Supporting Information

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Nicocembranoside A: A new neuroprotective cembrane glycoside from *Nicotiana tabacum* L.

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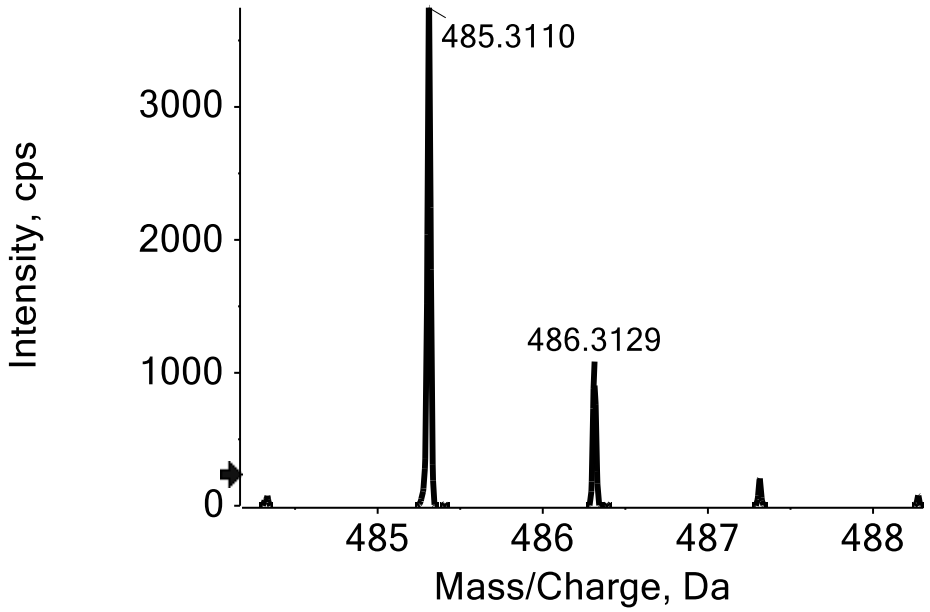

Figure S1: HRESIMS spectrum of **1**

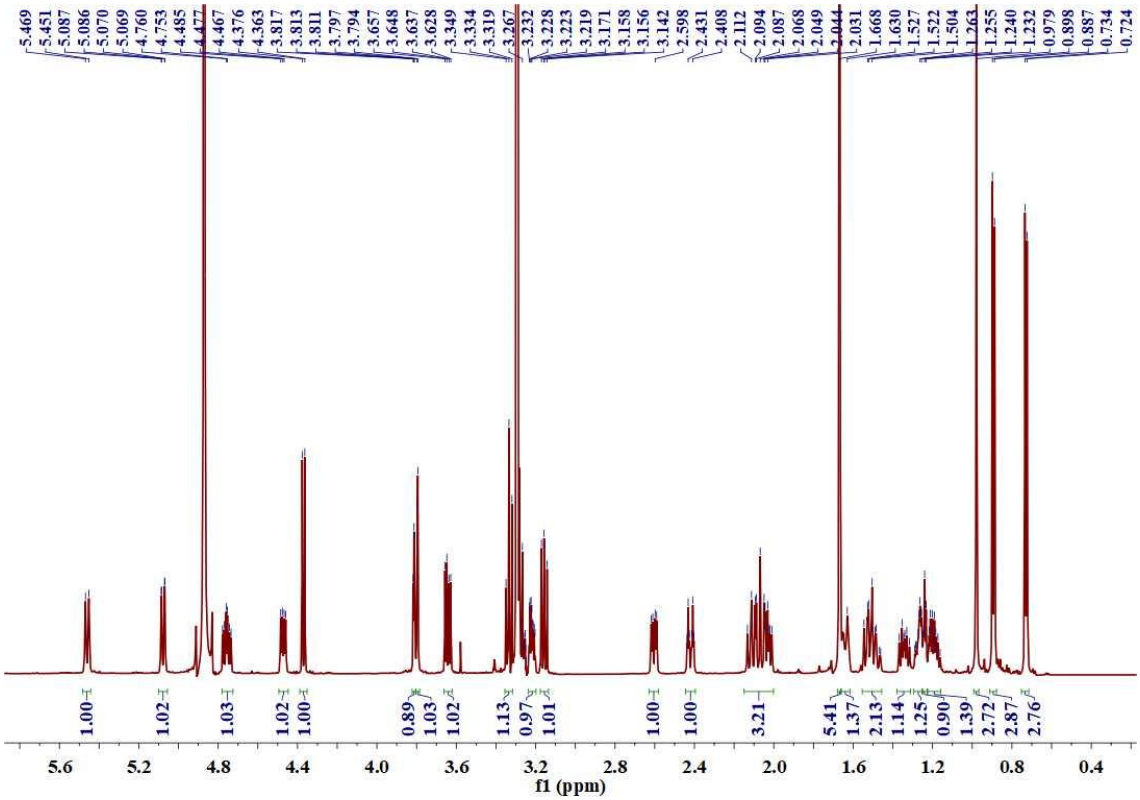

Figure S2: ^{1}H NMR (600 MHz, MeOH-d_4) spectrum of **1**

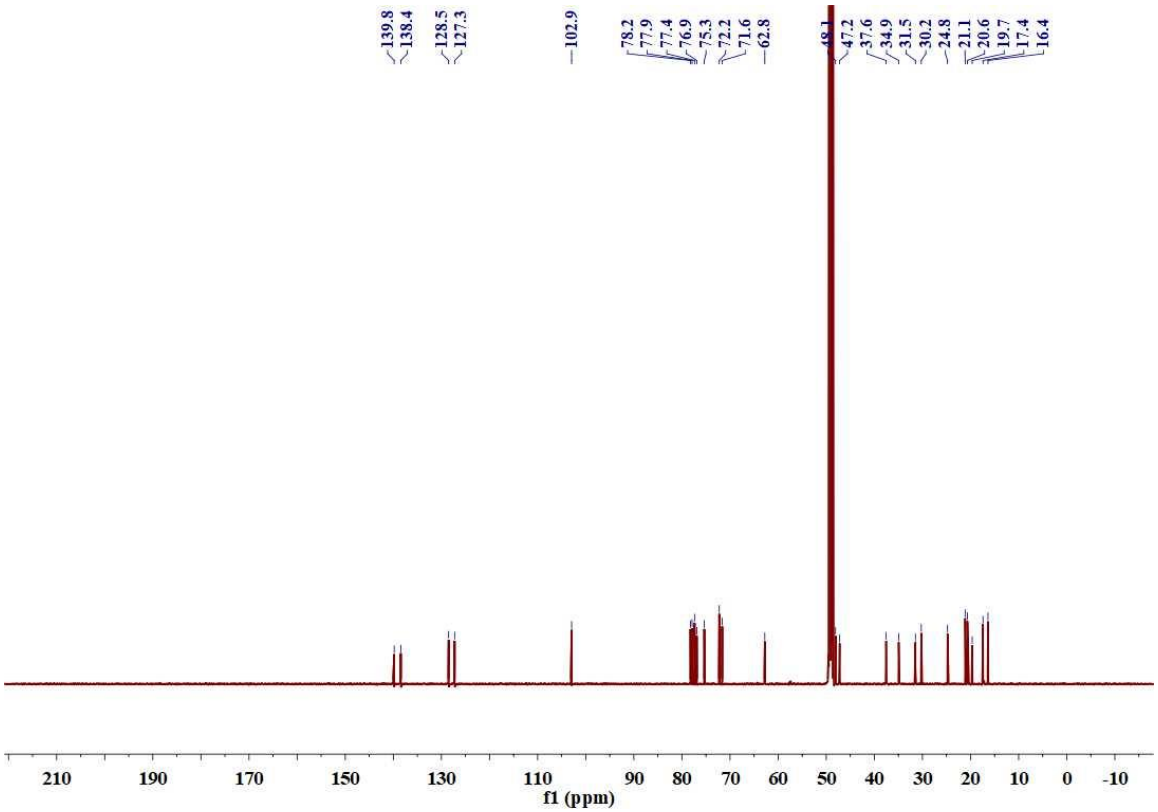

Figure S3: ^{13}C NMR (150 MHz, MeOH-d_4) spectrum of **1**

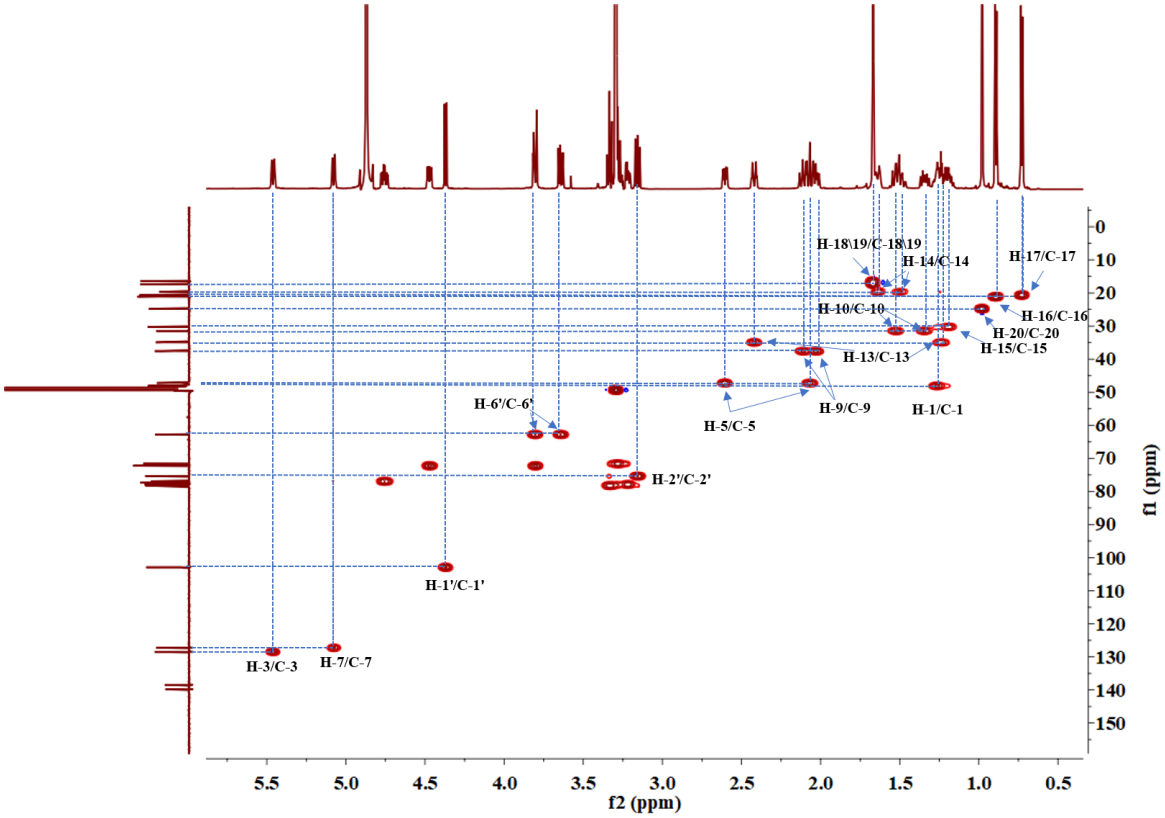

Figure S4: HSQC spectrum of **1**

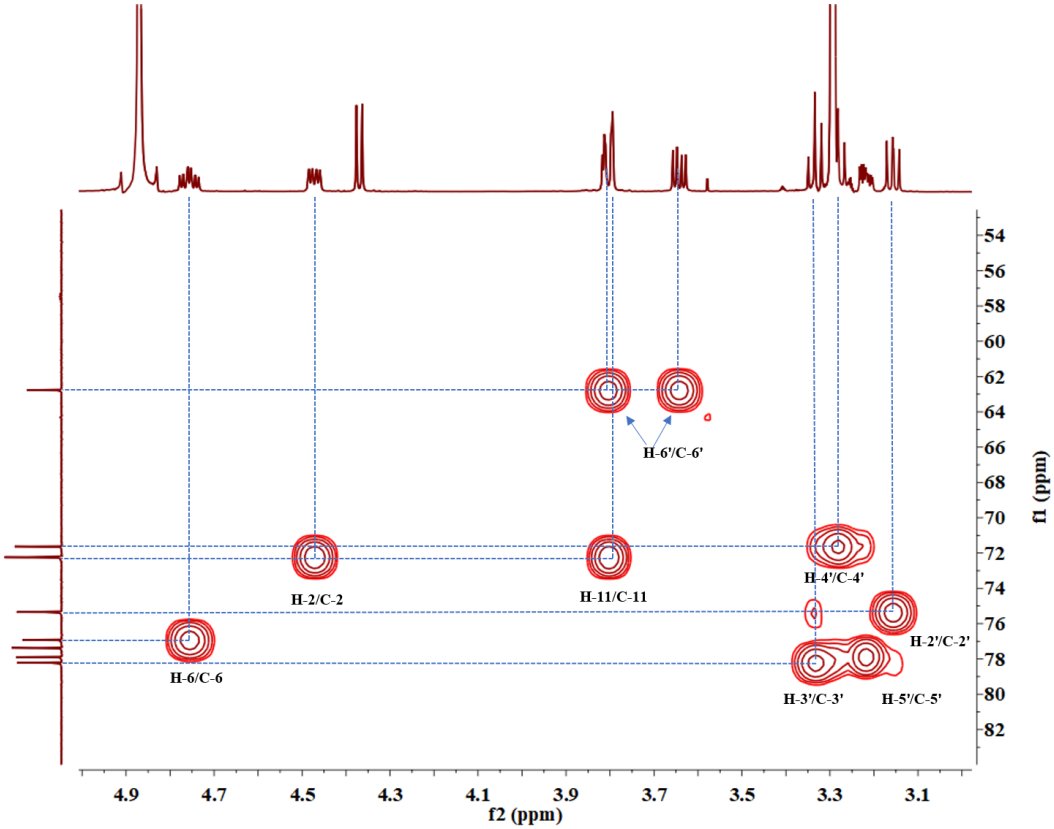

Figure S5: Enlarged HSQC spectrum of **1**

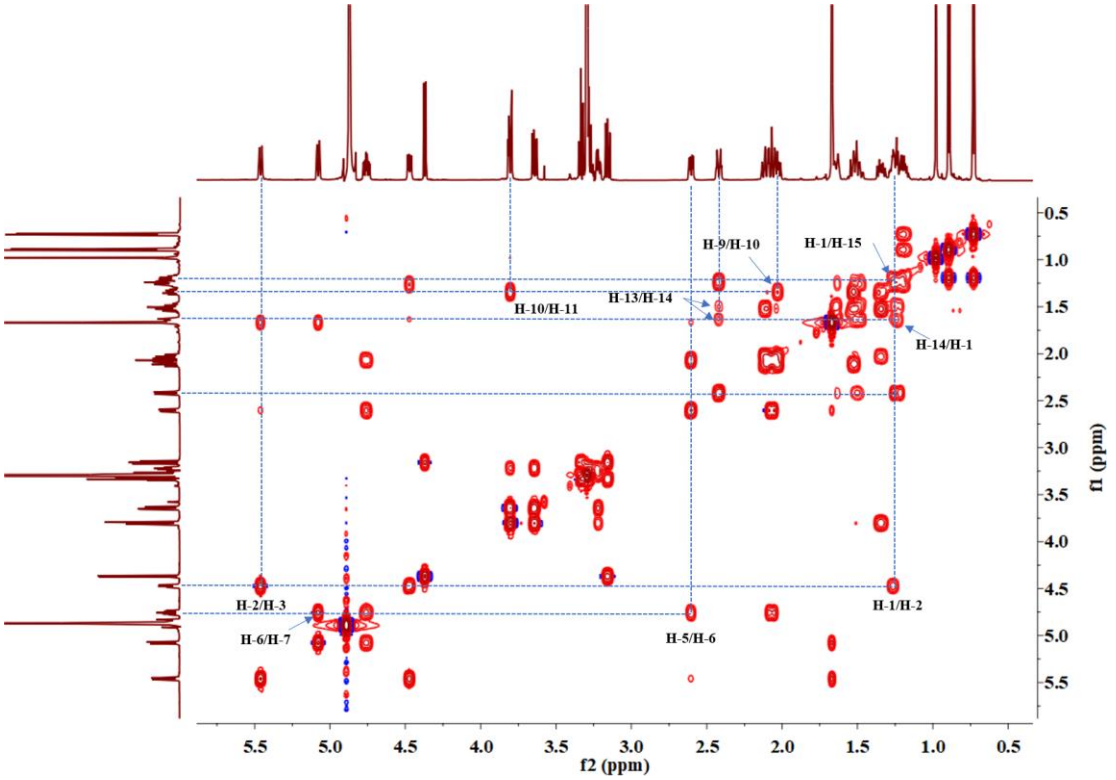

Figure S6: ^{1}H-^{1}H COSY spectrum of **1**

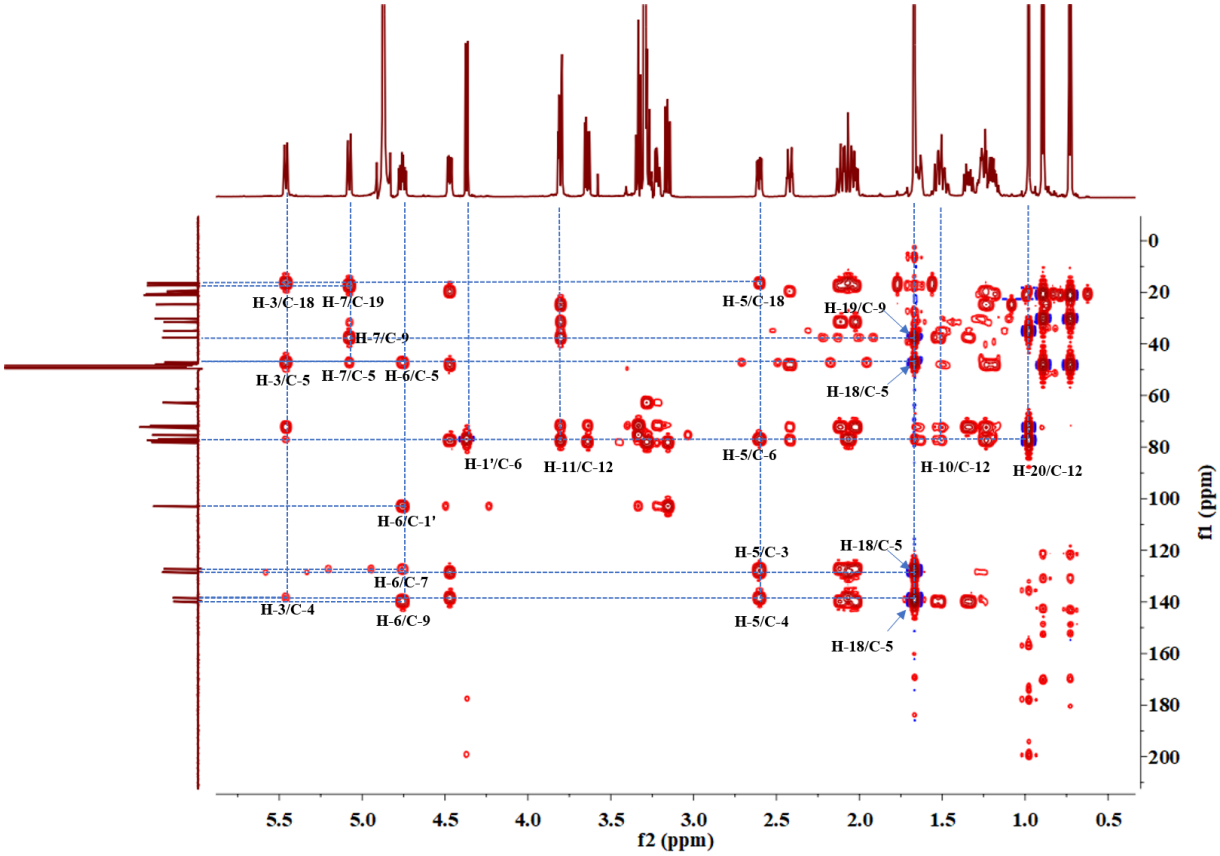

Figure S7: HMBC spectrum of **1**

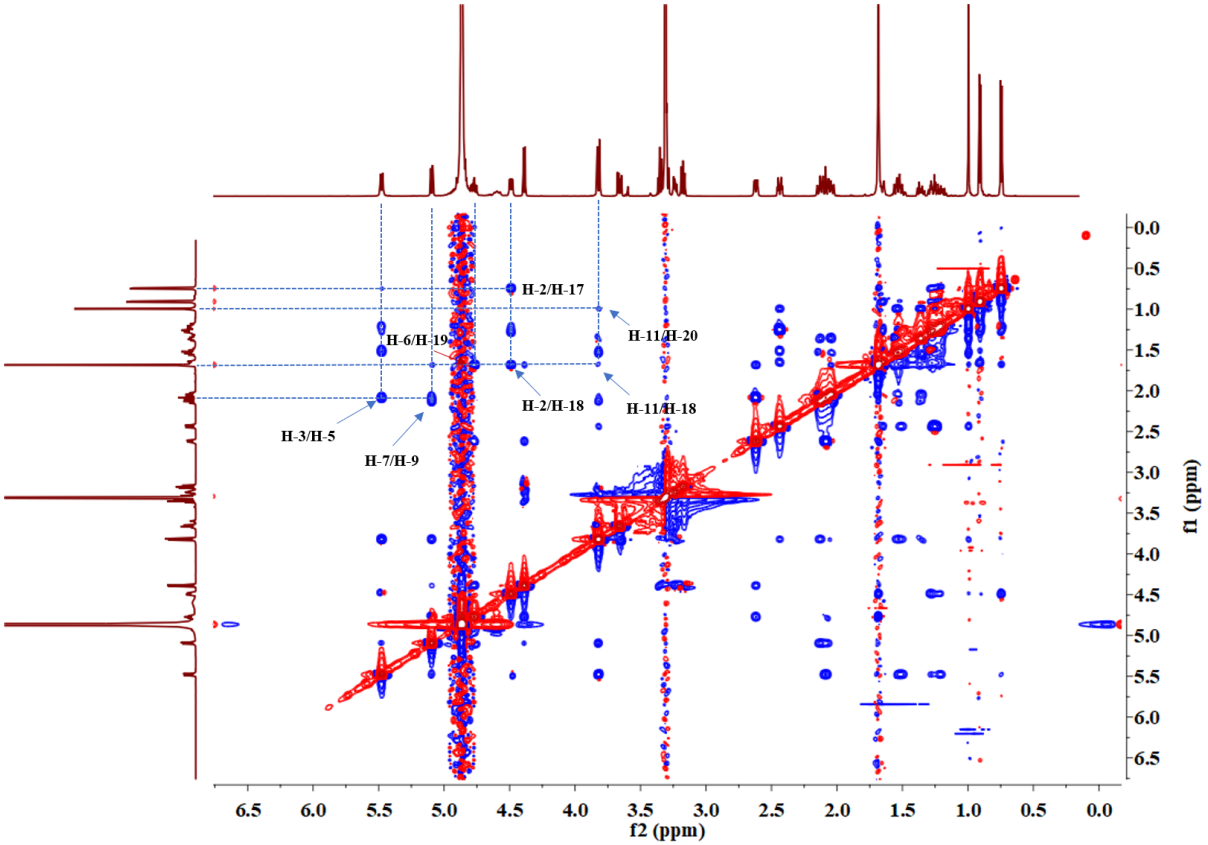

Figure S8: ROESY spectrum of **1**

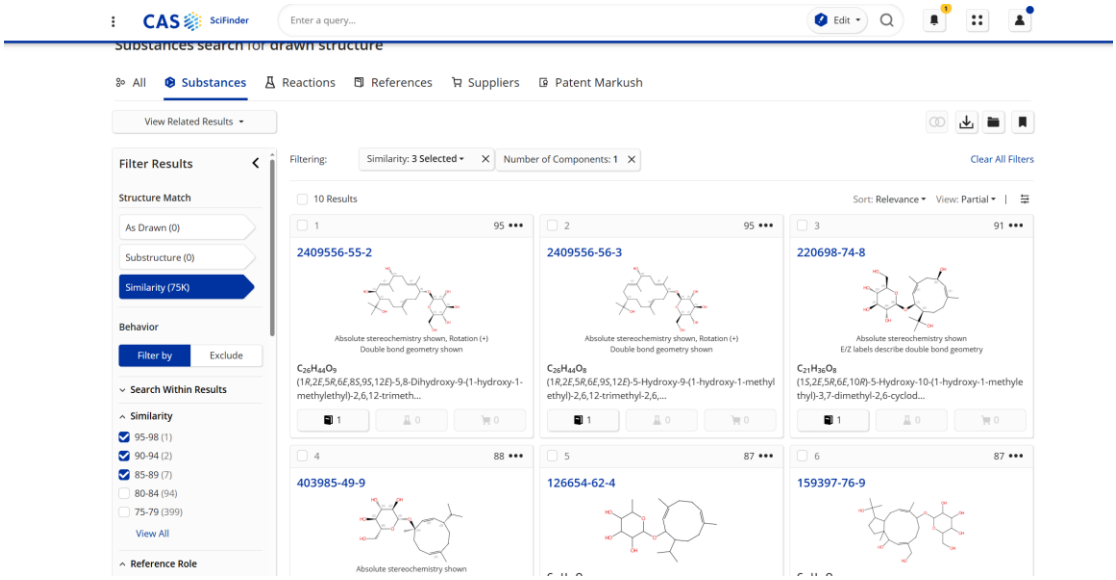

Figure S9: Scifinder search results of **1**

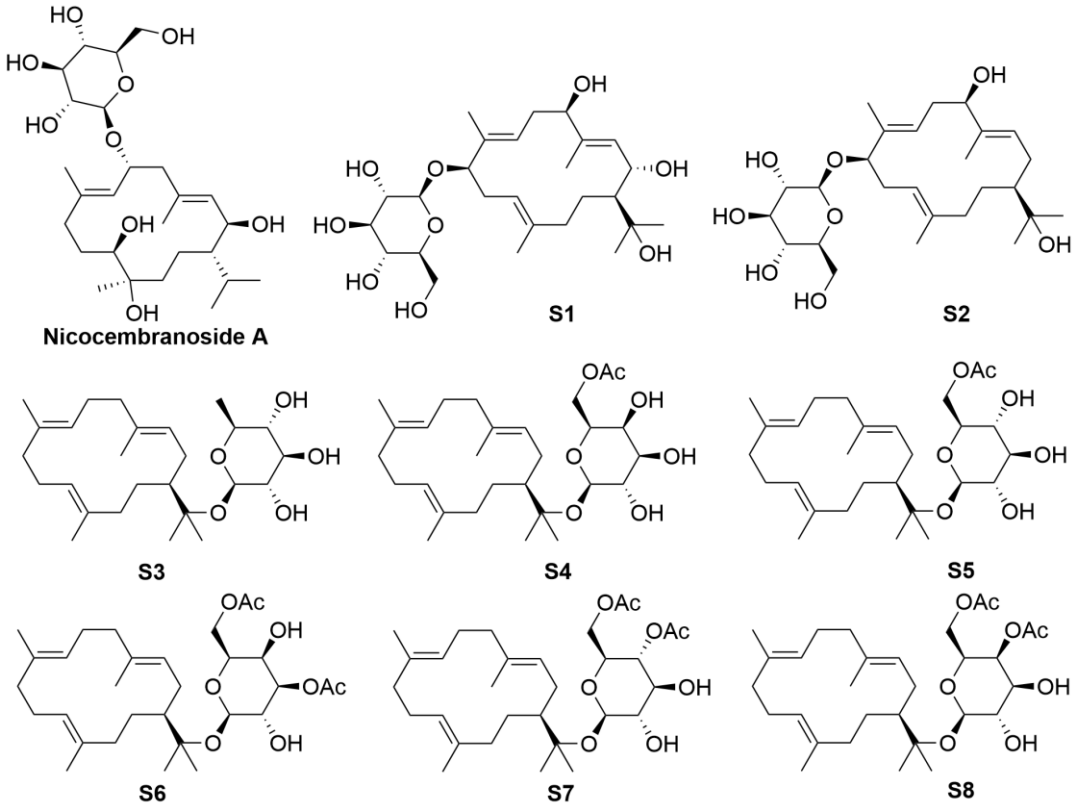

Figure S10: Structures of Nicocembranoside A and eight reported cembrane glycosides

Table S1. ^{1}H- and ^{13}C-NMR spectroscopic data of eight reported cembrane glycosides (δ, ppm; J, Hz)

Position	S1[a]		S2[b]		S3[c]		S4[c]	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
1	1.57, dd (9.6, 2.6)	53.7	1.55, m	48.7	1.50, m	47.6	1.45, m	47.7
2	4.64, t (9.6)	70.5	2.28, m 2.20, m	28.1	2.10, m 1.90, m	27.9	2.16, m 1.88, m	28.1
3	5.41, d (9.6)	132.6	5.68, d (7.7)	129.3	5.07, t (5.7)	126.7	5.07, t (6.2)	125.9
4		140.3		136.3		133.8		133.5
5	4.12, dd (11.1, 3.8)	79.1	4.40, d (11.0)	78.7	2.00-2.20, m	38.3	2.06, m	38.8
6	2.63, dd (14.5, 11.1) 2.26, d (14.5)	34.0	2.85, m 2.57, m	34.0	2.00-2.20, m	24.6	2.16, m	24.7
7	5.05, d (10.6)	125.1	5.17, d (9.9)	126.0	4.90, t (6.4)	125.8	4.93, t (6.0)	125.7
8		136.9		135.4		133.4		133.1
9	3.86, dd (11.1, 4.2)	88.5	4.23, t (7.0)	87.6	2.00-2.20, m	39.2	1.98, m	37.8
10	2.52, m 2.18, dt (12.5, 7.6)	30.3	2.82, m 2.38, m	31.0	2.05-2.15, m	24.0	2.10, m	24.0
11	4.74, t (7.6)	120.3	4.92, m	121.5	4.74, t (6.0)	125.4	4.99, t (6.0)	125.0
12		138.5		136.7		133.2		134.2
13	1.95, dd (11.2, 5.2) 1.90, d (11.2)	38.5	2.24, m 2.14, m	37.6	2.00-2.10, m	37.5	2.00, m	39.4
14	1.52, m 1.32, br s	28.6	1.74, m 1.40, m	28.9	1.25, m 1.60, m	27.7	1.28, m 1.65, m	28.2
15		75.5		72.8		81.5		81.4
16	1.28, s	29.9	1.37, s	28.1	1.17, s	22.1	1.22, s	23.8
17	1.34, s	26.0	1.38, s	28.8	1.28, s	26.2	1.22, s	24.8
18	1.70, s	10.5	1.81, s	10.7	1.55, s	15.5	1.56, s	15.6
19	1.67, s	11.3	1.82, s	11.7	1.56, s	15.9	1.56, s	15.3
20	1.61, s	16.0	1.59, s	15.6	1.54, s	15.4	1.56, s	15.5
1′	4.30, d (7.7)	103.2	4.90, d (7.7)	103.5	4.43, d (7.6)	96.6	4.40, d (7.2)	97.2
2′	3.20, d (7.7)	75.3	4.01, t (7.7)	75.8	3.30, dd (7.6, 9.0)	74.3	3.56, dd (7.2, 9.4)	72.2
3′	3.37, d (9.7)	78.3	4.24, m	78.4	3.50, t (9.0)	76.4	3.61, d (9.4)	73.3
4′	3.31, m	71.6	4.21, m	72.0	3.25, t (9.0)	75.3	3.89, d (2.2)	68.3
5′	3.19, d (8.0)	77.8	3.81, m	79.0	3.35, dd (6.1, 9.0)	71.3	3.65, t (6.4)	71.9
6′	3.81, d (11.8) 3.67, dd (11.8, 5.3)	62.7	4.40, d (11.0) 4.27, dd (11.0, 5.0)	63.1	1.30, d (6.1)	17.8	4.32, dd (3.4, 6.9)	62.8
1″							2.06, s	20.8
2″								171.0
1‴								
2‴								

[a] recorded in CD_3OD ; [b] recorded in C_5D_5N ; [c] recorded in $CDCl_3$.

Table S1-continued. ^{1}H- and ^{13}C-NMR spectroscopic data of eight reported cembrane glycosides (δ, ppm; J, Hz)

Position	S5[c]		S6[c]		S7[c]		S8[c]	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
1	1.45, m	47.8	1.45, m	47.8	1.46, m	47.7	1.47, m	47.7
2	2.19, m 1.87, m	28.2	2.14, m 1.87, m	28.2	2.14, m 1.87, m	28.2	2.17, m 1.88, m	28.2
3	5.06, t (6.5)	125.9	5.06, t (6.3)	125.8	5.07, t (6.6)	125.8	5.07, t (6.6)	125.8
4		133.4		133.5		133.5		133.6
5	2.12, m	38.9	2.07, m	38.9	2.08, m	38.8	2.08, m	38.8
6	2.17, m	24.7	2.10, m	24.7	2.14, m	24.7	2.13, m	24.7
7	4.91, t (6.0)	125.7	4.94, t (6.6)	125.7	4.93, t (6.6)	125.7	4.93, t (6.7)	125.7
8		133.0		133.1		133.1		133.1
9	1.95, m	37.9	1.97, m	37.9	2.00, m	37.8	2.00, m	37.8
10	2.10, m	24.0	2.06, m	24.0	2.10, m	24.0	2.08, m	24.0
11	4.99, t (6.1)	124.8	4.99, t (6.4)	125.0	5.00, t (6.9)	125.1	5.00, t (6.4)	125.0
12		134.3		134.2		134.1		134.1
13	2.02, m	39.4	1.99, m	39.4	2.00, m	39.4	2.03, m	39.4
14	1.27, m 1.63, m	28.2	1.22, m 1.62, m	28.2	1.24, m 1.62, m	28.3	1.23, m 1.61, m	28.2
15		81.4		81.7		81.6		81.6
16	1.21, s	24.1	1.22, s	23.8	1.22, s	24.0	1.22, s	23.8
17	1.21, s	24.6	1.23, s	24.8	1.22, s	24.5	1.23, s	24.8
18	1.54, s	15.6	1.54, s	15.6	1.56, s	15.6	1.56, s	15.6
19	1.54, s	15.3	1.56, s	15.3	1.56, s	15.3	1.56, s	15.3
20	1.54, s	15.5	1.54, s	15.6	1.56, s	15.5	1.56, s	15.6
1′	4.43, d (7.6)	96.8	4.51, d (7.8)	97.1	4.45, d (7.8)	96.7	4.44, d (7.8)	97.2
2′	3.32, d (8.4)	73.9	3.45, t (9.0)	72.2	3.41, t (8.7)	74.5	3.71, dd (7.6, 9.6)	72.0
3′	3.54, d (8.9)	76.5	4.93, dd (3.3, 9.3)	78.0	3.68, t (9.3)	74.7	3.45, dd (3.6, 9.7)	72.3
4′	3.38, d (9.1)	70.5	3.49, s	69.7	4.87, t (9.9)	70.9	5.30, dd (0.9, 3.6)	69.1
5′	3.44, ddd (2.6,5.5,8.9)	73.5	3.50, s	73.9	3.59, ddd (2.7, 6.0, 9.7)	71.6	3.81, dt (1.2, 6.9)	70.8
6′	4.33, dd (5.2,12.0) 4.29, dd (1.9,12.0)	63.8	4.34, s	63.5	4.10, dd (2.4, 12.0) 4.19, dd (6.0, 12.0)	62.8	4.11, s 4.13, s	62.1
1″	2.07, s	20.8	2.16, s	21.0	2.12, s	20.9	2.14, s	20.8
2″		171.4		172.4		170.6		171.1
1‴			2.08, s	20.8	2.06, s	20.7	2.03, s	20.7
2‴				171.3		170.7		170.5