

Lignans from the roots and rhizomes of *Dysosma versipellis* and their cytotoxic activities

Yanjuan Sun ^{1,2,3*}, Haojie Wang ^{1,2}, Ruijie Han ^{1,2}, Hongyun Bai ^{1,2}, Meng Li ^{1,2}, Junmin Wang ^{1,2}, and Weisheng Feng ^{1,2*}

¹ Collaborative Innovation Center for Respiratory Disease Diagnosis and Treatment & Chinese Medicine, Development of Henan Province, Henan University of Chinese Medicine, Zhengzhou 450046, China

² School of Pharmacy, Henan University of Chinese Medicine, Zhengzhou 450046, China

³ Henan Research Center for Special Processing Technology of Chinese Medicine, 450046, China

* Correspondence: sunyanjuan2011@hactcm.edu.cn (Y.S.); fwsh@hactcm.edu.cn (W.F.);
Tel.: +86-371-6596-2746 (Y.S. & W.F.)

Abstract: One new dibenzyltyrolactone lignan dysoslignan A (**1**), three new aryl-naphthalide lignans dysoslignan B–C (**2–4**), along with fourteen known metabolites (**5–18**), were isolated from the roots and rhizomes of *Dysosma versipellis*. Their structures and stereochemistry were determined from analysis of NMR spectroscopic and circular dichroism (CD) data. Compound **2** represents the first report of naturally occurring aryl-naphthalide lignan triglycoside. The cytotoxic activities of all isolated compounds were evaluated against A-549 and SMMC-7721 cell lines. Compounds **7–10**, and **14–16** were more toxic than cisplatin in two tumor cell lines. This investigation clarifies the potential effective substance basis of *D. versipellis* in tumor treatment.

Keywords: *Dysosma versipellis*; dibenzyltyrolactone; aryl-naphthalide; cytotoxic

Table of Contents

Figure S1. ¹ H NMR spectrum (500 MHz) of 1 in DMSO- <i>d</i> ₆	3
Figure S2. ¹³ C NMR spectrum (125 MHz) of 1 in DMSO- <i>d</i> ₆	3
Figure S3. HSQC spectrum of 1	4
Figure S4. HMBC spectrum of 1	4
Figure S5 DEPT spectrum of 1	5
Figure S6 ¹ H- ¹ H-COSY spectrum of 1	5
Figure S7. NOESY spectrum of 1	6
Figure S8. ECD spectrum of 1	6
Figure S9. HR-ESI-MS spectrum of 1	7
Figure S10. ¹ H NMR spectrum (500 MHz) of 2 in DMSO- <i>d</i> ₆	7
Figure S11. ¹³ C NMR spectrum (125 MHz) of 2 in DMSO- <i>d</i> ₆	8
Figure S12. HSQC spectrum of 2	8
Figure S13. HMBC spectrum of 2	9
Figure S14. DEPT spectrum of 2	9
Figure S15. ¹ H- ¹ H-COSY spectrum of 2	10
Figure S16. NOESY spectrum of 2	10
Figure S17. ECD spectrum of 2	11
Figure S18. HR-ESI-MS spectrum of 2	11
Figure S19. ¹ H NMR spectrum (500 MHz) of 3 in DMSO- <i>d</i> ₆	12
Figure S20. ¹³ C NMR spectrum (125 MHz) of 3 in DMSO- <i>d</i> ₆	12
Figure S21. HSQC spectrum of 3	13
Figure S22. HMBC spectrum of 3	13
Figure S23. HR-ESI-MS spectrum of 3	14
Figure S24. ¹ H NMR spectrum (500 MHz) of 3 in DMSO- <i>d</i> ₆	14
Figure S25. ¹³ C NMR spectrum (125 MHz) of 3 in DMSO- <i>d</i> ₆	15
Figure S26. HSQC spectrum of 4	15
Figure S27. HMBC spectrum of 4	16
Figure S28. HR-ESI-MS spectrum of 4	16

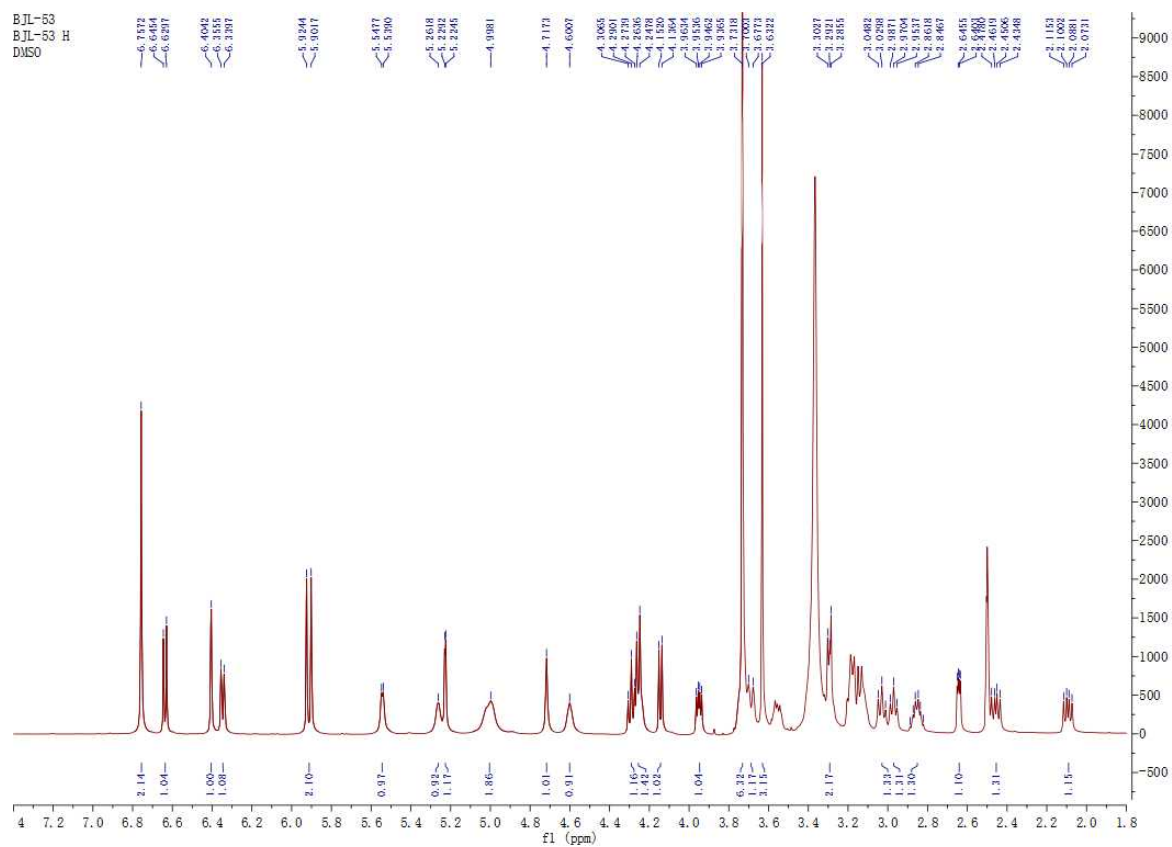


Figure S1. ^1H NMR spectrum of **1** (500 MHz, $\text{DMSO}-d_6$)

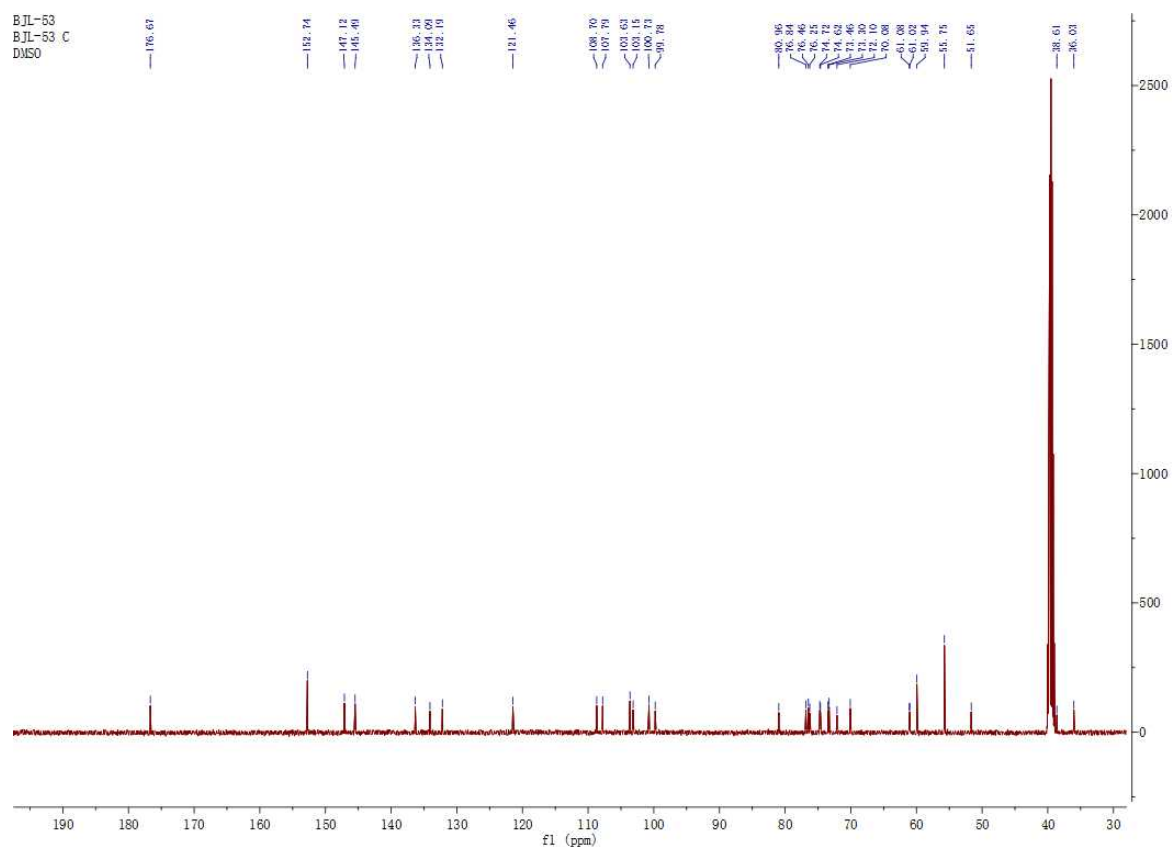


Figure S2. ^{13}C NMR spectrum of **1** (125 MHz, DMSO- d_6)

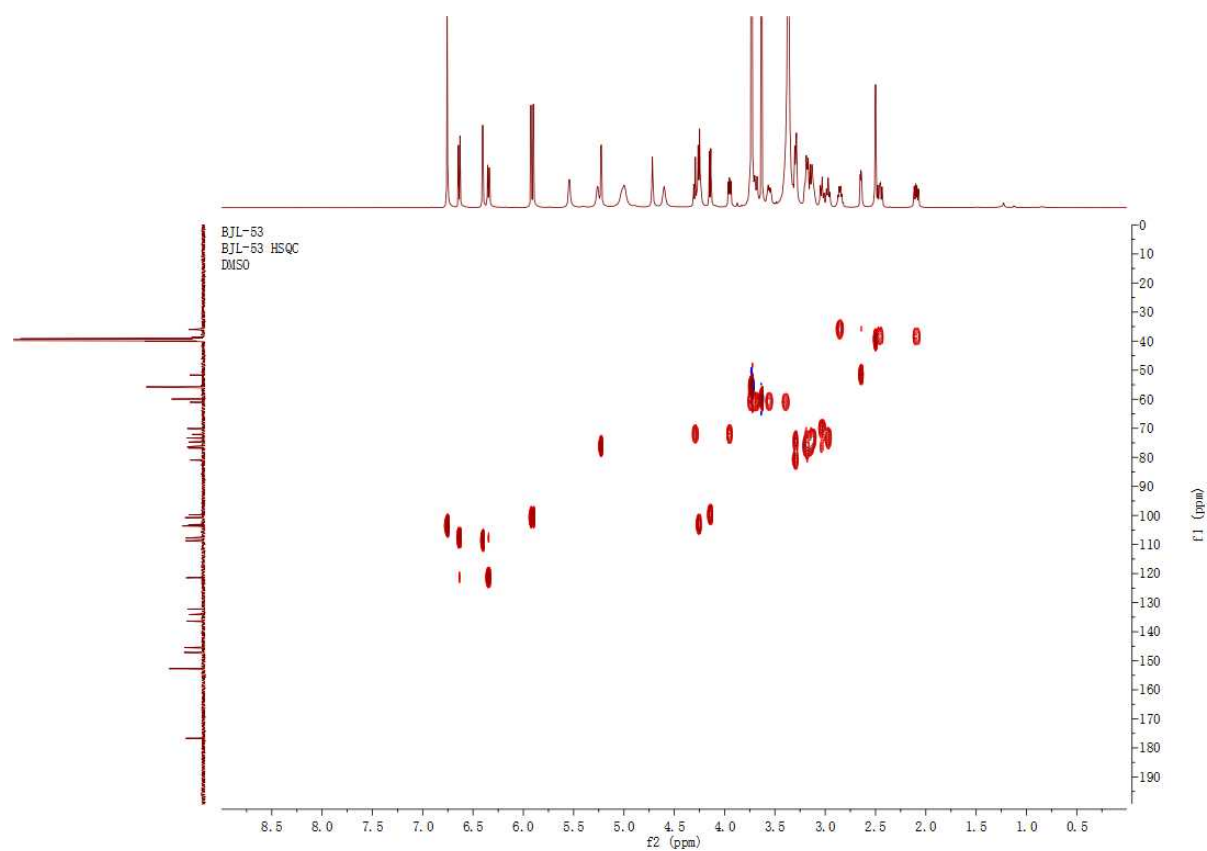


Figure S3. HSQC spectrum of **1**

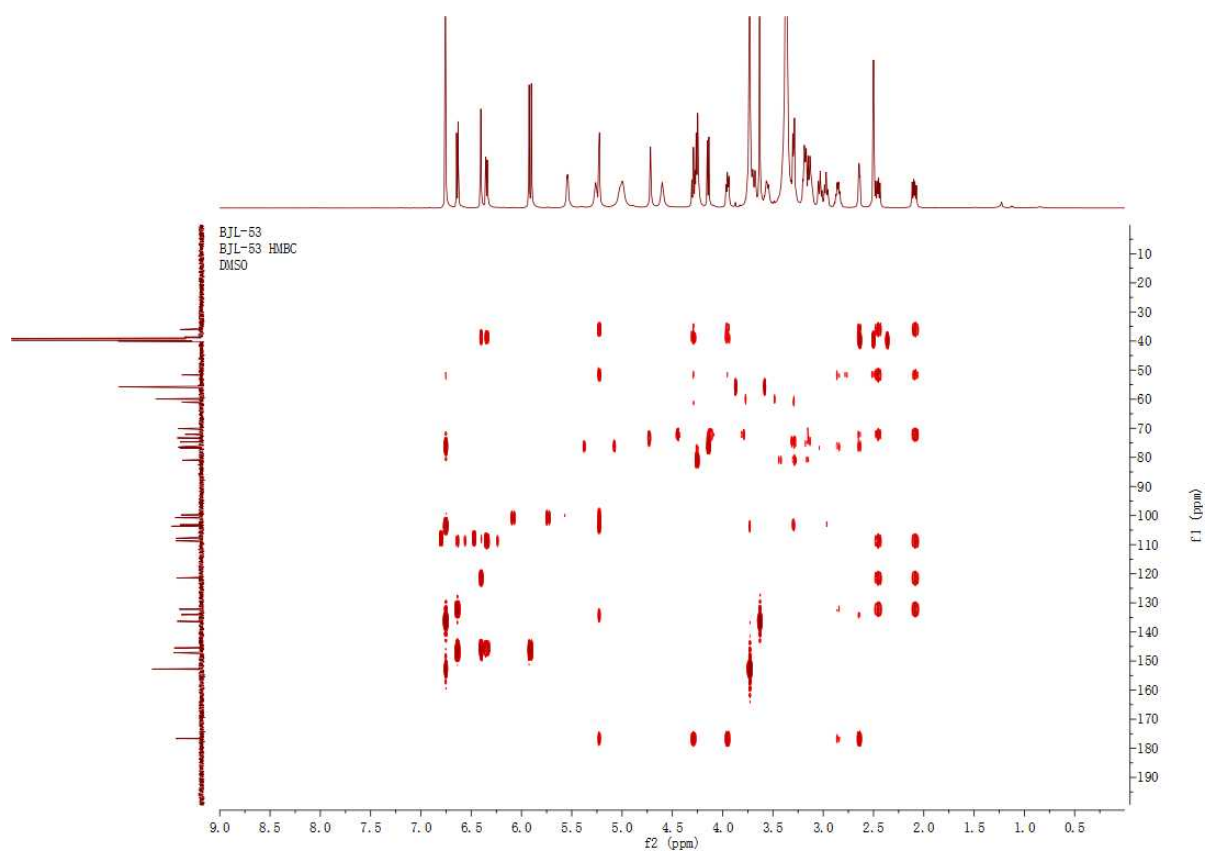


Figure S4. HMBC spectrum of **1**

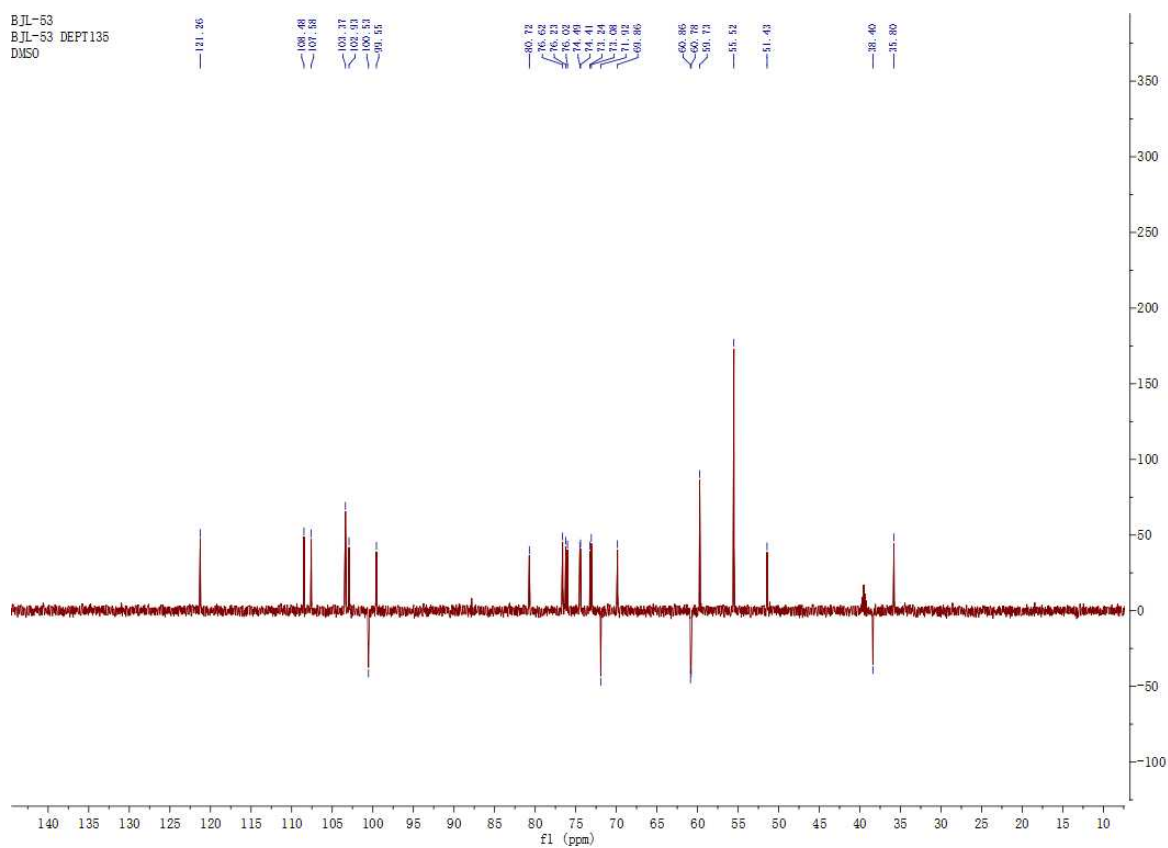


Figure S5. DEPT spectrum of **1**

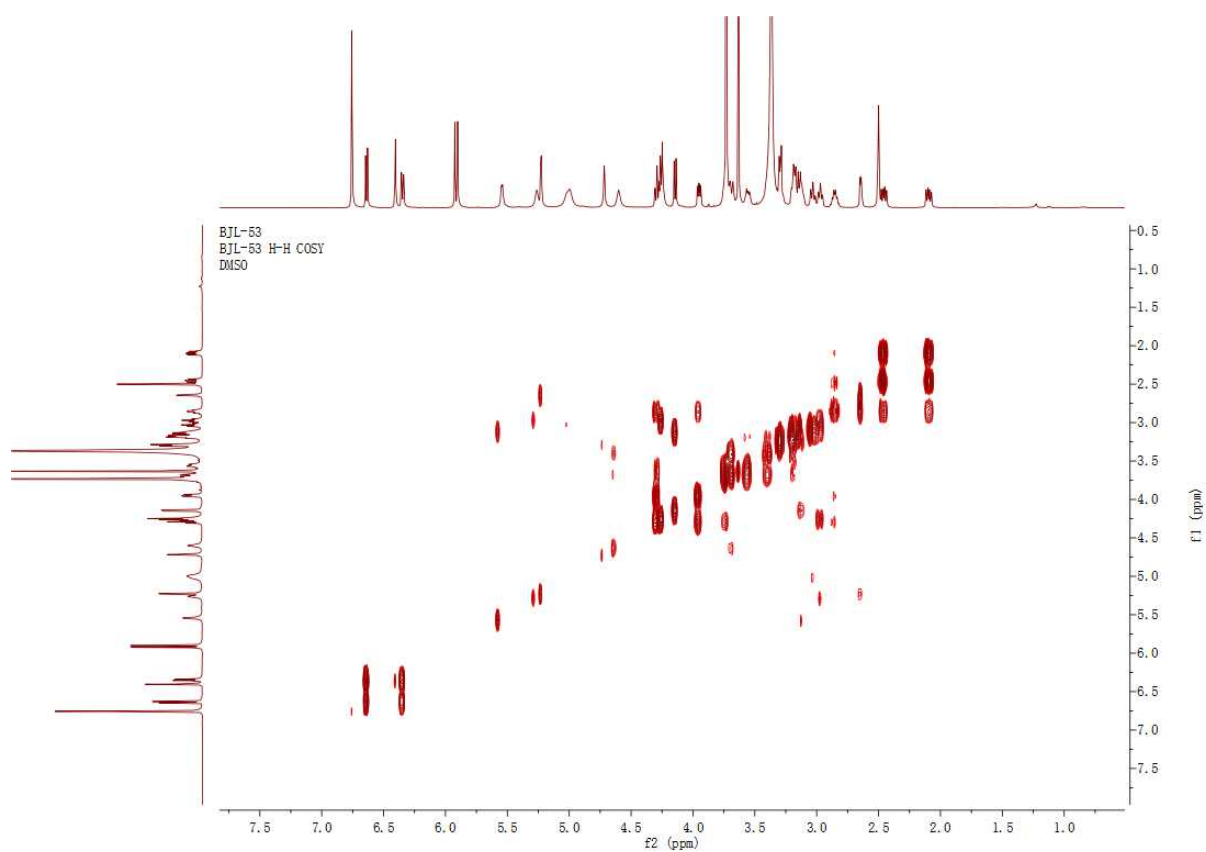


Figure S6. ^1H - ^1H -COSY spectrum of **1**

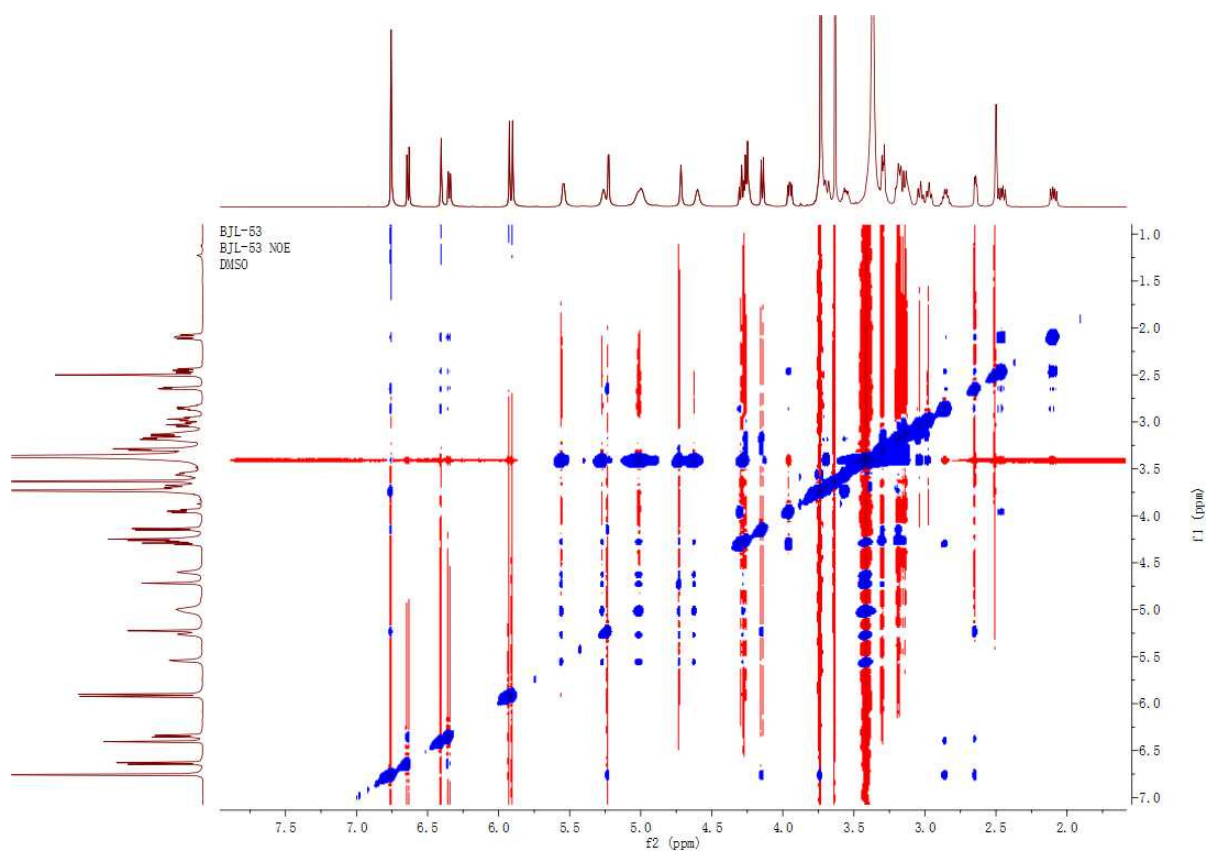


Figure S7. NOESY spectrum of **1**

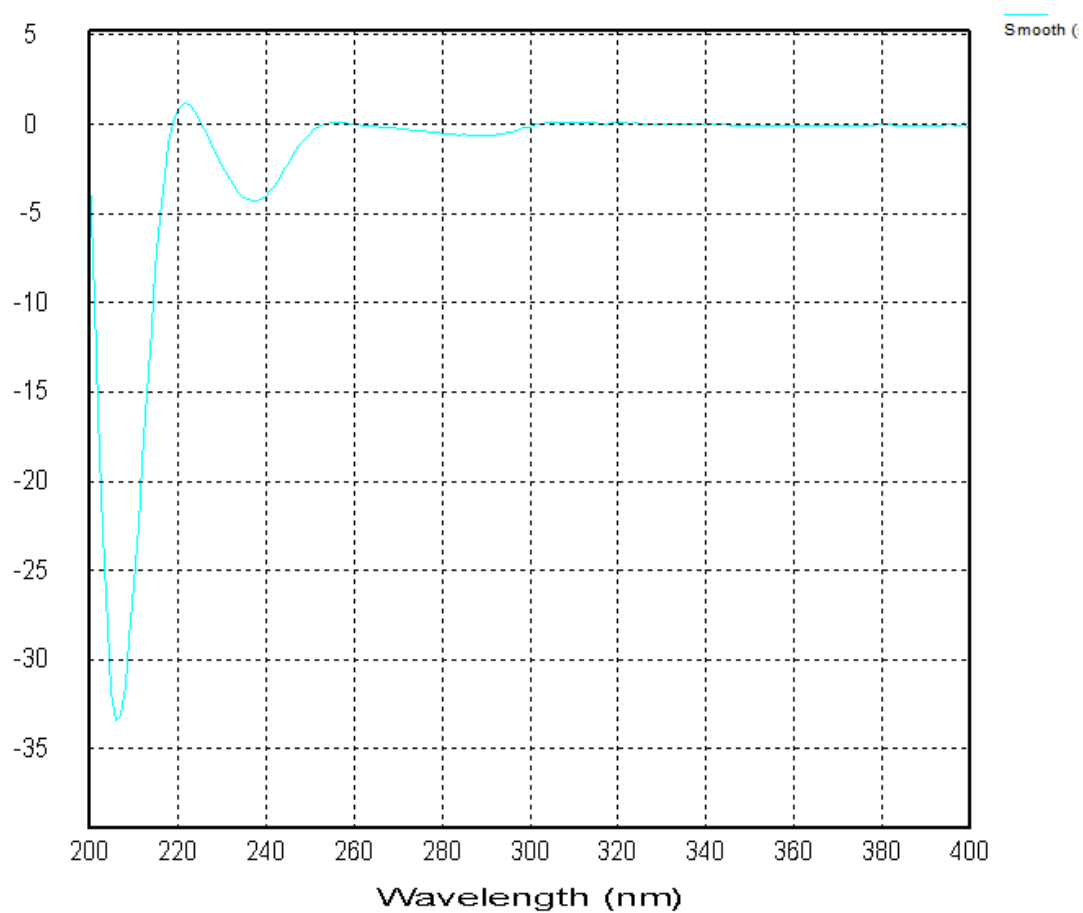


Figure S8. ECD spectrum of **1**

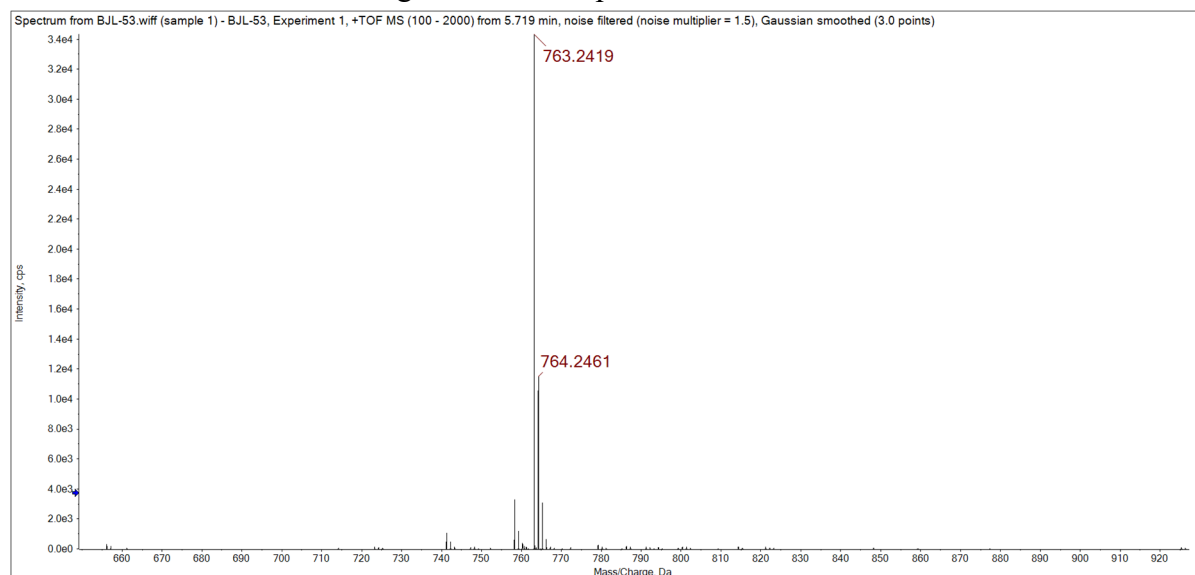


Figure S9. HR-ESI-MS spectrum of **1**

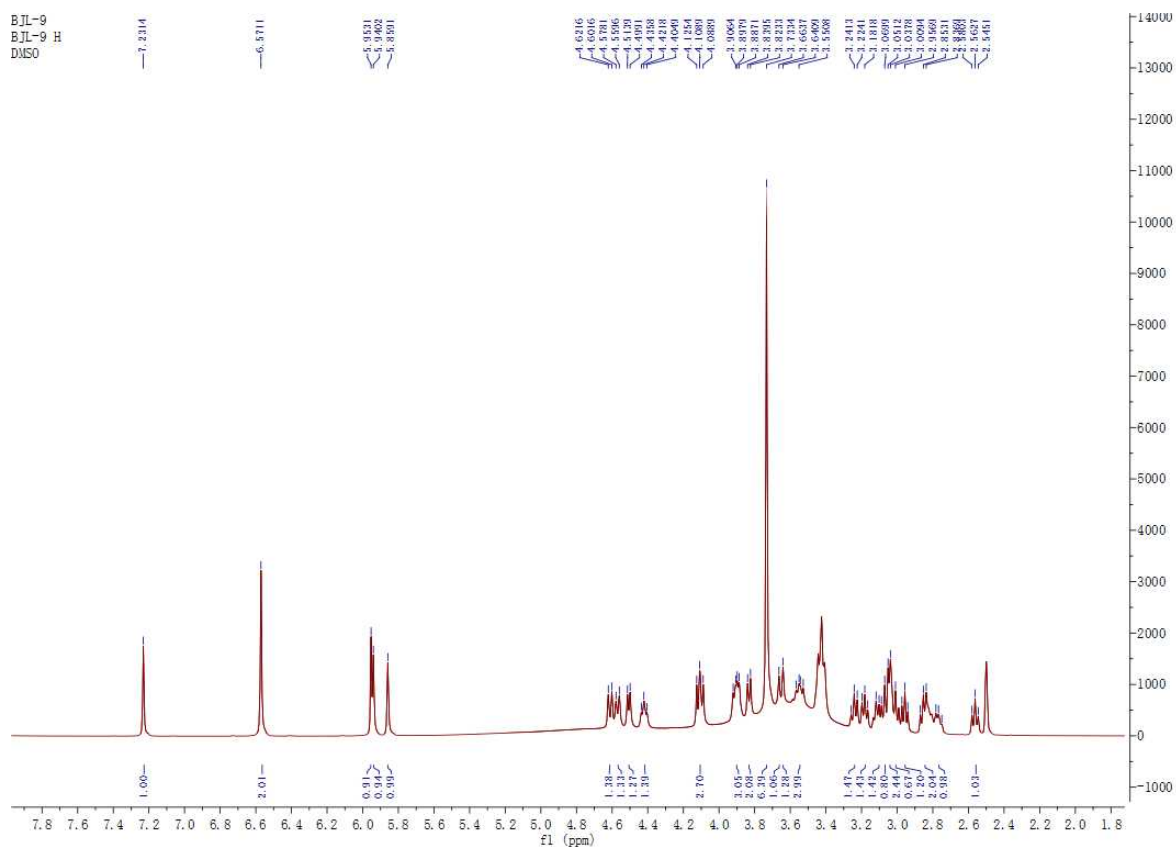


Figure S10. ^1H NMR spectrum of **2** (500 MHz, DMSO- d_6)

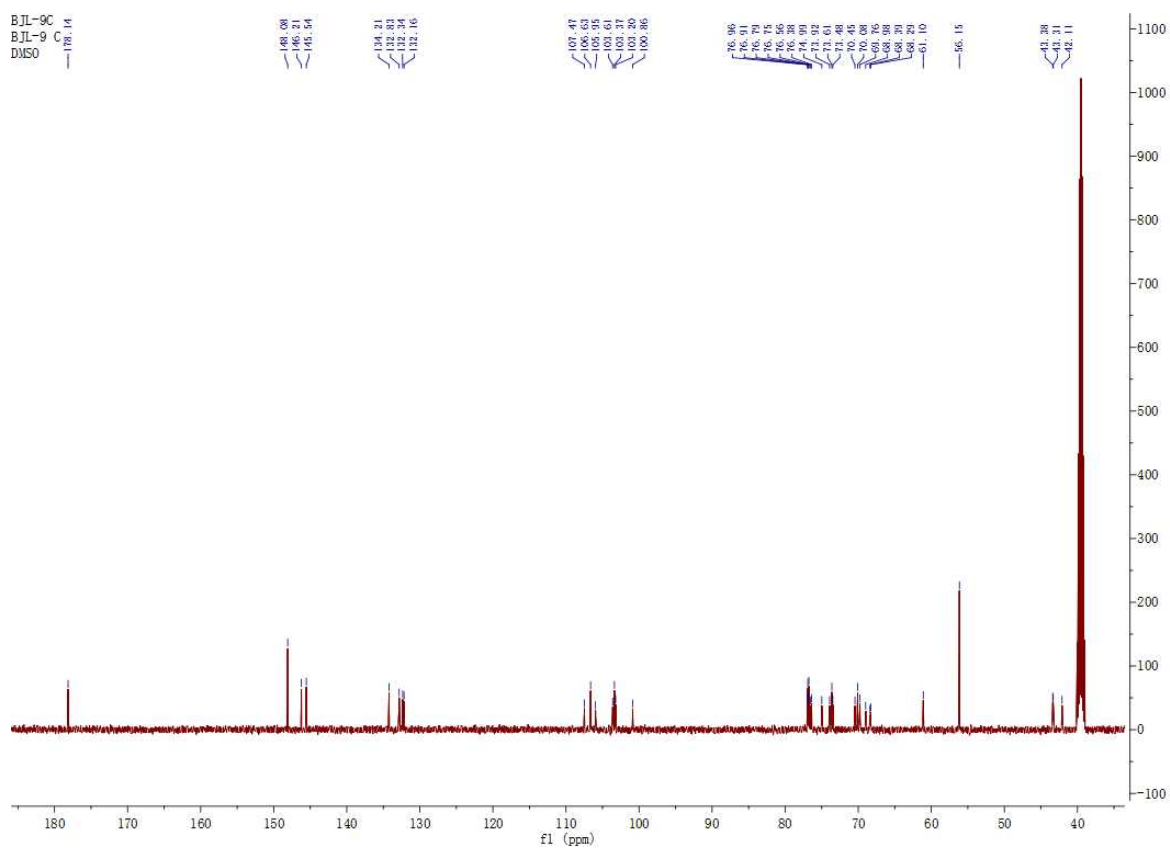


Figure S11. ^{13}C NMR spectrum of **2** (125 MHz, $\text{DMSO-}d_6$)

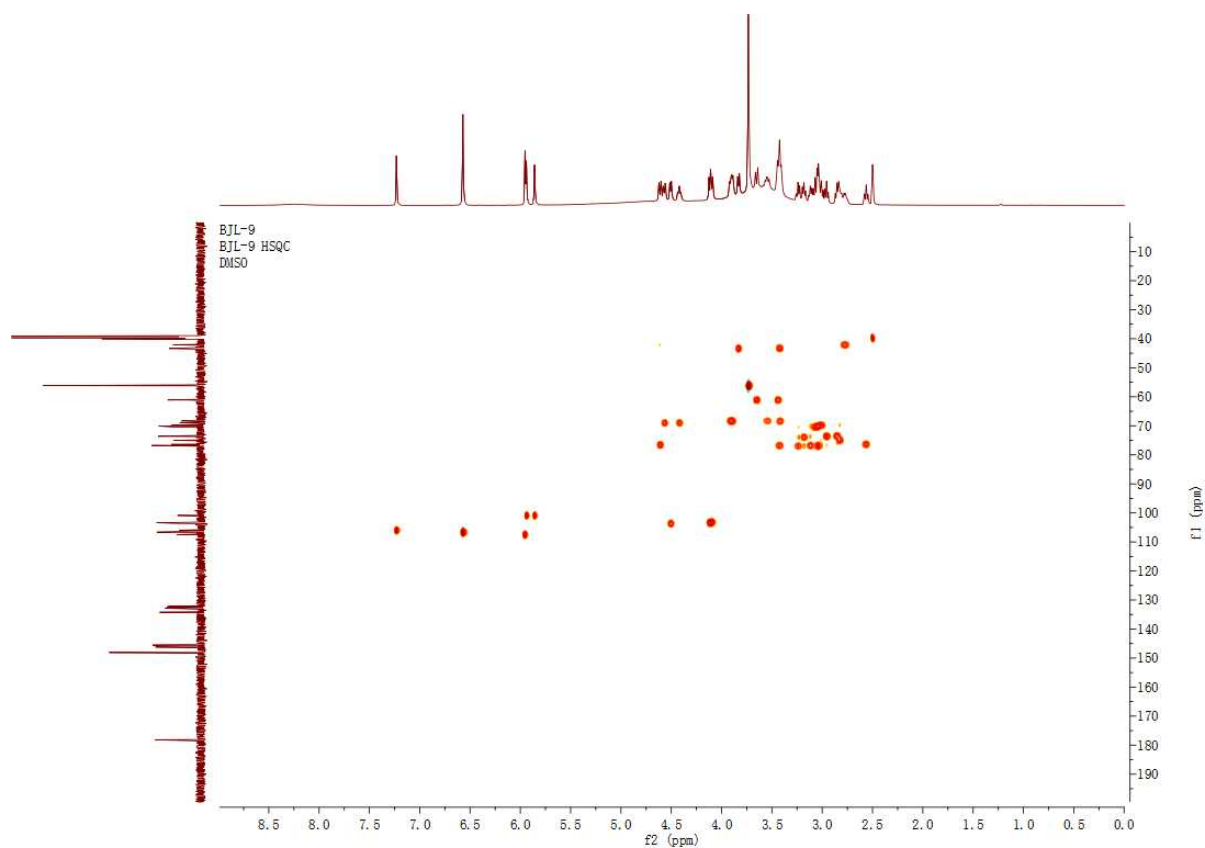


Figure S12. HSQC spectrum of **2**

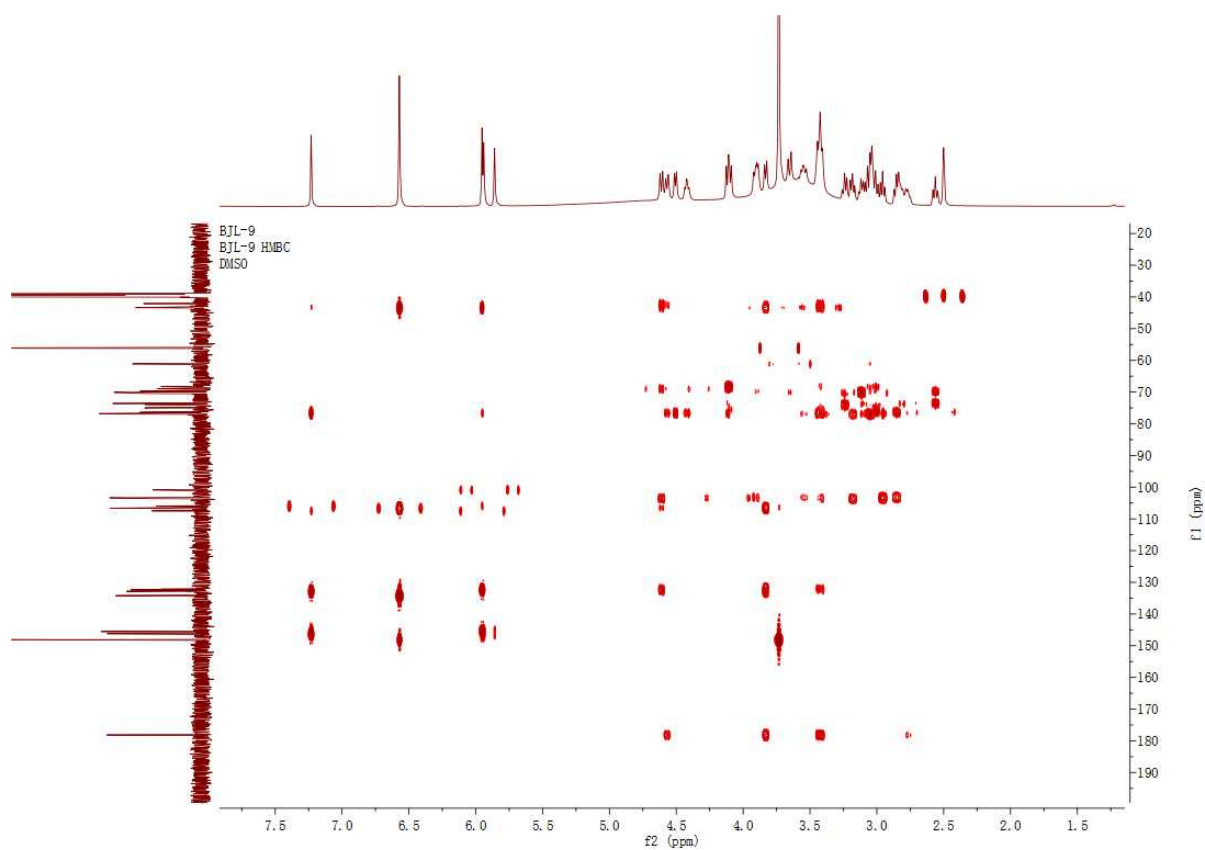


Figure S13. HMBC spectrum of **2**

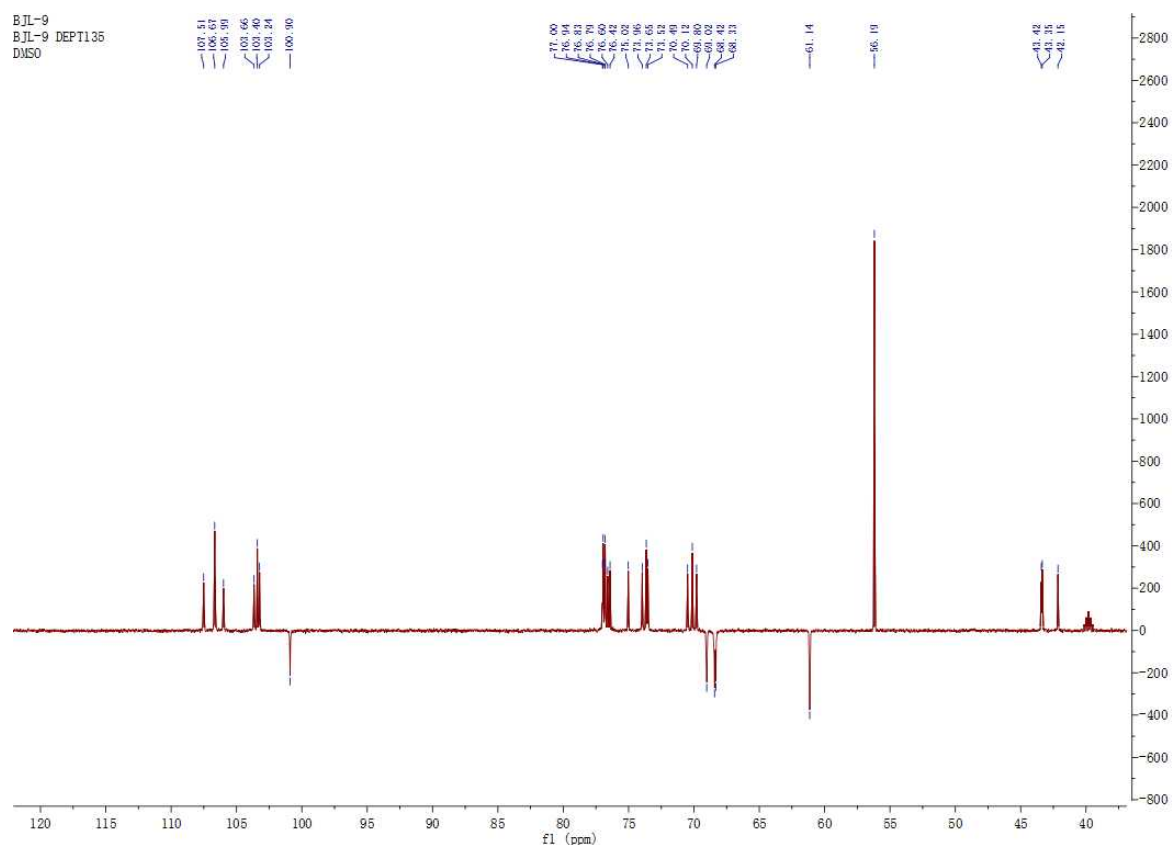


Figure S14. DEPT spectrum of **2**

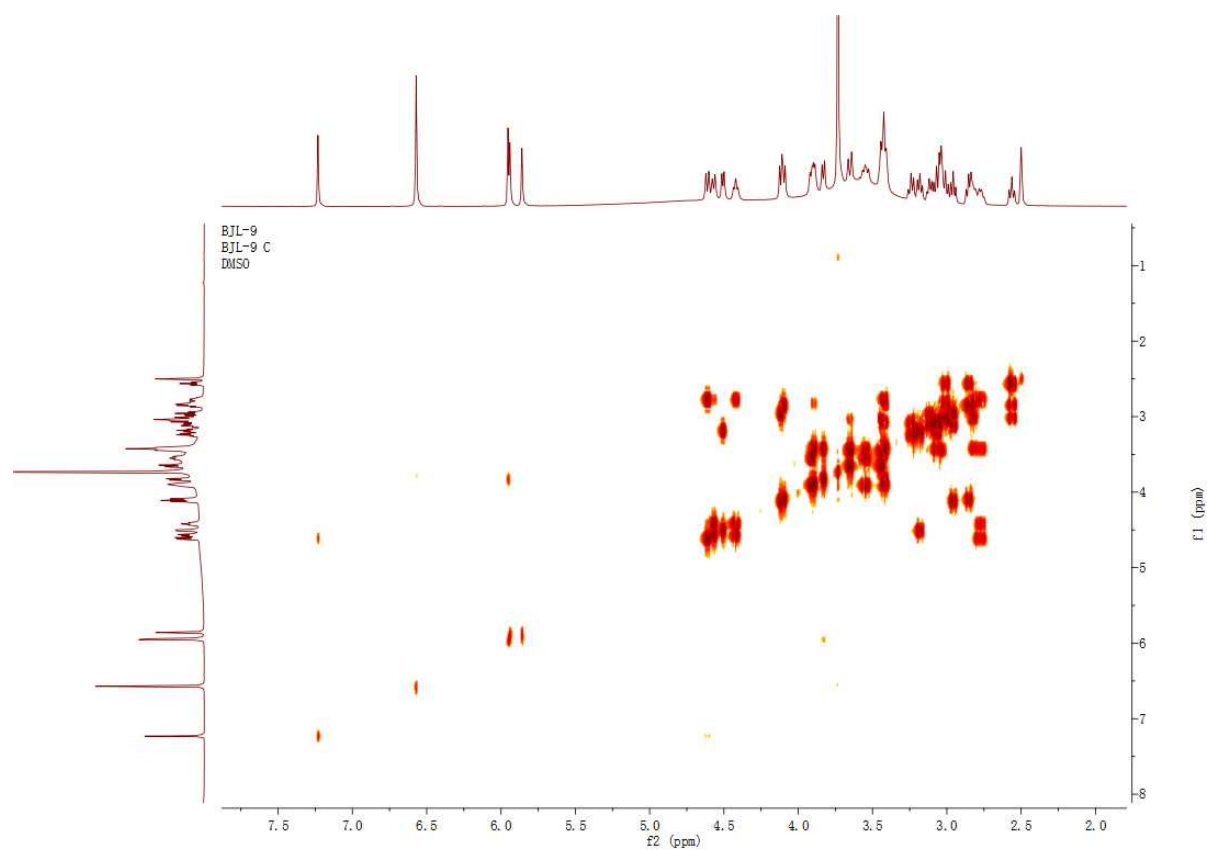


Figure S15. ^1H - ^1H -COSY spectrum of **2**

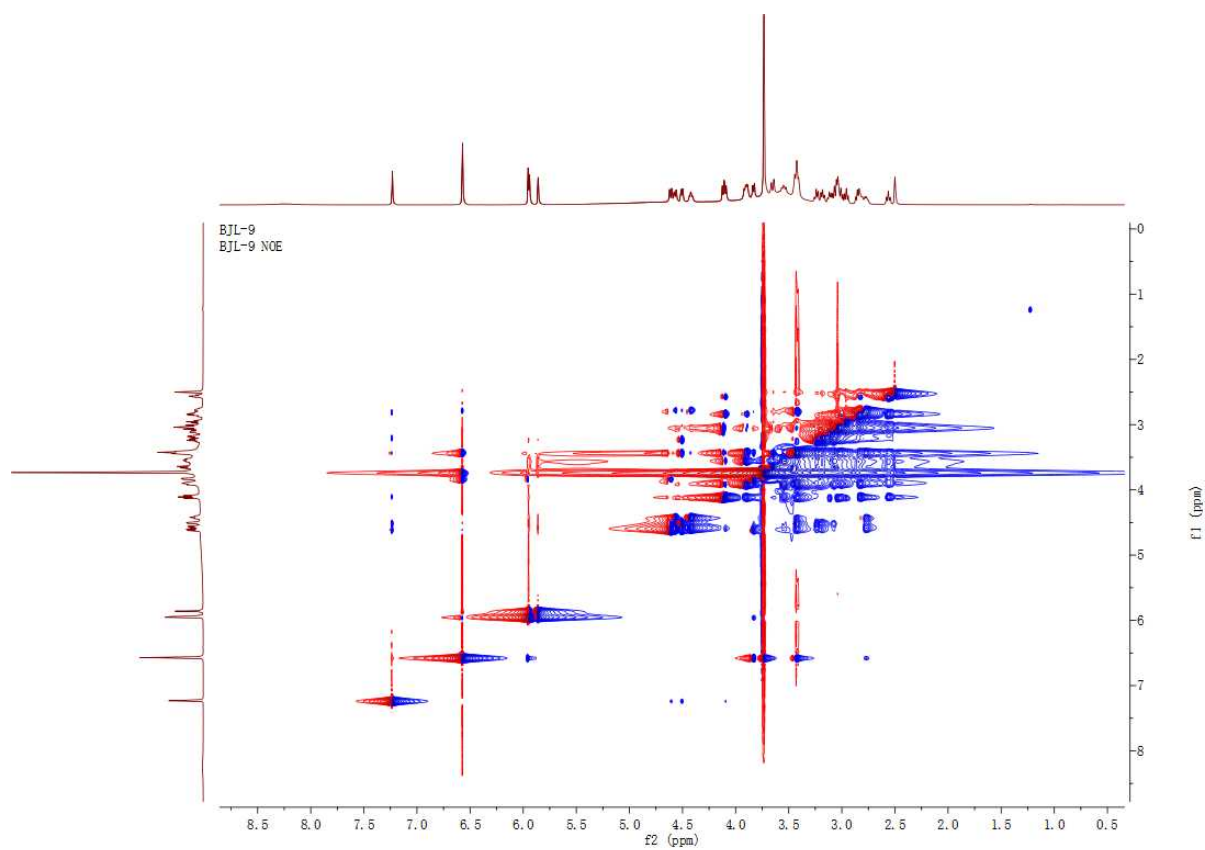


Figure S16. NOESY spectrum of **2**

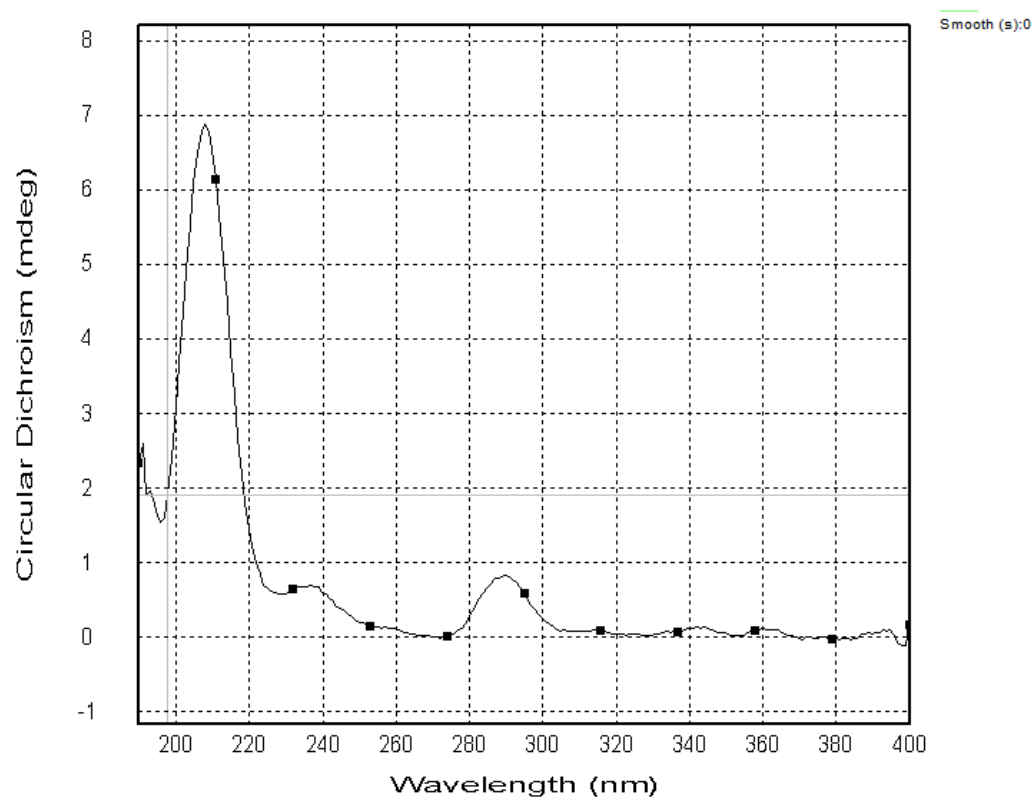


Figure S17. ECD spectrum of **2**

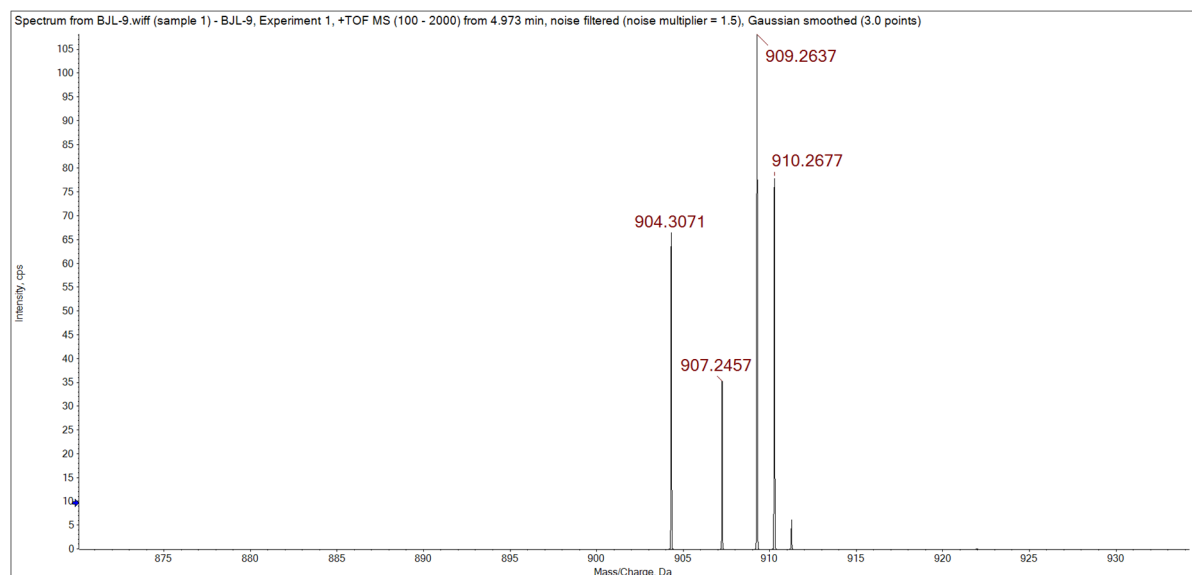


Figure S18. HR-ESI-MS spectrum of **2**

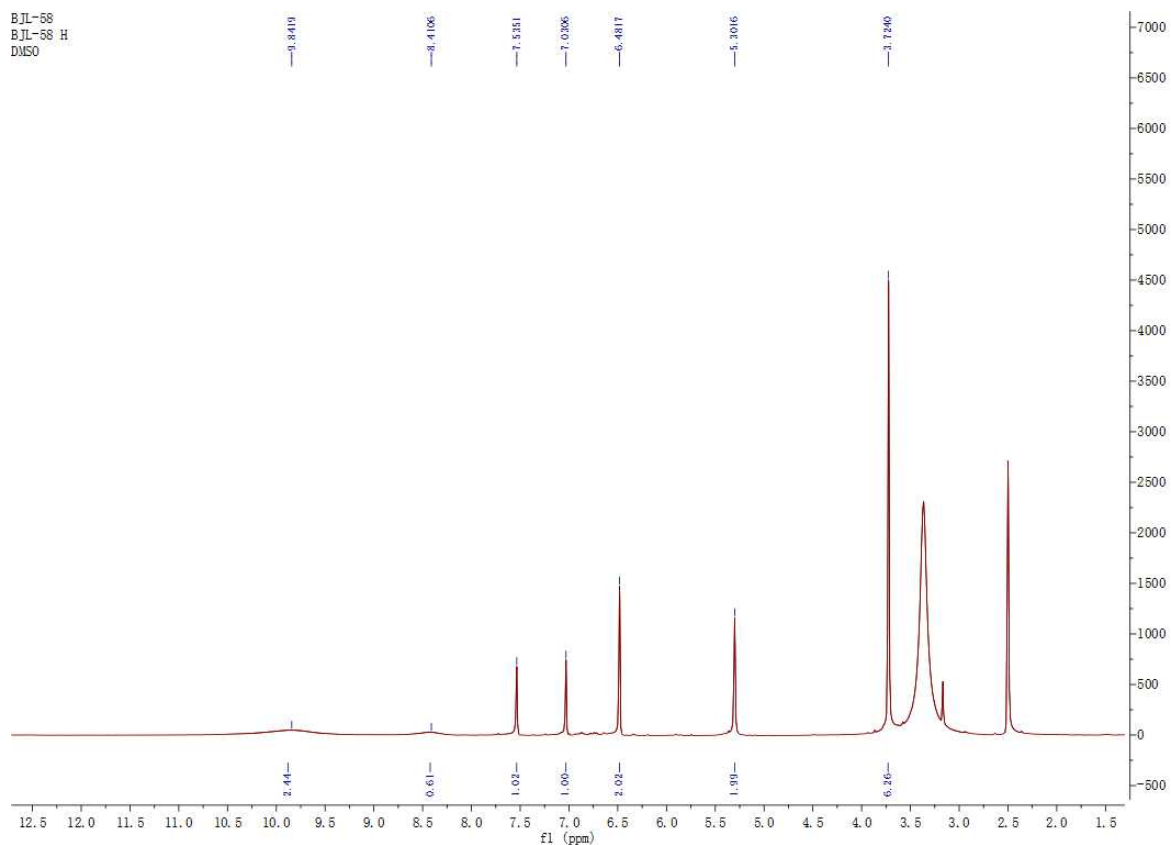


Figure S19. ^1H NMR spectrum of **3** (500 MHz, $\text{DMSO-}d_6$)

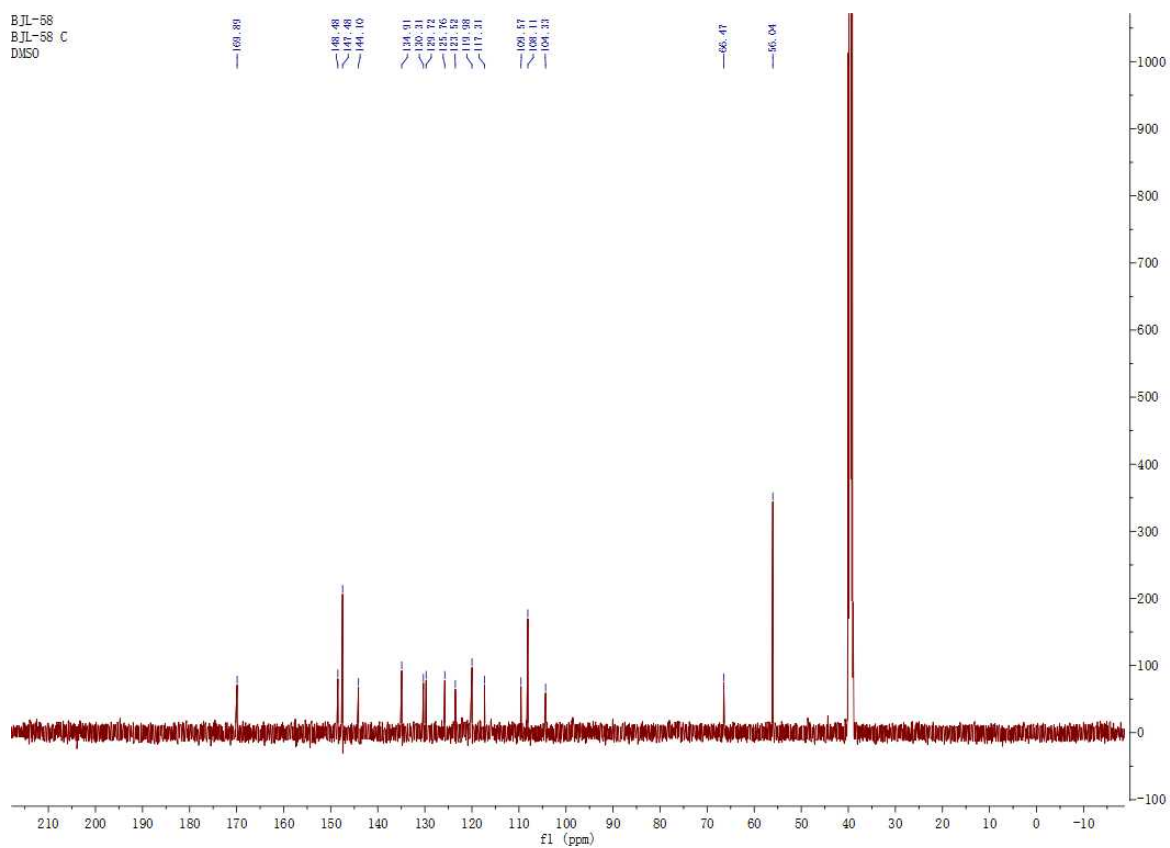


Figure S20. ^{13}C NMR spectrum of **3** (125 MHz, $\text{DMSO-}d_6$)

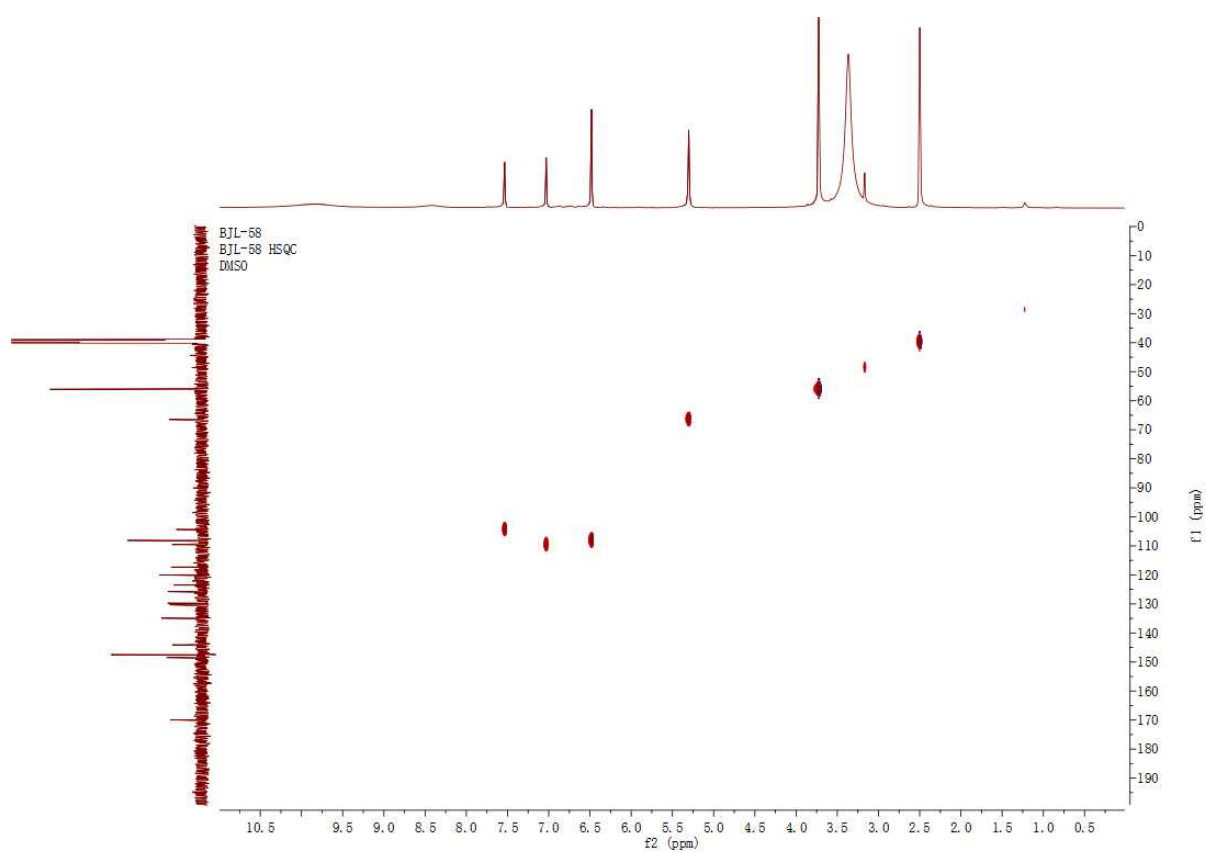


Figure S21. HSQC spectrum of **3**

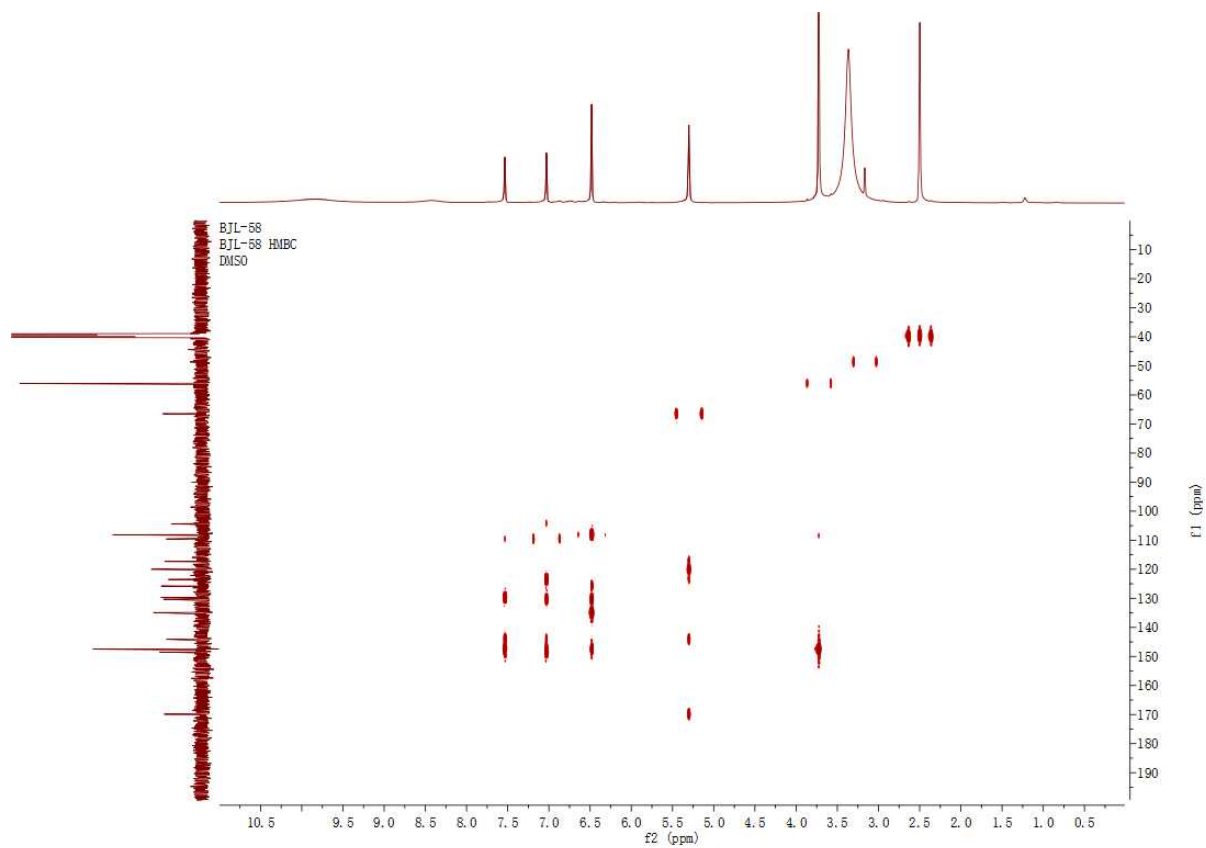


Figure S22. HMBC spectrum of **3**

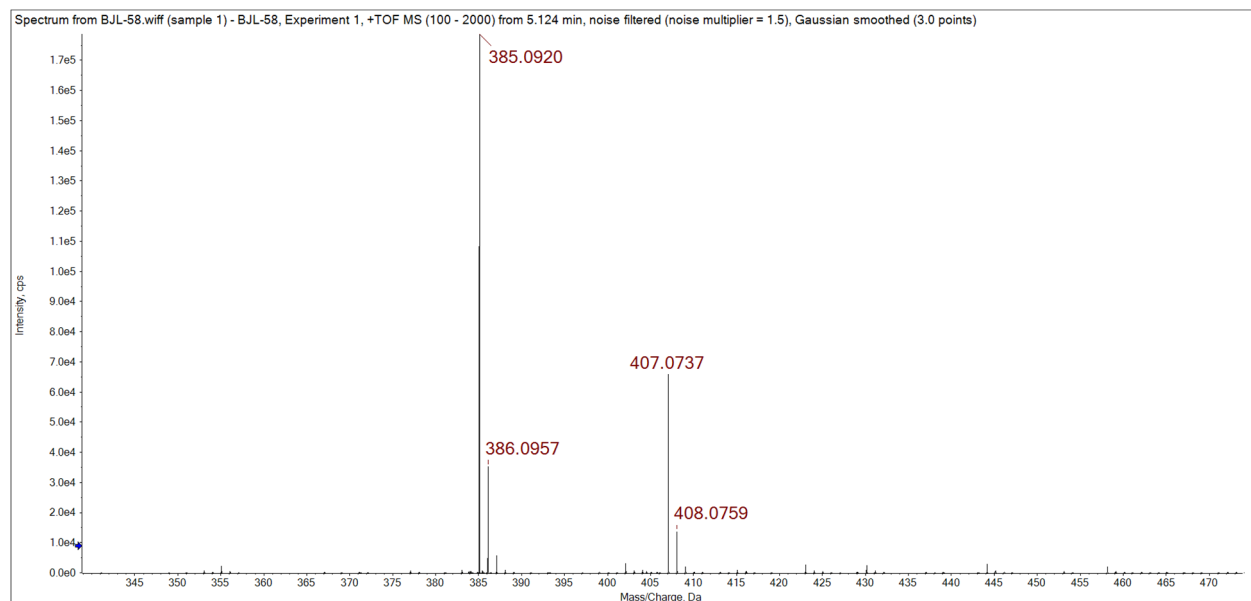


Figure S23. HR-ESI-MS spectrum of **3**

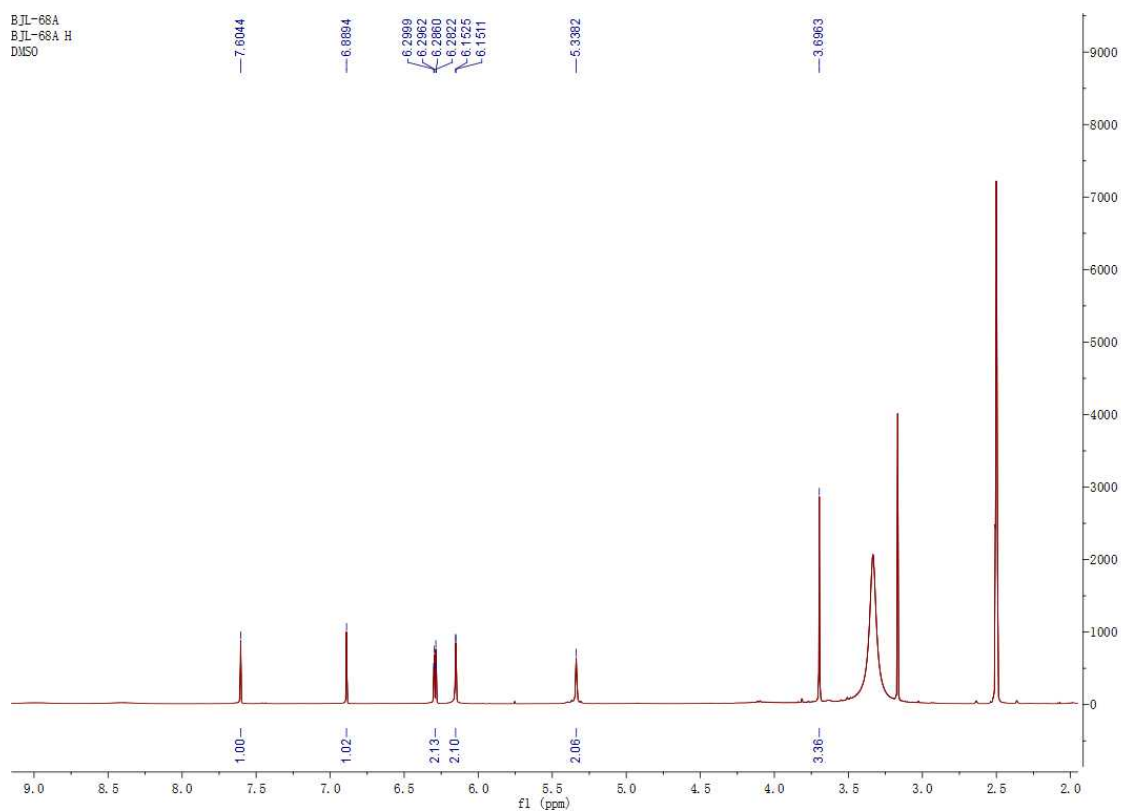


Figure S24. ¹H NMR spectrum of **4** (500 MHz, DMSO-*d*₆)

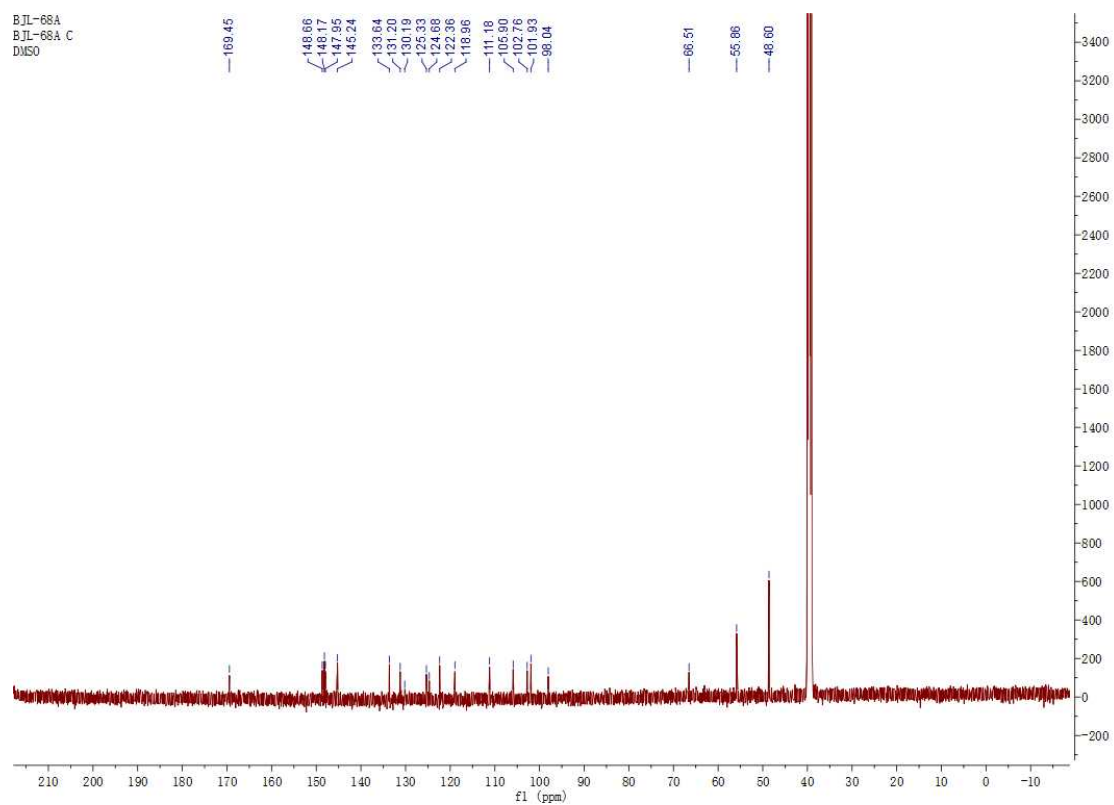


Figure S25. ^{13}C NMR spectrum of **4** (125 MHz, $\text{DMSO-}d_6$)

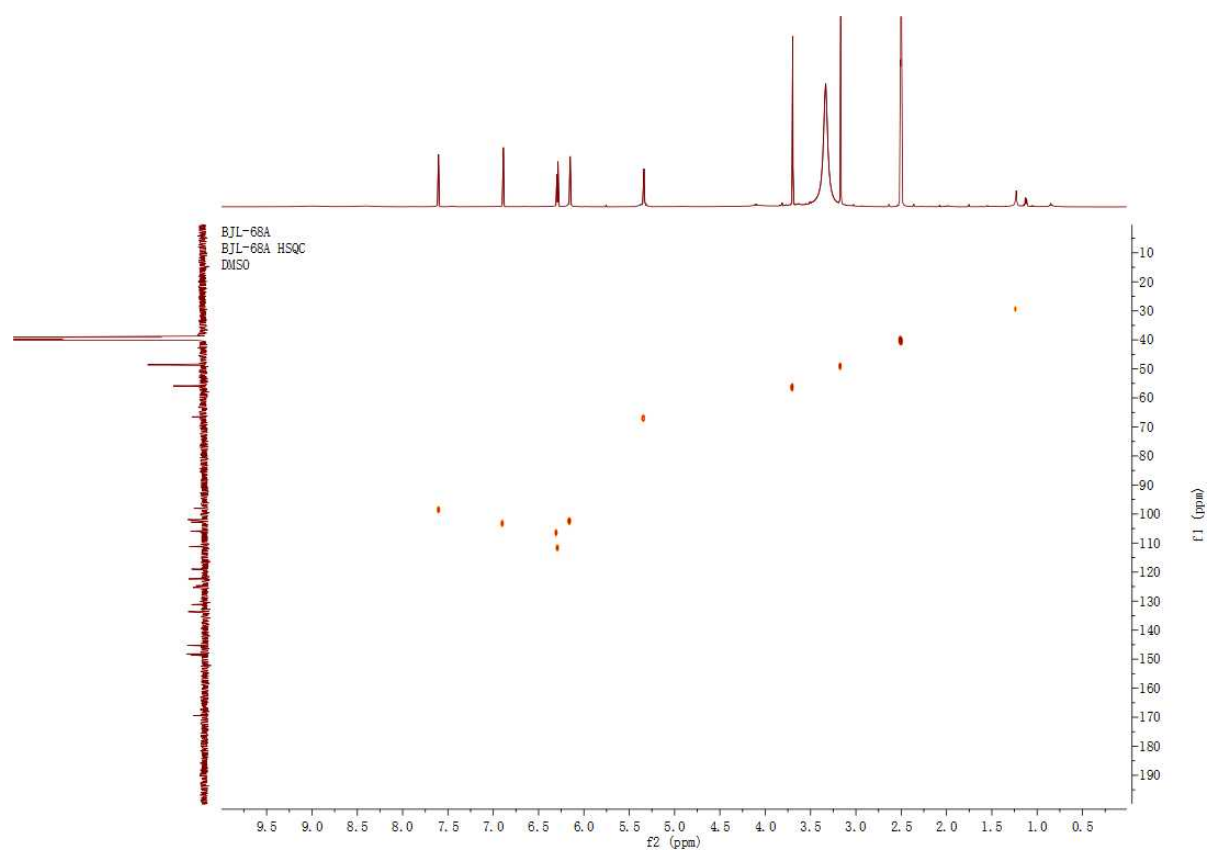


Figure S26. HSQC spectrum of **4**

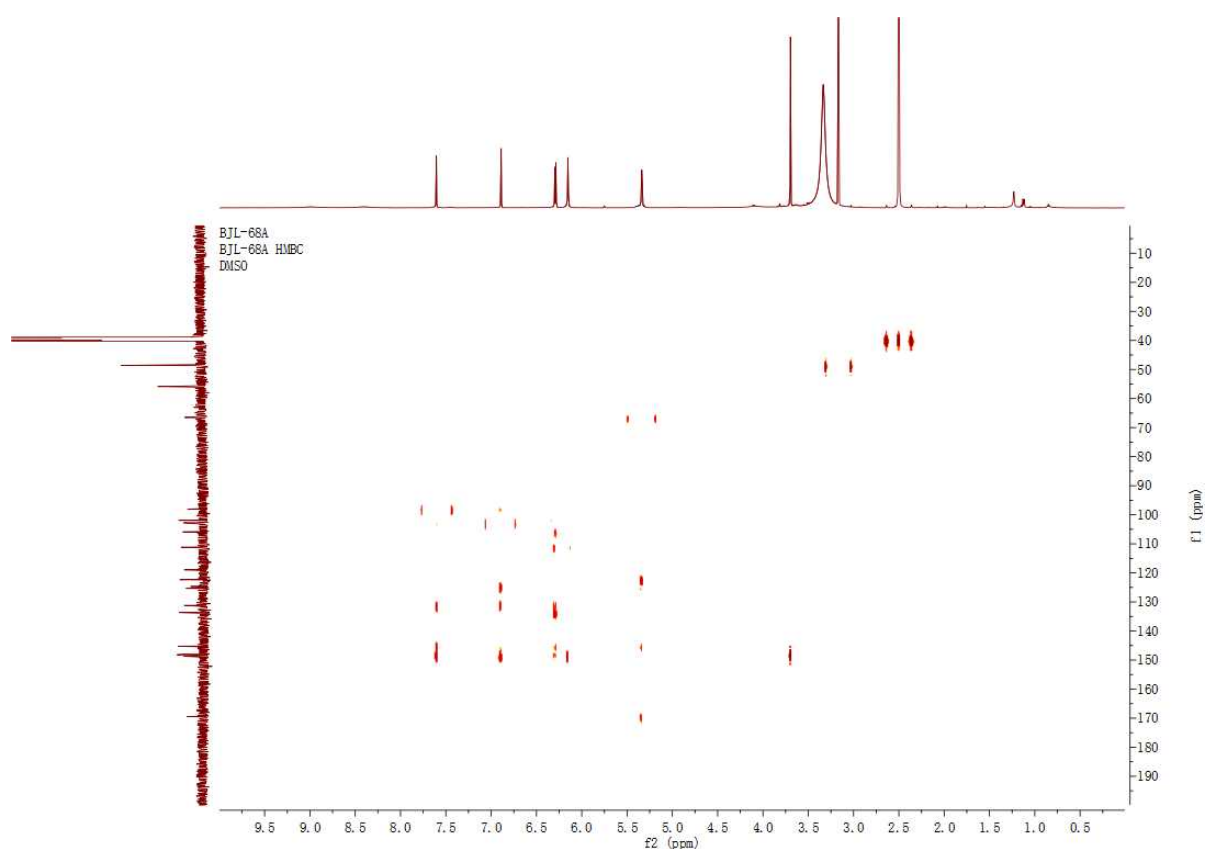


Figure S27. HMBC spectrum of **4**

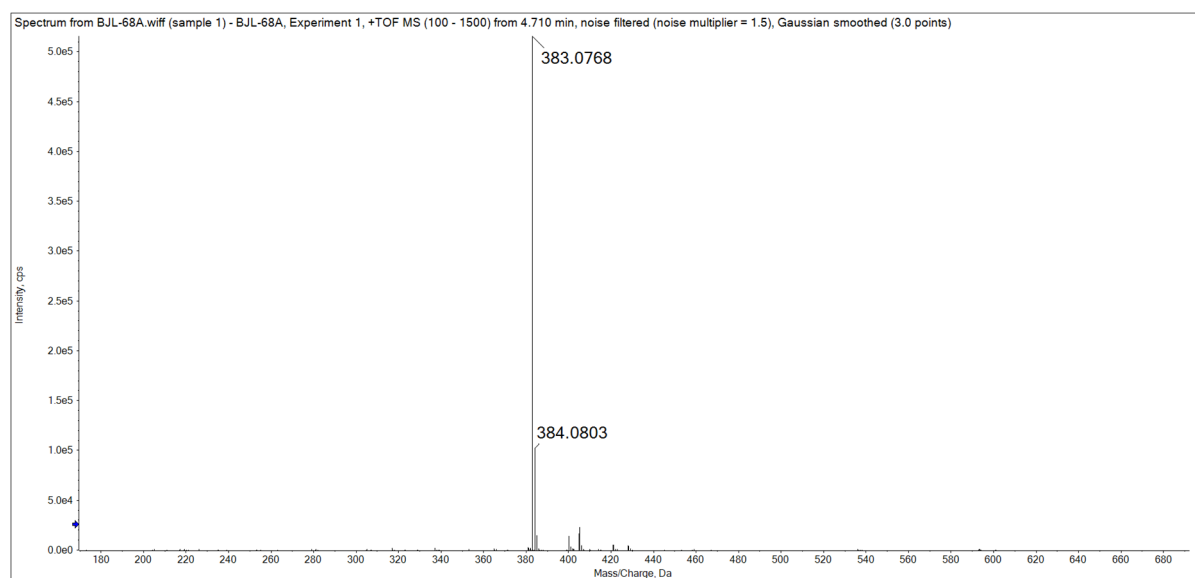


Figure S28. HR-ESI-MS spectrum of **4**