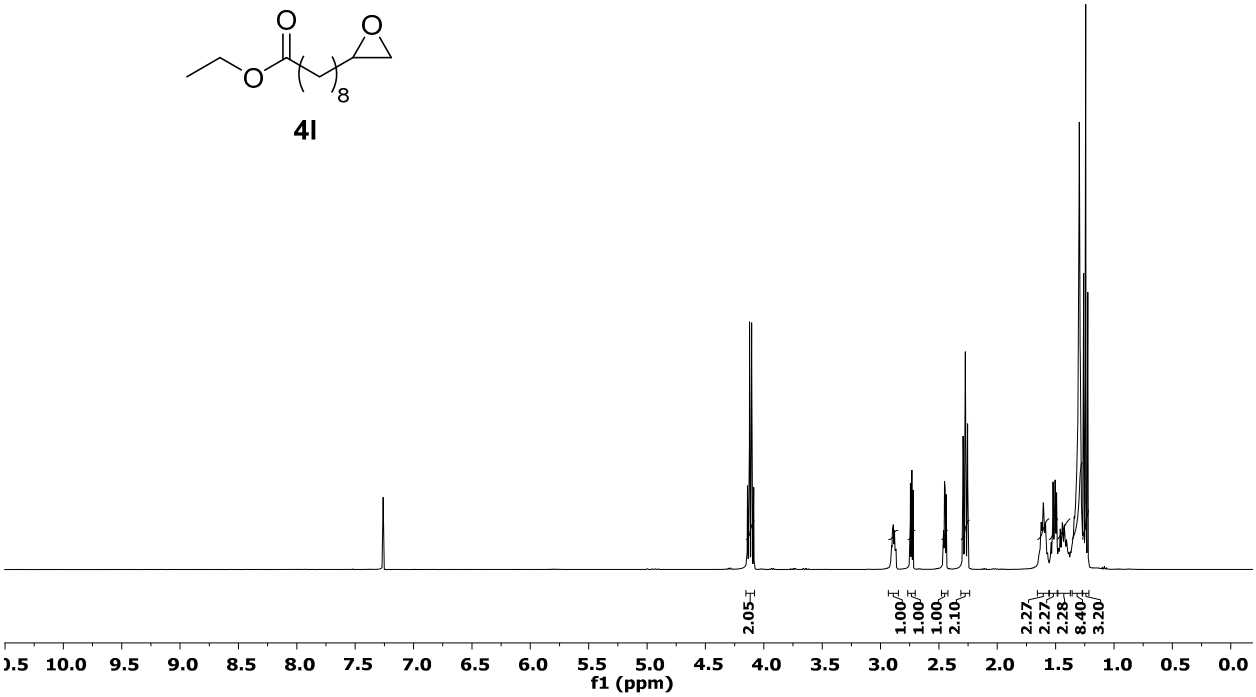
f1 (ppm)


MeO
OMe
N
Cl
N—Sn—N
Cl
N
MeO
OMe
2d
8.18
8.25
8.17
12.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


160.0
146.6
136.1
133.0
132.6
120.9
112.6
55.6
MeO
OMe
N
Cl
N—Sn—N
Cl
N
MeO
OMe
2d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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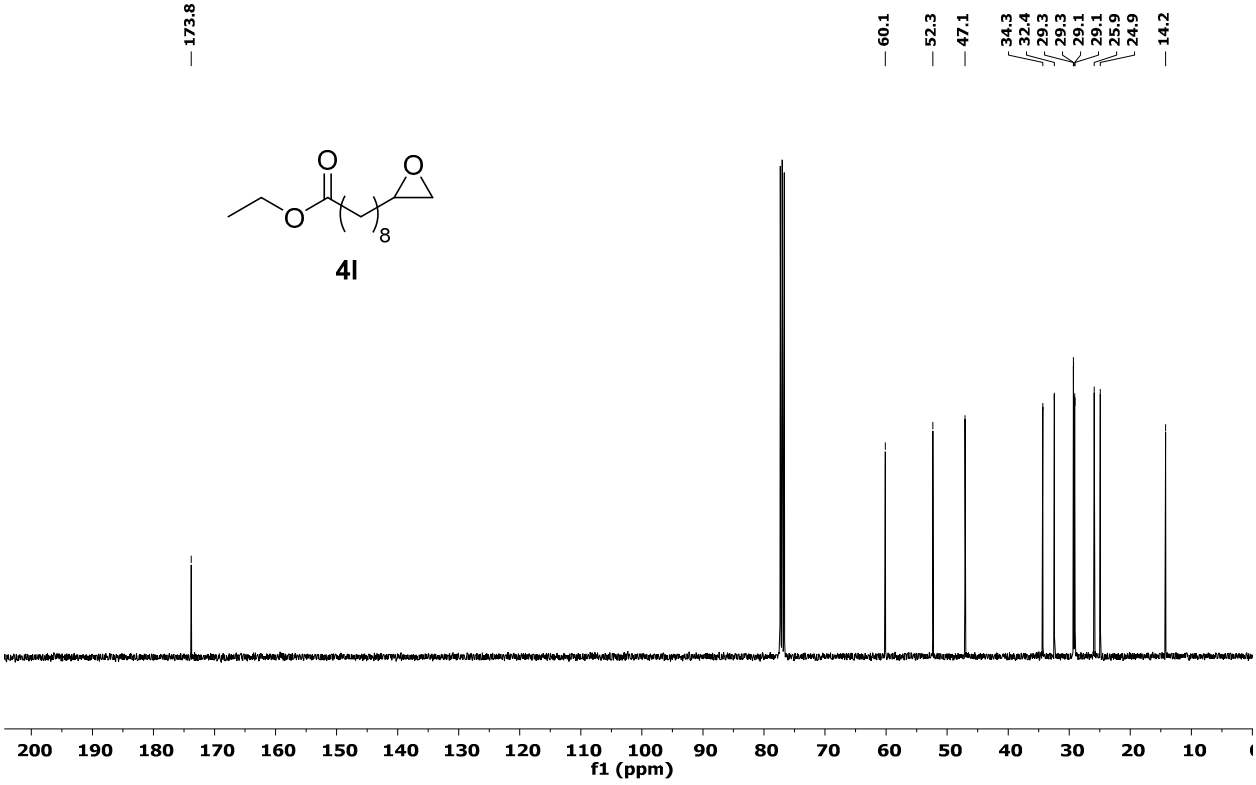
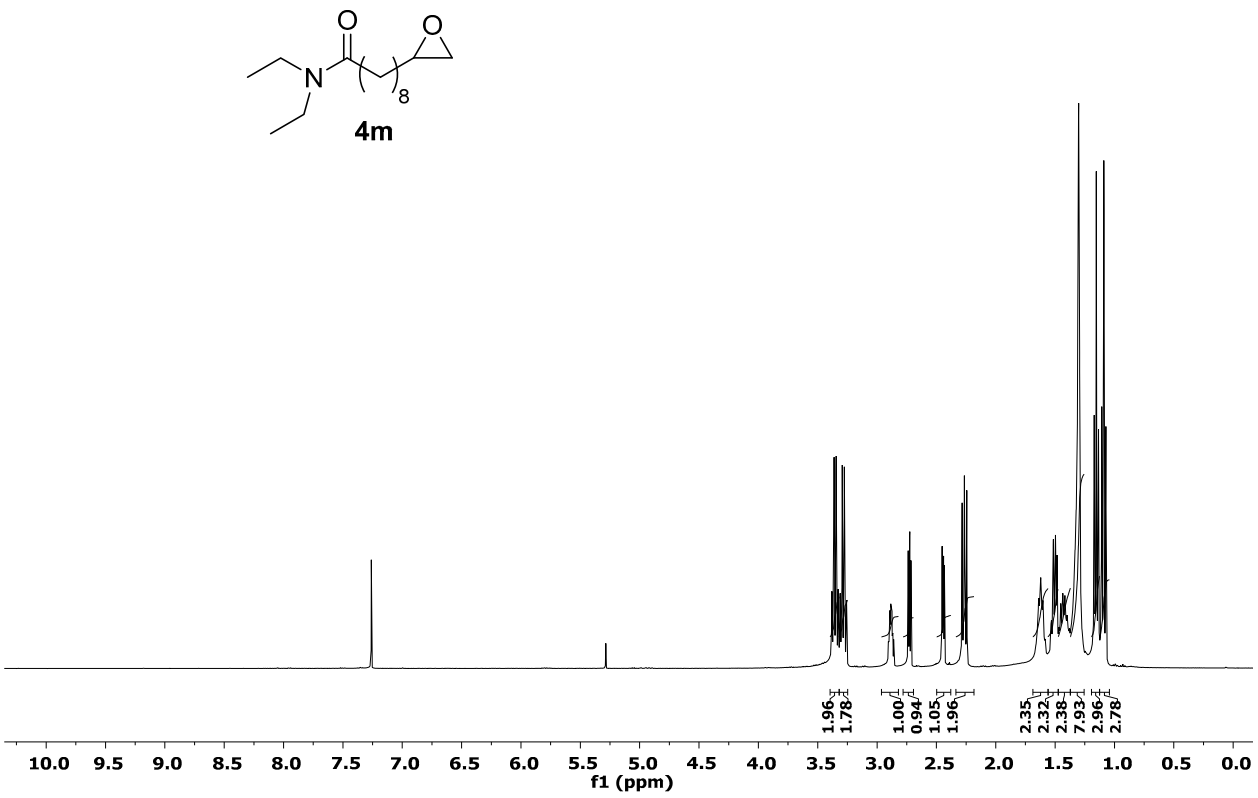
1.00
1.00
1.00
2.10
2.27
2.27
2.28
8.40
3.20
f1 (ppm)


173.8
60.1
52.3
47.1
34.3
32.4
29.3
29.3
29.1
29.1
25.9
24.9
14.2
4l
f1 (ppm)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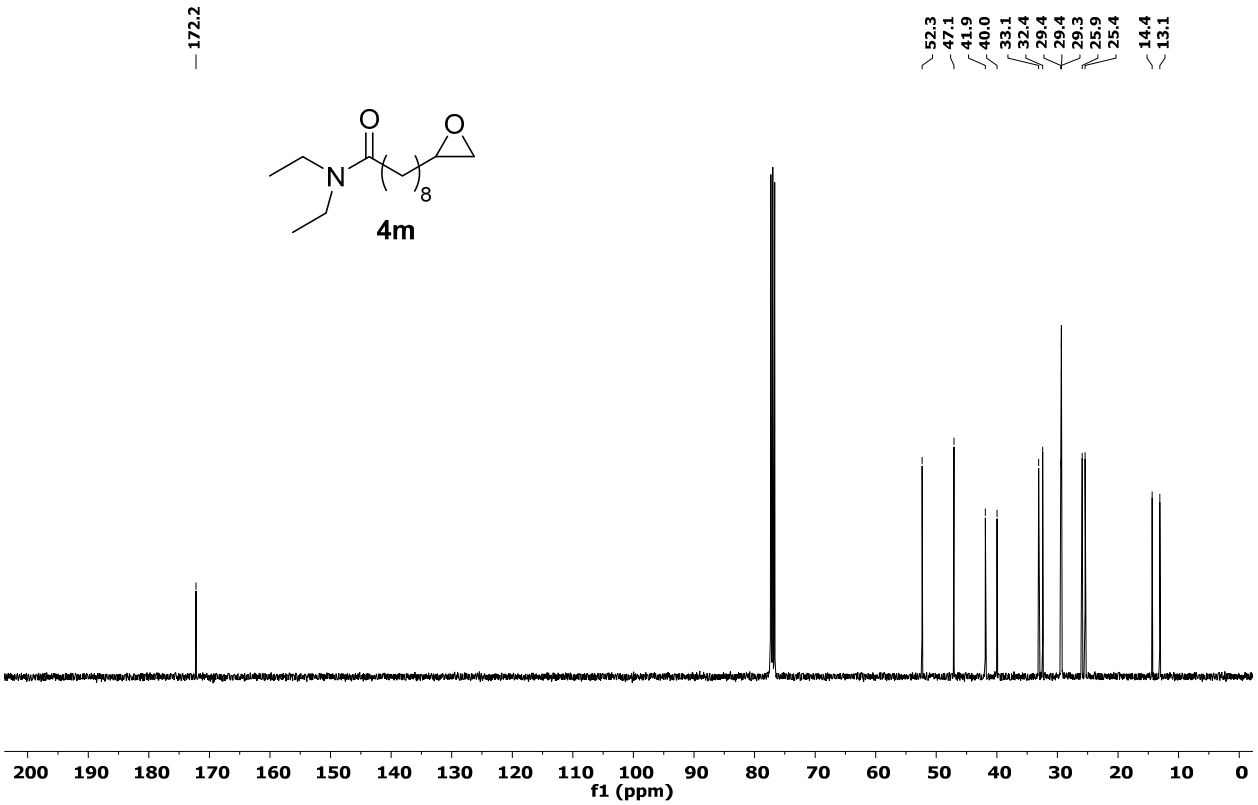
1.78
1.00
0.94
1.05
1.96
2.35
2.32
2.38
7.93
2.96
2.78
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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52.3
47.1
41.9
40.0
33.1
32.4
29.4
29.4
29.3
25.9
25.4
14.4
13.1
4m
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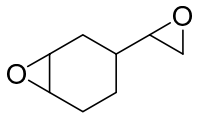
f1 (ppm)



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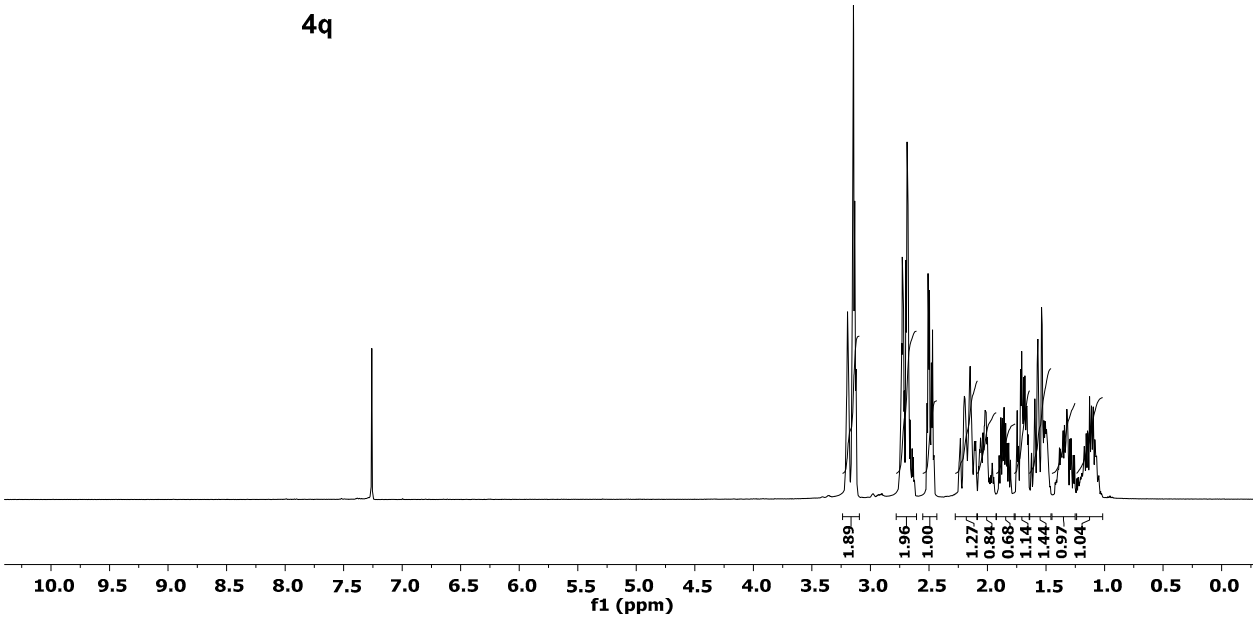
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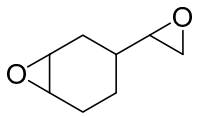
1.00
1.27
0.84
0.68
1.14
1.44
0.97
1.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



4q

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55.6
55.6
55.5
52.4
52.4
52.2
51.6
51.5
50.9
50.8
46.2
46.1
45.6
45.4
35.8
35.3
32.7
31.9
27.5
27.3
27.1
25.9
24.4
24.2
23.6
23.3
22.9
22.7
21.4
20.2
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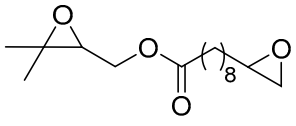
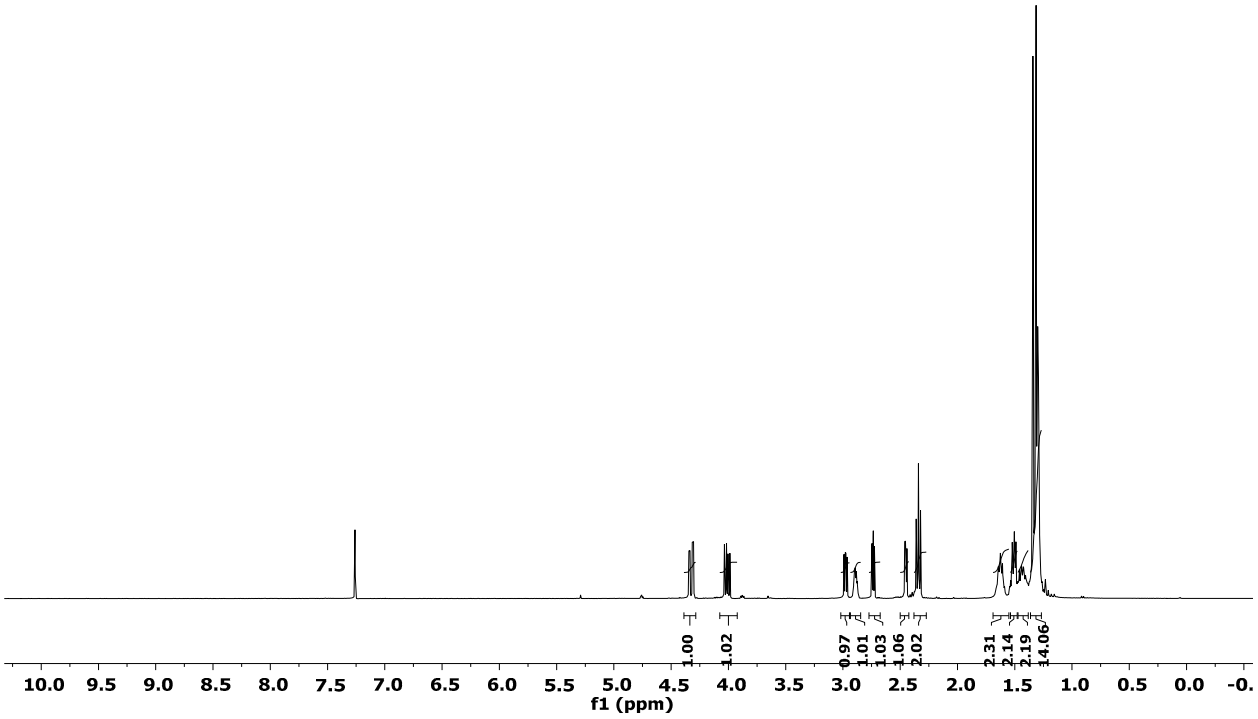
f1 (ppm)



4r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0.97
1.01
1.03
1.06
2.02
2.31
2.14
2.19
14.06
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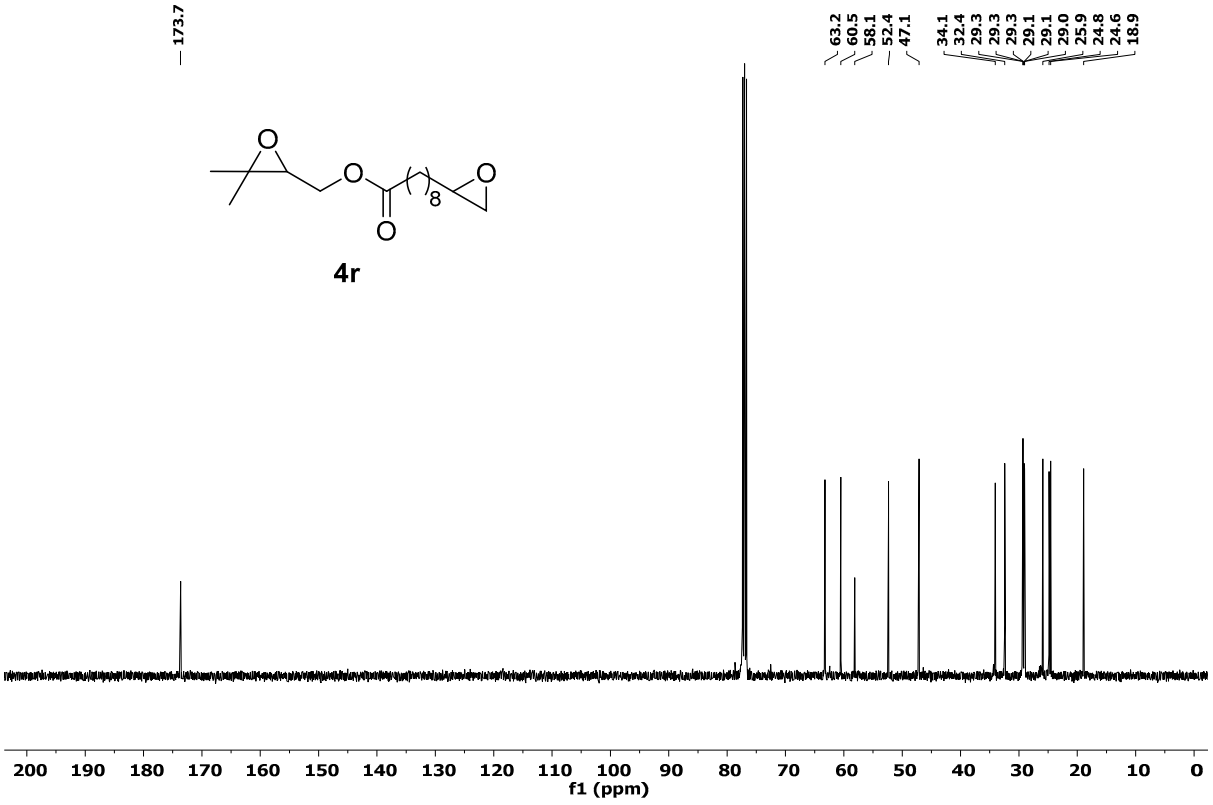
f1 (ppm)


173.7
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60.5
58.1
52.4
47.1
34.1
32.4
29.3
29.3
29.3
29.1
29.1
29.0
25.9
24.8
24.6
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O
O
O
8
O
4r
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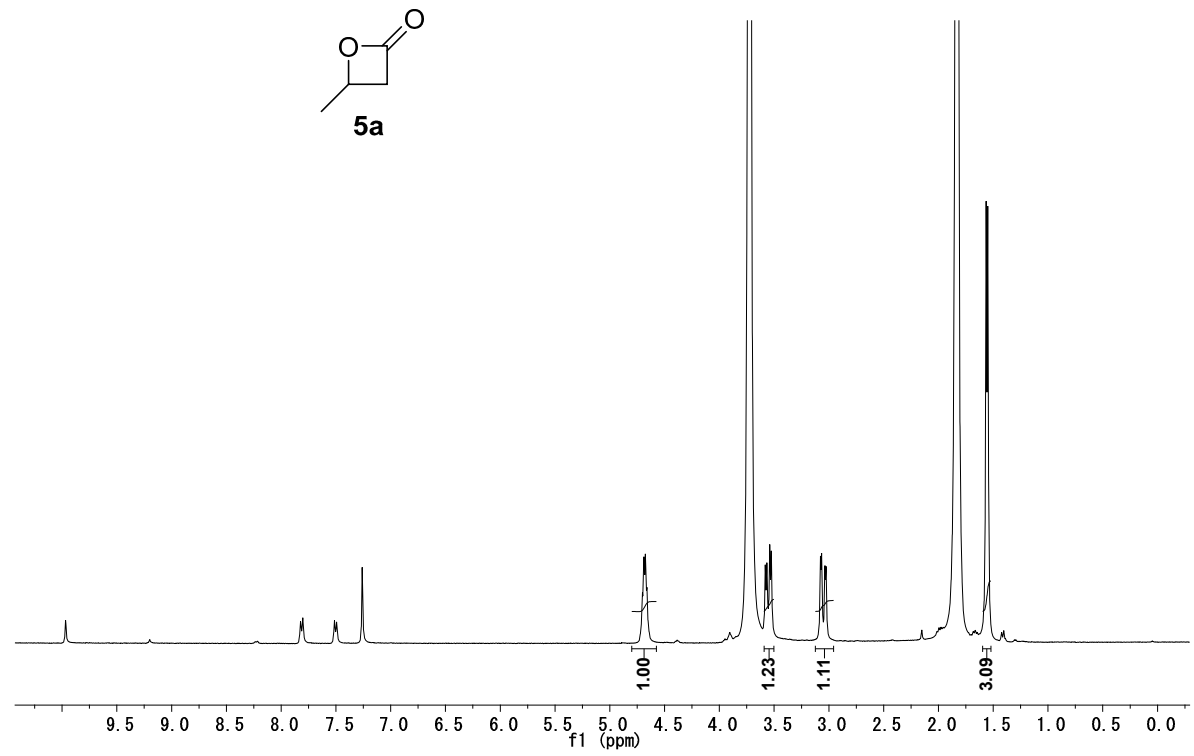
f1 (ppm)


5a
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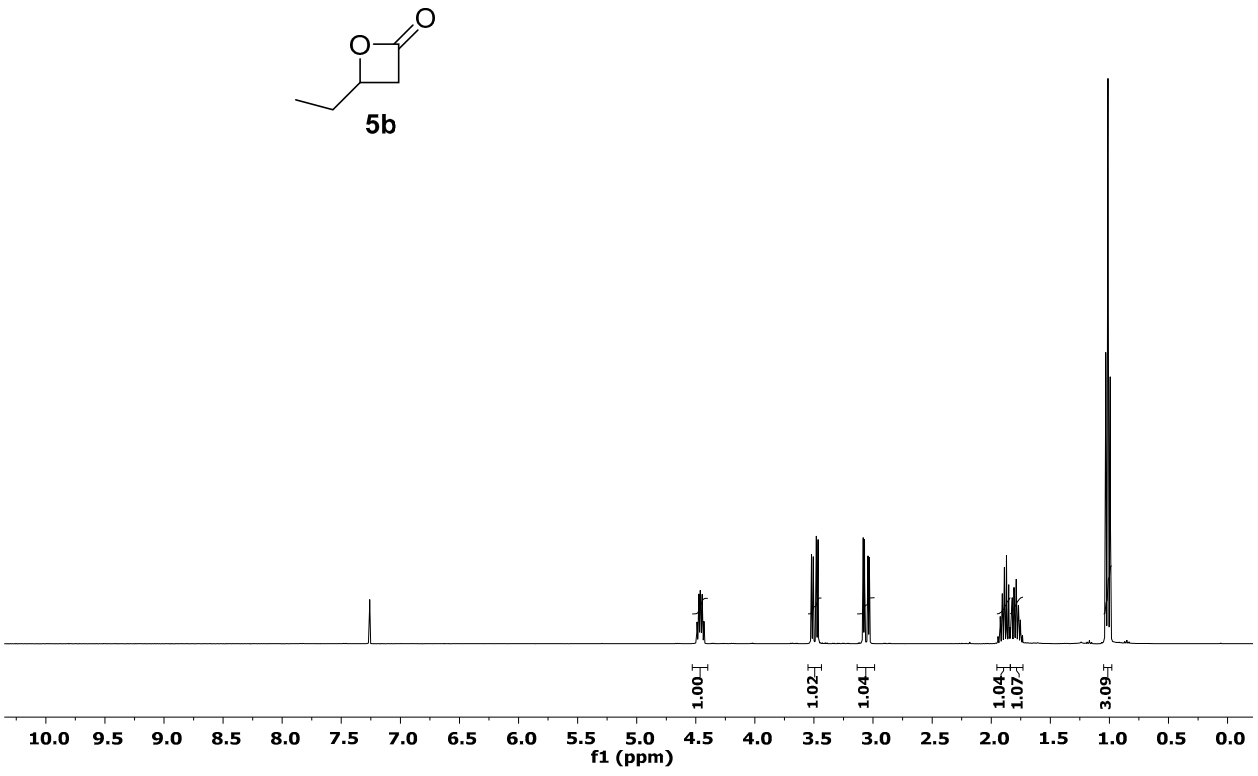
1.23
1.11
3.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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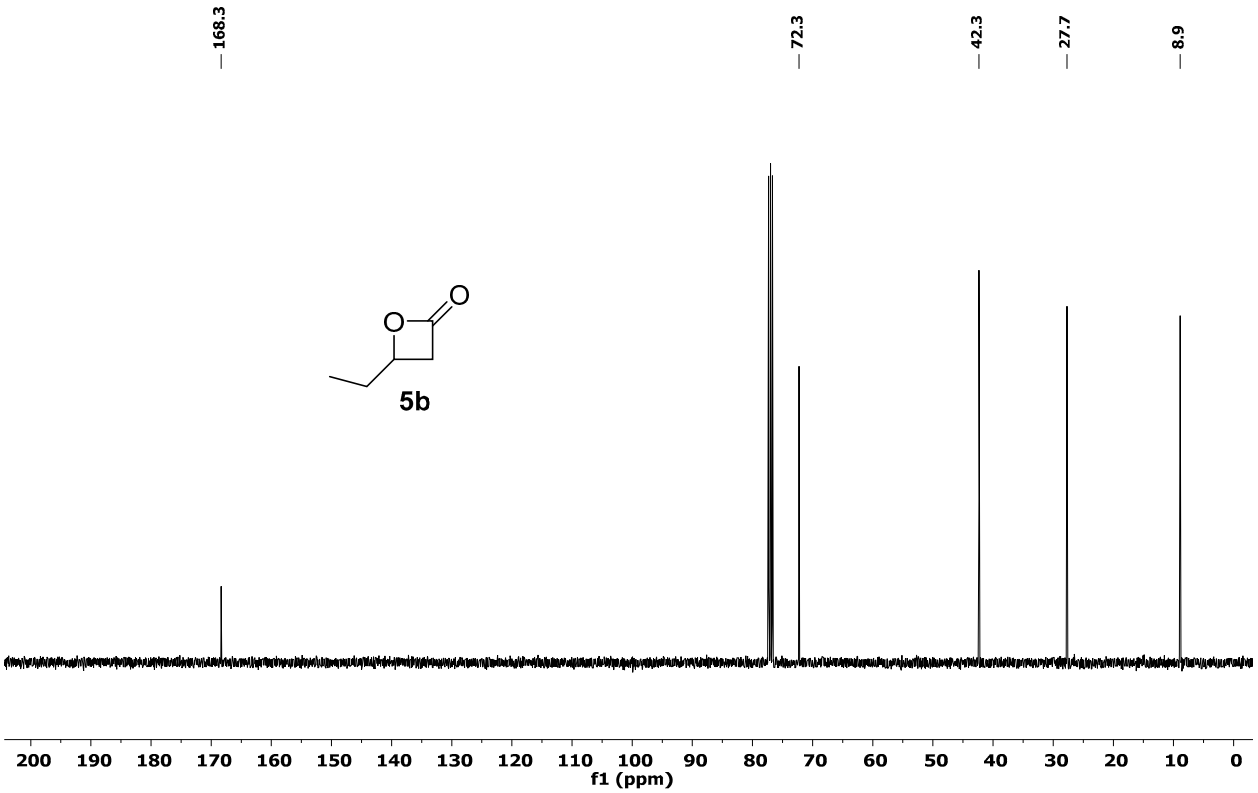
1.02
1.04
1.04
1.07
3.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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42.3
27.7
8.9
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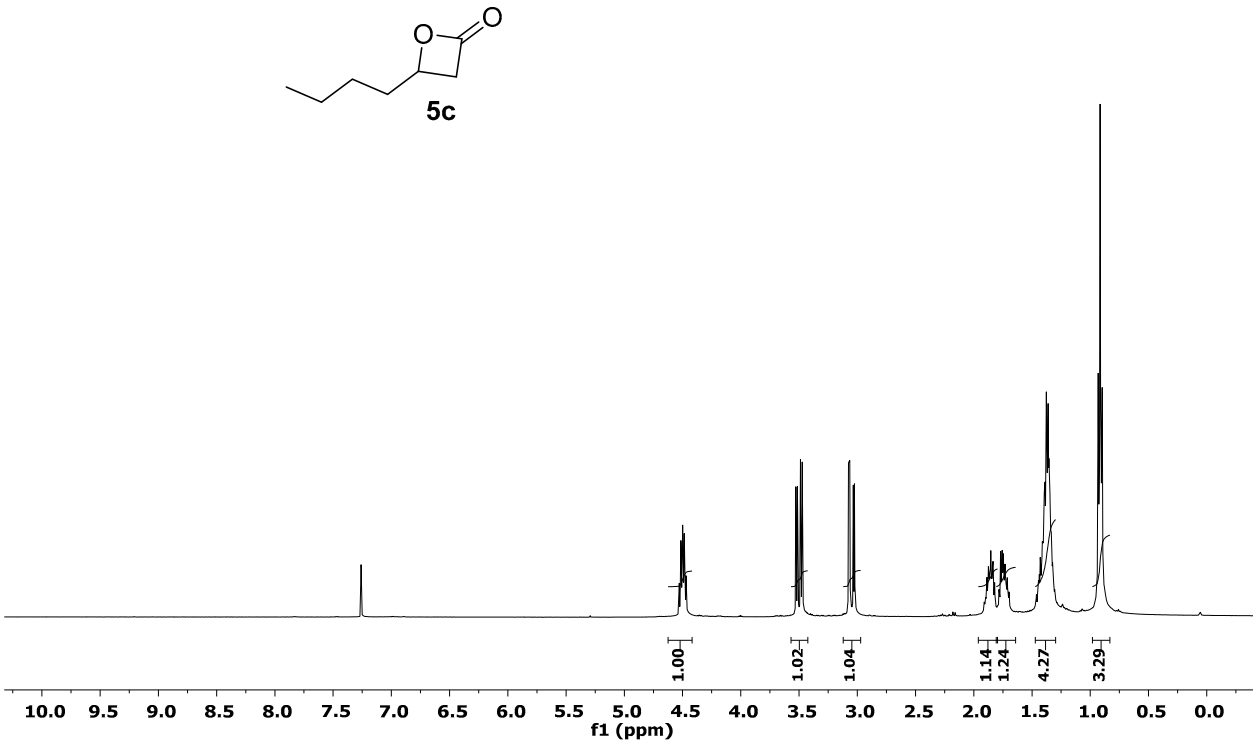
f1 (ppm)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1.04
1.14
1.24
4.27
3.29
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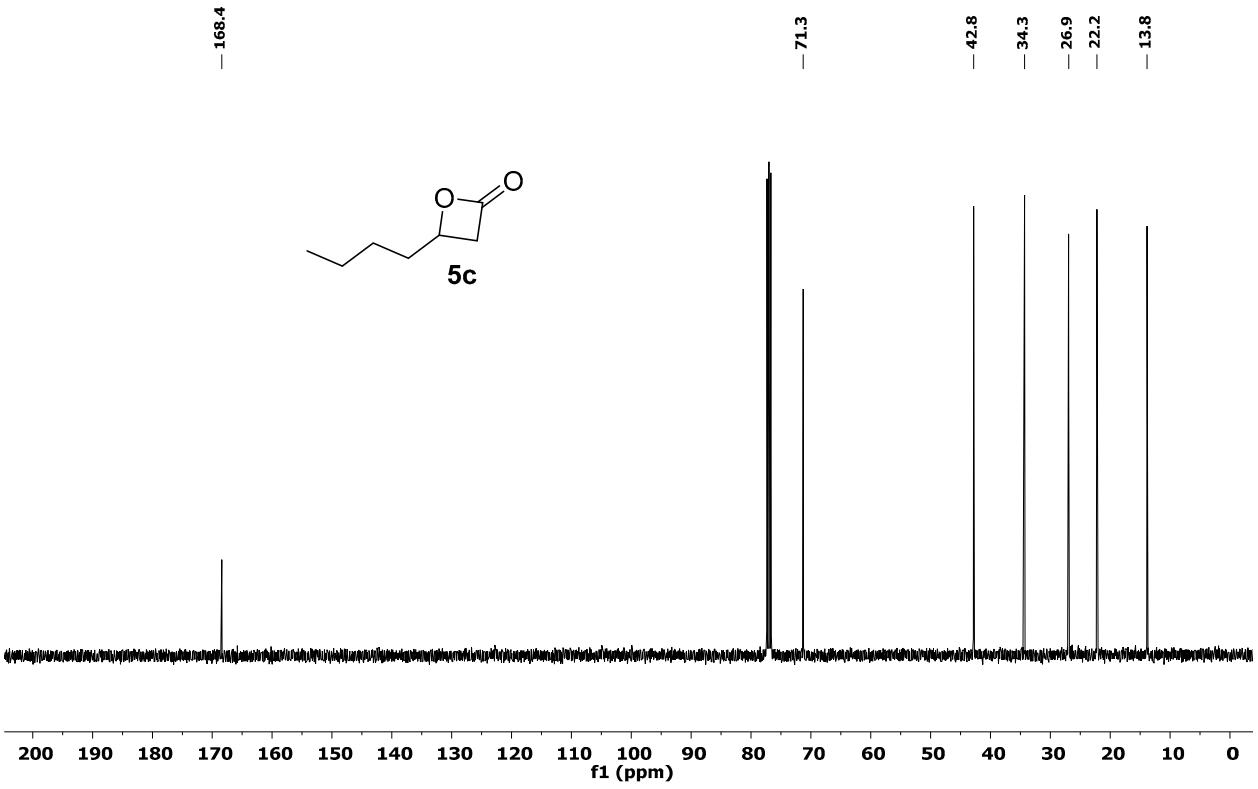
f1 (ppm)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34.3
26.9
22.2
13.8
5c
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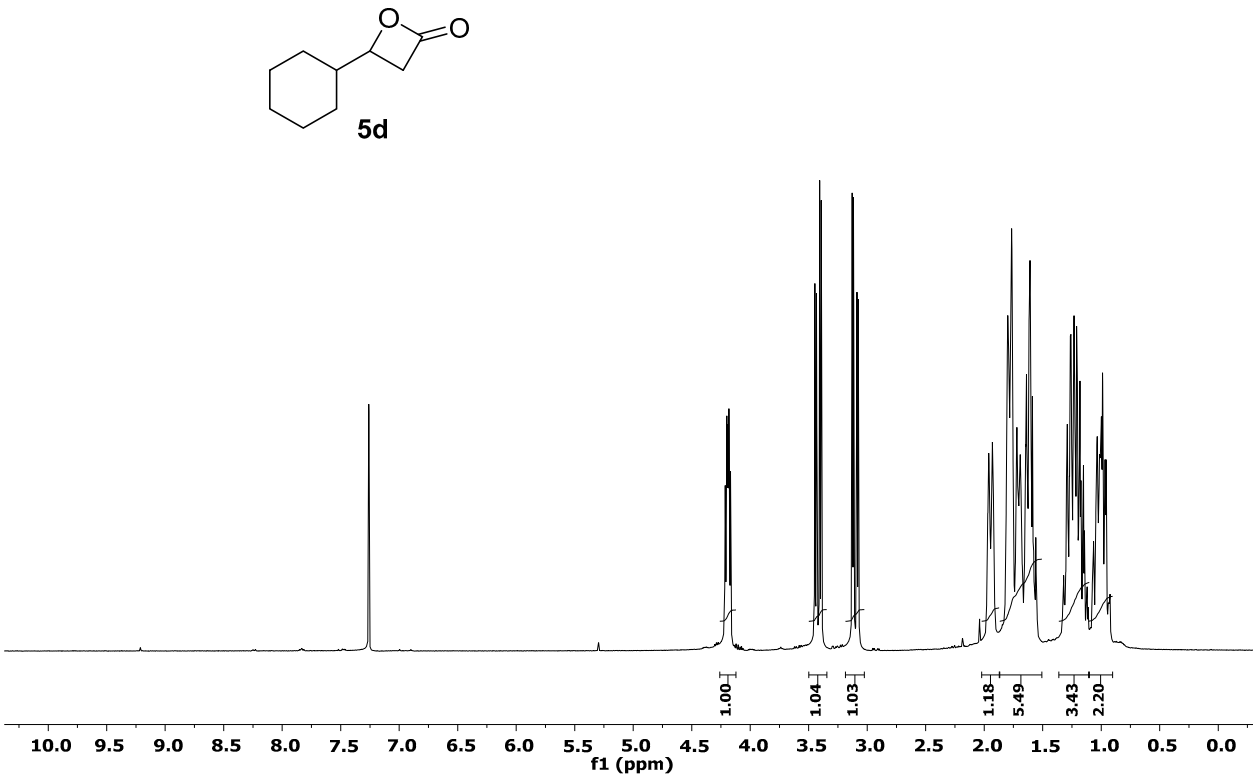
f1 (ppm)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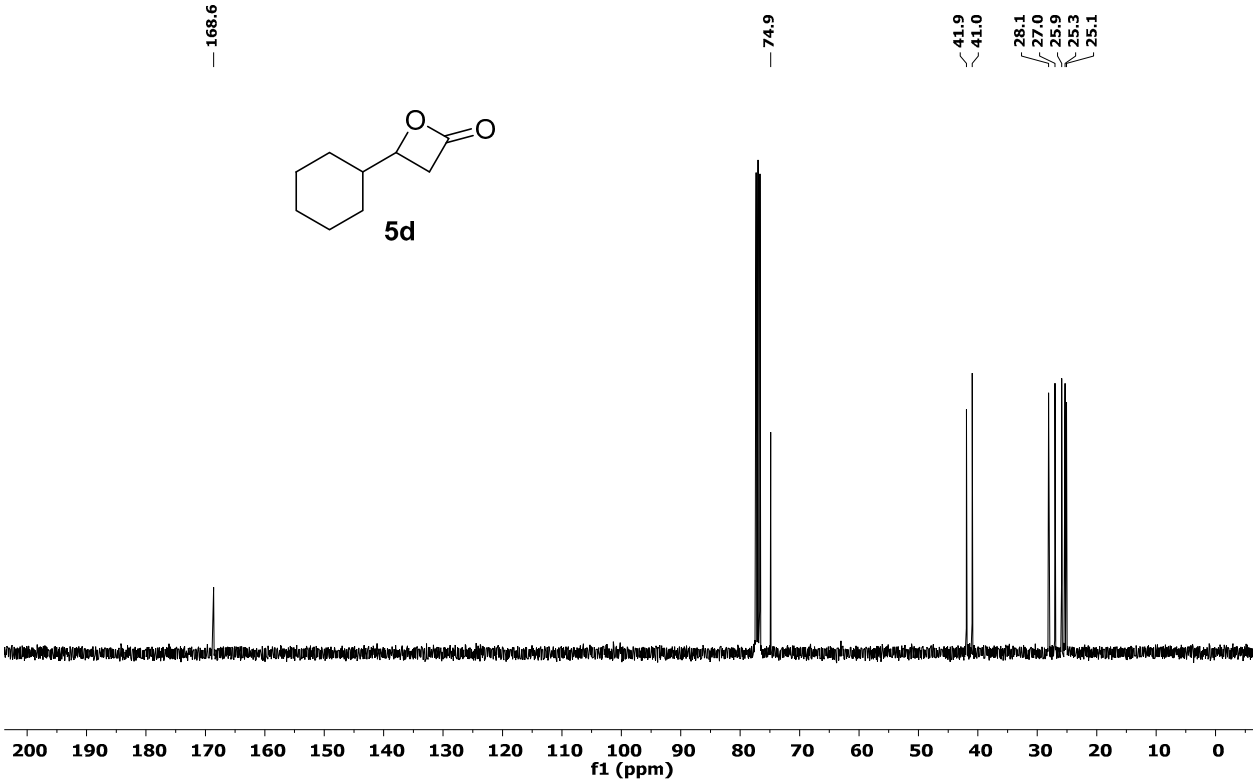
1.03
1.18
5.49
3.43
2.20
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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74.9
41.9
41.0
28.1
27.0
25.9
25.3
25.1
5d
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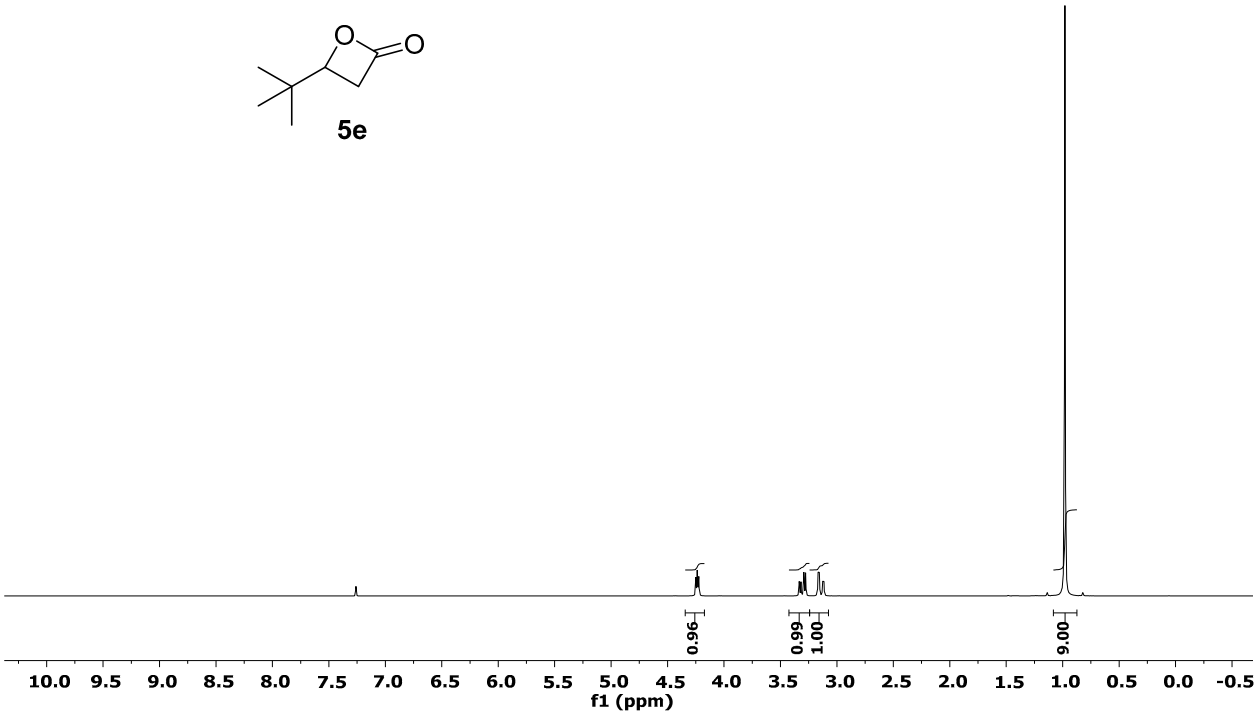
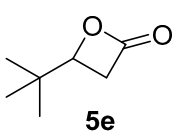
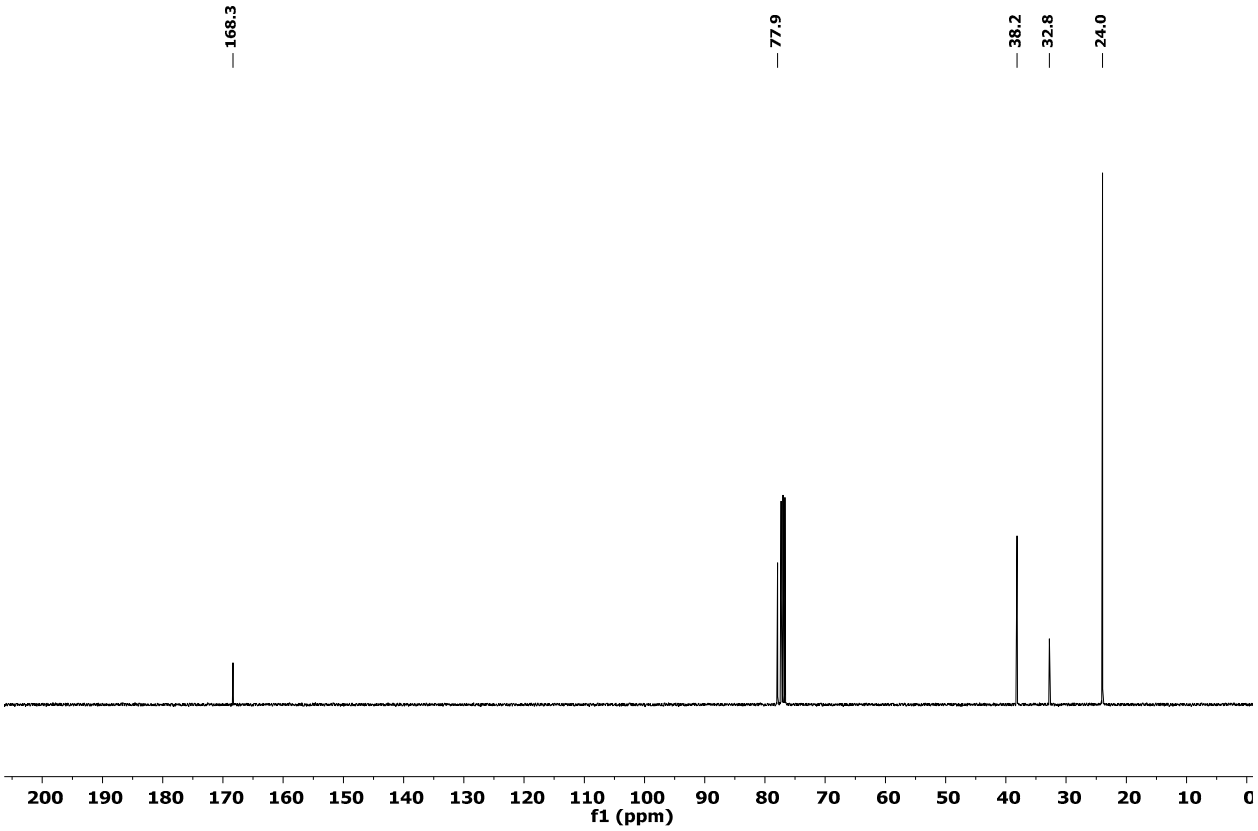
f1 (ppm)


5e
0.96
0.99
1.00
9.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


5e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77.9
38.2
32.8
24.0
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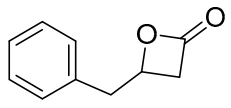
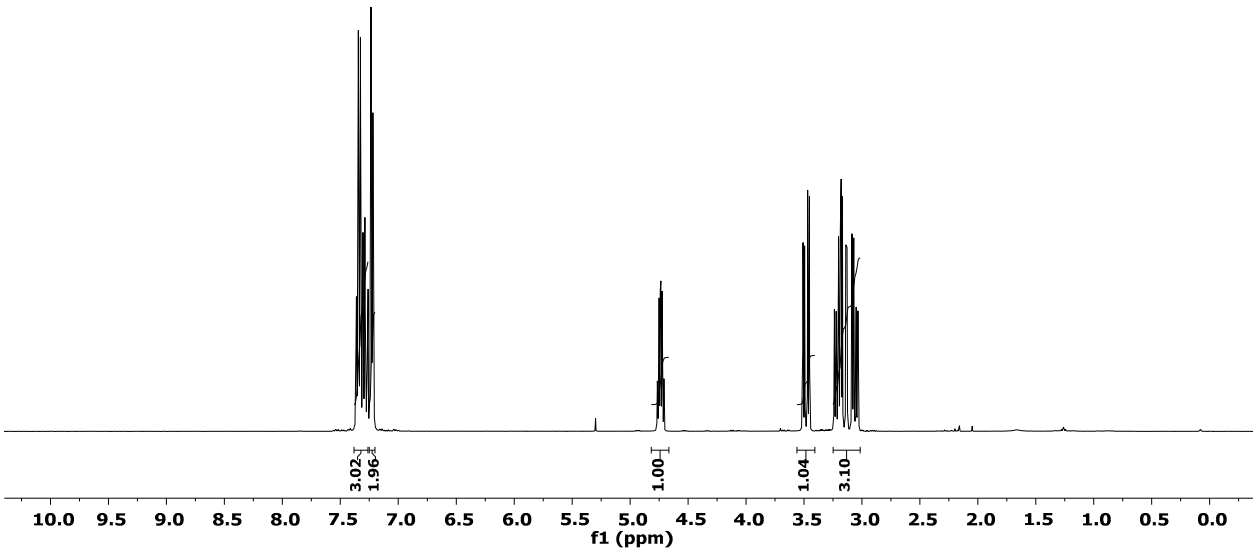
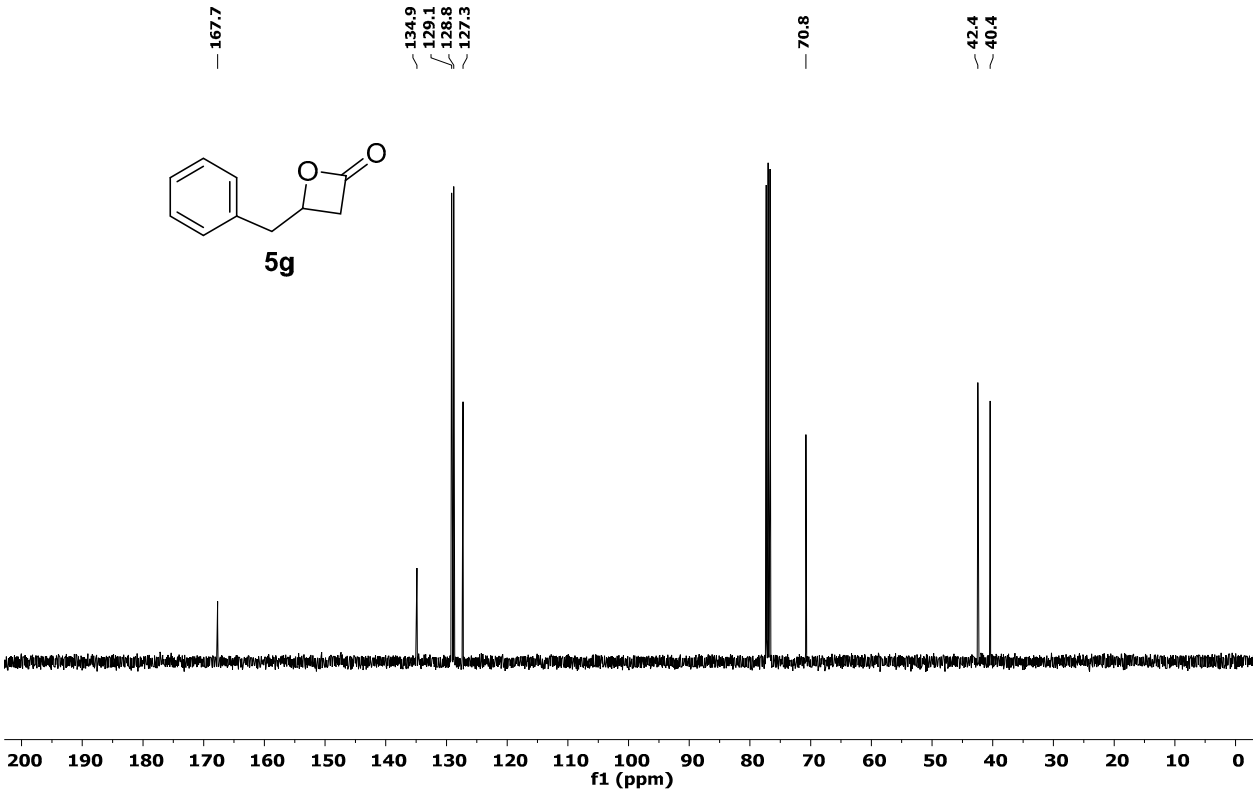
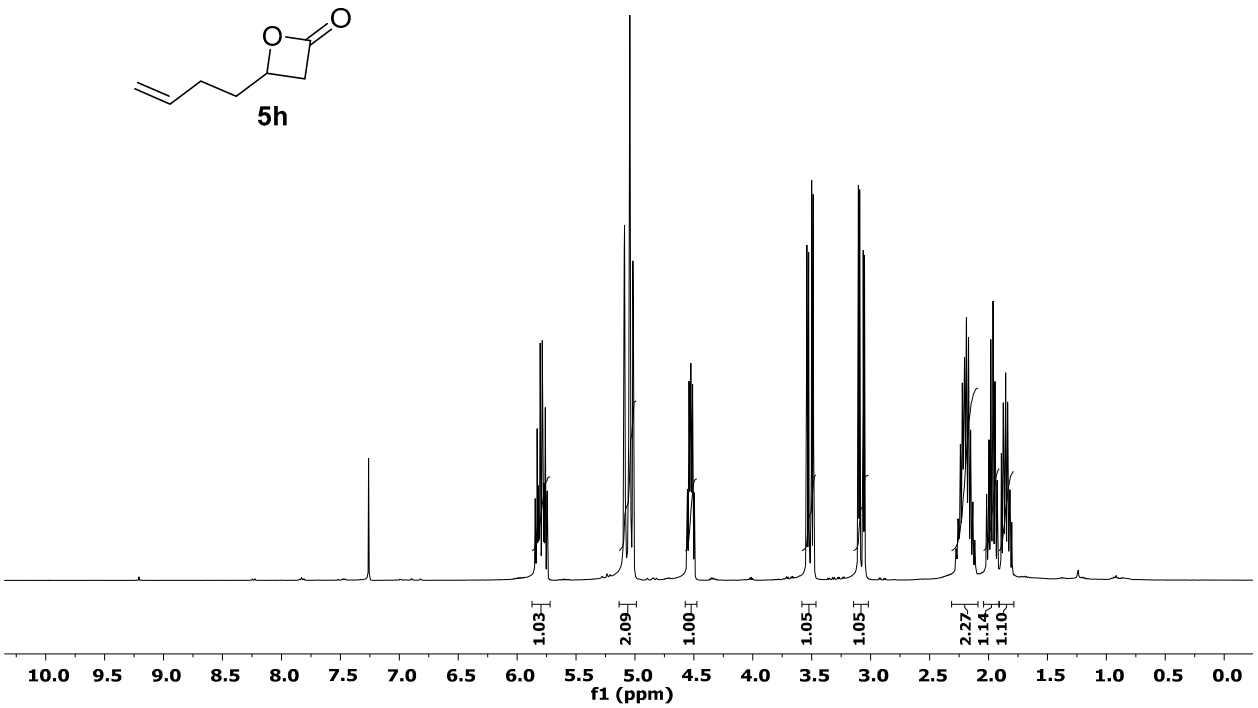
f1 (ppm)

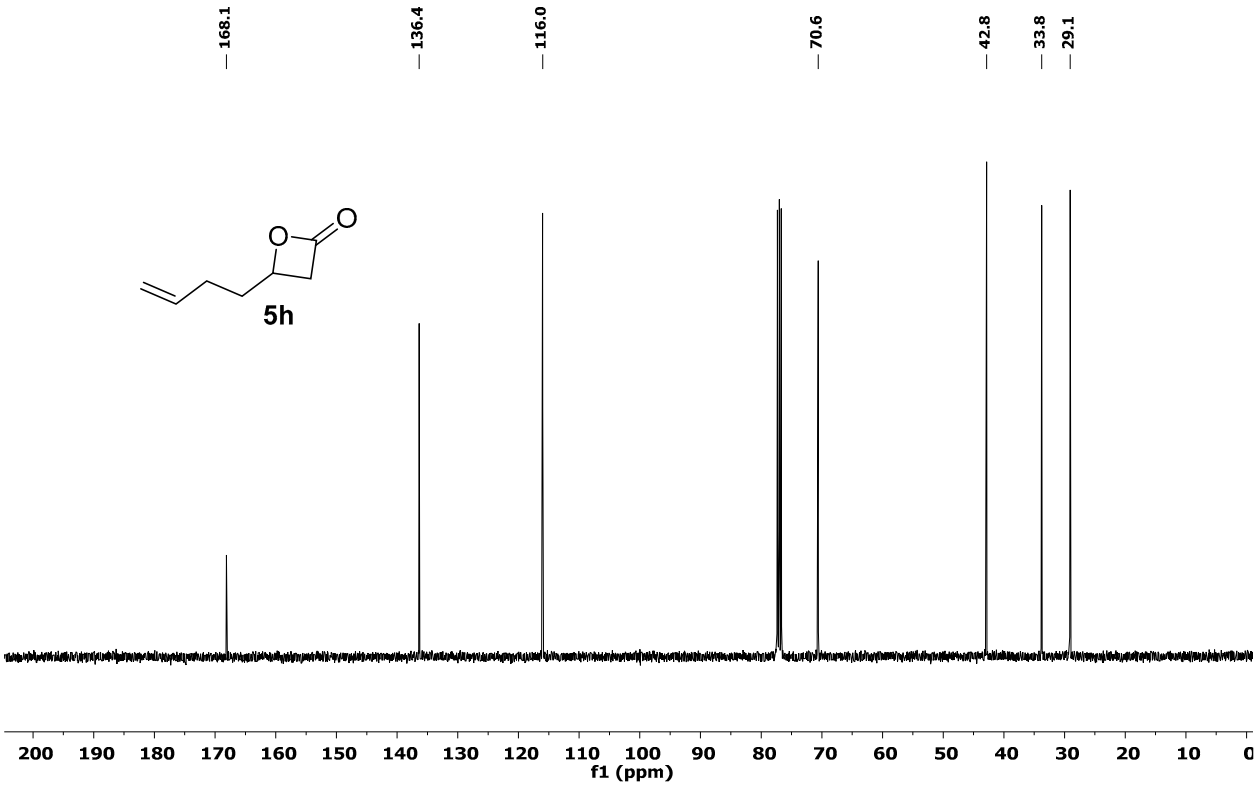

O
O

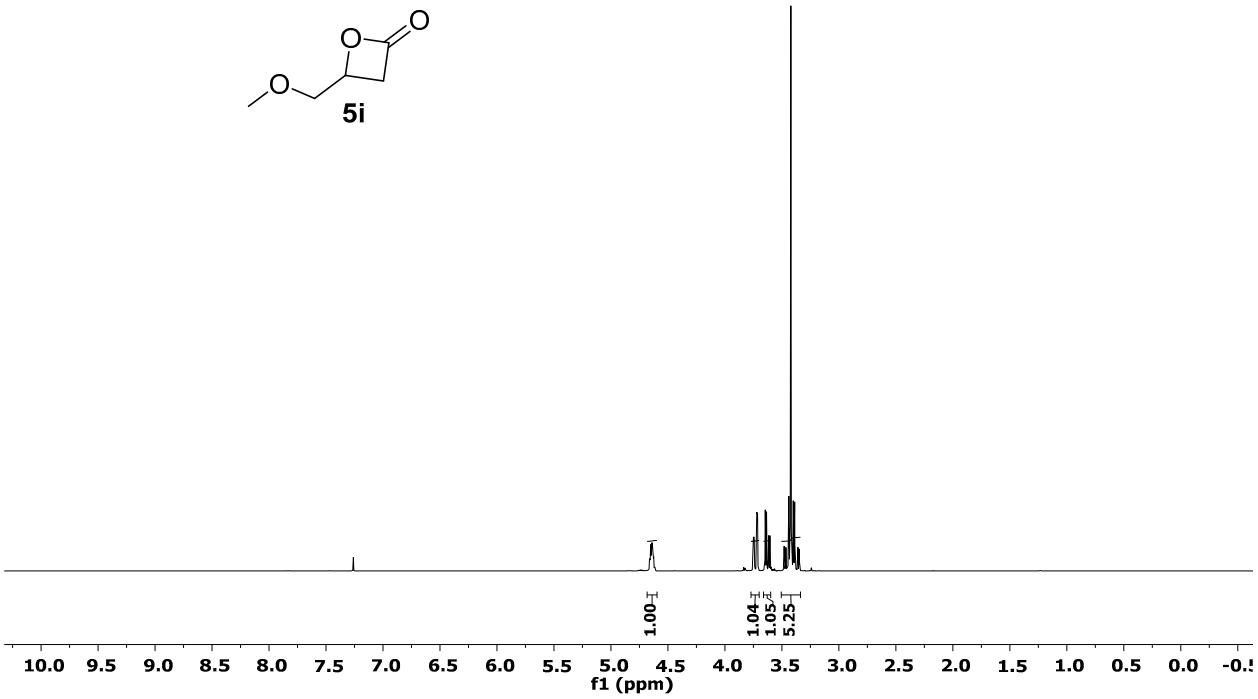
5g

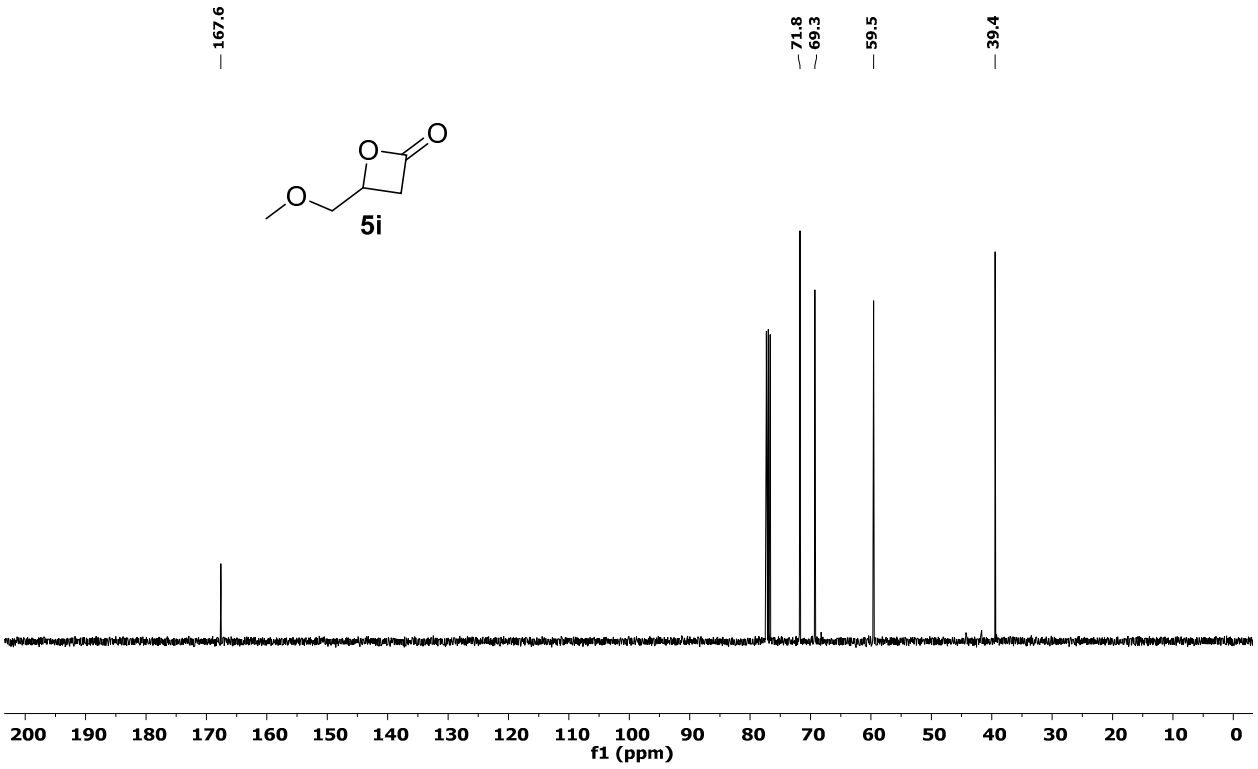

3.02
1.96
1.00
1.04
3.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

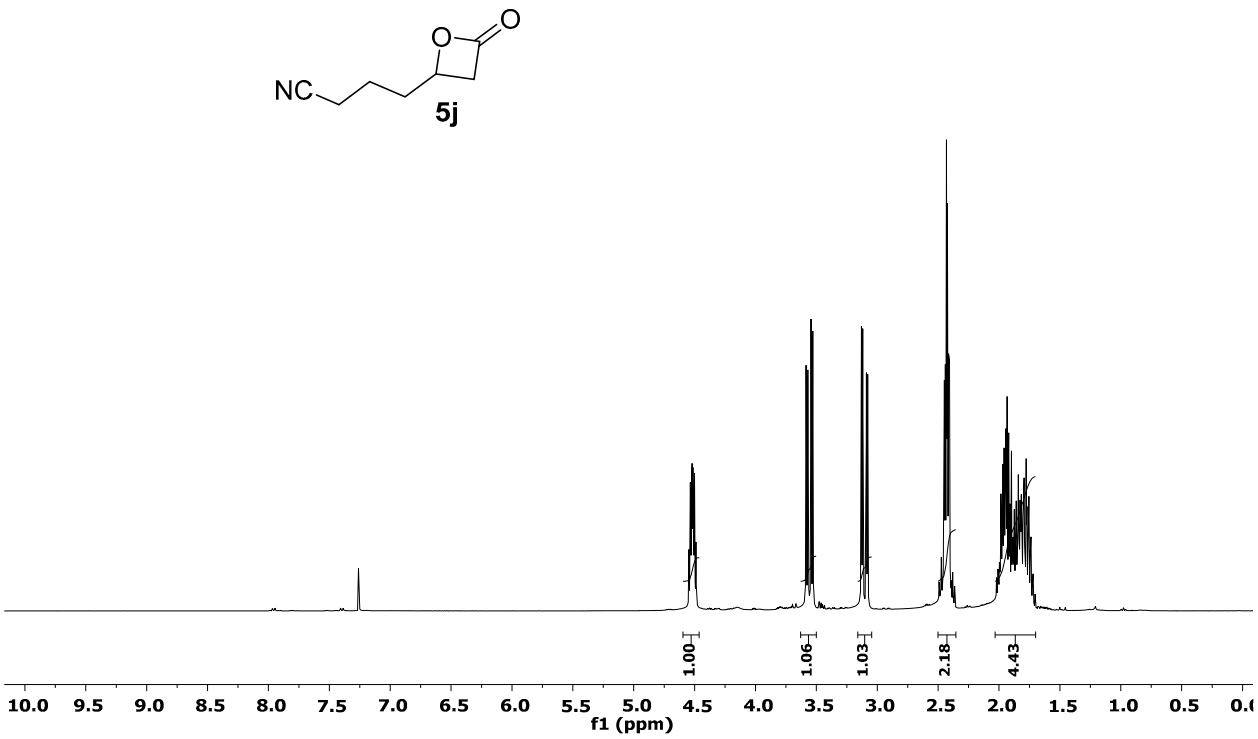

167.7
134.9
129.1
128.8
127.3
70.8
42.4
40.4
O
O
5g
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

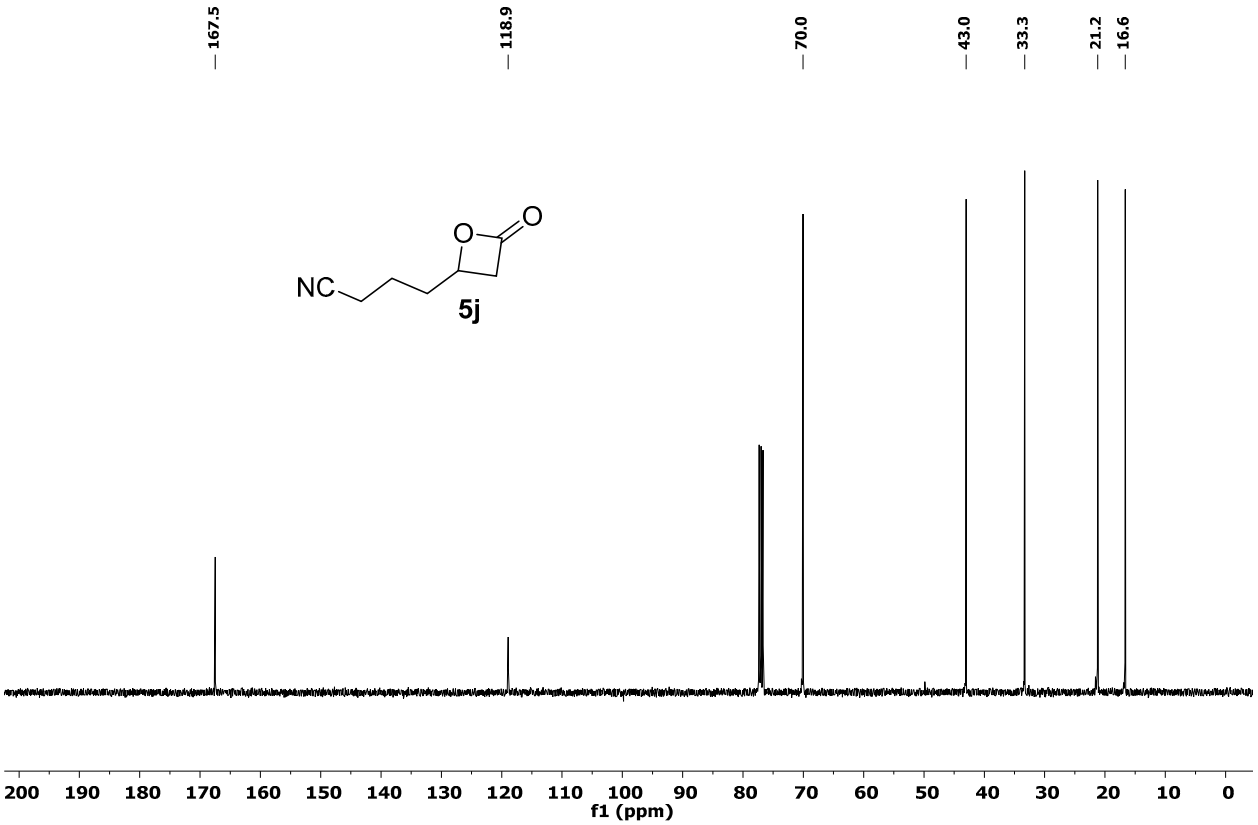

O
O
5h
1.03
2.09
1.00
1.05
1.05
2.27
1.14
1.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

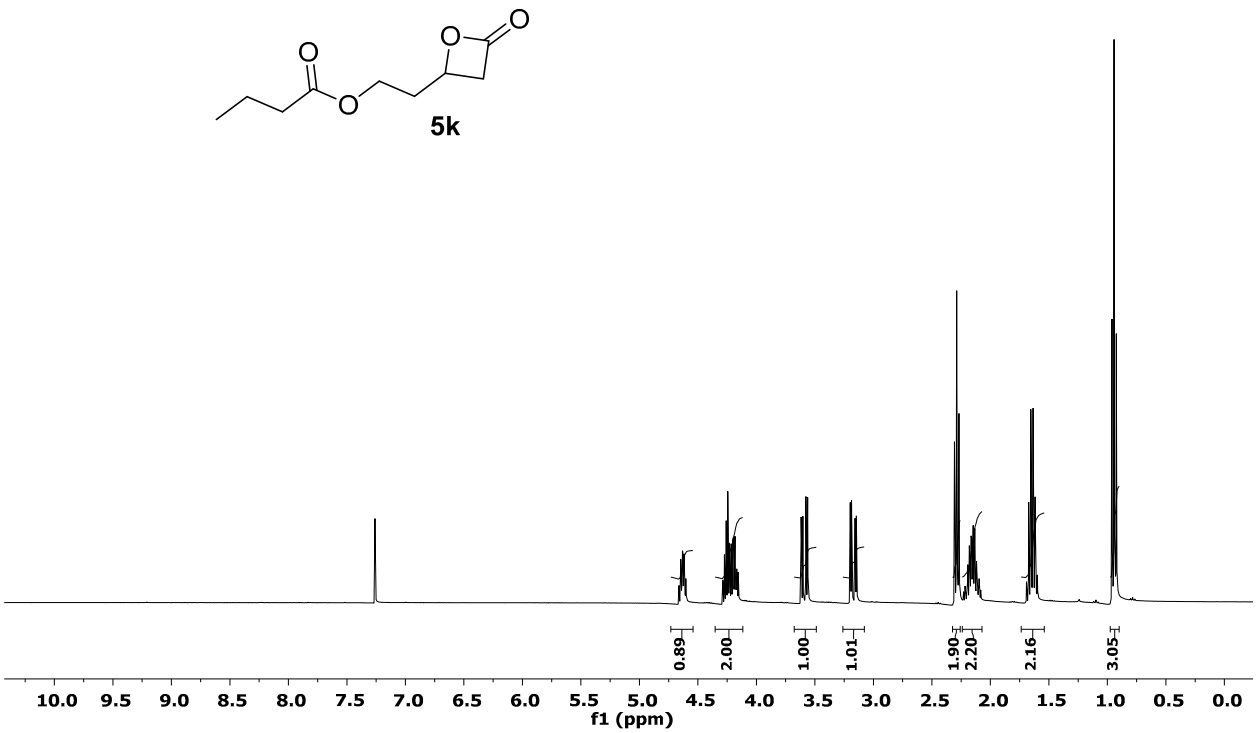

168.1
136.4
116.0
70.6
42.8
33.8
29.1
5h
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

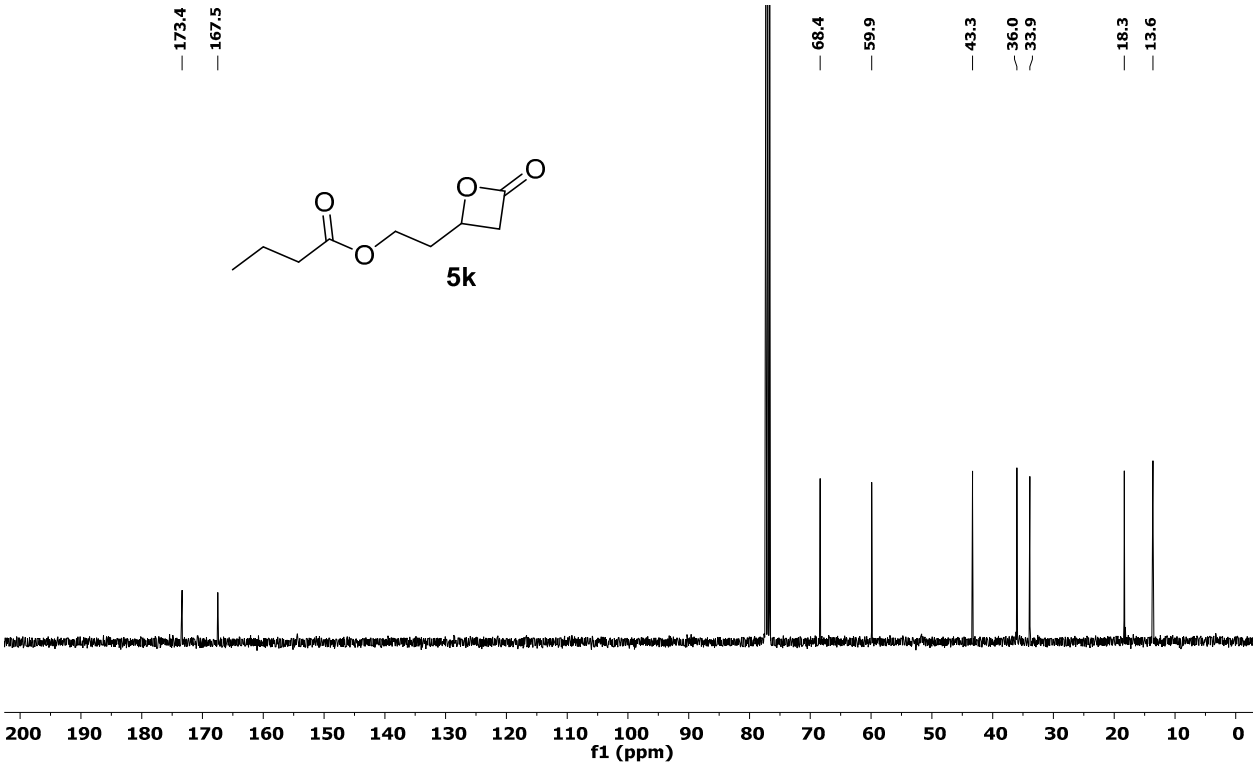

5i
1.00
1.04
1.05
5.25
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

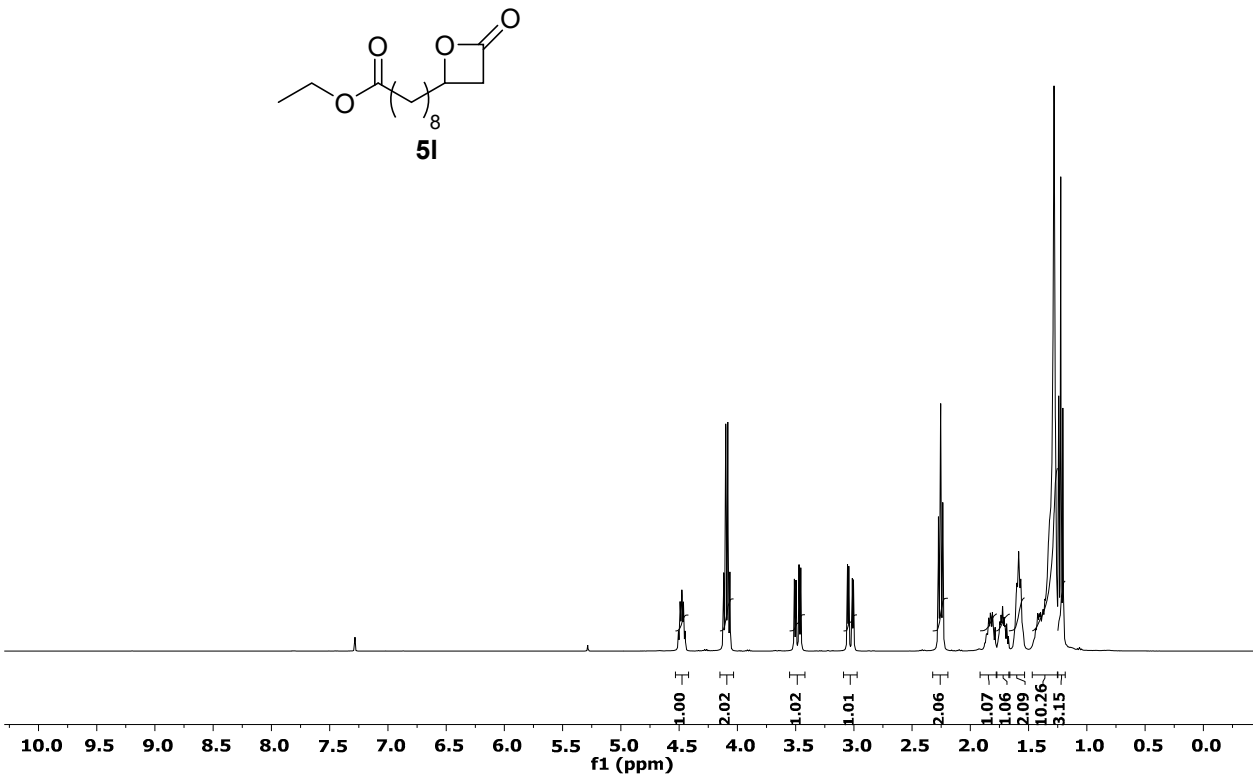

167.6
71.8
69.3
59.5
39.4
O
O
O
5i
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

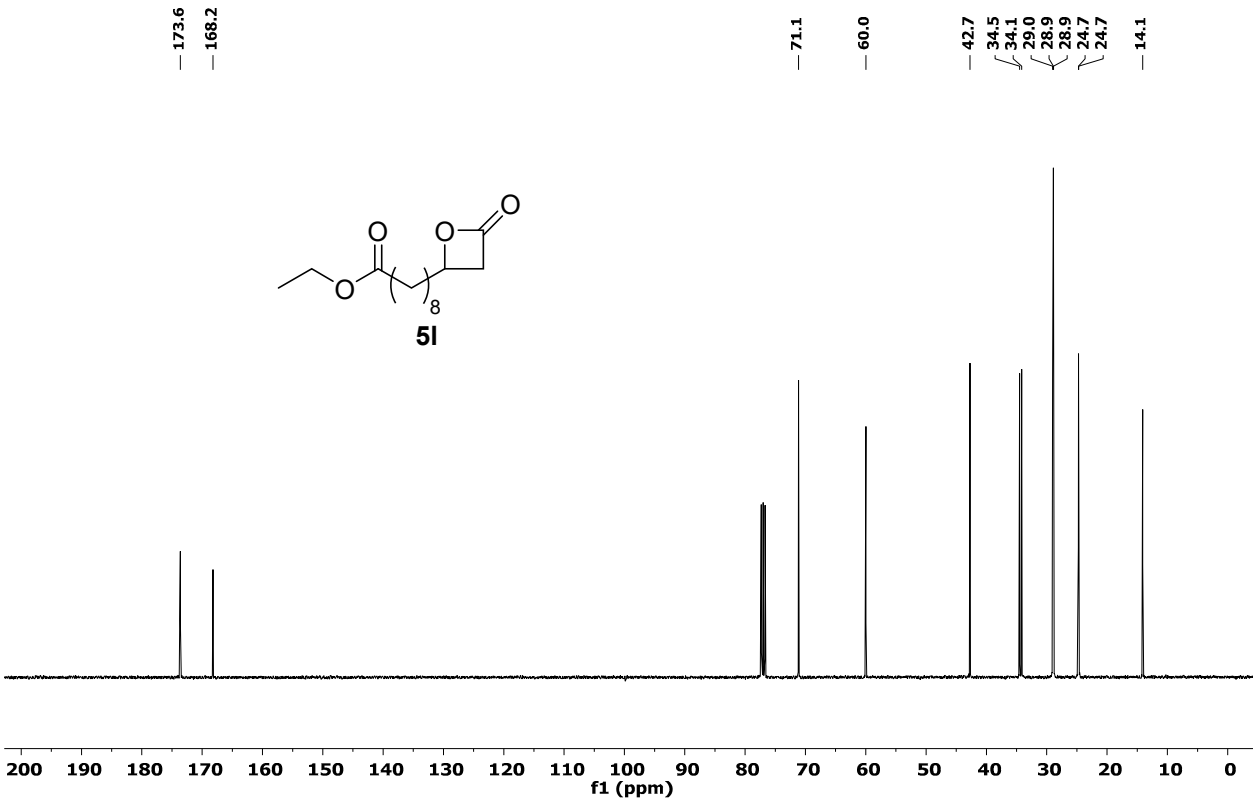

O
O
NC
5j
1.00
1.06
1.03
2.18
4.43
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

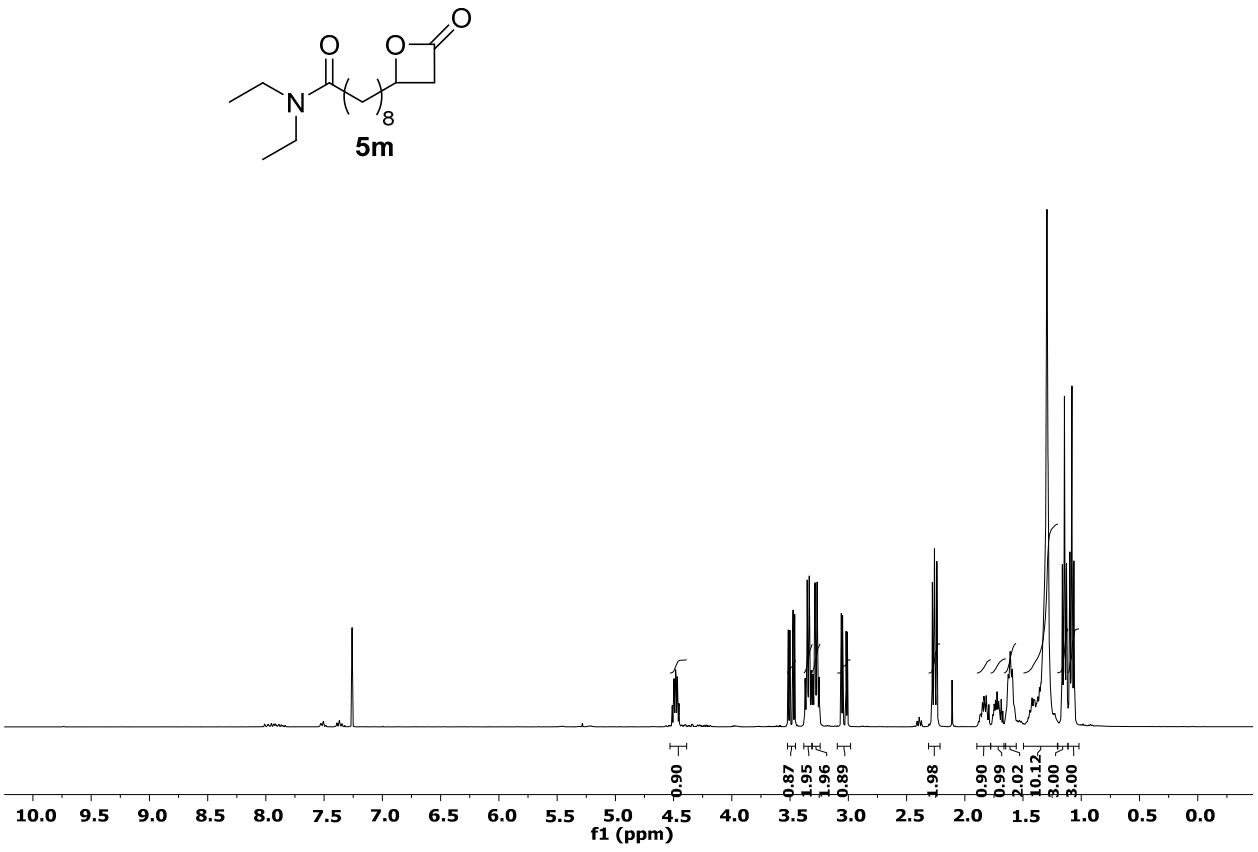

167.5
118.9
70.0
43.0
33.3
21.2
16.6
NC
5j
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

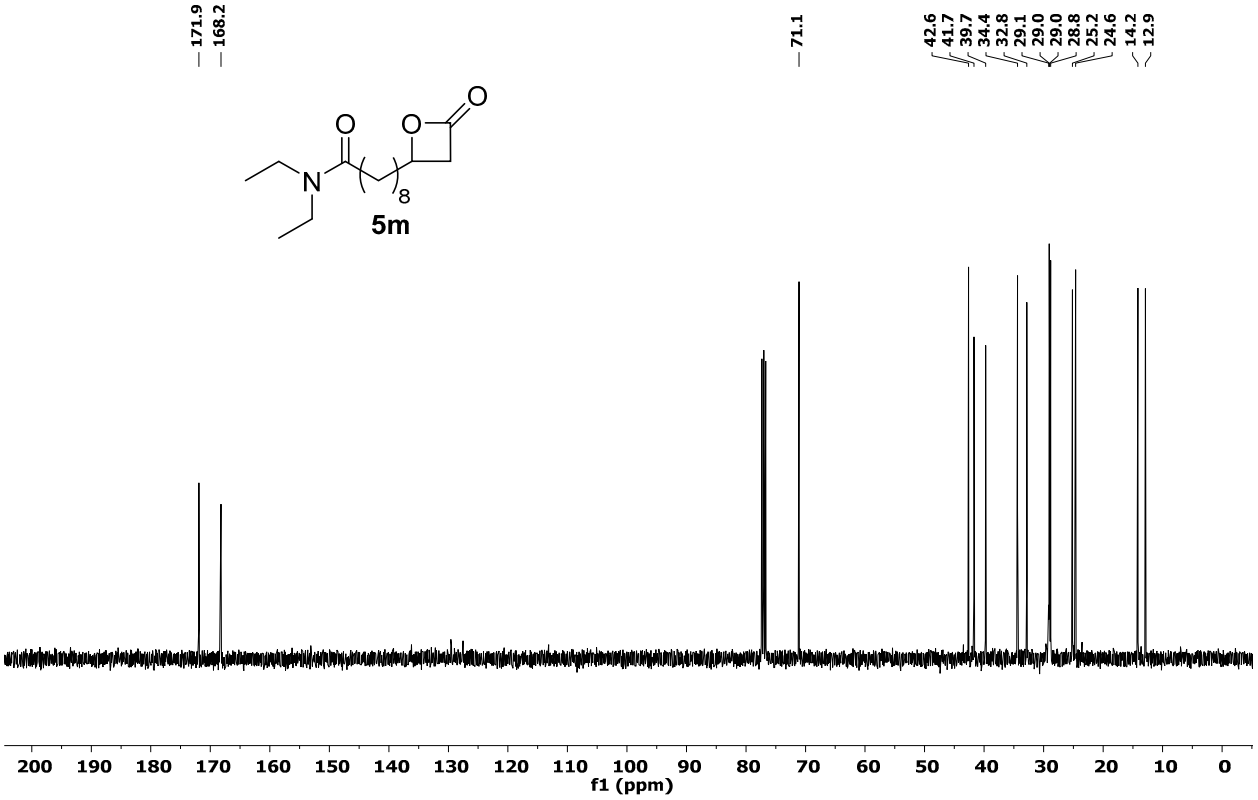

5k
0.89
2.00
1.00
1.01
1.90
2.20
2.16
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

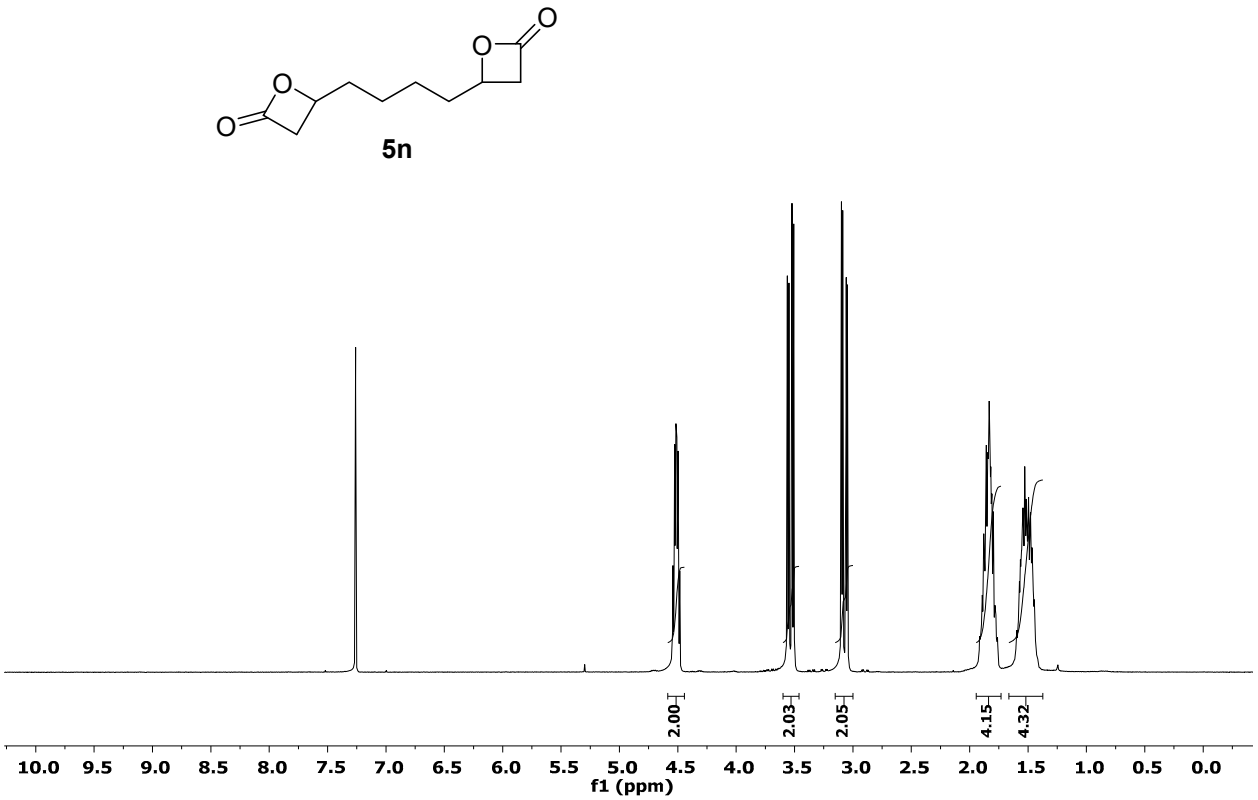

173.4
167.5
68.4
59.9
43.3
36.0
33.9
18.3
13.6
5k
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

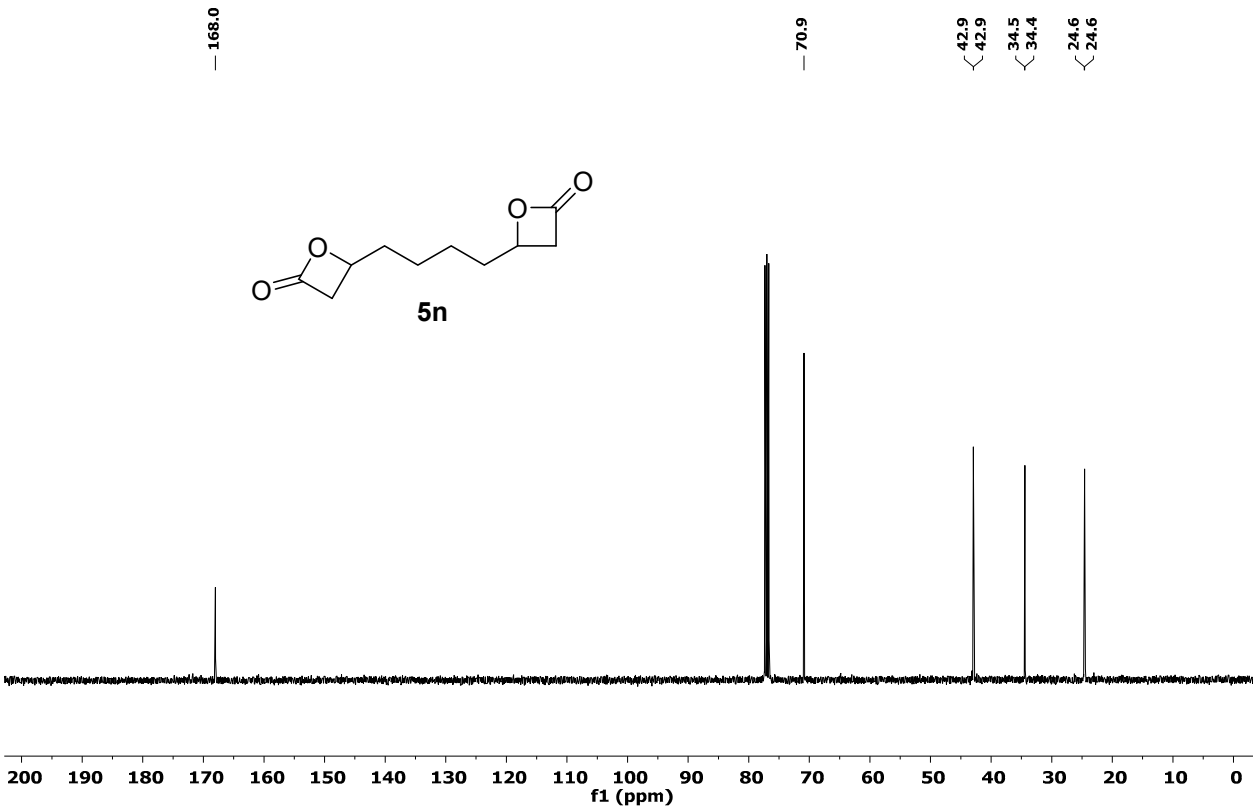

8
5l
1.00
2.02
1.02
1.01
2.06
1.07
1.06
2.09
10.26
3.15
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

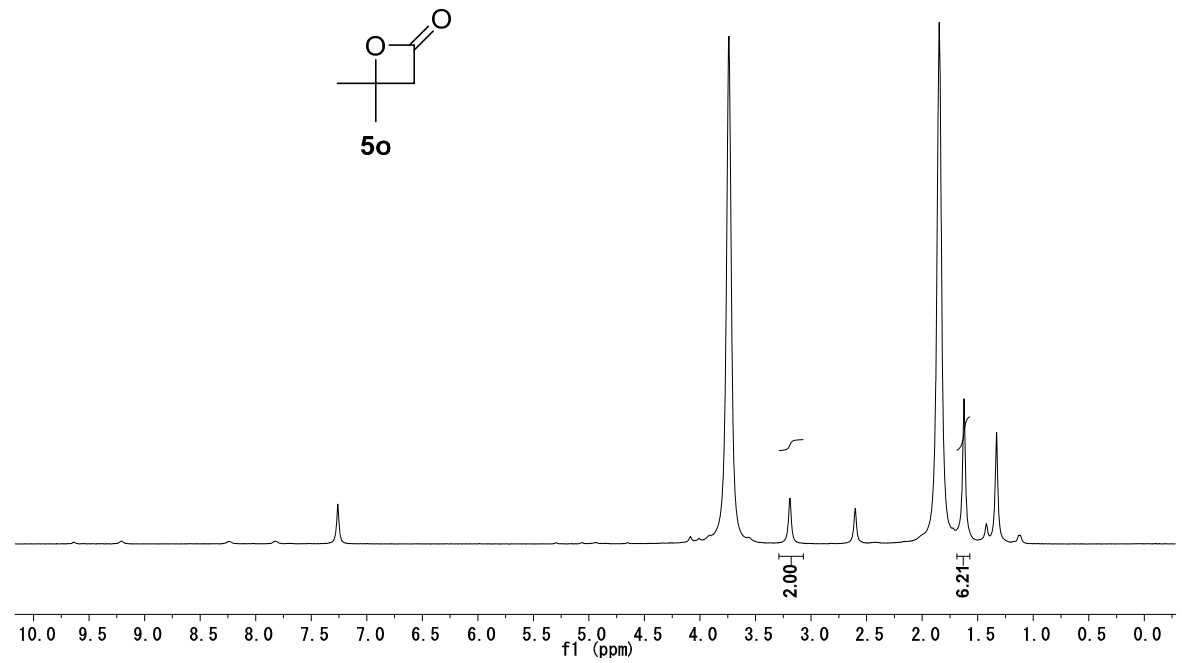

173.6
168.2
71.1
60.0
42.7
34.5
34.1
29.0
28.9
28.9
24.7
24.7
14.1
O
O
O
O
8
5l
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

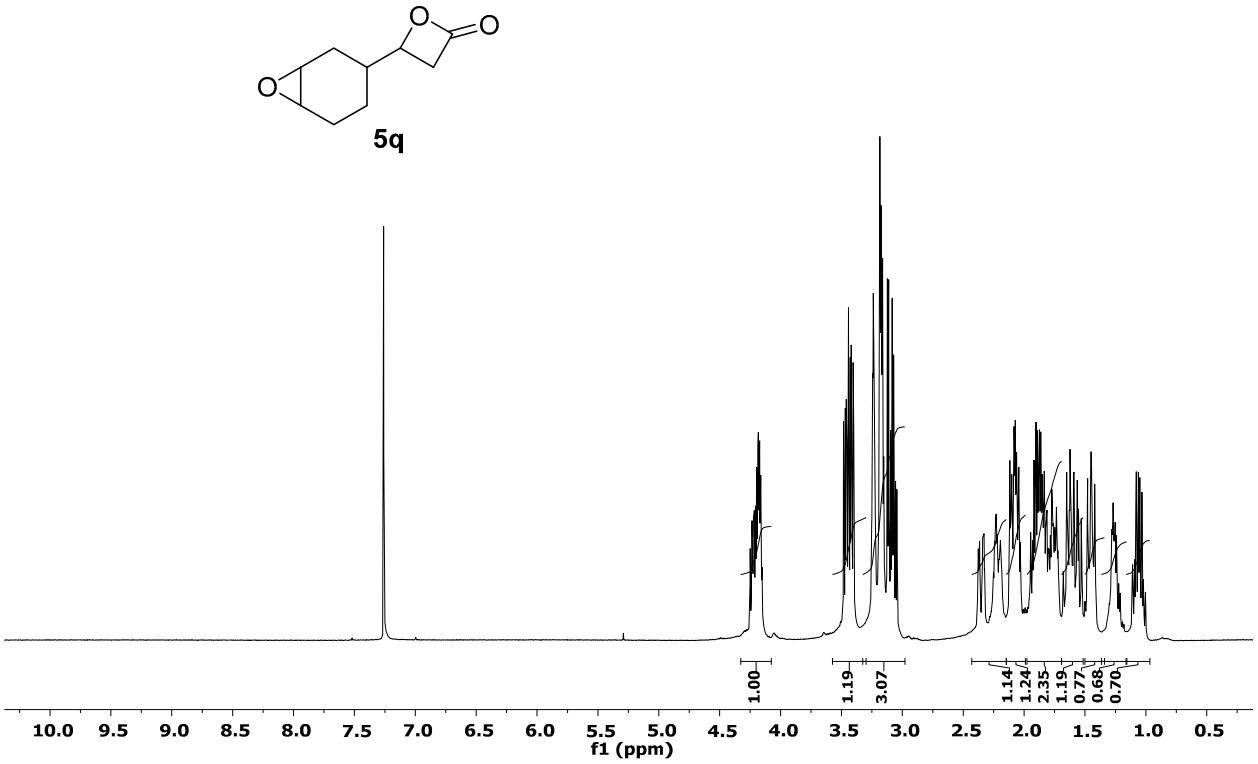

O
O
O
N
8
5m
0.90
0.87
1.95
1.96
0.89
1.98
0.90
0.99
2.02
10.12
3.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

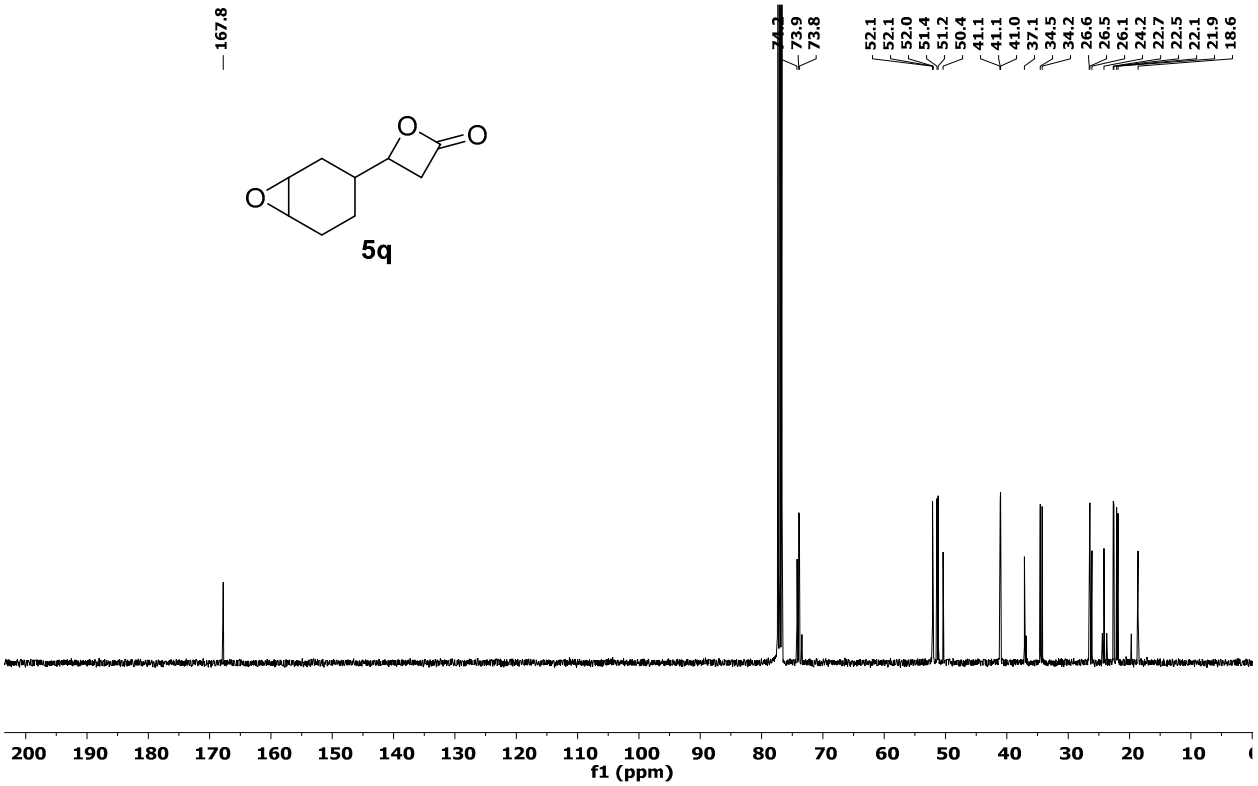

171.9
168.2
71.1
42.6
41.7
39.7
34.4
32.8
29.1
29.0
29.0
28.8
25.2
24.6
14.2
12.9
O
O
O
N
8
5m
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

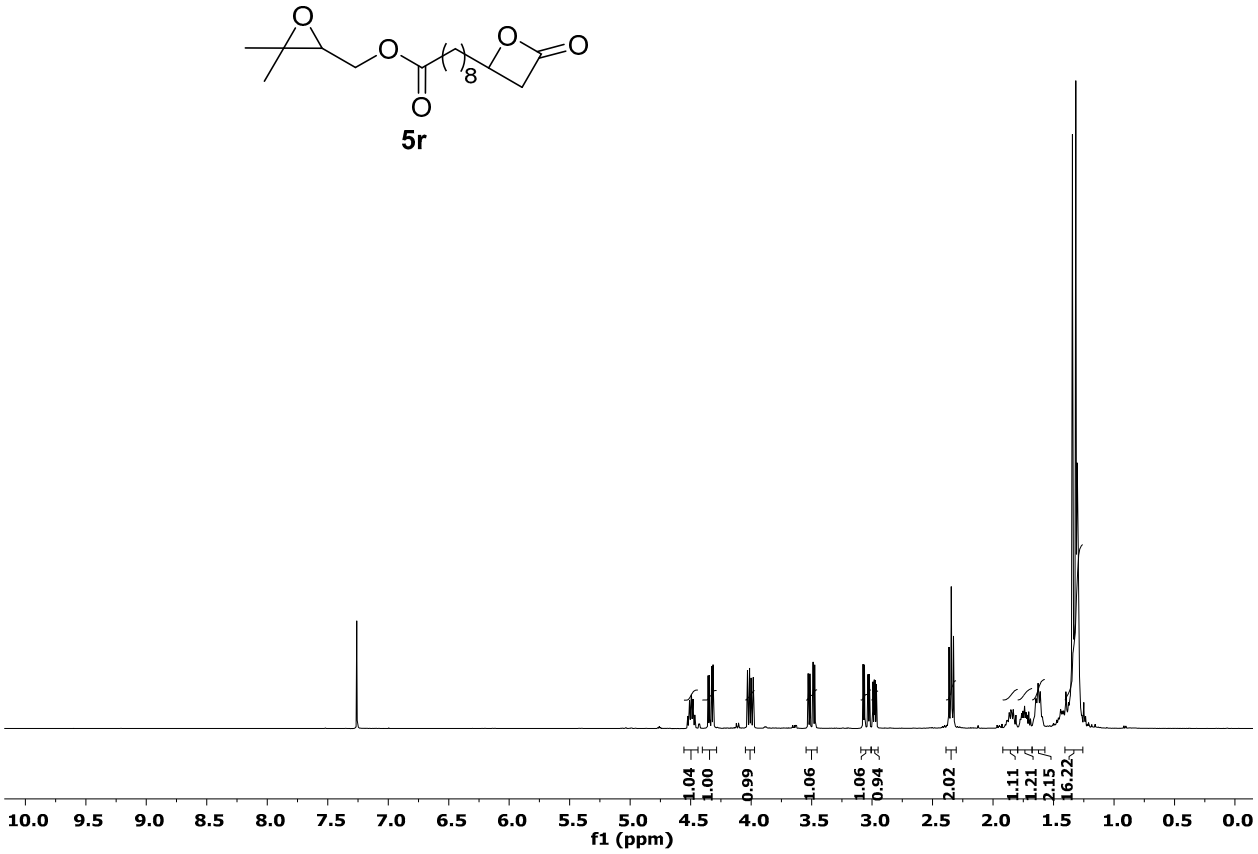

O
O
O
O
5n
2.00
2.03
2.05
4.15
4.32
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

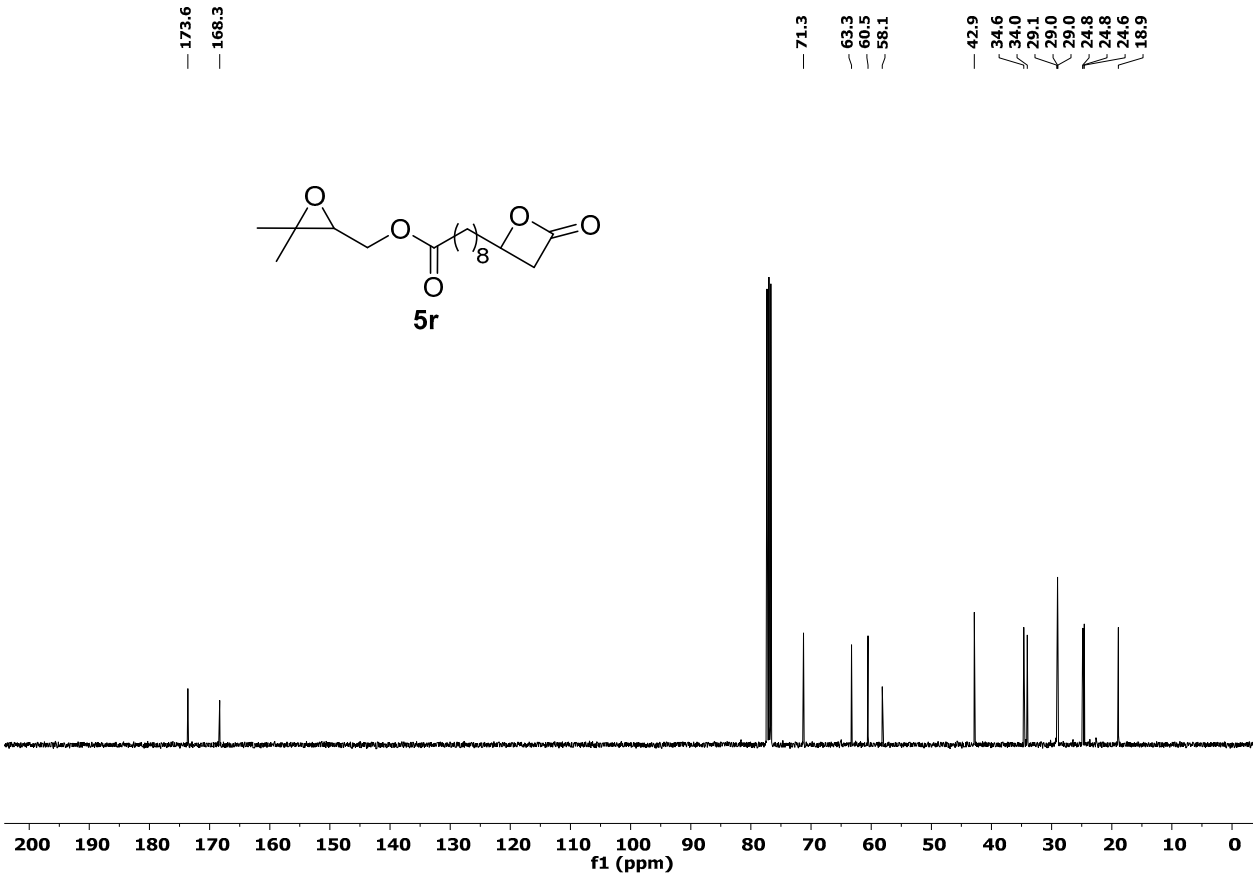

168.0
70.9
42.9
42.9
34.5
34.4
24.6
24.6
5n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


5o
2.00
6.21
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


5q
1.00
1.19
3.07
1.14
1.24
2.35
1.19
0.77
0.68
0.70
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


167.8
74.2
73.9
73.8
52.1
52.1
52.0
51.4
51.2
50.4
41.1
41.1
41.0
37.1
34.5
34.2
26.6
26.5
26.1
24.2
22.7
22.5
22.1
21.9
18.6
5q
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


5r
1.04
1.00
0.99
1.06
1.06
0.94
2.02
1.11
1.21
2.15
16.22
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


173.6
168.3
71.3
63.3
60.5
58.1
42.9
34.6
34.0
29.1
29.0
29.0
24.8
24.8
24.6
18.9
5r
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)