

Supporting Information

Rec. Nat. Prod. 20:3 (2026):e25113732

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

Jun-Zhang Wu¹, Bao-Min Lin¹, Ping-Zhang Yao¹, Cui-Ling Chen¹, Miao Liang², Ya-Ke Luo², Peng-Fei Yang^{2*} and Jun-Ping Gu^{1*}

¹*Technology Center, China Tobacco Guangdong Industrial Co., Ltd., Guangzhou 510000, People's Republic of China*

²*College of Tobacco Science and Engineering, Zhengzhou University of Light Industry, Zhengzhou 450000, People's Republic of China*

Table of Contents	Page
Figure S1: HRESIMS spectrum of 1	2
Figure S2: ¹ H NMR (600 MHz, MeOH- <i>d</i> ₄) spectrum of 1	3
Figure S3: ¹³ C NMR (150 MHz, MeOH- <i>d</i> ₄) spectrum of 1	4
Figure S4: HSQC spectrum of 1	5
Figure S5: Enlarged HSQC spectrum of 1	6
Figure S6: ¹ H- ¹ H COSY spectrum of 1	7
Figure S7: HMBC spectrum of 1	8
Figure S8: ROESY spectrum of 1	9
Figure S9: Scifinder search results of 1	10
Figure S10: Structures of Nicocembranoside A and eight reported cembrane glycosides	11
Table S1: NMR spectroscopic data of eight reported cembrane glycosides	12-13

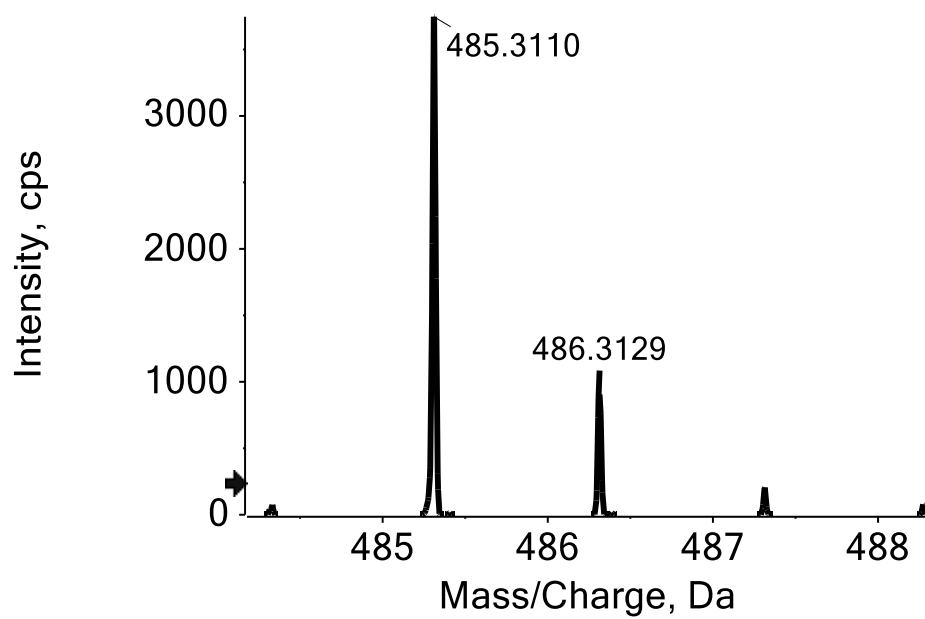


Figure S1: HRESIMS spectrum of **1**

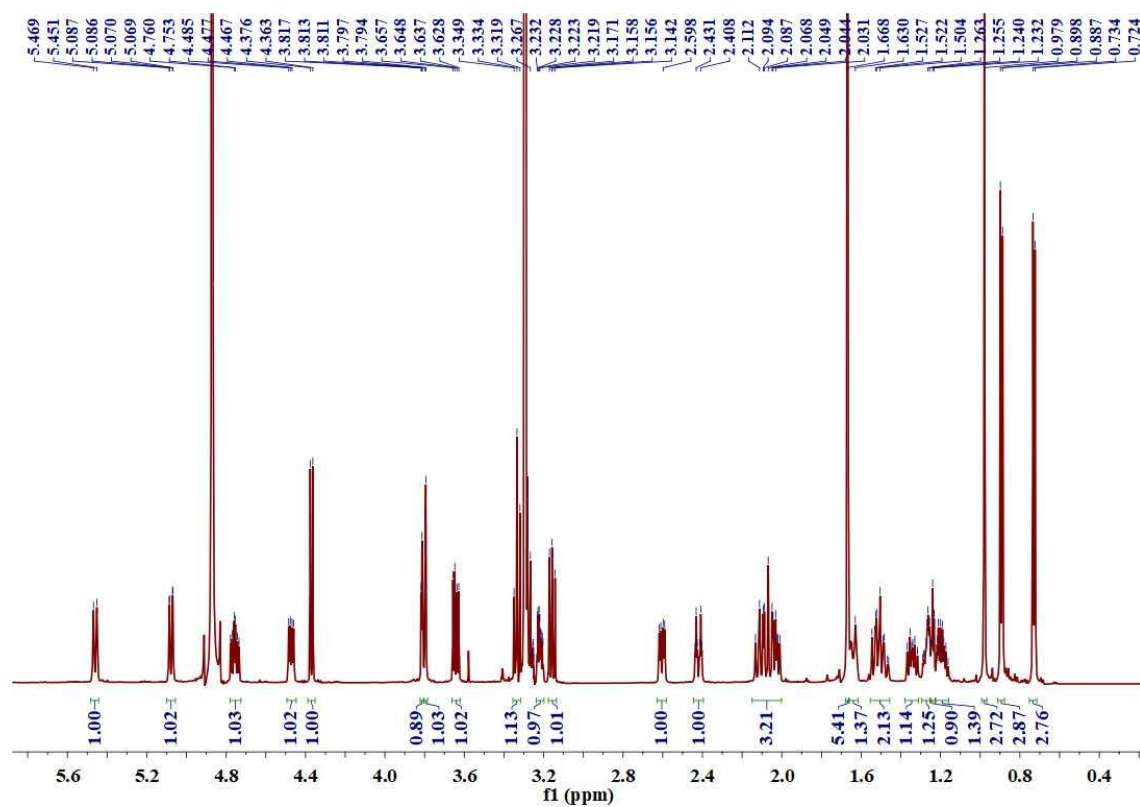


Figure S2: ^1H NMR (600 MHz, $\text{MeOH-}d_4$) spectrum of **1**

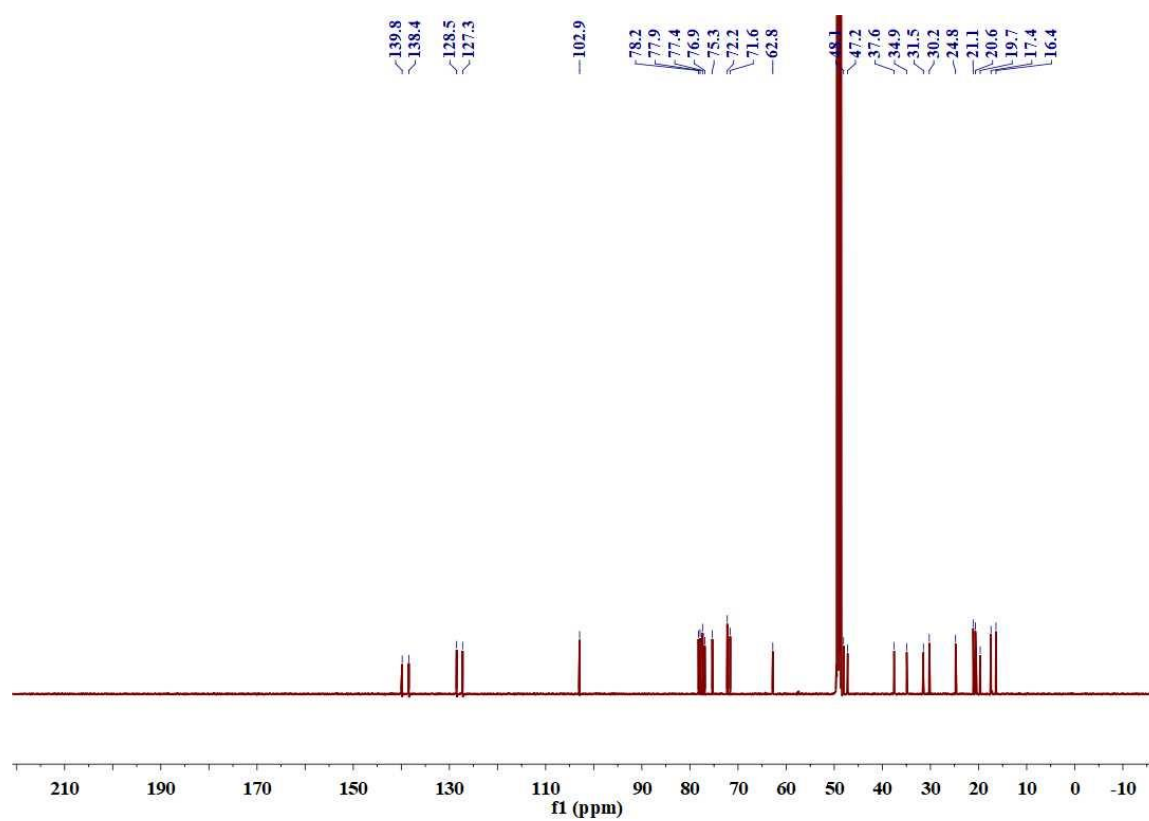


Figure S3: ¹³C NMR (150 MHz, MeOH-*d*₄) spectrum of **1**

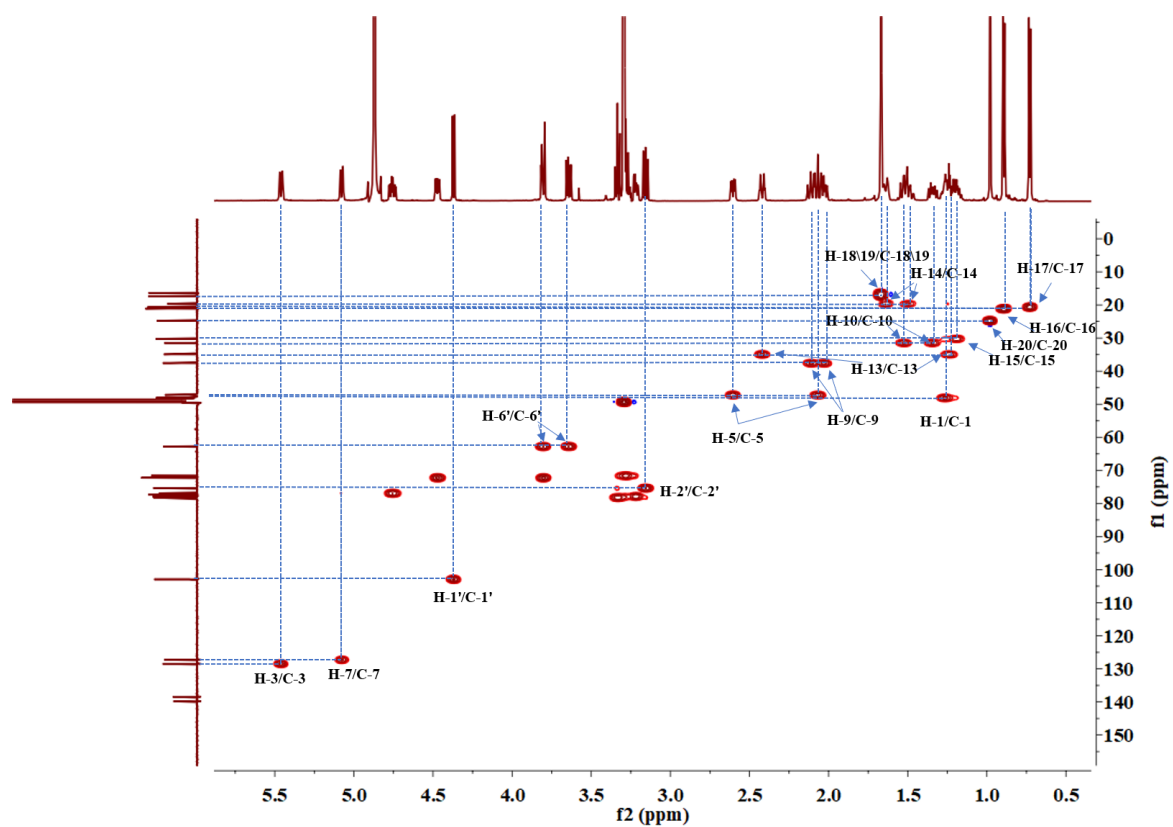


Figure S4: HSQC spectrum of **1**

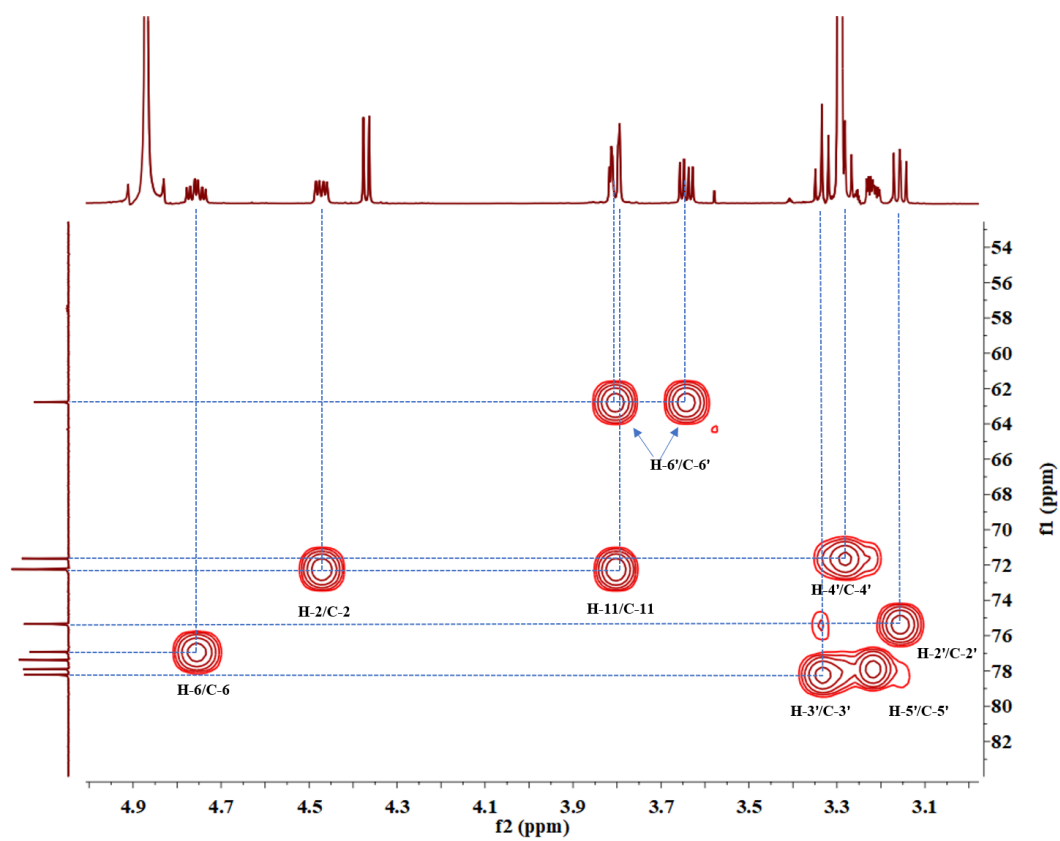


Figure S5: Enlarged HSQC spectrum of **1**

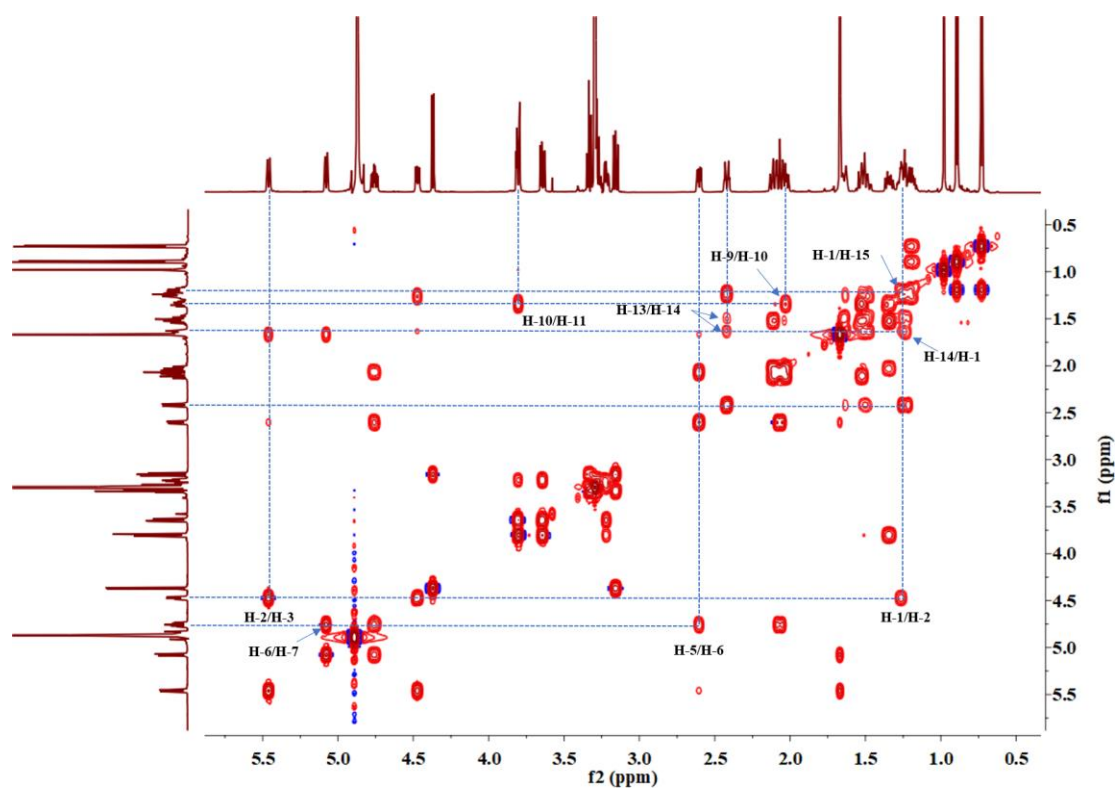


Figure S6: ^1H - ^1H COSY spectrum of **1**

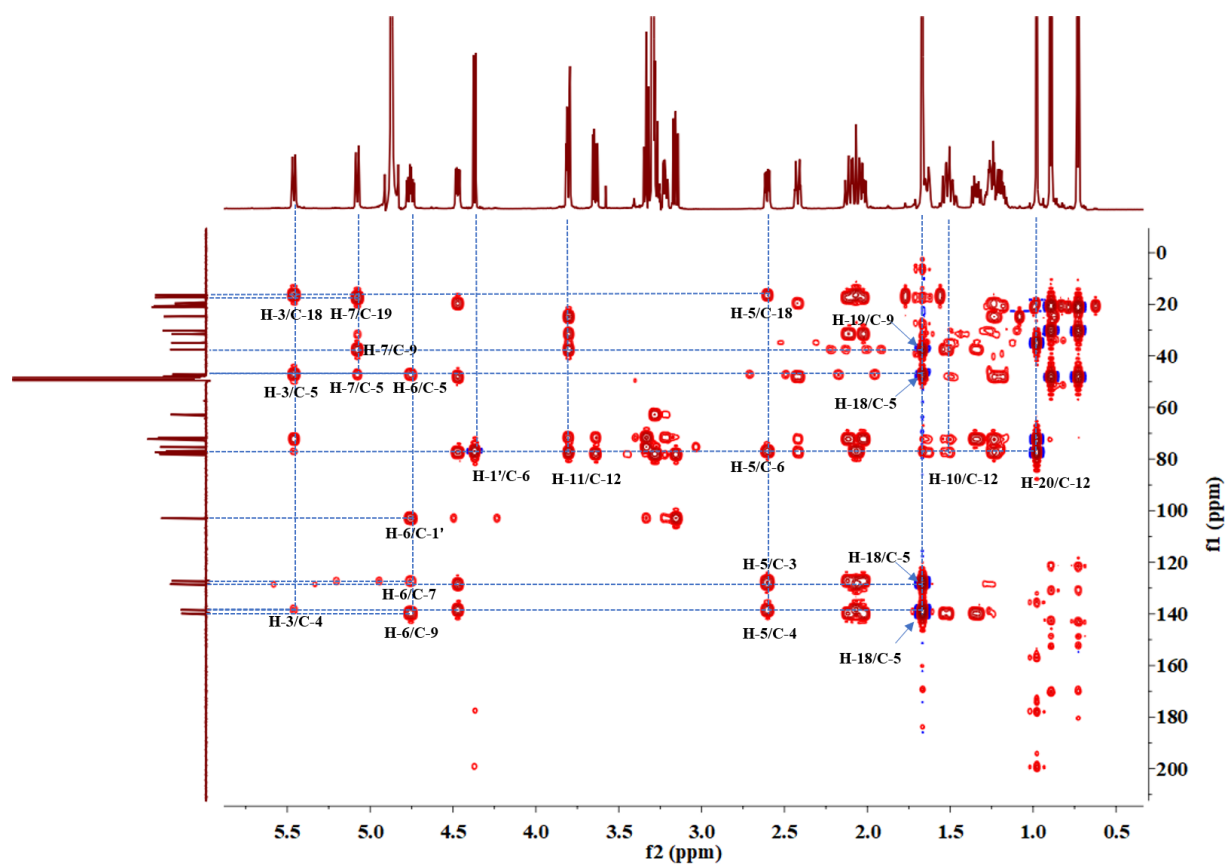


Figure S7: HMBC spectrum of 1

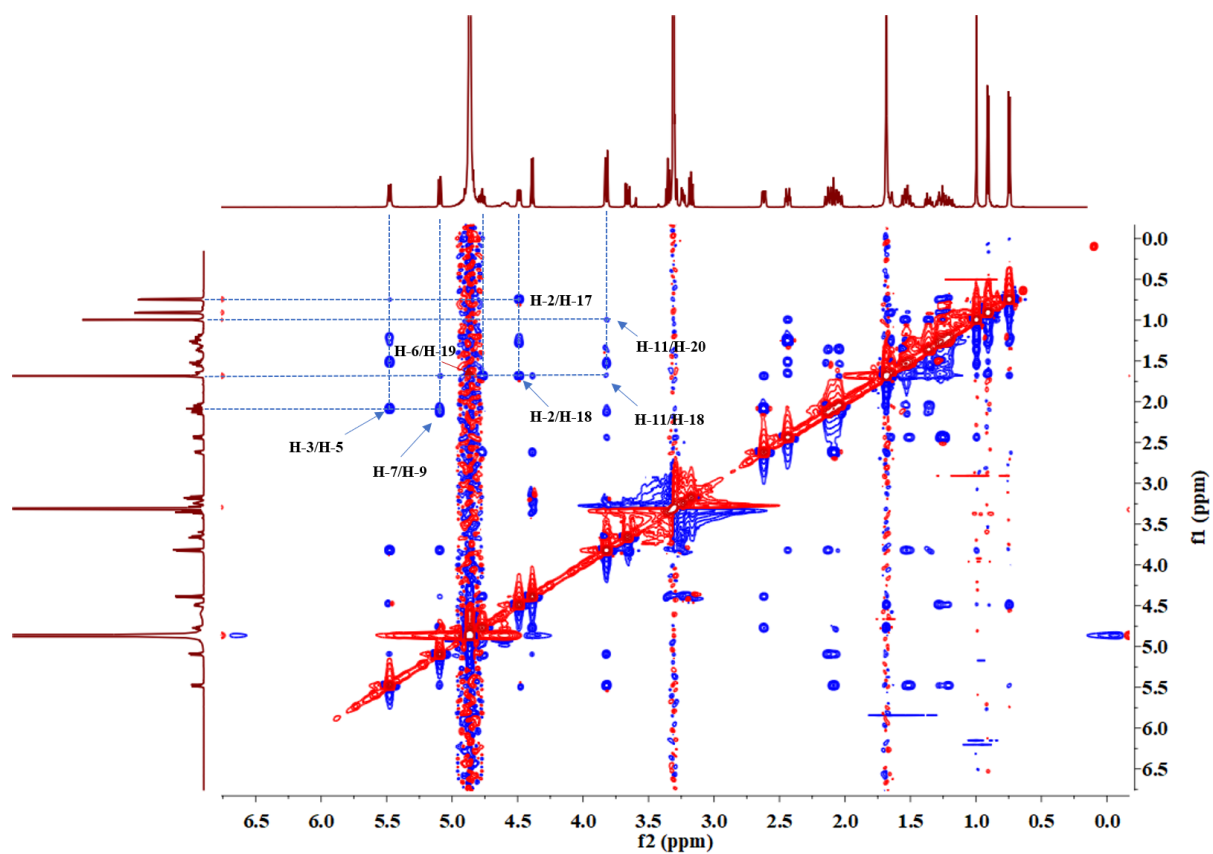


Figure S8: ROESY spectrum of **1**

CAS SciFinder

Enter a query...

Substances search for drawn structure

All Substances Reactions References Suppliers Patent Markush

View Related Results

Filter Results

Structure Match

As Drawn (0)

Substructure (0)

Similarity (75K)

Behavior

Filter by Exclude

Search Within Results

Similarity

95-98 (1)

90-94 (2)

85-89 (7)

80-84 (94)

75-79 (399)

View All

Reference Role

Filtering: Similarity: 3 Selected X Number of Components: 1 X

Clear All Filters

Sort: Relevance View: Partial

10 Results

1 2 3 4 5 6

2409556-55-2 95 ***

2409556-56-3 95 ***

220698-74-8 91 ***

403985-49-9 88 ***

126654-62-4 87 ***

159397-76-9 87 ***

The screenshot displays the CAS SciFinder search results for a chemical structure. The interface includes a search bar at the top, navigation tabs for 'All', 'Substances', 'Reactions', 'References', 'Suppliers', and 'Patent Markush'. The 'Substances' tab is selected. Below the search bar, there are filters for 'Similarity: 3 Selected' and 'Number of Components: 1'. The results are displayed in a grid of six cards, each showing a chemical structure, its name, and associated data. The cards are numbered 1 through 6. The first three cards (1, 2, 3) have a similarity score of 95, while the last three (4, 5, 6) have scores of 88, 87, and 87 respectively. The chemical structures are complex polycyclic compounds with various functional groups. The interface also includes a 'Filter Results' sidebar on the left with options for 'Structure Match', 'Behavior', and 'Search Within Results'. The 'Similarity' filter is expanded, showing a range of similarity scores from 95-98 to 75-79. The 'Reference Role' filter is also visible at the bottom of the sidebar.

Figure S9: Scifinder search results of 1

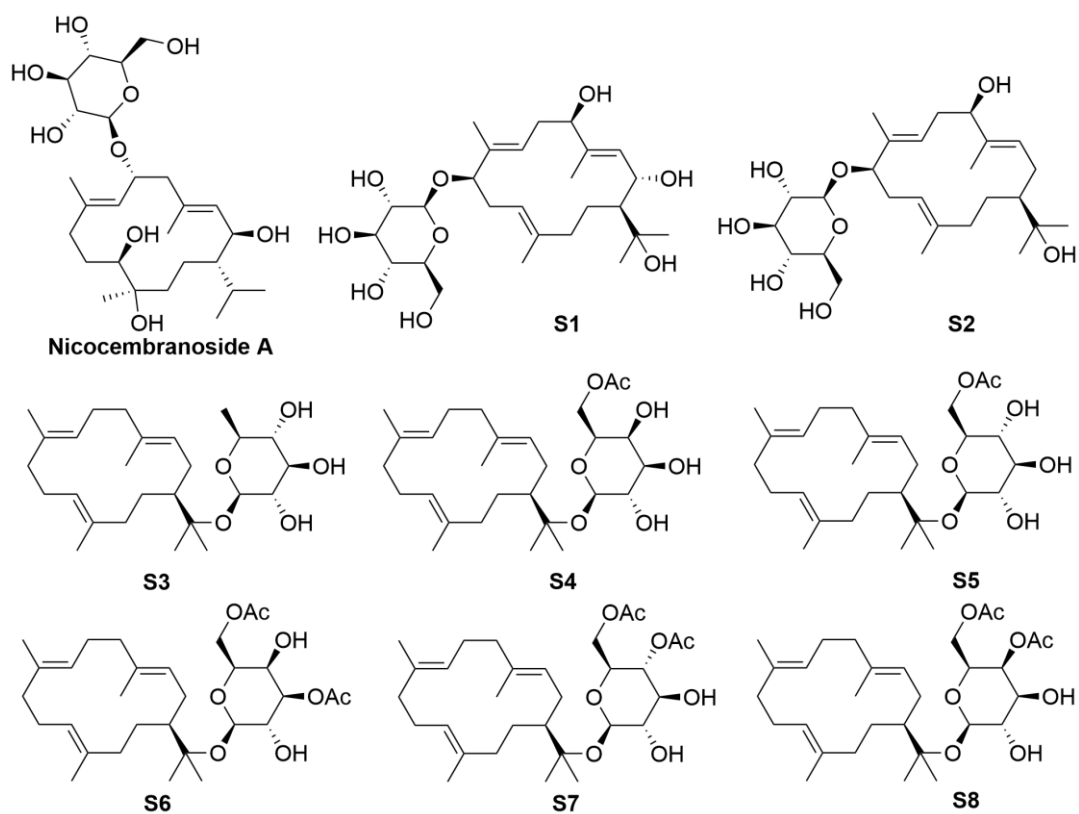


Figure S10: Structures of Nicocembranoside A and eight reported cembrane glycosides

Table S1. ¹H- and ¹³C-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 CD₃OD ; ^b recorded in C₅D₅N ; ^c recorded in CDCl₃ .

Table S1-continued. ¹H- and ¹³C-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