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Electronic Supporting Information

Development of Pyridine Based *o*-Aminophenolate Zinc Complexes as Structurally Tunable Catalysts for CO_2 Fixation into Cyclic Carbonates

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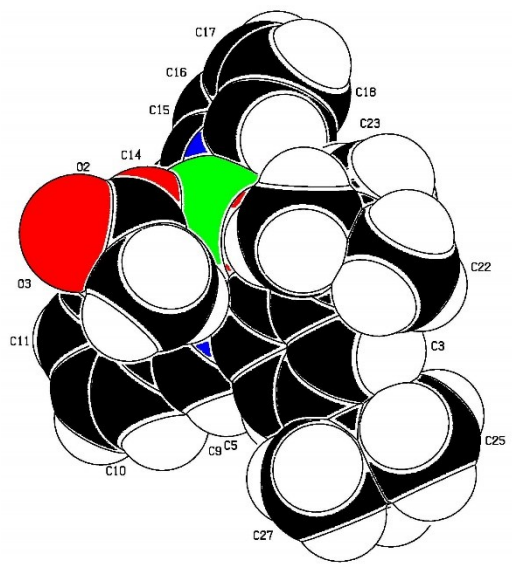
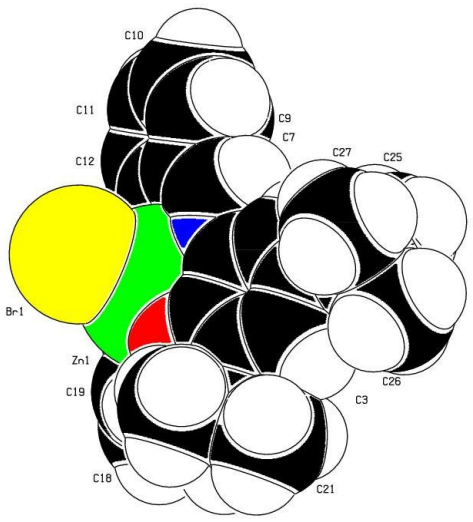
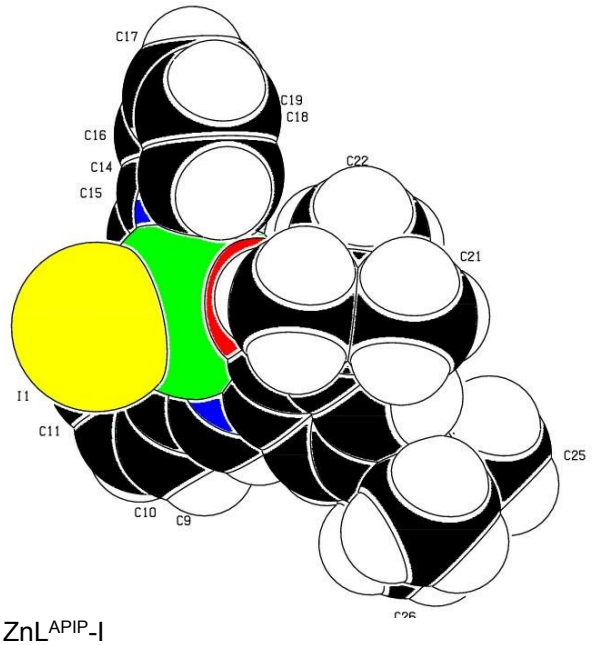
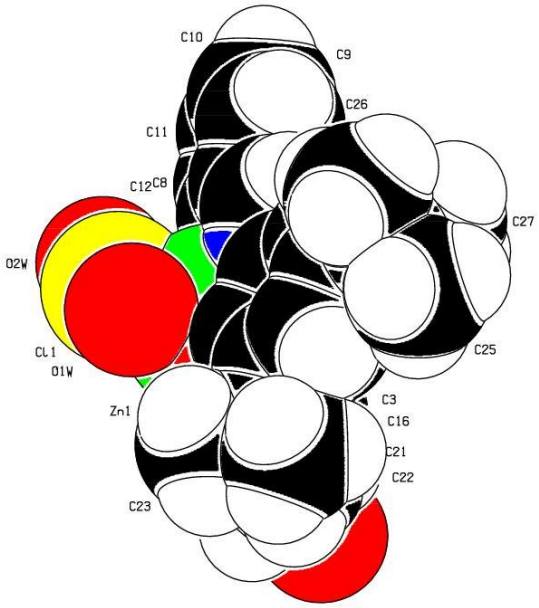




ZnL^{APIP} OAc

ZnL^{APIP}-Br





ZnL^{APIP}-I

ZnL^{APIP}-Cl

Figure S1. Space filling representation of $ZnL^{APIP}X$ (X = OAc, Br, I, Cl)

X-Ray Crystallography data of $ZnL^{APIP}X$ (X = OAc, Br, I)

In all complexes, the coordination sphere ZnN_3OX has a geometry of a distorted square pyramid, but *tau* parameters [1] of 0.31, 0.32 and 0.17 indicate the polyhedron being an intermediate between the square pyramid (SP) and the trigonal bypyramid (TB), with the deformation towards TB being smallest in $ZnL^{APIP}I$. The valence geometry of the L^{APIP} ligand found in $ZnL^{APIP}OAc$, $ZnL^{APIP}Br$ and $ZnL^{APIP}I$ is typical for such systems. However, the difference is found between the imine bond lengths with that involving N2 being significantly longer than that formed by N1. That difference in the bond lengths being the largest for acetate complex $ZnL^{APIP}OAc$ and the smallest for iodide complex $ZnL^{APIP}I$. That also reflects the internal strain imposed by the rigidity of the four-dentate L^{APIP} ligand.

With the four-dentate coordination, the L^{APIP} ligand is not flat. In $ZnL^{APIP}OAc$, the dihedral angles between C1--C6 (R1), C8--C13 (R2) and C15--N3 (R3) rings being R1-R2 18.1(3), R2-R3 30.7(2) and R1-R3 46.3(2)°. The dihedral angles between these ring planes and the N_3O_1 plane of the pyramid base are 24.8(2), 12.5(3) and 21.7(2)°, respectively. The dihedral angle between the best plane of acetate ligand and the N_3O_1 pyramid base plane is 85.1(2)°, but the acetate is slightly tilted towards N1 and O1, with the Zn1-O2-C28 angle being 129.3(4)°. The L^{APIP} conformation can be described with the torsion angles C1-C6-N1-C7 177.6(4)°, N1-C7-C8-C13 -13.9(7)° and C8-C13-N2-C14 -149.8(4)°. In $ZnL^{APIP}Br$, the significant effect of the bulk imposed by Br ligand is clearly visible. The dihedral angles R1-R2, R2-R3 and R1-R3 are 30.03(14), 37.74(15) and 65.05(14)° and are larger than these found in $ZnL^{APIP}OAc$. In $ZnL^{APIP}I$, the corresponding angles are 17.40(11), 31.55(12) and 47.07(11)°, almost identical to those in $ZnL^{APIP}OAc$. The reason for this similarity seems to be a Zn-I bond being the longest among the reported structures, and therefore minimizing the bulk of the axial ligand. In $ZnL^{APIP}Br$, angles between the N_3O_1 plane of the pyramid base and R1, R2 and R3 are 33.58(9), 13.7(1) and 31.7(1)°, respectively, and these values are again larger than these reported for $ZnL^{APIP}OAc$. In $ZnL^{APIP}I$, the corresponding angles are 25.11(9), 11.4(1) and 21.96(8)°.

The intramolecular Cg…Cg distances between the gravity centers of Zn1-O1-C1-C6-N1 chelate and N3--C19 pyridine rings as well as between Zn1-N2-C14-C15-N3 and C1--C6 phenolic rings are 4.675(3), 5.413(3) Å for $ZnL^{APIP}OAc$, 4.5044(16), 5.1743(15) Å in $ZnL^{APIP}Br$ and 4.6447(13), 5.2968(13) Å for $ZnL^{APIP}I$. These data indicate that the internal strain seems to be the largest for the Br complex $ZnL^{APIP}Br$. Analysis of the crystal packing of complexes revealed some intermolecular C-H…π interactions.

Table S1. Bond lengths [Å] and angles [°] for $ZnL^{APIP}OAc$

Bonds		Angles	
Zn1-O1	1.978(3)	**O1-Zn1-O2**	111.95(14)
Zn1-O2	1.991(4)	**O1-Zn1-N1**	81.73(12)
Zn1-N1	2.087(3)	**O2-Zn1-N1**	117.06(15)
Zn1-N3	2.109(4)	**O1-Zn1-N3**	96.71(13)
Zn1-N2	2.174(3)	**O2-Zn1-N3**	105.45(15)
O1-C1	1.311(5)	**N1-Zn1-N3**	134.79(14)
C1-C2	1.431(5)	**O1-Zn1-N2**	153.35(14)
C1-C6	1.432(5)	**O2-Zn1-N2**	94.67(13)
C2-C3	1.392(5)	**N1-Zn1-N2**	85.04(13)
C2-C20	1.543(5)	**N3-Zn1-N2**	76.60(13)
C3-C4	1.391(6)	**C1-O1-Zn1**	114.7(2)
C4-C5	1.390(6)	**O1-C1-C2**	123.0(3)
C4-C24	1.546(6)	**O1-C1-C6**	119.8(3)
C5-C6	1.386(5)	**C2-C1-C6**	117.1(3)
C6-N1	1.426(5)	**C3-C2-C1**	119.1(3)
N1-C7	1.281(5)	**C3-C2-C20**	121.3(4)
C7-C8	1.471(6)	**C1-C2-C20**	119.6(3)
C8-C9	1.394(6)	**C4-C3-C2**	123.5(4)
C8-C13	1.428(6)	**C5-C4-C3**	117.5(4)
C9-C10	1.390(6)	**C5-C4-C24**	121.5(4)
C10-C11	1.364(7)	**C3-C4-C24**	121.1(4)
C11-C12	1.383(7)	**C6-C5-C4**	121.8(4)
C12-C13	1.394(6)	**C5-C6-N1**	125.2(4)
C13-N2	1.419(5)	**C5-C6-C1**	121.1(4)
N2-C14	1.249(6)	**N1-C6-C1**	113.6(3)
C14-C15	1.465(6)	**C7-N1-C6**	123.5(3)
C15-N3	1.354(6)	**C7-N1-Zn1**	126.2(3)
C15-C16	1.374(6)	**C6-N1-Zn1**	110.1(2)
C16-C17	1.389(7)	**N1-C7-C8**	127.2(4)
C17-C18	1.400(8)	**C9-C8-C13**	116.8(4)
C18-C19	1.380(7)	**C9-C8-C7**	116.5(4)
C19-N3	1.326(6)	**C13-C8-C7**	126.7(4)
C20-C21	1.528(7)	**C10-C9-C8**	121.7(4)
C20-C23	1.531(7)	**C11-C10-C9**	120.9(4)
C20-C22	1.552(6)	**C10-C11-C12**	119.7(4)
C24-C27	1.493(9)	**C11-C12-C13**	120.6(4)
C24-C25	1.502(7)	**C12-C13-N2**	121.8(4)
C24-C26	1.569(8)	**C12-C13-C8**	120.4(4)
O2-C28	1.209(7)	**N2-C13-C8**	117.8(4)
C28-O3	1.246(7)	**C14-N2-C13**	121.6(4)
C28-C29	1.528(9)	**C14-N2-Zn1**	114.3(3)
		C13-N2-Zn1	124.0(3)
		N2-C14-C15	118.9(4)
		N3-C15-C16	122.5(4)
		N3-C15-C14	115.5(4)
		C16-C15-C14	121.9(4)
		C15-C16-C17	118.6(5)
		C16-C17-C18	118.7(5)
		C19-C18-C17	119.1(5)
		N3-C19-C18	122.0(5)
		C19-N3-C15	119.2(4)
		C19-N3-Zn1	126.4(3)
		C15-N3-Zn1	114.4(3)
		C21-C20-C23	109.7(4)
		C21-C20-C2	108.2(4)
		C23-C20-C2	110.4(4)
		C21-C20-C22	108.7(4)
		C23-C20-C22	108.0(4)
		C2-C20-C22	111.9(4)
		C27-C24-C25	111.7(6)
		C27-C24-C4	109.9(5)
		C25-C24-C4	113.4(4)
		C27-C24-C26	107.6(6)
		C25-C24-C26	105.3(5)
		C4-C24-C26	108.6(4)
		C28-O2-Zn1	129.3(4)
		O2-C28-O3	124.8(6)
		O2-C28-C29	118.7(5)
		O3-C28-C29	116.5(6)

Table S2. Bond lengths [Å] and angles [°] for ZnL^{APIP} Br

Number	Atom1	Atom2	Length
1	Zn1	Br1	2.4003(5)
2	Zn1	O1	1.960(2)
3	Zn1	N1	2.106(2)
4	Zn1	N2	2.170(2)
5	Zn1	N3	2.121(2)
6	O1	C1	1.308(3)
7	C1	C2	1.420(4)
8	C1	C6	1.426(3)
9	C2	C3	1.378(4)
10	C2	C20	1.535(4)
11	C3	H3A	0.93
12	C3	C4	1.405(4)
13	C4	C5	1.378(4)
14	C4	C24	1.530(4)
15	C5	H5A	0.93
16	C5	C6	1.382(4)
17	C6	N1	1.407(3)
18	C7	H7A	0.93
19	C7	N1	1.290(3)
20	C7	C8	1.461(3)
21	C8	C9	1.393(4)
22	C8	C13	1.407(3)
23	C9	H9A	0.93
24	C9	C10	1.370(4)
25	C10	H10A	0.93
26	C10	C11	1.387(5)
27	C11	H11A	0.93
28	C11	C12	1.378(4)
29	C12	H12A	0.93
30	C12	C13	1.384(4)
31	C13	N2	1.421(3)
32	N2	C14	1.271(4)
33	C14	H14A	0.929
34	C14	C15	1.468(3)
35	C15	C16	1.382(4)
36	C15	N3	1.349(4)
37	C16	H16A	0.93
38	C16	C17	1.382(4)

Number	Atom1	Atom2	Atom3	Angle
1	Br1	Zn1	O1	112.25(7)
2	Br1	Zn1	N1	111.95(7)
3	Br1	Zn1	N2	99.24(6)
4	Br1	Zn1	N3	116.74(7)
5	O1	Zn1	N1	81.12(9)
6	O1	Zn1	N2	148.01(9)
7	O1	Zn1	N3	93.67(9)
8	N1	Zn1	N2	82.03(9)
9	N1	Zn1	N3	129.02(9)
10	N2	Zn1	N3	76.37(9)
11	Zn1	O1	C1	115.0(2)
12	O1	C1	C2	123.0(2)
13	O1	C1	C6	119.9(2)
14	C2	C1	C6	117.1(2)
15	C1	C2	C3	118.4(3)
16	C1	C2	C20	119.5(2)
17	C3	C2	C20	122.1(3)
18	C2	C3	H3A	117.7
19	C2	C3	C4	124.5(3)
20	H3A	C3	C4	117.8
21	C3	C4	C5	116.7(3)
22	C3	C4	C24	122.3(3)
23	C5	C4	C24	121.1(2)
24	C4	C5	H5A	119.4
25	C4	C5	C6	121.3(2)
26	H5A	C5	C6	119.4
27	C1	C6	C5	122.0(2)
28	C1	C6	N1	113.5(2)
29	C5	C6	N1	124.5(2)
30	H7A	C7	N1	117.3
31	H7A	C7	C8	117.1
32	N1	C7	C8	125.6(2)
33	Zn1	N1	C6	110.0(2)
34	Zn1	N1	C7	124.9(2)
35	C6	N1	C7	124.3(2)
36	C7	C8	C9	117.0(2)
37	C7	C8	C13	125.8(2)
38	C9	C8	C13	117.1(2)
39	C8	C9	H9A	118.8
40	C8	C9	C10	122.5(3)
41	H9A	C9	C10	118.7
42	C9	C10	H10A	120.3
43	C9	C10	C11	119.4(3)
44	H10A	C10	C11	120.3
45	C10	C11	H11A	120.1
46	C10	C11	C12	119.9(3)
47	H11A	C11	C12	120
48	C11	C12	H12A	119.8
49	C11	C12	C13	120.4(3)
50	H12A	C12	C13	119.8
51	C8	C13	C12	120.7(2)
52	C8	C13	N2	118.7(2)
53	C12	C13	N2	120.7(2)
54	Zn1	N2	C13	122.4(2)
55	Zn1	N2	C14	114.4(2)
56	C13	N2	C14	123.1(2)
57	N2	C14	H14A	120.5
58	N2	C14	C15	119.0(3)
59	H14A	C14	C15	120.5
60	C14	C15	C16	122.6(3)
61	C14	C15	N3	114.8(2)
62	C16	C15	N3	122.5(3)
63	C15	C16	H16A	120.9
64	C15	C16	C17	118.3(3)
65	H16A	C16	C17	120.8
66	C16	C17	H17A	120.3
67	C16	C17	C18	119.4(3)
68	H17A	C17	C18	120.2
69	C17	C18	H18A	120.6
70	C17	C18	C19	118.9(3)
71	H18A	C18	C19	120.6

Table S3. Bond lengths [Å] and angles [°] for ZnL^{APIP} I

Number	Atom1	Atom2	Length
1	Zn1	I1	2.5765(4)
2	Zn1	O1	1.962(2)
3	Zn1	N1	2.116(2)
4	Zn1	N2	2.162(2)
5	Zn1	N3	2.126(2)
6	O1	C1	1.318(3)
7	C1	C2	1.429(4)
8	C1	C6	1.413(3)
9	C2	C3	1.368(3)
10	C2	C20	1.541(3)
11	C3	H3A	0.929
12	C3	C4	1.410(3)
13	C4	C5	1.377(4)
14	C4	C24	1.535(4)
15	C5	H5A	0.93
16	C5	C6	1.390(3)
17	C6	N1	1.417(3)
18	N1	C7	1.284(3)
19	C7	H7A	0.93
20	C7	C8	1.459(4)
21	C8	C9	1.398(3)
22	C8	C13	1.408(4)
23	C9	H9A	0.93
24	C9	C10	1.370(4)
25	C10	H10A	0.93
26	C10	C11	1.366(4)
27	C11	H11A	0.93
28	C11	C12	1.375(3)
29	C12	H12A	0.93
30	C12	C13	1.383(4)
31	C13	N2	1.418(3)
32	N2	C14	1.266(3)
33	C14	H14A	0.929
34	C14	C15	1.465(3)
35	C15	C16	1.379(3)
36	C15	N3	1.344(3)
37	C16	H16A	0.93
38	C16	C17	1.373(3)
39	C17	H17A	0.931
40	C17	C18	1.364(4)
41	C18	H18A	0.929
42	C18	C19	1.379(4)
43	C19	H19A	0.93
44	C19	N3	1.330(3)
45	C20	C21	1.525(4)
46	C20	C22	1.528(3)
47	C20	C23	1.528(4)

Number				
1	I1	Zn1	O1	114.73(5)
2	I1	Zn1	N1	117.60(5)
3	I1	Zn1	N2	101.16(5)
4	I1	Zn1	N3	106.81(5)
5	O1	Zn1	N1	81.23(7)
6	O1	Zn1	N2	144.10(7)
7	O1	Zn1	N3	92.04(7)
8	N1	Zn1	N2	82.99(7)
9	N1	Zn1	N3	133.75(7)
10	N2	Zn1	N3	76.22(7)
11	Zn1	O1	C1	114.7(1)
12	O1	C1	C2	121.4(2)
13	O1	C1	C6	120.7(2)
14	C2	C1	C6	117.8(2)
15	C1	C2	C3	117.8(2)
16	C1	C2	C20	120.0(2)
17	C3	C2	C20	122.3(2)
18	C2	C3	H3A	117.5
19	C2	C3	C4	124.9(2)
20	H3A	C3	C4	117.6
21	C3	C4	C5	116.7(2)
22	C3	C4	C24	119.4(2)
23	C5	C4	C24	123.9(2)
24	C4	C5	H5A	119.5
25	C4	C5	C6	121.0(2)
26	H5A	C5	C6	119.5
27	C1	C6	C5	121.7(2)
28	C1	C6	N1	113.5(2)
29	C5	C6	N1	124.8(2)
30	Zn1	N1	C6	109.5(1)
31	Zn1	N1	C7	126.8(2)
32	C6	N1	C7	123.6(2)
33	N1	C7	H7A	117
34	N1	C7	C8	125.9(2)
35	H7A	C7	C8	117.1
36	C7	C8	C9	116.7(2)
37	C7	C8	C13	126.1(2)
38	C9	C8	C13	117.2(2)
39	C8	C9	H9A	119
40	C8	C9	C10	122.0(2)
41	H9A	C9	C10	119
42	C9	C10	H10A	120.1
43	C9	C10	C11	119.8(2)
44	H10A	C10	C11	120.2
45	C10	C11	H11A	119.8
46	C10	C11	C12	120.4(2)
47	H11A	C11	C12	119.9
48	C11	C12	H12A	119.8
49	C11	C12	C13	120.5(2)
50	H12A	C12	C13	119.7
51	C8	C13	C12	120.1(2)
52	C8	C13	N2	119.0(2)
53	C12	C13	N2	120.9(2)
54	Zn1	N2	C13	123.4(1)
55	Zn1	N2	C14	114.6(2)
56	C13	N2	C14	122.1(2)
57	N2	C14	H14A	120.4
58	N2	C14	C15	119.2(2)
59	H14A	C14	C15	120.4
60	C14	C15	C16	123.2(2)
61	C14	C15	N3	114.7(2)
62	C16	C15	N3	122.1(2)
63	C15	C16	H16A	120.8
64	C15	C16	C17	118.4(2)
65	H16A	C16	C17	120.8
66	C16	C17	H17A	120
67	C16	C17	C18	119.9(2)
68	H17A	C17	C18	120
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70	C17	C18	C19	118.5(2)
71	H18A	C18	C19	120.7

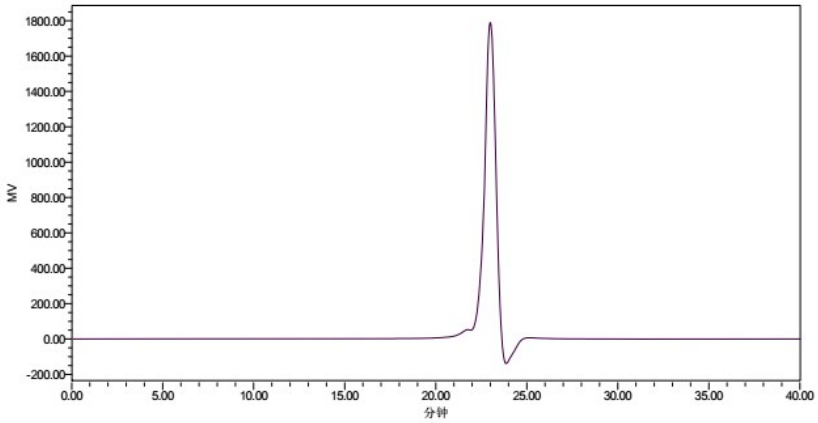


Figure S2. GPC analysis of Styrene Carbonate reaction mixture relevant to table 4 entry 12 showing no polymer chain

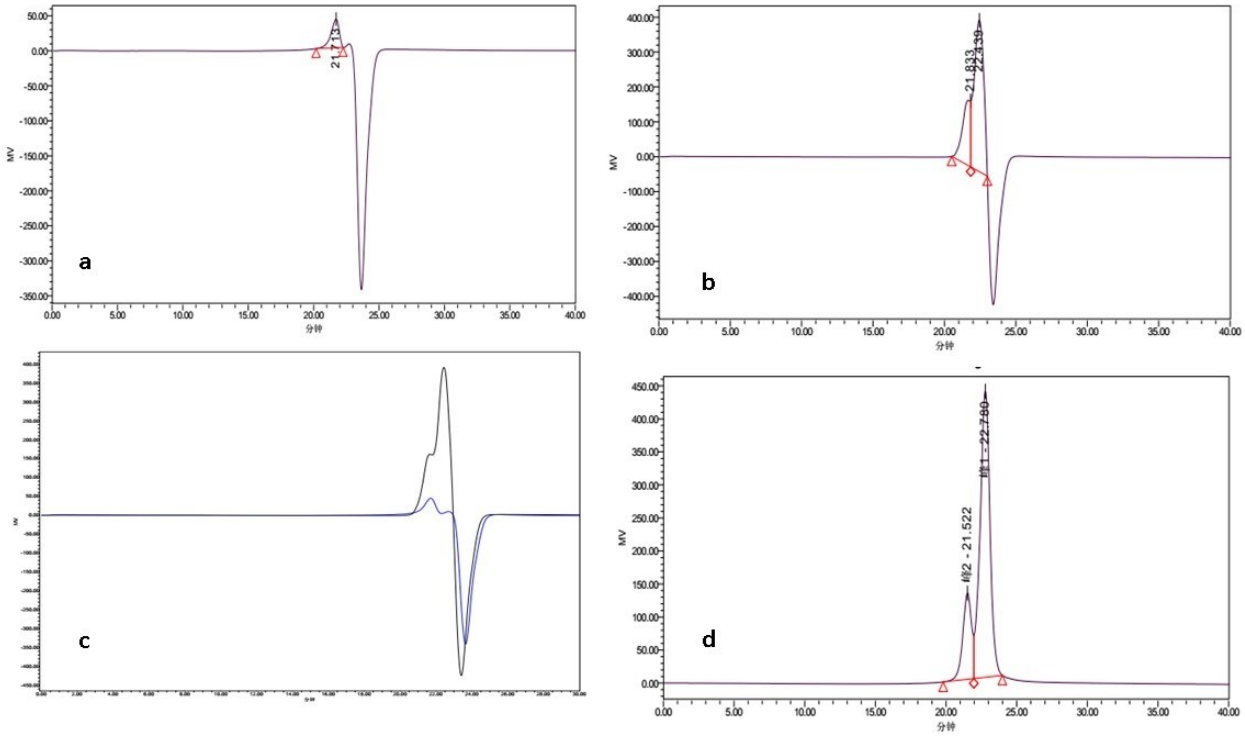


Figure S3. GPC analysis of **a)** typical polyether of cyclohexane oxide identified by ^{1}H NMR, **b)** Cyclohexane carbonate reaction mixture (Table 5, entries 6-10), **c)** Overlap spectra of **(a)** (blue) and **(b)** (black),**d)** Cyclohexane carbonate reaction catalyzed by TBAI relevant to table 5, entry 11.

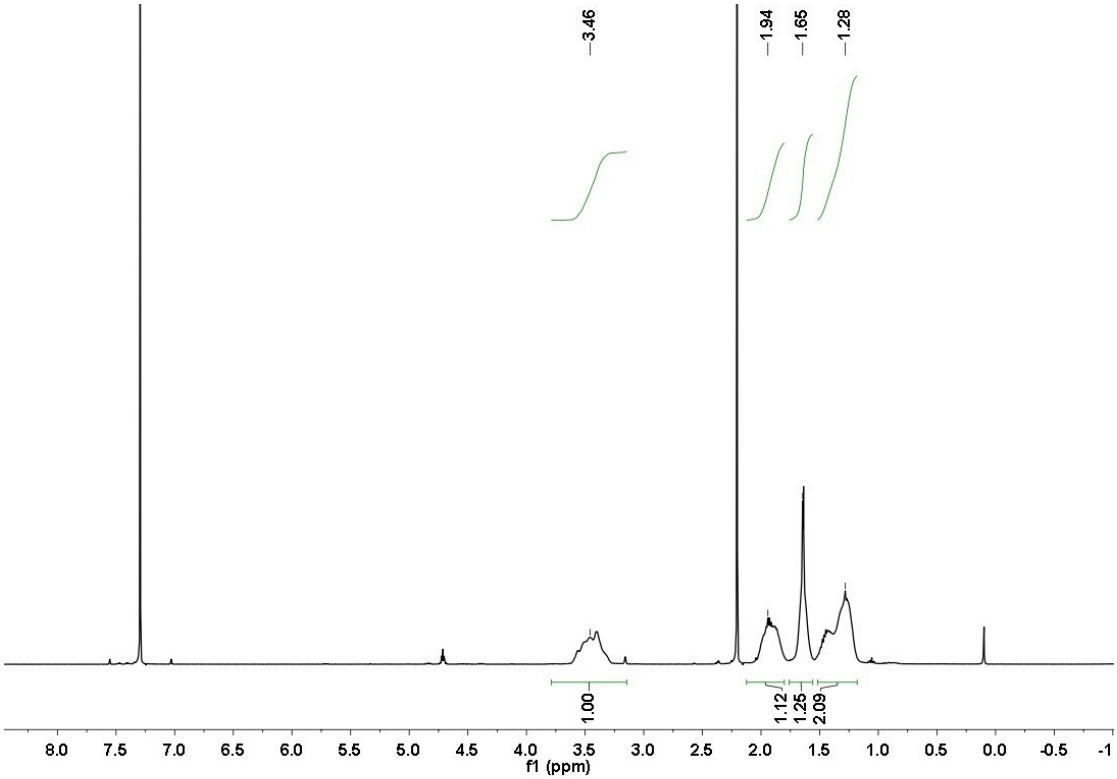


Figure S4. ^{1}H NMR spectrum of the cyclohexane oxide polyether chain (broad signal at δ = 3.45 ppm) (It was isolated by crystallization in THF in -1 °C)

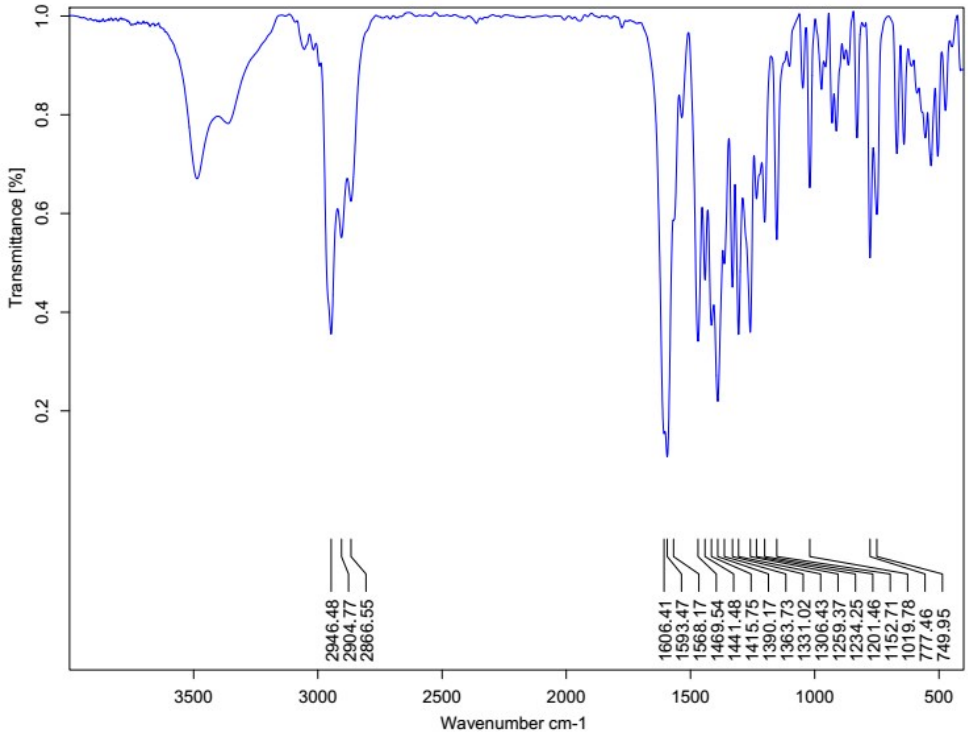


Figure S5. FT-IR of ZnL^{APIP}OAc

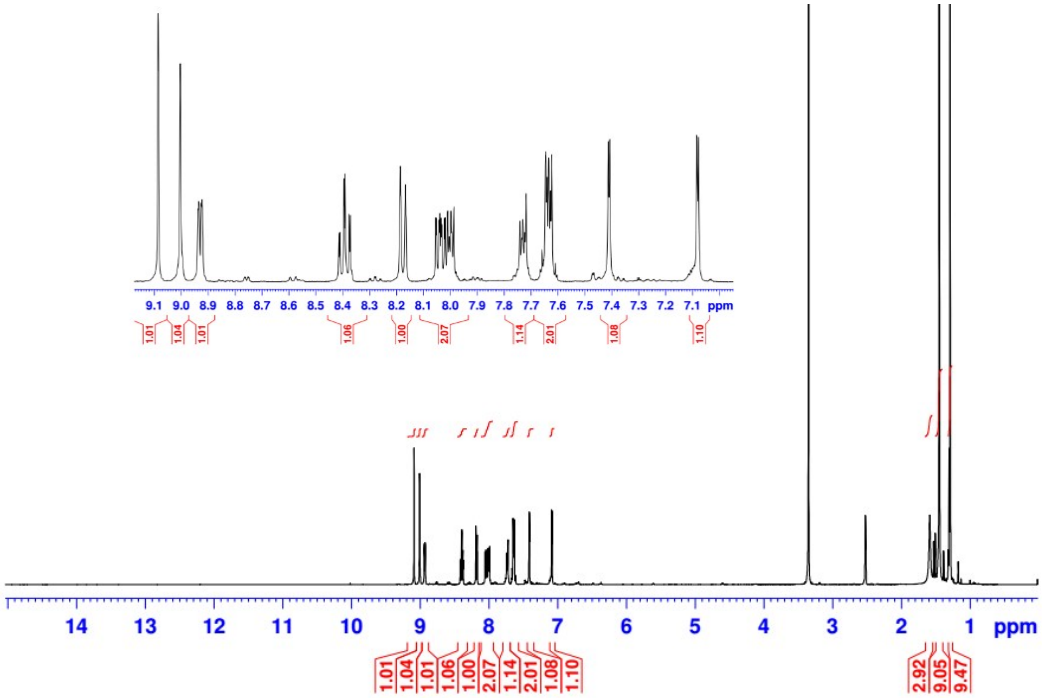


Figure S6. ^{1}H NMR of ZnL^{APIP}OAc

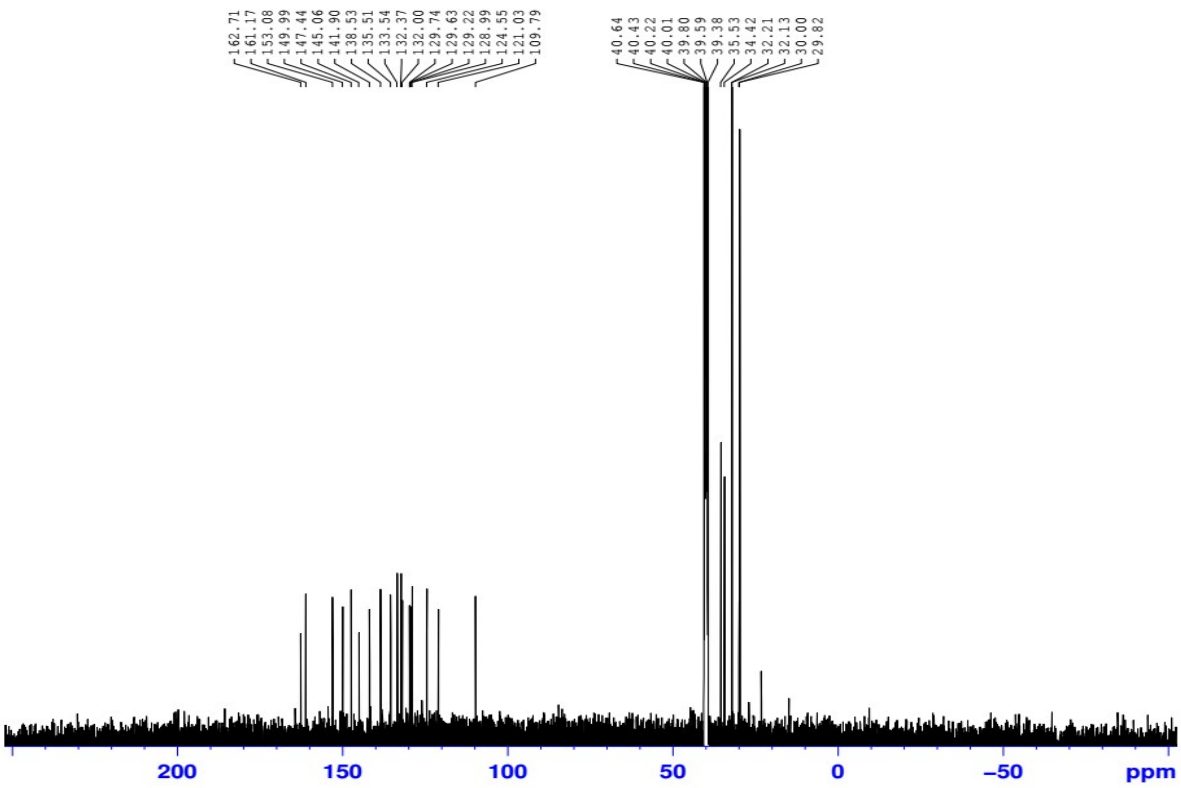


Figure S7. ^{13}C NMR of ZnL^{APIP}OAc

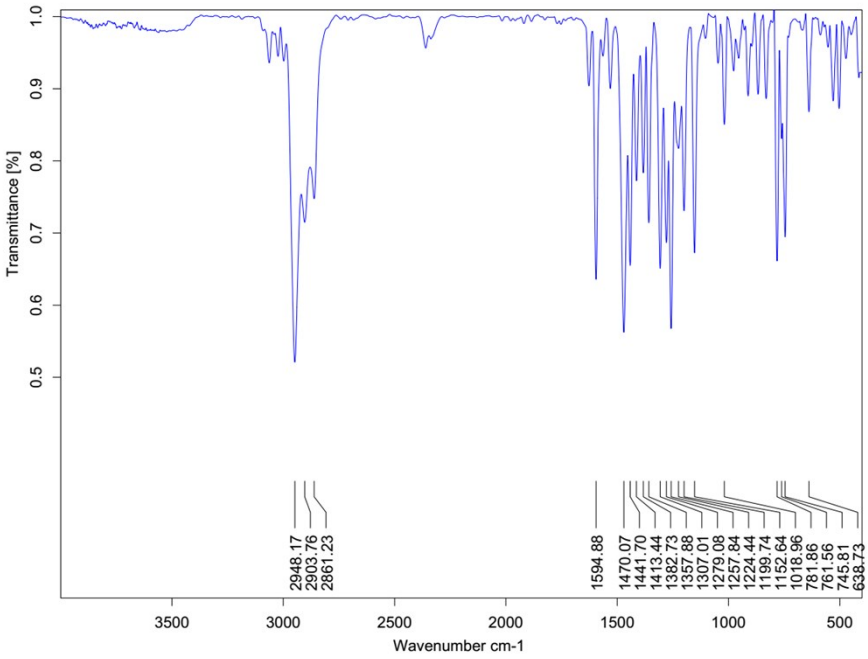


Figure S8. FTIR of ZnL^{APIP}Cl

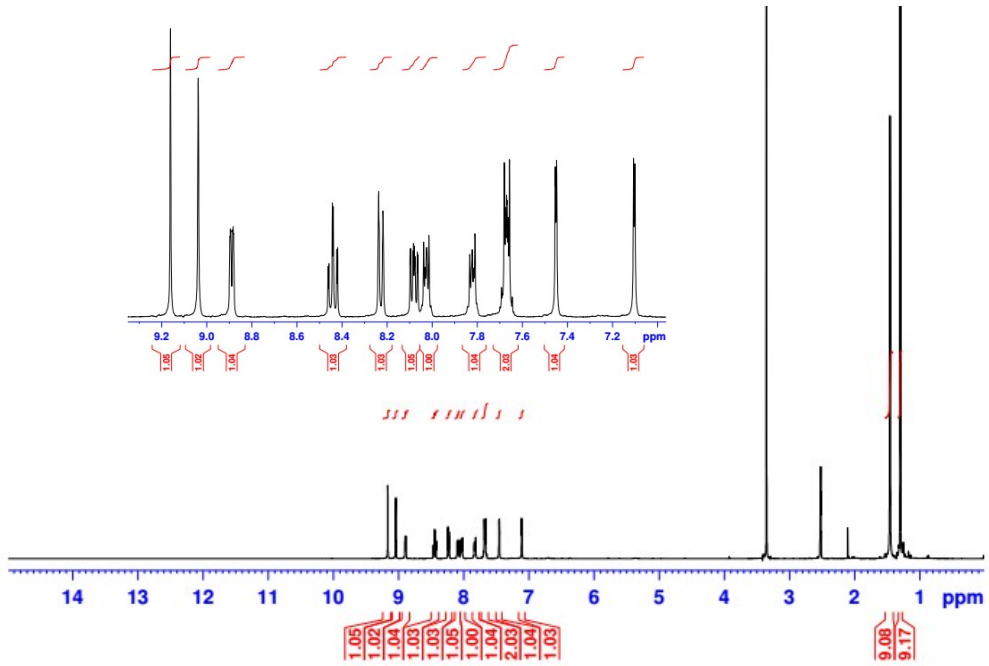


Figure S9. ^{1}H NMR of ZnL^{APIP}Cl

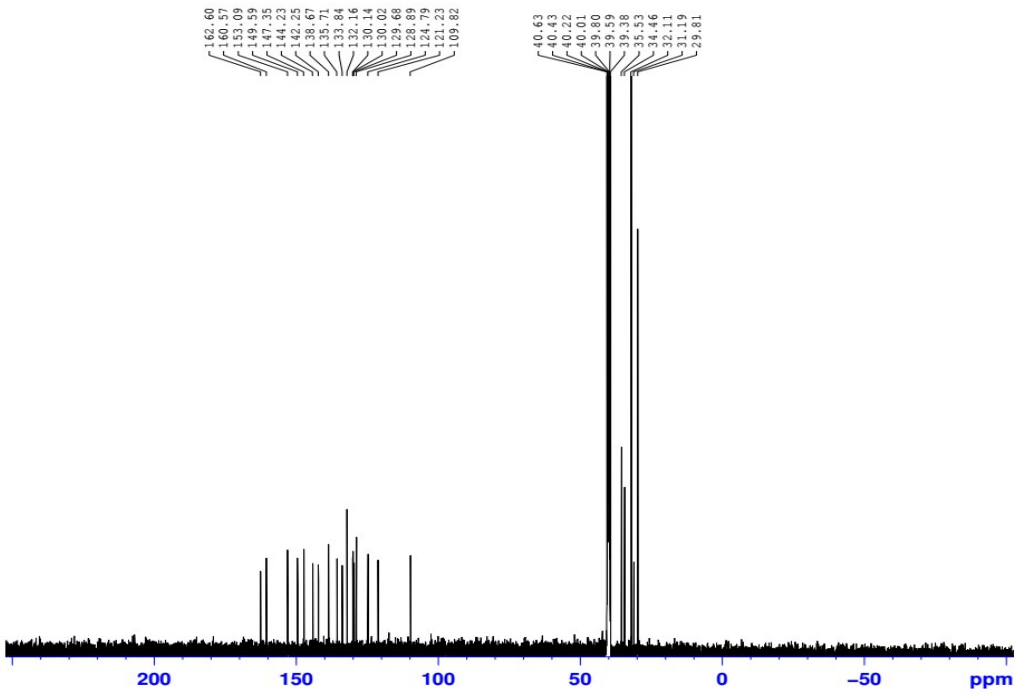
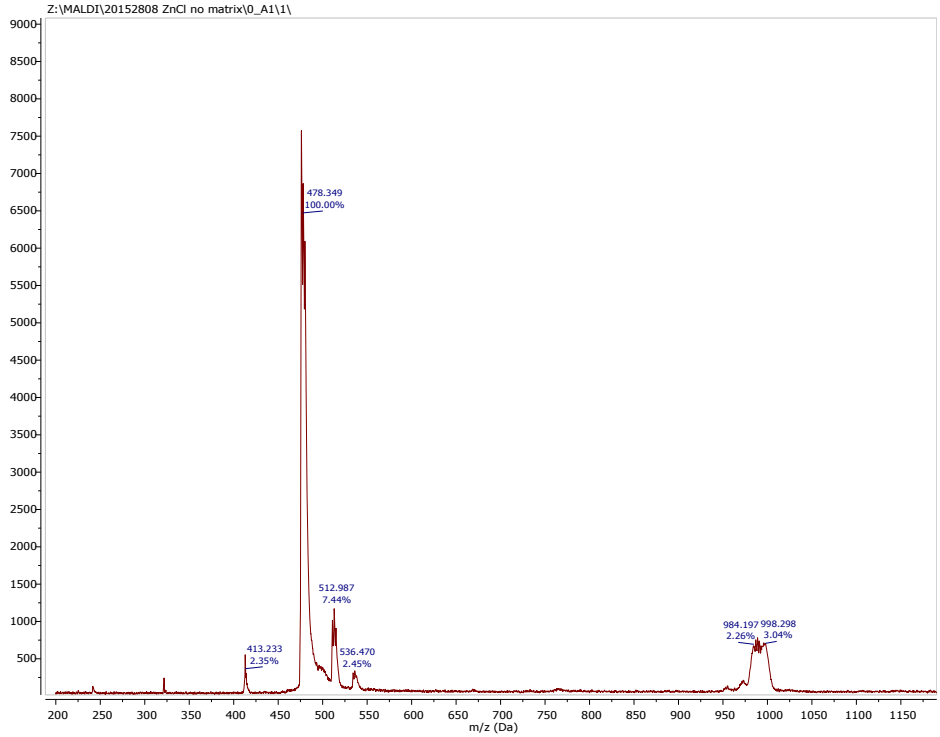
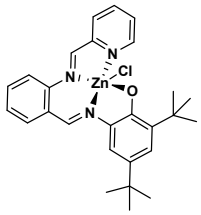


Figure S10. ^{13}C NMR of ZnL^{APIP}Cl





Molecular Weight: 513.39

Figure S11. MALDI-MS of ZnL^{APIP}Cl

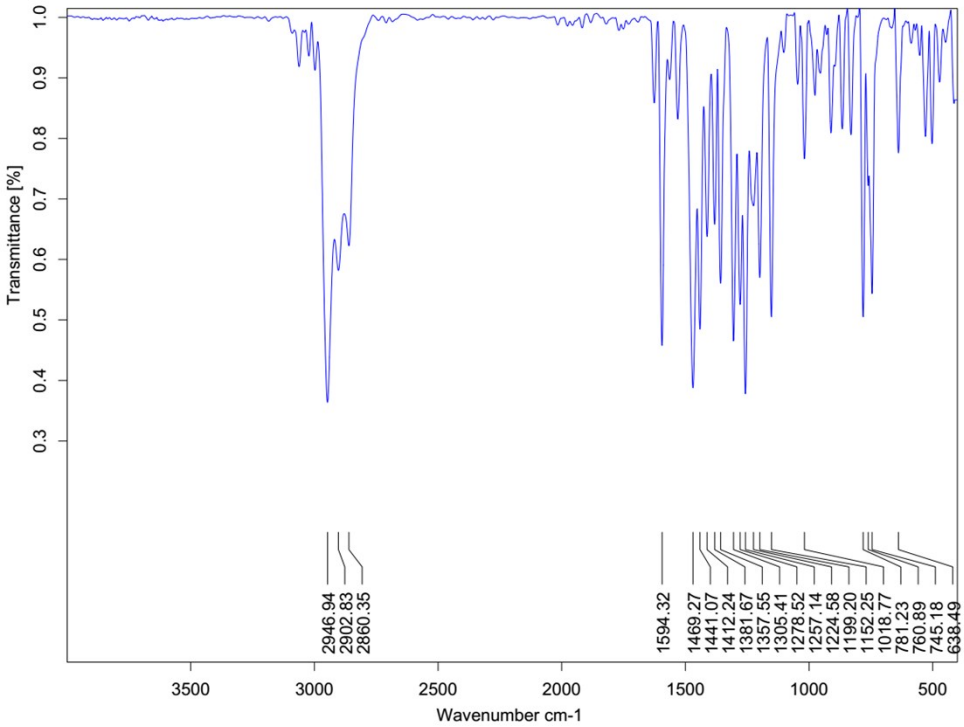


Figure S12. FTIR of ZnL^{APIP}Br

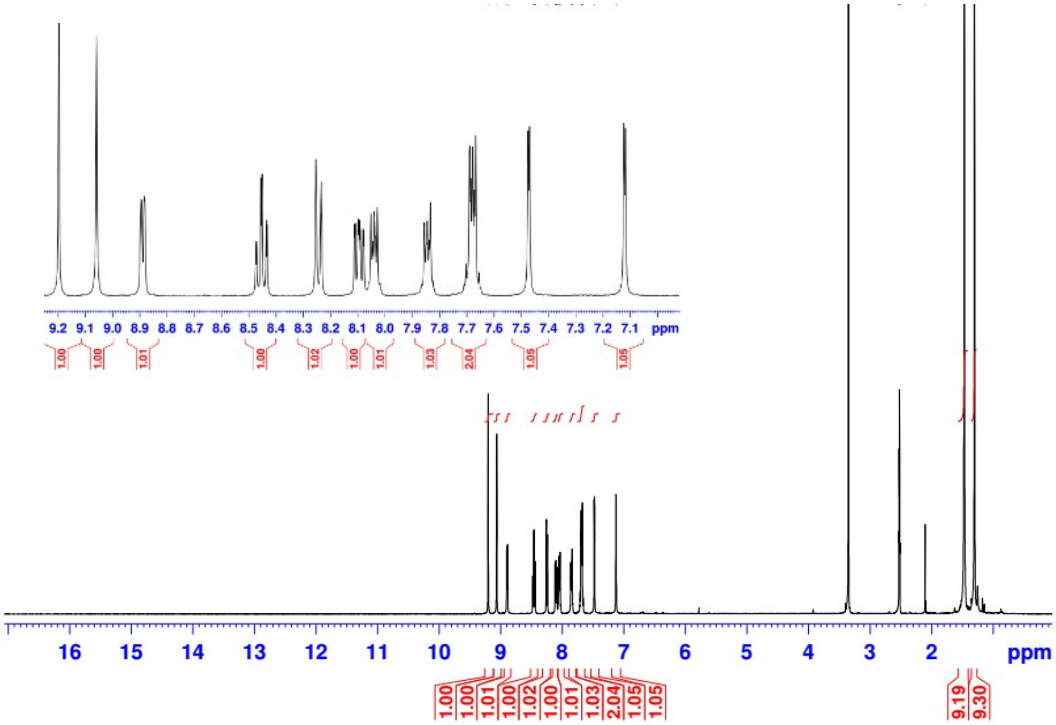


Figure S13. ^{1}H NMR of ZnL^{APIP}Br

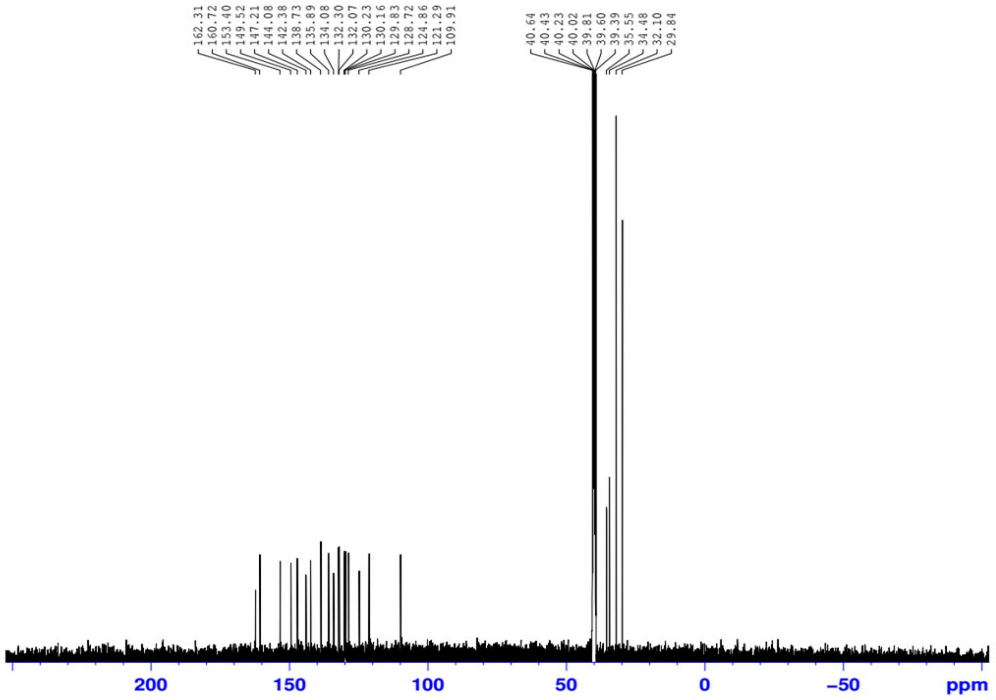
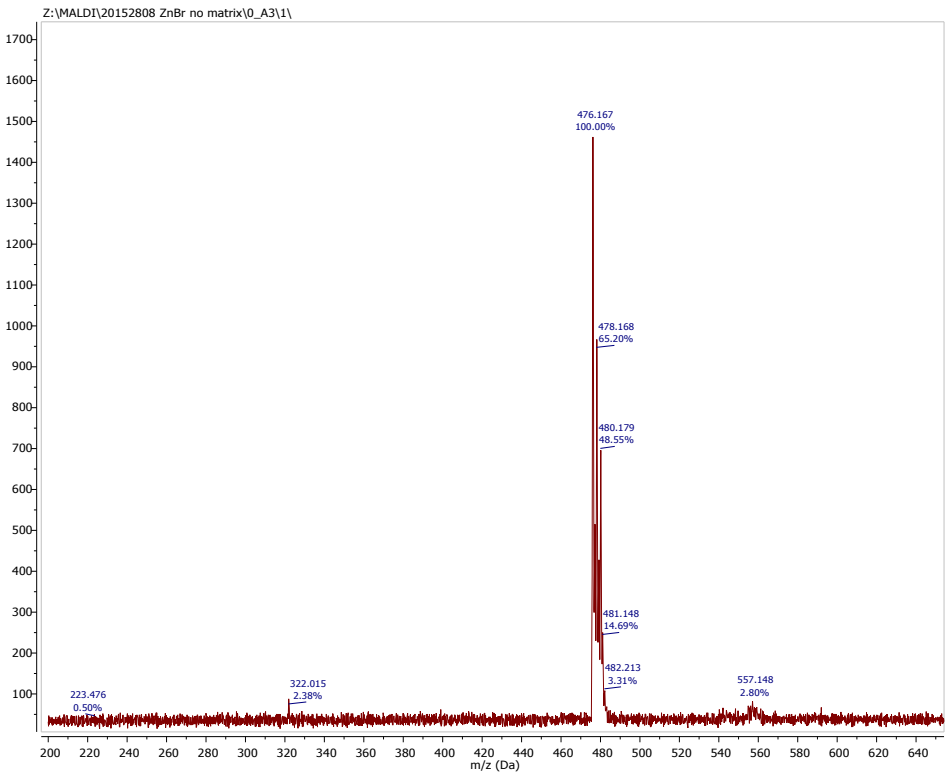
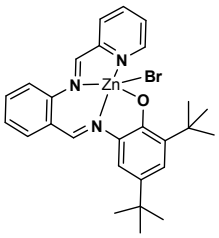


Figure S14. ^{13}C NMR of ZnL^{APIP}Br





$C_{27}H_{30}BrN_3OZn$
Exact Mass: 555.09

Figure S15. MALDI-MS of ZnL^{APIP}Br

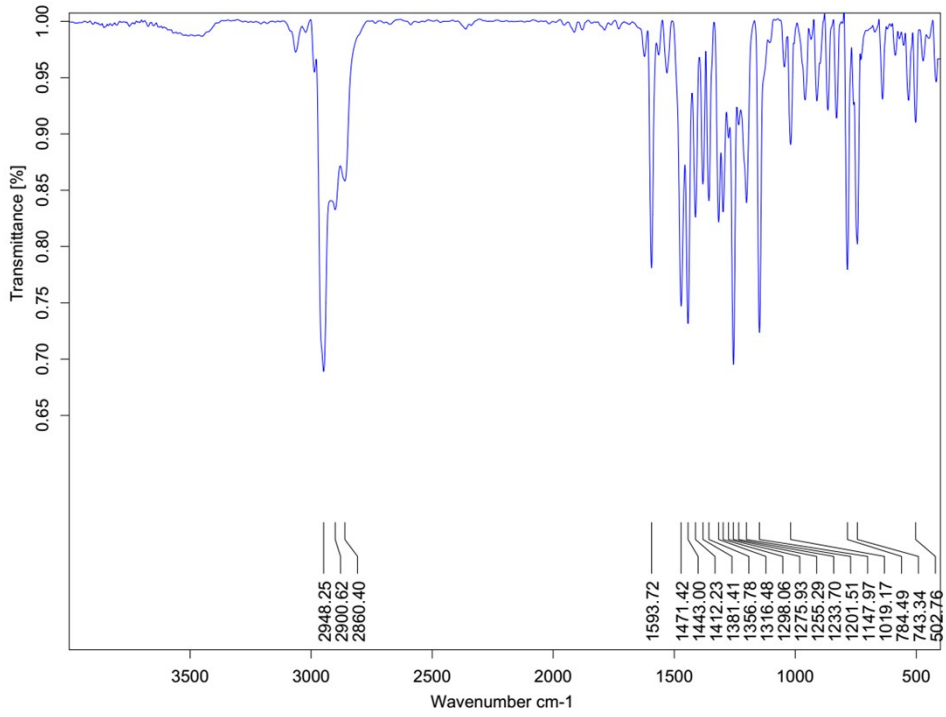


Figure S16. FTIR of ZnL^{APIP}I

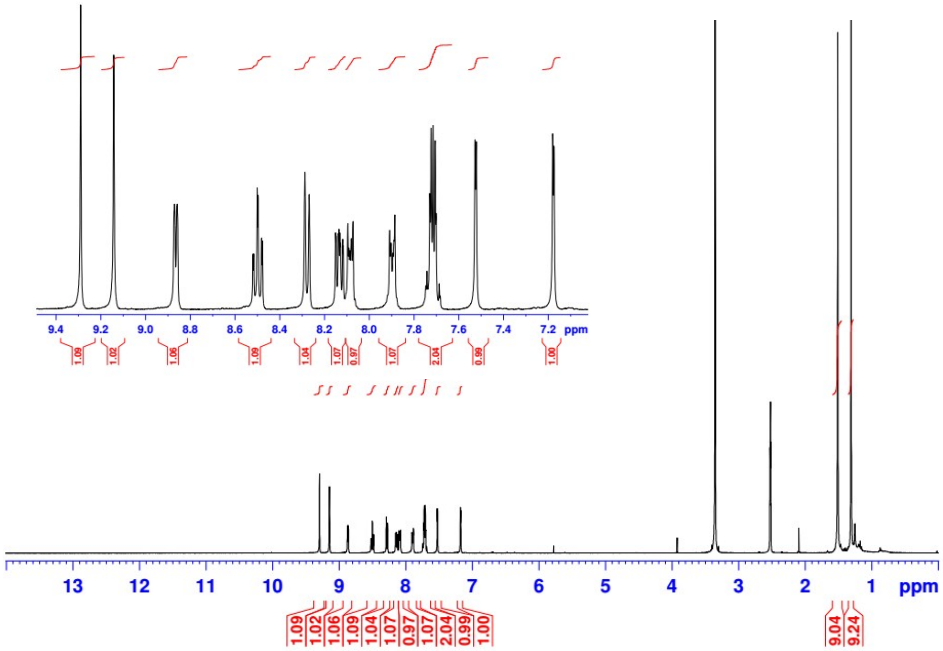


Figure S17. ^{1}H NMR of ZnL^{APIP} I

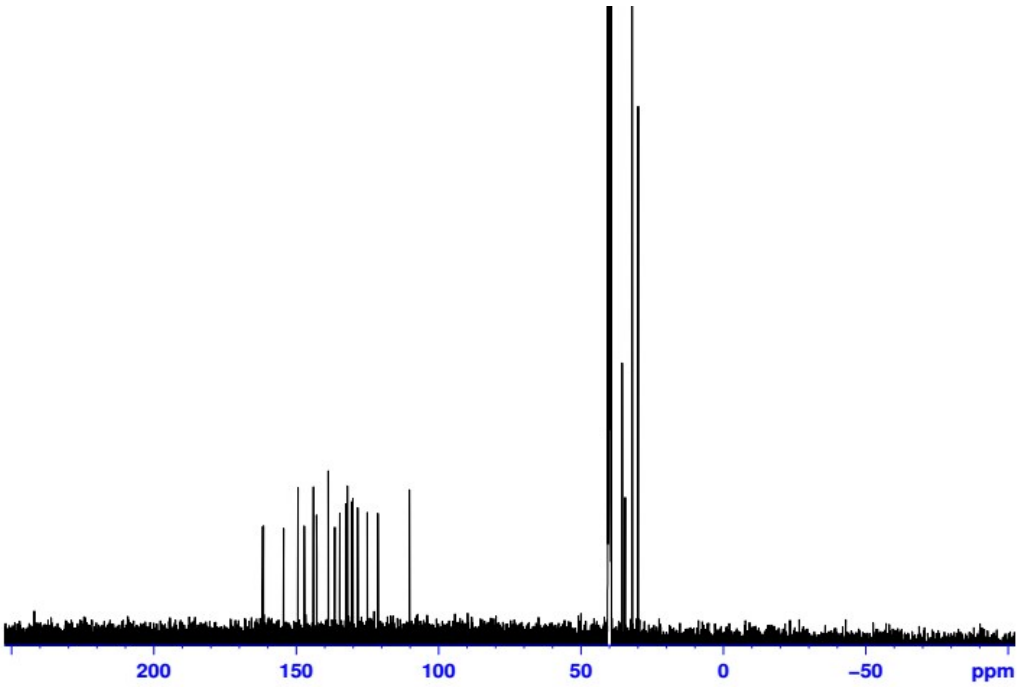
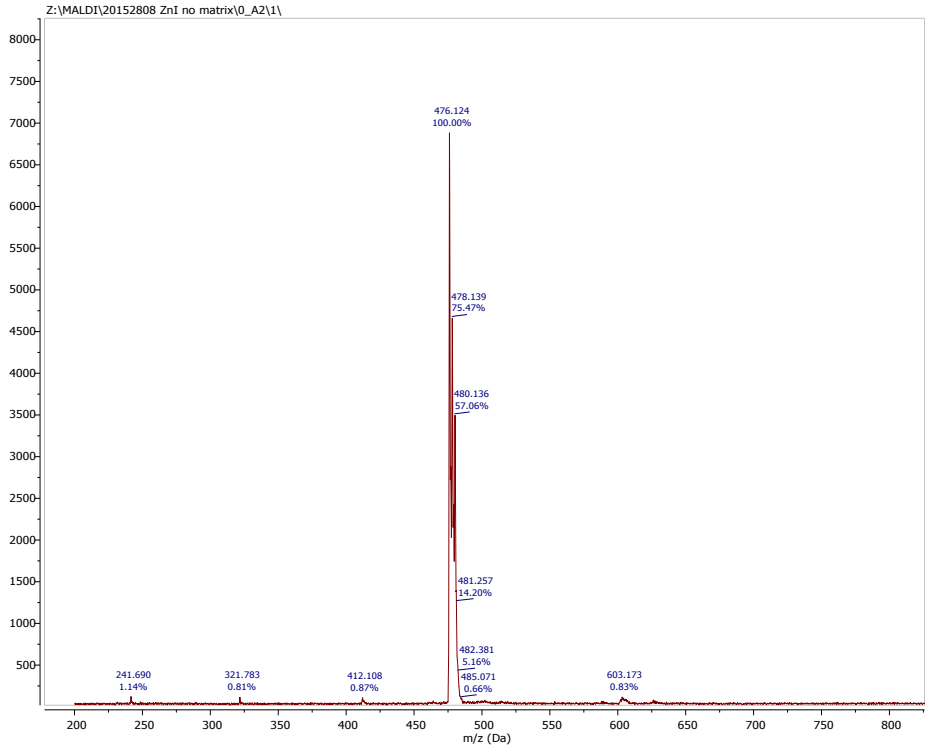
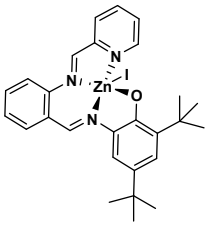


Figure S18. ^{13}C NMR of ZnL^{APIP} I



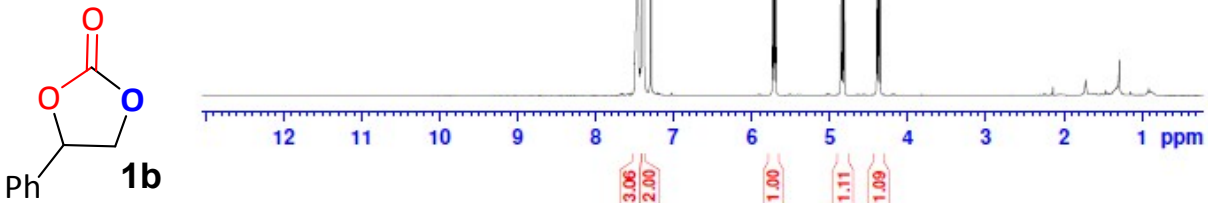


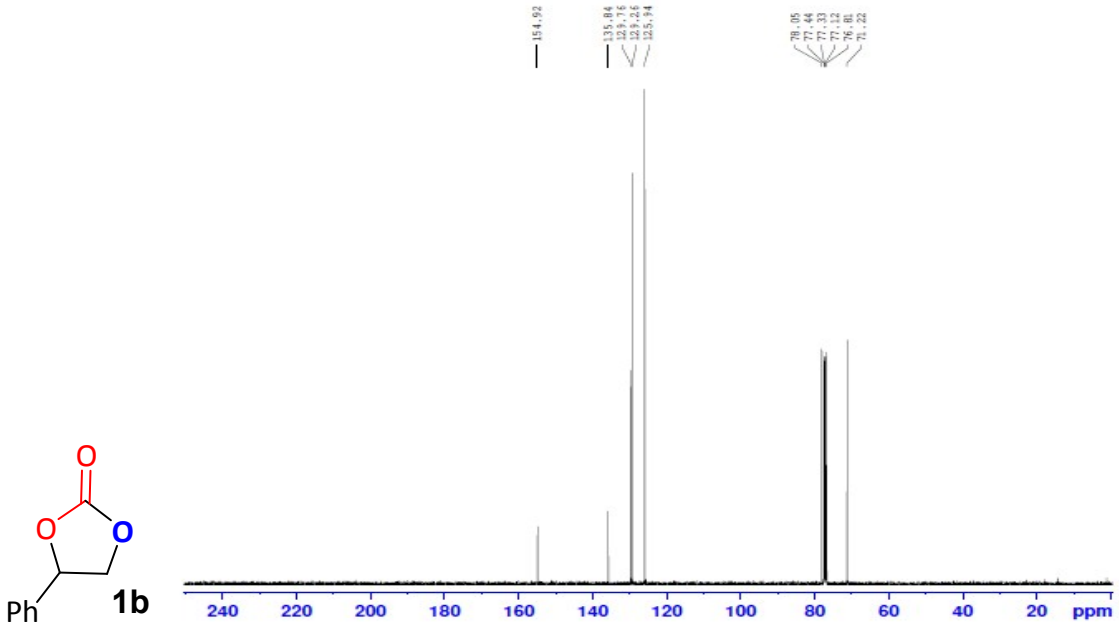
$C_{27}H_{30}IN_3OZn$
Exact Mass: 603.07

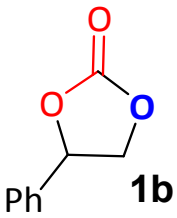
Figure S19. MALDI-MS of ZnL^{APIP} I

Additional IR, ^{1}H and ^{13}C NMR spectra of products

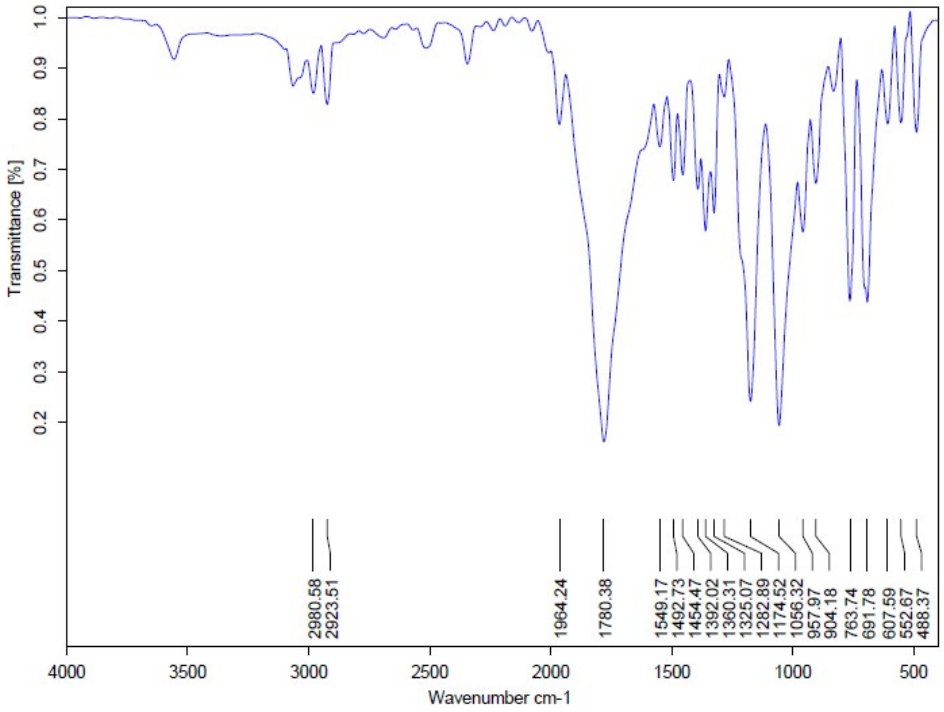
(1b) Styrene carbonate was isolated as a white powder. mp: 60 °C






O
O
O
Ph

1b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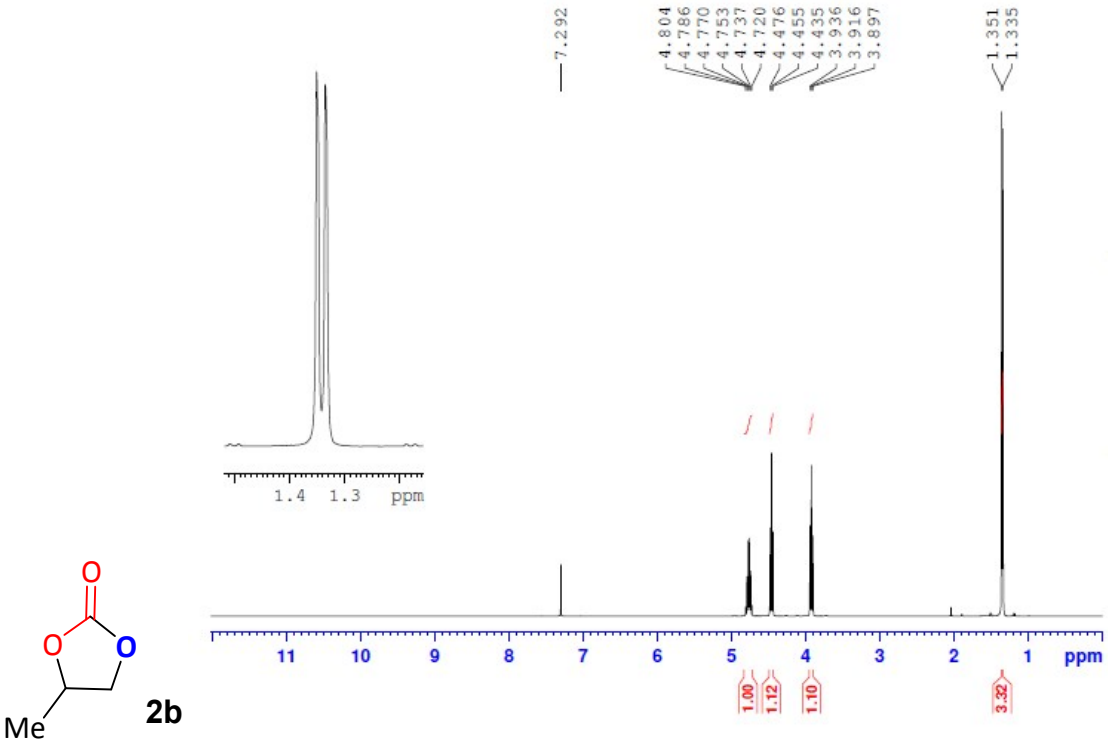
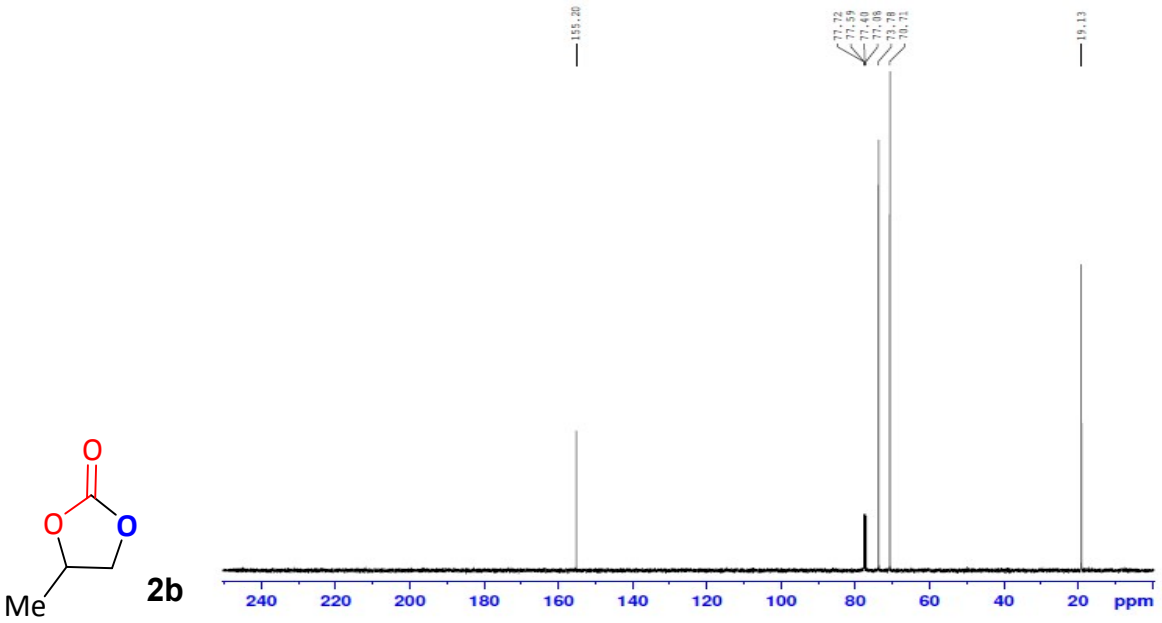
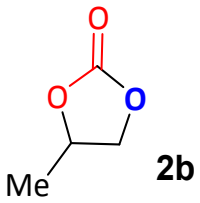
1780.38
1549.17
1492.73
1454.47
1392.02
1360.31
1325.07
1282.89
1174.52
1056.32
957.97
904.18
763.74
691.78
607.59
552.67
488.37
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

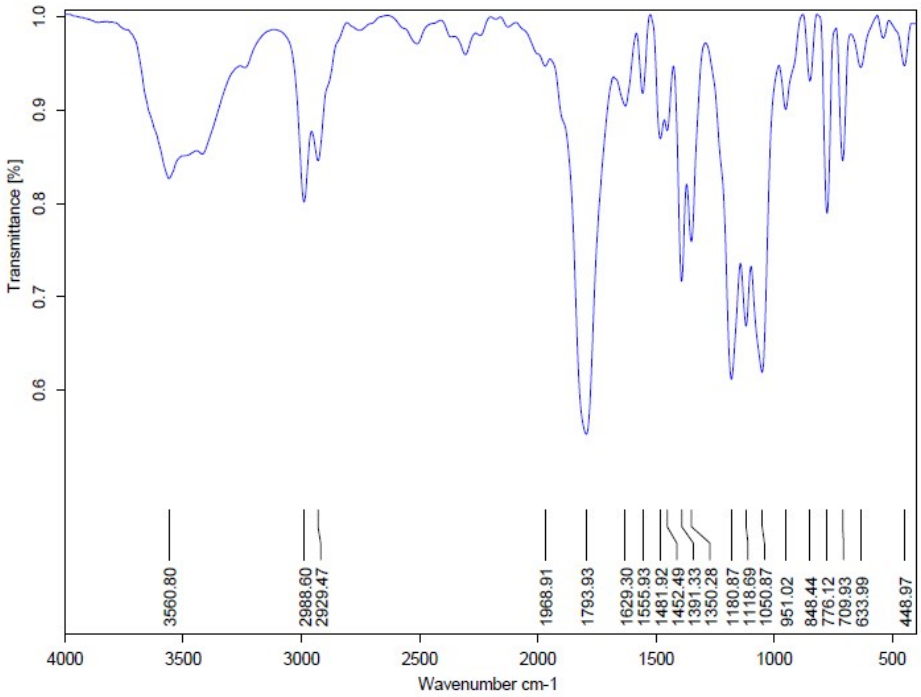
(2b) Propylene carbonate was isolated as colorless oil.






O
O
O
Me

2b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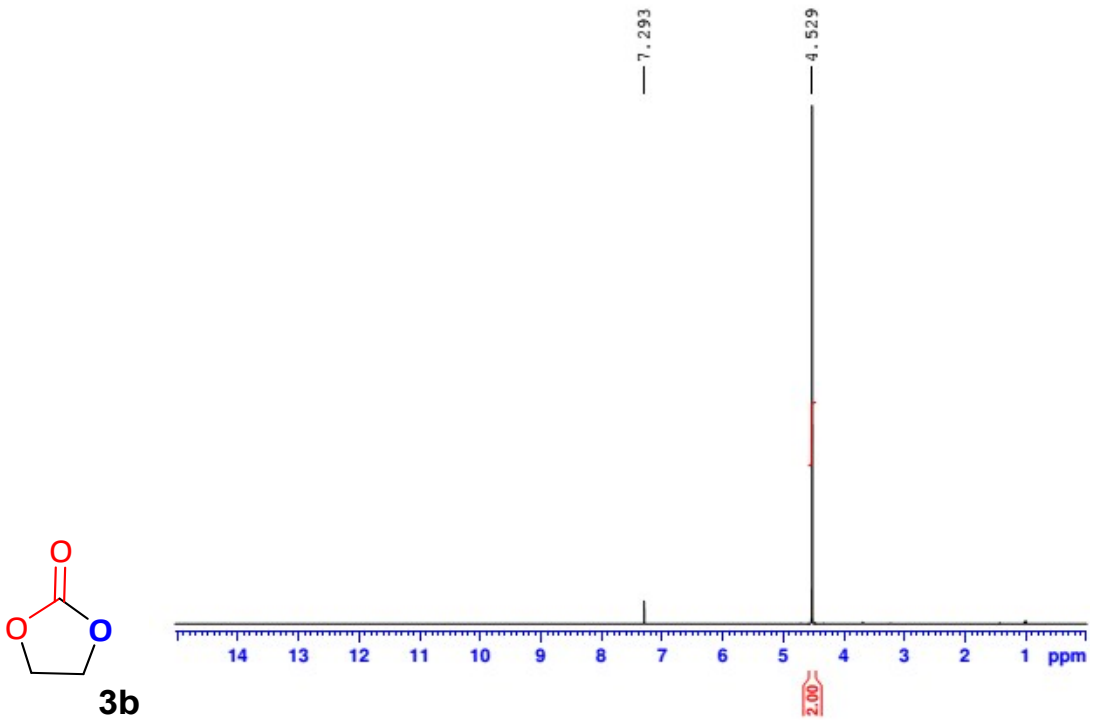
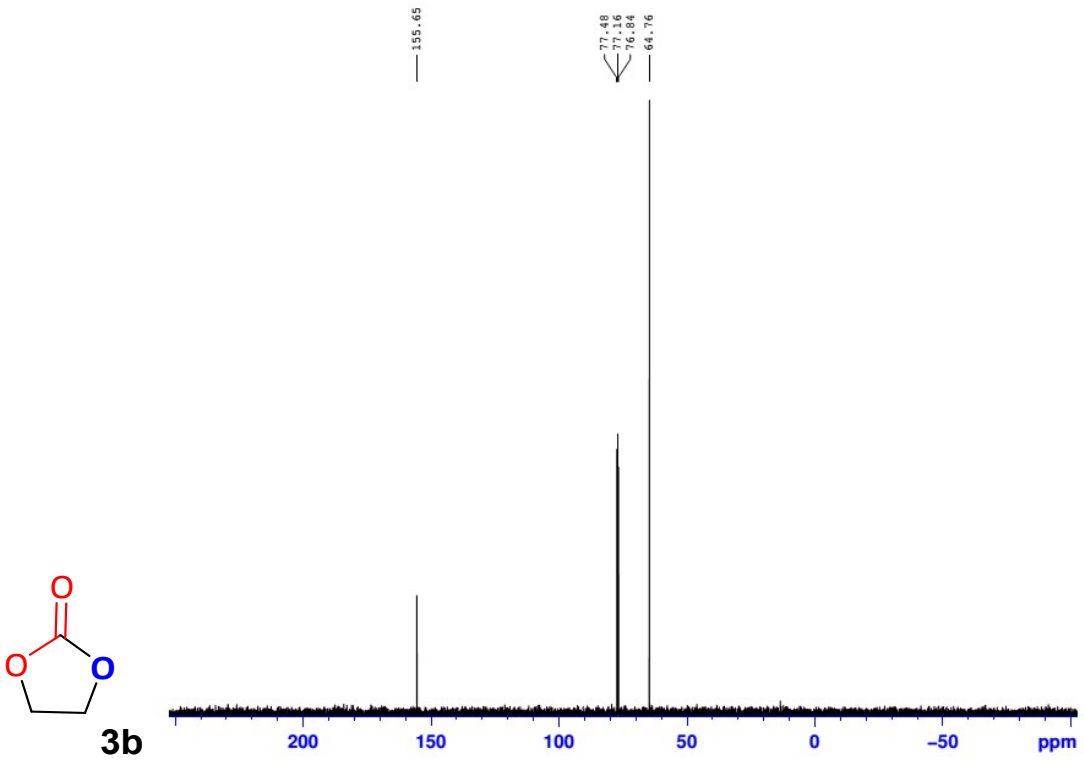
1481.92
1452.49
1391.33
1350.28
1180.87
1118.69
1050.87
951.02
848.44
776.12
709.93
633.99
448.97
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

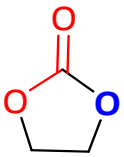
(3b) Ethylene Carbonate was isolated as white powder.



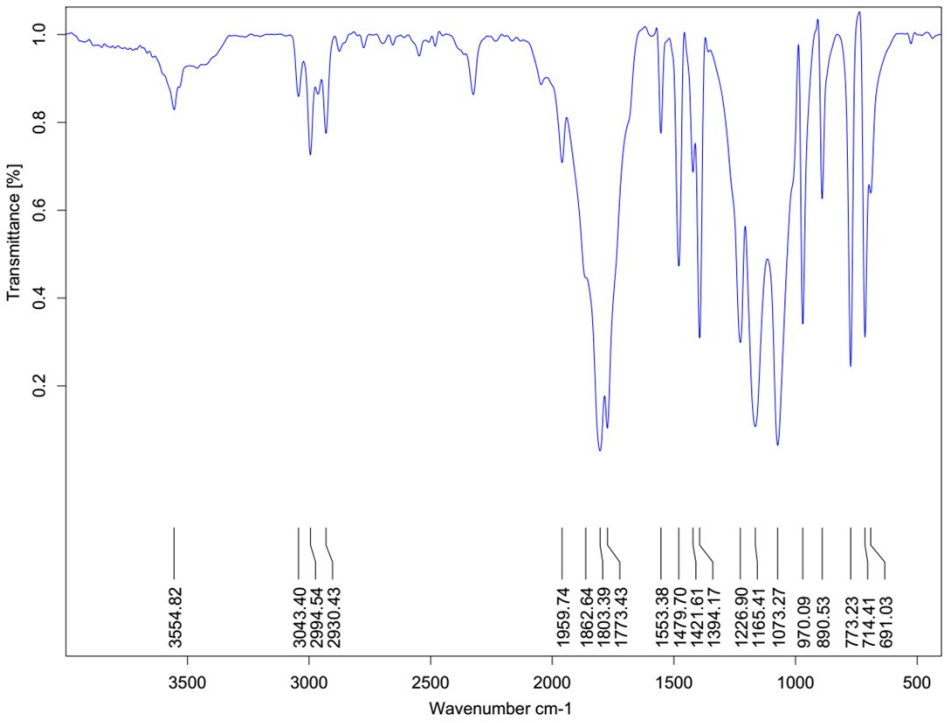
3b



3b



3b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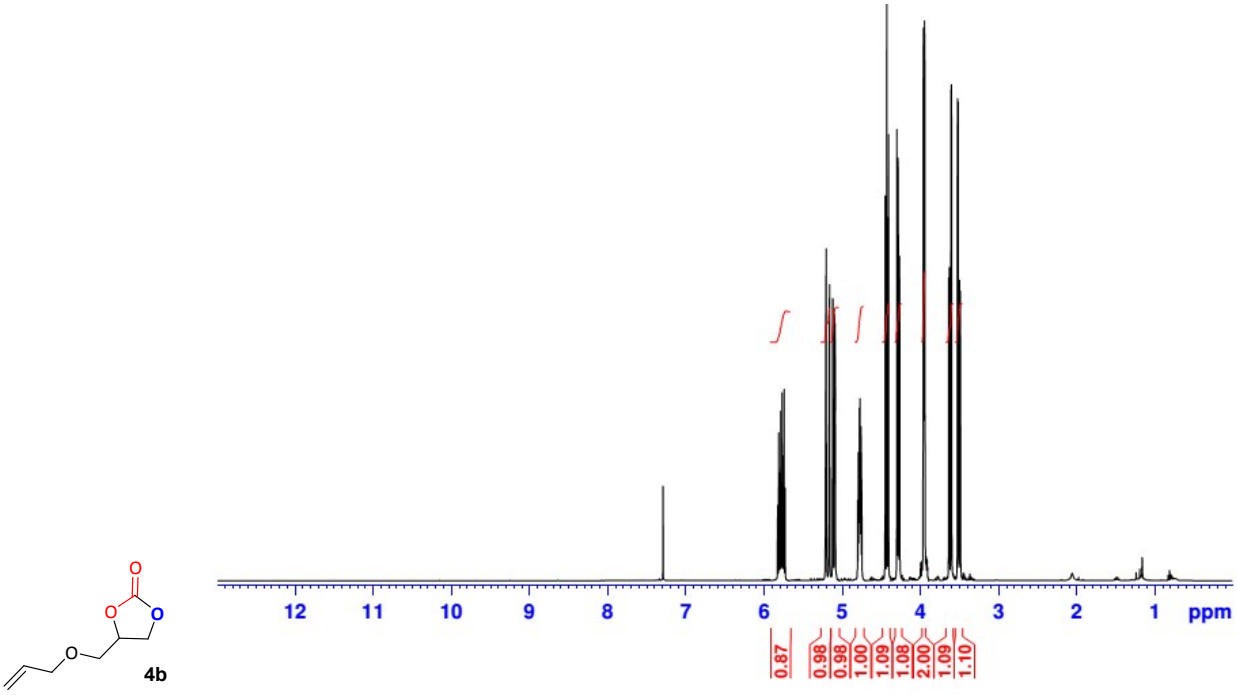
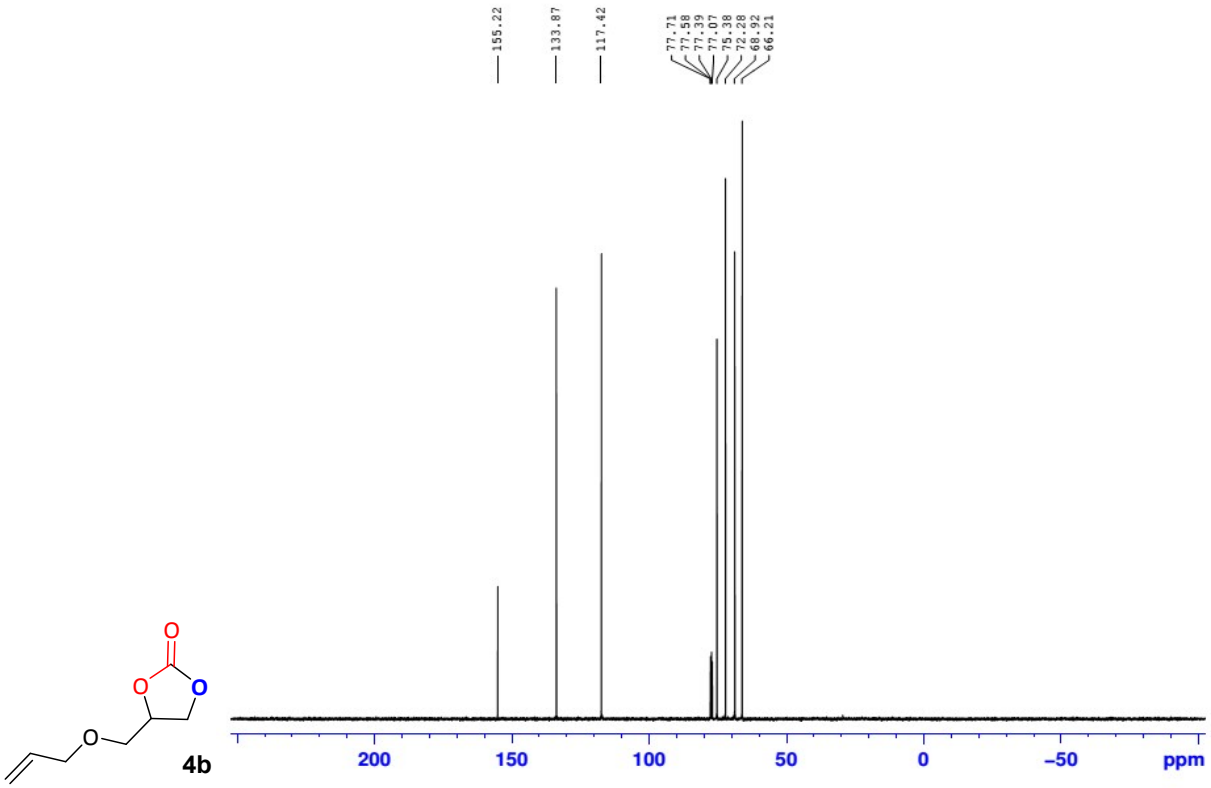
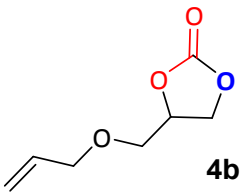
1803.39
1773.43
1553.38
1479.70
1421.61
1394.17
1226.90
1165.41
1073.27
970.09
890.53
773.23
714.41
691.03
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

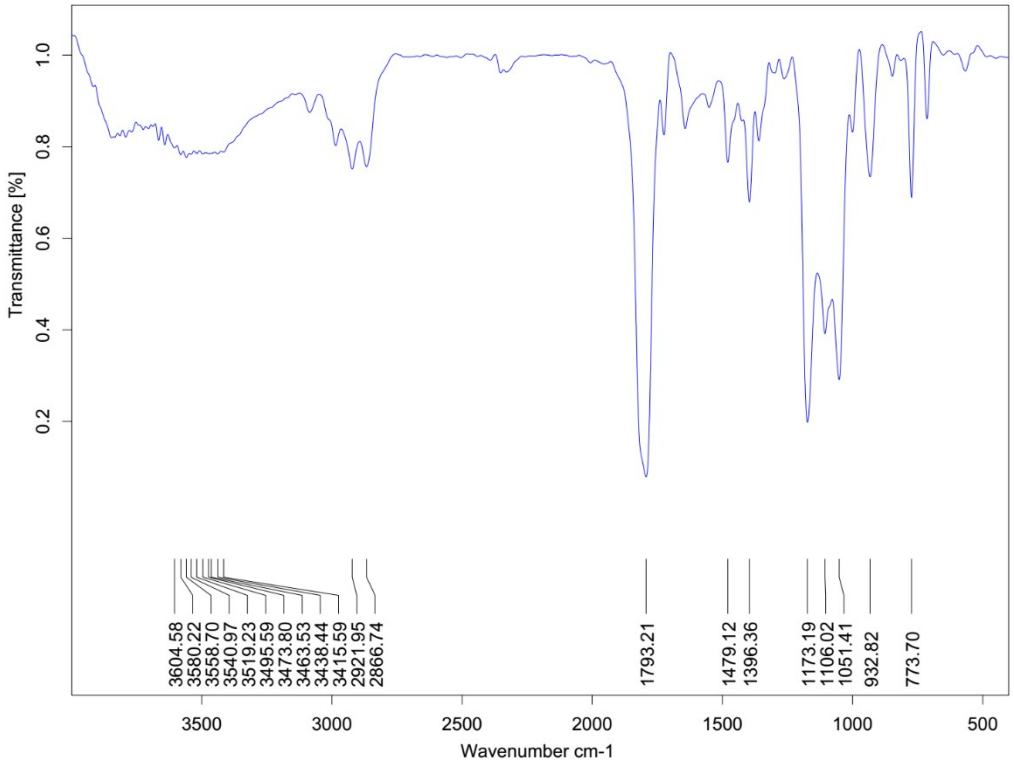
(4b) 4-((allyloxy)methyl)-1,3-dioxolan-2-one was isolated as pale yellow oil.






O
O
O
O

4b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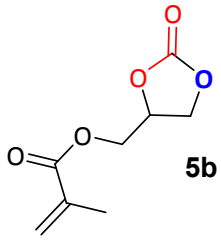
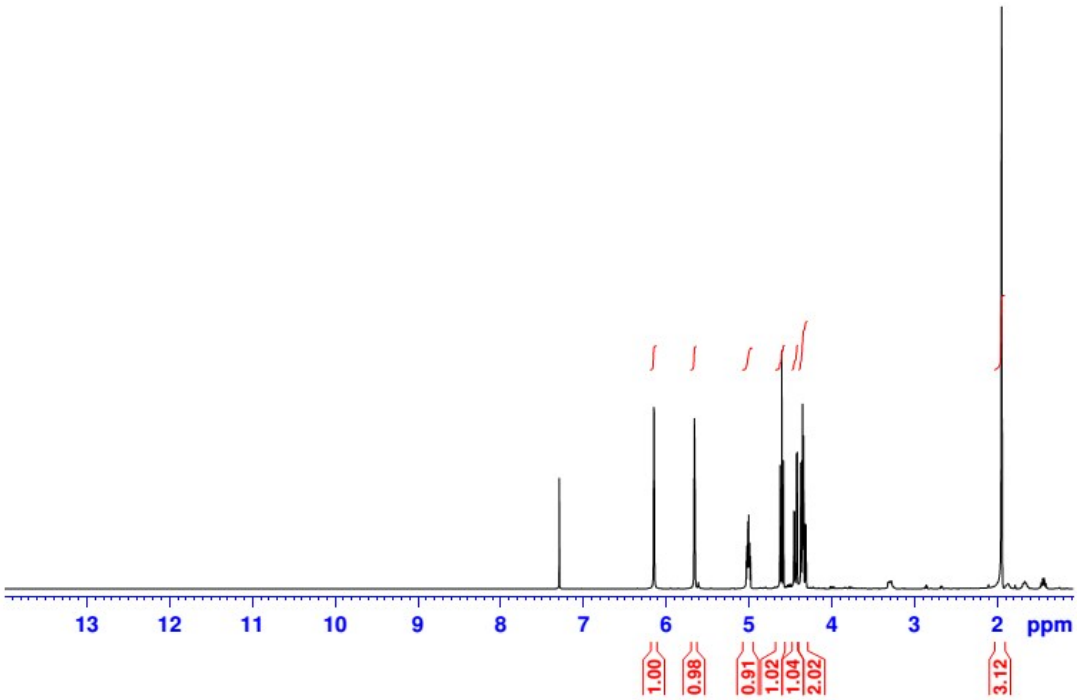
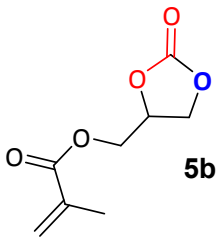
3473.80
3463.53
3438.44
3415.59
2921.95
2866.74
1793.21
1479.12
1396.36
1173.19
1106.02
1051.41
932.82
773.70
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

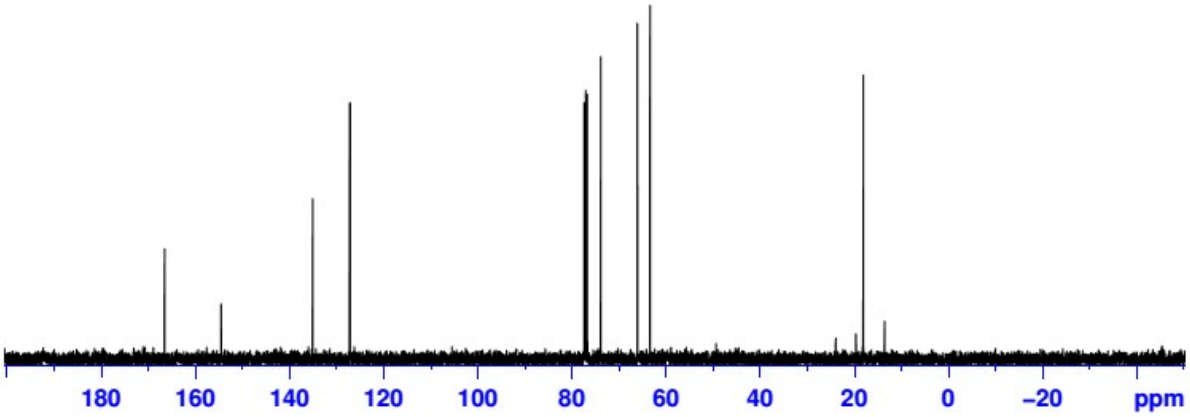
(5b) (2-oxo-1,3-dioxolan-4-yl)methyl methacrylate

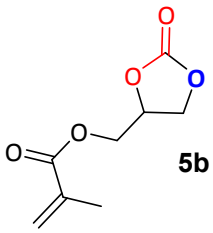




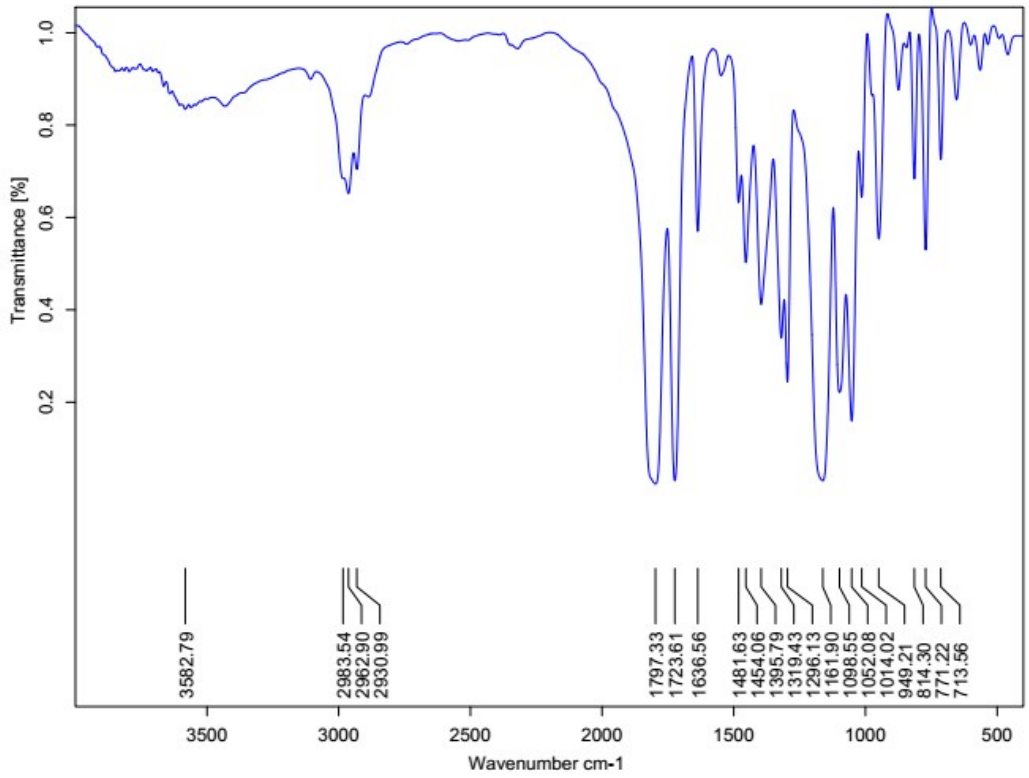


5b




O
O
O
O
O

5b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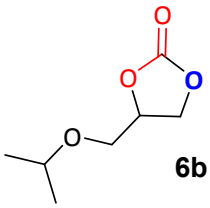
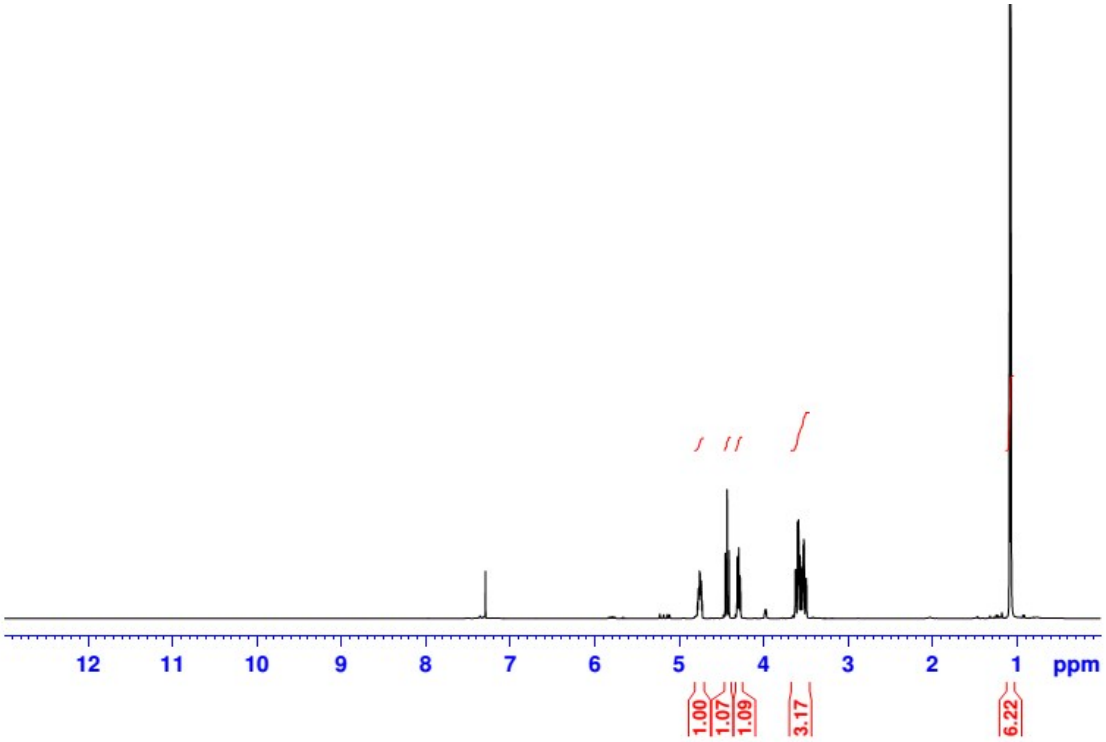
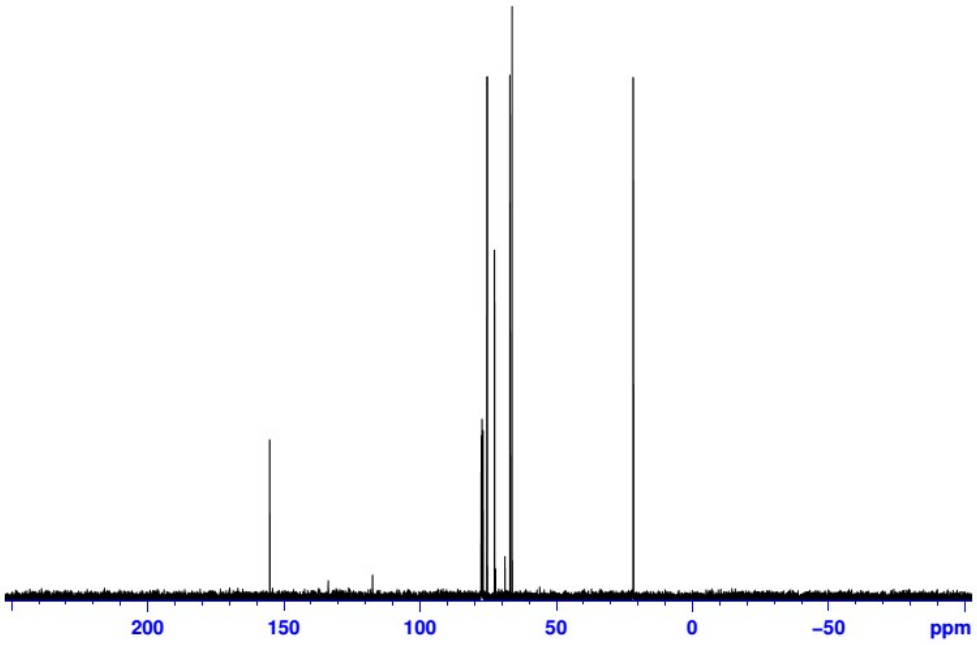
1454.06
1395.79
1319.43
1296.13
1161.90
1098.55
1052.08
1014.02
949.21
814.30
771.22
713.56
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

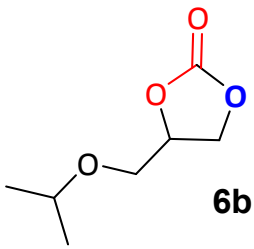
(6b) 4-(isopropoxymethyl)-1,3-dioxolan-2-one



6b







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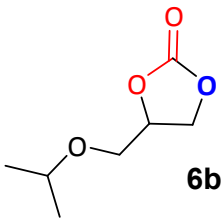

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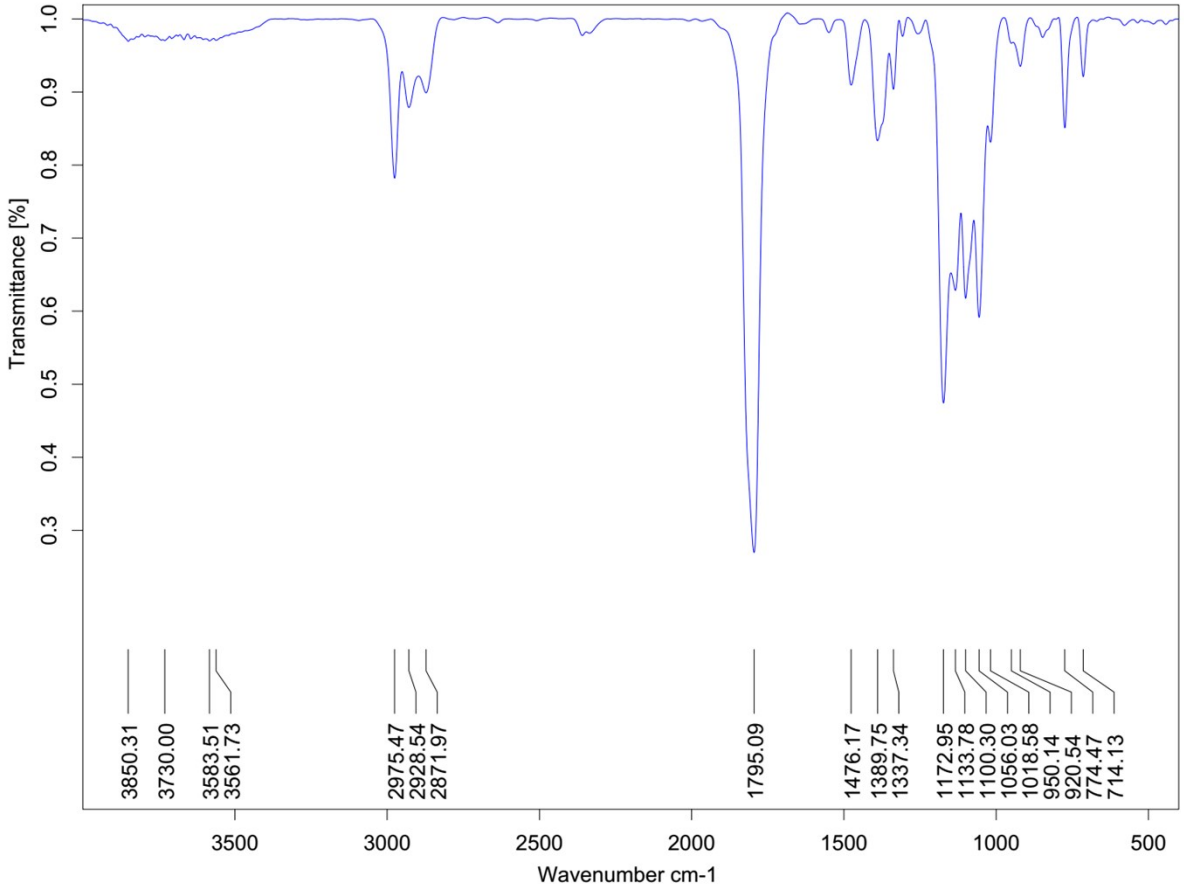
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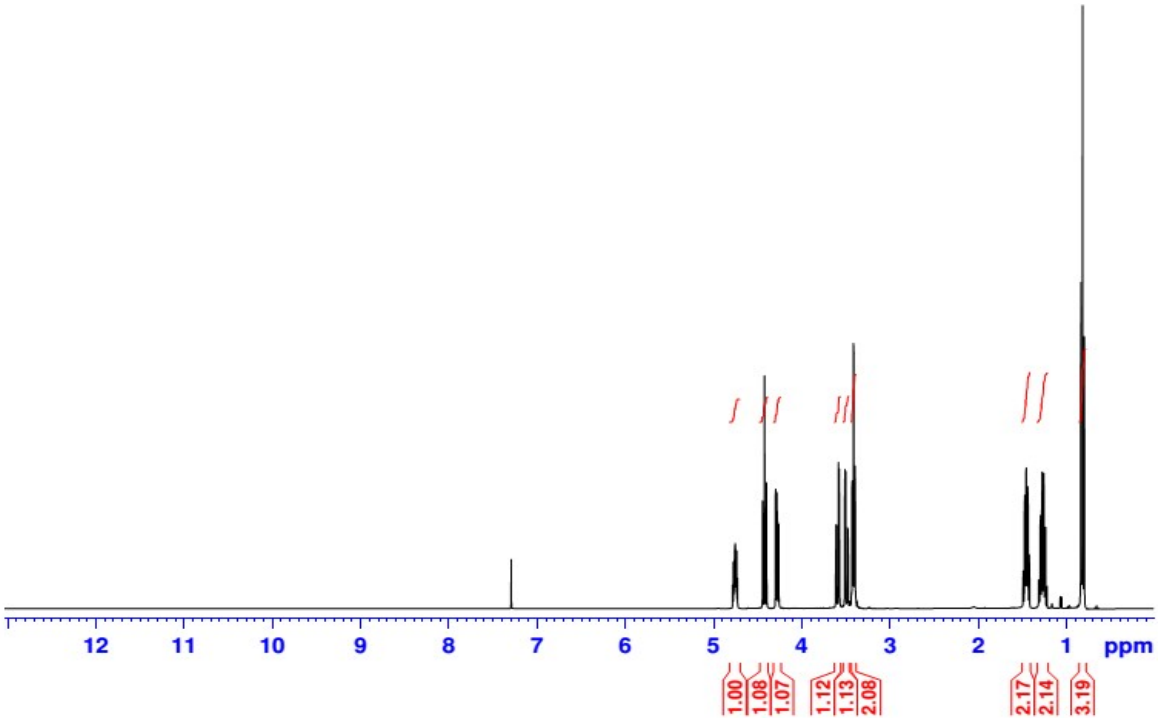
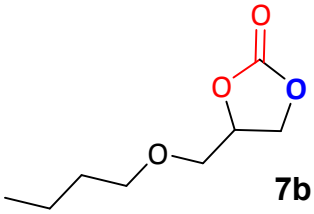
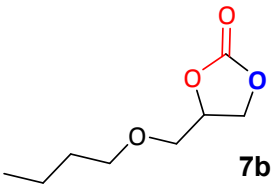
3561.73
2975.47
2928.54
2871.97
1795.09
1476.17
1389.75
1337.34
1172.95
1133.78
1100.30
1056.03
1018.58
950.14
920.54
774.47
714.13
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

(7b) 4-(butoxymethyl)-1,3-dioxolan-2-one

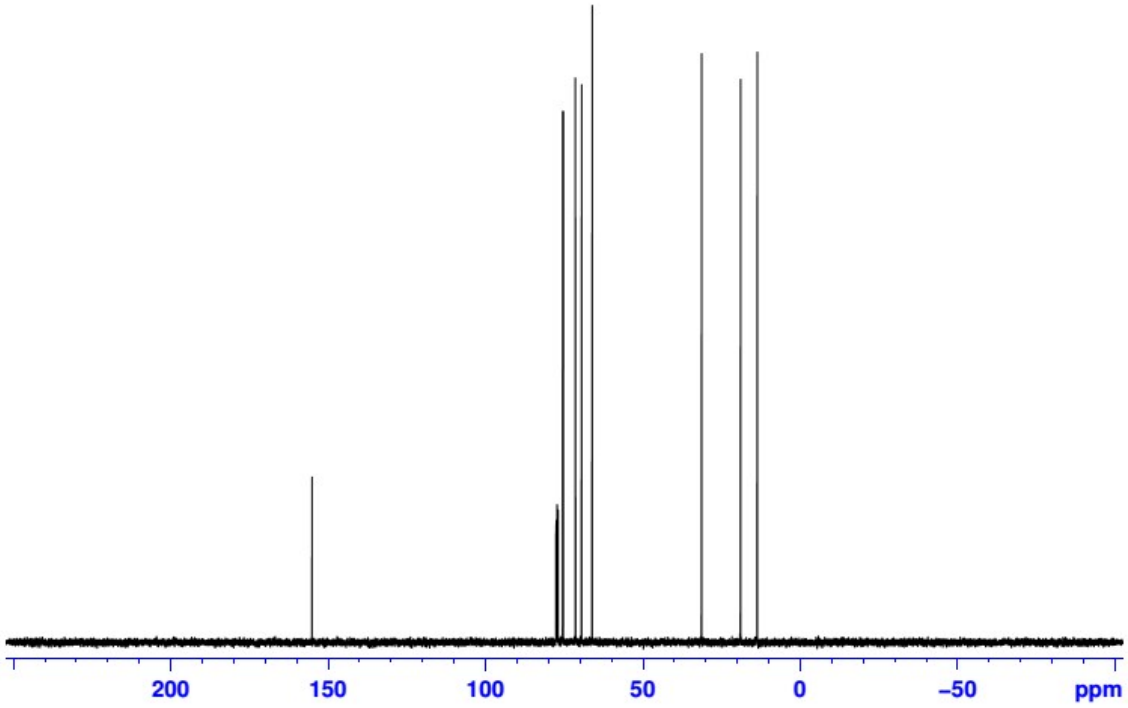


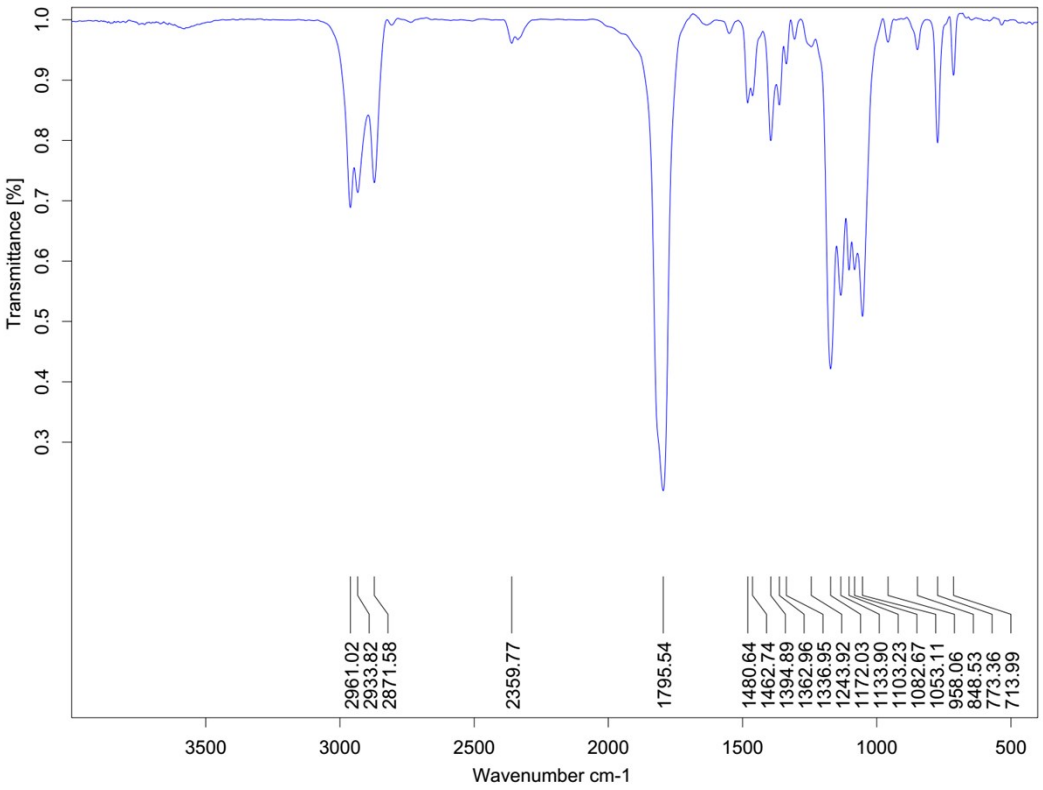


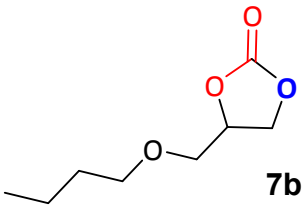
7b



7b

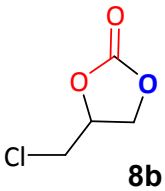



Transmittance [%]
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
2961.02
2933.82
2871.58
2359.77
1795.54
1480.64
1462.74
1394.89
1362.96
1336.95
1243.92
1172.03
1133.90
1103.23
1082.67
1053.11
958.06
848.53
773.36
713.99
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

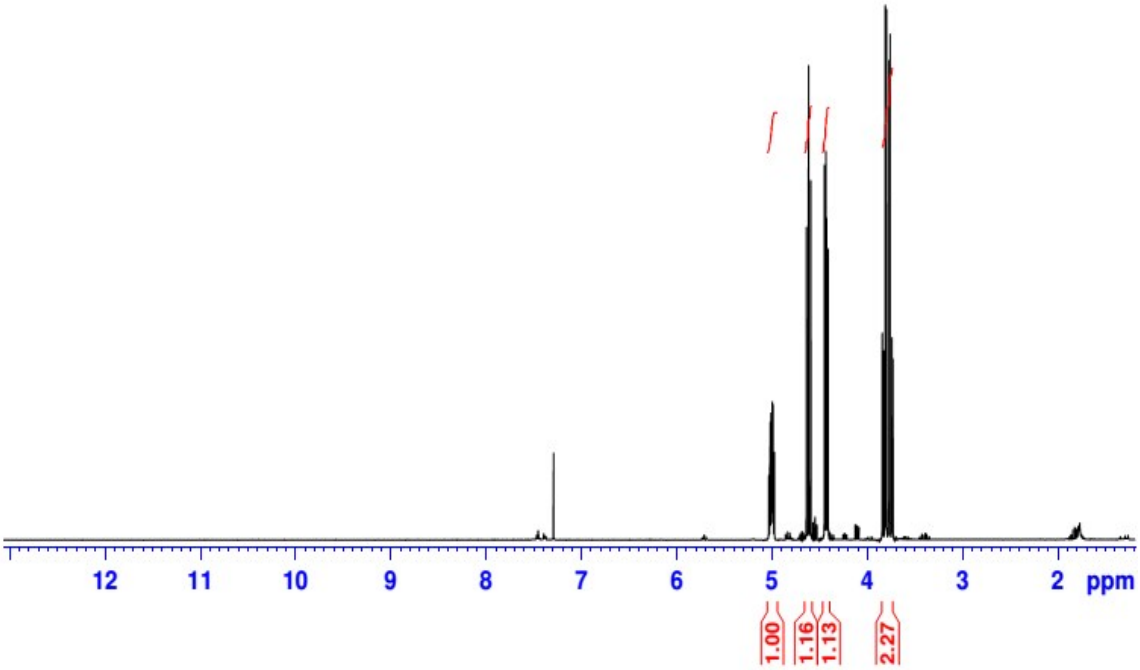

O
O
O
O

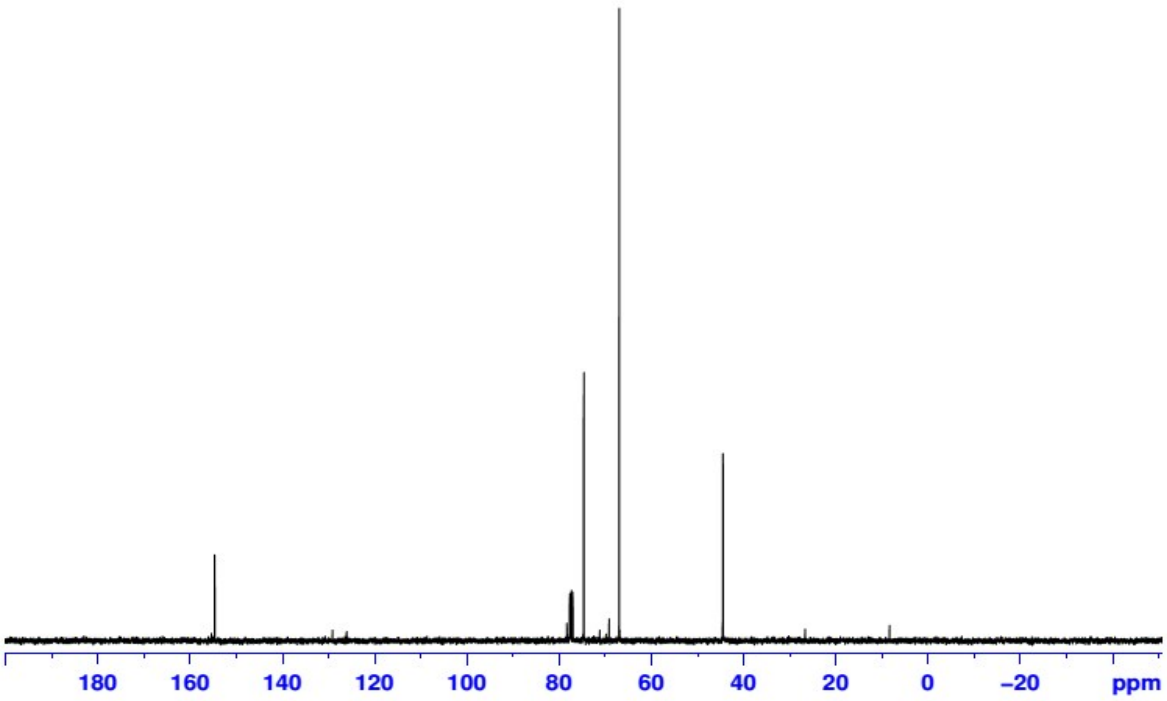
7b

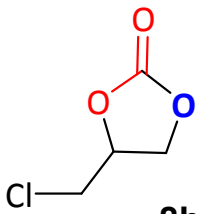
(8b) 4-(chloromethyl)-1,3-dioxolan-2-one



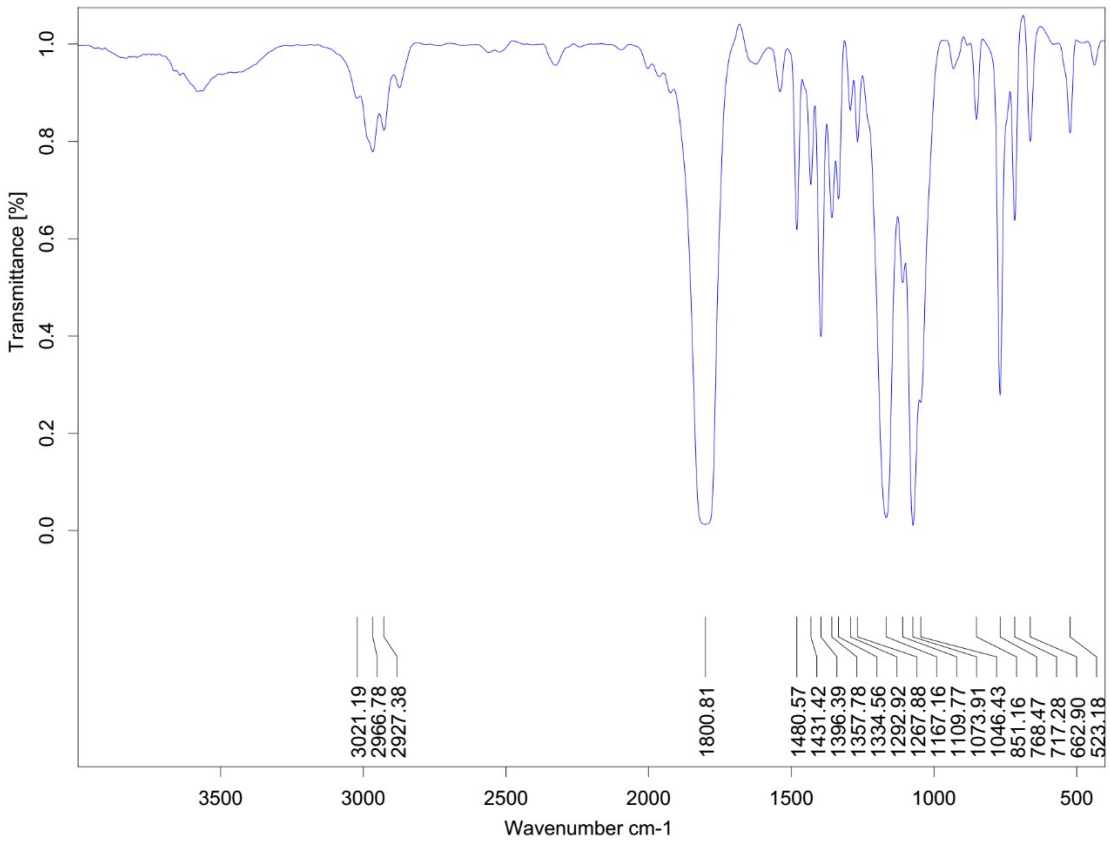
8b

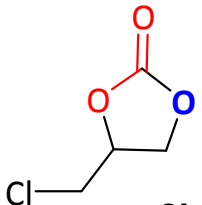






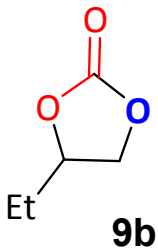
8b


Transmittance [%]
0.0
0.2
0.4
0.6
0.8
1.0
3021.19
2966.78
2927.38
1800.81
1480.57
1431.42
1396.39
1357.78
1334.56
1292.92
1267.88
1167.16
1109.77
1073.91
1046.43
851.16
768.47
717.28
662.90
523.18
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

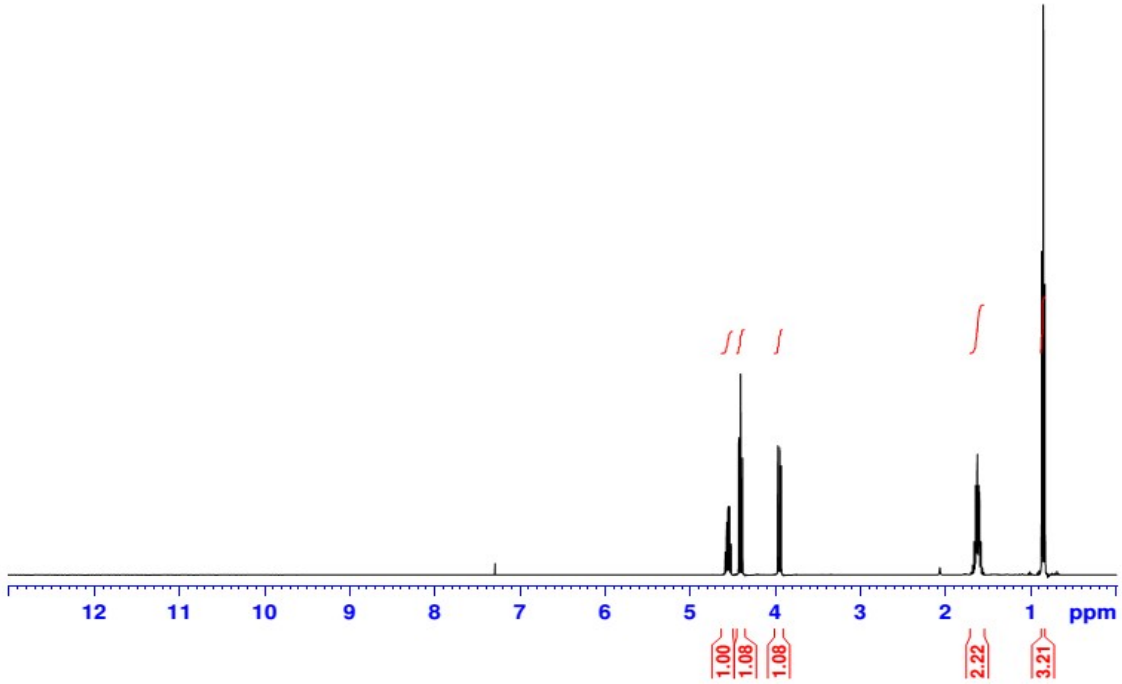

O
O
O
Cl

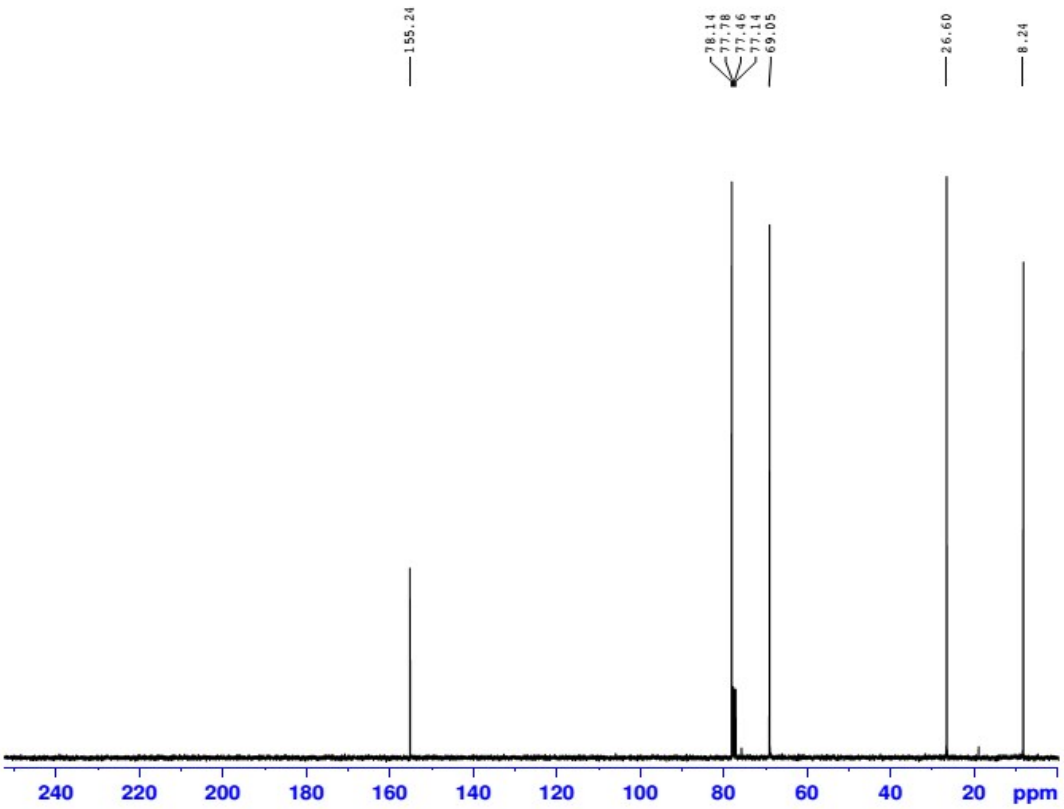
8b

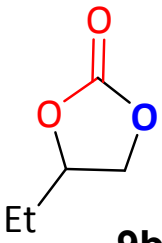
(9b) 4-ethyl-1,3-dioxolan-2-one



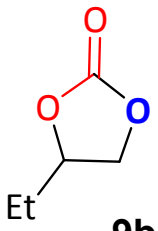
9b



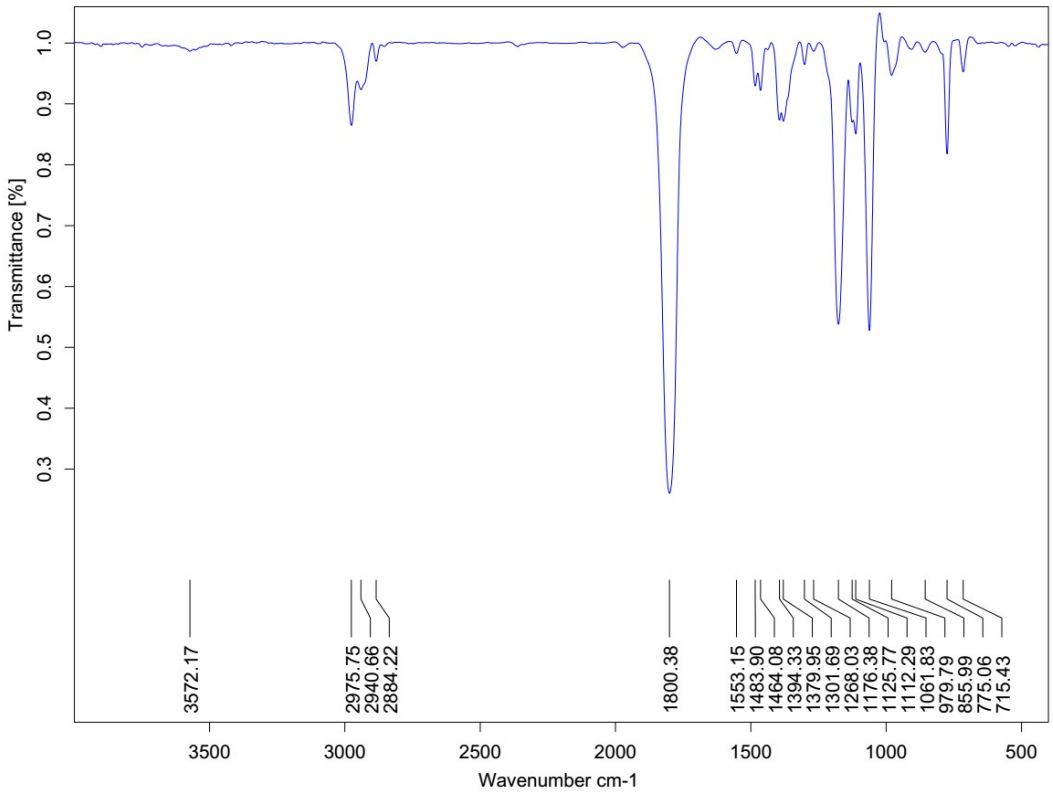

155.24
78.14
77.78
77.46
77.14
69.05
26.60
8.24
240
220
200
180
160
140
120
100
80
60
40
20
ppm


O
O
O
Et

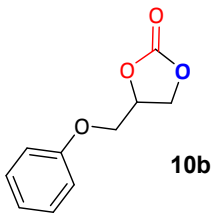
9b


O
O
O
Et

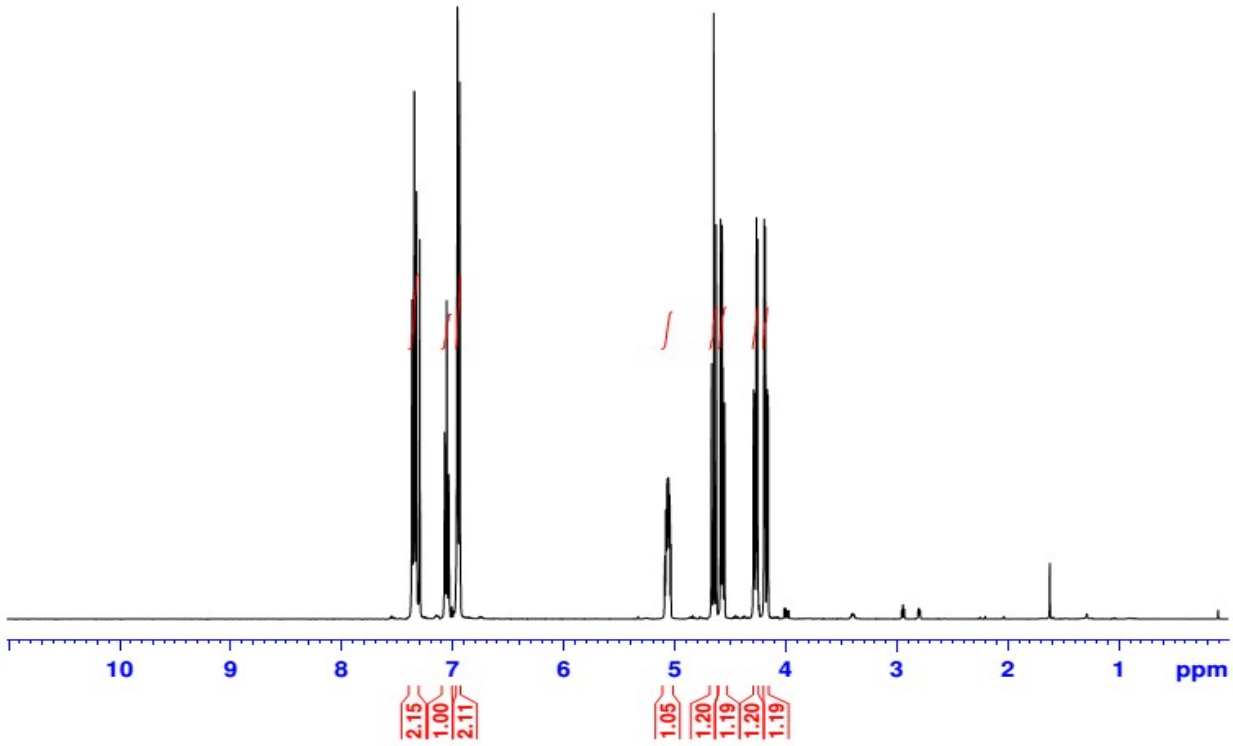
9b

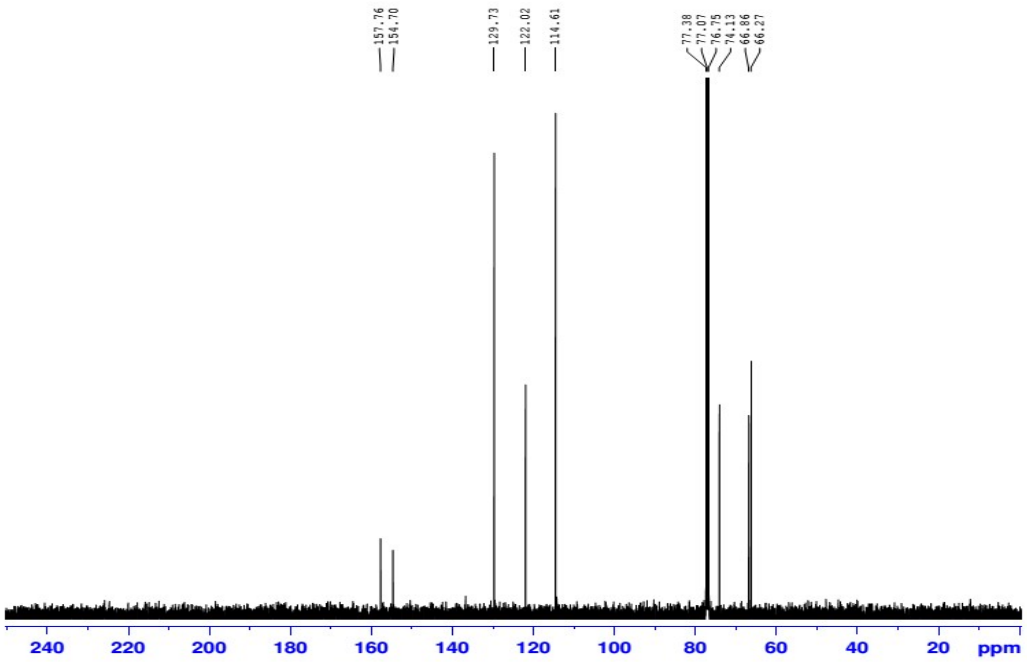

Transmittance [%]
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
3572.17
2975.75
2940.66
2884.22
1800.38
1553.15
1483.90
1464.08
1394.33
1379.95
1301.69
1268.03
1176.38
1125.77
1112.29
1061.83
979.79
855.99
775.06
715.43
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

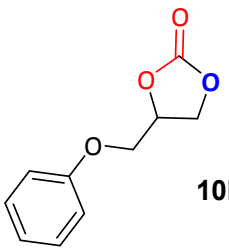
(10b) 4-(phenoxymethyl)-1,3-dioxolan-2-one was isolated as a white powder. mp: 108 °C



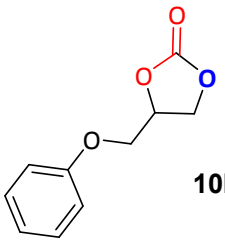
10b



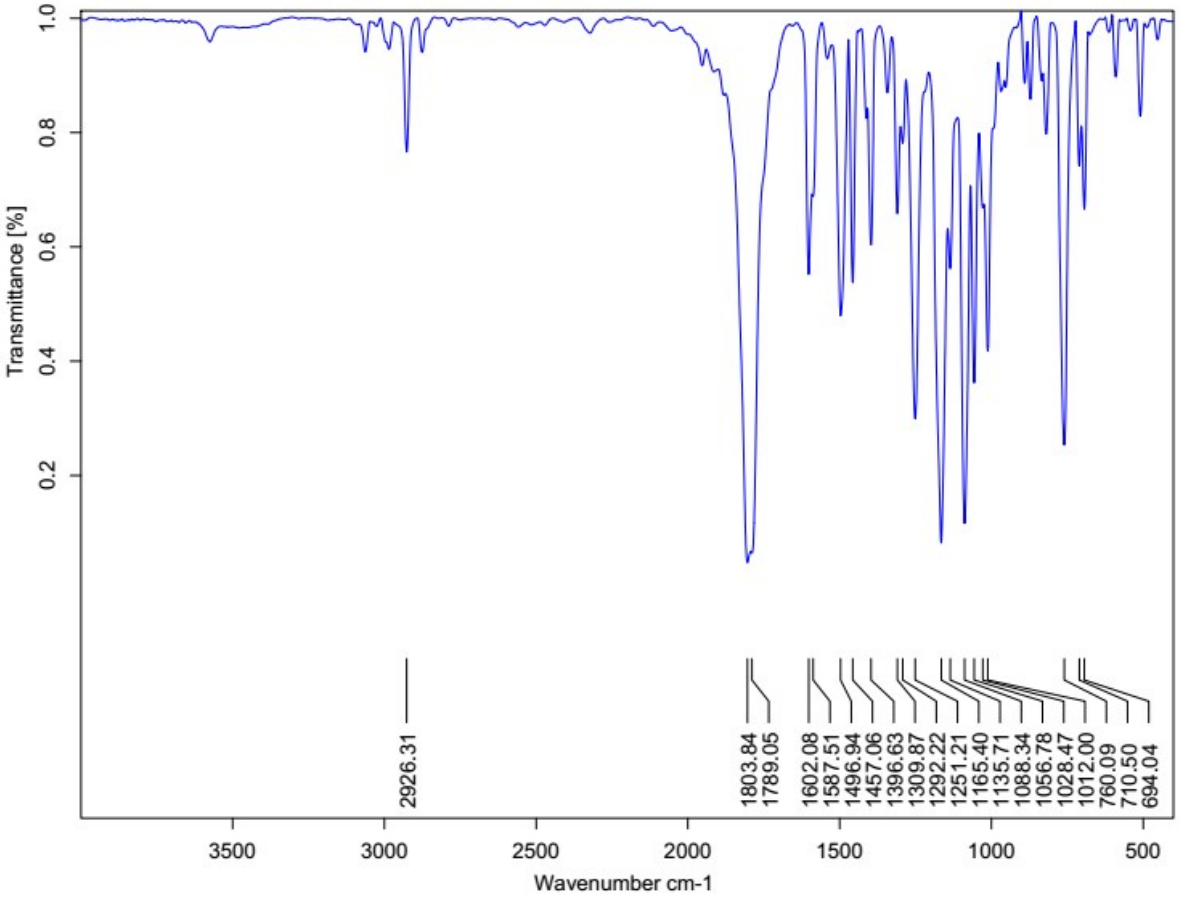

157.76
154.70
129.73
122.02
114.61
77.38
77.07
76.75
74.13
66.86
66.27
240
220
200
180
160
140
120
100
80
60
40
20
ppm



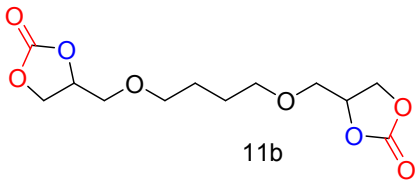
10b



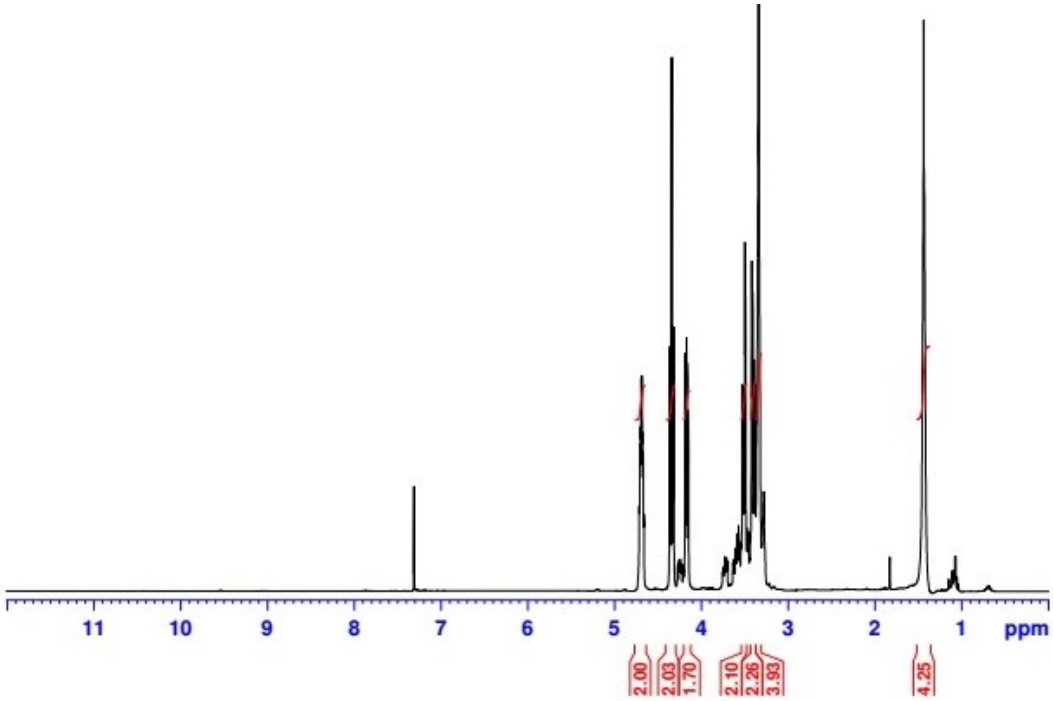
10b

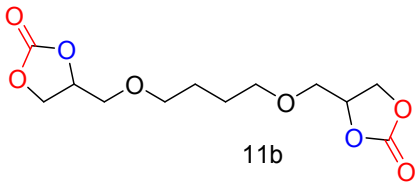

Transmittance [%]
1.0
0.8
0.6
0.4
0.2
2926.31
1803.84
1789.05
1602.08
1587.51
1496.94
1457.06
1396.63
1309.87
1292.22
1251.21
1165.40
1135.71
1088.34
1056.78
1028.47
1012.00
760.09
710.50
694.04
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

(11b) 4,4'-((butane-1,4-diylbis(oxy))bis(methylene))bis(1,3-dioxolan-2-one)

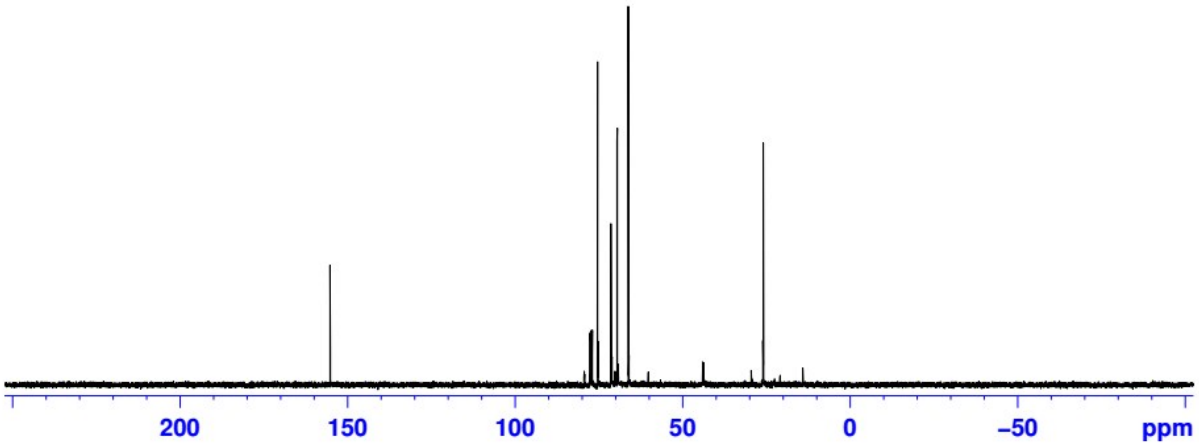


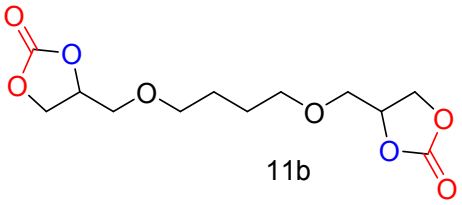
11b



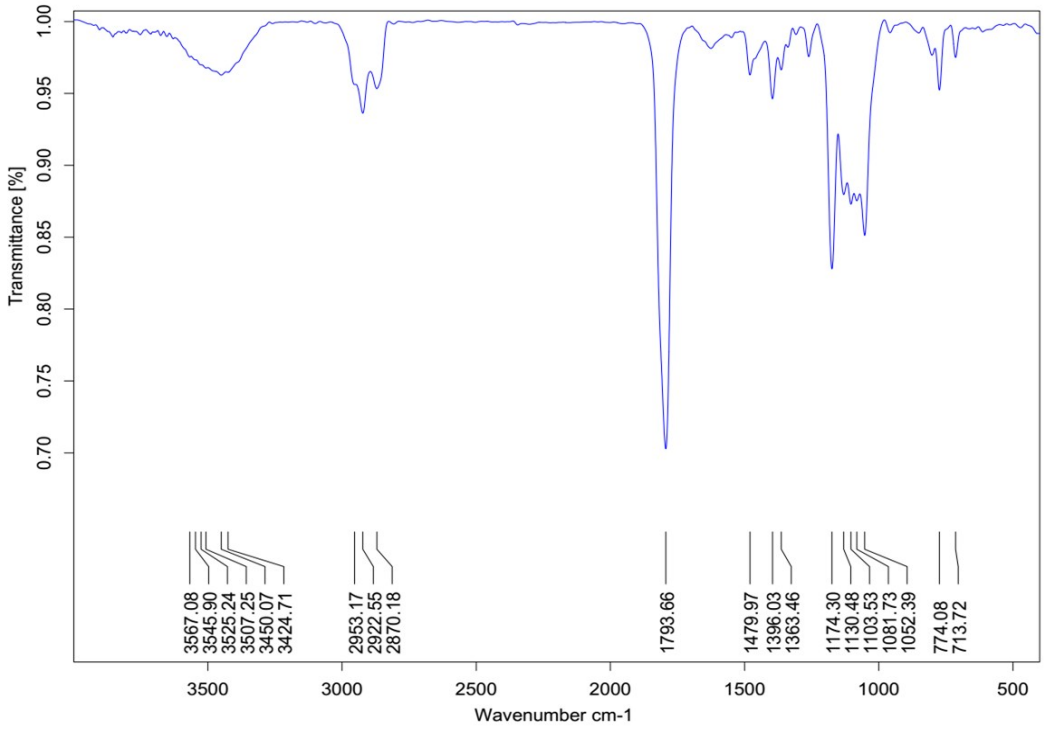


11b

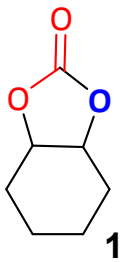




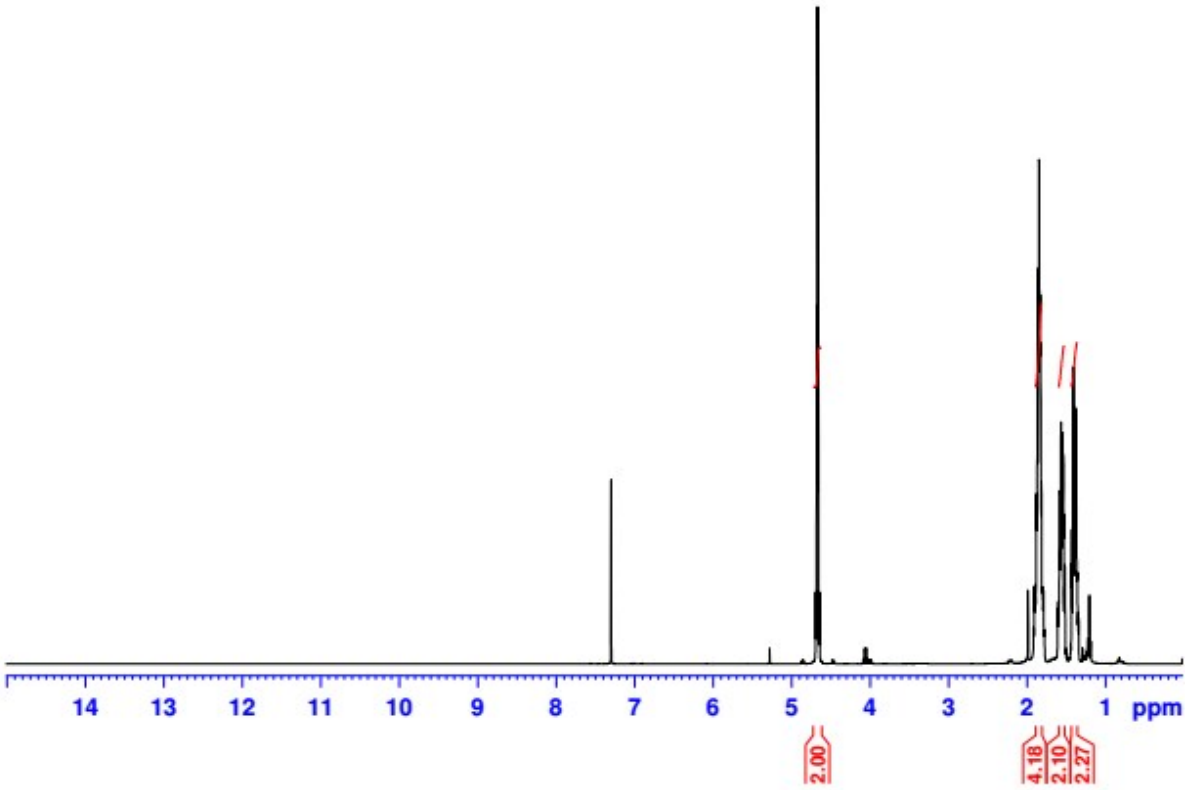
11b

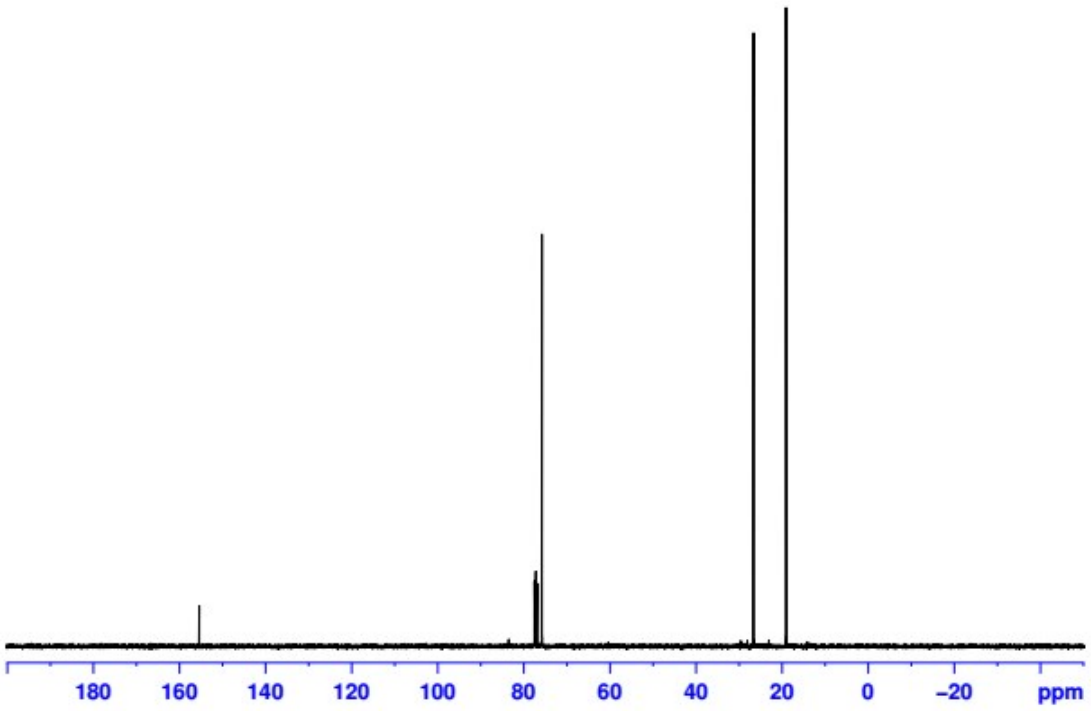

Transmittance [%]
1.00
0.95
0.90
0.85
0.80
0.75
0.70
3567.08
3545.90
3525.24
3507.25
3450.07
3424.71
2953.17
2922.55
2870.18
1793.66
1479.97
1396.03
1363.46
1174.30
1130.48
1103.53
1081.73
1052.39
774.08
713.72
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

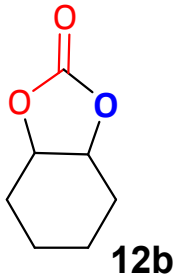
(12b) hexahydrobenzo[d][1,3]dioxol-2-one



12b







12b

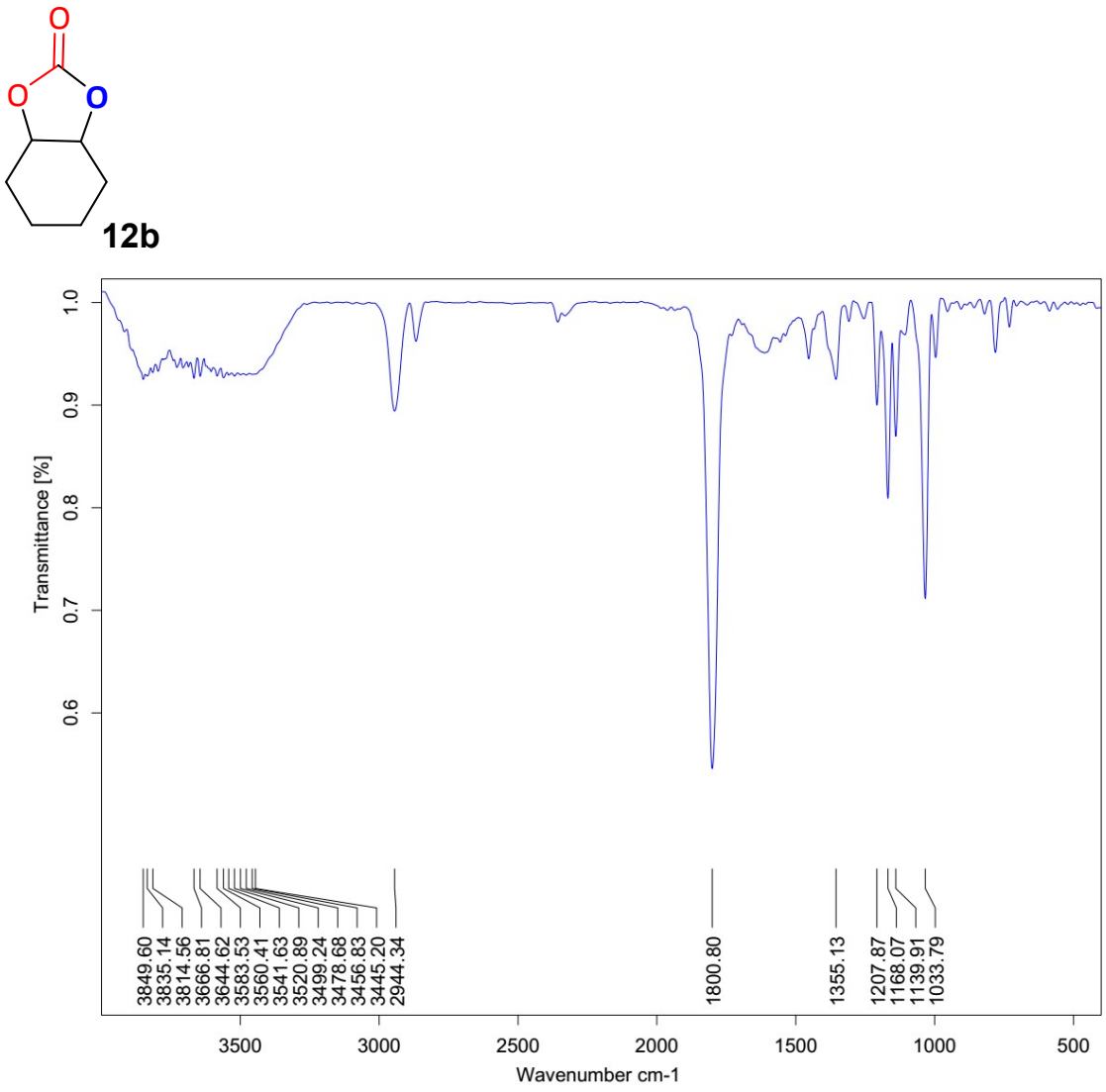


Figure S20. ^{1}H NMR, ^{13}C NMR and FTIR-spectra of cyclic carbonates