Supporting Information

Rec. Nat. Prod. **X:X (202X) XX-XX**

Heptaelliptoic acid A, a New Betulinic Acid Saponin from the Leaves of *Heptapleurum ellipticum*

Trong Nghia Ngo[1], Quoc Trung Nguyen[2], Hoang Diem Ly[1], Thi Hong Ngoc Dang[1], Thi Kim Phung Nguyen[1], Kim Yen Huynh[1], Van Son Dang[3], Thi Hong Tuoi Do[4], Thi Kim Dung Hoang[5,6] and Tan Phat Nguyen[*5,6]

[1]Kien Giang University, 320A Highway 61, 920000, Kien Giang Province, Vietnam
[2]University of Science, Vietnam National University HCM City, 227 Nguyen Van Cu, District 05, 700000, Ho Chi Minh City, Vietnam
[3]Institute of Tropical Biology, Vietnam Academy of Science and Technology, 85 Tran Quoc Toan, 700000, Ho Chi Minh City, Vietnam
[4]Faculty of Pharmacy, University of Medicine and Pharmacy at Ho Chi Minh City, 700000, Ho Chi Minh City, Vietnam
[5]Institute of Chemical Technology-Vietnam Academy of Science and Technology, 01A Thanh Loc 29, Thanh Loc, District 12, 700000, Ho Chi Minh City, Vietnam
[6]Graduate University of Science and Technology, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay, 100000, Hanoi, Vietnam

Table of Contents **Page**

Table S1: *In vitro* inhibitory properties of compounds **1-6** against *α*-glucosidase

Sample	IC_{50} (µM)
1	> 200.00
2	**11.53**
3	**28.75**
4	**10.90**
5	> 200.00
6	> 200.00
Acarbose	**214.50**

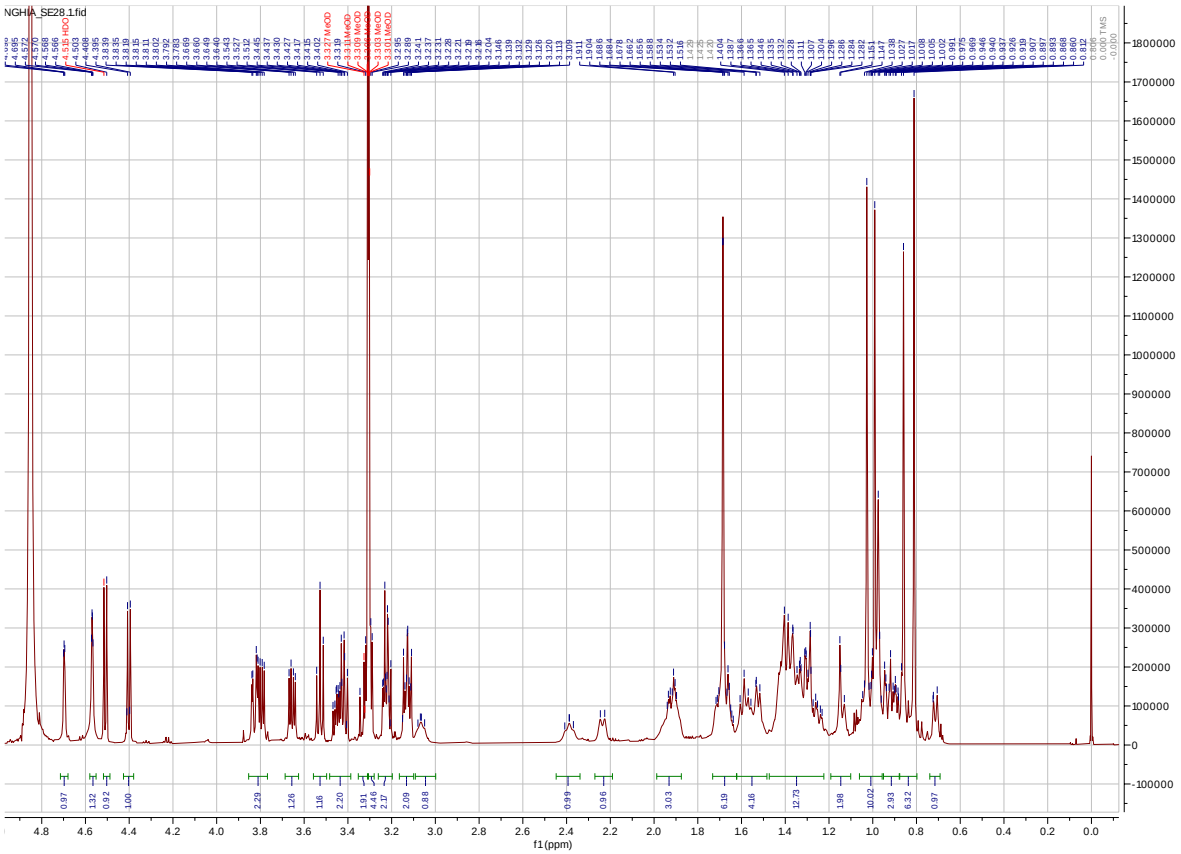


Figure S1: ^{1}H-NMR spectrum (600 MHz) of compound **1** in CD_3OD

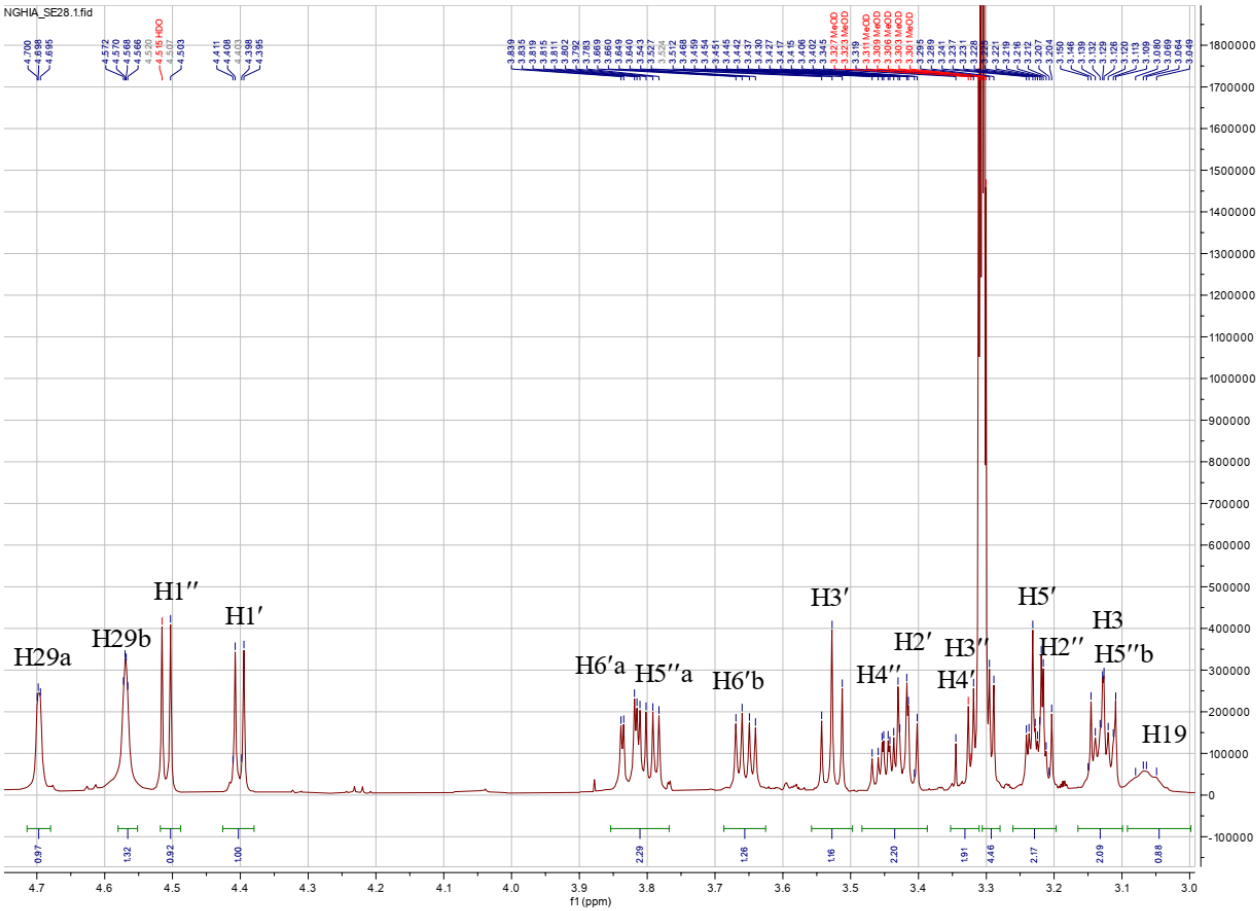


Figure S2: ^{1}H-NMR spectrum (600 MHz) of compound **1** in CD_3OD (Expanded)

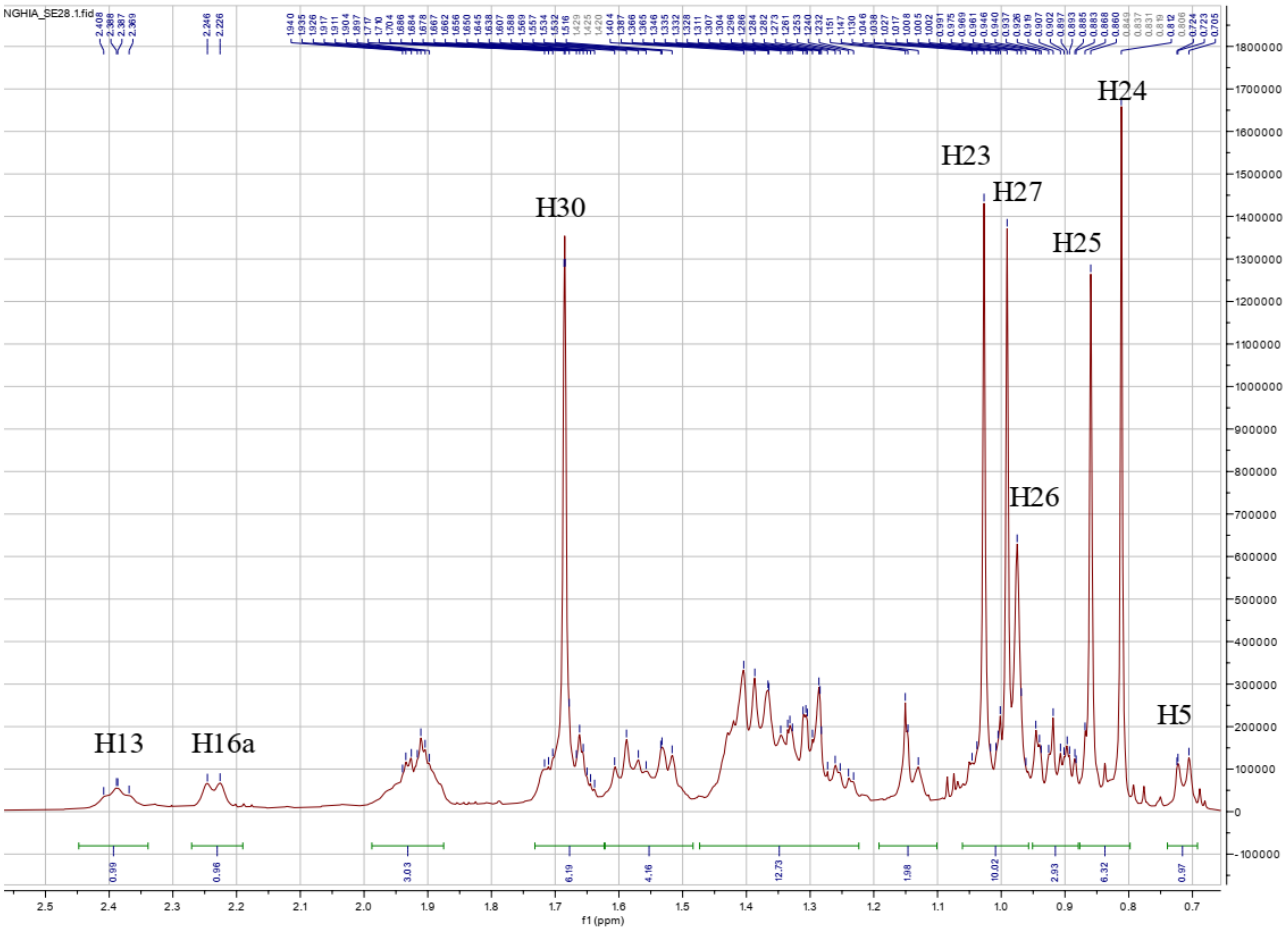


Figure S3: ^{1}H-NMR spectrum (600 MHz) of compound **1** in CD_3OD (Expanded)

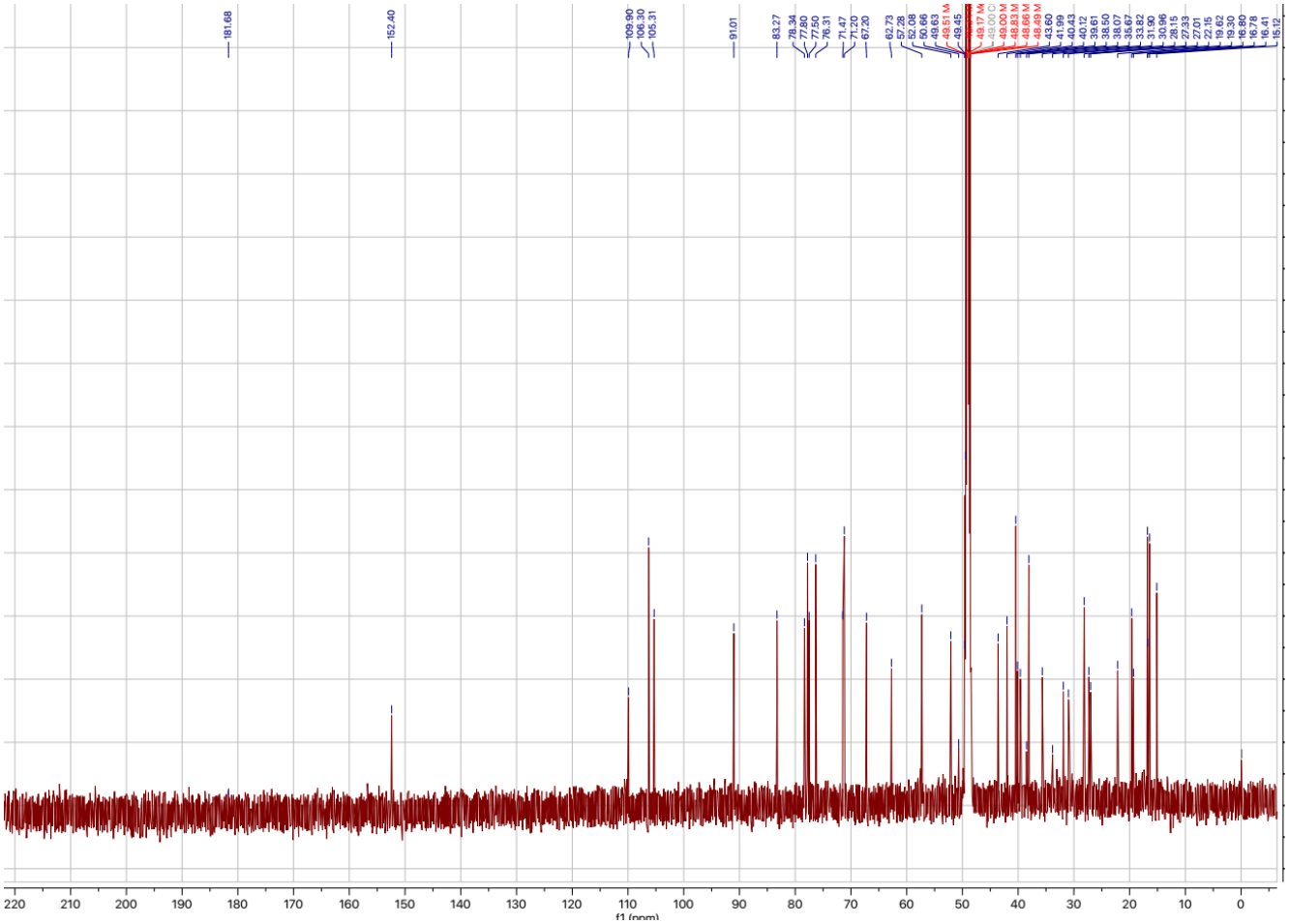


Figure S4: ^{13}C-NMR spectrum (150 MHz) of compound **1** in CD_3OD

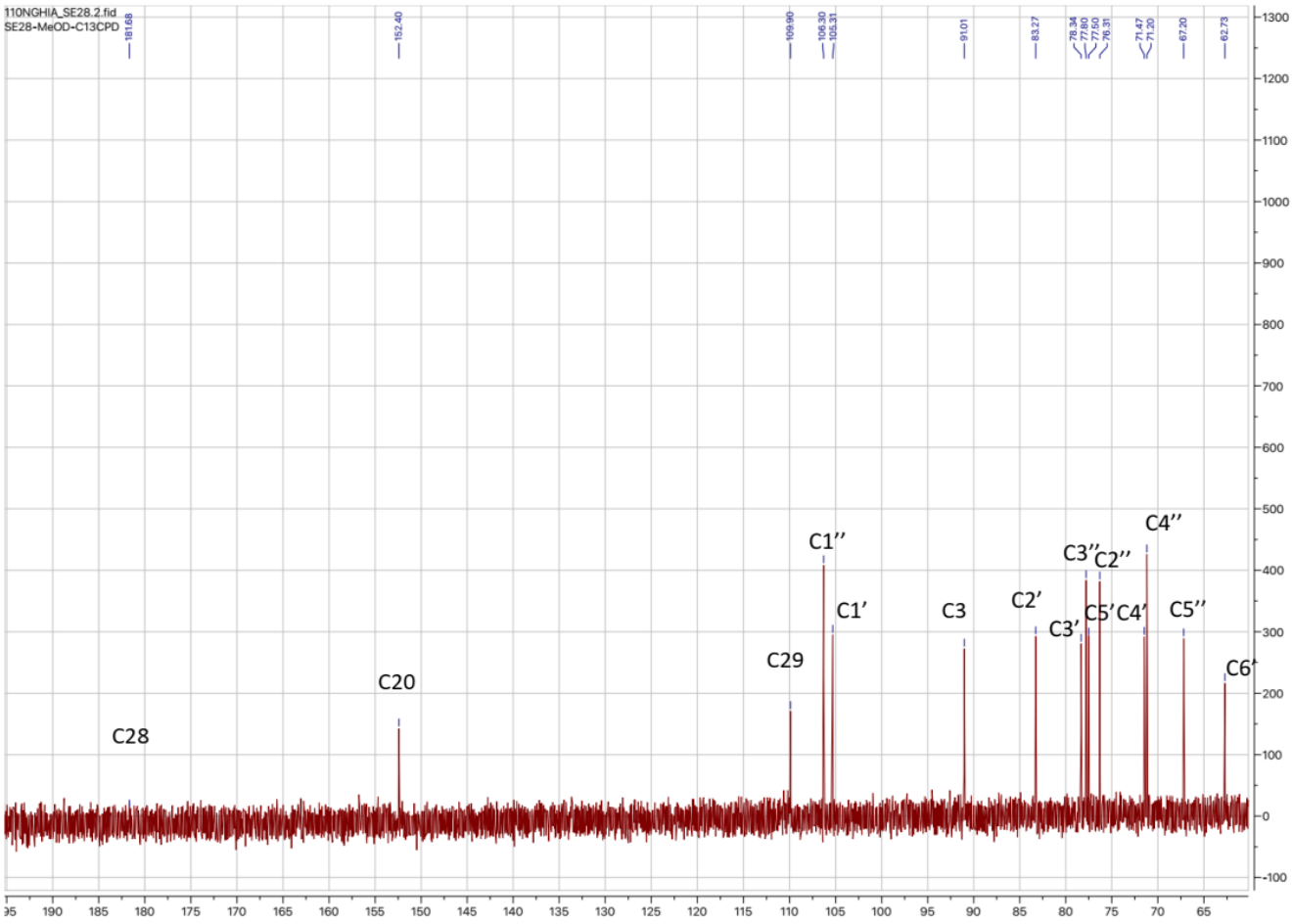


Figure S5: ^{13}C-NMR spectrum (150 MHz) of compound **1** in CD_3OD (Expanded)

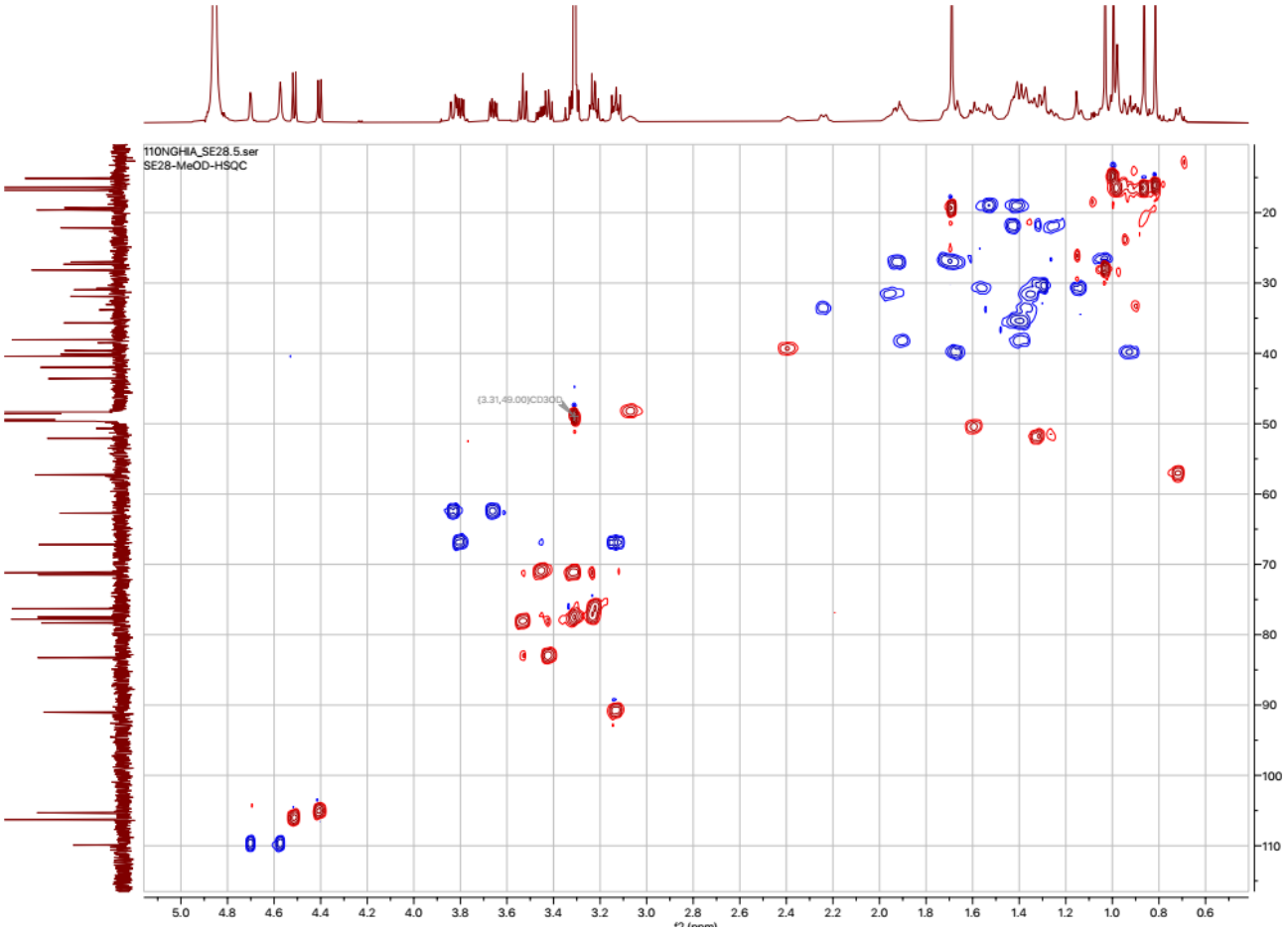


Figure S6: HSQC spectrum of compound **1** in CD_3OD

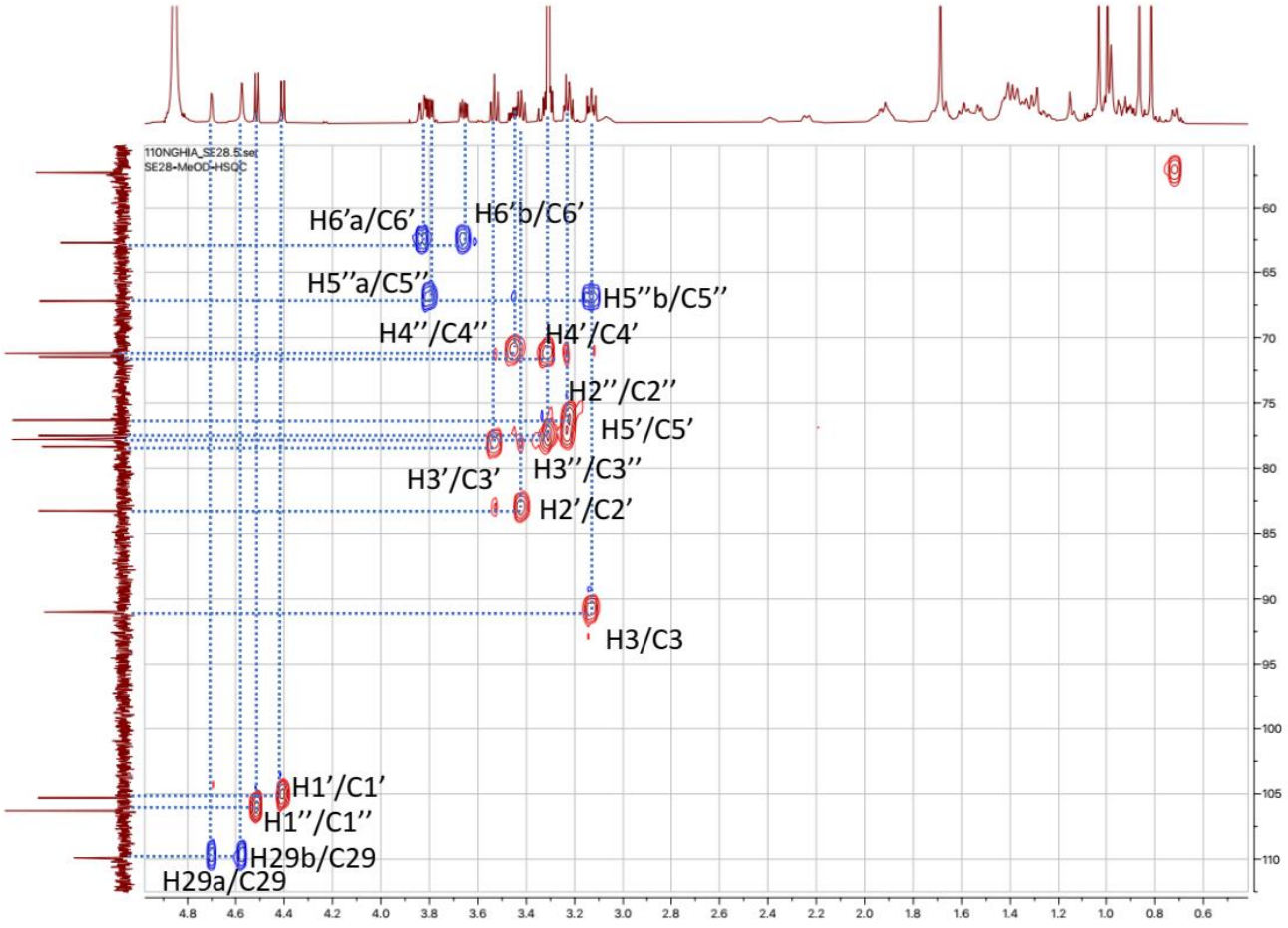


Figure S7: HSQC spectrum of compound **1** in CD_3OD
(Expanded)

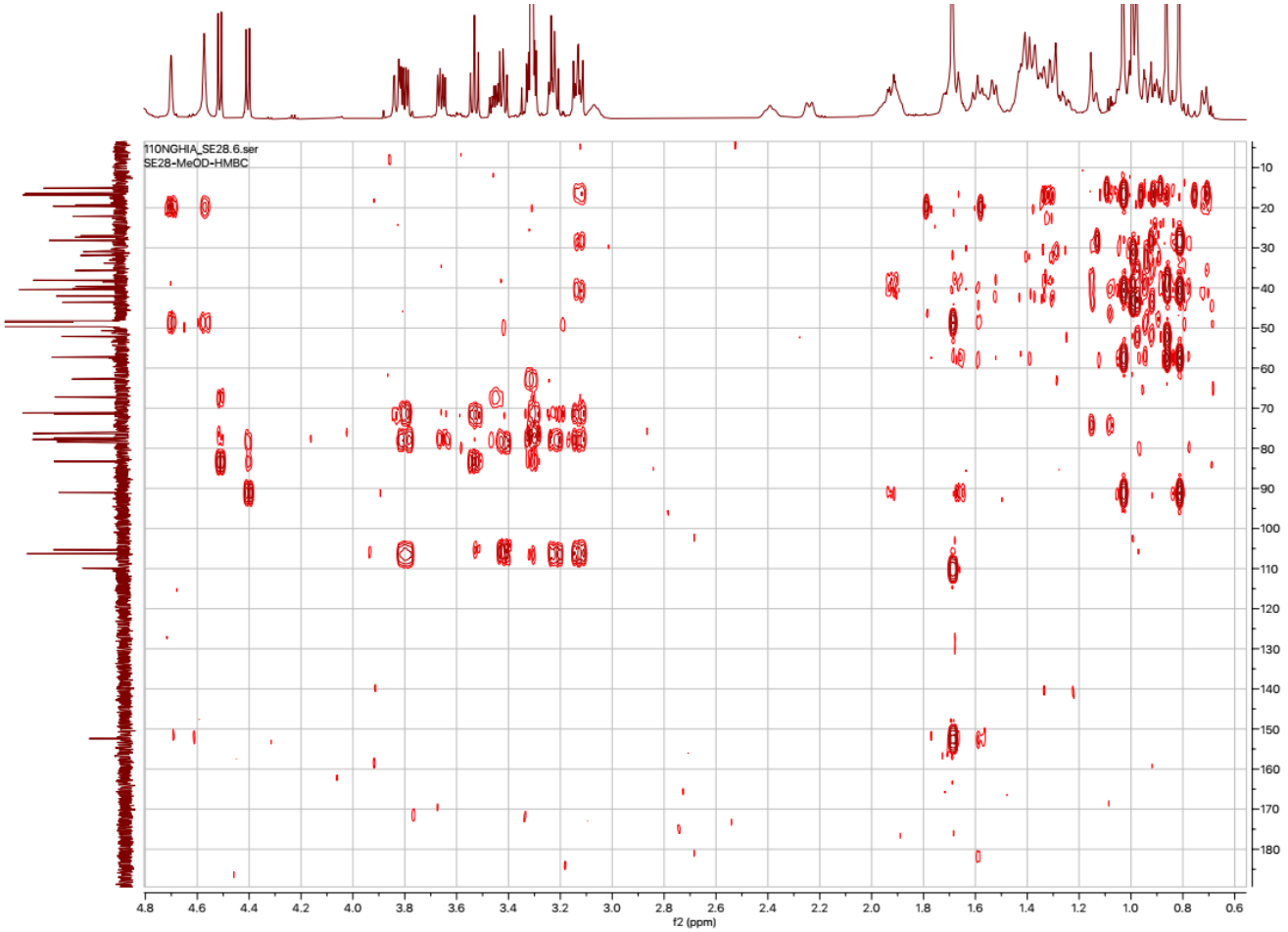


Figure S8: HMBC spectrum of compound **1** in CD_3OD

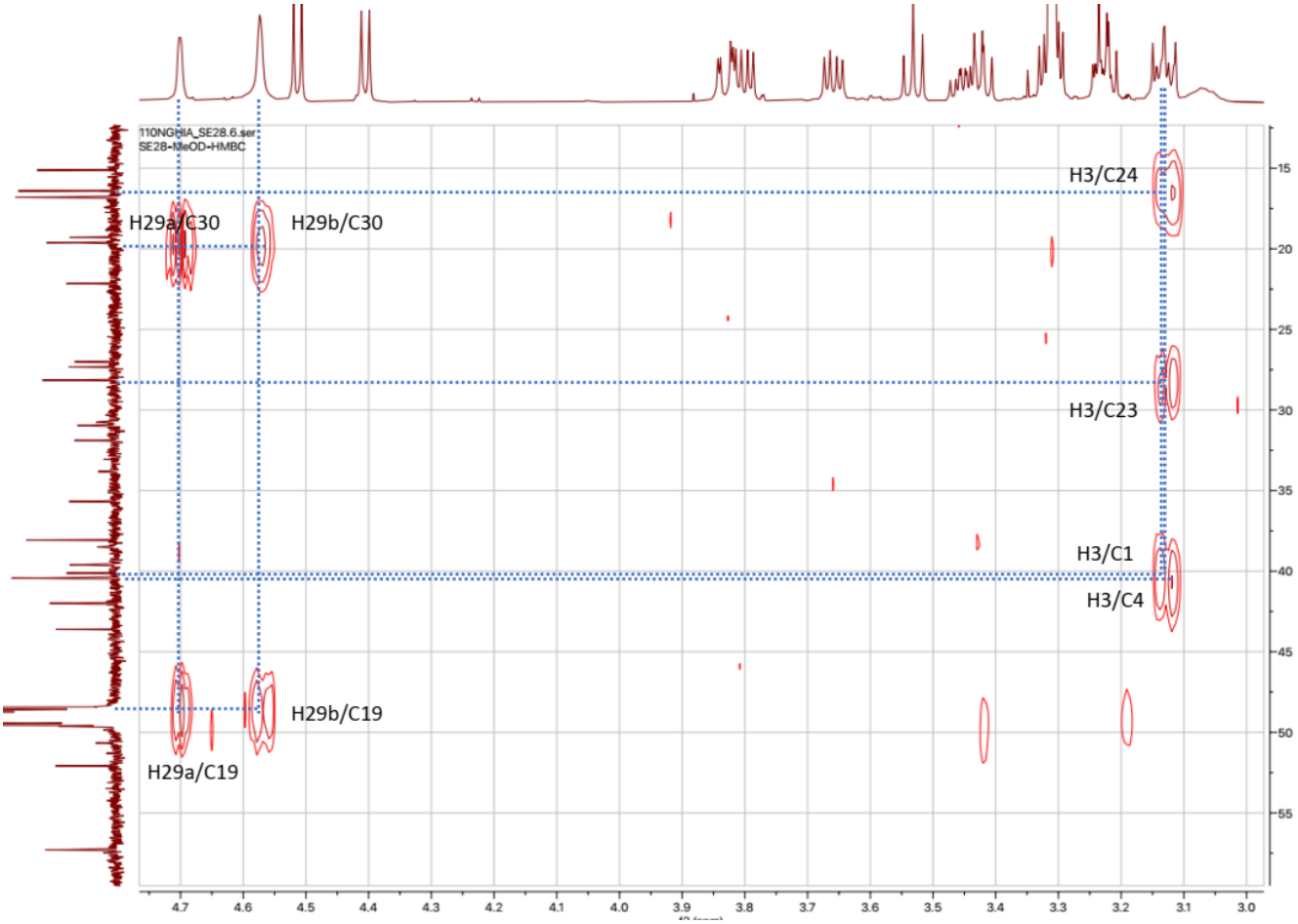


Figure S9: HMBC spectrum of compound **1** in CD_3OD (Expanded)

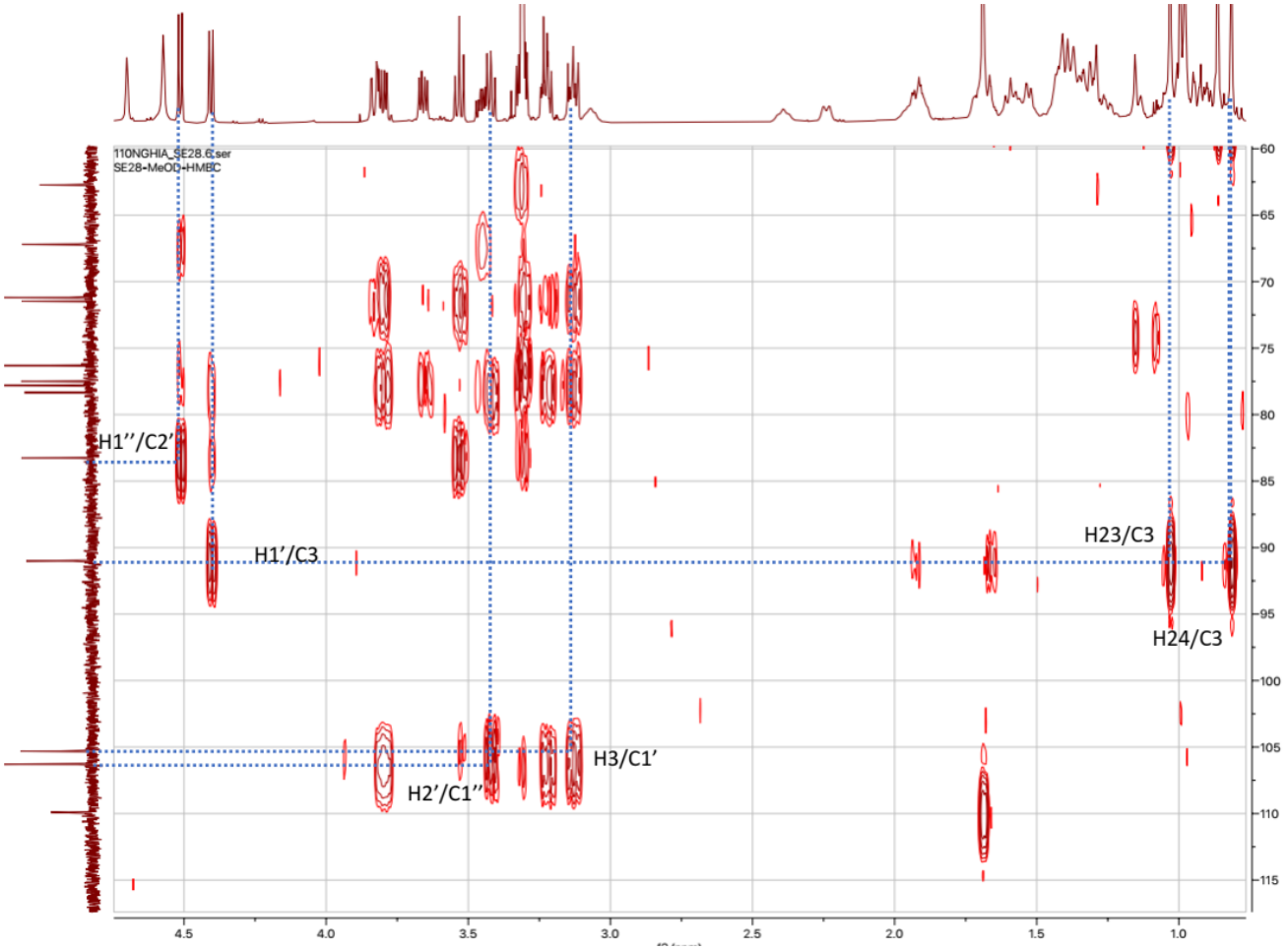


Figure S10: HMBC spectrum of compound **1** in CD_3OD (Expanded)

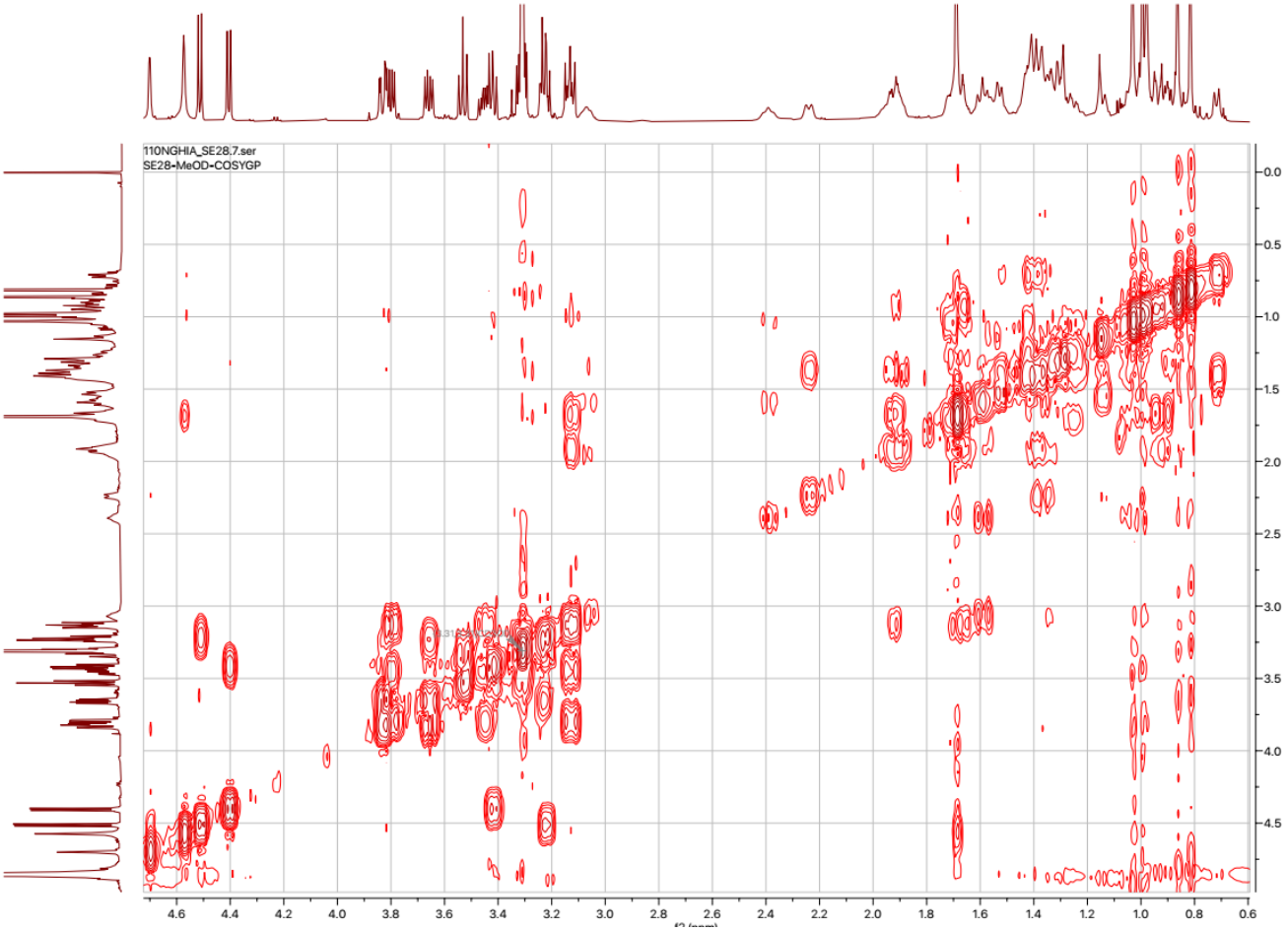


Figure S11: COSY spectrum of compound **1** in CD_3OD

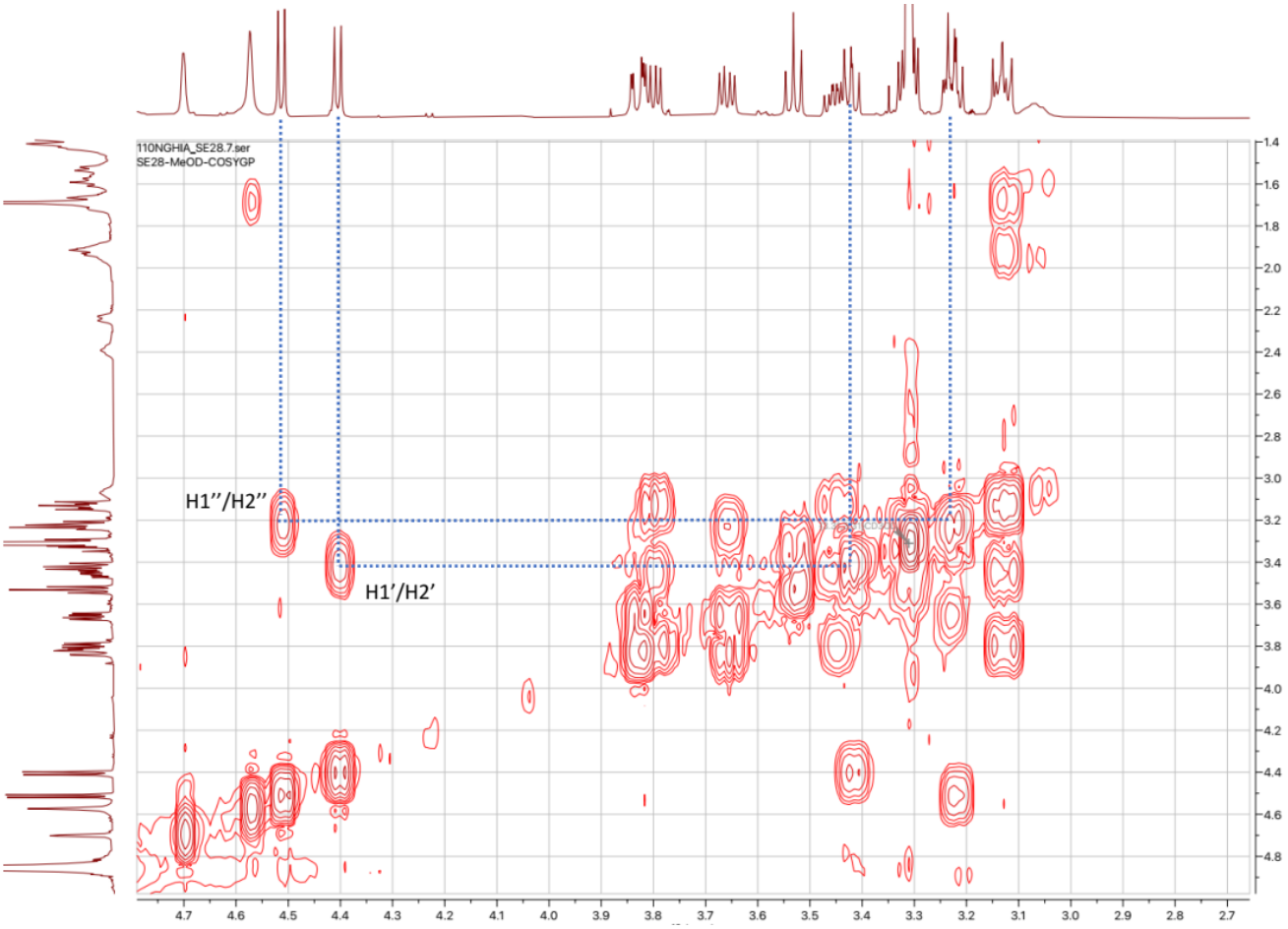


Figure S12: COSY spectrum of compound **1** in CD_3OD (Expanded)

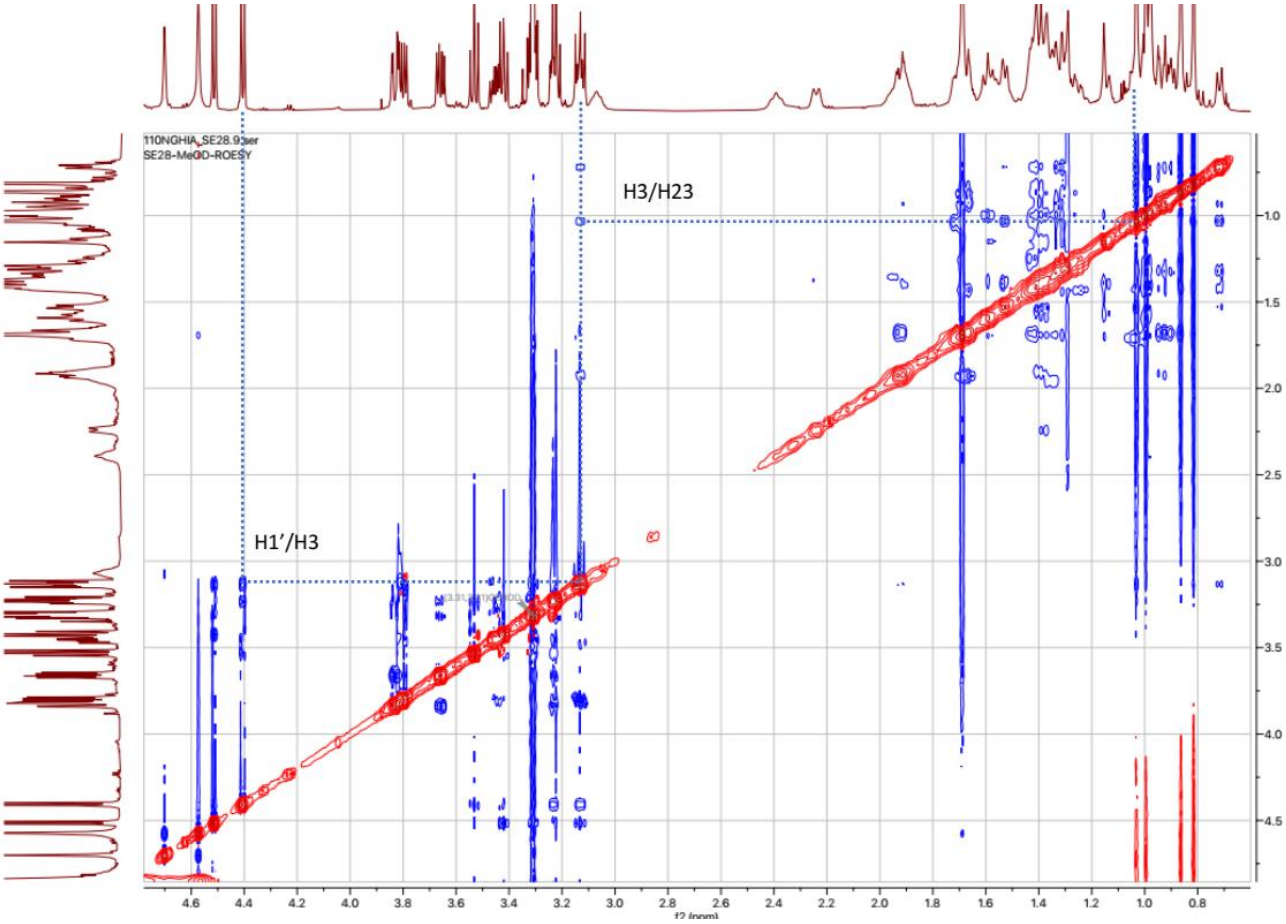


Figure S13: ROESY spectrum of compound **1** in CD_3OD

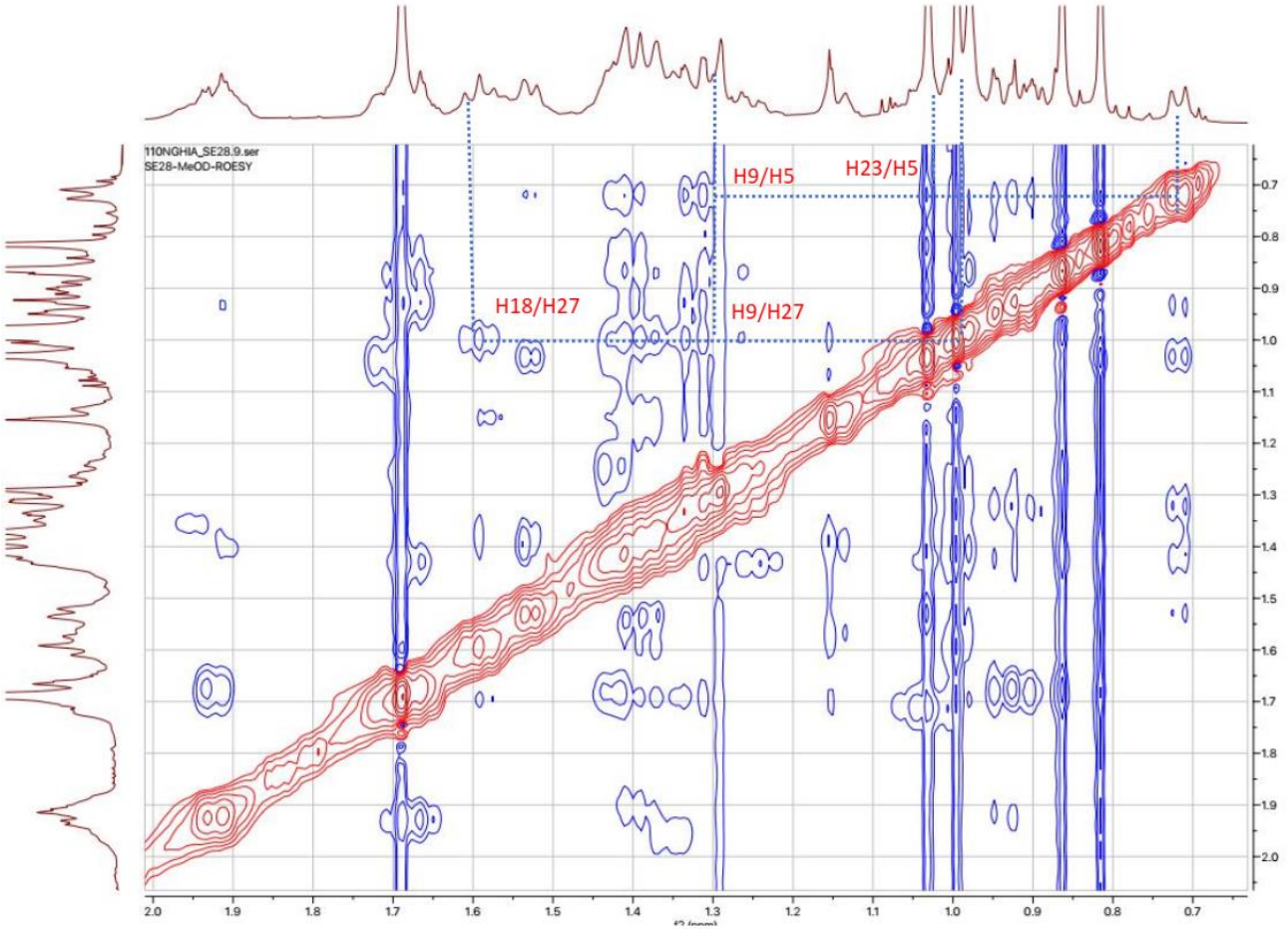


Figure S14: ROESY spectrum of compound **1** in CD_3OD (Expanded)

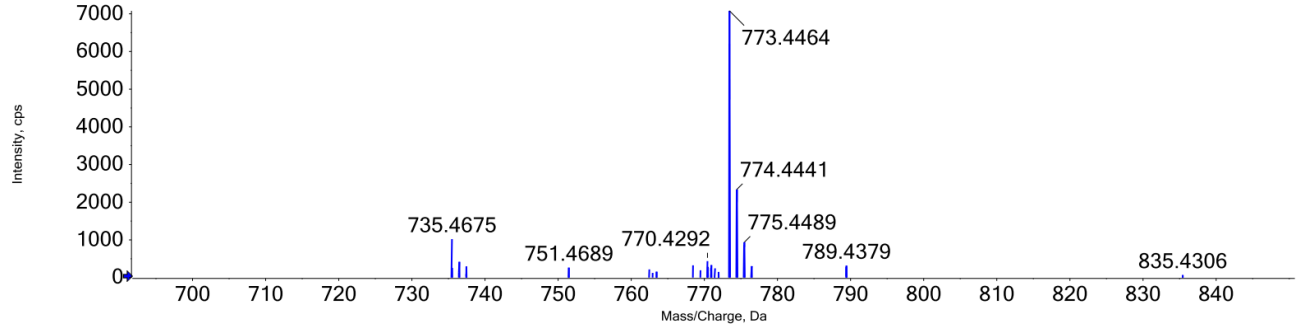


Figure S15: HR-ESI-MS spectrum (positive) of compound **1**

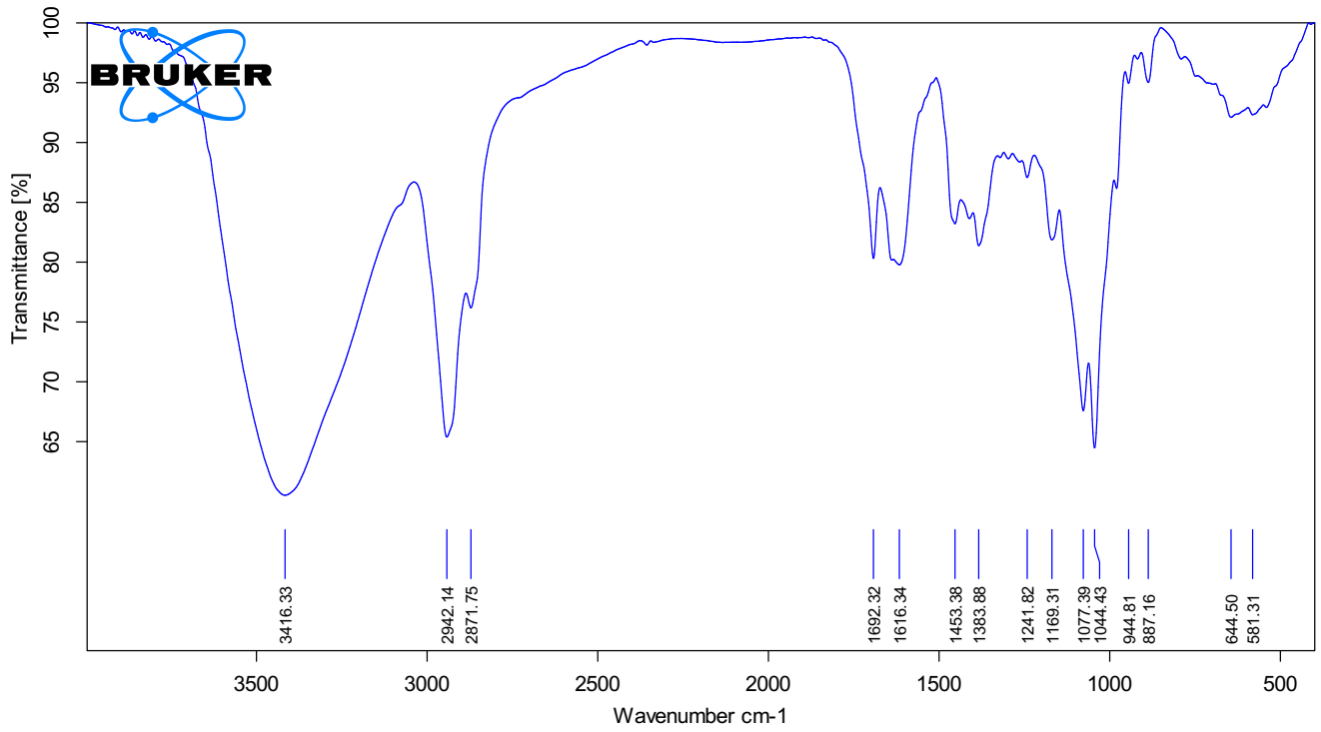


Figure S16: IR spectrum of compound **1**

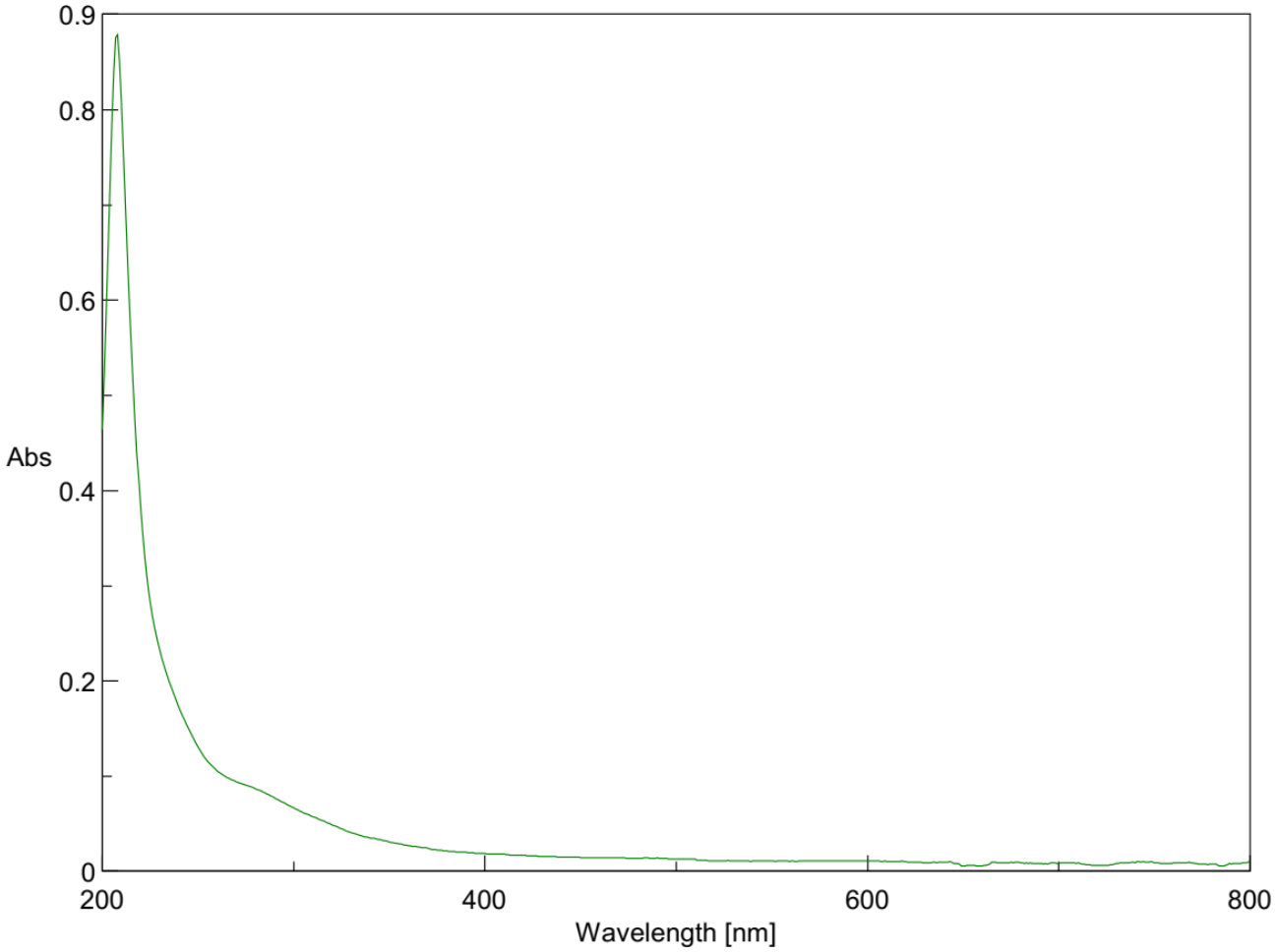


Figure S17: UV-VIS spectrum of compound **1**

CAS SciFinder

Task History

Initiating Search

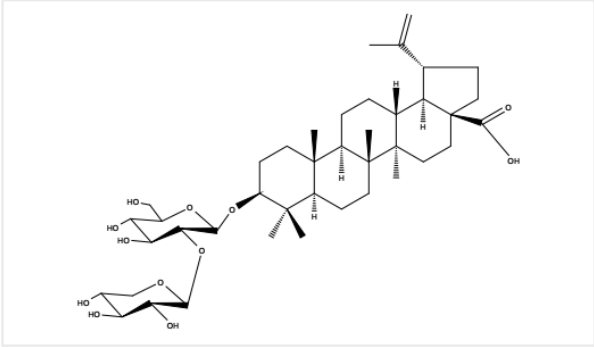
July 21, 2024, 6:32 PM

Substances:

Filtered By:

Similarity: >=99

Number of Components: 1



Structure Match: **Similarity**

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (12)	Substances	View Results

Figure S18: Search report from SciFinder for **1** (heptaelliptoic acid A) (Page 1) Accessed on July 21, 2024

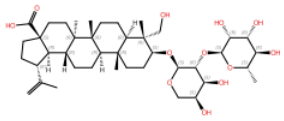
CAS SciFinder

Substances (12)

View in CAS SciFinder

1	Similarity Score: 100

129724-84-1



Absolute stereochemistry shown

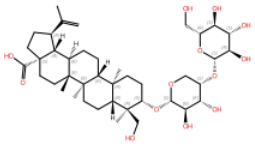
$C_{41}H_{66}O_{12}$

Anemoside A_3

73 References | 16 Reactions | 51 Suppliers

2	Similarity Score: 100

848784-89-4



Absolute stereochemistry shown, Rotation (-)

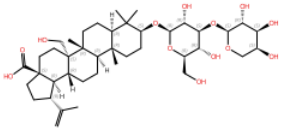
$C_{41}H_{66}O_{13}$

(3β,4α)-3-[(4-*O*-β-D-Glucopyranosyl-α-L-arabinopyranosyl)oxy]-23-hydroxylup-20(29)-en-28-oic acid

4 References | 0 Reactions | 0 Suppliers

3	Similarity Score: 100

137553-09-4



Absolute stereochemistry shown, Rotation (+)

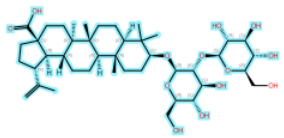
$C_{41}H_{66}O_{13}$

(3β)-3-[(3-*O*-α-L-Arabinopyranosyl-β-D-glucopyranosyl)oxy]-27-hydroxylup-20(29)-en-28-oic acid

2 References | 0 Reactions | 0 Suppliers

4	Similarity Score: 100

135757-66-3



Absolute stereochemistry shown

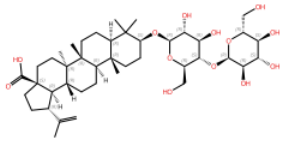
$C_{42}H_{68}O_{13}$

Lup-20(29)-en-28-oic acid, 3-[(2-*O*-β-D-glucopyranosyl-β-D-glucopyranosyl)oxy]-, (3β)-

2 References | 1 Reaction | 6 Suppliers

5	Similarity Score: 100

103482-16-2



Absolute stereochemistry shown

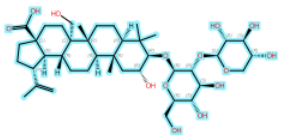
$C_{42}H_{68}O_{13}$

Lup-20(29)-en-28-oic acid, 3-[(4-*O*-α-D-glucopyranosyl-β-D-glucopyranosyl)oxy]-, (3β)-

2 References | 1 Reaction | 1 Supplier

6	Similarity Score: 100

2211959-71-4



Absolute stereochemistry shown, Rotation (+)

$C_{41}H_{66}O_{14}$

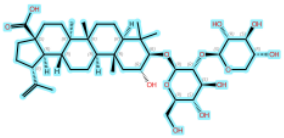
(2α,3β)-2,27-Dihydroxy-3-[(2-*O*-β-D-xylopyranosyl-β-D-glucopyranosyl)oxy]lup-20(29)-en-28-oic acid

1 Reference | 0 Reactions | 1 Supplier

Figure S19: Search report from SciFinder for **1** (heptaelliptoic acid A) (Page 2) Accessed on July 21, 2024

7 Similarity Score: **100**

2211959-69-0



Absolute stereochemistry shown, Rotation (+)

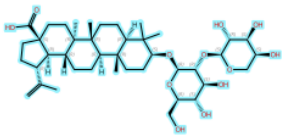
$C_{41}H_{66}O_{13}$

(2α,3β)-2-Hydroxy-3-[(2-*O*-β-D-xylopyranosyl-β-D-glucopyranosyl)oxy]lup-20(29)-en-28-oic acid

1 Reference | 0 Reactions | 1 Supplier

8 Similarity Score: **100**

420790-70-1



Absolute stereochemistry shown

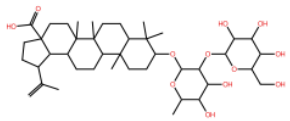
$C_{41}H_{66}O_{12}$

Lup-20(29)-en-28-oic acid, 3-[(2-*O*-α-L-arabinopyranosyl-β-D-glucopyranosyl)oxy]-, (3β)-

1 Reference | 0 Reactions | 0 Suppliers

9 Similarity Score: **100**

80312-31-8



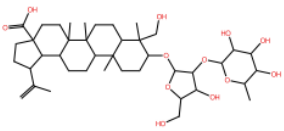
$C_{42}H_{68}O_{12}$

Lup-20(29)-en-28-oic acid, 3-[(6-deoxy-2-*O*-β-D-glucopyranosyl-α-L-mannopyranosyl)oxy]-, (3β)-

1 Reference | 0 Reactions | 0 Suppliers

10 Similarity Score: **100**

1041673-58-8

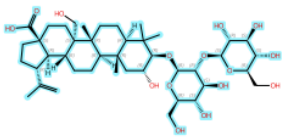


$C_{41}H_{66}O_{12}$

0 References | 0 Reactions | 0 Suppliers

11 Similarity Score: **99**

2211959-72-5



Absolute stereochemistry shown, Rotation (-)

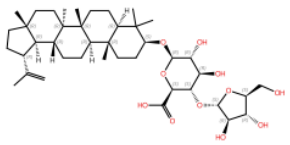
$C_{42}H_{68}O_{15}$

(2α,3β)-3-[(2-*O*-β-D-Glucopyranosyl-β-D-glucopyranosyl)oxy]-2,27-dihydroxylup-20(29)-en-28-oic acid

1 Reference | 0 Reactions | 1 Supplier

12 Similarity Score: **99**

78657-53-1



Absolute stereochemistry shown

$C_{41}H_{66}O_{11}$

β-D-Glucopyranosiduronic acid, (3β)-lup-20(29)-en-3-yl 4-*O*-α-L-arabinofuranosyl-

1 Reference | 0 Reactions | 0 Suppliers

Figure S20: Search report from SciFinder for **1** (heptaelliptoic acid A) (Page 3) Accessed on July 21, 2024

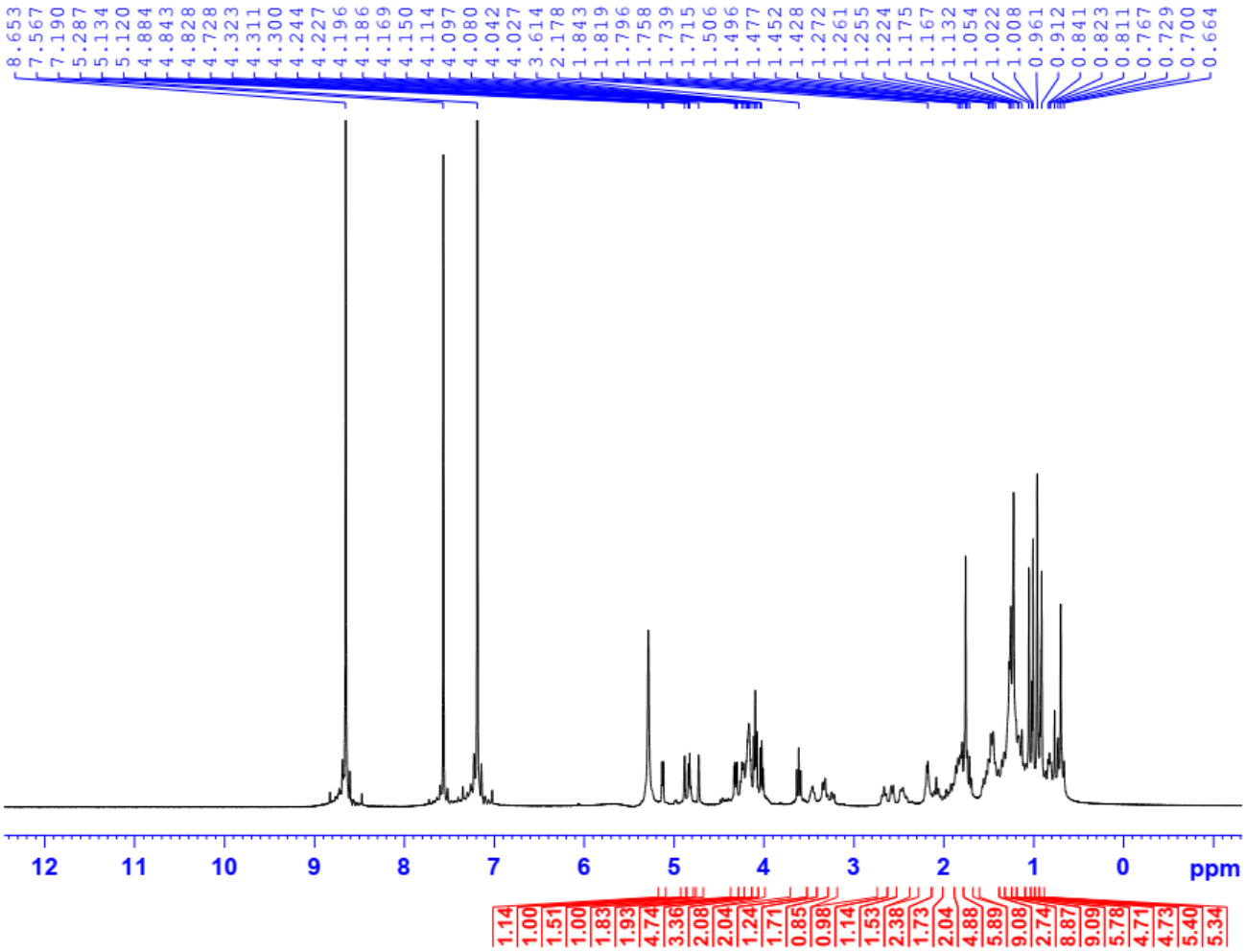


Figure S21: ^{1}H-NMR spectrum (500 MHz) of compound **2** in C_5D_5N

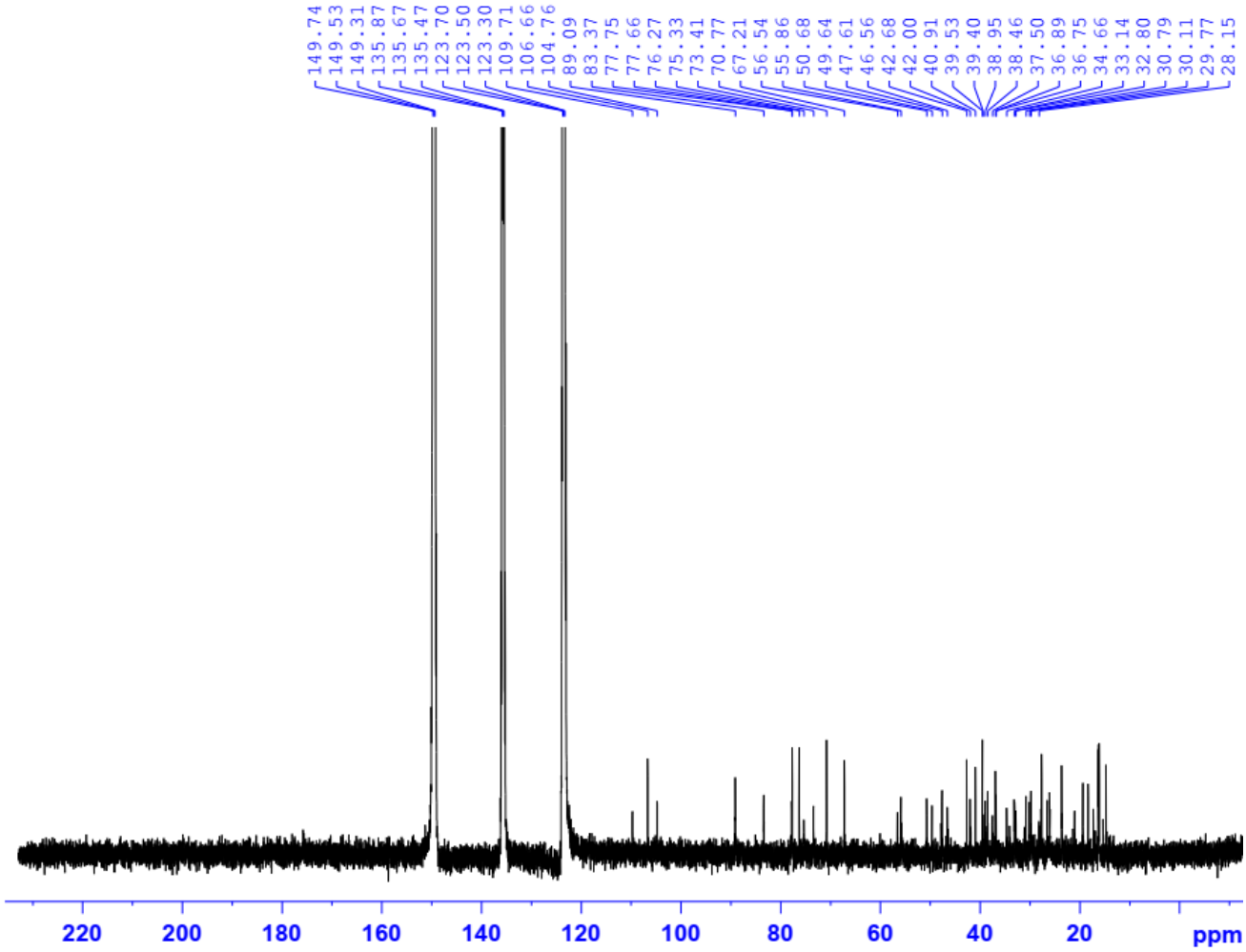


Figure S22: ^{13}C-NMR spectrum (125 MHz) of compound **2** in C_5D_5N

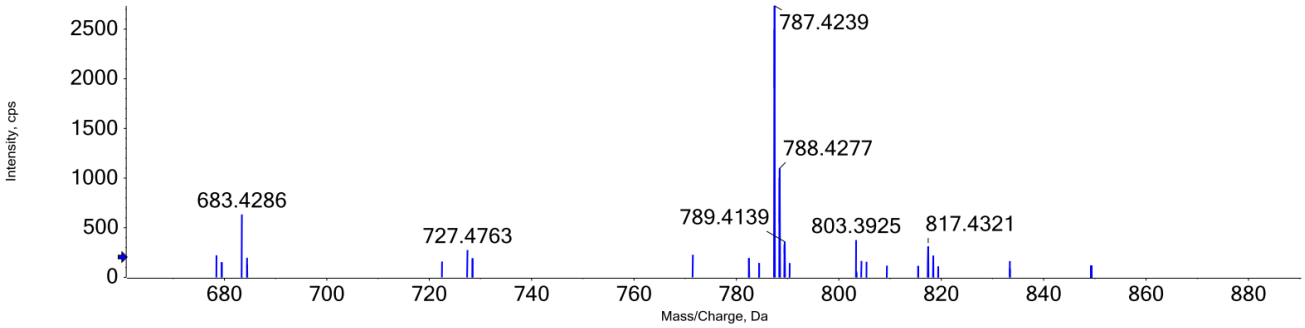


Figure S23: HR-ESI-MS spectrum (positive mode) of compound **2**

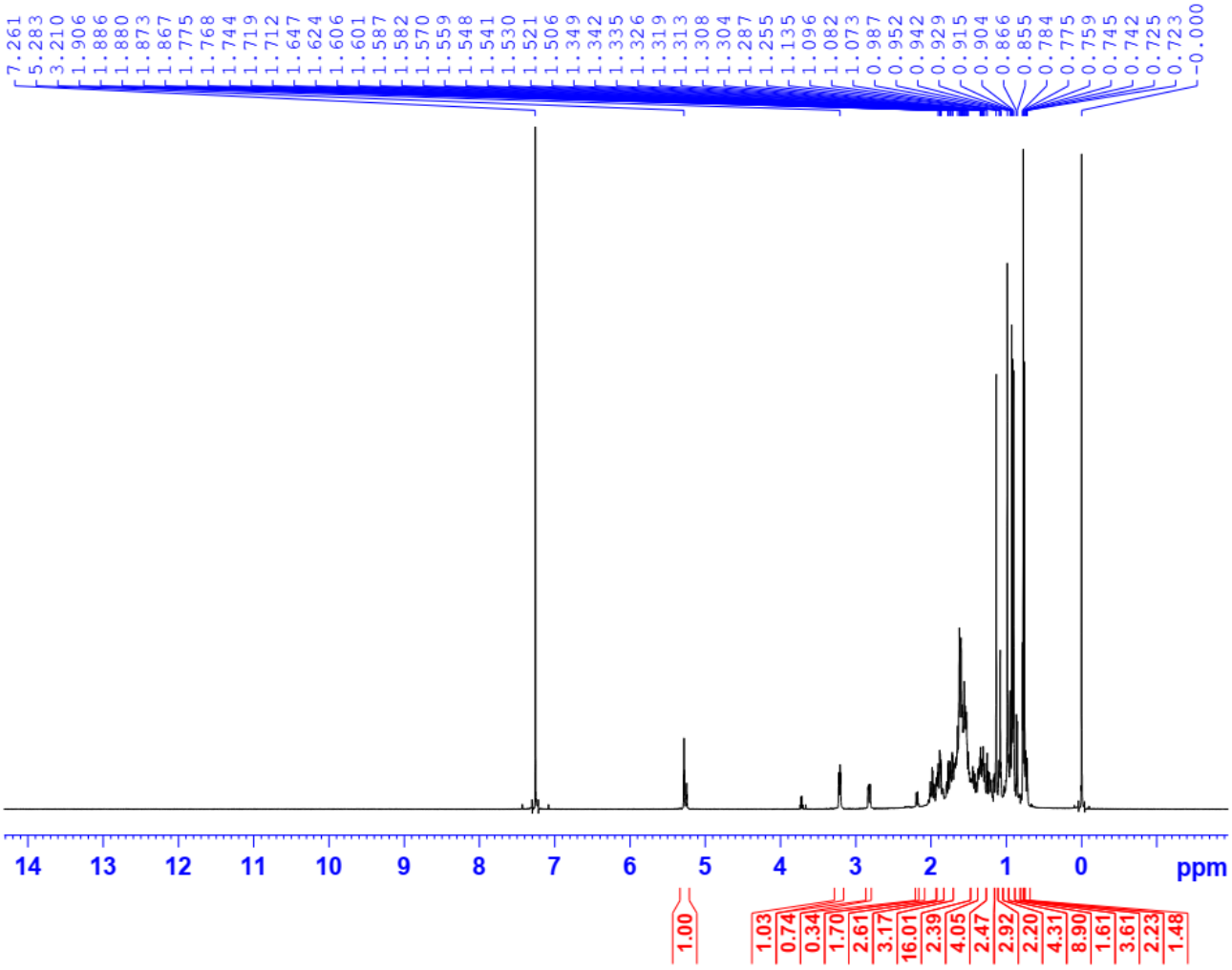


Figure S24: ^{1}H-NMR spectrum (600 MHz) of compound **3** in $CDCl_3$

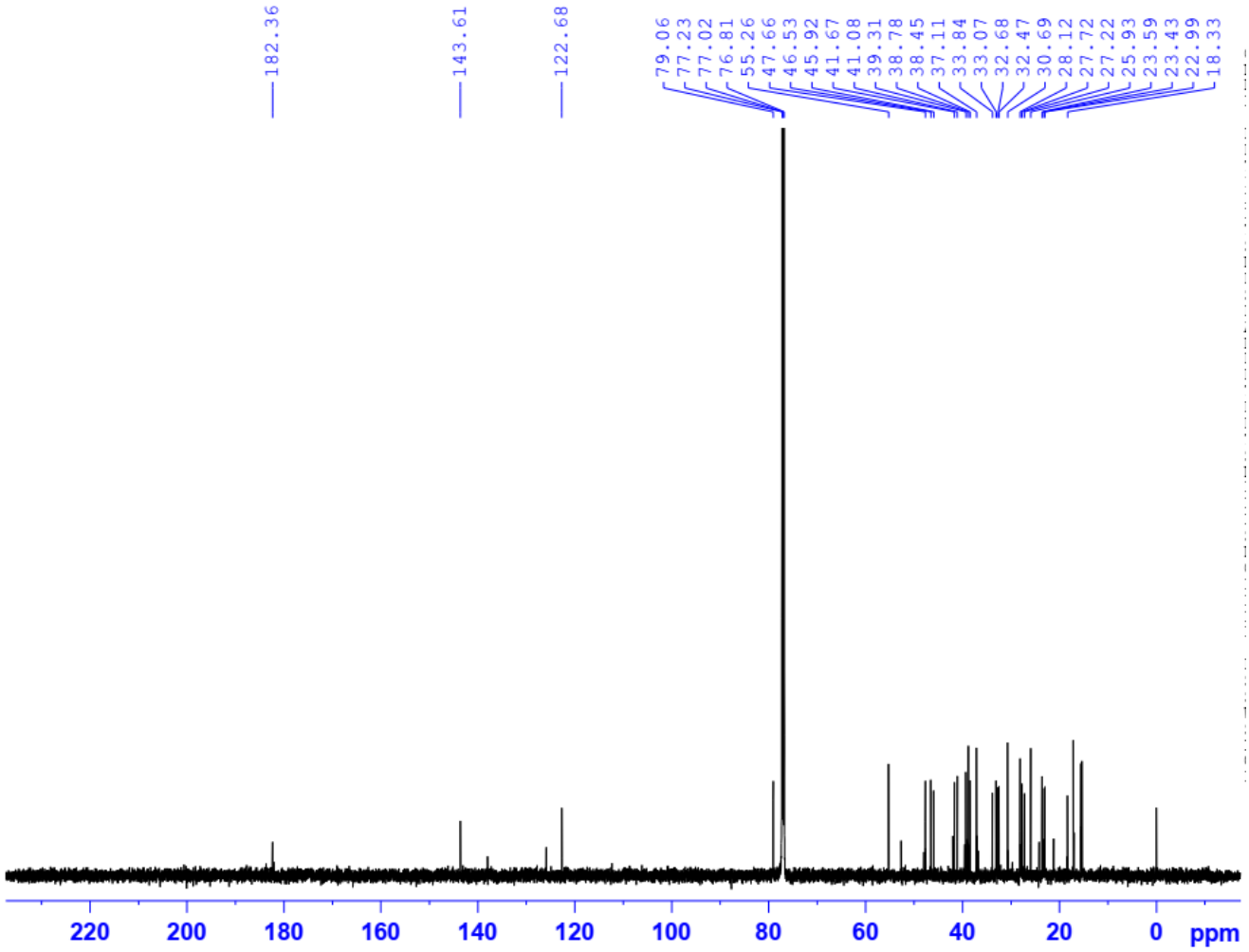


Figure S25: ^{13}C-NMR spectrum (150 MHz) of compound **3** in $CDCl_3$

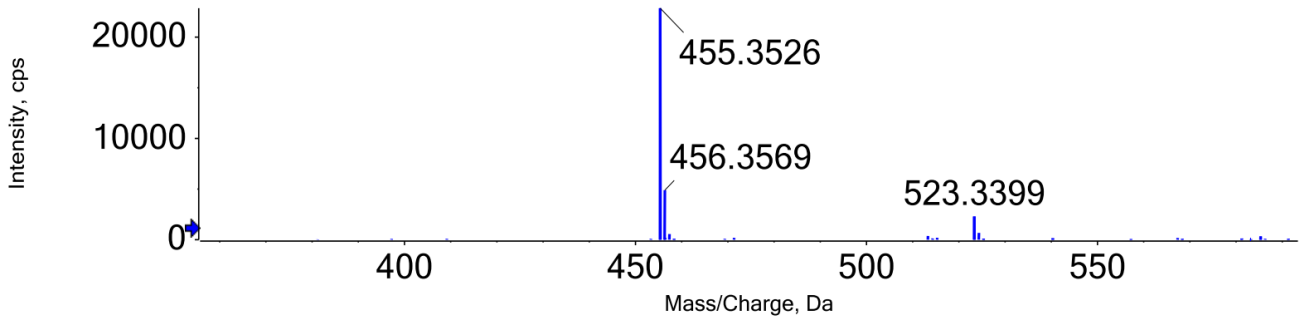


Figure S26: HR-ESI-MS spectrum (negative mode) of compound **3**

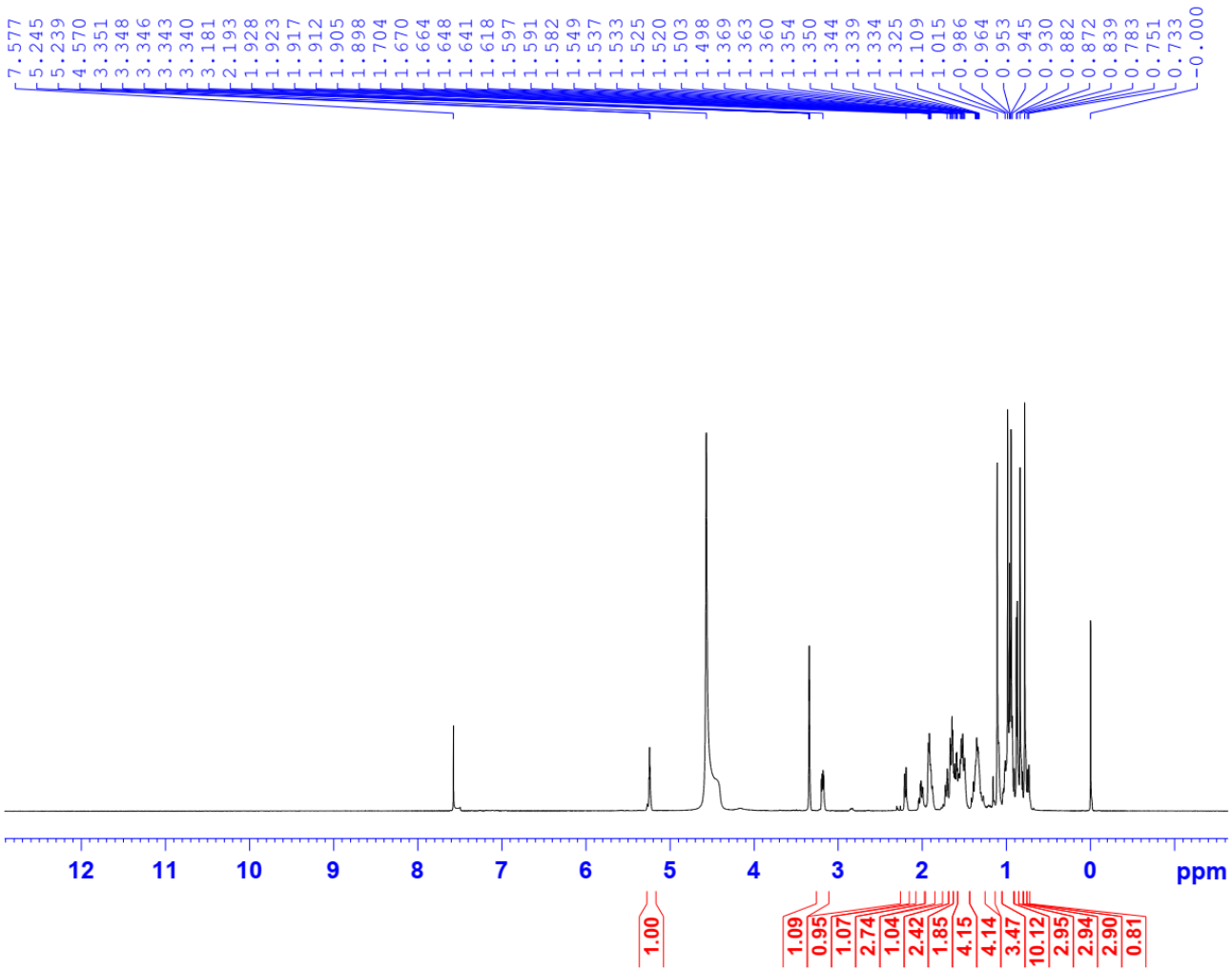


Figure S27: ^{1}H-NMR spectrum (600 MHz) of compound **4** in $CDCl_3$ + CD_3OD

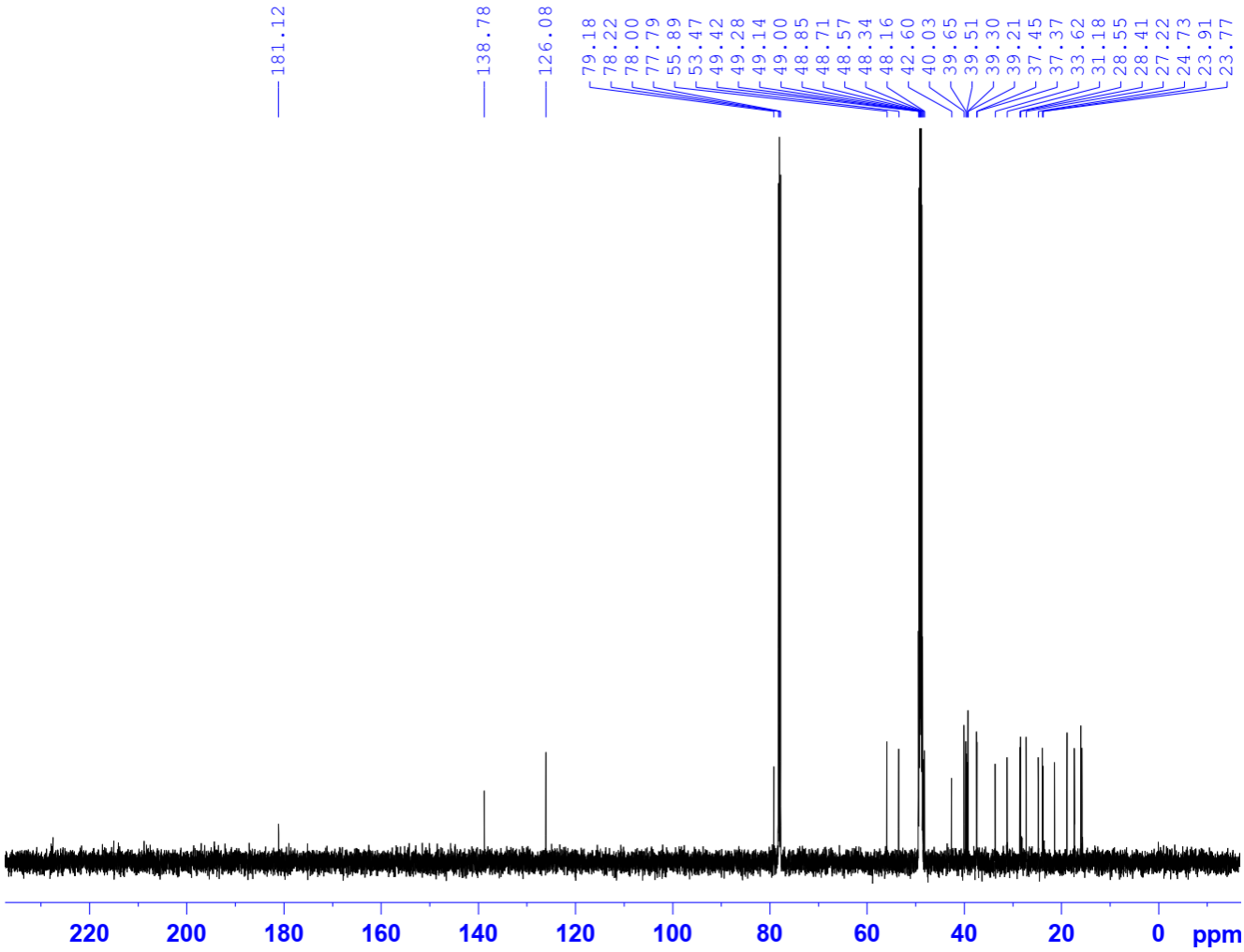


Figure S28: ^{13}C-NMR spectrum (150 MHz) of compound **4** in $CDCl_3$ + CD_3OD

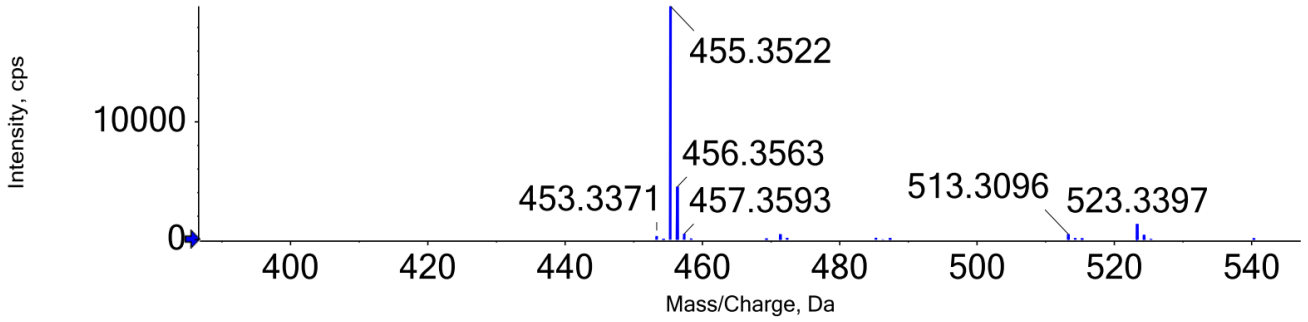


Figure S29: HR-ESI-MS spectrum (negative mode) of compound **4**

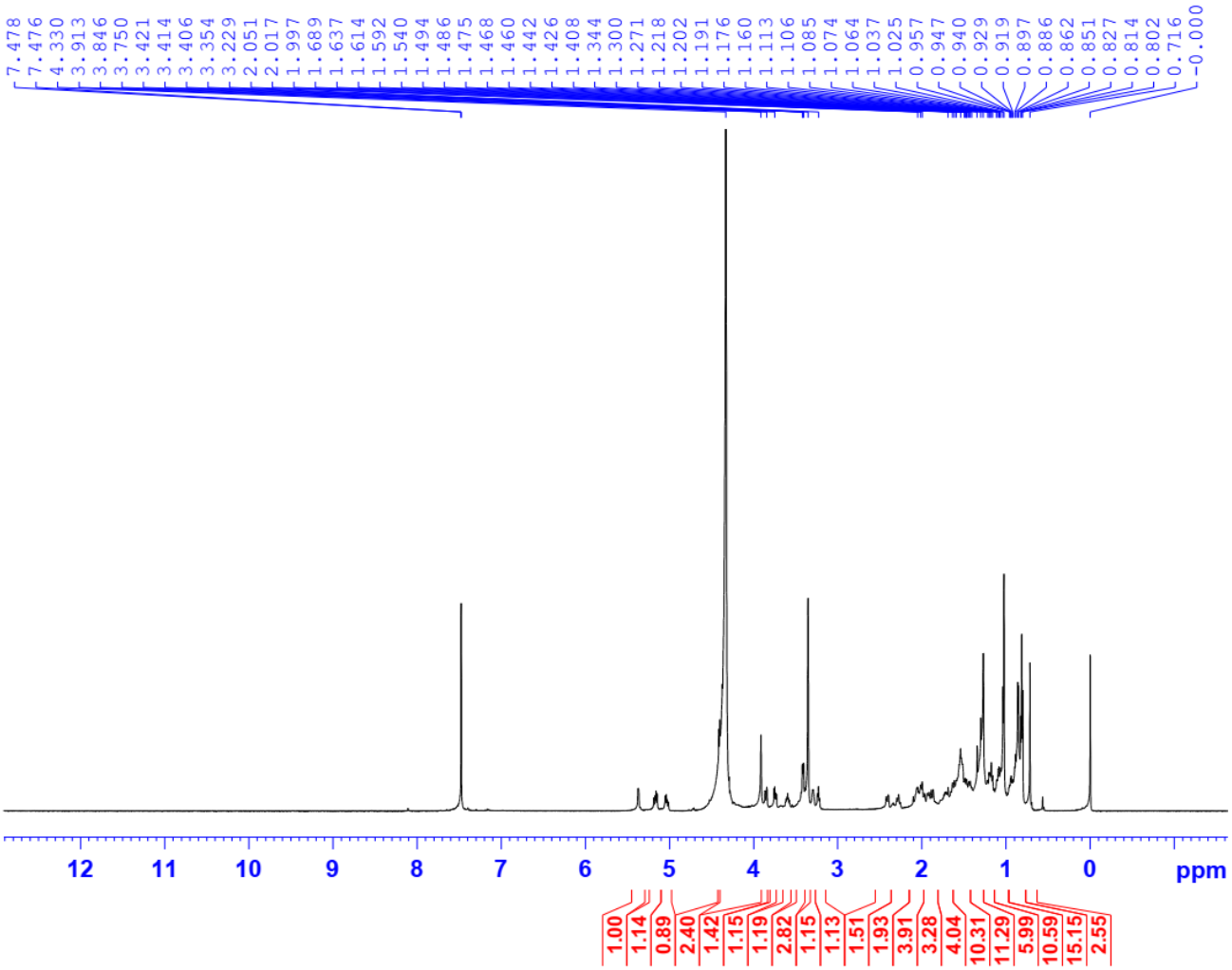


Figure S30: ^{1}H-NMR spectrum (600 MHz) of compound **5** in $CDCl_3$ + CD_3OD

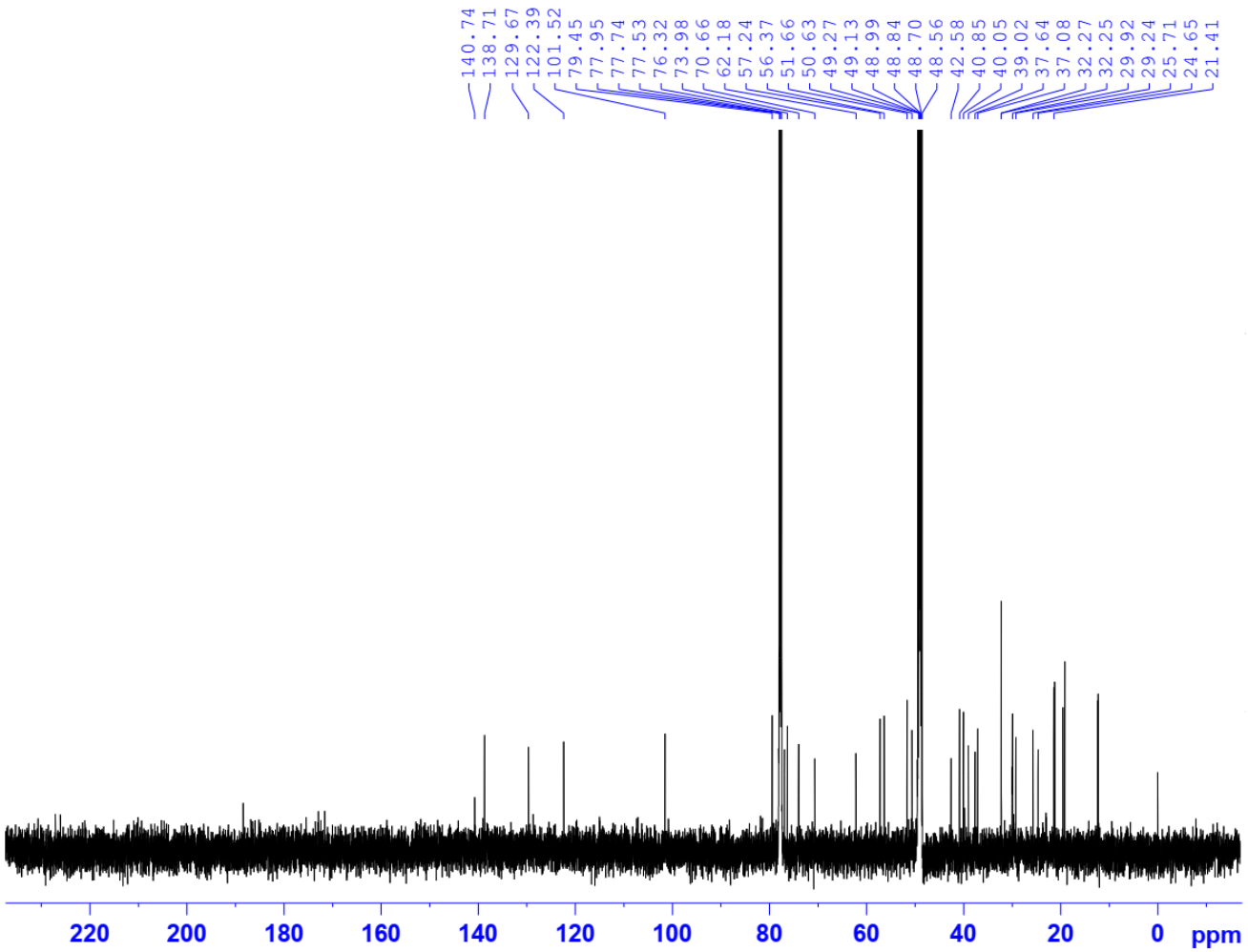


Figure S31: ^{13}C-NMR spectrum (150 MHz) of compound **5** in $CDCl_3$ + CD_3OD

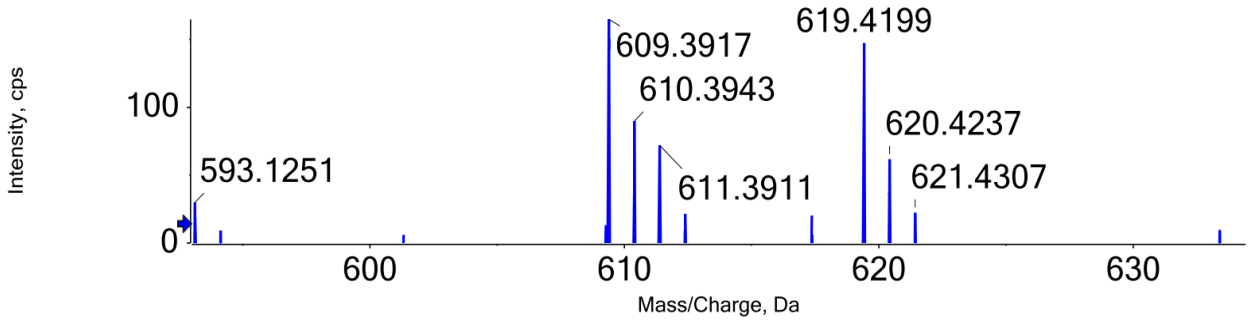


Figure S32: HR-ESI-MS spectrum (negative mode) of compound **5**

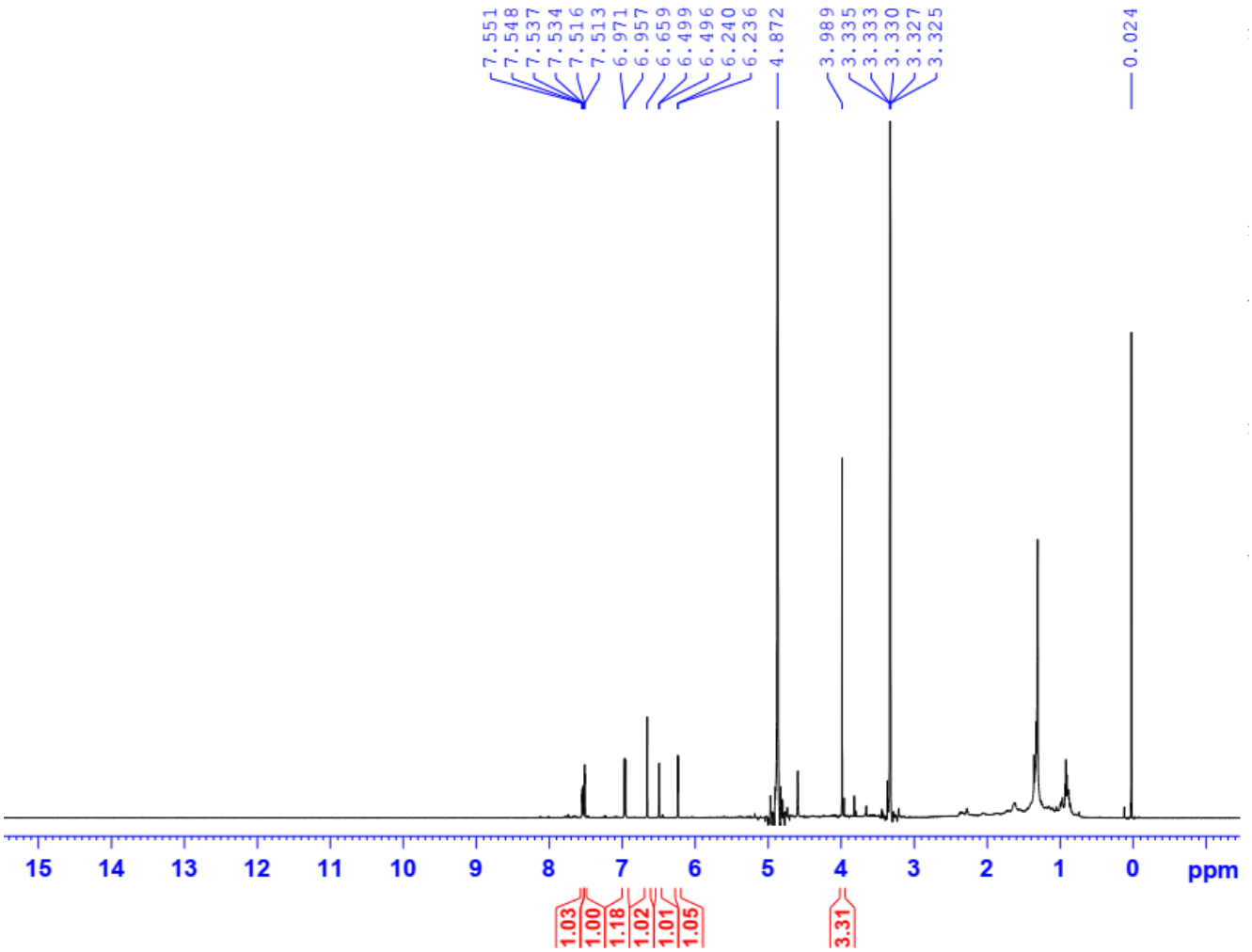


Figure S33: ^{1}H-NMR spectrum (600 MHz) of compound **6** in CD_3OD

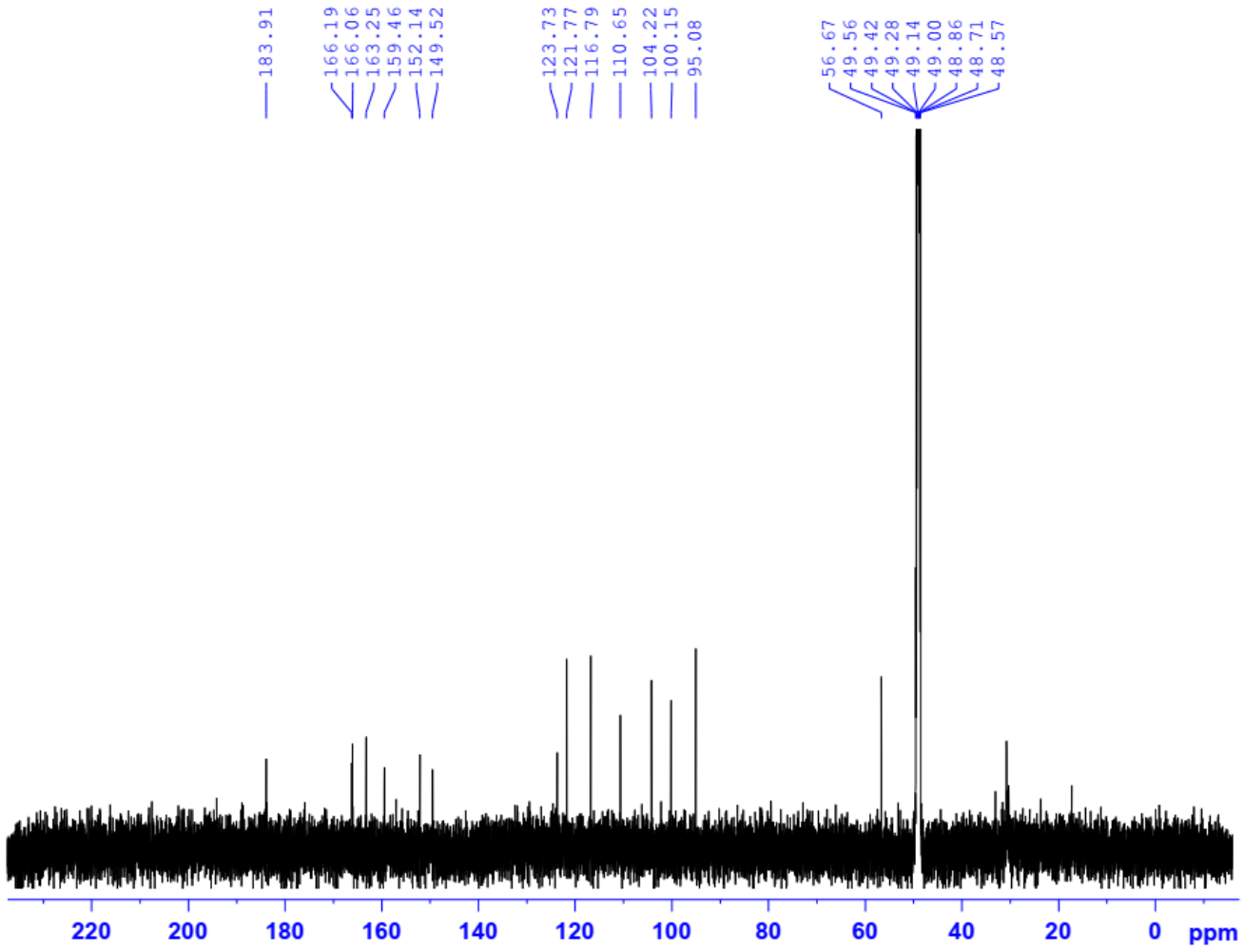


Figure S34: ^{13}C-NMR spectrum (150 MHz) of compound **6** in CD_3OD

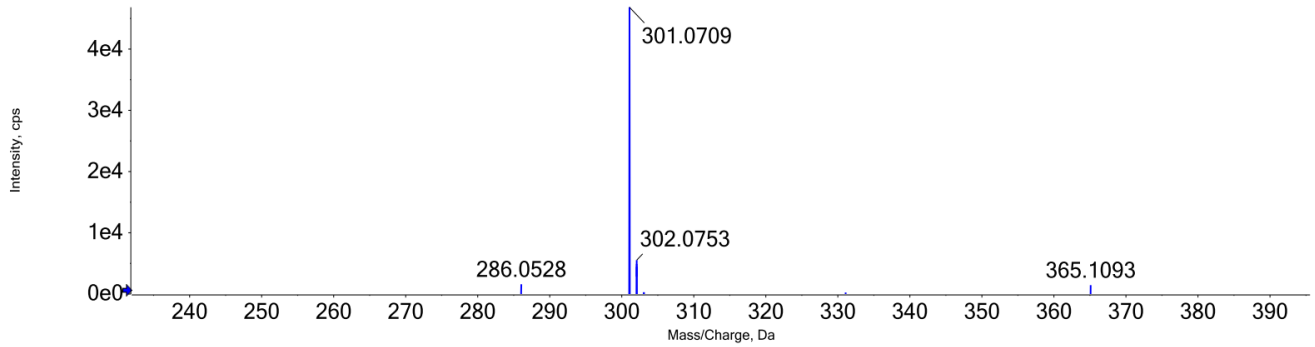


Figure S35: HR-ESI-MS spectrum (positive mode) of compound **6**

Table S1: NMR spectral data for compounds **1**, 28-*O*-*β*-D-glucopyranosylbetulinic acid 3-*O*-*β*-D-glucopyranoside, and 2*α*-hydroxy-3*β*-[(*O*-*β*-D-xylopyranosyl-(1→2)-*β*-D-glucopyranosyl)oxy]lup-20(29)-en-28-oic acid *α*-L-rhamnopyranosyl ester in methanol-d_4 (δ in ppm, J in Hz)

No.	**1**		**28-*O*-*β*-D-glucopyranosylbetulinic acid 3-*O*-*β*-D-glucopyranoside[5]**		**2*α*-hydroxy-3*β*-[(*O*-*β*-D-xylopyranosyl-(1→2)-*β*-D-glucopyranosyl)oxy]lup-20(29)-en-28-oic acid *α*-L-rhamnopyranosyl ester[6]**	
	δ_H	δ	δ_H	δ_C	δ_H	δ_C
1	1.69 (1H, m) 0.92 (1H, m)	40.1		40.1	-	47.7
2	1.94 (1H, m) 1.70 (1H, m)	27.3		27.2	3.69 (1H, dd, J = 11.8, 9.3)	68.2
3	3.12 (1H, dd, J = 10.2, 4.2)	91.0	3.15 (1H, m)	90.9	2.94 (1H, d, J = 9.3)	96.4
4	-	40.4		40.3		41.8
5	0.71 (1H, d, J =10.8)	57.3		57.2		56.9
6	1.55 1H, m) 1.42 (1H, m)	19.3		19.3		19.3
7	1.42 (1H, m)	35.7		35.5		35.4
8	-	42.0		42.1		42.0
9	1.30 (1H, m)	52.1		52.0		51.9

10	-	38.1		38.1	39.0
11	1.41 (1H, m) 1.26 (1H, m)	22.2		22.1	22.2
12	1.05 (1H, m) 1.71 (1H, m)	27.0		26.9	26.8
13	2.39 (1H, td, *J* = 12.0, 0.6)	39.6		39.4	40.0
14	-	43.6		43.6	43.7
15	1.15 (1H, m) 1.56 (1H, m)	31.0		30.9	30.8
16	2.23 (1H, d, *J* =12.0) 1.39 (1H, m)	33.8		32.8	33.1
17	-	57.3		58.0	58.2
18	1.61 (1H, m)	50.7		50.6	50.5
19	3.07 (1H, td, *J* = 12.0, 3.0)	48.5	3.01 (1H, td, *J*= 10.8, 4.5)	48.4	48.7
20	-	152.4		151.9	151.4
21	1.92 (1H, m) 1.34 (1H, m)	31.9		31.5	31.7

22	1.92 (1H, m) 1.40 (1H, m)	38.5		37.5		37.9
23	1.03 (3H, s)	28.2	1.03 (3H, s)	28.4	1.08 (3H, s)	28.4
24	0.81 (3H, s)	16.4	0.82 (3H, s)	16.8	0.87 (3H, s)	17.4
25	0.86 (3H, s)	16.8	0.86 (3H, s)	16.8	0.92 (3H, s)	17.9
26	0.98 (3H, s)	16.8	0.95 (3H, s)	16.7	0.94 (3H, s)	16.8
27	0.99 (3H, s)	15.1	0.99 (3H, s)	15.2	1.01 (3H, s)	15.1
28	-	181.7		176.2		175.6
29	4.70 (1H, d, *J* = 1.8) 4.57 (1H, d, *J* = 1.2)	109.9	4.71 (1H, brs) 4.60 (1H, brs)	110.3	4.75 (3H, s) 4.62 (3H, s)	110.6
30	1.69 (3H, s)	19.6	1.69 (3H, s)	19.5	1.70 (3H, s)	19.5
3-*O*-Glc						
1′	4.42 (1H, d, *J* = 7.8)	105.3	4.30 (1H, d, *J* = 7.6)	106.8	4.40 (1H, d, *J* = 7.5)	104.8
2′	3.42 (1H, dd, *J* = 9.0, 7.8)	83.3	3.18 (1H, m)	75.7	3.52 (1H, dd, *J* = 8.8, 7.5)	82.2
3′	3.53 (1H, m)	78.3	3.33 (1H, m)	78.3	3.57 (1H, t, *J* = 8.8)	78.5
4′	3.32 (1H, m)	71.5	3.28 (1H, m)	71.7	3.36 (1H, t, *J* = 8.8)	71.1
5′	3.22 (1H, m)	77.5	3.24 (1H, m)	77.7	3.35 (1H, m)	78.0

6′	3.84 (1H, m) 3.67 (1H, dd, *J* = 12.0, 5.4)	62.7	3.83 (1H, m) 3.65 (1H, dd, *J* = 11.9, 5.3)	62.8	3.84 (1H, dd, *J* =12.0, 1.8) 3.65 (1H, dd, *J* =12.0, 3.5)	62.3
Xyl						
1″	4.51 (1H, d, *J* = 7.2)	106.3			4.59 (1H, d, *J* = 7.6)	105.9
2″	3.21 (1H, m)	76.3			3.21 (1H, dd, *J* = 9.0, 7.6)	76.1
3″	3.34 (1H, m)	77.8			3.30 (1H, t, *J* = 9.0)	78.0
4″	3.45 (1H, ddd, *J* = 10.2, 8.4, 5.4)	71.2			3.43 (1H, ddd, *J* = 10.6, 9.0, 5.0)	71.2
5″	3.80 (1H, dd, *J* = 11.4, 5.4) 3.13 (1H, dd, *J* = 10.8, 6.0)	67.2			3.78 (1H, dd, *J* = 11.3, 5.0) 3.12 (1H, dd, *J* = 11.3, 10.6)	67.1
28-*O*-Glc/Rha						
1			5.49 (1H, d, *J* = 8.1)	95.2	5.99 (1H, brs)	95.1
			3.31 (1H, m)	74.1	3.79 (1H, brd, *J* = 3.5)	71.4
3			3.42 (1H, m)	78.4	3.65 (1H, dd, *J* = 9.6, 3.5)	72.5
4			3.39 (1H, m)	71.1	3.45 (1H, t, *J* = 9.6)	73.4
5			3.38 (1H, m)	78.8	3.67 (1H, qd, *J* = 9.6, 6.3)	72.8
6			3.84 (1H, m)	62.4	1.27 (3H, d, *J* = 6.3)	18.2

	3.70 (1H, dd, *J*= 11.9, 3.0)