

Three new compounds with their anti-glioma effects from the roots of *Arnebia guttata* Bunge

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ABSTRACT: Three new compounds, arneatas A-C (**1-3**), together with three known compounds (**4-6**) were isolated from the roots of *Arnebia guttata* Bunge. The structures were established on the basis of extensive spectroscopic data including NMR and HRESIMS. All the new compounds (**1-3**) were tested for their cytotoxic activity against two glioma cell lines (U118-MG and U373-MG) *in vitro* after treatment for 48h. Compound **1** exhibited moderate cytotoxic activity against U118-MG and U373-MG glioma cell lines, with IC₅₀ values of 10.4 and 17.5 μM, respectively.

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Table S1. ^1H (600 MHz) and ^{13}C -NMR (150 MHz) data of arneata A (1) in CDCl_3

Table S2. ^1H (600 MHz) and ^{13}C -NMR (150 MHz) data of arneata B (2) in CDCl_3

Table S3. ^1H (600 MHz) and ^{13}C -NMR (150 MHz) data of arneata C (3) in CDCl_3

Figure S1. Key ^1H - ^1H COSY and HMBC correlations of arneata A (1)

Figure S2. Key ^1H - ^1H COSY and HMBC correlations of arneata B (2)

Figure S3. Key ^1H - ^1H COSY and HMBC correlations of arneata C (3)

Figure S4. IR spectrum of compound **1**

Figure S5. ^1H -NMR spectrum of compound **1**

Figure S6. ^{13}C -NMR (150 MHz) spectrum of **1**

Figure S7. ^1H - ^1H COSY spectrum of compound **1**

Figure S8. HSQC spectrum of compound **1**

Figure S9. HMBC spectrum of compound **1**

Figure S10. ROESY spectrum of compound **1**

Figure S11. IR spectrum of compound **2**

Figure S12. ^1H -NMR spectrum of compound **2**

Figure S13. ^{13}C -NMR (150 MHz) spectrum of compound **2**

Figure S14. ^1H - ^1H COSY spectrum of compound **2**

Figure S15. HSQC spectrum of compound **2**

Figure S16. HMBC spectrum of compound **2**

Figure S17. ROESY spectrum of compound **2**

Figure S18. IR spectrum of compound **3**

Figure S19. ^1H -NMR spectrum of compound **3**

Figure S20. ^{13}C -NMR (150 MHz) spectrum of compound **3**

Figure S21. ^1H - ^1H COSY spectrum of compound **3**

Figure S22. HSQC spectrum of compound **3**

Figure S23. HMBC spectrum of compound **3**

Figure S24. ROESY spectrum of compound **3**

Table S1. ^1H (600 MHz) and ^{13}C - NMR (150 MHz) data of arneata A (**1**) in CDCl_3

No.	δ_{H} (J in Hz)	δ_{C}
1	-	127.5
2	7.53 (1H, s)	144.1
3	-	153.0
4	-	187.0
5	7.17 (1H, s)	116.3
6	5.71 (1H, t, 6.6Hz)	67.8
7	2.60 (1H, m), 2.49(1H, m)	33.4
8	5.02 (1H, m)	117.9
9	-	135.7
10	1.60 (3H,s)	18.0
11	1.70(3H,s)-	25.8
12	-	170.4
13	2.04(3H,s)	21.2
14	2.48(3H,s)	26.0

Table S2. ^1H (600 MHz) and ^{13}C - NMR (150 MHz) data of arneata B (**2**) in CDCl_3

No.	δ_{H} (J in Hz)	δ_{C}
1	-	187.1
2	5.89 (1H, s)	107.1
3	-	158.6
4	-	181.9
5	2.24 (1H, t, 10.2Hz)	47.4
6	2.58 (2H, m)	26.4
7	2.41 (2H, m)	34.3
8	-	38.0
9	5.79 (1H, dd, 10.8Hz, 17.4Hz)	146.3
10	4.99 (1H, d, 10.8Hz), 4.96 (1H,d,17.4Hz)	111.7
11	0.98 (3H, s)	20.1
12	-	145.8
13	4.91 (1H,s),4.72(1H,s)	113.4
14	1.75 (3H,s)	24.6
15	3.81 (3H,s)	56.2
4a	-	138.7
8a	-	141.4

Table S3. ^1H (600 MHz) and ^{13}C - NMR (150 MHz) data of arneata C (**3**) in CDCl_3

No.	δ_{H} (J in Hz)	δ_{C}
1	-	182.0
2	-	158.6
3	5.89 (1H, s)	107.2
4	-	187.2
5	2.24(1H,t,10.2Hz)	47.5
6	2.58(2H,m)	26.7
7	2.41(2H,m)	34.6
8	-	38.1
9	5.78(1H,dd,1.2Hz,2.4Hz)	146.3
10	4.98(1H,d,3.0Hz),4.95(1H,d,3.0Hz)	111.7
11	0.98(3H,s)	20.2
12	-	145.8
13	4.91(1H,d,2.4Hz),4.72(1H,d,6.0Hz)	113.4
14	1.75(3H,s)	24.6
15	3.81(3H,s)	56.2
4a	-	142.2
8a	-	139.4

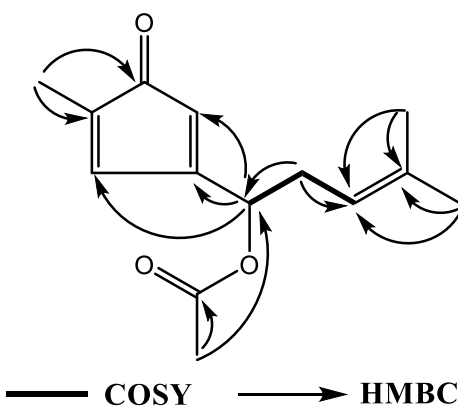


Figure S1. Key ^1H - ^1H COSY and HMBC correlations of arneata A(1)

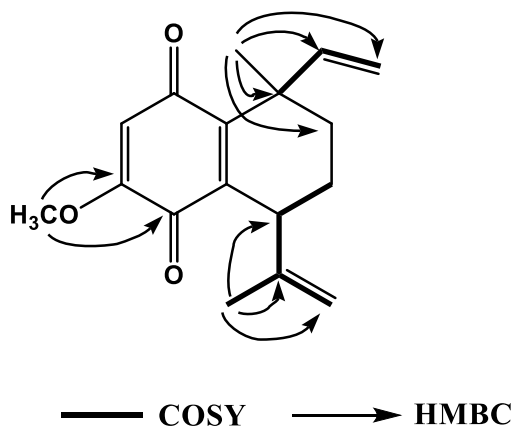


Figure S2. Key ^1H - ^1H COSY and HMBC correlations of arneata B (2)

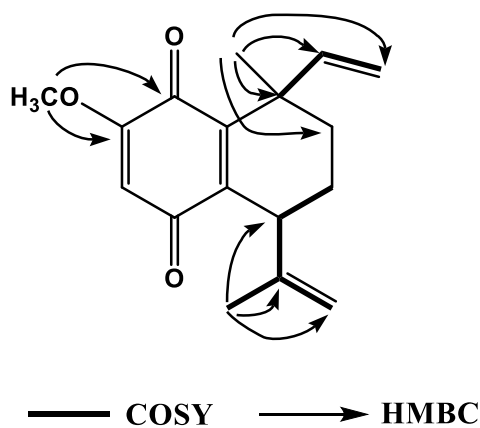


Figure S3. Key ^1H - ^1H COSY and HMBC correlations of arneata C (3)

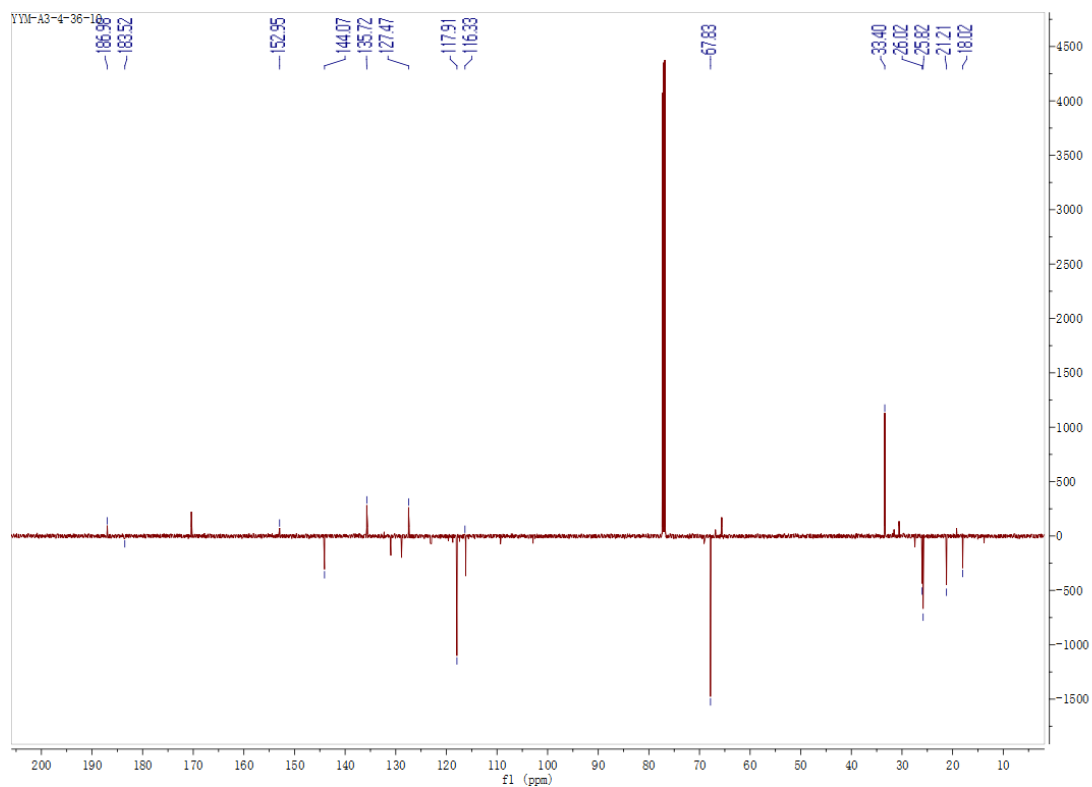


Figure S6. ^{13}C -NMR (150 MHz) spectrum of **1**

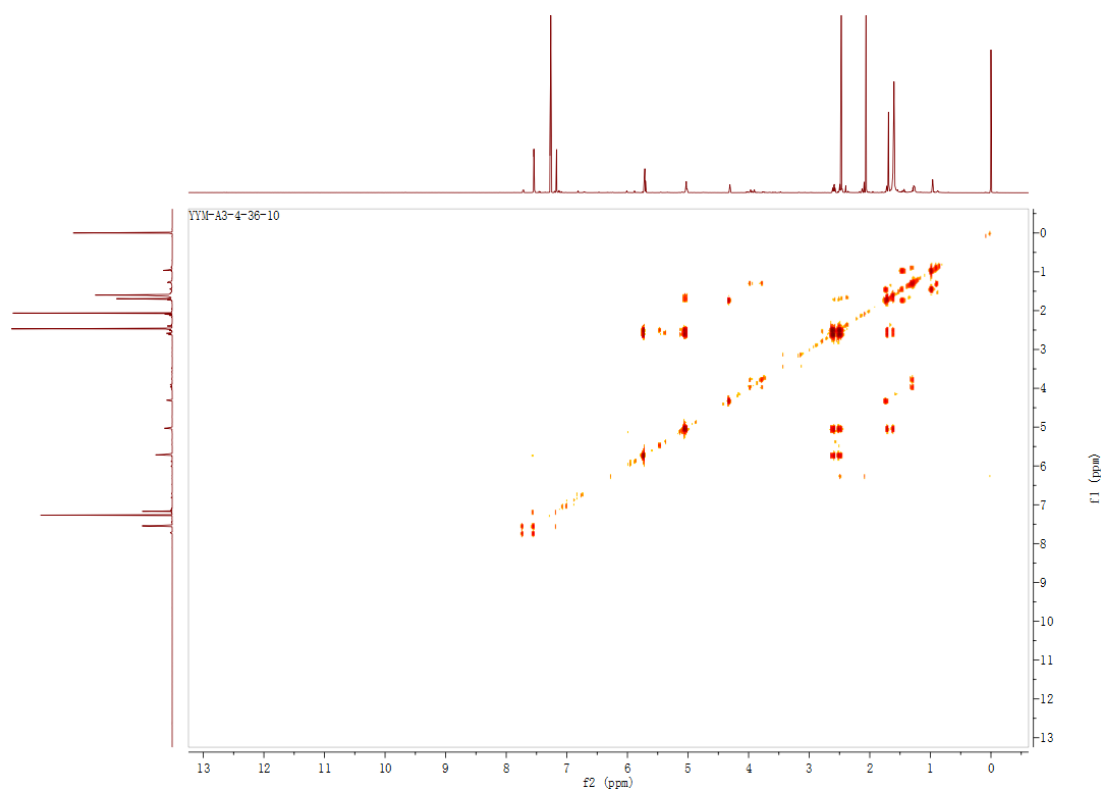


Figure S7. ^1H - ^1H COSY spectrum of compound **1**

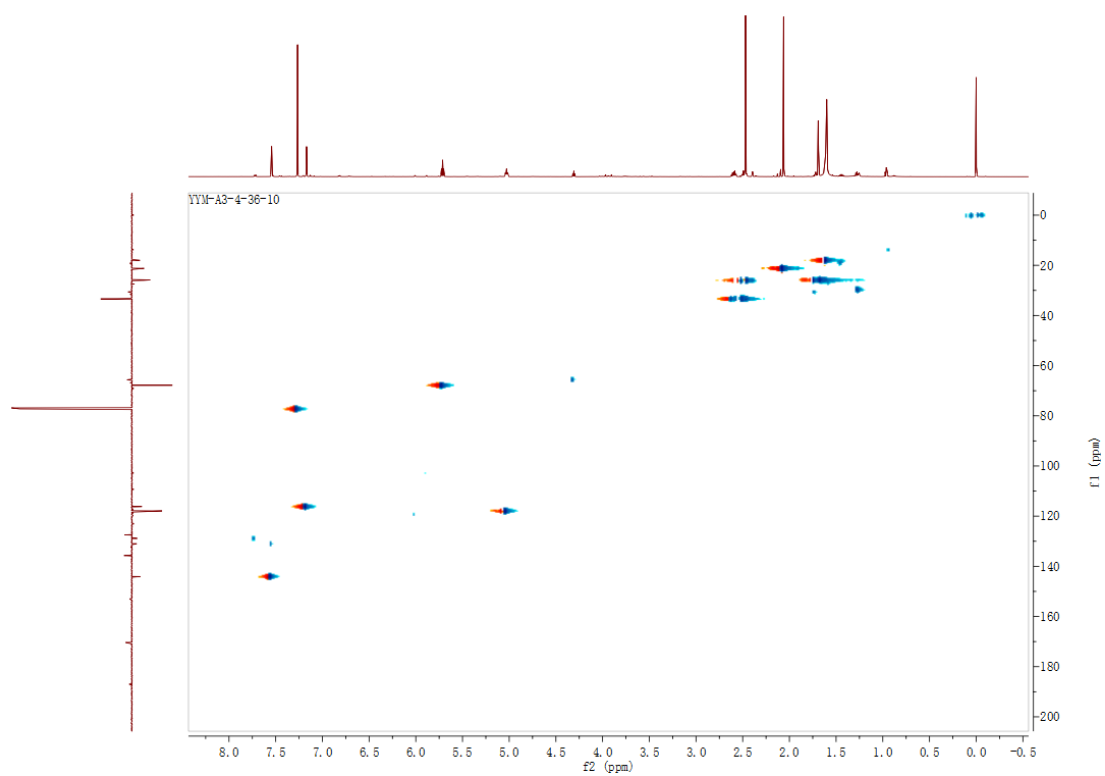


Figure S8. HSQC spectrum of compound **1**

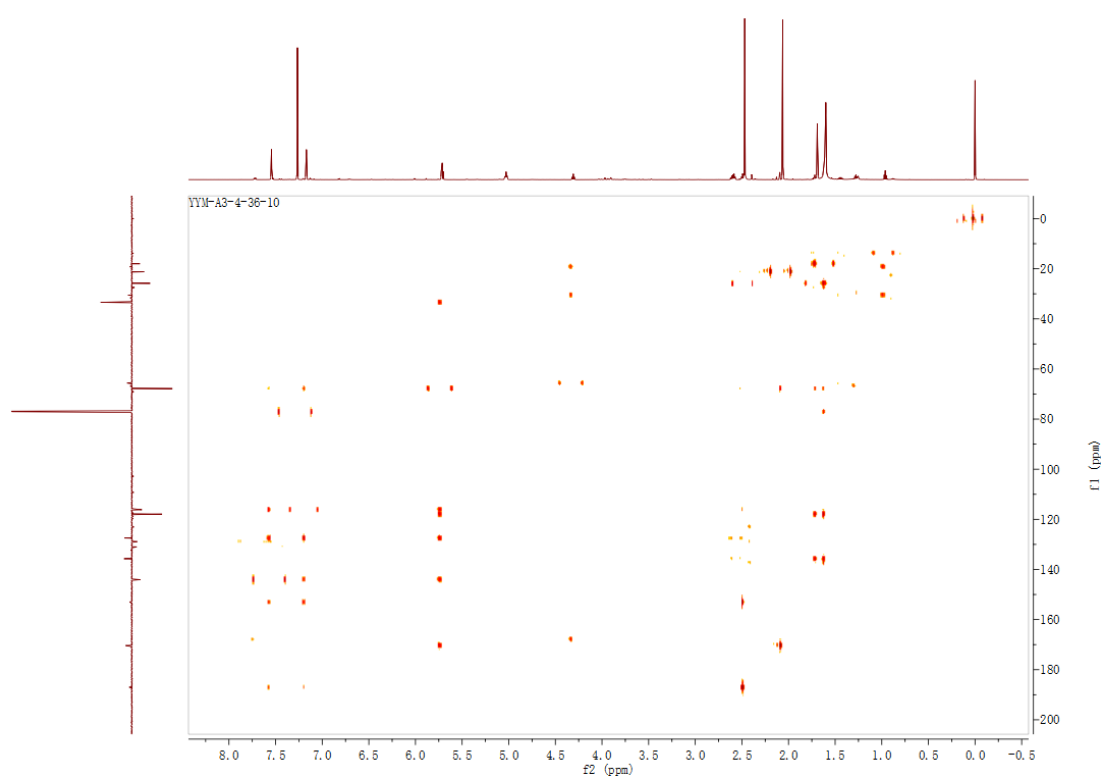


Figure S9. HMBC spectrum of compound **1**

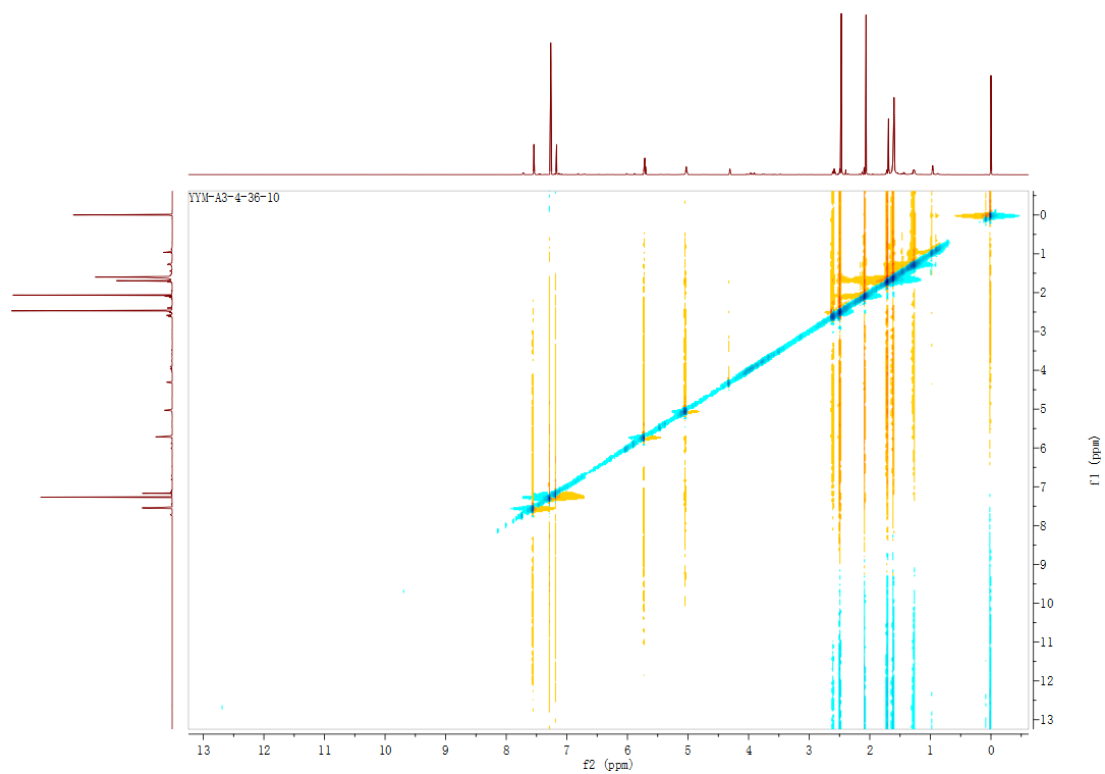


Figure S10. ROESY spectrum of compound **1**

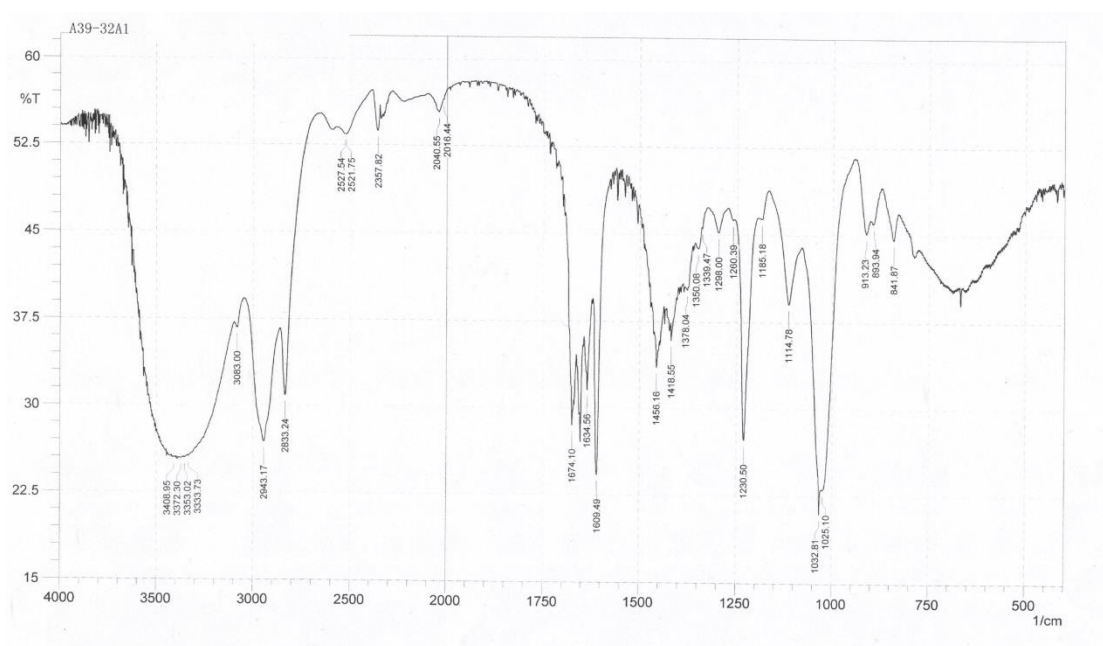


Figure S11. IR spectrum of compound **2**

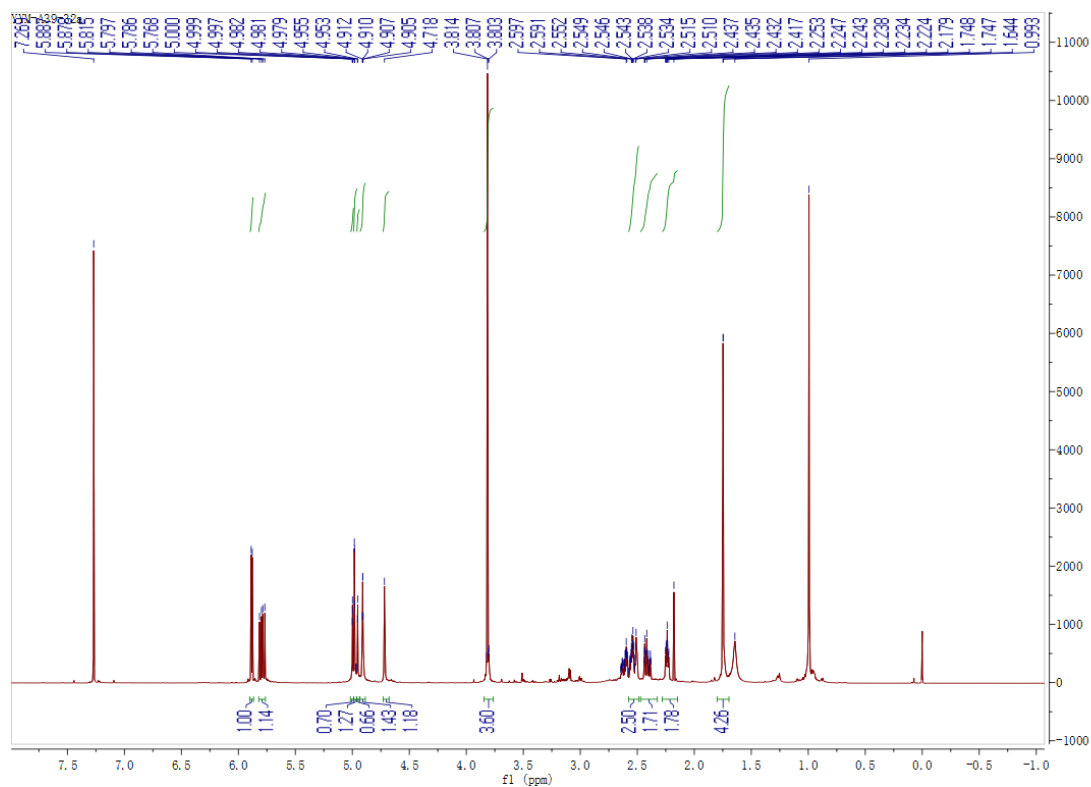


Figure S12. ^1H -NMR spectrum of compound 2

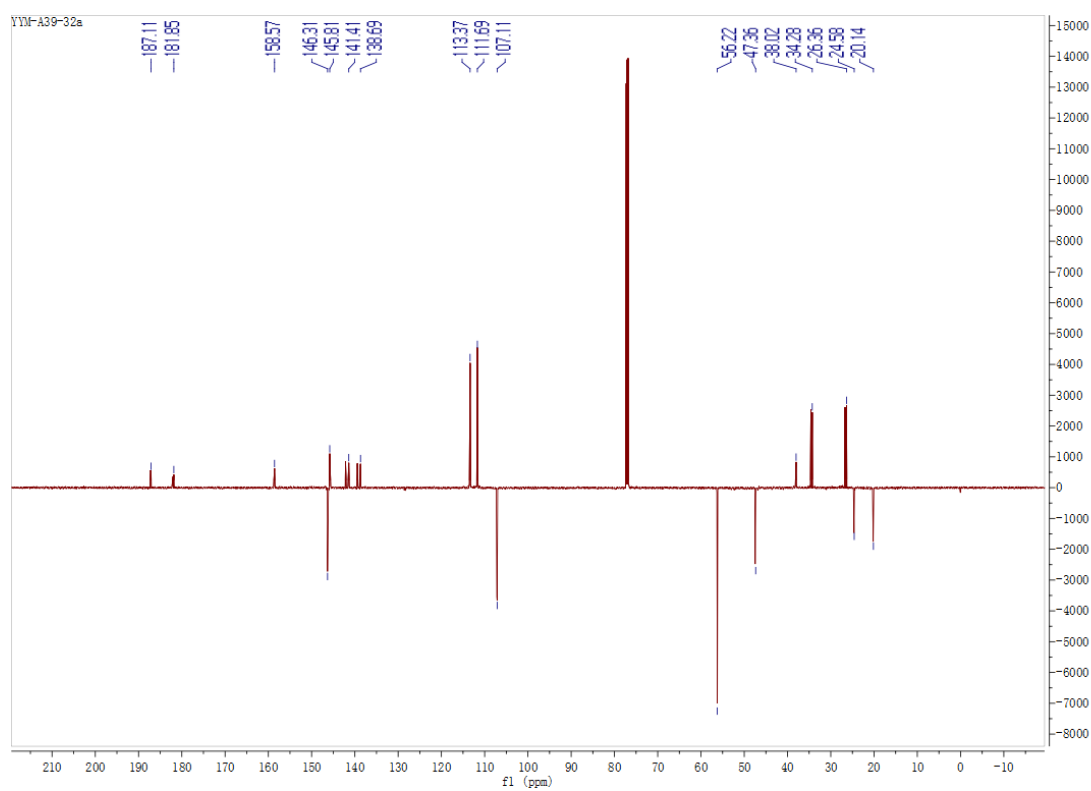


Figure S13. ^{13}C -NMR (150 MHz) spectrum of compound 2

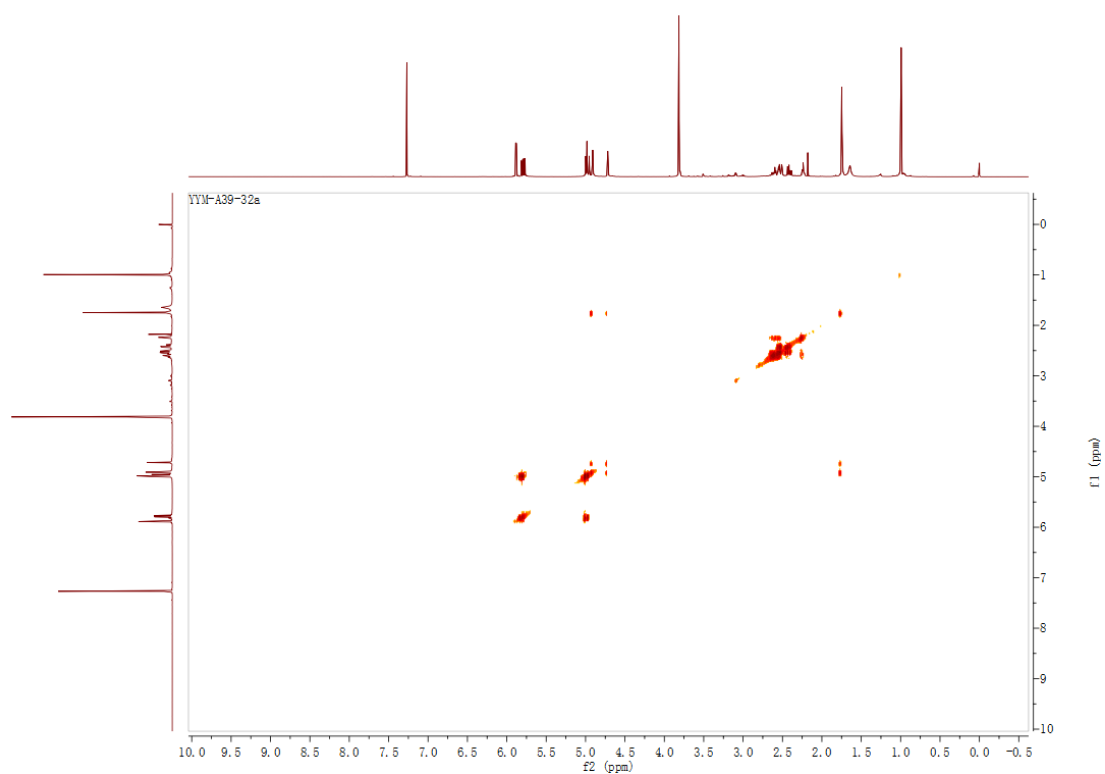


Figure S14. ^1H - ^1H COSY spectrum of compound **2**

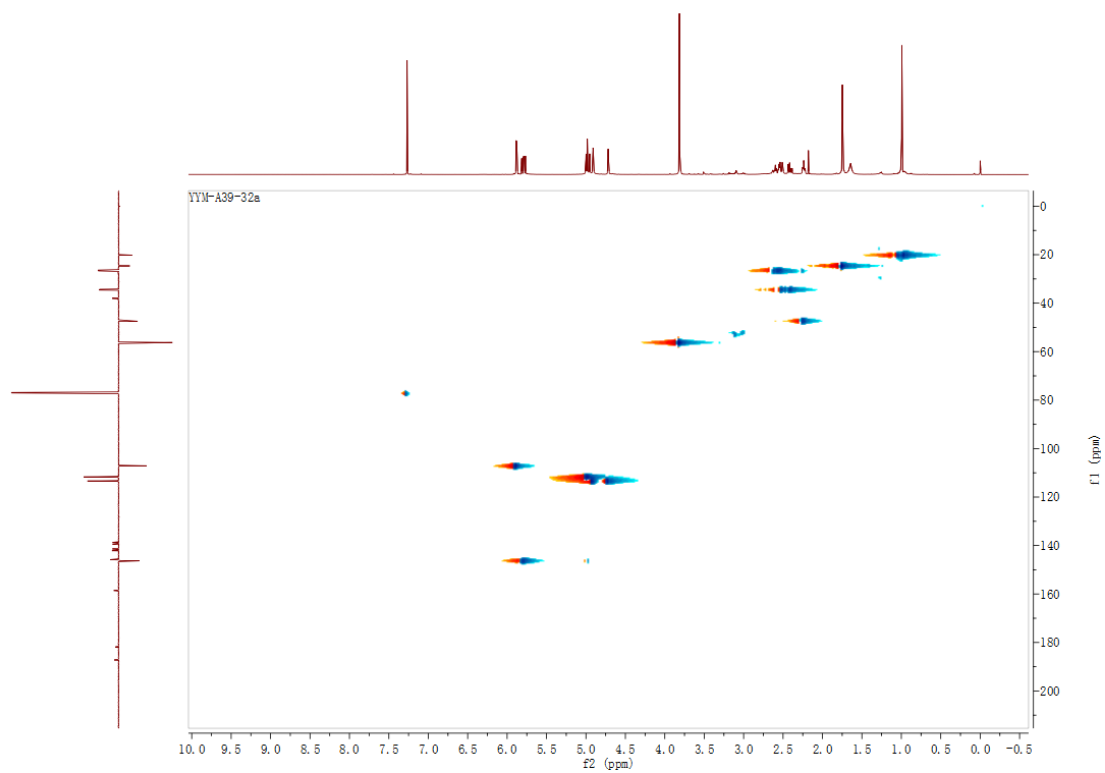


Figure S15. HSQC spectrum of compound **2**

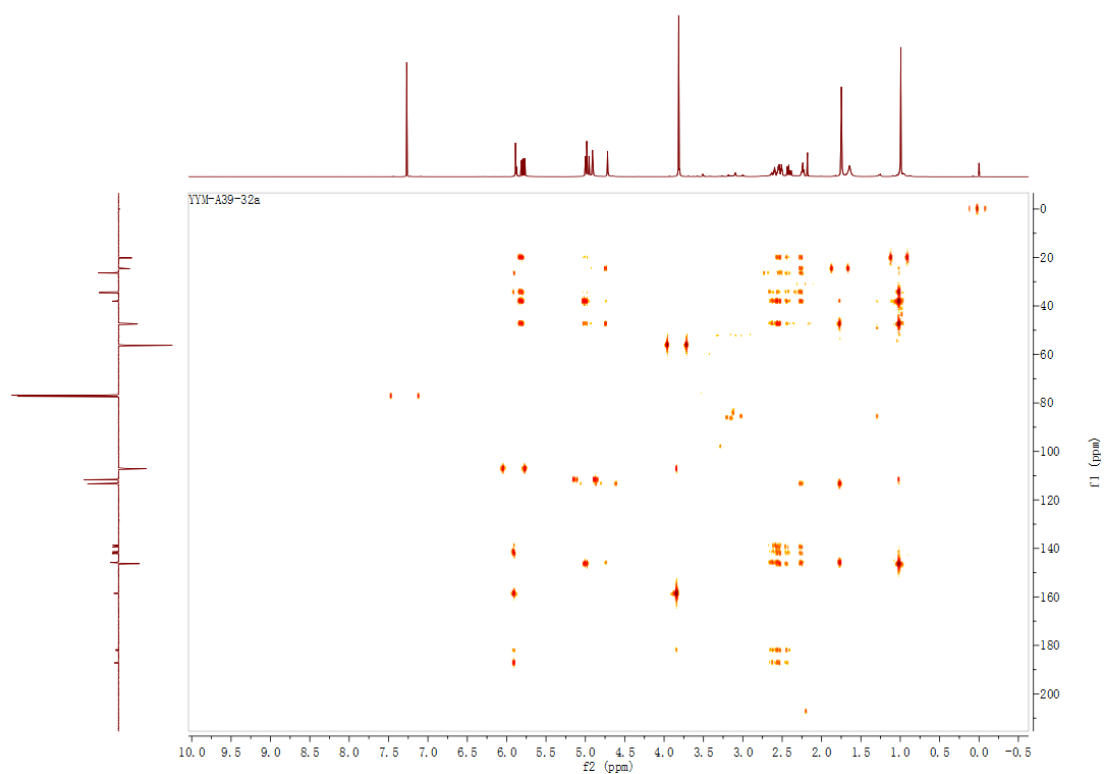


Figure S16. HMBC spectrum of compound **2**

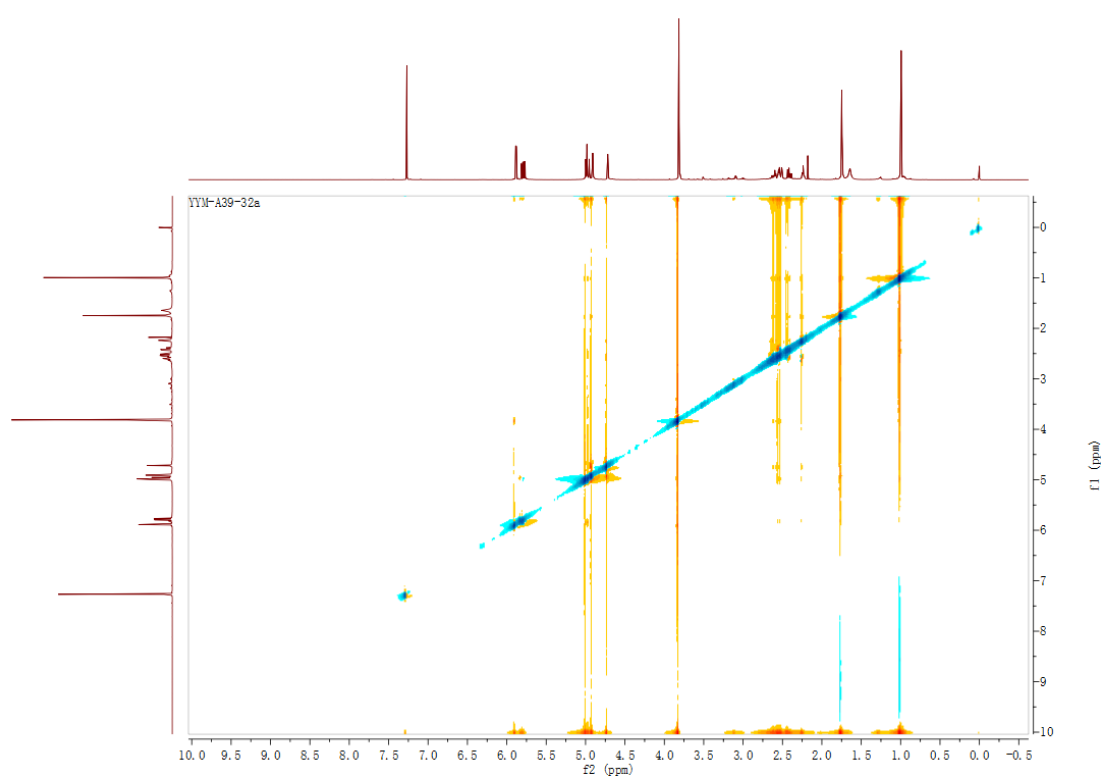


Figure S17. ROESY spectrum of compound **2**

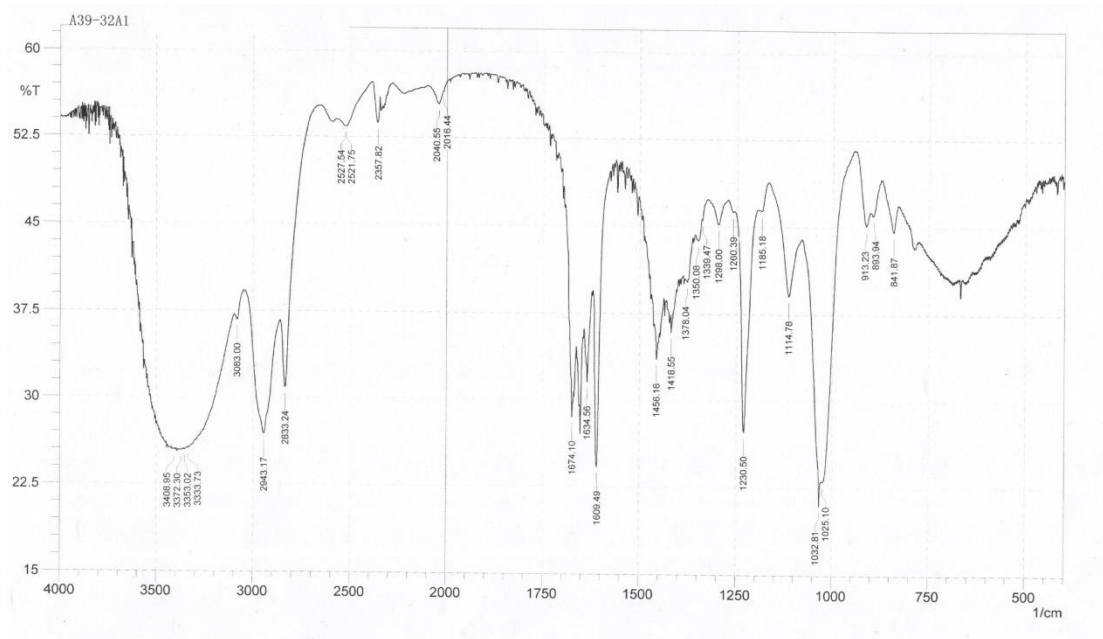


Figure S18. IR spectrum of compound 3

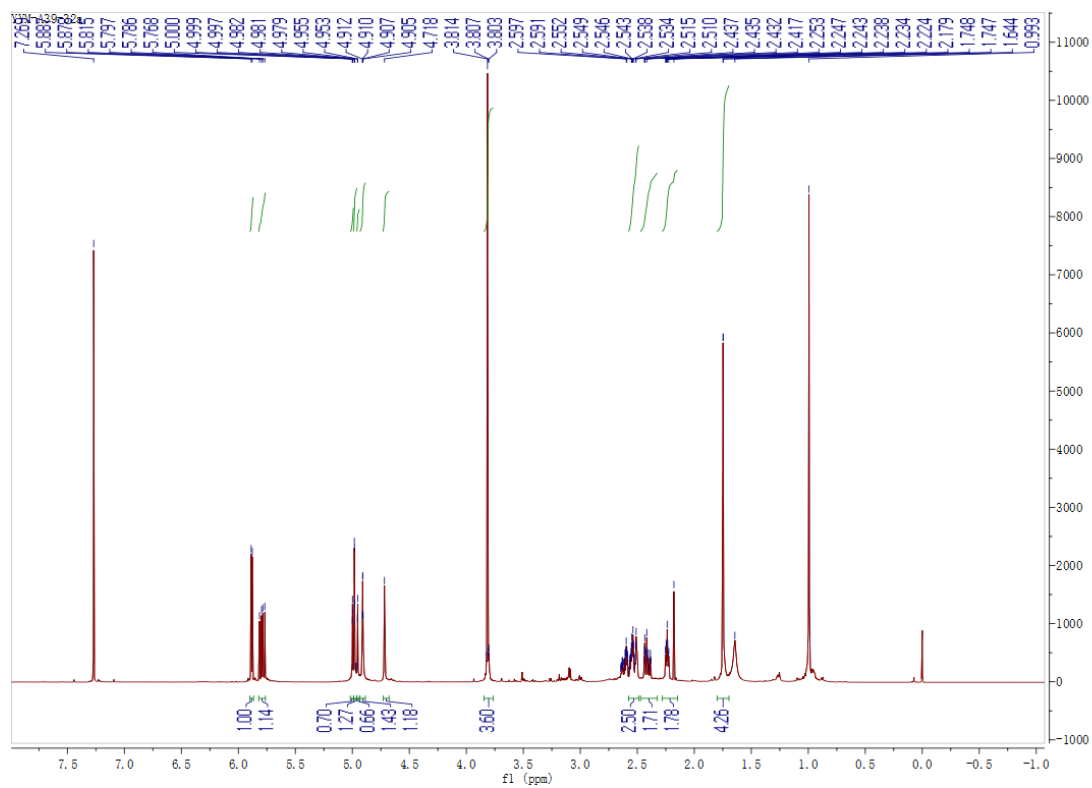


Figure S19. ¹H-NMR spectrum of compound 3



Figure S20. ^{13}C -NMR (150 MHz) spectrum of compound **3**

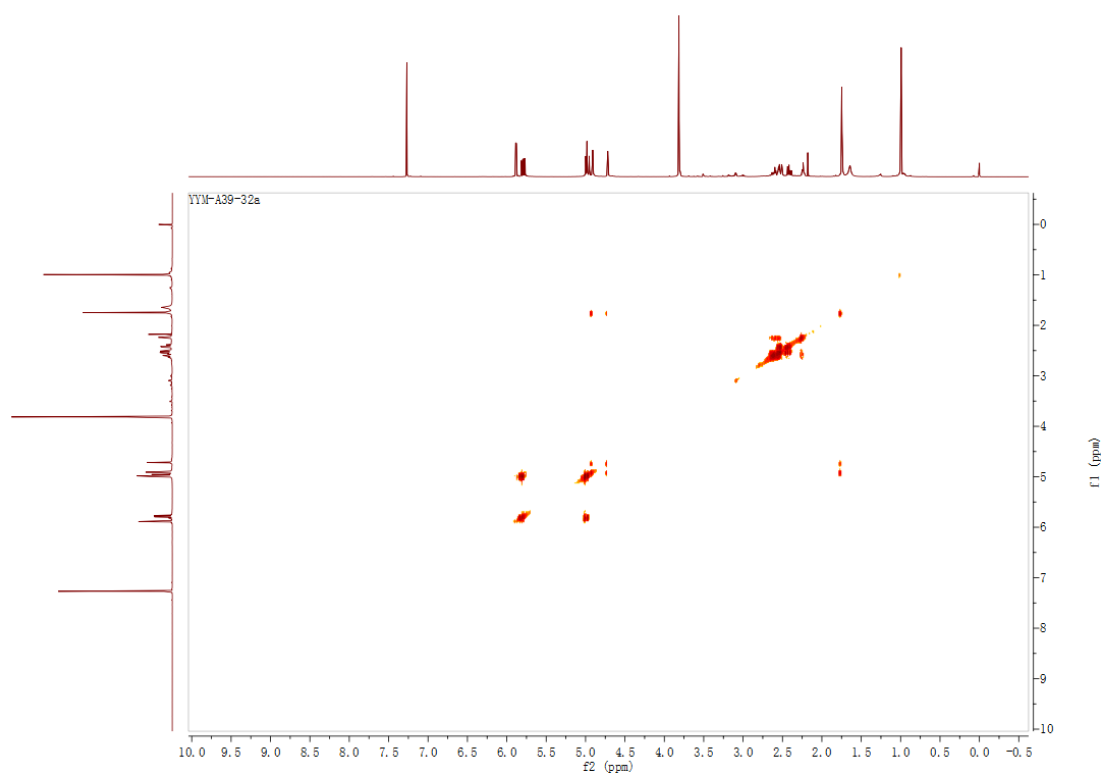


Figure S21. ^1H - ^1H COSY spectrum of compound **3**

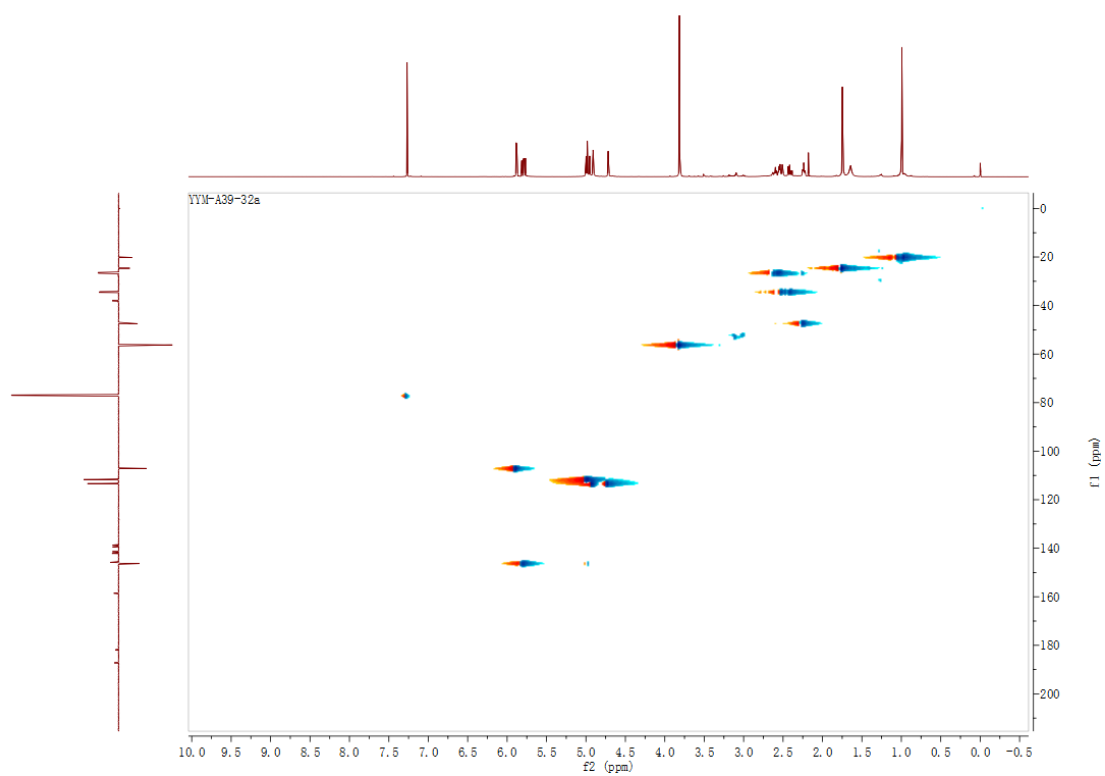


Figure S22. HSQC spectrum of compound **3**

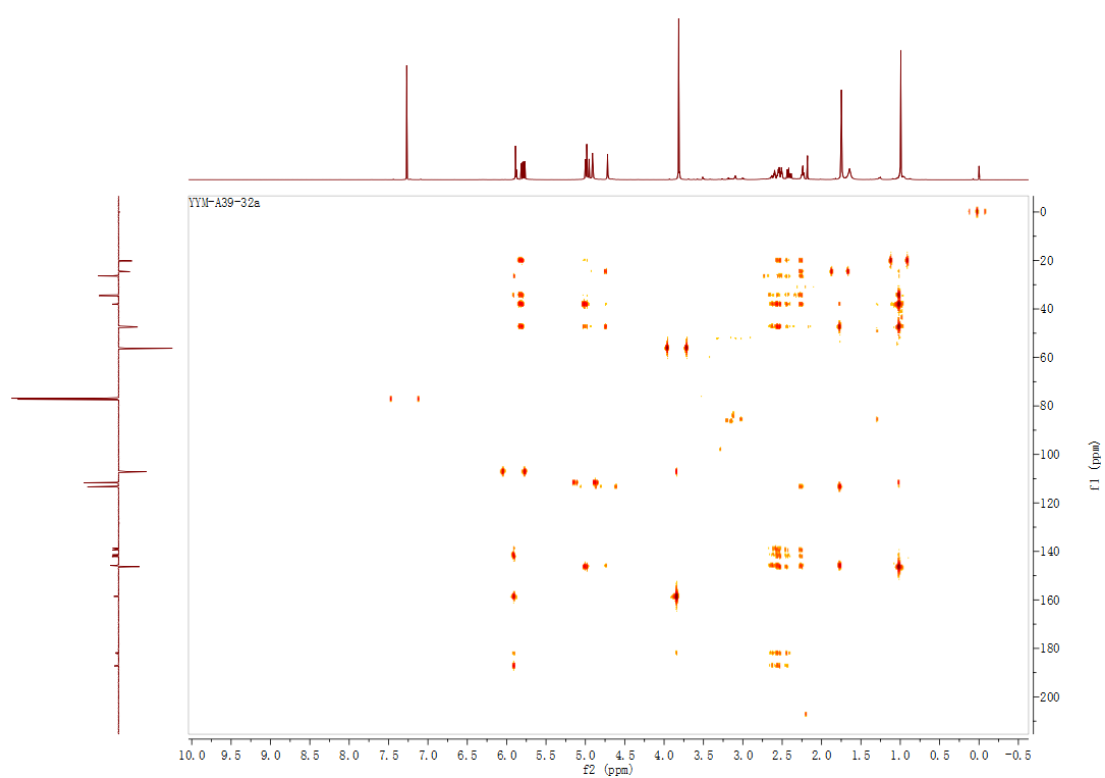


Figure S23. HMBC spectrum of compound **3**

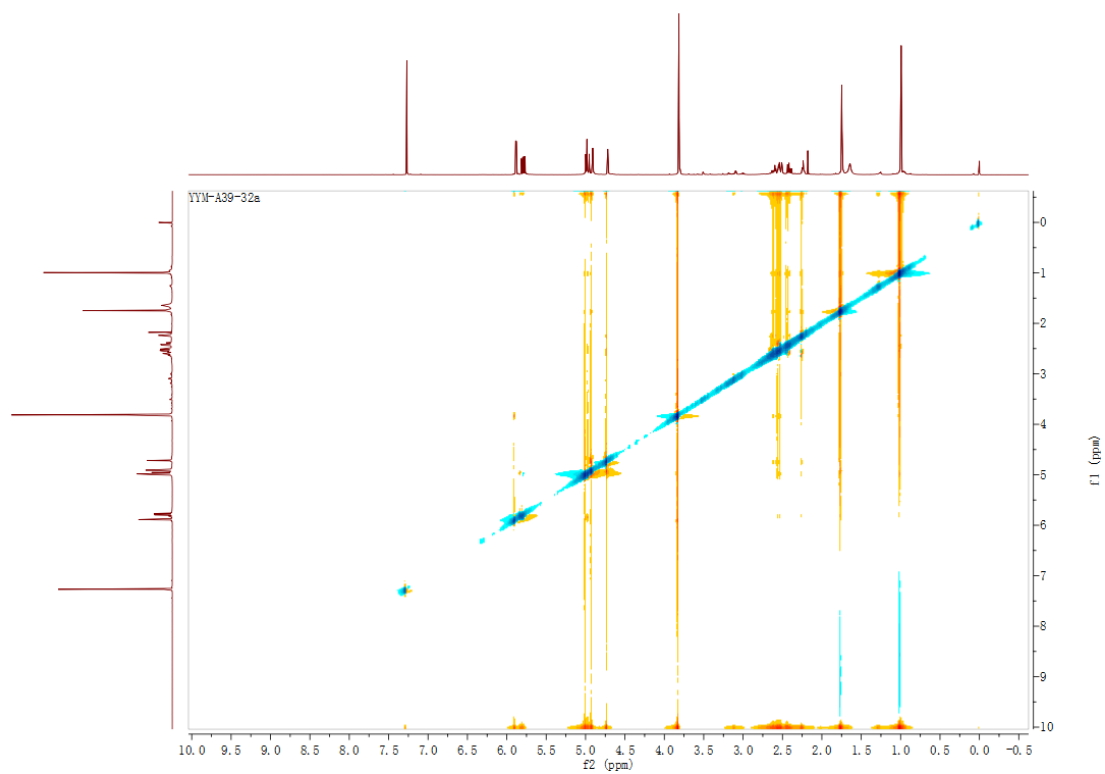


Figure S24. ROESY spectrum of compound **3**