Supporting Information

A Sustainable Flow Synthesis of a Versatile Cyclopentenone Building Block

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1. Materials and Methods

Unless otherwise stated, all solvents were purchased from Fisher Scientific and used without further purification. Substrates and reagents were purchased from Alfa Aesar or Sigma Aldrich and used as received.

^{1}H-NMR spectra were recorded on a Bruker Avance-400 instrument and are reported relative to residual solvent: $CHCl_3$ (δ 7.26 ppm). ^{13}C-NMR spectra were recorded on the same instrument and are reported relative to $CHCl_3$ (δ 77.16 ppm). Data for ^{1}H-NMR are reported as follows: chemical shift (δ/ ppm) (integration, multiplicity, coupling constant (Hz)). Multiplicities are reported as follows: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet, br. s = broad singlet, app = apparent. Data for ^{13}C-NMR are reported in terms of chemical shift (δ/ ppm) and multiplicity (C, CH, CH_2 or CH_3). DEPT-135, COSY, HSQC, HMBC and NOESY experiments were used in the structural assignment.

IR spectra were obtained by use of a Perkin Elmer RX1 spectrometer (neat, ATR sampling) with the intensities of the characteristic signals being reported as weak (w, <20% of tallest signal), medium (m, 21-70% of tallest signal) or strong (s, >71% of tallest signal).

Low and high resolution mass spectrometry was performed using the indicated techniques on either Waters LCT Premier XE or Waters TQD instruments equipped with Acquity UPLC and a lock-mass electrospray ion source. For accurate mass data the deviation from the calculated formula is reported.

Flow chemistry experiments were performed with a Vapourtec E-series system using set-ups as described in this article.

Microwave reactions were performed in a Biotage Initiator+ within 20 mL septum sealed vials containing the reagents and a Biotage microwave magnetic stirrer bar. No pre-stirring was set and reaction timing was commenced when the solution reached the specified reaction temperature.

2. Experimental Procedures

2.1 Microwave optimisation reactions: Transformation of compound **3** to **4**.

Two thermal methods (direct and indirect) catalysed by the Lewis acid $ZnCl_2$ were evaluated.

Direct route:

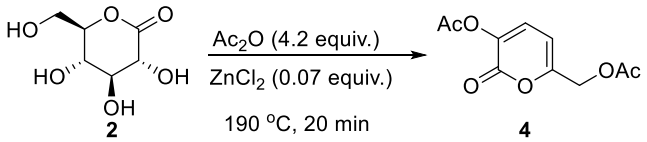
General procedure: To a 5 mL microwave via was added *D*-glucono-1,5-lactone (0.445 g, 2.8 mmol), acetic anhydride (1.0 mL, 10.5 mmol) and the acid component (0.1 mmol). 18-crown-6 (0.550 g) was added as an internal standard for assessment of conversion. The reaction was heated under microwave irradiation for X minutes at Y °C. A sample was taken for crude ^{1}H-NMR analysis selected results are tabulated in Table S1.

Table S1:

Entry	Lewis Acid additive	Time (min)	Temperature (°C)	Conversion to **4**
1	$Zn(OAc)_2$	30	150	17
2	$BF_3.Et_2O$	30	150	23
3	$BF_3.Et_2O$	15	170	28
4	$BF_3.Et_2O$	15	190	25
5	SiO_2-H_2SO_4	30	150	9
6	Titanium (IV) chloride	30	150	21
7	Titanium (IV) chloride	15	190	58 (38)
8	Tin(II) chloride	30	150	18
9	Tin(II) chloride	15	190	77 (45)
10	Iron(III) bromide	30	150	25
11	Iron(III) chloride	30	150	21
12	Iron(III) chloride	15	190	48 (42)
13	Iron(III) chloride	30	190	89 (60)
14	Aluminium chloride	30	150	34
15	Sulfuric acid	30	150	18
16	Hydrochloride acid	30	150	7
17	Zinc(II) chloride	30	150	58
18	Zinc(II) chloride	20	160	61
19	Zinc(II) chloride	20	170	78 (58)
20	Zinc(II) chloride	20	190	96 (73)
21	None	20	190	54

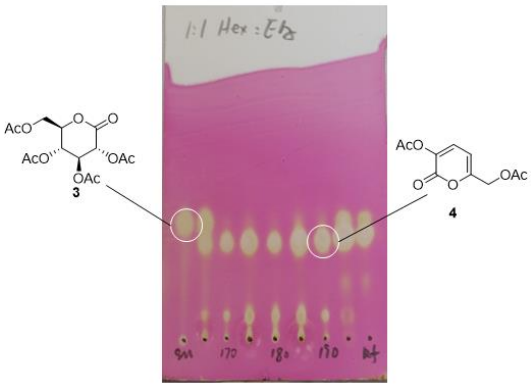
*Number in parentheses indicate isolated yield following chromatographic purification.

Optimized conditions using $ZnCl_2$ direct route:

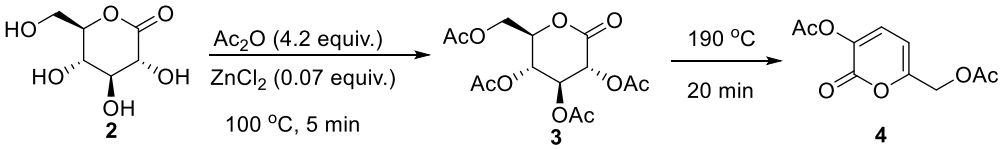


To a 5 mL microwave vial was added *D*-glucono-1,5-lactone (0.445 g, 2.8 mmol), acetic anhydride (1.0 mL, 10.5 mmol) and anhydrous $ZnCl_2$ (0.076 g, 0.07 mmol). The reaction was heated under microwave irradiation for 20 minutes at 190 °C. The crude reaction was diluted with EtOAc (20 mL) and extracted with water (20 mL) and washed with sat. aqu. sodium

hydrogen carbonate (2 × 15 mL). The organic phase was dried over anhydrous sodium sulfate. The solvent was removed by rotary evaporation and the compound purified by column chromatography (1:1 EtOAc/Hexane – visualization via $KMnO_4$ stain).

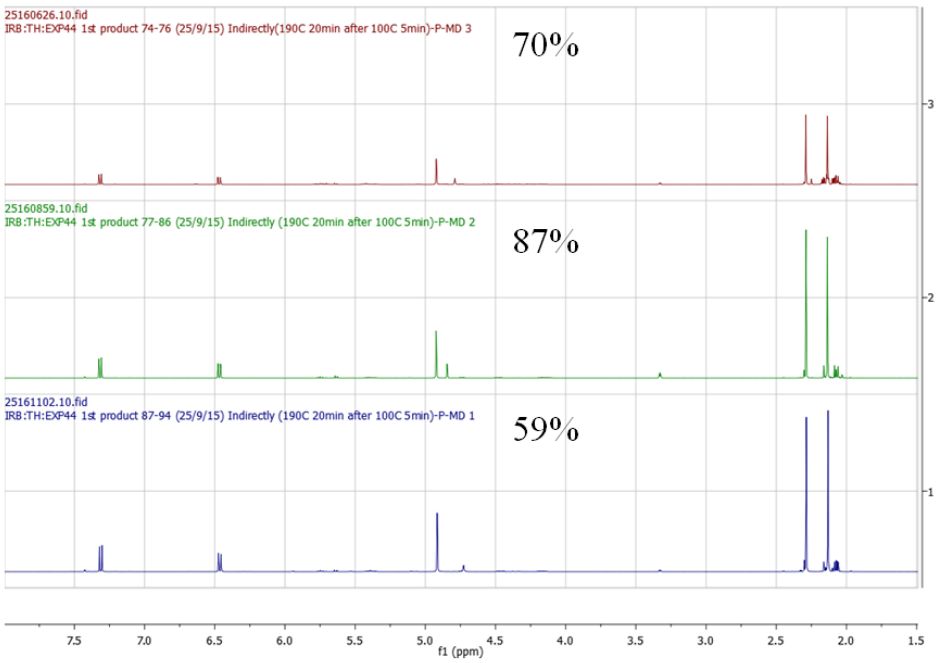


Indirect route:

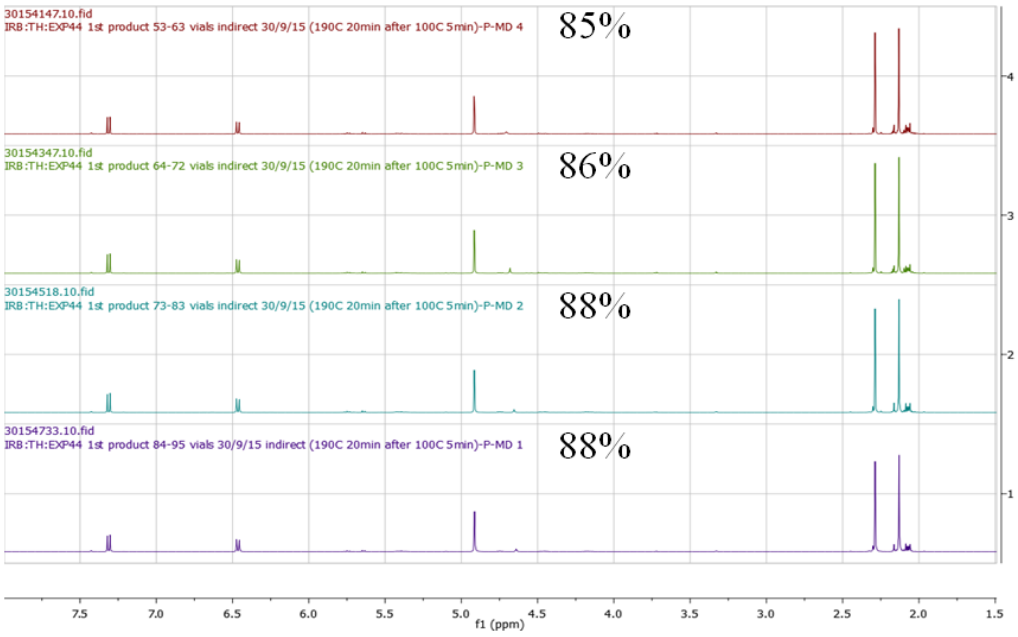


To a 5 mL microwave vial was added *D*-glucono-1,5-lactone (0.445 g, 2.8 mmol), acetic anhydride (1.0 mL, 10.5 mmol) and anhydrous $ZnCl_2$ (0.076 g, 0.07 mmol). The reaction was heated under microwave irradiation for 5 minutes at 100 °C and then at 190 °C for 20 min. The crude reaction was diluted with toluene (20 mL) and the mixture rotary evaporated to remove the solvent. The reaction was placed upon the high vacuum to remove residual acetic acid and then diluted with EtOAc (20 mL) before activated charcoal (1 g) was added. The crude material was filter over celite and the solvent removed using a rotary evaporator. The crude product was analyzed by ^{1}H NMR (see below with indicated crude mass yields).

Three examples are shown indicating the quality of material but also the variable recovery achieved.



Recovery was more consistent if the activated charcoal step was negated (removal of the acetic acid under high vacuum) and purification was performed by pouring the crude sample onto a pad of silica 3.5 g and eluting through with EtOAc. However, as seen in the NMR small traces of intermediates were still present. Full chromatographic purification allowed isolation of the clean product in 68-73%.



To perform a more robust analysis 3 reactions were performed at larger scale.

To a 20 mL microwave via was added *D*-glucono-1,5-lactone (4.24 g, 11.92 mmol), acetic anhydride (4.72 mL, 50.0 mmol) and anhydrous $ZnCl_2$ (95 mg).

Reaction 1: The reaction was heated under microwave irradiation for 20 minutes at 190 °C. The crude reaction was then diluted with toluene (20 mL) and the mixture rotary evaporated to remove the solvent. The reaction was placed upon the high vacuum to remove residual acetic acid and then diluted with EtOAc (20 mL) before activated charcoal (1 g) was added. The crude material was filter over celite and the solvent removed using a rotary evaporator to yield the crude product (3.0062 g).

Reaction 2: The reaction was heated under microwave irradiation for 5 minutes at 100 °C and then at 190 °C for 20 min. The crude reaction was diluted with toluene (20 mL) and the mixture rotary evaporated to remove the solvent. The reaction was placed upon the high vacuum to remove residual acetic acid and then diluted with EtOAc (20 mL) before activated charcoal (1 g) was added. The crude material was filter over celite and the solvent removed using a rotary evaporator to yield the crude product (3.0278 g).

Reaction 3: The reaction was heated under microwave irradiation for 5 minutes at 100 °C and then at 190 °C for 20 min. The sample was reduced in volume by rotary evaporator to yield the crude product (3.0464 g).

Each reaction was purified by column chromatography (1:1 EtOAc/Hexane – visualization via $KMnO_4$ stain). Reaction 1; 2.9216 g, 54%. Reaction 2; 3.2744 g, 61%. Reaction 3; 3.706 g, 69%.

2.2 Extraction of acetic acid.

To remove acetic acid and trace amounts of acetic anhydride liquid-liquid extraction was investigated. A rapid solubility screen was performed and indicated the product was almost completely insoluble in Et_2O and Hexane. Extraction of the acetic acid was evaluated by mixing different proportions of the solvent with the crude product and accessing the amount of acetic acid removed by NMR against an internal standard 1,3,5-trimethylbenzene after 20 min shaking (Table S2,S3).

Table S2: Extraction results for acetic acid with Et_2O.

Entry	Ratio of Et_2O (v/v)	% acetic acid removed
1	0	0
2	2	82
3	4	90
4	6	96
5	8	97
6	10	98
7	12	100

Table S3: Extraction results for acetic acid with Hexane.

Entry	Ratio of Hex (v/v)	% acetic acid removed
1	0	0
2	4	55
3	6	76

4	8	87
5	10	92
6	12	96
7	14	98
8	16	100

2.3 Base examination in the elimination to form compound 4.

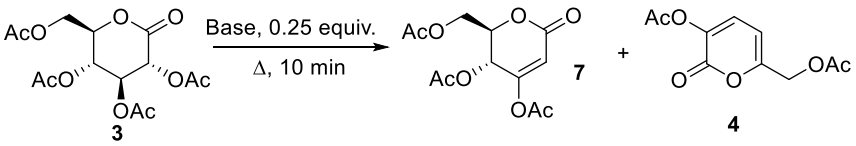


Table S4: Base evaluation for elimination

Entry	Base Catalyst	Temperature (°C)	Conversion	Yield*
1	SiO_2-Pyr	80 °C	8%	**7**: 5%
2		120 °C	84%	**7**: 61%
3	Et_3N	80 °C	96%	**7**: 93%
5		120 °C	100%	**7**: 46%; **4**: 7%
6	Pyridine	80 °C	77%	**7**: 45%; **4**: 8%
7		120 °C	100%	**7**: 5%; **4**: 51%
8	DMAP	80 °C	97%	**7**: 44%; **4**: 40%
9		120 °C	100%	**7**: 8%; **4**: 44%
10	Imidazole	80 °C	98%	**7**: 30%; **4**: 43%
11		120 °C	100%	**7**: 0%; **4**: 18%
12	NH_4OAc	80 °C	55%	**7**: 52%; **4**: 0%
13		120 °C	64%	**7**: 49%; **4**: 15%
14	DIPEA	80 °C	100%	**7**: 83%; **4**: 0%
15		120 °C	100%	**7**: 56%; **4**: 15%

***Reactions performed under MW irradiation using crude 3 as starting material; yields were determined by ^{1}H-NMR analysis using 18-crown-6 as analytical standard.*

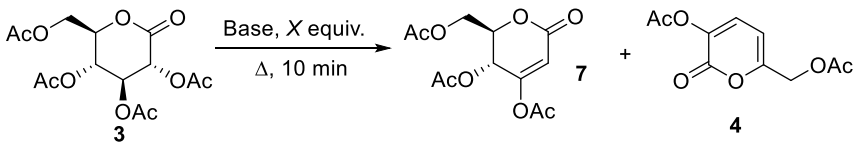


Table S5: Base stoichiometry optimisation

Entry	Catalyst		Temperature	Time	Conversion	Yield*
	Base	Equivalents				
1	Et_3N	0.25	80 °C	10 min	96%	**7**: 78%
2		0.5	80 °C	10 min	100%	**7**: 91%; **4**: 6%
3		0.75	80 °C	10 min	100%	**7**: 80%; **4**: 6%
4	Pyridine	0.125	120 °C	10 min	97%	**7**: 52%; **4**: 26%
5		0.25	120 °C	10 min	100%	**7**: 5%; **4**: 51%
6		0.25	120 °C	5 min	100%	**7**: 37%; **4**: 36%
7		0.5	120 °C	10 min	100%	**7**: 0%; **4**: 59%
8		0.5	120 °C	5 min	100%	**7**: 13%; **4**: 52%
9	DMAP	0.25	80 °C	10 min	97%	**7**: 44%; **4**: 40%
10		0.5	80 °C	10 min	100%	**7**: 0%; **4**: 19%
11		0.75	80 °C	10 min	100%	**7**: 0%; **4**: 6%

***Reactions performed under MW irradiation using crude 3 as starting material; yields were determined by ^{1}H-NMR analysis using 18-crown-6 as analytical standard.*

2.4 Conversion of enone 7 to compound 4

To a 5 mL microwave via was added triacetate **7** (0.495 g), acetic acid (0.5 mL, 5 equiv.) and triethylamine (0.06 mL, 0.25 equiv.). The base (X equiv.) and solvent (1 mL) were added and the reaction was heated under microwave irradiation at 90 °C for 20 min.

A crude 0.85 M solution of the triacetate **7** prepared as per Section 2.4 gave essentially identical results.

Table S6: Rearrangement process optimisation conditions

Entry	Base	Equivalents	Solvent (1 mL)[a)]	Conversion	Yield	**7**/**4** Ratio[b)]
1	NaOH	0.5	MeOH	83%	19%	0.52
2	NaOH	1	MeOH	100%	24%	0
3	-	-	H_2O	-	0%	- [c)]
4	-	-	MeOH	18%	Traces	5.26
5	NaOMe	1	H_2O	-	0%	- [d)]
6	NaOMe	0.5	MeOH	73%	13%	1.04
7	NaOMe	1	MeOH	92%	18%	0.21
8	NaOMe	2.5	MeOH	100%	21%	0
9	NaOMe	5	MeOH	100%	19%	0
10	NaOMe	7.5	MeOH	100%	20%	0

[a)] H_2O: ≈30 equiv.; MeOH: ≈15 equiv. [b)] Reactions performed using crude 2 as starting material; 2/3 ratios were determined by ^{1}H-NMR analysis of the crude reaction mixture. [c)] 0% conversion. [d)] 10-20% conversion.

2.5 Fully continuous synthesis of triacetate 3 from *D*-gluconolactone (2):

Note: For the conversion of **2** to **3** we found that lower quantities of acetic anhydride could be used than the theoretical required 4 equivalents per molecule of ***D***-gluconolactone. We assume under the high temperatures and acid catalysis the acetic acid formed could condense to generate more acetic anhydride or an alternative acid catalysed ester formation may occur accounting for the higher conversions.

A powder doser (HI-DOSER from LAMBDA Laboratory Instruments, Switzerland) was used to dispense *D*-gluconolactone **1** at a rate of 2 g/min into a CSTR (3 necked round bottom flask 104 mL, heated at 50 °C using a stirrer heating mantle – stir rate 900 rpm) containing silica-supported sulfuric acid (10 g). An HPLC pump (Knauer K120) was used to deliver a stream of acetic anhydride (neat, 4.5 mL/min) into the CSTR. After an initial 5 minutes fill cycle a second HPLC pump was turned on and used to withdraw the reaction solution from this CSTR at an equilibrium flow rate of 5.4 mL/min (calculated mean residence time of 20 min). A stainless steel filter frit was used to prevent removal of the silica-supported sulfuric acid. The reactor was run at steady state for 9 h with the output being sampled every 45 minutes and analysed by GC-MS for conversion which was shown to remain quantitative. A 2.5 h working exemplification batch was collected and the material worked up for assessment. The collected material was diluted with toluene 1 L and the solvent (toluene/acetic acid) removed under reduced pressure using a rotary evaporator. The residue was diluted with DCM

(1.5 L) and washed with sat. aqu. sodium hydrogen carbonate solution (3 × 500 mL). The organic phase was dried over anhydrous magnesium sulfate and the solvent removed with a rotary evaporator to yield the title compound in 96% isolated yield (559.8 g) and as a single compound by NMR.

2.6 Fully continuous synthesis of intermediate 7 from *D*-gluconolactone (2):

A powder doser (HI-DOSER from LAMBDA Laboratory Instruments, Switzerland) was used to dispense *D*-gluconolactone **1** at a rate of 2 g/min into a CSTR (3 necked round bottom flask 104 mL, heated at 50 °C using a stirrer heating mantle – stir rate 900 rpm) containing silica-supported sulfuric acid (10 g). The peristaltic pump channel A of a Vapourtec E-series was used to deliver a stream of acetic anhydride (neat, 4.5 mL/min) into the CSTR. After an initial 5 minutes fill cycle the peristaltic pump channel B of the Vapourtec E-series was turned on and used to withdraw the reaction solution from this CSTR at a flow rate of 5.4 mL/min (calculated mean residence time of 20 min). The exiting reaction solution was combined with a stream of triethylamine (neat, 0.7 mL/min, 3rd channel of the Vapourtec E-series pumping system) using a PEEK T-piece (IDEX corporation). The resulting reaction stream was progressed into two sequential tubular coil reactors installed on a Polar Bear plus reactor system (Cambridge Reactor Design, UK; 2 × 52 mL, 80 °C) prior to collection of the crude reaction mixture. LC-MS analysis indicated complete conversion of samples taken between 30 min and 6 h. A 2 h run was batched and worked up for assessment. The crude reaction mixture was diluted with toluene 1.7 L and washed with water (2 × 1 L), 1 M aqu. hydrochloric acid (1 L) and sat. aqu. sodium hydrogen carbonate (1 L). The organic phase was dried over anhydrous sodium sulfate and the solvent removed using a rotary evaporator to yield the title compound in 95% isolated yield (366.3 g) and as a single compound by NMR.

2.7 Fully continuous synthesis of cyclopentenone 1 from *D*-gluconolactone (2):

Acetic anhydride (neat, 2.2 mL/min) was pumped (Vapourtec E-series pump 1) into a CSTR (50 mL, 40 °C, 750 rpm stirring speed, which also contained silica-supported sulfuric acid (10 g)). Simultaneously a powder doser (HI-DOSER from LAMBDA Laboratory Instruments, Switzerland) was used to add *D*-gluconolactone (**2**) into the CSTR (addition rate of 0.95 g/min). After 12 minutes a pump was started to reaction mixture was then pumped (Vapourtec E-series pump 2, 2.5 mL/min) out of the CSTR and directed into a T-piece, where it was blended with a stream of triethylamine (Vapourtec E-series pump 2, neat, 0.5 mL/min). The resulting mixture was progressed into a sequence of connected coiled reactors (3 × 10 mL, 80 °C, 10 min residence time). The reactor solution was further combined with a stream of sodium hydroxide in MeOH (7% w/w, Knauer K120 HPLC pump, 2.5 mL/min) before entering passing through two linked Polar Bear plus reactor (2 × 52 mL, 90 °C, 18.9 min residence time). The crude reaction stream was diluted with a stream of EtOAc (5 mL/min) and directed into the bottom of the counter current extraction module (AMC technologies, UK, 100 mL). Into the top fitting of the extractor unit was continuously added aqu. hydrochloric acid (1 M, 5 mL/min) and the module which was agitated at a frequency of 6 Hz. The organic phase containing **1** was collected. After running this set-up for 8 h, the desired cyclopentenone product **1** was isolated after evaporation of all volatiles as a yellow oil (283.7 g, 71%, purity 79% as determined by ^{1}H-NMR). Further purification was accomplished by silica column chromatography (eluent: 4:6 EtOAc/Hexane) furnishing pure **1** with in an isolated yield of 50%.

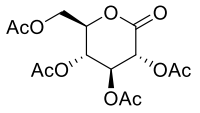
2.8 Heterogeneous flow synthesis of cyclopentenone 1 from 7 using Ambersep 900:

A solution of triacetate **7** (13 g; 0.73 M in MeOH) was pumped at 0.6 mL/min through a series of 3 sequentially linked and heated Omnifit glass column (85 °C; 100 mm length, 15 mm i.d.) each filled with 5 g of Ambersep 900 resin. Passage of the solution through the columns caused a discoloration of

the resin to a brown colour however the activity was still persistent. The reaction solution was collected after passing through a backpressure regulator (75 psi). After evaporation of the solvent the desired cyclopentenone **1** was isolated as a brown oil with moderate purity, which could be enhanced by high vacuum distillation (130 °C, 0.5 mbar) furnishing **1** as a yellow oil (71% yield, 8.00 g).

3. Spectroscopic Characterisation of Compounds 3, 7, 4 and 1

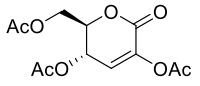
(2*R*, 3*R*, 4*S*, 5*R*)-2-(Acetoxymethyl)-6-oxotetrahydro-2*H*-pyran-3,4,5-triyl acetate, 3:



Chemical Formula: $C_{14}H_{18}O_{10}$
Exact Mass: 346.0900

Colourless oil. **^{1}H-NMR (400 MHz, $CDCl_3$)** δ/ppm: 5.54 (t, *J* = 9.1 Hz, 1H), 5.35 (t, *J* = 9.0 Hz, 1H), 5.11 (d, *J* = 9.1 Hz, 1H), 4.61 (ddd, *J* = 8.8, 3.7, 2.5 Hz, 1H), 4.39 (dd, *J* = 12.7, 3.7 Hz, 1H), 4.25 (dd, *J* = 12.7, 2.5 Hz, 1H), 2.15 (s, 3H), 2.10 (s, 3H), 2.07 (s, 3H), 2.06 (s, 3H). **^{13}C-NMR (101 MHz, $CDCl_3$)** δ/ppm: 170.3 (C), 170.0 (C), 169.5 (C), 169.2 (C), 164.6 (C), 75.8 (CH), 70.4 (CH), 70.3 (CH), 66.5 (CH), 61.3 (CH_2), 20.6 (CH_3), 20.5 ($2CH_3$), 20.3 (CH_3)**. IR (neat, ν/cm^{-1}):** 1739 (s), 1713 (s), 1372 (m), 1211 (s), 1038 (s), 973 (m), 925 (m), 732 (m), 597 (m). **HR-MS (AP+)** calculated for $C_{14}H_{19}O_{10}$ 347.0978, found 347.0973.

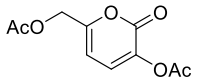
(2*R*, 3*S*)-2-(Acetoxymethyl)-6-oxo-3,6-dihydro-2*H*-pyran-3,5-diyl acetate, 7:



Chemical Formula: $C_{12}H_{14}O_8$
Exact Mass: 286.0689

Yellow oil. **^{1}H-NMR (400 MHz, $CDCl_3$)** δ/ppm: 6.44 (dd, *J* = 4.2, 0.6 Hz, 1H), 5.62 (dd, *J* = 5.8, 4.2 Hz, 1H), 4.71-4.80 (m, 1H), 4.38 (dd, *J* = 12.3, 4.8 Hz, 1H), 4.29 (dd, *J* = 12.3, 4.4 Hz, 1H), 2.25 (s, 3H), 2.12 (s, 3H), 2.09 (s, 3H). **^{13}C-NMR (101 MHz, $CDCl_3$)** δ/ppm: 170.4 (C), 169.7 (C), 168.1 (C), 157.2 (C), 139.6 (C), 126.1 (CH), 77.8 (CH), 64.2 (CH), 62.0 (CH_2), 20.7 (CH_3), 20.6 (CH_3), 20.3 (CH_3). **IR (neat, ν/cm^{-1}):** 1737 (s), 1672 (w), 1434 (w), 1370 (m), 1191 (s), 1129 (s), 1025 (s), 958 (m), 907 (m), 778 (m), 599 (m). **HR-MS (AP+)** calculated for $C_{12}H_{15}O_8$ 287.0767, found 287.0758.

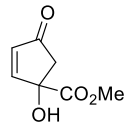
(3-Acetoxy-2-oxo-2*H*-pyran-6-yl) methyl acetate, 4:



Chemical Formula: $C_{10}H_{10}O_6$
Exact Mass: 226.0477

Colourless oil. **^{1}H-NMR (400 MHz, $CDCl_3$)** δ/ppm: 7.08 (d, *J* = 7.8 Hz, 1H), 6.26 (d, *J* = 7.8 Hz, 1H), 4.83 (s, 2 H), 2.30 (s, 3H), 2.12 (s, 3H). **^{13}C-NMR (101 MHz, $CDCl_3$) δ/ppm:** 170.0 (C), 167.9 (C), 157.2 (C), 155.6 (C), 136.8 (C), 130.7 (CH), 103.9 (CH), 61.3 (CH_2), 20.6 (CH_3), 20.4 (CH_3). **IR (neat, ν/cm^{-1}):** 2979 (w), 1732 (s) 1655 (m), 1586 (w), 1440 (w), 1369 (m), 1169 (s), 1099 (s), 1030 (s), 881 (m), 836 (m), 758 (m), 600 (m), 536 (m), 512 (m). **HR-MS (AP+)** calculated for $C_{10}H_{11}O_6$ 227.0556, found 227.0555.

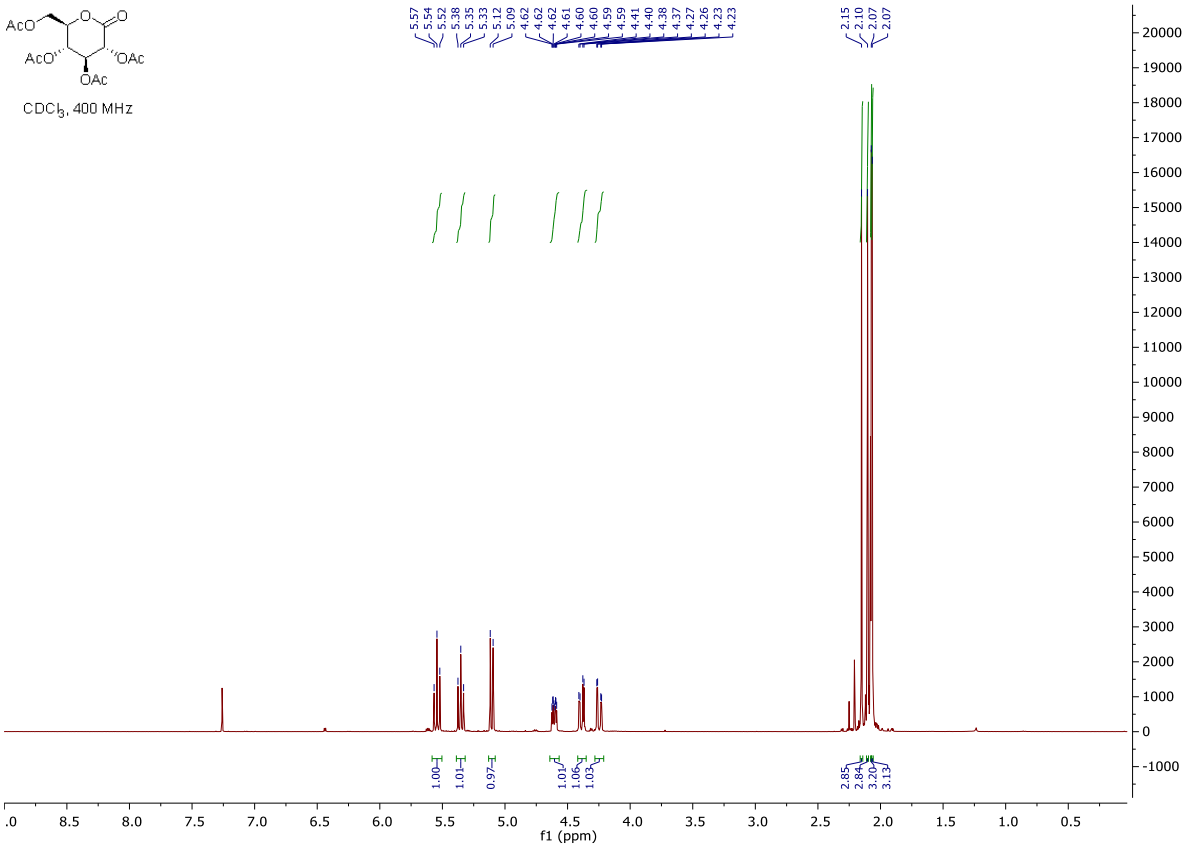
Methyl 1-hydroxy-4-oxocyclopent-2-enecarboxylate, 1:

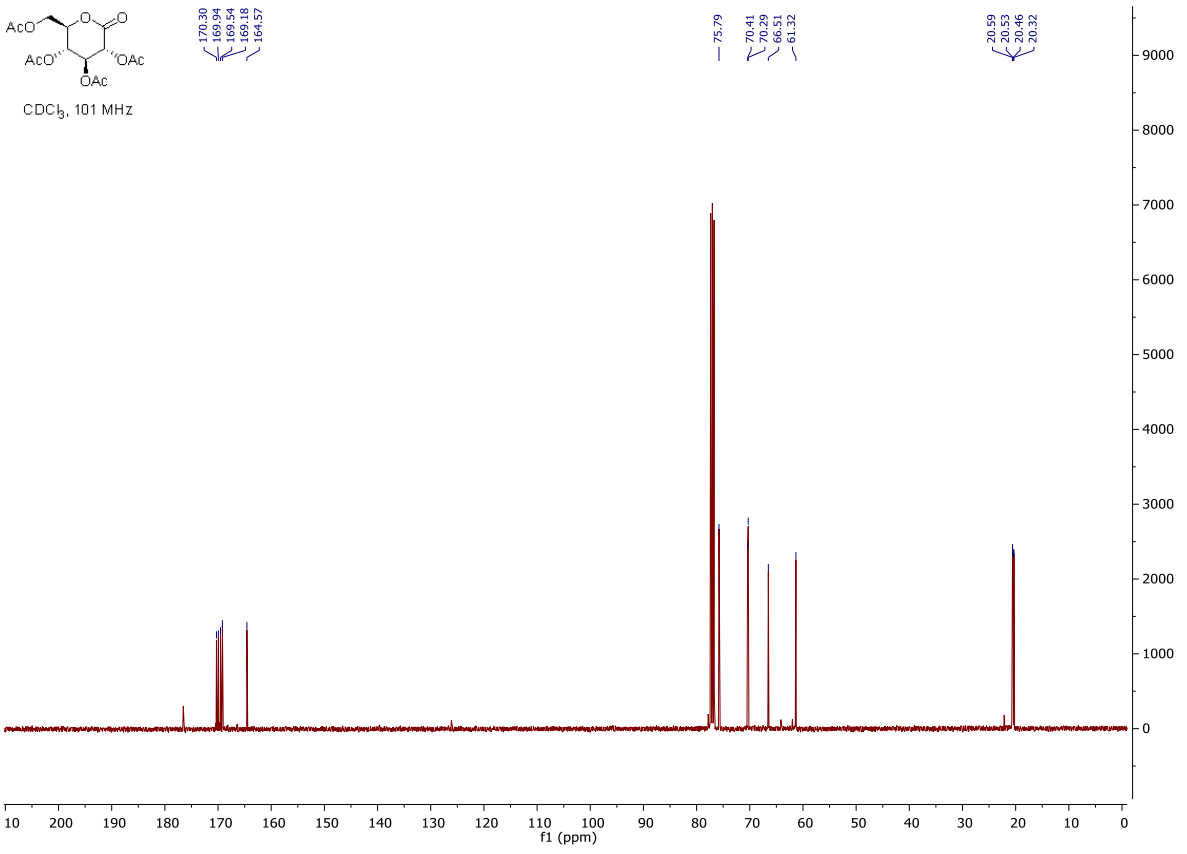


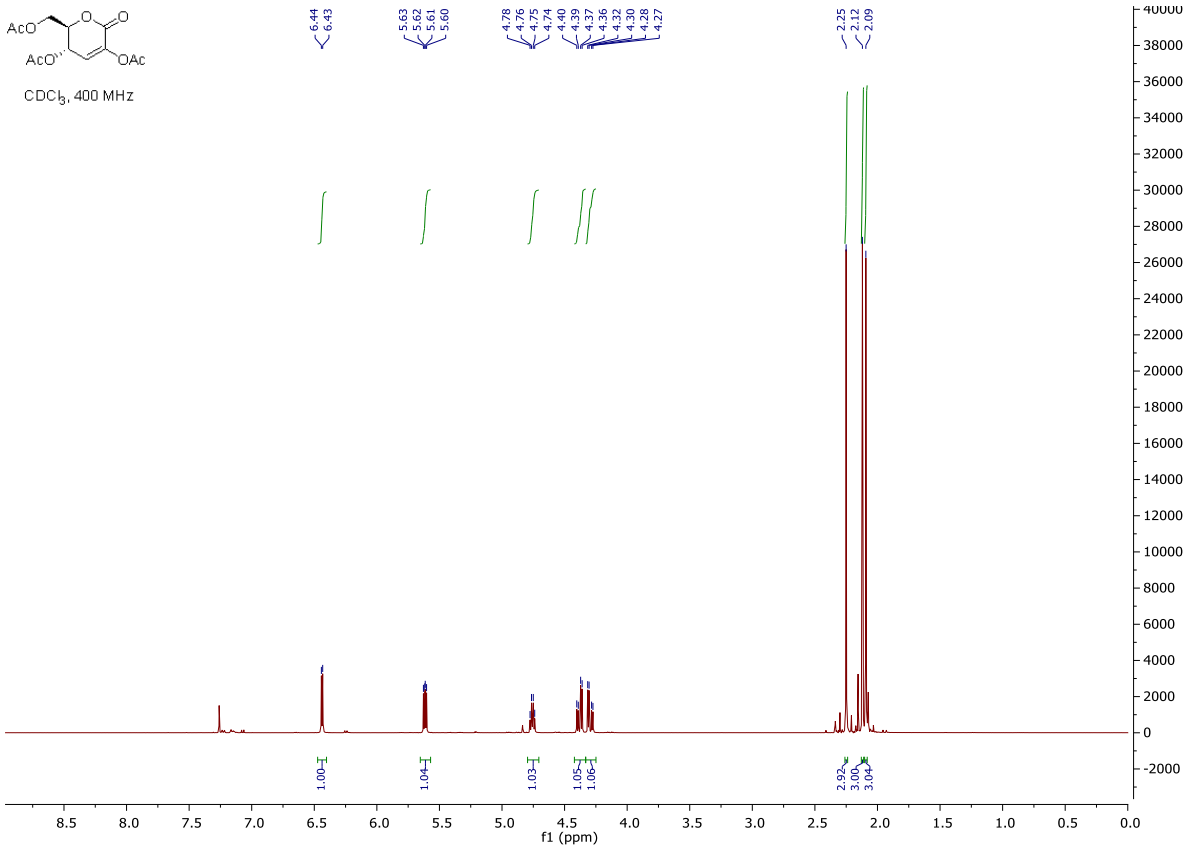
Chemical Formula: $C_7H_8O_4$
Exact Mass: 156.0423

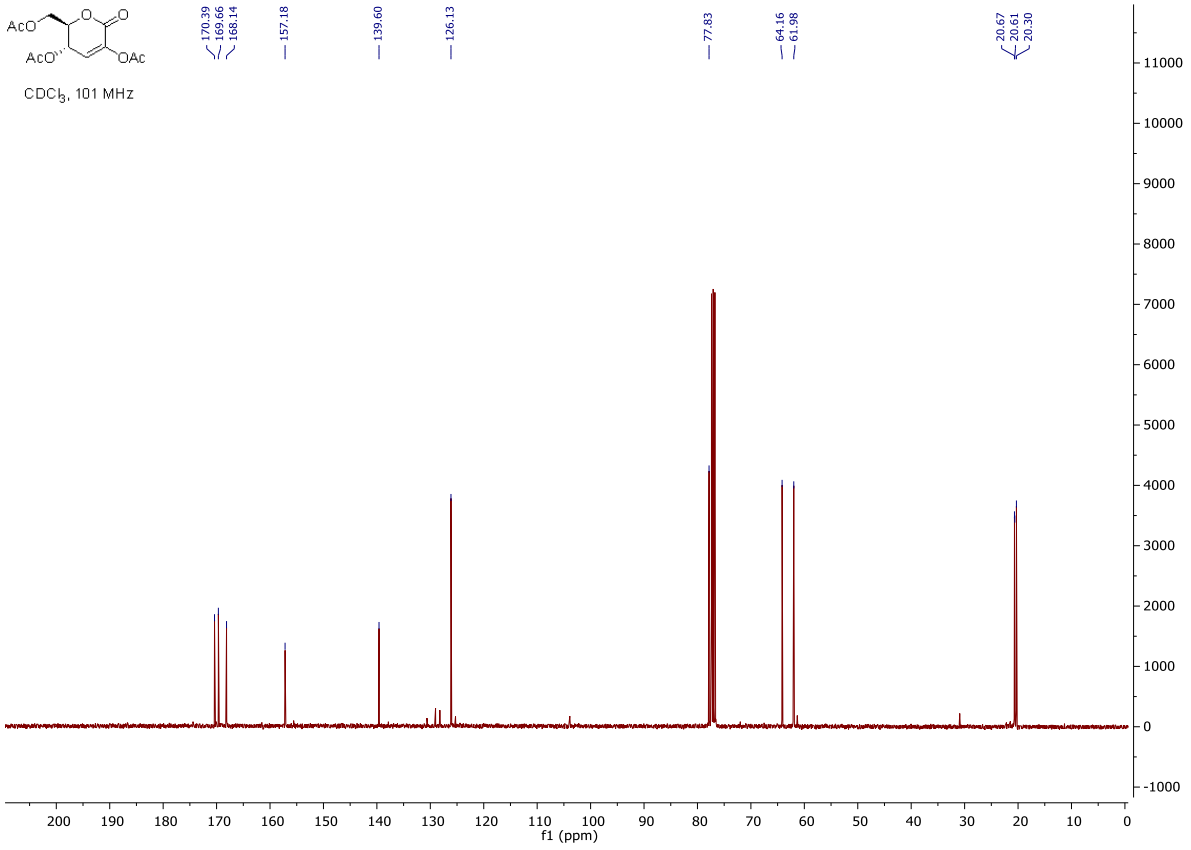
Yellow oil. **^{1}H-NMR (400 MHz, $CDCl_3$)** δ/ppm: 7.34 (d, *J* = 7.8 Hz, 1H), 6.29 (d, *J* = 7.8 Hz, 1H), 4.10 (br s, 1H), 3.78 (s, 3H), 2.86 (d, *J* = 16.0 Hz, 1H), 2.52 (d, *J* = 16.0 Hz, 1H). **^{13}C-NMR (101 MHz, $CDCl_3$)** δ/ppm: 205.3 (C), 173.8 (C), 160.3 (CH), 135.7 (CH), 79.0 (C), 53.8 (CH_2), 47.2 (CH_3). **IR (neat, ν/cm^{-1}):** 3424 (broad), 2958 (w), 1716 (s), 1438 (w), 1333 (w), 1252 (m), 1195 (m), 1172 (s), 1062 (m), 1027 (m), 814 (m), 758 (m), 670 (w). **HR-MS (AP+)** calculated for $C_7H_9O_4$ 157.0501, found 157.0493.

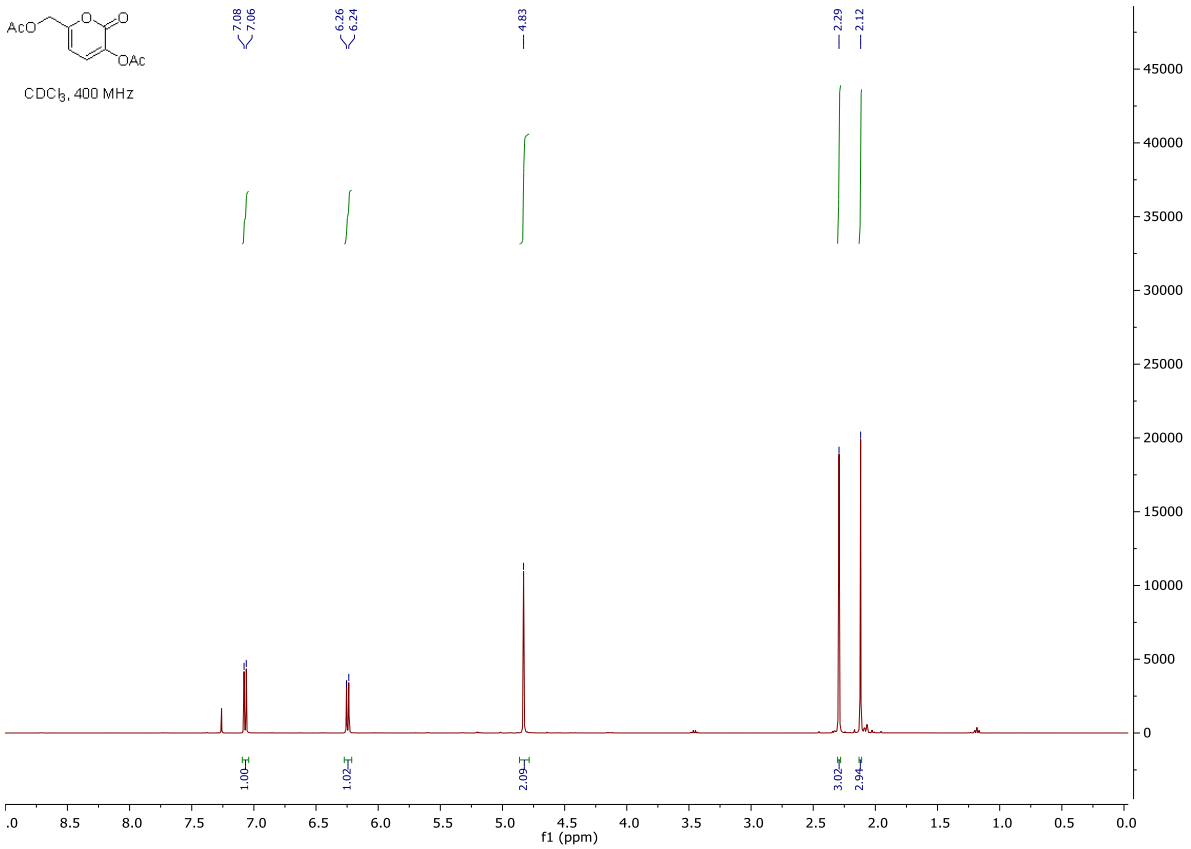
4. Copies of NMR-Spectra

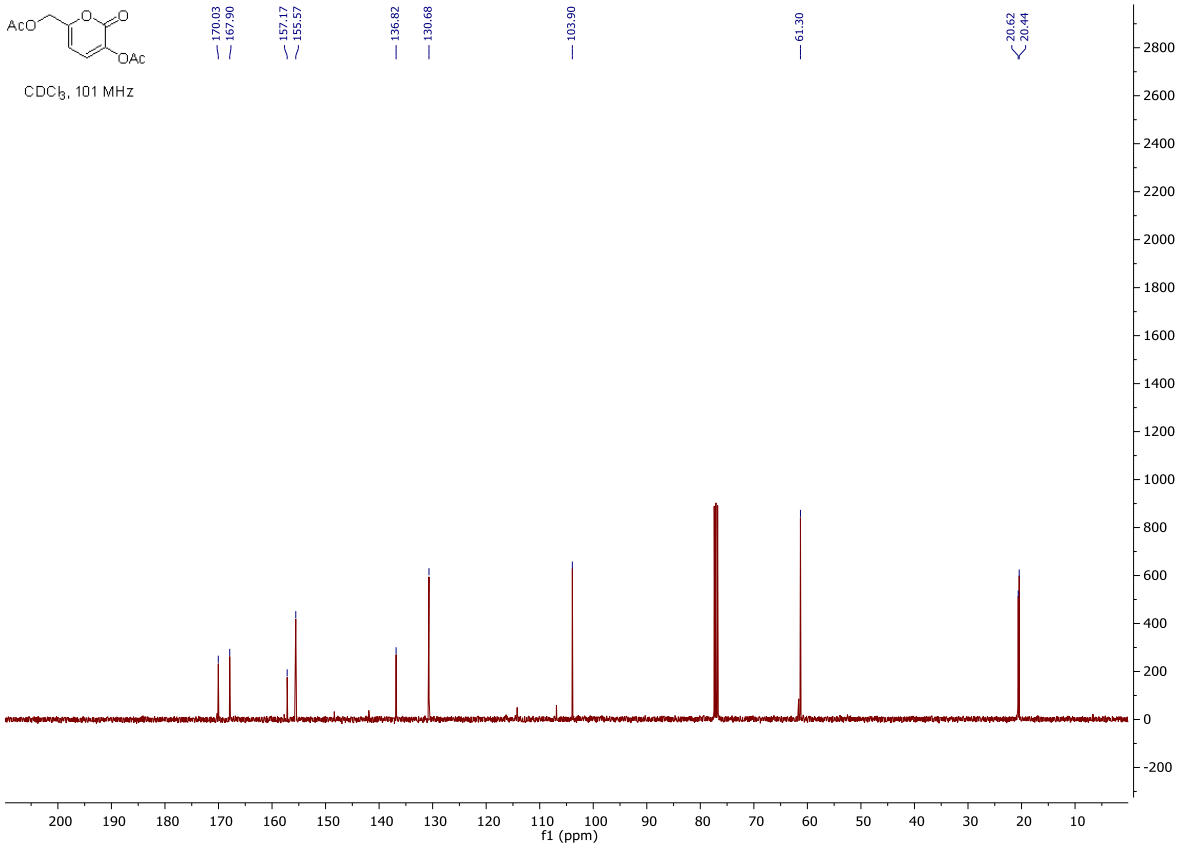


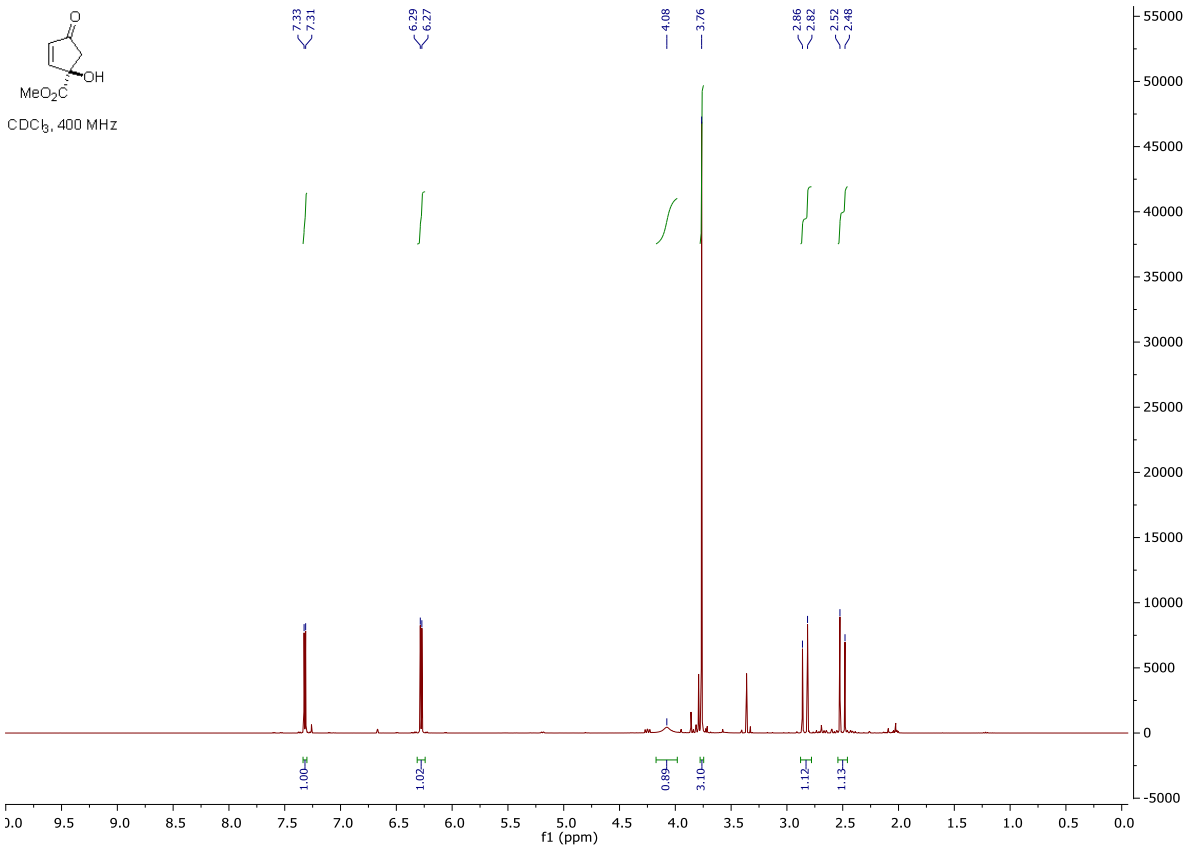


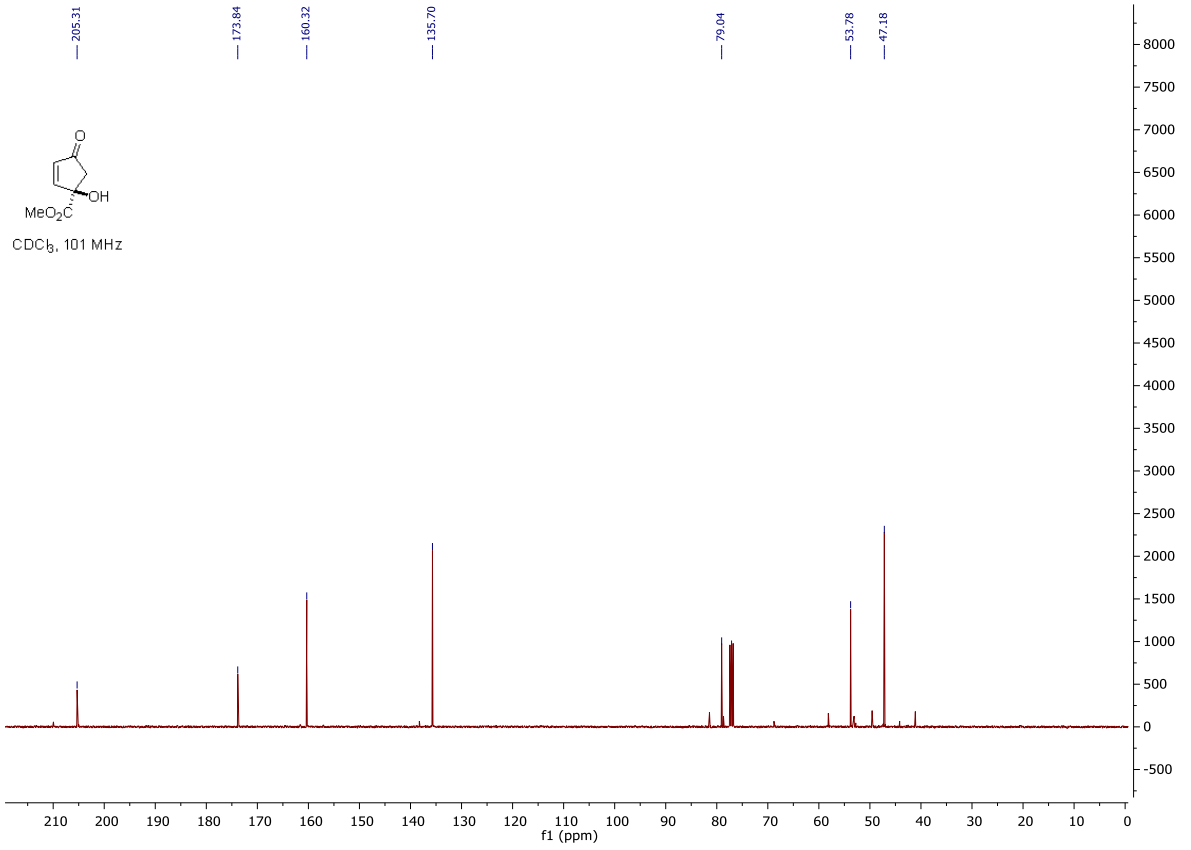

AcO
AcO
OAc
CDCl3, 400 MHz
6.44
6.43
5.63
5.62
5.61
5.60
4.78
4.76
4.75
4.74
4.40
4.39
4.37
4.36
4.32
4.30
4.28
4.27
2.25
2.12
2.09
1.00
1.04
1.03
1.05
1.06
2.92
3.00
3.04
f1 (ppm)


AcO
AcO
OAc
CDCl3, 101 MHz
170.39
169.66
168.14
157.18
139.60
126.13
77.83
64.16
61.98
20.67
20.61
20.30
f1 (ppm)


AcO
OAc
CDCl3, 400 MHz
7.08
7.06
6.26
6.24
4.83
2.29
2.12
1.00
1.02
2.09
3.02
2.94
f1 (ppm)


AcO
OAc
CDCl3, 101 MHz
170.03
167.90
157.17
155.57
136.82
130.68
103.90
61.30
20.62
20.44
f1 (ppm)


CDCl3, 400 MHz
7.33
7.31
6.29
6.27
4.08
3.76
2.86
2.82
2.52
2.48
1.00
1.02
0.89
3.10
1.12
1.13
f1 (ppm)


CDCl3, 101 MHz
205.31
173.84
160.32
135.70
79.04
53.78
47.18
f1 (ppm)