Electronic Supplementary Material (ESI) for Analytical Methods.

Electronic Supplementary Material

Simple and practical solvent system selection strategy for high-speed countercurrent chromatography based on the HPLC polarity parameter model

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Table of Contents

Table S1 Parameters of stationary phase of different columns under the same conditions

Column	Reference compound	p	Flow rate (mL/min)	B% (Methanol)	t_0	t_R	P_m^N	$(\log k)_0$	P_s^N
Column 1	Honokiol	4.31	1.0	80%	2.150	5.250	0.2267	5.9474	1.5217
	Magnolol	3.923				7.267			
Column 2	Honokiol	4.31			1.714	5.224	0.2267	4.9171	1.2013
	Magnolol	3.923				6.832			
Column 3	Honokiol	4.31			1.000	4.017	0.2267	5.8428	1.3262
	Magnolol	3.923				5.617			

Table S2 Parameters of stationary phase under different flow rates and methanol concentrations for compounds of group 1

Flow rate (mL/min)	Reference compound	p	Mobile phase composition (B% *v*/*v*)															
			75 ($P_m^N = 0.2625$)				80 ($P_m^N = 0.2267$)				85 ($P_m^N = 0.1922$)				90 ($P_{m=} 0.1588$)			
			t_0	t_R	$(\log k)_0$	P_S^N	t_0	t_R	$(\log k)_0$	P_S^N	t_0	t_R	$(\log k)_0$	P_S^N	t_0	t_R	$(\log k)_0$	P_S^N
0.8	Honokiol	4.31	1.25	7.483	6.8346	1.4755	1.25	5.033	5.8031	1.3162	1.25	3.633	4.7110	1.1356	1.25	2.817	3.7487	0.9761
	Magnolol	3.923		11.217				7.017				4.683				3.400		
0.9	Honokiol	4.31	1.11	6.700	6.8668	1.4809	1.11	4.467	5.8141	1.3193	1.11	3.233	4.7093	1.1348	1.11	2.517	3.8152	0.9894
	Magnolol	3.923		10.067				6.233				4.167				3.050		
1.0	Honokiol	4.31	1.00	6.050	6.8579	1.4779	1.00	4.017	5.8428	1.3262	1.00	2.900	4.6906	1.1316	1.00	2.200	3.6136	0.9549
	Magnolol	3.923		9.083				5.617				3.733				2.633		

Table S3 Parameters of stationary phase under different flow rates and methanol concentrations for compounds of group 2

Flow rate (mL/min)	Reference compound	*p*	Mobile phase composition (B% *v/v*)															
			60 ($P^N_m = 0.3775$)				65 ($P^N_m = 0.3378$)				70 ($P^N_m = 0.2995$)				75 ($P^N_m = 0.2625$)			
			t_0 (min)	t_R (min)	$(\log k)_0$	P^N_S	t_0 (min)	t_R (min)	$(\log k)_0$	P^N_S	t_0 (min)	t_R (min)	$(\log k)_0$	P^N_S	t_0 (min)	t_R (min)	$(\log k)_0$	P^N_S
0.8	vitexicarpin	4.31	1.25	19.716	8.9491	1.8291	1.25	16.589	8.5479	1.7393	1.25	12.500	7.8369	1.6080	1.25	7.917	6.9945	1.4969
	apigenin	3.923		33.635				27.635				19.917				12.000		
0.9	vitexicarpin	4.31	1.11	18.623	9.0150	1.8294	1.11	15.573	8.5649	1.7296	1.11	11.617	7.9115	1.6138	1.11	7.017	7.0099	1.5013
	apigenin	3.923		31.826				25.894				18.583				10.650		
1.0	vitexicarpin	4.31	1.00	17.603	9.0000	1.8138	1.00	14.457	8.6119	1.7328	1.00	10.150	7.9632	1.6335	1.00	6.283	6.9609	1.4913
	apigenin	3.923		29.946				24.089				16.333				9.500		

Table S4 HPLC analysis conditions for mangosteen peel and *H. sampsonii* Hance

Mobile phase composition (B%, v/v)	Flow rate (mL/min)	Column temperature (℃)	UV detector temperature (℃)	Wavelengths of the UV detector (nm)
90% Methanal	1.0	30	30	254, 280, 365
60% Methanal	1.0	30	30	254, 280, 365

Table S5 ^{1}H-NMR (4000MHz) data for Compound **1** and **2**

Compound **1**			Compound **2**		
Position	δ_H (J in Hz)	δc	Position	δ_H (J in Hz)	δc
1		160.1	1		
2		109.9	2		157.8
3		162.1	3		134.8
4	6.20, s	91.7	4		178.2
4a		154.7	5		161.8
4b		156.4	6	6.22, d, J = 1.9 Hz	93.3
5	6.65, s	101.3	7		164.6
6		155.2	8	6.38, d, J = 2.0 Hz	98.4
7		143.3	9		157.1
			10		104.4
8		136.9	1′		121.5
8a		110.7	2′	7.36, d, J = 2.0 Hz	114.9
8b		102.3	3′		145.0
9		181.6	4′		148.4

1′	3.27, d, J = 7.2 Hz	25.7	5′	6.93, d, J = 8.2 Hz	115.5
2′	5.24, m	123.8	6′	7.33, d, J = 8.4 Hz	121.4
3′		130.2	1′′	5.37, s	102.1
4′	1.67, s	24.6	2′′		70.6
5′	1.79, s	16.5	3′′		70.7
1′′	4.04, d, J = 4.6 Hz	20.8	4′′		71.8
2′′	5.24, m	122.5	5′′		70.5
3′′		130.2	6′′	0.96, d, J = 6.0 Hz	16.2
4′′	1.68, s	24.6			
5′′	1.82, s	16.9			
OCH_3-7	3.75, s	59.9			

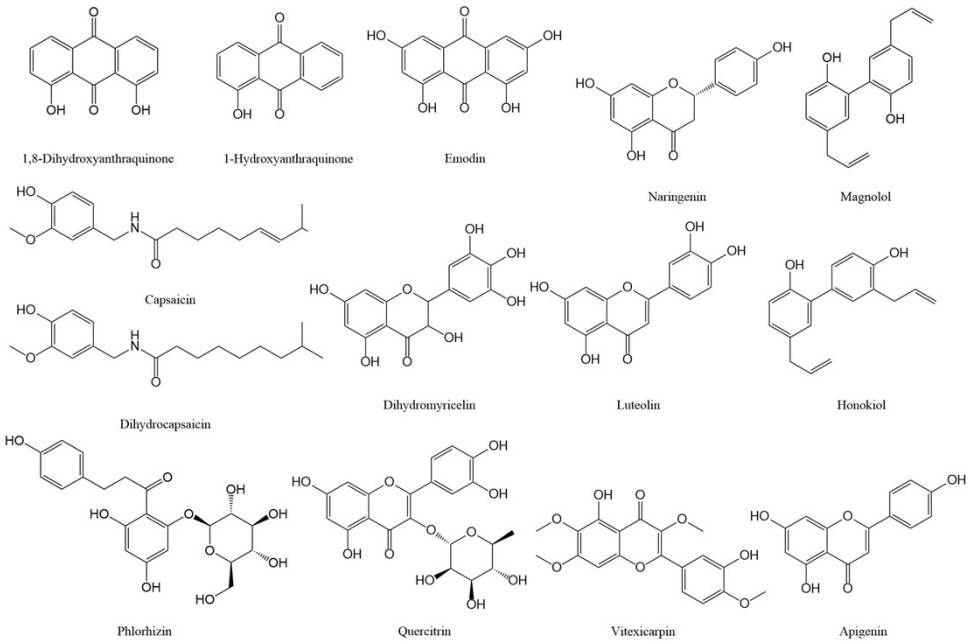

Figure S1. Chemical structure of standard compounds.

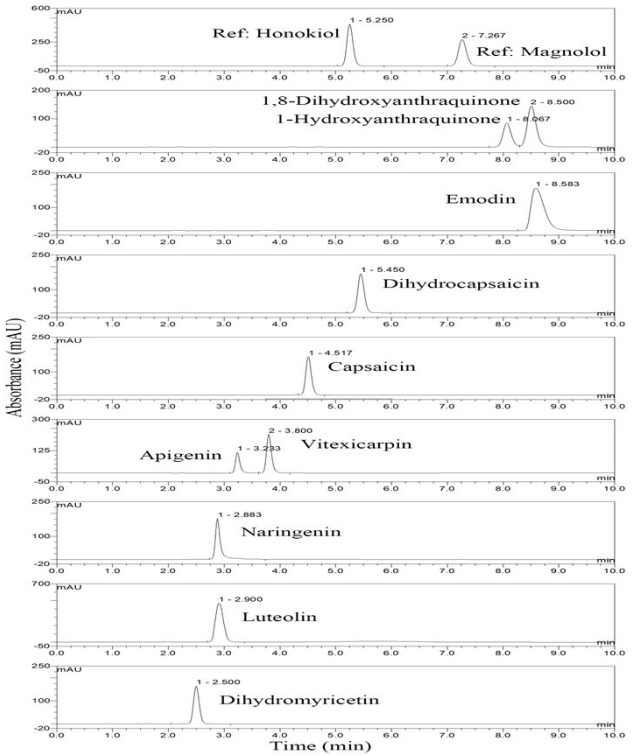

Figure S2. Representative HPLC chromatograms. Experimental conditions: column: Agilent ZORBAX SB-C18 column (5 μm particle size, 4.6 × 250 mm, marked as column 1); mobile phase: 80% methanol; flow rate: 1.0 mL/min; column temperature: 30℃; detector temperature: 30℃; detection wavelength: 254 nm.

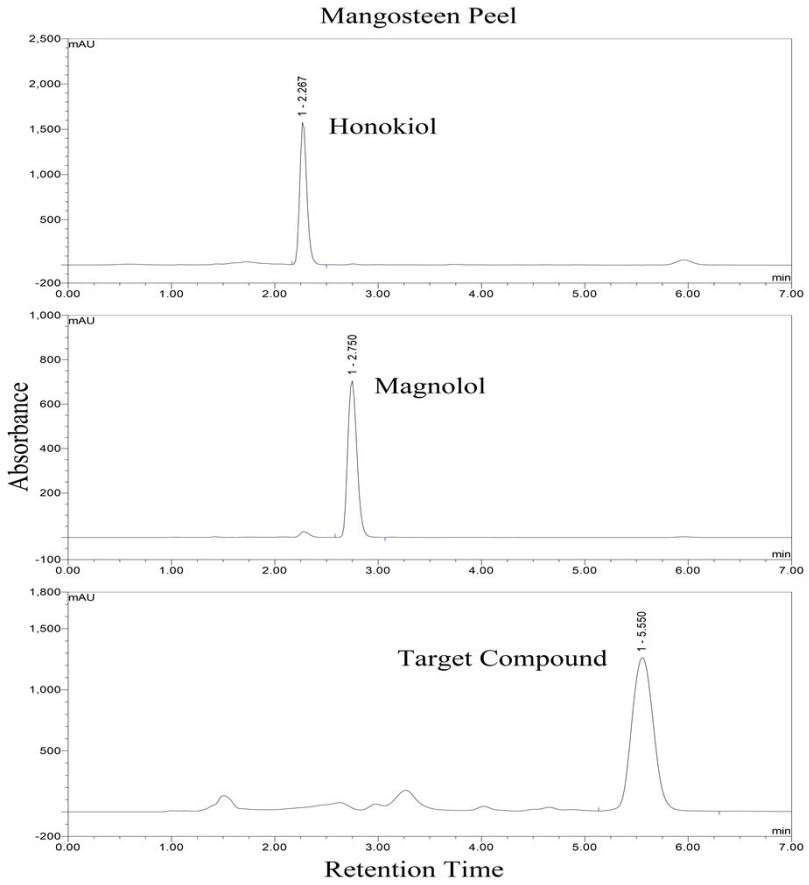

Figure S3. The HPLC chromatogram of mangosteen peel. Experimental conditions: column: Kromasil 100-5-C18 column (5 μm particle size, 4.6 × 150 mm); mobile phase: 90% methanol; column temperature: 30℃; detector temperature: 30℃; detection wavelength: 254 nm.

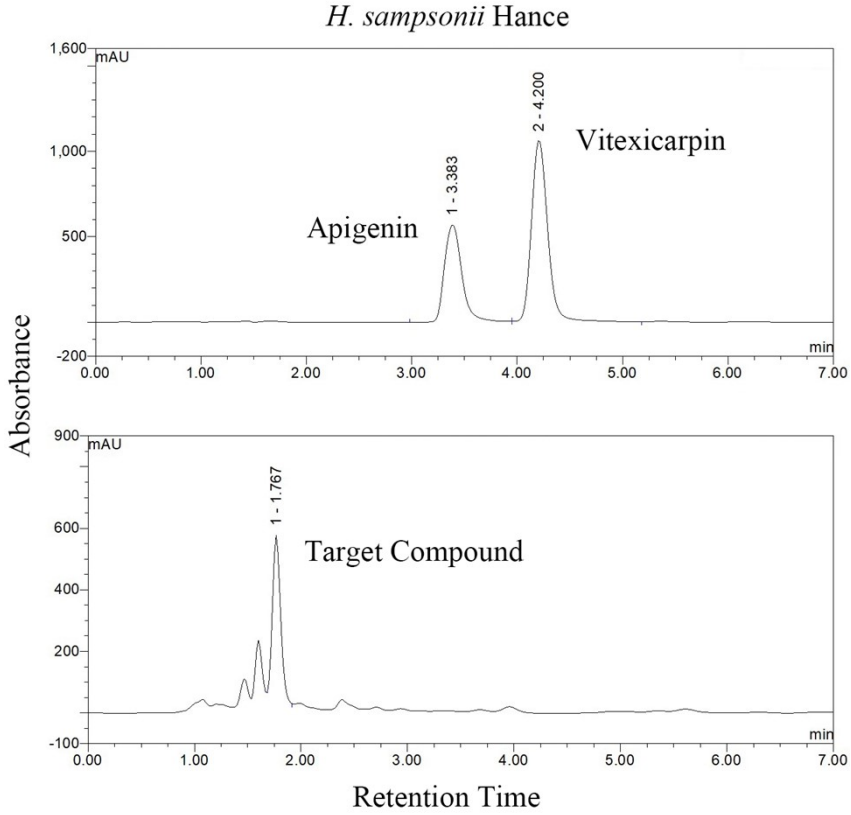

Figure S4. The HPLC chromatogram of *H. sampsonii* Hance. Experimental conditions: column: Agilent Eclipse XDB-C18 column (5 μm particle size, 9.4 × 250 mm); mobile phase: 60% methanol; column temperature: 30℃; detector temperature: 30℃; detection wavelength: 254 nm.

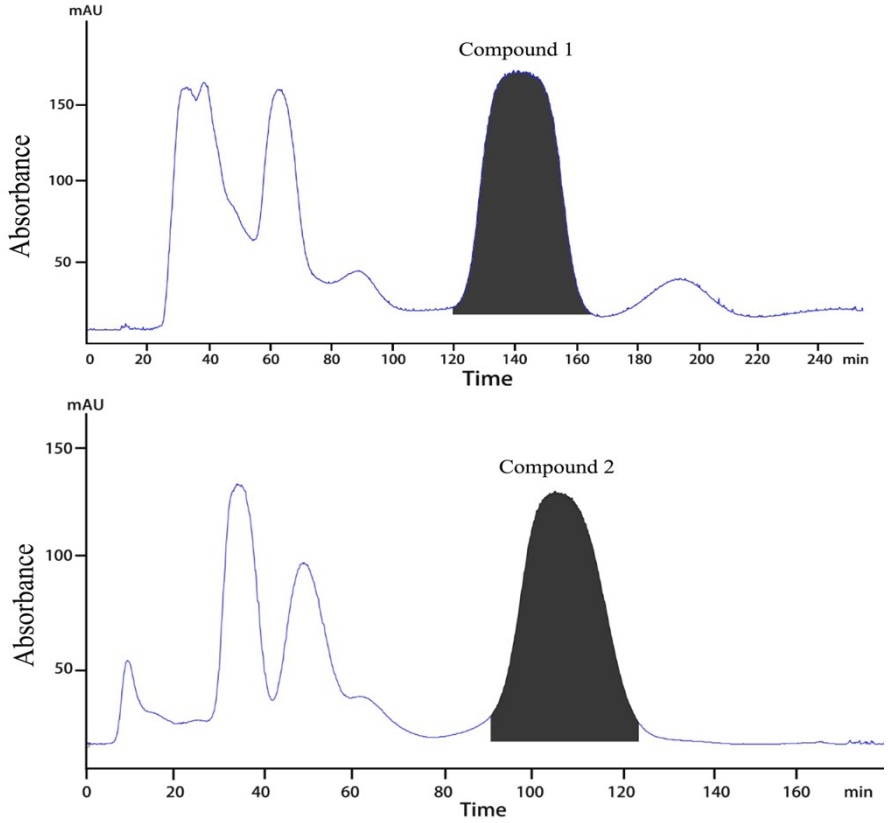

Figure S5. The HSCCC chromatogram of mangosteen peel and *H. sampsonii* Hance. Experimental conditions: solvent system: n-hexane-ethyl acetate-methanol-water (6:3:2:1 for mangosteen peel and 1:4:1:4 for *H. sampsonii* Hance, *v/v/v/v*); resolution speed: 900 rpm; separation temperature: 30℃; detection wavelength: 254 nm. The peaks marked in two chromatogram are mangostin and quercitrin.

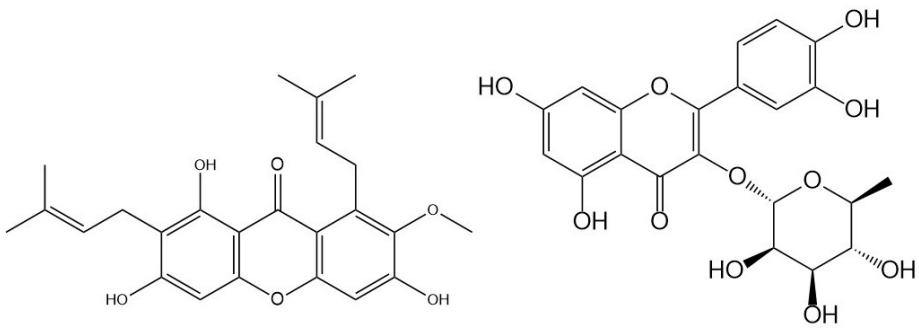

Figure S6. The structure of mangostin and quercitrin.

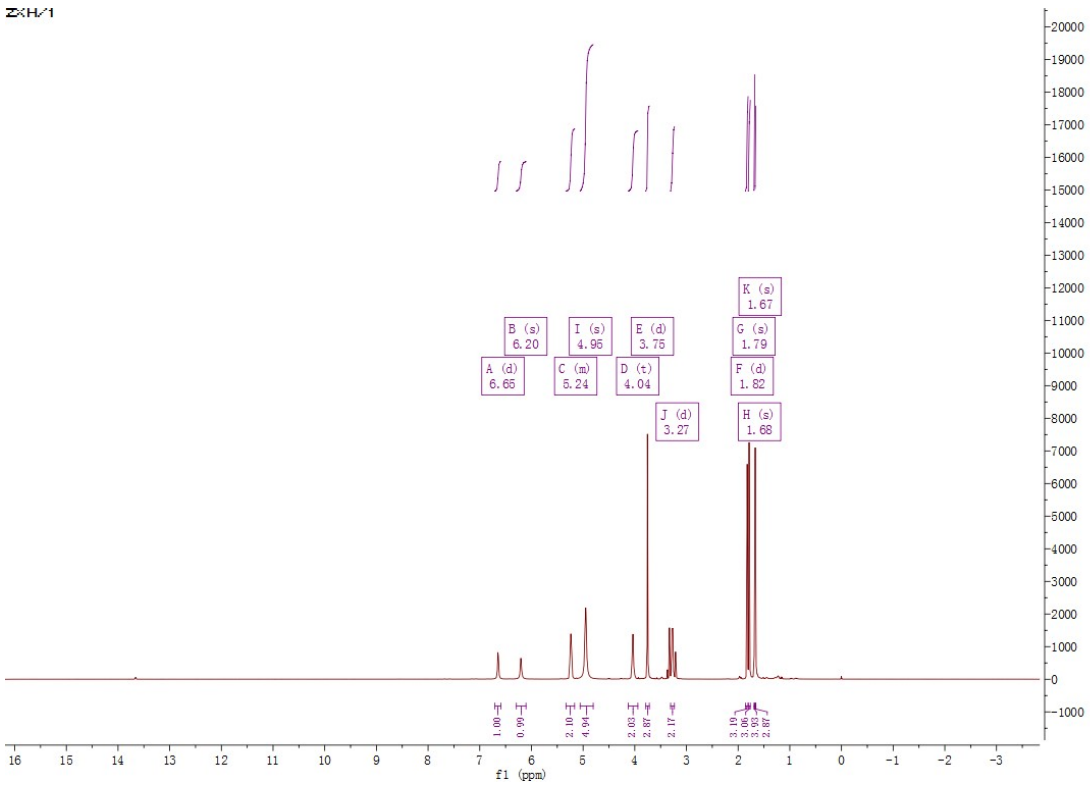

Figure S7. [1]H-NMR (400 MHz, CDCl3) Spectrum of Compound **1**.

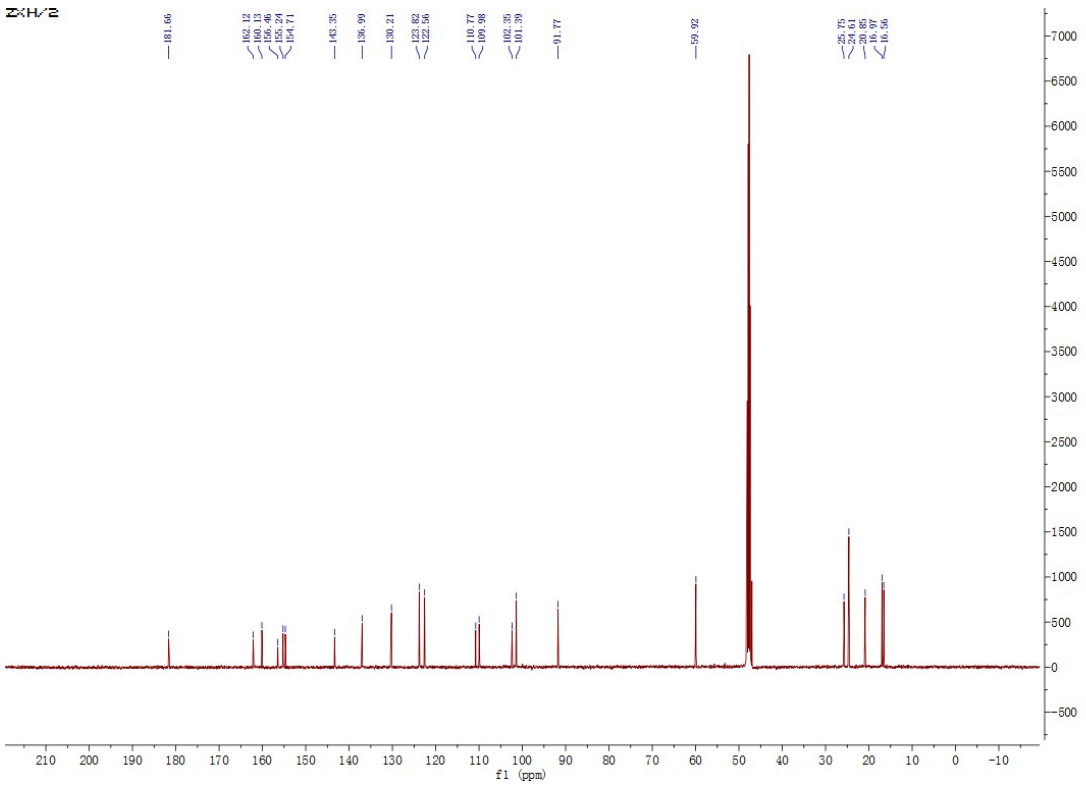

Figure S8. ^{13}C-NMR (100 MHz, $CDCl_3$) Spectrum of Compound **1**.

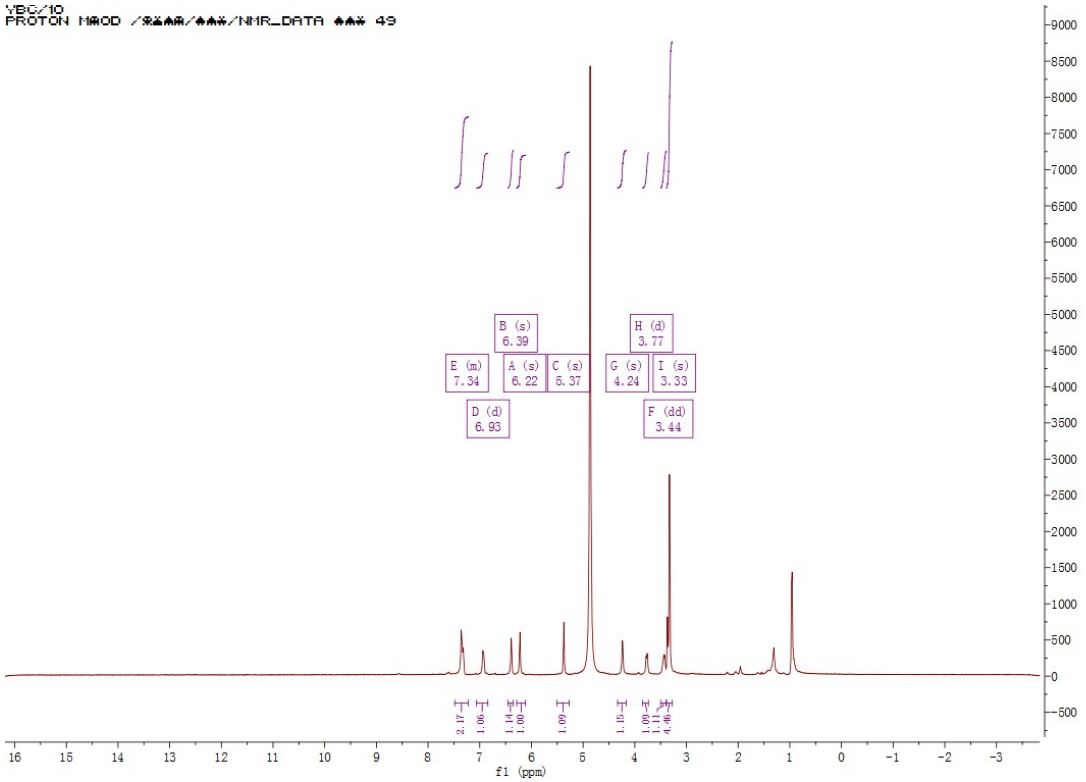

Figure S9. ^{1}H-NMR (400 MHz, CD_3OD) Spectrum of Compound **2**.

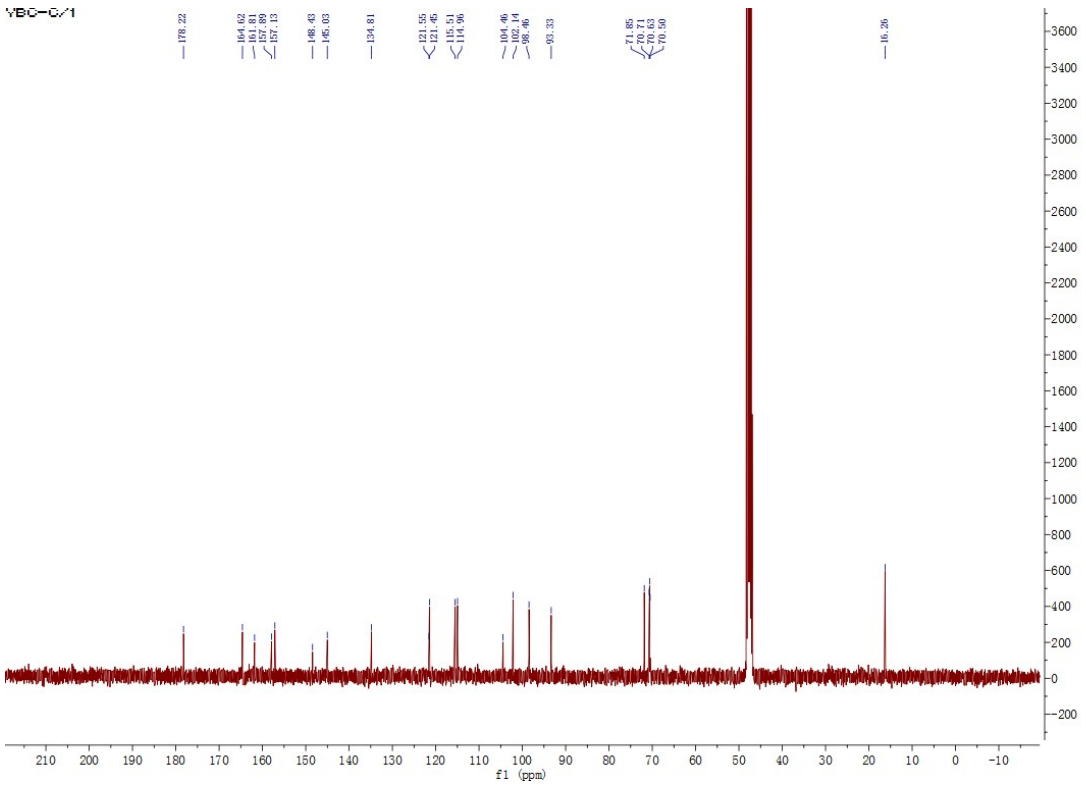

Figure S10. ^{1}H-NMR (100 MHz, CD_3OD) Spectrum of Compound **2**.