Supporting Information

Aluminum complexes derived from a hexadentate salen-type Schiff base: synthesis, structure, and catalysis for cyclic carbonate synthesis

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Table S1. Crystallographic data for complexes 1-3

Compound	4×**1**·C_4H_8O·0.5C_6H_{14}	2×**2**·7C_4H_8O	**3**·2C_4H_8O
Formula	$C_{187}H_{243}Al_4N_8O_{17}$	$C_{118}H_{170}Al_2N_4O_{15}$	$C_{52}H_{71}AlN_2O_6$
*F*w	2982.81	1938.54	847.09
T(K)	223(2)	223(2)	223(2)
crystal system	Triclinic,	Triclinic,	Triclinic,
space group	P -1	P -1	P -1
a (Å)	16.3401(8)	23.4700(2)	14.0607(8)
b (Å)	16.3450(7)	14.8888(11)	14.0829(7)
c (Å)	18.5163(8)	33.8790(3)	14.2229(7)
α (deg)	92.953(4)	90	110.791(5)
β (deg)	111.549(4)	103.819(8)	104.661(5)
γ (deg)	92.257(4)	90	99.320(4)
V (Å^3)	4584.5(4)	11496.0(17)	2446.5(2)
Z	1	4	2
D_{calcd} (g cm^{-3})	1.080	1.120	1.150
μ (mm^{-1})	0.086	0.087	0.090
F (000)	1609	4208	916
θ_{max} (deg)	26.37	25.50	26.37
Reflections collected	49887	26816	23790
unique reflections	18737	10676	9997
parameters refined	981	590	496
final *R* [I > 2.0σ(I)]	R1 = 0.0896, wR2 = 0.2430	R1 = 0.1189, wR2 = 0.3314	R1 = 0.0875, wR2 = 0.2400
R indices (all data)	R1 = 0.1697, wR2 = 0.2857	R1 = 0.1816, wR2 = 0.3750	R1 = 0.1349, wR2 = 0.2831
GOF on F^2	1.022	1.184	1.049

IR data of complexes **2-5**:

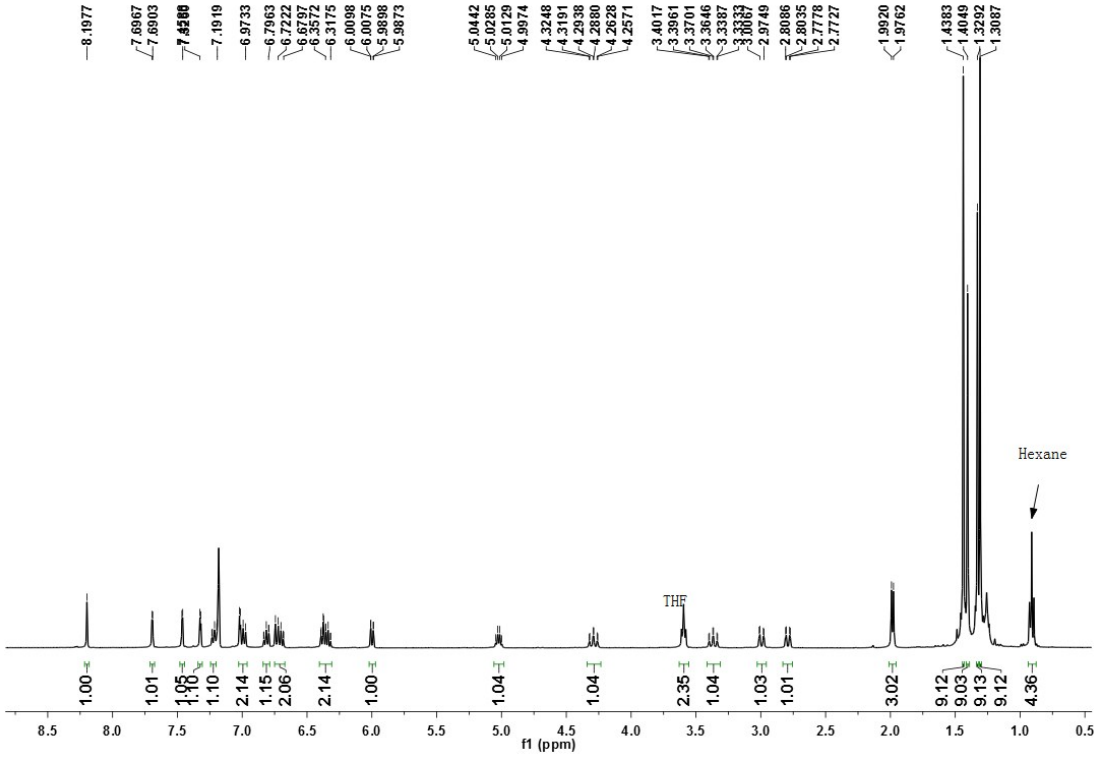
The IR spectra were recorded as KBr pellets on a Nicolet-550 FTIR spectrometer.

IR data of complex **2**: cm^{-1} 2953 (m), 2905 (w), 2868 (w), 1619(m), 1595 (m), 1555 (w), 1539 (m), 1490 (s), 1461 (s), 1436 (s), 1411 (w), 1389 (m), 1361 (m), 1334 (m), 1305 (w), 1276 (m), 1254 (s), 1202 (m), 1171 (s), 1134 (w), 1109 (w), 1096 (w), 1035 (m), 1022 (m), 984 (w), 911 (w), 894 (w), 877 (s), 848 (s), 808 (w), 783 (w), 768 (m), 752 (m), 731 (m), 693 (w), 670 (w), 646 (w), 612 (m).

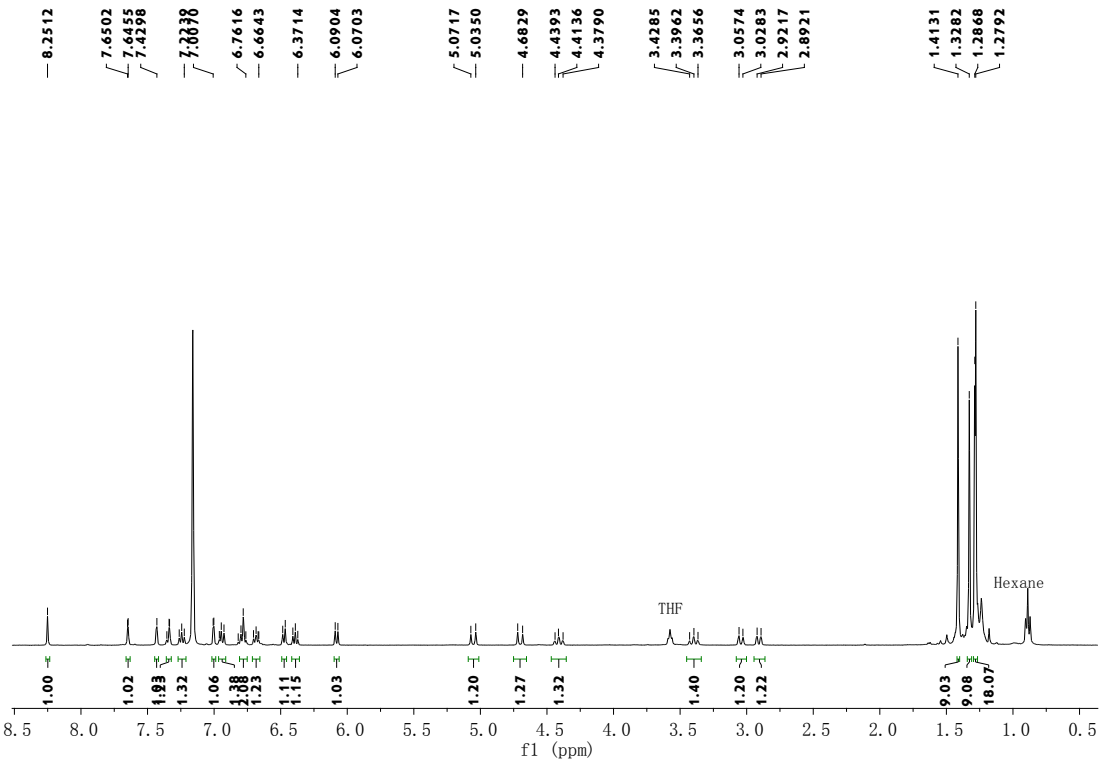
IR data of complex **3**: cm^{-1} 2949 (w), 2902 (w), 2865 (w), 1619(m), 1597 (m), 1555 (w), 1536 (m), 1494 (m), 1461 (m), 1437 (s), 1411 (w), 1389 (w), 1367 (w), 1342 (m), 1275 (m), 1253 (s), 1238 (m), 1202 (w), 1171 (s), 1127 (w), 1109 (m), 1035 (w), 1017 (m), 1001 (w), 911 (w), 899 (w), 877 (m), 847 (s), 813 (w), 789 (w), 765 (s), 748 (m), 733 (s), 688 (m), 667 (w), 644 (w), 613 (s).

IR data of complex **4**: cm^{-1} 2962 (w), 2946 (w), 1615(m), 1599 (w), 1577 (m), 1554 (w), 1536 (s), 1493 (m), 1478 (w), 1460 (w), 1434 (m), 1407 (w), 1387 (m), 1359 (w), 1324 (w), 1305 (w), 1290 (w), 1277 (w), 1250 (s), 1222 (w), 1203 (w), 1188 (s), 1174 (s), 1134 (w), 1121 (m), 1052 (w), 1029 (m), 985 (w), 929 (w), 879 (w), 844 (w), 820 (w), 787 (w), 775 (w), 756 (s), 672 (s), 639 (w).

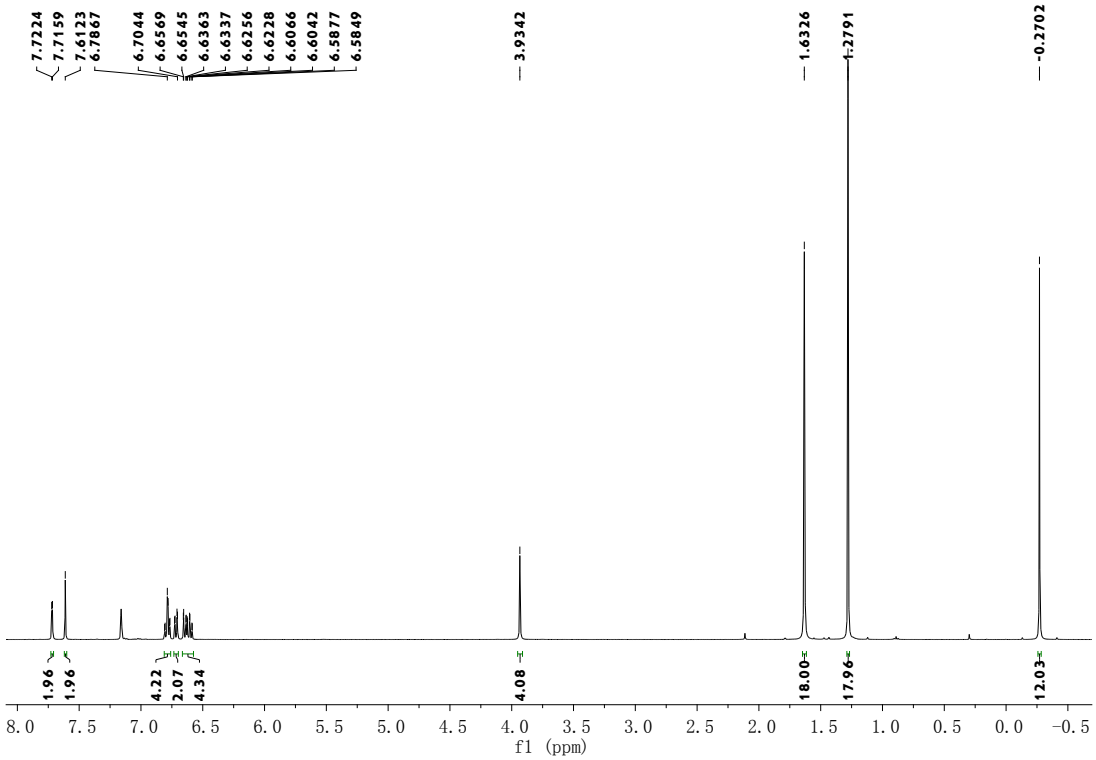
IR data of complex **5**: cm^{-1} 2954 (w), 2903 (w), 2862(w), 1614(s), 1596 (w), 1569 (w), 1558 (w), 1541 (s), 1532 (s), 1496 (m), 1477 (w), 1460 (m), 1436 (m), 1426 (m), 1409 (w), 1388 (w), 1375 (w), 1375 (w), 1360 (w), 1321 (w), 1281 (s), 1250 (m), 1191 (s), 1174 (m), 1119 (w), 1055 (w), 1035 (m), 982 (w), 946 (w), 930 (w), 918 (w), 880 (w), 852 (w), 786 (w), 748 (s), 653 (m), 637 (s).



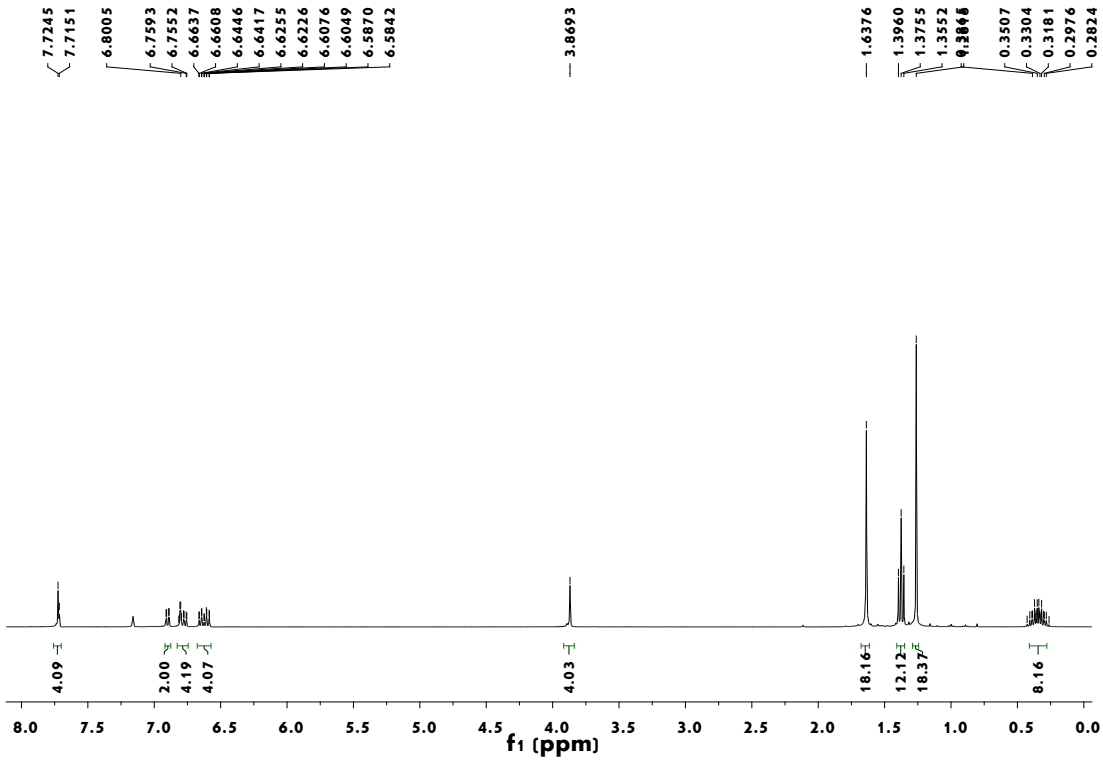
^{1}H NMR spectrum of complex 2 in C_6D_6



^{1}H NMR spectrum of complex 3 in C_6D_6



^{1}H NMR spectrum of complex 4 in C_6D_6



^{1}H NMR spectrum of complex 5 in C_6D_6

4-chloromethyl-1,3-dioxolan-2-one (7b)[1] : ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.98-4.93 (m, 1H, OCH), 4.59 (t, *J* = 8.6 Hz, 1H, OCH_2), 4.41 (q, 1H, OCH_2), 3.80-3.71 (m, 2H, $ClCH_2$).

4-phenyl-1,3-dioxolan-2-one (7c)[2] : ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.34-7.27 (m, 5H, ArH), 5.59 (t, *J* = 8.0 Hz, 1H, OCH), 4.70 (t, *J* = 8.5 Hz, 1H, OCH_2), 4.21 (t, *J* = 8.2 Hz, 1H, OCH_2).

4-(3-butenyl)-1,3-dioxolan-2-one (7d)[3] : ^{1}H NMR ($CDCl_3$, 400 MHz): δ 5.80-5.70 (m, 1H, C*H*=CH_2), 5.06-4.99 (m, 2H, CH=CH_2), 4.73-4.66 (m, 1H, OCH), 4.52-4.48 (t, *J* = 8.2 Hz ,1H, OCH_2), 4.07-4.03 (t, *J* = 7.8 Hz, 1H, OCH_2), 2.24-2.09 (m, 2H, CH_2CH_2), 1.92-1.83 (m, 1H, CH_2CH_2), 1.79-1.70 (m, 1H, CH_2CH_2).

4-phenoxymethyl-1,3-dioxolan-2-one (7e)[4] : ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.30 (t, *J* = 8.0 Hz, 2H, ArH), 7.01 (t, *J* = 7.4 Hz, 1H, ArH). 6.90 (d, *J* = 8.0 Hz, 2H, ArH). 5.04-4.99 (m, 1H, OCH), 4.59 (t, *J* = 8.5 Hz, 1H, OCH_2), 4.51 (q, 1H, OCH_2), 4.24-4.10 (m, 2H, OCH_2).

4-methoxymethyl-1,3-dioxolan-2-one (7f)[5] : ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.83-4.77 (m, 1H, OCH), 4.48 (t, *J* = 8.4 Hz, 1H, OCH_2), 4.36 (dd, *J* = 6.1 and 6.1 Hz, 1H, OCH_2), 3.65-3.54 (m, 2H, OCH_2), 3.41 (s, 3H, OCH_3)

4-allyoxymethyl-1,3-dioxolan-2-one (7g)[6] : ^{1}H NMR ($CDCl_3$, 400 MHZ): δ 5.90- 5.82 (m, 1H, C*H*=CH_2), 5.31-5.21 (m, 2H, CH=CH_2), 4.83-4.79 (m, 1H, OCH), 4.50 (t, *J* = 8.4 Hz, 1H, OCH_2), 4.40 (dd, *J* = 6.1 and 6.1 Hz, 1H, OCH_2), 4.07-4.04 (m, 2H, OCH_2), 3.71-3.60 (m, 2H, OCH_2).

4-butoxymethyl-1,3-dioxolan-2-one (7h)[7] : ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.76-4.71 (m, 1H, OCH), 4.40 (t, *J* = 8.4 Hz, 1H, OCH_2), 4.26 (dd, *J* = 6.0 and 6.0 Hz, 1H, OCH_2), 3.59-3.45 (m, 2H, OCH_2), 3.39 (t, *J* = 6.6 Hz, 2H, OCH_2), 1.43 (m, 2H, CH_2CH_2), 1.24 (m, 2H, CH_2CH_2), 0.81-0.77 (t, *J* = 7.4 Hz, 3H, CH_3).

4-tert-butyl-benzoic acid 2-oxo-[1,3]dioxolan-4-ylmethyl ester (7i)[7] : ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.94 (d, *J* = 8.6 Hz, 2H, ArH). 7.47 (d, *J* = 8.6 Hz, 2H,

ArH), 5.08-5.02 (m, 1H, OCH), 4.64-4.59 (m, 1H, OCH_2), 4.59-4.47 (m, 2H, OCH_2), 4.43-4.39 (m, 1H, OCH_2), 1.32 (s, 9H, $C(CH_3)_3$).

4-decyl-1,3-dioxolan-2-one (7j)[6]: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.73-4.65 (m, 1H, OCH), 4.54-4.49 (t, *J* = 8.2 Hz, 2H, OCH_2), 4.08-4.03 (t, *J* = 7.8 Hz, 2H, OCH_2), 1.85-1.75 (m, 1H, CH_2CH_2CH), 1.72–1.64 (m, 1H, CH_2CH_2CH), 1.30–1.49 (m, 16H, $CH_3(CH_2)_8$), 0.85–0.90 (t, 3H, *J* = 12 Hz, CH_3)

4- benzyloxymethyl-1,3-dioxolan-2-one (7k)[8] : ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.36-7.27 (m, 5H, Ar-H), 4.78-4.73 (m, 1H, OCH), 4.54 (q, *J* = 12.0 Hz, 2H, OCH_2), 4.41 (t, *J* = 8.4 Hz, 1H, OCH_2), 4.31 (dd, *J* = 8.3, 6.0 Hz, 1H, OCH_2), 3.62 (m, 2H, $ArCH_2$).

4,4'-(butane-1,4-diyl)-bis-1,3-dioxolan-2-one (7l)[9] : ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.75-4.68 (m, 2H, OCH), 4.54 (t, *J* = 8.2 Hz, 2H, OCH_2), 4.07 (t, *J* = 7.8 Hz, 2H, OCH_2), 1.45-1.83 (m, 8H, CH_2CH_2).

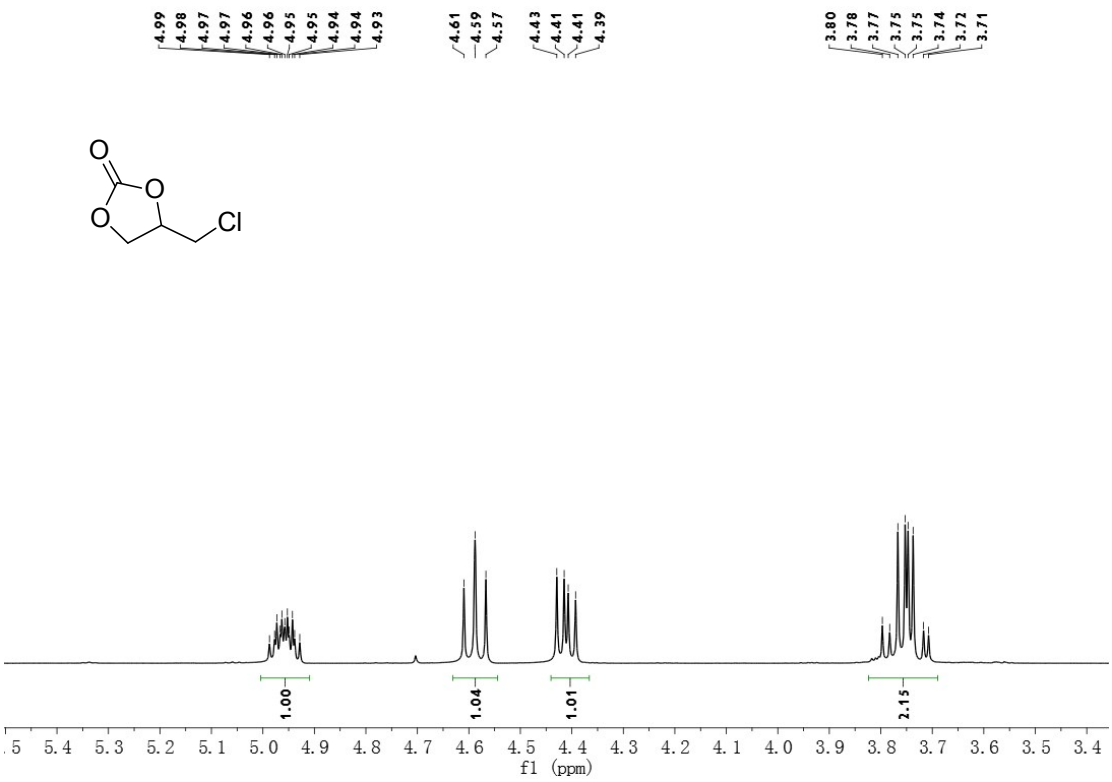


Figure S1. ^{1}H NMR spectrum of **7b** in $CDCl_3$.

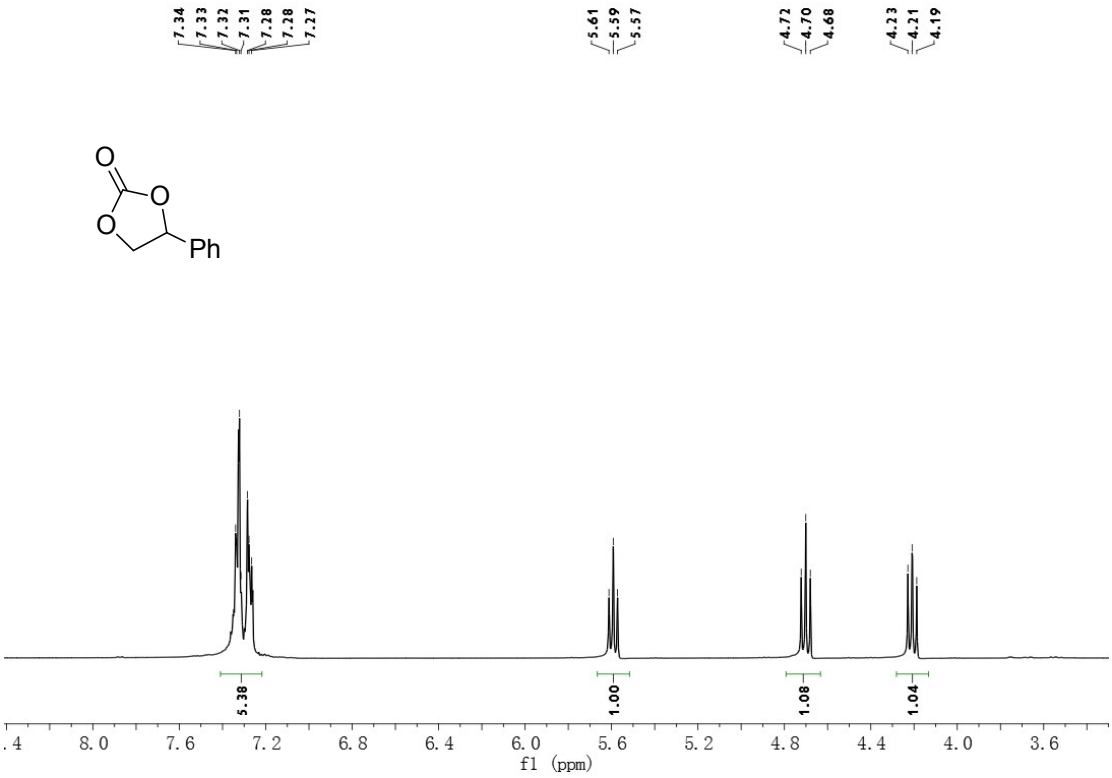


Figure S2. ^{1}H NMR spectrum of **7c** in $CDCl_3$.

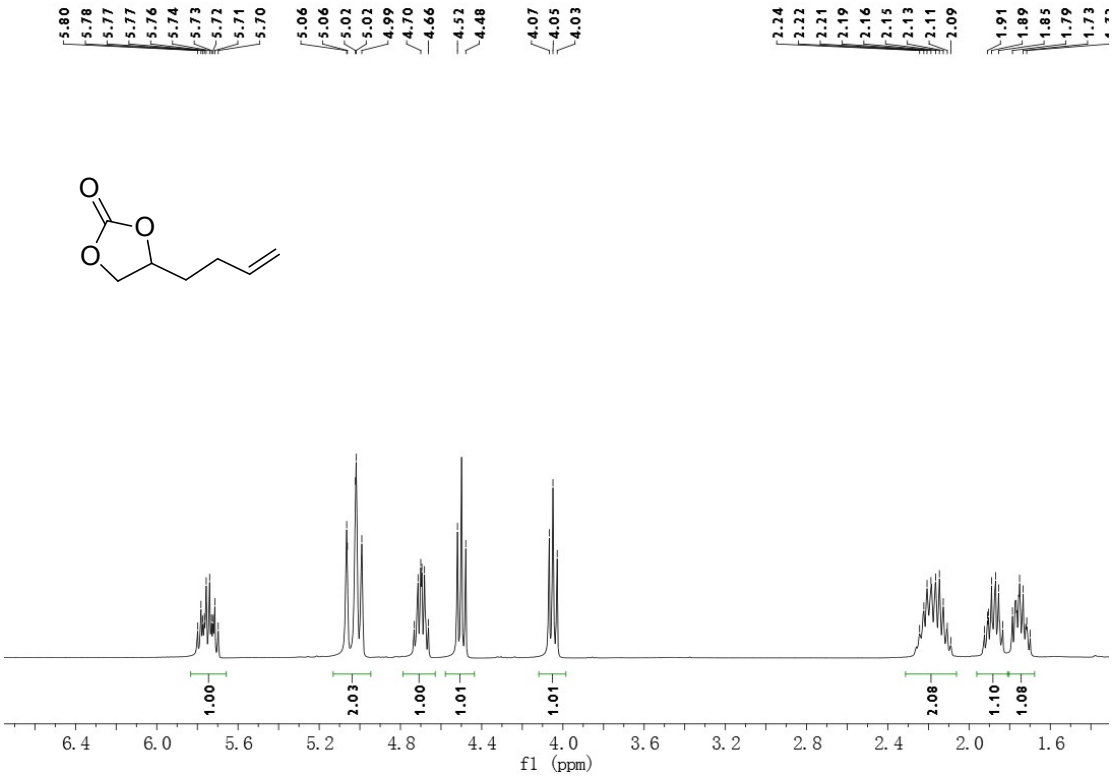


Figure S3. ^{1}H NMR spectrum of **7d** in $CDCl_3$.

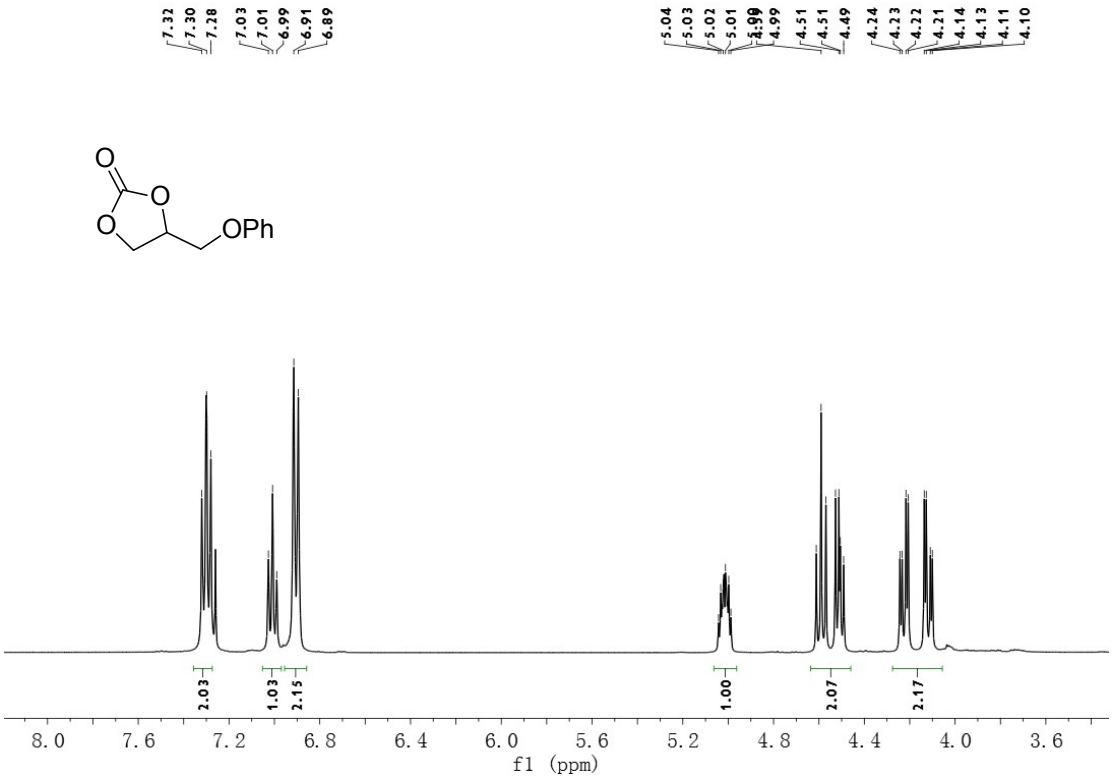


Figure S4. ^{1}H NMR spectrum of **7e** in $CDCl_3$.

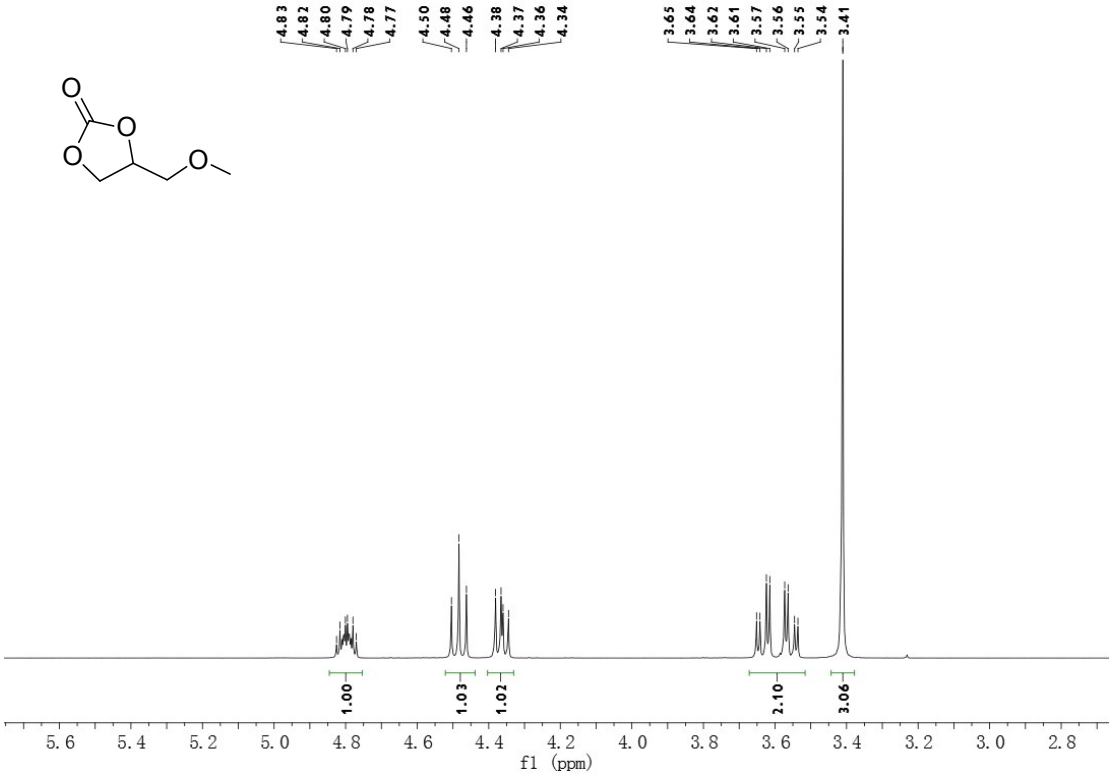


Figure S5. ^{1}H NMR spectrum of **7f** in $CDCl_3$.

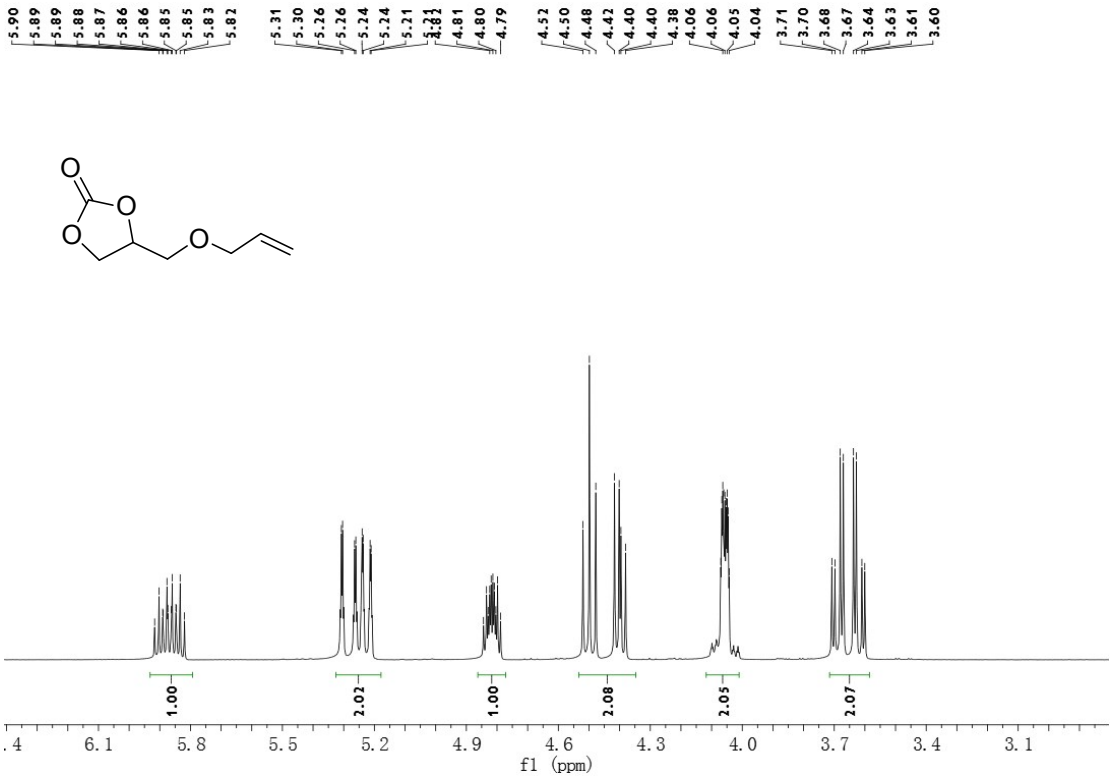


Figure S6. ^{1}H NMR spectrum of **7g** in $CDCl_3$.

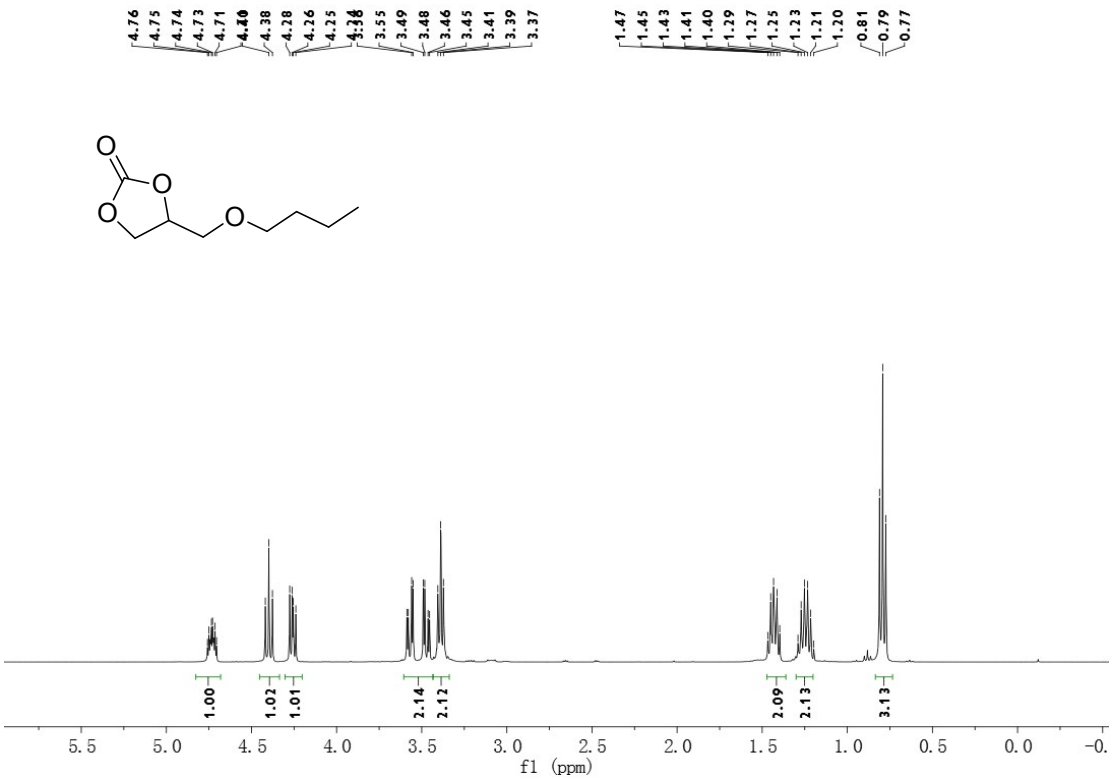


Figure S7. ^{1}H NMR spectrum of **7h** in $CDCl_3$.

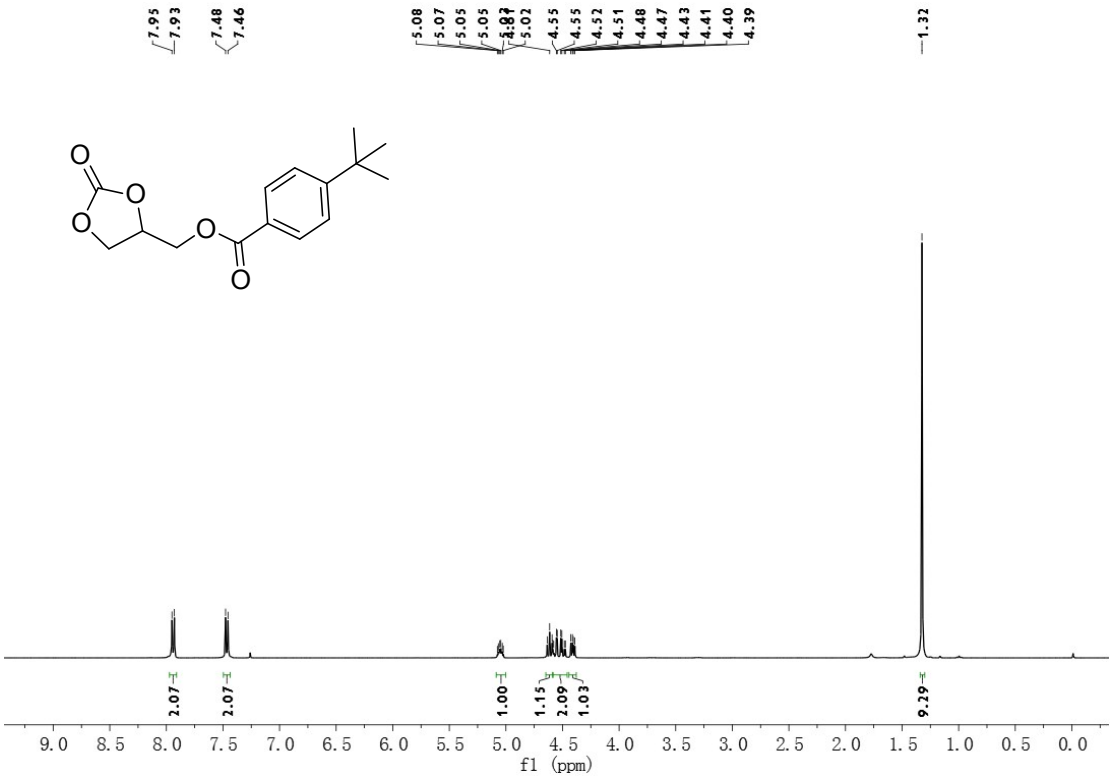


Figure S8. ^{1}H NMR spectrum of **7i** in $CDCl_3$.

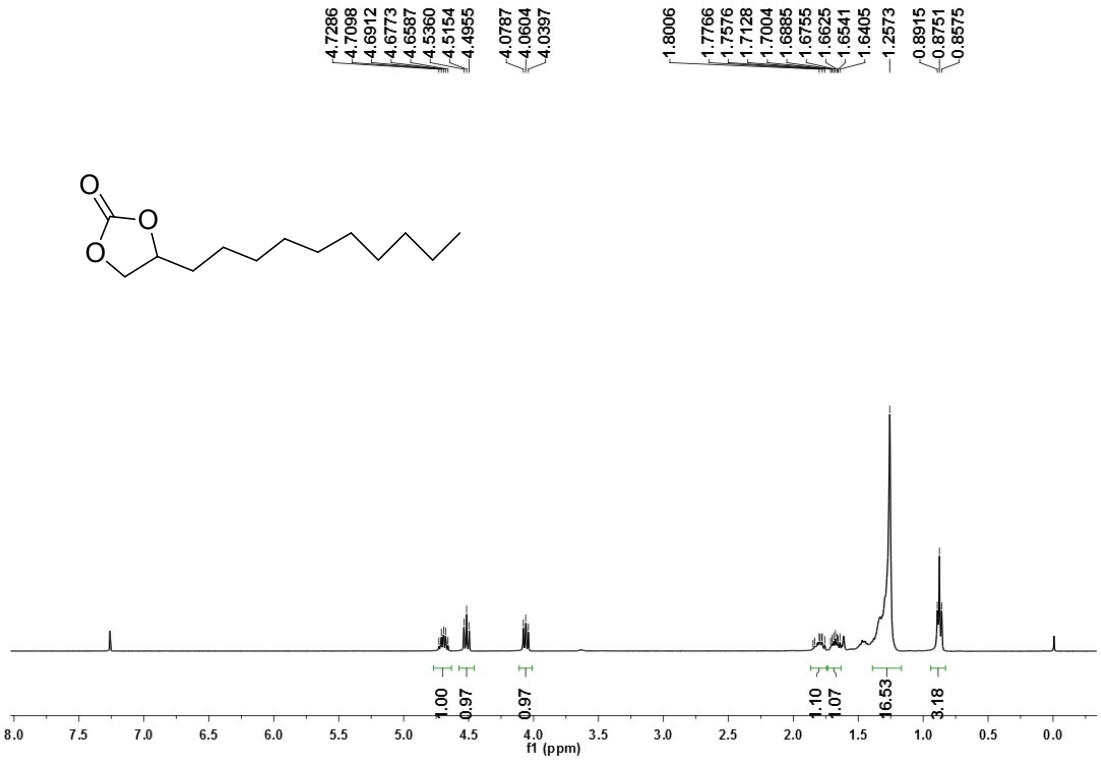


Figure S9. ^{1}H NMR spectrum of **7j** in $CDCl_3$.

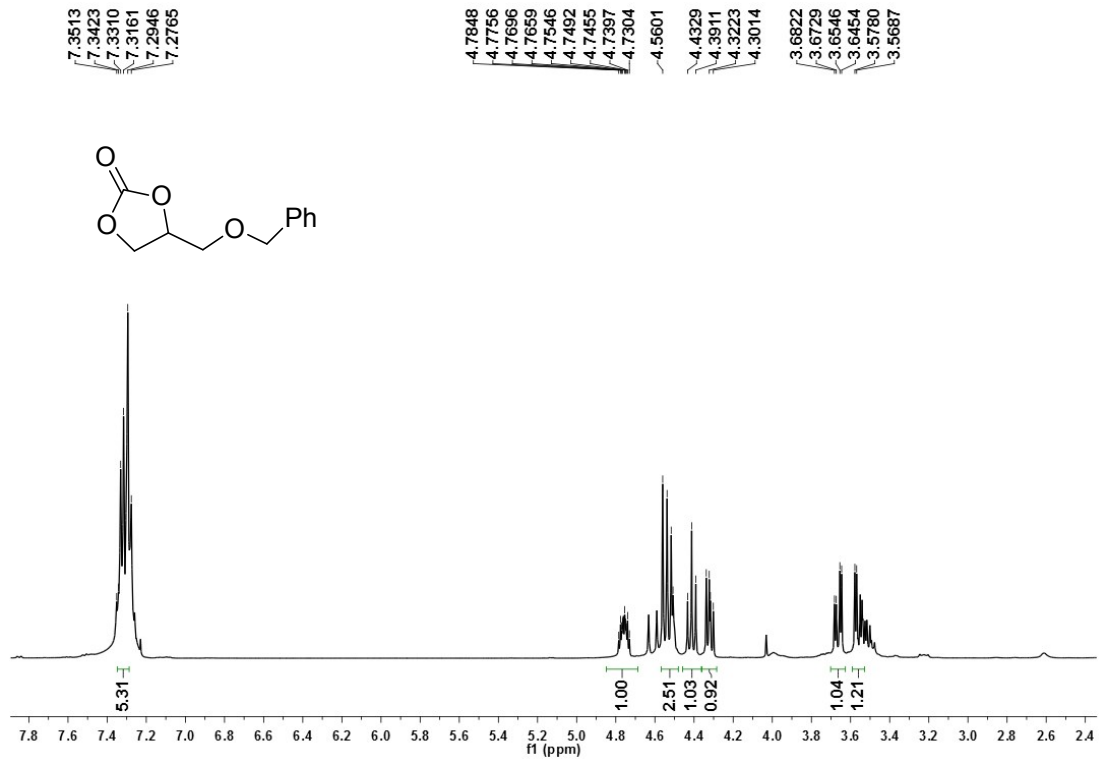


Figure S10. ^{1}H NMR spectrum of **7k** in $CDCl_3$.

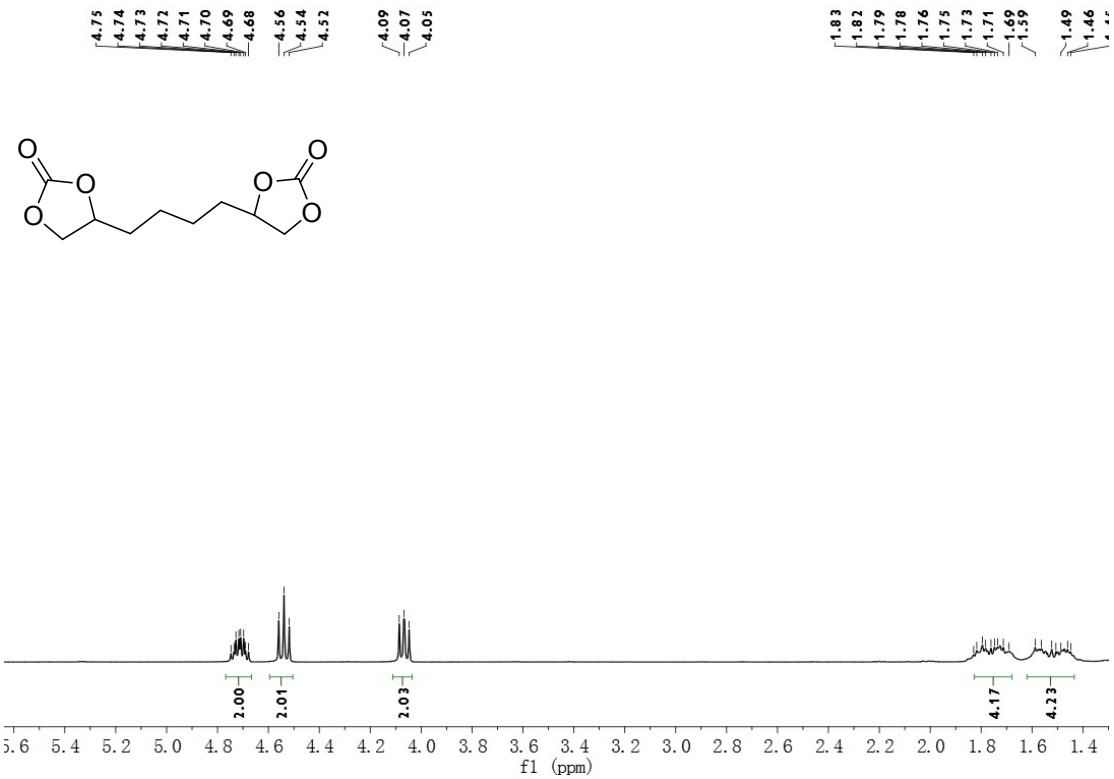


Figure S11. ^{1}H NMR spectrum of **7l** in $CDCl_3$.

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