Supporting Information

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Isolation of New Secondary Metabolites from *Kedrostis gijef* and Evaluation of Their *α*-Glucosidase Inhibitory Activity

Mahmoud M. Mubarek[1,2], Fahd M. Abdelkarem[1,3], Ahmed Othman[4], Masako Matsumoto [1], Fangjing Li [1] and Kuniyoshi Shimizu[*1]

[1]*Department of Agro-Environmental Sciences, Graduate School of Bioresource and Bioenvironmental Sciences, Kyushu University, Fukuoka, 819-0395, Japan*

[2]*Department of Medicinal and Aromatic plants, Desert Research Center, Matariya, Cairo, 11753, Egypt*

[3]*Department of Pharmacognosy, Faculty of Pharmacy, Al-Azhar University, Assiut, 71524, Egypt*

[4]*Department of Pharmacognosy and Medicinal Plants, Faculty of Pharmacy, Al-Azhar University, Cairo, 11884, Egypt*

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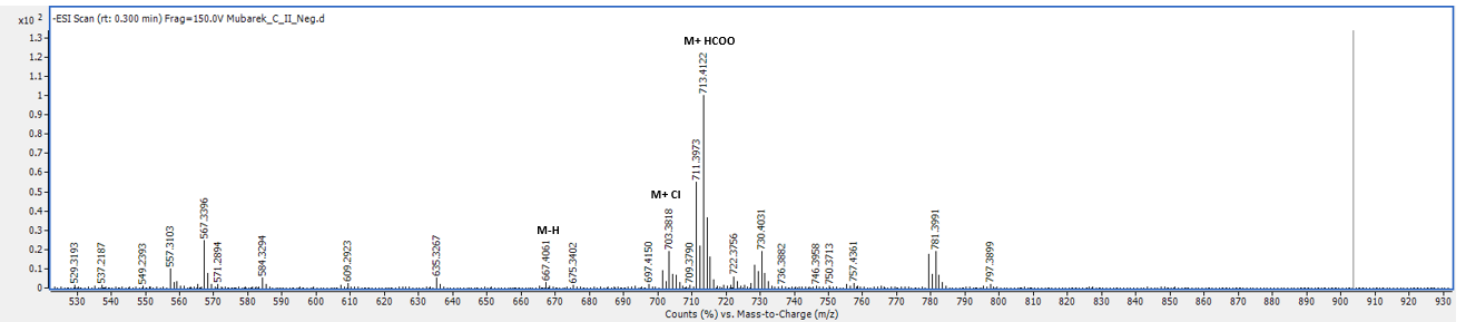


Ion Formula	Species	m/z	m/z (Calc.)	Diff (ppm)	DBE
C37 H61 O13	(M+HCOO)-	713.4122	713.4112	1.40171615	7

Figure S1: Negative HRESIMS for compound **4**

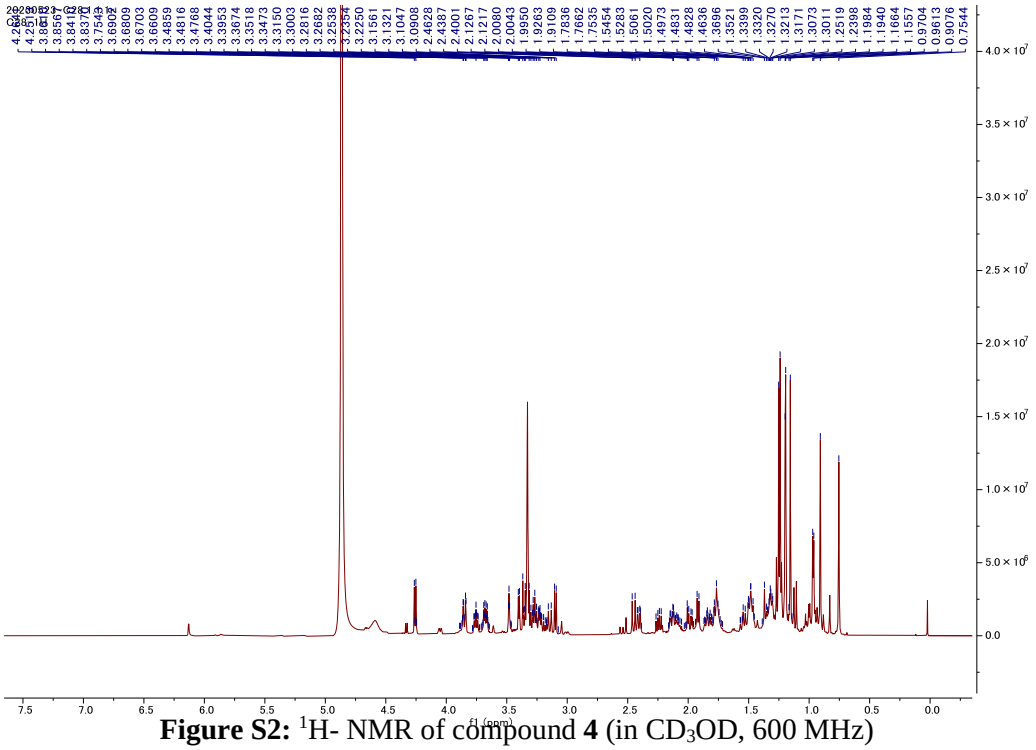


Figure S2: ^{1}H- NMR of compound **4** (in CD_3OD, 600 MHz)

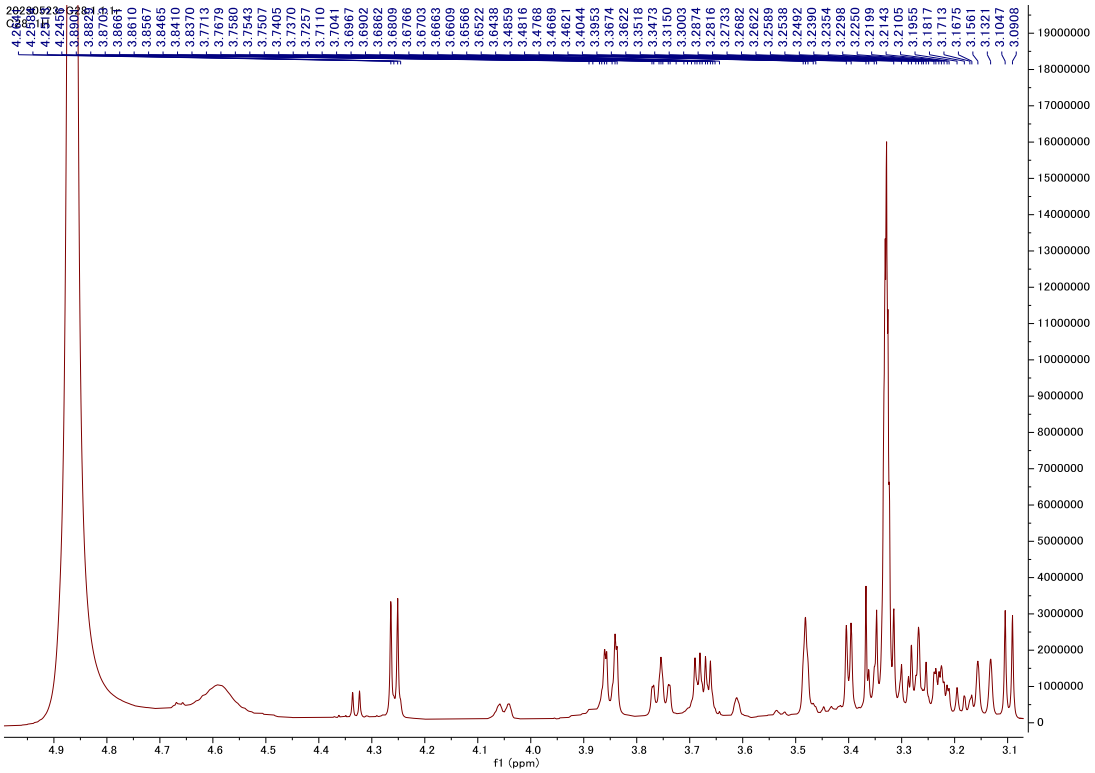


Figure S3: Expanded ^{1}H- NMR of compound **4** (in CD_3OD, 600 MHz)

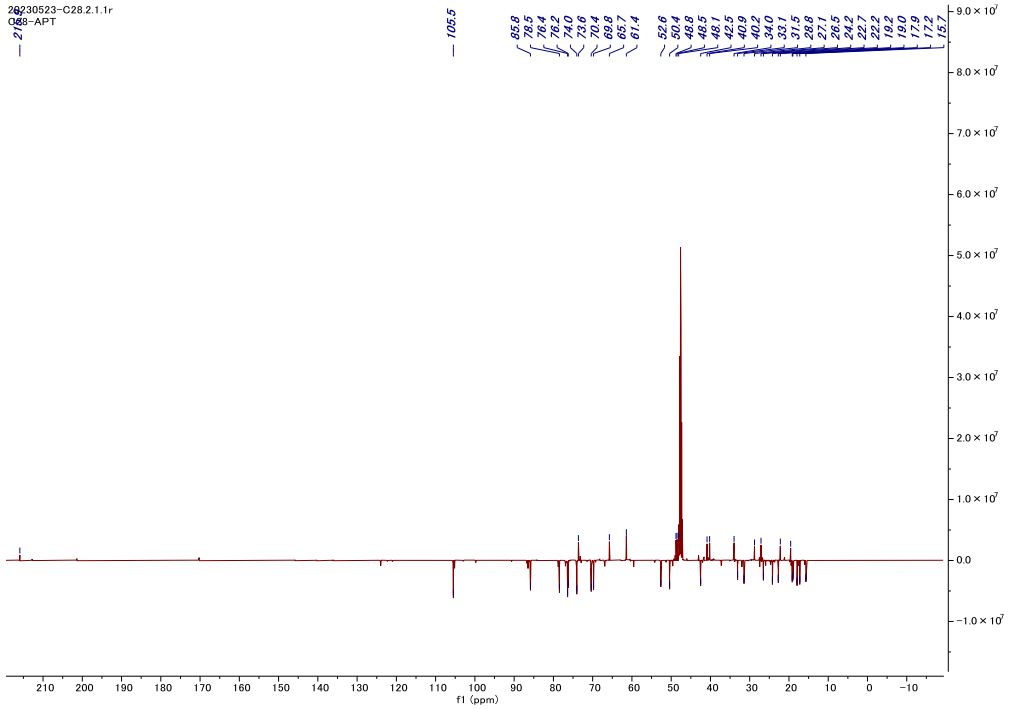


Figure S4: APT-NMR of compound **4** (in CD_3OD, 150 MHz)

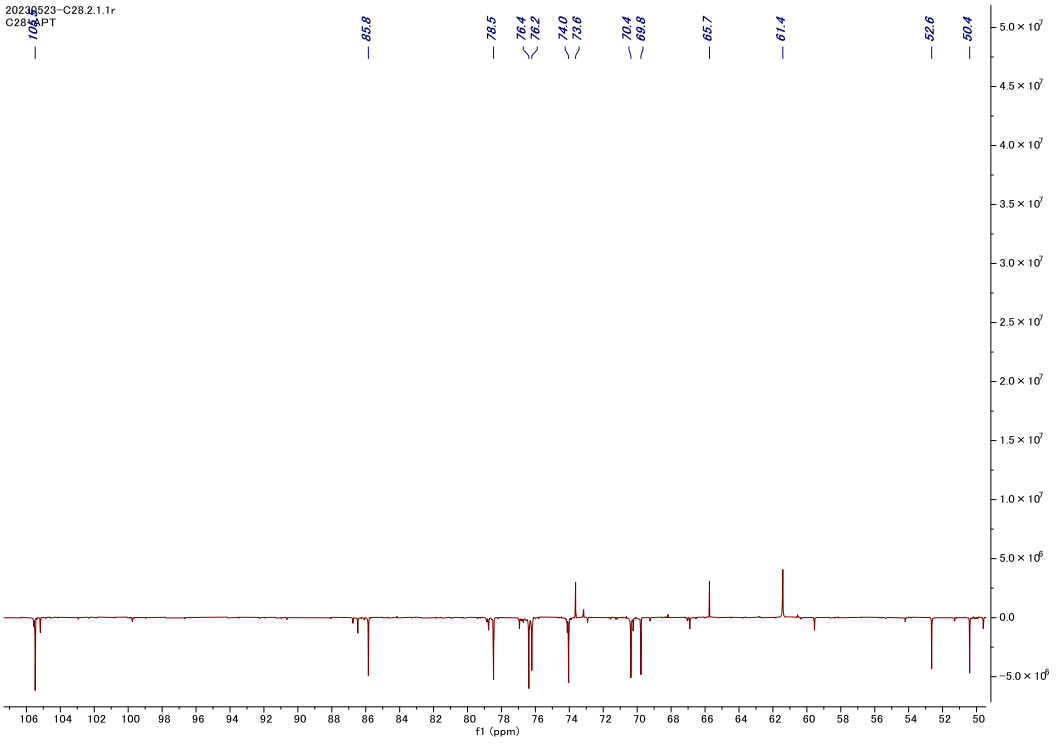


Figure S5: Expanded APT-NMR of compound **4** (in CD_3OD, 150 MHz)

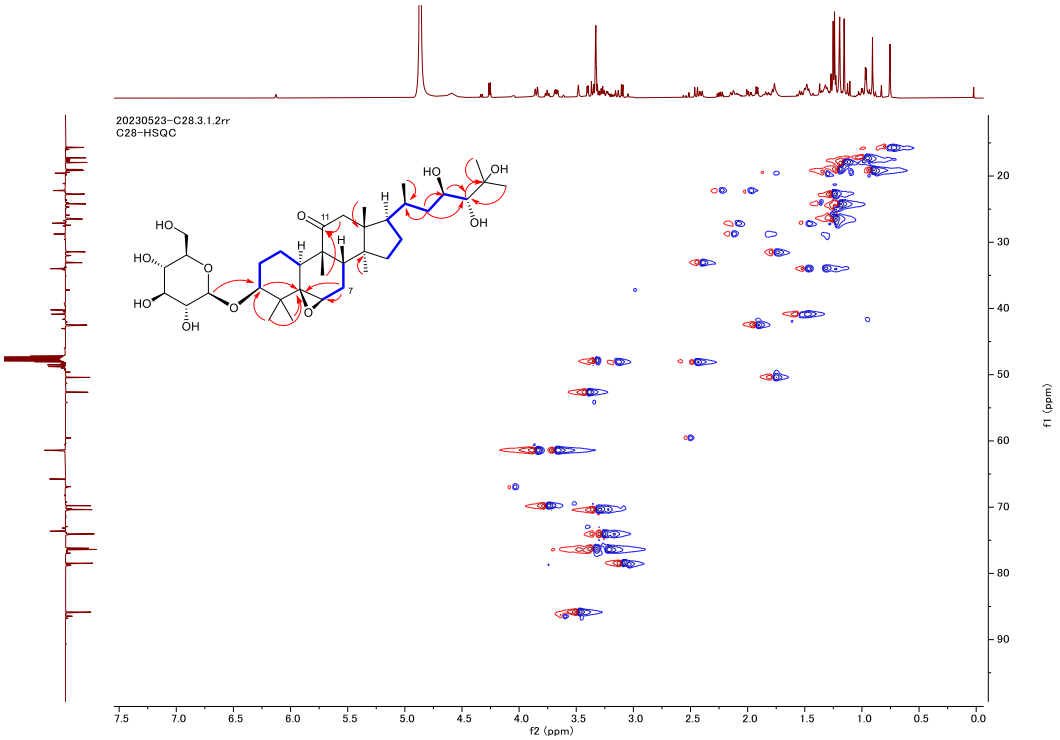


Figure S6: HSQC spectrum of compound **4**

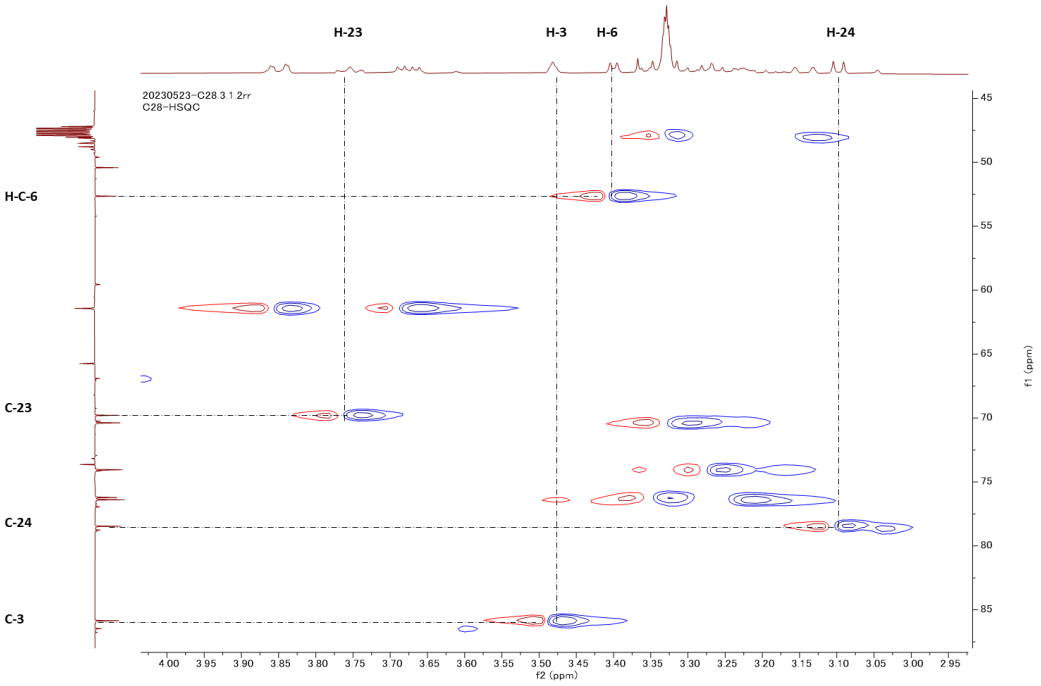


Figure S7: Expanded HSQC spectrum of compound **4**

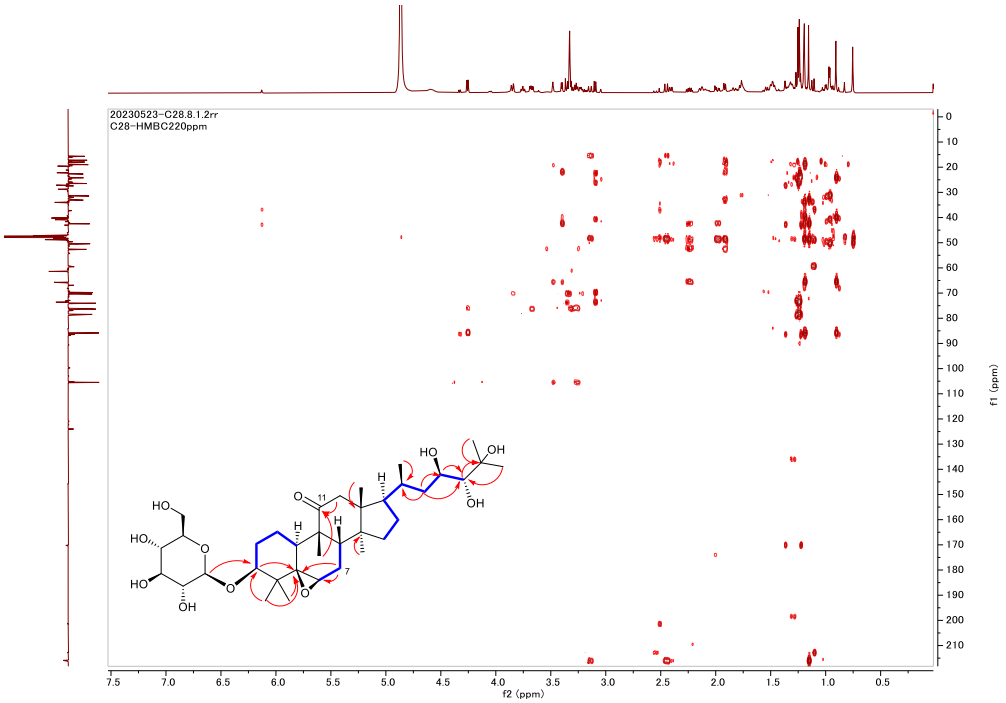


Figure S8: HMBC spectrum of compound **4**

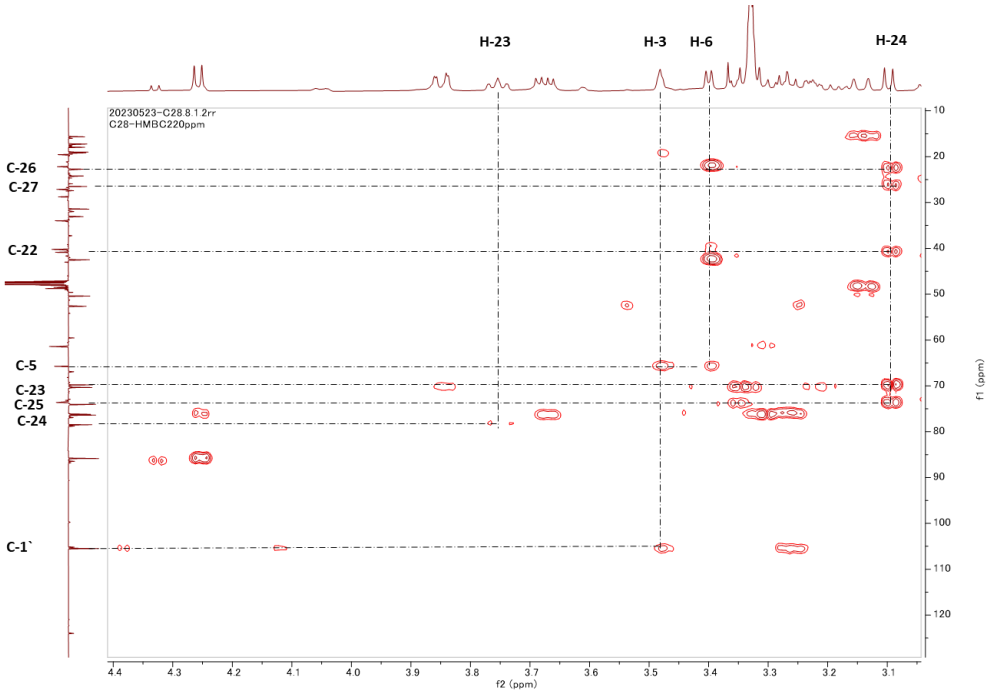


Figure S9: Expanded HMBC spectrum of compound **4**

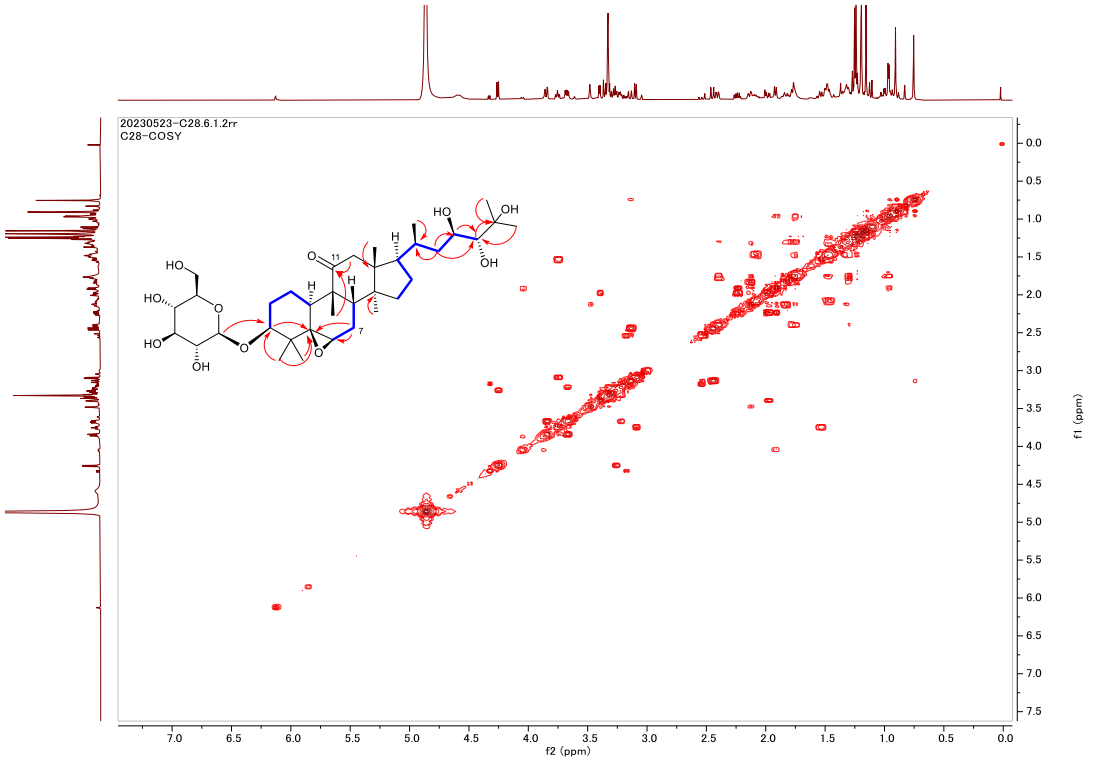


Figure S10: ^{1}H-^{1}H-COSY spectrum of compound **4**

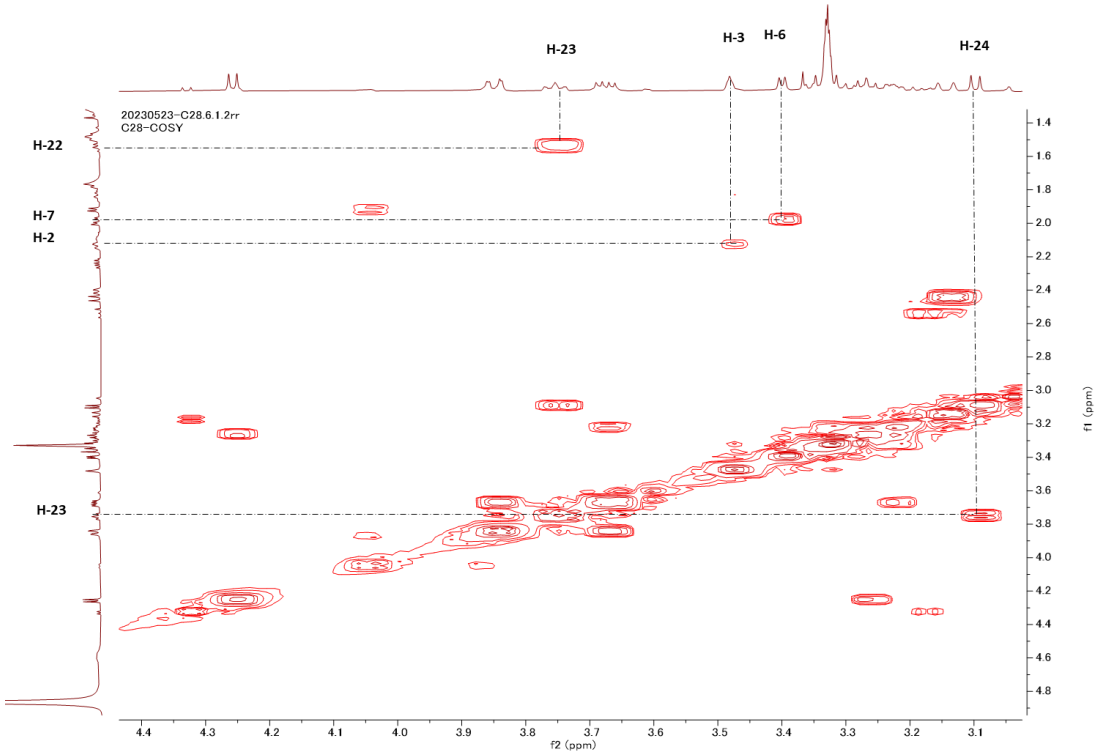


Figure S11: Expanded ^{1}H-^{1}H-COSY spectrum of compound **4**

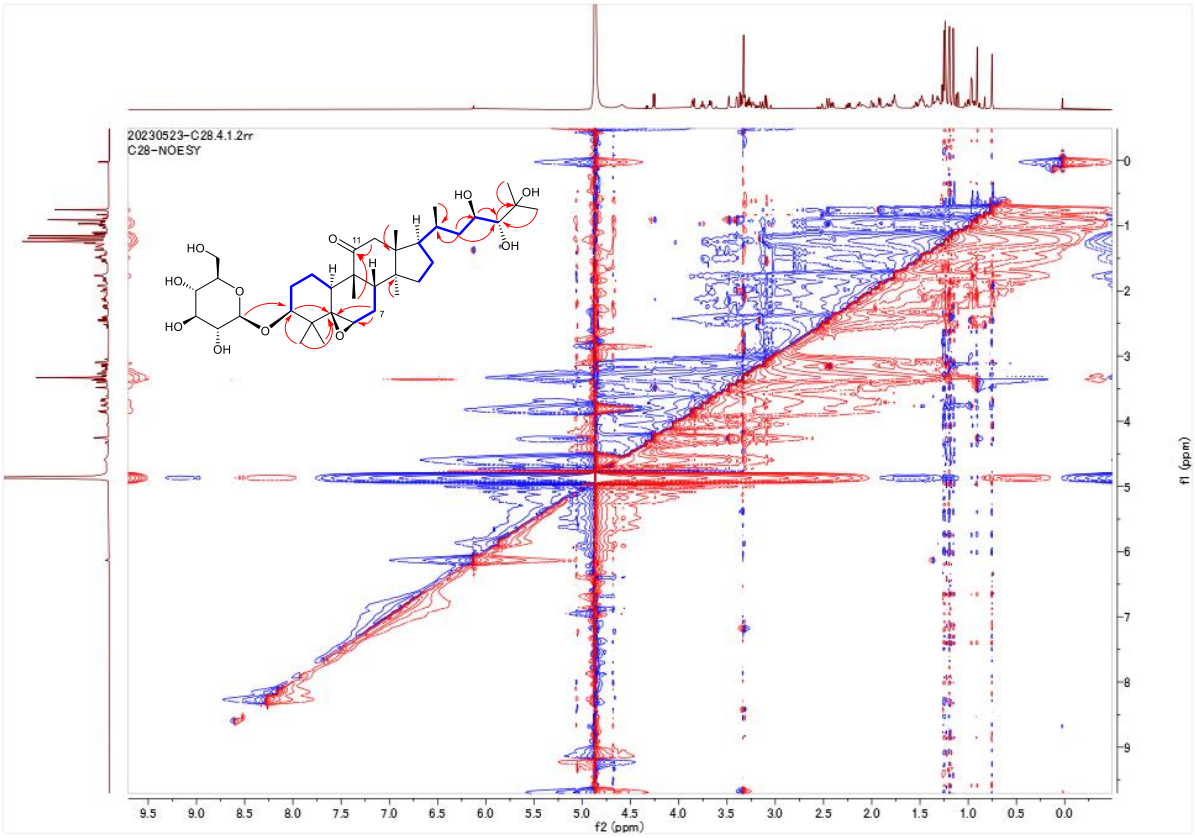


Figure S12: NOESY spectrum of compound **4**

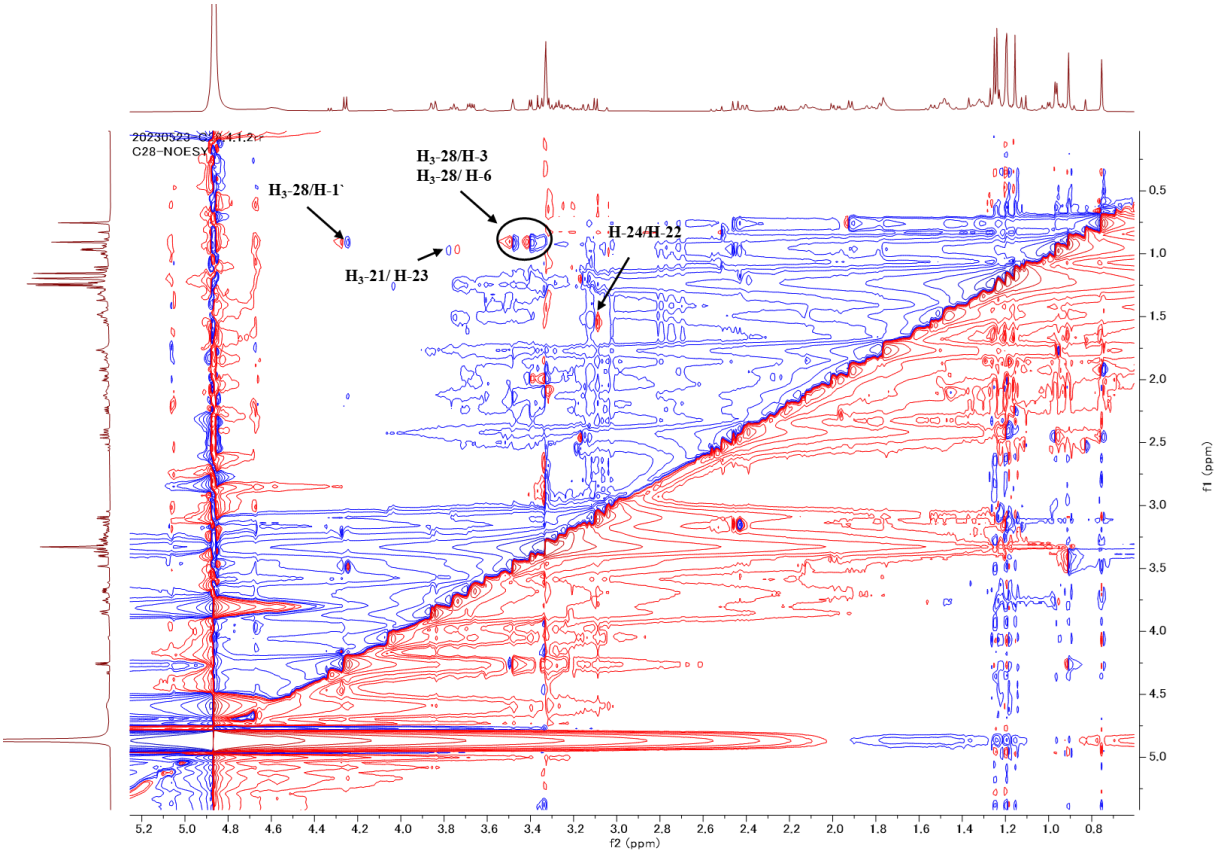
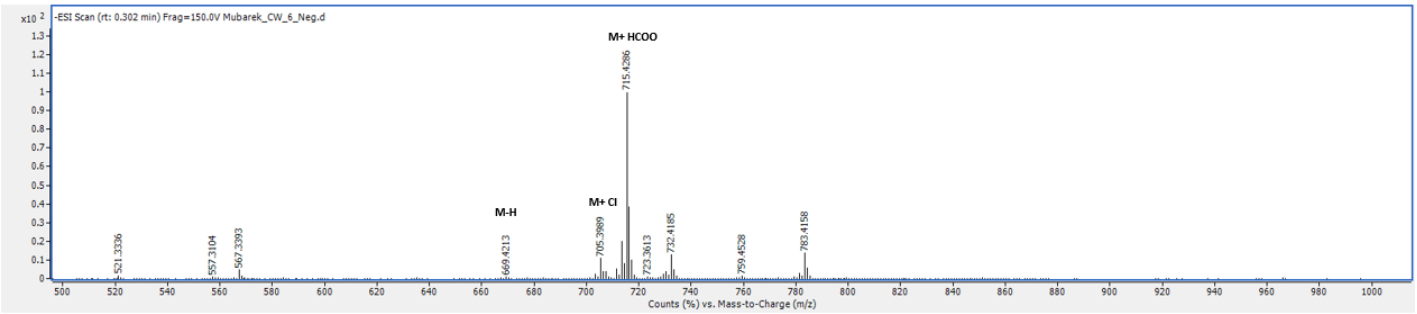


Figure S13: Expanded NOESY spectrum of compound **4**



Ion Formula	Species	m/z	m/z (Calc.)	Diff (ppm)	DBE
C36 H61 O11	(M-H)-	669.4213	669.4214	0.14938274	6

Figure S14: Negative HRESIMS for compound **5**

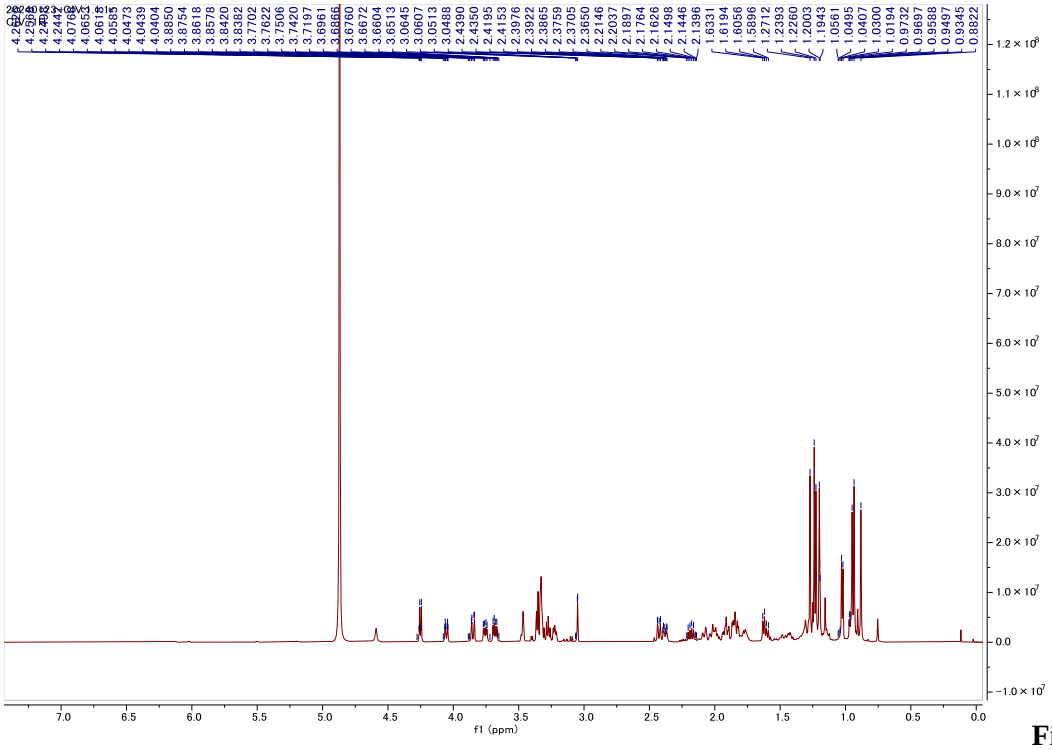


Figure S15: ^{1}H- NMR of compound **5** (in CD_3OD, 600 MHz)

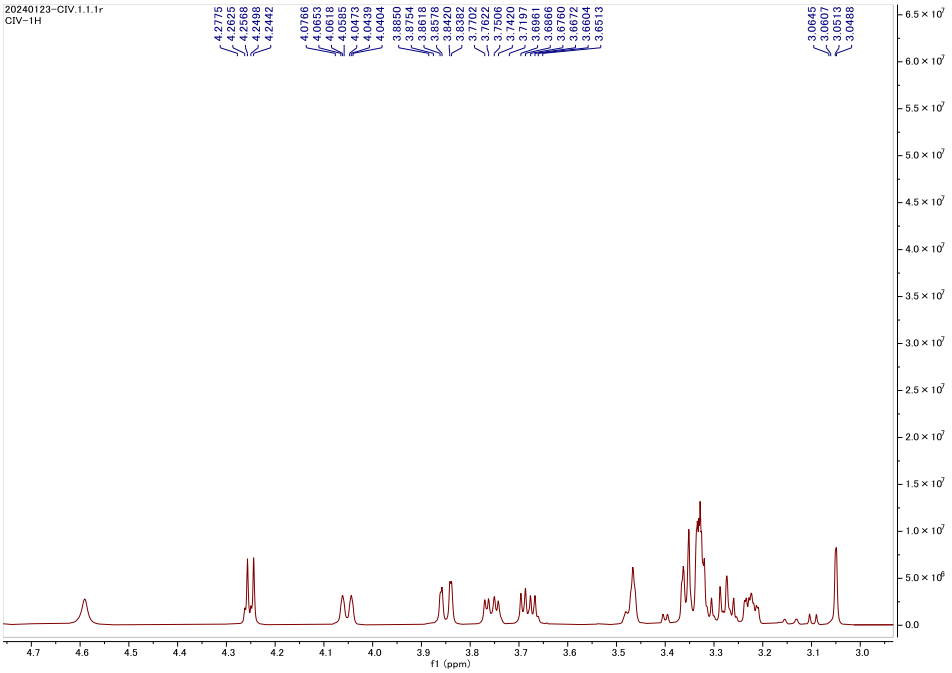


Figure S16: Expanded ^{1}H- NMR of compound **5** (in CD_3OD, 600 MHz)

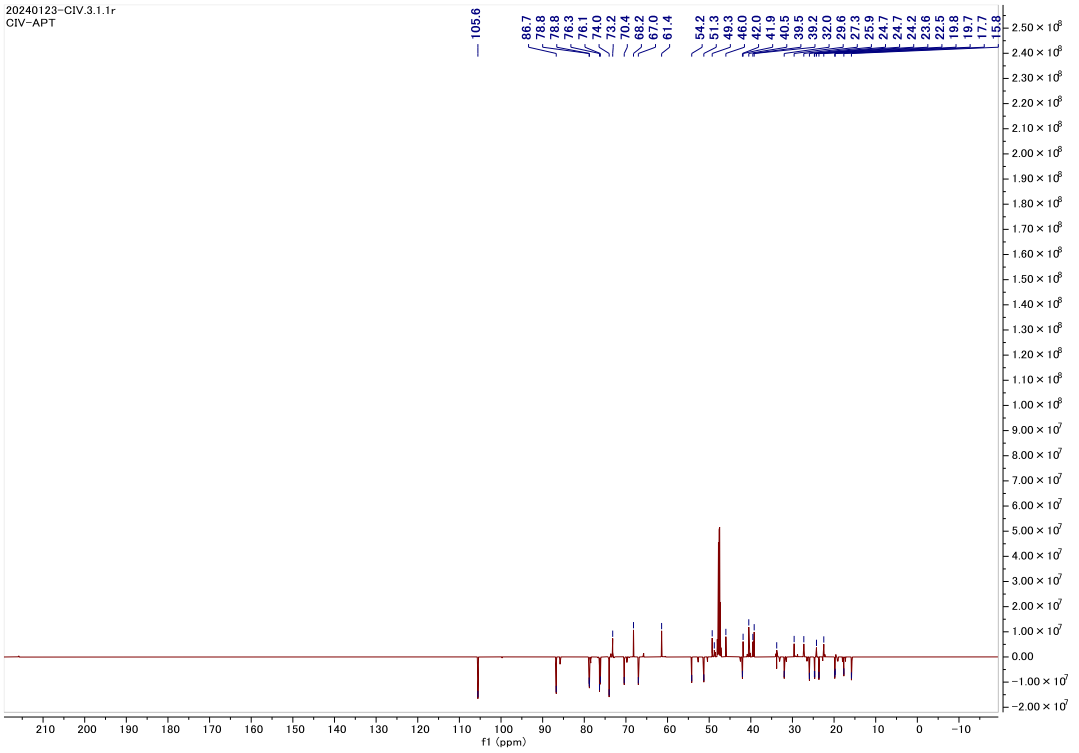


Figure S17: APT-NMR of compound **5** (in CD_3OD, 150 MHz)

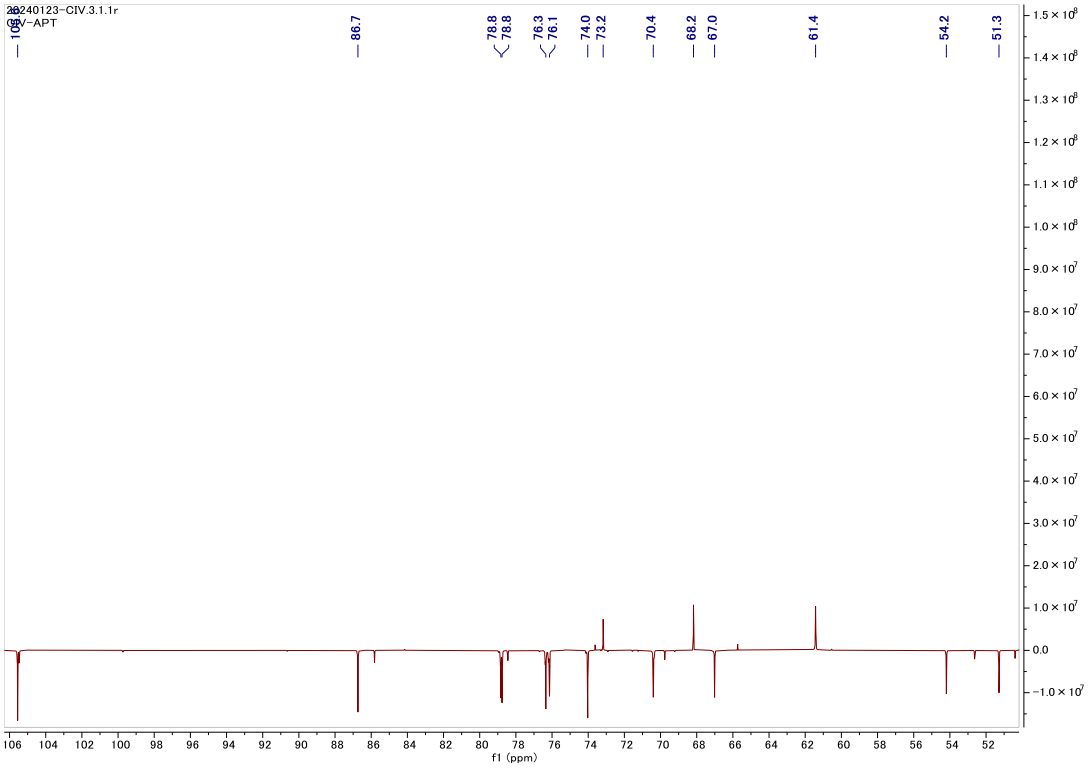


Figure S18: Expanded APT-NMR of compound **5** (in CD_3OD, 150 MHz)

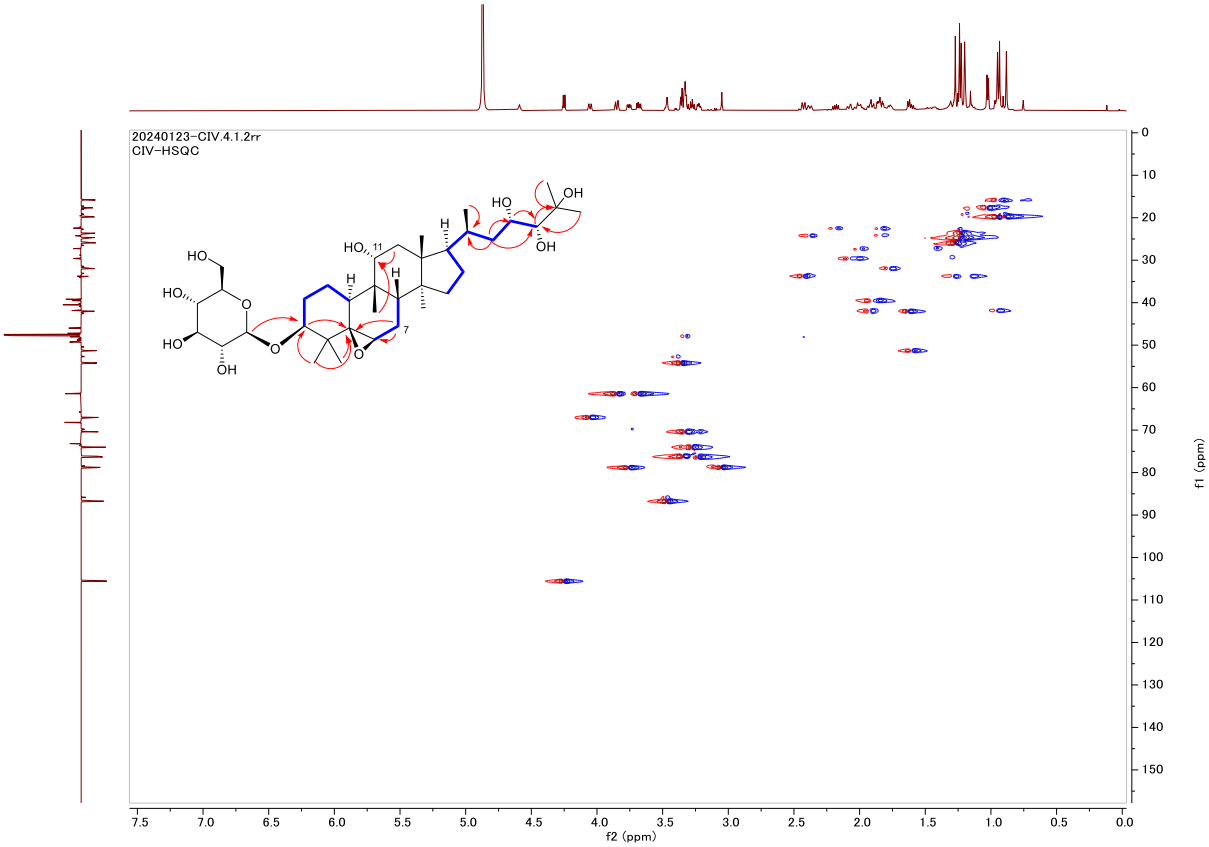


Figure S19: HSQC spectrum of compound **5**

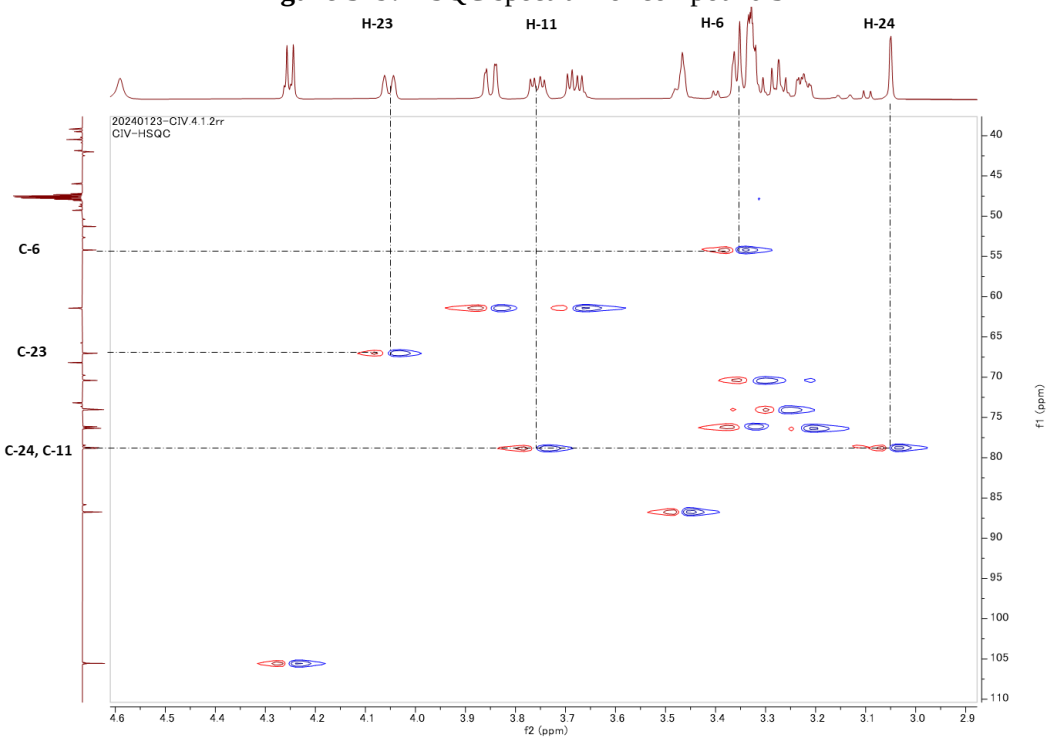


Figure S20: Expanded HSQC spectrum of compound **5**

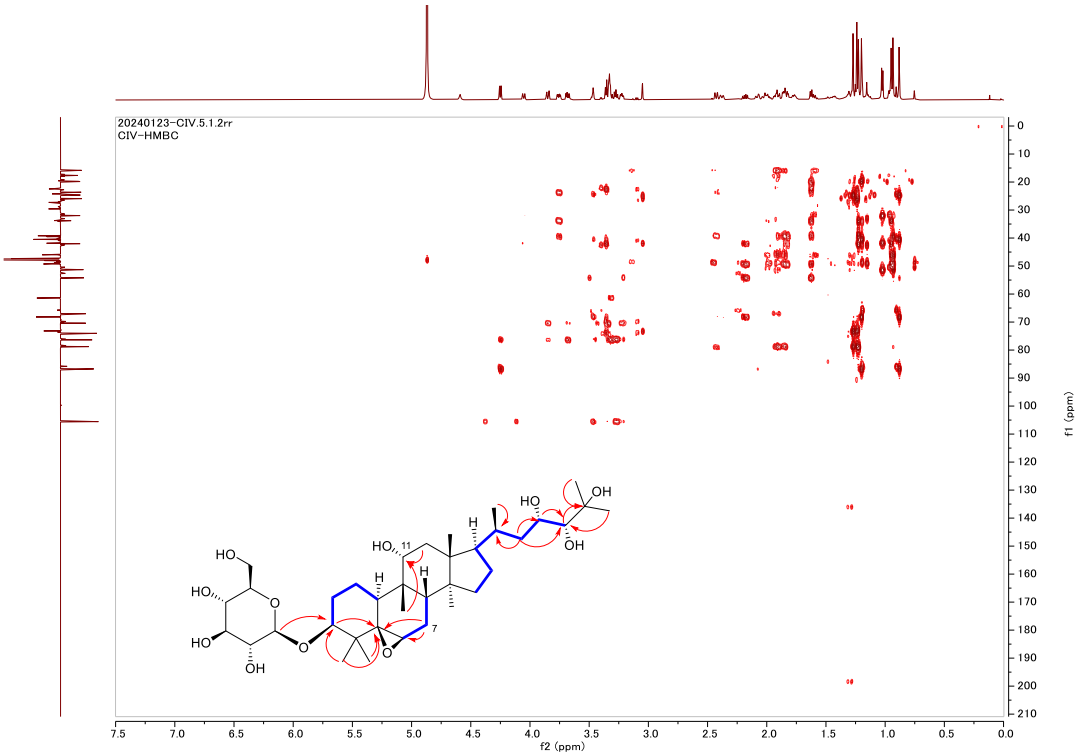


Figure S21: HMBC spectrum of compound **5**

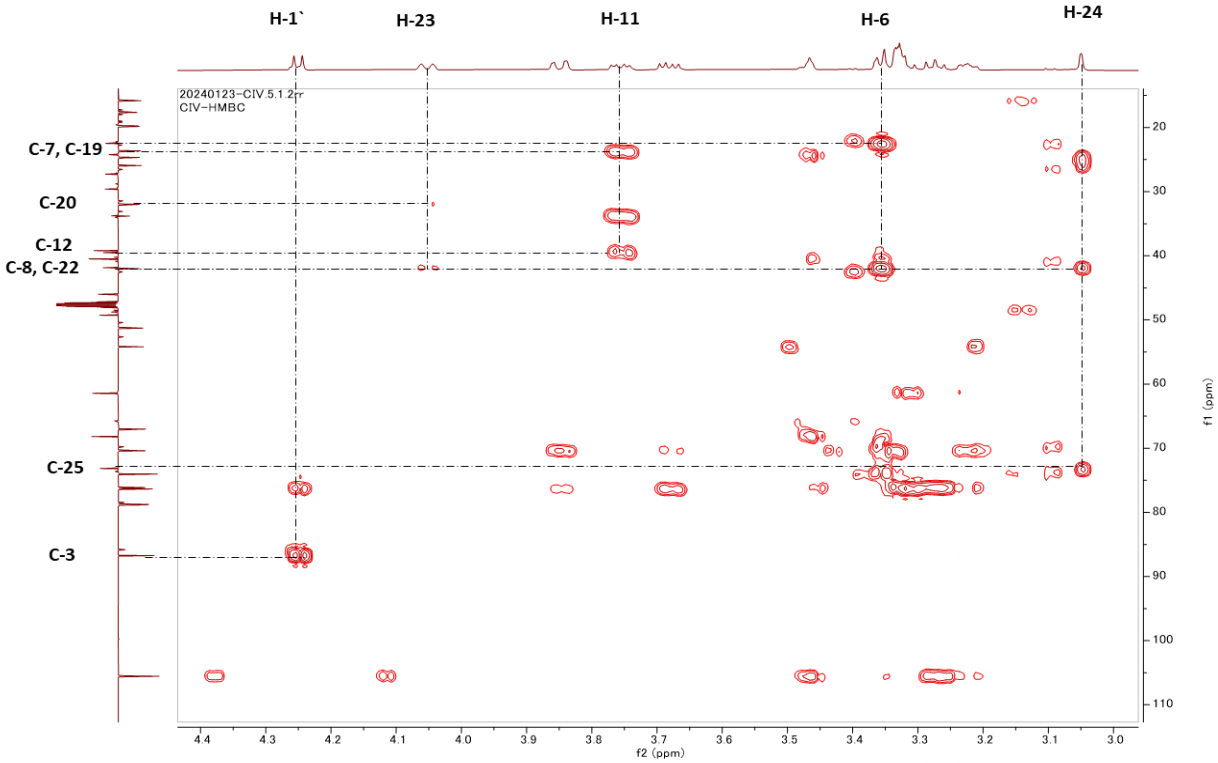


Figure S22: Expanded HMBC spectrum of compound **5**

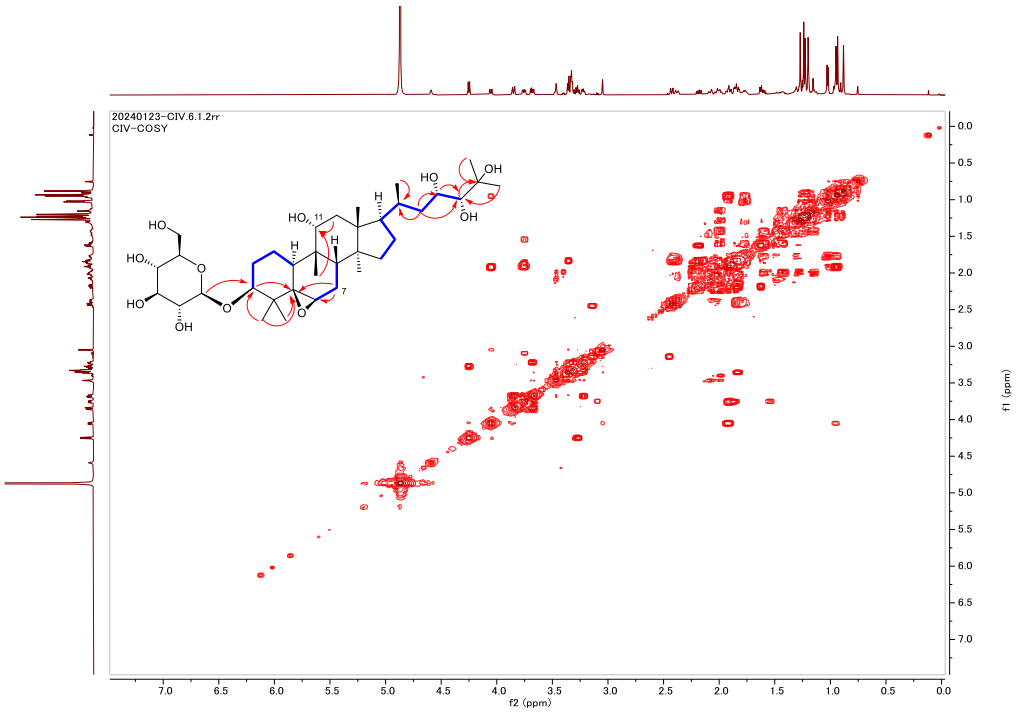


Figure S23: ^{1}H-^{1}H-COSY spectrum of compound **5**

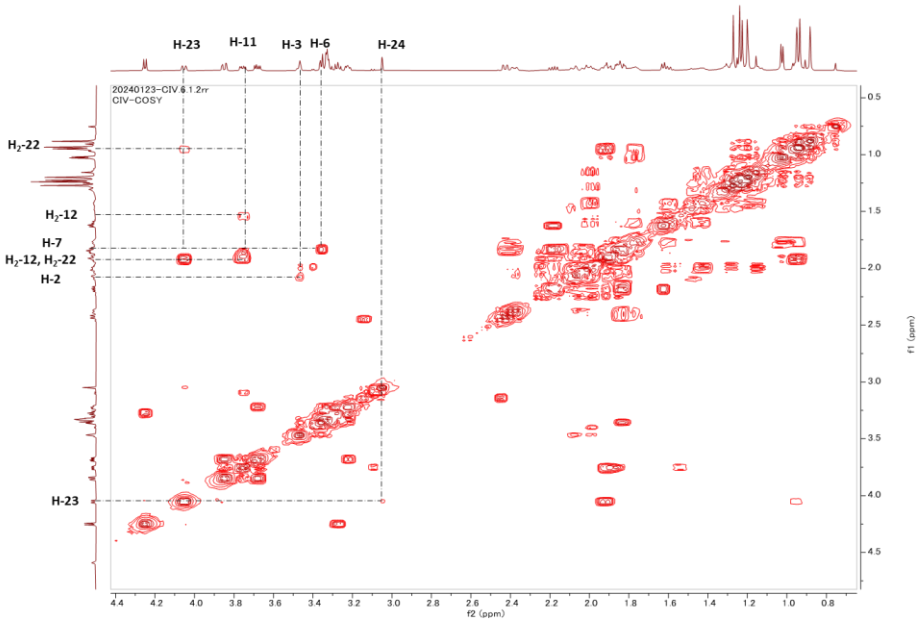


Figure S24: Expanded ^{1}H-^{1}H-COSY spectrum of compound **5**

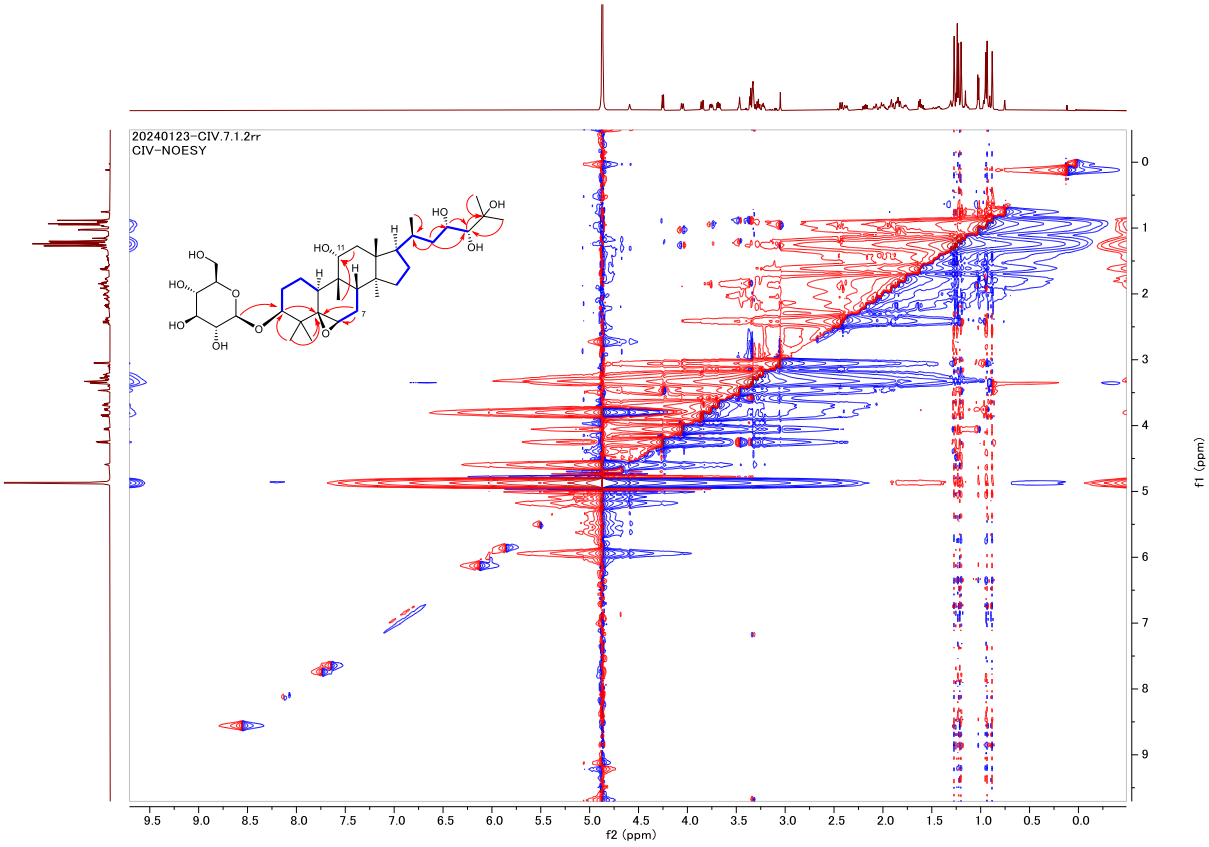


Figure S25: NOESY spectrum of compound **5**

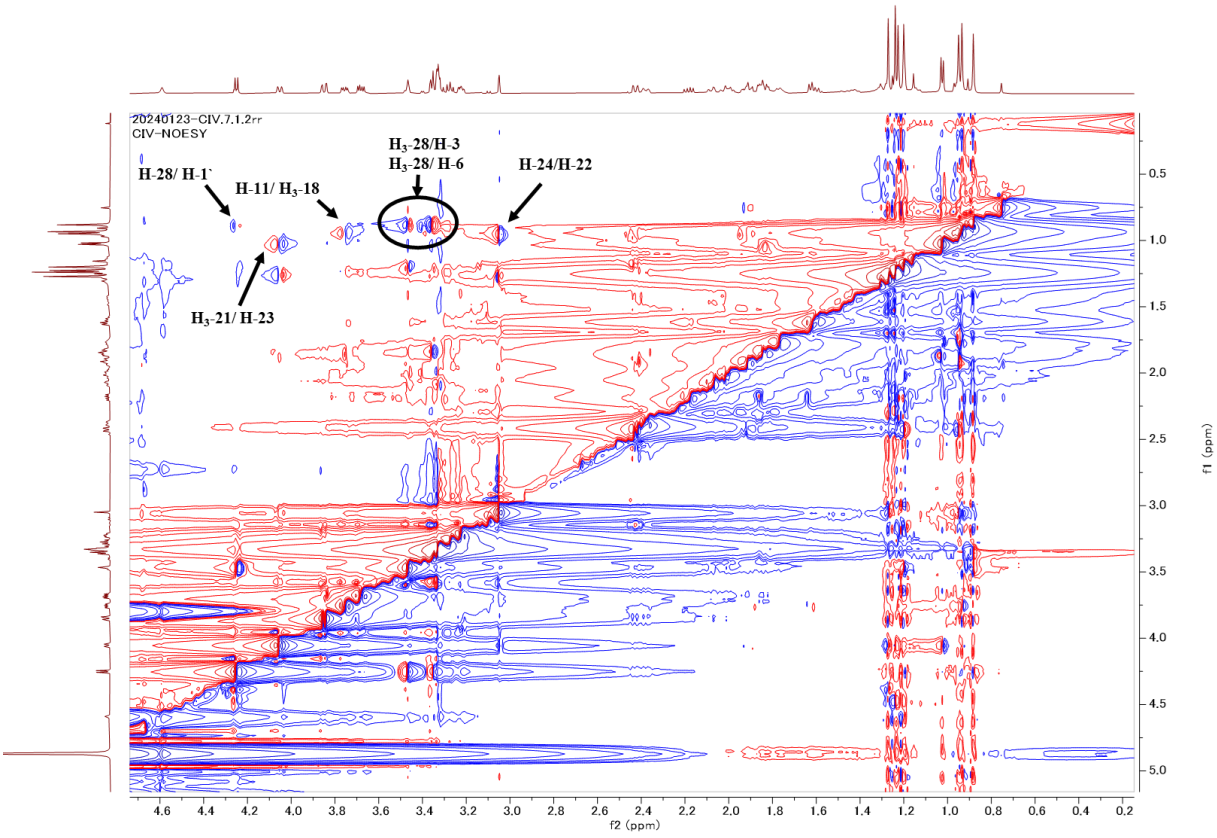
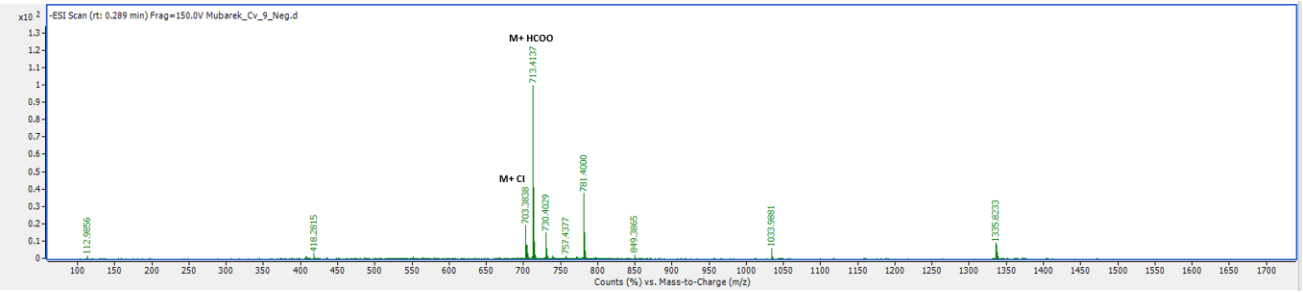


Figure S26: Expanded NOESY spectrum of compound **5**



Ion Formula	Species	m/z	m/z (Calc.)	Diff (ppm)	DBE
C37 H61 O13	(M+HCOO)-	713.4137	713.4112	3.50429037	7

Figure S27: Negative HRESIMS for compound **6**

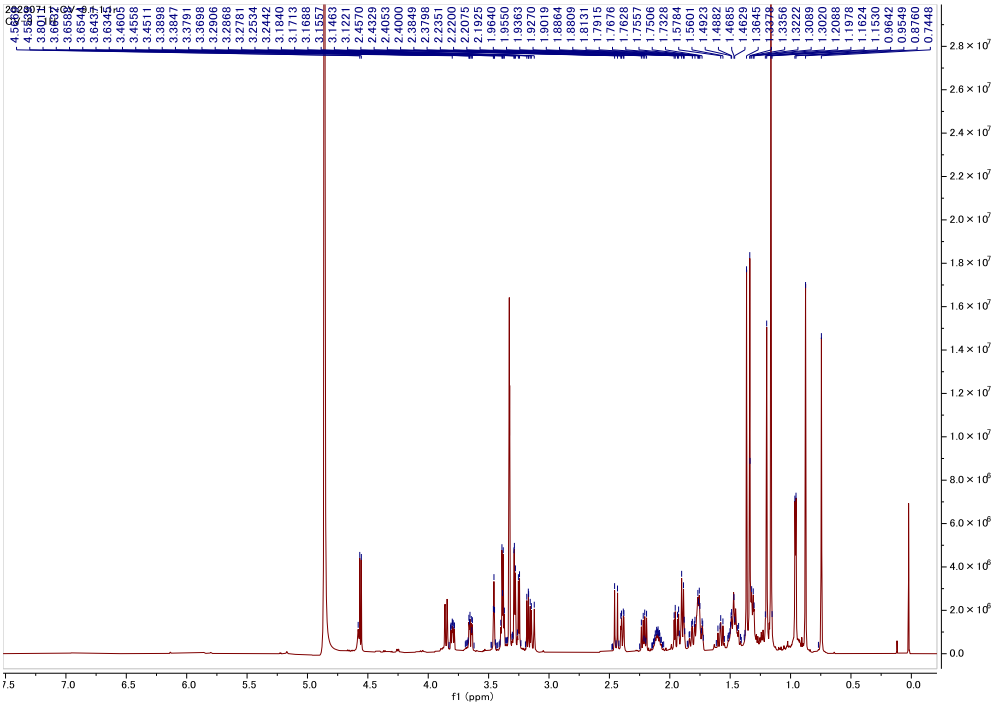


Figure S28: ^{1}H- NMR of compound **6** (in CD_3OD, 600 MHz)

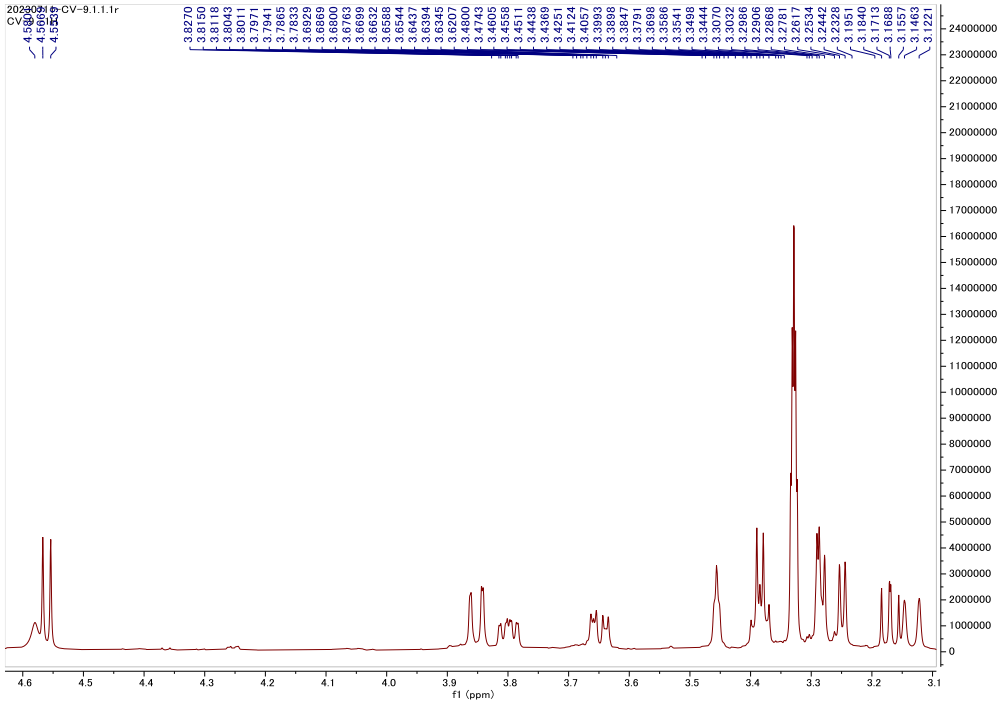


Figure S29: Expanded ^{1}H- NMR of compound **6** (in CD_3OD, 600 MHz)

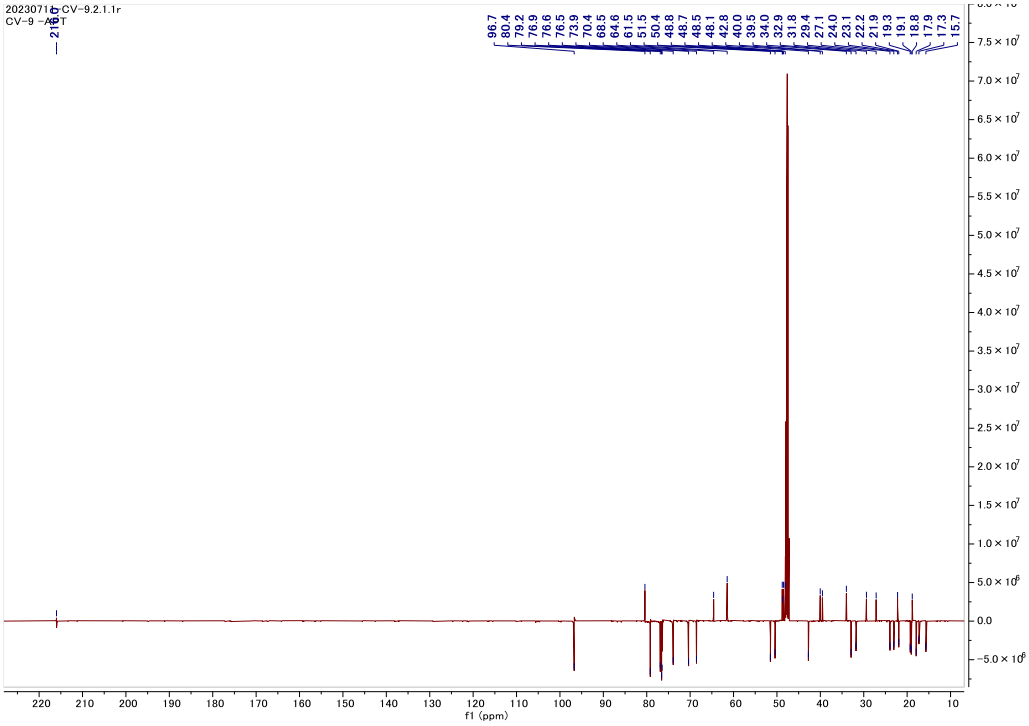


Figure S30: APT-NMR of compound **6** (in CD_3OD, 150 MHz)

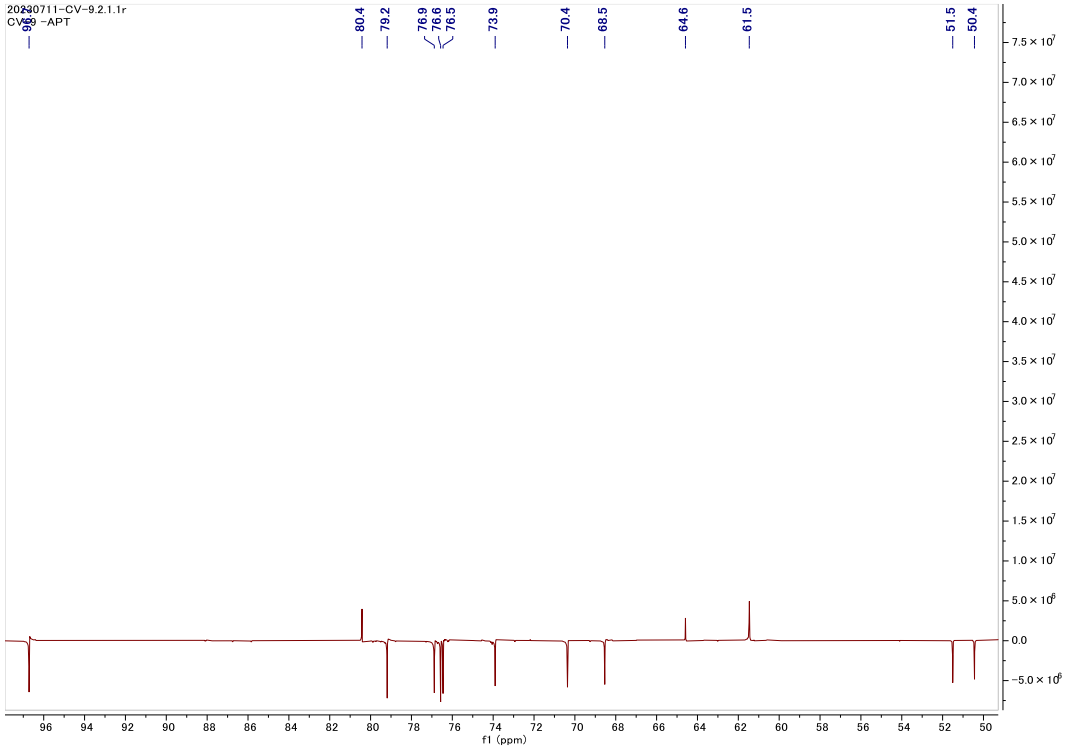


Figure S31: Expanded APT-NMR of compound **6** (in CD_3OD, 150 MHz)

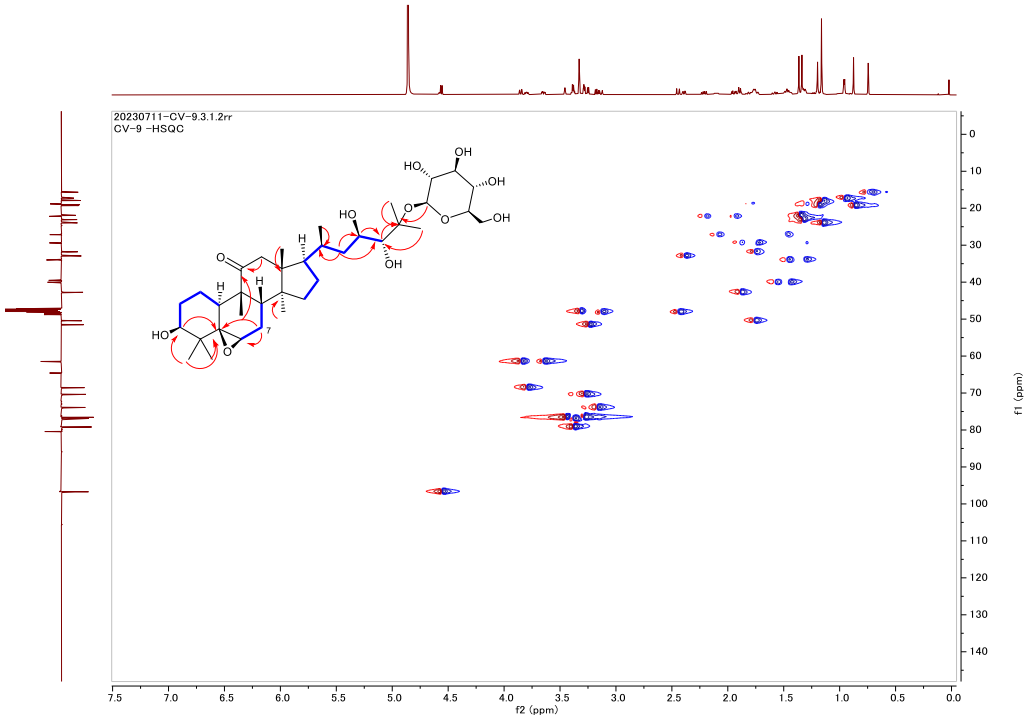


Figure S32: HSQC spectrum of compound **6**

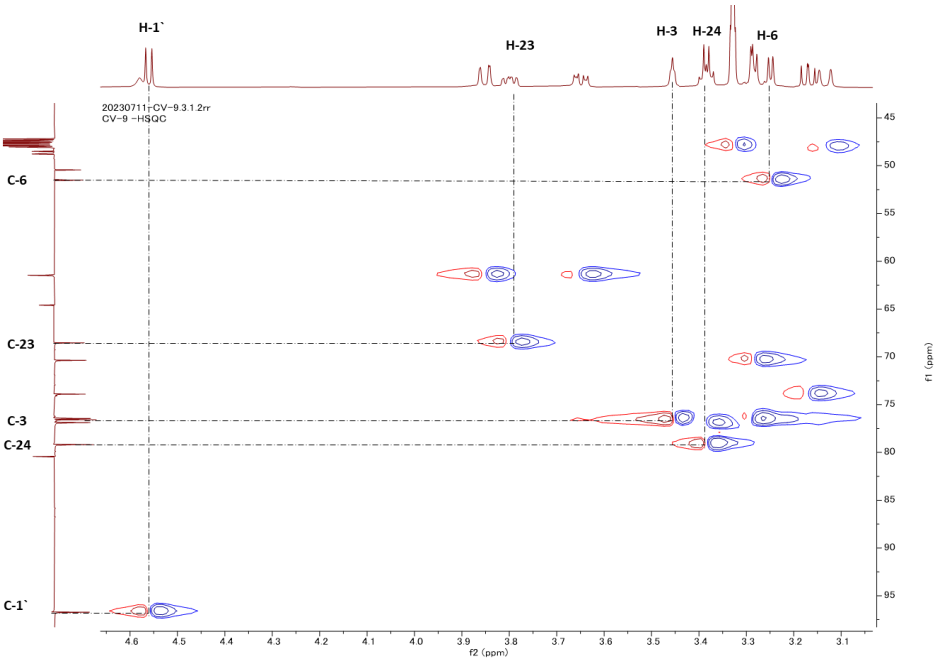


Figure S33: Expanded HSQC spectrum of compound **6**

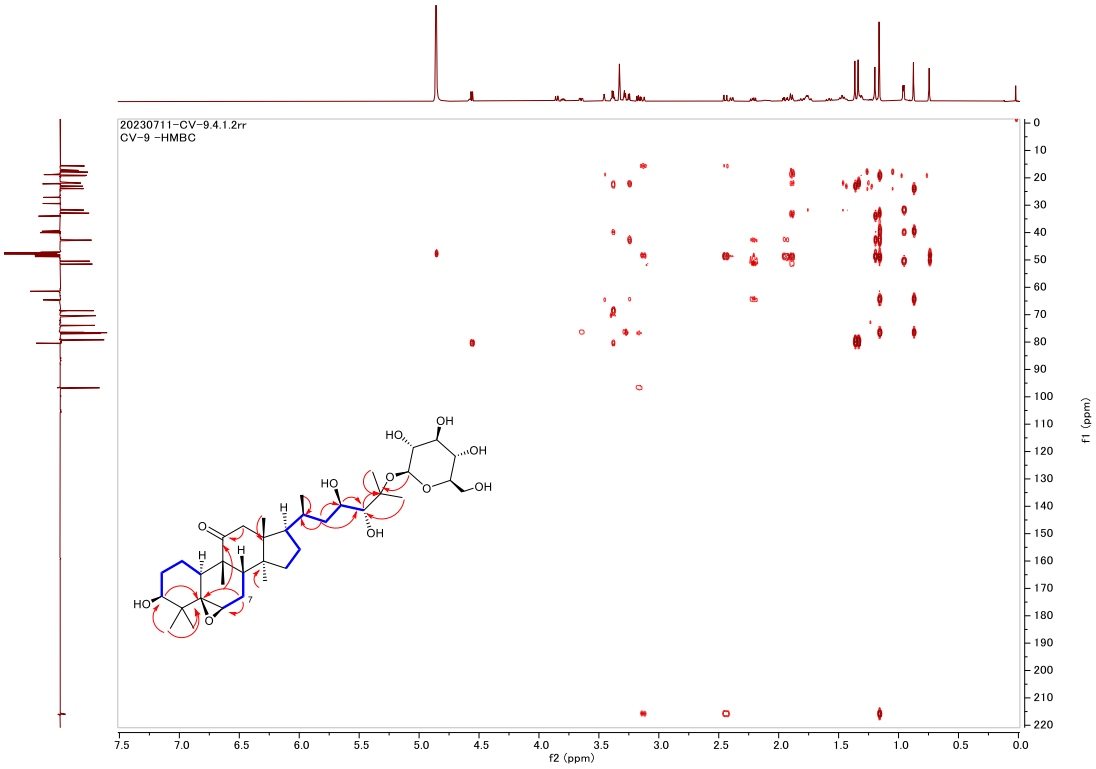


Figure S34: HMBC spectrum of compound **5**

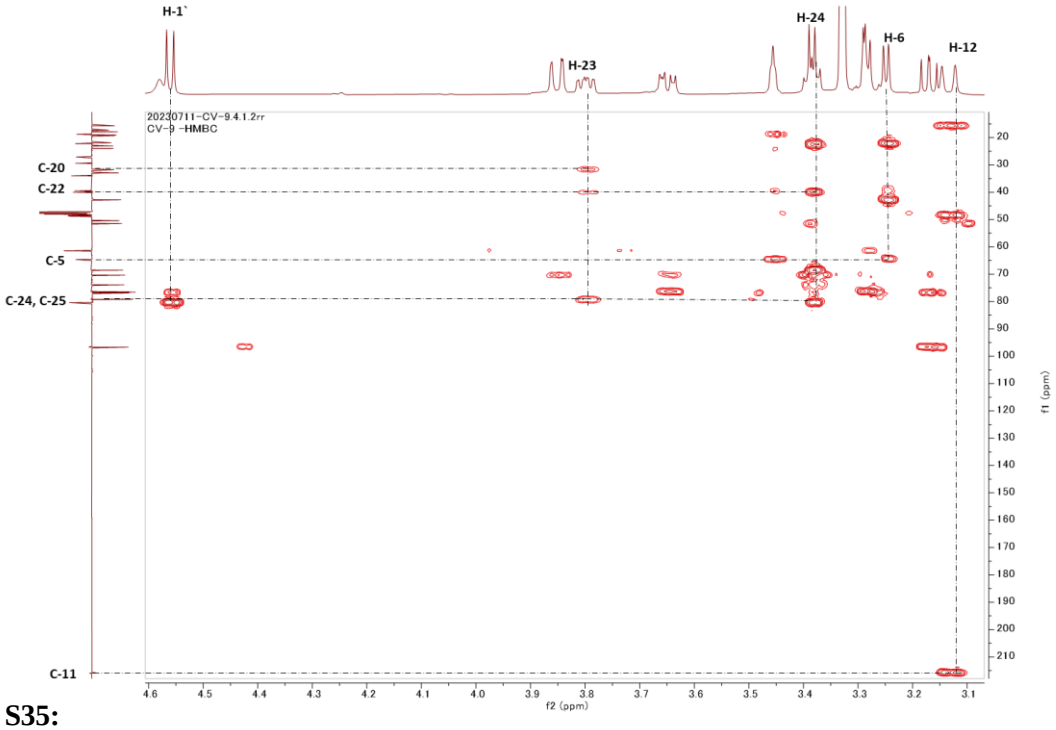


Figure S35: Expanded HMBC spectrum of compound **5**

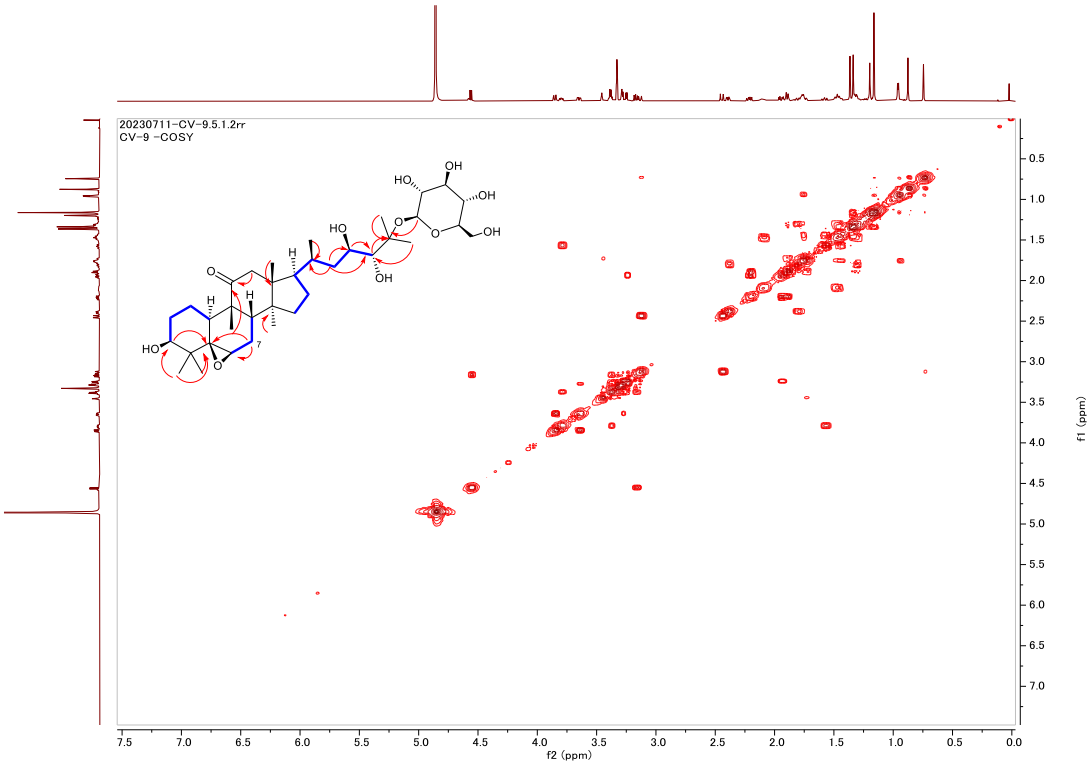


Figure S36: ^{1}H-^{1}H-COSY spectrum of compound **6**

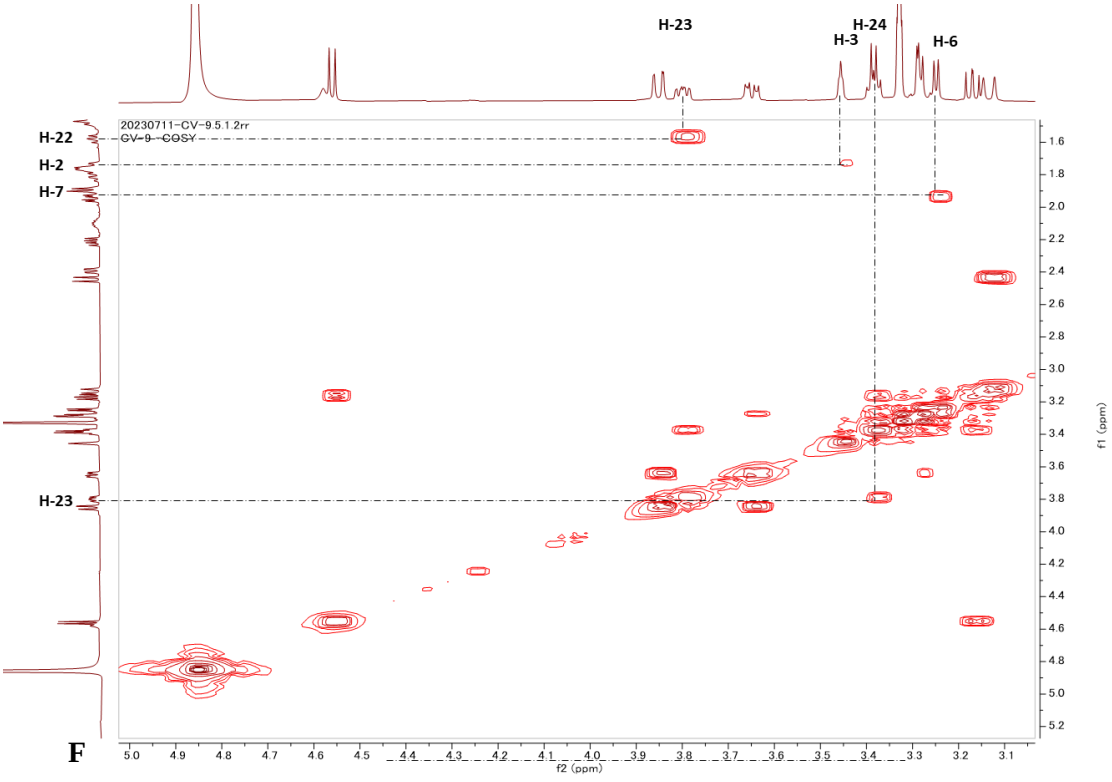
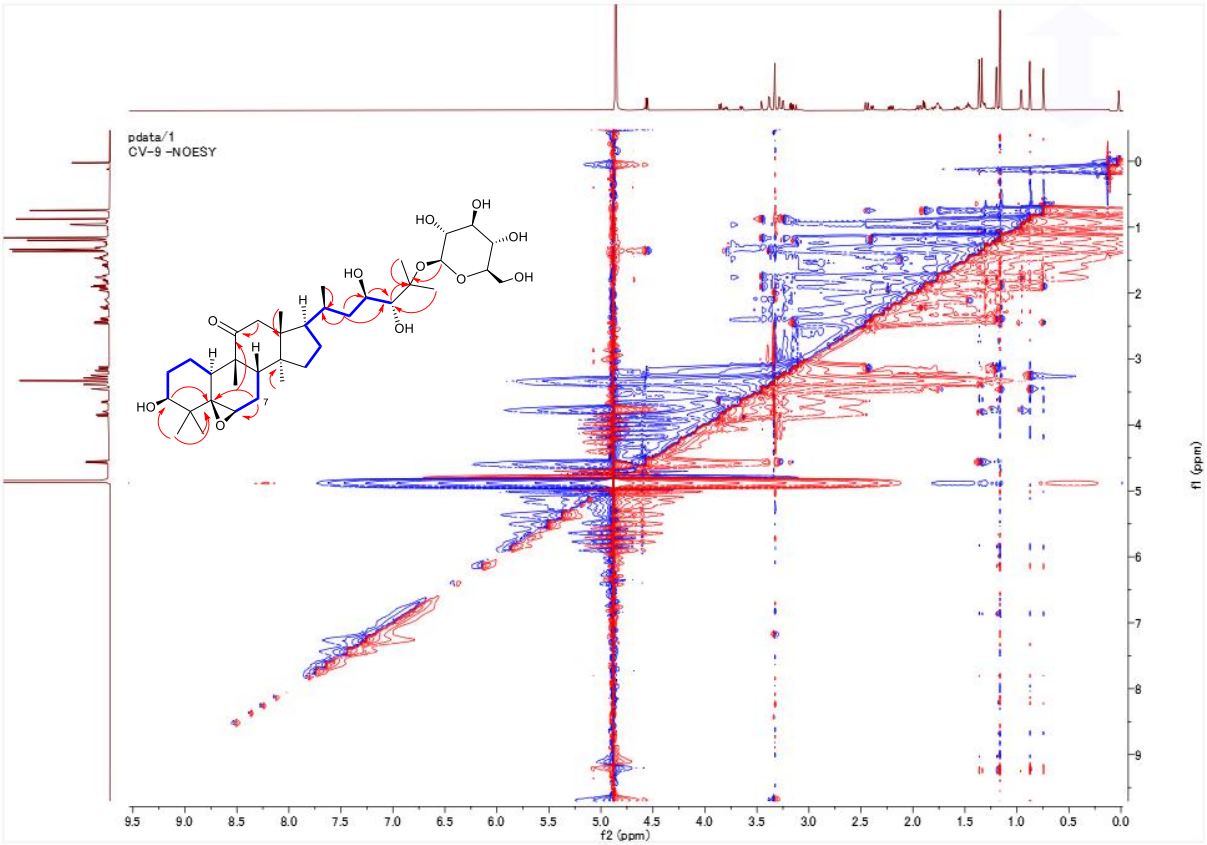


Figure S37: Expanded ^{1}H-^{1}H-COSY spectrum of compound **6**



S38: NOESY spectrum of compound **6**

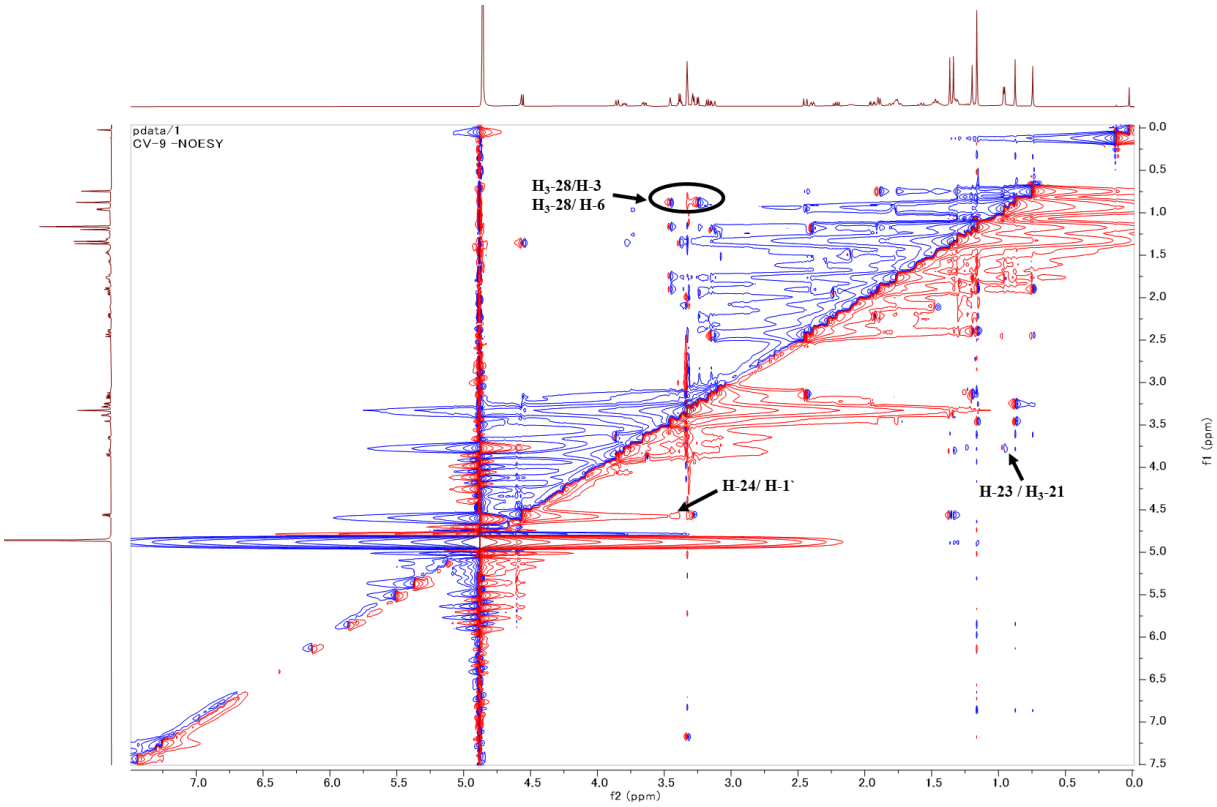
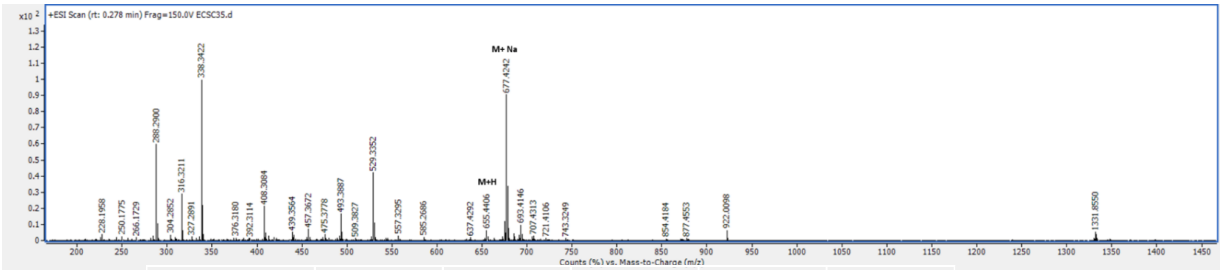


Figure S39: Expanded NOESY spectrum of compound **6**



Ion Formula	Species	m/z	m/z (Calc.)	Diff (ppm)	DBE
C36 H62 Na O10	(M+Na)+	677.4242	677.4241	0.29523607	6

Figure S40: Positive HRESIMS for compound **7**

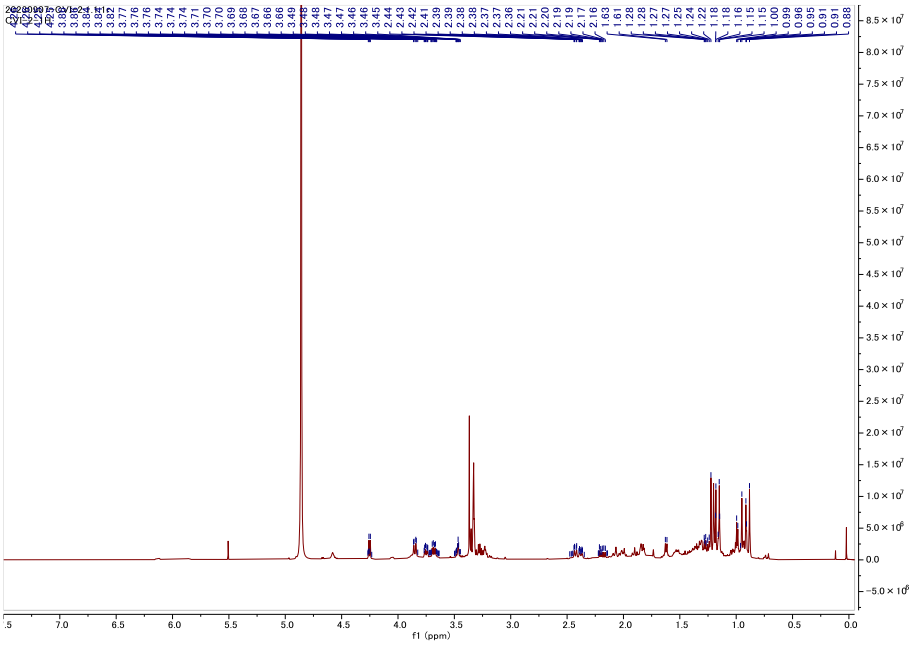


Figure S41: ^{1}H-NMR of compound **7** (in CD_3OD, 600 MHz)

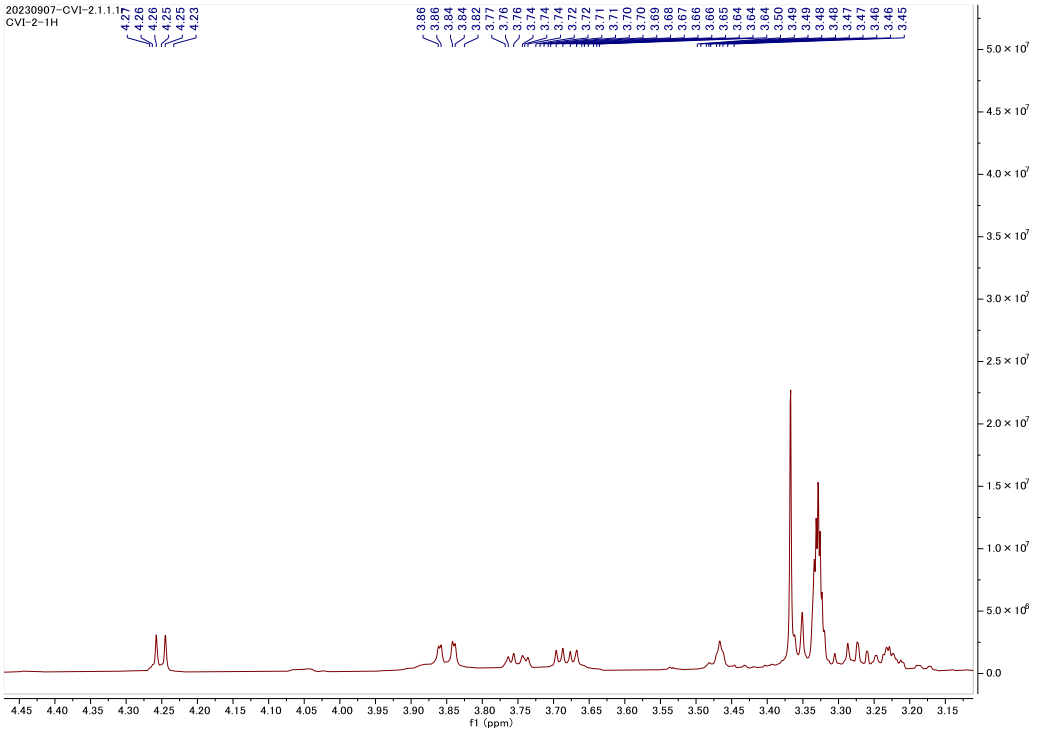


Figure S42: Expanded ^{1}H- NMR of compound **7** (in CD_3OD, 600 MHz)

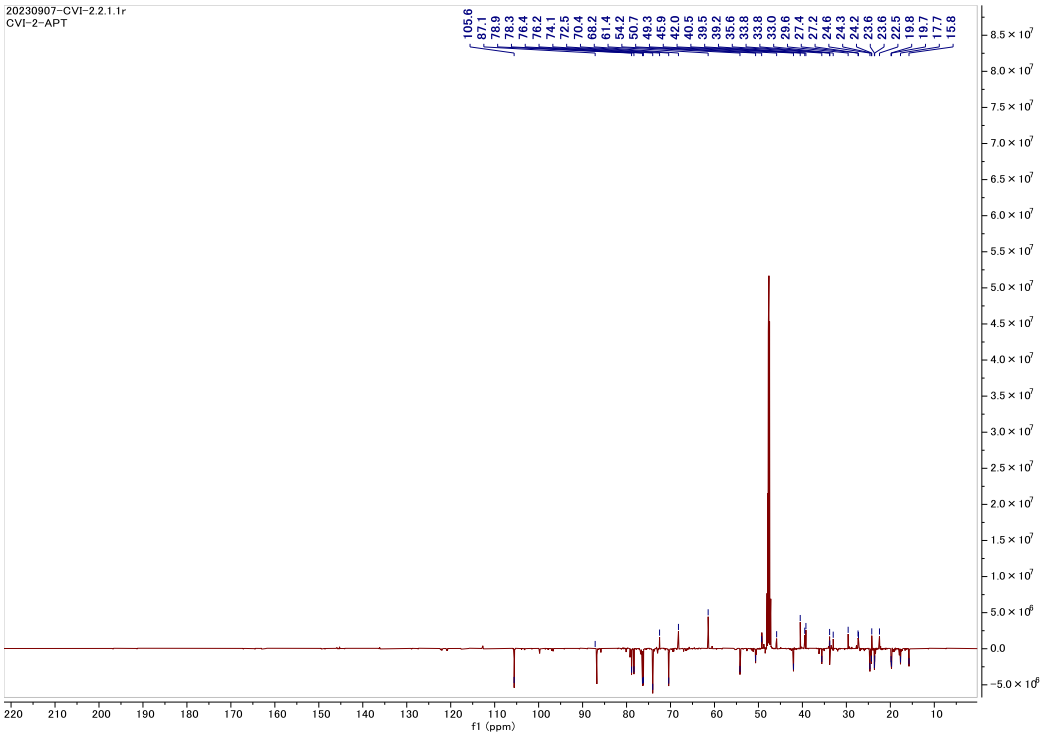


Figure S43: APT-NMR of compound **7** (in CD_3OD, 150 MHz)

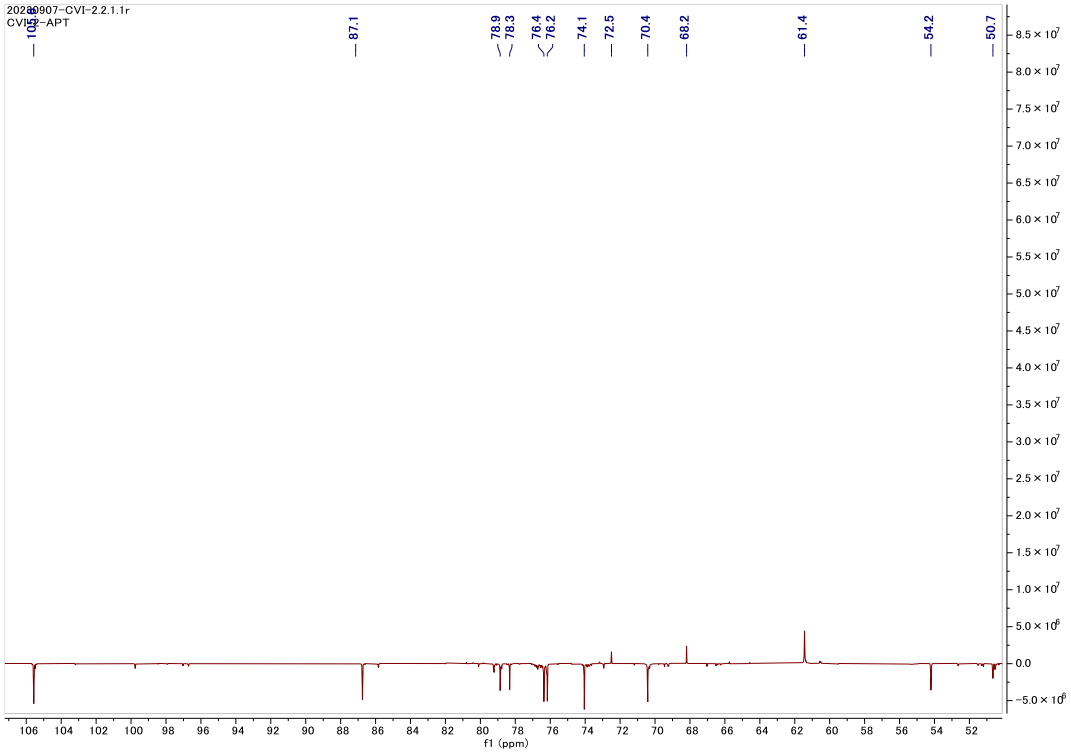
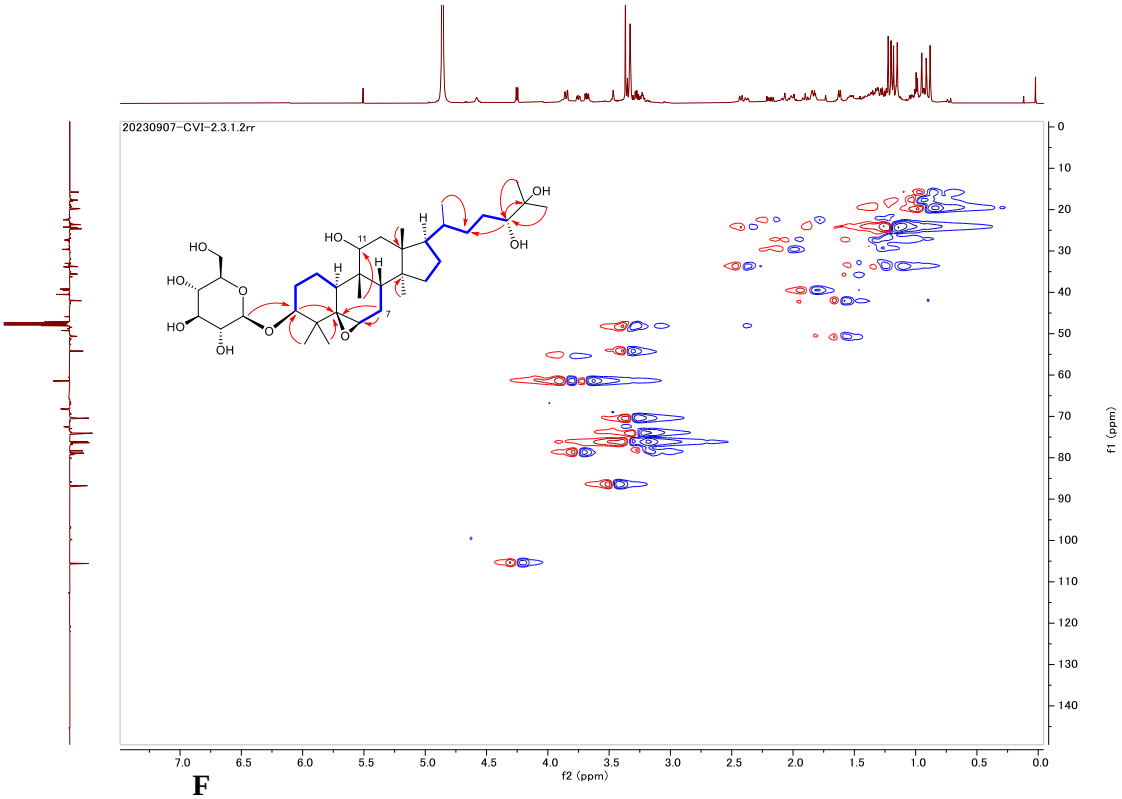


Figure S44: Expanded APT-NMR of compound **7** (in CD_3OD, 150 MHz)



F
igure S45: HSQC spectrum of compound **7**

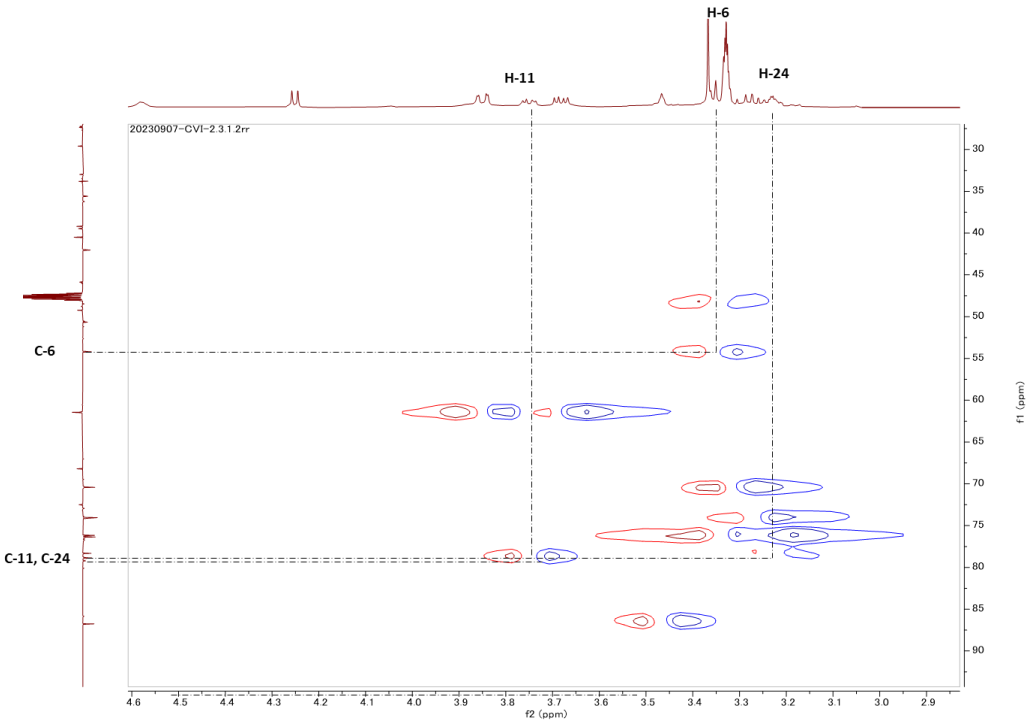


Figure S46: Expanded HSQC spectrum of compound **7**

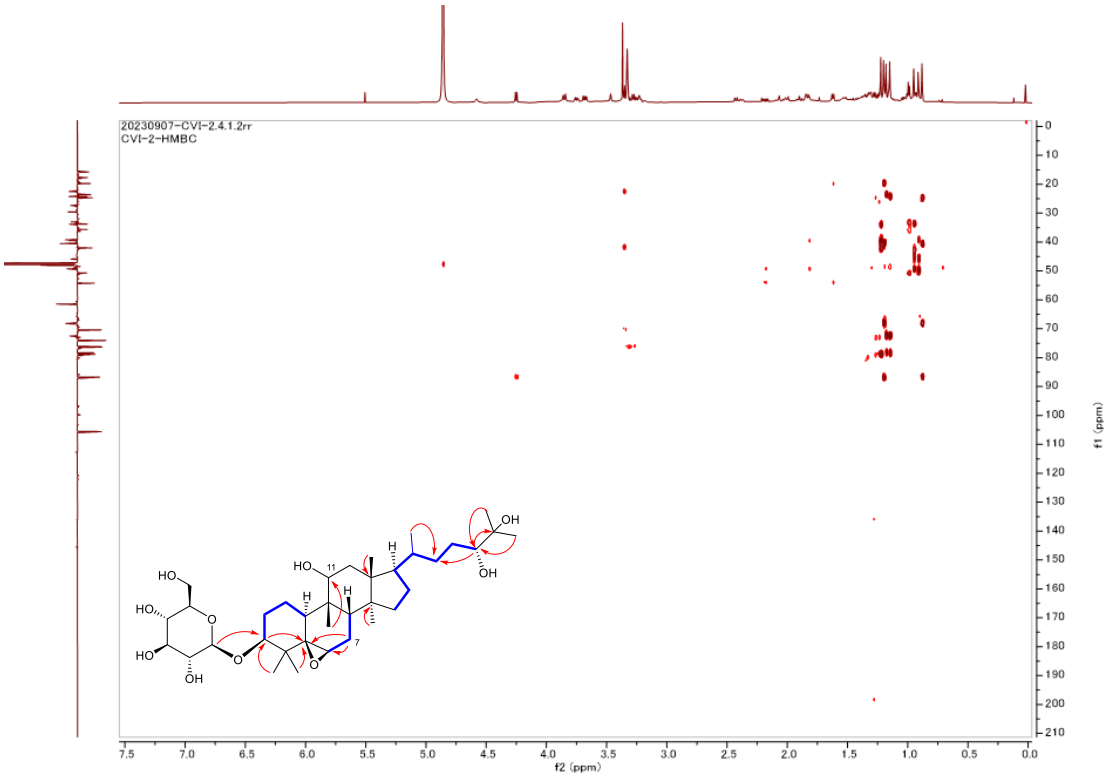


Figure S47: HMBC spectrum of compound **7**

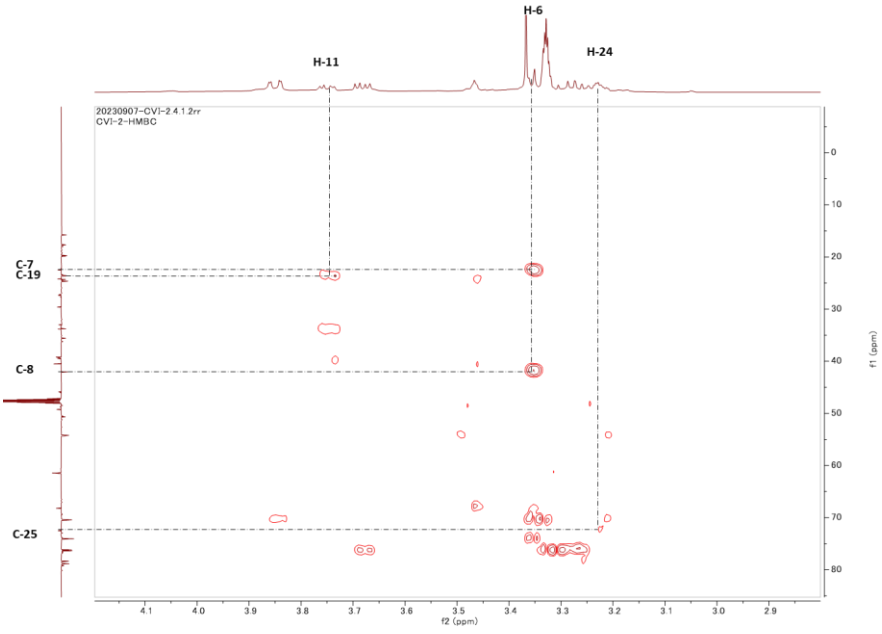


Figure S48: Expanded HMBC spectrum of compound **7**

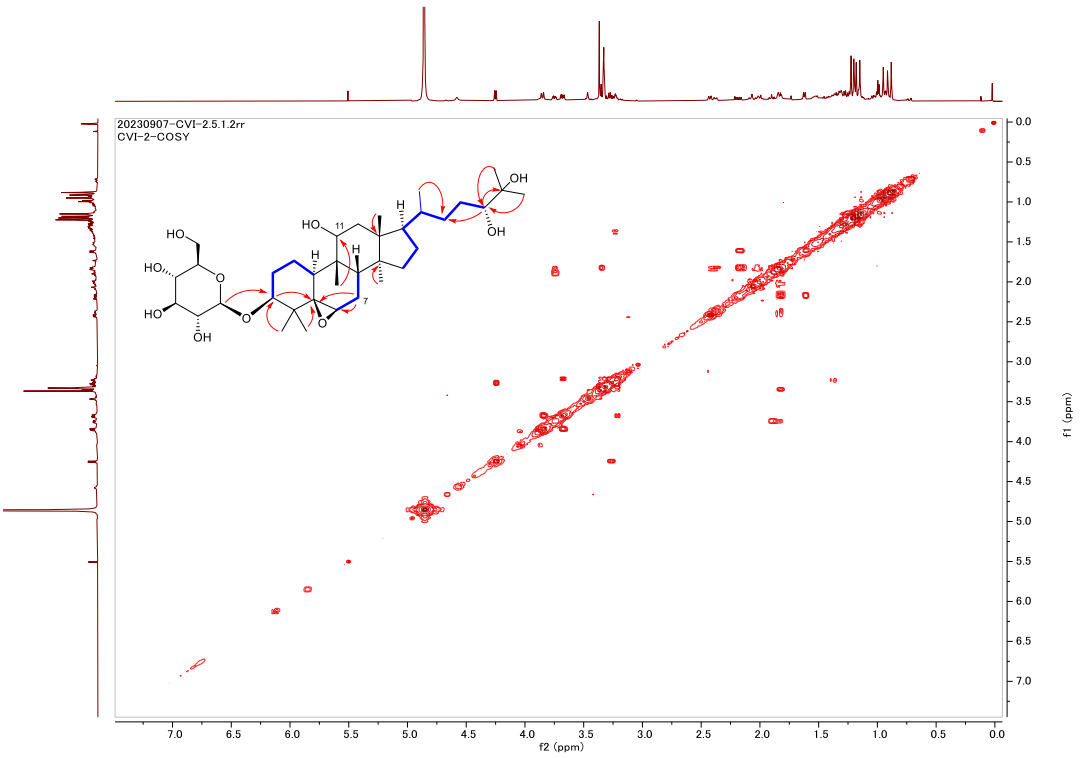


Figure S49: ^{1}H-^{1}H-COSY spectrum of compound **7**

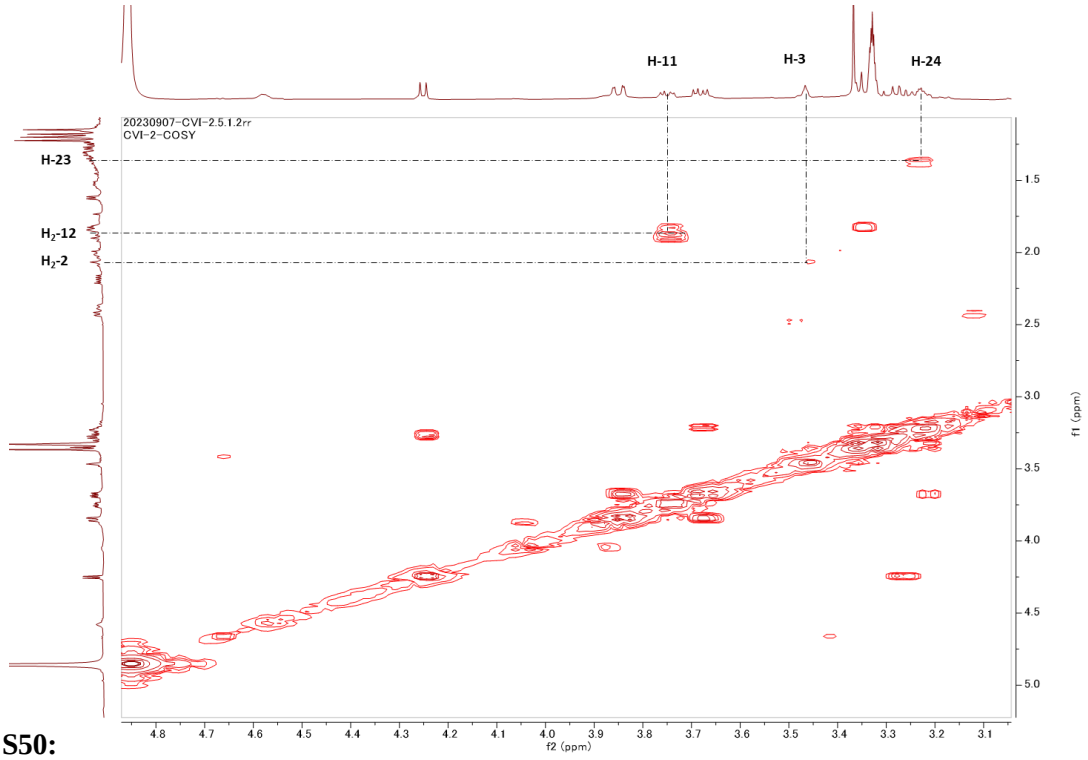


Figure S50: Expanded ^{1}H-^{1}H-COSY spectrum of compound **7**

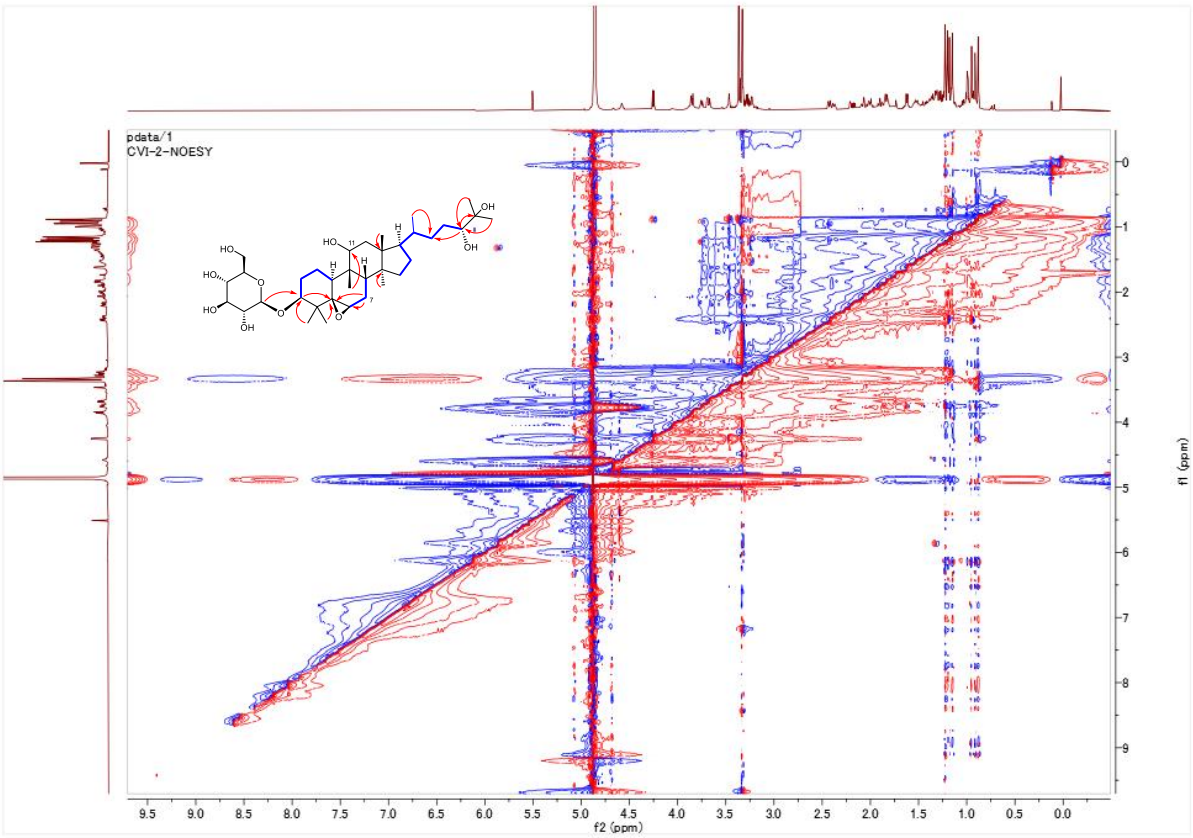


Figure S51: NOESY spectrum of compound **7**

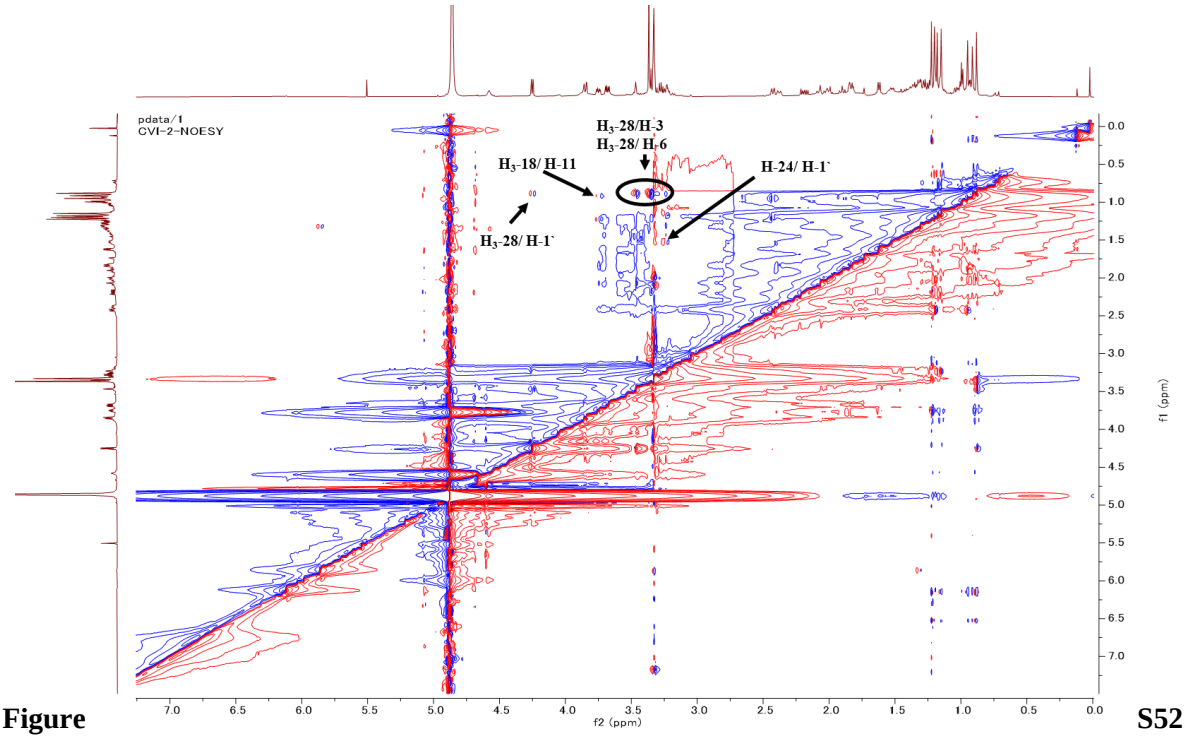


Figure S52: Expanded NOESY spectrum of compound **7**

CAS SciFinder^{n}

Task History

Initiating Search

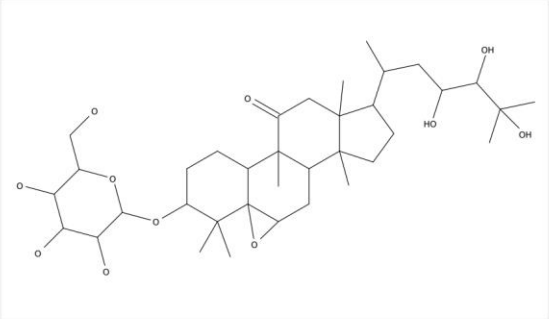
June 21, 2024, 3:12 PM

Substances:

Filtered By:

Similarity: 95-98

Number of Components: 1



Structure Match: **Similarity**

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (1)	Substances	View Results

Figure S53: Sci-Finder search for compound **4**

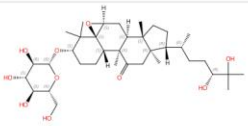
CAS SciFinder^{n}

Substances (1)

View in SciFinder^{n}

1 — Similarity Score: **99**

405281-91-6



Absolute stereochemistry shown, Rotation (+)

$C_{36}H_{60}O_{10}$

19-Norlanostan-11-one, 5,6-epoxy-3-(β-D-glucopyranosyloxy)-24,25-dihydroxy-9-methyl-, (3β,6α,9β,10α,24*R*)-

1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	652.86	-
Melting Point (Experimental)	124-156 °C	-
Boiling Point (Predicted)	772.4±60.0 °C	Press: 760 Torr
Density (Predicted)	1.27±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.91±0.70	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Figure S54: Sci-Finder similarity report for compound **4**

CAS SciFinder^{n}

Task History

Initiating Search

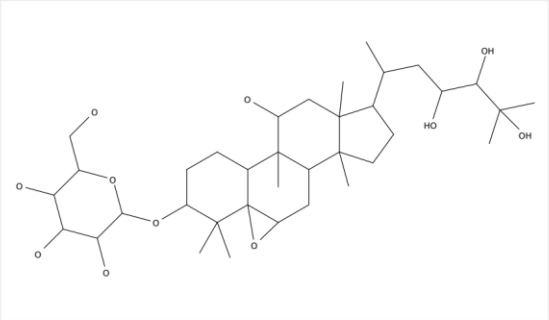
June 21, 2024, 3:13 PM

Substances:

Filtered By:

Similarity: 95-98

Number of Components: 1



Structure Match: **Similarity**

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (2)	Substances	View Results

Figure S55: Sci-Finder search for compound **5**

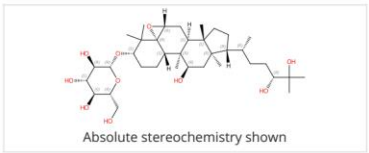
CAS SciFinder^{n}

Substances (2)

View in SciFinder^{n}

1 Similarity Score: 99

1283586-92-4



$C_{36}H_{62}O_{10}$

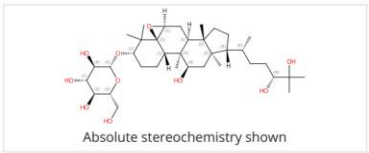
5*R*,6*R*-Epoxymogroside 1 E_1

1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	654.87	-
Boiling Point (Predicted)	773.2±60.0 °C	Press: 760 Torr
Density (Predicted)	1.27±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.92±0.70	Most Acidic Temp: 25 °C

2 Similarity Score: 99

476468-77-6



$C_{36}H_{62}O_{10}$

β-D-Glucopyranoside, (3β,6α,9β,10α,11α,24*R*)-5,6-epoxy-11,24,25-trihydroxy-9-methyl-19-norlanostan-3-yl

4 References | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	654.87	-
Boiling Point (Predicted)	773.2±60.0 °C	Press: 760 Torr
Density (Predicted)	1.27±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.92±0.70	Most Acidic Temp: 25 °C

Figure S56: Sci-Finder similarity report for compound **5**

CAS SciFinder^{n}

Task History

Initiating Search

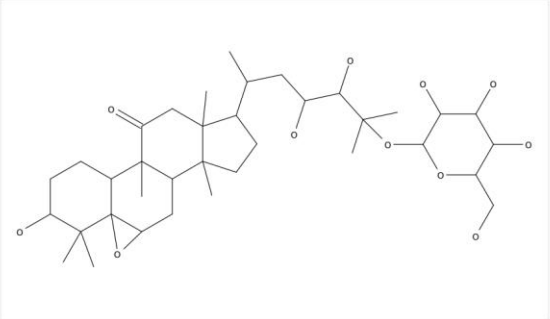
June 21, 2024, 3:22 PM

Substances:

Filtered By:

Similarity: 95-98

Number of Components: 1



Structure Match: **Similarity**

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (1)	Substances	View Results

Figure S57: Sci-Finder search for compound **6**

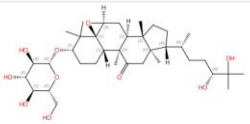
CAS SciFinder^{n}

Substances (1)

View in SciFinder^{n}

1 Similarity Score: **97**

405281-91-6



Absolute stereochemistry shown, Rotation (+)

$C_{36}H_{60}O_{10}$

19-Norlanostan-11-one, 5,6-epoxy-3-(β-D-glucopyranosyloxy)-24,25-dihydroxy-9-methyl-, (3β,6α,9β,10α,24*R*)-

1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	652.86	-
Melting Point (Experimental)	124-156 °C	-
Boiling Point (Predicted)	772.4±60.0 °C	Press: 760 Torr
Density (Predicted)	1.27±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.91±0.70	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Figure S58: Sci-Finder similarity report for compound **6**

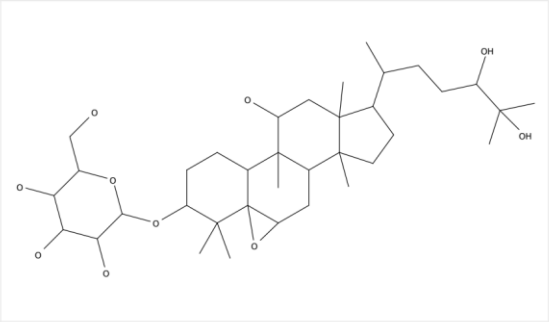
CAS SciFinder^{n}

Task History

Initiating Search June 21, 2024, 3:14 PM

Substances:

Filtered By:



Structure Match: **As Drawn**

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (2)	Substances	View Results

Figure S59: Sci-Finder search for compound **7**

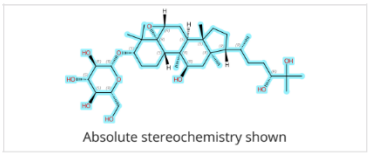
CAS SciFinder^{n}

Substances (2)

View in SciFinder^{n}

1

1283586-92-4



$C_{36}H_{62}O_{10}$

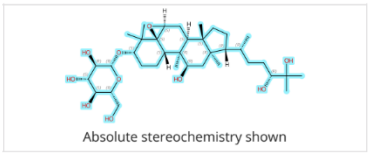
5*R*,6*R*-Epoxymogroside 1 E_1

1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	654.87	-
Boiling Point (Predicted)	773.2±60.0 °C	Press: 760 Torr
Density (Predicted)	1.27±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.92±0.70	Most Acidic Temp: 25 °C

2

476468-77-6



$C_{36}H_{62}O_{10}$

β-D-Glucopyranoside, (3β,6α,9β,10α,11α,24*R*)-5,6-epoxy-11,24,25-trihydroxy-9-methyl-19-norlanostan-3-yl

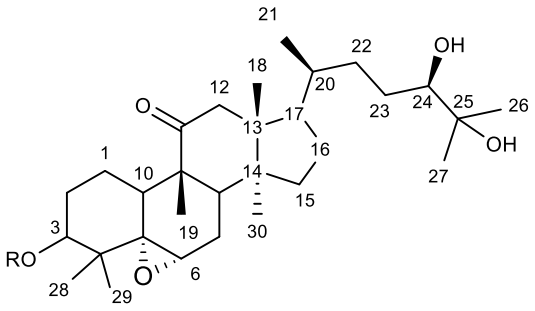
4 References | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	654.87	-
Boiling Point (Predicted)	773.2±60.0 °C	Press: 760 Torr
Density (Predicted)	1.27±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.92±0.70	Most Acidic Temp: 25 °C

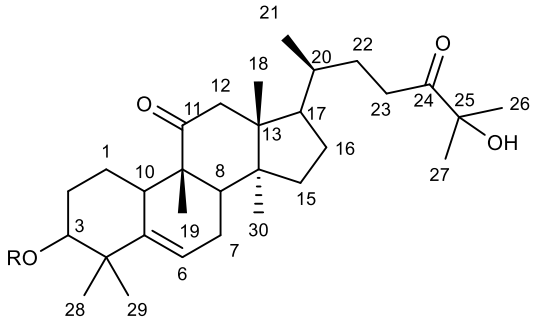
Figure S60: Sci-Finder similarity report for compound **7**

Table S1: The NMR data of similar compounds

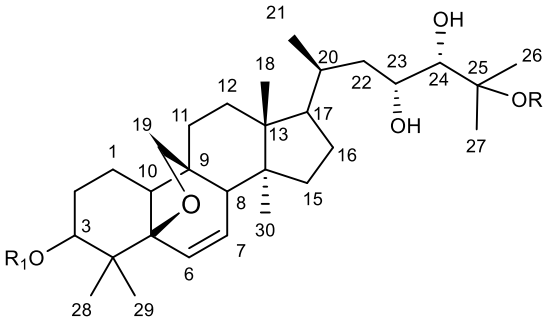
No.	**Bryonioside D**		**3-O-β-D-allopyranosyl-25-O-β-D-glucopyranosyl-5β,19-epoxycucurbita-6-ene-23(R),24(S)-diol**		**Bryonioside F**	
	δ_H	**δ_C**	**δ_H**	**δ_C**	**δ_H**	**δ_C**
1	1.60, 2.23	20.5	1.31, 1.72	18.5	1.52, 1.92	22.1
2	1.88, 2.42	29.7	1.74, 2.32	27.2	1.80, 2.39	28.5
3	3.71 (br si	86.4	3.64 br s	85.2	3.65 (br s)	87.2
		41.0		38.6		42.0
		64.8		85.8		141.2
6	3.16 (br d, 5.3)	51.5	6.14 dd (1.3 8.3)	133.8	5.53 (br d, 6.0)	118.5
7	1.73, 2.15	23.1	5.5 dd (3.3 9.8)	130.1	1.76, 2.17	24.1
8	1.77	42.7	2.26	51.9	1.80	43.9
		48.6		44.9		49.0
10	2.42	33.7	2.24	39.7	2.46	35.9
		213.8	1.29, 1.58	23.5		213.6
	2.93 (d, 15.0), 2.48 (d, 15.0)	48.7	1.44, 1.54	30.7	2.92 (d, 14.4), 2.46 (d, 14.4)	48.7
		49.1		45.2		49.1
		49.1		48.6		49.6
15	1.11, 1.30	34.5	1.09, 1.14	32.9	1.17, 1.27	34.5
16	1.76, 1.85	28.7	1.36, 1.86	28.1	1.35, 1.96	27.9
17	1.70	50.2	1.44	51.2	1.68	49.7
18	0.66 (s)	16.7	0.74 s	14.6	0.70 (s)	16.9
19	1.37 (s)	19.4	3.56 d (7.7) 3.74 d (7.7)	79.8	1.16 (s)	20.3
20	1.50	36.0	2.04	32.3	1.40	35.8
21	0.92 (d, 6.4)	18.6	1.06 d (6.0)	18.5	0.86 (d, 6.4)	18.4
22	1.67, 1.79	34.0	1.14, 2.26	42.3	1.40, 1.96	30.4
23	1.33, 2.01	27.7	4.48	66.6	2.92, 2.98	33.3
24	3.77 (d, 9.8)	79.1	3.61	79.7		216.4
		72.2	1.72 s	81.0		76.8
26	1.56 (s)	26.0	1.73 s	23.0	1.58 (s)	27.3
27	1.54 (s)	26.2	1.45 s	24.6	1.58 (s)	27.3
28	1.19 (s)	20.8	0.86 s	20.5	1.12 (s)	28.3
29	1.25 (s)	25.4	0.83 s	25.2	1.56 (s)	25.9
30	1.03 (s)	19.8	1.06 d (6.0)	19.8	0.96 (s)	18.2
1'	4.88 (d, 7.8)	106.8	5.34 d (7.7)	104.0	4.88 (d, 7.8)	107.4
2'	3.99	75.6	3.92	72.7	3.96	75.5
3'	4.23	78.6	4.67	72.3	4.19	78.8
4'	4.22	71.7	4.14	68.9	4.22	71.8
5'	3.95	78.5	4.44	75.8	3.96	78.3
6'	4.41, 4.55	62.9	4.32 4.50	62.9	4.40, 4.55	63.0
1"			5.21 d (7.8)	98.5		
2"			3.96	75.0		
3"			4.22	78.5		
4"			4.16	71.5		
5"			3.93	78.0		
6"			4.32 4.52	62.5		



Bryonioside D [1]



Bryonioside F[1]



3-O-*β*-D-allopyranosyl-25-O-*β*-D-glucopyranosyl -5*β*,19-epoxycucurbita-6-ene-23(*R*),24(*S*)-diol [2]

R= *β*-D-glucopyranosyl,
R1= *β*-D-allopyranosyl

Figure S61: Structure of compounds similar to 4 :7

References

[1] M. Ukiya, T. Akihisa, K. Yasukawa, H. Tokuda, M. Toriumi, K. Koike, Y. Kimura, T. Nikaido, W. Aoi and H. Nishino (2002). Anti-inflammatory and anti-tumor-promoting effects of cucurbitane glycosides from the roots of *Bryonia dioica*, *J. Nat. Prod.* **65**, 179-183.

[2] M.-J. Tan, J.-M. Ye, N. Turner, C. Hohnen-Behrens, C.-Q. Ke, C.-P. Tang, T. Chen, H.-C. Weiss, E.-R. Gesing and A. Rowland (2008). Antidiabetic activities of triterpenoids isolated from bitter melon associated with activation of the AMPK pathway, *Chem. Biol.* **15**, 263-273.