SUPPORTING INFORMATION

An indole diterpenoid isolated from the fungus *Drechmeria* sp. and its antimicrobial activity

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ABSTRACT: One new indole diterpenoid, drechmerin I (**1**), was isolated from the fermentation broth of *Drechmeria* sp. isolated from the root of *Panax notoginseng*. Its structure was elucidated based on 1D and 2D NMR, HRESIMS, and electronic circular dichroism (ECD) spectroscopic analyses as well as TD DFT calculations of ECD spectra. Drechmerin I (**1**) was assayed for its antimicrobial activities against *Candida albicans*, *Staphylococcus aureus*, *Bacillus cereus*, *B. subtillis*, *Pseudomonas aeruginosa*, and *Klebsiella pneumonia*, respectively. Drechmerin I (**1**) showed antimicrobial activities against *B. subtillis* with an MIC value of 200 μg/mL. The interaction of *S.*

aureus peptide deformylase with drechmerin I (**1**) was investigated by molecular docking.

Keywords: *Drechmeria* sp., indole diterpenoid, antimicrobial activity, molecular docking

Content

Table S1. ^{1}H (600 MHz) and ^{13}C NMR (150 MHz) data of compound 1 in MeOH-d_4

No.	δ_C	δ_H (J in Hz)	No.	δ_C	δ_H (J in Hz)
2	153.8		18	117.2	
3	52.1		19	126.5	
4	43.9		20	118.9	7.29 d (7.8)
5	27.4	2.62 m	21	119.8	6.92 td (7.8, 1.3)
		1.67 m	22	120.8	6.95 td (7.8, 1.3)
6	29.8	2.23 m	23	112.7	7.27 d (7.8)
		1.82 m	24	141.9	
7	73.1	4.33 d (9.1)			
9	72.9	3.55 (9.4)	25	16.6	1.28 s
10	72.8	3.94 (9.4)	26	19.0	1.16 s
11	61.8	3.63 s	27	76.0	
12	69.0		29	17.0	1.23 s
13	78.9		30	28.7	1.21 s
14	30.7	1.68 m	1'	97.8	4.83 d (5.5)
		1.53 td (13.2, 4.0)	2'	77.6	3.91 d (5.5)
15	22.0	1.96 m	3'	145.4	
		1.60 m	4'	114.3	4.98 br s
16	51.7	2.84 m			4.88 br s
17	28.2	2.65 dd (12.9, 6.1)	5'	19.1	1.76 s
		2.36 dd (12.9, 11.1)			

Table S2. Antibacterial and antifungal activities (MIC value, μg/mL) of compound 1

Compound	*C. albicans*	*S. aureus*	*B. cereus*	*B. subtillis*	*P. aeruginosa*	*K. pneumonia*
1	> 400	> 400	> 400	200	> 400	> 400
Ampicillin[a]	-	8	2.5	3.5	10	10
Geneticin[a]	6.3	-	-	-	-	-

[a]Positive control.

Table S3. The optimized conformers of 2′*S*-1

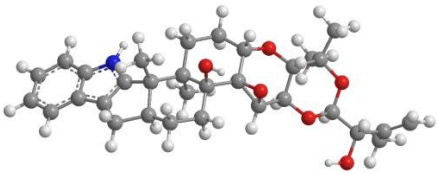
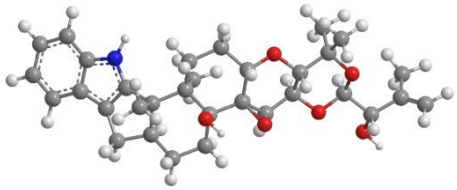
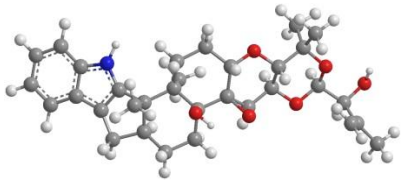
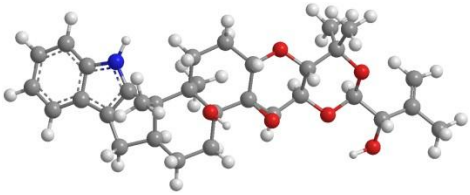
C1	C2
	
C3	C4
	

Table S4. B3LYP-calculated relative energies (Kcal/mol) and conformational population (%) for the most stable conformers of 2′*S*-1

Comound	conformer	ΔE (kcal/mol)[a]	Population (%)[b]
2′*S*-**1**	C1	0	83.29
	C2	0.001791	12.48
	C3	0.002891	3.88
	C4	0.005174	0.35

[a]Relative to conformer C1 with E6-31+G(d) = -1750.241046 Kcal/mol. [b]Calculated

using free energy values from Gaussian 09 according to ΔG = -RT In K.

Table S5. The optimized conformers of 2′*R*-1

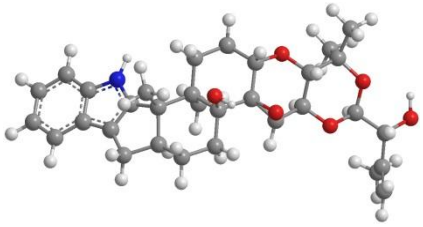
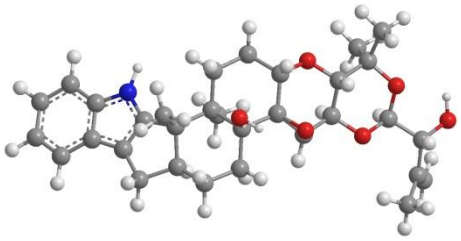
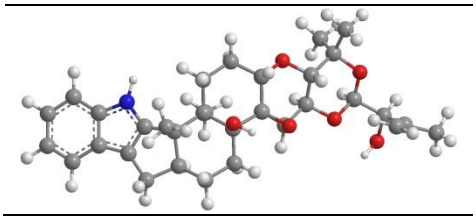
C1	C2
	
C3	
	

Table S6. B3LYP-calculated relative energies (Kcal/mol) and conformational population (%) for the most stable conformers of 2′*R*-1

Comound	conformer	ΔE (kcal/mol)[a]	Population (%)[b]
2′*R*-**1**	C1	0	73.75
	C2	0.000984	25.99
	C3	0.005312	0.26

[a]Relative to conformer C1 with E6-31+G(d) = -1750.2413581 Kcal/mol. [b]Calculated using free energy values from Gaussian 09 according to ΔG = -RT In K.

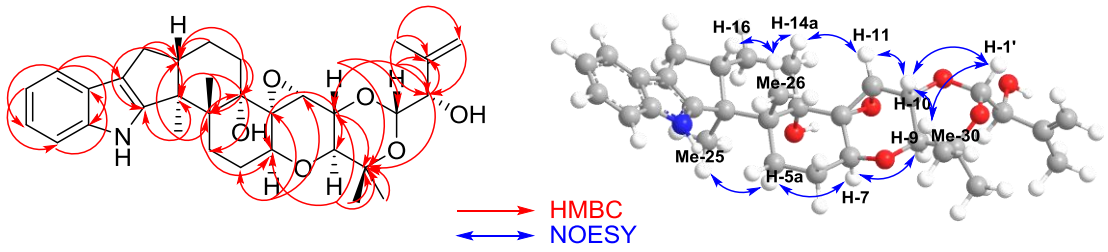


Figure S1. Selected HMBC and NOESY correlations of compound 1

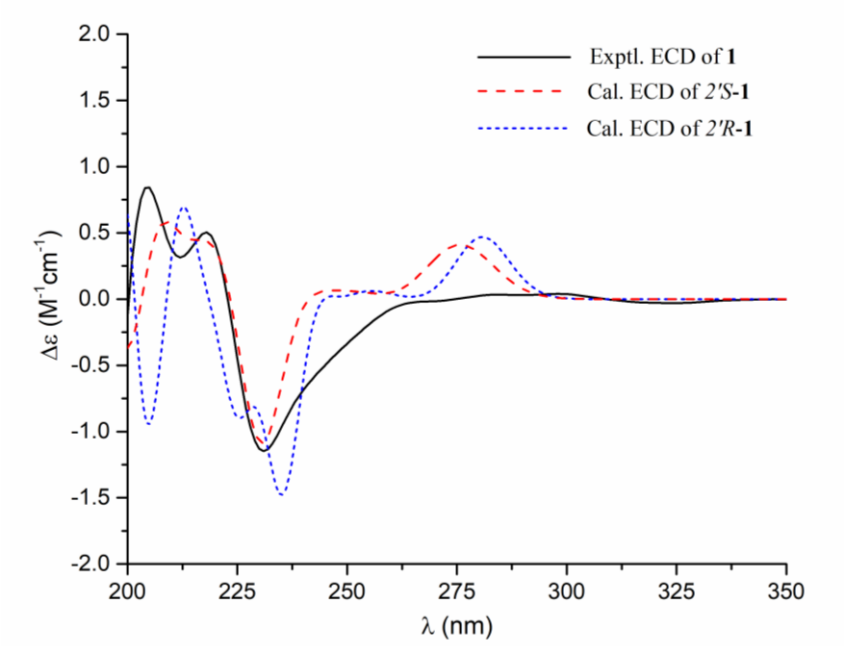


Figure S2. Calculated and experimental ECD spectra of 1 **at the B3LYP/6-311++G (d,p) level**

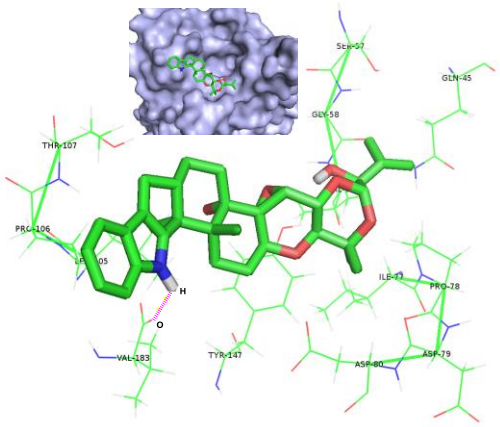


Figure S3. Interaction of compound 1 with PDF.

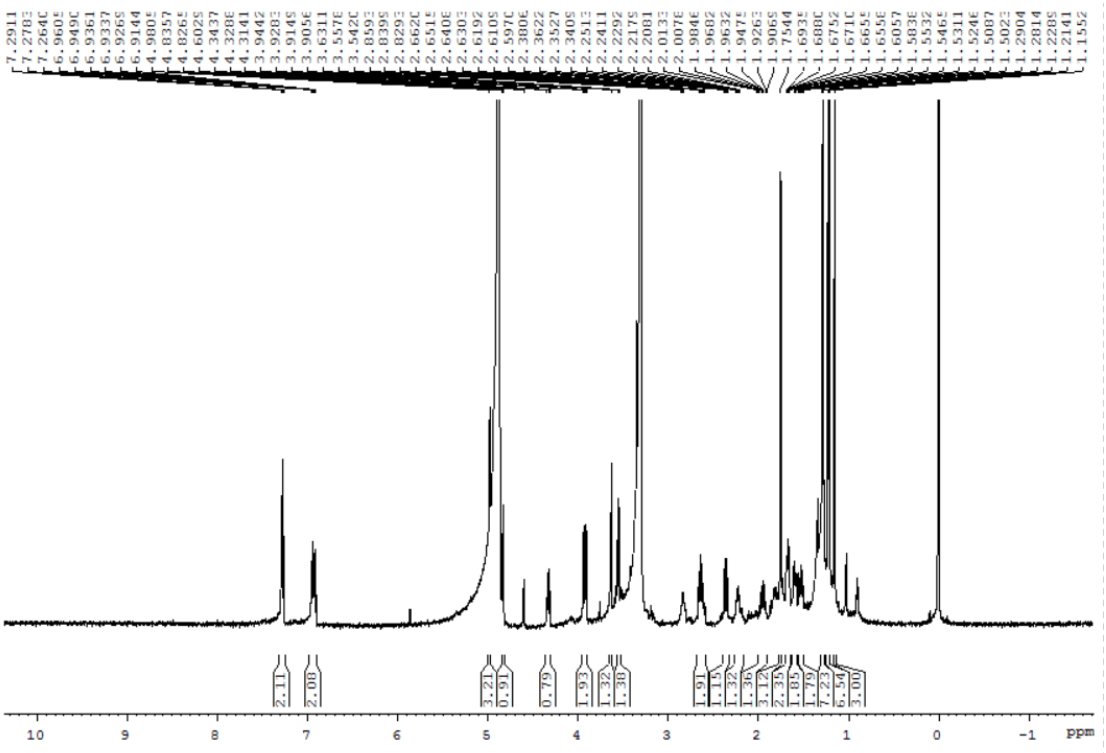


Figure S4. ^{1}H-NMR spectrum of 1 (600 MHz, MeOH-d_4)

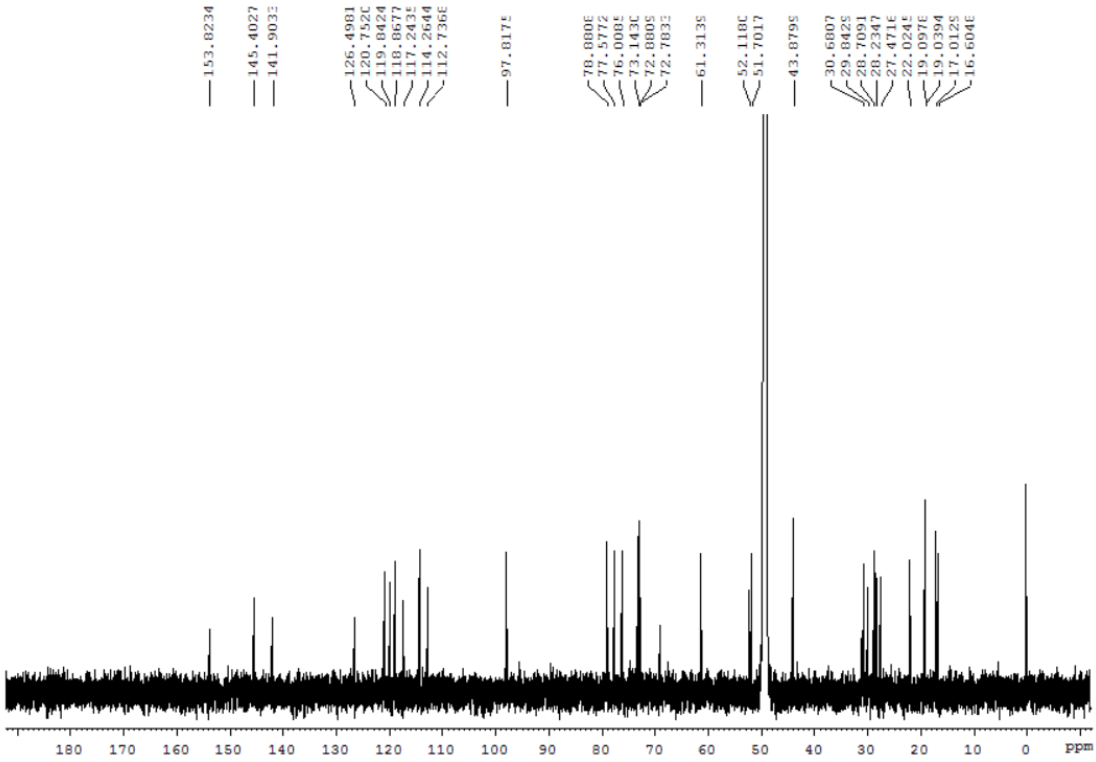


Figure S5. ^{13}C-NMR spectrum of 1 (150 MHz, MeOH-d_4)

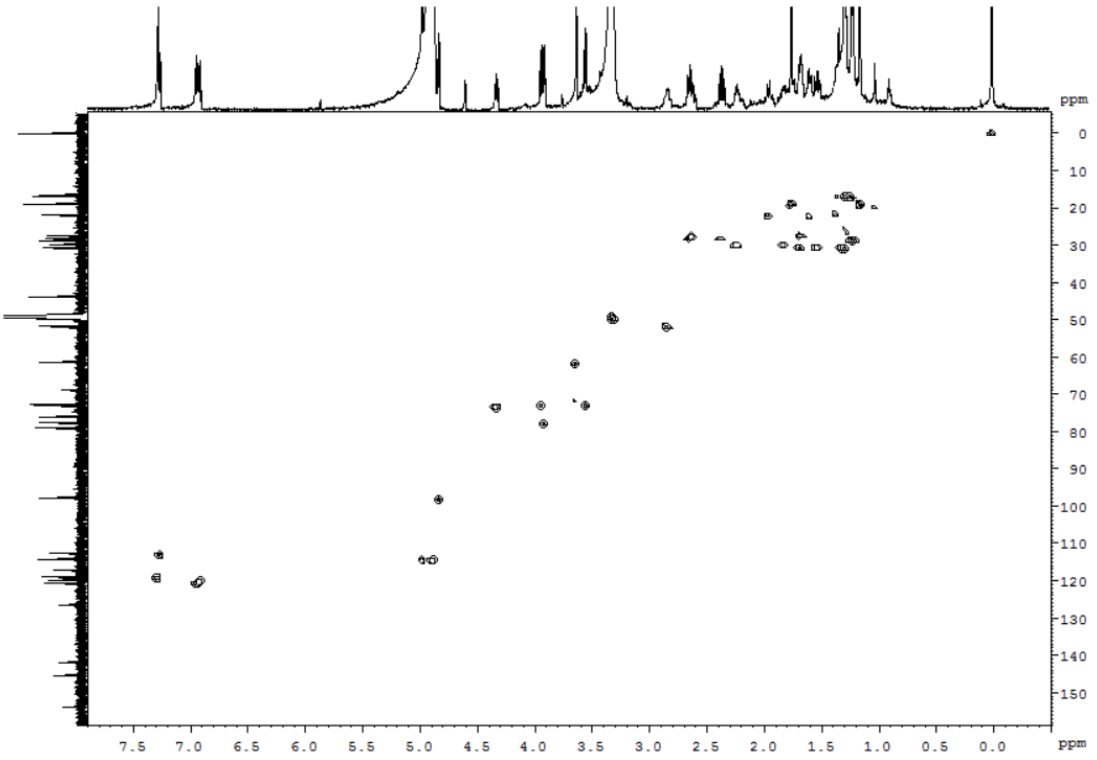
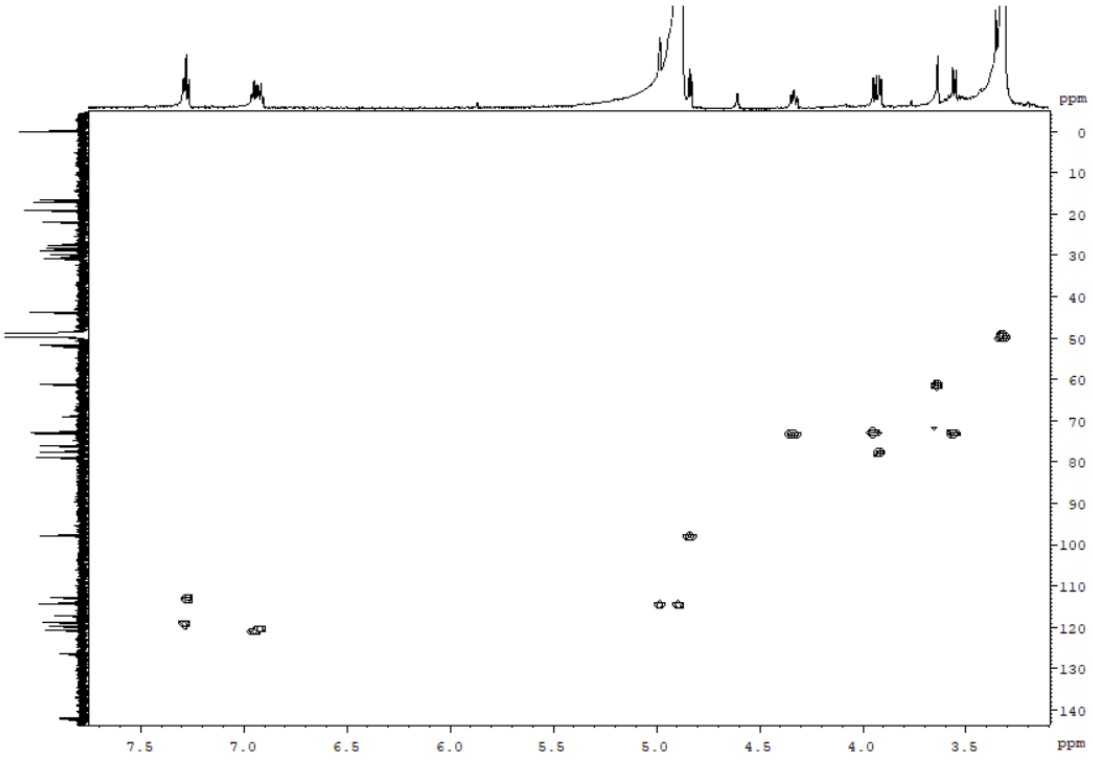


Figure S6. HSQC spectrum of 1 (600 MHz, MeOH-d_4)



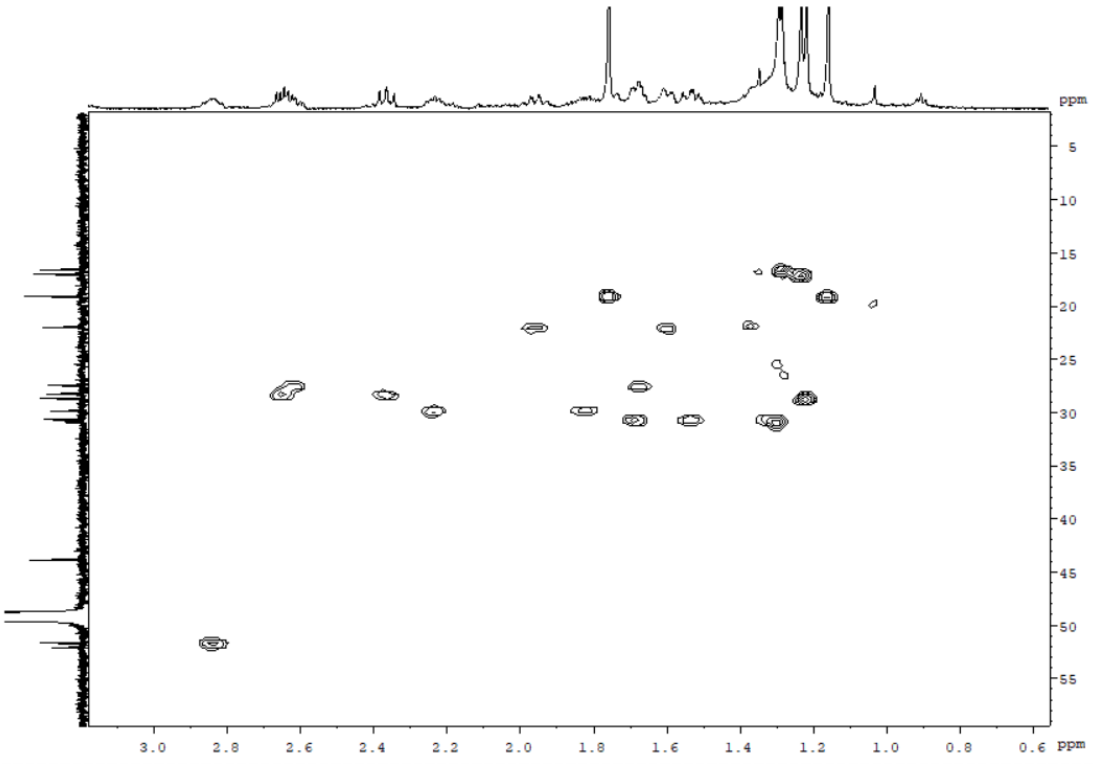


Figure S7. Amplified HSQC spectrum of 1 (600 MHz, MeOH-d_4)

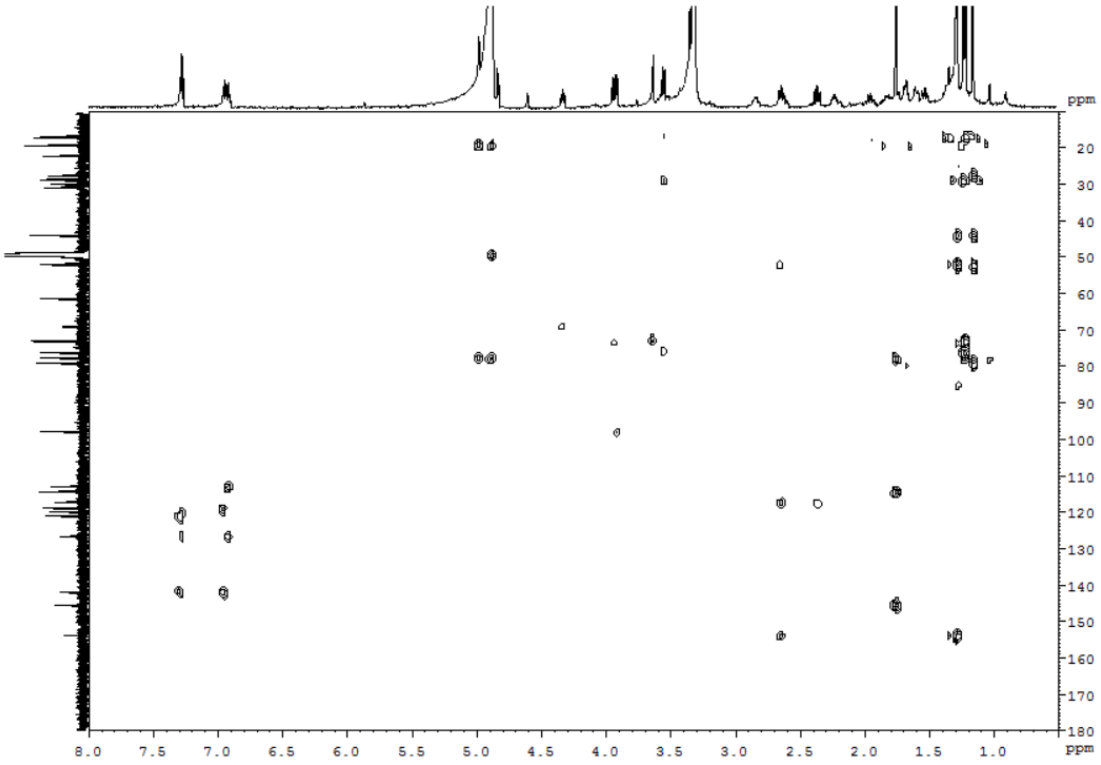
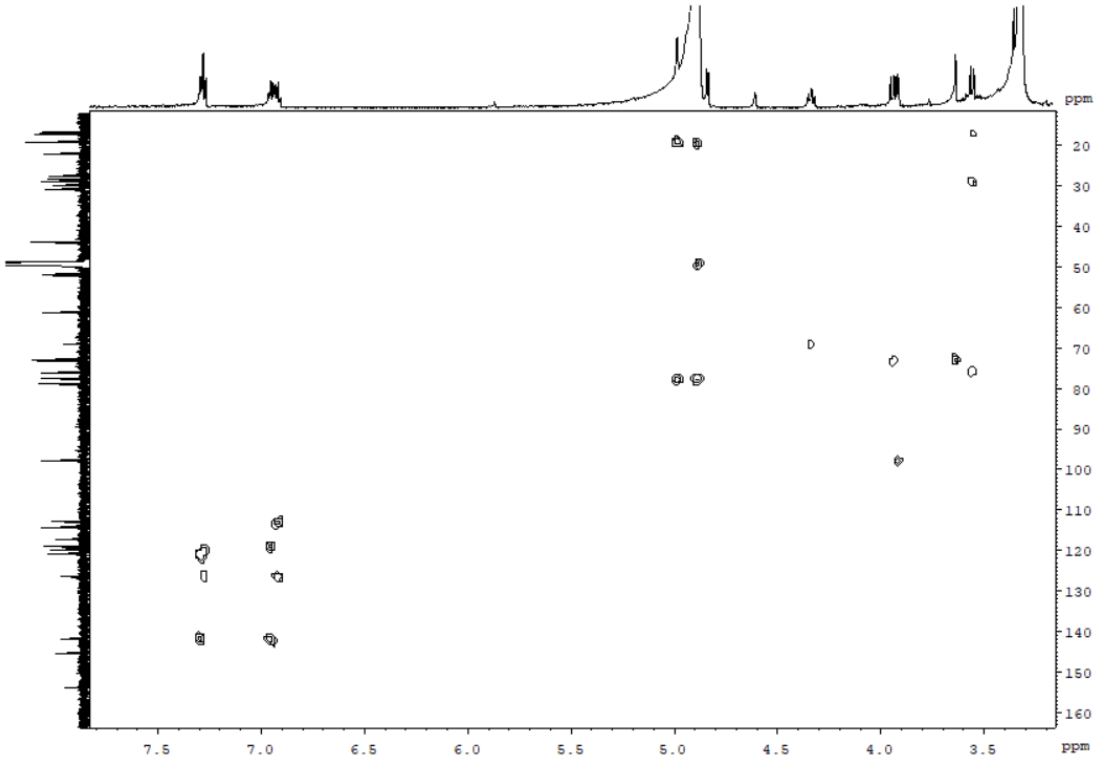


Figure S8. HMBC spectrum of 1 (600 MHz, MeOH-d_4)



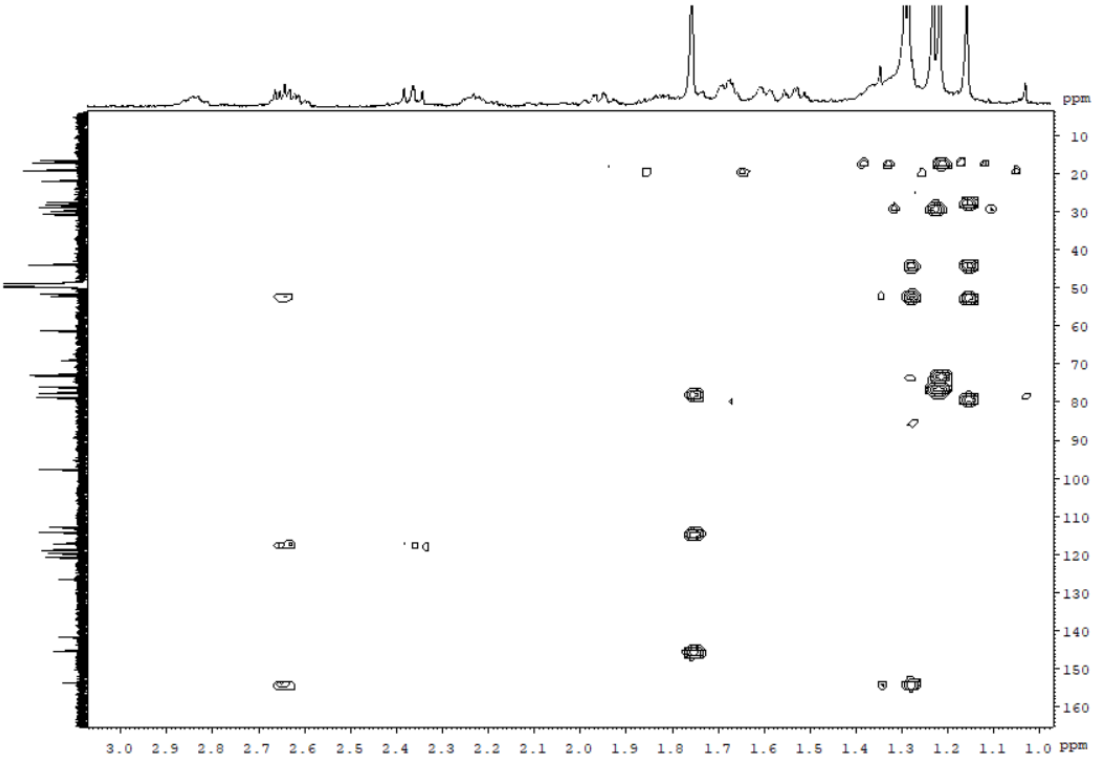


Figure S9. Amplified HMBC spectrum of 1 (600 MHz, MeOH-d_4)

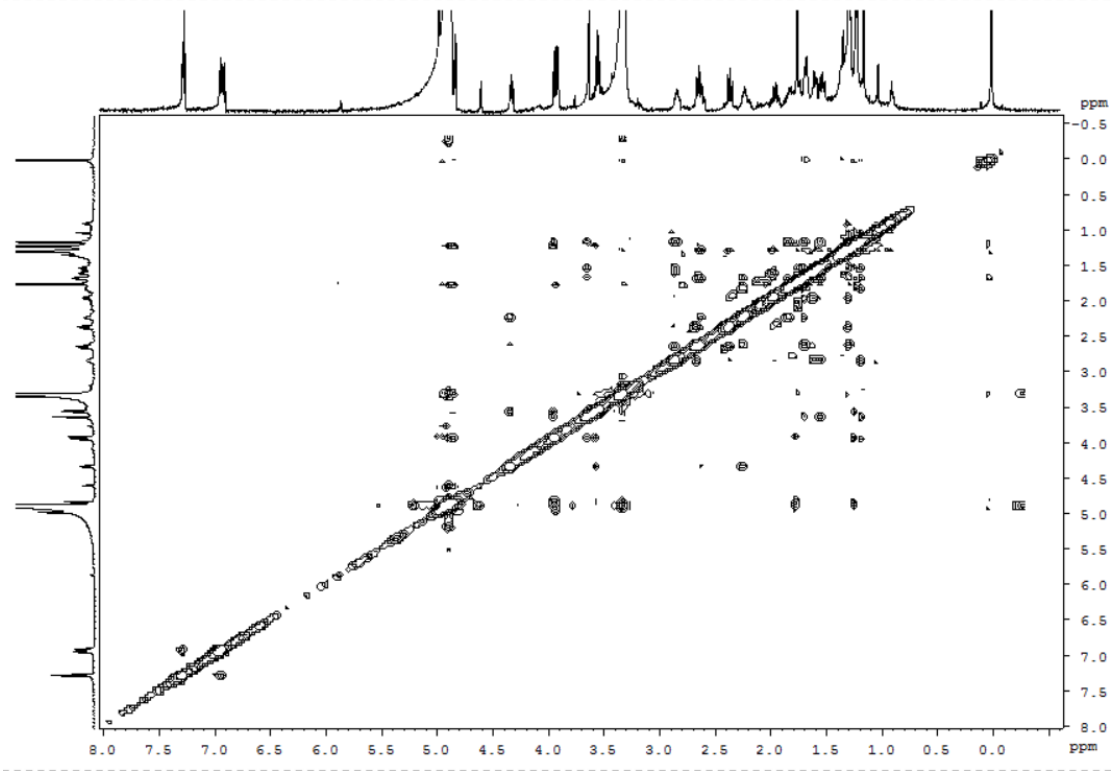


Figure S10. NOESY spectrum of 1 (600 MHz, MeOH-d_4)

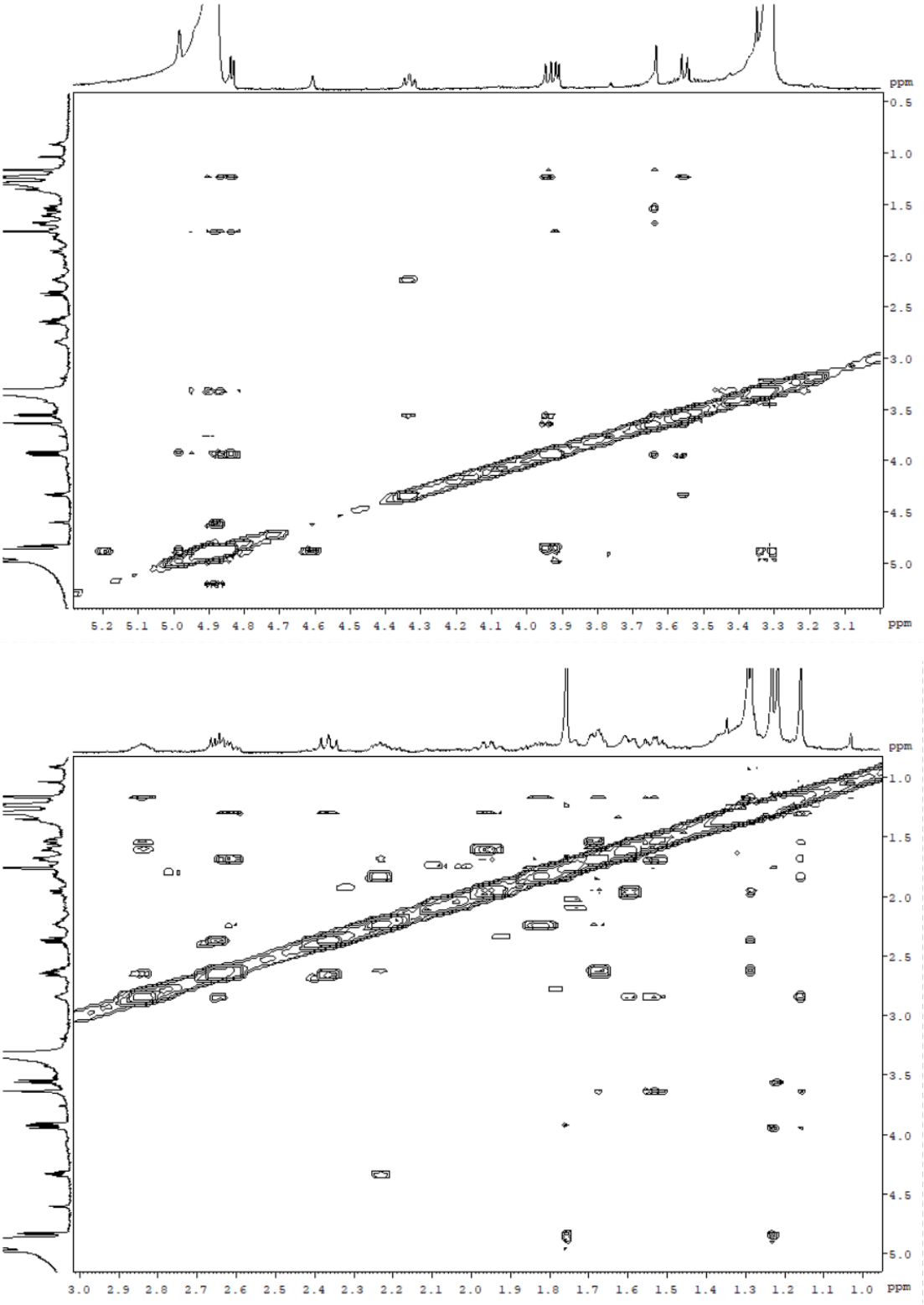


Figure S11. Amplified NOESY spectrum of 1 (600 MHz, MeOH-d_4)

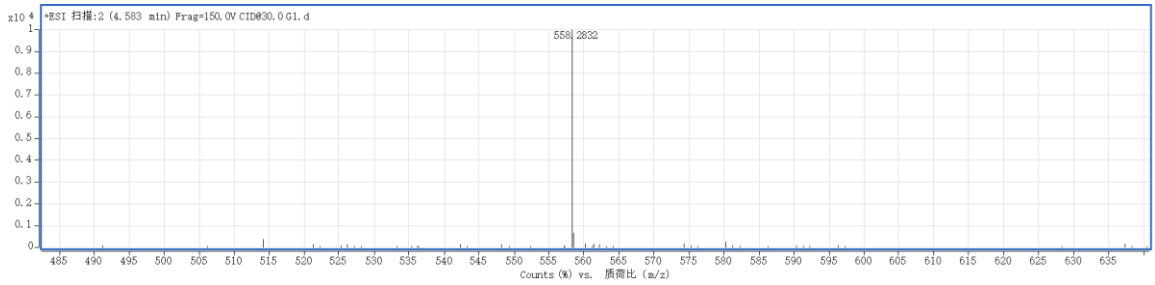


Figure S12. HRESIMS spectrum of 1