SUPPLEMENTARY MATERIAL

New flavonoid glycosides from seeds of *Baccharoides anthelmintica*

Yi Liu[a,b], Wen-Qiong Wang[a], Tong-Chen[a] and Li-jiang Xuan[a*]

[a] *State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 501 Haike Road, Shanghai 201203, People's Republic of China*

[b]*University of Chinese Academy of Sciences, No. 19A Yuquan Road, Beijing 100049, People's Republic of China*

*Corresponding Author

Prof. Dr. Li-jiang Xuan, Tel/fax: +86 21 20231968. E-mail: ljxuan@simm.ac.cn

Abstract: *Baccharoides anthelmintica* is the most popular traditional Uighur medicines used for vitiligo. The chemical investigation of the seeds of *B. anthelmintica* led to the isolation of three new flavonoid glycosides (Vernosides A-C). Their structures were determined by comprehensive analysis of spectroscopic data including 1D and 2D NMR and HRMS data. Vernosides A-C were evaluated for their effects on tyrosinase activity, Vernoside B can enhance tyrosinase activity.

Key words: *Baccharoides anthelmintica;* vitiligo; flavonoid glycosides

List of content

Abbreviations

HMBC: ^{1}H detected heteronuclear multiple-bond correlation

COSY: correlated spectroscopy

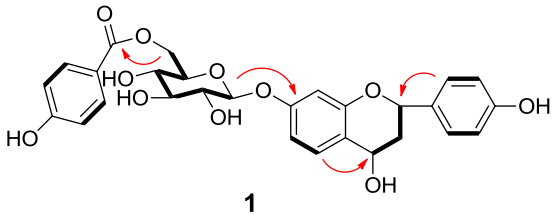
HSQC: ^{1}H detected heteronuclear single-quantum coherence

Table S1. ^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) data for Compounds **1-3** (δ_H, δ_C in ppm, *J* in Hz)

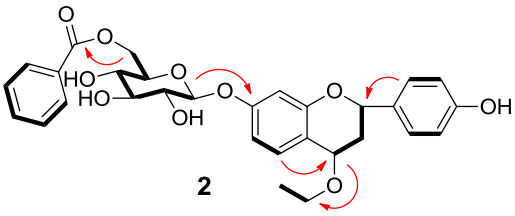
	1[a]		**2**[a]		**3**[b]	
position	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
2	5.12 (dd, 10.5, 3.6)	74.3	5.08 (d, 12.3)	74.8	4.99 (d, 12.1)	74.2
3	2.08 (m), 2.06 (m)	39.8	2.25 (m) 1.99 (m)	36.7	2.25 (m) 1.96 (m)	35.5
4	4.68 (dd, 2.4, 2.2)	64.2	4.37 (dd, 5.3, 2.7)	72.1	4.22 (m)	73.3
5	7.13 (d, 8.5)	132.4	7.06 (d, 8.4)	132.8	7.05 (d, 8.4)	132.4
6	6.68 (dd, 8.5, 2.5)	110.3	6.65 (dd, 8.4, 2.4)	110.4	6.64 (dd, 8.4, 2.5)	109.8
7		157.1		157.5		156.8
8	6.58 (d, 2.5)	105.4	6.62 (d, 2.4)	105.2	6.62 (d, 2.5)	105.0
9		159.8		160.2		159.5
10		119.1		117.0		115.8
11			3.63 (m) 3.69 (m)	64.6	3.41 (s)	56.1
12			1.24 (t, 7.0)	15.9		
1′		133.4		133.5		133.6
2′	7.25 (d, 8.5)	128.8	7.25 (d, 8.5)	128.8	6.87 (d, 1.9)	114.4
3′	6.80 (d, 8.5)	116.2	6.81 (d, 8.5)	116.2		145.7
4′		158.3		158.5		156.9
5′	6.80 (d, 8.5)	116.2	6.81 (d, 8.5)	116.2	6.80 (d, 8.1)	115.9
6′	7.25 (d, 8.5)	128.8	7.25 (d, 8.5)	128.8	6.75 (dd, 1.9, 8.1)	118.8
1″	5.02 (d, 5.6)	101.8	4.93 (d, 7.3)	102.0	4.91 (d, 6.5)	101.4
2″	3.78 (m)	74.8	3.49 (m)	74.8	3.52 (m)	74.0
3″	3.51 (m)	77.8	3.41 (m)	77.8	3.40 (m)	77.2
4″	3.43 (m)	72.0	3.40 (m)	72.0	3.42 (m)	74.2
5″	3.48 (m)	75.4	3.83 (m)	75.6	3.79 (m)	74.9
6″	4.64 (m), 4.33 (m)	65.0	4.72 (m) 4.35 (m)	65.6	4.71 (d, 12.3) 4.36 (dd, 11.8, 7.6)	65.2
1‴		121.8		131.1		130.3
2‴	7.86 (d, 8.7)	132.9	7.99 (d, 7.5)	130.6	7.97 (d, 7.8)	130.2
3‴	6.76 (d, 8.7)	116.3	7.28 (t, 7.5)	129.6	7.25 (t, 7.8)	129.1
4‴		163.9	7.48 (t, 7.5)	134.2	7.47 (t, 7.4)	133.9
5‴	6.76 (d, 8.7)	116.3	7.28 (t, 7.5)	129.6	7.25 (t, 7.8)	129.1
6‴	7.86 (d, 8.7)	132.9	7.99 (d, 7.5)	130.6	7.97 (d, 7.8)	130.2
7‴		168.1		167.9		167.7

[a] Recorded in CD_3OD. [b] Recorded in CD_3OD-$CDCl_3$ (1:1).

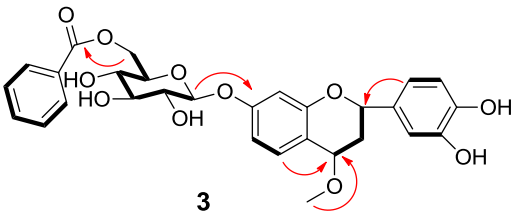
Figure S1. Key COSY and HMBC correlations of compounds **1-3**



1



2



3

Figure S2. ^{1}H NMR spectrum of compound **1** in CD_3OD

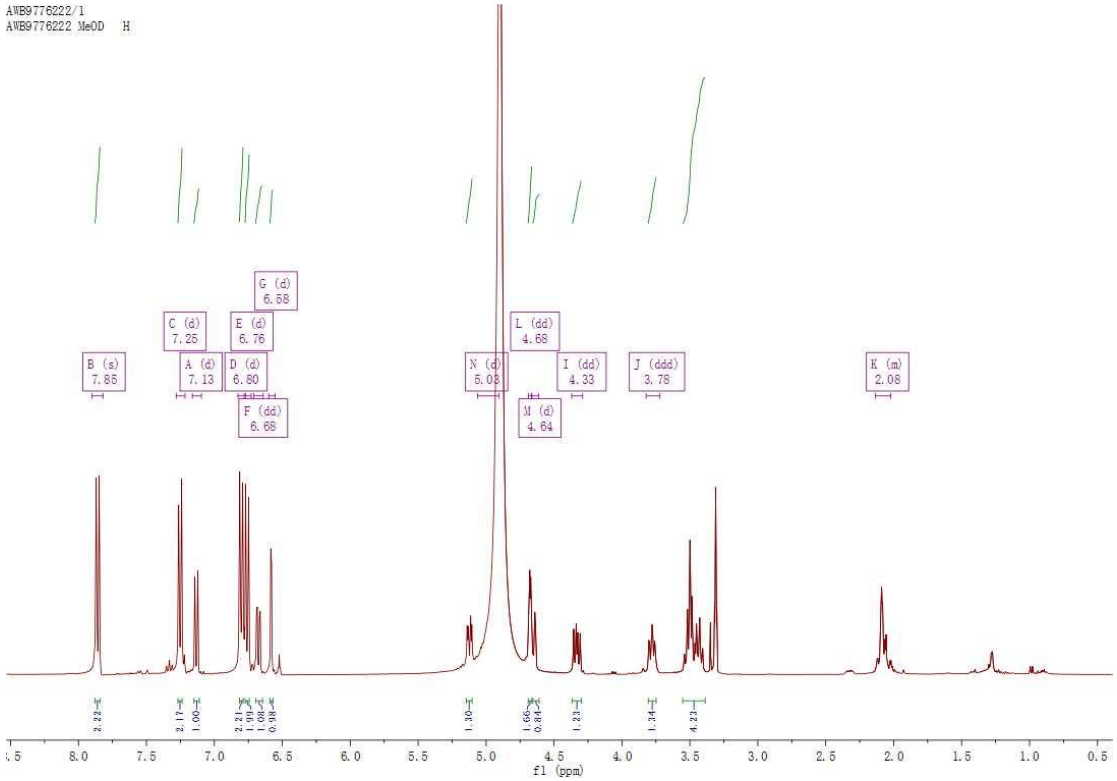


Figure S3. ^{13}C NMR spectrum of compound **1** in CD_3OD

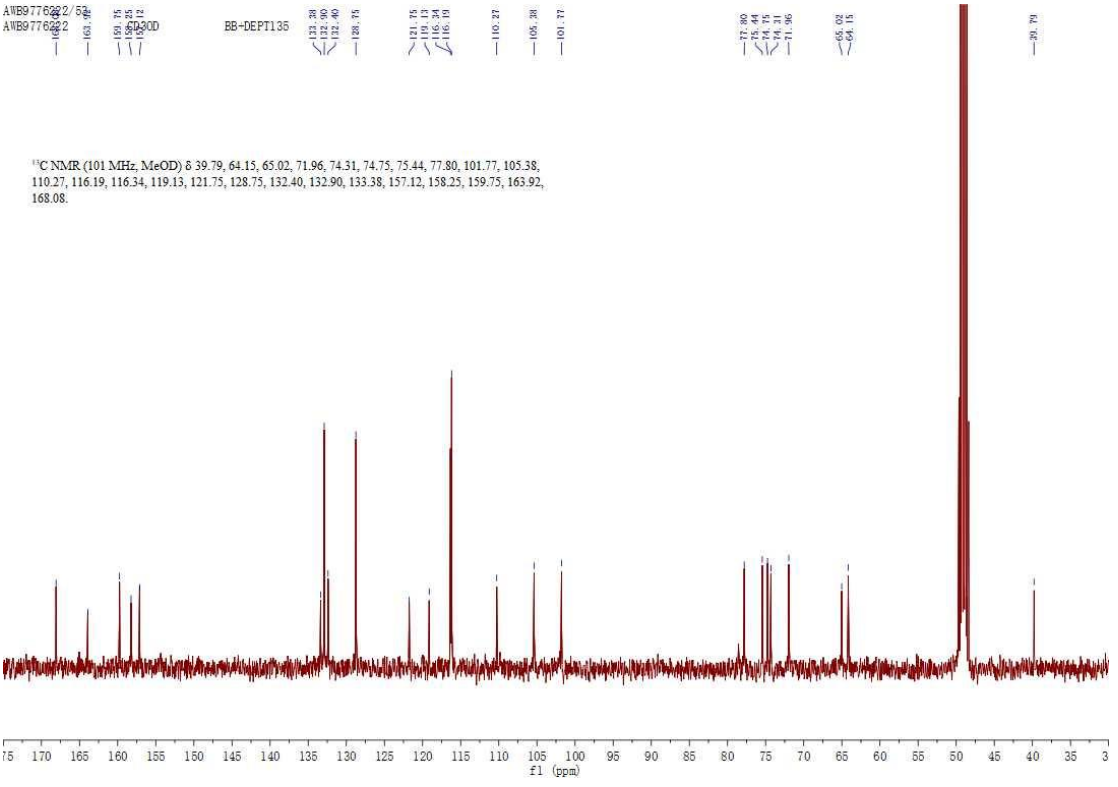


Figure S4. ^{1}H-^{1}H COSY spectrum of compound **1** in CD_3OD

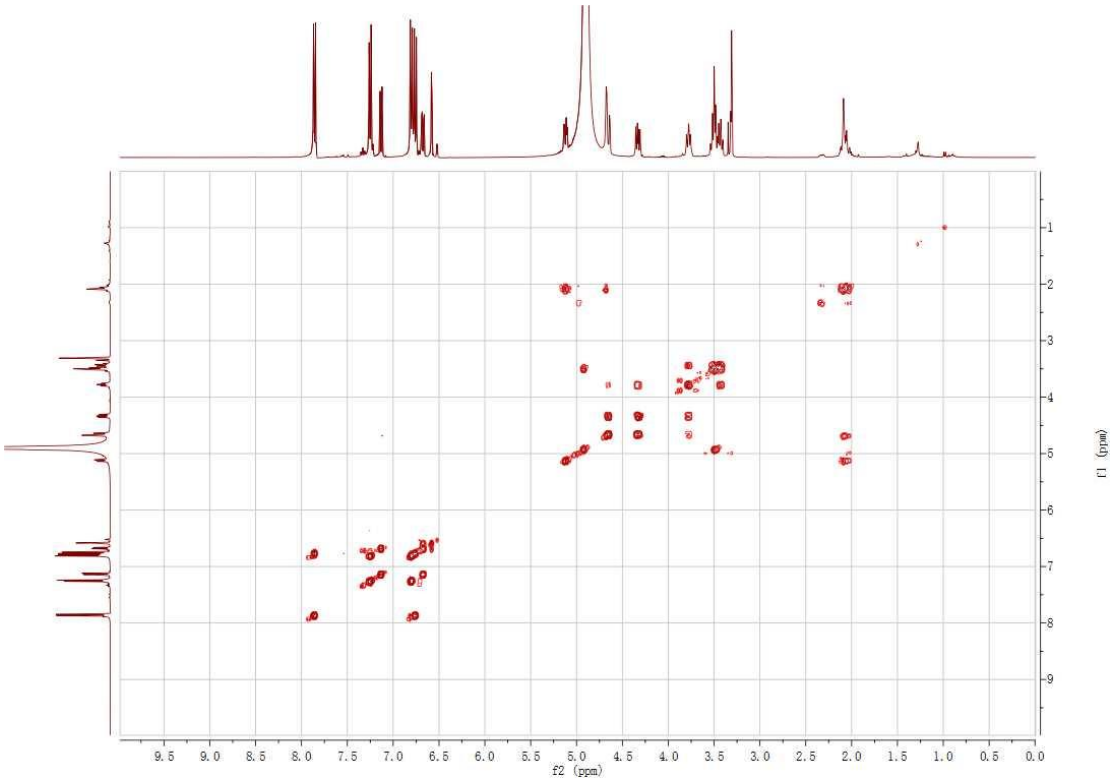


Figure S5. HSQC spectrum of compound **1** in CD_3OD

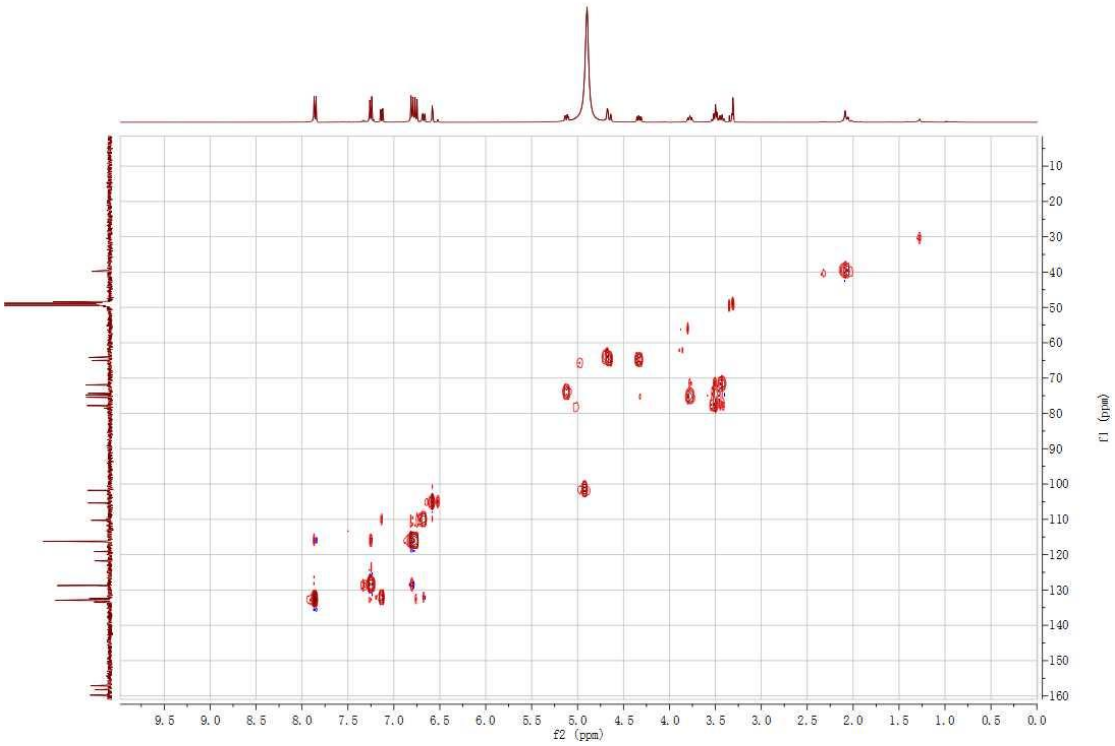


Figure S6. HMBC spectrum of compound **1** in CD_3OD

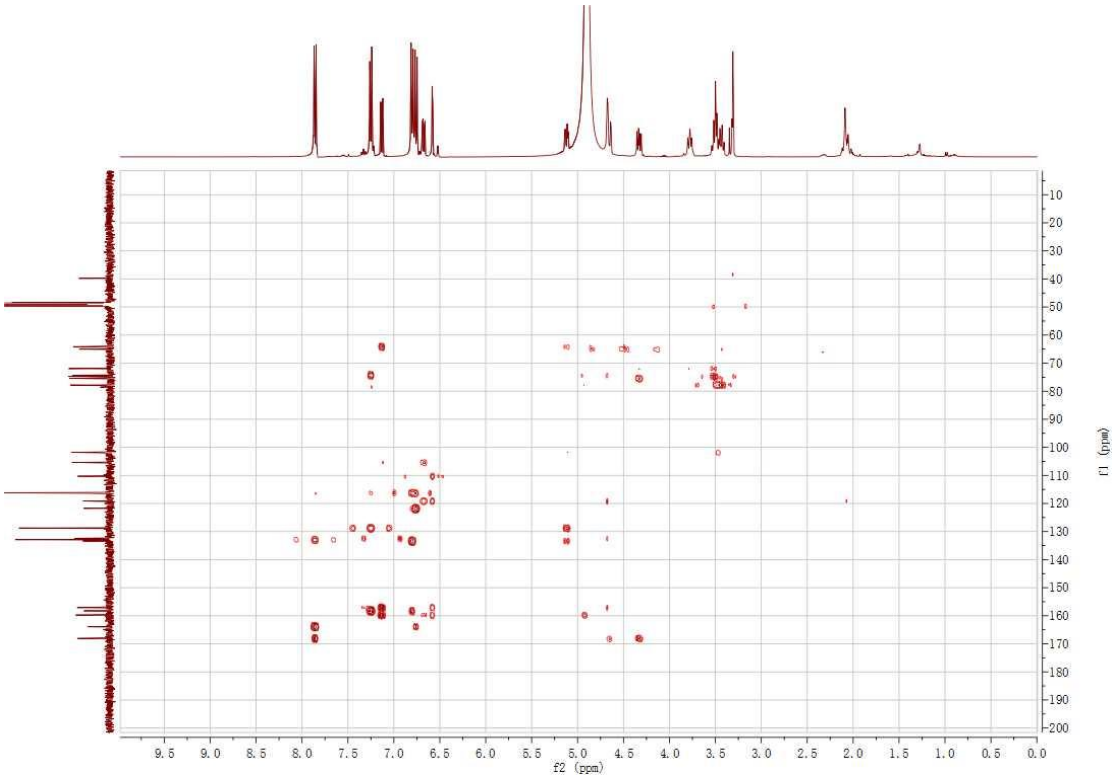


Figure S7. ^1H NMR spectrum of compound **2** in CD_3OD

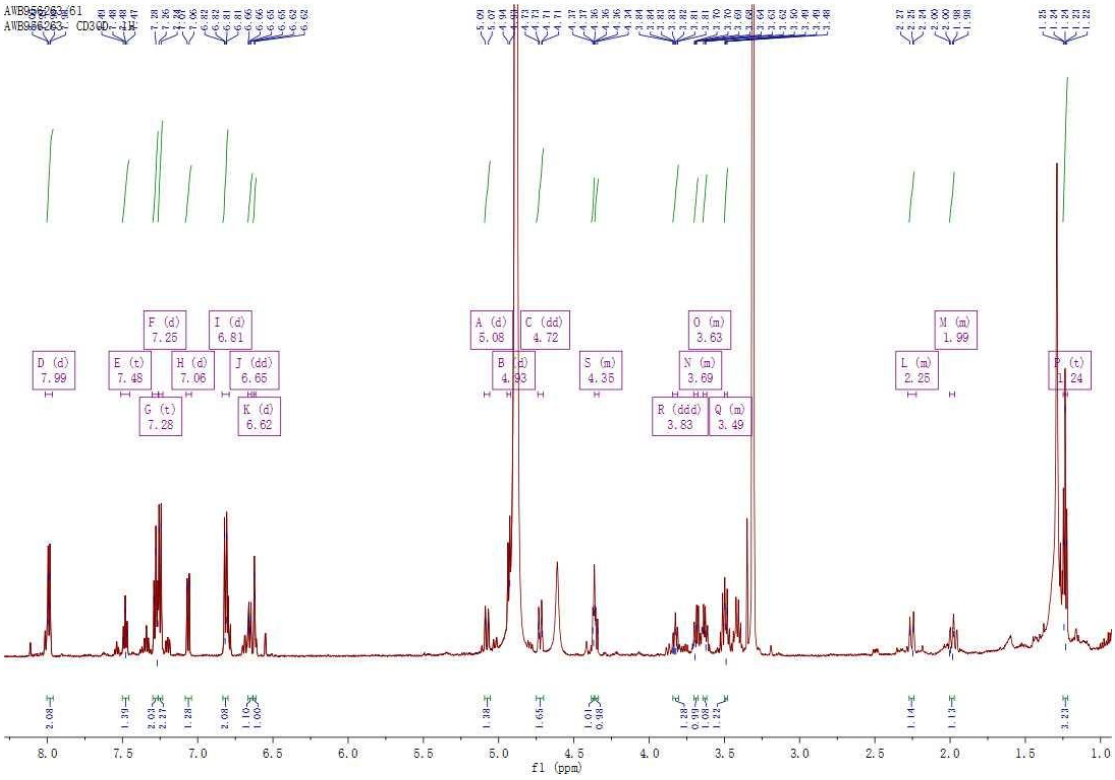


Figure S8. ^{13}C NMR spectrum of compound **2** in CD_3OD

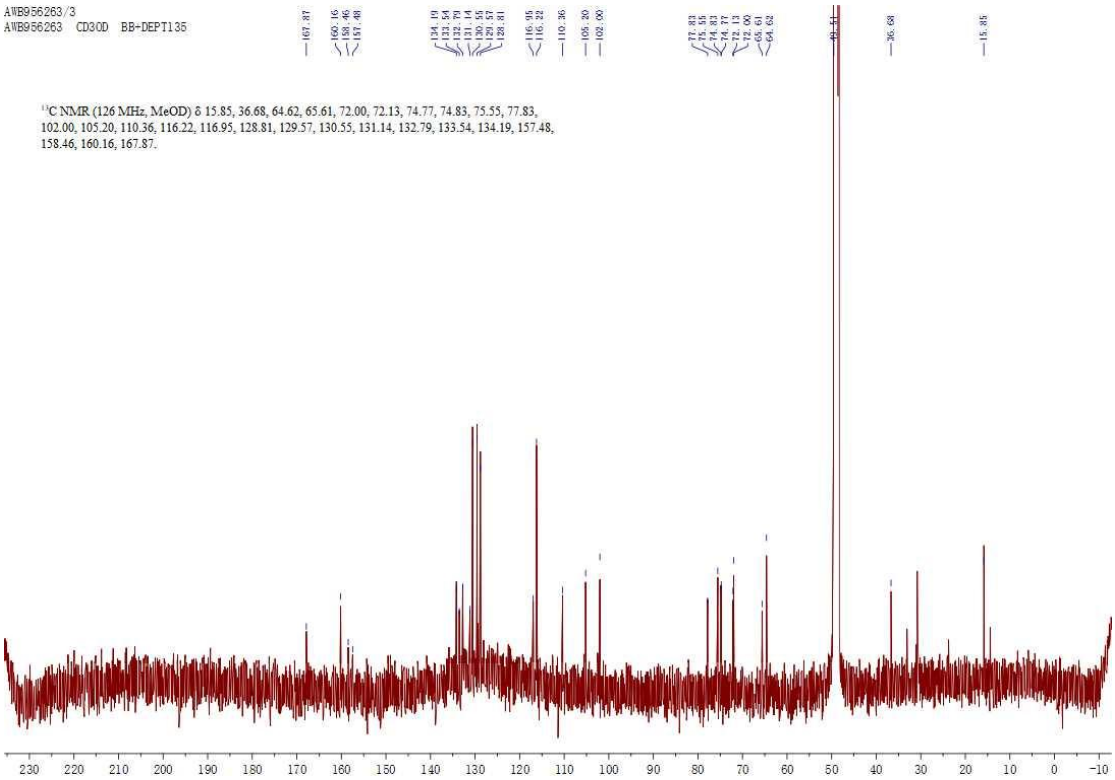


Figure S9. HSQC spectrum of compound **2** in CD_3OD

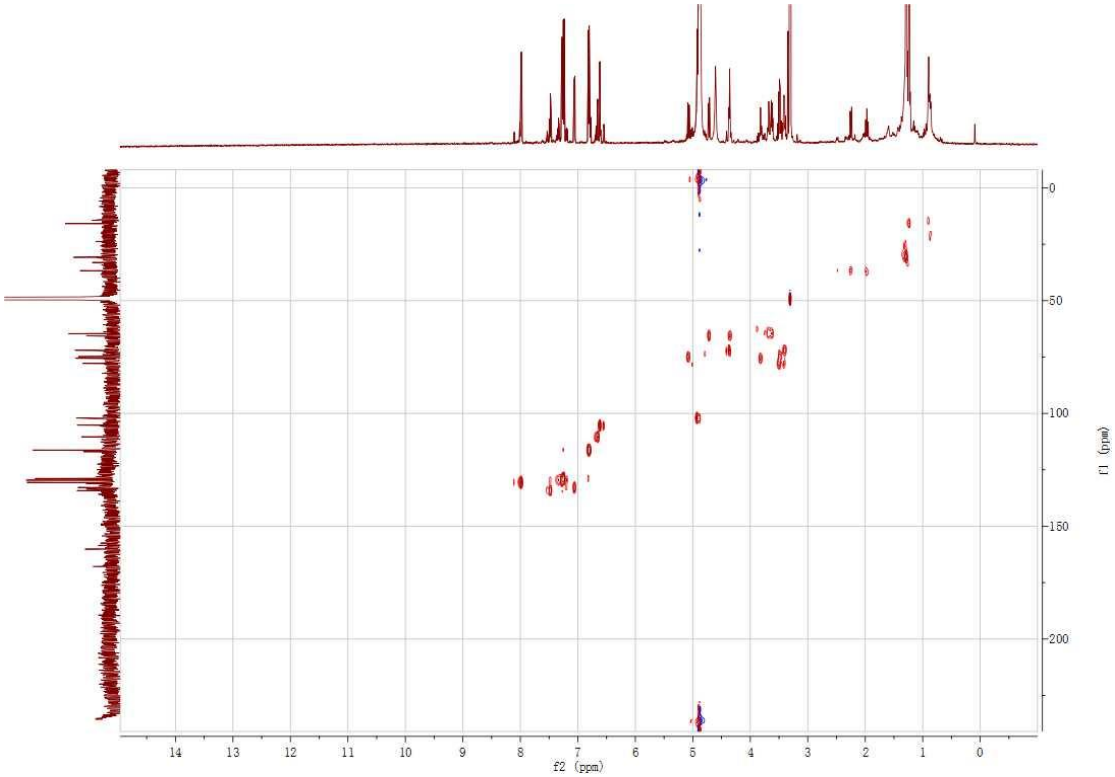


Figure S10. HMBC spectrum of compound **2** in CD_3OD

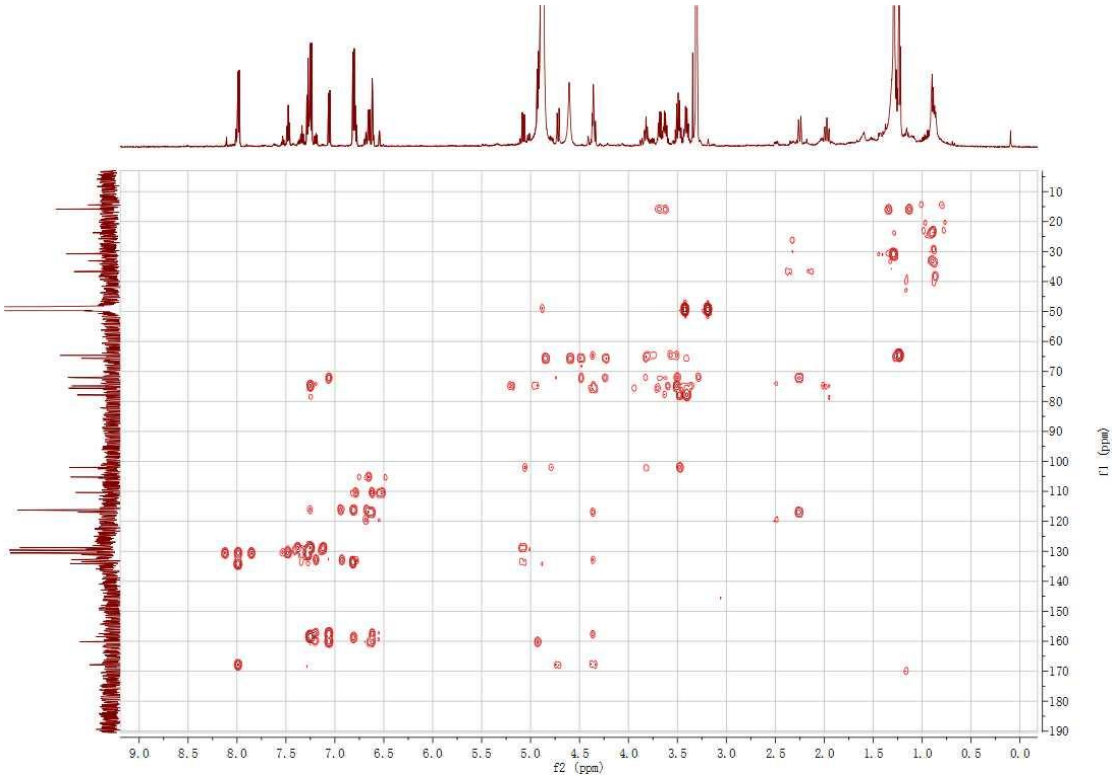


Figure S11. ^1H NMR spectrum of compound **3** in CD_3OD-$CDCl_3$ (1:1)

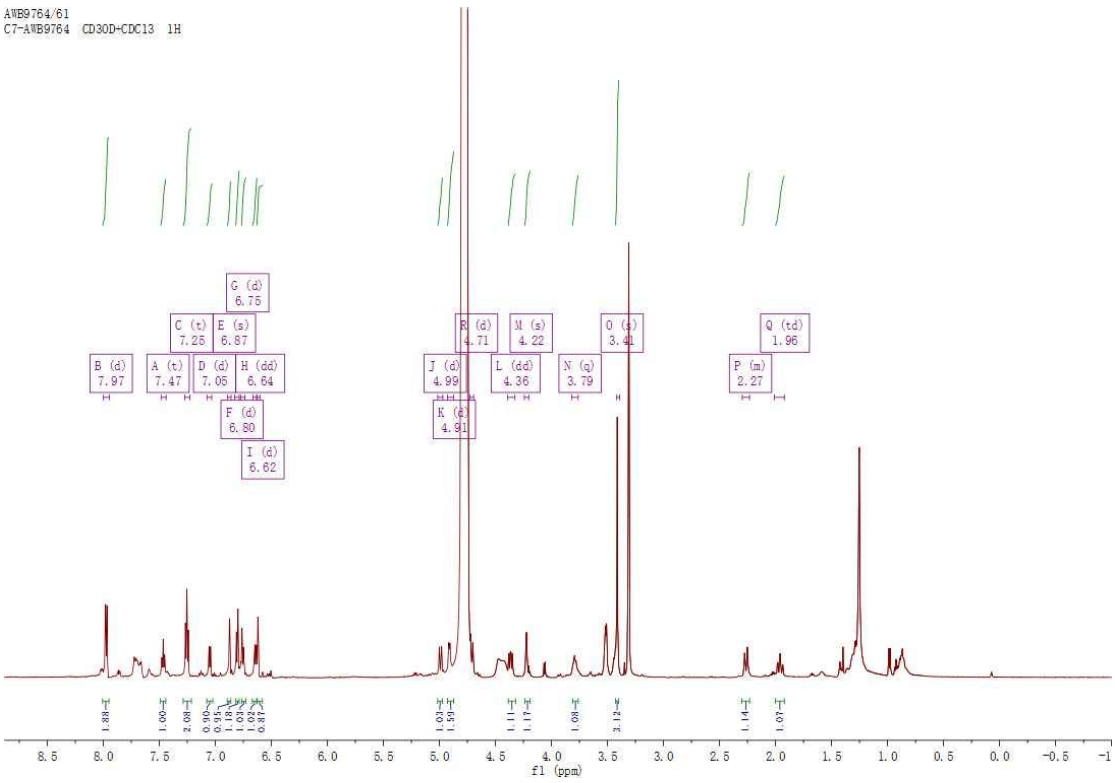


Figure S12. ^{13}C NMR spectrum of compound **3** in CD_3OD-$CDCl_3$ (1:1)

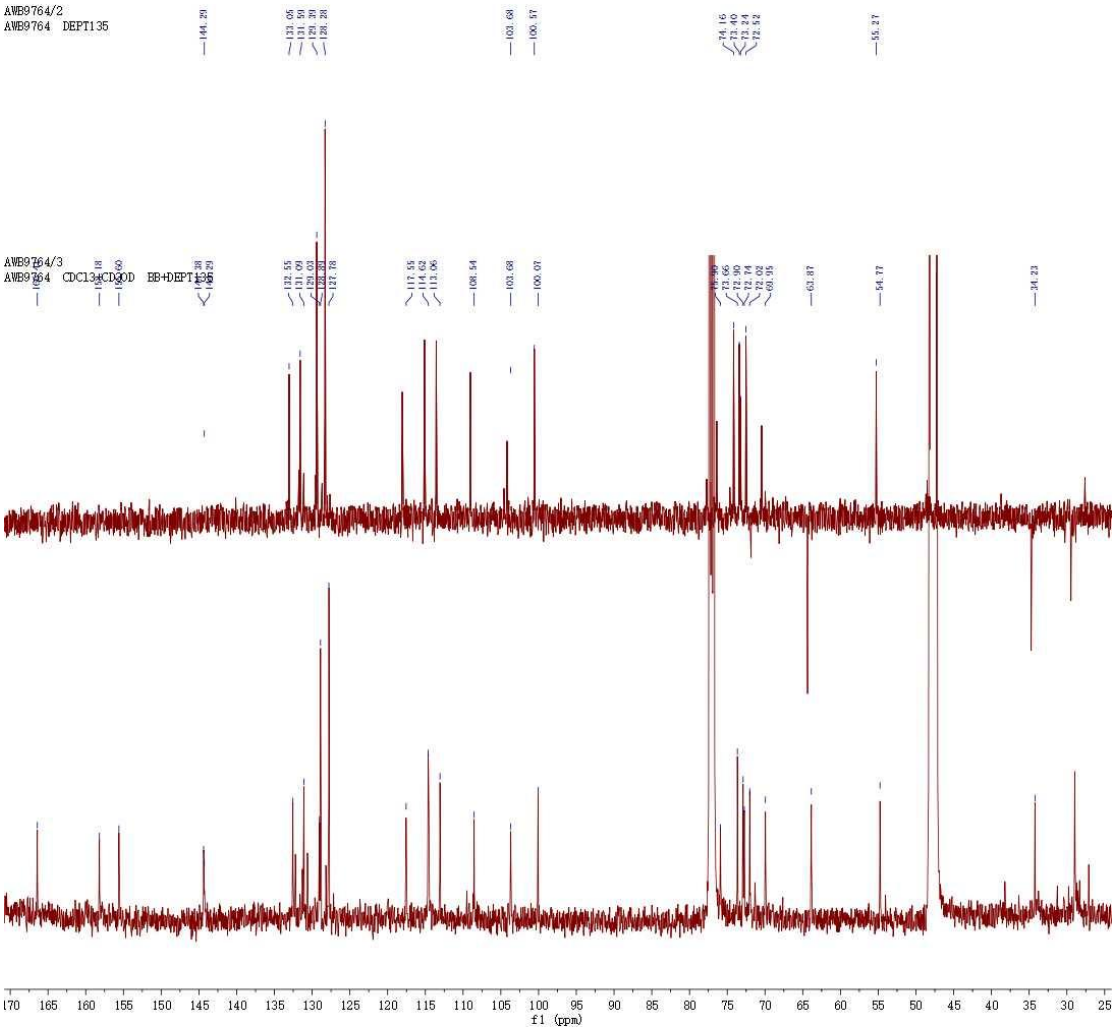


Figure S13. HSQC spectrum of compound **3** in CD_3OD-$CDCl_3$ (1:1)

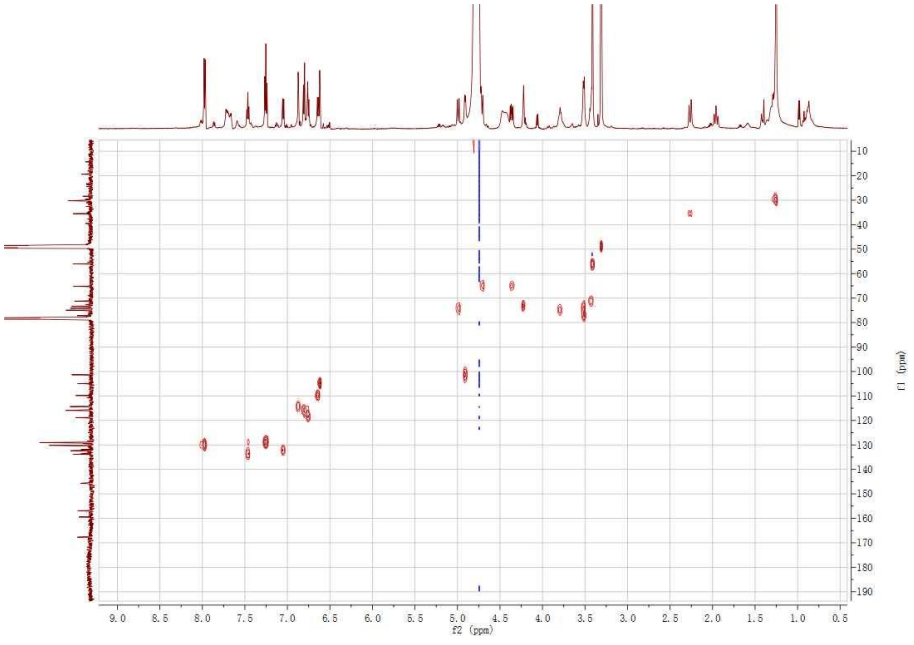


Figure S14. HMBC spectrum of compound **3** in CD_3OD-$CDCl_3$ (1:1)

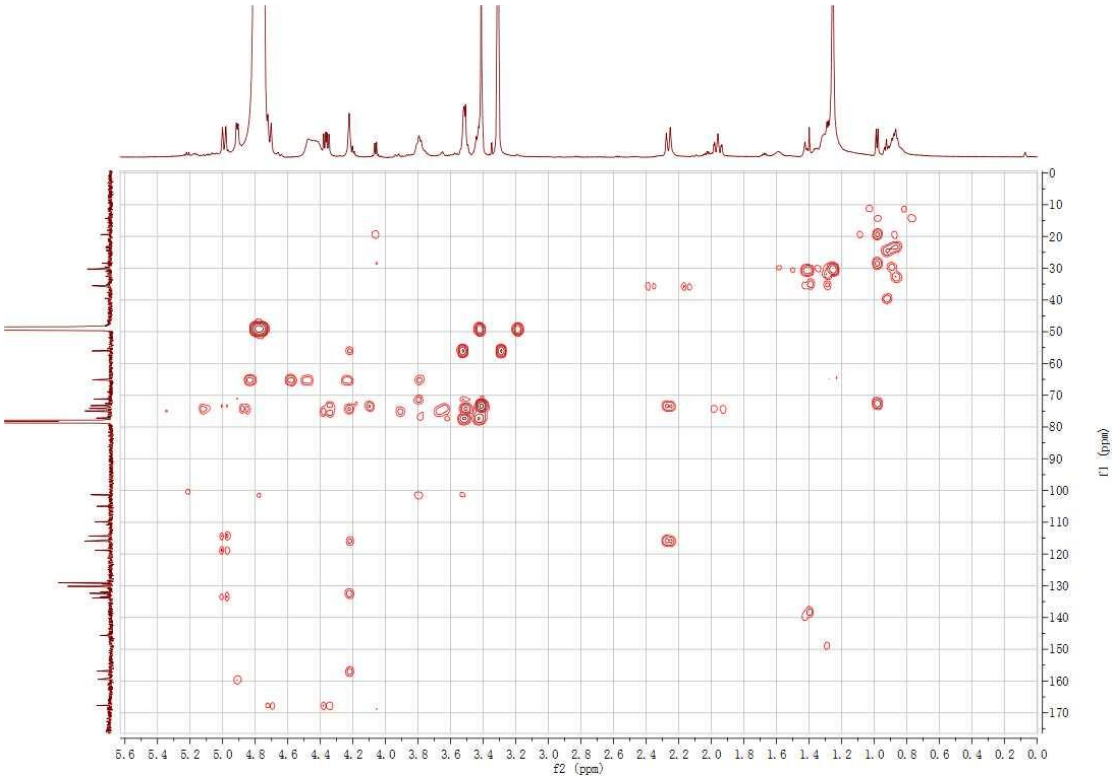


Figure S15. Activation of tyrosinase activity by compound **2**

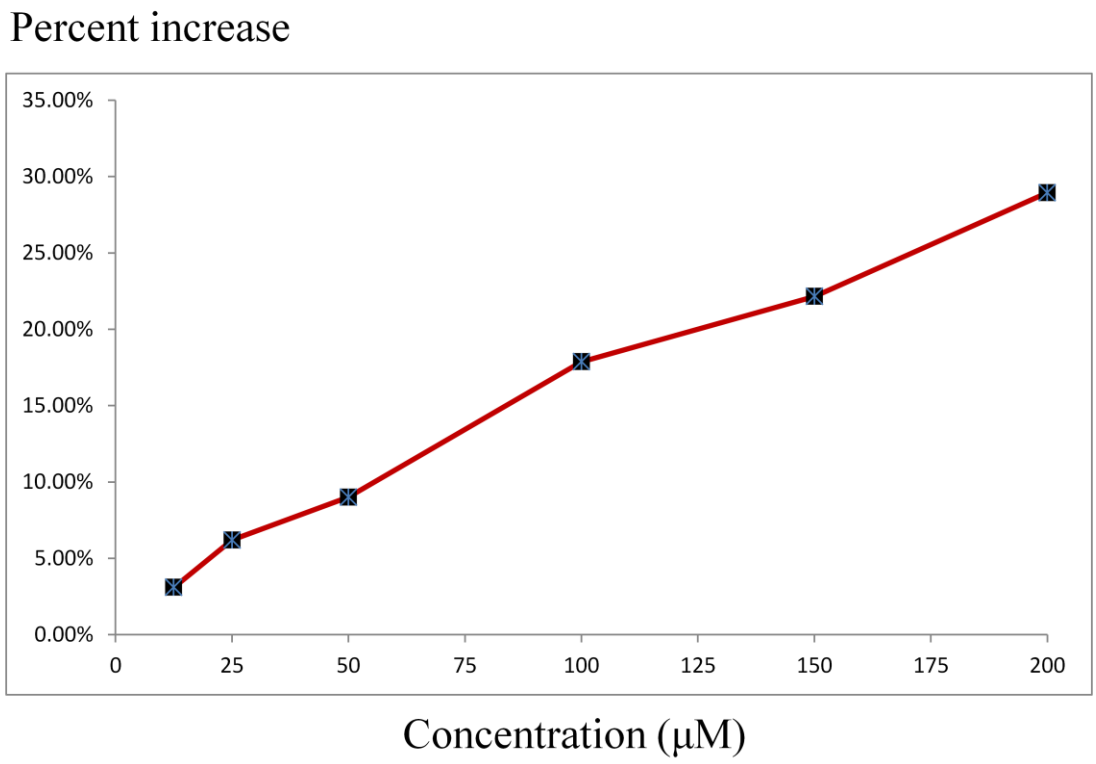


Figure S16. IR spectrum of compound **1**

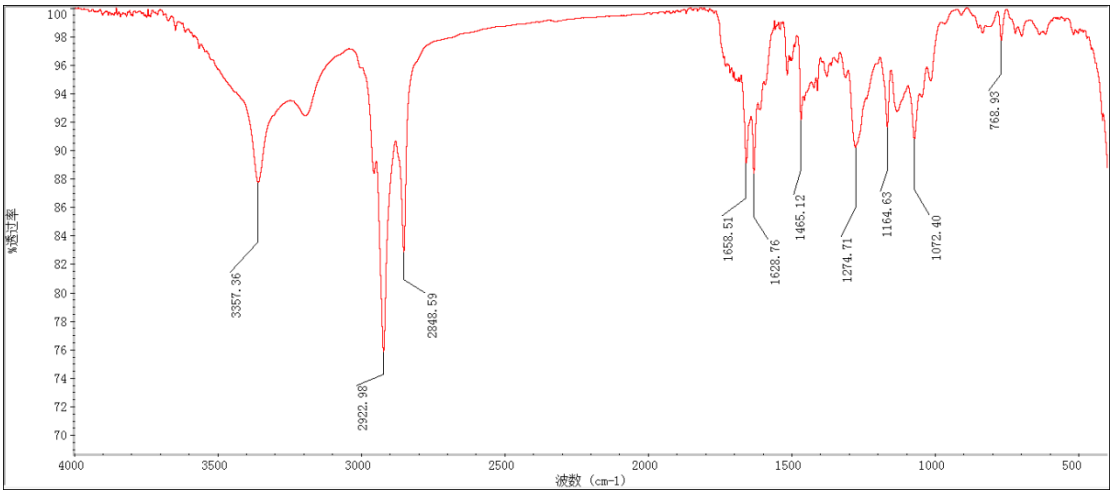
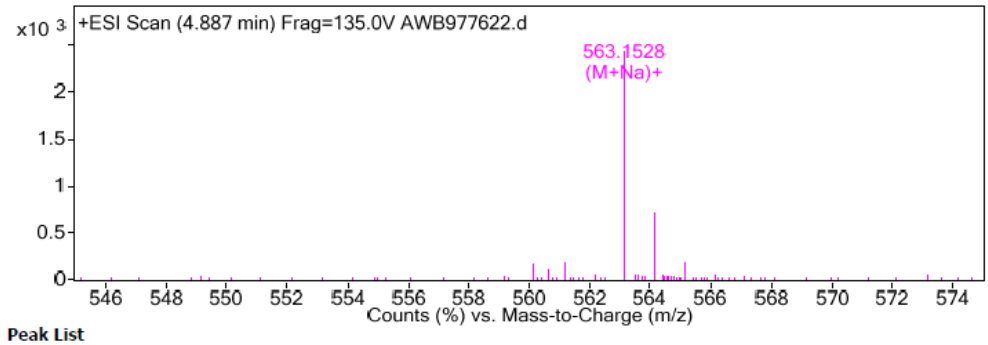


Figure S17. HR-ESI-MS spectrum of compound **1**

User Spectra

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
	135	0	Esi



Peak List

m/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
116.9865		169825					

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	0
S	0	0
Cl	0	0

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C28 H28 O11	TRUE	540.1636	540.1632	-0.73	C28 H28 Na O11	97.04

Figure S18. IR spectrum of compound **2**

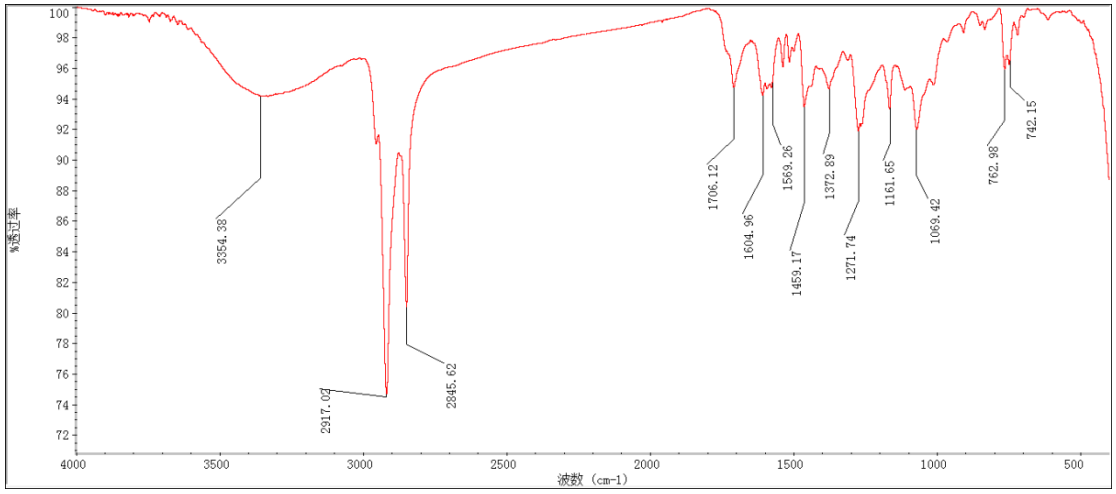
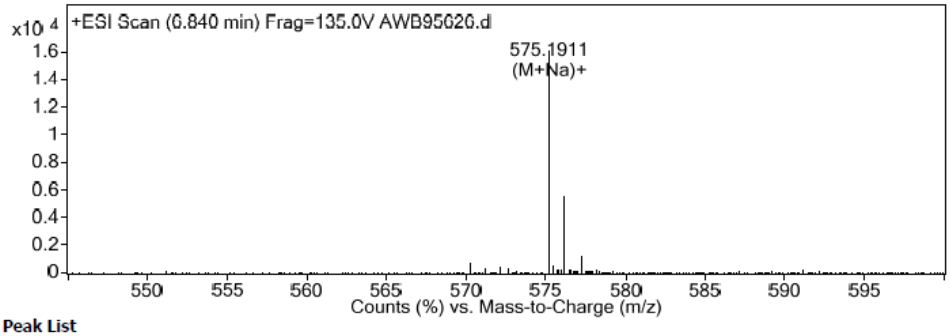


Figure S19. HR-ESI-MS spectrum of compound **2**

User Spectra

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
	135	0	Esi



Peak List

m/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
1127.3919	1	1855769					

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	0
S	0	0
Cl	0	0

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C30 H32 O10	TRUE	552.2019	552.1995	-4.31	C30 H32 Na O10	90.13
C23 H36 O15		552.2019	552.2054	6.33	C23 H36 Na O15	73.18

--- End Of Report ---

Figure S20. IR spectrum of compound **3**

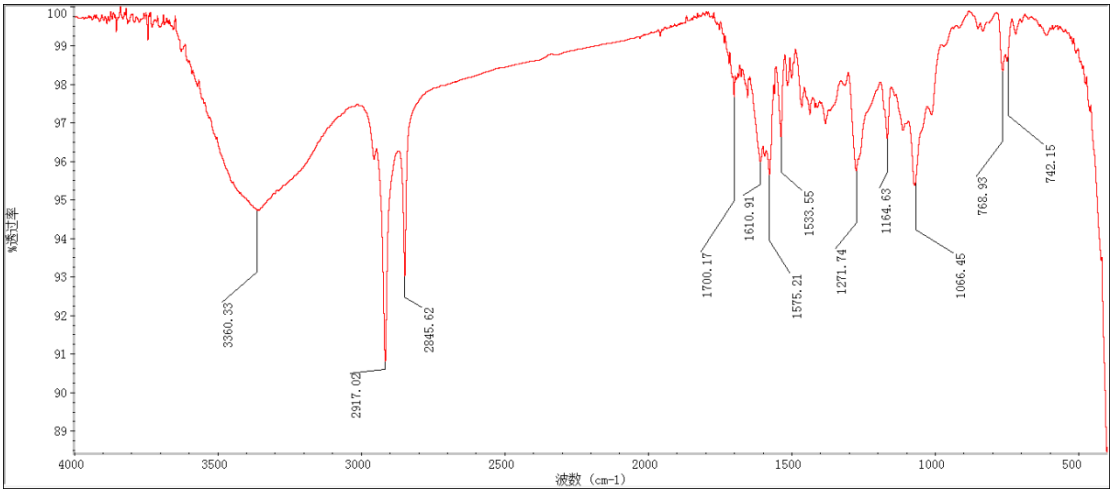
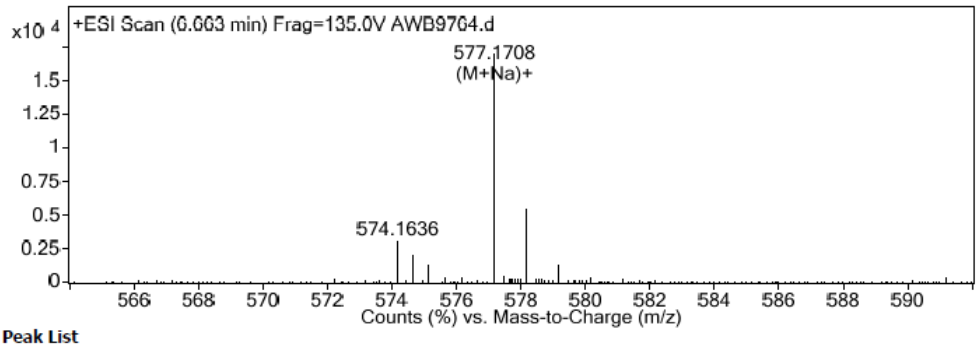


Figure S21. HR-ESI-MS spectrum of compound **3**

User Spectra

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
	135	0	Esi



Peak List

m/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
577.1708	1	820033		C29 H30 Na O11	(M+Na)+		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	0
S	0	0
Cl	0	0

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C29 H30 O11	TRUE	554.1816	554.1788	-5	C29 H30 Na O11	87.25
C22 H34 O16		554.1816	554.1847	5.6	C22 H34 Na O16	78.24

--- End Of Report ---