Supporting information

Three new compounds from the flower branch of Gastrodia elata Blume and anti-microbial activity

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Abstract: Three new compounds (**1**–**3**), including novel tetra-*p*-cresol substituted cyclopenta[a]naphthalene derivatives, named gastrodinol (**1**), 2-(4′-hydroxybenzoyl)-3-hydroxyethyl indole (**2**), 2-(4′-hydroxybenzoyl)-3-(4″-hydroxybenzyl)indole (**3**) were isolated from the flower branch of *G. elata*, along with five known compounds (**4**–**8**). Among them, compound **1** exhibited the most anti-microbial activity against *Streptococcus agalactiae*, with the minimum inhibitory concentration of 1 μg·ml^{-1}. This study demonstrated that the novel compound **1** found in the flower branch of *G. elata* may be responsible for anti-microbial effect. It will lead to the development of new antibiotics, and how to utilize the TCM (″Tianma″) better.

Keywords: *Gastrodia elata*; phenolic compounds; anti-microbial activity

Qualitative Analysis Report

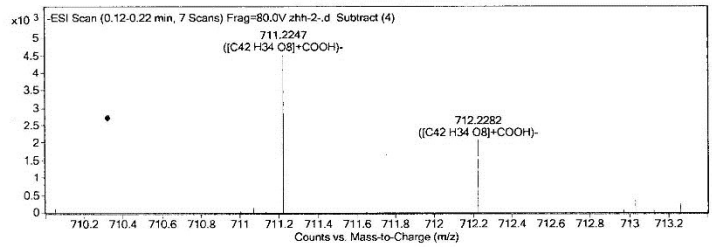
Data Filename	zhh-2-.d	**Sample Name**	zhh-2
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	s-.m	**Acquired Time**	6/20/2019 10:09:17 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
80	0	ESI



Peak List

m/z	z	Abund
89.0244		15483.73
339.2342	1	99244.21
340.2376	1	25692
347.1728	1	18513.32
365.2476	1	19452.87
375.2767	1	46418.15
393.2792	1	15546.55
403.3082	1	38207.61
453.2274	1	21337.53
713.476	1	18583.38

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C42 H34 O8	666.2254	711.2236	711.2247	-1.10	-1.55	26.0000

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Figure S1. HRESIMS of compound **1**.

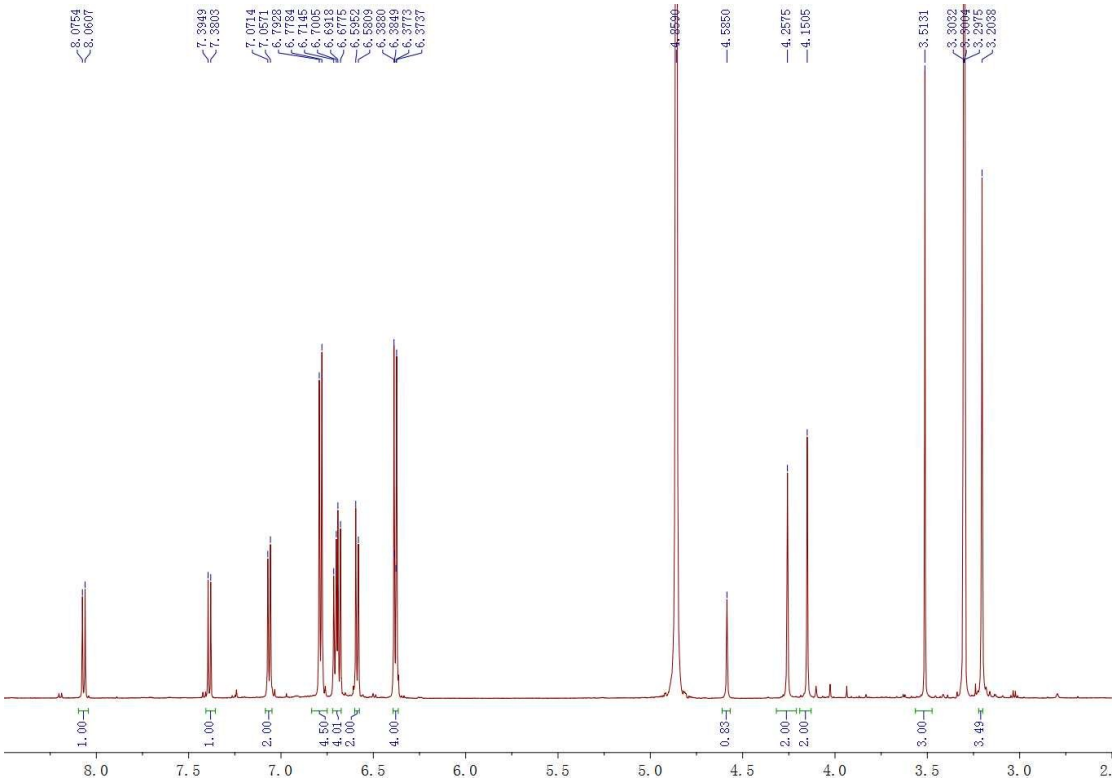


Figure S2. ^{1}H-NMR of compound **1**.

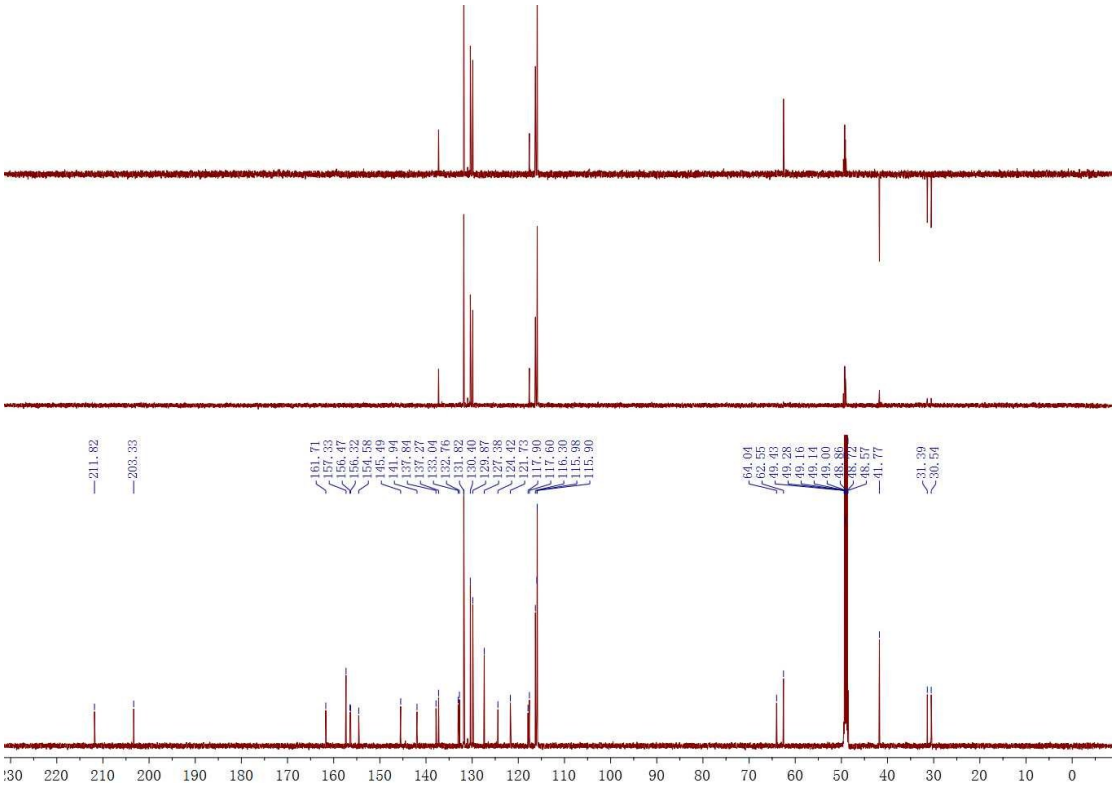


Figure S3. ^{13}C-NMR of compound **1**.

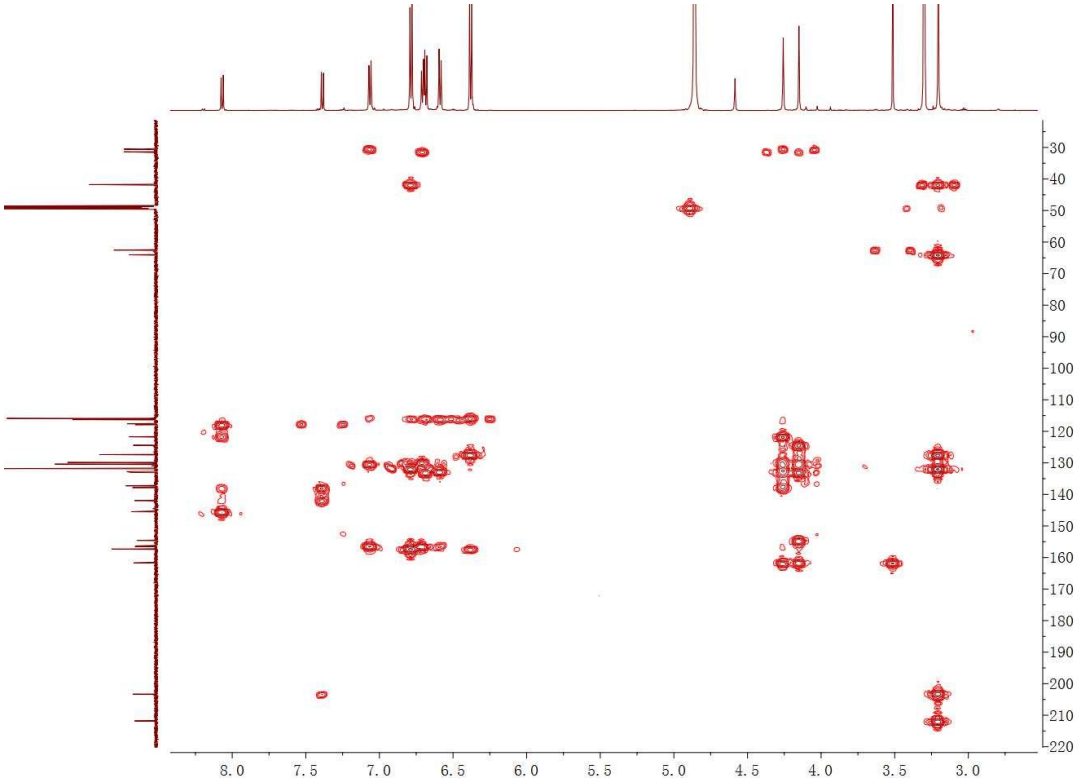


Figure S4. HMBC of compound **1**.

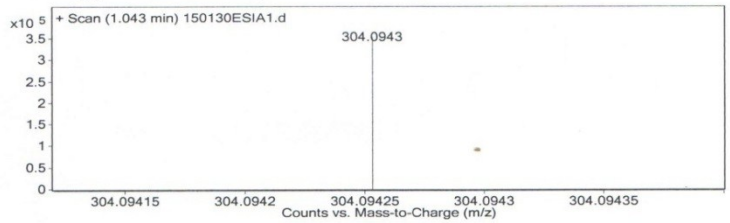
Qualitative Analysis Report

Data Filename	150130ESIA1.d	**Sample Name**	zhh-1
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	1/30/2015 12:27:32 PM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage 200 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund	Formula	Ion
121.0338		21475.58		
299.1095	1	51949.55		
301.1397		21687.71		
304.0943	1	351650.47	C17 H15 N Na O3	M+
305.0975	1	59522.75	C17 H15 N Na O3	M+
345.1204	1	80263.8		
413.2669	1	27380.66		
585.1992	1	112360.64		
586.2019	1	38124.55		
694.3715	1	26222.6		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	8
Na	1	1
N	1	1

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C17 H15 N Na O3	304.0950	304.0944	304.0943	0.2	0.6	10.5000

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Figure S5. HRESIMS of compound **2**.

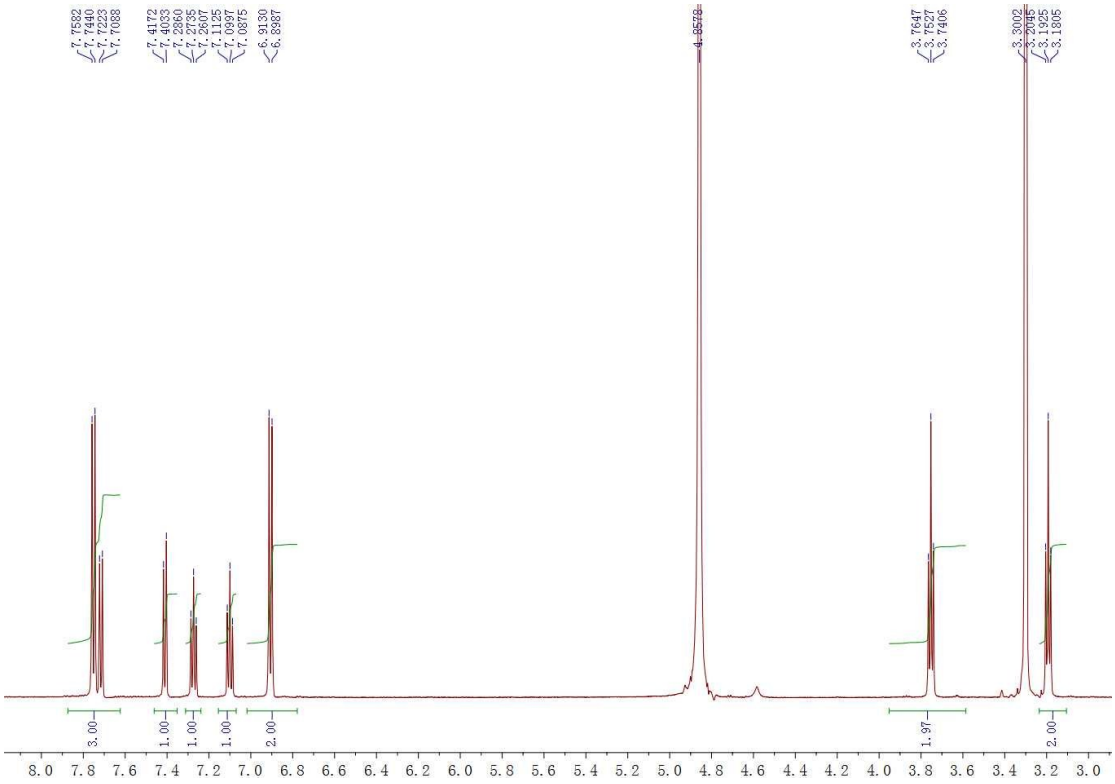


Figure S6. ^{1}H-NMR of compound **2**.

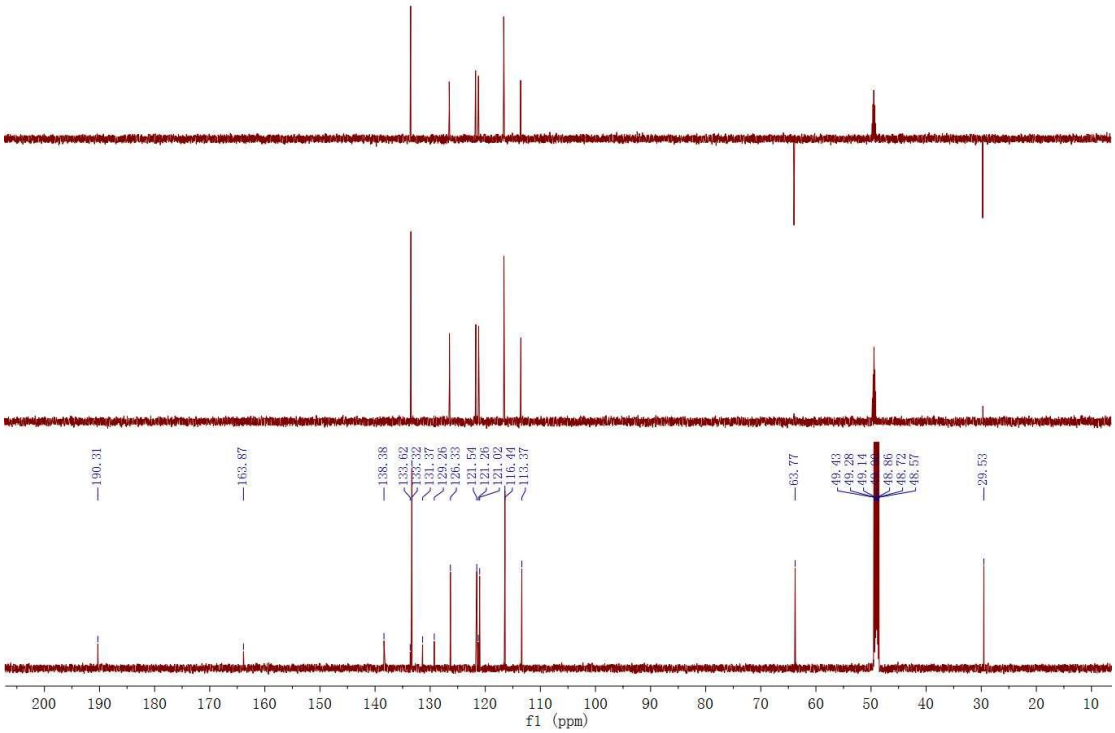


Figure S7. ^{13}C-NMR of compound **2**.

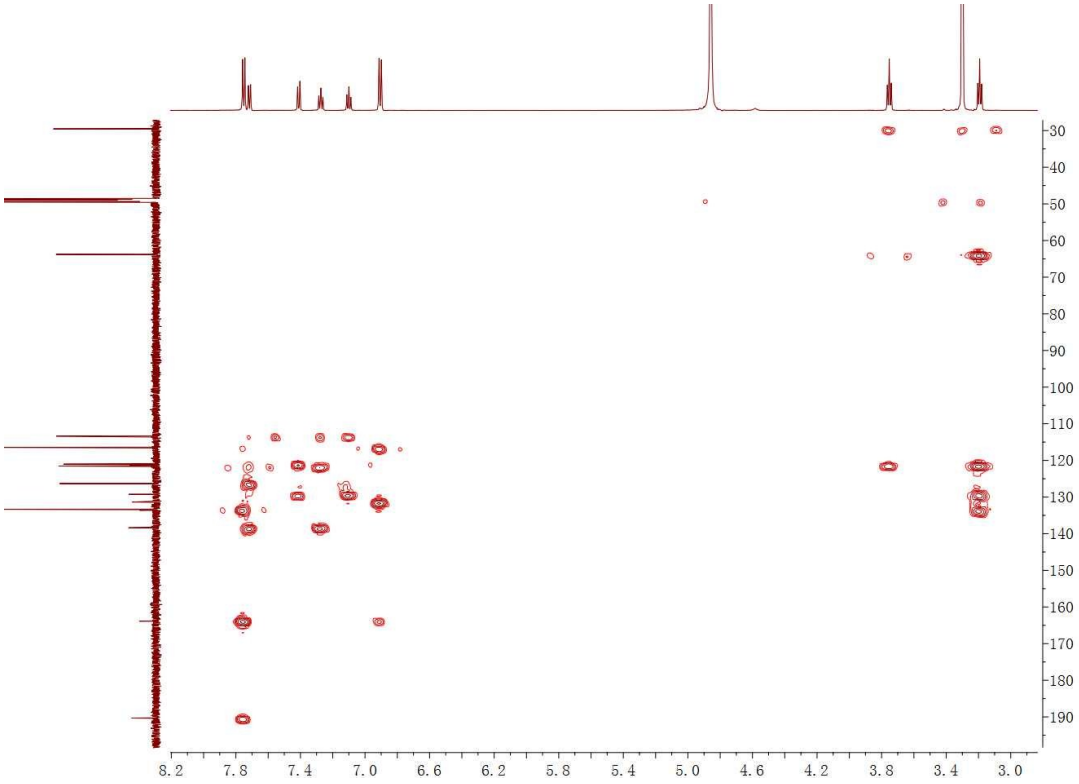


Figure S8. HMBC of compound **2**.

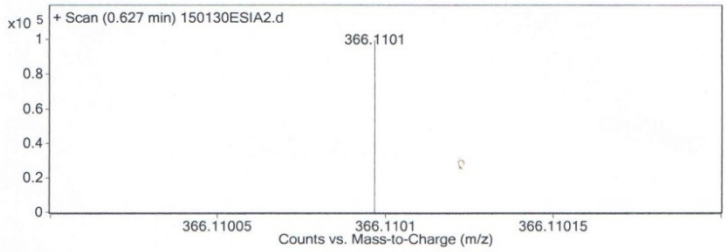
Qualitative Analysis Report

Data Filename	150130ESIA2.d	**Sample Name**	zhh-17
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	1/30/2015 12:29:27 PM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
121.0509	1	40675.41		
250.0861	1	17193.38		
360.3234	1	24369.18		
363.1021	2	16409.66		
366.1101	1	99525.78	C22 H17 N Na O3	M+
367.1132	1	20320.97	C22 H17 N Na O3	M+
382.0837	1	30991.05		
709.23	1	53005.6		
710.2331	1	24449.06		
922.0098	1	74399.55		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	8
Na	1	1
N	1	1

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C22 H17 N Na O3	366.1106	366.1101	366.1101	0.0	0.0	14.5000

--- End Of Report ---

Figure S9. HRESIMS of compound **3**.

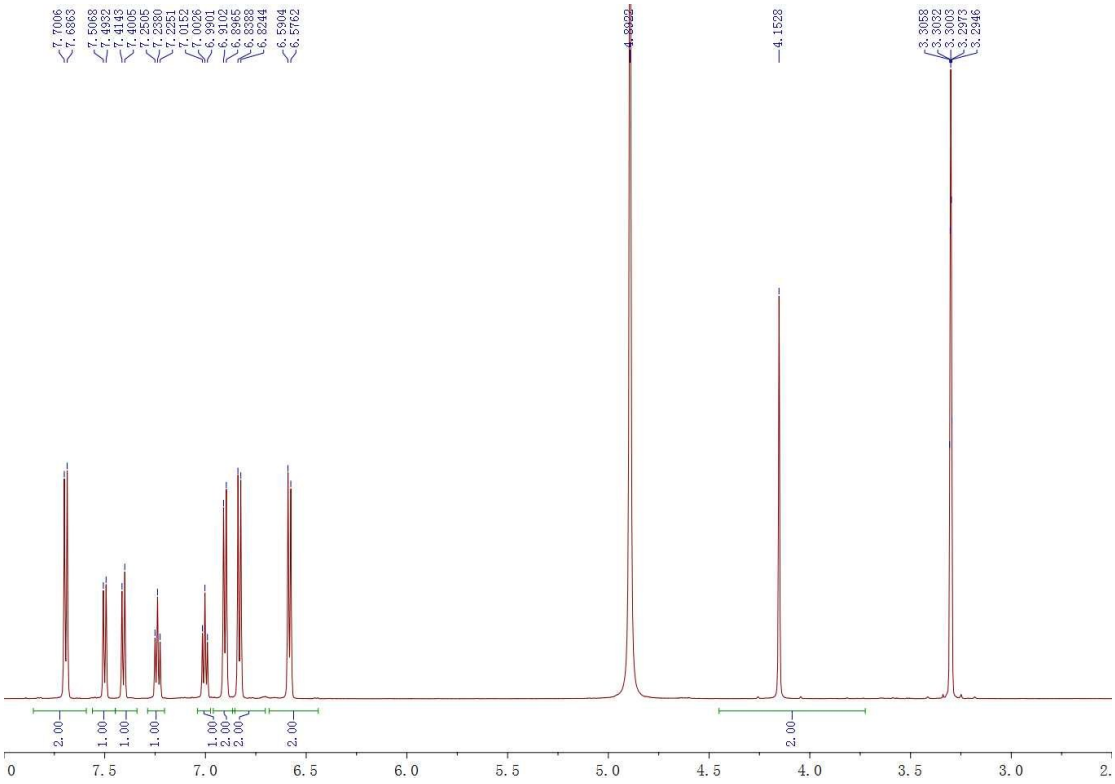


Figure S10. ^{1}H-NMR of compound **3**.

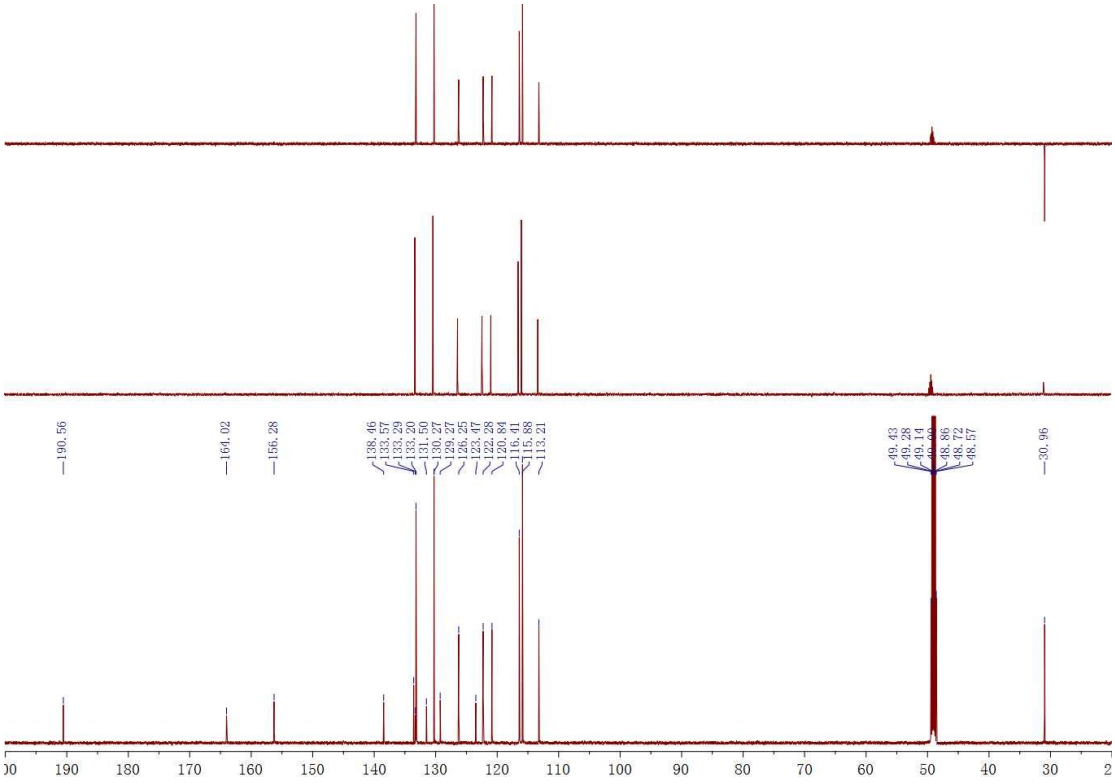


Figure S11. ^{13}C-NMR of compound **3**.

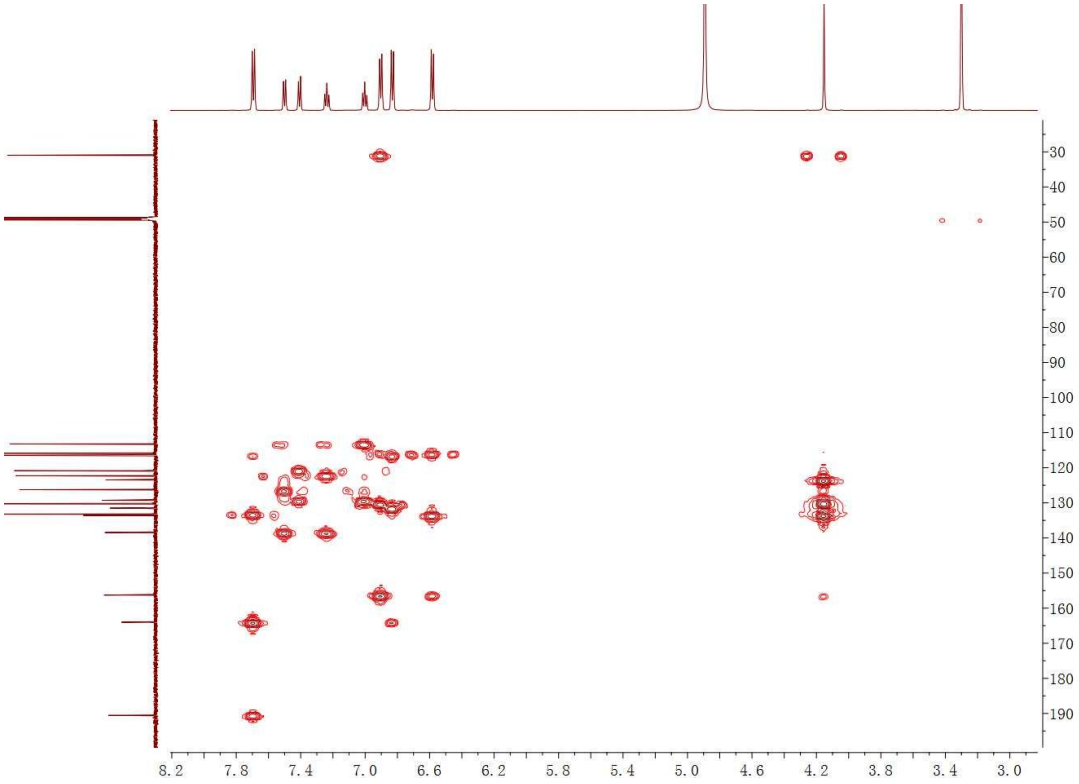


Figure S12. HMBC of compound **3**.