

Supporting Information

Rec. Nat. Prod. 17:3 (2023) 549-554

Anti-inflammatory Benzofurans from the Heartwood of *Dalbergia cochinchinensis* Pierre ex Laness

Qiwan Zheng¹, Chan yue Ouyang², Yang Liu¹, Jiahui Ren¹,

Xianwen Wei¹, Ronghua Liu^{1*} and Lanying Chen^{2*}

¹School of Pharmacy, Jiangxi University of Chinese Medicine, Nanchang, 330004, China

²National Pharmaceutical Engineering Center for Solid Preparation of Chinese Herbal Medicine, Jiangxi University of Chinese Medicine, Nanchang, 330006, China

Table of Contents	page
Table S1: The most similar compound data to compound 1	2
Table S2: Molecular mass information of compound 1 in HR-ESI-MS spectrum	3
Figure S1: HR-ESI-MS spectrum of compound 1	3
Figure S2: ¹ H-NMR (600 MHz, Acetone- <i>d</i> ₆) spectrum of 1 (Cochinfuran A)	4
Figure S3: The labeled ¹ H-NMR spectrum of compound 1	4
Figure S4: ¹³ C-NMR (151 MHz, Acetone- <i>d</i> ₆) spectrum of 1 (Cochinfuran A)	5
Figure S5: The labeled ¹³ C-NMR spectrum of compound 1	5
Figure S6: HMQC spectrum of 1 (Cochinfuran A)	6
Figure S7: The labeled HMQC spectrum of compound 1	6
Figure S8: HMBC spectrum of 1 (Cochinfuran A)	7
Figure S9: The labeled HMBC spectrum of compound 1	7
Figure S10: UV spectra of compound 1	8
Figure S11: IR spectra of compound 1	9
Figure S12: ¹ H-NMR (600 MHz, Acetone- <i>d</i> ₆) spectrum of 2	10
Figure S13: ¹³ C-NMR (151 MHz, Acetone- <i>d</i> ₆) spectrum of 2	11
Figure S14: ¹ H-NMR (600 MHz, Acetone- <i>d</i> ₆) spectrum of 3	12
Figure S15: ¹³ C-NMR (151 MHz, Acetone- <i>d</i> ₆) spectrum of 3	13
Figure S16: ¹ H-NMR (600 MHz, Acetone- <i>d</i> ₆) spectrum of 4	14
Figure S17: ¹³ C-NMR (151 MHz, Acetone- <i>d</i> ₆) spectrum of 4	15
Figure S18: ¹ H-NMR (600 MHz, Acetone- <i>d</i> ₆) spectrum of 5	16
Figure S19: ¹³ C-NMR (151 MHz, Acetone- <i>d</i> ₆) spectrum of 5	17
Figure S20: Effects of compounds on the production of NO and LDH in LPS-induced RAW 264.7 macrophages	18
Figure S21: 3D visualization of the docking of compound 4 with MPO	20
Table S3: Docking scores of compounds 1-5 with protein	20
Table S4: Annotation table	21
Table S5: SciFinder report of compound 1	22

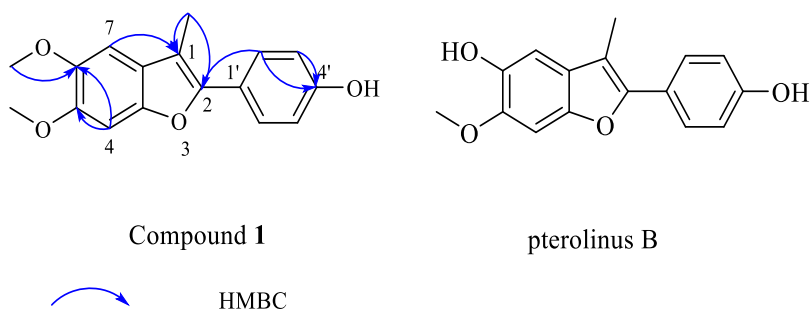


Table S1: The most similar compound data to compound 1

Position	1 ^a		pterolinus B ^b	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1	-	109.3	-	110.0
2	-	150.1	-	151.1
3	-	-	-	-
4	7.00 (1H, s)	95.4	7.13 (1H, s)	95.7
5	-	148.5	-	147.1
6	-	148.1	-	148.5
7	6.97 (1H, s)	101.8	6.96 (1H, s)	104.2
8	-	123.3	-	124.8
9	-	146.9	-	144.8
1'	-	123.2	-	123.3
2',6'	7.49 (2H, d, $J = 8.8$ Hz)	127.6	7.63 (2H, d, $J = 8.0$ Hz)	128.6
3',5'	6.84 (2H, d, $J = 8.8$ Hz)	115.5	6.96 (2H, d, $J = 8.0$ Hz)	116.5
4'	-	157.0	-	158.0
4'-OH	8.48 (1H, s)	-	8.6 (1H, s)	-
1-CH ₃	2.27 (3H, s)	8.6	2.36 (3H, s)	9.6
5-OCH ₃	3.74 (3H, s)	55.7	3.92 (3H, s)	56.8
6-OCH ₃	3.73 (3H, s)	55.9	-	-

^aMeasured in Acetone-*d*₆, -600 MHz

^bMeasured in Acetone-*d*₆, -500 MHz

References

S. F. Wu, F. R. Chang, S. Y. Wang, T. L. Hwang, C. L. Lee, S. L. Chen, C. C. Wu and Y. C. Wu (2011). Anti-inflammatory and cytotoxic neoflavonoids and benzofurans from *Pterocarpus santalinus*, *J. Nat. Prod.* **74**, 989-996

Table S2 : Molecular mass information of compound **1** in HR-ESI-MS spectrum

Compounds	Ionic mode	Formula	Measured value (m/z)	Calculated value (m/z)	Error (ppm)
1	$[M+H]^+$	$C_{17}H_{14}O_4$	285.1120	285.1121	-0.370

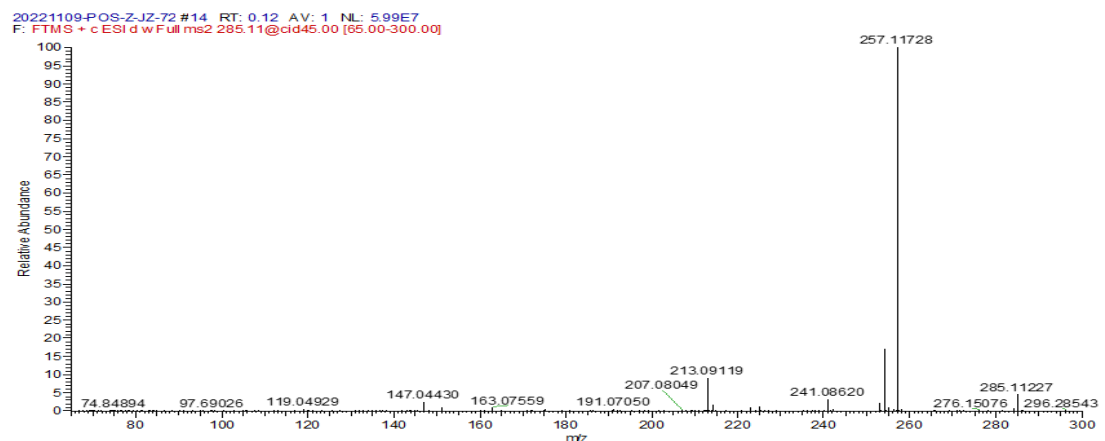
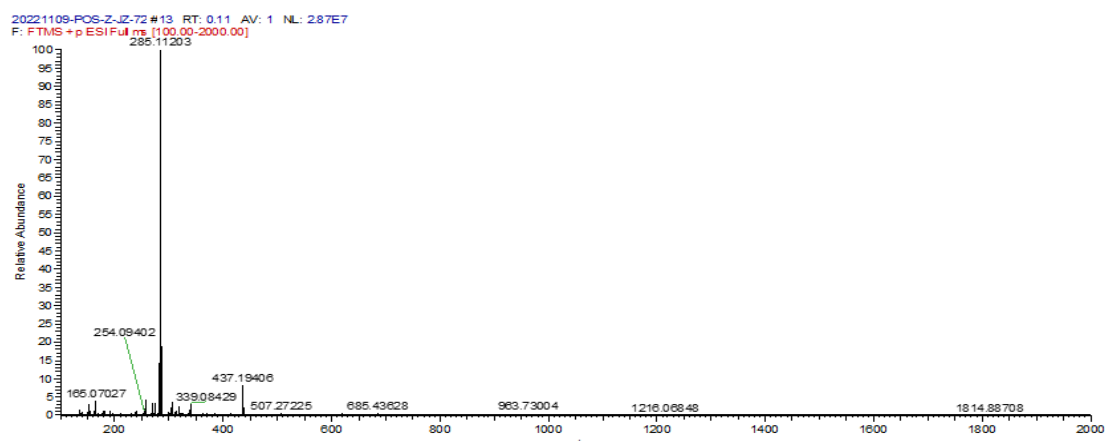
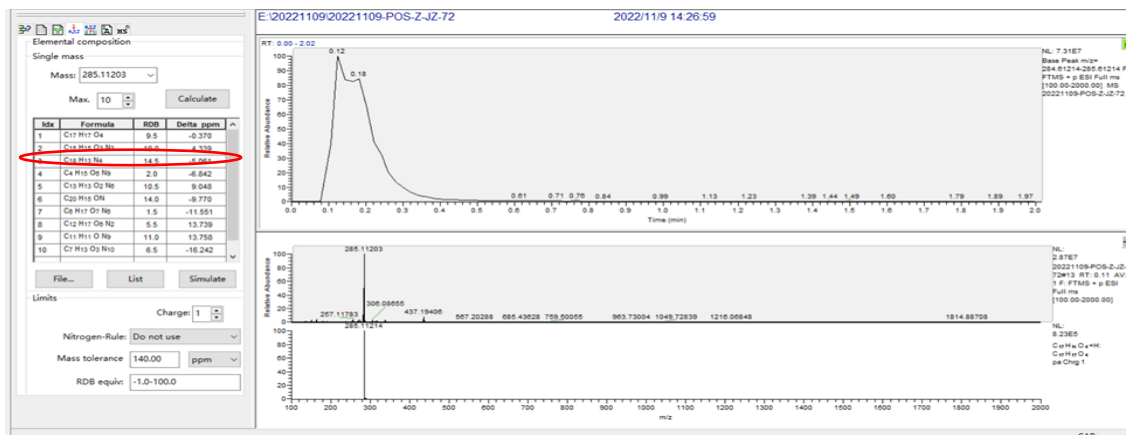


Figure S1: HR-ESI-MS spectrum of compound **1**

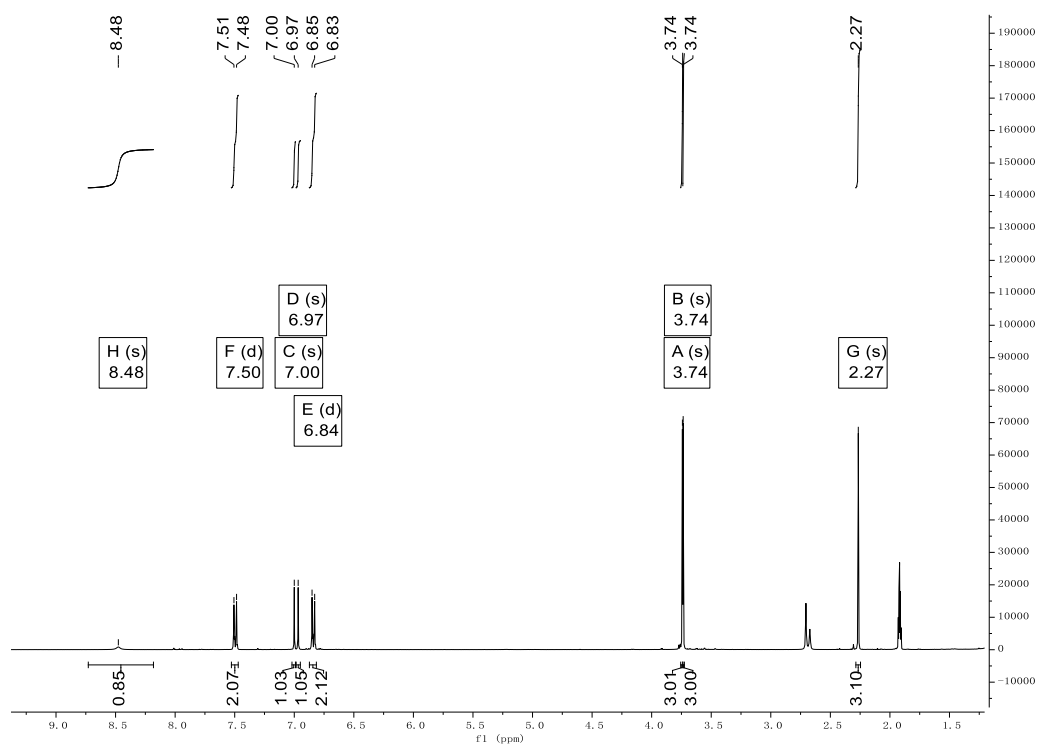


Figure S2: $^1\text{H-NMR}$ (600 MHz, Acetone- d_6) spectrum of **1** (Cochinfuran A)

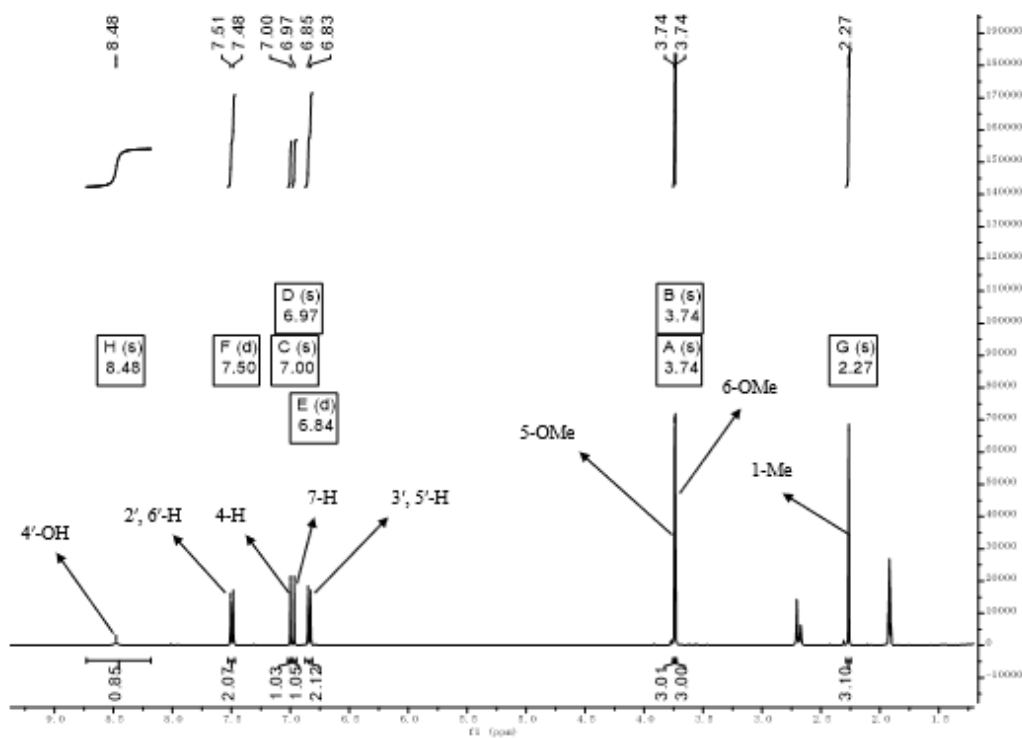


Figure S3: The labeled $^1\text{H-NMR}$ spectrum of compound **1**

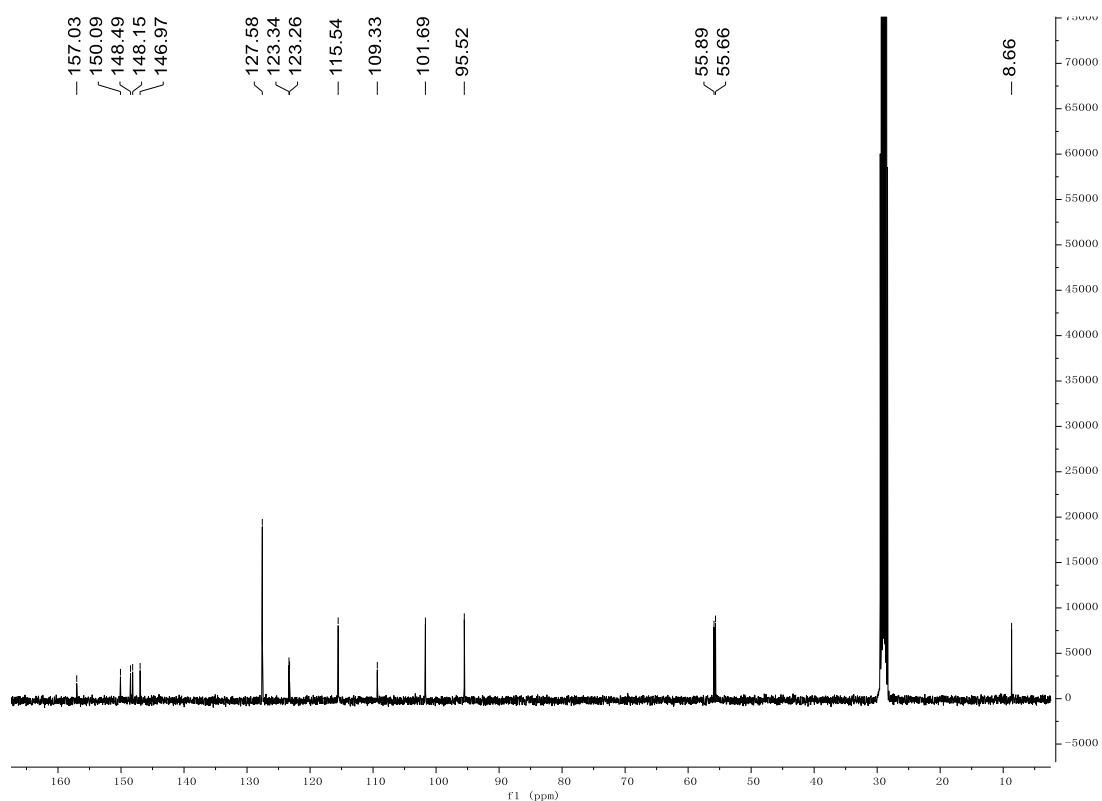


Figure S4: ^{13}C -NMR (151 MHz, Acetone- d_6) spectrum of **1** (Cochinfuran A)

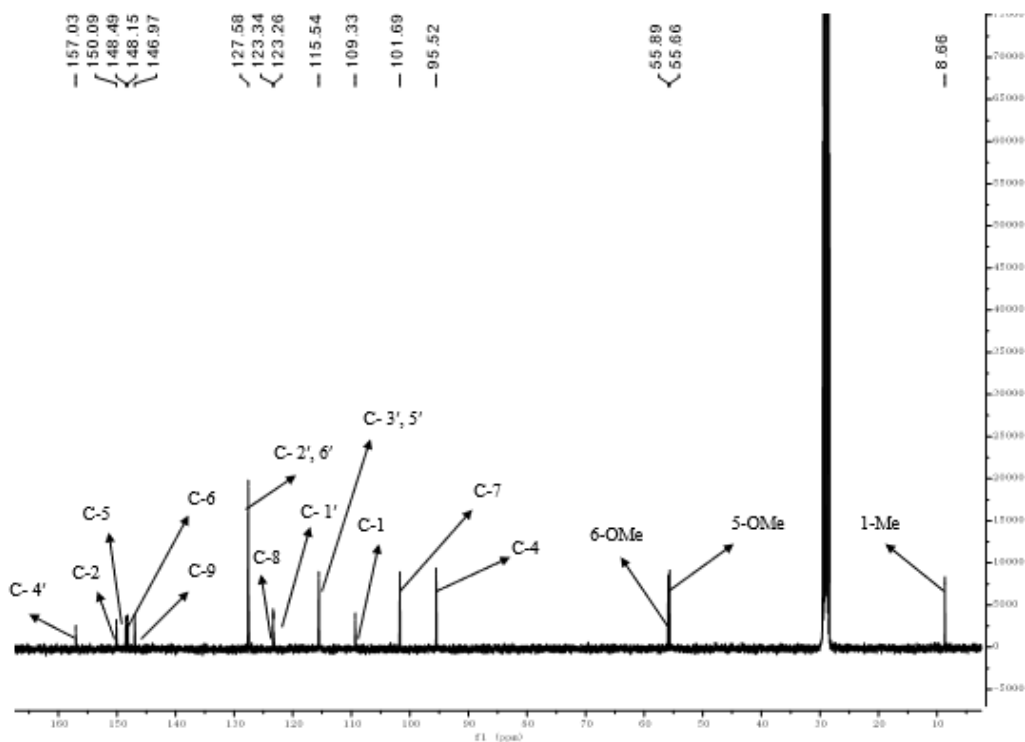


Figure S5: The labeled ^{13}C -NMR spectrum of compound **1**

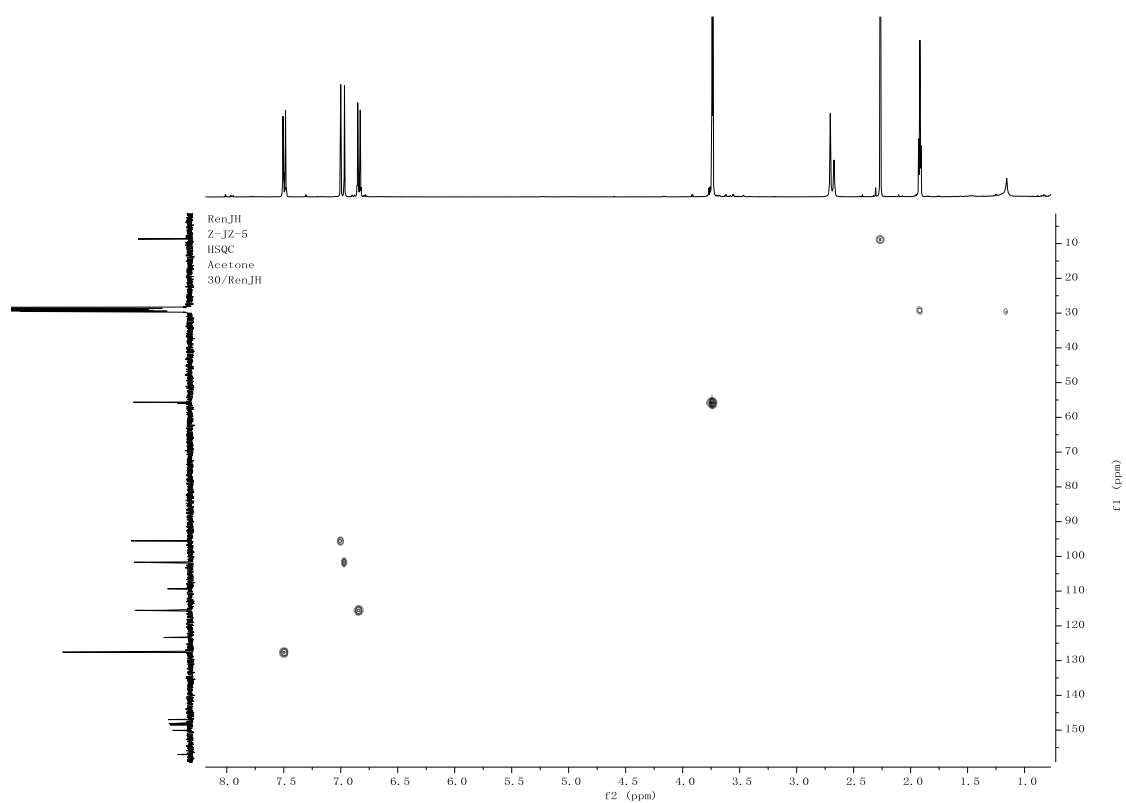


Figure S6: HMQC spectrum of **1** (Cochinfuran A)

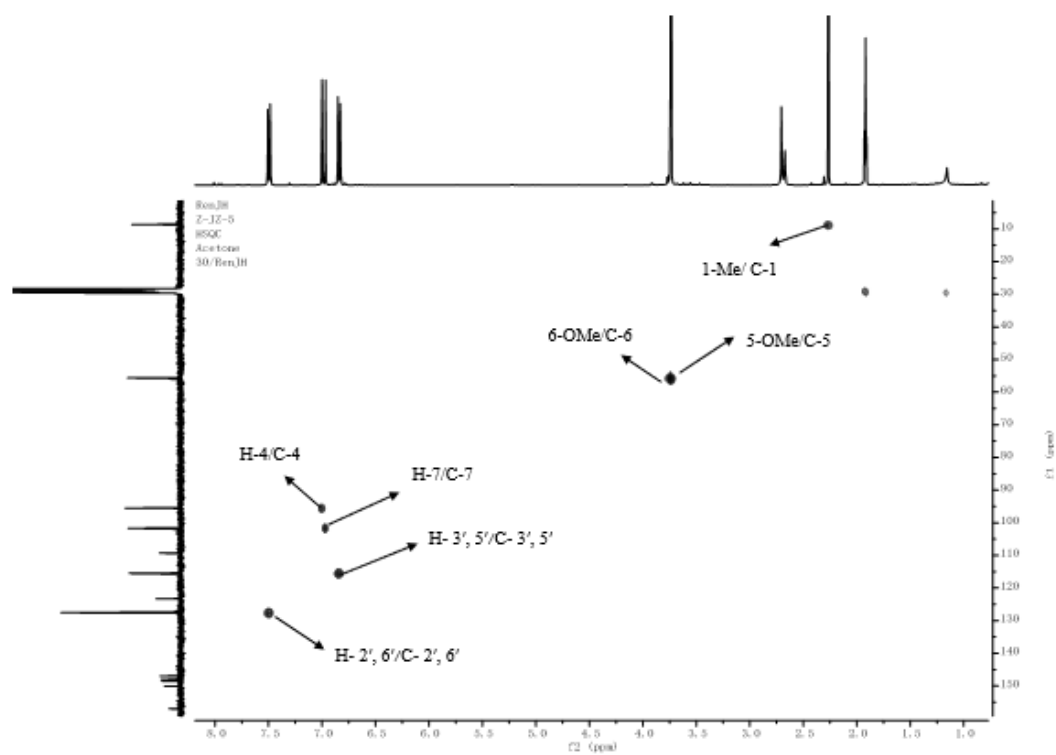


Figure S7: The labeled HMQC spectrum of compound **1**

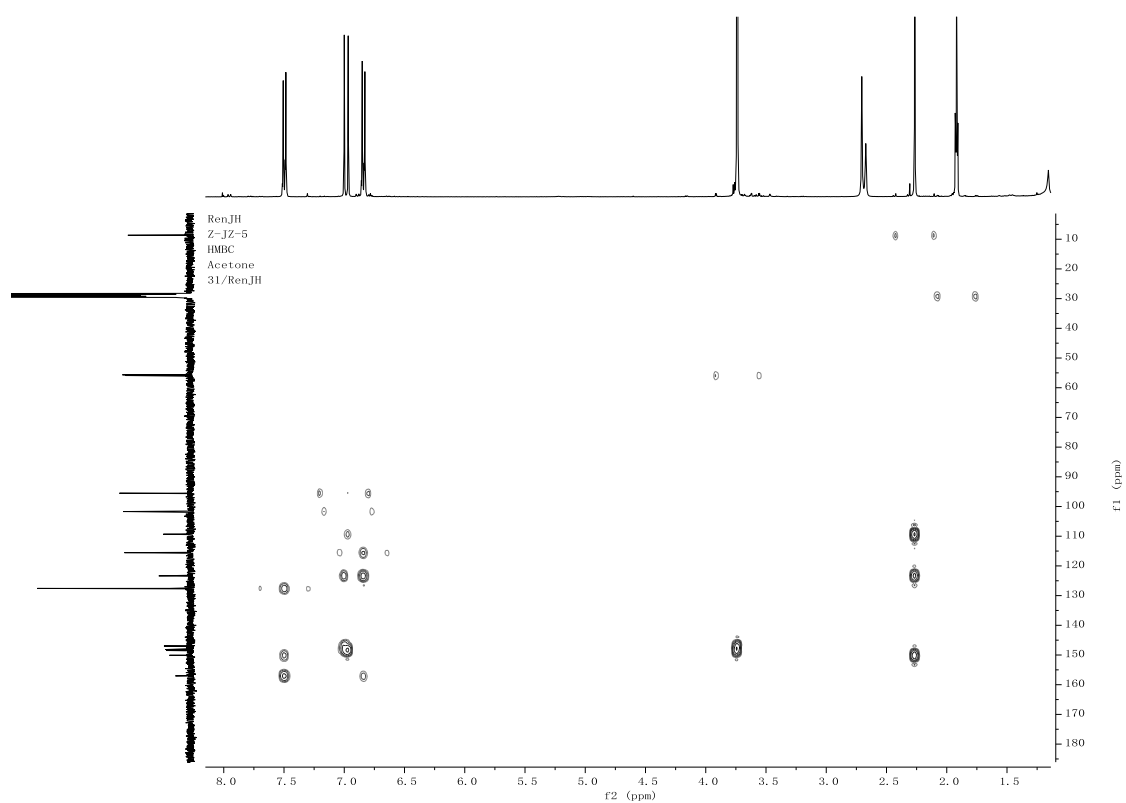


Figure S8: HMBC spectrum of **1** (Cochinfuran A)

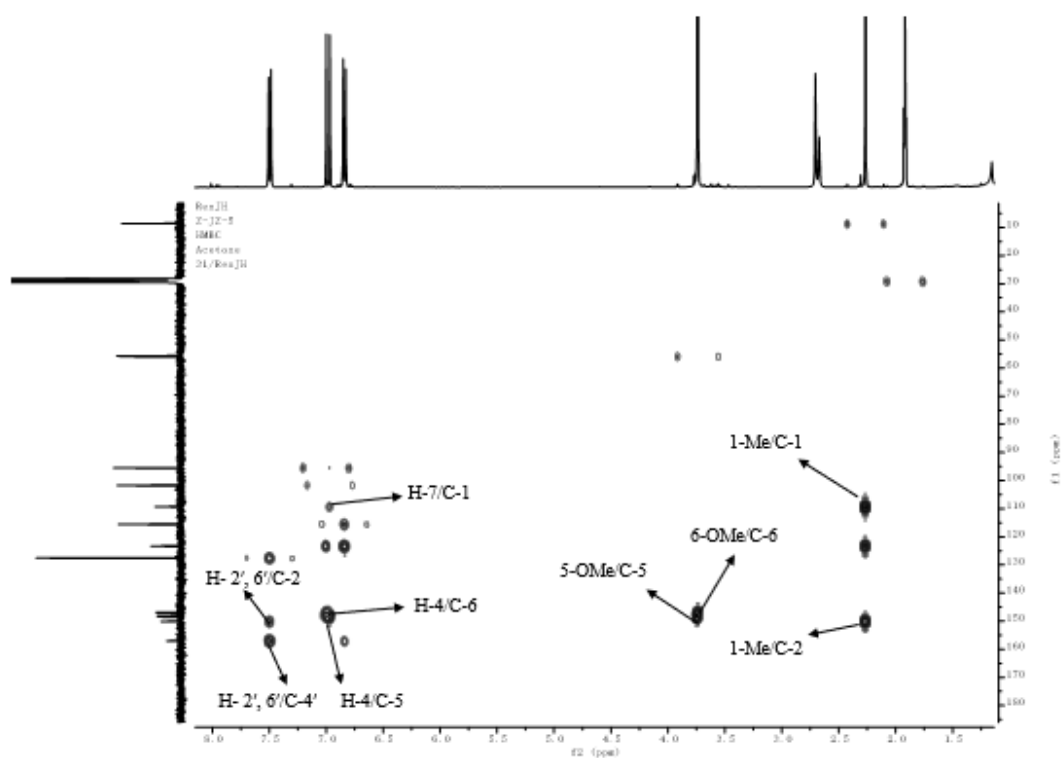


Figure S9: The labeled HMBC spectrum of compound **1**

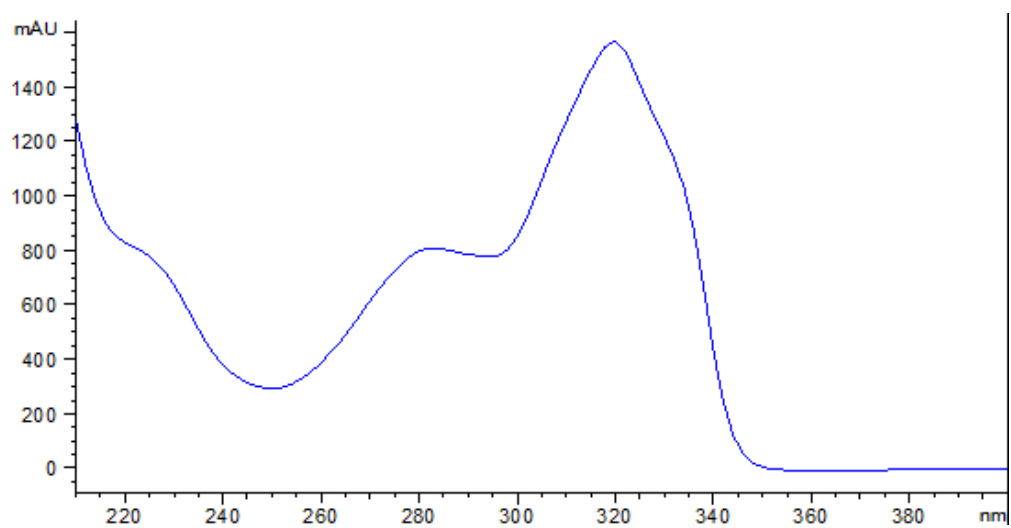


Figure S10: UV spectra of compound **1**

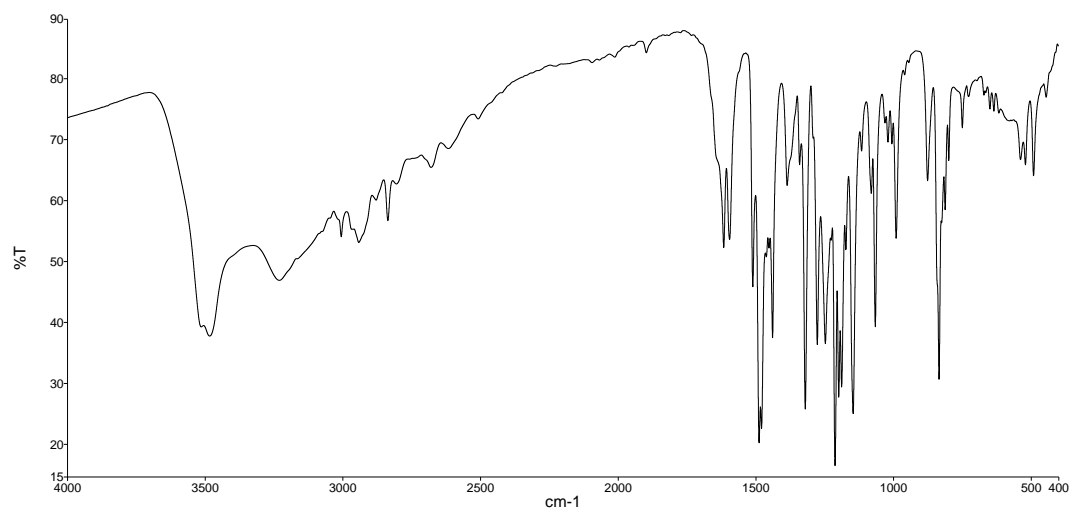


Figure S11: IR spectra of compound **1**

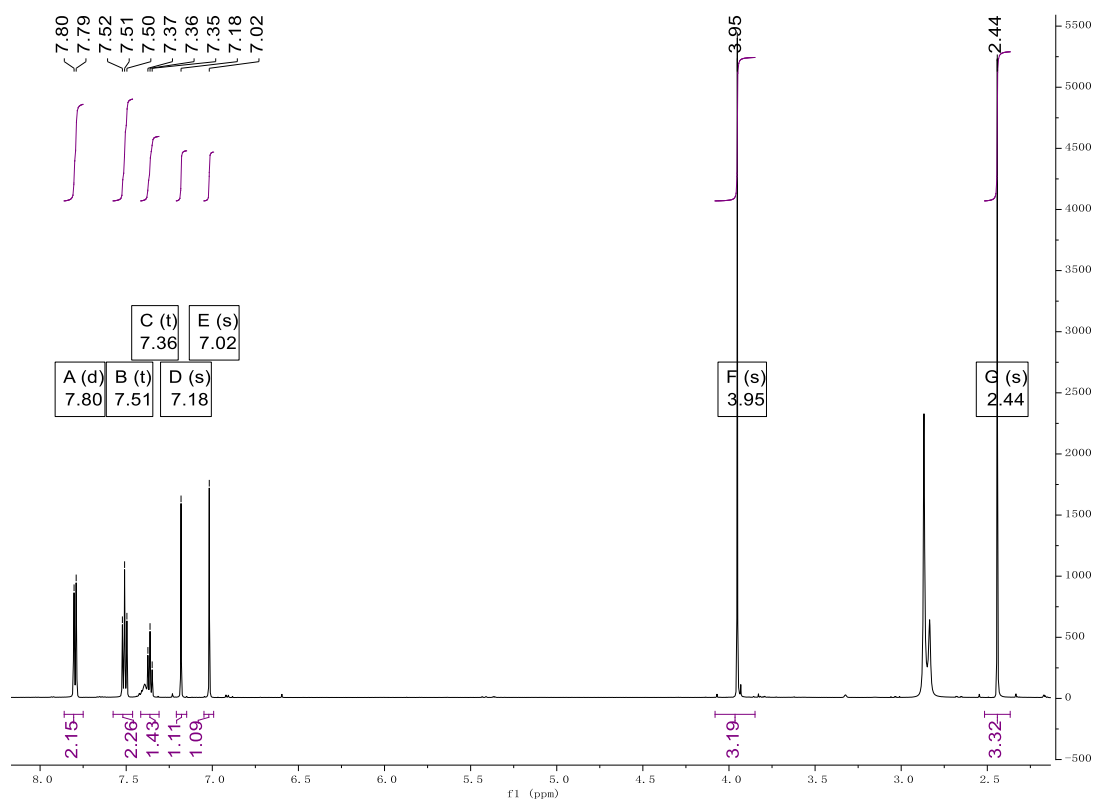


Figure S12: $^1\text{H-NMR}$ (600 MHz, Acetone- d_6) spectrum of **2**

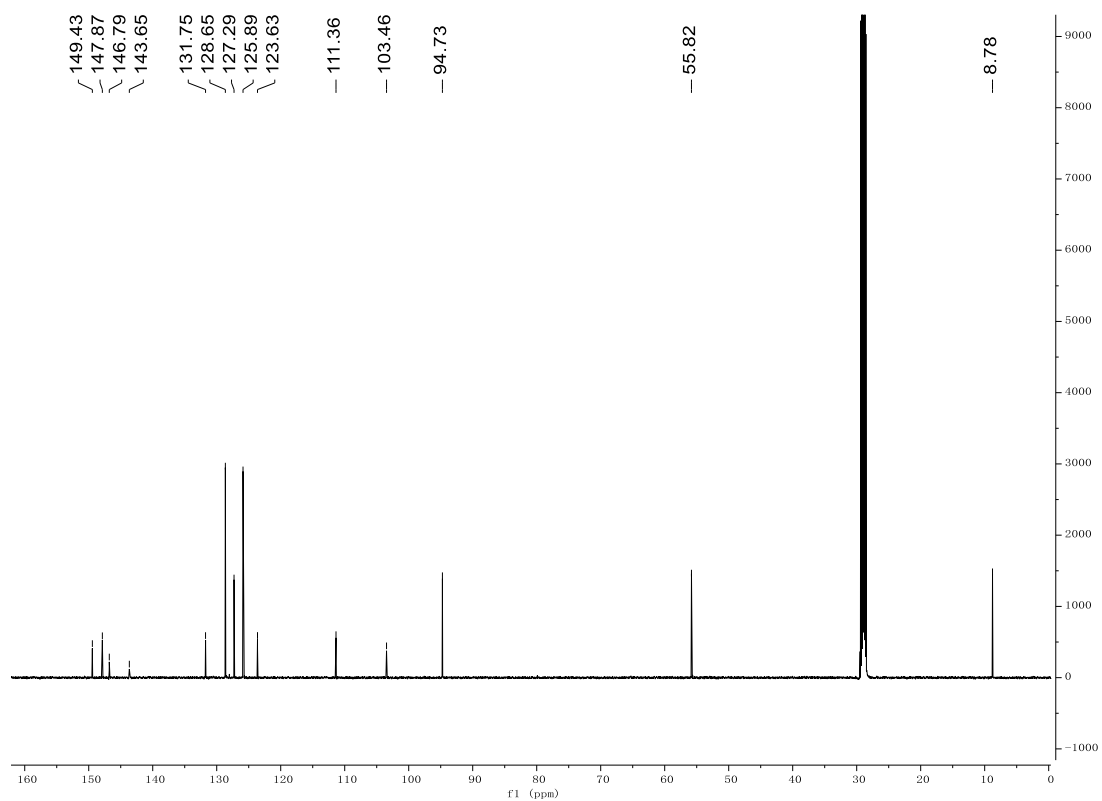


Figure S13: ^{13}C -NMR (151 MHz, Acetone- d_6) spectrum of **2**

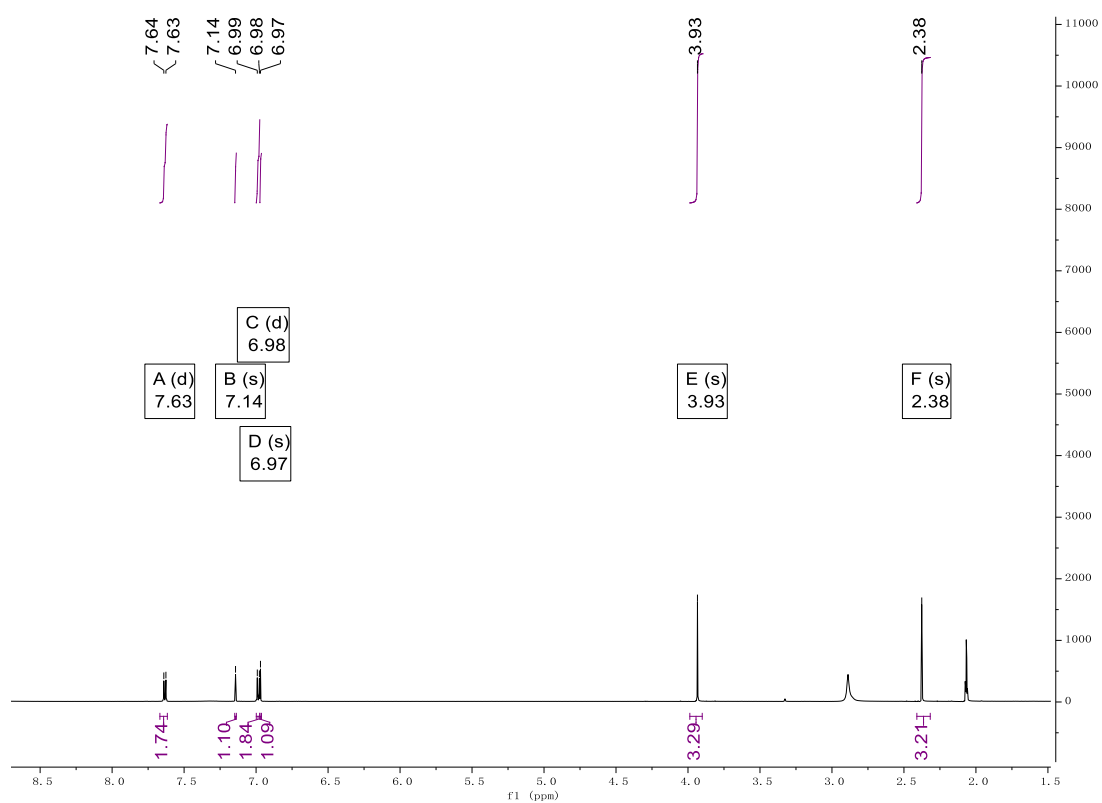


Figure S14: $^1\text{H-NMR}$ (600 MHz, $\text{Acetone-}d_6$) spectrum of **3**

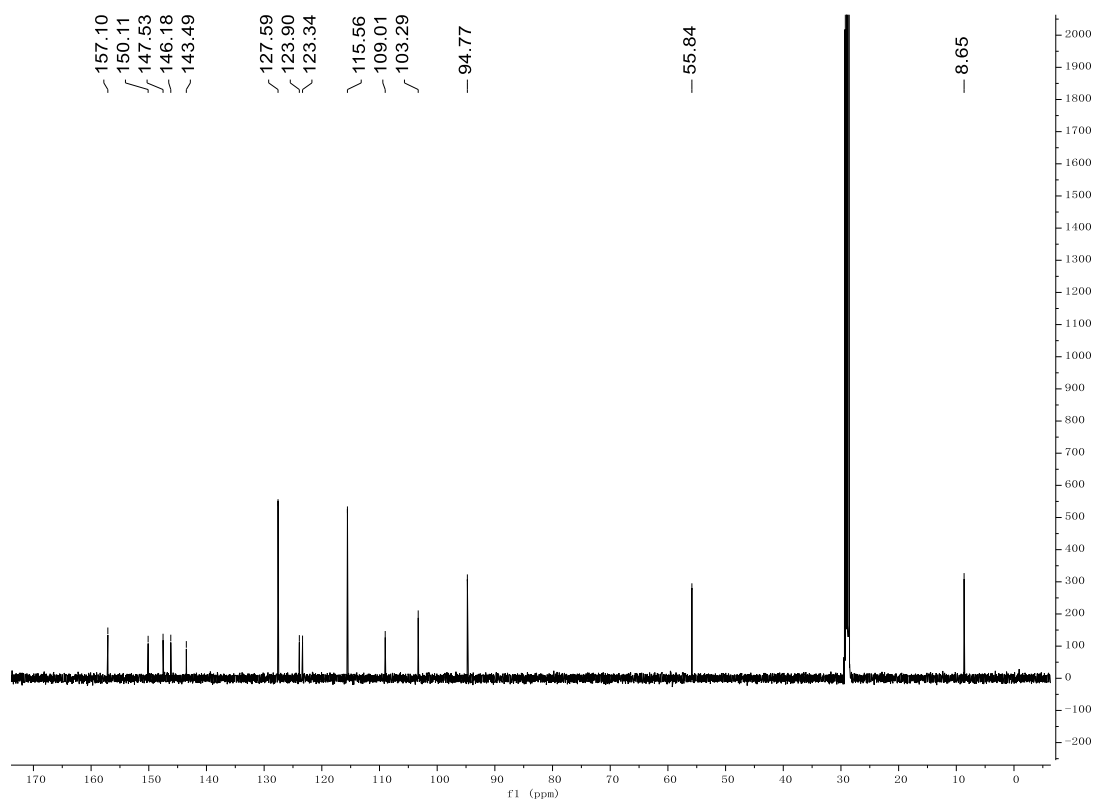


Figure S15: ^{13}C -NMR (151 MHz, Acetone- d_6) spectrum of **3**

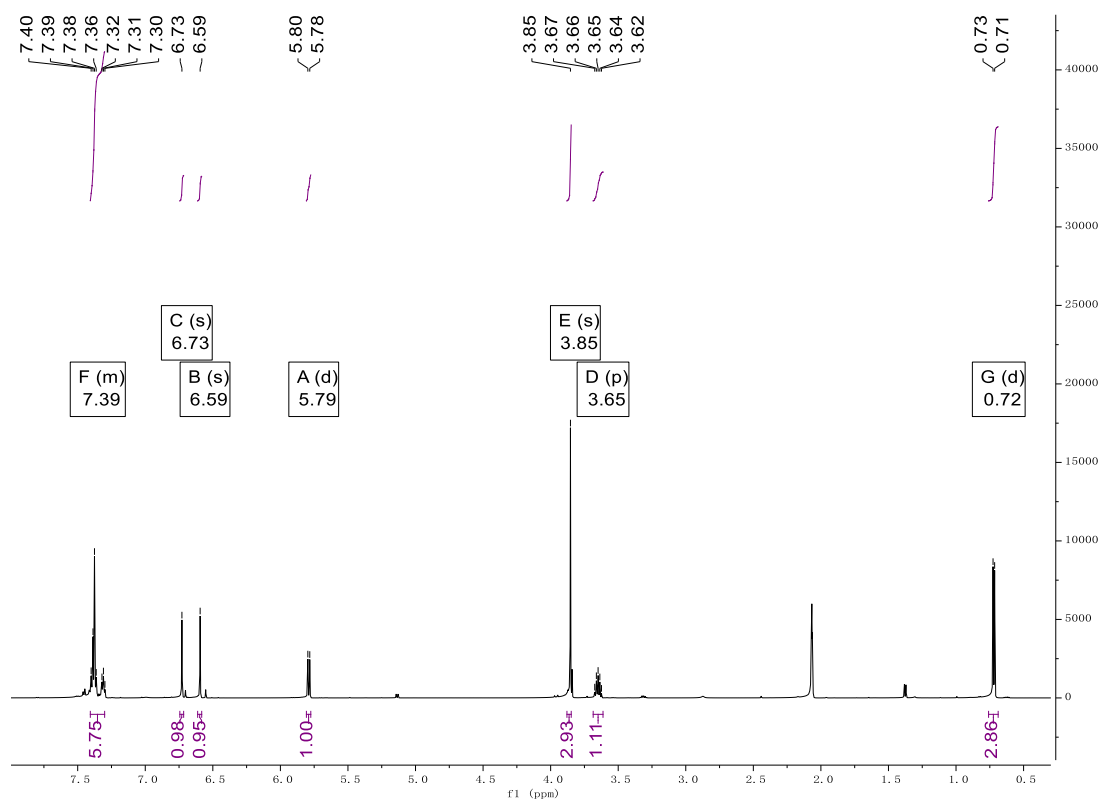


Figure S16: $^1\text{H-NMR}$ (600 MHz, $\text{Acetone-}d_6$) spectrum of **4**

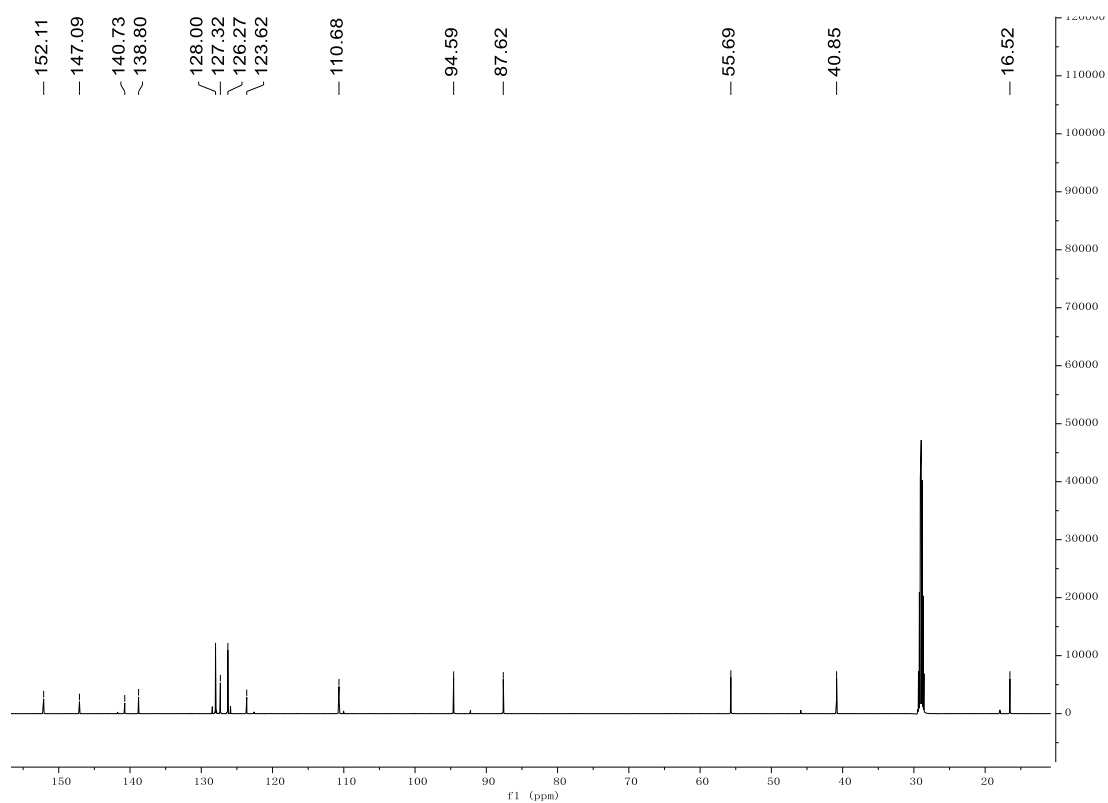


Figure S17: ^{13}C -NMR (151 MHz, Acetone- d_6) spectrum of **4**

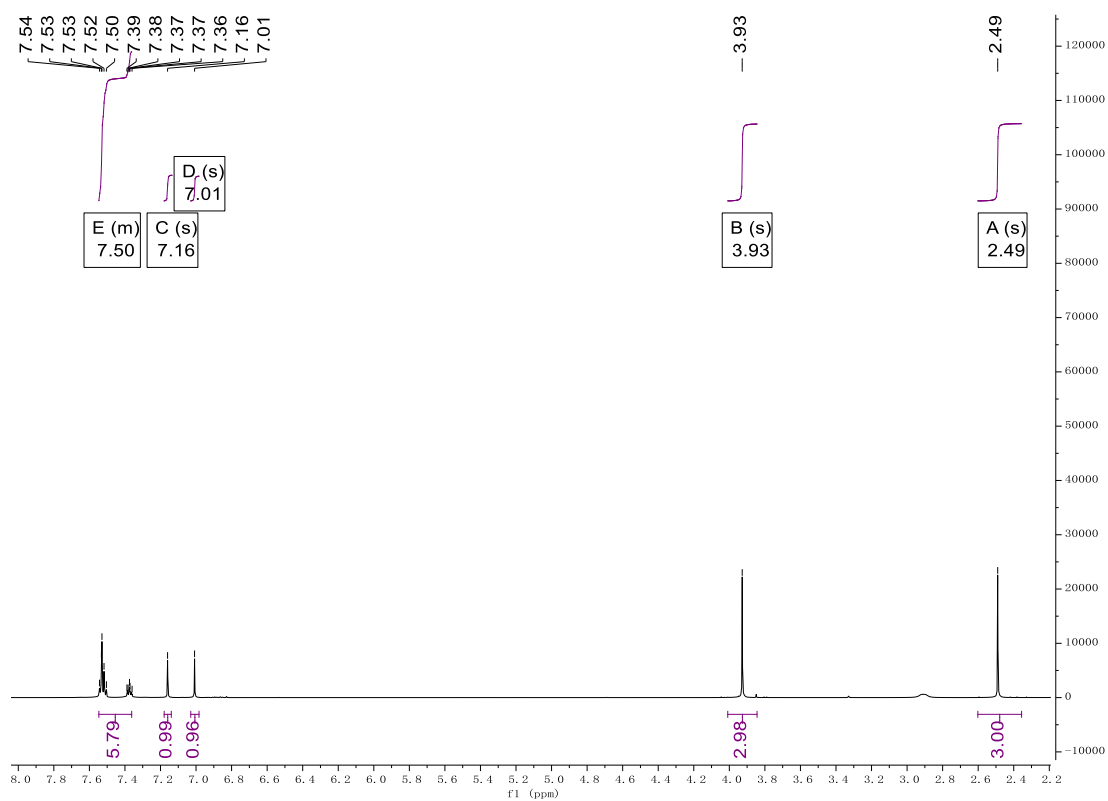


Figure S18: ¹H-NMR (600 MHz, Acetone-*d*₆) spectrum of **5**

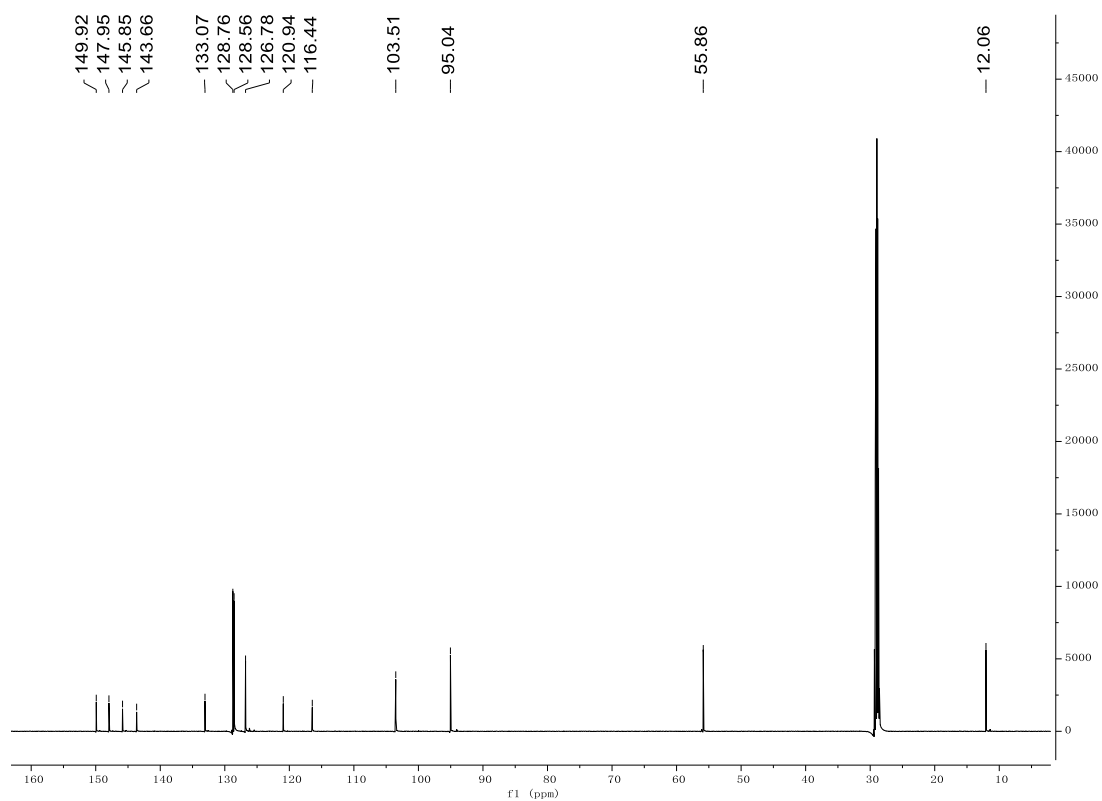
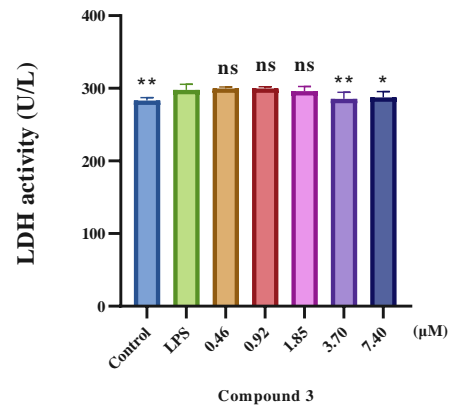
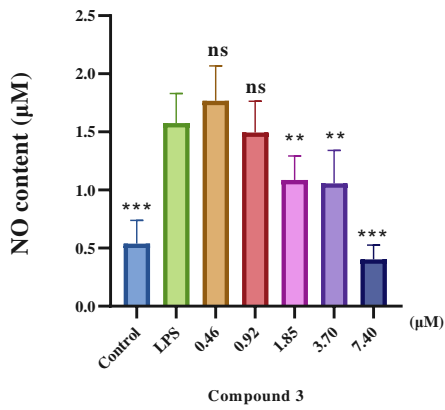
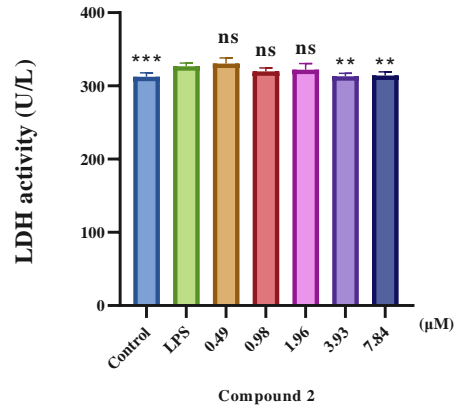
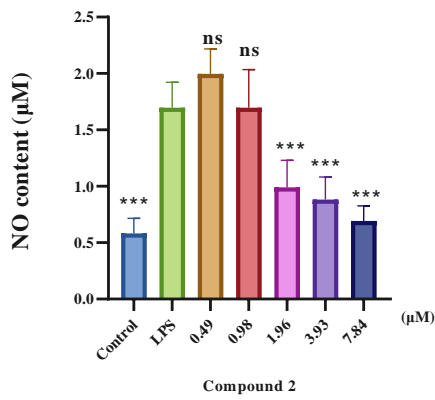
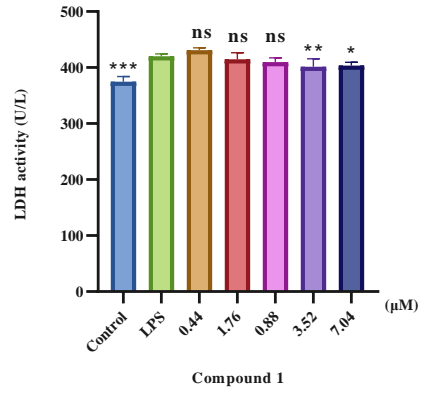
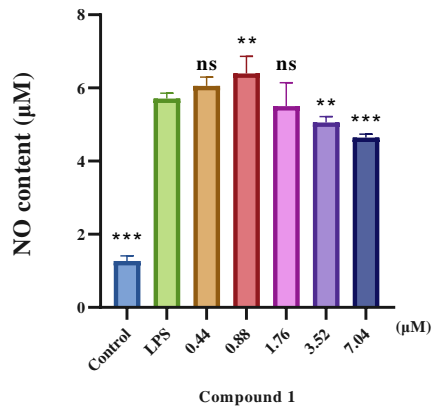


Figure S19: ^{13}C -NMR (151 MHz, Acetone- d_6) spectrum of **5**



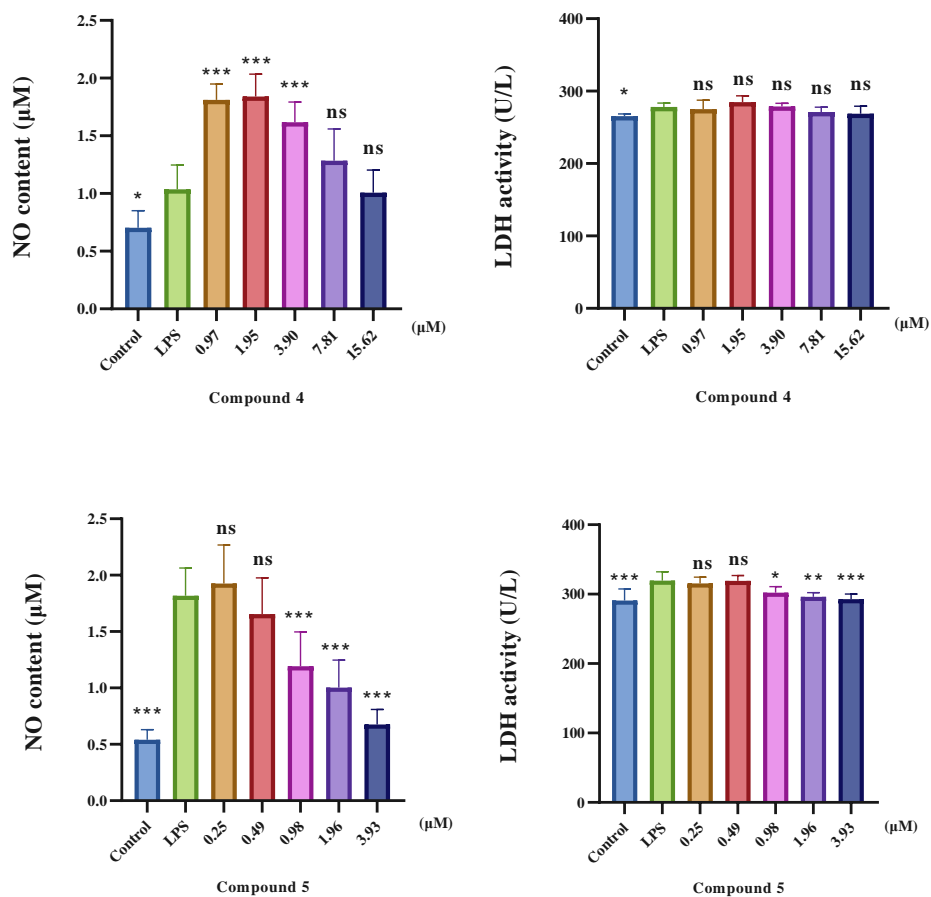


Figure S20: Effects of compounds on the production of NO and LDH in LPS-induced RAW 264.7 macrophages. The values shown represent the mean (n=6). * $P < 0.05$, ** $P < 0.01$, *** $P < 0.001$, compared to the LPS group.

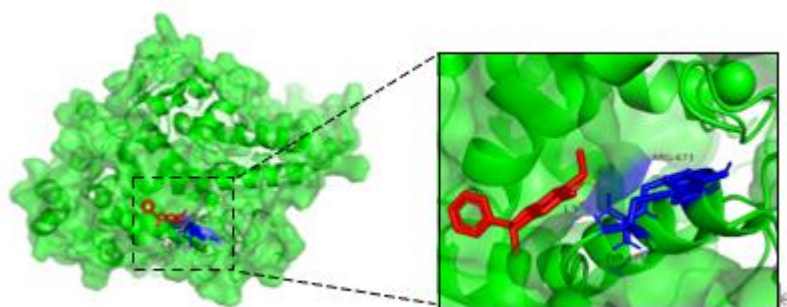


Figure 21: 3D visualization of the docking of compound 4 with MPO

Table S3. Docking scores of compounds 1-5 with protein

Compound		Total score					
Target spot	PLG	PSEN1	ADA	TERT	HDAC2	FGFR1	MPO
1	-5.27	-5.8	-6.25	-5.71	-5.17	-5.86	-7.97
2	-4.98	-5.48	-6.6	-5.65	-4.95	-5.99	-7.66
3	-4.94	-5.24	-6.9	-5.36	-5.96	-6.08	-8.63
4	-4.85	-5.32	-5.61	-5.35	-4.86	-5.83	-4.79
5	-5.19	-5.4	-6.81	-5.87	-4.53	-6.45	-7.89

Table S4. Annotation table

abbreviation	full name
NO	Nitric oxide
LDH	Lactate dehydrogenase
LPS	Lipopolysaccharide
PE	Petroleumether
CH ₂ Cl ₂	Pichloromethane
EtOAc	Ethyl acetate
n-BuOH	n-Butanol

Table S5. SciFinder report of compound 1

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<input checked="" type="checkbox"/> 95-98	2
<input type="checkbox"/> 90-94	9
<input type="checkbox"/> 85-89	46
<input type="checkbox"/> 80-84	210
<input type="checkbox"/> 75-79	727
<input type="checkbox"/> 70-74	2750
<input type="checkbox"/> 65-69	9371
<input type="checkbox"/> 0-64 (least similar)	25339

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