

Supporting Information

Rec. Nat. Prod. X:X (202X) XX-XX

A New Benzofuran from the Heartwood of *Dalbergia odorifera* T. Chen and Its Protective Effect on Hypoxia/Reoxygenation Injury in H9c2

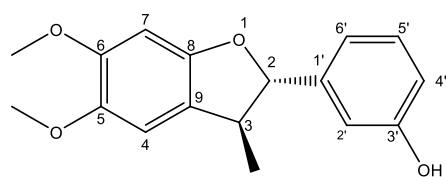
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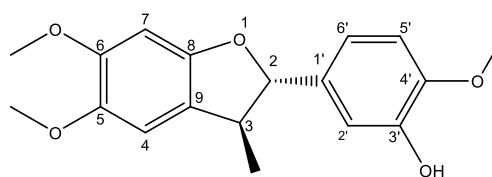
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compound 1



pterolinuses C

Table S1: The most similar compound data to compound 1

position	compound 1 ^a		pterolinuses C ^b	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1	-	-	-	-
2	5.08 (1H, d, $J = 8.0$ Hz)	91.6	5.02 (1H, d, $J = 8.0$)	94.0
3	3.26-3.20 (1H, m)	45.4	3.29 (1H, m, $J = 8.0, 6.8, 0.8$ Hz)	47.2
4	6.85 (1H, s)	109.1	6.83 (1H, d, $J = 0.8$ Hz)	111.0
5	-	143.4	-	145.6
6	-	149.4	-	151.8
7	6.59 (1H, s)	95.3	6.51 (1H, s)	96.8
8	-	152.7	-	155.1
9	-	121.6	-	123.6
1'	-	142.9	-	135.9
2'	6.78 (1H, t, $J = 2.1$ Hz)	112.4	6.91 (1H, d, $J = 2.0$ Hz)	114.4
3'	-	157.5	-	148.2
4'	6.71 (1H, dd, $J = 7.6, 2.1$ Hz)	114.9	-	149.0
5'	7.17 (1H, t, $J = 7.8$ Hz)	129.6	6.93 (1H, d, $J = 8.0$ Hz)	112.9
6'	6.80 (1H, d, $J = 7.5$ Hz)	116.3	6.80 (1H, dd, $J = 8.0, 2.0$ Hz)	118.9
3-CH ₃	1.33 (3H, d, $J = 6.8$ Hz)	18.6	1.34 (1H, d, $J = 6.8$ Hz)	19.4
5-OCH ₃	3.69 (3H, s)	56.6	3.78 (1H, s)	57.0
6-OCH ₃	3.73 (3H, s)	55.8	3.74 (1H, s)	58.1
3'-OH	9.44 (1H, s)	-	7.73 (1H, s)	-
4'-OCH ₃	-	-	3.84 (1H, s)	56.9

^a Measured in DMSO-*d*₆, -600 MHz

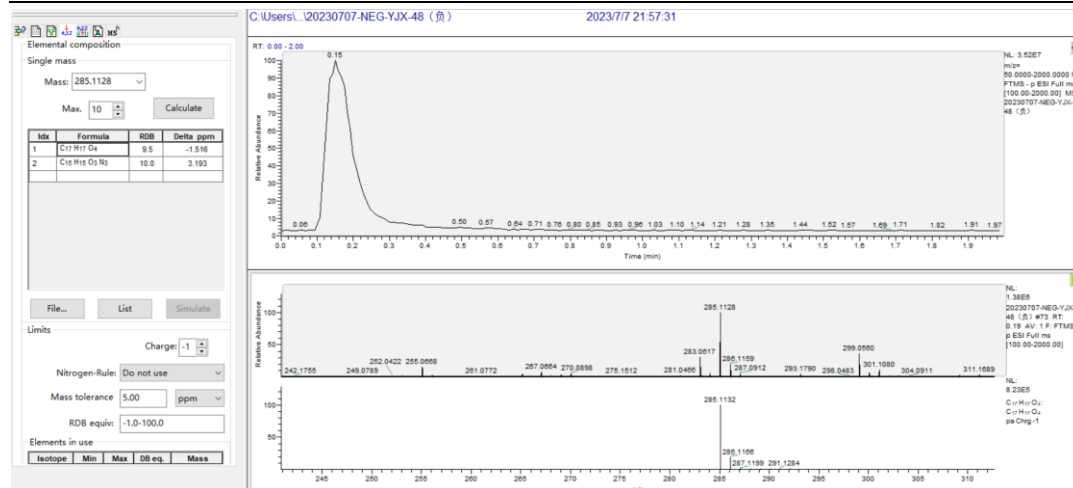
^b Measured in Acetone-*d*₆, -500 MHz

References

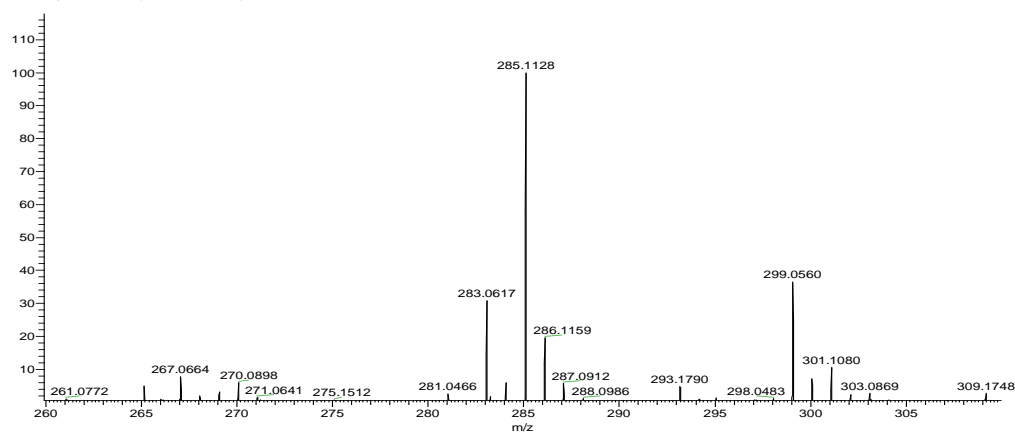
S.F. Wu, F.R. Chang, S.Y. Wang, T.L. Hwang, C.L. Lee, S.L. Chen, C.C. Wu and Y.C. Wu (2011). Anti-inflammatory and cytotoxic neoflavonoids and benzofurans from *Pterocarpus santalinus*, *J. Nat. Prod.* **74**, 989-996

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

compound	Ionic mode	Formula	Measured value (m/z)	Calculated value (m/z)	Error (ppm)
1	[M-H]⁻	C₁₇H₁₇O₄	285.1128	285.1132	-1.516



20230707-NEG-YJX-48 (负) #73 RT: 0.19 AV: 1 NL: 1.38E6
 F: FTMS - p ESI Full ms [100.00-2000.00]



20230707-NEG-YJX-48 (负) #70 RT: 0.19 AV: 1 NL: 1.59E6
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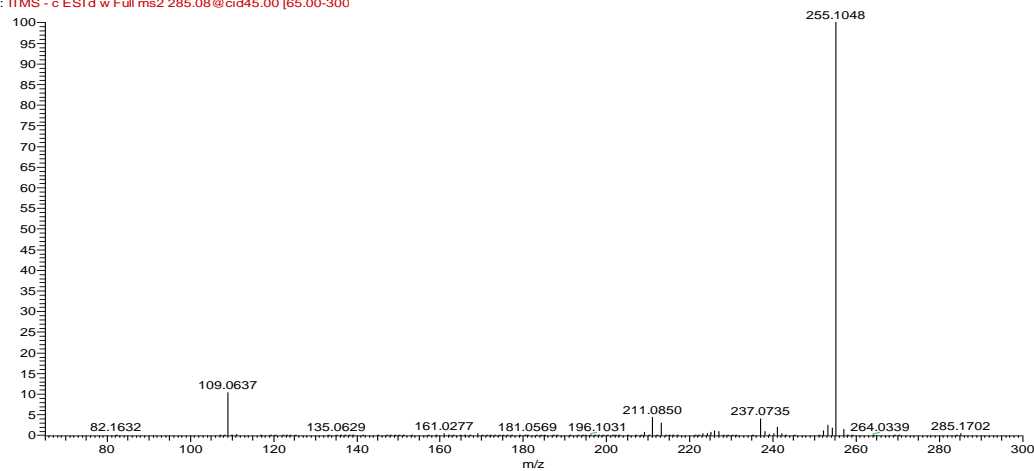


Figure S1: HR-ESI-MS spectrum of compound **1**

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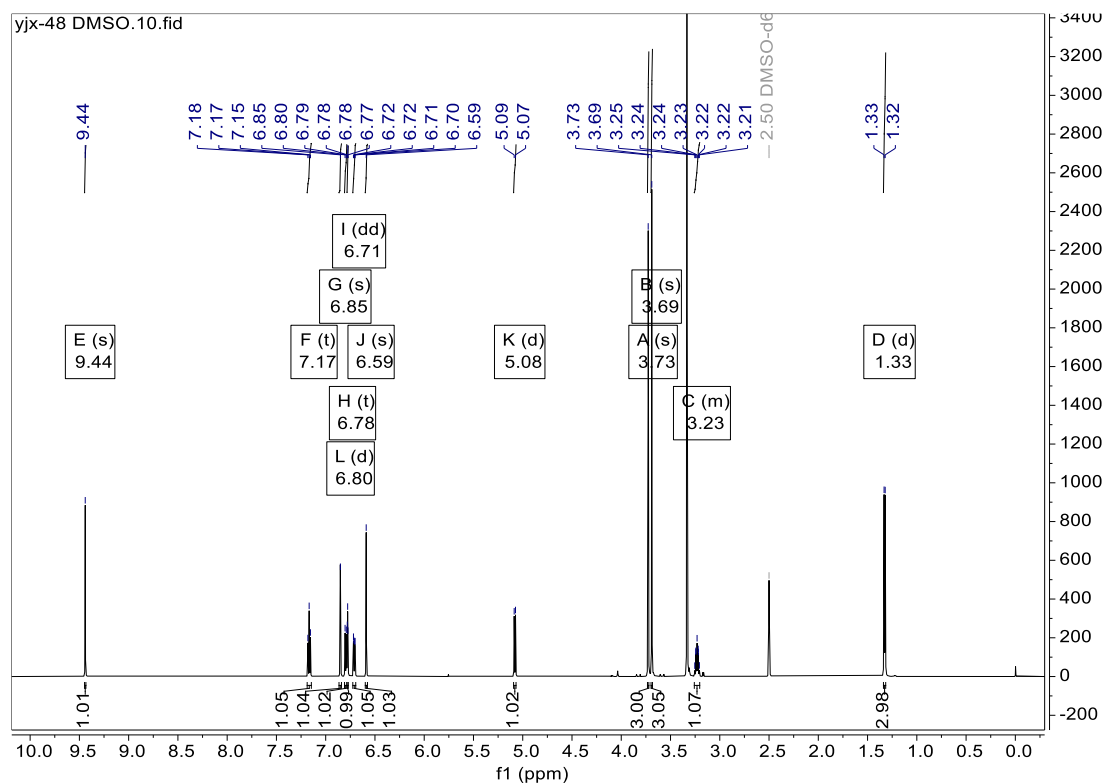


Figure S2: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) spectrum of compound **1**

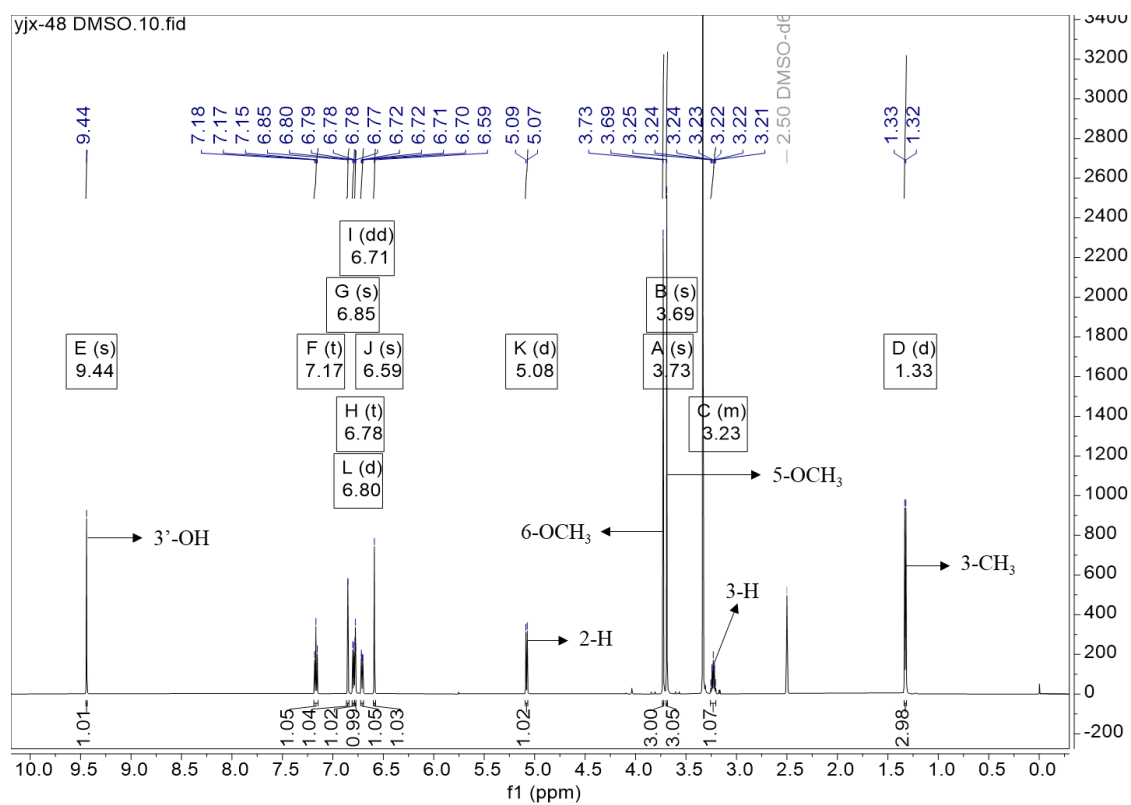


Figure S3: The labeled $^1\text{H-NMR}$ spectrum of compound **1**

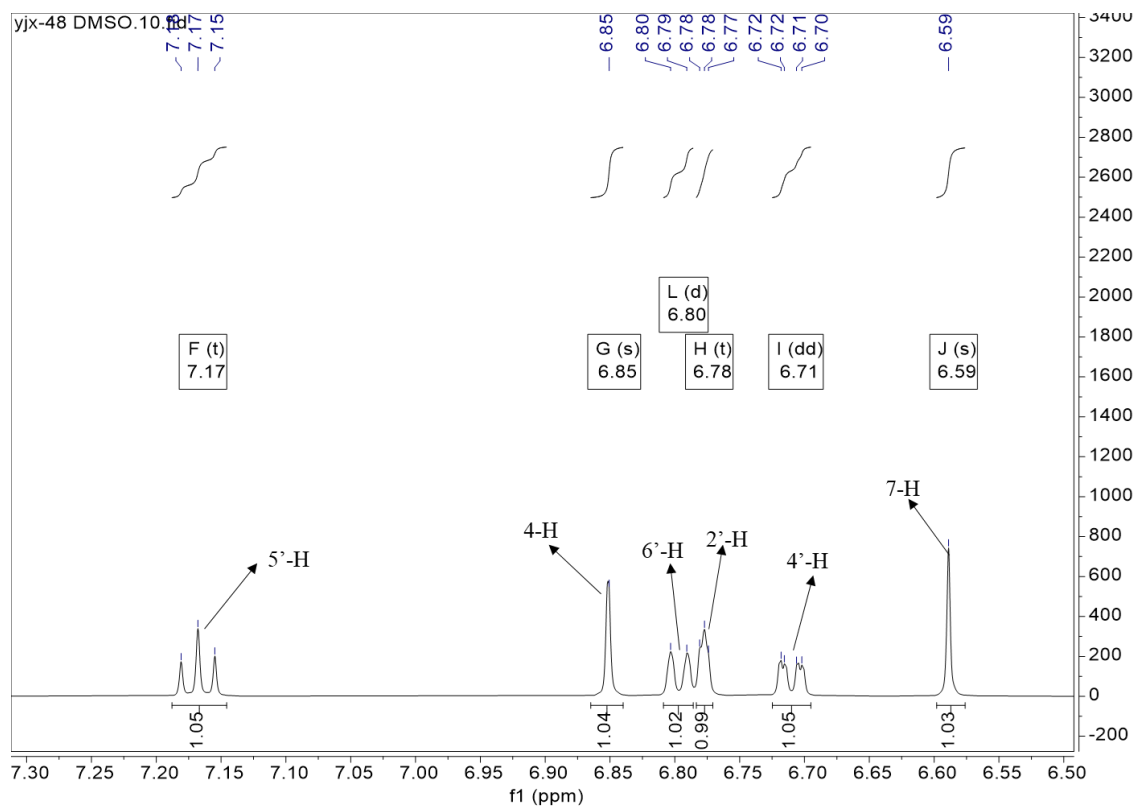


Figure S4: The labeled ^1H -NMR spectrum of compound **1** (From δ_{H} 6.5 ppm to δ_{H} 7.3 ppm)

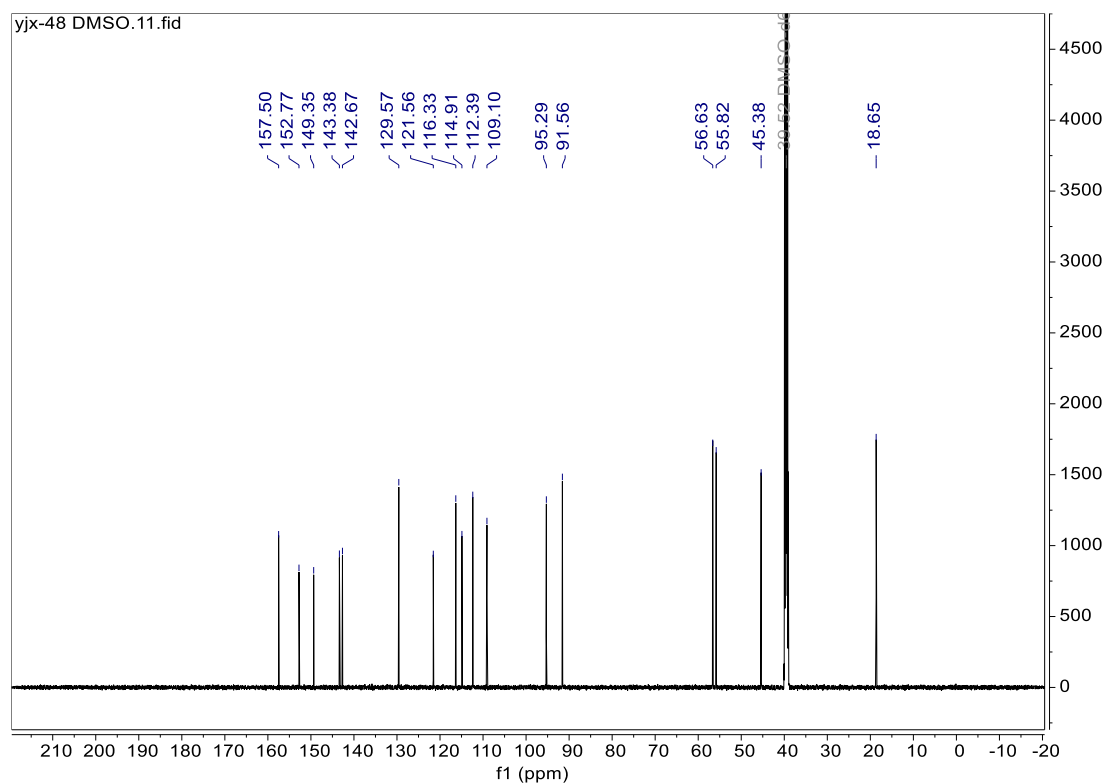


Figure S5: ^{13}C -NMR (151 MHz, $\text{DMSO-}d_6$) spectrum of compound **1**

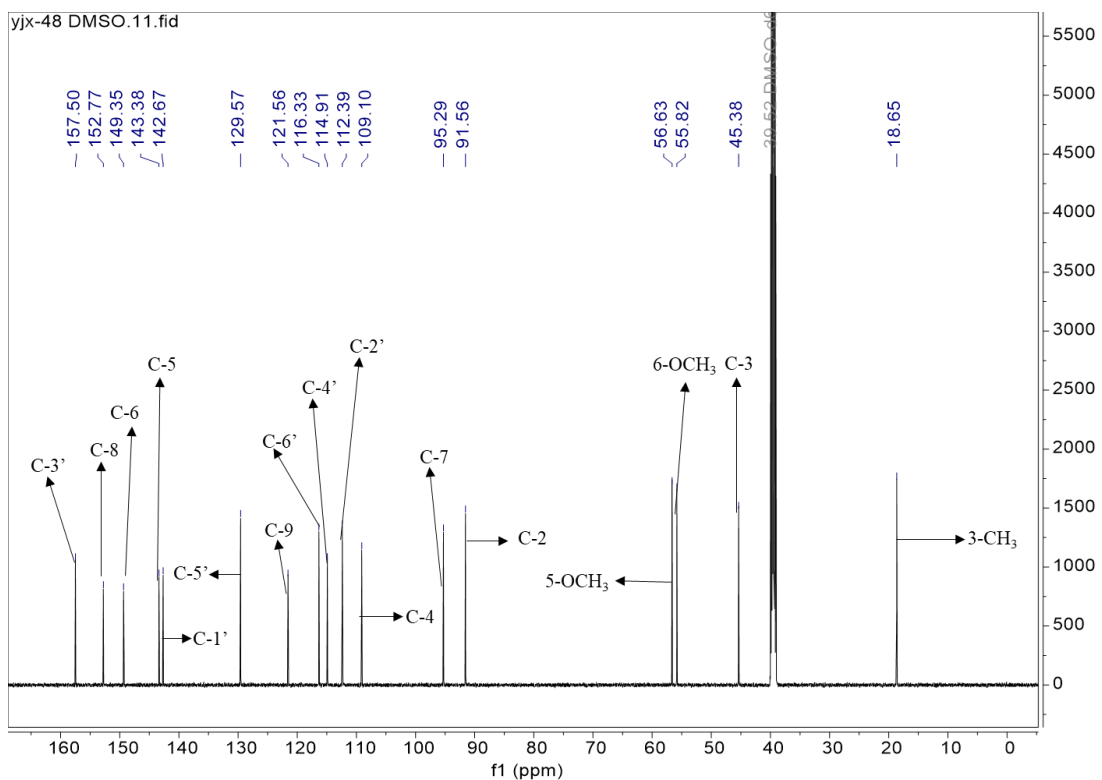


Figure S6: The labeled ¹³C-NMR spectrum of compound **1**

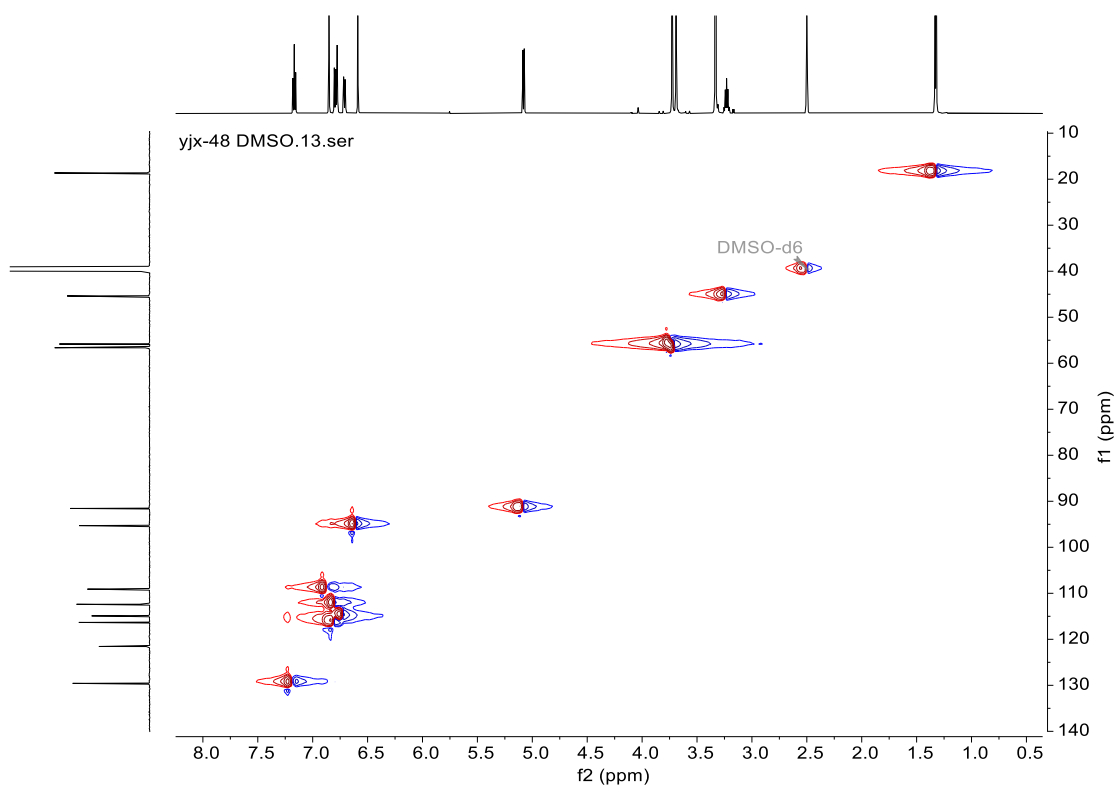


Figure S7: HSQC spectrum of compound **1**

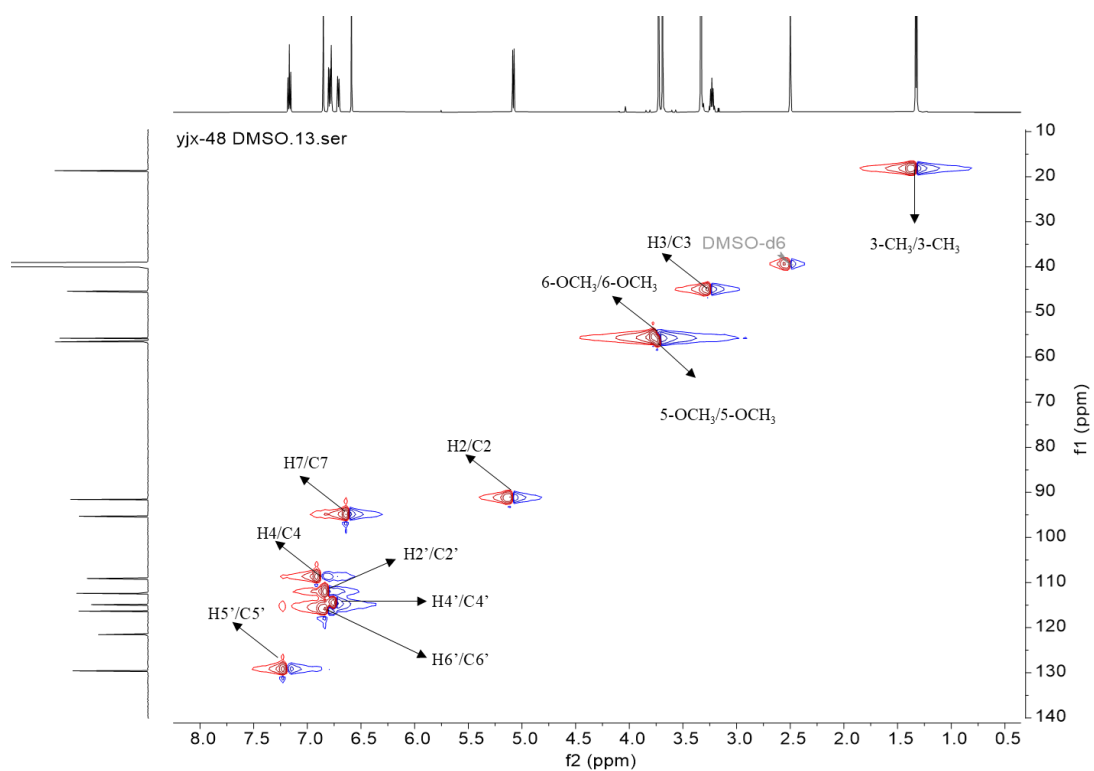


Figure S8: The labeled HSQC spectrum of compound **1**

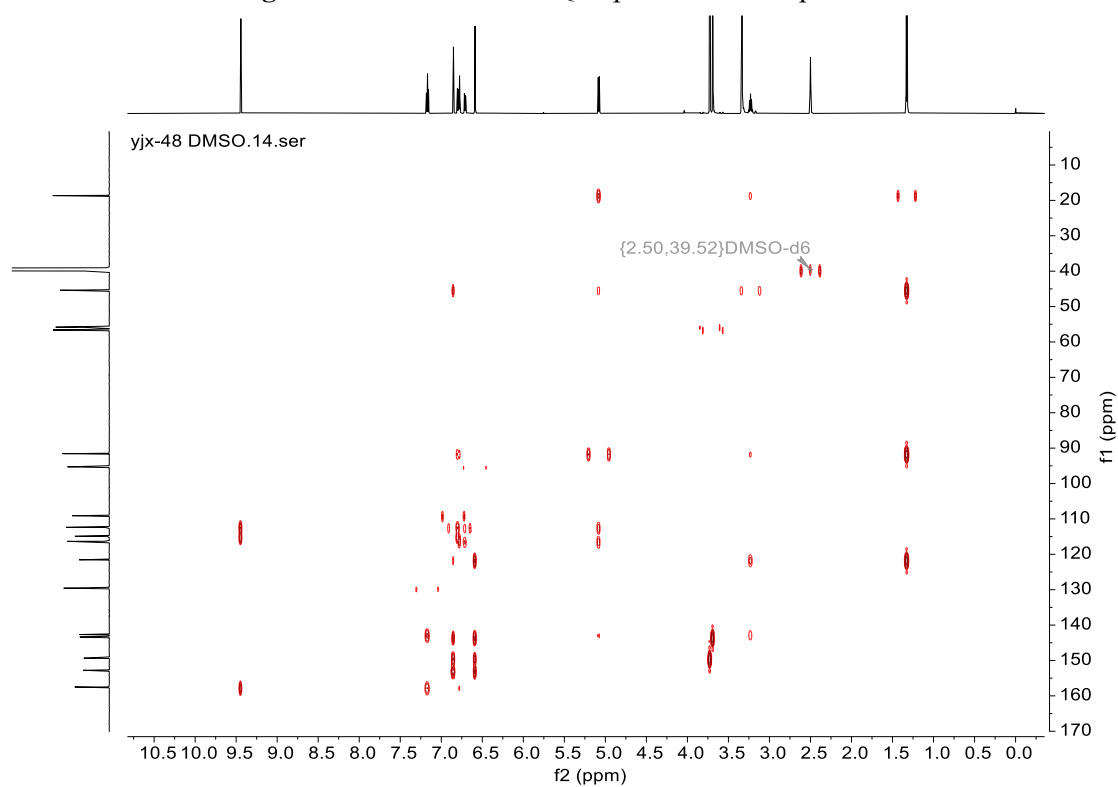


Figure S9: HMBC spectrum of compound **1**

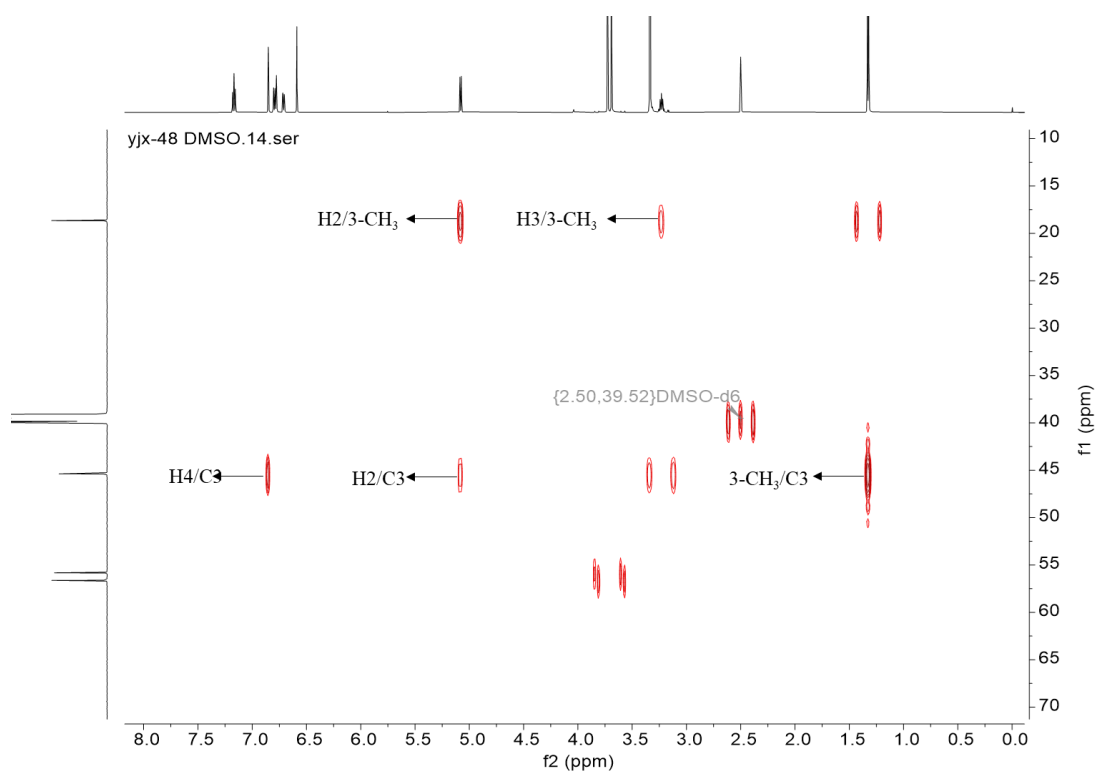


Figure S10: The labeled HMBC spectrum of compound **1** (From δ_C 10 ppm to δ_C 70 ppm)

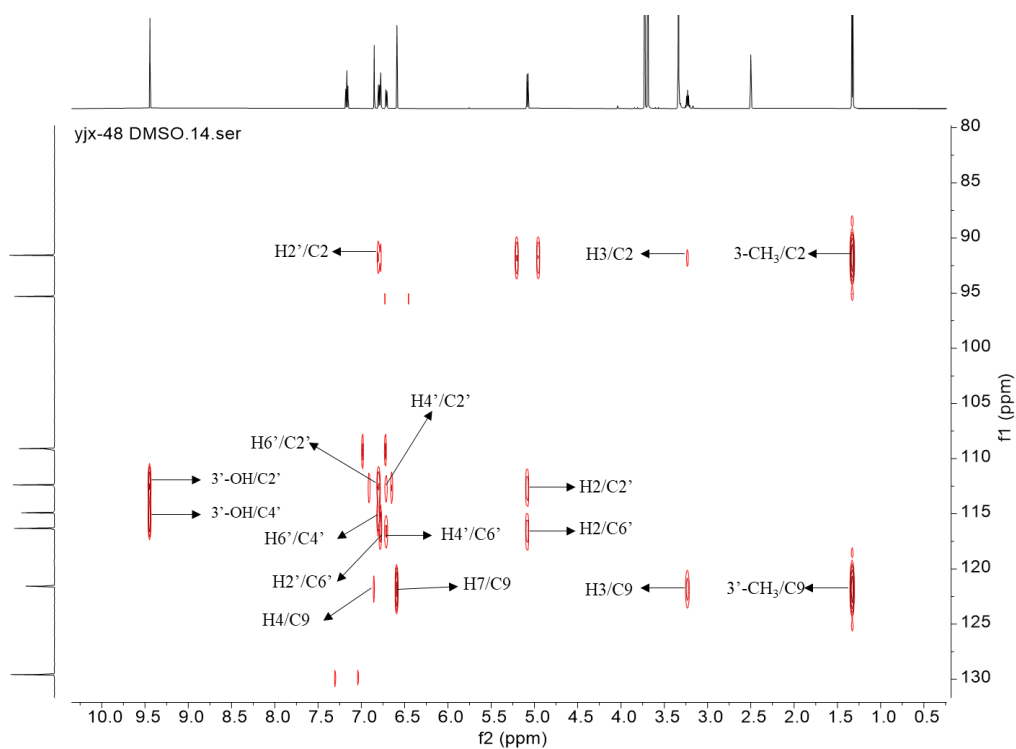


Figure S11: The labeled HMBC spectrum of compound **1** (From δ_C 80 ppm to δ_C 130 ppm)

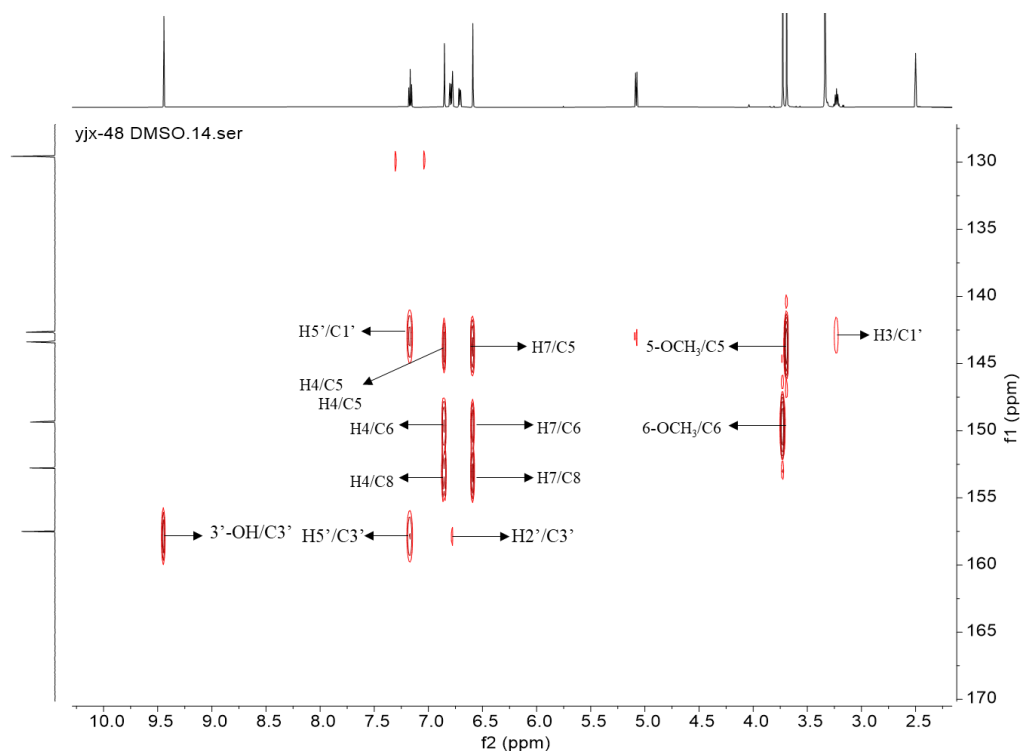


Figure S12: The labeled HMBC spectrum of compound **1** (From δ_{C} 130 ppm to δ_{C} 170 ppm)

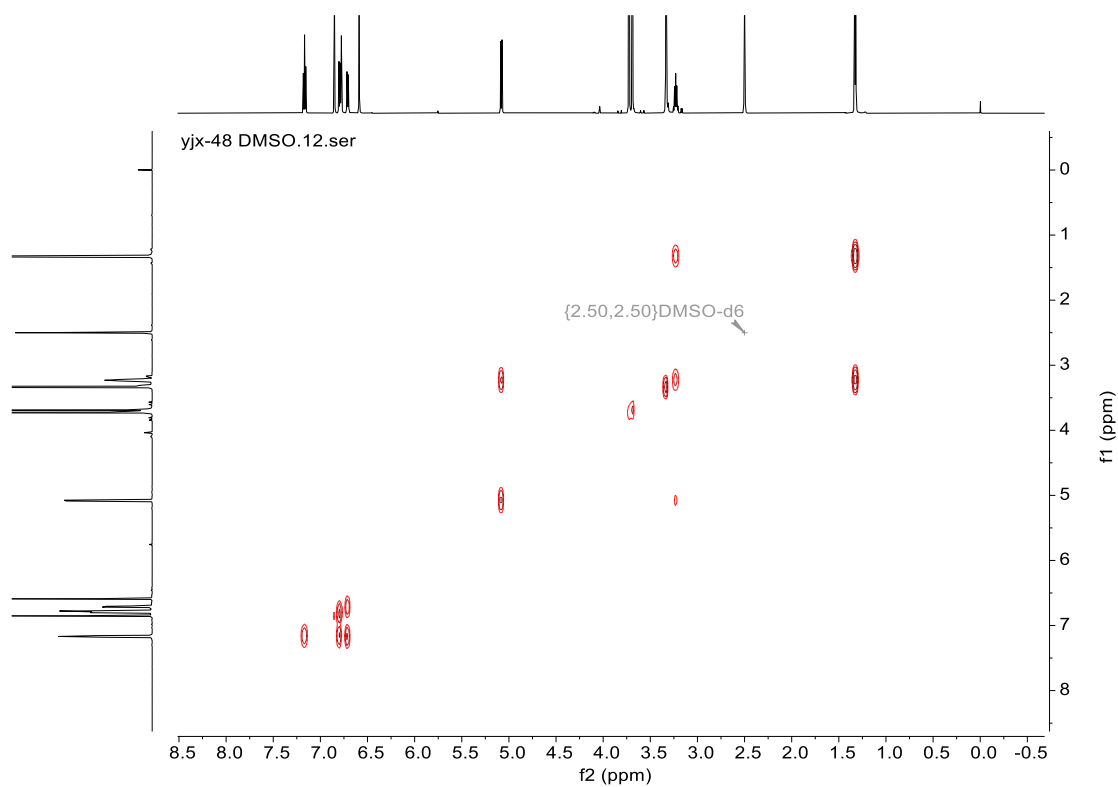


Figure S13: ^1H - ^1H COSY spectrum of compound **1**

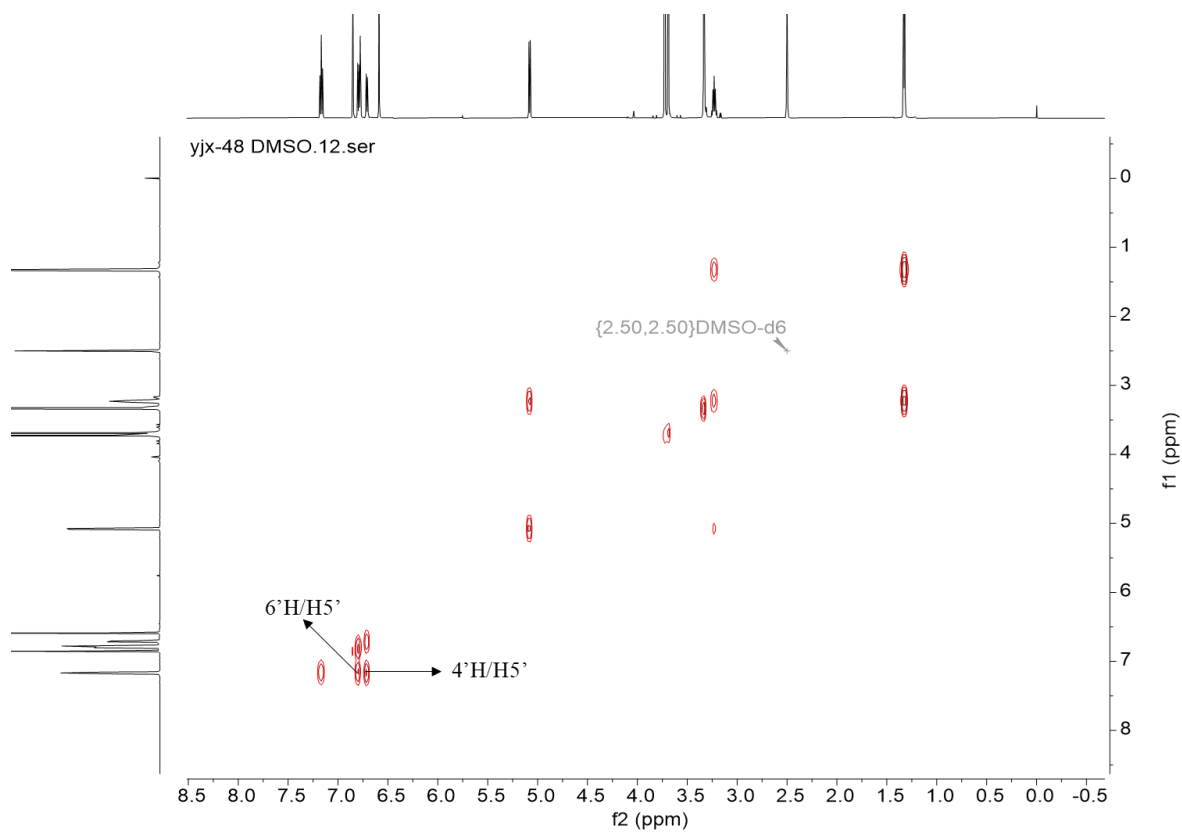


Figure S14: The labeled ^1H - ^1H COSY spectrum of compound **1**

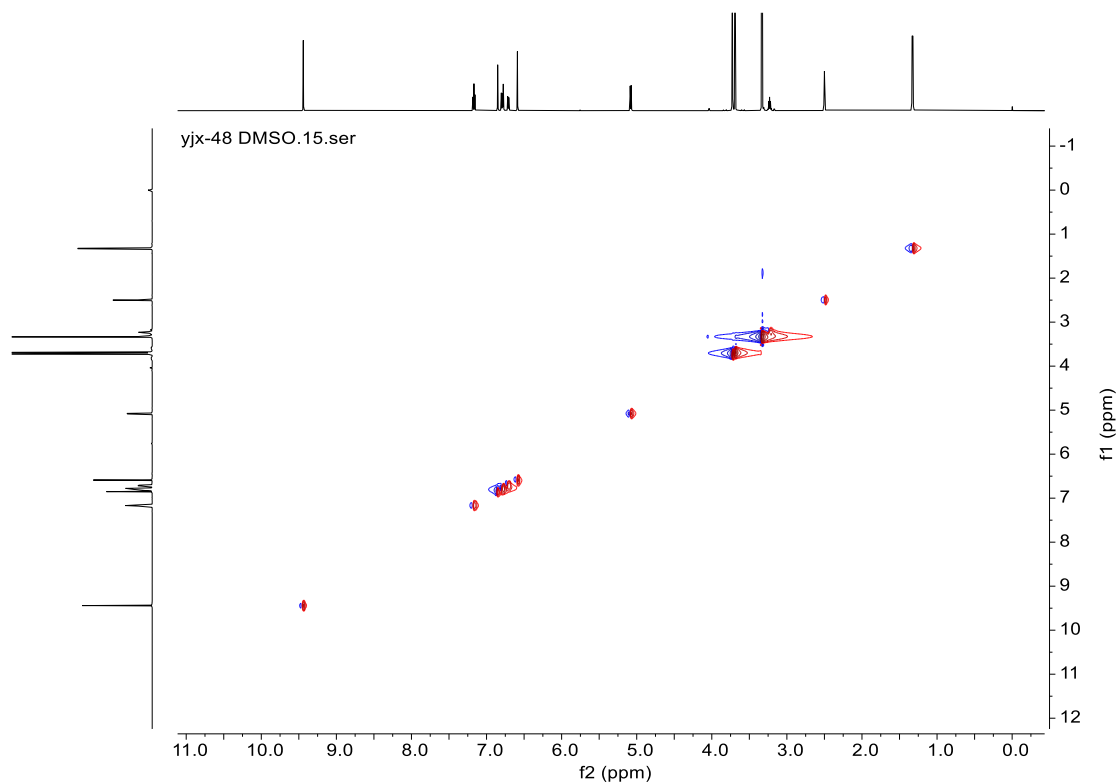


Figure S15: NOESY spectrum of compound **1**

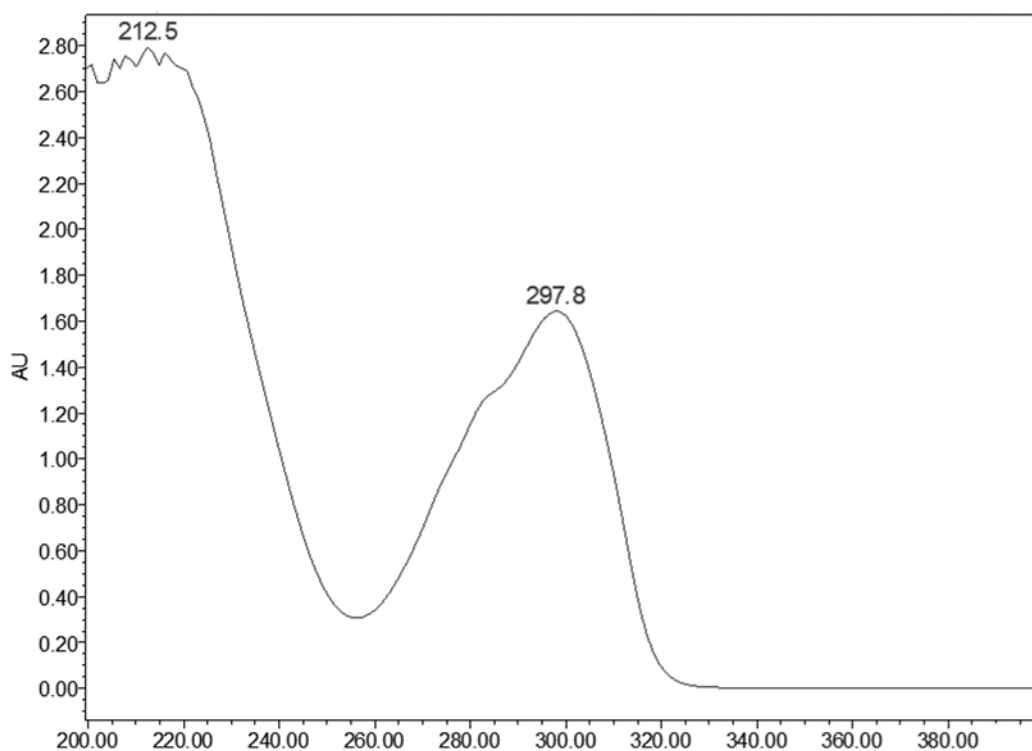


Figure S16: UV spectra of compound 1

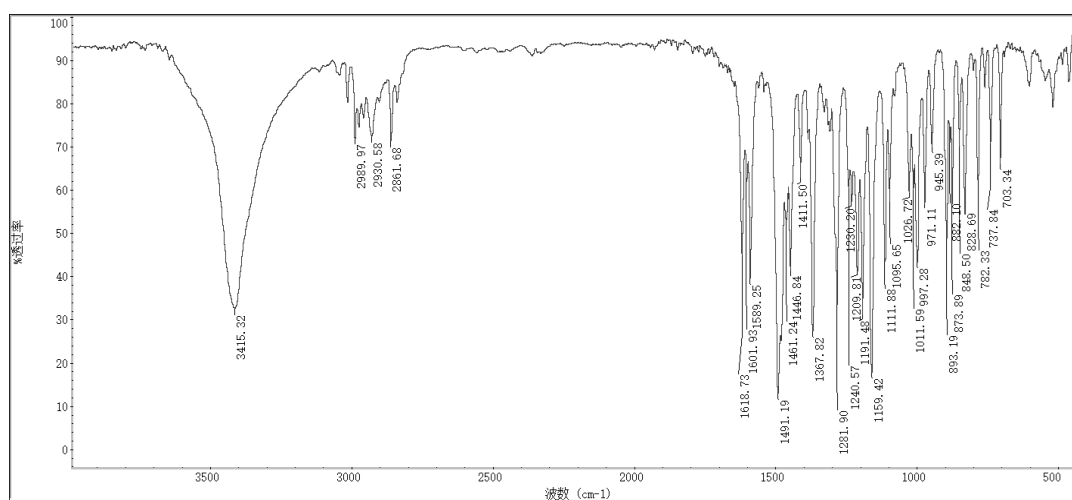


Figure S17: IR spectra of compound 1

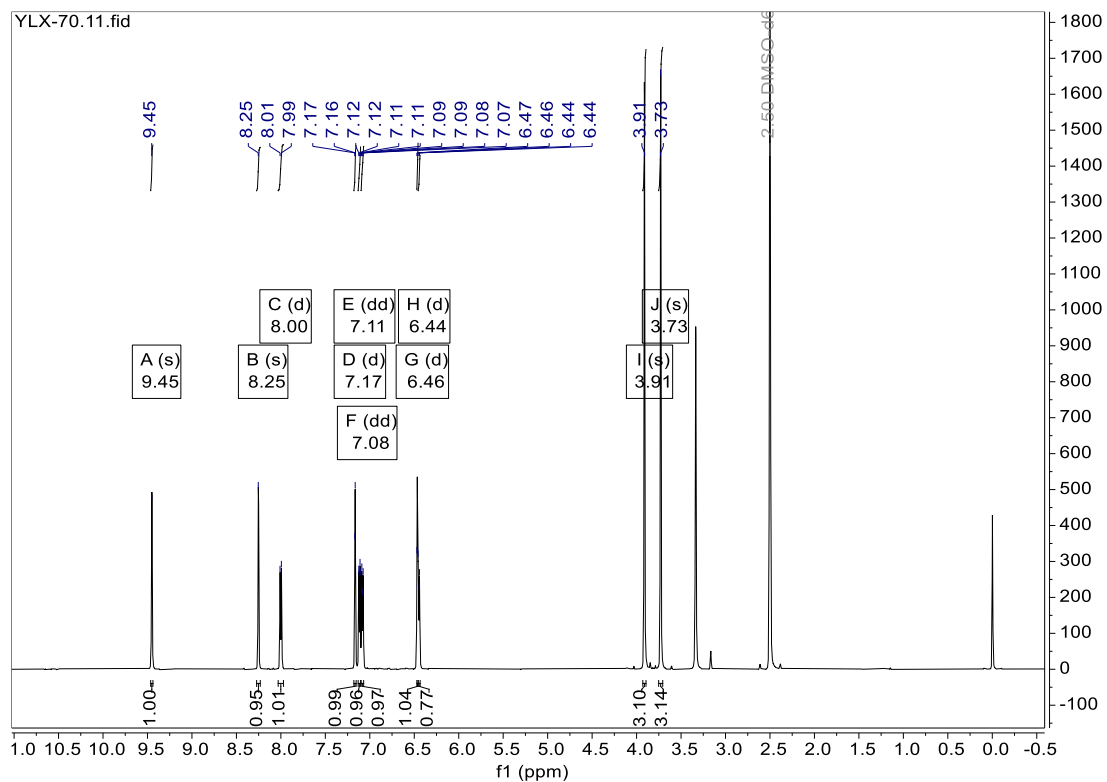


Figure S18: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) spectrum of compound 2

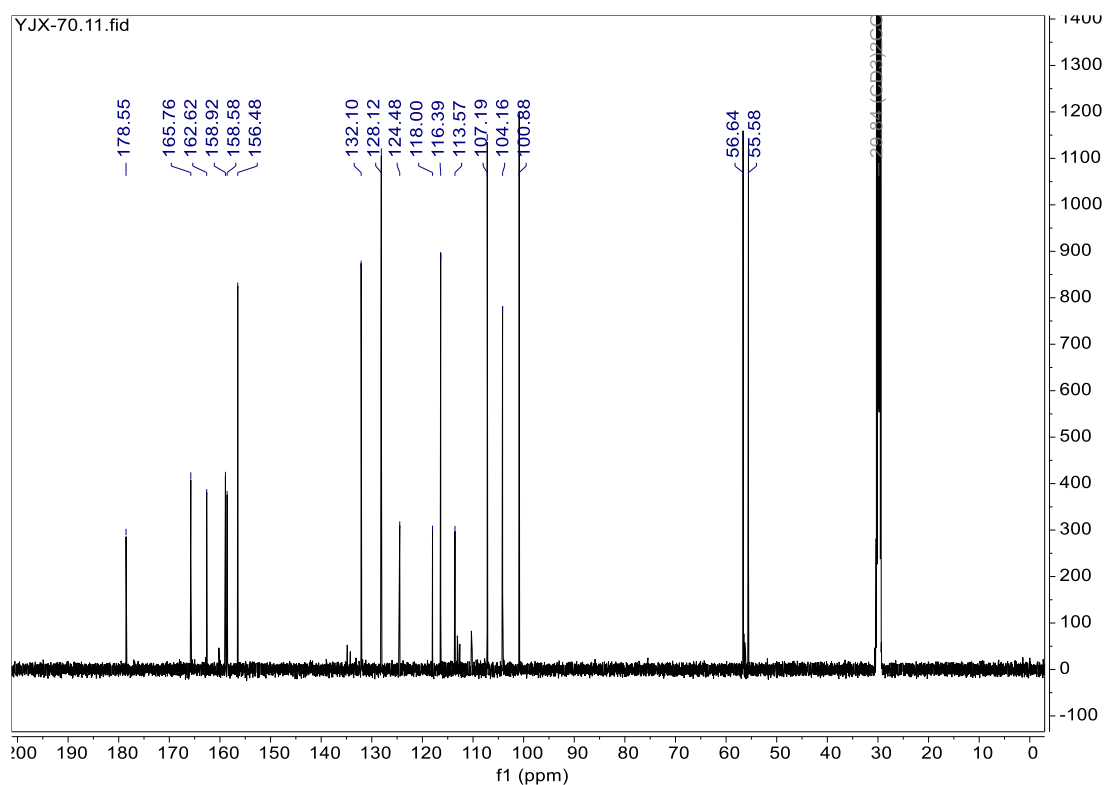


Figure S19: $^{13}\text{C-NMR}$ (151 MHz, $\text{DMSO-}d_6$) spectrum of compound 2

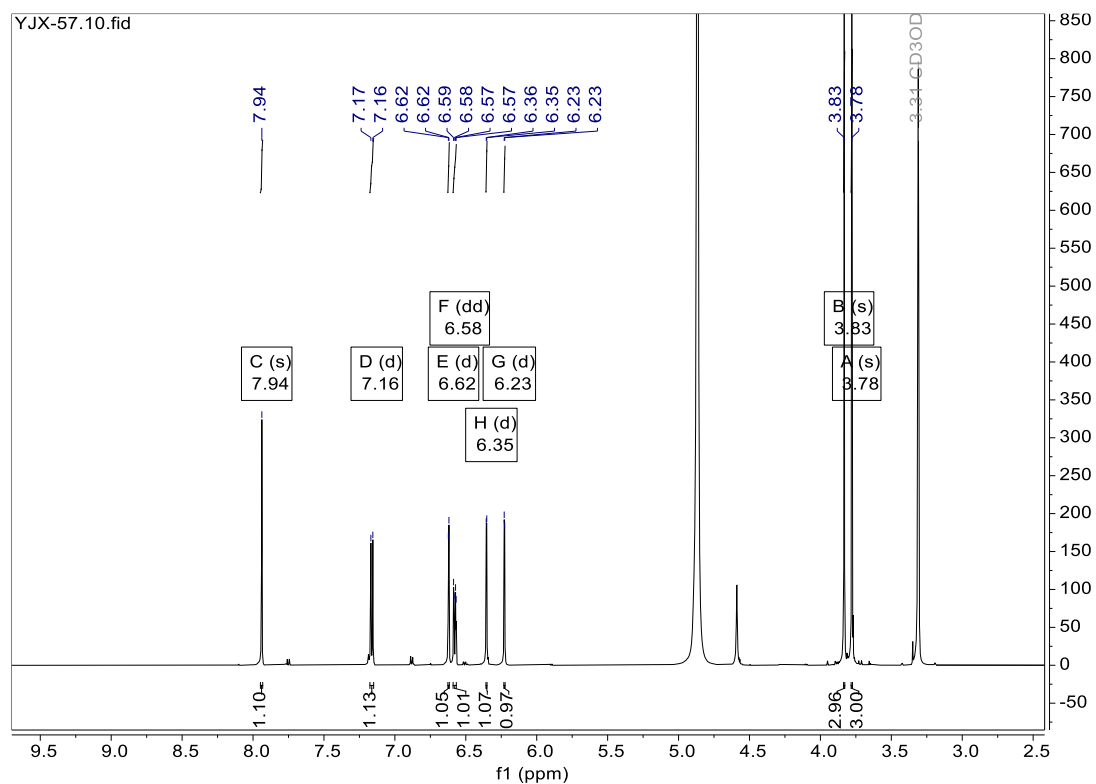


Figure S20: $^1\text{H-NMR}$ (600 MHz, Methanol- d_4) spectrum of compound **3**

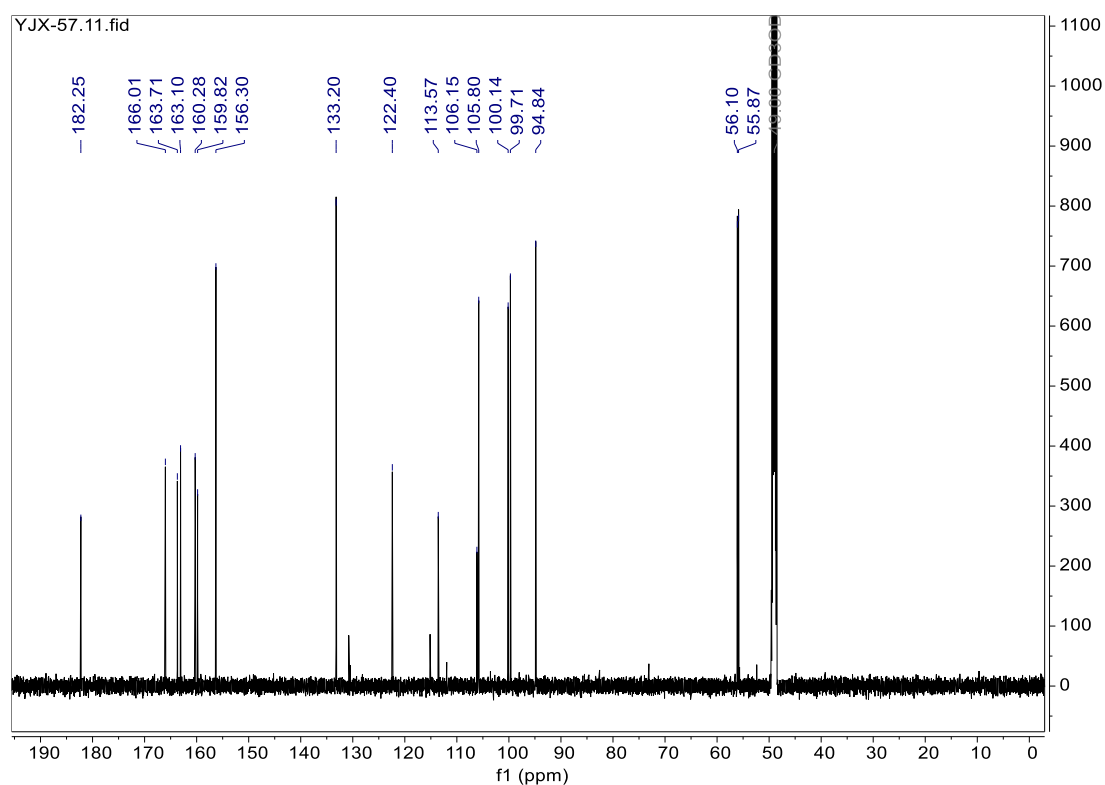


Figure S21: $^{13}\text{C-NMR}$ (151 MHz, Methanol- d_4) spectrum of compound **3**

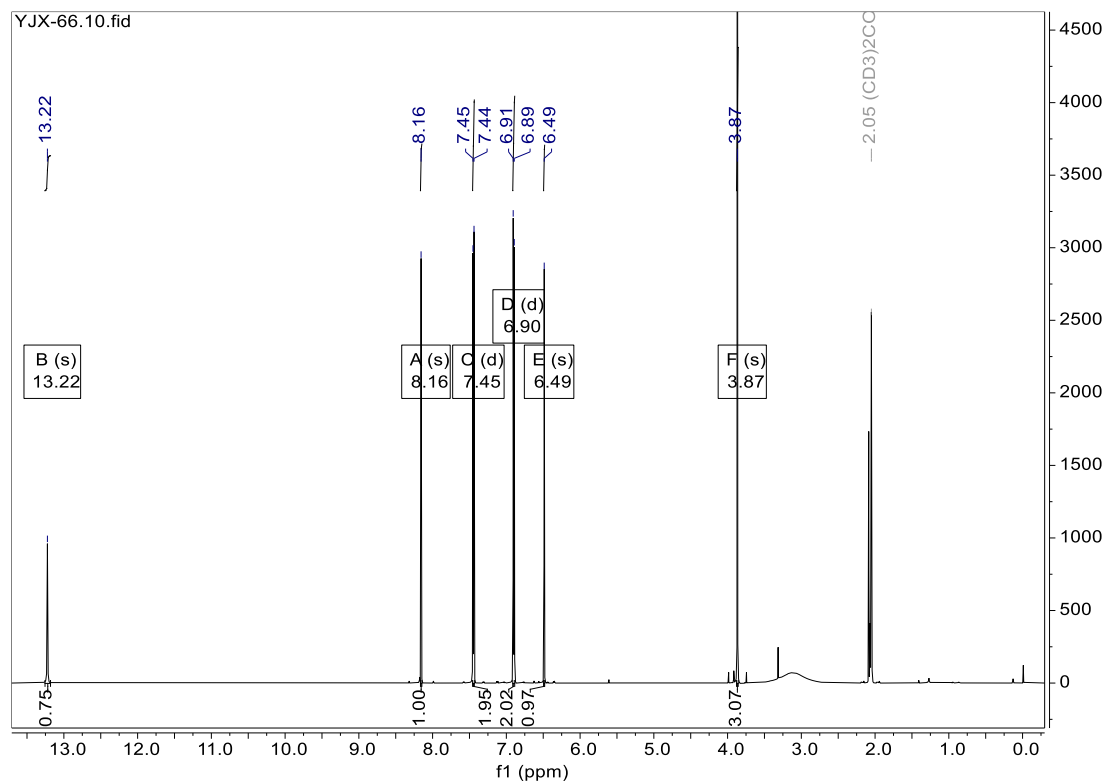


Figure S22: ¹H-NMR (600 MHz, Acetone-*d*₆) spectrum of compound 4

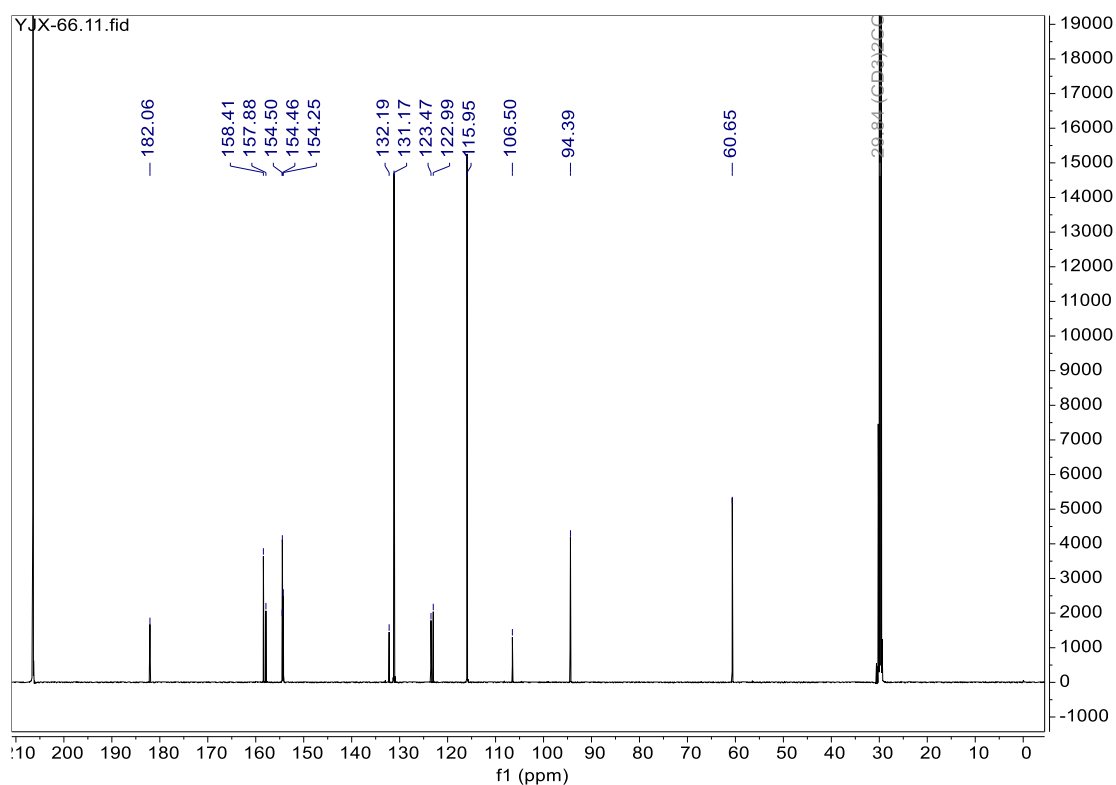


Figure S23: ¹³C-NMR (151 MHz, Acetone-*d*₆) spectrum of compound 4

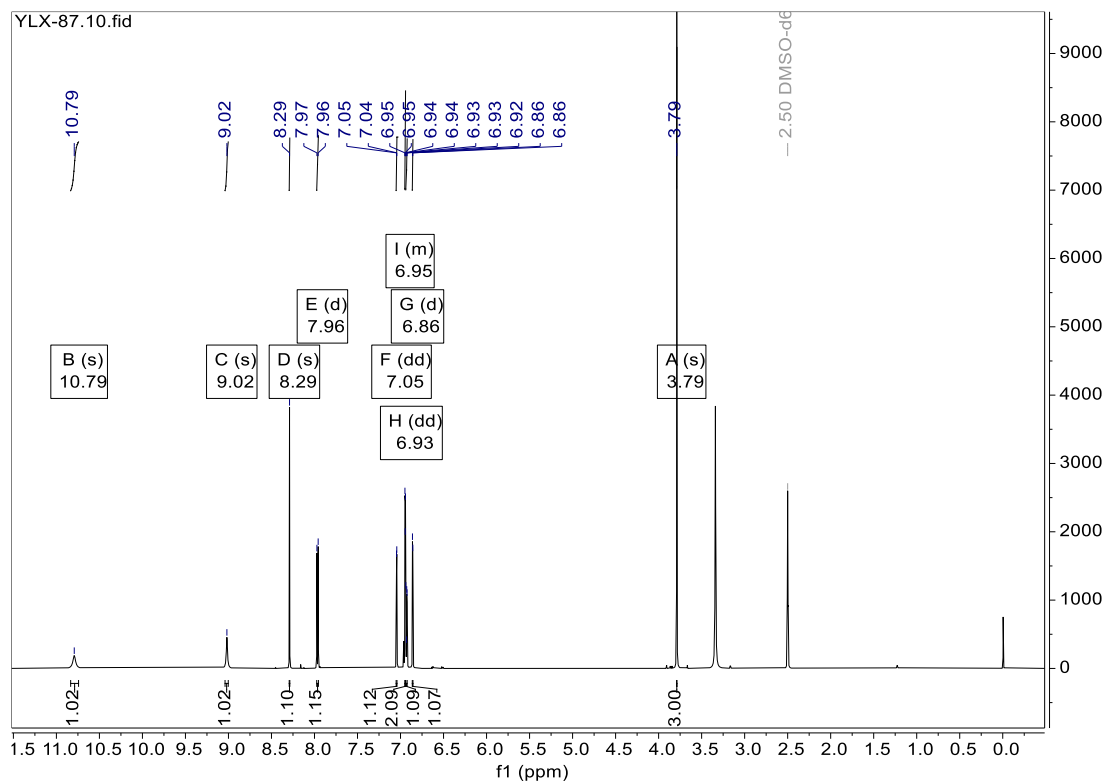


Figure S24: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) spectrum of compound **5**

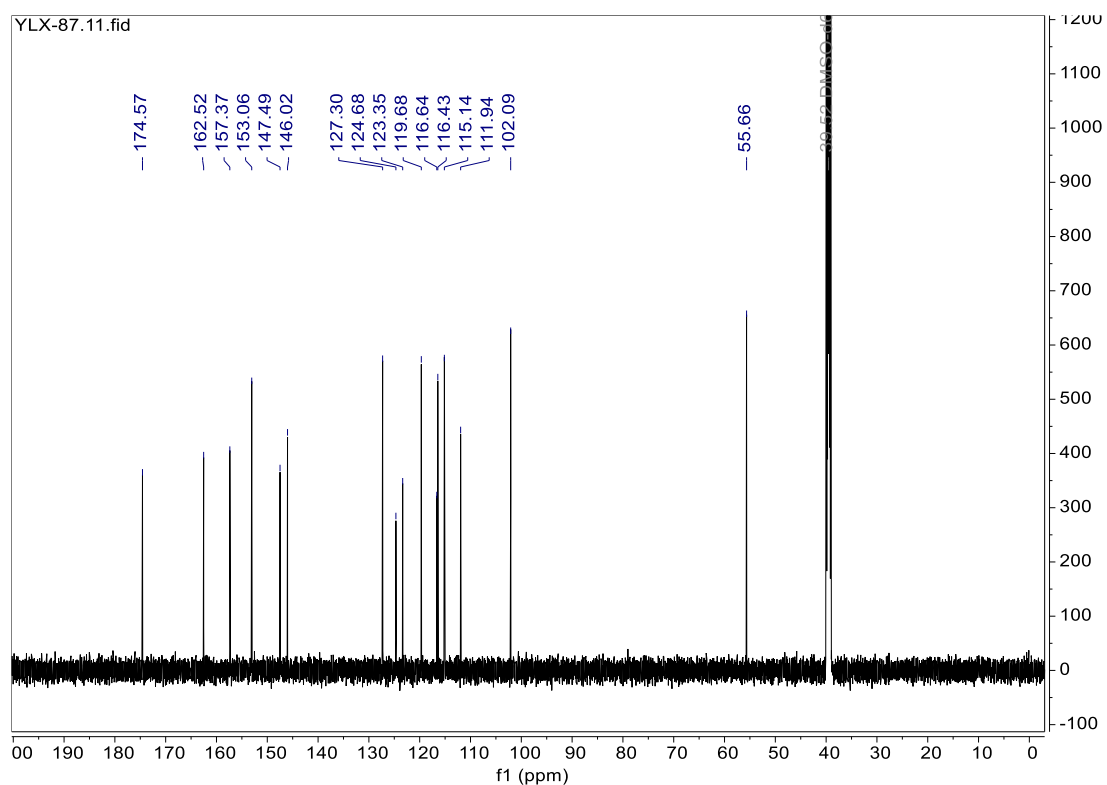


Figure S25: $^{13}\text{C-NMR}$ (151 MHz, $\text{DMSO-}d_6$) spectrum of compound **5**

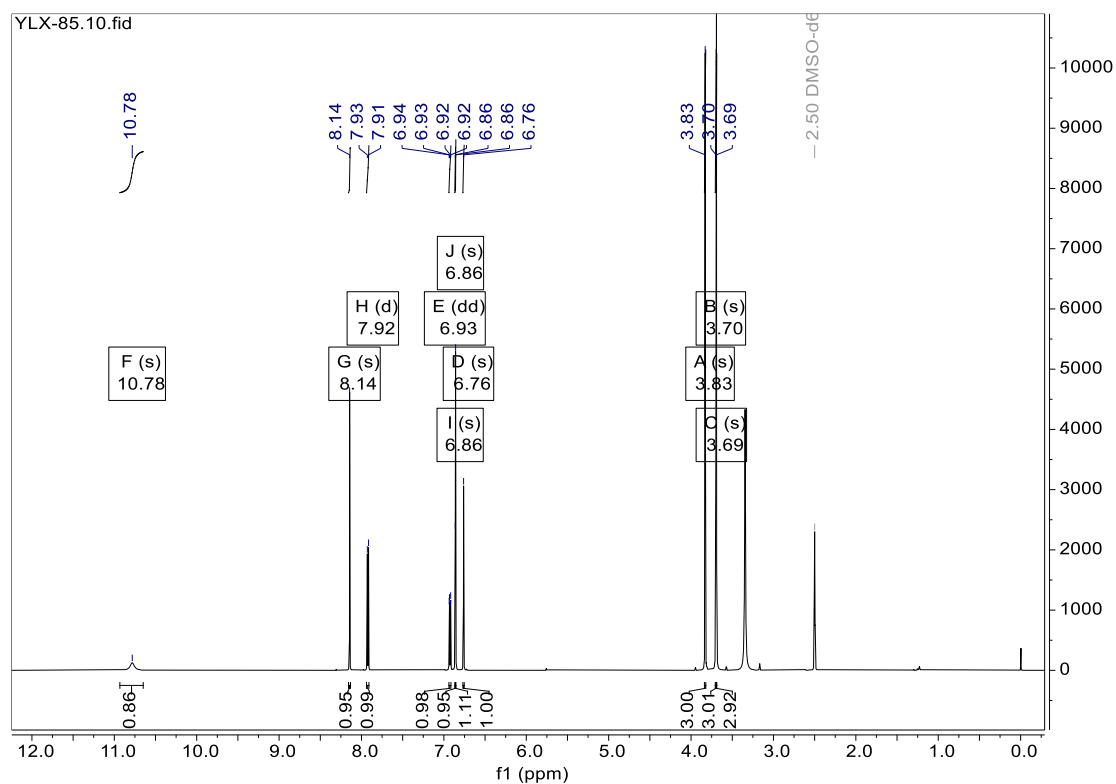


Figure S26: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) spectrum of compound **6**

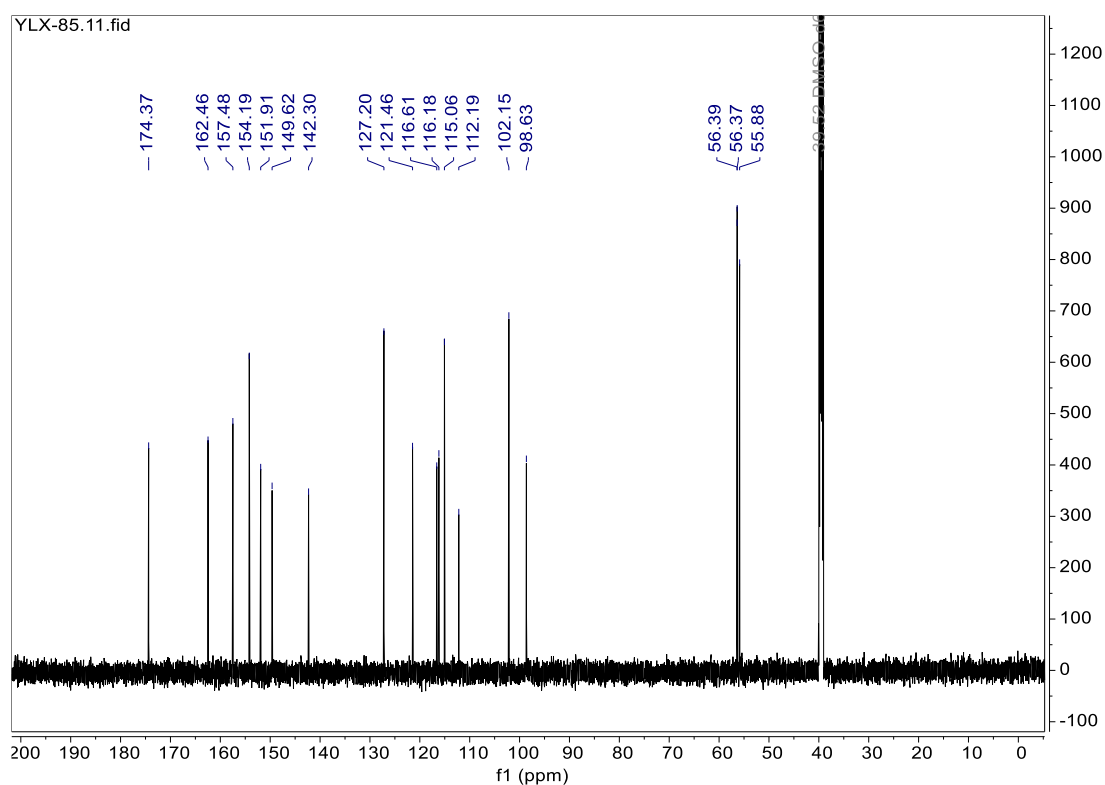


Figure S27: $^{13}\text{C-NMR}$ (151 MHz, $\text{DMSO-}d_6$) spectrum of compound **6**

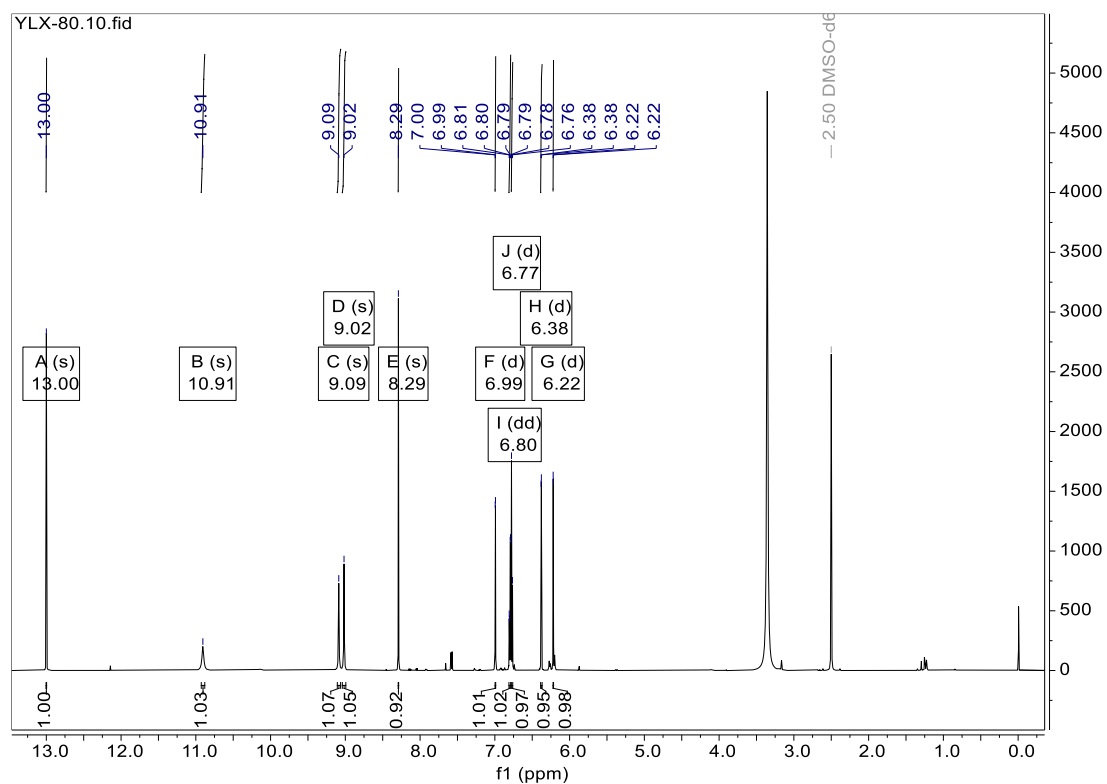


Figure S28: $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$) spectrum of compound 7

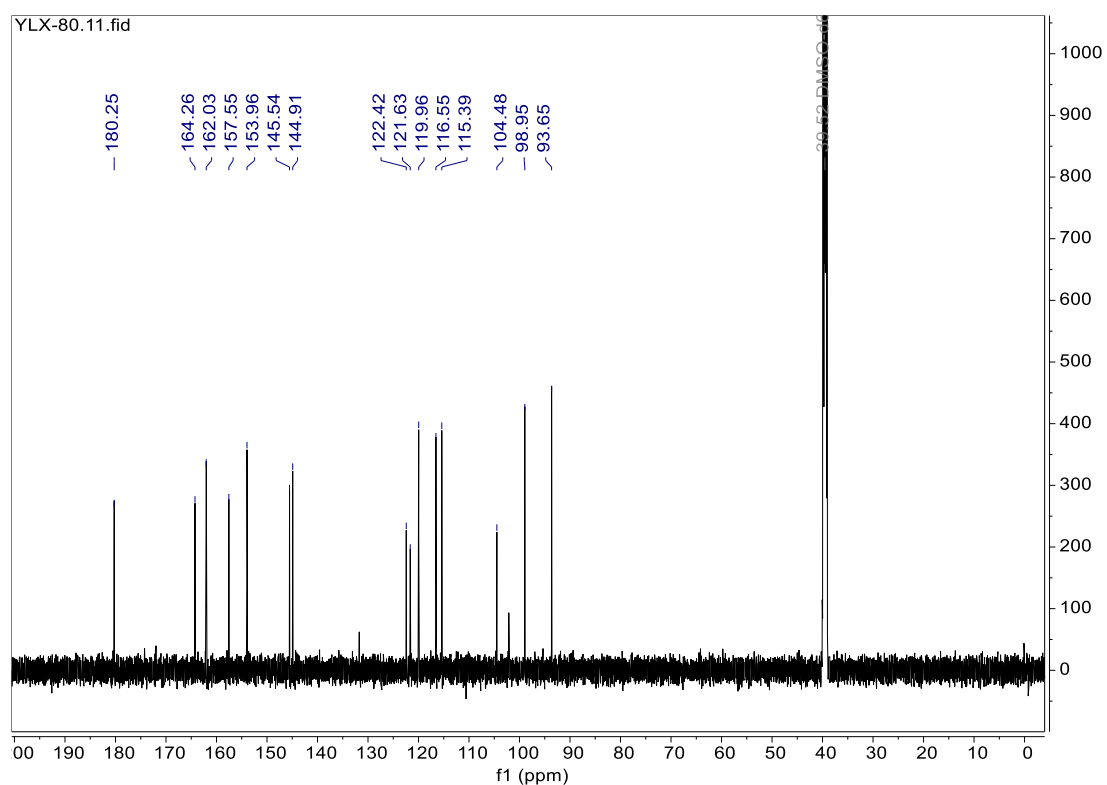


Figure S29: $^{13}\text{C-NMR}$ (151 MHz, $\text{DMSO-}d_6$) spectrum of compound 7

The screenshot displays the Scifinder search results page for compound 1. The URL is <https://scifinder-n.cas.org/search/substance/6619f0f1643c682c0e8d333e/1>. The page title is "Substances search for drawn structure".

Search Filters:

- Structure Match: As Drawn (0), **Substructure (7)**, Similarity (159K)
- Filtering: Stereochemistry: Absolute Stereo Match
- Search Patent Markush:
- Clear All Filters
- View: Partial

Chemical Structure:

C17H21O5
5-[(2S,3S)-2,3-Dihydro-5,6-dimethoxy-3-methyl-2-benzofuran-1-yl]-2-methoxy phenol

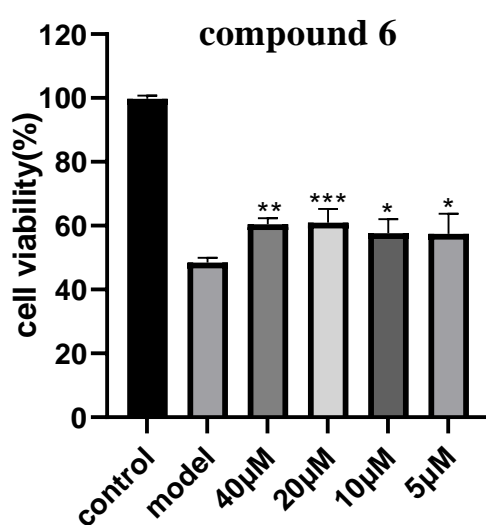
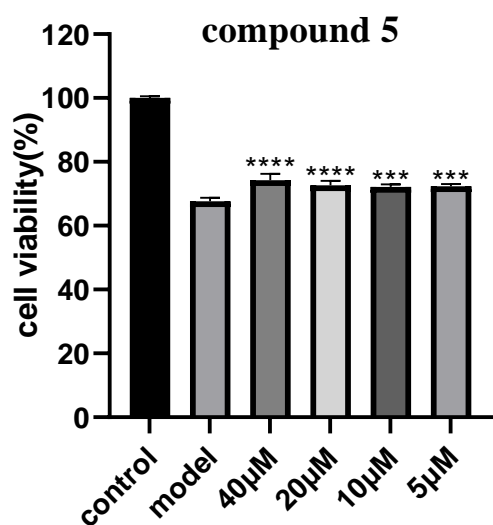
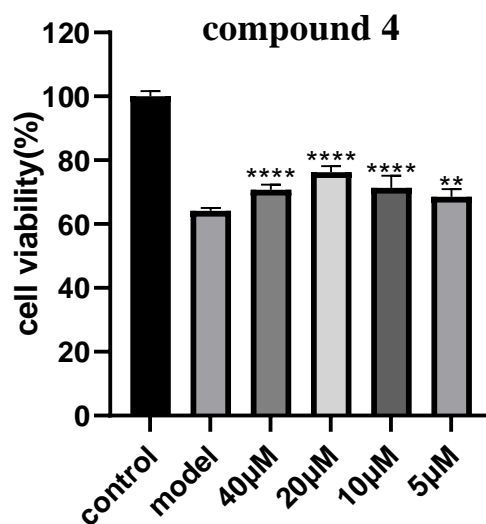
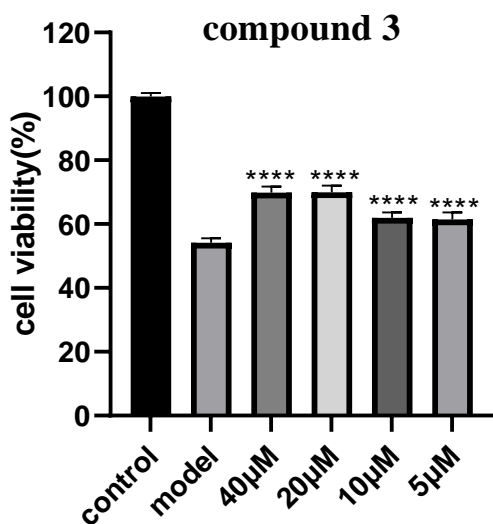
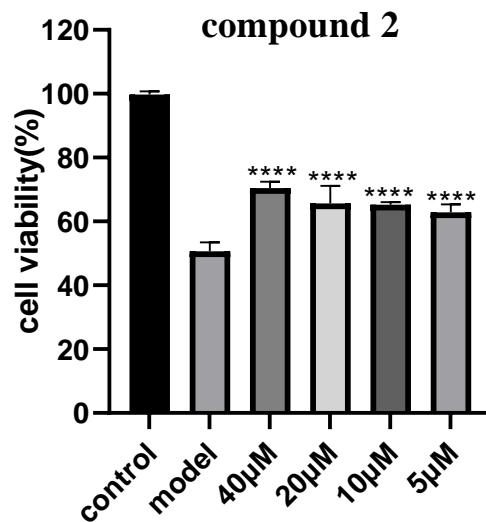
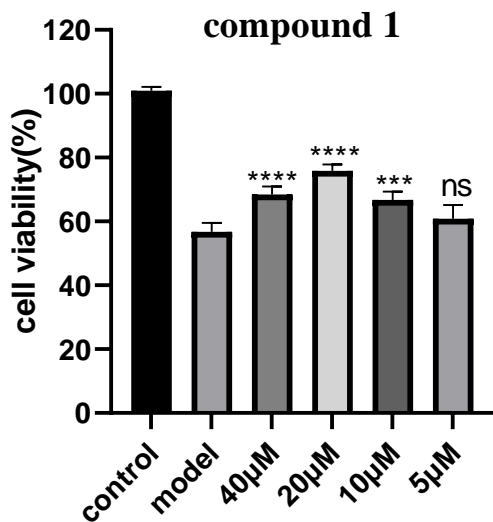
Results:

- 1 Result
- 1 Reference
- 0 Reactions
- 1 Supplier

Left Panel:

- Structure Match: As Drawn (0), **Substructure (7)**, Similarity (159K)
- Analyze Structure Precision
- Chemescape Analysis: Visually explore structure similarity with a powerful new tool. Learn more about Chemescape. [Create Chemescape Analysis](#)
- Filter Behavior: [Filter by](#), [Exclude](#)
- Search Within Results: Reference Role, Biological Study (1)

Figure S30: Scifinder search report of compound 1



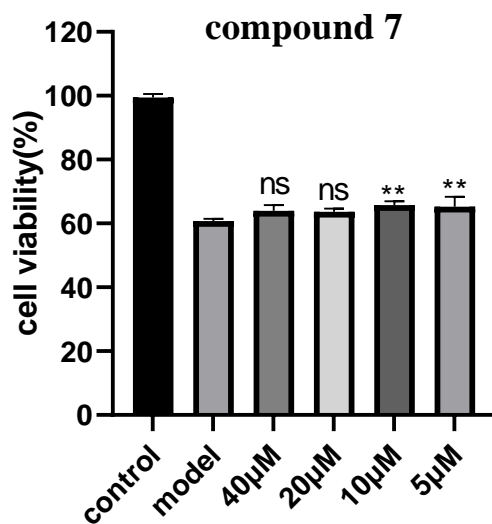


Figure S31: Protective effects of compounds 1-7 on H/R(hypoxia/reoxygenation) induced injury in H9c2 (Values are expressed as the mean \pm SD of 4 replicates; * $P < 0.05$, ** $P < 0.01$, *** $P < 0.001$ **** $P < 0.0001$ versus model group cell).