SUPPLEMENTARY MATERIAL

A Novel Sesquiterpene Derivative with a Seven-membered B Ring from *Illigera aromatica*

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Abstract: A novel sesquiterpene derivative with a seven-membered B ring, illigerine (**1**), along with four known compounds, 1-*epi*-chiliophyllin (**2**), 3,4-dihydroxyphenethyl alcohol (**3**), coniferyl alcohol (**4**), and phenylpropionic acid (**5**), were isolated from *Illigera aromatica* S. Z. Huang et S. L. Mo. Their structures were identified by 1D/2D NMR, HRESIMS, and electronic circular dichroism spectra, and the cytotoxic activity and inhibitory effect of NO production in LPS-stimulated RAW264.7 were also evaluated. This is the first report of sesquiterpene isolated from the genus *Illigera*.

Keywords: *Illigera aromatica*; sesquiterpene; illigerine; bioactivity

Table S1 The ^{1}H and ^{13}C NMR (^{1}H, 500 MHz; ^{13}C, 125 MHz) spectral data for **1** in $CDCl_3$.

No	δ_C	δ_H mult. (*J* in Hz)	No	δ_C	δ_H mult. (*J* in Hz)
1	152.8 s		12	31.8 t	2.60 dd (16.5, 5.5)
					2.48 m
2	35.6 t	2.42 dd (10.0, 3.0)	13	21.1 q	1.15 s
		2.12 dd (10.0, 3.0)			
3	36.7 t	1.69 dd (10.0, 3.0)	14	30.4 q	0.97 s
		1.61 dd (10.0, 3.0)			
4	34.0 s		15	22.3 q	1.00 s
5	53.8 d	1.92 m	16	110.1 t	4.88 s
					4.85 s
6	22.7 t	1.40 m	17	122.5 s	
		1.86 m			
7	38.8 t	2.09 m	18	154.1 s	
		1.83 m			
8	80.4 s		19	116.9 d	6.79 dd (8.0, 2.1)
9	34.8 d	2.07 m	20	127.2 d	7.09 dt (8.0, 2.1)
10	33.7 t	1.49 ddd (10.0, 8.5, 3.5)	21	119.4 d	6.82 dt (8.0 2.1)
		1.70 m			
11	41.9 d	2.45 m	22	128.7 d	7.03 dd (8.0, 2.1)

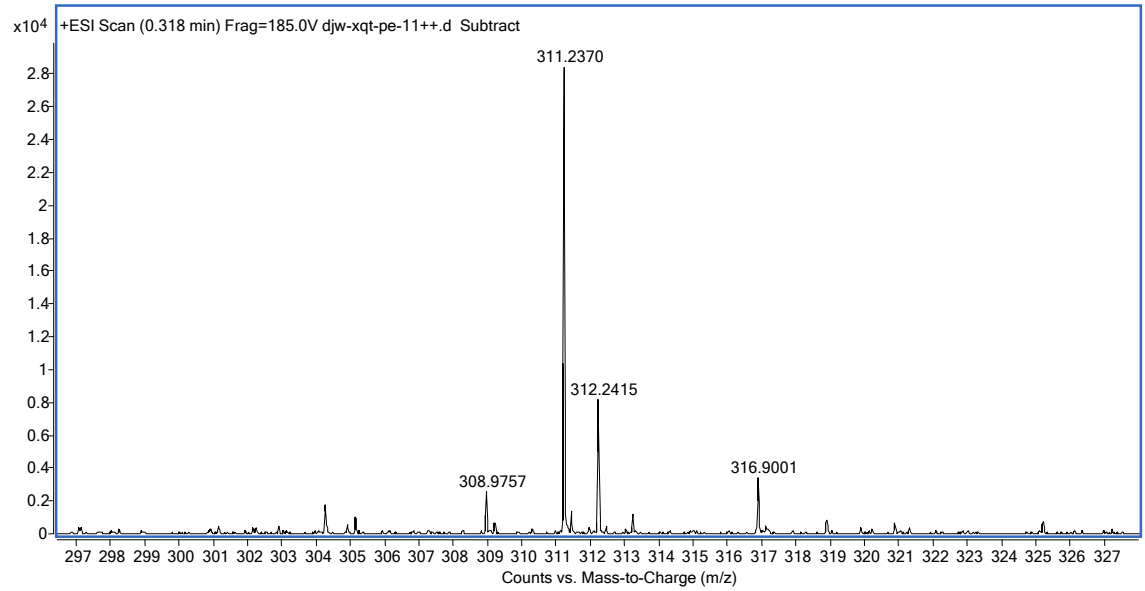


Figure S1 HRESIMS spetrum of illigerate D (1)

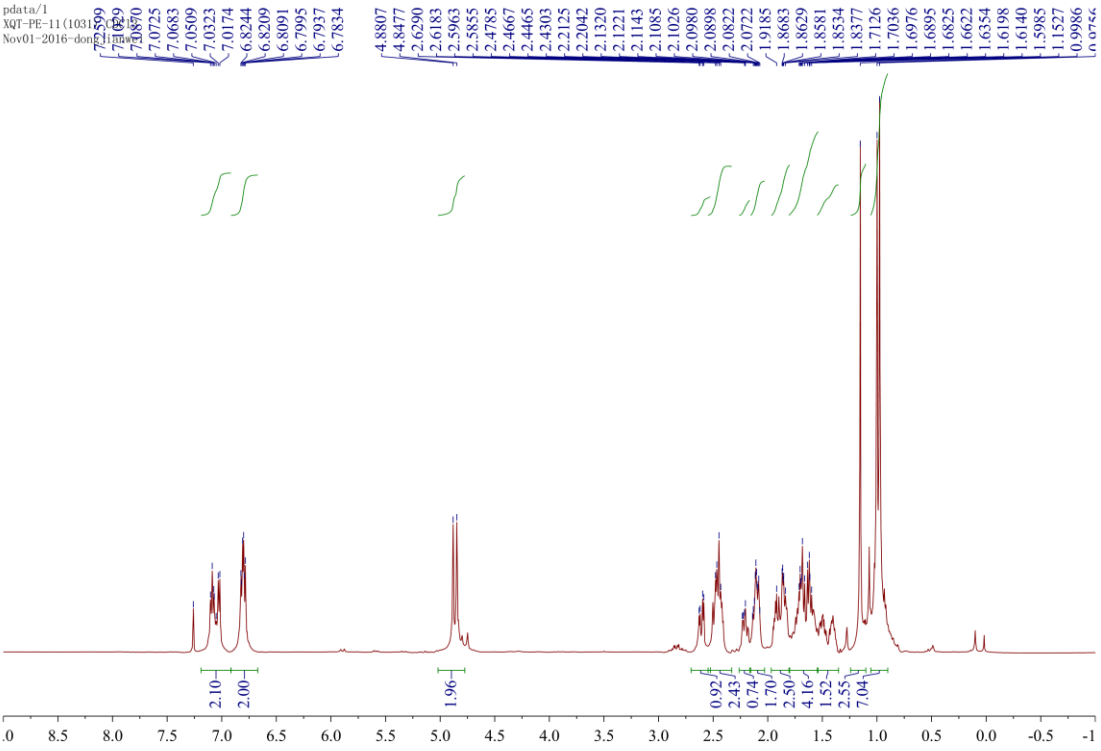


Figure S2 ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of illigerate D (1)

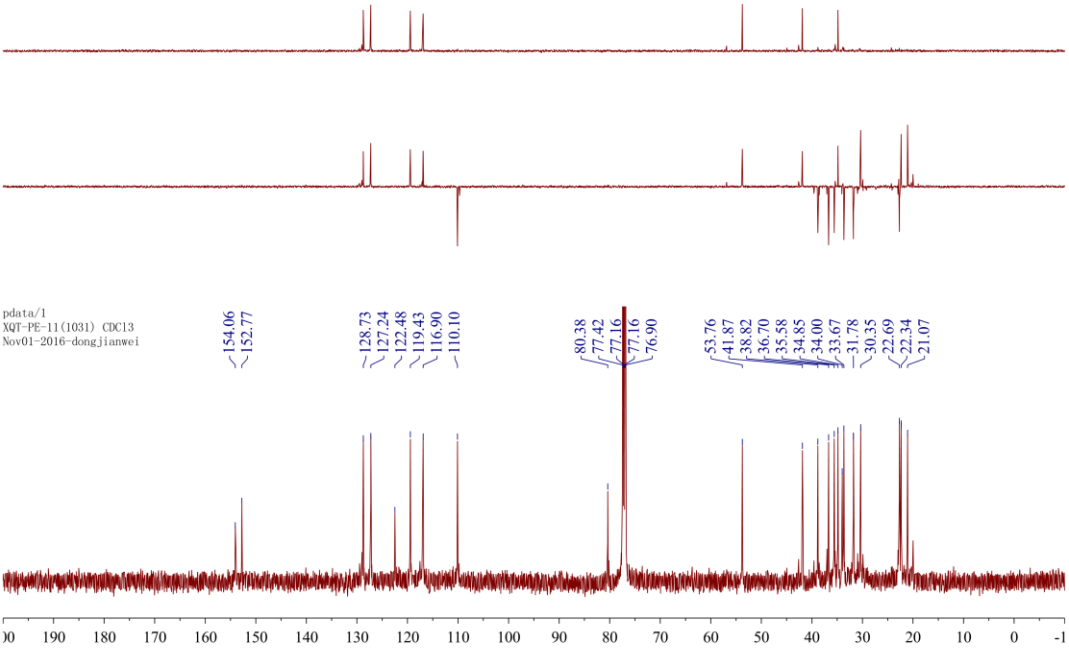


Figure S3 ^{13}C NMR and DEPT spectra ($CDCl_3$, 125 MHz) of illigerate D (1)



Figure S4 ^{1}H-^{1}H COSY spectrum ($CDCl_3$, 500 MHz) of illigerate D (1)

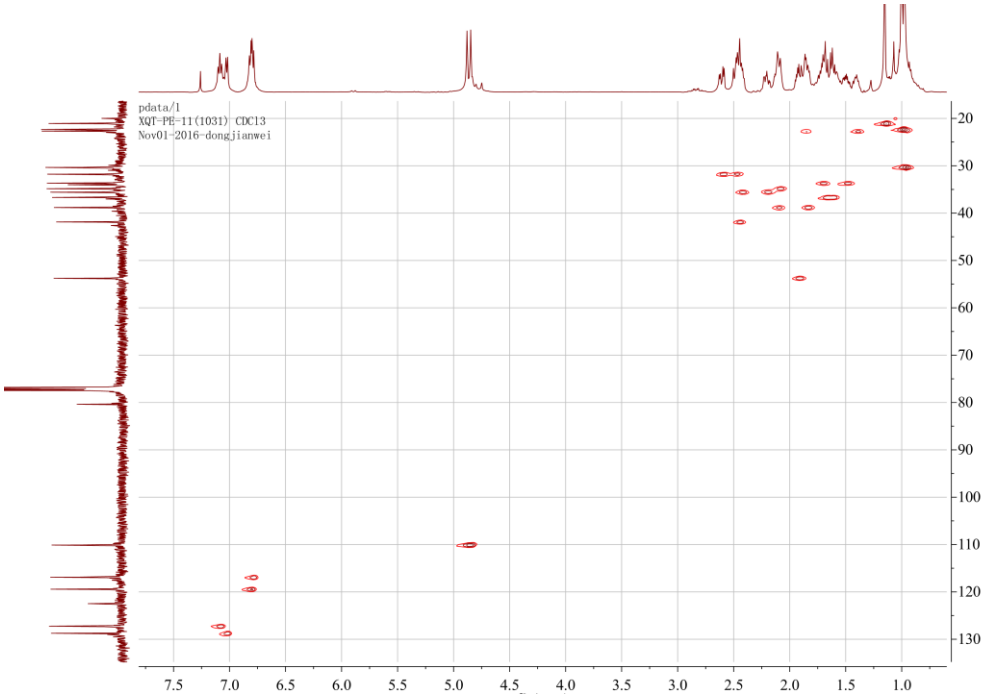


Figure S5 HSQCspectrum ($CDCl_3$, 500 MHz) of illigerate D (1)

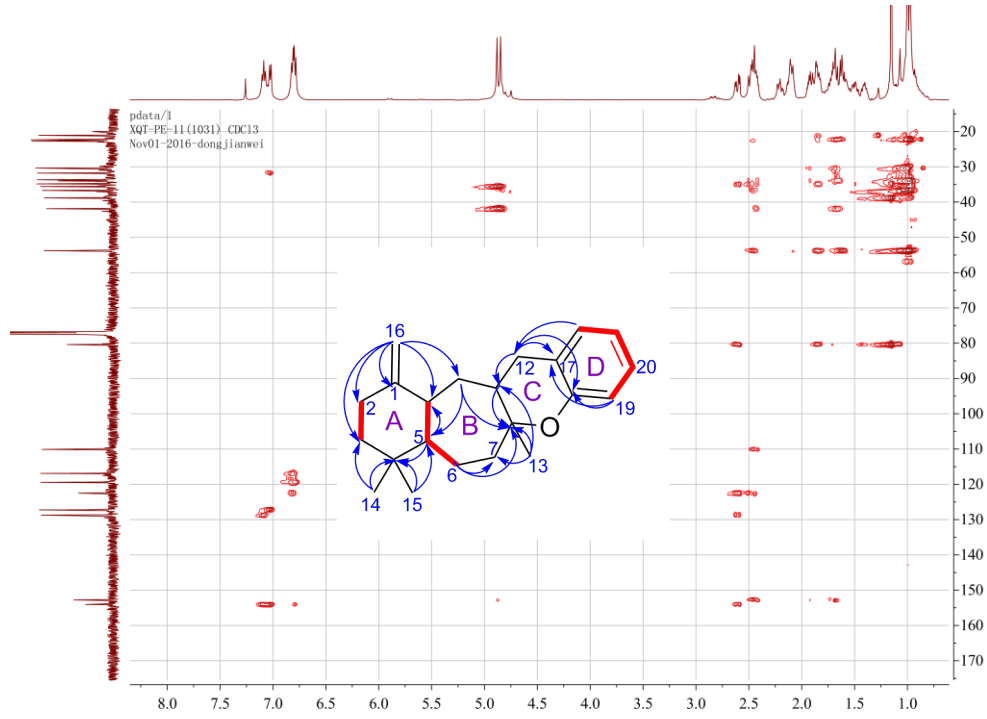


Figure S6 HMBC spectrum ($CDCl_3$, 500 MHz) of illigerate D (1)

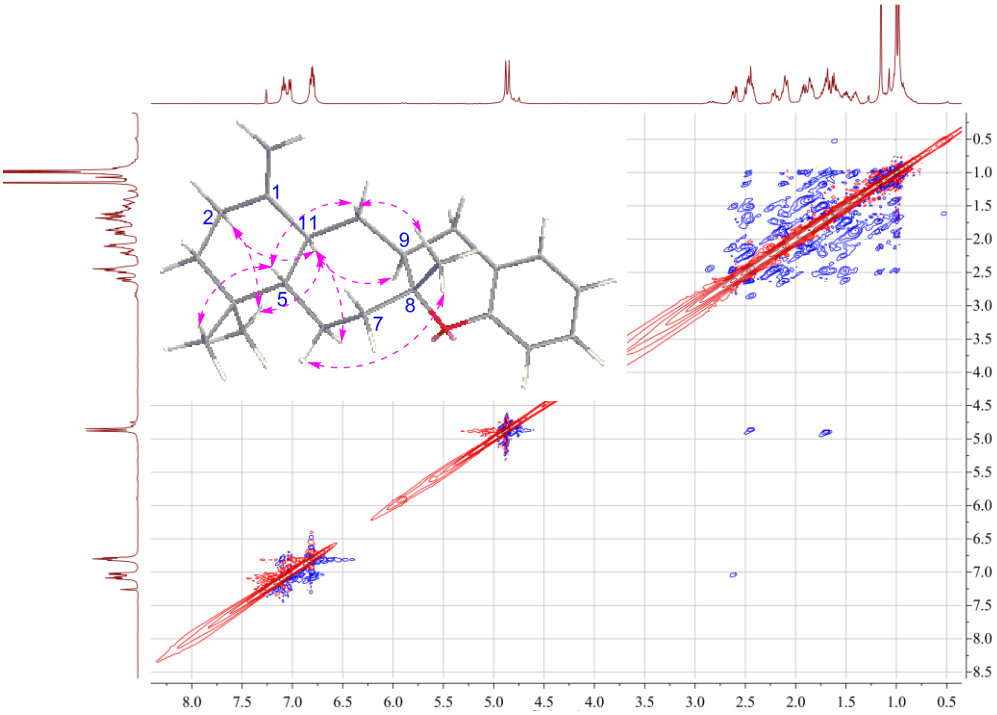


Figure S7 ROESY spectrum ($CDCl_3$, 500 MHz) of illigerate D (1)

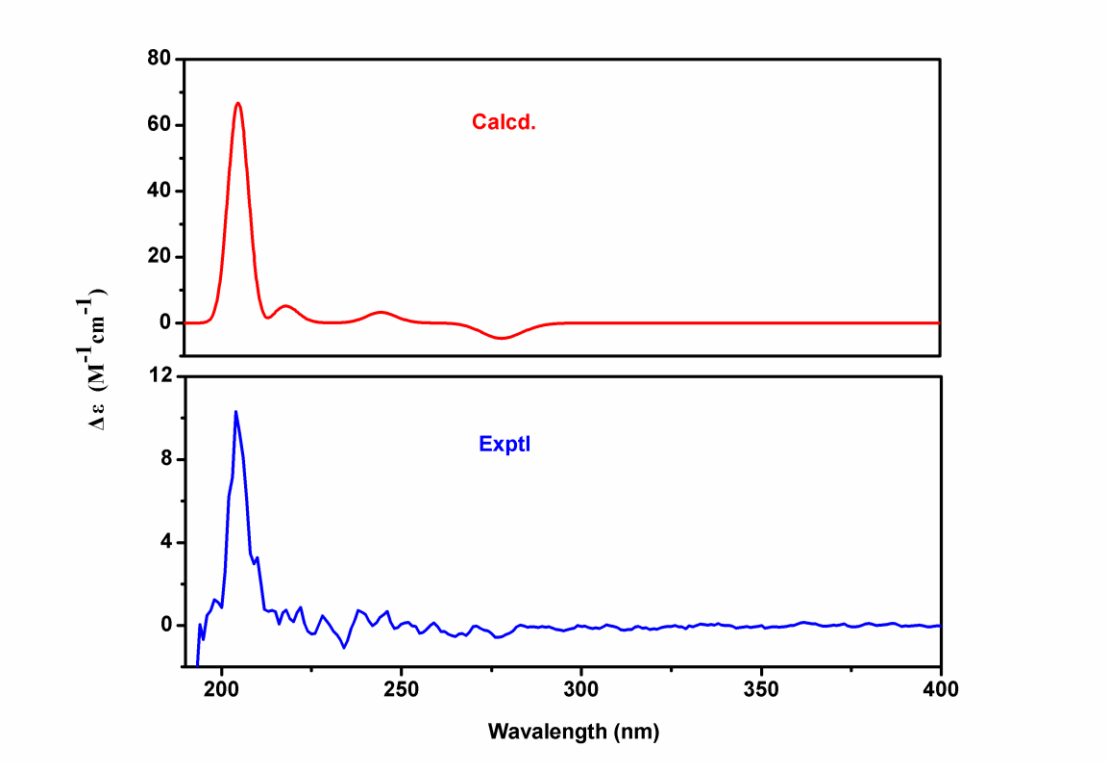


Figure S8 Experimental and calculated ECD spectra of **1**

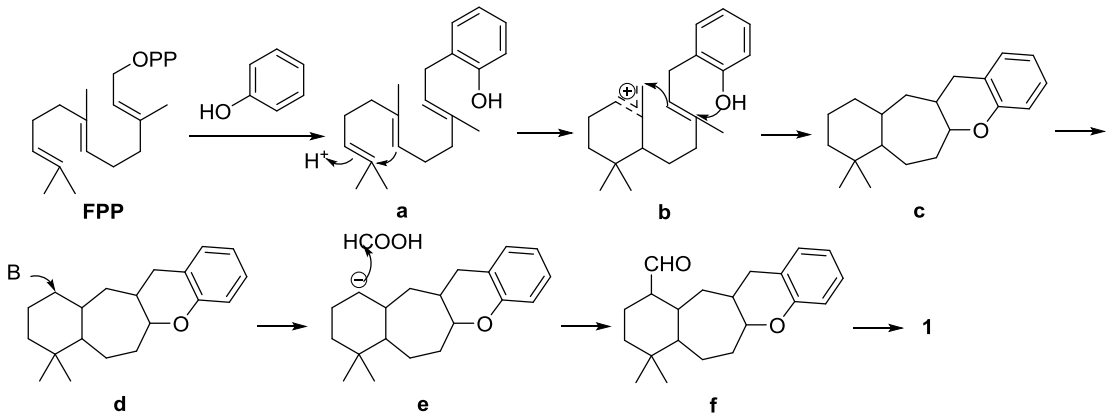
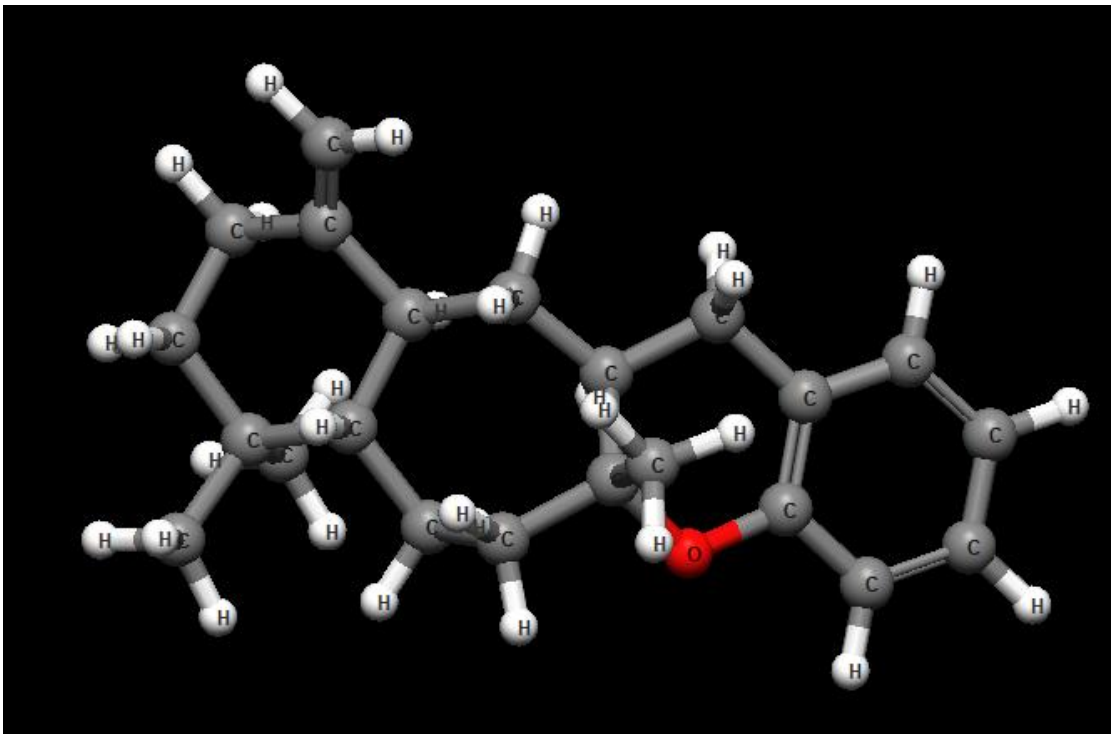


Figure S9 Plausible biosynthetic pathway of **1**.

Optimal conformer (population, 95.7%) obtained from CONFLEX 7.0



Atomic coordinate for the optimal conformer

C,0,-4.2364093458,1.3781672044,-0.8743591909
C,0,-4.6695064873,-0.0328772937,-0.4509822359
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C,0,-2.2825677266,-0.5744026988,0.2646267135
C,0,-1.854054682,0.8686653732,-0.1753499078
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