

Supporting Information

Rec. Nat. Prod. 18:4 (2024) 446-451

Two Cationic Indole Alkaloids from *Ophiorrhiza japonica* and Their Xanthine Oxidase Inhibitory Activity

Yu He ¹, Fan Xu ¹, Chun Tian ¹, Hong-Lian Ai ¹, Bao-Bao Shi, ^{1,2,*}
and Ji-Kai Liu ^{1,2,*}

¹*School of Pharmaceutical Sciences, South-Central MinZu University, Wuhan 430074,
People's Republic of China*

²*International Cooperation Base for Active Substances in Traditional Chinese Medicine in
Hubei Province, School of Pharmaceutical Sciences, South-Central Minzu University*

Table of Contents	page
Figure S1: HRESIMS spectrum of 1	2
Figure S2: ¹ H NMR spectrum of 1	3
Figure S3: Enlarged ¹ H NMR spectrum of 1	3
Figure S4: ¹³ C NMR spectrum of 1	4
Figure S5: Enlarged ¹³ C NMR spectrum of 1	4
Figure S6: HSQC spectrum of 1	5
Figure S7: HMBC spectrum of 1	6
Figure S8: Enlarged HMBC spectrum of 1	6
Figure S9: ¹ H- ¹ H COSY spectrum of 1	7
Figure S10: ROESY spectrum of 1	8
Figure S11: X-ray structure of compound 1	9
Figure S12: The Scifinder similarity report for 1	10
Figure S13: HRESIMS spectrum of 2	11
Figure S14: ¹ H NMR spectrum of 2	12
Figure S15: Enlarged ¹ H NMR spectrum of 2	12
Figure S16: ¹³ C NMR spectrum of 2	13
Figure S17: HSQC spectrum of 2	14
Figure S18: HMBC spectrum of 2	15
Figure S19: ¹ H- ¹ H COSY spectrum of 2	16
Figure S20: ROESY spectrum of 2	17
Figure S21: The Scifinder similarity report for 2	18
Table S1: ¹ H and ¹³ C NMR data for compound 1 and 2	19
Table S2: ¹ H and ¹³ C NMR data for compound 1 and Ophiorrhizine	20

*Corresponding author(s): shibb0505@163.com (B. B. Shi); liujikai@mail.scuec.edu.cn (J.K. Liu)

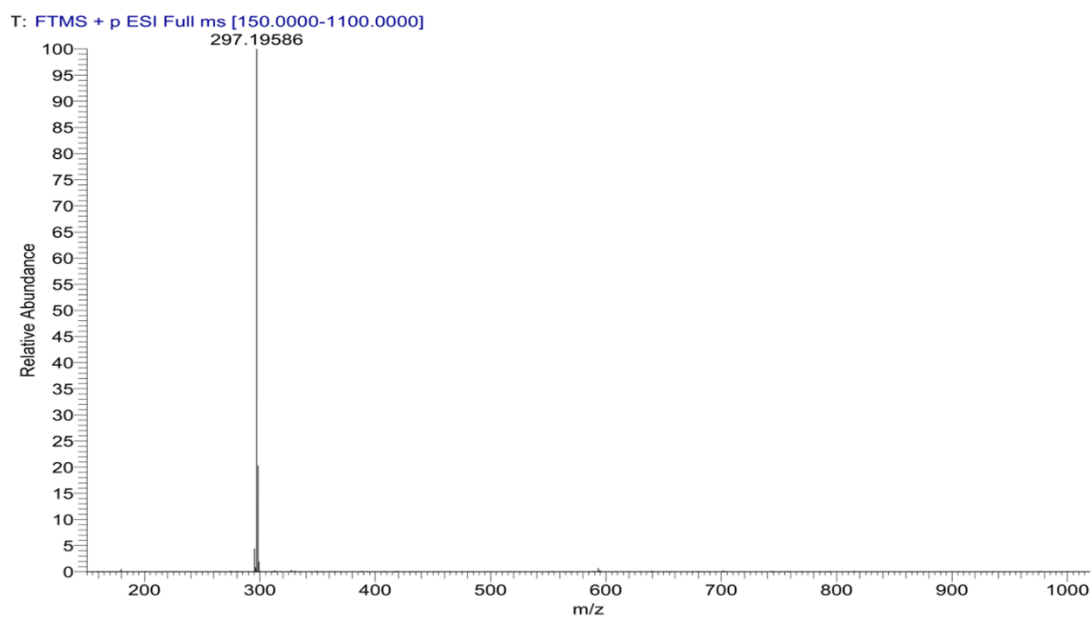


Figure S1: HRESIMS spectrum of 1

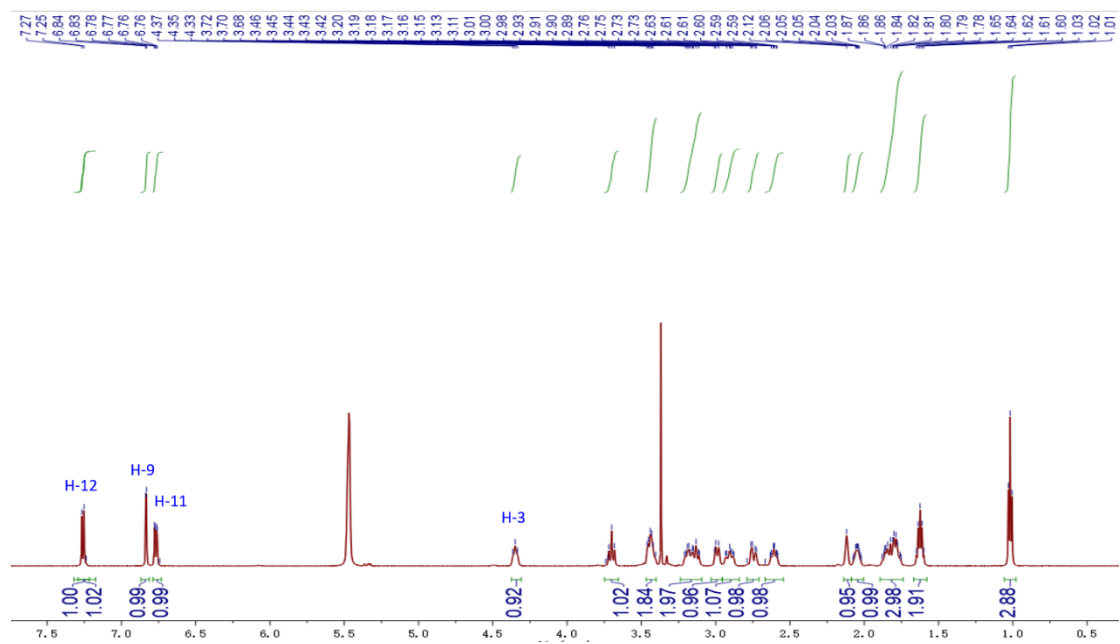


Figure S2: ^1H NMR spectrum of **1**

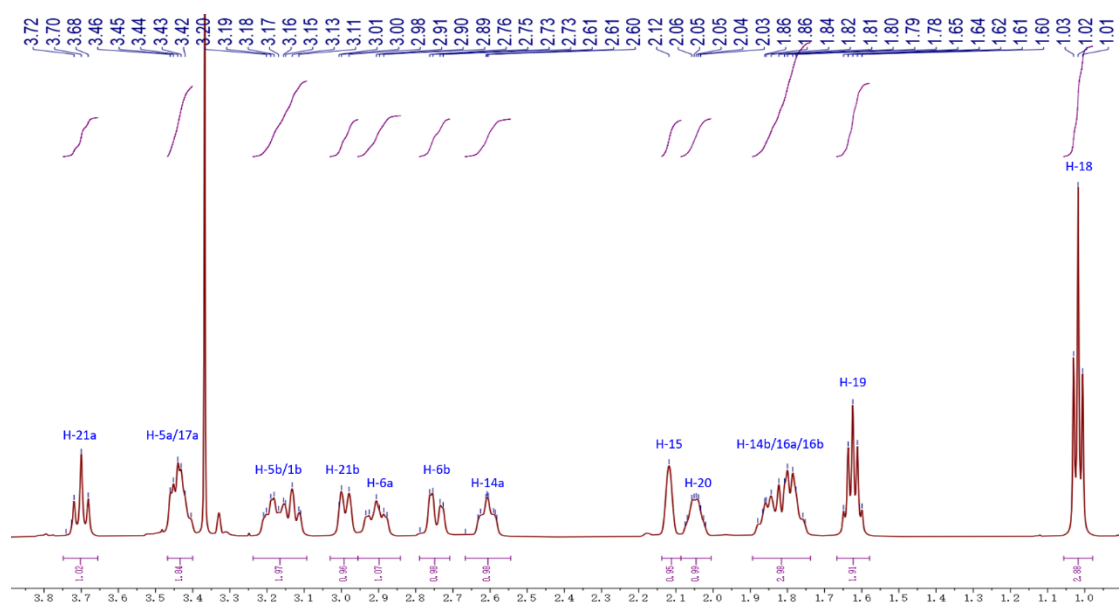


Figure S3: Enlarged ^1H NMR spectrum of **1**

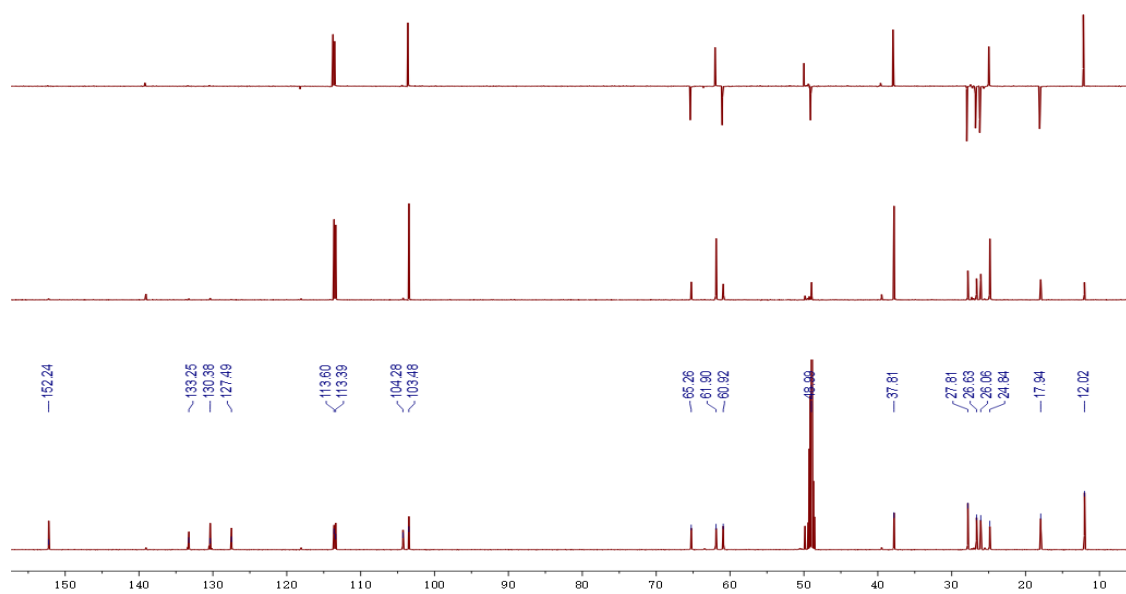


Figure S4: ^{13}C NMR spectrum of **1**

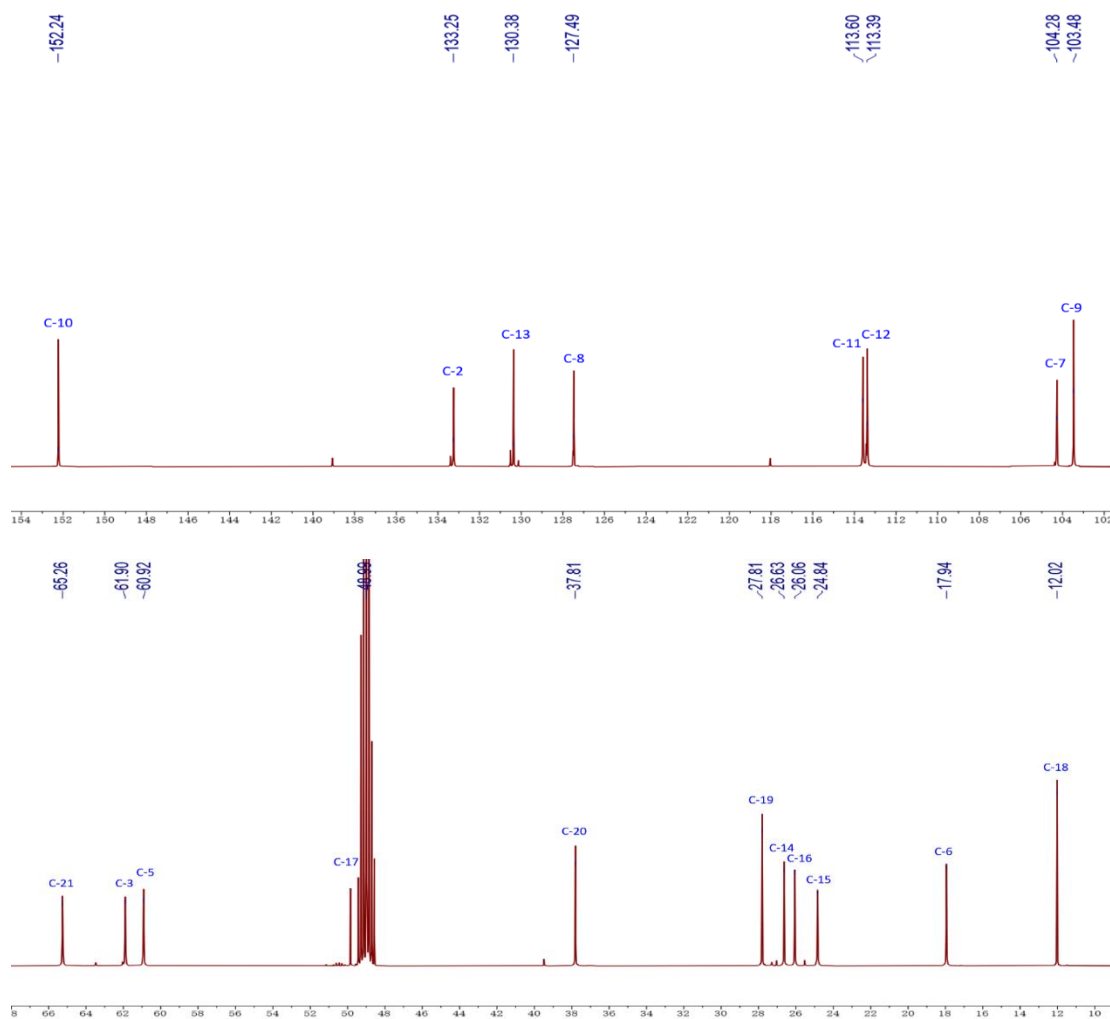


Figure S5: Enlarged ^{13}C NMR spectrum of **1**

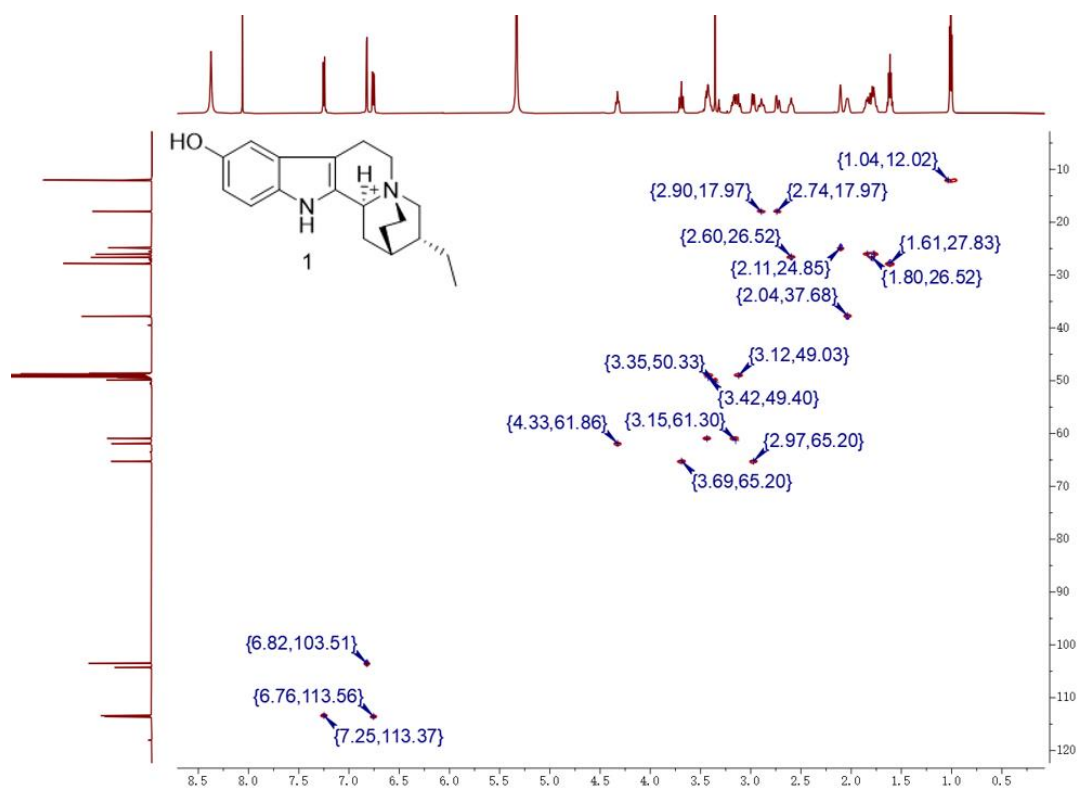


Figure S6: HSQC spectrum of **1**

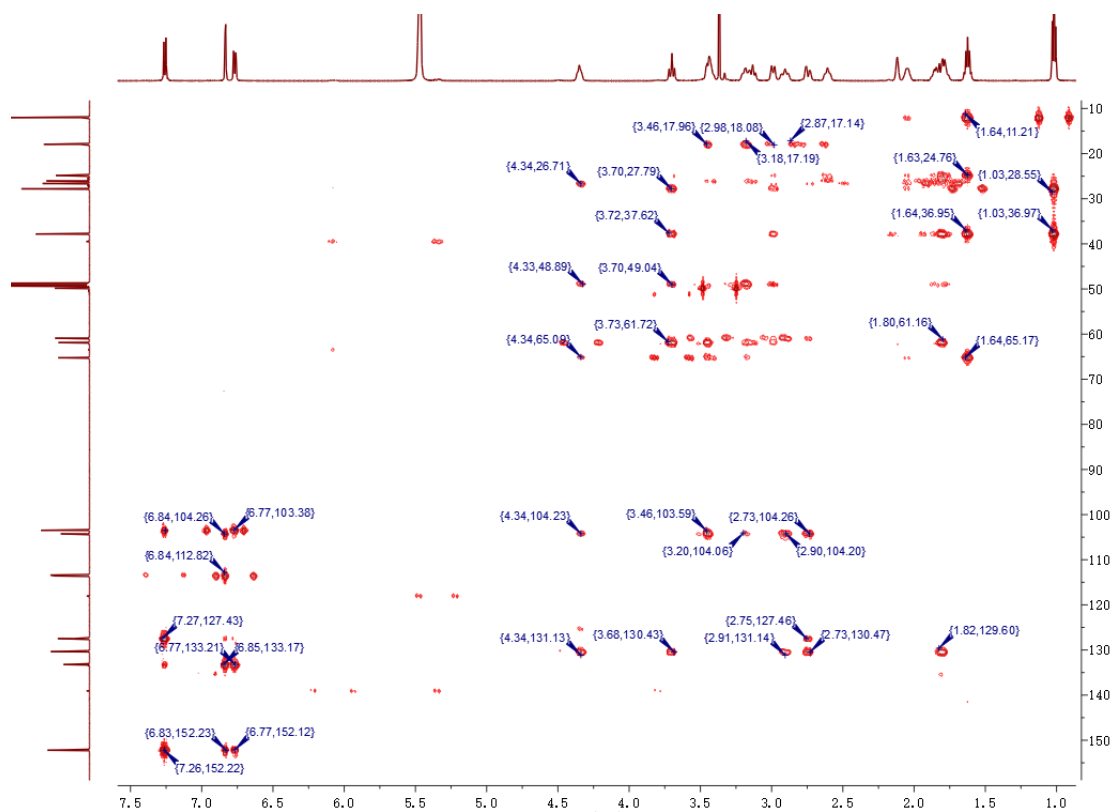


Figure S7: HMBC spectrum of **1**

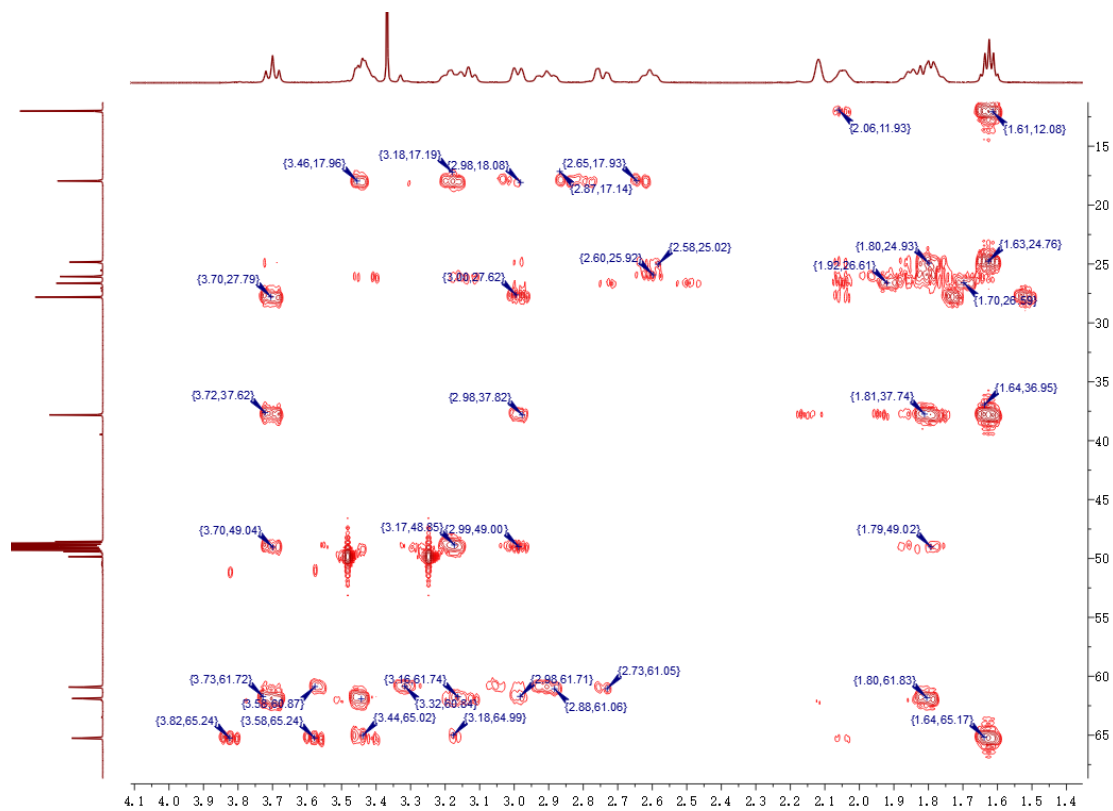


Figure S8: Enlarged HMBC spectrum of **1**

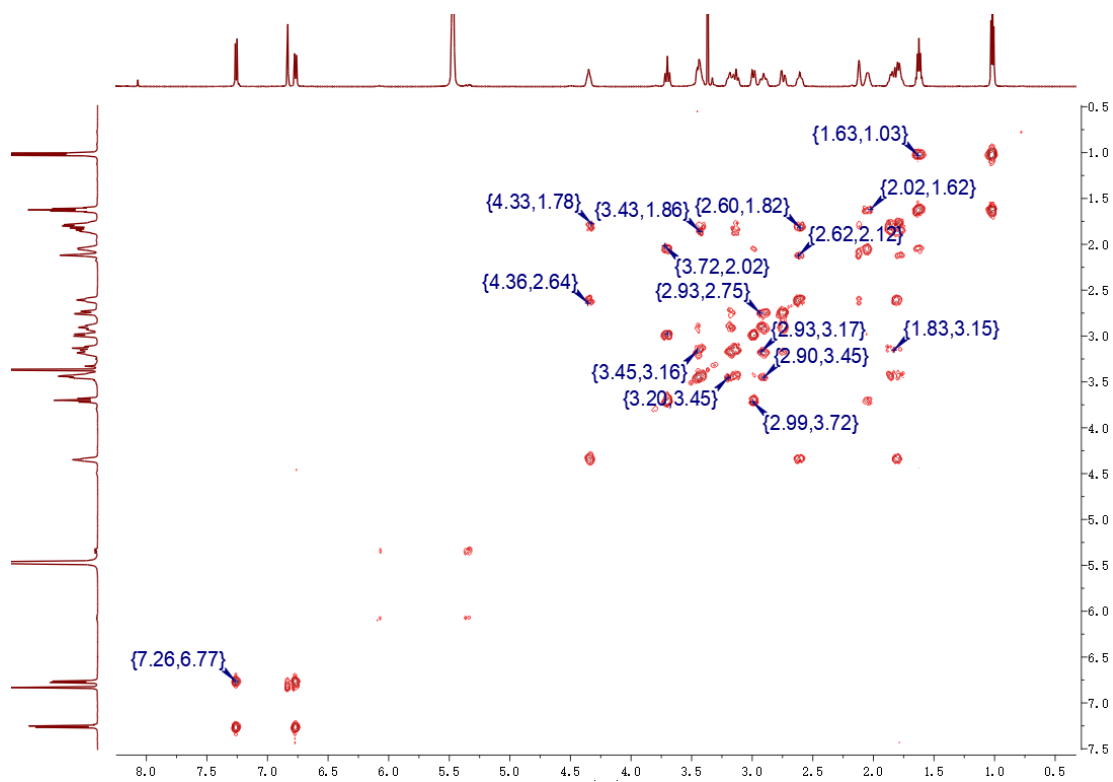


Figure S9: ^1H - ^1H COSY spectrum of **1**

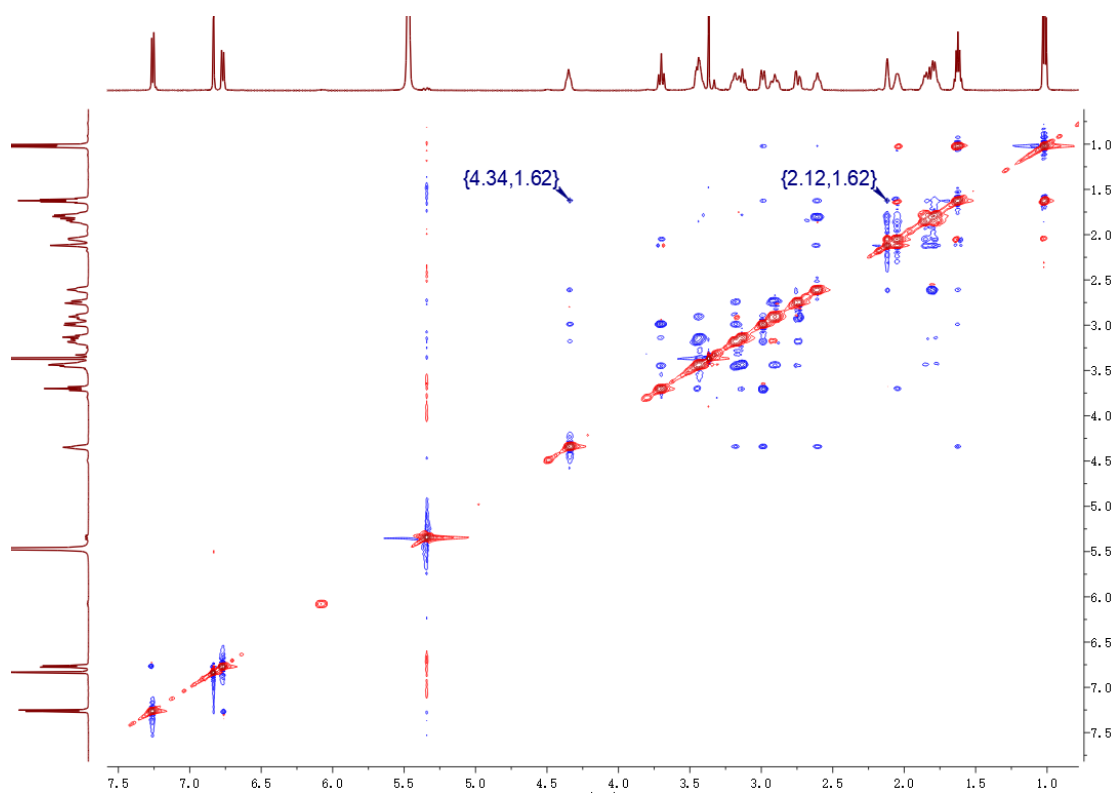


Figure S10: ROESY spectrum of 1

Crystal data for lzob20: $C_{19}H_{25}N_2O \cdot CHO_2 \cdot 4(H_2O)$, $M = 414.49$, $a = 8.1868(3) \text{ \AA}$, $b = 12.3654(4) \text{ \AA}$, $c = 20.9849(7) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 2124.37(13) \text{ \AA}^3$, $T = 150.(2) \text{ K}$, space group $P212121$, $Z = 4$, $\mu(\text{Cu K}\alpha) = 0.809 \text{ mm}^{-1}$, 21387 reflections measured, 4015 independent reflections ($R_{int} = 0.0625$). The final R_I values were 0.0303 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0784 ($I > 2\sigma(I)$). The final R_I values were 0.0331 (all data). The final $wR(F^2)$ values were 0.0801 (all data). The goodness of fit on F^2 was 1.053. Flack parameter = 0.02(4).

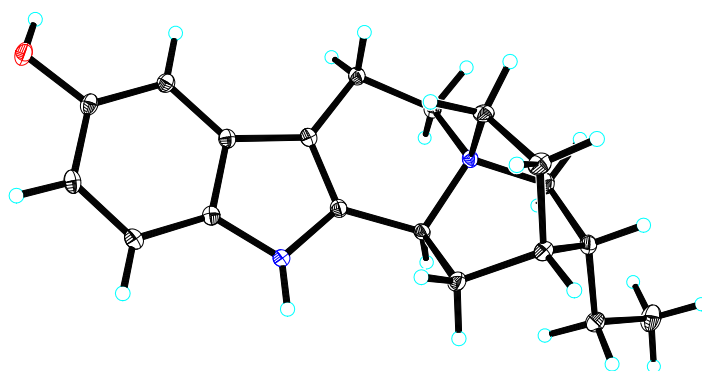
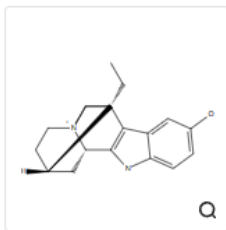


Figure S11: X-ray structure of compound **1**

May 18, 2024

Substances
9:14 PM



As Drawn (0)
Substructure (8)
Similarity (198K)

Rerun Search

Edit Search

Substances search for drawn structure

References Reactions Suppliers

Filtering: Similarity: 4 Selected X Number of Components: 1 X Clear All Filters

203 Results Sort: Relevance View: Partial

Structure Match

As Drawn (0)

Substructure (8)

Similarity (198K)

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Search Within Results

Similarity

- >=99 (1)
- 95-98 (2)
- 90-94 (6)
- 85-89 (194)
- 80-84 (1,779)

View All

Reaction Role

- Product (44)
- Reactant (9)

Item	Count	Similarity	References	Reactions	Suppliers
1	99	214702-40-6	2	0	0
2	97	47257-27-2	0	0	0
3	97	47257-26-1	0	0	0
4	91	2539272-59-6	0	0	1
5	91	2644483-30-5	0	0	1
6	90	2572971-35-6	0	0	1

Chemical structures and names for items 1-6 are shown in the report.

Figure S12: The Scifinder similarity report for 1

LOS-58 #15 RT: 0.20 AV: 1 SB: 10 1.40-1.66 NL: 2.30E9
T: FTMS + p ESI Full lock ms [100.0000-700.0000]

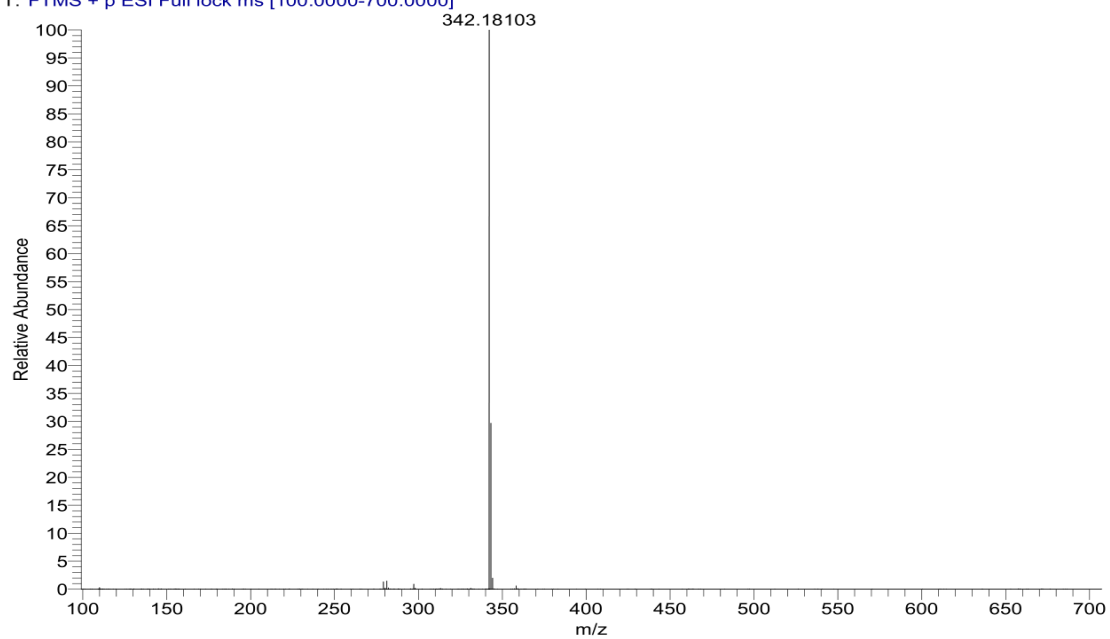


Figure S13: HRESIMS spectrum of 2

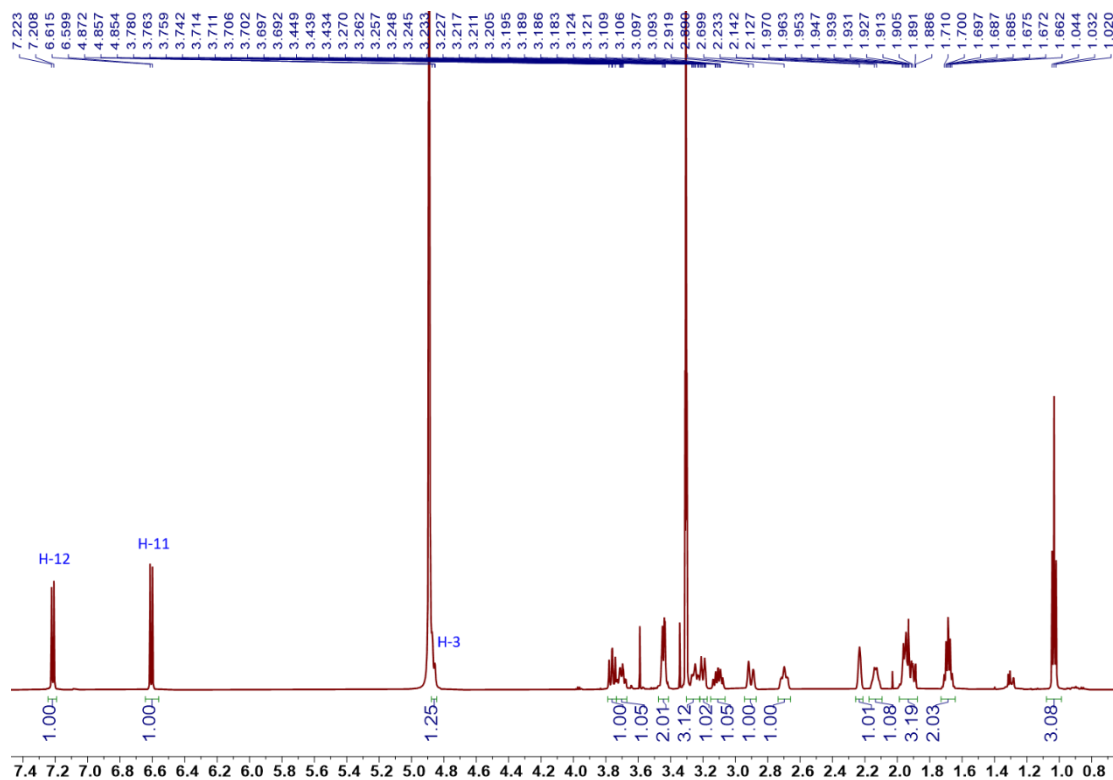


Figure S14: ^1H NMR spectrum of 2

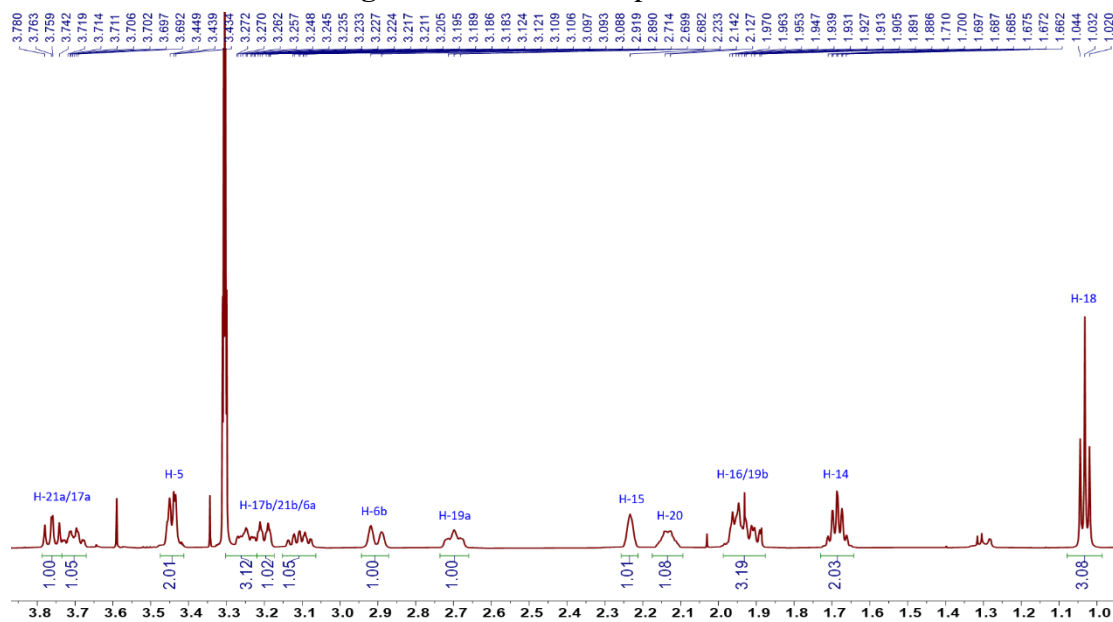


Figure S15: Enlarged ^1H NMR spectrum of 2

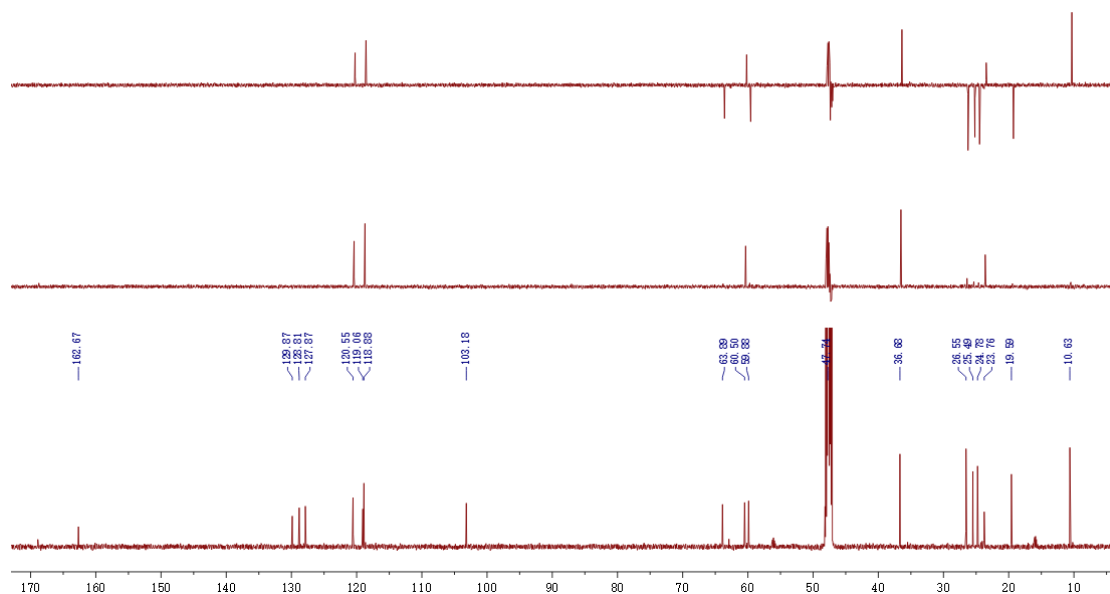


Figure S16: ^{13}C NMR spectrum of **2**

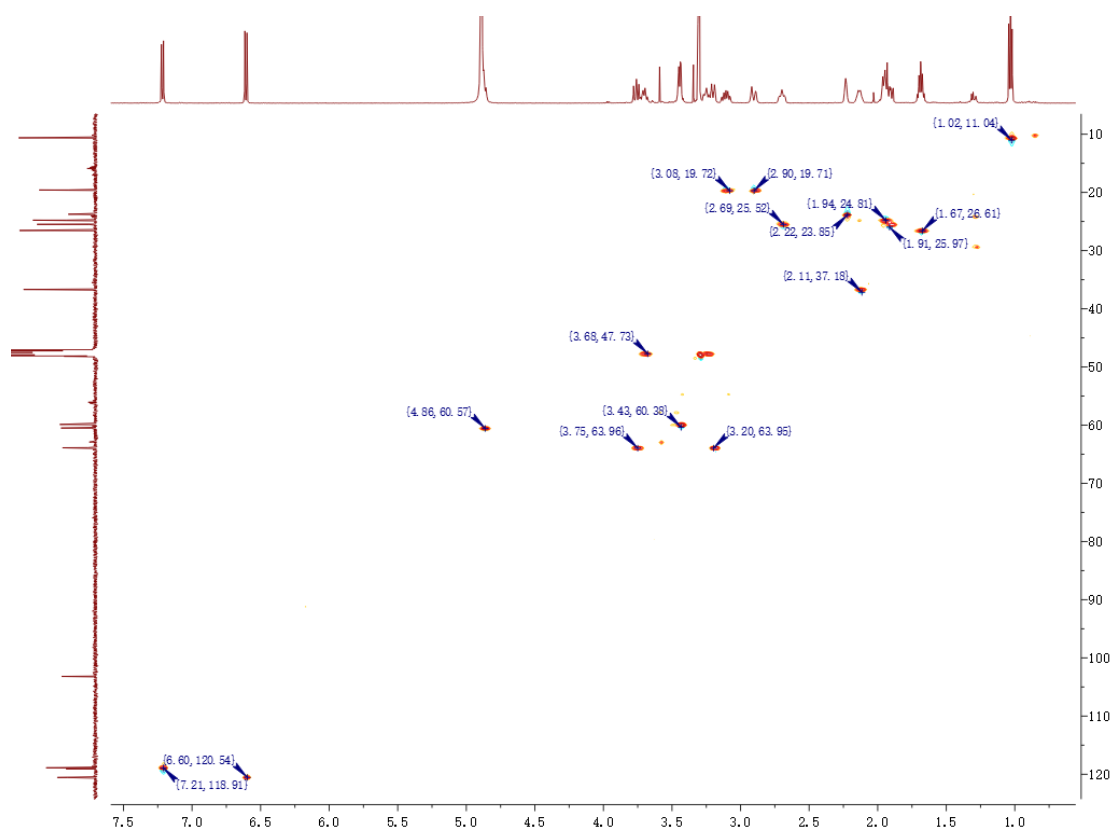


Figure S17: HSQC spectrum of **2**

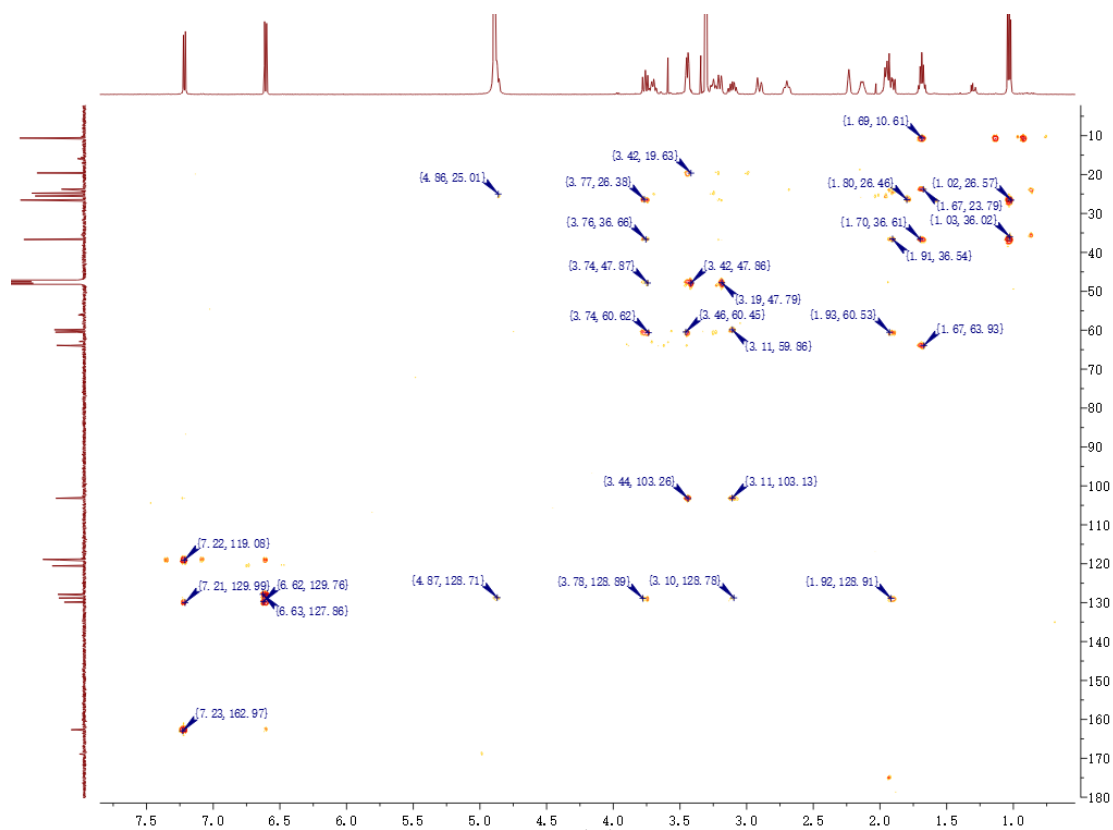


Figure S18: HMBC spectrum of 2

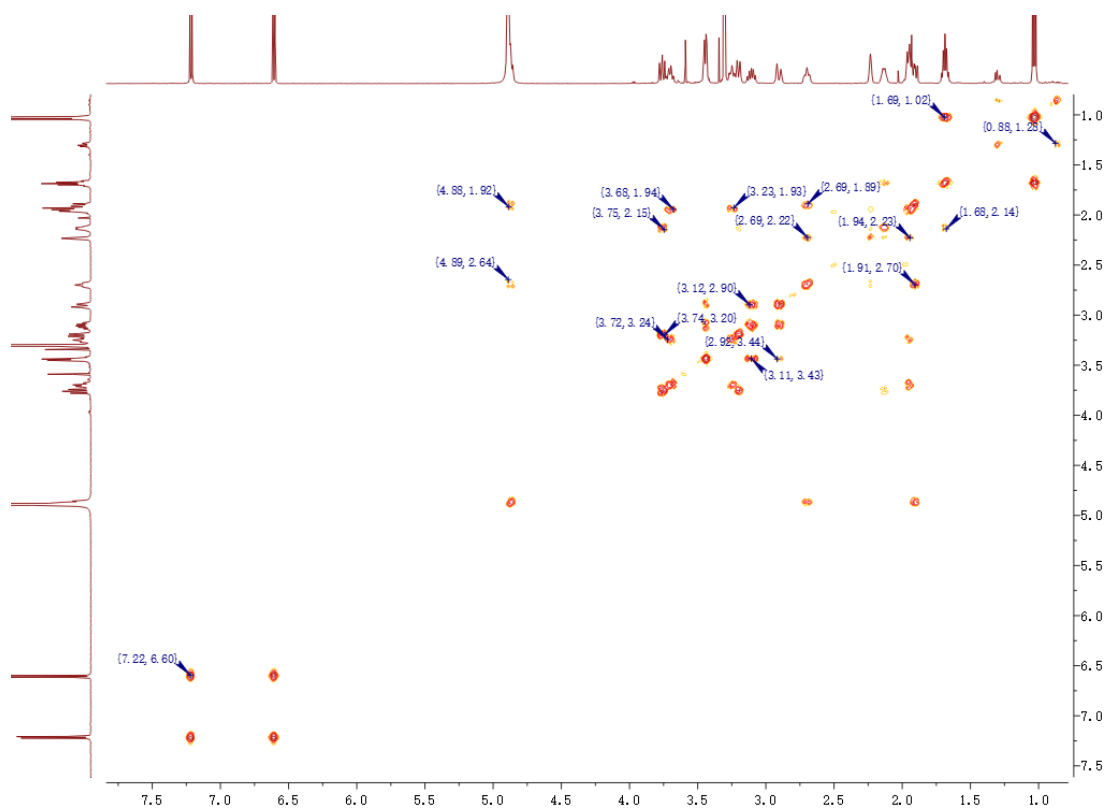


Figure S19: ^1H - ^1H COSY spectrum of **2**

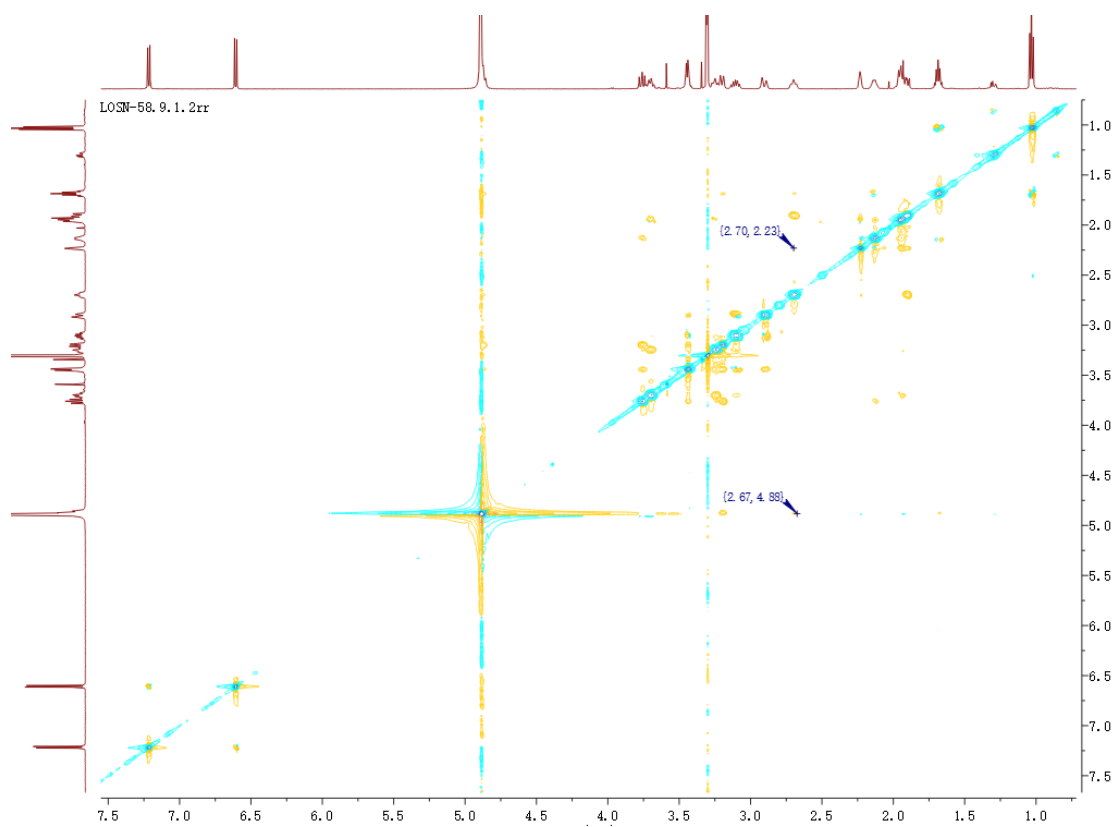
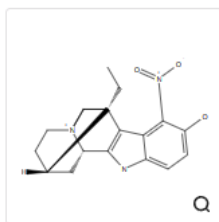


Figure S20: ROESY spectrum of 2

May 18, 2024

Substances
9:16 PM



As Drawn (0)
Substructure (0)
Similarity (52K)

Rerun Search

Edit Search

[Return to Home](#)

Substances search for drawn structure

References - Reactions - Suppliers -

Structure Match

As Drawn (0)

Substructure (0)

Similarity (52K)

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

[Learn more about Chemscape.](#)

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Search Within Results

Similarity

- 80-84 (7)
- 75-79 (171)
- 70-74 (1,745)
- 65-69 (10K)
- 60-64 (36K)

Reaction Role

- Product (17K)
- Reactant (4,526)
- Reagent (10)

Filtering: Number of Components: 1 X [Clear All Filters](#)

48,078 Results Sort: Relevance View: Partial

Result ID	Similarity	Chemical Name	References	Reactions	Suppliers
214403-96-0	85	2.5-Ethanoindolo[2,3-a]quinolizin-5-ium, 11-carboxy-3-ethyl-1,2,3,4,6,7,12,12b-o...	2	0	0
214702-40-6	83	2.5-Ethanoindolo[2,3-a]quinolizin-5-ium, 3-ethyl-1,2,3,4,6,7,12,12b-octahydro-10...	2	0	0
133146-16-4	81	Yohimban-16-methanol, 17-hydroxy-12-nitro-, (16a,17a)-	1	1	0
47257-27-2	81	2.5-Ethanoindolo[2,3-a]quinolizin-5-ium, 3-ethyl-1,2,3,4,6,7,12,12b-octahydro-9-...	0	0	0
47257-26-1	81	2.5-Ethanoindolo[2,3-a]quinolizin-5-ium, 3-ethyl-1,2,3,4,6,7,12,12b-octahydro-9-...	0	0	0
2626998-63-6	80	3-Ethyl-2',3',4',9'-tetrahydro-5'-nitrospiro [cyclopentane-1,1'-[1H]pyrido[3,4-b]...	0	0	1

Figure S21: The Scifinder similarity report for 2

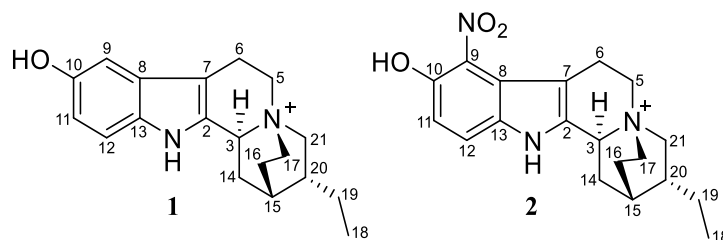


Table S1: ^1H and ^{13}C NMR data for compound **1** and **2**.

1			2	
No.	δ_{H}	δ_{C}	δ_{H}	δ_{C}
2	–	133.3, C	–	130.2, C
3	4.33 t (9.5)	61.9, CH	4.88 m	61.9, CH
5	3.16 m	60.9, CH ₂	3.45 m	61.3, CH ₂
	3.43 dd (11.8, 10.4)			
6	2.74 m	17.9, CH ₂	2.90 d (17.4)	20.9, CH ₂
	2.90 m		3.11 m	
7	–	104.3, C	–	104.6, C
8	–	127.5, C	–	131.3, C
9	6.82 d (2.4)	103.5, CH	–	120.5, C
10	–	152.2, C	–	164.1, C
11	6.76 dd (8.7, 2.4)	113.6, CH	6.61 d (9.0)	122.0, CH
12	7.25 d (8.7)	113.4, CH	7.23 d (9.0)	120.3, CH
13	–	130.4, C	–	129.3, C
14	1.80 m	26.6, CH ₂	1.69 m	27.9, CH ₂
	2.59 m			
15	2.10 s	24.8, CH	2.24 m	25.2, CH
16	1.77 m	26.1, CH ₂	1.96 m	26.2, CH ₂
	1.83 m			
17	3.12 m	49.0, CH ₂	3.25 m	49.1, CH ₂
	3.41 m		3.71 m	
18	1.01 t (7.3)	12.0, CH ₃	1.04 t (7.4)	12.0, CH ₃
19	1.61 m	27.8, CH ₂	1.91 m	26.9, CH ₂
			2.70 m	
20	2.04 m	37.8, CH	2.14 m	38.1, CH
21	2.97 m	65.3, CH ₂	3.20 m	65.3, CH ₂
	3.69 t (11.5)		3.77 m	

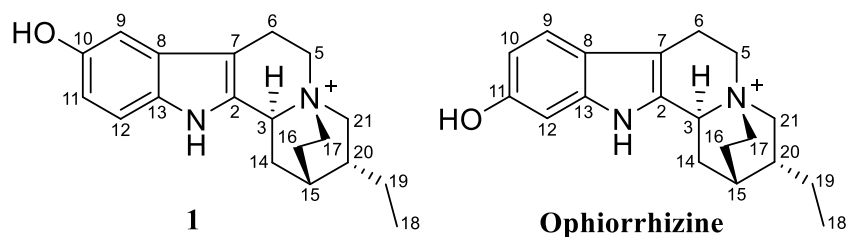


Table S2: ^1H and ^{13}C NMR data for compound **1** and **ophiorrhizine**.

No.	1		ophiorrhizine	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
2	–	133.3, C	–	127.7, C
3	4.33 t (9.5)	61.9, CH	4.90 t (9.0)	62.5, CH
5	3.16 m 3.43 dd (11.8, 10.4)	60.9, CH ₂	3.54 ddd (12.5, 12.5) 3.58 dd (12.5, 6.5)	61.3, CH ₂
6	2.74 m 2.90 m	17.9, CH ₂	2.96 d (18) 3.11 ddd (18, 12, 6.5, 2.5)	18.3, CH ₂
7	–	104.3, C	–	105.4, C
8	–	127.5, C	–	120.7, C
9	6.82 d (2.4)	103.5, CH	7.28 d (8.4)	119.7, C
10	–	152.2, C	6.64 dd (8.4, 2.1)	111.1, C
11	6.76 dd (8.7, 2.4)	113.6, CH	–	155.2 CH
12	7.25 d (8.7)	113.4, CH	6.79 d (2.1)	98.0, CH
13	–	130.4, C	–	140.0, C
14	1.80 m 2.59 m	26.6, CH ₂	1.79 dd (13.5, 9.0) 2.71 ddd (13.5, 9.4)	26.9, CH ₂
15	2.10 s	24.8, CH	2.24 m	25.1, CH
16	1.77 m 1.83 m	26.1, CH ₂	1.9 -1.98 m	26.3, CH ₂
17	3.12 m 3.41 m	49.0, CH ₂	3.28 m 3.67 m	49.1, CH ₂
18	1.01 t (7.3)	12.0, CH ₃	1.04 t (7.5)	12.0, CH ₃
19	1.61 m	27.8, CH ₂	1.70	28.0, CH ₂
20	2.04 m	37.8, CH	2.15 m	38.1, CH
21	2.97 m 3.69 t (11.5)	65.3, CH ₂	3.25 m 3.83 dd (12.5, 10.5)	65.2, CH ₂