Supporting Information

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

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

Qiwan Zheng [1], Chan yue Ouyang [2], Yang Liu [1], Jiahui Ren [1], Xianwen Wei [1], Ronghua Liu [1*] and Lanying Chen [2*]

[1]School of Pharmacy, Jiangxi University of Chinese Medicine, Nanchang, 330004, China
[2]National Pharmaceutical Engineering Center for Solid Preparation of Chinese Herbal Medicine, Jiangxi University of Chinese Medicine, Nanchang, 330006, China

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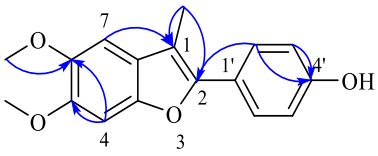
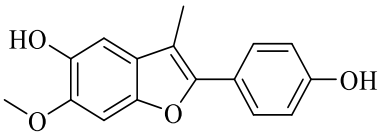


Compound **1**



pterolinus B

HMBC

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	-	-

[a]Measured in Acetone-d_6.-600 MHz

[b]Measured 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

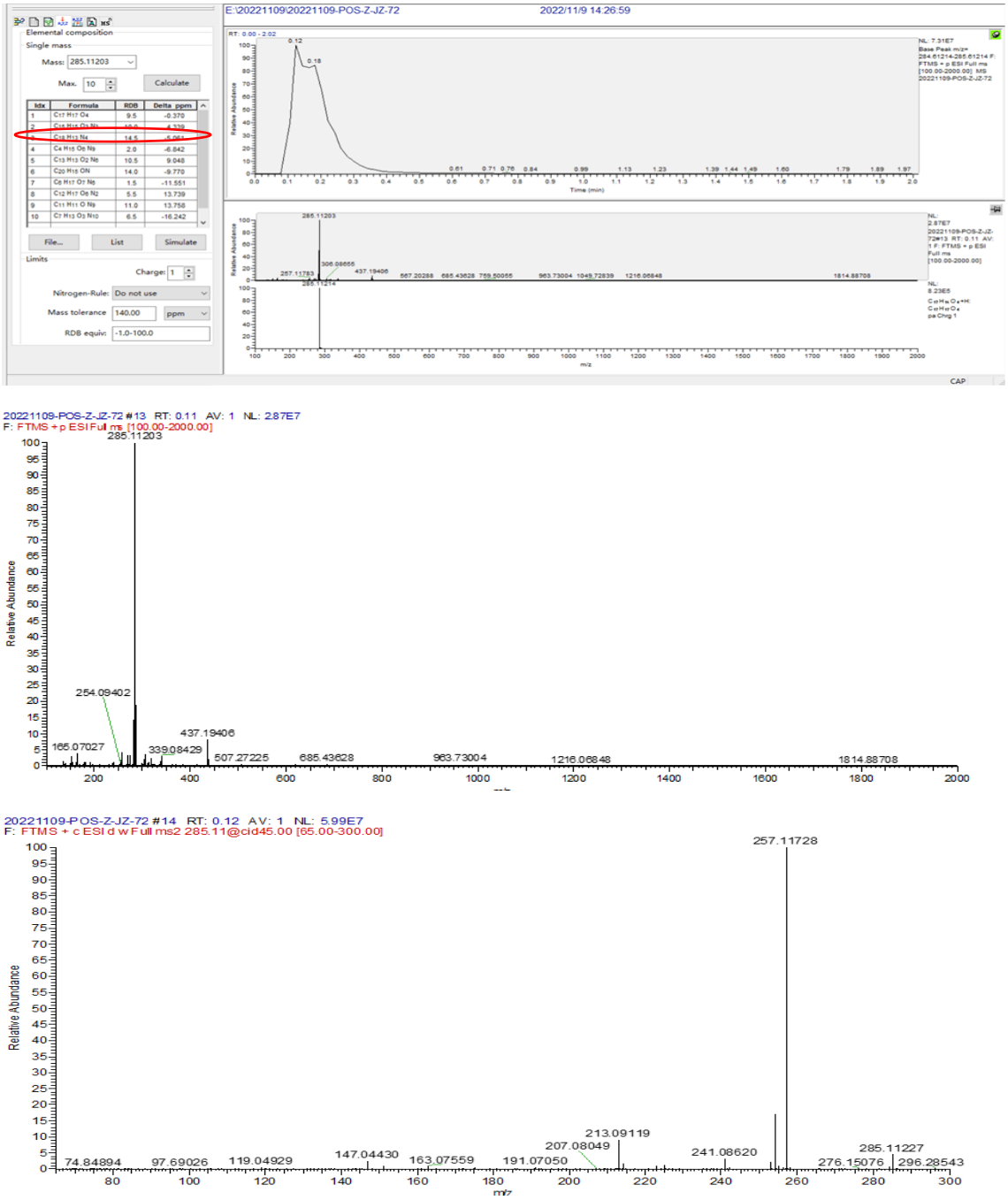


Figure S1: HR-ESI-MS spectrum of compound **1**

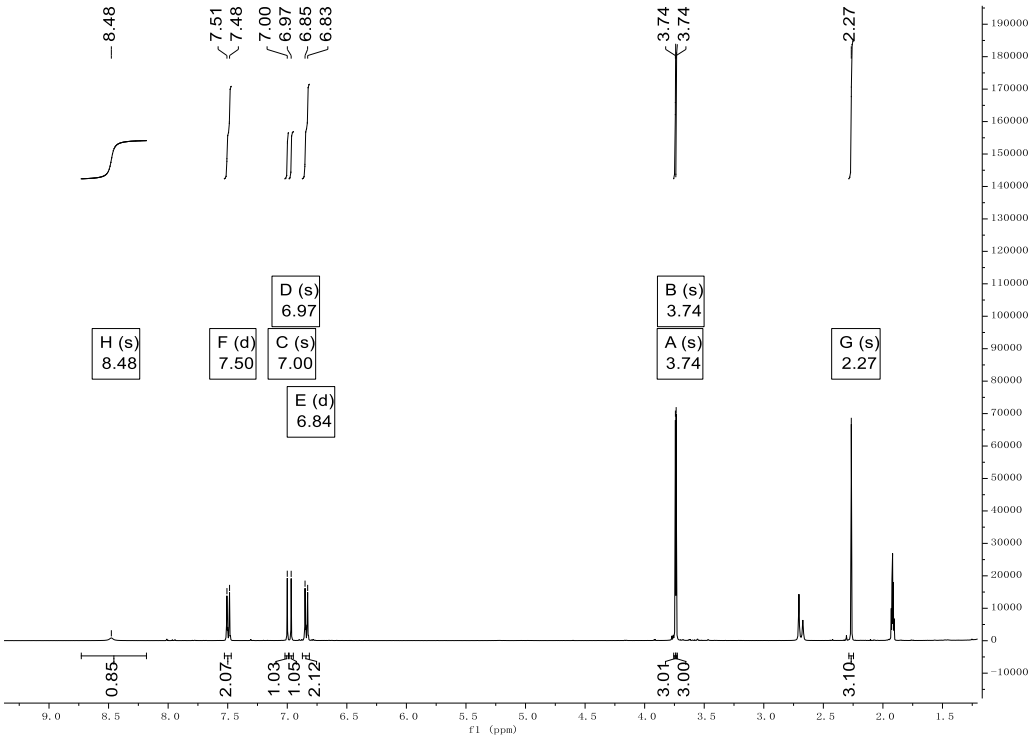


Figure S2: ^{1}H-NMR (600 MHz, Acetone-d_6) spectrum of **1** (Cochinfuran A)

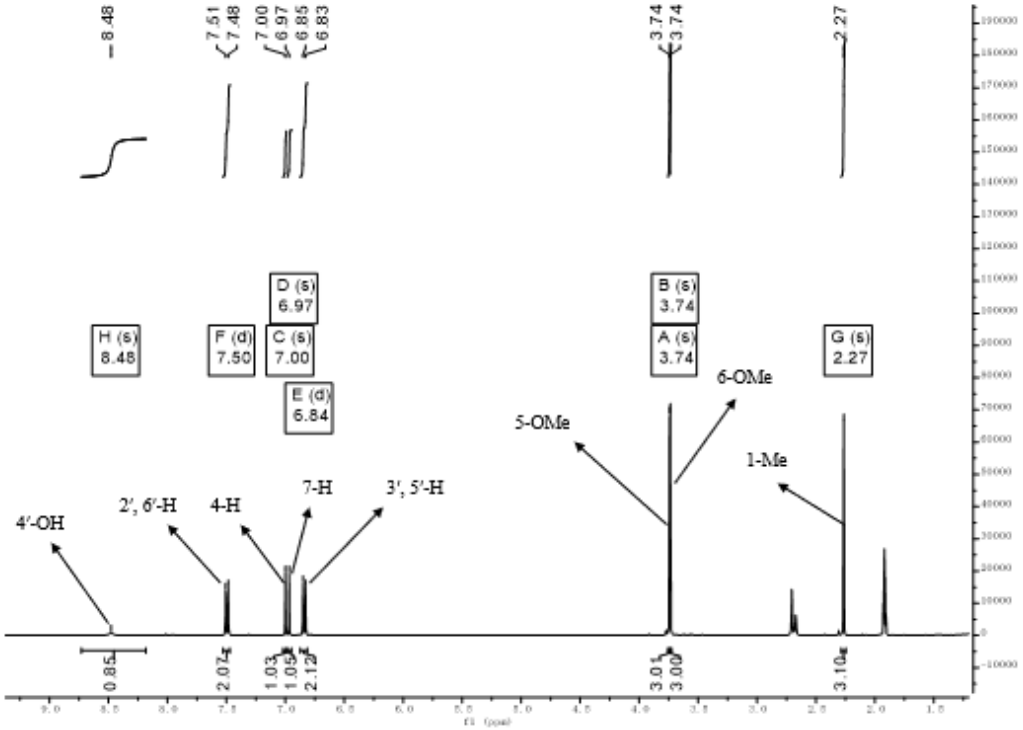


Figure S3: The labeled ^{1}H-NMR spectrum of compound **1**

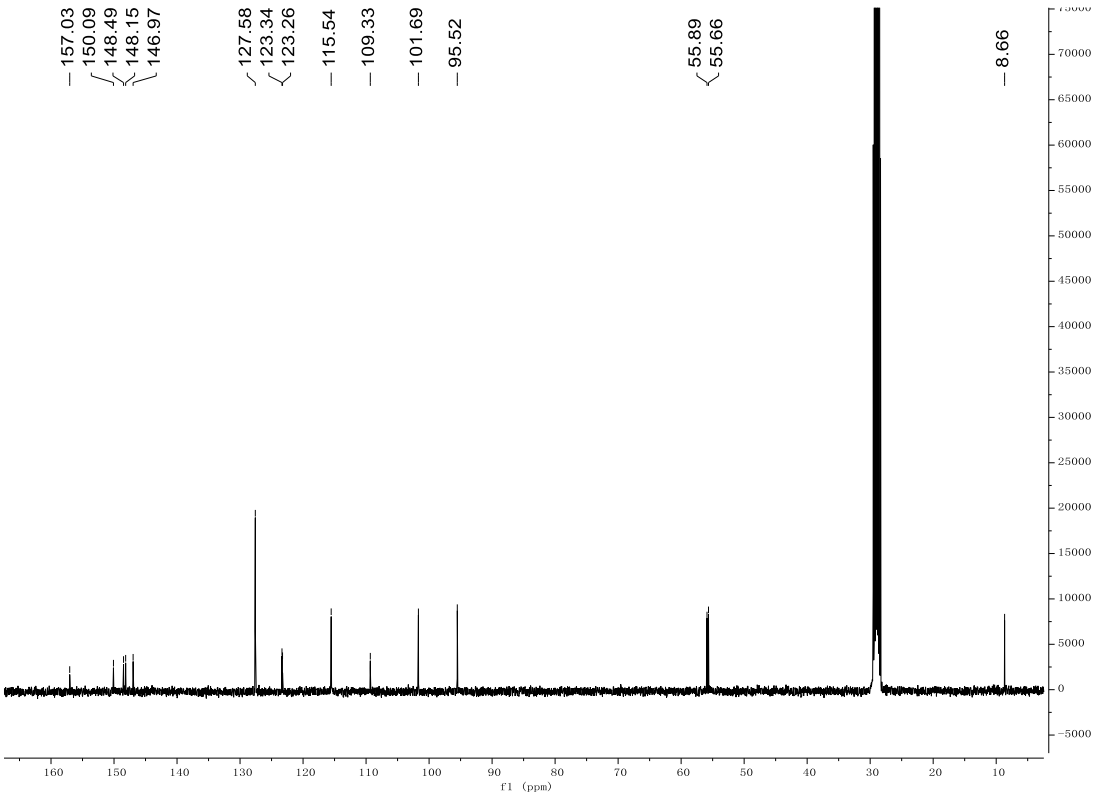


Figure S4: ^{13}C-NMR (151 MHz, Acetone-d_6) spectrum of **1** (Cochinfuran A)

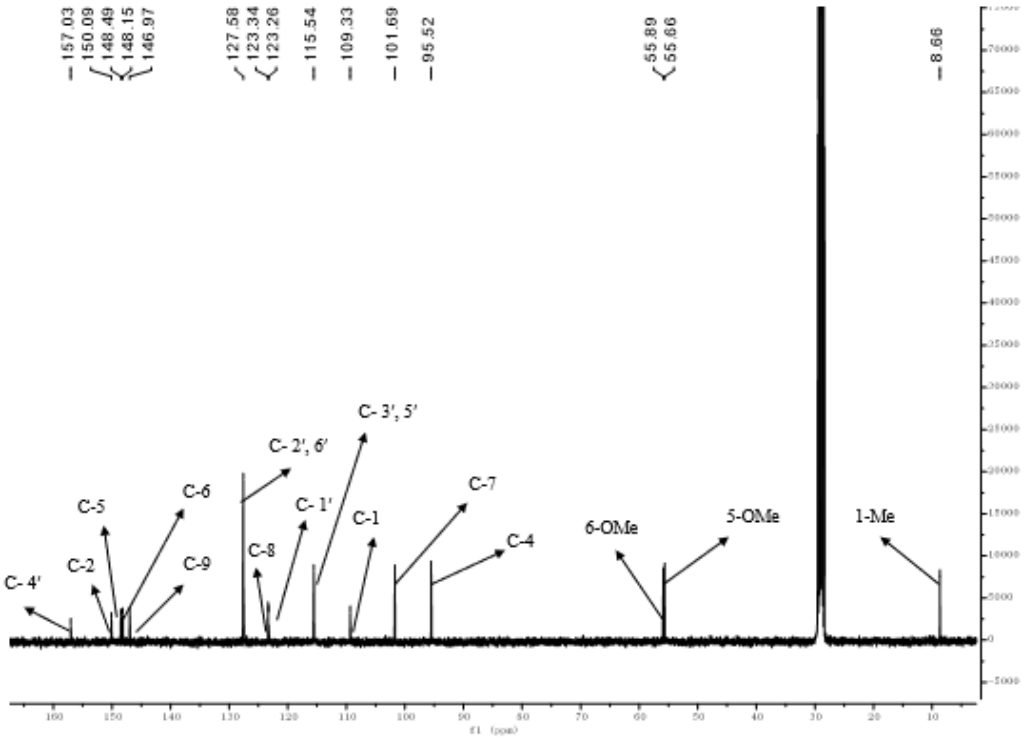


Figure S5: The labeled ^{13}C-NMR spectrum of compound **1**

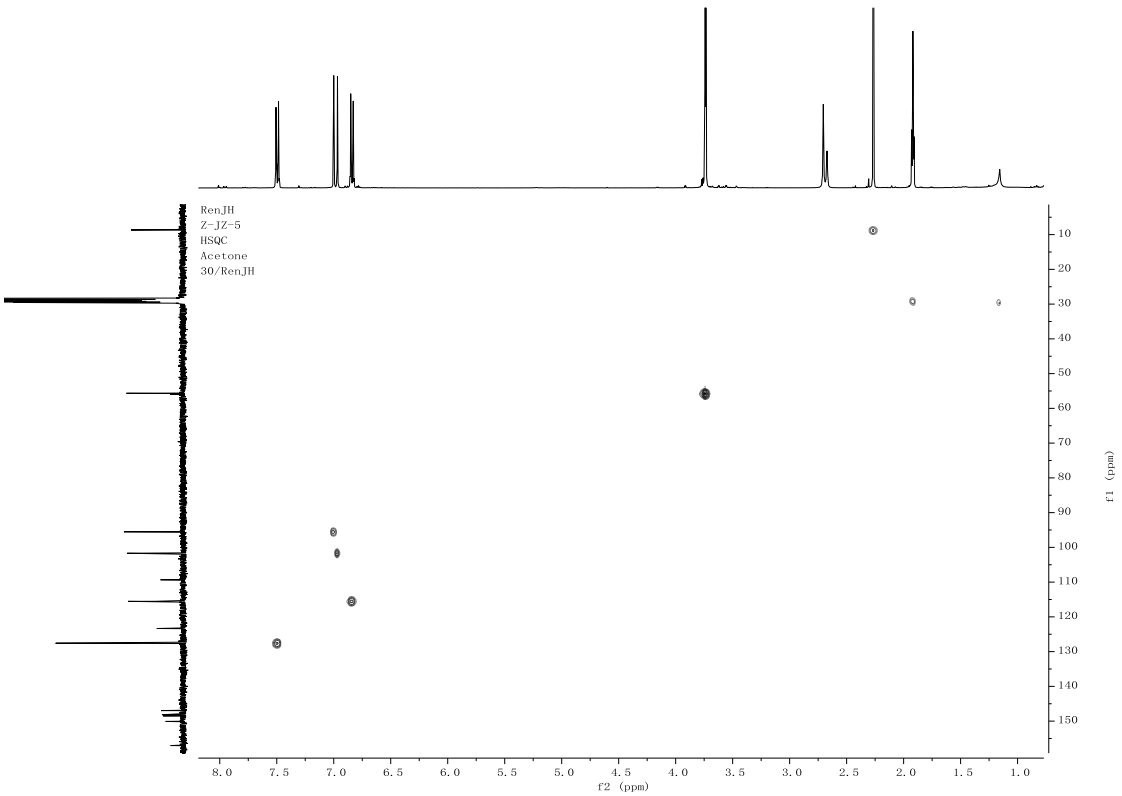


Figure S6: HMQC spectrum of **1** (Cochinfuran A)

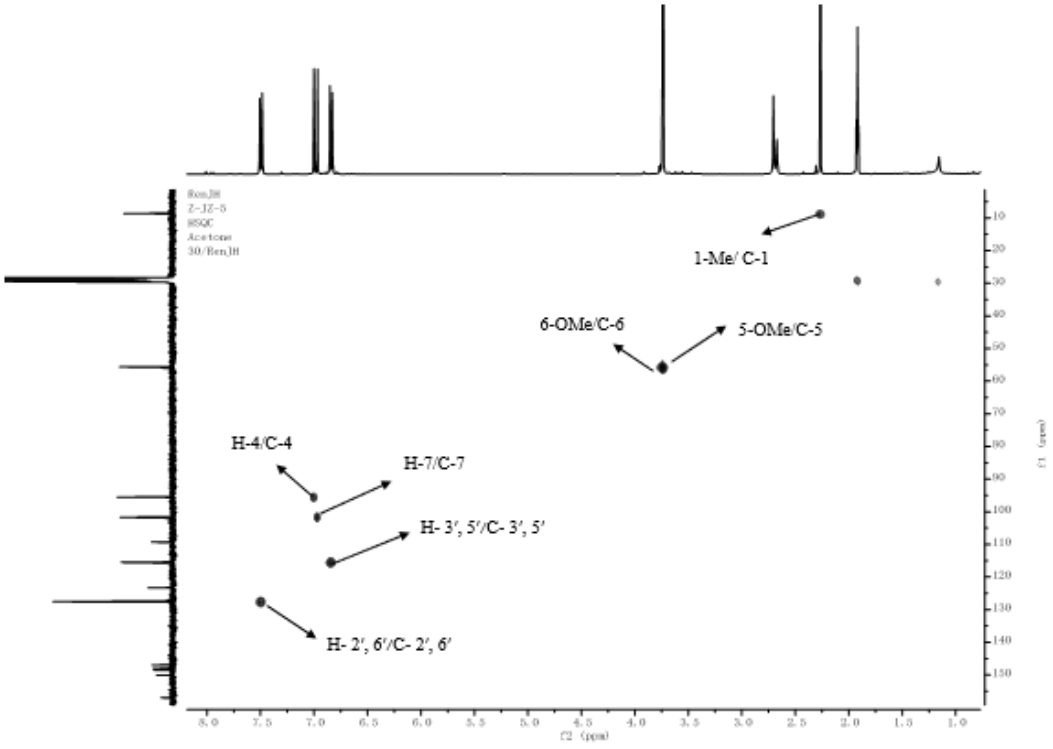


Figure S7: The labeled HMQC spectrum of compound **1**

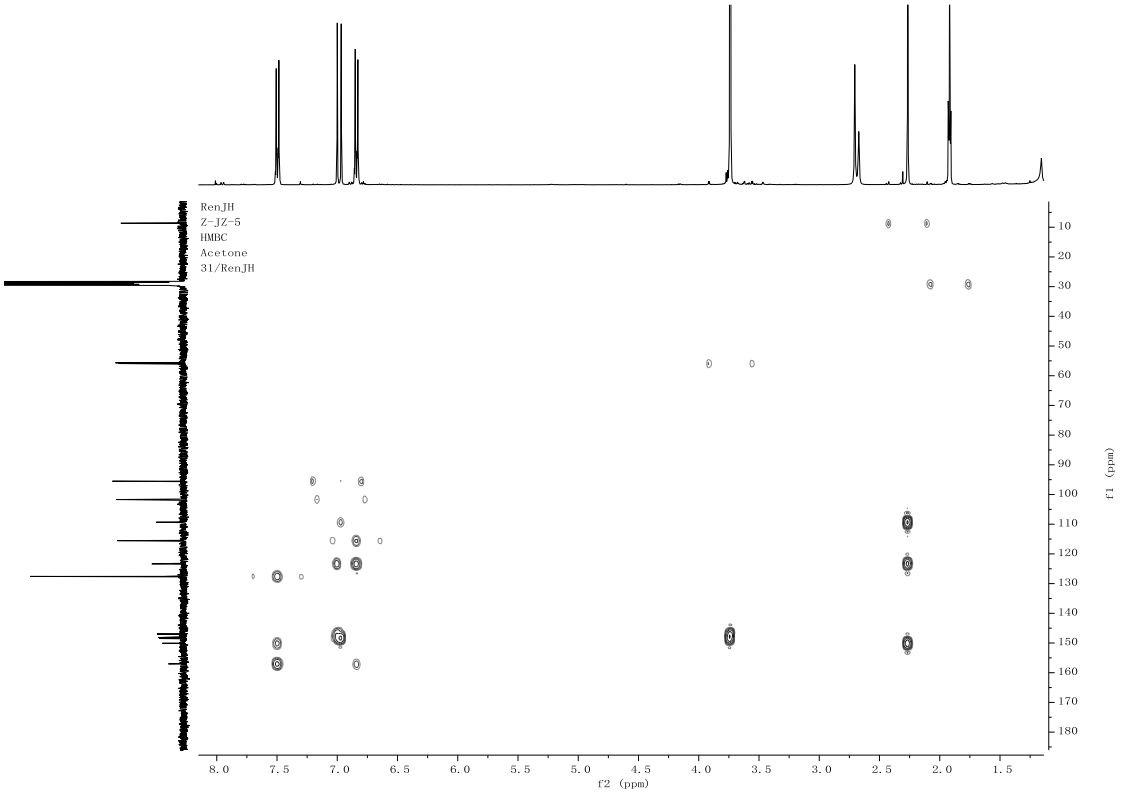


Figure S8: HMBC spectrum of **1** (Cochinfuran A)

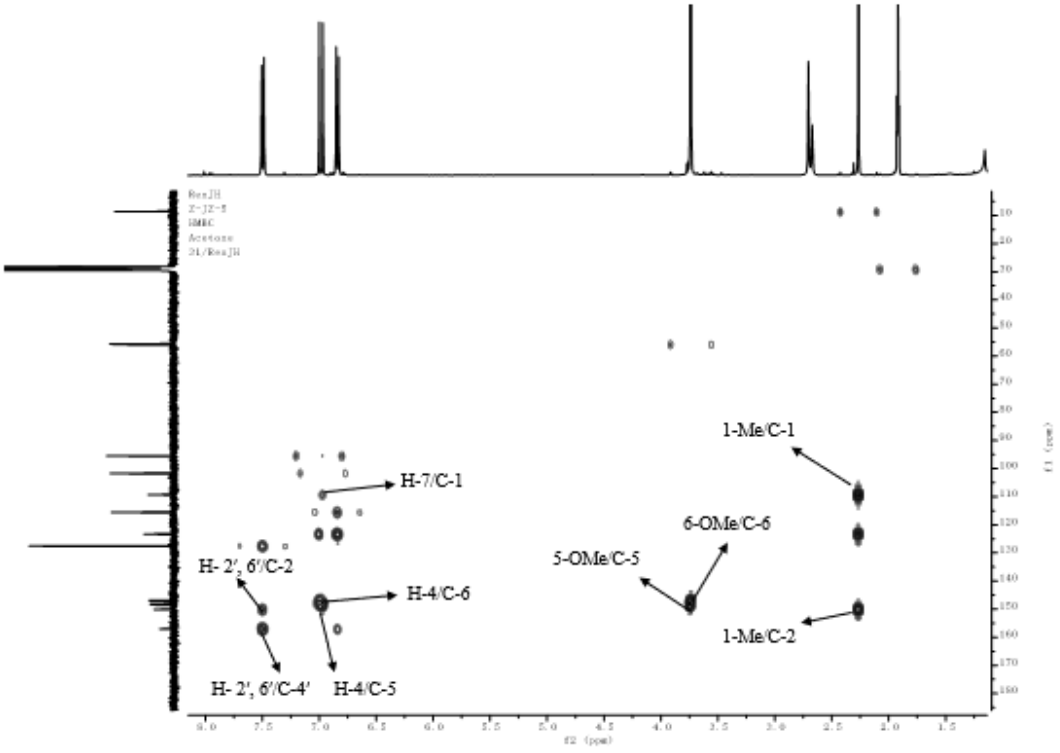


Figure S9: The labeled HMBC spectrum of compound **1**

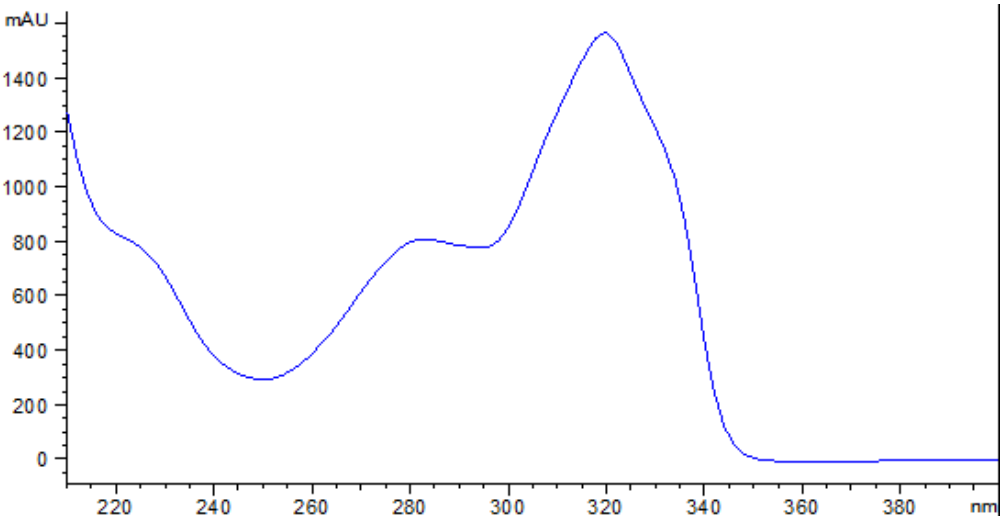


Figure S10: UV spectra of compound **1**

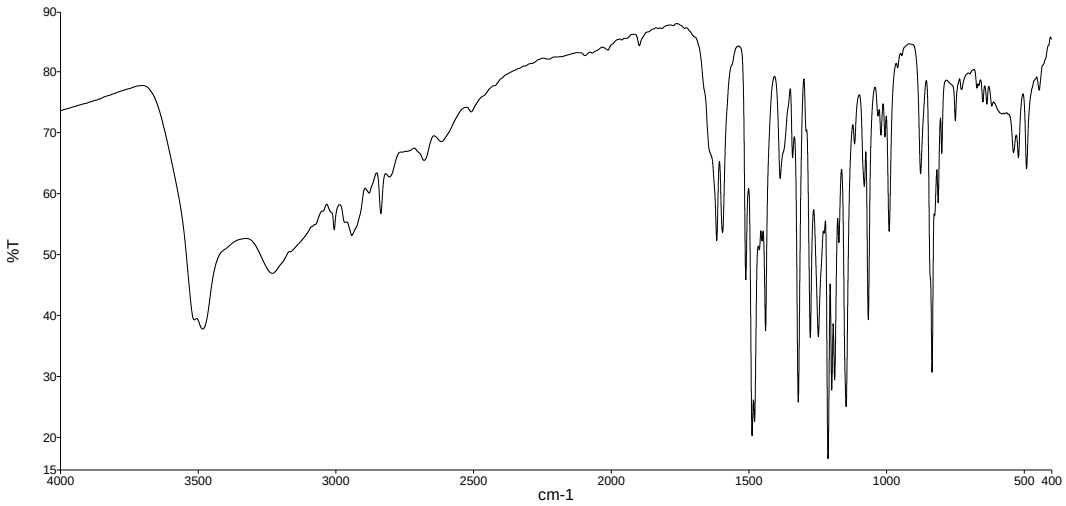


Figure S11: IR spectra of compound **1**

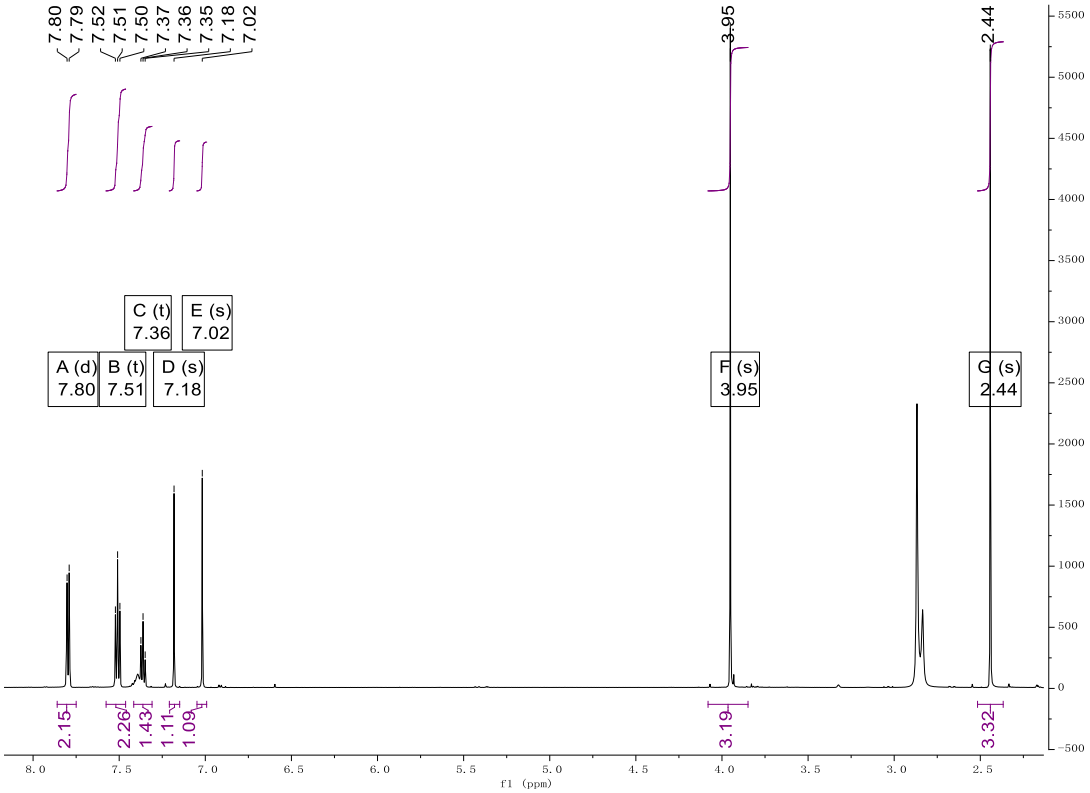


Figure S12: ^{1}H-NMR (600 MHz, Acetone-d_6) spectrum of **2**

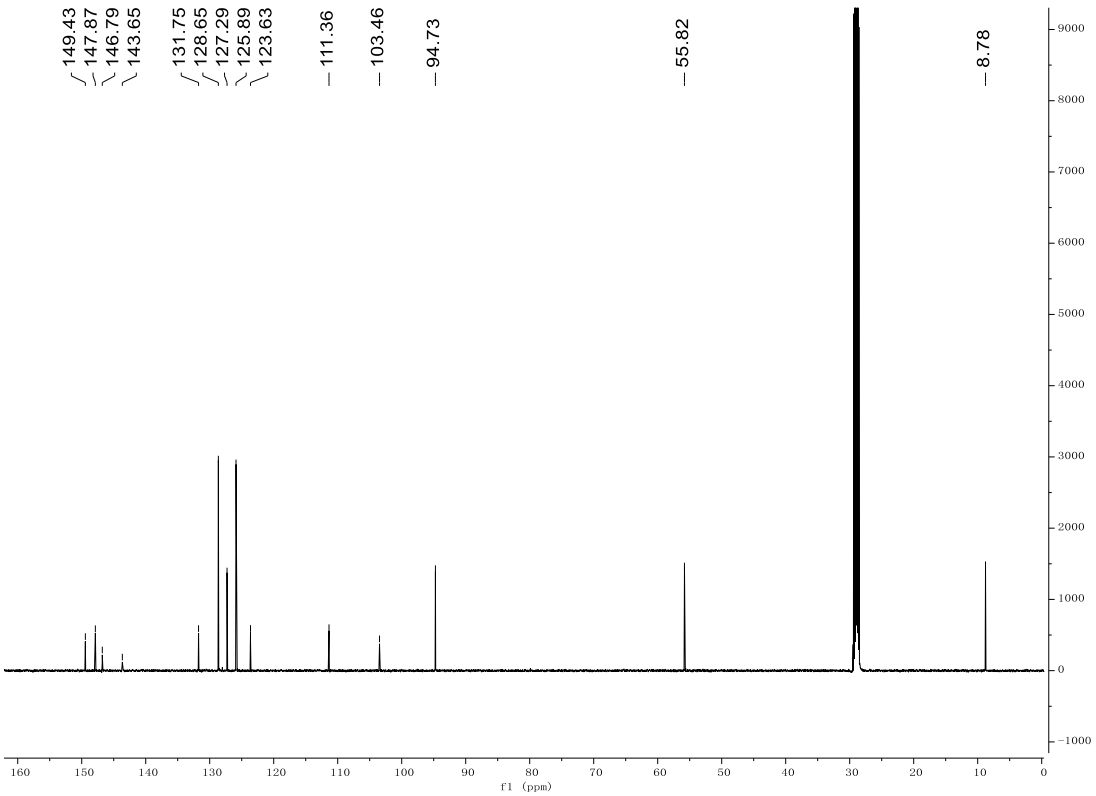


Figure S13: ^{13}C-NMR (151 MHz, Acetone-d_6) spectrum of **2**

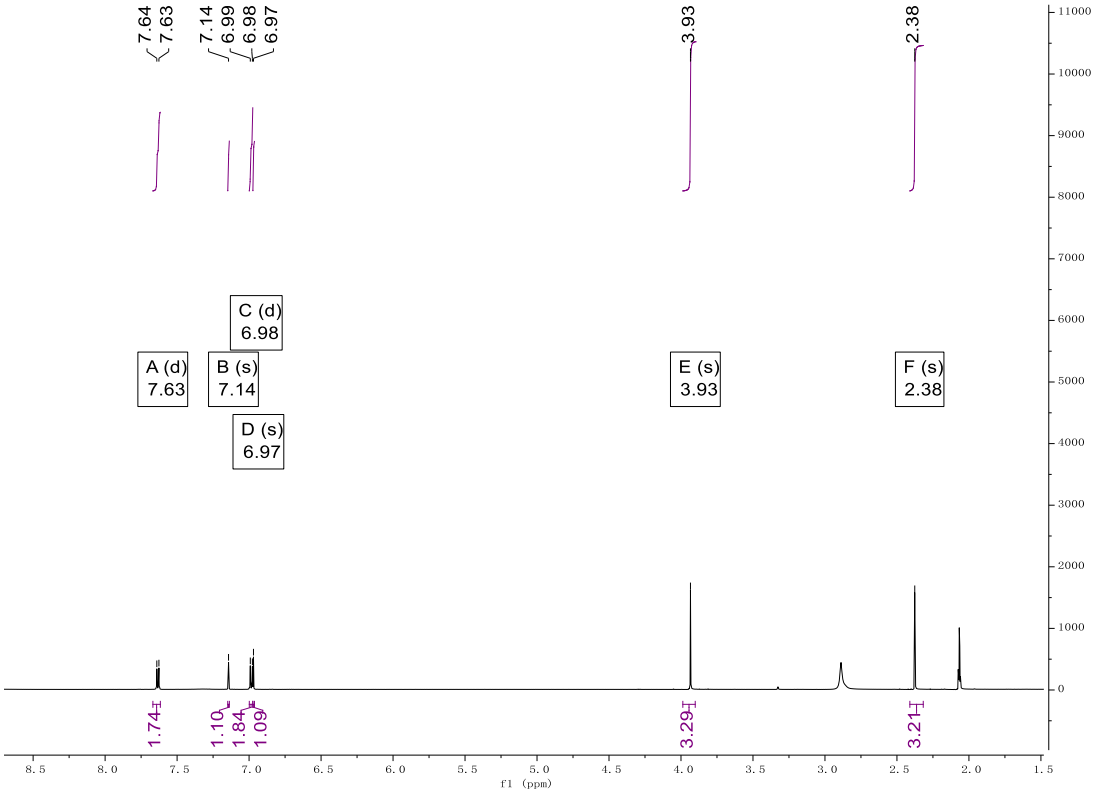


Figure S14: ^{1}H-NMR (600 MHz, Acetone-d_6) spectrum of **3**

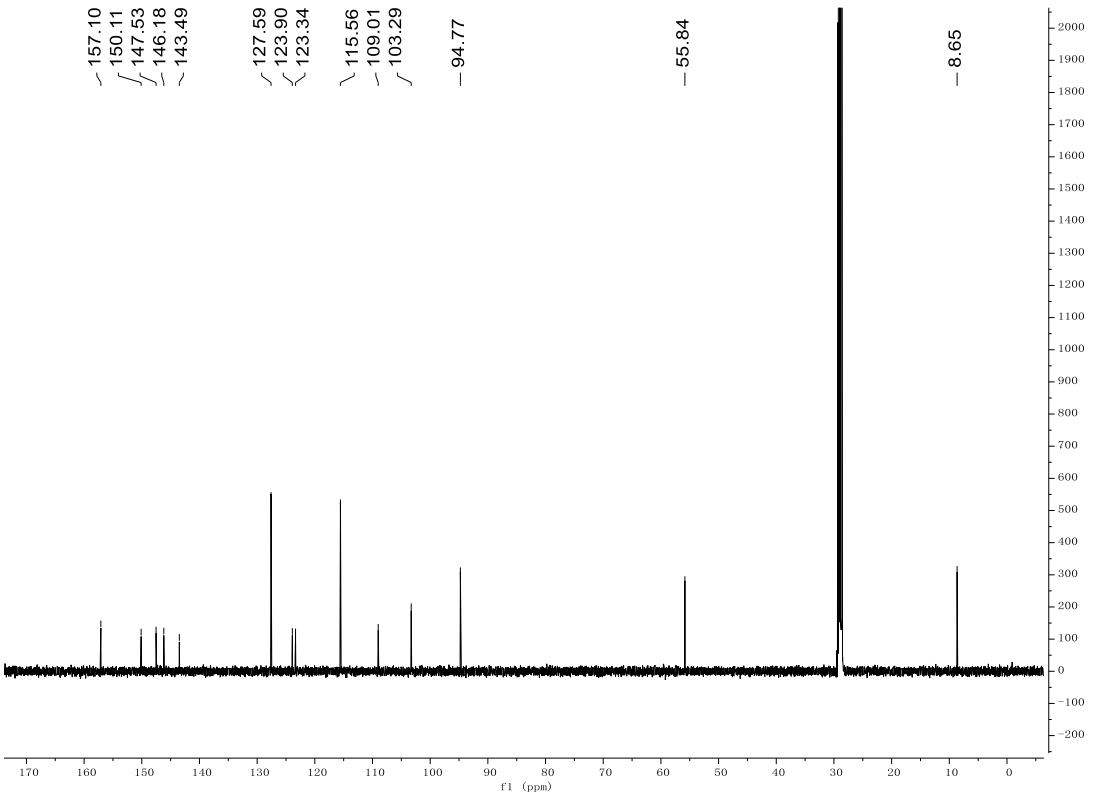


Figure S15: ^{13}C-NMR (151 MHz, Acetone-d_6) spectrum of **3**

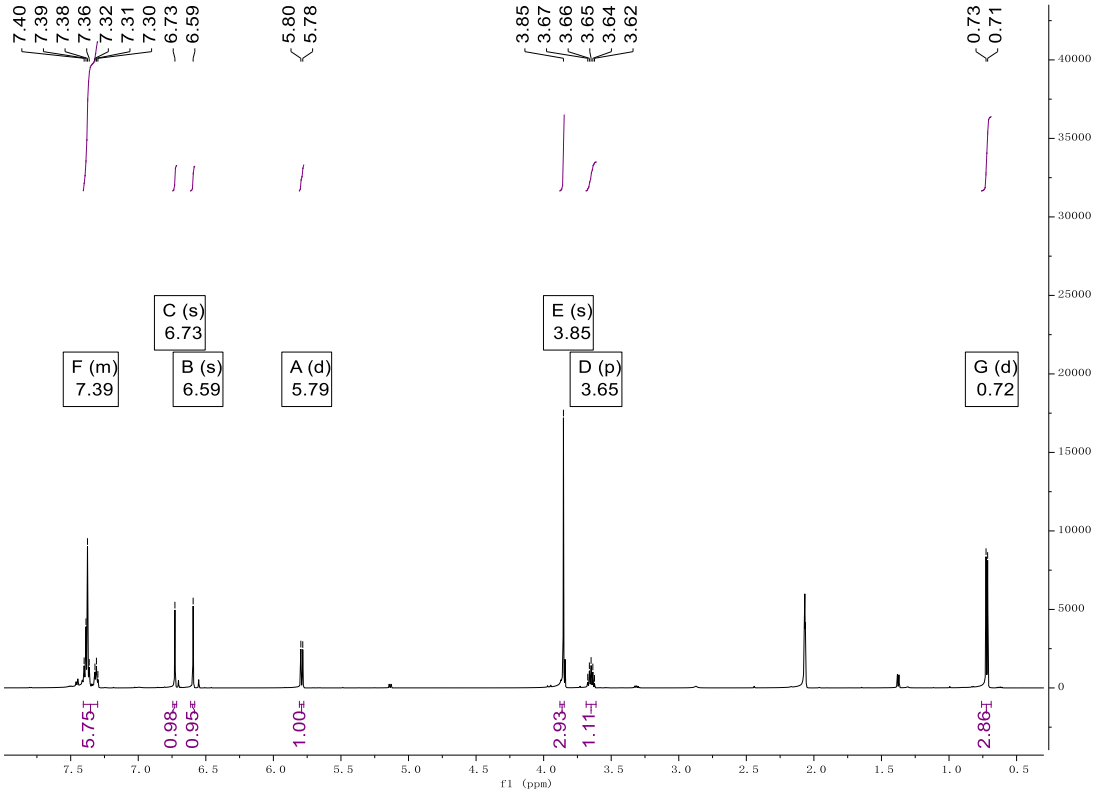


Figure S16: ^{1}H-NMR (600 MHz, Acetone-d_6) spectrum of **4**

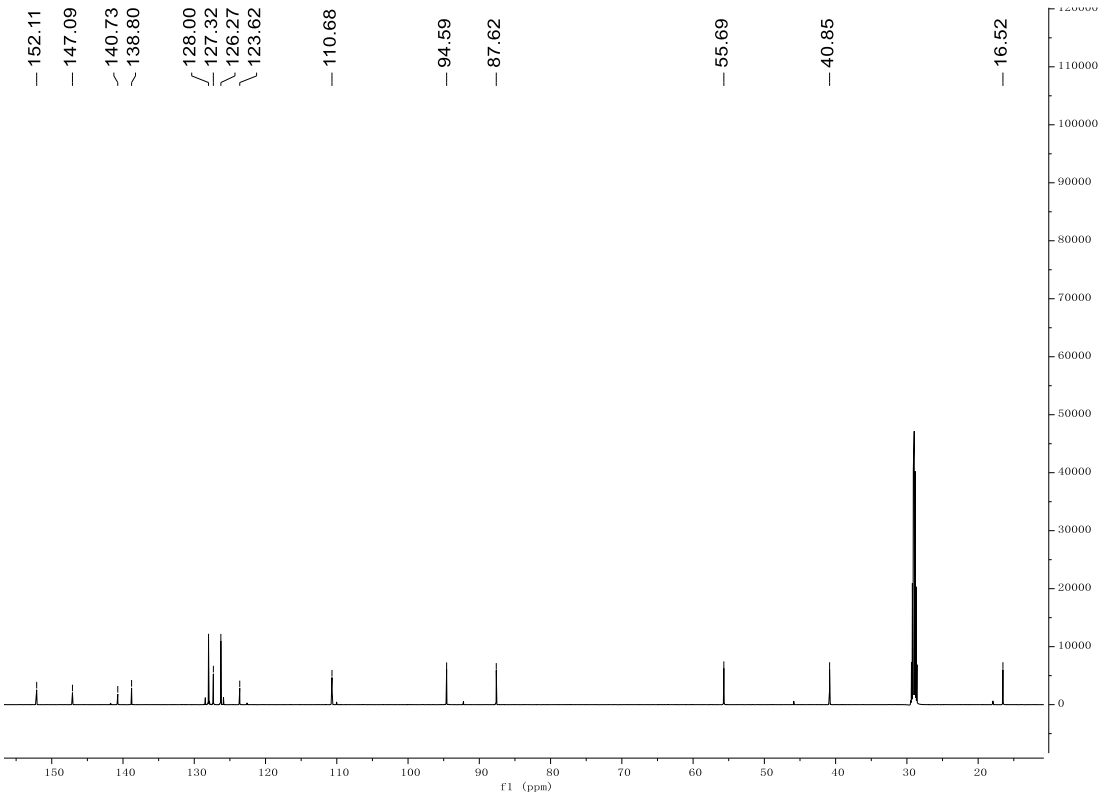


Figure S17: ^{13}C-NMR (151 MHz, Acetone-d_6) spectrum of **4**

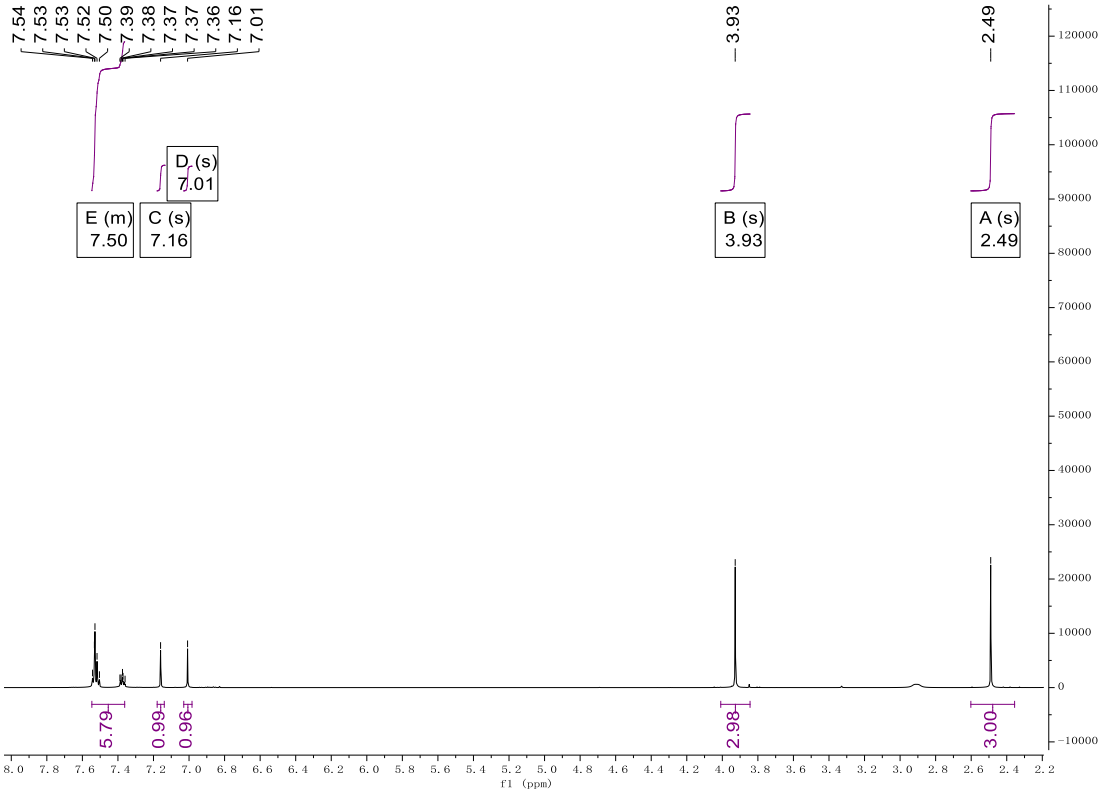


Figure S18: ^{1}H-NMR (600 MHz, Acetone-d_6) spectrum of **5**

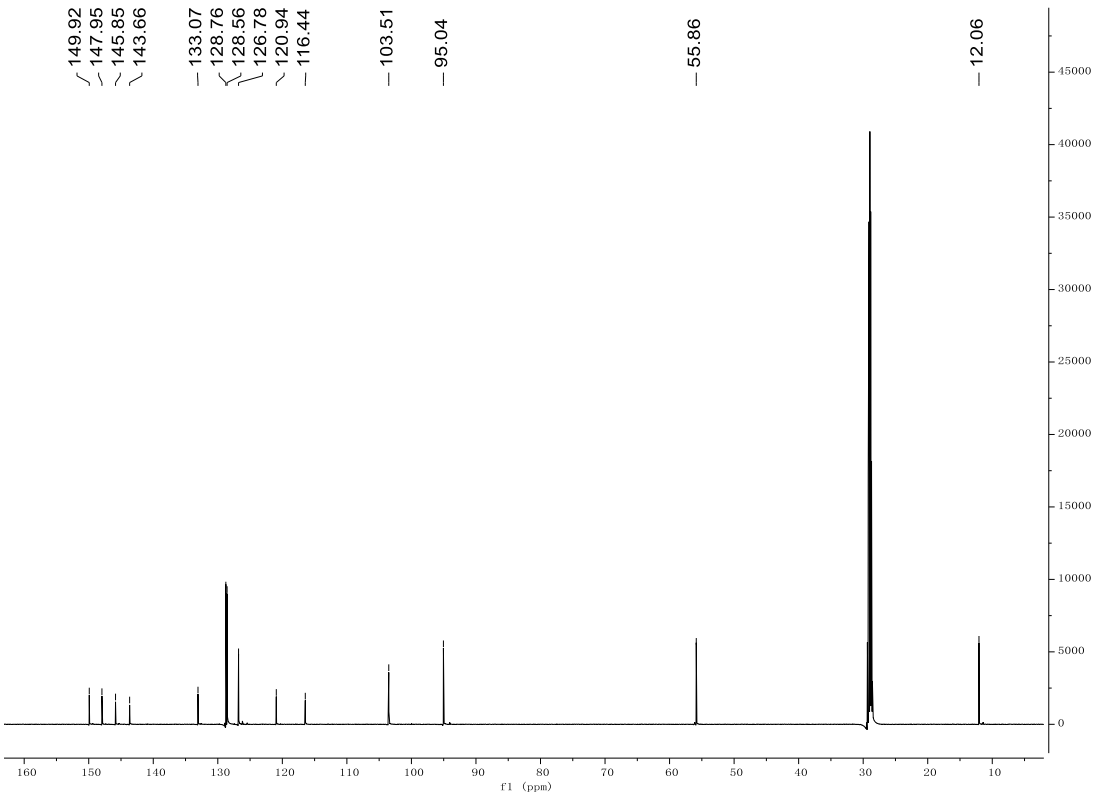
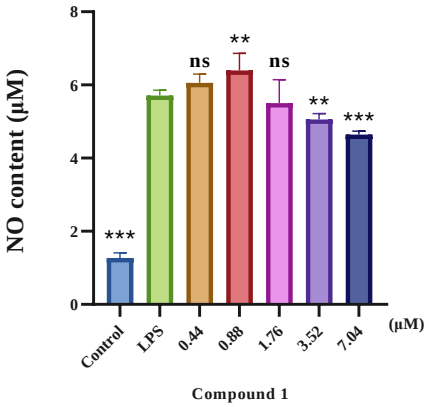
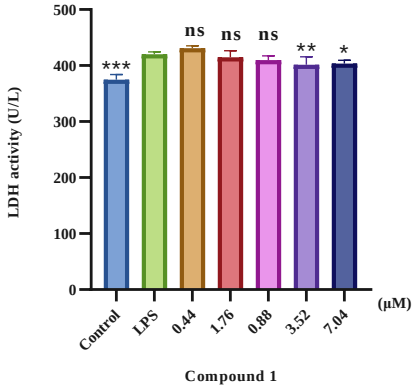
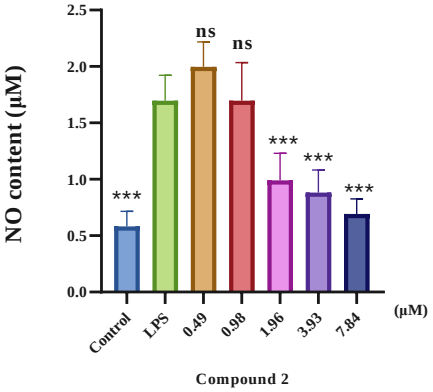
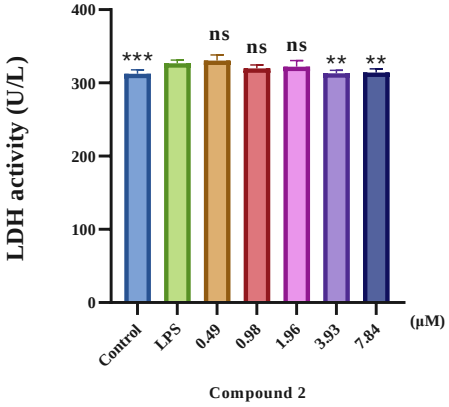


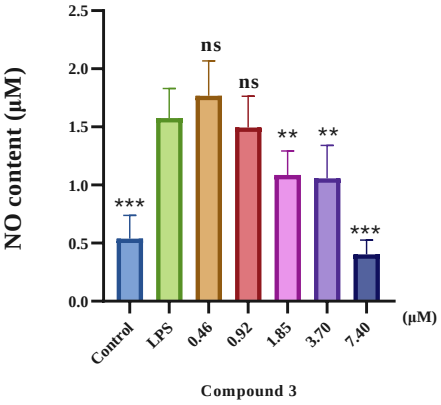
Figure S19: ^{13}C-NMR (151 MHz, Acetone-d_6) spectrum of **5**

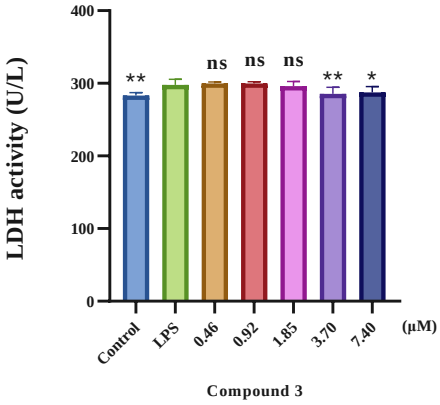












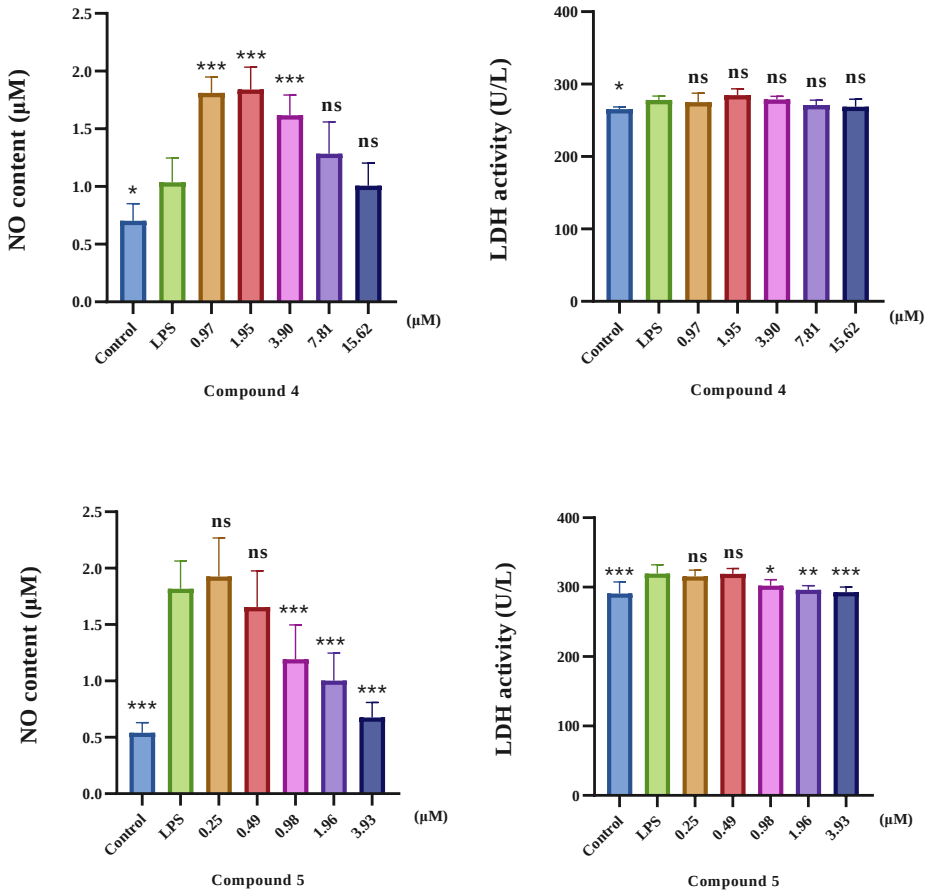


Figure S20: Effects of compounds on the production of NO and LDH in LPS-induced RAW 264.7 macrophages. The values shown represent the mean (n=6). **P*<0.05, ***P*<0.01, ****P*<0.001, compared to the LPS group.

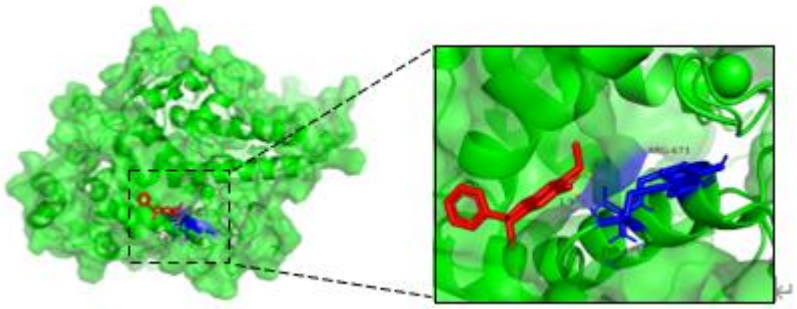


Figure 21: 3D visualization of the docking of compound **4** with MPO

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_2Cl_2	Pichloromethane
EtOAc	Ethyl acetate
n-BuOH	n-Butanol

Table S5. SciFinder report of compound **1**