

SUPPLEMENTARY MATERIAL

Secondary Metabolites from Marine-Derived Fungus *Penicillium rubens* BTBU20213035

Xiuli Xu ¹, Yifei Dong ², Jinpeng Yang ¹, Long Wang ³, Linlin Ma ⁴, Fuhang Song ^{2,*}, Xiaoli Ma ^{5,*}

¹ Key Laboratory of Marine Mineral Resources and Polar Geology, Ministry of Education, School of Ocean Sciences, China University of Geosciences, Beijing 100083, China

² Key Laboratory of Geriatric Nutrition and Health, Ministry of Education of China, School of Light Industry Science and Engineering, Beijing Technology and Business University, Beijing 100048, China

³ State Key Laboratory of Mycology, Institute of Microbiology, Chinese Academy of Sciences, Beijing 100101, China

⁴ Griffith Institute for Drug Discovery, School of Environment and Science, Griffith University, Brisbane 4111, Australia

⁵ School of Chemistry and Chemical Engineering, North Minzu University, Yinchuan 750021, China

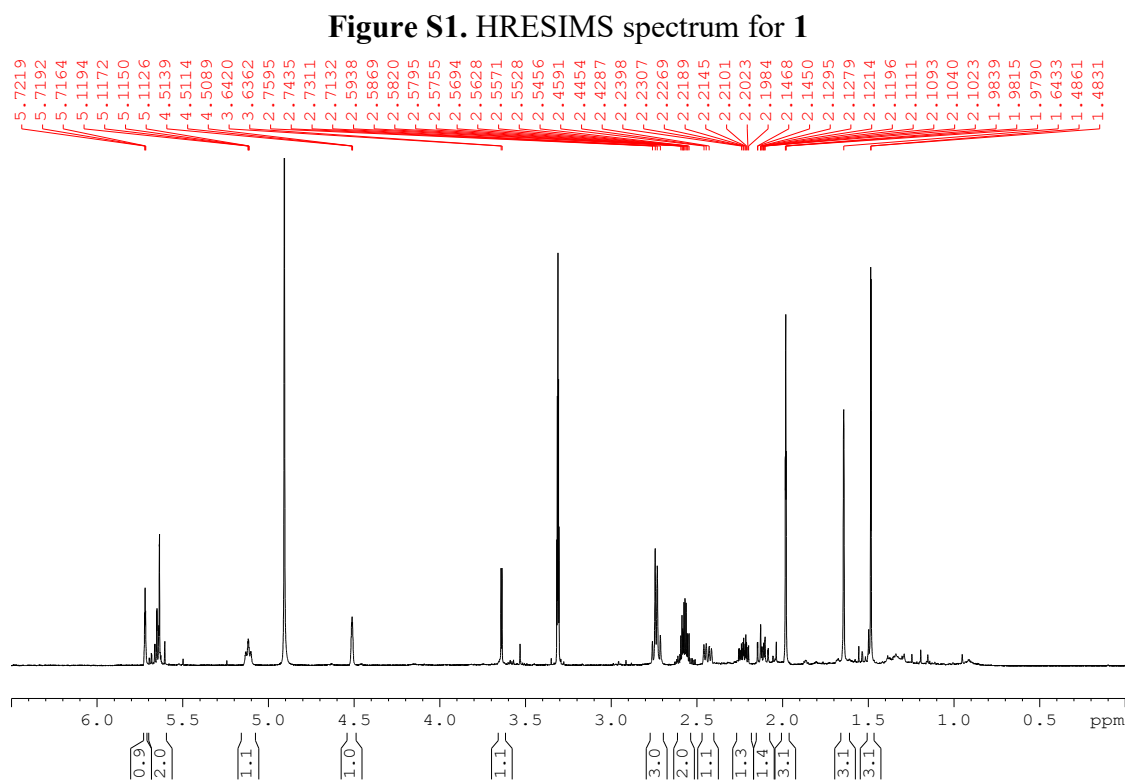
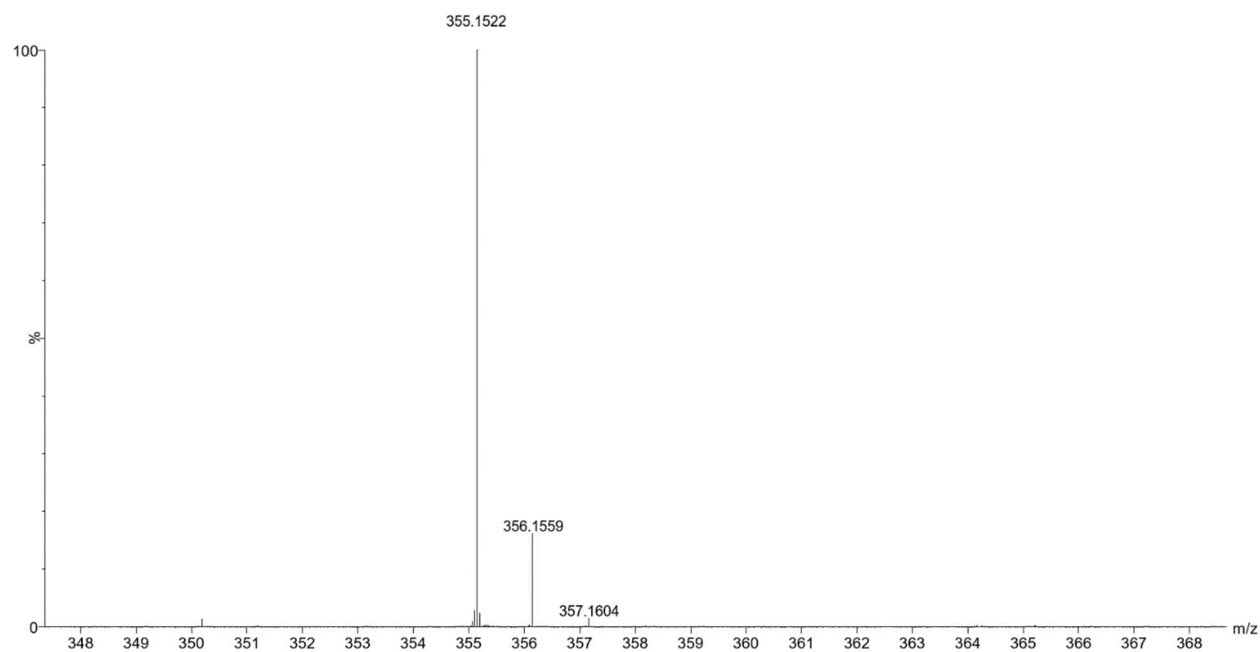
* Correspondence: songfuhang@btbu.edu.cn (F.S.); mxl@nmu.edu.cn (X.M.)

Table of Contents

Figure S1. HRESIMS spectrum for 1	3
Figure S2. ^1H NMR spectrum (500 MHz, CD_3OD) of 1	3
Figure S3. ^{13}C NMR spectrum (125 MHz, CD_3OD) of 1	4
Figure S4. HSQC spectrum (500 MHz, CD_3OD) of 1	4
Figure S5. ^1H - ^1H COSY spectrum (500 MHz, CD_3OD) of 1	5
Figure S6. HMBC spectrum (500 MHz, CD_3OD) of 1	5
Figure S7. ROESY spectrum (500 MHz, CD_3OD) of 1	6
Figure S8. HRESIMS spectrum for 2	6
Figure S9. ^1H NMR spectrum (500 MHz, CDCl_3) of 2	7
Figure S10. ^{13}C NMR spectrum (125 MHz, CDCl_3) of 2	7
Figure S11. HSQC spectrum (500 MHz, CDCl_3) of 2	8
Figure S12. ^1H - ^1H COSY spectrum (500MHz, CDCl_3) of 2	8
Figure S13. HMBC spectrum (500MHz, CDCl_3) of 2	9
Figure S14. ROESY spectrum (500MHz, CDCl_3) of 2	9
Figure S15. HRESIMS spectrum for 3	10
Figure S16. ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of 3	10
Figure S17. ^{13}C NMR spectrum (125 MHz, $\text{DMSO}-d_6$) of 3	11
Figure S18. HSQC spectrum (500 MHz, $\text{DMSO}-d_6$) of 3	11
Figure S19. ^1H - ^1H COSY spectrum (500MHz, $\text{DMSO}-d_6$) of 3	12
Figure S20. HMBC spectrum (500 MHz, $\text{DMSO}-d_6$) of 3	12
Figure S21. ROESY spectrum (500 MHz, $\text{DMSO}-d_6$) of 3	13
Figure S22. HRESIMS spectrum for 4	13
Figure S23. ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of 4	14
Figure S24. ^{13}C NMR spectrum (125 MHz, $\text{DMSO}-d_6$) of 4	14
Figure S25. HSQC spectrum (500 MHz, $\text{DMSO}-d_6$) of 4	15
Figure S26. ^1H - ^1H COSY spectrum (500MHz, $\text{DMSO}-d_6$) of 3	15
Figure S27 HMBC spectrum (500 MHz, $\text{DMSO}-d_6$) of 4	16

Figure S28. ROESY spectrum (500 MHz, DMSO- d_6) of **4** 16

Figure S29. The structures of compounds **5-13** 17



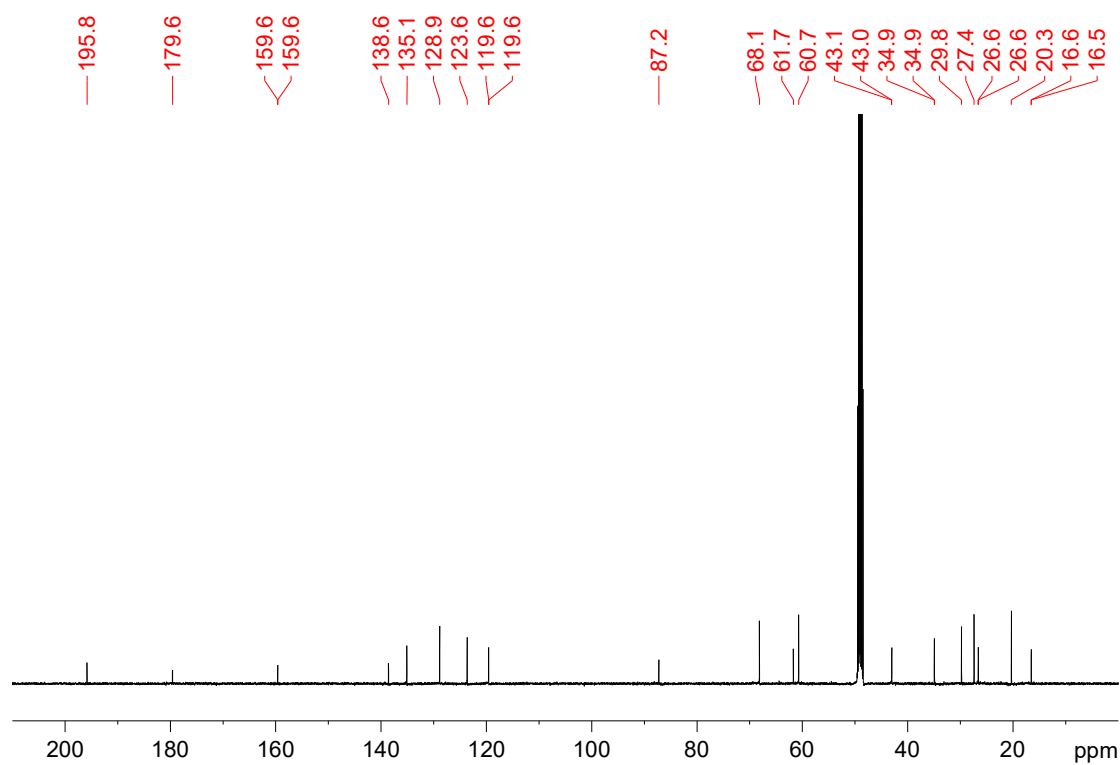


Figure S3. ¹³C NMR spectrum (125 MHz, CD₃OD) of **1**

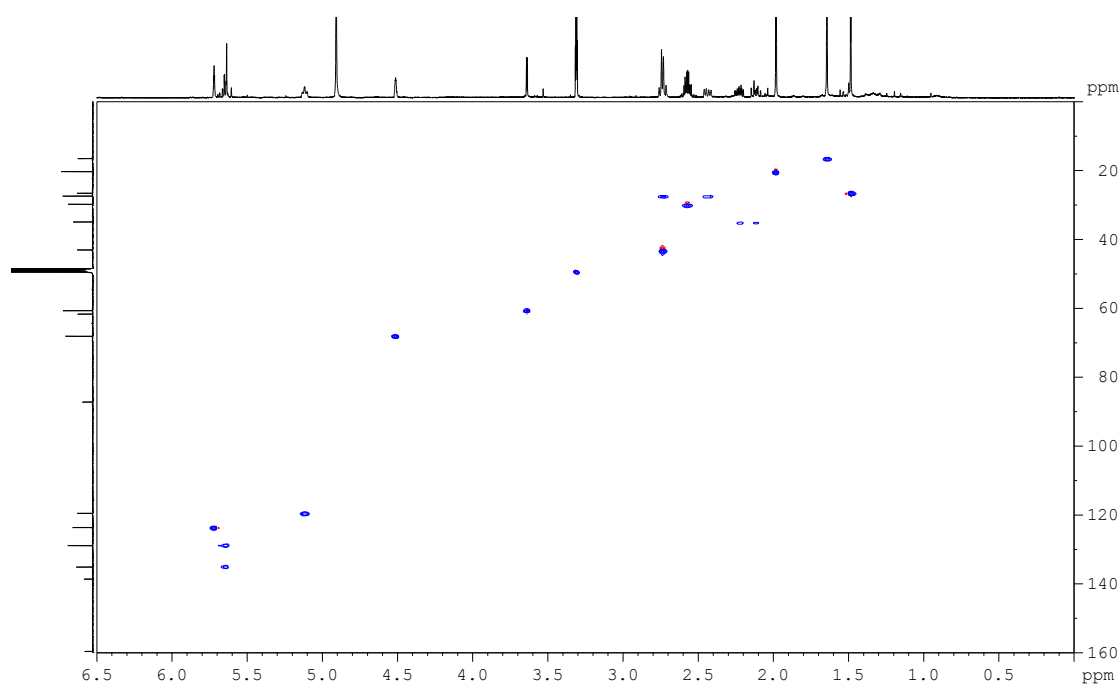


Figure S4. HSQC spectrum (500 MHz, CD₃OD) of **1**

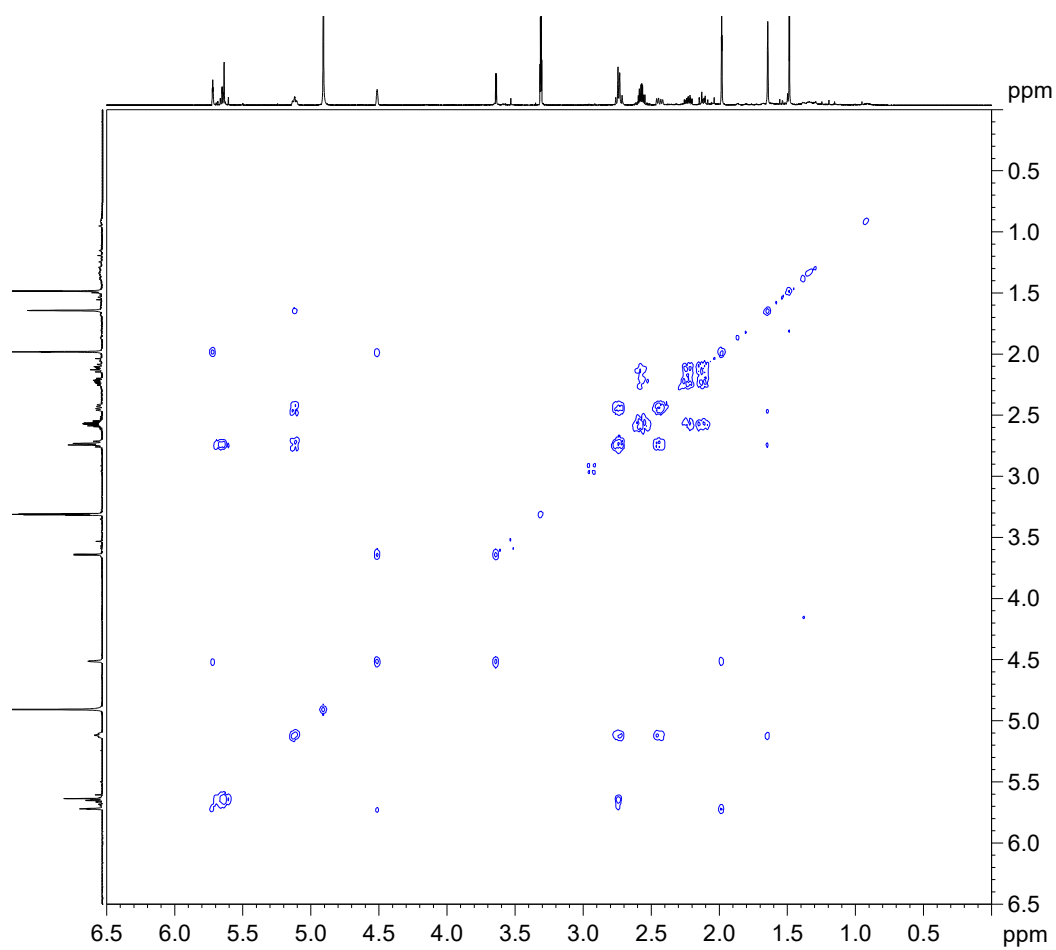


Figure S5. ^1H - ^1H COSY spectrum (500 MHz, CD_3OD) of **1**

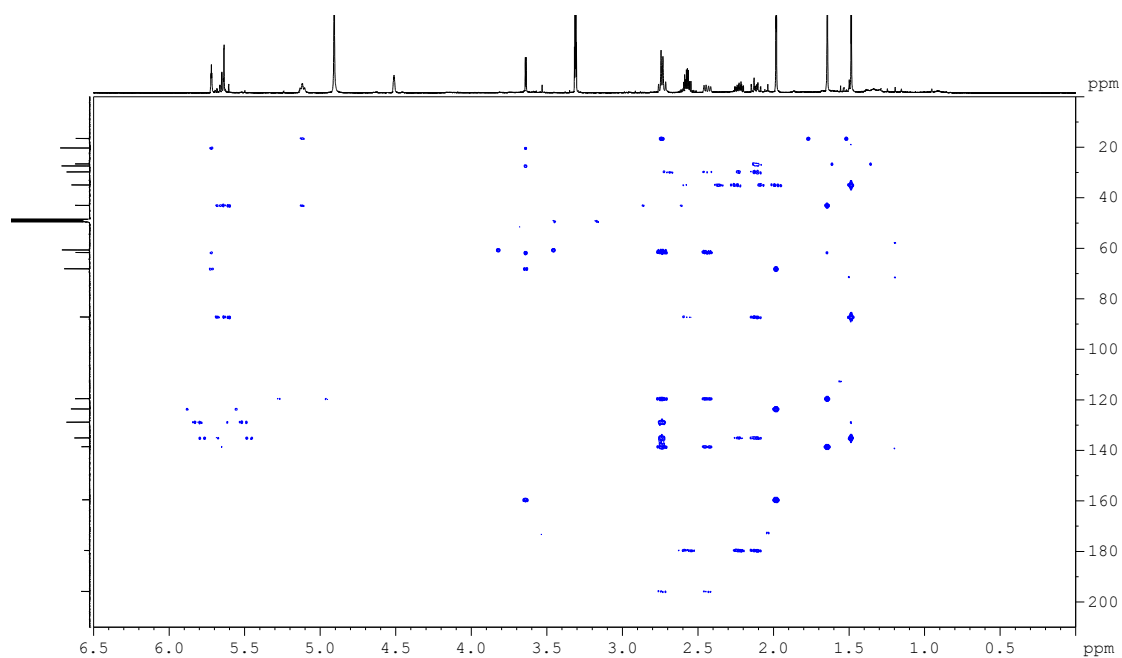


Figure S6. HMBC spectrum (500 MHz, CD_3OD) of **1**

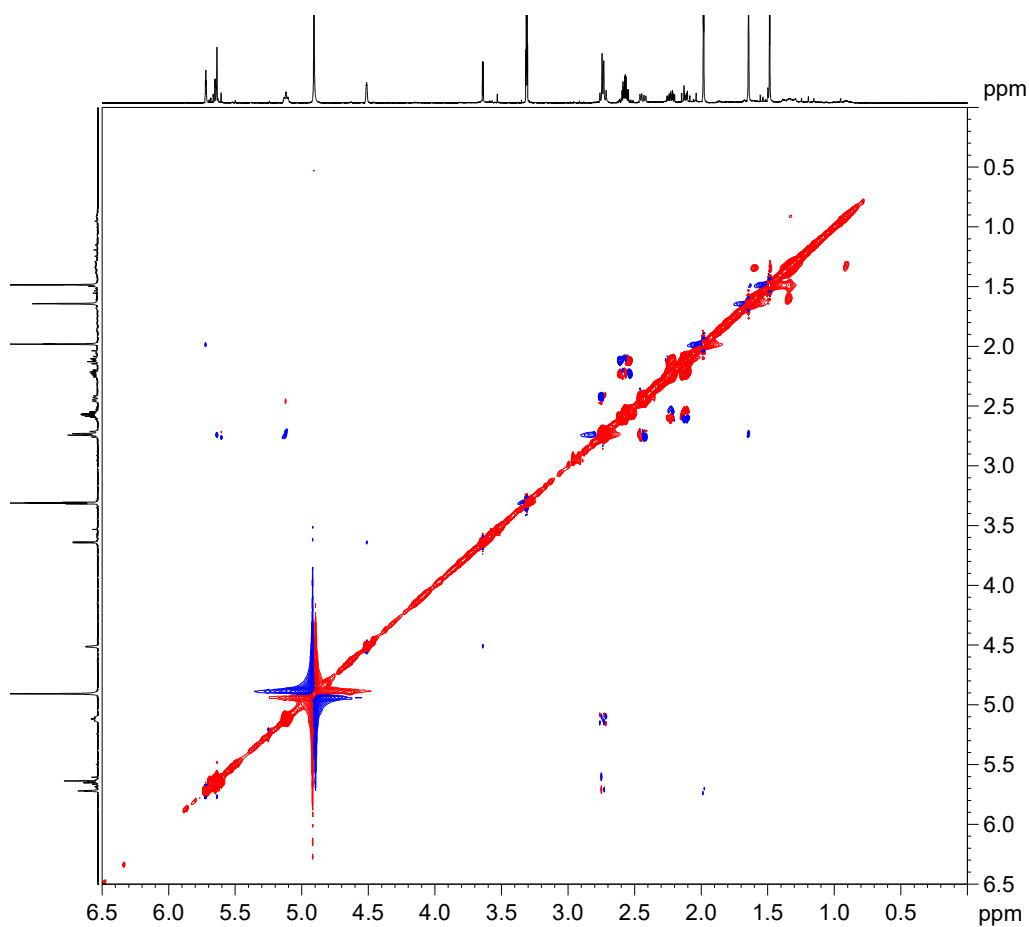


Figure S7. ROESY spectrum (500 MHz, CD₃OD) of **1**

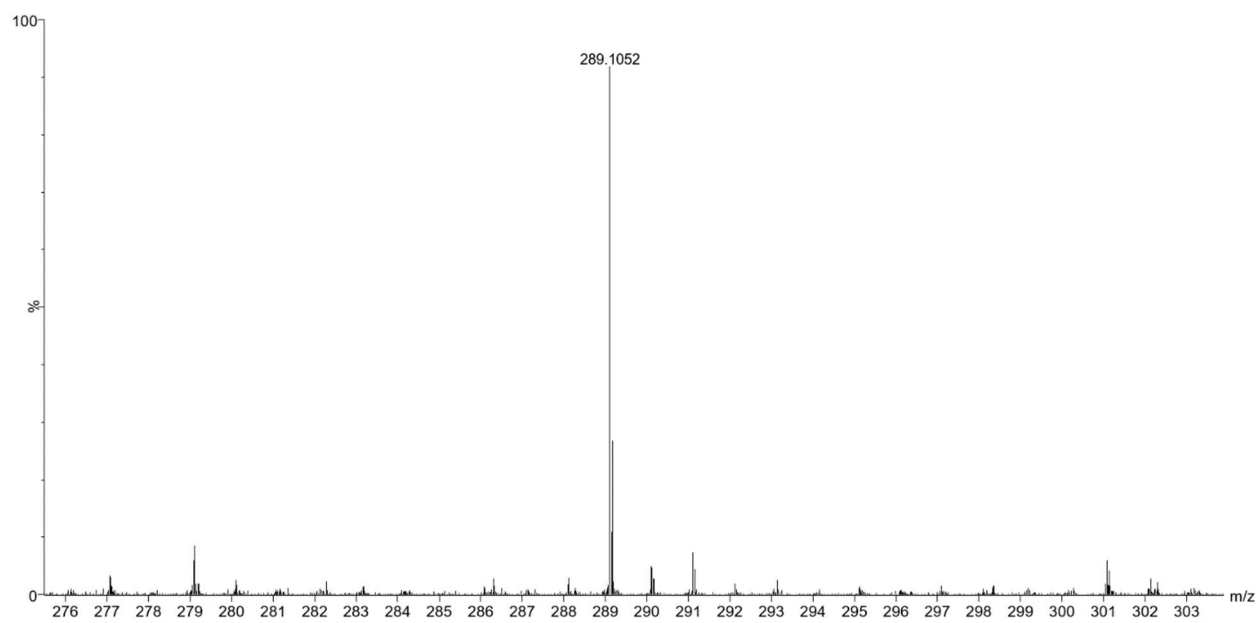


Figure S8. HRESIMS spectrum of **2**

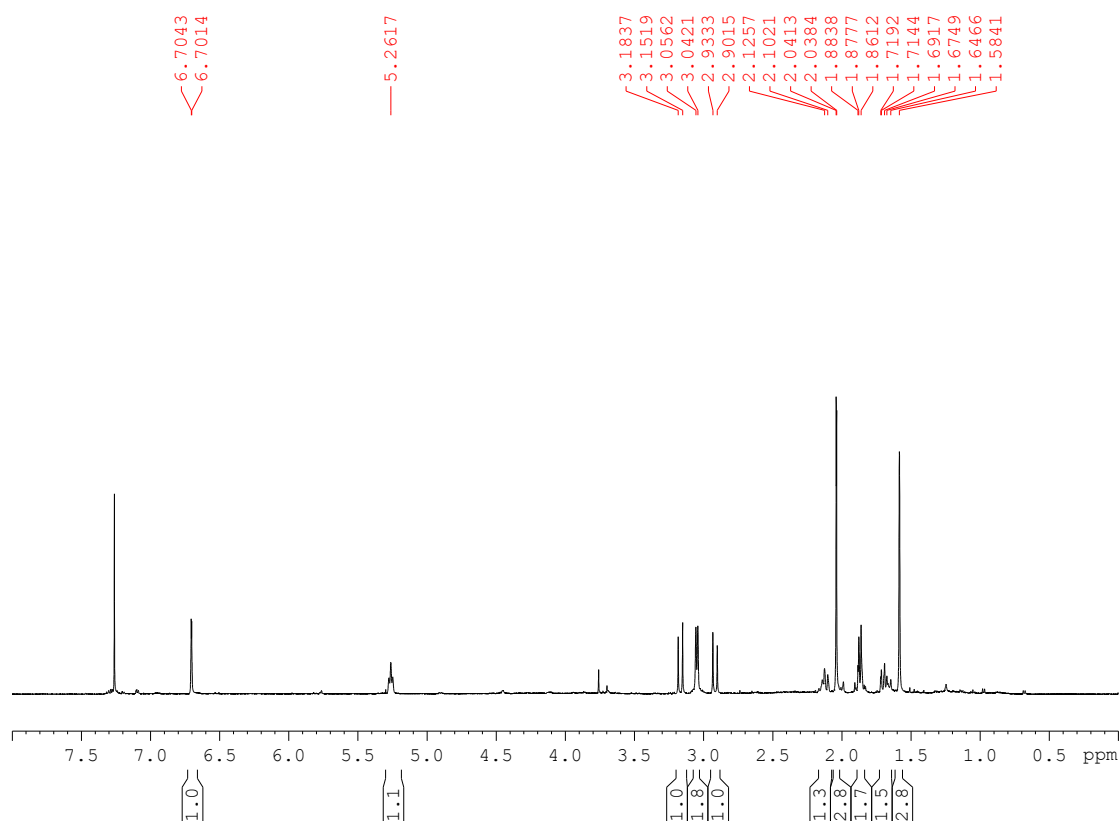


Figure S9. ^1H NMR spectrum (500 MHz, CDCl_3) of **2**

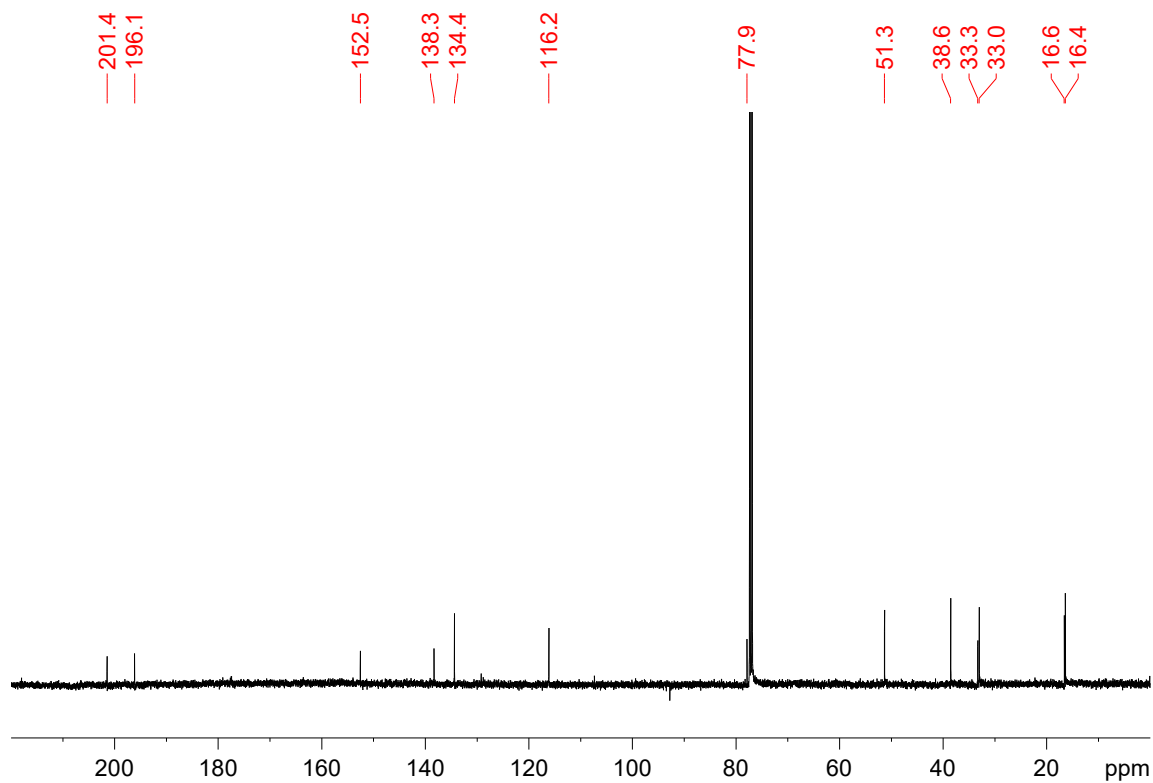


Figure S10. ^{13}C NMR spectrum (125 MHz, CDCl_3) of **2**

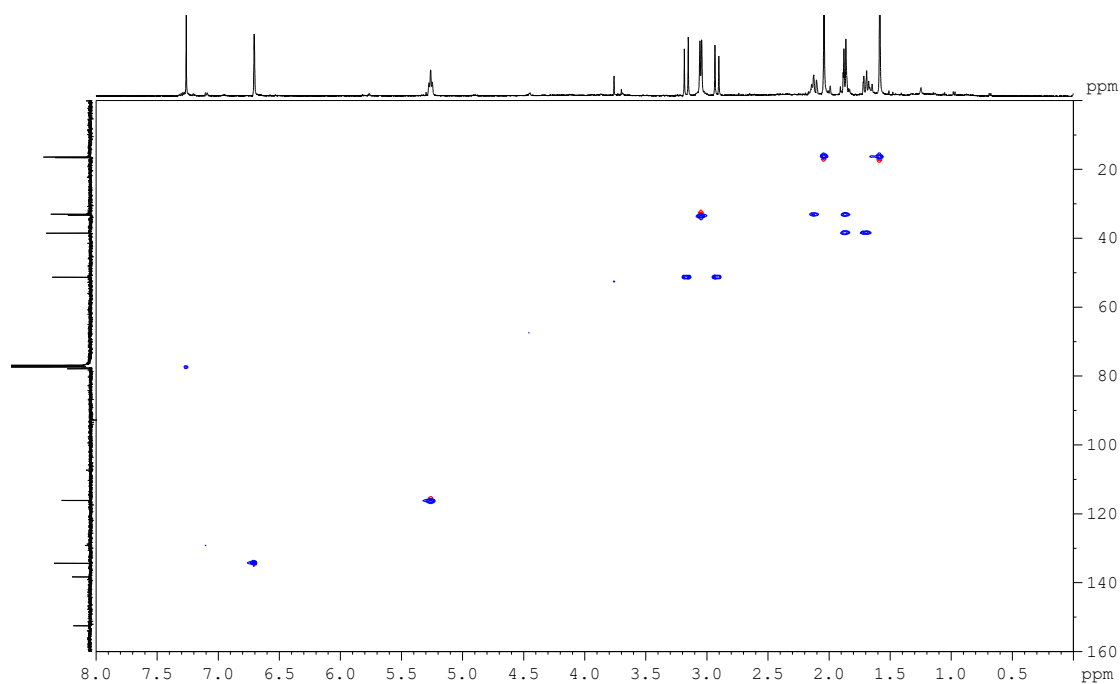


Figure S11. HSQC spectrum (500 MHz, CDCl₃) of **2**

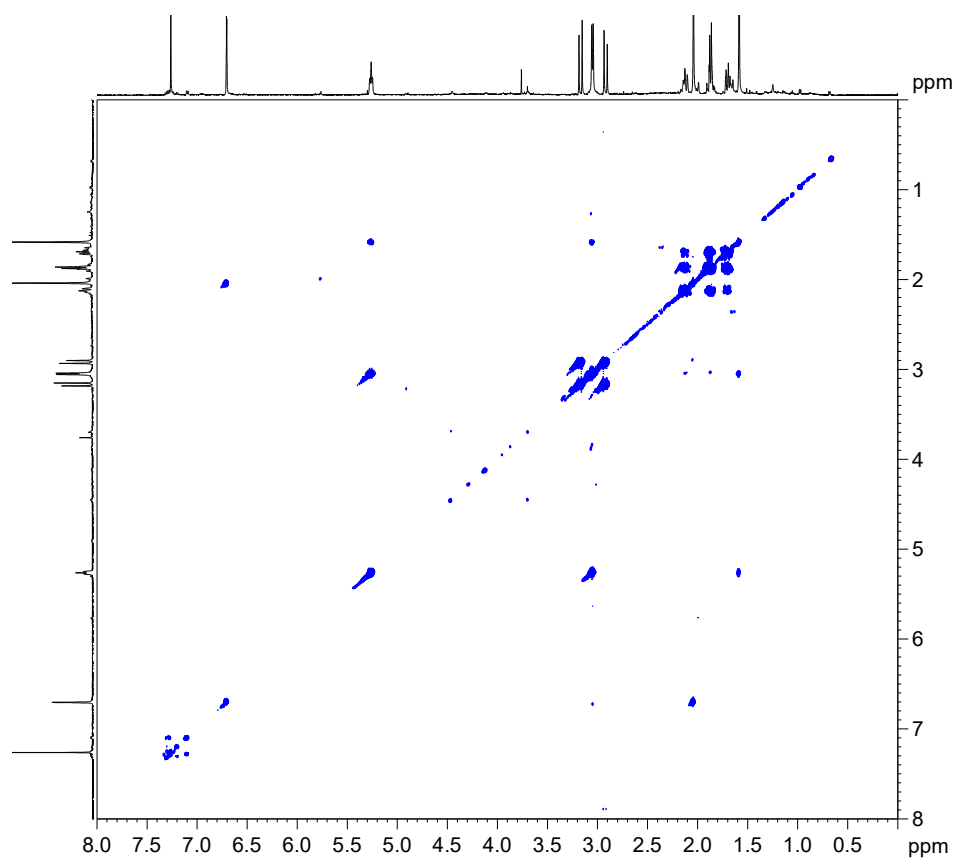


Figure S12. ¹H-¹H COSY spectrum (500 MHz, CDCl₃) of **2**

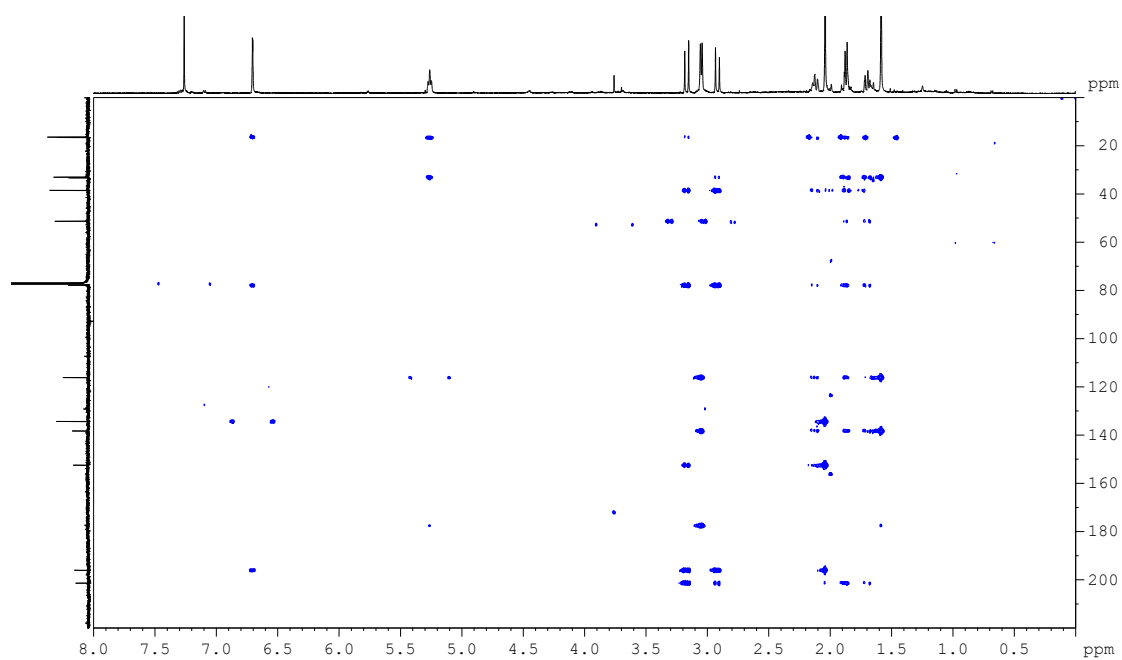


Figure S13. HMBC spectrum (500 MHz, CDCl_3) of **2**

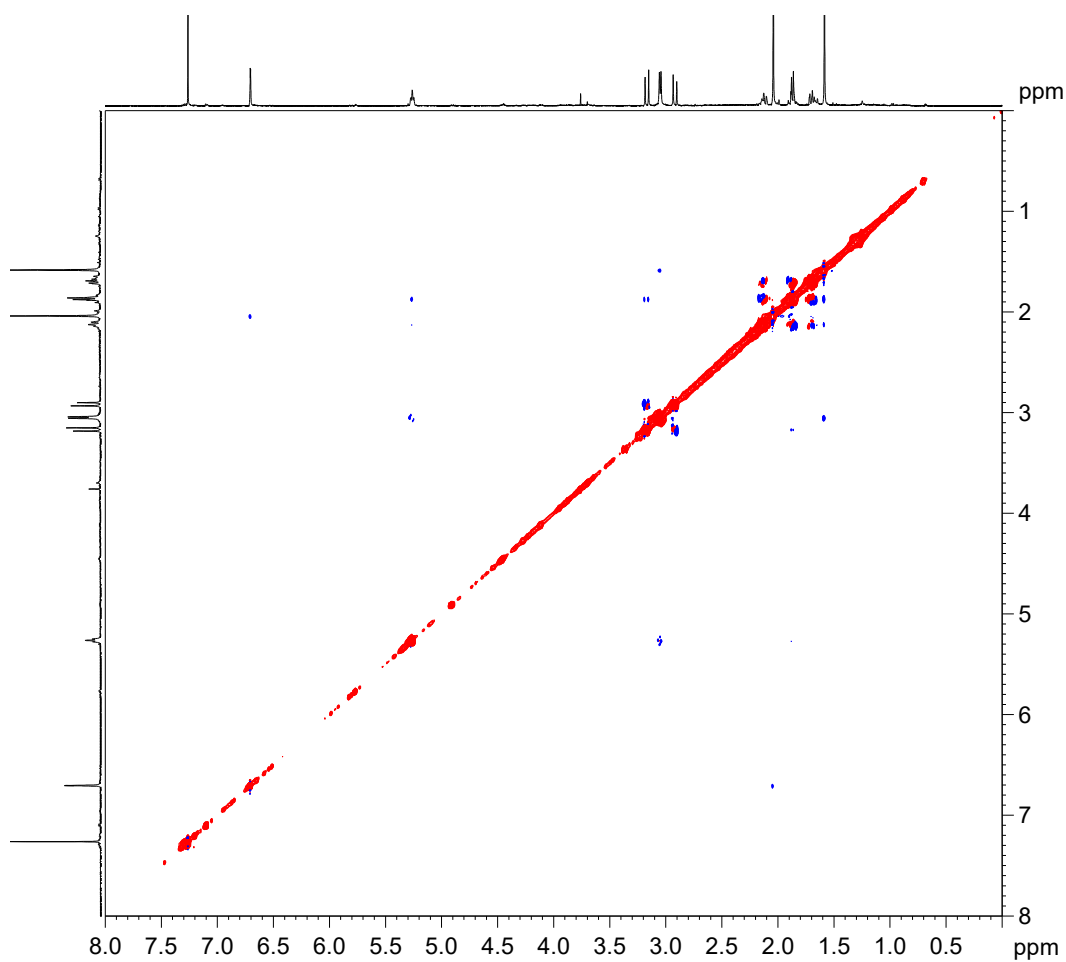


Figure S14. ROESY spectrum (500 MHz, CDCl_3) of **2**

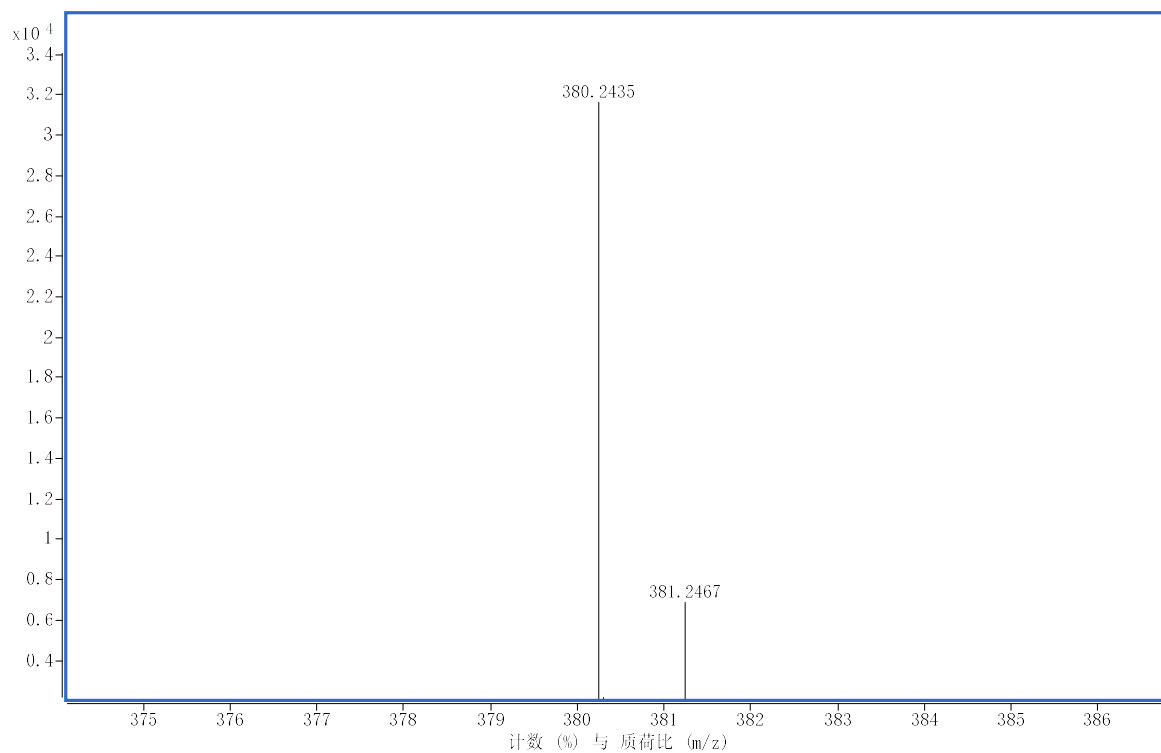
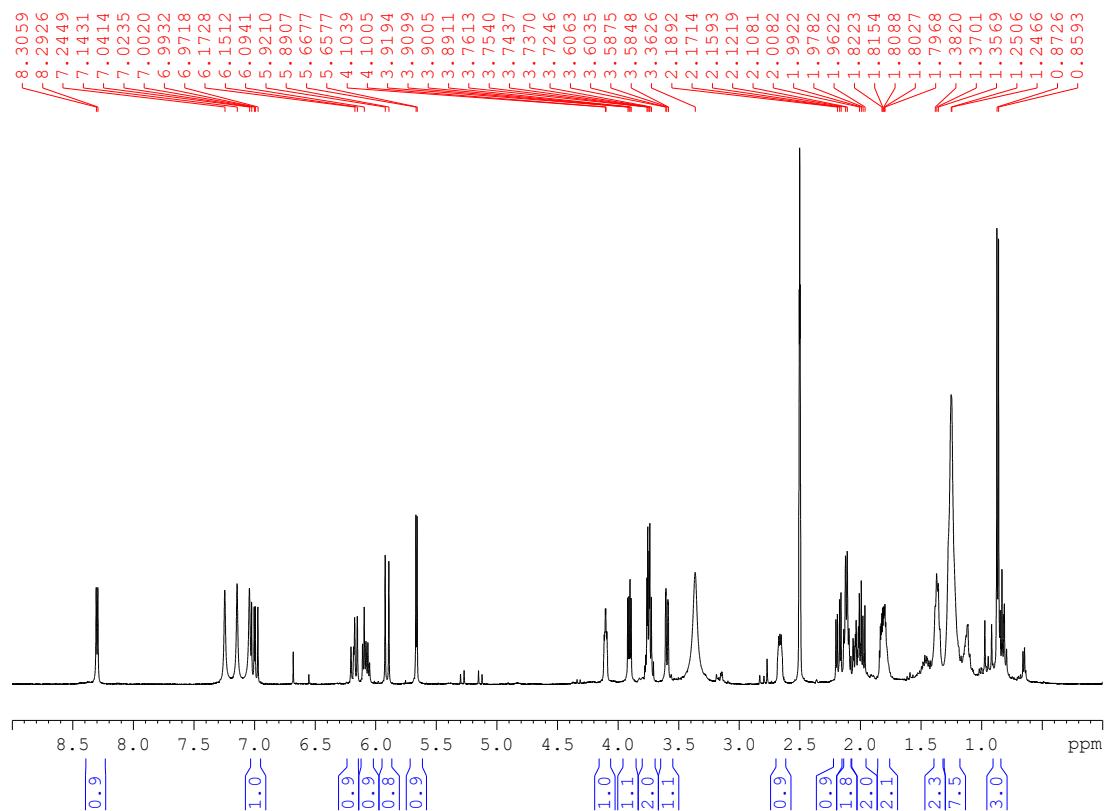


Figure S15. HRESIMS spectrum of 3

Figure S16. ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of 3

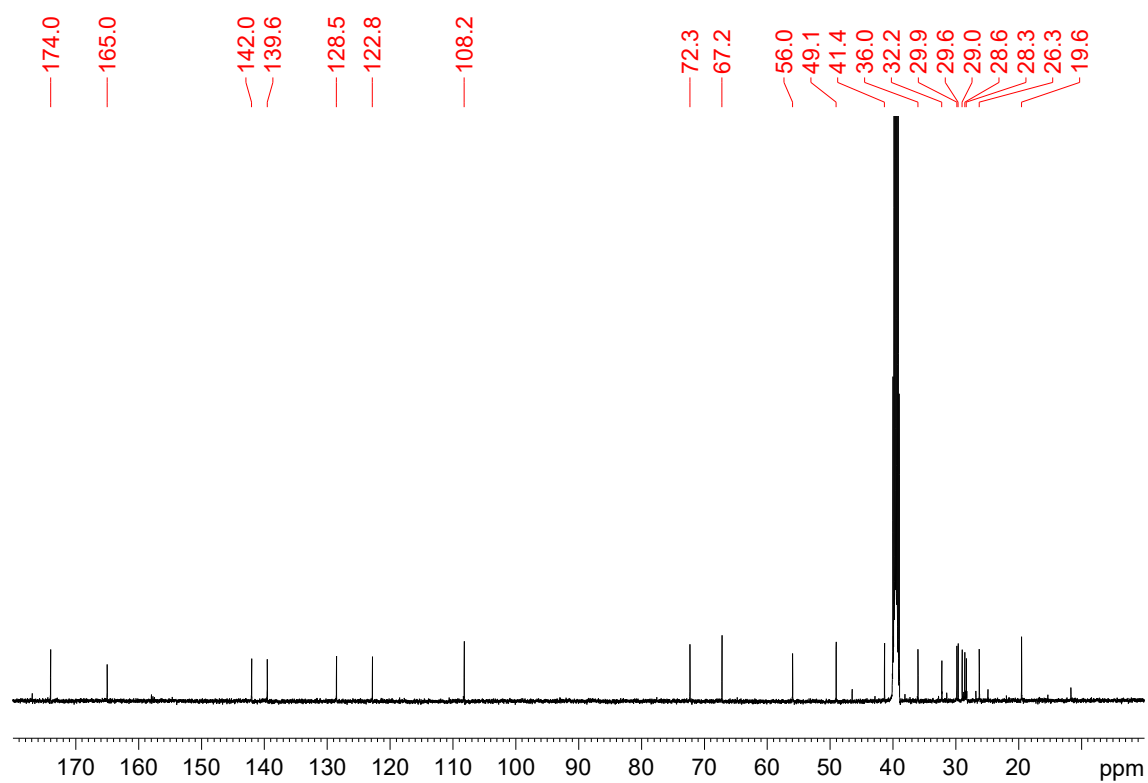


Figure S17. ^{13}C NMR spectrum (125 MHz, $\text{DMSO-}d_6$) of **3**

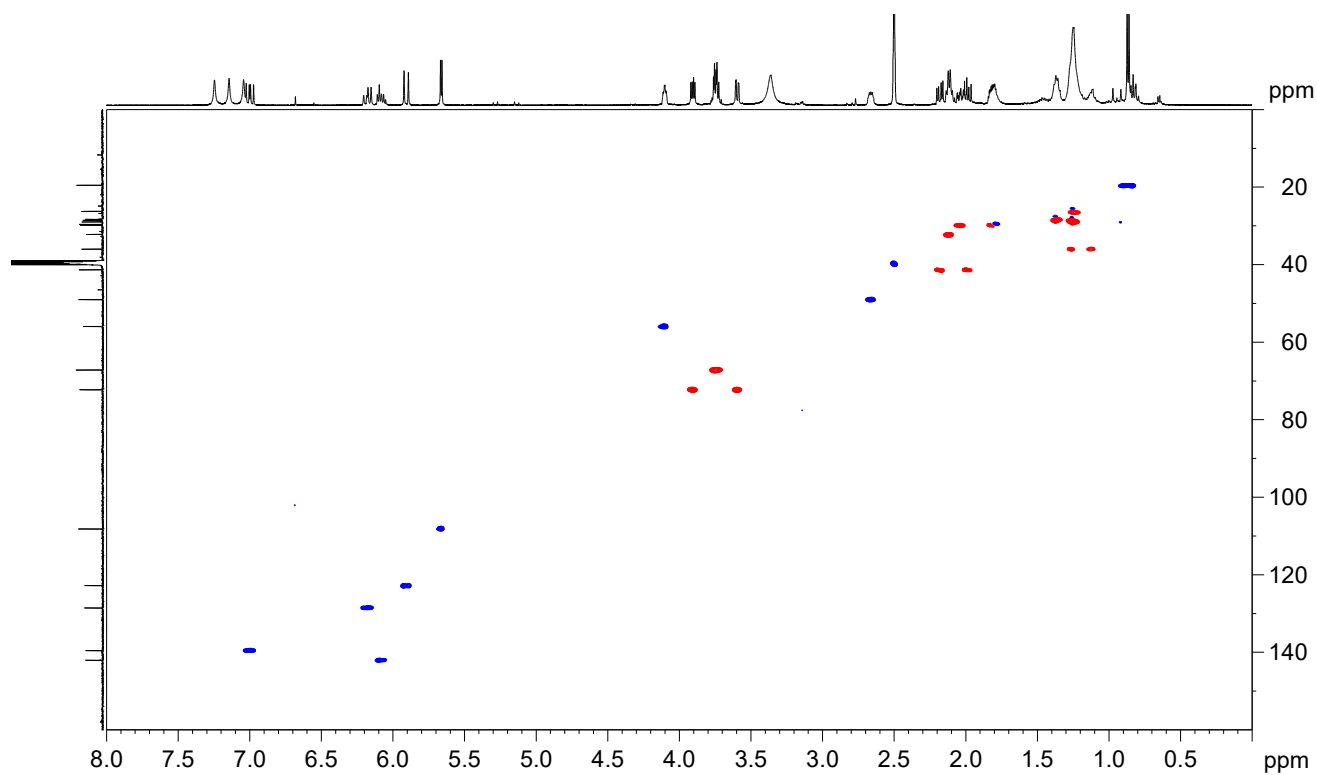


Figure S18. HSQC spectrum (500 MHz, $\text{DMSO-}d_6$) of **3**

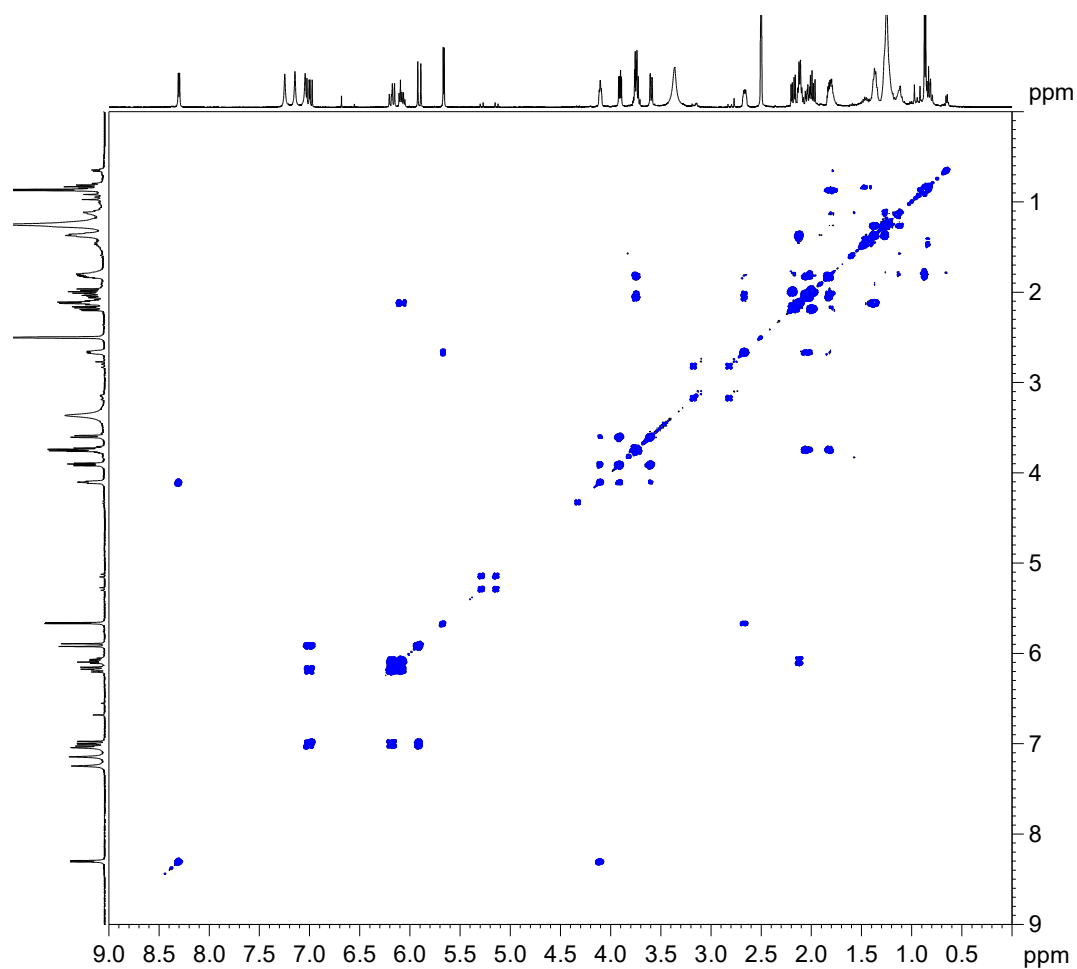


Figure S19. ^1H - ^1H COSY spectrum (500 MHz, $\text{DMSO-}d_6$) of **3**

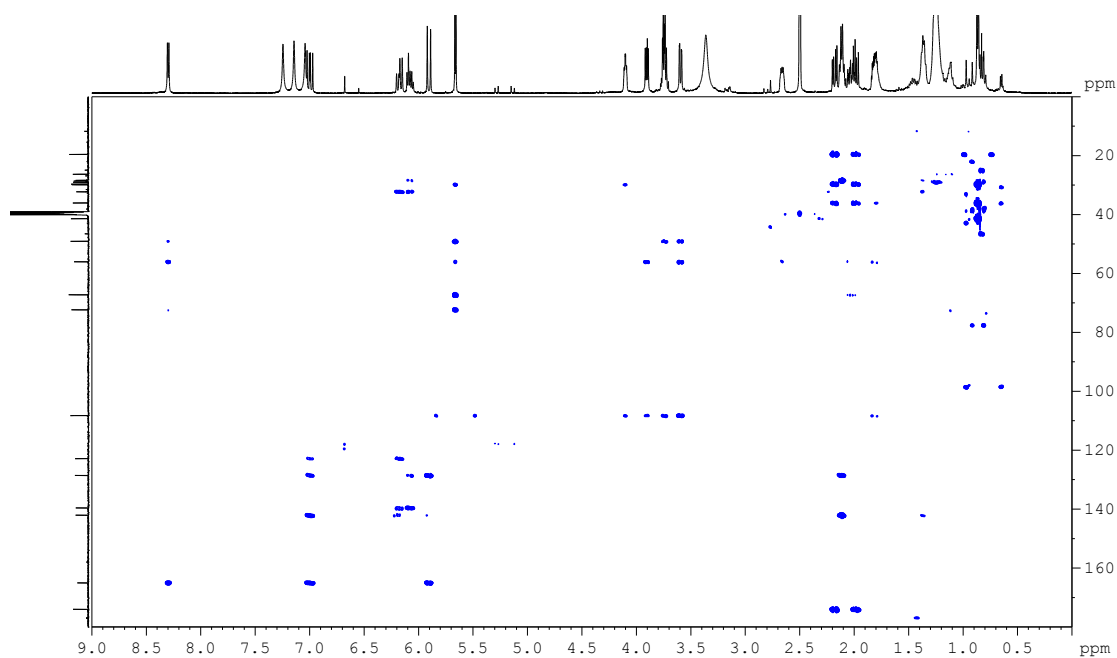


Figure S20. HMBC spectrum (500 MHz, $\text{DMSO-}d_6$) of **3**

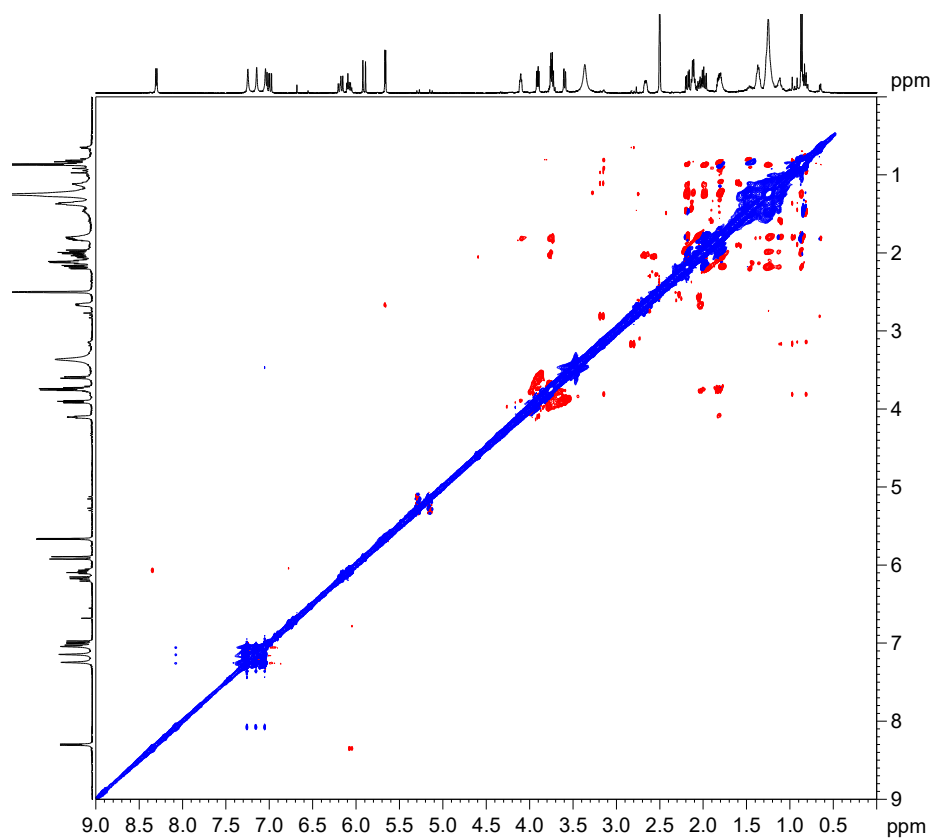


Figure S21. ROESY spectrum (500 MHz, DMSO- d_6) of **3**

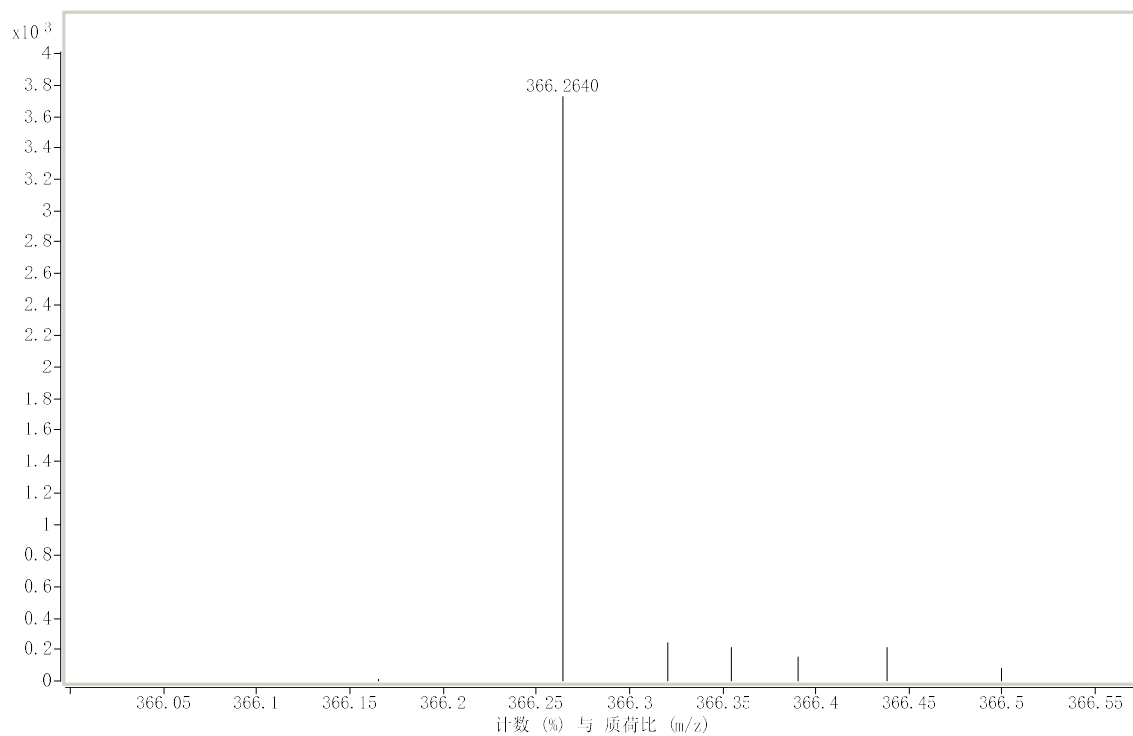


Figure S22. HRESIMS spectrum of **4**

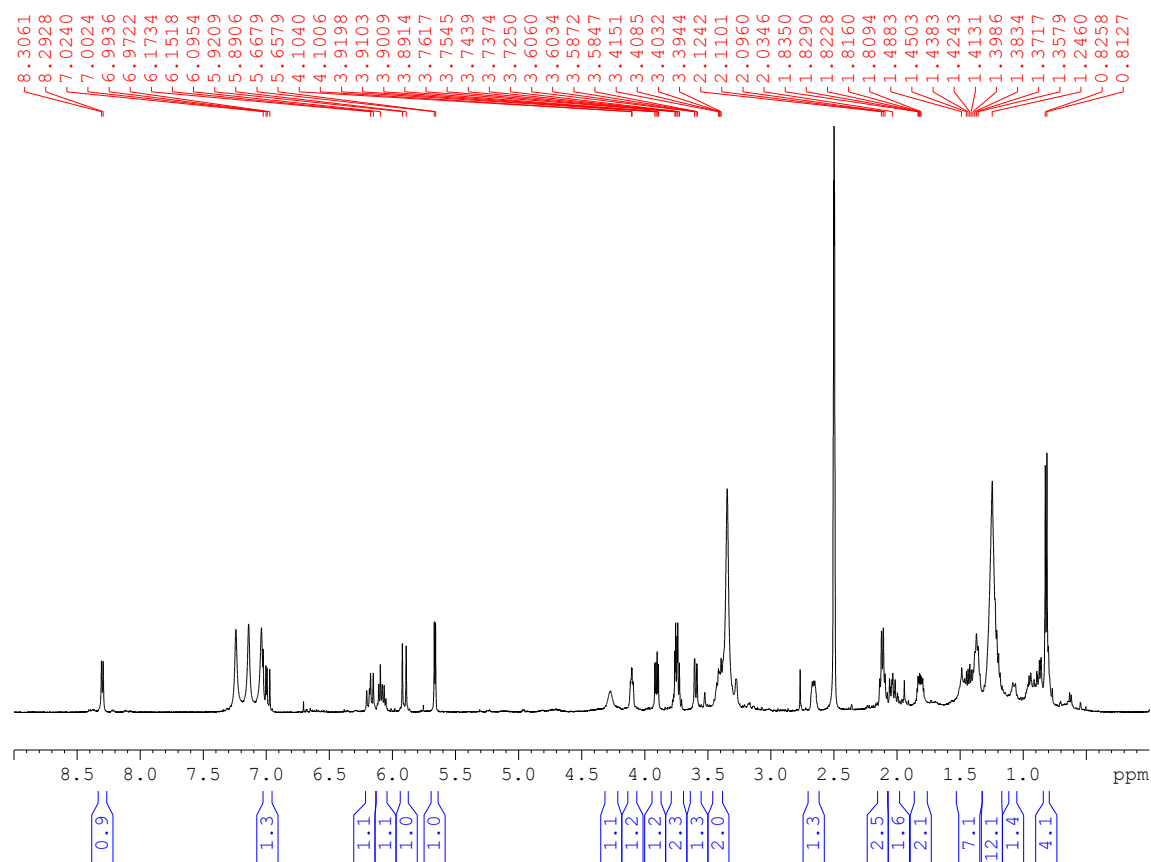


Figure S23. ¹H NMR spectrum (500 MHz, DMSO-*d*₆) of **4**

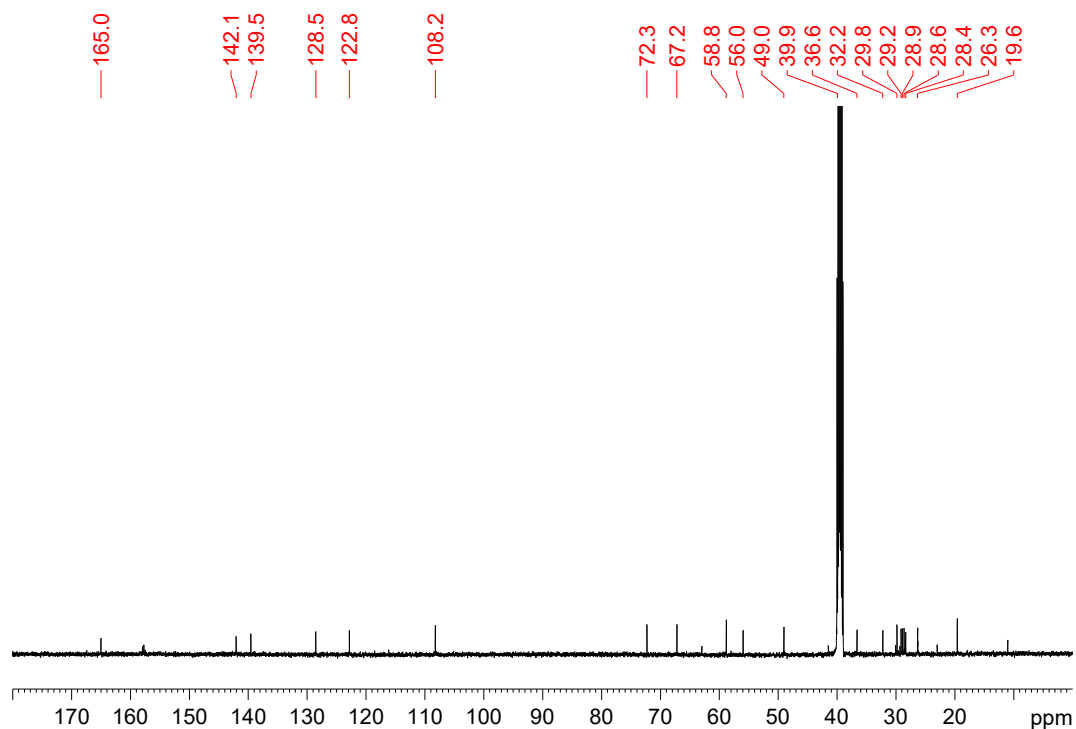


Figure S24. ¹³C NMR spectrum (125 MHz, DMSO-*d*₆) of **4**

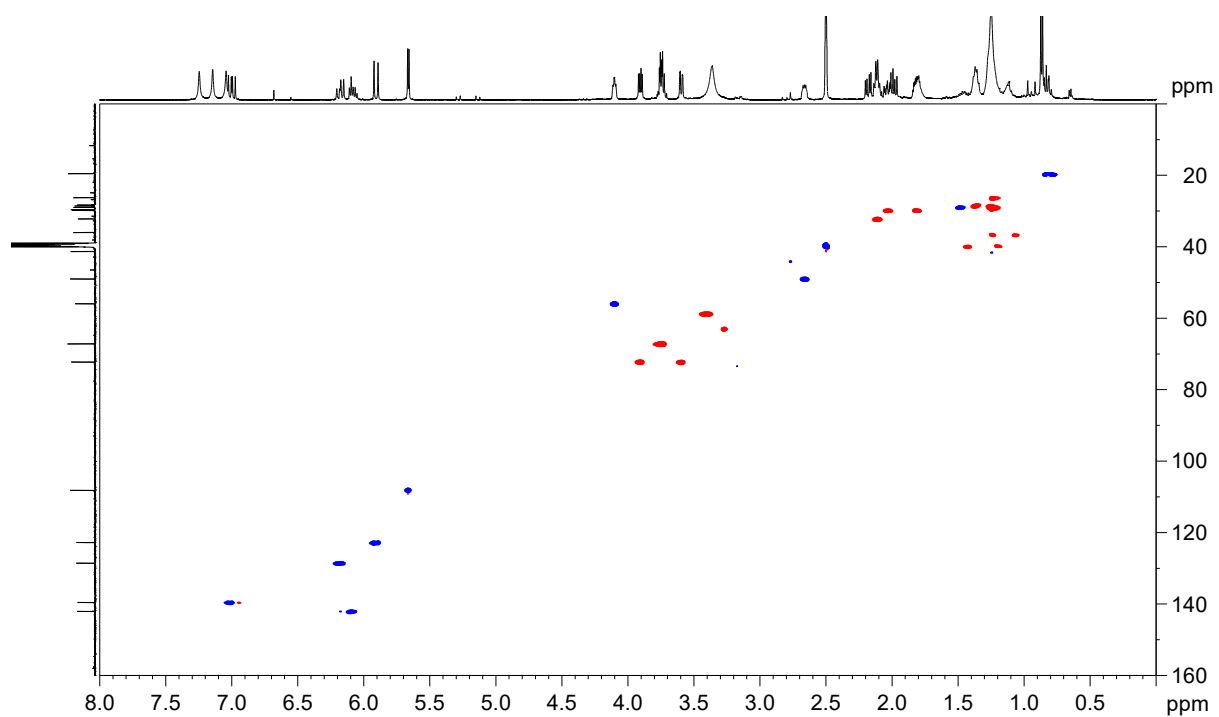


Figure S25. HSQC spectrum (500 MHz, DMSO- d_6) of **4**

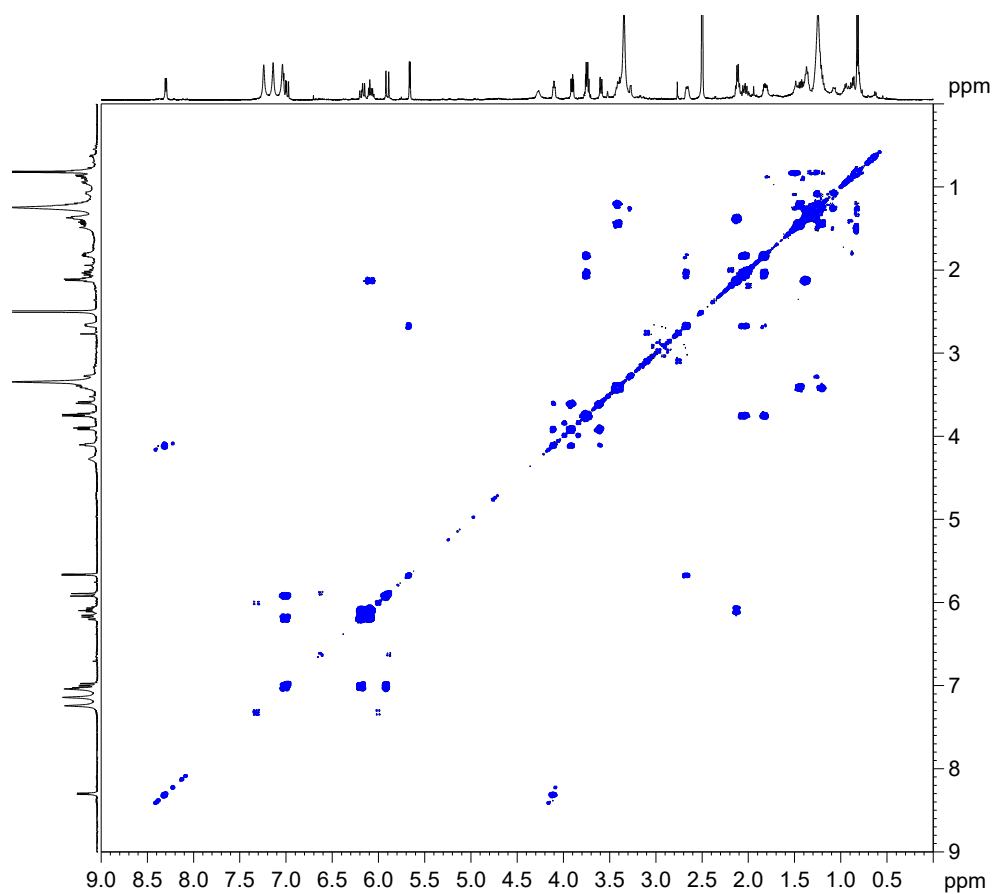


Figure S26. ^1H - ^1H COSY spectrum (500 MHz, DMSO- d_6) of **4**

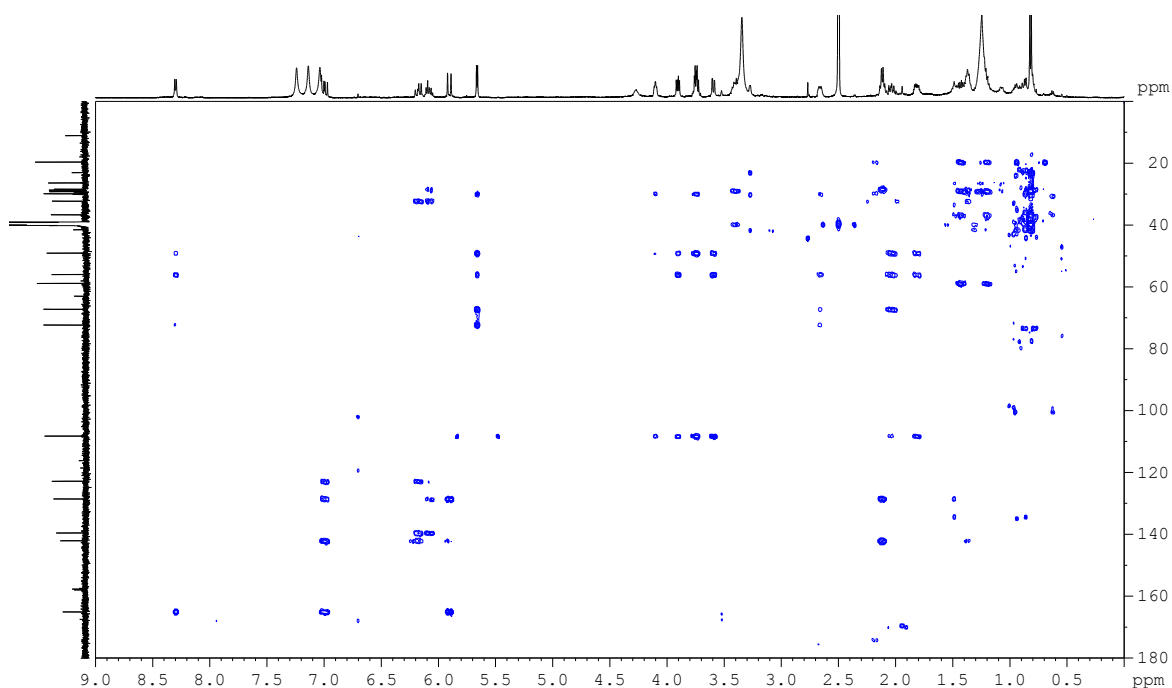


Figure S27. HMBC spectrum (500 MHz, DMSO-*d*₆) of **4**

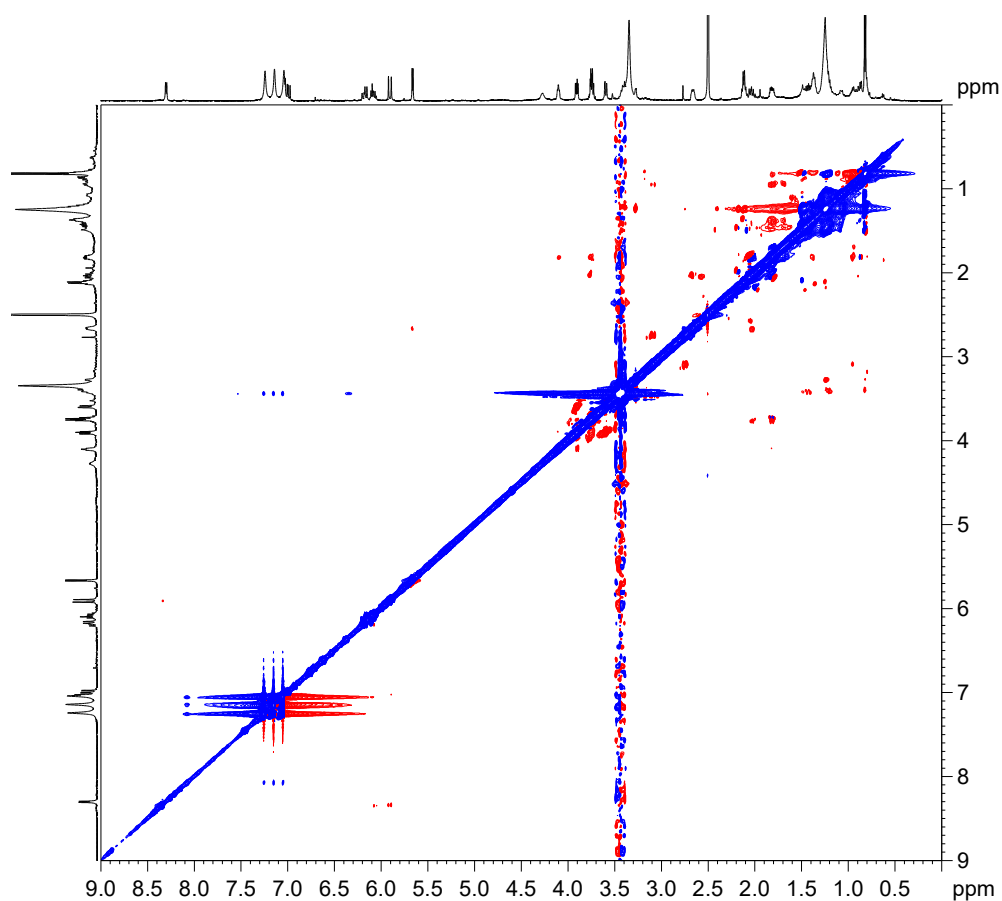


Figure S28. ROESY spectrum (500 MHz, DMSO-*d*₆) of **4**

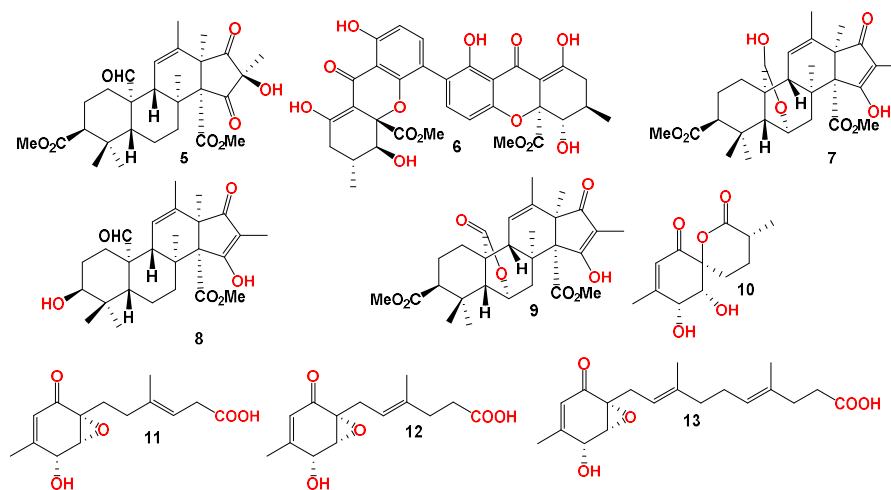


Figure S29. The structures of compounds 5-13.