Supporting Information

Synthesis of di-mycoloyl tri-arabinofuranosyl glycerol fragment of mycobacterial cell wall based on synthetic mycolic acids

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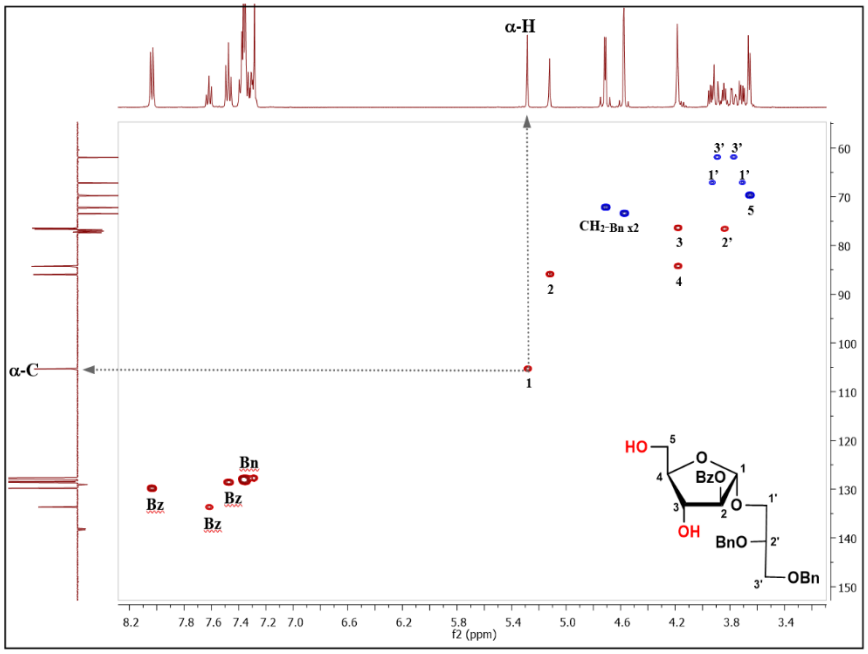


Figure S0: HSQC-NMR spectrum for TAG's acceptor **(5)**.

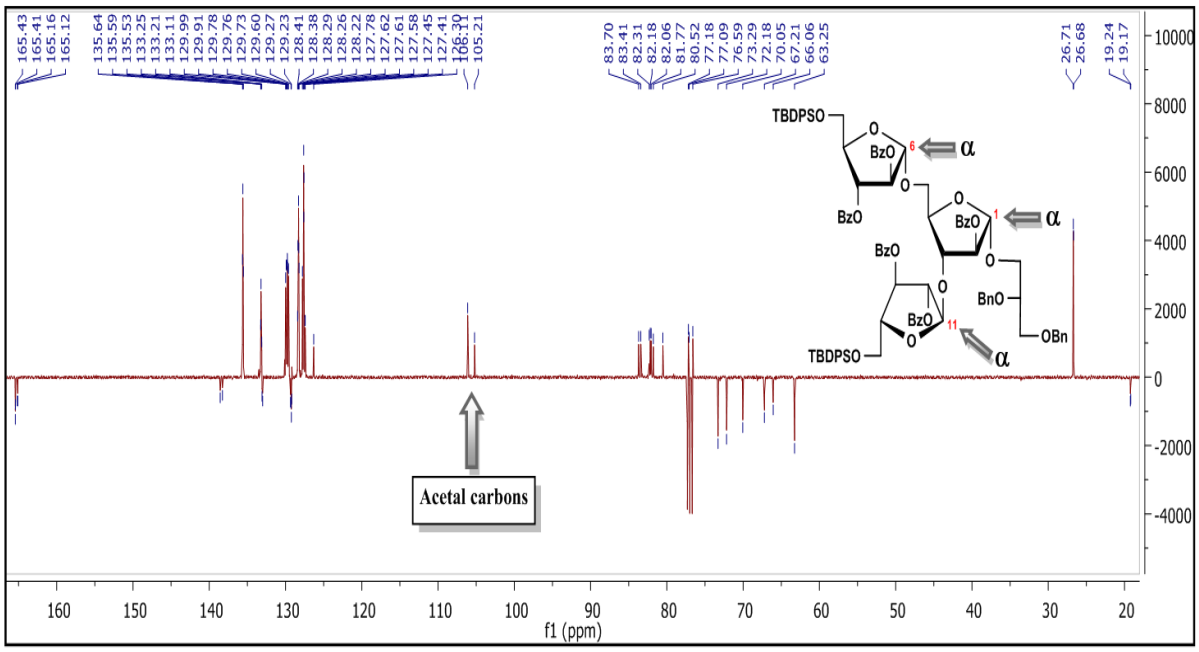


Figure S1: ^{13}C-NMR spectrum for fully protected tri-arabino glycerol **(6)**.

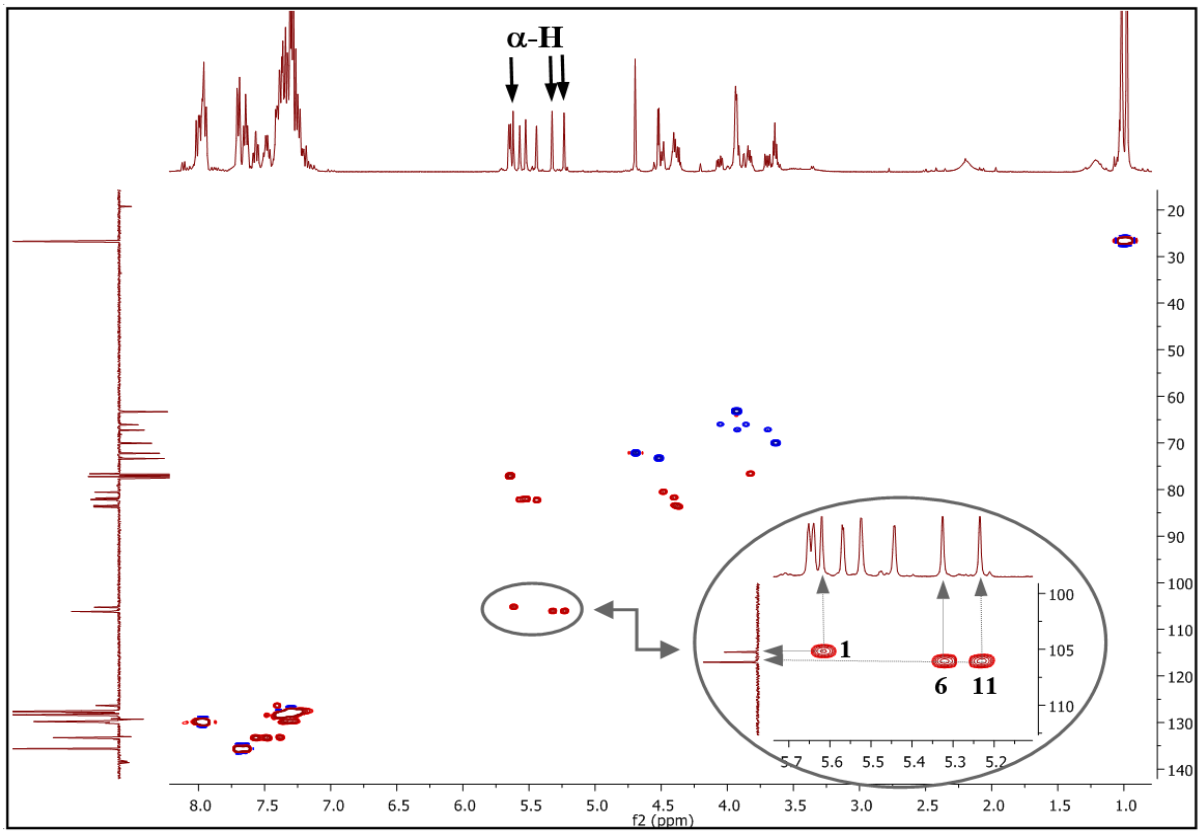


Figure S2: HSQC-NMR spectrum for tri-arabino glycerol **(6)**.

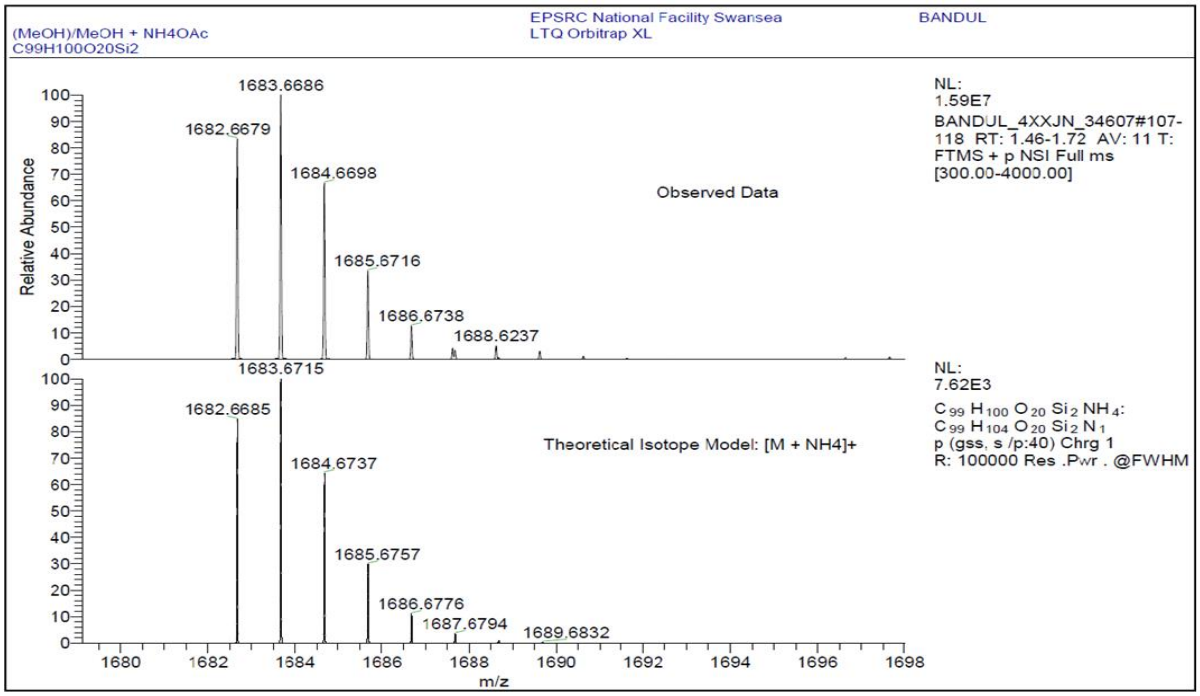


Figure S3: Mass spectrum of the tri-saccharide compound **(6)**.

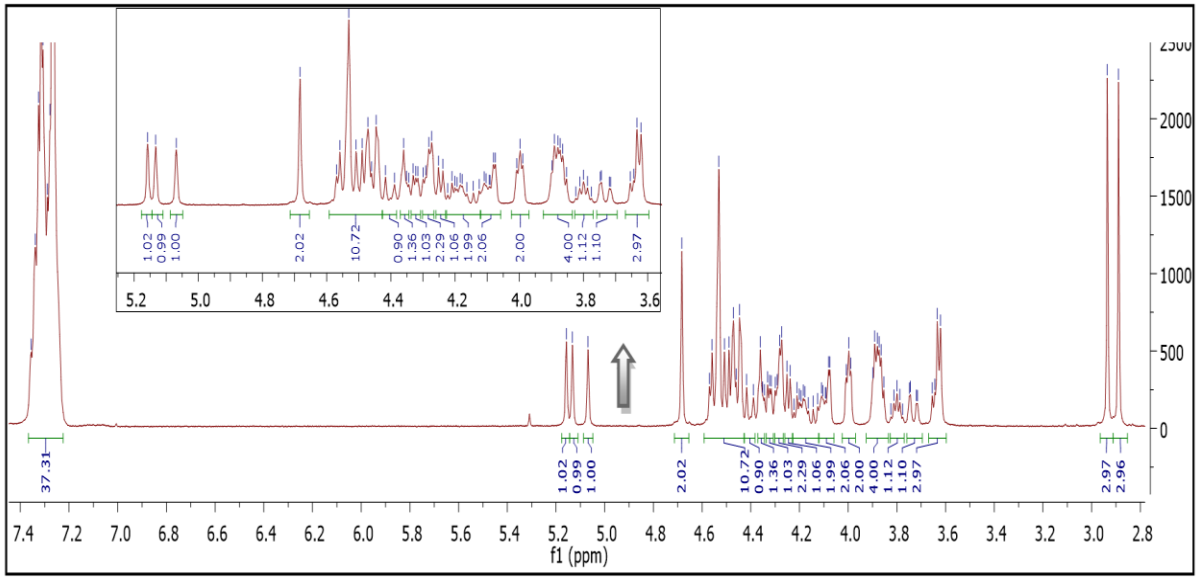


Figure S4: ^{1}H-NMR spectrum for compound **(10)**.

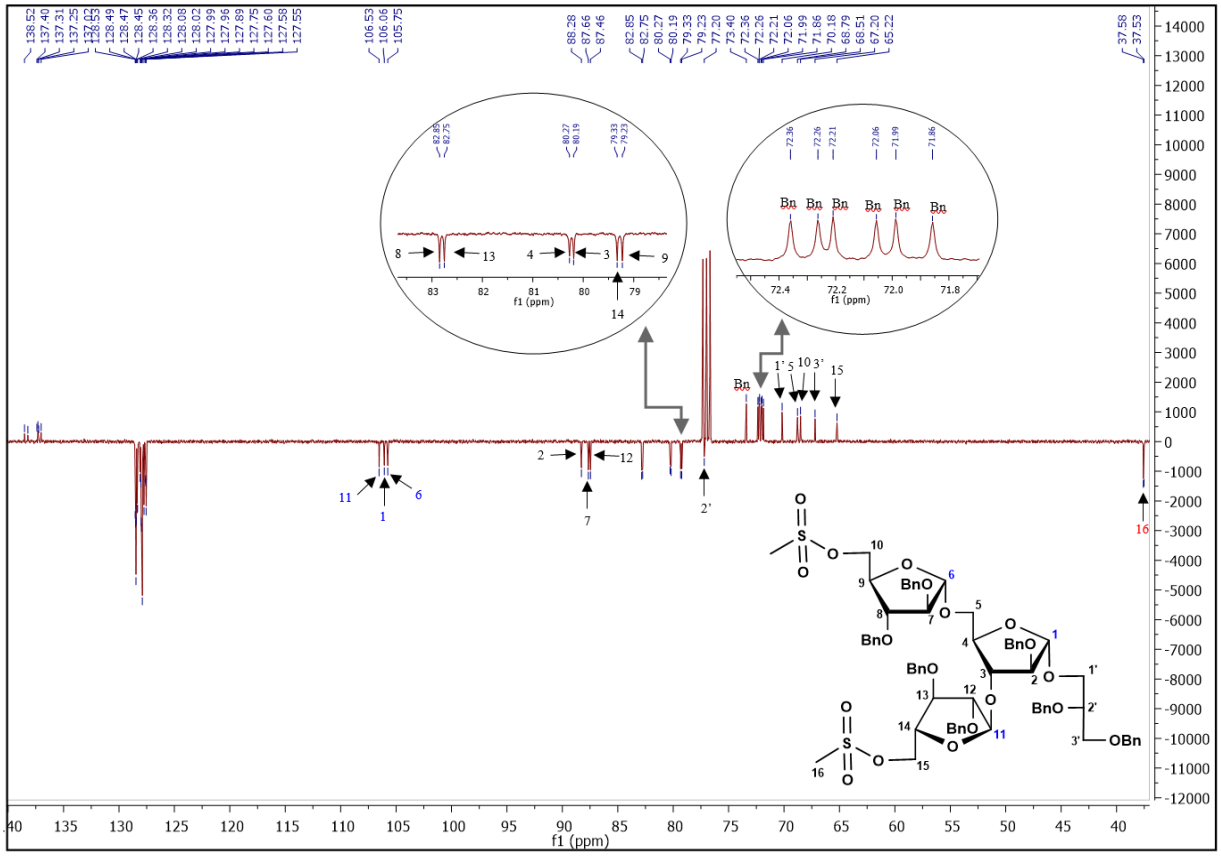


Figure S5: ^{13}C-NMR spectrum for compound **(10)**.

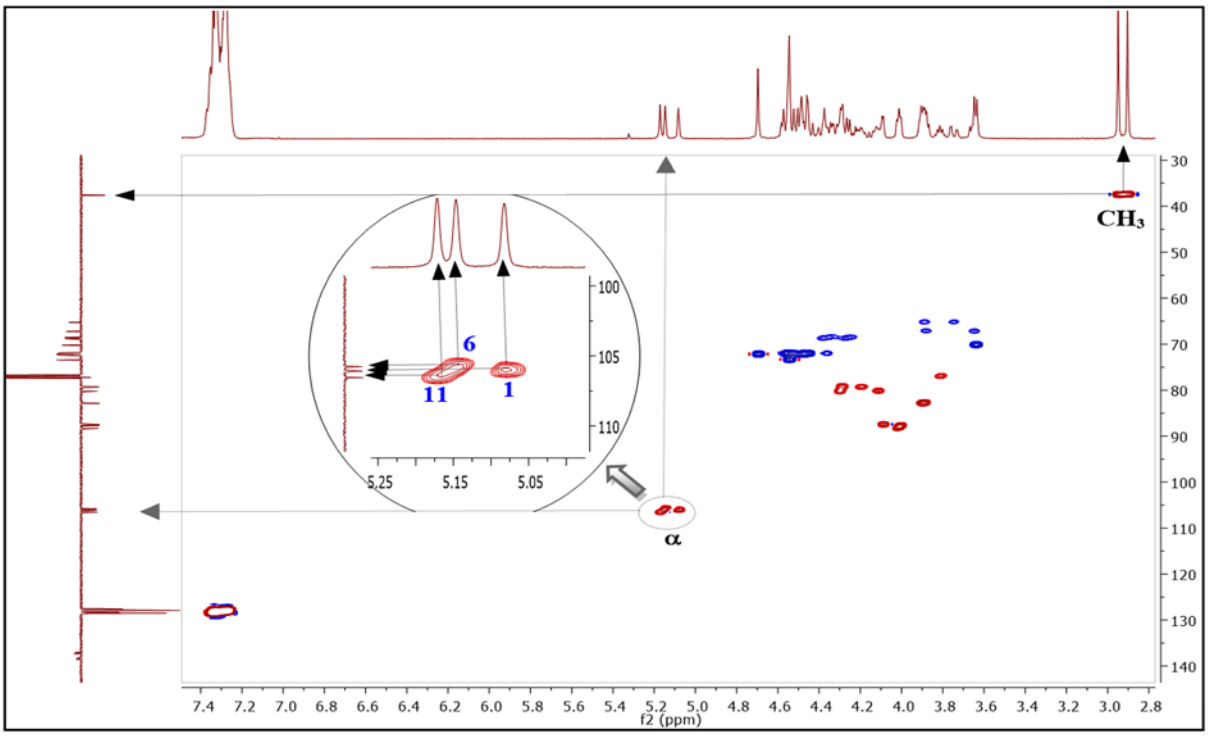
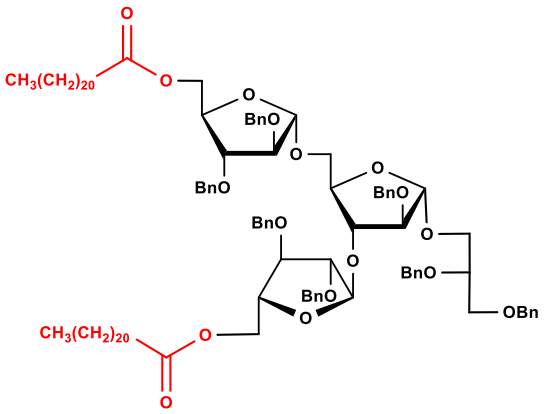
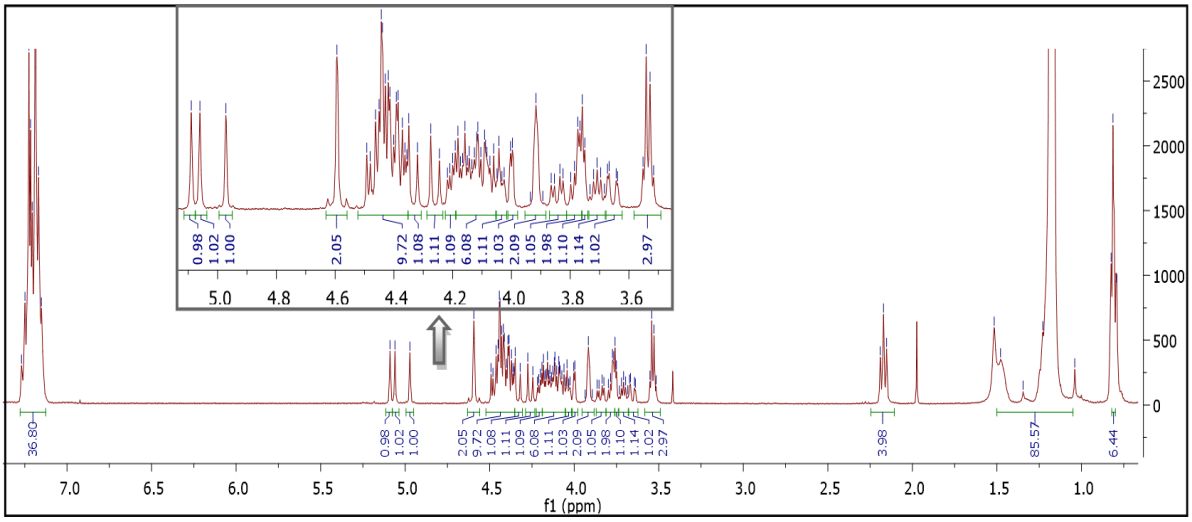
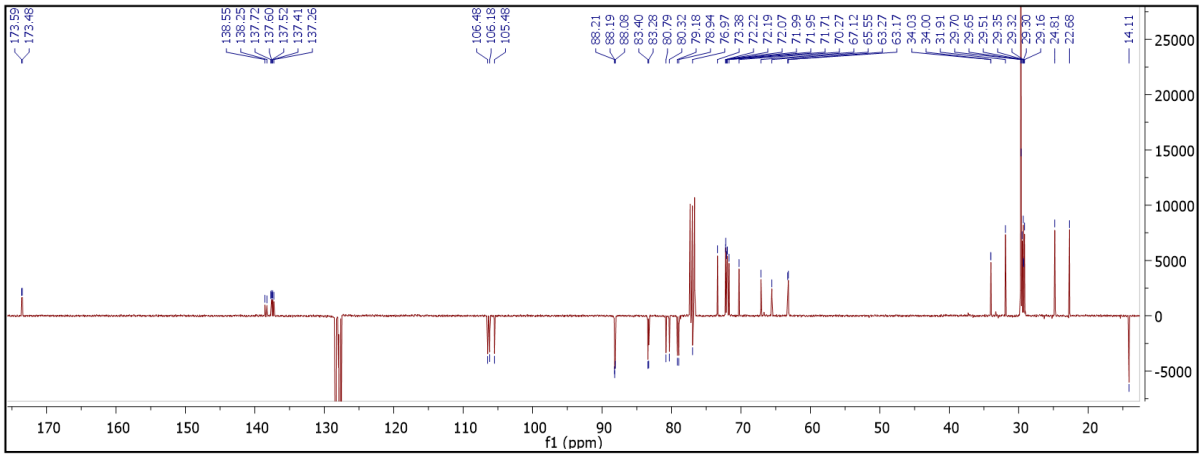


Figure S6: 2D-NMR spectrum for compound (**10**).


O
CH3(CH2)20
O
O
BnO
BnO
O
O
BnO
BnO
O
BnO
O
BnO
OBn
BnO
O
CH3(CH2)20
O
O


0.98
1.02
1.00
2.05
9.72
1.08
1.11
1.09
6.08
1.11
1.03
2.09
1.05
1.98
1.10
1.14
1.02
2.97
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
36.80
3.98
85.57
6.44
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
f1 (ppm)
2500
2000
1500
1000
500
0


173.59
173.48
138.55
138.25
137.72
137.60
137.52
137.41
137.36
106.48
106.18
105.48
88.21
88.19
88.08
83.40
83.28
80.79
80.32
79.18
78.94
76.97
73.38
72.22
72.19
72.07
71.99
71.95
71.71
70.27
67.12
65.55
63.27
63.17
34.03
34.00
31.91
29.70
29.65
29.51
29.35
29.32
29.30
29.16
24.81
22.68
14.11
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)
25000
20000
15000
10000
5000
0
-5000

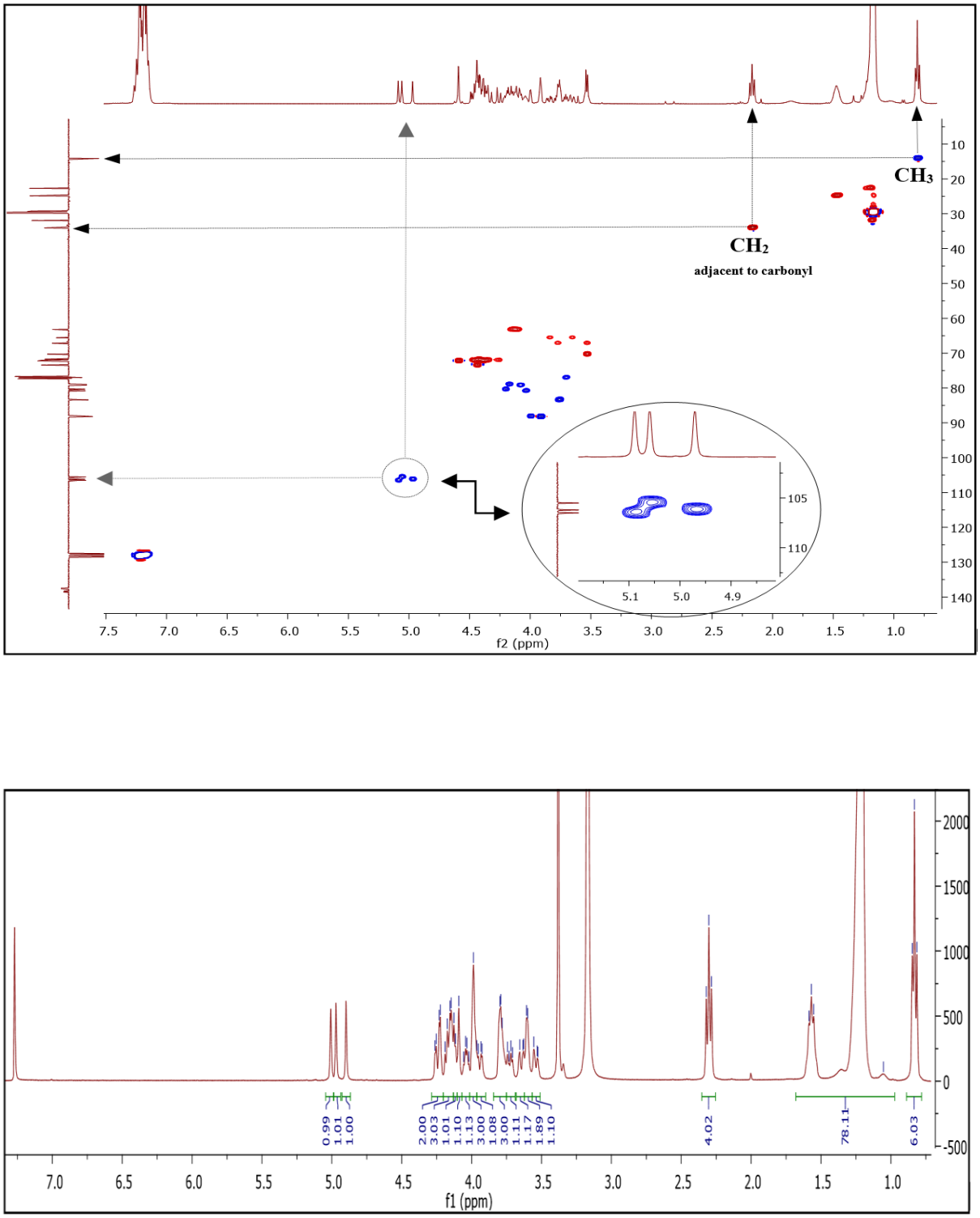


Figure S7: ^{1}H-NMR spectrum for compound **(11,** R = H**)**.

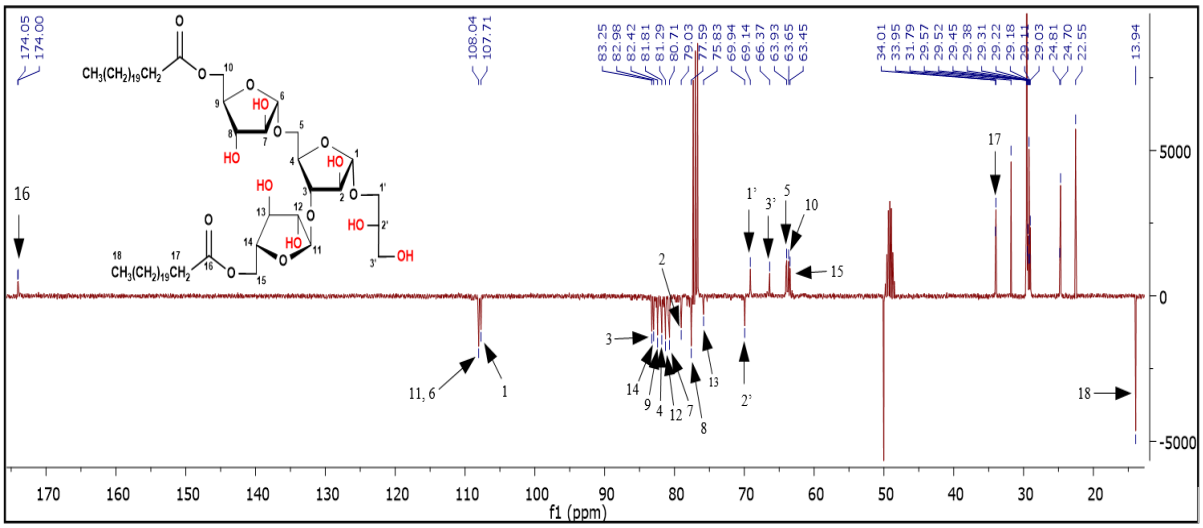


Figure S8: ^{13}C-NMR spectrum for compound **(11,** R = H**)**.

Table S1: The 1H and 13C-NMR data analysis of the glycolipid compound (**11,** R = H).

Proton	Shift	H's	Class	*J*/Hz	Carbon	*δ/ppm*
H_{11}	5.01	1	br. s	-	C_{16}	174.05
H_1	4.90	1	br. s	-	C_1	107.7
$H_{10,\,3}$	4.24	2	br.dd	3.2, 11.7	C_3	83.3
$H_{15,\,1'',\,13}$	4.17	3	br.dd	5.0, 11.8	C_{14}	83.0
$H_{15`}$	4.12	1	br.d	4.3	C_9	82.4
$H_{10`}$	4.09	1	m	-	C_4	81.8
H_4	4.04	1	br.q	5.5	C_{12}	81.3
$H_{2,\,7,\,9}$	3.95	3	br.m	-	C_7	80.7
$H_{5`}$	3.94	1	dd	3.6, 11.5	C_2	79.0
$H_{5,\,2',\,8}$	3.79	3	m	-	C_8	77.6
$H_{1'}$	3.73	1	br.dd	4.8, 10.1	C_{13}	75.8
$H_{3''}$	3.64	1	m	-	$C_{2'}$	69.9
$H_{3',\,12}$	3.60	2	br.d	3.1	$C_{1'}$	69.1
H_{14}	3.54	1	m	-	$C_{3'}$	66.4
$CH_{2\text{-Next to carbonyl}}$	2.30	4	t	7.6	C_5	63.9
$CH_{2\text{-Chain}}$	1.39	83	m	-	C_{10}	63.7
$CH_{3\text{-Terminal}}$	0.83	6	t	6.5	C_{15}	63.5
-	-	-	-	-	C_{17}	34.0
-	-	-	-	-	C_{18}	13.9

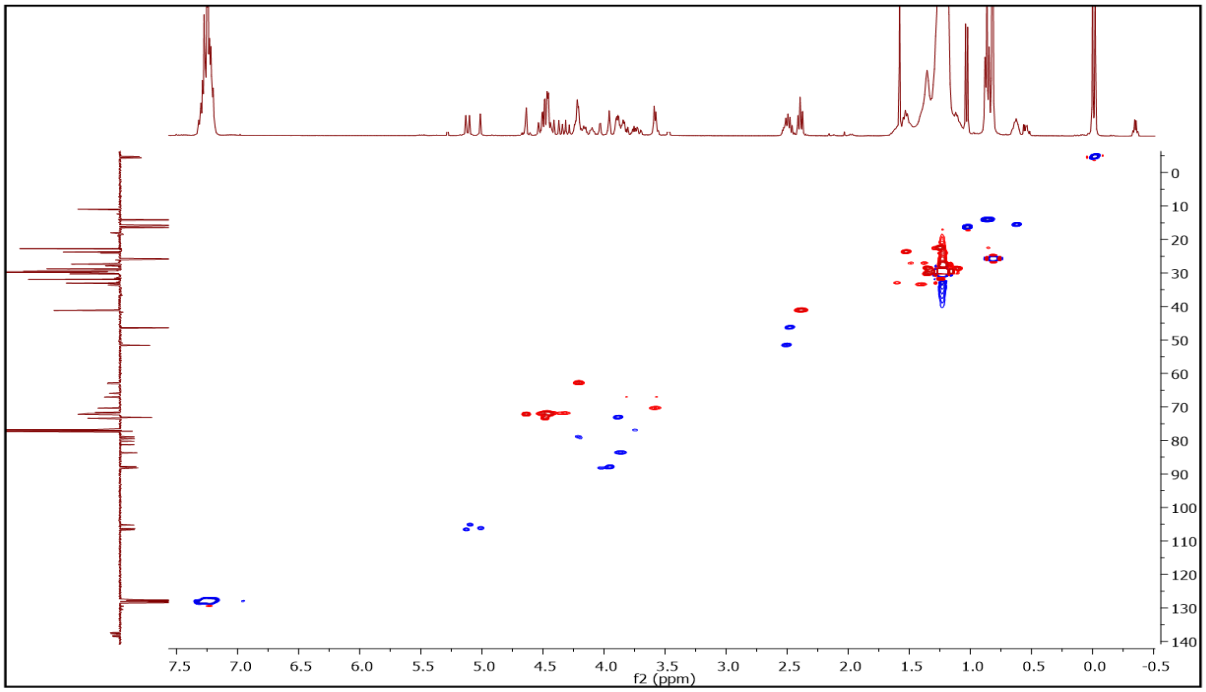


Figure S9: HSQC-NMR spectrum for compound **(13a (R` = TBDMS))**.

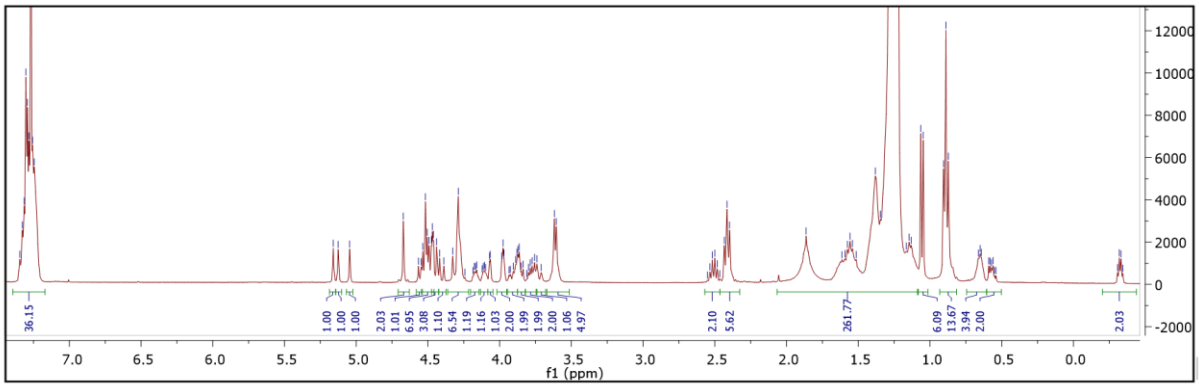


Figure S10: ^{1}H-NMR spectrum for compound **(14a (R` = H)**.

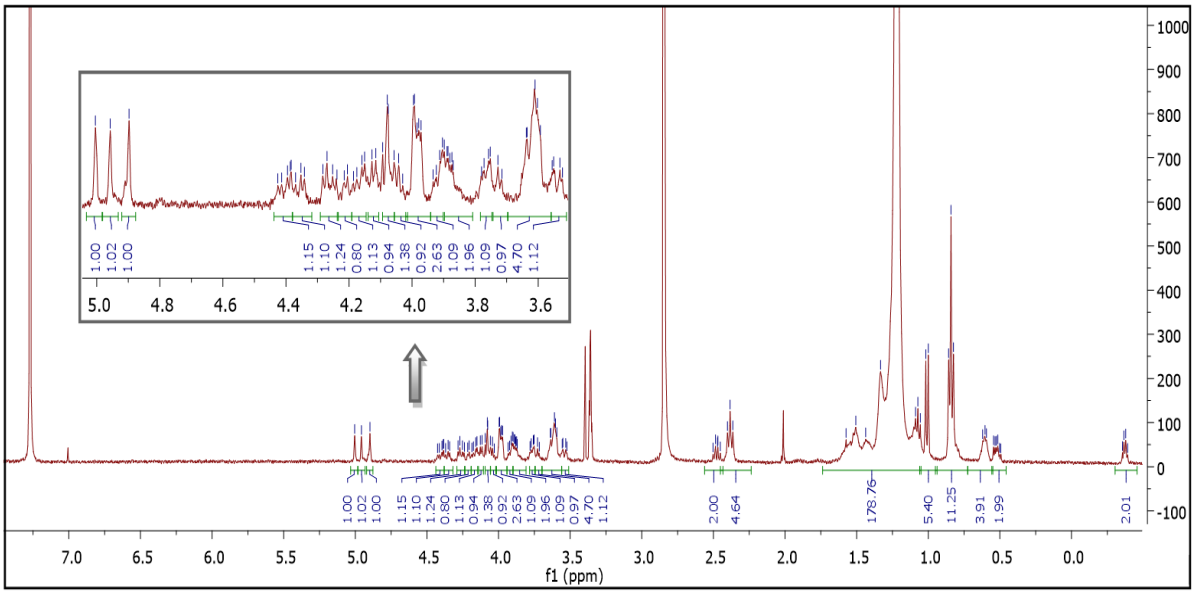


Figure S11: ^{1}H-NMR spectrum for compound **(15a (R` = H))**.

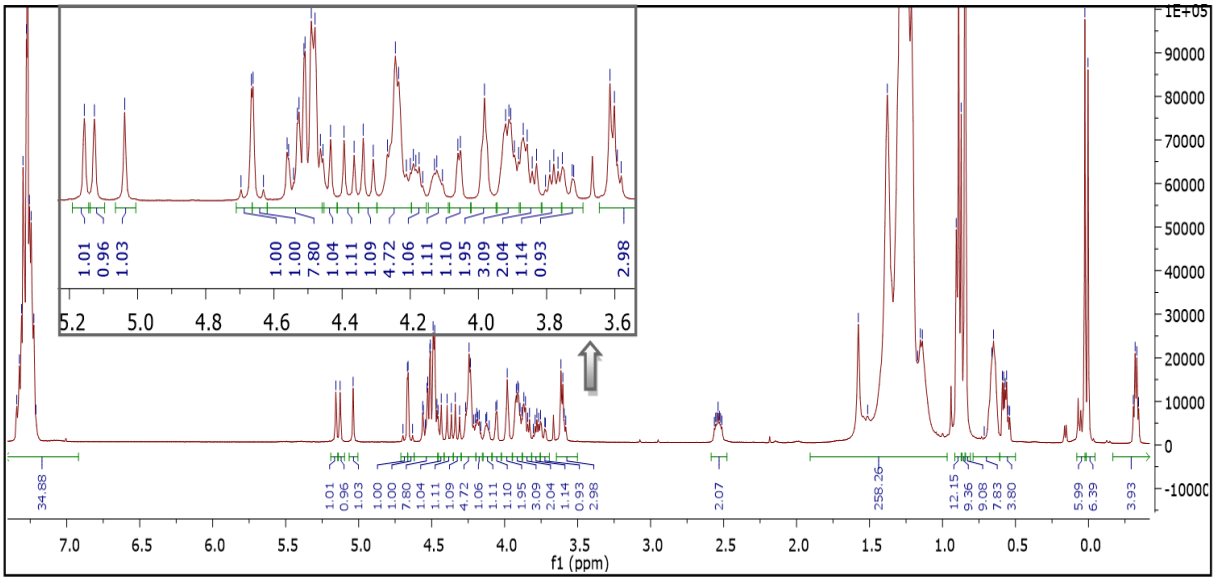


Figure S12: ^{1}H-NMR spectrum for compound **(13b (R` = TBDMS))**.

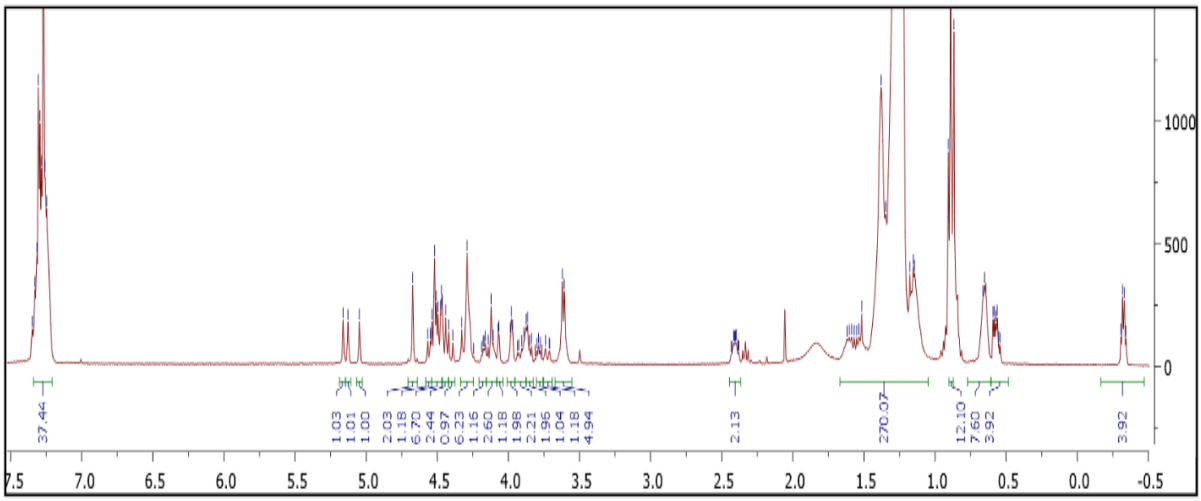


Figure S13: ^{1}H-NMR spectrum for compound **(14b (R` = H))**.

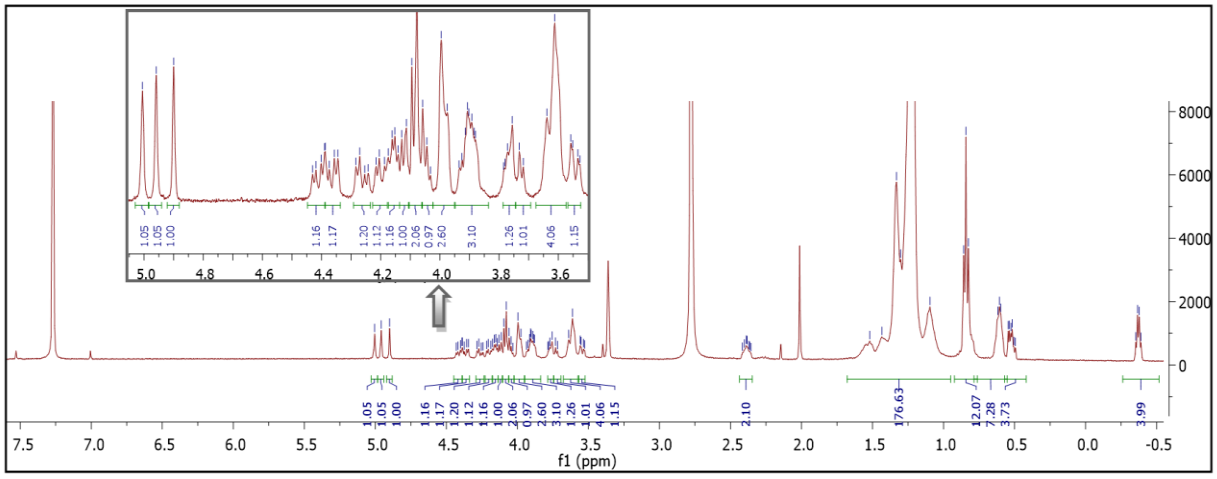


Figure S14: ^{1}H-NMR spectrum for compound **(15b (R` = H))**.

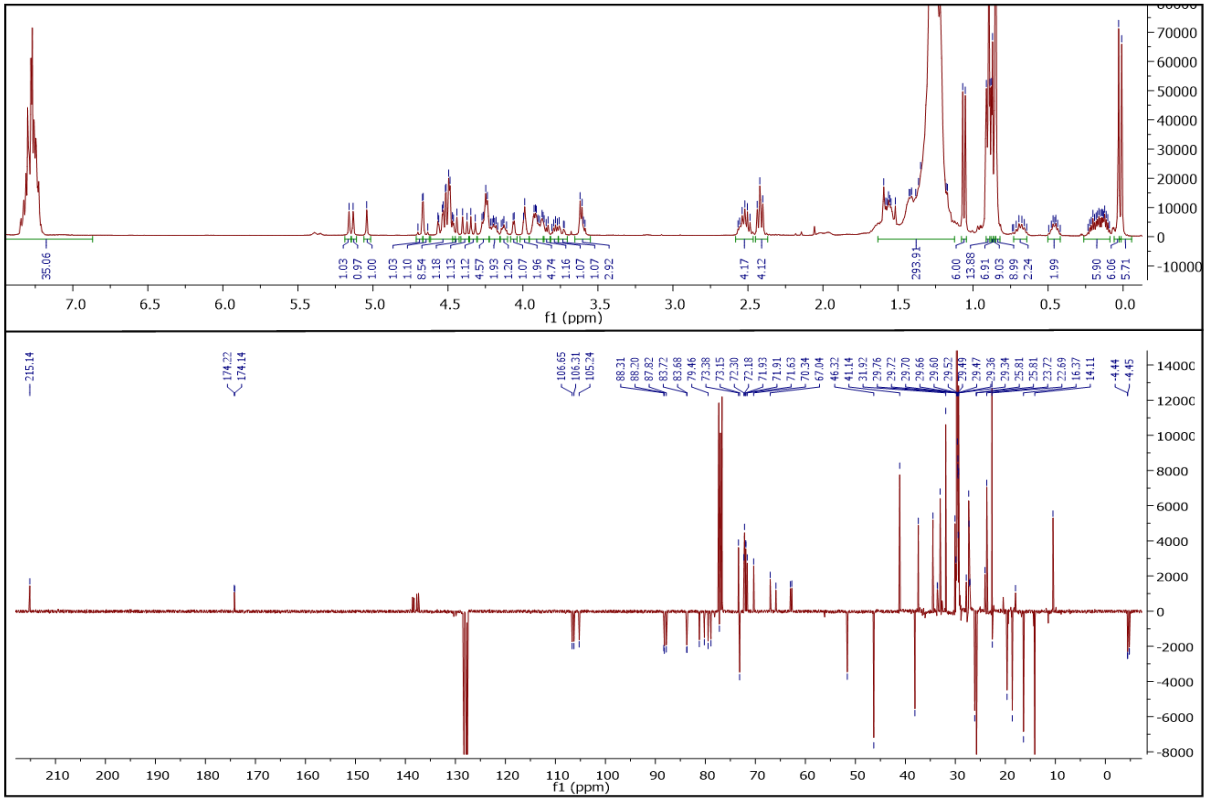


Figure S15: ^{1}H and ^{13}C-NMR spectra for compound **(13c (R` = TBDMS))**.

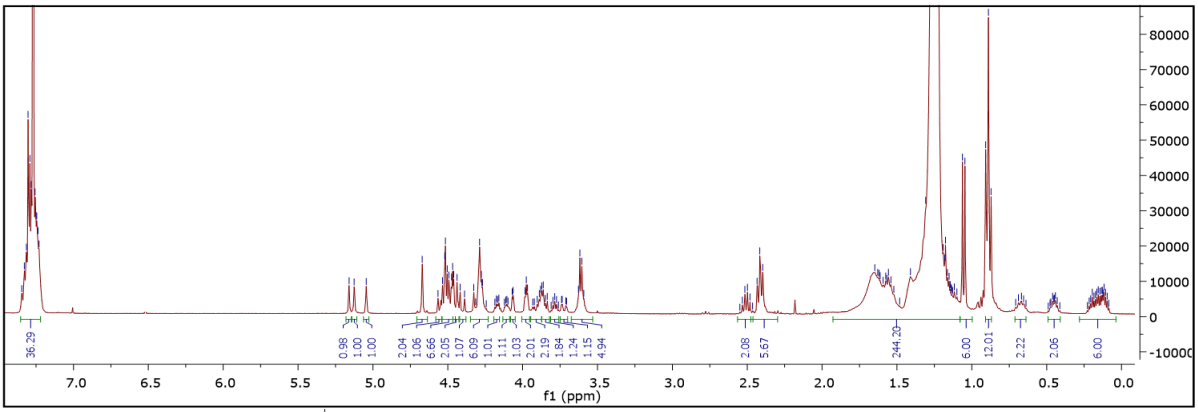


Figure S16: ^{1}H-NMR spectrum for compound **(14c (R` = H))**.

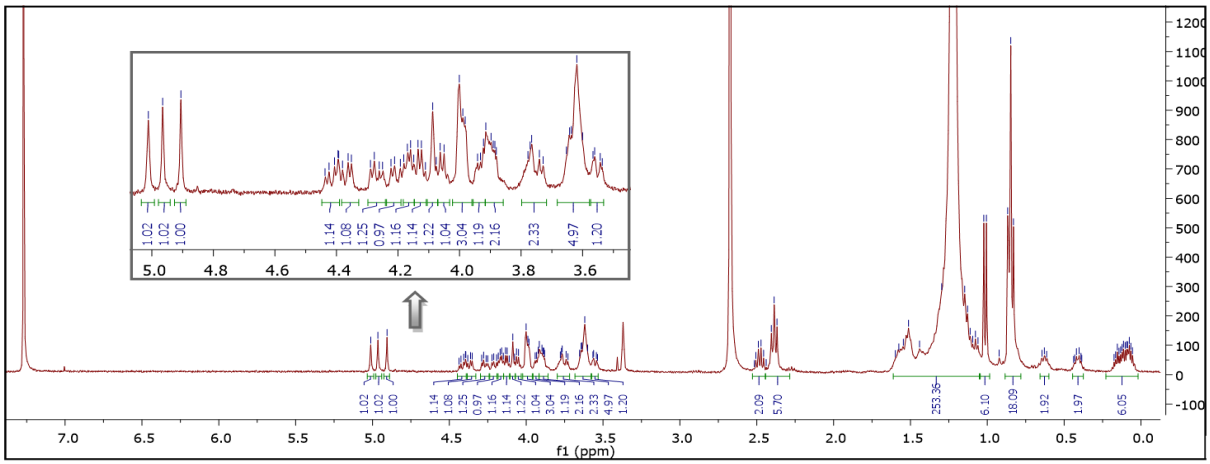


Figure S17: ^{1}H-NMR spectrum for compound **(15c (R` = H))**.