

# Supporting Information

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

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People's Republic of China*

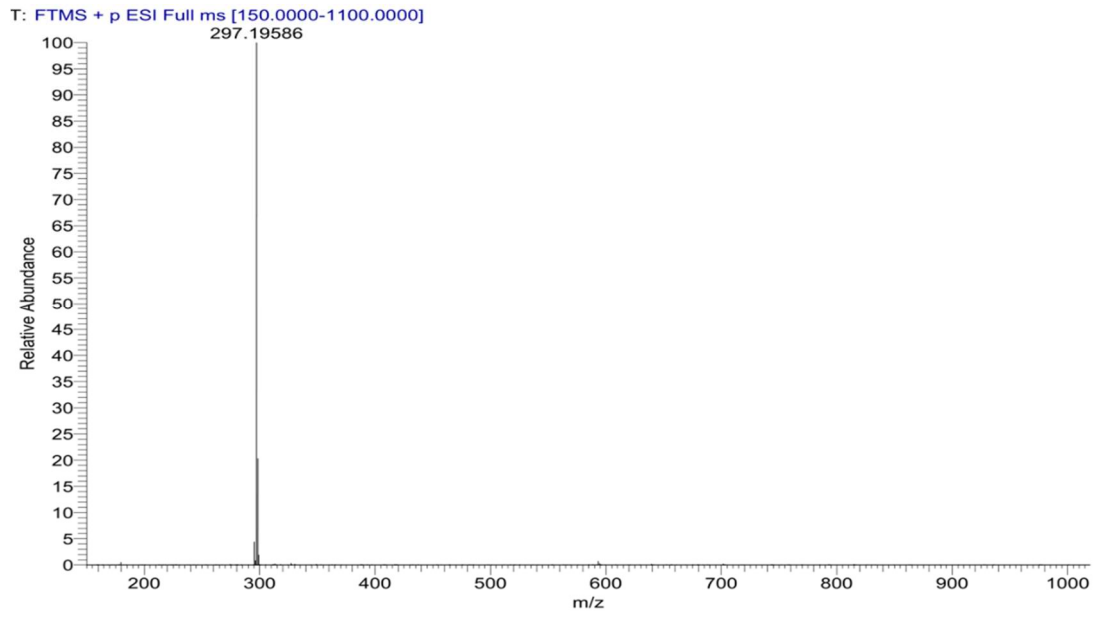
<sup>2</sup>*International Cooperation Base for Active Substances in Traditional Chinese Medicine in  
Hubei Province, School of Pharmaceutical Sciences, South-Central Minzu University*

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**Figure S1: HRESIMS spectrum of 1**

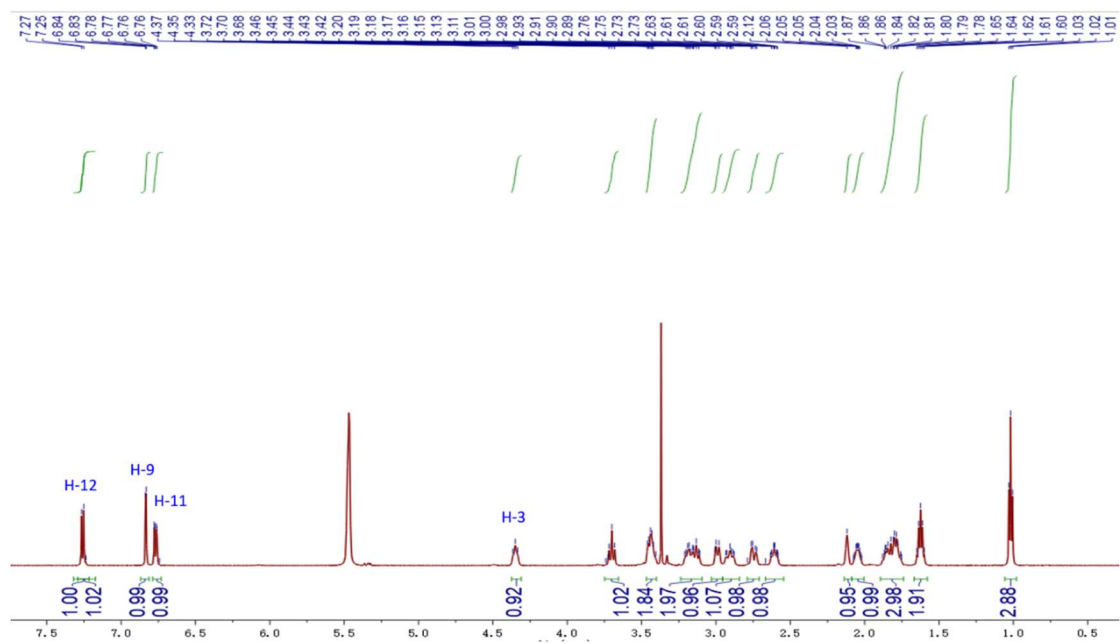


Figure S2:  $^1\text{H}$  NMR spectrum of **1**

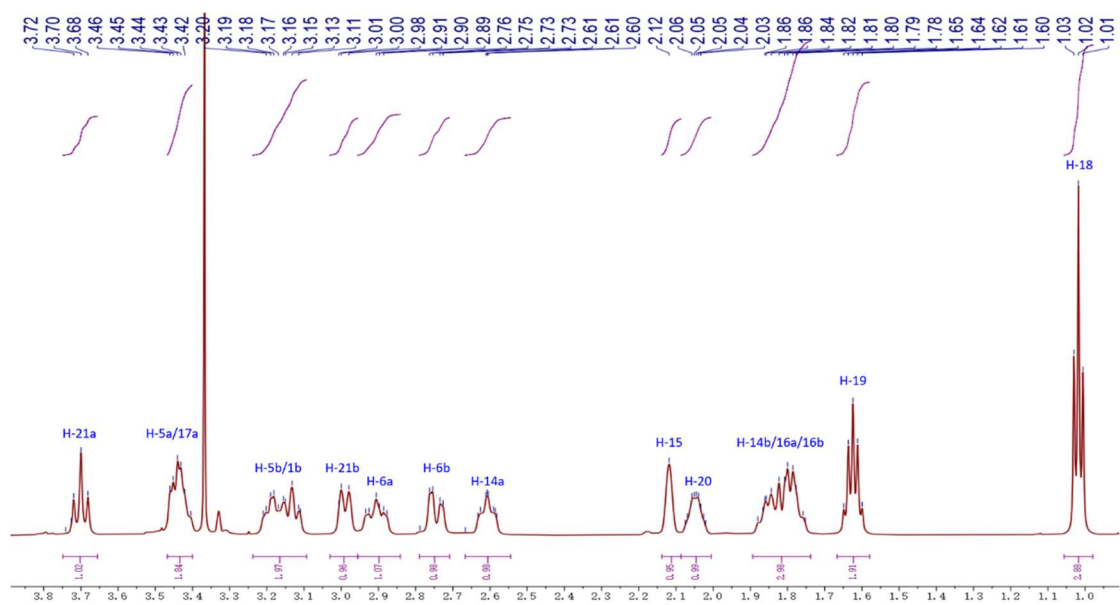


Figure S3: Enlarged  $^1\text{H}$  NMR spectrum of **1**

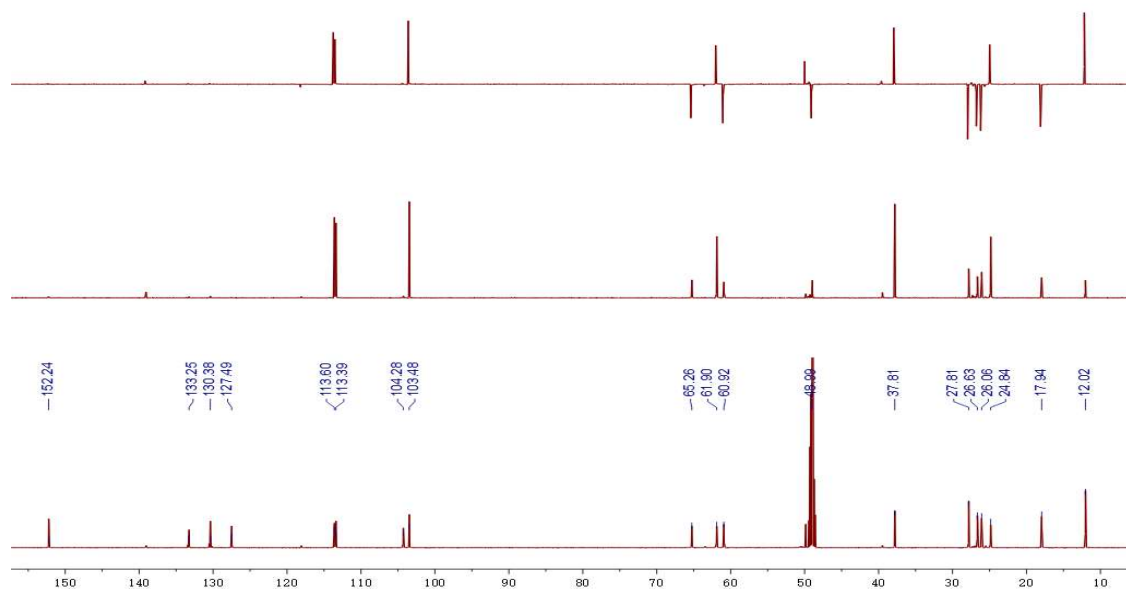


Figure S4:  $^{13}\text{C}$  NMR spectrum of **1**

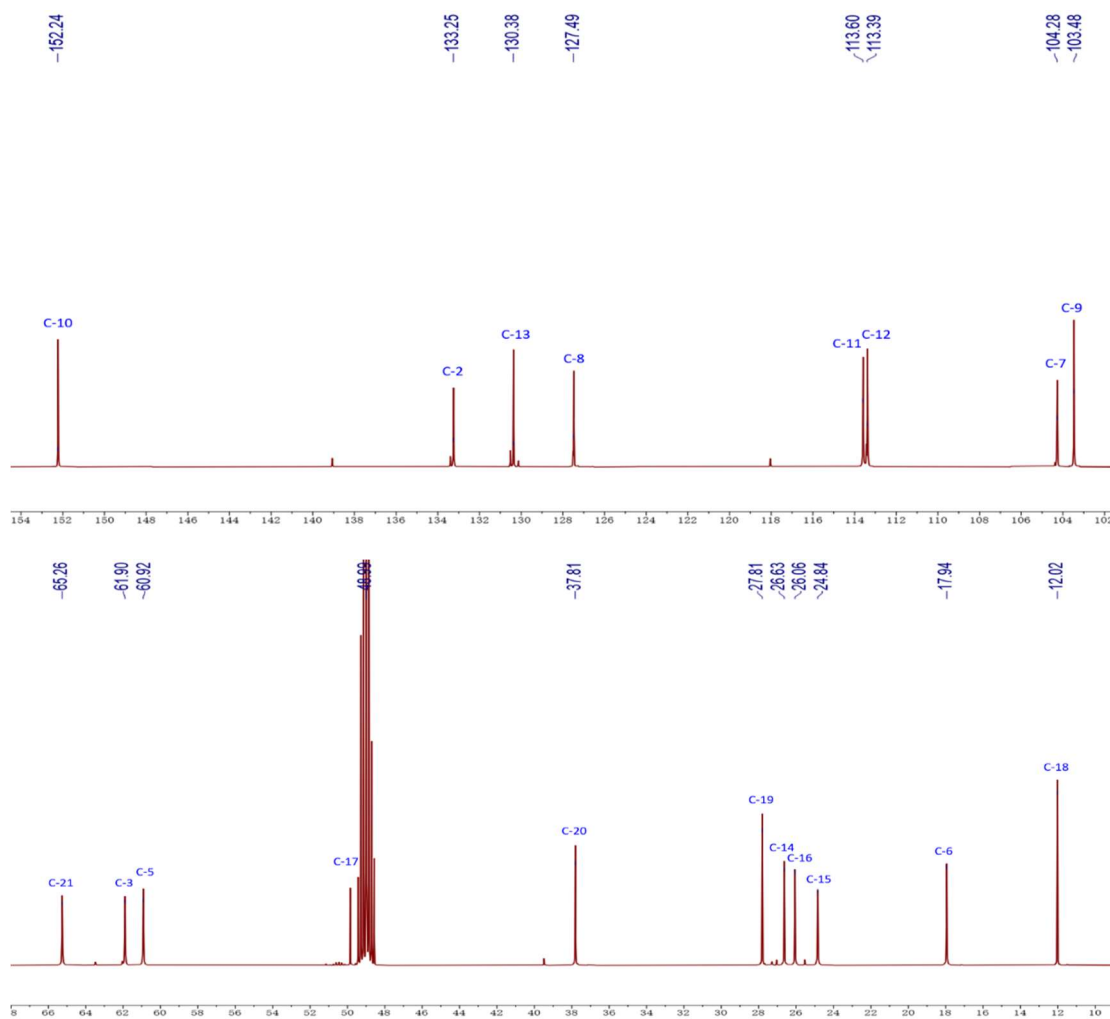
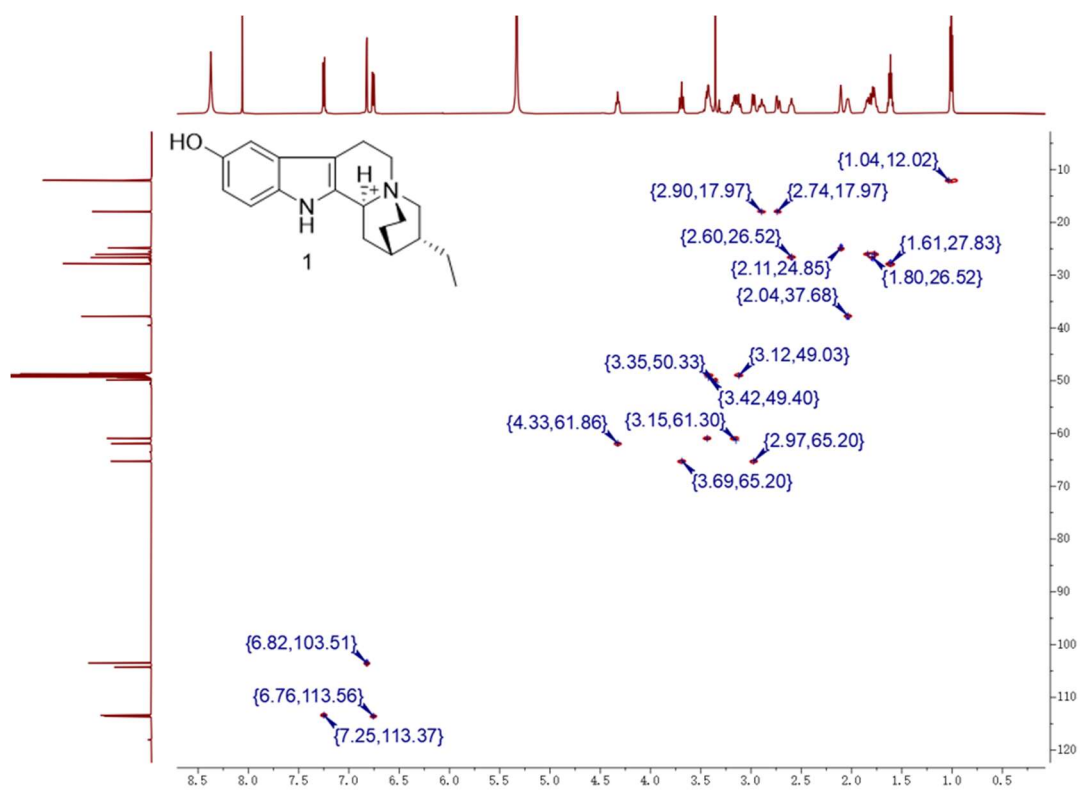


Figure S5: Enlarged  $^{13}\text{C}$  NMR spectrum of **1**



**Figure S6:** HSQC spectrum of **1**

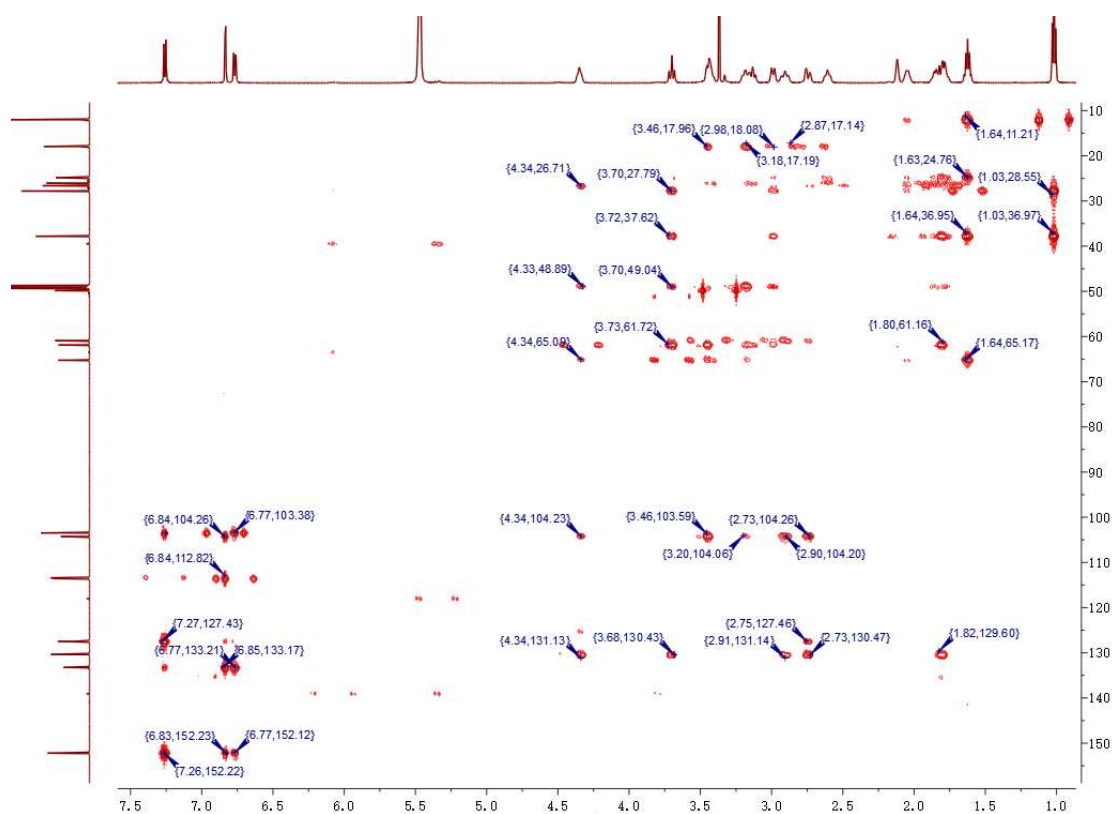


Figure S7: HMBC spectrum of **1**

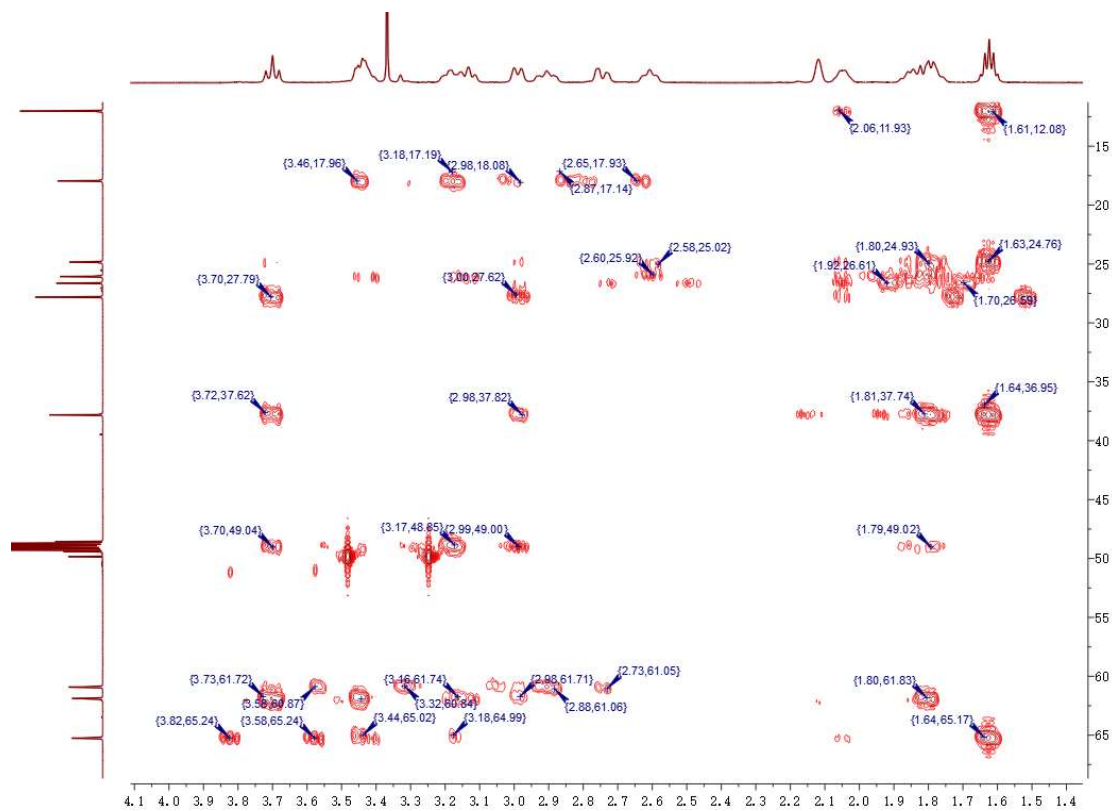
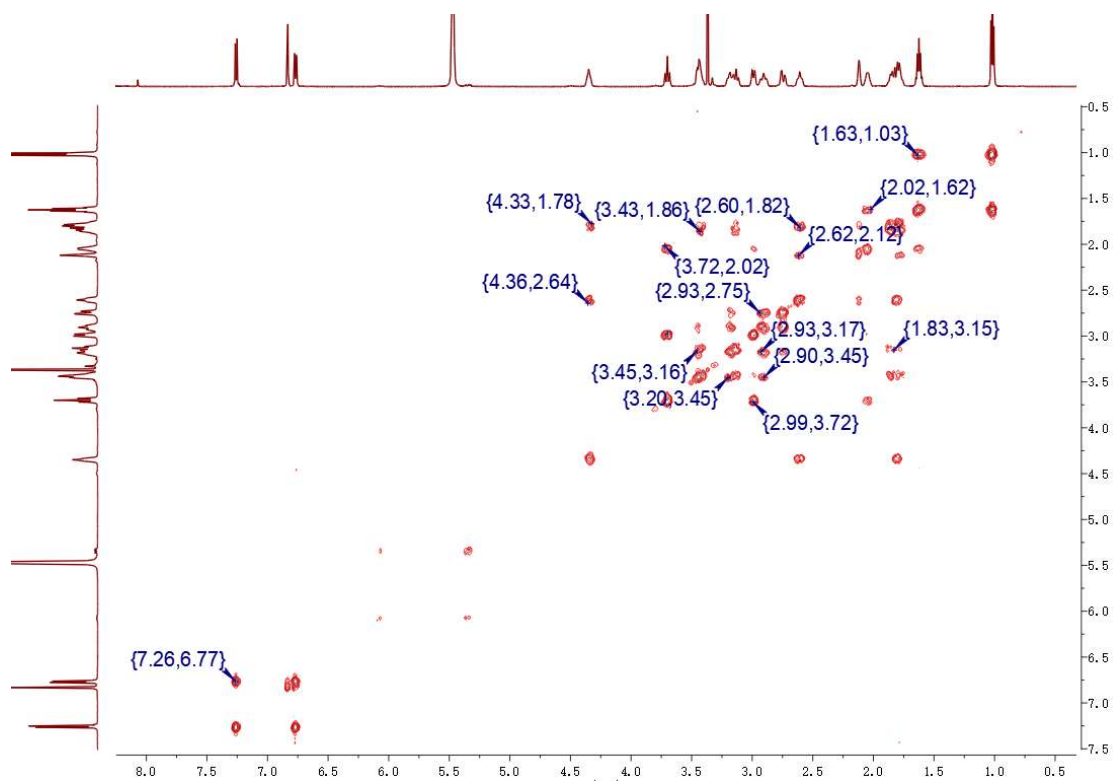
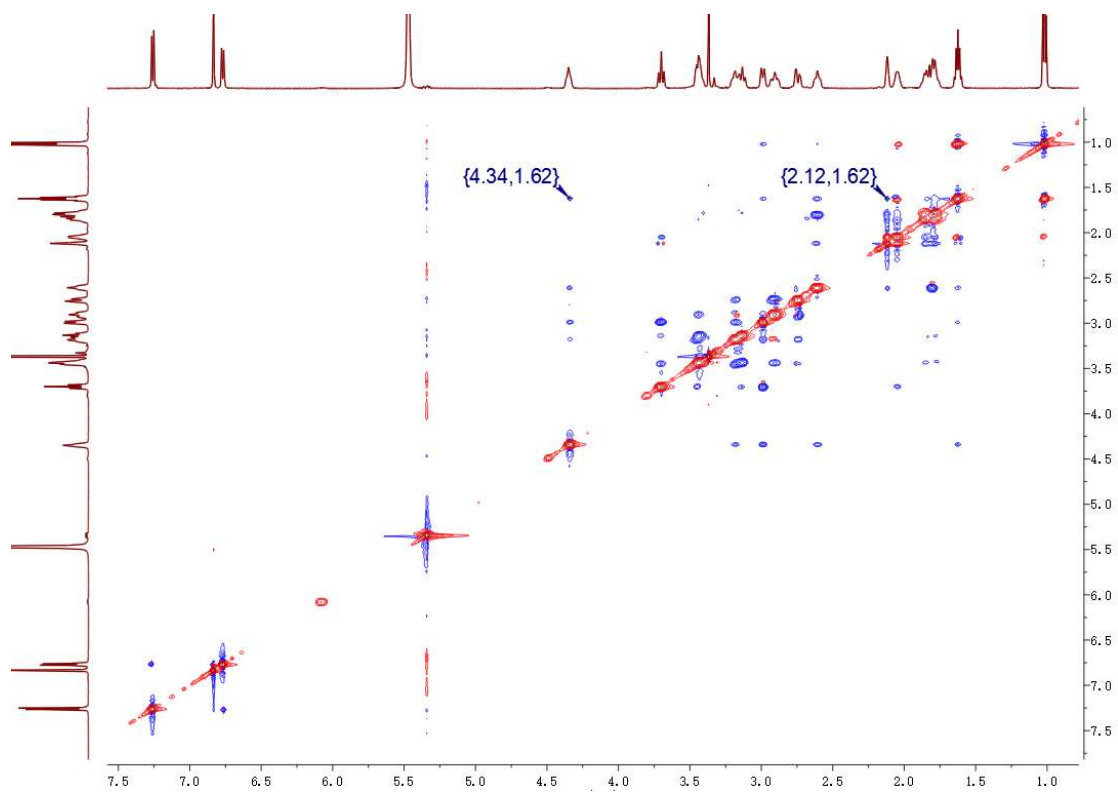


Figure S8: Enlarged HMBC spectrum of **1**



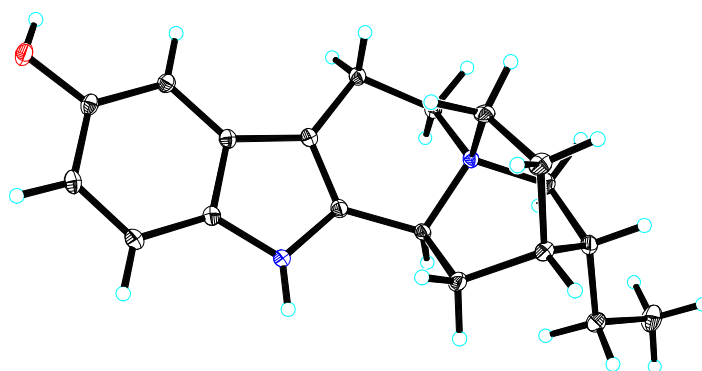
**Figure S9:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1**



**Figure S10:** ROESY spectrum of **1**



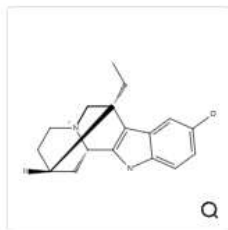
Crystal data for lzob20:  $C_{19}H_{25}N_2O \cdot CHO_2 \cdot 4(H_2O)$ ,  $M = 414.49$ ,  $a = 8.1868(3) \text{ \AA}$ ,  $b = 12.3654(4) \text{ \AA}$ ,  $c = 20.9849(7) \text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 90^\circ$ ,  $V = 2124.37(13) \text{ \AA}^3$ ,  $T = 150.(2) \text{ K}$ , 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**

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Substances  
9:14 PM



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

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Structure Match

As Drawn (0)

Substructure (8)

Similarity (198K)

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Similarity

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

View All

Reaction Role

- Product (44)
- Reactant (9)

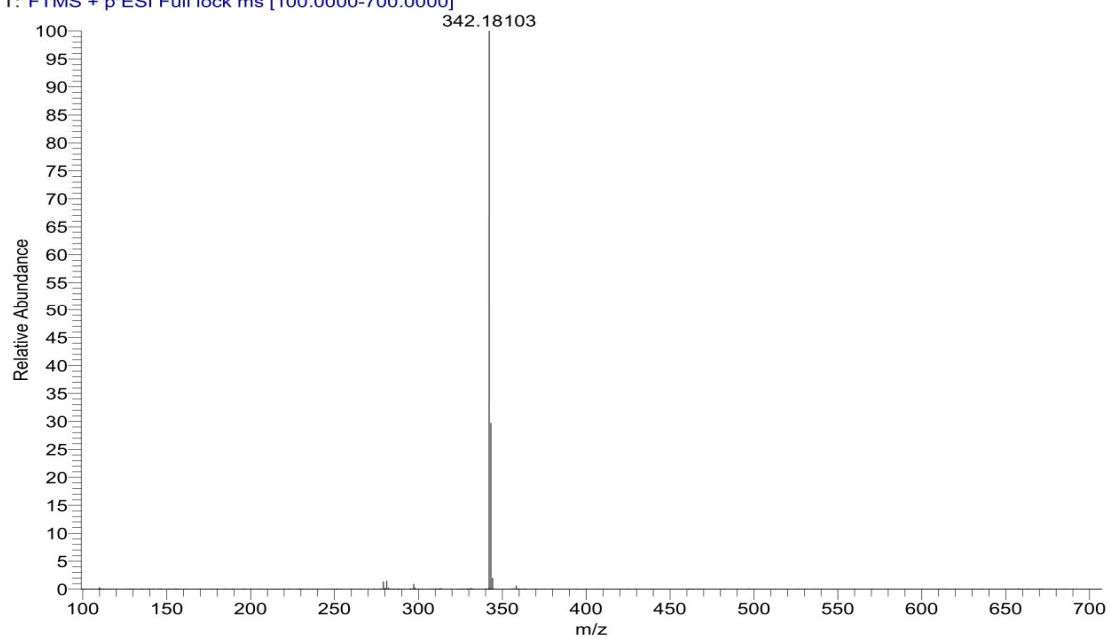
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203 Results Sort: Relevance View: Partial

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47257-27-2	97		$C_{20}H_{27}N_2O$ 2,5-Ethanoindolo[2,3-σ]quinolizin-5-ium, 3-ethyl-1,2,3,4,6,7,12,12b-octahydro-9...	0	0	0
47257-26-1	97		$C_{20}H_{27}N_2O$ 2,5-Ethanoindolo[2,3-σ]quinolizin-5-ium, 3-ethyl-1,2,3,4,6,7,12,12b-octahydro-9...	0	0	0
2539272-59-6	91		$C_{19}H_{26}N_2O$ 2',3',4',9'-Tetrahydro-4-propylspiro[cyclohexane-1,1'-[1H]pyrido[3,4-b]indol]-6...	0	0	1
2644483-30-5	91		$C_{18}H_{24}N_2O$ 4-Ethyl-2',3',4',9'-tetrahydrospiro[cyclohexane-1,1'-[1H]pyrido[3,4-b]indol]-6...	0	0	1
2572971-35-6	90		$C_{19}H_{26}N_2O$ 2',3',4',9'-Tetrahydro-2-propylspiro[cyclohexane-1,1'-[1H]pyrido[3,4-b]indol]-6...	0	0	1

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**

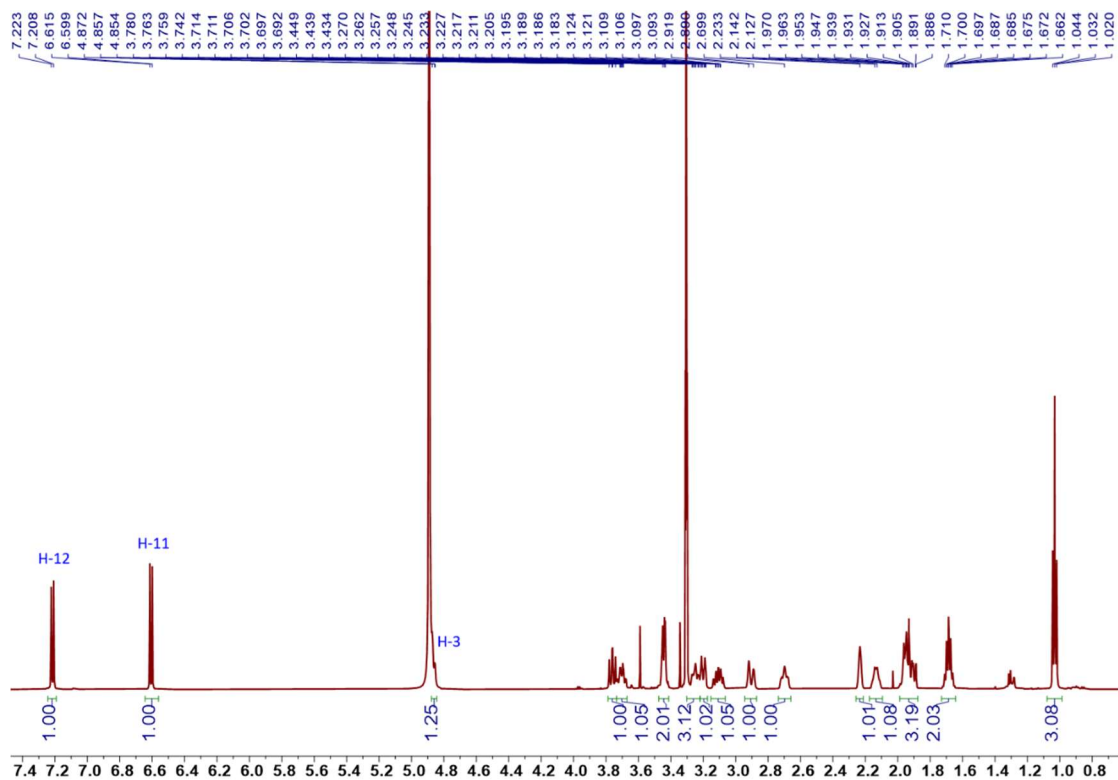


Figure S14:  $^1\text{H}$  NMR spectrum of **2**

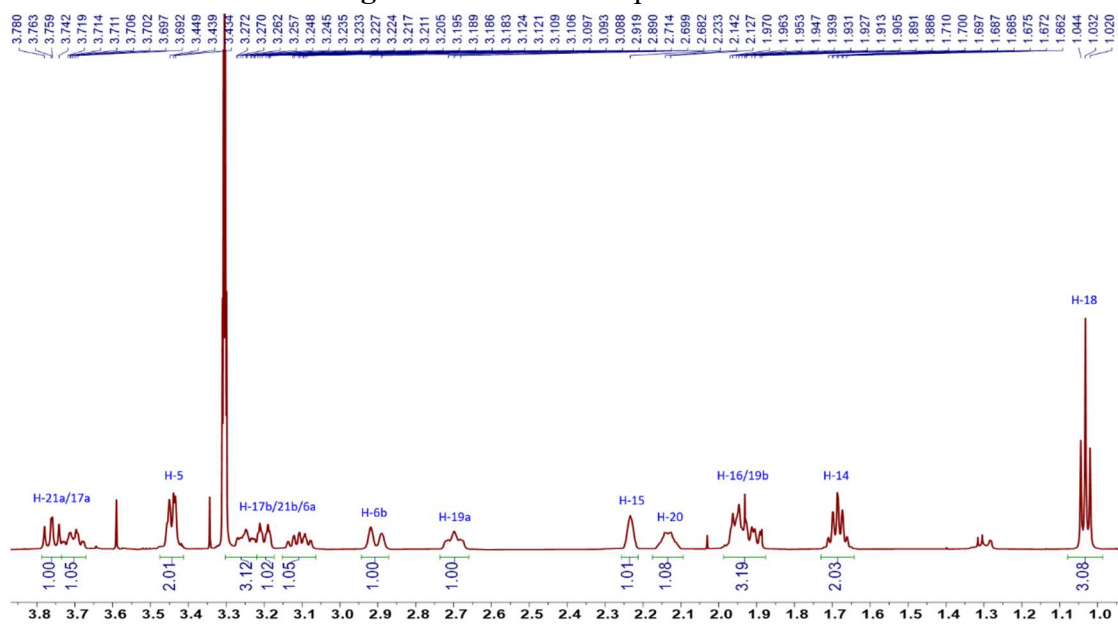
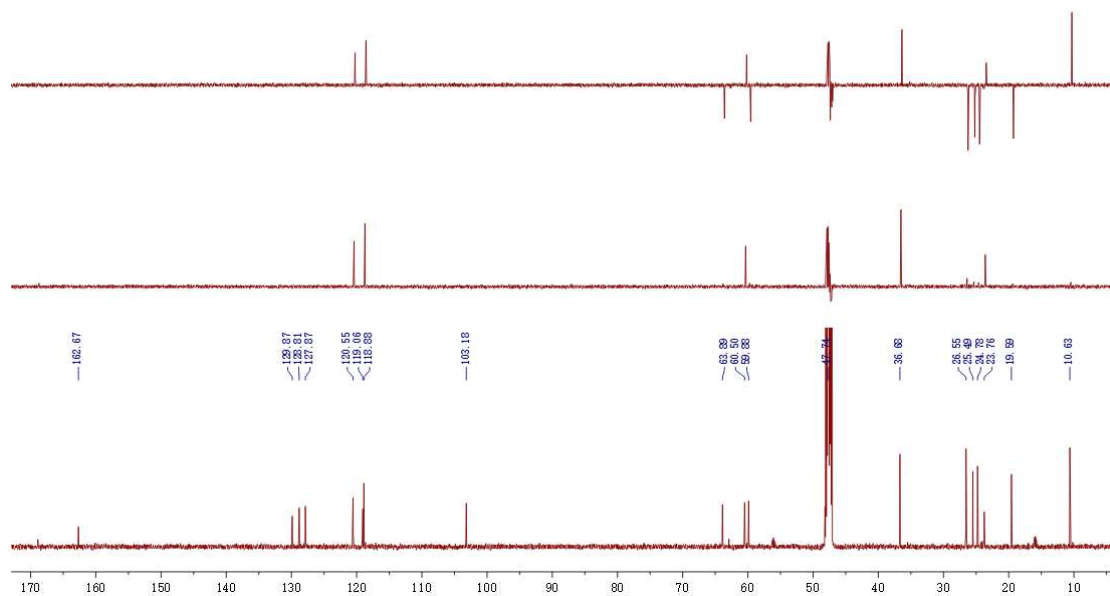


Figure S15: Enlarged  $^1\text{H}$  NMR spectrum of **2**



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

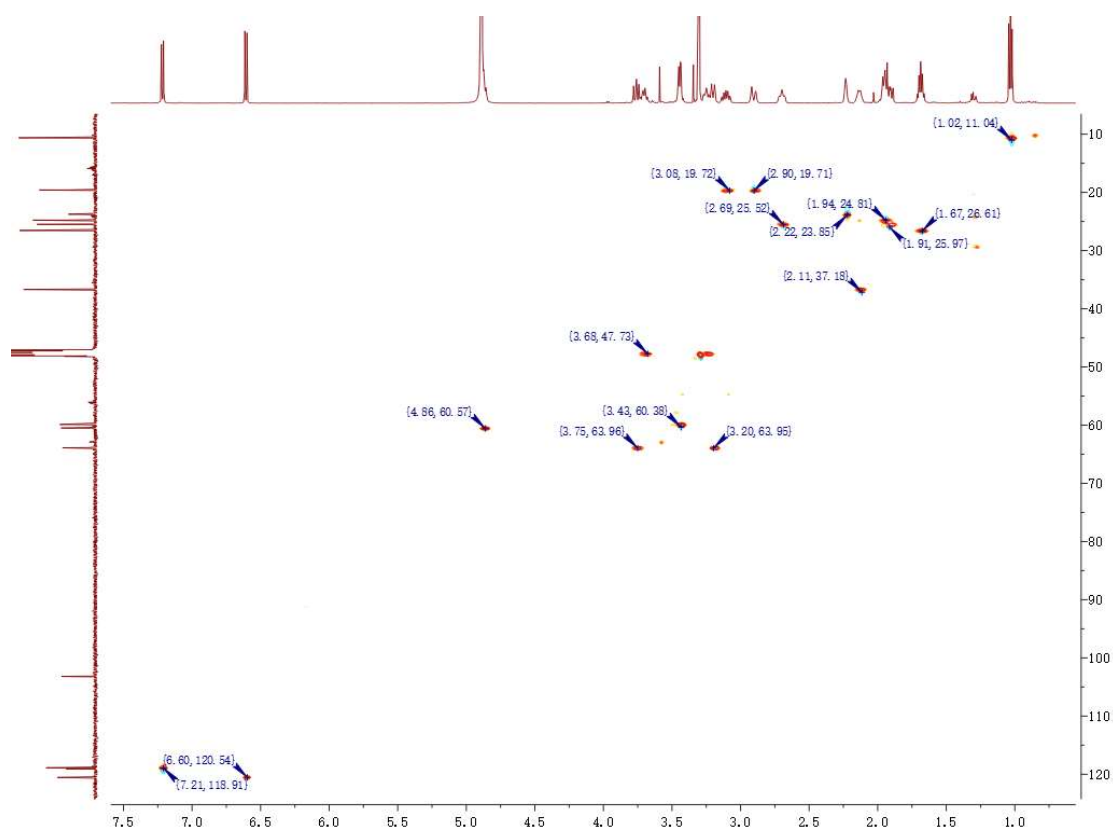
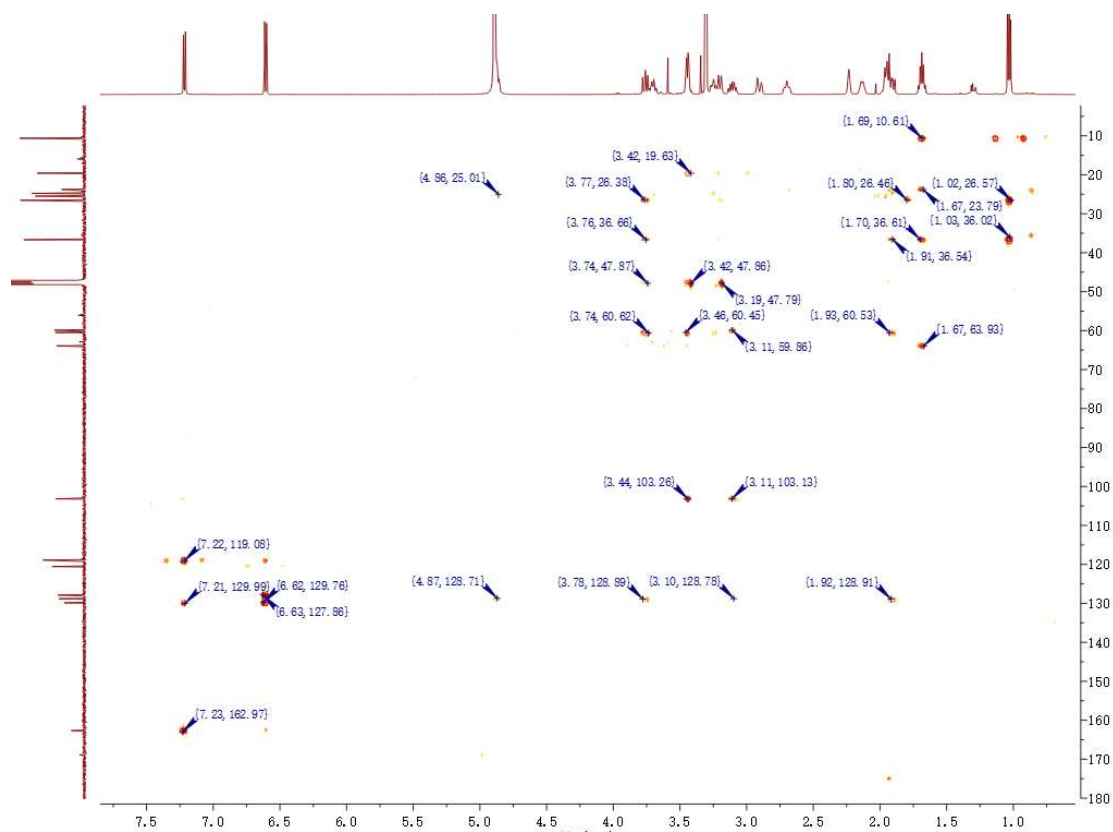
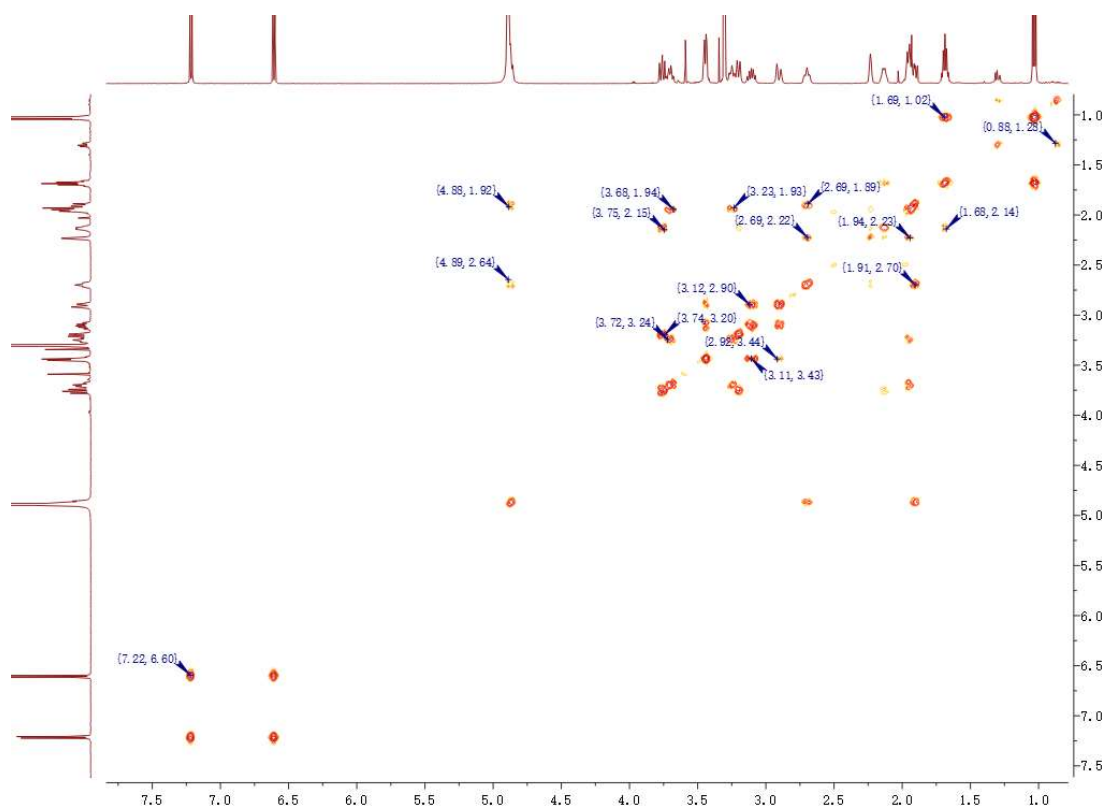


Figure S17: HSQC spectrum of 2

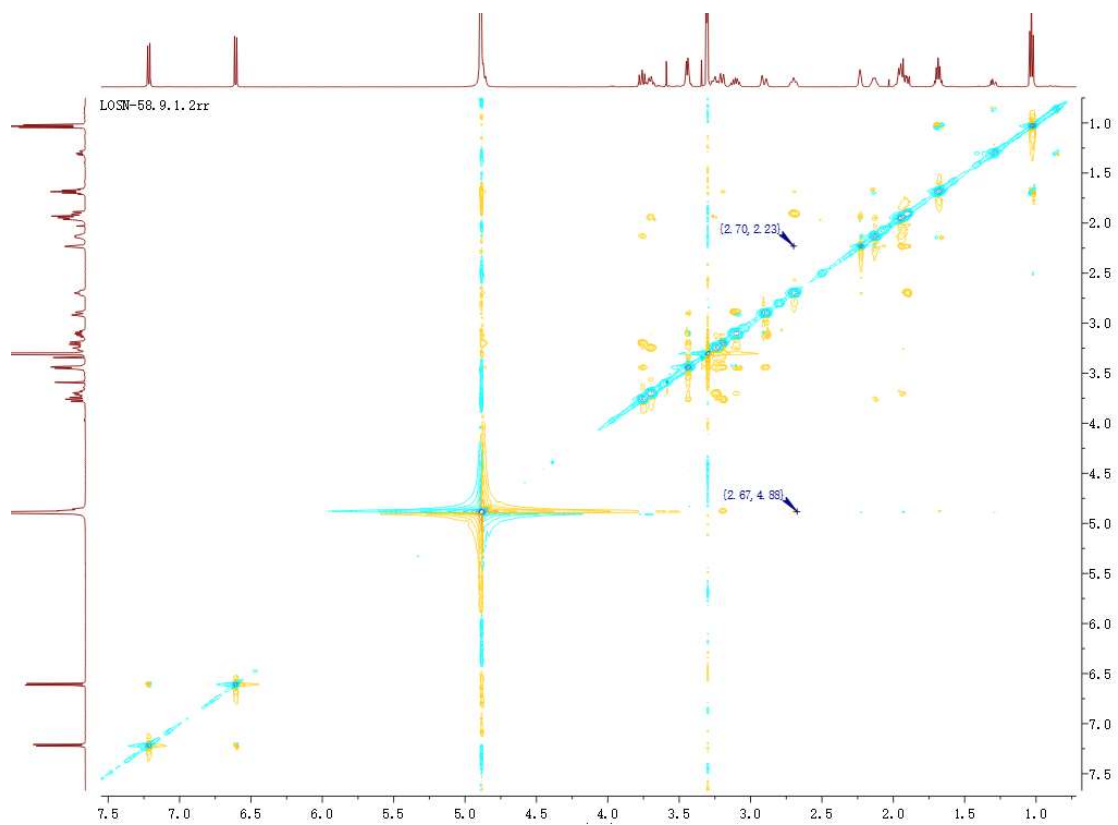


**Figure S18: HMBC spectrum of 2**



**Figure S19:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2**

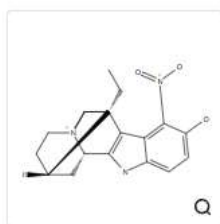




**Figure S20: ROESY spectrum of 2**

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

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

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  - 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

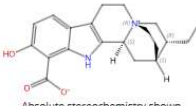
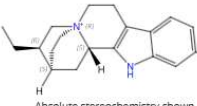
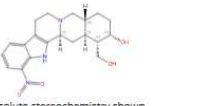
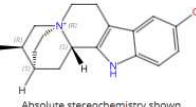
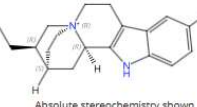
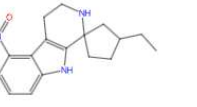
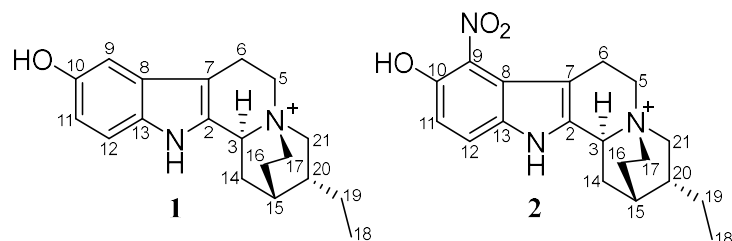
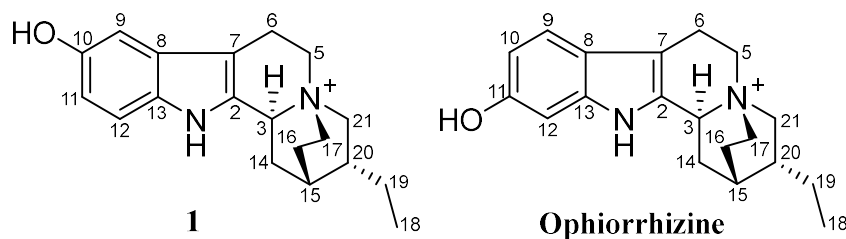
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214702-40-6	83		$C_{19}H_{22}N_2O$ 2,5-Ethanoindolo[2,3-a]quinolizin-5-ium, 3-ethyl-1,2,3,4,6,7,12,12b-octahydro-10...	2	0	0
133146-16-4	81		$C_{20}H_{25}N_3O_4$ Yohimban-16-methanol, 17-hydroxy-12-nitro-, (16a,17a)-	1	1	0
47257-27-2	81		$C_{20}H_{27}N_2O$ 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		$C_{20}H_{27}N_2O$ 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		$C_{17}H_{21}N_3O_2$ 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:**  $^1\text{H}$  and  $^{13}\text{C}$  NMR data for compound **1** and **2**.

No.	<b>1</b>		<b>2</b>	
	$\delta_{\text{H}}$	$\delta_{\text{C}}$	$\delta_{\text{H}}$	$\delta_{\text{C}}$
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 <sub>2</sub>	3.45 m	61.3, CH <sub>2</sub>
6	3.43 dd (11.8, 10.4)			
	2.74 m	17.9, CH <sub>2</sub>	2.90 d (17.4)	20.9, CH <sub>2</sub>
	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 <sub>2</sub>	1.69 m	27.9, CH <sub>2</sub>
	2.59 m			
15	2.10 s	24.8, CH	2.24 m	25.2, CH
16	1.77 m	26.1, CH <sub>2</sub>	1.96 m	26.2, CH <sub>2</sub>
	1.83 m			
17	3.12 m	49.0, CH <sub>2</sub>	3.25 m	49.1, CH <sub>2</sub>
	3.41 m		3.71 m	
18	1.01 t (7.3)	12.0, CH <sub>3</sub>	1.04 t (7.4)	12.0, CH <sub>3</sub>
19	1.61 m	27.8, CH <sub>2</sub>	1.91 m	26.9, CH <sub>2</sub>
			2.70 m	
20	2.04 m	37.8, CH	2.14 m	38.1, CH
21	2.97 m	65.3, CH <sub>2</sub>	3.20 m	65.3, CH <sub>2</sub>
	3.69 t (11.5)		3.77 m	



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

No.	<b>1</b>		<b>ophiorrhizine</b>	
	$\delta_{\text{H}}$	$\delta_{\text{C}}$	$\delta_{\text{H}}$	$\delta_{\text{C}}$
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 <sub>2</sub>	3.54 ddd (12.5, 12.5) 3.58 dd (12.5, 6.5)	61.3, CH <sub>2</sub>
6	2.74 m 2.90 m	17.9, CH <sub>2</sub>	2.96 d (18) 3.11 ddd (18, 12, 6.5, 2.5)	18.3, CH <sub>2</sub>
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 <sub>2</sub>	1.79 dd (13.5, 9.0) 2.71 ddd (13.5, 9.4)	26.9, CH <sub>2</sub>
15	2.10 s	24.8, CH	2.24 m	25.1, CH
16	1.77 m 1.83 m	26.1, CH <sub>2</sub>	1.9 -1.98 m	26.3, CH <sub>2</sub>
17	3.12 m 3.41 m	49.0, CH <sub>2</sub>	3.28 m 3.67 m	49.1, CH <sub>2</sub>
18	1.01 t (7.3)	12.0, CH <sub>3</sub>	1.04 t (7.5)	12.0, CH <sub>3</sub>
19	1.61 m	27.8, CH <sub>2</sub>	1.70	28.0, CH <sub>2</sub>
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 <sub>2</sub>	3.25 m 3.83 dd (12.5, 10.5)	65.2, CH <sub>2</sub>