Supporting Information

Rec. Nat. Prod. X:X (2024) XX-XX

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**

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

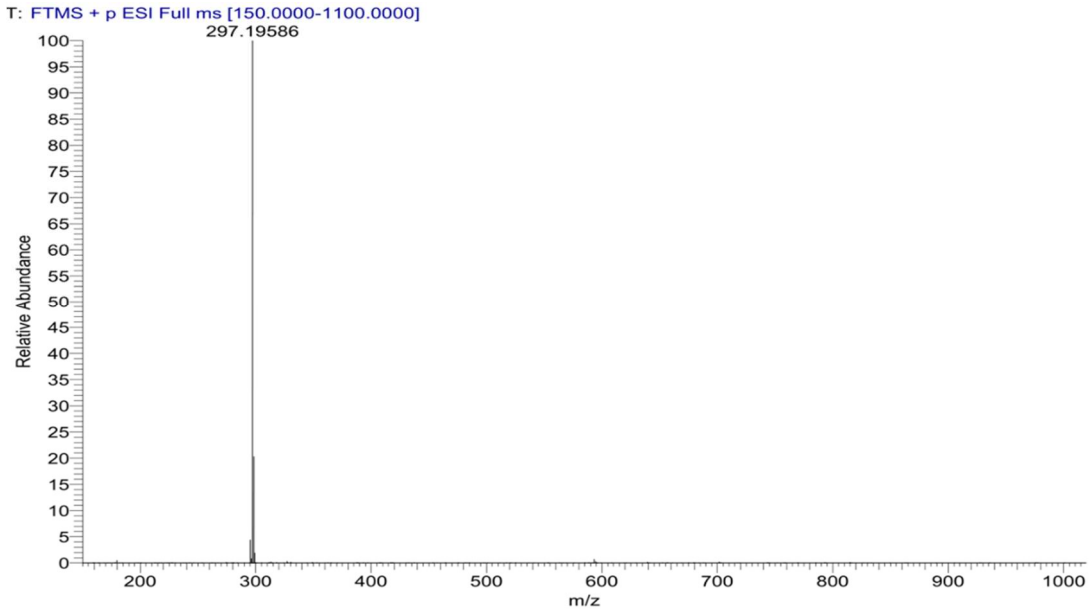


Figure S1: HRESIMS spectrum of **1**

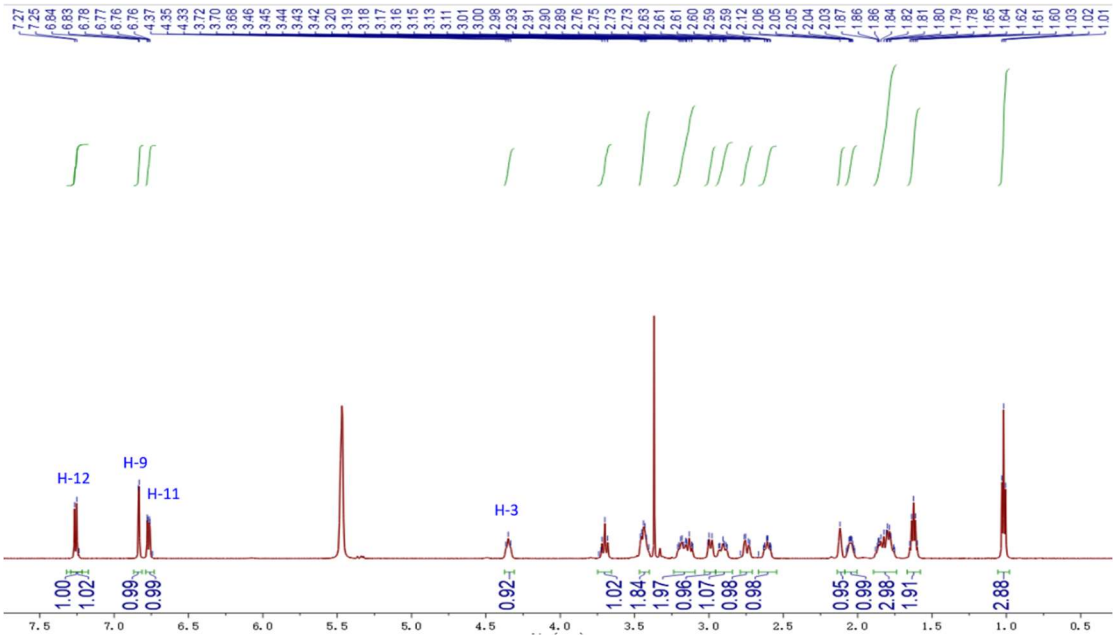


Figure S2: ^{1}H NMR spectrum of **1**

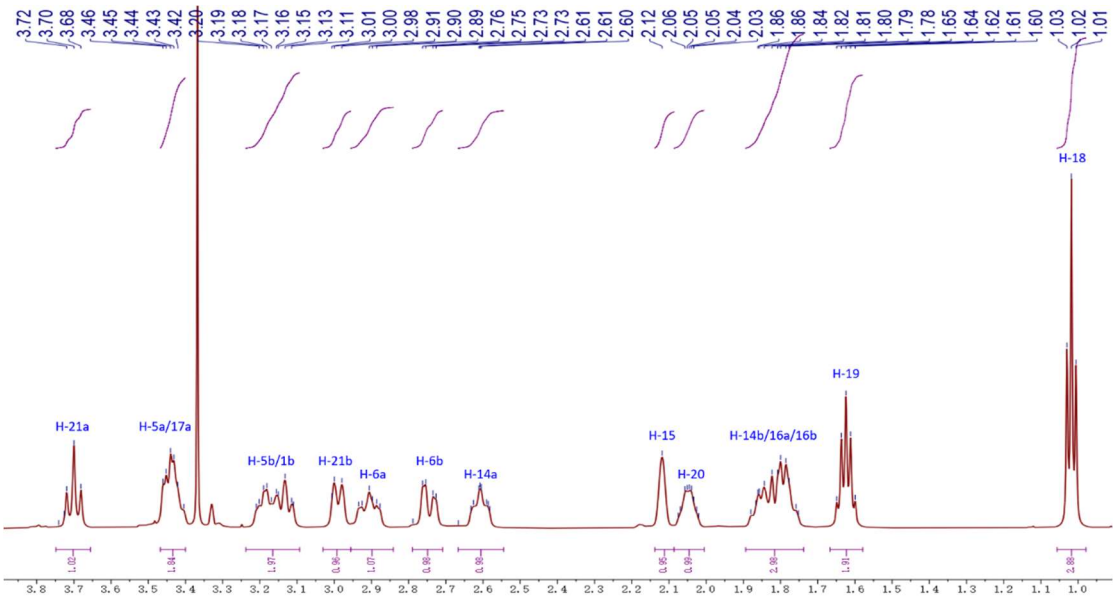


Figure S3: Enlarged ^{1}H NMR spectrum of **1**

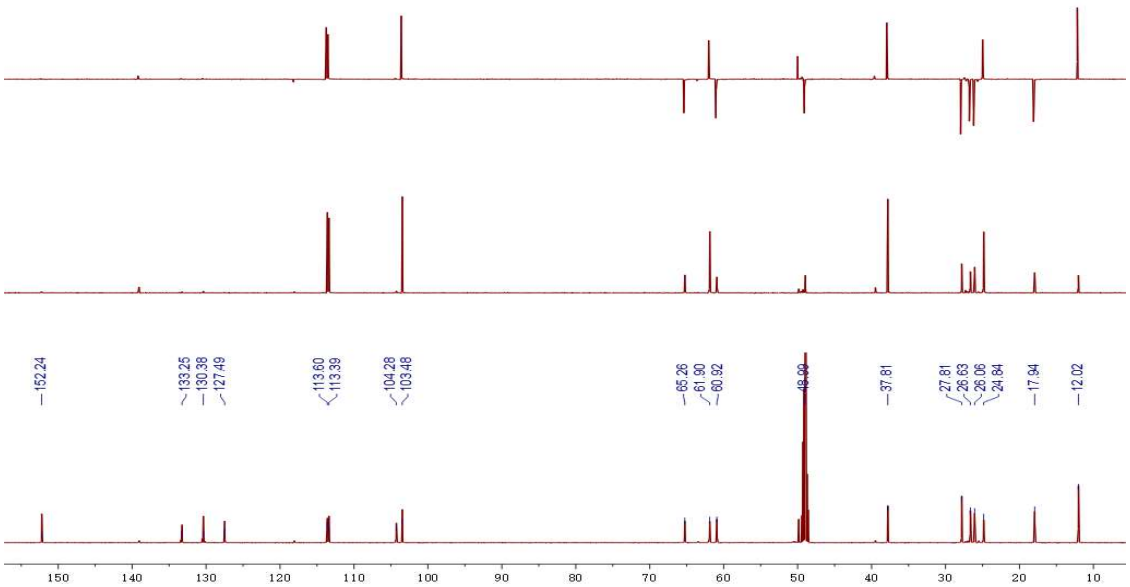


Figure S4: ^{13}C NMR spectrum of **1**

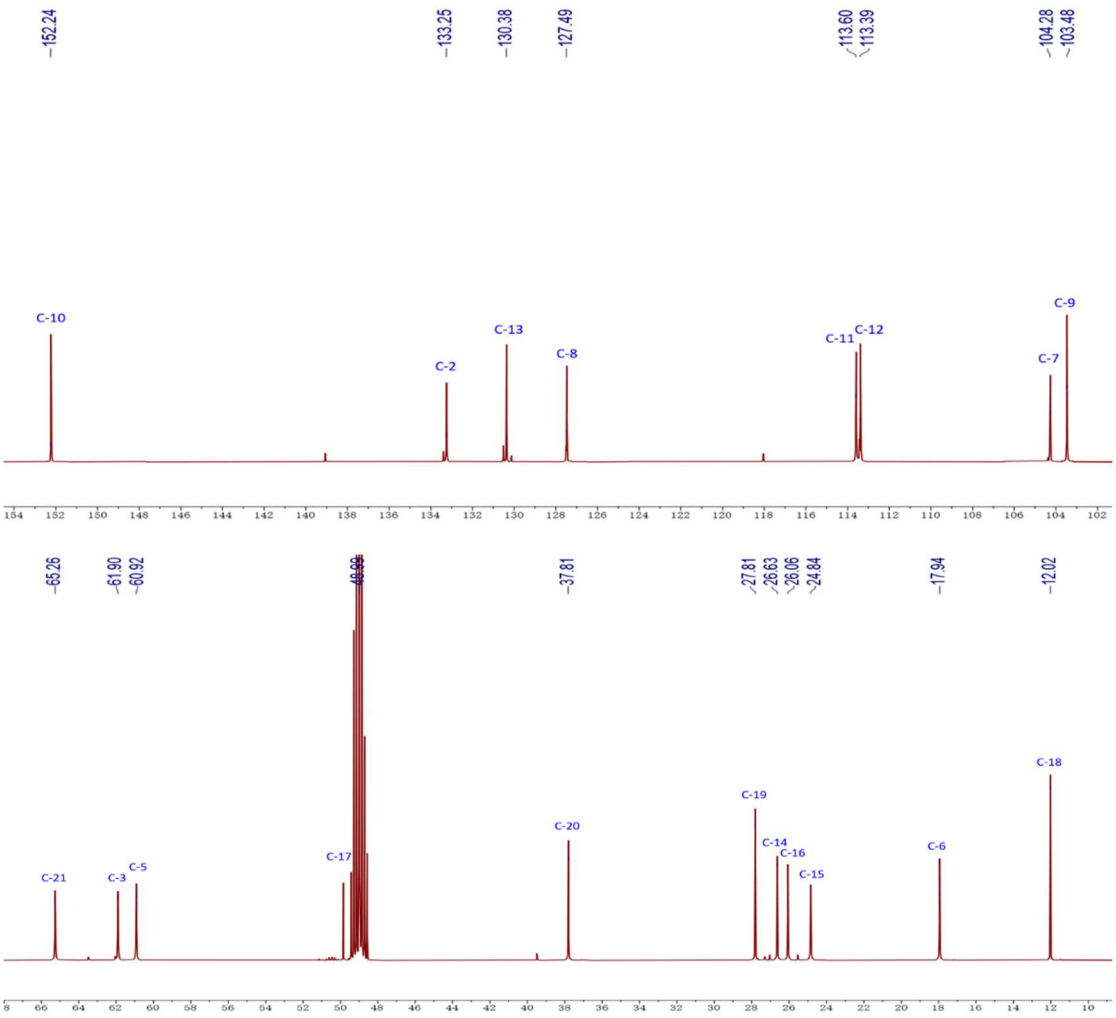


Figure S5: Enlarged ^{13}C NMR spectrum of **1**

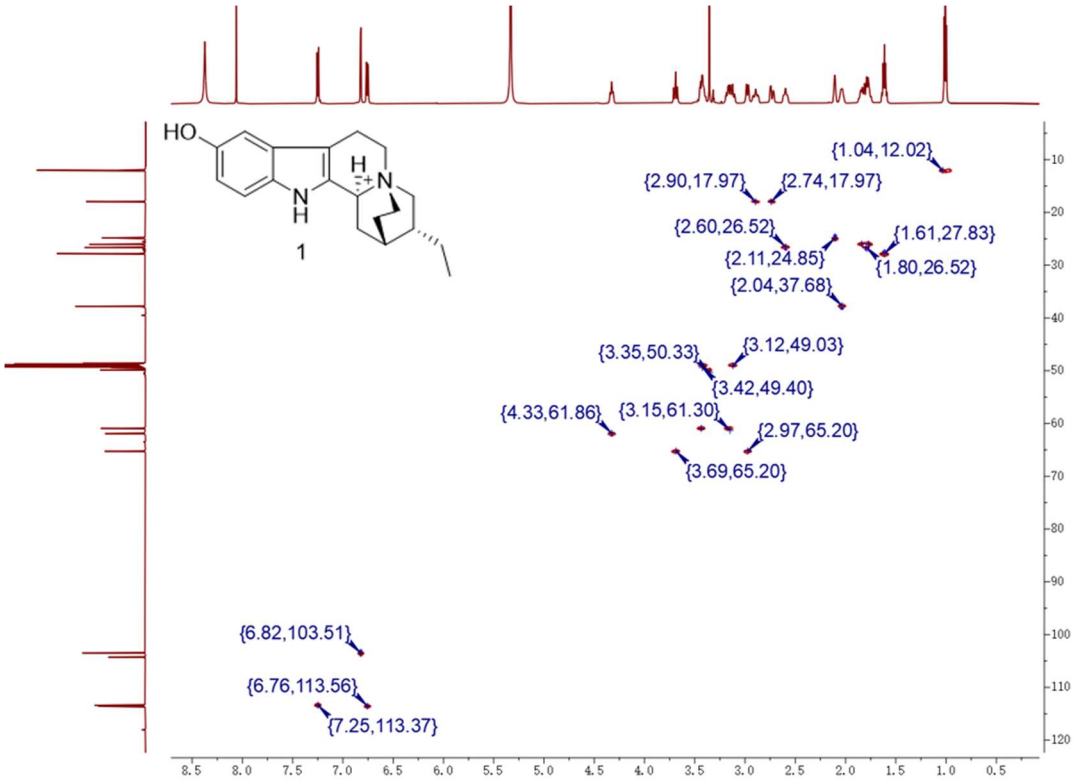


Figure S6: HSQC spectrum of **1**

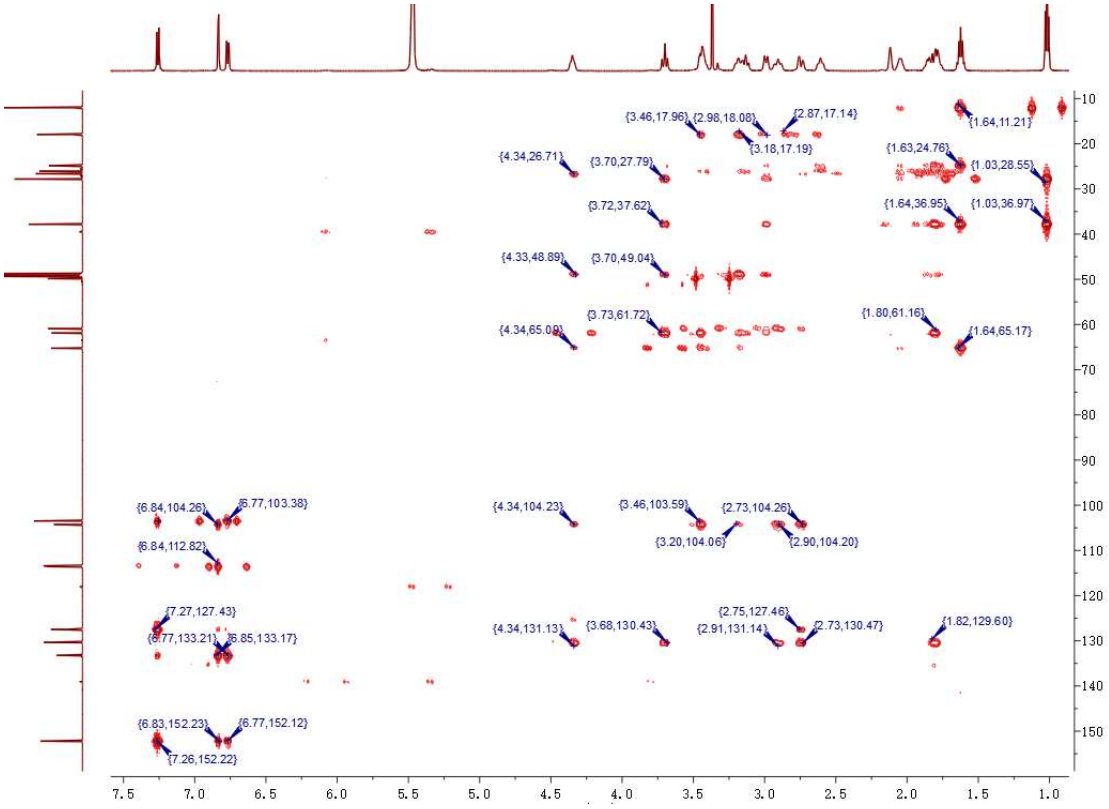


Figure S7: HMBC spectrum of **1**

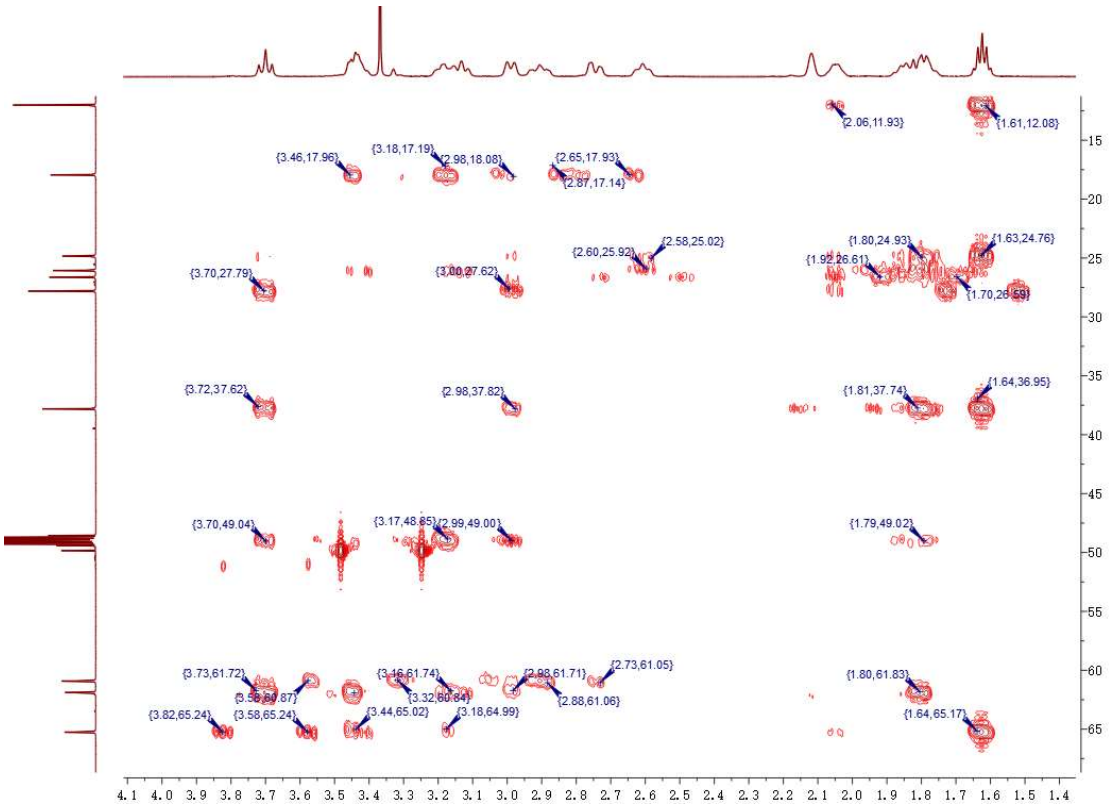


Figure S8: Enlarged HMBC spectrum of **1**

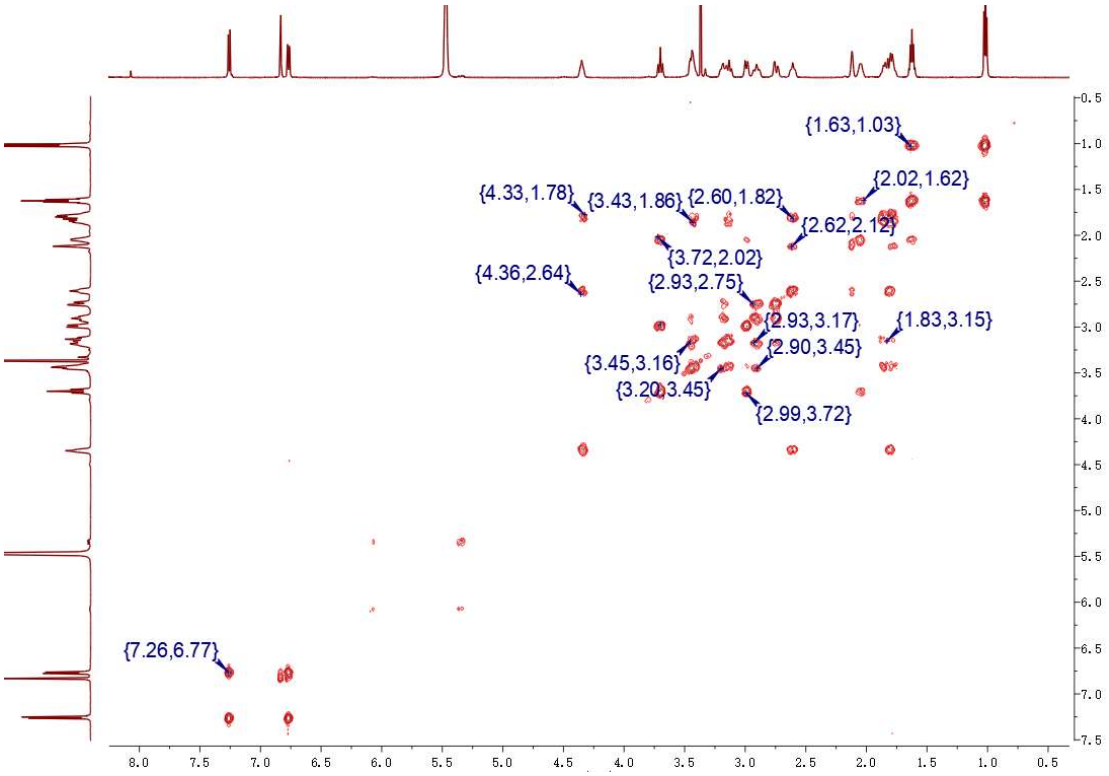


Figure S9: ^{1}H-^{1}H COSY spectrum of **1**

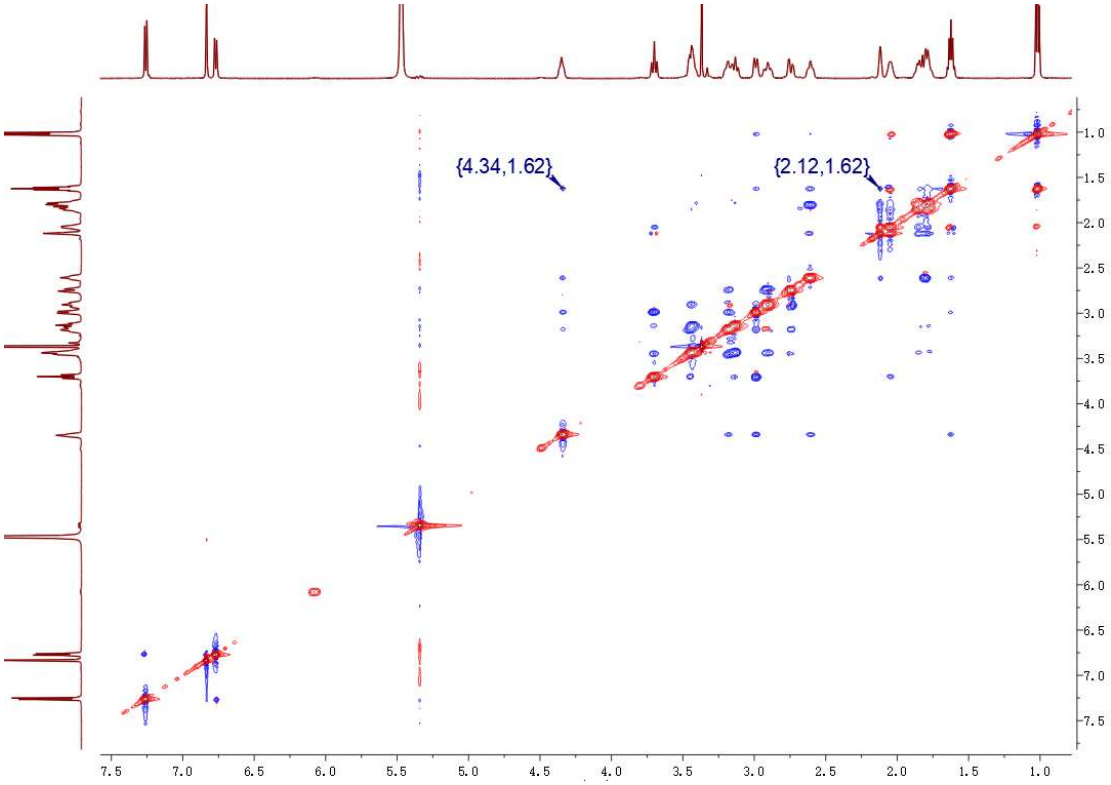


Figure S10: ROESY spectrum of **1**

Crystal data for lzob20: $C_{19}H_{25}N_2O•CHO_2•4(H_2O)$, M = 414.49, a = 8.1868(3) Å, b = 12.3654(4) Å, c = 20.9849(7) Å, α = 90°, β = 90°, γ = 90°, V = 2124.37(13) Å^3, T = 150.(2) K, space group $P212121$, Z = 4, μ(Cu Kα) = 0.809 mm^{-1}, 21387 reflections measured, 4015 independent reflections (R_{int} = 0.0625). The final R_1 values were 0.0303 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0784 ($I > 2\sigma(I)$). The final R_1 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).

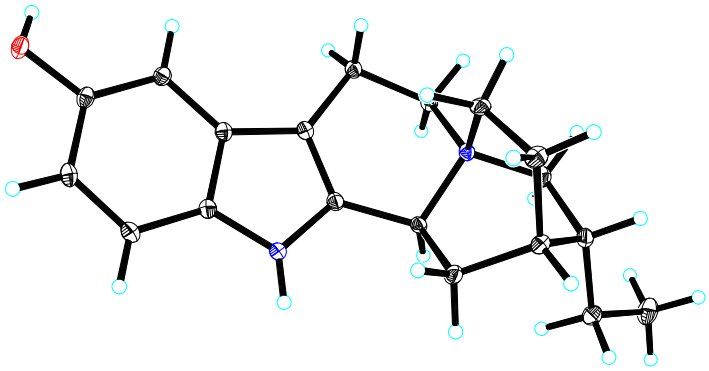


Figure S11: X-ray structure of compound **1**

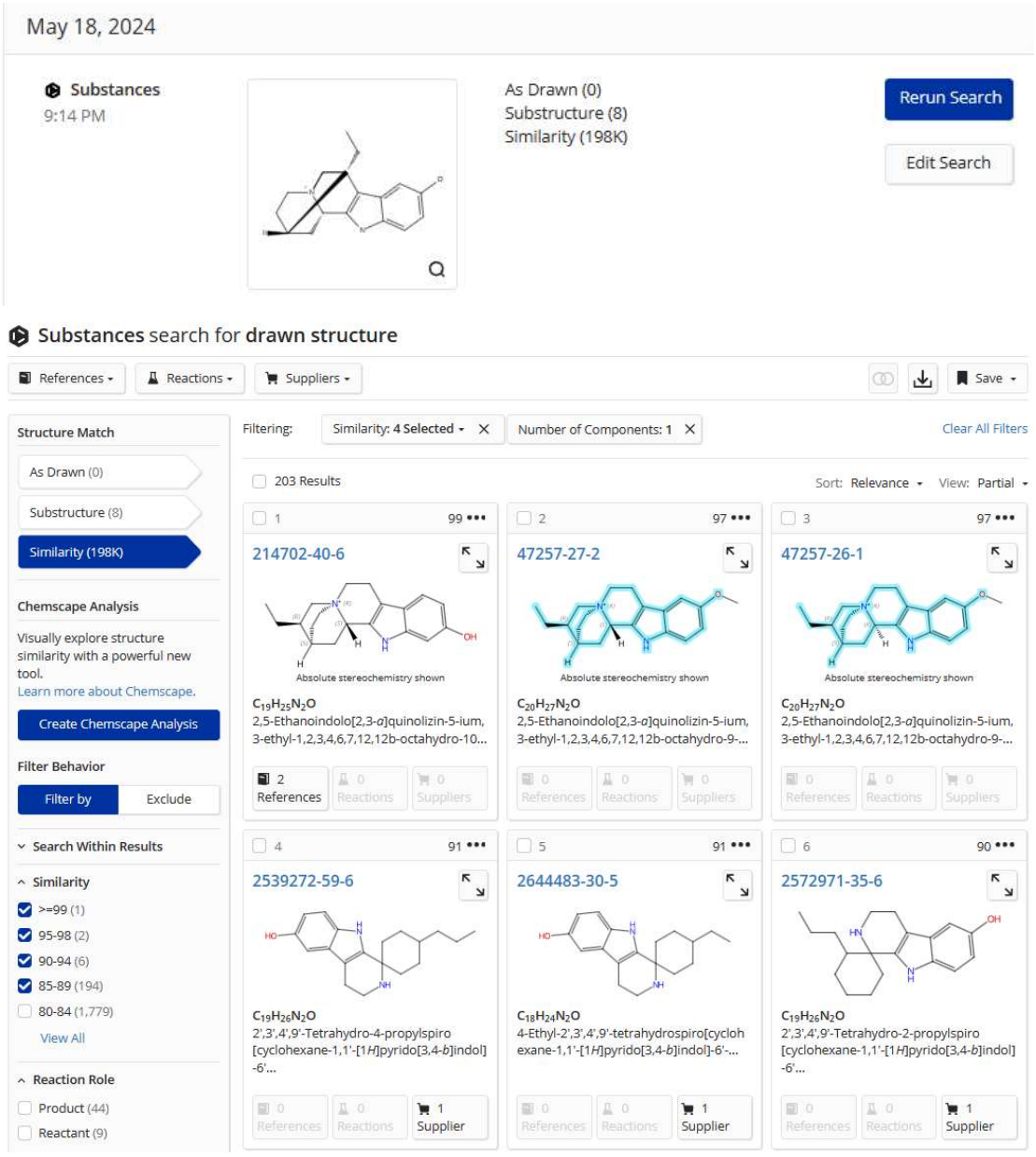


Figure S12: The Scifinder similarity report for **1**

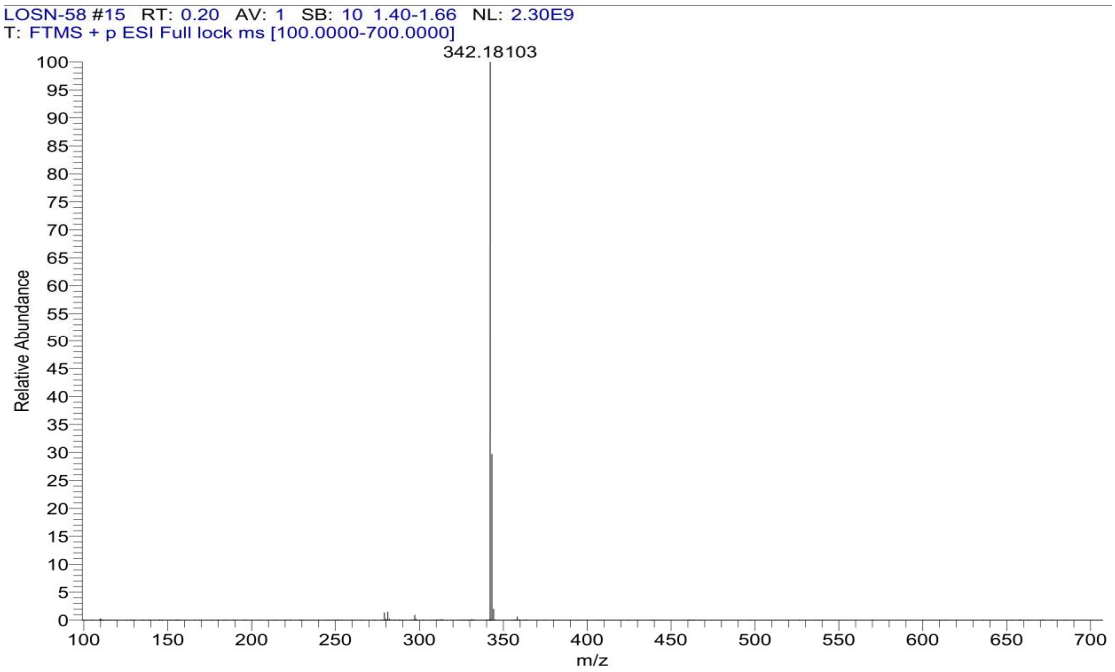


Figure S13: HRESIMS spectrum of **2**

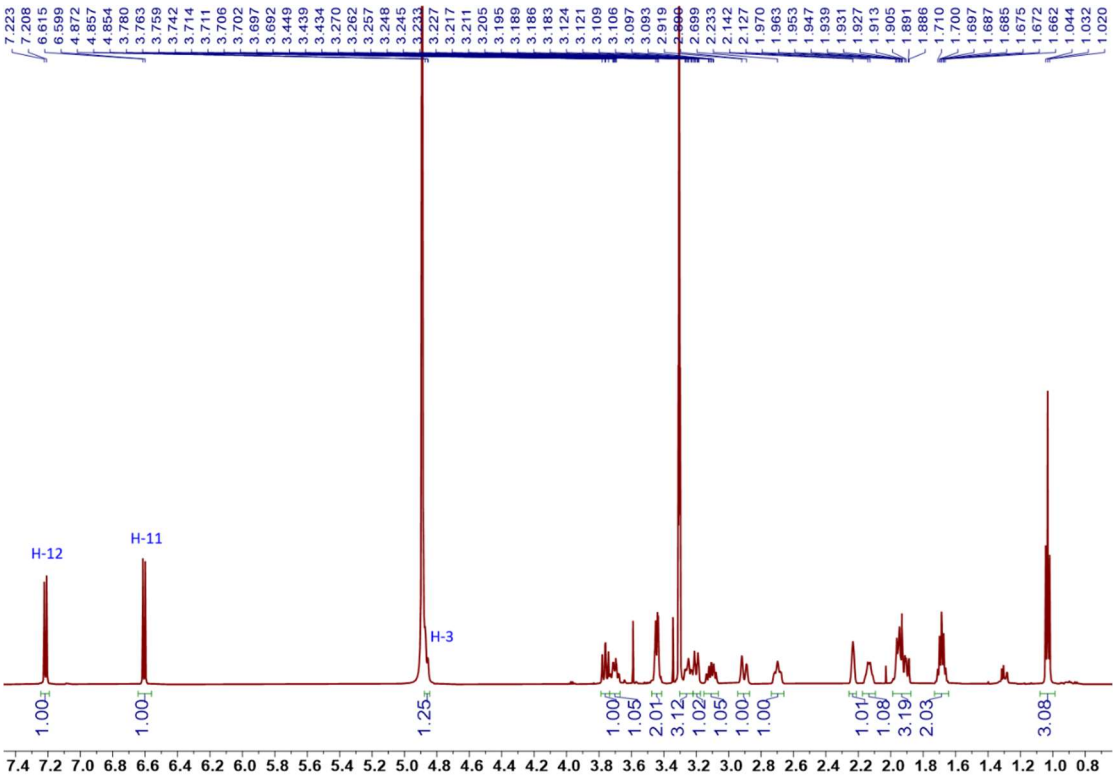


Figure S14: ^{1}H NMR spectrum of **2**

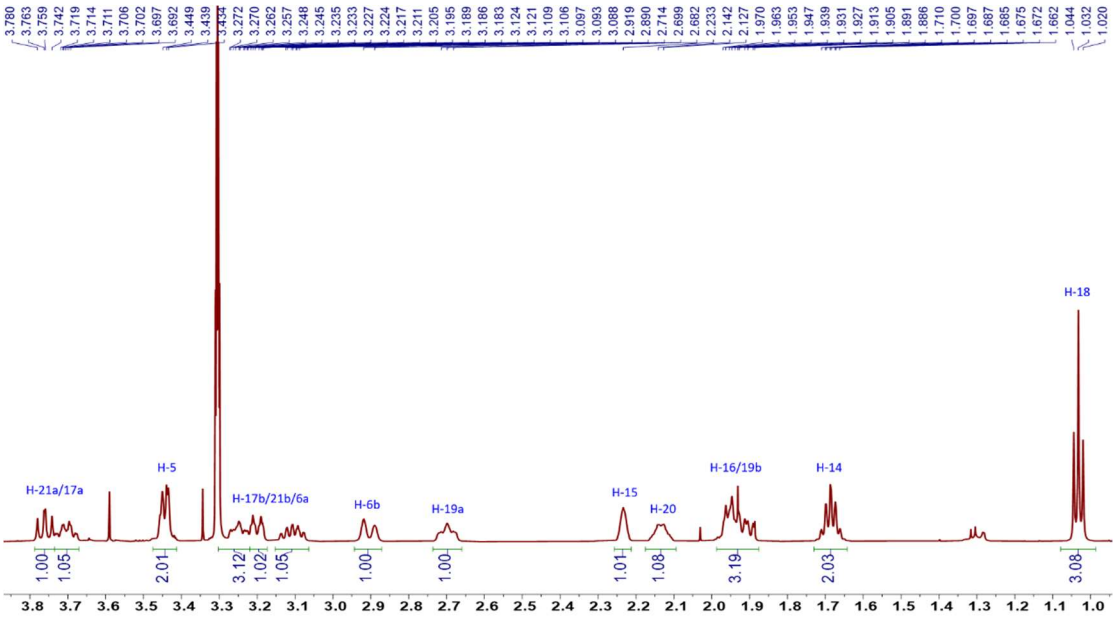


Figure S15: Enlarged ^{1}H NMR spectrum of **2**

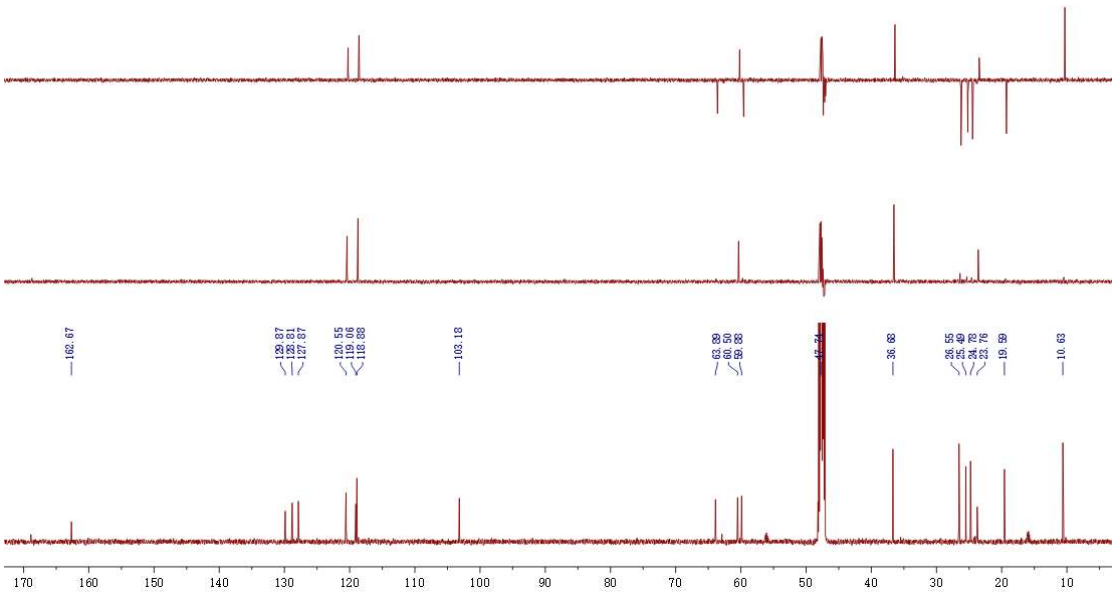


Figure S16: ^{13}C NMR spectrum of **2**

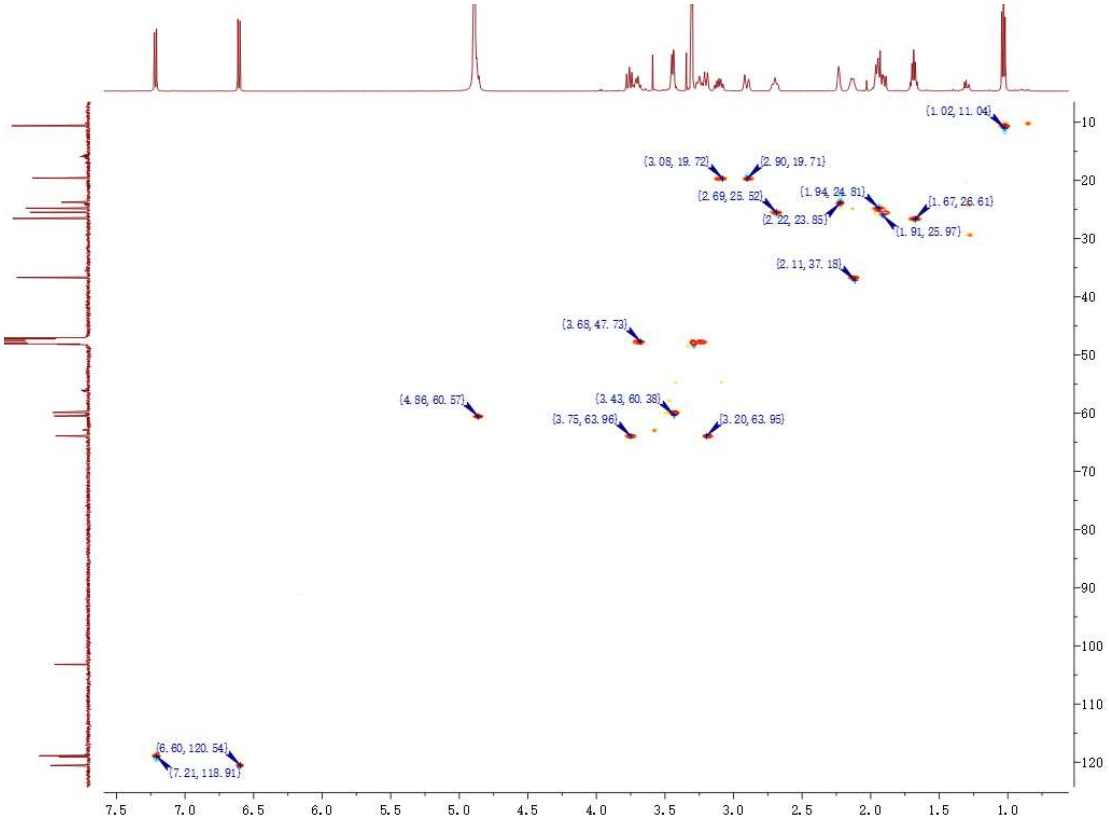


Figure S17: HSQC spectrum of **2**

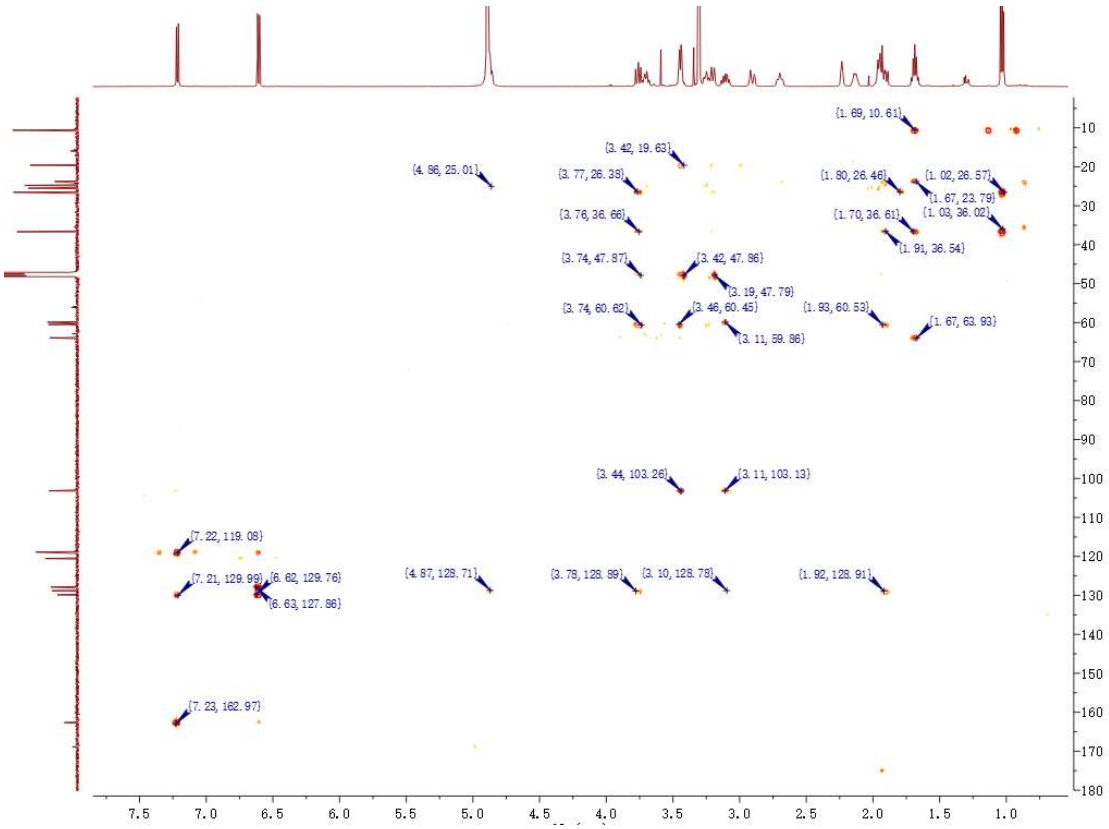


Figure S18: HMBC spectrum of **2**

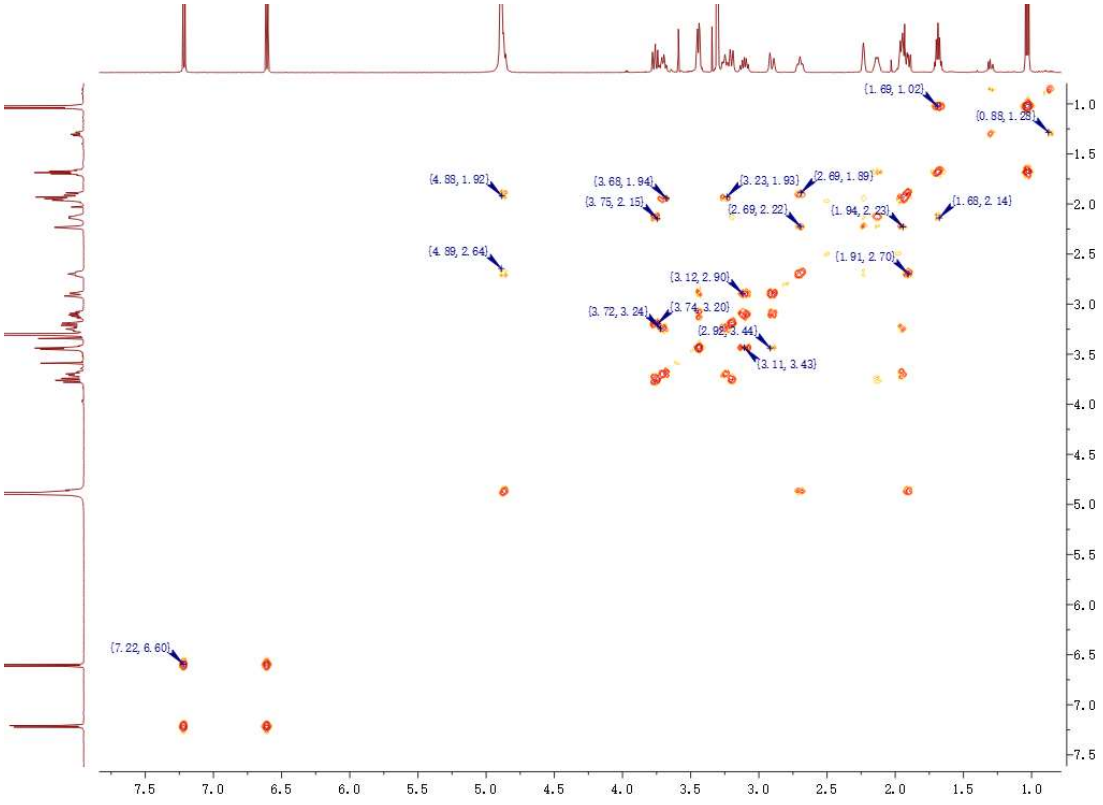


Figure S19: ^{1}H-^{1}H COSY spectrum of **2**

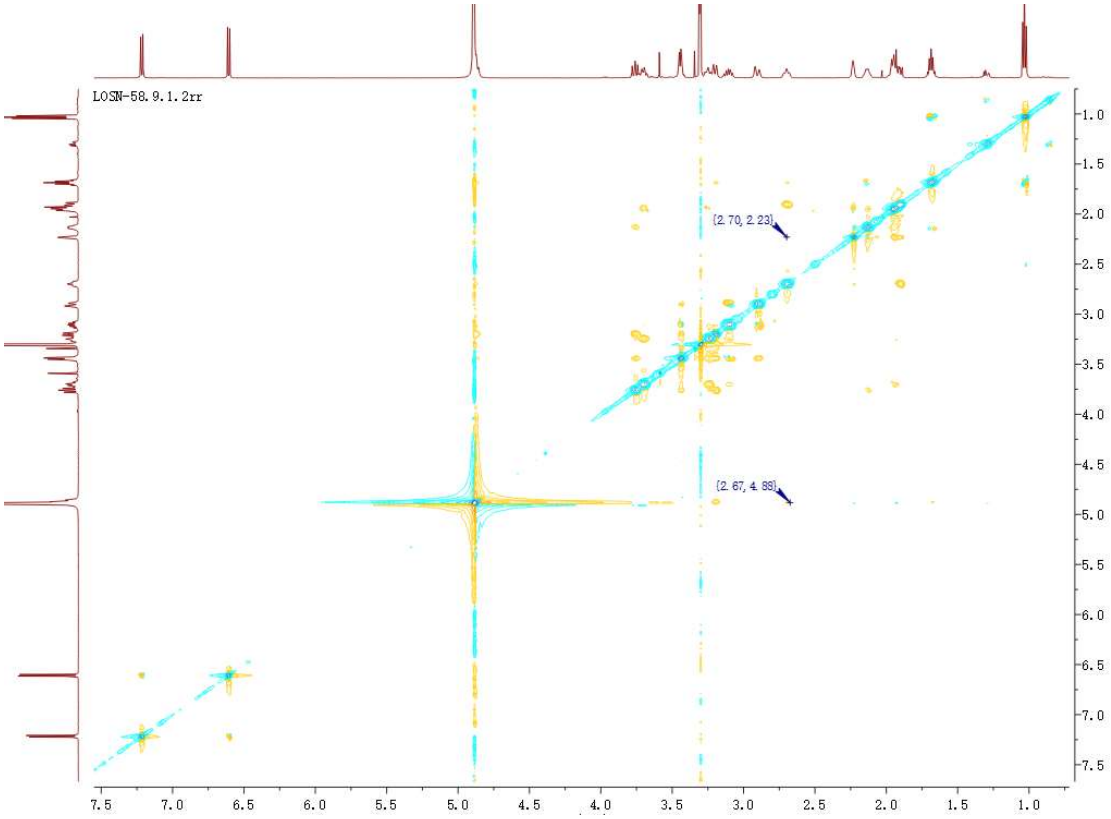


Figure S20: ROESY spectrum of **2**

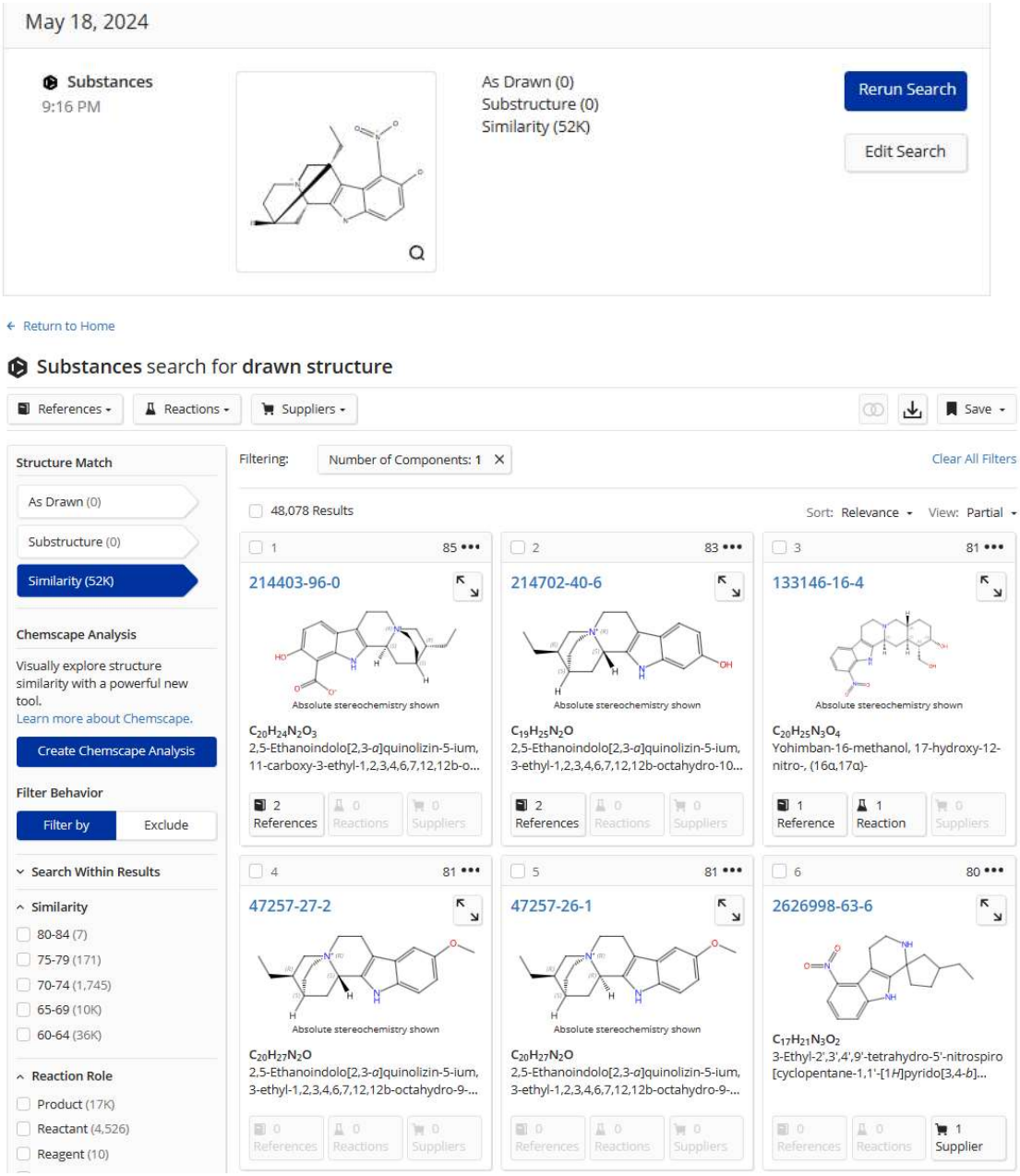
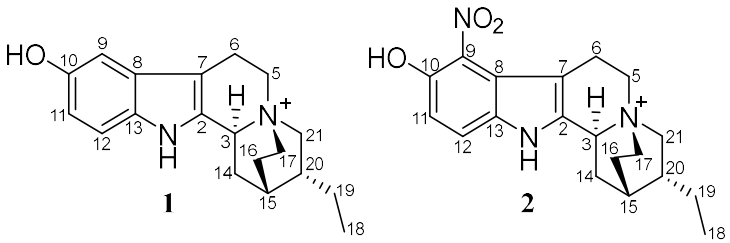


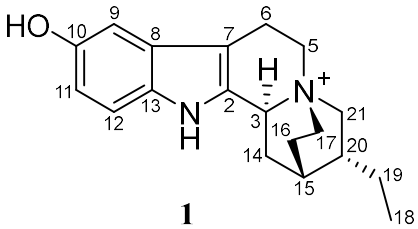
Figure S21: The Scifinder similarity report for **2**



1 **2**

Table S1: ^{1}H 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	



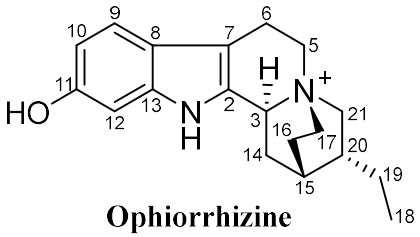


Table S2: ^{1}H and ^{13}C NMR data for compound **1** and **ophiorrhizine.**

	1		**ophiorrhizine**	
No.	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	60.9, CH_2	3.54 ddd (12.5,12,5)	61.3, CH_2
	3.43 dd (11.8, 10.4)		3.58 dd (12.5,6.5)	
6	2.74 m	17.9, CH_2	2.96 d (18)	18.3, CH_2
	2.90 m		3.11 ddd (18,12,6.5,2.5)	
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	26.6, CH_2	1.79 dd (13.5, 9.0)	26.9, CH_2
	2.59 m		2.71ddd(13.5, 9,4)	
15	2.10 s	24.8, CH	2.24 m	25.1, CH
16	1.77 m	26.1, CH_2	1.9 -1.98 m	26.3, CH_2
	1.83 m			
17	3.12 m	49.0, CH_2	3.28 m	49.1, CH_2
	3.41 m		3.67 m	
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	65.3, CH_2	3.25 m	65.2, CH_2
	3.69 t (11.5)		3.83 dd (12.5,10.5)	