

Supporting Information

Isocoumarins and Benzofurans from the Mangrove Endophytic Fungus

Talaromyces amestolkiae Possessing α -Glucosidase Inhibitory and Antibacterial

Activities

Senhua Chen¹, Yayue Liu¹, Zhaoming Liu¹, Runlin Cai¹, Yongjun Lu^{2,3}, Xishan Huang^{1,*} and Zhigang She^{1,2,*}

Affiliation

¹ School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, China

² Key Laboratory of Functional Molecules from Oceanic Microorganisms (Sun Yat-Sen University), Department of Education of Guangdong Province, Guangzhou 510080, China

³School of Life Sciences and Biomedical Center, Sun Yat-Sen University, Guangzhou 510275, China;

Correspondence

Dr. Xishan Huang, E-mail: huangxishan13@foxmail.com; Prof. Zhigang She, School of Chemistry and Chemical Engineering, Sun Yat-Sen University, 135 West Xingang Road, Guangzhou 510275, P. R. China. E-mail: ceshzhg@mail.sysu.edu.cn. Tel/Fax: +86 20 84113356.

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Fig. S1 HREIMS spectrum of **1**

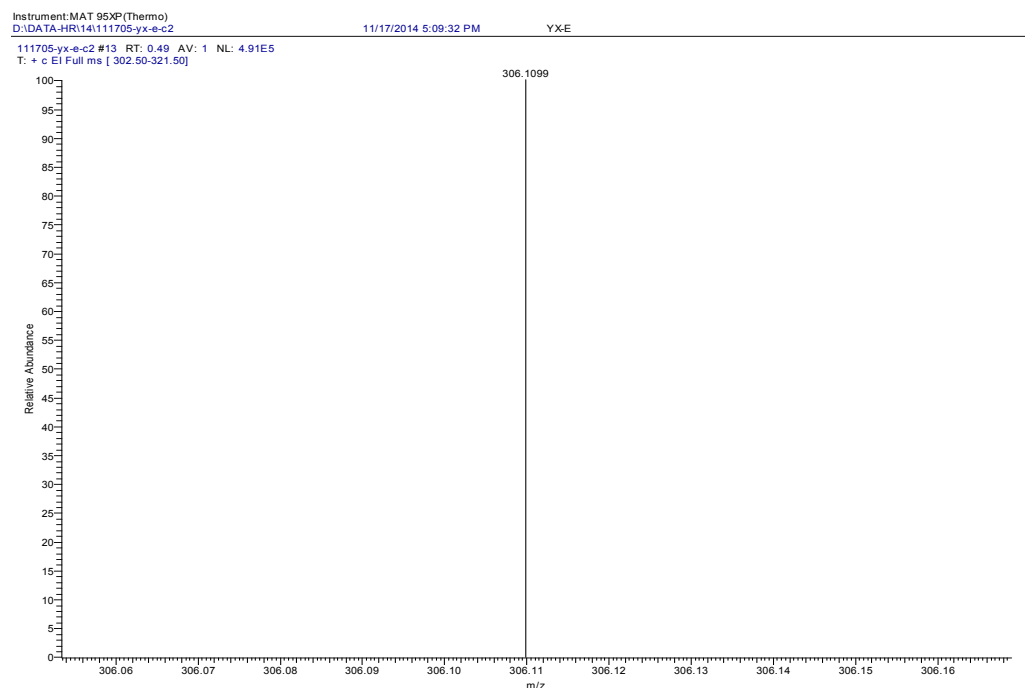


Fig. S2 ^1H NMR spectrum of **1** in CDCl_3

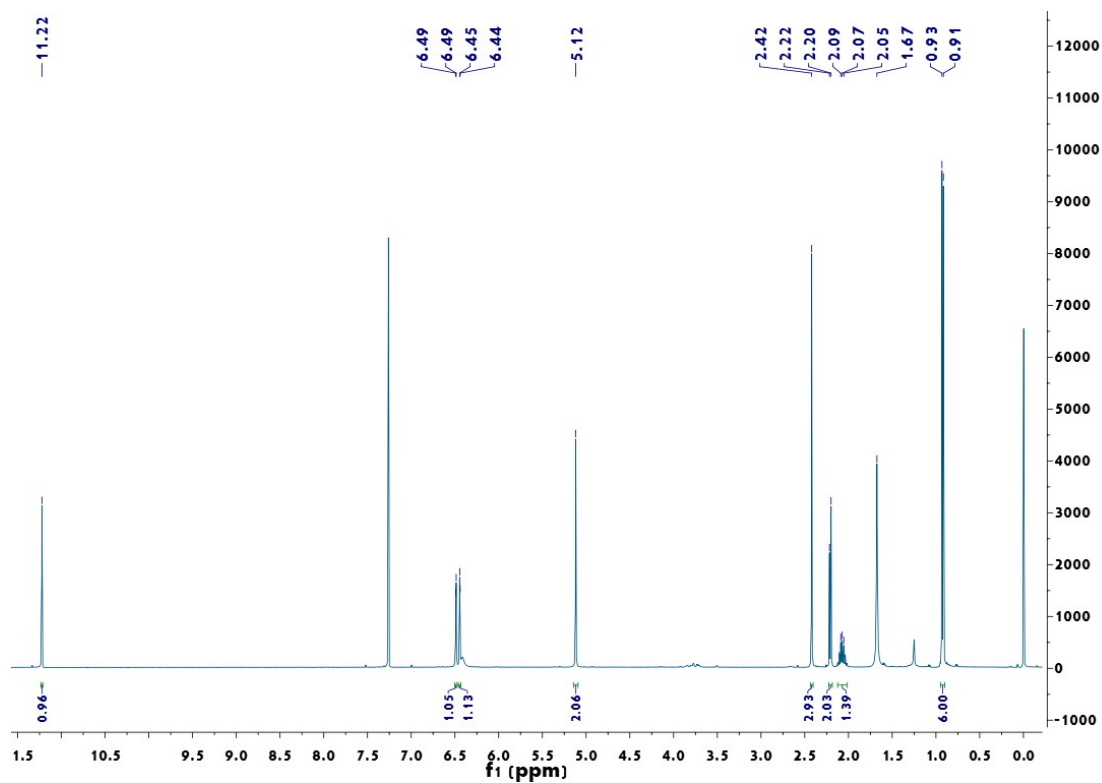


Fig. S3 ^{13}C NMR spectrum of **1** in CDCl_3

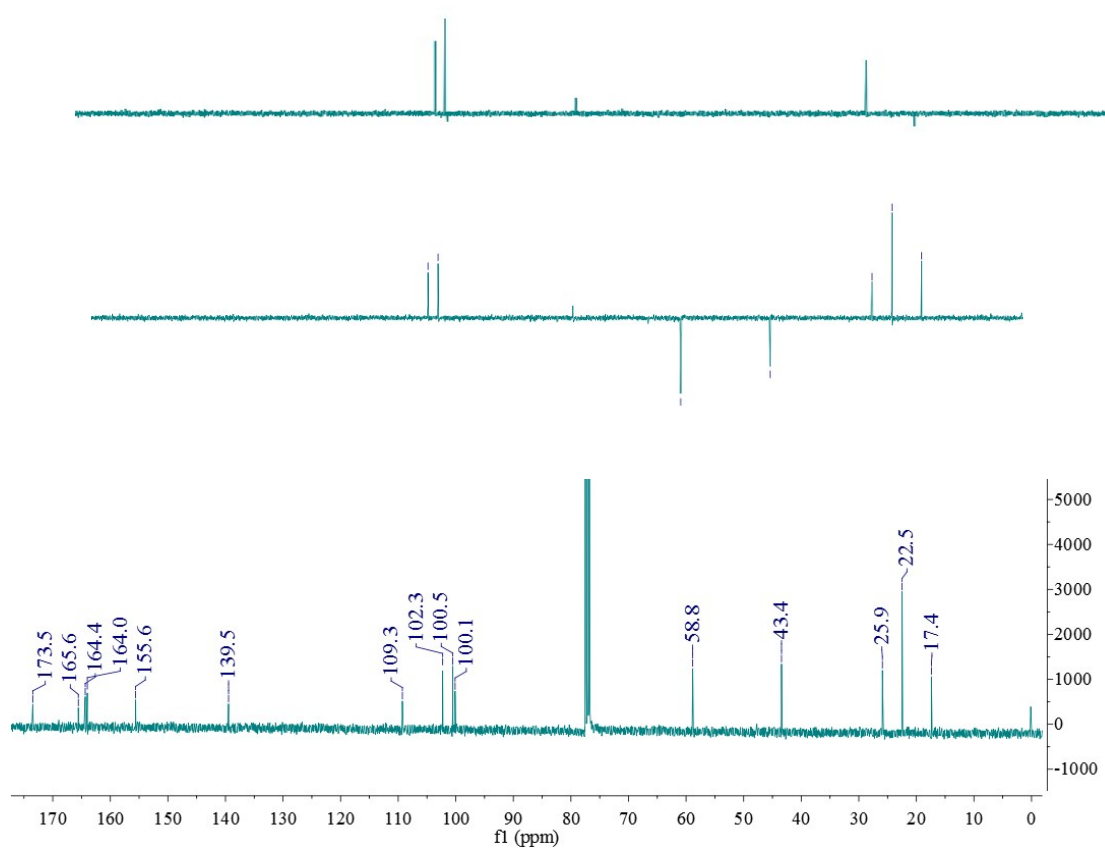


Fig. S4 HSQC spectrum of **1** in CDCl_3

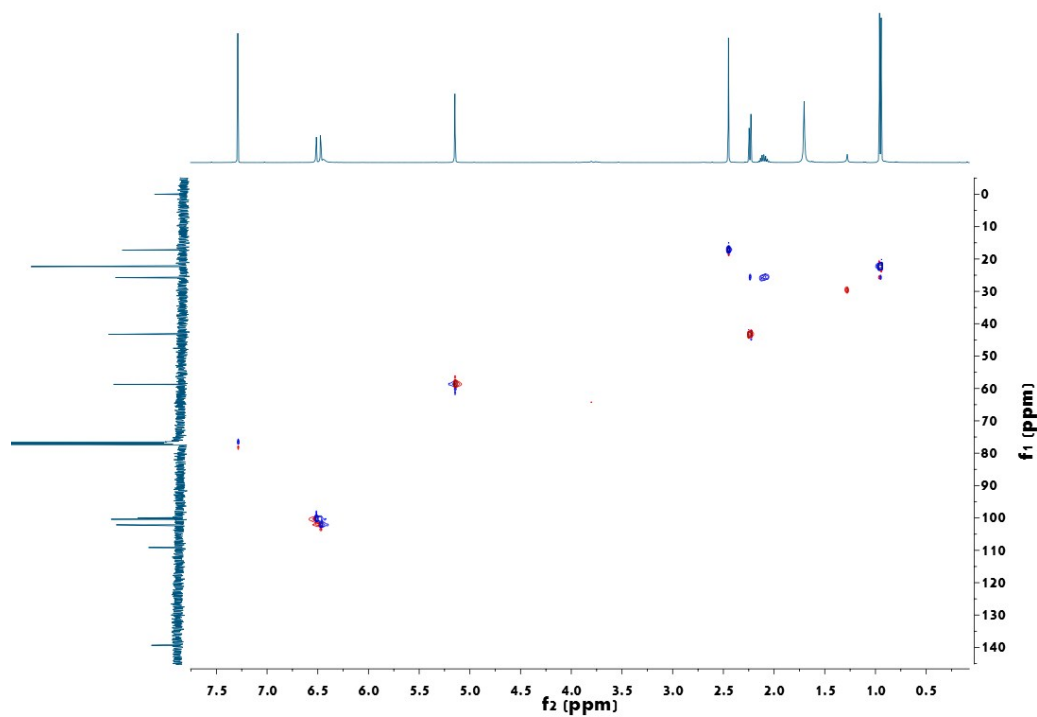


Fig. S5 ^1H - ^1H COSY spectrum of **1** in CDCl_3

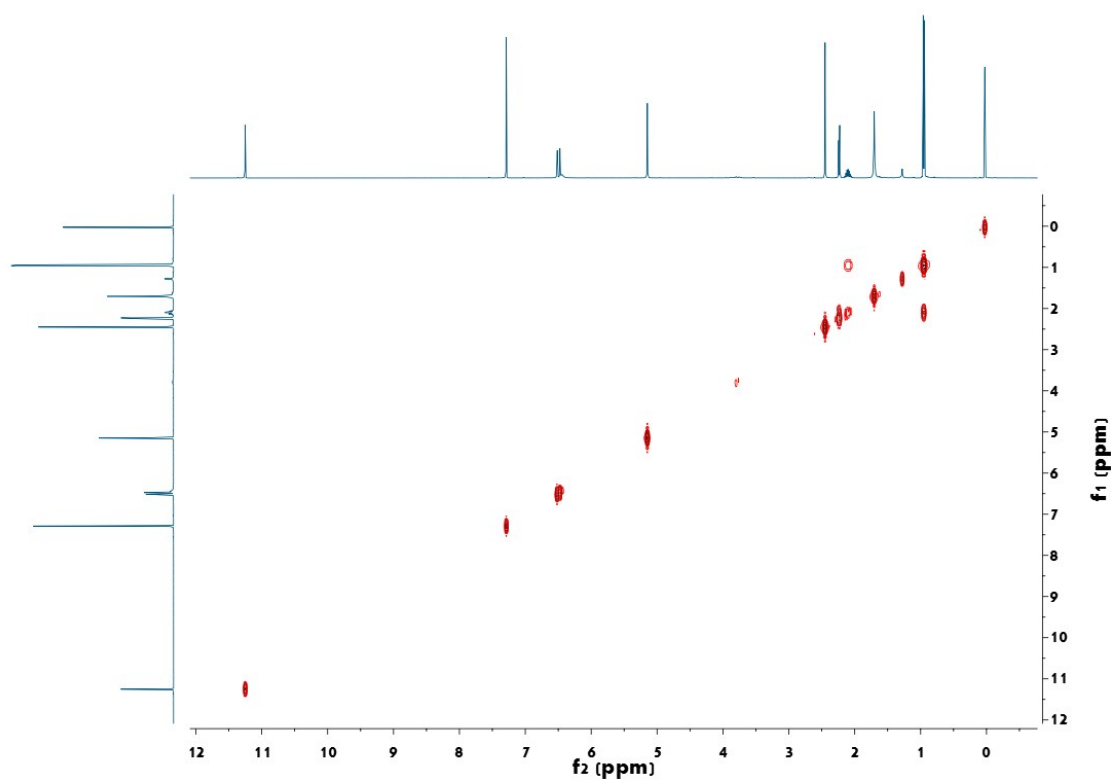


Fig. S6 HMBC spectrum of **1** in CDCl_3

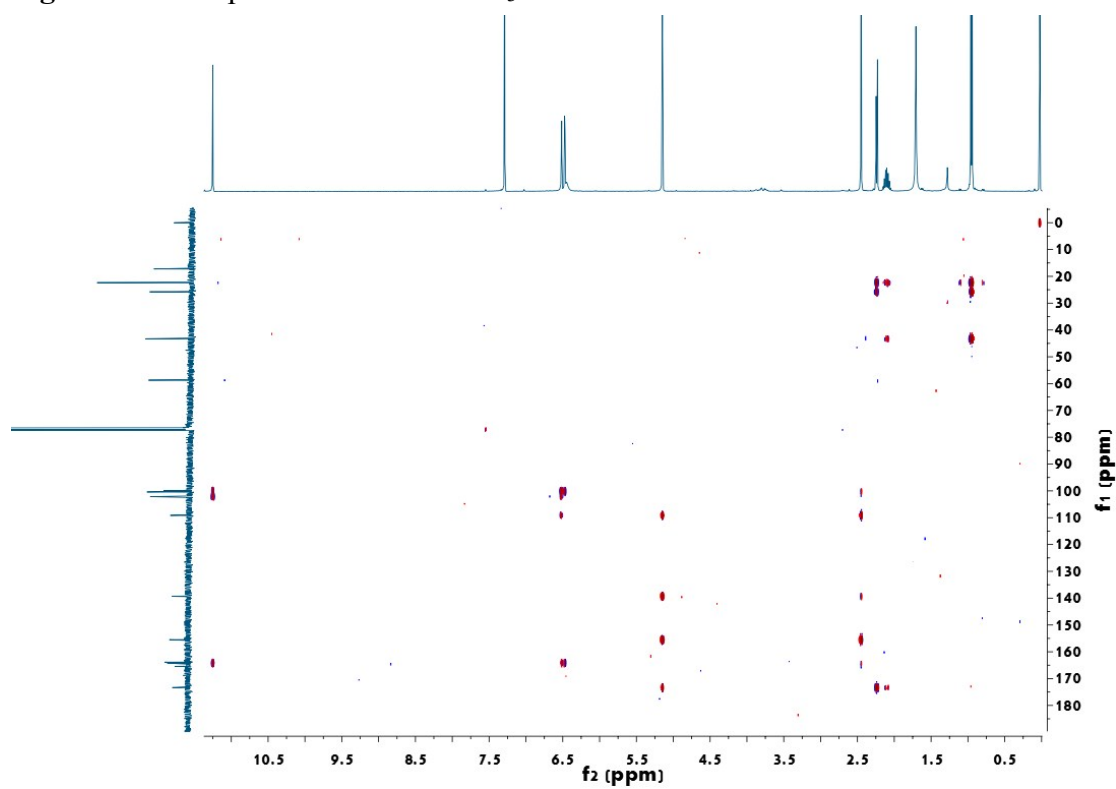


Fig. S7 HRESIMS spectrum of **2**

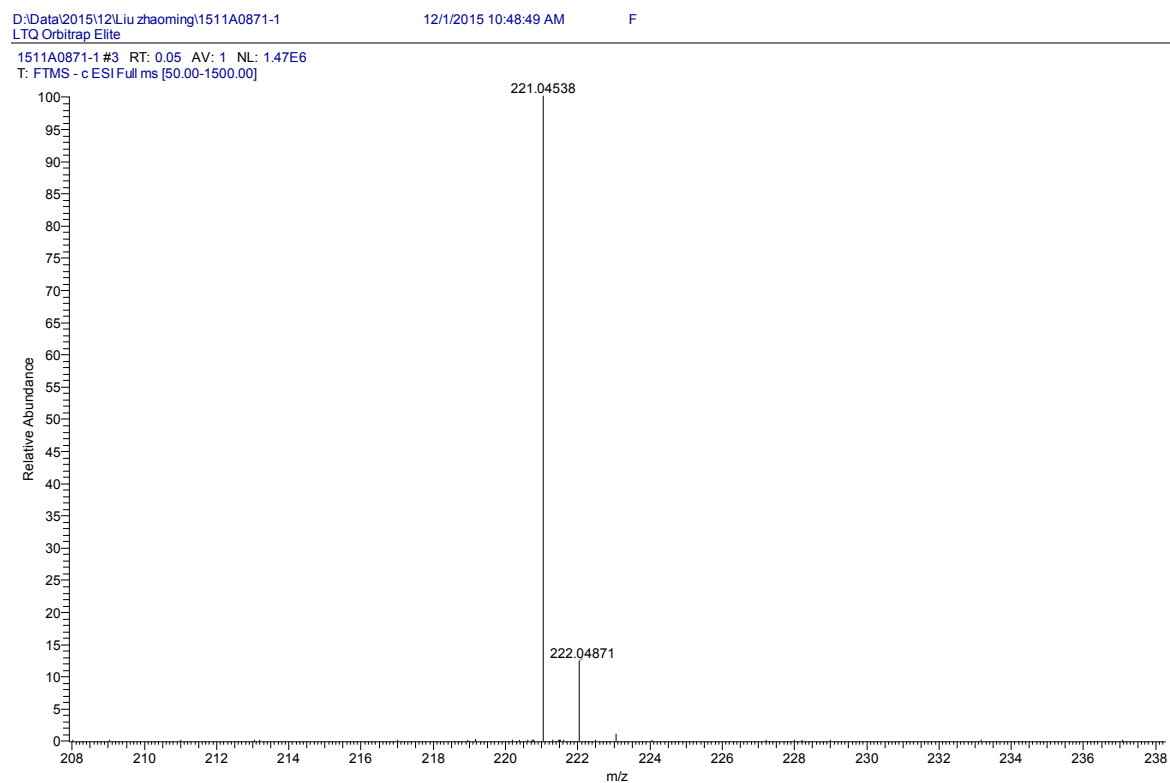


Fig. S8 ^1H NMR spectrum of **2** in CDCl_3

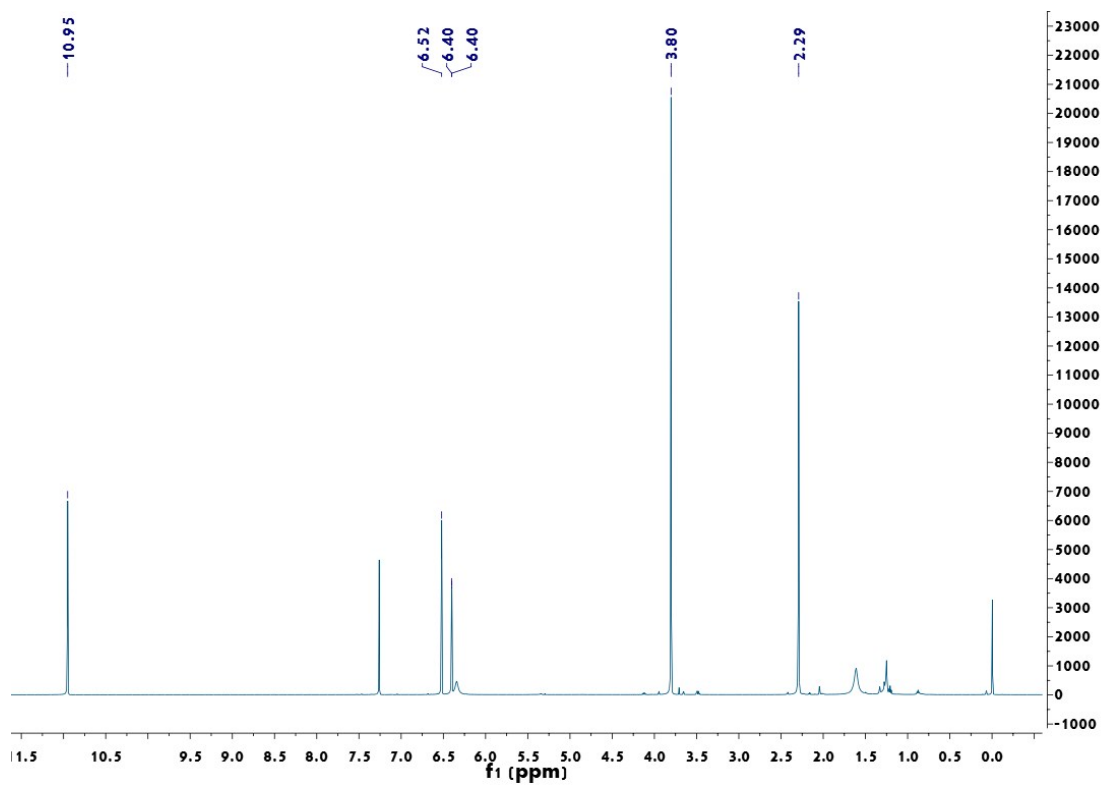


Fig. S9 ^{13}C NMR spectrum of **2** in CDCl_3

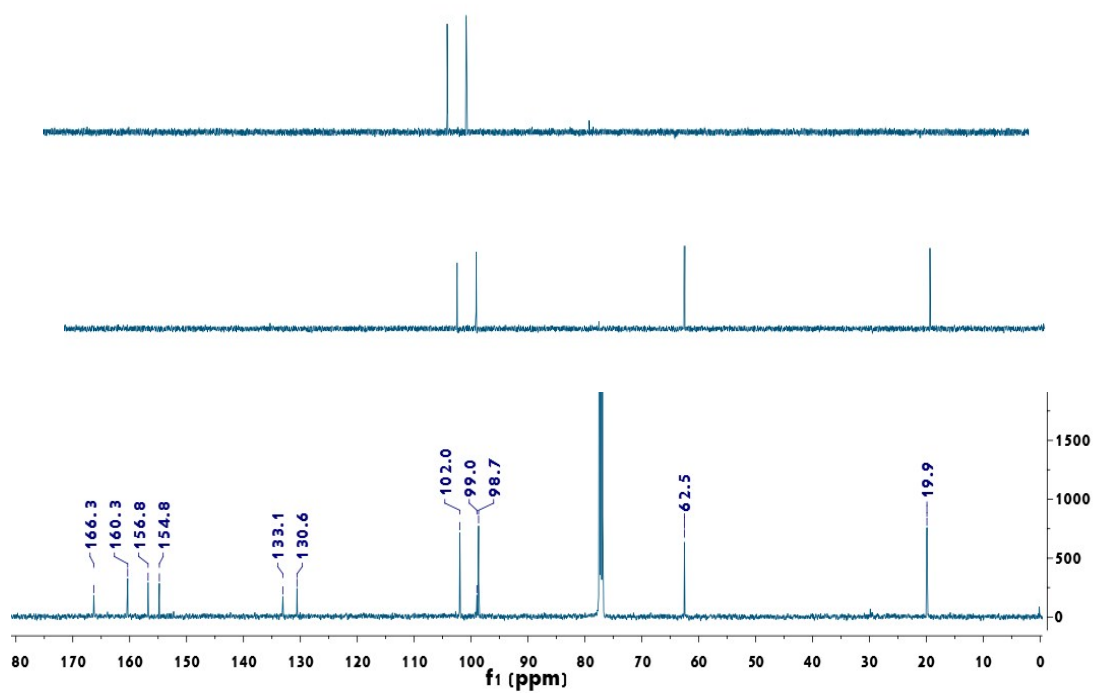


Fig. S10 HSQC spectrum of **1** in CDCl_3

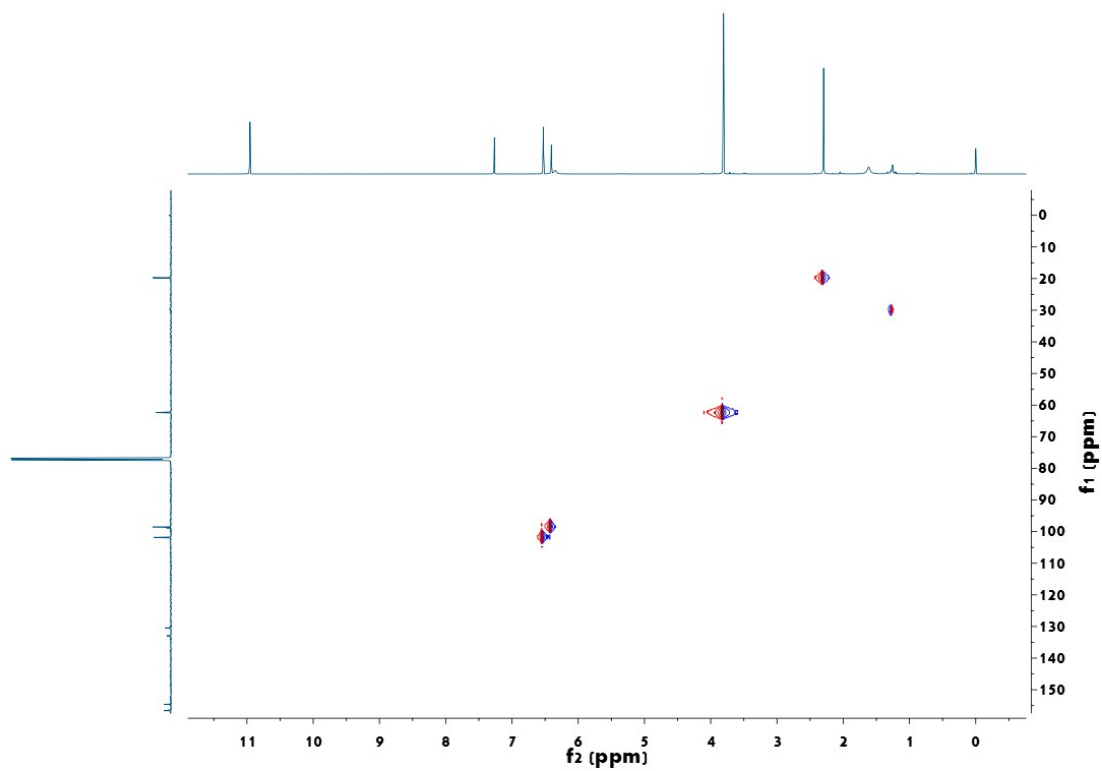


Fig. S11 ^1H - ^1H COSY spectrum of **2** in CDCl_3

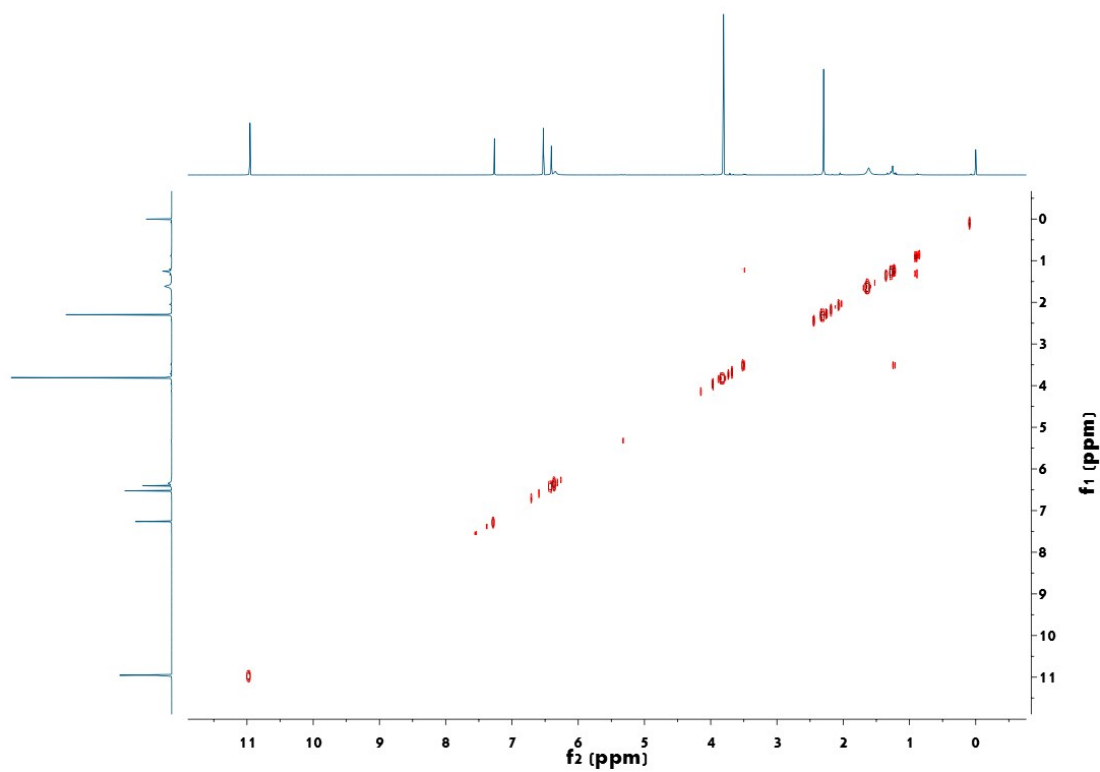


Fig. S12 HMBC spectrum of **2** in CDCl_3

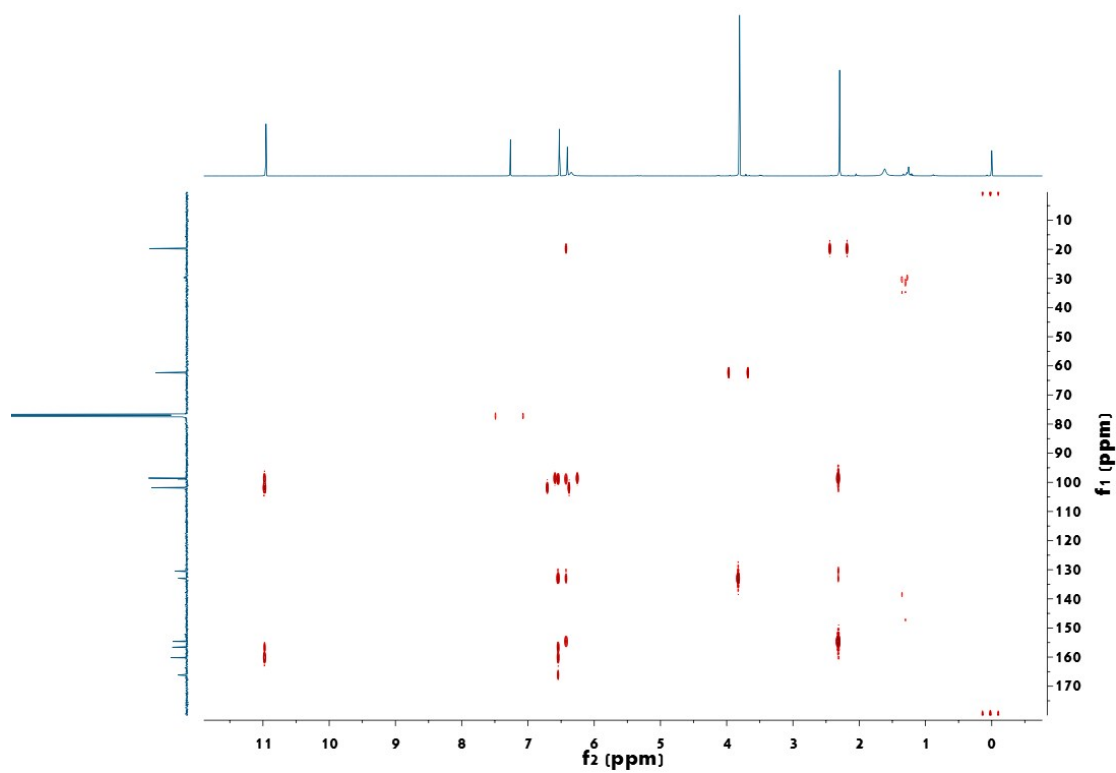


Fig. S13 HRESIMS spectrum of **3**

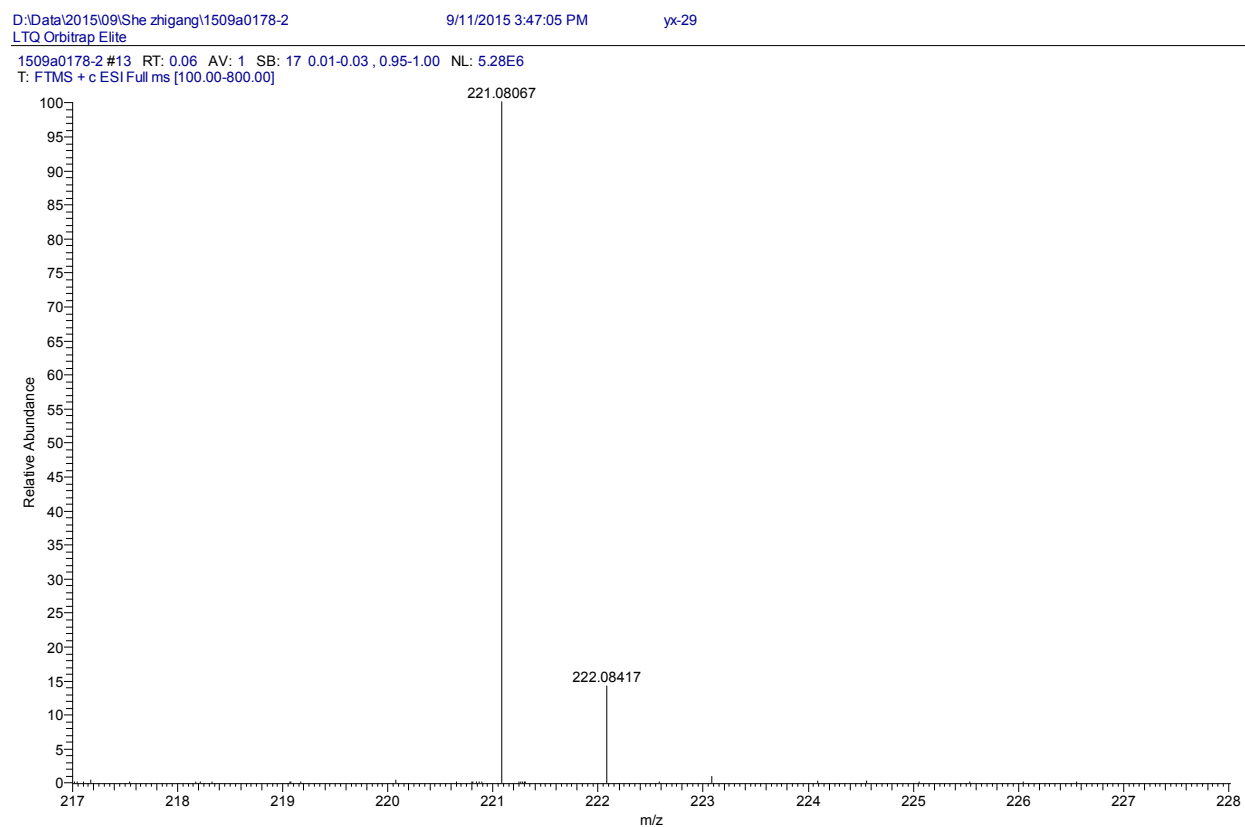


Fig. S14 ^1H NMR spectrum of **3** in $\text{DMSO}-d_6$

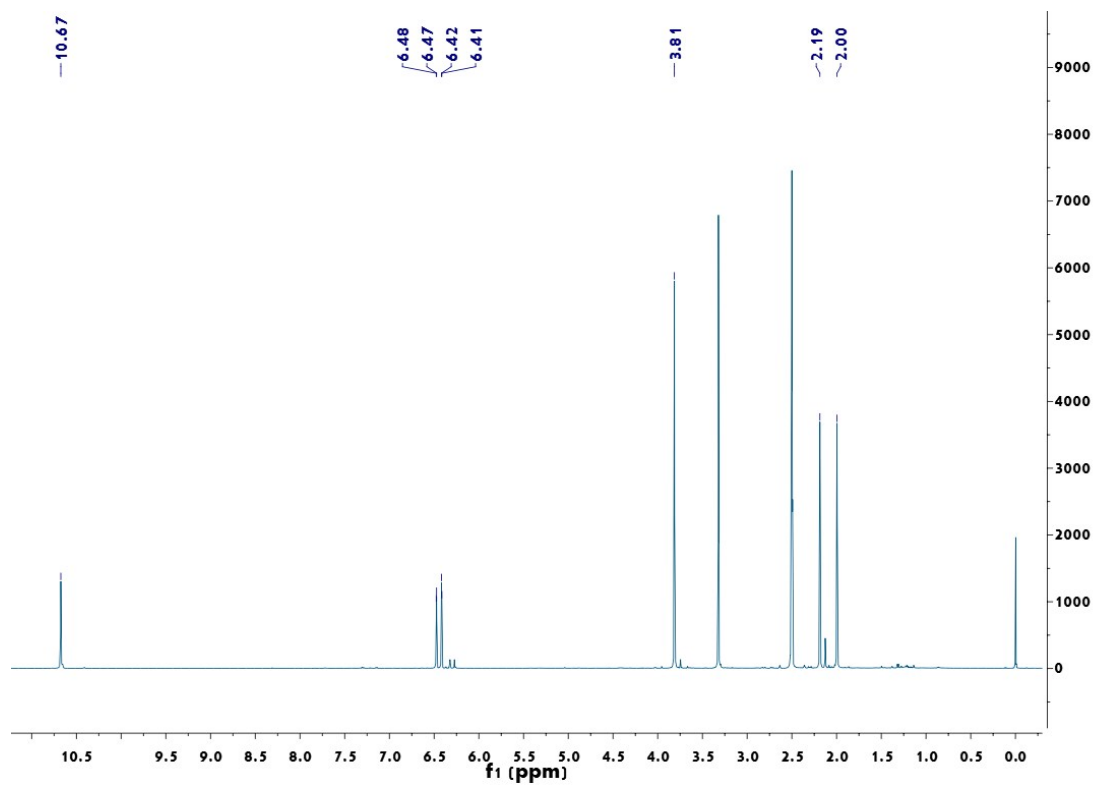


Fig. S15 ^{13}C NMR spectrum of **3** in $\text{DMSO-}d_6$

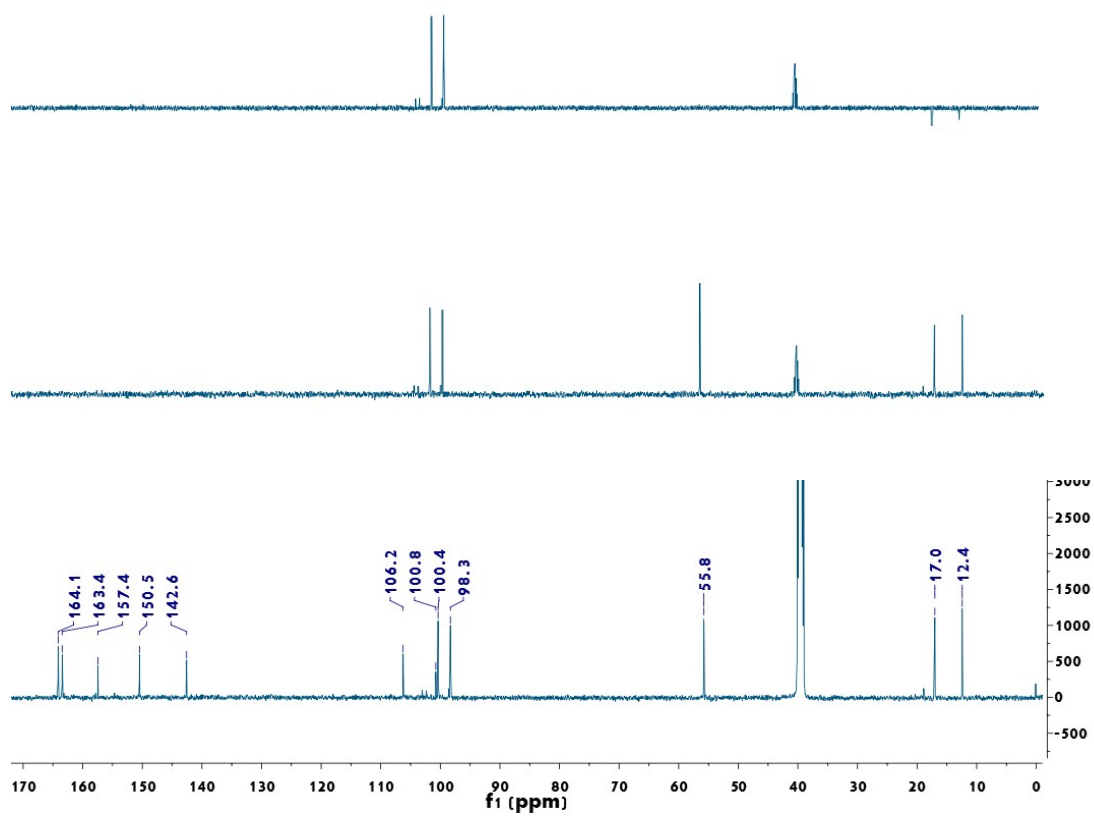


Fig. S16 HSQC spectrum of **3** in $\text{DMSO-}d_6$

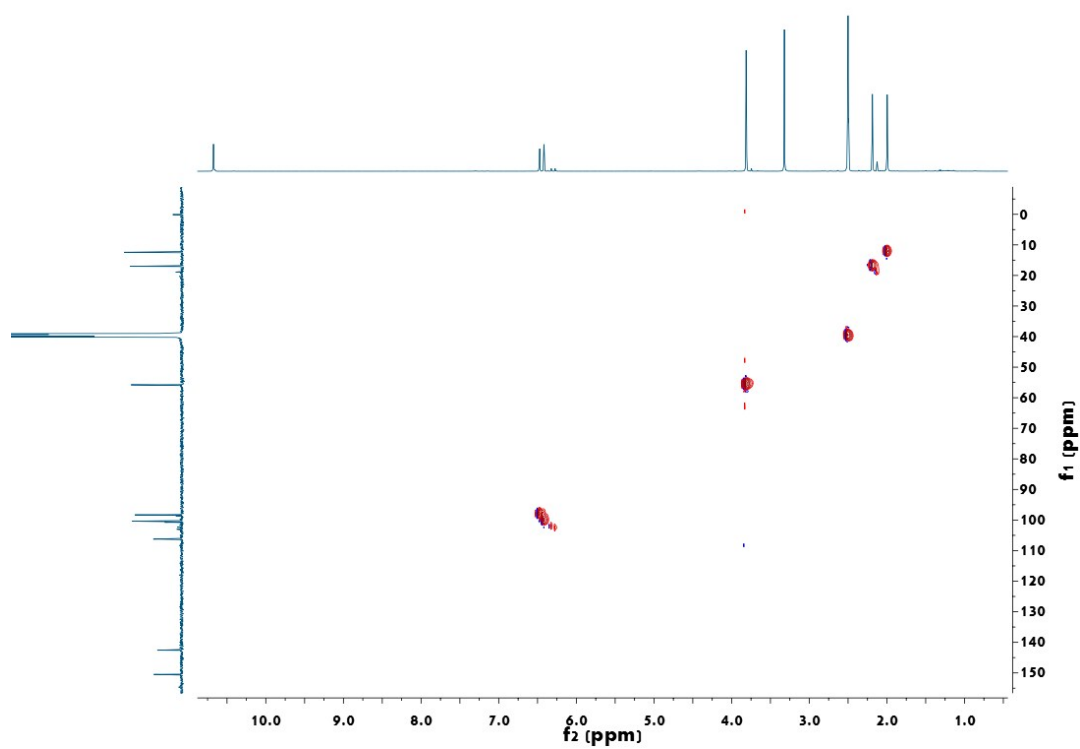


Fig. S17 ^1H - ^1H COSY spectrum of **3** in $\text{DMSO-}d_6$

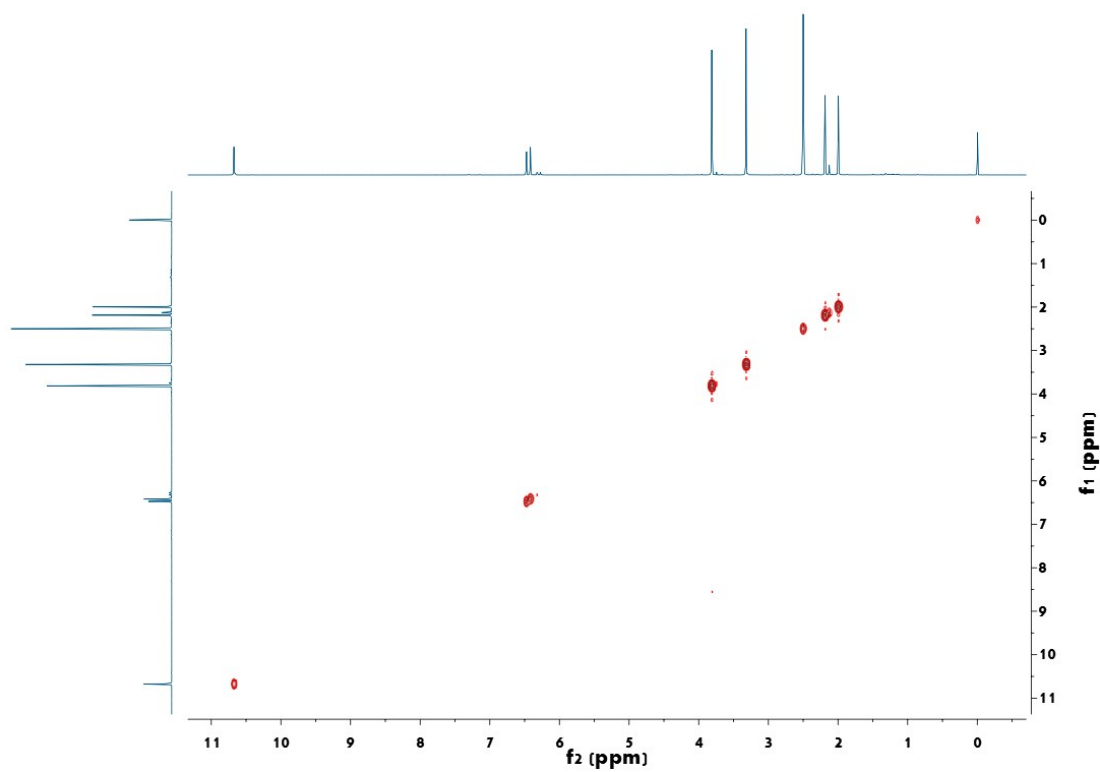


Fig. S18 HMBC spectrum of **3** in $\text{DMSO-}d_6$

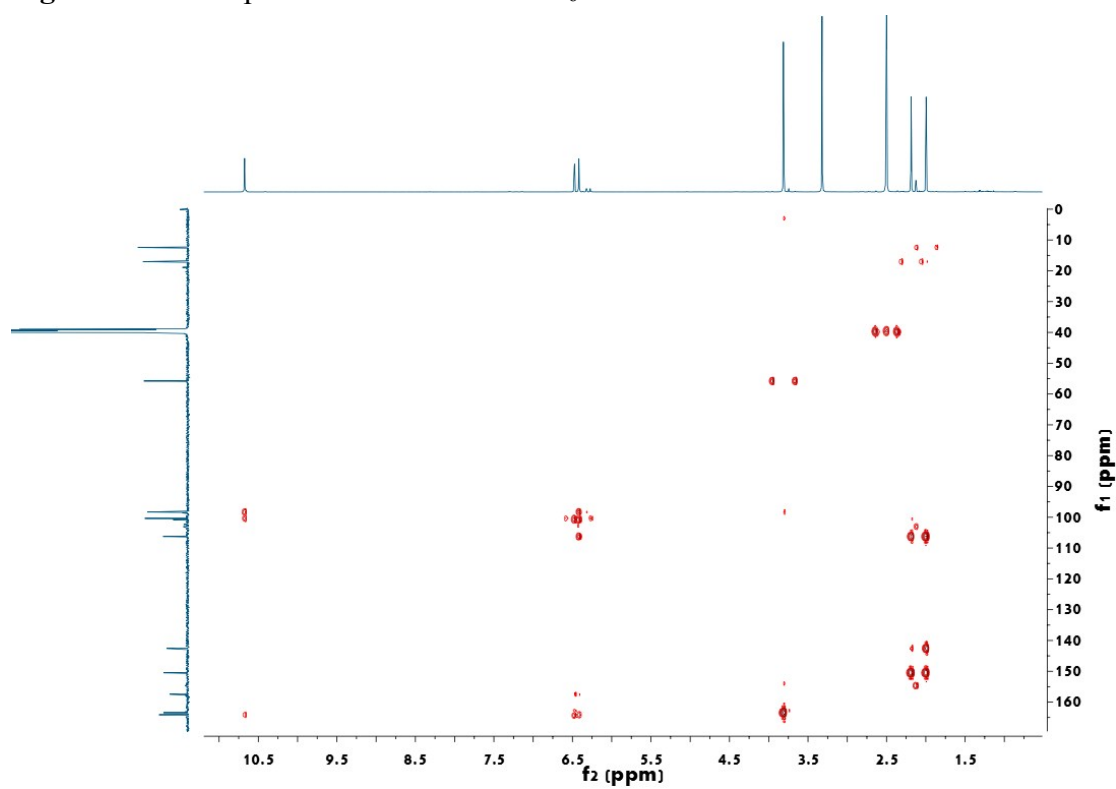


Fig. S19 HRESIMS spectrum of **4**

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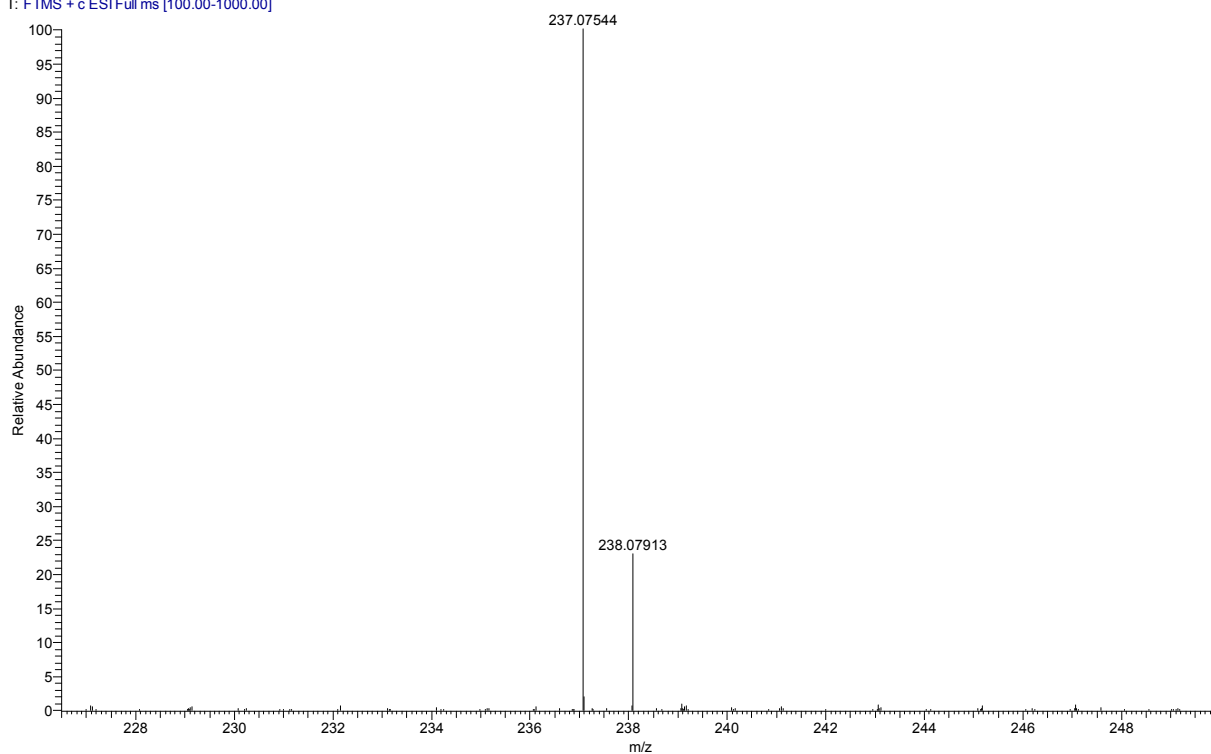


Fig. S20 ^1H NMR spectrum of **4** in $\text{DMSO}-d_6$

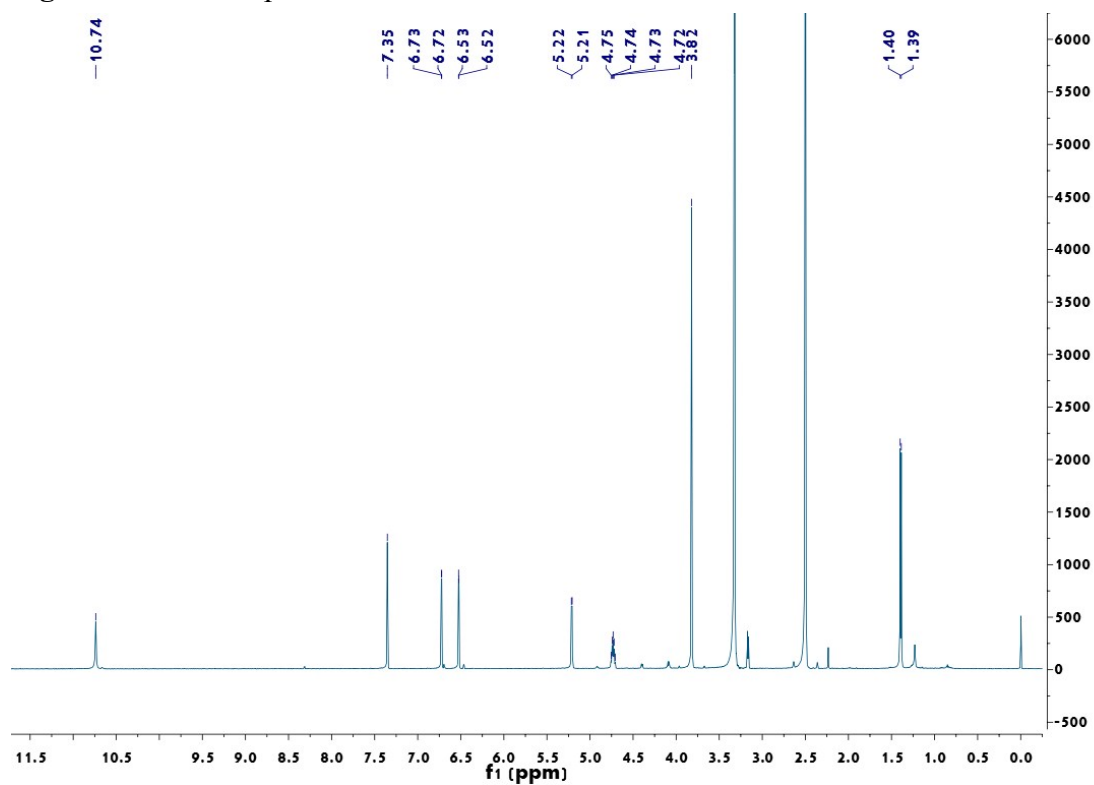


Fig. S21 ^{13}C NMR spectrum of **4** in $\text{DMSO-}d_6$

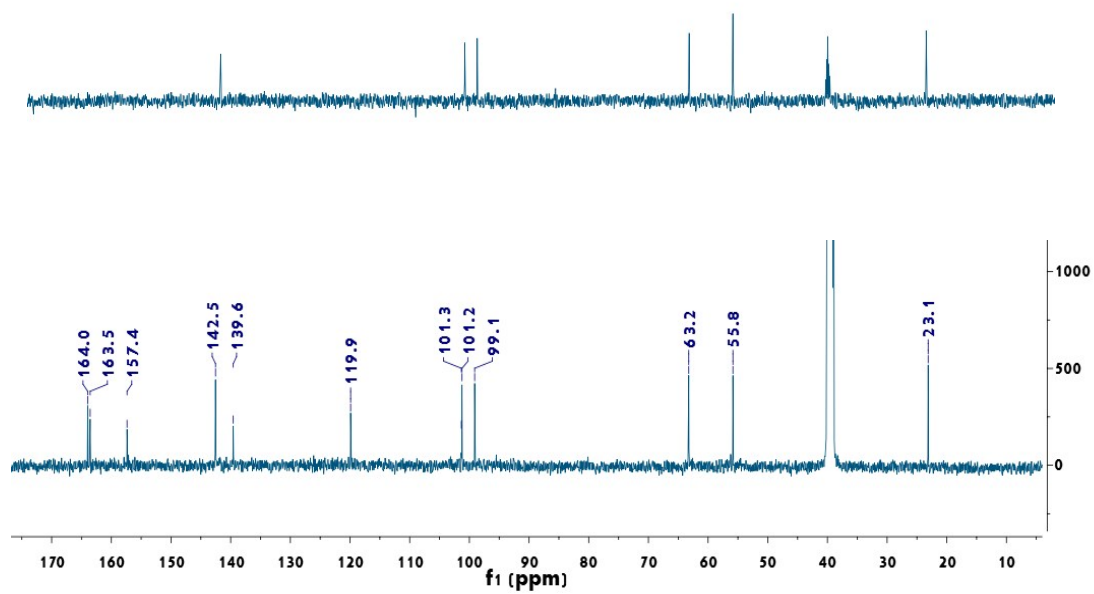


Fig. S22 HSQC spectrum of **4** in $\text{DMSO-}d_6$

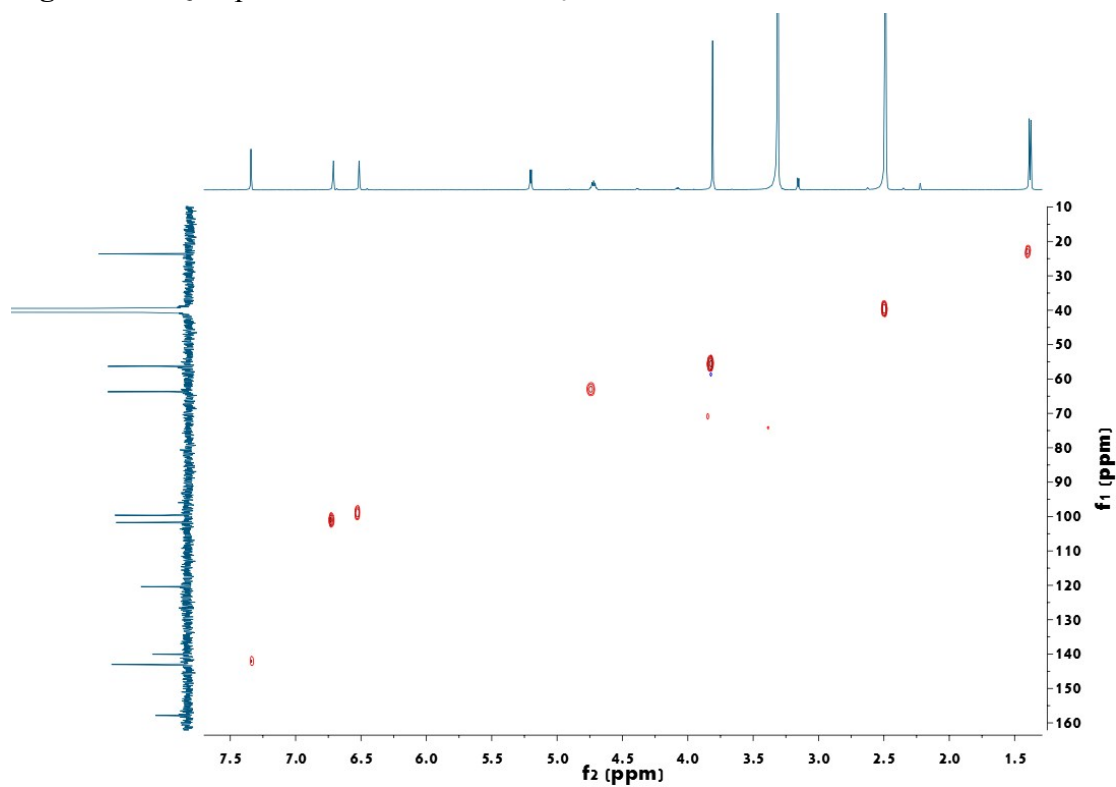


Fig. S23 ^1H - ^1H COSY spectrum of **4** in $\text{DMSO-}d_6$

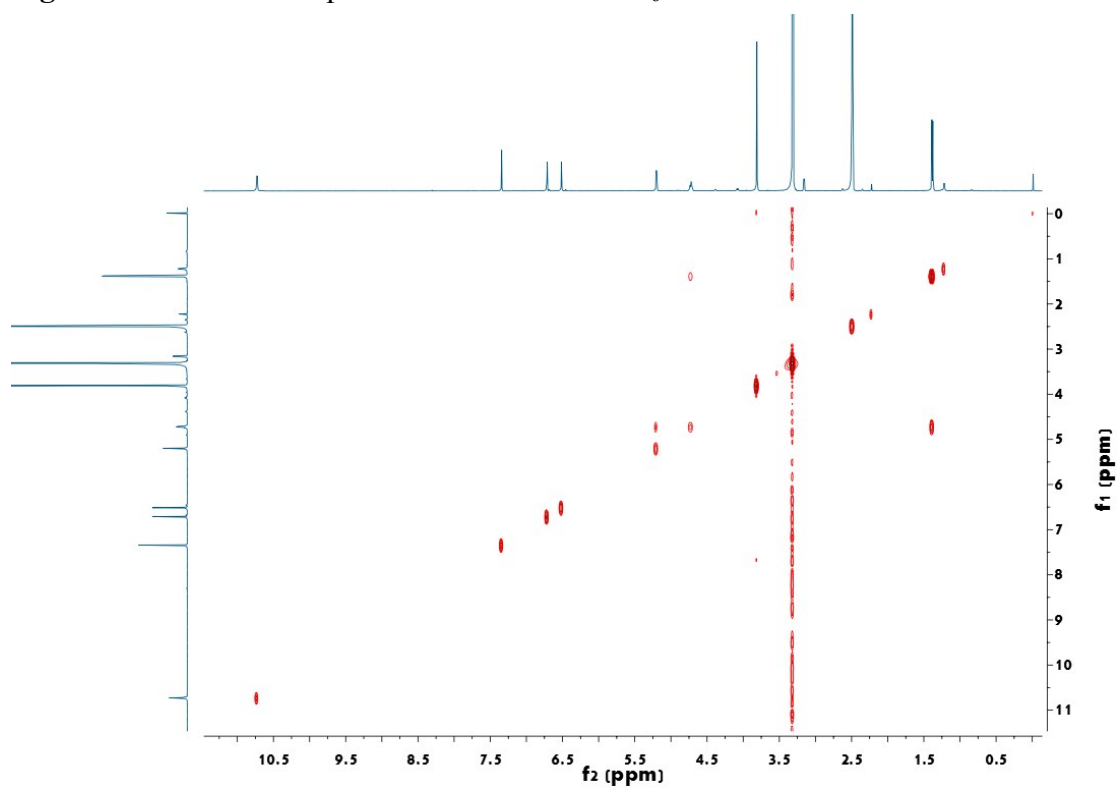


Fig. S24 HMBC spectrum of **4** in $\text{DMSO-}d_6$

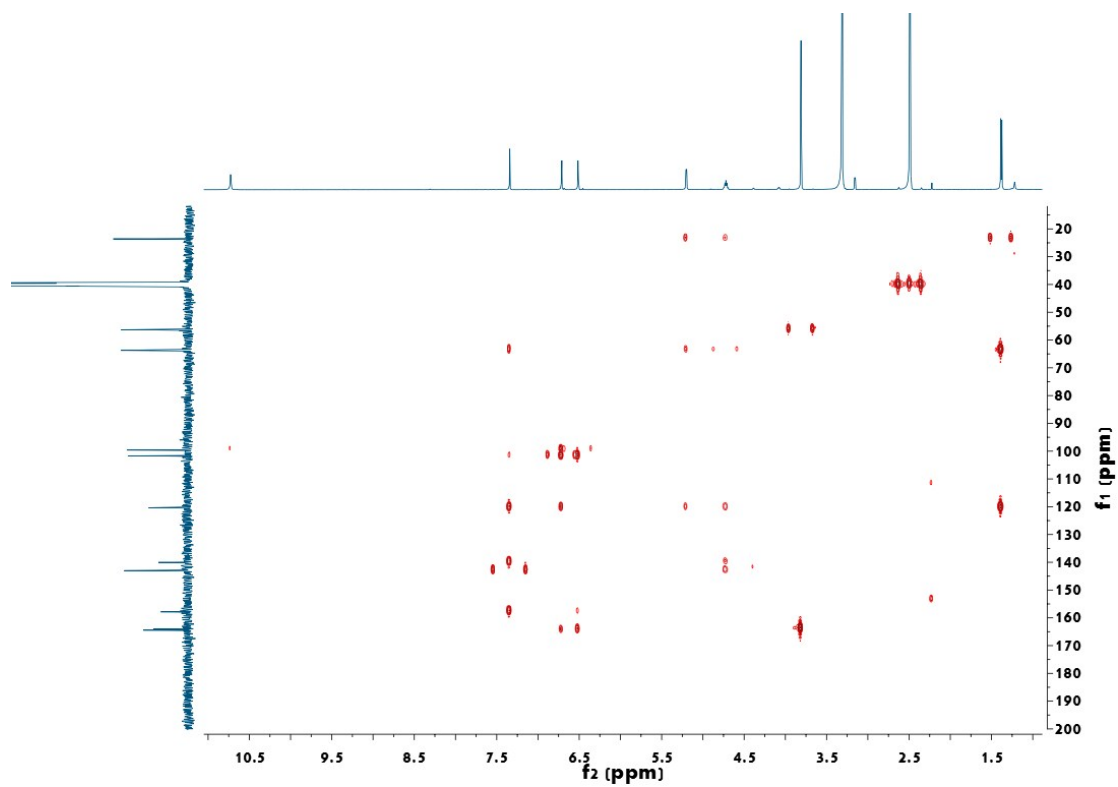


Fig. S25 HRESIMS spectrum of **14**

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LTQ Orbitrap Elite

12/10/2015 10:00:27 AM

yx-9

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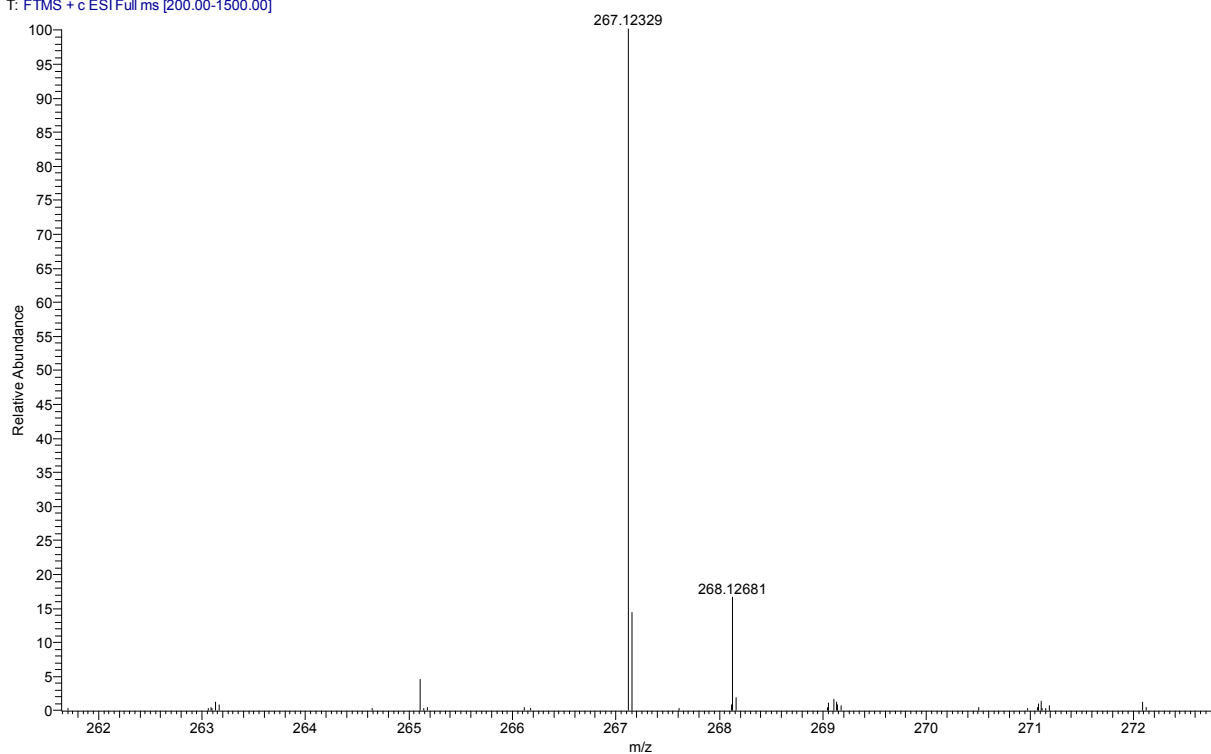


Fig. S26 ^1H NMR spectrum of **14** MeOH- d_4 .

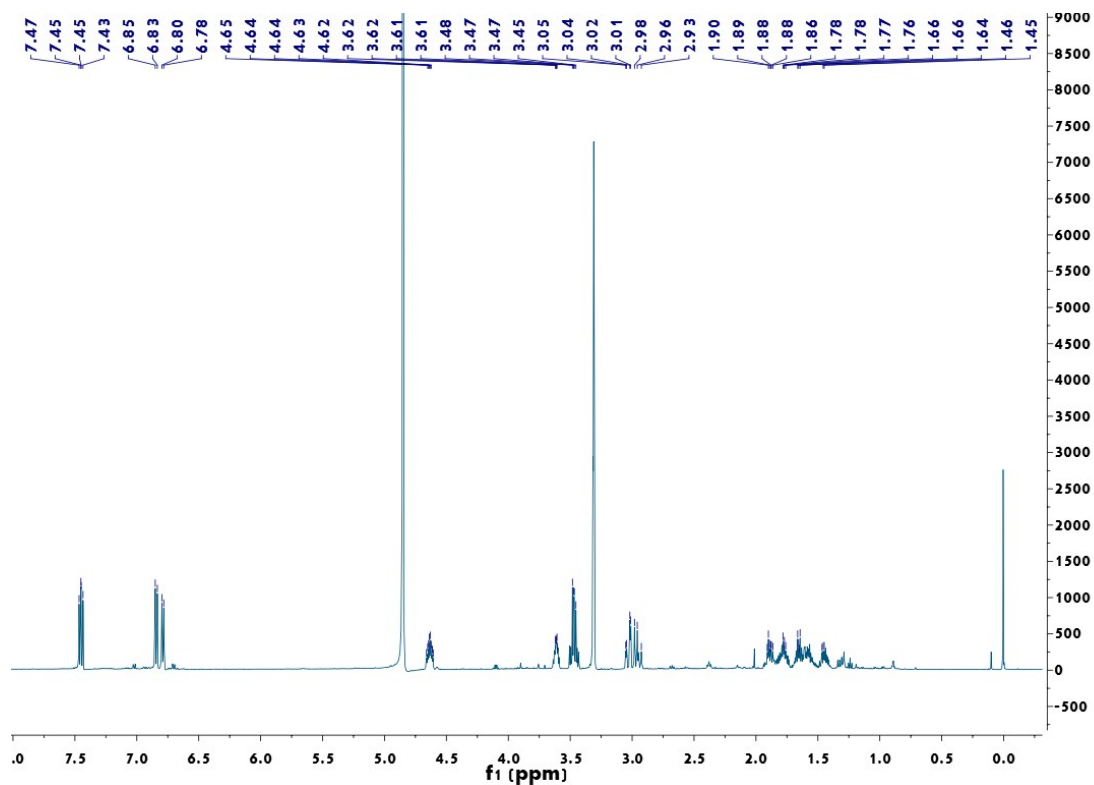


Fig. S27 ^{13}C NMR spectrum of **14** in $\text{MeOH-}d_4$.

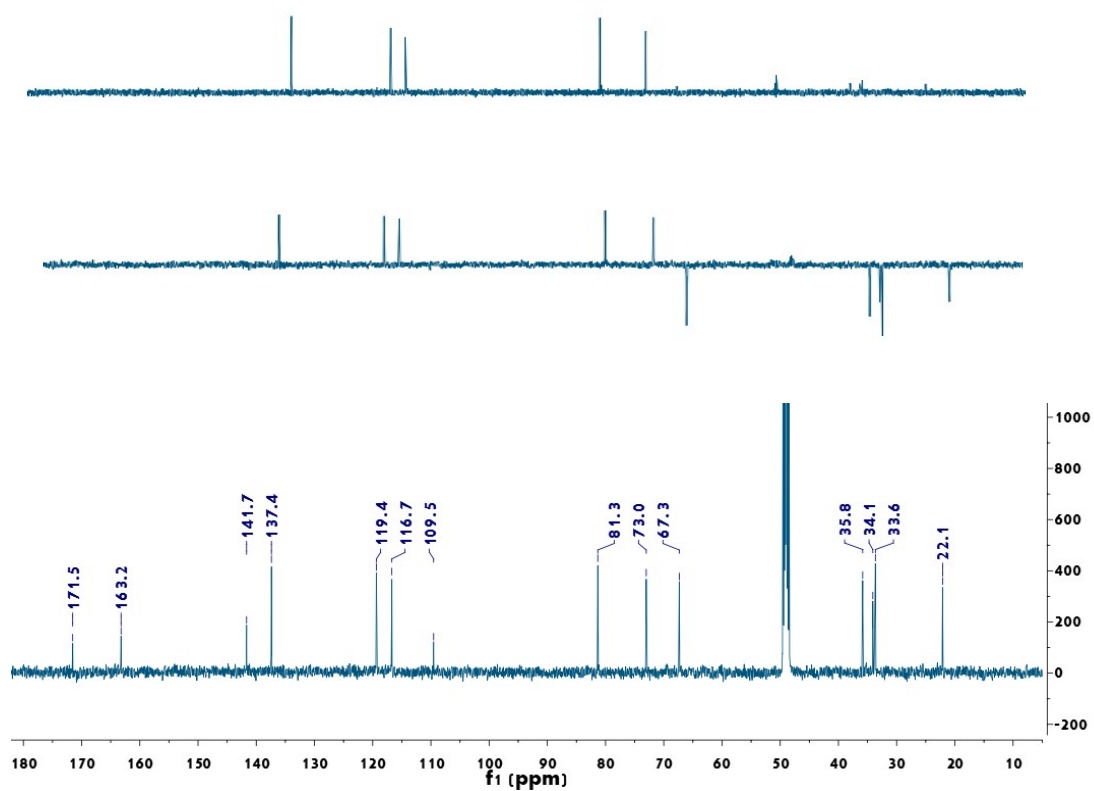


Fig. S28 HSQC spectrum of **14** in $\text{MeOH-}d_4$.

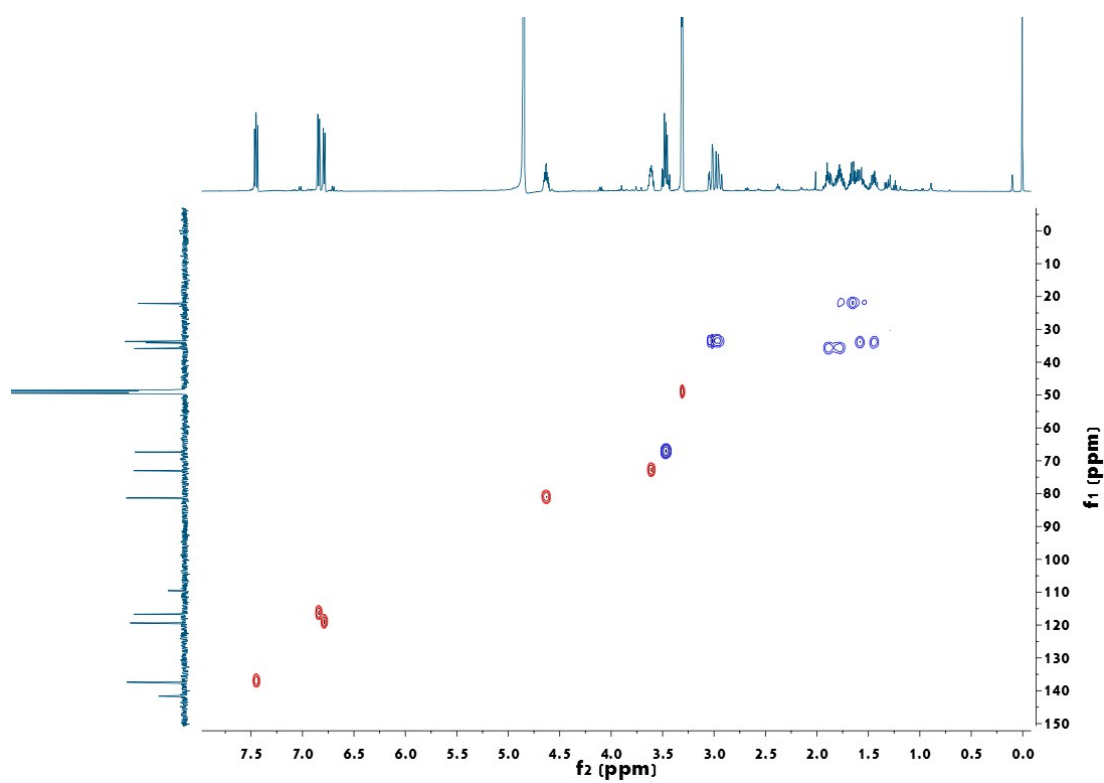


Fig. S29 ^1H - ^1H COSY spectrum of **14** in $\text{MeOH-}d_4$.

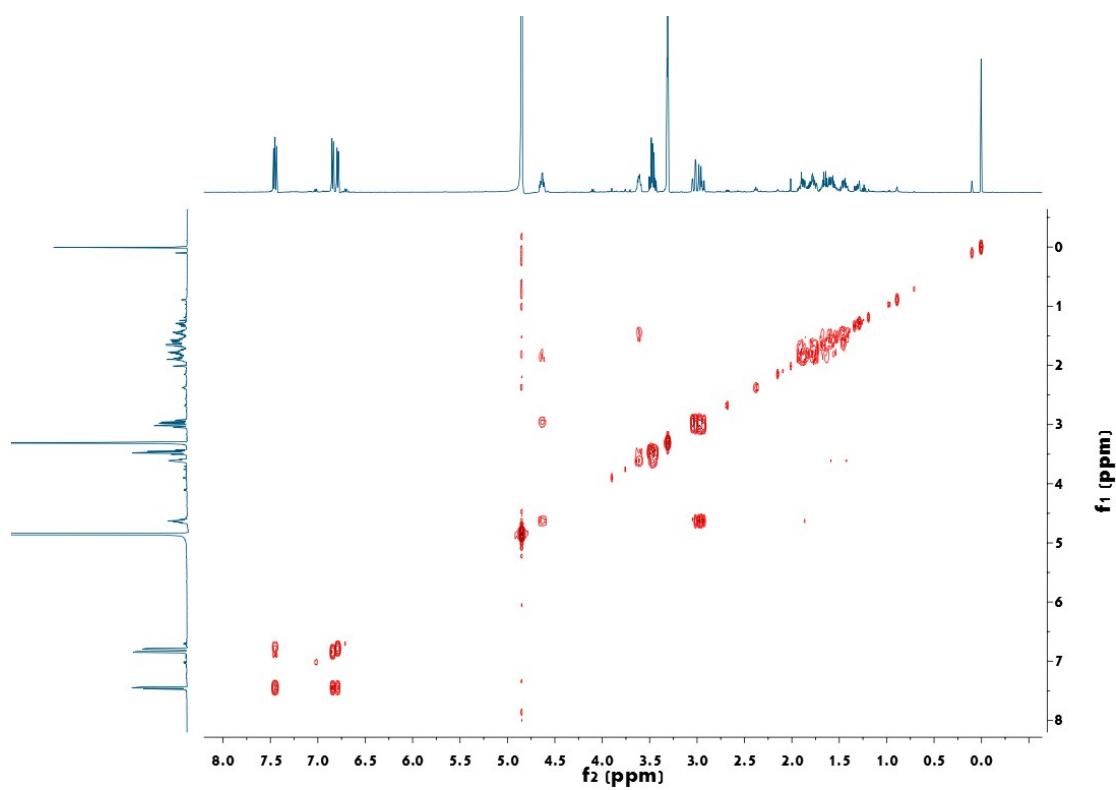


Fig. S30 HMBC spectrum of **14** in $\text{MeOH-}d_4$.

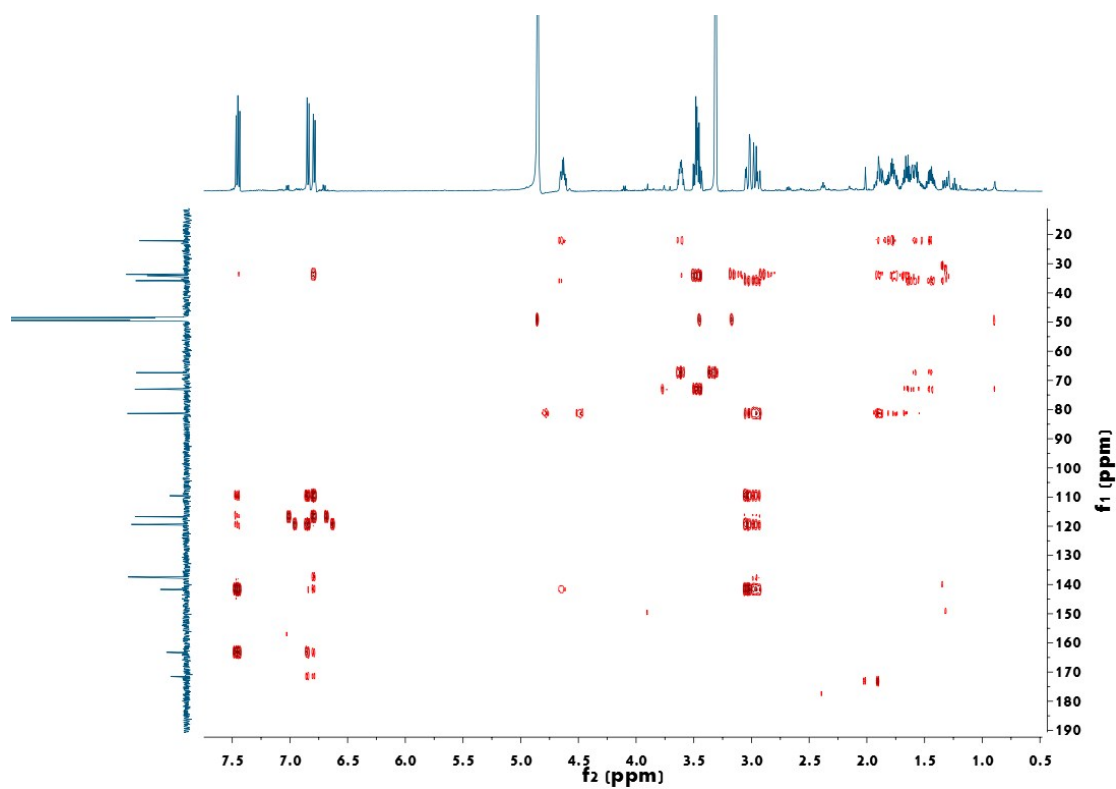


Fig. S31 HREIMS spectrum of **15**

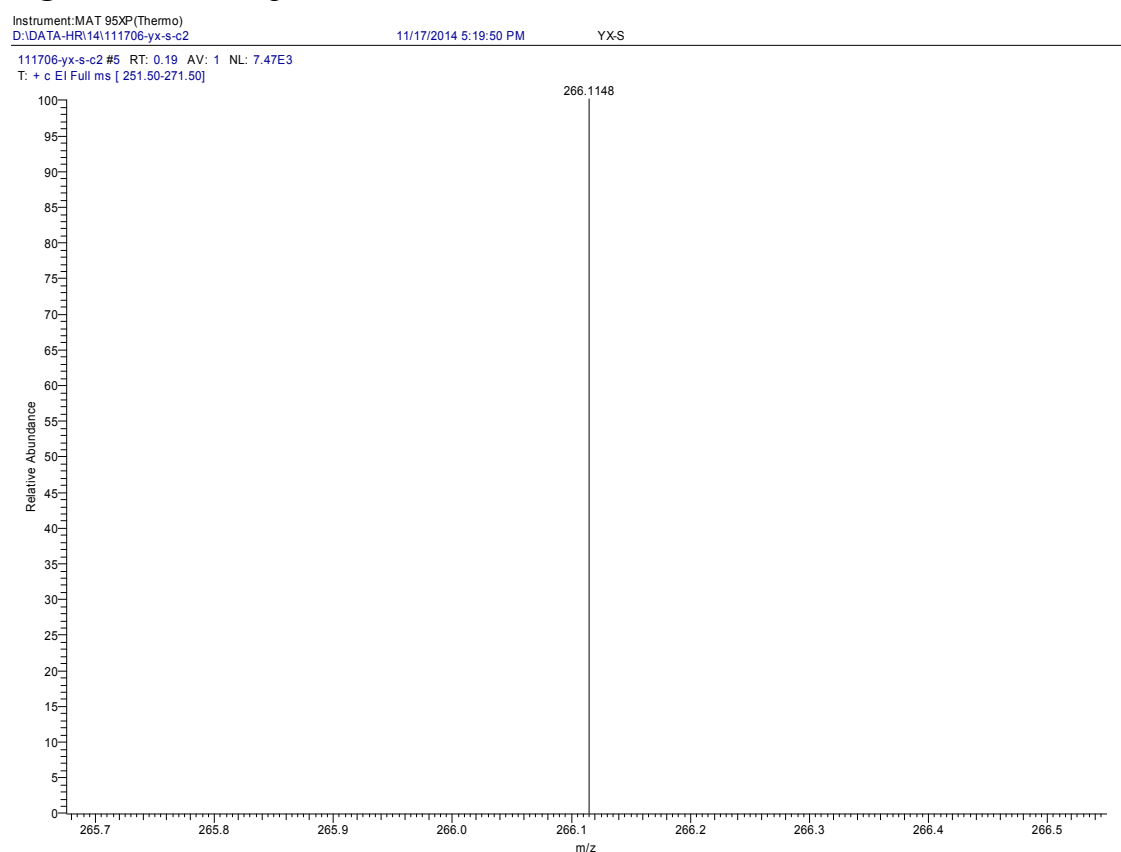


Fig. S32 ^1H NMR spectrum of **15** MeOH- d_4 .

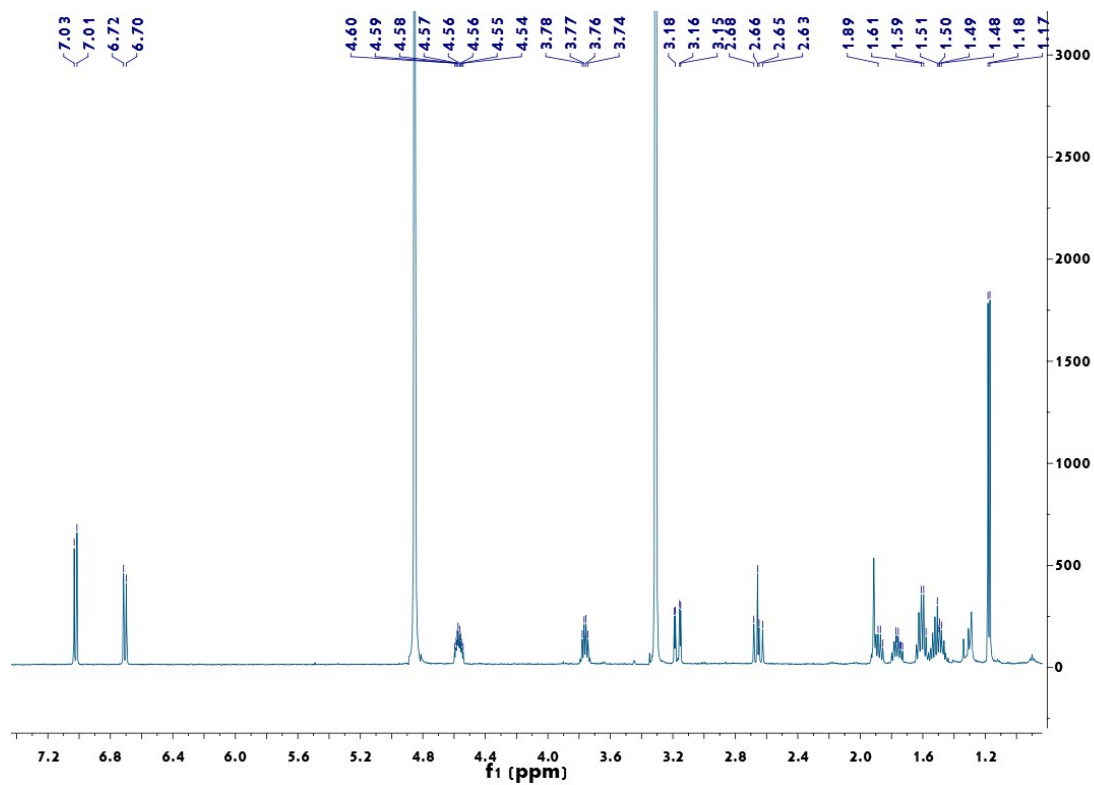


Fig. S33 ^{13}C NMR spectrum of **15** in $\text{MeOH-}d_4$.

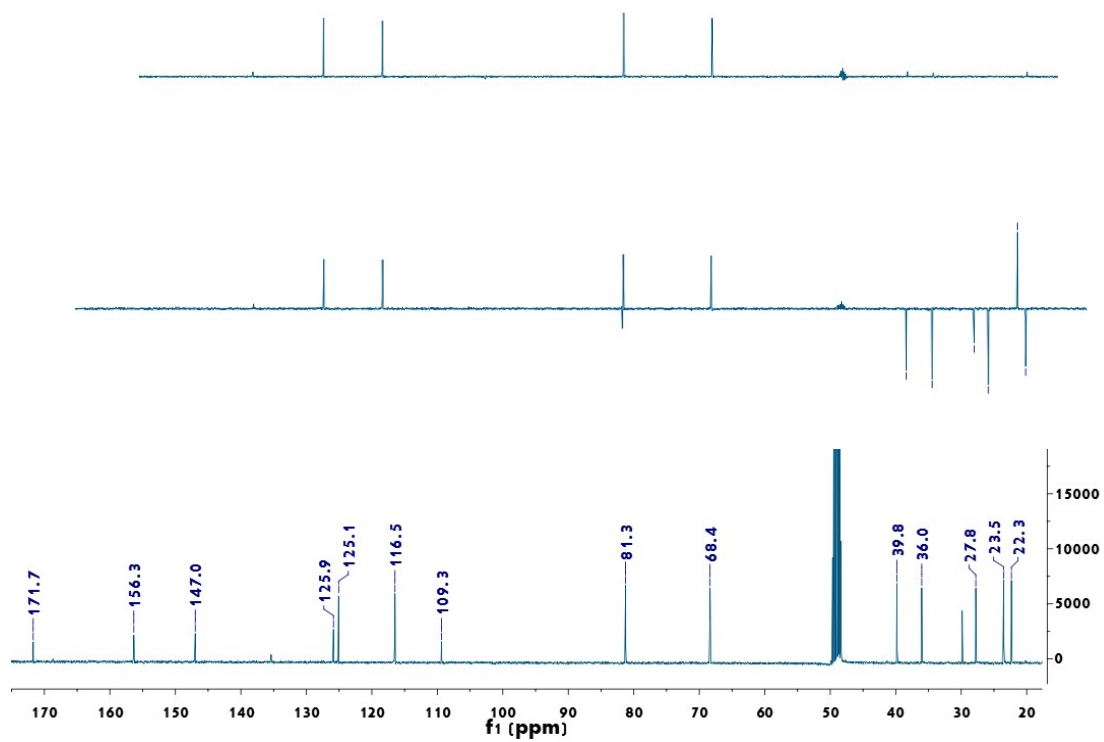


Fig. S34 HSQC spectrum of **15** in $\text{MeOH-}d_4$.

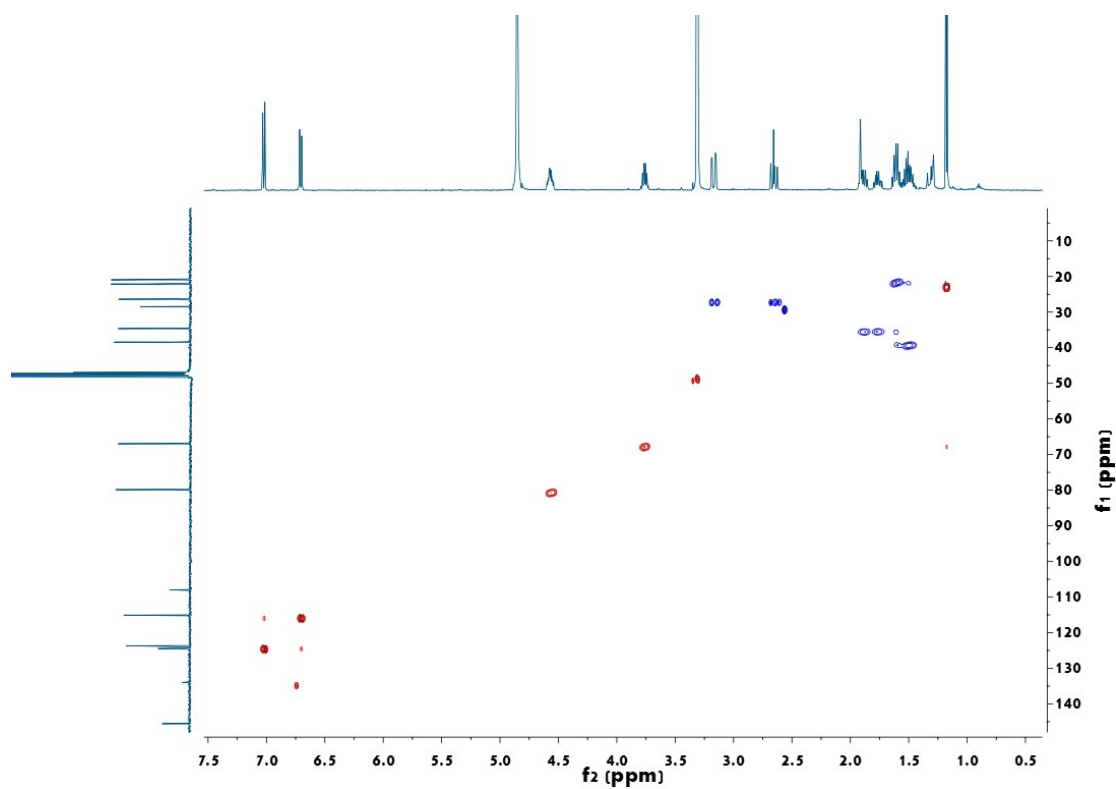


Fig. S35 ^1H - ^1H COSY spectrum of **15** in $\text{MeOH-}d_4$.

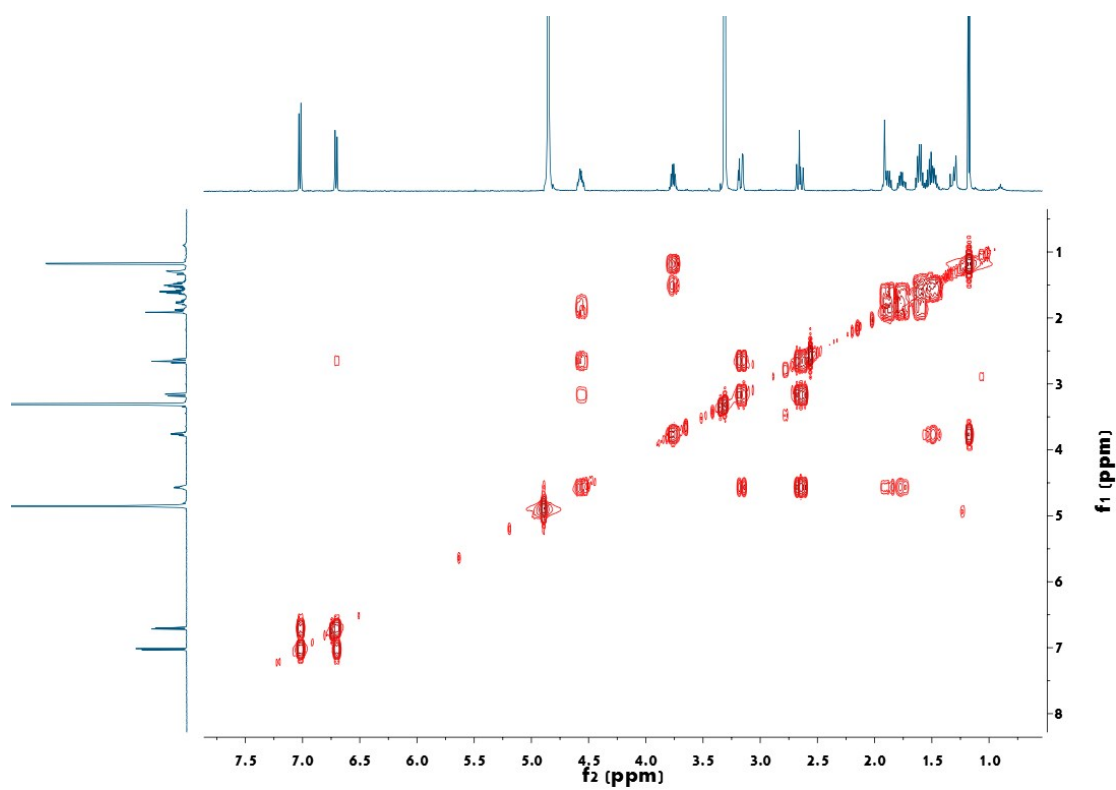


Fig. S36 HMBC spectrum of **15** in $\text{MeOH-}d_4$.

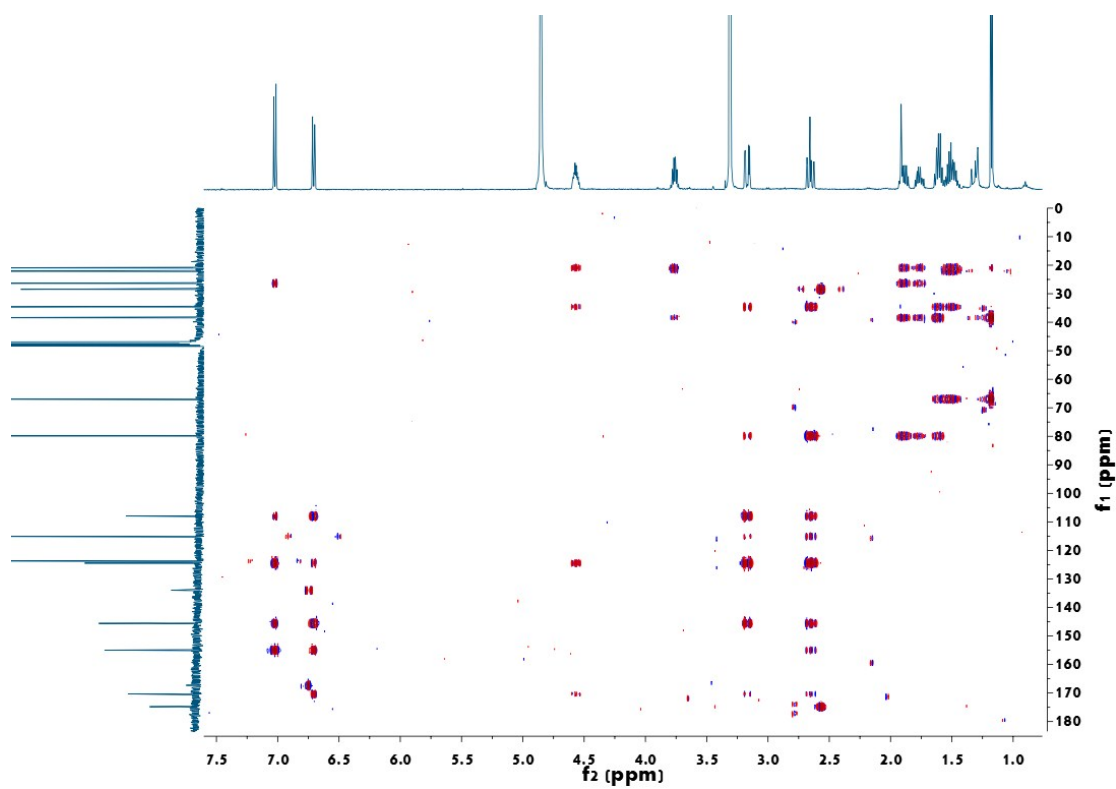


Fig. S37 HREIMS spectrum of **16**

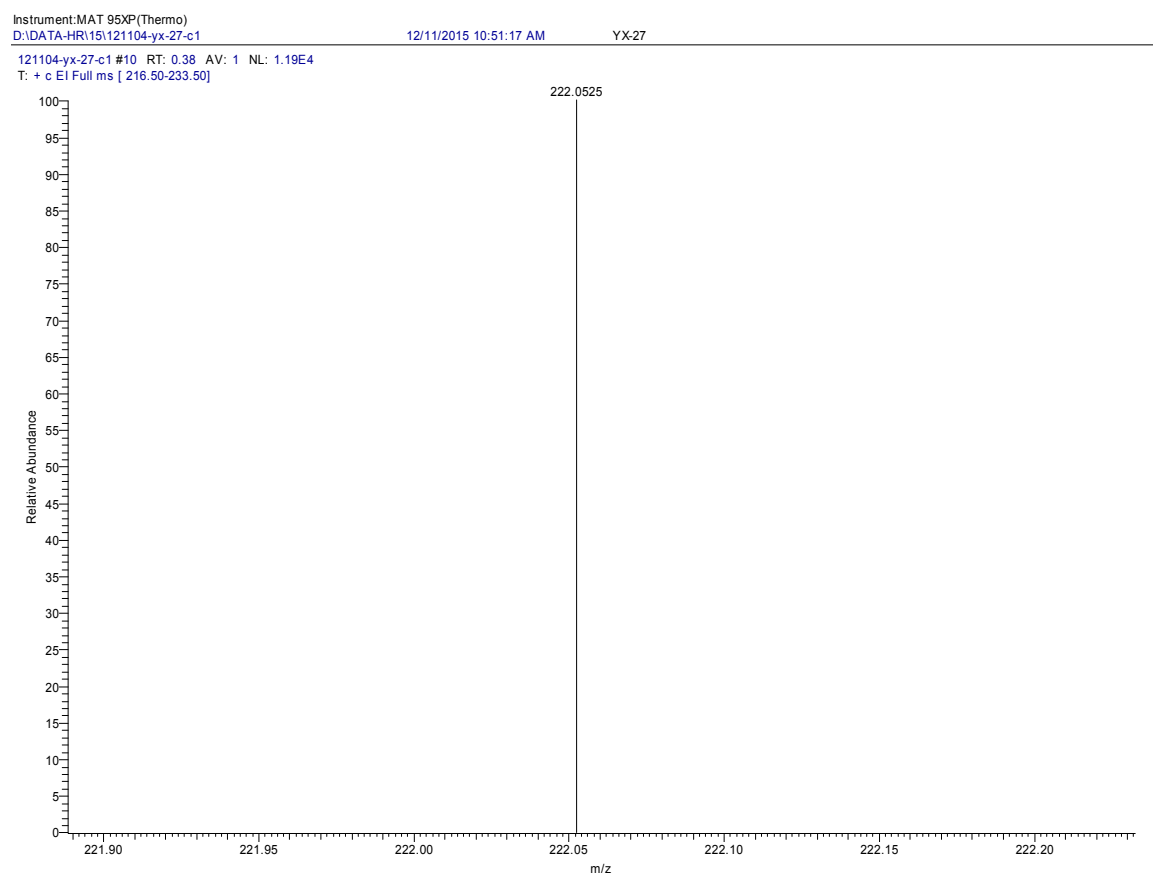


Fig. S38 ^1H NMR spectrum of **16** MeOH- d_4 .

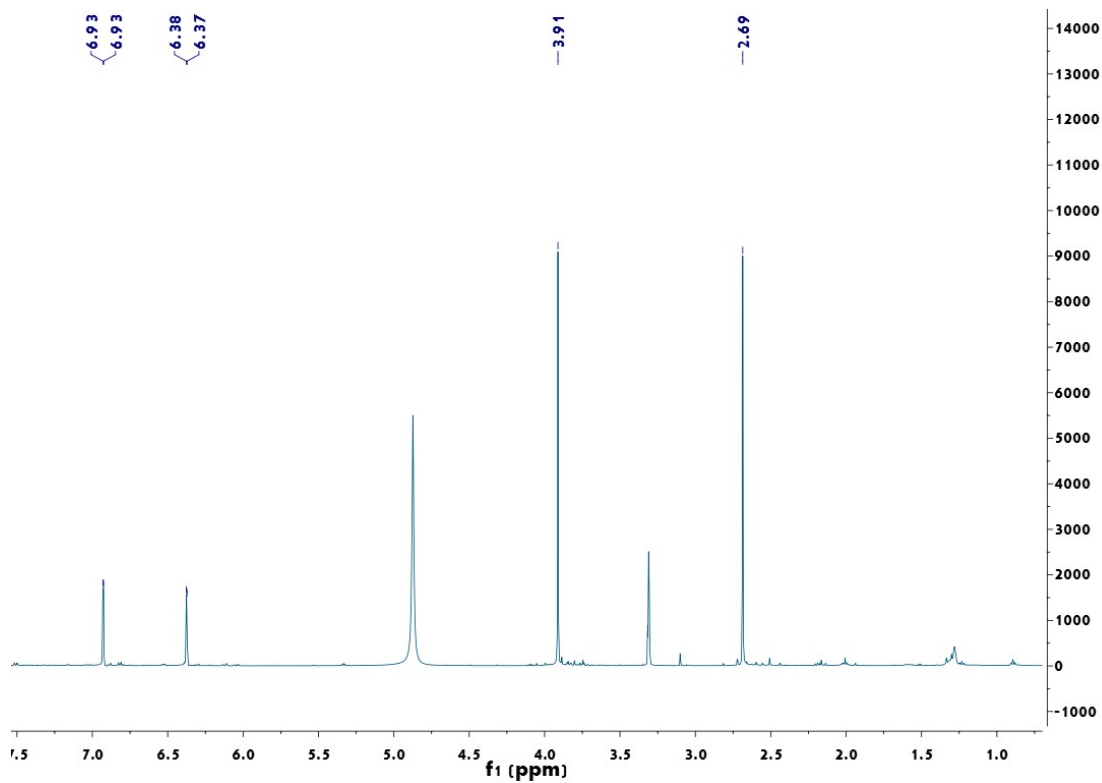


Fig. S39 ^{13}C NMR spectrum of **16** in $\text{MeOH-}d_4$.

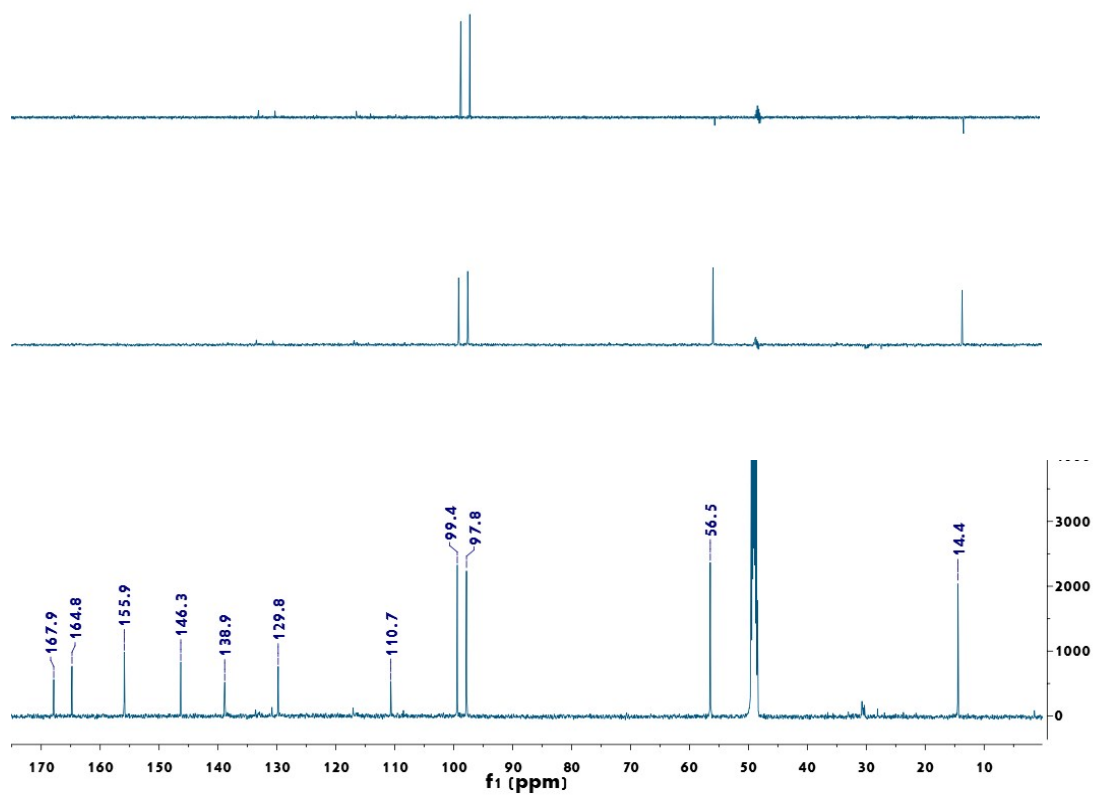


Fig. S40 HSQC spectrum of **16** in $\text{MeOH-}d_4$.

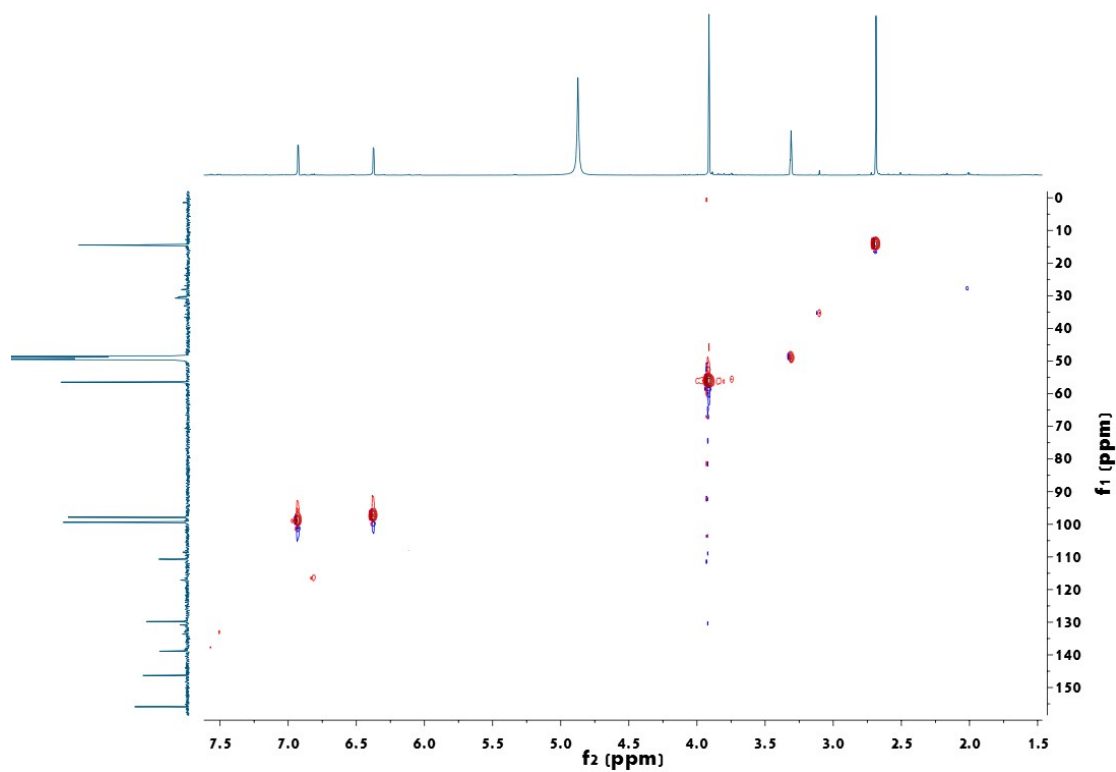


Fig. S41 ^1H - ^1H COSY spectrum of **16** in $\text{MeOH-}d_4$.

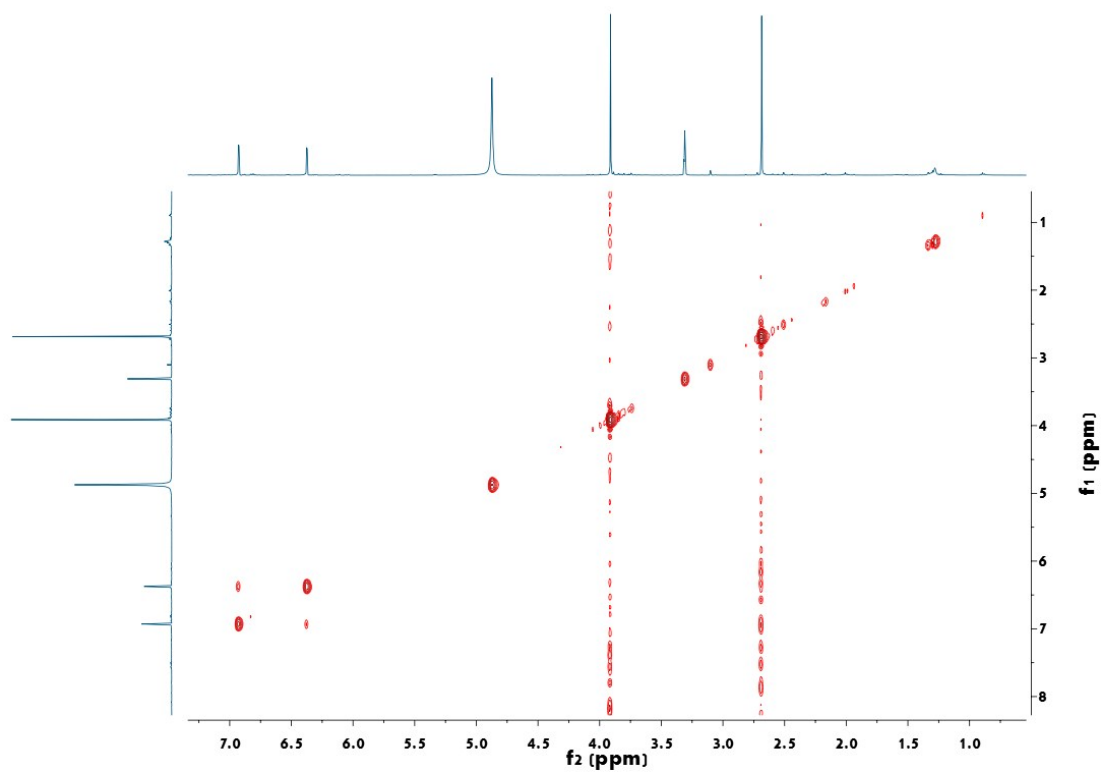


Fig. S42 HMBC spectrum of **16** in $\text{MeOH-}d_4$.

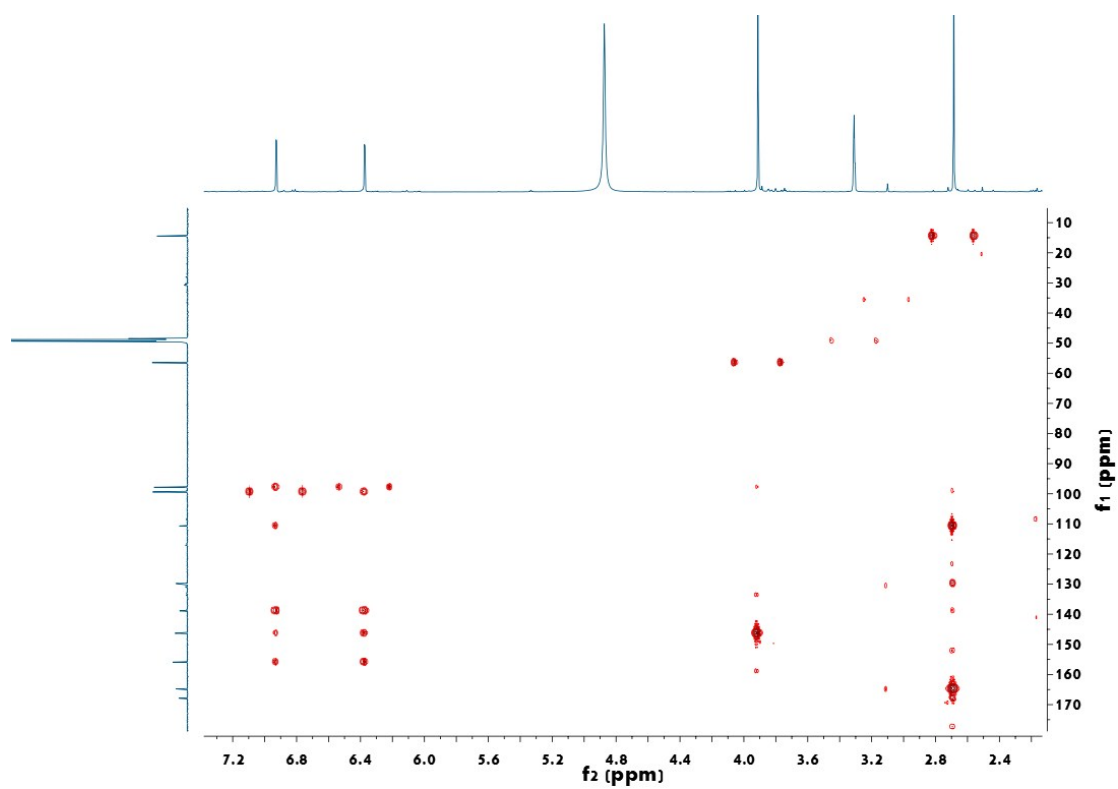


Fig. S43 HRESIMS spectrum of **17**

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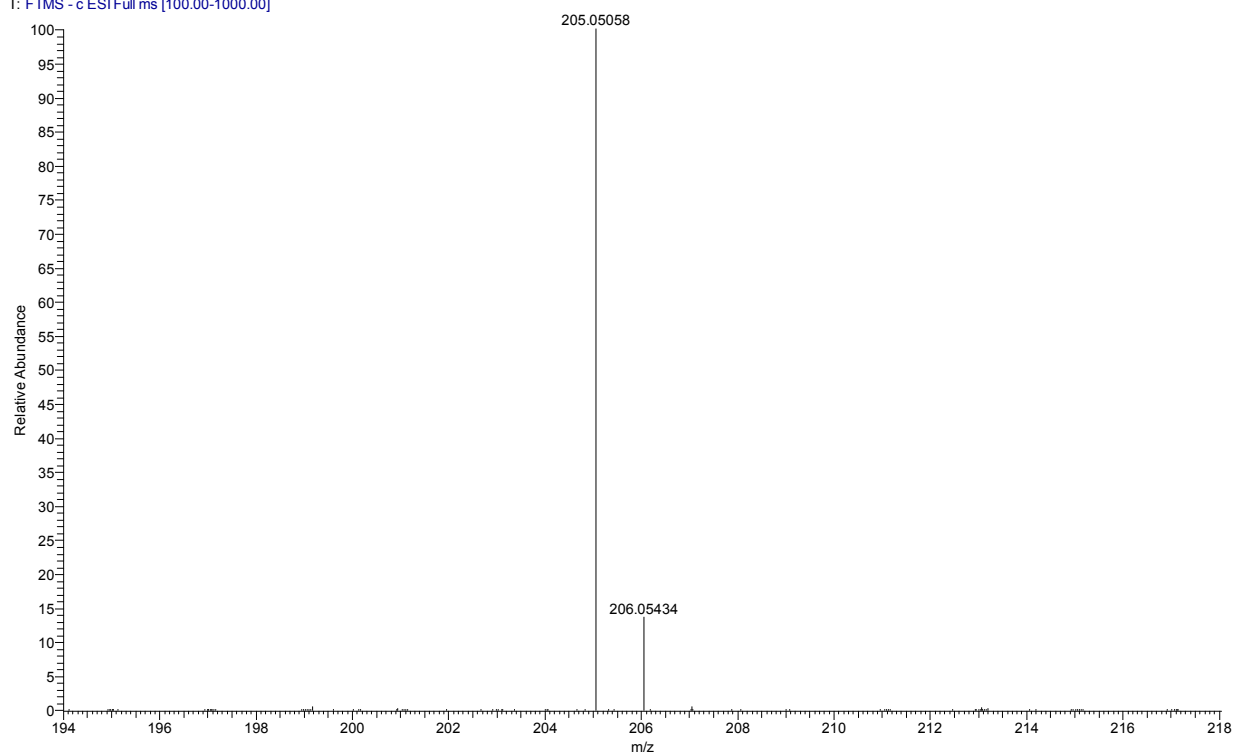


Fig. S44 ^1H NMR spectrum of **17** MeOH- d_4 .

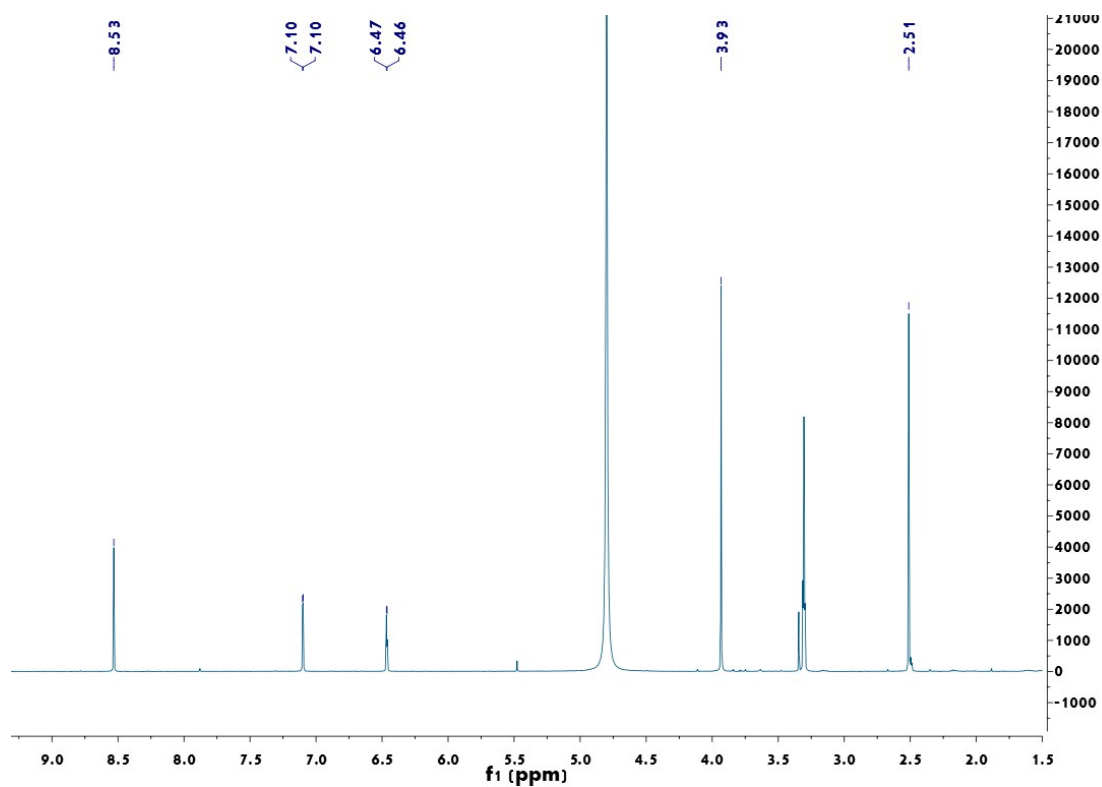


Fig. S45 ^{13}C NMR spectrum of **17** in $\text{MeOH-}d_4$.

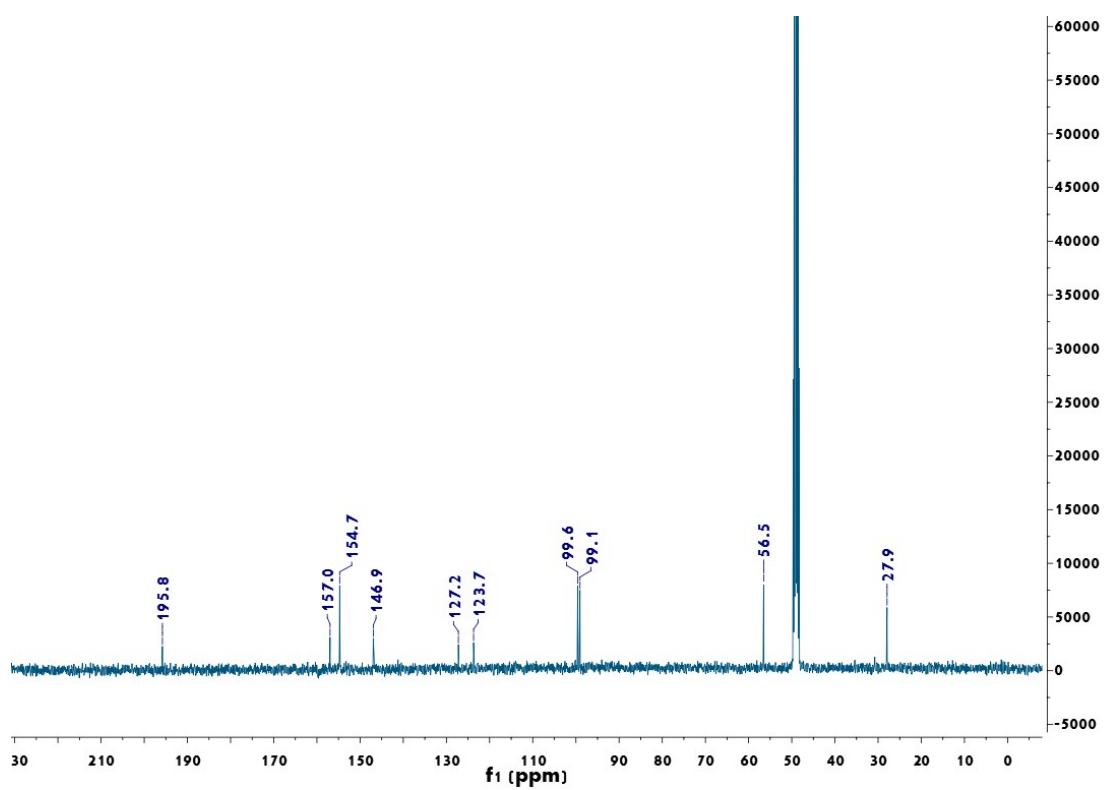


Fig. S46 HSQC spectrum of **17** in $\text{MeOH-}d_4$.

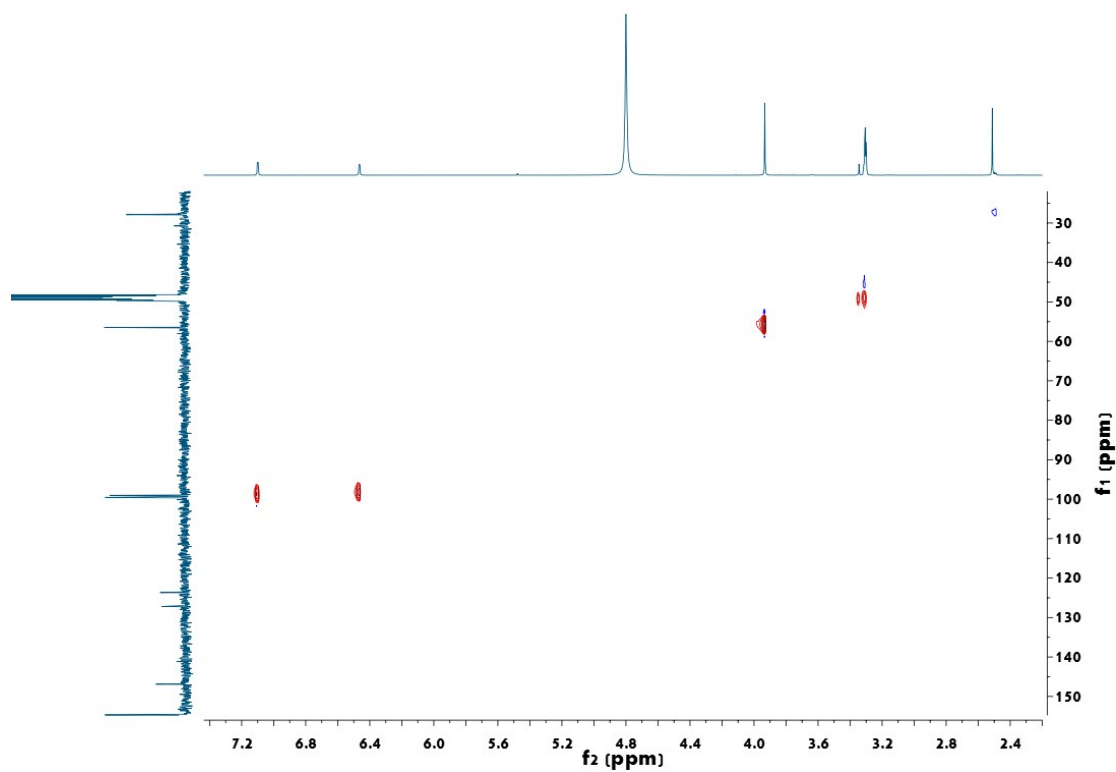


Fig. S47 ^1H - ^1H COSY spectrum of **17** in $\text{MeOH-}d_4$.

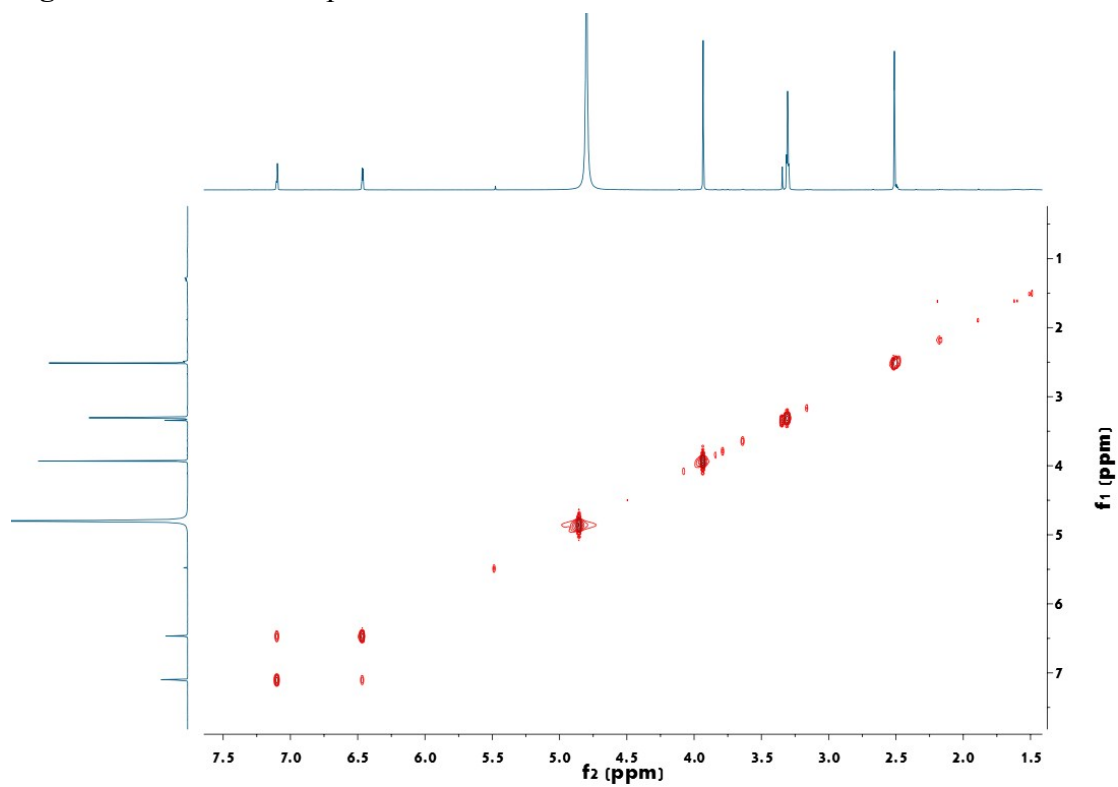


Fig. S48 HMBC spectrum of **17** in $\text{MeOH-}d_4$.

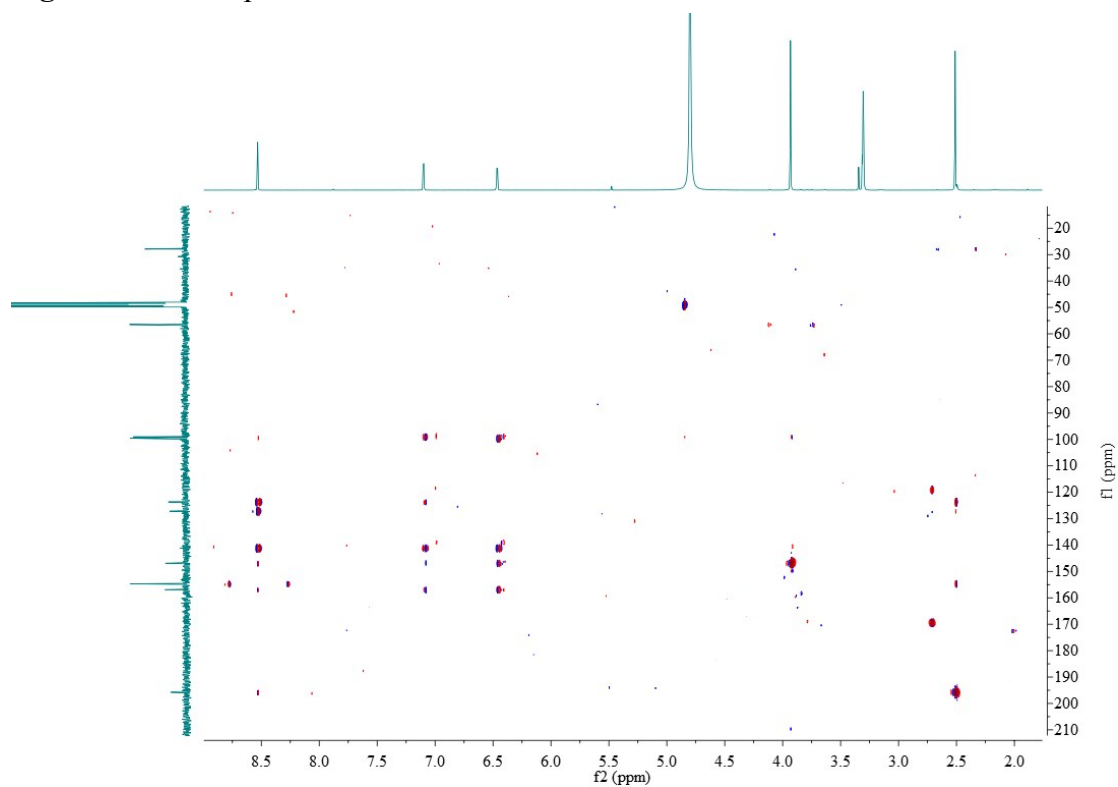


Fig. S49 ^1H NMR spectrum of **4a** CDCl_3

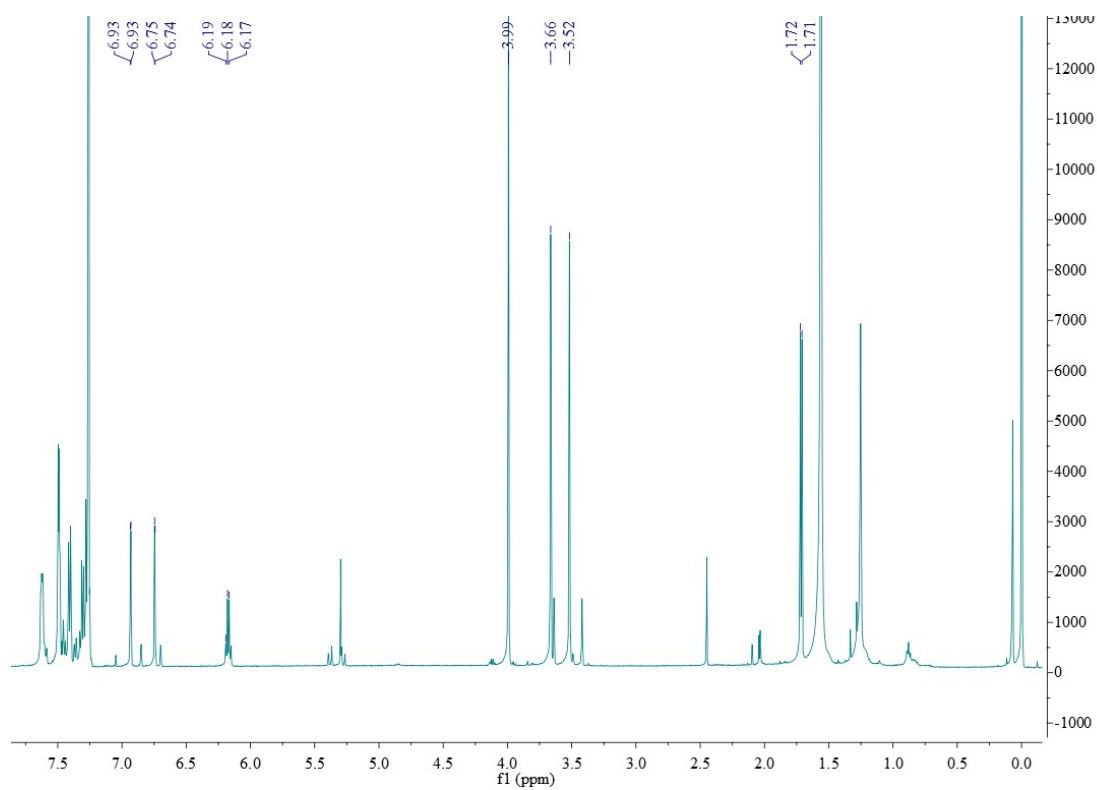


Fig. S50 ^1H NMR spectrum of **4b** CDCl_3

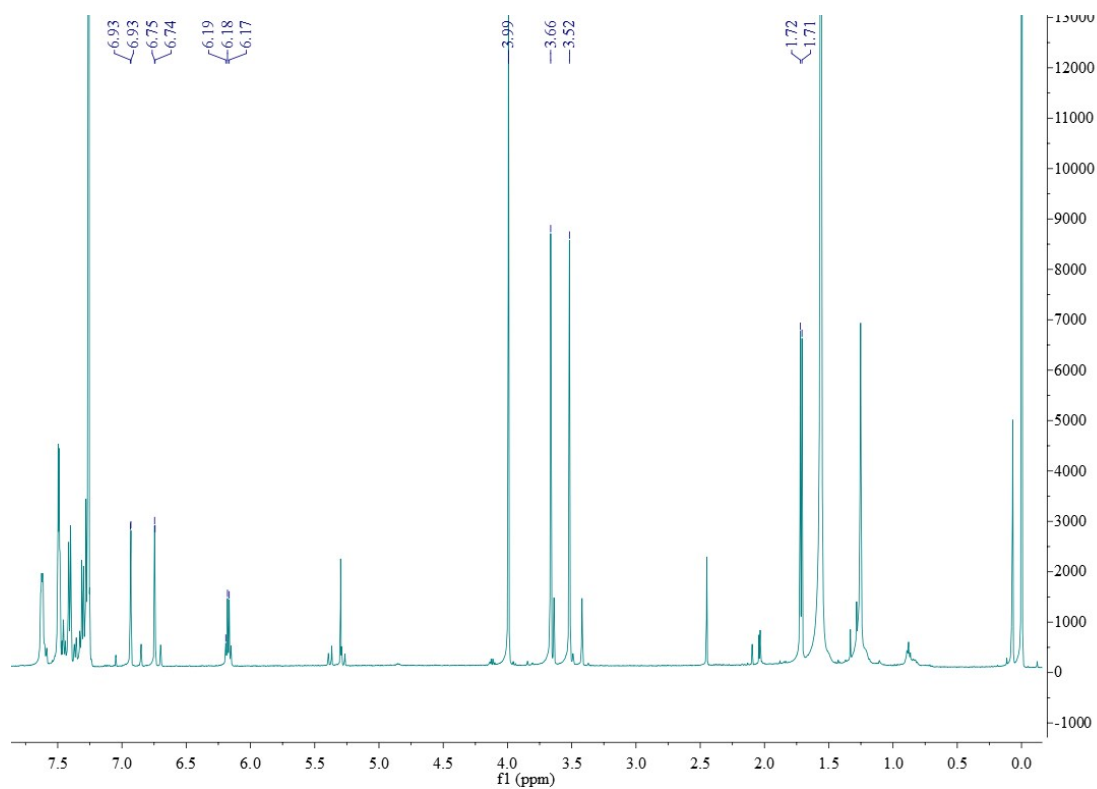


Fig. S51 ^1H NMR spectrum of **14a** CDCl_3

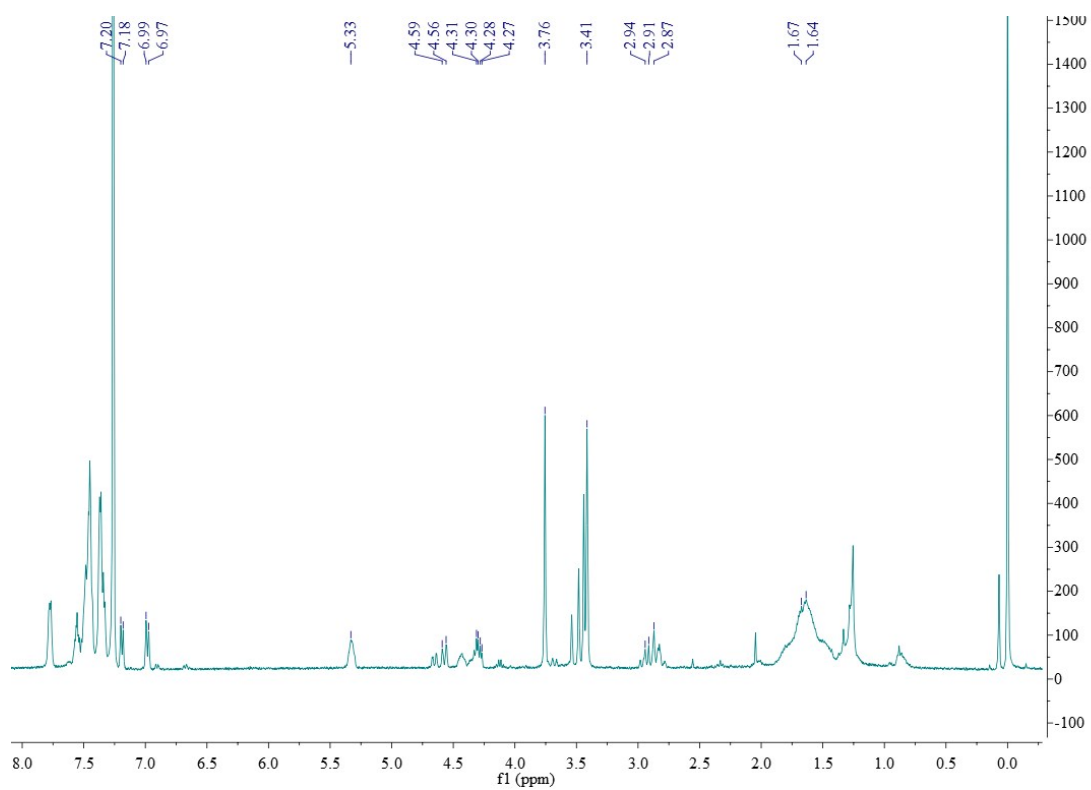


Fig. S52 ^1H NMR spectrum of **14b** CDCl_3

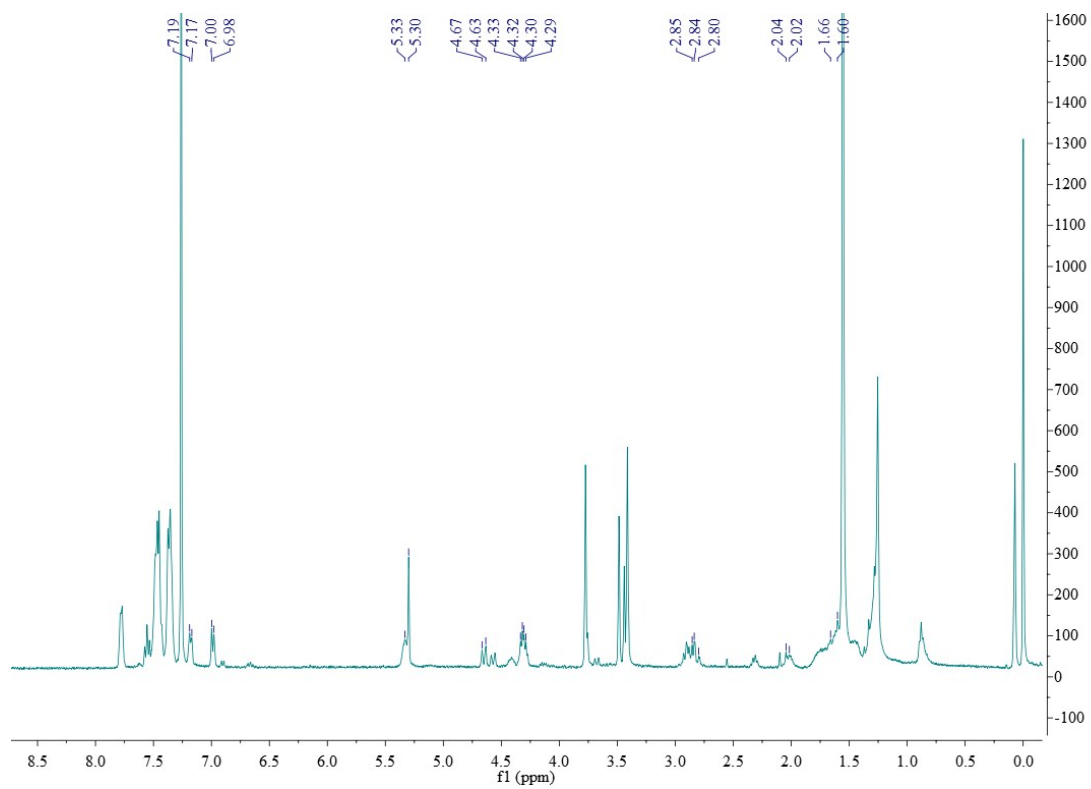


Fig. S53 ^1H NMR spectrum of **15a** CDCl_3

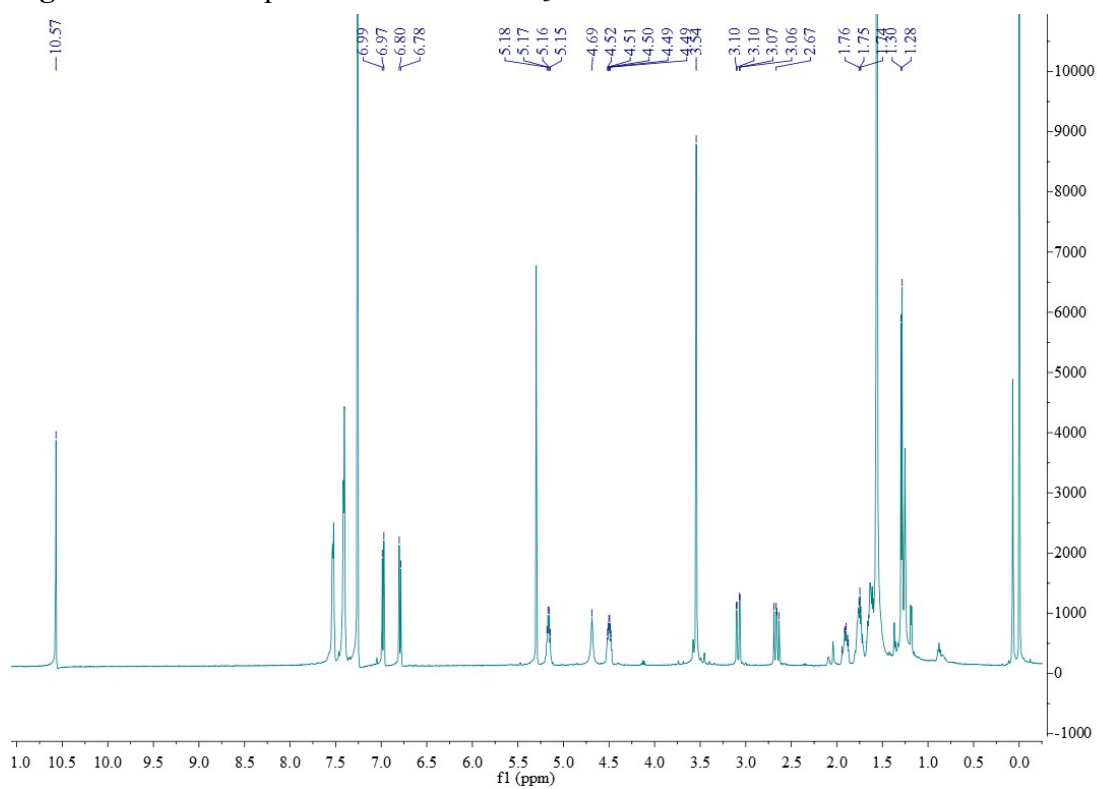


Fig. S54 ^1H NMR spectrum of **15b** CDCl_3

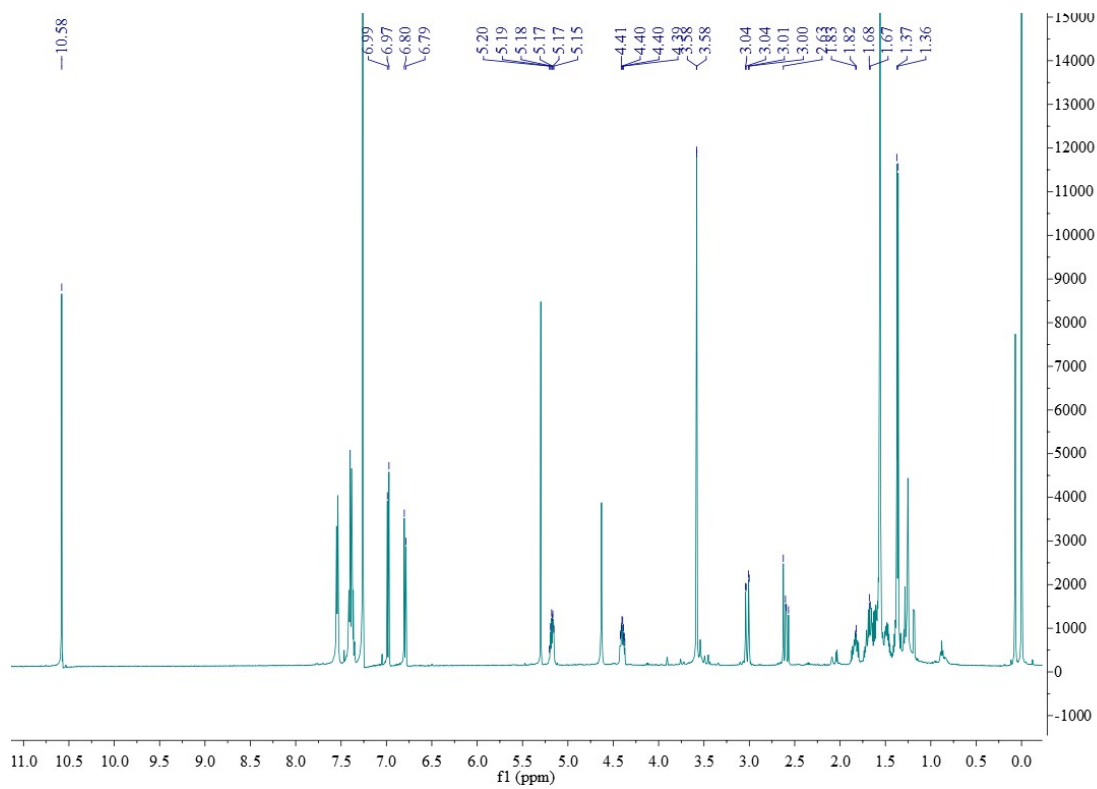


Fig. S55 X-ray crystallographic analysis of compound **5**

Colorless crystals of **5** were obtained by recrystallization from MeOH. $C_{22}H_{20}O_{12}$, $M_r = 476.38$, orthorhombic, $a = 7.0831(2)$ Å, $b = 10.0442(2)$ Å, $c = 28.1976(5)$ Å, $\alpha = 90.00$, $\beta = 90.00$, $\gamma = 90.00$, $V = 2006.09(8)$ Å³, space group $P2_12_12_1$, $Z = 4$, $D_{calcd} = 1.286$ mg/m³, $\mu(\text{Cu K}\alpha) = 1.577$ m⁻¹, and $F(000) = 992.0$. Crystal dimensions: $0.42 \times 0.32 \times 0.26$ mm³. Independent reflections: 3561 ($R_{int} = 0.0307$). The final R_1 values were 0.0286, $\omega R_2 = 0.0722$ ($I > 2\sigma(I)$). Flack parameter value was 0.06(13). CCDC number: 1444470. The single crystal X-ray diffraction data was collected at 123 K on an Agilent Gemini Ultra diffractometer with Cu K α radiation ($\lambda = 1.54178$ Å). The structures were solved by direct methods (SHELXS-97) and refined using full-matrix least-squares difference Fourier techniques. Hydrogen atoms bonded to carbons were placed on the geometrically ideal positions by the “ride on” method. Hydrogen atoms bonded to oxygen were located by the difference Fourier method and were included in the calculation of structure factors with isotropic temperature factors. Crystallographic data for **5** has been deposited with the Cambridge Crystallographic Data Centre. Copies of the data can be obtained, free of charge, on application to the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: 44-(0)1223-336033, or e-mail: deposit@ccdc.cam.ac.uk).

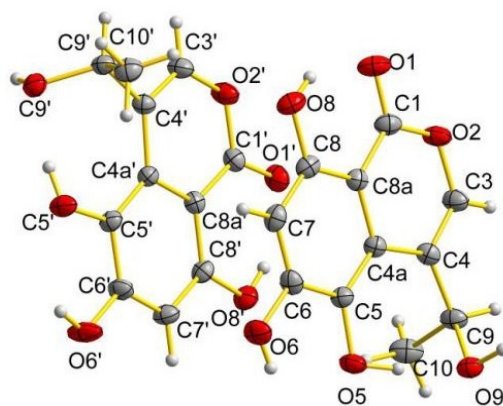


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