

Supplementary Information

2-Picolinic acid as a naturally occurred hydrogen bond donor for the preparation of cyclic carbonates from terminal/internal epoxides and CO₂

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Table of Contents

I. ¹ H NMR titration of pyridine-2-carboxylic acid (3a) –epichlorhydrin (1n) solutions-----	S2
II. Details of computational studies-----	S3
III. References-----	S27
IV. ¹ H NMR, ¹³ C NMR selected spectra -----	S28

I. ^1H NMR titration of pyridine-2-carboxylic acid (**3a**) and epichlorohydrin (**1n**)

The ^1H NMR investigation was carried out in $\text{DMSO-}d_6$ because of the insolubility of pyridine-2-carboxylic acid (**3a**) in CDCl_3 . The spectra of the pure substances were measured by dissolving 0.25 mmol of each compound in 0.5 mL $\text{DMSO-}d_6$. For the spectra containing mixtures of epichlorohydrin (**1n**) and pyridine-2-carboxylic acid (**3a**), **1n** (0.25 mmol) was dissolved in 0.5 mL $\text{DMSO-}d_6$ and the suitable amount of **3a** was added in order to establish epichlorohydrin with pyridine-2-carboxylic acid molar ratios of 1:0, 1:1, 1:2 and 1:3.

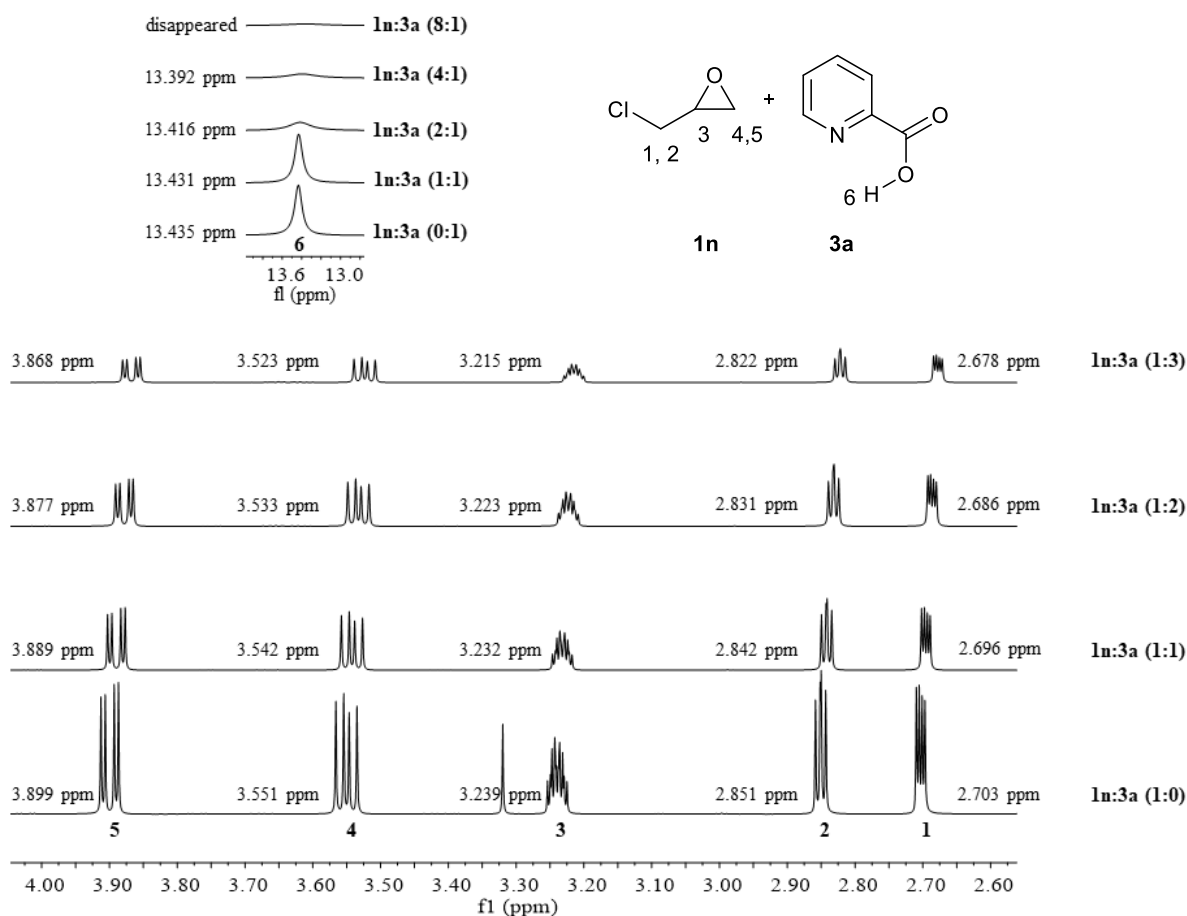


Figure S1. (a) Up field changes in the ^1H NMR spectrum of epichlorohydrin (**1n**) upon addition of pyridine-2-carboxylic acid (**3a**) at room temperature (below): (i) free **1n**, (ii) **1n:3a** = 1:1, (iii) **1n:3a** = 1:2, (iv) **1n:3a** = 1:3; (b) Up field changes of the OH proton signal of **3a** upon addition of **1n** (above): (**1n:3a** = 0:1 \rightarrow 8:1)

II. Details of computational studies

All calculations were carried out using Gaussian 16 software package.¹ The M06-2X² functional of density functional theory and Def-TZVPP^{3, 4} basis set has been used for all optimizations and frequency calculations. In addition of DFT, the gas-phase acidities were calculated using high-level compound energy calculation method G3MP2⁴ and the results are compared. The gas-phase acidities were calculated as the differences in SCF energy of the neutral and anionic form of the investigated molecules. The intrinsic reaction coordinate (IRC) calculation is carried out, in addition to the presence of one imaginary frequency, for the transition state structures. The implicit solvation effects were included using the PCM solvation model⁵ with standard parameters of cyclohexanone ($\epsilon = 15.619$) and styrene oxide using parameters $\epsilon = 16.0$, $n^2 = 1.865956$; these parameters have been used previously for styrene oxide as the media for similar reactions.⁶ The solvation effects calculated using single point energy at M06-2X/Def2-QZVPP level of theory and thermal correction to free energy is taken from the gas phase optimization. Interestingly, both solvents (cyclohexanone and styrene oxide) showed very similar results which can be contributed to the similar dielectric constant. The noncovalent interaction plots were obtained using NCI plot software.⁷ Snapshots were generated with the Visual Molecular Dynamics (VMD) package.⁸

i) Conformational studies of 3a

Pyridine-2-carboxylic acid can exhibit two different conformations (conformer **I** and **II**) with respect to the rotation of acidic OH group. Conformer **I** that holds an intramolecular hydrogen bond with the pyridine nitrogen atom is more stable by ~ 2.9 kcal/mol (ΔG). Note that the zwitterionic form (conformer **III**) is around 19.6 kcal/mol less stable, thus we did not consider conformer **III** for the mechanistic studies

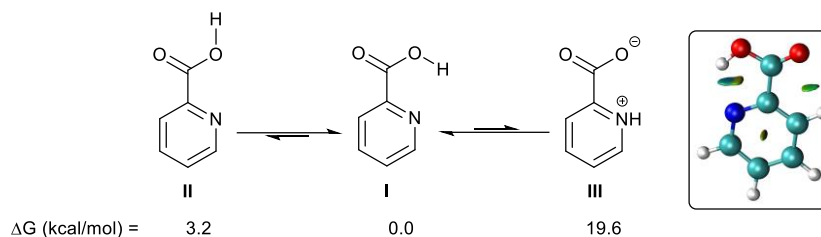


Figure S2. The relative energies (ΔG , in kcal/mol) of the two conformers and zwitterion of 2-picolinic acid calculated at the M06-2X/Def2-TZVPP level of theory; The NCI plot of most stable conformer showing intramolecular hydrogen-bond interaction.

ii) **Potential energy surfaces of the reaction of propylene oxide (PO) and CO₂ by different pyridine carboxylic acid regioisomers**

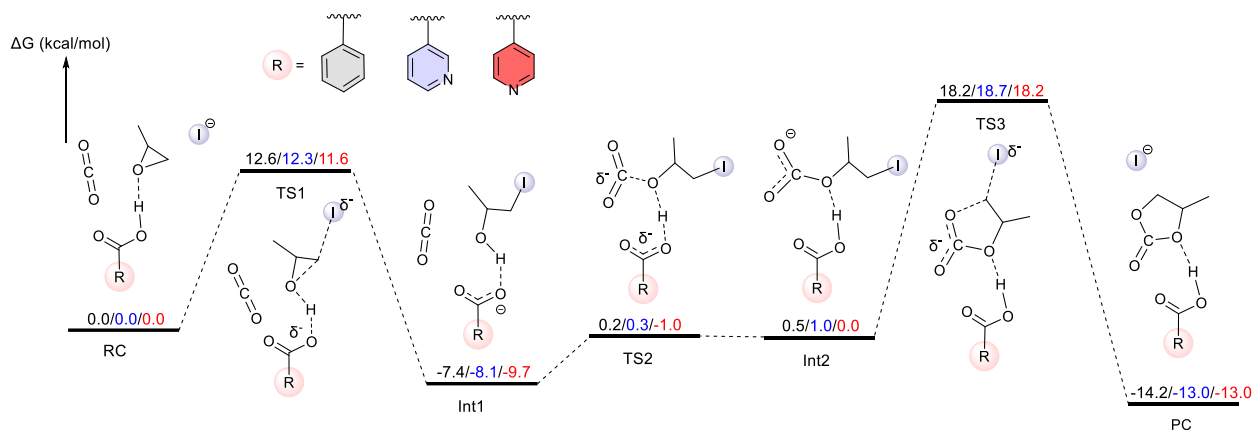


Figure S3. The relative energy profile (ΔG , in kcal/mol) of benzoic acid (**3f**) and pyridine-3 (**3b**), and -4- (**3c**) carboxylic acid-catalyzed [3 + 2] cycloaddition of propylene epoxide (PO) and CO₂ calculated at the M06-2X/Def2-TZVPP level of theory. Energies of reactants in comparison to the energies of complexed reactants were used to define the relative energies.

3a: $\Delta G_{\text{Int 1}} = 2.6$ kcal/mol; $\Delta G_{\text{RDS}} = 19.2$ kcal/mol

3b: $\Delta G_{\text{Int 1}} = -8.1$ kcal/mol; $\Delta G_{\text{RDS}} = 26.8$ kcal/mol

3c: $\Delta G_{\text{Int 1}} = -9.7$ kcal/mol; $\Delta G_{\text{RDS}} = 27.9$ kcal/mol

	3f		3a		3b		3c	
	CYC	SO	CYC	SO	CYC	SO	CYC	SO
RC	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS1	19.5	19.5	23.4	23.5	19.3	19.3	18.3	18.4
Int1	0.6	0.6	3.0	3.0	0.3	0.3	-1.3	-1.3
TS2	9.5	9.5	13.7	13.7	9.6	9.6	8.3	8.3
Int2	3.7	3.7	9.8	9.8	4.7	4.7	3.9	3.9
TS3	23.5	23.5	22.6	22.6	24.5	24.5	24.0	24.0
PC	-12.6	-12.6	-12.4	-12.4	-11.3	-11.3	-11.5	-11.5

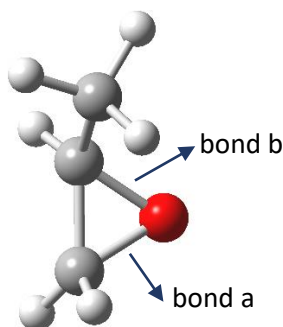
Table S1. The relative energy (ΔG , in kcal/mol) of benzoic acid (**3f**) and pyridine-2 (**3a**), -3- (**3b**) and -4- (**3c**) carboxylic acid-catalyzed [3 + 2] cycloaddition of propylene epoxide (PO) and CO₂ calculated at the M06-2X/Def2-QZVPP+PCM(solvent)//M06-2X/Def2-TZVPP level of theory; solvent = cyclohexanone (CYC) and styrene oxide (SO).

iii) The dimerization energy of 3a–c, and 3f:

	Benzoic acid (3f)	Pyridine-2-carboxylic acid (3a) ^b	Pyridine-3-carboxylic acid (3b)	Pyridine-4-carboxylic acid (3c)
M06-2X	-17.4	-8.0	-17.1	-17.1

Table S2. Dimerization energy ($\Delta E + \text{ZPE}$, in kcal/mol = $E_{\text{dimer}} - E_{\text{monomer} \times 2}$). All data are from the optimized structures at the M06-2X/Def2-TZVPP level of theory

iv) Gas-phase bond length changes upon hydrogen bond interaction between propylene oxide (PO) and different acids



	bond a (Å)	bond b (Å)	Complexation Energy
Propylene oxide (PO)	1.417	1.417	
Benzoic acid (3f)	1.429	1.431	-10.3
Pyridine-2-carboxylic acid (3a)	1.421	1.423	-5.7
Pyridine-3-carboxylic acid (3b)	1.430	1.432	-10.6
Pyridine-4-carboxylic acid (3c)	1.430	1.432	-10.8

Table S3. Gas-phase bond length changes upon hydrogen bond interaction between epoxide and different acids (the bonds **a** and **b** shown in the 2D structure of epoxide) and complexation energy ($\Delta E + \text{ZPE}$, in kcal/mol = $E_{\text{complex}} - E_{\text{epoxide+acid}}$). All data are from the optimized structures at the M06-2X/Def2-TZVPP level of theory.

v) **Gas-phase acidities of 3a–c, and 3f employed in the cycloaddition of CO₂ to epoxides**

	Benzoic acid (3f)	Pyridine-2- carboxylic acid (3a)^b	Pyridine-3- carboxylic acid (3b)	Pyridine-4- carboxylic acid (3c)
M06-2X	348.4	353.2	343.8	341.5
G3MP2	339.1	343.7	334.5	332.5
Experimental ^a	340.1 ± 2.2	---	334.4 ± 2.0	

Table S4. Gas-phase acidities (kcal/mol) using M06-2X/Def2-TZVPP and G3MP2 methods.

^aThe experimental gas-phase acidity values are obtained from the NIST Database (<http://webbook.nist.gov>).

^bCalculated using the most stable conformer (conformer I).

vi) **Cartesian Coordinates (M06-2X/Def2-TZVPP)**

Benzoic Acid (3f)

RC

-1 1

C	-4.08623300	-0.74439500	-0.06621300
C	-4.66511100	-1.79656600	0.63447100
C	-6.03828100	-1.97954500	0.60108500
H	-4.01884700	-2.45665200	1.19676400
H	-6.48817300	-2.79850600	1.14632300
H	-1.14410500	0.52011500	-0.60355000
C	1.20229600	-0.37497700	-0.47204700
C	0.97379200	0.32695900	0.78584500
H	0.24355400	-0.10966300	1.45861100
O	0.35771700	0.79912500	-0.43582100
H	2.15182900	-0.23830900	-0.97397600
H	0.65763600	-1.29250100	-0.65687000
C	2.01210800	1.22599000	1.37487500
H	1.54490100	2.04134700	1.92941700
H	2.65216700	0.64962300	2.04251800
H	2.65865900	1.61818700	0.59156200
I	4.98467800	-0.66844800	-0.18981800
C	-6.25911200	-0.06017400	-0.83431300
H	-6.88060300	0.61522400	-1.40703100
C	-2.59822900	-0.58098700	-0.00518100
O	-2.15500800	0.44919600	-0.70056200
O	-1.88886800	-1.33111300	0.62217900

C	-1.20597400	3.06364100	0.19710700
O	-1.17277100	2.68231200	1.28752100
O	-1.25674900	3.47968600	-0.87836700
C	-4.88437500	0.12466400	-0.80192700
H	-4.41929300	0.93636800	-1.34298400
C	-6.83614100	-1.11085700	-0.13365200
H	-7.90864500	-1.25364600	-0.16031300

TS1

-1 1

C	-3.33711400	-0.89997700	-0.07608300
C	-3.58328300	-2.19104500	0.37676400
C	-4.88628000	-2.64410200	0.51731500
H	-2.73418500	-2.81869900	0.61155900
H	-5.07454200	-3.64943600	0.87127400
H	-0.68663800	1.10291600	-0.70389700
C	1.77301200	0.33713200	-0.83200200
C	1.33165900	1.16863300	0.27452000
H	0.80011000	0.61985600	1.05260600
O	0.47679900	1.60120700	-0.77380800
H	2.41903900	0.76833600	-1.57532000
H	1.23060400	-0.57111800	-1.03419000
C	2.25331400	2.23100300	0.80415400
H	1.69057000	2.95837700	1.38971100
H	3.01889400	1.77203400	1.42893000
H	2.74146500	2.74242900	-0.02636400
I	3.94774300	-1.09389600	0.00581000
C	-5.70711500	-0.51731200	-0.25057000
H	-6.53514700	0.13508700	-0.49613200
C	-1.90727300	-0.43729300	-0.21736300
O	-1.78352800	0.78918100	-0.61999400
O	-0.98734200	-1.19197800	0.03623100
C	-1.35786900	3.40938900	0.30620800
O	-1.05446500	3.04501300	1.36056900
O	-1.68875200	3.83508700	-0.71486300
C	-4.40256100	-0.06389400	-0.38988700
H	-4.19114400	0.93569700	-0.74342000
C	-5.95034600	-1.80703700	0.20353100
H	-6.96797000	-2.16003900	0.31268600

Int1

-1 1

C	-3.11080800	-0.77412600	-0.18747500
C	-3.27921300	-2.12524000	0.09367500
C	-4.53980400	-2.63460500	0.37339900
H	-2.39879600	-2.75400300	0.08606200
H	-4.66292800	-3.68803100	0.59320300
H	-0.16551000	1.55475600	-1.00720400
C	2.11032200	0.09455000	-0.95836400
C	1.56343200	1.25524600	-0.13606800
H	0.97617000	0.84105100	0.69063600
O	0.73640900	1.99118100	-1.00338900
H	2.72351900	0.44854200	-1.78240600
H	1.29049300	-0.53497700	-1.28832600
C	2.63411700	2.18981000	0.39454100
H	2.15691000	3.01408800	0.92365400
H	3.31716000	1.68081400	1.07320100
H	3.20544900	2.60104000	-0.44092000
I	3.38411900	-1.23953900	0.17163000
C	-5.48386200	-0.44235300	0.09029300
H	-6.34409300	0.21580900	0.08786300
C	-1.71736100	-0.22563200	-0.49284100
O	-1.66021000	1.01767800	-0.70183100
O	-0.78225400	-1.03457400	-0.51109000
C	-1.12841600	3.33122100	0.58400000
O	-0.68903900	2.81675000	1.52221500
O	-1.58625000	3.92905100	-0.29164900
C	-4.22070800	0.06337600	-0.18734900
H	-4.06523900	1.11044200	-0.41084900
C	-5.64606200	-1.79320800	0.37202500
H	-6.63052200	-2.18892100	0.58964500

TS2

-1 1

C	3.61017200	-0.40680700	-0.06407100
C	4.03726400	-1.65237100	-0.50941300
C	5.38907300	-1.96345900	-0.52865900
H	3.28642800	-2.35921500	-0.83609900
H	5.71680800	-2.93520100	-0.87573300
H	0.66974000	1.38370500	0.37428000
C	-1.79773900	0.01785700	-0.44296500
C	-1.43940600	0.84089000	0.78968700

H	-2.32310500	1.40315300	1.10257200
O	-0.46063200	1.76542500	0.39002600
H	-0.97537200	-0.62744000	-0.73764100
H	-2.11149300	0.66965300	-1.25046900
C	-0.91746900	-0.00420100	1.94218500
H	-0.56836400	0.65138800	2.73943200
H	-1.70110200	-0.65210700	2.33422900
H	-0.08557100	-0.62256800	1.60321800
I	-3.49518200	-1.27851100	-0.11236900
C	5.90020700	0.21957100	0.34057200
H	6.62665000	0.95153900	0.67005000
C	2.12711200	-0.09023000	-0.05175600
O	1.83985300	1.06639500	0.41716900
O	1.33570200	-0.92970500	-0.46585800
C	-0.99020400	3.25169600	-0.47765600
O	-2.17829400	3.20520000	-0.50556800
O	0.01378600	3.81586600	-0.74596400
C	4.54691100	0.52856200	0.36062500
H	4.19294600	1.49221000	0.69964100
C	6.32323400	-1.02680100	-0.10317800
H	7.37881300	-1.26771500	-0.11861100

Int2

-1 1

C	3.68246900	-0.39992400	-0.06168700
C	4.06635900	-1.67858500	-0.44873900
C	5.40761000	-2.02885700	-0.46103100
H	3.29428500	-2.37920300	-0.73658600
H	5.70439300	-3.02507500	-0.76211100
H	0.98386100	1.39524700	0.33181700
C	-1.88713000	0.05795900	-0.45560800
C	-1.52373700	0.88579500	0.76949200
H	-2.39199300	1.47346100	1.07022100
O	-0.49812800	1.77121300	0.36922900
H	-1.06947700	-0.59401900	-0.74807600
H	-2.20053200	0.71102800	-1.26170100
C	-0.99508600	0.05486400	1.92481900
H	-0.65348700	0.71676800	2.72001500
H	-1.77150500	-0.59964000	2.31945100
H	-0.15691000	-0.55876700	1.59103700
I	-3.58222100	-1.23284300	-0.10742000
C	5.98898200	0.17972300	0.29606700
H	6.73875000	0.90535200	0.58304500
C	2.21780600	-0.05500400	-0.06187100

O	1.97753500	1.15048100	0.37834800
O	1.38350400	-0.85231300	-0.43504600
C	-0.88379800	3.00013400	-0.41022800
O	-2.09003300	3.10935900	-0.57873600
O	0.11330200	3.62856700	-0.70855700
C	4.64632600	0.53058500	0.31045100
H	4.32937700	1.52167100	0.60250500
C	6.37070200	-1.09898600	-0.08821300
H	7.41850600	-1.37082500	-0.09894100

TS3

-1 1

C	3.47058900	-0.35643200	-0.05328300
C	3.70954900	-1.43953300	-0.89142100
C	4.96092700	-2.03465200	-0.91653900
H	2.89858300	-1.79579100	-1.51202800
H	5.14547500	-2.87832400	-1.56834000
H	1.05903600	1.62791800	0.74422300
C	-2.16641700	0.83180800	-0.49146300
C	-1.62520800	1.30436900	0.85201900
H	-2.40614800	1.90108000	1.33172300
O	-0.50486000	2.15912800	0.61052000
H	-1.48619900	0.34922000	-1.17361400
H	-3.13104800	1.13325000	-0.83967900
C	-1.10981800	0.24647800	1.81225800
H	-0.53915600	0.74794400	2.59494000
H	-1.92685400	-0.31102600	2.25698500
H	-0.46100900	-0.45162900	1.28355100
I	-3.35023800	-1.42579200	-0.02625200
C	5.74053600	-0.46397800	0.73182500
H	6.53295900	-0.08287700	1.36244900
C	2.10189200	0.25738800	-0.05711600
O	1.97371600	1.23799500	0.81765100
O	1.22403500	-0.13012700	-0.78845200
C	-0.60154900	2.93887400	-0.57201500
O	-1.61850400	2.64231400	-1.24589100
O	0.29559900	3.73379100	-0.74138100
C	4.48763800	0.13191500	0.75920300
H	4.28609300	0.97674000	1.40206200
H	6.95550300	-2.01069300	-0.12430200
C	5.97777100	-1.54684300	-0.10450200

PC

-1 1

C	-4.07424500	-0.37087800	-0.00158700
C	-4.51985500	-0.81103200	1.23984000
C	-5.80379000	-1.31344000	1.37563900
H	-3.84368200	-0.74902400	2.08145700
H	-6.15077400	-1.65615900	2.34117800
H	-1.44526200	0.90223800	-1.31506700
C	1.36080000	0.80466900	0.96282000
C	1.24612100	0.57694300	-0.54214100
H	2.15882100	0.88984400	-1.04683400
O	0.19424600	1.51563200	-0.90642800
H	0.80976700	0.05564600	1.53072500
H	2.39421100	0.85847000	1.28901200
C	0.86140100	-0.82050700	-0.94876500
H	0.70143500	-0.87506700	-2.02567300
H	1.68750300	-1.48233200	-0.68755800
H	-0.04498000	-1.13158200	-0.42768300
I	4.61431800	-0.80093200	0.03174200
C	-6.20003900	-0.93617900	-0.96878000
H	-6.85552300	-0.98472300	-1.82798000
C	-2.68192100	0.16239900	-0.10275400
O	-2.35732000	0.54099000	-1.33450800
O	-1.93412000	0.23162500	0.84026600
C	-0.02915300	2.38328600	0.10966800
O	0.71810700	2.07672800	1.16342200
O	-0.79194500	3.29488600	0.03354200
C	-4.91487100	-0.43282400	-1.10750500
H	-4.55511600	-0.08530100	-2.06519100
H	-7.64742700	-1.76854800	0.37690000
C	-6.64437900	-1.37626500	0.27090700

Pyridine-2-carboxylic acid (3a)**RC**

-1 1

C	2.40596600	-1.98348900	-0.00639700
C	2.54819200	-3.35950900	-0.10107000
C	1.39394500	-4.12786500	-0.13016000
C	0.16308800	-3.49496300	-0.06240300
H	3.53940600	-3.78592900	-0.14914900
H	1.45572600	-5.20591400	-0.20521000
H	-0.76492800	-4.04884200	-0.08349000

H	2.45251000	0.42794900	0.10487200
C	-0.02516900	1.35242600	1.02913900
C	-0.18178700	1.43114700	-0.41271800
H	-0.19705400	0.49324700	-0.95236600
O	1.09131200	1.71041400	0.20152600
H	-0.40439100	2.16494600	1.63730100
H	0.05033500	0.38284900	1.50107900
C	-0.88541700	2.58050500	-1.06264500
H	-0.42668200	2.82855100	-2.02065400
H	-1.92464600	2.29134500	-1.22348000
H	-0.86325000	3.46048800	-0.41739500
I	-3.37705200	-0.37787400	0.03421500
C	0.12263700	-2.10788200	0.03342200
H	-0.82898900	-1.58111500	0.08667400
N	1.23003900	-1.37068500	0.05928200
C	3.63142800	-1.10321400	0.02750300
O	3.40947100	0.19617800	0.09413600
O	4.74235800	-1.56623400	-0.00358500
C	1.78046200	4.26071400	0.05902700
O	2.21473100	4.12781300	-1.00243500
O	1.36280000	4.47024600	1.11676300

TS1

-1 1

C	-2.95371200	-0.85898400	-0.04254200
C	-3.83451900	-1.93520700	0.00667600
C	-3.31024700	-3.20657400	0.16116900
C	-1.93444400	-3.35954100	0.25950900
H	-4.89376000	-1.74324200	-0.07794000
H	-3.96385800	-4.06870200	0.20355700
H	-1.48144000	-4.33389300	0.37891600
H	-1.62219000	1.42693800	-0.12254400
C	1.02392600	0.49686000	-0.52759000
C	0.58681300	1.01394100	0.76653400
H	0.07293200	0.27478100	1.38379900
O	-0.27322200	1.76804500	-0.03760200
H	1.67609700	1.12236200	-1.11547900
H	0.38611600	-0.20756200	-1.02920200
C	1.57793400	1.82850200	1.56231200
H	1.05232400	2.41692900	2.31515900
H	2.30182000	1.17457000	2.04864200
H	2.11871800	2.50857400	0.90026600
I	2.87949800	-1.33425200	-0.15673800

C	-1.13630600	-2.22549100	0.19892500
H	-0.05353700	-2.29312400	0.26697300
N	-1.63932200	-1.00270900	0.05117700
C	-3.51758800	0.54423300	-0.21278200
O	-2.68958700	1.53602600	-0.22815700
O	-4.72058600	0.66956300	-0.32586800
C	0.24952700	4.31852800	-0.24782200
O	-0.33119300	4.57803100	0.71673000
O	0.85963200	4.16822300	-1.21880400

Int1

-1 1

C	-2.97219000	-0.31958000	0.13261300
C	-4.09101200	-1.07471700	-0.22503600
C	-3.91818500	-2.24787800	-0.93392000
C	-2.62850500	-2.64634400	-1.26059700
H	-5.06016000	-0.70656600	0.07732300
H	-4.77122500	-2.84836600	-1.22629800
H	-2.43651300	-3.55936800	-1.80785800
H	-0.78530500	1.86500500	0.49878200
C	1.40819300	0.14836200	-0.39561400
C	0.91734500	0.94629400	0.80639100
H	0.25198600	0.31015900	1.39676100
O	0.18758200	2.01526900	0.26655300
H	2.14602400	0.70076500	-0.97043300
H	0.56363100	-0.14188400	-1.00896400
C	2.04926600	1.47825100	1.67065800
H	1.62786300	2.08506700	2.47097500
H	2.63866200	0.67278100	2.10929000
H	2.70584500	2.10937100	1.06827200
I	2.37852700	-1.70976000	0.13738100
C	-1.57781900	-1.83638600	-0.86034900
H	-0.55411100	-2.12173400	-1.08750700
N	-1.73609600	-0.69862500	-0.18747700
C	-3.19023400	0.98419700	0.93583700
O	-2.18619200	1.70916100	1.12553500
O	-4.34997300	1.16986800	1.31579200
C	1.09990900	3.85236800	-1.26417800
O	0.09073500	4.40877000	-1.30222600
O	2.15577600	3.37630800	-1.29615400

TS2

-1 1

C	-2.73128400	-0.79745600	0.28438000
C	-3.71373400	-1.54344200	-0.36553400
C	-3.33024400	-2.62084300	-1.14063400
C	-1.98084700	-2.93897200	-1.22083000
H	-4.74679500	-1.25753900	-0.23373800
H	-4.06820400	-3.21029400	-1.67019600
H	-1.63085600	-3.77837900	-1.80593300
H	-1.40056100	1.50422200	0.65369700
C	1.41674000	0.42772400	-0.54661500
C	0.73614900	1.19430900	0.58390700
H	0.38749600	0.46414000	1.32034200
O	-0.40628800	1.80488800	0.04488700
H	1.97870300	1.07314300	-1.21134900
H	0.68367000	-0.15315700	-1.09436300
C	1.65467900	2.20240600	1.26029800
H	1.09634300	2.72499300	2.03642100
H	2.50956800	1.70453800	1.72001500
H	2.01160900	2.93152100	0.53407000
I	2.84048600	-1.02756800	0.17941800
C	-1.07970800	-2.14863100	-0.52513100
H	-0.01688600	-2.37179600	-0.55009700
N	-1.43787100	-1.09243800	0.20134900
C	-3.17380700	0.36916800	1.16783900
O	-2.33888400	1.31611600	1.36520700
O	-4.29829700	0.30000800	1.63830000
C	-0.35549900	3.04356800	-1.28841600
O	-1.48631400	3.34464400	-1.43314200
O	0.78735600	3.15306600	-1.59938400

Int2

-1 1

C	2.37639100	-1.04355900	-0.27892900
C	2.60222100	-1.24399700	1.07797300
C	1.69209600	-2.00993800	1.78243000
C	0.61321900	-2.56499500	1.10563000
H	3.44718500	-0.76797800	1.55199200
H	1.81495300	-2.16558500	2.84620500
H	-0.12513300	-3.16766100	1.61660100
H	2.09714900	1.12890700	-1.22157000
C	-1.22709900	0.61595400	0.57778700
C	-0.52019100	1.40621200	-0.52379700
H	-0.53973100	0.80472500	-1.43581000

O	0.85793800	1.53929300	-0.23555800
H	-1.61993400	1.23771500	1.36957300
H	-0.58504500	-0.15891300	0.98261400
C	-1.18013200	2.75165400	-0.77952800
H	-0.66950500	3.26310200	-1.59475900
H	-2.22789000	2.61542600	-1.05315300
H	-1.11298500	3.35930600	0.12115200
I	-2.94350800	-0.45036100	-0.20638800
C	0.48046400	-2.30333400	-0.24909200
H	-0.36040800	-2.70081300	-0.80599200
N	1.33324100	-1.54469000	-0.93440600
C	3.37399000	-0.26569800	-1.11022600
O	2.92038400	0.82331600	-1.69221100
O	4.49653600	-0.67656900	-1.25457500
C	1.30222700	1.98127800	1.10012600
O	2.51070800	1.84914600	1.21162000
O	0.39887100	2.37634500	1.83176300

TS3

-1 1

C	2.49843700	-1.01920800	-0.31041500
C	2.63066200	-1.50241000	0.98351600
C	1.58089600	-2.23161400	1.51599400
C	0.46558800	-2.47479800	0.72767500
H	3.52195400	-1.26943300	1.54692800
H	1.62636100	-2.59503400	2.53414100
H	-0.38769000	-3.02300500	1.10270700
H	2.34296700	1.10944100	-1.34487100
C	-1.11086800	0.79772300	0.81172900
C	-0.49417800	1.43418700	-0.42482400
H	-0.60912700	0.76128700	-1.27173000
O	0.91181400	1.56772900	-0.25292900
H	-1.78309900	1.35227900	1.43801800
H	-0.70980600	-0.12507800	1.19108500
C	-1.12142300	2.78441900	-0.71837400
H	-0.65035000	3.23056300	-1.59280700
H	-2.18857800	2.66698200	-0.90652500
H	-0.97483300	3.44398400	0.13761400
I	-3.08098200	-0.41675100	-0.20494400
C	0.44201300	-1.96333900	-0.56319000
H	-0.42279300	-2.11959800	-1.19703400
N	1.43002300	-1.23504100	-1.07368400
C	3.61909500	-0.21483800	-0.92478600
O	3.24811200	0.85320100	-1.61294200
O	4.76551700	-0.56182800	-0.82845800

C	1.32712100	1.72995100	1.08681100
O	2.52525900	1.81688500	1.25552600
O	0.36090000	1.73154900	1.89323900

PC

-1 1

C	2.30054400	-1.47644900	-0.18482400
C	2.10954300	-2.26788200	0.93360500
C	0.83523200	-2.77097300	1.16266600
C	-0.17739400	-2.47005200	0.26859800
H	2.94460600	-2.46120200	1.59104500
H	0.63438500	-3.37760500	2.03577700
H	-1.19964800	-2.78779600	0.41716500
H	2.76006200	0.08676000	-1.78894300
C	-0.17676700	1.25997100	1.03260400
C	-0.17515900	1.72550400	-0.42075000
H	-0.42173200	0.92076400	-1.10448700
O	1.21684400	2.06489300	-0.61720200
H	-1.05783500	1.58010700	1.57899300
H	-0.06222100	0.18178700	1.13187900
C	-1.04164900	2.93832800	-0.66813600
H	-0.87601000	3.32551600	-1.67261100
H	-2.08494300	2.64058300	-0.56237900
H	-0.81108100	3.72405800	0.05461000
I	-3.23493200	-0.32980300	-0.06296100
C	0.12092700	-1.67391900	-0.83374000
H	-0.66635900	-1.40578500	-1.52702400
N	1.33337600	-1.17958200	-1.05443900
C	3.66350200	-0.91108500	-0.49130800
O	3.67854600	-0.03533600	-1.49033300
O	4.65333800	-1.23871600	0.10157900
C	1.80172800	2.28026100	0.57408000
O	2.89048300	2.73664500	0.72320300
O	0.98522900	1.91091500	1.57365900

Pyridine-3-carboxylic acid (3b)

RC

-1 1

C	-3.90809100	-0.82916300	-0.04896000
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C	-4.36884000	-1.91923800	0.67498400
C	-5.72580800	-2.18733900	0.67637500
H	-3.65561200	-2.52686300	1.21592400
H	-6.13351300	-3.02482200	1.22493500
H	-1.12108100	0.69674600	-0.72079900
C	1.31559000	0.04958900	-0.77239400
C	1.09626200	0.64413200	0.53637900
H	0.47520400	0.08275900	1.22503000
O	0.33925600	1.11004300	-0.61179400
H	2.19969100	0.32854400	-1.32717500
H	0.88284700	-0.91962000	-0.98345600
C	2.06259400	1.62385800	1.11703200
H	1.54933200	2.34035700	1.76033600
H	2.81411500	1.07960500	1.68881400
H	2.58824800	2.14782800	0.31990800
I	4.77712800	-0.81530000	-0.10150300
C	-2.44181800	-0.52869600	-0.05733700
O	-2.12791200	0.52906000	-0.77700500
O	-1.64703400	-1.20955800	0.54445200
C	-1.35752500	3.15799900	0.28191900
O	-1.26762500	2.67945400	1.33002500
O	-1.46645600	3.66796100	-0.74781900
C	-4.83113200	-0.05360100	-0.74317000
H	-4.49076800	0.79995000	-1.31552100
C	-6.56416000	-1.35052800	-0.04895100
H	-7.63314600	-1.53299800	-0.06845000
N	-6.13819800	-0.30262000	-0.74828500

TS1

-1 1

C	-3.30818500	-0.92722200	-0.08349100
C	-3.54273200	-2.22224800	0.35267400
C	-4.85188700	-2.64735300	0.50453800
H	-2.69388200	-2.86028000	0.56094900
H	-5.08385600	-3.64798500	0.84296600
H	-0.62674600	1.13077100	-0.74928600
C	1.73979000	0.35648600	-0.86123500
C	1.30297000	1.17648200	0.25207600
H	0.75185700	0.63050100	1.01620400
O	0.46251200	1.59829800	-0.82533800
H	2.41078400	0.77765300	-1.58767200
H	1.21581300	-0.56431400	-1.05577000
C	2.20793200	2.24778300	0.78525900
H	1.63553100	2.97043400	1.36667400

H	2.97108800	1.79177800	1.41483400
H	2.70068700	2.76099600	-0.04103700
I	3.95746800	-1.06407700	0.02559000
C	-1.88944700	-0.44042900	-0.25535100
O	-1.78657700	0.78510400	-0.63892300
O	-0.96259400	-1.20161100	-0.03231700
C	-1.45693000	3.37156200	0.32390300
O	-1.11281000	2.98920900	1.35935400
O	-1.81744800	3.81094000	-0.68078200
C	-4.40459600	-0.11402000	-0.35107200
H	-4.23850900	0.89891700	-0.69609700
C	-5.87392000	-1.75487900	0.21087400
H	-6.91049100	-2.05677200	0.31955900
N	-5.66867300	-0.50972700	-0.21036800

Int1

-1 1

C	-3.09799500	-0.79082300	-0.18714900
C	-3.26134500	-2.13704100	0.09872700
C	-4.53146600	-2.61470500	0.38342500
H	-2.38546600	-2.77274100	0.09005400
H	-4.70429500	-3.65785900	0.61375800
H	-0.16611400	1.56712200	-1.01816400
C	2.11161300	0.10704300	-0.96217400
C	1.55357800	1.25892500	-0.13495200
H	0.95916800	0.83667200	0.68231000
O	0.73298900	2.00187100	-1.00349800
H	2.73675300	0.46958400	-1.77343000
H	1.29693000	-0.51828900	-1.31171900
C	2.61716300	2.19100800	0.41368300
H	2.13392800	3.00855500	0.94760600
H	3.29600100	1.67658200	1.09243600
H	3.19401200	2.61207900	-0.41295900
I	3.36623800	-1.23973800	0.17241300
C	-1.71617000	-0.22606700	-0.50499300
O	-1.67552700	1.01574800	-0.71351400
O	-0.77771900	-1.03082100	-0.52991600
C	-1.13881600	3.33649400	0.58188000
O	-0.70947600	2.81349100	1.52017700
O	-1.58572500	3.93858000	-0.29612400
C	-4.23043900	0.01768900	-0.17501900
H	-4.11767100	1.07145900	-0.39879700
C	-5.59208300	-1.72014600	0.36786200
H	-6.59916600	-2.06194300	0.58589700

N	-5.45932200	-0.42433200	0.09433500
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TS2

-1 1

C	3.60995800	-0.41420200	-0.07716800
C	4.04326900	-1.63539900	-0.56895900
C	5.39924200	-1.91858800	-0.55527900
H	3.30619700	-2.33044000	-0.94913700
H	5.78331400	-2.85828300	-0.92876800
H	0.69259700	1.38513500	0.37257500
C	-1.80496800	0.02781500	-0.44701600
C	-1.42749500	0.83816600	0.78795000
H	-2.30318400	1.40338800	1.11623800
O	-0.44687200	1.76139400	0.38435100
H	-0.98802400	-0.61539300	-0.76024700
H	-2.12896100	0.68826600	-1.24326400
C	-0.89363800	-0.01756800	1.92655200
H	-0.52740700	0.62964100	2.72285800
H	-1.67613500	-0.66212000	2.32590400
H	-0.07189300	-0.64074100	1.57184100
I	-3.49801900	-1.26875900	-0.10331000
C	2.13357300	-0.08002900	-0.07769100
O	1.85421100	1.06453400	0.42238100
O	1.34421200	-0.90021600	-0.52966700
C	-0.96422800	3.22113700	-0.47031500
O	-2.15567400	3.19457100	-0.49533100
O	0.03747500	3.78611100	-0.75544500
C	6.26726600	-0.96223200	-0.04715700
H	7.33536100	-1.15265200	-0.02114400
N	5.87138500	0.21574600	0.42800300
H	4.24153800	1.43403900	0.79109500
C	4.56453600	0.47457000	0.40761000

Int2

-1 1

C	3.67533000	-0.40765500	-0.07596900
C	4.07032500	-1.65916700	-0.52288300
C	5.41699800	-1.97832700	-0.50200300
H	3.31436400	-2.34845300	-0.87509200
H	5.77335000	-2.94147200	-0.84045900
H	0.98100000	1.39499200	0.33755700
C	-1.88655600	0.06269600	-0.45838200
C	-1.50115200	0.87731700	0.76889900

H	-2.36204100	1.46612100	1.08808200
O	-0.47798700	1.76266100	0.36196600
H	-1.07501100	-0.58738700	-0.77114400
H	-2.21080800	0.72453600	-1.25290700
C	-0.96027700	0.03316500	1.90896200
H	-0.59926600	0.68559100	2.70337100
H	-1.73564300	-0.61759400	2.31149200
H	-0.13345100	-0.58585200	1.55701500
I	-3.57820900	-1.22775400	-0.09633700
C	2.21607500	-0.04731300	-0.09085600
O	1.97865500	1.13936900	0.39125900
O	1.38910300	-0.82782700	-0.51255800
C	-0.86897500	2.99911100	-0.41374900
O	-2.07653800	3.11270000	-0.56109200
O	0.12834100	3.61841500	-0.72580000
C	6.31225500	-1.02655200	-0.03279300
H	7.37456100	-1.24496800	-0.00211000
N	5.95116100	0.17898000	0.39758200
H	4.36318200	1.45885700	0.71818300
C	4.65333000	0.47525900	0.37187300

TS3

-1 1

C	3.44248300	-0.36914400	-0.05829700
C	3.68814100	-1.42348300	-0.92512500
C	4.94399400	-2.00405600	-0.92279700
H	2.89184600	-1.76052900	-1.57545700
H	5.18390500	-2.82880600	-1.57928000
H	1.05604500	1.62787300	0.77658700
C	-2.14371500	0.84056500	-0.49070200
C	-1.61571200	1.31620400	0.85699900
H	-2.39761800	1.92183800	1.32340100
O	-0.48653900	2.16210900	0.62297500
H	-1.45832200	0.35464200	-1.16488500
H	-3.10589700	1.13998700	-0.84764300
C	-1.11995300	0.26145200	1.83070000
H	-0.55656200	0.76389800	2.61799400
H	-1.94655200	-0.28791700	2.26779100
H	-0.46961700	-0.44545300	1.31571300
I	-3.32755100	-1.42186700	-0.03525500
C	2.08506600	0.26482400	-0.05236800
O	1.96749600	1.22232900	0.84512200
O	1.21111600	-0.09731900	-0.80080200
C	-0.56364800	2.93117400	-0.56937800

O	-1.58160700	2.64292400	-1.24499400
O	0.34757100	3.70874900	-0.74121800
C	5.90109500	-1.50199100	-0.05097600
H	6.89529700	-1.93519700	-0.02419400
N	5.68210700	-0.49120900	0.78533800
H	4.29838000	0.88377200	1.45536100
C	4.47062200	0.05994600	0.77479400

PC

-1 1

C	-4.07392900	-0.38293400	0.00907500
C	-4.52756900	-0.82343900	1.24408600
C	-5.82180100	-1.30072900	1.34044000
H	-3.85948200	-0.78107800	2.09390500
H	-6.22201700	-1.65552700	2.27967600
H	-1.44732000	0.86656900	-1.32703900
C	1.36588600	0.80034900	0.95083600
C	1.24410600	0.56768700	-0.55335500
H	2.14860200	0.89234600	-1.06507600
O	0.17584300	1.49012900	-0.91284800
H	0.83902300	0.03853700	1.52459700
H	2.40016600	0.87908300	1.26870000
C	0.87552300	-0.83554500	-0.95529600
H	0.70916000	-0.89398300	-2.03105500
H	1.71151200	-1.48634400	-0.69810100
H	-0.02324900	-1.15775600	-0.42774300
I	4.61832200	-0.77504400	0.03770700
C	-2.67809800	0.13332400	-0.10454700
O	-2.36198900	0.50811000	-1.33687000
O	-1.92792000	0.18935700	0.83691500
C	-0.06309600	2.34968600	0.10709100
O	0.69412200	2.05668100	1.15680200
O	-0.84786100	3.24285900	0.03618100
C	-6.60639200	-1.31548300	0.19425800
H	-7.62558400	-1.68387400	0.23585600
N	-6.18605400	-0.89555900	-0.99553800
H	-4.60560100	-0.09702100	-2.04972700
C	-4.93987300	-0.43821300	-1.07844100

Pyridine-4-carboxylic acid (3c)

RC

-1 1

C	-3.93234400	-0.80759200	-0.04236100
C	-4.44797900	-1.83609000	0.73170100
C	-5.81159000	-2.08028200	0.68150200
H	-3.78535500	-2.42234600	1.35254800
H	-6.24628200	-2.87688600	1.27435700
H	-1.09021800	0.63798400	-0.69088100
C	1.39051600	0.10003700	-0.79674800
C	1.14186100	0.58619100	0.55049500
H	0.55602100	-0.05505600	1.19889100
O	0.35442800	1.08767700	-0.56278600
H	2.25435700	0.46843400	-1.33029100
H	1.01923300	-0.87586600	-1.08052500
C	2.05545500	1.57465200	1.19773600
H	1.50951500	2.20894800	1.89749100
H	2.84330700	1.03149200	1.71974800
H	2.53841900	2.18908100	0.43881000
I	4.78801300	-0.80713600	-0.12227000
C	-6.15017700	-0.39744700	-0.80904000
H	-6.85632200	0.15915900	-1.41472100
C	-2.45561100	-0.52974200	0.00147500
O	-2.09533300	0.46940300	-0.77611000
O	-1.70508700	-1.17713200	0.68804500
C	-1.34793400	3.12292800	0.27395600
O	-1.27385400	2.64921800	1.32528200
O	-1.44442300	3.62881700	-0.75929800
N	-6.65816700	-1.38047900	-0.07115700
C	-4.80145100	-0.06995400	-0.83214600
H	-4.43049600	0.73656300	-1.44751800

TS1

-1 1

C	-3.31477600	-0.91829300	-0.08741900
C	-3.56000400	-2.20756900	0.36081100
C	-4.87503800	-2.62176100	0.50783700
H	-2.72594400	-2.85798000	0.58457900
H	-5.09651400	-3.62408700	0.85787800
H	-0.59704700	1.13570200	-0.76282400
C	1.73775200	0.35812100	-0.87030300
C	1.30759900	1.17553200	0.24632300

H	0.75075300	0.63205600	1.00734200
O	0.47019400	1.59351900	-0.84005600
H	2.41584700	0.77339000	-1.59332200
H	1.21960000	-0.56741500	-1.05889400
C	2.20987500	2.24911000	0.77680000
H	1.63673700	2.97212000	1.35684400
H	2.97275100	1.79364900	1.40699200
H	2.70351400	2.76051600	-0.04995600
I	3.97983600	-1.05239600	0.02603500
C	-5.67898400	-0.61558900	-0.19047900
H	-6.54753700	-0.00193900	-0.40420900
C	-1.88728600	-0.43696300	-0.25690500
O	-1.78154700	0.78332500	-0.64753600
O	-0.96645900	-1.20241900	-0.02435900
C	-1.49171600	3.34936100	0.33928900
O	-1.11503300	2.96339800	1.36176900
O	-1.88288400	3.79211400	-0.65255400
N	-5.92756400	-1.85008500	0.24063400
C	-4.40149600	-0.10399200	-0.36978200
H	-4.24022800	0.90432900	-0.72388000

Int1

-1 1

C	-3.10781600	-0.77826900	-0.18602500
C	-3.29095300	-2.12350900	0.09993500
C	-4.56965200	-2.58276000	0.37766200
H	-2.43265300	-2.78114700	0.09957800
H	-4.73708600	-3.63054600	0.60571600
H	-0.15537900	1.56678500	-1.01808300
C	2.11358500	0.10090400	-0.96214000
C	1.56541500	1.25997300	-0.13842700
H	0.97430600	0.84508200	0.68505600
O	0.74241700	2.00238100	-1.00569000
H	2.73446500	0.45634600	-1.77976400
H	1.29459700	-0.52359400	-1.30325100
C	2.63577500	2.19088900	0.39858400
H	2.15887100	3.01355700	0.93033700
H	3.31627800	1.67768800	1.07648500
H	3.20962200	2.60467400	-0.43377900
I	3.36994900	-1.24291000	0.17275300
C	-5.46478900	-0.51526900	0.10913200
H	-6.35466000	0.10602000	0.11897700
C	-1.71396900	-0.22733500	-0.49880400
O	-1.66546700	1.01378000	-0.70683700

O	-0.78485700	-1.04094200	-0.51972300
C	-1.12581800	3.33865800	0.58245000
O	-0.68787500	2.82057500	1.51929800
O	-1.58270700	3.93559100	-0.29414600
N	-5.65180300	-1.80491300	0.38609600
C	-4.22724500	0.04155200	-0.17944800
H	-4.11230800	1.09370500	-0.40056300

TS2

-1 1

C	3.61344100	-0.41334000	-0.06635900
C	4.05539700	-1.64907100	-0.51483400
C	5.41662000	-1.91237300	-0.50933500
H	3.33311400	-2.37671900	-0.85764400
H	5.78963900	-2.87111400	-0.85352700
H	0.68828000	1.37869700	0.37849700
C	-1.80733000	0.02743000	-0.44618200
C	-1.43884800	0.84129600	0.78897100
H	-2.31482700	1.41200300	1.10603900
O	-0.44988400	1.76005500	0.39247100
H	-0.99062500	-0.62152200	-0.74814700
H	-2.11961700	0.68611700	-1.24857600
C	-0.91781700	-0.01068200	1.93601200
H	-0.56079800	0.63889800	2.73455300
H	-1.70480400	-0.65391200	2.32845600
H	-0.09247900	-0.63533600	1.59242300
I	-3.50921900	-1.25880200	-0.11256600
C	5.89992400	0.14203100	0.32848600
H	6.66222000	0.83983700	0.65808200
C	2.12857900	-0.09415700	-0.05748700
O	1.84888300	1.05822900	0.42271500
O	1.34342900	-0.93003000	-0.48377200
C	-0.94644900	3.21105500	-0.46431800
O	-2.13846700	3.19496200	-0.50682000
O	0.06027600	3.77449000	-0.73937900
C	4.56062600	0.50348700	0.36476200
H	4.24356100	1.47509000	0.71554500
N	6.33660100	-1.04160100	-0.09710300

Int2

-1 1

C	3.68051300	-0.40822700	-0.06469100
C	4.08588200	-1.67311500	-0.46271100
C	5.44013900	-1.96873500	-0.45280300
H	3.34510000	-2.39746600	-0.77091800
H	5.78786800	-2.94976400	-0.75701600
H	0.96936100	1.37980200	0.34768300
C	-1.88828500	0.06101900	-0.45767700
C	-1.50972300	0.87679800	0.77087700
H	-2.36972000	1.47241200	1.07947600
O	-0.47701800	1.75510200	0.37186400
H	-1.07835500	-0.59610200	-0.76001900
H	-2.19925700	0.72254900	-1.25782000
C	-0.98559900	0.03300300	1.91893600
H	-0.63100900	0.68569900	2.71600800
H	-1.76836900	-0.61335400	2.31407000
H	-0.15767900	-0.59059400	1.57783900
I	-3.59211700	-1.21589900	-0.10818200
C	5.97907700	0.10897600	0.29251800
H	6.76021500	0.80128700	0.58626900
C	2.21083800	-0.06622200	-0.06690100
O	1.97057400	1.12654500	0.39469200
O	1.38955500	-0.86498500	-0.46196400
C	-0.85236400	2.99677300	-0.40668100
O	-2.05719300	3.11771100	-0.56557900
O	0.15279900	3.60910500	-0.70675300
C	4.64937500	0.50585600	0.32132000
H	4.36336700	1.50063200	0.63049500
N	6.38168700	-1.10243100	-0.08337500

TS3

-1 1

C	3.47848300	-0.37713300	-0.04690600
C	3.74307400	-1.43540100	-0.90274000
C	5.01385900	-1.98914400	-0.89541900
H	2.96180800	-1.80474100	-1.55202700
H	5.25209900	-2.81845300	-1.55172700
H	1.05784700	1.58842200	0.78200200
C	-2.15012000	0.84585800	-0.49593800
C	-1.61042300	1.30410900	0.85314100
H	-2.38071900	1.91872900	1.32683300
O	-0.46842500	2.13397100	0.62140700
H	-1.47834400	0.34208700	-1.17090300

H	-3.10614800	1.16619000	-0.85096100
C	-1.12702100	0.23440200	1.81675800
H	-0.55171100	0.72178100	2.60496000
H	-1.96009800	-0.30471600	2.25401300
H	-0.49060400	-0.47896100	1.29318600
I	-3.39187400	-1.38692300	-0.03513400
C	5.73331400	-0.54290600	0.70346800
H	6.55038000	-0.20708300	1.33218300
C	2.10380000	0.23341800	-0.04368100
O	1.97307700	1.18844000	0.85297500
O	1.23872500	-0.14553800	-0.79232000
C	-0.53059200	2.90577100	-0.57055700
O	-1.54982200	2.63190400	-1.24983800
O	0.39206600	3.67052500	-0.73776500
C	4.49598200	0.08157500	0.77604600
H	4.32181800	0.90671700	1.45078000
N	6.00084600	-1.56011100	-0.11099100

PC

-1 1

C	-4.08748500	-0.37722600	0.00243600
C	-4.56061200	-0.79769100	1.23604900
C	-5.86452400	-1.26087400	1.31813700
H	-3.91395000	-0.75691400	2.10103200
H	-6.26601000	-1.59764500	2.26685100
H	-1.42969500	0.82984800	-1.32134000
C	1.38019900	0.81015500	0.95443000
C	1.25108900	0.54257700	-0.54328900
H	2.15236000	0.85647700	-1.06713300
O	0.17941600	1.45535800	-0.91810300
H	0.85744200	0.06118700	1.54857700
H	2.41611000	0.89760200	1.26474700
C	0.88167700	-0.86988200	-0.91053700
H	0.71072200	-0.95375000	-1.98391000
H	1.71951100	-1.51376000	-0.64227800
H	-0.01436700	-1.18059900	-0.37139800
I	4.63079500	-0.76589100	0.03700100
C	-6.22342200	-0.91642100	-0.90082400
H	-6.91282800	-0.97539400	-1.73524800
C	-2.67899400	0.12578300	-0.09958600
O	-2.34757900	0.47726300	-1.33354900
O	-1.94241400	0.18875700	0.85054300
C	-0.05544400	2.33828800	0.08325300
O	0.70746200	2.07011900	1.13509300

O	-0.84235800	3.22792100	-0.00463500
C	-4.93541400	-0.43617900	-1.09321100
H	-4.59787800	-0.11403600	-2.06711800
N	-6.69031000	-1.32390000	0.27574800

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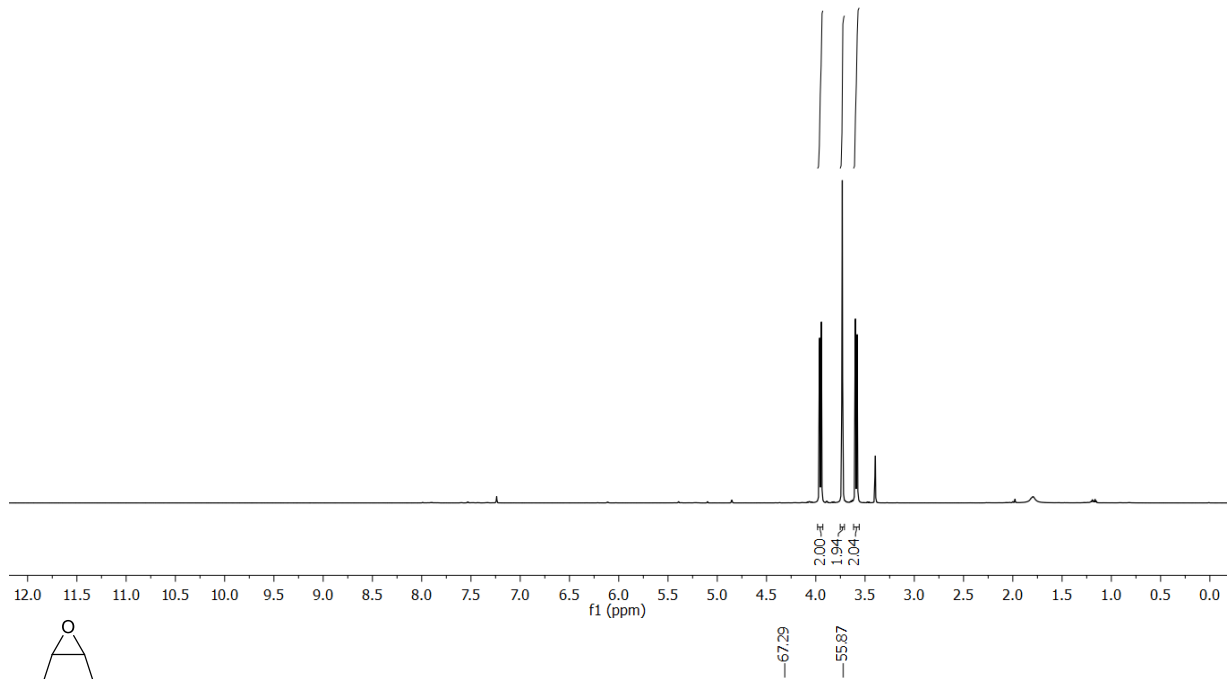
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IV. ^1H NMR, ^{13}C NMR selected spectra



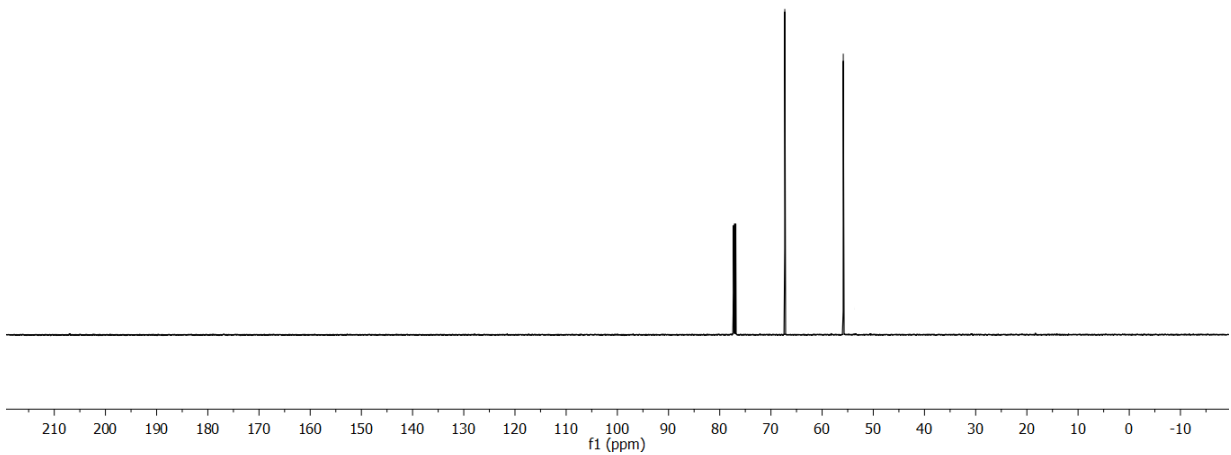
1b

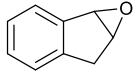
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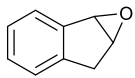
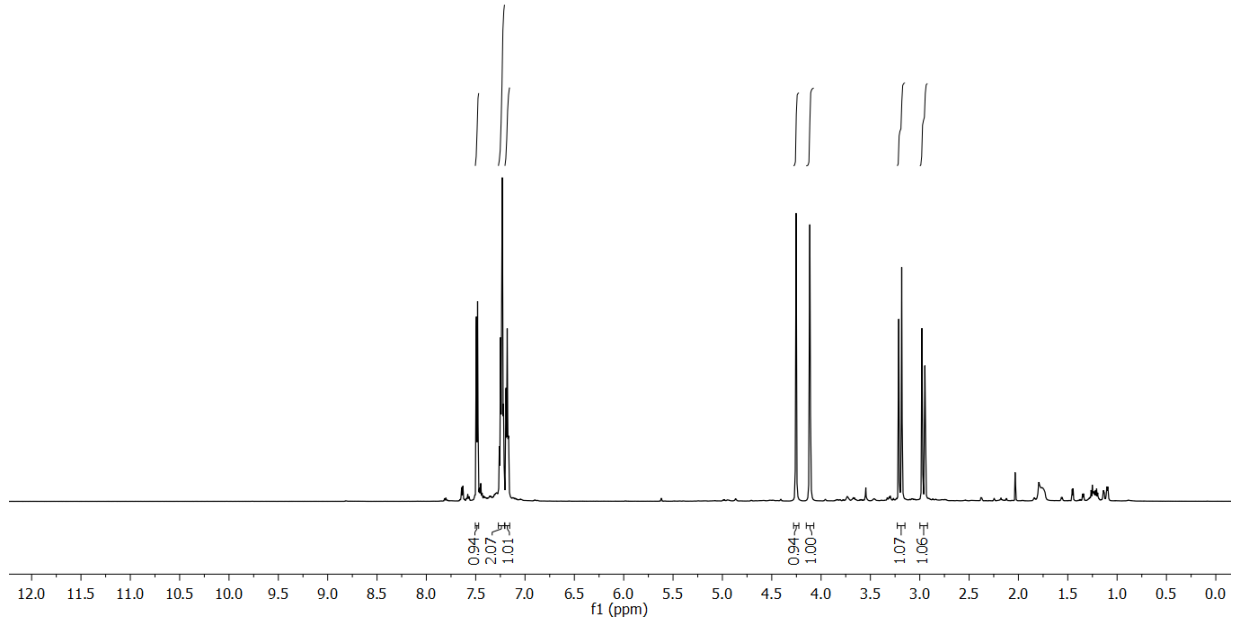
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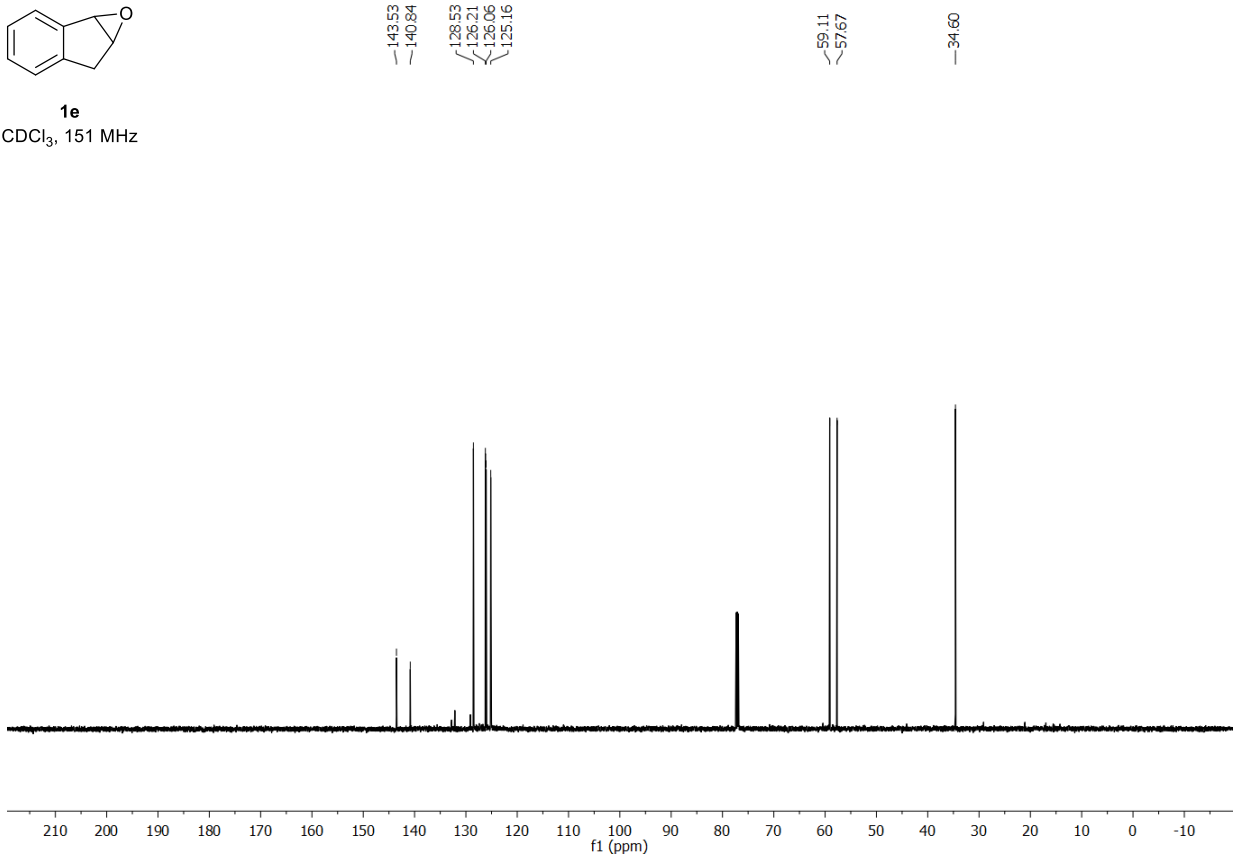


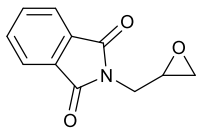


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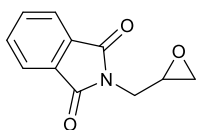
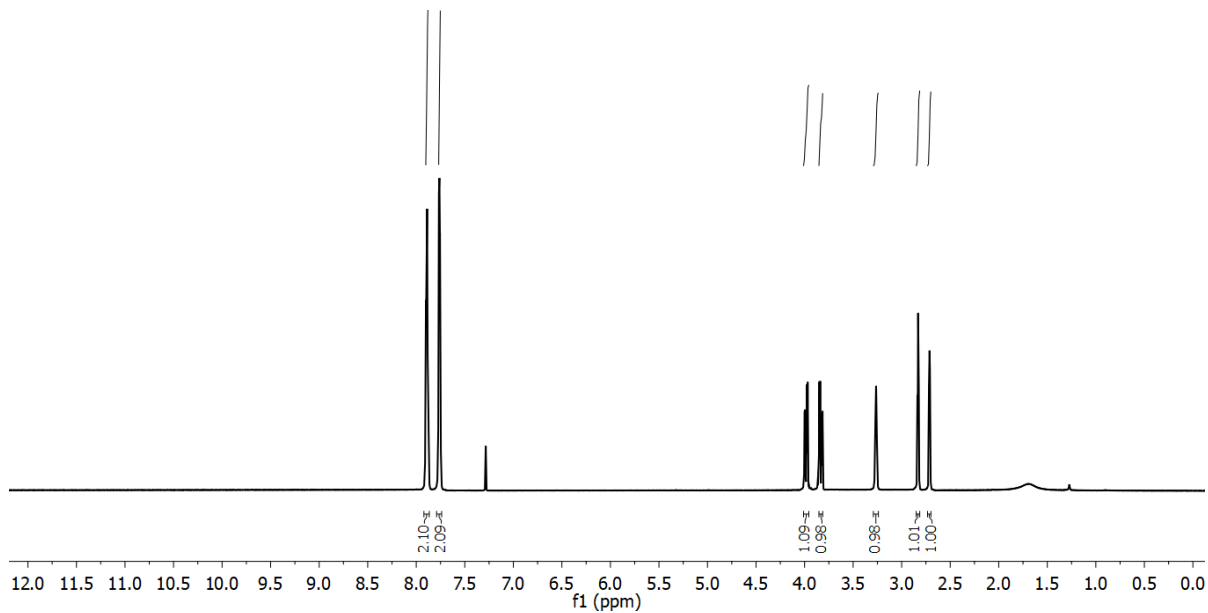


1e
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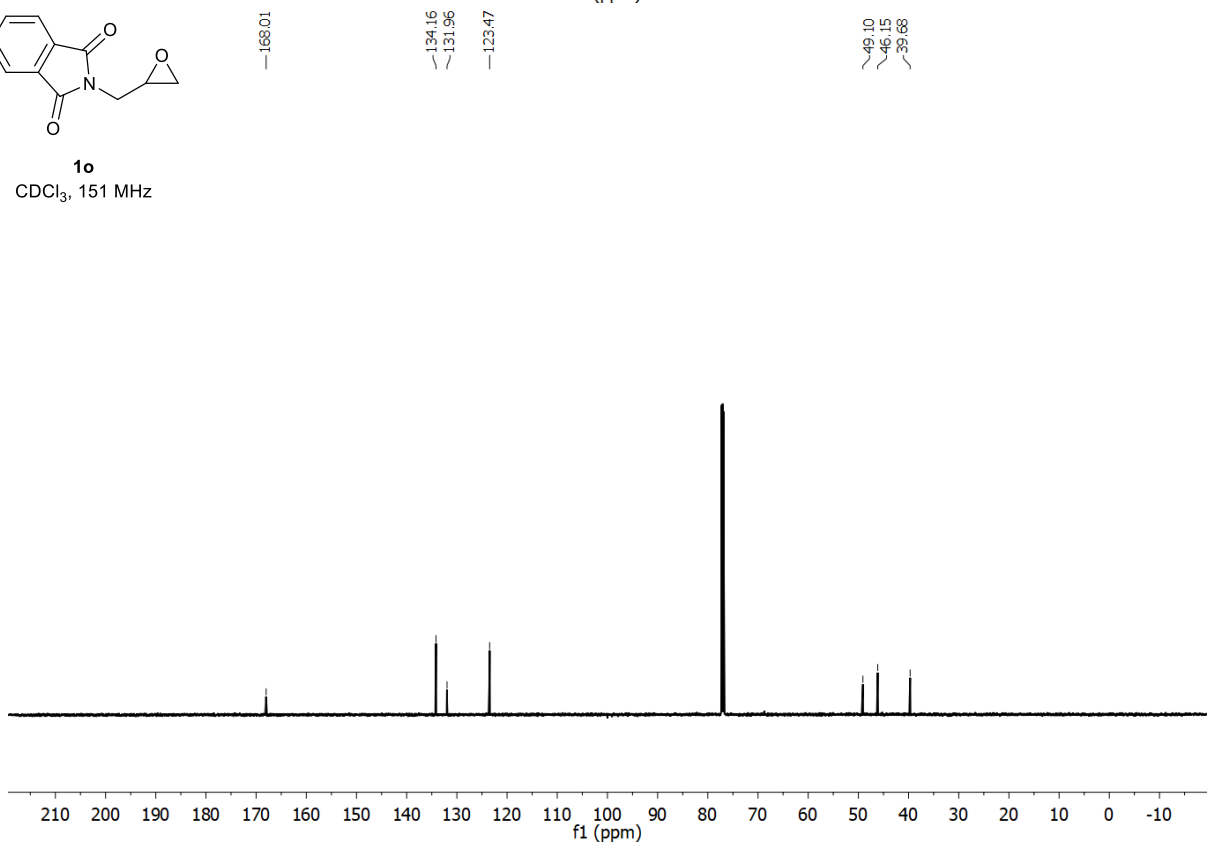


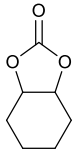


1o
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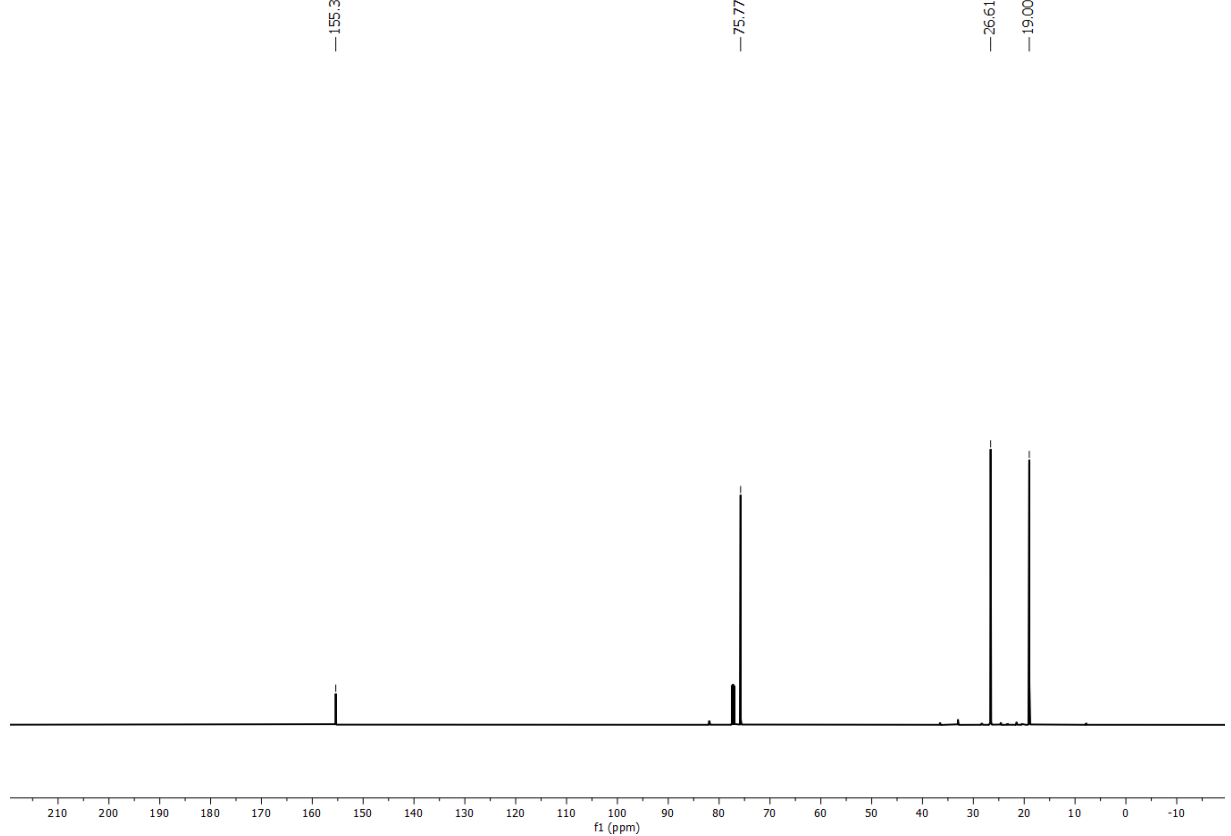
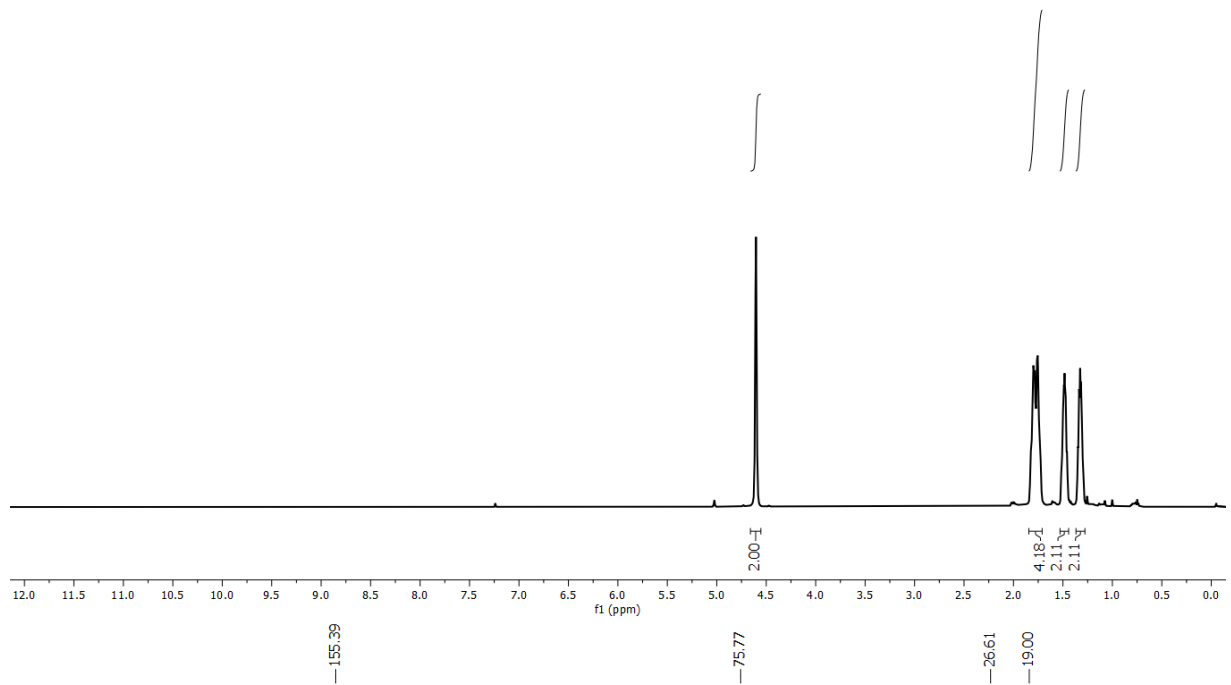


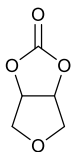
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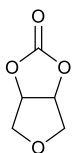
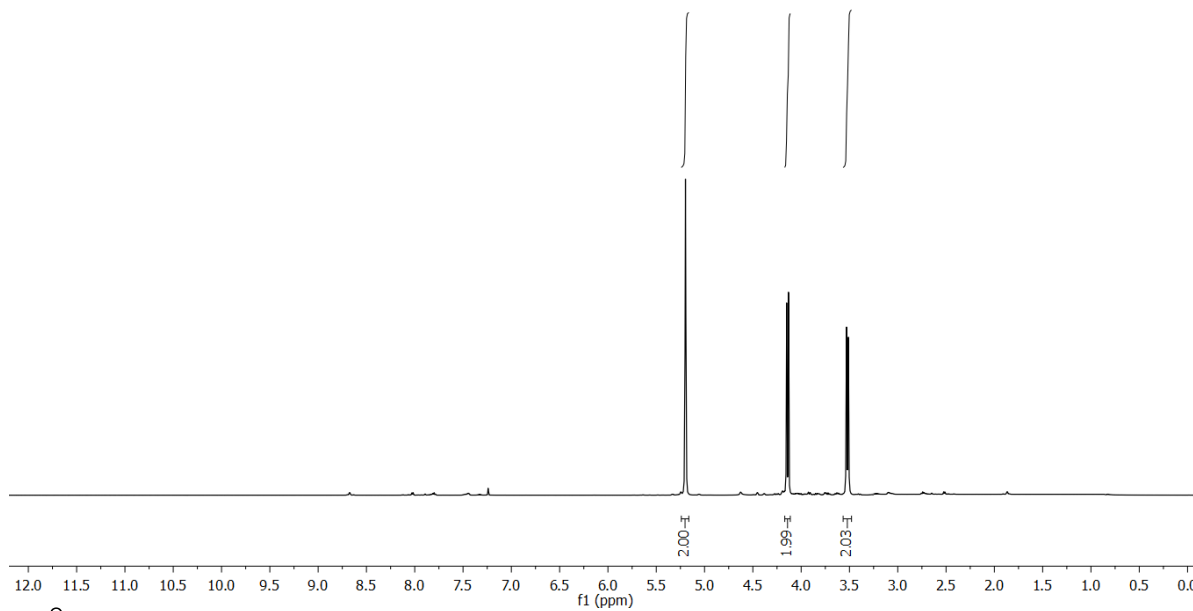


2a
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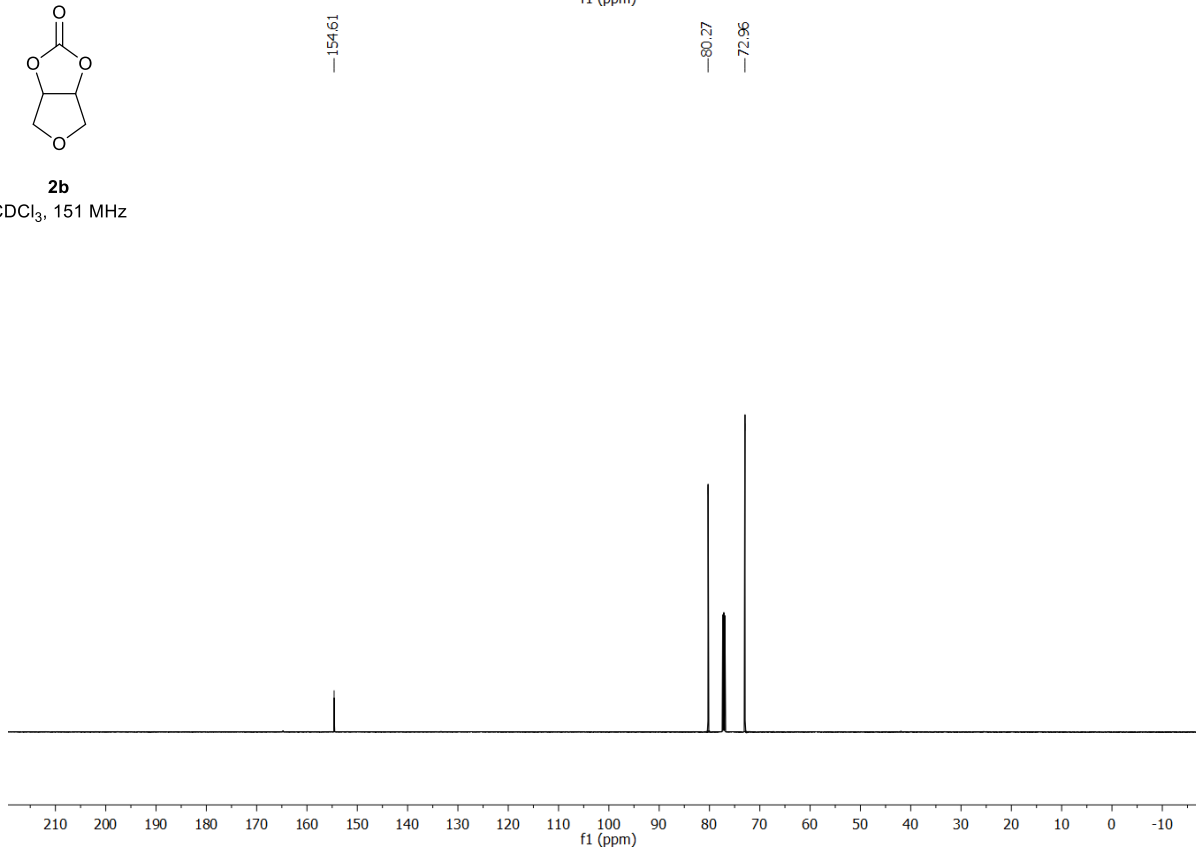


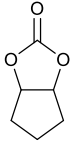


2b
CDCl₃, 600 MHz

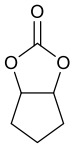
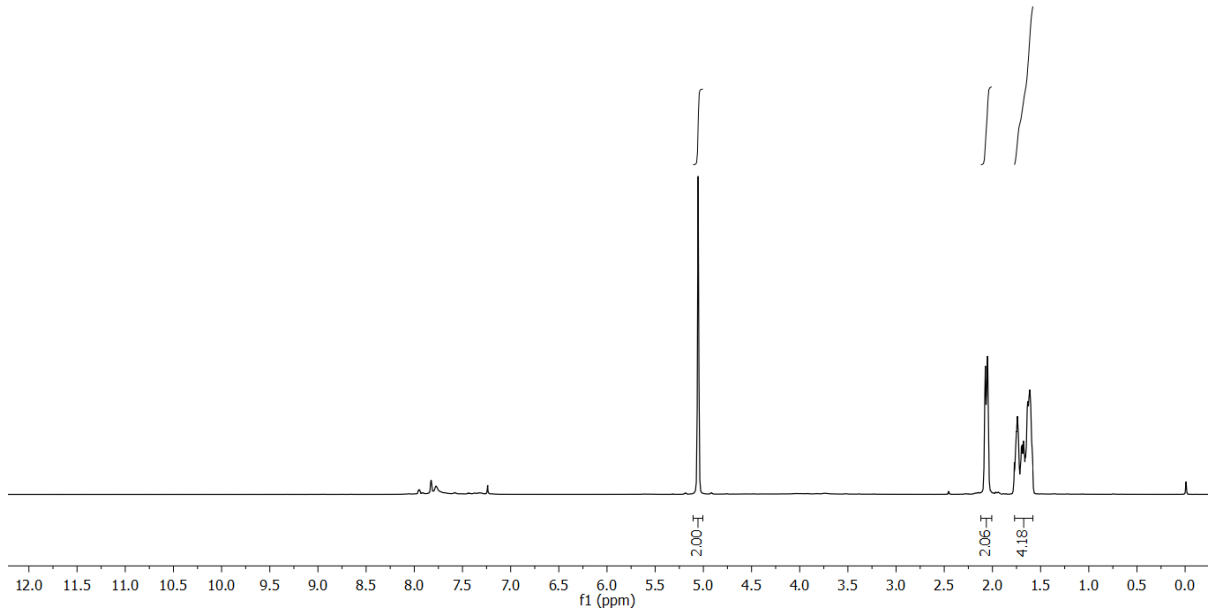


2b
CDCl₃, 151 MHz

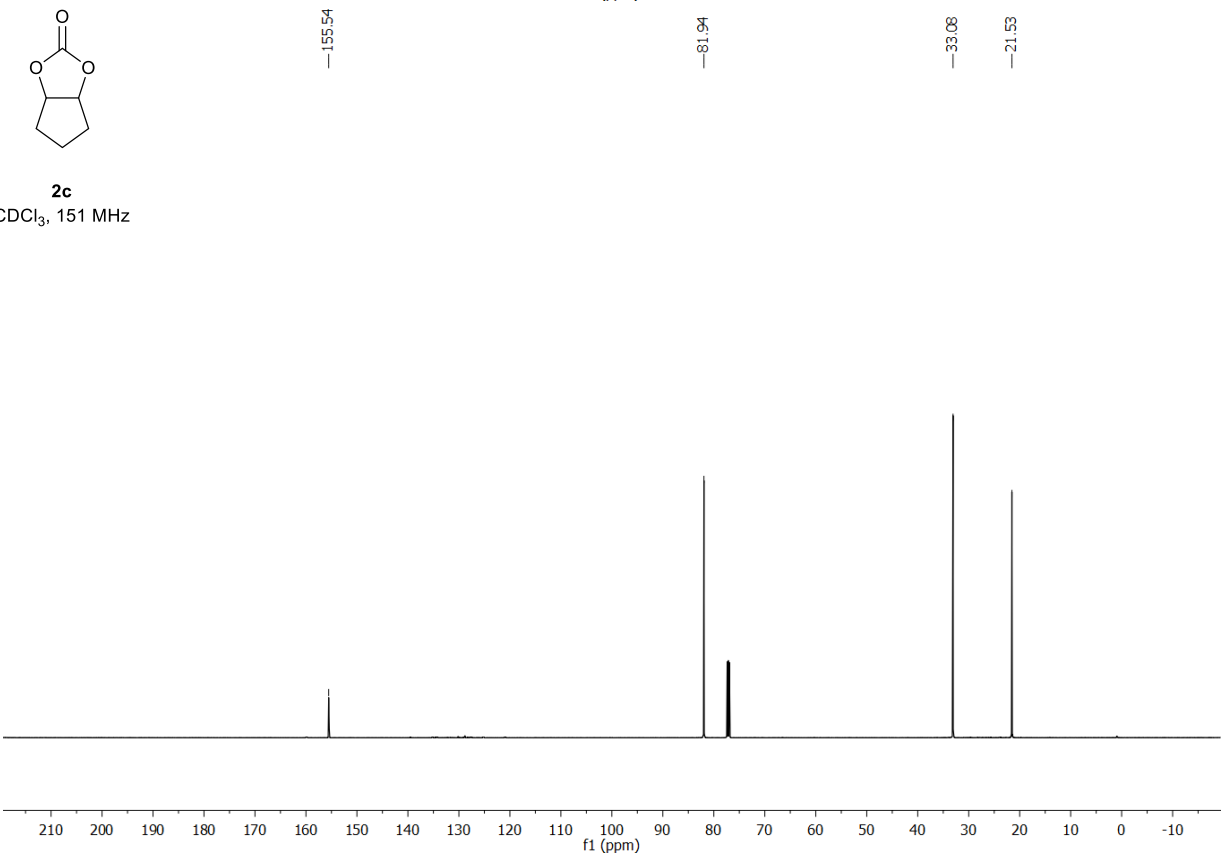


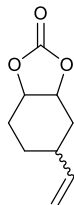


2c
CDCl₃, 600 MHz

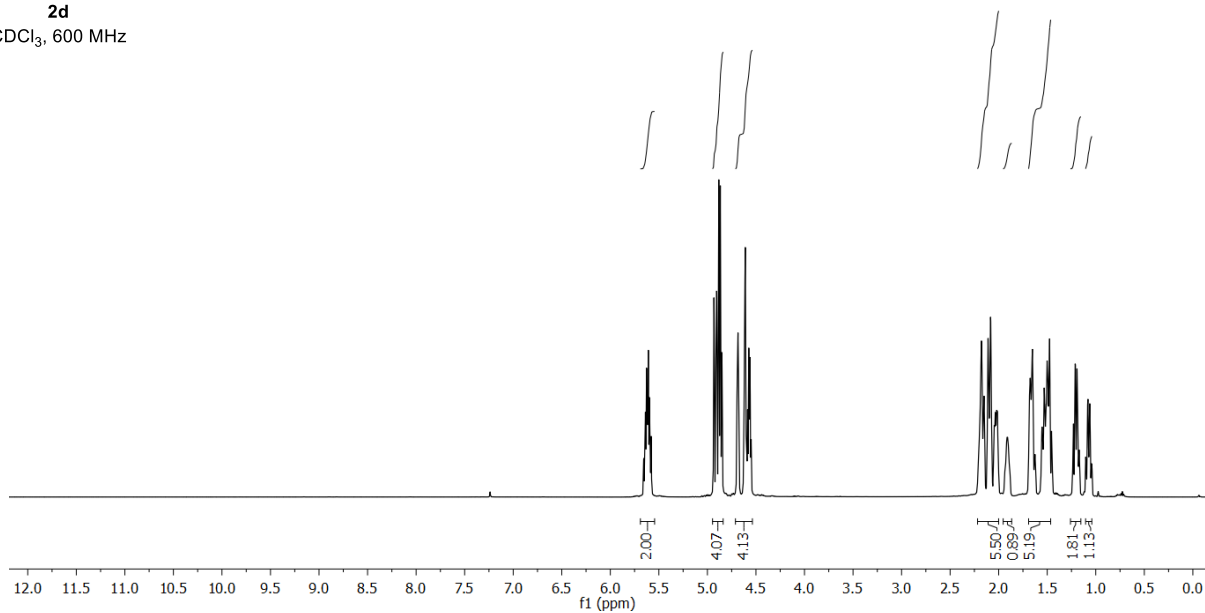


2c
CDCl₃, 151 MHz

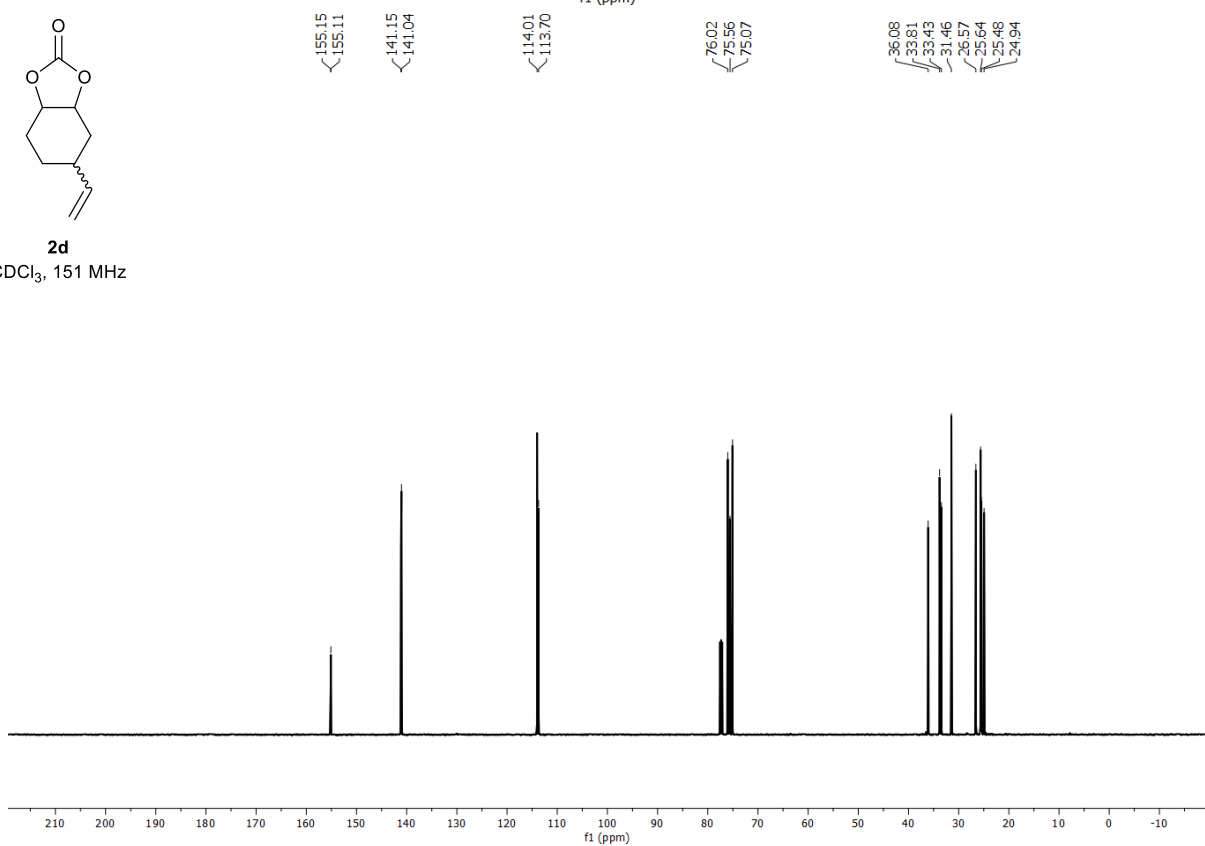


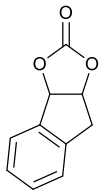


2d
CDCl₃, 600 MHz

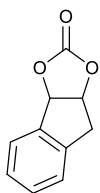
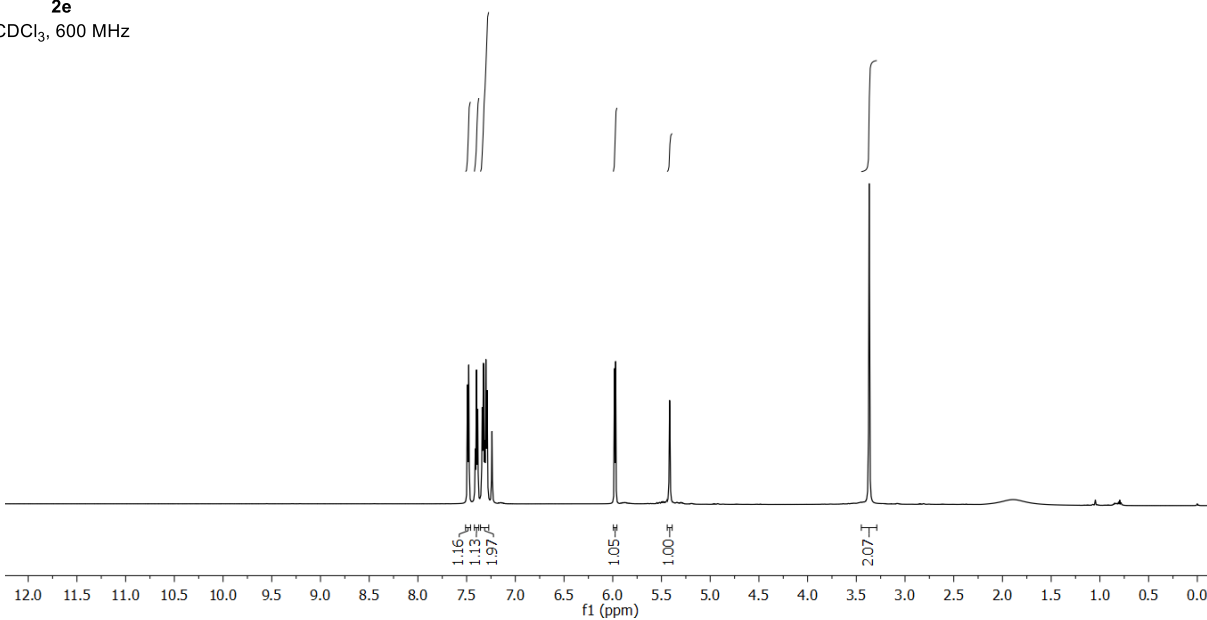


2d
CDCl₃, 151 MHz

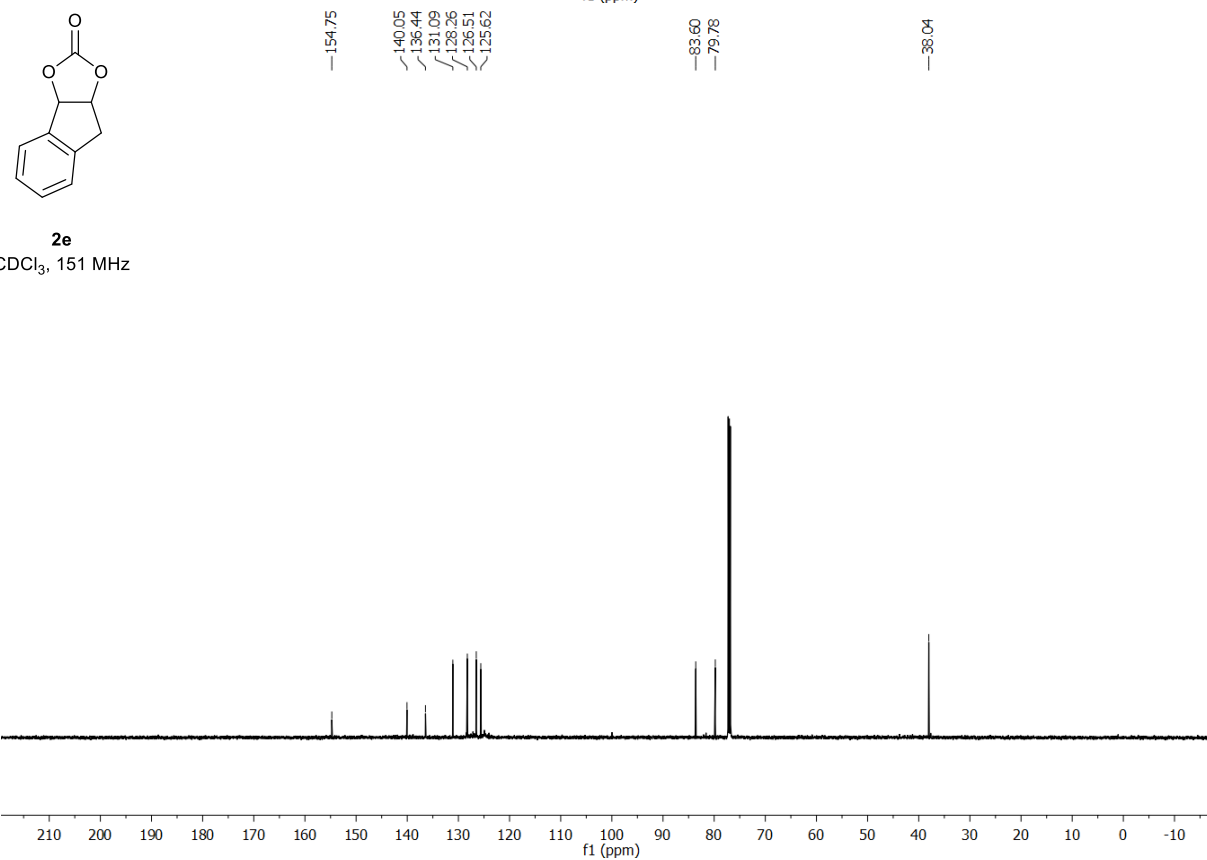


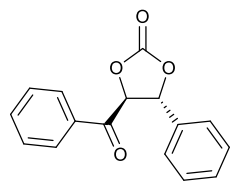


2e
CDCl₃, 600 MHz

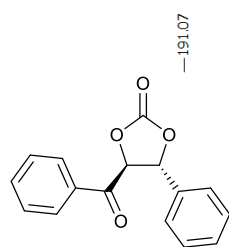
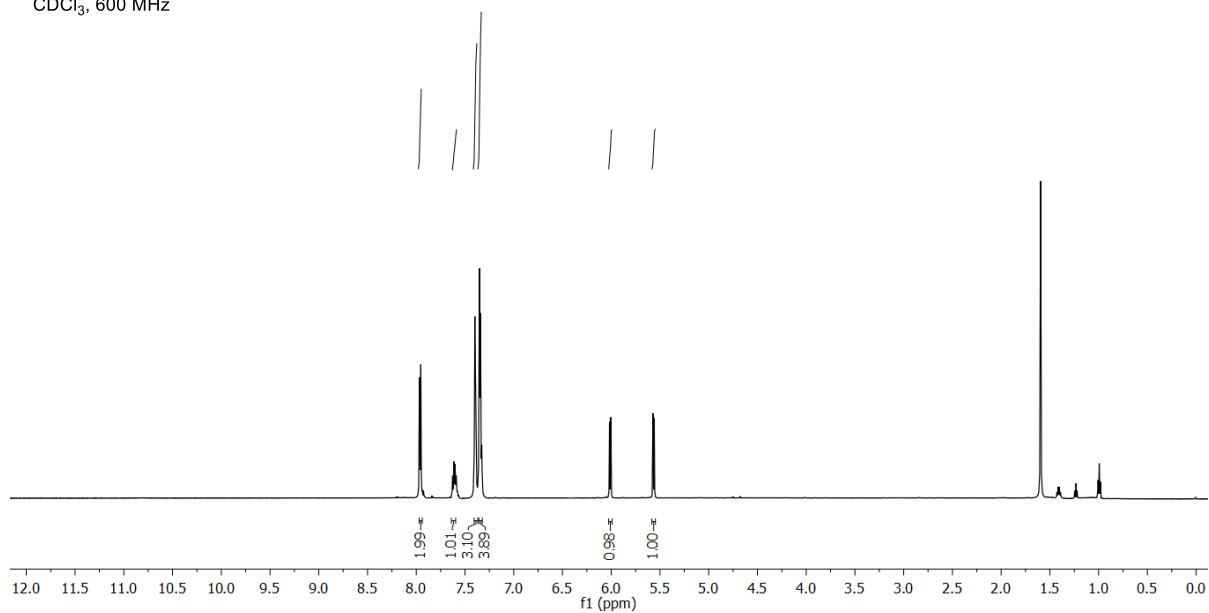


2e
CDCl₃, 151 MHz

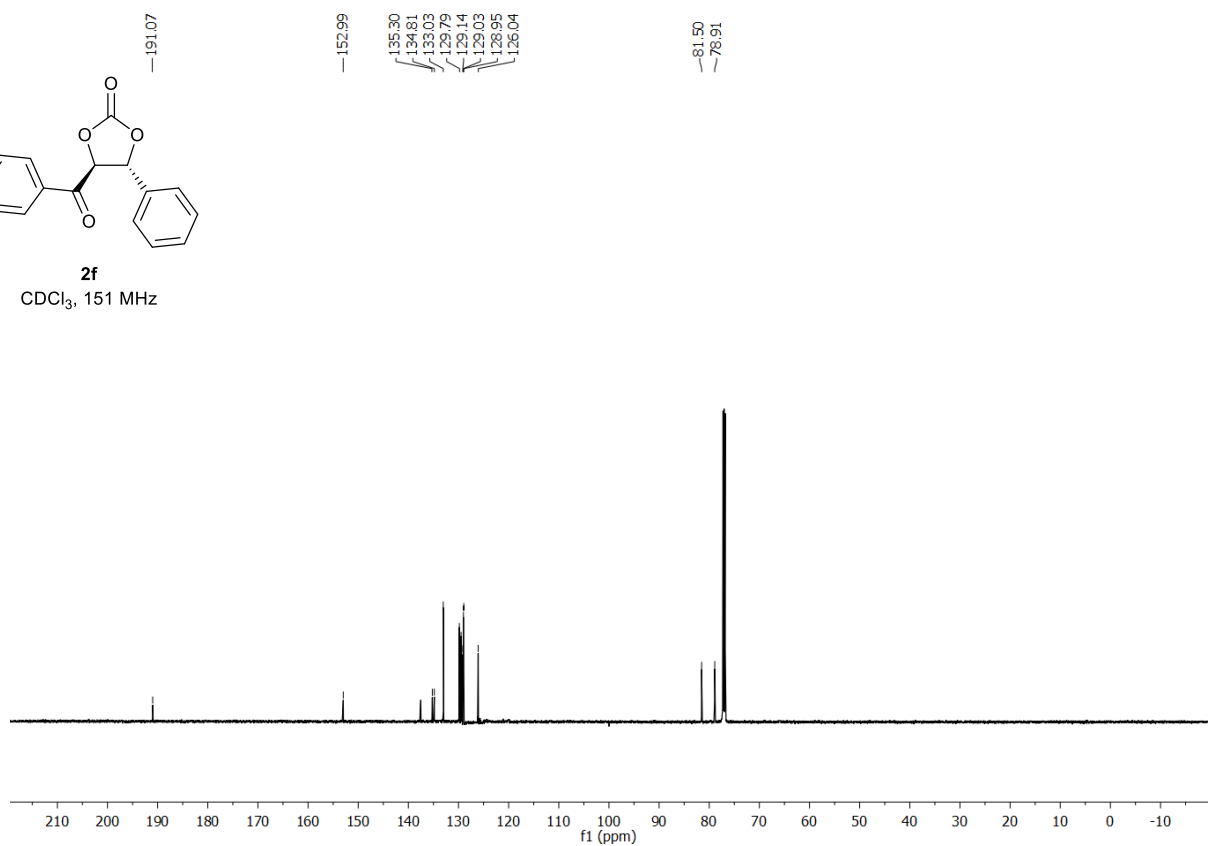


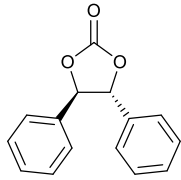


2f
CDCl₃, 600 MHz

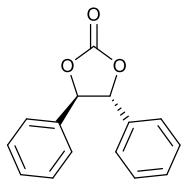
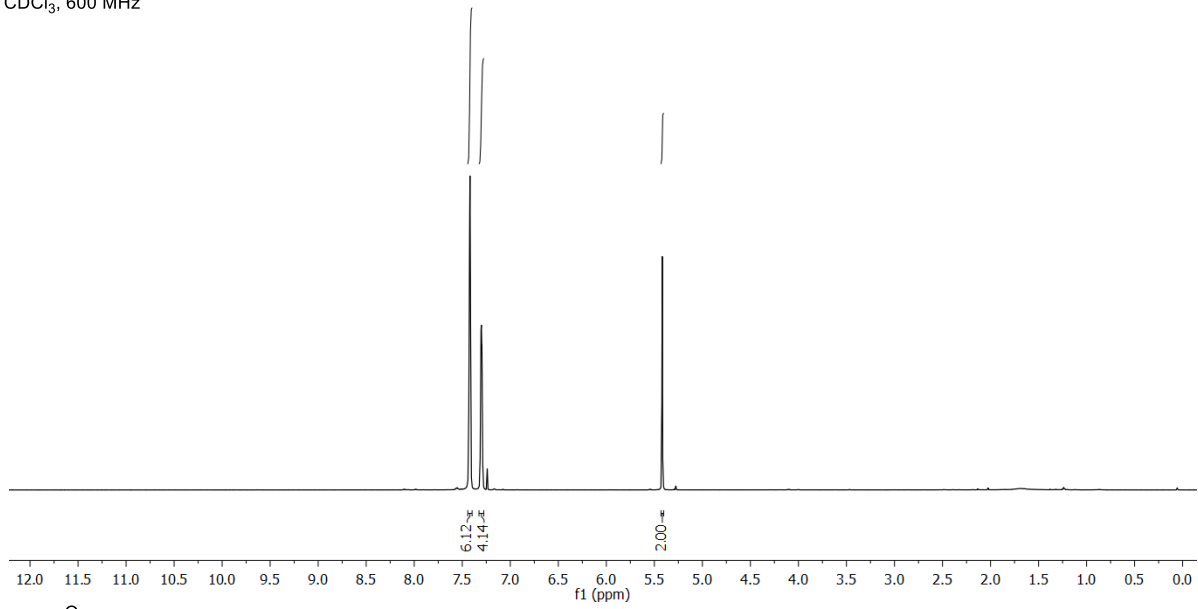


2f
CDCl₃, 151 MHz

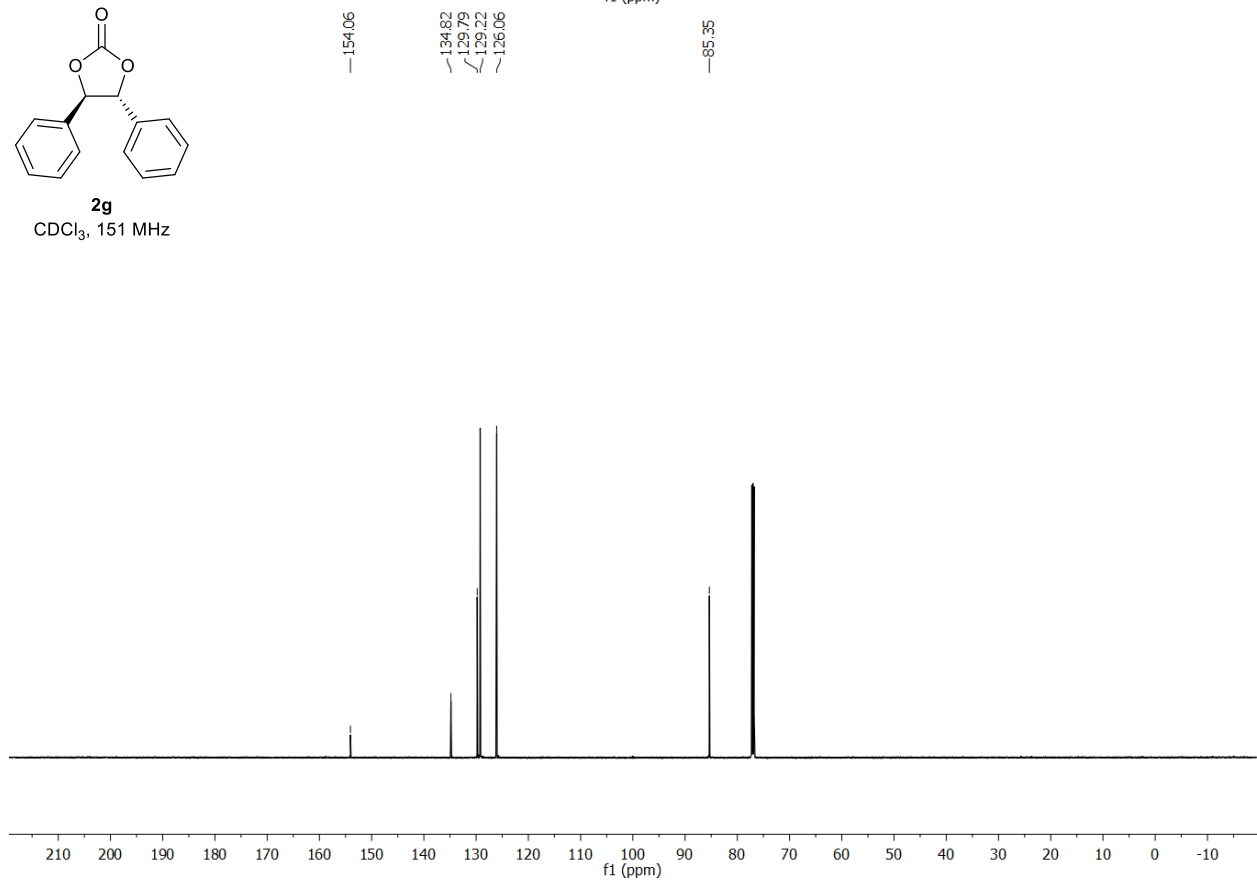


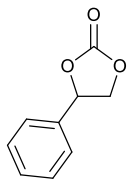


2g
CDCl₃, 600 MHz

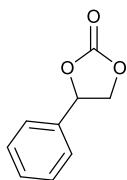
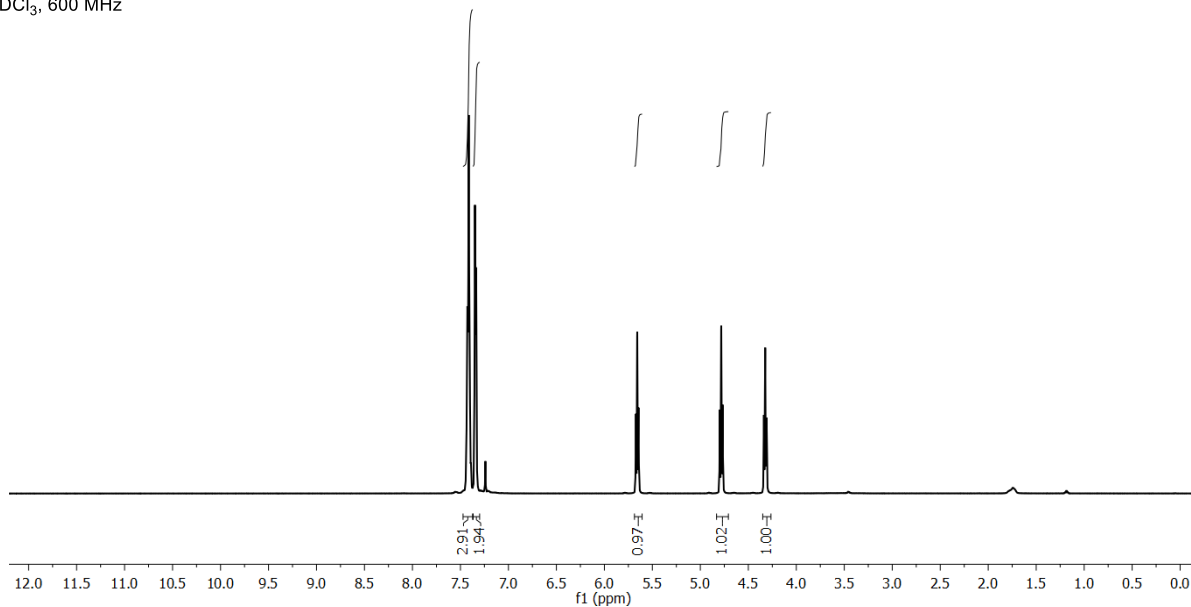


2g
CDCl₃, 151 MHz

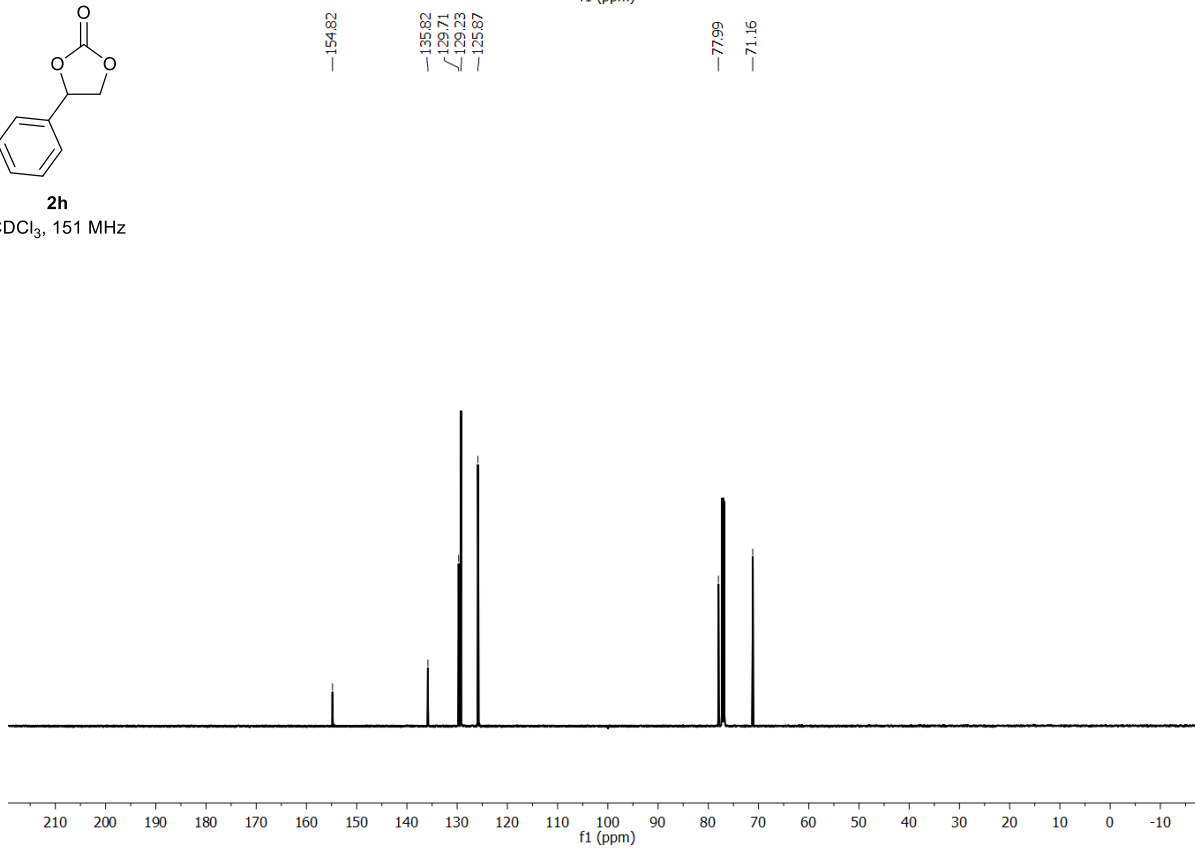


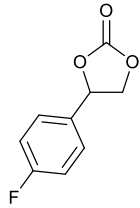


2h
CDCl₃, 600 MHz

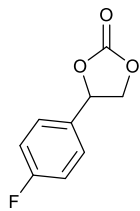
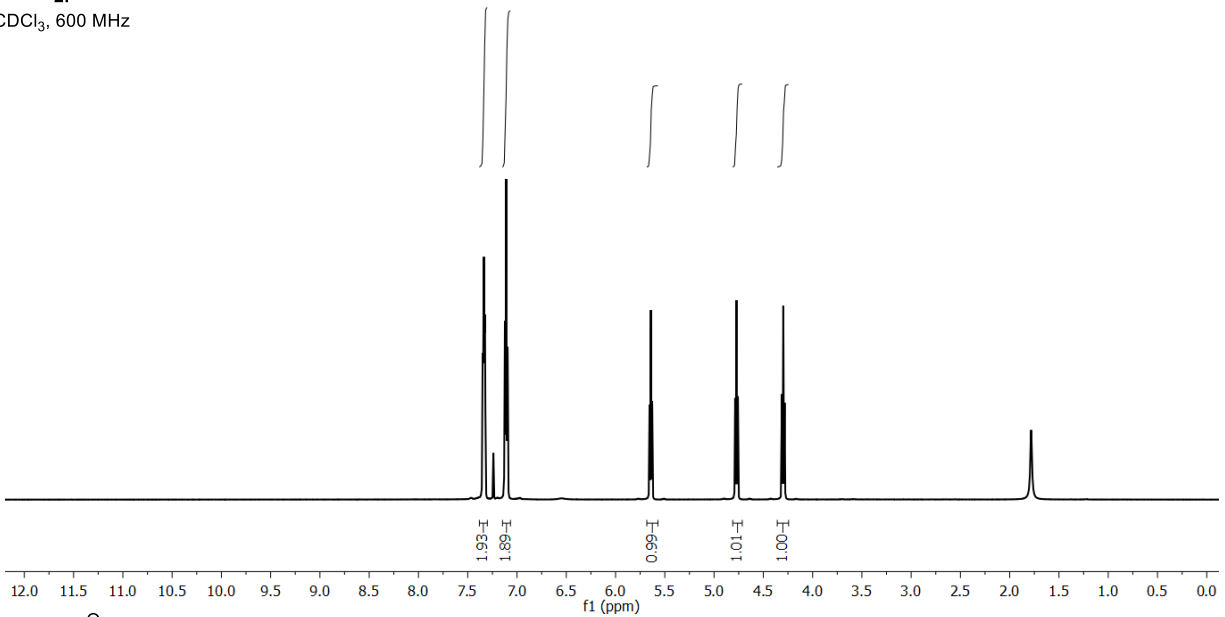


2h
CDCl₃, 151 MHz

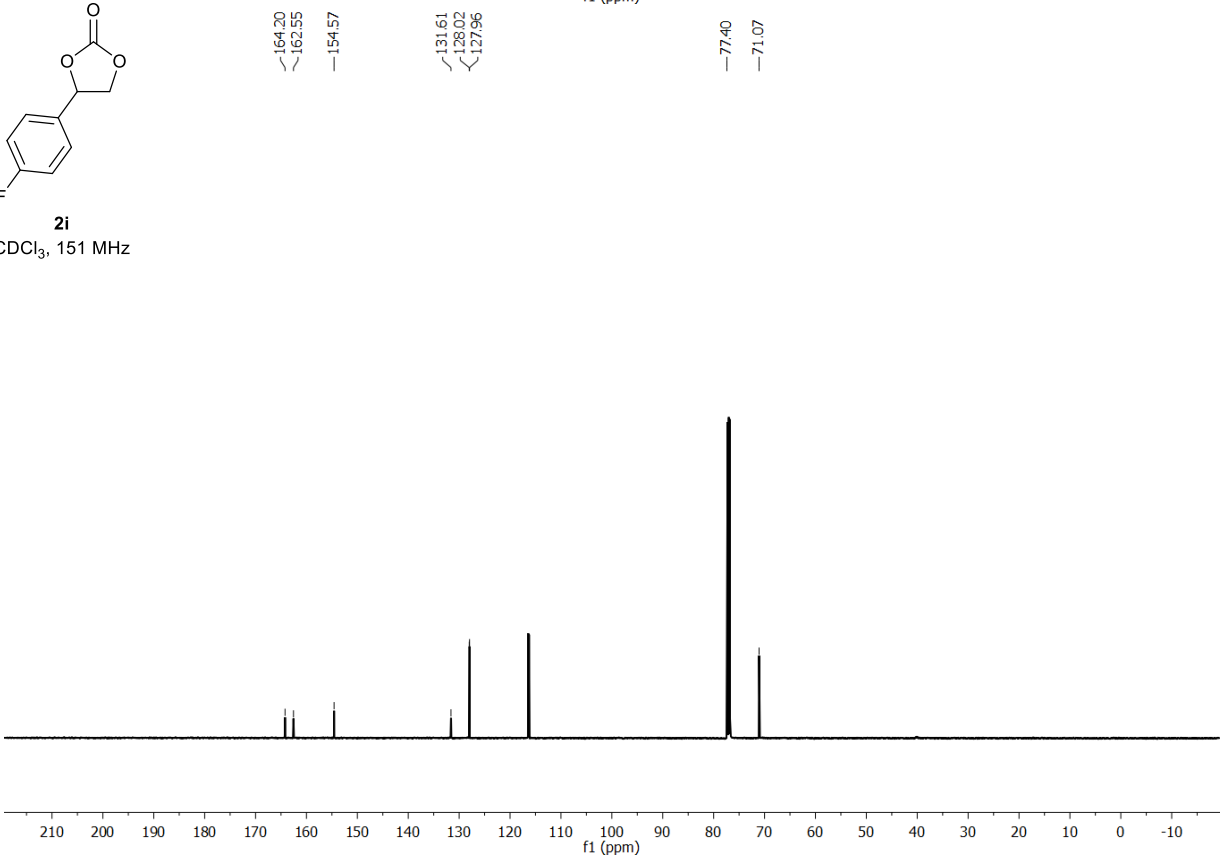


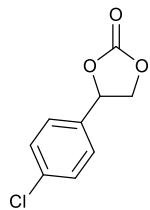


2i
CDCl₃, 600 MHz



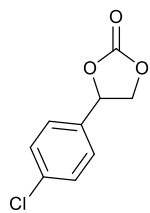
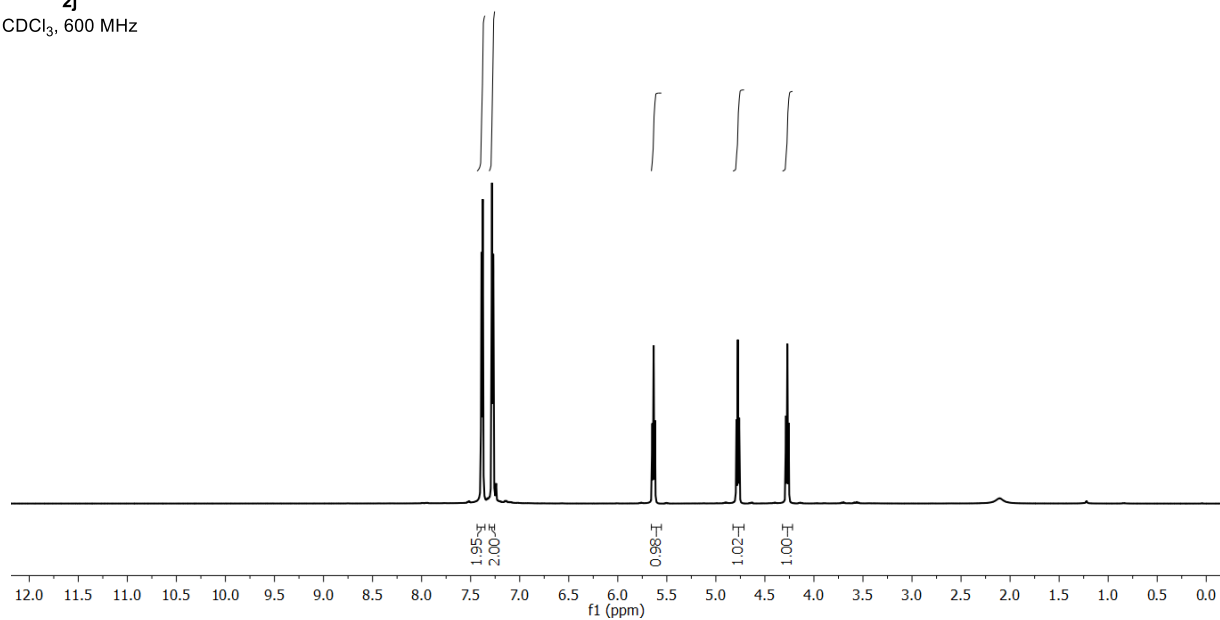
2i
CDCl₃, 151 MHz





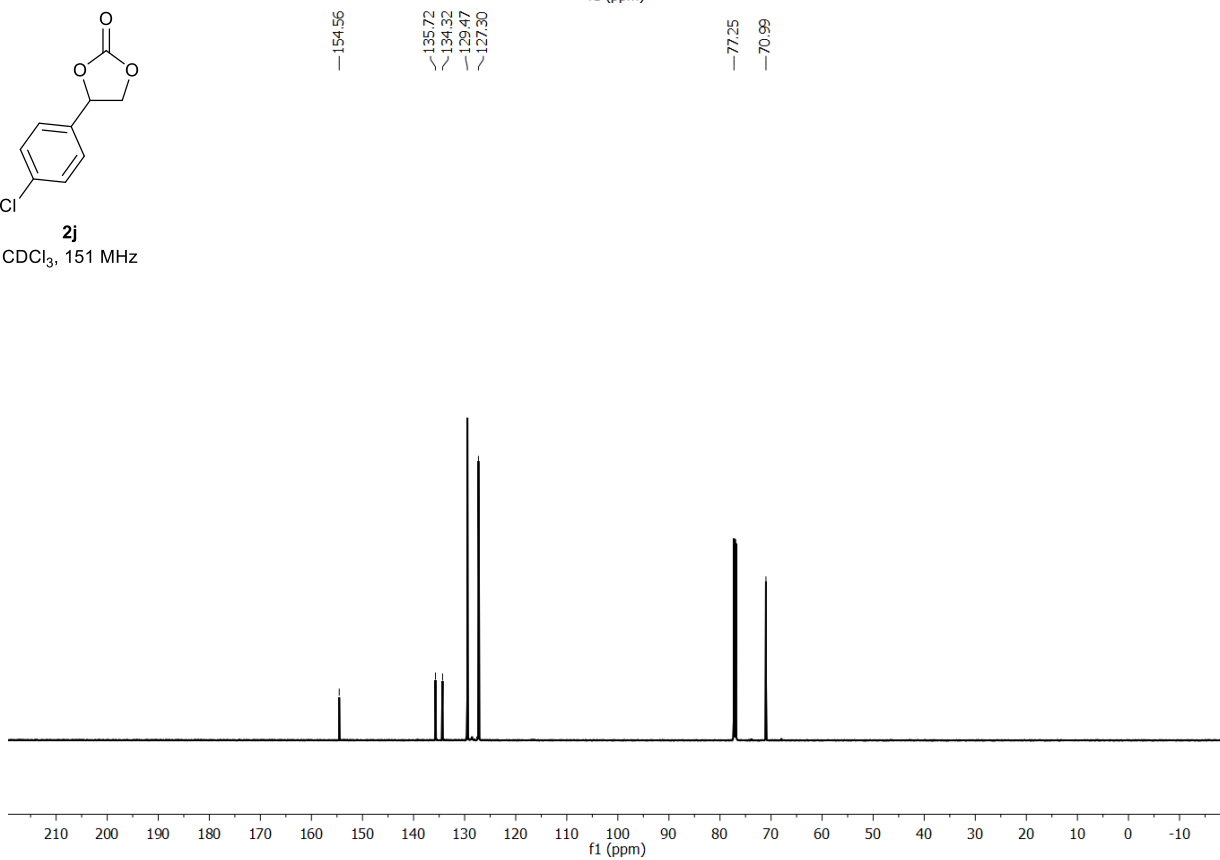
2j

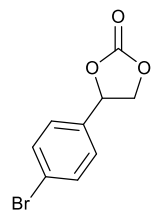
CDCl₃, 600 MHz



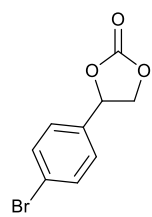
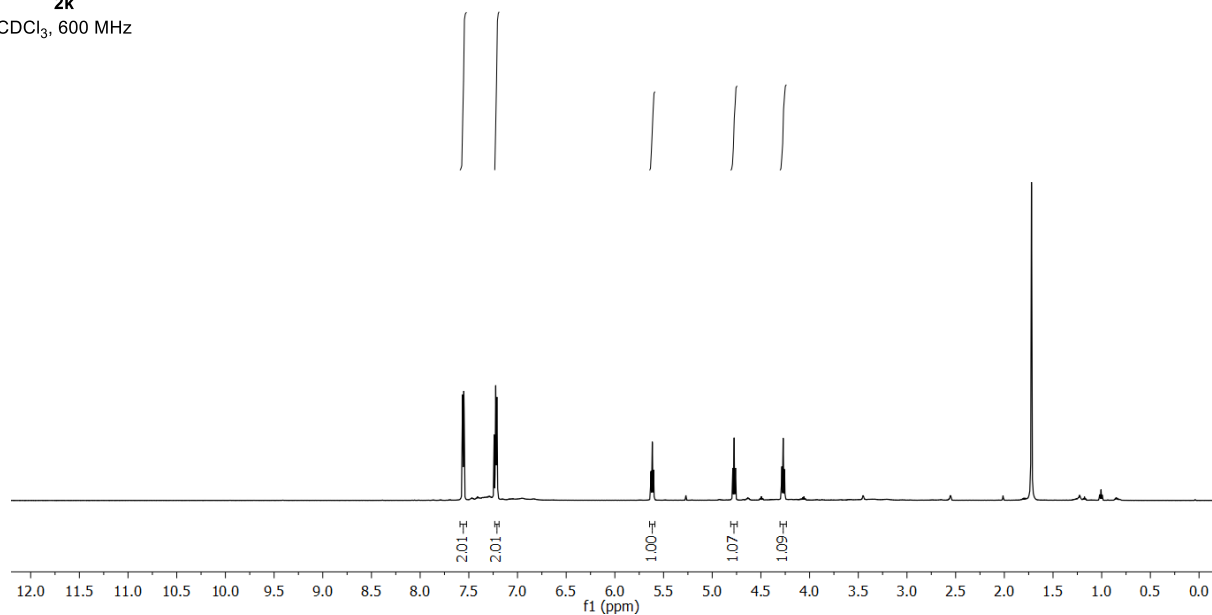
2j

CDCl₃, 151 MHz

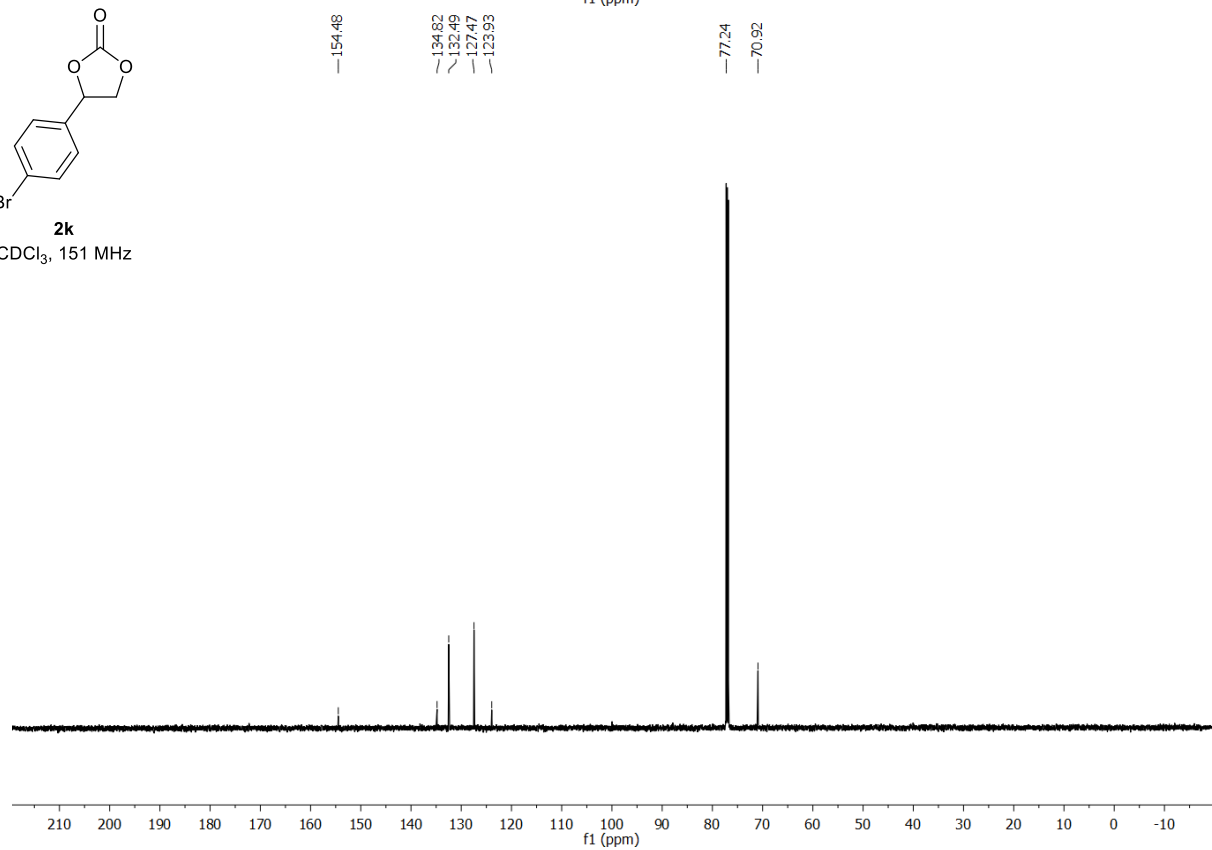


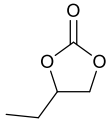


2k
CDCl₃, 600 MHz

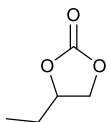
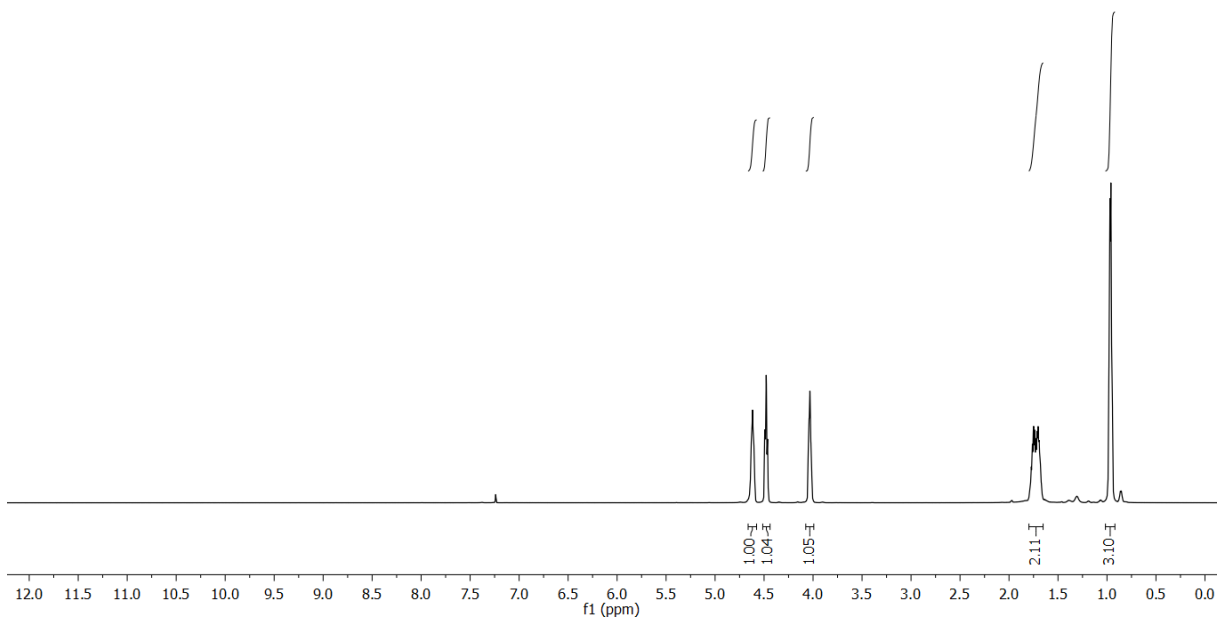


2k
CDCl₃, 151 MHz

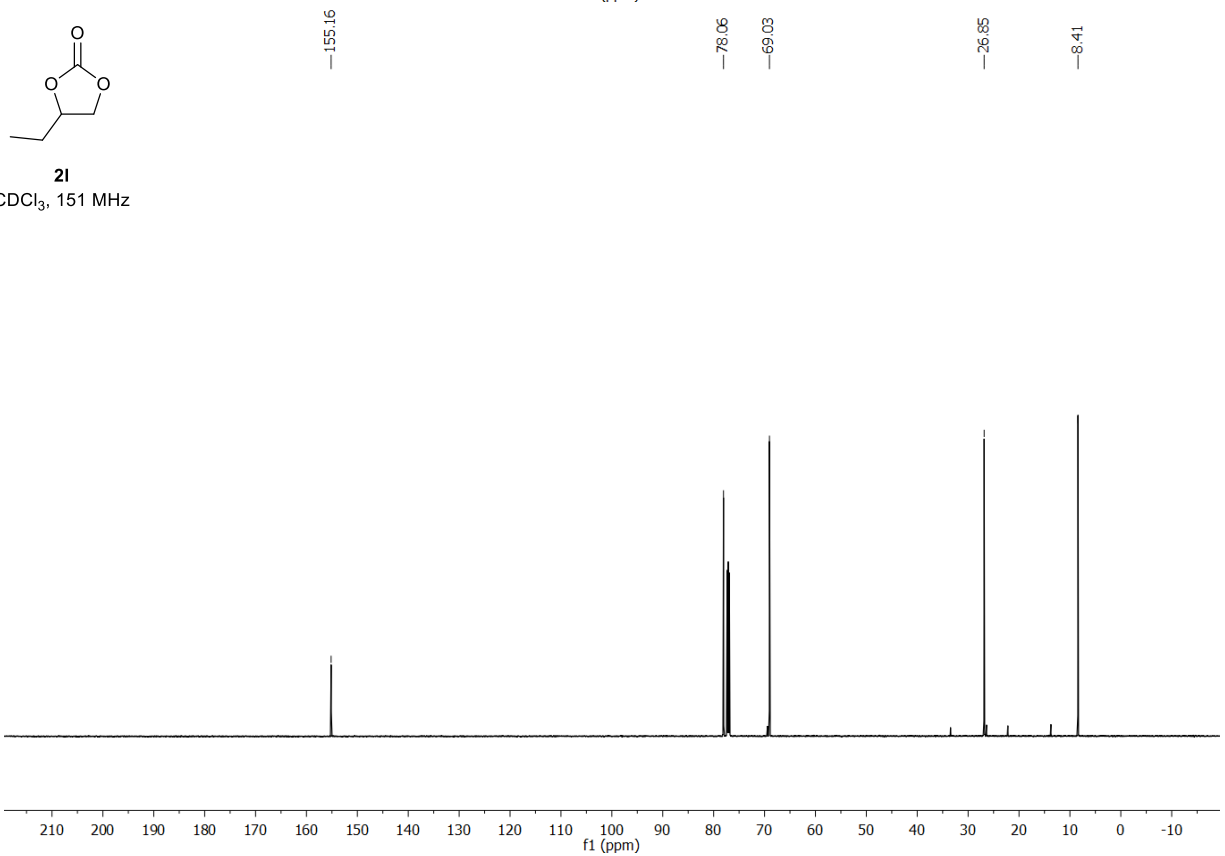


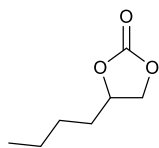


21
CDCl₃, 600 MHz

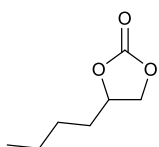
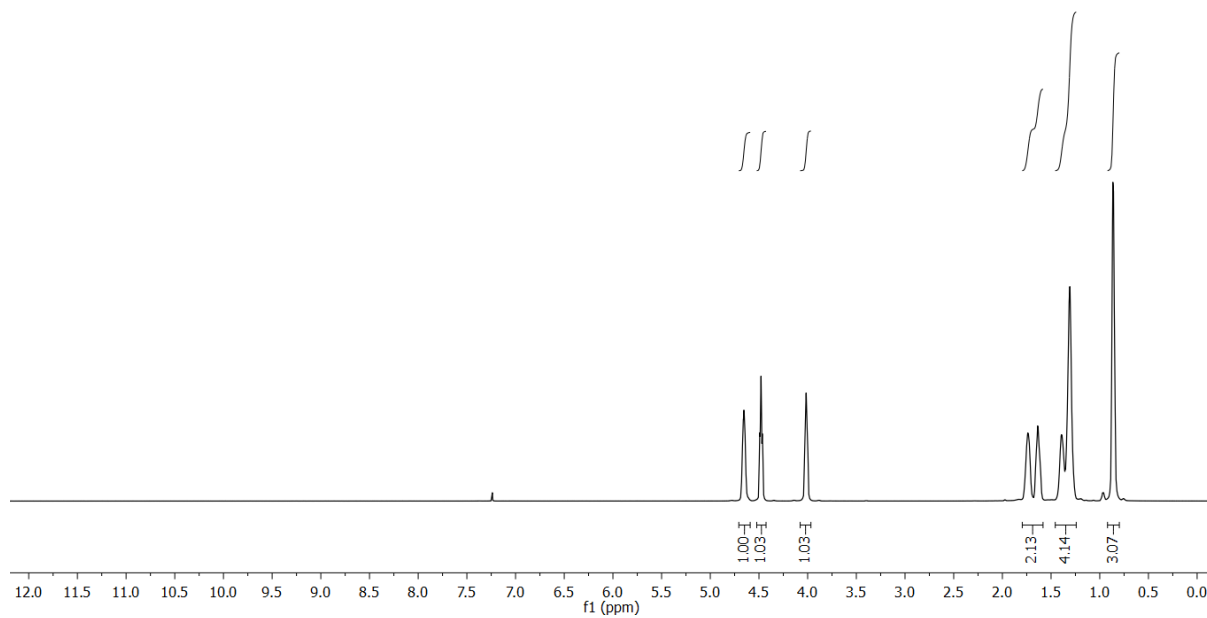


21
CDCl₃, 151 MHz

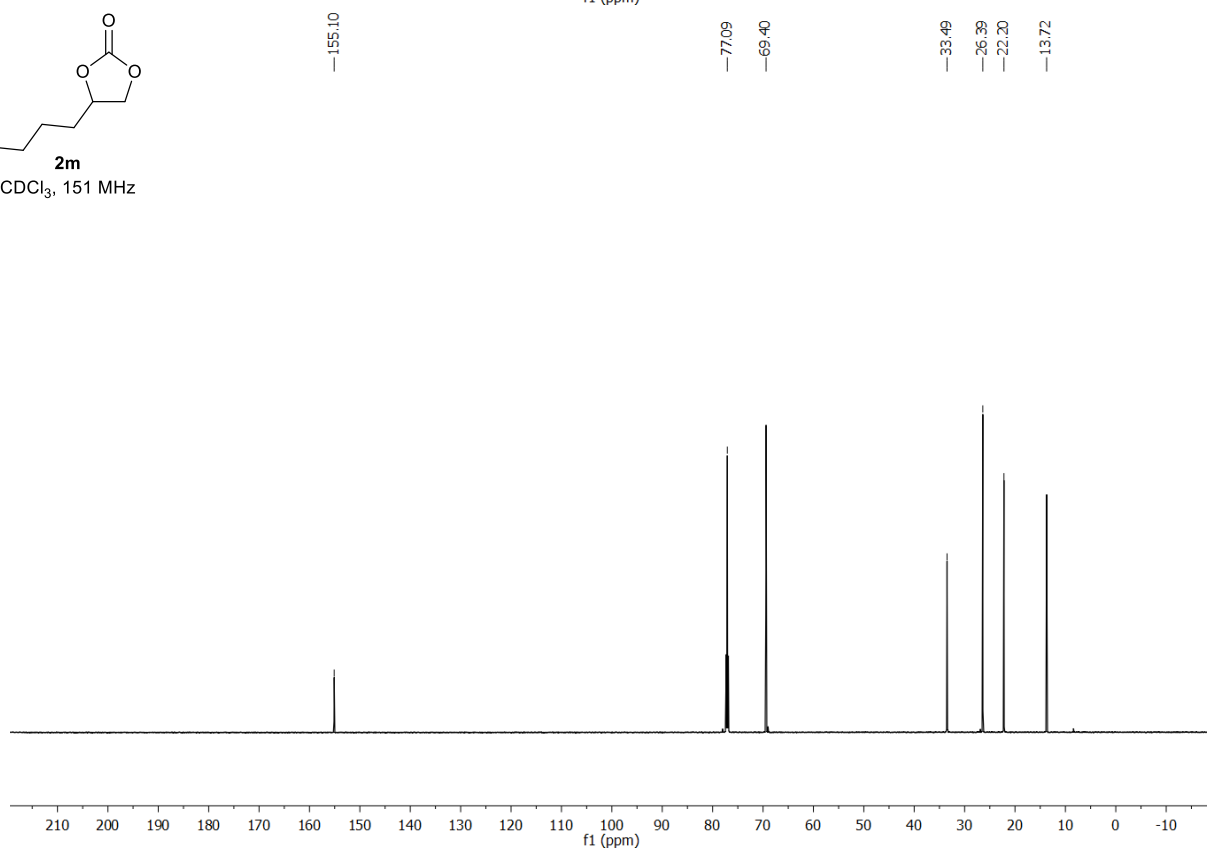


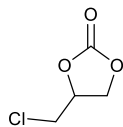


2m
CDCl₃, 600 MHz

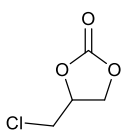
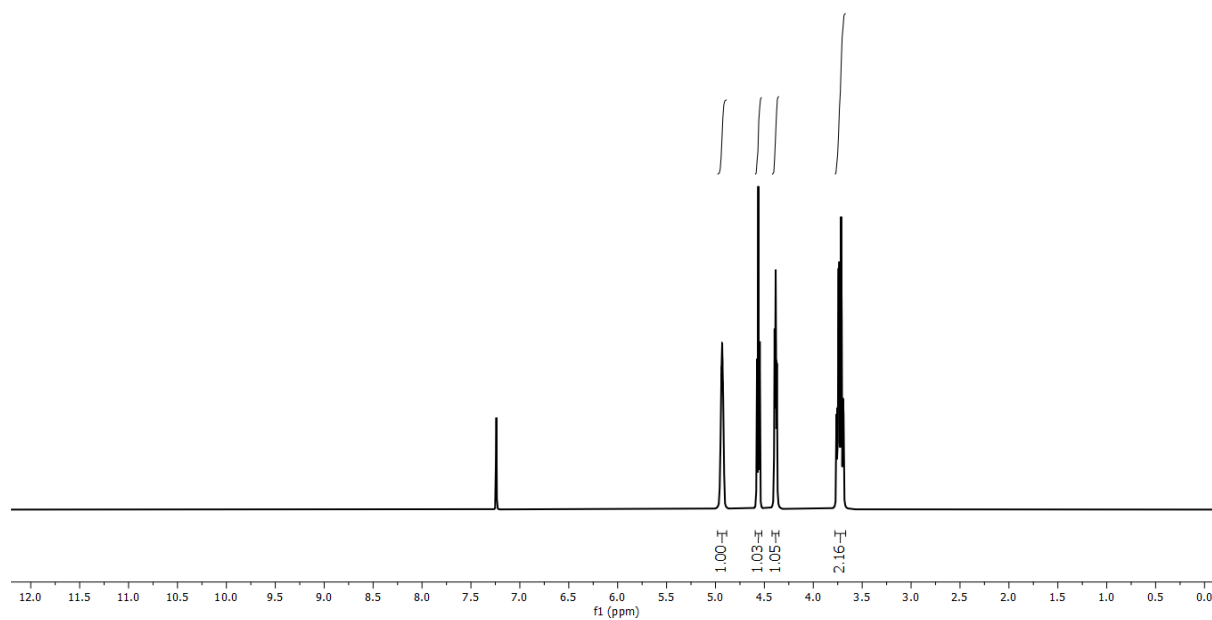


2m
CDCl₃, 151 MHz

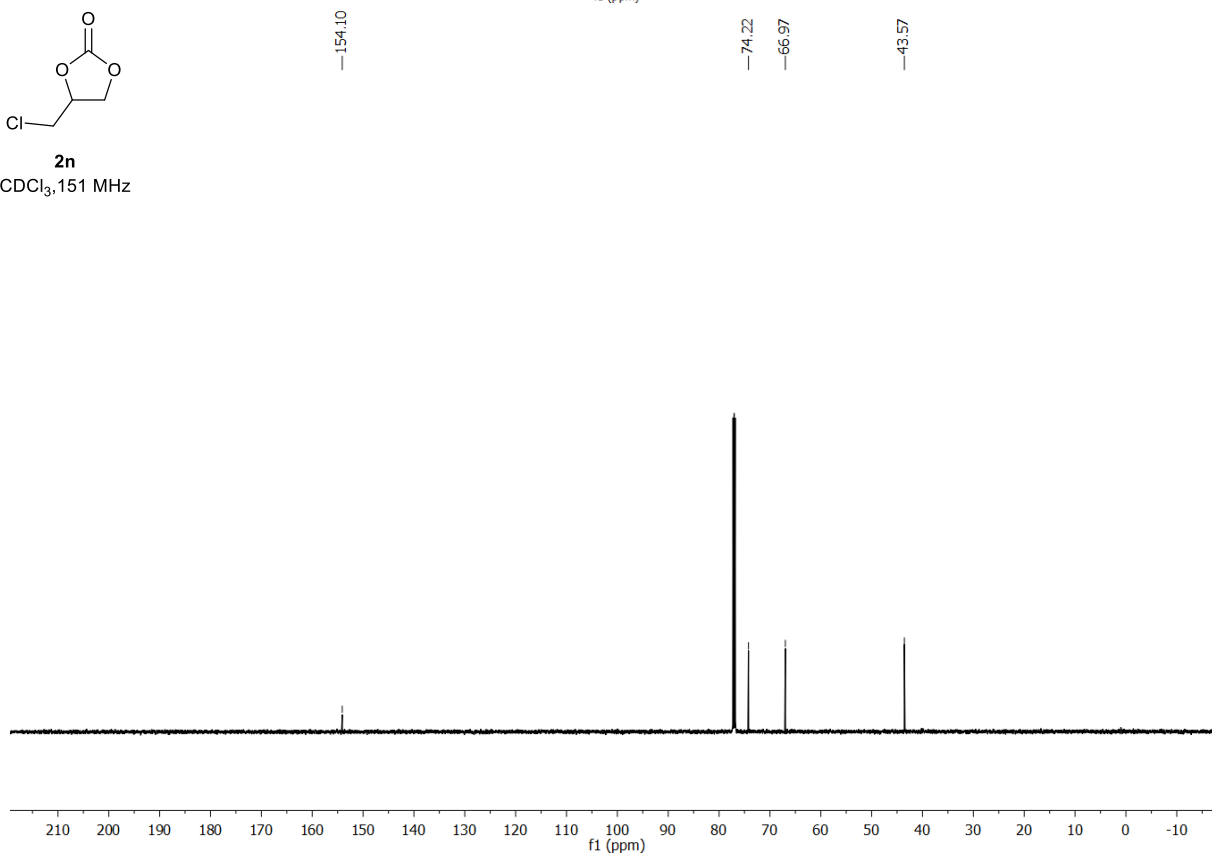


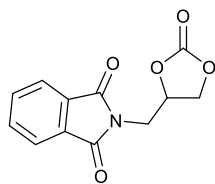


2n
CDCl₃, 600 MHz

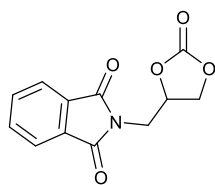
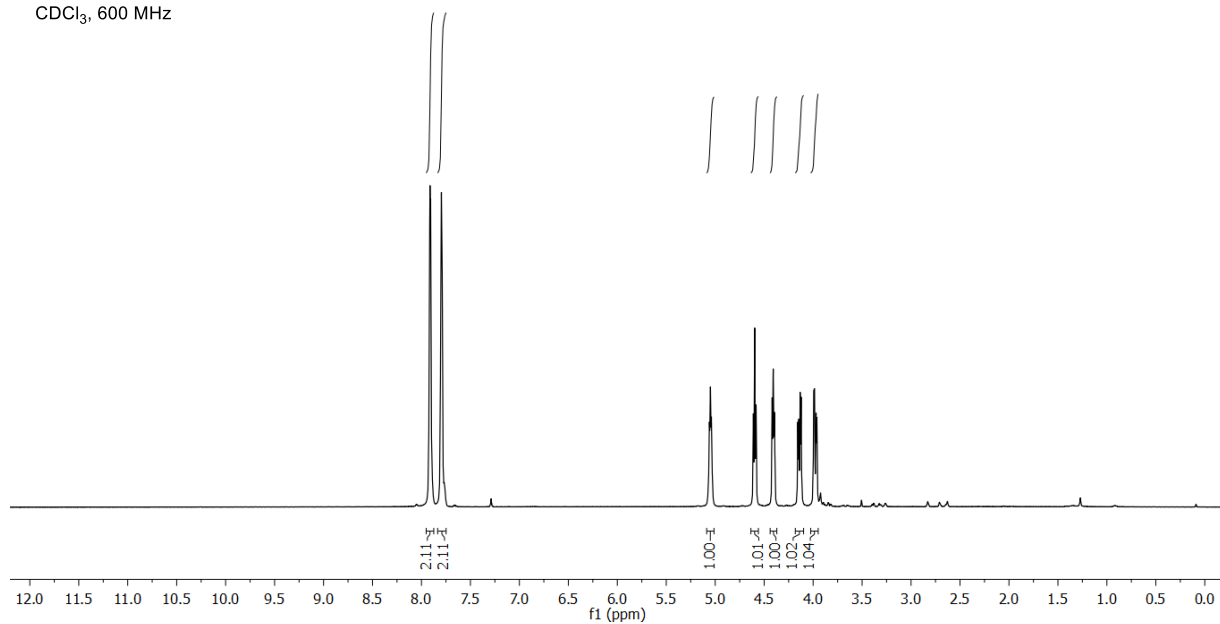


2n
CDCl₃, 151 MHz

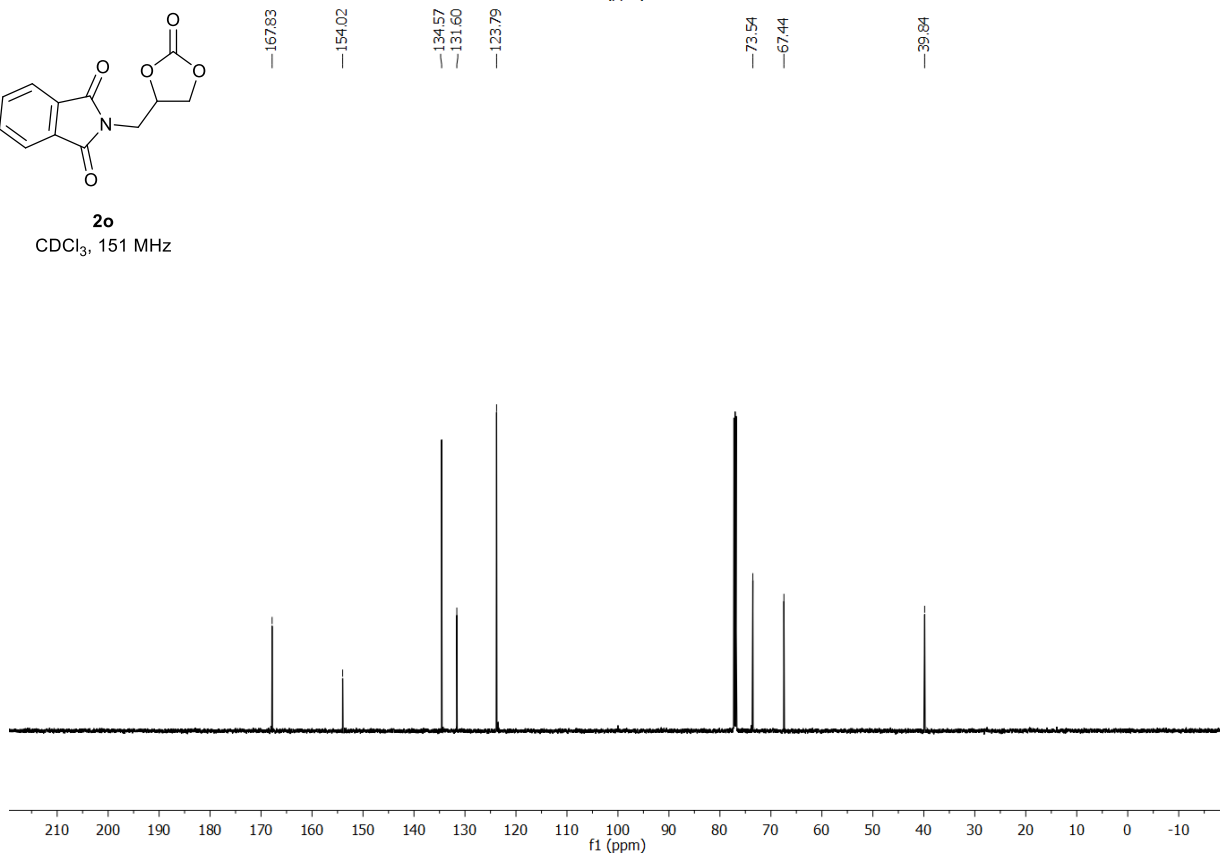


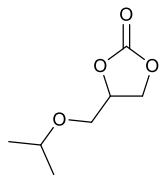


2o
CDCl₃, 600 MHz



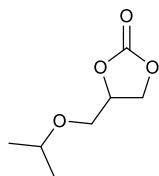
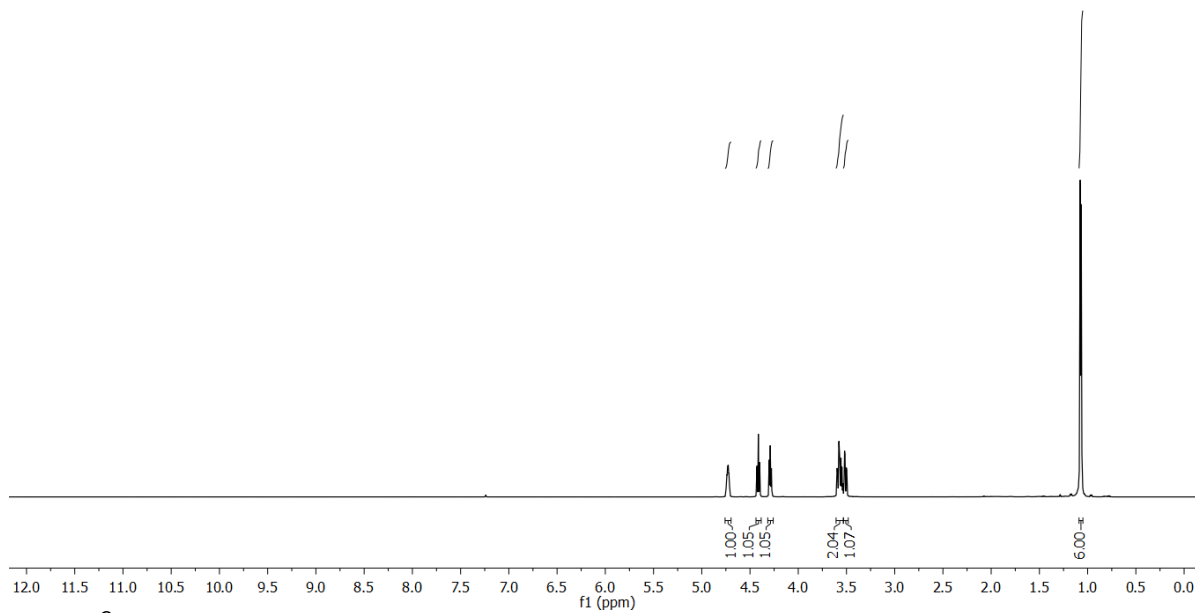
2o
CDCl₃, 151 MHz





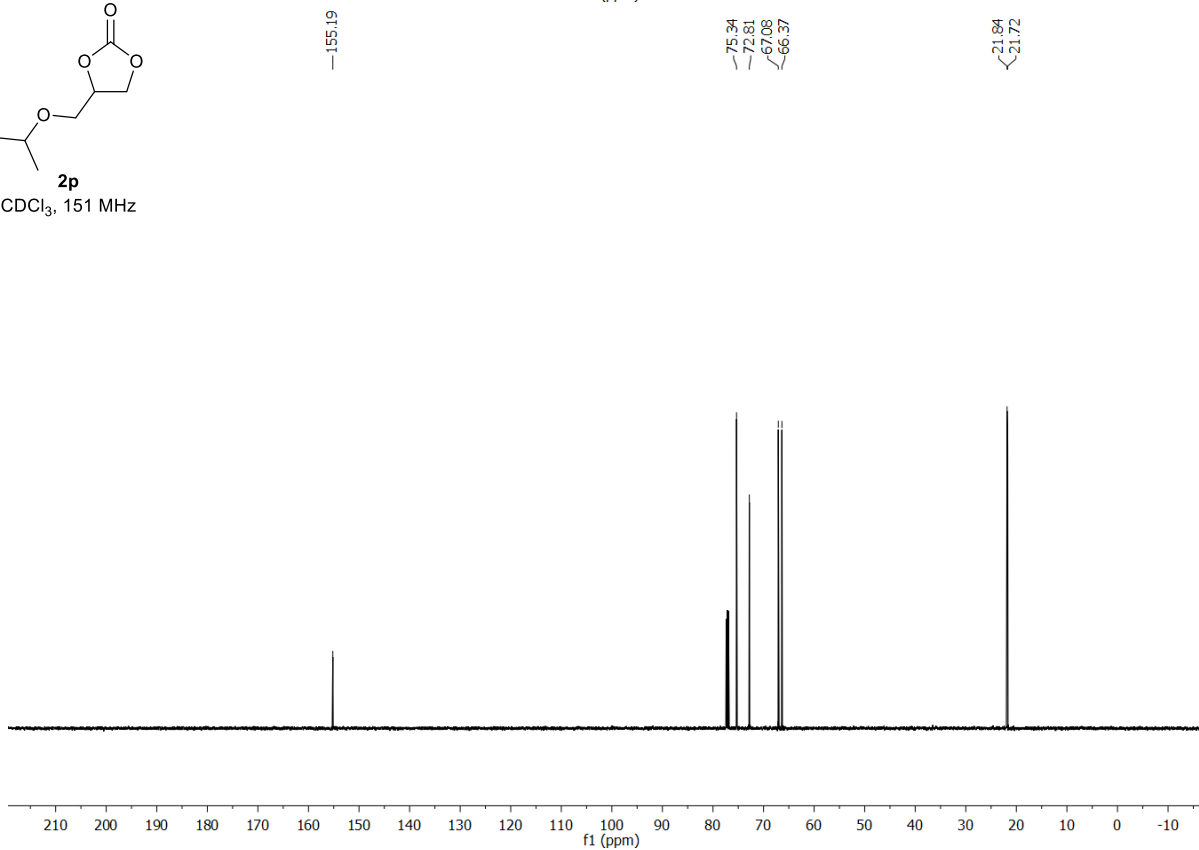
2p

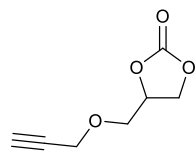
CDCl₃, 600 MHz



2p

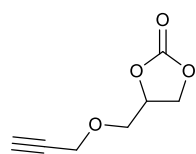
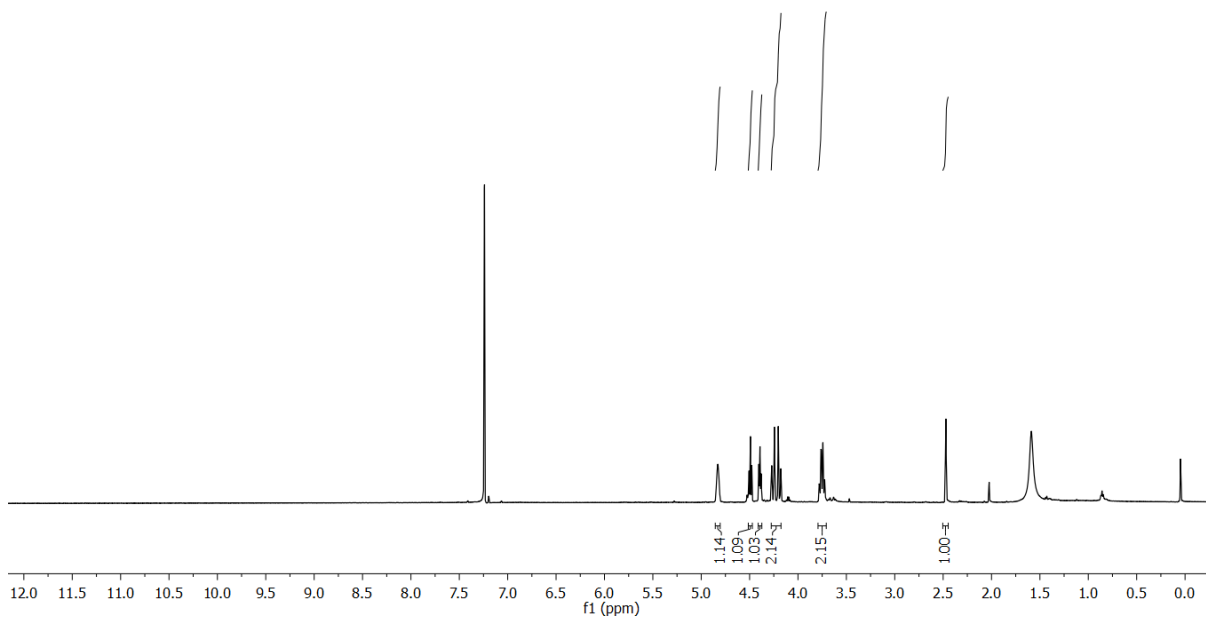
CDCl₃, 151 MHz





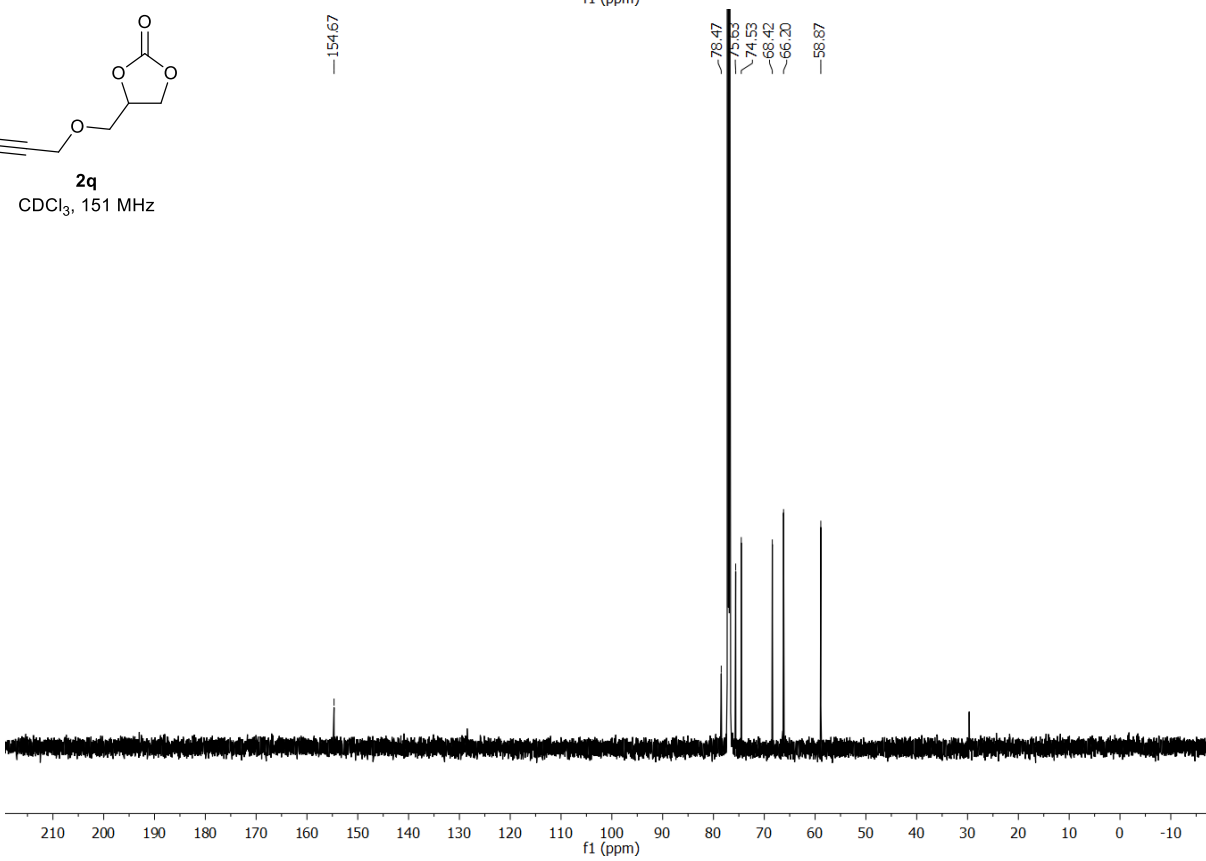
2q

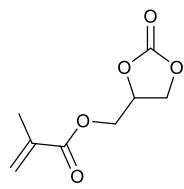
CDCl₃, 600 MHz



2q

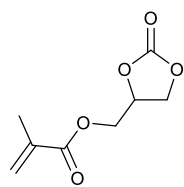
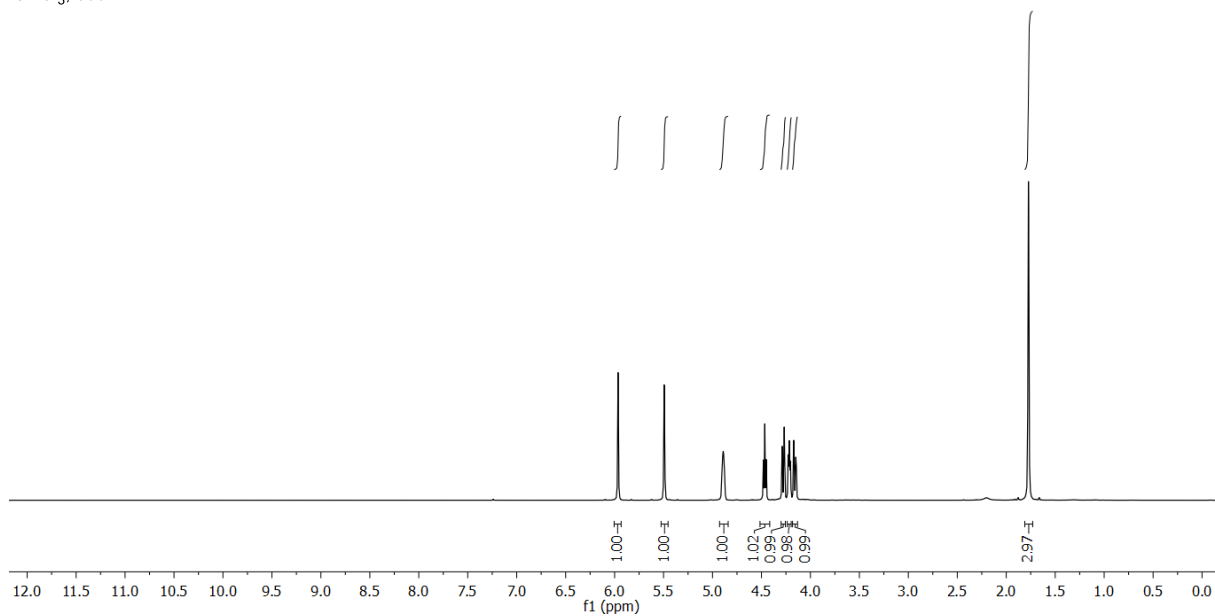
CDCl₃, 151 MHz





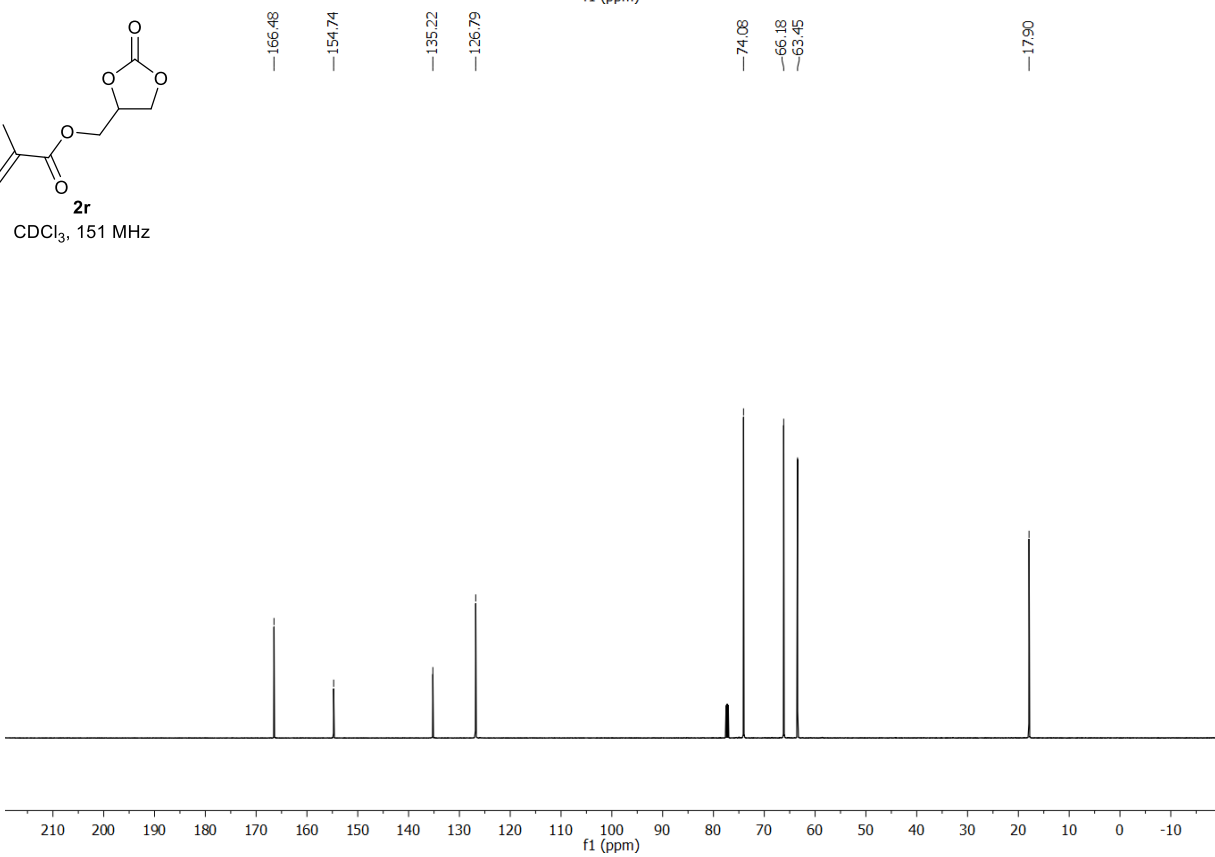
2r

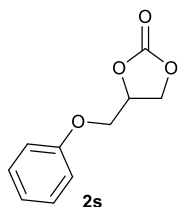
CDCl₃, 600 MHz



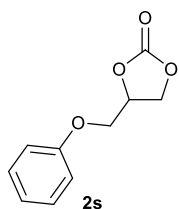
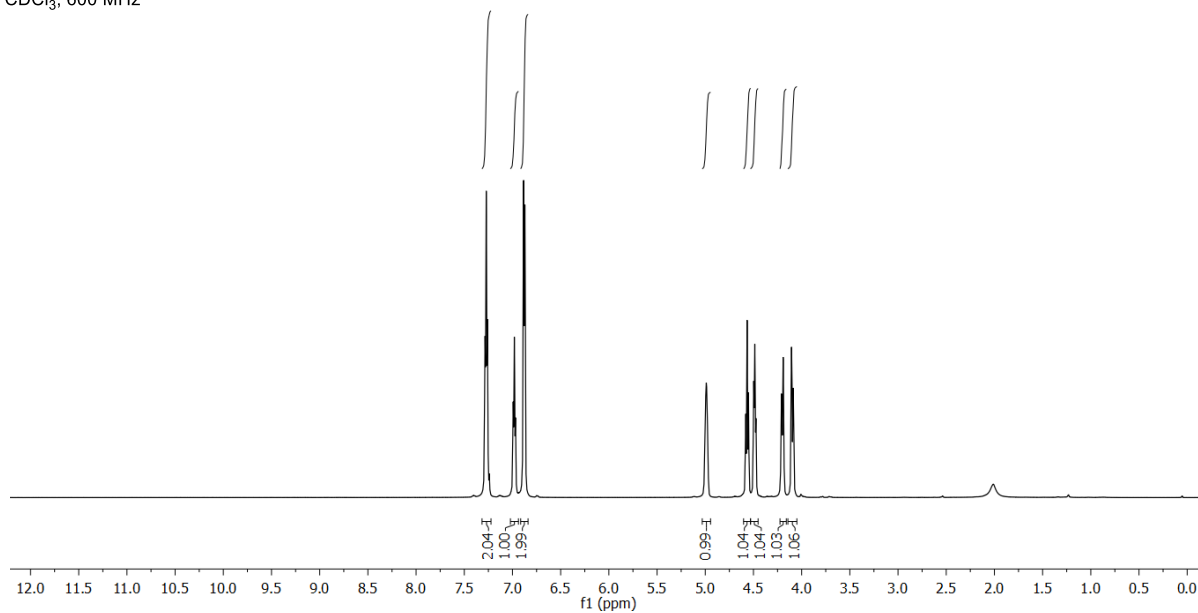
2r

CDCl₃, 151 MHz

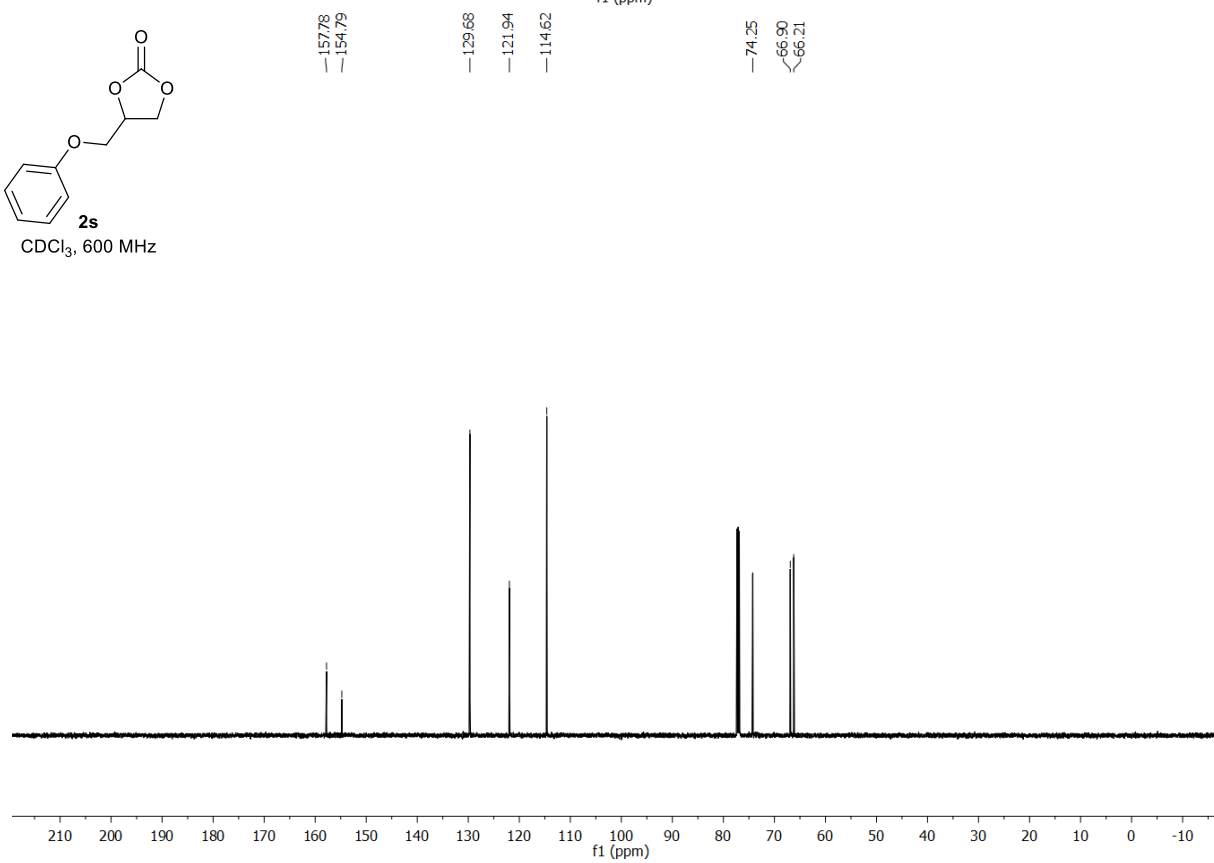


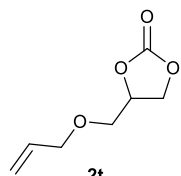


CDCl₃, 600 MHz

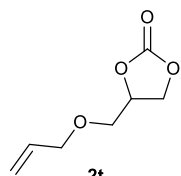
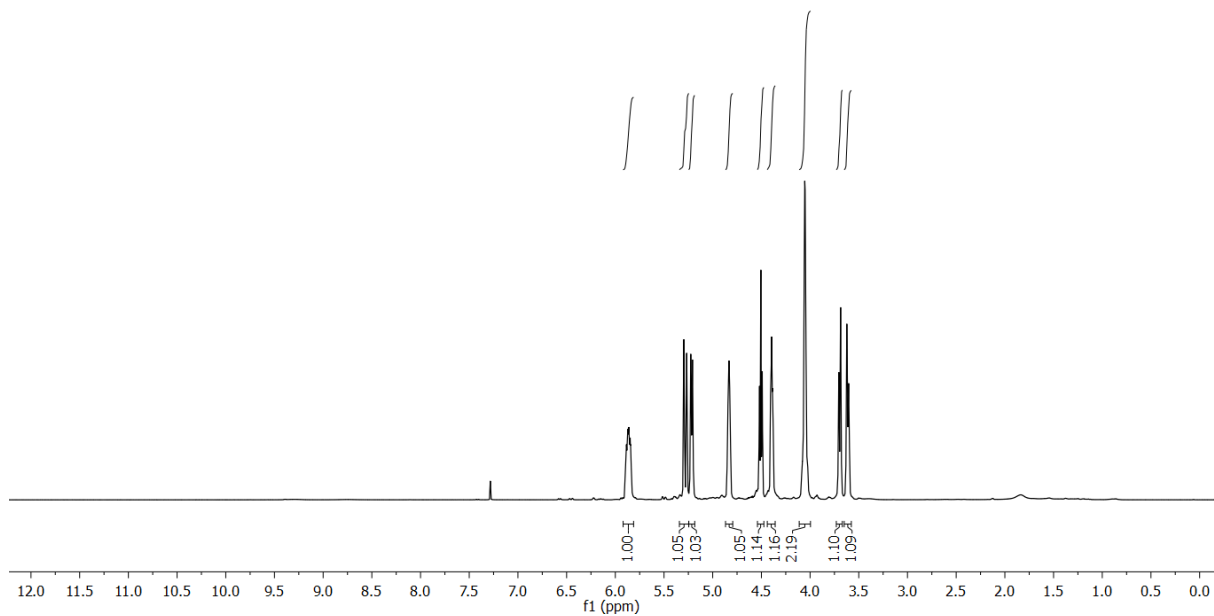


CDCl₃, 600 MHz





CDCl₃, 600 MHz



CDCl₃, 151 MHz

