

Supplementary Materials: Five 2-(2-Phenylethyl)chromones from Sodium Chloride-Elicited *Aquilaria sinensis* Cell Suspension Cultures

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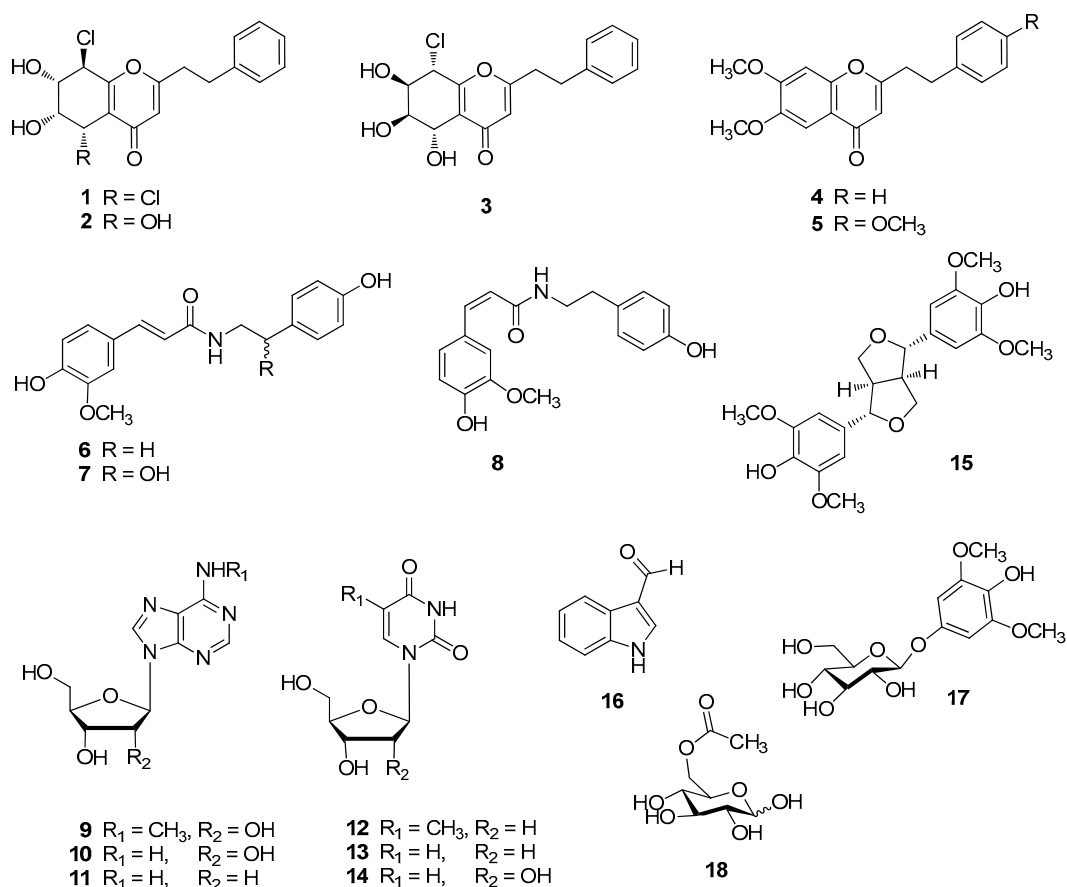


Figure S1. Structures of Compounds 1–18.

Formula Predictor Report - Compound 1.lcd

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Data File: D:\Data\张钟秀\Compound 1.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	20	O	2	0	5	S	2	0	0	H
C	4	0	20	F	1	0	0	Cl	1	0	2	
N	3	0	0	P	3	0	0					

Error Margin (ppm): 5

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0

Apply N Rule: no

Isotope RI (%): 1.00

MSn Logic Mode: AND

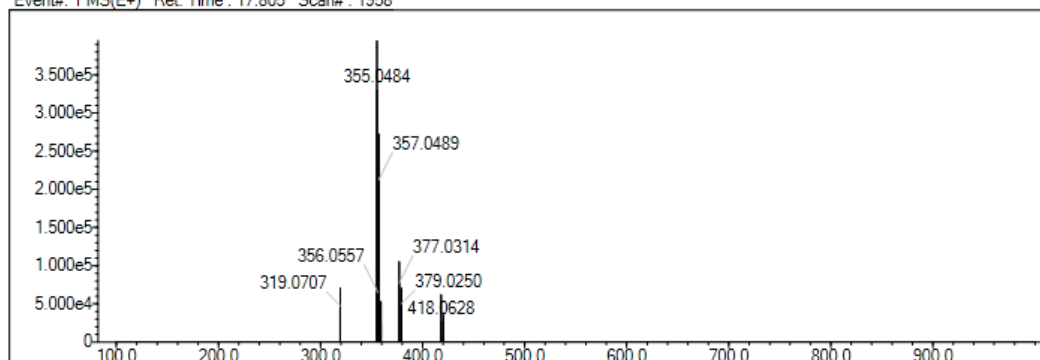
Electron Ions: both

Use MSn Info: yes

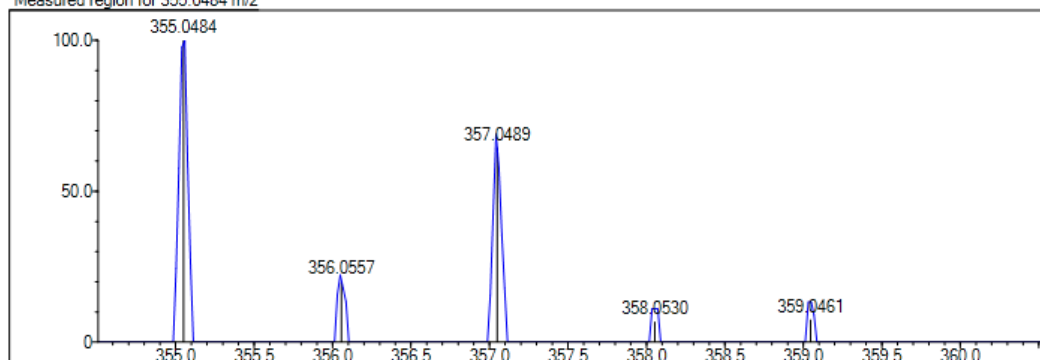
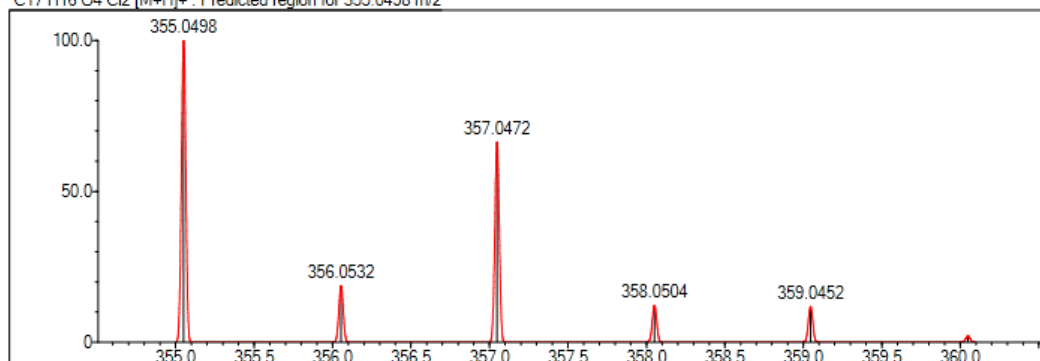
Isotope Res: 10000

Max Results: 100

Event#: 1 MS(E+) Ret. Time: 17.805 Scan#: 1958



Measured region for 355.0484 m/z

C17 H16 O4 Cl2 [M+H]⁺: Predicted region for 355.0498 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	92.65	C17 H16 O4 Cl2	[M+H] ⁺	355.0484	355.0498	-1.4	-3.94	100.00	9.0

Figure S2. HRESIMS spectrum of Compound 1.

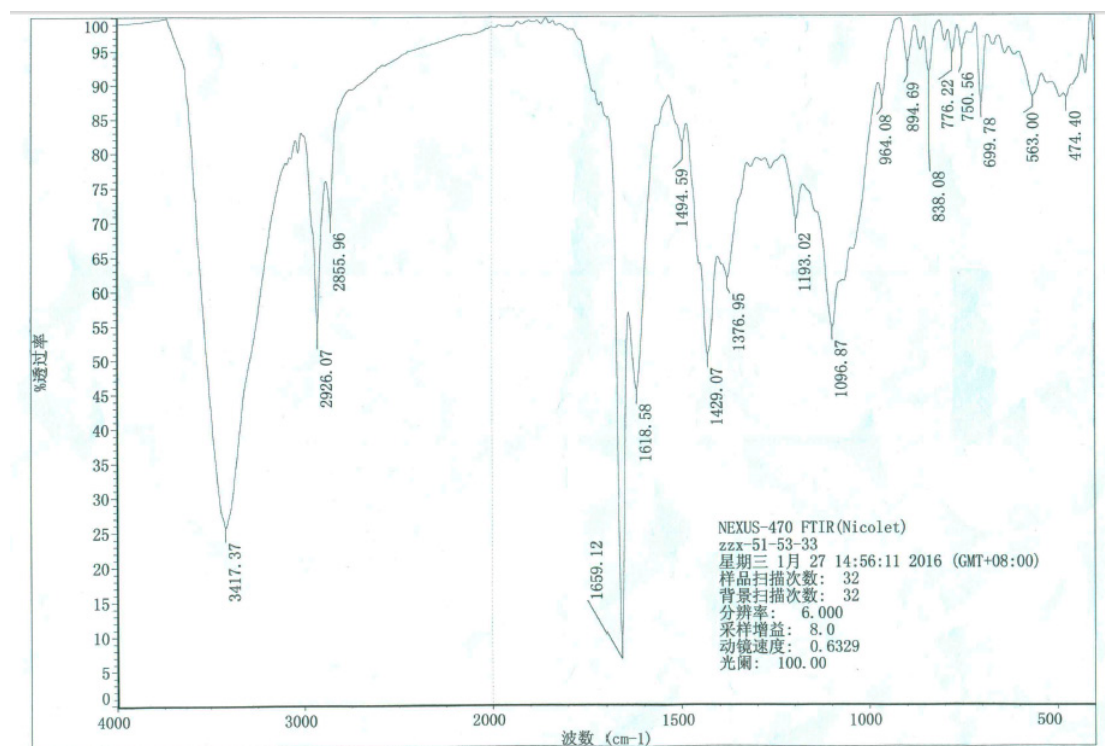
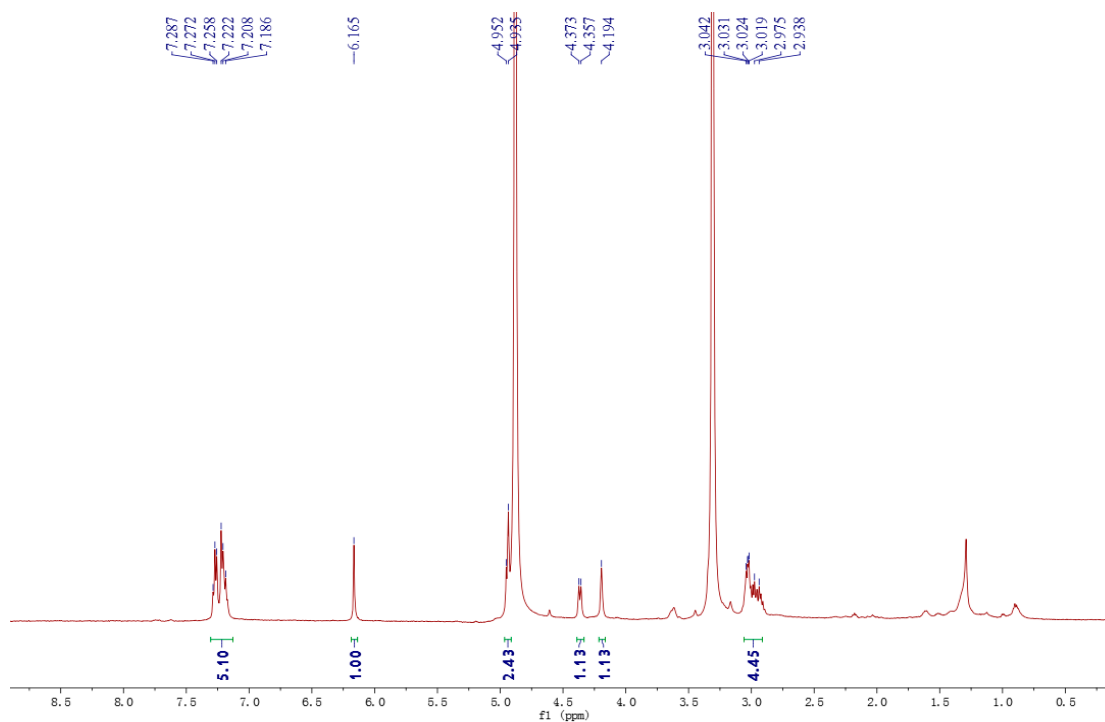


Figure S3. IR spectrum of Compound 1.

Figure S4. ¹H NMR spectrum of Compound 1 (CD₃OD, 500 MHz).

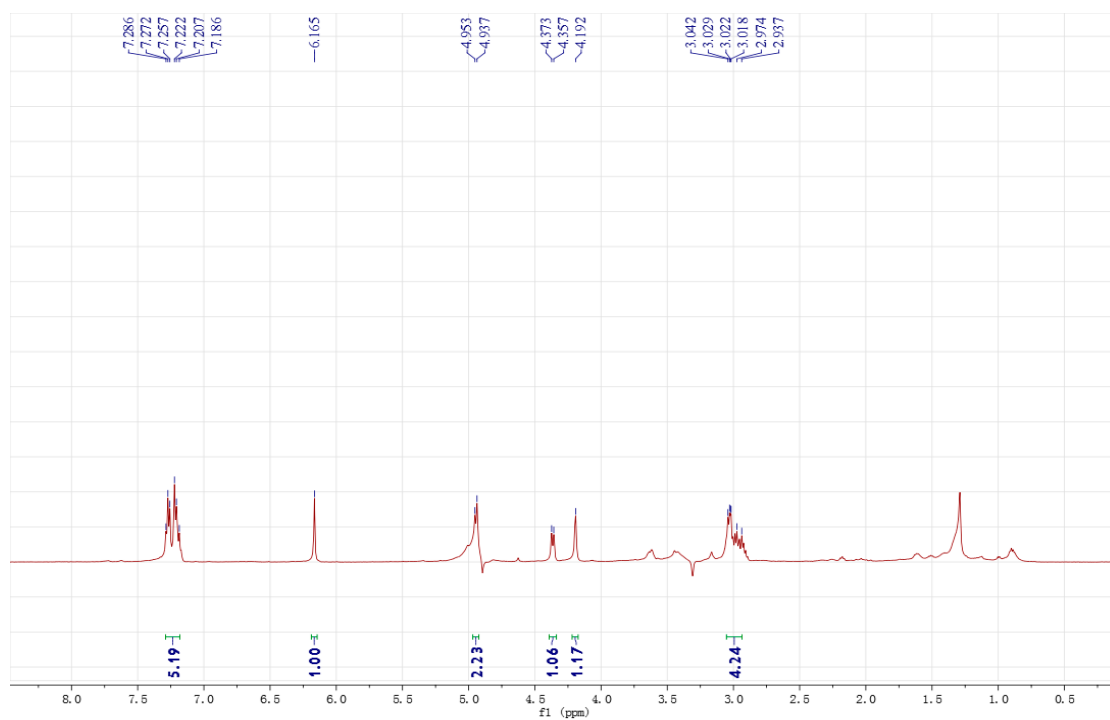


Figure S5. WET-¹H NMR spectrum of Compound 1 (CD₃OD, 500 MHz).

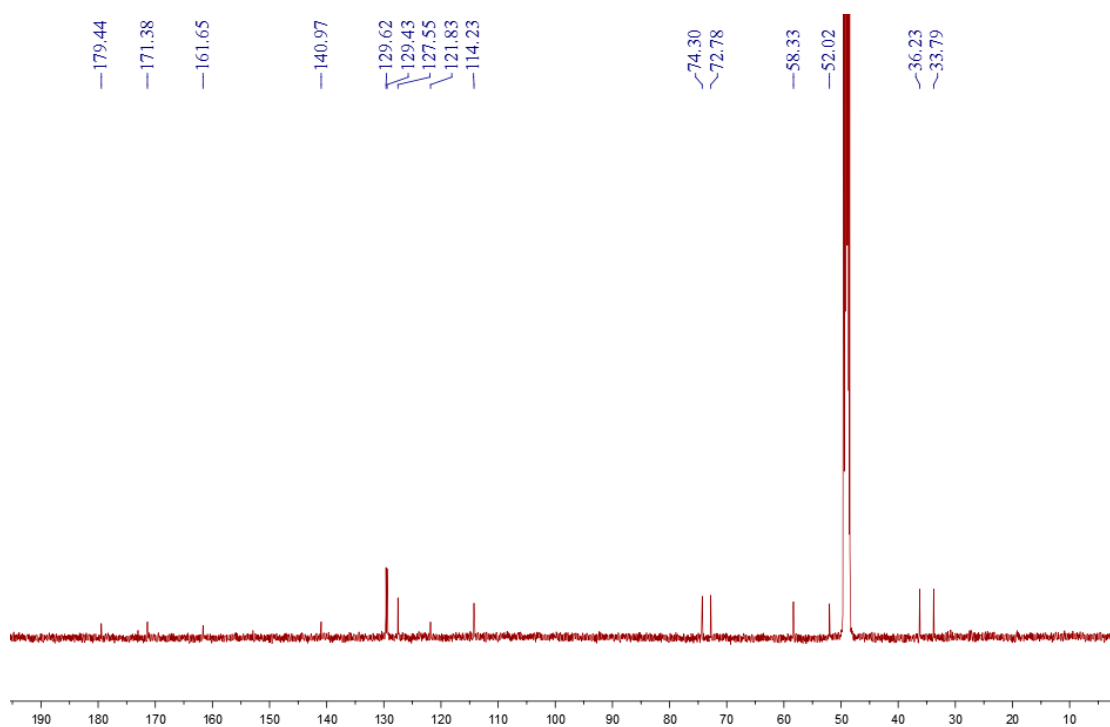


Figure S6. ¹³C-NMR spectrum of Compound 1 (CD₃OD, 125 MHz).

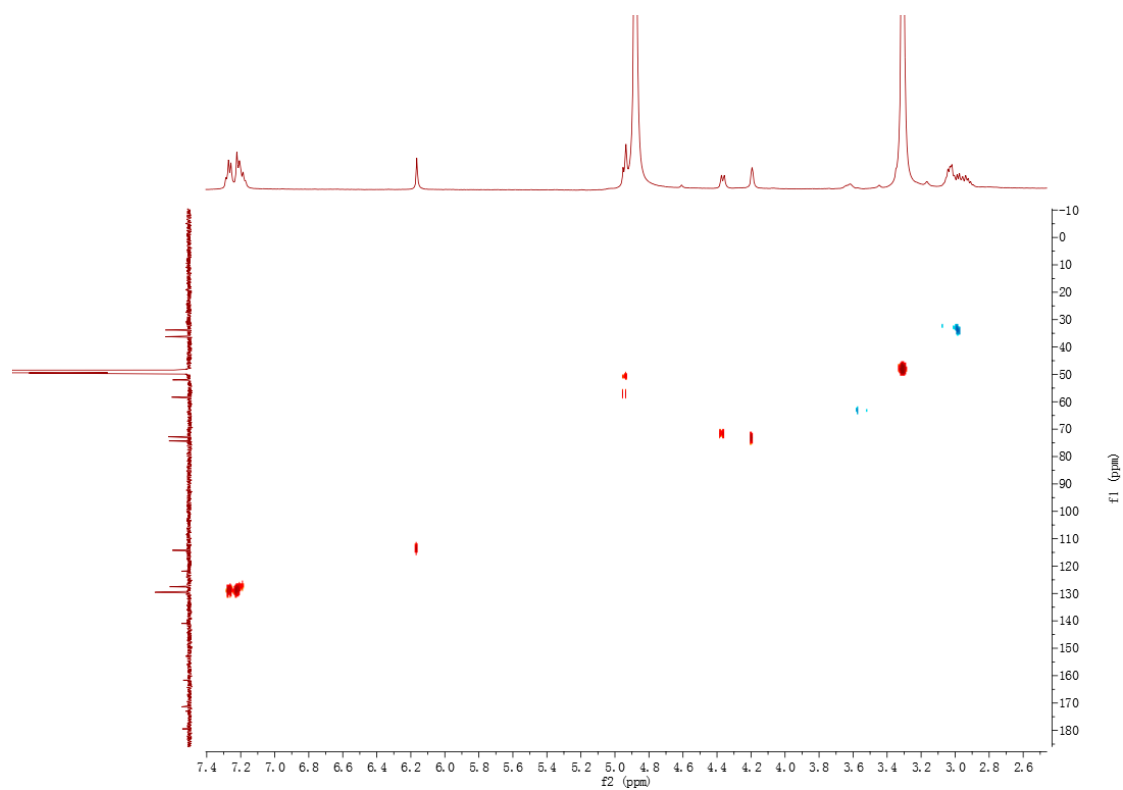


Figure S7. gHSQC spectrum of Compound 1.

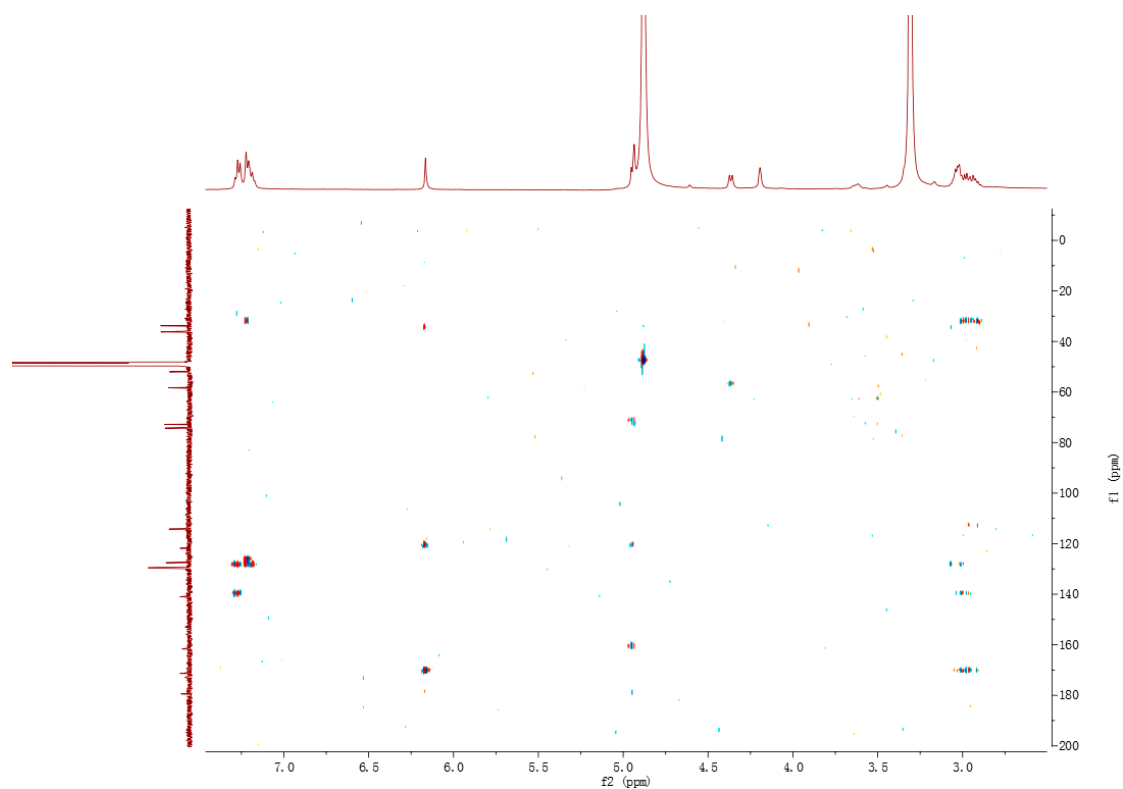


Figure S8. gHMBC spectrum of Compound 1.

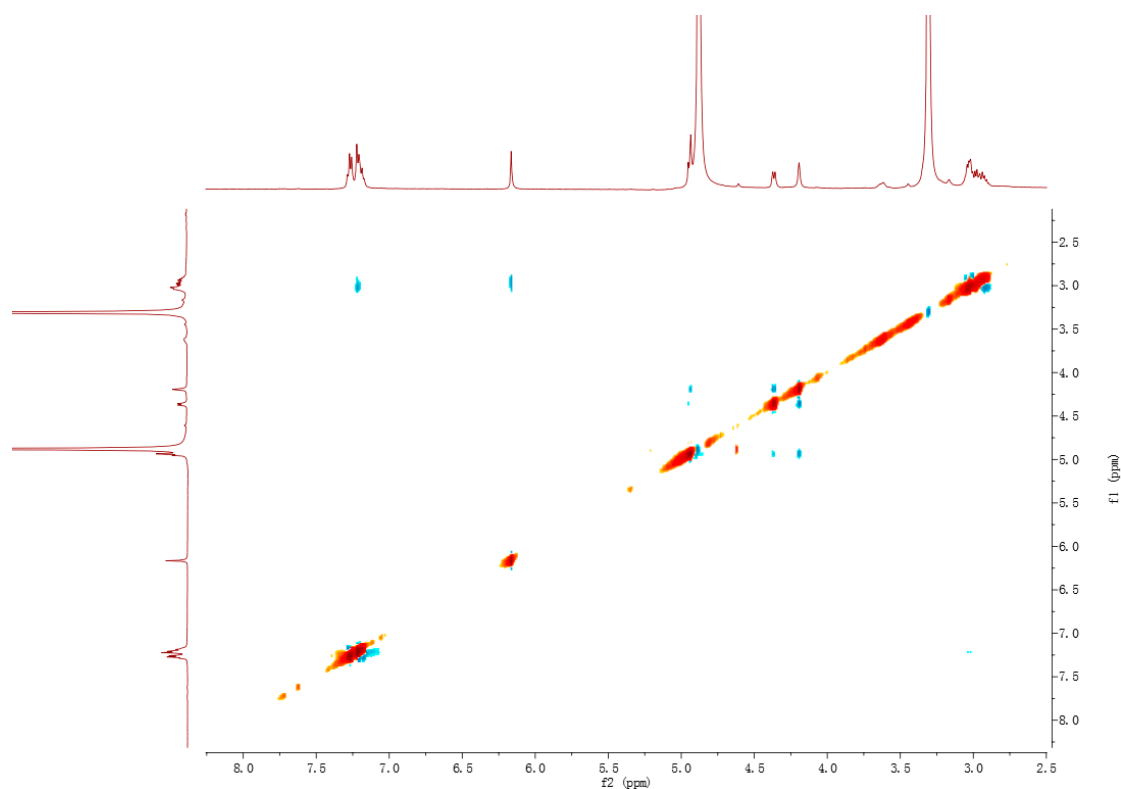


Figure S9. NOESY spectrum of Compound 1.

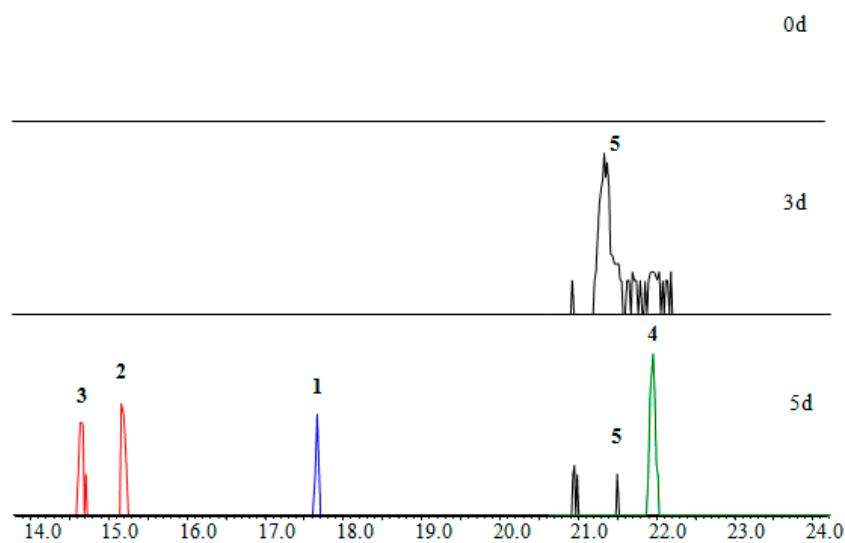


Figure S10. Extracted ion chromatogram of extracts from 0 d, 3 d, and 5 d NaCl-treated *A. sinensis* cell suspensions. The extracted ion chromatogram corresponding to Compound 1: m/z 377.0318 $[M + Na]^+$, 2: m/z 359.0657 $[M + Na]^+$, 3: m/z 359.0657 $[M + Na]^+$, 4: m/z 311.1278 $[M + H]^+$, and 5: m/z 341.1384 $[M + H]^+$. Column: Agilent-ZORBAX SB-C₁₈ (5 μ m, 250 mm $\times$ 4.6 mm i.d.). Mobile phase: 0–30 min, 5–95% acetonitrile.

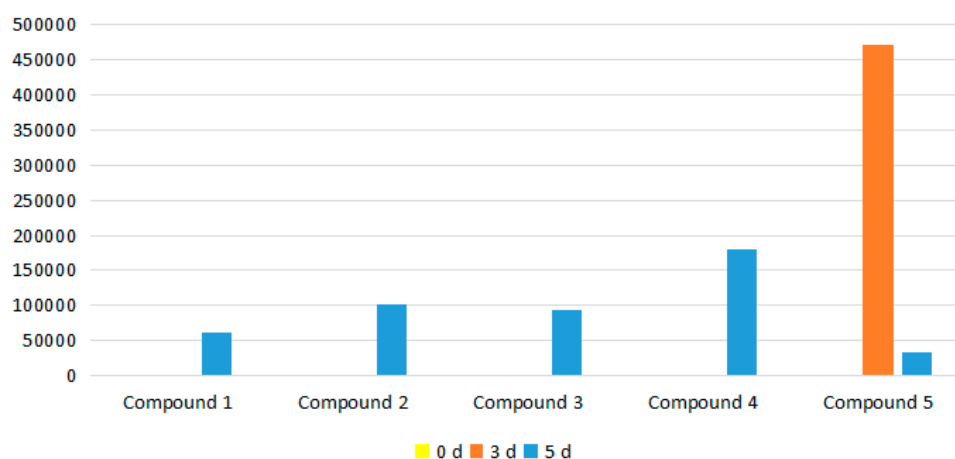


Figure S11. Accumulation of Compounds 1-5 in *Aquilaria sinensis* cell cultures treated with 150 mM NaCl for 0, 3 and 5 days. Relative production was calculated from the peak area presented in the extracted ion chromatograms.