

Structure Elucidation and Antiviral Properties of Pannosides from the Halophyte *Aster tripolium* L.

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pannoside F

Chemical shifts (ppm): 12.312, 10.615, 10.600, 10.486, 9.939, 8.640, 8.664, 8.143, 8.094, 7.534, 7.517, 7.484, 7.464, 7.438, 7.421, 7.317, 7.218, 7.197, 7.177, 7.066, 7.014, 6.915, 6.917, 6.894, 6.891, 6.857, 6.857, 6.827, 6.805, 5.497, 5.265, 4.749, 4.676, 4.297, 4.175, 4.159, 3.486, 3.121, 2.605, 2.605, 2.403, 2.377, 2.377, 2.381, 2.104, 2.086, 1.908, 1.889, 1.873, 1.834, 1.760, 1.739, 1.625, 1.625, 1.388.

Figure S3. COSY NMR spectrum of pannoside F (**1**) in CD₃OD-*d*₄.

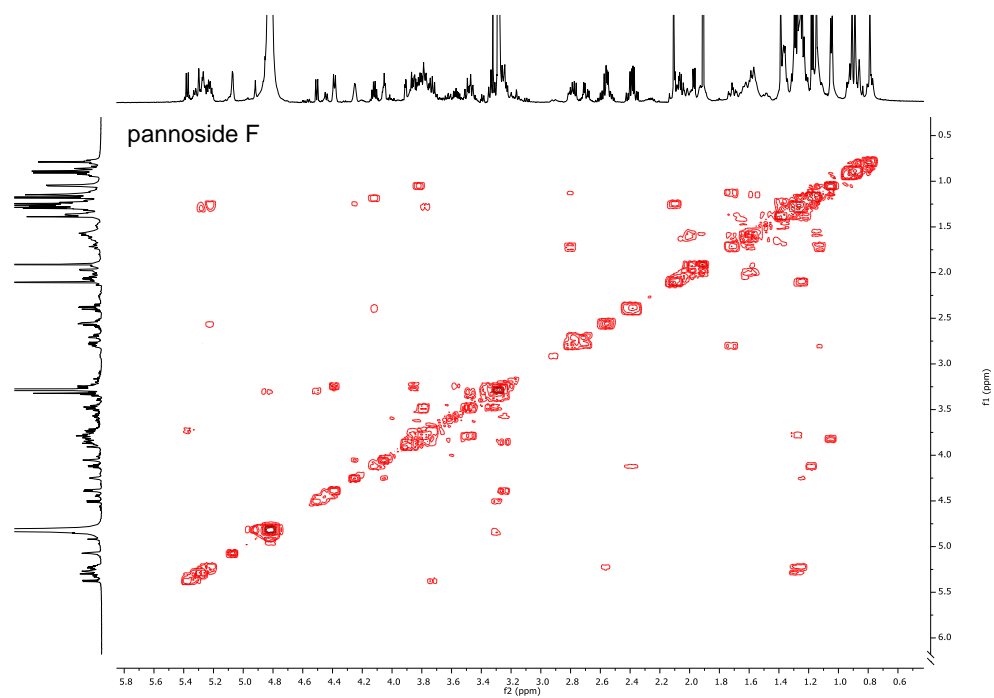


Figure S4. ROESY NMR spectrum of pannoside F (**1**) in CD₃OD-*d*₄.

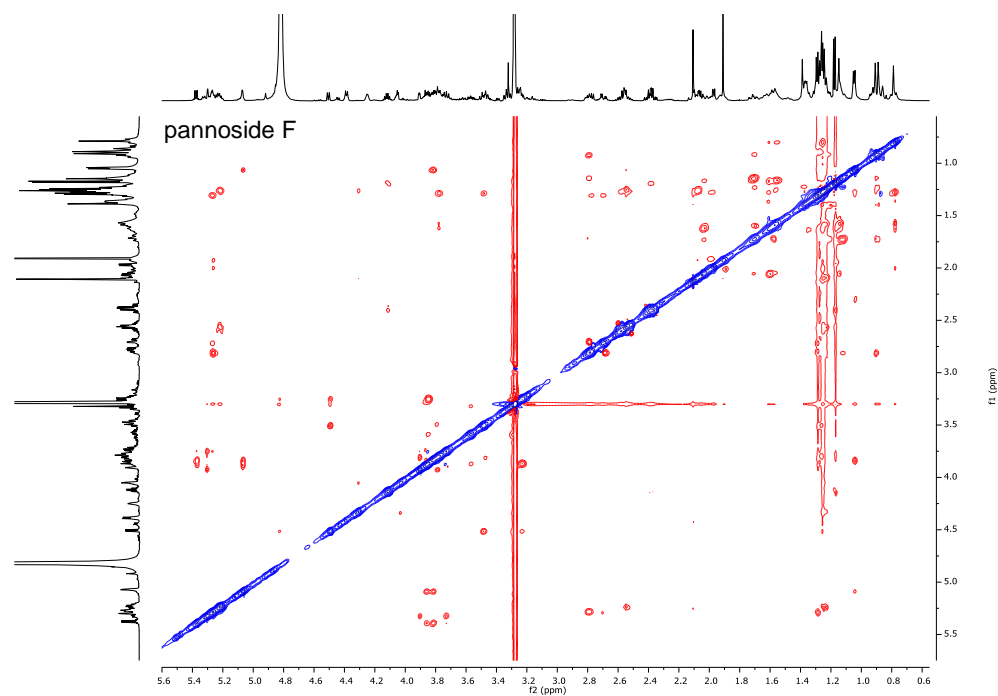


Figure S5. TOCSY NMR spectrum of pannoside F (**1**) in CD₃OD-*d*₄.

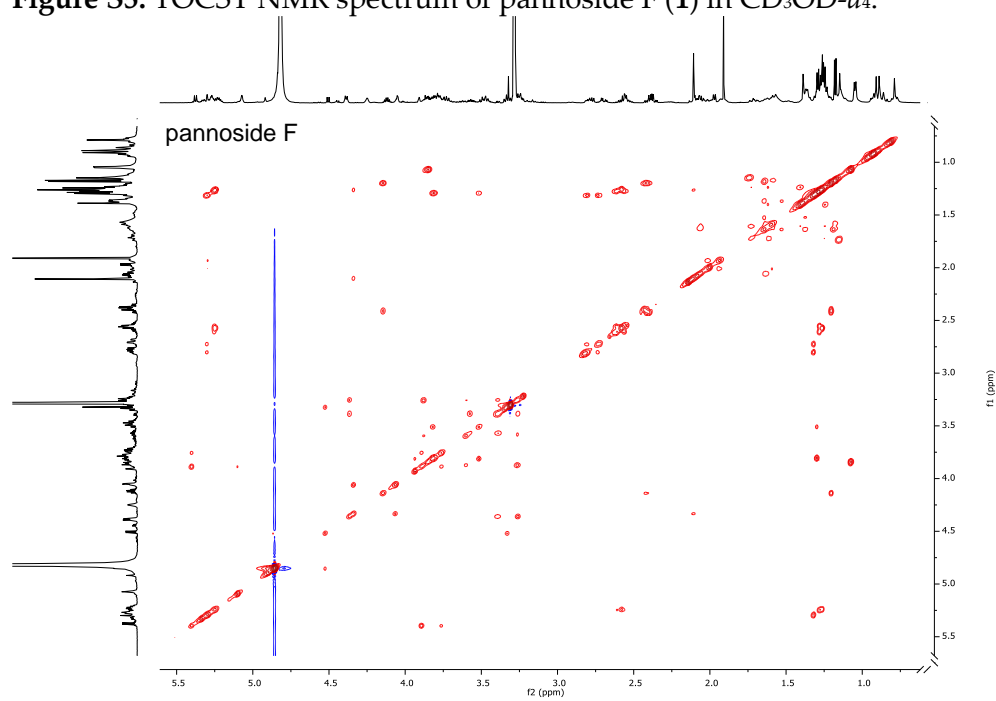


Figure S6. HSQC NMR spectrum of pannoside F (**1**) in CD₃OD-*d*₄.

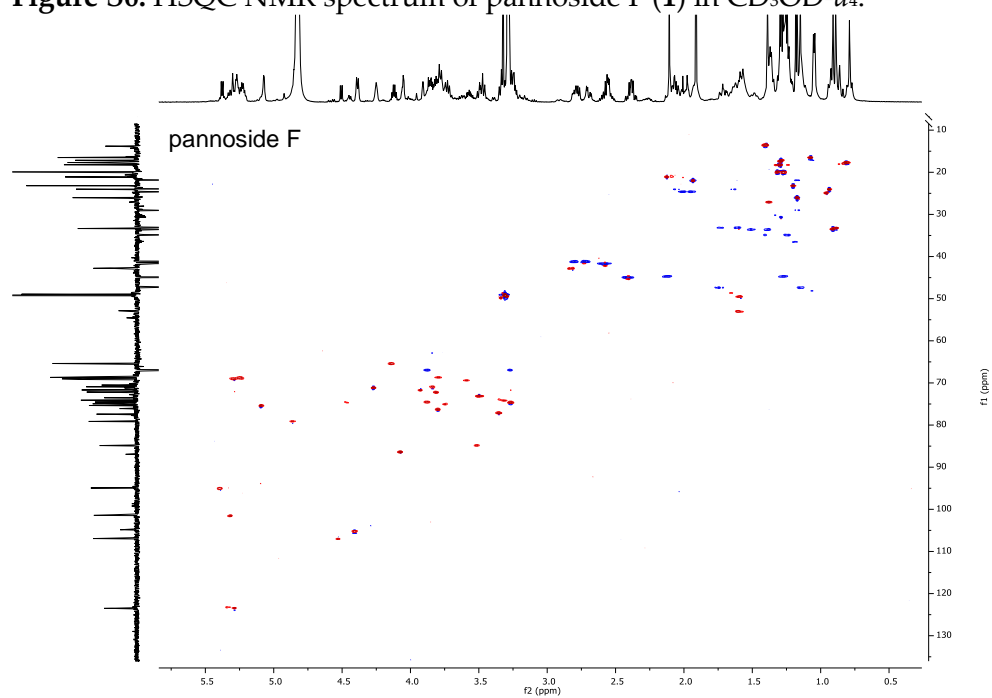
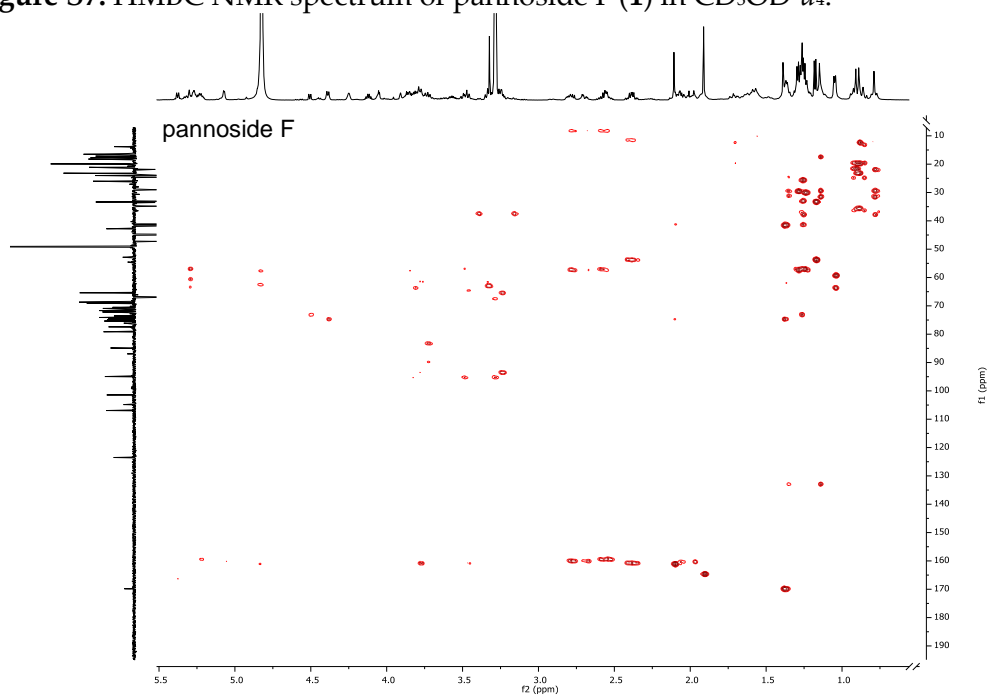


Figure S7. HMBC NMR spectrum of pannoside F (**1**) in CD₃OD-*d*₄.



1H NMR spectrum of compound 10b (a panoside C derivative) in CDCl₃.

Chemical Shifts (ppm): 5.5, 5.4, 5.3, 5.2, 5.1, 5.0, 4.9, 4.8, 4.7, 4.6, 4.5, 4.4, 4.3, 4.2, 4.1, 4.0, 3.9, 3.8, 3.7, 3.6, 3.5, 3.4, 3.3, 3.2, 3.1, 3.0, 2.9, 2.8, 2.7, 2.6, 2.5, 2.4, 2.3, 2.2, 2.1, 2.0, 1.9, 1.8, 1.7, 1.6, 1.5, 1.4, 1.3, 1.2, 1.1, 1.0, 0.9, 0.8, 0.7, 0.6, 0.5.

Peak Assignments and Integration:

Assignment	Chemical Shift (ppm)	Integration
L (dd)	5.31	5.31
I (m)	5.25	5.25
A (m)	5.40	5.40
H (m)	5.09	5.09
K (m)	5.34	5.34
F (m)	4.41	4.41
C (m)	4.14	4.14
O (d)	3.93	3.93
T (m)	3.74	3.74
V (m)	3.51	3.51
Y (m)	3.27	3.27
D (m)	4.52	4.52
B (t)	4.27	4.27
M (m)	4.07	4.07
Q (m)	3.86	3.86
U (m)	3.59	3.59
X (m)	3.40	3.40
G (q)	4.40	4.40
N (m)	4.04	4.04
R (m)	3.81	3.81
W (s)	3.47	3.47
S (m)	3.79	3.79
D1 (m)	2.71	2.71
A1 (dd)	2.79	2.79
F1 (m)	2.56	2.56
I1 (m)	2.30	2.30
M1 (d)	2.12	2.12
N1 (m)	1.99	1.99
P1 (m)	1.39	1.39
D2 (d)	1.62	1.62
J1 (td)	1.73	1.73
E (m)	1.40	1.40
R1 (dd)	1.19	1.19
J (m)	1.07	1.07
Z1 (d)	0.88	0.88
B1 (m)	2.82	2.82
E1 (m)	2.61	2.61
H1 (m)	2.39	2.39
L1 (d)	2.15	2.15
O1 (s)	1.93	1.93
U1 (d)	1.30	1.30
S1 (m)	1.25	1.25
W1 (d)	0.95	0.95
X1 (s)	0.93	0.93
A2 (m)	0.82	0.82
B2 (d)	0.78	0.78
Y1 (d)	0.90	0.90

pannosit G

123.512

104.833

103.518

94.508

86.774

77.453

75.337

74.666

74.110

73.585

73.299

71.366

70.888

70.589

69.245

68.750

65.431

54.595

52.886

44.803

42.782

34.881

33.881

33.394

33.058

29.942

28.692

24.126

24.650

20.803

20.721

18.907

17.726

16.404

13.751

Figure S10. COSY NMR spectrum of pannoside G (**2**) in CD₃OD-*d*₄.

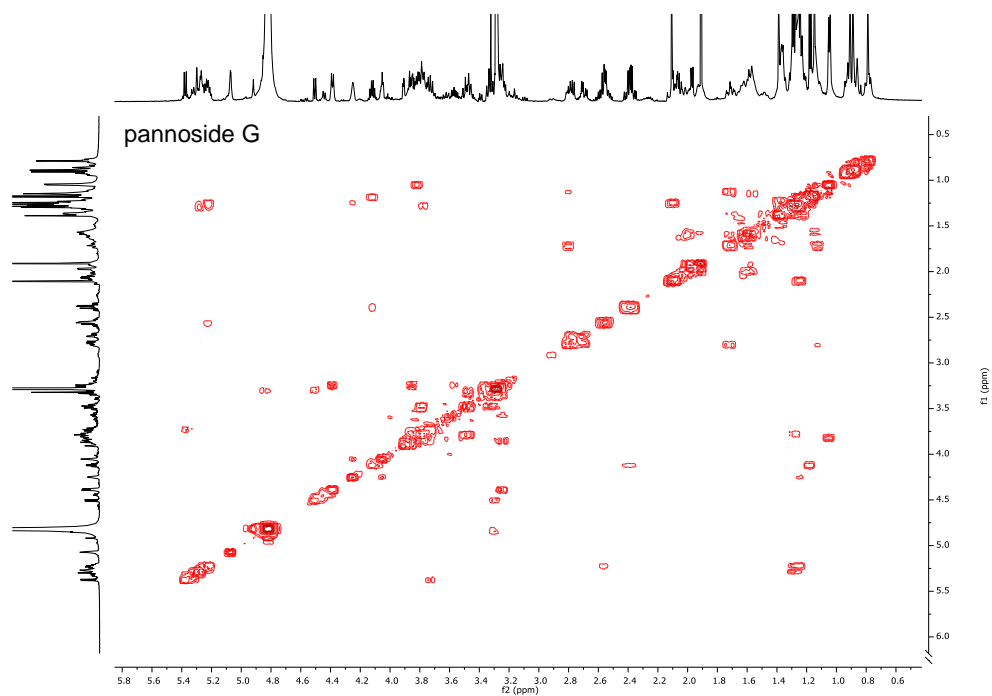


Figure S11. ROESY NMR spectrum of pannoside G (**2**) in CD₃OD-*d*₄.

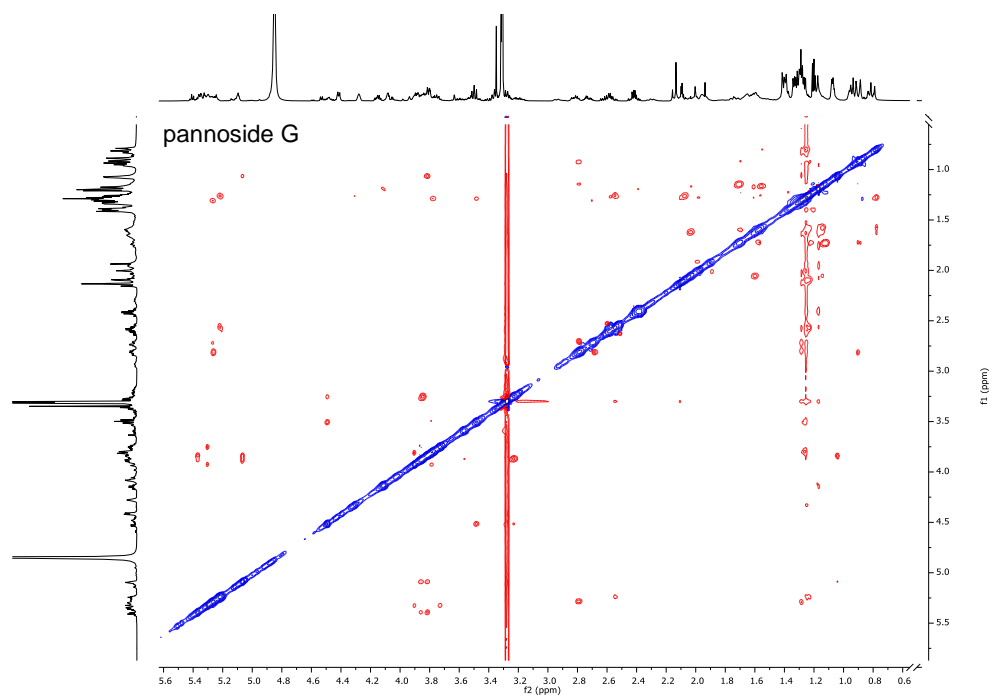


Figure S12. TOCSY NMR spectrum of pannoside G (**2**) in CD₃OD-*d*₄.

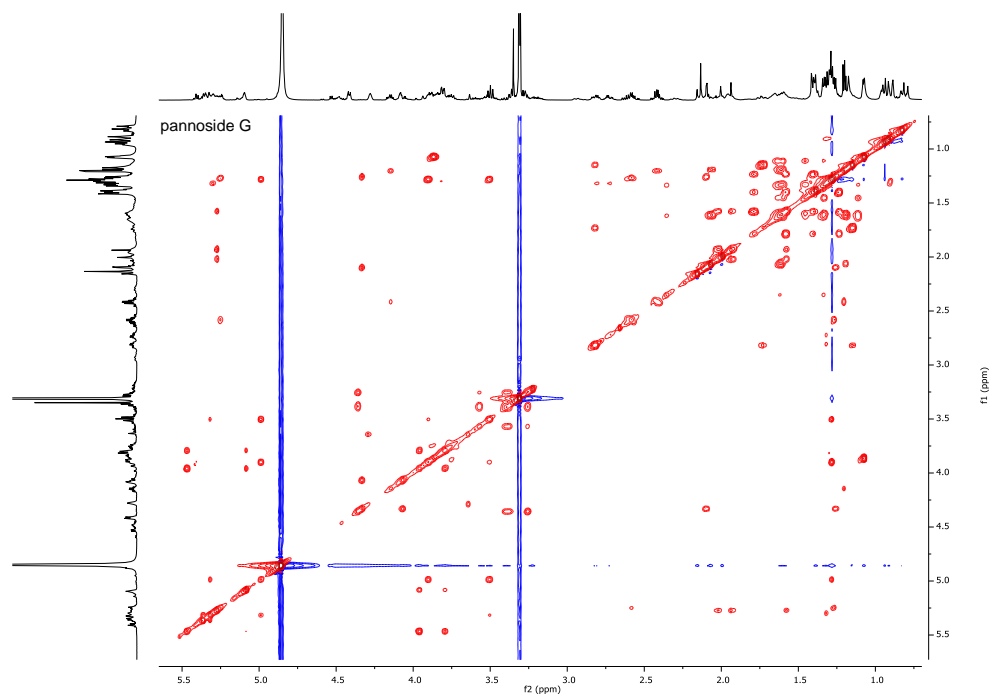


Figure S13. HSQC NMR spectrum of pannoside G (**2**) in CD₃OD-*d*₄.

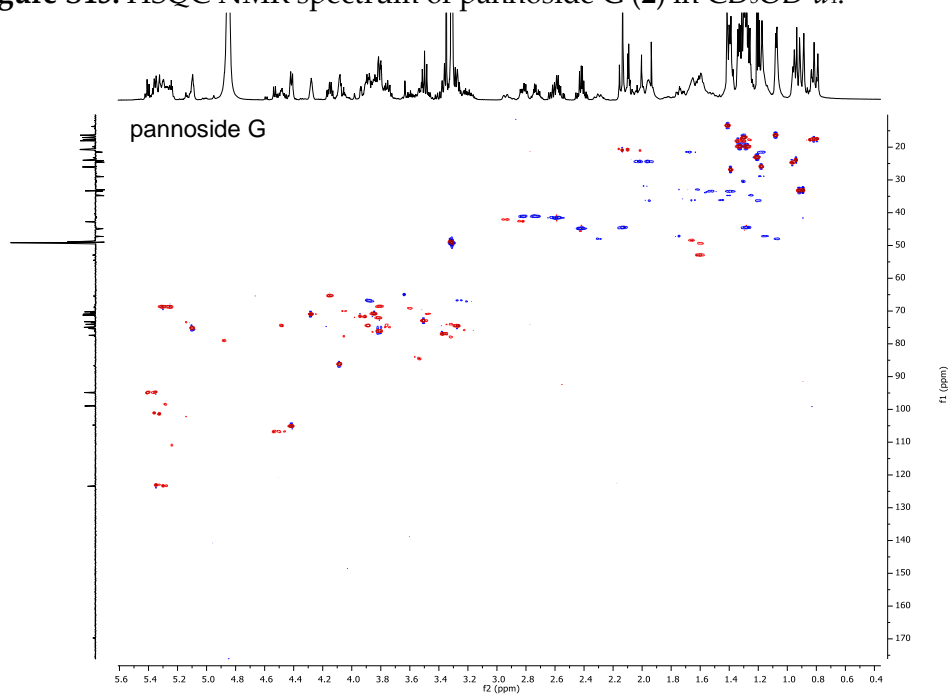


Figure S14. HMBC NMR spectrum of pannoside G (**2**) in CD₃OD-*d*₄.

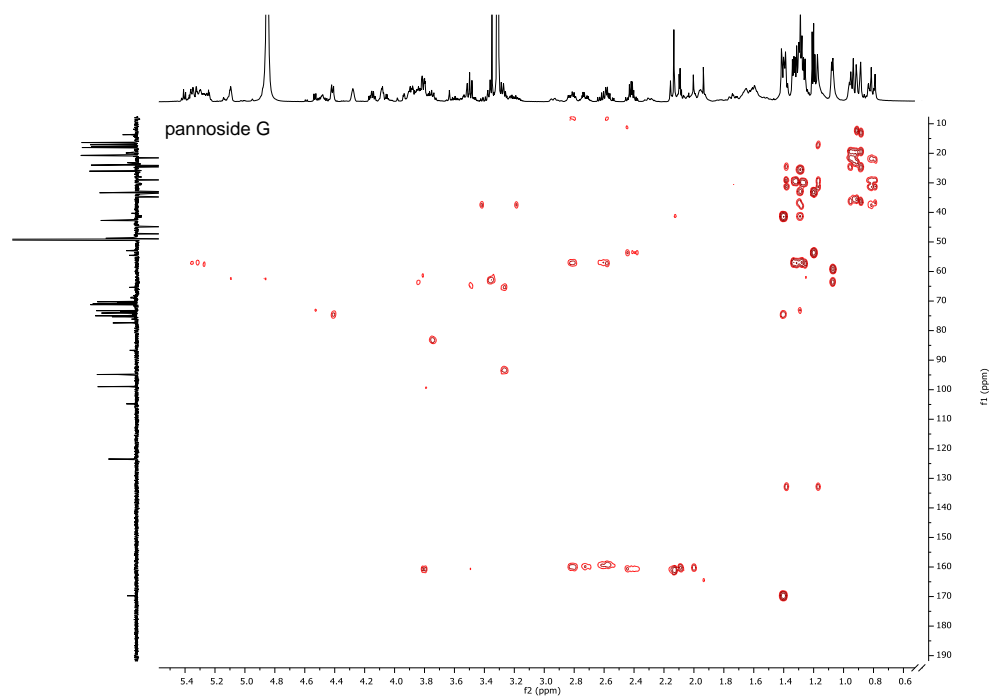


Figure S15. ^1H NMR spectrum (600 MHz) of pannoside H (3) in $\text{CD}_3\text{OD}-d_4$.

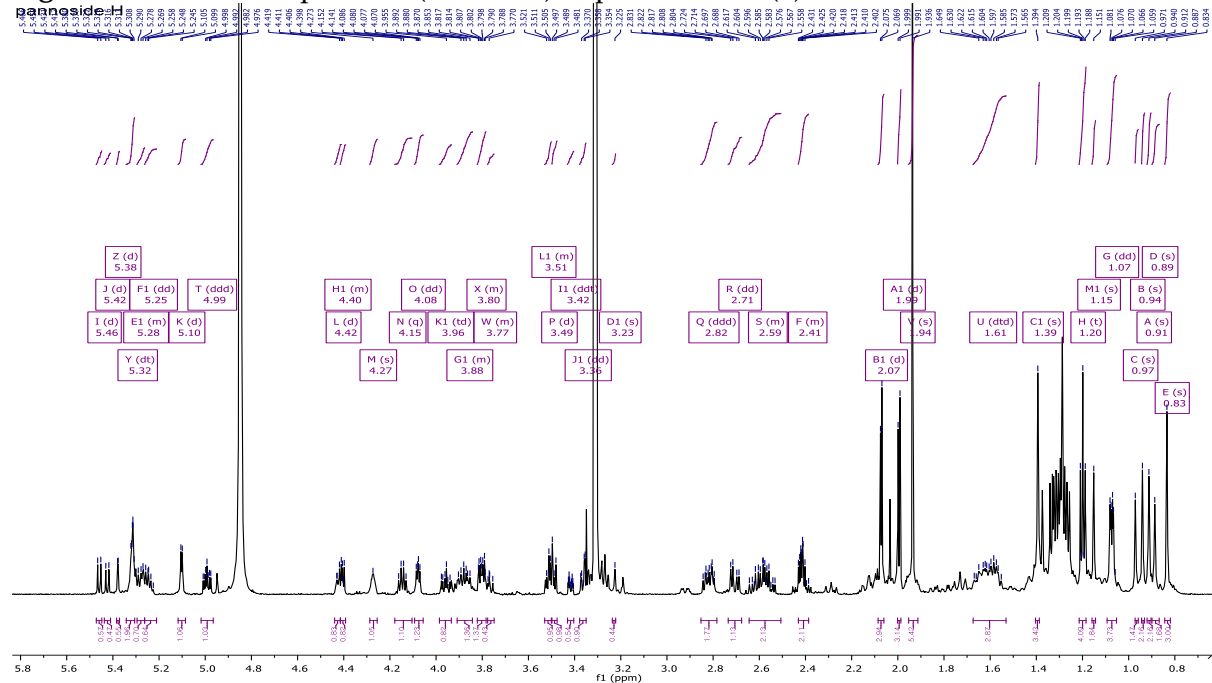


Figure S16. ^{13}C NMR spectrum (150 MHz) of pannoside H (3) in $\text{CD}_3\text{OD}-d_4$.

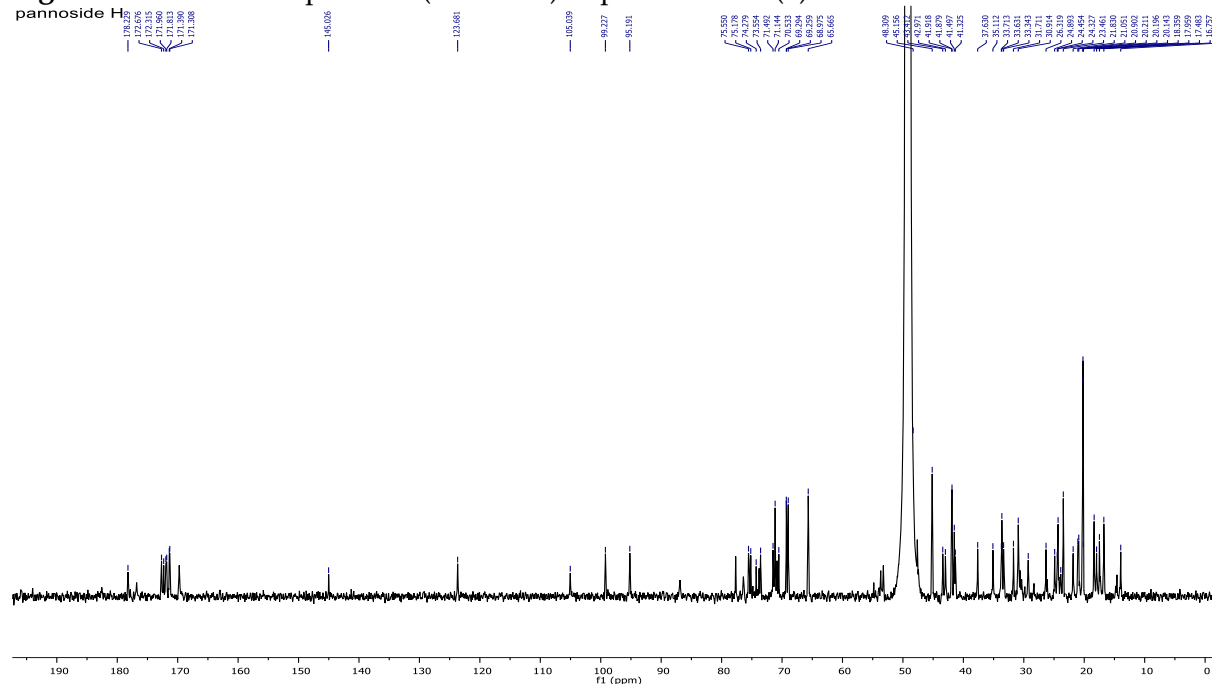


Figure S17. COSY NMR spectrum of pannoside H (3) in CD₃OD-*d*₄.

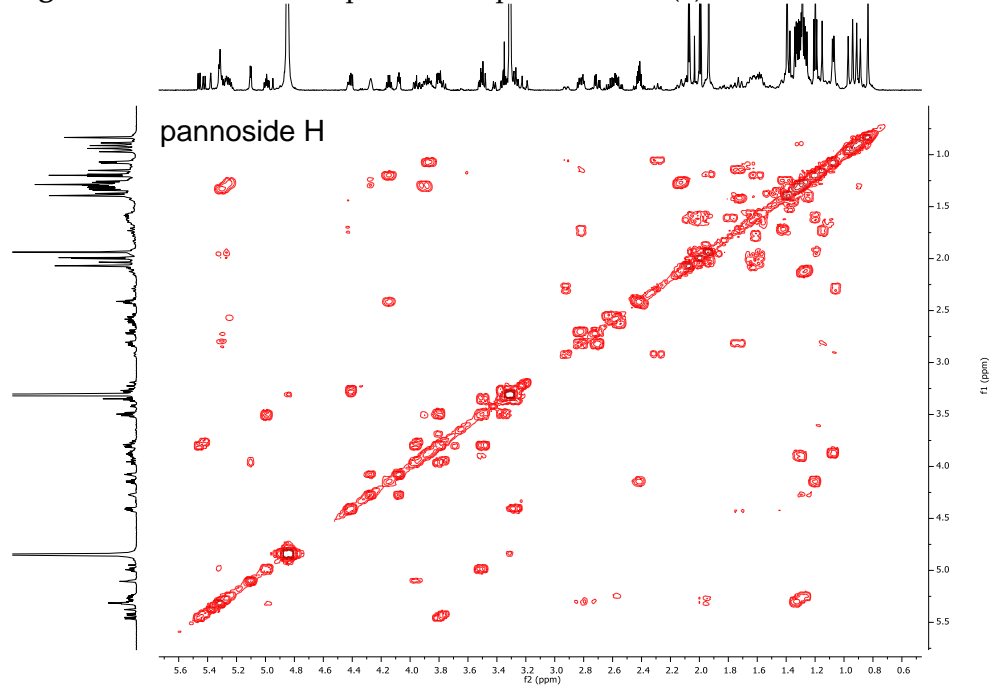


Figure S18. ROESY NMR spectrum of pannoside H (3) in CD₃OD-*d*₄.

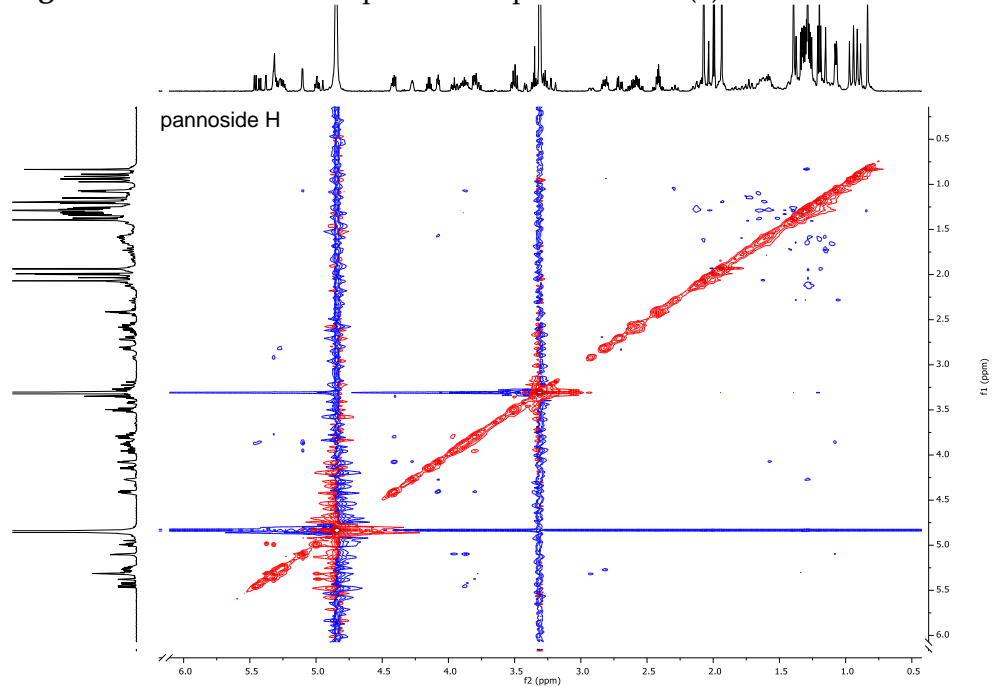


Figure S19. TOCSY NMR spectrum of pannoside H (3) in CD₃OD-*d*₄.

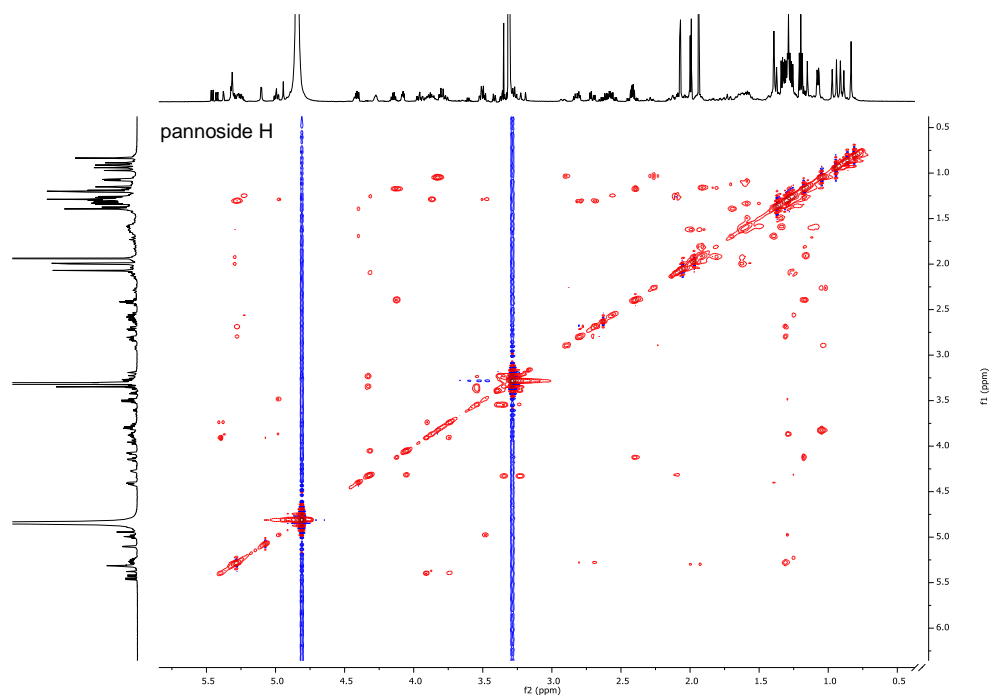


Figure S20. HSQC NMR spectrum of pannoside H (3) in CD₃OD-*d*₄.

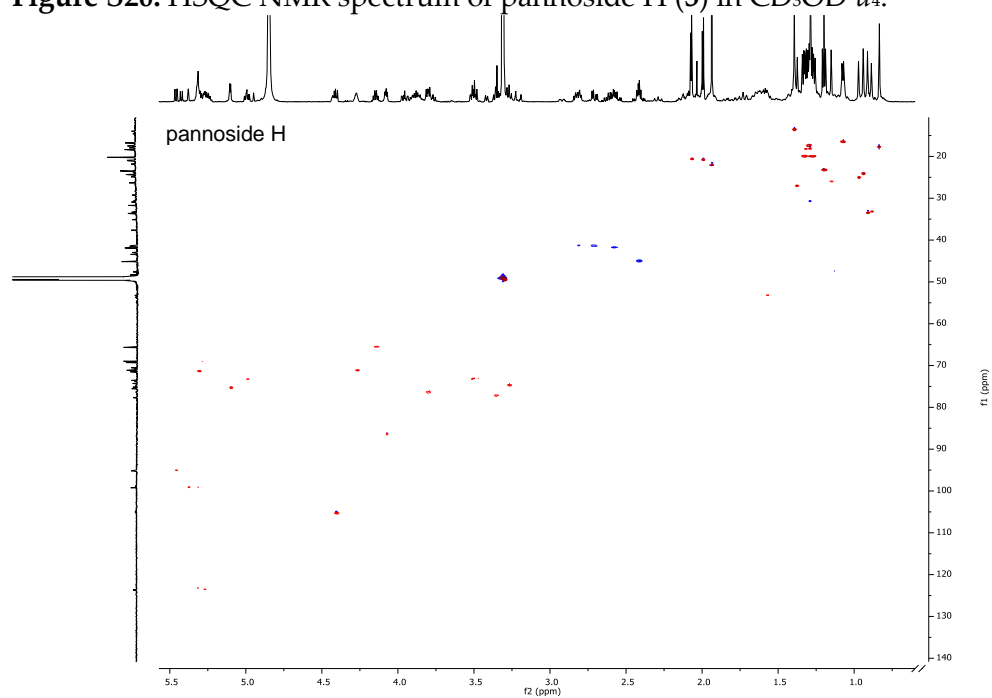


Figure S21. HMBC NMR spectrum of pannoside H (**3**) in CD₃OD-*d*₄.

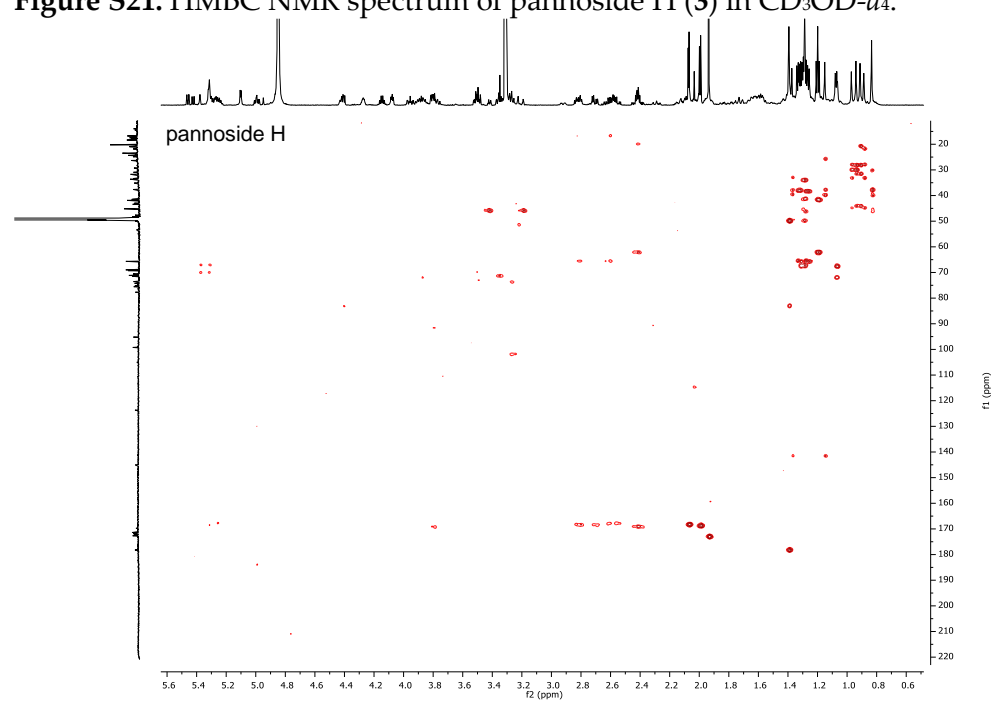


Figure S22. ^1H NMR spectrum (600 MHz) of pannoside I (**4**) in $\text{CD}_3\text{OD}-d_4$.

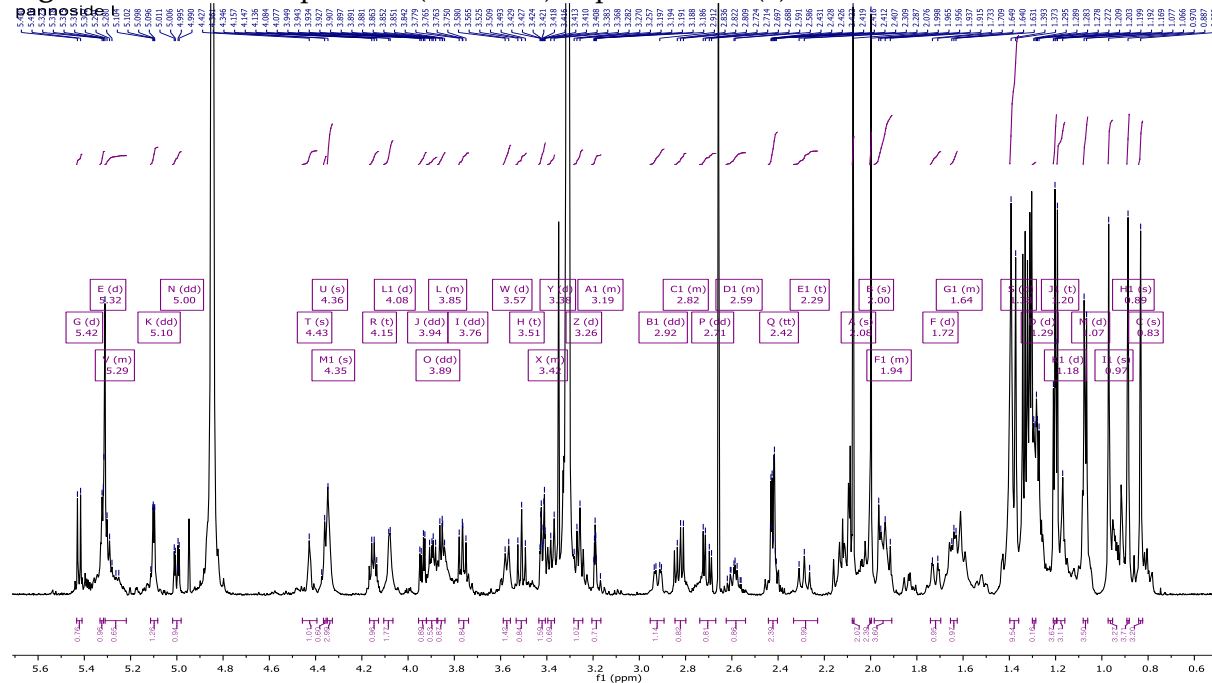


Figure S23. DEPT-135 spectrum (150 MHz) of pannoside I (**4**) in $\text{CD}_3\text{OD}-d_4$.

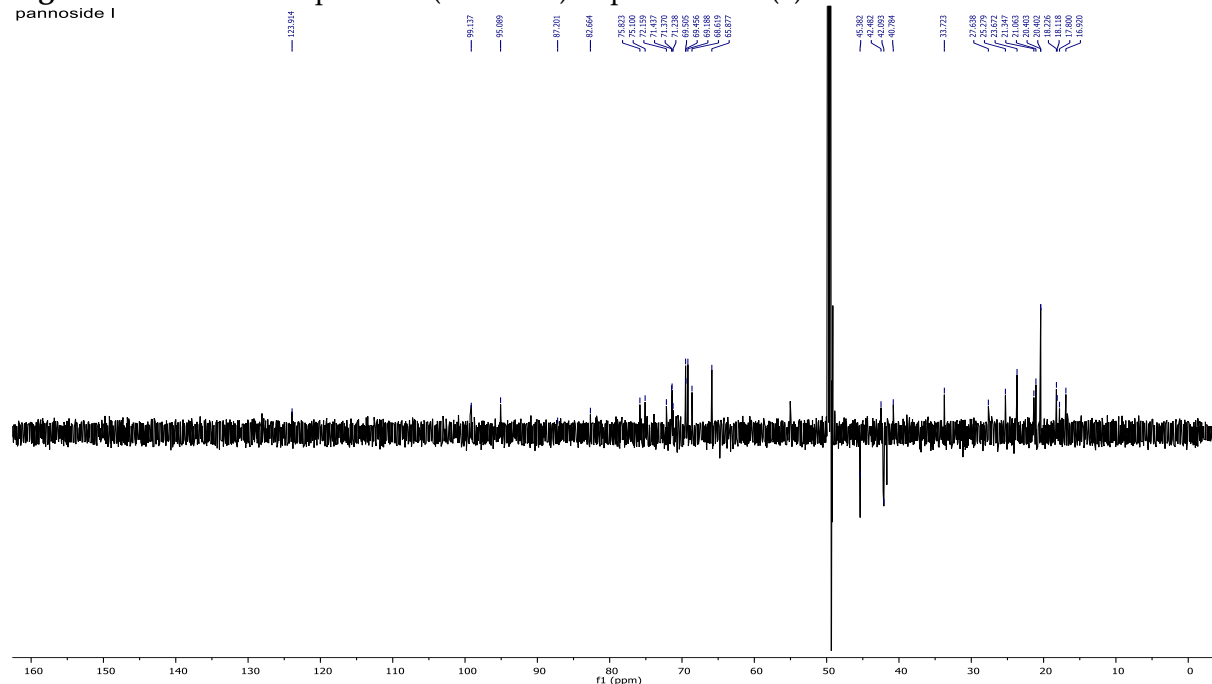


Figure S24. COSY NMR spectrum of pannoside I (**4**) in CD₃OD-*d*₄.

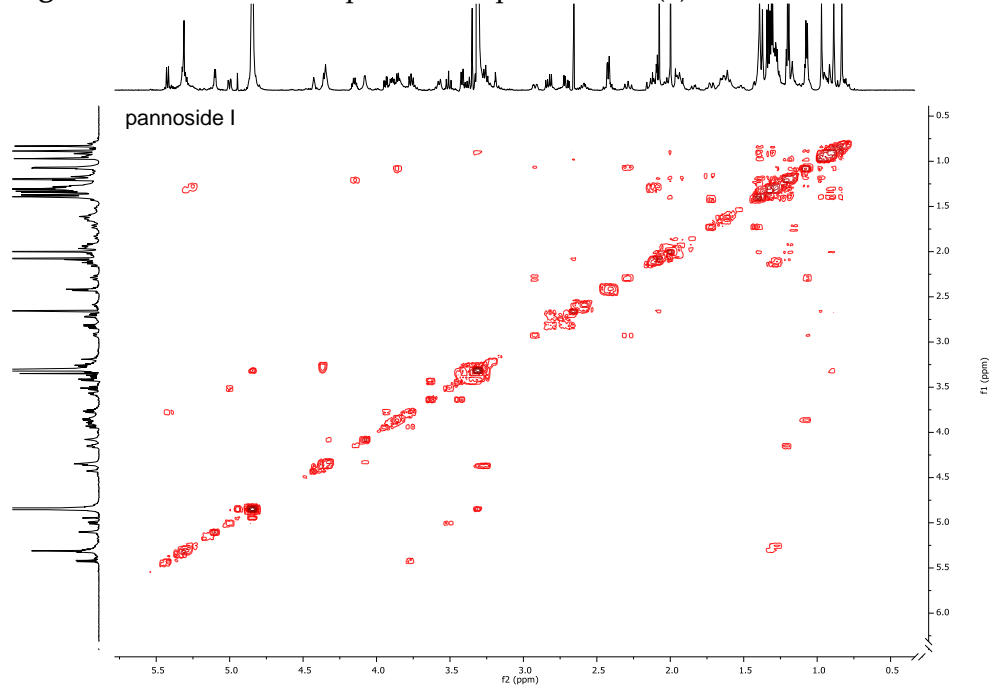


Figure S25. ROESY NMR spectrum of pannoside I (**4**) in CD₃OD-*d*₄.

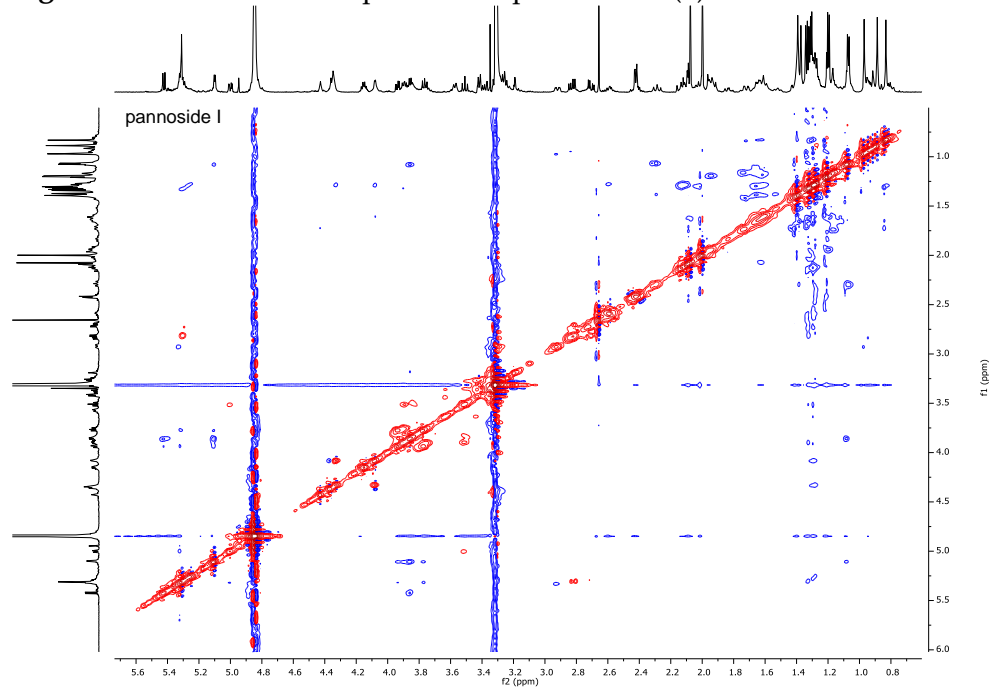


Figure S26. TOCSY NMR spectrum of pannoside I (**4**) in CD₃OD-*d*₄.

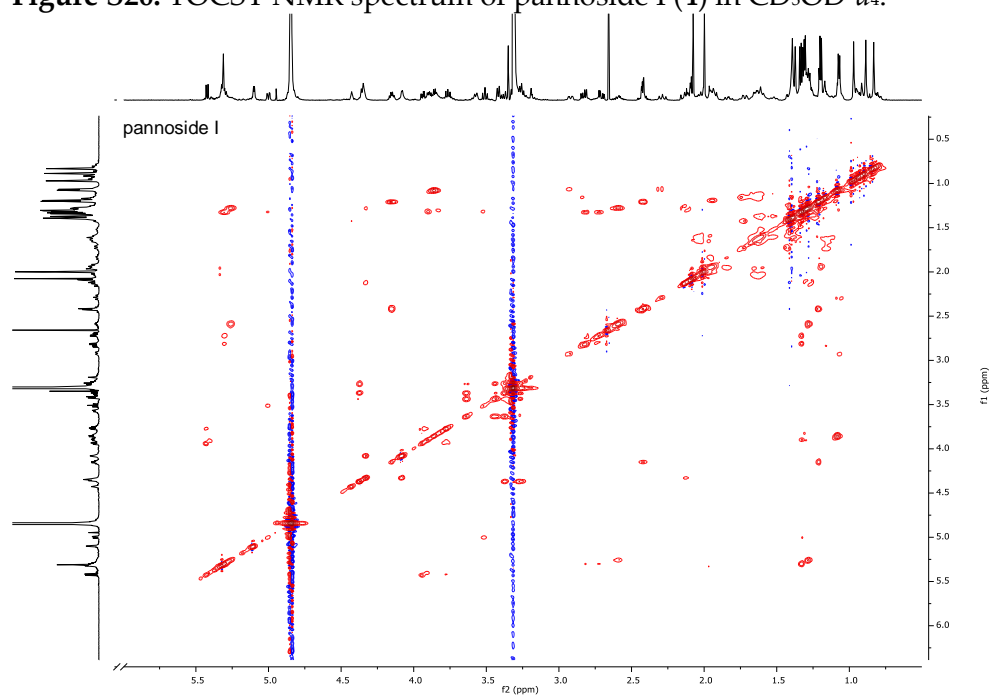


Figure S27. HSQC NMR spectrum of pannoside I (**4**) in CD₃OD-*d*₄.

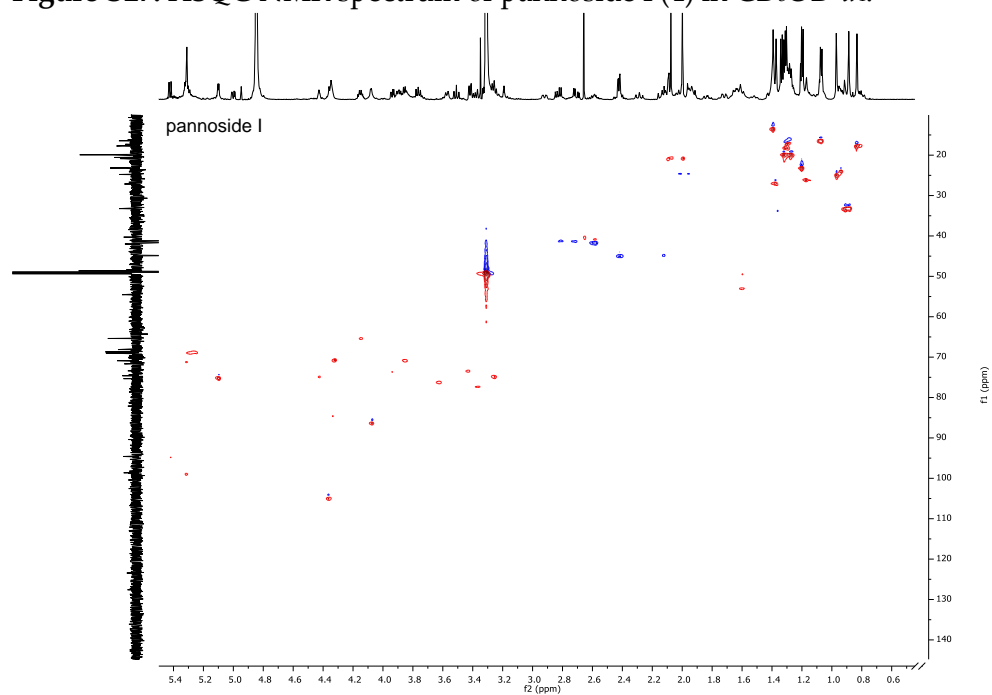


Figure S28. HMBC NMR spectrum of pannoside I (4) in CD₃OD-*d*₄.

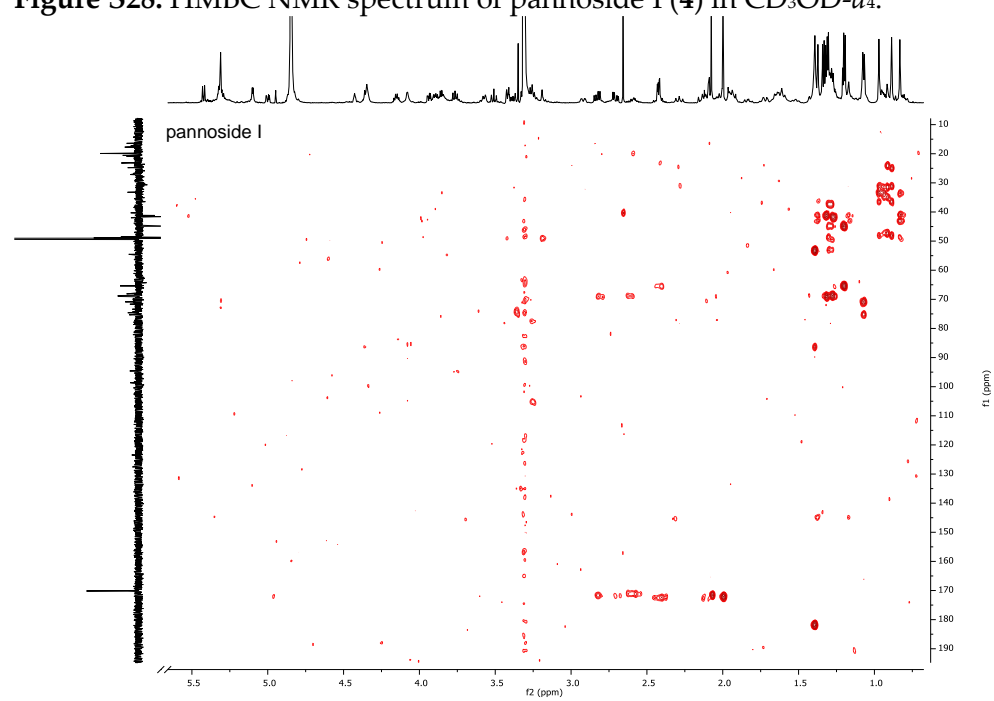


Figure S29. Extracted-ion chromatogram (EIC) of pannosides F–I (1–4).

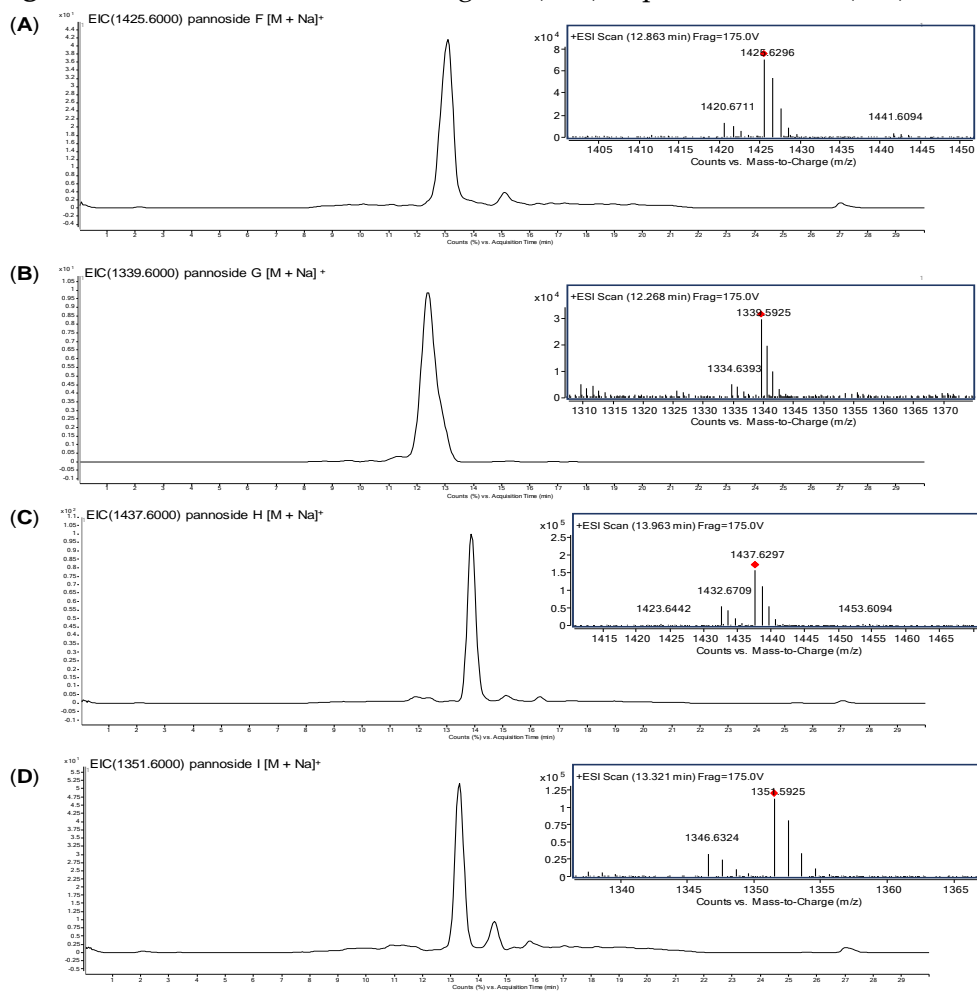
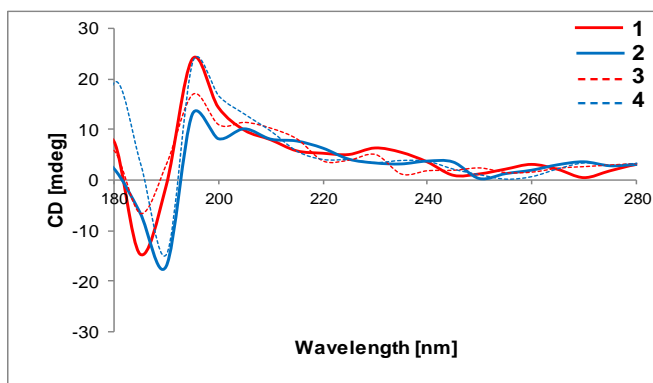


Figure S30. The experimental CD spectra of pannosides F–I (1–4).



1a

Label	Multiplicity	Chemical Shift (ppm)	Integration
G	t	5.26	1.00
I	d	4.07	0.91
H	d	3.97	0.91
L	dd	2.85	1.00
N	m	~2.01	1.00
M	dd	~2.10	0.92
O	m	~1.95	1.00
P	m	~1.75	1.00
Q	m	~1.69	0.92
R	m	~1.60	1.00
S	dt	~1.54	0.92
T	q	~1.38	1.00
U	q	~1.17	0.92
V	s	~1.06	1.00
W	s	~0.91	0.92
X	s	~0.82	1.00
Y	s	~0.74	0.92
Z	s	~0.68	1.00

1a

¹³C NMR spectrum (CDCl₃) of compound **1a**. The x-axis represents the chemical shift in ppm, ranging from 10 to 180. The spectrum shows several sharp peaks, with the following chemical shifts labeled:

- 182.26
- 165.42
- 122.705
- 76.584
- 72.204
- 54.331
- 52.823
- 50.000
- 48.661
- 48.212
- 47.863
- 47.514
- 46.060
- 39.587
- 38.771
- 38.377
- 33.396
- 32.933
- 32.580
- 28.902
- 28.456
- 24.301
- 23.795
- 22.159
- 17.795
- 17.253
- 11.188

Figure S33. COSY NMR spectrum (400 MHz) of an aglycone of **1** (**1a**) in CD₃OD-*d*₄.

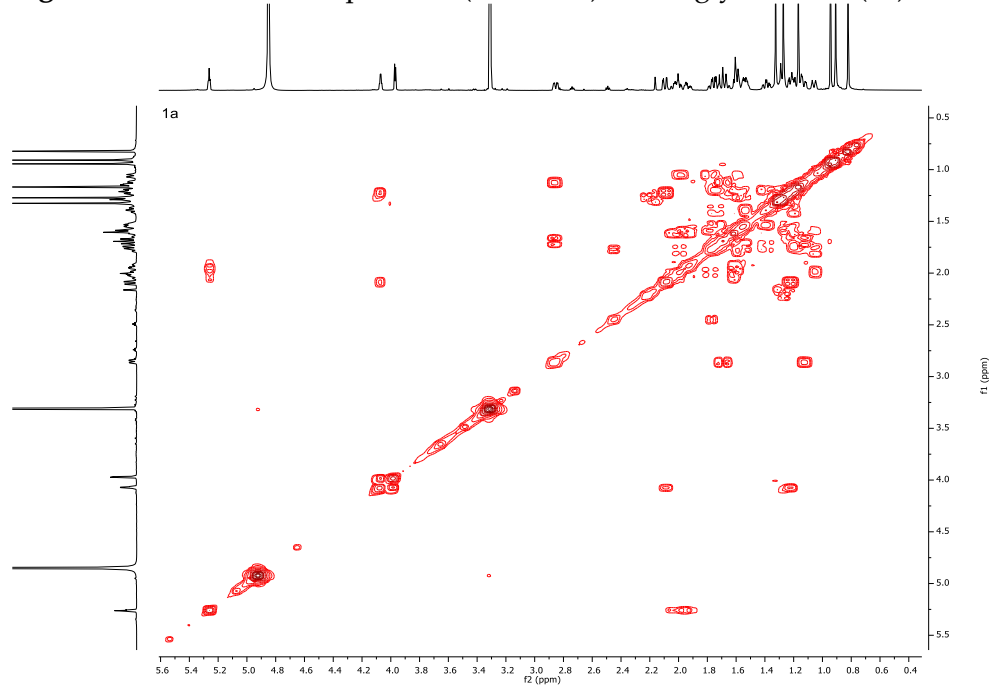


Figure S34. ROESY NMR spectrum (400 MHz) of an aglycone of **1** (**1a**) in CD₃OD-*d*₄.

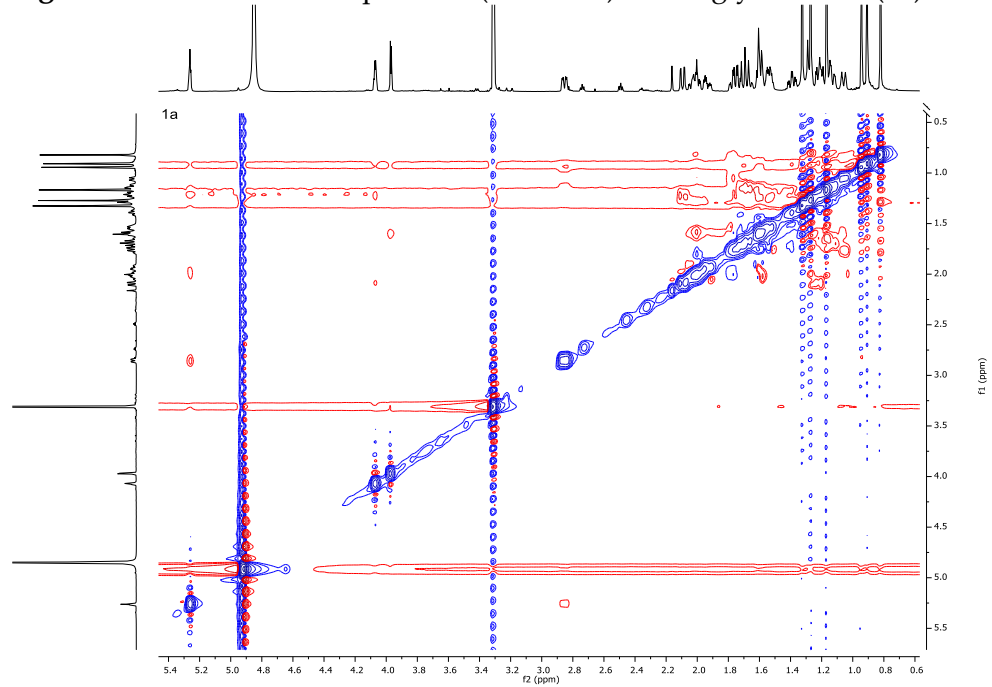


Figure S35. ^1H NMR spectrum (400 MHz) of an aglycone of **3** (**3a**) in $\text{CD}_3\text{OD}-d_4$.

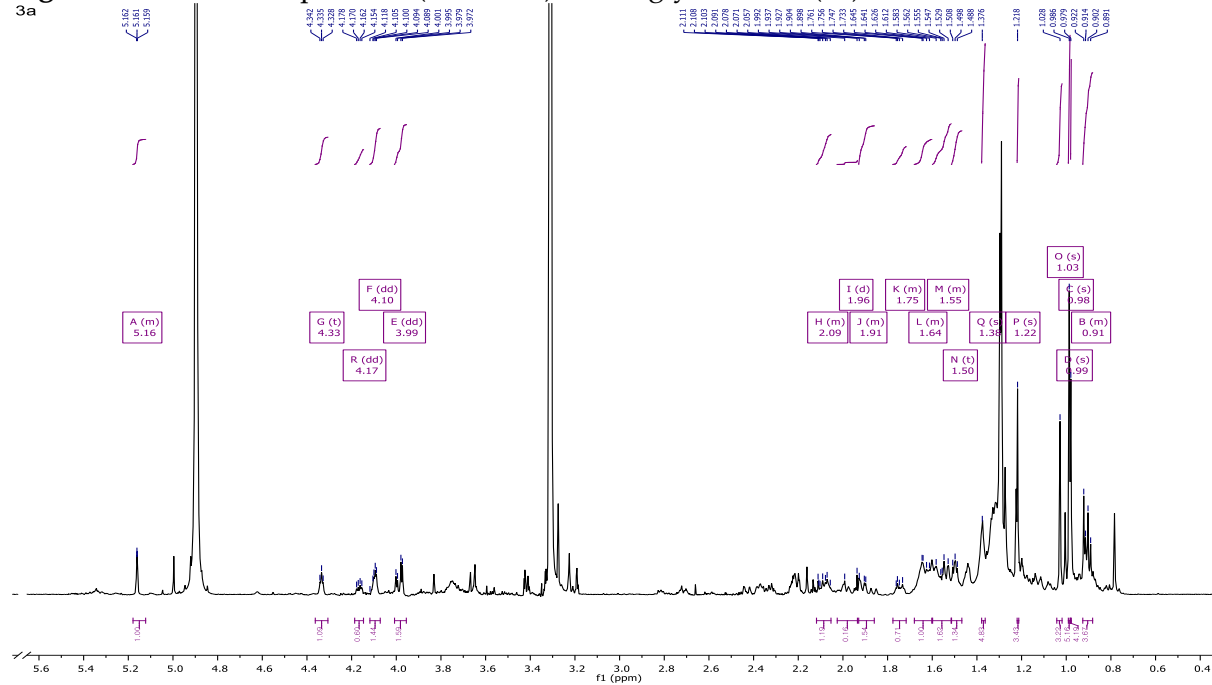


Figure S36. COSY NMR spectrum of an aglycone of **3** (**3a**) in $\text{CD}_3\text{OD}-d_4$.

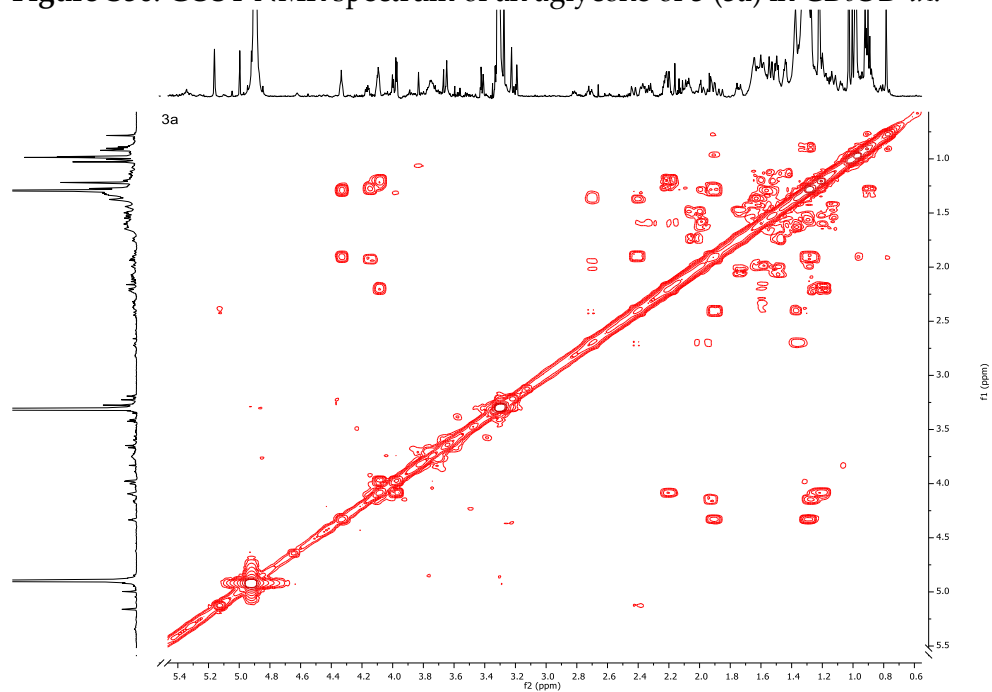


Figure S37. ROESY NMR spectrum of an aglycone of 3 (3a) in CD₃OD-*d*₄.

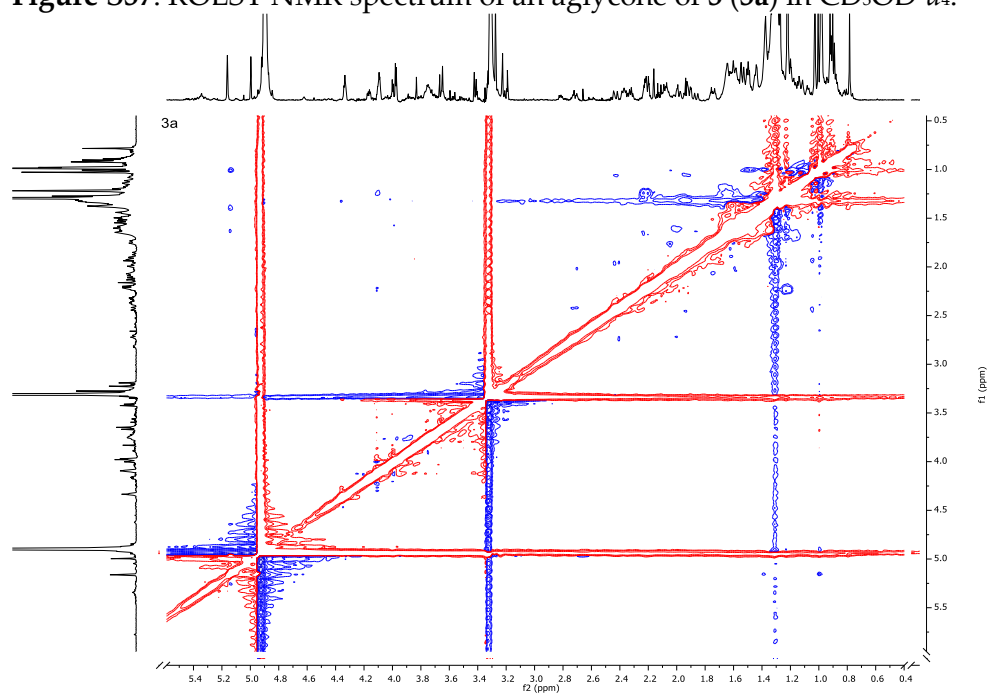


Figure S38. Extracted-ion chromatograms (EIC) of **1a** and **3a**.

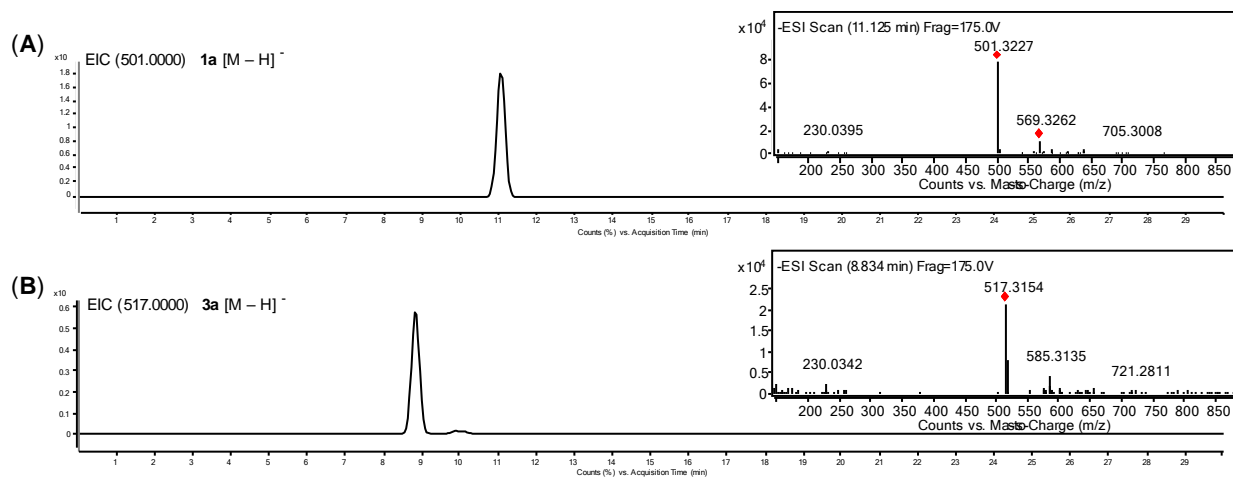


Figure S39. EIC of *S*-PGME derivatives; authentic (*S*)-, (*R*)-3-HB and 3-HB residues in hydrolysate of **1**.

