Figure S1 Map of sampling sites in the northwestern area of Yunnan province, China (A). In the picture B, the green dot is sampling site for *Astragalus acaulis* (Aa) growing in high altitude grassland of 4,353 m; as shown in the yellow dot, *A. ernestii* (AE) grows in the steep slopes of flowstone beaches of 4,048 m; The blue dot shows the *A. forrestii* (Af) survival environment, surrounded by more pine trees and deciduous foliage of 3,225 m [1].
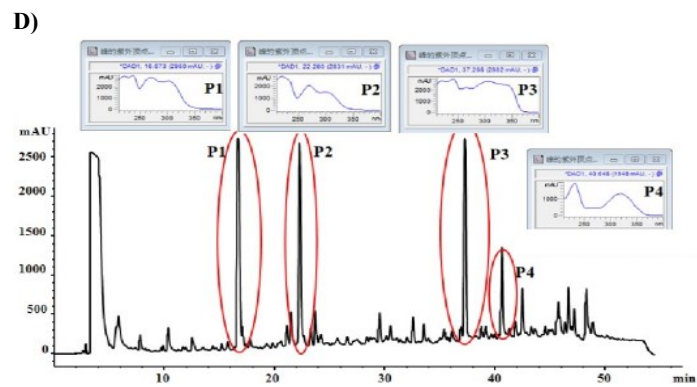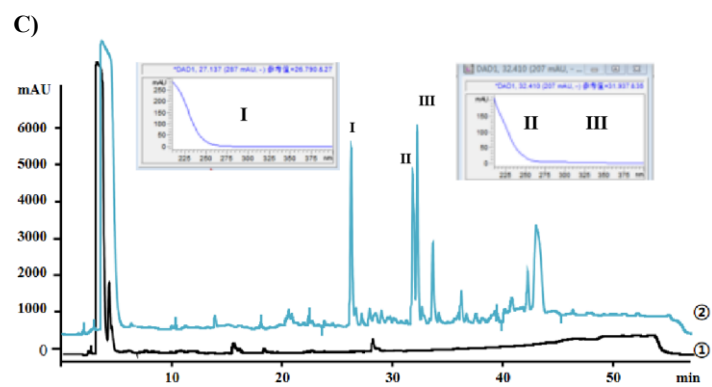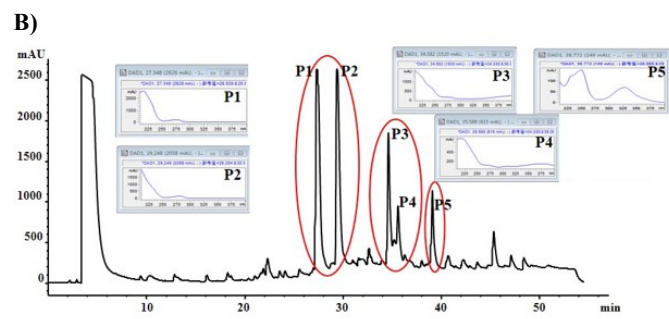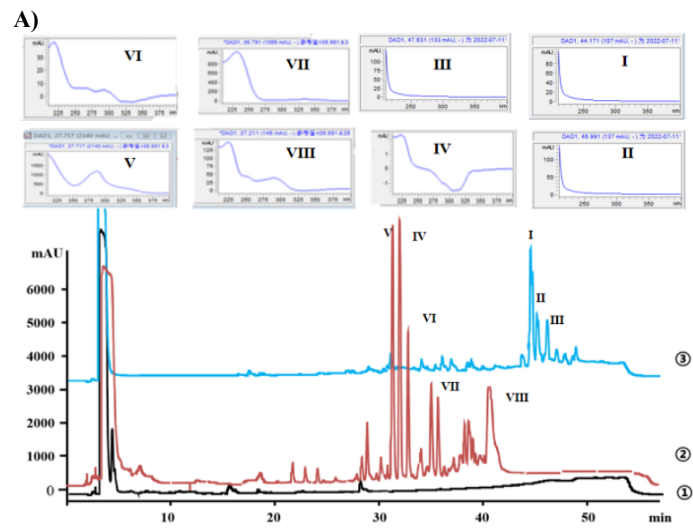

Figure S2 The plants of *Astragalus acaulis* (Aa) grows in alpine grassland (A), *A. forrestii* (Af) is surrounded by more pine trees and deciduous foliage (B), *A. ernestii* (Ae) grows in the steep slopes of flowstone beaches (C) [1].

Table S1 A total of 7, 2 and 4 unique genera identified in the rhizosphere fungal community of *Astragalus acaulis* (Aa), *A. forrestii* (Af) and *A. ernestii* (Ae), respectively.

the name of fungal genera of Aa rhizosphere	the name of fungal genera of Af rhizosphere	the name of fungal genera of Ae rhizosphere
Truncatella	*Lecanicillium*	*Leptosphaeria*
Cordyceps	*Umbelopsis*	*Fusarium*
Exophiala		*Nemania,*
Beauveria		*Aporospora*
Samsoniella		
Neonectria		
Pseudogymnoascus		

Table S2 A total of 10, 15 and 7 unique species identified in the rhizosphere fungal community of *Astragalus acaulis* (Aa), *A. forrestii* (Af) and *A. ernestii* (Ae), respectively.

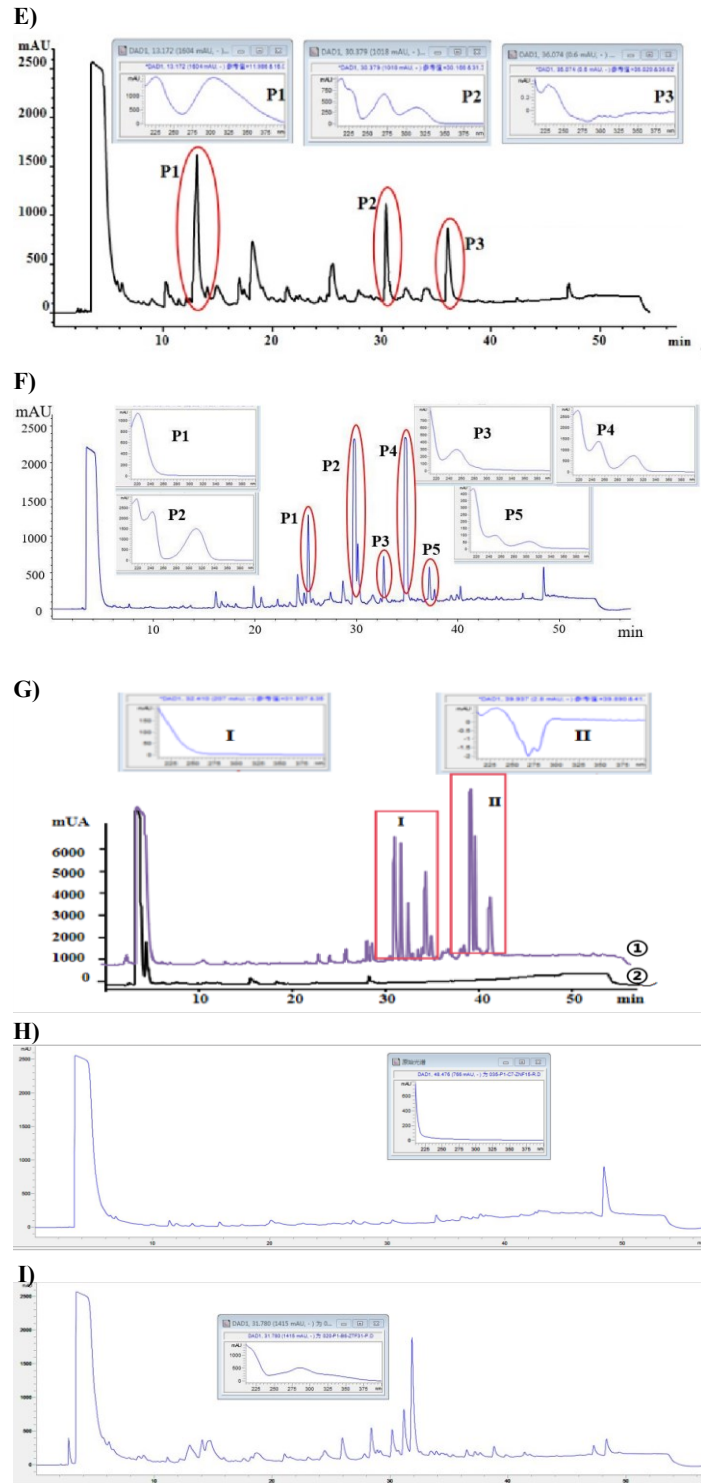| the name of fungal species of Aa rhizosphere	the name of fungal species of Af rhizosphere	the name of fungal species of Ae rhizosphere
Penicillium wellingtonense	*Penicillium vasconiae*	*Penicillium brevicompactum*
Aspergillus calidoustus	*P. suaveolens*	*Aspergillus niger*
Mortierella clonocystis	*P. thomii*	*Trichoderma longibrachiatum*
Truncatella angustata	*Aspergillus versicolor*	*Leptosphaeria sclerotioides*
Cordyceps farinosa	*A. tabacinus*	*Fusarium solani*
Exophiala tremulae	*Mortierella minutissima*	*Nemania diffusa*
Beauveria pseudobassiana	*M. verticillata*	*Aporospora terricola*
Samsoniella hepiali	*Trichoderma paraviridescens*	
Neonectria radicicola	*T. koningiopsis*	
Pseudogymnoascus roseus	*T. viride*	
	T. longipile	
	Lecanicillium aphanocladii	
	Umbelopsis vinacea	
	U. ramanniana	
	U. nana	

A)

B)

C)

D)

Figure S3 HPLC spectra of the crude ethyl acetate (EA) extracts of fermented substrates of *Aspergillus calidoustus* AA12 (A③) and other nine target fungal strains of *A. fumigatus* AA15 (A②), *A. tabacinus* AF16 (B), *Penicillium polonicum* AA17 (C②), *Penicillium vasconiae* AF5 (D), *P. glabrum* AF3-1 (E), *P. brevicompactum* AE7 (F), *Cordyceps farinosa* AA8 (G), *Lecanicillium aphanocladii* AF15 (H), and *Umbelopsis nana* AF31 (I).
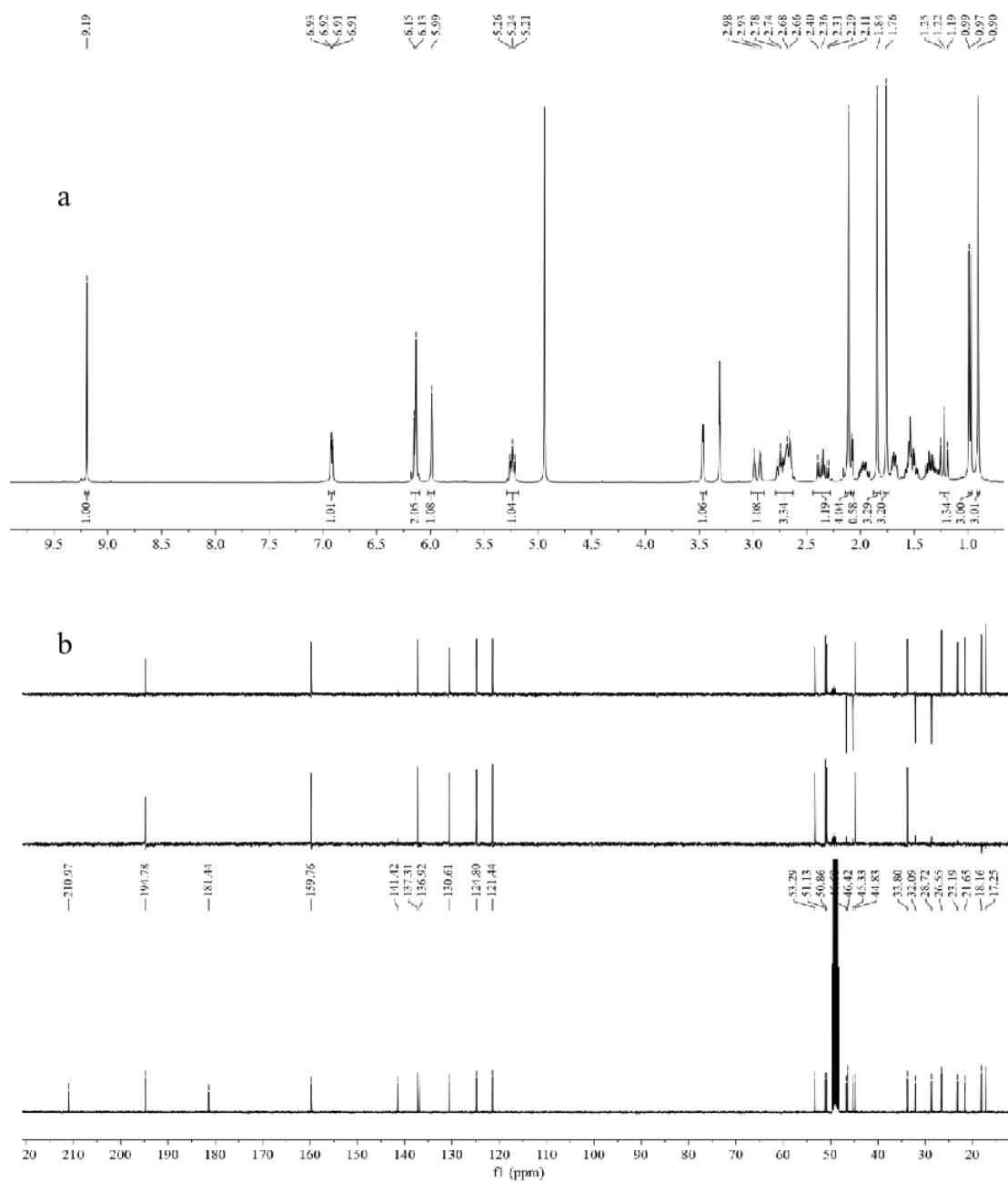
Figure S4 ¹H (a) and ¹³C (b) NMR spectrum of 6-epi-ophiobolin G (**1**).
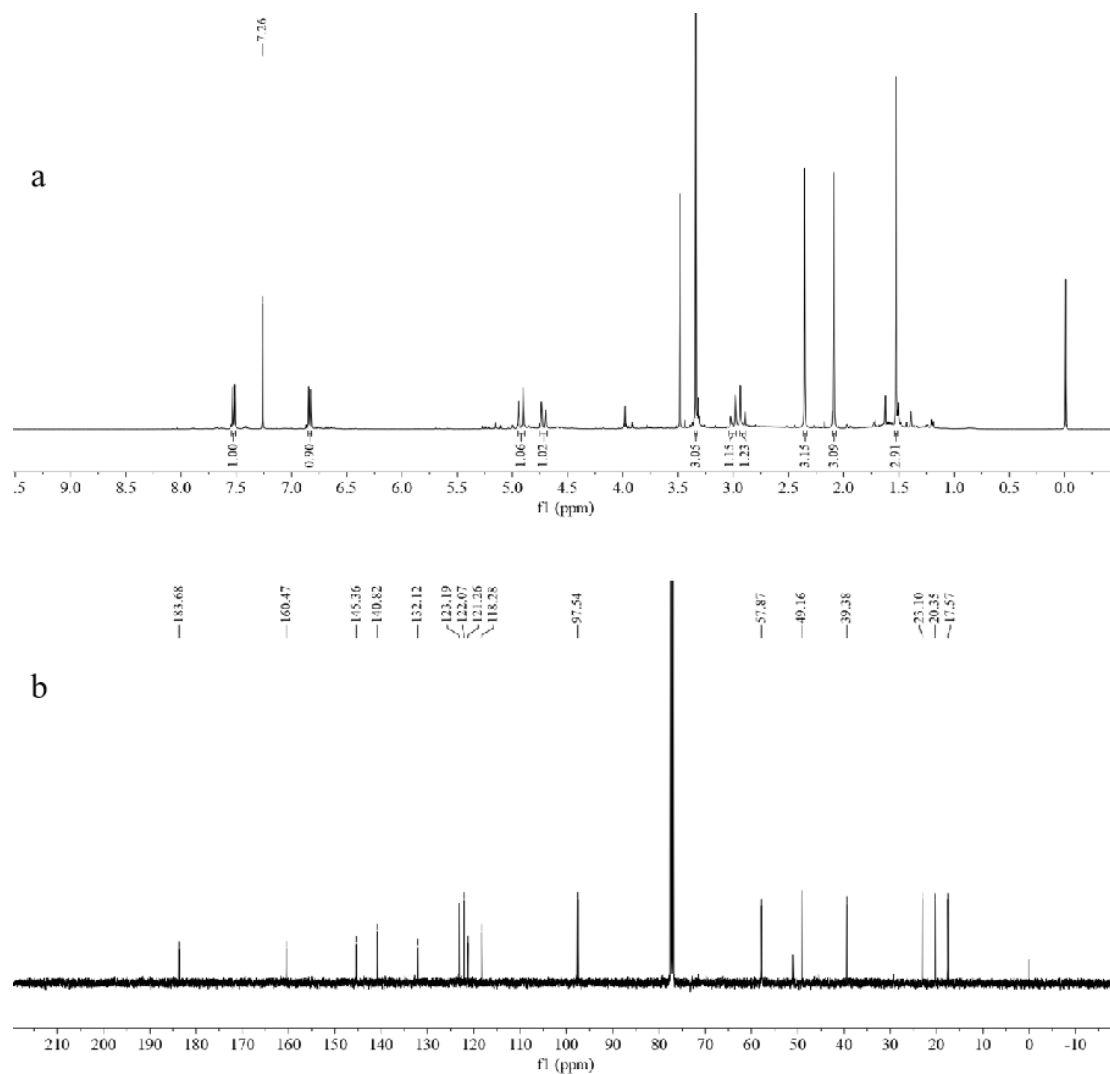
a

b

Figure S5 ^{1}H (a) and ^{13}C (b) NMR spectrum of penicisochroman A (**2**).

Figure S6 ^{1}H (a) and ^{13}C (b) NMR spectrum of pergillin (**3**).

a

b

Figure S7 ^{1}H (a) and ^{13}C (b) NMR spectrum of 7-methyl-2-(1-methylethylethlidene)-furo[3,2-H]isoquinoline-3-one (**4**).

Figure S8 ^{1}H (a) and ^{13}C (b) NMR spectrum of trypacidin (**5**).

Figure S9 ^{1}H (a) and ^{13}C (b) NMR spectrum of 1,2-seco-trypacidin (**6**).

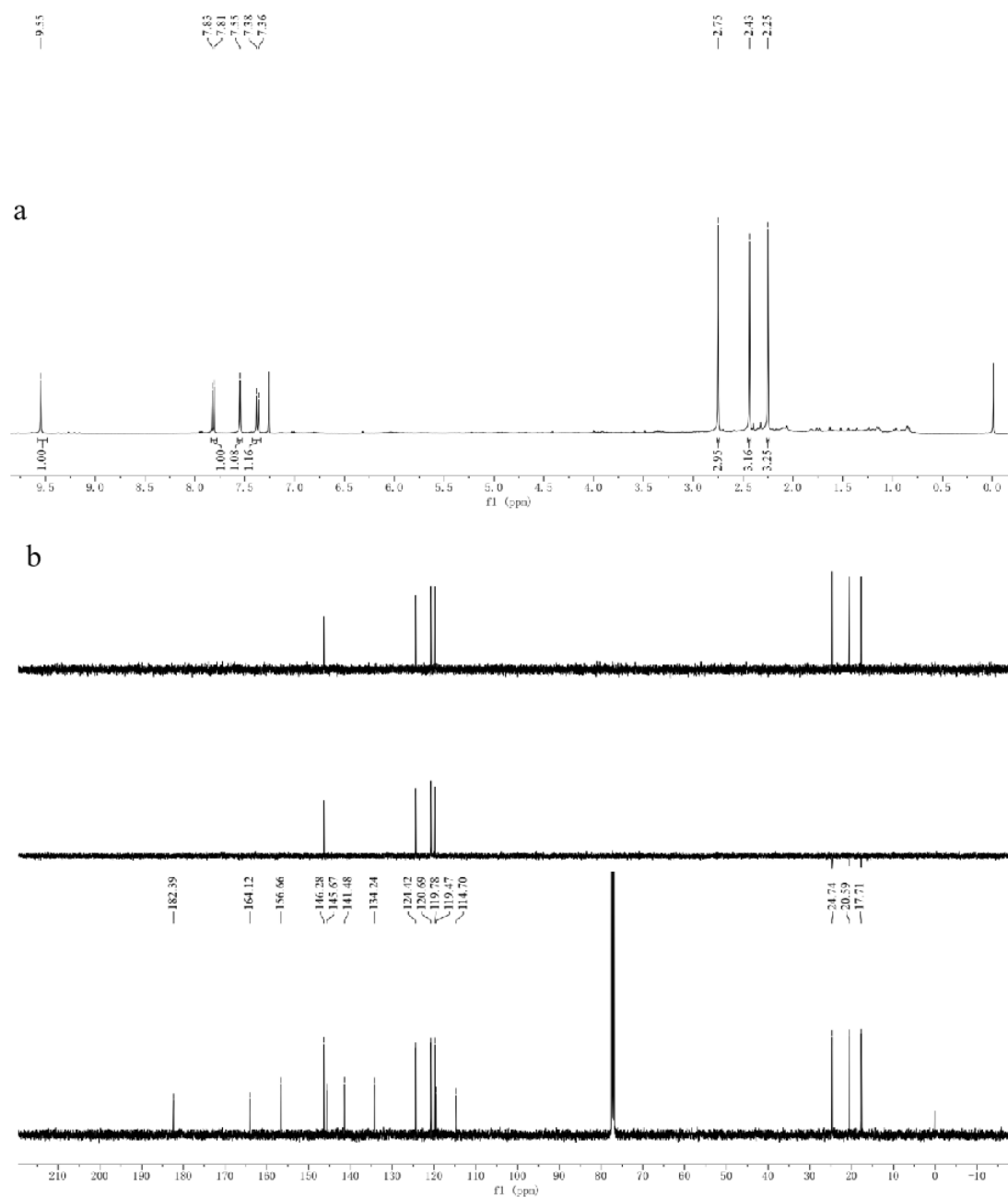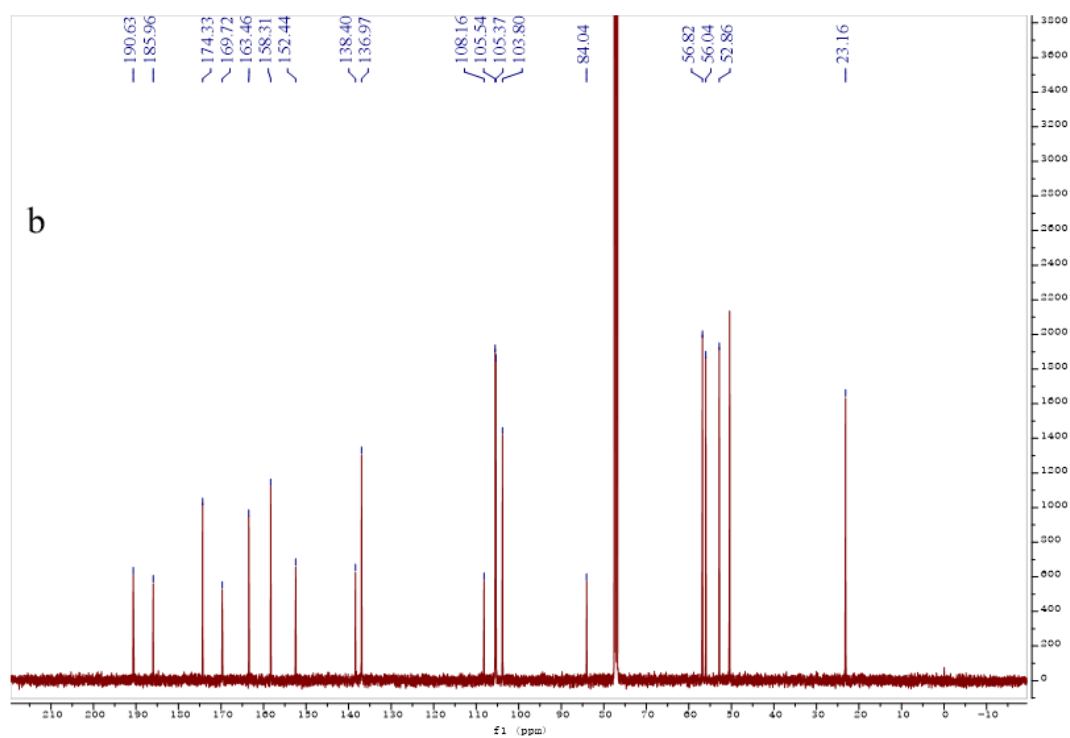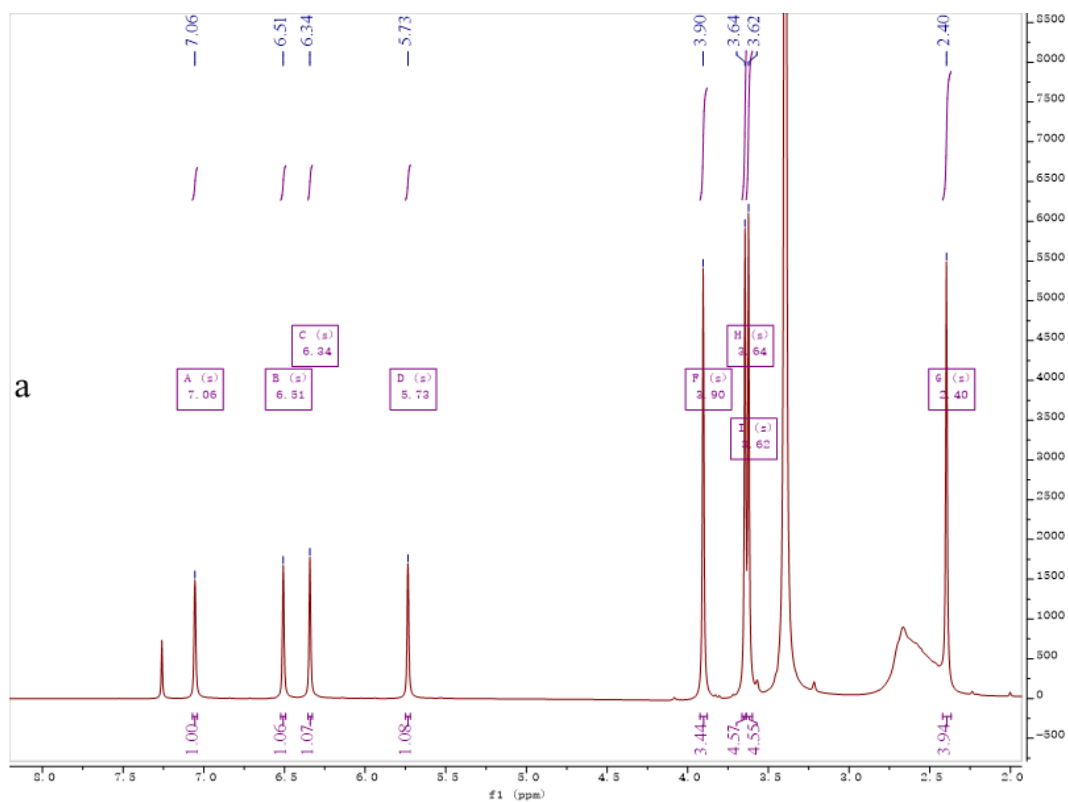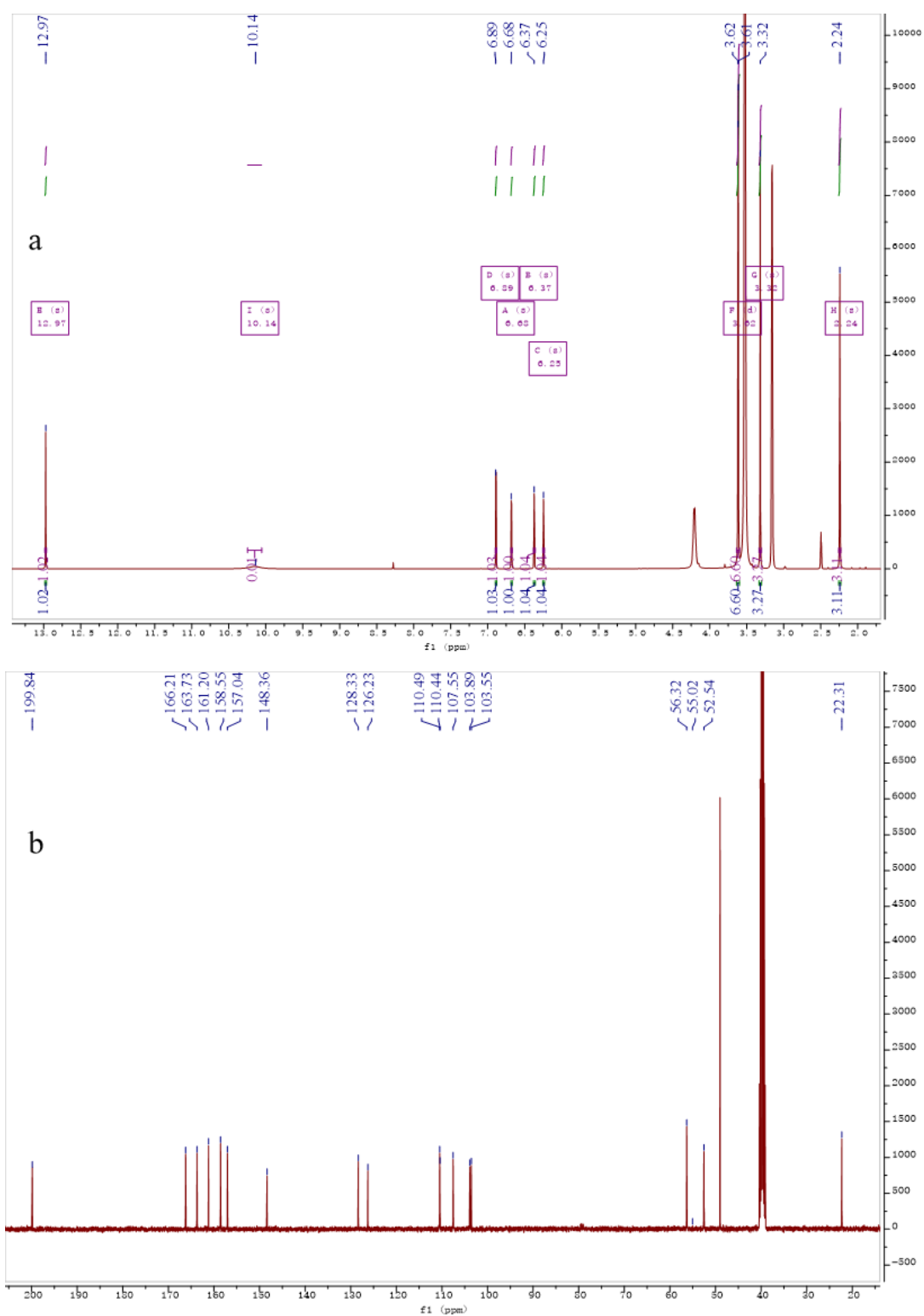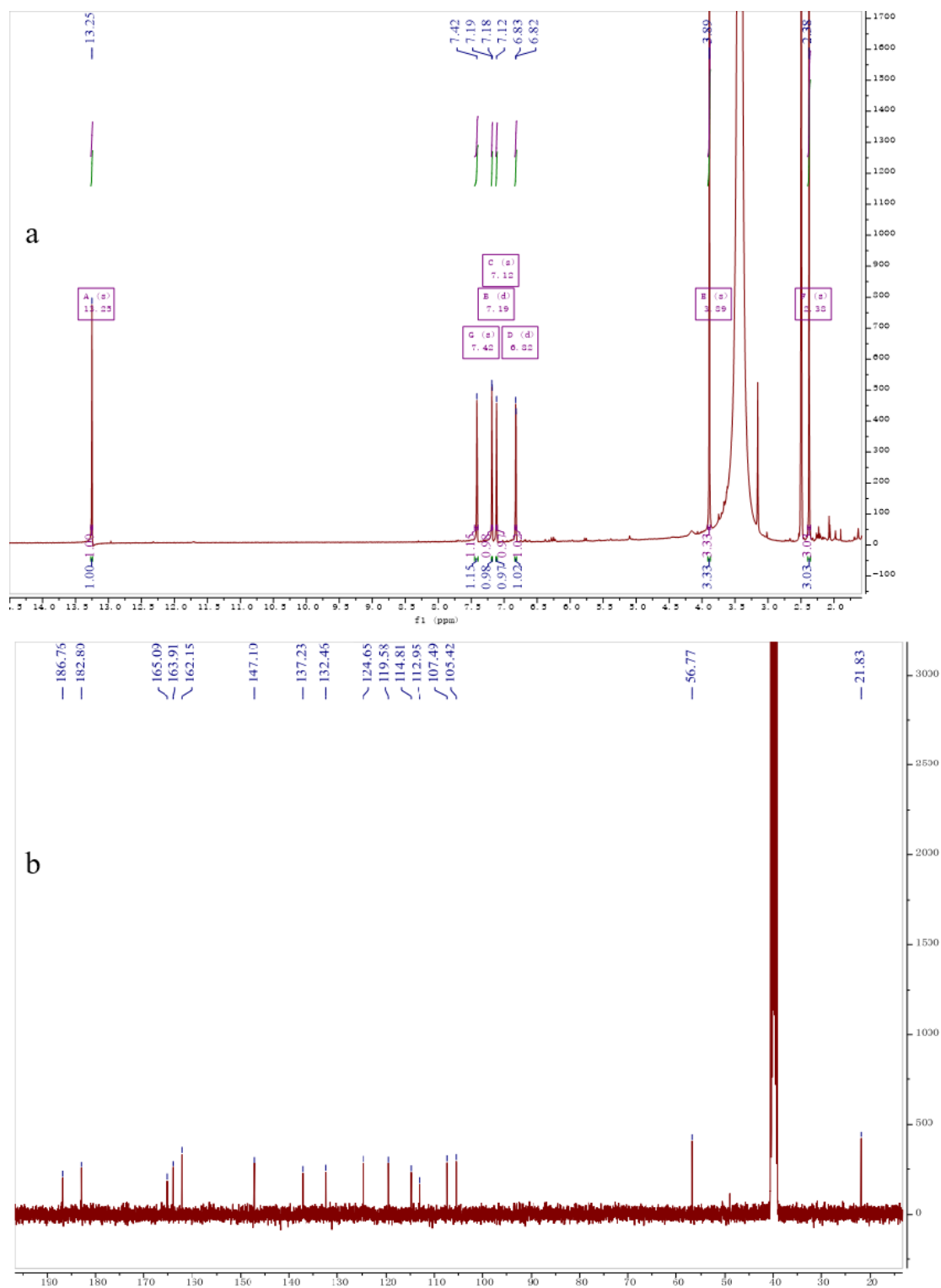**Figure S10** ^{1}H (a) and ^{13}C (b) NMR spectrum of questin (**7**).

Table S3 ^{1}H and ^{13}C NMR data of compounds **1** and **7** (δ in ppm).

No.	1 (In CD₃OD)		7 (In DMSO-d6)	
	$\delta_H{}^a$	$\delta_C{}^b$	$\delta_H{}^a$	$\delta_C{}^b$
1	1.19 t	45.33 CH₂		162.15 C
2	2.66 m	50.86 CH₂	7.12 s	124.65 CH
3		181.44 C		147.10 C
3-Me			2.38 s	21.83 CH₃
4	5.99 s	130.61 CH	7.42 s	119.58 CH
5		210.97 C	7.19 s	107.49 CH
6	3.46 d	51.13 CH		165.09 C
7		141.42 C	6.82 s	105.42 CH
8	6.91 d	159.76 CH		163.91 C
8-OMe			3.89 s	56.77 CH₃
9	2.93 d	32.09 CH₂		186.76 C
10	2.61 m	44.83 CH		182.80 C
11		46.68 C		137.23 C
12	1.49 m; 1.52 m	46.42 CH₂		112.95 C
13	1.28 m	28.72 CH₂		114.81 C
14	1.87 m	50.29 CH		132.46 C
15	2.68 m	33.80 CH		
16	5.21 t	137.31 CH		
17	6.13 t	124.80 CH		
18	5.99 t	121.44 CH		
19		136.92 C		
20	2.11 s	17.20 CH₃		
21	9.19 s	194.78 CH		
22	0.90 s	23.19 CH₃		
23	0.97 d	21.65 CH₃		
24	1.76 s	18.16 CH₃		
25	1.84 s	26.55 CH₃		

a Recorded at 400 MHz; b Recorded at 100 MHz.

Table S4 ^{1}H and ^{13}C NMR data of compounds **2−4** (δ in ppm).

No.	2 (In CDCl$_3$)		3 (In CDCl$_3$)		4 (In CDCl$_3$)	
	$\delta_H{}^a$	$\delta_C{}^b$	$\delta_H{}^a$	$\delta_C{}^b$	$\delta_H{}^a$	$\delta_C{}^b$
2		145.34 C		145.34 C		145.67 C
3		183.59 C		183.40 C		182.39 C
3a		121.28 C		121.42 C		119.47 C
4	7.53 d	122.02 CH	7.53 d	122.14 CH	7.78 d	124.42 CH
5	6.85 d	123.16 CH	6.87 d	123.34 CH	7.36 d	119.78 CH
5a		140.77 C		140.71 C		141.48 C
6	3.00 dd	39.38 CH$_2$	2.93 dd	38.77 CH$_2$	7.55 s	120.69 CH
7		97.50 C		94.96 C		156.66 C
9	4.93 dd	57.86 CH$_2$	4.92 dd	57.77 CH$_2$	9.51 s	146.28 CH
9a		118.29 C		118.30 C		114.70 C
9b		160.45 C		160.52 C		164.12 C
10	1.53 s	23.10 CH$_3$	1.63 s	29.39 CH$_3$	2.75 s	24.74 CH$_3$
11		131.85 C		132.22 C		134.22 C
12	2.09 s	20.31 CH$_3$	2.09 s	17.58 CH$_3$	2.43 s	17.71 CH$_3$
13	2.36 s	17.53 CH$_3$	2.36 s	20.37 CH$_3$	2.55 s	20.59 CH$_3$
7-OMe	3.55 s	49.13 CH$_3$				

a Recorded at 400 MHz; b Recorded at 100 MHz.

Table S5 ^{1}H and ^{13}C NMR data NMR data of compounds **5** and **6** (δ in ppm).

No.	5 (In CDCl$_3$)		6 (In DMSO-d6)	
	$\delta_H{}^a$	$\delta_C{}^b$	$\delta_H{}^a$	$\delta_C{}^b$
2		84.04 C		126.23 C
3		190.63 C		199.84 C
3a		108.16 C		110.44 C
4		158.31 C		161.20 C
5	6.34 s	105.37 CH	6.37 s	110.49 CH
6		152.44 C		148.36 C
6a	2.40 s	23.16 CH$_3$	2.24 s	22.31 CH$_3$
7	6.51 s	105.54 CH	6.68 s	103.89 CH
7a		174.33 C		163.73 C
1′		138.40 C		128.33 C
2′	7.06 s	136.97 CH	6.89 s	107.55 CH
3′		185.96 C		158.55 C
4′	5.73 s	103.80 CH	6.25 s	103.55 CH
5′		169.72 C		157.04C
1′-COOMe		163.46 C		166.21 C
4-OMe	3.90 s	56.04 CH$_3$	3.32 s	52.54CH$_3$
5′-OMe	3.62 s	56.82 CH$_3$	3.62 s	56.32CH$_3$
1′-COOMe	3.64 s	52.86 CH$_3$	3.61 s	55.02 CH$_3$

a Recorded at 400 MHz; b Recorded at 100 MHz.

References

1. Ding, J.J.; Zhou, G.J.; Chen, X.J.; Xu, W.; Gao, X.M.; Zhang, Y.Z.; Jiang, B.; Li, H.F.; Wang, K.L. Analysis of microbial diversity and community structure of rhizosphere soil of three *Astragalus* species grown in special high-cold environment of northwestern Yunnan, China. Microorganisms **2024**, 12, 539.