

## Supporting Information

*Rec. Nat. Prod.* 18:4 (2024) 452-457

### 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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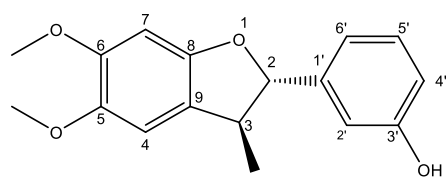
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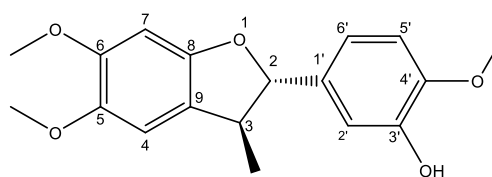
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compound 1



pterolinuses C

**Table S1:** The most similar compound data to compound 1

position	compound 1 <sup>a</sup>		pterolinuses C <sup>b</sup>	
	$\delta_{\text{H}}$	$\delta_{\text{C}}$	$\delta_{\text{H}}$	$\delta_{\text{C}}$
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 <sub>3</sub>	1.33 (3H, d, $J = 6.8$ Hz)	18.6	1.34 (1H, d, $J = 6.8$ Hz)	19.4
5-OCH <sub>3</sub>	3.69 (3H, s)	56.6	3.78 (1H, s)	57.0
6-OCH <sub>3</sub>	3.73 (3H, s)	55.8	3.74 (1H, s)	58.1
3'-OH	9.44 (1H, s)	-	7.73 (1H, s)	-
4'-OCH <sub>3</sub>	-	-	3.84 (1H, s)	56.9

<sup>a</sup> Measured in DMSO-*d*<sub>6</sub>, -600 MHz

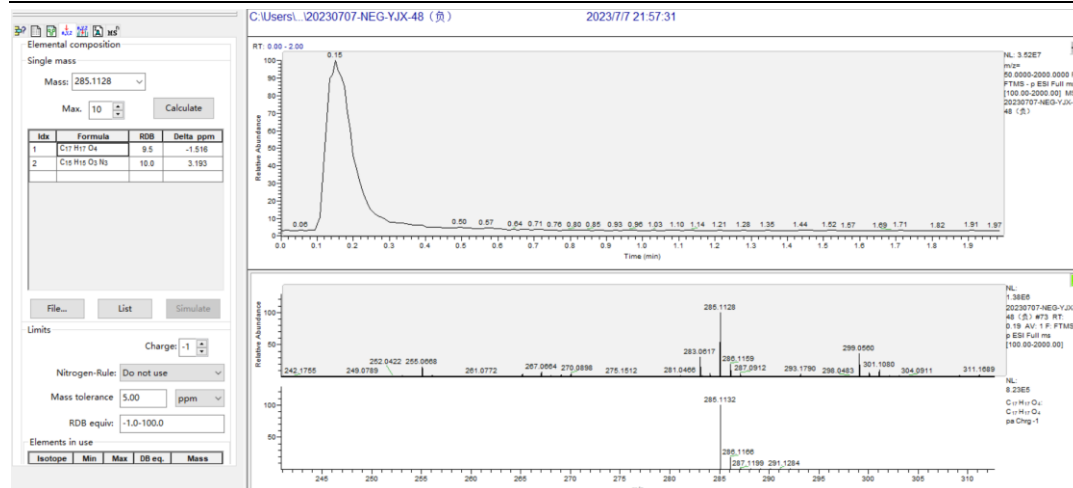
<sup>b</sup> Measured in Acetone-*d*<sub>6</sub>, -500 MHz

### References

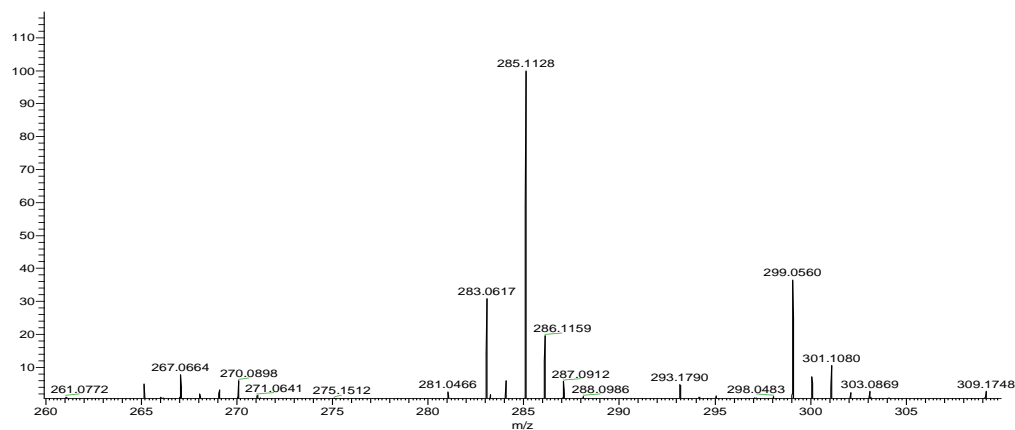
S.F. Wu, F.R. Chang, S.Y. Wang, T.L. Hwang, C.L. Lee, S.L. Chen, C.C. Wu and Y.C. Wu (2011). Anti-inflammatory and cytotoxic neoflavonoids and benzofurans from *Pterocarpus santalinus*, *J. Nat. Prod.* **74**, 989-996

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

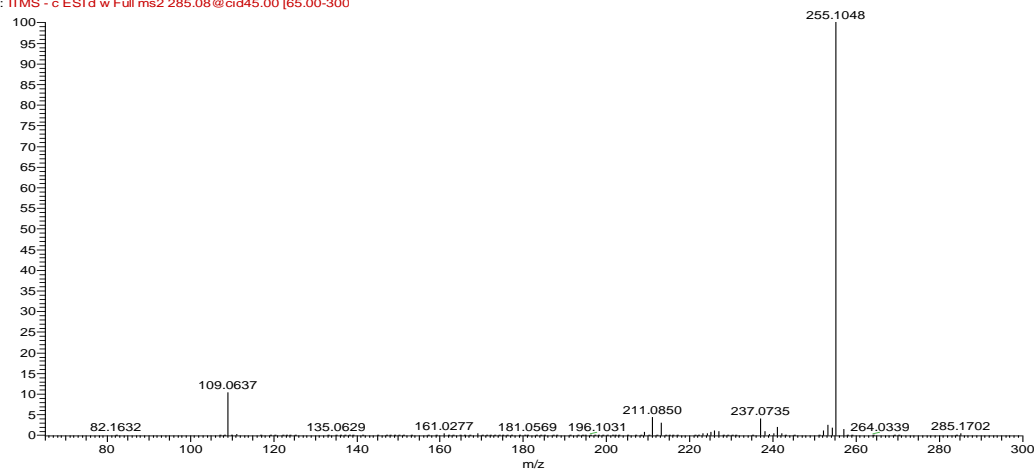
compound	Ionic mode	Formula	Measured value (m/z)	Calculated value (m/z)	Error (ppm)
<b>1</b>	<b>[M-H]<sup>-</sup></b>	<b>C<sub>17</sub>H<sub>17</sub>O<sub>4</sub></b>	<b>285.1128</b>	<b>285.1132</b>	<b>-1.516</b>



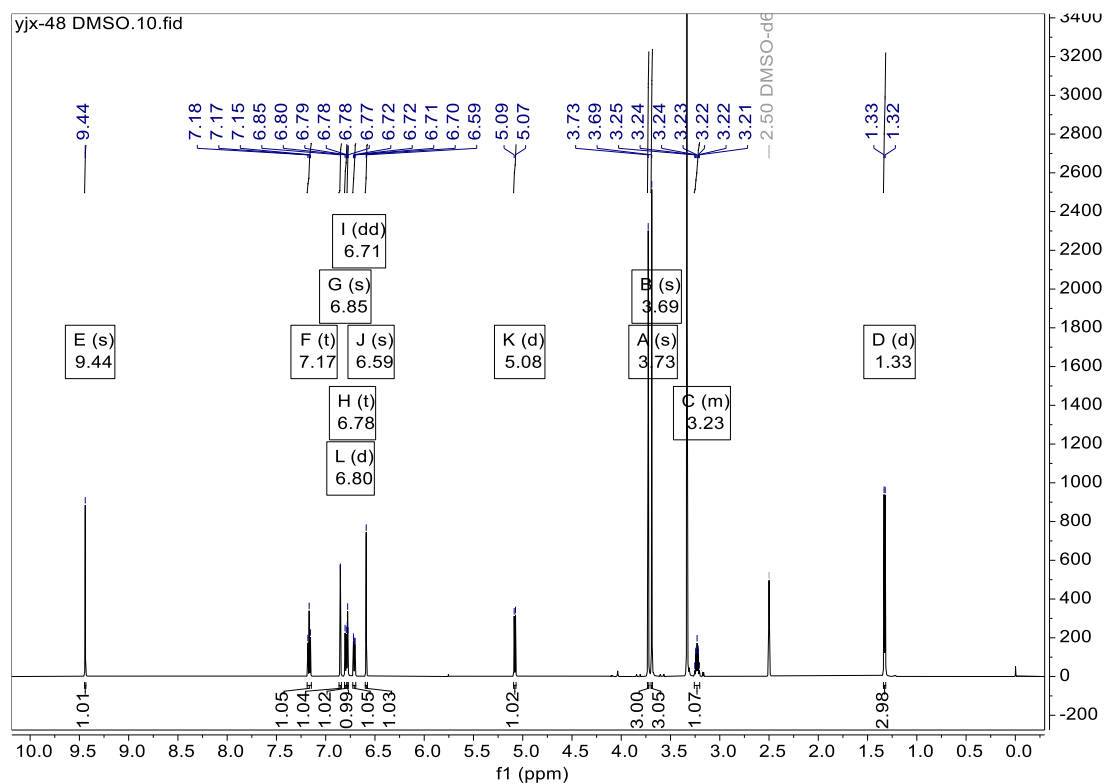
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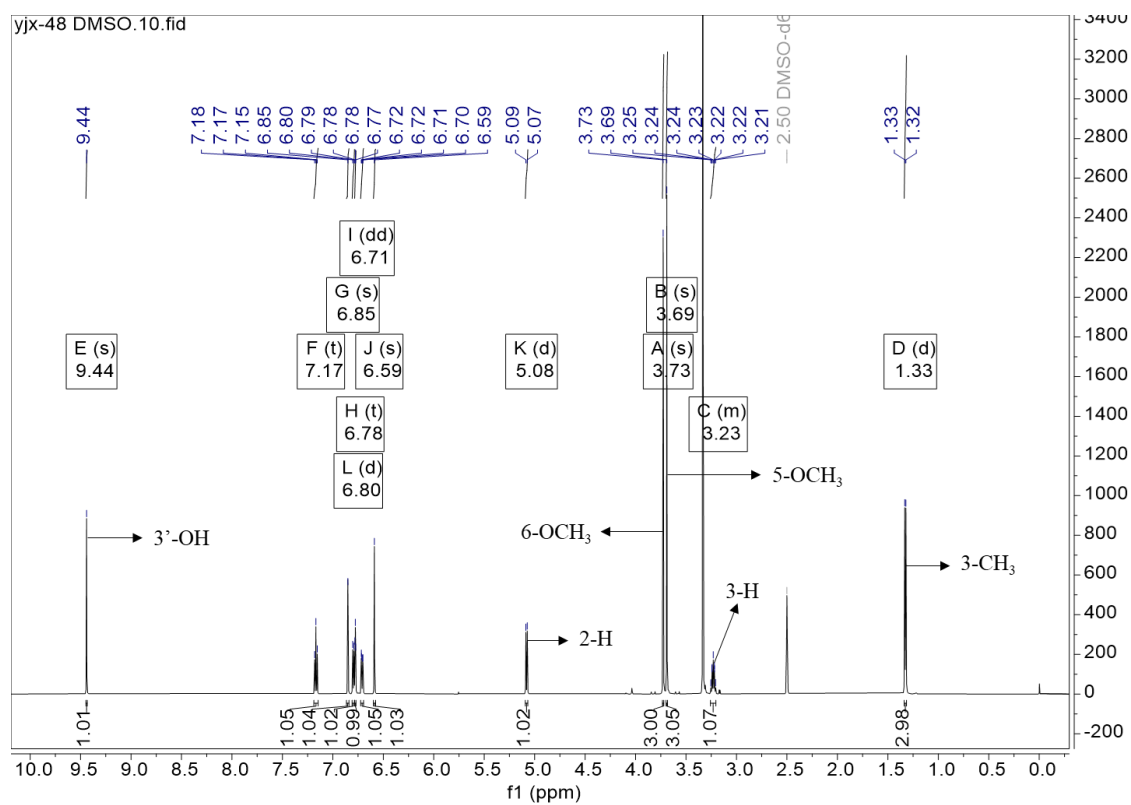
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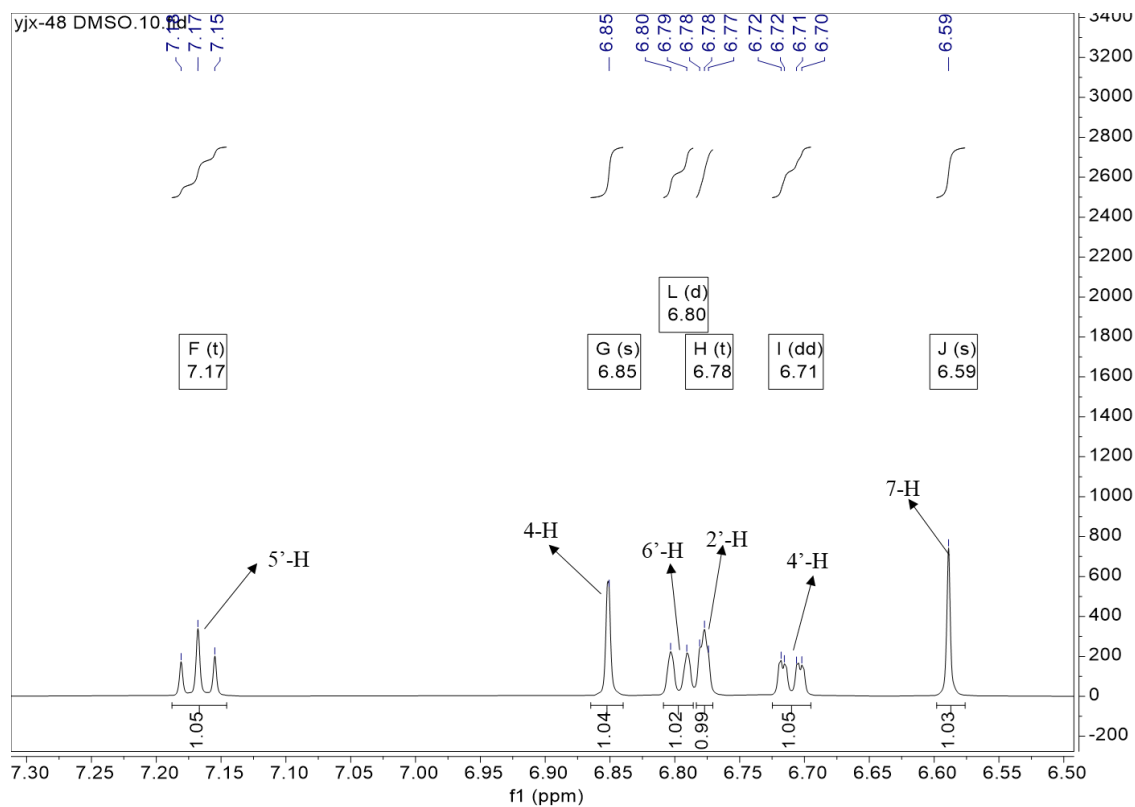
**Figure S1:** HR-ESI-MS spectrum of compound **1**



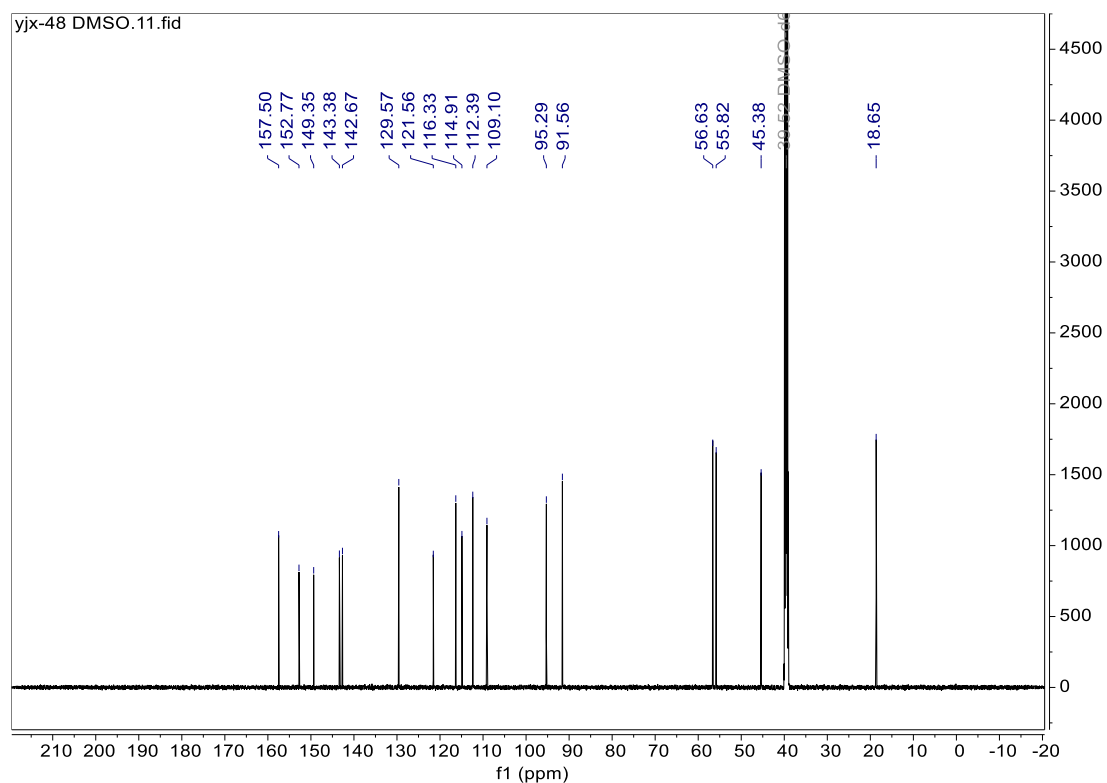
**Figure S2:**  $^1\text{H-NMR}$  (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **1**



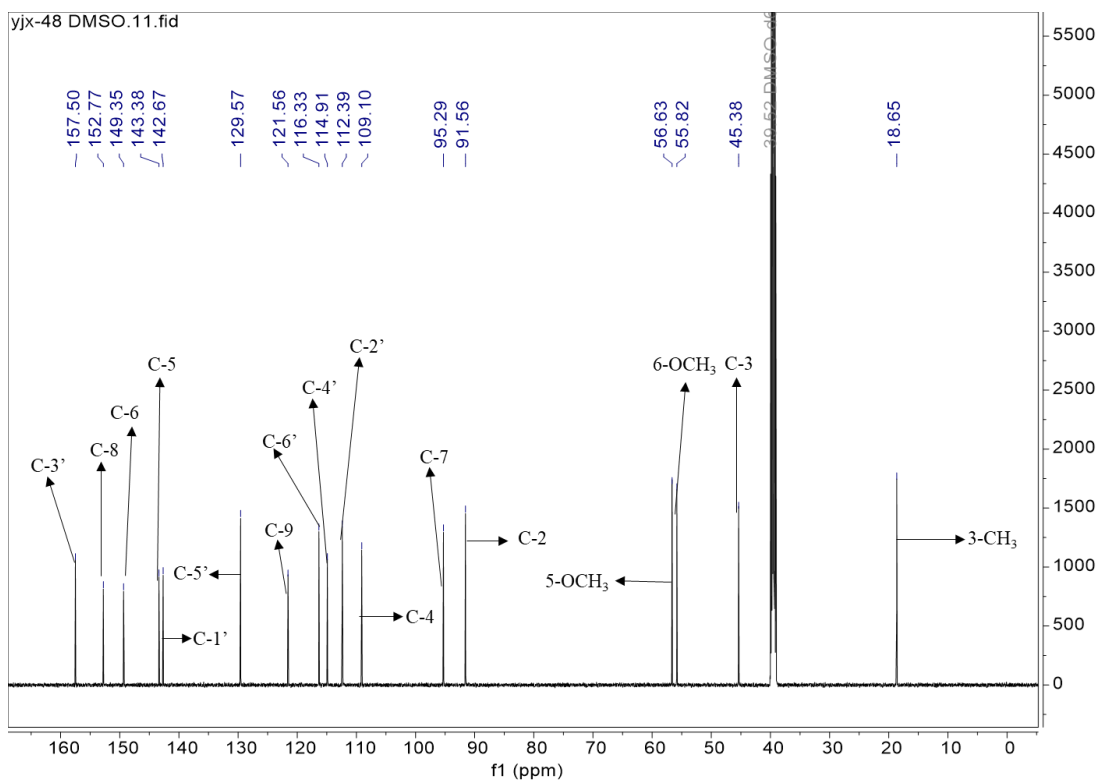
**Figure S3:** The labeled  $^1\text{H-NMR}$  spectrum of compound **1**



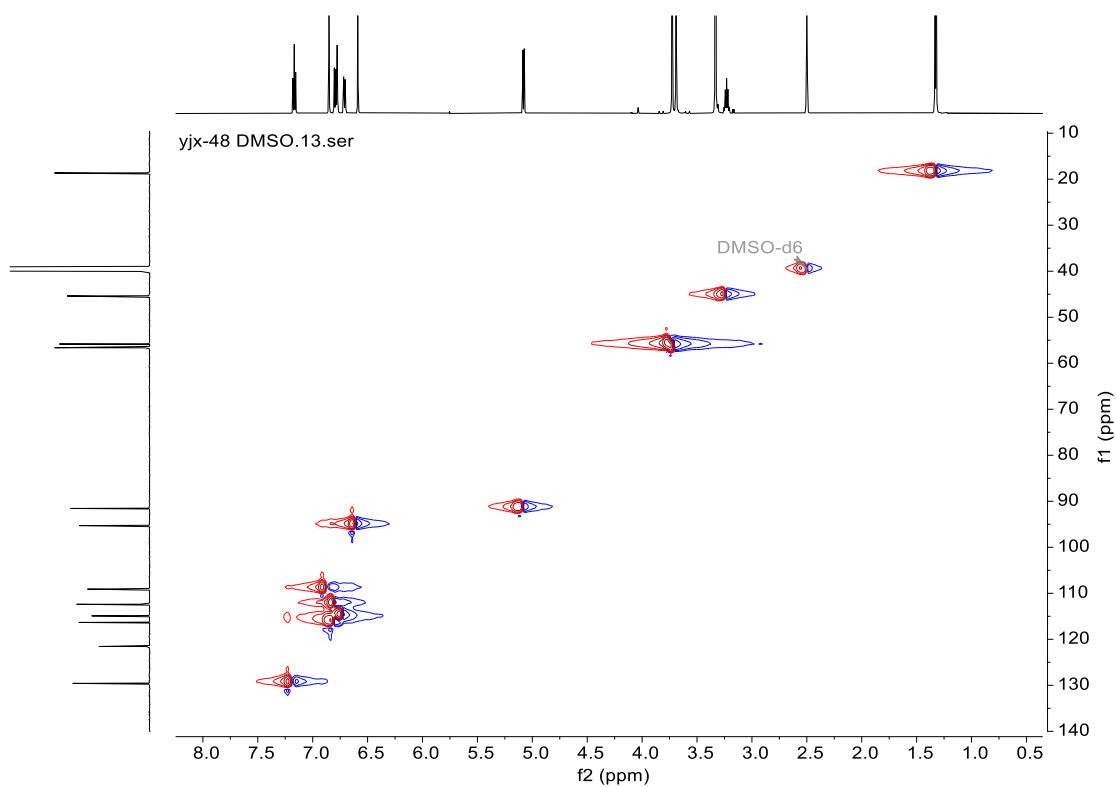
**Figure S4:** The labeled  $^1\text{H-NMR}$  spectrum of compound **1** (From  $\delta_H$  6.5 ppm to  $\delta_H$  7.3 ppm)



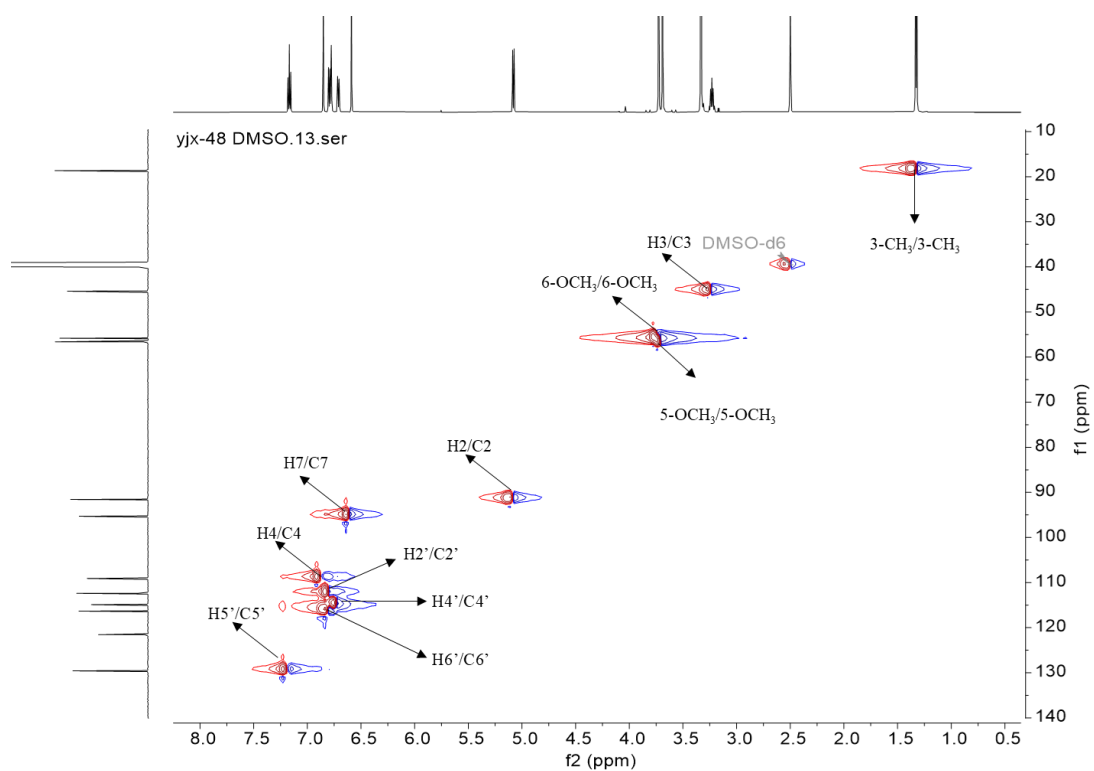
**Figure S5:**  $^{13}\text{C-NMR}$  (151 MHz, DMSO- $d_6$ ) spectrum of compound **1**



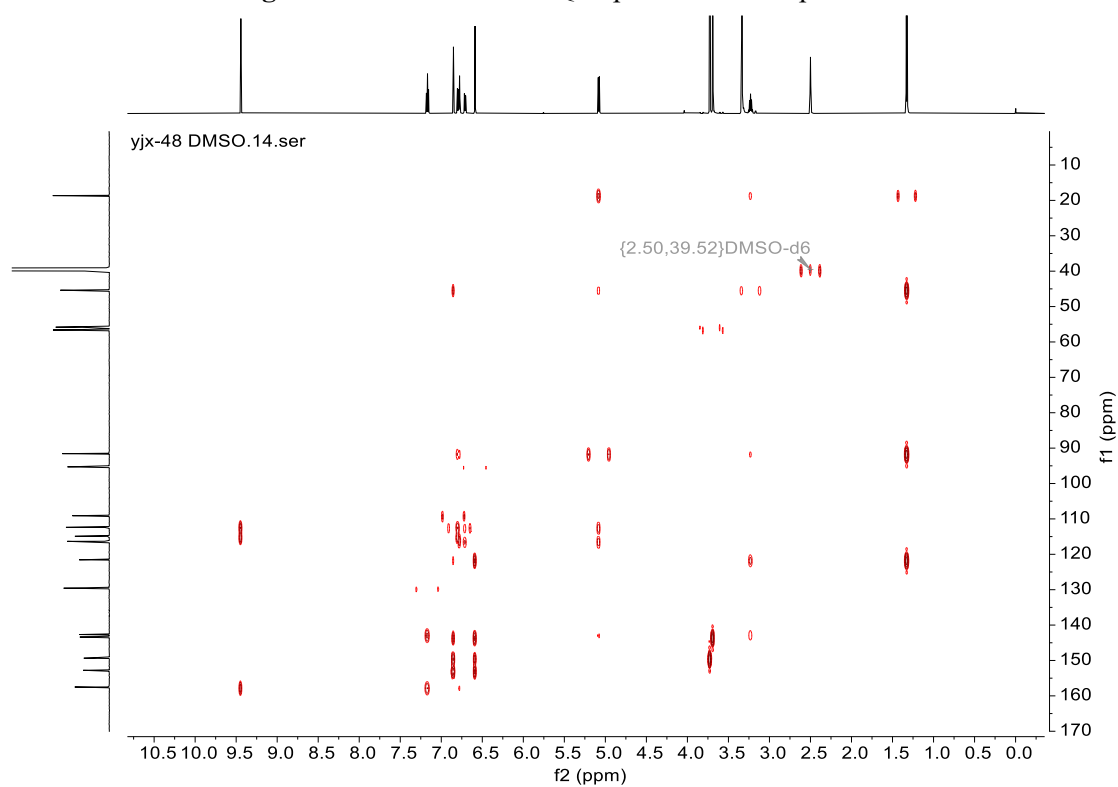
**Figure S6:** The labeled  $^{13}\text{C}$ -NMR spectrum of compound **1**



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

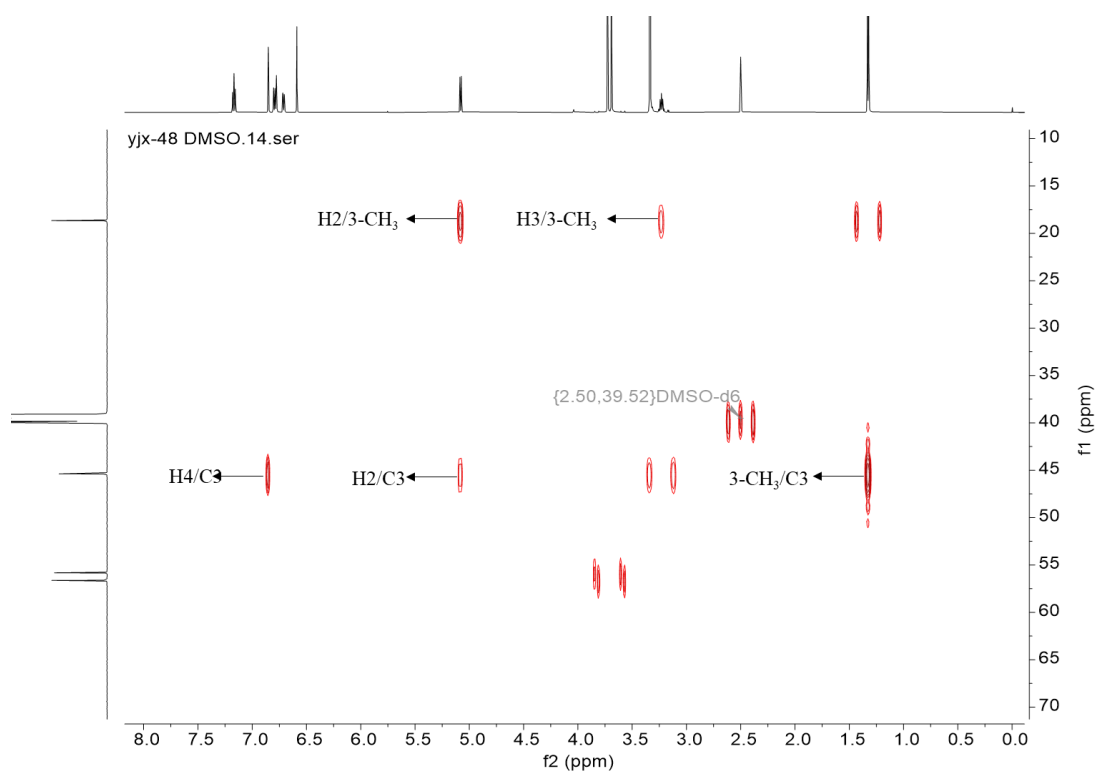


**Figure S8:** The labeled HSQC spectrum of compound **1**

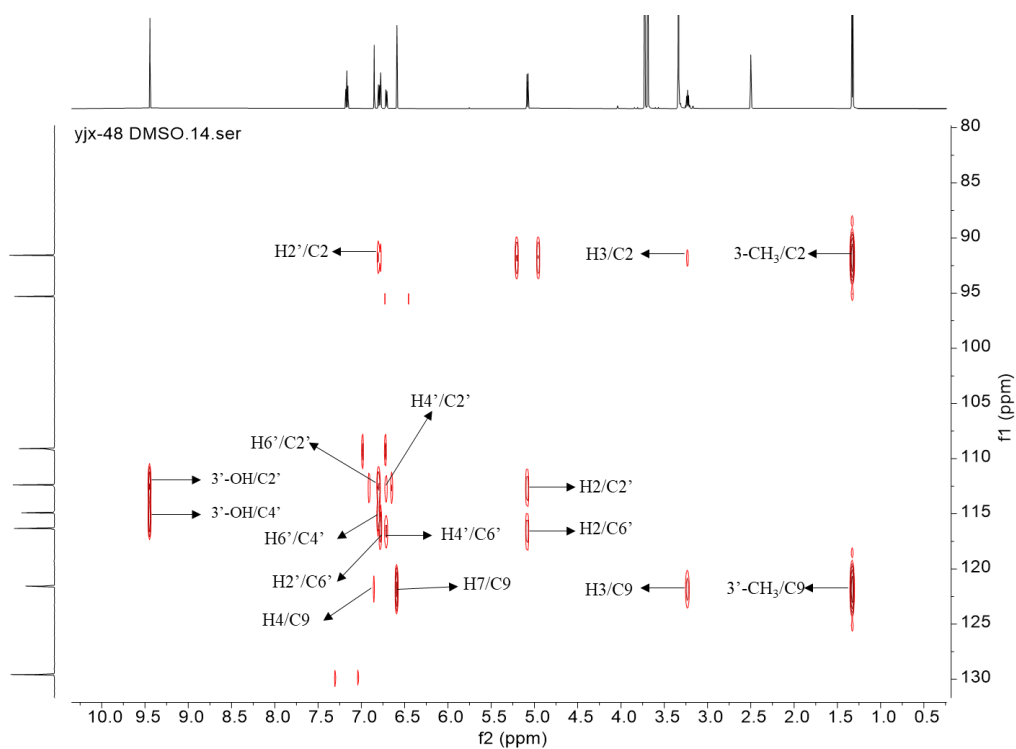


**Figure S9:** HMBC spectrum of compound **1**

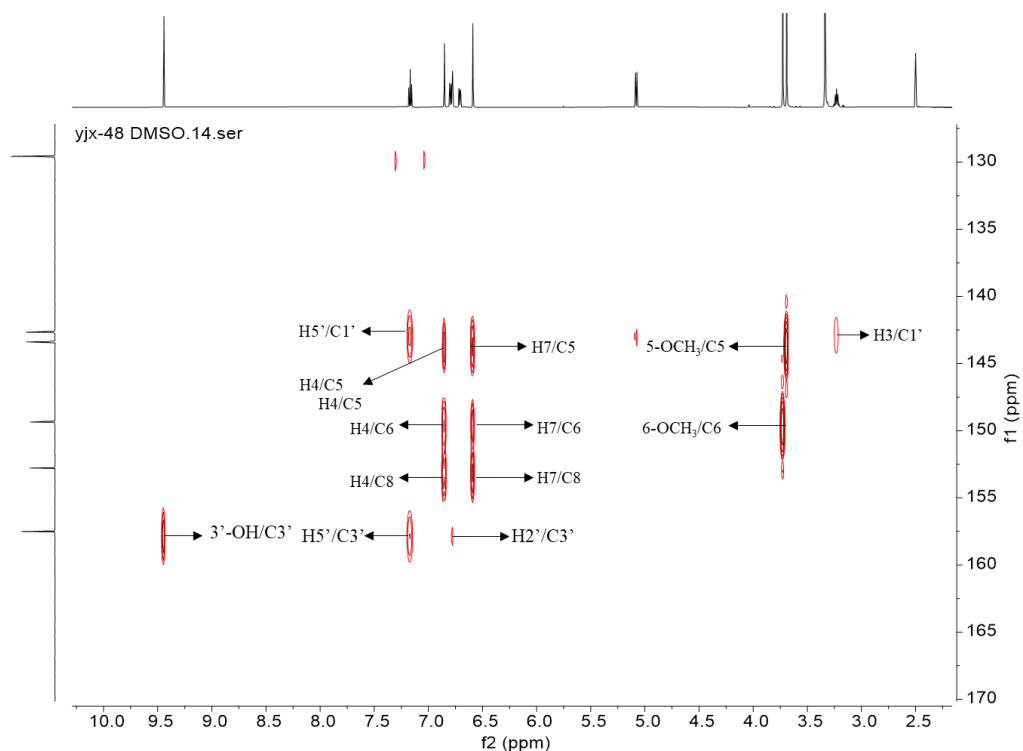




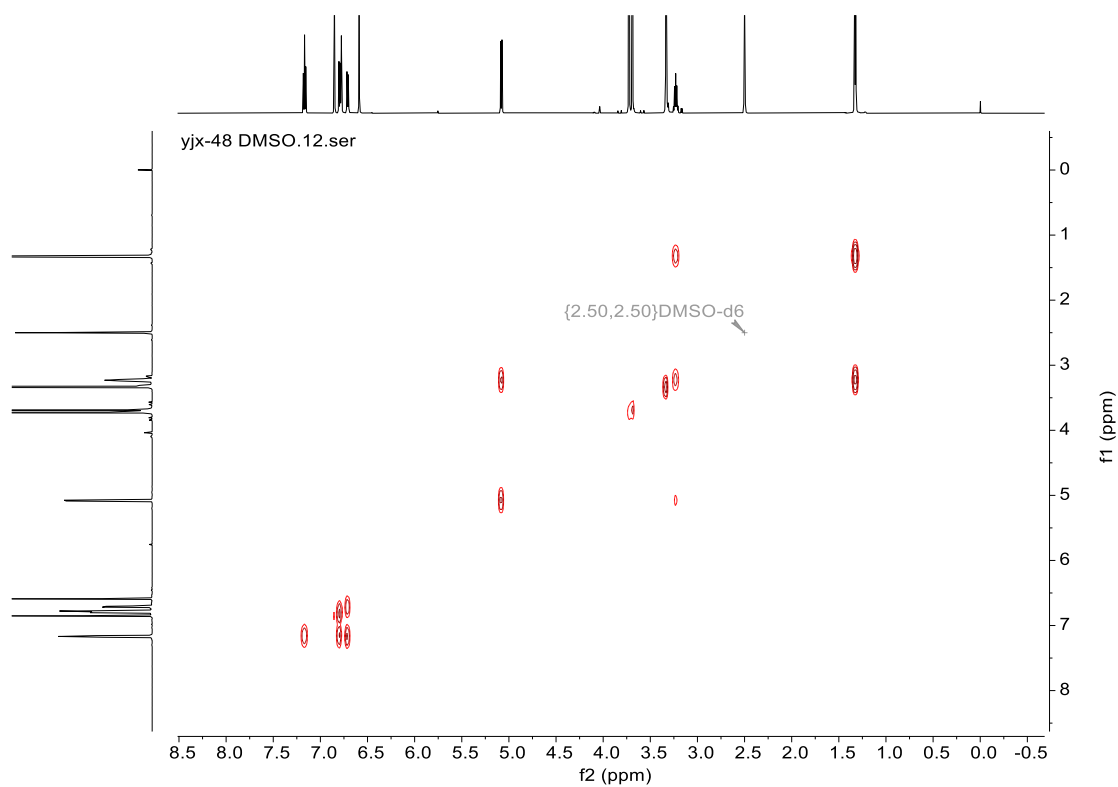
**Figure S10:** The labeled HMBC spectrum of compound **1** (From  $\delta_C$  10 ppm to  $\delta_C$  70 ppm)



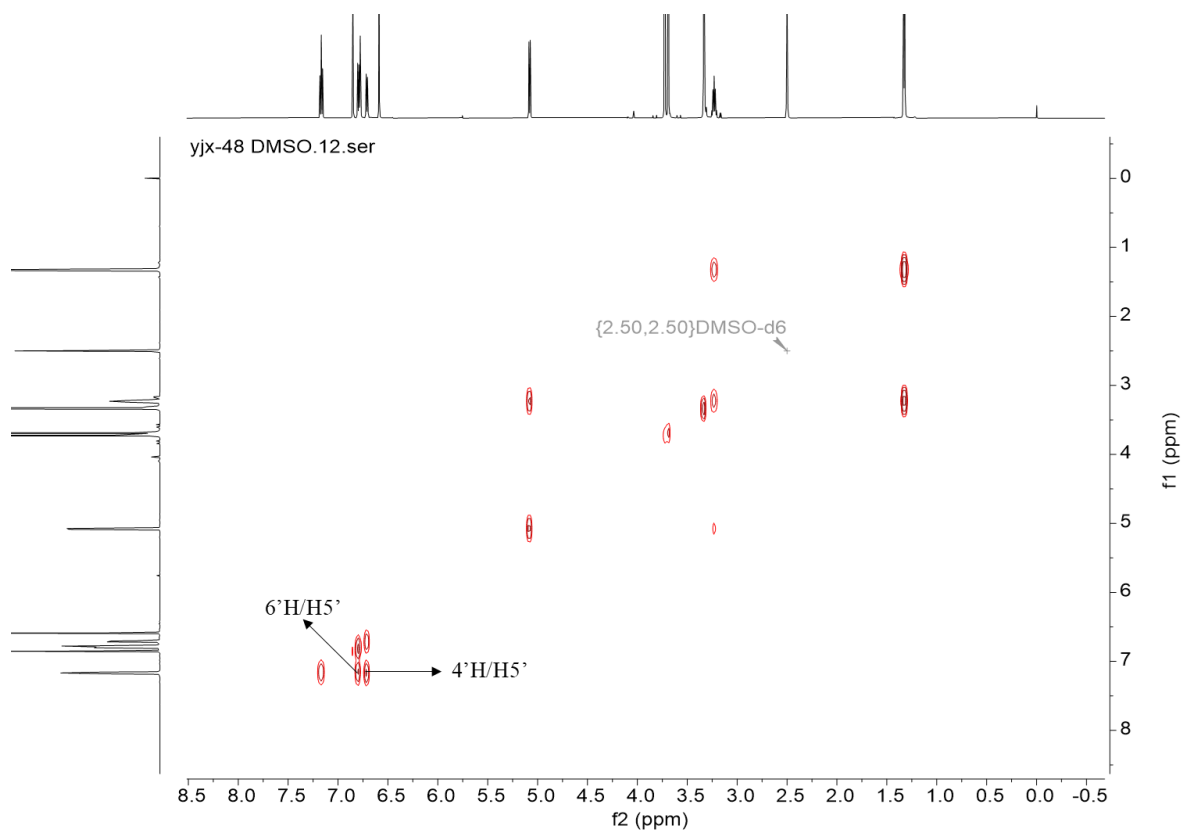
**Figure S11:** The labeled HMBC spectrum of compound **1** (From  $\delta_C$  80 ppm to  $\delta_C$  130 ppm)



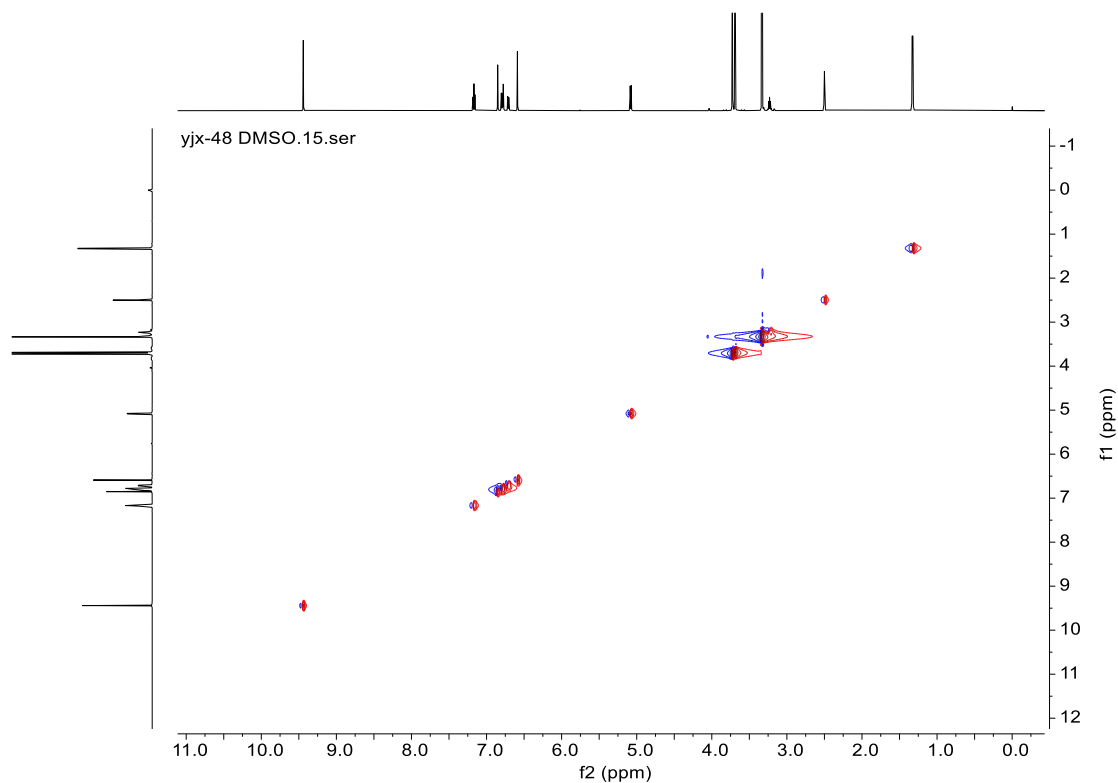
**Figure S12:** The labeled HMBC spectrum of compound **1** (From  $\delta_C$  130 ppm to  $\delta_C$  170 ppm)



**Figure S13:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1**



**Figure S14:** The labeled  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1**



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

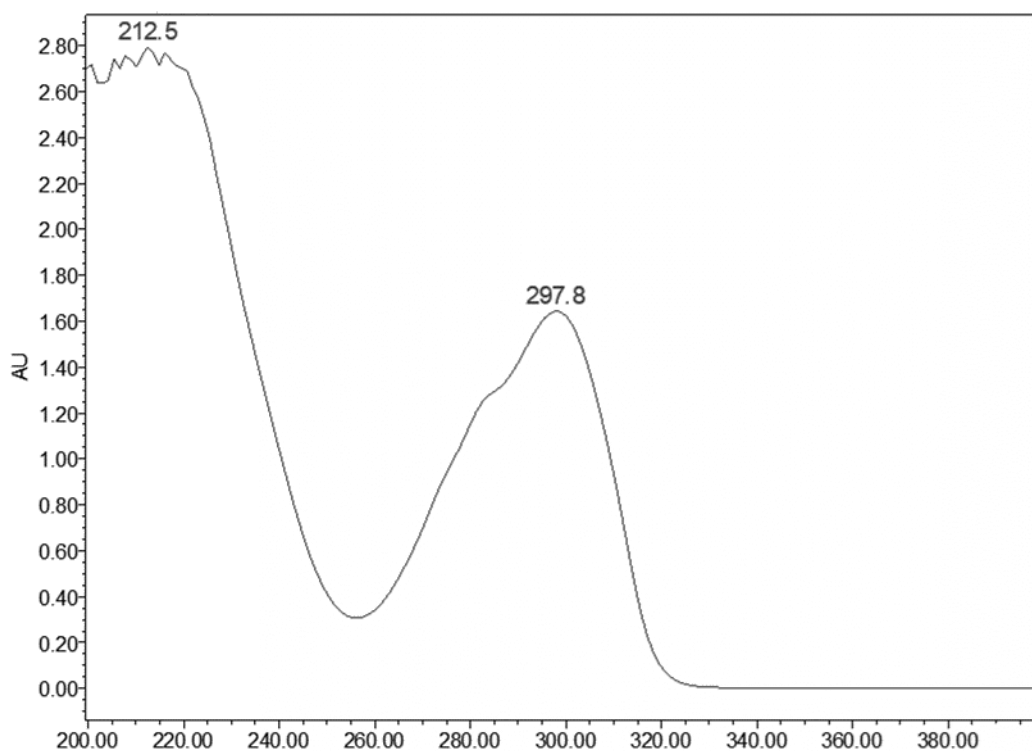


Figure S16: UV spectra of compound 1

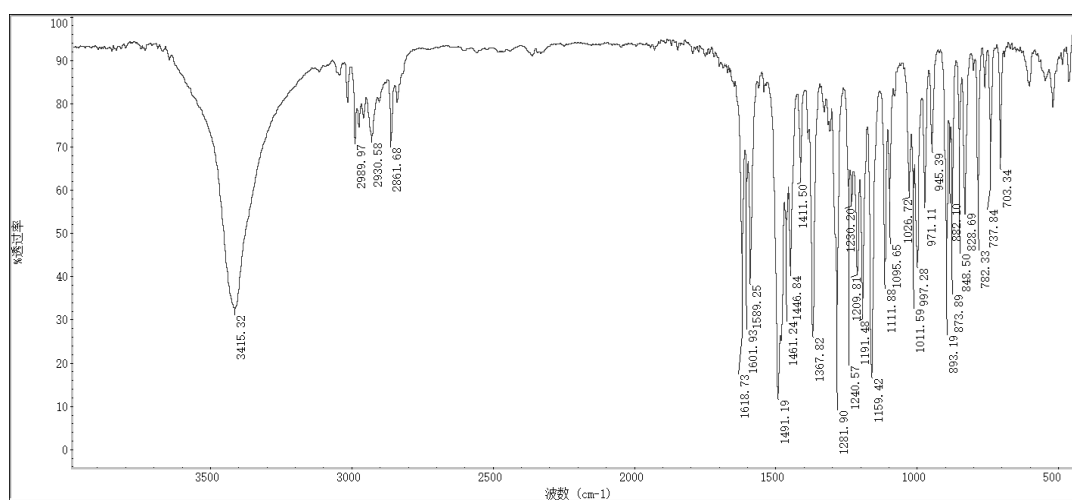


Figure S17: IR spectra of compound 1

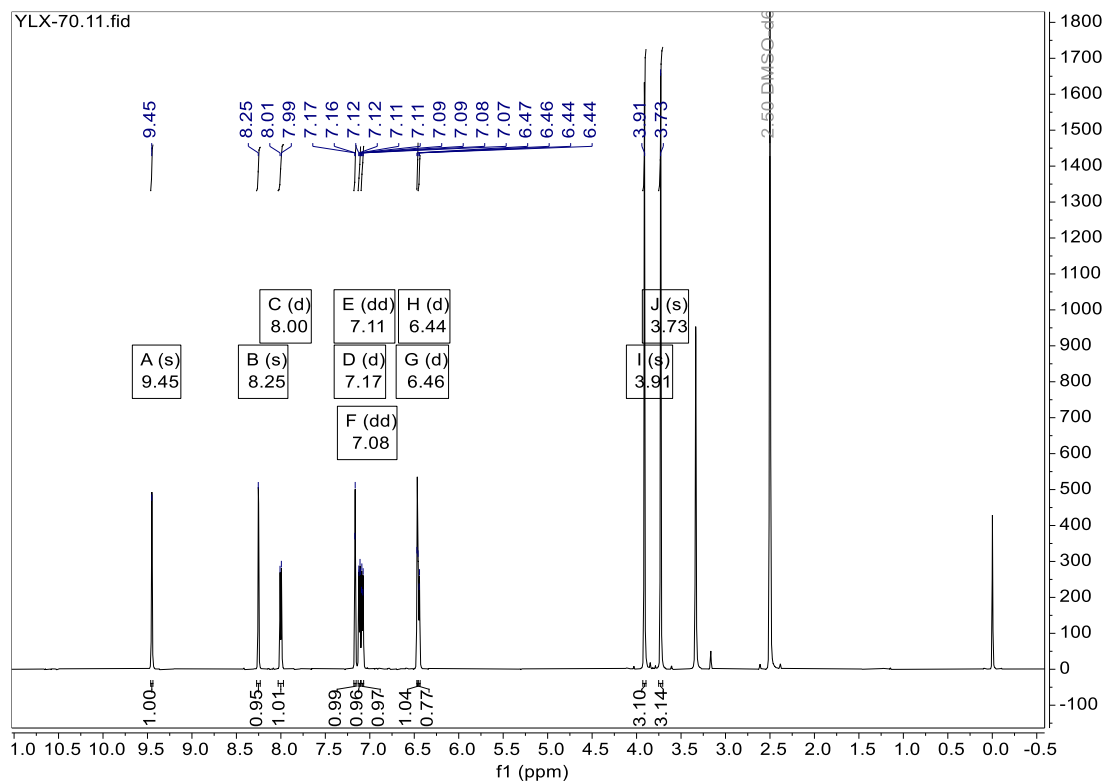


Figure S18: <sup>1</sup>H-NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 2

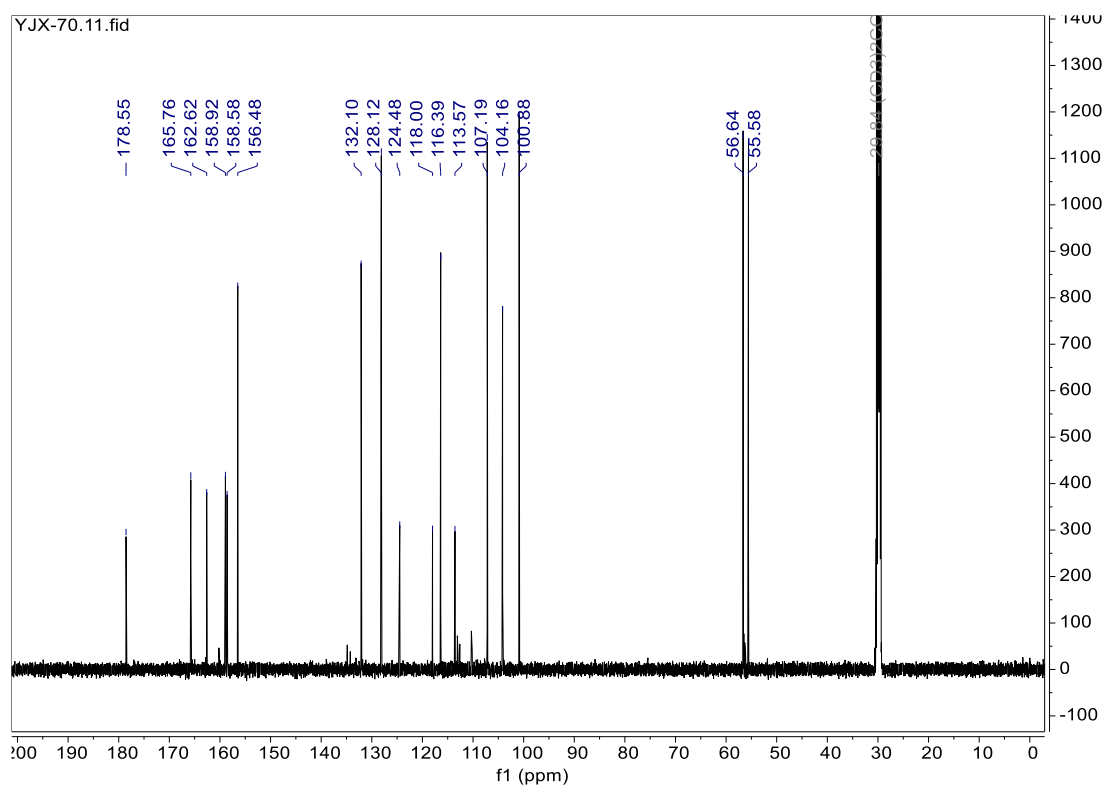


Figure S19: <sup>13</sup>C-NMR (151 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 2

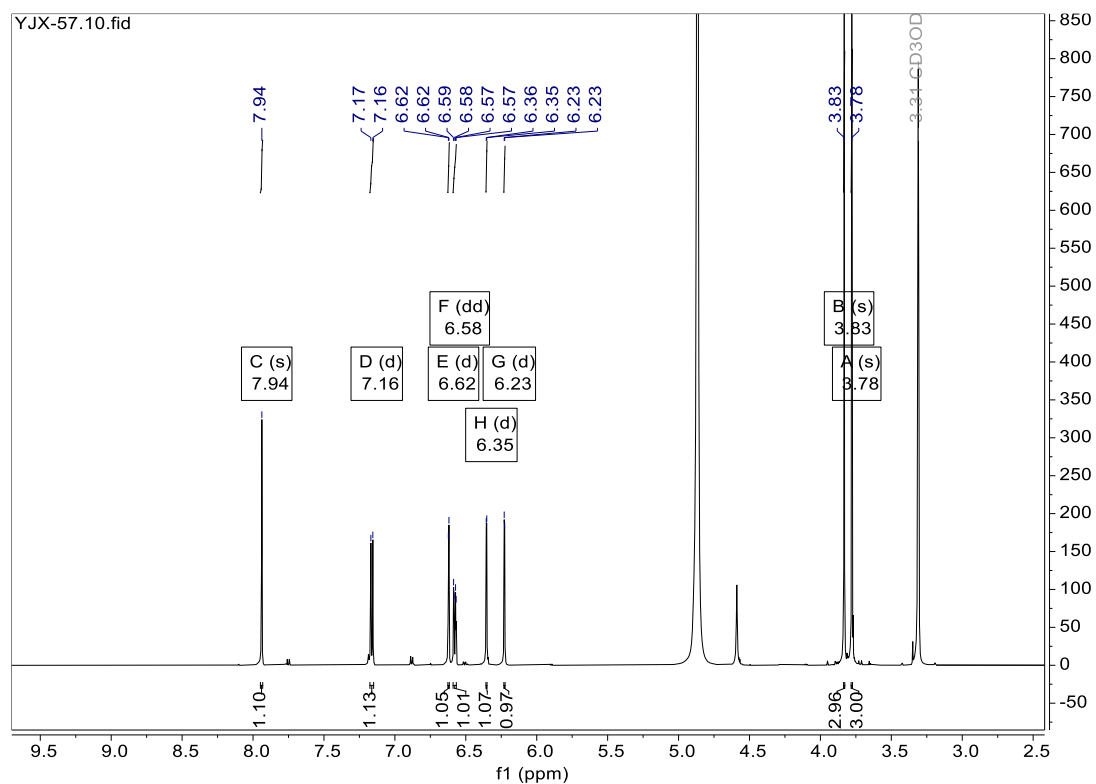


Figure S20:  $^1\text{H-NMR}$  (600 MHz, Methanol- $d_4$ ) spectrum of compound **3**

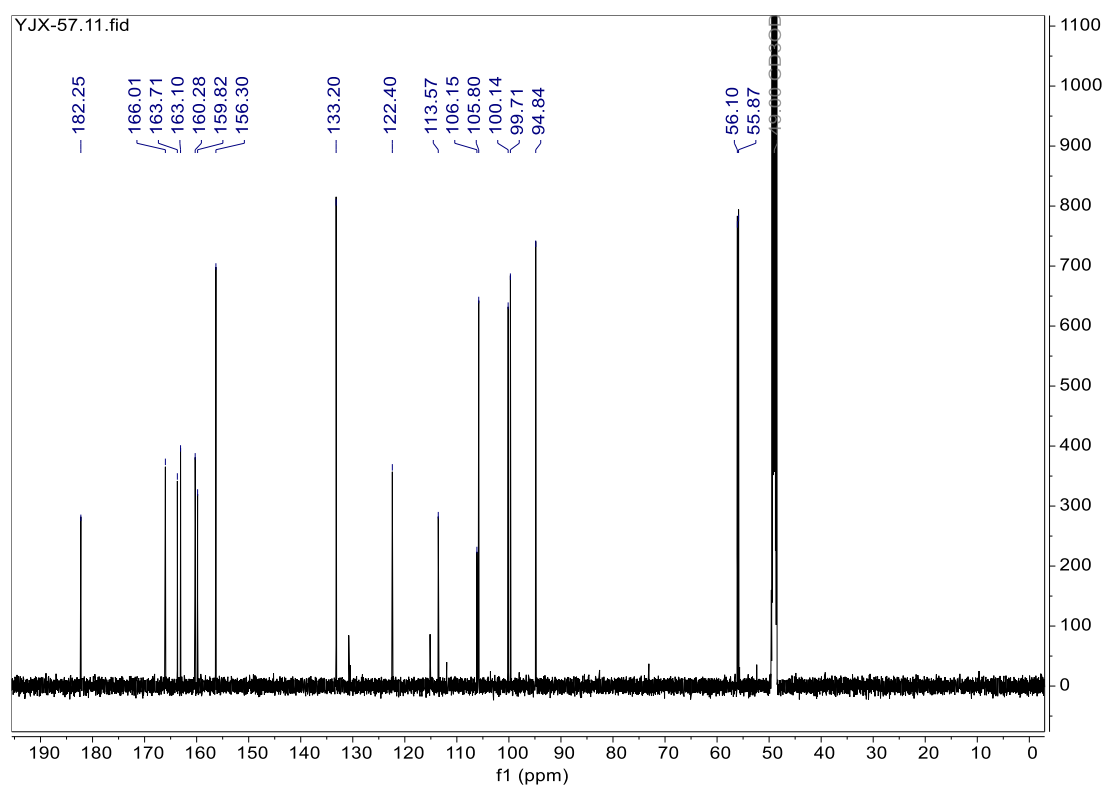


Figure S21:  $^{13}\text{C-NMR}$  (151 MHz, Methanol- $d_4$ ) spectrum of compound **3**

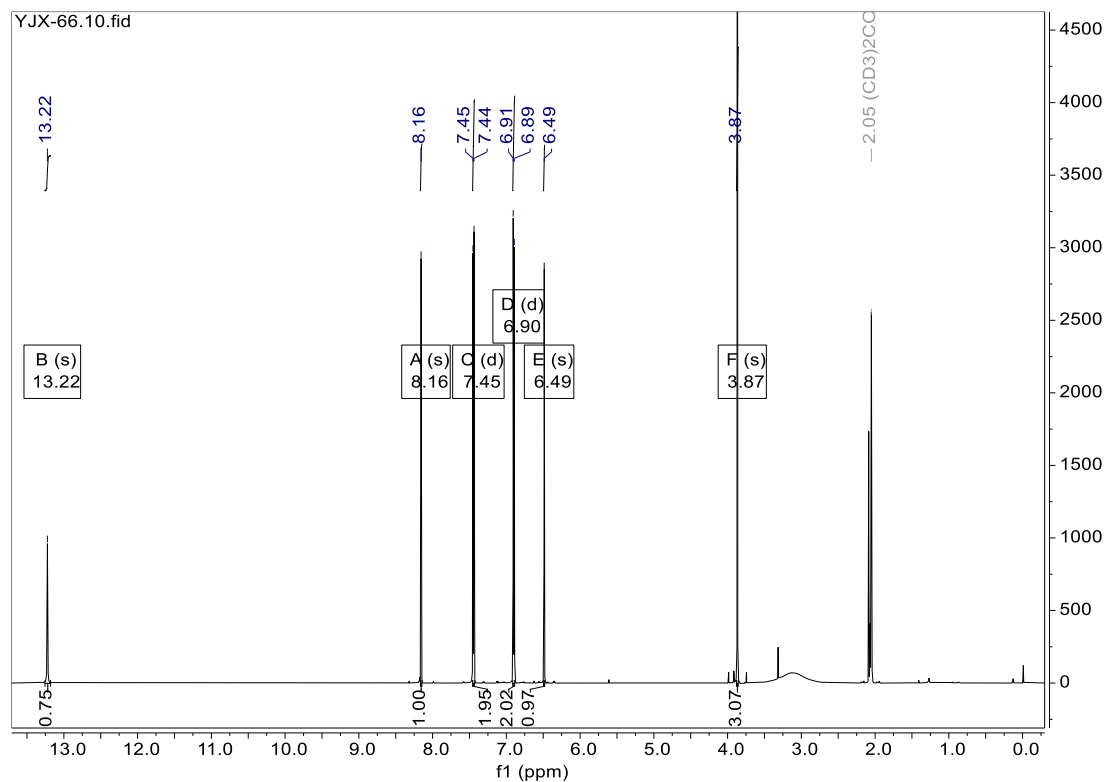


Figure S22:  $^1\text{H-NMR}$  (600 MHz, Acetone- $d_6$ ) spectrum of compound 4

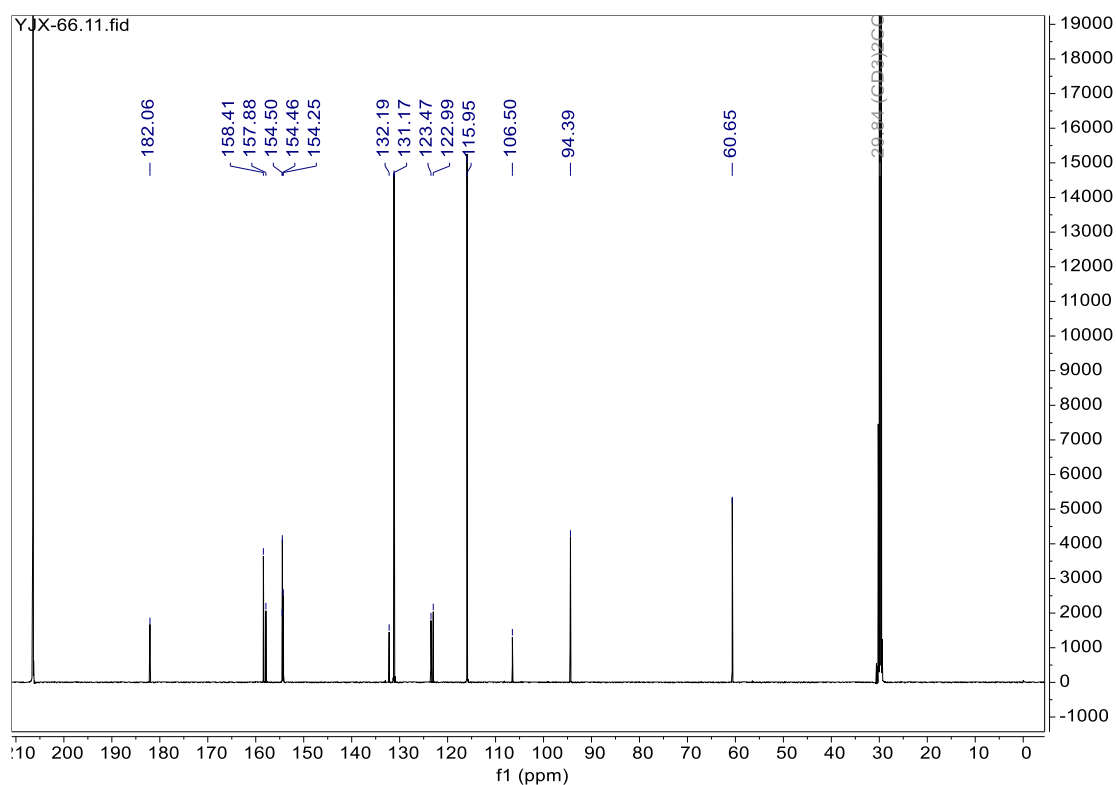


Figure S23:  $^{13}\text{C-NMR}$  (151 MHz, Acetone- $d_6$ ) spectrum of compound 4

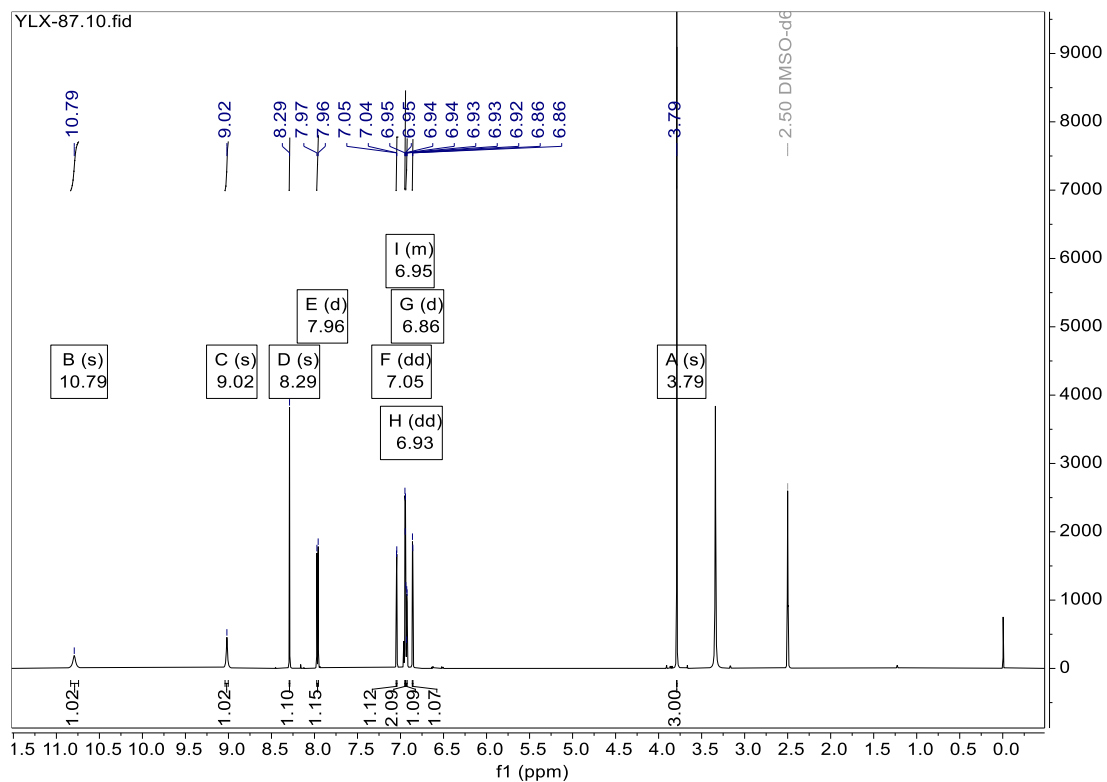


Figure S24:  $^1\text{H-NMR}$  (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **5**

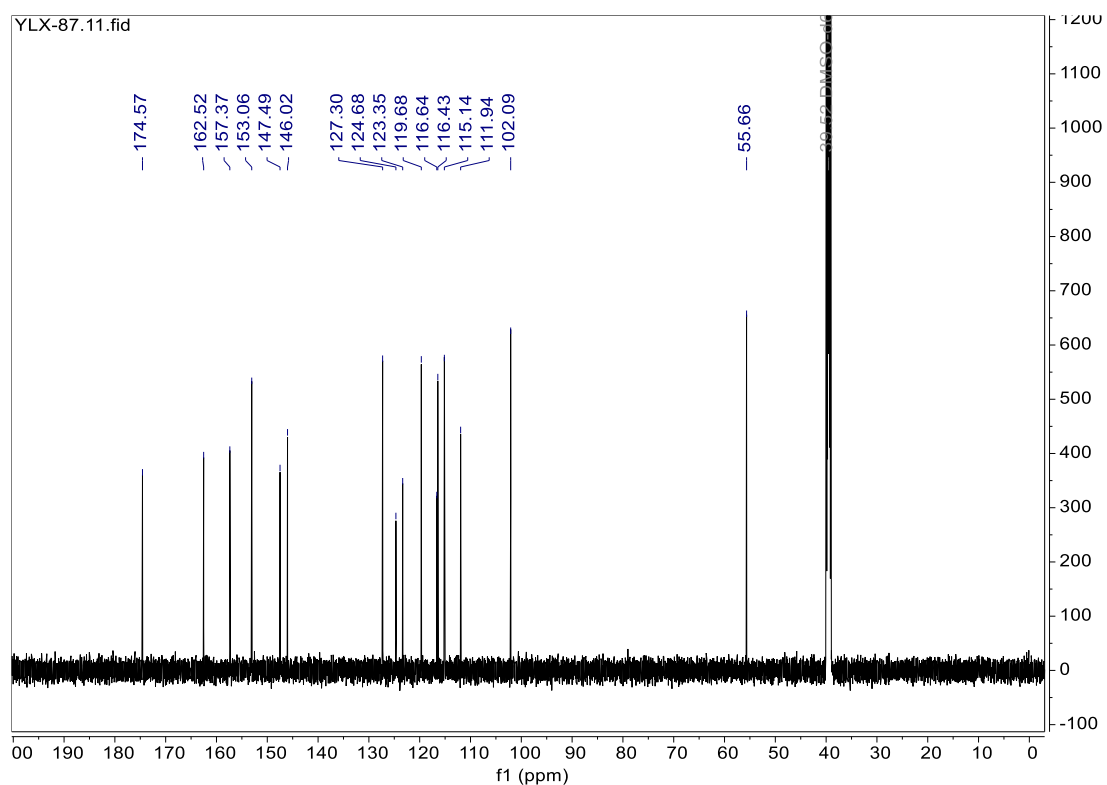


Figure S25:  $^{13}\text{C-NMR}$  (151 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **5**



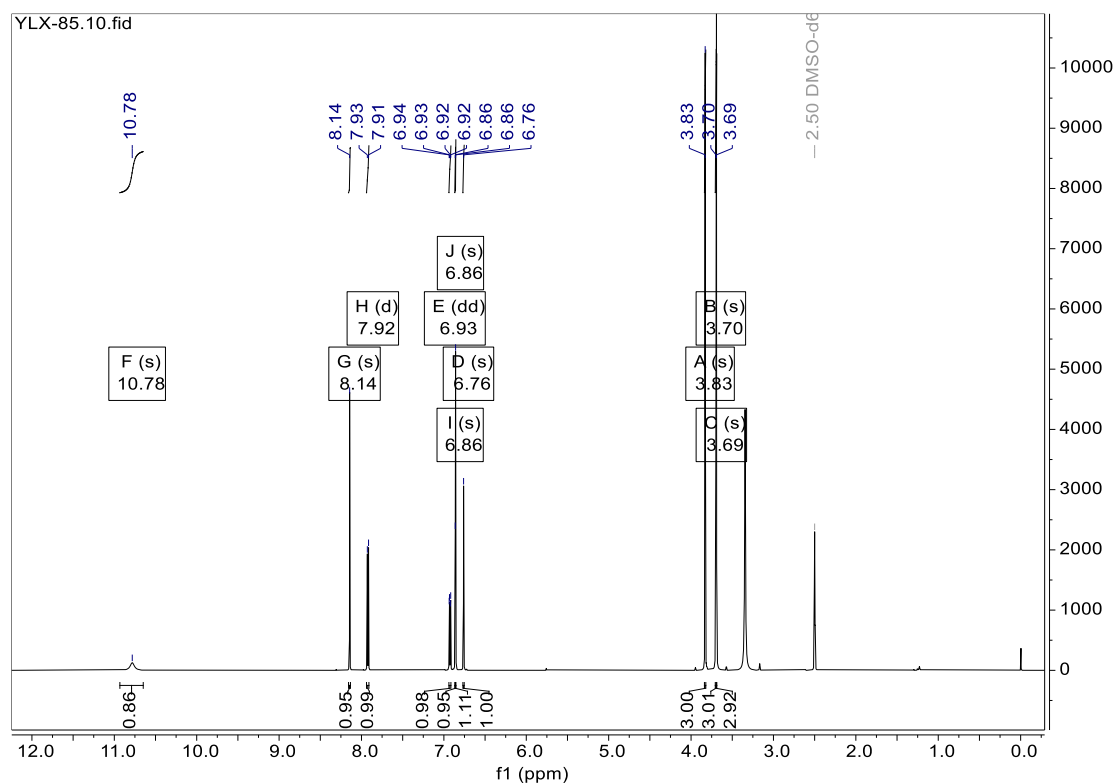


Figure S26:  $^1\text{H-NMR}$  (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **6**

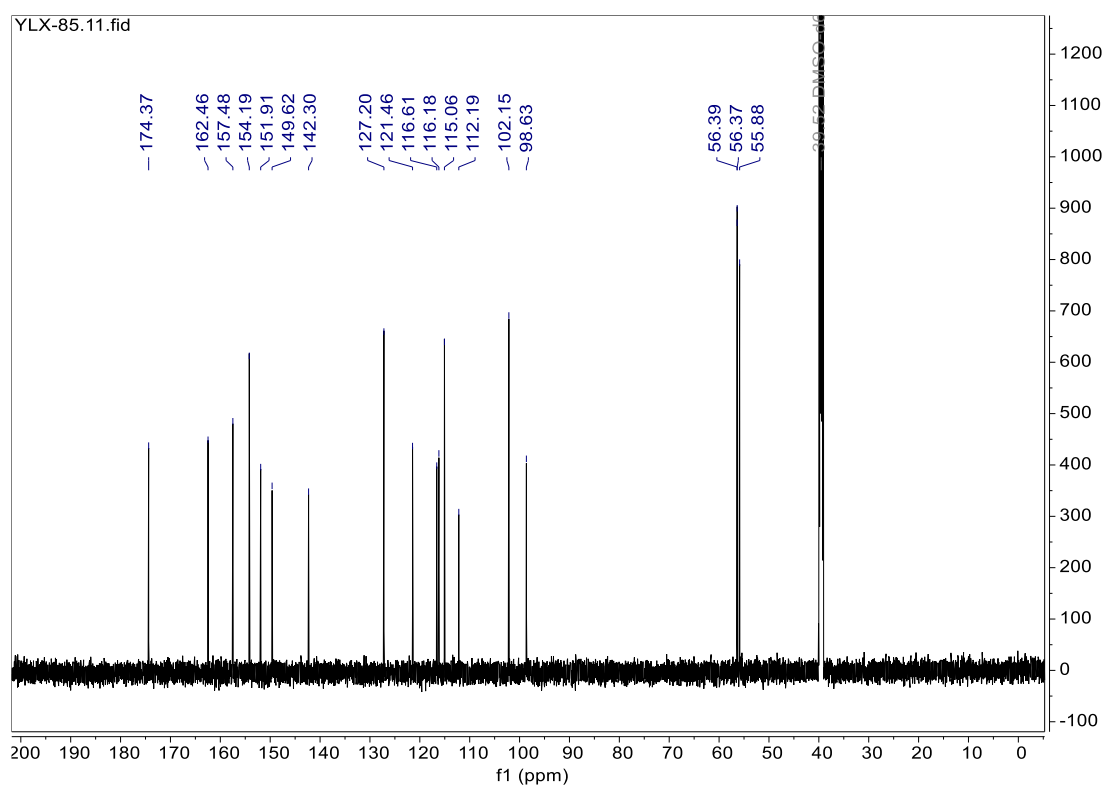


Figure S27:  $^{13}\text{C-NMR}$  (151 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **6**

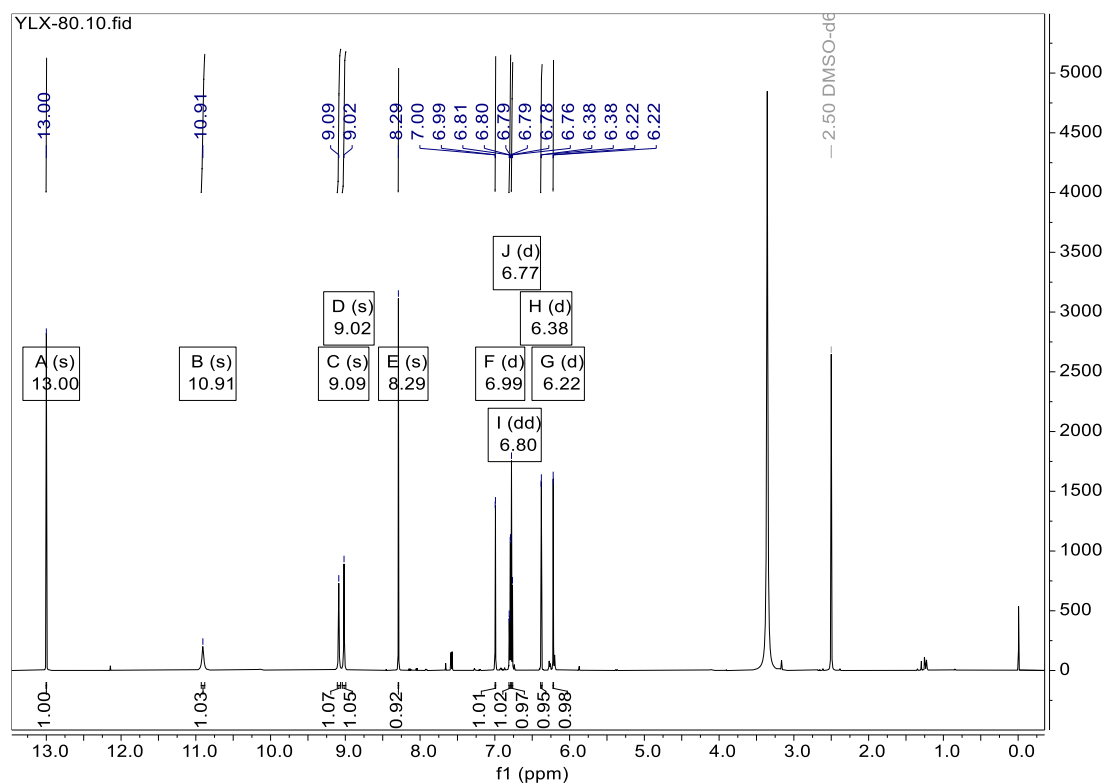


Figure S28:  $^1\text{H-NMR}$  (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 7

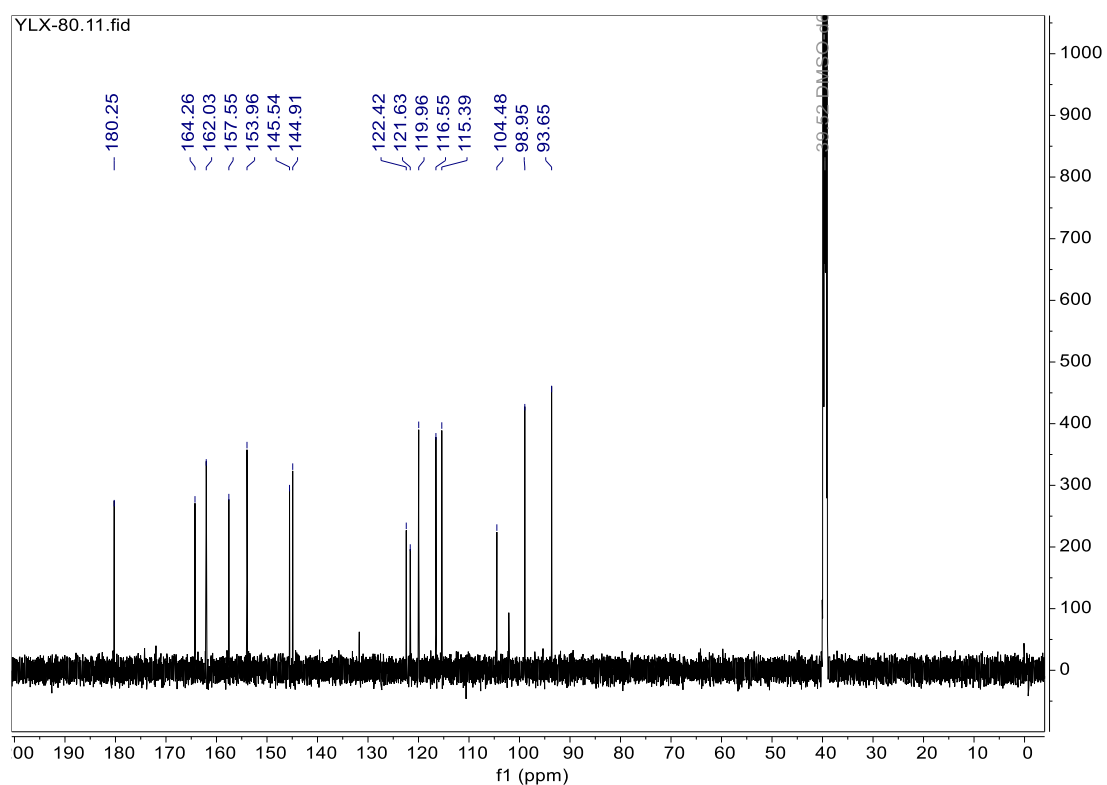


Figure S29:  $^{13}\text{C-NMR}$  (151 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 7

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

On the left side, there are several filter sections:

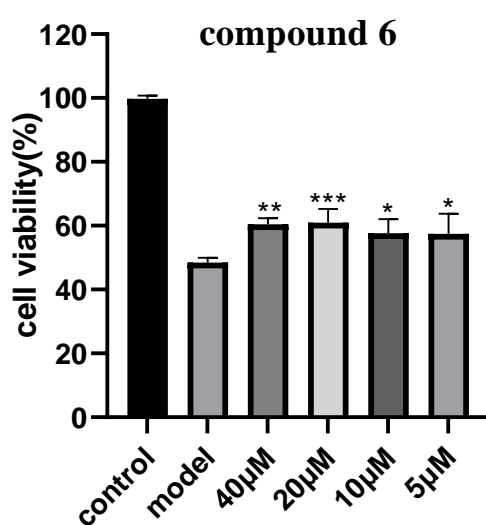
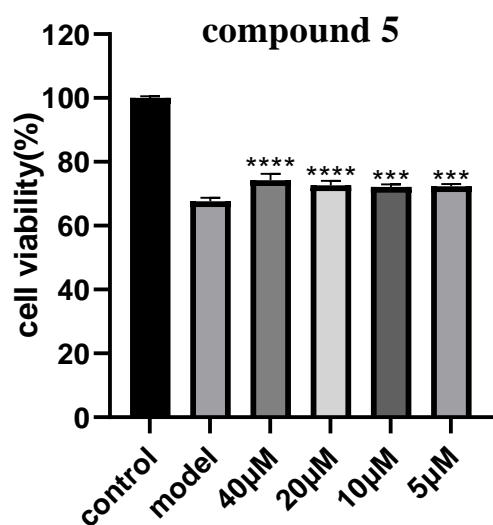
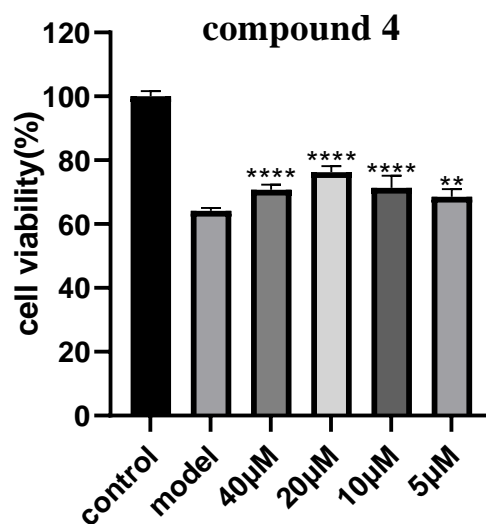
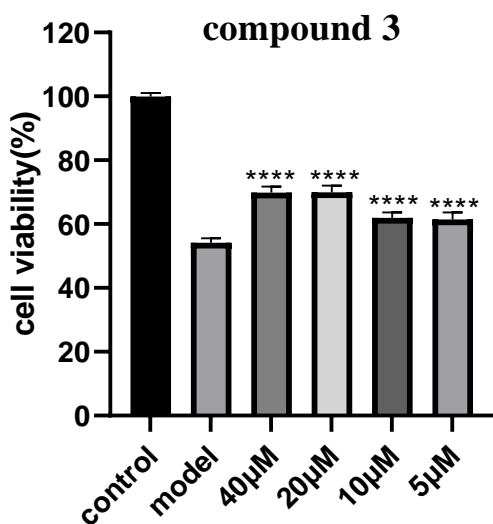
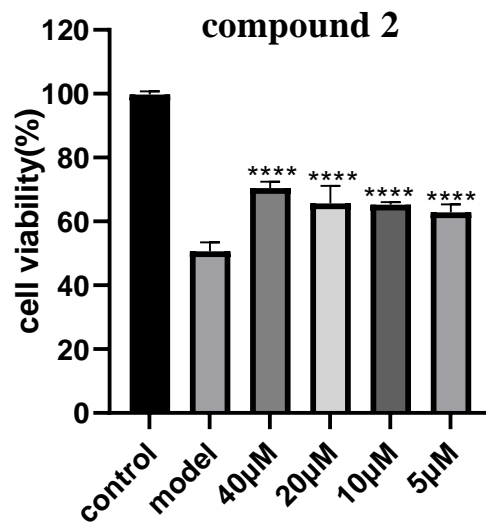
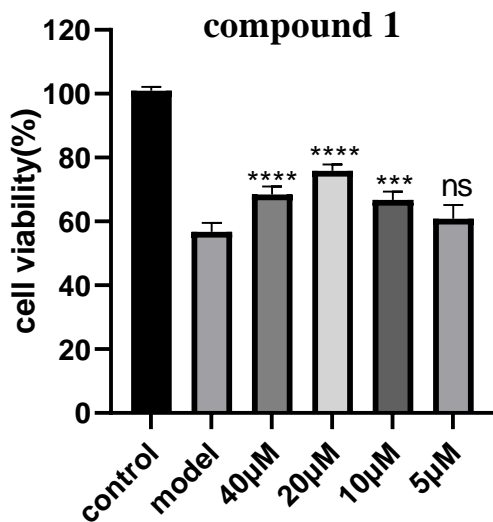
- Structure Match:** Includes "As Drawn (0)", "Substructure (7)", and "Similarity (159K)".
- Chemscape Analysis:** Includes a "Create Chemscape Analysis" button.
- Filter Behavior:** Includes "Filter by" and "Exclude" buttons.
- Search Within Results:** Includes "Reference Role" and "Biological Study (1)".

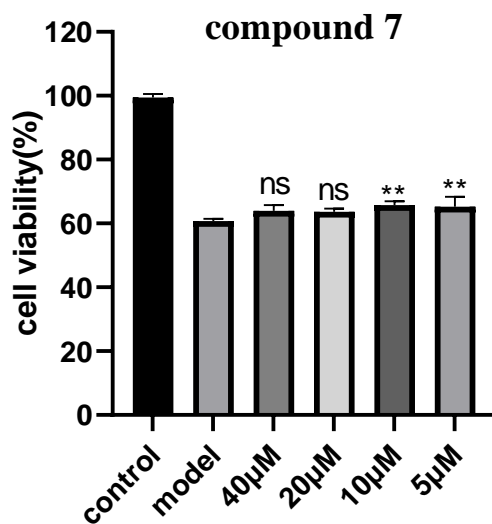
The main search area shows a filter for "Stereochemistry: Absolute Stereo Match". Below this, it indicates "1 Result". The result is displayed as a card with the following information:

- Reference ID: 1297315-13-9
- Chemical structure: A complex polycyclic aromatic system with multiple methoxy groups.
- Chemical formula:  $C_{21}H_{21}O_6$
- Chemical name: 5-[(2S,3S)-2,3-Dihydro-5,6-dimethoxy-3-methyl-2-benzofuran-1-yl]-2-methoxyphenol
- Buttons: Reference (1), Reactions (0), Supplier (1)

At the top right, there are options for "Edit Drawing", "Remove", and "Save". A "Search Patent Markush" checkbox is also present.

**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).