Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Oxidation of Terminal Diols Using an Oxoammonium Salt: A Systematic Study

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Supporting Information: Experimental Studies

Key to Abbreviated Terms:

$CDCl_3$: deuterated chloroform

CH_2Cl_2: dichloromethane

TLC: Thin layer chromatography

General Considerations:

General:

NMR Spectra (^{1}H, ^{13}C) were performed at 298 K on a Brüker DRX-400 400 MHz NMR. ^{1}H-NMR Spectra obtained in $CDCl_3$ were referenced to residual non-deuterated chloroform (7.26 ppm) in the deuterated solvent. ^{13}C-NMR Spectra obtained in $CDCl_3$ were referenced to chloroform (77.3 ppm). ^{19}F-NMR spectra were referenced to hexafluorobenzene (–164.9 ppm). Reactions in CH_2Cl_2 could be monitored with ^{1}H NMR by irradiating the solvent peak at 5.30 ppm. Flash chromatography and silica plugs utilized Dynamic Adsorbents Inc. Flash Silica Gel (60Å porosity, 32-63 µm). TLC analysis was performed using hexanes/ethyl acetate as the eluent and visualized using iodine. IR spectra were obtained on a Brüker ALPHA FT-IR spectrometer. High-resolution mass spectra were performed on either a JEOL AccuTOF-DART SVP 100 in positive direct analysis in real time (DART) ionization method, using PEG as the internal standard.

Chemicals:

Deuterated chloroform was purchased from Cambridge Isotope Laboratories and stored over 4Å molecular sieves. All chemicals were purchased from commercial suppliers with exception of the oxoammonium salt 4-acetamido-2,2,6,6-tetramethylpiperidine-1-oxoammonium tetrafluoroborate, **1**, which was prepared according to an established protocol.[1]

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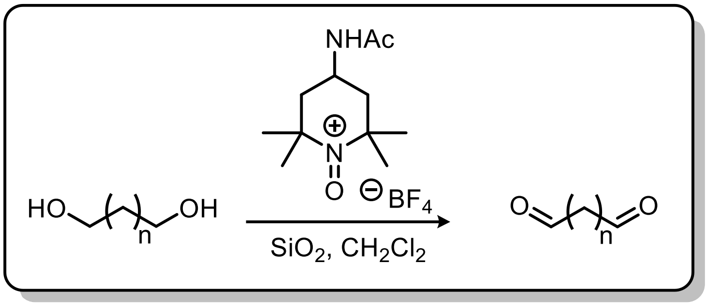
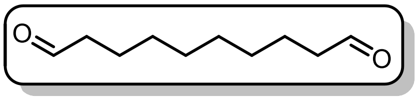
[1] M. A. Mercadante, C. B. Kelly, J. M. Bobbitt, L. J. Tilley and N. E. Leadbeater, *Nat. Protoc.* **2013**, *8*, 666-676.

Oxidation of Diols

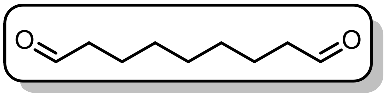


GENERAL PROCEDURE



1,10-Decanedial (3a) (1.294 g, 76%) was prepared from 1,10-decanediol (1.743 g, 10 mmol, 1 equiv). To a 250-mL round bottom flask equipped with a stir bar was added 1,10-decanediol and dichloromethane (100 mL, 0.1 M in diol). After stirring for 5 min, the oxoammonium salt (6.302 g, 21 mmol, 2.1 equiv) was added, followed by silica gel (2.644 g, 2 mass equiv to substrate). The flask was sealed with a rubber septa and the mixture was allowed to stir until the slurry became white. Once white, the slurry was filtered through a thin pad of silica gel. The solid was washed using CH_2Cl_2. The CH_2Cl_2 was removed *in vacuo* by rotary evaporation to afford the pure dialdehyde product, 1,10-decanedial, as a pale yellow oil.[2]

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 1.30 (s, 8 H) 1.56 - 1.65 (m, 4 H) 2.40 (td, *J*=1.77, 7.30 Hz, 4 H) 9.74 (t, *J*=1.82 Hz, 2 H)
^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm 22.25 (CH_2) 29.29 (CH_2) 29.36 (CH_2) 44.10 (CH_2) 203.04 (CHO)



1,9-Nonanedial (3b) (0.690g, 83%) was prepared from 1,9-nonanediol (0.801 g, 5 mmol, 1 equiv) using the general procedure to afford the product as a colorless oil.[3]

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 1.19 (bs, 6H) 1.48 (m, 4H) 2.29 (t, *J* = 7.0 Hz, 4H) 9.61 (bs, 2H)
^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm 21.15 (CH_2) 28.10 (CH_2) 28.28 (CH_2) 43.00 (CH_2) 201.89 (CO)

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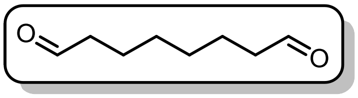
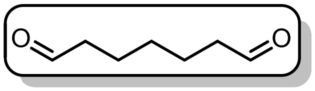
[2] T. Suzuki, M. Tokunaga, Y. Wakatsuki, *Org. Lett.* **2001**, *3*, 735-737.
[3] A. Ozanne, L. Pouységu, D. Depernet, B. François, S. Quideau, *Org. Lett.* **2003**, *5*, 2903-2906.



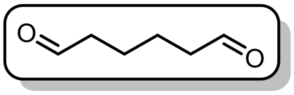
1,8-Octanedial (3c) (1.201 g, 84%) was prepared from 1,8-octanediol (1.462 g, 10 mmol, 1 equiv) using the general procedure to afford the product as a colorless oil.[4]

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 1.27 - 1.35 (m, 4 H) 1.54 - 1.64 (m, 4 H) 2.39 (td, *J*=1.70, 7.25 Hz, 4 H) 9.72 (t, *J*=1.75 Hz, 2 H)
^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm 21.96 (CH_2) 29.01 (CH_2) 43.90 (CH_2) 202.78 (CHO)



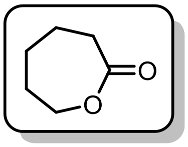
Heptanedialdehyde (3d) (0.826 g, 64%) was prepared from 1,7-heptanediol (1.322 g, 10 mmol, 1 equiv) using the general procedure to afford the product as a pale yellow oil.[5]

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 1.28 - 1.39 (m, 2 H) 1.62 (quin, *J*=7.52 Hz, 4 H) 2.41 (td, *J*=1.61, 7.27 Hz, 4 H) 9.73 (t, *J*=1.63 Hz, 2 H)
^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm 21.94 (CH_2) 28.79 (CH_2) 43.79 (CH_2) 202.49 (CHO)



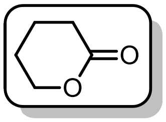
Adipaldehyde (3e) (26%) was prepared from 1,6-hexanediol (1.182 g, 10 mmol, 1 equiv) using the general procedure to afford the products adipaldehyde and caprolactone (**4e**) as an inseparable mixture of a colorless oil (0.874 g, 87%).[5]

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 1.62 (m, 4H) 2.44 (m, 4H) 9.73 (t, *J* = 1.5 Hz, 2H)
^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm 21.63 (CH_2) 43.71 (CH_2) 202.12 (CHO)



Caprolactone (4e) (74%)[6]

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 2.24 (quin, *J*=7.58 Hz, 2 H) 2.47 (t, *J*=8.26 Hz, 2 H) 4.32 (t, *J*=7.06 Hz, 2 H)
^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm 29.12 (CH_2) 29.47 (CH_2) 23.11 (CH_2) 34.73 (CH_2) 69.48 (CH_2) 176.42 (CHO)



δ-Valerolactone (4f) (0.817 g, 82%) was prepared from 1,5-pentanediol (0.994 g, 10 mmol, 1 equiv) using the general procedure to afford the product as a white solid.[6]

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 1.86 (m, 1H) 2.53 (t, *J*=6.97 Hz, 1H) 4.32 (t, *J*=5.62 Hz, 1H)
^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm 19.03 (CH_2) 22.26 (CH_2) 29.79 (CH_2) 69.44 (OCH_2) 171.46 (CO)

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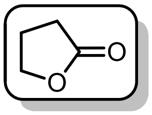
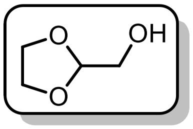
[4] X. Jiang, J. Zhang, S. Ma *J. Am. Chem. Soc.* **2016**, *138*, 8344-8347.
[5] B. Hong, H. Tseng, S. Chen, *Tetrahedron* **2007**, *63*, 2840-2850.
[6] T. Miyazawa, T. Endo *J. Org. Chem.* **1985**, *50*, 3930-3931.



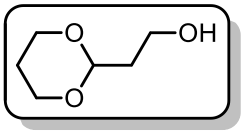
Butyrolactone (4g) (0.523 g, 61%) was prepared from 1,4-butanediol (0.901 g, 10 mmol, 1 equiv) using the general procedure to afford the product as a colorless oil.[6]

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 2.24 (quin, *J*=7.58 Hz, 2 H) 2.47 (t, *J*=8.26 Hz, 2 H) 4.32 (t, *J*=7.06 Hz, 2 H)
^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm 22.38 (CH_2) 27.98 (CH_2) 68.72 (CH_2) 177.92 (CO)



2-Hydroxymethyl-1,3-dioxolane (6) (1.363g, 65%) was prepared from freshly distilled ethylene glycol (2.483 g, 40 mmol, 1 equiv), using the following modification the general procedure: Ethylene glycol was stirred in CH_2Cl_2 (200 mL, 0.2 M in diol), then 0.55 equiv (6.602 g, 22 mmol) oxoammonium salt was added, followed by 1.98 g silica gel (0.8 mass equiv to the substrate). The mixture was refluxed for 20 h, at which point the white slurry was filtered through a pad of silica gel. Due to volatility, the solvent was removed *via* evaporation through a 30 cm Vigreux column to afford the product as a pale yellow oil.[7]

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 3.64 (br. d, *J*=2.40 Hz, 2 H) 3.67 (br. s, 1 H) 3.85 - 4.04 (m, 4 H) 4.96 (t, *J*=3.24 Hz, 1 H)
^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm 62.68 (CH_2O) 65.09 (CH_2O) 103.21 (OCHO)



2-Hydroxyethyl-1,3-dioxane (7) (0.485 g, 73%) was prepared from 1,3-propanediol (0.761 g, 10 mmol, 1 equiv) using the following modifications to the general procedure: 0.5 equiv (1.501 g, 5 mmol) oxoammonium salt was added, followed by 1.501 g silica gel (1 mass equiv to the oxoammonium salt). The product was afforded as a yellow oil.[8]

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 1.30 - 1.37 (dm, *J*=1.28, 13.42 Hz, 1 H) 1.84 (q, *J*=5.28 Hz, 2 H) 2.01 - 2.14 (qt, *J*=1.28, 13.42 Hz, 1 H) 2.62 (br. s, 1 H) 3.69 - 3.80 (m, 4 H) 4.09 (dd, *J*=5.06, 10.56 Hz, 2 H) 4.73 (t, *J*=4.84 Hz, 1 H)
^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm 25.91 (CH_2) 37.35 (CH_2) 58.87 (CH_2O) 67.10 (CH_2O) 102.01 (OCHO)

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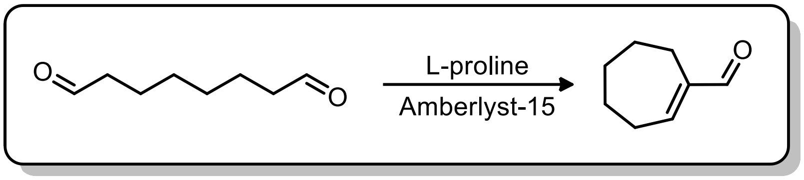
[7] J. R. Sanderson, E. L. Yeakey, J. J. Lin, R. Duranleau, E. T. Marquis *J. Org. Chem.* **1987**, *52*, 3243-3246.
[8] C. S. Shiner, T. Tsunoda, B. A. Goodman, S. Ingham, S.-H. Lee, P. E. Vorndam *J. Am. Chem. Soc.* **1989**, *111*, 1381-1392.

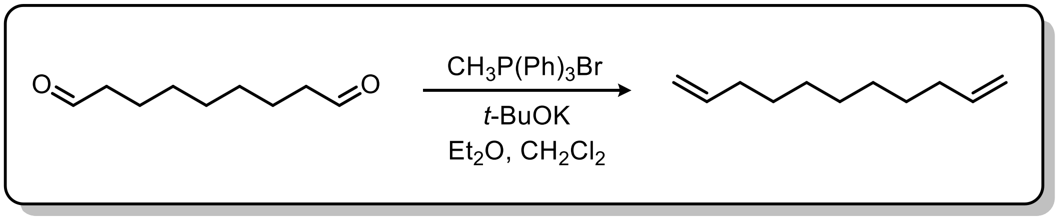
Aldol Reaction



1-Cycloheptene-1-carboxaldehyde (9) (1.06 g, 50%) was prepared from the oxidation of 1,8-octanediol (2.5 g, 17.1 mmol, 1 equiv) using the procedure outlined above for oxidation, followed by a subsequent Aldol reaction. To the resulting solution of 1,8-octanedial, filtered off from the silica gel and oxoammonium salt, was added L-proline (1.5 g, 13 mmol, 0.76 eq) and 1.5 g of activated 4Å molecular sieves. The mixture was refluxed for 2 days, then filtered through a pad of silica gel. Due to volatility, the solvent was removed *via* evaporation through a 30 mm Vigreux column to afford the product as an orange oil.[9]

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 1.45 (m, 1H) 1.56 (m, 1H) 1.75 (m, 1H) 2.37 (t, J = 5.6 Hz, 1H) 2.42 (q, J = 5.9 Hz, 1H) 6.83 (t, J = 6.3 Hz, 1H)
^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm 24.01 (CH_2) 26.17 (CH_2) 26.23 (CH_2) 30.08 (CH_2) 31.89 (CH_2) 147.64 (C) 157.22 (CH) 194.54 (CHO)

Wittig Reaction



1,10-Undecadiene (10) (0.655 g, 86%) was prepared from the oxidation of 1,9-nonanediol (0.801 g, 5 mmol, 1 equiv) using the procedure outlined above for oxidation, followed by a subsequent Wittig reaction. The Wittig reagent, methylenetriphenylphosphorane, was prepared by stirring methyltriphenylphosphonium bromide (5.355 g, 15 mmol, 3 equiv to diol) and potassium t-butoxide (1.68 g, 15 mmol, 3 equiv to diol) in dry diethyl ether (75 mL, 0.2 M) for 7 hours. The filtered solution of 1,9-nonanedial was added directly to this solution and the mixture was filtered overnight. The solution was filtered and the solvent was removed *in vacuo*, resulting in a thick oil. Pentane (50 mL) was added to precipitate excess triphenylphosphine and the oxide byproduct. The resulting slurry was filtered through silica and the solvent was removed *in vacuo* to afford the product as a colorless oil.[10]

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 1.34 (m, 10H). 2.05 (q, J = 7.1 Hz, 4H), 4.94 (dd, J=1.4, 8.00 Hz, 2H) 5.00 (dd, J = 1.9, 17.1 Hz, 2H) 5.84 (tq, J = 6.8, 14.8 Hz, 2H),
^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm 29.25 (CH_2) 29.41 (CH_2) 29.66 (CH_2) 34.12 (CH_2) 114.41 (CH_2) 139.46 (CH)

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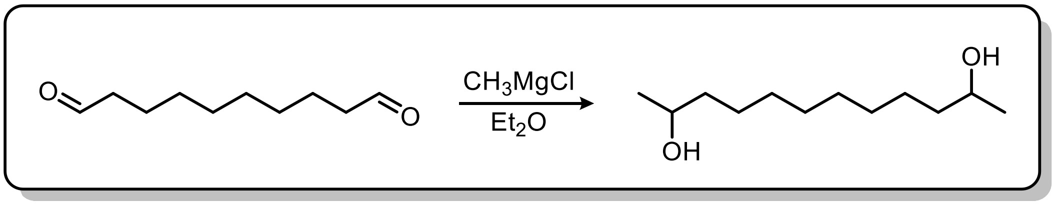
[9] I. G. Molnár, E. Tanzer, C. Daniliuc, R. Gilmour, *Chem. Eur. J.* **2014**, *20*, 794-800.
[10] X. Li, C. E. Burrell, R. J. Staples, B. Borhan, *J. Am. Chem. Soc.* **2012**, *134*, 9026-9029.

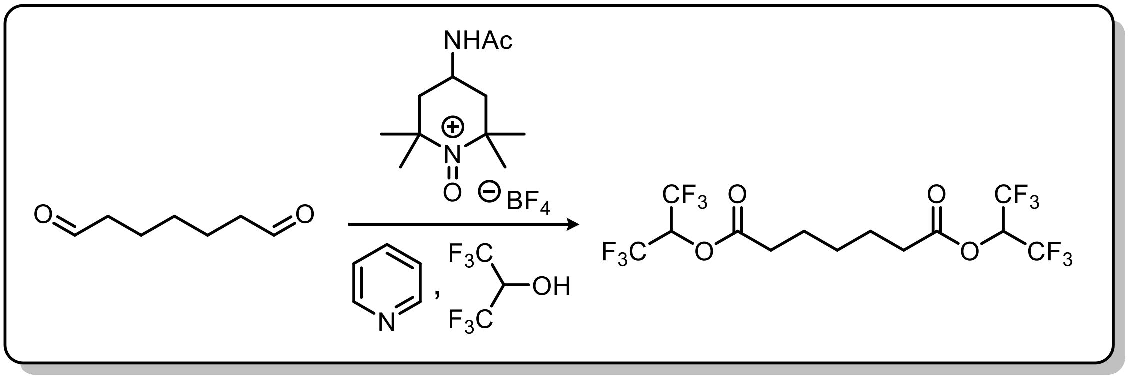
Grignard Reaction



2,11-Dodecanediol (11) (0.900 g, 89%) was prepared from 1,10-decanediol (0.870 g, 5 mmol, 1 equiv) using the procedure outlined above for oxidation, followed by a subsequent Grignard reaction. A solution of 1,10-decanedial, filtered off of the silica gel and oxoammonium salt, was added to a solution of commercially available 3 M methylmagnesium chloride in anhydrous diethyl ether (7 mL, 21 mmol, 4.2 equiv). The solution was stirred overnight, then aliquots (~25 drops) of aqueous saturated potassium carbonate were added dropwise about 10 min apart. After 5 aliquots a white precipitate formed. The solution was filtered, and the solvent removed *in vacuo* to afford the product as white solid.[10]

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 1.13 (d, *J*=8.00 Hz, 6H) 1.33 (m, 16H) 1.98 (br. s, 2 H) 3.72 (m, 2H)
^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm 23.62 (CH_2) 25.95 (CH_2) 29.73 (CH_2) 29.83 (CH_2) 29.53 (CH_3) 68.21 (CHOH)

Oxidative Functionalization



Bis(1,1,1,3,3,3-hexafluoropropan-2-yl) heptanedioate (12) (0.768 g, 77%) was prepared from 1,7-heptanediol (0.676 g, 5 mmol, 1 equiv) using the procedure outlined above for oxidation, followed by subsequent oxidative functionalization using previously published method.[11] To the resulting solution of 1,7-heptanedialdehyde (5 mmol), filtered off the silica gel and oxoammonium salt slurry, was added pyridine (10.085 g, 127.5 mmol, 25.5 equiv) and hexafluoroisopropanol (5.041 g, 30 mmol, 6 equiv). After stirring for 5 min, the oxoammonium salt (7.502 g, 25 mmol, 5 equiv) was added all at once. The flask was sealed with a rubber septum and stirred until the solution turned red. Once the reaction was determined complete by TLC, the hexafluoroisopropanol and CH_2Cl_2 was removed *in vacuo*. Pentane or diethyl ether was

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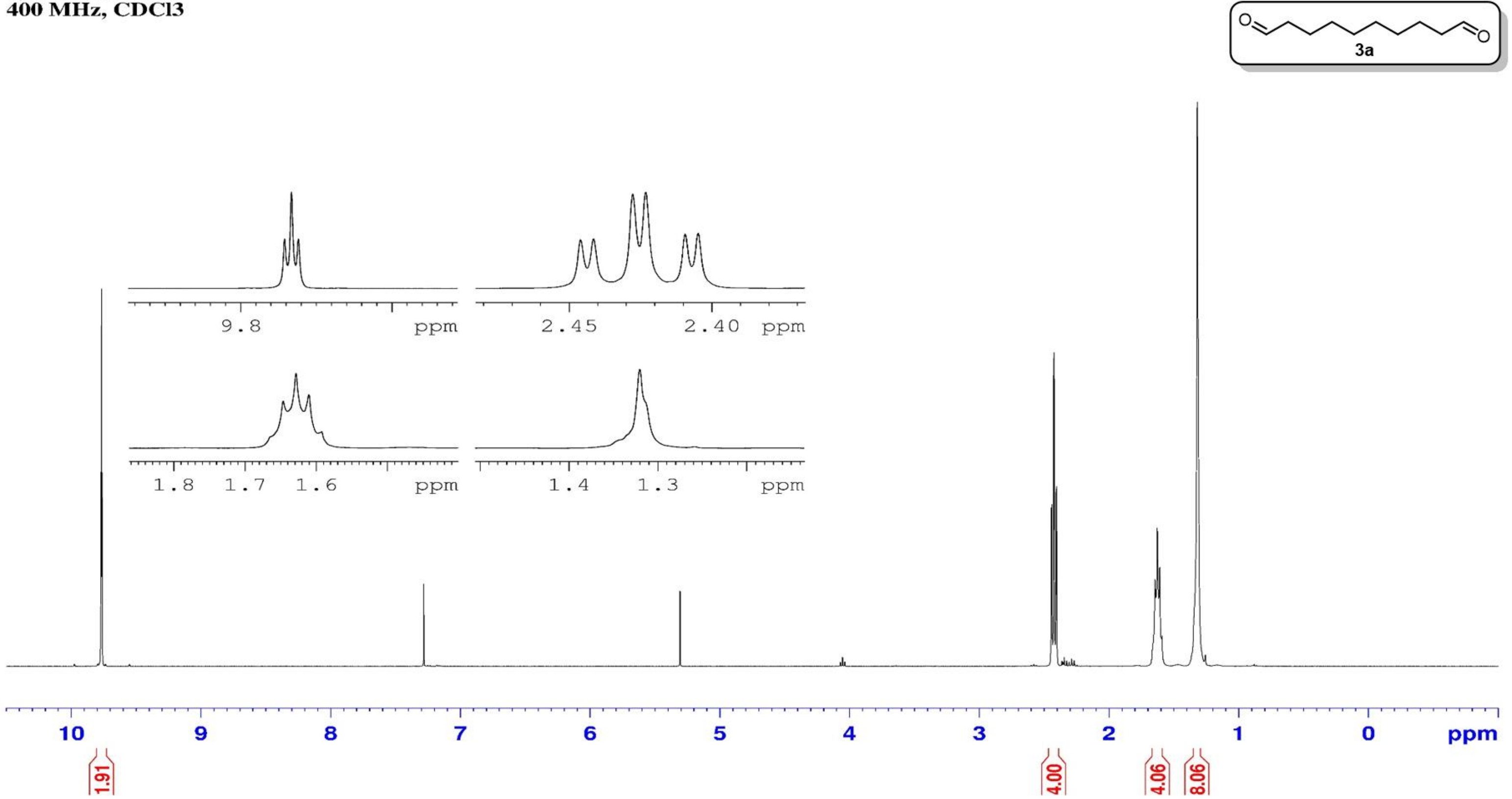
[11] C. B. Kelly, M. A. Mercadante, R. J. Wiles, N. E. Leadbeater, *Org. Lett.* **2013**, *15*, 2222-2225.

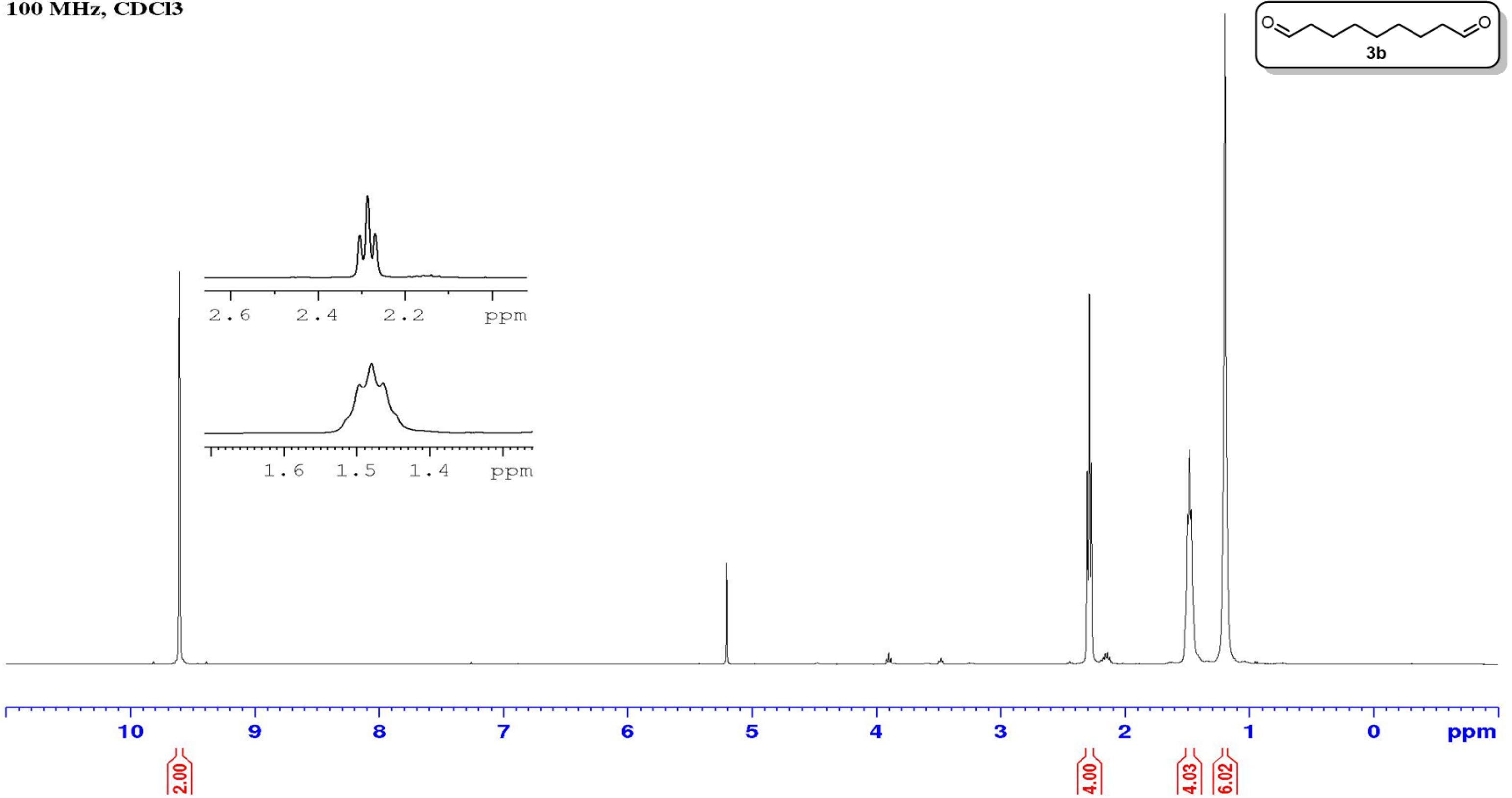
added to the resulting slurry to precipitate the nitroxide. After stirring for 5 min, the solution was filtered through a fritted funnel with medium porosity and transferred to a separatory funnel. The organic layer was washed with 1 M HCl (2×150 mL), deionized water (150 mL), and brine (150 mL). The organic layer was dried over sodium sulfate, and the solvent was removed *in vacuo*, affording the ester as a pale yellow oil. (Note: The CH_2Cl_2 may be removed *in vacuo* before the oxidative functionalization, however the reaction is slightly exothermic. With this particular substrate, the formation of the nitroxide, and subsequent red color, occurs within 5 min when concentrated and within 30 min when dilute).

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 1.42 (m, 2H) 1.74 (m, J = 7.6 Hz, 2H), 2.53 (t, J = 7.3 Hz, 4H), 5.77 (m, J = 6.1 Hz, 2H),
^{13}C NMR ($CDCl_3$, 100 MHz) δ ppm 24.29 (CH_2) 28.17 (CH_2) 33.23 (CH_2) 66.69 (m, $J_{O\text{-}CH\text{-}(CF3)2}$=34.74 Hz) 120.71 (q, $J_{C\text{-}F3)2}$ = 282.77 Hz) 170.25 (CO)
^{19}F NMR ($CDCl_3$, 377 MHz) δ ppm -76.56 (s, 6 F), -76.57 (s, 6 F)
HRMS (ESI+), calcd for $C_{13}H_{12}F_{12}O_4$ [MH]+, calc. 461.0622, obs. 461.0635; [MNH4]+, calc. 478.0888, obs. 478.0888
FT-IR (neat, ATR, cm^{-1}) 2996-2852 (w, b) 1774 (s) 1381 (m) 1357 (m) 1287 (s) 1267 (m) 1229 (s) 1193 (vs) 1103 (vs) 901 (s) 730 (w) 689 (s) 529 (w) 488 (w)

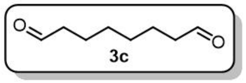
1,10–Decanedial
400 MHz, CDCl3



1,9-Nonanedial
100 MHz, CDCl3



1,8–Octanedial
400 MHz, CDCl3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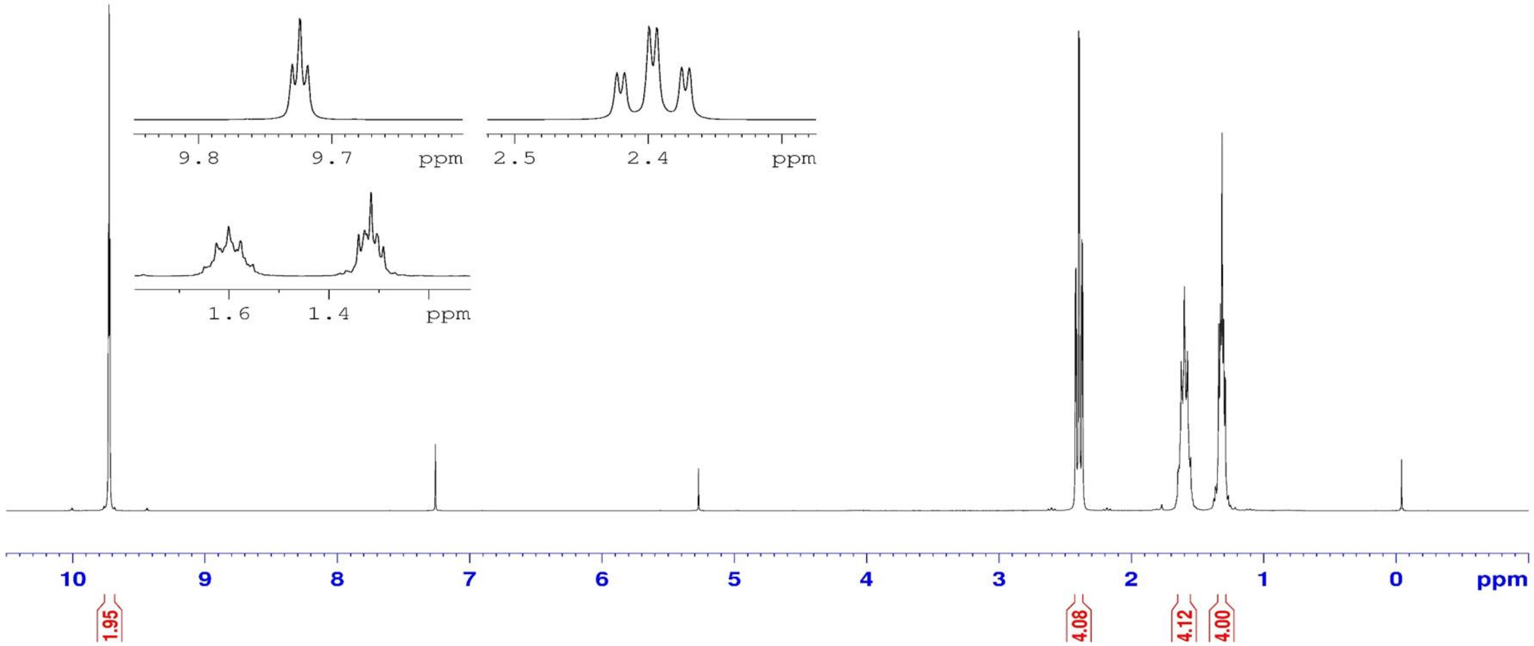
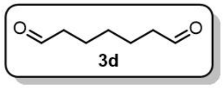
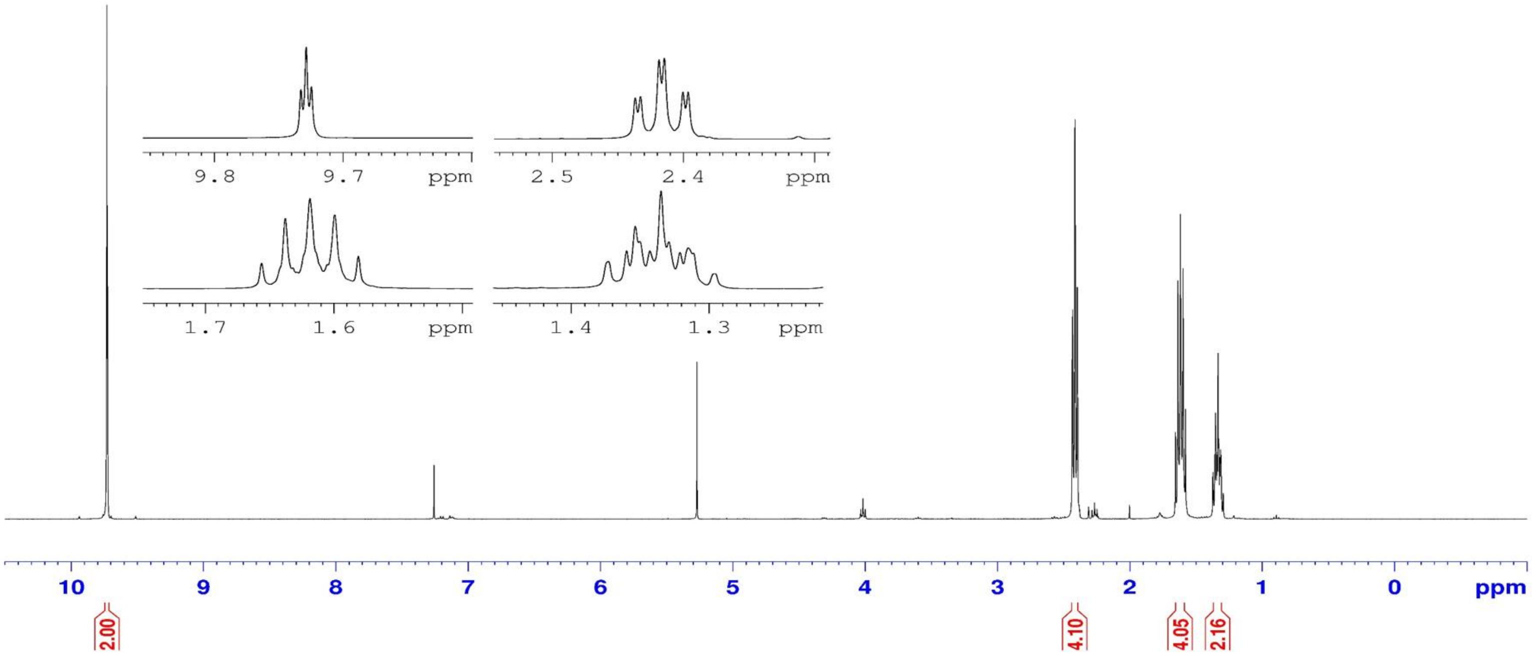
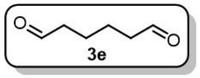


Heptanedialdehyde
400 MHz, CDCl3

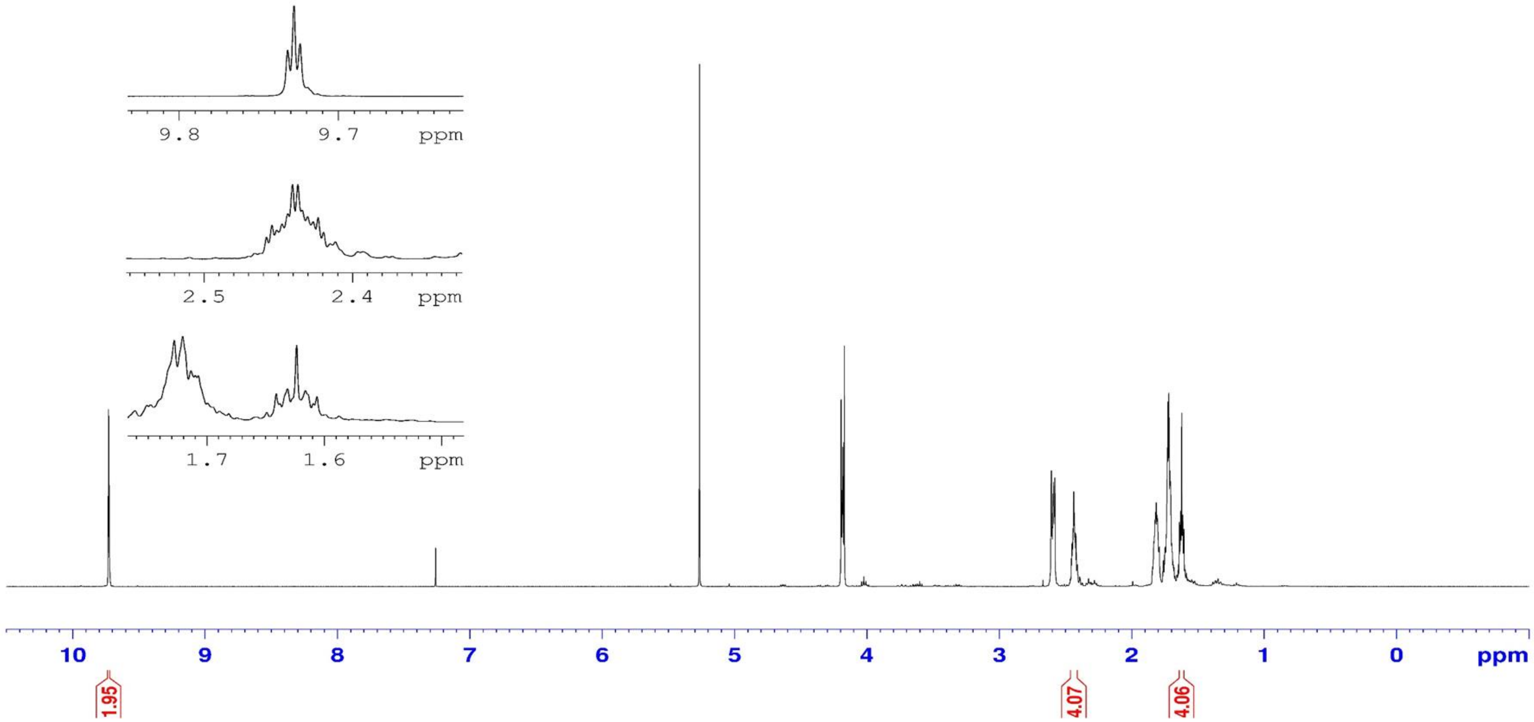

3d



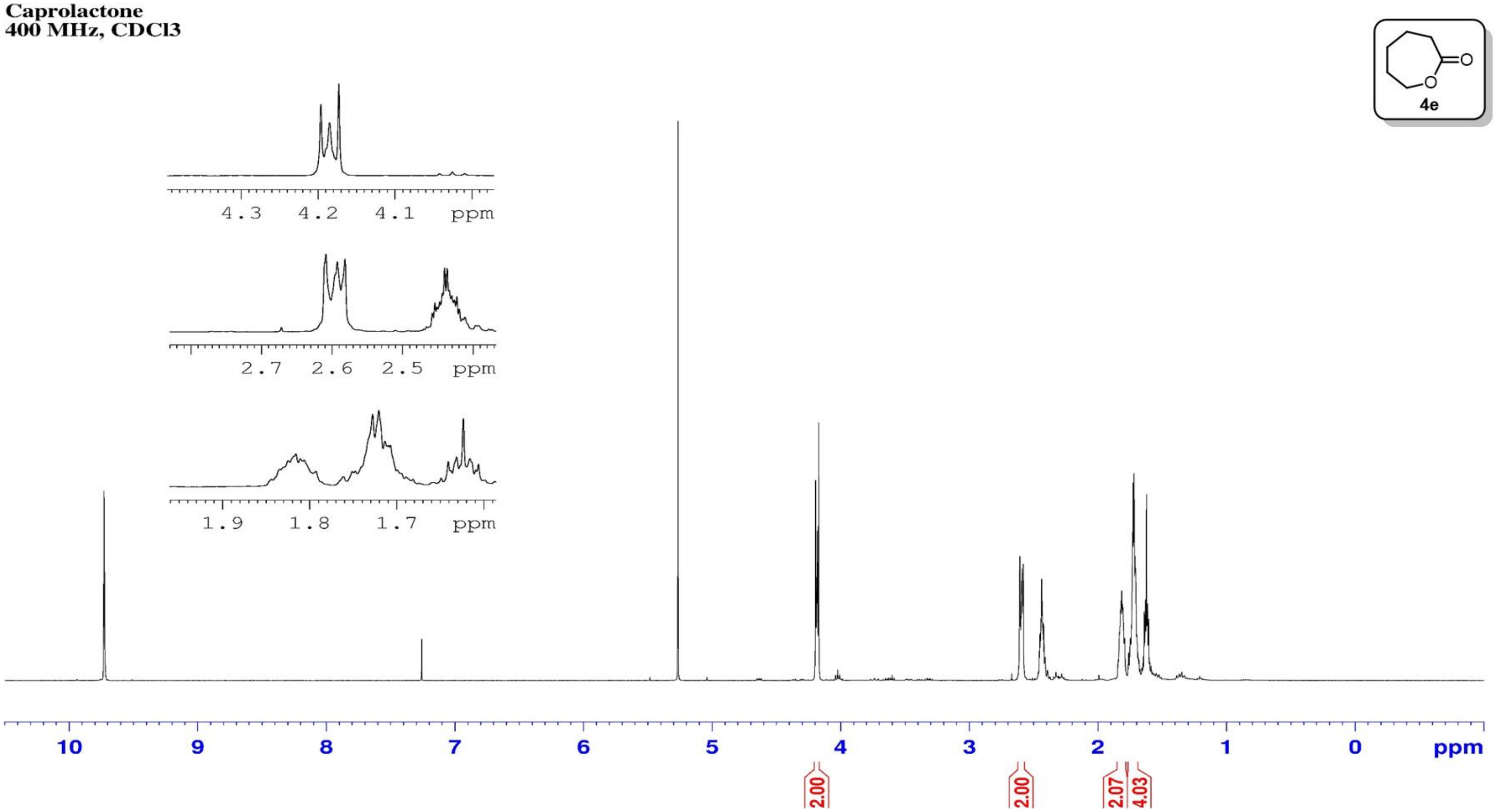
Adipaldehyde
400 MHz, CDCl3



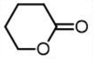
3e



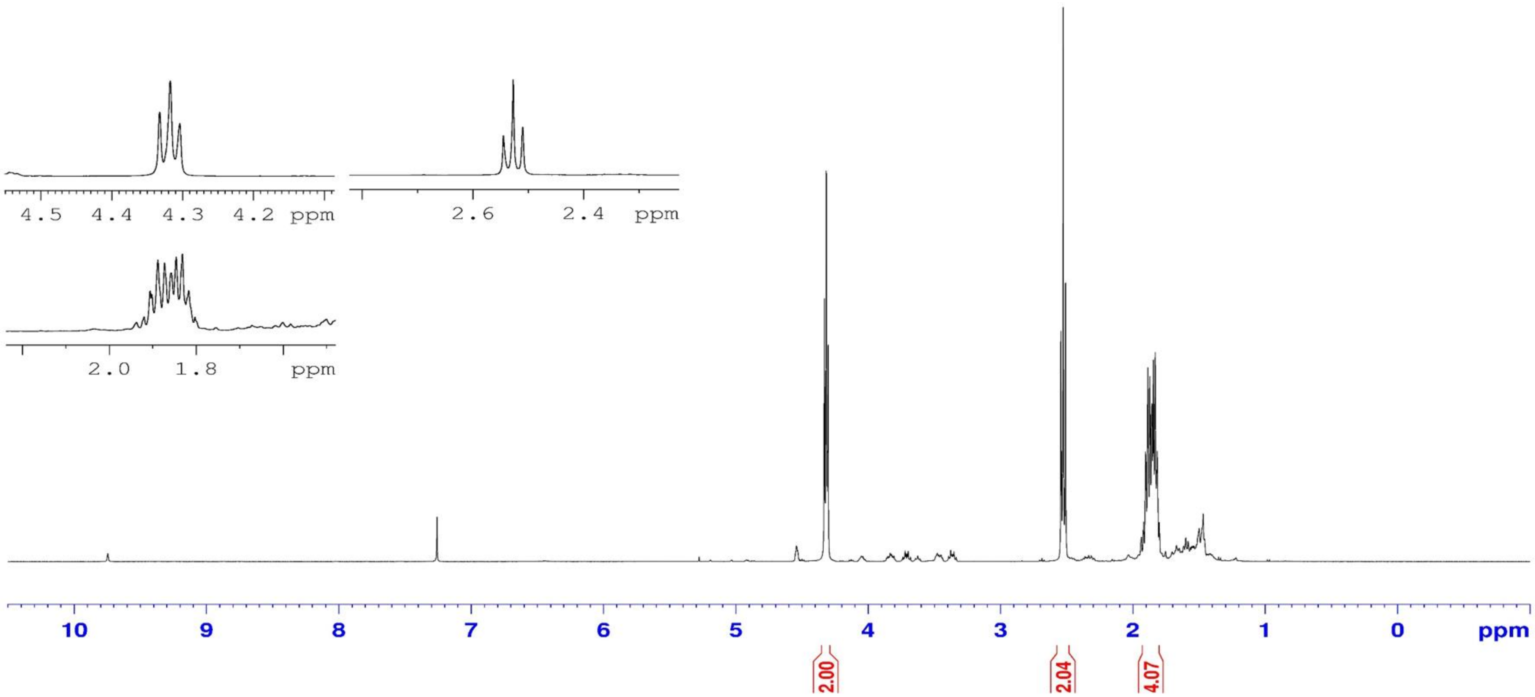
Caprolactone
400 MHz, CDCl3

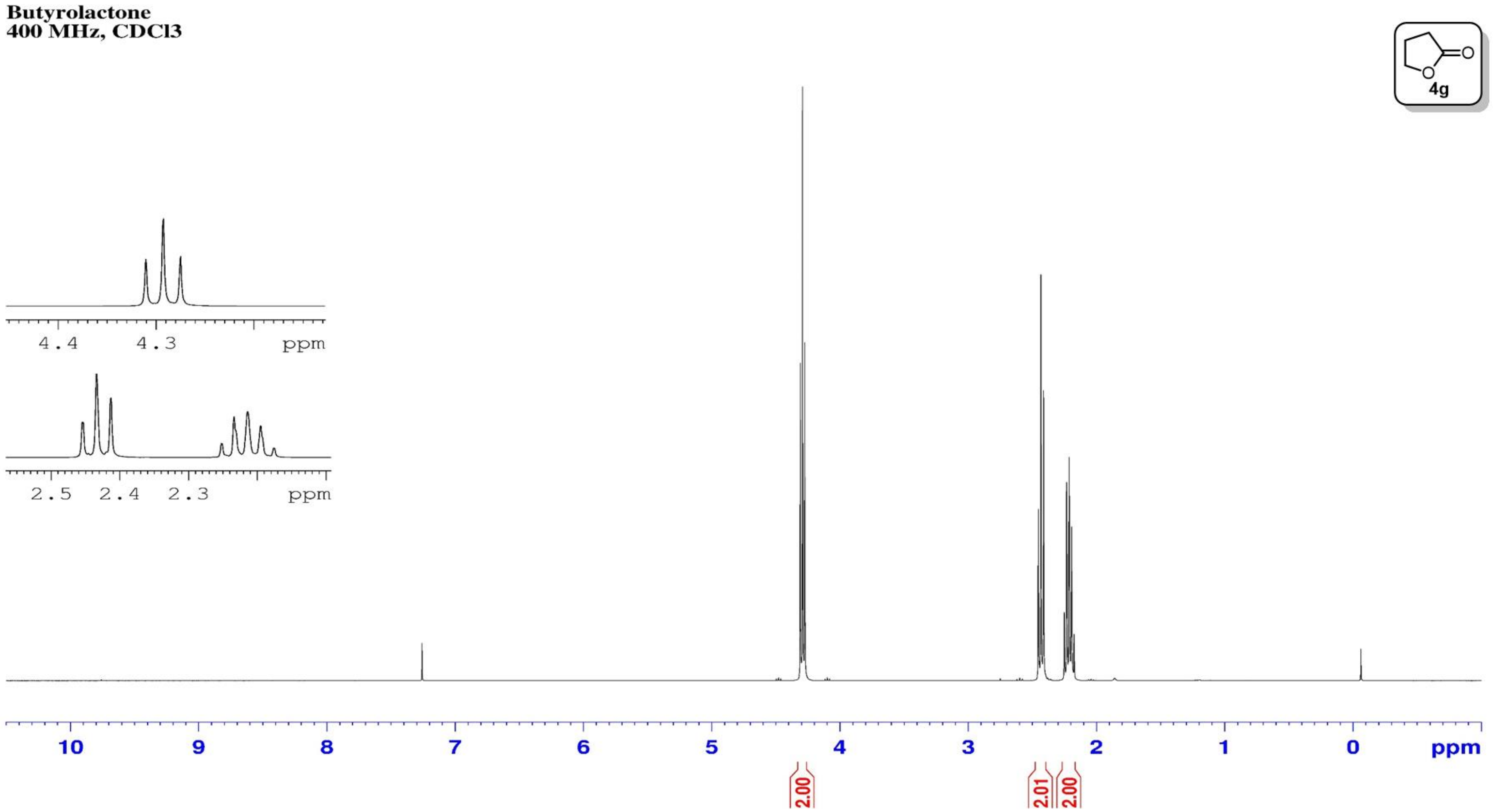


δ−Valerolactone
400 MHz, CDCl3

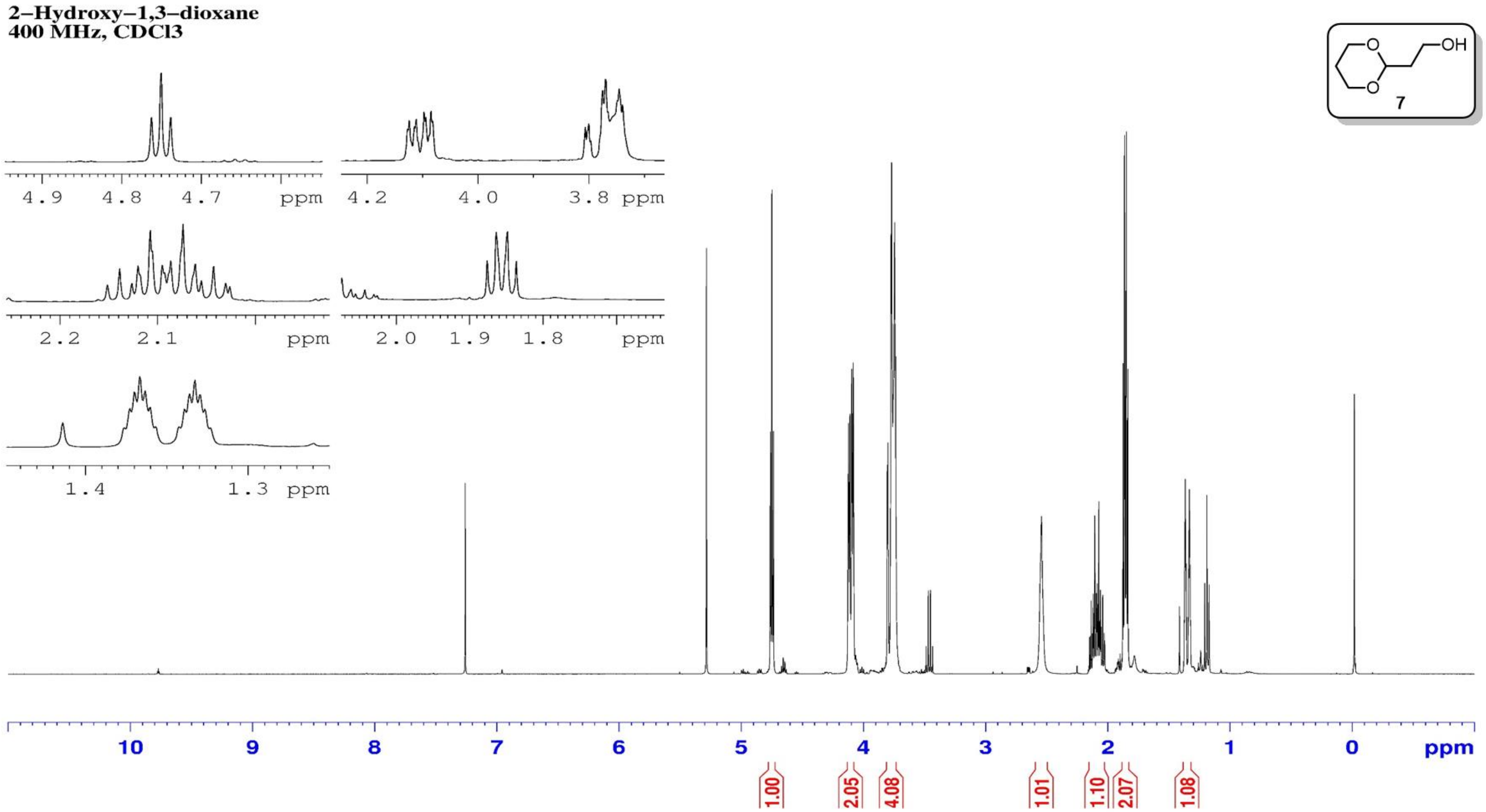


4f

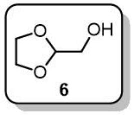




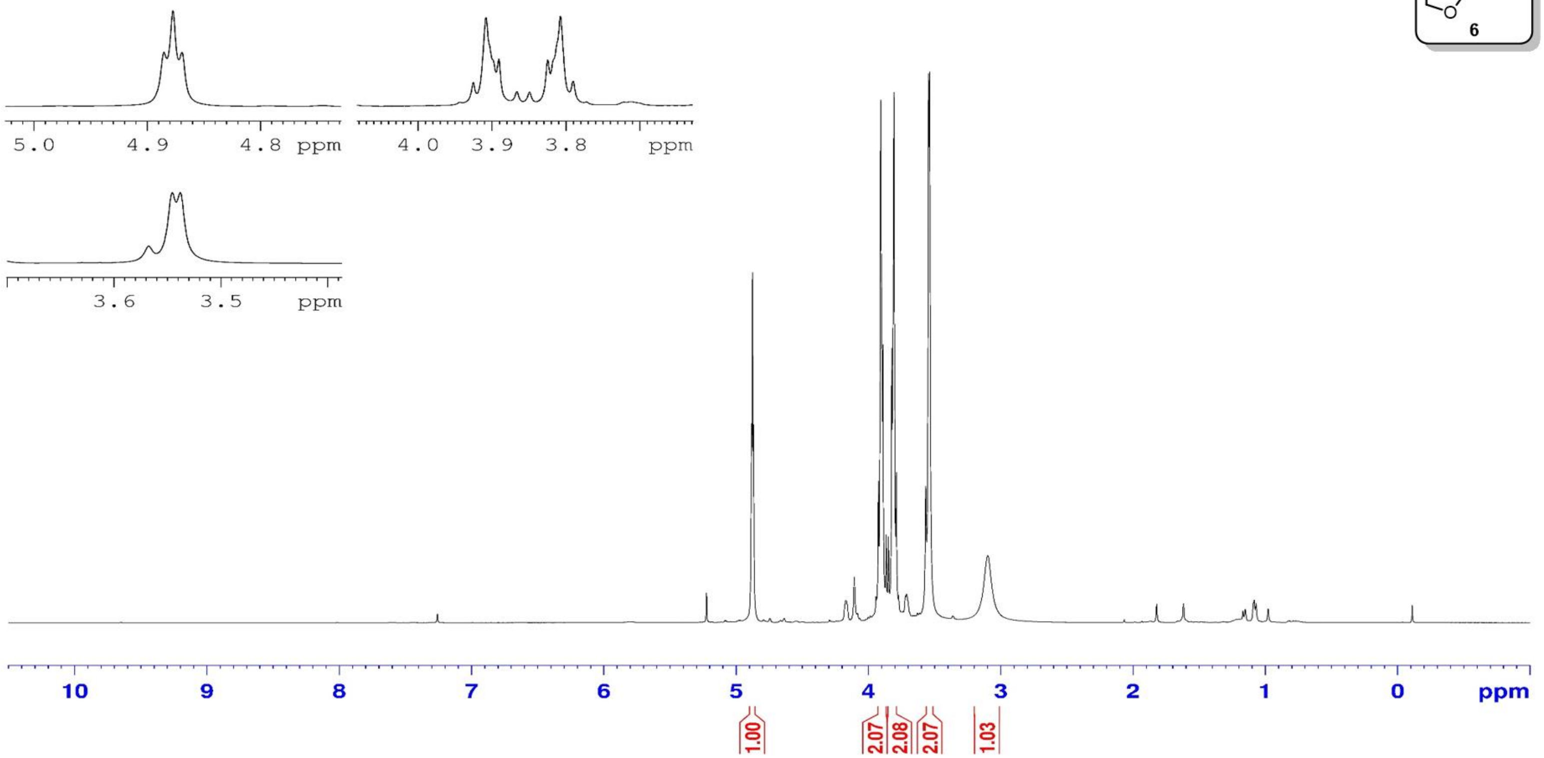
Butyrolactone
400 MHz, CDCl3


2–Hydroxy–1,3–dioxane
400 MHz, CDCl3
O
O
OH
7
4.9
4.8
4.7
ppm
4.2
4.0
3.8 ppm
2.2
2.1
ppm
2.0
1.9
1.8
ppm
1.4
1.3 ppm
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.05
4.08
1.01
1.10
2.07
1.08

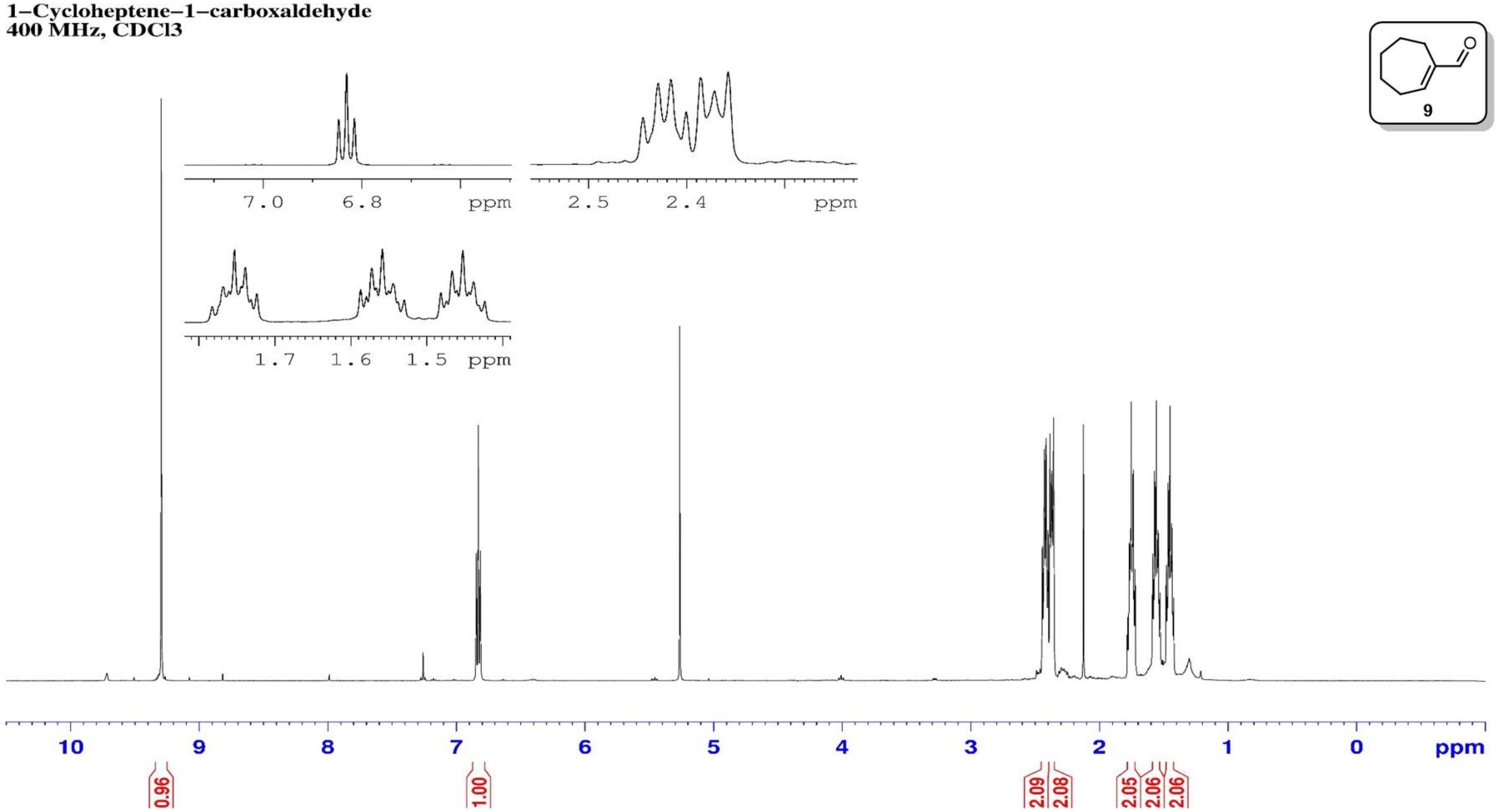
2–Hydroxymethyl–1,3–dioxolane
400 MHz, CDCl3

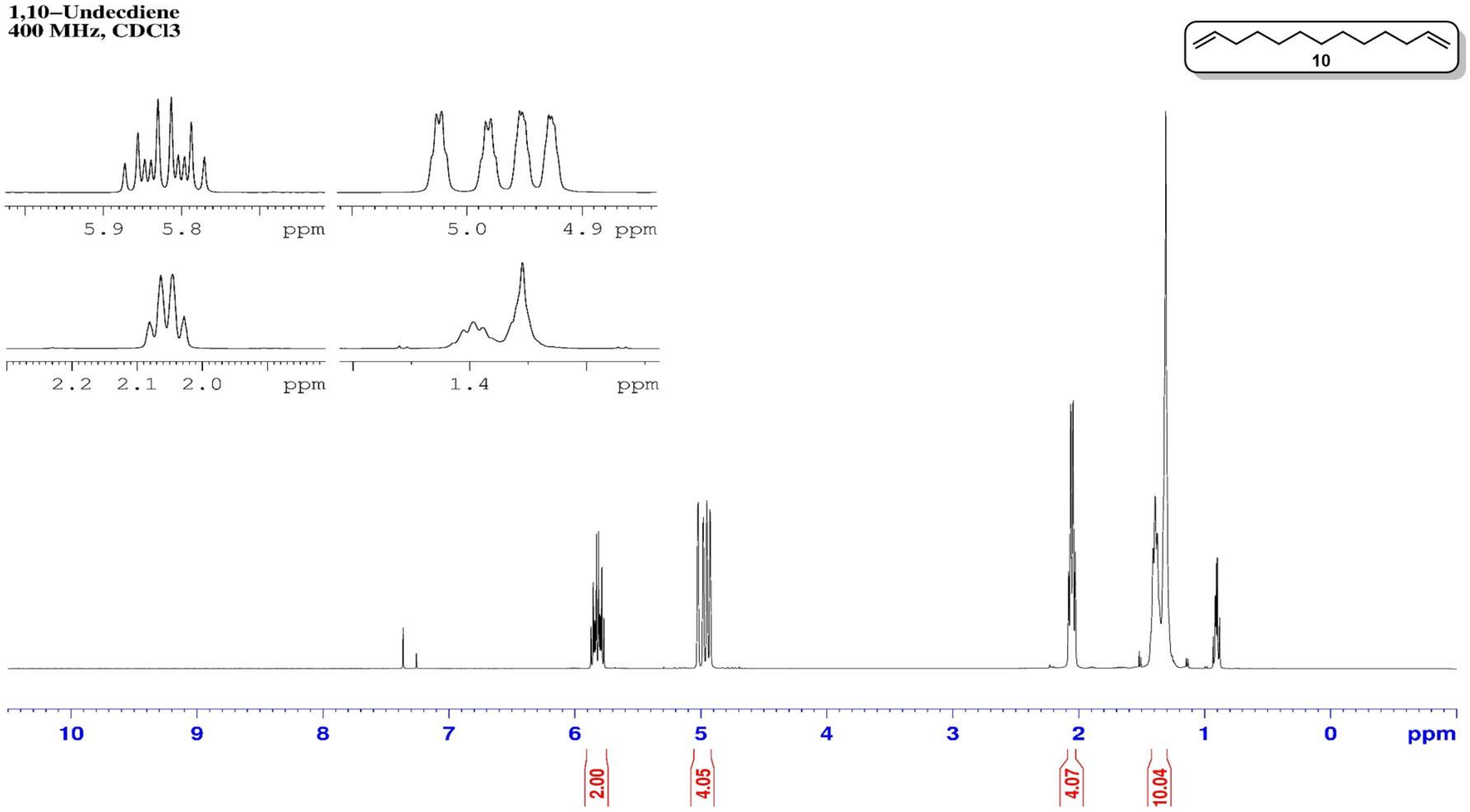


6

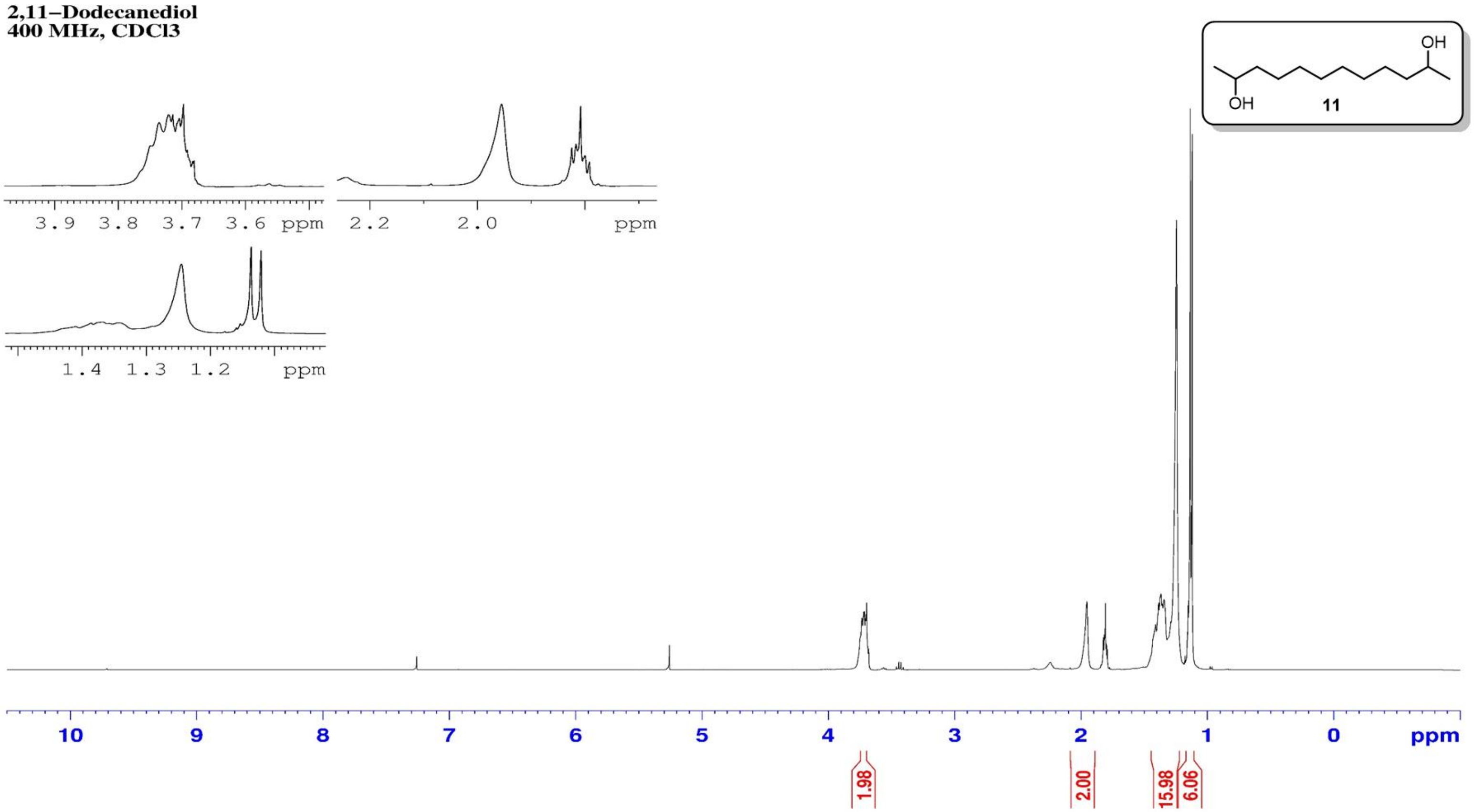


1–Cycloheptene–1–carboxaldehyde
400 MHz, CDCl3

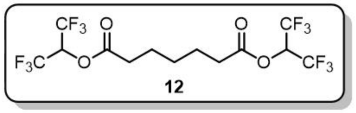




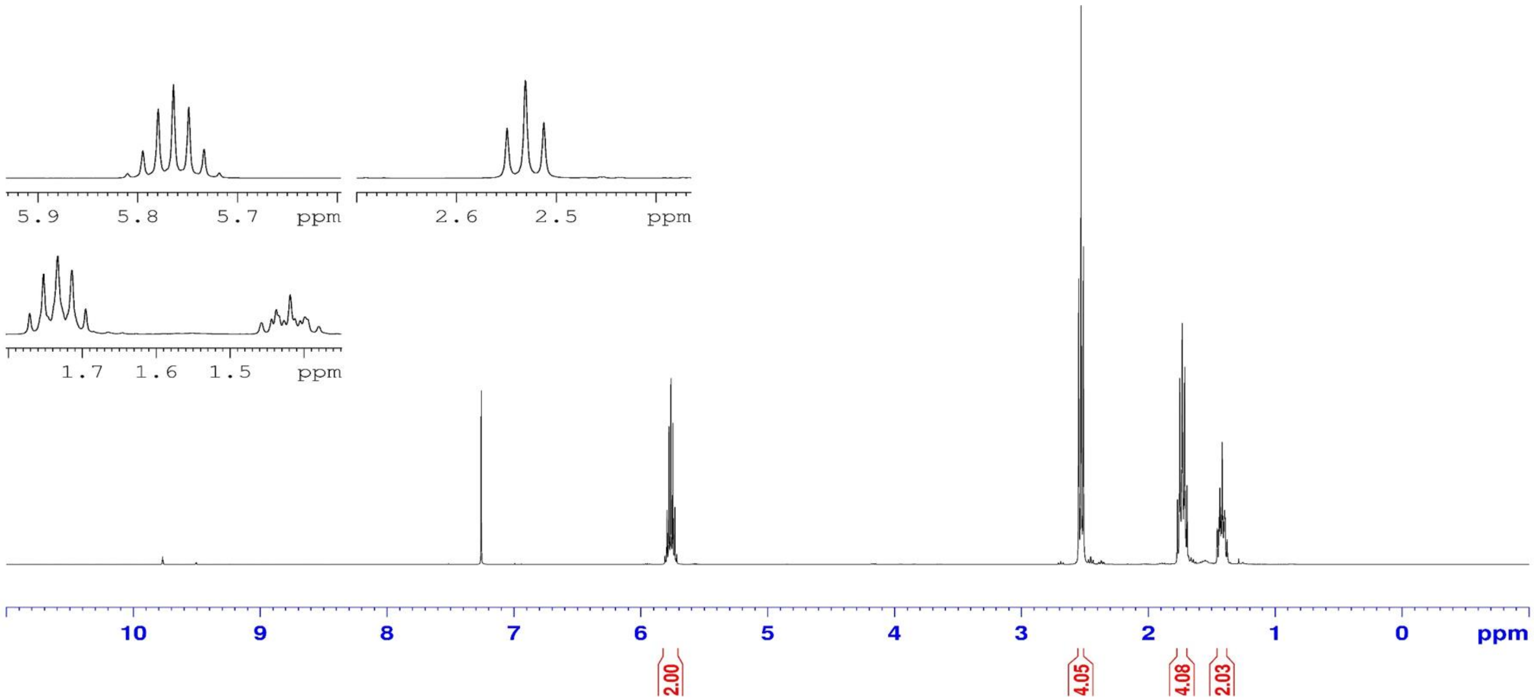
1,10–Undecdiene
400 MHz, CDCl3

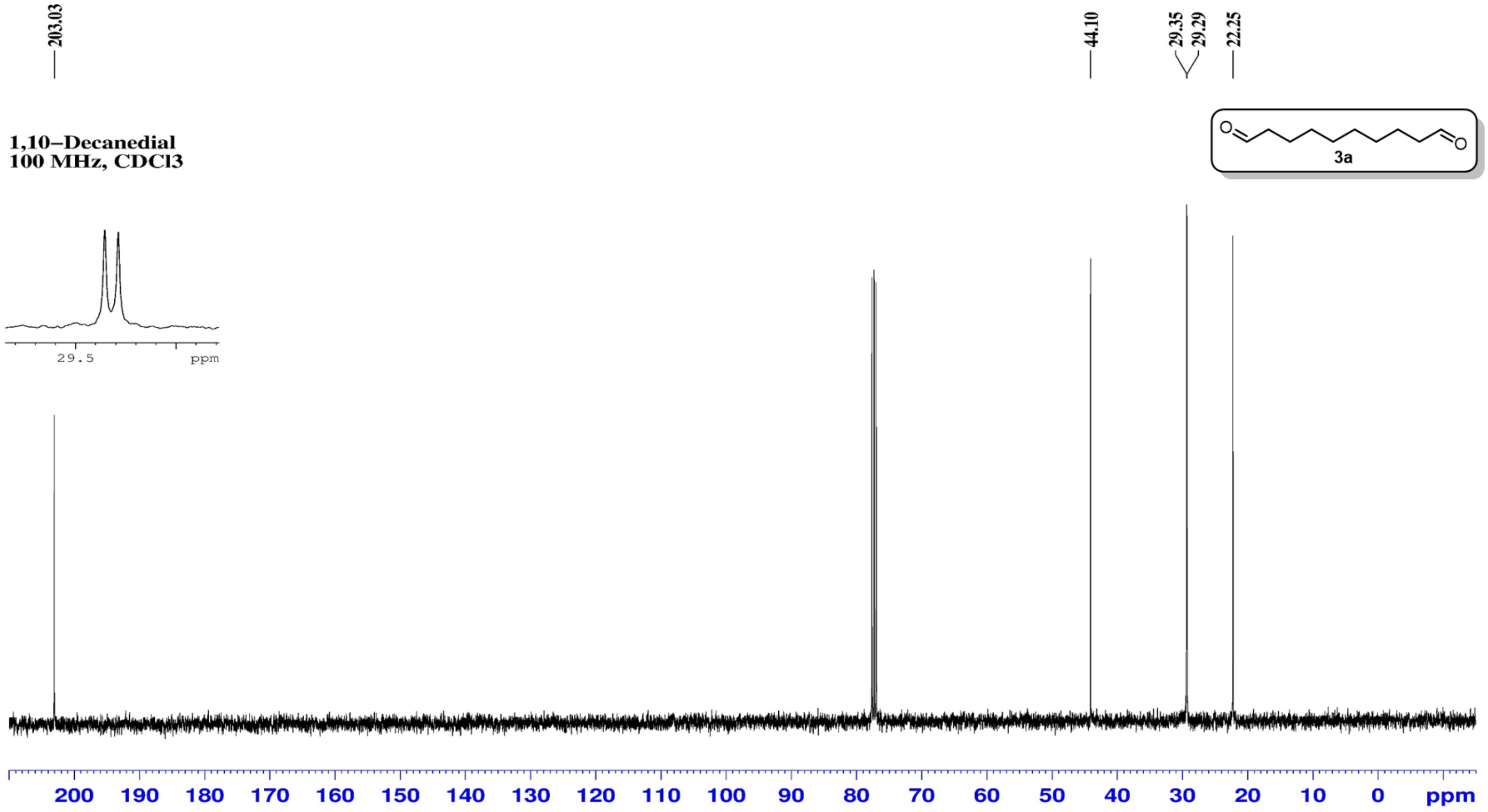

2,11−Dodecanediol
400 MHz, CDCl3
OH
OH
11
3.9 3.8 3.7 3.6 ppm
2.2 2.0 ppm
1.4 1.3 1.2 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.98
2.00
15.98
6.06

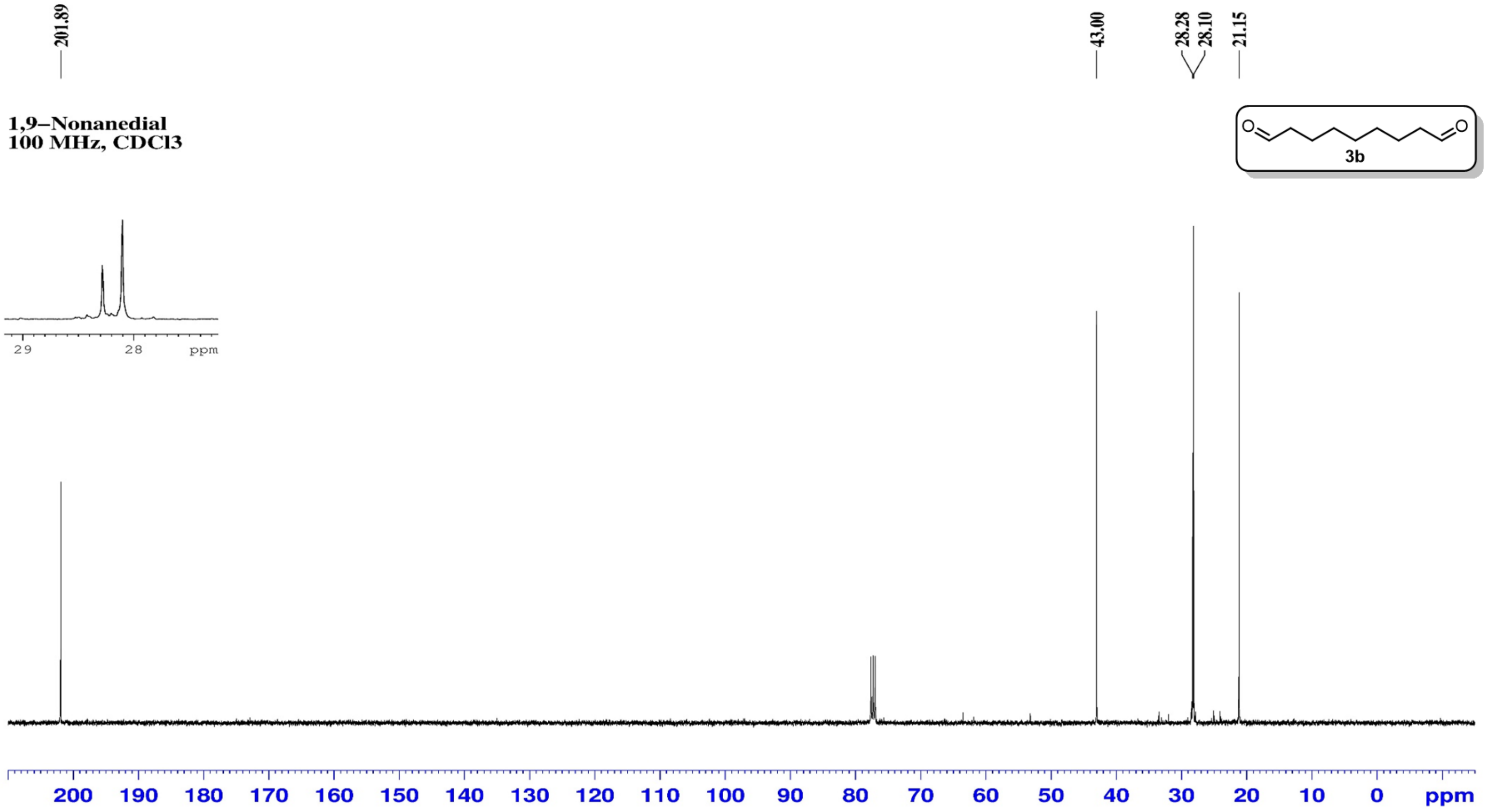
Bis(1,1,1,3,3,3−hexafluoropropan−2−yl) heptanedioate
400 MHz, CDCl3

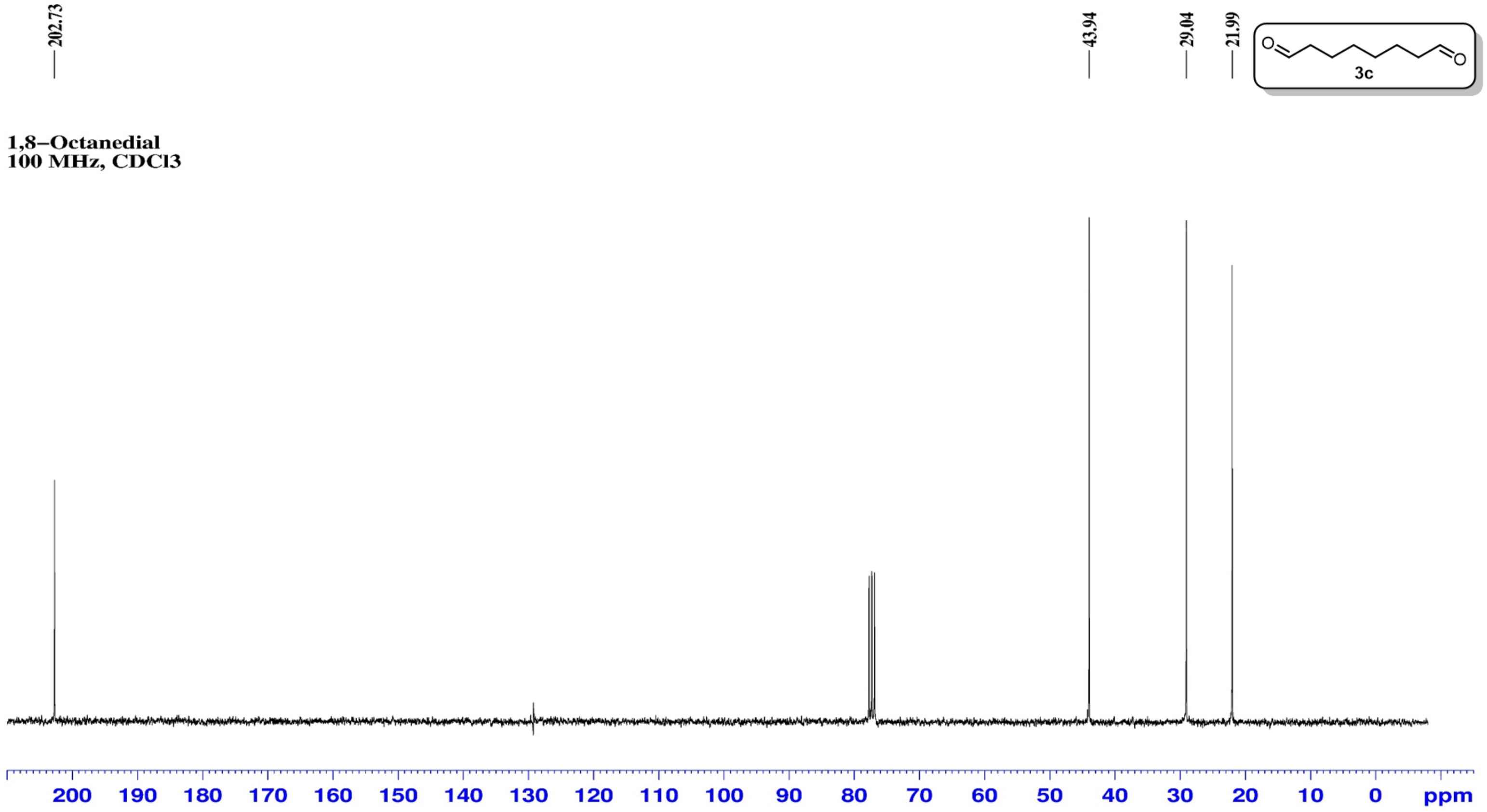


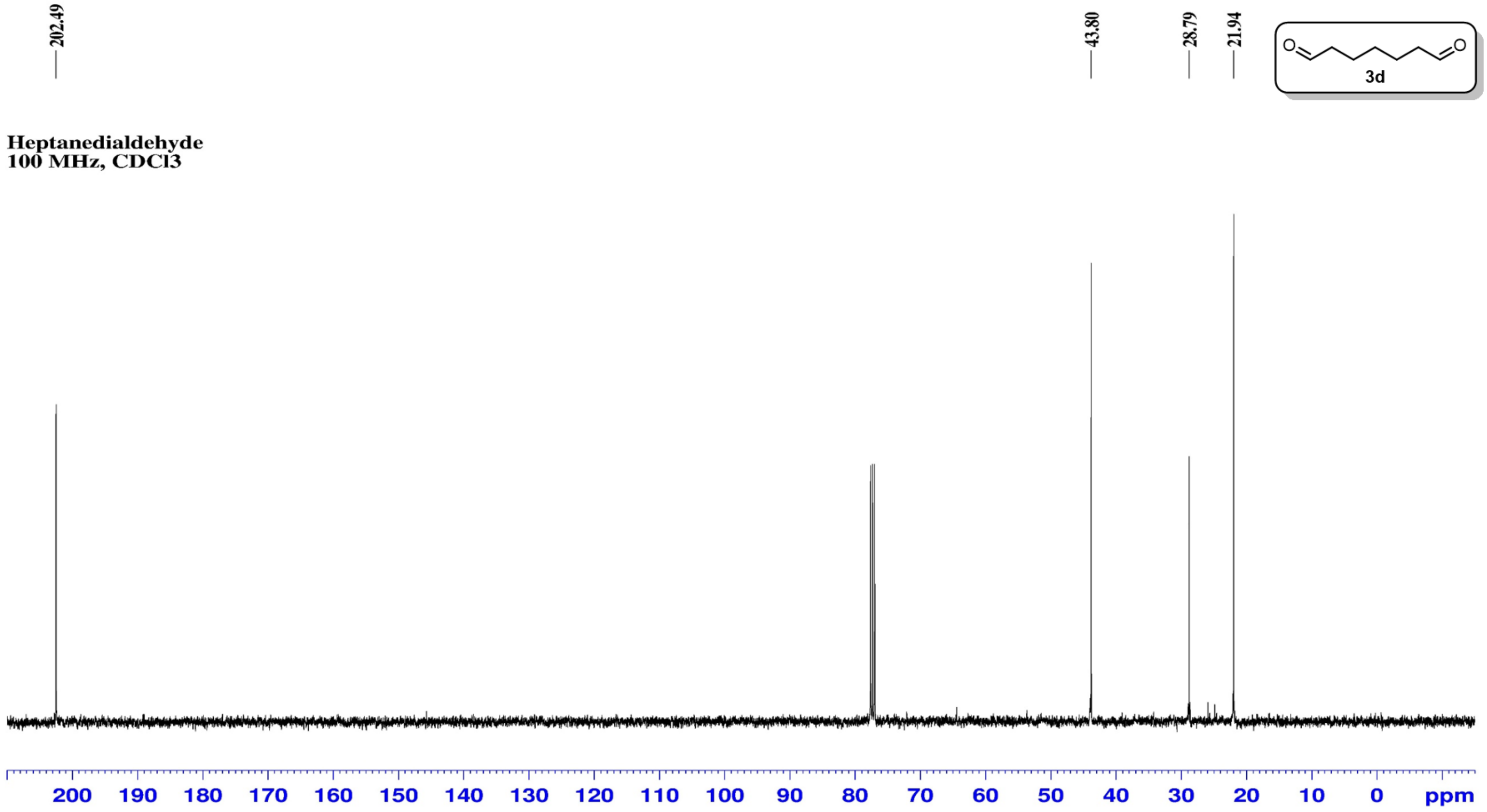
12

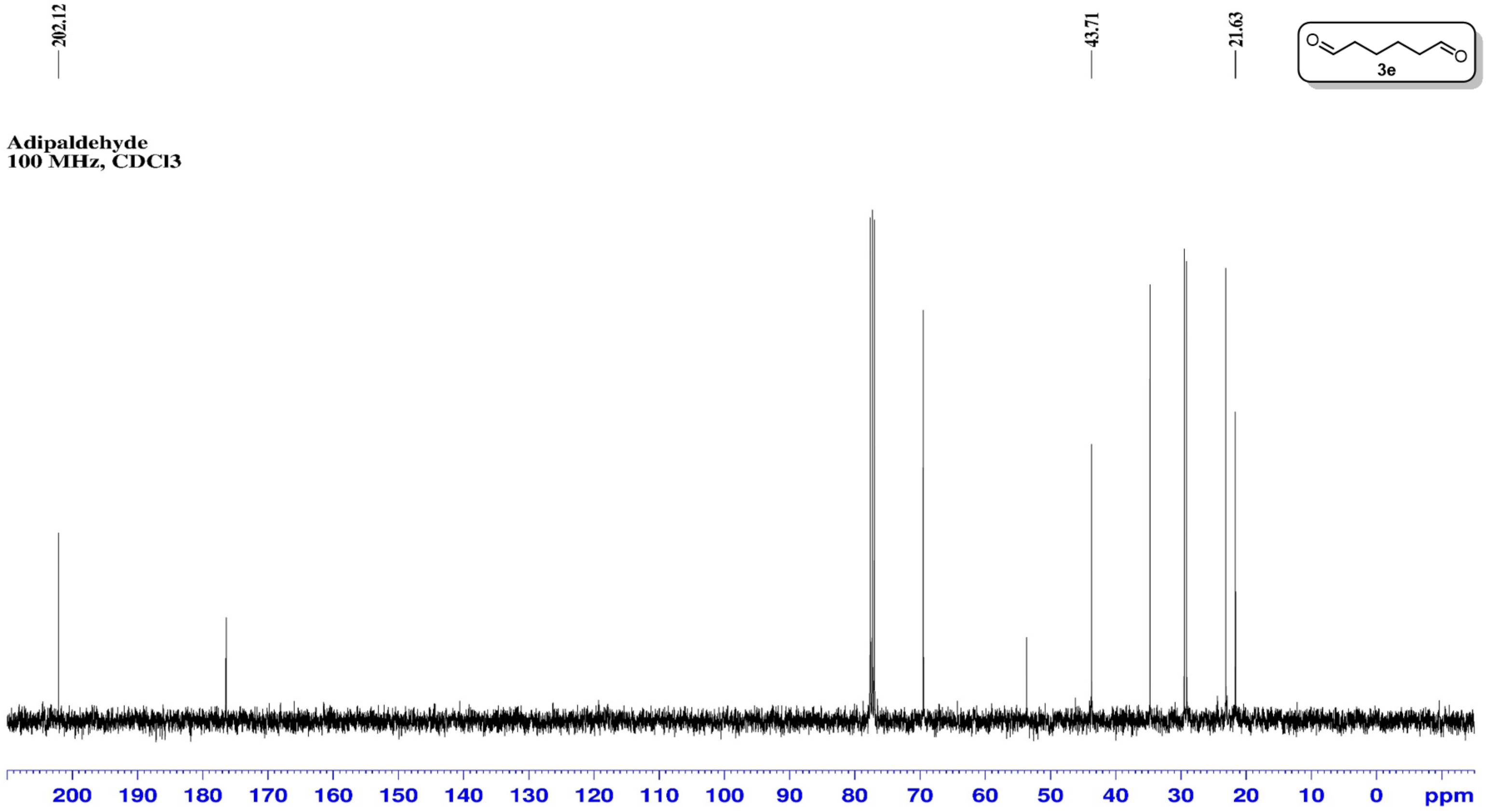



203.03
44.10
29.35
29.29
22.25
1,10−Decanedial
100 MHz, CDCl3
29.5
ppm
3a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

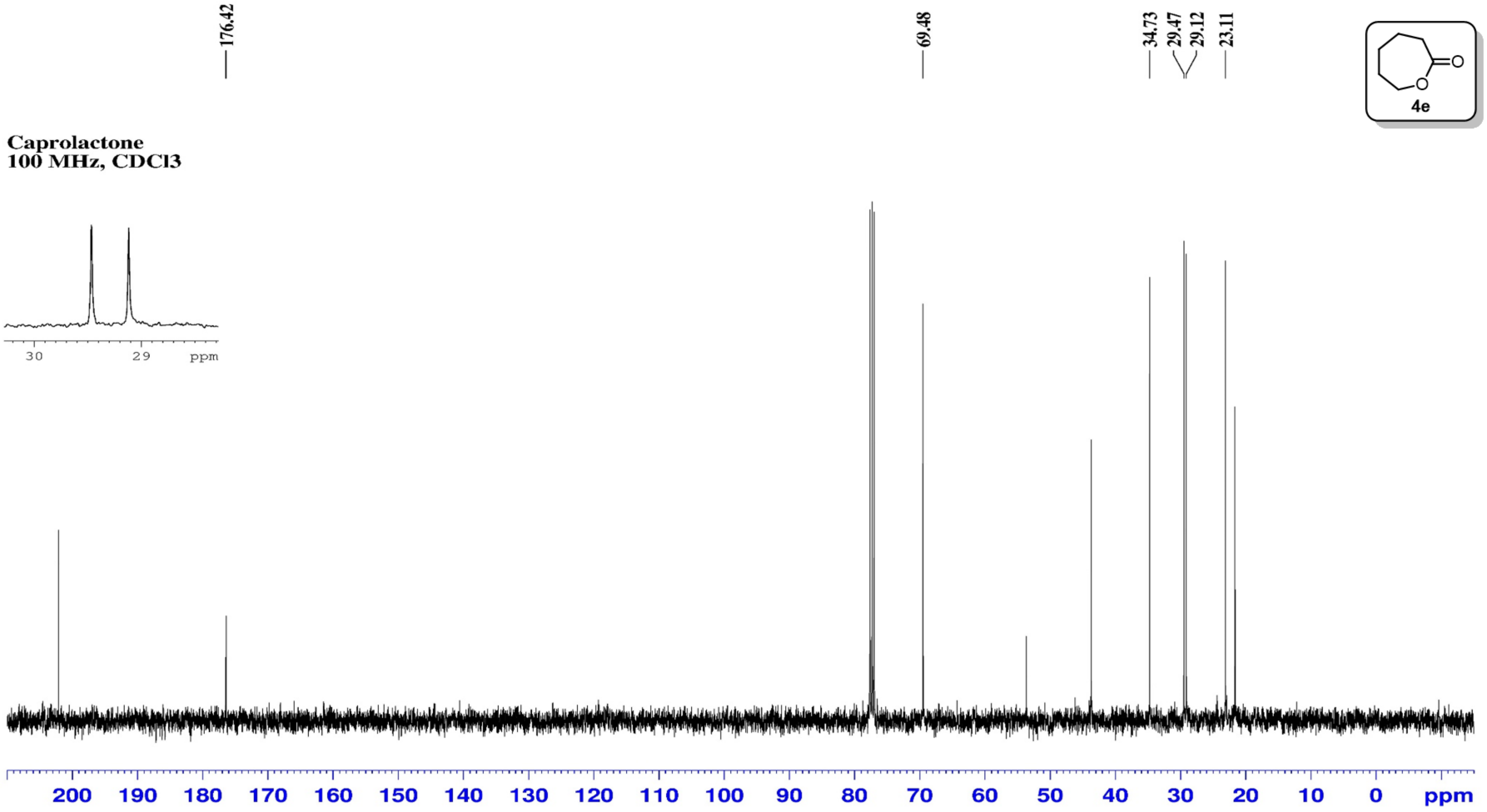

201.89
43.00
28.28
28.10
21.15
1,9–Nonanedial
100 MHz, CDCl3
O
O
3b
29
28
ppm
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

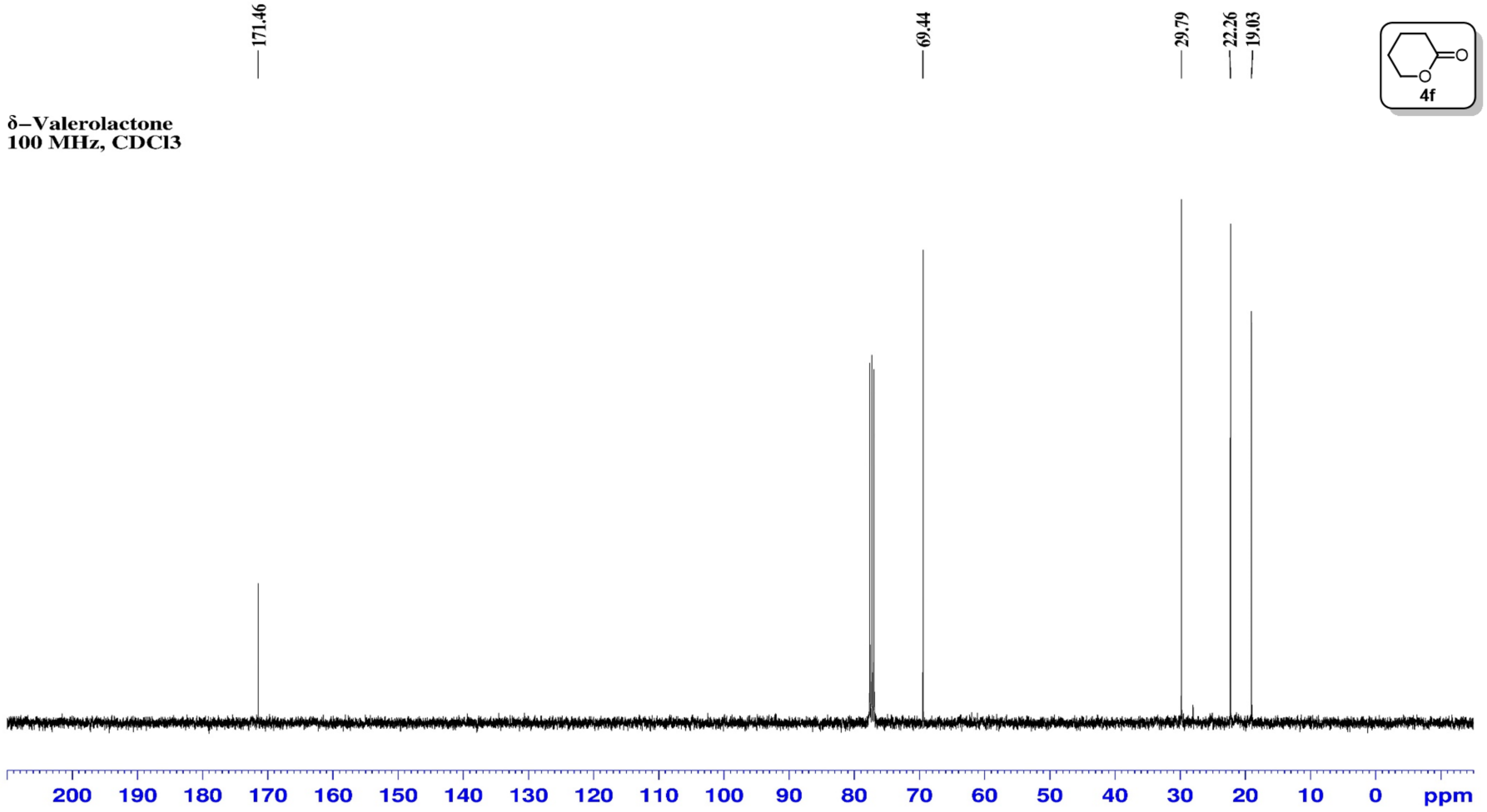

202.73
43.94
29.04
21.99
3c
1,8−Octanedial
100 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

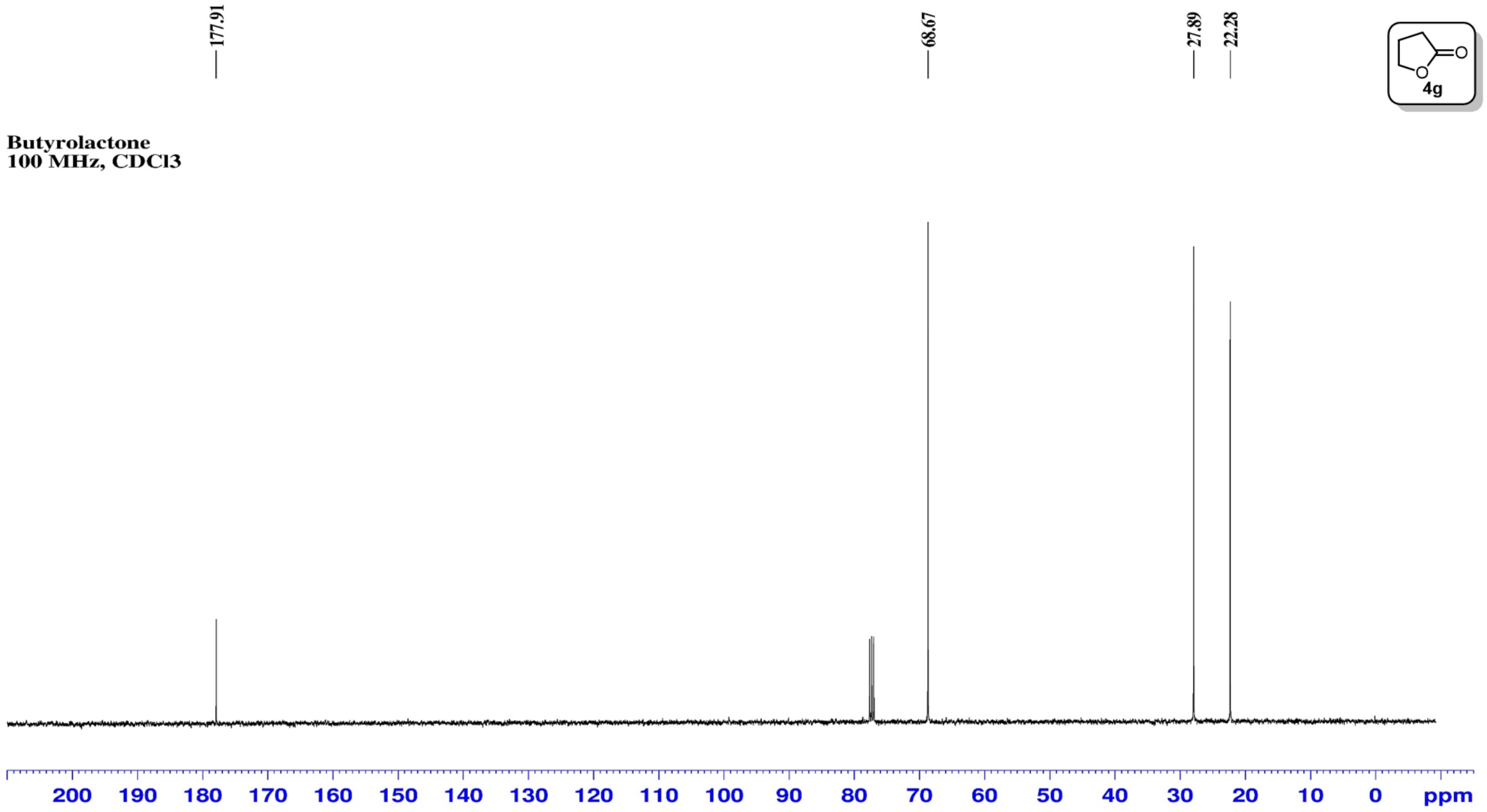

202.49
43.80
28.79
21.94
O
O
3d
Heptanedialdehyde
100 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

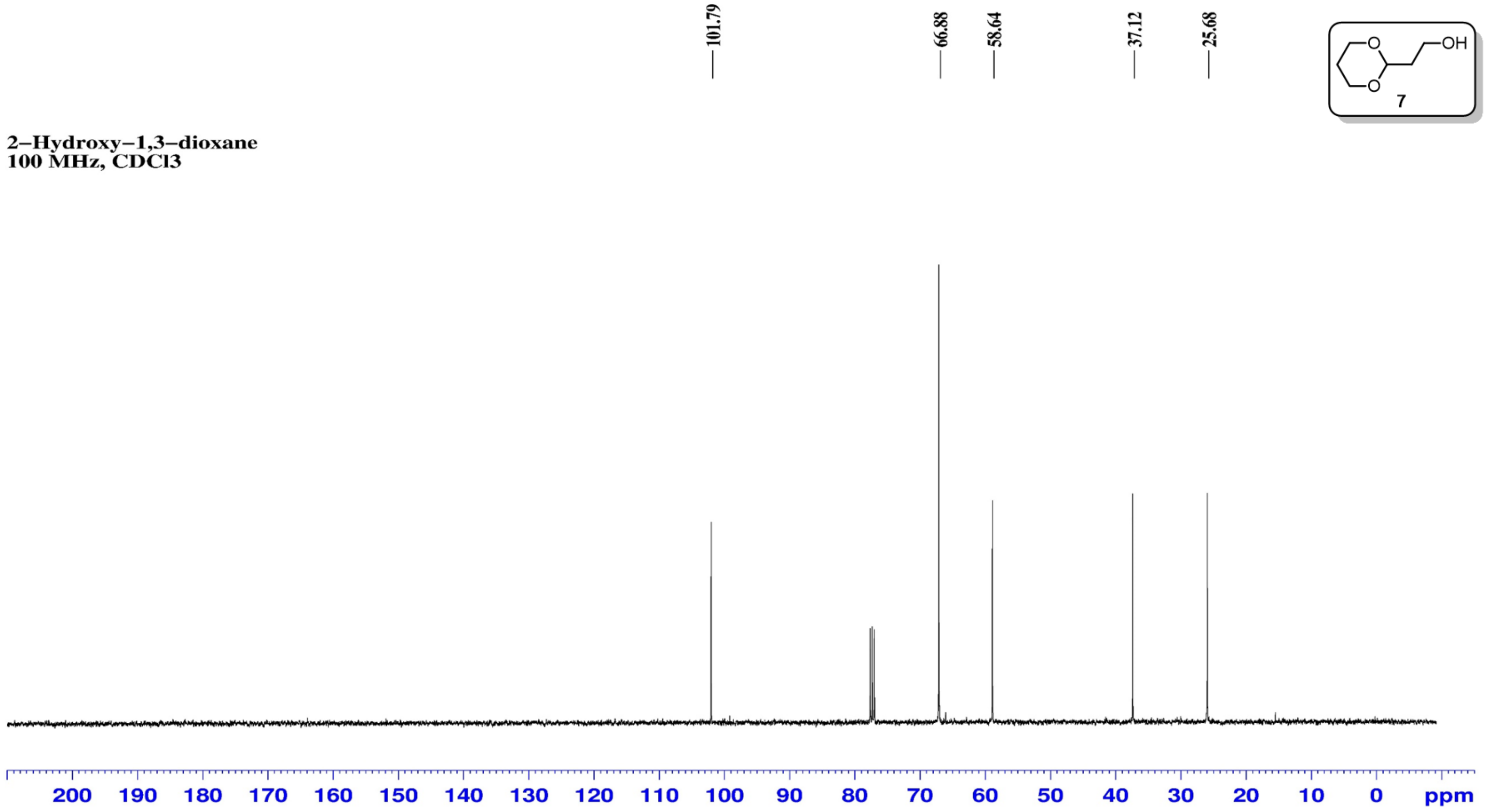

202.12
43.71
21.63
3e
Adipaldehyde
100 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

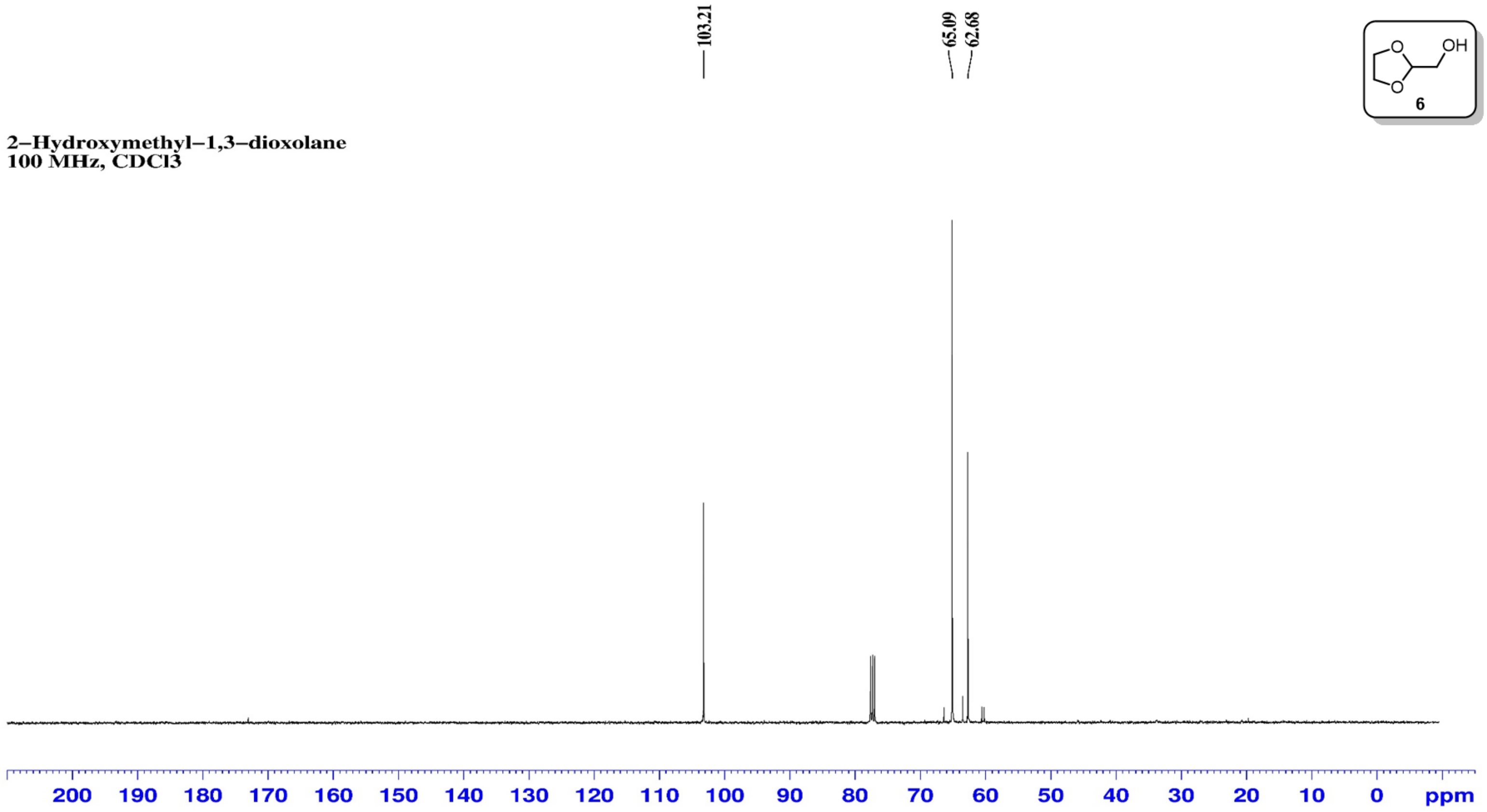
Caprolactone
100 MHz, CDCl3

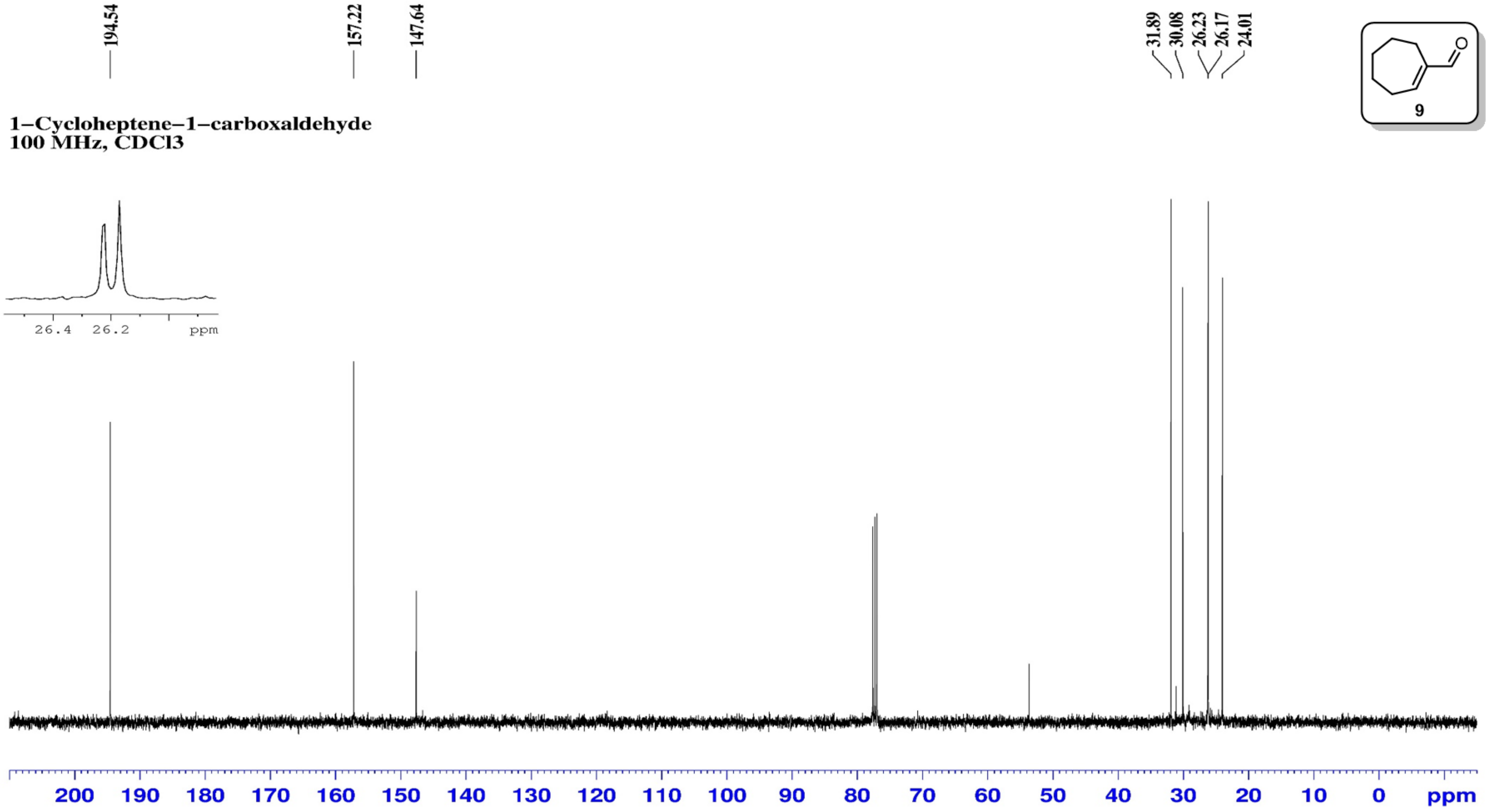


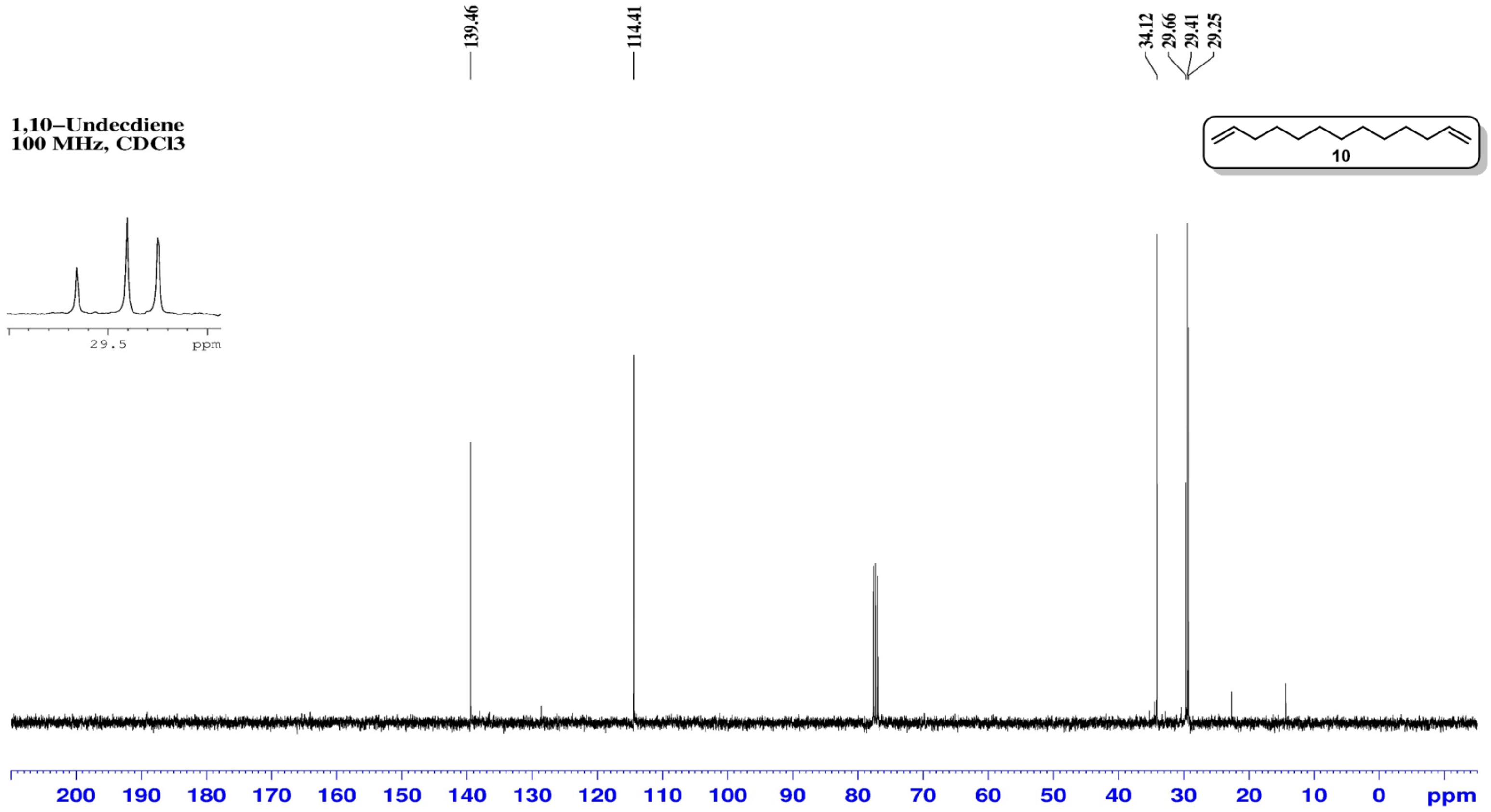

171.46
69.44
29.79
22.26
19.03
4f
δ−Valerolactone
100 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

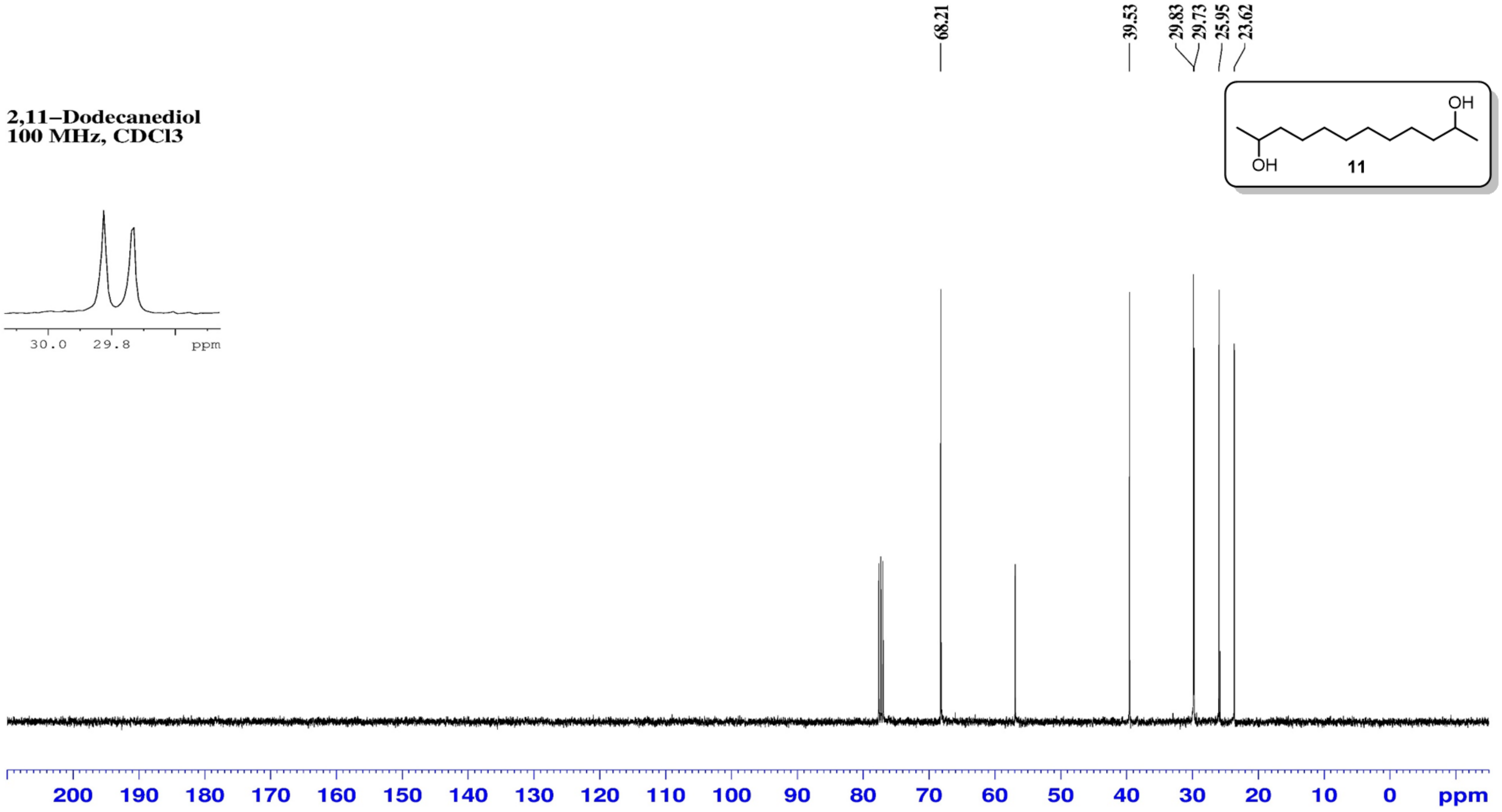

177.91
68.67
27.89
22.28
4g
Butyrolactone
100 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


101.79
66.88
58.64
37.12
25.68
2−Hydroxy−1,3−dioxane
100 MHz, CDCl3
O
O
OH
7
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

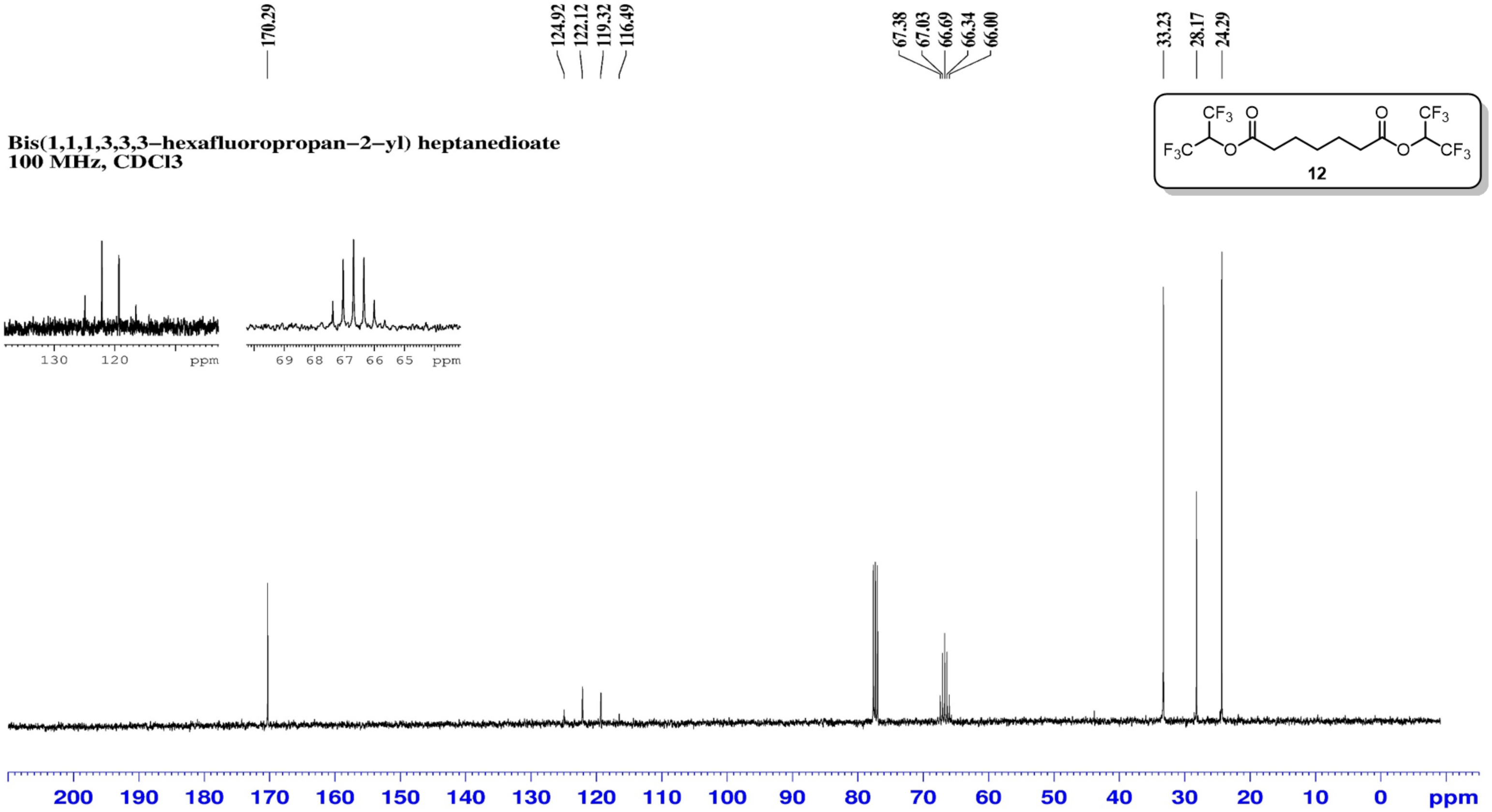

2−Hydroxymethyl−1,3−dioxolane
100 MHz, CDCl3
103.21
65.09
62.68
OH
O
O
6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


194.54
157.22
147.64
31.89
30.08
26.23
26.17
24.01
1−Cycloheptene−1−carboxaldehyde
100 MHz, CDCl3
26.4
26.2
ppm
9
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

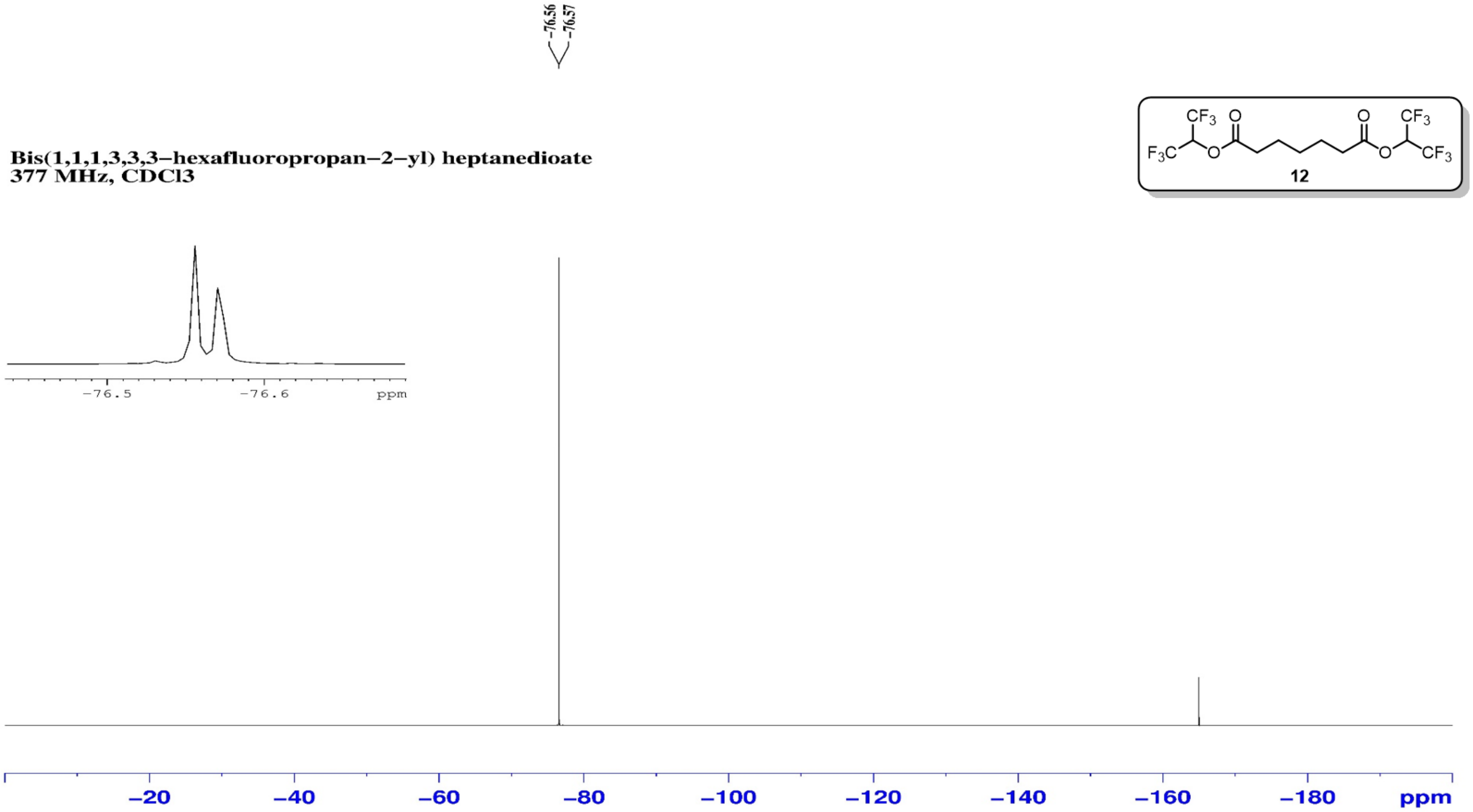

1,10–Undecdiene
100 MHz, CDCl3
139.46
114.41
34.12
29.66
29.41
29.25
10
29.5
ppm
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


2,11−Dodecanediol
100 MHz, CDCl3
68.21
39.53
29.83
29.73
25.95
23.62
OH
OH
11
30.0
29.8
ppm
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

Bis(1,1,1,3,3,3-hexafluoropropan-2-yl) heptanedioate
100 MHz, CDCl3



12


-76.56
-76.57
Bis(1,1,1,3,3,3-hexafluoropropan-2-yl) heptanedioate
377 MHz, CDCl3
-76.5
-76.6
ppm
CF3
O
F3C
12
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm