

Supplementary Material:

Anti-Inflammatory Phenolic Acid Esters from the Roots and Rhizomes of *Notopterygium incisum* and Their Permeability in the Human Caco-2 Monolayer Cell Model

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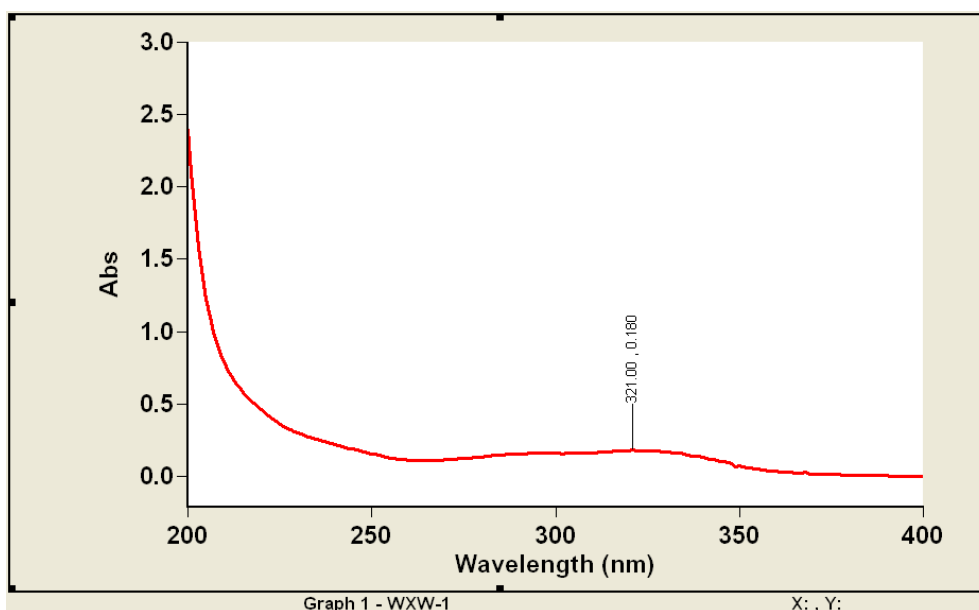


Figure S1. UV spectrum of 1 in MeOH.

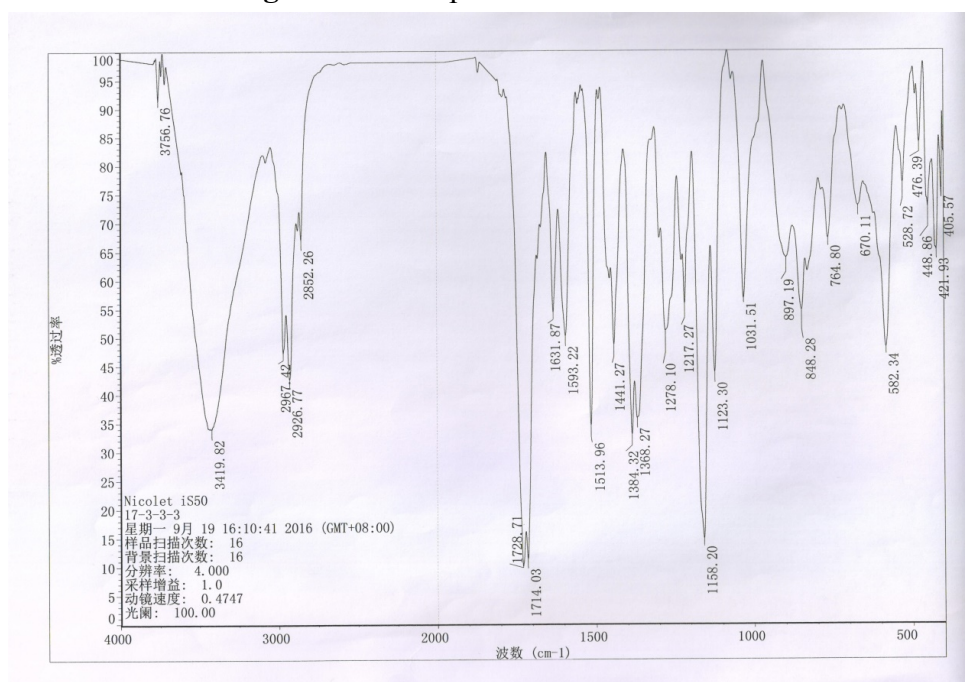


Figure S2. IR spectrum of 1.

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

92 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

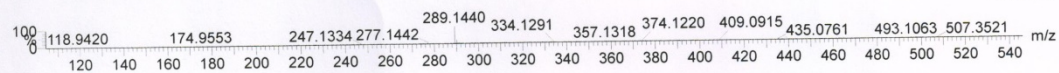
C: 0-100 H: 0-200 O: 0-50 Na: 0-1

24-Nov-2015

Xevo G2 Q-TOF/YCA166#

17-3-3 NEG 13 (0.237) Cm (11:15-(2:6+27:53))

Waters
 TOF MS ES-
 1.45e+006



Minimum: -1.5
 Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
289.1440	289.1440	0.0	0.0	7.5	359.3	n/a	n/a	C17 H21 O4

Figure S3. HR-ESI-MS spectrum of **1**.

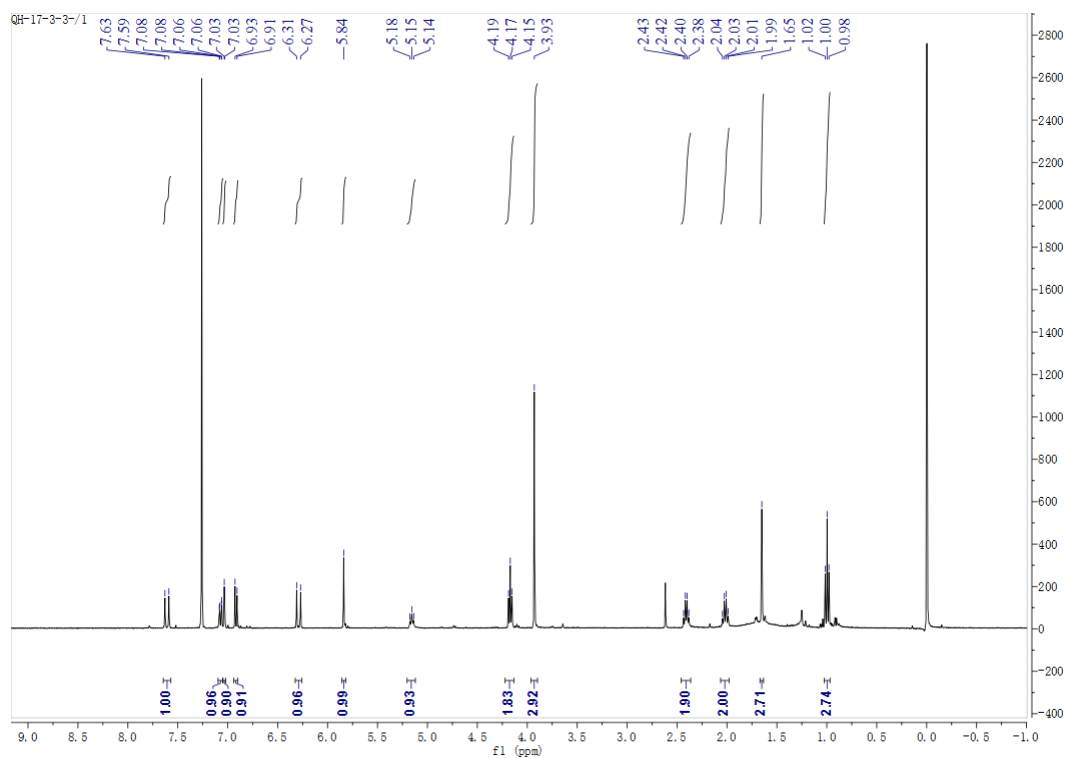


Figure S4. ¹H NMR spectrum of **1** in CDCl₃.

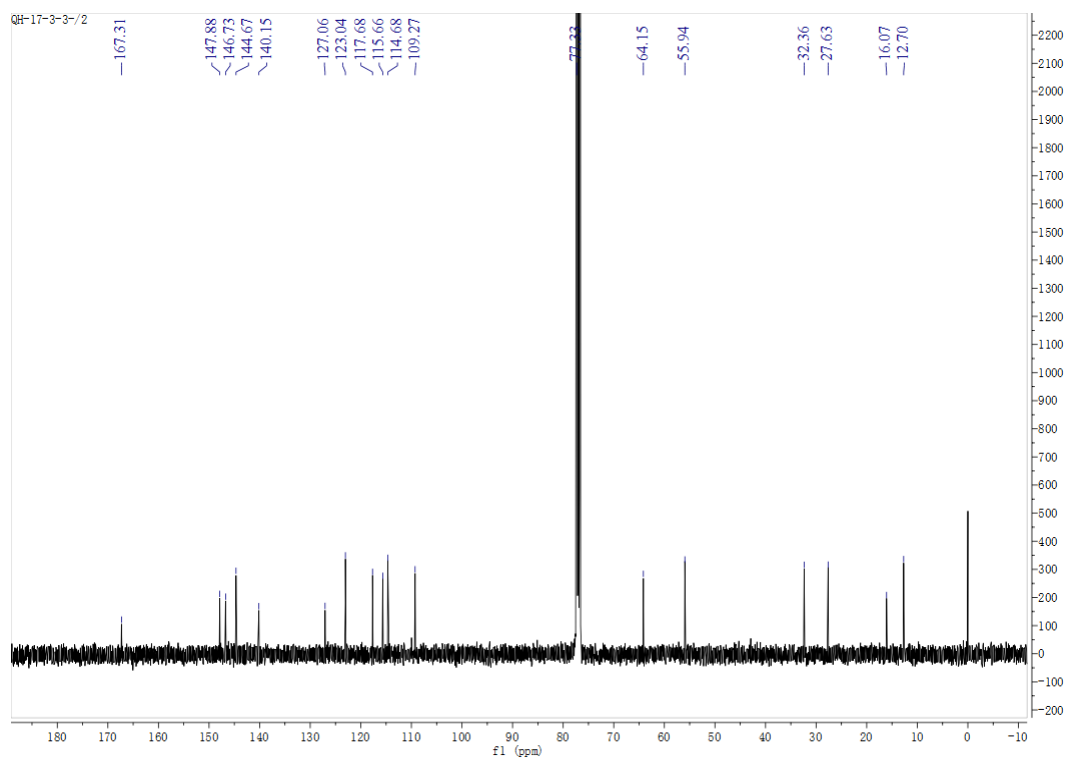


Figure S5. ^{13}C NMR spectrum of **1** in CDCl_3 .

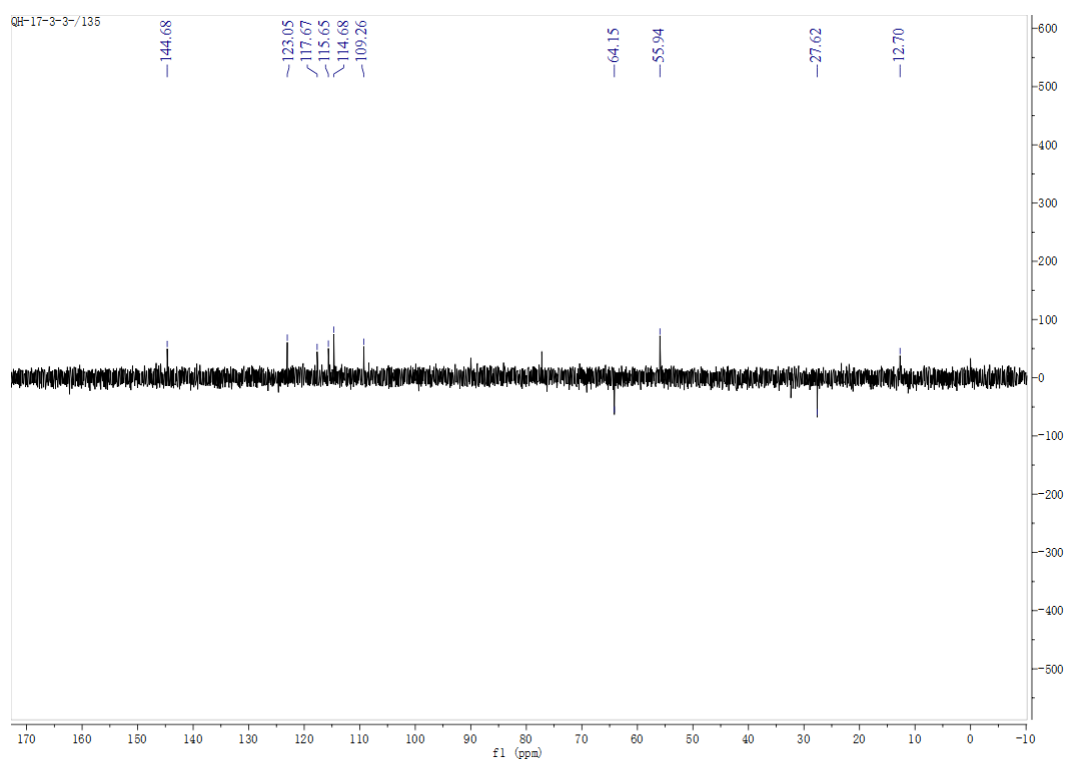


Figure S6. DEPT 135 spectrum of **1** CDCl_3 .

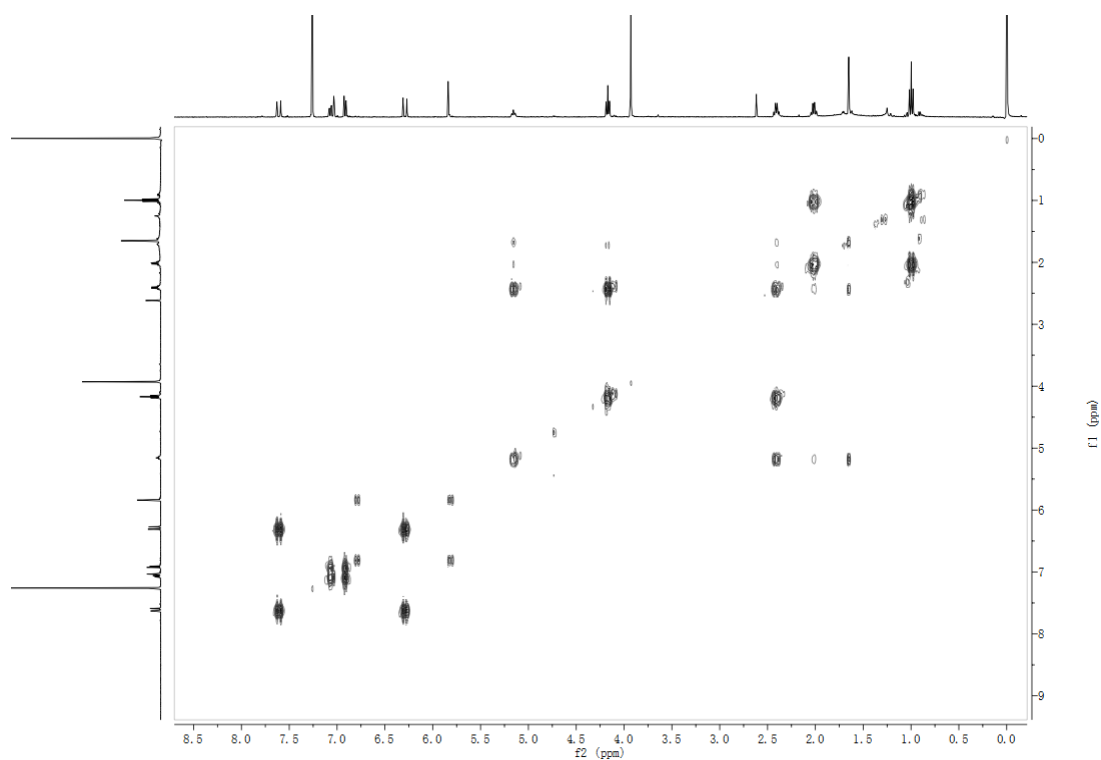


Figure S7. ^1H - ^1H COSY spectrum of **1** CDCl_3 .

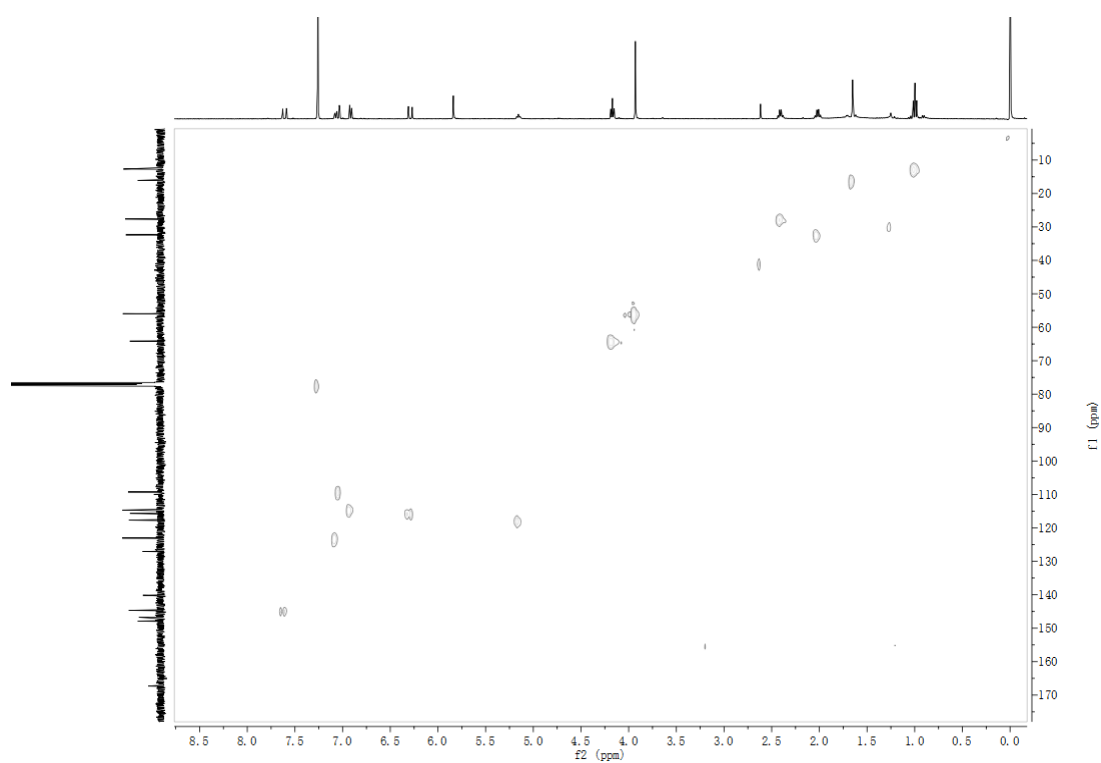


Figure S8. HSQC spectrum of **1** CDCl_3 .

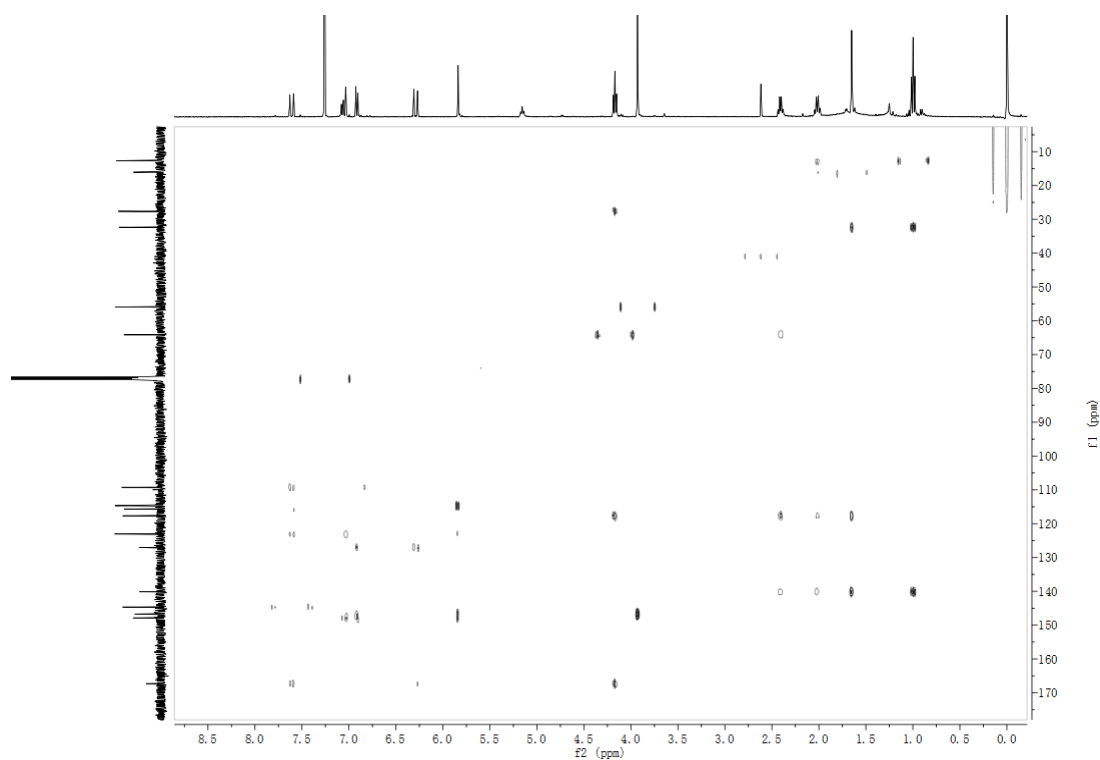


Figure S9. HMBC spectrum of **1** CDCl₃.

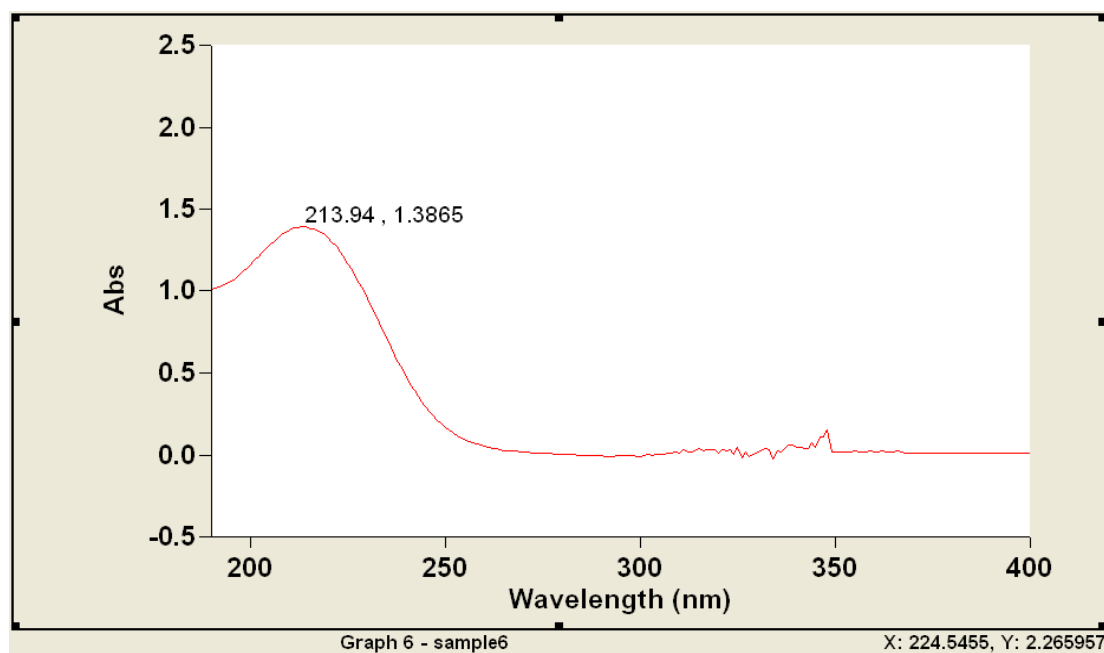


Figure S10. UV spectrum of **8** in MeOH.

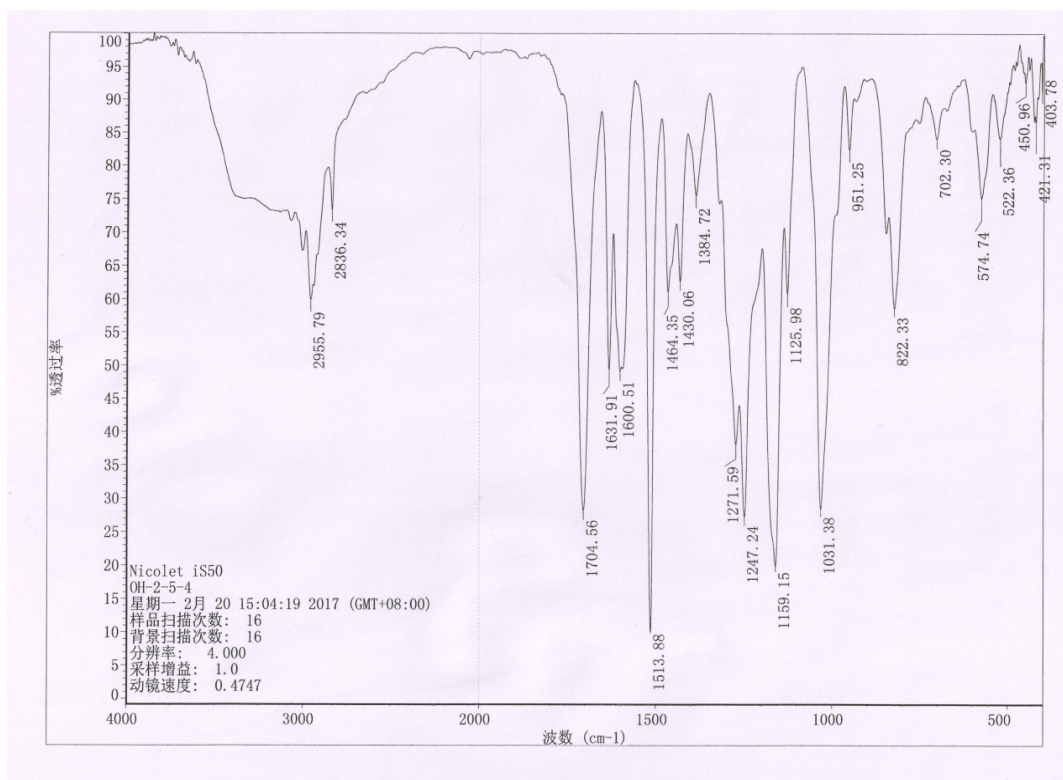


Figure S11. IR spectrum of **8**.

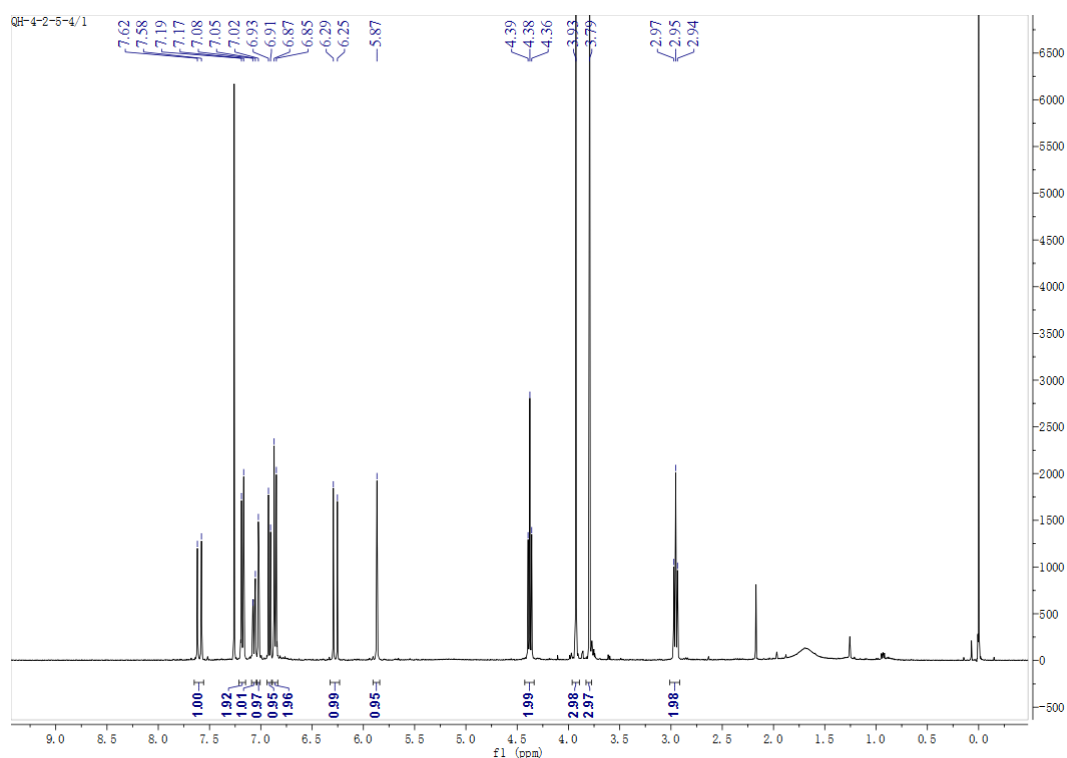


Figure S12. ¹H NMR spectrum of **8** in CDCl₃.

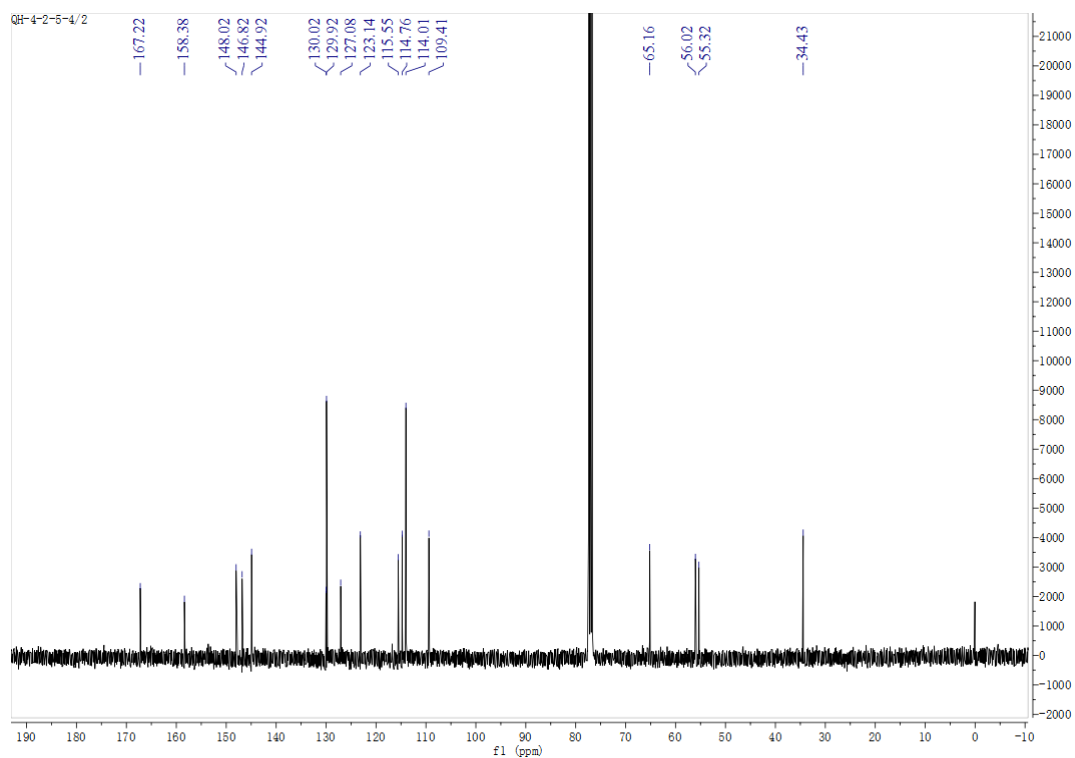


Figure S13. ^{13}C NMR spectrum of **8** in CDCl_3 .

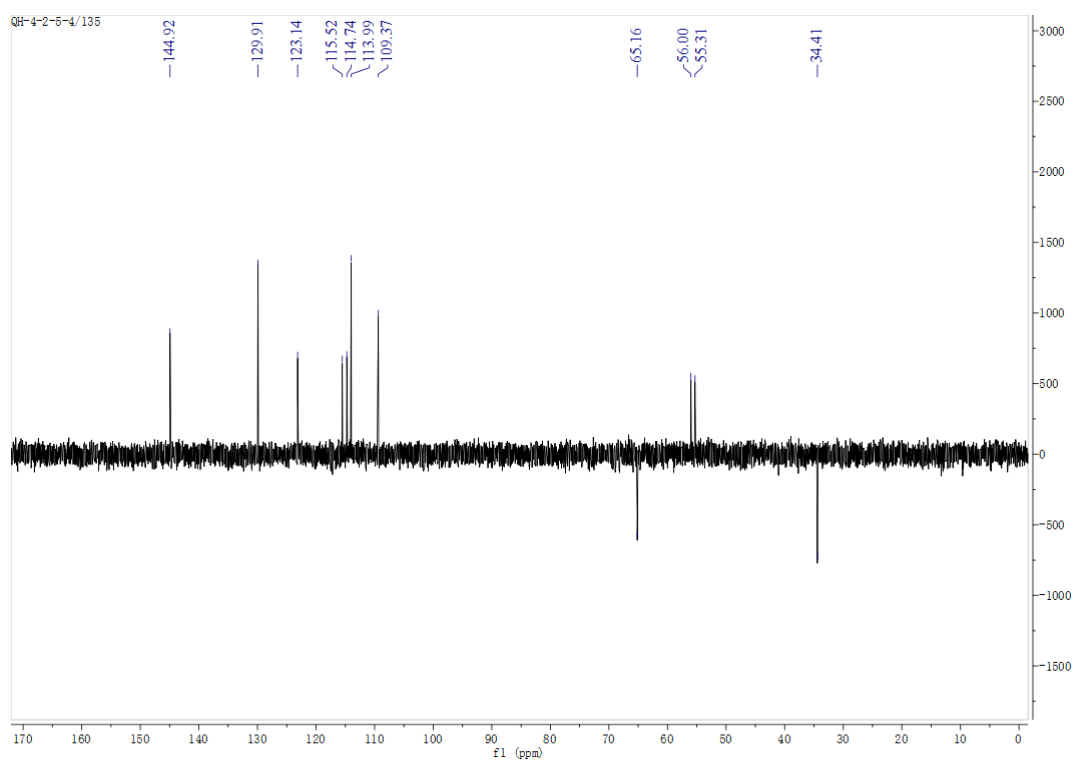


Figure S14. DEPT 135 spectrum of **8** in CDCl_3 .

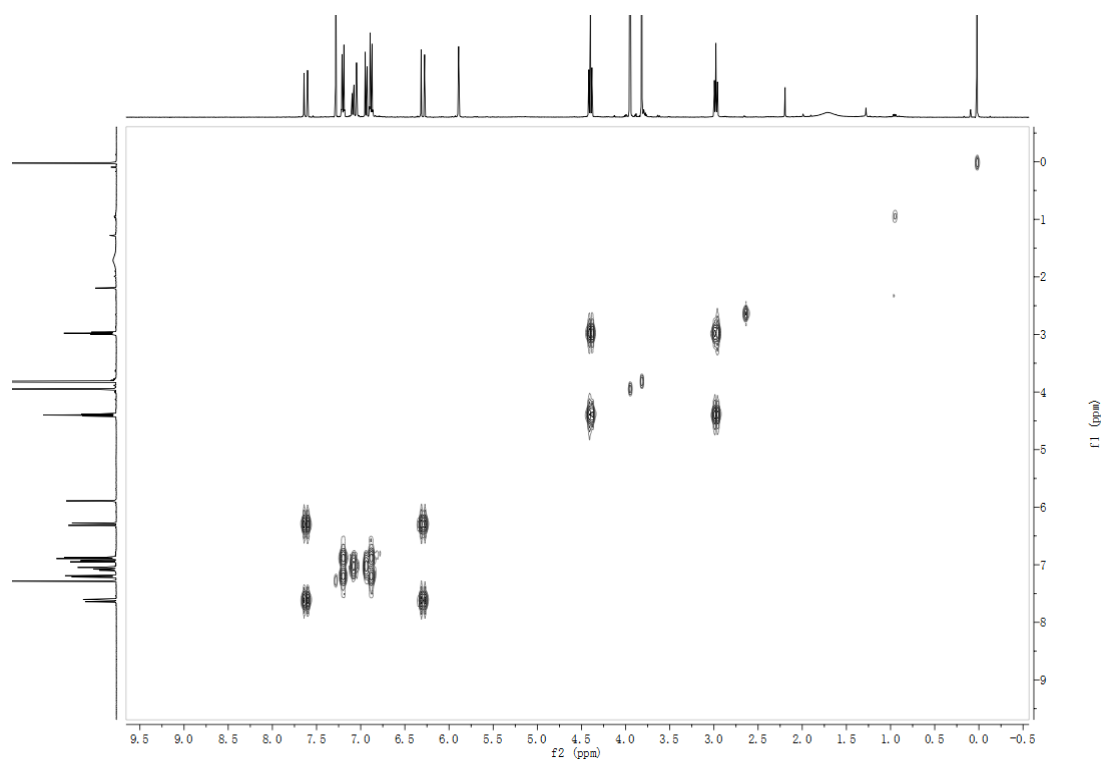


Figure S15. ^1H - ^1H COSY spectrum of **8** in CDCl_3 .

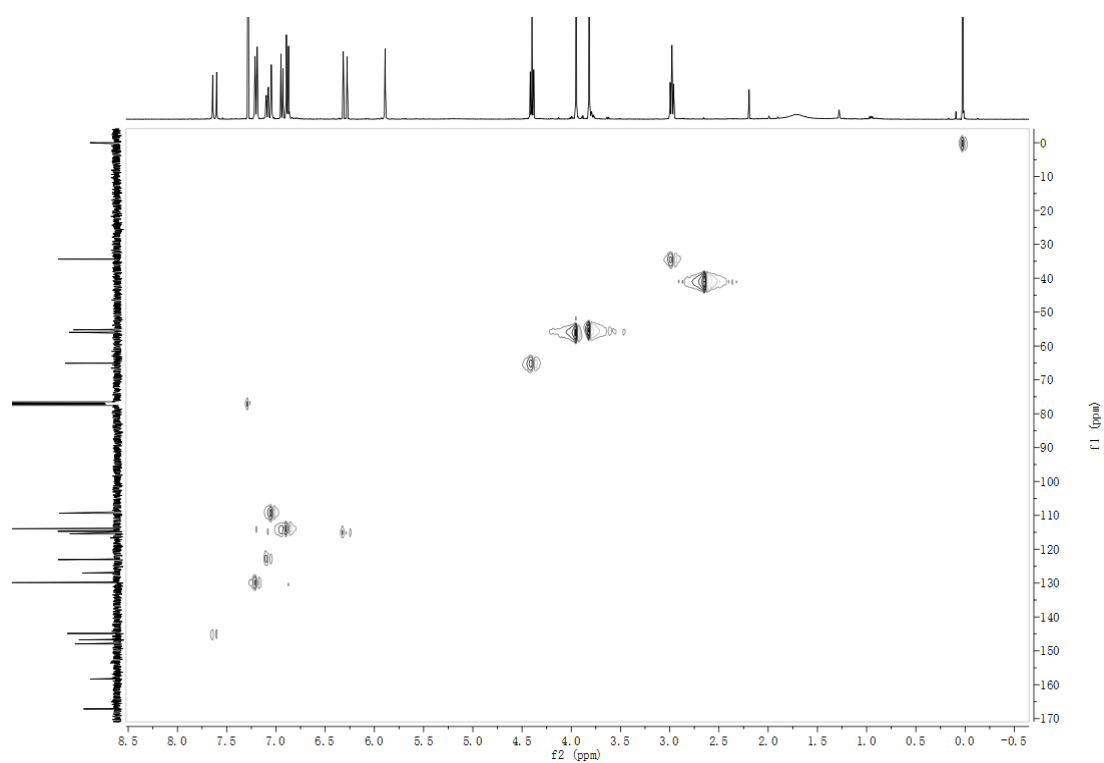


Figure S16. HSQC spectrum of **8** in CDCl_3 .

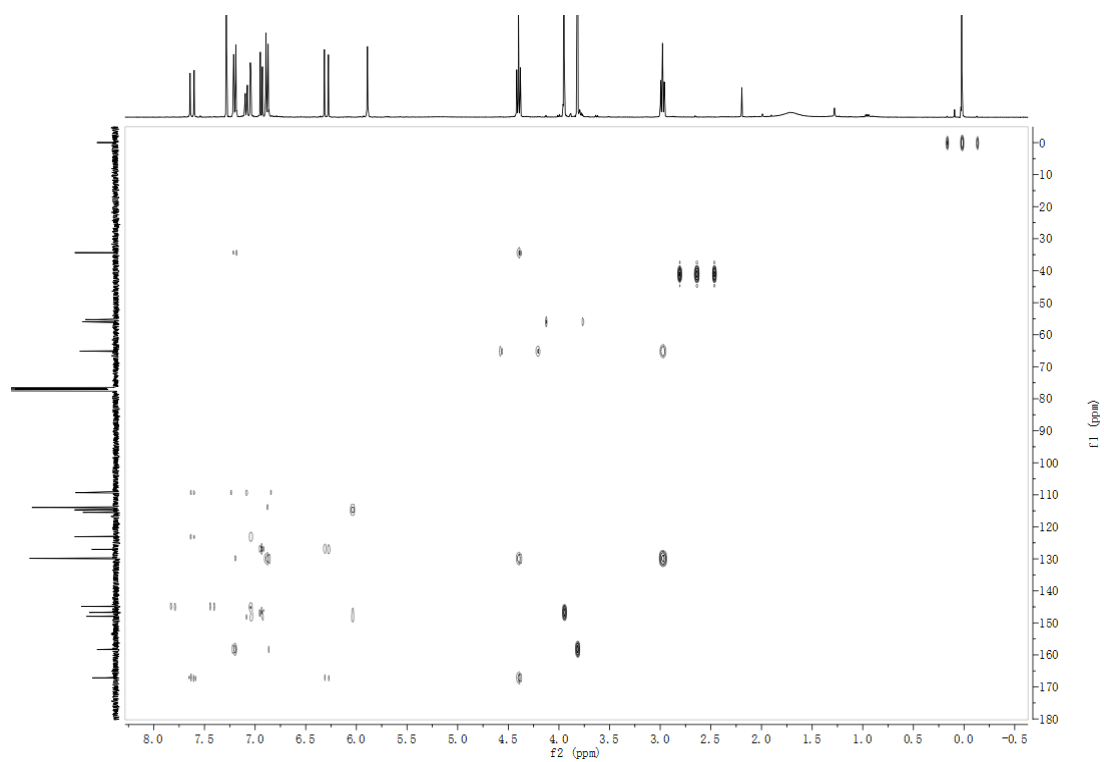


Figure S17. HMBC spectrum of **8** in CDCl₃.

Table S1. Precision, accuracy, recovery, and stability of the phenolic acid esters.

No.	QC/ μM	Precision RSD(%)		Accuracy (%)		Recovery (%)	Stability (%)
		Intra-day	Inter-day	Intra-day	Inter-day		
1	5	1.98	2.88	89.54	95.72	85.13 \pm 2.45	93.56 \pm 1.02
	25	0.63	1.54	82.13	96.86	86.66 \pm 1.33	95.65 \pm 0.56
	50	1.23	1.36	86.04	96.23	86.25 \pm 1.17	92.25 \pm 1.63
2	5	2.30	1.99	89.65	92.58	85.56 \pm 1.70	98.84 \pm 2.09
	25	1.26	2.33	96.98	101.59	80.50 \pm 1.87	94.57 \pm 1.85
	50	1.69	2.01	96.22	93.25	83.39 \pm 1.68	97.25 \pm 2.09
4	5	2.03	2.35	104.24	92.27	82.28 \pm 1.93	92.28 \pm 2.07
	25	2.20	2.14	105.16	104.15	90.41 \pm 1.94	100.74 \pm 2.15
	50	1.28	1.35	109.74	97.14	91.97 \pm 1.24	95.85 \pm 2.01
5	5	2.51	1.74	89.74	93.72	85.72 \pm 1.49	96.29 \pm 0.99
	25	1.08	2.58	82.58	86.69	96.68 \pm 2.49	94.56 \pm 0.96
	50	1.54	2.27	86.27	92.35	86.23 \pm 1.96	95.85 \pm 1.01
6	5	1.02	2.75	89.75	93.56	85.56 \pm 2.35	95.08 \pm 1.56
	25	1.32	2.35	96.35	98.50	90.50 \pm 2.13	102.02 \pm 1.96
	50	1.55	2.14	96.14	101.39	89.25 \pm 1.91	102.05 \pm 1.39
8	5	1.47	2.86	108.87	108.07	80.18 \pm 2.29	93.28 \pm 2.17
	25	2.01	2.51	95.80	90.41	90.14 \pm 2.26	95.45 \pm 1.12
	50	1.69	1.97	89.74	101.14	101.79 \pm 2.00	102.58 \pm 1.54
9	5	1.37	3.27	86.60	102.09	92.45 \pm 3.02	92.26 \pm 2.89
	25	0.98	2.91	88.43	103.08	93.50 \pm 2.72	93.71 \pm 1.88
	50	1.03	2.04	96.06	98.92	96.91 \pm 1.98	101.99 \pm 1.32