Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

A One–Pot and Two–stage Baeyer–Villiger Reaction Using 2,2'-Diperoxyphenic Acid under Biomolecule-Compatible Conditions

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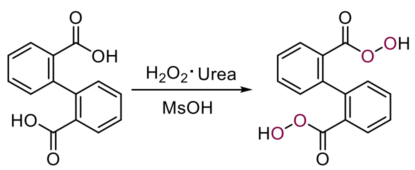
1. General Methods and Materials

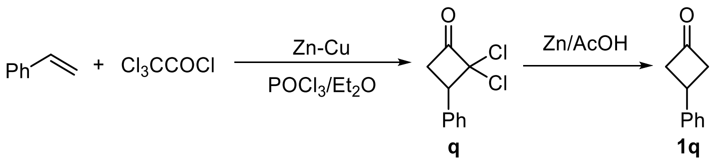
All reactions were carried out directly under open air unless otherwise noted. Commercially available reagents, starting materials and solvents were used without further purification. All reactions were monitored by TLC and visualized by UV lamp (254 nm) or by staining with a solution of 10 g phosphomolybdic acid and 100 mL EtOH followed by heating. Flash column chromatography was performed using 200-300 mesh silica gel. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz or 150 MHz) spectra were obtained on Bruker 400M or 600M nuclear resonance spectrometers or Zhongke-Niujin ((Quantum-I Plus 400M)). HRMS (ESI) was recorded using an Agilent 6520 accurate-Mass Q-TOF spectrometer and HRMS (EI) was recorded using waters GTC. Coupling constants are reported in Hertz (Hz). The enantiomeric excesses were determined by HPLC analysis using an Agilent 1260 Infinity II LC system (column Daicel Co. CHIRALCEL AS-H; eluent: hexane/2-propanol). Data for ^{1}H-NMR spectra were reported as follows: chemical shift *(*ppm, referenced to protium; s = singlet, br s= broad singlet, d = doublet, t = triplet, q = quartet, p = quintet, dd = doublet of doublets, td = triplet of doublets, m = multiplet, coupling constant (Hz), and integration). Data for ^{1}H-NMR were reported in (ppm) relative to residual solvent peak ($CDCl_3$: 7.26 ppm, $(CD_3)_2SO$: 2.50 ppm) and $(CD_3)_2CO$: 2.05 ppm). Data for ^{13}C-NMR were reported in (ppm) relative to residual solvent peak ($CDCl_3$: 77.16 ppm, $(CD_3)_2SO$: 39.52 ppm and $(CD_3)_2CO$: 29.84 ppm).

2. General procedure for the preparation of the 2,2'-Diperoxyphenic Acid



Methane sulfonic acid (30 mL) was placed in a round bottomed flask equipped with a large magnetic stirrer bar and immersed in a bath of water at 22 °C. Urea hydrogen peroxide (9.82 g, 104 mmol) was added in a single portion and stirred for 30 seconds. Diphenic acid (35 mmol) was added in a single portion and the reaction stirred vigorously for 24 h. The reaction mixture was poured into a mixture of ice (80 g) and ethyl acetate (100 mL) and the layers separated. The aqueous layer was extracted with ethyl acetate (2 × 100 mL) and the combined organics were washed with $NaHCO_3$ (2 × 50 mL), brine (20 mL) and dried over Na_2SO_4. Removal of the solvent under reduced pressure gave the 2,2'-Diperoxyphenic Acid. 1H NMR (400 MHz, Chloroform-d) δ 11.28 (s, 2H), 8.03 (dd, J = 7.9, 1.3 Hz, 2H), 7.70 (td, J = 7.6, 1.4 Hz, 2H), 7.58 (td, J = 7.7, 1.3 Hz, 2H), 7.32 (dd, J = 7.7, 1.3 Hz, 2H). 13C NMR (101 MHz, CDCl3) δ 168.3, 142.1, 133.3, 130.9, 129.9, 128.39, 124.69. HRMS (ESI), m/z calcd for $C_{14}H_9O_6$ $[M–H]^-$: 273.0404; found: 273.0402

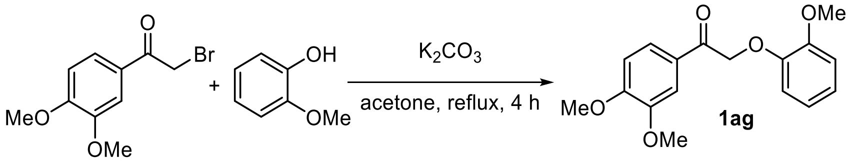
3. General procedure for the preparation of substrates.



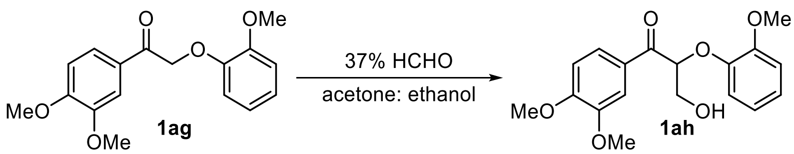
Experimental procedure for the synthesis of the **q**: To a stirred suspension of activated Zn-Cu (1.60 g, 25 mmol) and styrene (10 mmol) in dry Et_2O (20 mL) was added dropwise through an addition funnel, during 2 h at reflux, a solution of trichloroacetic chloride (2.2 mL, 20 mmol) and phosphorus oxychloride (1.9 mL, 20 mmol) in Et_2O (10 mL). The suspension was stirred overnight at reflux. The mixture was cooled to room temperature and then filtered through a pad of Celite. The residue was washed with Et_2O (3 × 15 mL). The organic phase was concentrated in vacuo to give crude products **B**, which were routinely used without further purification to the next step.

Experimental procedure for the synthesis of the cyclobutanones **1q**: The cyclobutanones **1q** were prepared according to the methods reported in the literature with a minor modification.[4] The solution of the previous crude products **q** in acetic acid (10 mL) was added dropwise to a vigorously stirred suspension of zinc dust (2.6 g, 40 mmol) in acetic acid (8 mL) at 0 °C. After the addition, the reaction mixture was heated at 70 °C for 2 h. The mixture was allowed to cool to room temperature and then evacuated to get rid of most of the acetic acid. The residue was dissolved in Et_2O (20 mL) and then poured into a separation funnel containing water (20 mL) and Et_2O

(20 mL). The organic layer was washed with water (3 × 10 mL), saturated sodium bicarbonate solution (2 × 10 mL), brine (50 mL) and dried over Na_2SO_4. The solution was then filtered and concentrated, followed by purification with flash chromatography (petroleum ether/EtOAc = 8/1) to afford the desired pure sample products **1q** which have been reported previously.[1]

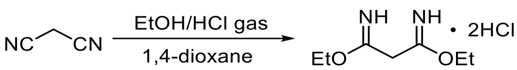


A mixture of 2-methoxyphenol (6.5 g, 25.12 mmol) and K_2CO_3 (5.21 g, 37.68 mmol) was dissolved in acetone (250 ml) with stirred at room temperature for 20 min. After addition of2-Bromo-1-(3,4-dimethoxyphenyl) ethan-1-one in acetone (250 ml), the reaction mixture was reflux for 4 h and cooled to room temperature. The suspension was collected by filtration and washed with acetone and concentrated in vacuo. The solid was dissolved in ethyl acetate and wash with water. The combined organic phases were washed with brine, dried with MgSO4, and concentrated in vacuo. The crude residue was purified by recrystallization from ethanol to give a white solid 1-(3,4-dimethoxyphenyl)-2-(2-methoxyphenoxy) ethan-1-one (**1ag**, 78%). 1H NMR (400 MHz, Chloroform-d) δ 7.70 – 7.64 (m, 1H), 7.59 (d, J = 1.9 Hz, 1H), 6.99 – 6.87 (m, 3H), 6.86 – 6.80 (m, 2H), 5.29 (d, J = 0.9 Hz, 2H), 3.94 (d, J = 7.2 Hz, 6H), 3.88 (d, J = 0.9 Hz, 3H). 13C NMR (101 MHz, CDCl3) δ 193.38, 153.90, 149.78, 149.29, 147.64, 127.91, 122.86, 122.43, 120.90, 114.68, 112.19, 110.48, 110.21, 77.48, 77.16, 76.84, 72.05, 56.22, 56.10, 55.98.

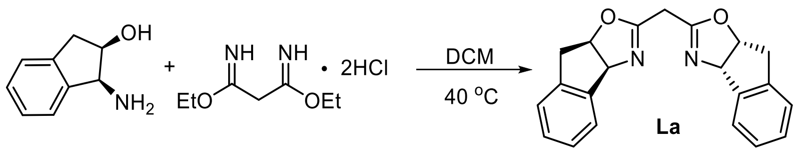


A mixture of 1-(3,4-dimethoxyphenyl)-2-(2-methoxyphenoxy) ethanone (2.0 g, 6.62 mmol), potassium carbonate (1 g, 7.28 mmol) and acetone: ethanol (v/v=1:1, 34 ml) was added a water solution of formaldehyde (37%) (0.4 g, 13.23 mmol) at room temperature for 4 h. After the reaction mixture was filtered and concentrated in vacuo. The syrup product was poured into water and extracted with ethyl acetate. The crude was purified by column chromatography (petroleum ether/ethyl acetate, 1:1) to give adduct 1-(3,4-dimethoxyphenyl)-3-hydroxy-2-(2-methoxyphenoxy) propan-1-one (**1ah**, 68%) which have been reported previously.[2] 1H NMR (400 MHz, Chloroform-d) δ 7.70 – 7.64 (m, 1H), 7.59 (d, J = 1.9 Hz, 1H), 6.99 – 6.87 (m, 3H), 6.86 – 6.80 (m, 2H), 5.29 (d, J = 0.9 Hz, 2H), 3.94 (d, J = 7.2 Hz, 6H), 3.88 (d, J = 0.9 Hz, 3H). 13C NMR (101 MHz, CDCl3) δ 195.11, 154.01, 150.14, 149.25, 146.96, 128.06, 123.67, 123.31, 121.23, 117.49, 112.31, 110.98, 110.20, 84.15, 77.48, 77.16, 76.84, 63.78, 56.17, 56.02, 55.85.

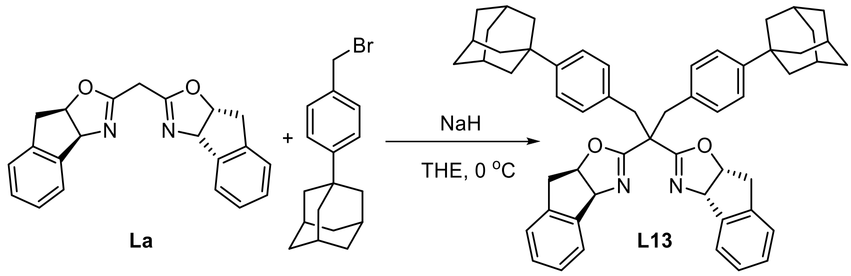
4. General experimental procedures for catalyst



A solution of malonodinitrile (10.00 g, 151 mmol) in dry 1,4-dioxane (200 mL) was added dropwise to a mixture of dry ethanol (18.0 mL, 312 mmol) and 1,4-dioxane (350 mL) over 4.5 h at 0–5 °C, while gaseous HCl was continuously passed through the reaction vessel. The stream of HCl was continued for 1.5 h after addition was completed, whereupon the reaction mixture was allowed to warm up to r.t. and stirred for 12 h. The precipitate formed was filtered off, washed thoroughly with dry 1,4-dioxane and ether, and dried in high vacuum to afford dihydrochloride salt (22.18 g, 93%) as a white powder.



(1*S*,2*R*)-(–)-*cis*-1-Amino-2-indanol (1.08 g, 7.24 mmol, 2.1 equiv) and diethyl malonimidate dihydrochloride (0.80 g, 3.46 mmol, 1.0 equiv) were taken up in CH_2Cl_2 (80 mL), and the resulting suspension was refluxed for 16 h. Upon completion, the reaction contents were poured into water (160 mL) and extracted with CH_2Cl_2 (4 × 40 mL). The combined organic layers were dried ($MgSO_4$), filtered and concentrated. The resultant crude product was recrystallized from *i*-PrOH (100 mL). The mother liquor was concentrated, and a second recrystallization was performed with *i*-PrOH (30 mL) to provide ligand **Ligand a** (0.853 g from first crop, 0.071 g from second crop, 81% yield overall) as thin white needles, 1H NMR (400 MHz, Chloroform-d) δ 7.39 (dd, J = 6.6, 2.1 Hz, 2H), 7.18 (m, J = 5.9, 3.7, 2.8 Hz, 6H), 5.49 (d, J = 8.0 Hz, 2H), 5.27 (m, J = 8.2, 7.0, 1.8 Hz, 2H), 3.31 (dd, J = 18.0, 7.0 Hz, 2H), 3.19 (d, J = 1.1 Hz, 2H), 3.09 (dd, J = 18.0, 1.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 141.7, 139.8, 128.6, 127.6, 125.6, 125.4, 83.7, 76.8, 39.8, 28.8.



NaH [60 % dispersion in mineral oil] (0.12 g, 3.0 mmol) was added to a solution of **La** (0.20 g, 0.6 mmol) in anhydrous THF (20 mL) at room temperature under N_2 atmosphere. The mixture was then cooled to 0 ℃ and a solution of 4-AdaMantyl benzyl bromide (0.68 g, 3.0 mmol) in THF (10 mL) was slowly added with stirring. The reaction mixture was slowly warmed to room temperature. When the reaction was complete (monitored by TLC), the reaction mixture was poured into saturated aqueous NH4Cl (15 mL) and H2O (50 mL), extracted with CH2Cl2 (50 mL×3). The combined organic layers were dried over anhydrous Na2SO4, filtered, and concentrated. The residue was purified by flash chromatography (hexane/acetone, 10/1) affording **L13** as white solid (336 mg, 90%),1H NMR (400 MHz, Chloroform-d) δ 7.47 (d, J = 7.4 Hz, 1H), 7.34 (m, J = 15.7, 7.8 Hz, 3H), 6.81 (d, J = 8.2 Hz, 2H), 6.73 (d, J = 8.2 Hz, 2H), 5.60 (d, J = 7.9 Hz, 1H), 5.31 (t, J = 7.2 Hz, 1H), 3.34 (dd, J = 18.1, 6.8 Hz, 1H), 3.21 (d, J = 14.1 Hz, 1H), 3.10 – 2.96 (m, 2H), 2.11 – 2.03 (m, 3H), 1.85 – 1.71 (m, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.6, 149.2, 141.7, 140.0, 133.2, 130.1, 128.5, 127.6, 126.0, 125.2, 124.2, 83.4, 76.6, 47.8, 43.2, 39.5, 38.0, 37.0, 36.9, 36.9, 29.1. HRMS (ESI), m/z calcd for $C_{55}H_{59}N_2O_2$ $[M + H]^+$: 779.4572; found: 779.4572.

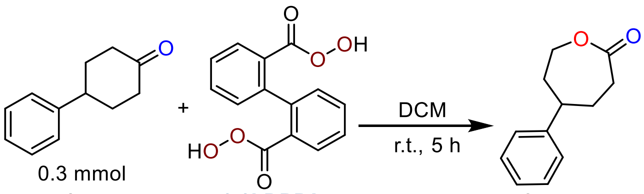
5. General experimental procedures for lactones

A solution of appropriate ketones (0.3 mmol) and **2,2'-DPPA** (0.225 mmol) in 3 mL DCM, H_2O and 1× PBS, in a standard Schlenk tube at room temperature, respectively. After the completion of the reaction monitored by TLC, the reaction was concentrated in vacuum and purified by column chromatography using petroleum ether/ethyl acetate to afford corresponding products, partially known compounds date is consistent with literature.

6. Procedure and Results of Sensitivity Assessment

Table S1 General description of experiments included in one sensitivity assessment

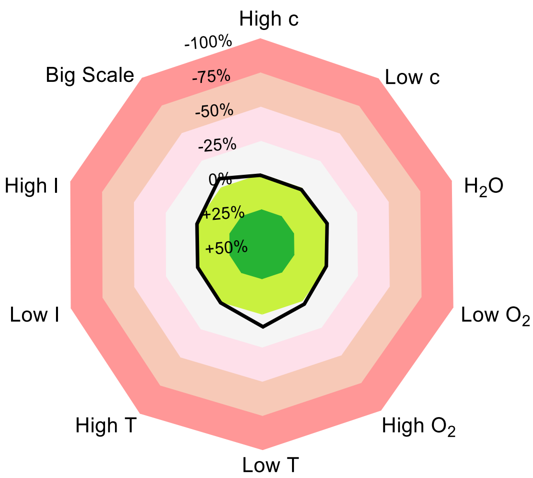
High *c*	2.7 mL solvent	Low *T*	35 °C
Low c	3.3 mL solvent	High *T*	15 °C
High H_2O	30 μL H_2O_2	Low *I*	dark
Low O_2	N_2	High *I*	blue LED
High O_2	O_2	Big scale	6 mol (1.032 g)



0.3 mmol **1a** + **2,2'-DPPA** → **2a**

Number	Experiment	Yield 1 / %	Yield 2 / %	Average Y. / %	Deviation / %
1	High *c*	99	99	99	0
2	Low c	98	98	98	-1
3	High H_2O	97	99	98	-1
4	Low O_2	99	99	99	0
5	High O_2	98	96	97	-2
6	Low *T*	91	89	90	-9
7	High *T*	97	99	98	-1
8	Low *I* (dark)	99	98	98.5	-0.5
9	High *I* (blue LED)	99	99	99	0
10	control	99	99	99	
11	Big scale	92	93	92.5	-6.5

Radar diagram:

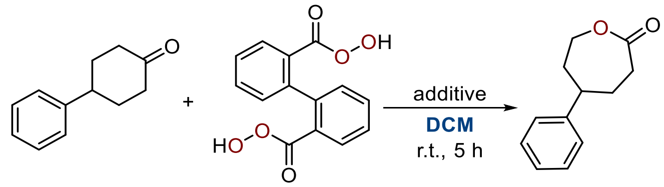


7. Additive-Based Robustness Screen

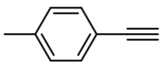
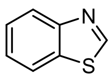
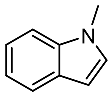
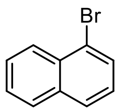
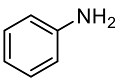
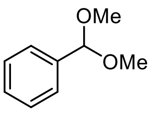
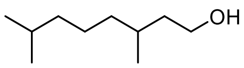
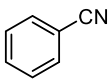
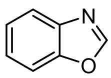
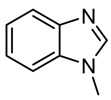
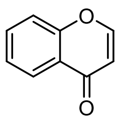
In order to evaluate the robustness and the functional group preservation of the investigated reactions, we decided to apply an intermolecular additive-based screen to these transformations. This screening evaluates the tolerance of a given reaction to a series of additives (robustness), as well as the stability of these additives to the reaction conditions (functional group preservation).

A solution of appropriate **1a** (52.3 mg, 0.3 mmol), **2,2'-DPPA** (62 mg, 0.225 mmol) and additives (0.3 mmol) in DCM, H_2O and 1XPBS in a standard Schlenk tube at room temperature, After the completion of the reaction monitored by TLC, the reaction was concentrated in vacuum and purified by column chromatography using petroleum ether/ethyl acetate to afford corresponding products.

Table S2. Robustness Screen in DCM

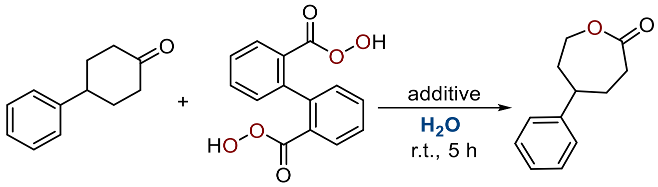


1a + **2,2'-DPPA** → **2a**

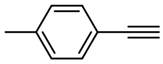
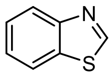
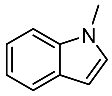
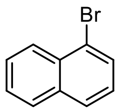
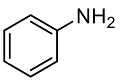
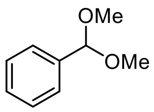
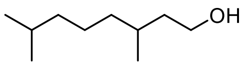
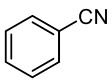
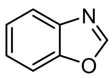
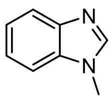
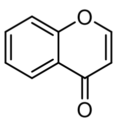
Entry	Additive	yield of **C** (%)	Additive remainning (%)	SM remainning (%)
1	None	99	–	
2		99 √	97 √	0
3		42 –	80 √	56
4		0 x	0 x	96
5		99 √	98 √	0
6		26 x	10 x	70
7		95 √	13 x	0
8		97 √	98 √	0
9		98 √	95 √	0
10		84 √	0 x	13
11		37 –	0 x	61
12		76 √	99 √	21

The standard reaction is undertaken in the presence of one molar equivalent of the given additive.The yield of **2a**, and the additive and starting material remaining after reaction is given. Colour coding should helpthe ready assessment of the data: green '✓' (above 66%), yellow '-' (34 - 66%), red 'x' (below 34%). Isolated yield. SM is starting material.

Table S3. Robustness Screen in pure water.

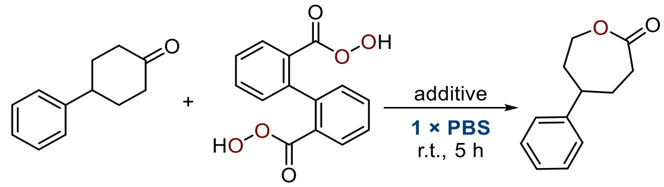


1a **2,2'-DPPA** **2a**

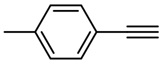
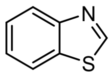
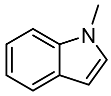
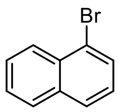
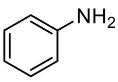
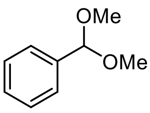
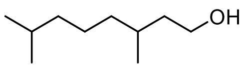
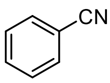
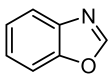
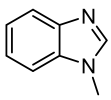
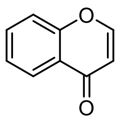
Entry	Additive	yield of **C** (%)	Additive remainning (%)	SM remainning (%)
1	None	99	–	
2		99 √	96 √	0
3		53 –	84 √	43
4		0 ×	0 ×	97
5		99 √	97 √	0
6		13 ×	18 ×	84
7		84 √	16 ×	13
8		97 √	95 √	0
9		99 √	95 √	0
10		79 √	0 ×	18
11		47 –	0 ×	50
12		84 √	99 √	13

The standard reaction is undertaken in the presence of one molar equivalent of the given additive.The yield of **2a**, and the additive and starting material remaining after reaction is given. Colour coding should helpthe ready assessment of the data: green '✓' (above 66%), yellow '-' (34 - 66%), red 'x' (below 34%). Isolated yield. SM is starting material.

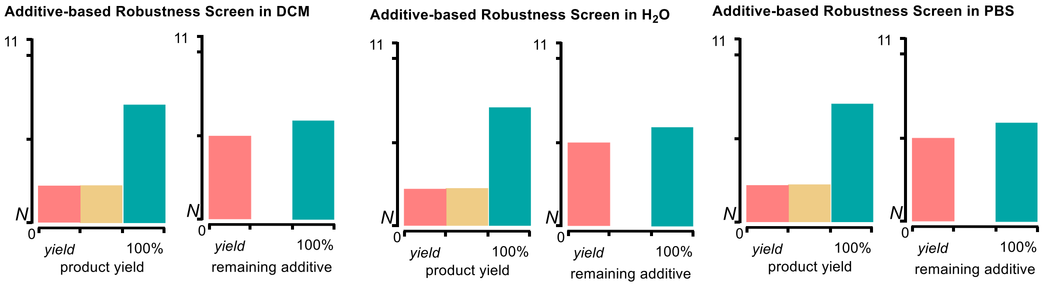
Table S4. Robustness Screen in 1XPBS.



1a **2,2'-DPPA** **2a**

Entry	Additive	yield of **c** (%)	Additive remainning (%)	SM remainning (%)
1	None	99	–	
2		97 √	96 √	0
3		37 –	85 √	60
4		0 ×	0 ×	97
5		95 √	97 √	0
6		0 ×	0 ×	96
7		87 √	11 ×	10
8		97 √	95 √	0
9		98 √	95 √	0
10		89 √	0 ×	10
11		55 –	0 ×	41
12		71 √	97 √	23

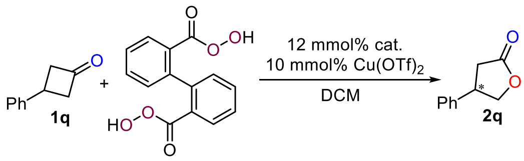
The standard reaction is undertaken in the presence of one molar equivalent of the given additive.The yield of **2a**, and the additive and starting material remaining after reaction is given. Colour coding should helpthe ready assessment of the data: green '✓' (above 66%), yellow '-' (34 - 66%), red 'x' (below 34%). Isolated yield. SM is starting material.

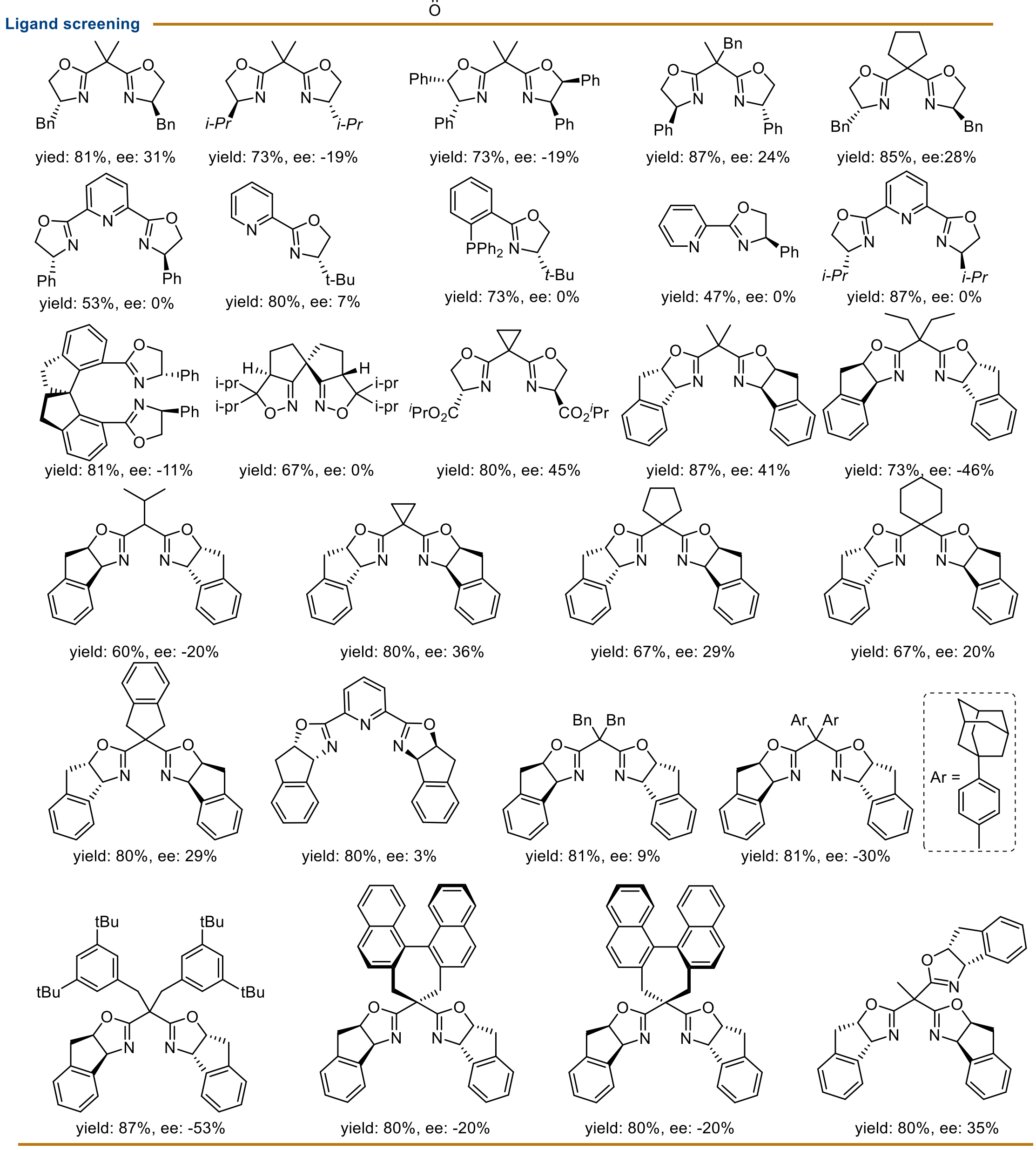


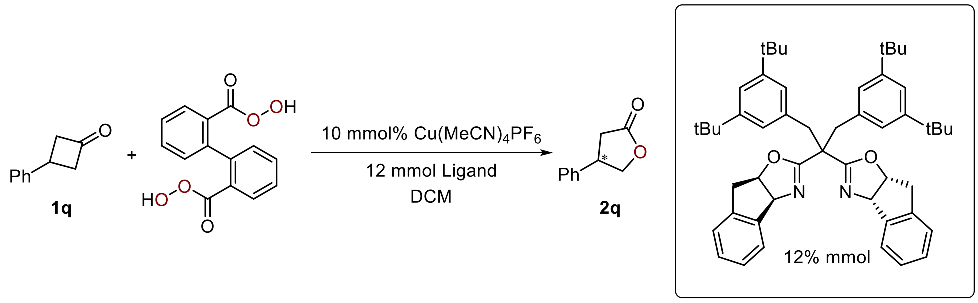
Scheme S1 Additive-based Robustness screen in DCM, H_2O and PBS.

8. A catalytic asymmetric version of the BV reaction.

Table S5 Ligand screening



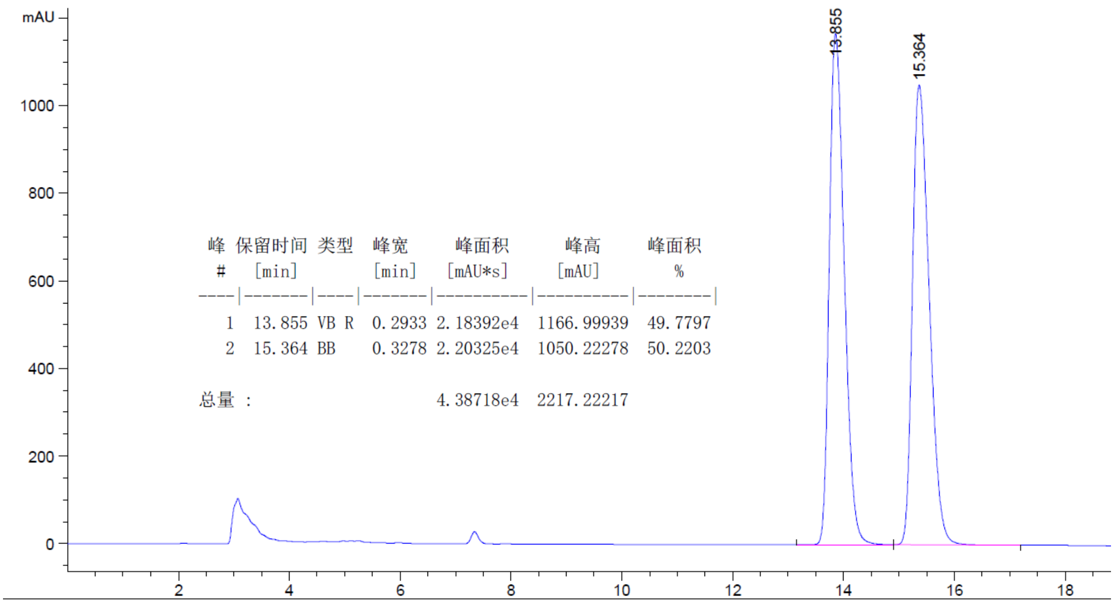




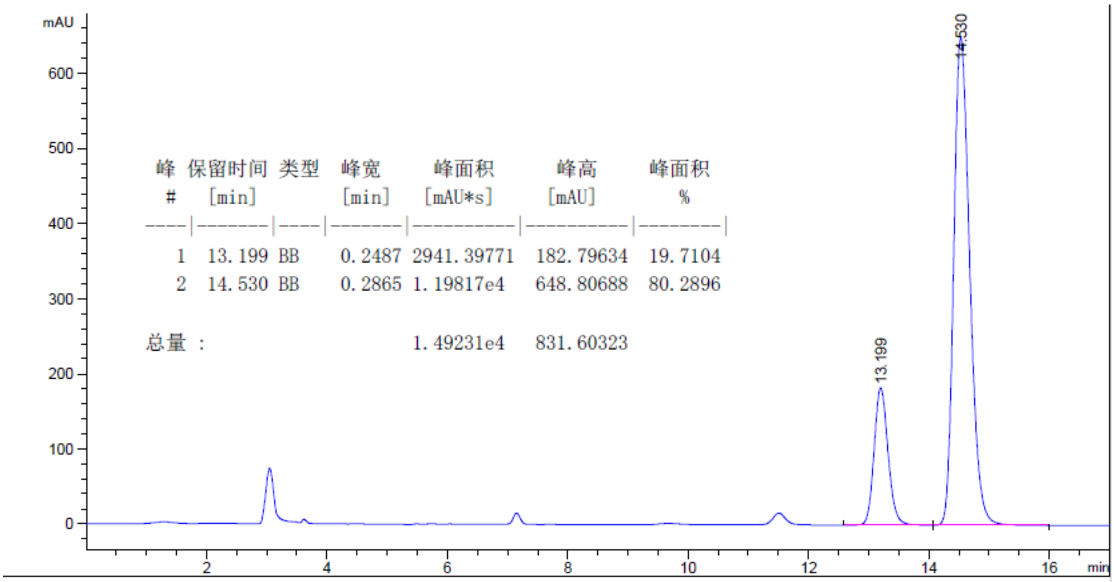
In a dried sealed 25 mL Schlenk tube, **L12** (8.8 mg, 0.012 mmol, 12 mmol %), $Cu(CH_3CN)_4PF_6$ (3.6 mg, 0.01 mmol, 10 mmol %) were dissolved in dry DCM under N_2, and the mixture was stirred for 1 h at room temperature. Then **1q** (14.6 mg, 0.1 mmol) and 2,2'-DPPA (15 mg, 0.055mmol) were added sequentially at room temperature and stirred for 3 h. According to the same workup procedure, the residue was purified by chromatography (PE/EA = 15:1) to give product 2q (14 mg, 87% yield, 60% ee) as light-yellow oil.

HPLC analysis: DAICEL CHIRALPAK AS-H, n-hexane/isopropanol = 80/20, 1.0 mL/min, λ = 210 nm, t_R (major) = 13.2 min, t_R (minor) = 14.5 min, ee = 60%.

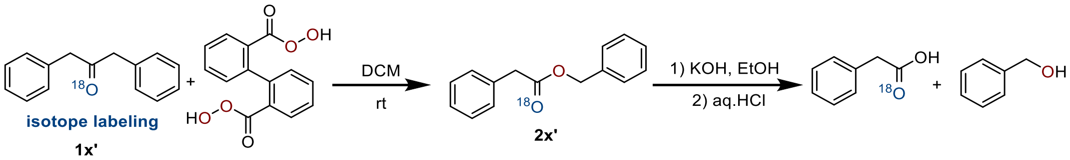
Chiral HPLC spectrum of (rac)-**2q**



Chiral HPLC spectrum of (S)-**2q**



9. Oxygen Labelling Experiment



A solution of **1x'** and **2,2'-DPPA** in DCM, after stirred for 16 h, After the completion of the reaction monitored by TLC, the reaction was concentrated in vacuum and purified by column chromatography using petroleum ether/ethyl acetate to afford corresponding products.

A solution of **2x'** (0.4 mmol, 90 mg) and KOH (90 mg, 1.6 mmol, 4 equiv) in a mixture 4 mL EtOH and 2 mL water, reflux for 8 hours, then reduced pressure to remove the solvent. The residue was extracted twice with ethyl acetate and then the combined organic phases were washed with brine and dried over Na_2SO_4. After removal of the solvent, the crude mixture was purified by column chromatography on silica gel to afford the compound benzyl alcohol. The water phases were added HCl and extracted twice with ethyl acetate, then the combined organic phases were washed with brine and dried over Na_2SO_4. After removal of the solvent, the crude mixture was purified by column chromatography on silica gel to afford the compound phenylacetic acid. The benzyl alcohol was analyzed by GC mass, and the phenylacetic was analyzed by HR-EI-MS spectra. The result is shown below:

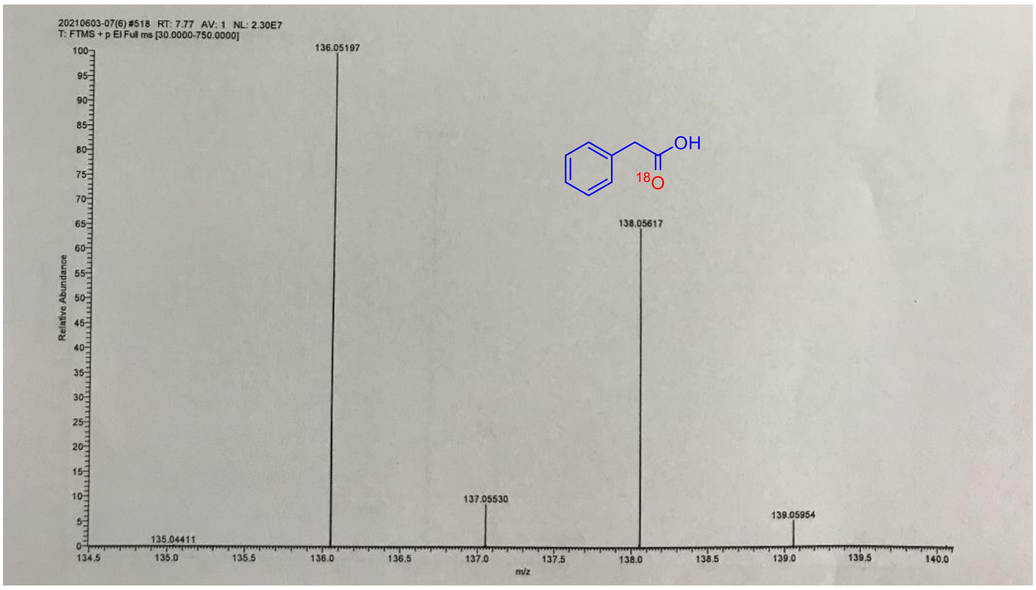
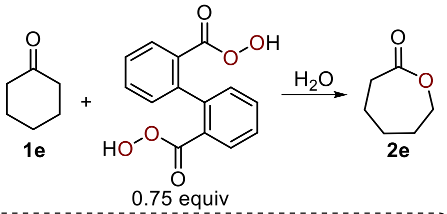


Figure S1 The ^{18}O-labeled result.

10. Green chemistry metrics analysis

Table S6. E-Factor, AE, RME, PMI, CE and atom efficiency for 1e, 1ae, 1af and 1ag using 2,2'-DPPA (This Work):



98.15	274.23	114.14
29.4 mg	61.7 mg	31.8 mg

Total amount of reactants: 29.4 mg + 61.7 mg = 91.1 mg
Amount of final product: 31.8 mg
Amount of waste: 91.1 mg - 31.8 mg = 59.3 mg
E-Factor = Amount of waste/Amount of product = 59.3/31.8 = 1.86

Molecular weight of product: 114.14
Sum of molecular weight of reagent: 98.15 + 274.23 ×0.75 = 303.82
Atom economy = Molecular weight of product/Sum of molecular weight of reagent = 114.14/303.82 = 37.6%

Mass of product: 31.8 mg
Total mass of reagent: 29.4 mg + 61.7 mg = 91.1 mg
RME = Mass of product/Total mass of reagent = 31.8 mg/ 91.1 mg = 34.9%

Total mass in process: 29.4 mg + 61.7 mg = 91.1 mg
Mass of product: 31.8 mg
PMI = Total mass in process/Mass of product = 91.1/31.8 = 2.86

Amount of carbon in desired product : 6

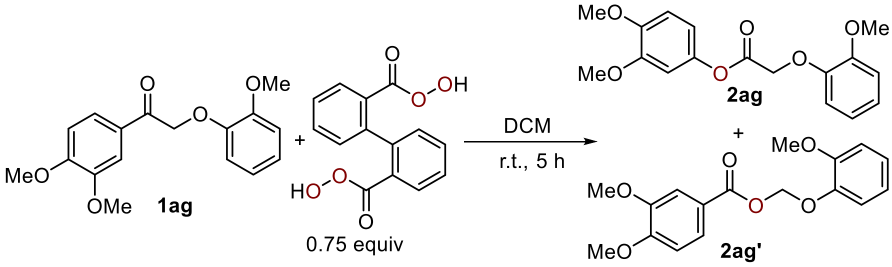
Total amount of carbon presenten in all reactants: 6 + 14 × 0.75 = 16.5

$$\text{Carbon Efficiency (\%)} = \frac{\text{amount of carbon in desired product}}{\text{total amount of carbon presenten in all reactants}} \times 100\% = \frac{6}{16.5} \times 100\% = 36.4\%$$

Yield of product: 93%

Atom economy: 37.6%

Atom Efficiency (%) = (% yield of product × % atom economy) × 100 = (93% × 37.6%) × 100 = 35.0%



302.33	274.23	318.33
151 mg	103 mg	150 mg

Total amount of reactants: 151 mg + 103 mg = 254 mg
Amount of final product: 150 mg
Amount of waste: 254 mg - 150 mg = 104 mg
E-Factor = Amount of waste/Amount of product = 104/150 = 0.69

Molecular weight of product: 318.33
Sum of molecular weight of reagent: 302.33 + 274.23 × 0.75 = 508.00
Atom economy = Molecular weight of product/Sum of molecular weight of reagent = 318.33/508.00 = 62.7%

Mass of product: 150 mg
Total mass of reagent: 151 mg + 103 mg = 254 mg
RME = Mass of product/Total mass of reagent = 150/254 = 59.1%

Total mass in process: 151 mg + 103 mg = 254 mg
Mass of product:150 mg
PMI = Total mass in process/Mass of product = 254/150 = 1.69

Amount of carbon in desired product : 17

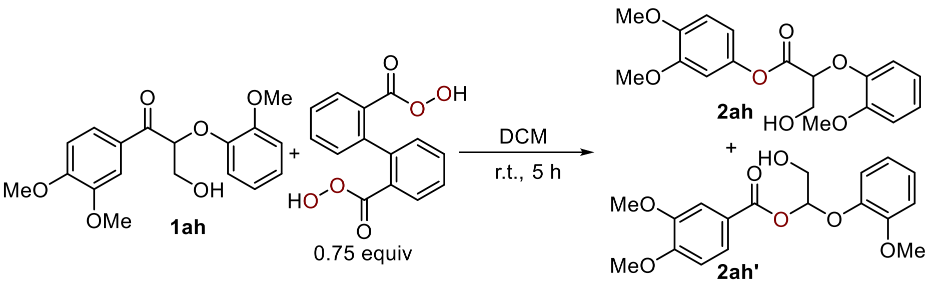
Total amount of carbon presenten in all reactants: 17 + 14 × 0.75 = 28.5

$$\text{Carbon Efficiency (\%)} = \frac{\text{amount of carbon in desired product}}{\text{total amount of carbon presenten in all reactants}} \times 100\% = \frac{17}{27.5} \times 100\% = 61.8\%$$

Yield of product: 94%

Atom economy: 62.7%

Atom Efficiency (%) = (% yield of product × % atom economy) × 100 = (94% × 62.7%) × 100 = 58.9%



332.35	274.23	348.35
166 mg	103 mg	152 mg

Total amount of reactants: 166 mg + 103 mg = 269 mg
Amount of final product: 152mg
Amount of waste:269 mg - 152 mg = 117 mg
E-Factor = Amount of waste/Amount of product = 117/152 = 0.77

Molecular weight of product: 348.35
Sum of molecular weight of reagent: 332.35 + 274.23 × 0.75 = 538.02
Atom economy = Molecular weight of product/Sum of molecular weight of reagent = 348.35/538.02 = 64.7%

Mass of product: 152 mg
Total mass of reagent: 166 mg + 103 mg = 269 mg
RME = Mass of product/Total mass of reagent = 152/269 = 57.0 %

Total mass in process: 166 mg + 103 mg = 269 mg
Mass of product:152 mg
PMI = Total mass in process/Mass of product = 269/152 = 1.77

Amount of carbon in desired product : 18

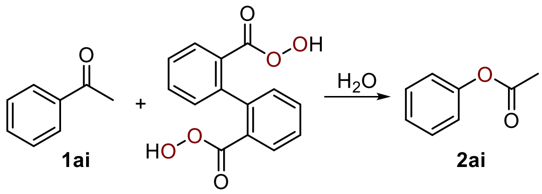
Total amount of carbon presenten in all reactants: 18 + 14 × 0.75 = 28.5

$$\text{Carbon Efficiency (\%)} = \frac{\text{amount of carbon in desired product}}{\text{total amount of carbon presenten in all reactants}} \times 100\% = \frac{18}{28.5} \times 100\% = 63.2\%$$

Yield of product: 87%

Atom economy: 64.7%

Atom Efficiency (%) = (% yield of product × % atom economy) × 100 = (93% × 37.6%) × 100 = 56.3%



0.75 equiv

120.15	274.23	136.15
36.0 mg	61.7 mg	38.8 mg

Total amount of reactants: 36.0 mg + 61.7 mg = 97.7 mg
Amount of final product: 38.8 mg
Amount of waste: 97.7 mg - 38.8 mg = 58.9 mg
E-Factor = Amount of waste/Amount of product =58.9/38.8 = 1.52

Molecular weight of product: 136.15
Sum of molecular weight of reagent:120.15 + 274.23 ×0.75 = 325.8
Atom economy = Molecular weight of product/Sum of molecular weight of reagent = 136.15/325.8 = 41.8%

Mass of product:
Total mass of reagent: 36.0 mg + 61.7 mg = 97.7 mg
RME = Mass of product/Total mass of reagent = 38.8 mg/ 97.7 mg = 39.7%

Total mass in process: 36.0 mg + 61.7 mg = 97.7 mg
Mass of product: 38.8 mg
PMI = Total mass in process/Mass of product = 97.7/38.8 = 2.52

Amount of carbon in desired product : 8

Total amount of carbon presenten in all reactants: 8 + 14 × 0.75 = 18.5

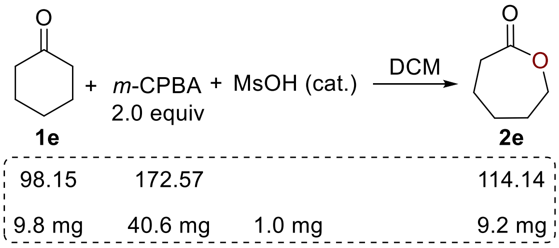
$$\text{Carbon Efficiency (\%)} = \frac{\text{amount of carbon in desired product}}{\text{total amount of carbon presenten in all reactants}} \times 100\% = \frac{6}{18.5} \times 100\% = 32.4\%$$

Yield of product: 95%

Atom economy: 41.8%

Atom Efficiency (%) = (% yield of product × % atom economy) × 100 = (95% × 41.8%) × 100 = 39.7%

Table S7. E-Factor, AE, RME, PMI, CE and atom efficiency for 1e, 1ae, 1af and 1ag using *m*-CPBA:



Total amount of reactants: 9.8 mg + 40.6 mg +1.0 mg = 51.4 mg
Amount of final product: 9.2 mg
Amount of waste:51.4 - 9.2 mg = 42.2 mg
E-Factor = Amount of waste/Amount of product = 42.2/9.2 = 4.59

Molecular weight of product: 114.14
Sum of molecular weight of reagent: 98.15 + 172.57 ×2 = 443.29
Atom economy = Molecular weight of product/Sum of molecular weight of reagent = 114.14/443.29 = 25.7%

Mass of product: 9.2 mg
Total mass of reagent: 9.8 mg + 40.6 mg = 50.4 mg
RME = Mass of product/Total mass of reagent = 9.2 mg/50.4 mg = 18.3%

Total mass in process: 9.8 mg + 40.6 mg +1.0 mg = 51.4 mg
Mass of product: 9.2 mg
PMI = Total mass in process/Mass of product = 51.4 mg/9.2 mg = 5.59

Amount of carbon in desired product : 6

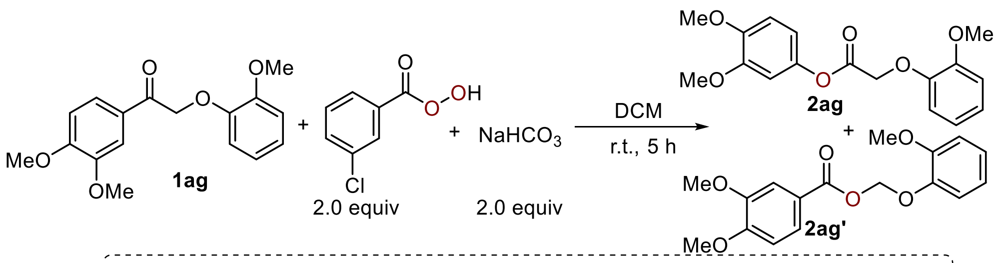
Total amount of carbon presenten in all reactants: 6 + 7 × 2 = 20

$$\text{Carbon Efficiency (\%)} = \frac{\text{amount of carbon in desired product}}{\text{total amount of carbon presenten in all reactants}} \times 100\% = \frac{6}{20} \times 100\% = 30\%$$

Yield of product: 81%

Atom economy: 25.7%

Atom Efficiency (%) = (% yield of product × % atom economy) × 100 = (81% × 25.7%) × 100 = 20.8%



302.33	172.56	84.01	318.33
30 mg	41 mg	17 mg	28 mg

Total amount of reactants: 30mg + 41 mg + 17 mg = 88 mg
Amount of final product: 28mg
Amount of waste:88mg - 28 mg = 60 mg
E-Factor = Amount of waste/Amount of product = 60/28 = 2.14

Molecular weight of product: 318.33
Sum of molecular weight of reagent: 302.33 + 172.56 × 2 + 84.01 × 2 = 815.47
Atom economy = Molecular weight of product/Sum of molecular weight of reagent = 318.33/815.47 = 39.0%

Mass of product: 28 mg
Total mass of reagent: 30 mg + 41 mg = 71 mg
RME = Mass of product/Total mass of reagent = 28/71 = 39.4%

Total mass in process: 30 mg + 41 mg + 17 mg = 88 mg
Mass of product: 28mg
PMI = Total mass in process/Mass of product = 88/28 = 3.14

Amount of carbon in desired product : 17

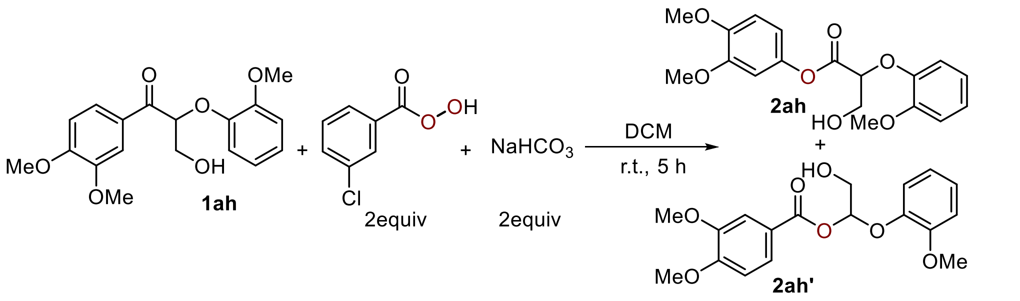
Total amount of carbon presenten in all reactants: 17 + 7 × 2 = 28.5

$$\text{Carbon Efficiency (\%)} = \frac{\text{amount of carbon in desired product}}{\text{total amount of carbon presenten in all reactants}} \times 100\% = \frac{17}{31} \times 100\% = 54.8\%$$

Yield of product: 89%

Atom economy: 39.0%

Atom Efficiency (%) = (% yield of product × % atom economy) × 100 = (94% × 62.7%) × 100 = 34.1%



332.35	172.56	84.01	348.35
33 mg	41 mg	17 mg	32 mg

Total amount of reactants: 33mg + 41 mg + 17 mg = 91 mg
Amount of final product: 32mg
Amount of waste:91mg - 32 mg = 59 mg
E-Factor = Amount of waste/Amount of product = 59/32 = 1.84

Molecular weight of product: 348.35
Sum of molecular weight of reagent: 332.35 + 172.56 × 2 + 84.01 × 2 = 845.49
Atom economy = Molecular weight of product/Sum of molecular weight of reagent = 348.35/845.49 = 41.2%

Mass of product: 32 mg
Total mass of reagent: 33 mg + 41 mg = 74 mg
RME = Mass of product/Total mass of reagent = 32/74 = 43.2%

Total mass in process: 33 mg + 41 mg + 17 mg = 91 mg
Mass of product: 32 mg
PMI = Total mass in process/Mass of product = 91/32 = 2.84

Amount of carbon in desired product : 18

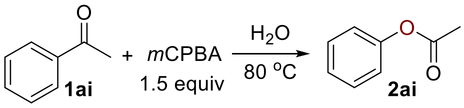
Total amount of carbon presenten in all reactants: 18 + 7 × 2 = 32

$$\text{Carbon Efficiency (\%)} = \frac{\text{amount of carbon in desired product}}{\text{total amount of carbon presenten in all reactants}} \times 100\% = \frac{18}{32} \times 100\% = 56.3\%$$

Yield of product: 92%

Atom economy: 41.2%

Atom Efficiency (%) = (% yield of product × % atom economy) × 100 = (92% × 41.2%) × 100 = 37.9%



120.15	172.57	136.15
120.1 mg	304.5 mg	121.2 mg

Total amount of reactants: 120.1 mg + 304.5 mg = 424.6 mg
Amount of final product: 121.2 mg
Amount of waste: 424.6 - 121.2 mg = 303.4 mg
E-Factor = Amount of waste/Amount of product = 303.4/121.2 = 2.5

Molecular weight of product: 136.15
Sum of molecular weight of reagent: 120.15 + 172.57 × 1.5 = 379.0
Atom economy = Molecular weight of product/Sum of molecular weight of reagent = 136.15/379.0 = 35.9%

Mass of product: 121.2 mg
Total mass of reagent: 120.1 mg + 304.5 mg = 424.6 mg
RME = Mass of product/Total mass of reagent = 121.2 mg/424.6 mg = 28.5%

Total mass in process: 120.1 mg + 304.5 mg = 424.6 mg
Mass of product: 121.2 mg
PMI = Total mass in process/Mass of product = 424.6/121.2 = 3.5

Amount of carbon in desired product : 8

Total amount of carbon presenten in all reactants: 8 + 7 × 1.5 = 18.5

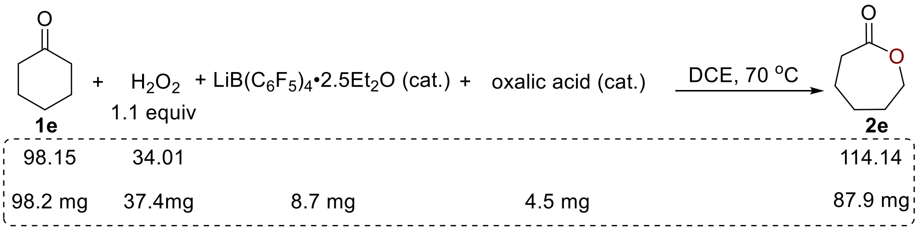
$$\text{Carbon Efficiency (\%)} = \frac{\text{amount of carbon in desired product}}{\text{total amount of carbon presenten in all reactants}} \times 100\% = \frac{8}{18.5} \times 100\% = 43.2\%$$

Yield of product: 89%

Atom economy: 35.9%

Atom Efficiency (%) = (% yield of product × % atom economy) × 100 = (89% × 35.9%) × 100 = 32.0%

Table S8. E-Factor, AE, RME, PMI, CE and atom efficiency for 1e, 1ae, 1af and 1ag using H_2O_2:



Total amount of reactants: 98.2 mg + 37.4 mg +8.7 mg + 4.5 mg = 148.8 mg
Amount of final product: 89.7 mg
Amount of waste: 148.8 mg - 89.7 mg = 59.1 mg
E-Factor = Amount of waste/Amount of product = 59.1/ 89.7 = 0.66

Molecular weight of product: 114.14
Sum of molecular weight of reagent: 98.15 + 34.01 × 1.1 = 135.55
Atom economy = Molecular weight of product/Sum of molecular weight of reagent = 114.14/135.55 = 84.2%

Mass of product: 87.9 mg
Total mass of reagent: 98.2 mg + 37.4 mg mg = 135.6 mg
RME = Mass of product/Total mass of reagent = 87.9 mg/135.6 mg = 64.8%

Total mass in process: 98.2 mg + 37.4 mg +8.7 mg + 4.5 mg = 148.8 mg
Mass of product: 89.7 mg
PMI = Total mass in process/Mass of product = 148.8/89.7 = 1.66

Amount of carbon in desired product : 6

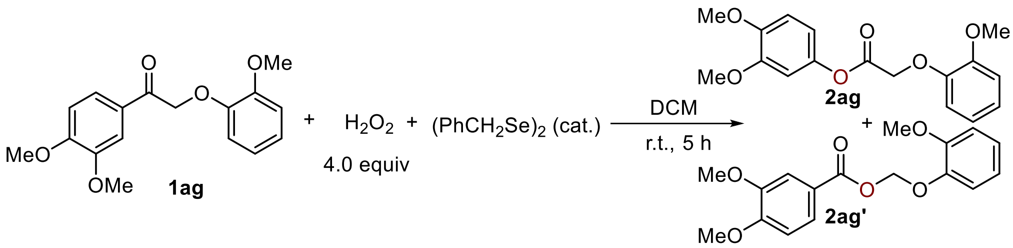
Total amount of carbon presenten in all reactants: 6

$$\text{Carbon Efficiency (\%)} = \frac{\text{amount of carbon in desired product}}{\text{total amount of carbon presenten in all reactants}} \times 100\% = \frac{6}{6} \times 100\% = 100\%$$

Yield of product: 77%

Atom economy: 84.2%

Atom Efficiency (%) = (% yield of product × % atom economy) × 100 = (77% × 84.2%) × 100 = 64.8%



302.33	34.01		318.33
30 mg	13.6 mg	1.7 mg	29 mg

Total amount of reactants: 30 mg + 13.6 mg + 1.7 mg = 45.3 mg
Amount of final product: 29 mg
Amount of waste:45.3mg - 29 mg = 16.3 mg
E-Factor = Amount of waste/Amount of product = 16.3/29 = 0.56

Molecular weight of product: 318.33
Sum of molecular weight of reagent: 302.33 + 34.01 × 4 = 438.37
Atom economy = Molecular weight of product/Sum of molecular weight of reagent = 318.33/438.37 = 72.6%

Mass of product: 29 mg
Total mass of reagent: 30 mg + 13.6 mg = 43.6 mg
RME = Mass of product/Total mass of reagent = 29/43.6 = 66.5%

Total mass in process: 30 mg + 13.6 mg + 1.7 mg = 45.3 mg
Mass of product: 29mg
PMI = Total mass in process/Mass of product = 45.3/29 = 1.56

Amount of carbon in desired product : 17

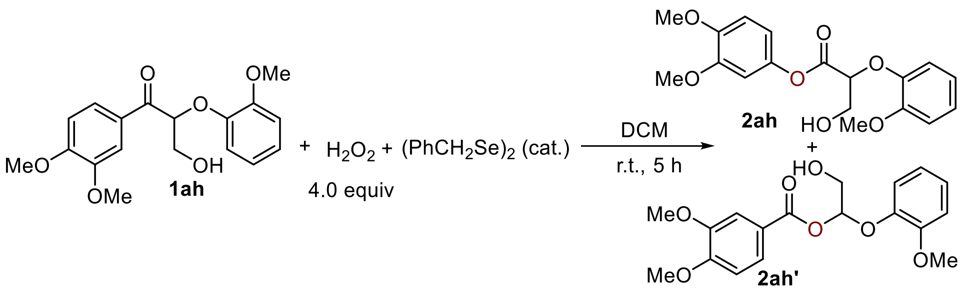
Total amount of carbon presenten in all reactants: 17

$$\text{Carbon Efficiency (\%)} = \frac{\text{amount of carbon in desired product}}{\text{total amount of carbon presenten in all reactants}} \times 100\% = \frac{17}{17} \times 100\% = 100\%$$

Yield of product: 92%

Atom economy: 41.2%

Atom Efficiency (%) = (% yield of product × % atom economy) × 100 = (91% × 72.6%) × 100 = 66.1%



332.35	34.01		348.35
33 mg	13.6 mg	1.7 mg	28 mg

Total amount of reactants: 33mg + 13.6 mg + 1.7 mg = 48.3 mg
Amount of final product: 28 mg
Amount of waste:48.3 mg - 28 mg = 20.3 mg
E-Factor = Amount of waste/Amount of product = 20.3/28 = 0.73

Molecular weight of product: 348.35
Sum of molecular weight of reagent: 332.35 + 34.01 × 4 = 468.39
Atom economy = Molecular weight of product/Sum of molecular weight of reagent = 348.35/468.39 = 74.4%

Mass of product: 28 mg
Total mass of reagent: 33 mg + 13.6 mg = 46.6 mg
RME = Mass of product/Total mass of reagent = 28/46.4 = 60.1%

Total mass in process: 33 mg + 13.6 mg + 1.7 mg = 48.3 mg
Mass of product: 28 mg
PMI = Total mass in process/Mass of product = 48.3/28 = 1.73

Amount of carbon in desired product : 18

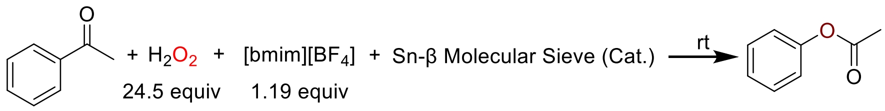
Total amount of carbon presenten in all reactants: 18

$$\text{Carbon Efficiency (\%)} = \frac{\text{amount of carbon in desired product}}{\text{total amount of carbon presenten in all reactants}} \times 100\% = \frac{18}{18} \times 100\% = 100\%$$

Yield of product: 81%

Atom economy: 74.4%

Atom Efficiency (%) = (% yield of product × % atom economy) × 100 = (81% × 74.4%) × 100 = 60.3%



1ai				**2ai**
120.15	34.01	226.02		136.15
448 mg	832.5 mg	1000 mg	100 mg	330 mg

Total amount of reactants: 448 mg + 832.5 mg +1000 mg + 100 mg = 2380.5 mg
Amount of final product: 330 mg
Amount of waste: 2380.5 mg - 330 mg = 2030.5 mg
E-Factor = Amount of waste/Amount of product =2050.5/330 = 6.21

Molecular weight of product: 136.15
Sum of molecular weight of reagent: 120.15 + 34.01×24.5 + 226.02 × 1.19 = 1,222.34
Atom economy = Molecular weight of product/Sum of molecular weight of reagent = 136.15/1,222.34 = 11.1%

Mass of product: 330 mg
Total mass of reagent: 448 mg + 832.5 mg +1000 mg = 2280.5 mg
RME = Mass of product/Total mass of reagent = 330/2280.5 = 14.5%

Total mass in process: 448 mg + 832.5 mg +1000 mg + 100 mg = 2380.5 mg
Mass of product: 330 mg
PMI = Total mass in process/Mass of product = 2380.5/330 = 7.21

Amount of carbon in desired product : 8

Total amount of carbon presenten in all reactants: 8 + 8 × 1.19 = 17.52

$$\text{Carbon Efficiency (\%)} = \frac{\text{amount of carbon in desired product}}{\text{total amount of carbon presenten in all reactants}} \times 100\% = \frac{8}{17.52} \times 100\% = 45.7\%$$

Yield of product: 72%

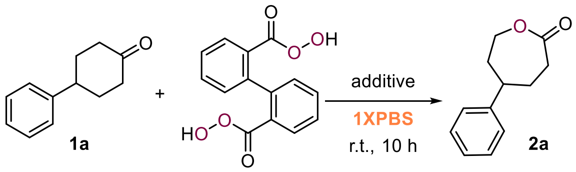
Atom economy: 11.1%

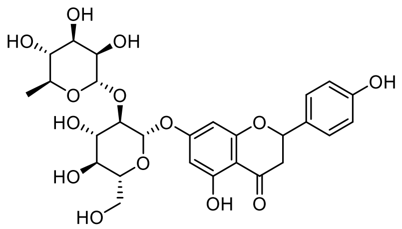
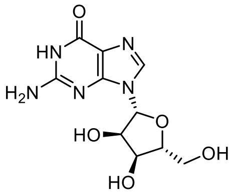
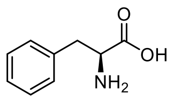
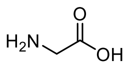
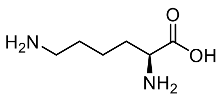
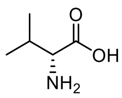
Atom Efficiency (%) = (% yield of product × % atom economy) × 100 = (72% × 11.1%) × 100 = 8.0%

11. Biomolecule-Compatibility Experiments

To a solution of 4-Phenylcyclohexanone (34.8 mg, 0.2 mmol), 2,2'-DPPA (0.2 mmol, 55 mg) and additives (0.2 mmol) in 1XPBS, and stirred at room temperature.

Table S9. Compatibility with Biomolecules in 1× PBS



Entry	Additive	yield of **c** (%)[a]	Additive remainning (%)
1		97	99[b]
2		94	95[a]
3		93	77[c]
4		94	69[c]
5		87	85[c]
6		97	75[c]

Reaction conditions: 1g (0.2 mmol, 34.8 mg), 2,2'-DPPA (0.2 mmol, 55 mg), additives (0.2 mmol, 1 equiv.) in 2 mL 1× PBS. [a]Isolated yields. [a]additive remaining was determined by LC-MS. [c] additives remainning were determined by ^{1}H NMR analysis.

11.1 The stability of nucleic acids in the oxidation

1a (0.004 mmol, 0.7 mg), 2,2'-DPPA (0.0024mol, 0.7 mg) and 20 μL pCVD442 were oscillation in 40 μL 1XPBS for 10 h. Then a portion of the reaction mixture was extracted with EA then subjected to GC analysis monitored 254 nm, internal standard is naphthalene. The agarose gel electrophoresis was conducted to confirm the pCVD442 was not degraded.

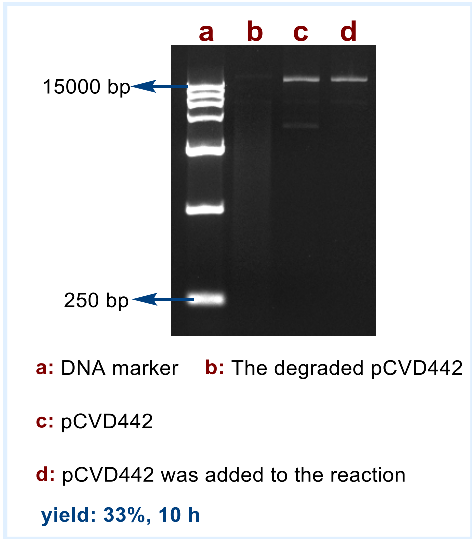


Figure S2. The electrophoretic of pCVD442

11.2 The stability of proteins in the oxidation

1a (0.001 mmol, 0.17 mg), 2,2'-DPPA (0.0006 mmol, 0.16 mg) and 10 mg (0.15 μmol) Bovine serum albumin were oscillation in 10 mL 1XPBS for 10 h. Then a portion of the reaction mixture was extracted with EA then subjected to GC analysis monitored 254 nm, internal standard is naphthalene. The other reaction mixture was diluted four times, and the amount of albumin bovine serum remaining was determined by BCA Protein Assay Ki (Bio TeKe).

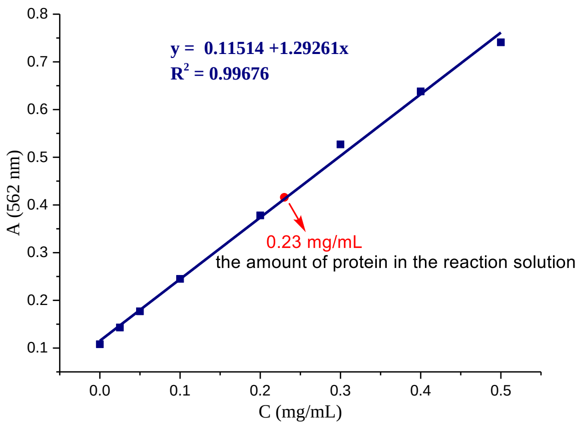


Figure S3. BSA concentration test by BCA Protein Assay Ki

11.3 The activity of DNase I in the reaction

We treated 100 μM of **1g,** 55 μM of 2,2'-DPPA and 0.032 μM DNase I were oscillation in 1XPBS for 10 h. Then a portion of the reaction mixture was extracted with EA then subjected to GC analysis monitored 254 nm, internal standard is naphthalene. 10 μL the reaction mixture was added 10 μL pCVD442, incubated at 37 °C for 3 h, then examined by agarose gel electrophoresis.

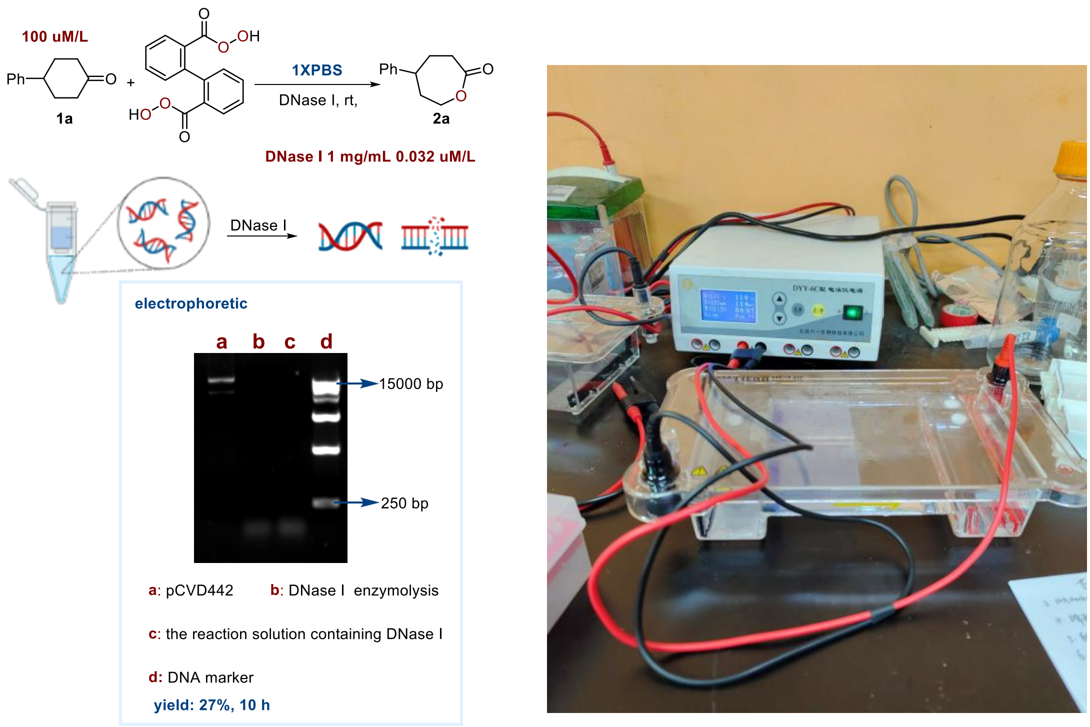
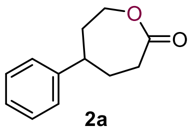


Figure S4. The activity of DNase I

12. Physical data

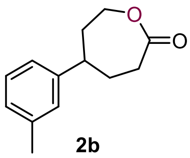
5-phenyloxepan-2-one (2a)



2a

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 (dd, *J* = 8.1, 6.7 Hz, 2H), 7.25 – 7.21 (m, 1H), 7.20 – 7.16 (m, 2H), 4.42 – 4.26 (m, 2H), 2.90 – 2.72 (m, 3H), 2.15 – 2.01 (m, 3H), 1.89 – 1.82 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.8, 144.1, 127.9, 126.0, 125.7, 67.4, 46.4, 35.9, 32.8, 29.4.

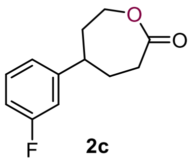
5-(m-tolyl) oxepan-2-one (2b)



2b

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.21 (t, *J* = 7.5 Hz, 1H), 7.10 – 6.92 (m, 3H), 4.42 – 4.24 (m, 2H), 2.87 – 2.65 (m, 3H), 2.34 (s, 3H), 2.18 – 1.94 (m, 3H), 1.83 (d, *J* = 12.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.9, 145.0, 138.5, 128.7, 127.7, 127.5, 123.7, 68.4, 47.3, 36.8, 33.8, 30.4, 21.6.

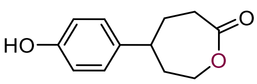
5-(3-fluorophenyl)oxepan-2-one (2c)



2c

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.23 (m, 1H), 7.06 – 6.77 (m, 3H), 4.44 – 4.24 (m, 2H), 2.91 – 2.68 (m, 3H), 2.19 – 1.91 (m, 3H), 1.87 – 1.73 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.6, 164.3, 161.9, 147.5 (d, *J* = 7.0 Hz), 130.4 (d, *J* = 8.3 Hz), 122.4 (d, *J* = 2.9 Hz), 113.8 (dd, *J* = 17.0 Hz), 68.1, 47.0, 36.7, 33.7, 30.3.

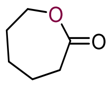
5-(4-hydroxyphenyl)oxepan-2-one (2d)



2d

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.23 (s, 1H), 7.04 (d, *J* = 8.5 Hz, 2H), 6.69 (d, *J* = 8.5 Hz, 2H), 4.40 (dd, *J* = 12.9, 10.4 Hz, 1H), 4.23 (m, *J* = 12.9, 5.5, 1.9 Hz, 1H), 2.93 (t, *J* = 12.5 Hz, 1H), 2.85 – 2.72 (m, 1H), 2.53 (d, *J* = 6.6 Hz, 1H), 1.98 (dt, *J* = 16.6, 4.1 Hz, 1H), 1.92 – 1.73 (m, 2H), 1.61 (q, *J* = 12.6 Hz, 1H). ^{13}C NMR (101 MHz, DMSO) δ 175.5, 155.8, 136.2, 127.5, 115.1, 67.6, 45.0, 36.7, 33.2, 30.2.

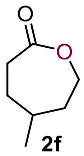
oxepan-2-one (2e)



2e

^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.26 – 4.16 (m, 2H), 2.63 (d, *J* = 7.2 Hz, 2H), 1.85 (s, 2H), 1.75 (d, *J* = 6.0 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.4, 69.4, 34.7, 29.4, 29.1, 23.0.

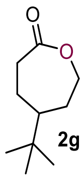
5-methyloxepan-2-one (2f)



2f

^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.29 – 4.20 (m, 1H), 4.15 (dd, *J* = 12.9, 10.3 Hz, 1H), 2.72 – 2.49 (m, 2H), 1.96 – 1.80 (m, 2H), 1.73 (m, *J* = 11.0, 7.1, 3.8 Hz, 1H), 1.55 – 1.41 (m, 1H), 1.38 – 1.23 (m, 1H), 0.96 (dd, *J* = 6.6, 1.4 Hz, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 176.2, 68.2, 37.3, 35.3, 33.3, 30.8, 22.2.

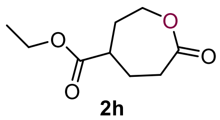
5-(tert-butyl)oxepan-2-one (2g)



2g

^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.30 (m, *J* = 12.9, 5.9, 1.8 Hz, 1H), 4.12 (dd, *J* = 12.9, 10.4 Hz, 1H), 2.67 (m, *J* = 14.3, 7.5, 1.5 Hz, 1H), 2.54 (m, *J* = 14.0, 11.7, 2.1 Hz, 1H), 2.12 – 1.93 (m, 2H), 1.48 (m, *J* = 15.5, 12.0, 10.4, 1.9 Hz, 1H), 1.37 – 1.27 (m, 2H), 0.86 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.4, 68.7, 50.8, 33.5, 33.0, 30.4, 27.5, 23.8.

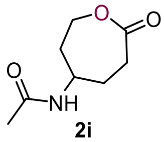
ethyl 7-oxooxepane-4-carboxylate (2h)



2h

^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.35 (m, *J* = 13.3, 7.1, 1.7 Hz, 1H), 4.26 – 4.07 (m, 3H), 2.84 – 2.53 (m, 3H), 2.21 – 2.00 (m, 3H), 1.92 (m, *J* = 14.7, 11.2, 9.3, 1.8 Hz, 1H), 1.24 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.2, 173.7, 66.8, 61.0, 44.1, 32.2, 31.4, 24.9, 14.2.

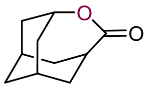
N-(7-oxooxepan-4-yl)acetamide (2i)



2i

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.95 (d, *J* = 7.7 Hz, 1H), 4.38 – 4.14 (m, 2H), 3.89 (dt, *J* = 8.1, 4.1 Hz, 1H), 2.74 (m, *J* = 14.0, 11.9, 1.8 Hz, 1H), 2.57 – 2.48 (m, 1H), 2.01 (m, *J* = 16.0, 4.9 Hz, 1H), 1.95 – 1.86 (m, 1H), 1.81 (s, 3H), 1.67 – 1.54 (m, 1H), 1.51 – 1.36 (m, 1H). ^{13}C NMR (101 MHz, DMSO) δ 175.2, 168.4, 65.2, 48.1, 34.8, 30.1, 28.3, 22.7. HRMS (ESI), m/z calcd for $C_8H_{14}NO_3$ $[M + H]^+$: 172.0969; found: 172.0969.

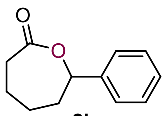
(1R,3r,8S)-4-oxatricyclo[4.3.1.13,8]undecan-5-one (2j)



2j

^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.43 (s, 1H), 3.01 (s, 1H), 2.05 (s, 2H), 1.96 (s, 4H), 1.87 (d, *J* = 14.2 Hz, 2H), 1.79 (s, 2H), 1.68 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.0, 73.2, 41.2, 35.7, 33.7, 30.9, 25.8.

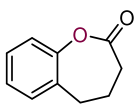
7-phenyloxepan-2-one (2k)



2k

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 (m, 5H), 5.32 (d, *J* = 9.3 Hz, 1H), 2.78 (t, *J* = 5.9 Hz, 2H), 2.20 – 1.97 (m, 4H), 1.88 – 1.63 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.0, 140.8, 128.6, 128.1, 125.9, 82.1, 37.5, 35.0, 28.6, 22.9.

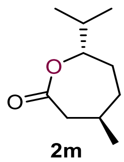
4,5-dihydrobenzo[b]oxepin-2(3H)-one (2l)



2l

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.27 (m, 1H), 7.25 – 7.15 (m, 2H), 7.11 (d, *J* = 7.9 Hz, 1H), 2.86 (t, *J* = 7.3 Hz, 2H), 2.50 (t, *J* = 7.2 Hz, 2H), 2.22 (q, *J* = 7.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 151.9, 130.2, 129.8, 128.4, 126.0, 119.4, 31.2, 28.4, 26.6.

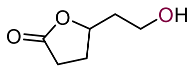
(4R,7S)-7-isopropyl-4-methyloxepan-2-one (2m)



2m

^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.01 (dd, *J* = 9.2, 4.4 Hz, 1H), 2.59 – 2.37 (m, 2H), 1.95 – 1.72 (m, 4H), 1.62 – 1.48 (m, 1H), 1.33 – 1.18 (m, 1H), 1.03 – 0.97 (m, 3H), 0.93 (t, *J* = 6.2 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.1, 84.8, 42.6, 37.5, 33.3, 31.0, 30.4, 24.0, 18.4, 17.1.

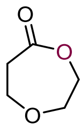
5-(2-hydroxyethyl)dihydrofuran-2(3H)-one (2n)



2n

^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.74 – 4.57 (m, 1H), 3.71 (td, *J* = 6.7, 2.2 Hz, 2H), 2.92 (dd, *J* = 14.2, 8.6 Hz, 2H), 2.56 – 2.43 (m, 2H), 2.33 (m, *J* = 13.4, 6.7 Hz, 1H), 1.86 (td, *J* = 12.4, 6.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.8, 78.7, 58.7, 38.1, 28.7, 28.0.

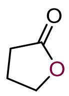
1,4-dioxepan-5-one (2o)



2o

^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.37 – 4.27 (m, 2H), 3.96 – 3.88 (m, 2H), 3.88 – 3.80 (m, 2H), 2.96 – 2.85 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.2, 70.8, 70.4, 64.8, 39.4.

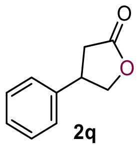
dihydrofuran-2(3H)-one (2p)



2p

^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.18 (t, *J* = 7.7 Hz, 2H), 2.32 (t, *J* = 7.9 Hz, 2H), 2.21 – 2.03 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.7, 68.3, 27.4, 21.8.

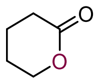
4-phenyldihydrofuran-2(3H)-one (2q)



2q

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 (dd, *J* = 8.2, 6.6 Hz, 2H), 7.37 – 7.31 (m, 1H), 7.27 (dd, *J* = 7.3, 1.7 Hz, 2H), 4.70 (dd, *J* = 9.0, 7.9 Hz, 1H), 4.30 (dd, *J* = 9.0, 8.0 Hz, 1H), 3.83 (p, *J* = 8.4 Hz, 1H), 2.96 (dd, *J* = 17.5, 8.7 Hz, 1H), 2.71 (dd, *J* = 17.5, 9.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.6, 139.5, 129.2, 127.8, 126.8, 74.1, 41.1, 35.8.

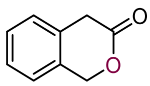
tetrahydro-2H-pyran-2-one (2r)



2r

^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.21 – 4.06 (m, 2H), 2.39 – 2.26 (m, 2H), 1.81 – 1.57 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.1, 69.1, 29.4, 21.8, 18.6.

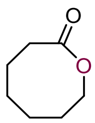
isochroman-3-one (2s)



2s

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.27 (m, 1H), 7.25 – 7.15 (m, 2H), 7.11 (d, *J* = 7.9 Hz, 1H), 2.86 (t, *J* = 7.3 Hz, 2H), 2.50 (t, *J* = 7.2 Hz, 2H), 2.22 (q, *J* = 7.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 151.9, 130.2, 129.8, 128.4, 126.0, 119.4, 31.2, 28.4, 26.6.

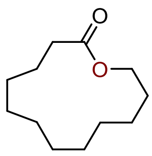
oxocan-2-one (2t)



2t

^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.41 – 4.30 (m, 2H), 2.59 – 2.50 (m, 2H), 1.83 (m, *J* = 25.1, 5.7 Hz, 4H), 1.67 – 1.52 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.0, 68.0, 31.4, 31.0, 28.5, 25.9, 24.0.

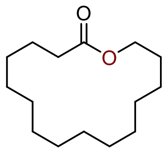
oxacyclotridecan-2-one (2u)



2u

[1]H NMR (400 MHz, Chloroform-*d*) δ 4.19 – 4.10 (m, 2H), 2.41 – 2.29 (m, 2H), 1.72 – 1.59 (m, 4H), 1.43 – 1.29 (m, 14H). [13]C NMR (101 MHz, $CDCl_3$) δ 174.4, 64.7, 34.8, 27.5, 26.7, 26.5, 26.5, 25.5, 25.4, 25.0, 24.6, 24.3.

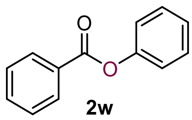
oxacyclohexadecan-2-one (2v)



2v

[1]H NMR (400 MHz, Chloroform-*d*) δ 4.12 (t, *J* = 5.5 Hz, 2H), 2.31 (t, *J* = 6.8 Hz, 2H), 1.63 (m, 4H), 1.30 (m, 20H). [13]C NMR (101 MHz, $CDCl_3$) δ 174.2, 64.1, 34.5, 28.5, 27.8, 27.2, 27.2, 27.0, 26.7, 26.4, 26.1, 26.0, 25.9, 25.2, 25.0.

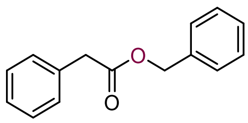
phenyl benzoate (2w)



2w

[1]H NMR (400 MHz, Chloroform-*d*) δ 8.31 – 8.22 (m, 2H), 7.72 – 7.64 (m, 1H), 7.56 (t, *J* = 7.6 Hz, 2H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.37 – 7.23 (m, 3H). [13]C NMR (101 MHz, $CDCl_3$) δ 165.3, 151.1, 133.7, 130.3, 129.67, 129.6, 128.7, 126.0, 121.8.

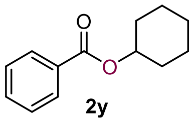
benzyl 2-phenylacetate (2x)



2x

[1]H NMR (400 MHz, Chloroform-*d*) δ 7.40 (dd, *J* = 9.3, 4.0 Hz, 10H), 5.22 (s, 2H), 3.76 (s, 2H). [13]C NMR (101 MHz, $CDCl_3$) δ 171.5, 135.9, 134.0, 130.4, 128.6, 128.6, 128.3, 128.2, 127.2, 66.7, 41.4.

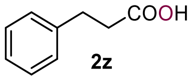
cyclohexyl benzoate (2y)



2y

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 (d, *J* = 7.6 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 5.04 (m, *J* = 8.6, 3.8 Hz, 1H), 1.94 (d, *J* = 12.4 Hz, 2H), 1.80 (d, *J* = 13.4 Hz, 2H), 1.60 (q, *J* = 9.3 Hz, 3H), 1.53 – 1.35 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.1, 132.8, 131.1, 129.6, 128.4, 7 73.1, 31.7, 25.6, 23.8.

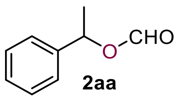
3-phenylpropanoic acid (2z)



2z

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.26 (d, *J* = 608.6 Hz, 1H), 7.41 – 7.32 (m, 2H), 7.32 – 7.21 (m, 3H), 3.02 (t, *J* = 7.8 Hz, 2H), 2.75 (t, *J* = 7.8 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.49, 140.27, 128.69, 128.39, 126.51, 77.48, 77.16, 76.84, 35.75, 30.67.

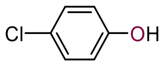
1-phenylethyl formate (2aa)



2aa

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.10 (s, 1H), 7.42 – 7.28 (m, 5H), 6.02 (qd, *J* = 6.6, 1.1 Hz, 1H), 1.60 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.51, 141.01, 128.72, 128.28, 126.28, 77.48, 77.16, 76.84, 72.36, 22.24.

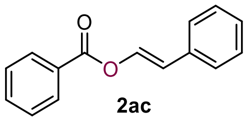
4-chlorophenol (2ab)



2ab

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.19 (d, *J* = 8.5 Hz, 2H), 6.77 (d, *J* = 8.7 Hz, 2H), 5.02 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.33, 129.65, 125.72, 116.80, 77.48, 77.16, 76.84.

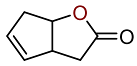
(E)-styryl benzoate (2ac)



2ac

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.15 (dd, *J* = 8.4, 1.4 Hz, 2H), 8.10 (d, *J* = 12.7 Hz, 1H), 7.62 (d, *J* = 7.4 Hz, 1H), 7.50 (dd, *J* = 8.3, 7.1 Hz, 2H), 7.42 – 7.38 (m, 2H), 7.37 – 7.31 (m, 2H), 7.29 – 7.23 (m, 1H), 6.60 (d, *J* = 12.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.8, 136.6, 134.3, 133.8, 130.2, 129.0, 128.9, 128.7, 127.6, 126.4, 116.0.

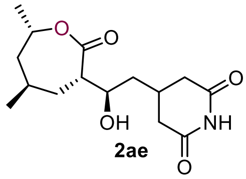
3,3a,6,6a-tetrahydro-2H-cyclopenta[b]furan-2-one (2ad)



2ad

^{1}H NMR (400 MHz, Chloroform-*d*) δ 5.79 (dd, *J* = 5.6, 2.5 Hz, 1H), 5.61 – 5.56 (m, 1H), 5.13 (td, *J* = 5.1, 4.1, 2.5 Hz, 1H), 3.51 (m, *J* = 7.8, 5.9, 2.0 Hz, 1H), 2.77 (dd, *J* = 18.0, 9.6 Hz, 1H), 2.71 (q, *J* = 2.2 Hz, 2H), 2.45 (dd, *J* = 18.0, 1.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.9, 131.4, 129.9, 83.2, 45.72, 39.68, 33.43.

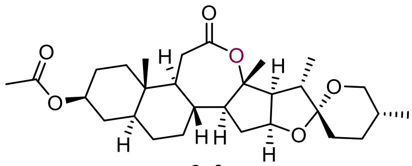
4-((R)-2-((3S,5R,7S)-5,7-dimethyl-2-oxooxepan-3-yl)-2-hydroxyethyl)piperidine-2,6-dione (2ae)



2ae

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.73 (s, 1H), 4.66 – 4.52 (m, 1H), 4.10 (d, *J* = 8.5 Hz, 1H), 3.41 (s, 1H), 2.87 – 2.74 (m, 2H), 2.71 (d, *J* = 4.5 Hz, 1H), 2.45 (dd, *J* = 9.4, 4.8 Hz, 1H), 2.31 (m, *J* = 17.0, 10.6 Hz, 2H), 1.93 – 1.72 (m, 3H), 1.66 (m, *J* = 15.7, 10.8, 5.1 Hz, 1H), 1.47 (dd, *J* = 14.5, 7.6 Hz, 2H), 1.32 (d, *J* = 6.1 Hz, 3H), 1.26 – 1.18 (m, 1H), 1.00 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.2, 172.8, 172.7, 72.6, 67.8, 44.2, 42.2, 38.4, 37.9, 37.2, 28.4, 28.1, 27.4, 22.0, 20.4. HRMS (ESI), m/z calcd for $C_{15}H_{24}NO_5$ $[M + H]^+$: 298.1649; found: 298.1647.

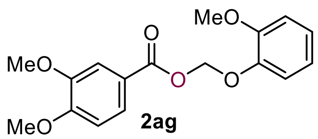
(2S,4aS,4bS,5'R,7aS,7bS,8S,9R,10aS,11aS,11bR,13aS)-4a,5',7a,8-tetramethyl-6-oxodocosahydrospiro[furo[2',3':4,5]cyclopenta[1,2-b]naphtho[2,1-d]oxepine-9,2'-pyran]-2-yl acetate (2af)



2af

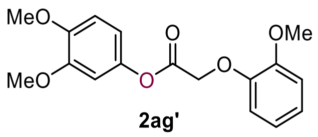
^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.67 (m, *J* = 10.5, 4.6 Hz, 1H), 4.37 (q, *J* = 7.9 Hz, 1H), 3.47 (d, *J* = 9.1 Hz, 1H), 3.31 (t, *J* = 10.9 Hz, 1H), 2.73 (d, *J* = 13.7 Hz, 1H), 2.60 – 2.40 (m, 2H), 2.31 (m, *J* = 13.5, 7.1 Hz, 1H), 2.01 (s, 4H), 1.95 – 1.80 (m, 4H), 1.80 – 1.65 (m, 4H), 1.62 – 1.54 (m, 2H), 1.47 (d, *J* = 11.4 Hz, 1H), 1.44 (s, 3H), 1.39 – 1.29 (m, 4H), 1.28 – 1.18 (m, 3H), 1.12 (t, *J* = 10.9 Hz, 2H), 1.04 (d, *J* = 7.0 Hz, 3H), 0.78 (d, *J* = 7.5 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.8, 170.7, 108.9, 86.4, 75.7, 73.1, 67.1, 63.1, 56.8, 50.3, 43.6, 42.7, 38.3, 36.8, 36.6, 34.5, 34.0, 32.2, 31.5, 30.2, 28.8, 28.2, 27.4, 21.5, 18.7, 17.2, 14.1, 11.6. HRMS (ESI), m/z calcd for $C_{29}H_{45}O_6$ $[M + H]^+$: 489.3211; found: 489.3208.

(2-methoxyphenoxy)methyl 3,4-dimethoxybenzoate (2ag)



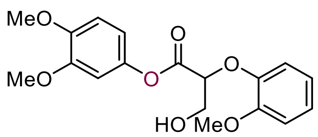
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.55 (d, *J* = 2.0 Hz, 1H), 7.15 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.06 (td, *J* = 7.8, 1.6 Hz, 1H), 6.01 (s, 2H), 3.94 (s, 3H), 3.91 (s, 3H), 3.85 (s, 3H). ^{13}C NMR (101 MHz, CDC^{l3}) δ 165.4, 153.5, 150.5, 148.8, 146.2, 124.2, 124.2, 122.1, 120.99, 118.0, 112.4, 112.3, 110.4, 87.7, 56.2, 56.0.

3,4-dimethoxyphenyl 2-(2-methoxyphenoxy)acetate (2ag')



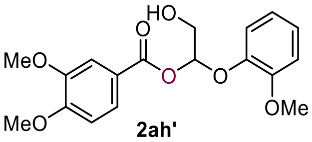
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.04 – 6.86 (m, 4H), 6.81 (d, *J* = 8.3 Hz, 1H), 6.68 – 6.61 (m, 2H), 4.90 (s, 2H), 3.88 (s, 3H), 3.84 (s, 3H), 3.82 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 149.8, 149.4, 147.1, 147.0, 143.8, 123.0, 120.8, 115.1, 112.6, 112.3, 111.1, 105.4, 66.7, 56.2, 56.0, 55.9.

3,4-dimethoxyphenyl 3-hydroxy-2-(2-methoxyphenoxy)propanoate (2ah)



^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.13 – 7.01 (m, 2H), 6.91 (m, *J* = 15.4, 7.9, 1.5 Hz, 2H), 6.81 (d, *J* = 8.4 Hz, 1H), 6.67 – 6.59 (m, 2H), 4.89 (t, *J* = 4.4 Hz, 1H), 4.18 (d, *J* = 4.4 Hz, 2H), 3.87 (s, 3H), 3.84 (s, 3H), 3.82 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7, 150.6, 149.4, 147.1, 146.8, 143.9, 124.1, 121.2, 118.8, 112.7, 112.4, 111.1, 105.5, 80.8, 63.3, 56.2, 56.1, 55.9.

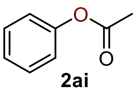
2-hydroxy-1-(2-methoxyphenoxy)ethyl 3,4-dimethoxybenzoate (2ah')



2ah'

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.53 (d, *J* = 2.0 Hz, 1H), 7.14 – 7.03 (m, 2H), 6.96 – 6.82 (m, 3H), 6.54 (dd, *J* = 6.3, 3.8 Hz, 1H), 4.02 (dd, *J* = 11.8, 6.3 Hz, 1H), 3.95 (d, *J* = 4.0 Hz, 1H), 3.93 (s, 3H), 3.91 (s, 3H), 3.85 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.1, 153.6, 151.0, 148.8, 145.3, 125.1, 124.3, 121.7, 121.3, 120.6, 112.3, 112.2, 110.4, 97.7, 63.4, 56.2, 56.2, 55.9.

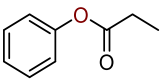
phenyl acetate (2ai)



2ai

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.34 (m, 2H), 7.24 (m, *J* = 8.6, 7.1, 1.4 Hz, 1H), 7.13 – 7.06 (m, 2H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.6, 150.8, 129.5, 126.0, 121.7, 21.2.

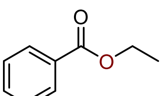
phenyl propionate (2aj)



2aj

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 (t, *J* = 7.9 Hz, 2H), 7.26 (td, *J* = 7.3, 1.2 Hz, 1H), 7.15 – 7.09 (m, 2H), 2.64 (q, *J* = 7.5 Hz, 2H), 1.31 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.1, 150.9, 129.5, 125.8, 121.7, 27.9, 9.2.

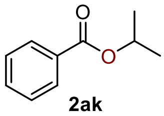
ethyl benzoate (2aj')



2aj'

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12 – 8.04 (m, 2H), 7.62 – 7.57 (m, 1H), 7.48 (dd, *J* = 8.4, 7.0 Hz, 2H), 4.43 (q, *J* = 7.1 Hz, 2H), 1.43 (d, *J* = 7.1 Hz, 3H).

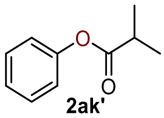
isopropyl benzoate (2ak)



2ak

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.08 – 8.01 (m, 2H), 7.55 – 7.51 (m, 1H), 7.45 – 7.40 (m, 2H), 5.26 (m, *J* = 6.2 Hz, 1H), 1.37 (d, *J* = 6.3 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2, 132.8, 131.0, 129.6, 128.4, 68.4, 22.0.

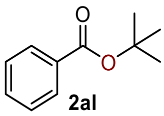
phenyl isobutyrate (2ak')



2ak'

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.33 (m, 2H), 7.24 – 7.18 (m, 1H), 7.07 (d, *J* = 7.4 Hz, 2H), 2.80 (m, *J* = 7.0 Hz, 1H), 1.32 (d, *J* = 7.0 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.8, 151.0, 129.5, 125.8, 121.6, 34.3, 19.0.

tert-butyl benzoate (2al)

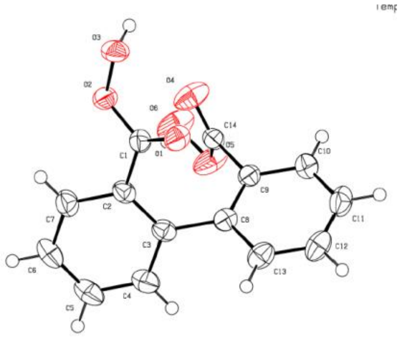


2al

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 (dd, *J* = 7.8, 2.3 Hz, 2H), 7.56 – 7.48 (m, 1H), 7.41 (td, *J* = 7.8, 2.1 Hz, 2H), 1.60 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9, 132.6, 132.2, 129.5, 128.3, 81.1, 28.3.

13. Crystal data and structure refinement

2,2'-Diperoxyphenic Acid: The crystal structure of compound **2,2'-Diperoxyphenic Acid** has been deposited at the Cambridge Crystallographic Data Centre (**CCDC** 2089219).



X-ray crystal structure of **2,2'-Diperoxyphenic Acid**

Crystal data and structure refinement for **2,2'-Diperoxyphenic Acid.**

Identification code	GSY2021329-S (2,2'-Diperoxyphenic Acid)
Empirical formula	$C_{14}H_{10}O_6$
Formula weight	274.22
Temperature	230 K
Wavelength	1.54184 Å
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	13.5207(4)
b/Å	11.7590(3)
c/Å	7.7352(2)
α/°	90
β/°	97.600(2)
γ/°	90
Volume/Å3	1219.02(6)
Z	4
ρcalcg/cm3	1.494
μ/mm-1	1.014
F(000)	568.0
Crystal size/mm^3	0.3 × 0.3 × 0.2
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.596 to 143.558
Index ranges	$-16 \le h \le 16$, $-10 \le k \le 14$, $-9 \le l \le 9$
Reflections collected	6127
Independent reflections	2317 [R_{int} = 0.0352, R_{sigma} = 0.0369]
Data/restraints/parameters	2317/0/183
Goodness-of-fit on F^2	1.052
Final R indexes [I>=2σ (I)]	R_1 = 0.0522, wR_2 = 0.1475
Final R indexes [all data]	R_1 = 0.0556, wR_2 = 0.1525

Largest diff. peak/hole / e Å^{-3} 0.320/ -0.368

14. DFT Computations Methods:

All the DFT computations were performed with the Gaussian16 program suite.[3] Geometries were optimized with dispersion corrections [DFT-D3(BJ)][4] in conjunction with the B3LYP functional combining a 6-31G(d) basis set.[5] Vibrational frequencies were computed for each optimized structure to verify the stationary structures as minima or saddle points. Solvent effects were included by single-point energy computations with the SMD model at the level of B3LYP/6-311G(d,p) for the optimized geometry.[6] All energies discussed are Gibbs free relative energies at 298.15 K and 1 atm in kcal mol^{-1}. Effects of zero-point vibrational energy (ZPVE) corrections are included.

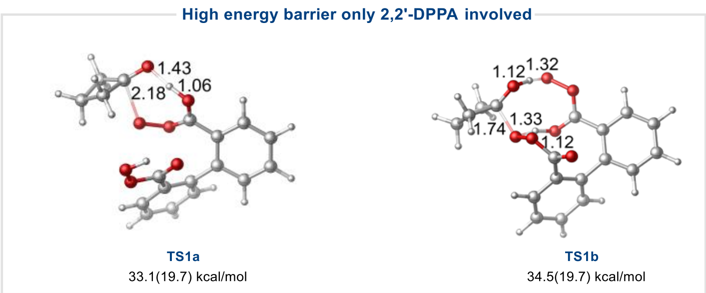


Figure S5. Computed geometries and relative free energies of the transition states for the addition step in pathway a and b without external acid.

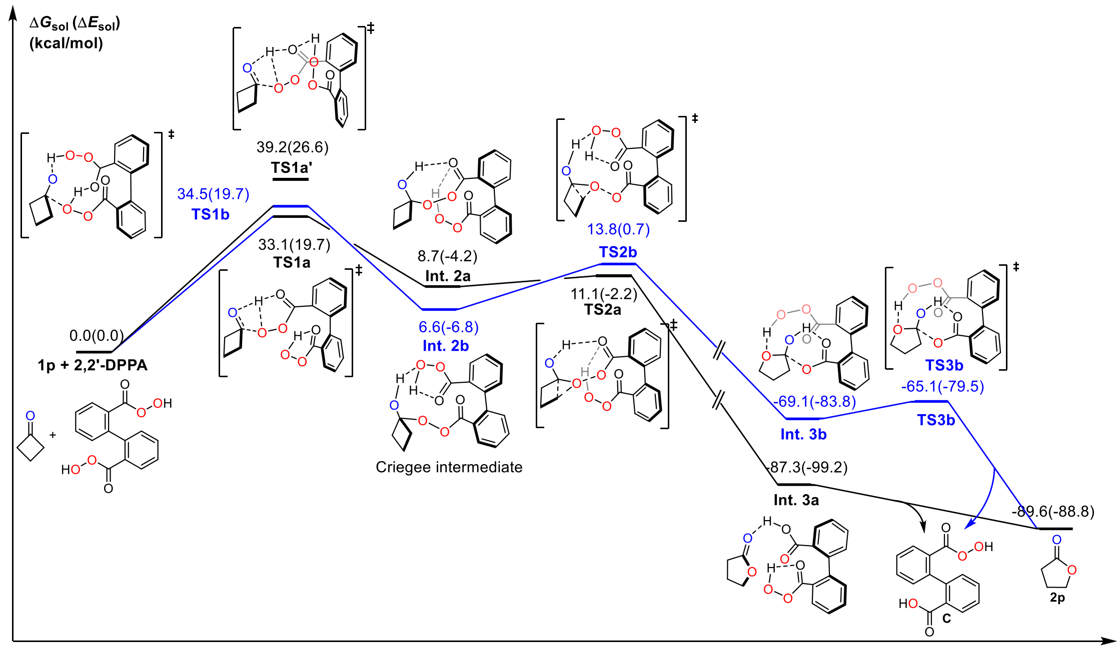


Figure S6. Potential energy profiles of the reaction of **1q** and 2,2'-DPPA.

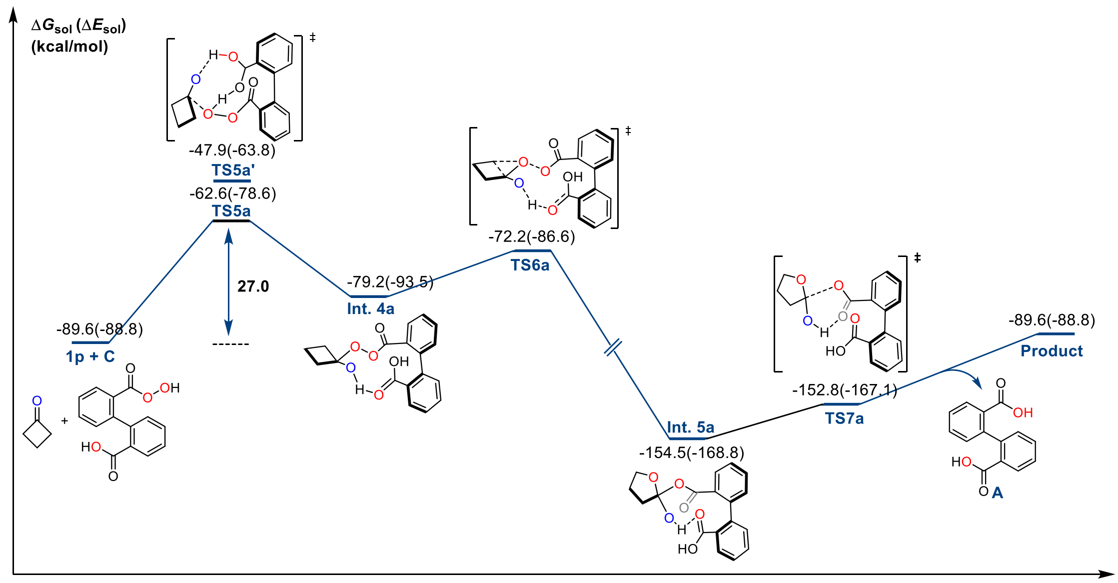


Figure S7. Potential energy profiles of the reaction of **1p** and monoperacid.

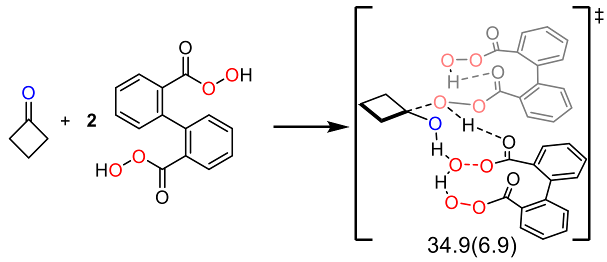


Figure S8. Potential energy profiles of two molecular of 2,2'-DPPA in presence.

Energies

Geometries	E (SCF Done)	E(correction)	G(correction)

1p	-231.241627	-231.150355	-231.179533
TS1a	-1221.969253	-1221.659764	-1221.711385
TS1apri	-1221.950693	-1221.643180	-1221.695964
TS1b	-1221.965222	-1221.658829	-1221.708072
Int. 2a	-1222.013477	-1221.700134	-1221.752441
Int. 2b	-1222.018470	-1221.704761	-1221.756280
TS2a	-1222.005916	-1221.694822	-1221.746518
TS2b	-1221.990969	-1221.680212	-1221.732193
Int. 3a	-1222.166980	-1221.851187	-1221.905011
Int. 3b	-1222.146474	-1221.828560	-1221.878063
TS3b	-1222.131000	-1221.817990	-1221.867881
1q	-306.507981	-306.408828	-306.437442
C	-915.629556	-915.414921	-915.460344
TS4a	-1146.858774	-1146.555288	-1146.603160
TS4apri	-1146.846738	-1146.538918	-1146.587048
Int. 4a	-1146.889565	-1146.579359	-1146.630025
TS5a	-1146.865194	-1146.557458	-1146.607962
Int. 5a	-1147.014932	-1146.701028	-1146.751572
TS6a	-1222.131000	-1221.817990	-1221.867881
A	-840.502263	-840.290229	-840.332324
TSI	-2062.520671	-2061.999430	-2062.071981
B	-2062.546360	-2062.019115	-2062.092290
TSII	-2062.531228	-2062.006143	-2062.077243
TSIII	-1987.393152	-1986.874460	-1986.946112
D	-1987.425815	-1986.901341	-1986.973010
TSIV	-1987.400197	-1986.878799	-1986.949557
Me-TS2c-ph	-2216.205802	-2215.634857	-2215.707859
Me-TS2c-R	-2216.194470	-2215.624434	-2215.700234
Me-TS4c-ph	-2141.072888	-2140.505846	-2140.578743
Me-TS4c-R	-2141.067784	-2140.501268	-2140.575131
tBu-TS2c-ph	-2334.159462	-2333.503643	-2333.583287
tBu-TS2c-R	-2334.166464	-2333.511209	-2333.592880
tBu-TS4c-ph	-2259.038185	-2258.385682	-2258.462038
tBu-TS4c-R	-2259.042758	-2258.390646	-2258.470793

Cartesian coordinates (Å)

1p

C	-0.040686	-0.384021	-1.110488
C	-0.040686	-1.478826	-0.000000
C	-0.040686	-0.384021	1.110488
C	0.025815	0.679126	0.000000
H	-0.955260	-0.321213	-1.711061
H	0.816533	-0.375344	-1.792368
H	0.854514	-2.104990	-0.000000
H	-0.920046	-2.126599	0.000000
H	-0.955260	-0.321213	1.711061
H	0.816533	-0.375344	1.792368
O	0.115055	1.878894	-0.000000

TS1a

O	-0.515595	-0.007850	-2.061062
O	0.911134	-1.735408	-2.009640
O	1.531474	-1.020728	-3.093427
H	0.950663	-0.215675	-3.114964
O	0.534947	2.417062	-0.375965
O	0.426692	0.558002	0.934624
O	1.663387	0.068031	0.362216
H	1.765339	2.486719	0.149225
C	-0.165022	-1.054450	-1.539065
C	-0.795322	-1.731515	-0.383464
C	-1.764114	-1.077424	0.415554
C	-2.301481	-1.788493	1.497646
H	-3.031027	-1.292421	2.129565
C	-1.907438	-3.091443	1.793343
H	-2.343410	-3.604421	2.645610
C	-0.955797	-3.725852	0.998895
H	-0.639807	-4.741195	1.216551
C	-0.405577	-3.043149	-0.079880
H	0.337130	-3.526233	-0.702846
C	-2.323076	0.295184	0.201804
C	-1.585672	1.502345	0.172538
C	-2.235415	2.731653	0.010084
H	-1.631171	3.631306	-0.026401
C	-3.619185	2.797426	-0.104885
H	-4.112468	3.757036	-0.222732
C	-4.358886	1.616463	-0.077869

H	-5.439889	1.645134	-0.179644
C	-3.715249	0.388587	0.071368
H	-4.298543	-0.526537	0.069318
C	-0.112898	1.532114	0.212710
C	3.972383	0.581290	-0.371471
C	4.481038	-0.501708	0.627553
C	3.870767	0.313277	1.807211
C	3.114415	1.139183	0.774104
H	3.444535	0.248116	-1.268527
H	4.745053	1.309224	-0.644604
H	5.560920	-0.663344	0.659449
H	3.973658	-1.457543	0.482476
H	3.261672	-0.213332	2.544367
H	4.608390	0.938506	2.323745
O	2.658978	2.336356	0.966048

TS1b

O	2.824337	-1.734882	0.800958
O	1.870988	0.623235	0.313998
H	2.232441	-2.265228	0.088532
C	-0.146155	0.723149	1.604536
O	1.187914	0.316836	1.561115
O	-0.774765	0.297399	2.535425
O	1.468344	-2.704866	-1.046613
O	0.207797	-0.396412	-1.273692
H	1.240400	0.203541	-0.397779
C	-0.644433	1.646462	0.550416
C	-0.033522	2.892619	0.393135
C	-1.766139	1.289073	-0.221585
C	-0.552012	3.818977	-0.508968
H	0.840560	3.136021	0.988344
C	-2.267915	2.231807	-1.124746
C	-1.673109	3.485296	-1.266826
H	-0.082162	4.791507	-0.618420
H	-3.122819	1.962961	-1.737294
H	-2.081931	4.196391	-1.978703
C	3.307475	-0.705216	0.246177
C	4.405160	0.207485	0.755410
C	3.644080	-0.420556	-1.212383
C	4.554263	0.741412	-0.705261
H	5.257000	-0.396581	1.087238
H	4.135169	0.909171	1.545919

H	4.208655	-1.270454	-1.612069
H	2.818281	-0.217649	-1.895787
H	5.570074	0.760194	-1.103515
H	4.093150	1.721667	-0.837925
C	-0.404496	-1.364853	-0.789273
O	0.118316	-2.549837	-0.573256
C	-1.827896	-1.280572	-0.357279
C	-2.569014	-2.463736	-0.221332
C	-2.447651	-0.032944	-0.108141
C	-3.908939	-2.431058	0.147861
H	-2.077888	-3.408615	-0.420796
C	-3.799397	-0.023809	0.258494
C	-4.527188	-1.204248	0.386631
H	-4.466951	-3.357327	0.244401
H	-4.273343	0.930679	0.465386
H	-5.572762	-1.163797	0.677794

Int. 2a

O	2.027711	-0.109025	2.245426
O	0.151160	-1.416221	2.132670
O	-0.234382	-0.799601	3.377465
H	-0.595456	0.045396	3.029764
O	-0.980620	1.314628	1.372416
O	-0.861745	0.137850	-0.581526
O	-1.968406	-0.699337	-0.122143
H	-2.842891	1.030823	1.333216
C	1.352942	-0.931190	1.682956
C	1.611415	-1.530154	0.336800
C	1.923933	-0.687683	-0.750045
C	2.210213	-1.279032	-1.985656
H	2.433725	-0.638599	-2.833530
C	2.179134	-2.663476	-2.146659
H	2.401710	-3.097107	-3.117199
C	1.847925	-3.485342	-1.070443
H	1.814074	-4.563596	-1.192117
C	1.555128	-2.915315	0.166780
H	1.292819	-3.541275	1.012998
C	1.961861	0.794831	-0.629334
C	0.910915	1.564098	-0.081819
C	1.053521	2.945895	0.090094
H	0.238513	3.501323	0.541859
C	2.212486	3.593265	-0.323865

H	2.310838	4.666703	-0.196811
C	3.244409	2.849660	-0.896361
H	4.158188	3.341211	-1.217059
C	3.120158	1.468665	-1.034876
H	3.946554	0.887709	-1.431847
C	-0.391123	0.991622	0.352226
C	-4.343933	-0.909090	-0.782434
C	-4.776149	0.276144	-1.689792
C	-3.396324	0.945871	-1.438214
C	-3.227242	-0.001800	-0.223978
H	-3.926275	-1.744155	-1.349051
H	-5.050892	-1.272063	-0.034234
H	-5.595901	0.847087	-1.247801
H	-5.021106	0.037904	-2.727612
H	-2.676401	0.727283	-2.229880
H	-3.380951	2.013338	-1.203516
O	-3.608990	0.521230	1.002012

Int. 2b

O	2.914964	-2.118896	0.543320
O	1.766281	-0.112579	0.219238
H	2.275105	-2.484990	-0.101394
C	-0.021896	0.512349	1.580482
O	1.138593	-0.206009	1.555612
O	-0.756760	0.333704	2.522045
O	0.939374	-2.719274	-1.488574
O	-0.312125	-0.612354	-1.993717
H	0.955657	-1.890604	-2.042240
C	-0.283222	1.499675	0.486490
C	0.612297	2.550671	0.269830
C	-1.495273	1.445815	-0.222940
C	0.296039	3.567647	-0.626789
H	1.548569	2.573179	0.817523
C	-1.799053	2.471410	-1.122932
C	-0.913820	3.529067	-1.321335
H	0.991034	4.387271	-0.782550
H	-2.727549	2.420886	-1.683539
H	-1.163515	4.316494	-2.026370
C	3.030934	-0.773344	0.296314
C	4.040476	-0.015967	1.175209
C	3.753361	-0.238099	-0.977896
C	4.456874	0.810035	-0.073860

H	4.826971	-0.695658	1.511243
H	3.620966	0.511860	2.034148
H	4.437698	-1.004918	-1.350466
H	3.116801	0.124404	-1.790137
H	5.528290	0.952562	-0.232648
H	3.958633	1.782051	-0.115907
C	-0.817576	-1.280124	-1.112005
O	-0.240282	-2.448159	-0.698309
C	-2.074352	-1.014748	-0.376928
C	-2.939120	-2.081305	-0.097189
C	-2.432921	0.306716	-0.036506
C	-4.177545	-1.841301	0.489773
H	-2.642892	-3.090148	-0.362219
C	-3.683772	0.525534	0.545244
C	-4.552356	-0.534354	0.801818
H	-4.847308	-2.669649	0.697972
H	-3.956459	1.537424	0.827466
H	-5.516812	-0.339703	1.261516

TS2a

C	2.953701	0.801364	-0.317331
O	2.753233	1.759538	0.564528
C	3.663942	-0.464122	0.164966
H	4.149332	-0.271910	1.122481
H	2.956592	-1.288431	0.275319
O	2.250062	0.782698	-1.408198
C	-0.129745	1.523784	-0.446817
O	0.420678	0.431943	-0.845480
O	0.464572	2.588727	-0.166585
H	1.929055	2.284585	0.235461
C	4.654177	-0.566651	-1.017173
H	5.686184	-0.790789	-0.728917
H	4.329939	-1.284213	-1.772919
C	4.451412	0.854524	-1.491045
H	4.298073	1.092569	-2.539344
H	4.951194	1.643979	-0.929956
C	-1.631630	1.486148	-0.289483
C	-2.267492	2.726474	-0.168567
C	-2.394964	0.300745	-0.229757
C	-3.646291	2.820717	-0.007288
H	-1.647449	3.614383	-0.202172
C	-3.782709	0.416262	-0.055740

C	-4.408013	1.656104	0.053046
H	-4.118523	3.795087	0.077774
H	-4.374121	-0.491681	0.012993
H	-5.484487	1.706742	0.190241
C	-1.873152	-1.091803	-0.372849
C	-2.441464	-1.880922	-1.381347
C	-0.909048	-1.698415	0.463930
C	-2.082266	-3.215424	-1.563397
H	-3.170407	-1.423907	-2.042796
C	-0.552551	-3.040213	0.280548
C	-1.137839	-3.803218	-0.725355
H	-2.543334	-3.792109	-2.360164
H	0.182734	-3.484482	0.941501
H	-0.856598	-4.844202	-0.851282
C	-0.238110	-0.926078	1.532219
O	-0.656607	0.033422	2.151511
O	1.014842	-1.418075	1.772164
O	1.669405	-0.669355	2.816085
H	1.014591	0.067567	2.928222

TS2b

O	3.041914	-2.193611	0.420251
O	1.971046	-0.182238	0.137433
H	2.183928	-2.516092	0.051675
C	-0.081420	0.358771	1.652328
O	1.071009	-0.269360	1.751385
O	-0.984320	0.122740	2.444184
O	0.820098	-2.875595	-1.138127
O	-0.246345	-0.747663	-1.869956
H	0.893597	-2.105898	-1.770417
C	-0.238021	1.416637	0.590093
C	0.726030	2.421133	0.467163
C	-1.403064	1.471770	-0.196377
C	0.537151	3.485975	-0.410664
H	1.617921	2.365416	1.082188
C	-1.580498	2.541022	-1.080783
C	-0.620281	3.545363	-1.187919
H	1.287182	4.268403	-0.485527
H	-2.472662	2.569205	-1.699634
H	-0.773551	4.368165	-1.880315
C	3.077564	-0.862075	0.309055
C	4.264177	-0.131412	0.931330

C	3.572061	0.015739	-1.207024
C	4.401938	0.866380	-0.245296
H	5.119916	-0.804619	1.013935
H	4.023202	0.285316	1.913283
H	4.118714	-0.776151	-1.726774
H	2.798225	0.466270	-1.822484
H	5.427379	1.058950	-0.572386
H	3.908601	1.818292	-0.040491
C	-0.866174	-1.318298	-0.991330
O	-0.397650	-2.489882	-0.458399
C	-2.162013	-0.938865	-0.393455
C	-3.132407	-1.929729	-0.197077
C	-2.441252	0.412195	-0.101196
C	-4.402930	-1.582589	0.251170
H	-2.891415	-2.963482	-0.419349
C	-3.726440	0.738125	0.338675
C	-4.700630	-0.244346	0.508602
H	-5.155744	-2.351311	0.394300
H	-3.944454	1.772679	0.583868
H	-5.689599	0.034939	0.860176

Int. 3a

C	-3.213009	-1.457371	-0.369318
O	-2.892937	-2.596089	-0.083234
C	-3.591305	-0.328727	0.567427
H	-4.635355	-0.477076	0.873518
H	-2.968036	-0.347813	1.461963
O	-3.288060	-1.047063	-1.648719
C	0.195839	-1.557729	-0.424750
O	-0.578968	-0.610236	-0.428393
O	-0.211428	-2.825490	-0.542903
H	-1.203742	-2.837546	-0.528484
C	-3.409748	0.916415	-0.306033
H	-4.109488	1.722426	-0.071647
H	-2.391360	1.291943	-0.198356
C	-3.622659	0.359300	-1.722303
H	-2.969346	0.805737	-2.473953
H	-4.663260	0.435270	-2.057449
C	1.674306	-1.427565	-0.280839
C	2.441893	-2.592665	-0.150243
C	2.313370	-0.166696	-0.264627
C	3.823933	-2.534417	-0.001267

H	1.933894	-3.548788	-0.167059
C	3.706686	-0.130133	-0.126276
C	4.459023	-1.294930	0.010856
H	4.397736	-3.450142	0.104222
H	4.200704	0.836494	-0.111978
H	5.537082	-1.229449	0.126987
C	1.642720	1.155552	-0.459369
C	2.002422	1.895995	-1.590617
C	0.729897	1.738261	0.444935
C	1.476515	3.165942	-1.831618
H	2.698092	1.455409	-2.297897
C	0.205756	3.012883	0.204162
C	0.577495	3.730457	-0.930495
H	1.774035	3.710444	-2.723131
H	-0.489444	3.441327	0.917159
H	0.168727	4.721064	-1.104190
C	0.299102	0.992571	1.646804
O	0.917570	0.148088	2.267610
O	-0.955473	1.365181	2.032152
O	-1.363635	0.635578	3.207546
H	-0.570205	0.048079	3.319232

Int. 3b

O	2.662750	-0.870559	2.166551
O	2.674457	-1.162793	-0.107600
H	1.711766	-1.111978	2.217130
C	0.543018	0.571400	0.905049
O	1.858167	0.831543	0.752212
O	0.124412	-0.422215	1.482233
O	0.952883	-2.930485	-1.343762
O	-0.146869	-0.578891	-1.718449
H	1.562600	-2.408495	-0.769211
C	-0.302345	1.626185	0.286170
C	0.273689	2.882455	0.052614
C	-1.646744	1.387053	-0.080924
C	-0.454924	3.915293	-0.526854
H	1.306112	3.040928	0.338707
C	-2.354292	2.439484	-0.680264
C	-1.776773	3.687552	-0.901174
H	0.009072	4.882984	-0.691091
H	-3.377114	2.259143	-0.994611
H	-2.360020	4.474857	-1.369985

C	2.823878	-0.260441	0.966715
C	4.187994	0.370540	0.748607
C	3.292252	-0.591894	-1.288538
C	4.232686	0.527109	-0.780218
H	4.935127	-0.339767	1.113109
H	4.291473	1.308497	1.296456
H	3.824369	-1.408957	-1.782165
H	2.502726	-0.224121	-1.947521
H	5.244695	0.425833	-1.179419
H	3.849250	1.506984	-1.075113
C	-0.749390	-1.371355	-1.033230
O	-0.300782	-2.621324	-0.707630
C	-2.054923	-1.153710	-0.344211
C	-2.909525	-2.245016	-0.150478
C	-2.417346	0.124497	0.133723
C	-4.125309	-2.095953	0.511547
H	-2.610777	-3.216125	-0.527139
C	-3.638622	0.246353	0.811060
C	-4.485192	-0.844127	1.002831
H	-4.778213	-2.952711	0.647192
H	-3.917670	1.218459	1.205192
H	-5.422310	-0.710287	1.535475

TS3b

O	2.398099	-1.032468	2.004850
O	2.787766	-1.045396	-0.219599
H	1.298813	-0.907649	1.848524
C	0.550256	0.742969	0.850233
O	1.787322	1.042616	0.688184
O	0.163265	-0.301754	1.456646
O	1.074442	-2.811883	-1.590743
O	-0.116075	-0.492002	-1.737156
H	1.706272	-2.300286	-1.039156
C	-0.439238	1.694339	0.264571
C	0.010746	2.997516	0.019587
C	-1.761687	1.331963	-0.072649
C	-0.822478	3.959500	-0.540672
H	1.033999	3.240876	0.280621
C	-2.579510	2.313995	-0.652932
C	-2.126336	3.610440	-0.884512
H	-0.454432	4.966345	-0.713866
H	-3.588670	2.039300	-0.942971

H	-2.791452	4.340282	-1.337302
C	2.923463	-0.450831	0.990611
C	4.223534	0.307173	1.010509
C	3.512952	-0.292107	-1.233207
C	4.390344	0.721684	-0.461944
H	5.001054	-0.392675	1.339925
H	4.181075	1.139138	1.712322
H	4.088113	-1.025814	-1.802081
H	2.766432	0.175280	-1.876105
H	5.431383	0.688888	-0.790590
H	4.010186	1.733121	-0.611366
C	-0.659657	-1.343492	-1.075240
O	-0.133679	-2.589928	-0.840689
C	-1.951605	-1.236551	-0.338072
C	-2.705582	-2.397634	-0.125619
C	-2.407781	0.004443	0.159055
C	-3.906482	-2.356901	0.577193
H	-2.340446	-3.337832	-0.520888
C	-3.612941	0.017014	0.874940
C	-4.355939	-1.142584	1.088145
H	-4.478695	-3.267299	0.727322
H	-3.961905	0.960720	1.282029
H	-5.283214	-1.091485	1.651655

2p

C	-0.888603	-0.001612	-0.003731
O	-2.087779	-0.028213	0.073404
C	0.027734	1.207769	-0.172373
H	-0.006101	1.512877	-1.226073
H	-0.335660	2.044588	0.426867
O	-0.126585	-1.135099	0.044165
C	1.404071	0.668385	0.224410
H	2.237658	1.145465	-0.297102
H	1.563067	0.785701	1.301484
C	1.268922	-0.820476	-0.130039
H	1.841664	-1.486615	0.518371
H	1.541536	-1.019915	-1.173697

C

C	-1.152934	-0.933433	1.552512
O	-0.003033	-0.877011	1.942181

O	-2.047926	-1.776514	2.132661
H	-1.545802	-2.241652	2.826713
C	-1.746602	-0.138142	0.447008
C	-3.094868	-0.327837	0.114580
C	-0.975877	0.805819	-0.267414
C	-3.691619	0.400788	-0.909284
H	-3.672008	-1.054899	0.672251
C	-1.597922	1.538057	-1.284728
C	-2.938242	1.339355	-1.610902
H	-4.736563	0.236986	-1.154247
H	-1.008161	2.264375	-1.835239
H	-3.389052	1.917748	-2.412258
C	0.451593	1.143698	0.018138
C	0.719850	2.423512	0.513166
C	1.543695	0.288743	-0.241426
C	2.025040	2.849698	0.760021
H	-0.115187	3.086446	0.717530
C	2.852142	0.720975	0.004473
C	3.096285	1.997307	0.503789
H	2.200076	3.848286	1.149899
H	3.677669	0.051028	-0.205077
H	4.115945	2.321241	0.687537
C	1.311947	-1.069783	-0.777142
O	0.322205	-1.477716	-1.362026
O	2.375782	-1.887353	-0.554665
O	2.156221	-3.182418	-1.145636
H	1.232177	-3.054004	-1.483969

TS4a

O	2.597489	-1.940023	0.469565
O	1.979297	0.642130	0.319441
H	1.690948	-2.222146	-0.041366
C	-0.045696	0.577932	1.609885
O	1.314755	0.270939	1.558500
O	-0.652549	0.062764	2.510380
C	-0.202686	-1.408826	-0.712605
O	0.419148	-2.465372	-0.376096
O	0.344273	-0.391480	-1.238716
H	1.304139	0.278913	-0.400305
C	-0.595169	1.540657	0.614809
C	-0.031225	2.817036	0.547982
C	-1.708225	1.199919	-0.180565

C	-0.584254	3.790283	-0.281336
H	0.837314	3.045061	1.157246
C	-2.242395	2.191853	-1.011015
C	-1.694710	3.473390	-1.060950
H	-0.148780	4.784170	-0.318100
H	-3.087053	1.938838	-1.644177
H	-2.131348	4.219143	-1.719061
C	-1.672799	-1.361548	-0.422502
C	-2.351249	-0.146247	-0.175965
C	-2.373108	-2.571837	-0.369030
C	-3.726398	-0.197066	0.093350
C	-3.740419	-2.600829	-0.115023
H	-1.818378	-3.488321	-0.536348
C	-4.419383	-1.404962	0.116883
H	-4.248745	0.729853	0.309972
H	-4.270197	-3.548516	-0.089721
H	-5.484645	-1.410689	0.329660
C	3.242675	-0.977763	-0.019125
C	4.492005	-0.318328	0.520418
C	3.529399	-0.533303	-1.447187
C	4.642094	0.390954	-0.862652
H	5.261208	-1.075501	0.713061
H	4.365715	0.296878	1.412449
H	3.931337	-1.390581	-2.001708
H	2.710991	-0.105691	-2.027230
H	5.622280	0.311932	-1.335426
H	4.335169	1.437093	-0.825766

TS4apri

C	-2.932813	-0.732767	0.013599
O	-2.469655	-1.251211	1.116048
C	-3.257611	0.753099	-0.259502
H	-3.741775	1.196872	0.616040
H	-2.426818	1.393025	-0.561879
O	-1.920973	-1.166278	-1.177469
C	0.145759	-1.506866	-0.278884
O	-0.565804	-0.641947	-0.955938
O	-0.395968	-2.498950	0.301756
H	-1.419623	-2.227246	0.489265
C	-4.282755	0.286957	-1.331436
H	-5.261559	0.772507	-1.311389
H	-3.874349	0.340667	-2.342846

C	-4.215870	-1.153455	-0.753117
H	-4.149554	-2.003943	-1.437641
H	-5.003026	-1.347505	-0.016820
C	1.601259	-1.340219	-0.273235
C	2.345706	-2.526749	-0.258719
C	2.237464	-0.076343	-0.237436
C	3.735435	-2.488918	-0.266427
H	1.820966	-3.475435	-0.252721
C	3.638054	-0.074449	-0.231944
C	4.380554	-1.254516	-0.257296
H	4.303896	-3.413188	-0.266255
H	4.151357	0.879413	-0.174049
H	5.465345	-1.204171	-0.250492
C	1.557147	1.253066	-0.176365
C	1.989774	2.220248	-1.097220
C	0.551887	1.619349	0.748316
C	1.471667	3.512839	-1.100132
H	2.735120	1.940401	-1.835222
C	0.024808	2.915205	0.724947
C	0.488735	3.867294	-0.178025
H	1.829648	4.234591	-1.828449
H	-0.761436	3.162166	1.429006
H	0.074324	4.870880	-0.171349
C	-0.028239	0.620687	1.702839
O	0.581672	-0.354896	2.106226
O	-1.312129	0.857960	1.983377
H	-1.785417	-0.043224	1.983023

Int. 4a

O	2.551490	-2.219474	0.184198
O	1.881587	0.024604	0.191798
H	1.763038	-2.352900	-0.382015
C	0.033420	0.379136	1.588999
O	1.284851	-0.168779	1.533422
O	-0.672289	0.036458	2.506508
C	-0.577484	-1.298953	-1.275496
O	0.111377	-2.308962	-1.253244
O	-0.243715	-0.228160	-2.016624
H	0.646331	-0.405348	-2.373070
C	-0.339343	1.425152	0.588154
C	0.451034	2.571715	0.470328
C	-1.553045	1.325524	-0.114806

C	0.021746	3.642077	-0.310811
H	1.393438	2.624406	1.005390
C	-1.973025	2.408124	-0.891959
C	-1.197016	3.562553	-0.985257
H	0.633851	4.535654	-0.388332
H	-2.903279	2.326893	-1.446189
H	-1.537878	4.393691	-1.595820
C	-1.866612	-1.155904	-0.550751
C	-2.358870	0.075996	-0.067469
C	-2.610268	-2.329412	-0.370700
C	-3.619572	0.098639	0.536761
C	-3.860840	-2.287660	0.235075
H	-2.193147	-3.264805	-0.727571
C	-4.370256	-1.066619	0.679411
H	-3.991474	1.039795	0.929368
H	-4.434231	-3.200778	0.361077
H	-5.344291	-1.023757	1.158025
C	2.958388	-0.914754	0.085956
C	4.161111	-0.533346	0.967517
C	3.727226	-0.389415	-1.167040
C	4.705064	0.333426	-0.201773
H	4.776363	-1.415173	1.160874
H	3.919287	-0.039761	1.910882
H	4.185102	-1.236127	-1.684791
H	3.165050	0.222808	-1.880052
H	5.769991	0.241183	-0.427349
H	4.455496	1.391048	-0.085706

TS5a

O	2.363316	-1.700214	-0.865752
O	2.592430	0.336822	0.129079
H	1.489123	-1.288129	-1.147445
C	0.144724	0.126658	1.473326
O	1.410227	-0.159648	1.618909
O	-0.721859	-0.529535	2.053965
C	-0.932338	-1.589598	-0.758477
O	-0.090929	-0.925097	-1.360059
O	-0.711117	-2.868023	-0.409975
H	0.203662	-3.092978	-0.662531
C	-0.225343	1.304690	0.609317
C	0.630757	2.408423	0.575064
C	-1.435627	1.341598	-0.117288

C	0.321705	3.543851	-0.170419
H	1.547551	2.361207	1.150653
C	-1.720728	2.481870	-0.881503
C	-0.856052	3.574594	-0.913452
H	0.997568	4.394640	-0.173499
H	-2.635567	2.502253	-1.466507
H	-1.107394	4.444302	-1.514263
C	-2.267355	-1.094364	-0.373638
C	-2.479139	0.273337	-0.086654
C	-3.322027	-2.011416	-0.297742
C	-3.780775	0.665342	0.251362
C	-4.607772	-1.593081	0.028942
H	-3.124089	-3.056398	-0.507297
C	-4.833878	-0.246311	0.304449
H	-3.956774	1.705968	0.503502
H	-5.419651	-2.312285	0.074994
H	-5.828447	0.098010	0.573702
C	3.076191	-0.813826	-0.187046
C	4.323111	-1.326990	0.523006
C	4.406211	0.339232	-1.029137
C	5.244022	-0.147424	0.135937
H	4.643676	-2.271448	0.078274
H	4.137931	-1.464764	1.591911
H	4.464675	-0.234173	-1.955313
H	4.184283	1.391263	-1.174961
H	6.262761	-0.439000	-0.139298
H	5.290040	0.607567	0.922447

Int. 5a

O	1.898860	-2.886730	-1.075700
O	2.740528	-0.823018	-1.089262
H	1.199559	-3.407976	-0.626466
C	-0.475259	-1.796013	-0.049624
O	-0.385387	-2.973408	0.294814
O	0.574003	-1.059923	-0.418506
C	-0.288727	1.552936	1.783069
O	-1.171109	0.845370	2.223707
O	0.607527	2.157027	2.616655
H	0.339111	1.887632	3.514291
C	-1.779628	-1.080806	-0.120111
C	-2.918077	-1.868274	0.096084
C	-1.923499	0.296910	-0.386165

C	-4.193068	-1.318083	0.039308
H	-2.772162	-2.921683	0.306224
C	-3.214204	0.832481	-0.452660
C	-4.340396	0.039937	-0.240636
H	-5.064168	-1.943925	0.207898
H	-3.327138	1.892032	-0.661326
H	-5.329868	0.485311	-0.293401
C	-0.032100	1.857947	0.353597
C	-0.789712	1.232330	-0.658025
C	0.984936	2.759737	0.006022
C	-0.507851	1.540427	-1.992155
C	1.260086	3.044051	-1.327258
H	1.555645	3.235124	0.794645
C	0.510084	2.428903	-2.329729
H	-1.087812	1.055356	-2.770828
H	2.050886	3.743284	-1.581685
H	0.716751	2.639517	-3.374948
C	1.938050	-1.697915	-0.401005
C	2.431769	-1.727192	1.051182
C	3.489063	0.014162	-0.186366
C	2.991920	-0.313526	1.230309
H	3.225706	-2.479511	1.103612
H	1.644113	-2.001772	1.754062
H	4.551562	-0.223833	-0.315563
H	3.320131	1.055901	-0.469923
H	3.794513	-0.260836	1.971168
H	2.207468	0.382756	1.533542

TS6a

O	2.601069	2.641097	0.720598
O	3.823700	0.849359	1.136763
H	1.569971	2.801684	0.372674
C	-0.149031	1.588381	0.428003
O	0.292007	2.754363	0.074057
O	0.566100	0.668963	0.876697
C	-0.237086	-1.111558	-1.788480
O	-0.693471	-0.065975	-2.204480
O	0.687119	-1.800335	-2.529499
H	0.775123	-1.281571	-3.349933
C	-1.623903	1.377151	0.241650
C	-2.449588	2.491576	0.070421
C	-2.187178	0.086652	0.221713

C	-3.824193	2.350305	-0.104845
H	-1.985695	3.471144	0.076534
C	-3.569905	-0.043059	0.045249
C	-4.386422	1.075566	-0.118912
H	-4.450339	3.229076	-0.230995
H	-4.004096	-1.038685	0.026290
H	-5.456445	0.946745	-0.257265
C	-0.550880	-1.777067	-0.502350
C	-1.418705	-1.177423	0.438881
C	0.044688	-3.015261	-0.215282
C	-1.663745	-1.862750	1.635001
C	-0.200796	-3.669414	0.986895
H	0.700114	-3.462912	-0.952509
C	-1.060843	-3.086333	1.916443
H	-2.331893	-1.408083	2.359367
H	0.268531	-4.627045	1.191566
H	-1.266689	-3.583735	2.860224
C	2.979308	1.501960	0.373774
C	2.729888	0.779305	-0.922894
C	4.145552	-0.448514	0.536247
C	3.070551	-0.662572	-0.534113
H	3.452028	1.187970	-1.646741
H	1.725537	0.946427	-1.303723
H	5.157921	-0.365887	0.129177
H	4.133356	-1.172971	1.350370
H	3.424749	-1.271666	-1.367447
H	2.189351	-1.131934	-0.095083

TSI

O	-0.393273	1.214421	-3.081028
O	1.151130	0.433829	-1.164750
H	-1.219718	0.712706	-2.628891
C	2.956153	-1.082427	-1.364414
O	2.327991	0.021281	-1.896785
O	3.933871	-1.451449	-1.976821
C	-1.736733	-0.975418	-1.157982
O	-2.171688	0.060273	-1.772291
O	-0.536278	-1.358748	-1.158140
H	0.435058	-0.379141	-1.279740
C	2.348646	-1.797405	-0.207001
C	2.042954	-1.227327	1.047036
C	2.060664	-3.142564	-0.462483

C	1.394770	-2.035117	1.989576
C	1.404691	-3.920815	0.485384
C	1.061156	-3.358860	1.712289
H	1.180184	-1.619431	2.969057
H	1.166699	-4.956703	0.265752
H	0.552680	-3.954059	2.464785
C	-2.746507	-1.768630	-0.395999
C	-2.846698	-3.145903	-0.605147
C	-3.613885	-1.117301	0.498902
C	-3.850895	-3.876711	0.026142
C	-4.610092	-1.865023	1.133346
C	-4.741047	-3.231790	0.885577
H	-3.940067	-4.943860	-0.153799
H	-5.275700	-1.368822	1.833142
H	-5.528746	-3.794671	1.377618
C	0.226299	1.843740	-2.159595
C	1.354378	2.833647	-2.321991
C	-0.304807	2.513964	-0.898196
C	0.974074	3.407026	-0.920332
H	1.141802	3.505331	-3.160768
H	2.351896	2.410196	-2.447778
H	-1.235282	3.045480	-1.125390
H	-0.476218	1.887184	-0.022794
H	0.792611	4.482684	-0.888155
H	1.689532	3.131741	-0.147370
H	-2.143398	-3.629117	-1.275762
H	2.329092	-3.560213	-1.426870
C	-3.382856	0.304463	0.906679
C	-4.117892	1.392789	0.406344
C	-2.422892	0.539130	1.901353
C	-3.899378	2.676131	0.921389
C	-2.190211	1.824313	2.390043
C	-2.931595	2.899372	1.897220
H	-1.872475	-0.308026	2.301496
H	-4.507158	3.491696	0.543231
H	-1.450674	1.980051	3.170586
H	-2.767582	3.901800	2.281607
C	2.385251	0.164756	1.438405
C	3.659604	0.733853	1.244334
C	1.397596	0.955331	2.043199
C	3.914091	2.055854	1.628064
C	1.660057	2.259844	2.450275
C	2.923876	2.816281	2.244380

H	0.402191	0.542176	2.160903
H	4.901580	2.472058	1.459164
H	0.871410	2.849549	2.908390
H	3.134859	3.834902	2.555057
C	-5.180501	1.253750	-0.654720
O	-6.254041	1.806870	-0.550680
O	-4.867989	0.512302	-1.724950
H	-3.902693	0.290753	-1.734679
C	4.775611	-0.092337	0.687071
O	5.099744	-1.193452	1.045250
O	5.324960	0.596777	-0.363280
O	6.358873	-0.168523	-1.013482
H	5.800413	-0.832592	-1.478016

B

O	-0.051763	-1.471584	-2.812527
O	-1.217882	-0.425215	-1.080038
H	0.711699	-0.871631	-2.695378
C	-3.178338	0.814705	-1.512518
O	-2.446577	-0.269769	-1.871803
O	-4.197471	0.986259	-2.152425
C	1.735821	1.150640	-0.791579
O	1.933360	0.234275	-1.593688
O	0.530583	1.606541	-0.493809
H	-0.154272	1.031551	-0.922469
C	-2.689690	1.772352	-0.474509
C	-2.372681	1.460620	0.866507
C	-2.614432	3.096704	-0.926290
C	-1.954975	2.508758	1.698071
C	-2.174458	4.114643	-0.086903
C	-1.842942	3.815596	1.232773
H	-1.738161	2.287963	2.738182
H	-2.106108	5.132259	-0.458371
H	-1.513779	4.600312	1.907360
C	2.846208	1.839109	-0.089803
C	2.930157	3.234469	-0.119674
C	3.848953	1.067772	0.526169
C	4.046221	3.873079	0.415580
C	4.957580	1.726378	1.064079
C	5.065075	3.115965	0.994772
H	4.122254	4.955227	0.376235
H	5.731398	1.140305	1.549909

H	5.940063	3.607978	1.408840
C	-0.592239	-1.651247	-1.563793
C	-1.479880	-2.899337	-1.431670
C	0.347831	-2.165991	-0.440826
C	-0.443940	-3.502768	-0.440558
H	-1.624041	-3.427543	-2.375591
H	-2.449147	-2.676010	-0.983364
H	1.392809	-2.220117	-0.745857
H	0.273290	-1.603817	0.488476
H	0.123259	-4.339597	-0.854754
H	-0.851315	-3.793192	0.529956
H	2.131521	3.806284	-0.581113
H	-2.898262	3.313415	-1.950678
C	3.673925	-0.400614	0.755833
C	4.313943	-1.385559	-0.015856
C	2.890455	-0.798656	1.847456
C	4.186404	-2.734754	0.333289
C	2.739477	-2.146660	2.168637
C	3.391935	-3.119271	1.410411
H	2.412754	-0.035274	2.455397
H	4.717438	-3.473193	-0.258369
H	2.125674	-2.434966	3.017309
H	3.287750	-4.170768	1.660223
C	-2.442075	0.097141	1.454929
C	-3.549066	-0.761693	1.307391
C	-1.342165	-0.366013	2.191195
C	-3.523009	-2.052779	1.845627
C	-1.331457	-1.639557	2.754076
C	-2.421588	-2.492085	2.576329
H	-0.470190	0.274493	2.281948
H	-4.382273	-2.699688	1.704366
H	-0.462190	-1.973020	3.313360
H	-2.417119	-3.489159	3.005710
C	5.171649	-1.058178	-1.210273
O	6.264139	-1.554412	-1.369747
O	4.649070	-0.200583	-2.102441
H	3.695846	-0.034341	-1.914411
C	-4.786120	-0.275970	0.621313
O	-5.350582	0.766226	0.824341
O	-5.126272	-1.194557	-0.337792
O	-6.263098	-0.759048	-1.109136
H	-5.826410	-0.073317	-1.665498

TSII

O	0.006696	-1.649018	2.867777
O	0.692095	-0.839170	0.840085
H	-0.775371	-1.080855	2.643470
C	1.766898	1.680722	0.849487
O	1.482967	0.688977	1.658098
O	2.229999	2.724096	1.314857
C	-1.961058	1.017919	1.566559
O	-2.033139	-0.163124	1.926277
O	-0.964159	1.822979	1.883818
H	-0.178866	1.317235	2.217812
C	1.421863	1.609192	-0.615122
C	1.928190	0.678838	-1.545723
C	0.551586	2.619557	-1.044493
C	1.518175	0.793594	-2.884086
C	0.145141	2.706084	-2.372737
C	0.634149	1.785599	-3.299355
H	1.938299	0.109888	-3.615436
H	-0.537311	3.492204	-2.681565
H	0.344505	1.848394	-4.344175
C	-3.029216	1.643896	0.758616
C	-3.492983	2.922825	1.085996
C	-3.618519	0.906050	-0.285937
C	-4.586736	3.458709	0.412121
C	-4.712121	1.464442	-0.953824
C	-5.203405	2.721159	-0.599121
H	-4.958541	4.443043	0.678548
H	-5.167174	0.909059	-1.767869
H	-6.060461	3.130322	-1.125664
C	0.772831	-1.741115	1.772466
C	2.005316	-2.627734	1.934822
C	0.228627	-2.976824	0.560791
C	1.395168	-3.794628	1.118693
H	2.230240	-2.849568	2.978493
H	2.860440	-2.163227	1.443409
H	-0.788080	-3.193802	0.882122
H	0.280646	-2.652043	-0.470618
H	1.039646	-4.604320	1.760522
H	2.052738	-4.197397	0.347253
H	-3.008016	3.475960	1.883430
H	0.191164	3.334816	-0.313695
C	-3.027186	-0.365180	-0.813811

C	-3.597964	-1.629751	-0.583811
C	-1.932380	-0.263143	-1.680369
C	-3.110943	-2.749211	-1.267963
C	-1.432090	-1.387636	-2.334840
C	-2.031220	-2.633400	-2.140916
H	-1.485321	0.707859	-1.859720
H	-3.597799	-3.705148	-1.103794
H	-0.591055	-1.273832	-3.012041
H	-1.662856	-3.509360	-2.667550
C	2.893398	-0.405429	-1.218870
C	4.075799	-0.200051	-0.480694
C	2.642008	-1.698682	-1.701556
C	4.937859	-1.267209	-0.203965
C	3.521402	-2.751880	-1.462039
C	4.670845	-2.541758	-0.698903
H	1.732265	-1.873770	-2.267267
H	5.833194	-1.081081	0.379854
H	3.305812	-3.736789	-1.867103
H	5.357592	-3.358530	-0.498943
C	-4.733263	-1.849400	0.378923
O	-5.683317	-2.551332	0.114644
O	-4.615687	-1.245808	1.575837
H	-3.717155	-0.858906	1.684966
C	4.470568	1.183337	-0.062595
O	4.513628	2.147998	-0.778975
O	4.720677	1.163312	1.280813
O	4.980530	2.486355	1.790646
H	4.054722	2.834364	1.778080

TSIII

O	-0.336456	-1.276503	3.139070
O	1.242207	-0.490593	1.257542
H	-1.137826	-0.787846	2.694701
C	3.075120	1.008952	1.534738
O	2.421349	-0.121295	2.013060
O	4.054163	1.321633	2.161542
C	-1.625163	0.932770	1.170414
O	-2.092119	-0.109880	1.740187
O	-0.422913	1.312015	1.237183
H	0.528387	0.336558	1.372590
C	2.466748	1.783910	0.416256
C	2.215424	1.271183	-0.870773

C	2.127681	3.102342	0.731234
C	1.559246	2.095265	-1.791601
C	1.471504	3.904529	-0.197604
C	1.175436	3.392854	-1.458632
H	1.376973	1.716066	-2.792576
H	1.192012	4.920061	0.064853
H	0.662230	4.007263	-2.192356
C	-2.586634	1.751651	0.372013
C	-2.683121	3.126200	0.599760
C	-3.411798	1.126919	-0.579784
C	-3.644387	3.879747	-0.070496
C	-4.364758	1.897058	-1.252820
C	-4.494536	3.260612	-0.987481
H	-3.731093	4.944729	0.123347
H	-4.996833	1.420993	-1.996391
H	-5.248746	3.841222	-1.510516
C	0.300686	-1.891611	2.210489
C	1.407751	-2.900313	2.394818
C	-0.226703	-2.560289	0.947244
C	1.033612	-3.478705	0.993599
H	1.173096	-3.560683	3.236473
H	2.410044	-2.491583	2.528604
H	-1.170635	-3.071798	1.163171
H	-0.371517	-1.934121	0.066917
H	0.830263	-4.550760	0.969380
H	1.764472	-3.224957	0.227332
H	-2.009824	3.589416	1.313823
H	2.354424	3.479712	1.722768
C	-3.171694	-0.288729	-1.003661
C	-3.932365	-1.382695	-0.556957
C	-2.169561	-0.509535	-1.959131
C	-3.695648	-2.657274	-1.085580
C	-1.919136	-1.786638	-2.460336
C	-2.685713	-2.867217	-2.020827
H	-1.598344	0.342286	-2.317905
H	-4.322757	-3.476873	-0.750060
H	-1.144903	-1.930781	-3.208900
H	-2.508106	-3.863375	-2.415487
C	2.606044	-0.098893	-1.288853
C	3.905323	-0.622558	-1.125803
C	1.624298	-0.922291	-1.856609
C	4.177135	-1.948180	-1.494196
C	1.908985	-2.224737	-2.253466

C	3.190865	-2.745954	-2.066047
H	0.615589	-0.535894	-1.947712
H	5.180370	-2.333927	-1.353388
H	1.123964	-2.840619	-2.682868
H	3.420287	-3.764839	-2.363051
C	-5.040683	-1.258651	0.458420
O	-6.111311	-1.803659	0.294269
O	-4.772562	-0.541551	1.555820
H	-3.805656	-0.327028	1.614499
C	5.040717	0.244126	-0.690789
O	5.151445	1.426119	-0.931081
O	5.983051	-0.454059	-0.009934
H	6.671237	0.195879	0.226247

D

O	0.117904	-2.577837	1.111800
O	1.504146	-1.850727	-0.619284
H	-0.468205	-1.799713	0.997010
C	2.715988	-1.109867	1.311881
O	2.720218	-1.922306	0.187003
O	3.461861	-1.445073	2.195093
C	-1.224325	0.307730	-0.738026
O	-1.437338	-0.421574	0.233800
O	-0.143919	0.197021	-1.500272
H	0.501165	-0.433029	-1.085374
C	1.900033	0.138921	1.304120
C	2.180770	1.179982	0.398793
C	0.923045	0.300007	2.289190
C	1.407741	2.343807	0.464709
C	0.163280	1.465928	2.342061
C	0.397831	2.482906	1.415740
H	1.624464	3.153263	-0.226125
H	-0.624374	1.570782	3.080322
H	-0.199396	3.389211	1.442023
C	-2.144563	1.396707	-1.127229
C	-1.615655	2.594025	-1.626481
C	-3.526432	1.270927	-0.880858
C	-2.446556	3.687586	-1.847916
C	-4.345215	2.379943	-1.112120
C	-3.811708	3.581403	-1.579121
H	-2.030865	4.619185	-2.219063
H	-5.411276	2.289141	-0.929718

H	-4.466643	4.432337	-1.741398
C	0.601998	-2.889899	-0.133499
C	1.201348	-4.293608	-0.298364
C	-0.358726	-3.157313	-1.326733
C	0.513287	-4.389878	-1.688397
H	0.764008	-4.968482	0.440894
H	2.289139	-4.354644	-0.254582
H	-1.347957	-3.419812	-0.943273
H	-0.458843	-2.367847	-2.075105
H	-0.023036	-5.316485	-1.905043
H	1.203526	-4.177146	-2.508289
H	-0.548845	2.664302	-1.803148
H	0.745716	-0.509140	2.989721
C	-4.168454	-0.024798	-0.496455
C	-4.610457	-0.288902	0.811574
C	-4.430907	-0.961850	-1.502041
C	-5.338853	-1.451170	1.081366
C	-5.119533	-2.140792	-1.217989
C	-5.584290	-2.382266	0.075169
H	-4.102832	-0.751894	-2.516120
H	-5.693599	-1.617364	2.093383
H	-5.307329	-2.859567	-2.010393
H	-6.135621	-3.290645	0.298696
C	3.266528	1.059321	-0.613921
C	4.619954	0.880374	-0.252505
C	2.935163	1.081102	-1.973586
C	5.586751	0.678370	-1.245063
C	3.908197	0.903390	-2.956054
C	5.236552	0.689324	-2.592331
H	1.896812	1.211032	-2.258294
H	6.618631	0.532320	-0.947722
H	3.623434	0.919850	-4.004233
H	5.997727	0.538677	-3.351843
C	-4.304520	0.625460	1.965429
O	-5.139098	0.985119	2.763445
O	-3.012574	0.996288	2.080189
H	-2.453858	0.484575	1.450590
C	5.054086	1.011515	1.169052
O	4.481415	1.657515	2.019999
O	6.211841	0.350654	1.416090
H	6.398265	0.498148	2.361807

TSIV

O	0.058267	1.881064	-2.761971
O	0.790789	0.851369	-0.851495
H	-0.736360	1.322050	-2.560339
C	1.837121	-1.676308	-1.162104
O	1.499817	-0.601751	-1.859254
O	2.322117	-2.631717	-1.749418
C	-1.941361	-0.825830	-1.637141
O	-1.998129	0.386422	-1.878085
O	-0.971744	-1.615446	-2.052899
H	-0.163767	-1.101850	-2.330664
C	1.504193	-1.763324	0.305685
C	2.083342	-0.978623	1.320527
C	0.584532	-2.763538	0.641638
C	1.694285	-1.209858	2.648562
C	0.205009	-2.976574	1.964522
C	0.763831	-2.193442	2.974599
H	2.164995	-0.630278	3.437252
H	-0.515654	-3.753101	2.203494
H	0.489766	-2.356122	4.012911
C	-3.006742	-1.503098	-0.865426
C	-3.520580	-2.726925	-1.307061
C	-3.539682	-0.862135	0.269192
C	-4.609720	-3.298896	-0.655403
C	-4.629336	-1.455612	0.912927
C	-5.171172	-2.653899	0.447151
H	-5.020597	-4.239234	-1.009263
H	-5.040843	-0.975435	1.795176
H	-6.024040	-3.091446	0.957501
C	0.864651	1.842184	-1.691779
C	2.120615	2.702925	-1.814699
C	0.408200	2.961700	-0.339143
C	1.580779	3.797784	-0.861081
H	2.314999	3.023510	-2.838878
H	2.977338	2.165049	-1.407819
H	-0.611767	3.249912	-0.585974
H	0.491233	2.529753	0.649999
H	1.228382	4.678292	-1.403946
H	2.280402	4.104721	-0.082187
H	-3.077334	-3.207761	-2.172798
H	0.163004	-3.369009	-0.153023
C	-2.889797	0.329554	0.903144
C	-3.424398	1.627838	0.824549

C	-1.768477	0.105960	1.710853
C	-2.874317	2.655958	1.598366
C	-1.205174	1.141873	2.454202
C	-1.767602	2.418691	2.410837
H	-1.348551	-0.891271	1.772549
H	-3.332729	3.638480	1.550239
H	-0.342761	0.934132	3.080554
H	-1.349153	3.225086	3.006654
C	3.094382	0.078846	1.061932
C	4.254598	-0.128625	0.288090
C	2.895502	1.347959	1.624001
C	5.135673	0.932982	0.042336
C	3.802955	2.385131	1.423945
C	4.920263	2.185472	0.611750
H	2.003196	1.515544	2.219028
H	6.011793	0.752928	-0.570734
H	3.632415	3.350072	1.893405
H	5.624838	2.992411	0.434754
C	-4.583349	1.979815	-0.067982
O	-5.499954	2.679207	0.301495
O	-4.526498	1.500048	-1.323604
H	-3.645541	1.098867	-1.505255
C	4.655187	-1.500882	-0.148136
O	4.497261	-2.505241	0.508686
O	5.270272	-1.493746	-1.353690
H	5.448683	-2.429596	-1.563866

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O	-0.067486	1.067499	-2.911891
O	0.445573	0.827871	-0.682897
H	-0.789249	0.471979	-2.587508
C	1.615082	-1.894935	-0.430574
O	1.150577	-0.969706	-1.213109
O	1.842404	-3.025751	-0.887850
C	-2.073031	-1.571537	-1.480514
O	-2.075794	-0.389198	-1.845575
O	-1.070767	-2.400212	-1.662300
H	-0.233456	-1.898048	-1.879814
C	1.792125	-1.671175	1.046654
C	2.568915	-0.665970	1.656573
C	1.144046	-2.624971	1.843524
C	2.628069	-0.637540	3.060821

C	1.203063	-2.571738	3.232026
C	1.950098	-1.565973	3.845202
H	3.259315	0.105235	3.538335
H	0.683906	-3.316343	3.827906
H	2.026280	-1.517353	4.927502
C	-3.263909	-2.132891	-0.794537
C	-3.926716	-3.252701	-1.300871
C	-3.768121	-1.429599	0.315522
C	-5.135965	-3.652133	-0.734554
C	-4.981865	-1.844781	0.869328
C	-5.668571	-2.938053	0.339412
H	-5.662528	-4.512900	-1.134822
H	-5.374172	-1.315708	1.732326
H	-6.613796	-3.242631	0.778762
C	0.654291	1.476049	-1.840468
H	-3.506968	-3.787120	-2.147166
H	0.592244	-3.415835	1.346591
C	-2.952982	-0.373748	0.992653
C	-3.285890	0.992514	0.986855
C	-1.840382	-0.791406	1.733669
C	-2.563095	1.886036	1.786242
C	-1.080493	0.116356	2.468486
C	-1.458306	1.457708	2.513655
H	-1.574820	-1.843278	1.738998
H	-2.865886	2.925847	1.791951
H	-0.209899	-0.231042	3.012220
H	-0.887864	2.169701	3.102799
C	3.403942	0.331055	0.932793
C	4.304861	-0.009944	-0.096005
C	3.373868	1.669454	1.354022
C	5.115238	0.964385	-0.687575
C	4.204962	2.634034	0.786736
C	5.079476	2.283629	-0.242699
H	2.678217	1.948419	2.139728
H	5.790317	0.672436	-1.485387
H	4.165778	3.658892	1.145966
H	5.727752	3.028673	-0.693534
C	-4.320421	1.598743	0.084939
O	-5.022812	2.528788	0.419648
O	-4.373390	1.116476	-1.174109
H	-3.630189	0.496215	-1.354318
C	4.473178	-1.440418	-0.511887
O	4.745566	-2.358267	0.214534

O	4.214556	-1.519331	-1.852187
O	4.224936	-2.884139	-2.318257
H	3.357307	-3.178688	-1.938961
C	2.065789	1.828304	-2.248916
C	-0.116250	2.611060	-0.923738
C	0.575497	3.411396	-0.003588
C	-1.459584	2.866164	-1.243752
C	-0.048828	4.542982	0.508193
H	1.581578	3.145436	0.291438
C	-2.070306	4.002553	-0.728932
H	-1.992204	2.222890	-1.929084
C	-1.366541	4.840957	0.143183
H	0.484383	5.185977	1.201686
H	-3.103364	4.214921	-0.983265
H	-1.854380	5.720502	0.552701
H	2.040741	2.493965	-3.114298
H	2.557141	0.891618	-2.524661
H	2.619463	2.290800	-1.435404

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O	0.198712	2.487289	-1.933650
O	0.753495	0.919355	-0.333779
H	-0.737520	2.208915	-1.772975
C	1.375729	-1.536336	-1.321672
O	1.610821	-0.269480	-1.547693
O	1.754715	-2.348432	-2.169691
C	-2.097843	0.121845	-1.796801
O	-2.187321	1.328969	-1.541198
O	-1.100610	-0.397010	-2.501951
H	-0.394587	0.266918	-2.654033
C	0.626444	-2.013023	-0.109367
C	1.013284	-1.794231	1.228085
C	-0.486790	-2.814916	-0.387338
C	0.247217	-2.382527	2.245780
C	-1.249562	-3.371099	0.634788
C	-0.874159	-3.158972	1.960775
H	0.563961	-2.248052	3.275537
H	-2.125010	-3.965821	0.393767
H	-1.446728	-3.598521	2.772192
C	-3.109008	-0.856943	-1.359529
C	-3.411411	-1.953068	-2.177932
C	-3.783630	-0.660422	-0.138054

C	-4.411075	-2.846271	-1.808504
C	-4.782254	-1.572664	0.216062
C	-5.102344	-2.648409	-0.612047
H	-4.652882	-3.686780	-2.451139
H	-5.299252	-1.438334	1.160750
H	-5.887071	-3.338314	-0.316219
C	0.957465	2.117710	-0.859907
H	-2.868103	-2.085522	-3.107164
H	-0.749389	-2.991008	-1.423389
C	-3.389399	0.374138	0.872266
C	-4.109750	1.565243	1.069573
C	-2.339593	0.064514	1.744025
C	-3.803375	2.394681	2.153766
C	-2.020416	0.910895	2.804696
C	-2.758639	2.076034	3.018259
H	-1.784426	-0.852037	1.596267
H	-4.396204	3.291487	2.301799
H	-1.208027	0.643679	3.474908
H	-2.525655	2.730243	3.853208
C	2.223463	-1.032994	1.642513
C	3.518564	-1.360929	1.197877
C	2.087441	0.018939	2.559006
C	4.630663	-0.645583	1.656203
C	3.196055	0.720740	3.026715
C	4.474730	0.385706	2.578806
H	1.089906	0.293142	2.887930
H	5.616456	-0.913483	1.290427
H	3.061905	1.532399	3.735956
H	5.342649	0.929276	2.938976
C	-5.213797	2.005005	0.148027
O	-6.283648	2.403311	0.547447
O	-4.922974	1.958910	-1.167014
H	-3.965393	1.776388	-1.294338
C	3.706552	-2.509633	0.254719
O	3.281271	-3.624607	0.402051
O	4.383583	-2.042218	-0.837349
O	4.474478	-3.042680	-1.871642
H	3.550866	-2.981941	-2.217723
C	0.184485	2.790393	0.685426
H	0.852459	2.557176	1.508003
H	0.182785	3.843310	0.403752
H	-0.807083	2.359187	0.781330
C	2.342001	2.675325	-0.931882

C	3.401977	1.980810	-0.345173
C	2.568712	3.903730	-1.564114
C	4.688874	2.509741	-0.398051
H	3.218786	1.023079	0.117324
C	3.856967	4.431018	-1.607980
H	1.740243	4.429436	-2.026056
C	4.918987	3.735499	-1.024393
H	5.510356	1.955803	0.045367
H	4.033694	5.381650	-2.102579
H	5.923697	4.146779	-1.063858

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O	-0.441139	1.148098	3.029914
O	-1.429802	0.606919	0.968766
H	0.429791	1.344189	2.618871
C	-1.455679	-2.184188	0.955242
O	-1.935850	-1.141832	1.604221
O	-1.458563	-3.244910	1.568692
C	1.803868	-0.611982	1.833170
O	1.981784	0.613618	1.904448
O	0.832887	-1.238325	2.472519
H	0.217915	-0.577220	2.886507
C	-0.969563	-2.113553	-0.458221
C	-1.580574	-1.388958	-1.504924
C	0.111428	-2.958951	-0.737121
C	-1.064207	-1.546615	-2.801198
C	0.621514	-3.086302	-2.025126
C	0.020876	-2.380003	-3.065998
H	-1.548301	-1.020123	-3.617888
H	1.474791	-3.731322	-2.209377
H	0.391934	-2.474493	-4.082415
C	2.676958	-1.497436	1.038111
C	2.917341	-2.804068	1.483262
C	3.276910	-1.017484	-0.141270
C	3.784781	-3.634155	0.781789
C	4.144447	-1.869092	-0.833378
C	4.405958	-3.159694	-0.374642
H	3.976954	-4.642050	1.135755
H	4.602226	-1.512557	-1.750558
H	5.088157	-3.798271	-0.928143
C	-1.481532	1.357953	2.109129
H	2.422547	-3.152904	2.382845

H	0.543005	-3.520701	0.082200
C	2.932436	0.288903	-0.790186
C	3.781920	1.408022	-0.741575
C	1.801449	0.332005	-1.613513
C	3.533394	2.509259	-1.568556
C	1.538074	1.448091	-2.404594
C	2.417556	2.531662	-2.401785
H	1.141058	-0.523175	-1.646664
H	4.230229	3.340951	-1.542620
H	0.659347	1.454243	-3.042894
H	2.232529	3.390979	-3.040038
C	-2.726982	-0.448895	-1.349393
C	-3.949250	-0.760067	-0.717616
C	-2.568192	0.841361	-1.873367
C	-4.944615	0.218640	-0.595165
C	-3.573355	1.798487	-1.780356
C	-4.767070	1.491544	-1.128686
H	-1.616665	1.105343	-2.322503
H	-5.872355	-0.042412	-0.099409
H	-3.411642	2.788320	-2.195066
H	-5.556429	2.232676	-1.042370
C	4.963902	1.486547	0.183888
O	6.049554	1.889598	-0.167869
O	4.727870	1.113875	1.456326
H	3.763541	0.976803	1.601187
C	-4.248141	-2.141707	-0.252674
O	-3.755321	-3.156566	-0.698005
O	-5.184138	-2.168867	0.730102
H	-5.299240	-3.112581	0.947973
C	-2.790544	1.289931	2.877467
H	-2.774799	0.382126	3.481550
H	-2.891873	2.158338	3.533190
H	-3.633747	1.226711	2.188696
C	-1.290463	2.546713	1.148952
C	-2.385193	3.366000	0.810226
C	-0.023877	2.831051	0.601524
C	-2.199901	4.482361	0.006599
H	-3.370868	3.137114	1.193337
C	0.149591	3.945895	-0.212446
H	0.820124	2.179574	0.793308
C	-0.931830	4.777202	-0.506555
H	-3.044875	5.124410	-0.223984
H	1.131177	4.152824	-0.622081

H	-0.791394	5.649460	-1.138396

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O	-0.106088	2.871625	-1.480195
O	0.568617	0.944564	-0.461922
H	-0.949171	2.340216	-1.476991
C	1.716855	-0.977433	-1.648078
O	0.951079	0.013447	-2.112268
O	2.901977	-1.050912	-1.929950
C	-2.444680	0.202580	-1.705305
O	-2.268232	1.336266	-1.229411
O	-1.587276	-0.435741	-2.456852
H	-0.621613	-0.112293	-2.373290
C	1.045923	-1.998055	-0.765845
C	1.490577	-2.237134	0.548786
C	-0.021270	-2.744176	-1.276768
C	0.831388	-3.197221	1.324467
C	-0.644131	-3.724937	-0.507538
C	-0.220789	-3.947595	0.802543
H	1.174373	-3.372080	2.340191
H	-1.458465	-4.306652	-0.929553
H	-0.702574	-4.704180	1.415262
C	-3.715281	-0.517883	-1.441794
C	-4.443360	-1.081383	-2.492998
C	-4.203776	-0.556254	-0.122858
C	-5.695453	-1.640320	-2.247753
C	-5.458713	-1.127199	0.105505
C	-6.206707	-1.650780	-0.949542
H	-6.270609	-2.061160	-3.066642
H	-5.838992	-1.170403	1.121379
H	-7.184169	-2.081172	-0.753158
C	0.784296	2.214227	-0.724698
H	-4.034355	-1.055847	-3.497837
H	-0.364707	-2.558569	-2.287373
C	-3.357299	-0.147012	1.042003
C	-3.572653	1.038027	1.768221
C	-2.364814	-1.035675	1.473461
C	-2.843520	1.280925	2.938053
C	-1.617910	-0.771095	2.620392
C	-1.864863	0.384533	3.363626
H	-2.185392	-1.946819	0.912973
H	-3.056987	2.184583	3.499888

H	-0.860805	-1.482600	2.934000
H	-1.301403	0.585652	4.270380
C	2.576136	-1.434095	1.181747
C	3.933735	-1.540696	0.821585
C	2.219939	-0.518127	2.179516
C	4.886505	-0.717879	1.436220
C	3.175051	0.285057	2.801670
C	4.513882	0.191658	2.422655
H	1.172309	-0.427311	2.446855
H	5.924677	-0.809433	1.138467
H	2.873016	0.985804	3.575416
H	5.263714	0.819986	2.893554
C	-4.558802	2.090992	1.338862
O	-5.311698	2.630977	2.118372
O	-4.529931	2.431148	0.038178
H	-3.758400	2.020005	-0.416978
C	4.375150	-2.580119	-0.154031
O	3.804780	-3.627831	-0.364664
O	5.550939	-2.258094	-0.746265
H	5.742560	-2.993124	-1.357096
C	0.287777	2.327508	1.021744
H	1.078511	1.926492	1.644883
H	0.252818	3.417481	1.004424
H	-0.686508	1.875859	1.179789
C	2.172380	2.756453	-0.811401
C	3.257060	1.951464	-0.451169
C	2.379400	4.075562	-1.232177
C	4.549397	2.462763	-0.526932
H	3.095127	0.929085	-0.143086
C	3.674476	4.582916	-1.297353
H	1.530205	4.687134	-1.515820
C	4.760576	3.777448	-0.945359
H	5.387397	1.825169	-0.264880
H	3.836935	5.604242	-1.628748
H	5.770304	4.174074	-1.002937

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O	-0.146853	1.657989	-2.699450
O	0.635176	0.839584	-0.713730
H	-0.866098	1.039539	-2.415870
C	1.804800	-1.839626	-1.085218
O	1.364214	-0.748087	-1.654588

O	2.488689	-2.633447	-1.736073
C	-2.055822	-1.147625	-1.678879
O	-2.074926	0.088877	-1.723343
O	-1.047204	-1.874213	-2.110174
H	-0.226034	-1.314756	-2.225798
C	1.335067	-2.246228	0.292834
C	1.724650	-1.678509	1.520516
C	0.483029	-3.360899	0.288030
C	1.224963	-2.247994	2.704538
C	-0.012137	-3.901062	1.470107
C	0.364355	-3.340455	2.690423
H	1.558343	-1.838178	3.653224
H	-0.672307	-4.762784	1.437300
H	0.006127	-3.760504	3.625739
C	-3.225075	-1.889013	-1.158995
C	-3.753240	-2.963702	-1.880563
C	-3.862883	-1.409692	0.002657
C	-4.958199	-3.538708	-1.483860
C	-5.070192	-2.001368	0.383473
C	-5.623020	-3.044280	-0.361297
H	-5.379005	-4.362060	-2.052405
H	-5.563574	-1.650920	1.284656
H	-6.566444	-3.483569	-0.051041
C	0.719453	1.790941	-1.661643
H	-3.231439	-3.321105	-2.762366
H	0.210723	-3.801399	-0.664246
C	-3.197798	-0.444058	0.936215
C	-3.605305	0.890258	1.119615
C	-2.187796	-0.958617	1.759119
C	-3.055450	1.645570	2.161760
C	-1.610894	-0.180775	2.761013
C	-2.056692	1.122586	2.975581
H	-1.864130	-1.984312	1.622808
H	-3.417510	2.656979	2.301849
H	-0.831378	-0.610847	3.380078
H	-1.627554	1.729455	3.767381
C	2.673727	-0.542755	1.685437
C	3.976117	-0.536794	1.148979
C	2.294362	0.537952	2.494702
C	4.848986	0.525771	1.404860
C	3.175672	1.580861	2.774495
C	4.458808	1.579616	2.226969
H	1.283364	0.562571	2.888361

H	5.840592	0.509689	0.964940
H	2.855330	2.398565	3.415017
H	5.149486	2.390413	2.437523
C	-4.562925	1.616112	0.217790
O	-5.346263	2.444564	0.630372
O	-4.458898	1.358307	-1.099613
H	-3.657667	0.818618	-1.292739
C	4.459872	-1.699413	0.338803
O	4.444480	-2.853603	0.672718
O	4.871551	-1.213078	-0.872247
O	5.234315	-2.275832	-1.775731
H	4.326424	-2.612089	-1.978691
C	2.072481	2.358755	-2.181869
C	0.019584	2.628215	-0.401064
C	0.709343	3.027406	0.750204
C	-1.297183	3.061035	-0.635870
C	0.131838	3.967970	1.598407
H	1.663908	2.587295	0.989017
C	-1.859113	4.002250	0.217173
H	-1.840328	2.730045	-1.508825
C	-1.145738	4.463007	1.329487
H	0.673472	4.295344	2.480694
H	-2.863790	4.363133	0.019855
H	-1.598139	5.191051	1.996338
C	2.465812	1.560953	-3.449953
H	1.711374	1.664448	-4.231633
H	3.415807	1.955939	-3.825892
H	2.590615	0.501692	-3.218812
C	3.200973	2.212941	-1.158079
H	4.151795	2.448235	-1.647139
H	3.103483	2.898336	-0.313673
H	3.265103	1.192148	-0.782410
C	1.865117	3.835682	-2.559548
H	1.640091	4.448388	-1.680045
H	2.779795	4.225954	-3.017973
H	1.048038	3.948325	-3.278453

tBu-TS2c-R

O	-0.677101	2.358732	-1.571428
O	0.436034	0.927465	-0.170396
H	-1.364315	1.670607	-1.409568
C	1.682451	-1.238280	-0.786124

O	0.934319	-0.306951	-1.384651
O	2.334792	-1.990562	-1.490977
C	-2.521968	-0.812422	-1.484630
O	-2.553961	0.396610	-1.226104
O	-1.436224	-1.454018	-1.871517
H	-0.623526	-0.872930	-1.844432
C	1.572431	-1.348782	0.709752
C	2.651646	-1.180163	1.599324
C	0.298277	-1.643792	1.211755
C	2.403861	-1.300245	2.974852
C	0.080565	-1.793005	2.577024
C	1.139508	-1.612844	3.465320
H	3.233189	-1.163850	3.661950
H	-0.910419	-2.041633	2.941808
H	0.985409	-1.718072	4.535251
C	-3.740032	-1.651070	-1.411997
C	-3.985086	-2.592413	-2.418945
C	-4.686317	-1.425241	-0.393195
C	-5.194432	-3.280653	-2.451358
C	-5.892346	-2.130134	-0.440461
C	-6.152934	-3.038013	-1.467267
H	-5.389302	-3.997106	-3.243101
H	-6.622950	-1.969528	0.346048
H	-7.101378	-3.566425	-1.488546
C	0.372368	2.114504	-0.735942
H	-3.233169	-2.757739	-3.182964
H	-0.527319	-1.760480	0.518785
C	-4.397329	-0.583568	0.810971
C	-4.944071	0.697985	0.997329
C	-3.650707	-1.156620	1.848427
C	-4.778975	1.356345	2.220413
C	-3.455928	-0.477707	3.050663
C	-4.030746	0.778906	3.242442
H	-3.244274	-2.155077	1.712901
H	-5.242233	2.329194	2.348518
H	-2.873041	-0.937477	3.843183
H	-3.898715	1.304092	4.183685
C	4.027661	-0.771389	1.189950
C	4.875298	-1.553071	0.380944
C	4.514764	0.454512	1.665955
C	6.149854	-1.089364	0.036478
C	5.792129	0.905739	1.337549
C	6.612108	0.134391	0.514017

H	3.868000	1.064314	2.289176
H	6.780027	-1.703992	-0.596603
H	6.140779	1.860596	1.720296
H	7.607407	0.478843	0.250001
C	-5.715191	1.420652	-0.073866
O	-6.754441	1.998640	0.152059
O	-5.160139	1.420946	-1.298904
H	-4.248880	1.048219	-1.266757
C	4.416285	-2.901115	-0.065888
O	3.726412	-3.658980	0.566377
O	4.869200	-3.118790	-1.339248
O	4.258349	-4.292904	-1.902297
H	3.327991	-3.980534	-1.934193
C	-0.053386	2.813158	0.943463
C	1.640128	2.736258	-1.241626
C	2.874642	2.221666	-0.836458
C	1.598084	3.810527	-2.137708
C	4.058884	2.778821	-1.313196
H	2.908707	1.374840	-0.165261
C	2.784005	4.371368	-2.607591
H	0.639145	4.190183	-2.470203
C	4.016123	3.858880	-2.195798
H	5.008421	2.356954	-0.999365
H	2.745258	5.203925	-3.304095
H	4.938502	4.294096	-2.569889
C	-0.178032	4.294688	0.607602
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H	-0.558937	4.801171	1.504906
H	0.782774	4.741299	0.344550
C	1.060340	2.531992	1.934775
H	1.125240	1.471190	2.185165
H	2.028673	2.871954	1.558201
H	0.849923	3.092133	2.855877
C	-1.387432	2.218080	1.362587
H	-1.312757	1.156594	1.600363
H	-1.731982	2.745536	2.261017
H	-2.154577	2.354363	0.597489

tBu-TS4c-ph

O	-0.083792	1.659418	2.490933
O	-1.035677	0.735066	0.590730
H	0.825271	1.527344	2.132679

C	-1.741999	-1.847781	1.187216
O	-2.003854	-0.599800	1.544254
O	-2.081339	-2.694382	2.002589
C	1.916879	-0.606088	1.851206
O	2.266433	0.579127	1.803063
O	0.818770	-1.014477	2.472978
H	0.287037	-0.229192	2.758825
C	-1.106219	-2.205281	-0.113199
C	-1.579285	-1.790241	-1.374780
C	-0.040351	-3.106057	-0.026641
C	-0.918127	-2.265298	-2.516062
C	0.612142	-3.557939	-1.169709
C	0.170537	-3.130742	-2.420952
H	-1.290963	-1.972422	-3.492671
H	1.458882	-4.230083	-1.078232
H	0.663637	-3.476330	-3.324681
C	2.706730	-1.678580	1.215140
C	2.869543	-2.911952	1.855365
C	3.325062	-1.416905	-0.021722
C	3.683139	-3.887790	1.287553
C	4.138127	-2.410007	-0.576062
C	4.325038	-3.629700	0.074600
H	3.821511	-4.839607	1.790652
H	4.613232	-2.221771	-1.533557
H	4.966701	-4.383644	-0.371914
C	-0.986257	1.830734	1.427606
H	2.368882	-3.088920	2.801552
H	0.277356	-3.436425	0.954185
C	3.046664	-0.182916	-0.821260
C	4.000959	0.837316	-0.976681
C	1.836409	-0.092319	-1.516135
C	3.769344	1.879410	-1.878690
C	1.593383	0.974708	-2.378312
C	2.568230	1.950810	-2.579249
H	1.089556	-0.863327	-1.384266
H	4.535603	2.638040	-2.002333
H	0.644095	1.035724	-2.900648
H	2.385782	2.773728	-3.262547
C	-2.762345	-0.910420	-1.567608
C	-4.025757	-1.170118	-0.996299
C	-2.626431	0.222402	-2.379155
C	-5.086084	-0.278024	-1.199427
C	-3.695340	1.085601	-2.611051

C	-4.928915	0.844174	-2.007891
H	-1.654621	0.434206	-2.813094
H	-6.042949	-0.489897	-0.735977
H	-3.558959	1.953535	-3.250615
H	-5.763603	1.519093	-2.170036
C	5.251346	0.894989	-0.146643
O	6.348647	1.118329	-0.604991
O	5.062414	0.727103	1.179102
H	4.100883	0.712597	1.386795
C	-4.300277	-2.451104	-0.281078
O	-3.817314	-3.524774	-0.566907
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C	-2.324458	2.382806	2.043987
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C	0.808338	3.478517	0.576502
C	-0.512426	3.846867	-1.855988
H	-1.885775	2.349275	-1.156754
C	1.304492	4.381258	-0.360213
H	1.310468	3.372095	1.529855
C	0.644202	4.573957	-1.575350
H	-1.023993	3.977150	-2.805586
H	2.206786	4.941302	-0.134161
H	1.035909	5.281034	-2.300831
C	-2.140448	3.884071	2.336142
H	-3.021284	4.260081	2.867616
H	-1.264015	4.057454	2.968610
H	-2.025451	4.469296	1.418827
C	-3.507566	2.178857	1.089395
H	-3.411428	2.770155	0.175411
H	-3.626172	1.130047	0.815612
H	-4.425333	2.508380	1.589036
C	-2.630645	1.676384	3.384924
H	-3.554869	2.100936	3.793133
H	-2.771252	0.603701	3.255349
H	-1.831744	1.842666	4.110387
H	-5.294703	-3.177564	1.126781

tBu-TS4c-R

O	-0.628138	2.482254	-1.379202
O	0.449950	0.897225	-0.129185
H	-1.315641	1.780171	-1.297956

C	1.832396	-1.102443	-0.956571
O	0.941751	-0.229578	-1.459143
O	2.646719	-1.601871	-1.711132
C	-2.485741	-0.703448	-1.563622
O	-2.498955	0.480784	-1.204634
O	-1.412258	-1.338123	-1.983909
H	-0.577310	-0.786920	-1.893364
C	1.715730	-1.428869	0.501046
C	2.840997	-1.482517	1.347243
C	0.443060	-1.688594	1.025772
C	2.646149	-1.759236	2.706671
C	0.271990	-2.004494	2.368836
C	1.379064	-2.028889	3.216801
H	3.512441	-1.781660	3.360734
H	-0.721003	-2.217551	2.750654
H	1.258889	-2.260085	4.271380
C	-3.727312	-1.513214	-1.577917
C	-4.007370	-2.321924	-2.685154
C	-4.657908	-1.382610	-0.529468
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H	-5.459702	-3.578615	-3.653045
H	-6.604157	-1.954187	0.163553
H	-7.144983	-3.308423	-1.841577
C	0.416478	2.130614	-0.577319
H	-3.266006	-2.418252	-3.471153
H	-0.417789	-1.642399	0.370066
C	-4.329769	-0.698793	0.761379
C	-4.839896	0.563827	1.109729
C	-3.583303	-1.410905	1.709457
C	-4.642292	1.064424	2.401037
C	-3.356856	-0.888257	2.982265
C	-3.897028	0.349108	3.334001
H	-3.202999	-2.394353	1.447591
H	-5.078198	2.025672	2.652822
H	-2.779537	-1.456852	3.705326
H	-3.740061	0.752585	4.329885
C	4.220584	-1.138507	0.896757
C	4.973984	-1.927068	0.004669
C	4.794893	0.035440	1.399339
C	6.247824	-1.507019	-0.392827
C	6.074066	0.439192	1.015648

C	6.799847	-0.329766	0.107479
H	4.217182	0.643455	2.089346
H	6.806208	-2.120558	-1.089912
H	6.495655	1.354047	1.422603
H	7.792926	-0.020956	-0.204922
C	-5.603950	1.431992	0.146735
O	-6.620050	2.010188	0.461808
O	-5.070019	1.563695	-1.079819
H	-4.171816	1.158907	-1.116903
C	4.454802	-3.248070	-0.450688
O	3.632194	-3.918548	0.136205
O	5.058518	-3.675921	-1.586202
H	4.653036	-4.540013	-1.783269
C	-0.001329	2.669667	1.180802
C	1.698702	2.775521	-1.009414
C	2.921789	2.203069	-0.647277
C	1.682212	3.930942	-1.799015
C	4.118288	2.780807	-1.064748
H	2.937849	1.295749	-0.058409
C	2.880758	4.513210	-2.206583
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C	4.100626	3.940797	-1.840339
H	5.058078	2.311021	-0.792679
H	2.861252	5.409053	-2.820553
H	5.033199	4.391768	-2.167705
C	1.102506	2.256760	2.134887
H	1.145376	1.173676	2.266174
H	2.078758	2.617144	1.799929
H	0.900563	2.715736	3.112443
C	-1.351434	2.067191	1.526810
H	-1.695970	2.513008	2.468696
H	-2.105155	2.294070	0.769885
H	-1.301974	0.986462	1.661408
C	-0.085701	4.178519	0.992214
H	-0.456918	4.605107	1.934289
H	0.887372	4.623450	0.775465
H	-0.788810	4.443209	0.199363

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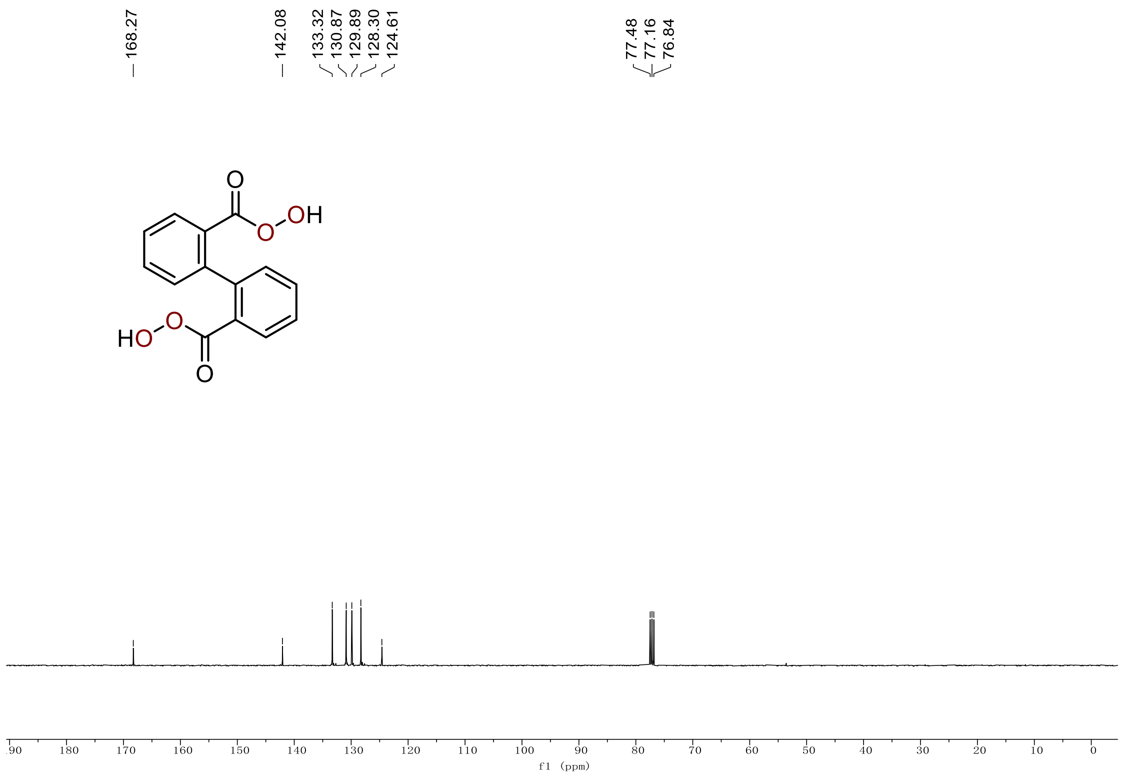
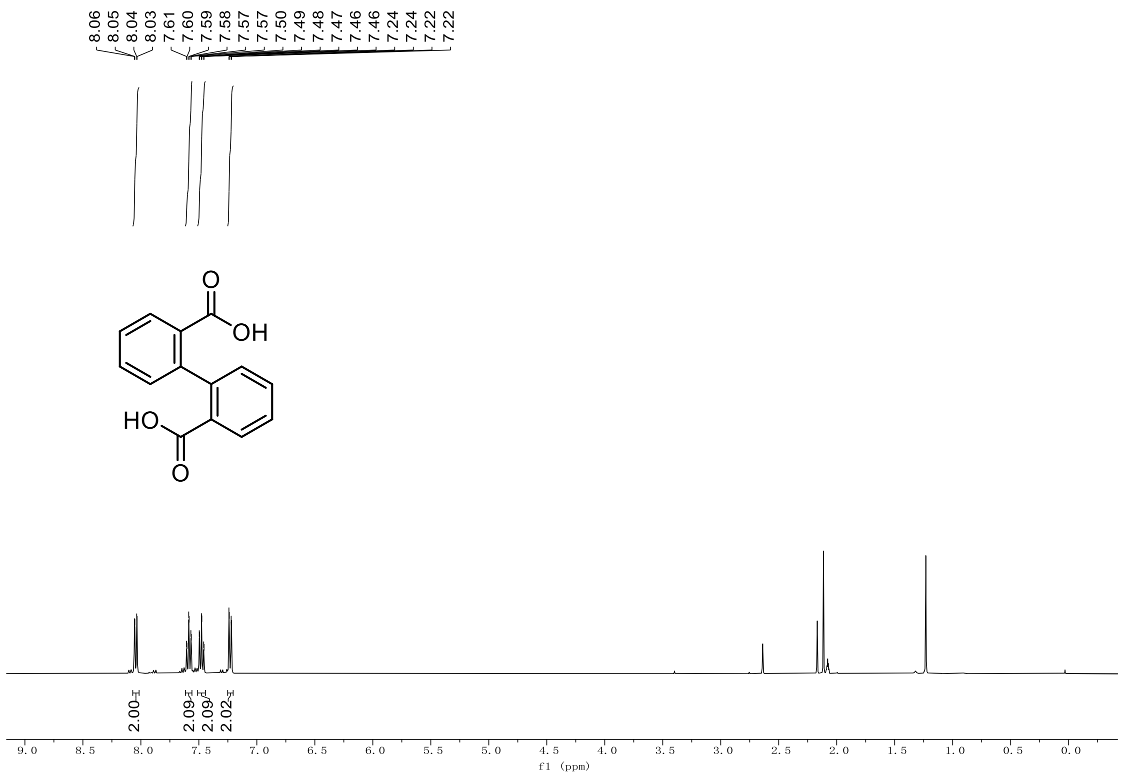
16NMR spectra

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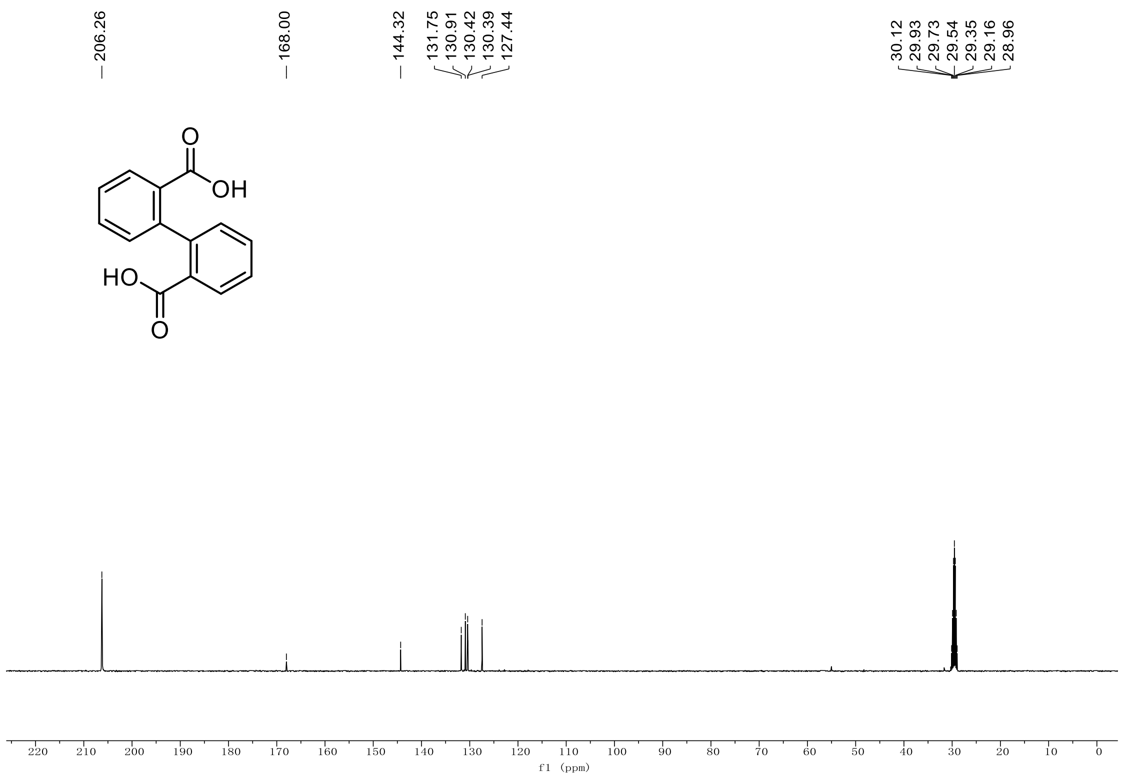
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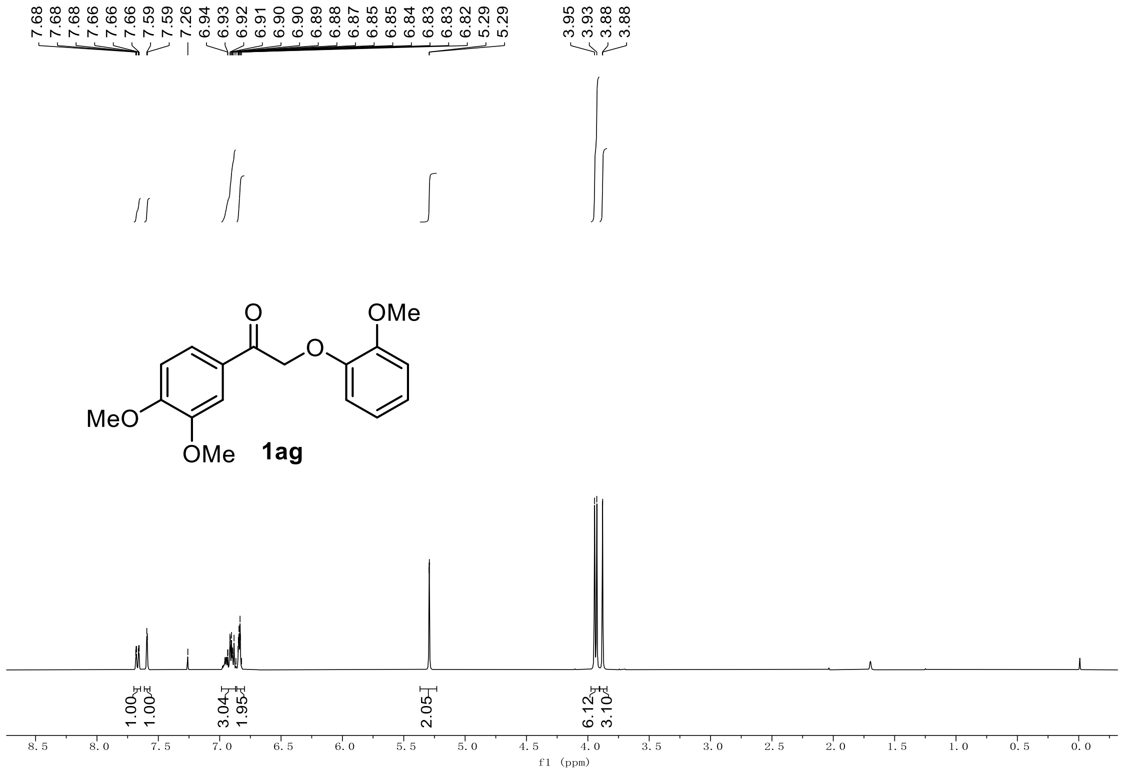
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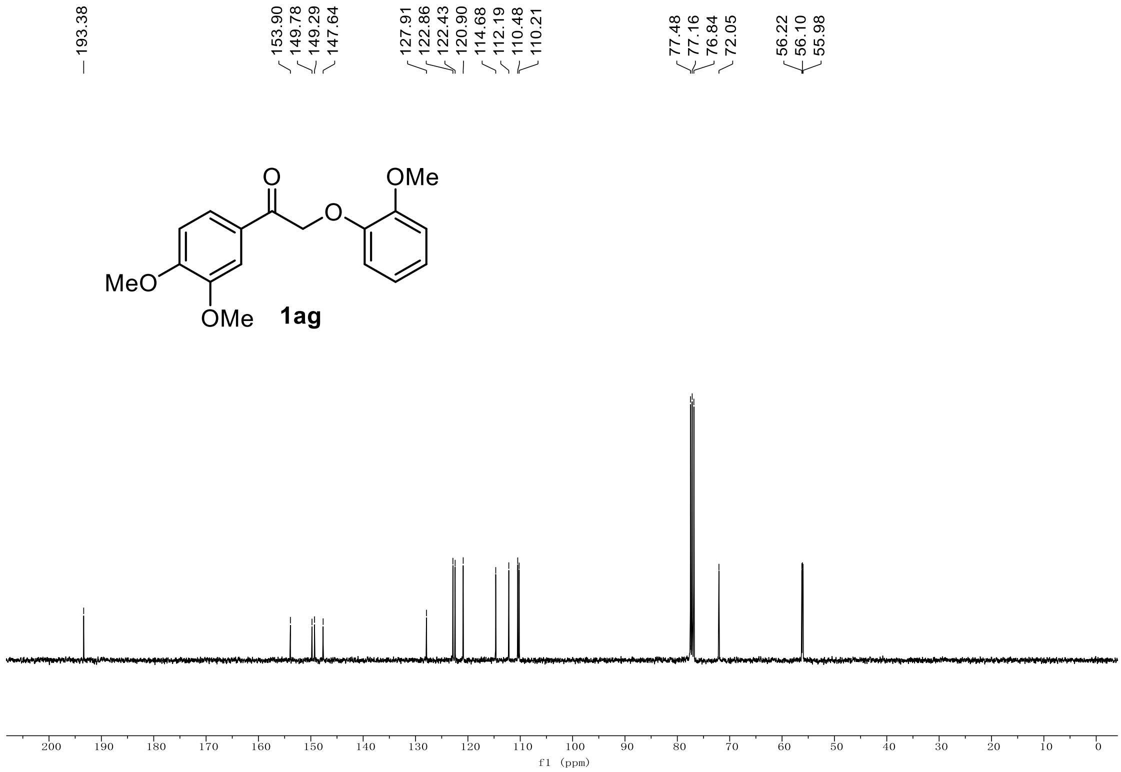
1.00
3.04
1.95
2.05
6.12
3.10
f1 (ppm)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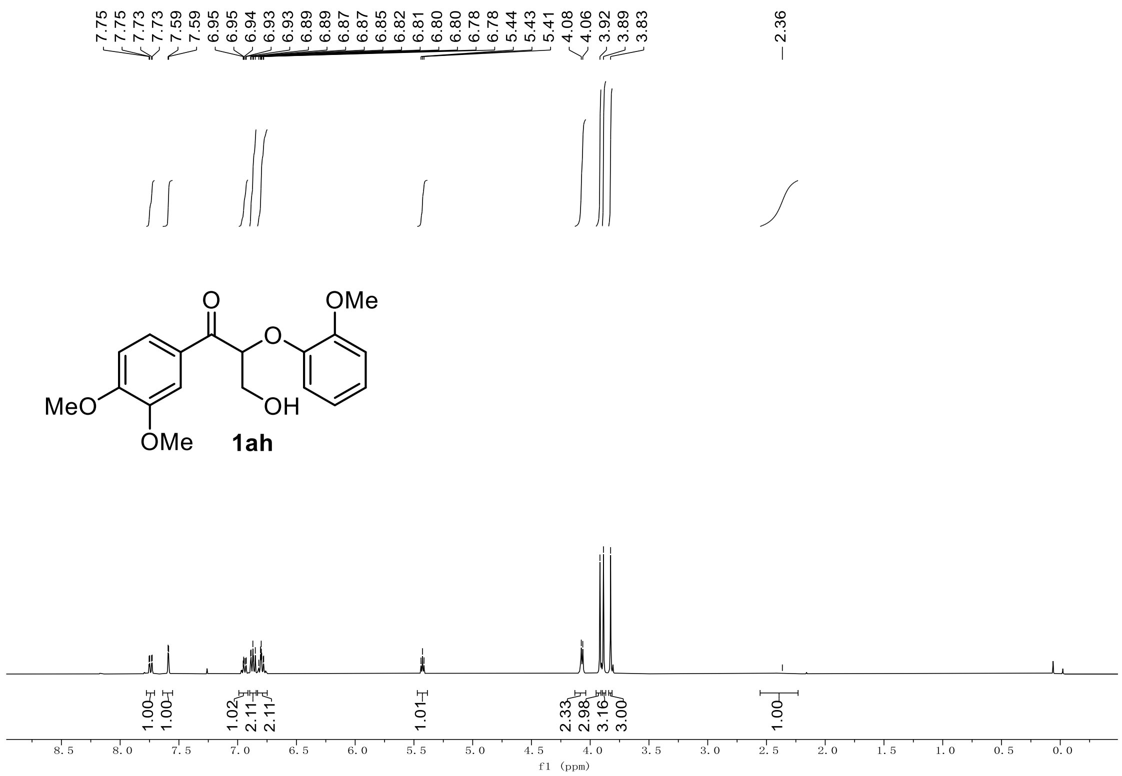
153.90 149.78 149.29 147.64
127.91 122.86 122.43 120.90 114.68 112.19 110.48 110.21
77.48 77.16 76.84 72.05
56.22 56.10 55.98
OMe
O
O
MeO
OMe
1ag
f1 (ppm)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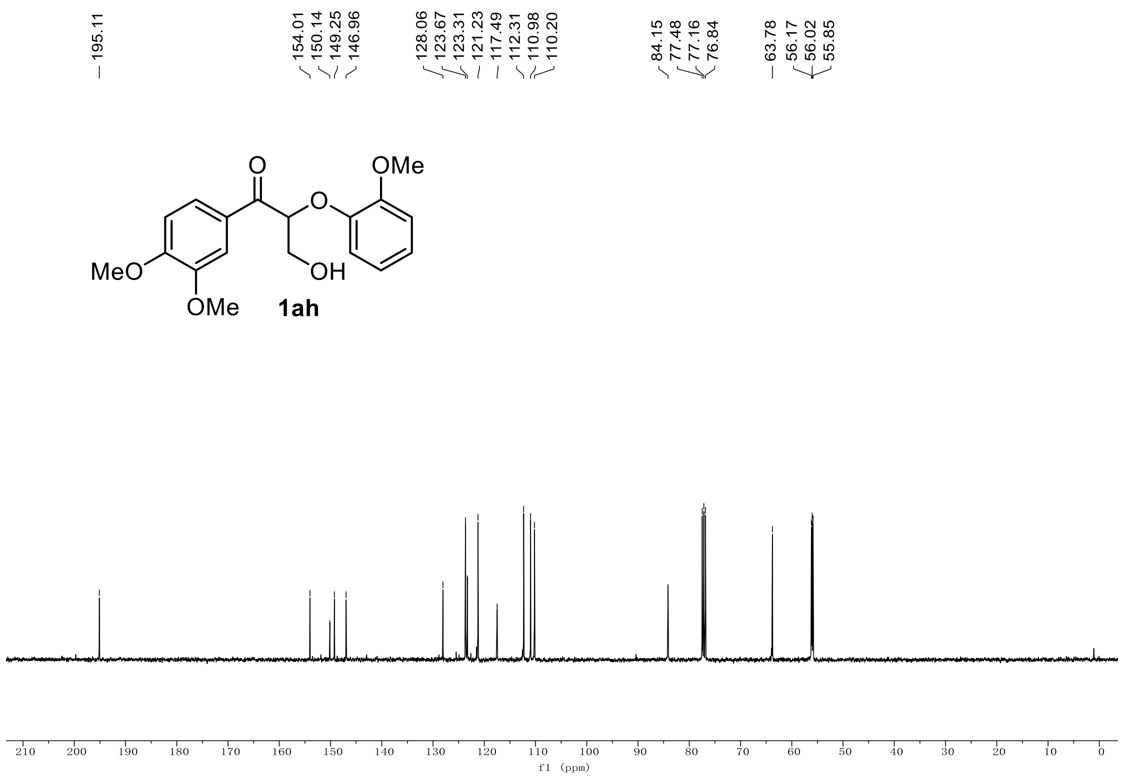
2.36
OMe
O
O
MeO
OMe
OH
1ah
1.00 1.00 1.02 2.11 2.11 1.01 2.33 2.98 3.16 3.00 1.00
f1 (ppm)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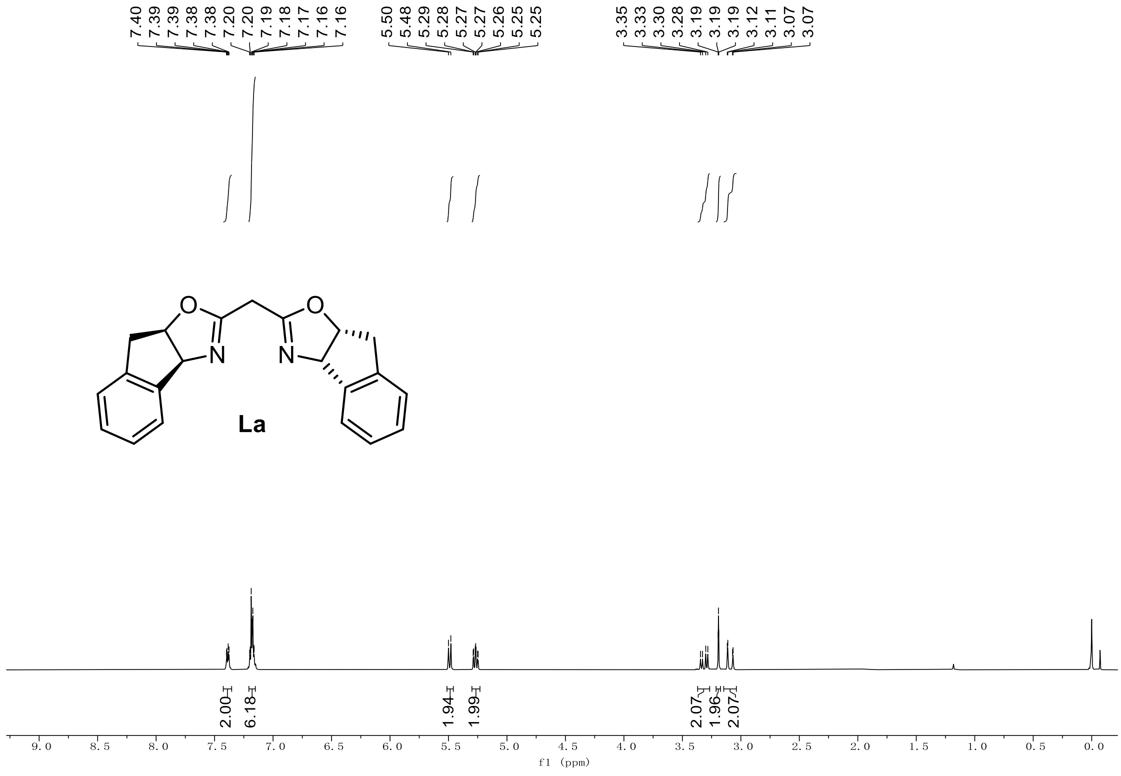
154.01 150.14 149.25 146.96
128.06 123.67 123.31 121.23 117.49 112.31 110.98 110.20
84.15 77.48 77.16 76.84
63.78 56.17 56.02 55.85
OMe
O
O
MeO
OMe
OH
1ah
f1 (ppm)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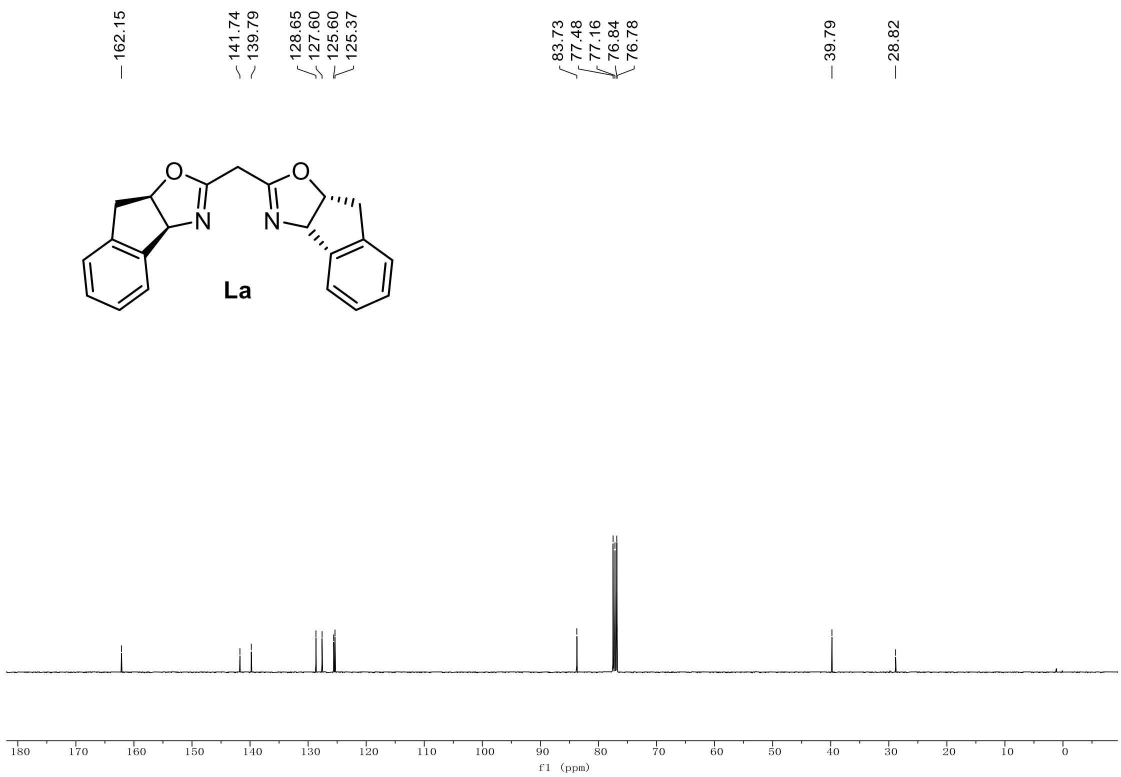
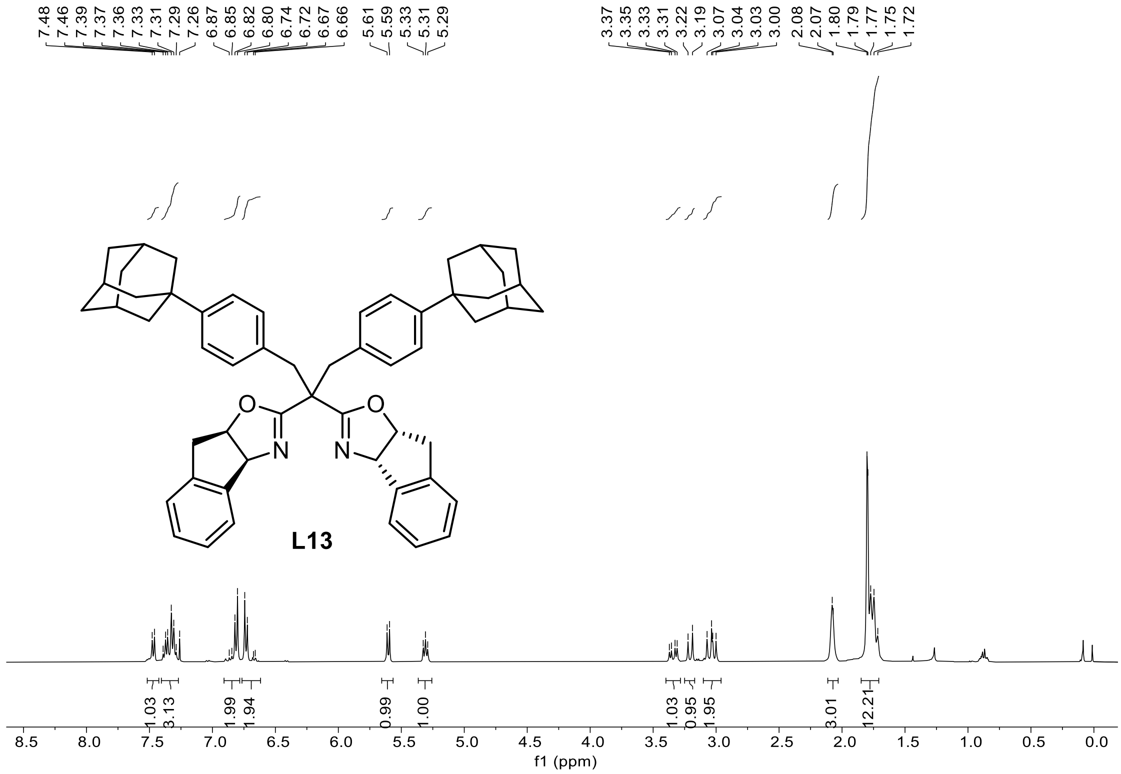
5.50 5.48 5.29 5.28 5.27 5.27 5.26 5.25 5.25
3.35 3.33 3.30 3.28 3.19 3.19 3.19 3.12 3.11 3.07 3.07
O
N
La
2.00
6.18
1.94
1.99
2.07
1.96
2.07
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


162.15
141.74 139.79
128.65 127.60 125.60 125.37
83.73 77.48 77.16 76.84 76.78
39.79
28.82
O
N
La
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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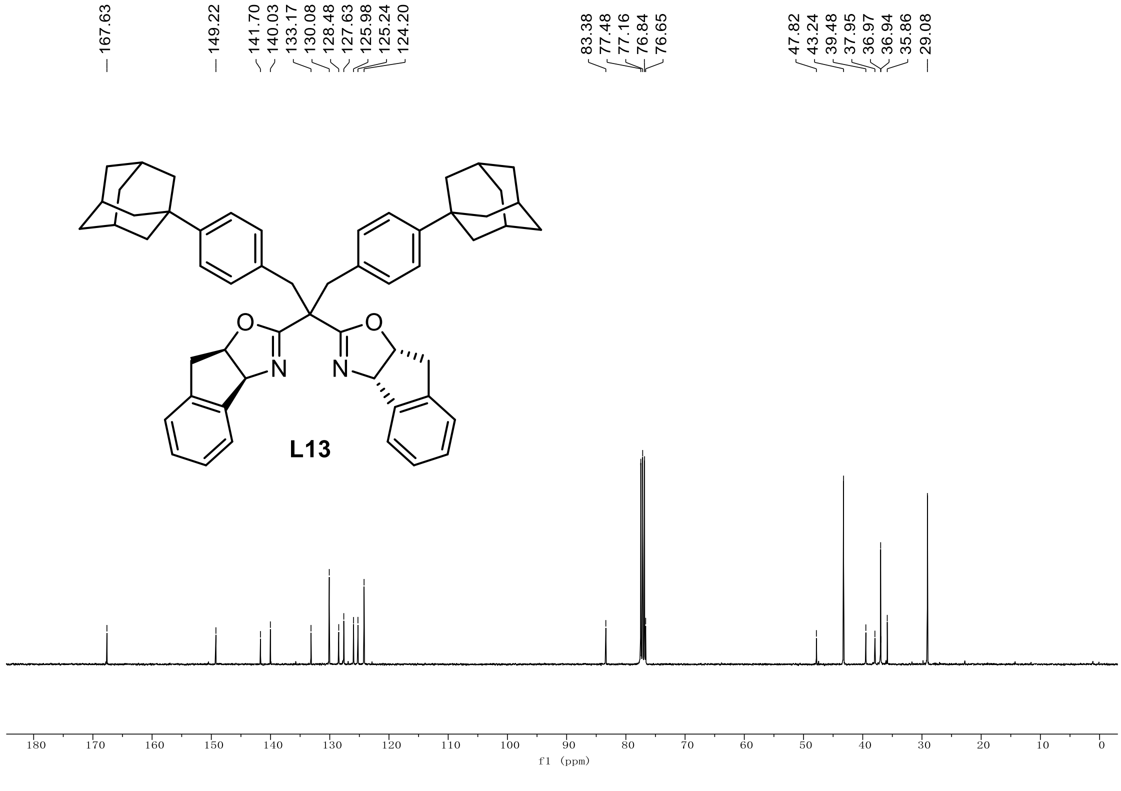
3.37 3.35 3.33 3.31 3.22 3.19 3.07 3.04 3.03 3.00 2.08 2.07 1.80 1.79 1.77 1.75 1.72
O
N
L13
1.03 3.13 1.99 1.94 0.99 1.00 1.03 0.95 1.95 3.01 12.21
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


167.63
149.22 141.70 140.03 133.17 130.08 128.48 127.63 125.98 125.24 124.20
83.38 77.48 77.16 76.84 76.65
47.82 43.24 39.48 37.95 36.97 36.94 35.86 29.08
O
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L13
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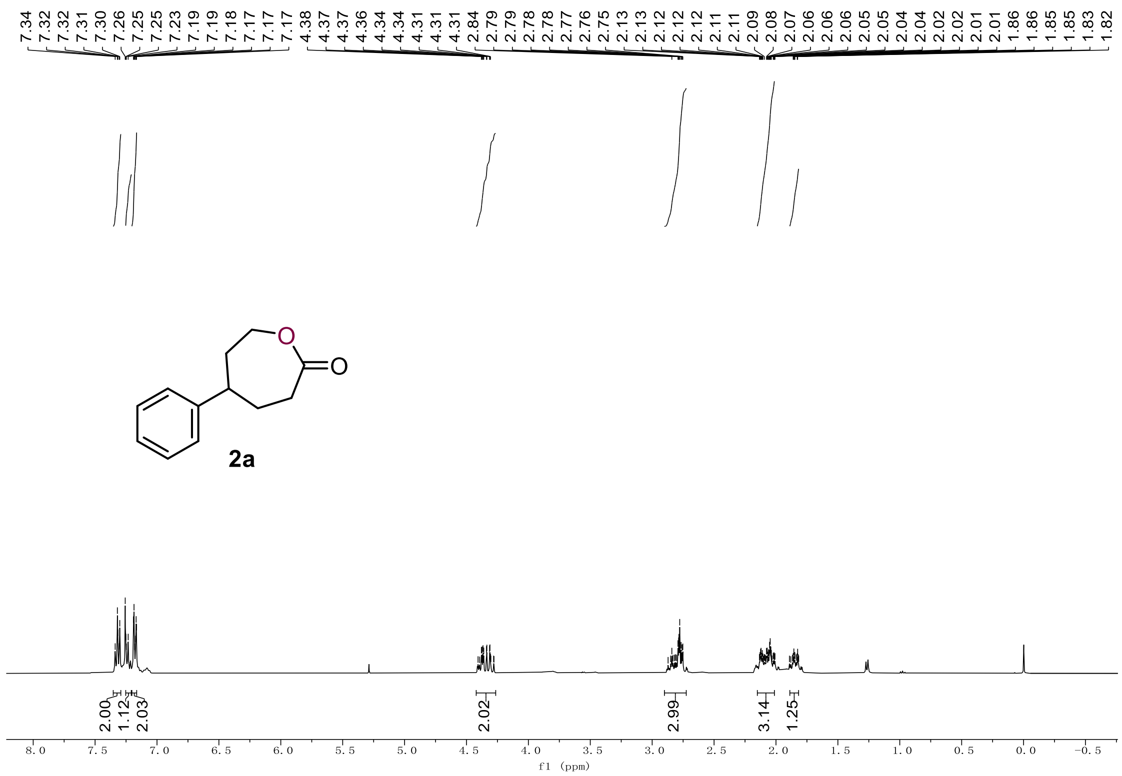
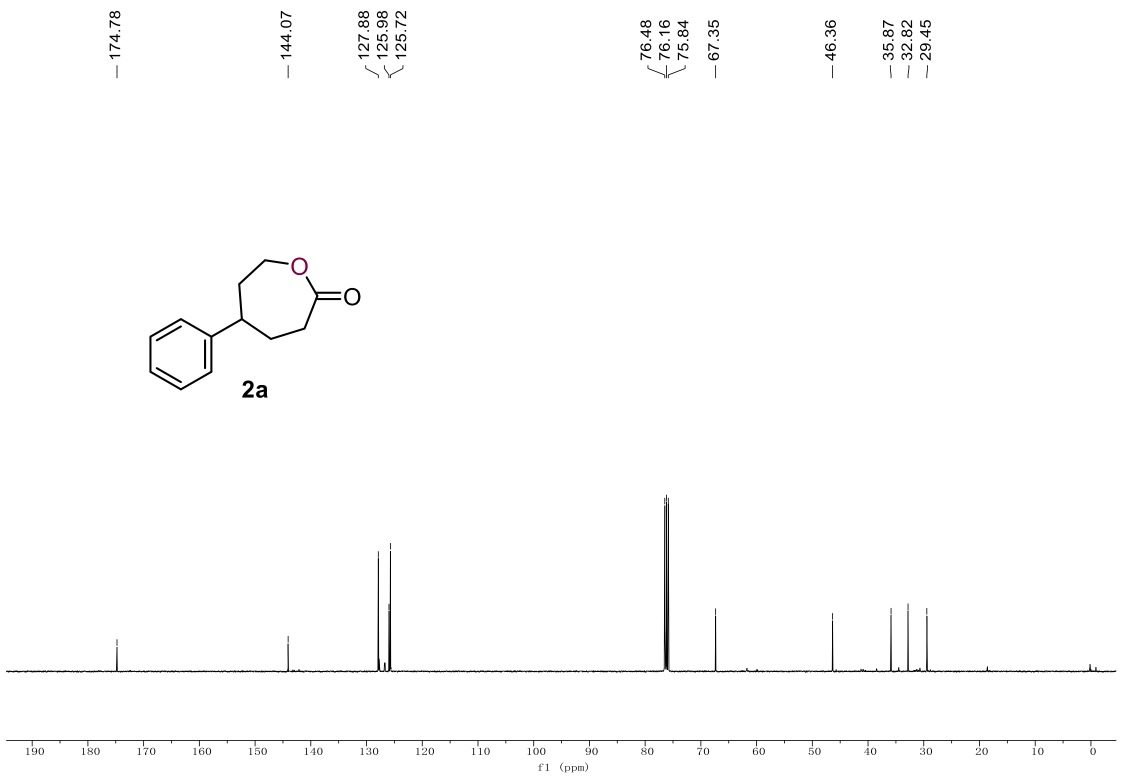
f1 (ppm)



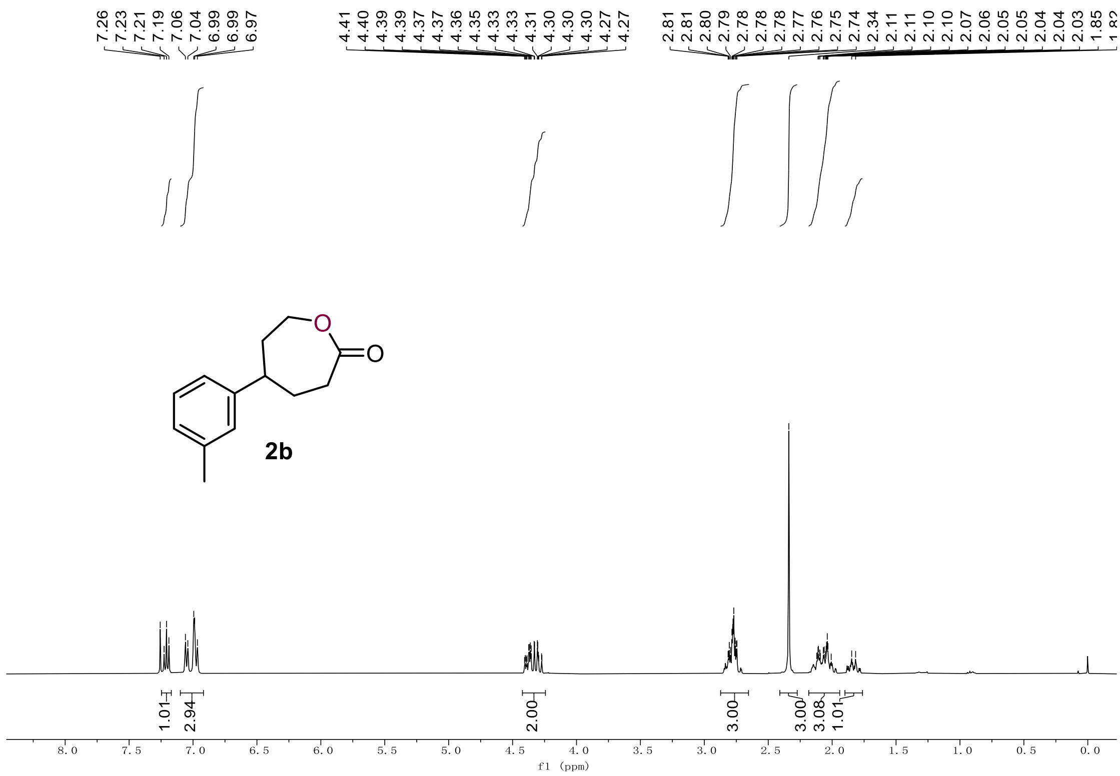
7.34 7.32 7.32 7.31 7.30 7.26 7.25 7.25 7.23 7.19 7.18 7.17 7.17 7.17 4.38 4.37 4.37 4.36 4.34 4.34 4.31 4.31 4.31 2.84 2.79 2.79 2.78 2.78 2.77 2.76 2.75 2.13 2.13 2.12 2.12 2.12 2.11 2.11 2.09 2.08 2.07 2.06 2.06 2.06 2.05 2.05 2.04 2.04 2.02 2.02 2.01 2.01 1.86 1.86 1.85 1.83 1.82
2.00 1.12 2.03 2.02 2.99 3.14 1.25
f1 (ppm)

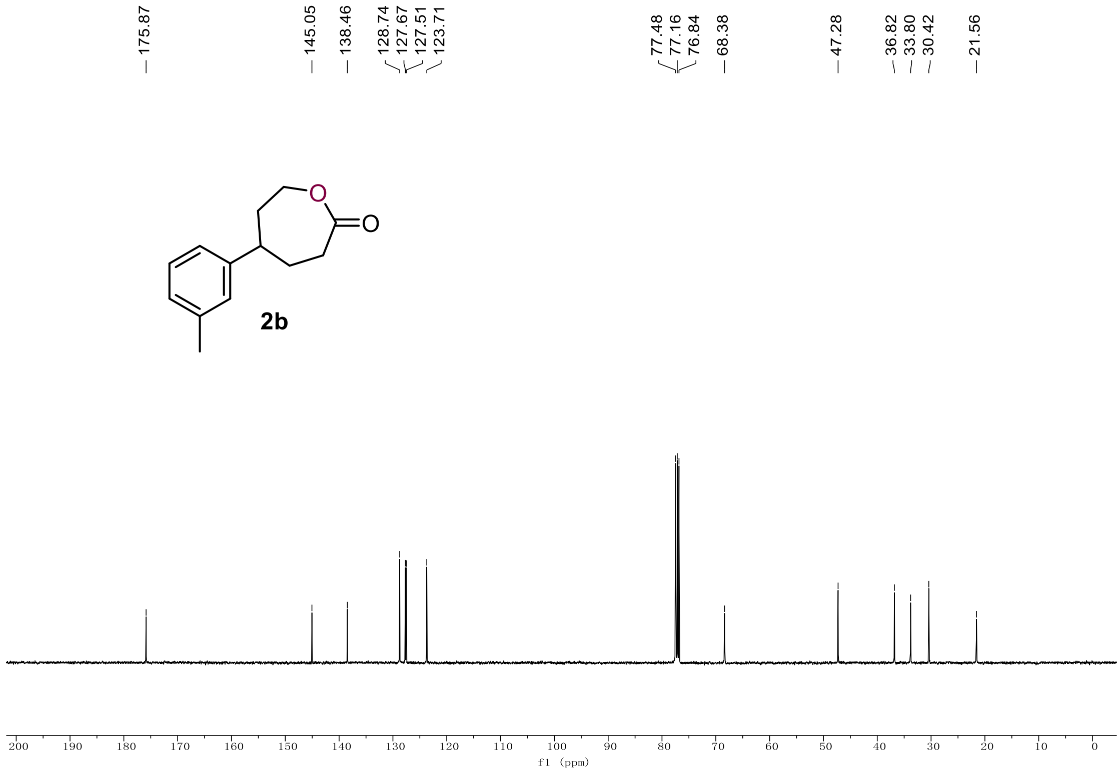
2a

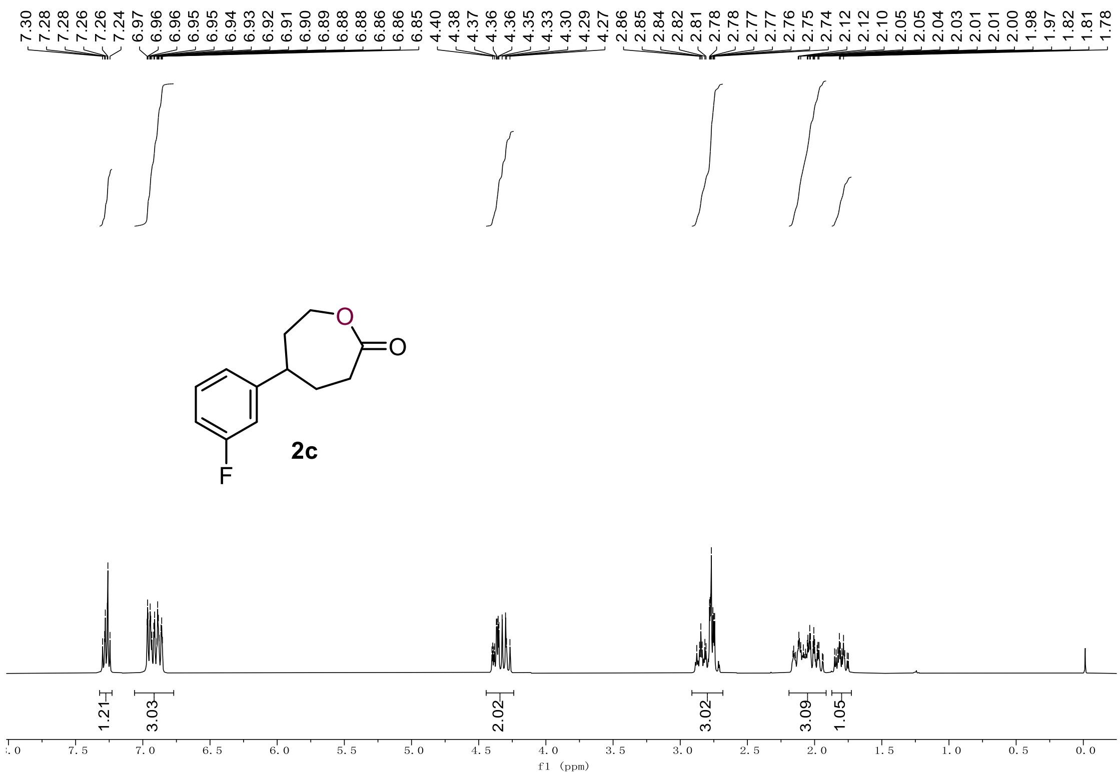


174.78 144.07 127.88 125.98 125.72 76.48 76.16 75.84 67.35 46.36 35.87 32.82 29.45
f1 (ppm)

2a



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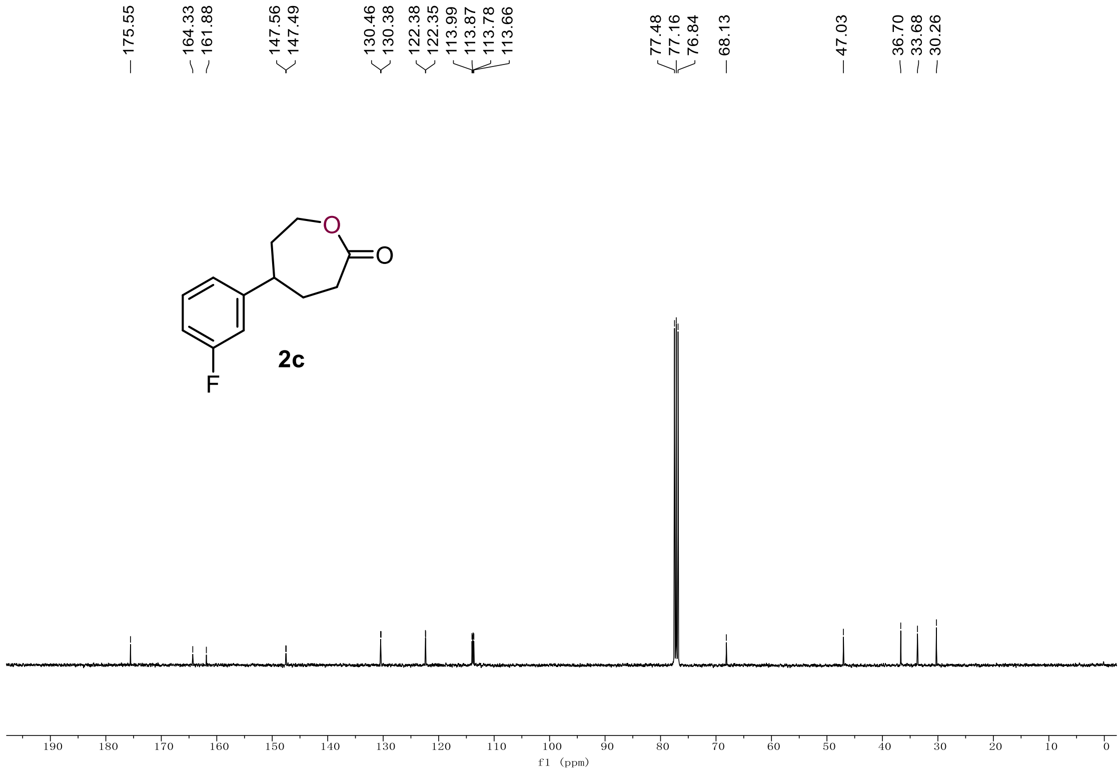
O
O
F
2c
1.21
3.03
2.02
3.02
3.09
1.05
f1 (ppm)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147.56 147.49
130.46 130.38 122.38 122.35 113.99 113.87 113.78 113.66
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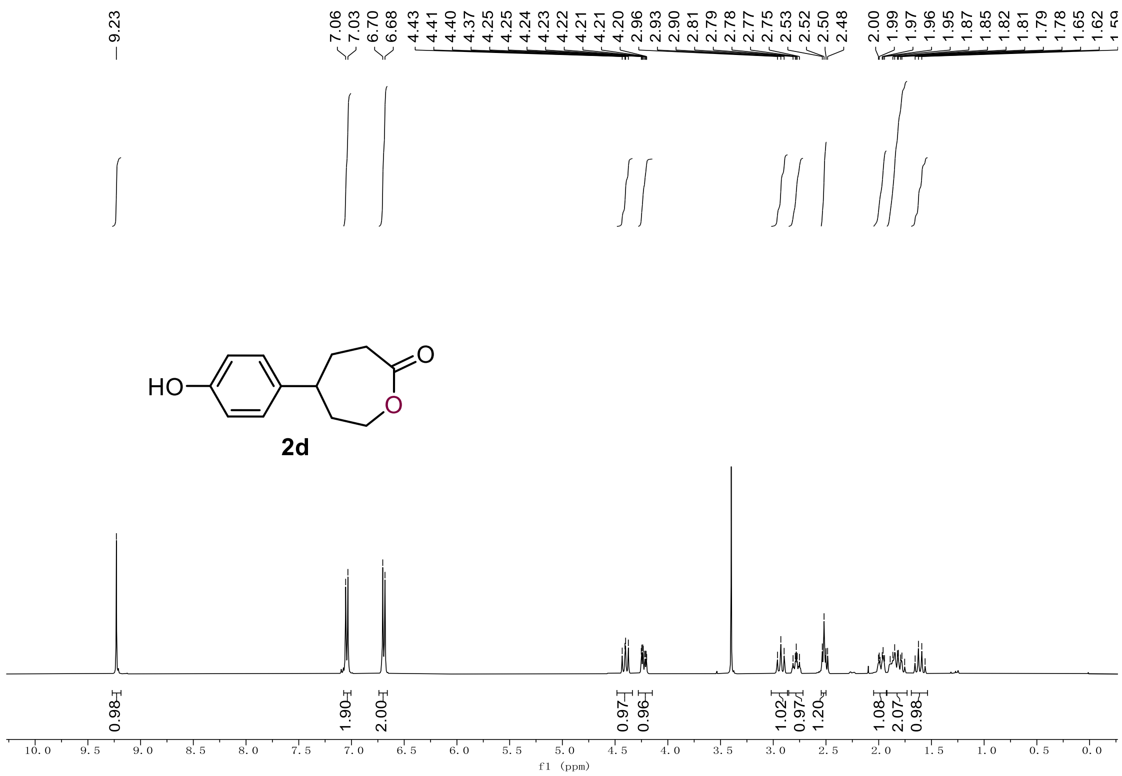
68.13
47.03
36.70 33.68 30.26
O
O
F
2c
f1 (ppm)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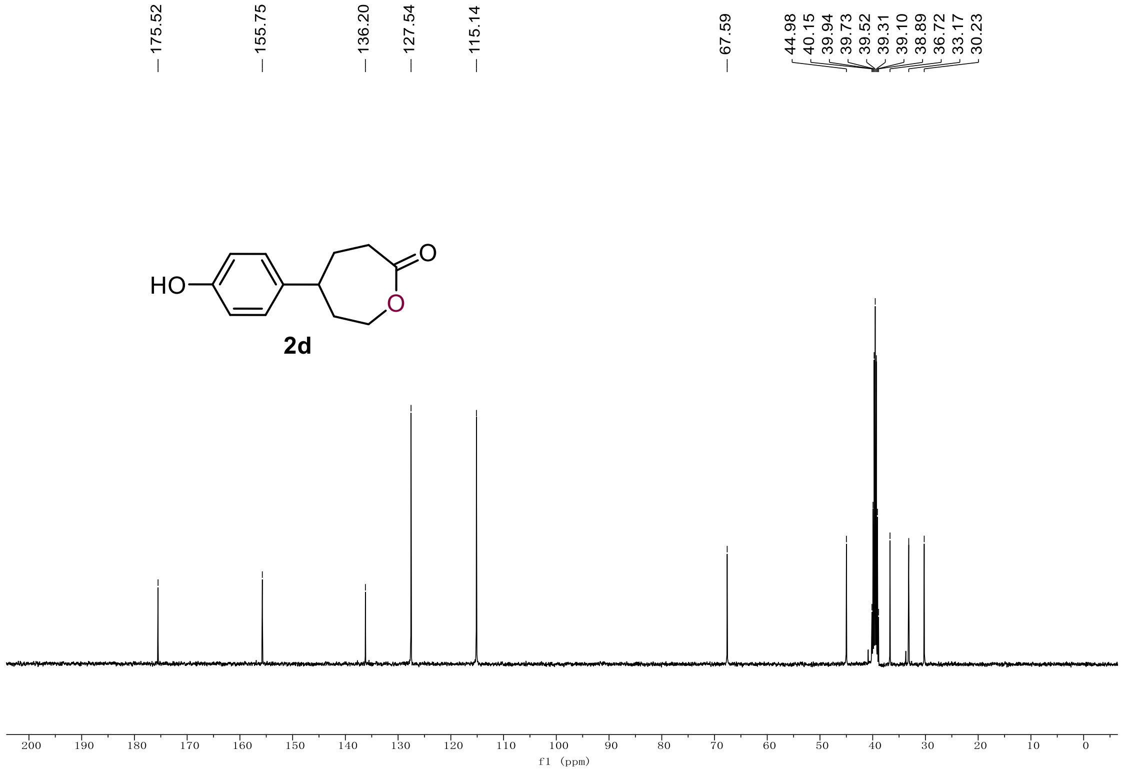
7.06
7.03
6.70
6.68
4.43
4.41
4.40
4.37
4.25
4.25
4.24
4.23
4.22
4.21
4.21
4.20
2.96
2.93
2.90
2.81
2.79
2.78
2.77
2.75
2.53
2.52
2.50
2.48
2.00
1.99
1.97
1.96
1.95
1.87
1.85
1.82
1.81
1.79
1.78
1.65
1.62
HO
O
O
2d
0.98
1.90
2.00
0.97
0.96
1.02
0.97
1.20
1.08
2.07
0.98
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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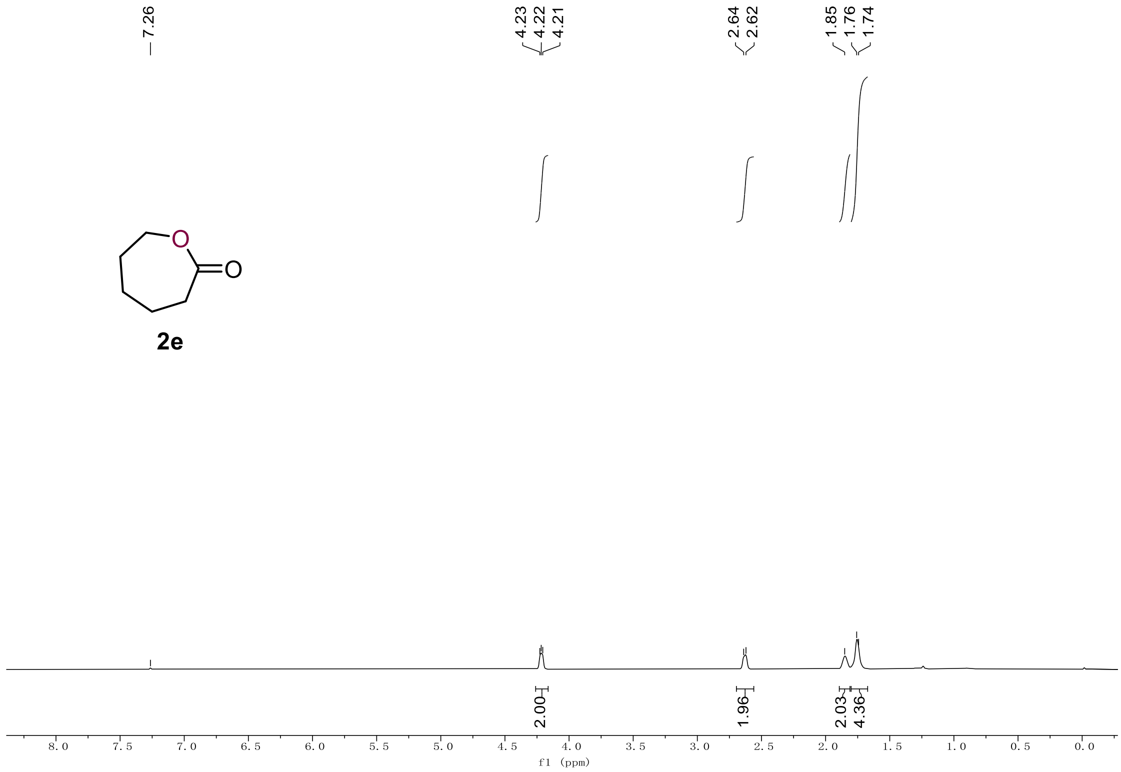
115.14
67.59
44.98
40.15
39.94
39.73
39.52
39.31
39.10
38.89
36.72
33.17
30.23
HO
O
O
2d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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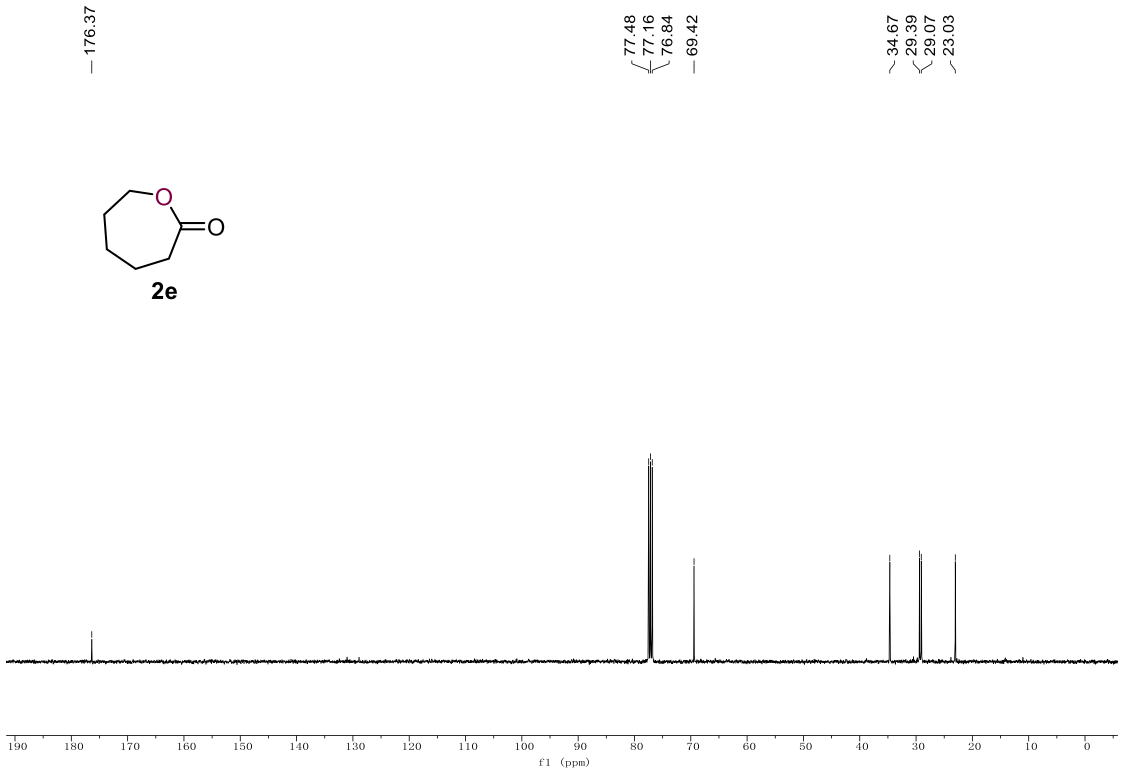
4.23
4.22
4.21
2.64
2.62
1.85
1.76
1.74
O
O
2e
2.00
1.96
2.03
4.36
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.48
77.16
76.84
69.42
34.67
29.39
29.07
23.03
O
O
2e
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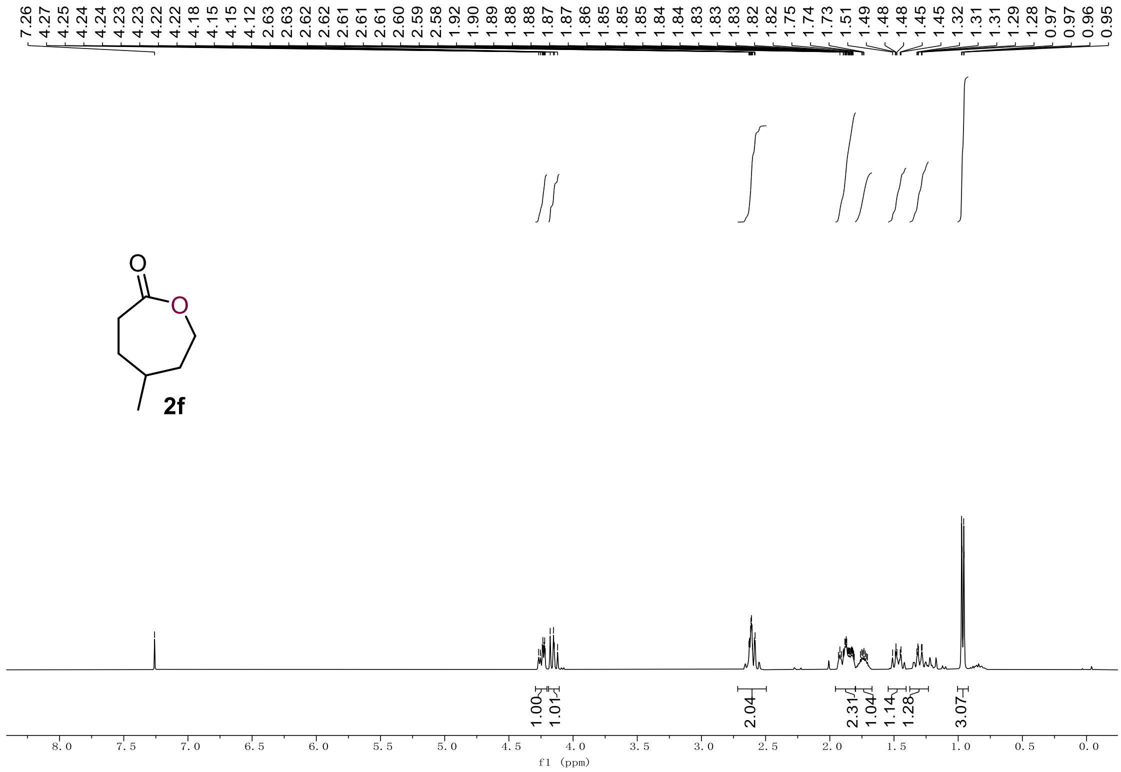
f1 (ppm)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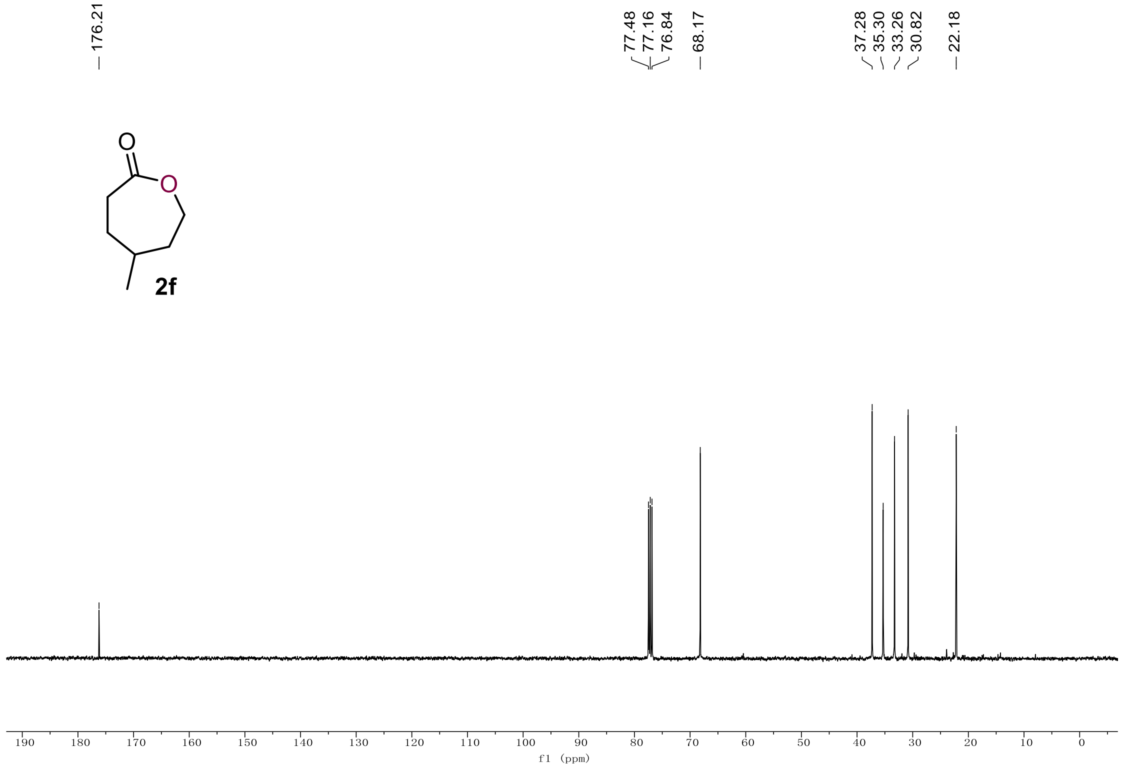
O
O
2f
1.00
1.01
2.04
2.31
1.04
1.14
1.28
3.07
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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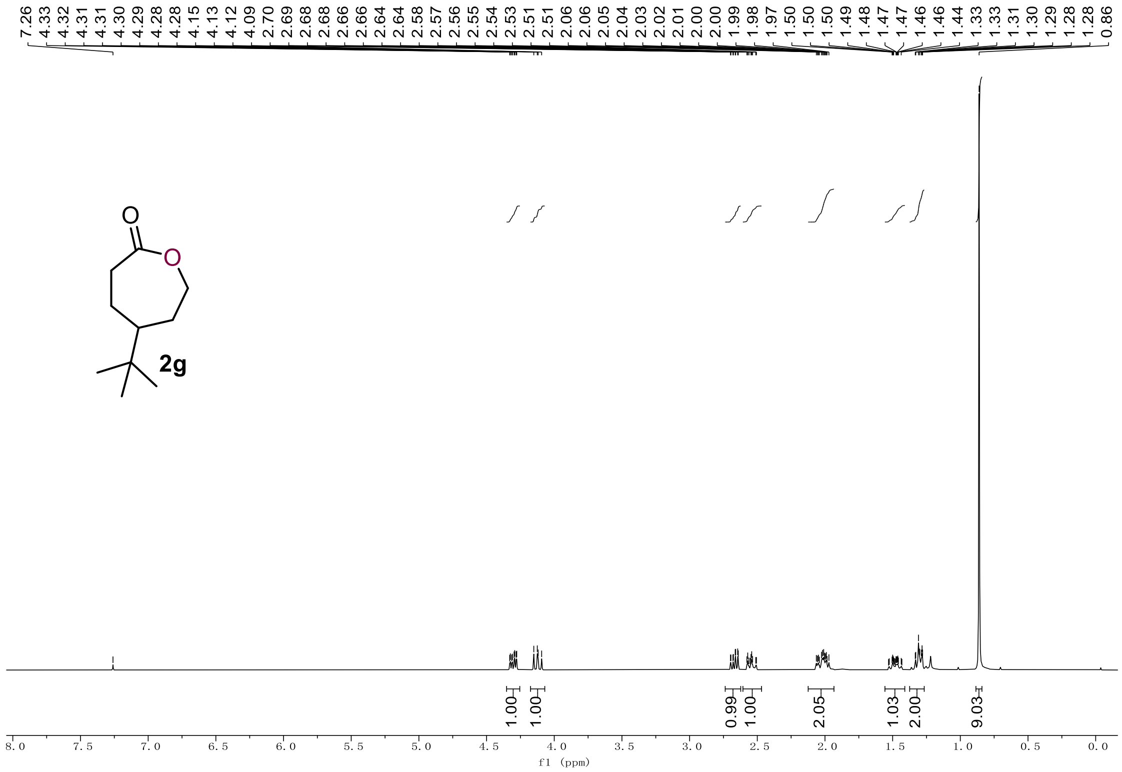
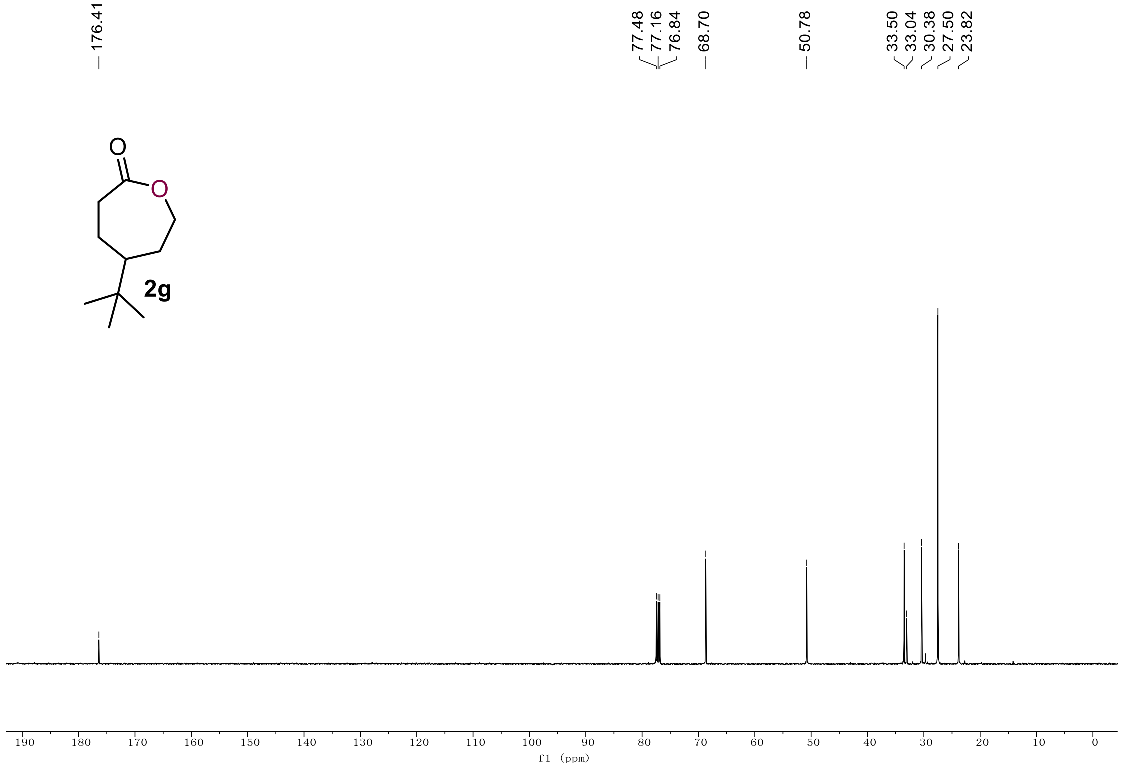
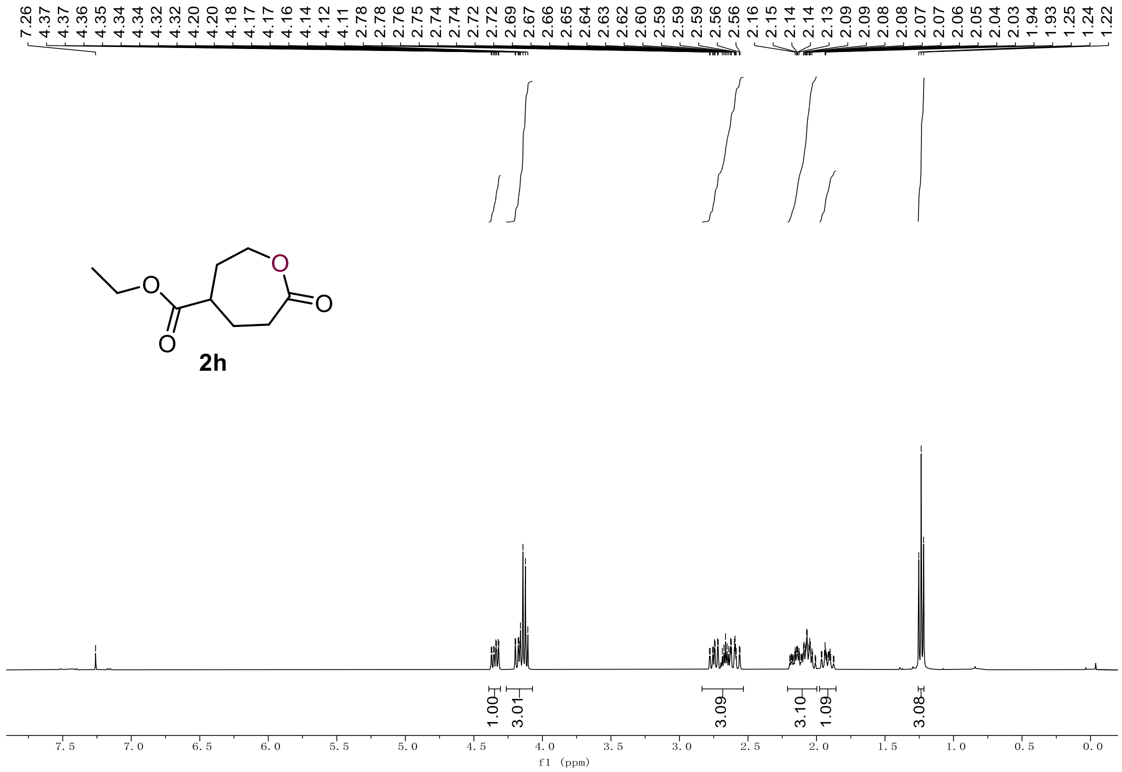
77.48 77.16 76.84
68.17
37.28 35.30 33.26 30.82
22.18
O
O
2f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



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O
O
O
O
2h
1.00
3.01
3.09
3.10
1.09
3.08
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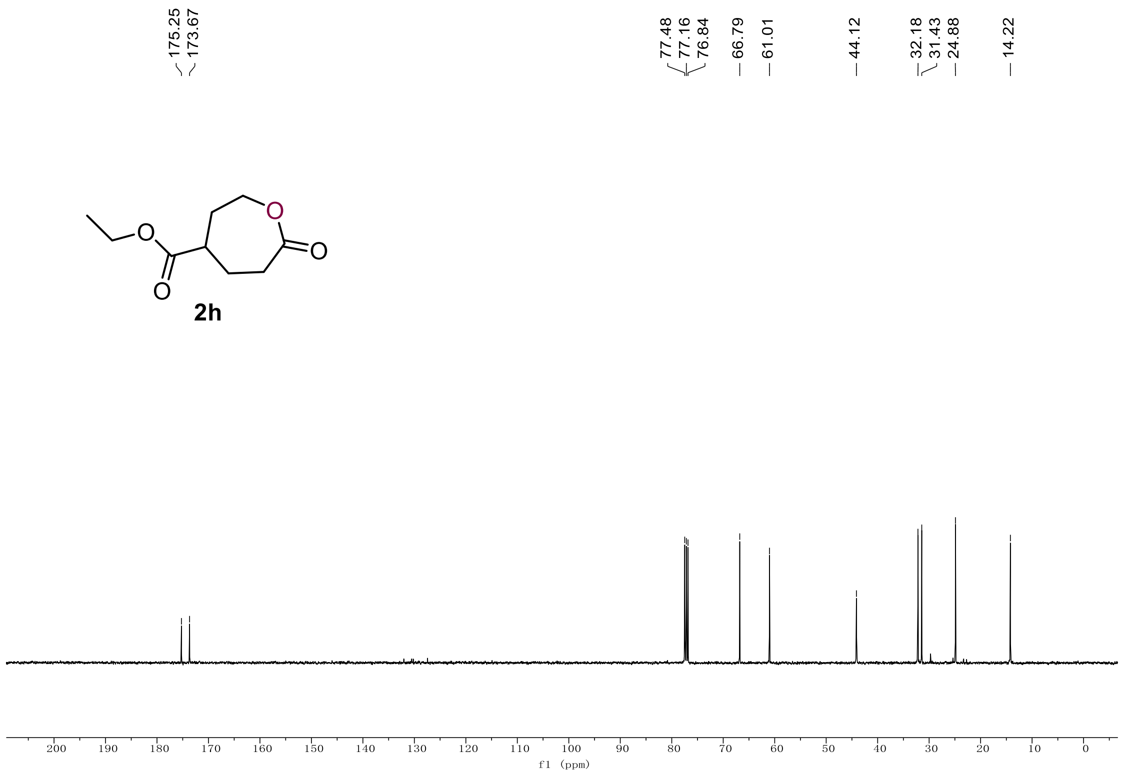
f1 (ppm)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O
O
O
O
2h
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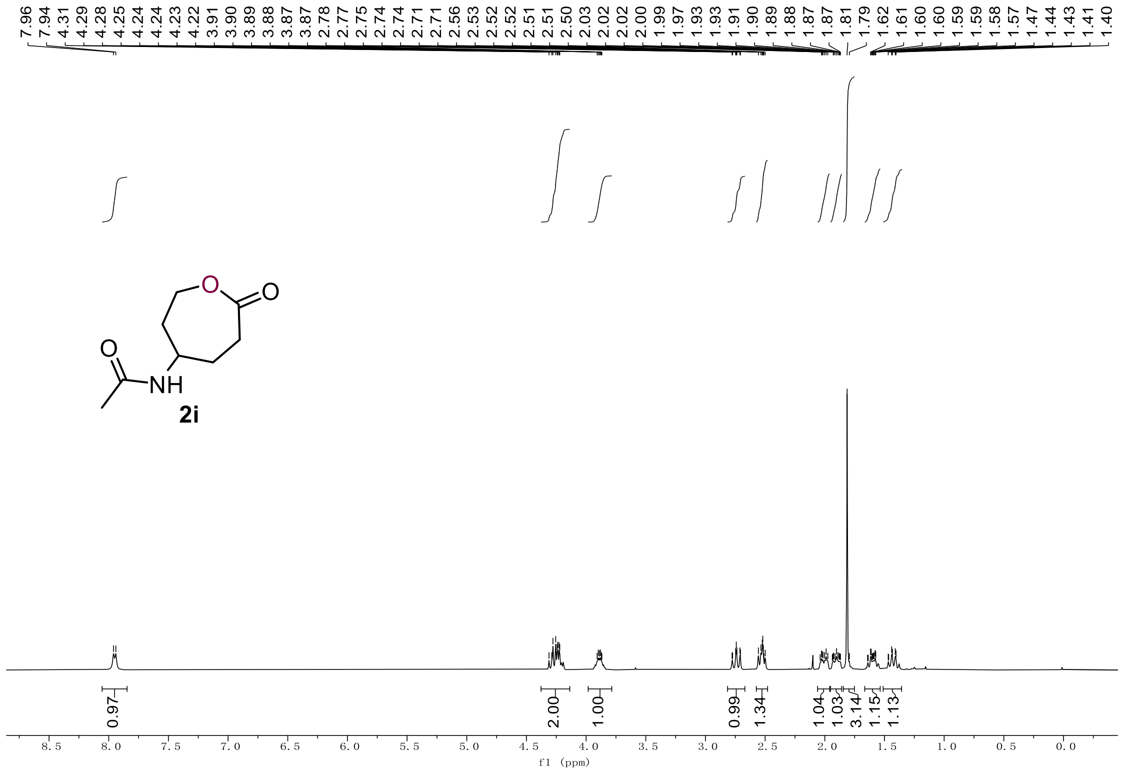
f1 (ppm)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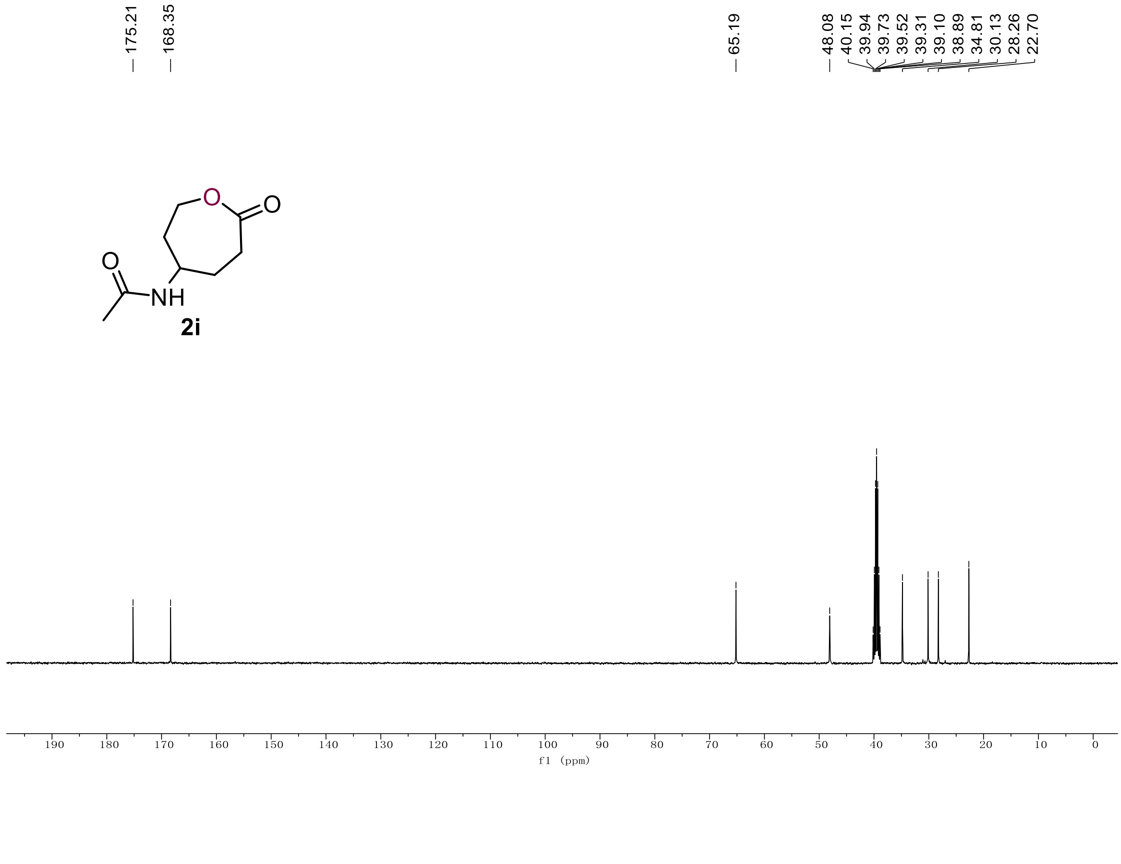
O
O
O
NH
2i
0.97
2.00
1.00
0.99
1.34
1.04
1.03
3.14
1.15
1.13
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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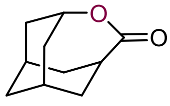
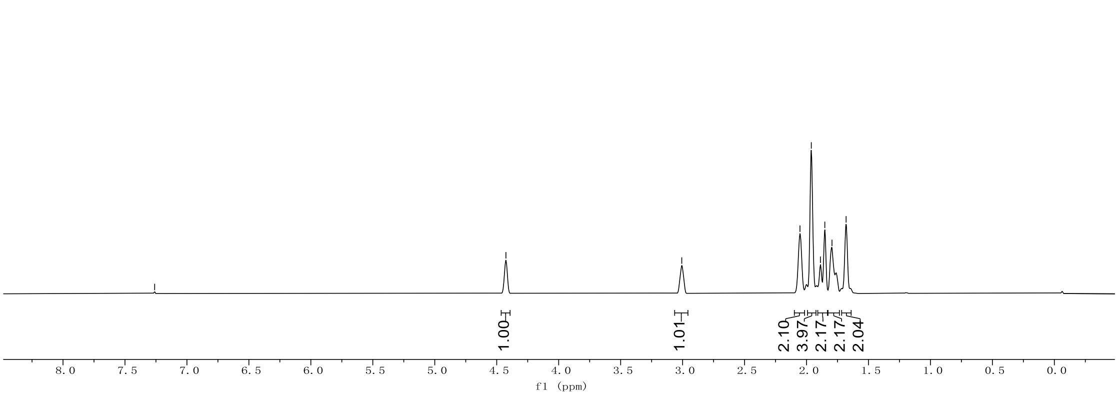
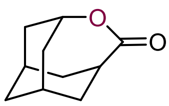
168.35
65.19
48.08 40.15 39.94 39.73 39.52 39.31 39.10 38.89 34.81 30.13 28.26 22.70
O
O
O
NH
2i
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



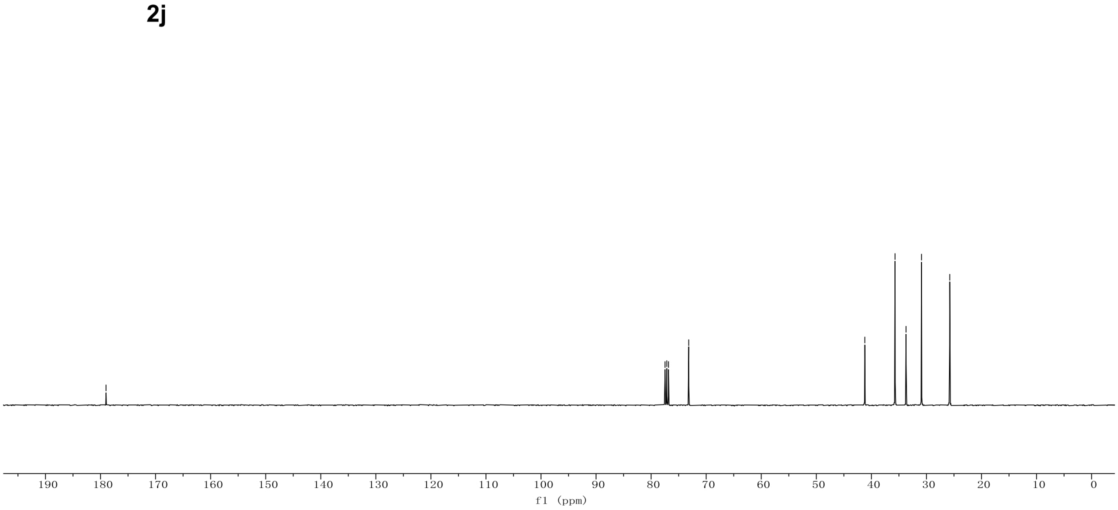
2j



7.26
4.43
3.01
2.05
1.96
1.89
1.85
1.79
1.68
1.00
1.01
2.10
3.97
2.17
2.17
2.04
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)



2j



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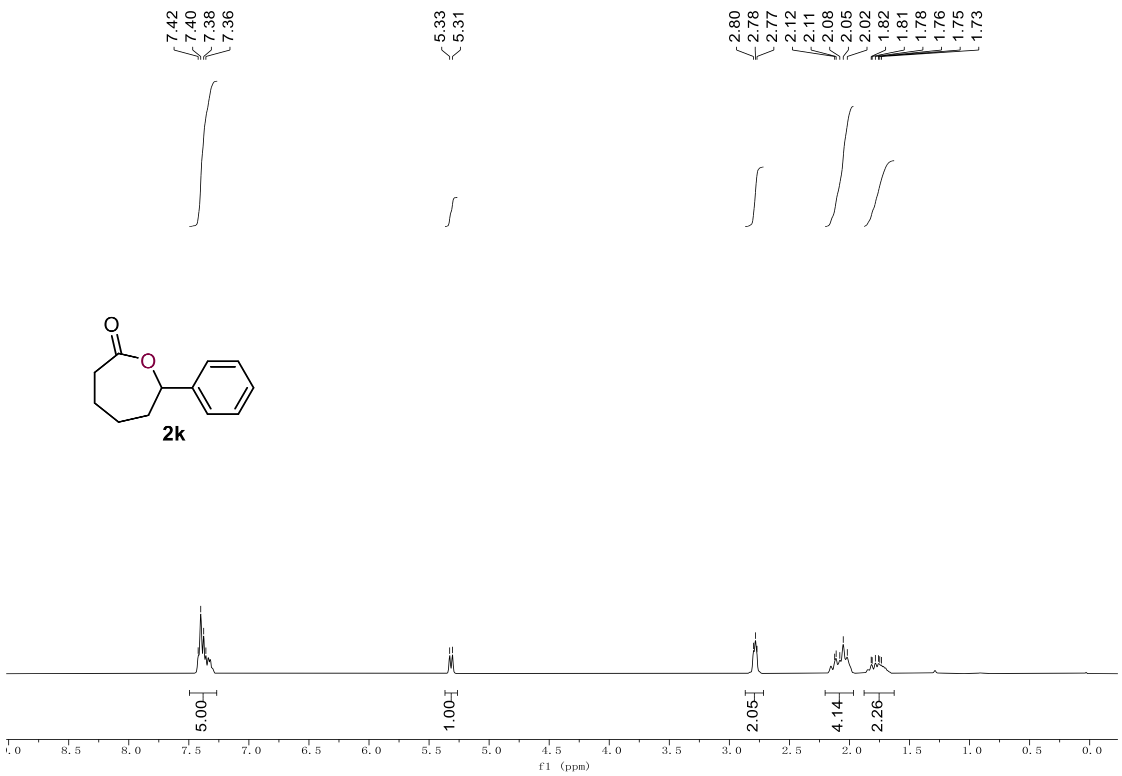
77.48
77.16
76.84
73.17
41.19
35.70
33.70
30.89
25.76
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.38
7.36
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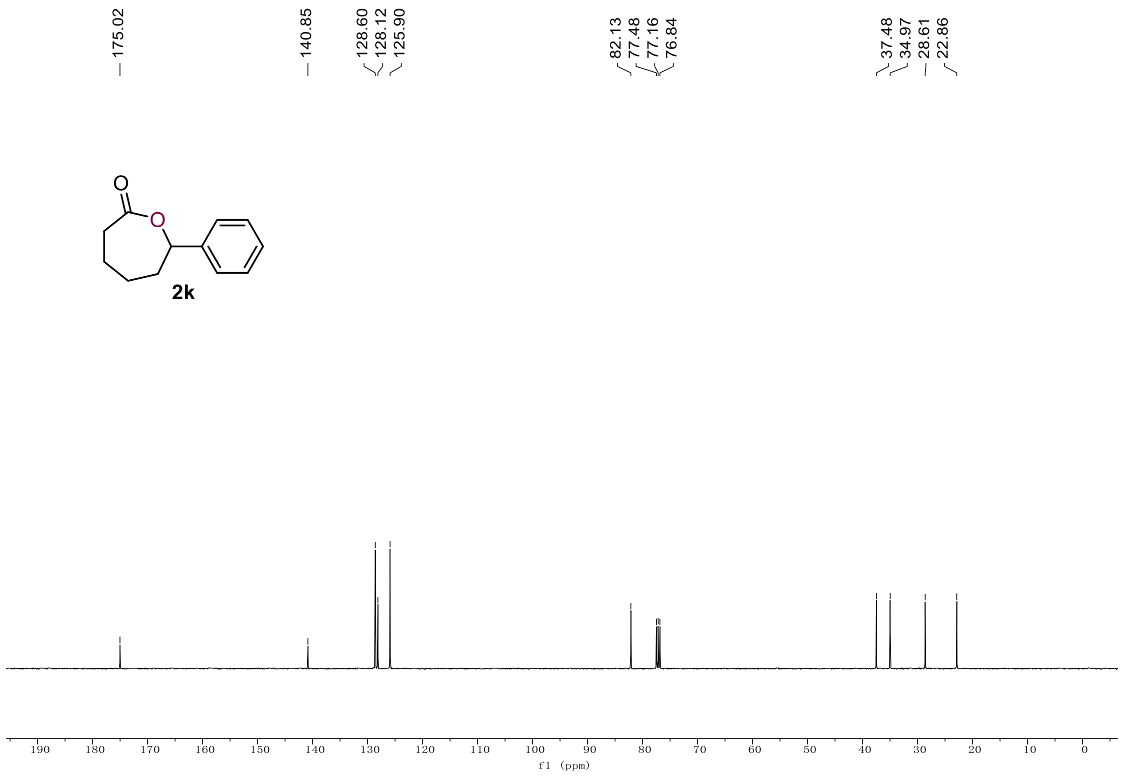
2.78
2.77
2.12
2.11
2.08
2.05
2.02
1.82
1.81
1.78
1.76
1.75
1.73
2k
5.00
1.00
2.05
4.14
2.26
f1 (ppm)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140.85
128.60
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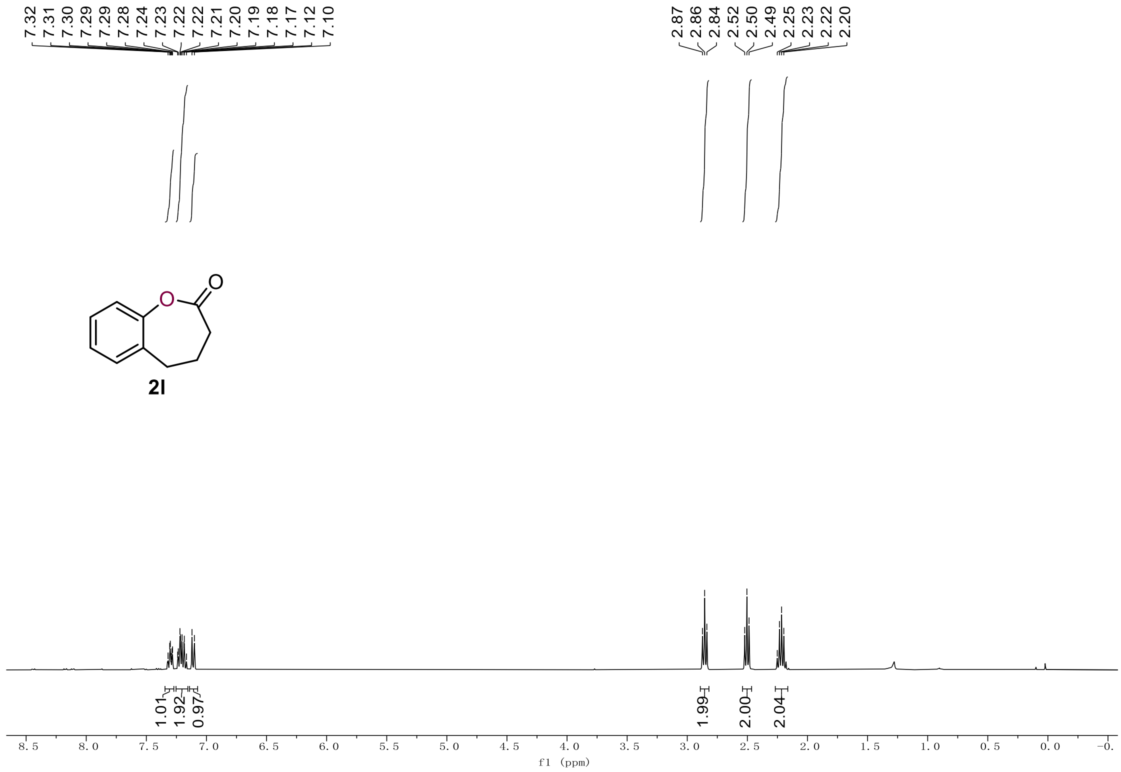
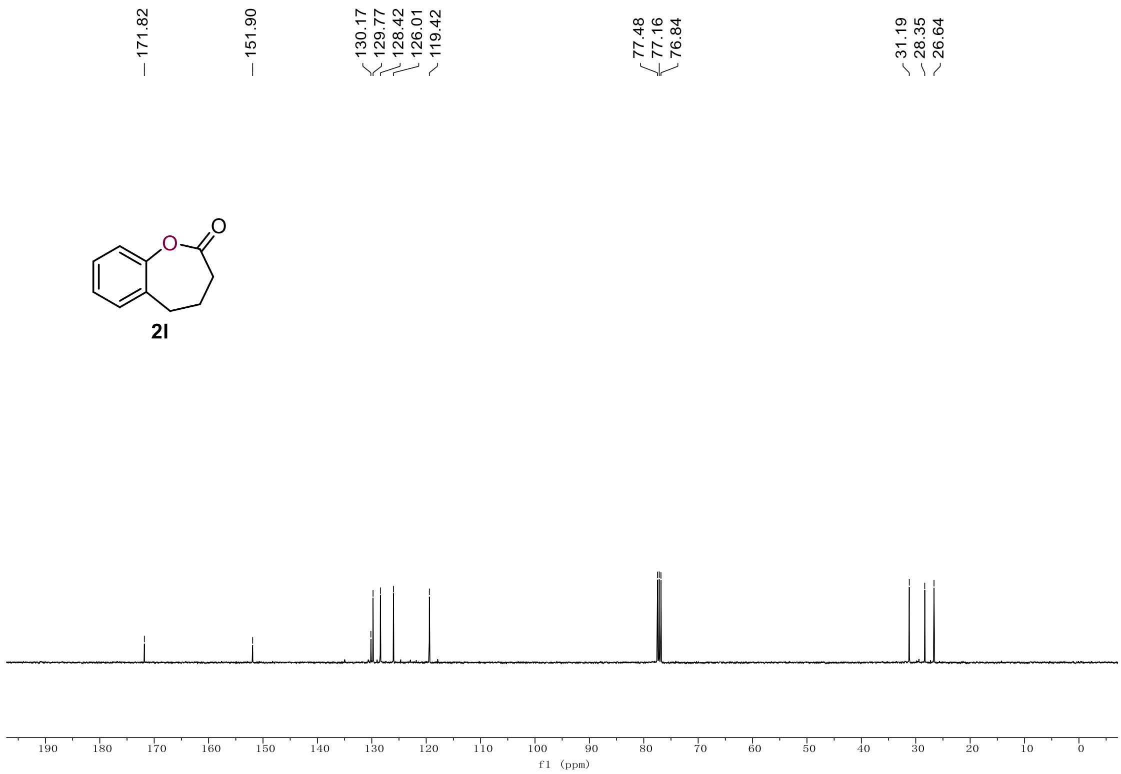
125.90
82.13
77.48
77.16
76.84
37.48
34.97
28.61
22.86
2k
f1 (ppm)


7.32 7.31 7.30 7.29 7.29 7.28 7.24 7.23 7.22 7.22 7.21 7.20 7.19 7.18 7.17 7.12 7.10
2.87 2.86 2.84 2.52 2.50 2.49 2.25 2.23 2.22 2.20
2l
1.01 1.92 0.97 1.99 2.00 2.04
f1 (ppm)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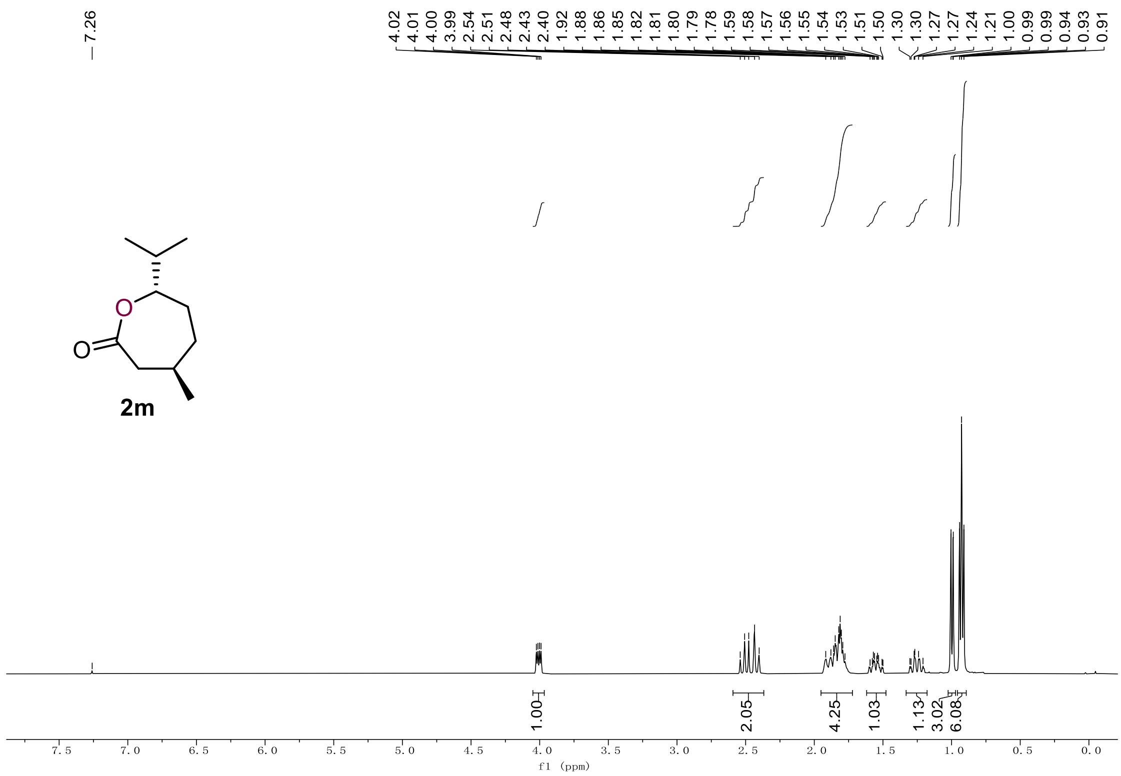
77.48 77.16 76.84
31.19 28.35 26.64
2l
f1 (ppm)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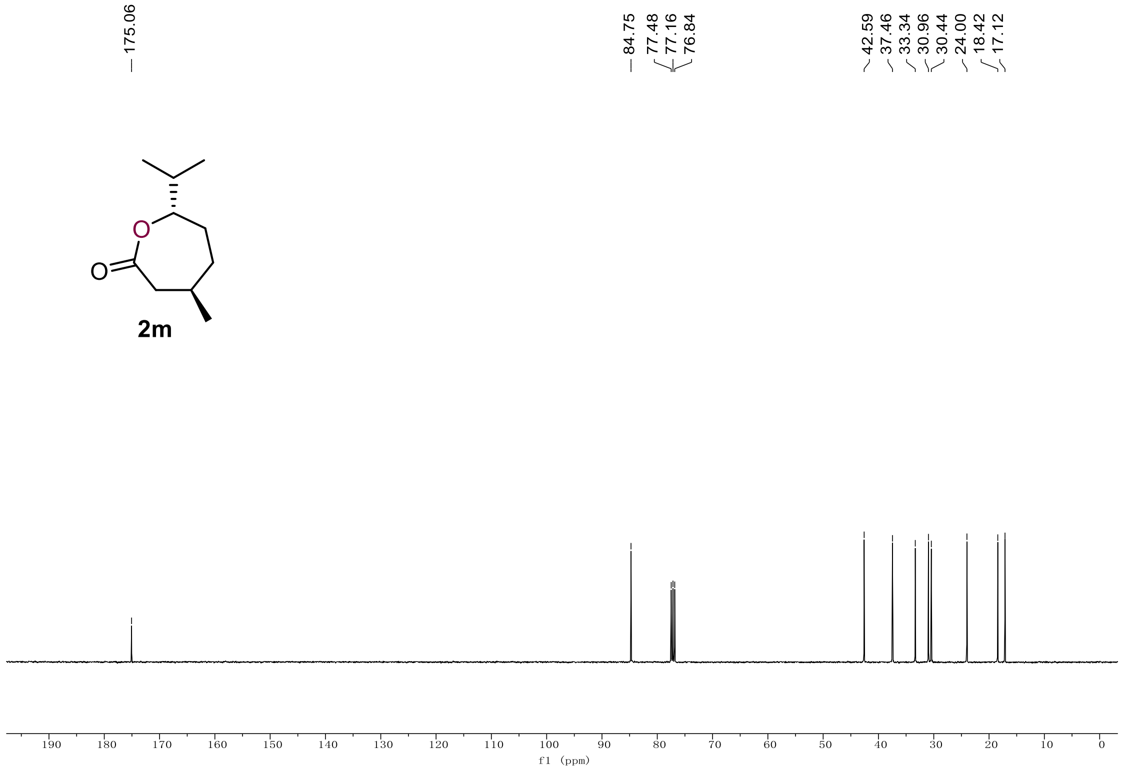
O
O
2m
1.00
2.05
4.25
1.03
1.13
3.02
6.08
f1 (ppm)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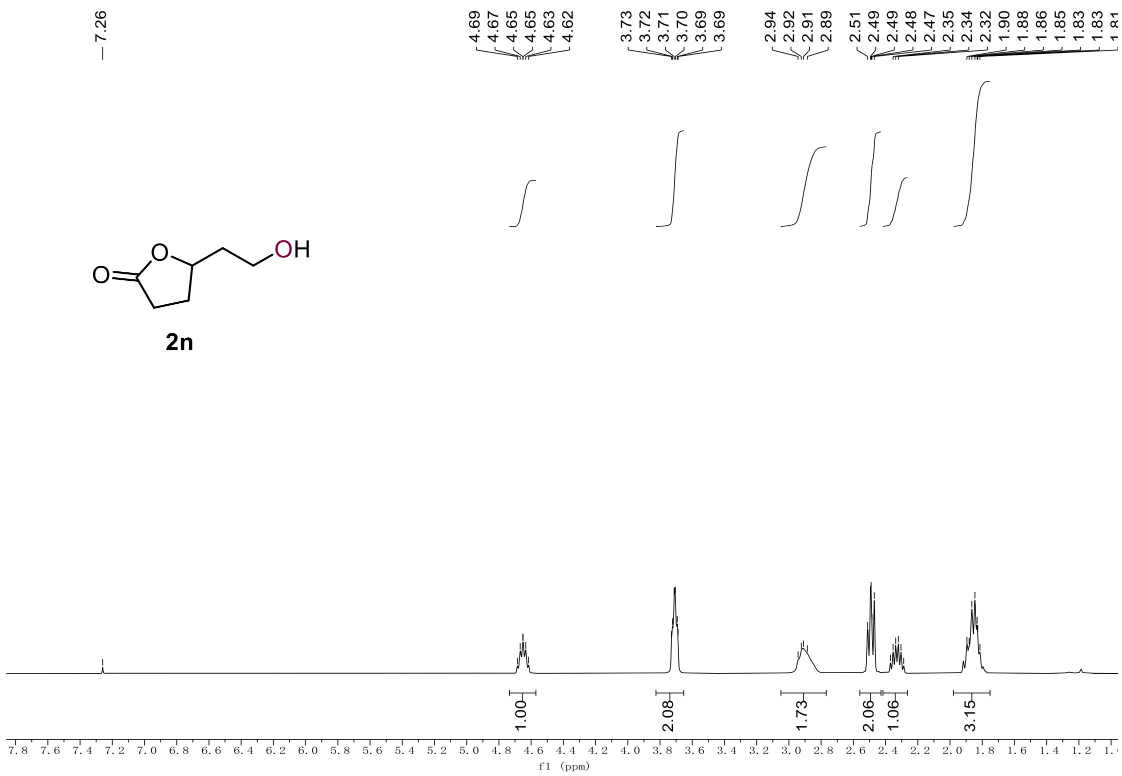
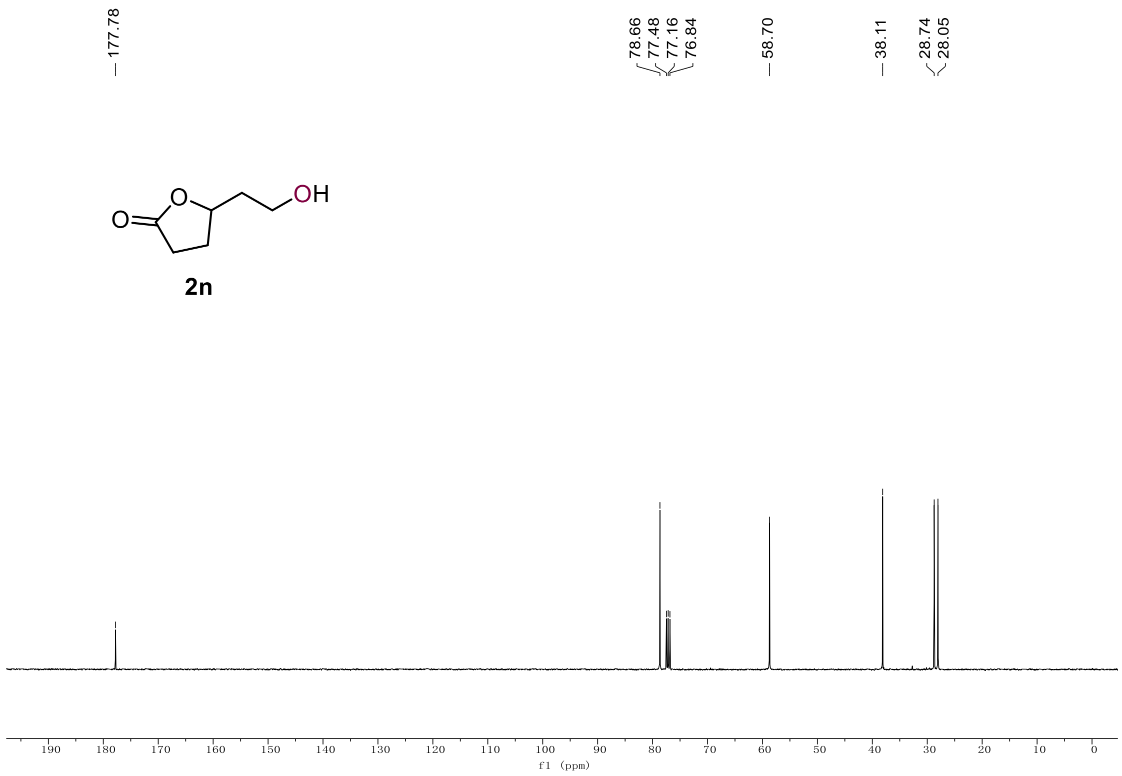
42.59 37.46 33.34 30.96 30.44 24.00 18.42 17.12
O
O
2m
f1 (ppm)


7.26
4.69 4.67 4.65 4.65 4.63 4.62
3.73 3.72 3.71 3.70 3.69 3.69
2.94 2.92 2.91 2.89
2.51 2.49 2.49 2.48 2.47 2.35 2.34 2.32 1.90 1.88 1.86 1.85 1.83
OH
O
2n
1.00
2.08
1.73
2.06
1.06
3.15
f1 (ppm)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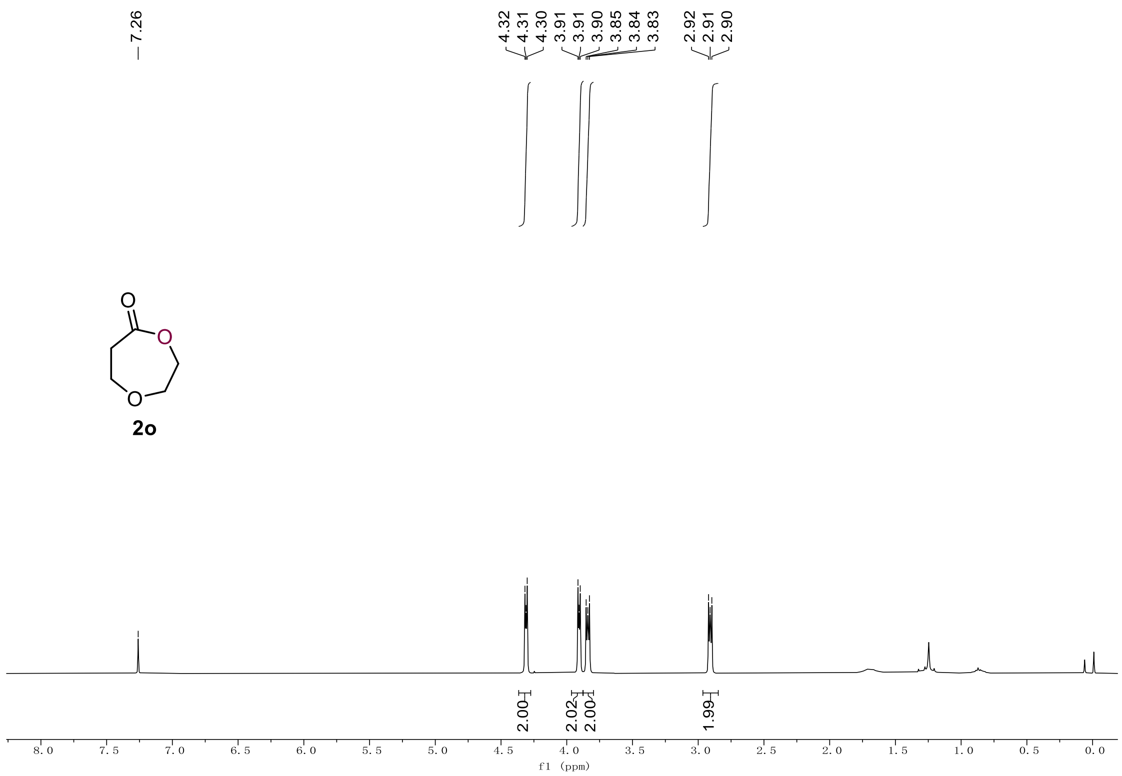
78.66 77.48 77.16 76.84
58.70
38.11
28.74 28.05
OH
O
2n
f1 (ppm)



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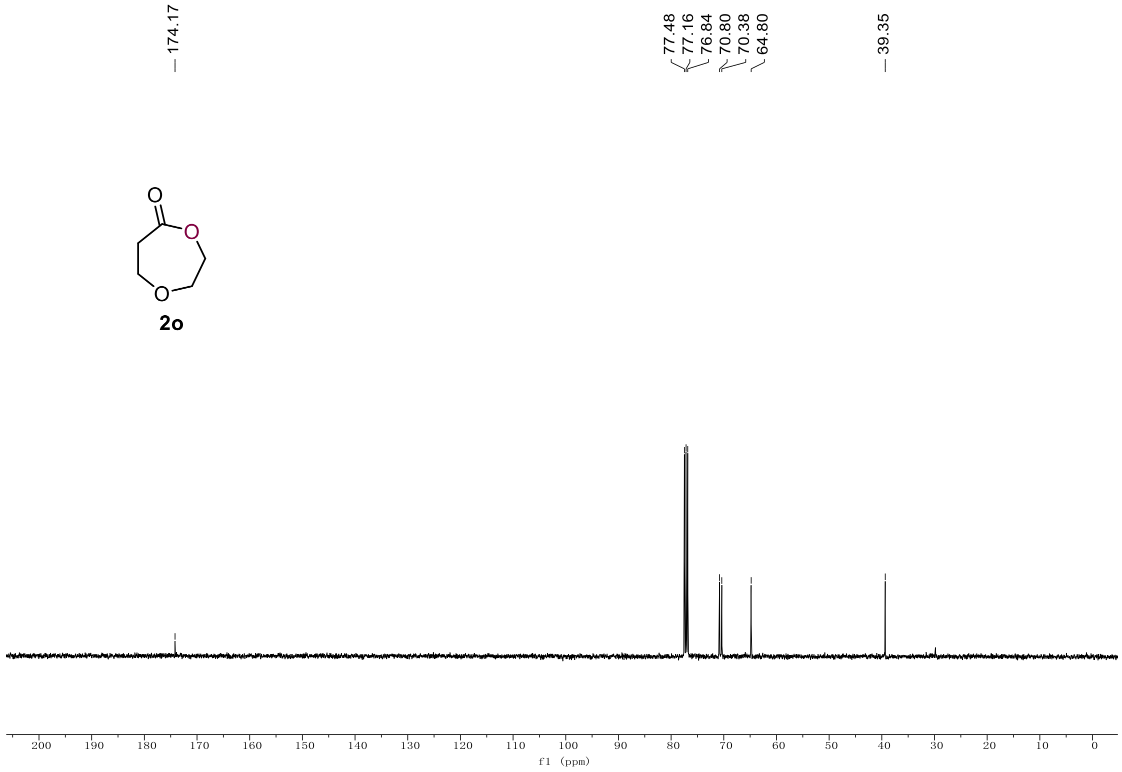
4.32
4.31
4.30
3.91
3.91
3.90
3.85
3.84
3.83
2.92
2.91
2.90
2.00
2.02
2.00
1.99
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

2o



174.17
77.48
77.16
76.84
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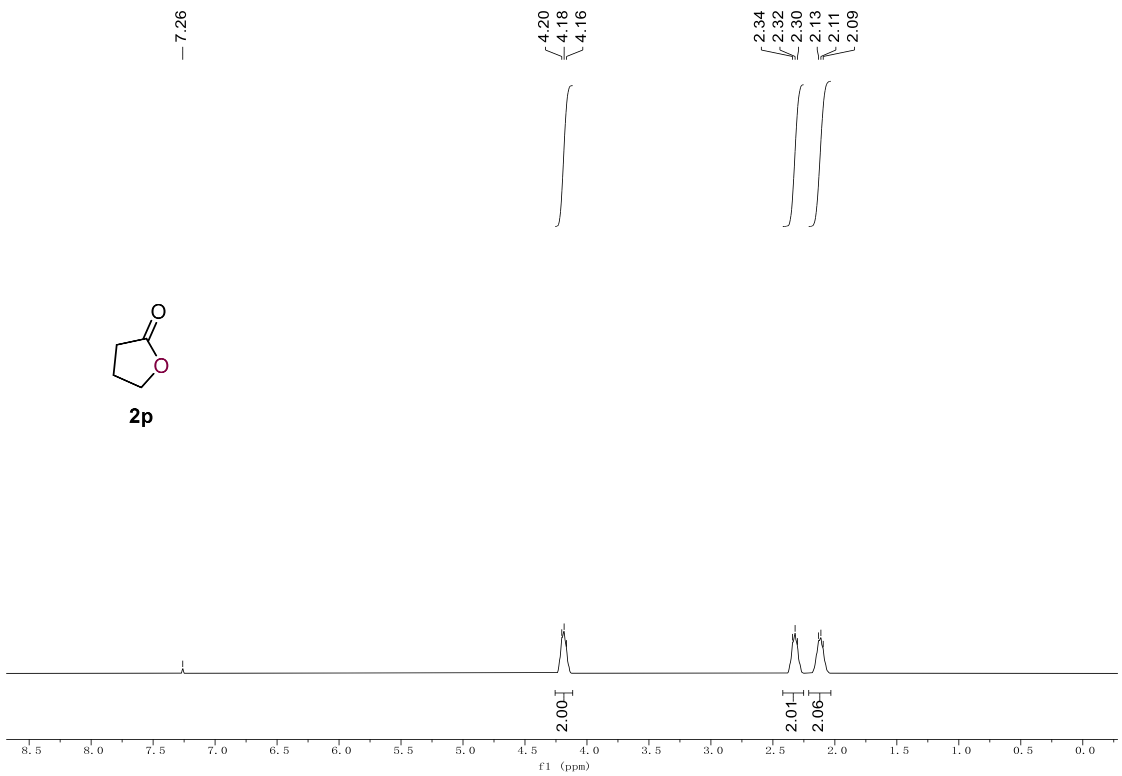
70.38
64.80
39.35
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

2o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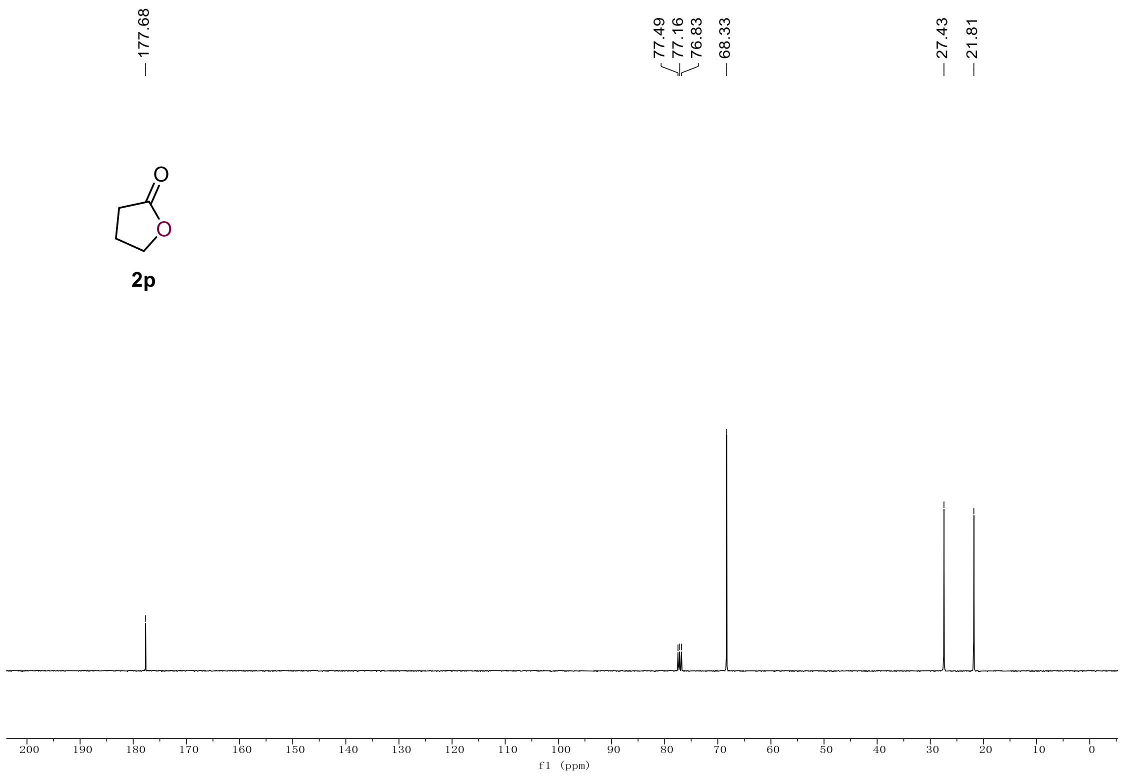
4.16
2.34
2.32
2.30
2.13
2.11
2.09
2p
2.00
2.01
2.06
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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27.43
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2p
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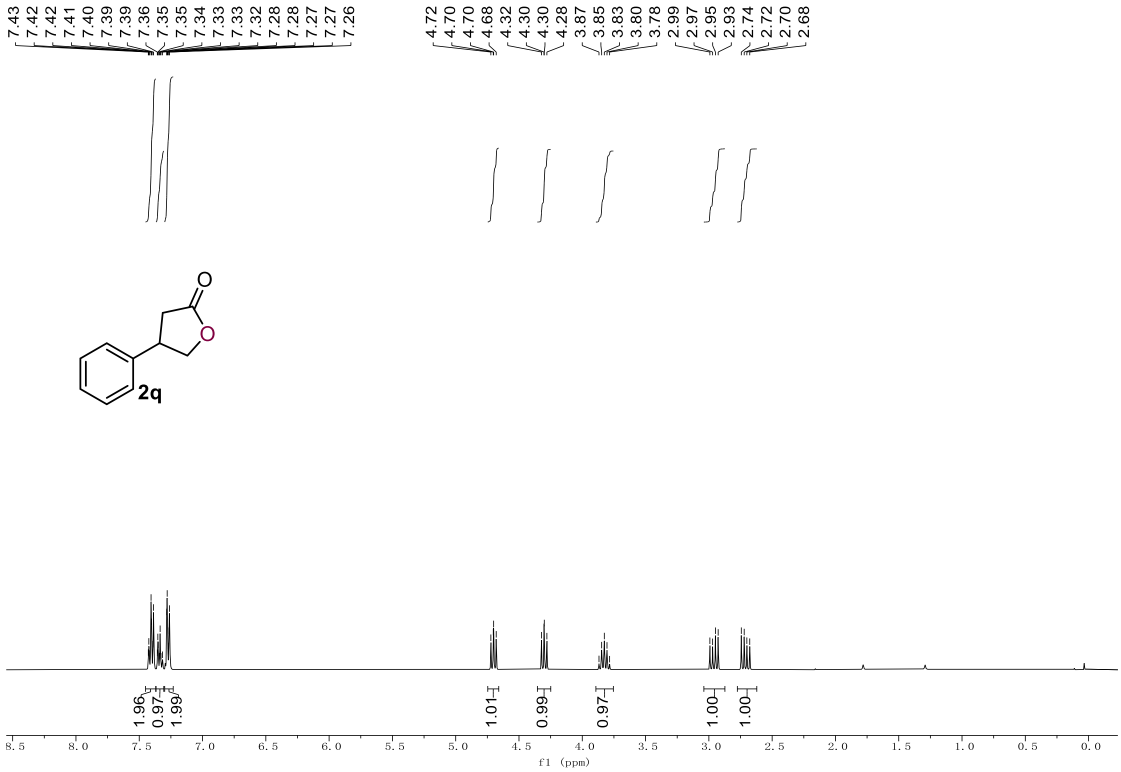
f1 (ppm)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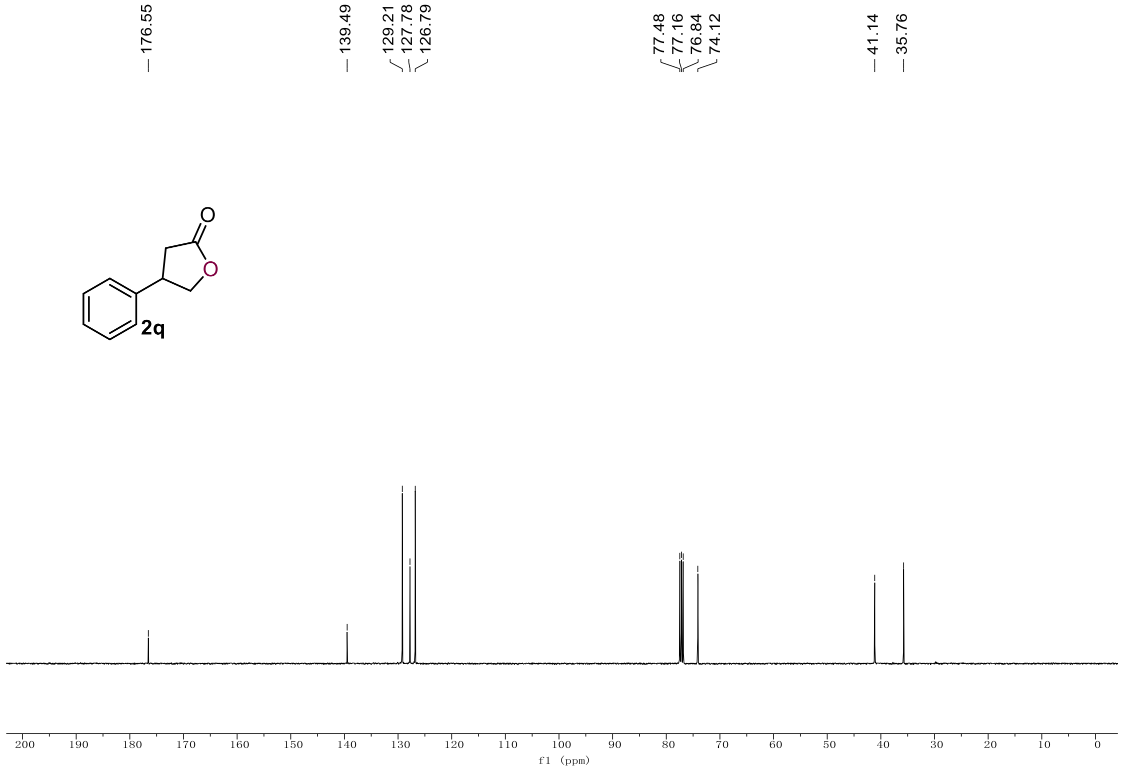
4.72 4.70 4.70 4.68 4.32 4.30 4.30 4.28 3.87 3.85 3.83 3.80 3.78 2.99 2.97 2.95 2.93 2.74 2.72 2.70 2.68
O
O
2q
1.96 0.97 1.99
1.01 0.99 0.97 1.00 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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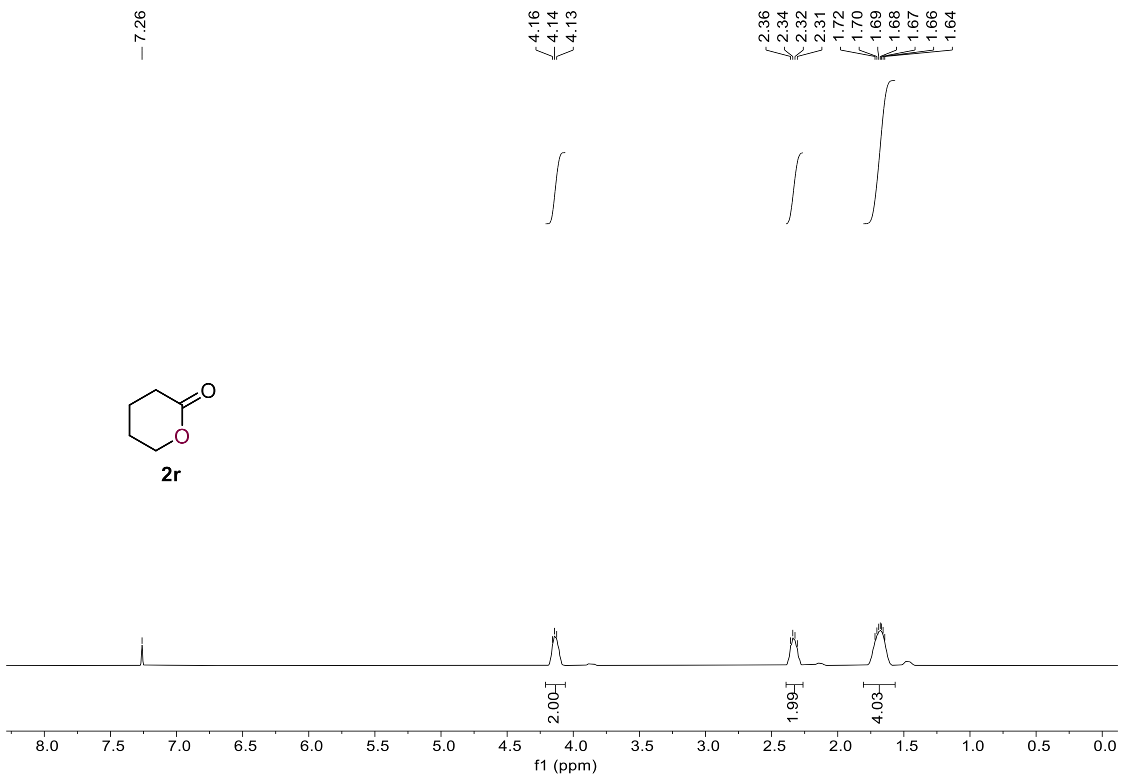
139.49
129.21 127.78 126.79
77.48 77.16 76.84 74.12
41.14
35.76
O
O
2q
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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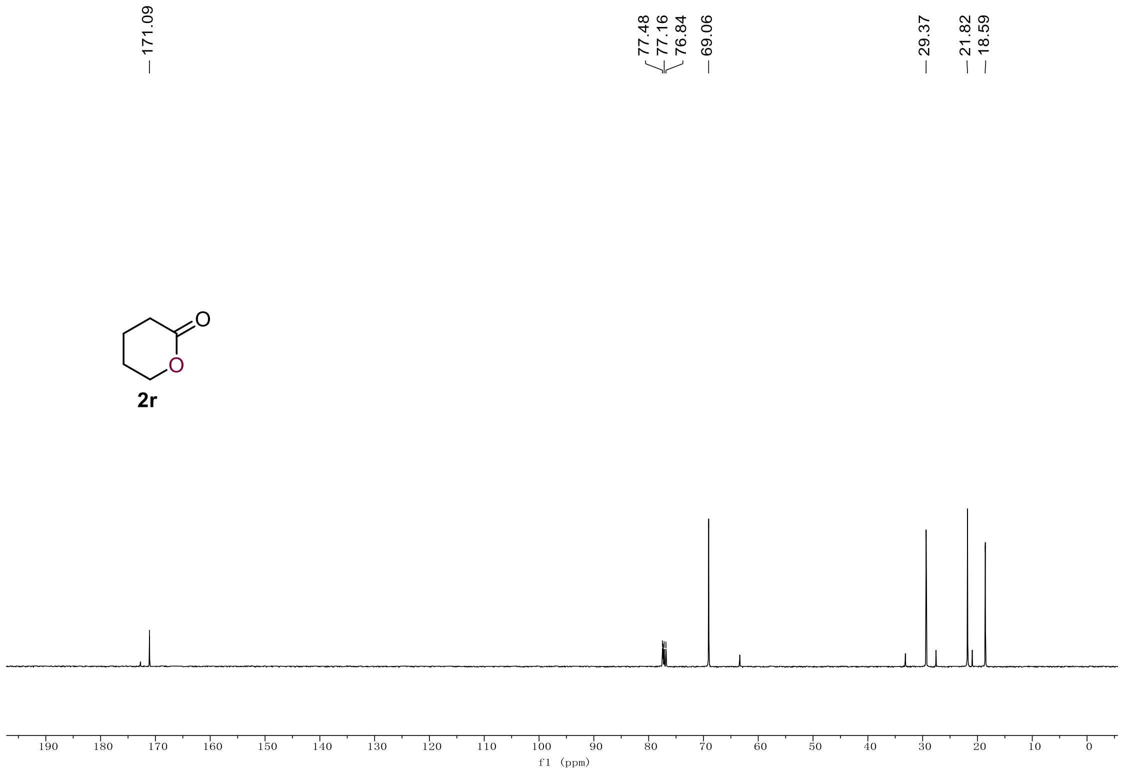
2.31
1.72
1.70
1.69
1.68
1.67
1.66
1.64
2r
2.00
1.99
4.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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21.82
18.59
2r
190
180
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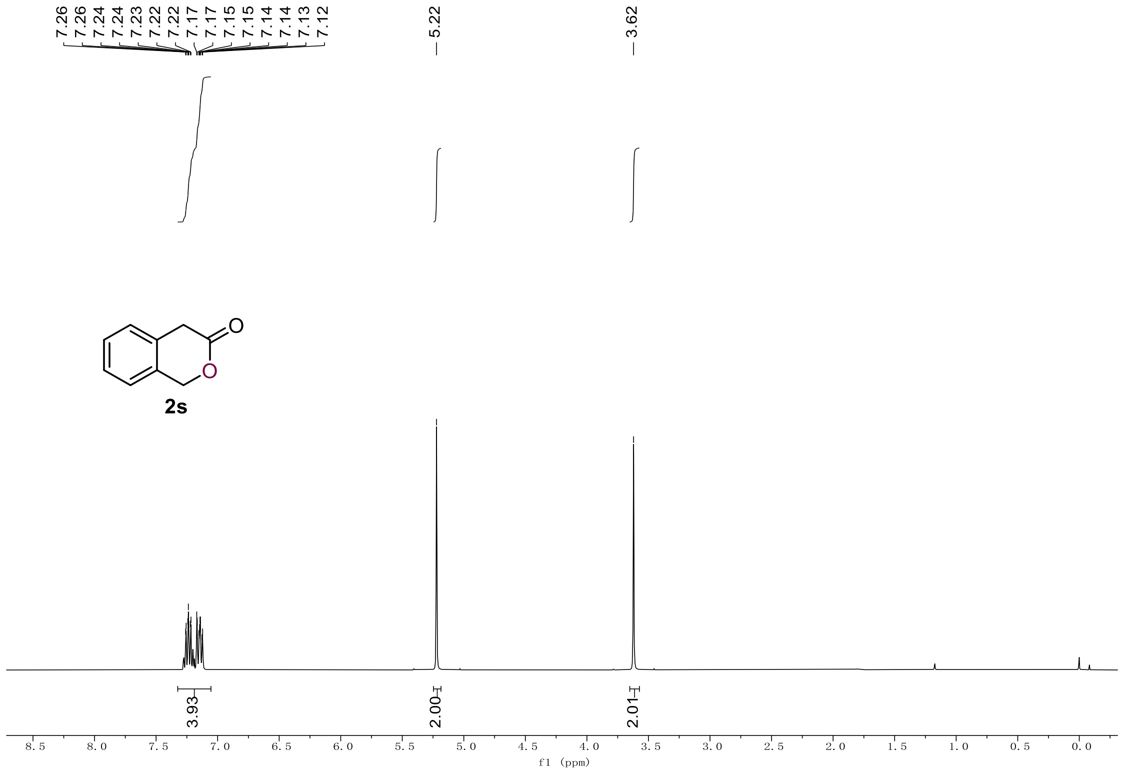
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.24
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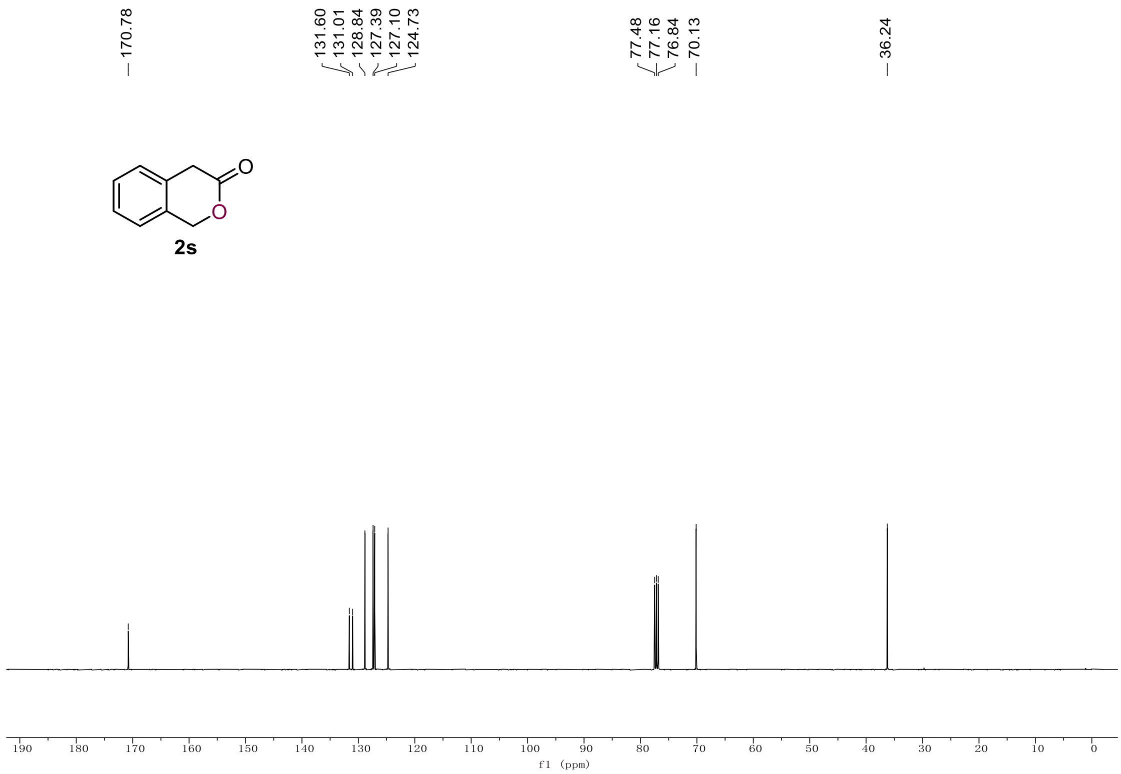
7.22
7.22
7.17
7.17
7.15
7.15
7.14
7.14
7.13
7.12
5.22
3.62
2s
3.93
2.00
2.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.39
127.10
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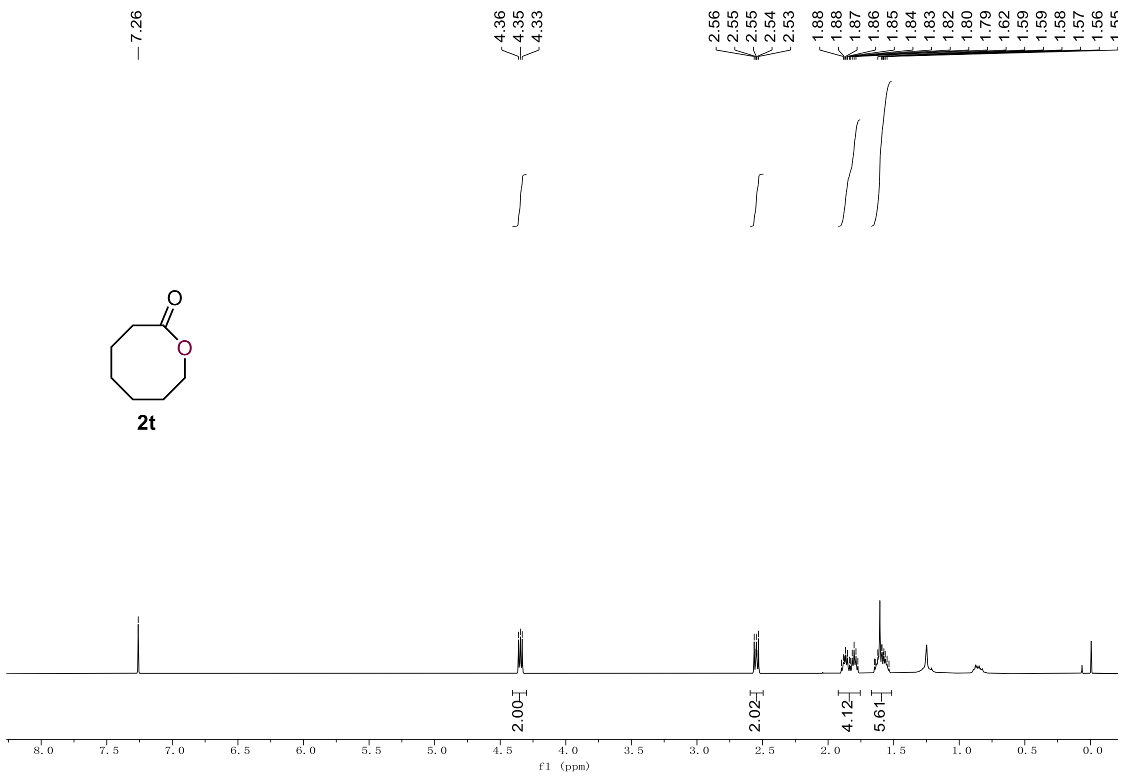
76.84
70.13
36.24
2s
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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1.87
1.86
1.85
1.84
1.83
1.82
1.80
1.79
1.62
1.59
1.59
1.58
1.57
1.56
2t
2.00
2.02
4.12
5.61
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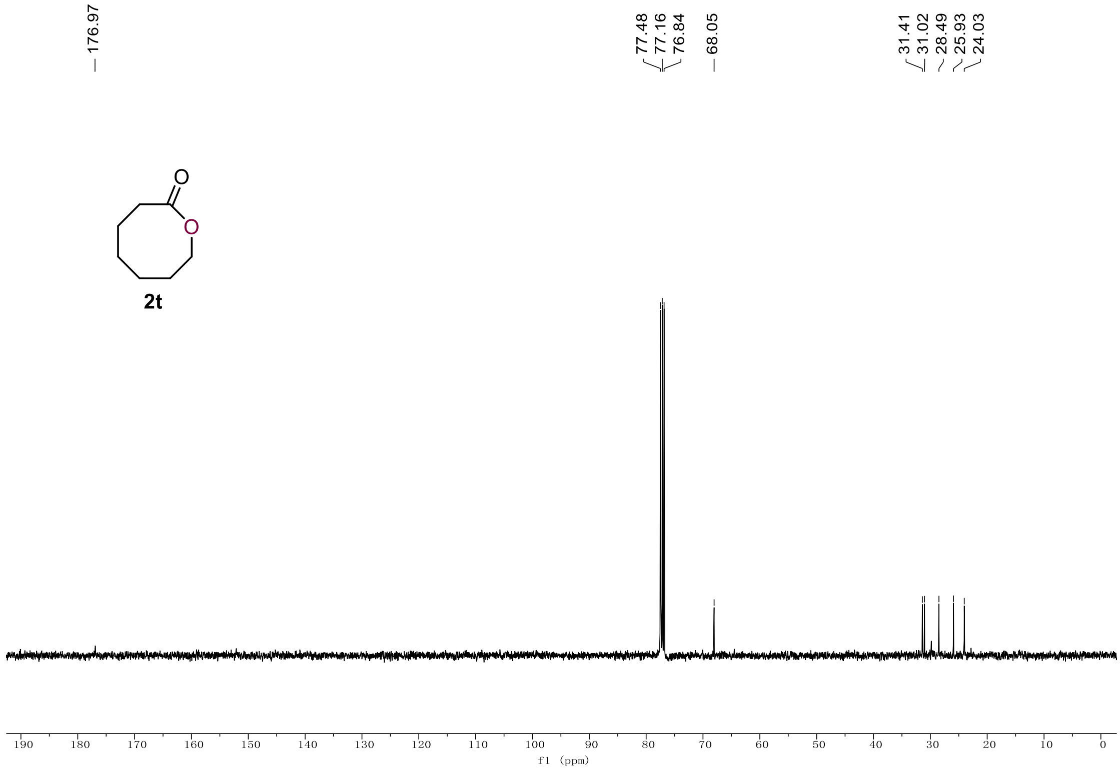
f1 (ppm)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76.84
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24.03
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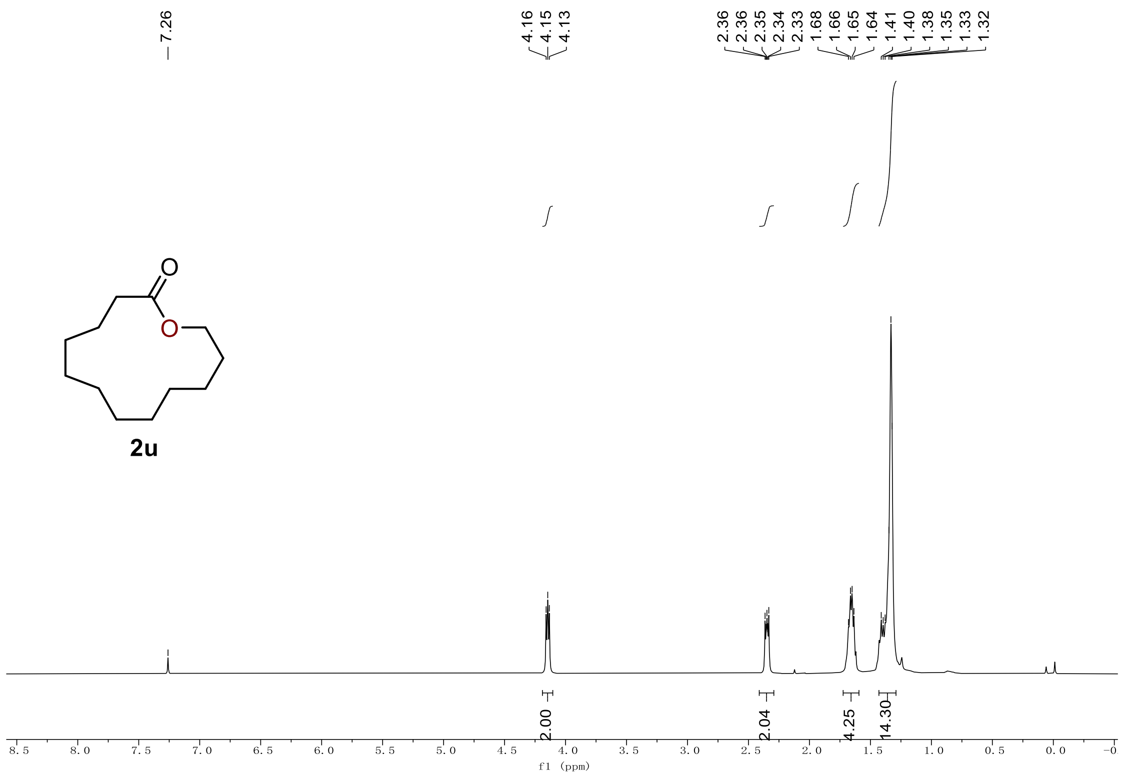
f1 (ppm)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4.16
4.15
4.13
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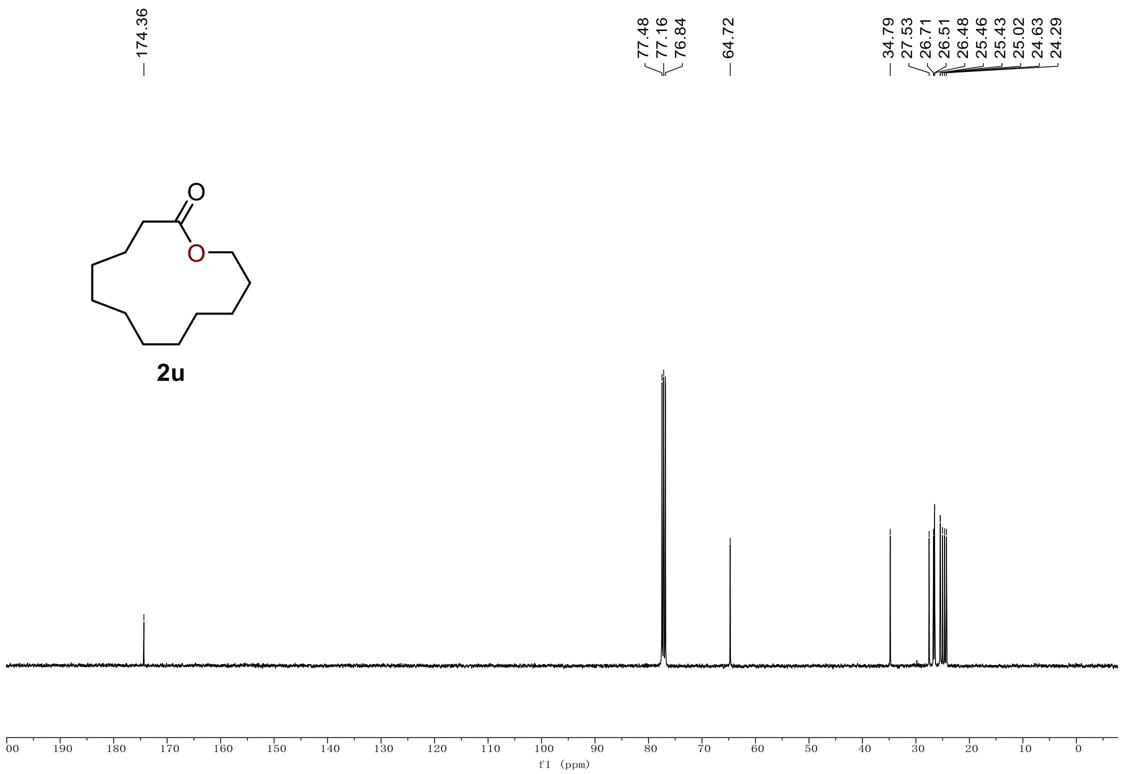
2.36
2.35
2.34
2.33
1.68
1.66
1.65
1.64
1.41
1.40
1.38
1.35
1.33
1.32
O
O
2u
2.00
2.04
4.25
14.30
f1 (ppm)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64.72
34.79
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26.48
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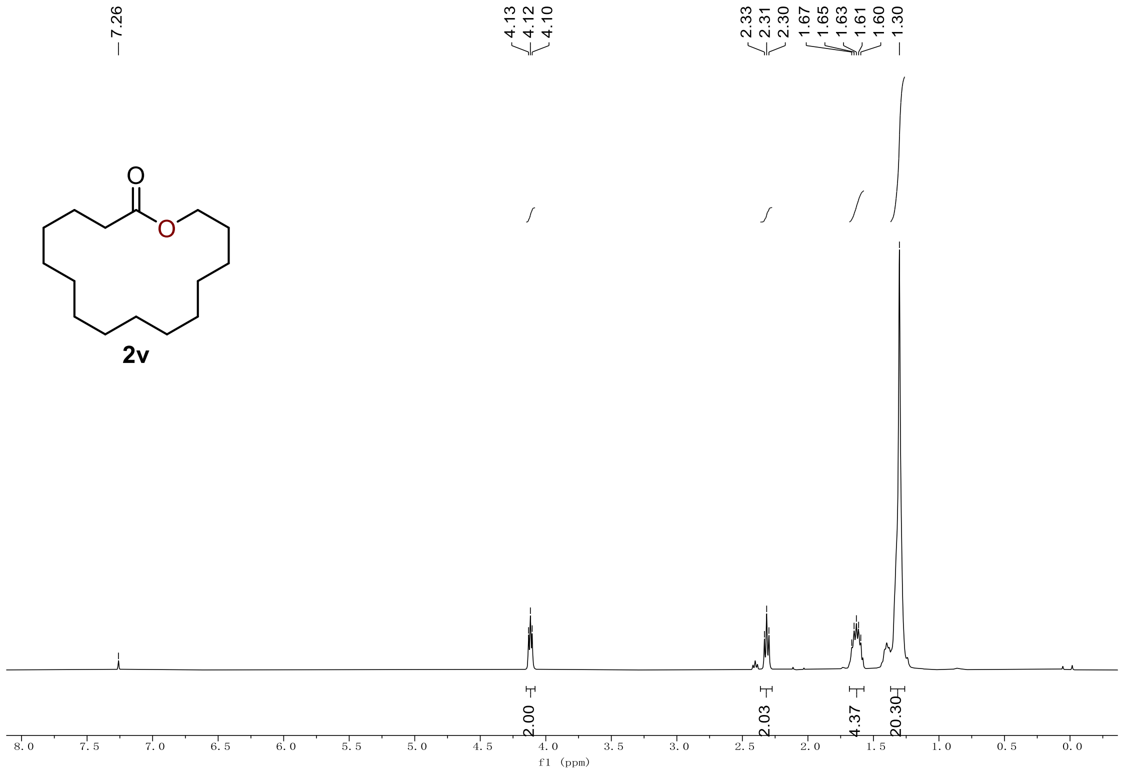
25.43
25.02
24.63
24.29
O
O
2u
f1 (ppm)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4.13
4.12
4.10
2.33
2.31
2.30
1.67
1.65
1.63
1.61
1.60
1.30
O
O
2v
2.00
2.03
4.37
20.30
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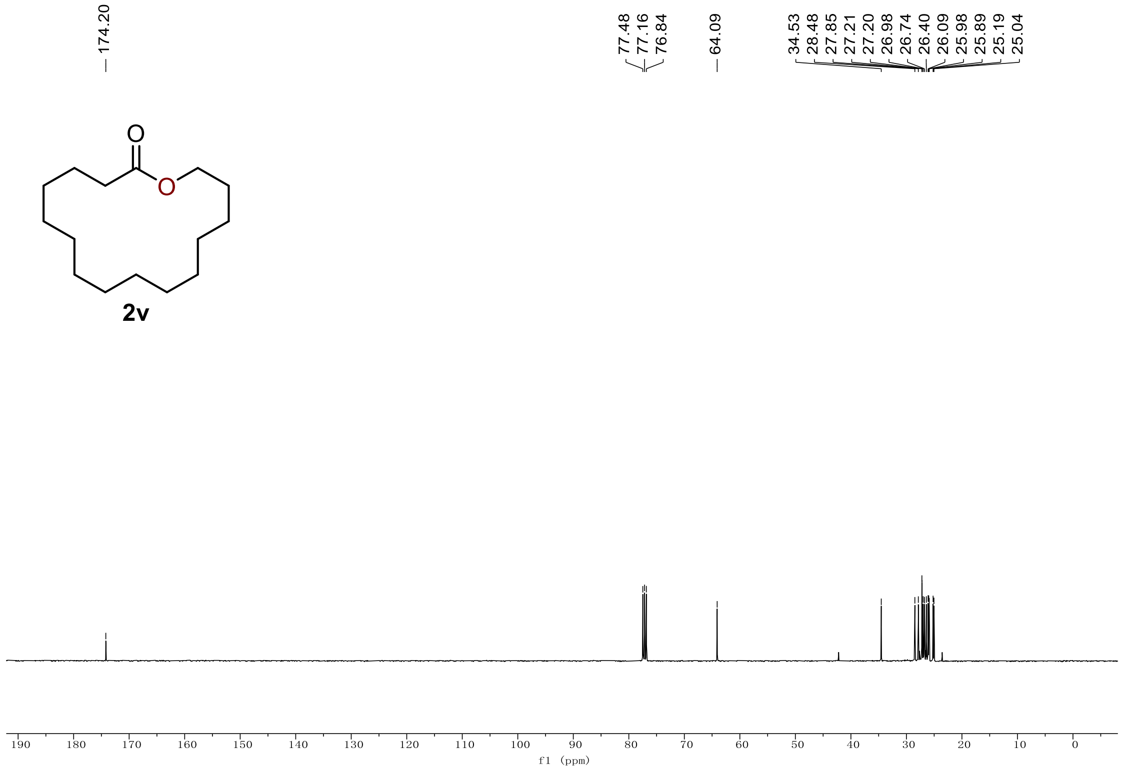
f1 (ppm)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34.53
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27.85
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27.20
26.98
26.74
26.40
26.09
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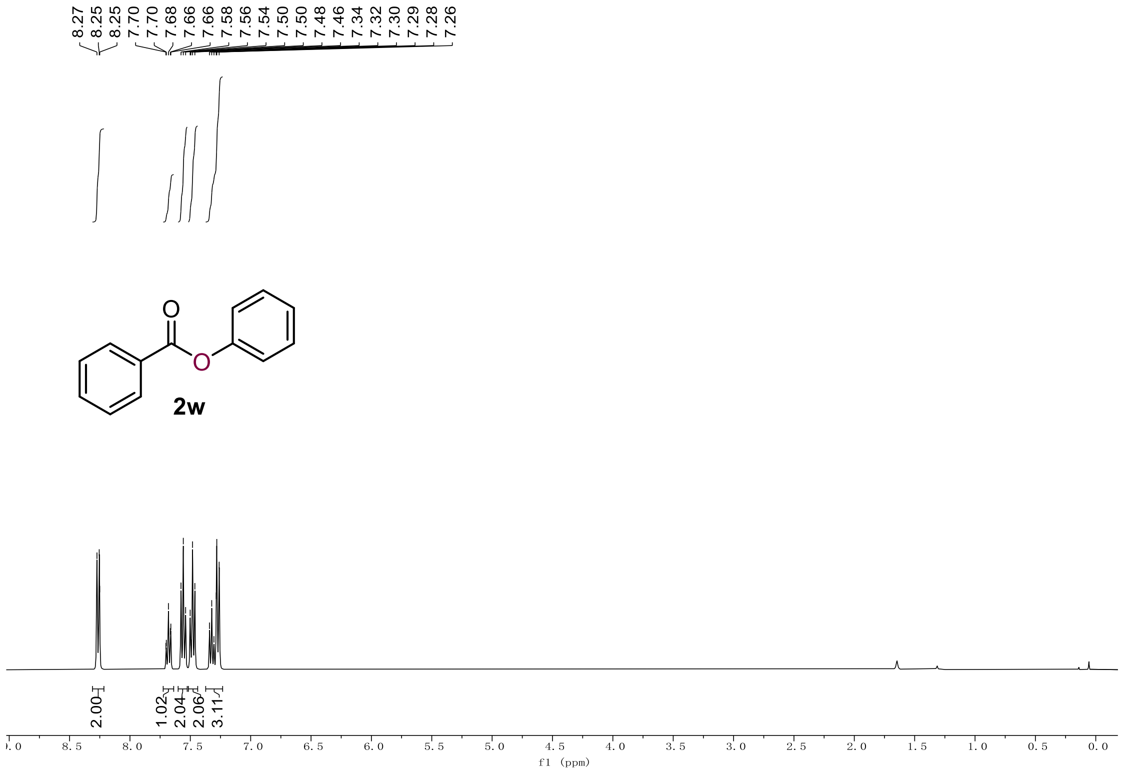
25.19
25.04
O
O
2v
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.66
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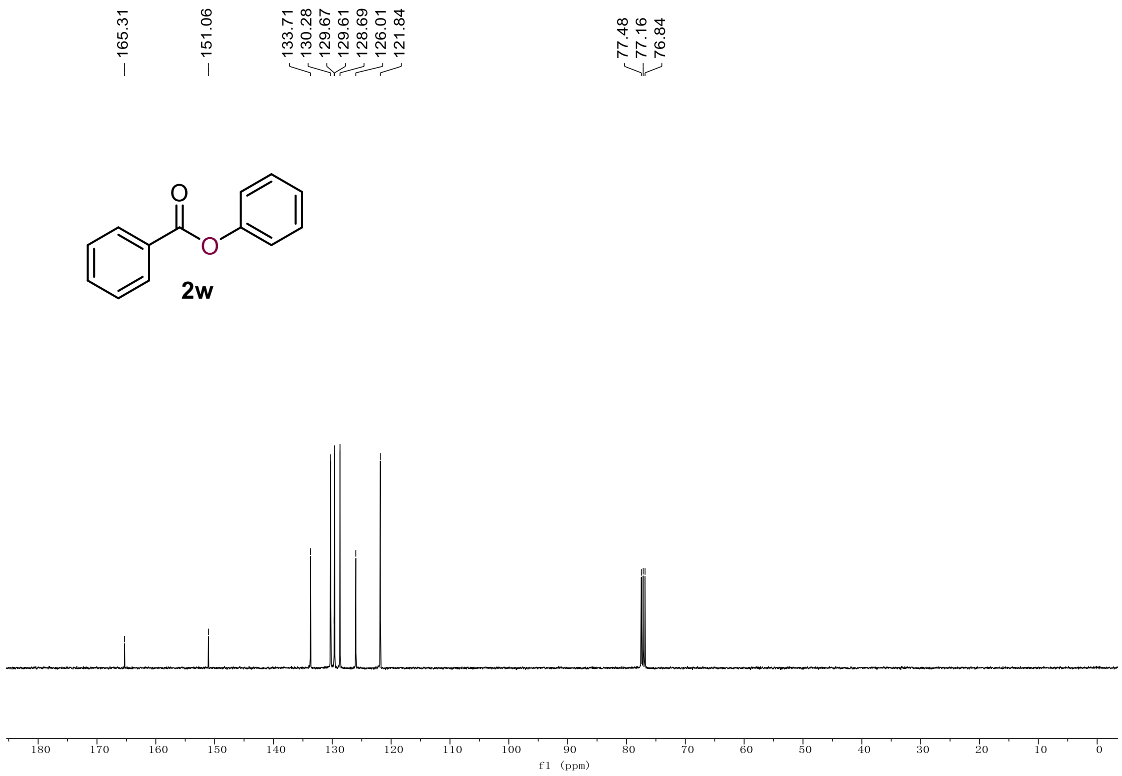
7.56
7.54
7.50
7.50
7.48
7.46
7.34
7.32
7.30
7.29
7.28
7.26
2w
2.00
1.02
2.04
2.06
3.11
f1 (ppm)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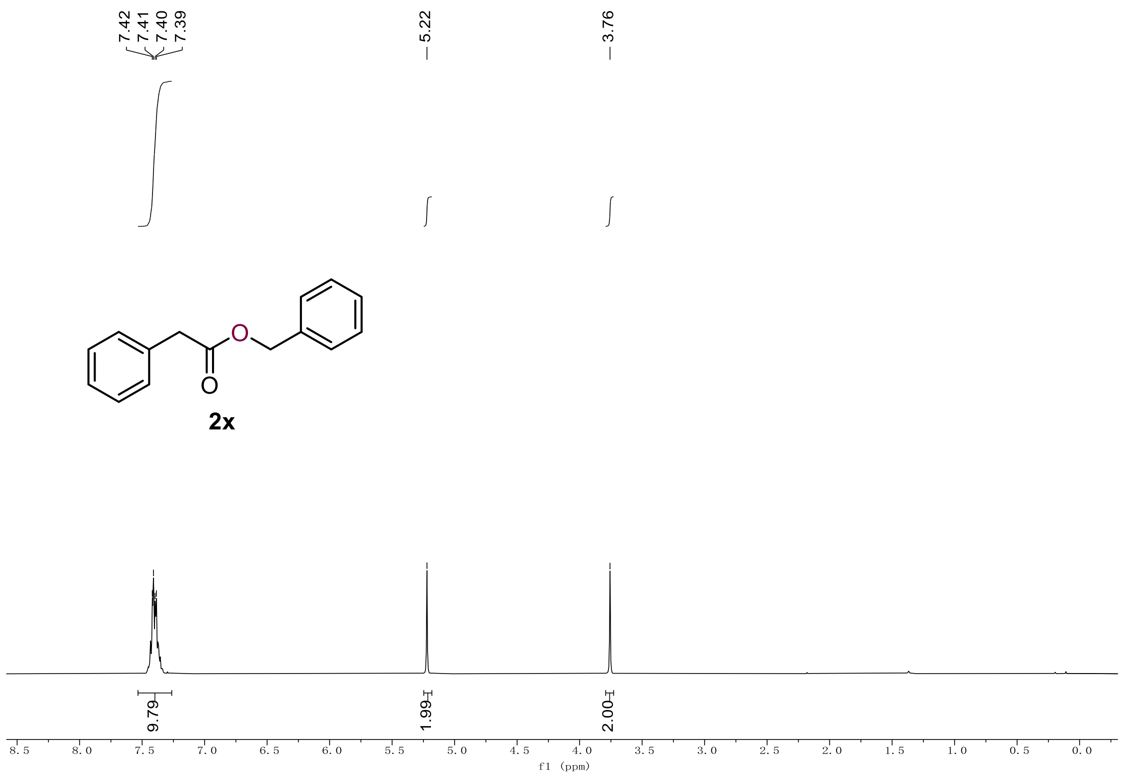
2w
f1 (ppm)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5.22
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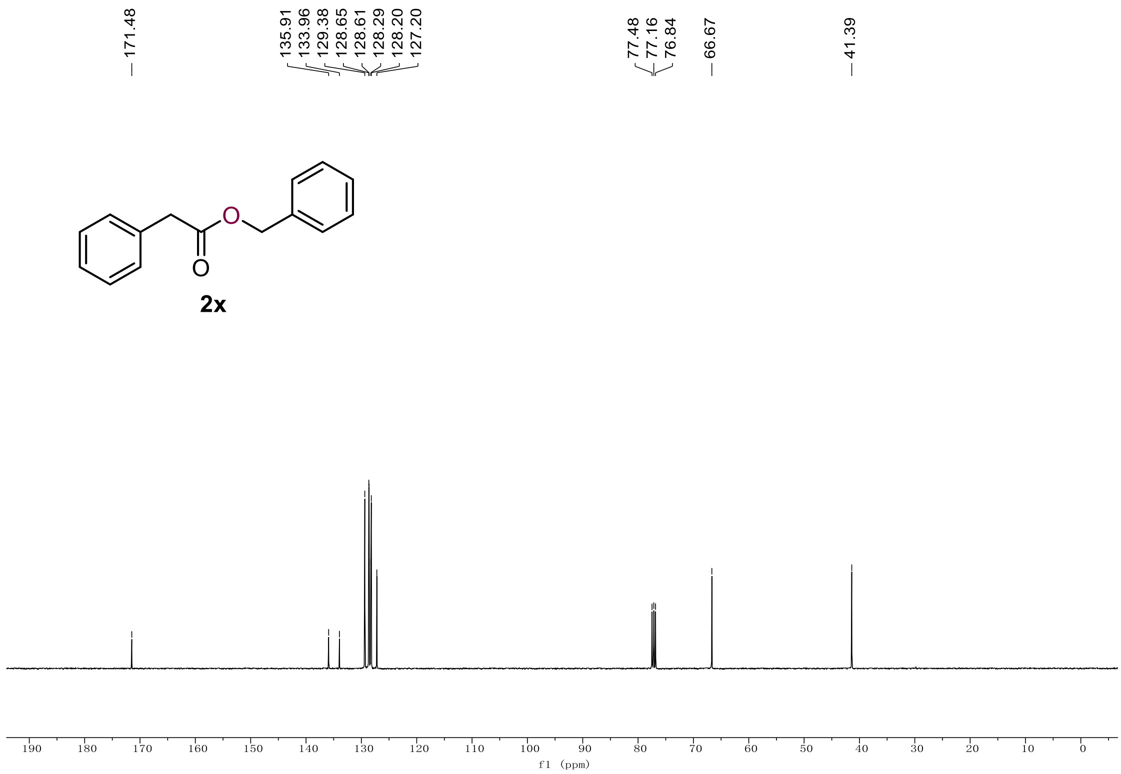
1.99
2.00
f1 (ppm)

2x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128.20
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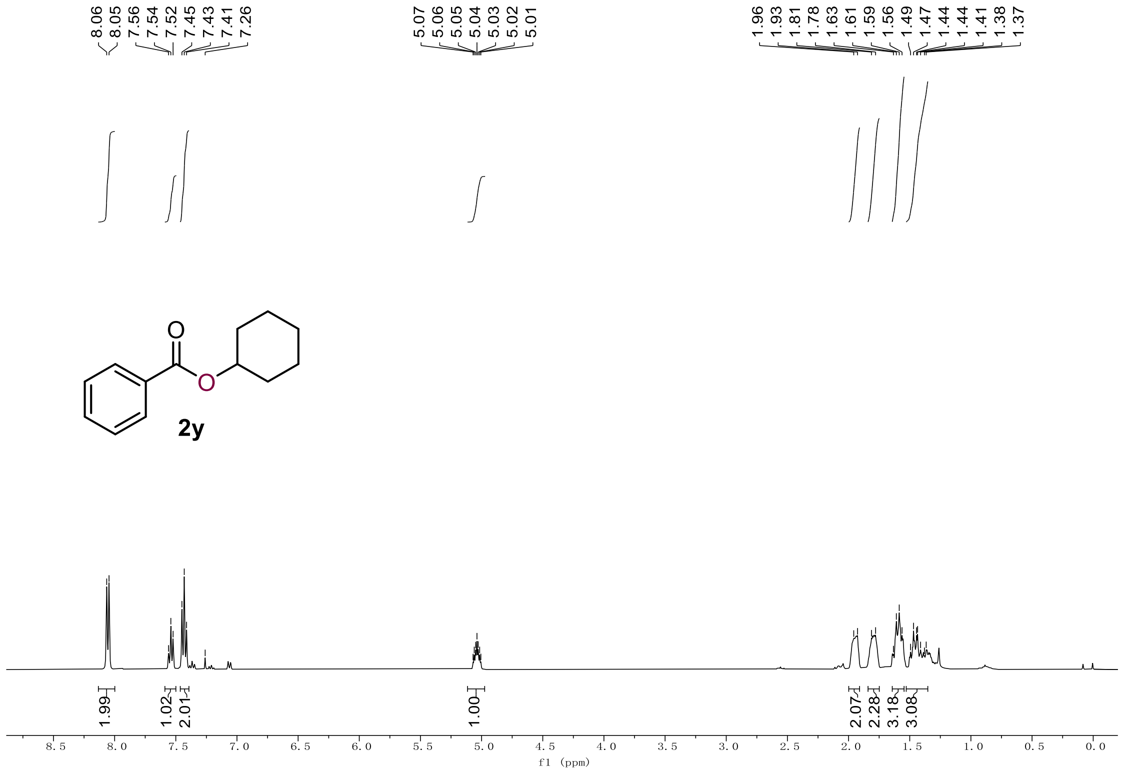
66.67
41.39
f1 (ppm)

2x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5.04
5.03
5.02
5.01
1.96
1.93
1.81
1.78
1.63
1.61
1.59
1.56
1.49
1.47
1.44
1.44
1.41
1.38
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O
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2.01
1.00
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2.28
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3.08
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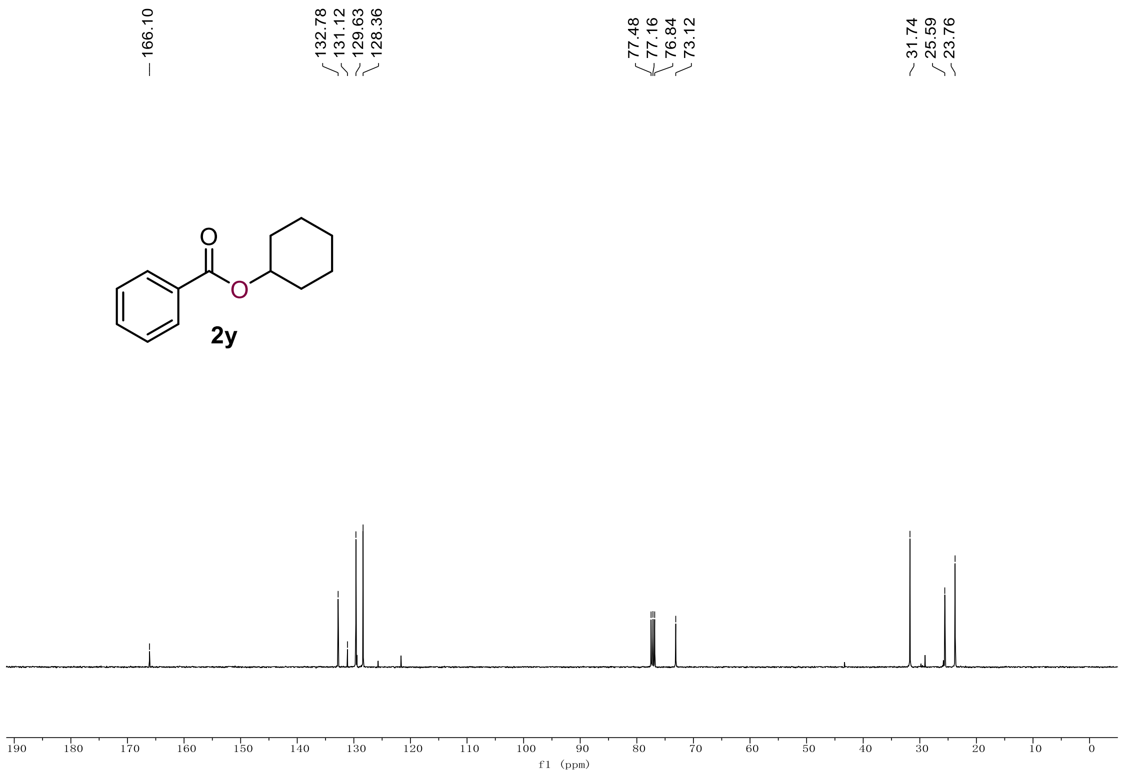
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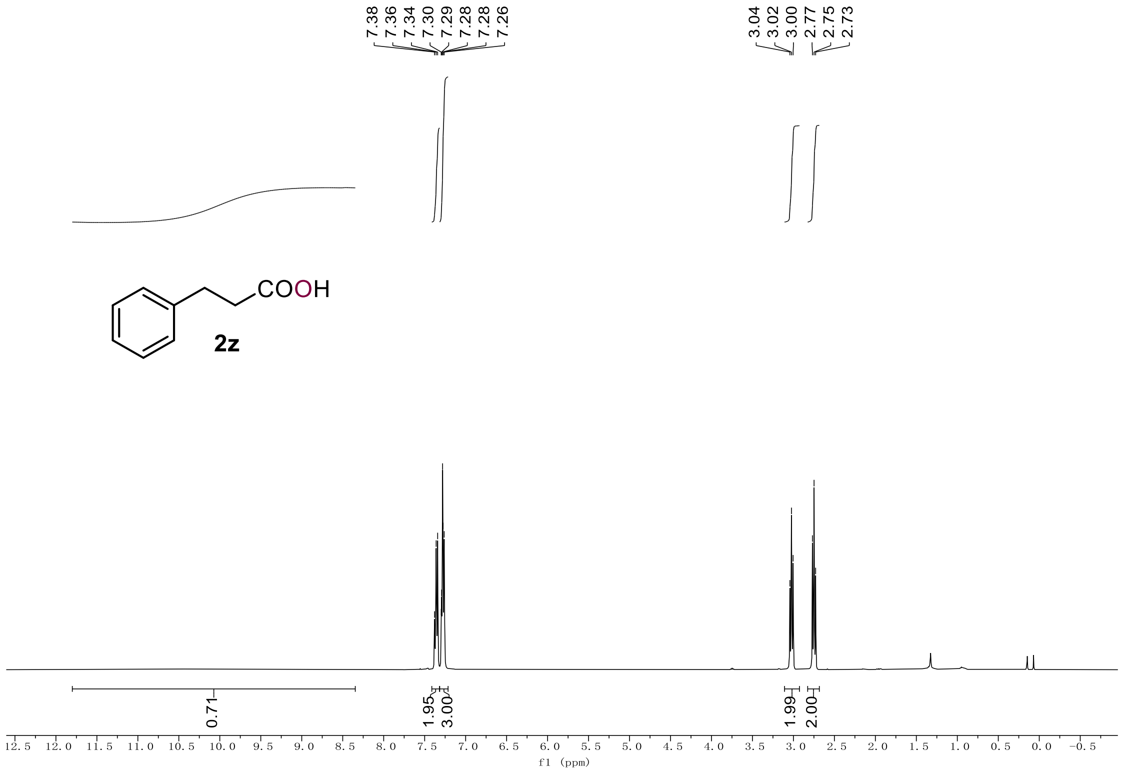
O
2y
f1 (ppm)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7.28
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7.26
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COOH
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3.00
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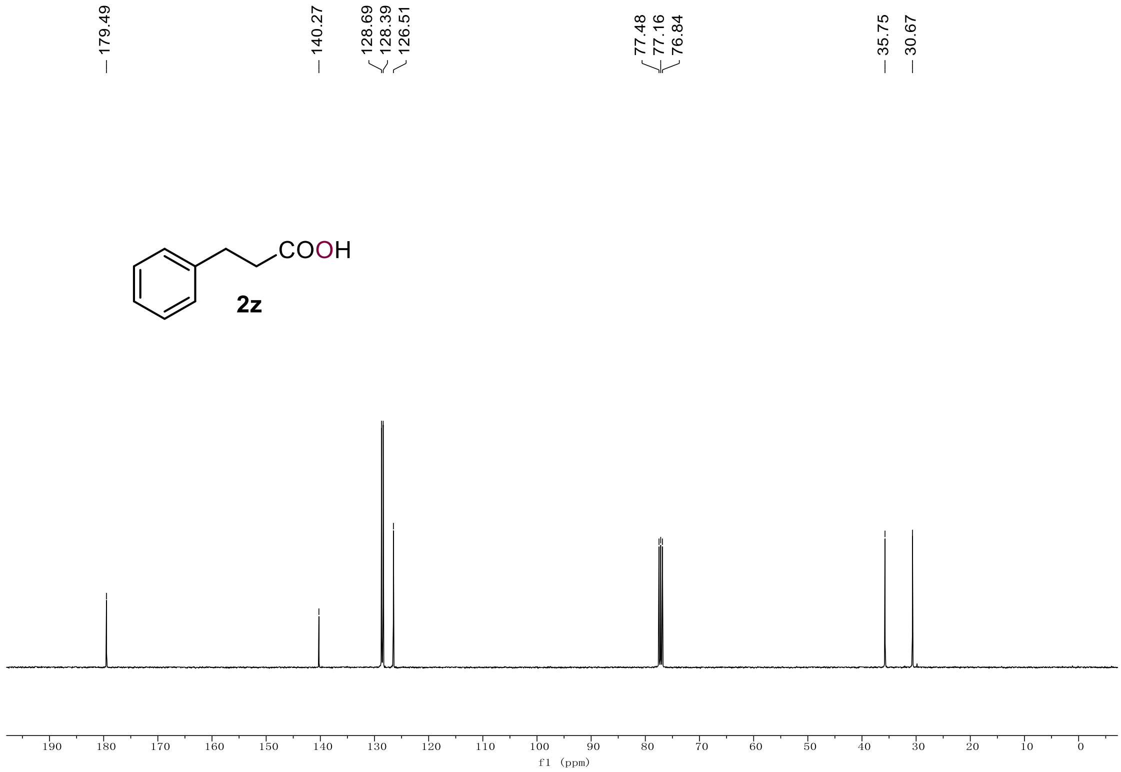
2.00
f1 (ppm)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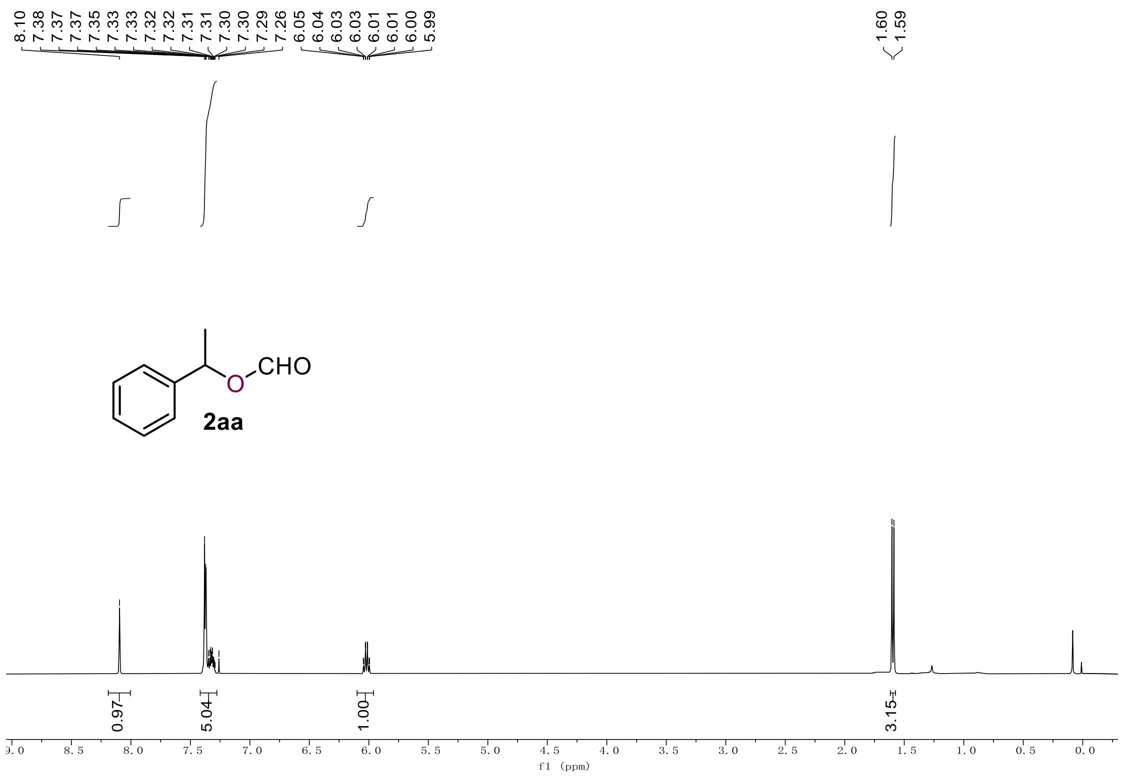
2z
f1 (ppm)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1.60 1.59
CHO
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1.00
3.15
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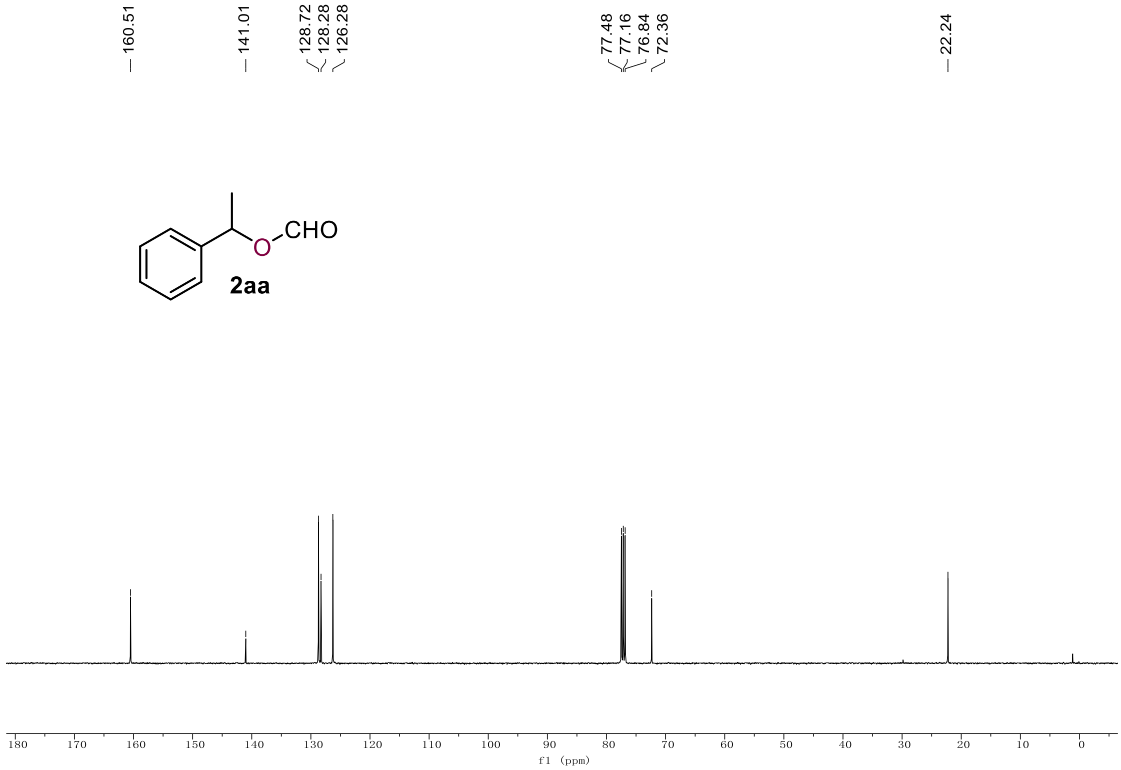
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22.24
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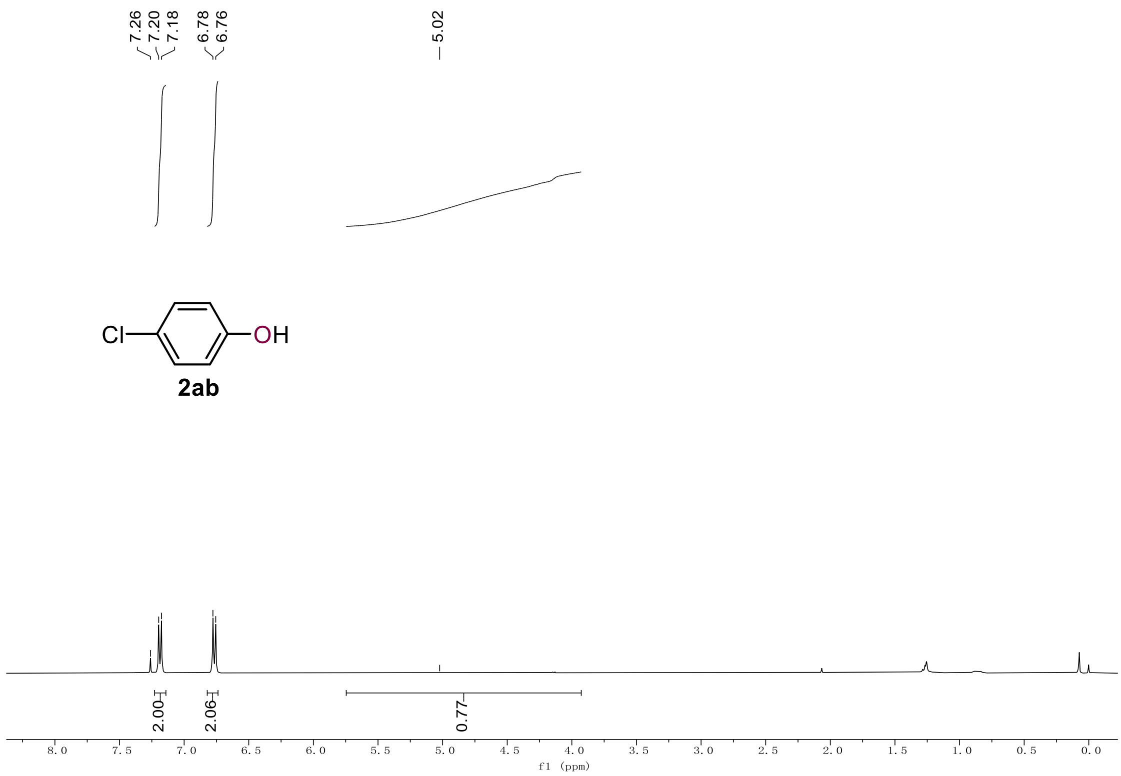
f1 (ppm)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7.20
7.18
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6.76
5.02
Cl
OH
2ab
2.00
2.06
0.77
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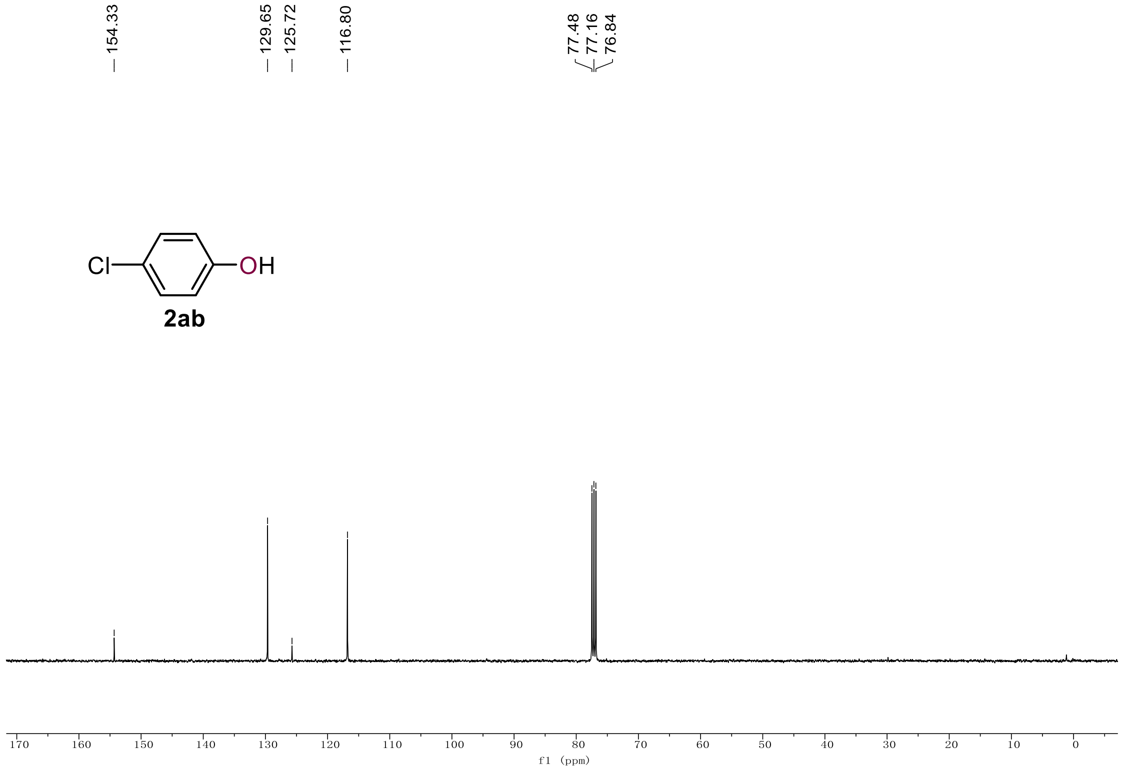
f1 (ppm)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Cl
OH
2ab
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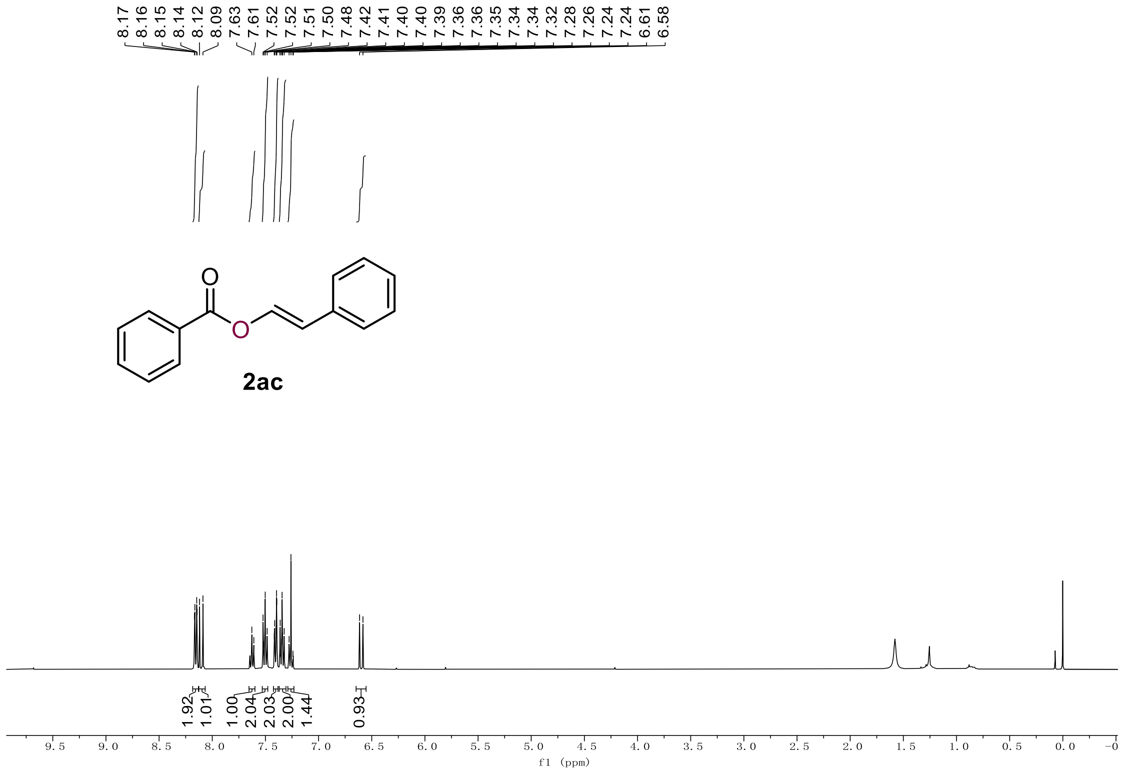
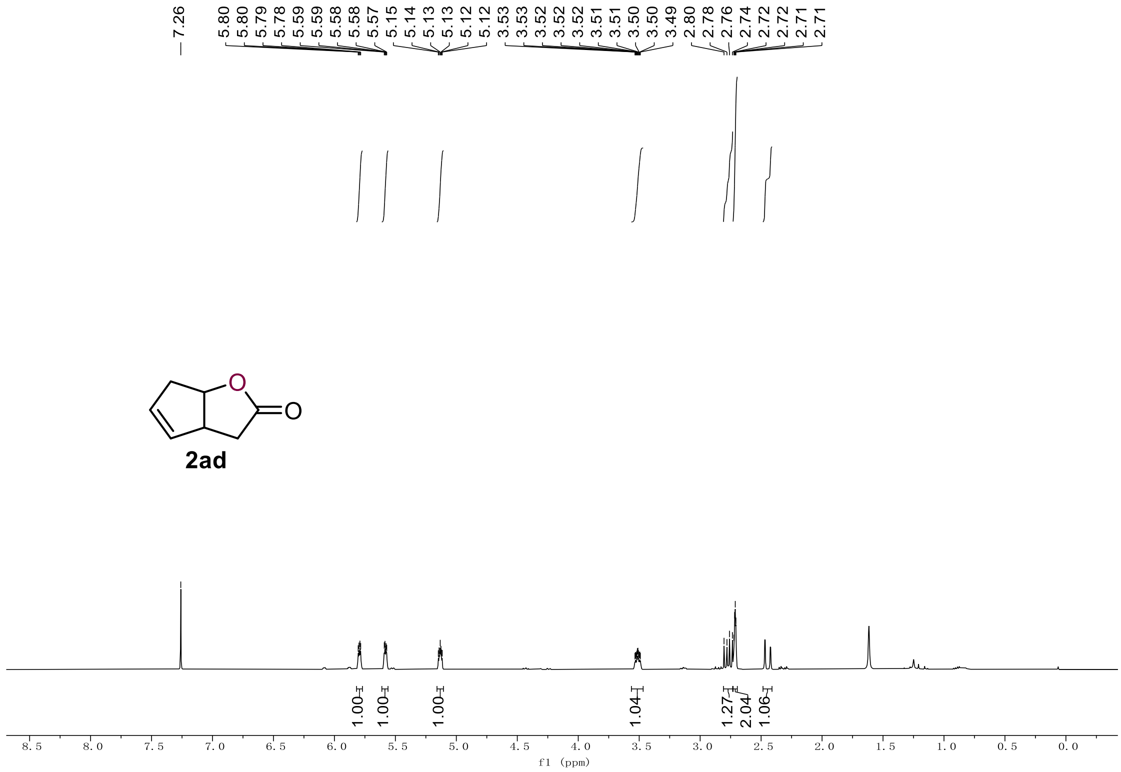
f1 (ppm)


2ac
f1 (ppm)


2ac
f1 (ppm)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2.74
2.72
2.72
2.71
2.71
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1.00
1.00
1.00
1.04
1.27
2.04
1.06
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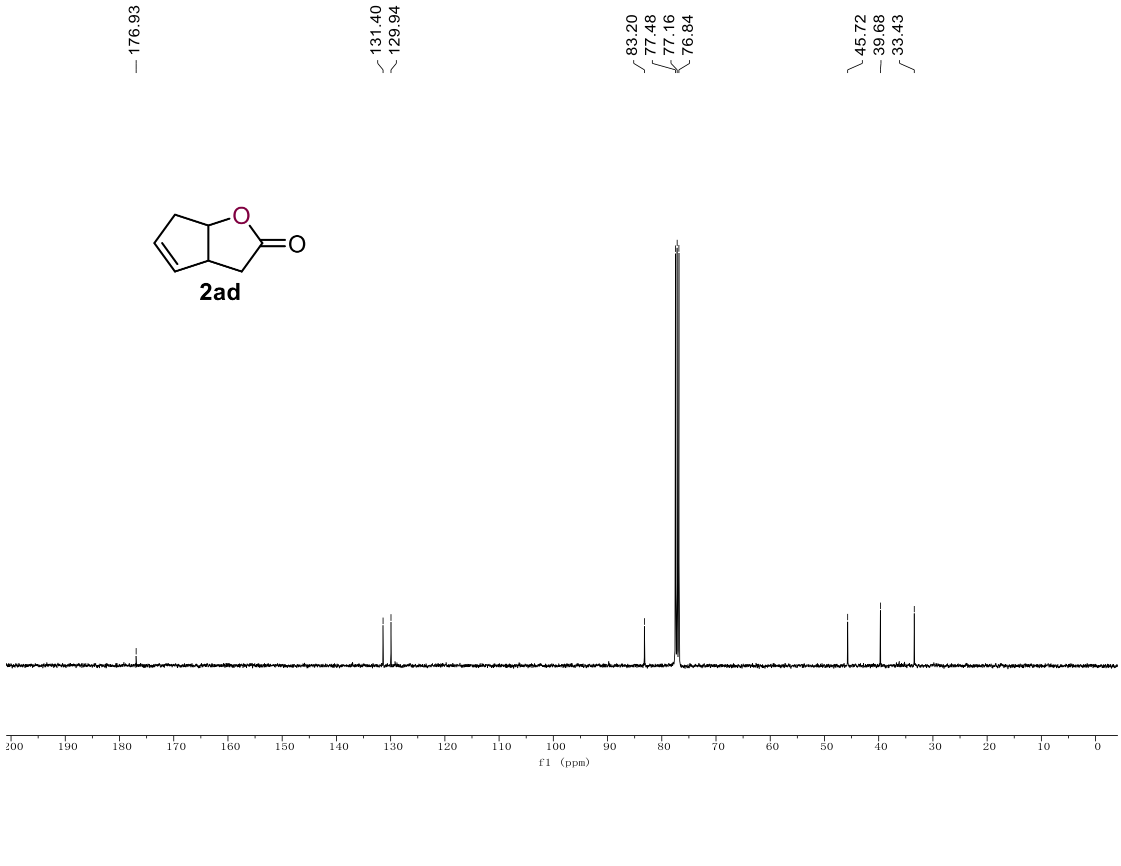
f1 (ppm)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33.43
2ad
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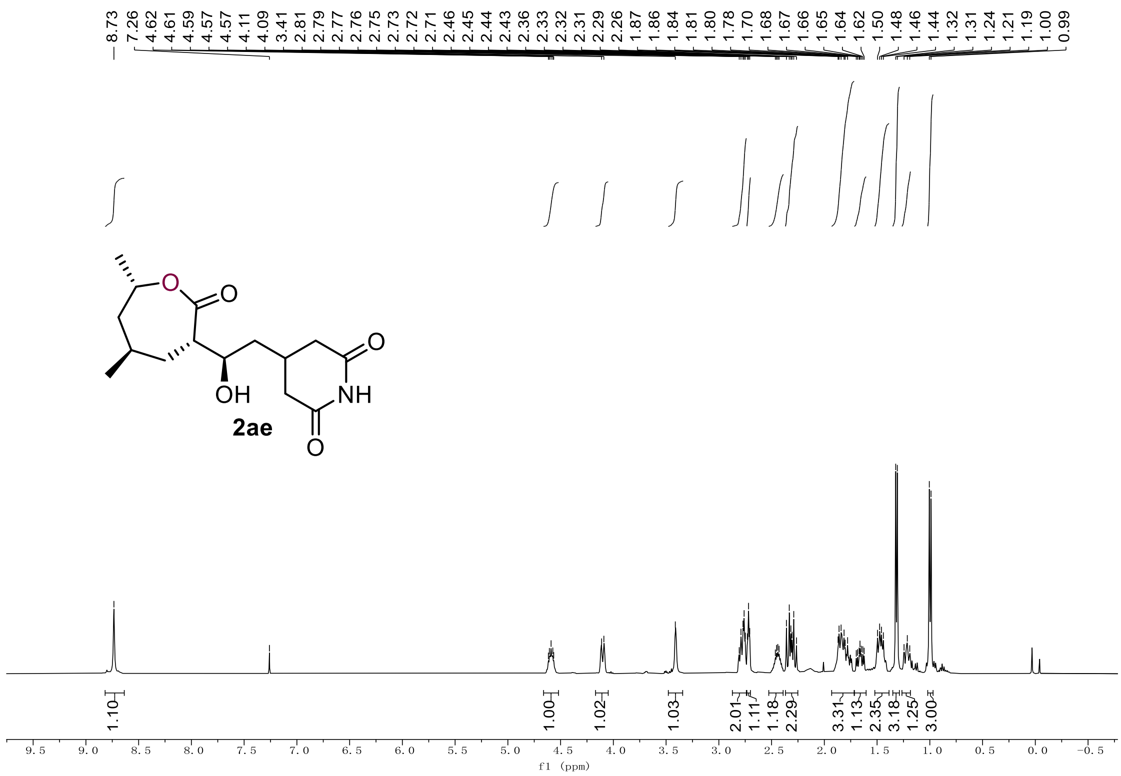
f1 (ppm)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2.77
2.76
2.75
2.73
2.72
2.71
2.46
2.45
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1.80
1.78
1.70
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1.67
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1.64
1.62
1.50
1.48
1.46
1.44
1.32
1.31
1.24
1.21
1.19
1.00
0.99
O
O
OH
O
NH
O
2ae
1.10
1.00
1.02
1.03
2.01
1.11
1.18
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3.31
1.13
2.35
3.18
1.25
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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3.0
2.5
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0.5
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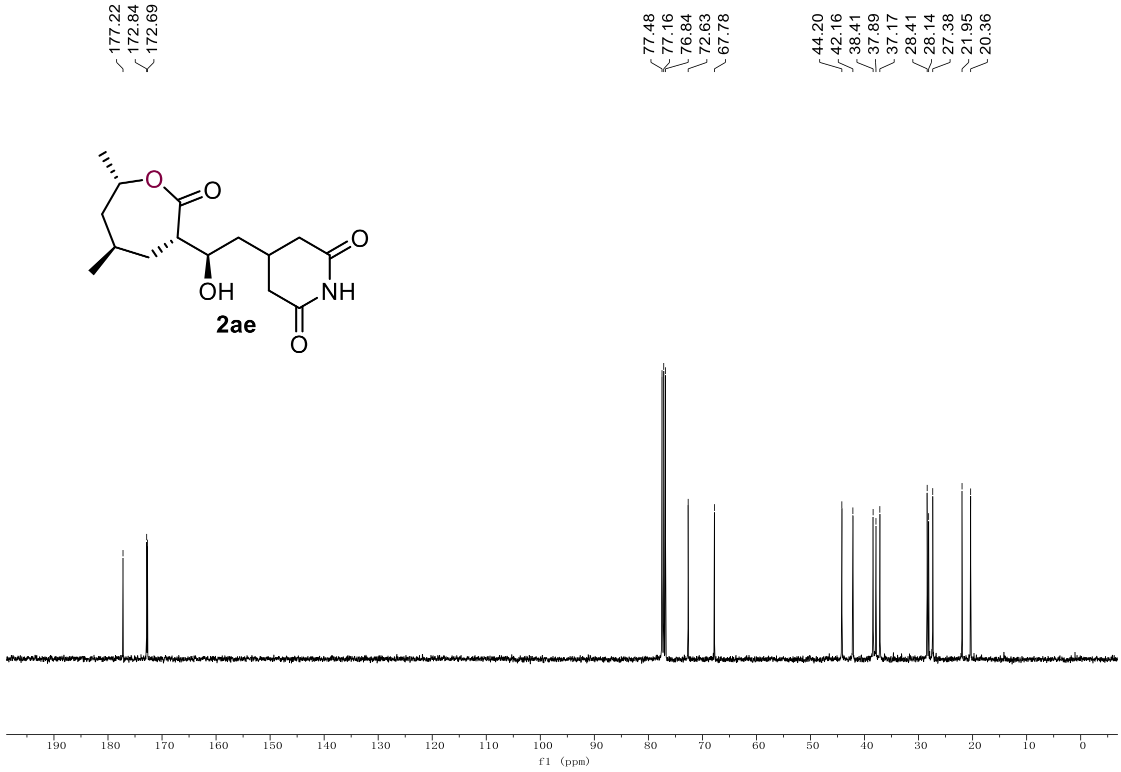
-0.5
f1 (ppm)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67.78
44.20
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38.41
37.89
37.17
28.41
28.14
27.38
21.95
20.36
O
O
OH
O
NH
O
2ae
190
180
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40
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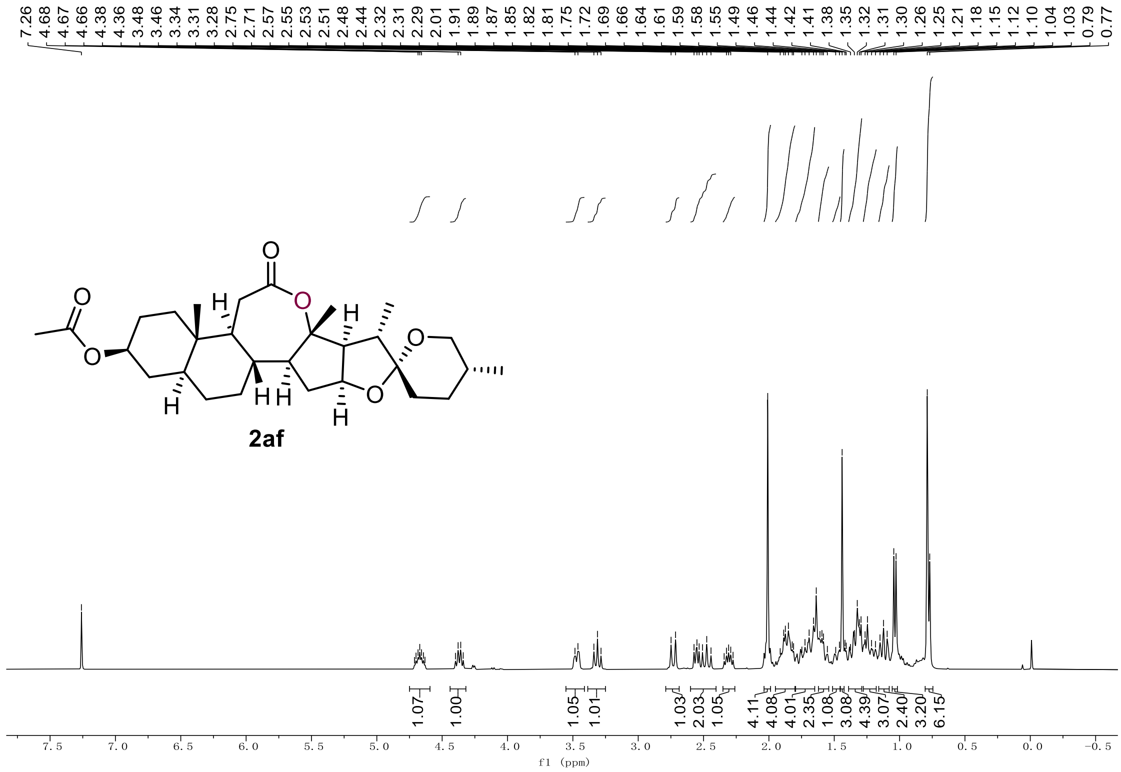
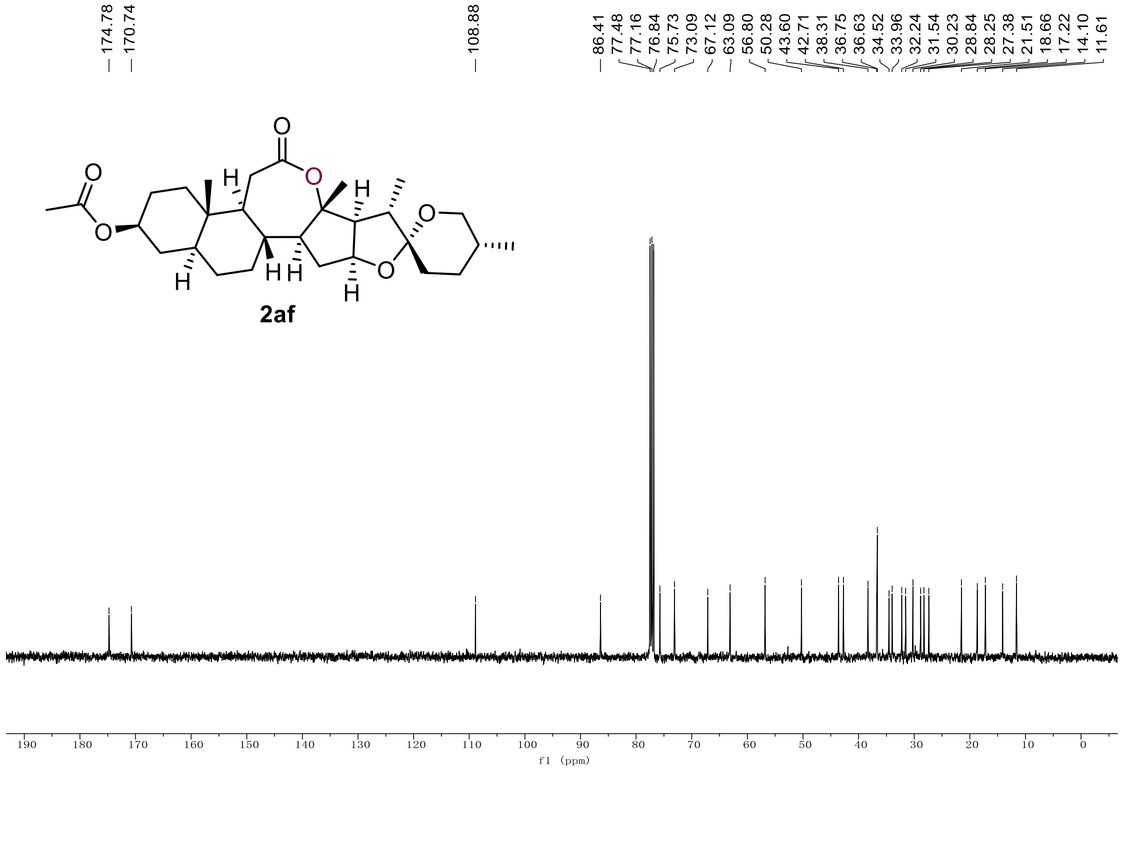
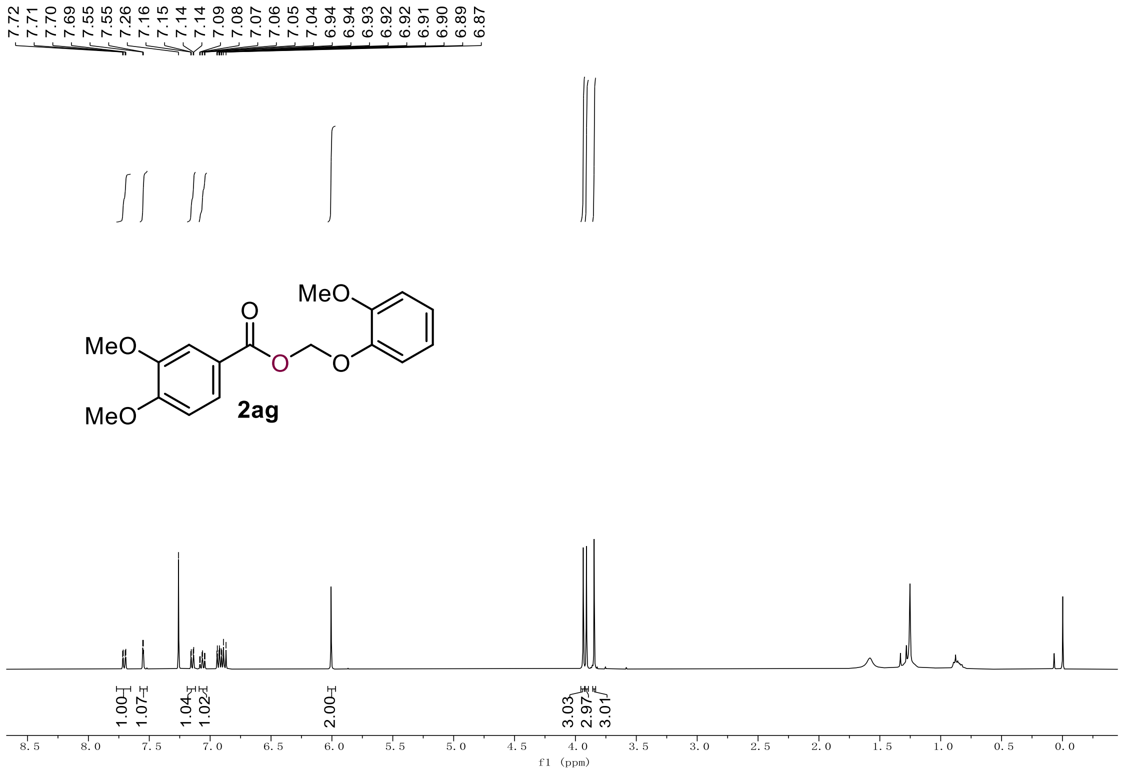
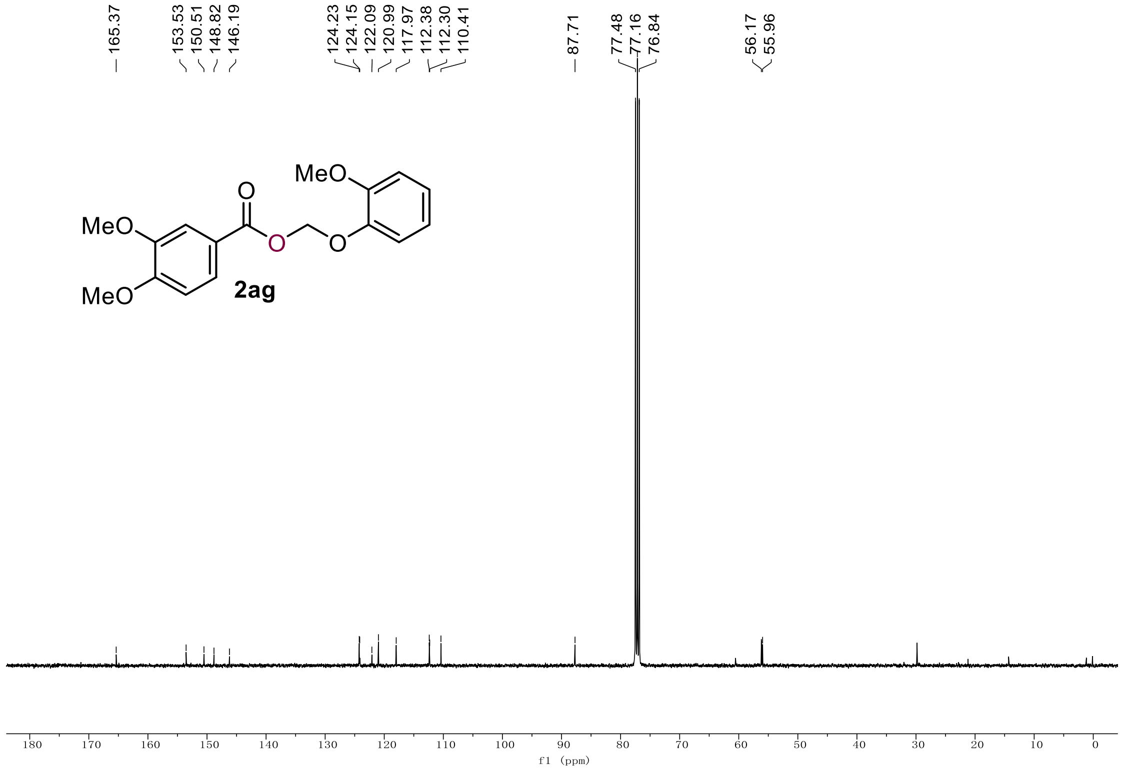
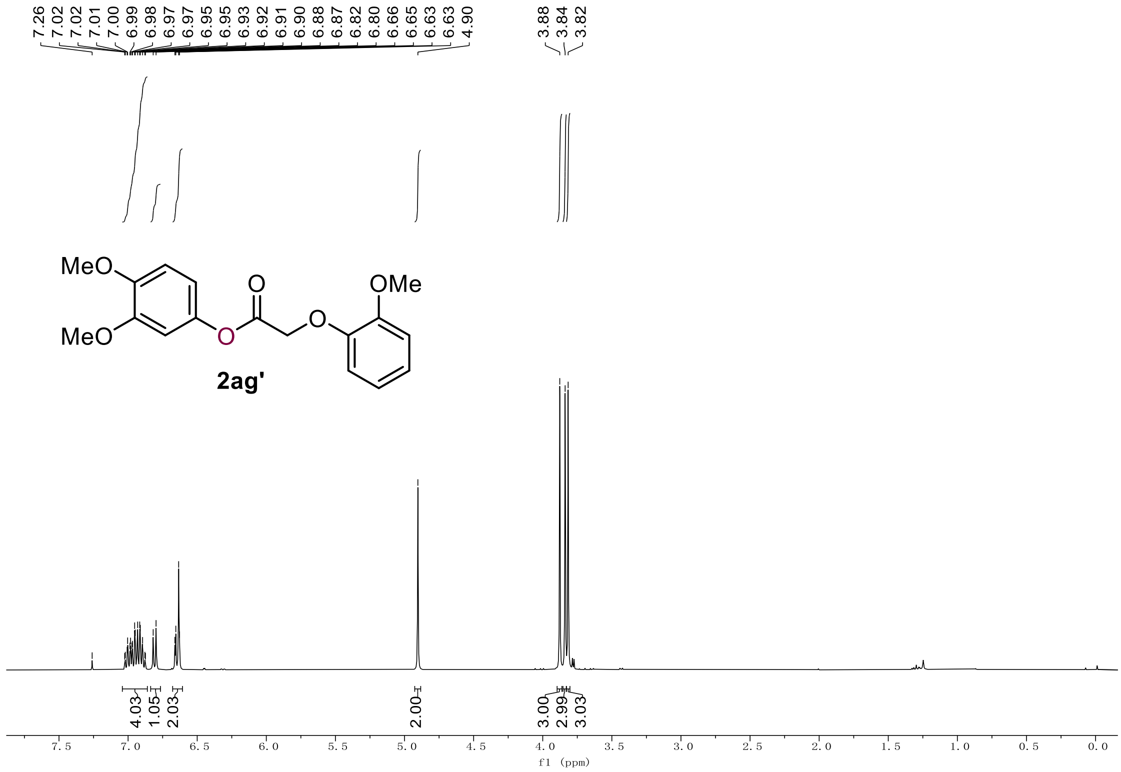
f1 (ppm)


7.26 4.68 4.67 4.66 4.38 4.36 3.48 3.46 3.34 3.31 3.28 2.75 2.71 2.57 2.55 2.53 2.51 2.48 2.44 2.32 2.31 2.29 2.01 1.91 1.89 1.87 1.85 1.82 1.81 1.75 1.72 1.69 1.66 1.64 1.61 1.59 1.58 1.55 1.49 1.46 1.44 1.42 1.41 1.38 1.35 1.32 1.31 1.30 1.26 1.25 1.21 1.18 1.15 1.12 1.10 1.04 1.03 0.79 0.77
2af
1.07 1.00 1.05 1.01 1.03 2.03 1.05 4.11 4.08 4.01 2.35 1.08 3.08 4.39 3.07 2.40 3.20 6.15
f1 (ppm)

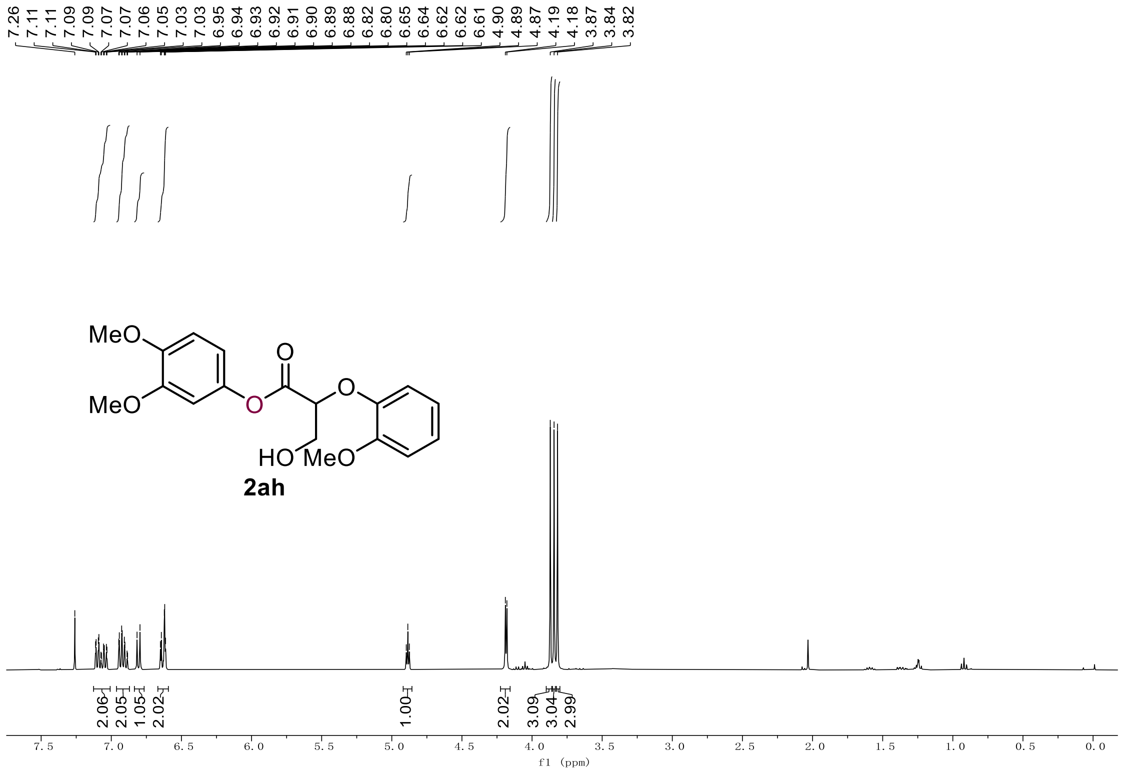

174.78 170.74 108.88 86.41 77.48 77.16 76.84 75.73 73.09 67.12 63.09 56.80 50.28 43.60 42.71 38.31 36.75 36.63 34.52 33.96 32.24 31.54 30.23 28.84 28.25 27.38 21.51 18.66 17.22 14.10 11.61
2af
f1 (ppm)

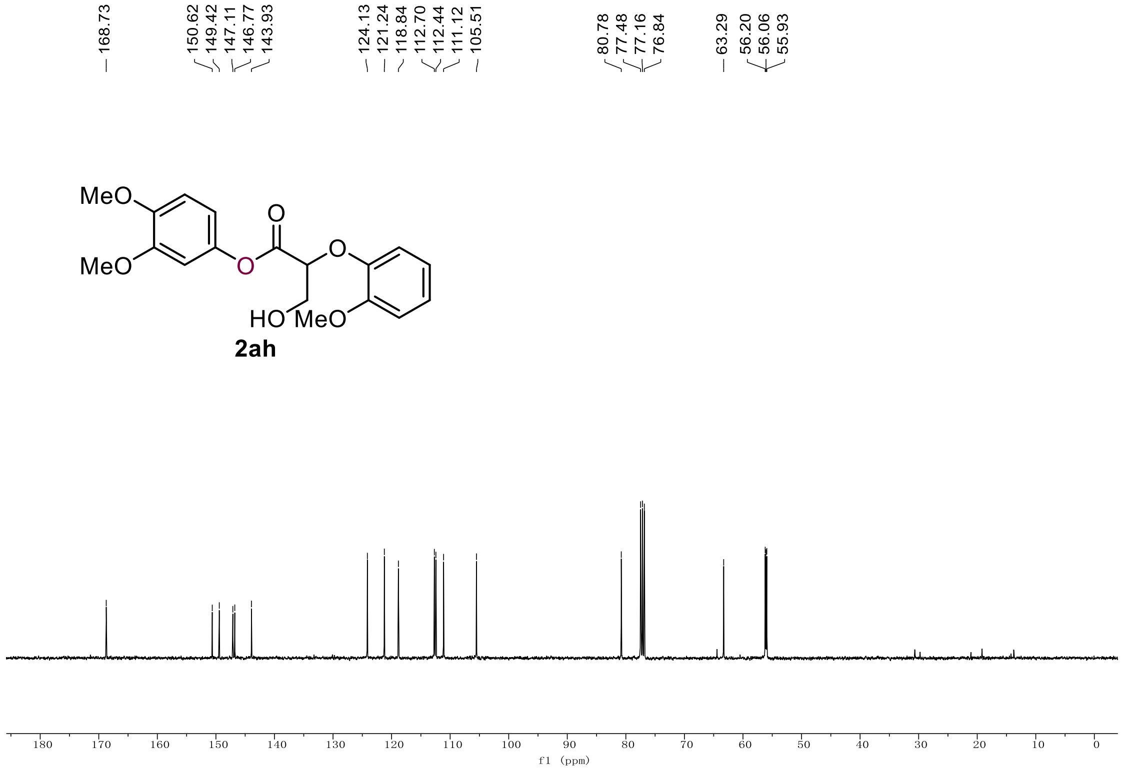

7.72 7.71 7.70 7.69 7.55 7.55 7.26 7.16 7.15 7.14 7.14 7.09 7.08 7.07 7.06 7.05 7.04 6.94 6.93 6.92 6.92 6.91 6.90 6.89 6.87
MeO
O
MeO
MeO
O
O
2ag
1.00
1.07
1.04
1.02
2.00
3.03
2.97
3.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

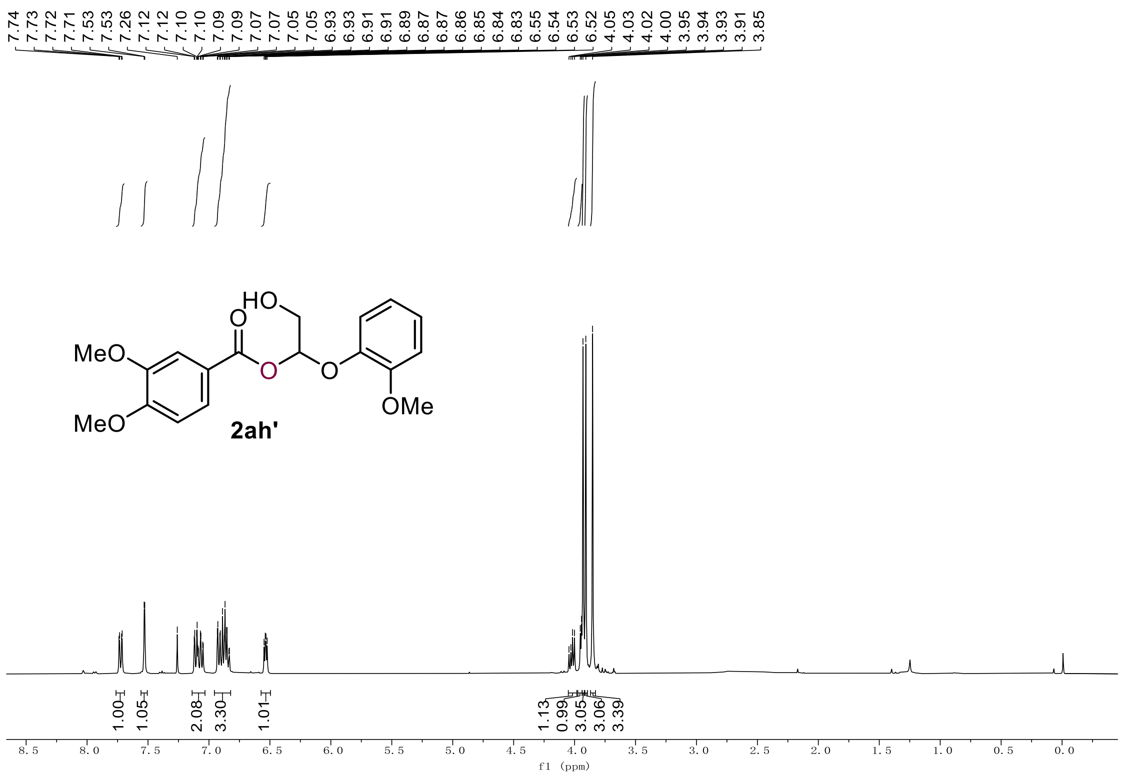

165.37
153.53 150.51 148.82 146.19
124.23 124.15 122.09 120.99 117.97 112.38 112.30 110.41
87.71
77.48 77.16 76.84
56.17 55.96
MeO
O
MeO
MeO
O
O
2ag
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

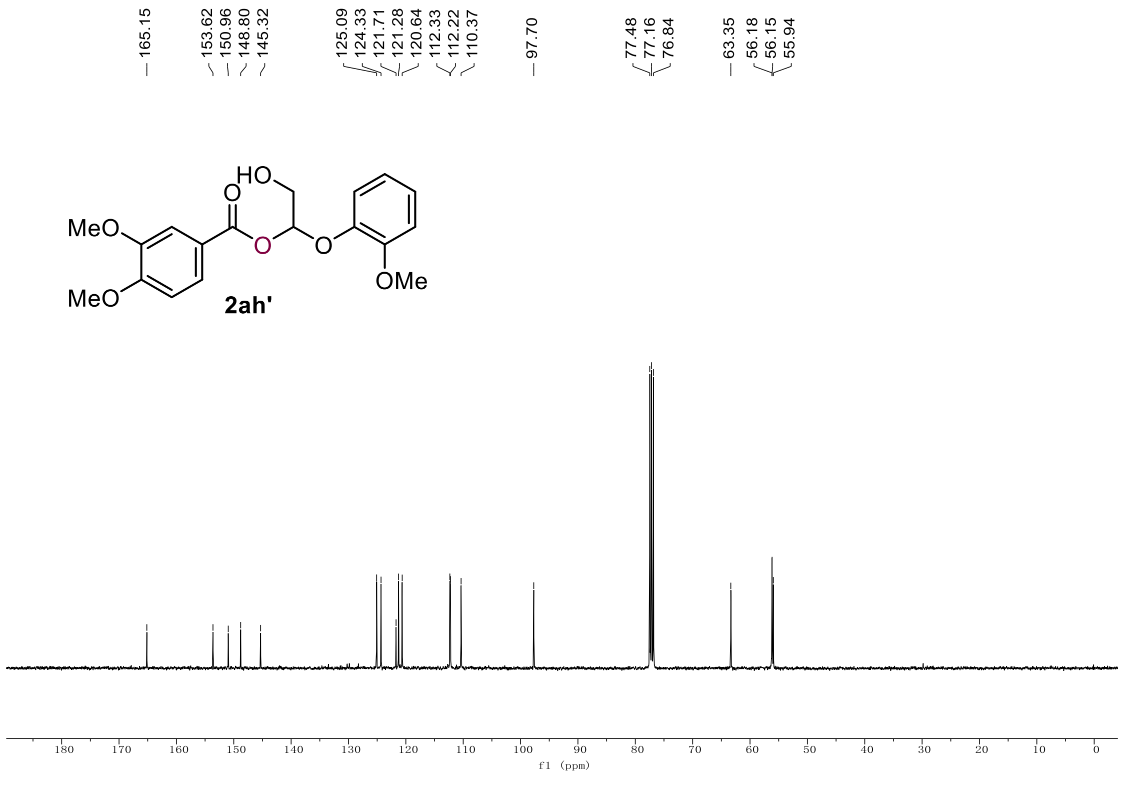

7.26
7.02
7.02
7.01
7.00
6.99
6.98
6.97
6.97
6.95
6.95
6.93
6.92
6.91
6.90
6.88
6.87
6.82
6.80
6.66
6.65
6.63
6.63
4.90
3.88
3.84
3.82
MeO
MeO
O
O
O
OMe
2ag'
4.03
1.05
2.03
2.00
3.00
2.99
3.03
f1 (ppm)

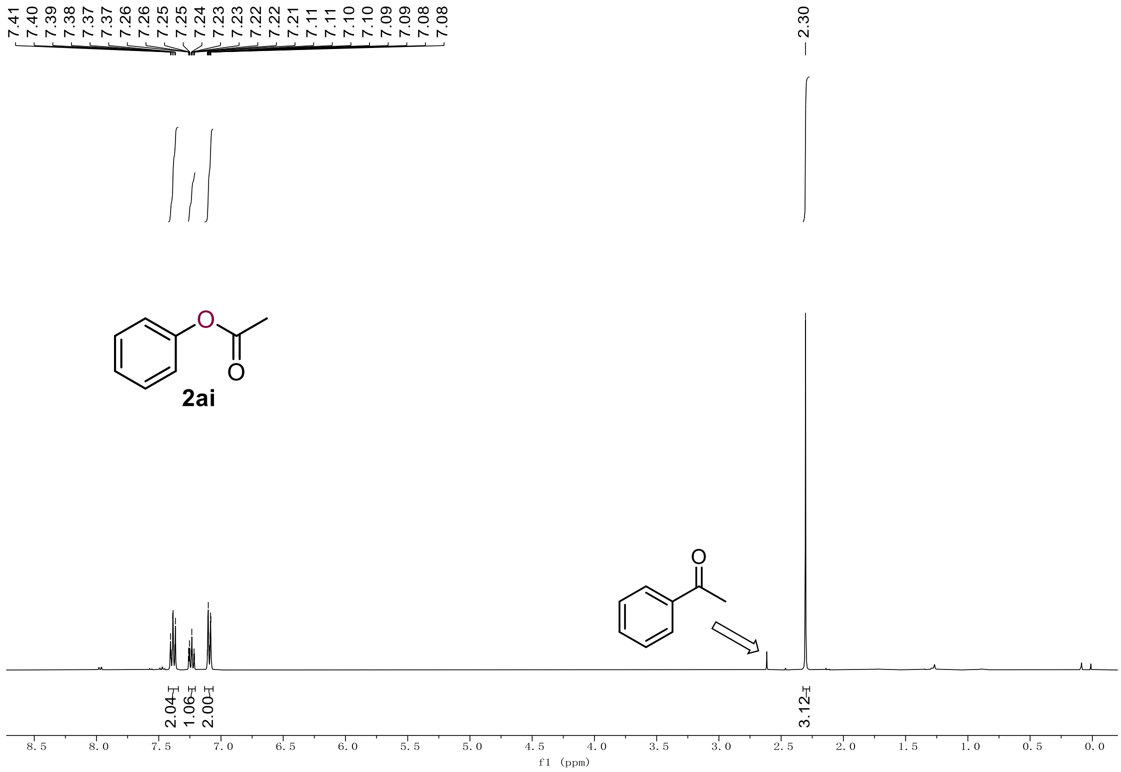

168.06
149.85
149.36
147.14
147.04
143.75
122.98
120.80
115.09
112.62
112.27
111.09
105.44
77.48
77.16
76.84
66.73
56.15
55.99
55.90
MeO
MeO
O
O
O
OMe
2ag'
f1 (ppm)

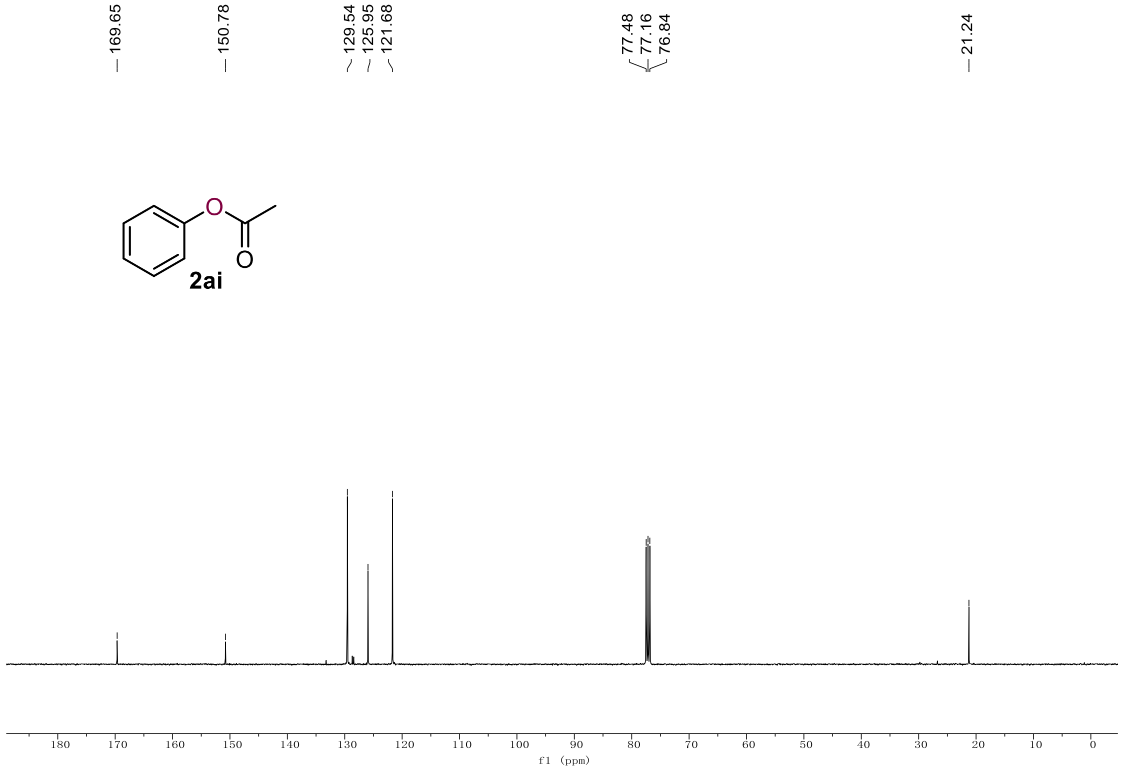

7.26
7.11
7.11
7.09
7.09
7.07
7.07
7.06
7.05
7.03
7.03
6.95
6.94
6.93
6.92
6.91
6.90
6.89
6.88
6.82
6.80
6.65
6.64
6.62
6.62
6.61
4.90
4.89
4.87
4.19
4.18
3.87
3.84
3.82
MeO
MeO
O
O
O
HO
MeO
2ah
2.06
2.05
1.05
2.02
1.00
2.02
3.09
3.04
2.99
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

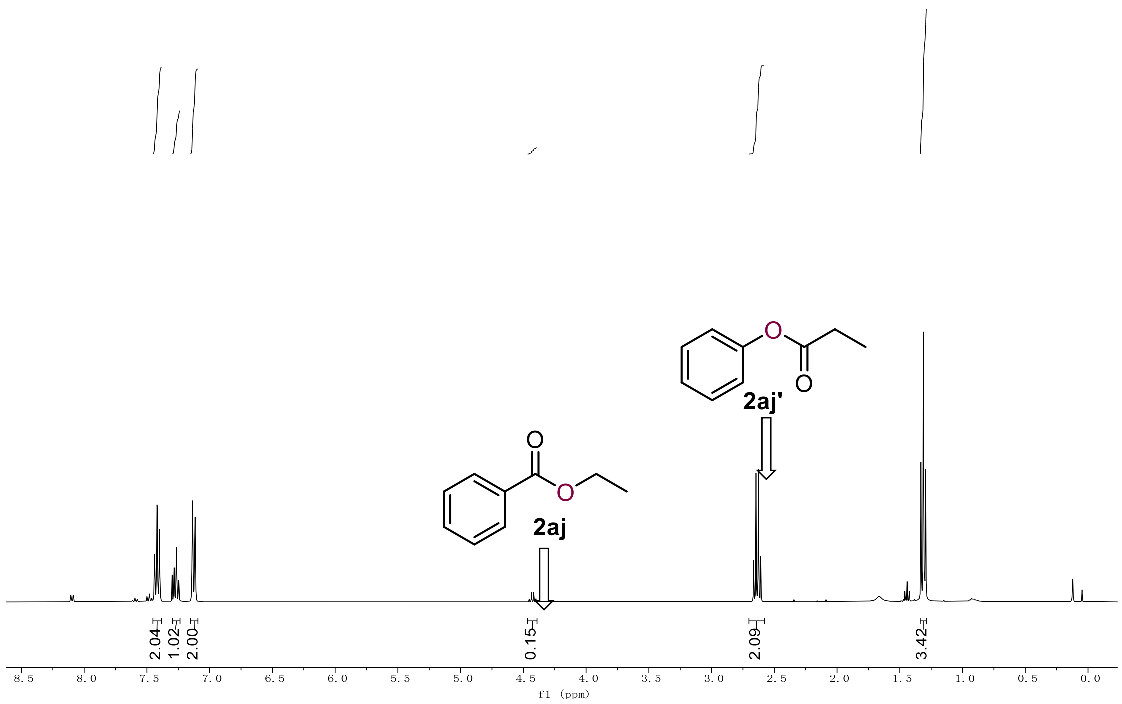

168.73
150.62
149.42
147.11
146.77
143.93
124.13
121.24
118.84
112.70
112.44
111.12
105.51
80.78
77.48
77.16
76.84
63.29
56.20
56.06
55.93
MeO
MeO
O
O
O
HO
MeO
2ah
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

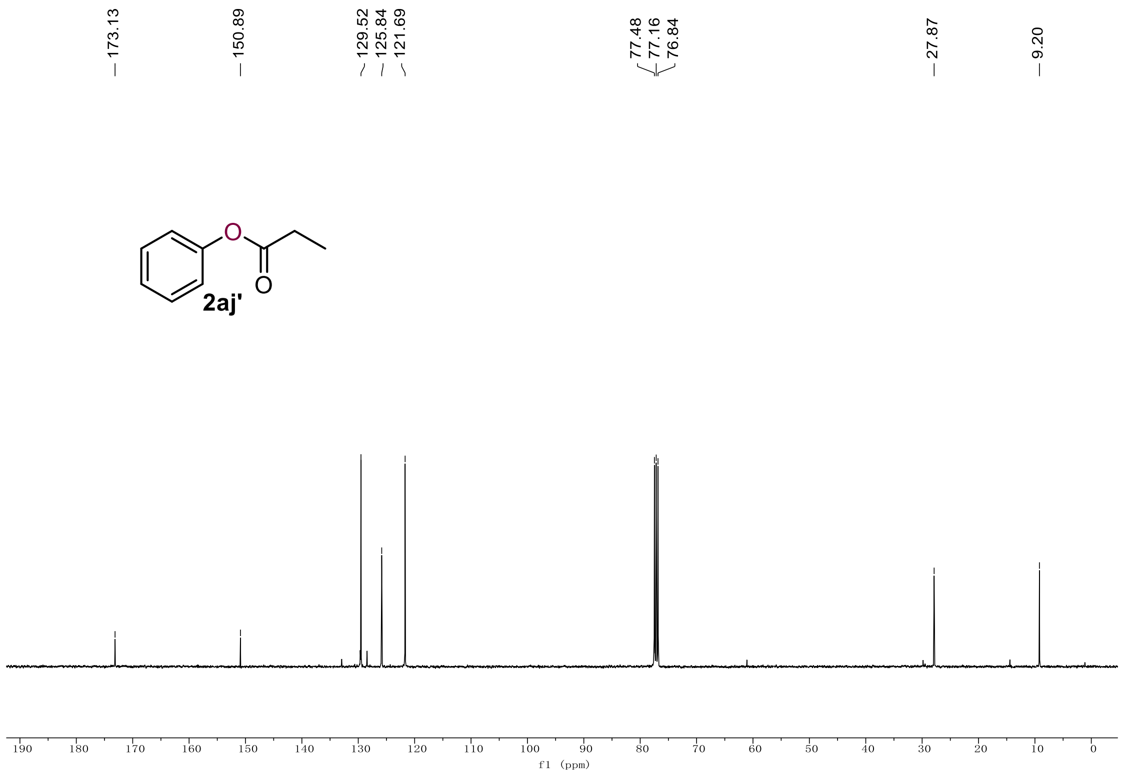


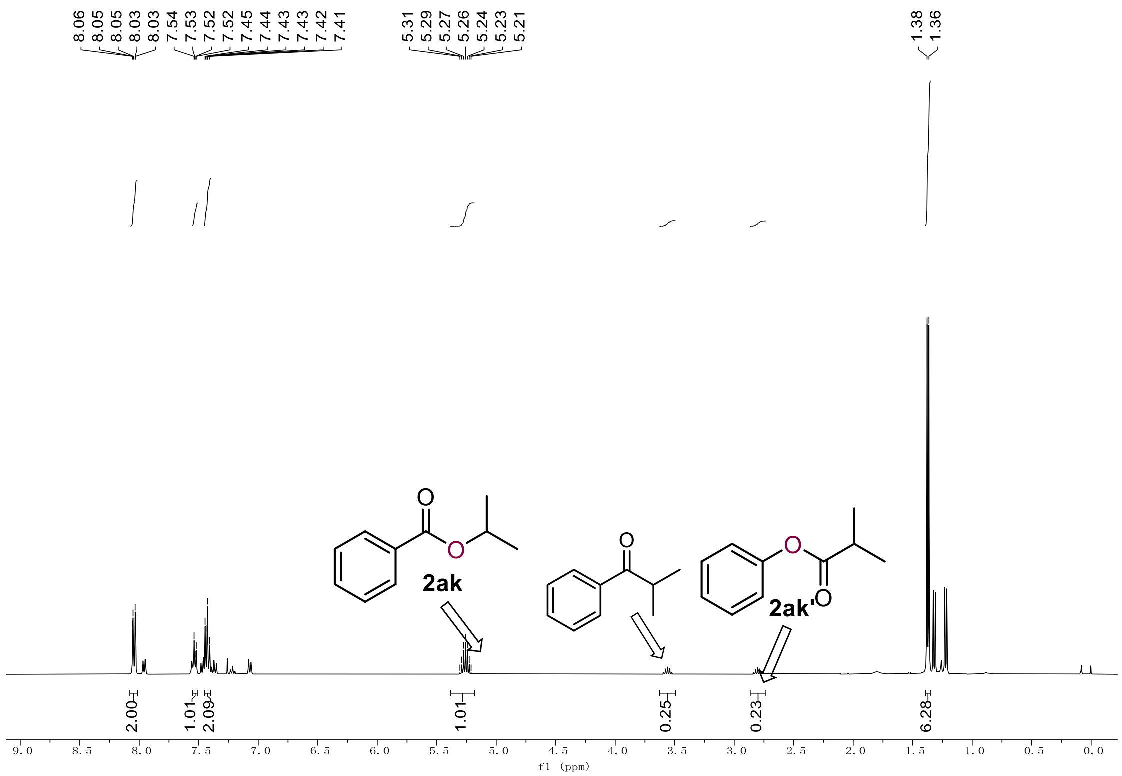


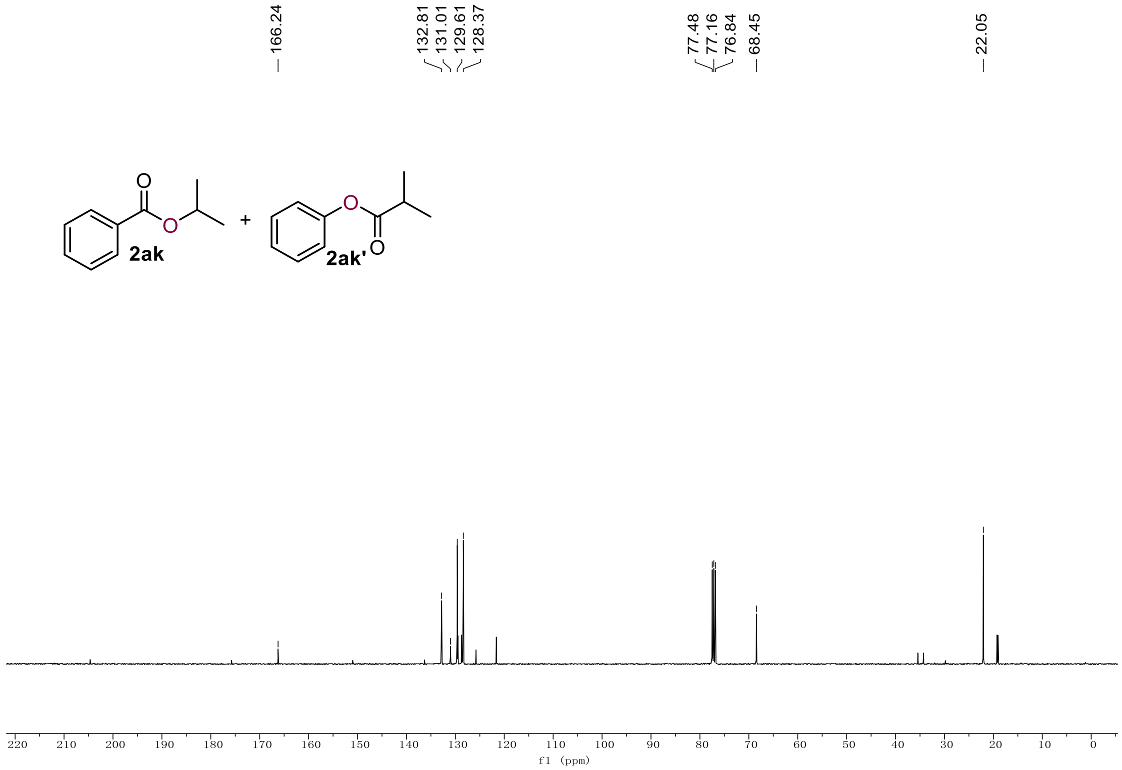

7.41 7.40 7.39 7.38 7.37 7.37 7.26 7.26 7.25 7.25 7.24 7.23 7.23 7.22 7.22 7.21 7.11 7.10 7.10 7.09 7.08 7.08
2.30
O
2ai
O
O
2.04
1.06
2.00
3.12
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

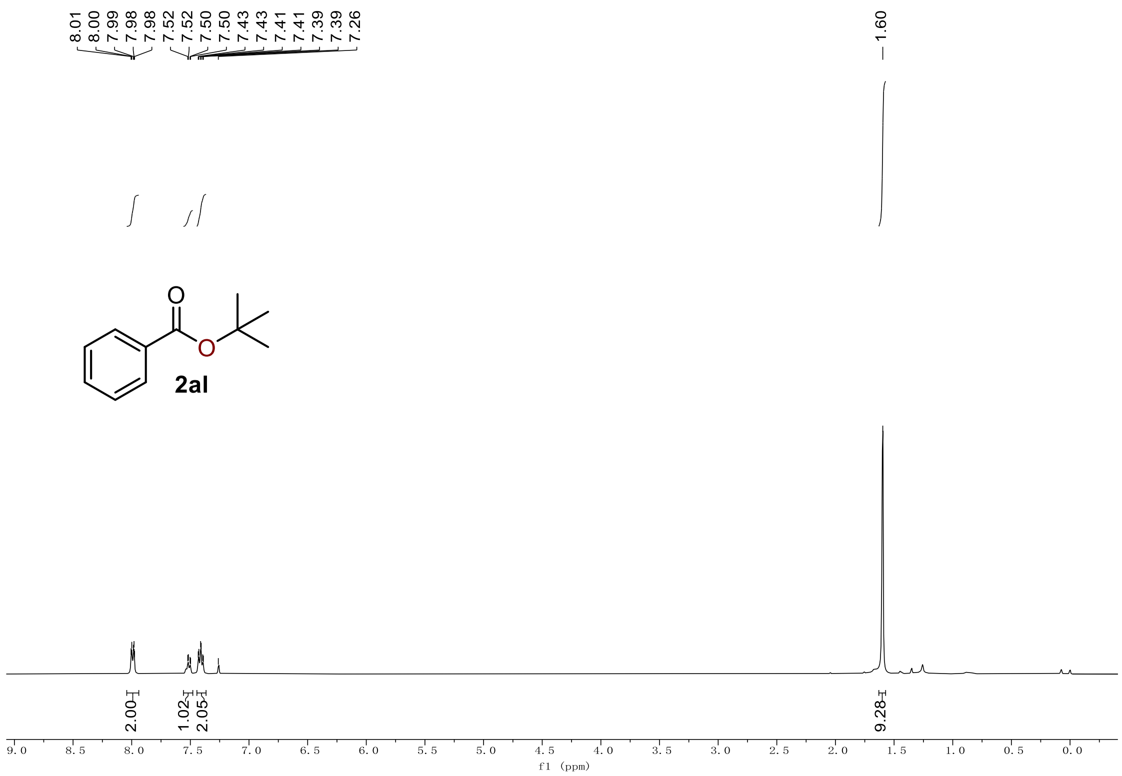

169.65
150.78
129.54 125.95 121.68
77.48 77.16 76.84
21.24
O
O
2ai
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

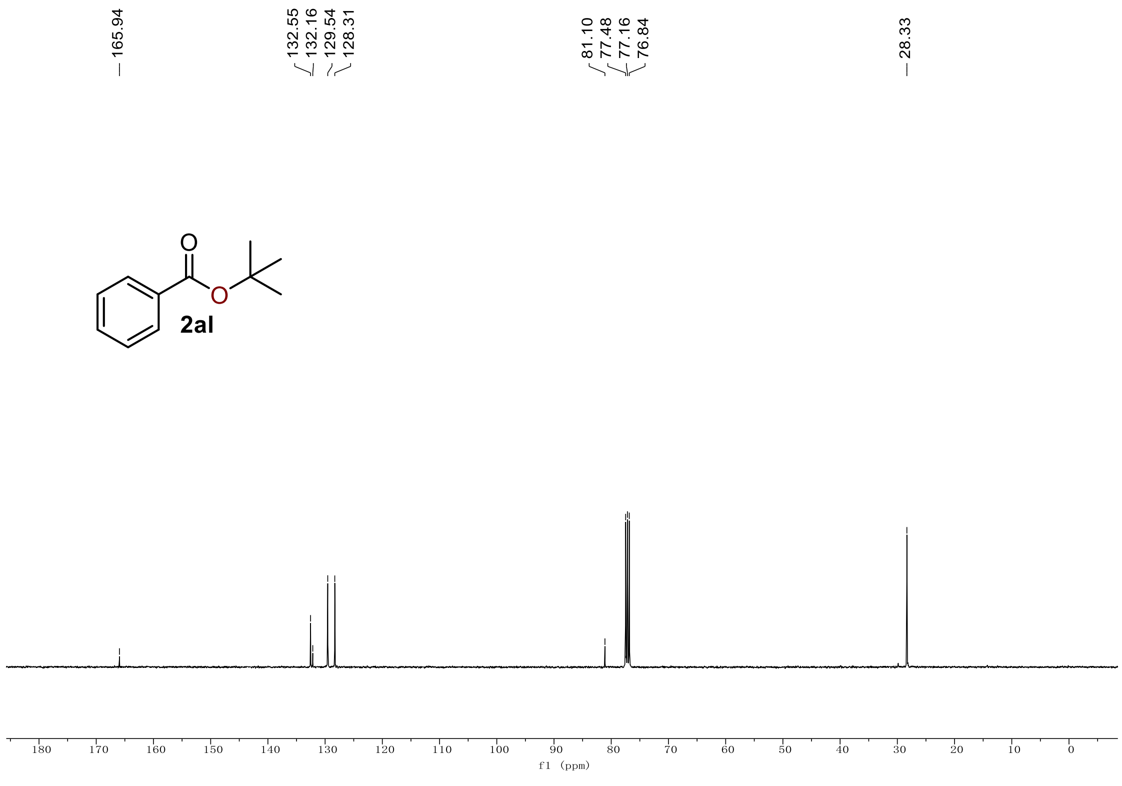

2aj'
2aj
2.04
1.02
2.00
0.15
2.09
3.42
f1 (ppm)


173.13
150.89
129.52
125.84
121.69
77.48
77.16
76.84
27.87
9.20
2aj'
f1 (ppm)


8.06 8.05 8.05 8.03 8.03 7.54 7.53 7.52 7.52 7.45 7.44 7.43 7.43 7.42 7.41
5.31 5.29 5.27 5.26 5.24 5.23 5.21
1.38 1.36
2ak
2ak'
2.00
1.01
2.09
1.01
0.25
0.23
6.28
f1 (ppm)


166.24
132.81 131.01 129.61 128.37
77.48 77.16 76.84 68.45
22.05
2ak
+
2ak'
f1 (ppm)


8.01
8.00
7.99
7.98
7.98
7.52
7.52
7.50
7.50
7.43
7.43
7.41
7.41
7.39
7.39
7.26
1.60
2al
2.00
1.02
2.05
9.28
f1 (ppm)


165.94
132.55
132.16
129.54
128.31
81.10
77.48
77.16
76.84
28.33
2al
f1 (ppm)