Supporting Information for

In situ capture and value-added utilization of CO_2 from flue gas using ionic liquid polymer supported Zn catalyst

Hongyan Ni, [ab] Kang Zhao, [a] Shujuan Liu, [a] Xingchao Dai, [a] Ce Liu, [a] Xionghou Gao, [c] Junyi Zhang, [c] Honghai Liu, [d] Kuowei Huang, [e] Xinjiang Cui*[a] and Feng Shi*[a]

[a] State Key Laboratory of Low Carbon Catalysis and Carbon Dioxide Utilization,

State Key Laboratory for Oxo Synthesis and Selective Oxidation

Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences

No.18, Tianshui Middle Road, Lanzhou, 730000, China

[b] University of Chinese Academy of Sciences, No. 19A, Yuquanlu, Beijing, 100049, People's Republic of China

[c] PetroChina Lanzhou Petrochemical Company,10 Yumen Street, Xigu District Lanzhou, Gansu 730060 China

[d] Petrochina Lanzhou Chemical Research Center,10 Yumen Street, Xigu District

Lanzhou, Gansu 730060 China

[e] Center of Excellence for Renewable Energy and Storage Technologies and Division of Physical Science and Engineering, King Abdullah University of Science and Technology, Thuwal, 23955-6900, Saudi Arabia.

E-mail: xinjangcui@licp.cas.cn

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1. General Information

Chemicals and materials

All solvents and chemicals, unless otherwise noted, were obtained commercially and were used as received without further purification. All glassware was dried before use. Flue gas was purchased from Lanzhou Yulon Gas Co., Ltd., where the flue gas is directly supplied from a coal power group. The flue gas composition is as follows: CO_2 (19.4%), O_2 (1.8%), N_2 (78.8%), and NO_x (≤20 ppm). Analytical thin layer chromatography (TLC) was performed using pre-coated Jiangyou silica gel HSGF254 (0.2mm ± 0.03mm). Flash chromatography was performed using silica gel 60, 0.063-0.2 mm, 200-300 mesh (Jiangyou, Yantai) with the indicated solvent system.

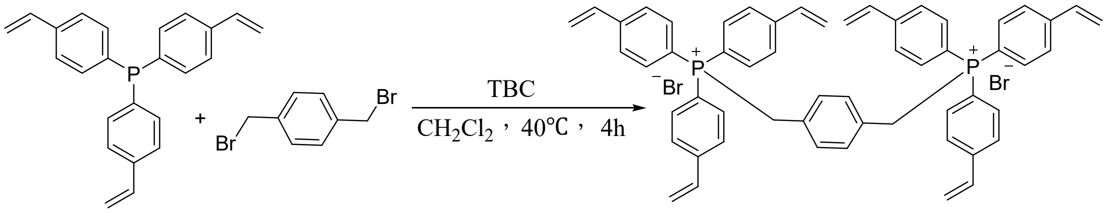
Characterization

Gas chromatography analysis was performed on Agilent 7890A GC equipped with a HP-5 capillary column and FID detector. GC-MS analysis was in general recorded on an Agilent 5977A MSD GC-MS. Fourier transform infrared (FT-IR) spectrum were recorded with a Bruker VERTEX 70FTIR spectrometer. The liquid nuclear magnetic resonance spectra (NMR) were recorded on a Bruker Avance TM III 400 MHz in deuterated chloroform unless otherwise noted. Data are reported in parts per million (ppm) as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiples, dd = doublet of doublet and br = broad signal), coupling constant in Hz and integration. Powder X-ray diffraction (PXRD) measurements were conducted by a STADIP automated transmission diffractometer (STOE) equipped with an incident beam curved germanium monochromator selecting CuKα1 radiation and a 6° position sensitive detector (PSD) (step size: 0.014, step time: 25.05 s). The XRD patterns were scanned in the 2θ range of 0-80°. Nitrogen adsorption-desorption isotherms were measured at 77 K using an American Quantachrome iQ2 automated gas sorption analyzer. The samples were outgassed at 120 ℃ for 12 h before the measurements. Surface areas were calculated from the adsorption data using Langmuir and Brunauer-Emmett-Teller (BET) methods. The pore-size-distribution curves were obtained from the adsorption branches using the non-local density functional theory (NLDFT) method. X-ray photoelectron spectroscopy (XPS) measurements were carried out by a VG ESCALAB 210 instrument equipped with a dual Mg/Al anode X-ray source, a hemispherical capacitor analyzer, and a 5 keV Ar^+ ion gun. All spectra were recorded by using AlKa (1361 eV) radiation. The electron binding energy was referenced to the C1s peak at 284.8 eV. The thermal properties of Zn@PIP-1 catalysts were evaluated using a METTLER TOLEDO simultaneous thermal analyzer over the temperature range from 30 to 800 °C under a nitrogen atmosphere (20 mL/min) with a heating rate of 5 °C/min. Field emission scanning electron microscopy (SEM) observations were performed on a Hitachi S-4800 microscope operated at an accelerating voltage of 5.0 kV. High-resolution transmission electron microscope (HR-TEM) analysis was carried out on a Talos F200S operating at 200 kV. Zn K-edge analysis was performed with Si (111) crystal monochromators at the BL11B beamlines at the Shanghai Synchrotron Radiation Facility (SSRF) (Shanghai, China). Before the analysis at the beamline, samples were pressed into thin sheets with 1 cm in diameter and sealed using Kapton tape film. The XAFS spectra were recorded at room temperature using a 4-channel Silicon Drift Detector (SDD) Bruker 5040. XX-edge extended X-ray absorption fine structure (EXAFS) spectra were recorded in transmission mode. Negligible changes in the line-shape and peak position of Zn K-edge XANES spectra were observed between two scans taken for a specific sample. The XAFS spectra of these standard samples (Zn Foil, ZnO) were recorded in transmission mode (fluorescence mode). The spectra were processed and analyzed by the software codes Athena and Artemis.

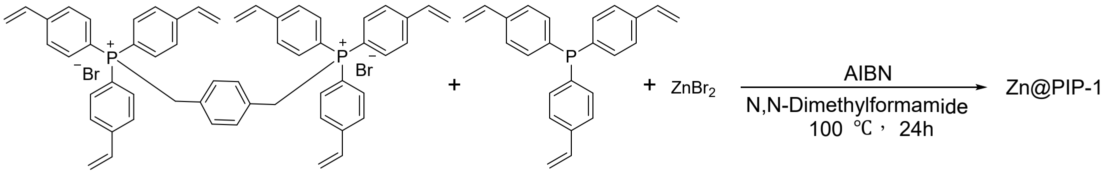
2. Synthetic procedures of the porous organic polymer catalysts

1. Preparation of Zn@2P2Br&*p*-3vPPh$_3$ porous ionic liquid polymer catalysts (Zn@PIP-1):

a. Synthesis of the quaternary phosphonium salt ionic liquid (2P2Br): Under argon protection, trivinylphenylphosphine (2.1 mmol), *p*-dibromobenzyl (1 mmol), and 4-5 g of TBC (*p*-tert-butylcatechol) were dissolved into a solution of anhydrous dichloromethane (20 mL). The mixture was stirred at 40 °C for 4 h, then washed with methyl tert-butyl ether and dried. A white solid was obtained in quantitative yield, noted as **2P2Br**.

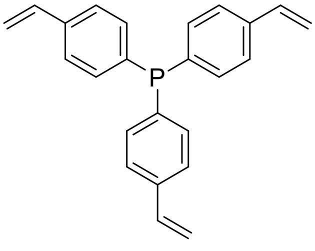


b. Under argon protection, **2P2Br** (0.36 mmol), trivinylphenylphosphine (1 mmol), zinc bromide (0.5 mmol), and 18 mg of AIBN were dissolved into a solution of anhydrous N, N-Dimethylformamide (8 mL). After stirring for 24 h at 100 ° C, the solution was washed with methyl tert-butyl ether and drained at room temperature. The white solid obtained was labeled as Zn@PIP-1.

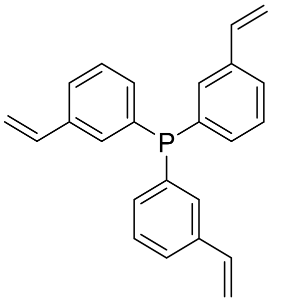


2. Preparation of Zn@2P2Br&*p*-3vPPh$_3$ porous ionic liquid polymer catalysts (Zn@PIP-2):

Synthesise in the same way as above, but replace monomer 1 with monomer 2.

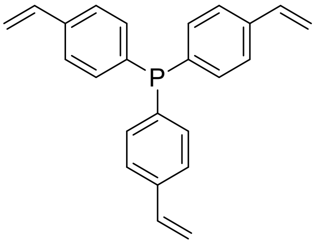


monomer 1

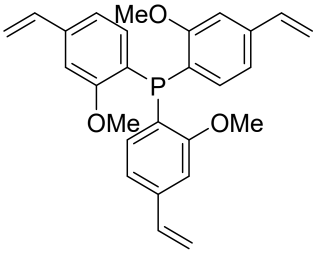


monomer 2

3. Preparation of Zn@2P2Br&*p*-3vPPh$_3$ porous ionic liquid polymer catalysts (Zn@PIP-3): Synthesise in the same way as above, but replace monomer 1 with monomer 3.

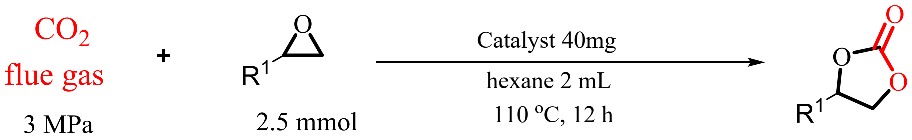


monomer 1



monomer 3

3. General procedures



In a typical procedure, a 100 mL stainless steel autoclave was filled with 40 mg of Zn@PIP-1 catalyst, 2.5 mmol of substrates, 3.0 MPa of flue gas, and 2 mL of hexane as solvent. At room temperature, the air in the autoclave was replaced three times with 1 MPa flue gas and then filled with 3.0 MPa flue gas. The autoclave was placed in the reactor and heated and stirred at 110 °C for 12 h. After the reaction, the autoclave was cooled down to room temperature, and the pressure in the autoclave was slowly released. Subsequently, the reaction mixture was diluted with ethyl acetate (6.0 mL), and the selectivity of the product was confirmed by gas chromatography (Agilent 7890A GC, HP-5 capillary column, 5 wt.% phenyl, FID detector). The quantitative yield of target product GC: The yield of the product can be obtained by GC analysis using biphenyl as an internal standard. Target product isolation yield: After the reaction mixture was concentrated in a vacuum to remove the solvent, the crude product was analyzed by GC using PE/EA as eluent. After the reaction mixture was concentrated in a vacuum to remove the solvent, the product yield could be obtained by using PE/EA (10:1-2:1) as eluent, and the crude product was purified by rapid column chromatography.

Recyclability Test for Zn@PIP-1.

After the cycloaddition reaction of epoxides with flue gas was completed, the recycled catalyst was separated by centrifugation, washed with degassed THF (tetrahydrofuran), and used directly for the next run.

4. Catalyst characterization

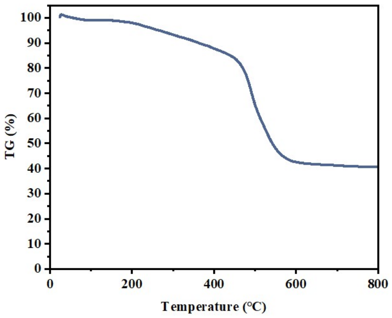


Figure S1. Thermal gravimetric analysis (TGA) curve of Zn@PIP-1

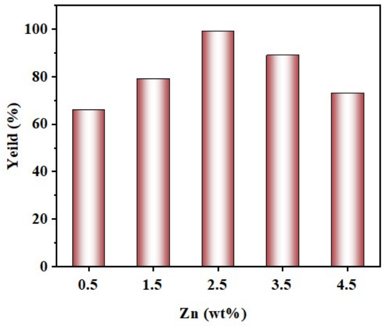


Figure S2. Metal loading optimization identified an ideal Zn content

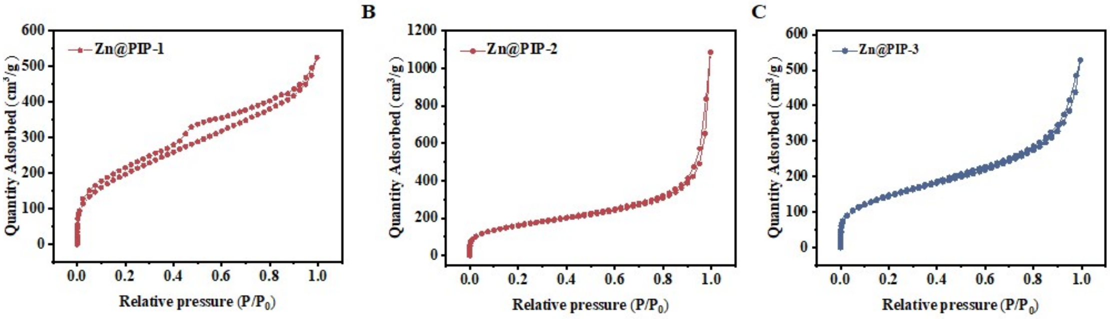


Figure S3. N_2 sorption isotherms measured at 77 K.

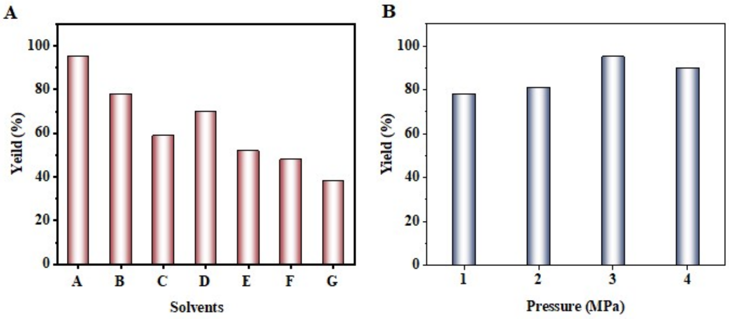


Figure S4. (A) Effect of reaction solvents on the yield of carbonates.: A. n-hexane. B. dioxane. C. acetonitrile. D. methyl tertbuty ether. E. dichloromethane. F. methylbenzene. G. dimethyl formamide. (B) Effect of reaction pressure on carbonate yield.

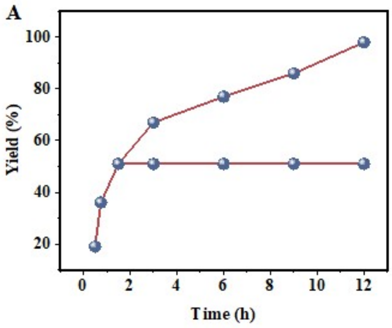


Figure S5. Hot filtrating experiments.

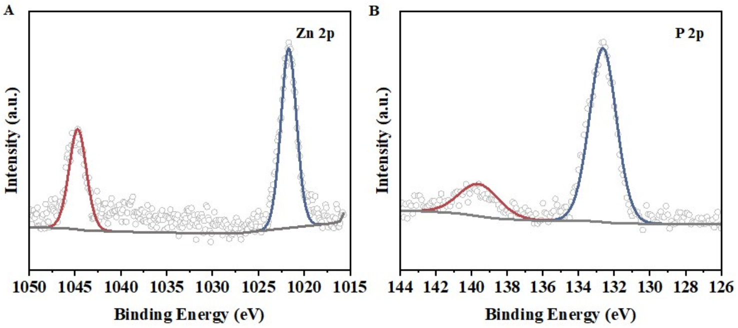


Figure S6. XPS spectra image of Zn@PIP-1-used

Table S1 ICP data for fresh and used catalysts.

Entry	Zn (wt%)
Zn@PIP-1	3.04
Zn@PIP-1-used	3.90

5.Performance Comparison of cycloaddition of PO using flue gas.

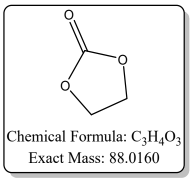
Table S2 Performance Comparison of cycloaddition of PO using flue gas.

Entry	Catalyst	Co-catalyst	Reaction condition	Flue gas composition	Num. of S	Y (%)	Cycle	Ref.
1^a	**Zn@PIP-1**	**-**	**110°C, 30bar, 12h**	**19.4% CO_2 ，78.8 % N_2, 1.8% O_2, NO_x (≤20ppm)**	**22**	**99**	**5**	**(1)**
2^a	**Al-MDC-NC**	**-**	**100°C, 1bar, 12h**	**15% CO_2, 85% N_2, 0.0200g fly ash, and 95% RH)**	**-**	**82**	**-**	**(2)**
5^a	**PBPILs**	**-**	**100°C, 20bar, 4h**	**15% CO_2 and 85% N_2**	**6**	**95**	**5**	**(3)**
7^a	**I_{C2}HCP-5$_b$**	**-**	**120°C, 30bar, 24h**	**15% CO_2 and 85% N_2**	**6**	**92**	**6**	**(4)**
11^b	**(3-aminobenzyl alcohol/n Bu_4NI**	**-**	**60°C, 10bar, 35h**	**14.5% CO_2, 2% H_2O, 1.5% O_2, 300 ppm CO, 207 ppm SO_x, 300 ppm NO_x and the other component was N_2**	**-**	**99**	**-**	**(5)**
12^b	**HBDs**	**Ammonium salt**	**60°C, 1bar, 10h**	**14.5% CO_2, 2% H_2O, 1.5% O_2, 300 ppm CO, 207 ppm SO_x, 300 ppm NO_x and the other component was N_2**	**-**	**99**	**-**	**(6)**
13^b	**$PP_{1,4}Br/ZnCl_2$**	**$ZnCl_2$**	**60°C, 40bar, 18h**	**19.4% CO_2, 78.8 % N_2 1.8% O_2, No_x(≤20ppm)**	**19**	**99**	**7**	**(7)**

^{a} Heterogeneous, ^{b} Homogeneous

(1). This work. (2). Ind.Eng.Chem.Res. 2024, 63, 16725−16735. (3). Molecular Catalysis 2023，544, 113157. (4). ChemSusChem 2020, 13, 341. (5). Journal of Environmental Chemical Engineering 2024, 12, 113614. (6). Catal. Sci. Technol. 2024, 14, 6215－6223. (7).Green Chem. 2023, 25, 2293－2298.

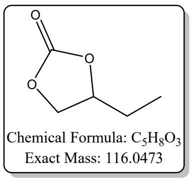
6. NMR data of the products



1,3-dioxolan-2-one

^{1}H NMR (400 MHz, CDCl$_3$) δ 4.51 (s, 1H).

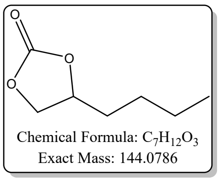
^{13}C NMR (101 MHz, CDCl$_3$) δ 155.60, 64.74.



4-Ethyl-1,3-Dioxolan-2-one

^{1}H NMR (400 MHz, CDCl$_3$) δ 4.78 – 4.64 (m, 1H), 4.56 (t, *J* = 8.2 Hz, 1H), 4.11 (dd, *J* = 8.4, 7.0 Hz, 1H), 1.91 – 1.72 (m, 2H), 1.03 (t, *J* = 7.5 Hz, 3H).

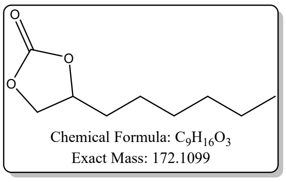
^{13}C NMR (101 MHz, CDCl$_3$) δ 155.19, 78.08, 69.04, 26.82, 8.41.



4-Butyl-1,3-dioxolan-2-one,

^{1}H NMR (400 MHz, CDCl$_3$) δ 4.72 (dd, *J* = 7.5, 5.5 Hz, 1H), 4.54 (t, *J* = 8.1 Hz, 1H), 4.08 (dd, *J* = 8.3, 7.3 Hz, 1H), 1.74 (dd, *J* = 23.8, 18.4 Hz, 2H), 1.50 – 1.24 (m, 4H), 0.93 (t, *J* = 7.0 Hz, 3H).

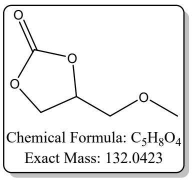
^{13}C NMR (101 MHz, CDCl$_3$) δ 155.21, 77.17,69.50, 33.66, 26.53, 22.35, 13.89.



4-Hexyl-1,3-dioxolan-2-one,

^{1}H NMR (400 MHz, CDCl$_3$) δ 4.69 (dd, *J* = 7.5, 5.4 Hz, 1H), 4.63 – 3.89 (m, 2H), 1.89 – 1.57 (m, 2H), 1.47 – 1.20 (m, 8H), 0.86 (t, *J* = 6.8 Hz, 3H).

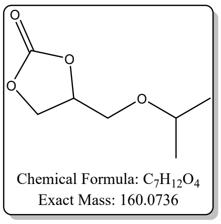
^{13}C NMR (101 MHz, CDCl$_3$) δ 155.19, 77.16, 69.48, 33.92, 31.56, 28.84, 24.38, 22.51, 14.04.



4-Methoxymethyl-1,3-dioxolan-2-one,

^{1}H NMR (400 MHz, CDCl$_3$) δ 4.85 – 4.75 (m, 1H), 4.55 – 4.27 (m, 2H), 3.67 – 3.48 (m, 2H), 3.39 (dd, *J* = 5.5, 2.2 Hz, 3H).

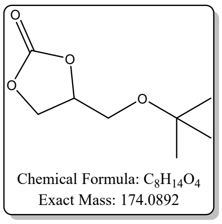
^{13}C NMR (101 MHz, CDCl$_3$) δ 155.09, 75.17, 71.51, 66.22, 59.64.



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

^{1}H NMR (400 MHz, CDCl$_3$) δ 4.83 – 4.79 (m, 1H), 4.56 – 4.36 (m, 1H), 3.72 – 3.55 (m, 1H), 1.17 (d, *J* = 6.1 Hz, 1H).

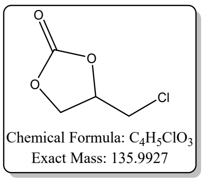
^{13}C NMR (101 MHz, CDCl$_3$) δ 155.20, 75.31, 72.98, 67.18, 66.48, 21.95, 21.84.



4-tert-butoxymethyl-1,3-dioxolan-2-one,

^{1}H NMR (400 MHz, CDCl$_3$) δ 4.77 – 4.54 (m, 1H), 4.41 – 4.14 (m, 1H), 3.42 (dd, *J* = 44.9, 2.4 Hz, 1H), 1.03 (d, *J* = 1.0 Hz, 1H).

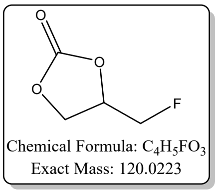
^{13}C NMR (101 MHz, CDCl$_3$) δ 155.11,75.27, 73.30, 66.10, 61.00, 26.92.



4-Chloromethyl-1,3-dioxolan-2-one,

^{1}H NMR (400 MHz, CDCl$_3$) δ 5.01 – 4.87 (m, 1H), 4.51 (td, *J* = 8.7, 2.6 Hz, 1H), 4.29 (ddd, *J* = 9.3, 5.6, 3.9 Hz, 1H), 3.77 (ddd, *J* = 12.5, 4.1, 1.3 Hz, 1H), 3.70 – 3.62 (m, 1H).

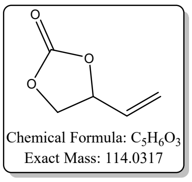
^{13}C NMR (101 MHz, CDCl$_3$) δ 154.49, 74.45, 66.75, 44.22.



4-(fluoromethyl)-1,3-dioxolan-2-one

^{1}H NMR (400 MHz, CDCl$_3$) δ 4.96 – 4.79 (m, 1H), 4.78 – 4.28 (m, 4H).

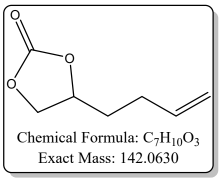
^{13}C NMR (101 MHz, CDCl$_3$) δ 154.71, 82.30, 80.55, 74.78, 74.59, 64.98, 64.91.



4-Vinyl-1,3-dioxolan-2-one,

^{1}H NMR (400 MHz, CDCl$_3$) δ 5.83 (s, 1H), 5.59 – 5.24 (m, 2H), 5.07 (d, *J* = 7.4 Hz, 1H), 4.54 (t, *J* = 8.4 Hz, 1H), 4.25 – 3.80 (m, 1H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 154.82, 132.15, 120.96, 77.30, 77.16, 69.03.

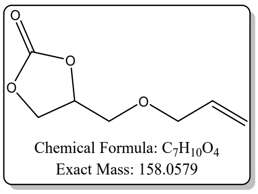


Chemical Formula: $C_7H_{10}O_3$
Exact Mass: 142.0630

4-(But-3-en-1-yl)-1,3-dioxolan-2-one,

^{1}H NMR (400 MHz, CDCl$_3$) δ 5.76 (ddd, *J* = 16.9, 7.6, 2.9 Hz, 1H), 5.18 – 4.94 (m, 2H), 4.71 (dt, *J* = 7.8, 4.0 Hz, 1H), 4.58 – 4.46 (m, 1H), 4.11 – 3.99 (m, 1H), 2.19 (ddd, *J* = 9.3, 8.3, 4.2 Hz, 2H), 1.95 – 1.74 (m, 2H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 155.06, 136.18, 116.43, 76.43, 69.40, 33.08, 28.70.

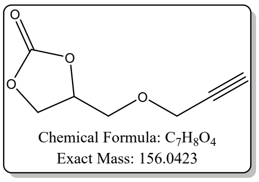


Chemical Formula: $C_7H_{10}O_4$
Exact Mass: 158.0579

4-((Allyloxy)methyl)-1,3-dioxolan-2-one,

^{1}H NMR (400 MHz, CDCl$_3$) δ 4.88 – 4.79 (m, 1H), 4.48 (t, *J* = 8.5 Hz, 1H), 4.35 (dd, *J* = 8.4, 6.1 Hz, 1H), 4.25 – 4.12 (m, 2H), 3.80 – 3.64 (m, 2H), 2.48 (t, *J* = 2.4 Hz, 1H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 154.97, 78.61, 75.63, 74.86, 68.47, 66.19, 58.78.

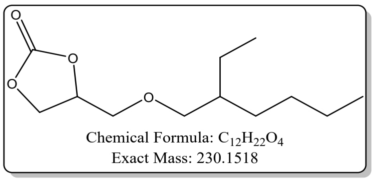


Chemical Formula: $C_7H_8O_4$
Exact Mass: 156.0423

4-((Prop-2-yn-1-yloxy) methyl)-1,3-dioxola n-2-one,

^{1}H NMR (400 MHz, CDCl$_3$) δ 4.88 – 4.79 (m, 1H), 4.48 (t, *J* = 8.5 Hz, 1H), 4.35 (dd, *J* = 8.4, 6.1 Hz, 1H), 4.25 – 4.12 (m, 2H), 3.80 – 3.64 (m, 2H), 2.48 (t, *J* = 2.4 Hz, 1H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 154.97, 78.61, 75.63, 74.86, 68.47, 66.19, 58.78.

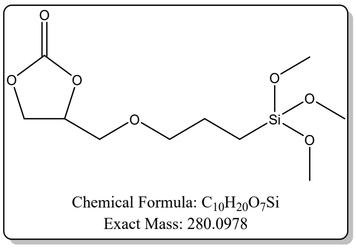


Chemical Formula: $C_{12}H_{22}O_4$
Exact Mass: 230.1518

4-(2-ethylhexyl) oxy) methyl)-1,3-dioxolan-2-one

^{1}H NMR (400 MHz, CDCl$_3$) δ 4.85 – 4.62 (m, 1H), 4.49 – 4.16 (m, 1H), 3.63 – 3.38 (m, 1H), 3.33 – 3.21 (m, 1H), 1.39 (d, *J* = 5.8 Hz, 1H), 1.31 – 1.01 (m, 1H), 0.77 (dt, *J* = 10.1, 6.7 Hz, 1H).

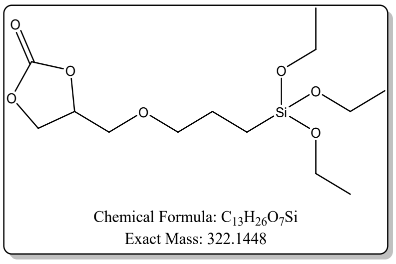
^{13}C NMR (101 MHz, CDCl$_3$) δ 155.03, 75.25, 74.44, 74.42, 69.75, 66.10, 39.39, 30.24, 28.86, 23.57, 22.82, 13.84, 10.82.



4-((3-(trimethoxy silyl) proxy) methyl)-1,3-dioxolan-2-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.80 (dd, *J* = 4.0, 2.0 Hz, 1H), 4.53 – 4.26 (m, 5H), 3.72 – 3.41 (m, 29H), 1.73 – 1.59 (m, 5H), 0.68 – 0.58 (m, 4H).

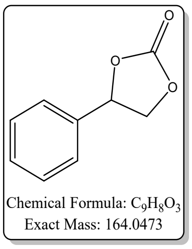
^{13}C NMR (101 MHz, $CDCl_3$) δ 155.07, 77.48, 75.14, 74.05, 69.71, 66.43, 50.67, 22.79, 5.21.



4-((3-(Triethoxysilyl) propoxy) methyl)-1,3-dioxolan-2-one,

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.73 – 4.66 (m, 1H), 4.41 – 4.21 (m, 1H), 3.67 (q, *J* = 7.0 Hz, 3H), 3.50 (ddd, *J* = 38.7, 11.1, 3.6 Hz, 1H), 3.34 (td, *J* = 6.6, 1.2 Hz, 1H), 1.59 – 1.48 (m, 1H), 1.07 (t, *J* = 7.0 Hz, 5H), 0.54 – 0.42 (m, 1H).

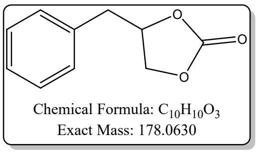
^{13}C NMR (101 MHz, $CDCl_3$) δ 156.94, 154.90, 75.09, 73.73, 69.39, 66.06, 58.11, 22.68, 18.04, 6.10.



4-phenyl-1,3-dioxolan-2-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.37 (m, 3H), 7.36 – 7.31 (m, 2H), 5.65 (t, *J* = 8.0 Hz, 1H), 4.82 – 4.69 (m, 1H), 4.29 (dd, *J* = 8.6, 7.8 Hz, 1H).

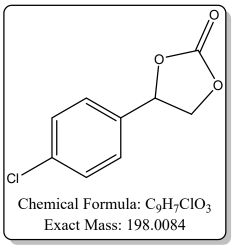
^{13}C NMR (101 MHz, $CDCl_3$) δ 154.90, 135.78, 129.55, 129.06, 125.87, 77.94, 71.08.



4-benzyl-1,3-dioxolan-2-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.18 (m, 1H), 5.03 – 4.65 (m, 1H), 4.42 (dd, *J* = 8.6, 7.9 Hz, 1H), 4.15 (dd, *J* = 8.6, 6.9 Hz, 1H), 3.05 (ddd, *J* = 55.9, 14.2, 6.4 Hz, 1H).

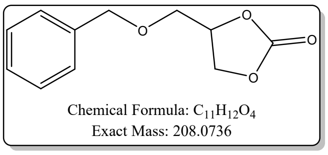
^{13}C NMR (101 MHz, $CDCl_3$) δ 154.90, 134.05, 129.40, 128.98, 127.55,76.93, 68.54, 39.54.



4-(4-chlorophenyl)-1,3-dioxolan-2-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (dd, *J* = 47.7, 8.5 Hz, 1H), 5.66 (s, 1H), 4.56 (d, *J* = 199.6 Hz, 1H).

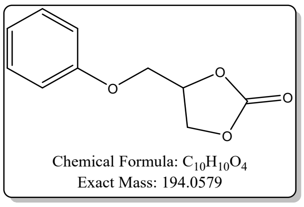
^{13}C NMR (101 MHz, $CDCl_3$) δ 154.62, 135.95, 134.42, 129.67, 127.38, 77.35, 77.16, 71.12.



4-((benzyloxy)methyl)-1,3-dioxolan-2-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (s, 1H), 4.75 (dd, *J* = 5.8, 2.6 Hz, 1H), 4.52 (d, *J* = 1.7 Hz, 1H), 4.46 – 4.20 (m, 1H), 3.61 (ddd, *J* = 46.2, 12.9, 7.2 Hz, 1H).

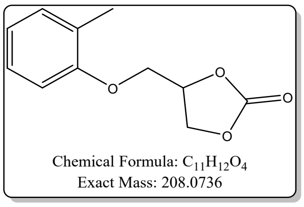
^{13}C NMR (101 MHz, $CDCl_3$) δ 155.06, 137.18, 128.56, 128.04, 127.73, 75.13, 68.88, 66.28.



4-(phenoxymethyl)-1,3-dioxolan-2-one

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.28 (m, 1H), 7.04 – 6.98 (m, 1H), 6.93 – 6.88 (m, 1H), 5.09 – 4.97 (m, 1H), 4.57 (ddd, *J* = 14.4, 12.7, 7.2 Hz, 1H), 4.19 (ddd, *J* = 39.3, 10.6, 3.9 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.87, 154.80, 129.82, 122.11, 74.24, 66.99, 66.35.

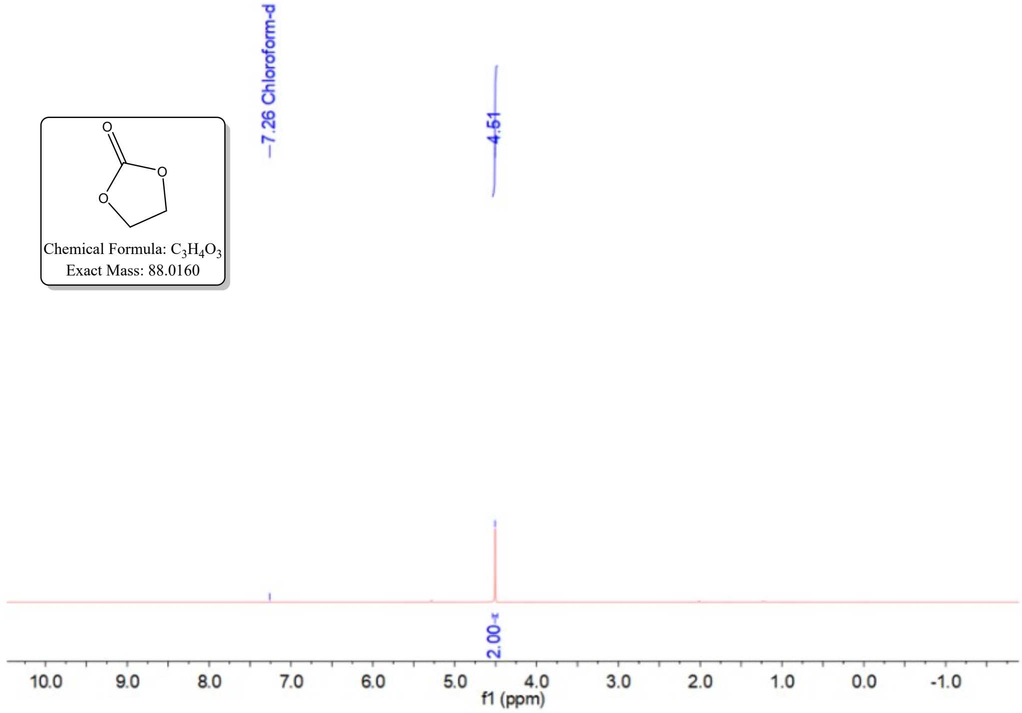


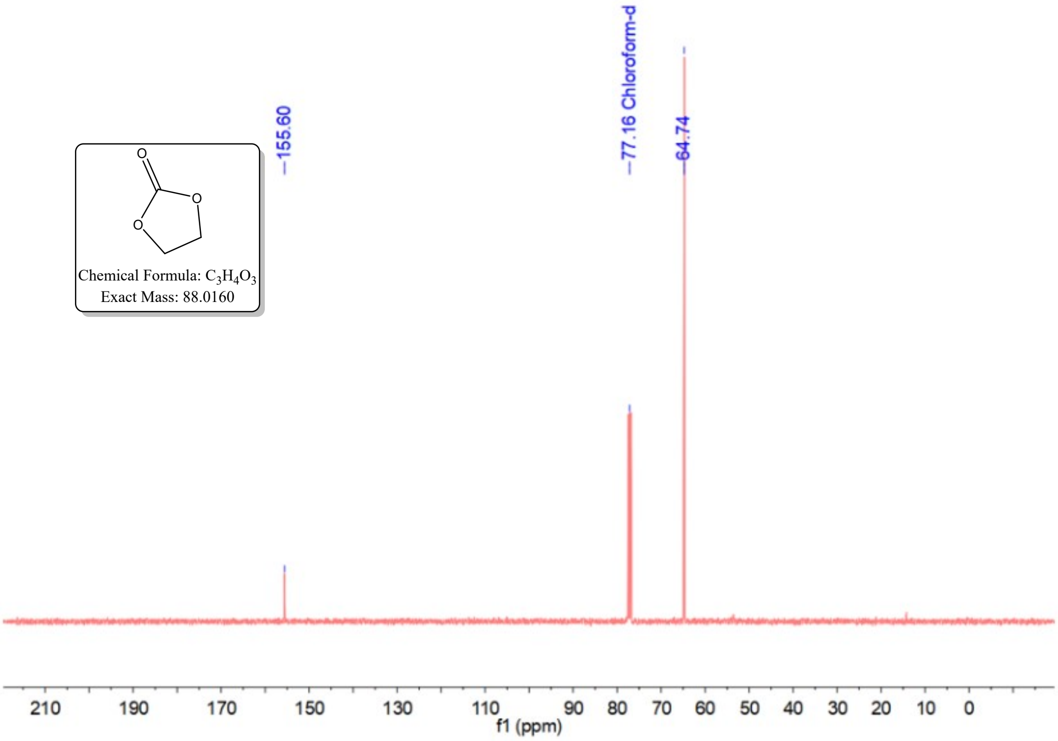
4-((o-tolyloxy) methyl)-1,3-dioxolan-2-one

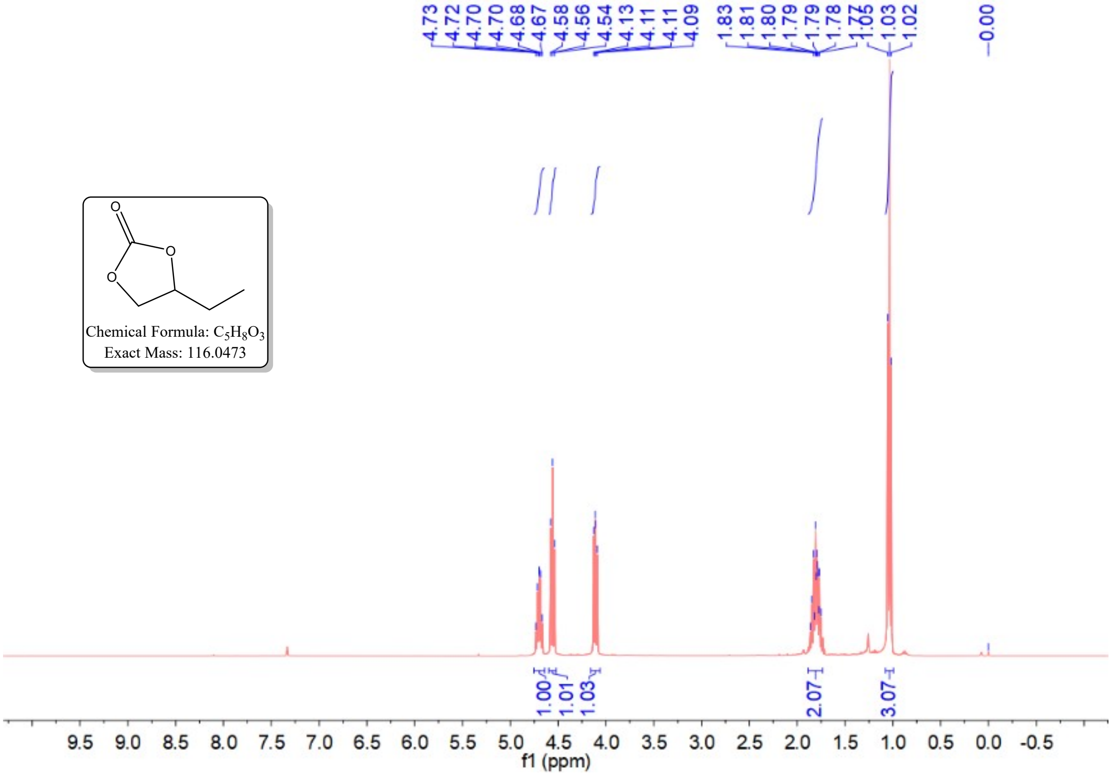
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 – 7.09 (m, 1H), 6.94 – 6.85 (m, 1H), 6.77 (s, 1H), 5.02 (d, *J* = 3.0 Hz, 1H), 4.56 (dd, *J* = 11.2, 6.9 Hz, 1H), 4.15 (dd, *J* = 45.7, 3.1 Hz, 1H), 2.20 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.84, 155.01, 131.07, 127.06, 126.94, 121.63, 110.91, 77.16, 74.41, 67.06, 66.30, 15.

7. NMR specture of the products



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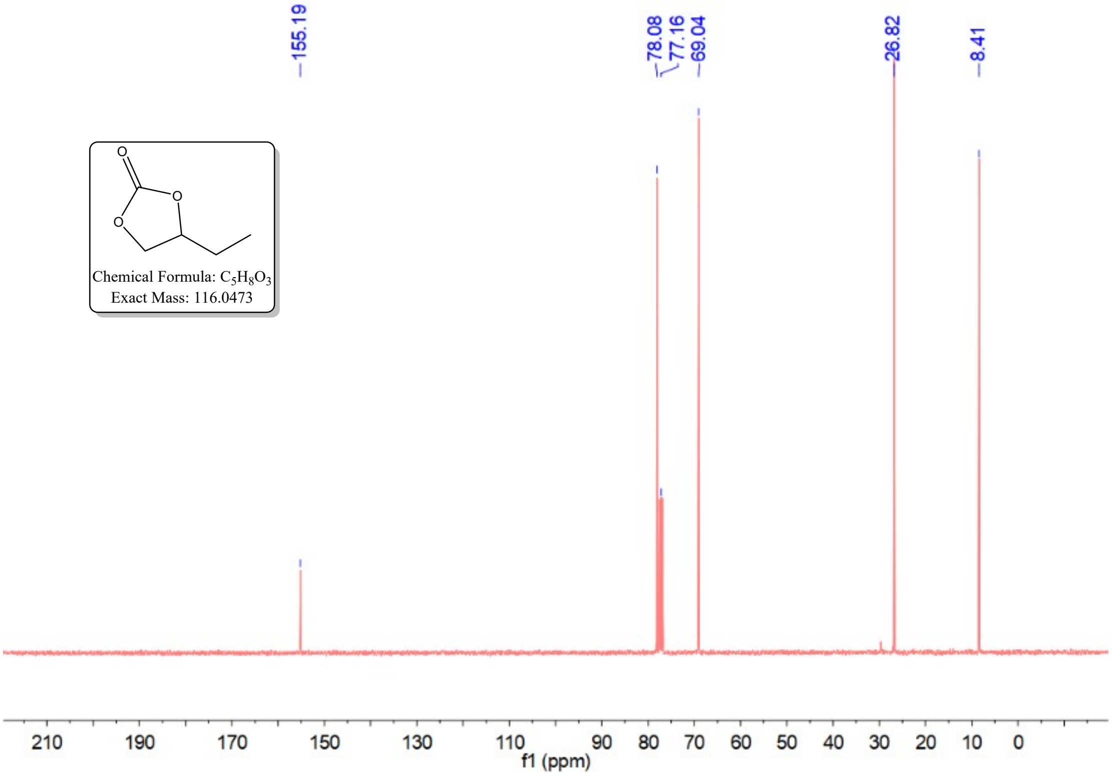
4.72
4.70
4.70
4.68
4.67
4.58
4.56
4.54
4.13
4.11
4.11
4.09
1.83
1.81
1.80
1.79
1.79
1.78
1.77
1.05
1.03
1.02
0.00
O
O
O
Chemical Formula: C5H8O3
Exact Mass: 116.0473
1.00
1.01
1.03
2.07
3.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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78.08
77.16
69.04
26.82
8.41
O
O
O
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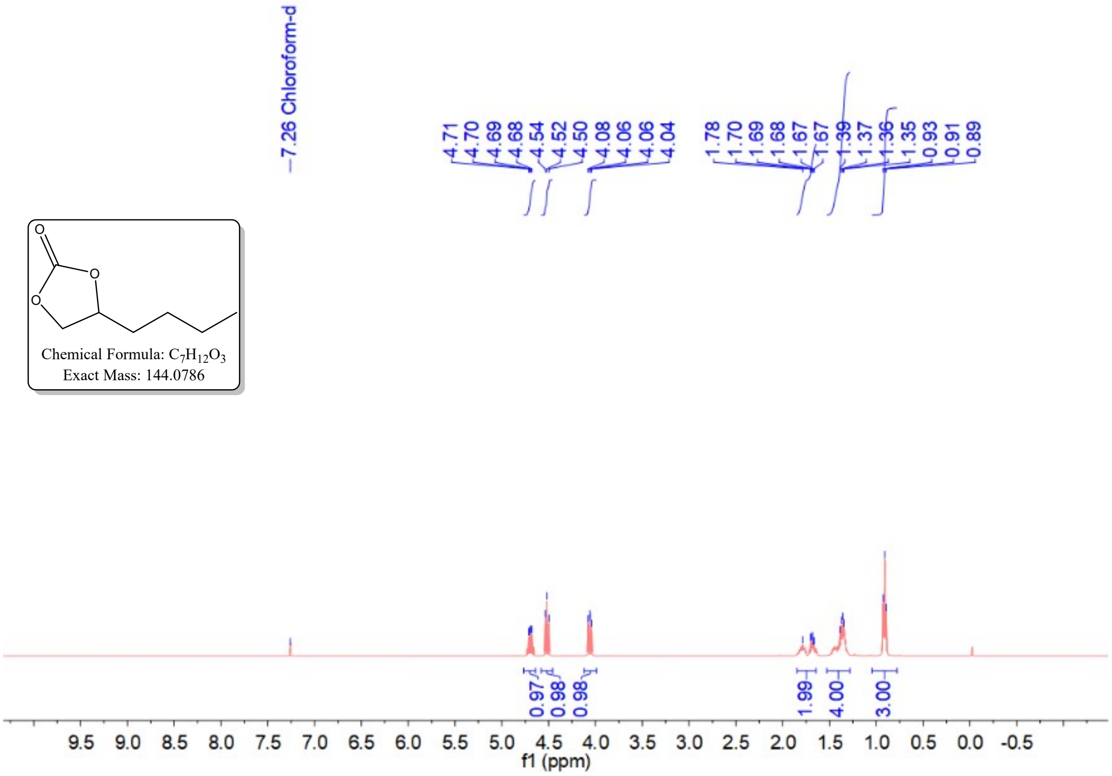
Exact Mass: 116.0473
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.26 Chloroform-d
4.71
4.70
4.69
4.68
4.54
4.52
4.50
4.08
4.06
4.06
4.04
1.78
1.70
1.69
1.68
1.67
1.67
1.39
1.37
1.36
1.35
0.93
0.91
0.89
O
O
O
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Exact Mass: 144.0786
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0.98
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
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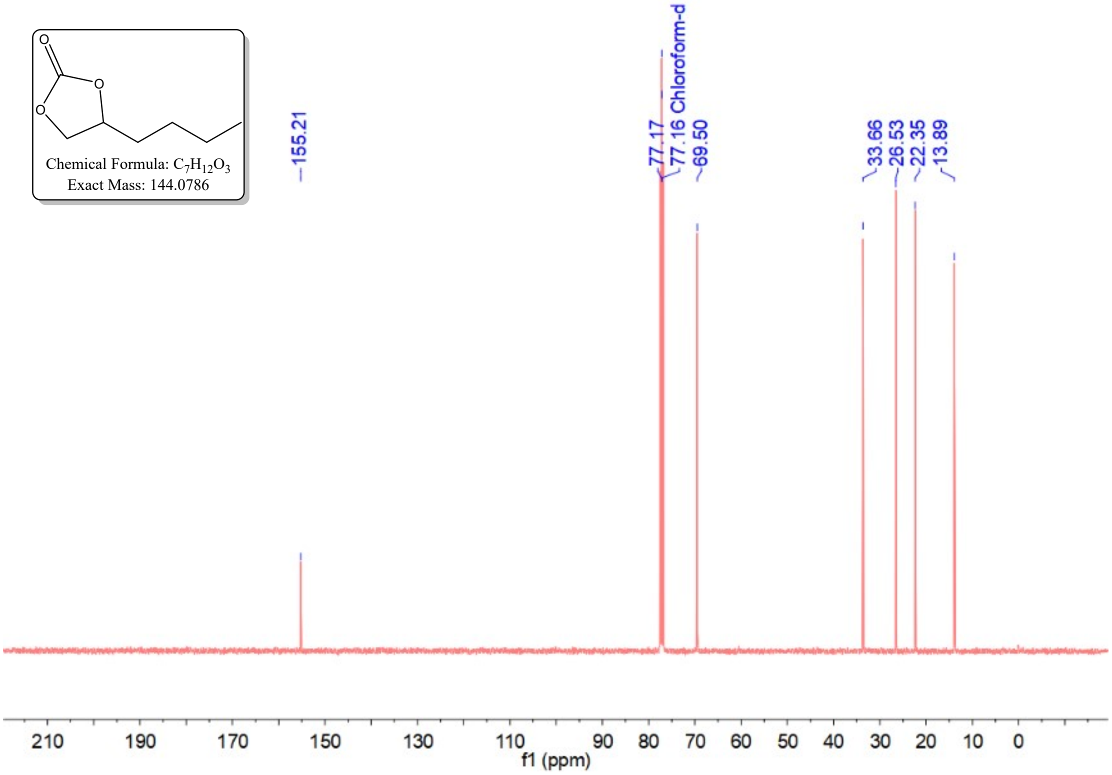
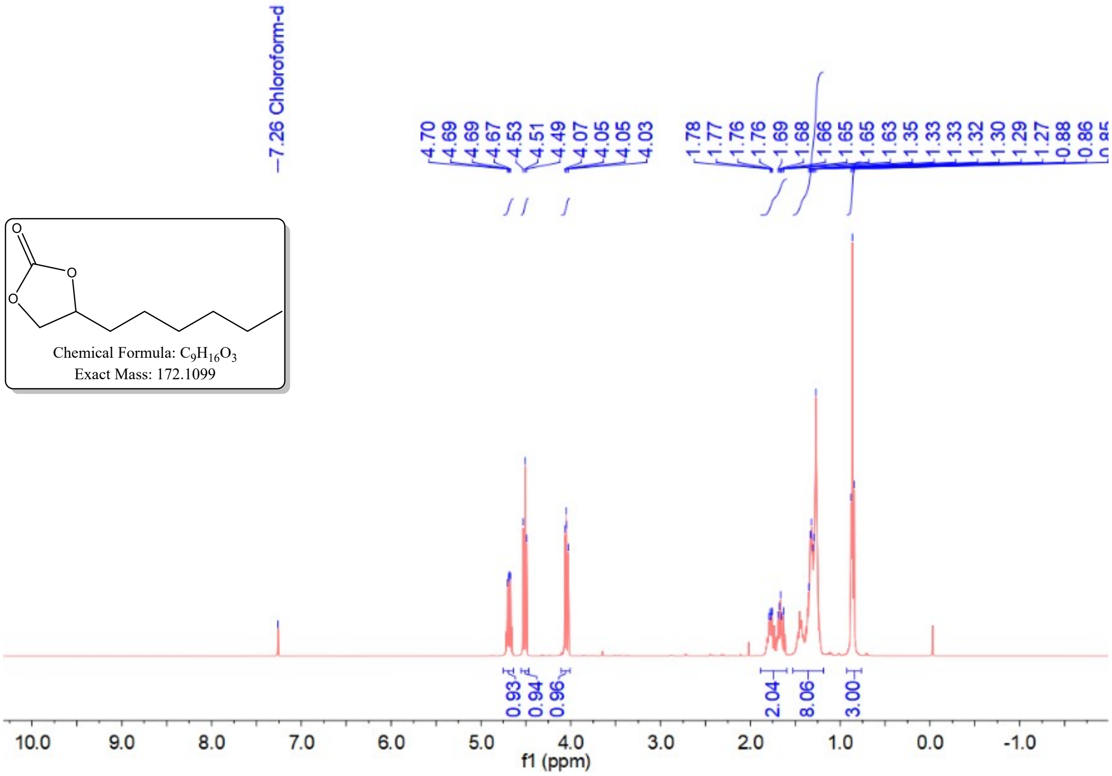
f1 (ppm)


O
O
O
Chemical Formula: $C_7H_{12}O_3$
Exact Mass: 144.0786
155.21
77.17
77.16 Chloroform-d
69.50
33.66
26.53
22.35
13.89
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.26 Chloroform-d
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4.69
4.69
4.67
4.53
4.51
4.49
4.07
4.05
4.05
4.03
1.78
1.77
1.76
1.76
1.69
1.68
1.66
1.65
1.65
1.63
1.35
1.33
1.32
1.30
1.29
1.27
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0.86
Chemical Formula: C9H16O3
Exact Mass: 172.1099
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0.94
0.96
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8.06
3.00
10.0
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5.0
4.0
3.0
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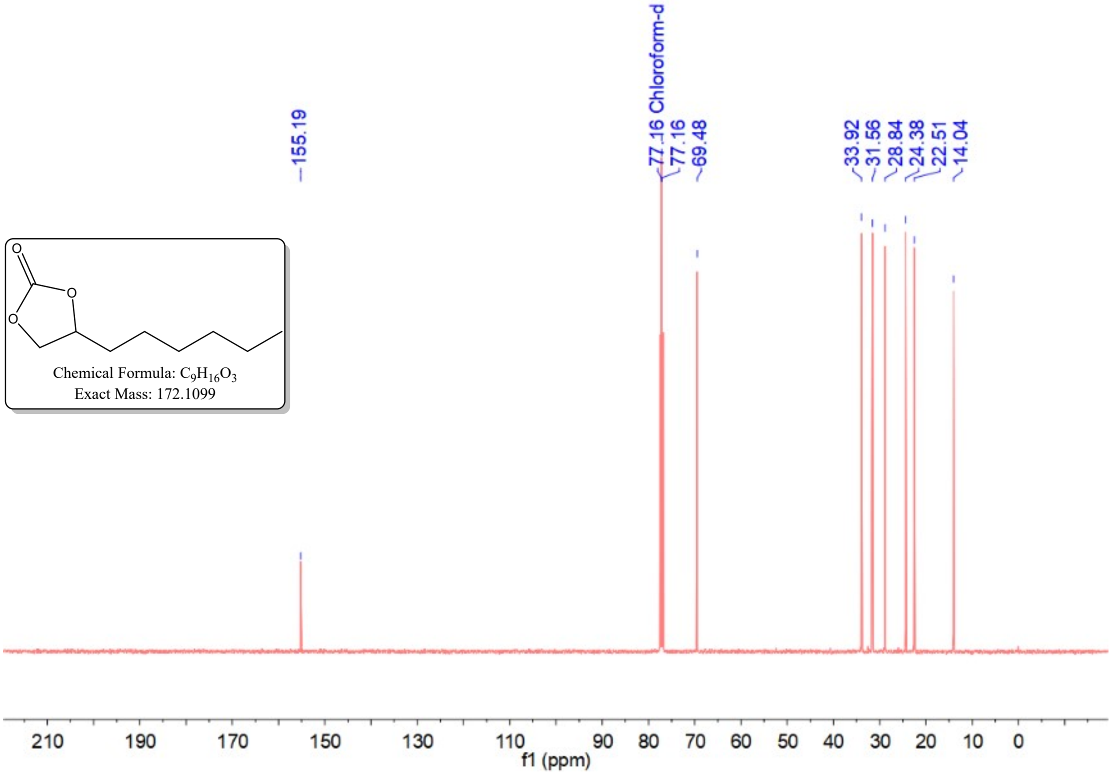
-1.0
f1 (ppm)


155.19
77.16 Chloroform-d
77.16
69.48
33.92
31.56
28.84
24.38
22.51
14.04
Chemical Formula: C9H16O3
Exact Mass: 172.1099
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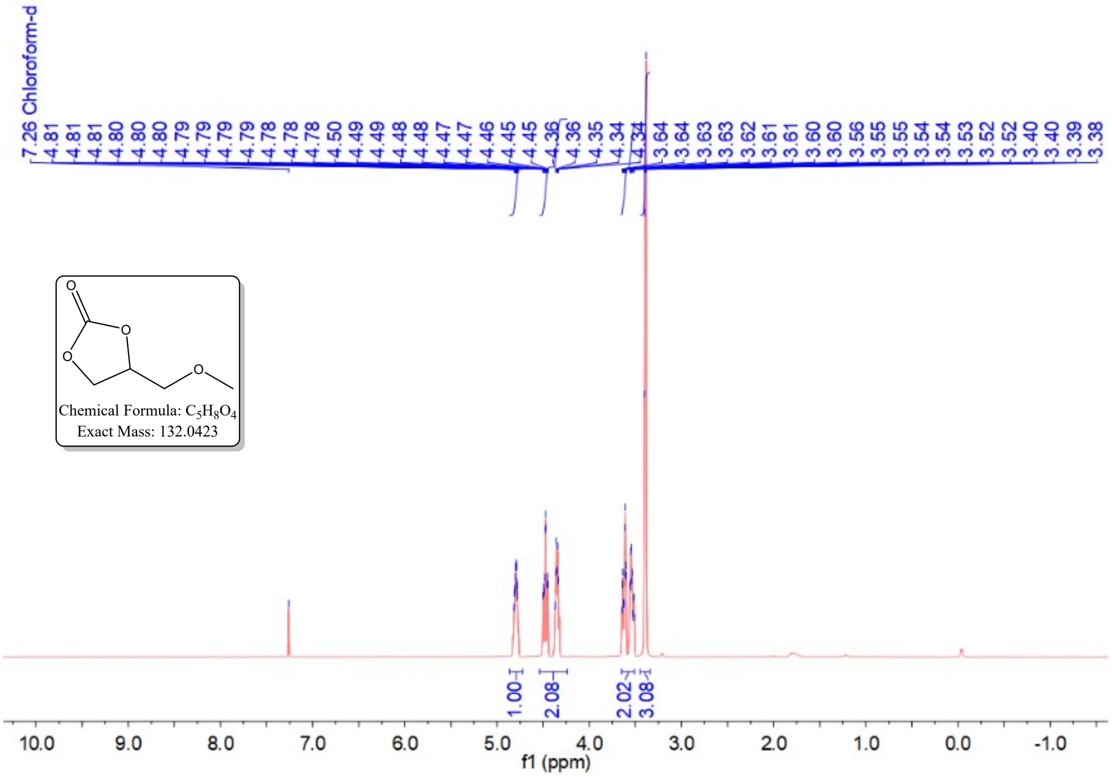
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.26 Chloroform-d
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4.81
4.81
4.80
4.80
4.80
4.79
4.79
4.79
4.79
4.78
4.78
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3.60
3.56
3.55
3.55
3.54
3.54
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3.52
3.52
3.40
3.40
3.39
3.38
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Exact Mass: 132.0423
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2.02
3.08
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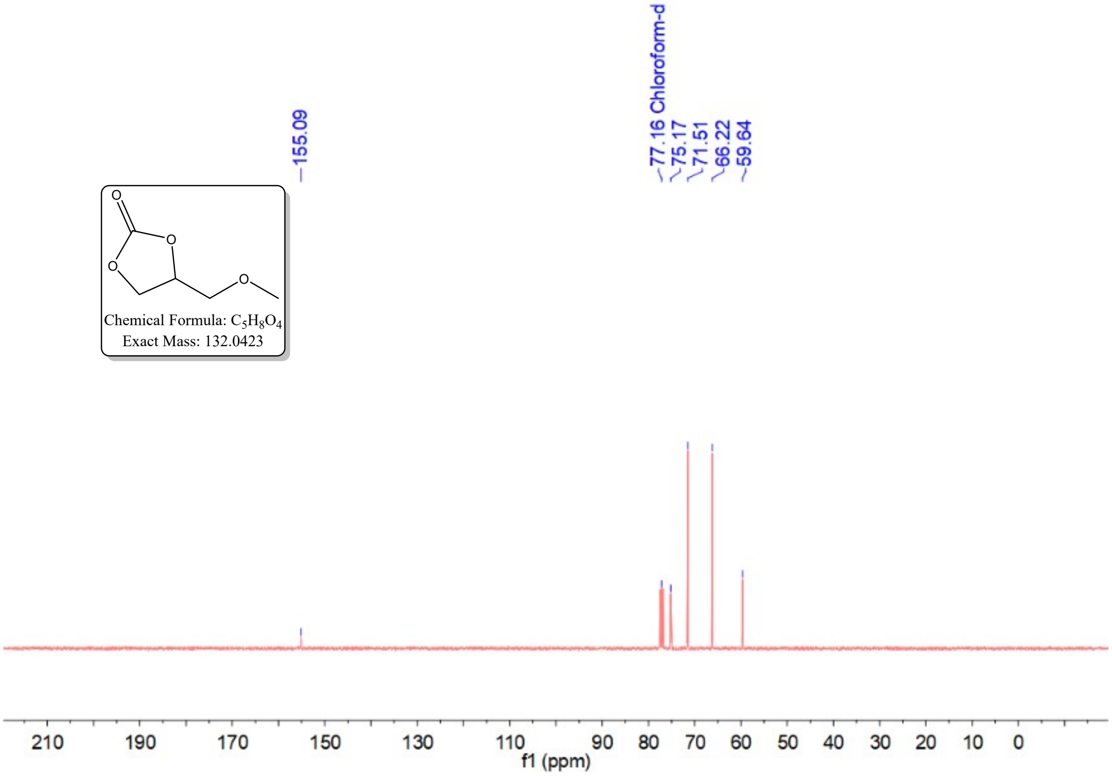
-1.0
f1 (ppm)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77.16 Chloroform-d
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66.22
59.64
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Exact Mass: 132.0423
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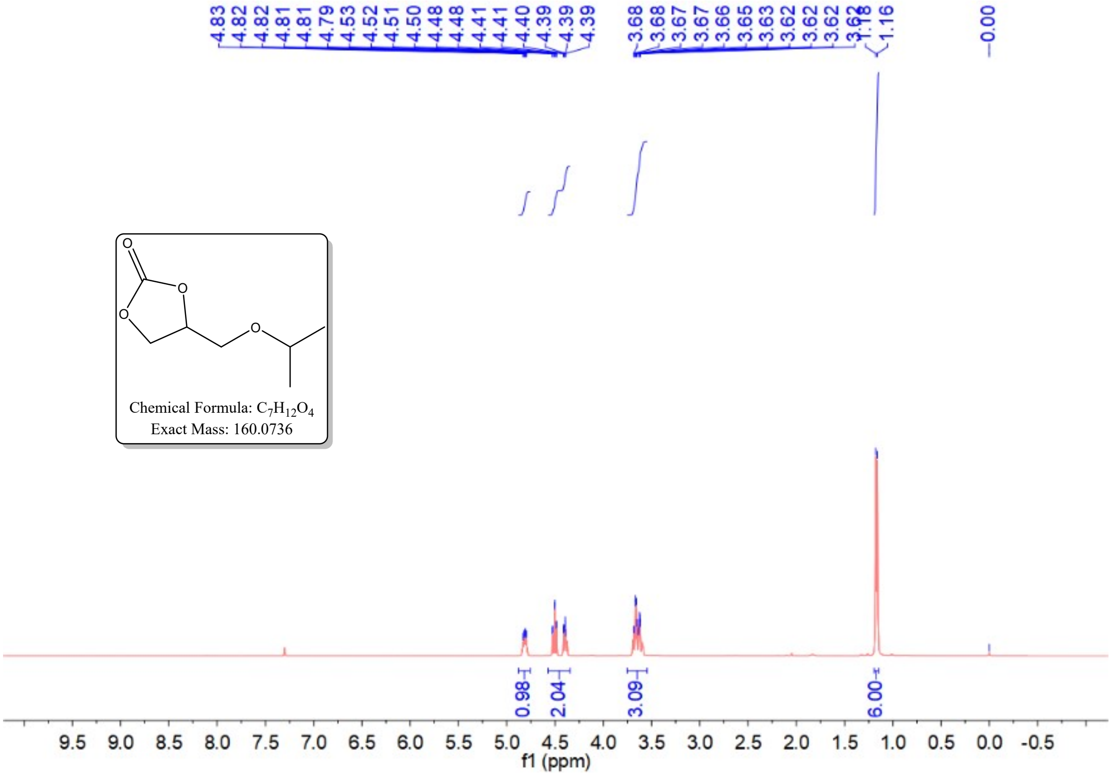
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


4.83
4.82
4.82
4.81
4.81
4.79
4.53
4.52
4.51
4.50
4.48
4.48
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3.68
3.68
3.67
3.67
3.66
3.65
3.63
3.62
3.62
3.62
1.18
1.16
-0.00
Chemical Formula: C7H12O4
Exact Mass: 160.0736
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3.09
6.00
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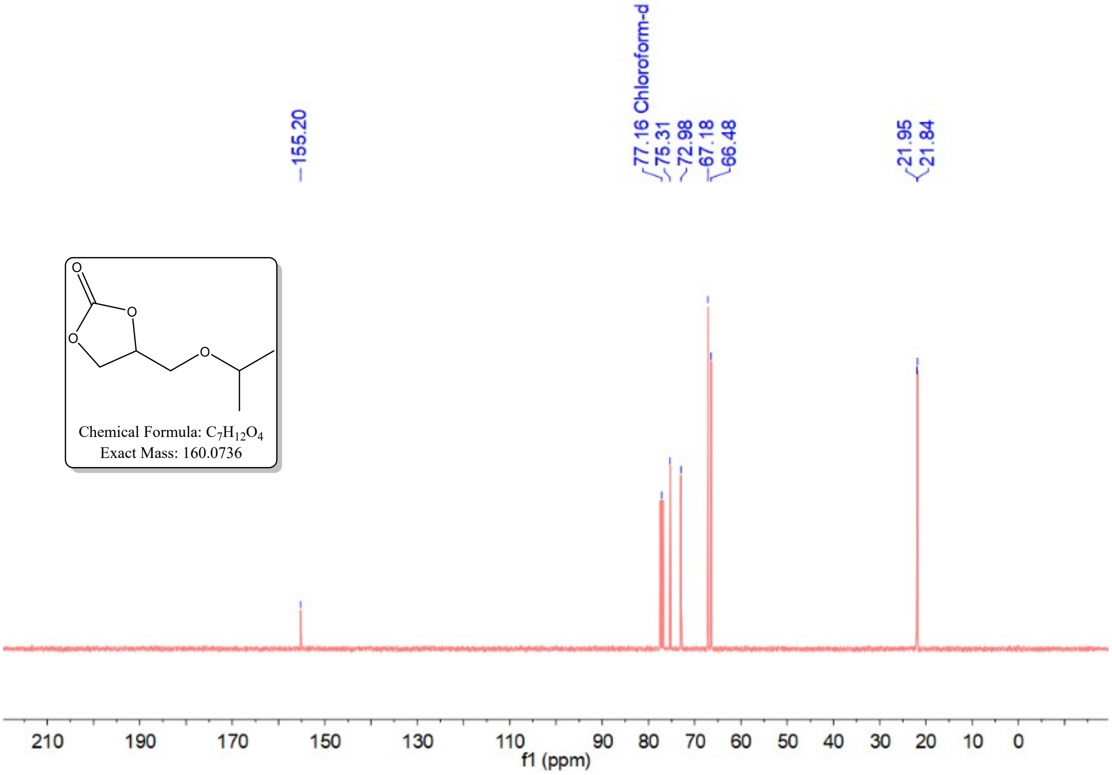
f1 (ppm)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72.98
67.18
66.48
21.95
21.84
Chemical Formula: C7H12O4
Exact Mass: 160.0736
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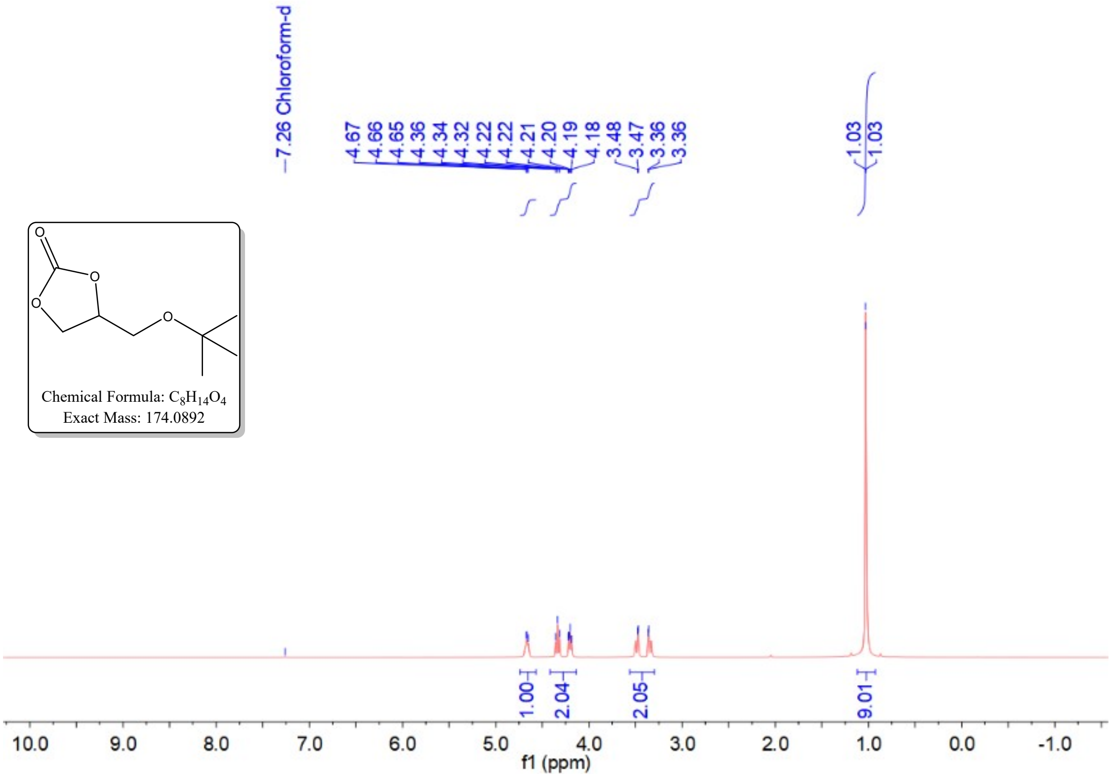
f1 (ppm)


7.26 Chloroform-d
4.67
4.66
4.65
4.36
4.34
4.32
4.22
4.22
4.21
4.20
4.19
4.18
3.48
3.47
3.36
3.36
1.03
1.03
Chemical Formula: $C_8H_{14}O_4$
Exact Mass: 174.0892
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2.05
9.01
10.0
9.0
8.0
7.0
6.0
5.0
4.0
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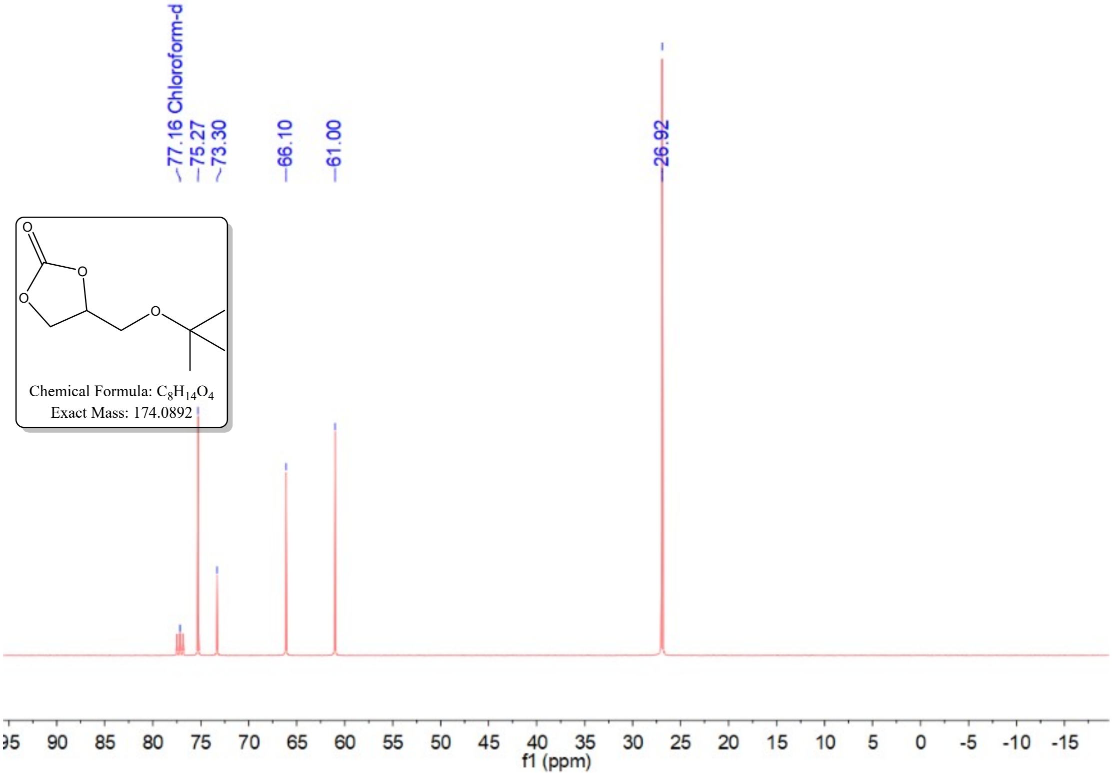
2.0
1.0
0.0
-1.0
f1 (ppm)


77.16 Chloroform-d
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73.30
66.10
61.00
26.92
Chemical Formula: $C_8H_{14}O_4$
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90
85
80
75
70
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60
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45
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25
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15
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5
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-5
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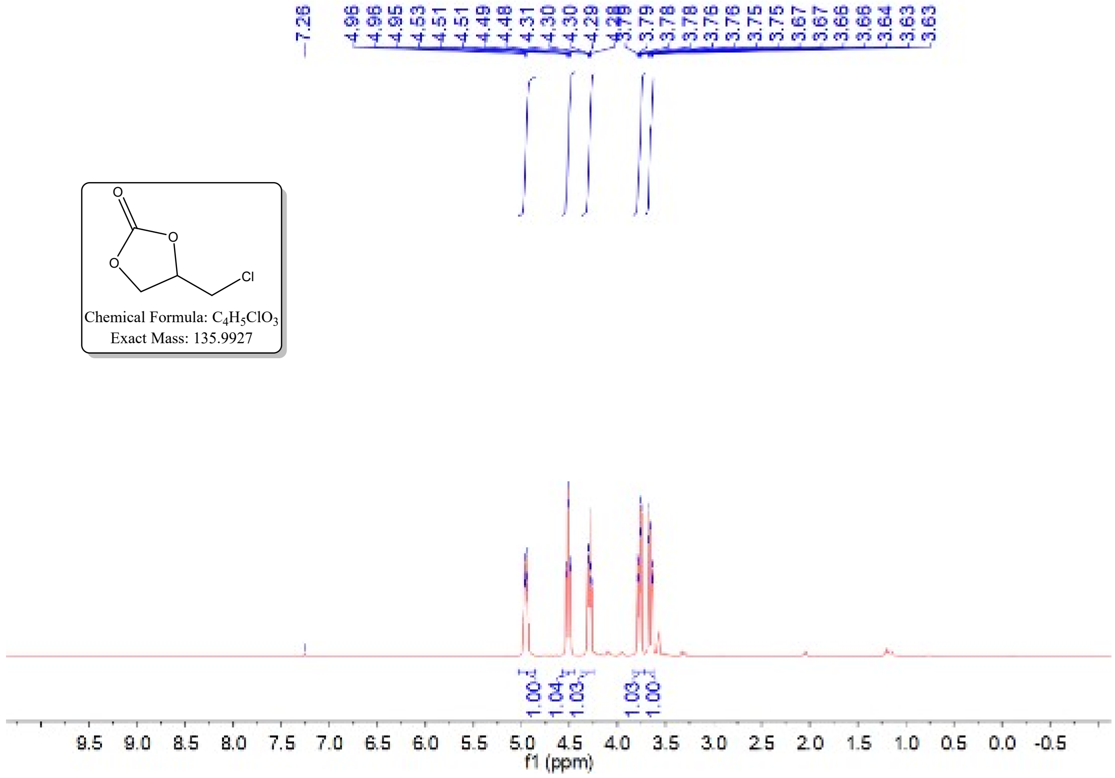
-15
f1 (ppm)


7.26
4.96 4.96 4.95 4.53 4.51 4.51 4.49 4.48 4.31 4.30 4.30 4.29 4.28 3.78 3.79 3.78 3.78 3.76 3.76 3.75 3.75 3.67 3.67 3.66 3.66 3.64 3.64 3.63 3.63
1.00 1.04 1.03 1.03 1.00
Chemical Formula: $C_4H_5ClO_3$
Exact Mass: 135.9927
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O
O
Cl
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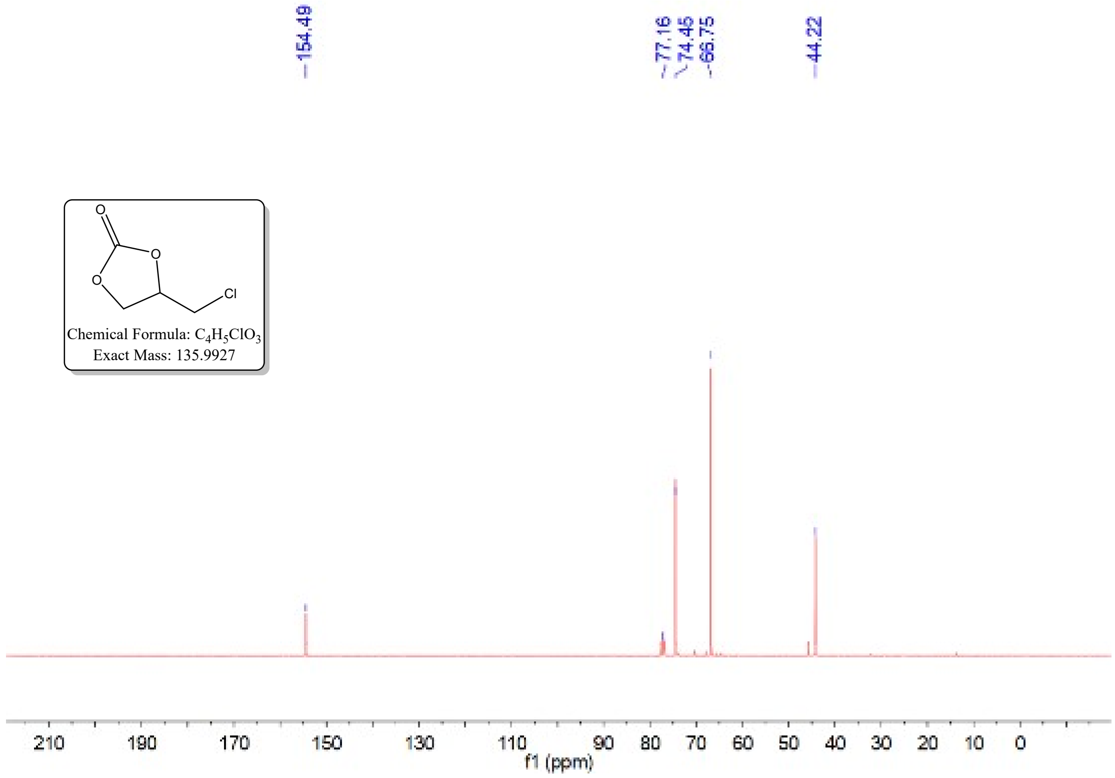
f1 (ppm)


154.49
77.16
74.45
66.75
44.22
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Exact Mass: 135.9927
O
O
O
Cl
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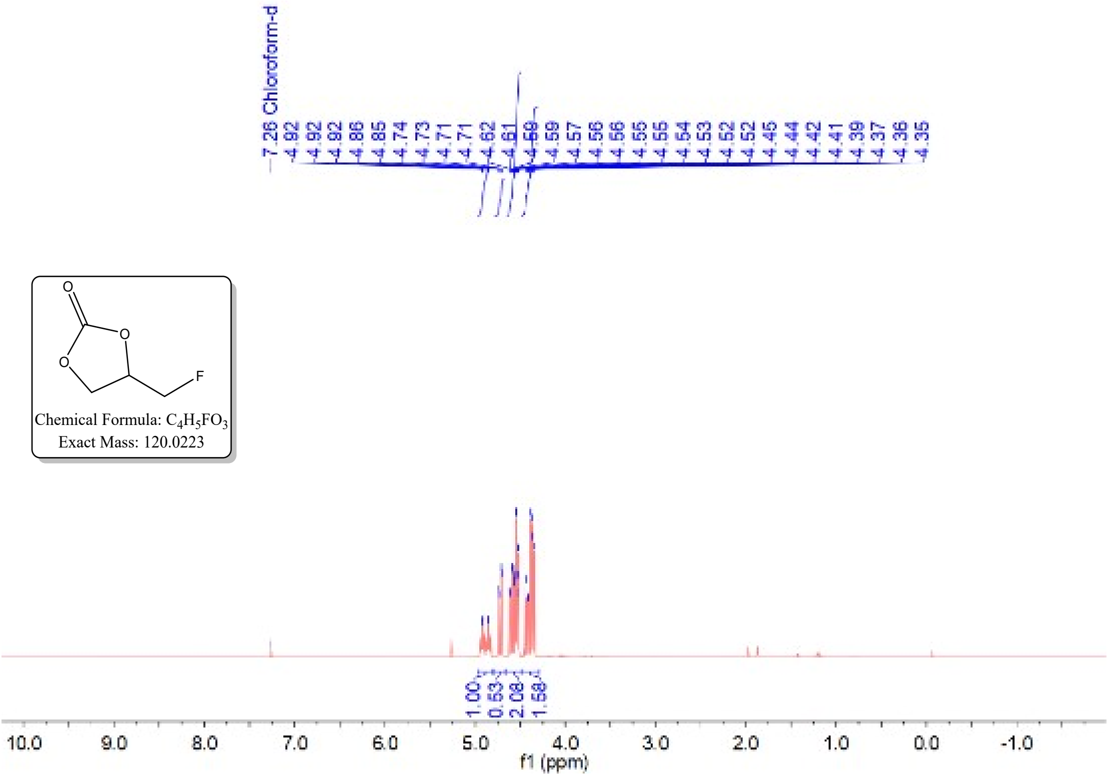
f1 (ppm)


7.26 Chloroform-d
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4.92
4.86
4.85
4.74
4.73
4.71
4.71
4.62
4.61
4.59
4.59
4.57
4.56
4.56
4.55
4.55
4.54
4.53
4.52
4.52
4.45
4.44
4.42
4.41
4.39
4.37
4.36
4.35
O
O
O
F
Chemical Formula: $C_4H_5FO_3$
Exact Mass: 120.0223
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2.08
1.58
10.0
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6.0
5.0
4.0
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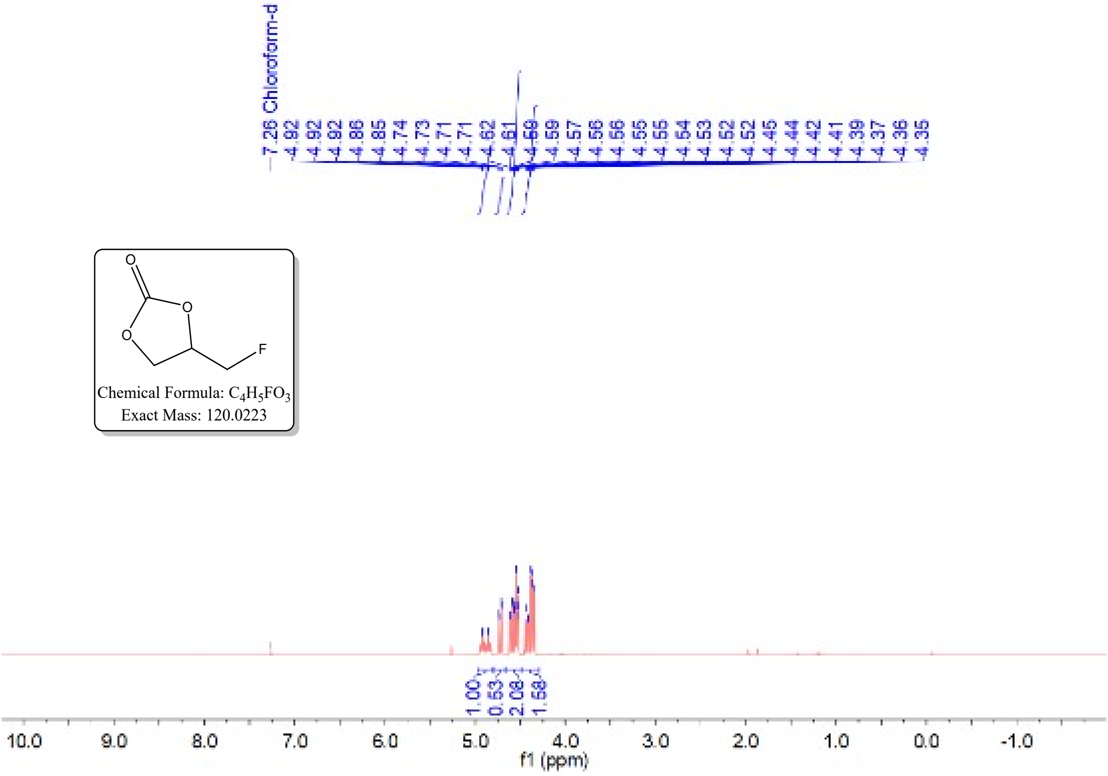
2.0
1.0
0.0
-1.0
f1 (ppm)


7.26 Chloroform-d
4.92
4.92
4.86
4.85
4.74
4.73
4.71
4.71
4.62
4.61
4.59
4.59
4.57
4.56
4.56
4.55
4.55
4.54
4.53
4.52
4.52
4.45
4.44
4.42
4.41
4.39
4.37
4.36
4.35
O
O
O
F
Chemical Formula: $C_4H_5FO_3$
Exact Mass: 120.0223
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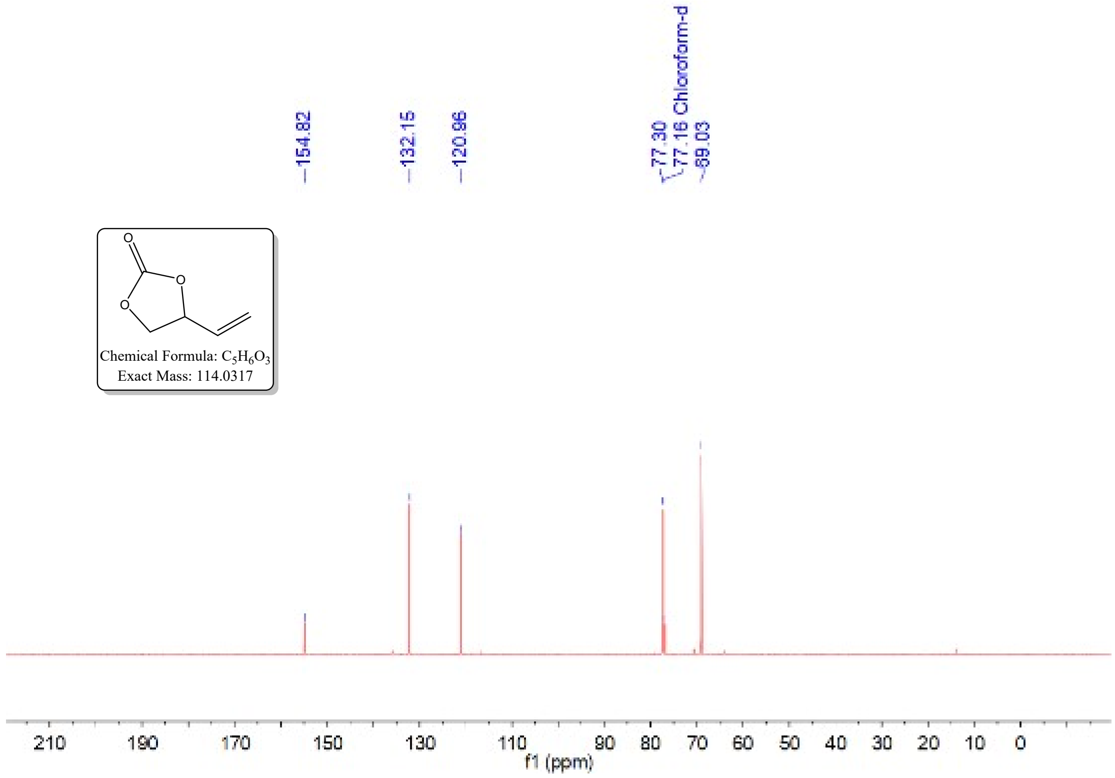
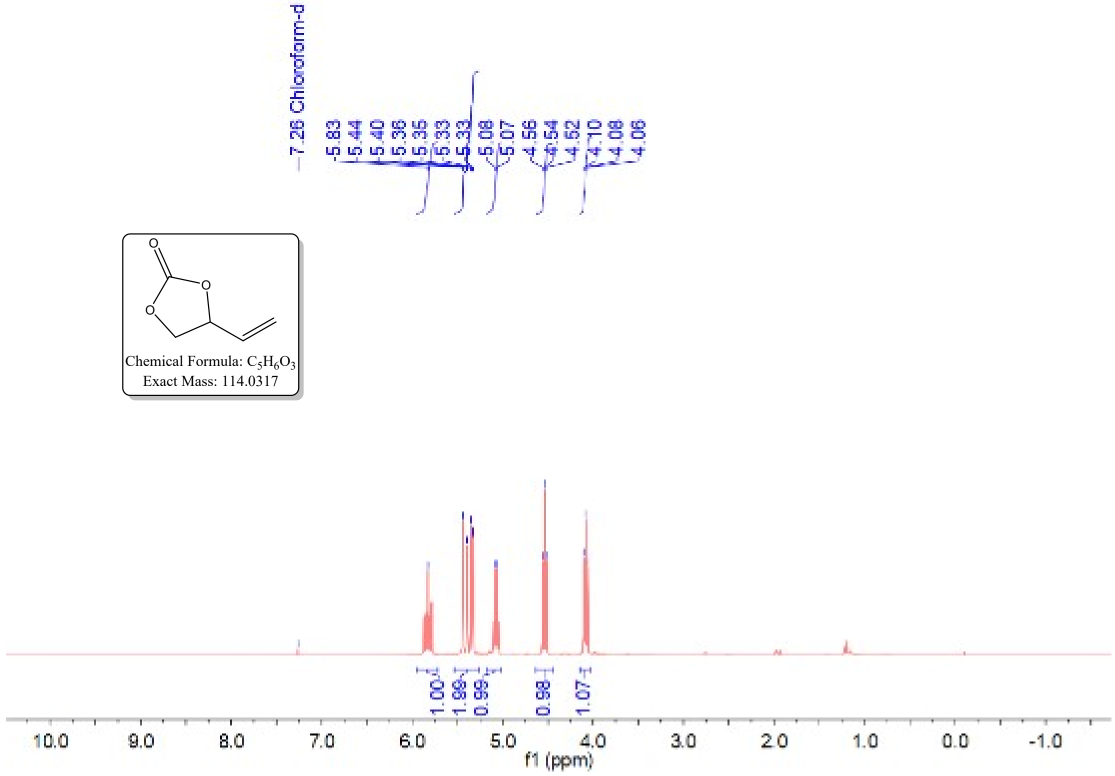
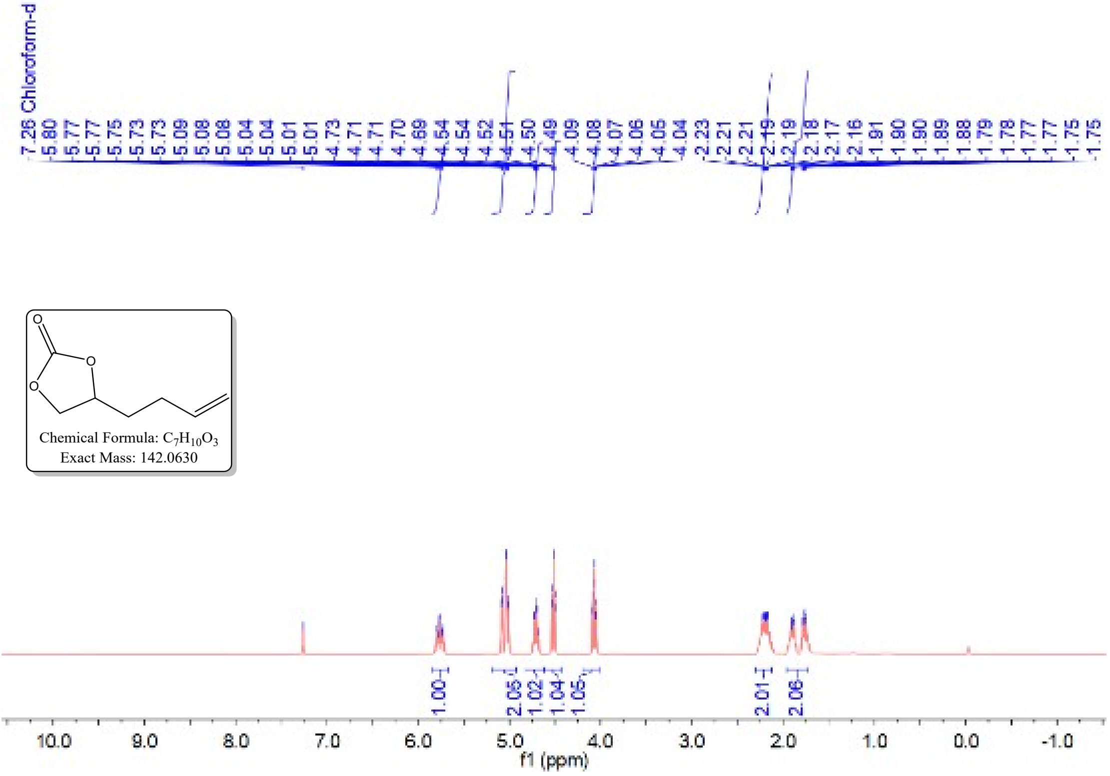
0.53
2.08
1.58
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

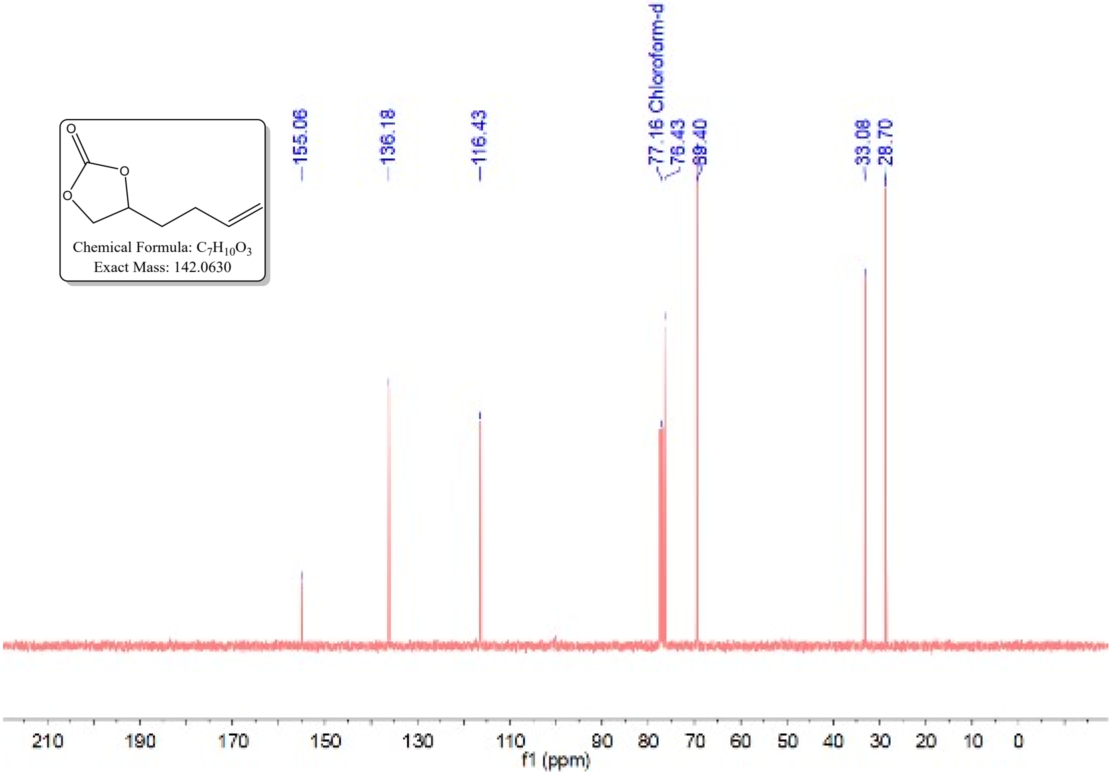


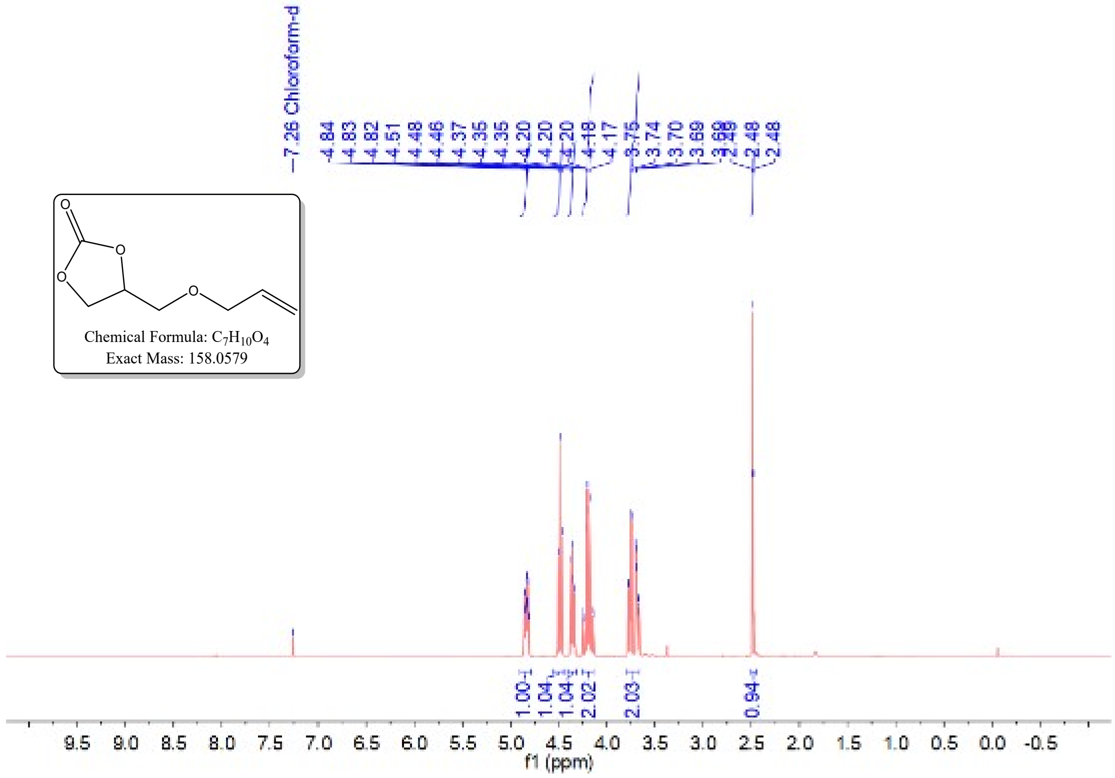
154.82
132.15
120.96
77.30
77.16 Chloroform-d
69.03
Chemical Formula: $C_5H_6O_3$
Exact Mass: 114.0317
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

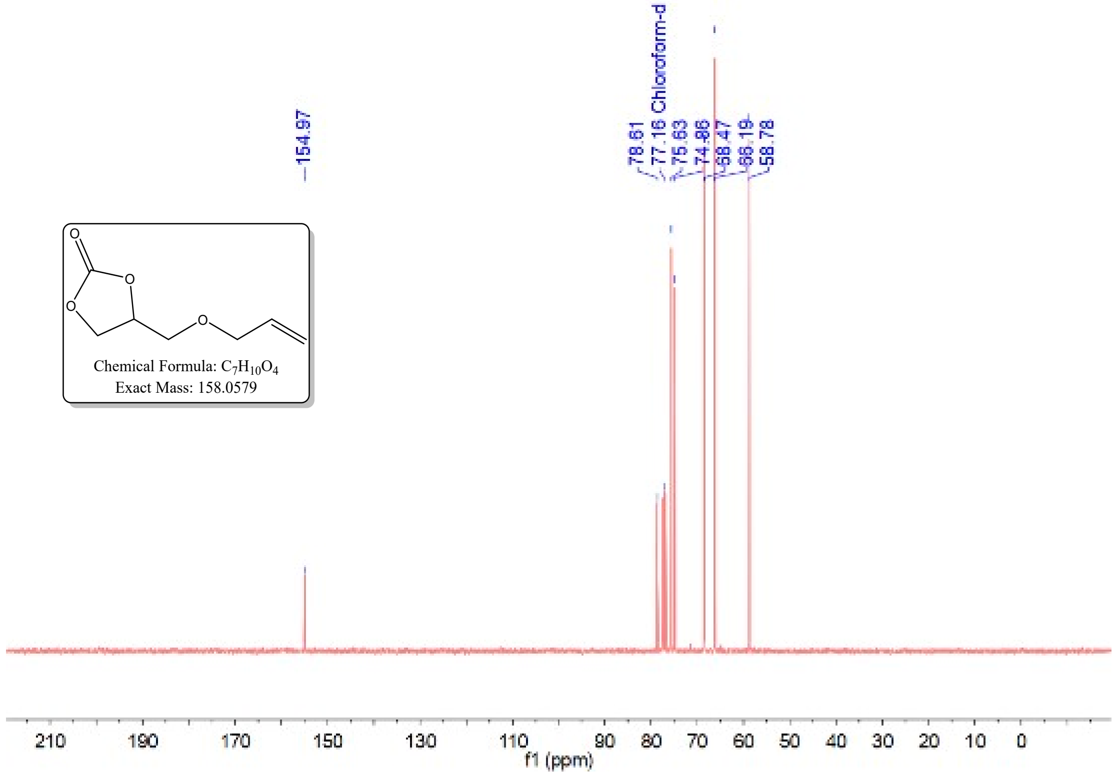


7.26 Chloroform-d
5.83
5.44
5.40
5.36
5.35
5.33
5.33
5.08
5.07
4.56
4.54
4.52
4.10
4.08
4.06
Chemical Formula: $C_5H_6O_3$
Exact Mass: 114.0317
1.00
1.99
0.99
0.98
1.07
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

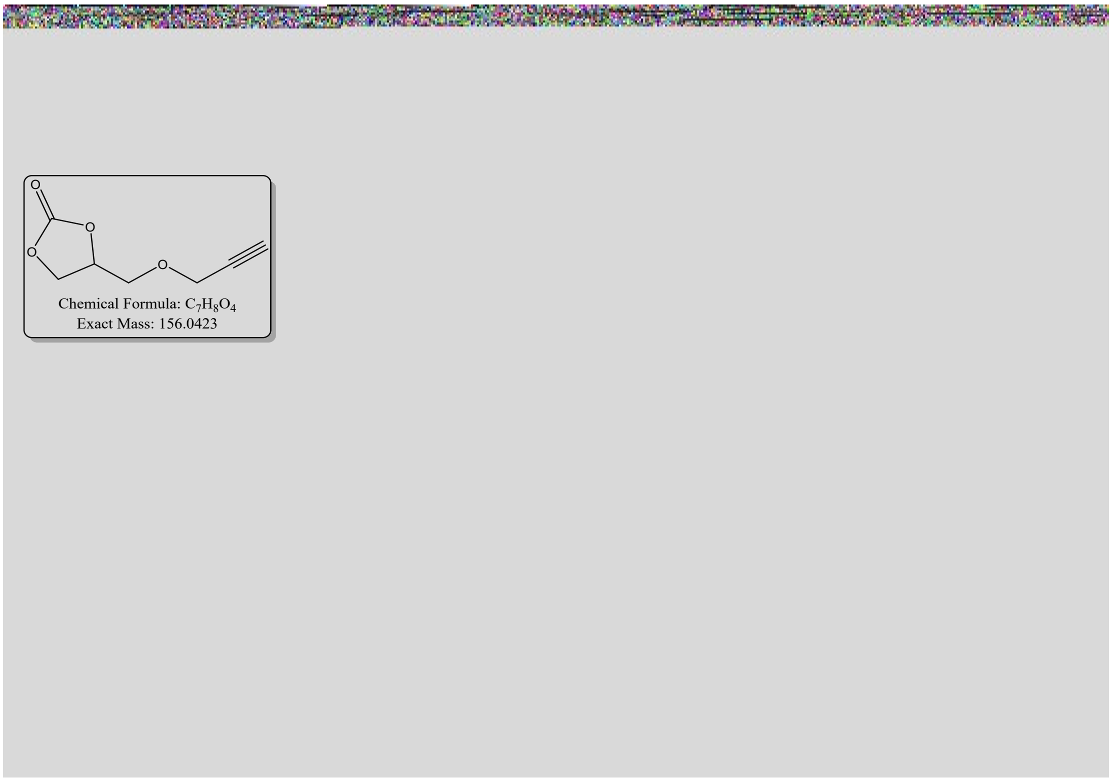

7.26 Chloroform-d
5.80
5.77
5.77
5.75
5.73
5.73
5.09
5.08
5.08
5.04
5.04
5.01
5.01
4.73
4.71
4.71
4.70
4.69
4.54
4.54
4.52
4.51
4.50
4.49
4.09
4.08
4.07
4.06
4.05
4.04
2.23
2.21
2.21
2.19
2.19
2.18
2.17
2.16
1.91
1.90
1.90
1.89
1.88
1.79
1.78
1.77
1.77
1.75
1.75
O
O
O
Chemical Formula: $C_7H_{10}O_3$
Exact Mass: 142.0630
1.00
2.05
1.02
1.04
1.05
2.01
2.06
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)

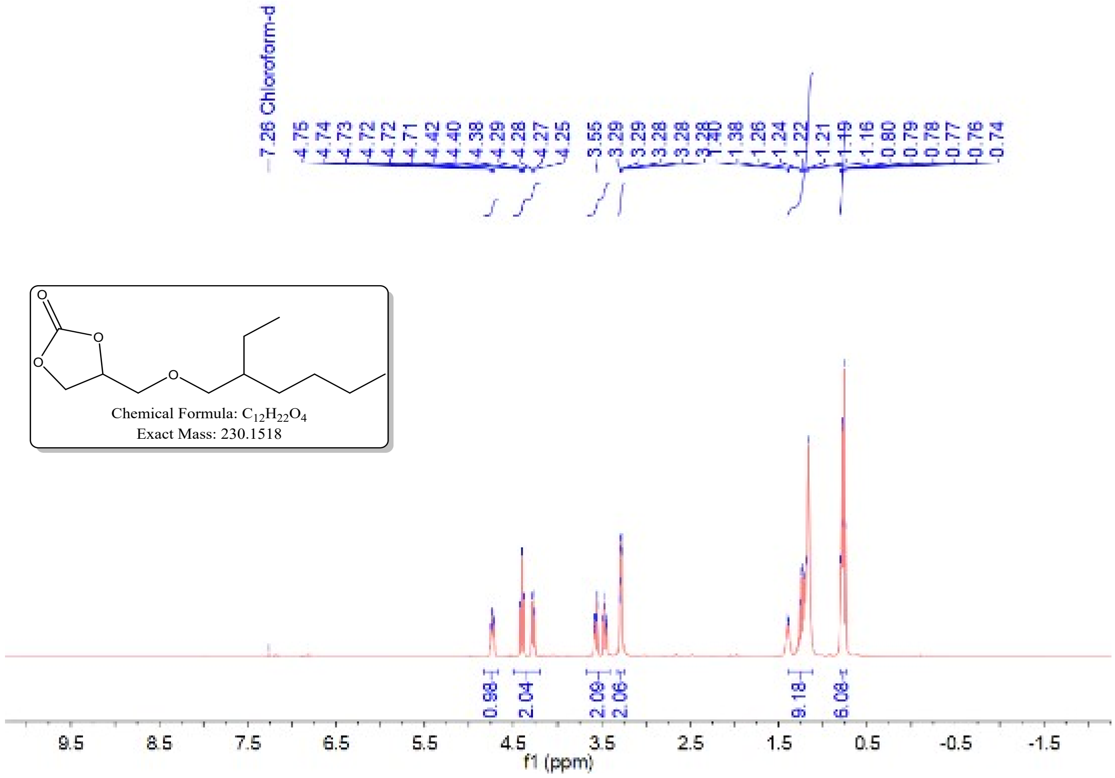

155.06
136.18
116.43
77.16 Chloroform-d
76.43
69.40
33.08
28.70
O
O
O
Chemical Formula: $C_7H_{10}O_3$
Exact Mass: 142.0630
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

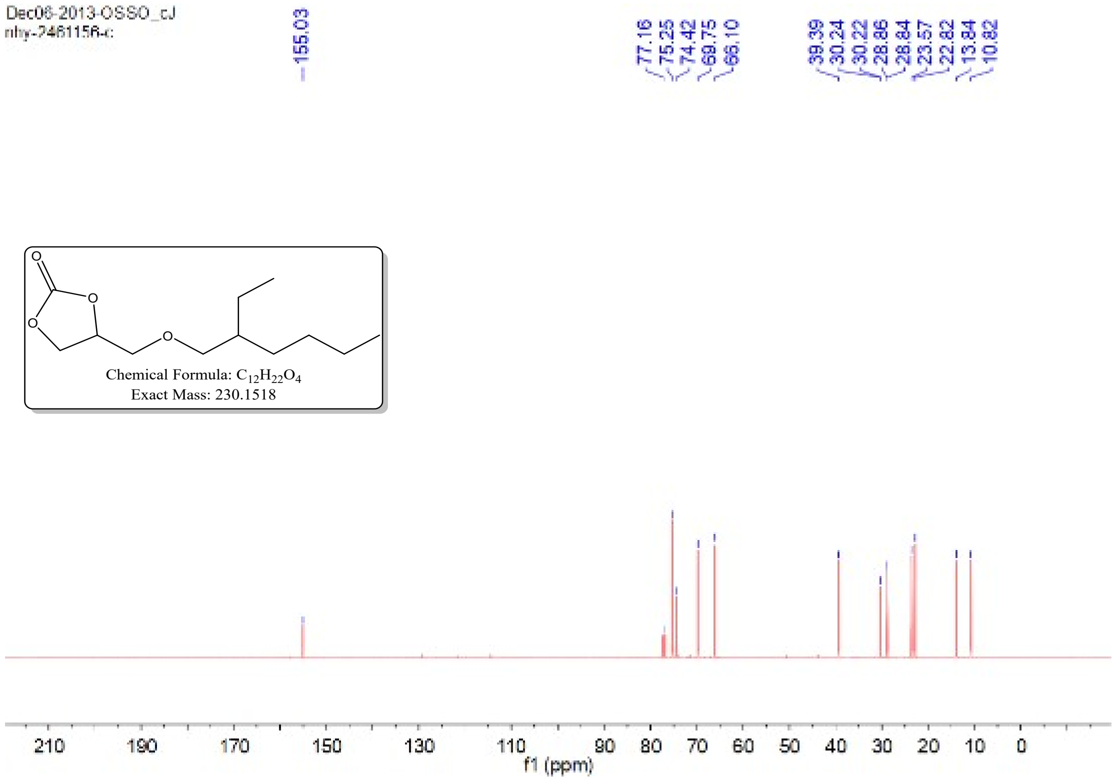

7.26 Chloroform-d
4.84
4.83
4.82
4.51
4.48
4.46
4.37
4.35
4.35
4.20
4.20
4.20
4.18
4.17
3.75
3.74
3.70
3.69
2.49
2.49
2.48
2.48
O
O
O
O
Chemical Formula: $C_7H_{10}O_4$
Exact Mass: 158.0579
1.00
1.04
1.04
2.02
2.03
0.94
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

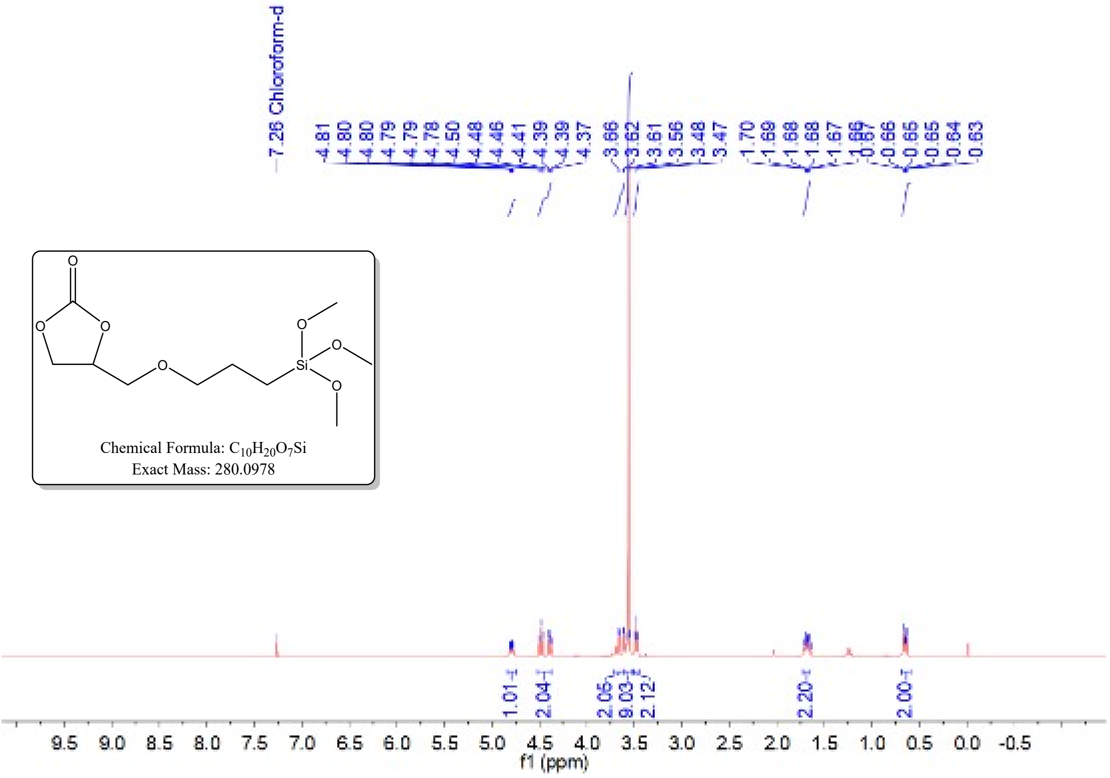

154.97
78.61
77.16 Chloroform-d
75.63
74.86
68.47
66.19
58.78
O
O
O
O
Chemical Formula: $C_7H_{10}O_4$
Exact Mass: 158.0579
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

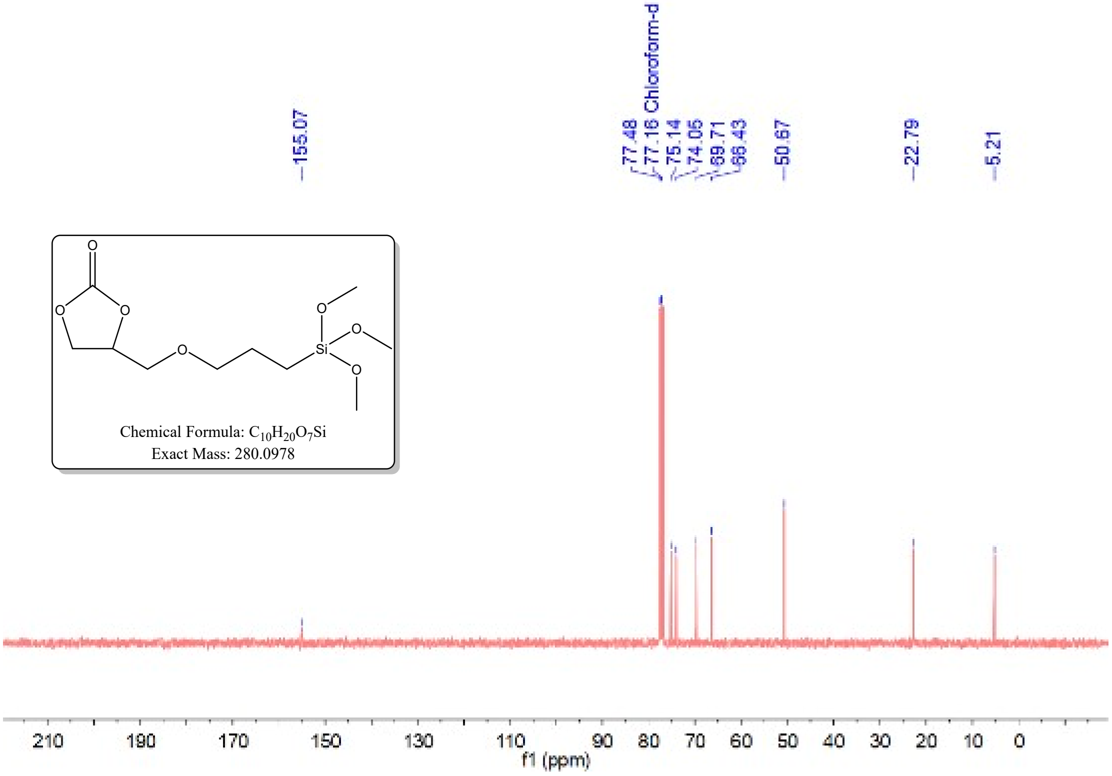

O
O
O
O
Chemical Formula: $C_7H_8O_4$
Exact Mass: 156.0423

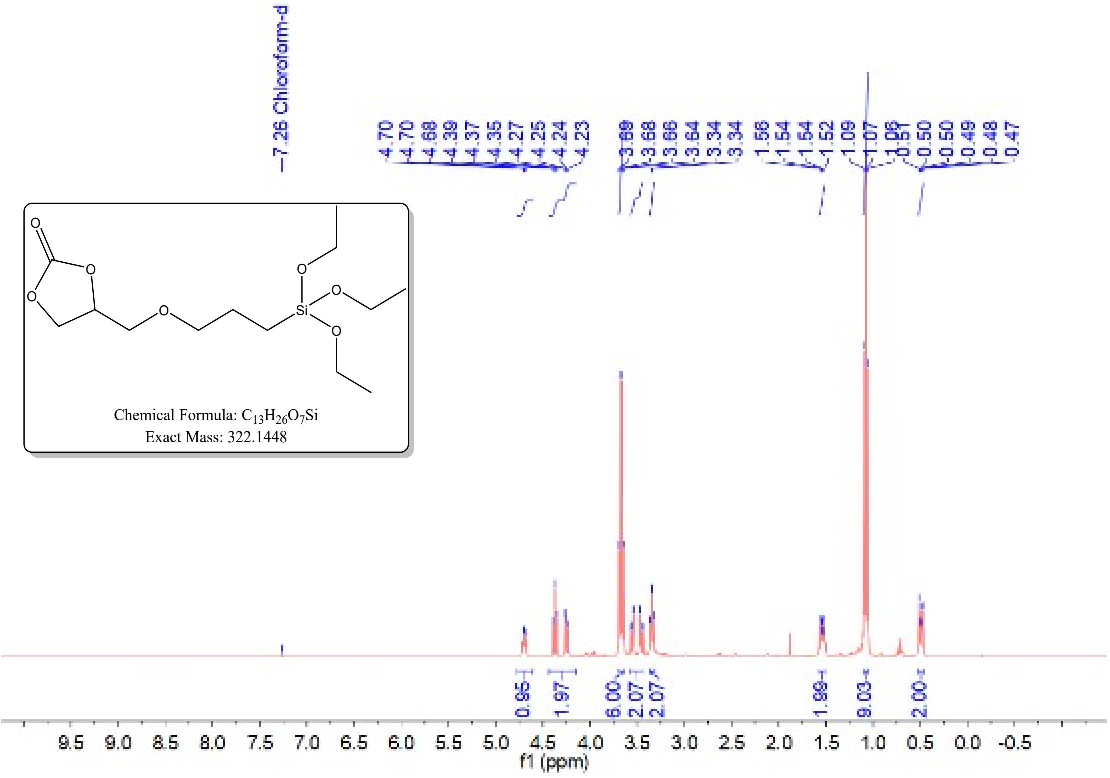

O
O
O
O
Chemical Formula: $C_7H_8O_4$
Exact Mass: 156.0423

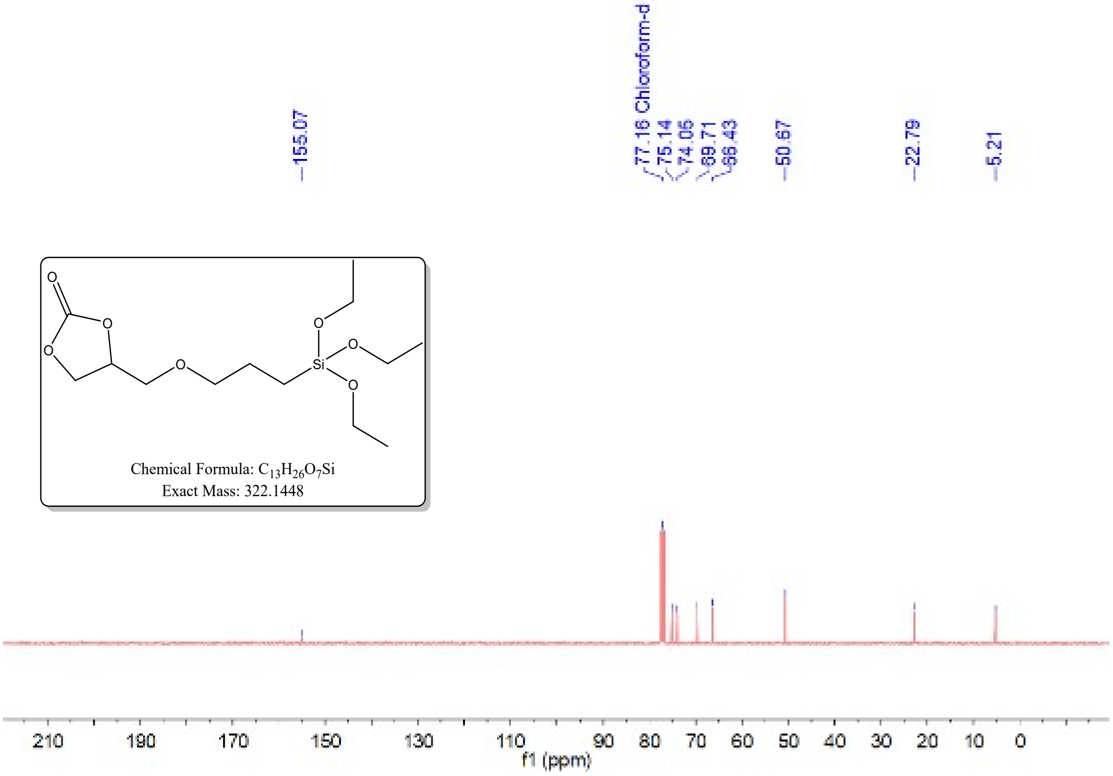

7.26 Chloroform-d
4.75
4.74
4.73
4.72
4.72
4.71
4.42
4.40
4.38
4.29
4.28
4.27
4.25
3.55
3.29
3.29
3.28
3.28
3.28
1.40
1.38
1.26
1.24
1.22
1.21
1.19
1.16
0.80
0.79
0.78
0.77
0.76
0.74
O
O
O
O
Chemical Formula: C12H22O4
Exact Mass: 230.1518
0.98
2.04
2.09
2.06
9.18
6.08
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)

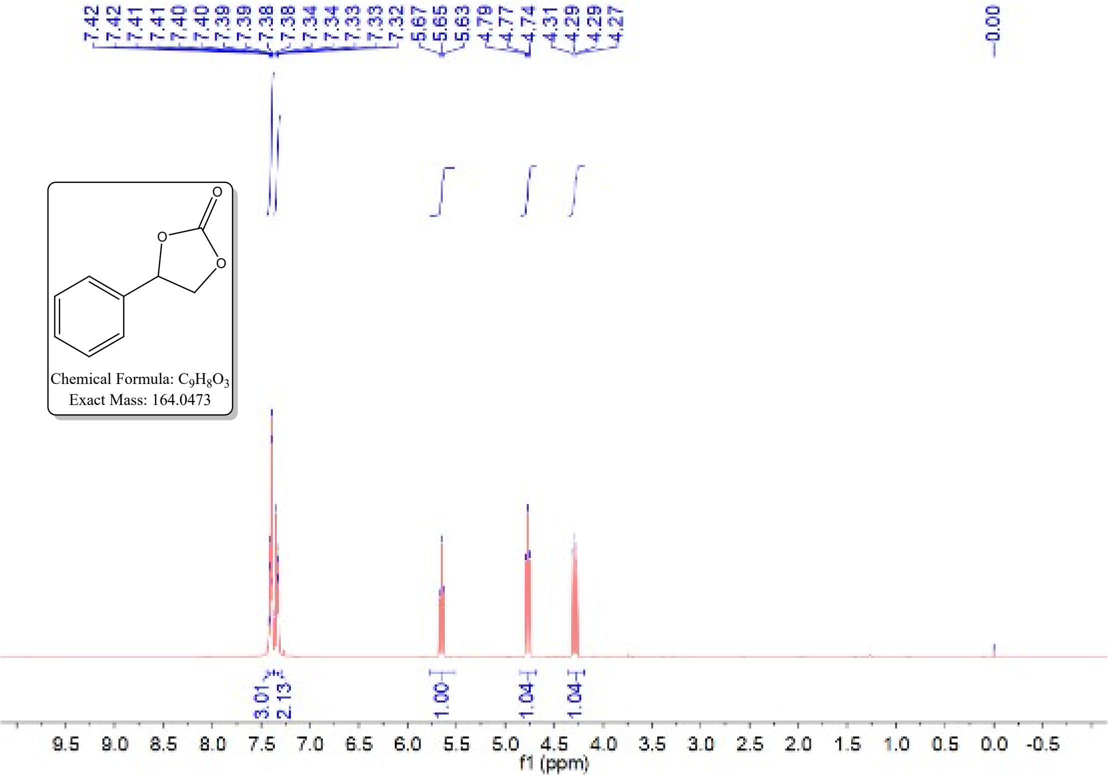

Dec06-2013-OSSO_cJ
nhy-2461156-c:
155.03
77.16
75.25
74.42
69.75
66.10
39.39
30.24
30.22
28.86
28.84
23.57
22.82
13.84
10.82
O
O
O
O
Chemical Formula: C12H22O4
Exact Mass: 230.1518
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

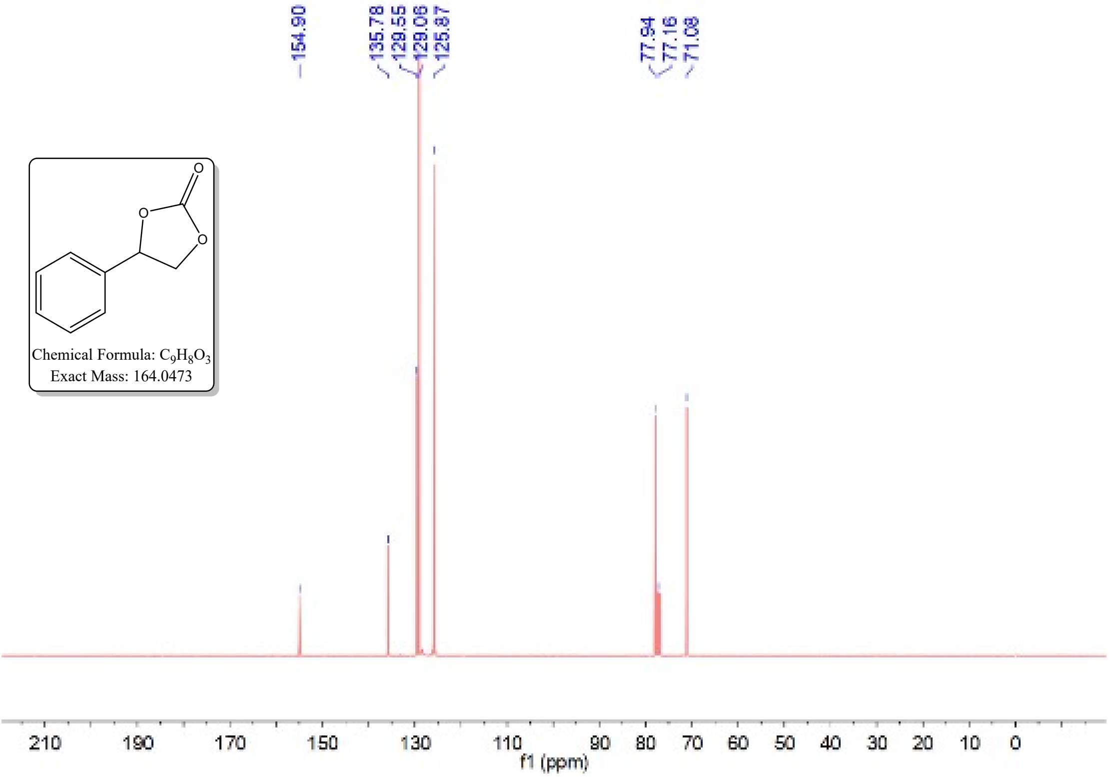

7.26 Chloroform-d
4.81
4.80
4.80
4.79
4.79
4.78
4.50
4.48
4.46
4.41
4.39
4.39
4.37
3.66
3.62
3.61
3.56
3.48
3.47
1.70
1.69
1.68
1.68
1.67
1.66
0.67
0.66
0.65
0.65
0.64
0.63
1.01
2.04
2.05
9.03
2.12
2.20
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
O
O
O
O
O
O
O
Si
Chemical Formula: C10H20O7Si
Exact Mass: 280.0978

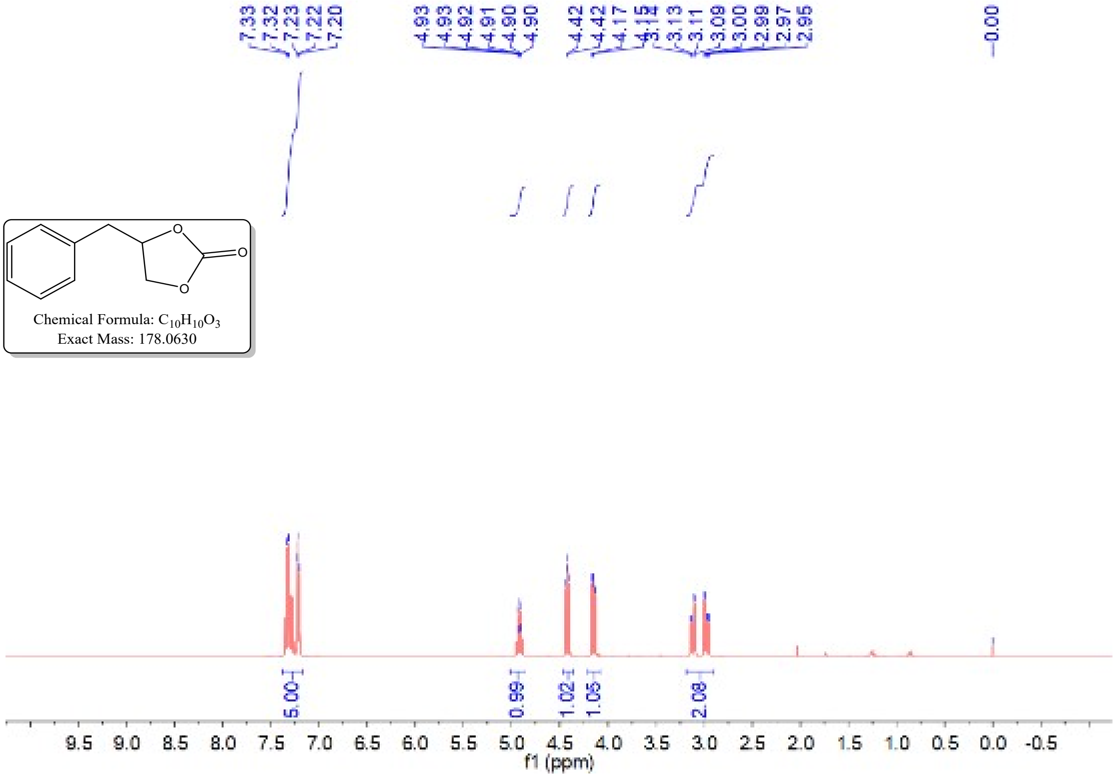

155.07
77.48
77.16 Chloroform-d
75.14
74.05
69.71
66.43
50.67
22.79
5.21
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
O
O
O
O
O
O
O
Si
Chemical Formula: C10H20O7Si
Exact Mass: 280.0978

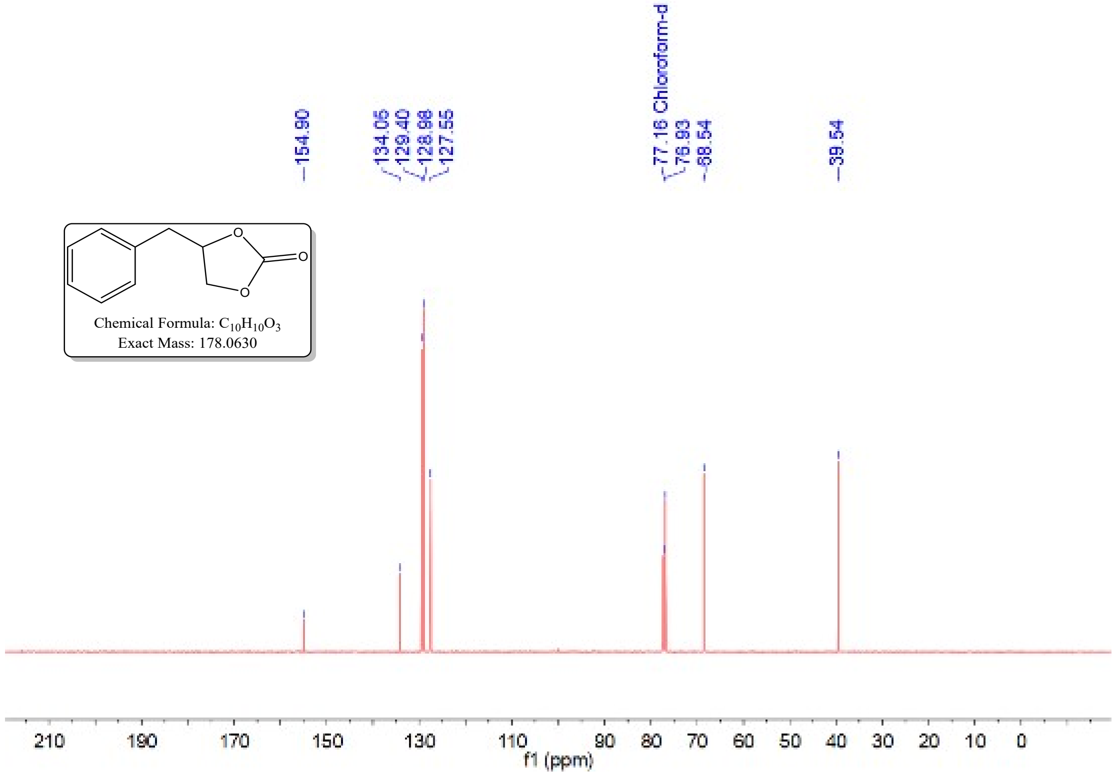

7.26 Chloroform-d
4.70
4.70
4.68
4.39
4.37
4.35
4.27
4.25
4.24
4.23
3.69
3.68
3.66
3.64
3.34
3.34
1.56
1.54
1.54
1.52
1.09
1.07
1.06
0.51
0.50
0.50
0.49
0.48
0.47
O
O
O
O
Si
O
O
O
Chemical Formula: $C_{13}H_{26}O_7Si$
Exact Mass: 322.1448
0.95
1.97
6.00
2.07
2.07
1.99
9.03
2.00
9.5
9.0
8.5
8.0
7.5
7.0
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)

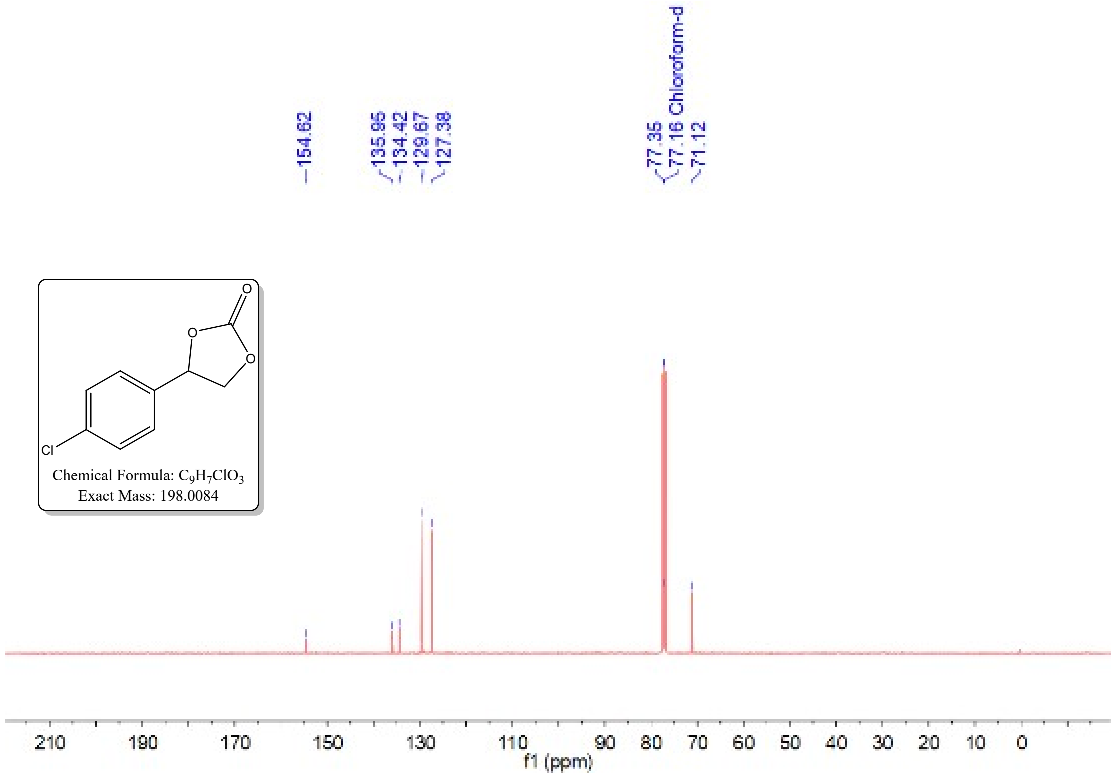

155.07
77.16 Chloroform-d
75.14
74.06
69.71
66.43
50.67
22.79
5.21
O
O
O
O
Si
O
O
O
Chemical Formula: $C_{13}H_{26}O_7Si$
Exact Mass: 322.1448
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

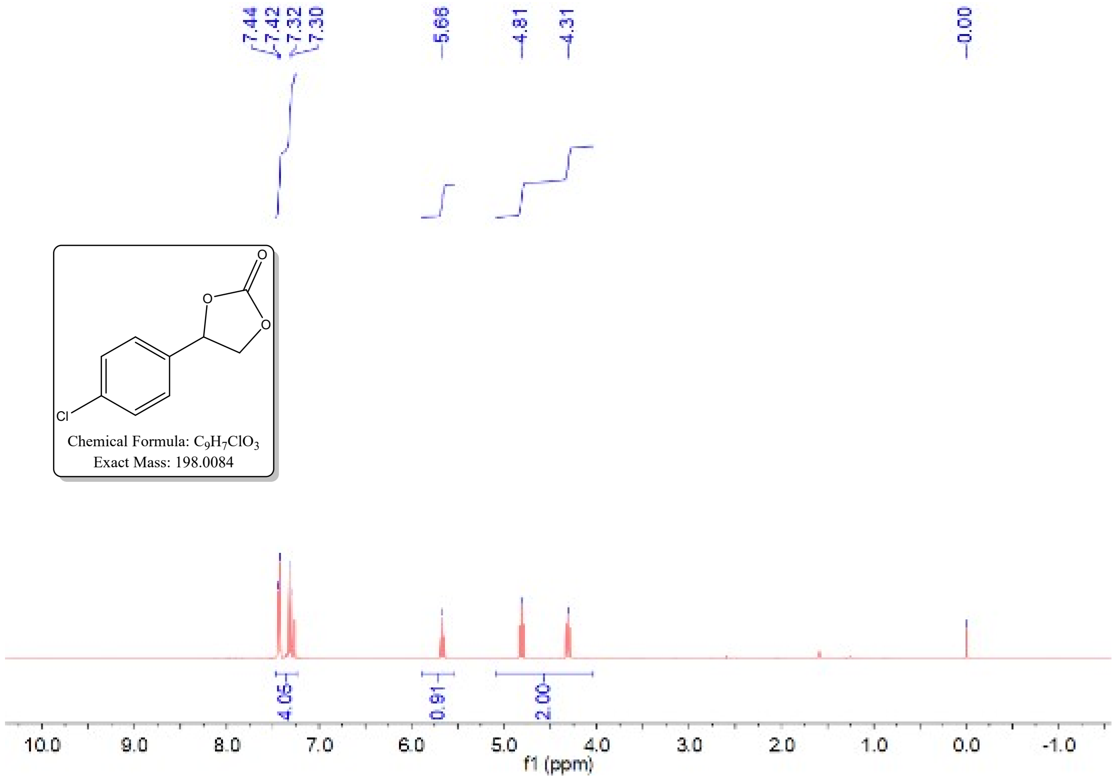

7.42
7.42
7.41
7.41
7.40
7.40
7.39
7.39
7.38
7.38
7.34
7.34
7.33
7.33
7.32
5.67
5.65
5.63
4.79
4.77
4.74
4.31
4.29
4.29
4.27
0.00
O
O
O
Chemical Formula: $C_9H_8O_3$
Exact Mass: 164.0473
3.01
2.13
1.00
1.04
1.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

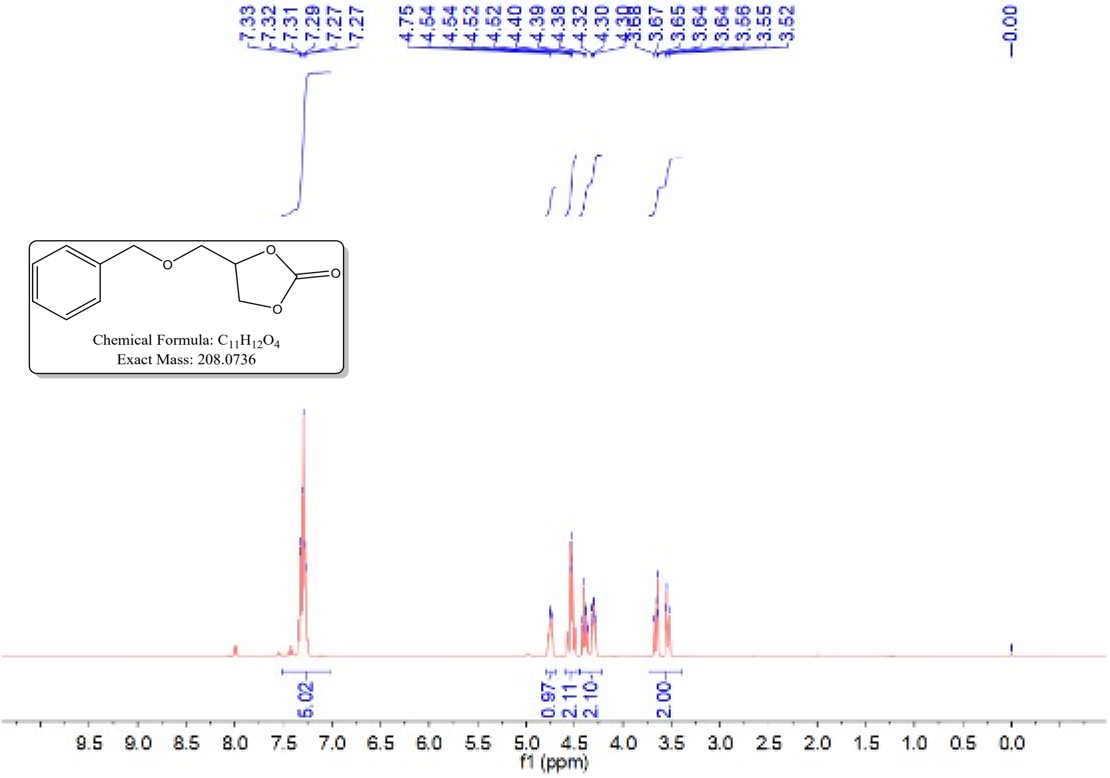

154.90
135.78
129.55
129.06
125.87
77.94
77.16
71.08
O
O
O
Chemical Formula: $C_9H_8O_3$
Exact Mass: 164.0473
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

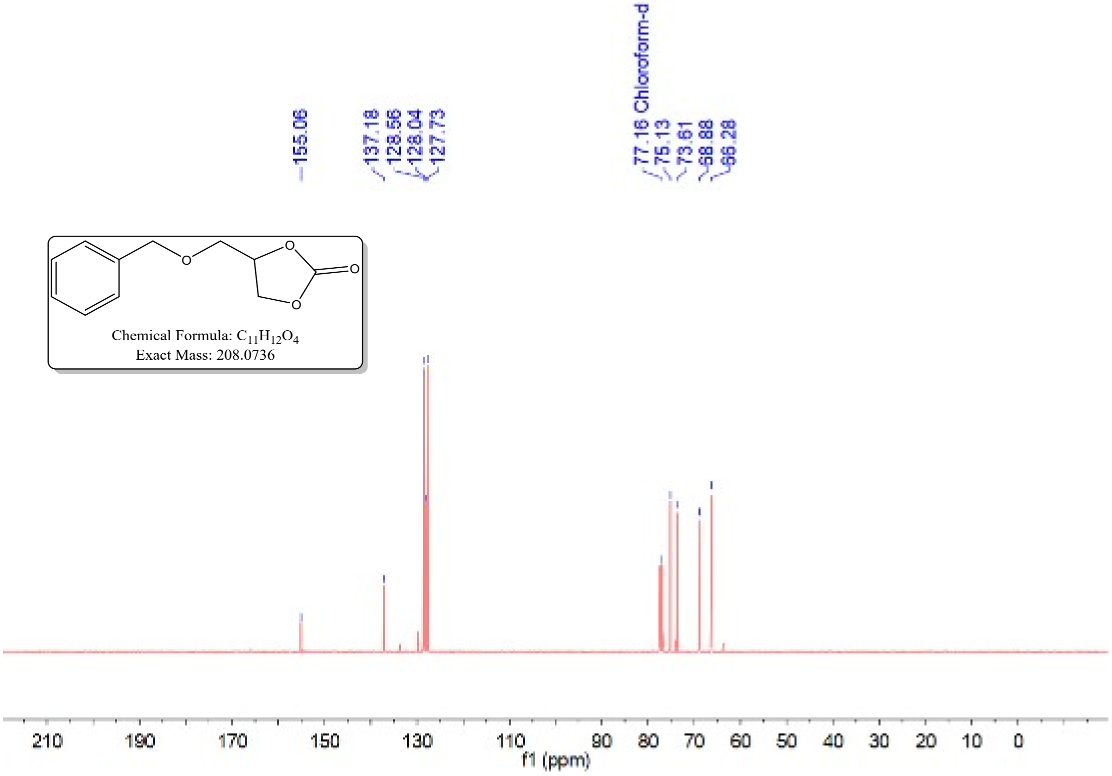

7.33
7.32
7.23
7.22
7.20
4.93
4.93
4.92
4.91
4.90
4.90
4.42
4.42
4.17
4.15
3.14
3.13
3.11
3.09
3.00
2.99
2.97
2.95
0.00
Chemical Formula: $C_{10}H_{10}O_3$
Exact Mass: 178.0630
5.00
0.99
1.02
1.05
2.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

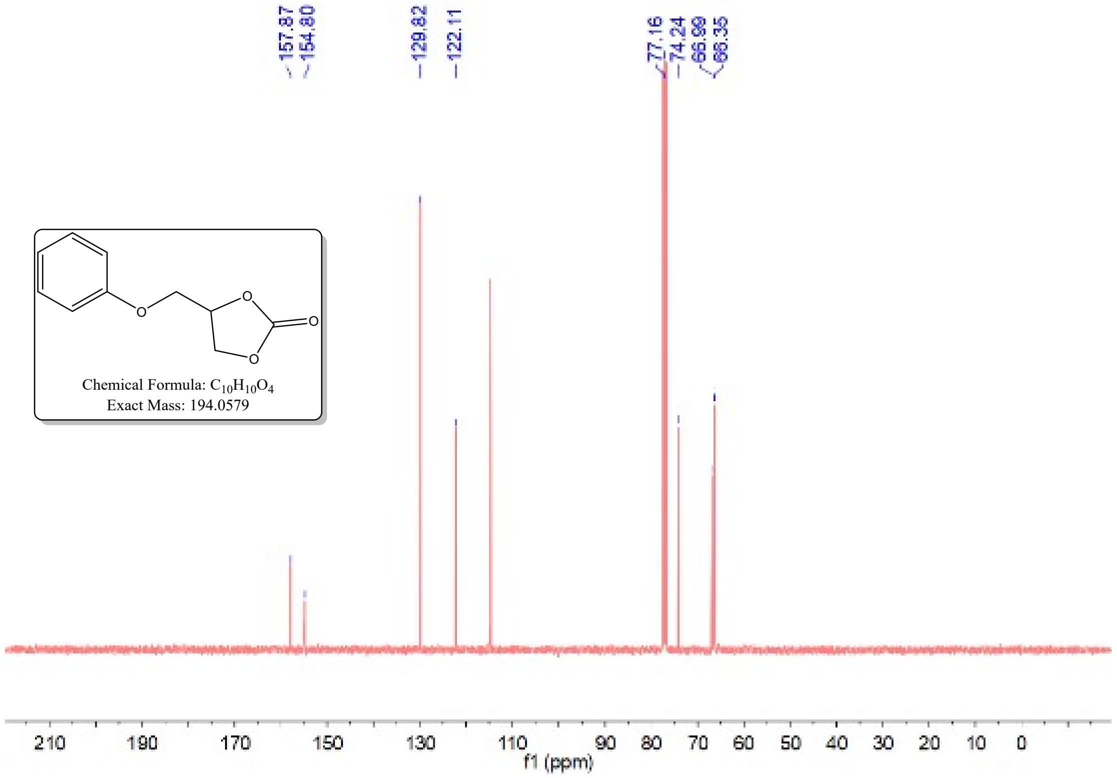

154.90
134.05
129.40
128.98
127.55
77.16 Chloroform-d
76.93
68.54
39.54
Chemical Formula: $C_{10}H_{10}O_3$
Exact Mass: 178.0630
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

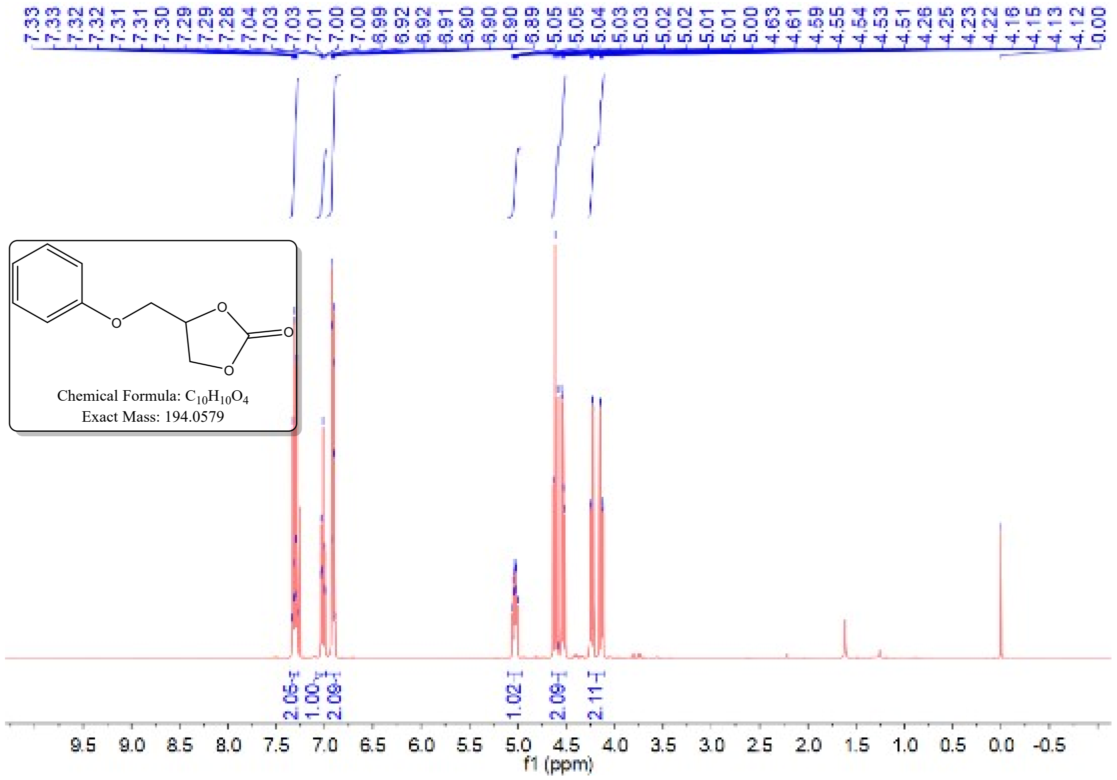

154.62
135.95
134.42
129.67
127.38
77.35
77.16 Chloroform-d
71.12
Cl
O
O
O
Chemical Formula: $C_9H_7ClO_3$
Exact Mass: 198.0084
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

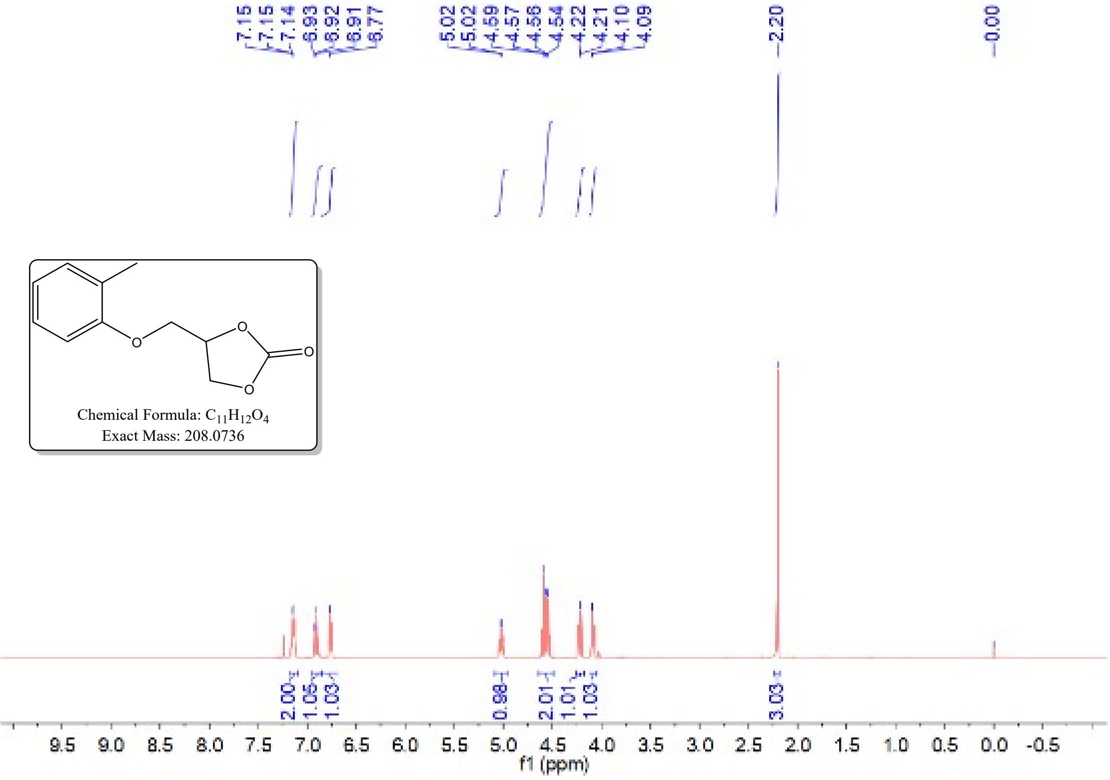

7.44
7.42
7.32
7.30
5.66
4.81
4.31
0.00
Cl
O
O
O
Chemical Formula: $C_9H_7ClO_3$
Exact Mass: 198.0084
4.05
0.91
2.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

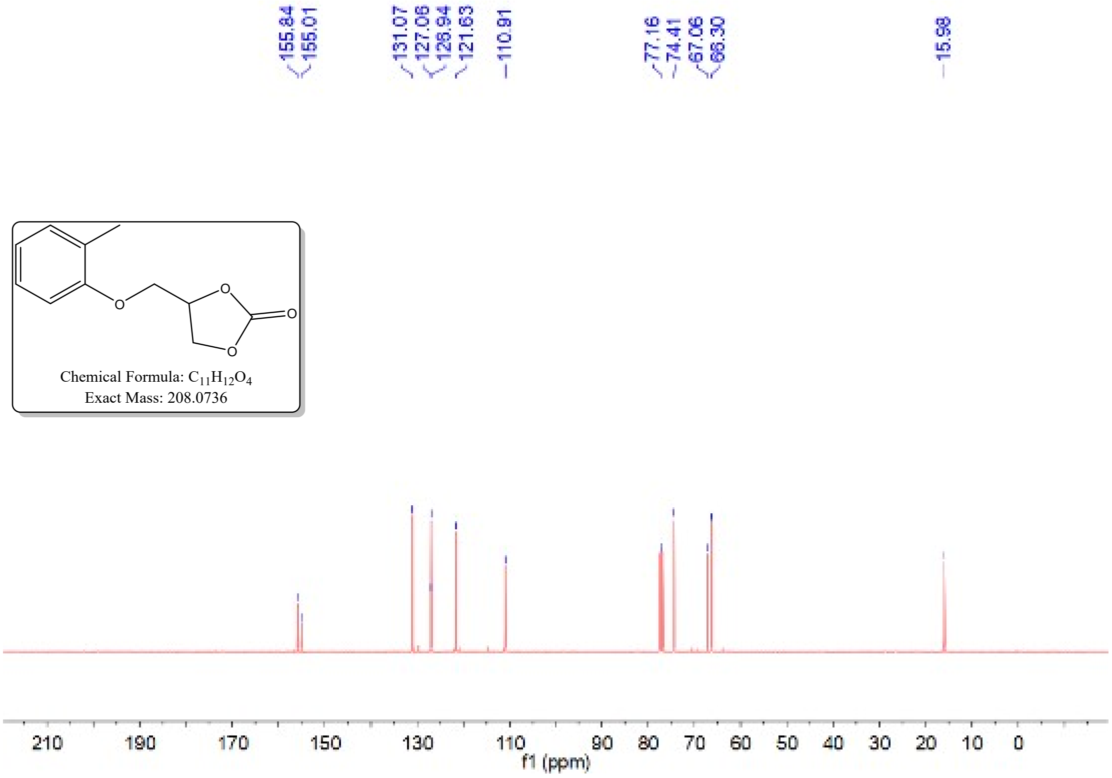

7.33
7.32
7.31
7.29
7.27
7.27
4.75
4.54
4.54
4.52
4.52
4.40
4.39
4.38
4.32
4.30
4.30
3.68
3.67
3.65
3.64
3.64
3.56
3.55
3.52
0.00
O
O
O
O
Chemical Formula: $C_{11}H_{12}O_4$
Exact Mass: 208.0736
5.02
0.97
2.11
2.10
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


155.06
137.18
128.56
128.04
127.73
77.16 Chloroform-d
75.13
73.61
68.88
66.28
O
O
O
O
Chemical Formula: $C_{11}H_{12}O_4$
Exact Mass: 208.0736
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


157.87
154.80
129.82
122.11
77.16
74.24
66.99
66.35
O
O
O
O
Chemical Formula: $C_{10}H_{10}O_4$
Exact Mass: 194.0579
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.33
7.33
7.32
7.32
7.31
7.31
7.30
7.29
7.29
7.28
7.04
7.03
7.03
7.01
7.00
7.00
6.99
6.92
6.92
6.91
6.91
6.90
6.90
6.90
6.89
5.05
5.05
5.04
5.03
5.03
5.02
5.02
5.01
5.01
5.00
4.63
4.61
4.59
4.55
4.54
4.53
4.51
4.26
4.25
4.23
4.22
4.16
4.15
4.13
4.12
0.00
O
O
O
O
Chemical Formula: $C_{10}H_{10}O_4$
Exact Mass: 194.0579
2.05
1.00
2.09
1.02
2.09
2.11
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)


7.15
7.15
7.14
6.93
6.92
6.91
6.77
5.02
5.02
4.59
4.57
4.56
4.54
4.22
4.21
4.10
4.09
2.20
0.00
Chemical Formula: $C_{11}H_{12}O_4$
Exact Mass: 208.0736
O
O
O
O
2.00
1.05
1.03
0.98
2.01
1.01
1.03
3.03
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)


155.84
155.01
131.07
127.06
126.94
121.63
110.91
77.16
74.41
67.06
66.30
15.58
Chemical Formula: $C_{11}H_{12}O_4$
Exact Mass: 208.0736
O
O
O
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)