

Supporting Information

Rec. Nat. Prod. 18:1 (2024) 161-164

Two Polyoxygenated Bipyrrrole Alkaloids from *Speranskia tuberculata*

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[†]Xu Tang and Fengqing Xu contributed equally to this work.

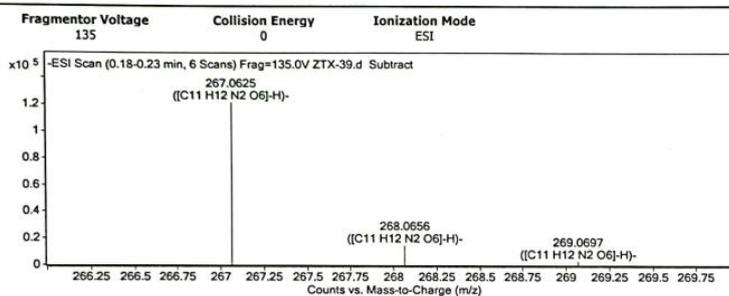
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Qualitative Analysis Report

Data Filename	ZTX-39.d	Sample Name	ZTX-39
Sample Type	Sample	Position	P1-F9
Instrument Name	Instrument 1	User Name	
Acq Method	s-.m	Acquired Time	5/18/2023 4:50:38 PM
IRM Calibration Status	Success	DA Method	PCDL.m
Comment			

Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.2)

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
209.0338	1	2816.58		
235.0358	1	9729.64		
267.0625	1	121359.35	C11 H12 N2 O6	(M-H)-
268.0656	1	14528.97	C11 H12 N2 O6	(M-H)-
270.0838	1	3141.56		
335.0498	1	8412.65		
403.0368	1	4803.73		
535.1317	1	2949.66		
982.9902	1	5705.52		
1033.9881	1	8808.86		

Formula Calculator Element Limits

Element	Min	Max
C	3	100
H	0	200
O	0	30
N	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C11 H12 N2 O6	268.0695	267.0623	267.0625	-0.20	-0.75	7.0000

--- End Of Report ---

Figure S1: HR-ESI-MS spectrum of **1** (speranberculatine B)

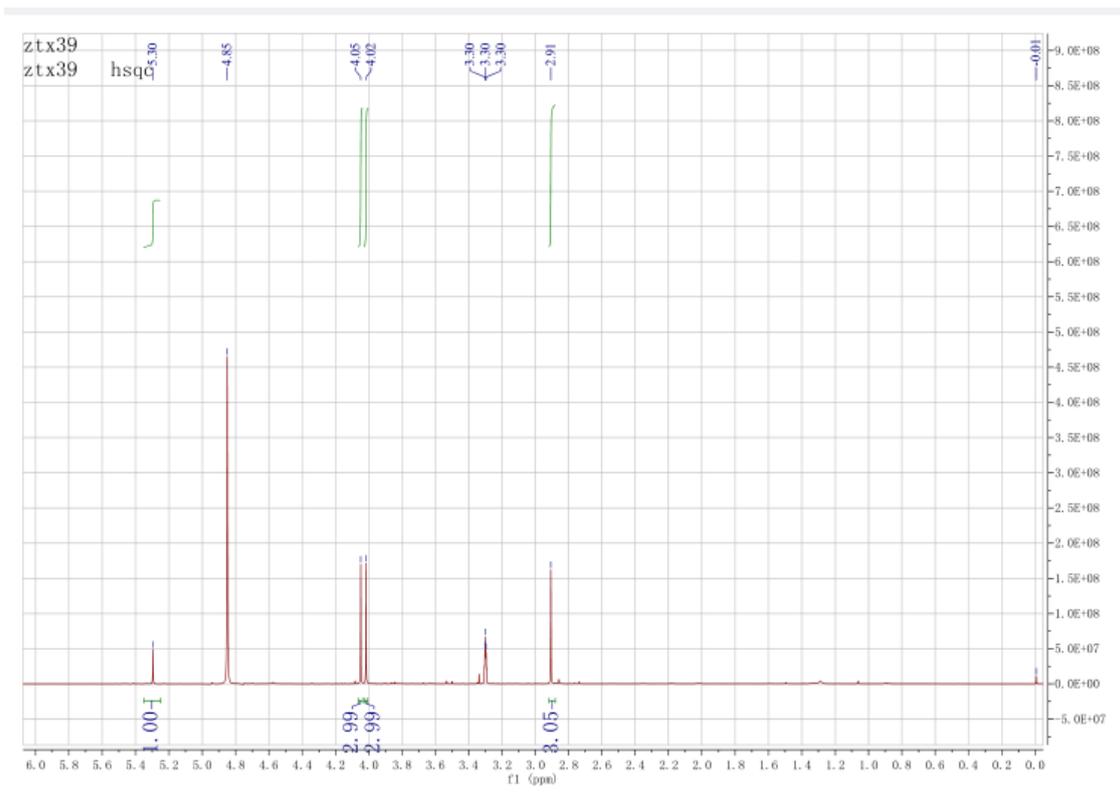


Figure S2: $^1\text{H-NMR}$ (600 MHz, CD_3OD) spectrum of **1** (speranberculatine B)

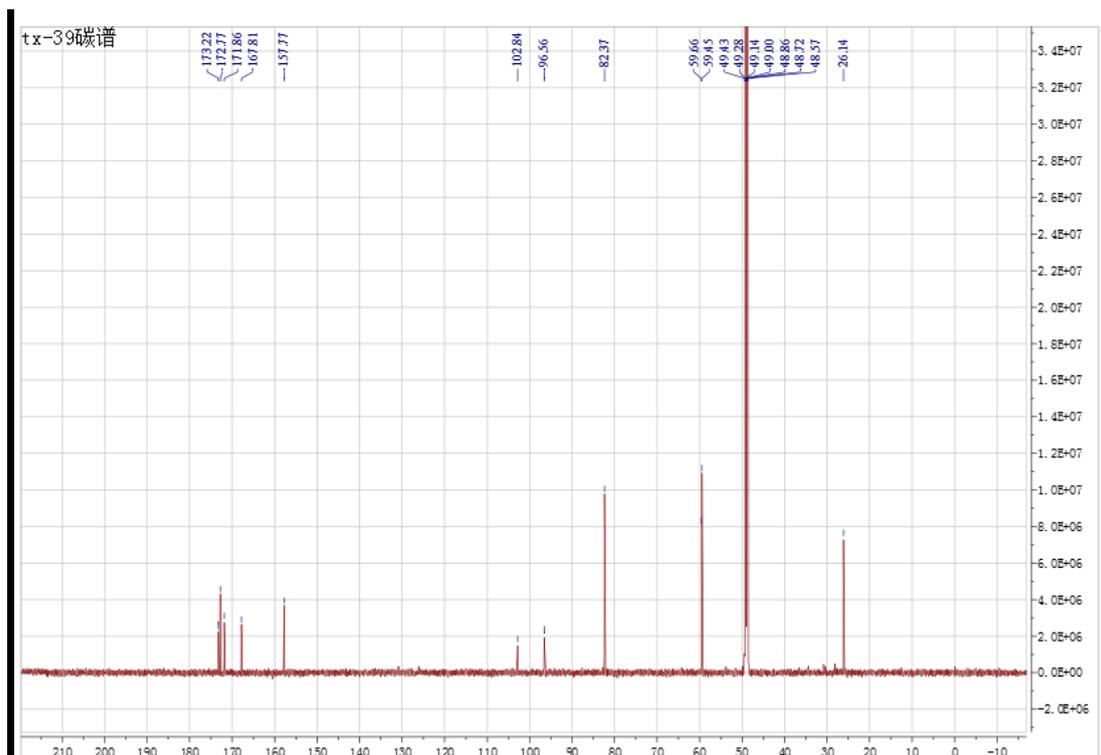


Figure S3: ^{13}C -NMR (150 MHz, CD_3OD) spectrum of **1** (speranberculatine B)

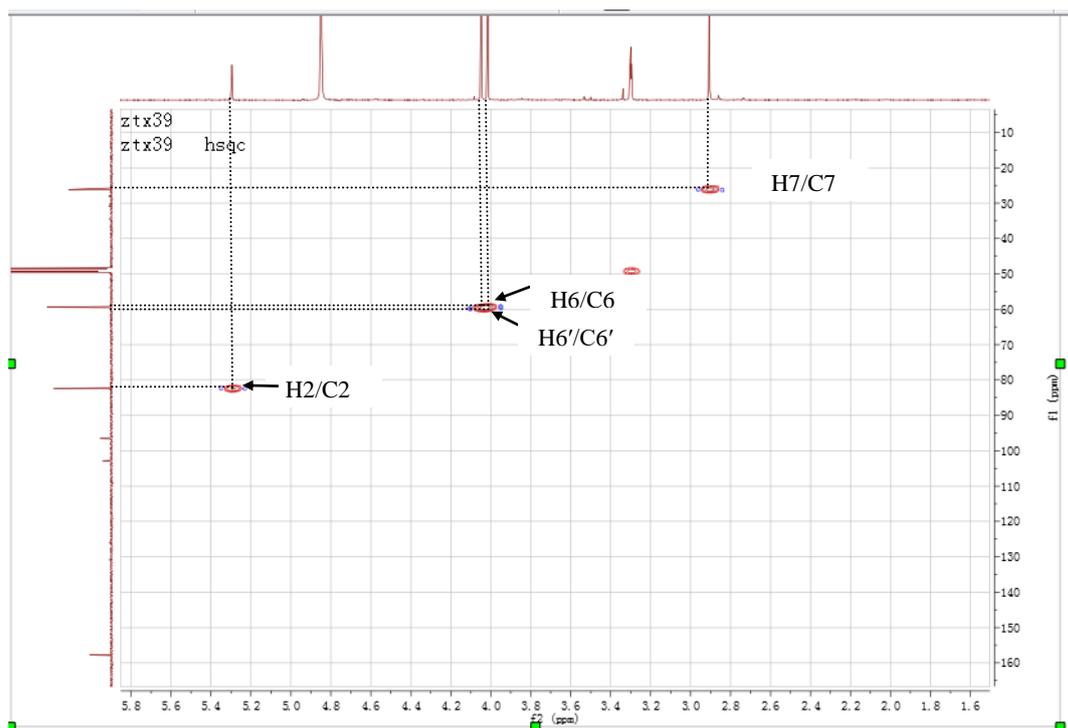


Figure S4: HSQC spectrum of **1** (speranberculatine B)

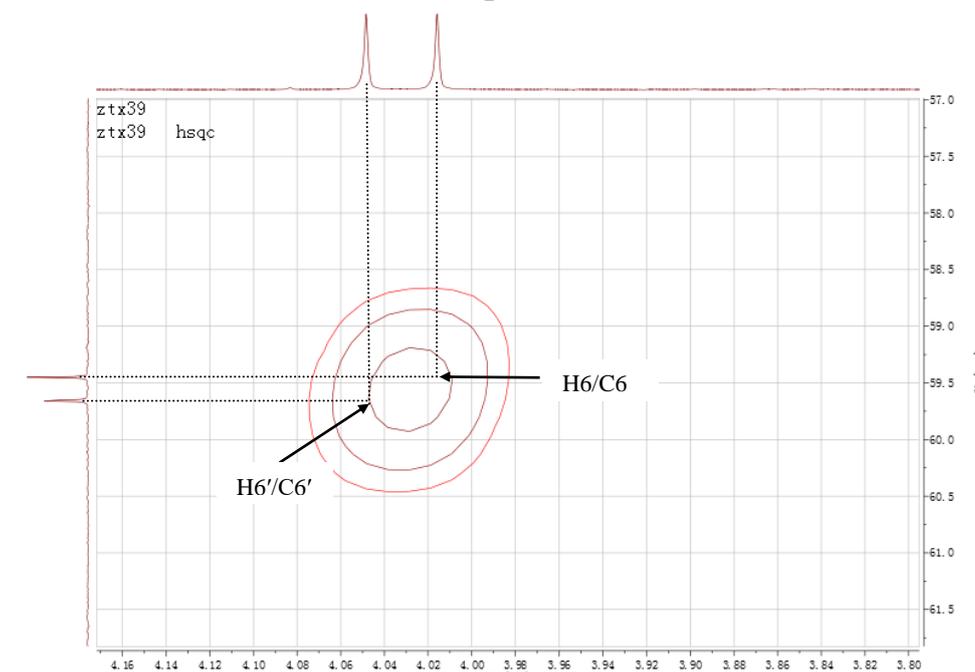


Figure S5: HSQC spectrum (δ 3.80-4.16 ppm) of **1** (speranberculatine B)

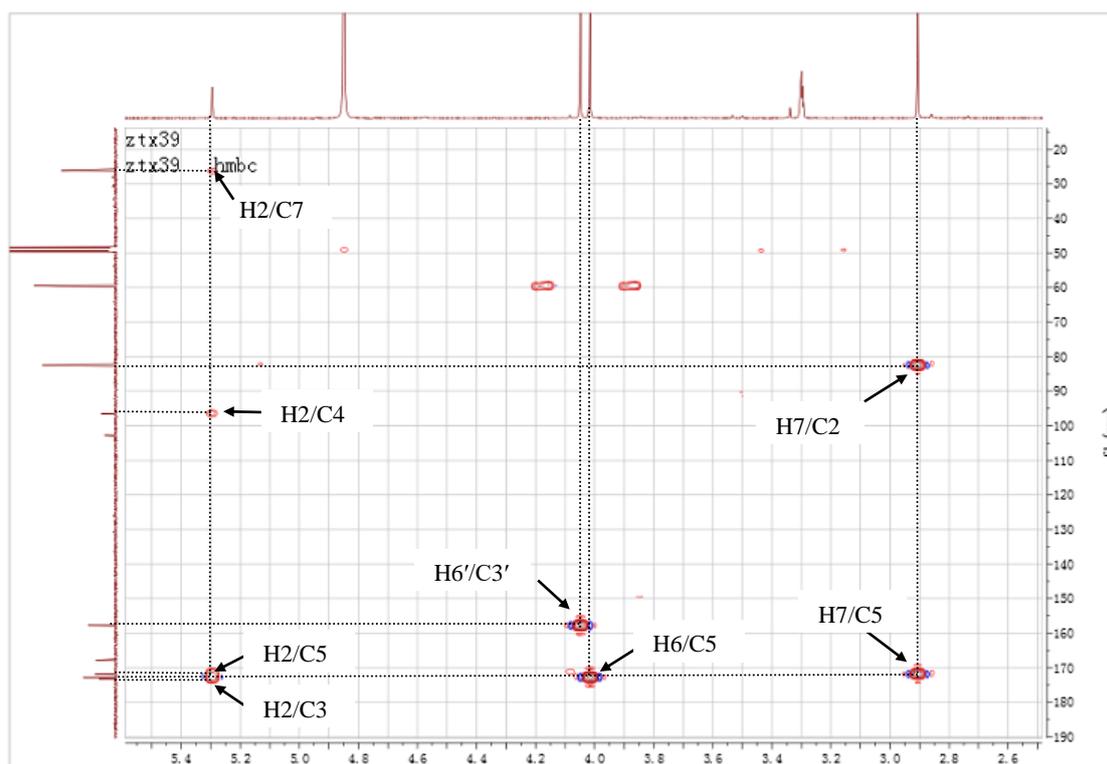


Figure S6: HMBC spectrum of **1** (speranberculatine B)

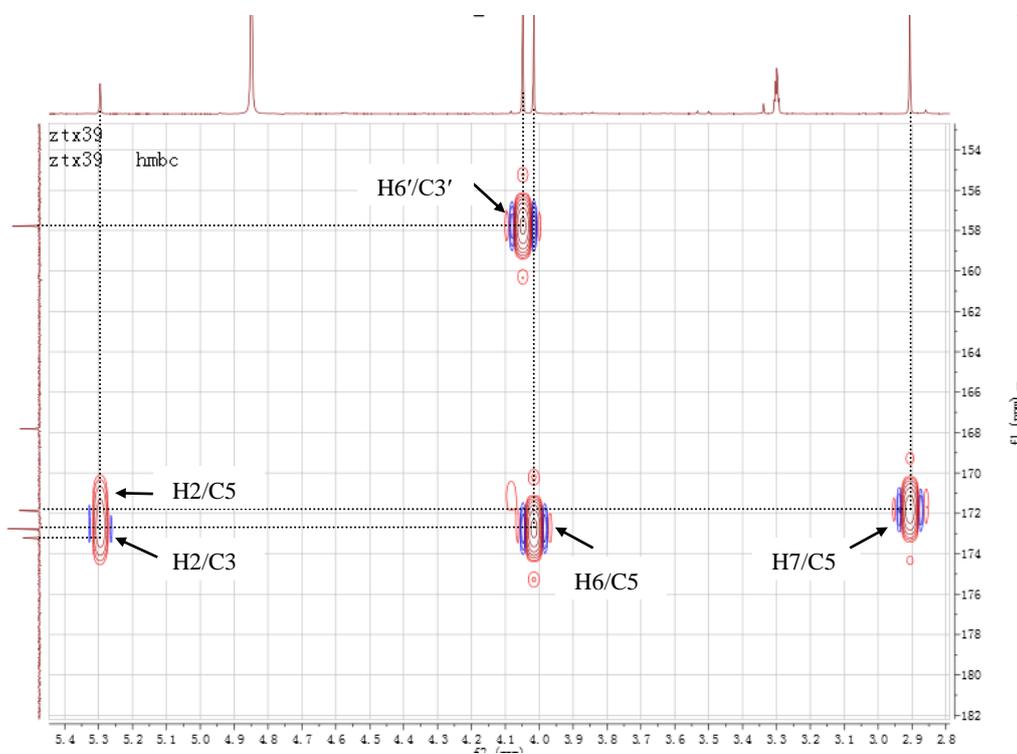


Figure S7: HMBC spectrum (δ 2.80-5.40 ppm) of **1** (speranberculatine B)

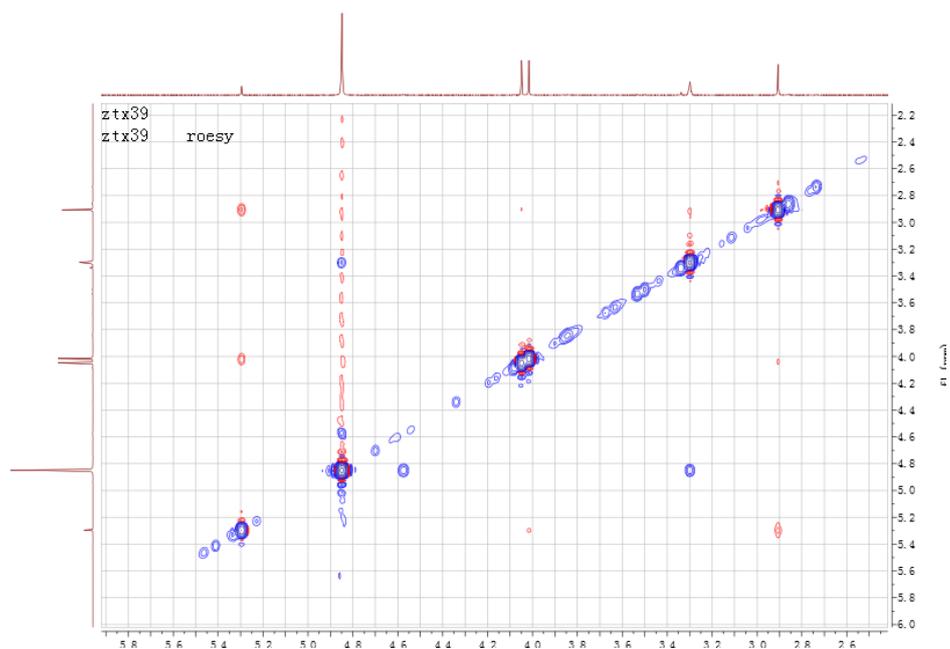


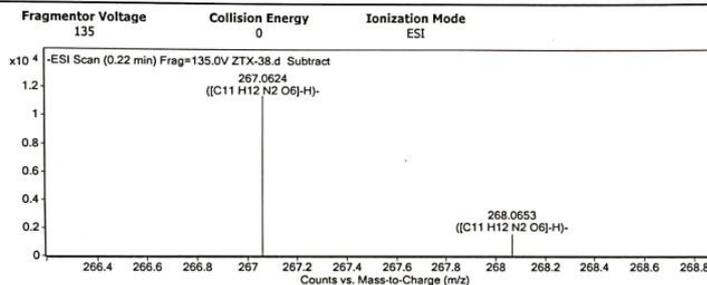
Figure S8: ROESY spectrum of **1** (speranberculatine B)

Qualitative Analysis Report

Data Filename	ZTX-38.d	Sample Name	ZTX-38
Sample Type	Sample	Position	P1-F8
Instrument Name	Instrument 1	User Name	
Acq Method	s-m	Acquired Time	5/18/2023 4:49:29 PM
IRM Calibration Status	Success	DA Method	PCDL.m
Comment			

Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.2)

User Spectra



Peak List				
m/z	z	Abund	Formula	Ion
112.9856	1	12364.33		
235.0356	1	13044.95		
253.0464	1	9036.88		
267.0624	1	11440.88	C11 H12 N2 O6	(M-H)-
313.068	1	41159.43		
314.0712	1	6498.47		
349.1181	1	2601.92		
381.0542	1	3627.93		
1033.9881	1	29397.3		
1034.9907	1	5856.94		

Formula Calculator Element Limits		
Element	Min	Max
C	3	100
H	0	200
O	0	30
N	0	3

Formula Calculator Results						
Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C11 H12 N2 O6	268.0695	267.0623	267.0624	-0.10	-0.37	7.0000

--- End Of Report ---

Figure S9: HR-ESI-MS spectrum of **2** (speranberculatine C)

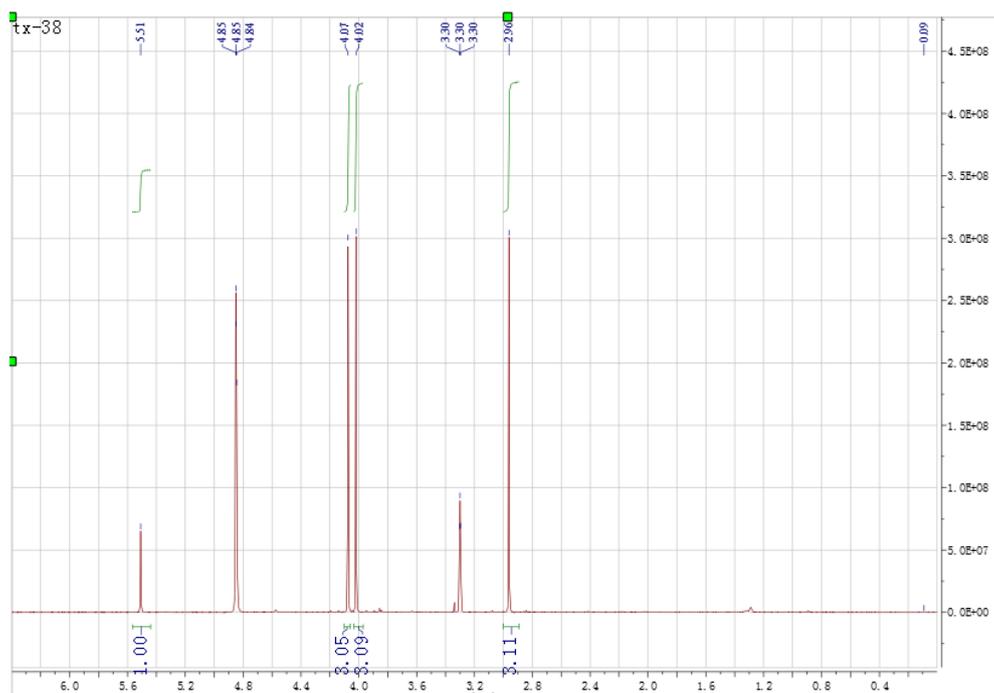


Figure S10: ¹H-NMR (600 MHz, CD₃OD) spectrum of **2** (speranberculatine C)

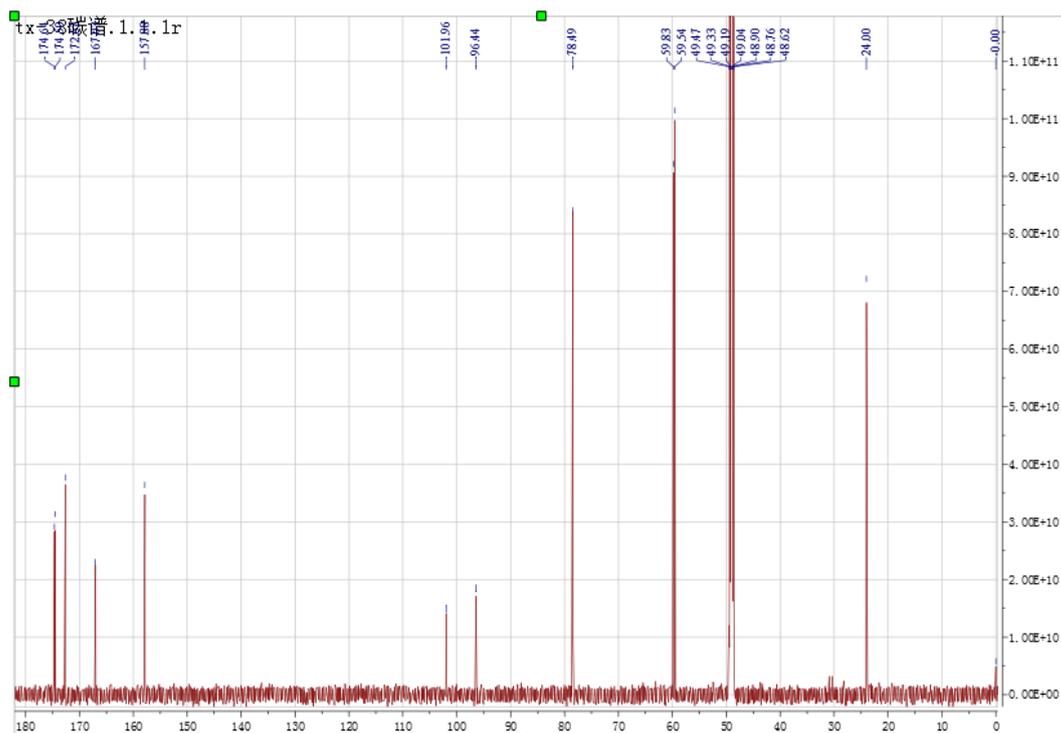


Figure S11: ^{13}C -NMR (150 MHz, CD_3OD) spectrum of **2** (speranberculatine C)

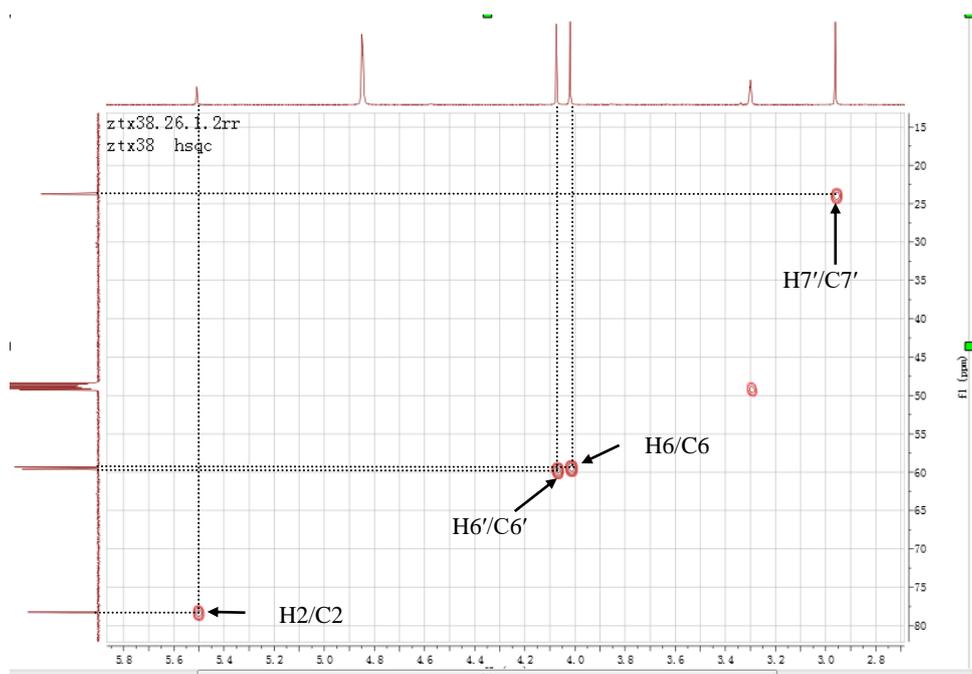


Figure S12: HSQC spectrum of **2** (speranberculatine C)

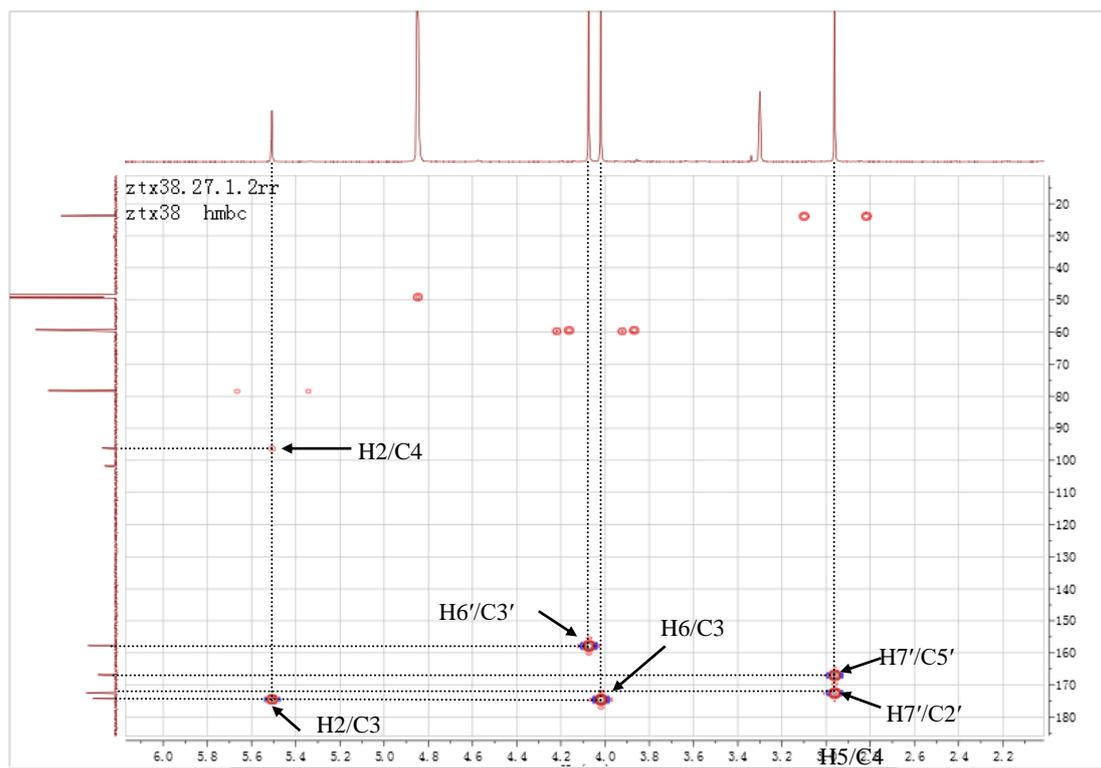


Figure S13: HMBC spectrum of **2** (speranberculatine C)

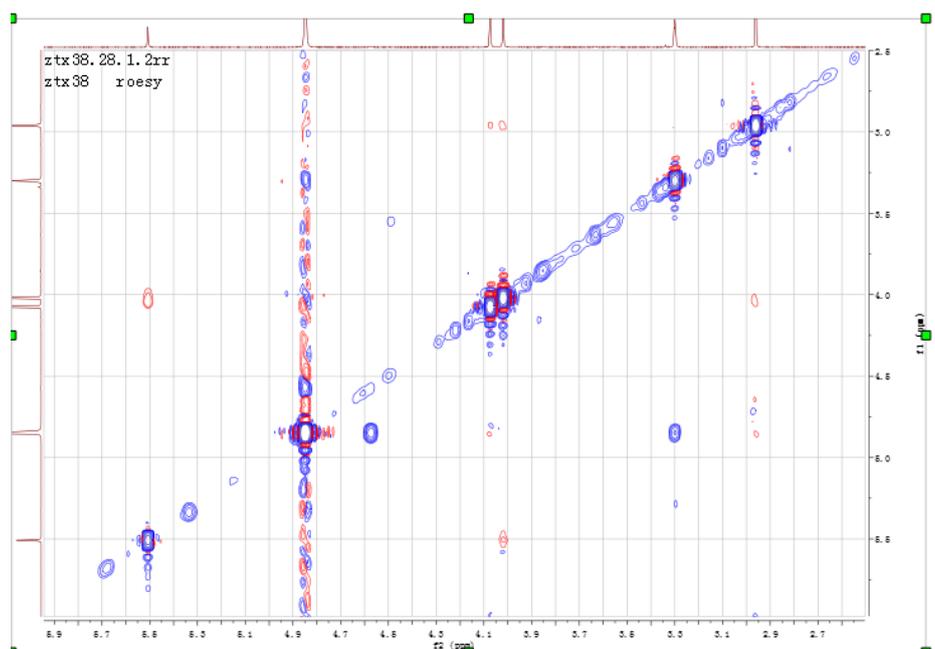


Figure S14: ROESY spectrum of **2** (speranberculatine C)

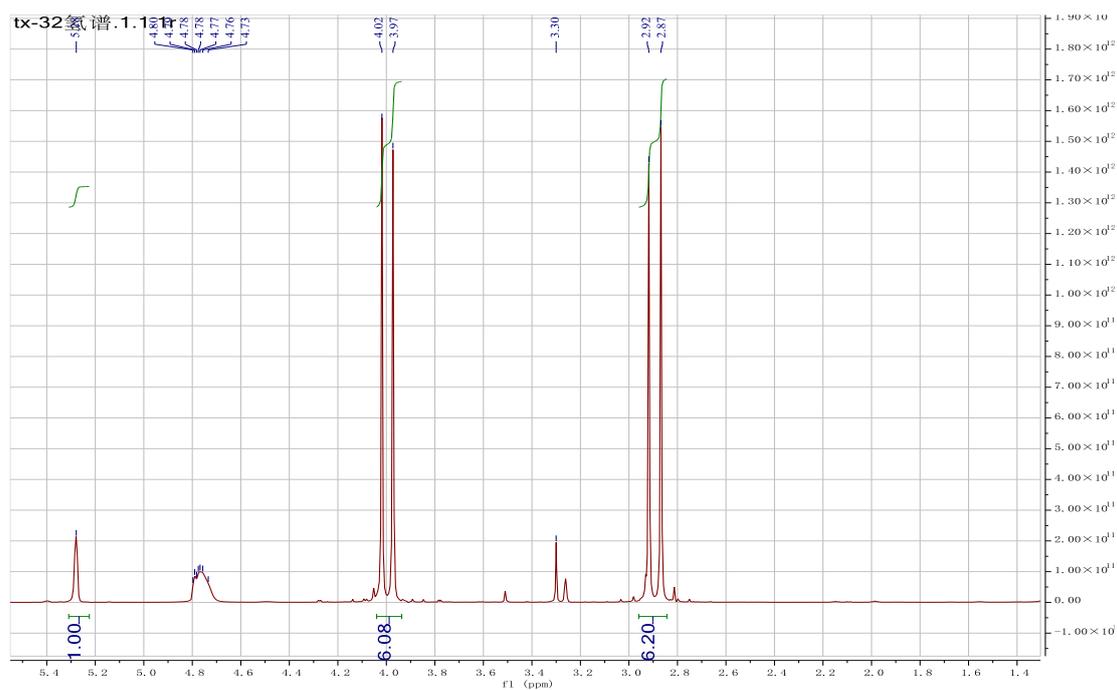


Figure S15: ¹H-NMR (600 MHz, CD₃OD) spectrum of **3** (speranberculatine A)

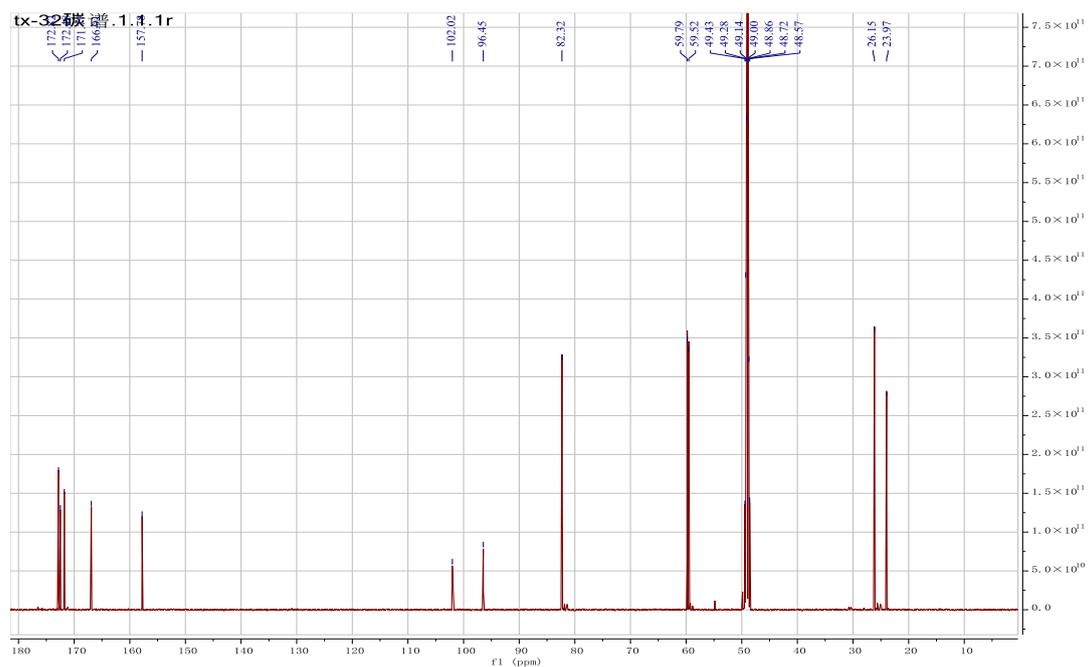


Figure S16: ¹³C-NMR (150 MHz, CD₃OD) spectrum of **3** (speranberculatine A)

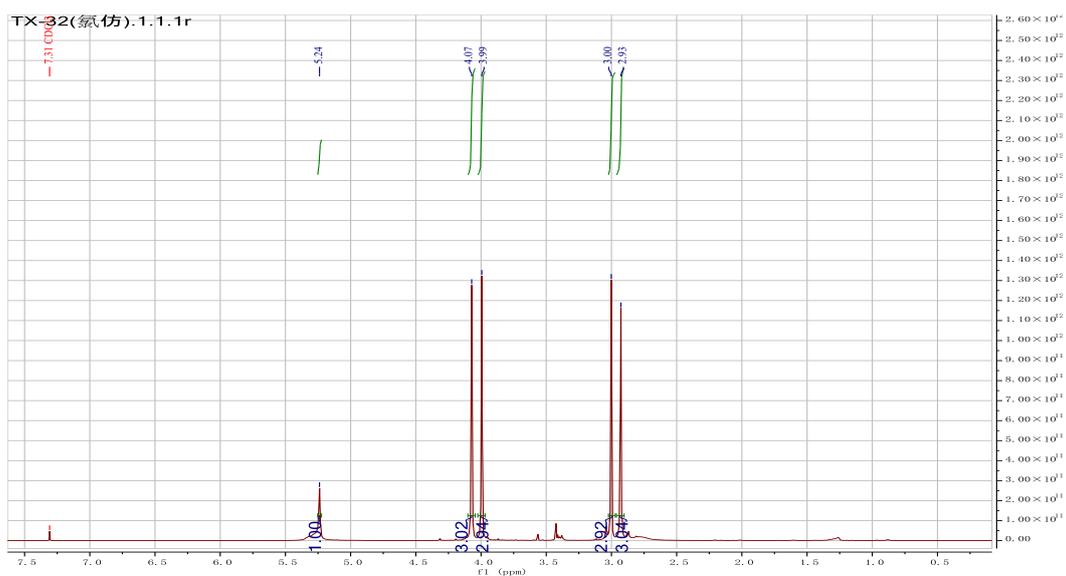


Figure S17: $^1\text{H-NMR}$ (600 MHz, CD_3Cl) spectrum of **3** (speranberculatine A)

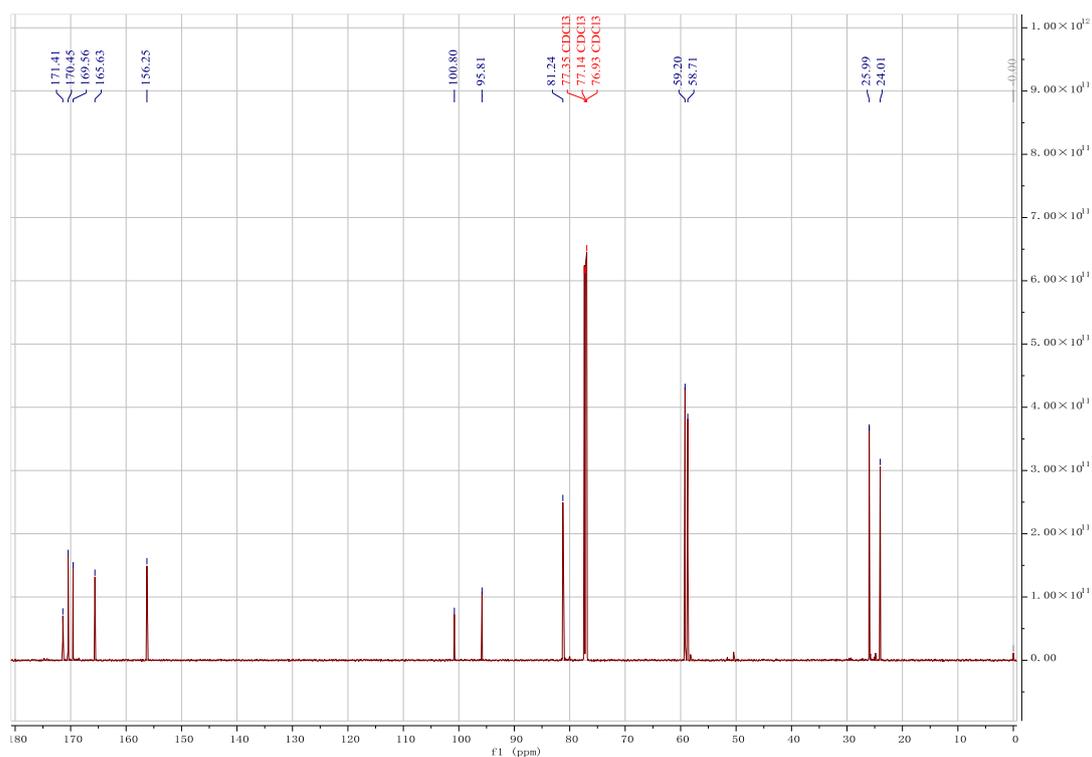


Figure S18: $^{13}\text{C-NMR}$ (150 MHz, CD_3Cl) spectrum of **3** (speranberculatine A)