SUPPLEMENTARY MATERIAL

Trienic α-pyrone and ochratoxin derivatives from a sponge-derived fungus *Aspergillus ochraceopetaliformis*

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Abstract: A new trienic α-pyrone derivative asteltoxin G (**1**) bearing a tetrahydrofuran ring and a new ochratoxin derivative named ochratoxin A_1 (**5**), along with seven known compounds were isolated from a sponge-derived fungus *Aspergillus ochraceopetaliformis*. The compounds (**1-9**) were evaluated on the basis of spectroscopic analyses and comparison with those of the reported data. The new compound ochratoxin A_1 (**5**) exhibited anti-inflammatory activity against IL-6 and TNF-α expression of the LPS-induced THP-1 cells with inhibitory rates of 74.4% and 67.7% at concentration of 10 μM, respectively.

Keywords: sponge-derived fungus; *Aspergillus ochraceopetaliformis*; trienic α-pyrone; ochratoxin; anti-inflammatory

Figure legends

Figure S1. HRESIMS of **1**

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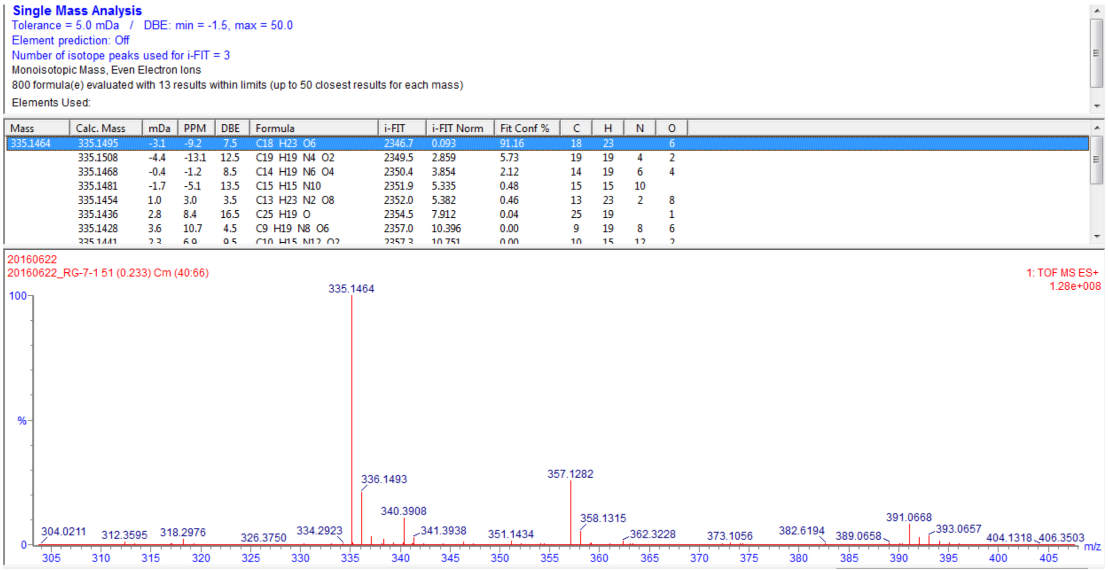
Figure S16. The key HMBC and COSY correlations of compound **5**

Figure S17. The levels of the inflammatory cytokines IL-6 (A) and IFN-α (B) in cell supernatant (pg/ml, mean ± SD)

Table S1. ^{1}H (600 MHz) and ^{13}C NMR (150 MHz) Data for **1** in CD_3OD

Table S2. ^{1}H (600 MHz) and ^{13}C NMR (150 MHz) Data for **5** in CD_3OD

Figure S1. HRESIMS of **1**


Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
800 formula(e) evaluated with 13 results within limits (up to 50 closest results for each mass)
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
335.1464	335.1495	-3.1	-9.2	7.5	C18 H23 O6	2346.7	0.093	91.16	18	23		6
	335.1508	-4.4	-13.1	12.5	C19 H19 N4 O2	2349.5	2.859	5.73	19	19	4	2
	335.1468	-0.4	-1.2	8.5	C14 H19 N6 O4	2350.4	3.854	2.12	14	19	6	4
	335.1481	-1.7	-5.1	13.5	C15 H15 N10	2351.9	5.335	0.48	15	15	10	
	335.1454	1.0	3.0	3.5	C13 H23 N2 O8	2352.0	5.382	0.46	13	23	2	8
	335.1436	2.8	8.4	16.5	C25 H19 O	2354.5	7.912	0.04	25	19		1
	335.1428	3.6	10.7	4.5	C9 H19 N8 O6	2357.0	10.396	0.00	9	19	8	6
	335.1441	2.3	6.9	9.5	C10 H15 N12 O2	2357.3	10.751	0.00	10	15	12	2

Figure S2.[1]H NMR (600 MHz, CD_3OD) of **1**

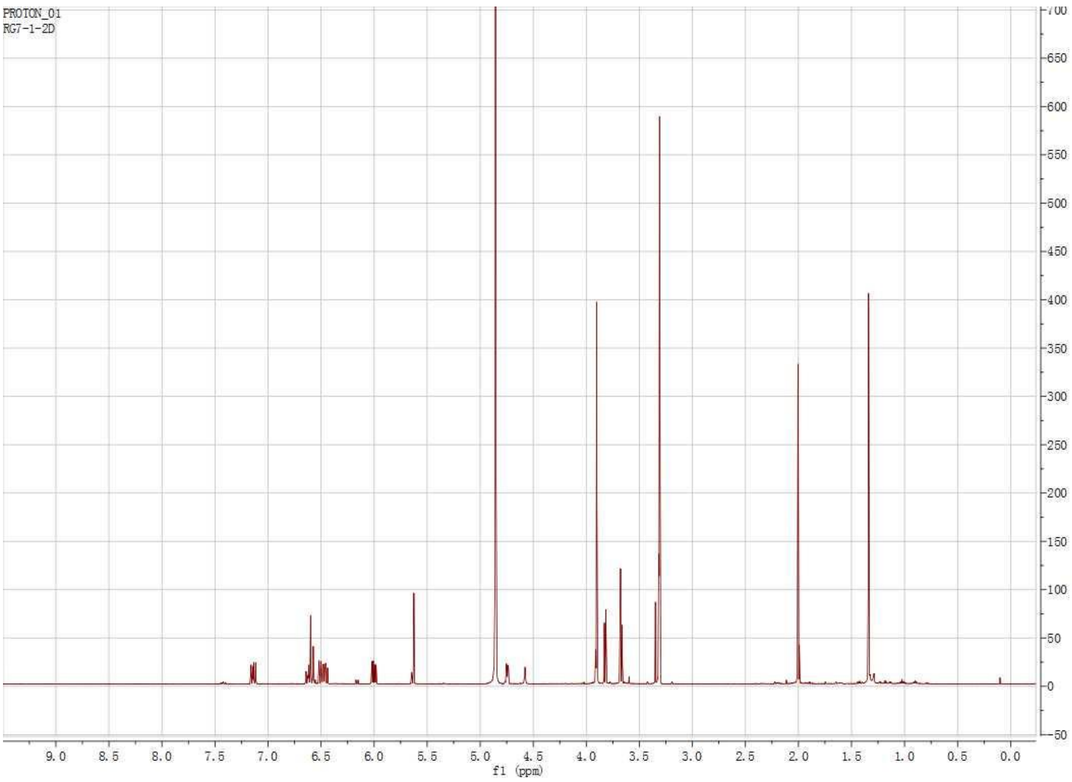


Figure S3. ^{13}CNMR (150 MHz, CD_3OD) of **1**

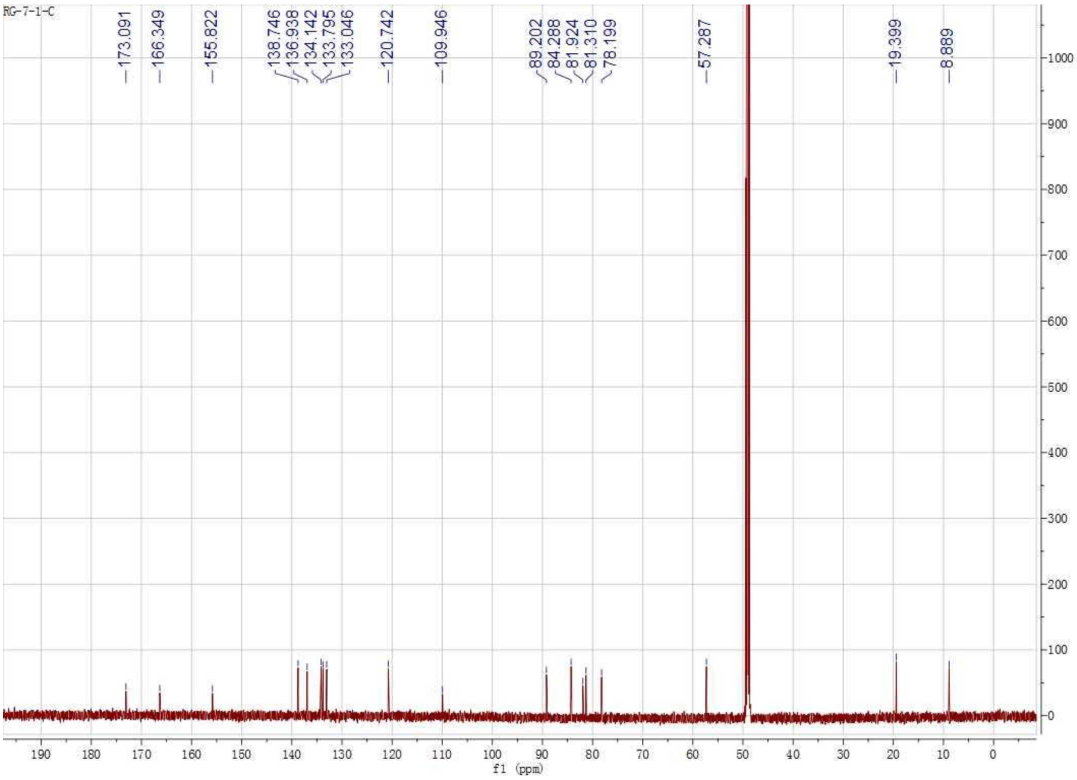


Figure S4. HSQC (600 MHz, CD_3OD) of **1**

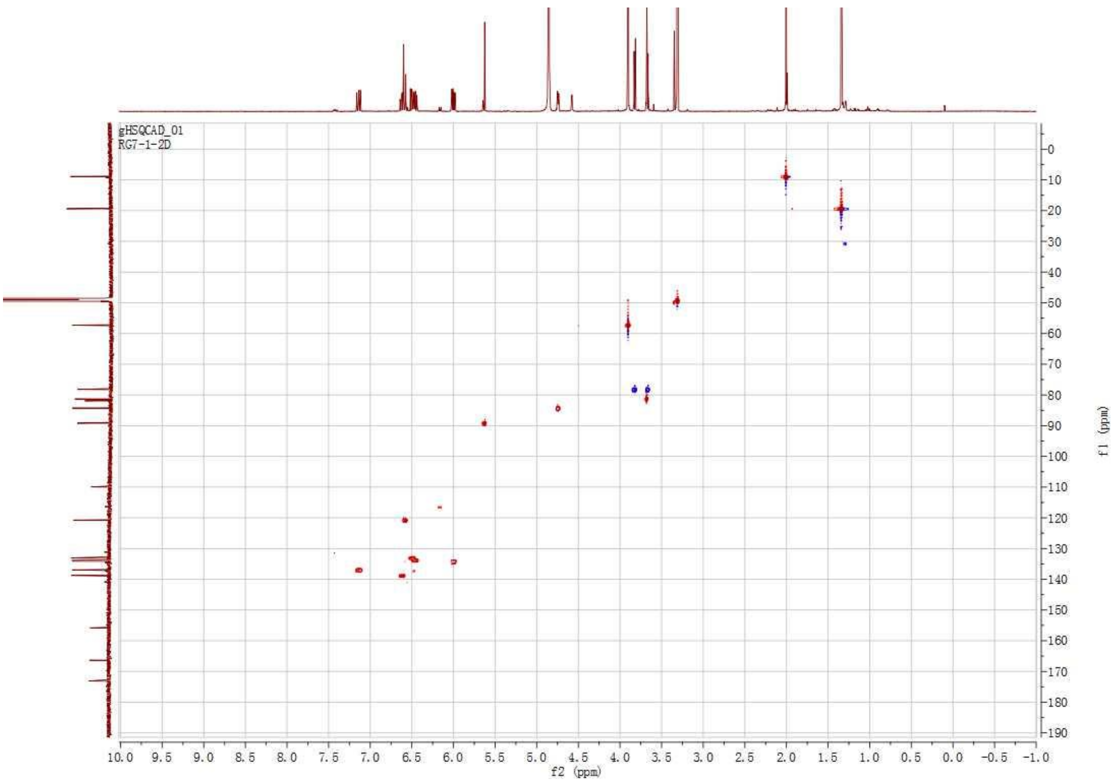


Figure S5. COSY (600 MHz, CD_3OD) of **1**

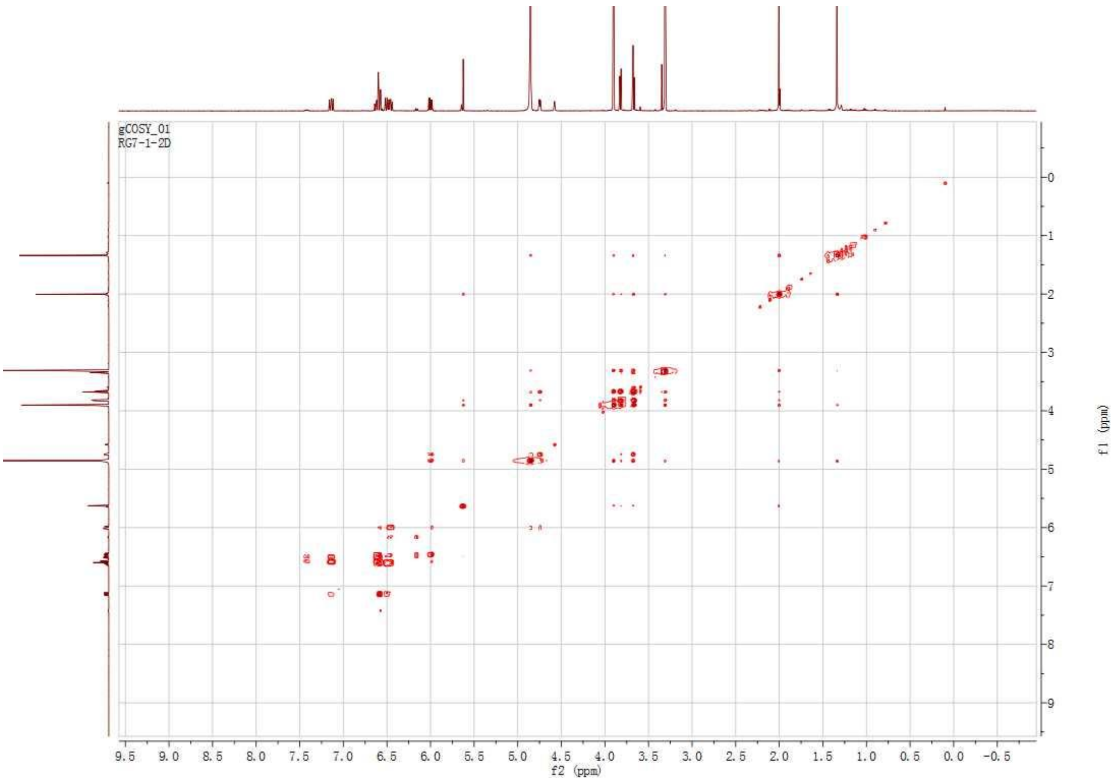


Figure S6. HMBC (600 MHz, CD_3OD) of **1**

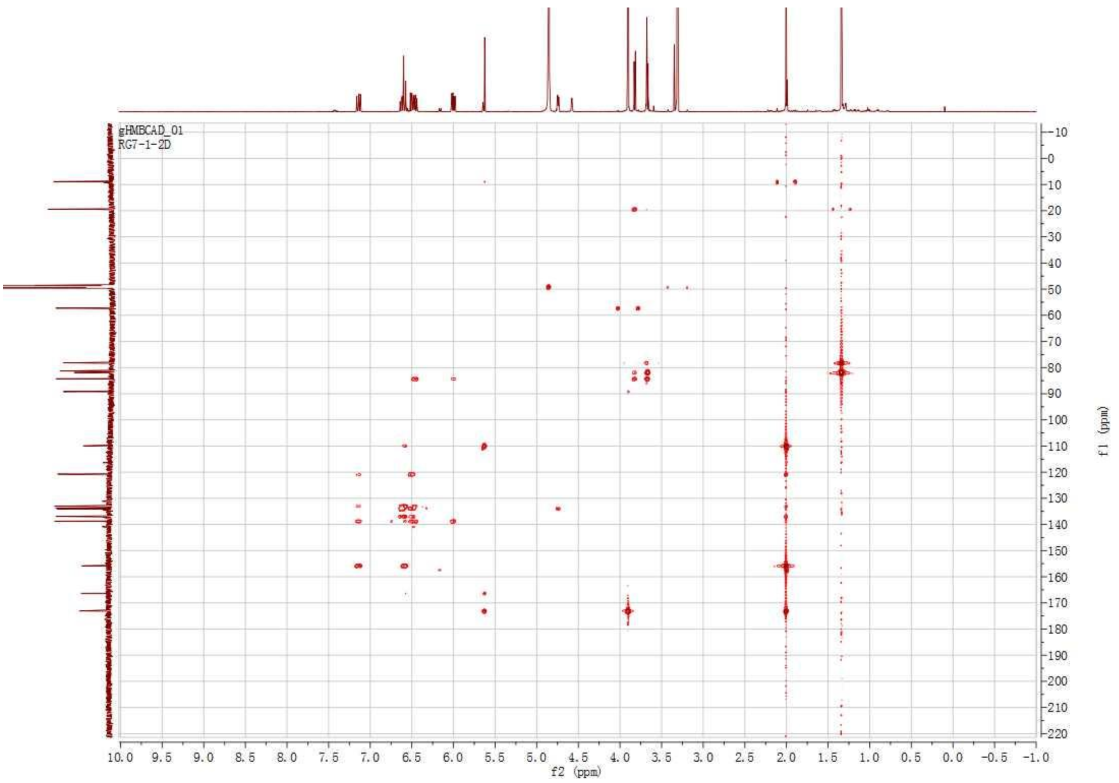


Figure S7.NOESY (600 MHz, CD_3OD) of **1**

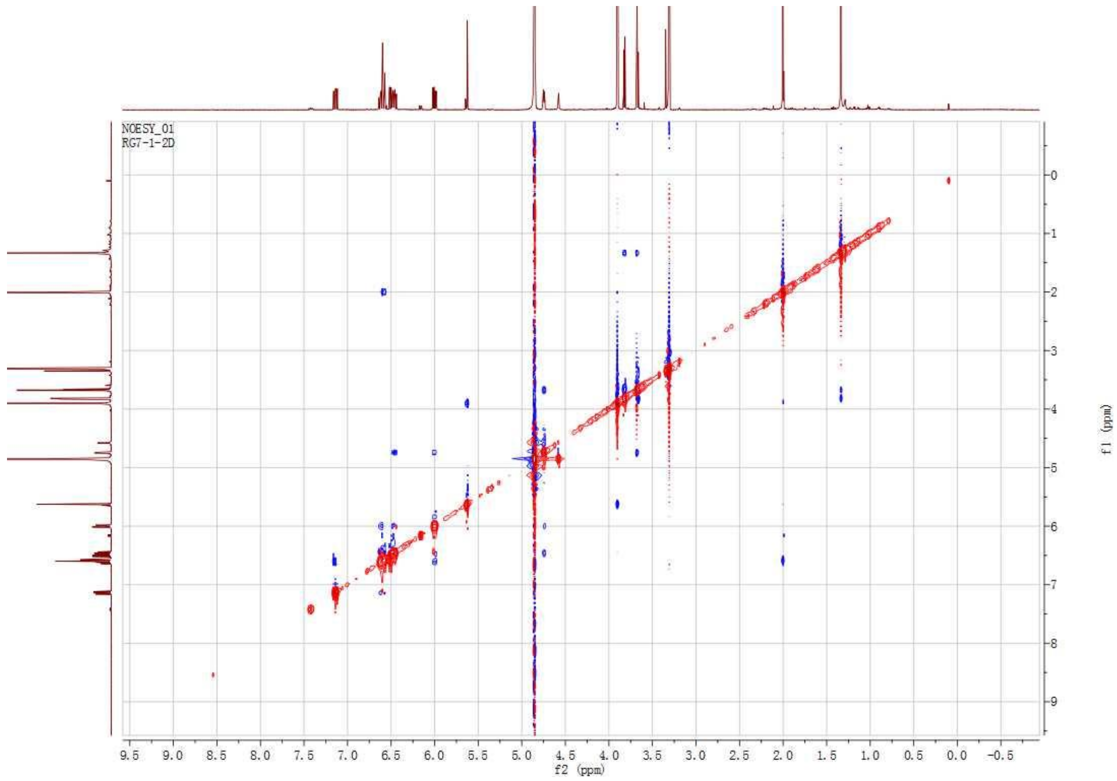


Figure S8. The key HMBC and COSY correlations of **1**

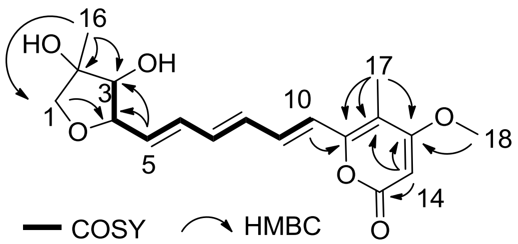


Figure S9. Key NOE correlations for compound **1**

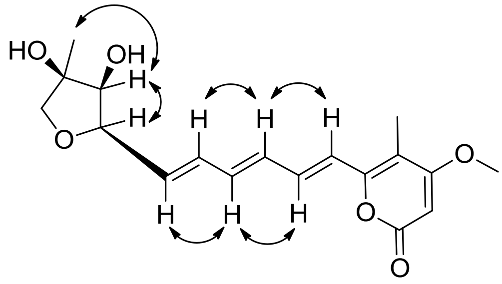


Figure S10. HRESIMS of **5**

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
450 formula(e) evaluated with 5 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Cl
506.1198	100.00	506.1218	-2.0	-4.0	12.5	C24 H25 N O9 Cl	961.2	0.000	100.00	24	25	1	9	1
		506.1137	6.1	12.1	12.5	C25 H26 N O6 Cl2	974.9	13.612	0.00	25	26	1	6	2
		506.1209	-1.1	-2.2	16.5	C30 H27 N Cl3	975.4	14.140	0.00	30	27	1		3
		506.1290	-9.2	-18.2	16.5	C29 H26 N O3 Cl2	975.9	14.667	0.00	29	26	1	3	2
		506.1240	-4.2	-8.3	21.5	C30 H20 N O7	984.1	22.851	0.00	30	20	1	7	

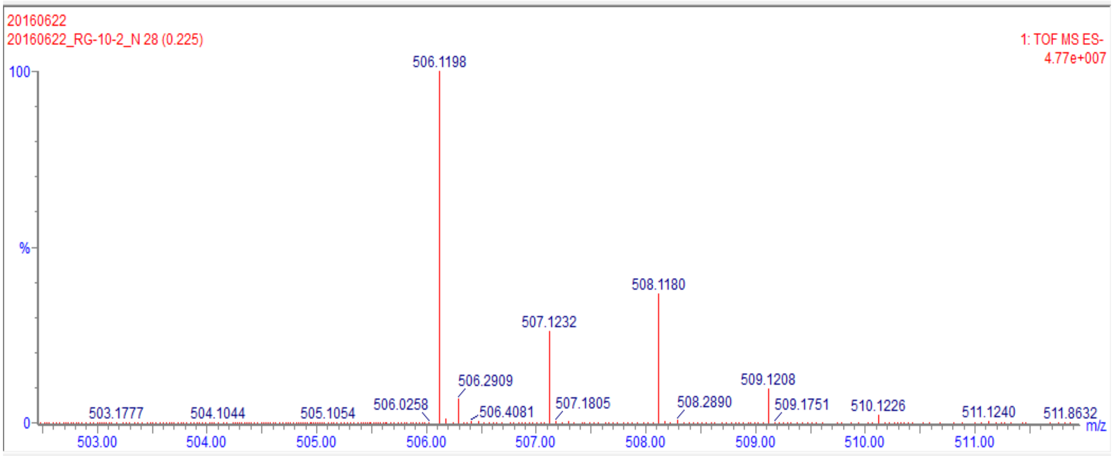


Figure S11. ^{1}H NMR (600 MHz, CD_3OD) of **5**

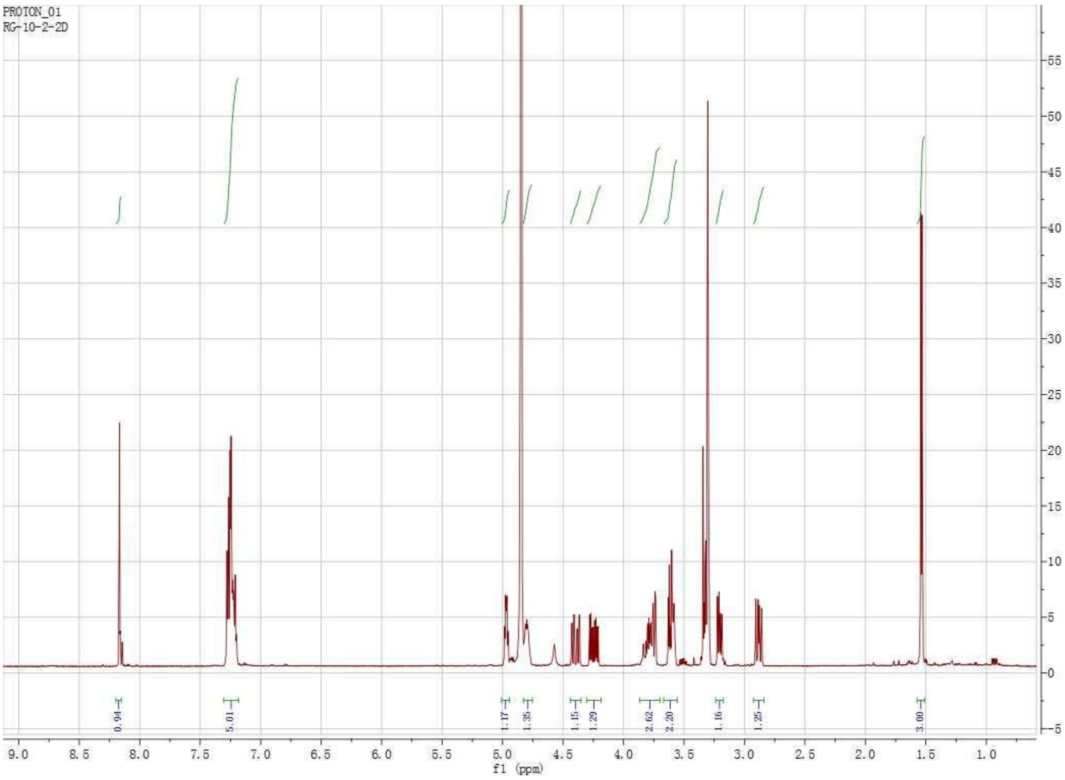


Figure S12. ^{13}CNMR (150 MHz, CD_3OD) of **5**

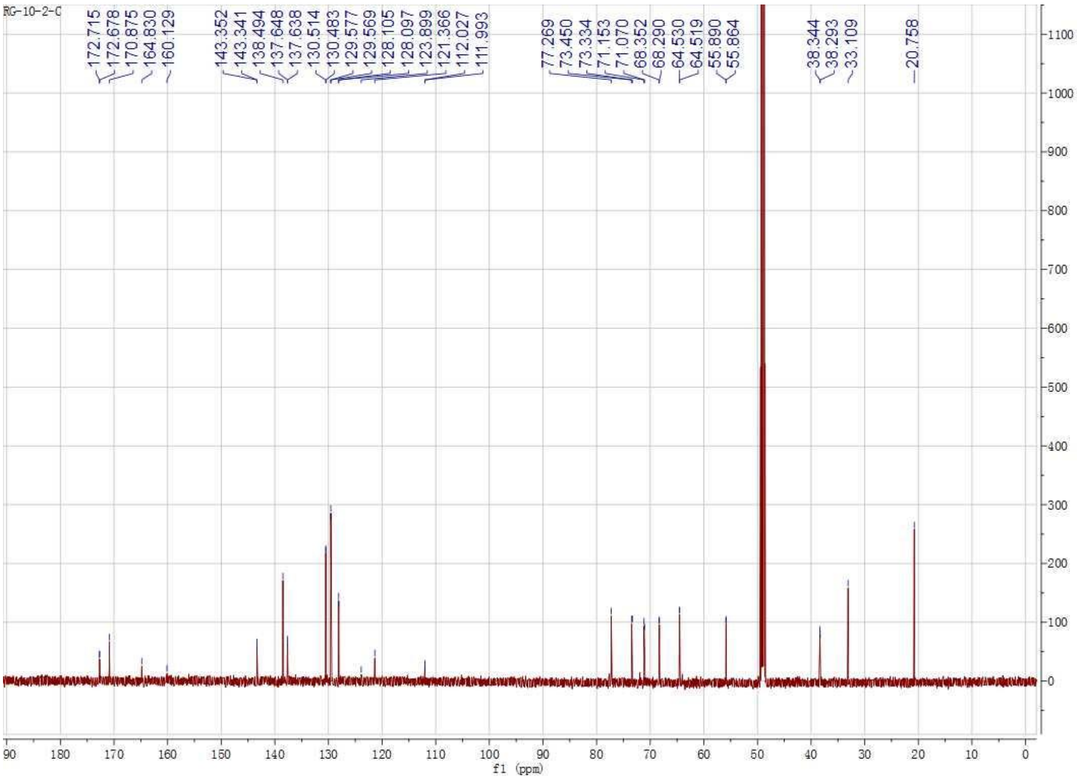


Figure S13. HSQC (600 MHz, CD_3OD) of **5**

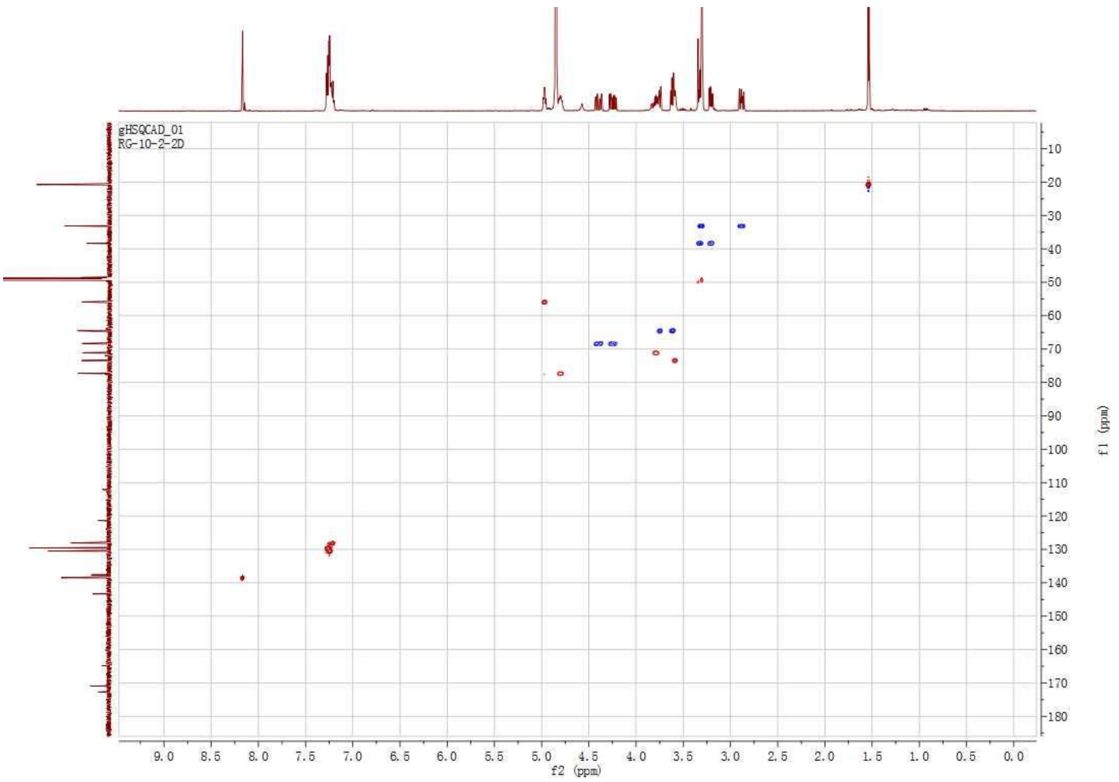


Figure S14. COSY (600 MHz, CD_3OD) of **5**

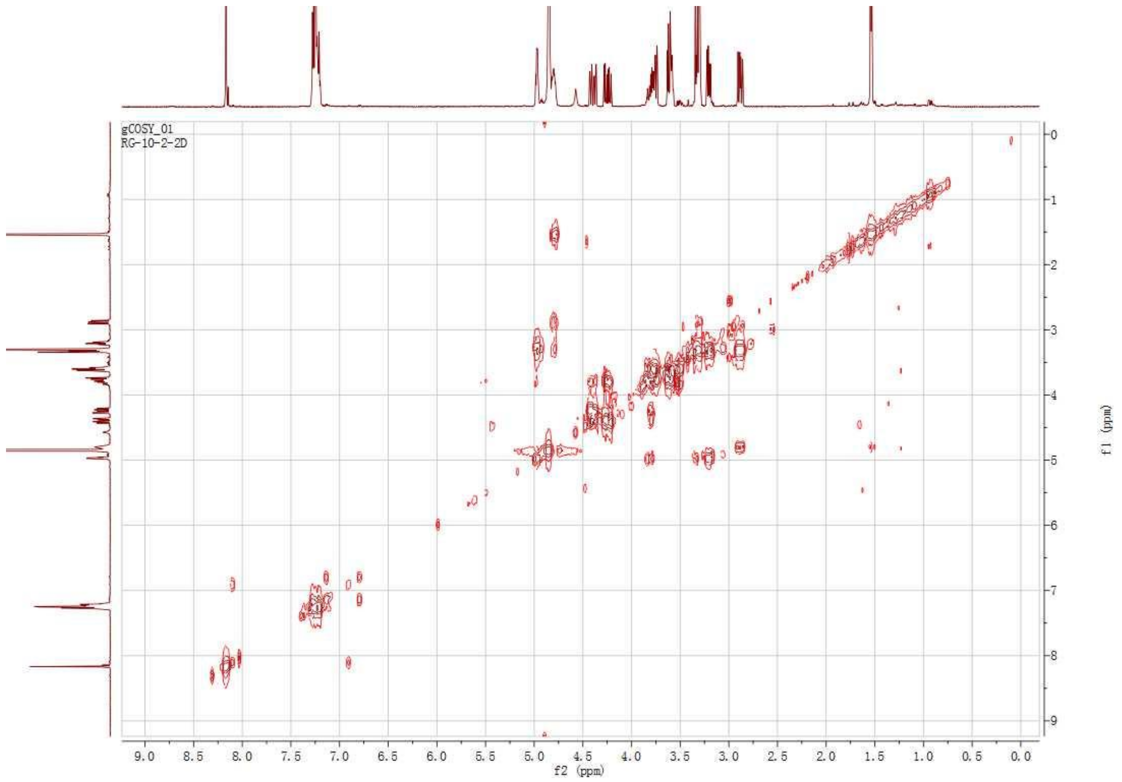


Figure S15. HMBC (600 MHz, CD_3OD) of **5**

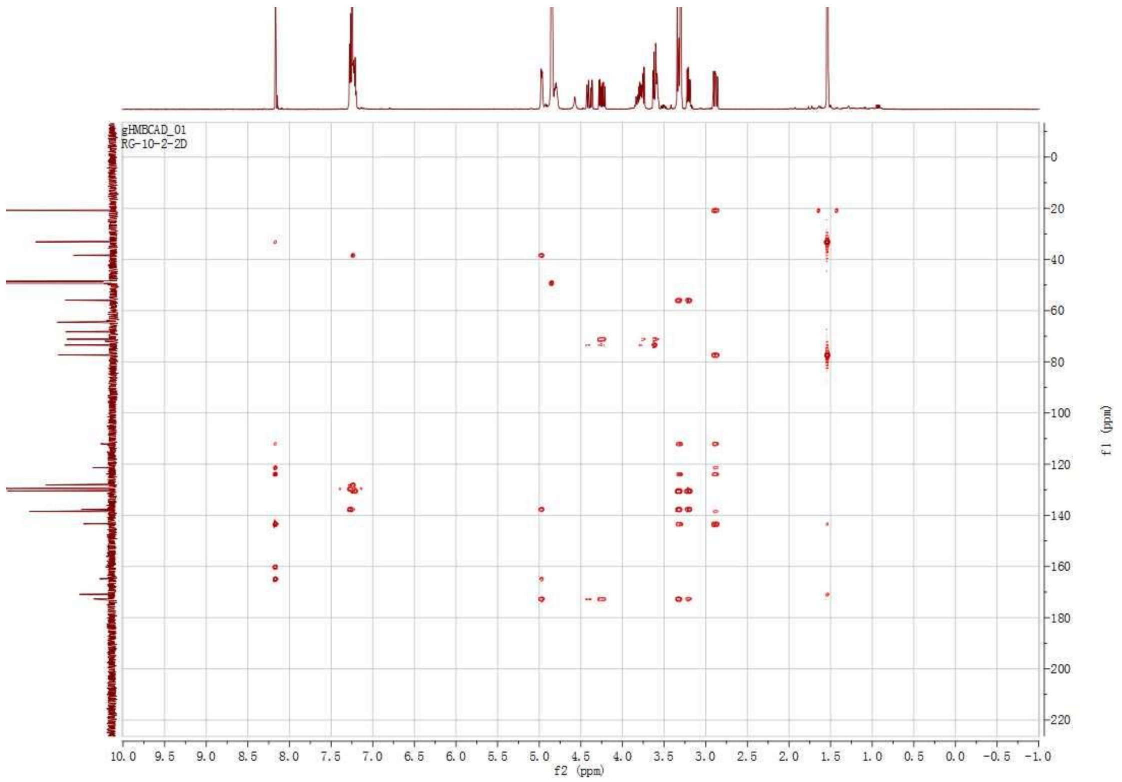


Figure S16. The key HMBC and COSY correlations of compound **5**.

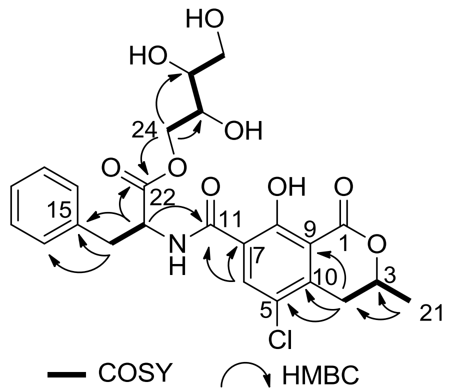


Figure S17. The levels of the inflammatory cytokines IL-6 (A) and IFN-α (B) in cell supernatant (pg/ml, mean ± SD)

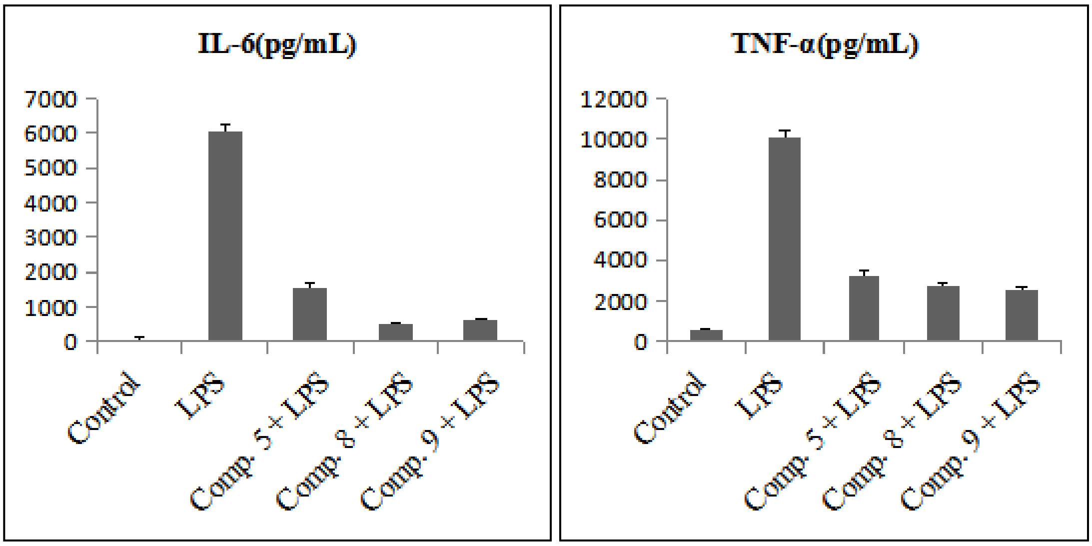


Table S1. ^{1}H (600 MHz) and ^{13}C NMR (150 MHz) Data for **1** in CD_3OD.

Position	δ_C	δ_H (J in Hz)
1	78.2, CH_2	3.82, d (8.9)
		3.67, d (8.9)
2	81.9, C	
3	81.3, CH	3.68, d (3.3)
4	84.3, CH	4.74, dd (7.3, 3.3)
5	134.1, CH	6.00, dd (15.2, 7.3)
6	133.8, CH	6.46, dd (15.2, 11.2)
7	138.7, CH	6.62, dd (14.9, 11.1)
8	133.0, CH	6.50, dd (14.8, 11.2)
9	136.9, CH	7.14, dd (14.9, 11.1)
10	120.7, CH	6.59, d (14.8)
11	155.8, C	
12	109.9, C	
13	173.1, C	
14	89.2, CH	5.63, s
15	166.3, C	
16	19.4, CH_3	1.34, s
17	8.9, CH_3	2.00, s
18	57.3, CH_3	3.90, s

Table S2. ^{1}H (600 MHz) and ^{13}C NMR (150 MHz) Data for **5** in CD_3OD.

Position	δ_C	δ_H (J in Hz)
1	170.9, C	
3	77.3, CH	4.81, m
4	33.1, CH_2	3.31, ov
		2.89, dd (17.3, 11.7)
5	123.9, C	
6	138.5, CH	8.17, s
7	121.4, C	
8	160.1, C	
9	112.0, C	
10	143.3, C	
11	164.8, C	
13	55.9, CH	4.98, m
14	38.3, CH_2	3.33, ov
		3.21, dd (13.8, 7.6)
15	137.6, C	
16	130.5, CH	7.24, m
17	129.6, CH	7.26, m
18	128.1, CH	7.21, m
19	129.6, CH	7.26, m
20	130.5, CH	7.24, m
21	20.8, CH_3	1.54, d (6.3)
22	172.7, C	
24	68.3, CH_2	4.40, ddd (26.8, 11.4, 2.9)
		4.25, ddd (25.0, 11.4, 6.5)
25	71.1, CH	3.79, m
26	73.4, CH	3.59, m
27	64.5, CH_2	3.75, m
		3.62, m