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# Supporting Information

## Cycloaddition of carbon dioxide and epoxides catalyzed by rare earth metal complexes bearing Trost ligand

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## Contents

**Solid state structures of complexes 2-5**

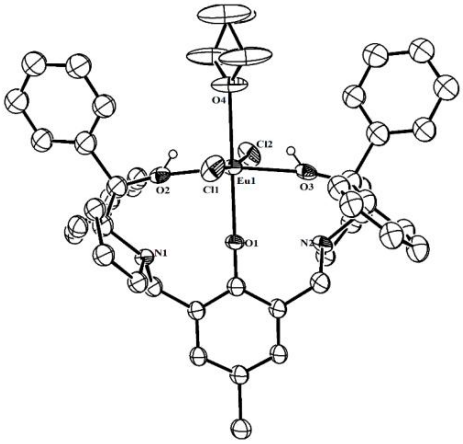


**Fig. S1** Solid state structure of complex **2.** Thermal ellipsoids are drawn at the 30% probability level, for clarity, all other hydrogen atoms and solvent molecules except alcohol hydroxyl hydrogen. Selected bond lengths [Å] and bond angles [deg]: Eu(1)-O(1) 2.176(8), Eu(1)-O(2) 2.196(18), Eu(1)-O(3) 2.196(19), Eu(1)-O(4) 2.442(19), Eu(1)-Cl(1) 2.727(6), Eu(1)-Cl(2) 2.727(6); O(1)-Eu(1)-O(2) 85.1(4), O(1)-Eu(1)-O(3) 85.1(4), O(1)-Eu(1)-O(4) 180.0(4), O(2)-Eu(1)-O(3) 170.2(8), O(2)-Eu (1)-O(4) 94.9(4), O(3)-Eu(1)-O(4) 94.9(4), Cl(1)-Eu(1)-Cl(2) 172.3(3), O(1)-Eu(1)-Cl(1) 93.9(2), O(1)-Eu(1)-Cl(2) 93.9(2), O(2)-Eu(1)-Cl(1) 94.1(4), O(2)-Eu(1)-Cl(2) 86.6(4), O(3)-Eu(1)-Cl(1) 94.1(4), O(3)-Eu(1)-Cl(2) 86.6(4), O(4)-Eu(1)-Cl(1) 86.1(2), O(4)-Eu(1)-Cl(2) 86.1(2).

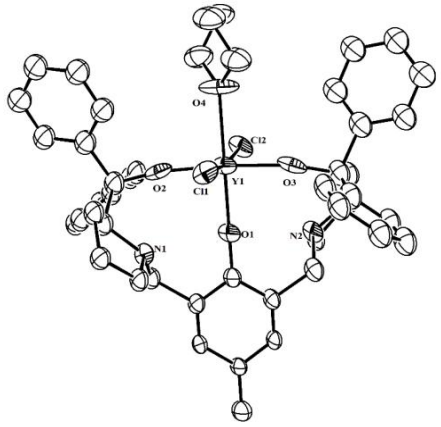


**Fig. S2** Solid state structure of complex **3.** Thermal ellipsoids are drawn at the 30% probability level, for clarity, all other hydrogen atoms and solvent molecules except alcohol hydroxyl hydrogen. Selected bond lengths [Å] and bond angles [deg]: Y(1)-O(1) 2.098(14), Y(1)-O(2) 2.086(15), Y(1)-O(3) 2.086(15), Y(1)-O(4) 2.422(17), Y(1)-Cl(1) 2.679(5), Y(1)-Cl(2) 2.679(5); O(1)-Y(1)-O(2) 87.7(4), O(1)-Y(1)-O(3) 87.7(4), O(1)-Y(1)-O(4) 180.0, O(2)-Y(1)-O(3) 175.3(7), O(2)-Y(1)-O(4) 92.3(4), Cl(1)-Y(1)-Cl(2) 171.2(3), O(1)-Y(1)-Cl(1) 94.39(13), O(1)-Y(1)-Cl(2) 94.39(13),

O(2)-Y(1)-Cl(1) 93.7(4), O(2)-Y(1)-Cl(2) 86.7(4), O(3)-Y(1)-Cl(1) 93.7(4), O(3)-Y(1)-Cl(2) 86.7(4), O(4)-Y(1)-Cl(1) 85.61(13), O(4)- Y(1)-Cl(2) 85.61(13).

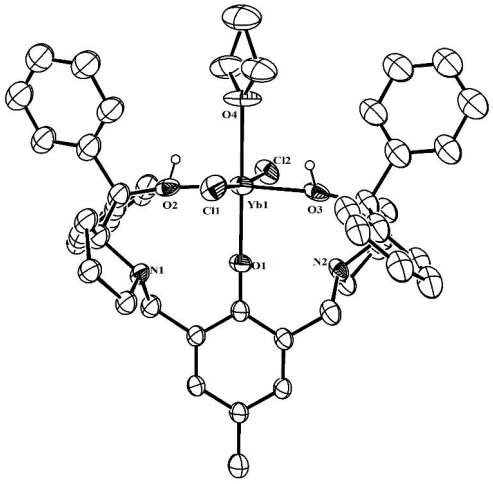


**Fig. S3** Solid state structure of complex **4**. Thermal ellipsoids are drawn at the 30% probability level, for clarity, all other hydrogen atoms and solvent molecules except alcohol hydroxyl hydrogen. Selected bond lengths [Å] and bond angles [deg]: Yb1-O1 2.126(11), Yb1-O4 2.369(11), Yb1-O2 2.075(11), Yb1-Cl1 2.651(4), Yb1-O3 2.075(11), Yb1-Cl2 2.651(4), O1-Yb1-O2 86.9(3), O1-Yb1-Cl1 93.53(10), O1-Yb1-O3 86.9(3), O1-Yb1-Cl2 93.53(10), O1-Yb1-O4 180.0, O2-Yb1-Cl1 94.4(3), O2-Yb1-O3 173.8(5), O2-Yb1-Cl2 86.0(3), O2-Yb1-O4 93.1(3), O3-Yb1-Cl1 94.3(3), O3-Yb1-O4 93.1(3), O3-Yb1-Cl2 86.0(3), Cl1-Yb1-Cl2 172.9(2), O4-Yb1-Cl1 86.47(10), O4-Yb1-Cl2 86.47(10).

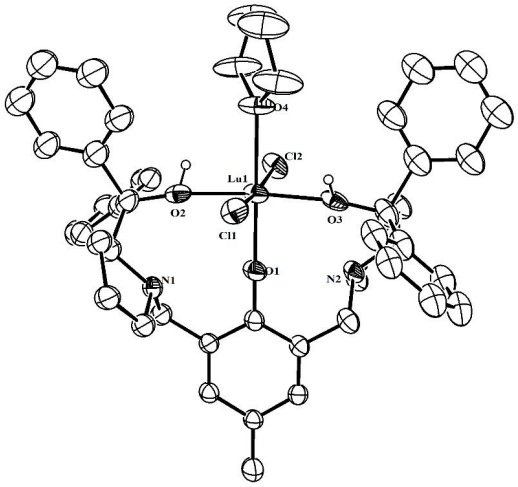


**Fig. S4** Solid state structure of complex **5**. Thermal ellipsoids are drawn at the 30% probability level, for clarity, all other hydrogen atoms and solvent molecules except alcohol hydroxyl hydrogen.Selected bond lengths [Å] and bond angles [deg]: Lu1-O1 2.125(8), Lu1-O4 2.359(9), Lu1-O2 2.093(8), Lu1-Cl1 2.629(3), Lu1-O3 2.093(8), Lu1-Cl2 2.629(3), O1-Lu1-O2 86.9(3), O1-Lu1-Cl1 93.60(8), O1-Lu1-O3 86.9(3), O1-Lu1-Cl2 93.60(8), O1-Lu1-O4 180.0, O2-Lu1-Cl1 86.51(19), O2-Lu1-O3

173.8(5), O2-Lu1-Cl2 93.81(19), O2-Lu1-O4 93.1(3), O3-Lu1-Cl1 86.51(19),O3-Lu1-O4 93.1(3), O3-Lu1-Cl2 93.81(19), Cl1-Lu1-Cl2 172.81(15), O4-Lu1-Cl1 86.5(5), O4-Lu1-Cl2 86.3(5).

**Crystallographic data for complexes 1-5**

| Complexes | **1** | **2** | **3** |
|---|---|---|---|
| Empirical formula | $C_{47}H_{51}Cl_2N_2O_4Sm\cdot THF$ | $C_{55}H_{69}Cl_2N_2O_6$ Eu·2THF | $C_{47}H_{53}Cl_2N_2O_4Y\cdot THF$ |
| Formula weight | 929.15 | 1072.80 | 869.72 |
| Temperature/K | 296.15 | 296(2) | 120.01 |
| Crystal system | orthorhombic | tetragonal | tetragonal |
| Space group | $P2_12_12_1$ | $P4_32_12$ | $P4_32_12$ |
| a/Å | 12.9665(12) | 12.9908(4) | 12.8764(6) |
| b/Å | 12.9771(12) | 12.9908(4) | 12.8764(6) |
| c/Å | 30.056(3) | 30.0245(16) | 29.6614(17) |
| α/° | 90 | 90 | 90 |
| β/° | 90 | 90 | 90 |
| γ/° | 90 | 90 | 90 |
| Volume/$Å^3$ | 5057.4(8) | 5067.0(4) | 4917.9(5) |
| Z | 4 | 4 | 4 |
| $\rho_{calc}$ g/$cm^3$ | 1.220 | 1.406 | 1.175 |
| μ/$mm^{-1}$ | 1.305 | 1.361 | 1.334 |
| F(000) | 1900.0 | 2225.0 | 1816.0 |
| Crystal size/$mm^3$ | 0.3/0.2/0.2 | 0.3/0.2/0.2 | 0.3/0.2/0.2 |
| Radiation | MoKα (λ =0.71073) | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) |
| Reflections collected | 139369 | 96947 | 80557 |
| Independent reflections | 9582 [$R_{int}$ = 0.1725] | 5853 [$R_{int}$ = 0.0516] | 4188 [$R_{int}$ = 0.1297] |
| Goodness-of-fit on $F^2$ | 1.037 | 1.077 | 1.040 |
| Final R indexes [I >= 2σ (I)] | $R_1$ = 0.1025, $wR_2$ = 0.2417 | $R_1$ = 0.1259, $wR_2$ = 0.2777 | $R_1$ = 0.1392, $wR_2$ = 0.3606 |
| Largest diff. peak/hole / e $Å^{-3}$ | 2.73/-2.49 | 5.21/-3.56 | 1.30/-1.35 |
| Flack parameter | 0.122(9) | 0.079(9) | 0.080(11) |

| Complexes | **4** | **5** |
|---|---|---|
| Empirical formula | $C_{47}H_{53}Cl_2N_2O_4Yb\cdot THF$ | $C_{55}H_{69}Cl_2N_2O_6Lu\cdot 2THF$ |
| Formula weight | 953.85 | 1100.04 |
| Temperature/K | 296.15 | 296.15 |
| Crystal system | tetragonal | tetragonal |
| Space group | $P4_32_12$ | $P4_32_12$ |
| a/Å | 12.9011(5) | 12.8865(5) |
| b/Å | 12.9011(5) | 12.8865(5) |
| c/Å | 29.9105(16) | 29.8955(17) |
| α/° | 90 | 90 |
| β/° | 90 | 90 |
| γ/° | 90 | 90 |
| Volume/$Å^3$ | 4978.3(5) | 4964.5(4) |
| Z | 4 | 4 |
| $\rho_{calc}$ g/$cm^3$ | 1.273 | 1.4717 |
| μ/$mm^{-1}$ | 2.025 | 2.148 |
| F(000) | 1940.0 | 2264.8 |
| Crystal size/mm3 | 0.3/0.25/0.2 | 0.2/0.2/0.1 |
| Radiation | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) |
| Reflections collected | 111202 | 97816 |
| Independent reflections | 4736<br>[$R_{int}$ = 0.0896] | 5742<br>[$R_{int}$ = 0.0933] |
| Goodness-of-fit on $F^2$ | 1.048 | 1.130 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0671,<br>$wR_2$ = 0.1542 | $R_1$ =0.0709,<br>$wR_2$ = 0.1555 |
| Largest diff. peak/hole / e $Å^{-3}$ | 2.00/-1.43 | 3.77/-2.99 |
| Flack parameter | 0.038(7) | 0.06(2) |

**The IR spectra of complexes 2-5.**

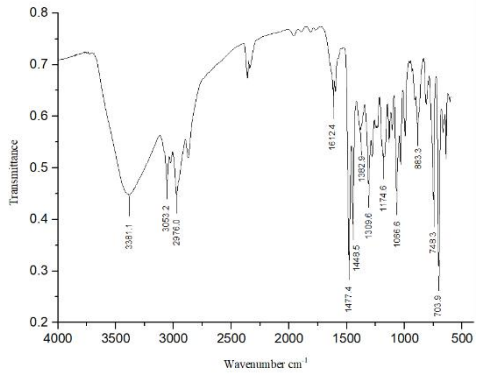


**Fig. S5** IR spectrum of complex **2**

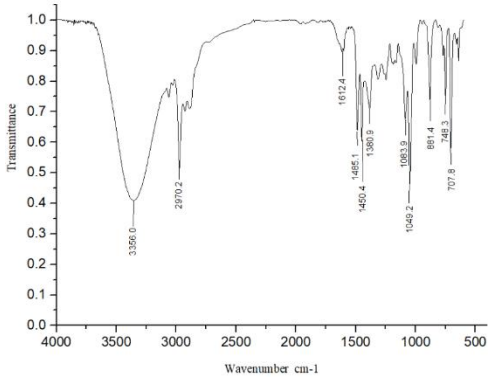


**Fig. S6** IR spectrum of complex **3**

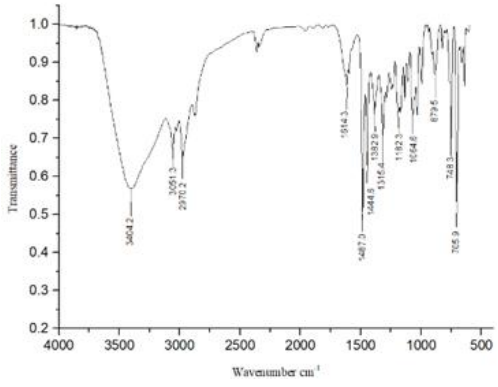


**Fig. S7** IR spectrum of complex **4**

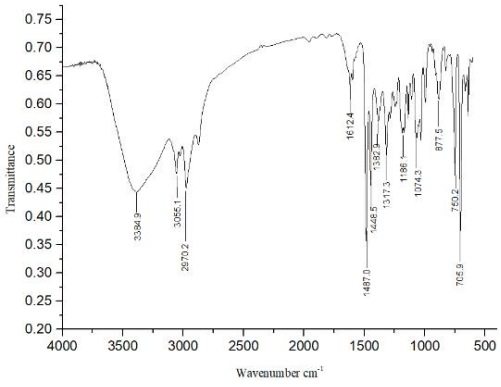


**Fig. S8** IR spectrum of complex **5**

**NMR spectra of complexes 3 and 5**

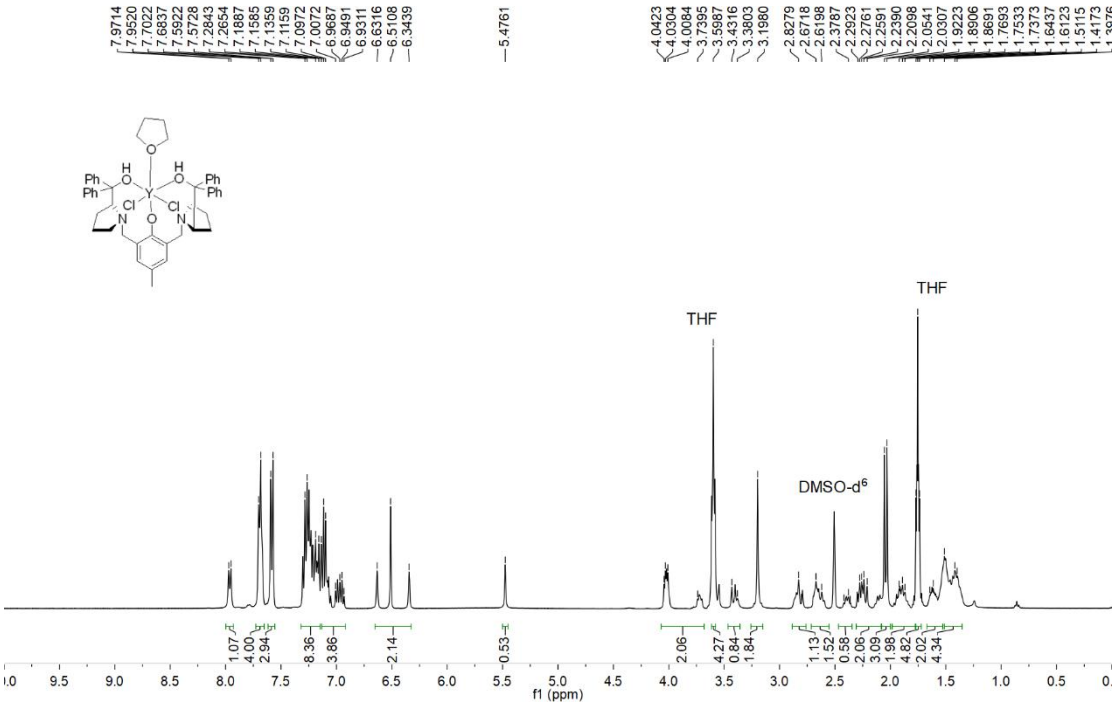


**Fig. S9** $^{1}$H NMR spectrum of complex **3** in DMSO-$d_6$

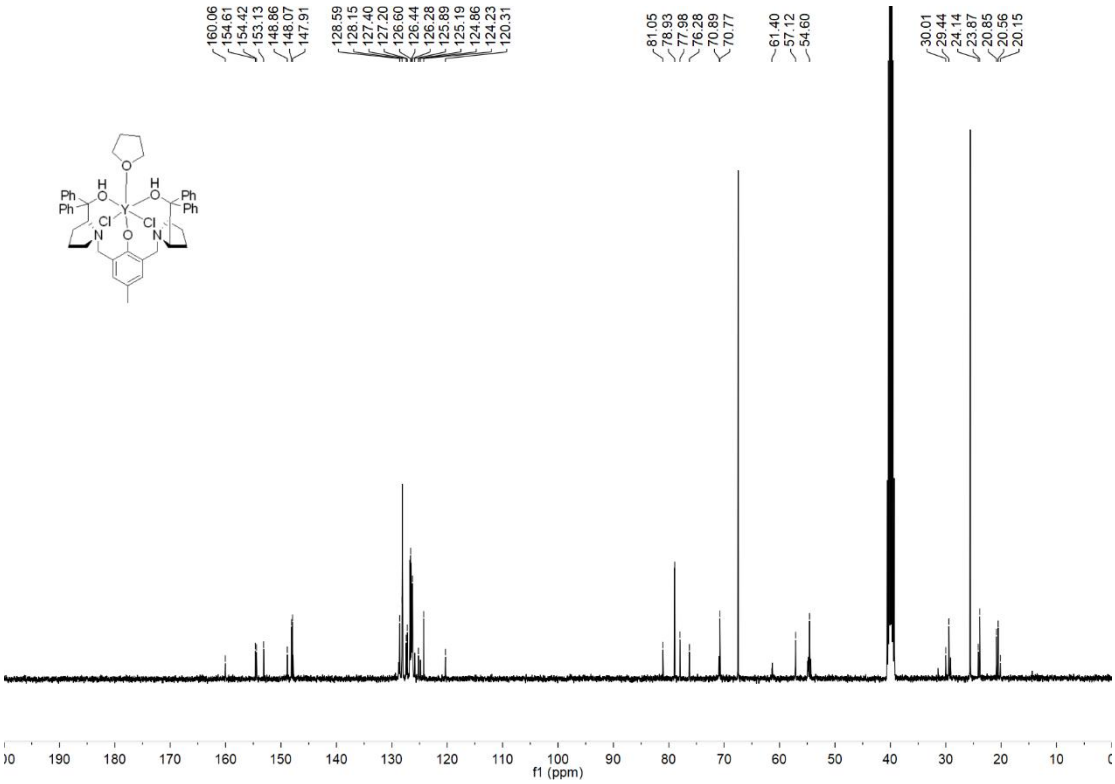


**Fig. S10** $^{13}$C NMR spectrum of complex **3** in DMSO-$d_6$

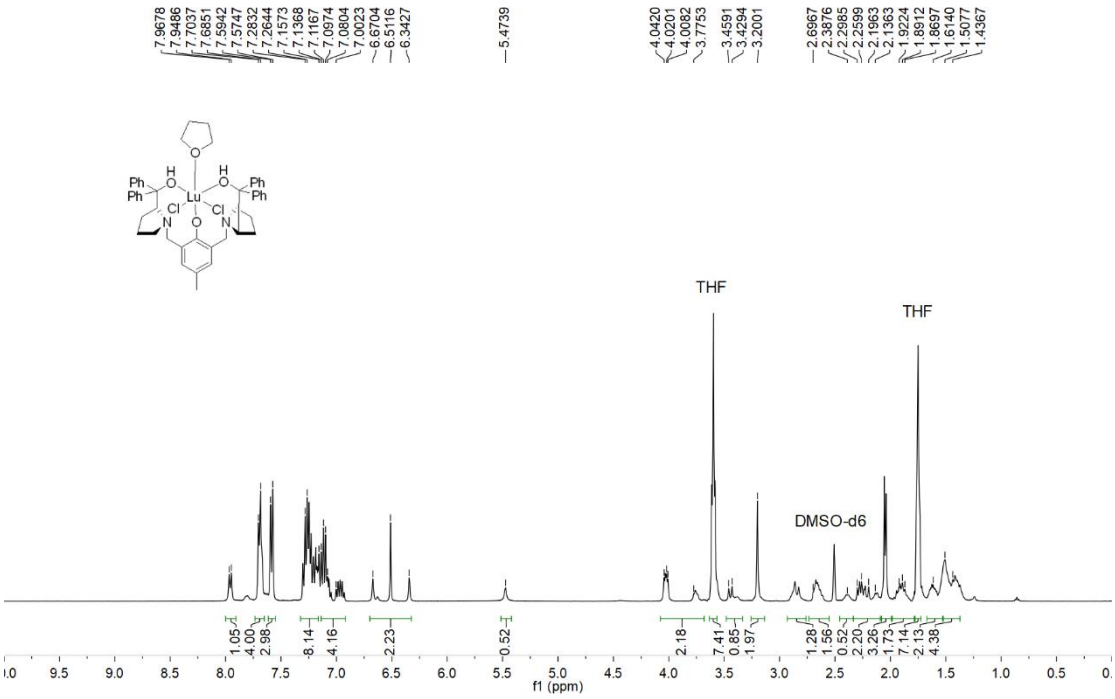


**Fig. S11** $^{1}$H NMR spectrum of complex **5** in DMSO-$d_6$

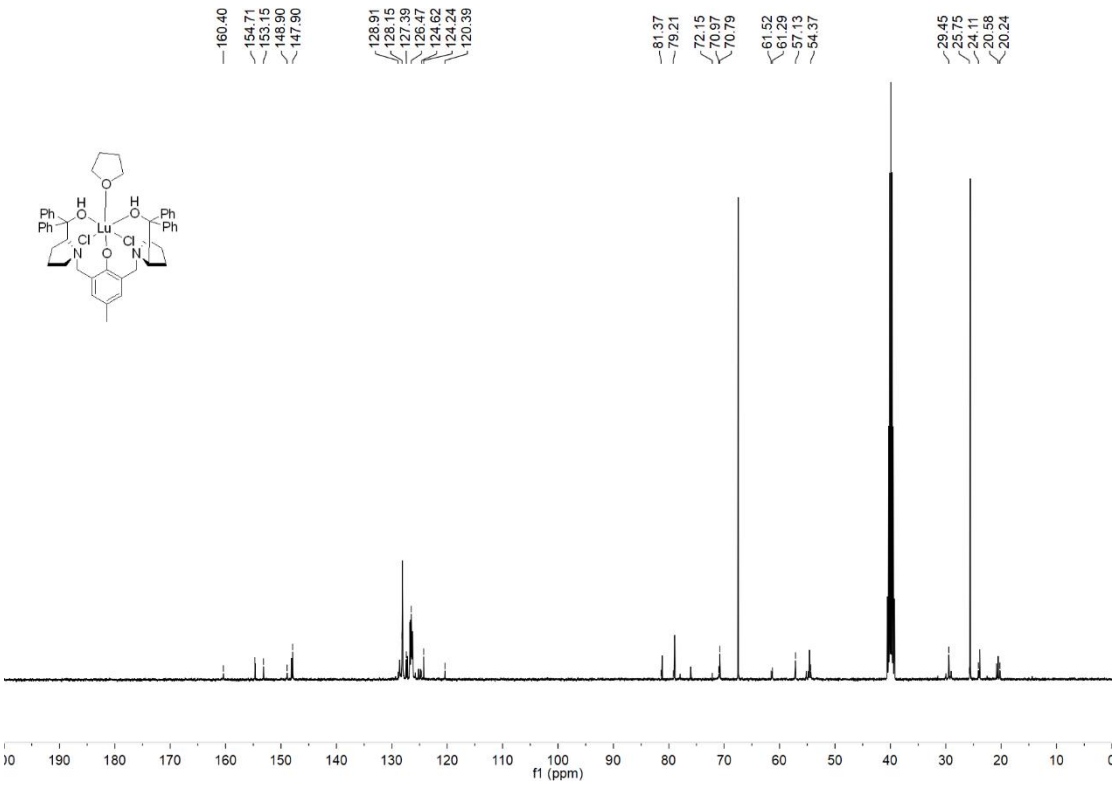


**Fig. S12** $^{13}C$ NMR spectrum of complex **5** in DMSO-$d_6$

## NMR spectra of the cyclic carbonates

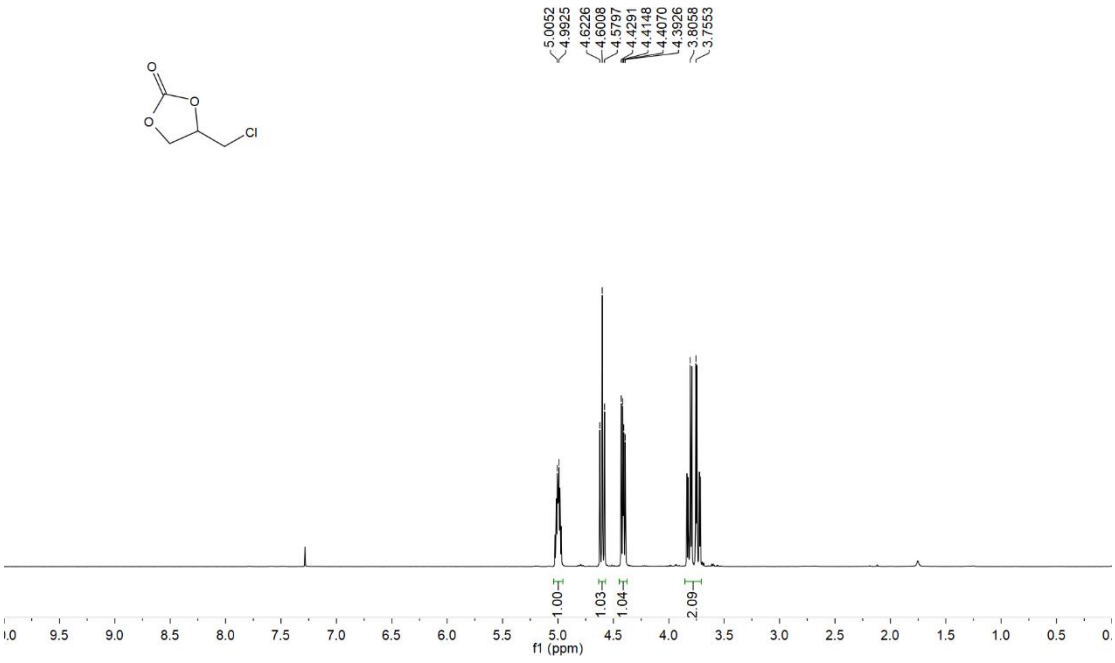


**Fig. S13** $^{1}H$ NMR spectrum of **7a** in $CDCl_3$

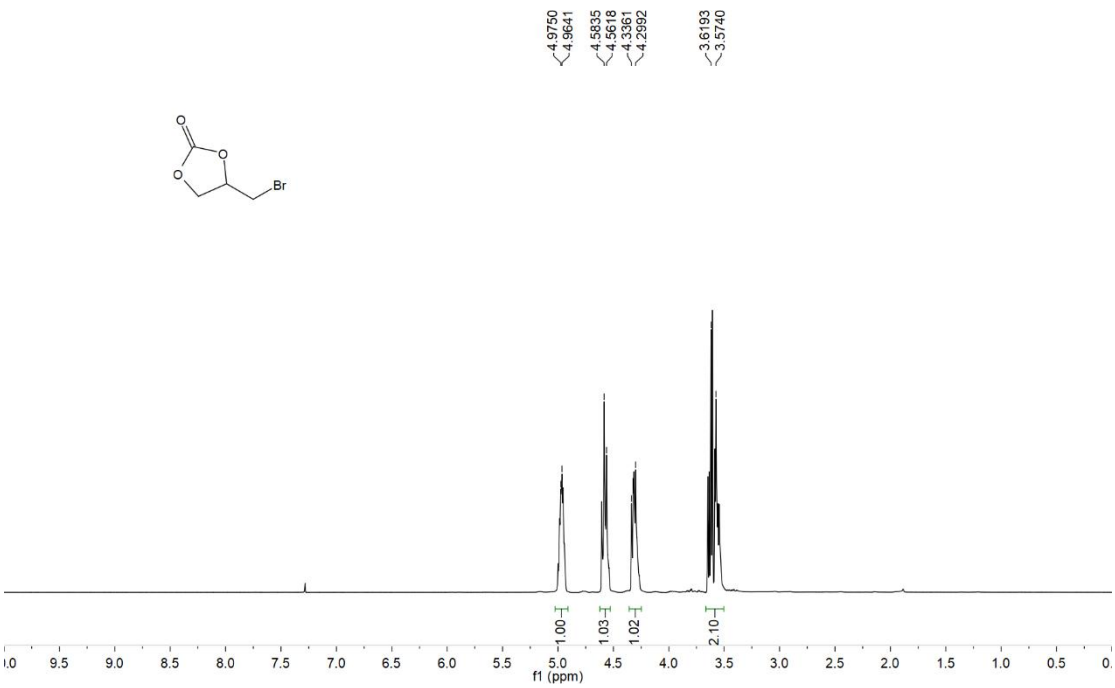


**Fig. S14** $^{1}$H NMR spectrum of **7b** in $CDCl_3$

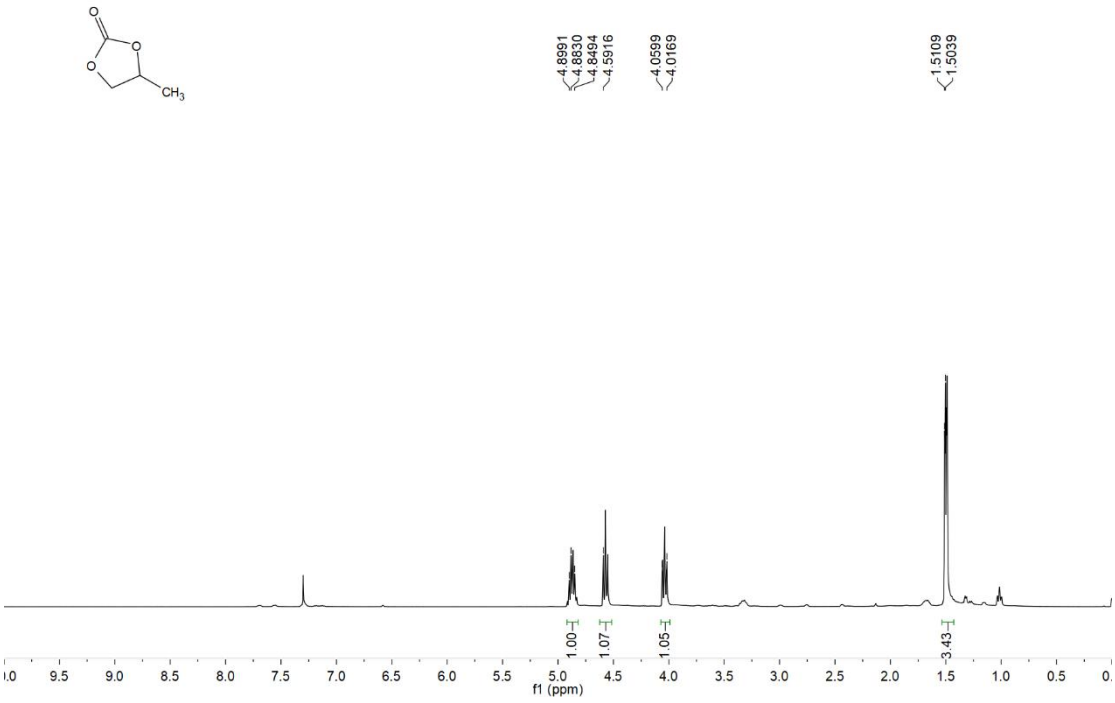


**Fig. S15** $^{1}$H NMR spectrum of **7c** in $CDCl_3$

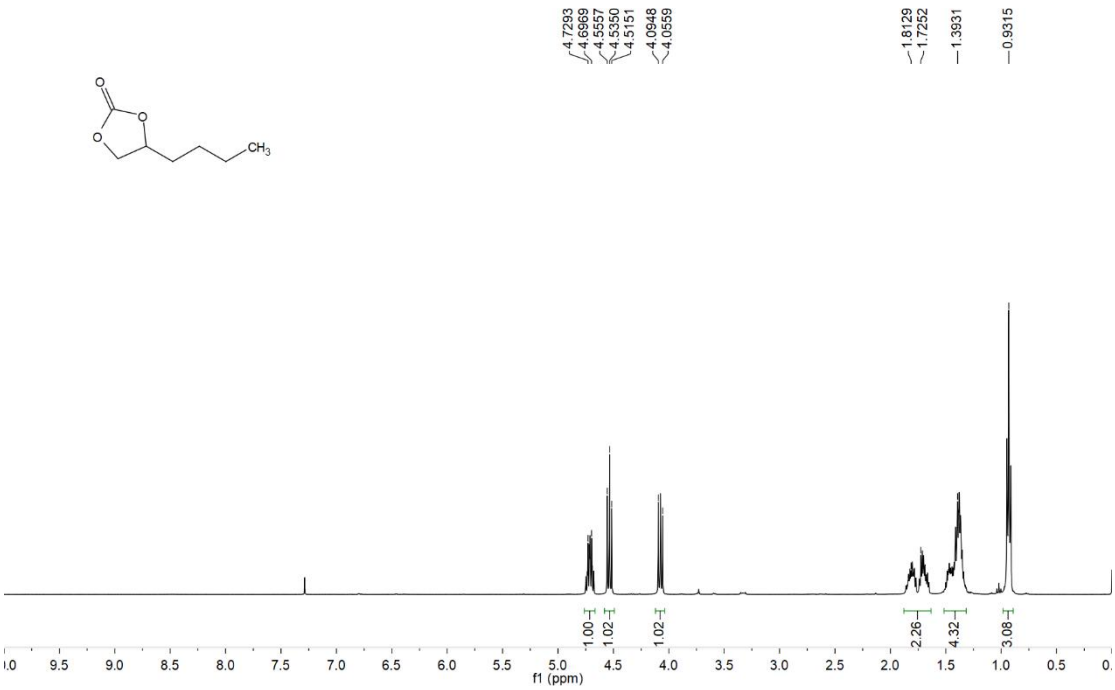


**Fig. S16** $^{1}$H NMR spectrum of **7d** in $CDCl_3$

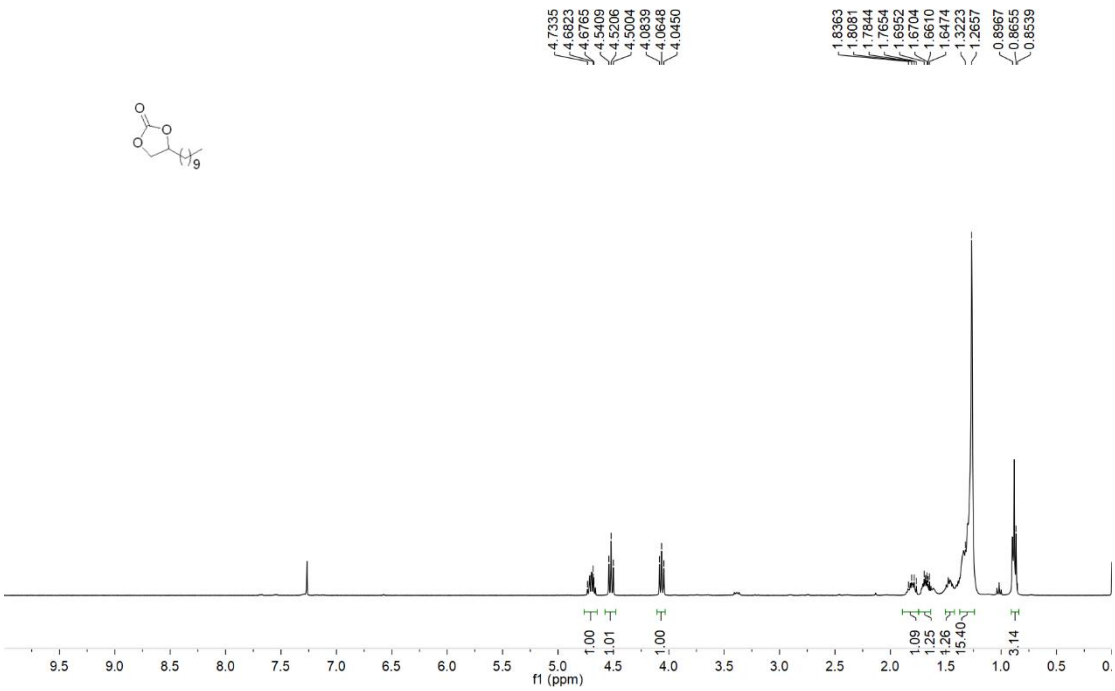


**Fig. S17** $^{1}$H NMR spectrum of **7e** in $CDCl_3$

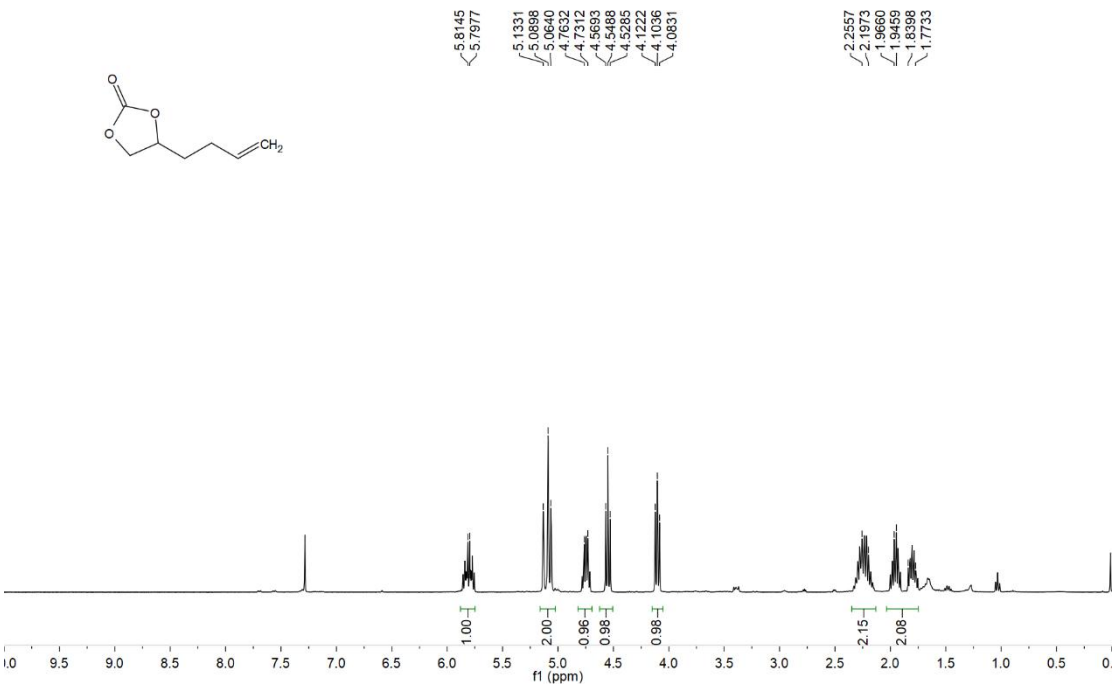


**Fig. S18** $^{1}$H NMR spectrum of **7f** in $CDCl_3$

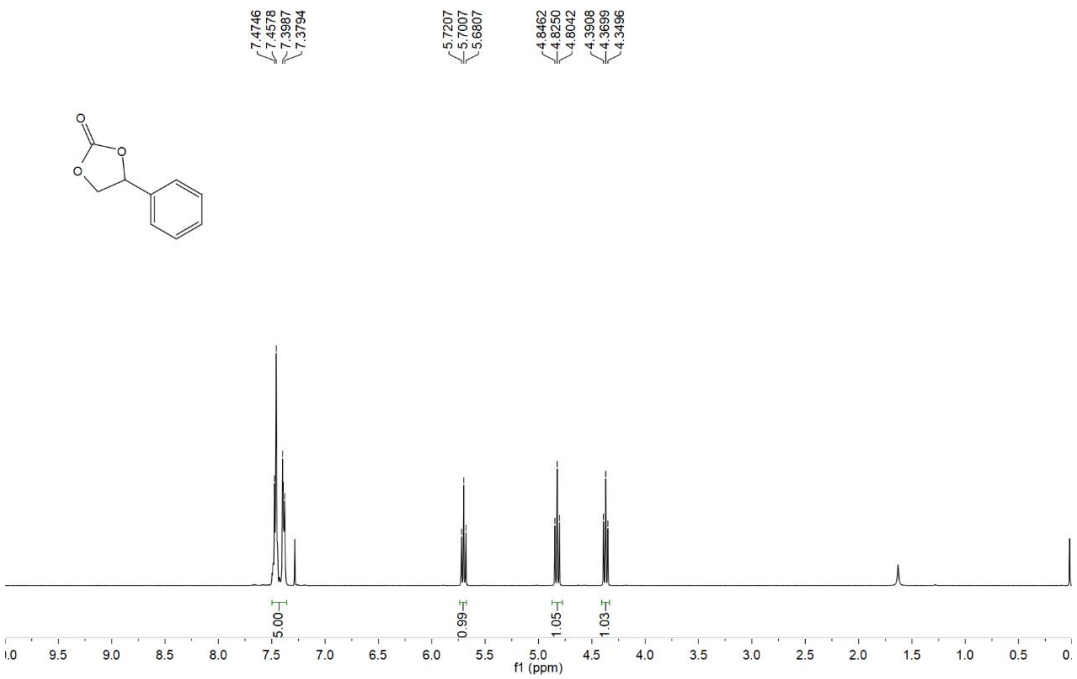


**Fig. S19** $^{1}$H NMR spectrum of **7g** in $CDCl_3$

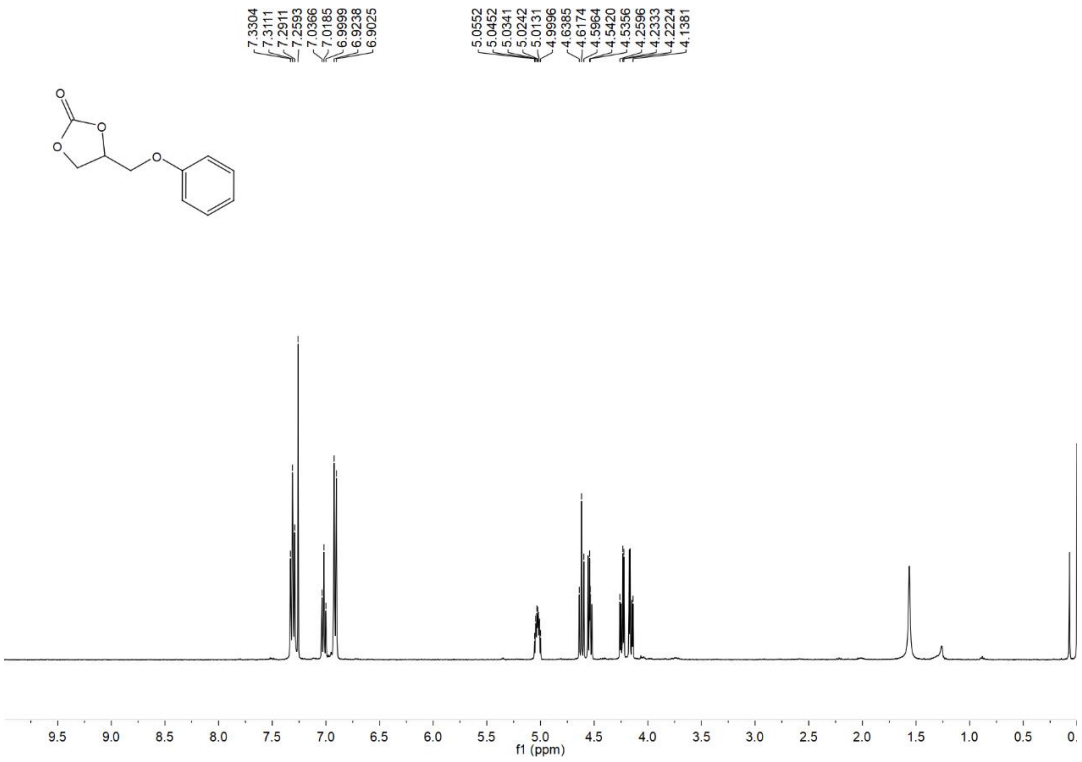


**Fig. S20** $^{1}$H NMR spectrum of **7h** in $CDCl_3$

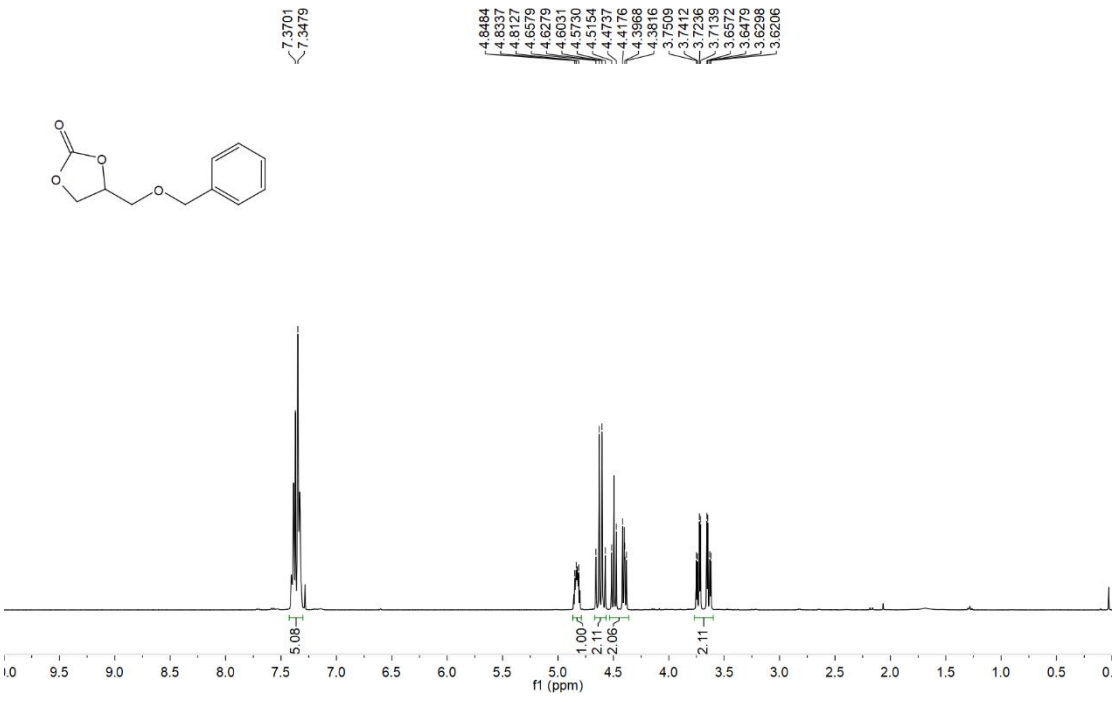


**Fig. S21** $^{1}$H NMR spectrum of **7i** in $CDCl_3$

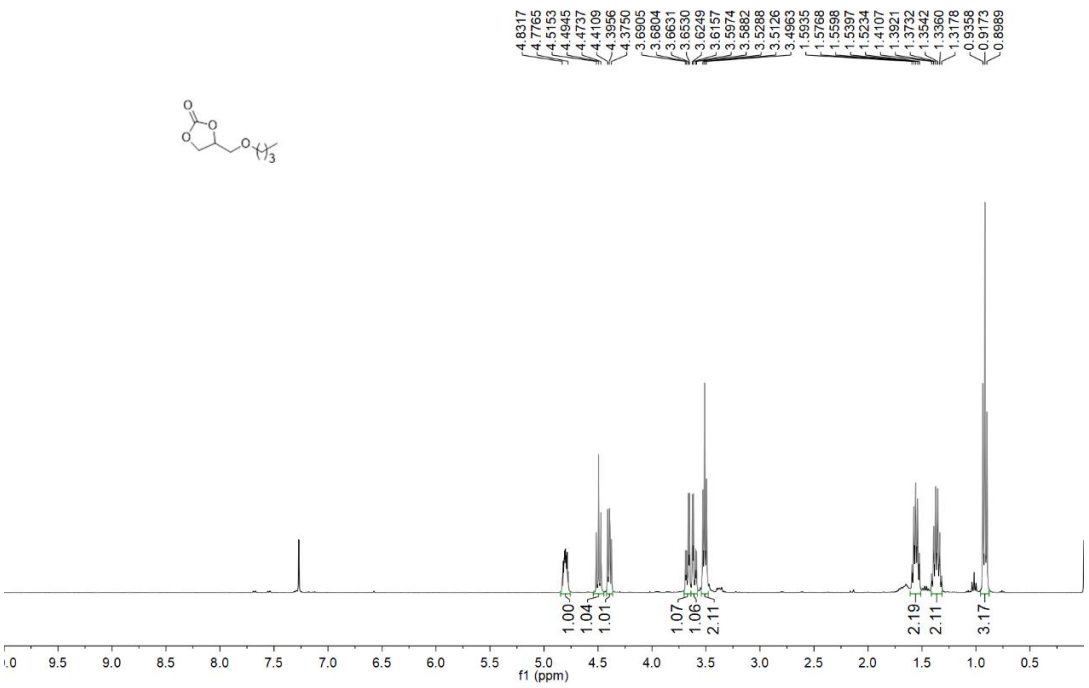


**Fig. S22** $^{1}$H NMR spectrum of **7j** in $CDCl_3$

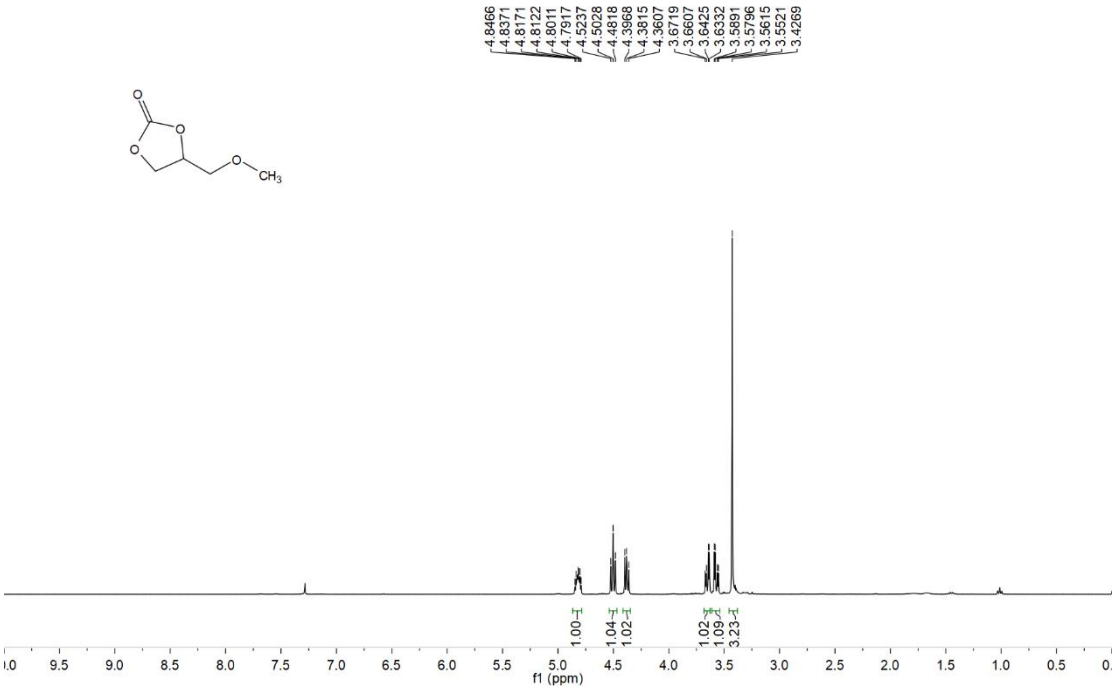


**Fig. S23** $^{1}$H NMR spectrum of **7k** in $CDCl_3$

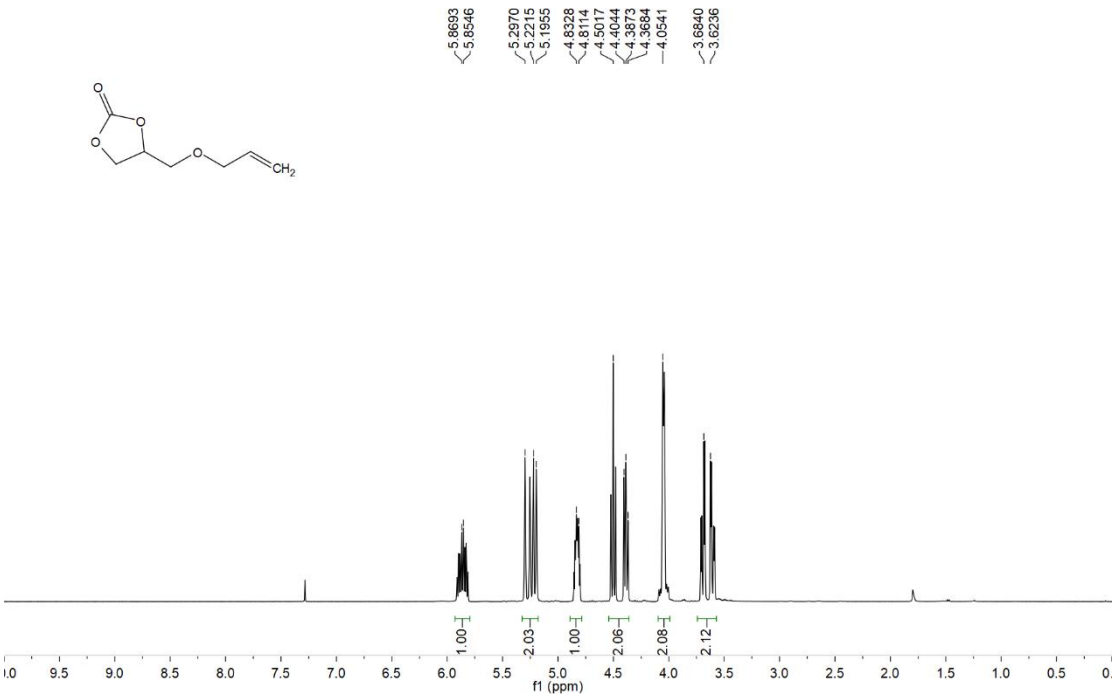


**Fig. S24** $^{1}$H NMR spectrum of **7l** in $CDCl_3$

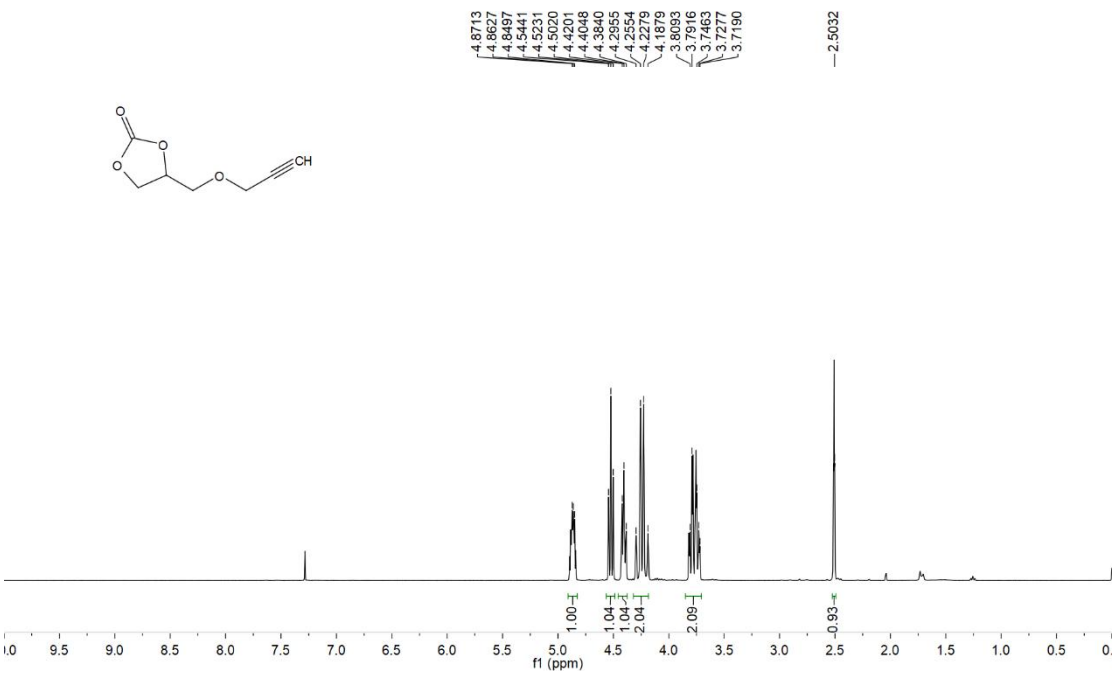


**Fig. S25** $^{1}$H NMR spectrum of **7m** in $CDCl_3$

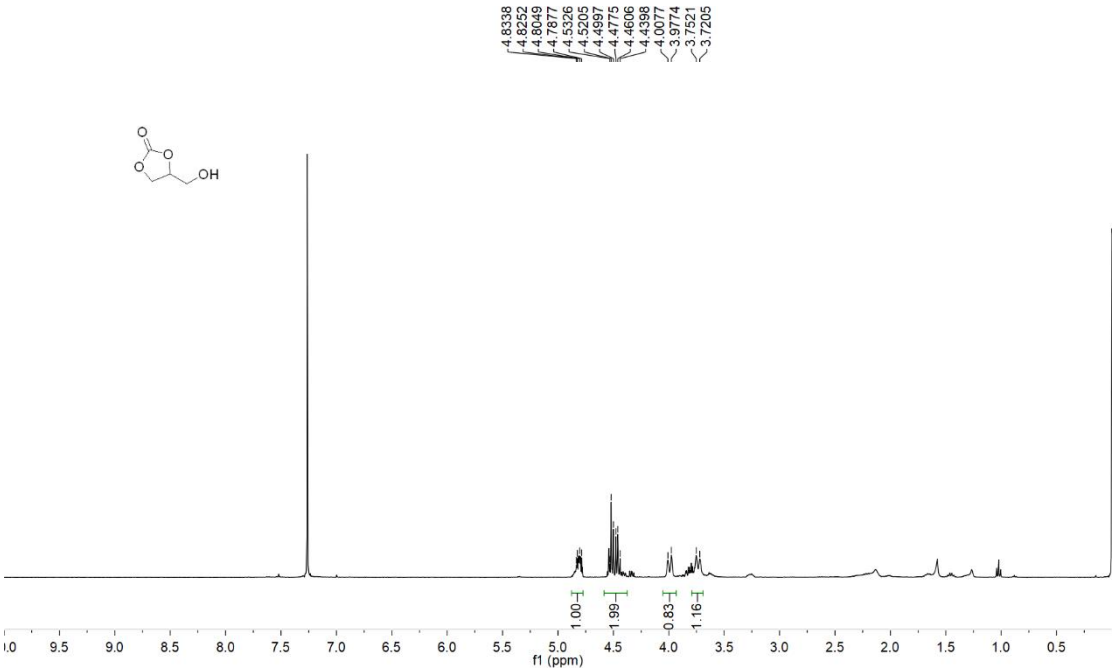


**Fig. S26** $^{1}$H NMR spectrum of **7n** in $CDCl_3$

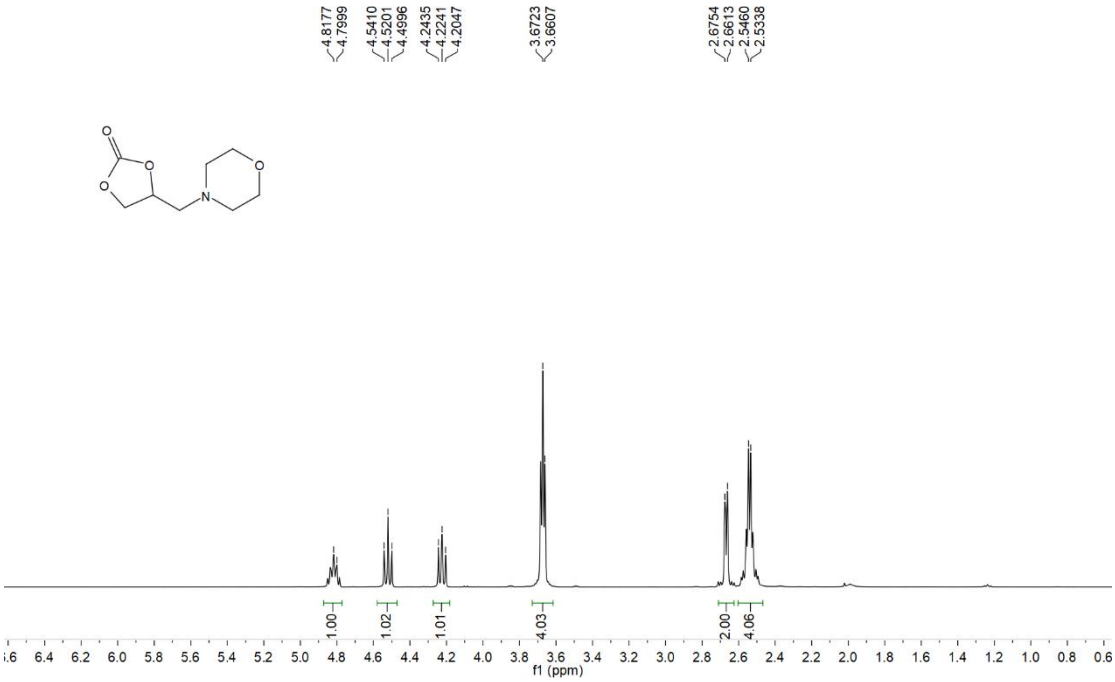


**Fig. S27** $^{1}$H NMR spectrum of **7o** in $CDCl_3$

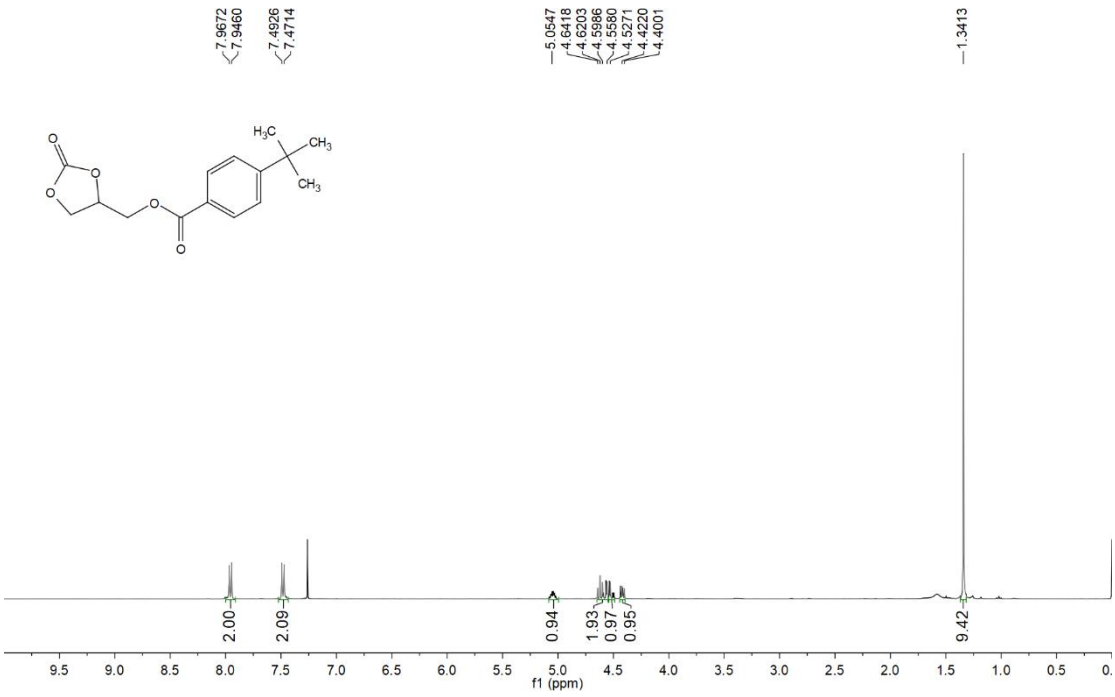


**Fig. S28** $^{1}$H NMR spectrum of **7p** in $CDCl_3$

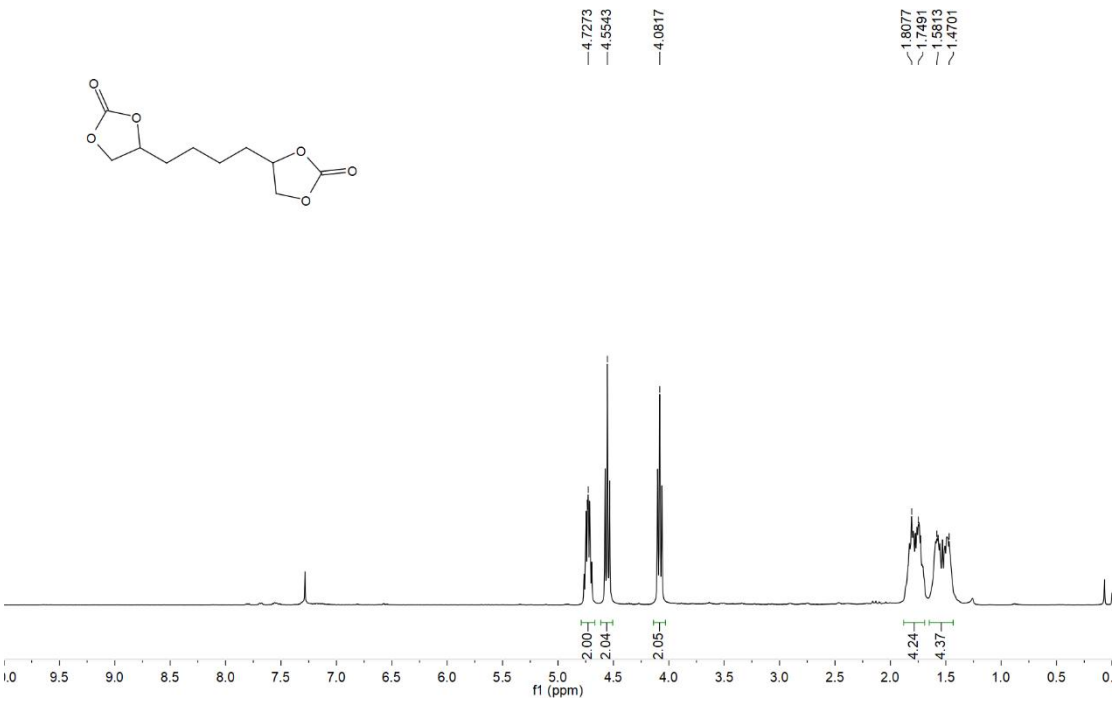


**Fig. S29** $^{1}$H NMR spectrum of **7q** in $CDCl_3$

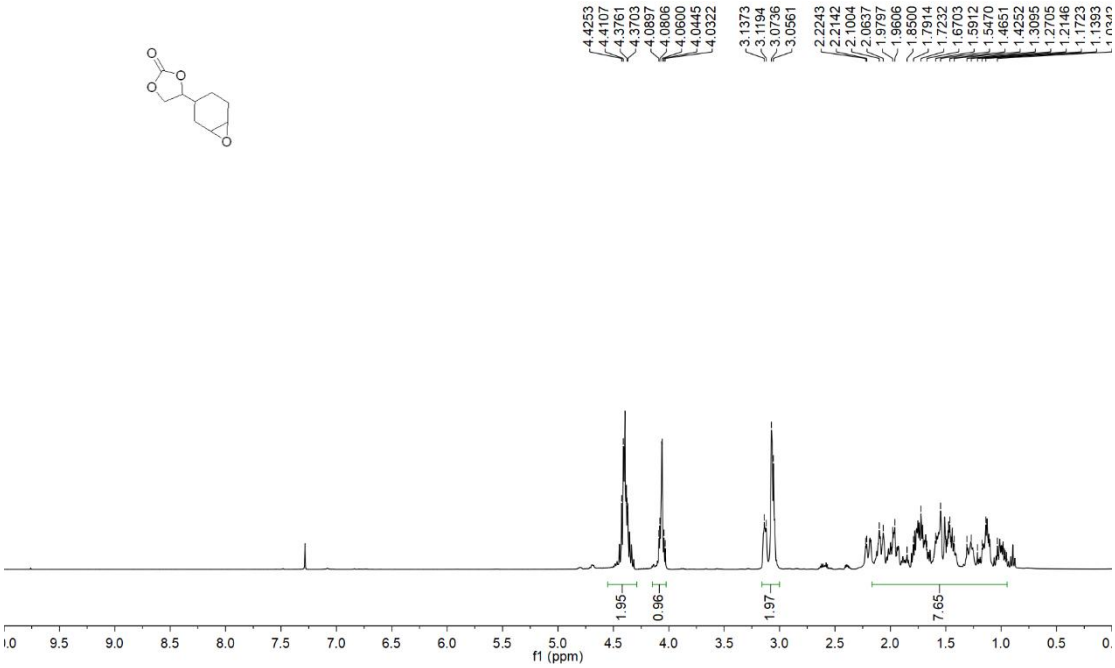


**Fig. S30** $^{1}$H NMR spectrum of **7r** in $CDCl_3$

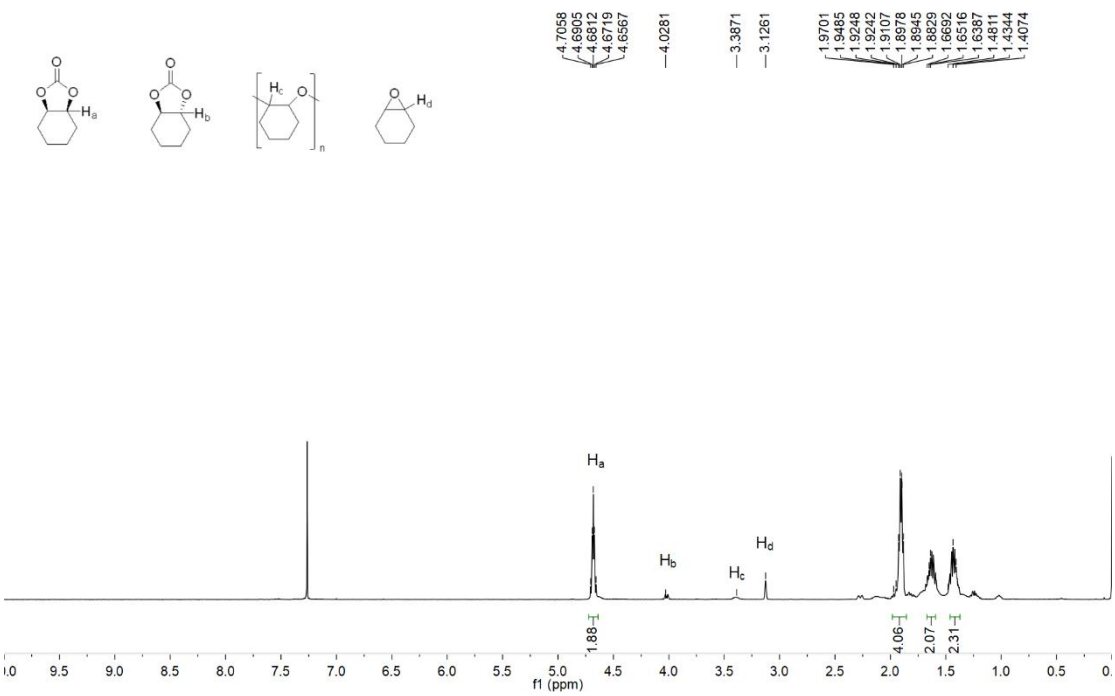


**Fig. S31** $^{1}$H NMR spectrum of **cis-9a** in $CDCl_3$

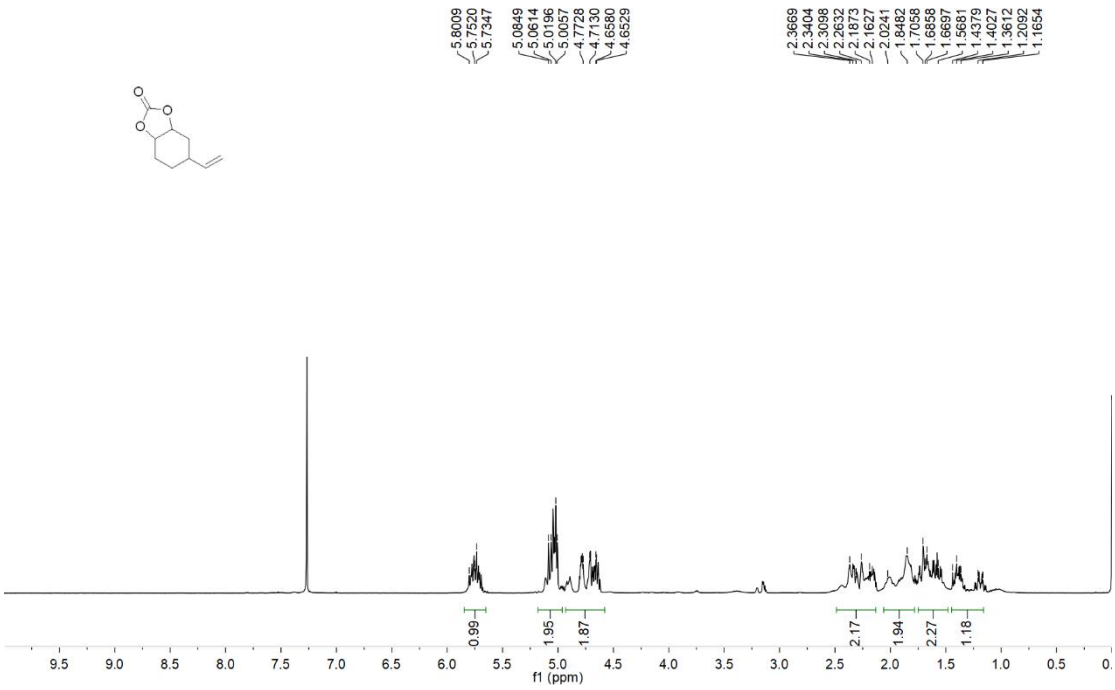


**Fig. S32** $^{1}$H NMR spectrum of **9b** in $CDCl_3$

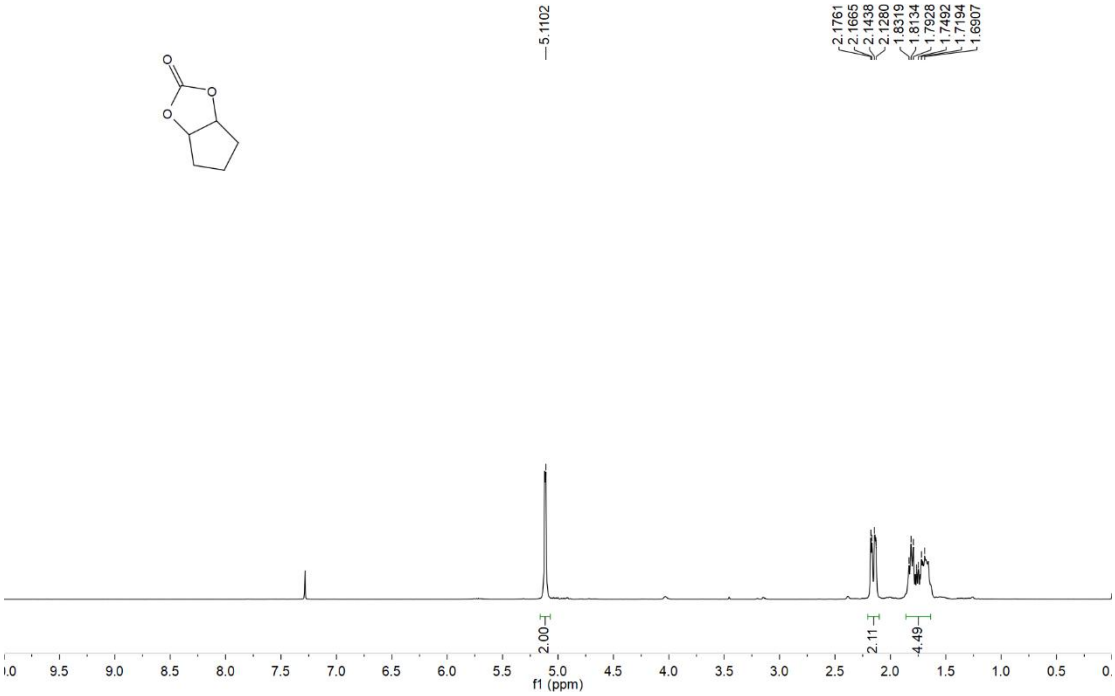


**Fig. S33** $^{1}$H NMR spectrum of **9c** in $CDCl_3$

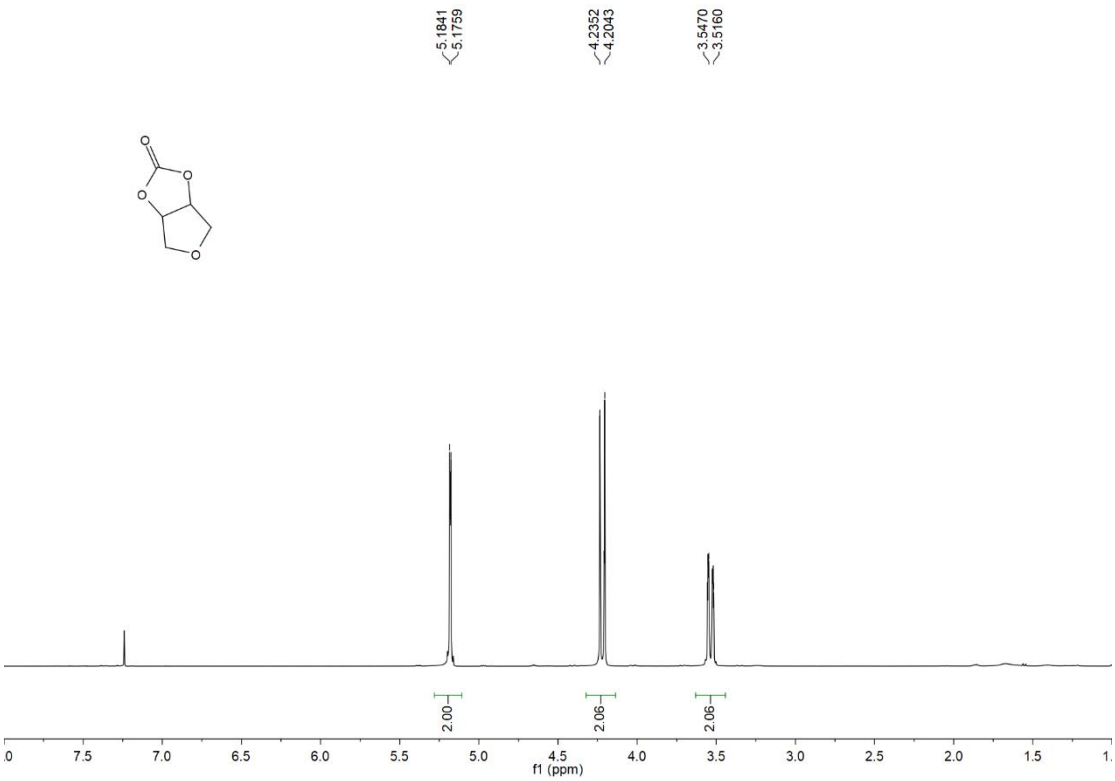


**Fig. S34** $^{1}$H NMR spectrum of **9d** in $CDCl_3$

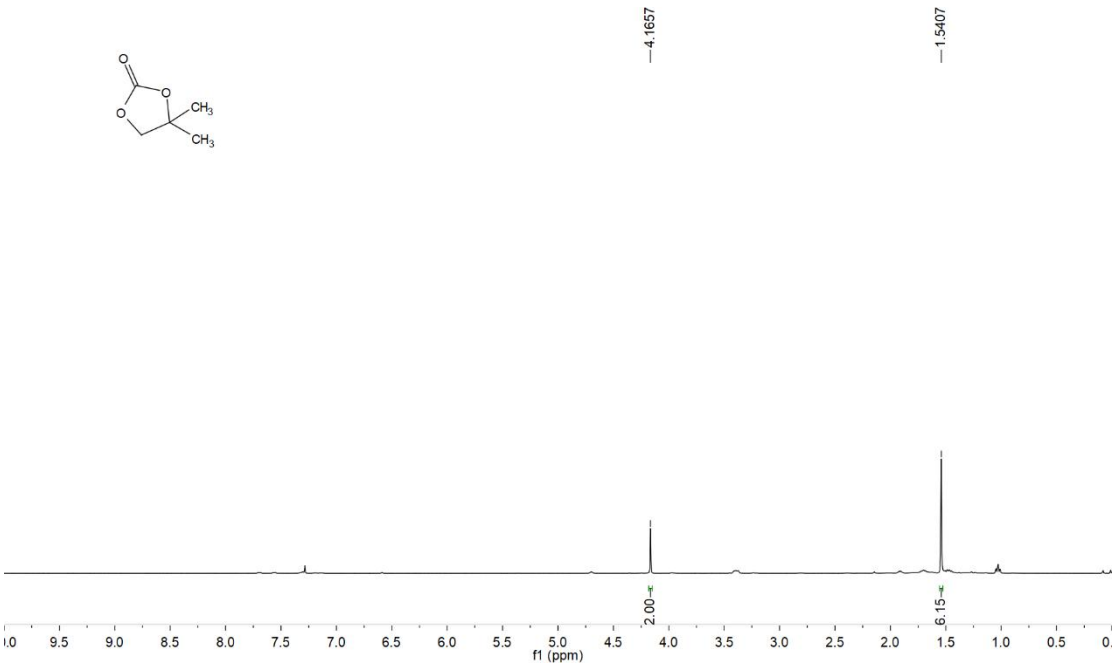


**Fig. S35** $^{1}$H NMR spectrum of **9e** in $CDCl_3$

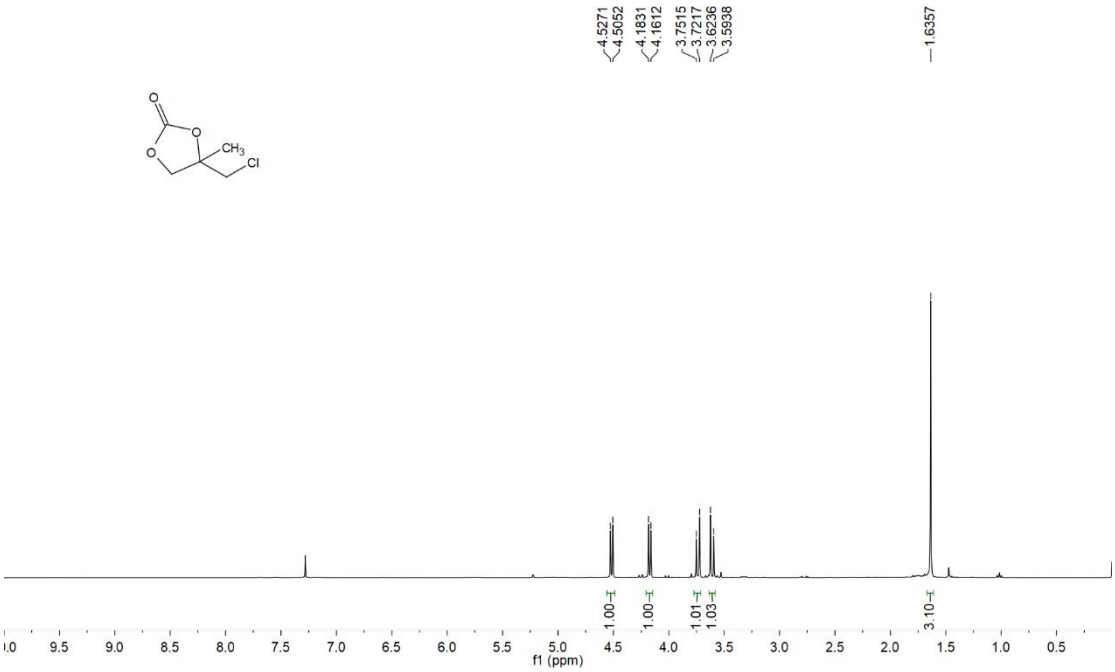


**Fig. S36** $^{1}$H NMR spectrum of **9f** in $CDCl_3$