Supporting Information for

Highly Regio- and Stereoselective Synthesis of Cyclic Carbonates from Biomass-derived Polyols via Organocatalytic Cascade Reaction

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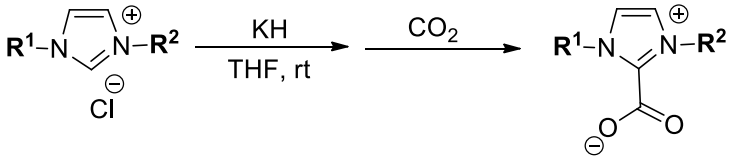
1. General information

Unless otherwise stated, all manipulations of oxygen- and/or moisture-sensitive materials were performed in a glove box or using standard Schlenk techniques under a dry nitrogen atmosphere. All commercially available chemicals were used without purification unless otherwise noted. All polyhydroxy chemicals were purchased from Energy chemical (purity ≥ 99%). Acetonitrile were distilled under N_2 atmosphere from P_2O_5. *N*,*N*-Dimethylformamide were distilled under N_2 atmosphere from CaH_2.

2. General procedure for the synthesis of Lewis base CO_2 adducts

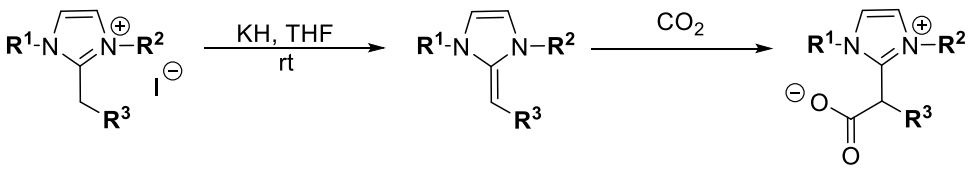
(1) The synthesis of **NHC-CO_2 1a-1c**



1a: $\mathbf{R^1}$ = ^{i}Pr, $\mathbf{R^2}$ = ^{i}Pr;
1b: $\mathbf{R^1}$ = 2,6-^{i}Pr$_2$C$_6$H$_3$, $\mathbf{R^2}$ = 2,6-^{i}Pr$_2$C$_6$H$_3$;
1c: $\mathbf{R^1}$ = IMes, $\mathbf{R^2}$ = IMes;

In a glove box, KH (2.4 mmol) was added to a suspension of *N,N′*-disubstituent imidazolium chloride (2.0 mmol) in THF (10 mL) respectively, and the mixture was stirred at room temperature for 4 h. After filtration, the filtrate was collected and exposed to 1.0 atm of CO_2 at ambient temperature for 2 h. The precipitate was collected by filtration and washed with ether (3×10 mL) and then dried under high vacuum to afford desired product **1a-1c**[S1].

(2) The synthesis of **NHO-CO_2 1d-1e**

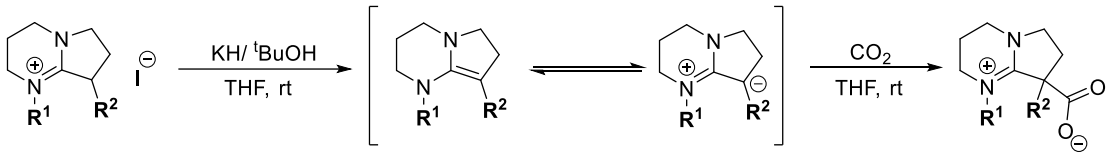


1d: $\mathbf{R^1}$ = Me, $\mathbf{R^2}$ = Me, $\mathbf{R^3}$ = Me;
1e: $\mathbf{R^1}$ = $\mathbf{R^2}$ = 2,6-^{i}Pr$_2$C$_6$H$_3$, $\mathbf{R^3}$ = H;

In a glove box, *N,N′*-disubstituent-2-alkyl imidazolium iodide (2 mmol) synthesized according to literature[S2] was added to a suspension of KH (0.16 g, 4 mmol) in THF (10 mL) and the mixture was stirred at ambient temperature for 48 h in the absence of light. After filtration to remove the salt, the filtrate was transferred to

the Schlenk flask equipped with a CO_2, and stirred to room temperature for 2 hours. The precipitate was formed and collected via filtration. Subsequent the solid was washed with *n*-hexane (10 mL) and then dried under high vacuum to afford the corresponding NHO-CO_2 adducts.

(3) The synthesis of **THPE-CO_2 1f-1i**



1f: R^1 = Me, R^2 = 2,6-^{i}Pr$_2$C$_6$H$_3$, R^3 = Me; **1g**: R^1 = Et, R^2 = 2,6-^{i}Pr$_2$C$_6$H$_3$, R^3 = Me;
1h: R^1 = Bn, R^2 = H; **1i** : R^1 = Me, R^2 = H;
1j : R^1 = Me, R^2 = Me; **1k**: R^1 = ^{n}Bu, R^2 = H;

In a glove box, KH (3.0 mmol) and KO*t*Bu (0.2 mmol) were added to a suspension of *N*-alkyl 1,5-diazabicyclo[4.3.0]non-5-ene (DBN) salts[S3] (2.0 mmol) in THF (10 mL) respectively, and the mixture was stirred at room temperature for 48 h in the absence of light. After filtration, the filtrate was collected and exposed to 1.0 atm of CO_2 at ambient temperature for 2 h. The resulting white precipitate was collected via filtration, washed with *n*-hexane (3×20 mL) and then dried under high vacuum to afford desired product **1f**-**1i**.

3. Determination for enantiomeric purity of cyclic carbonates

(*R*)-propylene carbonate: The *ee* value of the resultant propylene carbonate was determined by chiral GC analysis (GC column, Agilent HP-Chiral 19091G-B213, 80 ^{o}C, isothermal, t_R(major) = 10.6 min, t_R(minor) = 10.9 min).

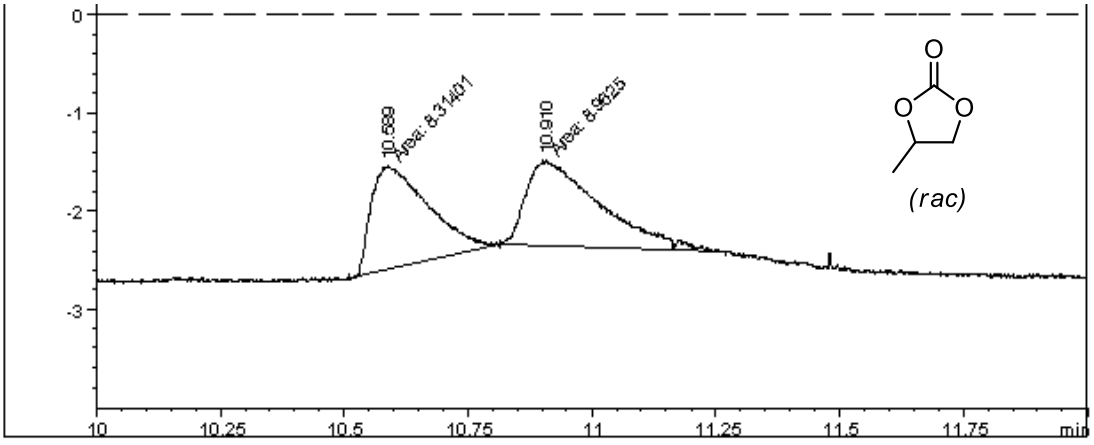


Figure S1. GC spectrum of *racemic* propylene carbonate

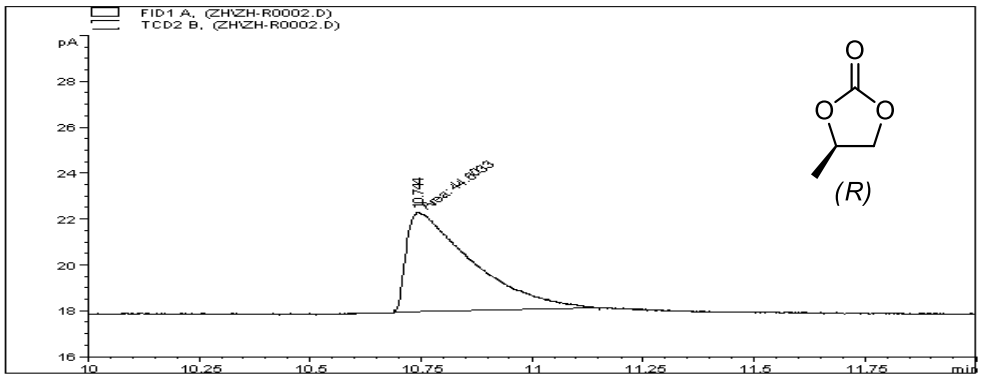
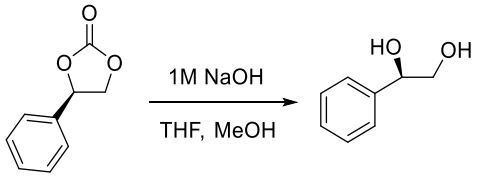


Figure S2. GC spectrum of (*R*)-propylene carbonate

***(R)*-1-Phenyl-1,2-ethanediol and *(S)*-1-Phenyl-1,2-ethanediol**: First, the hydrolysis of styrene carbonate **4p** was applied to obtain the corresponding 1-phenyl-1,2-ethanediol with retention of stereochemistry. The *ee* value of the resulting 1-phenyl-1,2-ethanediol was determined by chiral HPLC analysis (OD-H, 95:5 hexane : *i*-PrOH, t_R(major) = 17.1 min, t_R(minor) = 18.6 min).



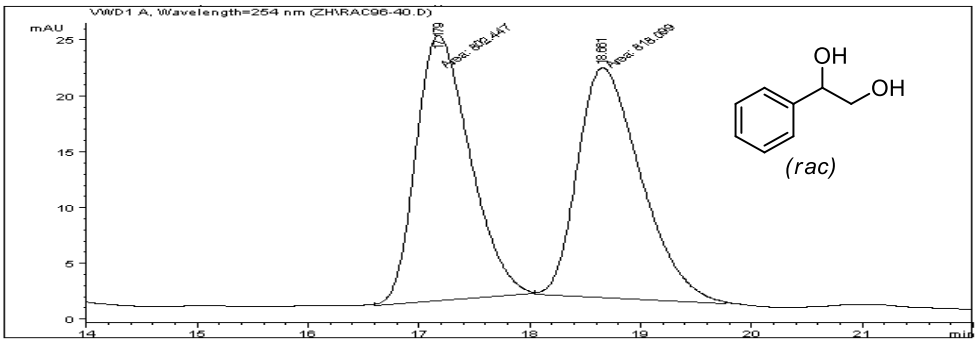


Figure S3. HPLC spectrum of *racemic* 1-phenyl-1,2-ethanediol

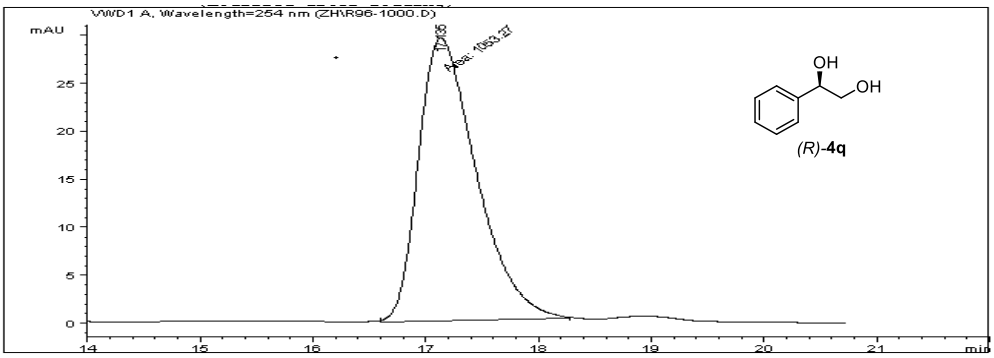


Figure S4. HPLC spectrum of (*R*)-1-phenyl-1,2-ethanediol

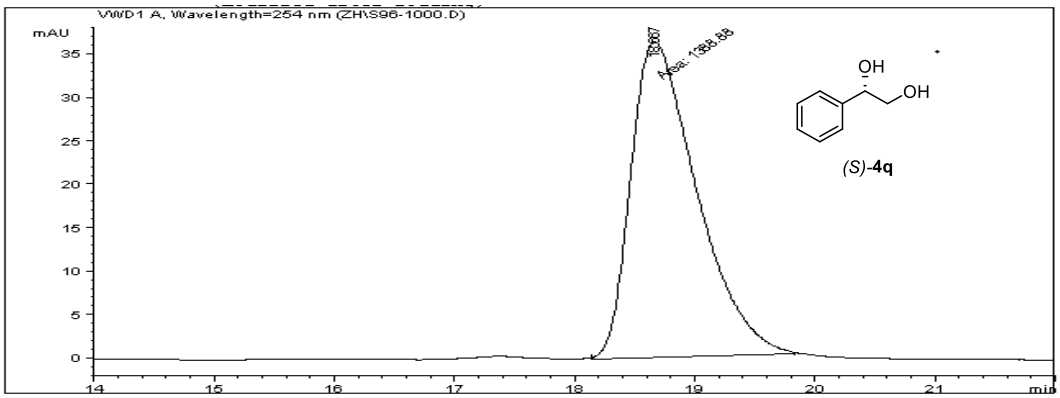


Figure S5. HPLC spectrum of (*S*)-1-phenyl-1,2-ethanediol

4. Reaction procedure for the one-pot synthesis of cyclic carbonate 4a,4q-4w

All operations involving air- and/or water-sensitive compounds were carried out in a glove box or with the standard Schlenk techniques under dry nitrogen. Solvents were dried and distilled prior to use. CO_2 (99.995%) was purchased from Dalian Institute of Special Gases. Propargylic alcohol **2** and all polyhydroxy chemicals were purchased from commercial sources and used without further purification.

(1) Under N_2 atmosphere, an oven-dried 10 mL Schlenk flask was charged with **Cat 1. 1h** (0.1 mmol, 10 mol%), propargylic alcohol **2** (1.0 mmol), 1,2,4,5-tetramethyl-benzen (33.5 mg, 0.25 mmol), and a magnetic stirring bar. The Schlenk flask was then recharged with CO_2 using a balloon. After 24 h, excessive CO_2 was carefully released, 1,2-dilol **3a** (1.0 mmol), **Cat. 2** MTBD (0.05 mmol, 5 mol%), and CH_3CN (0.5 mL) were added to the flask successively, and the reaction was left to continue at room temperature for 24 hours. The yields of **4a** and **5** were determined by ^{1}H NMR using 1,2,4,5-tetramethyl-benzen as the internal standard, and the residue was purified by column chromatography using petroleum ether/ethyl acetate as an eluent to give the desired products **4a** (5/1−5/3) and **5** (10/1−5/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.83 (dd, *J* = 13.4, 6.9 Hz, 1H), 4.53 (t, *J* = 8.0 Hz, 1H), 4.00 (dd, *J* = 8.3, 7.4 Hz, 1H), 1.46 (d, *J* = 6.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.1, 73.6, 70.6, 19.1.

(2) Under N_2 atmosphere, an oven-dried 10 mL Schlenk flask was charged with **Cat 1. 1h** (0.1 mmol, 10 mol%), propargylic alcohol **2** (1.0 mmol), 1,2,4,5-tetramethyl-benzen (33.5 mg, 0.25 mmol), and a magnetic stirring bar. The Schlenk flask was then recharged with CO_2 using a balloon. After 24 h, excessive CO_2 was

carefully released, glycerol **3q** (1.2 mmol), **Cat. 2** MTBD (0.05 mmol, 5 mol%), and CH_3CN (1.0 mL) were added to the flask successively, and the reaction was left to continue at room temperature for 24 hours. The yields of **4q** were determined by ^1H NMR using 1,2,4,5-tetramethyl-benzen as the internal standard, and the residue was purified by column chromatography to give the corresponding cyclic carbonate **4q**.

(3) Under N_2 atmosphere, an oven-dried 10 mL Schlenk flask was charged with **Cat 1. 1h** (0.1 mmol, 10 mol%), propargylic alcohol **2** (1.0 mmol), 1,2,4,5-tetramethyl- benzen (33.5 mg, 0.25 mmol), and a magnetic stirring bar. The Schlenk flask was then recharged with CO_2 using a balloon. After 24 h, excessive CO_2 was carefully released, glycerol **3q** (2.0 mmol), **Cat. 2** MTBD (0.1 mmol, 10 mol%), and CH_3CN (1.0 mL) were added to the flask successively, and the reaction was left to continue at 0 ^oC for 24 hours. The yields of **4q′** were determined by ^1H NMR in $CDCl_3$, and the residue was purified by column chromatography to give the corresponding cyclic carbonate **4q′**.

(4) Under N_2 atmosphere, an oven-dried 10 mL Schlenk flask was charged with **Cat 1. 1h** (0.1 mmol, 10 mol%), propargylic alcohol **2** (1.0 mmol), 1,2,4,5-tetramethyl-benzen (33.5 mg, 0.25 mmol), and a magnetic stirring bar. The Schlenk flask was then recharged with CO_2 using a balloon. After 24 h, excessive CO_2 was carefully released, alpha-Chloralose **3r** (4.0 mmol), **Cat. 2** MTBD (0.1 mmol, 10 mol%), and DMF (1.0 mL) were added to the flask successively, and the reaction was left to continue at room temperature for 24 hours. The yields of **4r** were determined by ^1H NMR in DMSO-d_6. All volatiles were removed under vacuum and the residue was recrystallized in Et_2O to give the corresponding cyclic carbonate **4r**.

(5) Under N_2 atmosphere, an oven-dried 10 mL Schlenk flask was charged with **Cat 1. 1h** (0.1 mmol, 10 mol%), propargylic alcohol **2** (1.0 mmol), 1,2,4,5-tetramethyl-benzen (33.5 mg, 0.25 mmol), and a magnetic stirring bar. The Schlenk flask was then recharged with CO_2 using a balloon. After 24 h, excessive CO_2 was carefully released, erythritol **3s** (1.0 mmol), **Cat. 2** MTBD (0.1 mmol, 10 mol%), and DMF (1.0 mL) were added to the flask successively, and the reaction was left to

continue at room temperature for 24 hours. The yields of **4s** were determined by ^{1}H NMR in $CDCl_3$, and the residue was purified by column chromatography to give the corresponding cyclic carbonate **4s**.

(6) Under N_2 atmosphere, an oven-dried 10 mL Schlenk flask was charged with **Cat 1. 1h** (0.1 mmol, 10 mol%), propargylic alcohol **2** (1.0 mmol), 1,2,4,5-tetramethyl-benzen (33.5 mg, 0.25 mmol), and a magnetic stirring bar. The Schlenk flask was then recharged with CO_2 using a balloon. After 24 h, excessive CO_2 was carefully released, erythritol **3s** (2.0 mmol), **Cat. 2** MTBD (0.1 mmol, 10 mol%), and DMF (1.0 mL) were added to the flask successively, and the reaction was left to continue at room temperature for 24 hours. The yields of **4s′** were determined by ^{1}H NMR in DMSO-*d*$_6$, and the residue was purified by column chromatography to give the corresponding cyclic carbonate **4s′**.

(7) Under N_2 atmosphere, an oven-dried 10 mL Schlenk flask was charged with **Cat 1. 1h** (0.1 mmol, 10 mol%), propargylic alcohol **2** (1.0 mmol), 1,2,4,5-tetramethyl-benzen (33.5 mg, 0.25 mmol), and a magnetic stirring bar. The Schlenk flask was then recharged with CO_2 using a balloon. After 24 h, excessive CO_2 was carefully released, adonitol **3t** (4.0 mmol), **Cat. 2** MTBD (0.1 mmol, 10 mol%), and DMF (1.0 mL) were added to the flask successively, and the reaction was left to continue at room temperature for 24 hours. The yields of **4t** were determined by ^{1}H NMR in DMSO-*d*$_6$. The resulting precipitate was collected via centrifuge, washed with DCM (3×2 mL) and then dried under high vacuum to afford desired product **4t**.

(8) Under N_2 atmosphere, an oven-dried 10 mL Schlenk flask was charged with **Cat 1. 1h** (0.1 mmol, 10 mol%), propargylic alcohol **2** (1.0 mmol), 1,2,4,5-tetramethyl-benzen (33.5 mg, 0.25 mmol), and a magnetic stirring bar. The Schlenk flask was then recharged with CO_2 using a balloon. After 24 h, excessive CO_2 was carefully released, xylitol **3u** (4.0 mmol), **Cat. 2** MTBD (0.1 mmol, 10 mol%), and DMF (1.0 mL) were added to the flask successively, and the reaction was left to continue at 0 ^{o}C for 24 hours. The yields of **4u** were determined by ^{1}H NMR in DMSO-*d*$_6$. The resulting precipitate was collected via centrifuge, washed with acetone

(3×2 mL) and then dried under high vacuum to afford desired product **4u**.

(9) Under N_2 atmosphere, an oven-dried 10 mL Schlenk flask was charged with **Cat 1. 1h** (0.1 mmol, 10 mol%), propargylic alcohol **2** (1.0 mmol), 1,2,4,5-tetramethyl-benzen (33.5 mg, 0.25 mmol), and a magnetic stirring bar. The Schlenk flask was then recharged with CO_2 using a balloon. After 24 h, excessive CO_2 was carefully released, D-sorbitol **3v** (4.0 mmol), **Cat. 2** MTBD (0.1 mmol, 10 mol%), and DMF (1.0 mL) were added to the flask successively, and the reaction was left to continue at room temperature for 24 hours. The yields of **4v** were determined by ^{1}H NMR in DMSO-*d*$_6$. The resulting precipitate was collected via centrifuge, washed with DCM (3×2 mL) and then dried under high vacuum to afford desired product **4v**.

(10) Under N_2 atmosphere, an oven-dried 10 mL Schlenk flask was charged with **Cat 1. 1h** (0.1 mmol, 10 mol%), propargylic alcohol **2** (1.0 mmol), 1,2,4,5-tetramethyl-benzen (33.5 mg, 0.25 mmol), and a magnetic stirring bar. The Schlenk flask was then recharged with CO_2 using a balloon. After 24 h, excessive CO_2 was carefully released, D-mannitol **3w** (4.0 mmol), **Cat. 2** MTBD (0.1 mmol, 10 mol%), and DMF (1.0 mL) were added to the flask successively, and the reaction was left to continue at room temperature for 24 hours. The yields of **4w** were determined by ^{1}H NMR in DMSO-*d*$_6$. The resulting precipitate was collected via centrifuge, washed with DCM (3×2 mL) and then dried under high vacuum to afford desired product **4w**.

5. Crystallography

Single crystals of complexes 4r, 4s′, 4t and 4u suitable for X-ray structural analysis were obtained from acetone solution at room temperature. Diffraction data were collected at 220 K on a Bruker SMART-CCD diffractometer using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The structures were solved by direct methods[S4] and refined by full-matrix least squares on F2. All nonhydrogen atoms were refined anisotropically, and the hydrogen atoms were included in idealized positions. All calculations were performed using the SHELXTL[S5] crystallographic software packages. **CCDC**: 1937067(**4r**), **CCDC**:

1940555 (**4s′**), **CCDC**: 1937066 (**4t**), **CCDC**: 1937068 (**4u**), **CCDC**: 1946539 (**4w**) contain supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

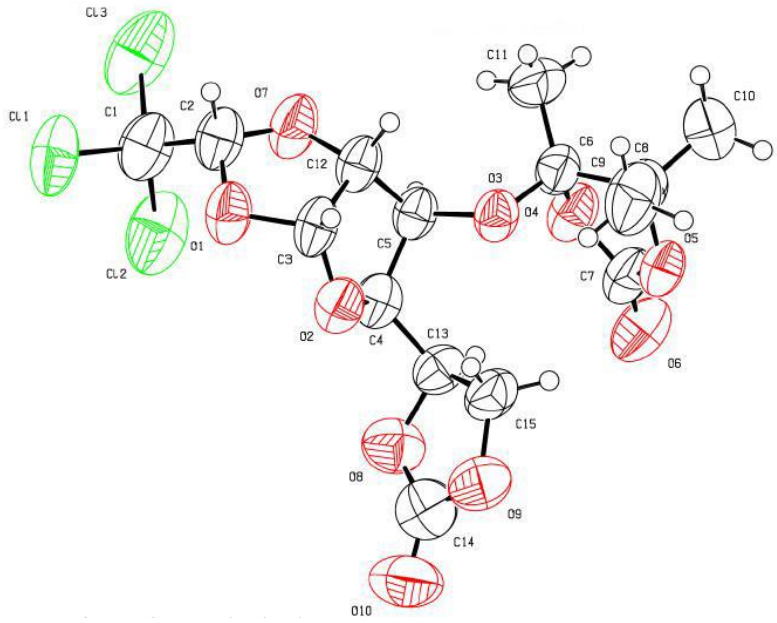


Figure S6. ORTEP Single Crystal X-Ray Diffraction of **4r**

Table S1. Crystal data and structure refinement for **4r**

Bond precision:	C-C = 0.0125 A	Wavelength=0.71073	
Cell:	a=8.238(7)	b=13.923(12)	c=17.649(15)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated		Reported
Volume	2024(3)		2024(3)
Space group	P 21 21 21		P 21 21 21
Hall group	P 2ac 2ab		P 2ac 2ab
Moiety formula	C15 H17 Cl3 O10		C15 H17 Cl3 O10
Sum formula	C15 H17 Cl3 O10		C15 H17 Cl3 O10
Mr	463.64		463.64
Dx,g cm-3	1.522		1.521
Z	4		4
Mu (mm-1)	0.502		0.502
F000	952.0		952.0
F000'	954.34		
h,k,lmax	9,16,21		9,16,21
Nref	3582[2060]		3582
Tmin,Tmax			0.463,0.746
Tmin'			

Correction method= # Reported T Limits: Tmin=0.463 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.74/1.00 Theta(max)= 25.023

R(reflections)= 0.0658(2013) wR2(reflections)= 0.1913(3582)

S = 1.031 Npar= 258

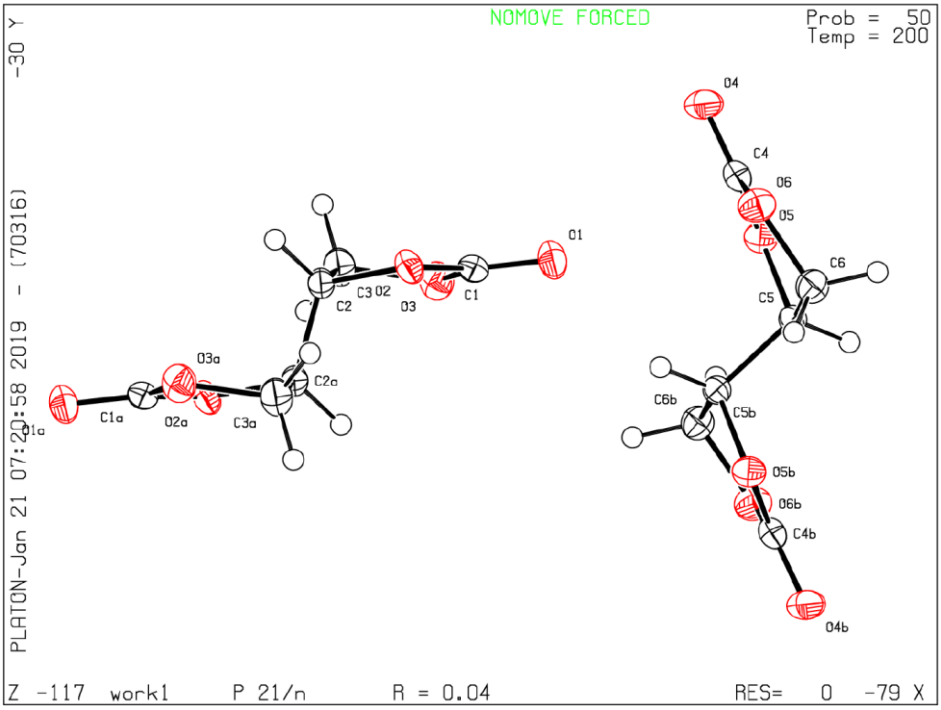


Figure S7. ORTEP Single Crystal X-Ray Diffraction of **4s'**

Table S2. Crystal data and structure refinement for **4s'**

Bond precision: C-C = 0.0023 A		Wavelength=0.71073	
Cell:	a=11.6926(10)	b=5.2936(5)	c=12.0745(11)
	alpha=90	beta=118.255(1)	gamma=90
Temperature:	200 K		
	Calculated		Reported
Volume	658.31(10)		658.31(10)
Space group	P 21/n		P 21/n
Hall group	-P 2yn		-P 2yn
Moiety formula	C6 H6 O6		?
Sum formula	C6 H6 O6		C6 H6 O6
Mr	174.11		174.11
Dx,g cm-3	1.757		1.757
Z	4		4
Mu (mm-1)	0.163		0.163
F000	360.0		360.0
F000'	360.30		
h,k,lmax	14,6,14		14,6,14
Nref	1197		1147
Tmin,Tmax	0.971,0.981		
Tmin'	0.968		
Correction method= Not given			
Data completeness= 0.958		Theta(max)= 25.248	
R(reflections)= 0.0380(1054)		wR2(reflections)= 0.1448(1147)	
S = 1.298		Npar= 109	

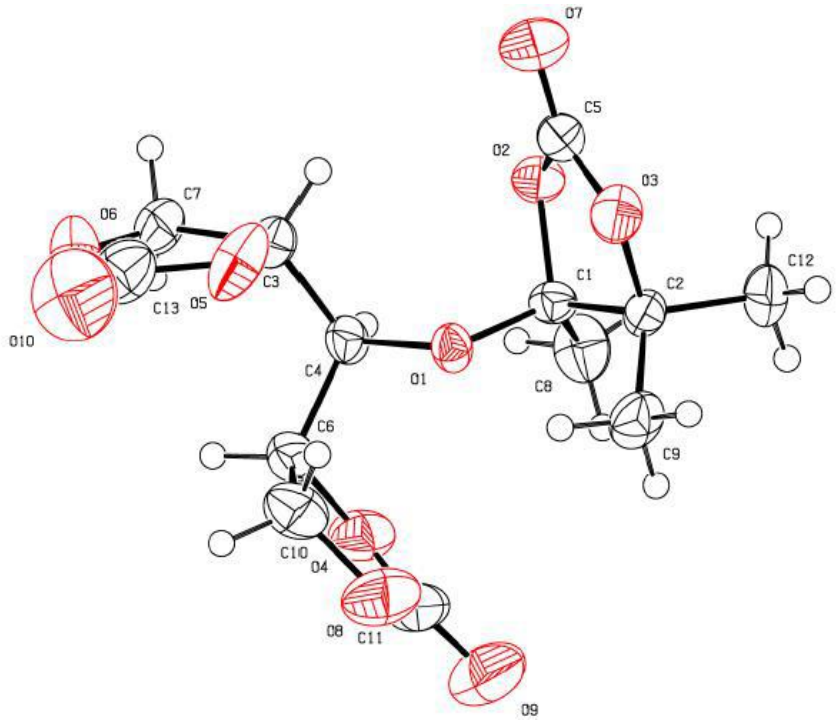


Figure S8. ORTEP Single Crystal X-Ray Diffraction of **4t**

Table S3. Crystal data and structure refinement for **4t**

Bond precision:	C-C = 0.0060 A	Wavelength=0.71073	
Cell:	a=14.095(2)	b=9.4714(14)	c=11.1536(18)
	alpha=90	beta=102.690(9)	gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	1452.6(4)	1452.6(4)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C13 H16 O10	C13 H16 O10	
Sum formula	C13 H16 O10	C13 H16 O10	
Mr	332.26	332.26	
Dx,g cm-3	1.519	1.519	
Z	4	4	
Mu (mm-1)	0.133	0.133	
F000	696.0	696.0	
F000'	696.53		
h,k,lmax	18,12,14	18,12,14	
Nref	3367	3280	
Tmin,Tmax		0.603,0.746	
Tmin'			

Correction method= # Reported T Limits: Tmin=0.603 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.974 Theta(max)= 27.585

R(reflections)= 0.0804(2129) wR2(reflections)= 0.2614(3280)

S = 1.088 Npar= 212

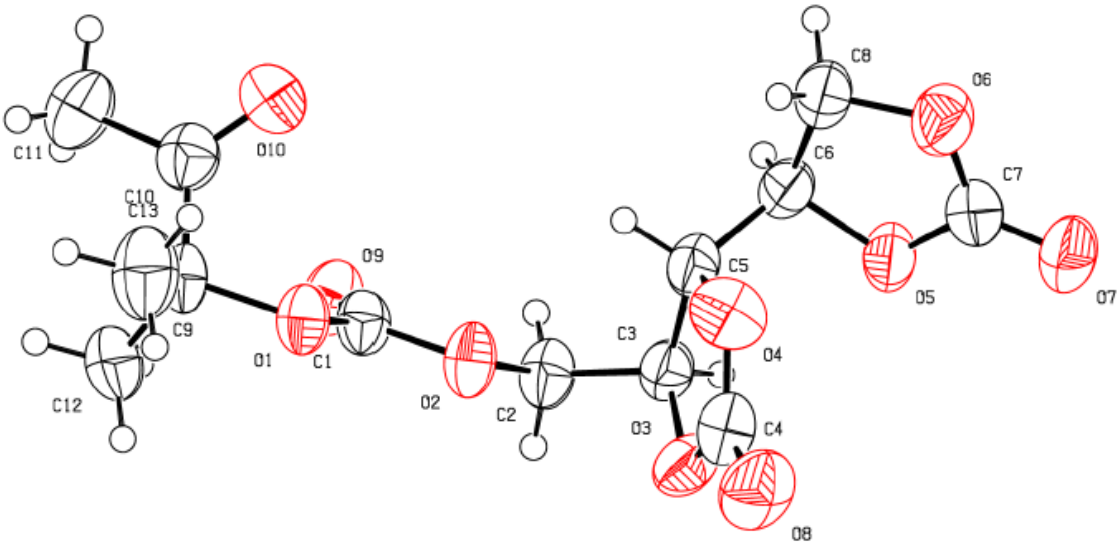


Figure S9. ORTEP Single Crystal X-Ray Diffraction of **4u**

Table S4. Crystal data and structure refinement for **4u**

Bond precision:	C-C = 0.0069 A	Wavelength=0.71073	
Cell:	a=10.764(8)	b=11.060(8)	c=25.394(19)
	alpha=90	beta=90	gamma=90
Temperature:	296 K		

	Calculated	Reported
Volume	3023(4)	3023(4)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C13 H16 O10	C13 H16 O10
Sum formula	C13 H16 O10	C13 H16 O10
Mr	332.26	332.26
Dx,g cm-3	1.460	1.460
Z	8	8
Mu (mm-1)	0.128	0.128
F000	1392.0	1392.0
F000'	1393.05	
h,k,lmax	12,13,30	12,13,30
Nref	2669	2670
Tmin,Tmax		0.336,0.746
Tmin'		

Correction method= # Reported T Limits: Tmin=0.336 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.026

R(reflections)= 0.0942(1415) wR2(reflections)= 0.2404(2670)

S = 1.021 Npar= 212

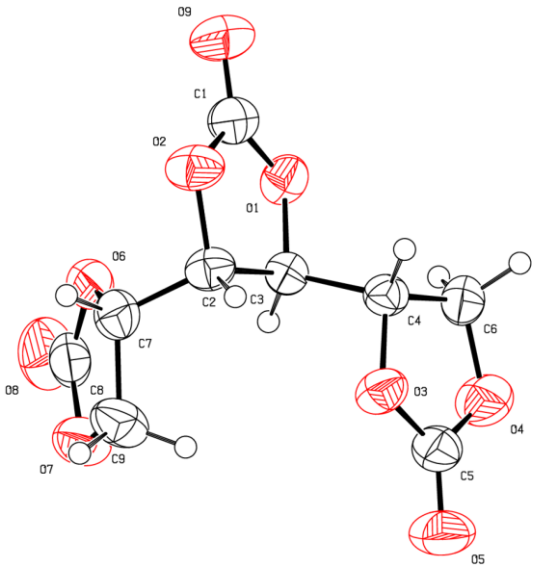


Figure S10. ORTEP Single Crystal X-Ray Diffraction of **4w**

Table S5. Crystal data and structure refinement for **4w**

Bond precision:	C-C = 0.0042 A		Wavelength=0.71073
Cell:	a=5.709(4)	b=12.143(8)	c=14.775(9)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	1024.3(12)	1024.3(12)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C9 H8 O9	C9 H8 O9
Sum formula	C9 H8 O9	C9 H8 O9
Mr	260.15	260.15
Dx,g cm-3	1.687	1.687
Z	4	4
Mu (mm-1)	0.157	0.157
F000	536.0	536.0
F000'	536.45	
h,k,lmax	7,15,19	7,15,19
Nref	2326[1372]	2326
Tmin,Tmax		0.657,0.746
Tmin'		

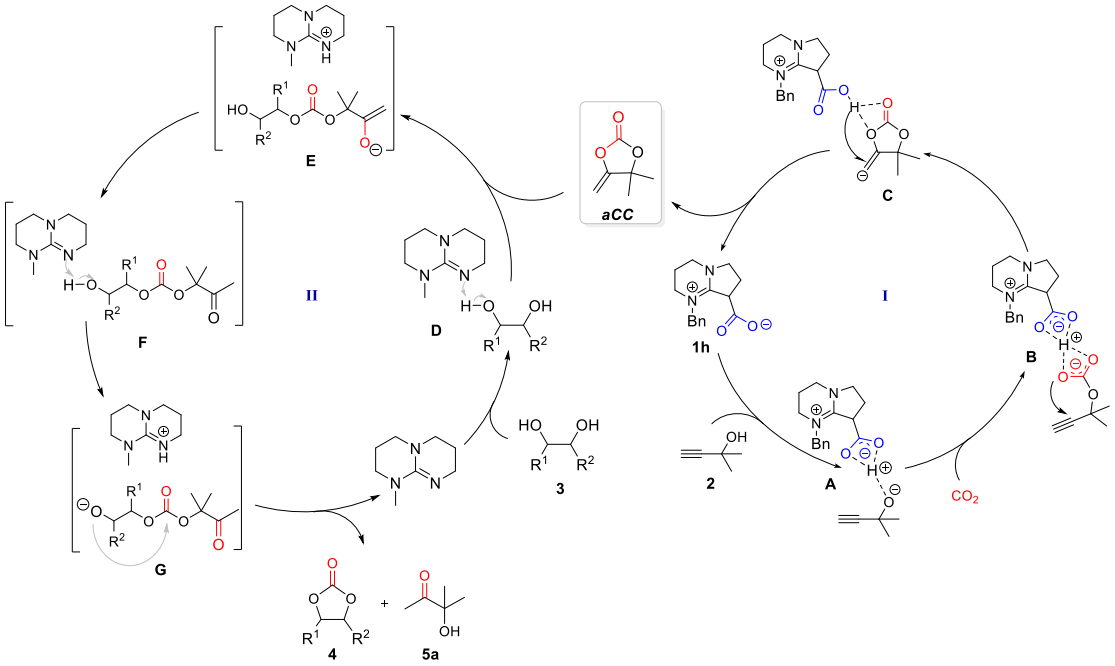
Correction method= # Reported T Limits: Tmin=0.657 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.70/1.00 Theta(max)= 27.352

R(reflections)= 0.0373(1555) wR2(reflections)= 0.0900(2326)

S = 0.989 Npar= 165

6. Possible reaction pathway for organocatalyzed cascade reaction

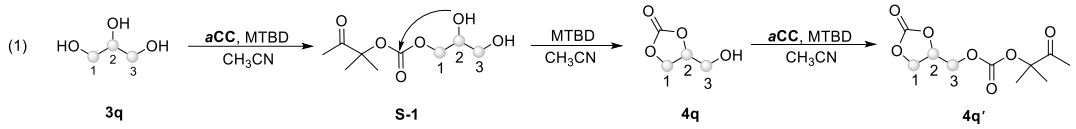


Scheme S1. Possible reaction pathway for organocatalytic relay cascade reaction of CO_2, vicinal diols and propargylic alcohols

Based on the experimental observations and previous literatures,[S2,S3] the reaction mechanism is proposed as above (Scheme S1). For the first catalytic cyclic, NHO-CO_2 adduct **1h** primarily acts as organic bases to activate the O-H bond of propargylic alcohols, which could favor the generation of the carboxylate intermediate **B**. Then, the [carbonate]$^-$ anion attacks the triple bond to give the alkenyl anion intermediate **C**. Finally, the protonation of intermediate **C** leads to the formation of α-alkylidene cyclic carbonate **aCC**, and regeneration of free NHO-CO_2 adduct.

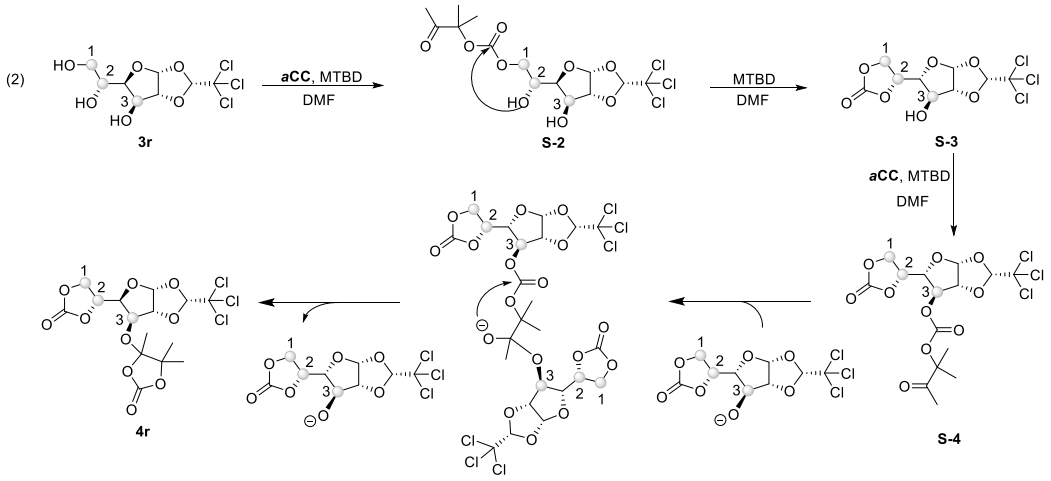
Afterwards, α-alkylidene cyclic carbonate **aCC** as carboxylation reagent, enters the another catalytic cycle. MTBD as organocatalyst firstly activated the O-H bond of vicinal diol to accelerate the nucleophilic ring opening of **aCC** and vicinal diol, thus forming intermediate **E**. Furthermore, the protonation of intermediate **E** lead to the formation of intermediate **F**. Next, MTBD catalyzed the cyclization of intermediate **F** *via* intramolecular transesterification, which could result in desired cyclic carbonate **4** and α-hydroxyl ketone **5**.

7 Possible reaction pathway for the formation of biomass-based cyclic carbonates Triol substrates



Scheme S2. Possible reaction pathway for **3q** involved reaction

With these results in hand, the reaction mechanisms have been proposed (Scheme S2). Because the primary OH group is more acidic than secondary OH group, when using glycerol **3q** as substrate, the transesterification reaction started from primary hydroxyl group, and intermediate **S-1** was formed. Then, as a result of the attack of the secondary alkoxy group (position 2) on the carbonyl group of linear carbonate, cyclic carbonate **4q** containing an additional hydroxyl group, was produced. For higher excesses of ***a*CC**, **4s** was transformed into the corresponding carbonate **4q′** as a result of the attack of the alkoxy group (position 3) in **4q** on the carbonyl group of ***a*CC** *via* transesterification.

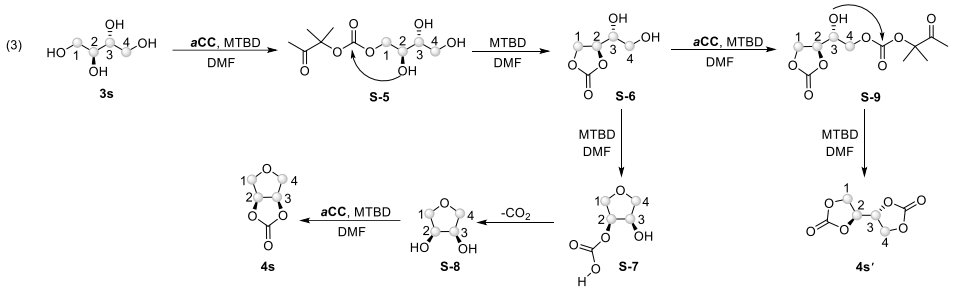


Scheme S3. Possible reaction pathway for **3r** involved reaction

As for **3r** as substrate, intermediate **S-4** should be firstly generated through the similar process (Scheme S3). Due to the lower reactivity of secondary OH group than primary OH group, the conversion of **S-3** to **S-4** could not be accomplished completely, even in the presence of excess amount of ***a*CC** generated in-situ. Furthermore, nucleophilic attack by nucleophilic oxygen of the residual **S-3** (position

3) to the carbonyl group of acetone in **S-4**, along with subsequent Intramolecular transesterfication, affords the final bicyclic carbonate **4r**, which structure have been proved by X-ray diffraction.

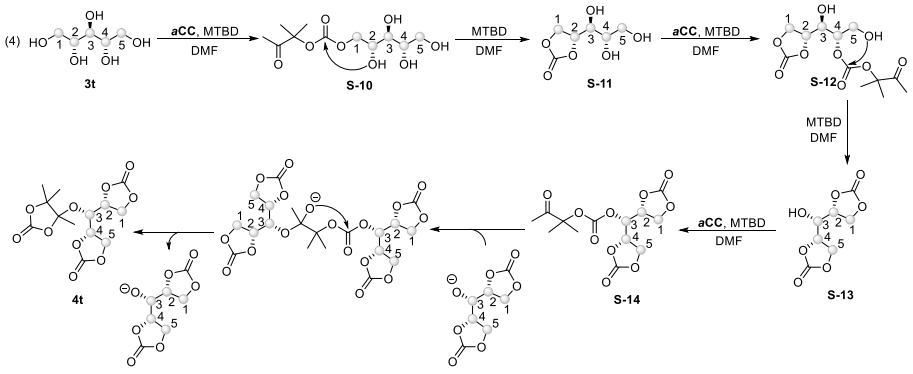
Tetrol substrates



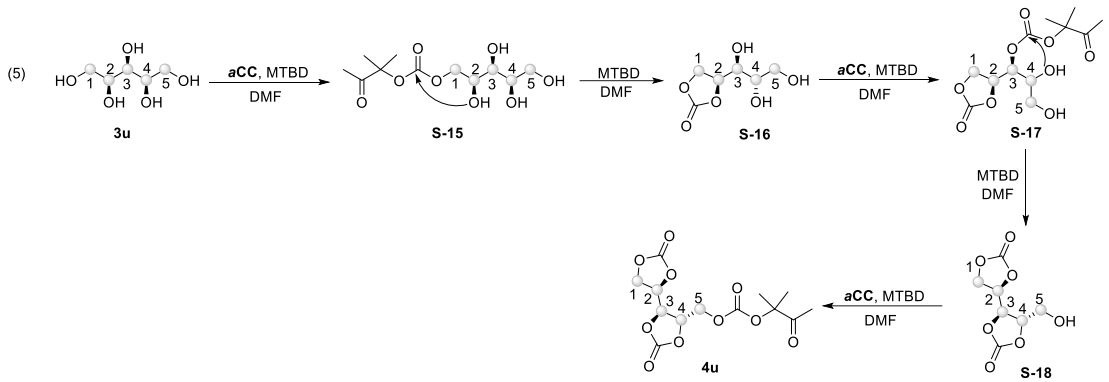
Scheme S4. Possible reaction pathway for **3s** involved reaction

The reaction of Erythritol **3s** with ***α*CC** in the presence of MTBD can proceed according to two reaction pathways, depending on molar ratio of substrates (Scheme S4). At the reaction beginning, 4-(1,2-dihydroxy-ethyl)-1,3-dioxolan-2-one (**S-6**) was formed as an intermediate *via* transesterification. Subsequently, the primary alkoxy group (position 4) could attack the alkyl carbon atom in the 1,3-dioxolan-2-one ring and as a result an unstable hydrocarbonate group is formed (**S-7**), which after decarboxylation is transformed into a hydroxyl group (**S-8**). When the reaction of the resulting 3,4-dihydroxytetrahydrofuran **S-8** was carried out with molar excess of ***α*CC** under the same reaction conditions, 2,4,7-trioxa-3-oxy-bicyclo[3.3.0]octane **4s** a bicyclic derivative of tetrahydrofuran was formed. Moreover, in the presence of excess amount of ***α*CC** (4.0 equivalents to **3s**), intermediate **S-6** selectively react with ***α*CC** to form biscyclic carbonate **4s′**.

Pentitol substrates



Scheme S5. Possible reaction pathway for **3t** involved reaction



Scheme S6. Possible reaction pathway for **3u** involved reaction

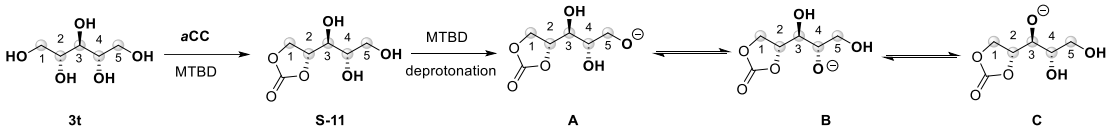
Based on the single crystal structure data of product and DFT calculation, the possible mechanism using pentitol as substrate is proposed (Scheme S5). As for adonitol, 1,2,3-trihydroxypropyl-1,3-dioxolan-2-one **S-11** was formed firstly via transesterification. Furthermore, the alkoxy group on carbon 4 preferentially react with ***α*CC** to form intermediate **S-12**, then the primary alkoxy group on carbon 5 attack the carbonyl group of linear carbonate *via* an intramolecular nucleophilic cyclization to afford bicyclic carbonate **S-13**. Then, **S-13** undergoes a nucleophilic ring-opening reaction by secondary OH group (position 3) to generate intermediate **S-14**. Finally, **4t** was selectively formed by ring-chain tautomerization of intermediate **S-14**.

As for xylitol, 1,2,3-trihydroxypropyl-1,3-dioxolan-2-one **S-16** was formed firstly via transesterification. Further, the alkoxy group on carbon 3 preferentially react with ***α*CC** to form intermediate **S-17**, then the neighboring alkoxy group on carbon 4 attack the carbonyl group of linear carbonate *via* an intramolecular nucleophilic cyclization to afford bicyclic carbonate **S-18**. Finally, **S-18** undergoes a nucleophilic ring-opening reaction by the remaining OH group (position 5) to generate the final product **4u** (Scheme S6).

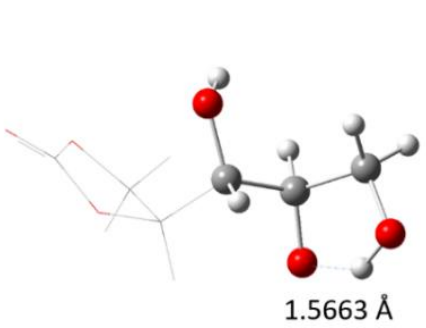
In order to illustrate the proposed reaction mechanism, DFT calculation was performed with Gaussian 16. All geometries of intermediates involving the deprotonation of **S-11** and **S-16** were fully optimized in DMF solution (experimentally used) with the continuum solvation model (SMD) at the M06-2X/6-31G** level of theory. To improve the accuracy of the energy, the single

point energy of each optimized structure was calculated at the M06-2X (SMD, DMF)/6-311G** level.

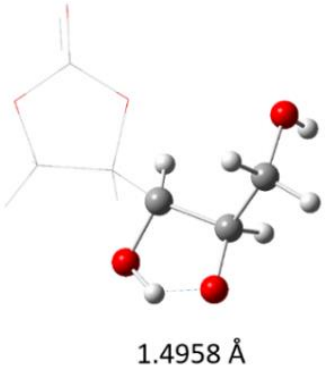
For **3t** based process, the formation of intermediate **B** is favored by strong intermolecular dihydrogen bonds (Scheme S7), while for **3u**, intermediate **F** is easily formed (Scheme S8). Noting that the origin of the chemoselectivity may be also closely related to the dihydrogen bonds.



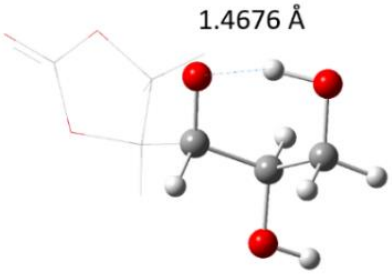
Scheme S7. Selective deprotonation process of **S-11**



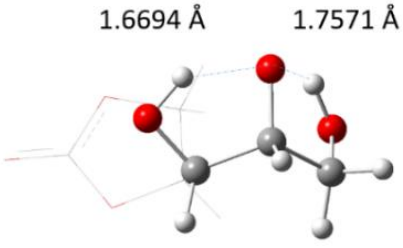
Intermediate 1: **6.8 kcal/mol**



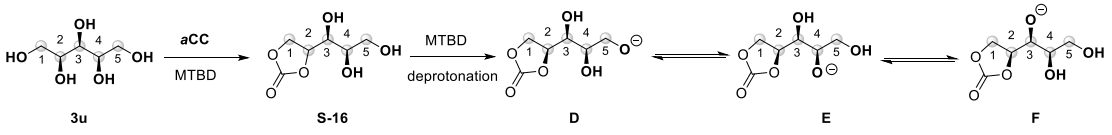
Intermediate 2: **9.7 kcal/mol**



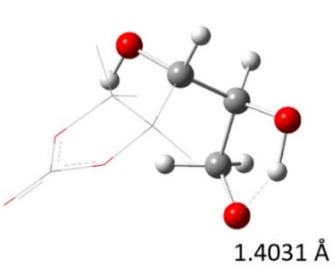
Intermediate 3: **1.7 kcal/mol**

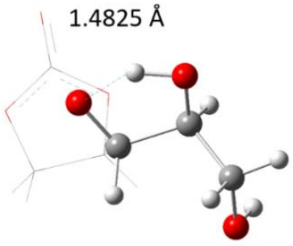


Intermediate 4: **0.0 kcal/mol**

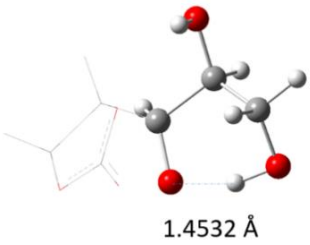


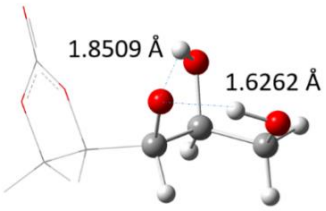
Scheme S8. Selective deprotonation process of **S-16**



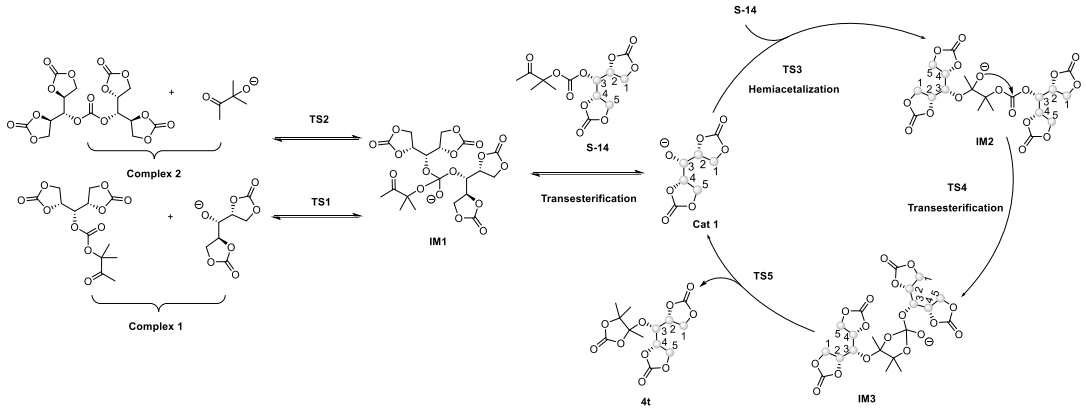


Intermediate 5: **10.9 kcal/mol** **Intermediate 6:** **5.2 kcal/mol**



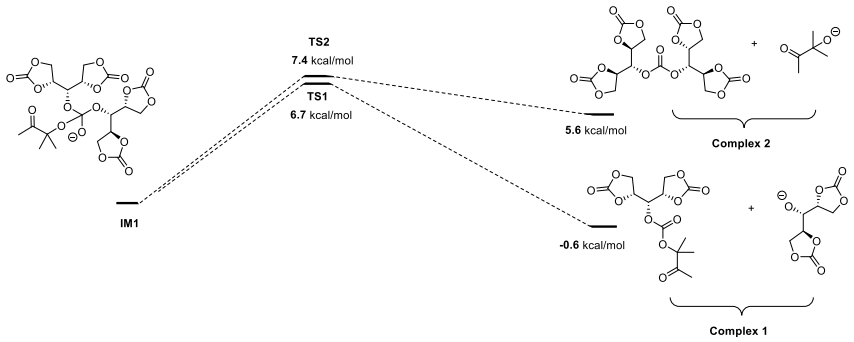


Intermediate 7: **4.0 kcal/mol** **Intermediate 8:** **0.0 kcal/mol**



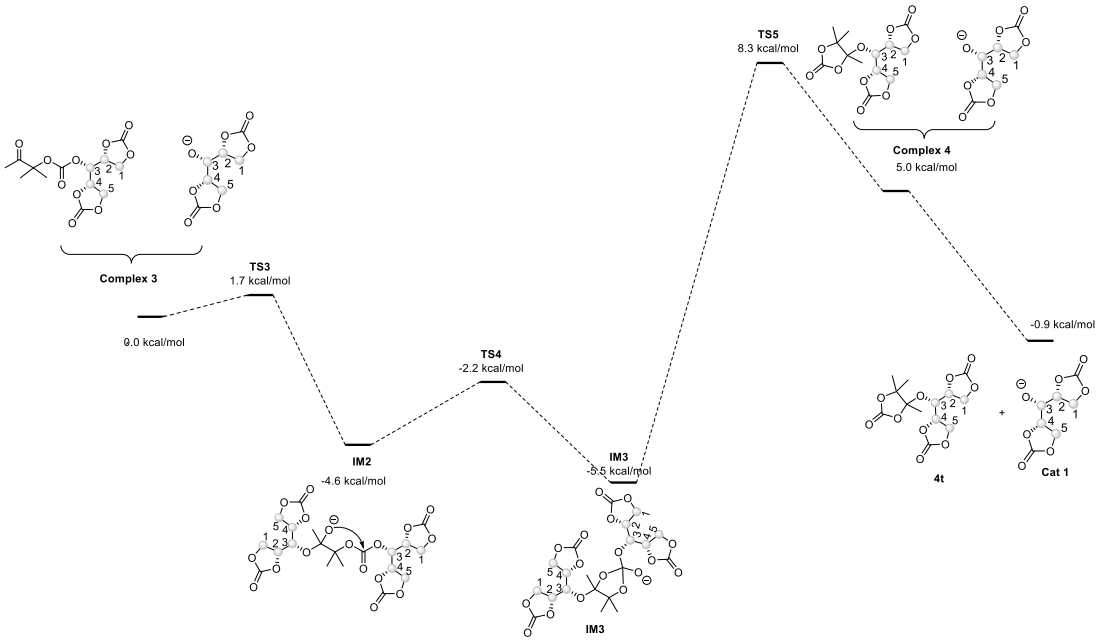
Scheme S9. Possible pathway for the formation of **4t**

The catalytic transformation of polyols is not as easy as it looks due to the presence of multiple reactive sites. Compared with reported methods, this process could smoothly take place under room temperature, which is beneficial to enhance the chemo-selectivity. For **3t**-involved process, the intermediate **S14** could be attacked by **Cat1** by different pathways (Scheme S9). One is through a transesterification process, in which the alcoholate **Cat1** attacks the ester group to form intermediate **IM1** (Scheme S10). Calculation results showed that the releasing ability of the alcoholate **Cat 1**(**TS1**: 6.7 kcal/mol) is better than α-hydroxyl ketone group (**TS2**: 7.4 kcal/mol). More importantly, **complex 1** is thermodynamically stable intermediate in this reversible transesterification.



Scheme S10. Possible pathway for reversible transesterification

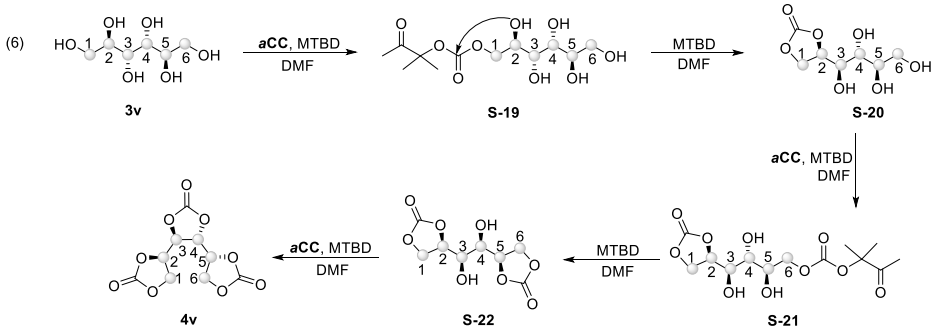
Alternatively, the catalytic reaction might proceed through a sequential hemiacetalization/transesterification process, in which the alcoholate **Cat 1** firstly attacks the β-carbonyl group of intermediate **IM1** to form hemiacetal intermediate **IM2** with an energy barrier of 1.7 kcal/mol and released energy of 4.6 kcal/mol. Subsequently, **IM2** was smoothly converted to **IM3** via intramolecular transesterification with an energy barrier of 2.4 kcal/mol. It is worth noting that **Cat1**-releasing step is the rate-determining step with an energy barrier of 13.8 kcal/mol, and the thermodynamically stable tetrasubstituted cyclic carbonate **4t** was generated, and the alcoholate **Cat 1** was released for the next catalytic cycle (Scheme S11).



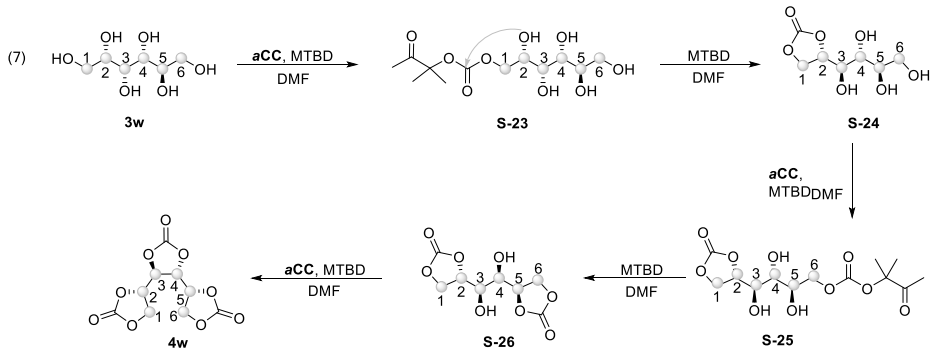
Scheme S11. Possible pathway for the sequential hemiacetalization/transesterification reaction.

Hexitol substrates

As for D-sorbitol **3v**/D-mannitol **3w** as substrates, the transesterification started from the primary OH group, and the corresponding bicyclic carbonates **S-22**/**S-26** were formed. Then the remaining vicinal diols on carbon 3 and 4 further reacted with excess ***a*CC** generated in-situ *via* transesterification, thus obtaining tricyclic carbonates **4v/4y** as the final products.

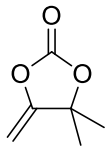


Scheme S12. Possible reaction pathway for **3v** involved reaction

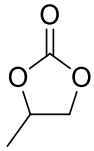


Scheme S3. Possible reaction pathway for **3w** involved reaction

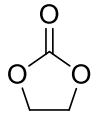
8. Characterization data



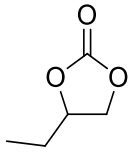
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.67 (d, *J* = 3.9 Hz, 1H), 4.28 (d, *J* = 4.0 Hz, 1H), 1.53 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 158.6, 151.1, 85.2, 84.6, 27.4.



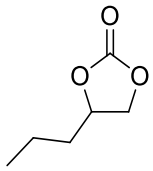
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.83 (dd, *J* = 13.4, 6.9 Hz, 1H), 4.53 (t, *J* = 8.0 Hz, 1H), 4.00 (dd, *J* = 8.3, 7.4 Hz, 1H), 1.46 (d, *J* = 6.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.1, 73.6, 70.6, 19.1.



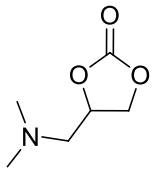
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.50 (s, 4H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.6, 64.7.



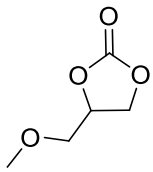
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.79 – 4.58 (m, 1H), 4.52 (t, *J* = 8.1 Hz, 1H), 4.08 (dd, *J* = 8.4, 7.0 Hz, 1H), 1.96 – 1.66 (m, 2H), 1.03 (t, *J* = 7.5 Hz, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.2, 78.1, 69.1, 27.1, 8.6.



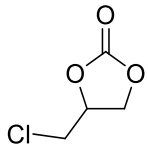
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.81 – 4.62 (m, 1H), 4.50 (t, *J* = 8.1 Hz, 1H), 4.04 (dd, *J* = 8.3, 7.3 Hz, 1H), 1.76 (ddd, *J* = 7.5, 4.5, 1.7 Hz, 1H), 1.69 –1.55(m, 1H), 1.53 – 1.32 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.2, 77.0, 69.5, 35.9, 17.9, 13.7.



^{1}H NMR (400 MHz, $CDCl_3$) δ 5.46 – 4.64 (m, 1H), 4.52 (t, *J* = 8.3 Hz, 1H), 4.21 (t, *J* = 7.8 Hz, 1H), 2.86 – 2.48 (m, 2H), 2.30 (d, *J* = 2.7 Hz, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.0, 75.2, 68.2, 61.3, 46.4.

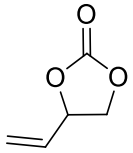


^{1}H NMR (400 MHz, $CDCl_3$) δ 4.77 (dt, *J* = 9.5, 3.6 Hz, 1H), 4.45 (t, *J* = 8.4 Hz, 1H), 4.31 (dd, *J* = 8.4, 6.1 Hz, 1H), 3.59 (dd, *J* = 11.2, 3.4 Hz, 1H), 3.49 (dd, *J* = 11.2, 3.8 Hz, 1H), 3.35 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.1, 75.2, 71.4, 66.1, 59.5.

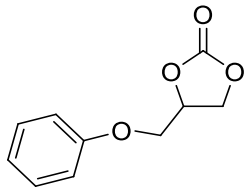


^{1}H NMR (400 MHz, $CDCl_3$) δ 4.96 (dt, *J* = 9.7, 5.7 Hz, 1H), 4.77 – 4.52 (m, 1H), 4.42 (dd, *J* = 8.9, 5.7 Hz, 1H), 4.00 – 3.34 (m, 2H). **^{13}C NMR** (101 MHz,

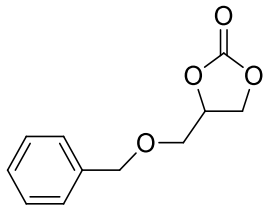
$CDCl_3$) δ 154.2, 74.3, 67.1, 43.7.



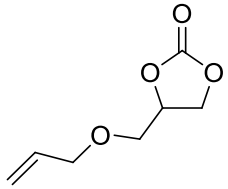
^{1}H NMR (400 MHz, $CDCl_3$) δ 5.82 (ddd, *J* = 17.3, 10.4, 7.0 Hz, 1H), 5.38 (dd, *J* = 30.8, 13.8 Hz, 2H), 5.07 (dd, *J* = 15.0, 7.5 Hz, 1H), 4.53 (t, *J* = 8.4 Hz, 1H), 4.21 – 4.03 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.8, 132.1, 120.9, 77.3, 69.0.



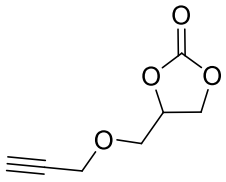
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (dt, *J* = 18.5, 9.2 Hz, 2H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.91 (d, *J* = 7.8 Hz, 2H), 5.03 (ddt, *J* = 8.1, 5.9, 4.0 Hz, 1H), 4.61 (t, *J* = 8.4 Hz, 1H), 4.53 (dd, *J* = 8.5, 5.9 Hz, 1H), 4.24 (dd, *J* = 10.6, 4.2 Hz, 1H), 4.15 (dd, *J* = 10.6, 3.6 Hz, 1H).**^{13}C NMR** (101 MHz, CDCl3) δ 157.9, 154.8, 129.8, 122.1, 114.7, 74.3, 67.0, 66.3.



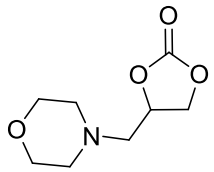
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.22 (m, 5H), 4.79 (ddt, *J* = 9.3, 6.9, 3.5 Hz, 1H), 4.57 (q, *J* = 12.0 Hz, 2H), 4.43 (t, *J* = 8.4 Hz, 1H), 4.34 (dd, *J* = 8.3, 6.0 Hz, 1H), 3.69 (dd, *J* = 11.1, 3.4 Hz, 1H), 3.57 (dd, *J* = 11.1, 3.6 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.1, 137.2, 128.5, 127.9, 127.6, 75.1, 73.4, 68.8, 66.2.



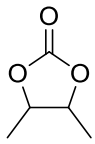
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.82 (dtd, *J* = 20.1, 10.0, 5.5 Hz, 1H), 6.20 (dd, *J* = 27.6, 13.8 Hz, 2H), 5.93 – 5.61 (m, 1H), 5.46 (td, *J* = 8.4, 4.0 Hz, 1H), 5.39 – 5.11 (m, 1H), 5.00 (s, 2H), 4.61 (ddt, *J* = 38.3, 11.1, 3.8 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.1, 133.7, 117.8, 75.2, 72.5, 68.8, 66.2.



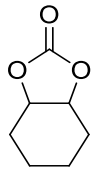
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.85 (dt, *J* = 9.8, 3.8 Hz, 1H), 4.50 (t, *J* = 8.4 Hz, 1H), 4.43 – 4.34 (m, 1H), 4.22 (q, *J* = 16.0 Hz, 2H), 3.75 (ddd, *J* = 23.8, 10.9, 3.8 Hz, 2H), 2.49 (t, *J* = 2.3 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.0, 78.6, 75.7, 74.8, 68.5, 66.3, 58.9.



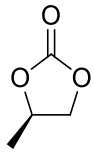
^{1}H NMR (400 MHz, $CDCl_3$) δ 5.02 – 4.68 (m, 1H), 4.51 (t, *J* = 8.3 Hz, 1H), 4.36 – 4.03 (m, 1H), 3.66 (t, *J* = 4.6 Hz, 4H), 2.66 (dd, *J* = 5.4, 1.5 Hz, 2H), 2.53 (dd, *J* = 9.7, 4.7 Hz, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.9, 75.1, 67.9, 66.9, 60.4, 54.5.



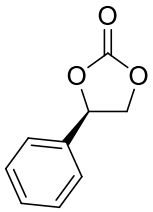
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.89 – 4.77 (m, 2H), 1.39 – 1.32 (m, 6H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.7, 76.1, 14.5.



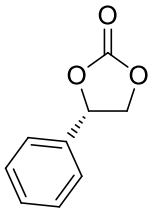
^{1}H NMR (400 MHz, $CDCl_3$) δ 5.04 – 4.08 (m, 2H), 1.89 (dd, *J* = 11.0, 5.1 Hz, 4H), 1.61 (dt, *J* = 13.2, 5.4 Hz, 2H), 1.42 (dt, *J* = 9.5, 5.9 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.5, 75.9, 26.9, 19.3.



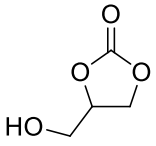
^{1}H NMR (400 MHz, $CDCl_3$) δ 5.01 – 4.69 (m, 1H), 4.55 (t, *J* = 8.0 Hz, 1H), 4.02 (dd, *J* = 8.3, 7.4 Hz, 1H), 1.49 (d, *J* = 6.3 Hz, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.1, 73.6, 70.7, 19.5.



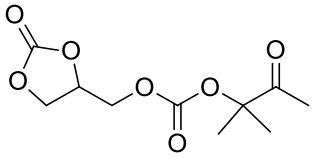
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.31 (m, 5H), 5.68 (t, *J* = 8.0 Hz, 1H), 4.80 (t, *J* = 8.4 Hz, 1H), 4.35 (t, *J* = 8.2 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.9, 135.9, 129.8, 129.3, 126.0, 78.1, 71.2.



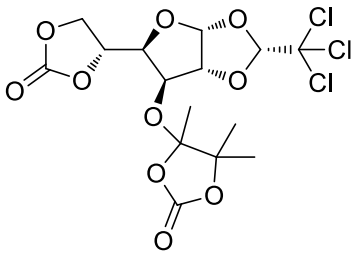
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (m, *J* = 8.2, 7.0, 4.3 Hz, 5H), 5.68 (t, *J* = 8.0 Hz, 1H), 4.80 (t, *J* = 8.4 Hz, 1H), 4.35 (t, *J* = 8.2 Hz, 1H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.9, 135.9, 129.9, 129.4, 126.0, 78.1, 71.3.



^{1}H NMR (400 MHz, $CDCl_3$) δ 4.81 (ddt, *J* = 8.4, 6.6, 3.3 Hz, 1H), 4.49 (dt, *J* = 15.1, 8.4 Hz, 2H), 4.00 (dd, *J* = 12.8, 3.0 Hz, 1H), 3.72 (dd, *J* = 12.8, 3.4 Hz, 1H), 2.36 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.3, 76.6, 65.8, 61.8.

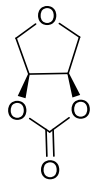


^{1}H NMR (400 MHz, $CDCl_3$) δ 4.92 (tdd, *J* = 6.3, 4.3, 3.3 Hz, 1H), 4.54 (t, *J* = 8.7 Hz, 1H), 4.39 (dd, *J* = 12.5, 3.2 Hz, 1H), 4.29 (dd, *J* = 8.8, 6.2 Hz, 1H), 4.23 (dd, *J* = 12.5, 4.4 Hz, 1H), 2.11 (s, 3H), 1.46 (d, *J* = 2.4 Hz, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 206.0, 154.4, 153.3, 86.4, 77.4, 77.2, 76.9, 73.7, 66.1, 65.7, 23.7, 23.1. For $C_{10}H_{14}O_7$: 269.0637 $[M + Na]^+$. Found: 269.0640 $[M + Na]^+$. **IR** (KBr): 2992, 2949, 1809, 1723, 1463, 1391, 1366, 1289, 1163, 946, 921, 790 cm^{-1}.

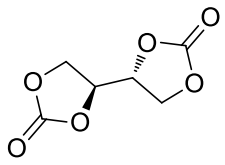


^{1}H NMR (400 MHz, DMSO-d_6) δ 6.26 (d, *J* = 3.9 Hz,

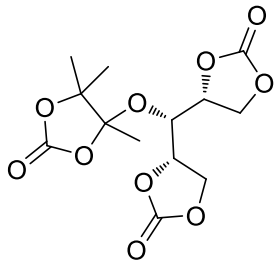
1H), 5.55 (s, 1H), 4.95 – 4.87 (m, 2H), 4.84 (dd, *J* = 11.6, 5.9 Hz, 1H), 4.77 (d, *J* = 4.0 Hz, 1H), 4.43 (dt, *J* = 16.7, 8.1 Hz, 2H), 1.68 (s, 3H), 1.39 (d, *J* = 8.4 Hz, 6H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 154.0, 151.9, 108.8, 106.4, 105.7, 96.7, 88.0, 85.9, 80.5, 75.8, 73.8, 65.2, 24.1, 19.5, 16.0. **HRMS** (ESI, m/z): calcd. For $C_8H_9Cl_3O_5$: 484.9785 $[M + Na]^+$ .Found: 484.9789 $[M + Na]^+$. **IR** (KBr): 2972, 2919, 1811, 1684, 1377, 1269, 803, 763, 745, 700 cm^{-1}.



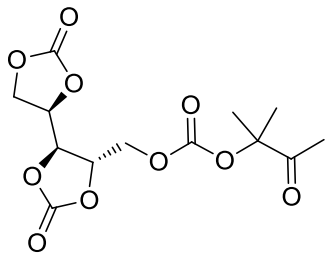
^{1}H NMR (400 MHz, $CDCl_3$) δ 5.31 – 5.09 (m, 2H), 4.26 (d, *J* = 12.2 Hz, 2H), 3.67 – 3.45 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.5, 80.2, 73.1.



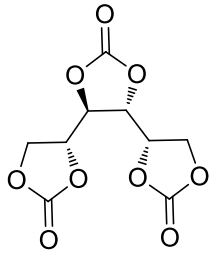
^{1}H NMR (400 MHz, DMSO-d_6) δ 5.14 (t, *J* = 6.3 Hz, 2H), 4.61 (t, *J* = 8.7 Hz, 2H), 4.40 (dd, *J* = 8.8, 5.7 Hz, 2H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 154.2 74.9, 64.7.



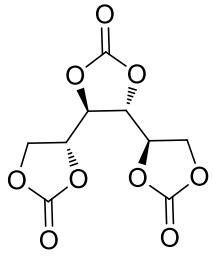
^{1}H NMR (400 MHz, DMSO-d_6) δ 5.14 (ddd, *J* = 8.5, 6.1, 2.2 Hz, 1H), 4.97 (td, *J* = 8.1, 3.7 Hz, 1H), 4.93 – 4.88 (m, 1H), 4.58 (t, *J* = 8.6 Hz, 2H), 4.52 – 4.39 (m, 2H), 1.59 (s, 3H), 1.39 (d, *J* = 3.8 Hz, 6H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 154.3, 153.7, 151.7, 108.6, 88.3, 75.2, 74.7 71.8, 65.9, 65.1, 23.9, 19.6, 16.0. **HRMS** (ESI, m/z): calcd. For $C_{13}H_{16}O_{10}$: 355.0641 $[M + Na]^+$. Found: 355.0646 $[M + Na]^+$. **IR** (KBr): 1801, 1393, 1278, 1164, 1124, 1066, 992, 768 cm^{-1}.



^{1}H NMR (400 MHz, DMSO-d_6) δ 5.17 (ddd, *J* = 8.9, 5.5, 1.9 Hz, 1H), 5.08 – 5.02 (m, 1H), 5.00 (dd, *J* = 4.9, 1.9 Hz, 1H), 4.66 (t, *J* = 8.9 Hz, 1H), 4.50 – 4.42 (m, 2H), 4.40 (dd, *J* = 12.4, 3.9 Hz, 1H), 2.14 (s, 3H), 1.47 (s, 6H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 205.9, 154.2, 153.3, 152.9, 85.7, 76.4, 75.4, 75.0, 66.6, 66.0, 23.9, 22.9, 22.9. **HRMS** (ESI, m/z): calcd. For $C_{13}H_{16}O_{10}$: 355.0641 [M + Na]$^+$. Found: 355.0645 [M + Na]$^+$. **IR** (KBr): 1814, 1748, 1721, 1458, 1389, 1287, 1159, 1120, 1075, 919, 792, 764 cm^{-1}.



^{1}H NMR (400 MHz, DMSO-d_6) δ 5.44 – 4.98 (m, 4H), 4.65 (dt, *J* = 13.8, 8.9 Hz, 2H), 4.54 – 4.28 (m, 2H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 154.0, 153.9, 152.8, 76.1, 75.3, 75.2, 74.7, 66.1, 64.7.



^{1}H NMR (400 MHz, DMSO-d_6) δ 5.21 (d, *J* = 8.8 Hz, 1H), 4.64 (t, *J* = 8.8 Hz, 1H), 4.44 (dd, *J* = 8.9, 5.9 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 154.0, 152.6, 75.2, 74.4, 64.8.

9. Rerferences

[S1] Arduengo, A. J.; Krafczyk, R.; Schmutzler, R. *Tetrahedron* **1999**, *55*, 14523-l4534.

[S2] Wang, Y. B.; Wang, Y. M.; Zhang, W. Z.; Lu, X. B. *J Am Chem Soc* **2013**, *135*, 11996-12003.

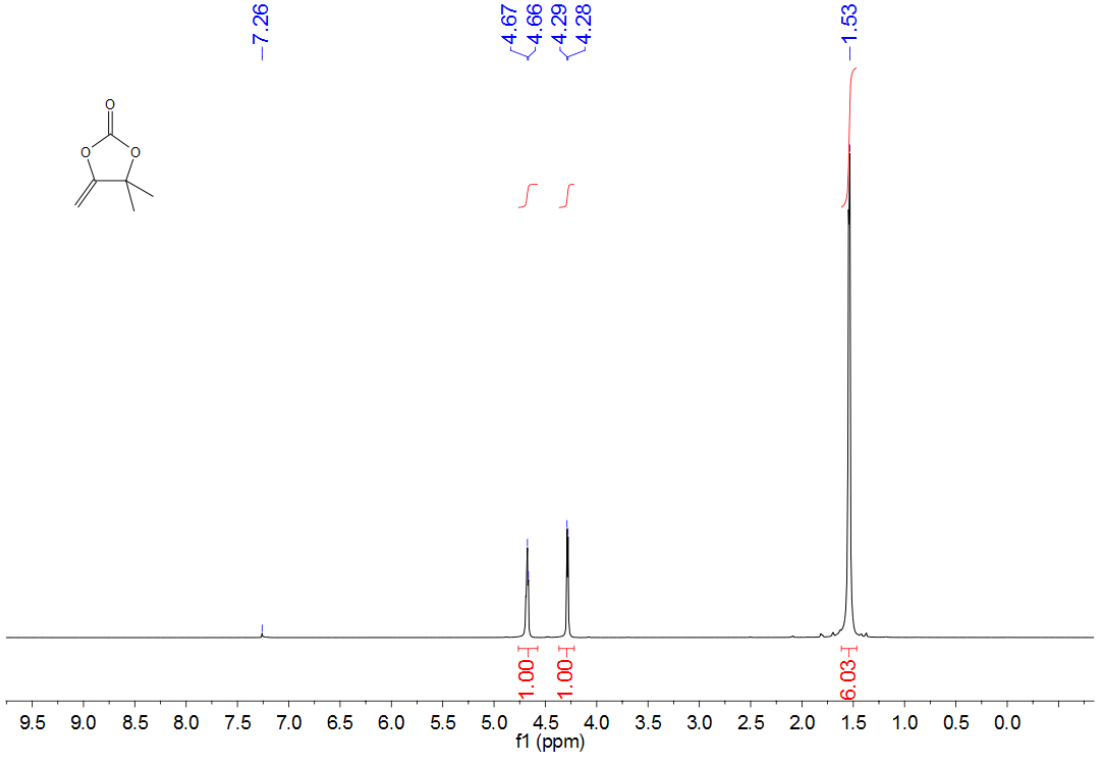
[S3] Zhou, H.; Zhang, R.; Lu, X.-B. *Advanced Synthesis & Catalysis*, **2019**, *361(2)*,

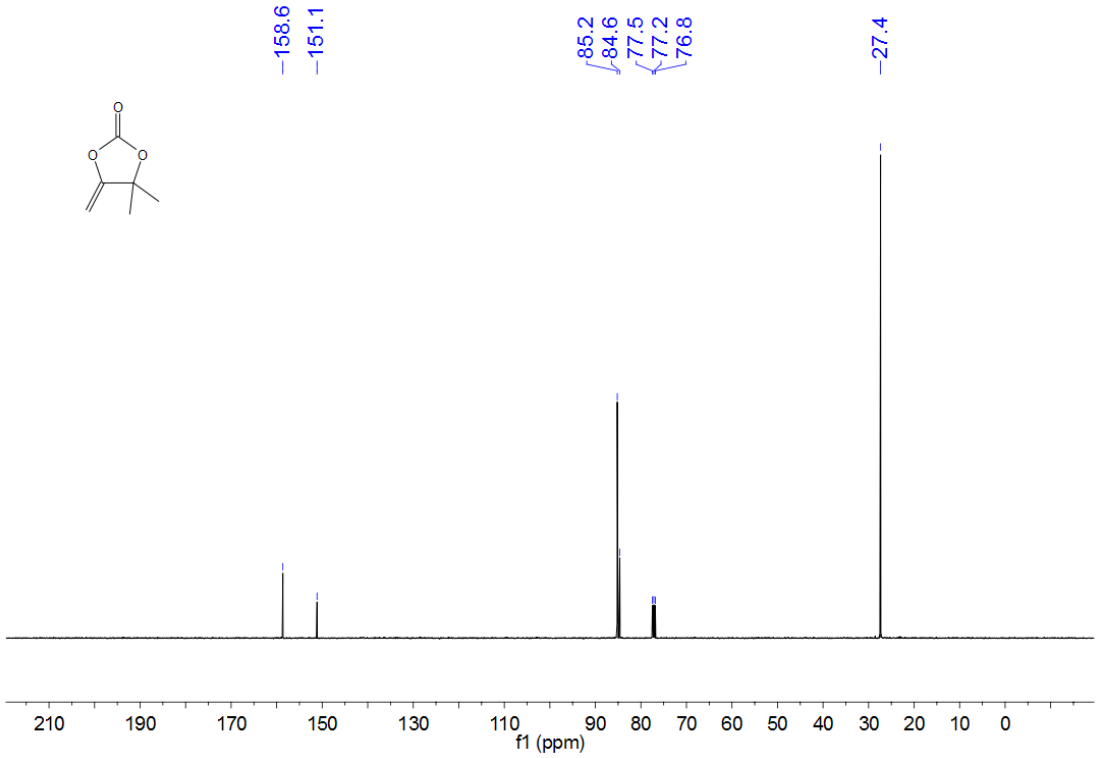
326-334.

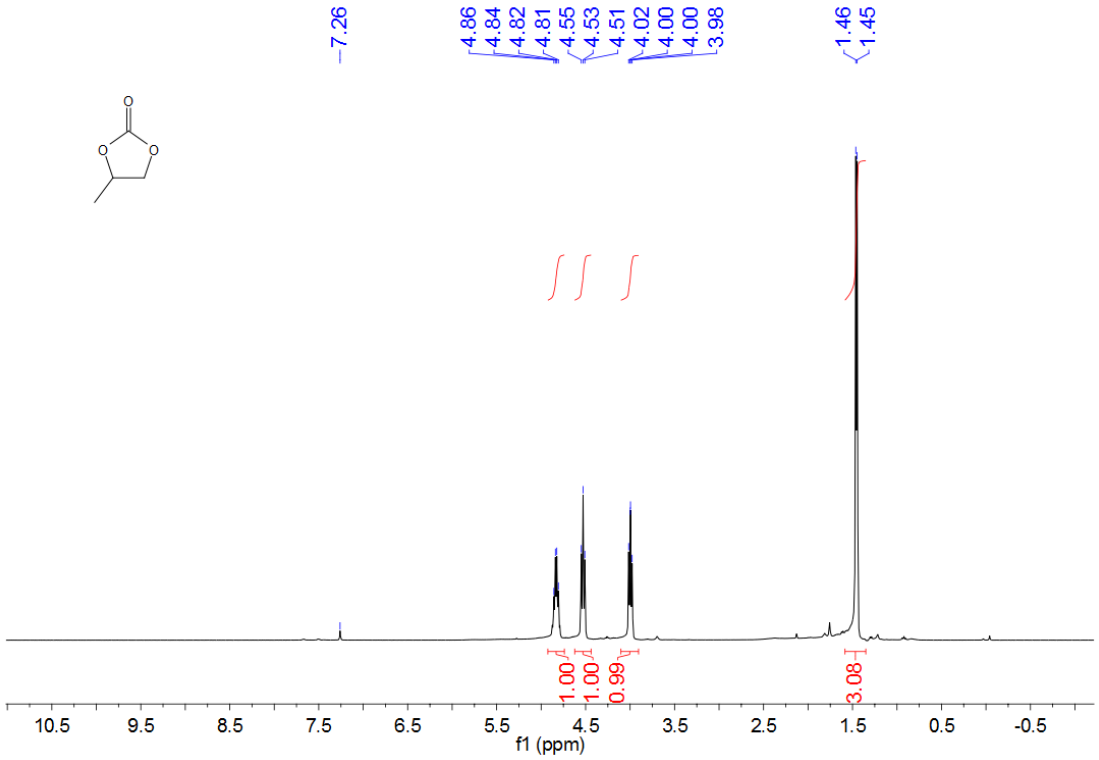
[S4] SHELXTL PC; Siemens Analytical X-ray Instruments, Madison, WI, 1993.

[S5] Sheldrick, G. M. SHELXTL Structure Determination Programs, version 5.0, PC; Siemens Analytical Systems, Madison, WI, 1994.

10. NMR spectra



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4.82
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4.53
4.51
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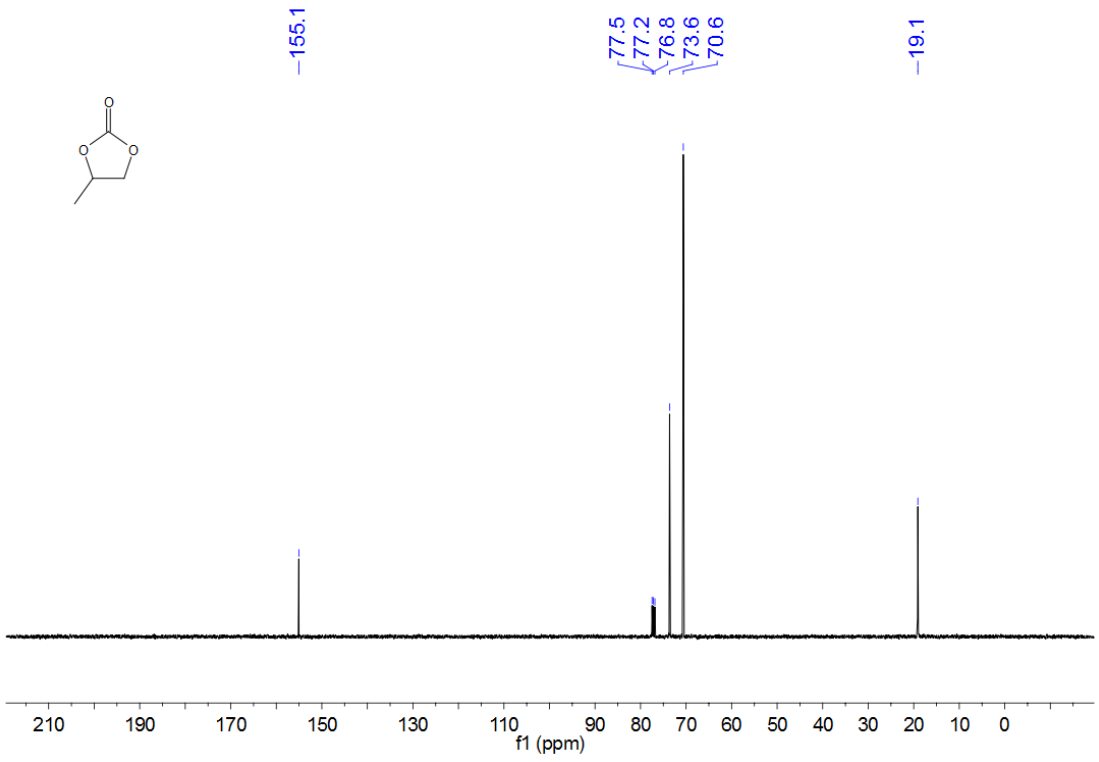
4.00
4.00
3.98
1.46
1.45
1.00
1.00
0.99
3.08
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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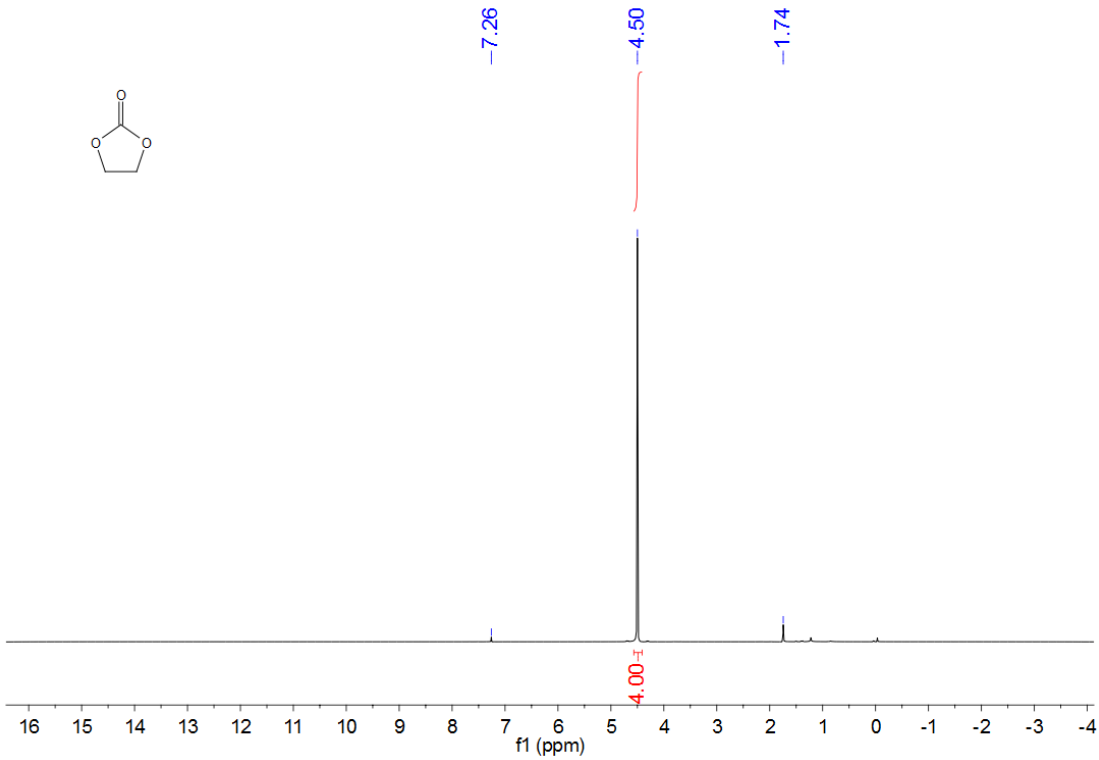
77.5
77.2
76.8
73.6
70.6
19.1
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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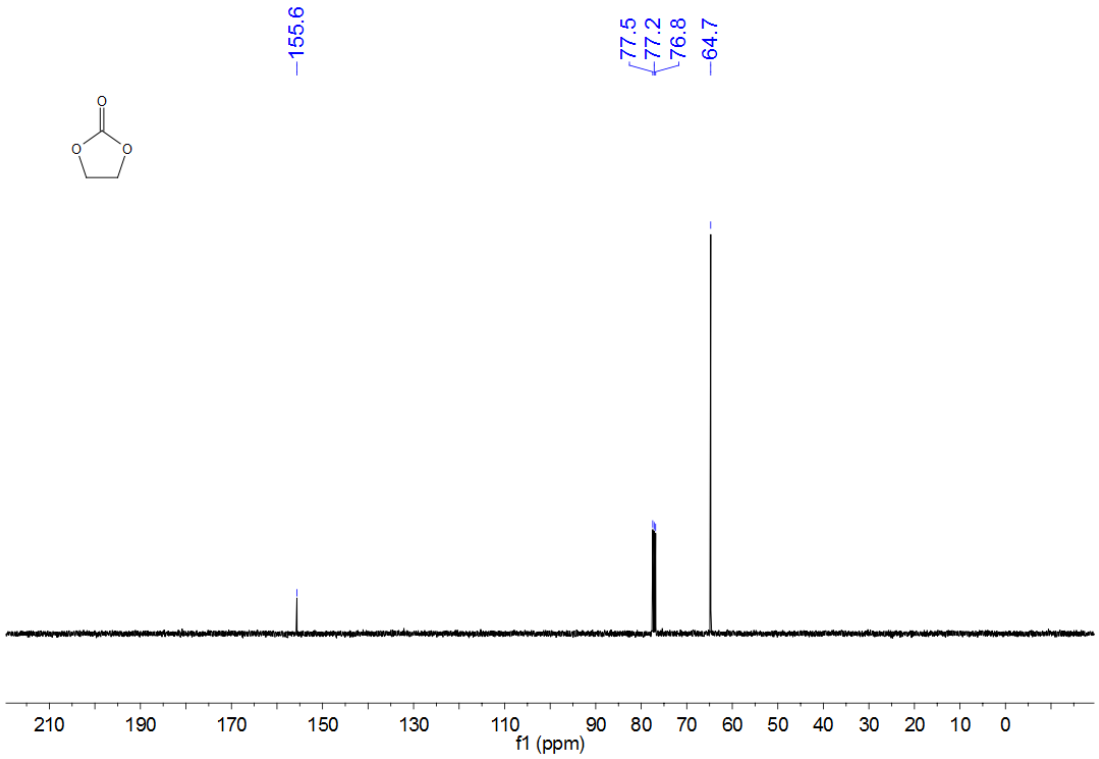
4.50
1.74
4.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


155.6
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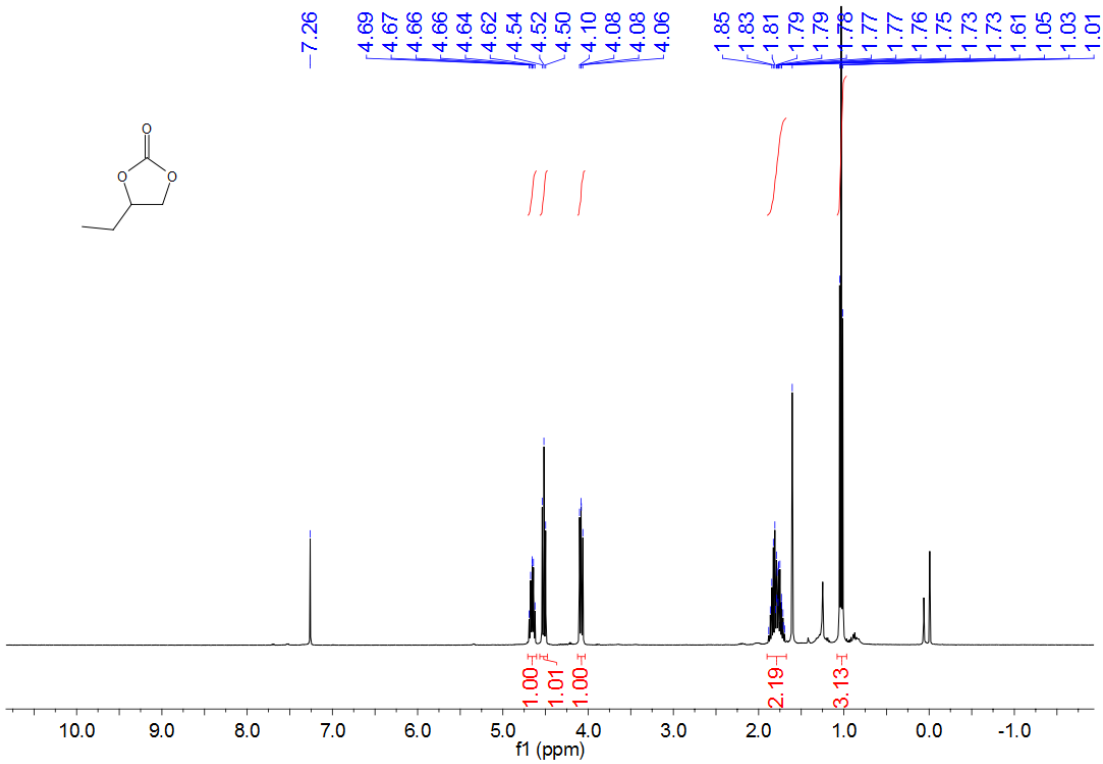
77.2
76.8
64.7
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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4.54
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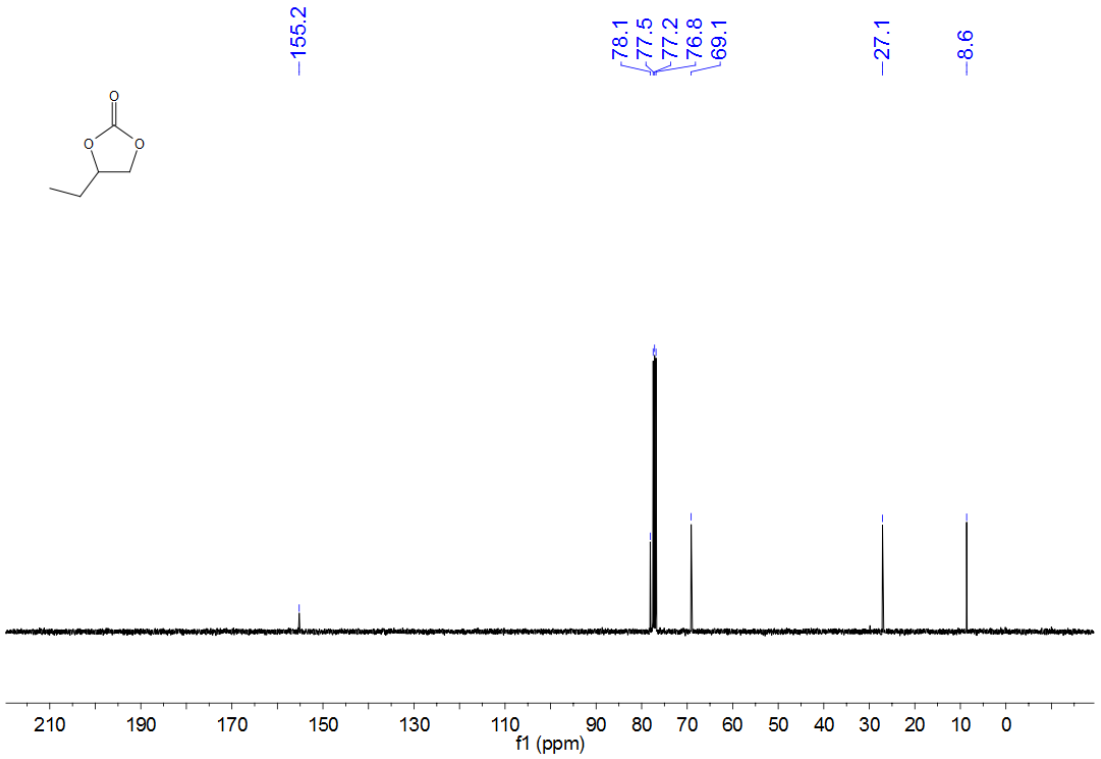
1.77
1.76
1.75
1.73
1.73
1.61
1.05
1.03
1.01
1.00
1.01
1.00
2.19
3.13
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)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77.5
77.2
76.8
69.1
27.1
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170
150
130
110
90
80
70
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50
40
30
20
10
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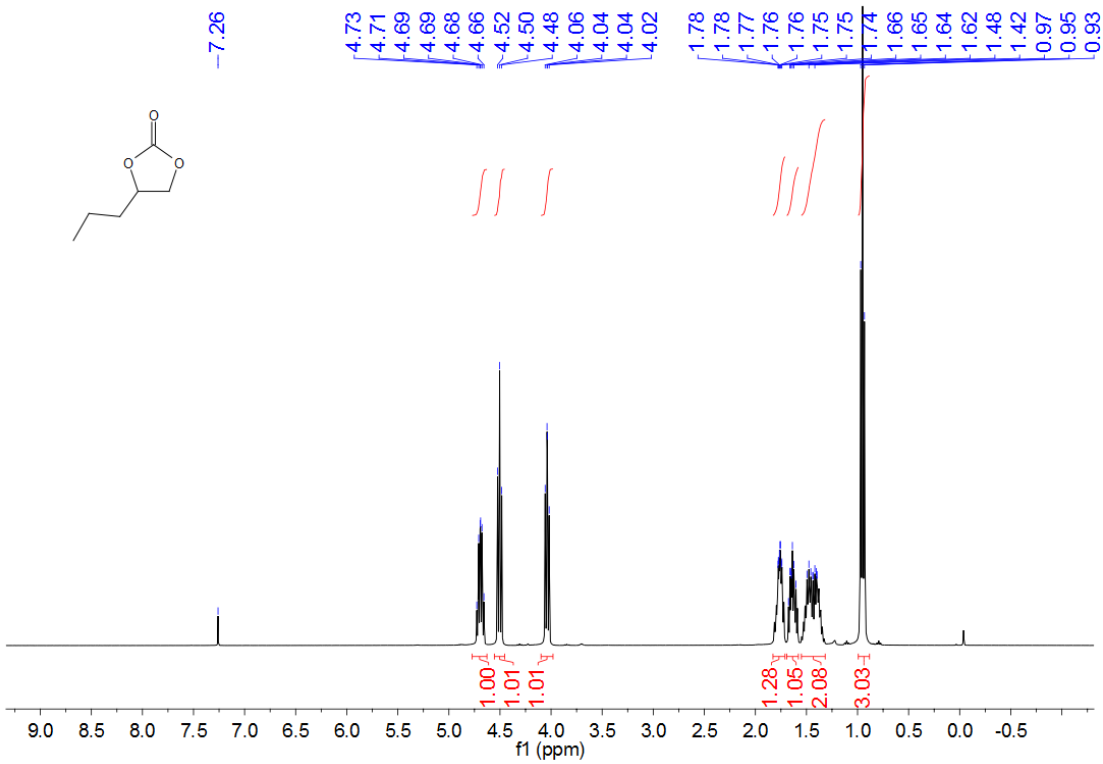
f1 (ppm)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4.71
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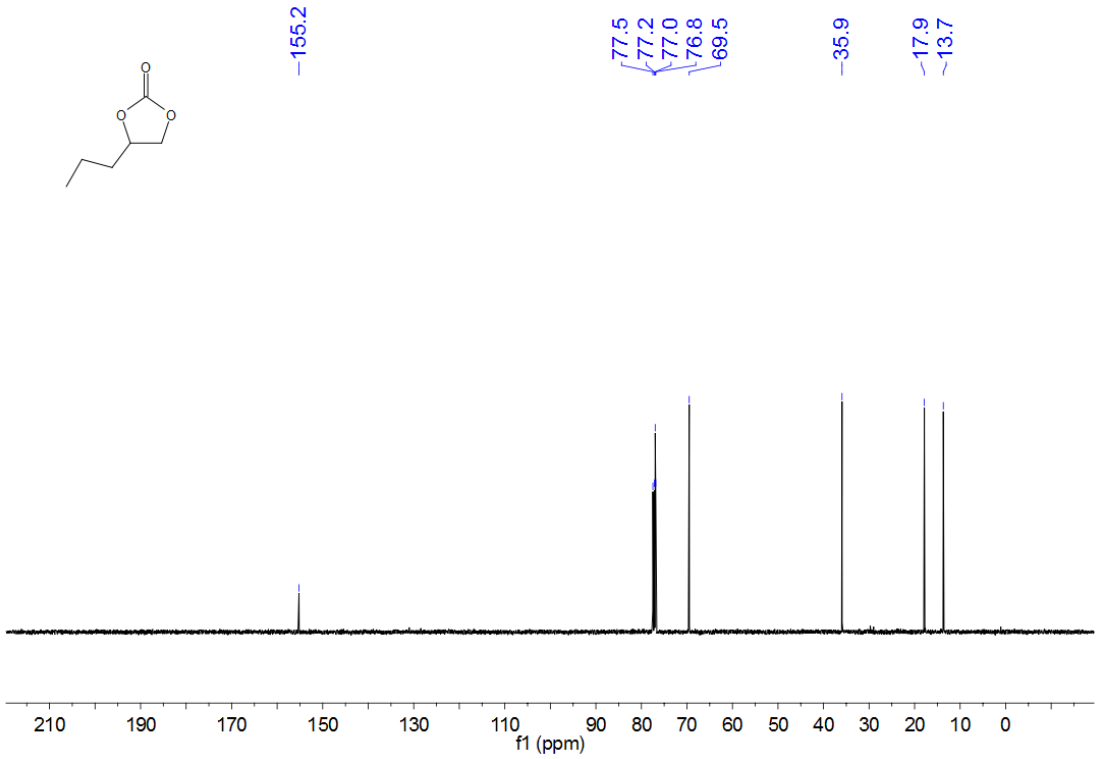
4.68
4.66
4.52
4.50
4.48
4.06
4.04
4.04
4.02
1.78
1.78
1.77
1.76
1.76
1.75
1.75
1.74
1.66
1.65
1.64
1.62
1.48
1.42
0.97
0.95
0.93
1.00
1.01
1.01
1.28
1.05
2.08
3.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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77.5
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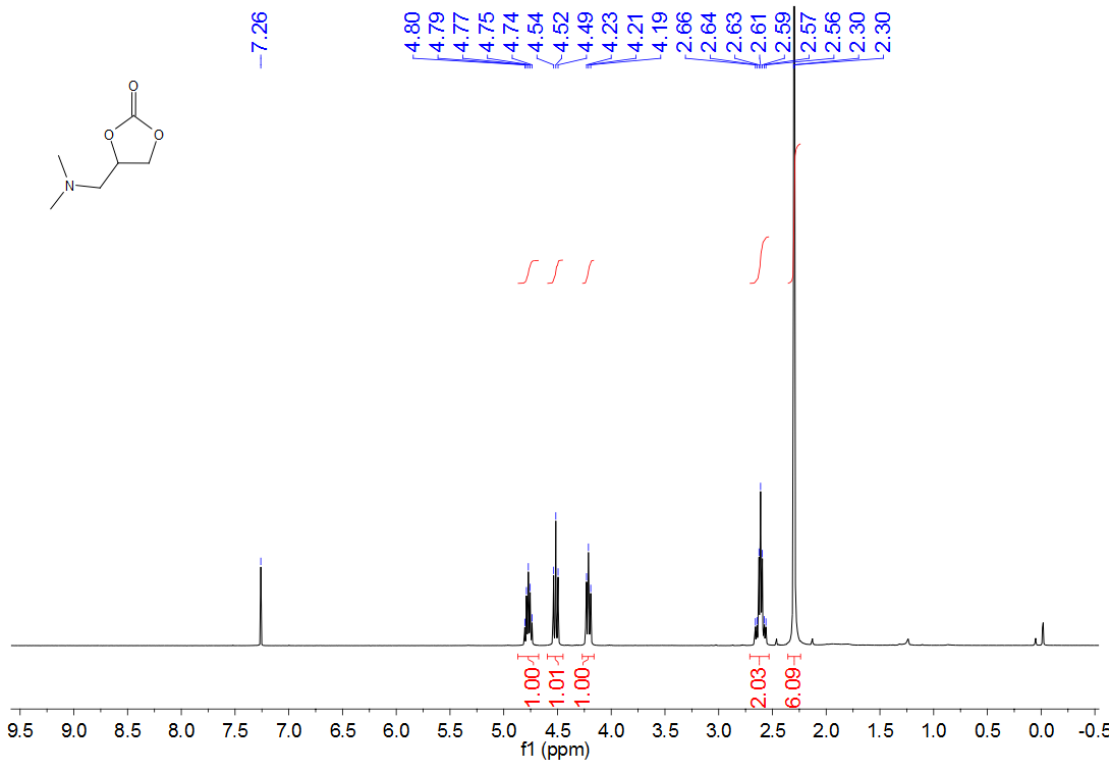
76.8
69.5
35.9
17.9
13.7
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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4.52
4.49
4.23
4.21
4.19
2.66
2.64
2.63
2.61
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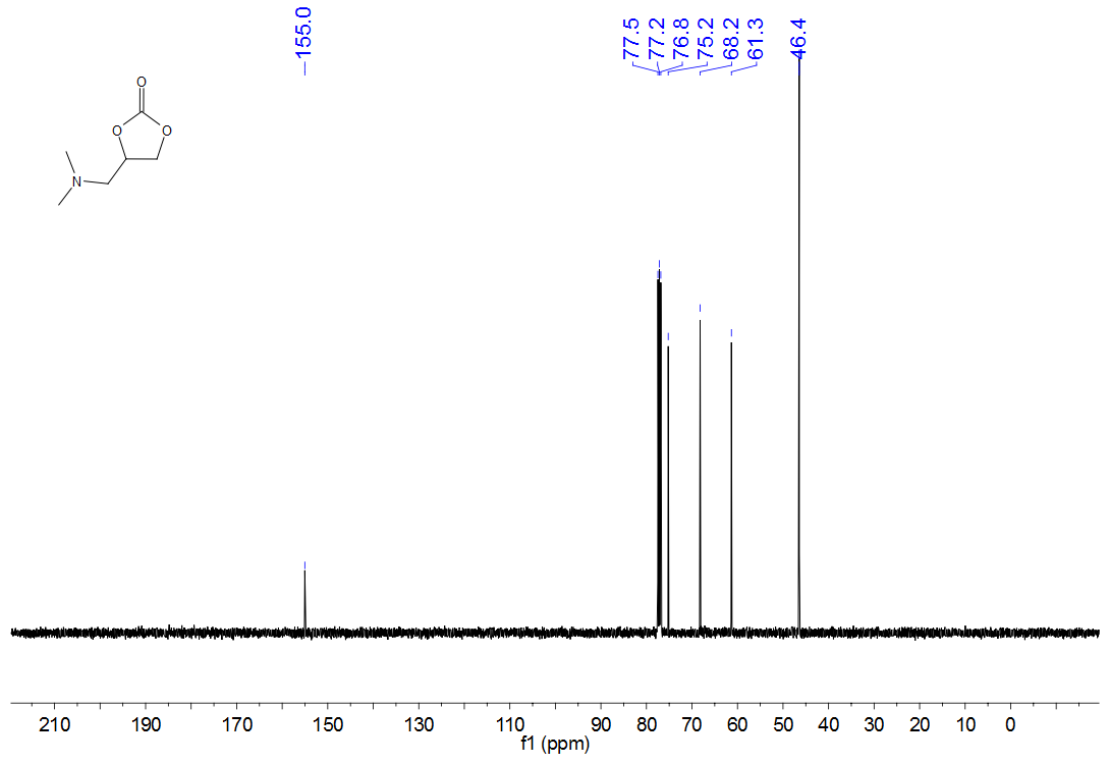
2.56
2.30
2.30
1.00
1.01
1.00
2.03
6.09
f1 (ppm)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75.2
68.2
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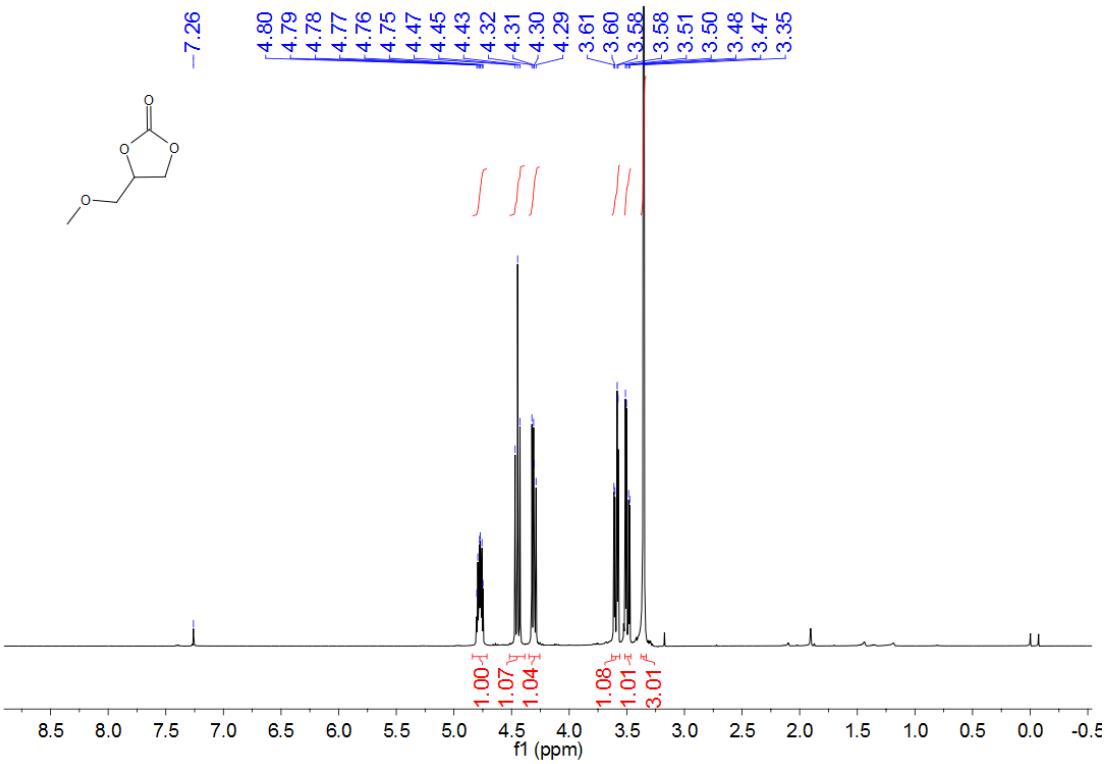
46.4
f1 (ppm)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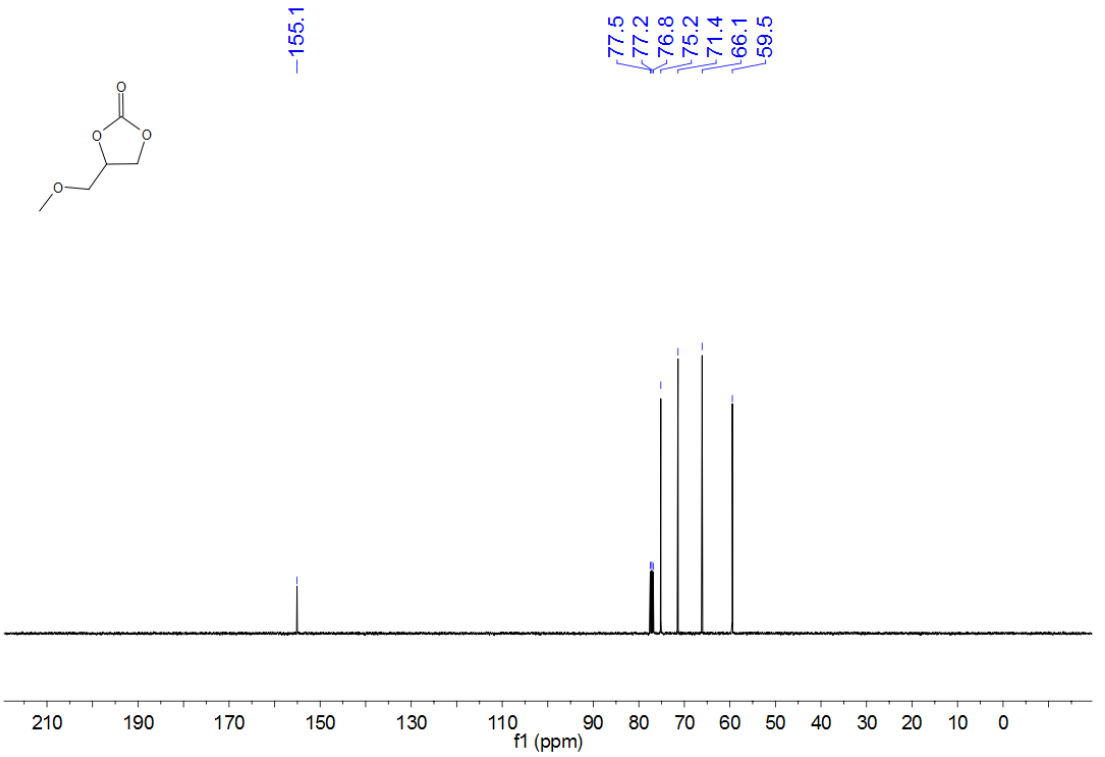
4.76
4.75
4.47
4.45
4.43
4.32
4.31
4.30
4.29
3.61
3.60
3.58
3.58
3.51
3.50
3.48
3.47
3.35
1.00
1.07
1.04
1.08
1.01
3.01
f1 (ppm)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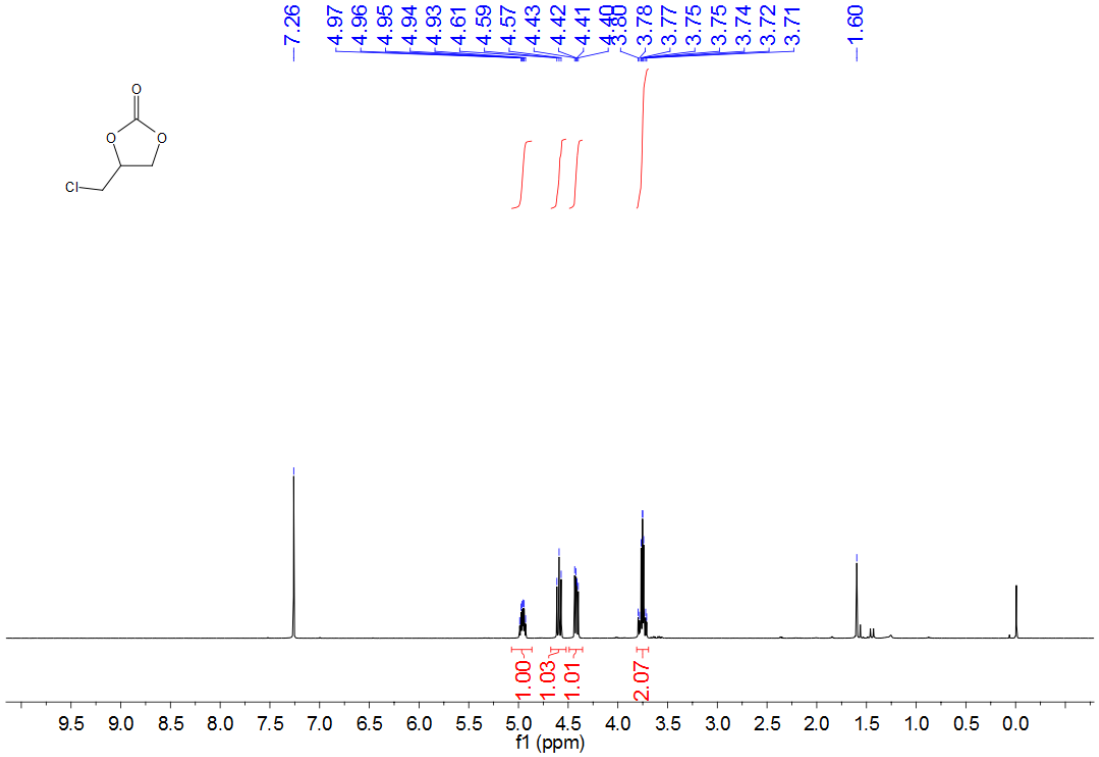
76.8
75.2
71.4
66.1
59.5
f1 (ppm)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4.95
4.94
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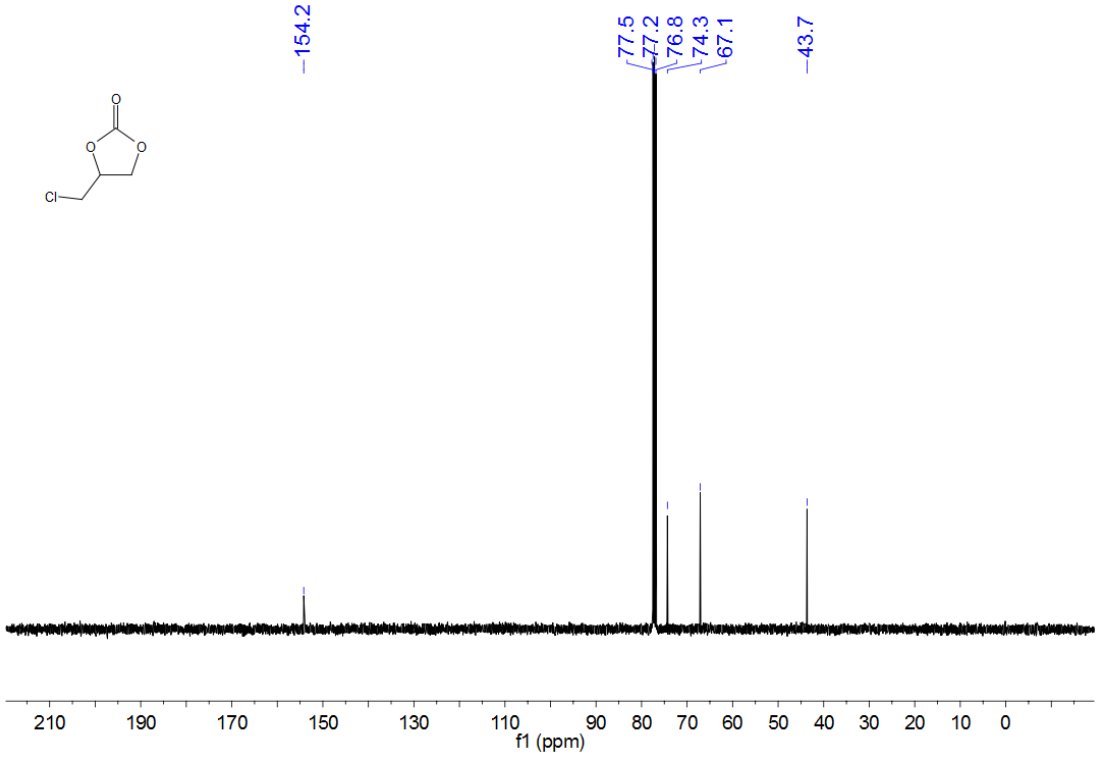
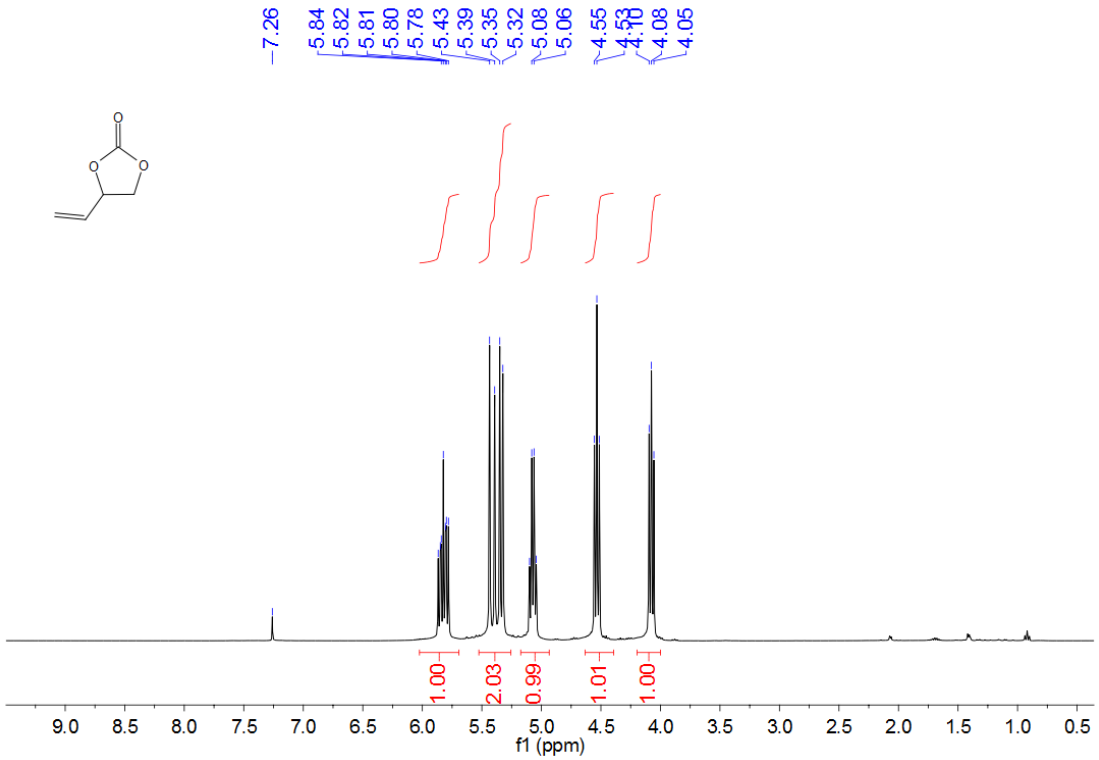
4.59
4.57
4.43
4.42
4.41
3.78
3.77
3.75
3.75
3.74
3.72
3.71
1.60
Cl
1.00
1.03
1.01
2.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


154.2
77.5
77.2
76.8
74.3
67.1
43.7
Cl
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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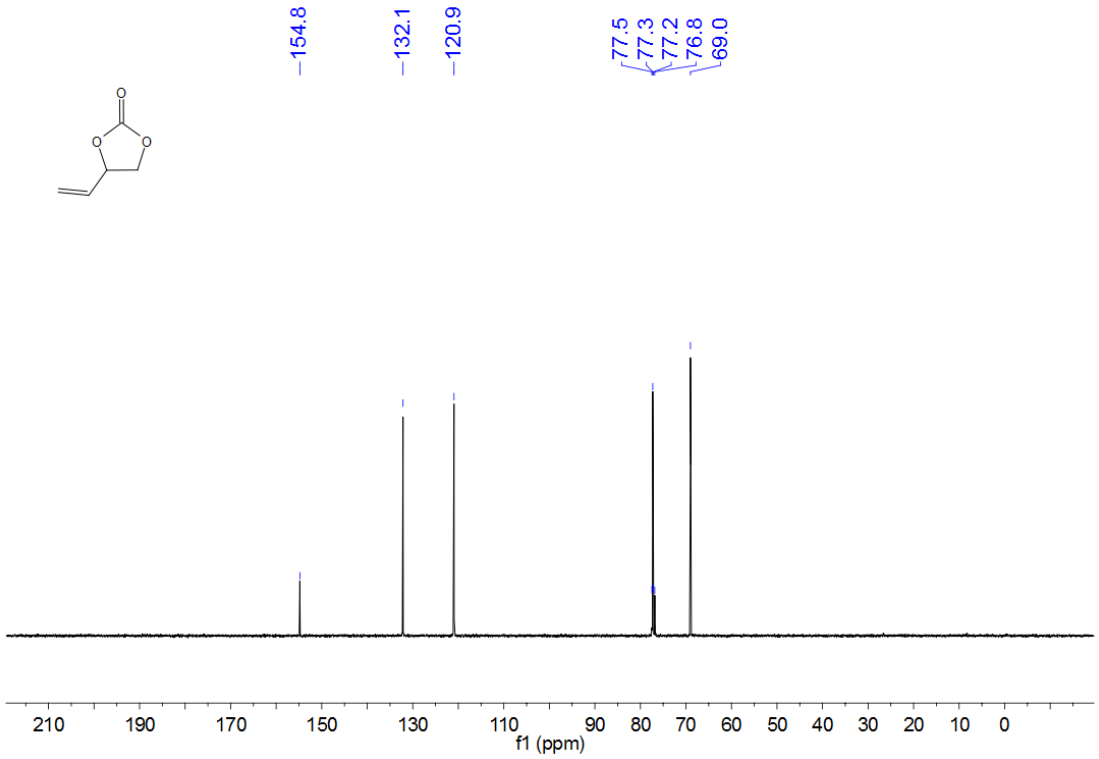
5.84
5.82
5.81
5.80
5.78
5.43
5.39
5.35
5.32
5.08
5.06
4.55
4.53
4.10
4.08
4.05
1.00
2.03
0.99
1.01
1.00
f1 (ppm)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132.1
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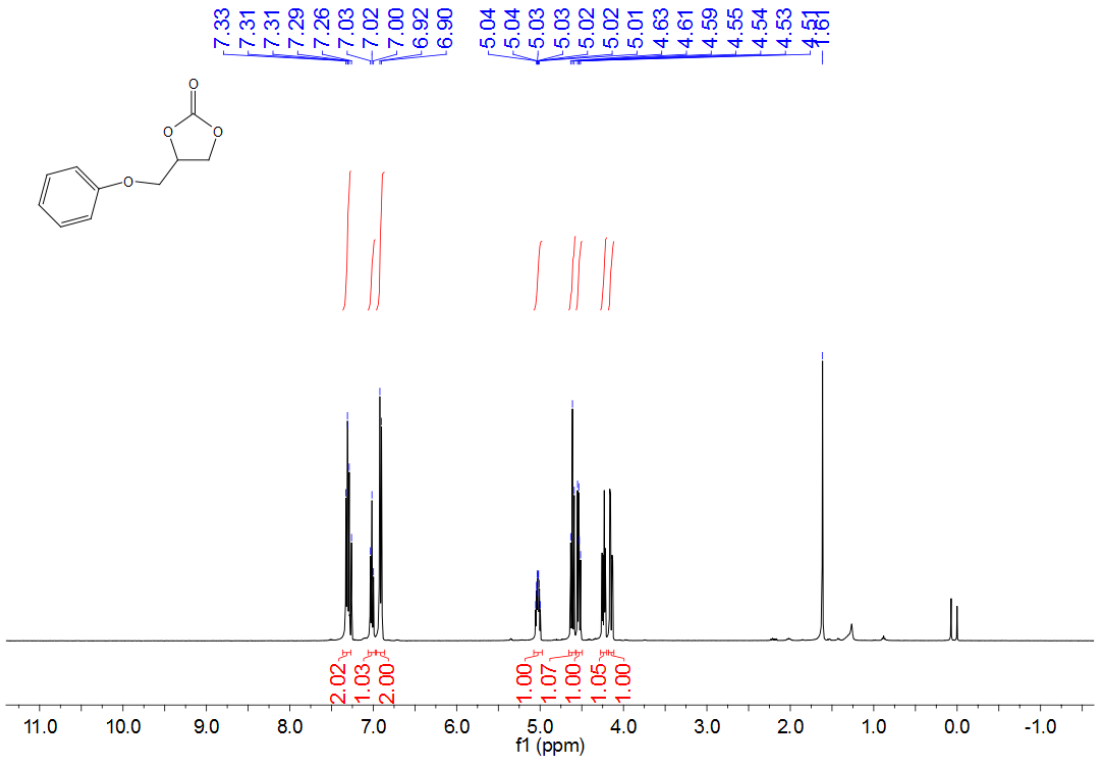
77.5
77.3
77.2
76.8
69.0
f1 (ppm)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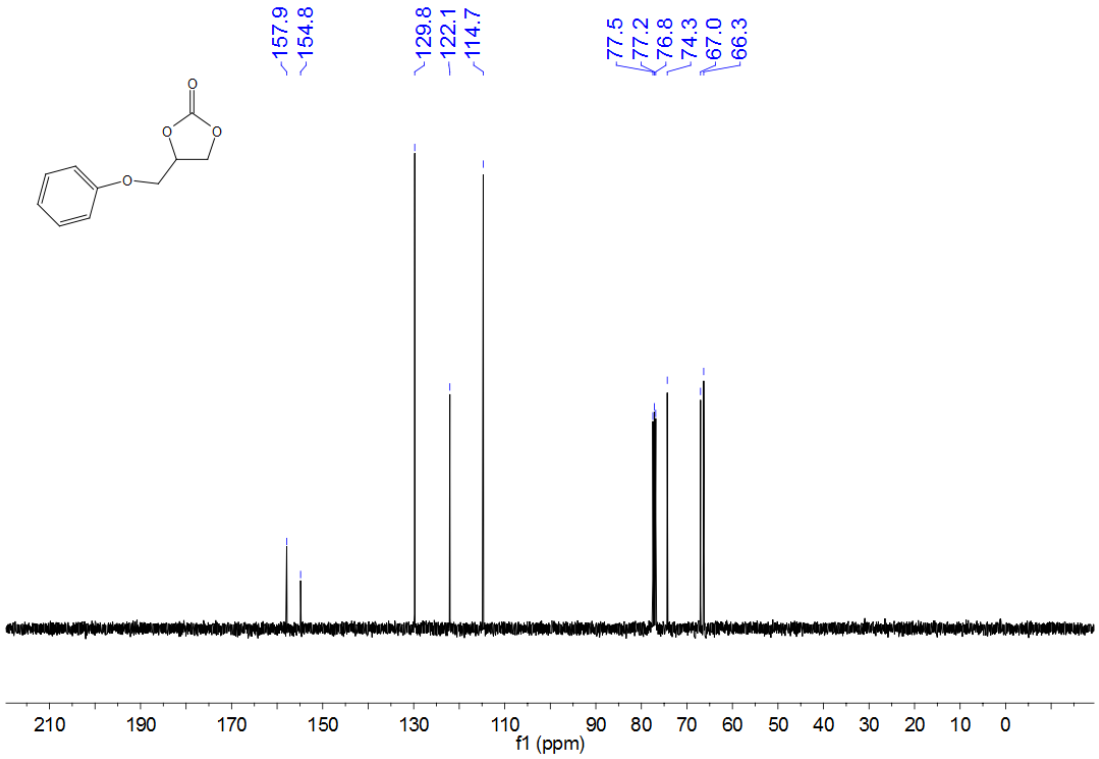
7.31
7.31
7.29
7.26
7.03
7.02
7.00
6.92
6.90
5.04
5.04
5.03
5.03
5.02
5.02
5.01
4.63
4.61
4.59
4.55
4.54
4.53
4.51
4.51
2.02
1.03
2.00
1.00
1.07
1.00
1.05
1.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)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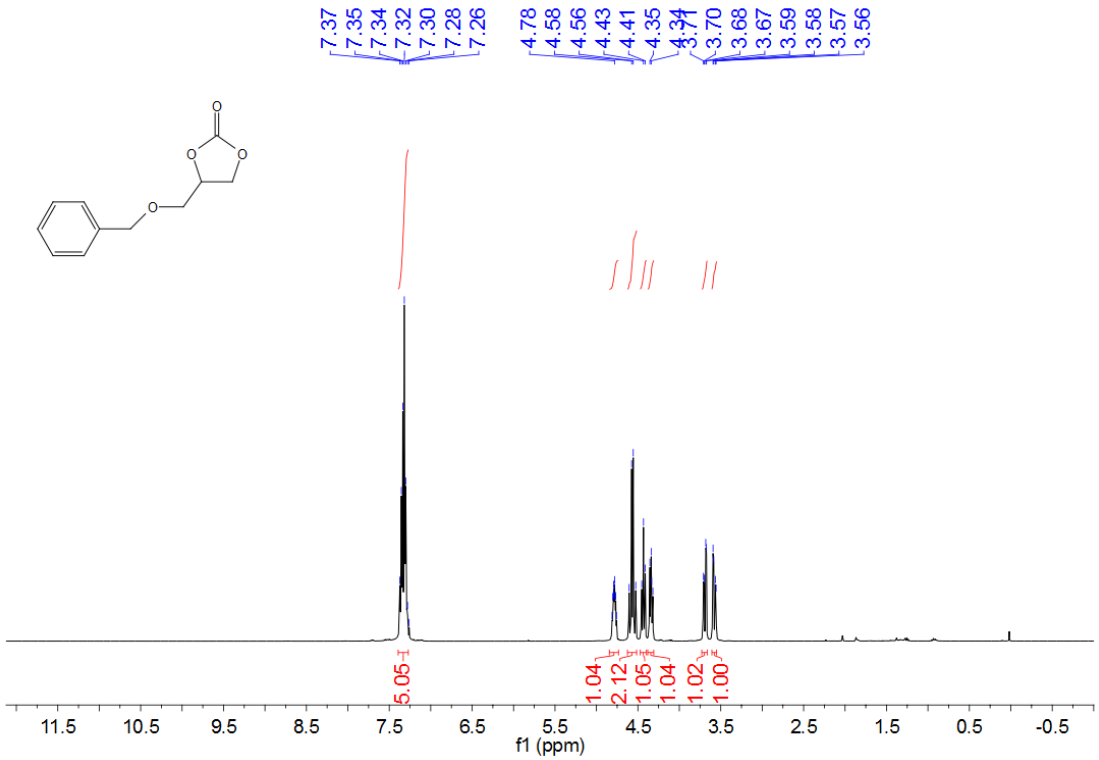
154.8
129.8
122.1
114.7
77.5
77.2
76.8
74.3
67.0
66.3
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.32
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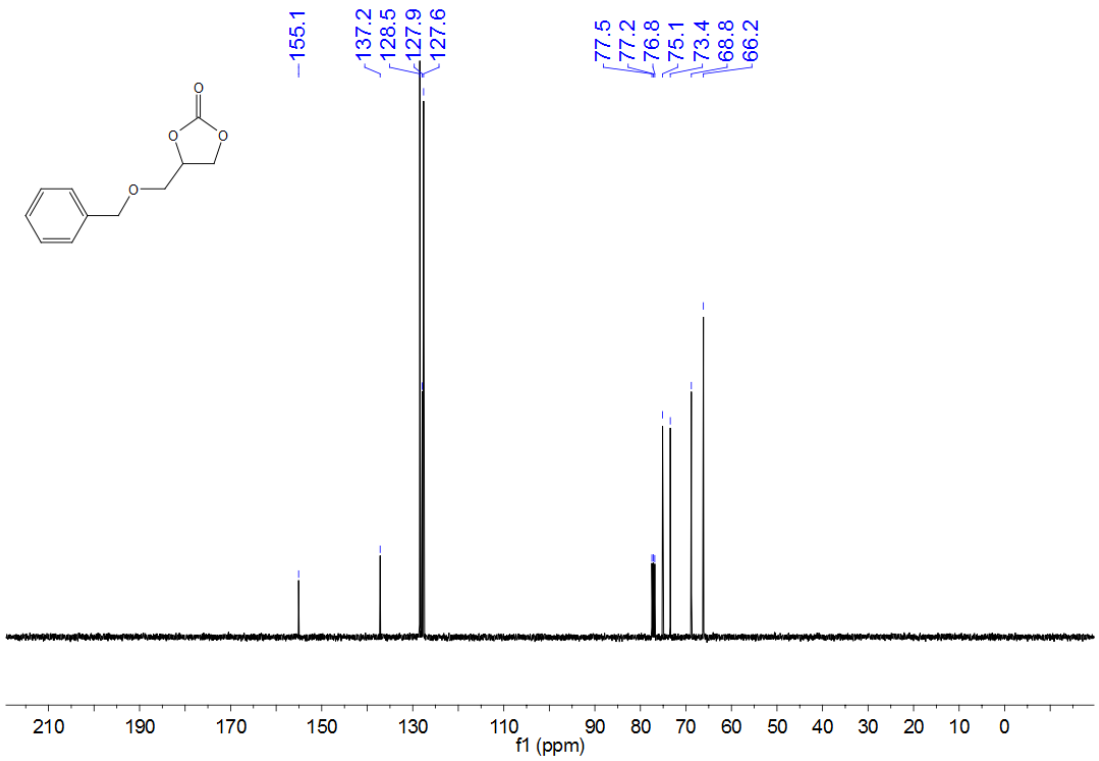
4.58
4.56
4.43
4.41
4.35
4.34
3.71
3.70
3.68
3.67
3.59
3.58
3.57
3.56
5.05
1.04
2.12
1.05
1.04
1.02
1.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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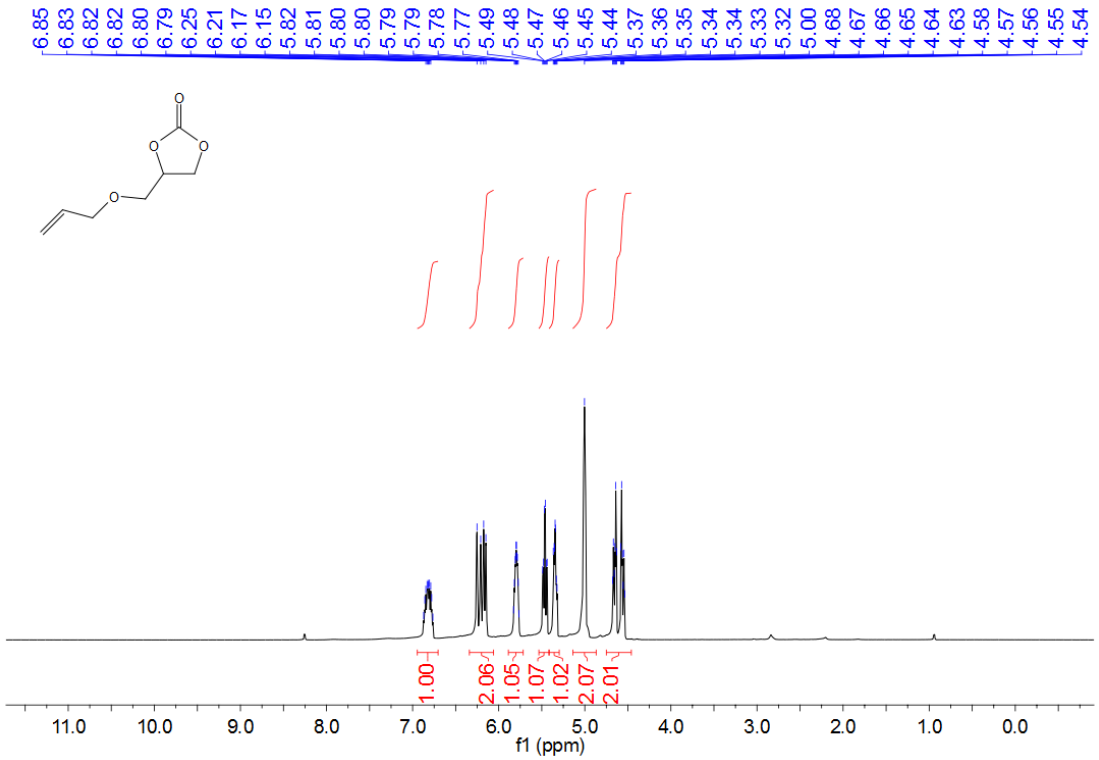
137.2
128.5
127.9
127.6
77.5
77.2
76.8
75.1
73.4
68.8
66.2
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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6.82
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5.82
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5.80
5.80
5.79
5.79
5.78
5.77
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5.48
5.47
5.46
5.45
5.44
5.37
5.36
5.35
5.34
5.34
5.33
5.32
5.00
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4.67
4.66
4.65
4.64
4.63
4.58
4.57
4.56
4.55
4.54
1.00
2.06
1.05
1.07
1.02
2.07
2.01
11.0
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7.0
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3.0
2.0
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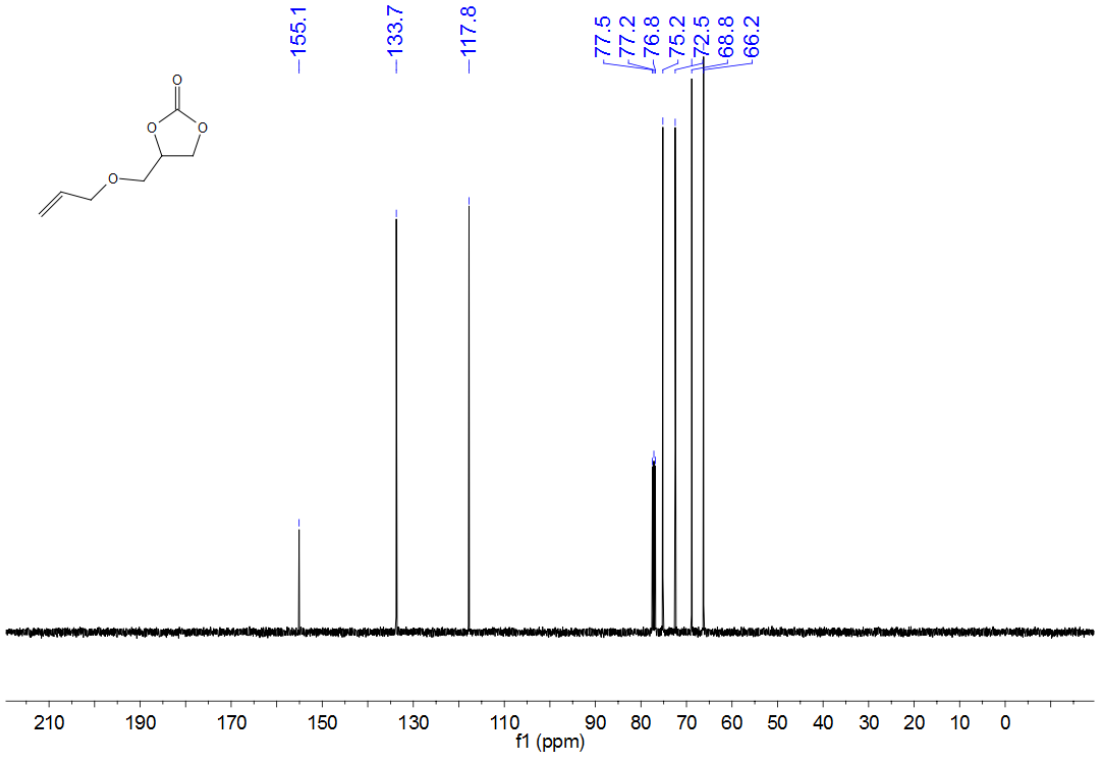
0.0
f1 (ppm)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133.7
117.8
77.5
77.2
76.8
75.2
72.5
68.8
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170
150
130
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90
80
70
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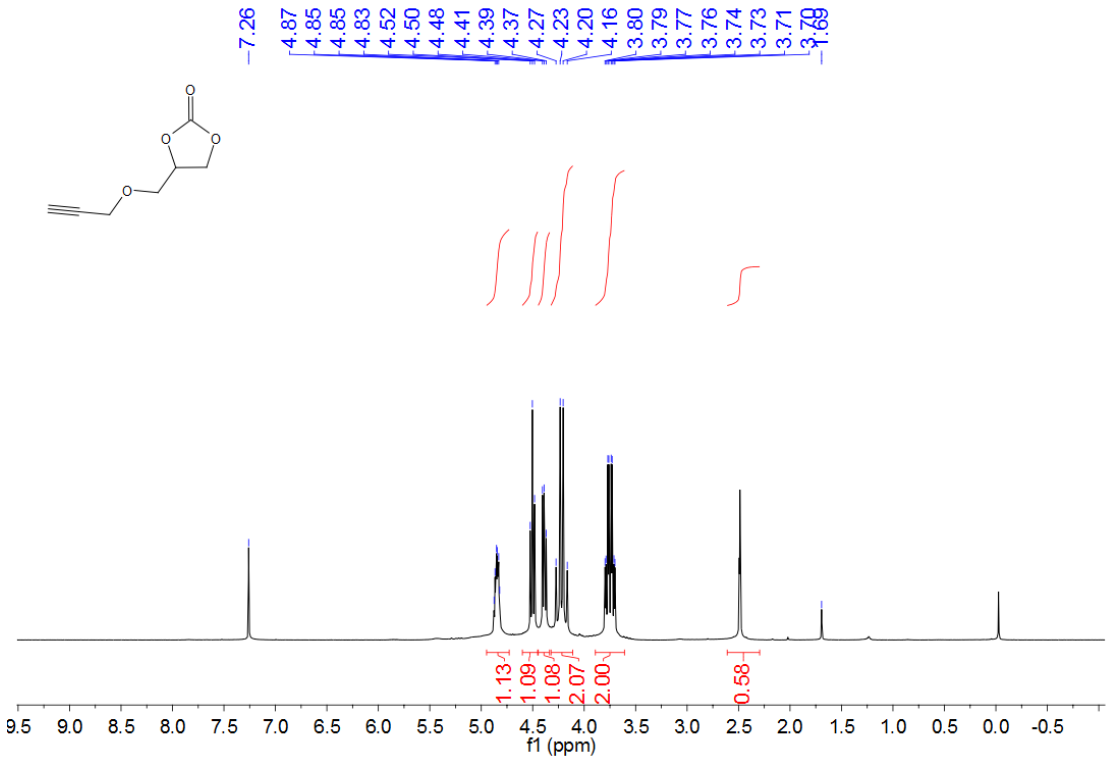
50
40
30
20
10
0
f1 (ppm)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4.85
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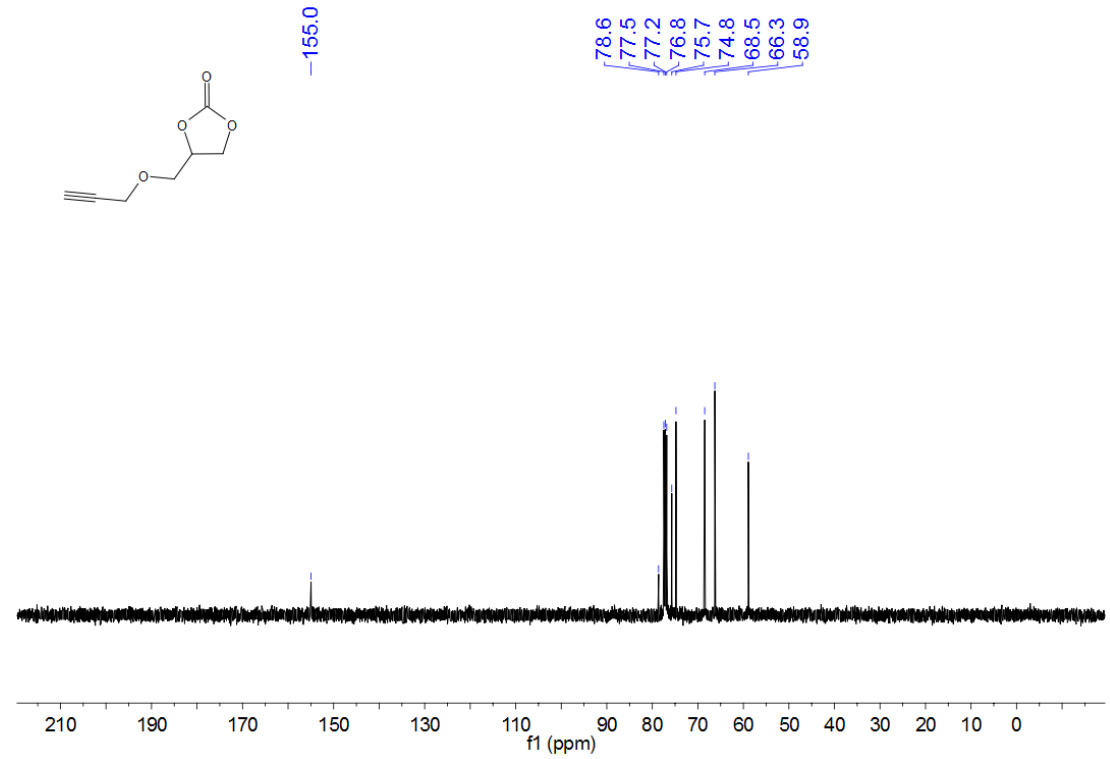
4.48
4.41
4.39
4.37
4.27
4.23
4.20
4.16
3.80
3.79
3.77
3.76
3.74
3.73
3.71
1.69
1.13
1.09
1.08
2.07
2.00
0.58
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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76.8
75.7
74.8
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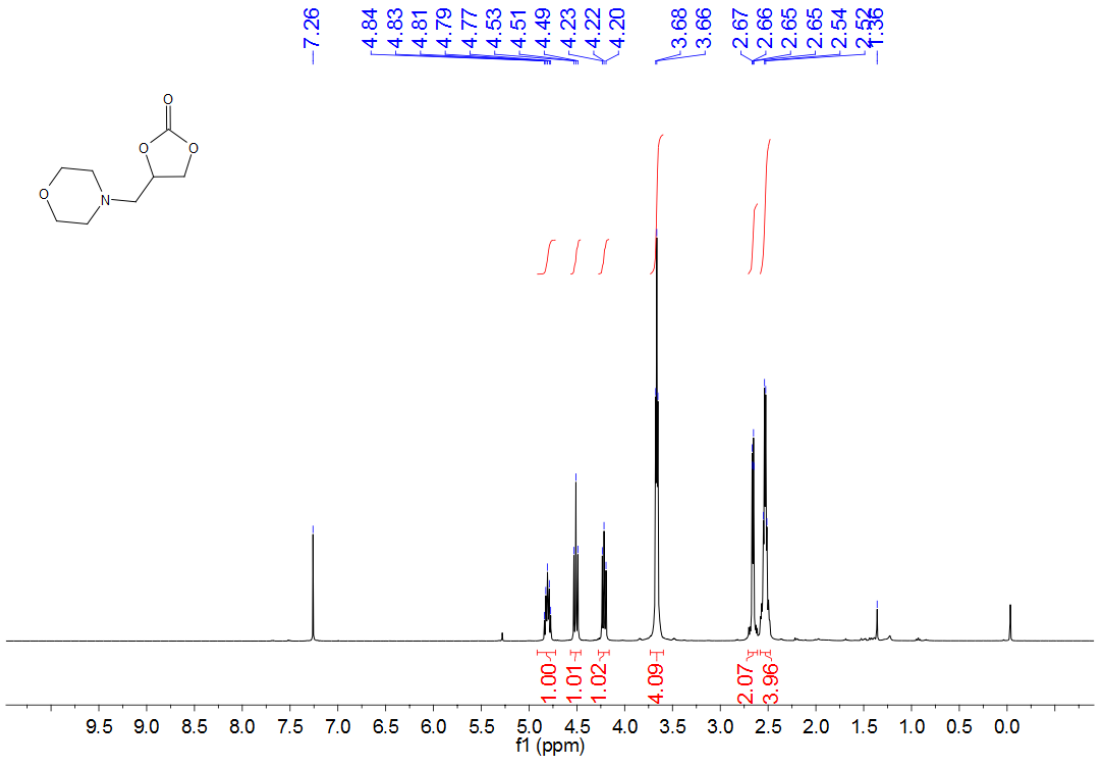
66.3
58.9
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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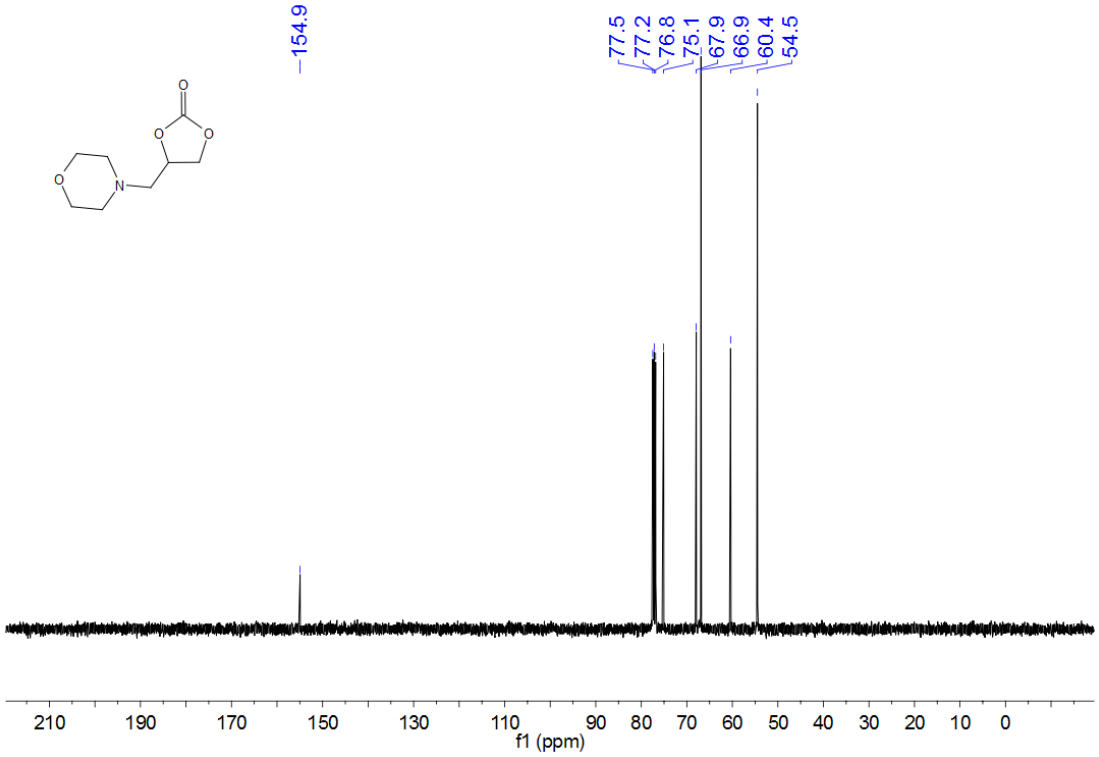
4.23
4.22
4.20
3.68
3.66
2.67
2.66
2.65
2.65
2.54
1.36
1.00
1.01
1.02
4.09
2.07
3.96
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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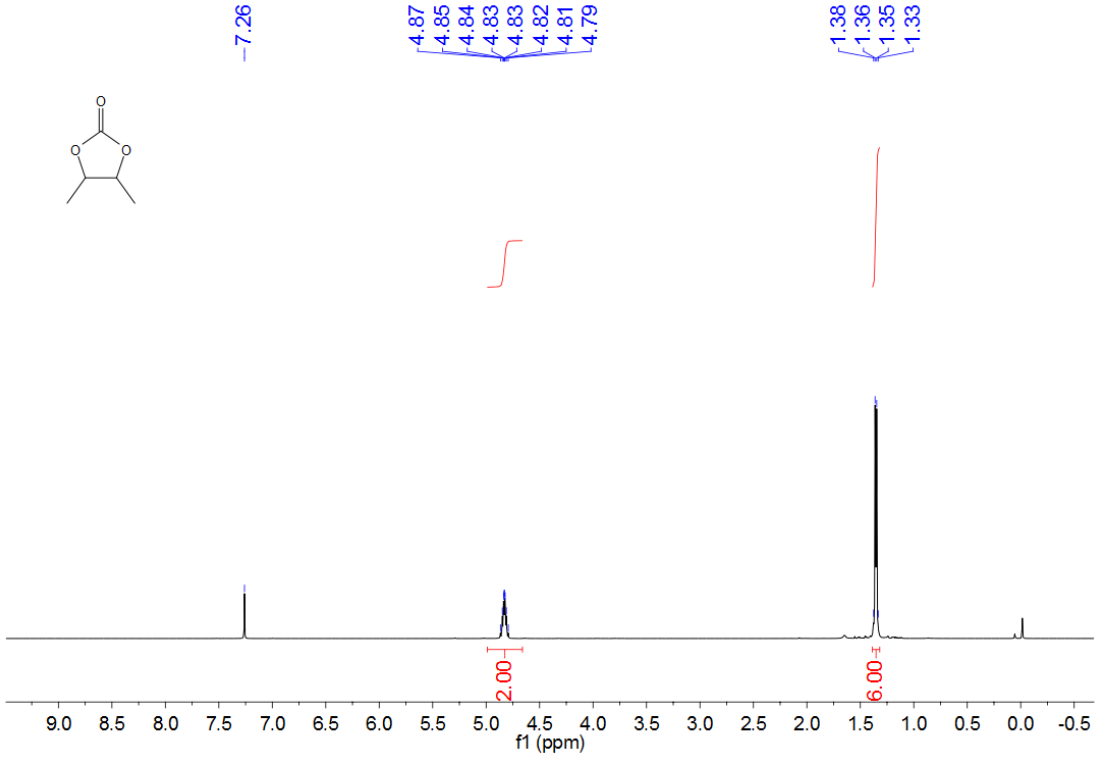
77.5
77.2
76.8
75.1
67.9
66.9
60.4
54.5
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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4.83
4.82
4.81
4.79
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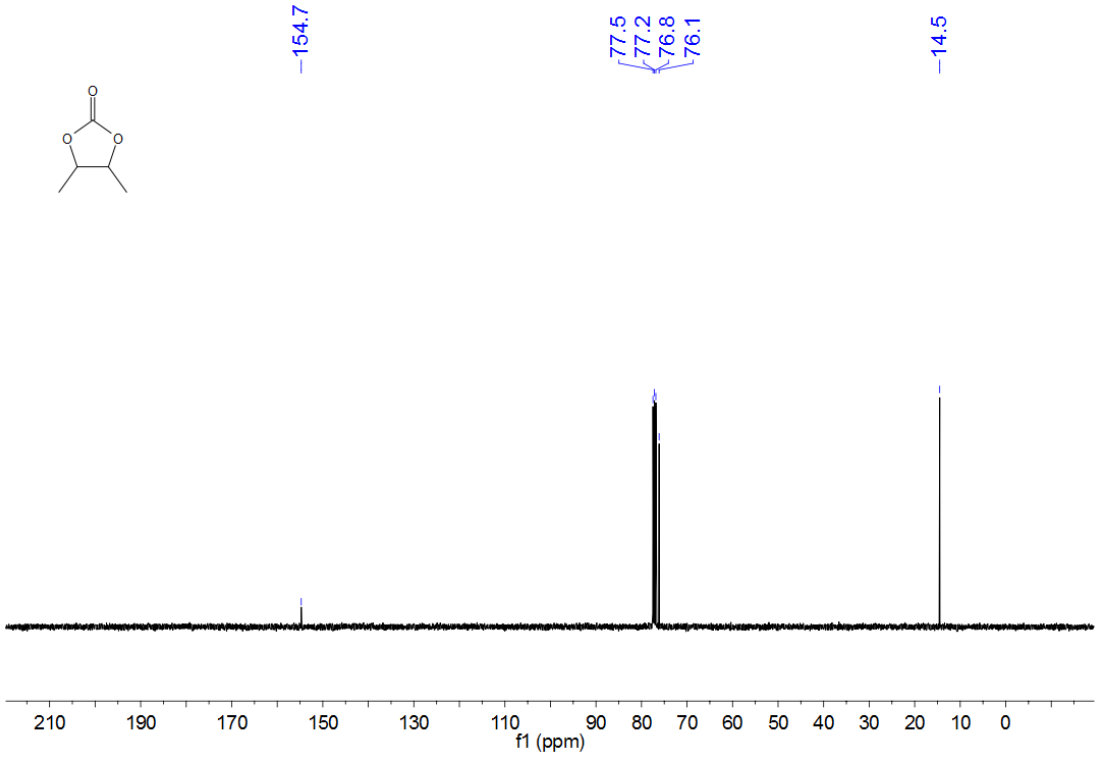
1.36
1.35
1.33
2.00
6.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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76.1
14.5
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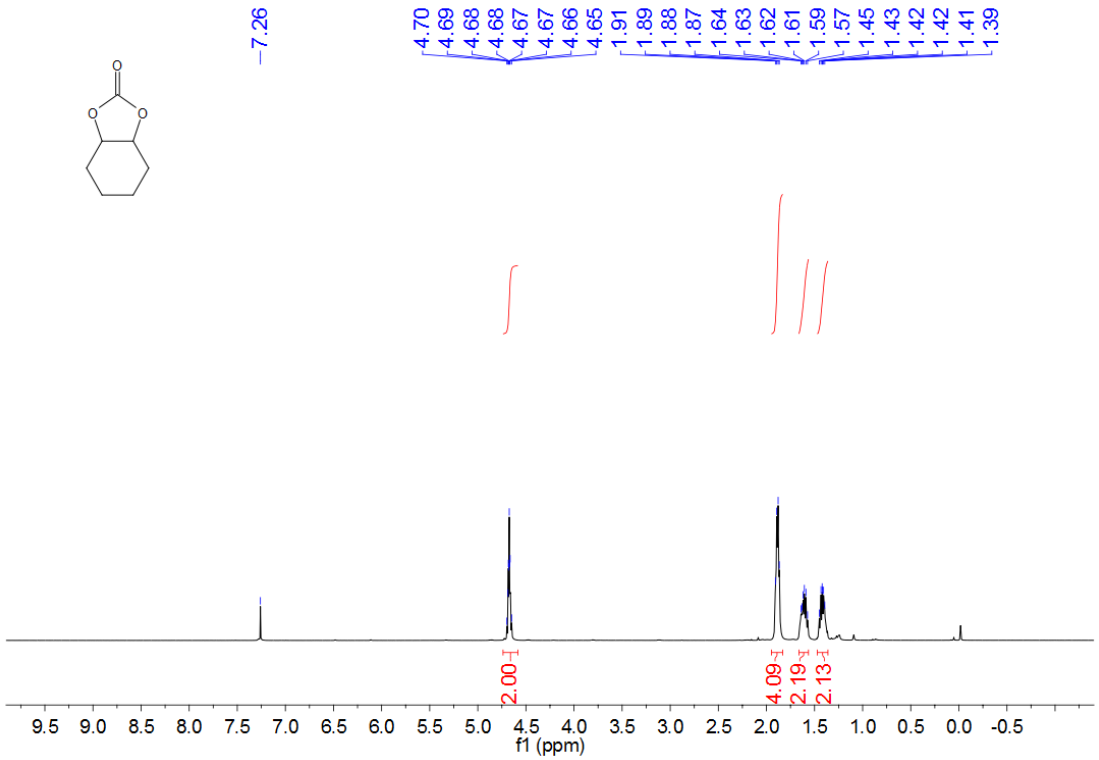
f1 (ppm)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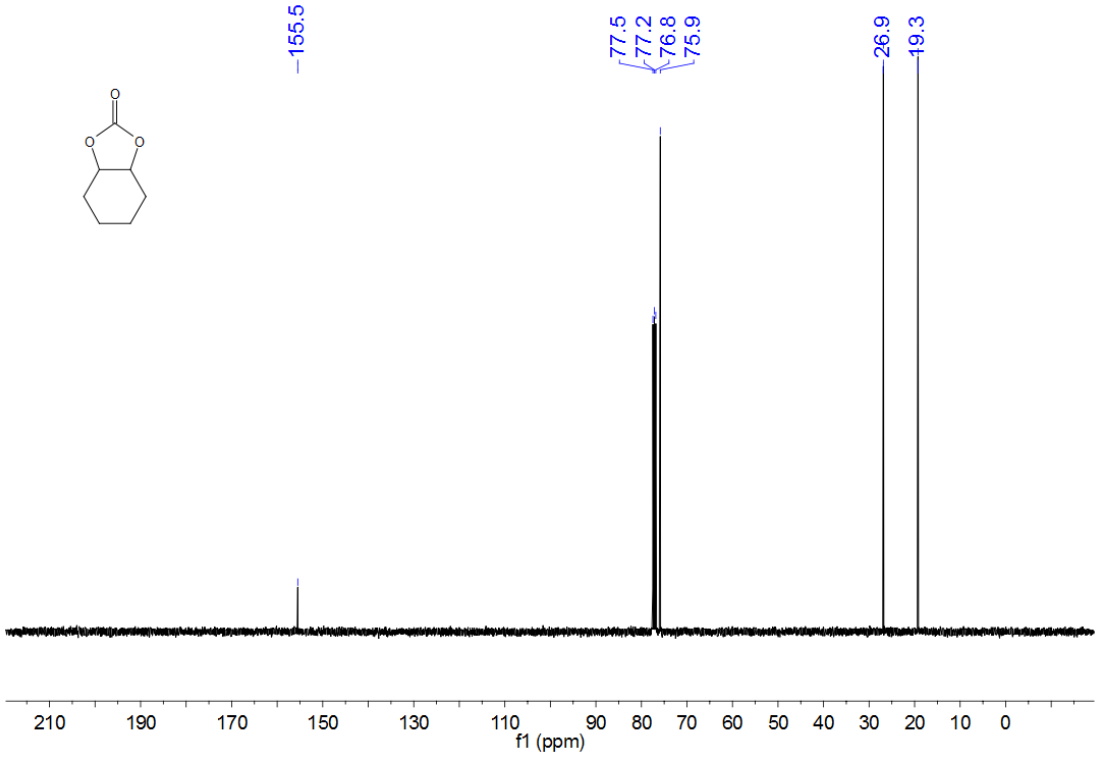
1.87
1.64
1.63
1.62
1.61
1.59
1.57
1.45
1.43
1.42
1.42
1.41
1.39
2.00
4.09
2.19
2.13
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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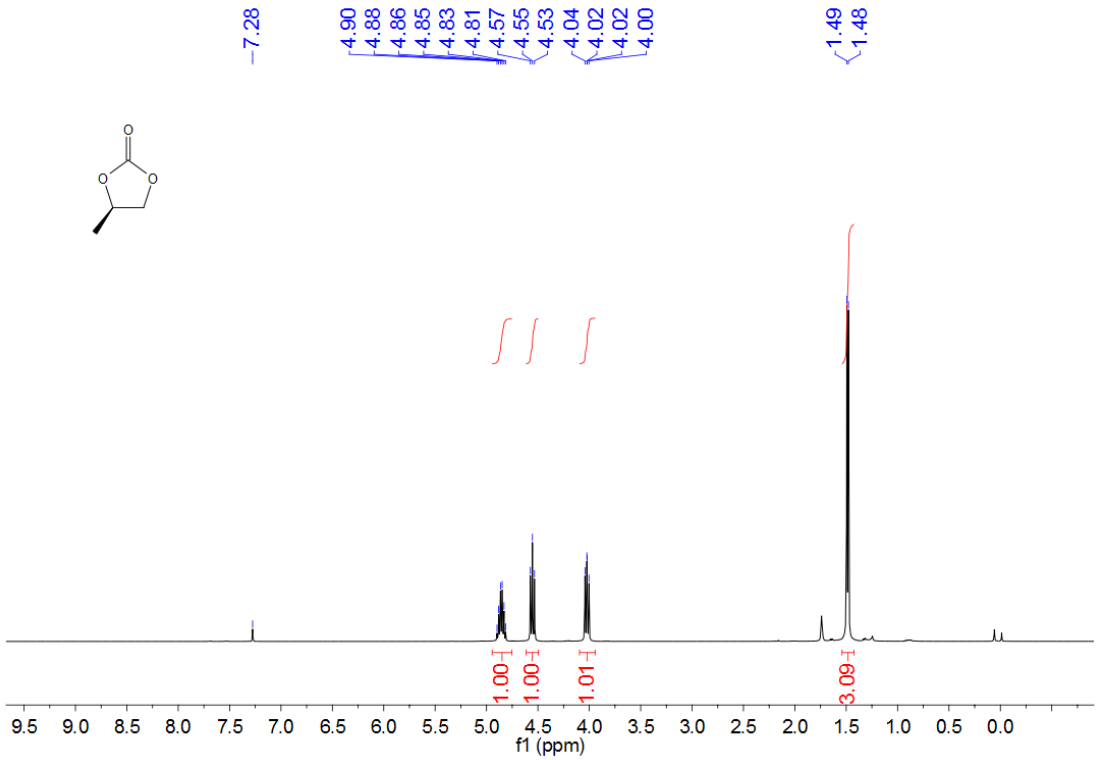
76.8
75.9
26.9
19.3
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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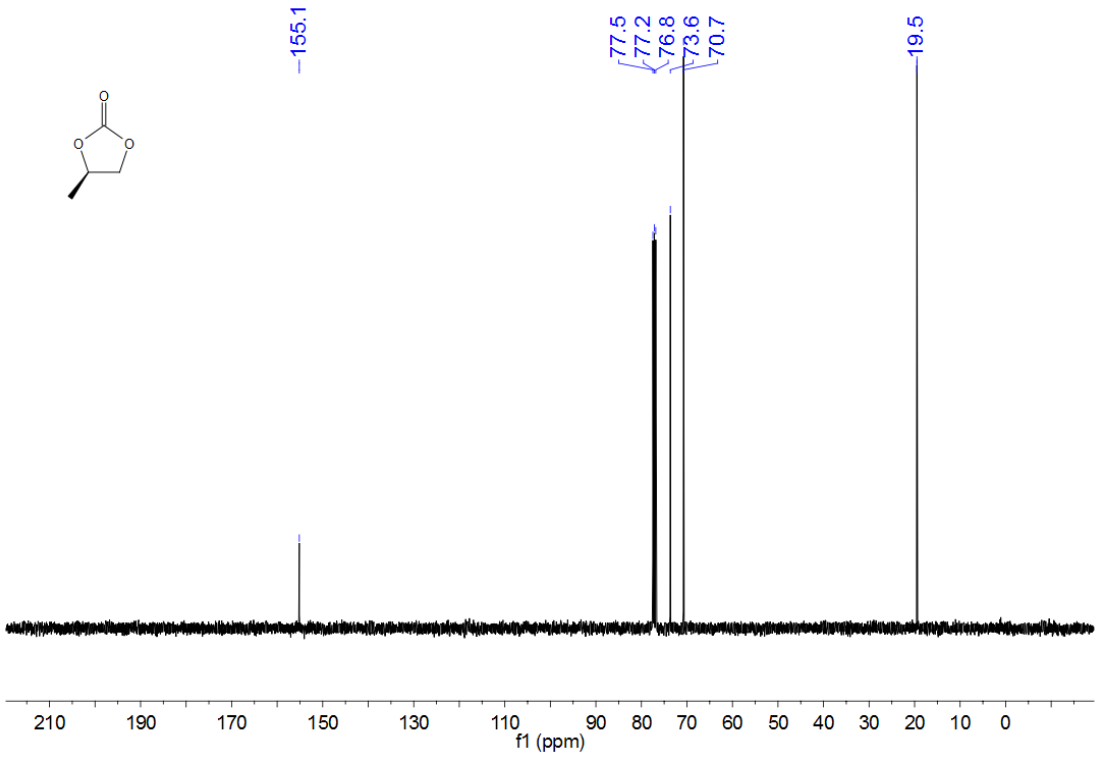
4.00
1.49
1.48
1.00
1.00
1.01
3.09
f1 (ppm)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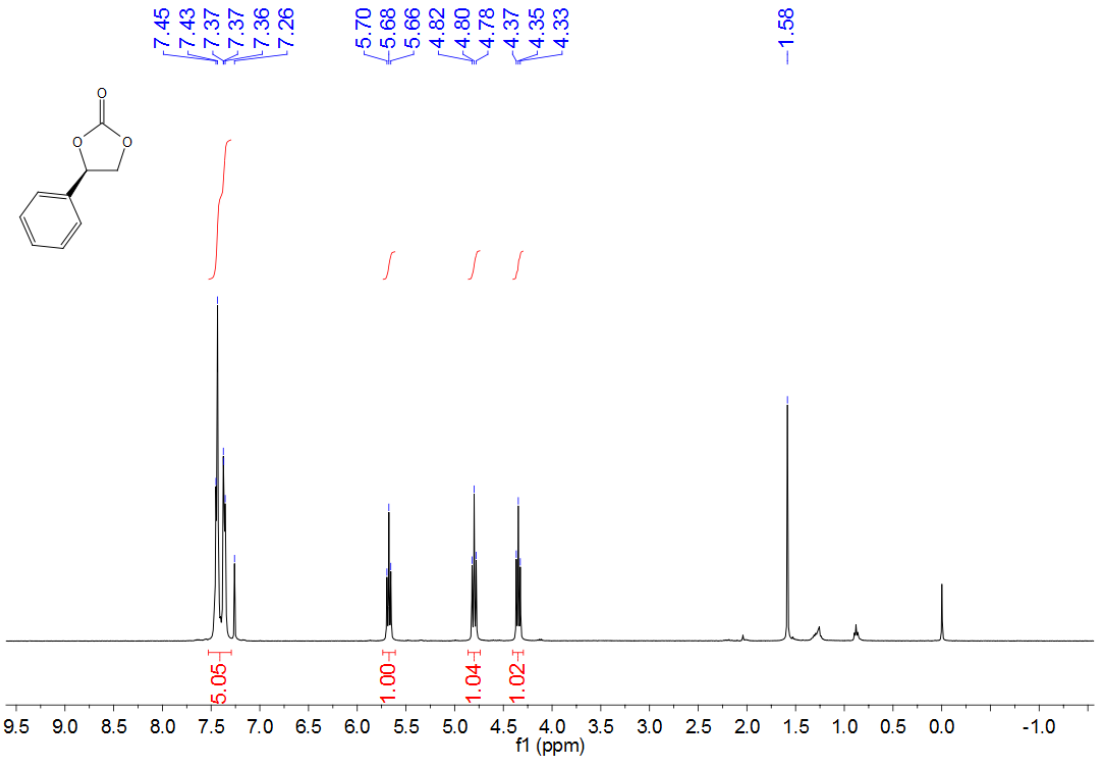
77.2
76.8
73.6
70.7
19.5
f1 (ppm)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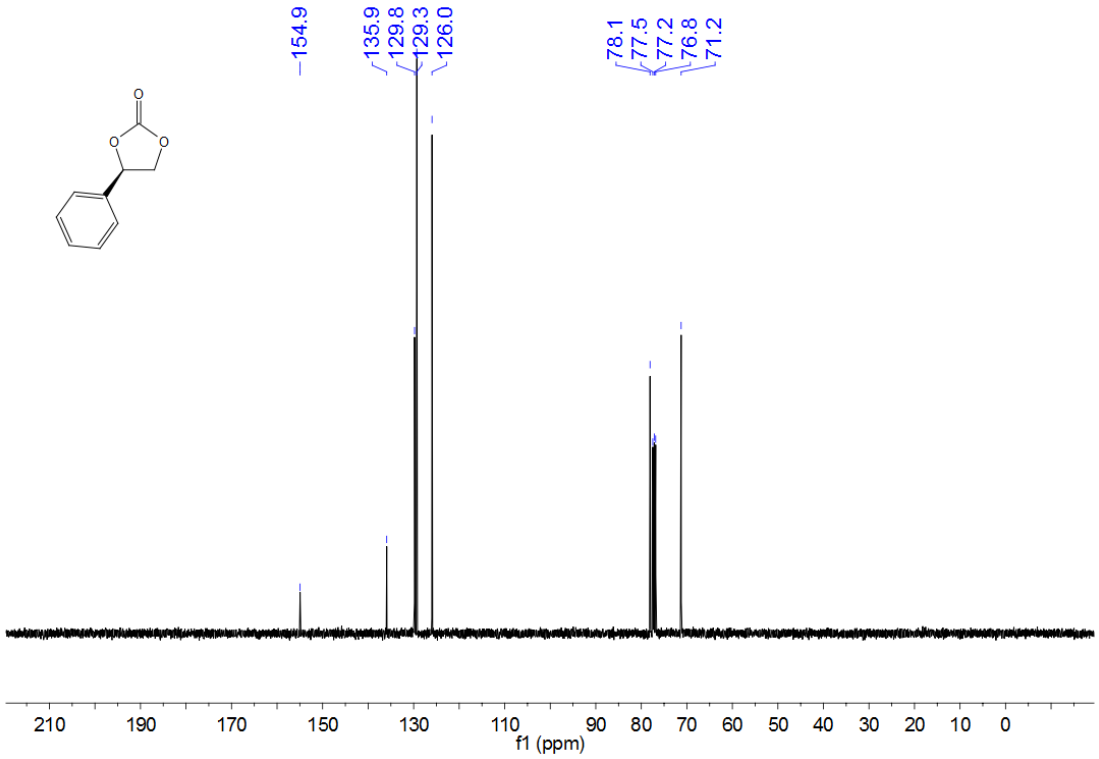
4.80
4.78
4.37
4.35
4.33
1.58
5.05
1.00
1.04
1.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)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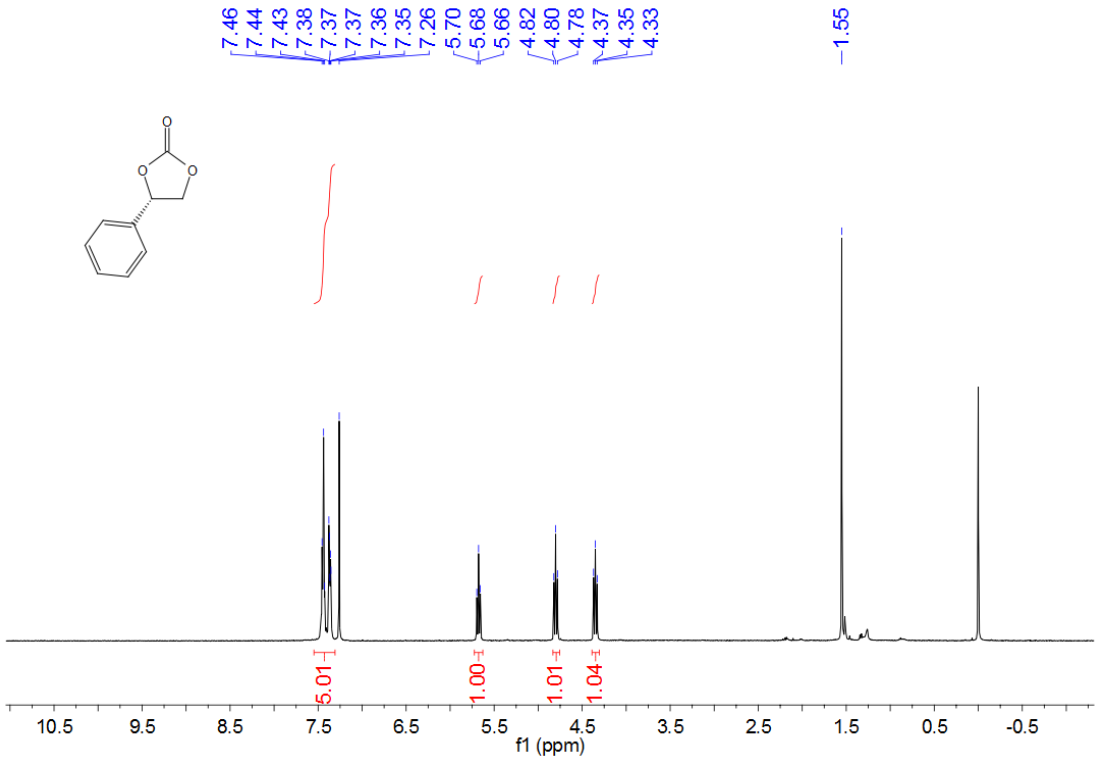
77.2
76.8
71.2
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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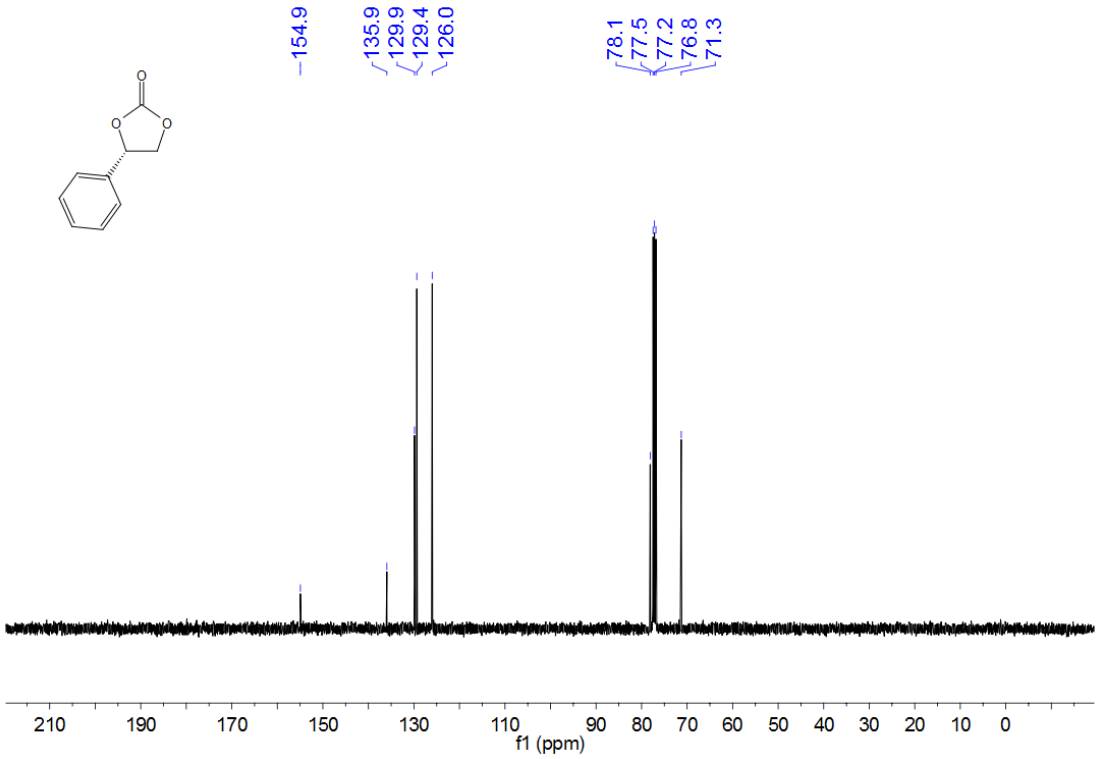
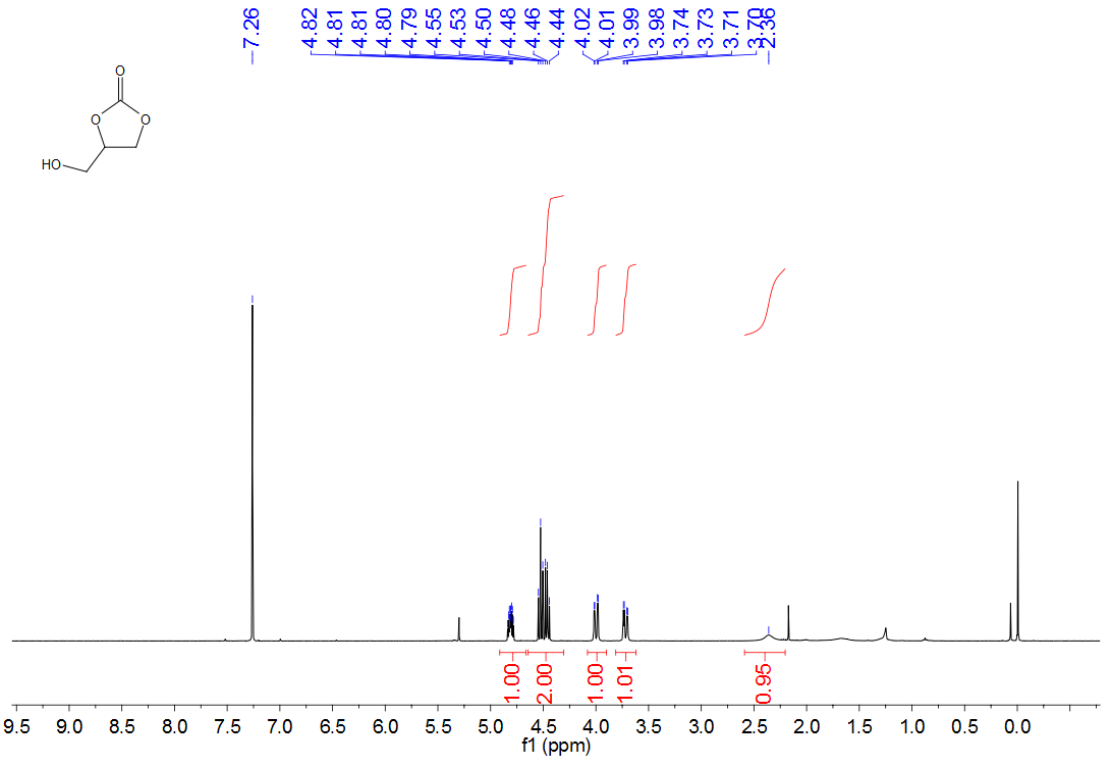
4.80
4.78
4.37
4.35
4.33
1.55
5.01
1.00
1.01
1.04
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


154.9
135.9
129.9
129.4
126.0
78.1
77.5
77.2
76.8
71.3
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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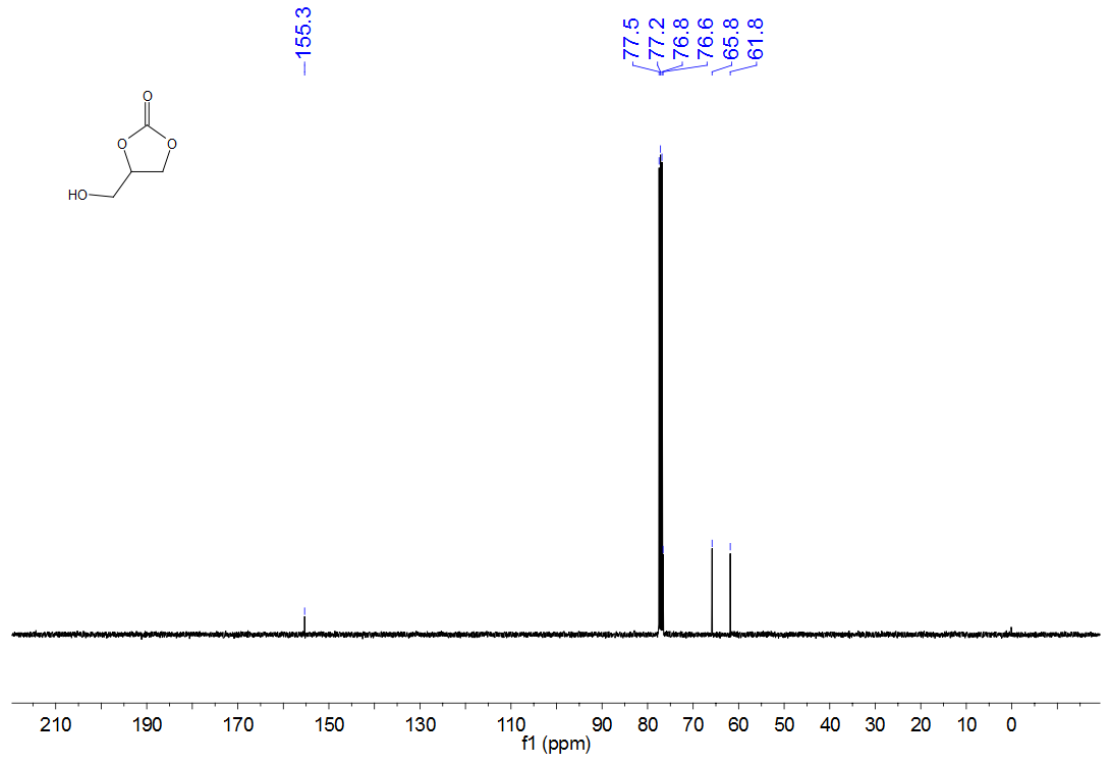
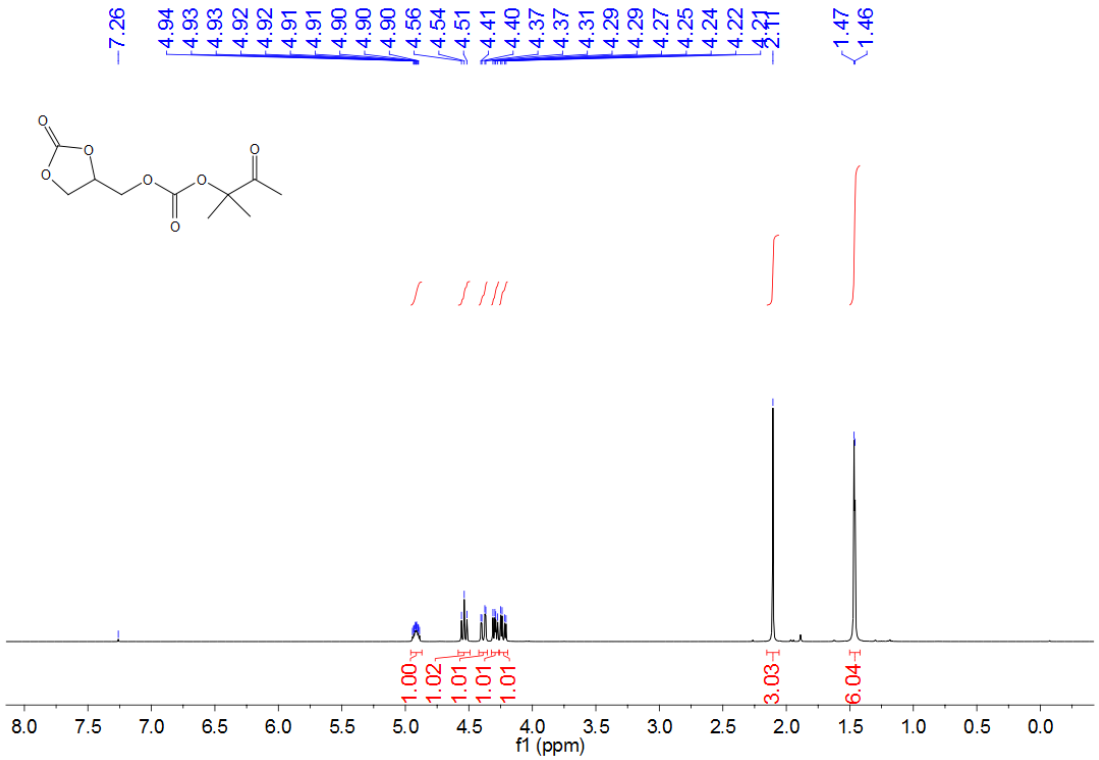
4.82
4.81
4.81
4.80
4.79
4.55
4.53
4.50
4.48
4.46
4.44
4.02
4.01
3.99
3.98
3.74
3.73
3.71
3.70
2.38
HO
1.00
2.00
1.00
1.01
0.95
f1 (ppm)


155.3
77.5
77.2
76.8
76.6
65.8
61.8
HO
f1 (ppm)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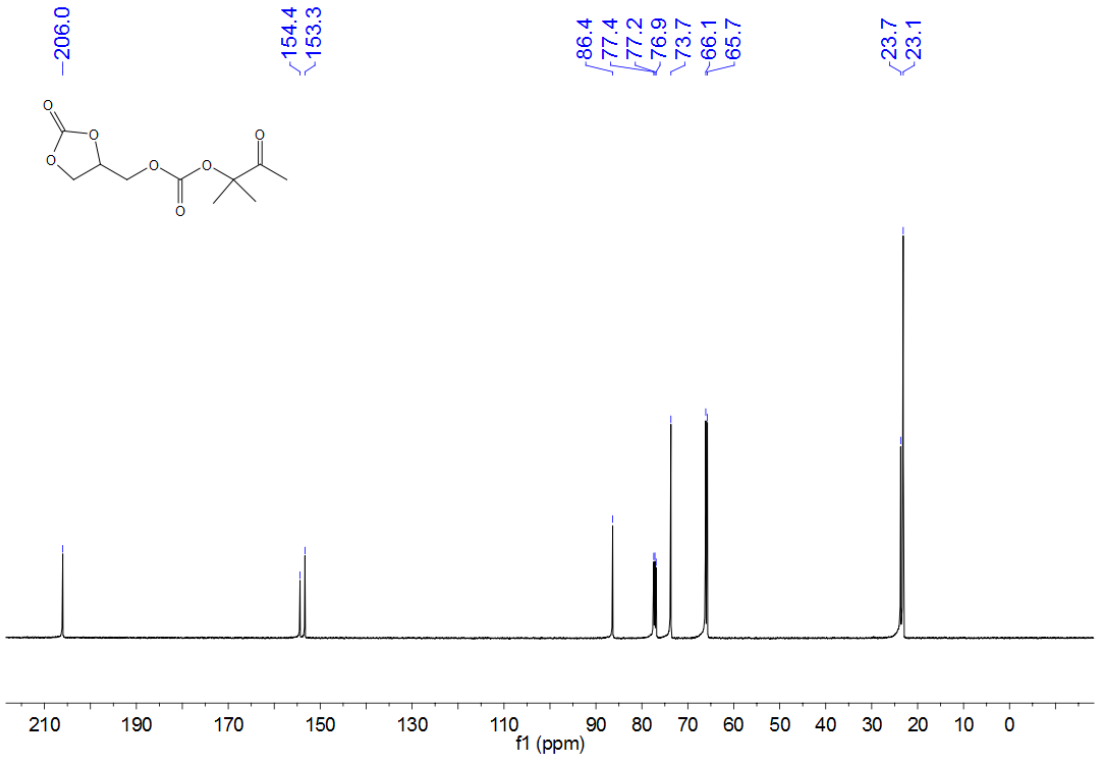
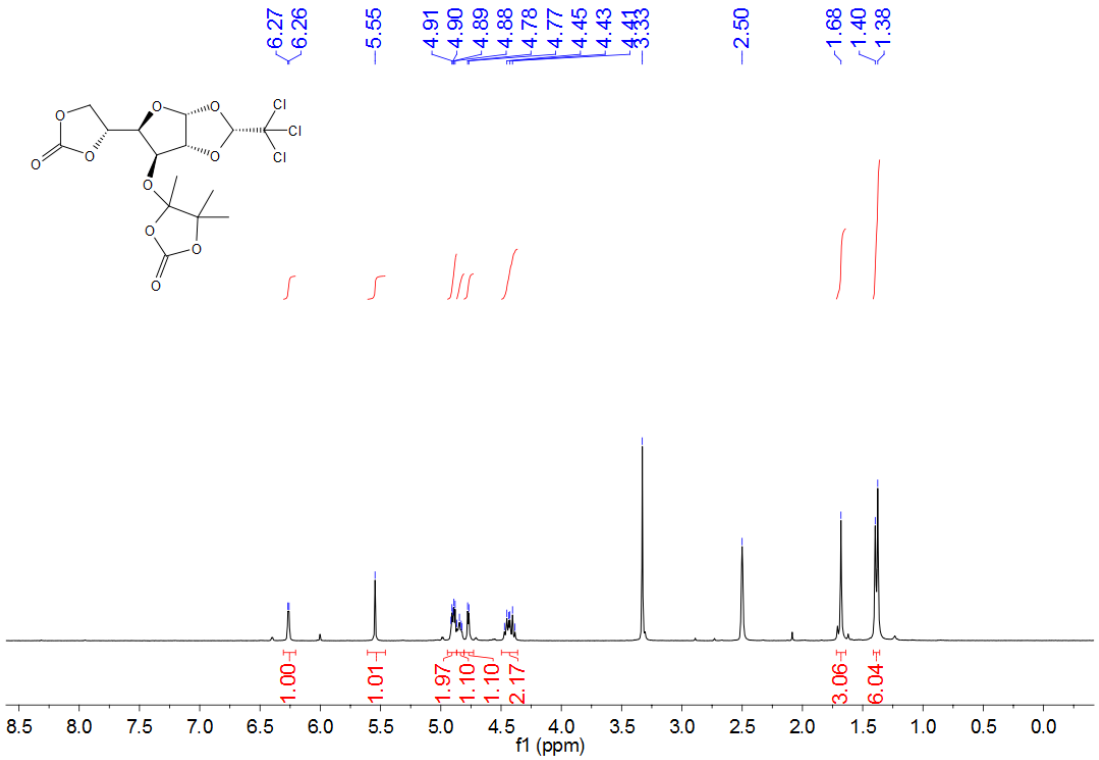
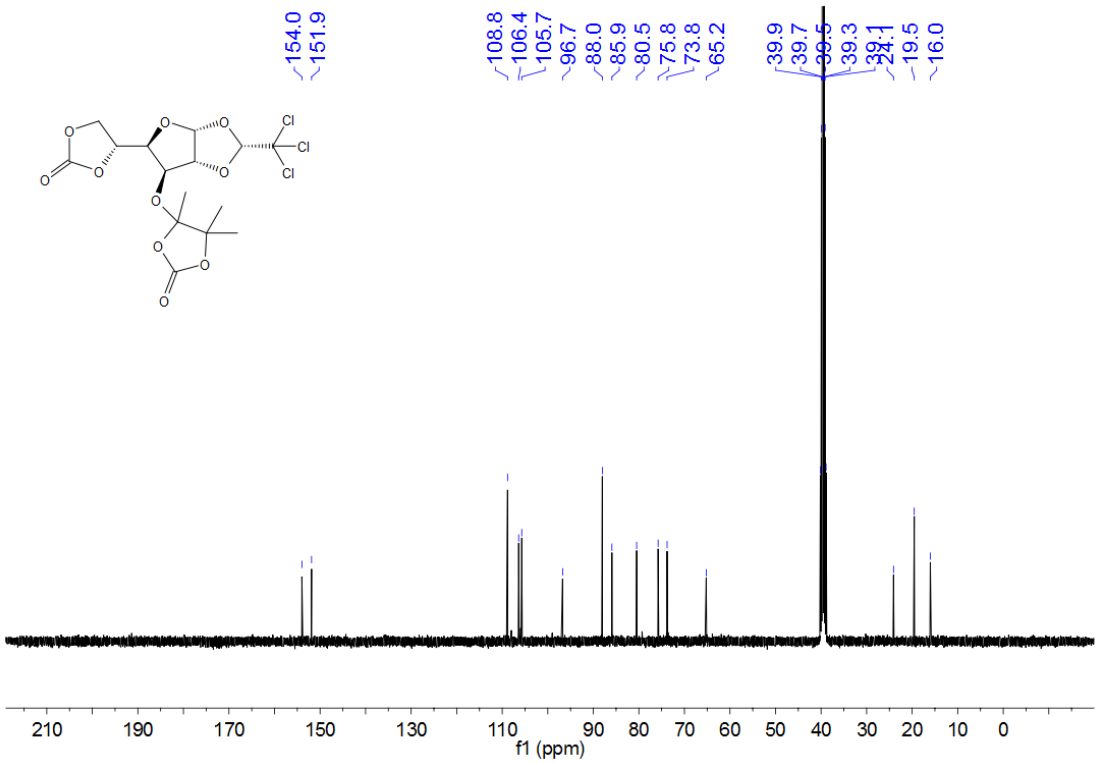
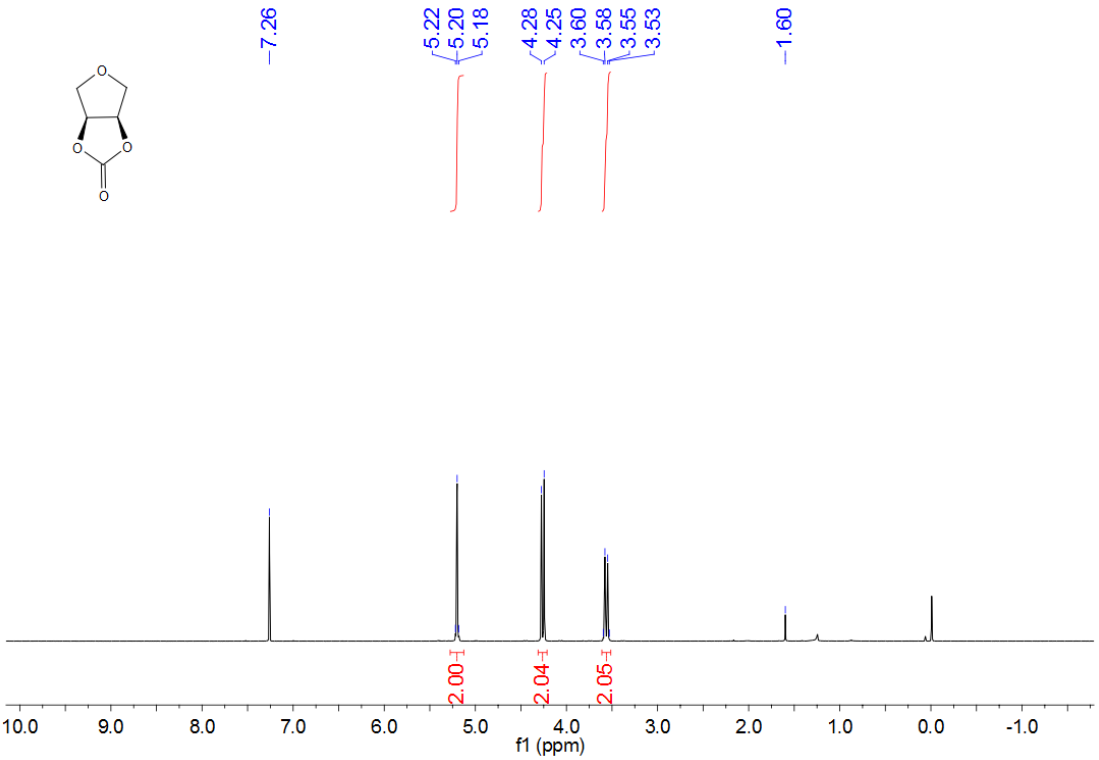
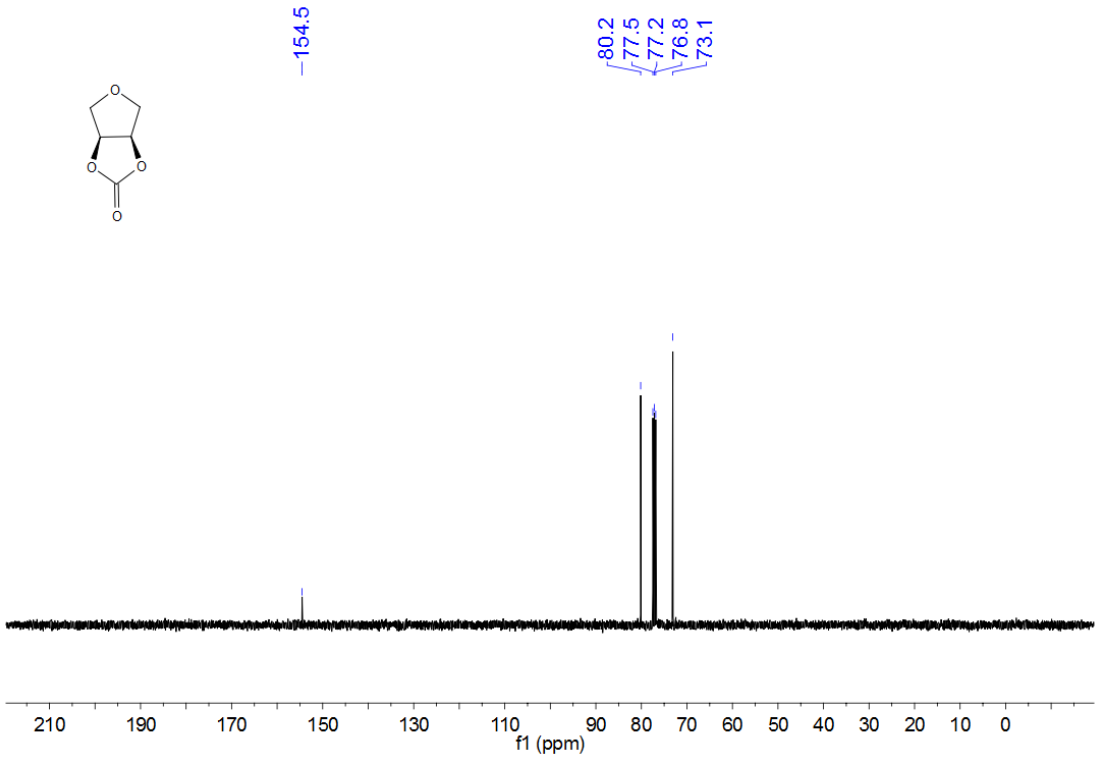
4.94
4.93
4.93
4.92
4.92
4.91
4.91
4.90
4.90
4.90
4.56
4.54
4.51
4.41
4.40
4.37
4.37
4.31
4.29
4.29
4.27
4.25
4.24
4.22
4.21
2.11
1.47
1.46
1.00
1.02
1.01
1.01
1.01
1.01
3.03
6.04
f1 (ppm)

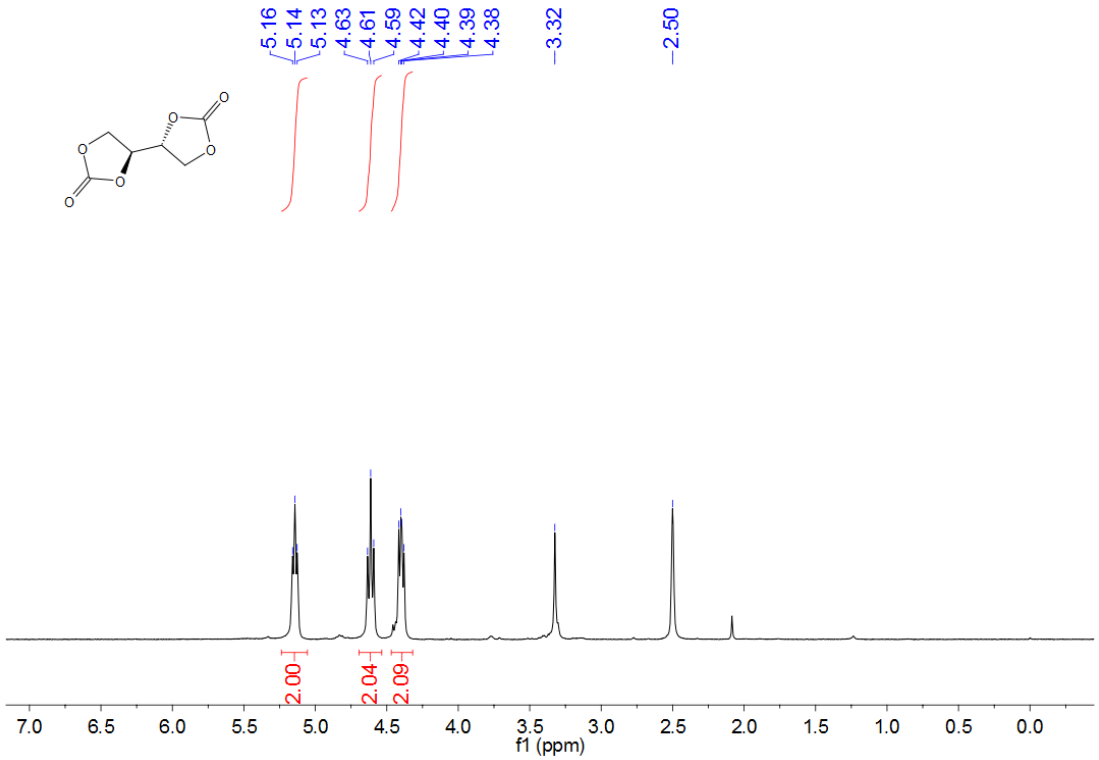

206.0
154.4
153.3
86.4
77.4
77.2
76.9
73.7
66.1
65.7
23.7
23.1
f1 (ppm)

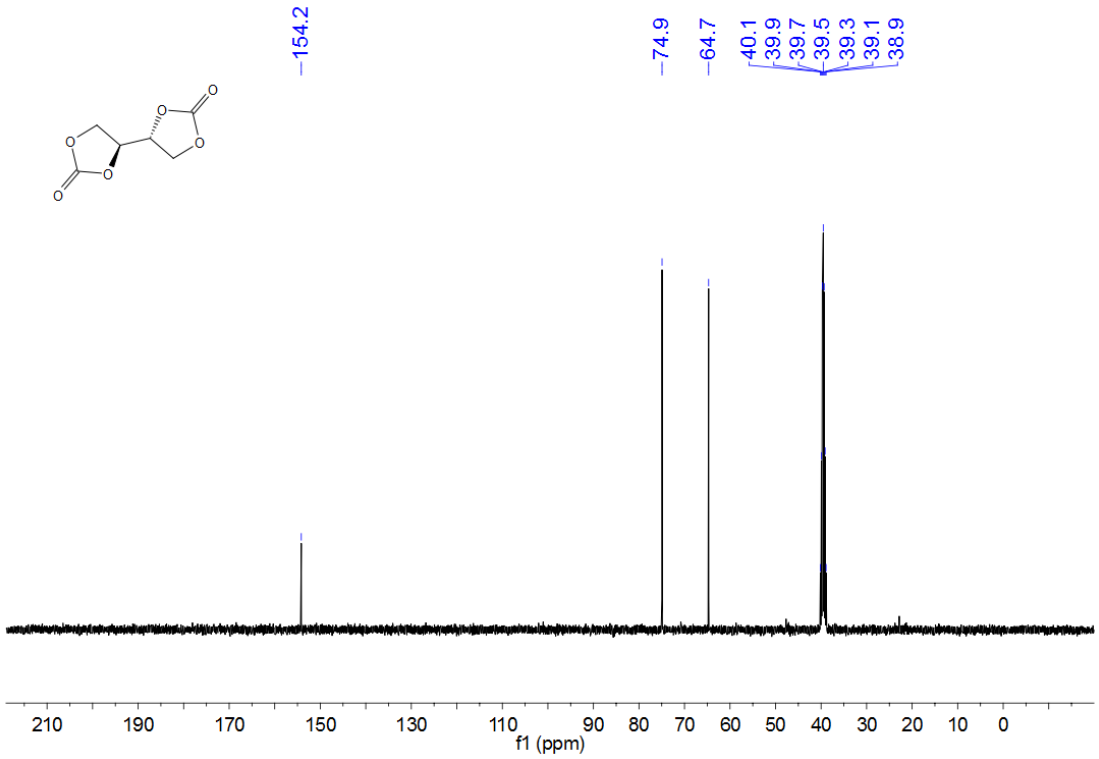

6.27
6.26
5.55
4.91
4.90
4.89
4.88
4.78
4.77
4.45
4.43
4.41
3.33
2.50
1.68
1.40
1.38
Cl
Cl
Cl
O
O
O
O
O
O
O
O
O
O
O
1.00
1.01
1.97
1.10
1.10
2.17
3.06
6.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

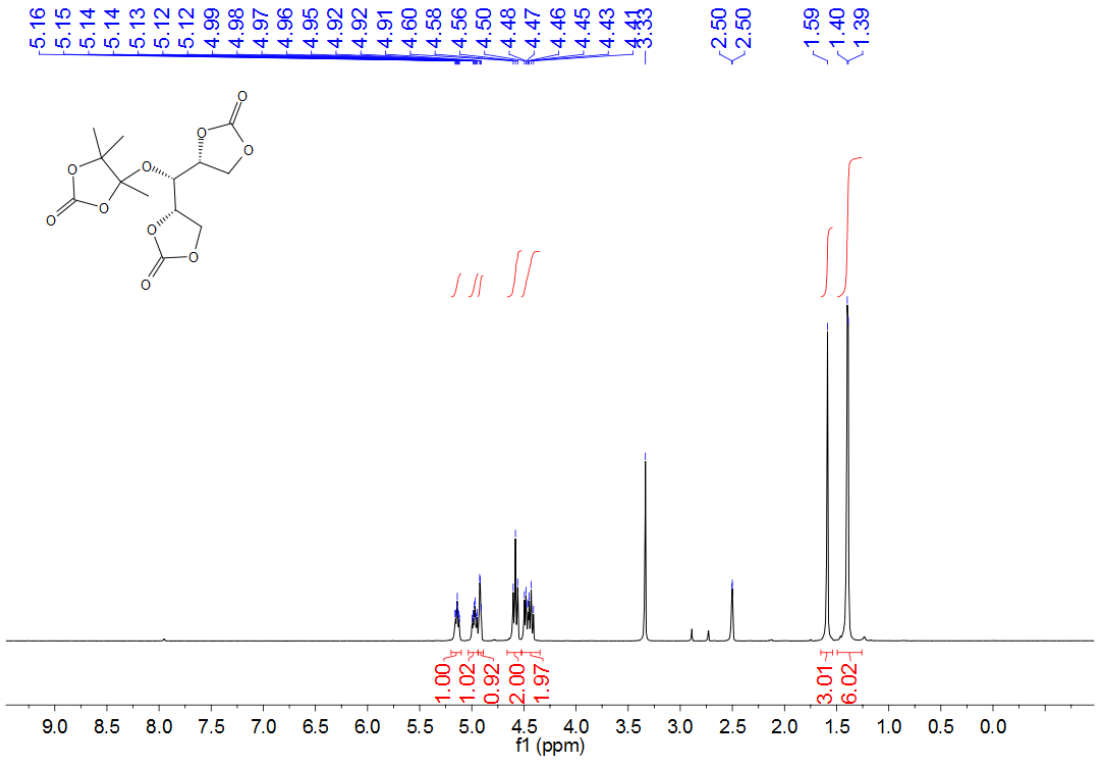

154.0
151.9
108.8
106.4
105.7
96.7
88.0
85.9
80.5
75.8
73.8
65.2
39.9
39.7
39.5
39.3
39.1
24.1
19.5
16.0
Cl
Cl
Cl
O
O
O
O
O
O
O
O
O
O
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

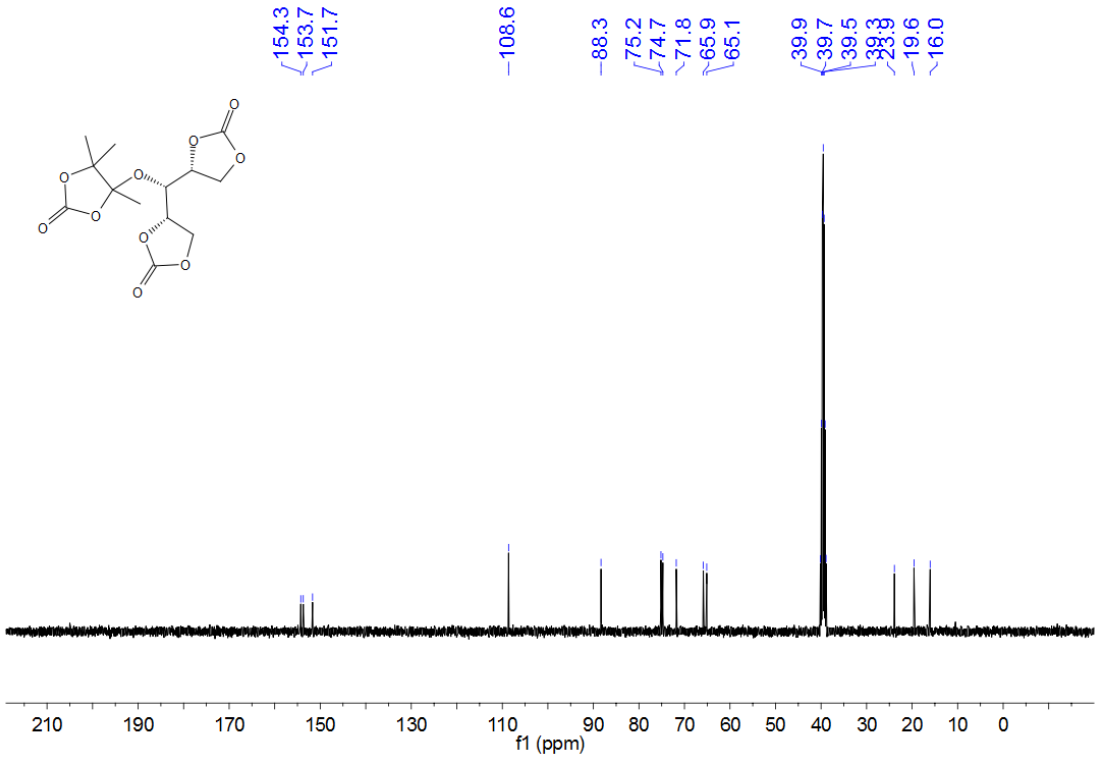

7.26
5.22
5.20
5.18
4.28
4.25
3.60
3.58
3.55
3.53
1.60
2.00
2.04
2.05
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

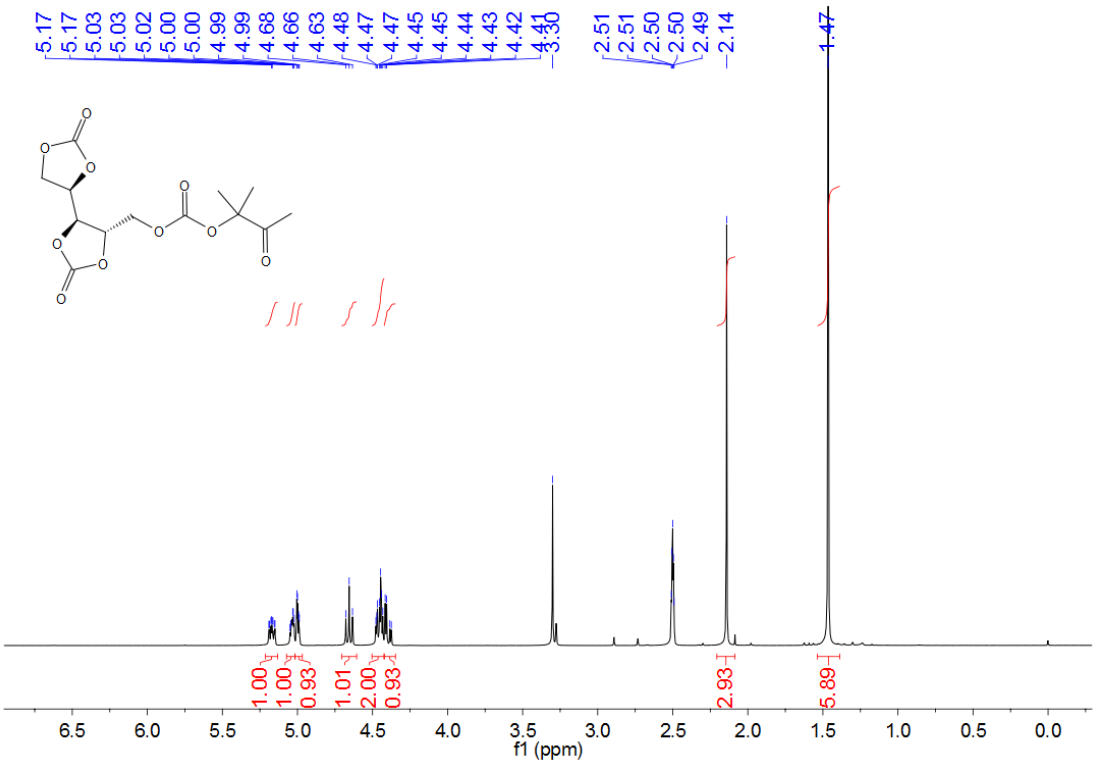

154.5
80.2
77.5
77.2
76.8
73.1
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

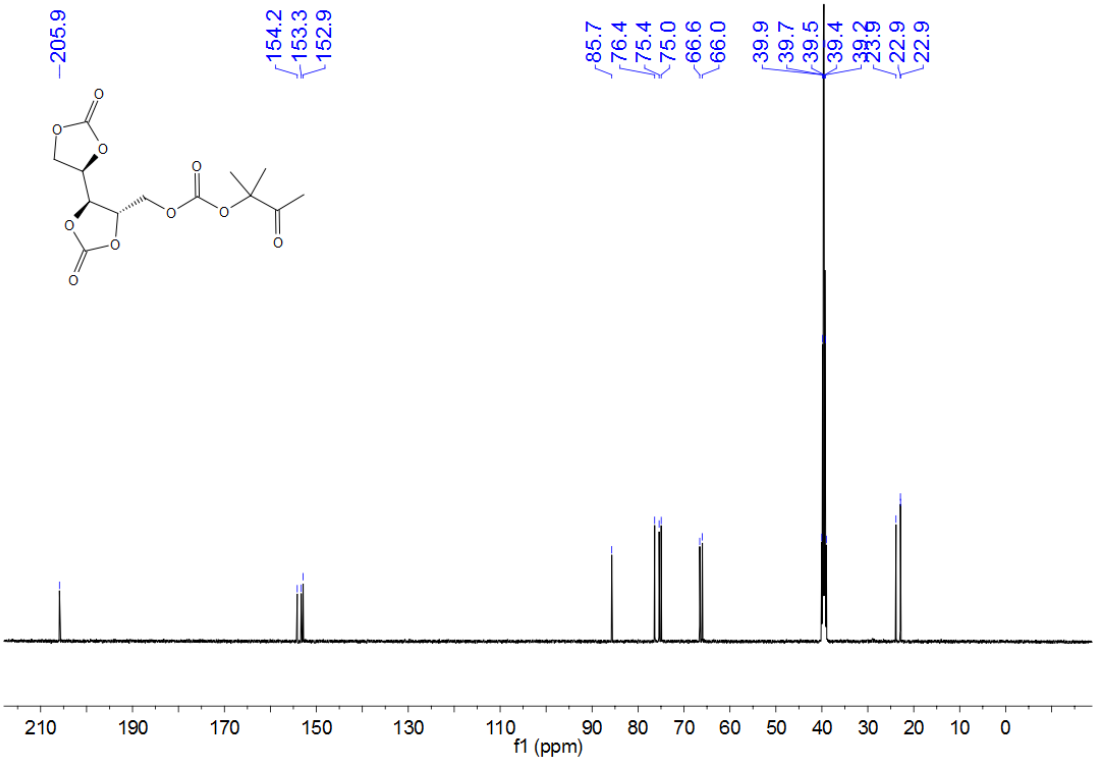

5.16
5.14
5.13
4.63
4.61
4.59
4.42
4.40
4.39
4.38
3.32
2.50
2.00
2.04
2.09
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

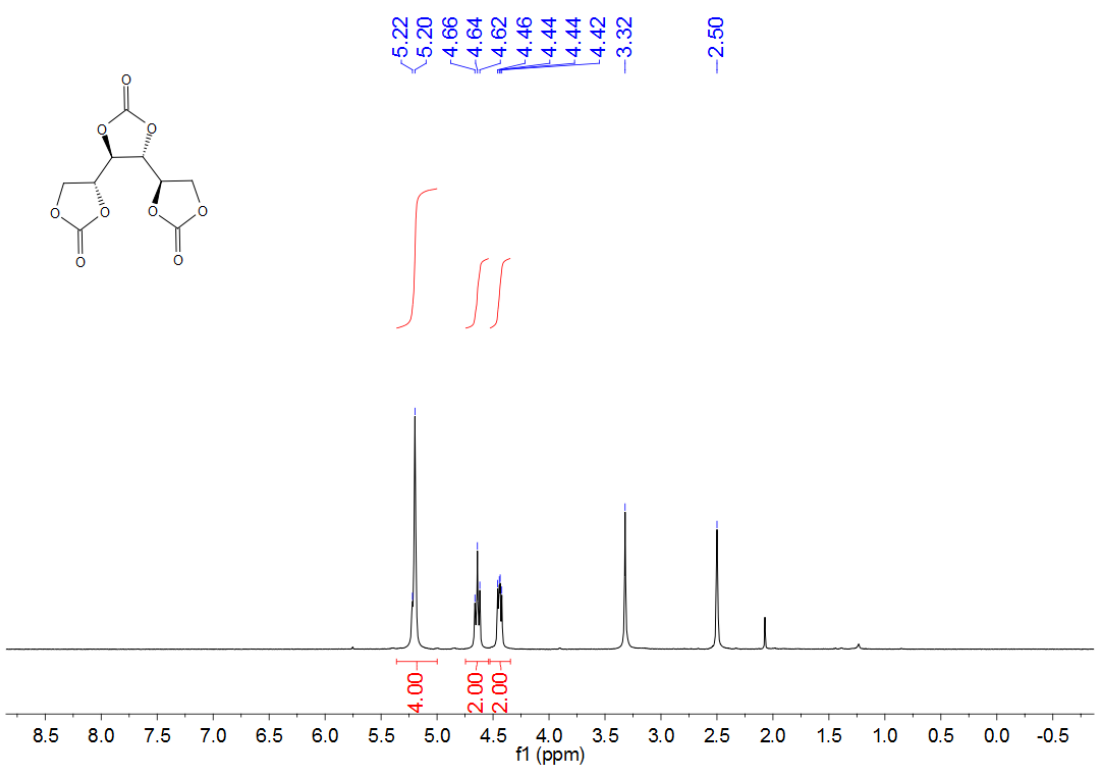

154.2
74.9
64.7
40.1
39.9
39.7
39.5
39.3
39.1
38.9
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

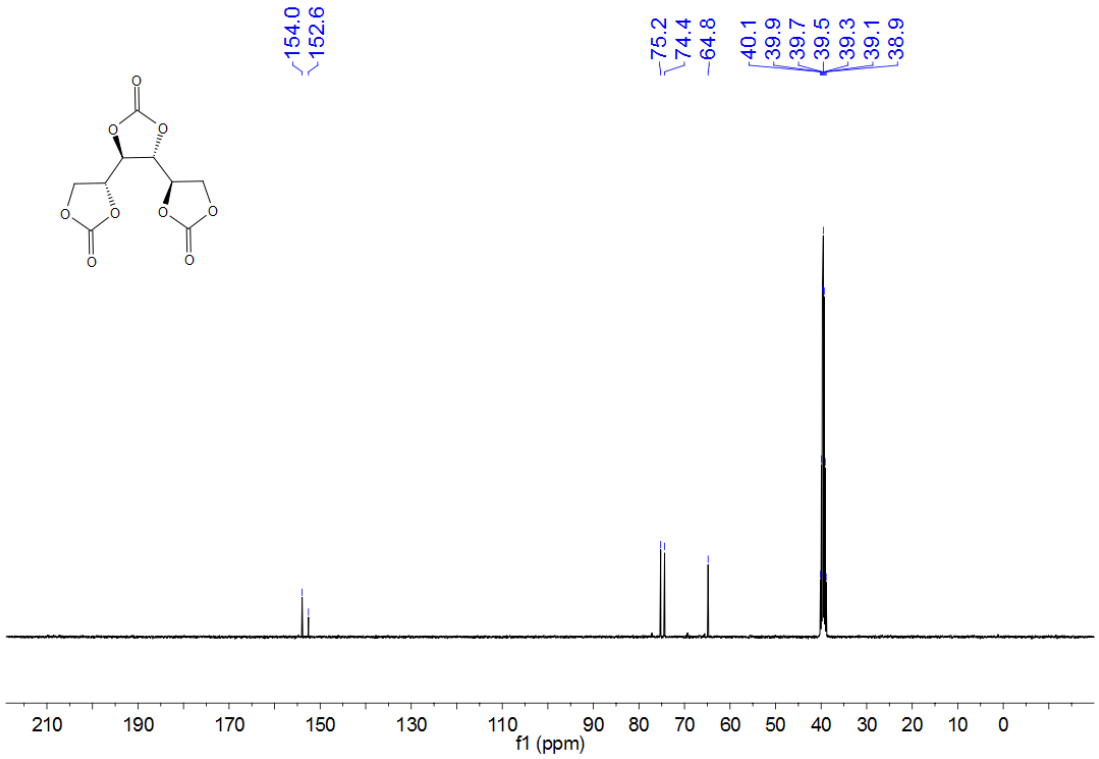

5.16
5.15
5.14
5.14
5.13
5.12
5.12
4.99
4.98
4.97
4.96
4.95
4.92
4.92
4.91
4.60
4.58
4.56
4.50
4.48
4.47
4.46
4.45
4.43
4.41
3.33
2.50
2.50
1.59
1.40
1.39
1.00
1.02
0.92
2.00
1.97
3.01
6.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

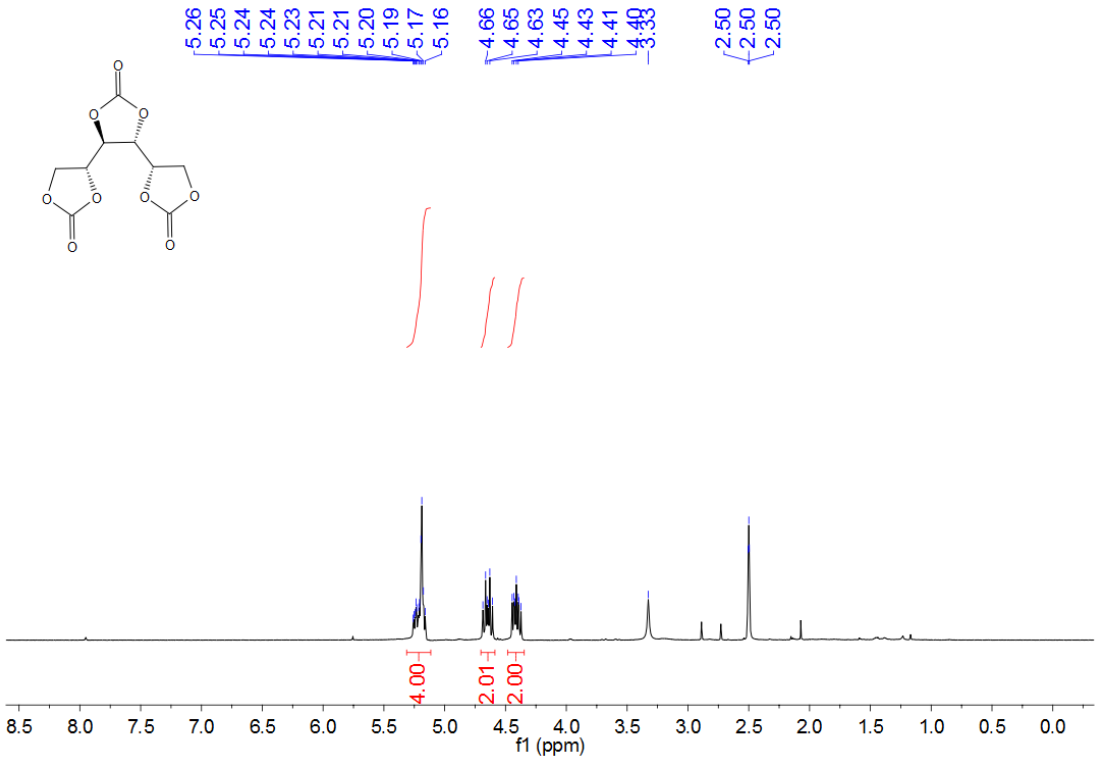

154.3
153.7
151.7
108.6
88.3
75.2
74.7
71.8
65.9
65.1
39.9
39.7
39.5
39.3
23.9
19.6
16.0
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

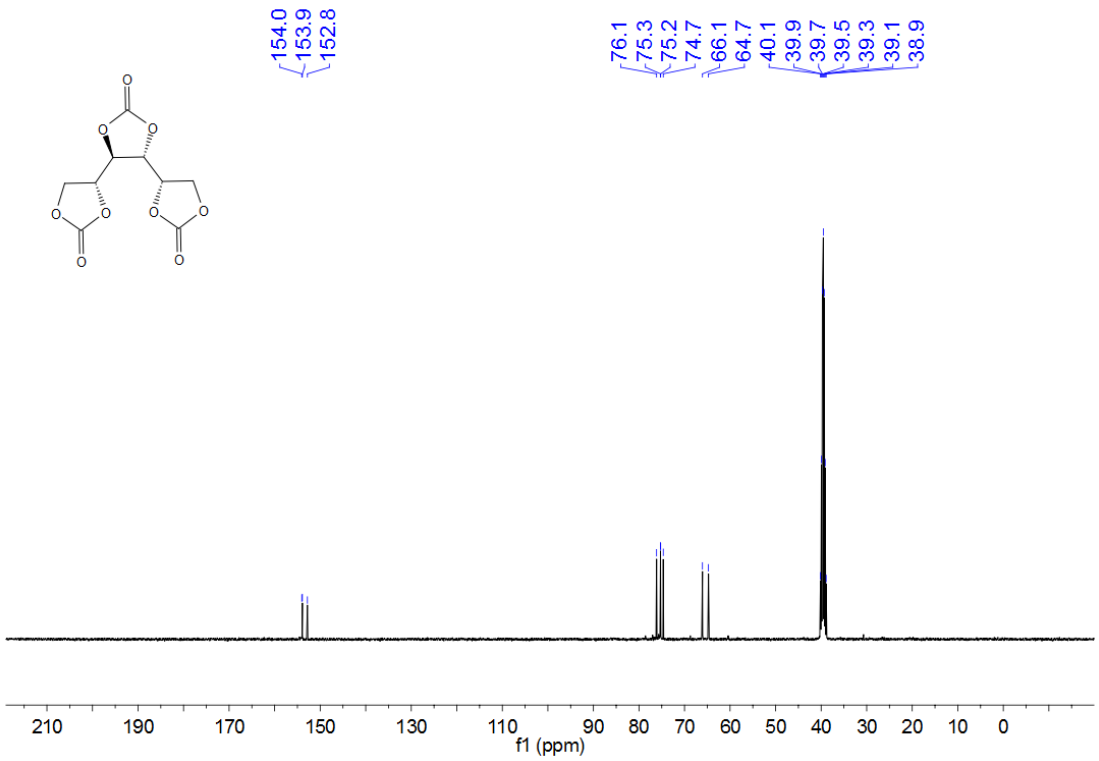

5.17
5.17
5.03
5.03
5.02
5.00
5.00
4.99
4.99
4.68
4.66
4.63
4.48
4.47
4.47
4.45
4.45
4.44
4.43
4.42
4.41
4.30
2.51
2.51
2.50
2.50
2.49
2.14
1.47
1.00
1.00
0.93
1.01
2.00
0.93
2.93
5.89
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


205.9
154.2
153.3
152.9
85.7
76.4
75.4
75.0
66.6
66.0
39.9
39.7
39.5
39.4
39.2
23.9
22.9
22.9
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

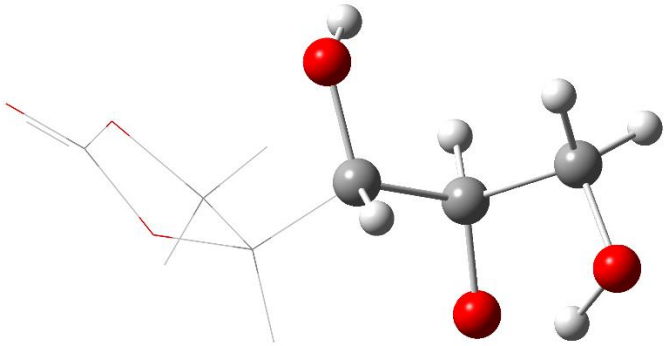

5.22
5.20
4.66
4.64
4.62
4.46
4.44
4.44
4.42
3.32
2.50
4.00
2.00
2.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


154.0
152.6
75.2
74.4
64.8
40.1
39.9
39.7
39.5
39.3
39.1
38.9
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


5.26
5.25
5.24
5.24
5.23
5.21
5.21
5.20
5.19
5.17
5.16
4.66
4.65
4.63
4.45
4.43
4.41
4.40
4.33
2.50
2.50
2.50
4.00
2.01
2.00
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)

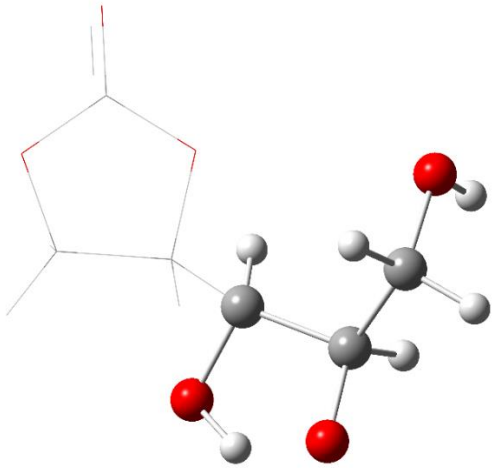

154.0
153.9
152.8
76.1
75.3
75.2
74.7
66.1
64.7
40.1
39.9
39.7
39.5
39.3
39.1
38.9
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

11. Cartesian coordinates of intermediates



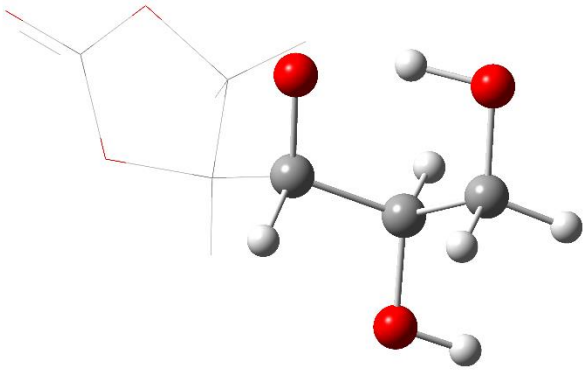
Intermediate 1

C	2.95865400	-0.69206100	0.47953300
H	2.61514500	-1.73252500	0.58607200
H	3.61654000	-0.47104600	1.34119500
C	1.75748100	0.31513700	0.45625000
H	1.49282200	0.55293900	1.52304400
C	0.52163000	-0.40229800	-0.12586800
H	0.83493900	-0.96009600	-1.01847200
C	-0.51965100	0.61522800	-0.55921200
H	-0.08929500	1.29383800	-1.29097900
C	-1.19871300	1.34018000	0.60326200
H	-1.50760400	2.35605400	0.34478300
H	-0.60132800	1.35927600	1.51586900
O	-0.05692100	-1.34925400	0.76380400
H	3.21429100	0.44277000	-0.90709800
O	2.11457400	1.37832300	-0.29994200
O	-1.64038100	-0.08022400	-1.15308500
O	3.61854900	-0.48687000	-0.73649800
O	-2.37234000	0.54665400	0.83976500
C	-2.59755400	-0.23461000	-0.23048800
O	-3.55676300	-0.94604700	-0.35076400
H	0.03967300	-0.99132400	1.65847400



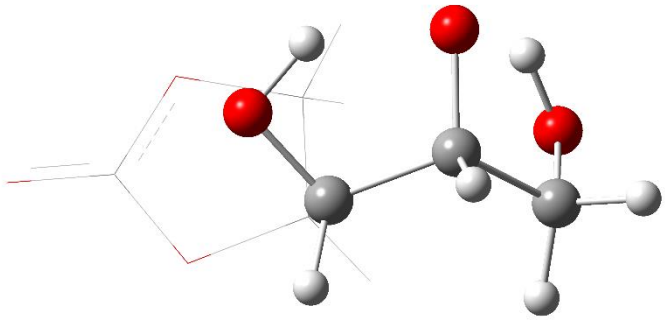
Intermediate 2

C	1.90060000	1.43442000	0.44565800
H	2.81815500	1.78335800	0.94616200
H	1.09457100	1.46589600	1.18716900
C	2.13997000	0.00322800	-0.02916700
H	2.85057400	0.10277100	-0.90269600
C	0.86543400	-0.68694100	-0.62954900
H	0.61941900	-0.35491100	-1.64913900
C	-0.35906100	-0.52830000	0.25869300
H	-0.04464700	-0.60020400	1.30645600
C	-1.45571200	-1.53671200	-0.07417100
H	-1.47584500	-2.40004600	0.58836300
H	-1.40512100	-1.86653000	-1.11609900
O	1.19177200	-2.05218600	-0.57833500
H	1.89745100	-1.92086500	0.19255500
O	2.58569600	-0.82692200	0.94557000
O	-1.04678100	0.73085400	0.07784200
O	1.52292800	2.31502900	-0.60387400
O	-2.66584300	-0.78053600	0.11346800
C	-2.37015600	0.52980700	0.09383100
O	-3.19299600	1.40411900	0.09180800
H	2.16078000	2.17466100	-1.31638400



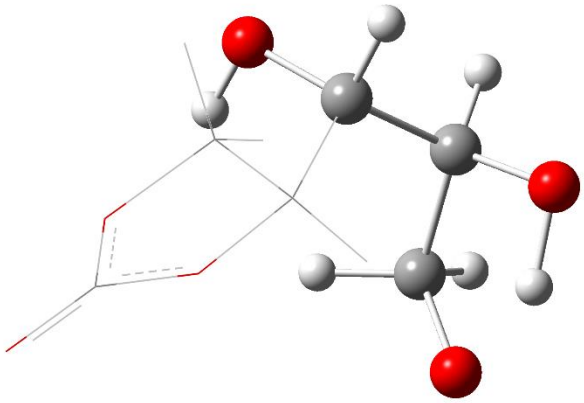
Intermediate 3

C	2.95623000	-0.52706600	-0.16704400
H	3.91427300	-0.21204400	0.28171400
H	3.10820800	-0.50720000	-1.26604900
C	1.87466400	0.50490400	0.15818000
H	1.73689700	0.50609000	1.25363200
C	0.55596400	0.07657100	-0.51555400
H	0.69028400	0.34791900	-1.59470700
C	-0.58883300	0.97334500	-0.02205800
H	-0.36797500	2.04036400	-0.09517500
C	-1.07732100	0.54000700	1.36511600
H	-1.37341900	1.37328600	2.00696800
H	-0.34690800	-0.09872900	1.86188200
O	0.25167900	-1.23191700	-0.29799600
H	1.56278400	-1.76686100	0.08765400
O	2.21887200	1.80290900	-0.30721000
O	-1.74374300	0.70153600	-0.84553400
O	2.58554100	-1.78462200	0.30900900
O	-2.23750500	-0.25445800	1.08639100
C	-2.53869600	-0.16892300	-0.21616800
O	-3.45578600	-0.75144600	-0.73142700
H	3.03135100	2.06813400	0.14338900



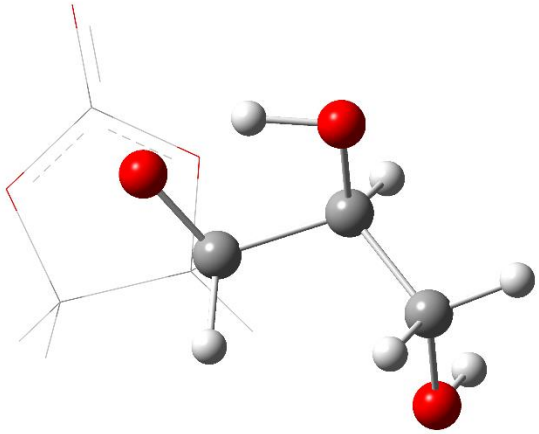
Intermediate 4

C	-2.65808400	-0.44688400	-0.76282900
H	-2.32869900	-0.67341100	-1.78616200
H	-3.74933200	-0.29101200	-0.79374500
C	-1.97546600	0.80857200	-0.17885300
H	-2.48595500	1.70410900	-0.60057600
C	-0.47402900	0.93502600	-0.60488900
H	-0.38327000	1.42604200	-1.58460700
C	0.27367800	-0.39409700	-0.69300900
H	-0.15903900	-1.07781500	-1.42409800
C	0.50271500	-1.05681300	0.67125400
H	0.42887700	-2.14531700	0.63212600
H	-0.16014500	-0.64419800	1.42971700
O	0.13104700	1.71825000	0.39617200
H	-2.21801800	-0.97739500	0.93227500
O	-2.01743800	0.74922300	1.18894300
O	1.62764100	-0.10718700	-1.11956300
O	-2.33052800	-1.51441400	0.10177500
O	1.85672200	-0.70018400	0.99906900
C	2.45061700	-0.14837200	-0.06510400
O	3.59350500	0.22366900	-0.08173400
H	-0.54860100	1.53955700	1.11836000



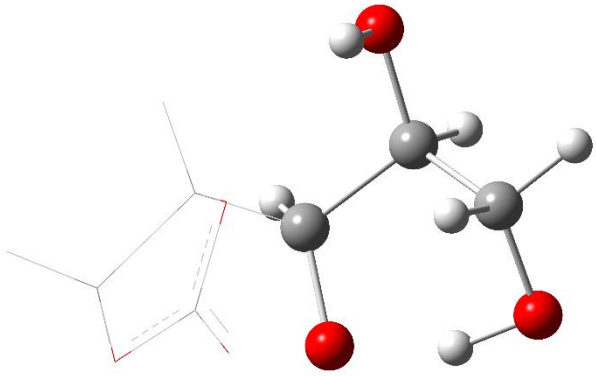
Intermediate 5

C	-1.49125500	-1.34249200	-0.78903500
H	-1.55977600	-2.14275100	-0.04589100
H	-1.51368500	-1.75778900	-1.79607200
C	-0.28499500	-0.43832300	-0.53199700
H	0.17393200	-0.04460300	-1.43930400
C	0.76878900	-1.10549700	0.35098300
H	0.89782100	-2.12360700	-0.04033700
C	2.13858100	-0.41936700	0.27126200
H	2.79580600	-0.93744600	0.98991300
C	2.06926300	1.12870800	0.55663200
H	3.01029900	1.40987100	1.09477100
H	1.25418300	1.33768300	1.28650200
O	0.27338500	-1.24466600	1.66946600
O	-0.89117400	0.66890100	0.17354500
O	2.60645300	-0.49726300	-1.03737000
H	2.39164200	0.54608000	-1.24015400
O	-2.61773300	-0.46940800	-0.61975700
O	1.92169000	1.73132400	-0.65457000
C	-2.22319600	0.63202300	0.03896300
O	-2.97090600	1.47713400	0.44594000
H	0.11293200	-0.34592000	1.99168200



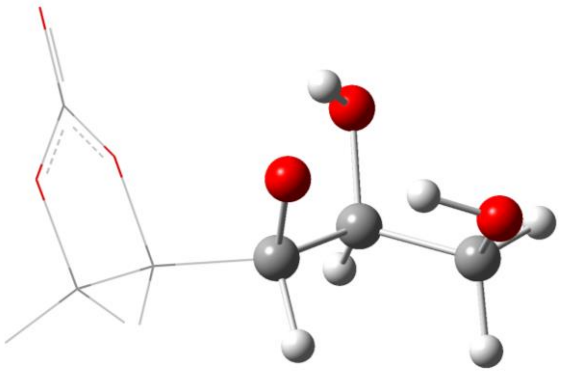
Intermediate 6

C	1.50998200	1.49421700	0.74326800
H	1.24426400	1.49564400	1.80113000
H	1.86172800	2.48356900	0.43735500
C	0.37739900	0.94712600	-0.13100900
H	-0.14756100	1.71906100	-0.69967600
C	-0.56128500	0.04663200	0.67433000
H	-1.09049800	0.75312700	1.36869900
C	-1.66473400	-0.61451600	-0.24837100
H	-1.35441000	-0.53389100	-1.31203000
C	-3.01161100	0.07458900	-0.11224100
H	-3.30965400	0.07680100	0.94277700
H	-3.78329300	-0.47392800	-0.67420900
O	0.12602000	-0.94129000	1.29391200
O	1.10862100	0.12461300	-1.06429300
O	-1.73151100	-1.94202700	0.16282000
H	-0.88592900	-1.89411200	0.77809800
O	2.56964200	0.55101300	0.54068000
O	-2.95228200	1.43579600	-0.52078600
C	2.25574000	-0.25177000	-0.48819900
O	2.96720200	-1.13312300	-0.89030500
H	-2.66912900	1.43620900	-1.44503400



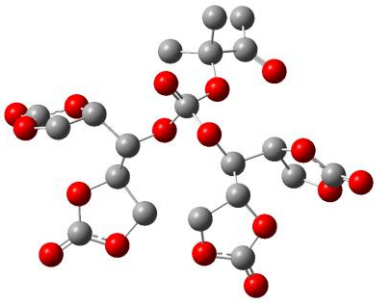
Intermediate 7

C	-1.90657800	1.16763000	-0.72867200
H	-1.70151900	1.23948700	-1.79644800
H	-2.64398100	1.91105700	-0.41571300
C	-0.61560400	1.20243300	0.09327000
H	-0.49145000	2.12145400	0.66806100
C	0.59835200	0.84297500	-0.77897700
H	0.79338100	1.79573500	-1.34007300
C	1.86052900	0.59219300	0.11353600
H	2.74162700	0.95628500	-0.42942200
C	2.08344500	-0.90505200	0.35951000
H	1.25000800	-1.28473000	0.98229700
H	3.00219800	-1.02485400	0.95568000
O	0.29485300	-0.21648100	-1.58052900
O	-0.83827100	0.12867300	1.03698300
O	1.84189500	1.31733100	1.34126600
H	1.38247500	-1.15094100	-1.34438300
O	-2.43940400	-0.13791300	-0.46306500
O	2.19706700	-1.58565300	-0.85404800
C	-1.74191400	-0.71778300	0.52145200
O	-1.95253200	-1.82474600	0.93786800
H	1.16901700	0.89244200	1.89148000



Intermediate 8

C	1.70165300	-1.61022800	0.18496400
H	1.20810700	-2.28334100	-0.51680600
H	2.36985900	-2.16771100	0.84670800
C	0.69354600	-0.72877000	0.93416000
H	0.58981200	-0.99567000	1.98900000
C	-0.63910600	-0.68301600	0.18142400
H	-1.04220100	-1.72146500	0.28561300
C	-1.69229100	0.27185200	0.81181400
H	-1.71106000	0.22214600	1.91049000
C	-3.06067700	-0.12079100	0.25219900
H	-3.79493400	0.65110800	0.53369600
H	-3.38273600	-1.06360200	0.73308900
O	-0.43530000	-0.28209000	-1.11069500
O	1.32944500	0.56294800	0.86867400
O	-1.36334000	1.58556600	0.40523400
H	-0.86007400	1.37976200	-0.41512000
O	2.48095100	-0.66922900	-0.56260000
O	-3.02187600	-0.25772300	-1.14898400
C	2.18902600	0.57504100	-0.15448100
O	2.69884000	1.56458100	-0.60784600
H	-2.03944000	-0.27816700	-1.37740800

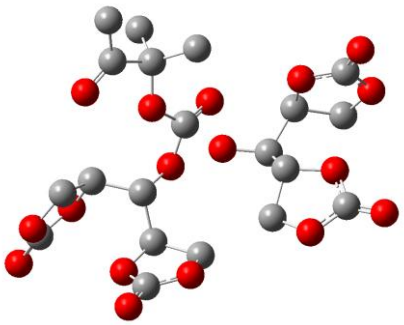


IM1

O	3.1251	-2.44593	0.4139
C	2.23514	-1.68383	1.25196
C	1.13383	-2.6938	1.53995
O	1.22357	-3.58167	0.4094
C	2.4342	-3.45181	-0.15894
O	2.84725	-4.13751	-1.04838
C	1.76823	-0.43148	0.50428
C	2.98505	0.34656	-0.0362
O	1.00193	0.25581	1.45527
O	4.12591	0.18391	0.83391
C	5.14595	-0.39318	0.18155
O	4.8532	-0.5899	-1.10978
C	3.5133	-0.1692	-1.38866
O	6.19691	-0.67527	0.68658
O	-3.46605	-1.75038	-0.48875
C	-2.29994	-0.95452	-0.77279
C	-1.29453	-1.99852	-1.24803
O	-2.13993	-3.09116	-1.64913
C	-3.35424	-2.94619	-1.10031
O	-4.22664	-3.76431	-1.14758
C	-1.87905	-0.16001	0.45564
C	-3.05775	0.66584	1.00204
O	-0.8062	0.60755	-0.01466
O	-3.89274	1.13653	-0.07528

C	-5.13187	0.62926	0.02585
O	-5.27518	-0.0926	1.14349
C	-4.04333	-0.13617	1.87334
O	-6.00519	0.81894	-0.7741
C	0.02424	1.25972	1.0284
O	0.81411	2.13639	0.21881
C	0.34726	3.43666	-0.07406
C	1.28903	3.94176	-1.18219
C	0.89317	5.19529	-1.92814
O	-0.60082	1.71759	2.01613
O	2.32569	3.36589	-1.44461
C	-1.10562	3.47063	-0.55743
H	2.77846	-1.39093	2.14913
H	1.31878	-3.27012	2.44875
H	0.14094	-2.24546	1.56976
H	1.14829	-0.71616	-0.36092
H	2.74136	1.40517	-0.08283
H	3.54541	0.61908	-2.14251
H	2.95556	-1.02572	-1.77433
H	-2.55879	-0.25762	-1.57418
H	-0.7073	-1.67668	-2.10667
H	-0.63847	-2.34656	-0.4478
H	-1.56097	-0.84297	1.25952
H	-2.64785	1.52554	1.52487
H	-4.20329	0.32426	2.84918
H	-3.75207	-1.18031	1.99846
H	0.14528	4.93316	-2.68482
H	0.44572	5.94558	-1.27261
H	1.77049	5.60632	-2.42866

H	-1.39858	4.4934	-0.80822
H	-1.75267	3.10696	0.2418
H	-1.24195	2.83104	-1.43297
C	0.54395	4.35801	1.14174
H	1.59508	4.34666	1.4467
H	0.25077	5.38808	0.92079
H	-0.0637	3.96624	1.95791

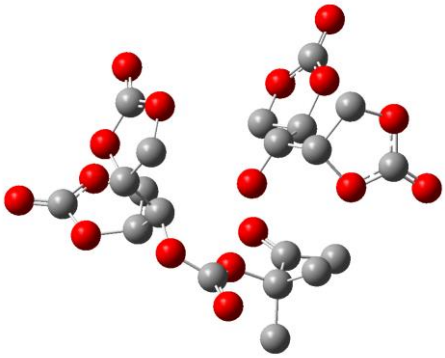


TS1

O	-3.02513	-2.57399	-0.3918
C	-2.19403	-1.75158	-1.25135
C	-0.96857	-2.64099	-1.46143
O	-1.01962	-3.54289	-0.32625
C	-2.26101	-3.52388	0.20202
O	-2.6452	-4.2519	1.07884
C	-1.90619	-0.40439	-0.56882
C	-3.20142	0.31758	-0.14621
O	-1.16085	0.31348	-1.55245
O	-4.30241	0.00691	-1.04478
C	-5.35677	-0.47827	-0.35587
O	-5.10468	-0.52452	0.96552
C	-3.75236	-0.09547	1.23484
O	-6.39842	-0.81343	-0.86072
O	3.75576	-1.79647	0.53779
C	2.59115	-0.95835	0.83411

C	1.66011	-1.94276	1.54237
O	2.55986	-2.99461	1.98407
C	3.71604	-2.91182	1.2955
O	4.60109	-3.72908	1.35301
C	1.97026	-0.30561	-0.40946
C	2.99079	0.58025	-1.17342
O	0.86742	0.36483	0.0658
O	3.81106	1.36621	-0.25478
C	5.11687	1.09347	-0.42625
O	5.31488	0.21877	-1.43132
C	4.04821	-0.17159	-2.00883
O	6.00603	1.57785	0.23119
C	-0.30511	1.35359	-1.16091
O	-0.91811	2.04414	-0.14044
C	-0.49086	3.36332	0.24887
C	-1.38398	3.69098	1.47231
C	-0.9807	4.85485	2.35179
O	0.37096	1.86326	-2.04888
O	-2.39424	3.05091	1.71187
C	0.99641	3.40725	0.61557
H	-2.74106	-1.58188	-2.17798
H	-1.03724	-3.23615	-2.37519
H	-0.02902	-2.09389	-1.43533
H	-1.27254	-0.54147	0.31365
H	-3.03216	1.38982	-0.18741
H	-3.78296	0.74774	1.92577
H	-3.21319	-0.92761	1.69122
H	2.93142	-0.17421	1.51475
H	1.16745	-1.52432	2.41871

H	0.92038	-2.38788	0.87308
H	1.73365	-1.12408	-1.12971
H	2.41876	1.28348	-1.77463
H	4.04548	0.12848	-3.05931
H	3.96199	-1.25697	-1.93849
H	-0.16633	4.53953	3.01521
H	-0.616	5.70943	1.77599
H	-1.83411	5.15233	2.96407
H	1.2658	4.39588	0.99598
H	1.59485	3.19908	-0.27024
H	1.22883	2.64746	1.36321
C	-0.84102	4.38086	-0.85615
H	-1.90951	4.33708	-1.09053
H	-0.59544	5.39959	-0.54306
H	-0.27307	4.1379	-1.75501

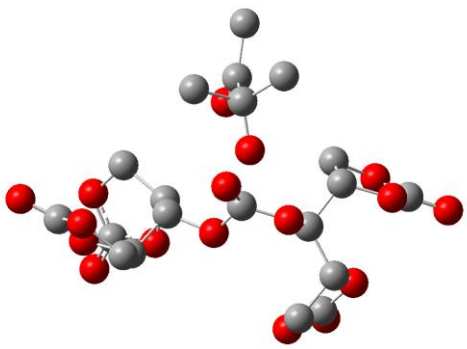


Complex1

O	-2.29502	-2.35154	-0.66434
C	-2.41609	-1.19963	-1.53164
C	-1.27769	-1.39964	-2.54851
O	-0.88983	-2.78568	-2.33756
C	-1.42201	-3.24589	-1.19607
O	-1.17805	-4.31587	-0.70053
C	-2.24627	0.06952	-0.69621
C	-3.26536	0.24318	0.43375

O	-2.38815	1.12629	-1.68616
O	-4.57252	-0.25367	0.04897
C	-4.97483	-1.23607	0.8878
O	-4.07862	-1.44162	1.86931
C	-2.95189	-0.55117	1.72134
O	-6.00945	-1.84049	0.77072
O	3.33655	-1.66426	1.22125
C	2.28383	-0.71803	0.82123
C	1.12611	-1.13363	1.7307
O	1.77522	-1.88131	2.79327
C	3.01383	-2.2386	2.39519
O	3.73772	-2.97685	3.01812
C	1.89115	-0.77583	-0.66569
C	3.0716	-0.44172	-1.61531
O	0.83696	0.05916	-0.83729
O	3.72951	0.80176	-1.22412
C	5.01339	0.57551	-0.89378
O	5.36271	-0.70869	-1.10463
C	4.24913	-1.43422	-1.67731
O	5.7652	1.41745	-0.46494
C	-1.75697	2.30672	-1.48876
O	-1.39329	2.44861	-0.21557
C	-0.45265	3.48025	0.21682
C	-0.22356	3.12942	1.70924
C	0.90673	3.83493	2.42339
O	-1.62908	3.0957	-2.39845
O	-0.93166	2.32287	2.28646
C	0.84184	3.36557	-0.59322
H	-3.40486	-1.23232	-1.99515

H	-1.60449	-1.29452	-3.58289
H	-0.41355	-0.76703	-2.30678
H	-1.22267	0.0949	-0.30126
H	-3.36896	1.30546	0.65047
H	-2.90164	0.09495	2.59836
H	-2.04605	-1.15292	1.65176
H	2.65211	0.2815	1.06907
H	0.59547	-0.29536	2.17877
H	0.42152	-1.79926	1.2232
H	1.68176	-1.85932	-0.88633
H	2.63744	-0.26757	-2.60236
H	4.51416	-1.7129	-2.70032
H	4.08411	-2.33258	-1.08189
H	1.84189	3.30054	2.21544
H	1.04105	4.86779	2.09374
H	0.72405	3.80324	3.49922
H	1.62518	3.98371	-0.14833
H	0.67216	3.71856	-1.61274
H	1.15685	2.31443	-0.62585
C	-1.12069	4.85891	0.12722
H	-2.04569	4.87948	0.71185
H	-0.45001	5.63229	0.50975
H	-1.35295	5.08456	-0.91492

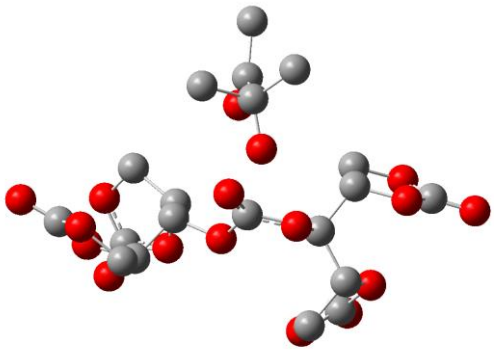


TS2

O	-3.73165	-2.19752	0.36718
C	-2.94671	-1.68546	-0.73674
C	-2.33323	-2.95825	-1.34065
O	-3.15247	-4.01483	-0.78624
C	-3.87418	-3.54023	0.24724
O	-4.56103	-4.21303	0.96981
C	-1.91069	-0.6829	-0.23028
C	-2.46595	0.55879	0.47339
O	-1.21884	-0.31248	-1.44049
O	-3.64269	1.06368	-0.22
C	-4.73639	0.95949	0.56456
O	-4.42094	0.50499	1.79204
C	-2.98928	0.33757	1.90522
O	-5.85368	1.2435	0.21182
O	4.24491	-1.58463	0.04591
C	2.84313	-1.72836	-0.2868
C	2.89889	-2.31087	-1.70564
O	4.23034	-1.95078	-2.15217
C	4.98805	-1.61748	-1.09034
O	6.16635	-1.38005	-1.13254
C	2.13612	-0.36819	-0.21678
C	2.29194	0.40319	1.09605
O	0.74814	-0.67024	-0.40089
O	2.2026	-0.49154	2.23777
C	3.3529	-0.47502	2.94557
O	4.22649	0.41841	2.44566
C	3.64737	1.10666	1.31558
O	3.56446	-1.16724	3.90895
C	0.11962	0.01743	-1.41709

O	0.07386	1.74331	-0.37443
C	0.06131	2.97607	-0.97655
C	-0.39637	4.06661	0.03895
C	-0.11353	5.53276	-0.26214
O	0.66669	0.21314	-2.51381
O	-0.9894	3.77084	1.06681
C	1.46685	3.34026	-1.53311
H	-3.63188	-1.19882	-1.43541
H	-2.40477	-2.99824	-2.42683
H	-1.29883	-3.12081	-1.02544
H	-1.2265	-1.17933	0.46153
H	-1.67342	1.3194	0.41603
H	-2.61128	1.09444	2.59672
H	-2.78965	-0.65762	2.30349
H	2.39924	-2.41858	0.43061
H	2.81294	-3.39989	-1.71561
H	2.17406	-1.86242	-2.38491
H	2.47568	0.2758	-1.03286
H	1.45299	1.10453	1.11649
H	3.52309	2.15826	1.58305
H	4.33314	1.02177	0.47207
H	0.94017	5.75301	-0.05096
H	-0.28916	5.78636	-1.31125
H	-0.7334	6.16325	0.3803
H	1.50973	4.30664	-2.04877
H	1.75843	2.56044	-2.24231
H	2.20505	3.35423	-0.72177
C	-0.97151	3.04908	-2.14671
H	-1.97993	2.83755	-1.77558

H	-0.98772	4.02168	-2.6532
H	-0.71082	2.27953	-2.87811

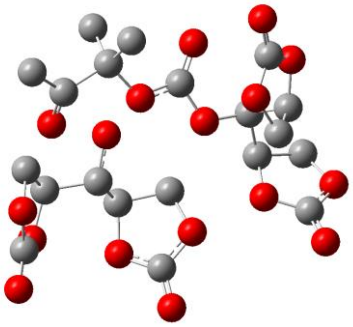


Complex 2

O	-3.47101	-2.12257	0.04376
C	-2.7247	-1.85588	-1.15635
C	-1.78733	-3.06221	-1.22245
O	-1.70979	-3.46425	0.15762
C	-2.77013	-2.9795	0.81873
O	-3.06492	-3.27006	1.94122
C	-1.98035	-0.54442	-0.94437
C	-2.90372	0.6572	-0.67958
O	-1.23166	-0.31363	-2.14969
O	-4.29201	0.31601	-0.90392
C	-4.9571	0.26105	0.26658
O	-4.18538	0.67323	1.27781
C	-2.91041	1.12617	0.7799
O	-6.09732	-0.09309	0.37341
O	4.10411	-1.13337	-0.06808
C	2.90443	-1.40358	-0.80935
C	3.39743	-1.35973	-2.25216
O	4.55554	-0.50865	-2.1438
C	4.9812	-0.49513	-0.87113
O	6.00087	0.00635	-0.49174
C	1.87079	-0.32151	-0.50131

C	1.67428	-0.05631	0.98705
O	0.64337	-0.81001	-1.05273
O	1.78659	-1.29076	1.72364
C	2.83171	-1.24562	2.57822
O	3.40716	-0.03998	2.57346
C	2.75845	0.82856	1.63688
O	3.18047	-2.16831	3.25994
C	0.09345	-0.12372	-2.07451
O	-0.42017	1.56632	-0.27837
C	-0.14971	2.87887	-0.25681
C	-0.19545	3.42836	1.18078
C	-0.38699	4.91309	1.41227
O	0.69858	0.53293	-2.87689
O	-0.0657	2.67373	2.13536
C	1.29702	3.19195	-0.75522
H	-3.41917	-1.80188	-1.99338
H	-2.21201	-3.88453	-1.80937
H	-0.78595	-2.81774	-1.57194
H	-1.28664	-0.64386	-0.10938
H	-2.63195	1.45516	-1.3633
H	-2.87711	2.21556	0.86448
H	-2.11376	0.69476	1.38077
H	2.52958	-2.382	-0.51131
H	3.71821	-2.33519	-2.61383
H	2.68798	-0.89843	-2.93582
H	2.13405	0.62307	-0.99138
H	0.68017	0.38541	1.10625
H	2.30782	1.65909	2.18368
H	3.50711	1.19544	0.93601

H	-0.16679	5.16648	2.45523
H	0.24713	5.50544	0.74658
H	-1.42334	5.18119	1.19462
H	1.53307	4.26344	-0.81718
H	1.40135	2.74387	-1.7486
H	2.03094	2.71898	-0.09237
C	-1.11875	3.68259	-1.16932
H	-2.15049	3.59389	-0.82084
H	-0.88275	4.75327	-1.25089
H	-1.06185	3.23977	-2.17206

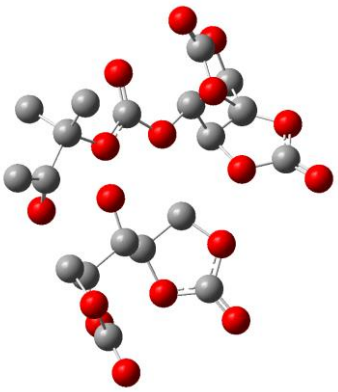


Complex 3

O	-3.28314	2.06215	-0.8982
C	-3.83466	0.88597	-1.51065
C	-5.33839	1.20114	-1.55029
O	-5.47108	2.28769	-0.62059
C	-4.26351	2.79968	-0.33326
O	-4.07239	3.77138	0.33543
C	-3.4658	-0.34454	-0.69038
C	-3.85643	-0.19538	0.78718
O	-2.04785	-0.47698	-0.84429
O	-4.02986	-1.48084	1.3997
C	-2.92625	-1.79174	2.10716
O	-2.08004	-0.74357	2.15241
C	-2.76462	0.42387	1.66608

O	-2.736	-2.84287	2.64532
C	-1.53009	-1.71677	-0.69775
O	-0.22501	-1.62877	-0.86799
C	0.58321	-2.82648	-0.67092
C	1.99115	-2.42936	-1.16248
O	-2.19585	-2.69383	-0.4611
O	2.10815	-1.70608	-2.13356
C	0.52941	-3.24741	0.78902
C	0.13531	-3.93504	-1.63274
H	-3.40864	0.78948	-2.50935
H	-5.65549	1.53769	-2.53606
H	-5.96723	0.37415	-1.21669
H	-3.97396	-1.21623	-1.11179
H	-4.80773	0.33173	0.87721
H	-3.18903	0.96739	2.51031
H	-2.06057	1.04767	1.12347
H	1.11863	-4.15803	0.92569
H	-0.49913	-3.46768	1.07703
H	0.94663	-2.44508	1.39833
H	0.01882	-3.52558	-2.64067
H	0.89789	-4.71843	-1.66844
H	-0.80272	-4.38501	-1.30782
C	3.15332	-3.21166	-0.60157
H	4.07502	-2.84943	-1.07076
H	3.20723	-3.08641	0.48297
O	2.13513	2.39155	-0.80196
C	1.76604	1.01367	-0.52152
C	0.44289	1.20484	0.20124
O	0.58822	2.52042	0.7756

C	1.53208	3.18848	0.08648
O	1.78144	4.35126	0.2446
C	2.77978	0.3008	0.39386
C	4.13314	0.10251	-0.32154
O	2.29088	-0.88832	0.78236
O	4.82708	1.34298	-0.58905
C	5.73552	1.55828	0.36898
O	5.89244	0.46887	1.14121
C	5.11604	-0.61283	0.59943
O	6.34638	2.58069	0.52139
H	1.65924	0.48179	-1.46648
H	-0.42043	1.21882	-0.46946
H	0.32002	0.4623	0.98742
H	2.99529	1.03308	1.23088
H	3.98044	-0.40944	-1.27453
H	5.79286	-1.29853	0.08176
H	4.58716	-1.12315	1.4049
H	3.03378	-4.28333	-0.84115

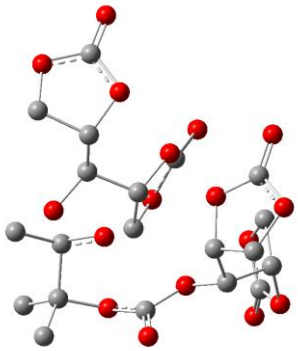


TS3

O	-3.2846	2.06124	-0.90084
C	-3.84081	0.88476	-1.5112
C	-5.34126	1.20138	-1.54698
O	-5.47209	2.28929	-0.61862
C	-4.26376	2.80053	-0.33611

O	-4.0711	3.77301	0.33098
C	-3.46941	-0.34191	-0.68944
C	-3.85857	-0.19304	0.78823
O	-2.05171	-0.47295	-0.84158
O	-4.02945	-1.47735	1.40306
C	-2.92538	-1.78792	2.10997
O	-2.08126	-0.73735	2.15254
C	-2.76856	0.42682	1.66517
O	-2.73547	-2.83826	2.64678
C	-1.52906	-1.71	-0.69113
O	-0.22419	-1.61478	-0.84689
C	0.59476	-2.80693	-0.64882
C	2.00764	-2.38598	-1.11224
O	-2.19516	-2.69203	-0.46311
O	2.12385	-1.69167	-2.1097
C	0.51817	-3.24714	0.80382
C	0.1645	-3.90612	-1.62729
H	-3.41573	0.78642	-2.51011
H	-5.66185	1.53992	-2.53294
H	-5.97063	0.37545	-1.21176
H	-3.97582	-1.21674	-1.10904
H	-4.81239	0.33196	0.87817
H	-3.19186	0.97181	2.51201
H	-2.06465	1.0524	1.12099
H	1.10531	-4.15997	0.93891
H	-0.51562	-3.47007	1.07706
H	0.92475	-2.4542	1.43308
H	0.07089	-3.48739	-2.63302
H	0.92719	-4.68938	-1.65194

H	-0.78131	-4.35543	-1.32751
C	3.16216	-3.2023	-0.57481
H	4.09118	-2.80105	-0.98495
H	3.19233	-3.17168	0.51225
O	2.13872	2.38205	-0.80533
C	1.75913	1.00678	-0.54246
C	0.4399	1.19635	0.18886
O	0.59328	2.50702	0.7739
C	1.53496	3.17585	0.08669
O	1.78811	4.3392	0.25045
C	2.772	0.2747	0.35765
C	4.13299	0.09278	-0.34425
O	2.2823	-0.92748	0.72205
O	4.82053	1.34274	-0.5938
C	5.72637	1.55274	0.36678
O	5.88271	0.4625	1.1362
C	5.11292	-0.62188	0.58314
O	6.33453	2.57704	0.52305
H	1.64608	0.48612	-1.49341
H	-0.42502	1.21676	-0.47777
H	0.31716	0.44836	0.97259
H	2.9746	0.97783	1.21856
H	3.99532	-0.4132	-1.3013
H	5.79797	-1.3004	0.0668
H	4.58404	-1.1387	1.38319
H	3.06388	-4.24356	-0.90653

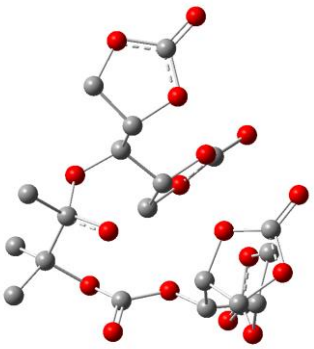


IM2

O	1.12921	-1.03735	-2.01134
C	1.97116	0.1283	-2.0817
C	2.96263	-0.27154	-3.17858
O	2.89976	-1.71142	-3.15877
C	1.76888	-2.0961	-2.54768
O	1.38612	-3.22663	-2.47312
C	2.65812	0.42045	-0.74209
C	3.2639	-0.79223	-0.03944
O	1.75934	1.00933	0.19406
O	3.91634	-0.30195	1.14425
C	3.10439	-0.49049	2.20569
O	2.10743	-1.33455	1.89897
C	2.29225	-1.81925	0.56158
O	3.26801	0.01036	3.28116
C	1.36548	2.26981	-0.10694
O	0.46191	2.66343	0.79168
C	-0.74513	3.33419	0.30093
C	-1.47449	2.2326	-0.57191
O	1.88297	2.92531	-0.97708
O	-0.62716	1.51401	-1.25147
C	-1.46978	3.78323	1.56058
C	-0.39242	4.5653	-0.53107
H	1.32567	0.97223	-2.34078

H	2.65314	0.08029	-4.16287
H	3.9925	0.03083	-2.97605
H	3.46615	1.13033	-0.95066
H	4.01545	-1.25935	-0.67836
H	2.7521	-2.81019	0.60858
H	1.31848	-1.8763	0.08435
H	-2.46156	4.15371	1.29301
H	-0.92106	4.59492	2.0481
H	-1.59464	2.96008	2.2628
H	-0.01906	4.29307	-1.51635
H	-1.28443	5.18834	-0.63974
H	0.37385	5.1544	-0.01482
C	-2.58628	2.87346	-1.43075
H	-3.09945	2.07371	-1.97579
H	-3.32968	3.42743	-0.84491
O	-0.81806	-1.82394	1.30239
C	-0.8107	-0.41683	0.98233
C	-0.45838	0.23237	2.33192
O	-0.51318	-0.85217	3.26833
C	-0.65885	-2.01381	2.62062
O	-0.66778	-3.08873	3.15469
C	-2.17895	0.04565	0.4712
C	-2.57008	-0.53177	-0.89765
O	-2.28054	1.44137	0.4748
O	-2.57839	-1.97142	-0.86862
C	-3.82748	-2.41254	-0.68349
O	-4.71591	-1.40974	-0.78611
C	-4.0324	-0.21945	-1.2206
O	-4.12483	-3.55342	-0.46697

H	-0.06377	-0.23108	0.21579
H	0.54317	0.65999	2.34988
H	-1.19362	0.98265	2.6272
H	-2.92827	-0.31457	1.20225
H	-1.85933	-0.1938	-1.6463
H	-4.21404	-0.08275	-2.29039
H	-4.41535	0.63014	-0.65668
H	-2.14447	3.54167	-2.17576

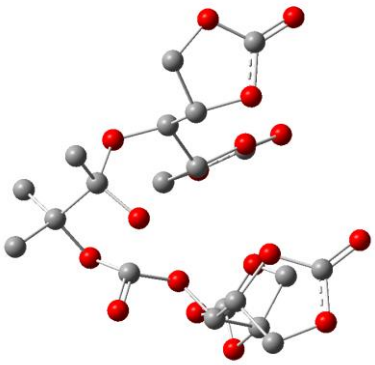


TS4

O	1.1399	-1.04072	-2.03141
C	1.98586	0.12348	-2.0935
C	3.00105	-0.28563	-3.16464
O	2.93011	-1.72156	-3.14557
C	1.7888	-2.1016	-2.54923
O	1.40438	-3.23293	-2.47367
C	2.63279	0.43153	-0.73867
C	3.25284	-0.77103	-0.03038
O	1.70843	0.99608	0.17608
O	3.89337	-0.27757	1.15816
C	3.07813	-0.47756	2.21351
O	2.09097	-1.33331	1.89877
C	2.29206	-1.81326	0.56326
O	3.23167	0.01937	3.29054
C	1.23541	2.23316	-0.19839

O	0.44848	2.7052	0.79526
C	-0.75962	3.35624	0.33188
C	-1.45433	2.24101	-0.53775
O	1.81684	2.90018	-1.03039
O	-0.5188	1.55004	-1.16594
C	-1.50601	3.78593	1.58292
C	-0.43245	4.59612	-0.50353
H	1.35744	0.96372	-2.38239
H	2.71698	0.06452	-4.15903
H	4.02575	0.01364	-2.94041
H	3.43252	1.15506	-0.93423
H	4.01705	-1.2308	-0.66114
H	2.76278	-2.79879	0.61163
H	1.32183	-1.88269	0.07949
H	-2.50489	4.14122	1.31127
H	-0.97399	4.60732	2.0756
H	-1.61679	2.96115	2.28601
H	-0.03206	4.33417	-1.4823
H	-1.33767	5.19851	-0.6317
H	0.30979	5.20305	0.0245
C	-2.52452	2.82628	-1.47079
H	-2.99482	2.00949	-2.02706
H	-3.30434	3.36912	-0.92504
O	-0.83624	-1.82932	1.31944
C	-0.81193	-0.42621	0.99152
C	-0.47068	0.23211	2.33969
O	-0.50836	-0.85342	3.27838
C	-0.66081	-2.01544	2.63741
O	-0.66541	-3.09052	3.17107

C	-2.17031	0.04313	0.46212
C	-2.55135	-0.53205	-0.9077
O	-2.2579	1.44187	0.46274
O	-2.55032	-1.97148	-0.87664
C	-3.80112	-2.42102	-0.69881
O	-4.69212	-1.42079	-0.80874
C	-4.01403	-0.23017	-1.2435
O	-4.09197	-3.56351	-0.48231
H	-0.04718	-0.25864	0.2393
H	0.52229	0.67826	2.35622
H	-1.21864	0.96549	2.64059
H	-2.93106	-0.30144	1.18538
H	-1.83982	-0.20091	-1.66238
H	-4.19092	-0.10039	-2.31457
H	-4.40961	0.61958	-0.68659
H	-2.06757	3.49834	-2.20177

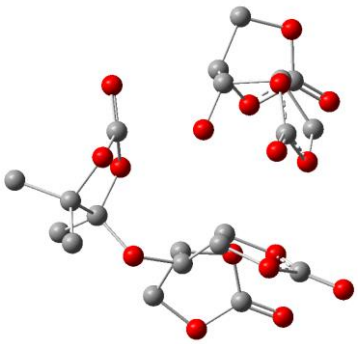


IM3

O	-1.8579	0.48399	-2.07026
C	-2.08193	-0.94913	-2.00358
C	-3.38273	-1.08552	-2.80274
O	-3.95867	0.22935	-2.71983
C	-3.0018	1.10915	-2.37848
O	-3.16221	2.29881	-2.34239
C	-2.15703	-1.46009	-0.55194

C	-3.27381	-0.73708	0.227
O	-0.98958	-1.38344	0.13975
O	-3.44075	-1.42179	1.48306
C	-2.71201	-0.79704	2.41785
O	-2.3952	0.44849	2.02508
C	-2.90278	0.67973	0.70747
O	-2.43443	-1.26053	3.48664
C	0.43865	-2.52367	-0.69537
O	1.01791	-3.00002	0.45658
C	2.44086	-2.80741	0.33283
C	2.48824	-1.46777	-0.47172
O	-0.18703	-3.22001	-1.4754
O	1.25988	-1.48673	-1.1661
C	3.05221	-2.74567	1.71907
C	3.02092	-3.97965	-0.45335
H	-1.23619	-1.42992	-2.4908
H	-3.21537	-1.3261	-3.85352
H	-4.0825	-1.79976	-2.36664
H	-2.51969	-2.50706	-0.68247
H	-4.23981	-0.75806	-0.28629
H	-3.77657	1.33551	0.77719
H	-2.11331	1.15164	0.12529
H	4.10742	-2.45778	1.65029
H	2.99074	-3.73151	2.18442
H	2.5313	-2.02238	2.34647
H	2.57937	-4.05677	-1.45151
H	4.10857	-3.88966	-0.55368
H	2.79939	-4.90169	0.08976
C	3.62859	-1.35988	-1.4745

H	3.53751	-0.45095	-2.07062
H	4.58758	-1.3361	-0.94298
O	0.13061	2.12966	1.29915
C	0.59279	0.80974	0.97149
C	0.61312	0.0993	2.33449
O	0.12766	1.0881	3.25666
C	-0.16026	2.21878	2.60855
O	-0.59672	3.21014	3.13323
C	1.99145	0.86242	0.35565
C	2.04885	1.42438	-1.06745
O	2.6021	-0.41329	0.48098
O	1.27074	2.63106	-1.13516
C	2.07597	3.69226	-0.97204
O	3.36828	3.32164	-1.01751
C	3.44894	1.94305	-1.4108
O	1.70129	4.81711	-0.82313
H	-0.11702	0.32134	0.30184
H	-0.04812	-0.76649	2.34
H	1.6212	-0.177	2.65241
H	2.60071	1.51942	0.99634
H	1.63371	0.72803	-1.794
H	3.66616	1.89114	-2.4839
H	4.24159	1.46045	-0.83847
H	3.62324	-2.2022	-2.16519

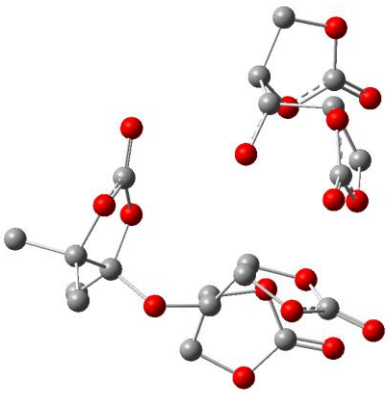


TS5

O	1.87789	-0.4746	-2.06976
C	2.10747	0.95612	-1.98062
C	3.39827	1.10267	-2.78751
O	3.9781	-0.2127	-2.71901
C	3.02242	-1.09557	-2.37767
O	3.18647	-2.28432	-2.34805
C	2.19823	1.44202	-0.51643
C	3.33168	0.71882	0.24489
O	1.05548	1.33274	0.18665
O	3.47763	1.40885	1.50287
C	2.71994	0.79339	2.4196
O	2.42121	-0.46023	2.03833
C	2.93638	-0.68978	0.72128
O	2.41521	1.26431	3.48124
C	-0.55593	2.59819	-0.75261
O	-1.09353	3.06172	0.40186
C	-2.51474	2.80617	0.32919
C	-2.53517	1.46293	-0.47214
O	0.17055	3.22152	-1.47876
O	-1.31143	1.52779	-1.19002
C	-3.07789	2.72839	1.73151
C	-3.14211	3.96301	-0.44398
H	1.256	1.44744	-2.44648

H	3.22462	1.34972	-3.83783
H	4.10028	1.81581	-2.35095
H	2.56043	2.49468	-0.64373
H	4.30626	0.73799	-0.25117
H	3.79453	-1.36411	0.79501
H	2.14284	-1.14166	0.12889
H	-4.12318	2.40968	1.69473
H	-3.03457	3.71824	2.19321
H	-2.51638	2.0244	2.34264
H	-2.72143	4.05165	-1.45019
H	-4.22527	3.84226	-0.52411
H	-2.93449	4.89	0.09577
C	-3.67552	1.32562	-1.46649
H	-3.55749	0.42454	-2.06969
H	-4.62625	1.27031	-0.9303
O	-0.11769	-2.12813	1.29335
C	-0.58647	-0.80638	0.96764
C	-0.60965	-0.10278	2.33586
O	-0.1292	-1.09499	3.25334
C	0.16643	-2.22259	2.60327
O	0.60295	-3.21291	3.12308
C	-1.98364	-0.86513	0.35274
C	-2.03891	-1.42826	-1.07168
O	-2.59248	0.41532	0.48001
O	-1.25056	-2.62444	-1.14137
C	-2.0468	-3.69653	-0.98134
O	-3.34219	-3.33669	-1.02662
C	-3.43423	-1.95811	-1.41745
O	-1.659	-4.81851	-0.83512

H	0.12919	-0.30484	0.3078
H	0.0587	0.75871	2.34121
H	-1.61604	0.17569	2.65205
H	-2.59475	-1.52258	0.99092
H	-1.63271	-0.72706	-1.80016
H	-3.65444	-1.90609	-2.487
H	-4.23157	-1.48707	-0.84141
H	-3.69814	2.17133	-2.15368

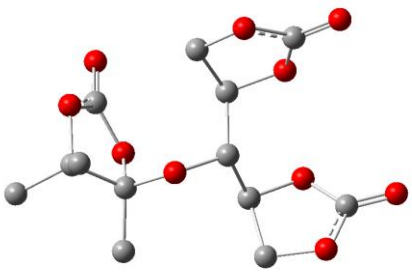


Complex 4

O	-1.95956	-0.07001	-2.12296
C	-2.18527	-1.4739	-1.81994
C	-3.45109	-1.75245	-2.62934
O	-4.04176	-0.4475	-2.77347
C	-3.1	0.48586	-2.54383
O	-3.27426	1.66435	-2.69591
C	-2.30491	-1.71637	-0.29885
C	-3.47702	-0.90159	0.30984
O	-1.1864	-1.47487	0.38792
O	-3.65798	-1.41553	1.64683
C	-2.92824	-0.67768	2.49129
O	-2.62976	0.51825	1.95724
C	-3.08394	0.55675	0.59743
O	-2.64948	-0.99934	3.61498

C	1.20703	-2.63856	-0.68432
O	1.80588	-3.0229	0.45209
C	3.14283	-2.45927	0.46716
C	2.92331	-1.15001	-0.36115
O	0.39366	-3.26593	-1.29189
O	1.76329	-1.47822	-1.13059
C	3.57753	-2.24428	1.90039
C	4.04745	-3.46698	-0.23239
H	-1.31154	-2.01961	-2.1727
H	-3.24937	-2.15208	-3.62665
H	-4.15925	-2.39968	-2.10795
H	-2.67476	-2.78179	-0.26455
H	-4.43941	-0.99265	-0.20292
H	-3.93122	1.2458	0.53507
H	-2.25565	0.90251	-0.01794
H	4.53083	-1.70956	1.91866
H	3.71543	-3.21421	2.38456
H	2.84066	-1.66836	2.45689
H	3.71783	-3.66427	-1.25706
H	5.08092	-3.11388	-0.25511
H	4.01264	-4.40559	0.32534
C	4.05865	-0.80434	-1.30812
H	3.80013	0.03877	-1.94803
H	4.9479	-0.54893	-0.72663
O	-0.223	2.0212	1.03425
C	0.45297	0.76536	0.82964
C	0.43571	0.14812	2.23573
O	0.02779	1.23163	3.08692
C	-0.41923	2.24738	2.34533

O	-0.90231	3.25381	2.78611
C	1.87415	1.03677	0.32881
C	1.95311	1.56533	-1.11041
O	2.685	-0.11396	0.56055
O	0.96922	2.58957	-1.30429
C	1.53245	3.79356	-1.09521
O	2.87047	3.68003	-1.00449
C	3.25075	2.34088	-1.35618
O	0.93182	4.82446	-1.01779
H	-0.14068	0.13156	0.16023
H	-0.29935	-0.65529	2.28094
H	1.41707	-0.18446	2.57137
H	2.30838	1.80693	0.98544
H	1.74843	0.78441	-1.84192
H	3.56235	2.32287	-2.40394
H	4.07225	2.0336	-0.70837
H	4.28808	-1.64382	-1.96394

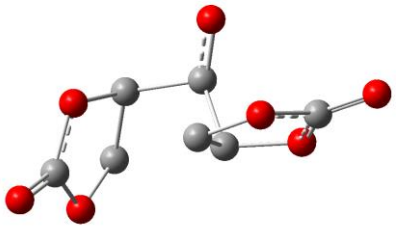


4t

C	1.20691	-2.60823	-0.64274
O	1.76331	-3.00487	0.51055
C	3.15217	-2.57471	0.50874
C	3.0505	-1.27523	-0.34903
O	0.29837	-3.13493	-1.20632
O	1.89537	-1.54407	-1.14668
C	3.61945	-2.36828	1.93215

C	3.94809	-3.67917	-0.17656
H	4.63174	-1.95503	1.92496
H	3.64463	-3.33157	2.44739
H	2.96753	-1.68721	2.47585
H	3.60312	-3.8505	-1.2011
H	5.0128	-3.43604	-0.19862
H	3.81409	-4.60317	0.39045
C	4.24047	-1.02171	-1.25451
H	4.0792	-0.15245	-1.89178
H	5.12575	-0.84511	-0.6384
O	-0.08893	1.94946	0.81926
C	0.57535	0.6786	0.68043
C	0.48101	0.11659	2.10314
O	0.23062	1.28413	2.90608
C	-0.19897	2.27652	2.12197
O	-0.59244	3.33915	2.51545
C	2.02649	0.93712	0.25072
C	2.20281	1.45133	-1.18591
O	2.8424	-0.1972	0.5354
O	1.25301	2.48842	-1.45943
C	1.82715	3.68802	-1.25169
O	3.15319	3.5525	-1.06876
C	3.53038	2.19695	-1.35453
O	1.24393	4.73163	-1.24791
H	-0.00564	0.04695	0.00138
H	-0.36187	-0.57095	2.1709
H	1.40796	-0.33595	2.4509
H	2.41778	1.71513	0.9244
H	2.03777	0.66604	-1.9221

H	3.91847	2.14374	-2.37515
H	4.29444	1.88981	-0.63925
H	4.42208	-1.87506	-1.90762



Cat1

O	-2.32528	-0.21679	-2.12332
C	-2.56944	-1.56057	-1.62535
C	-3.89947	-1.89355	-2.30245
O	-4.45183	-0.59931	-2.6042
C	-3.47144	0.32035	-2.55255
O	-3.61748	1.47355	-2.85431
C	-2.58474	-1.59862	-0.08148
C	-3.65253	-0.62688	0.48882
O	-1.4049	-1.35204	0.48654
O	-3.80869	-0.985	1.87876
C	-2.9922	-0.22259	2.61507
O	-2.61628	0.87662	1.94361
C	-3.10731	0.80613	0.59755
O	-2.69856	-0.44547	3.7589
H	-1.73831	-2.17971	-1.96214
H	-3.78455	-2.44656	-3.2381
H	-4.59194	-2.42171	-1.6435
H	-3.01975	-2.62062	0.12032
H	-4.64521	-0.67742	0.03027
H	-3.87929	1.57043	0.47088
H	-2.26541	0.97831	-0.06972