Supplementary Information

Coastal halophyte plant *Atriplex maximowicziana* with previously undescribed terpenoids and anti-colorectal cancer chlorophyll stereoisomers utilizing a molecular networking approach

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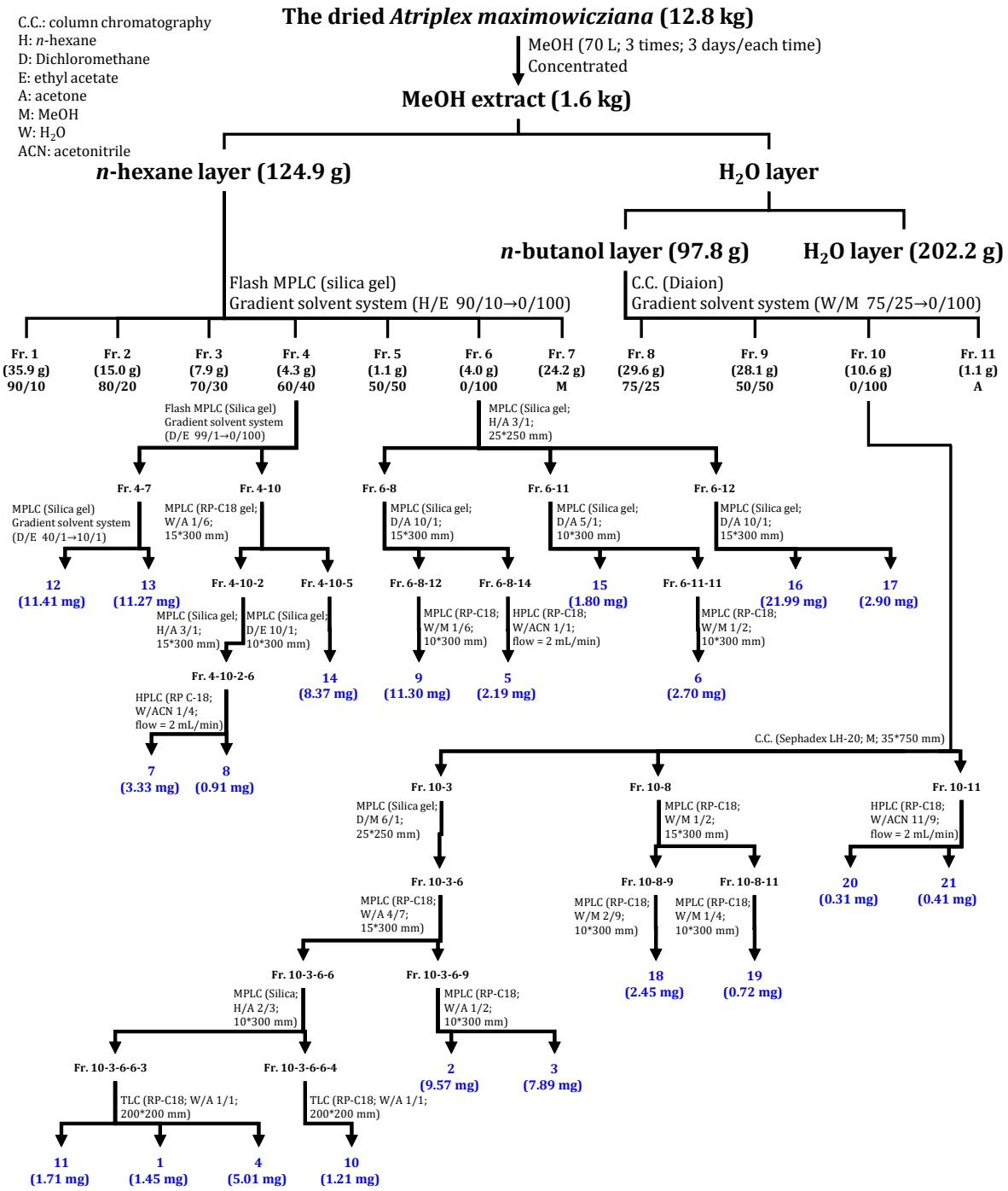

Fig. S1 The isolation flow chart of compounds **1**–**21** from *Atriplex maximowicziana*.

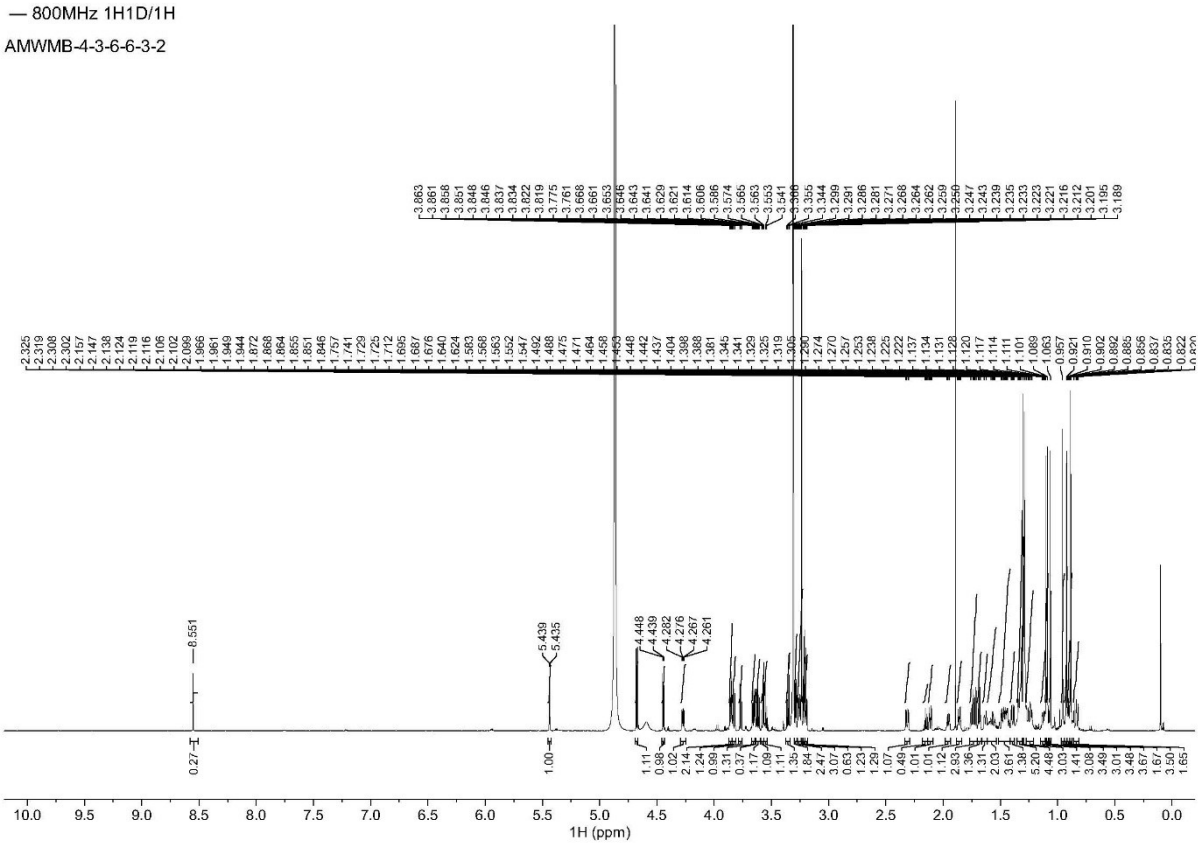

Fig. S2 ^{1}H NMR spectrum (800 MHz, CD_3OD) of **1**.

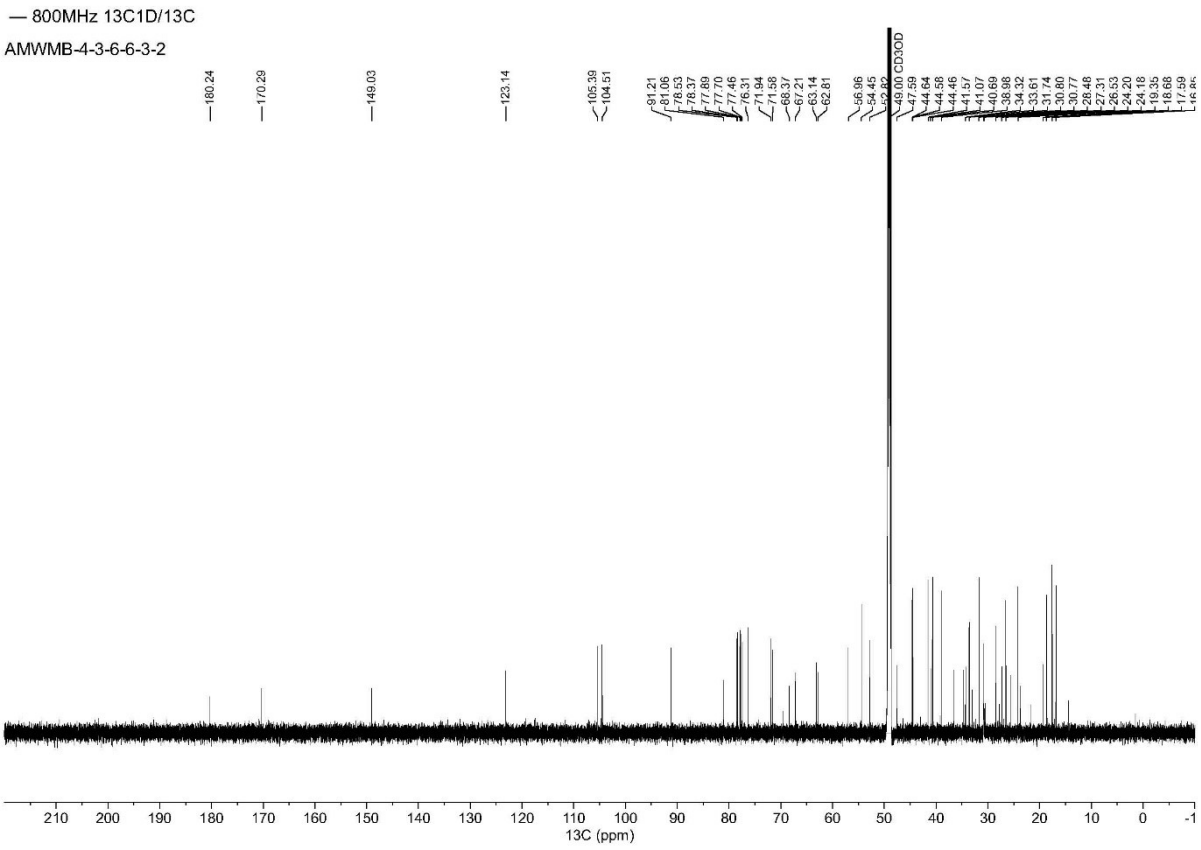

Fig. S3 ^{13}C NMR spectrum (200 MHz, CD_3OD) of **1**.

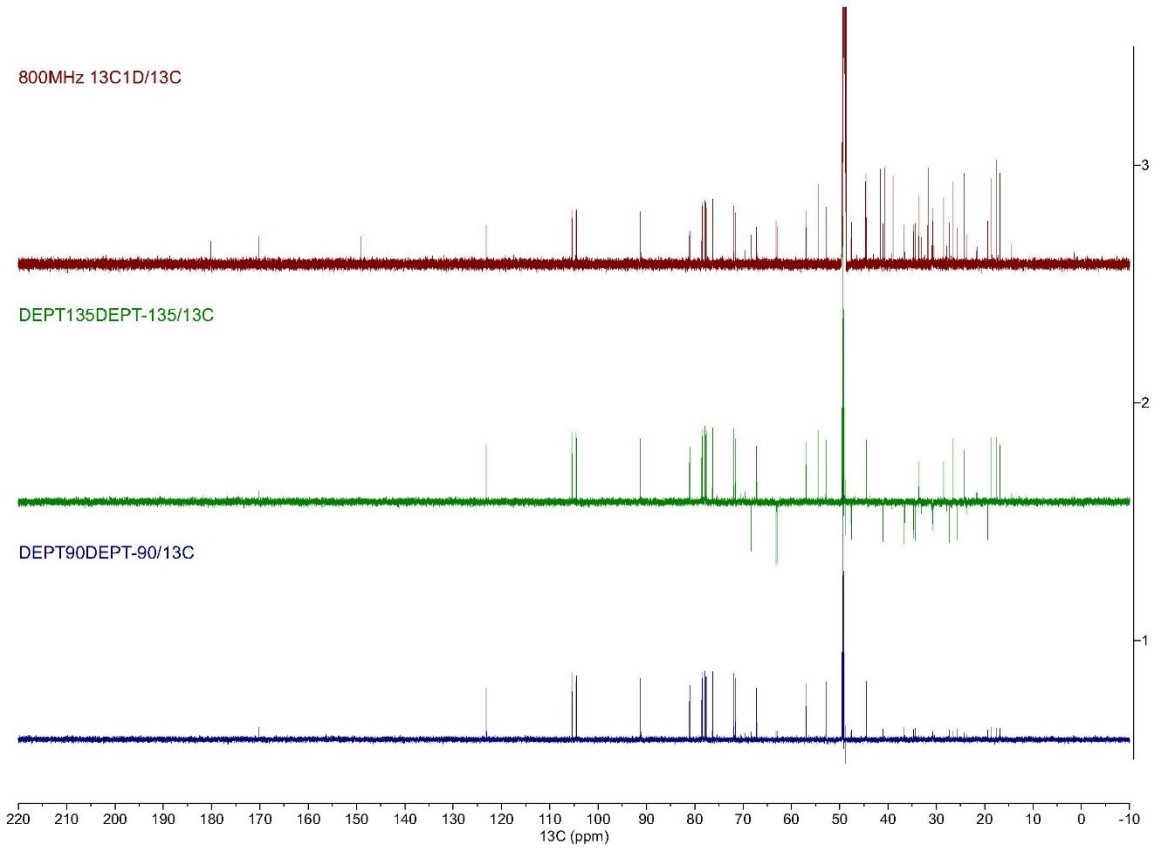

Fig. S4 DEPT spectrum of **1**.

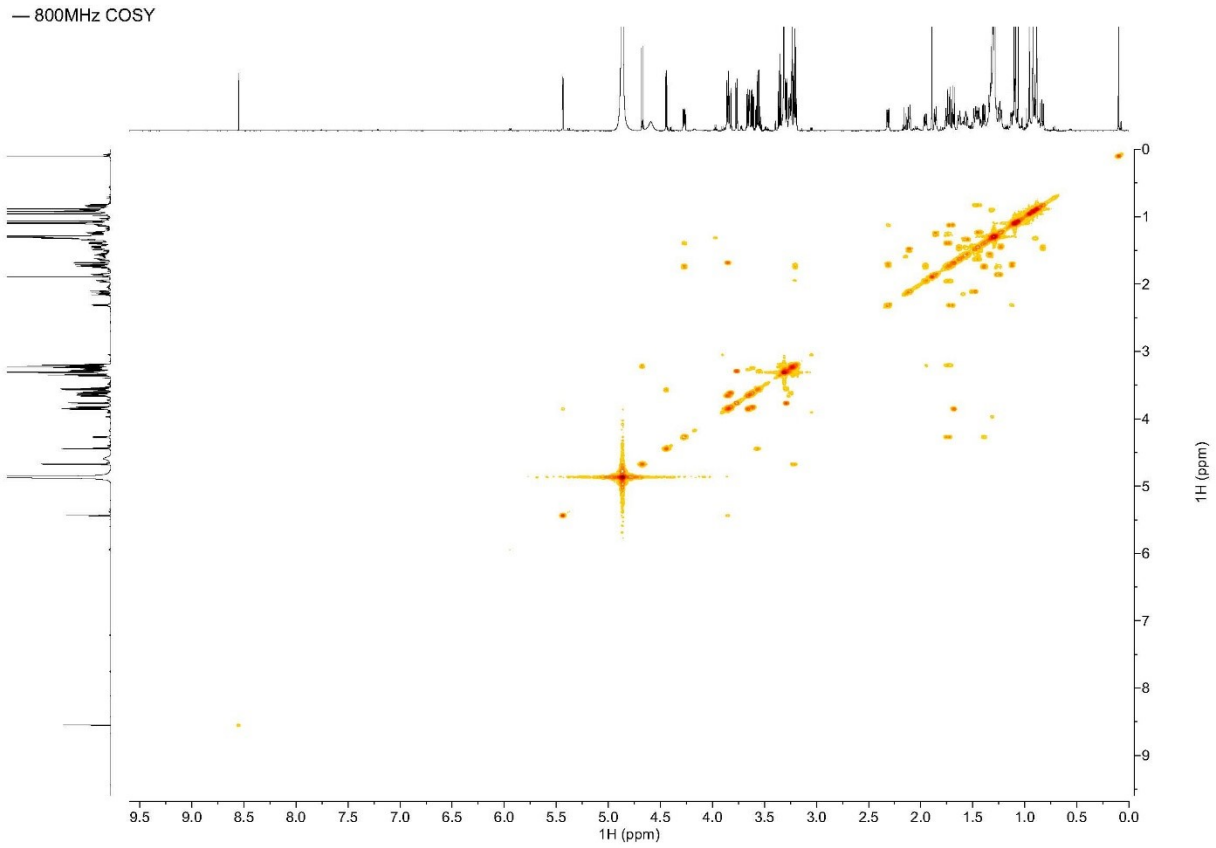

Fig. S5 COSY spectrum of **1**.

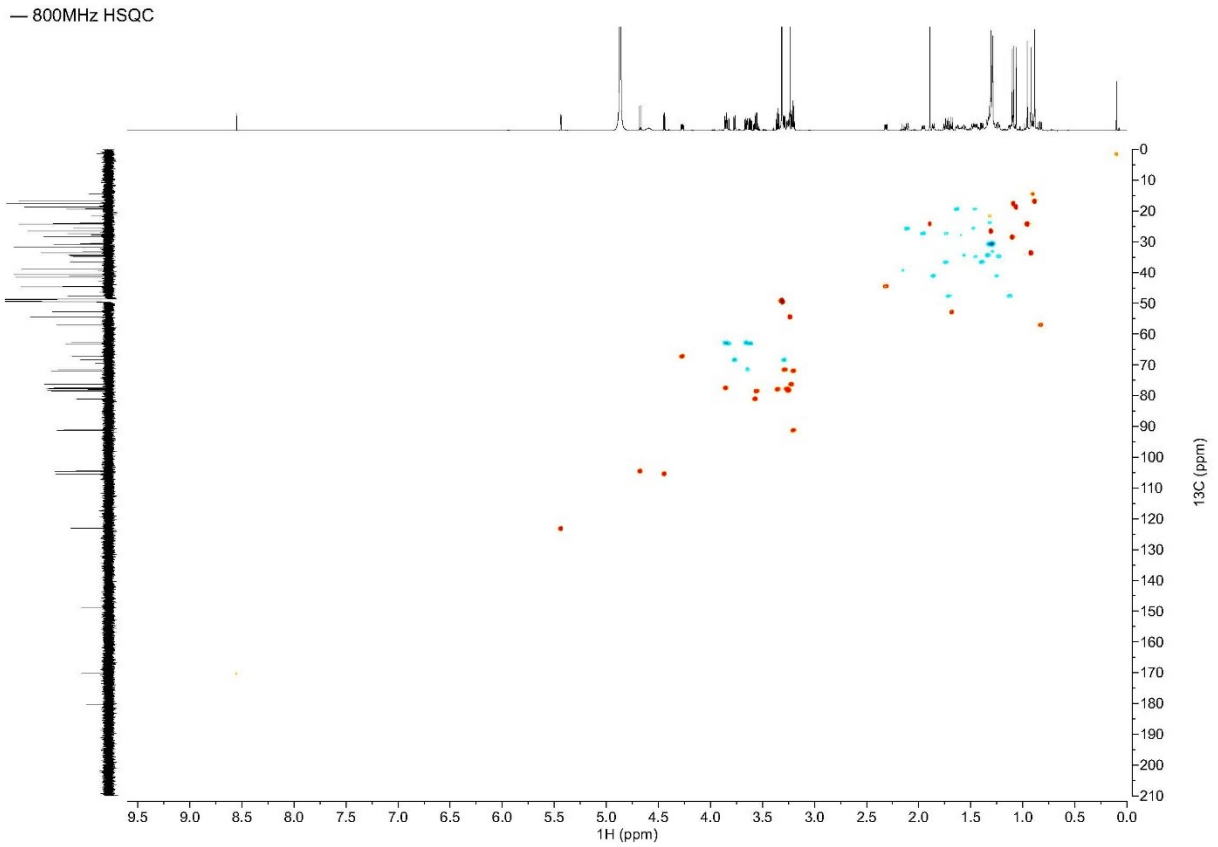

Fig. S6 HSQC spectrum of **1**.

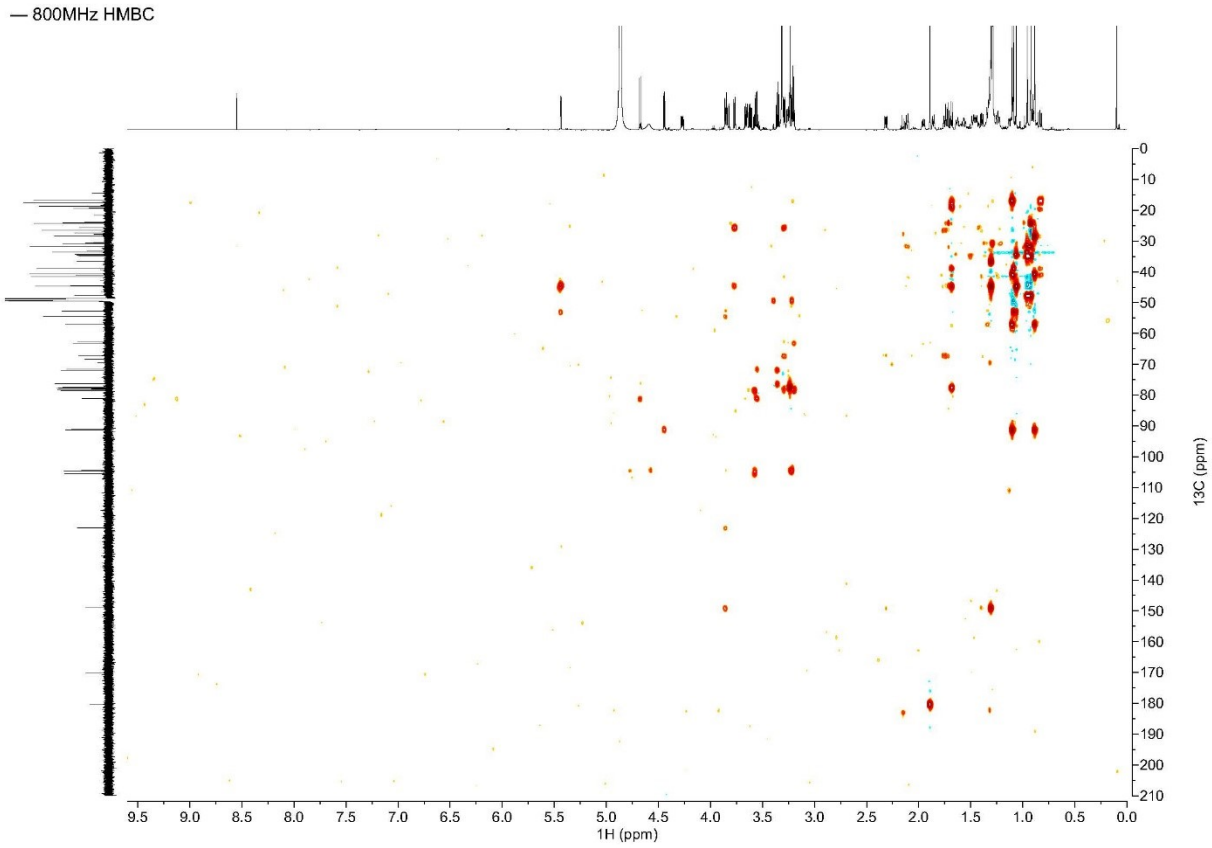

Fig. S7 HMBC spectrum of **1**.

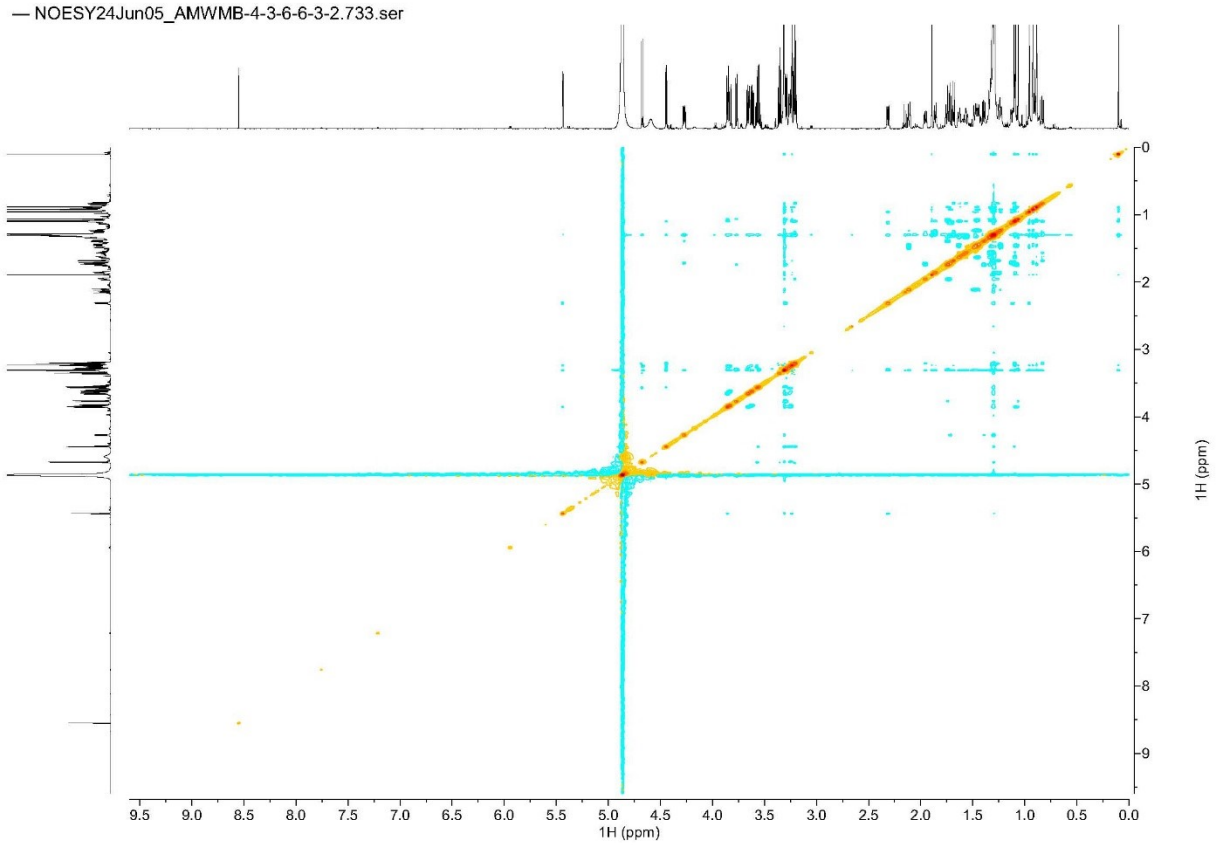

Fig. S8 NOESY spectrum of **1**.

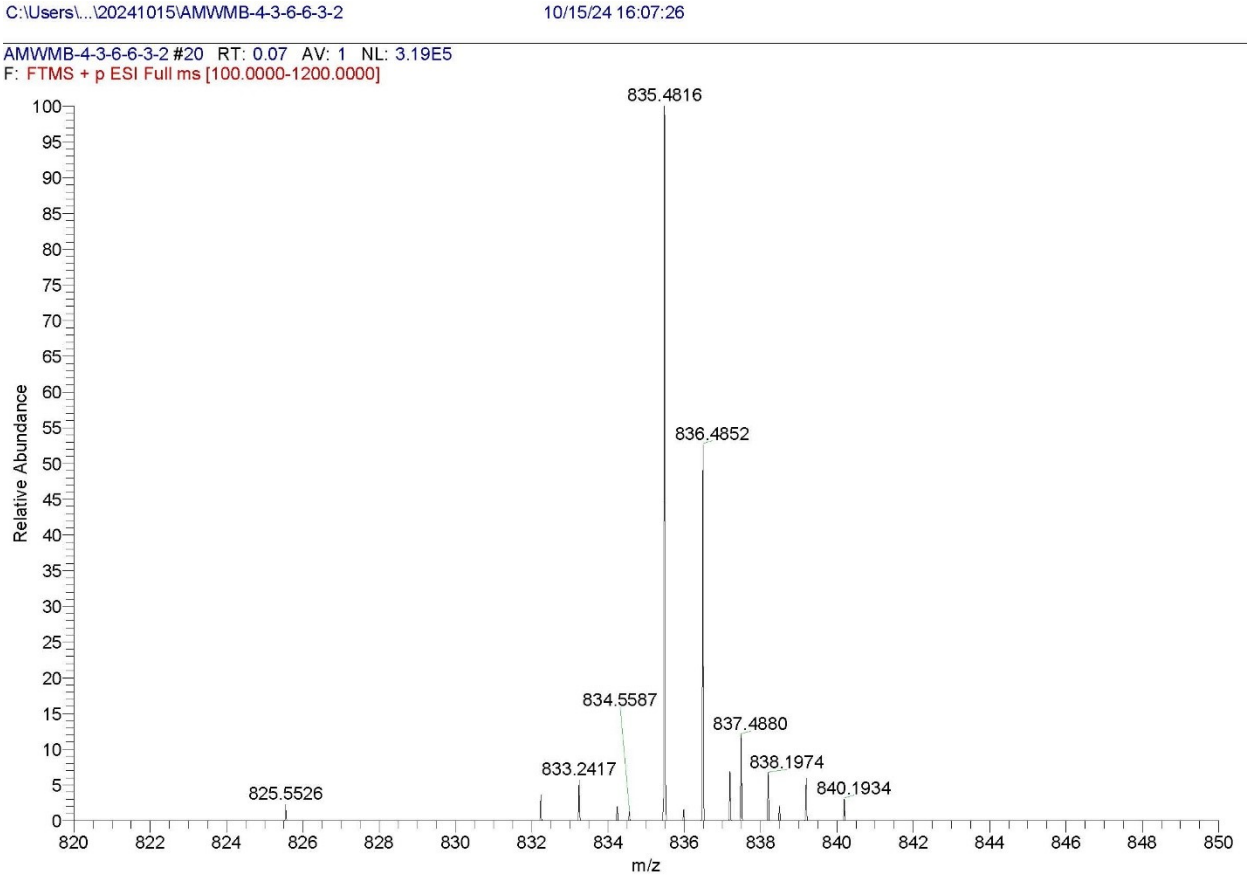

Fig. S9 HRESIMS spectrum of **1**.

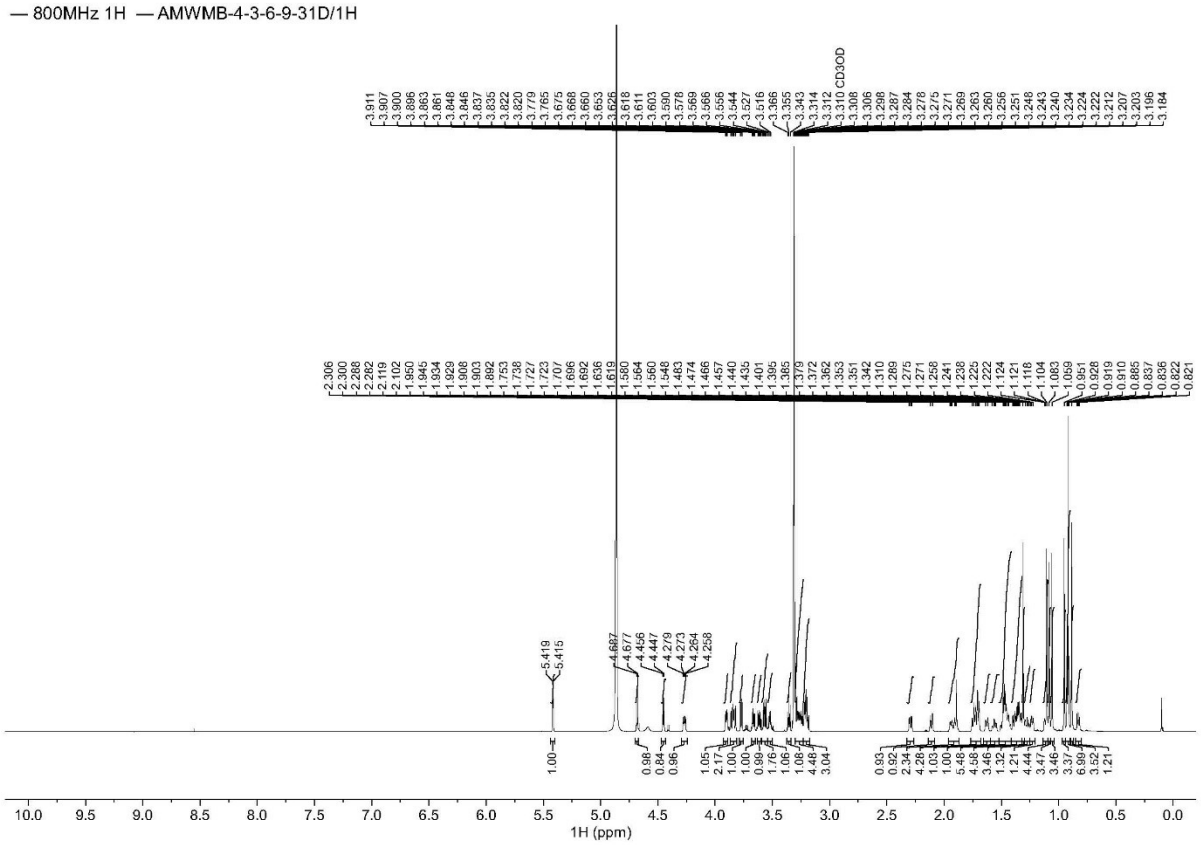

Fig. S10 ^{1}H NMR spectrum (800 MHz, CD_3OD) of **2**.

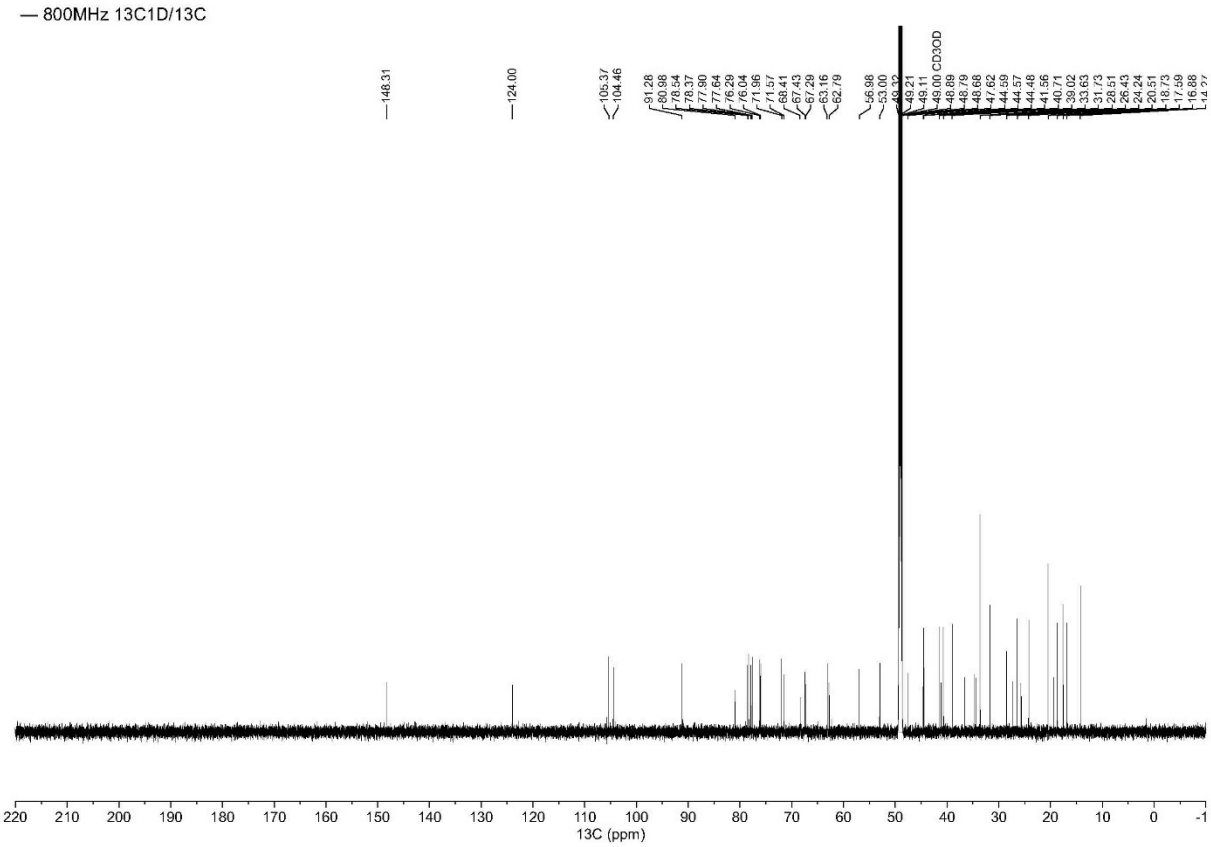

Fig. S11 ^{13}C NMR spectrum (200 MHz, CD_3OD) of **2**.

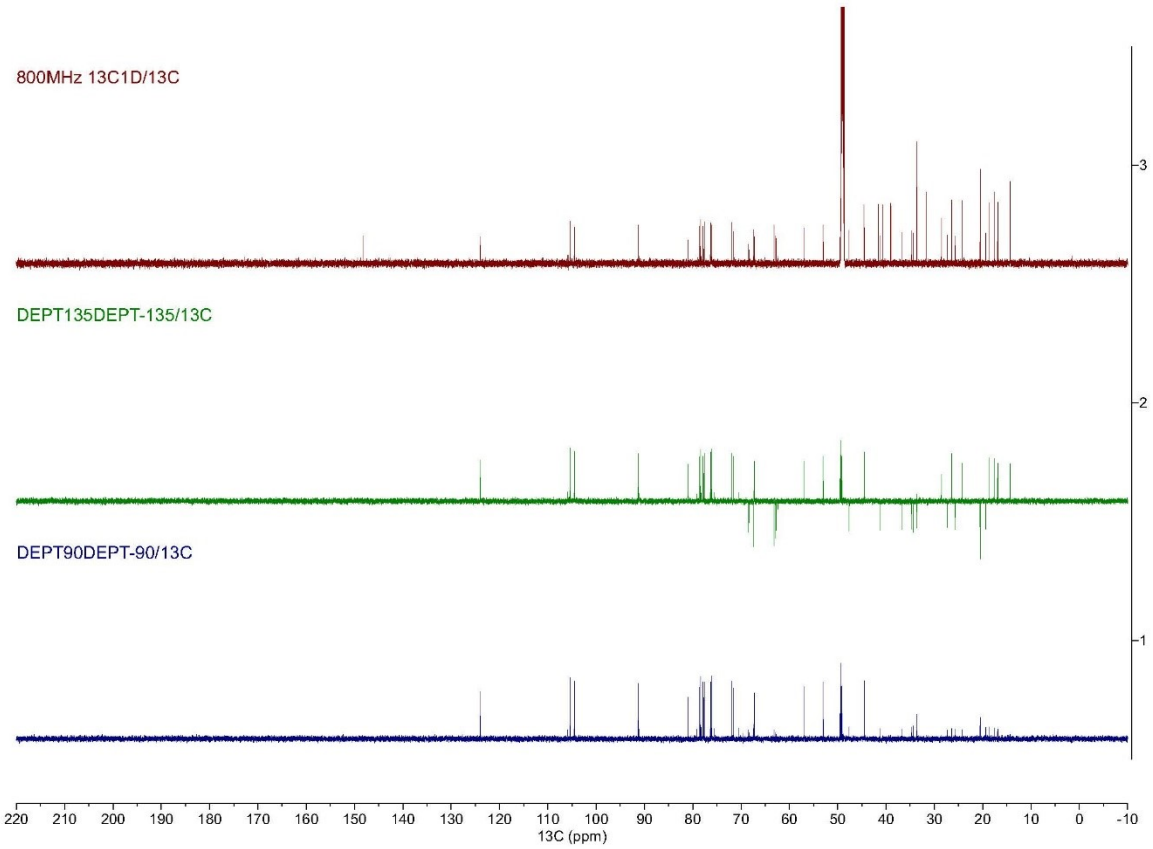

Fig. S12 DEPT spectrum of **2**.

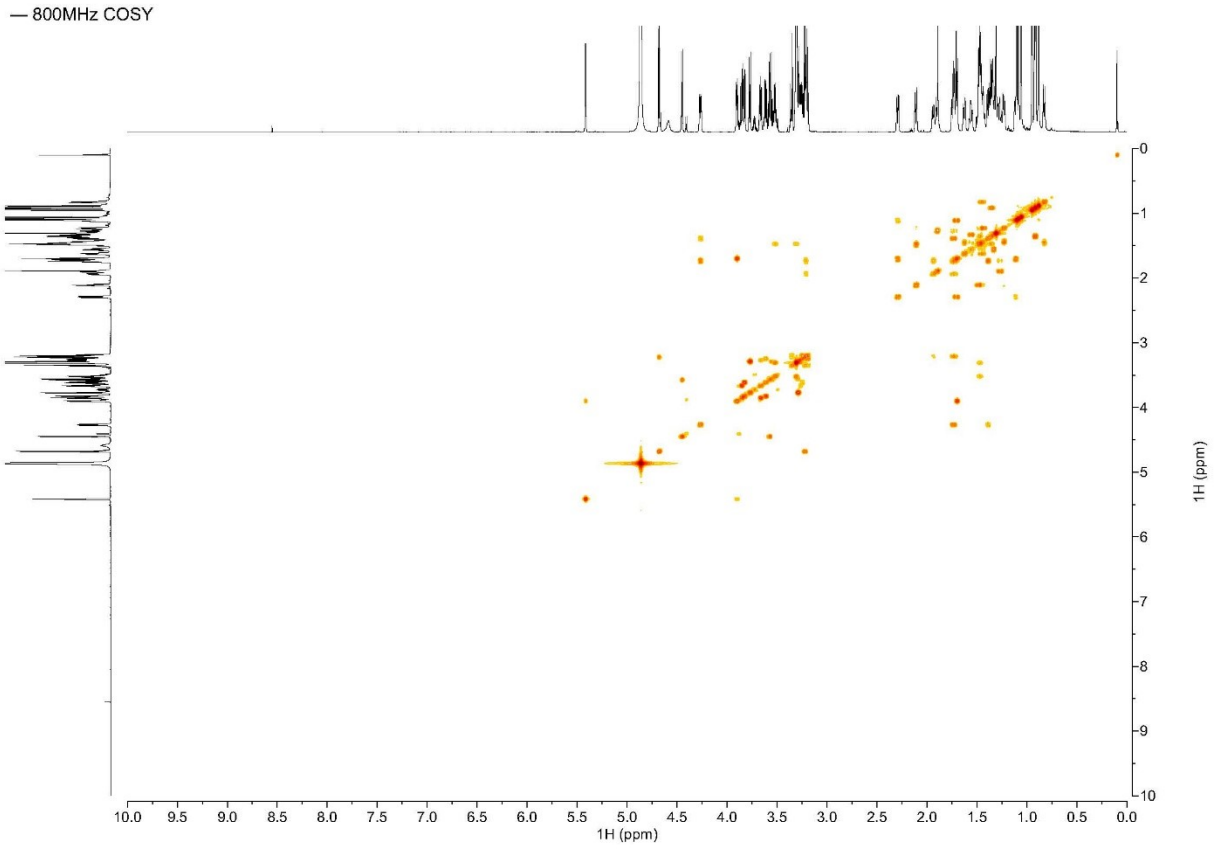

Fig. S13 COSY spectrum of **2**.

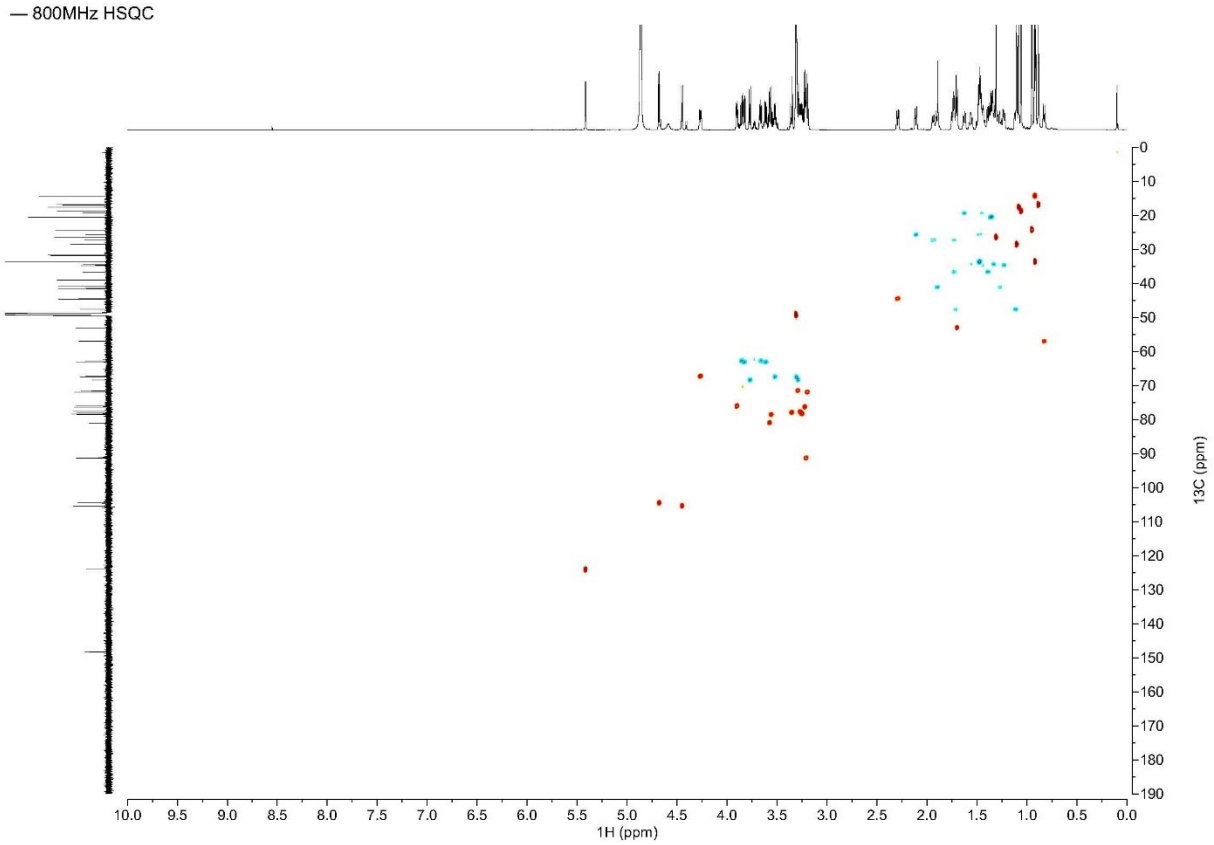

Fig. S14 HSQC spectrum of **2**.

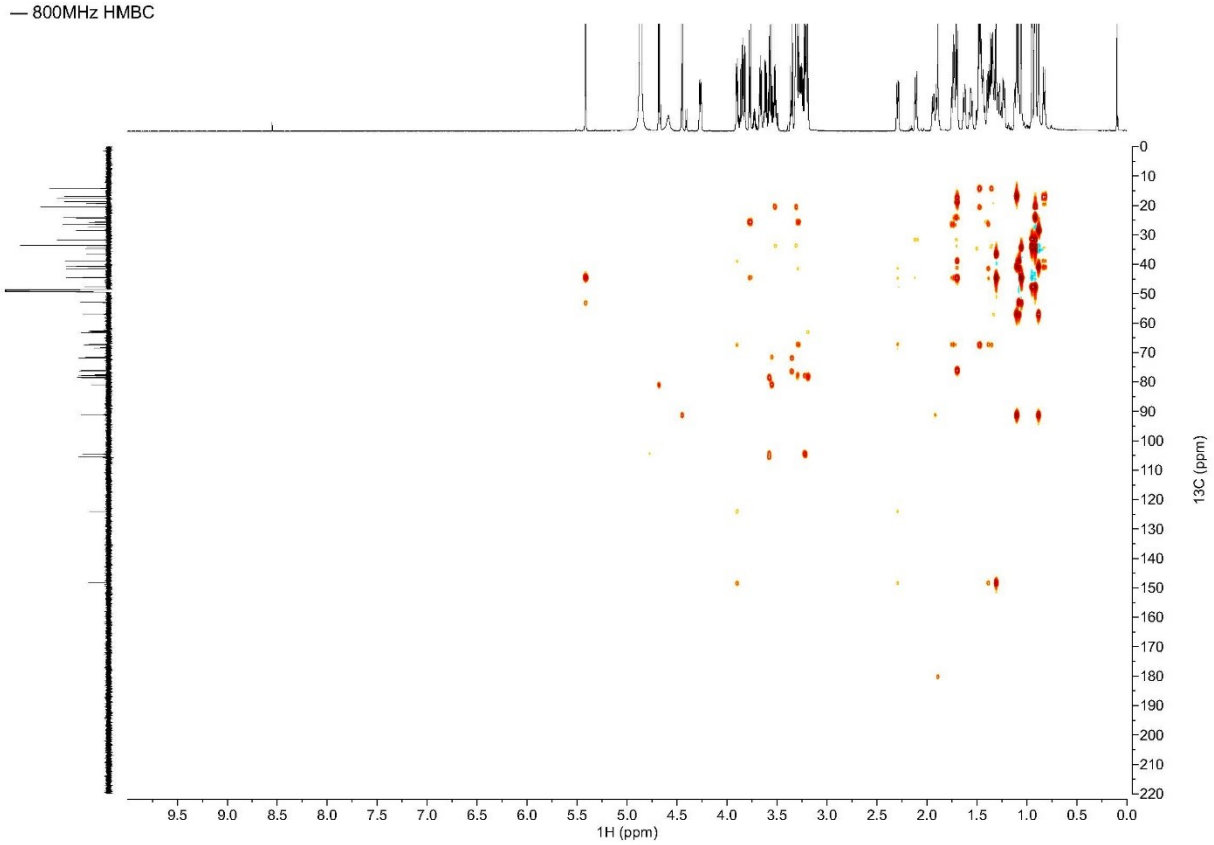

Fig. S15 HMBC spectrum of **2**.

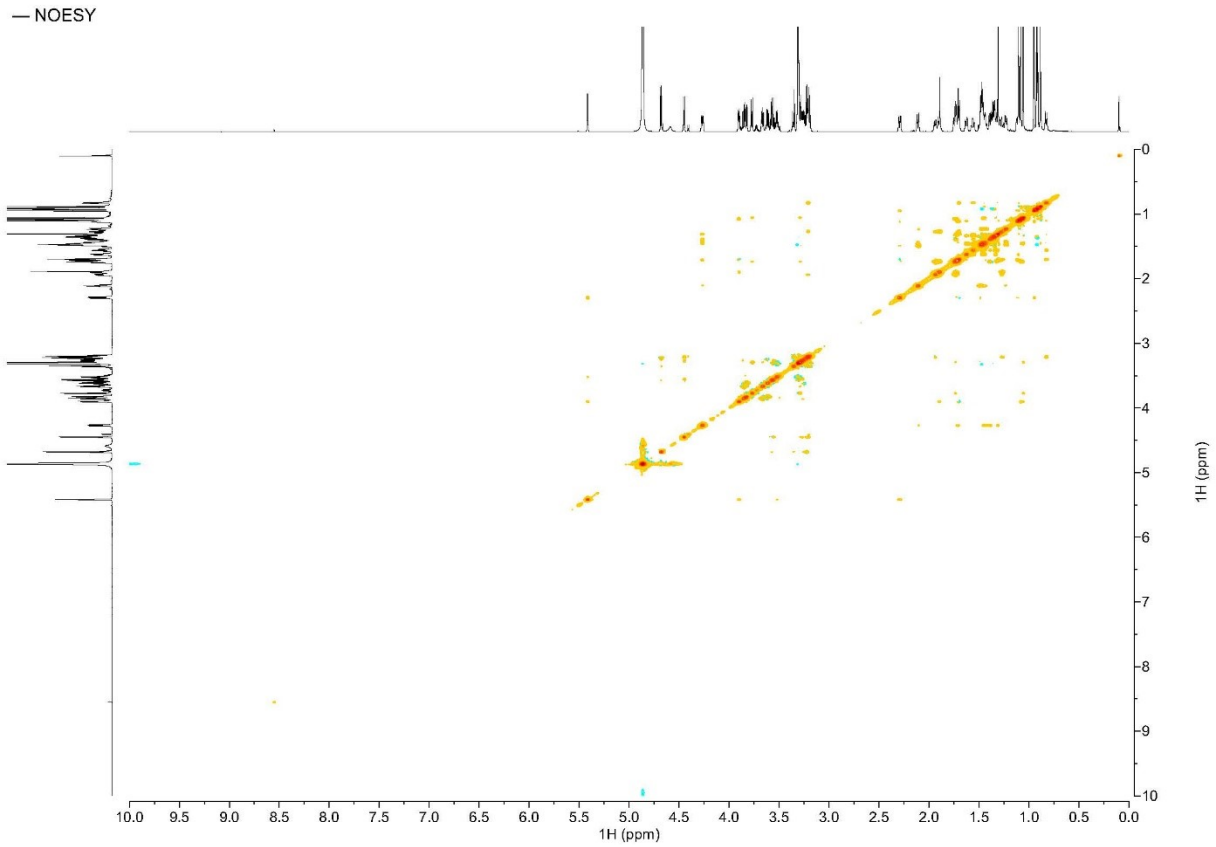

Fig. S16 NOESY spectrum of **2**.

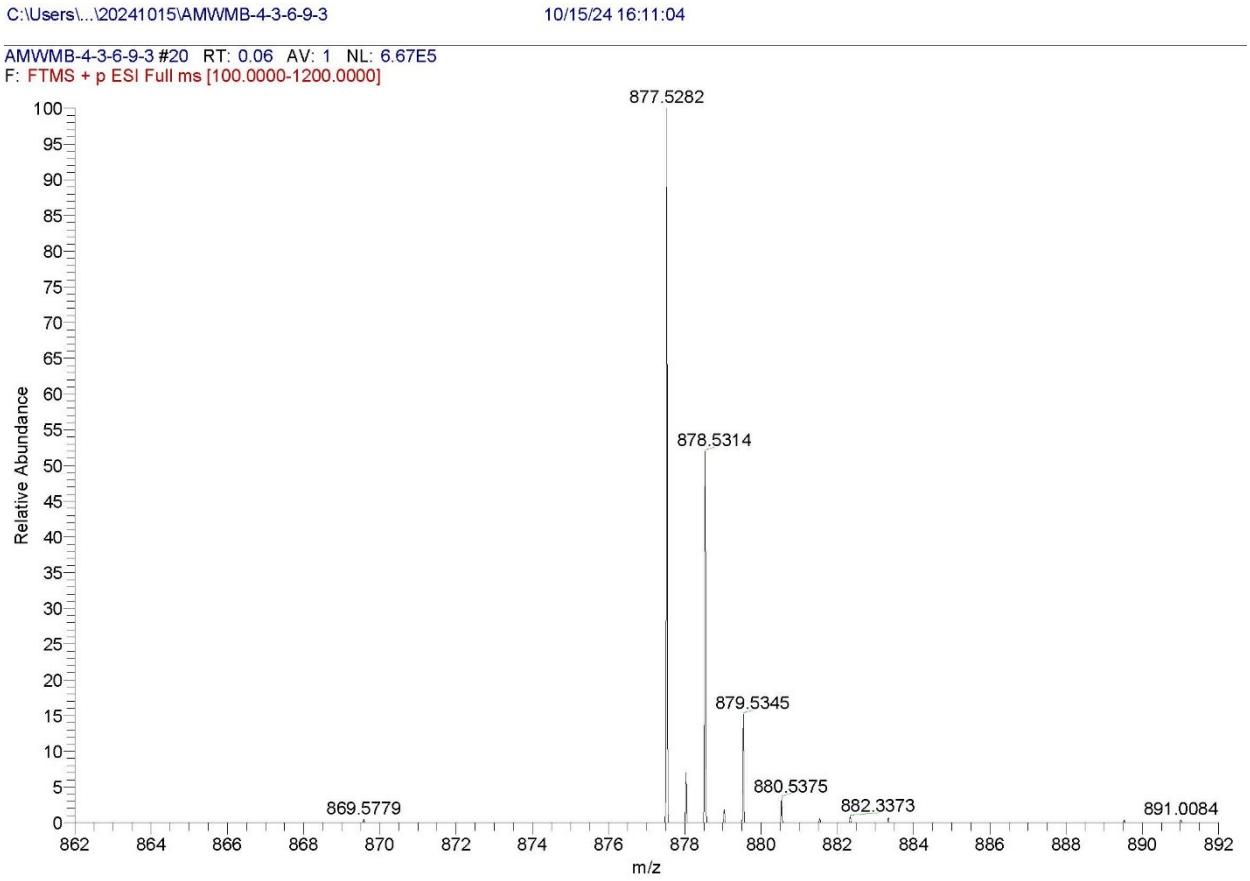

Fig. S17 HRESIMS spectrum of **2**.

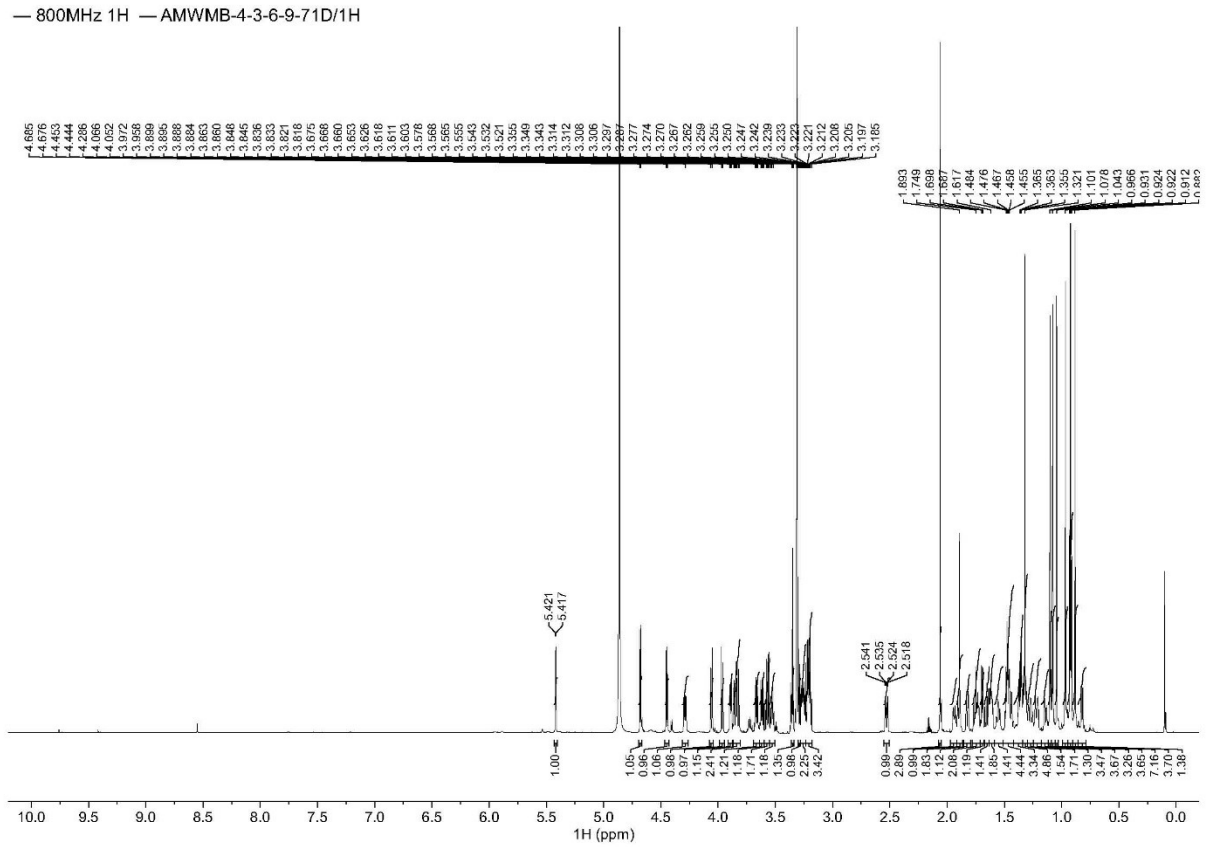

Fig. S18 ^{1}H NMR spectrum (800 MHz, CD_3OD) of **3**.

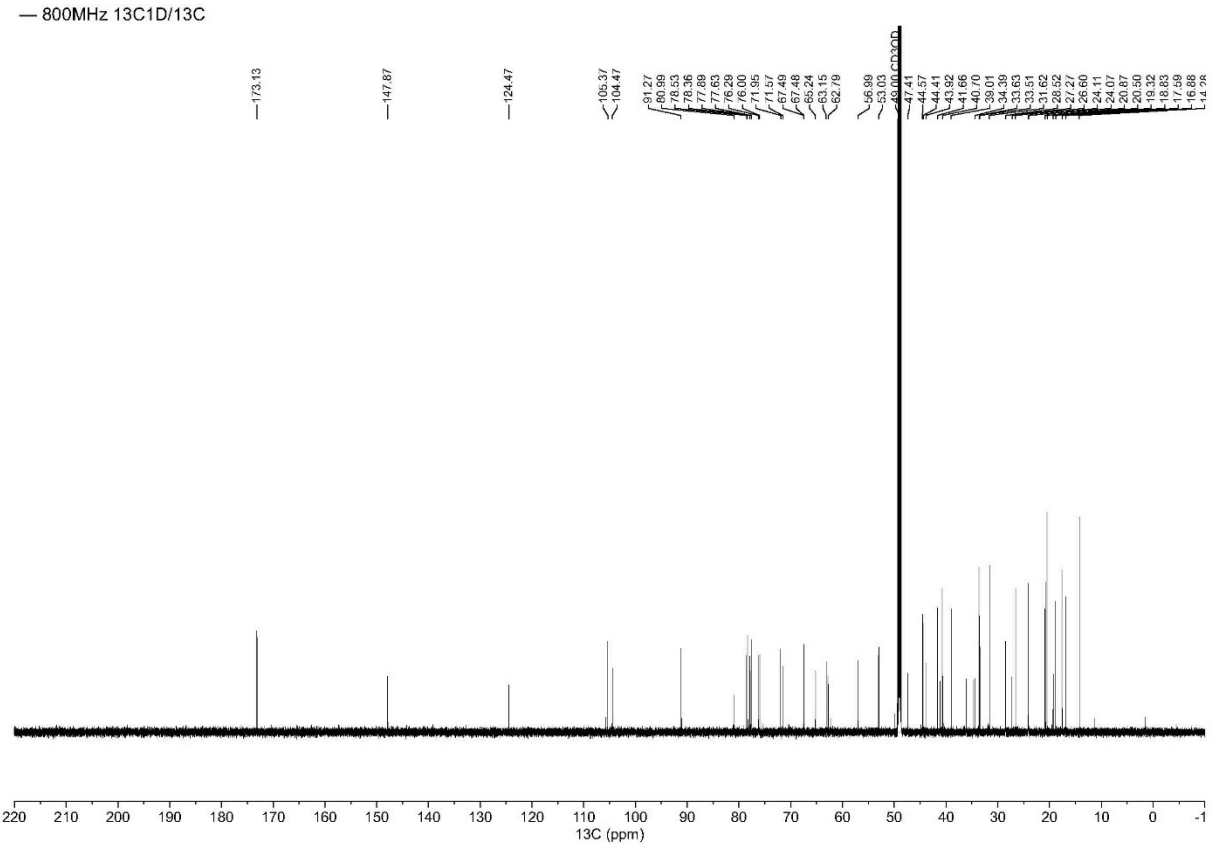

Fig. S19 ^{13}C NMR spectrum (200 MHz, CD_3OD) of **3**.

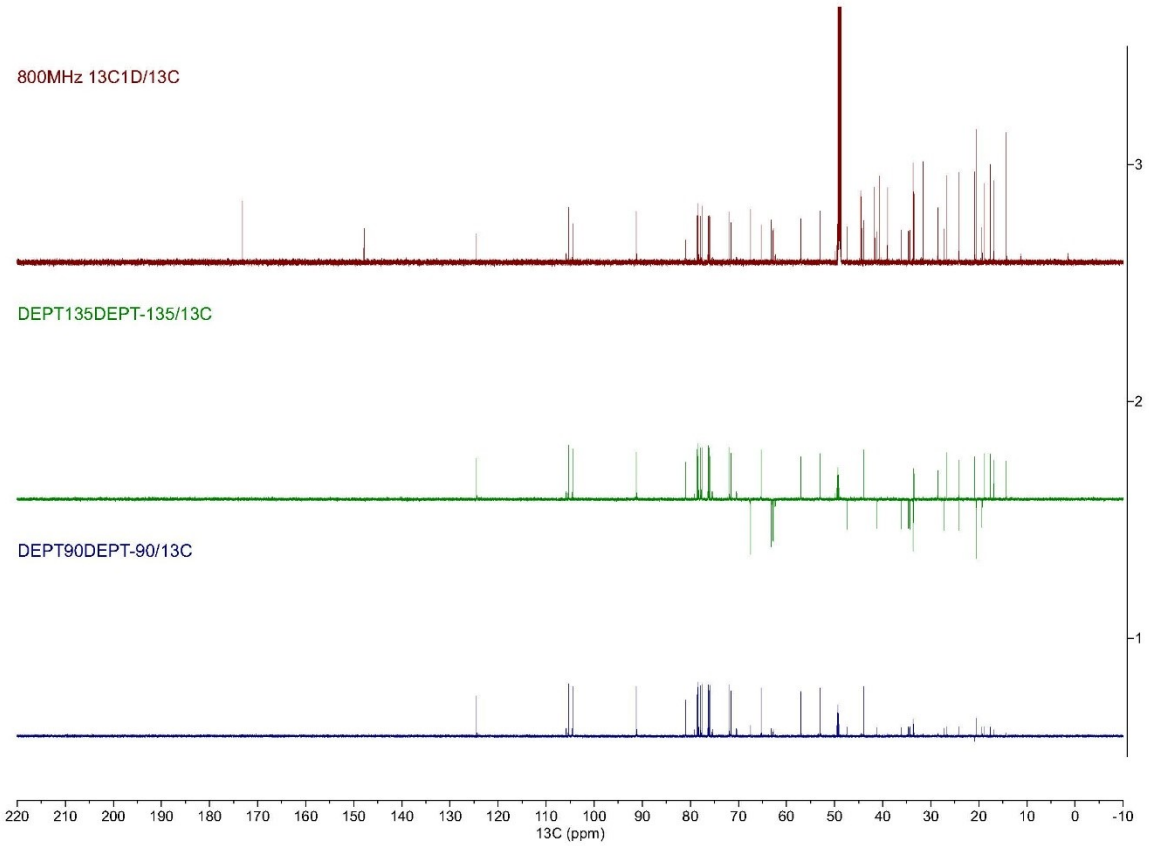

Fig. S20 DEPT spectrum of **3**.

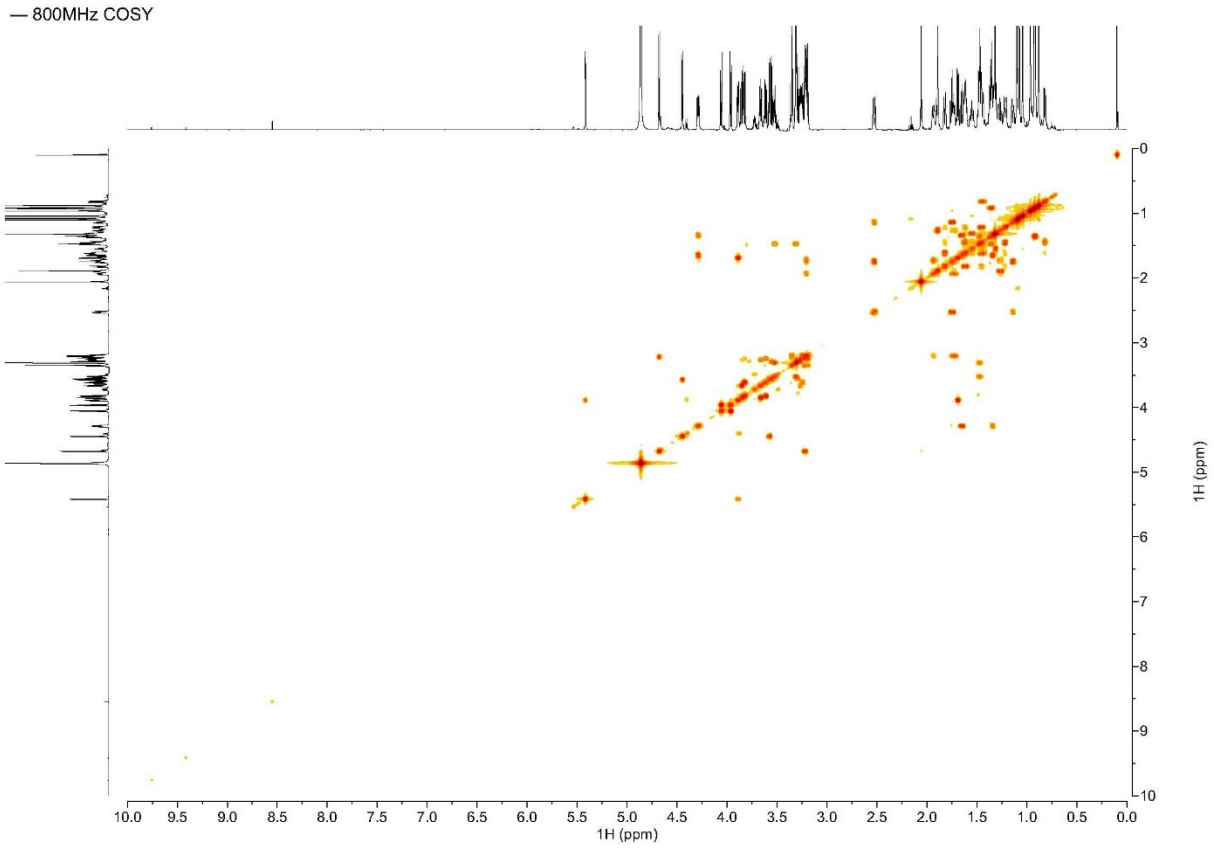

Fig. S21 COSY spectrum of **3**.

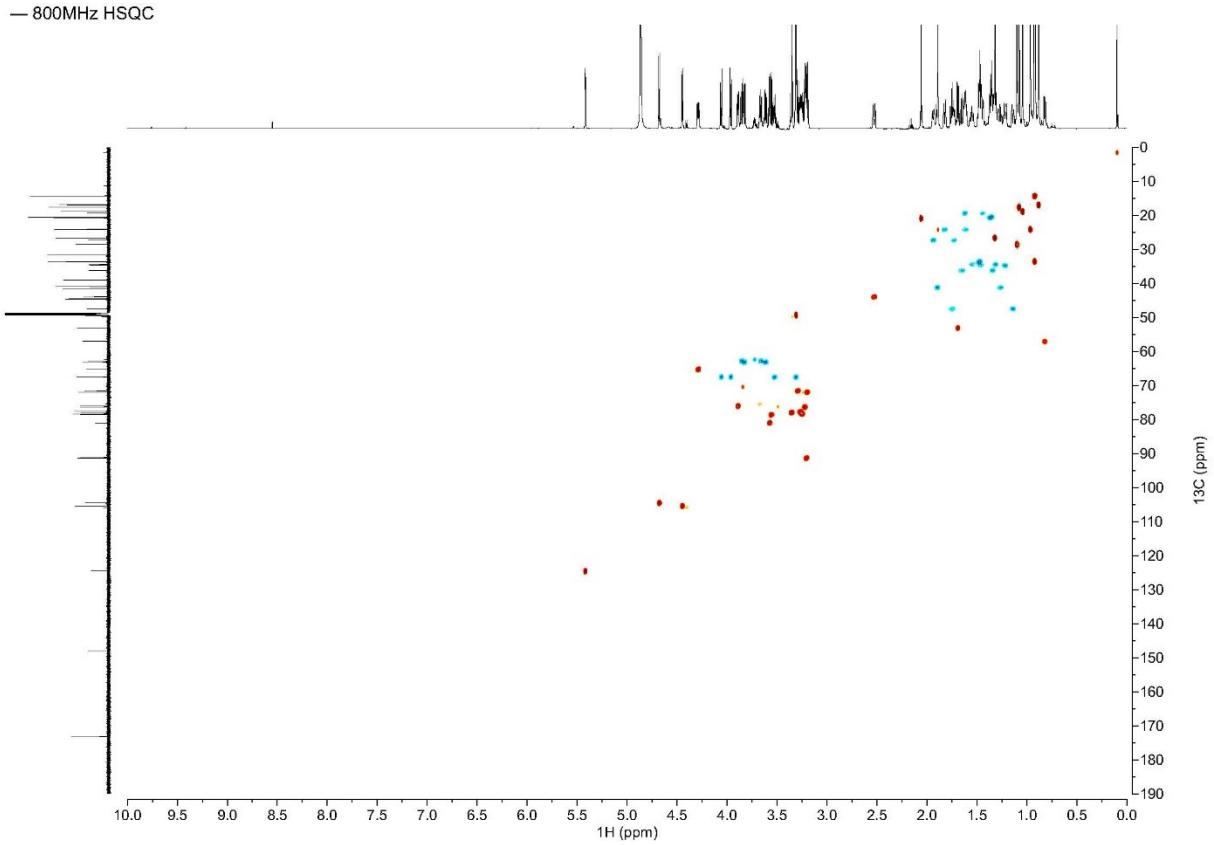

Fig. S22 HSQC spectrum of **3**.

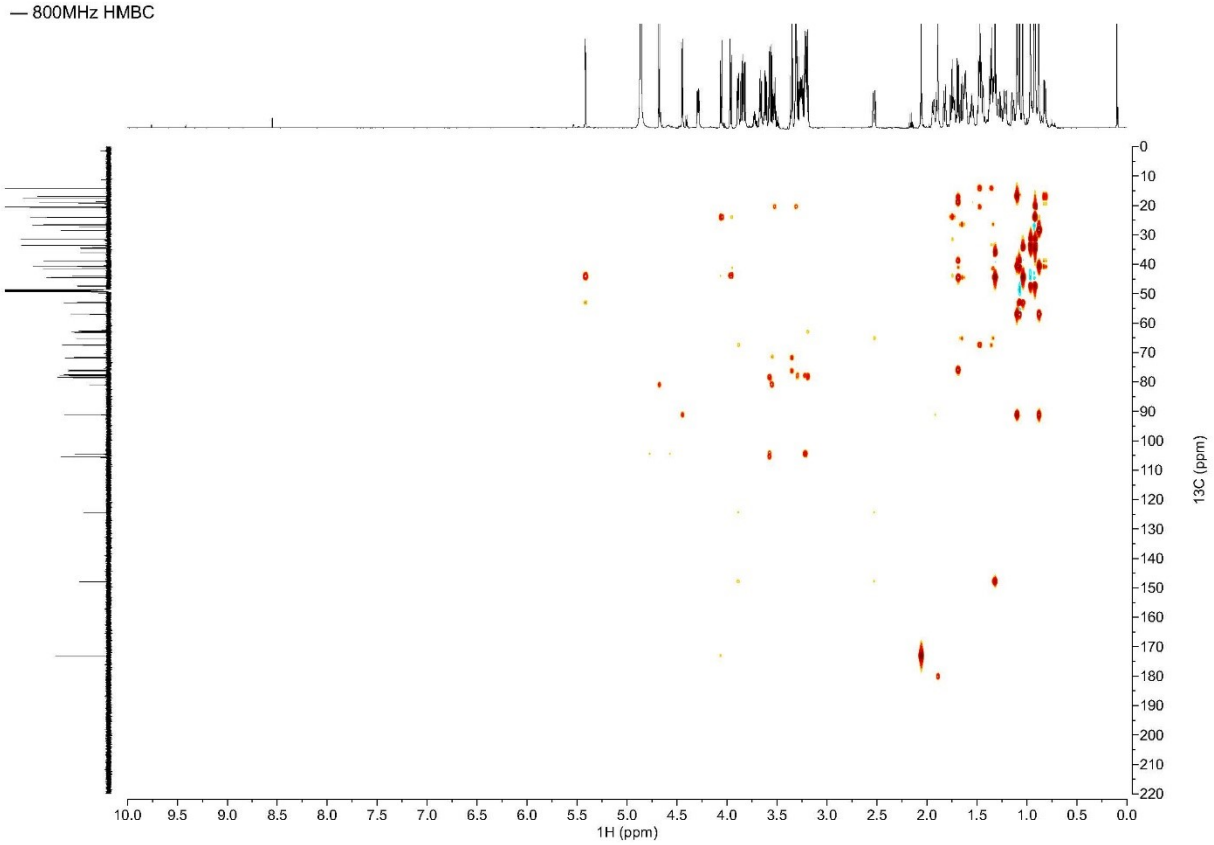

Fig. S23 HMBC spectrum of **3**.

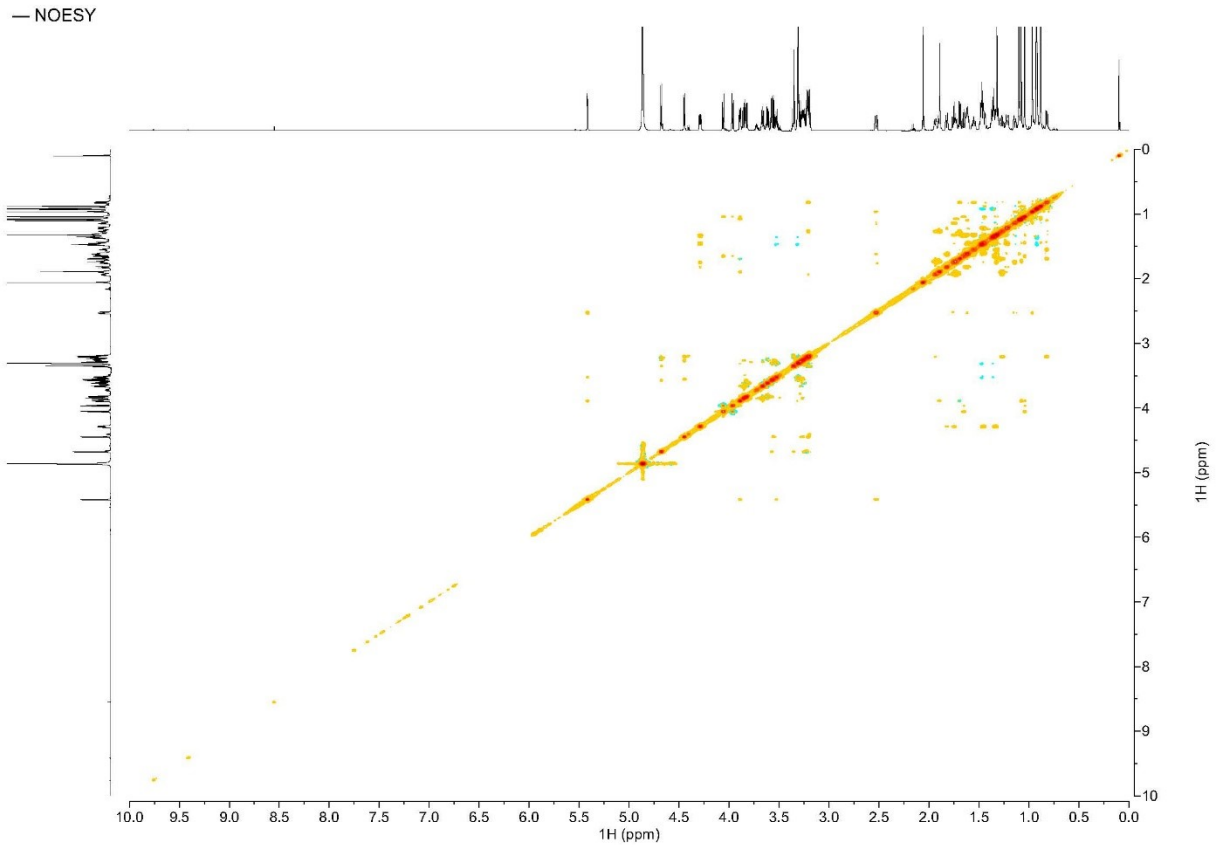

Fig. S24 NOESY spectrum of **3**.

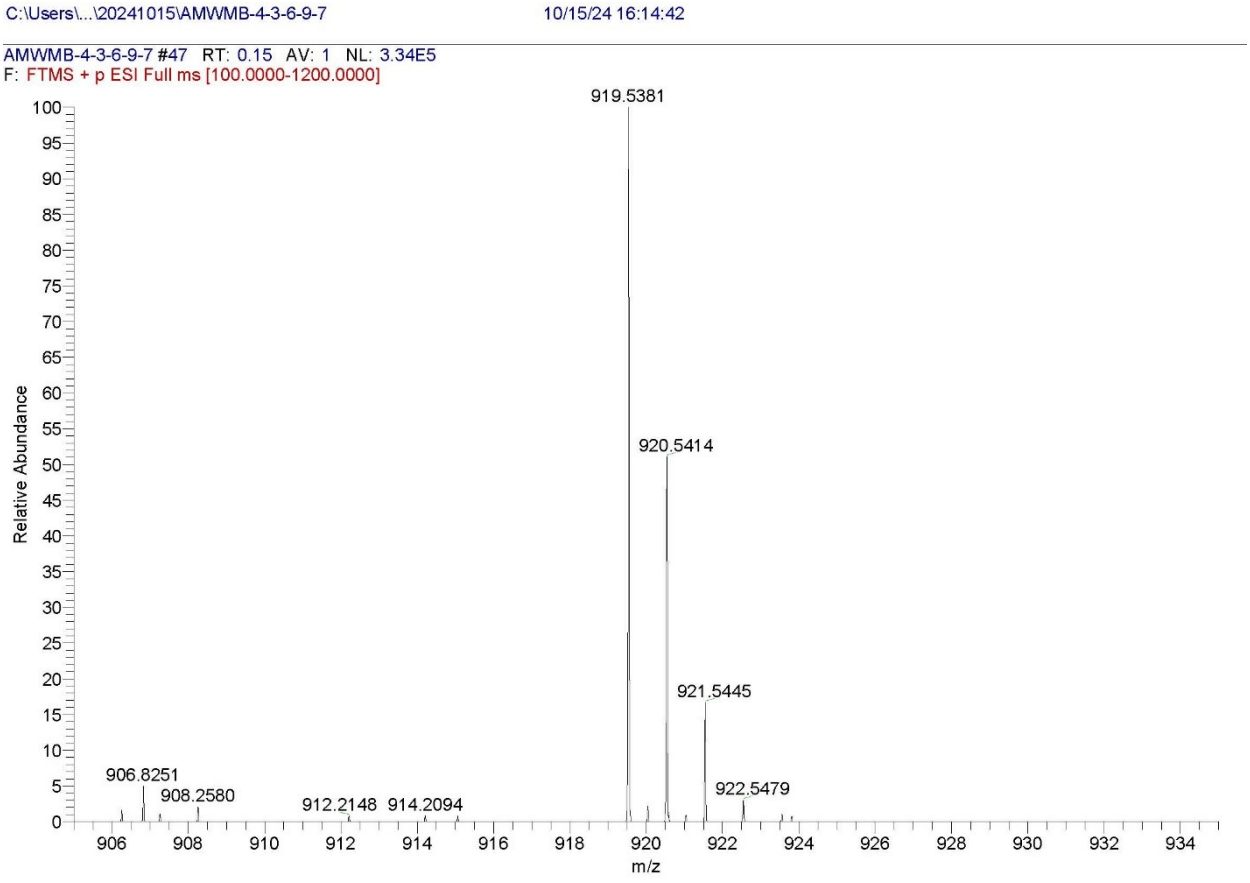

Fig. S25 HRESIMS spectrum of **3**.

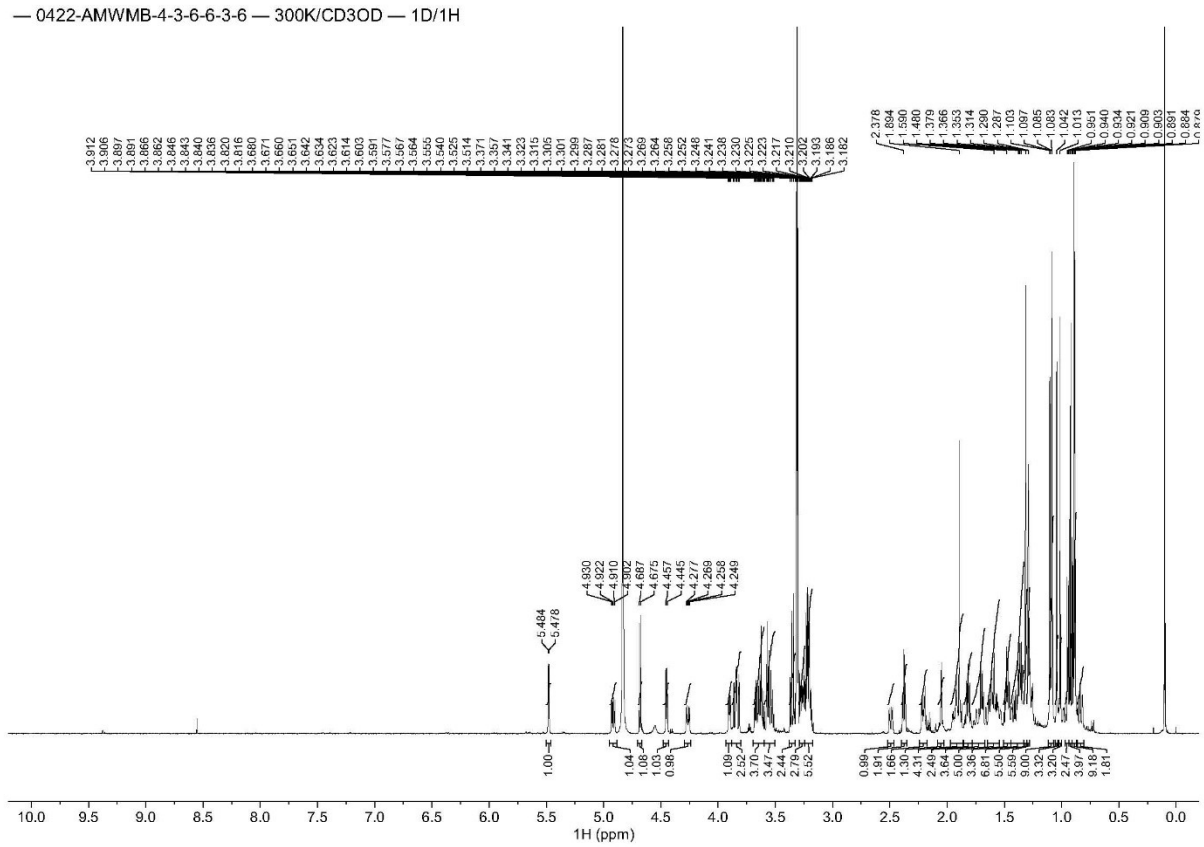

Fig. S26 ^{1}H NMR spectrum (600 MHz, CD_3OD) of **4**.

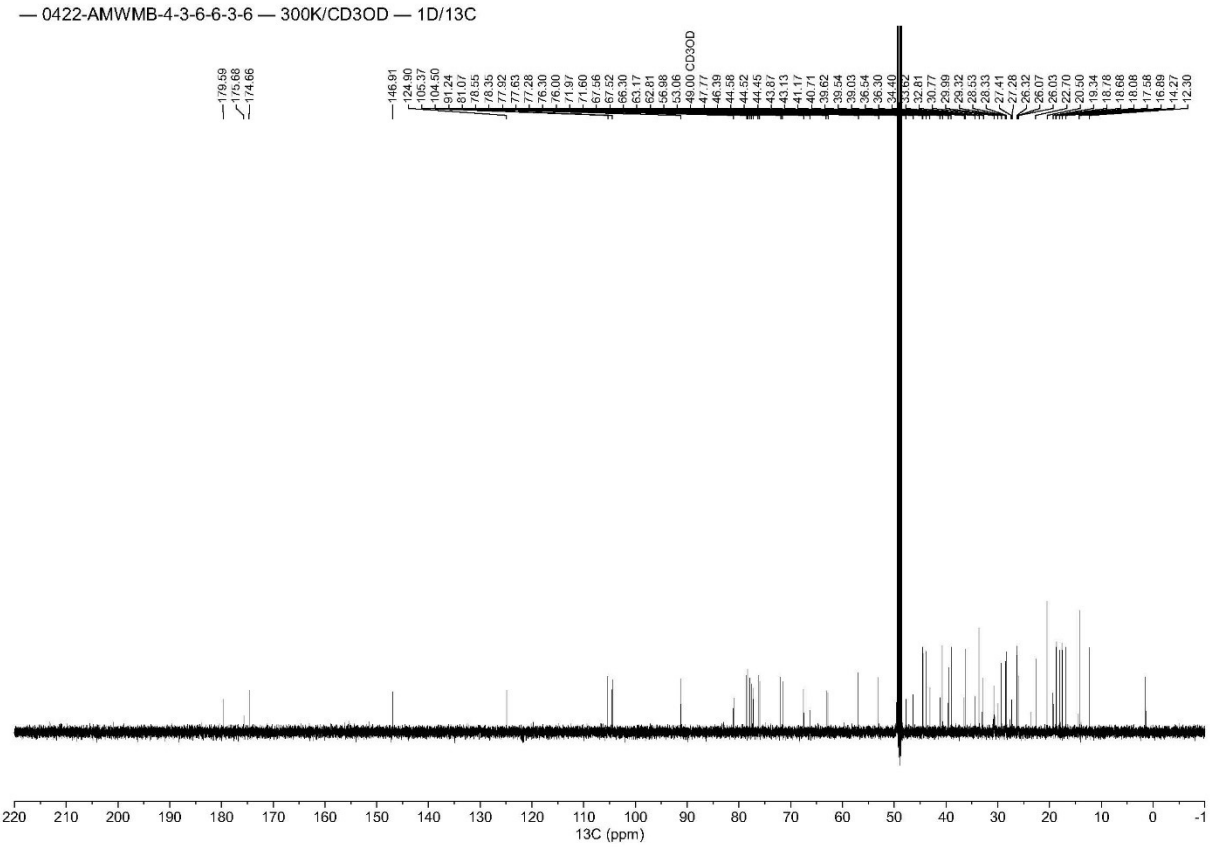

Fig. S27 ^{13}C NMR spectrum (150 MHz, CD_3OD) of **4**.

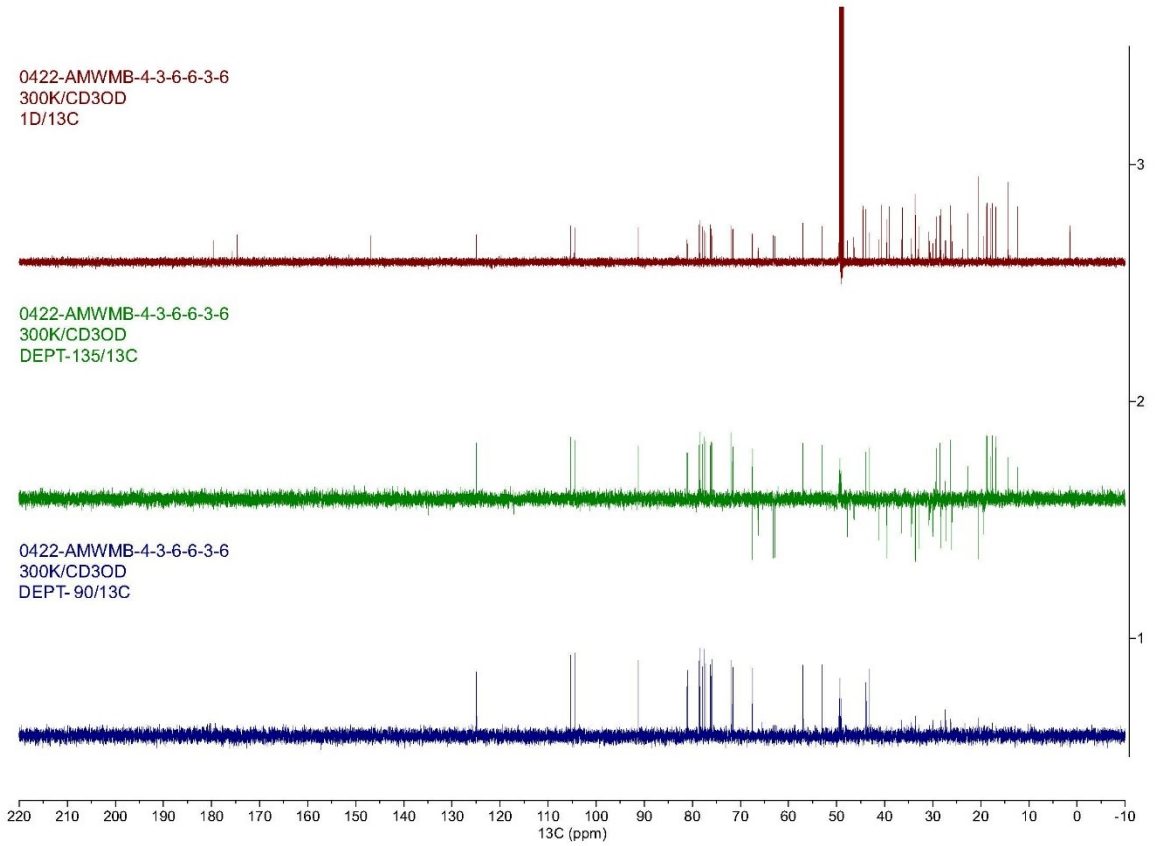

Fig. S28 DEPT spectrum of **4**.

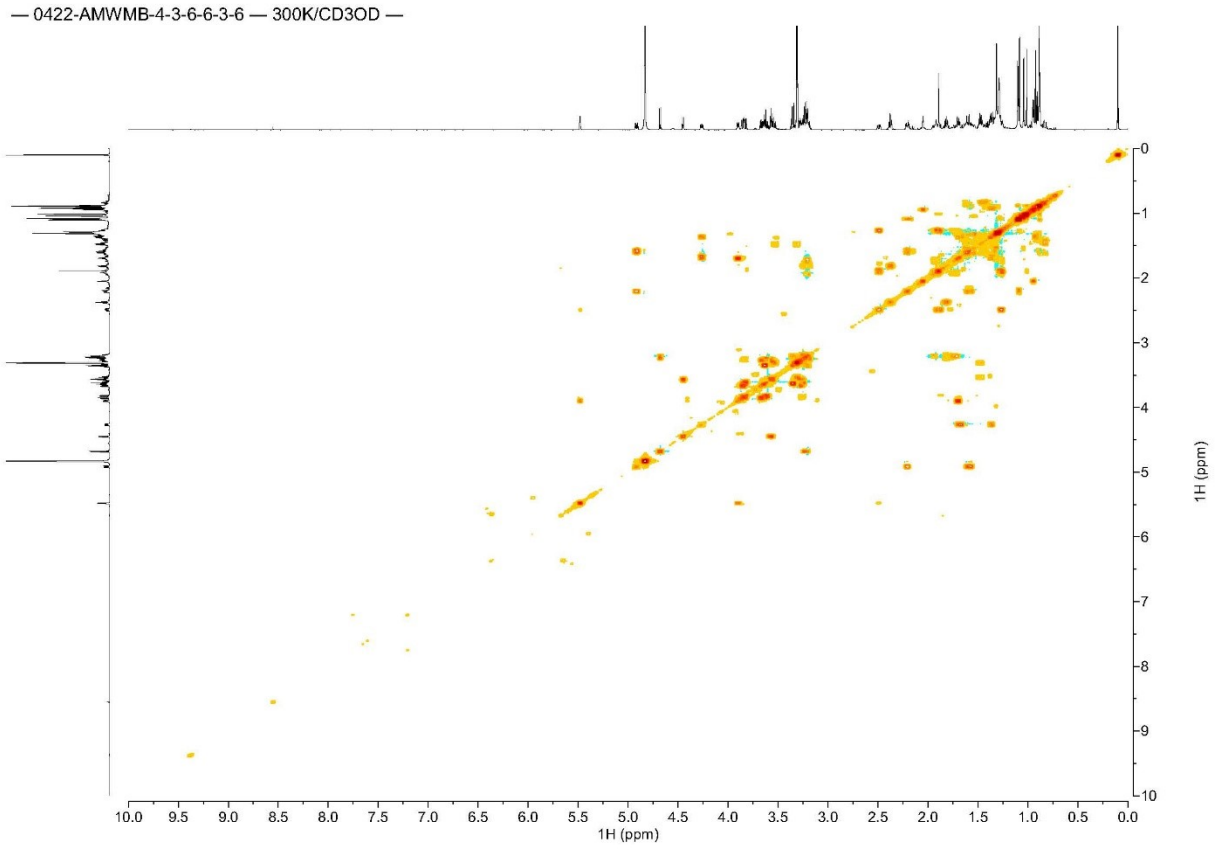

Fig. S29 COSY spectrum of **4**.

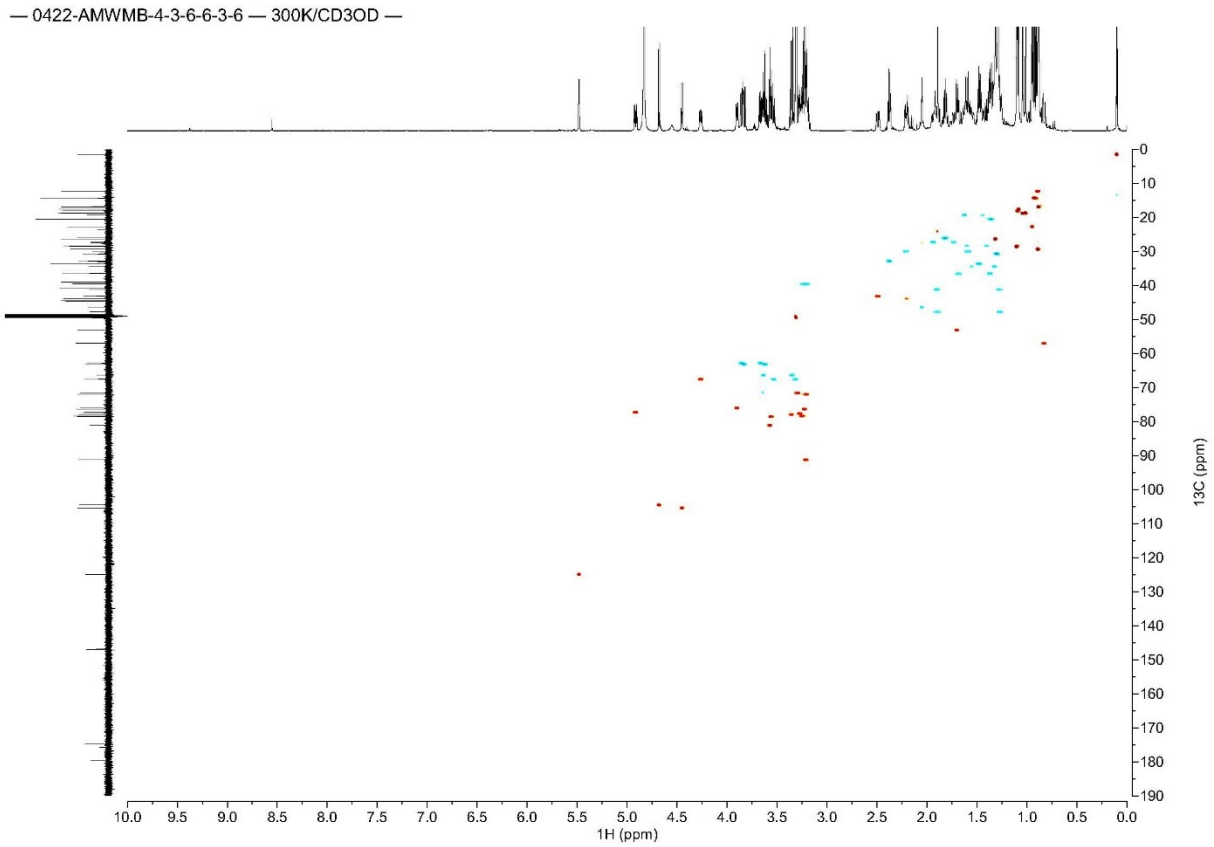

Fig. S30 HSQC spectrum of **4**.

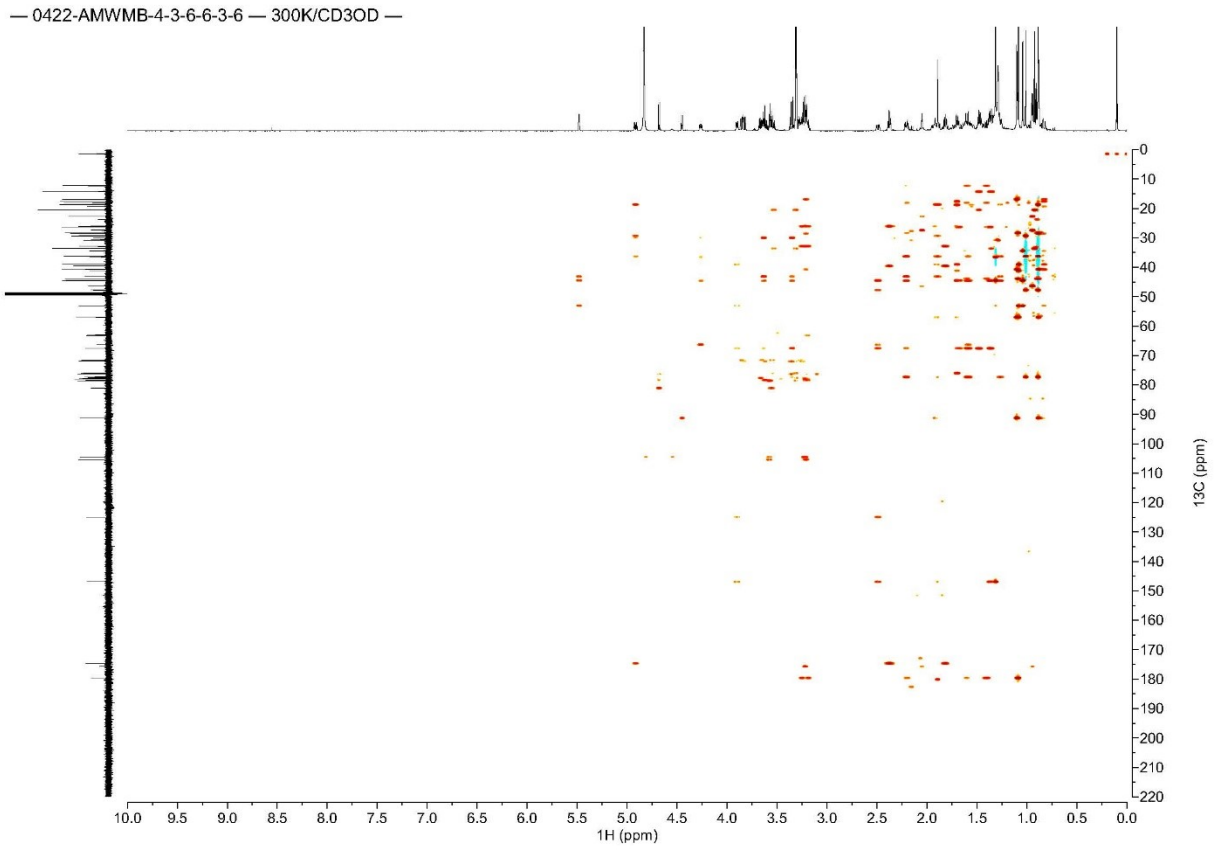

Fig. S31 HMBC spectrum of **4**.

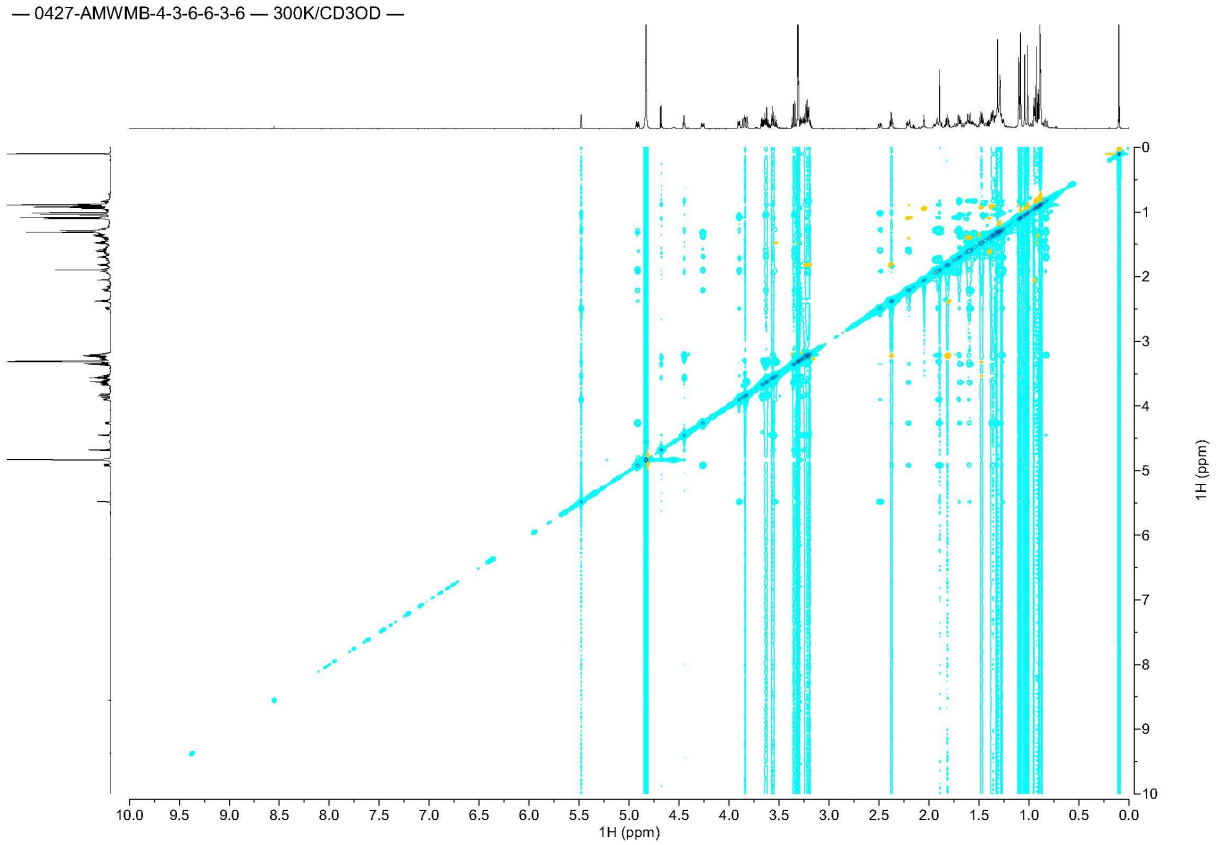

Fig. S32 NOESY spectrum of **4**.

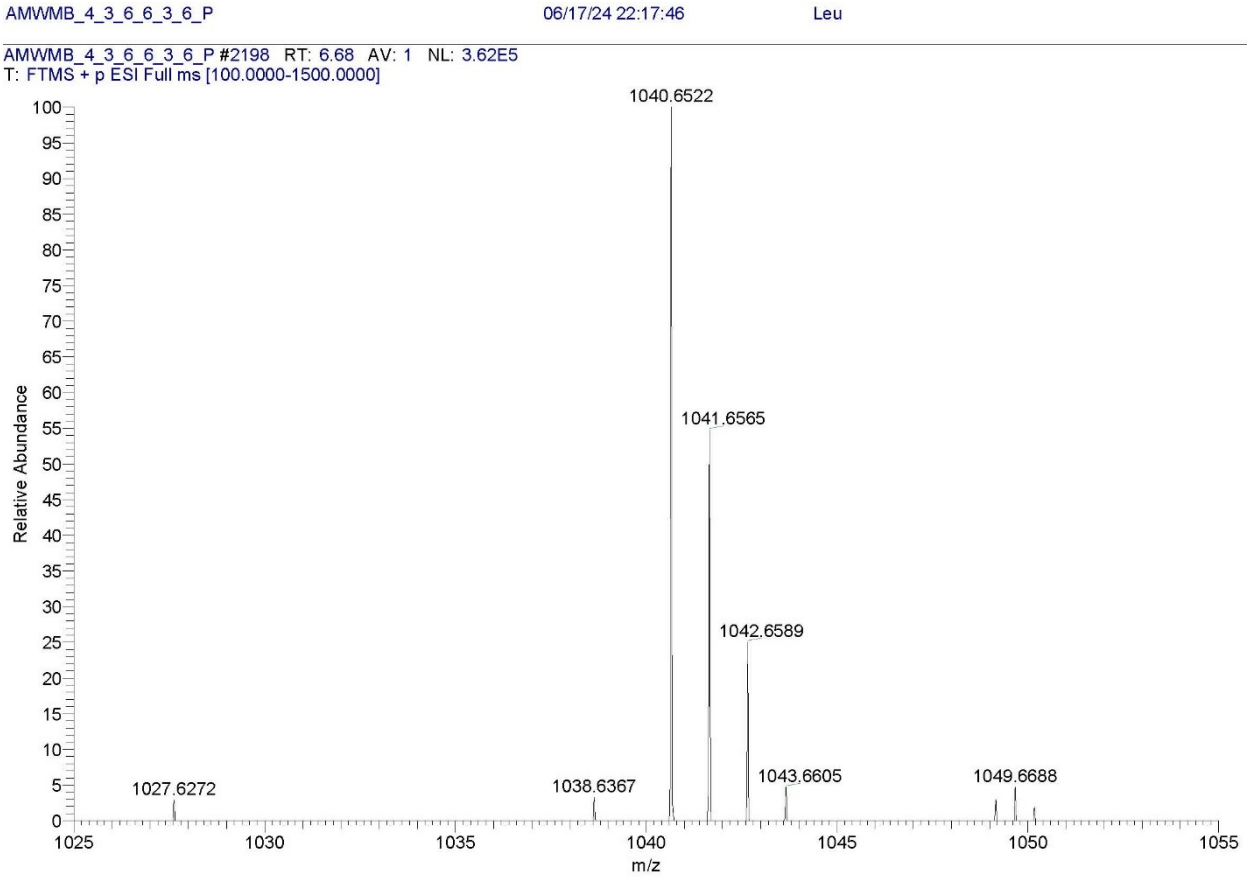

Fig. S33 HRESIMS spectrum of **4**.

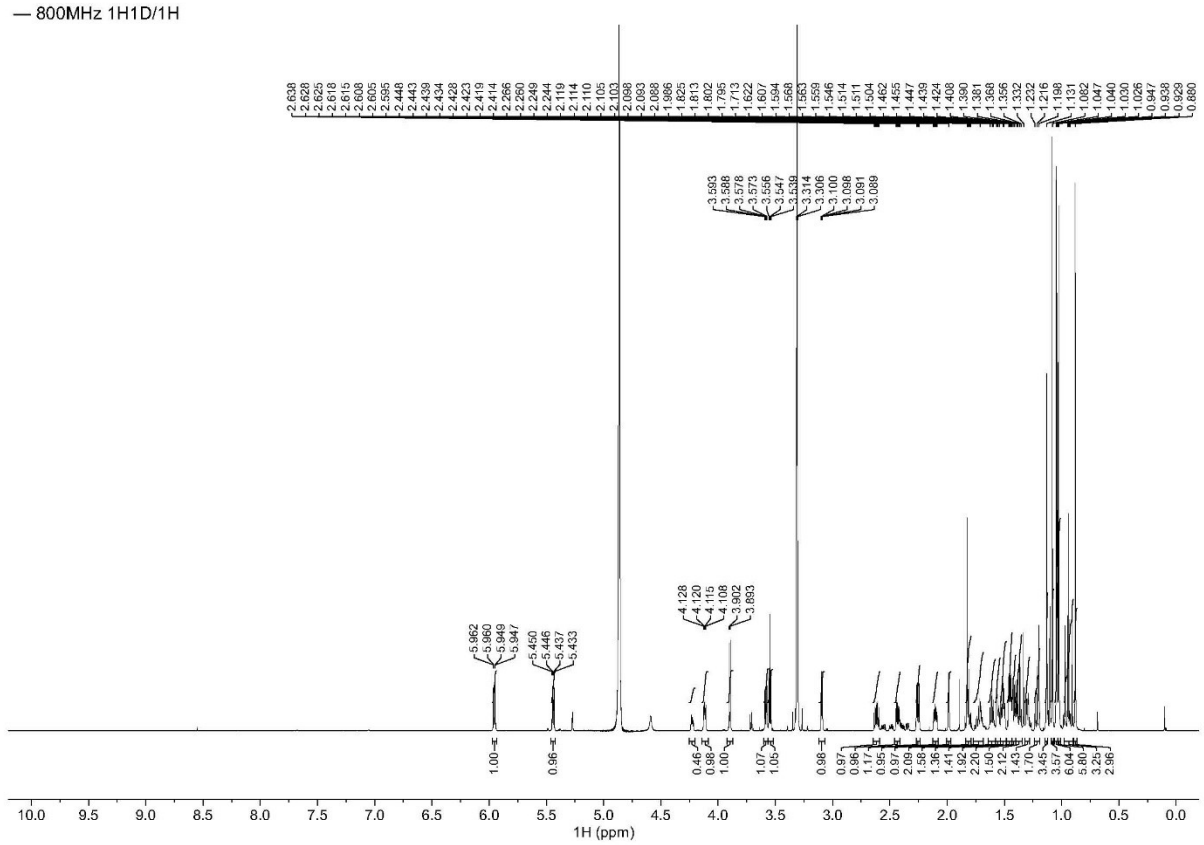

Fig. S34 ^{1}H NMR spectrum (800 MHz, CD_3OD) of **5**.

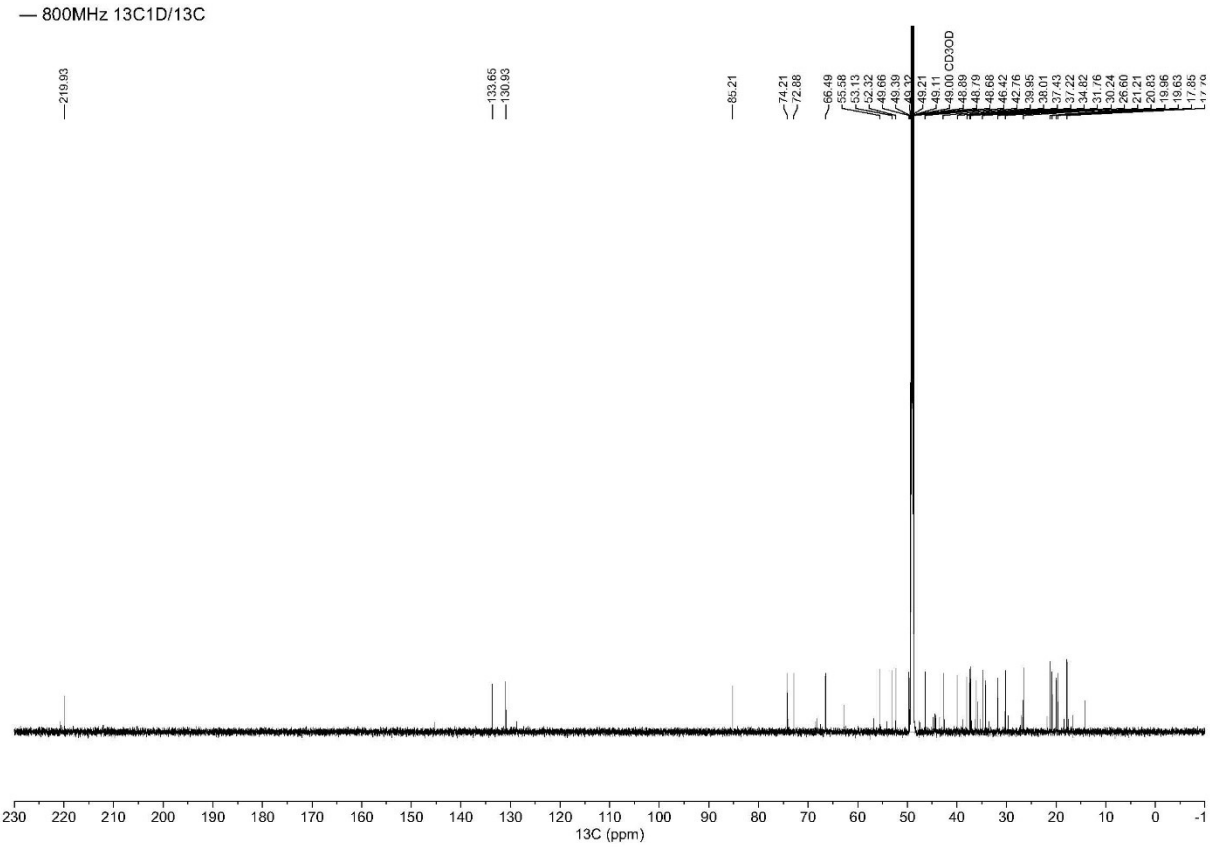

Fig. S35 ^{13}C NMR spectrum (200 MHz, CD_3OD) of **5**.

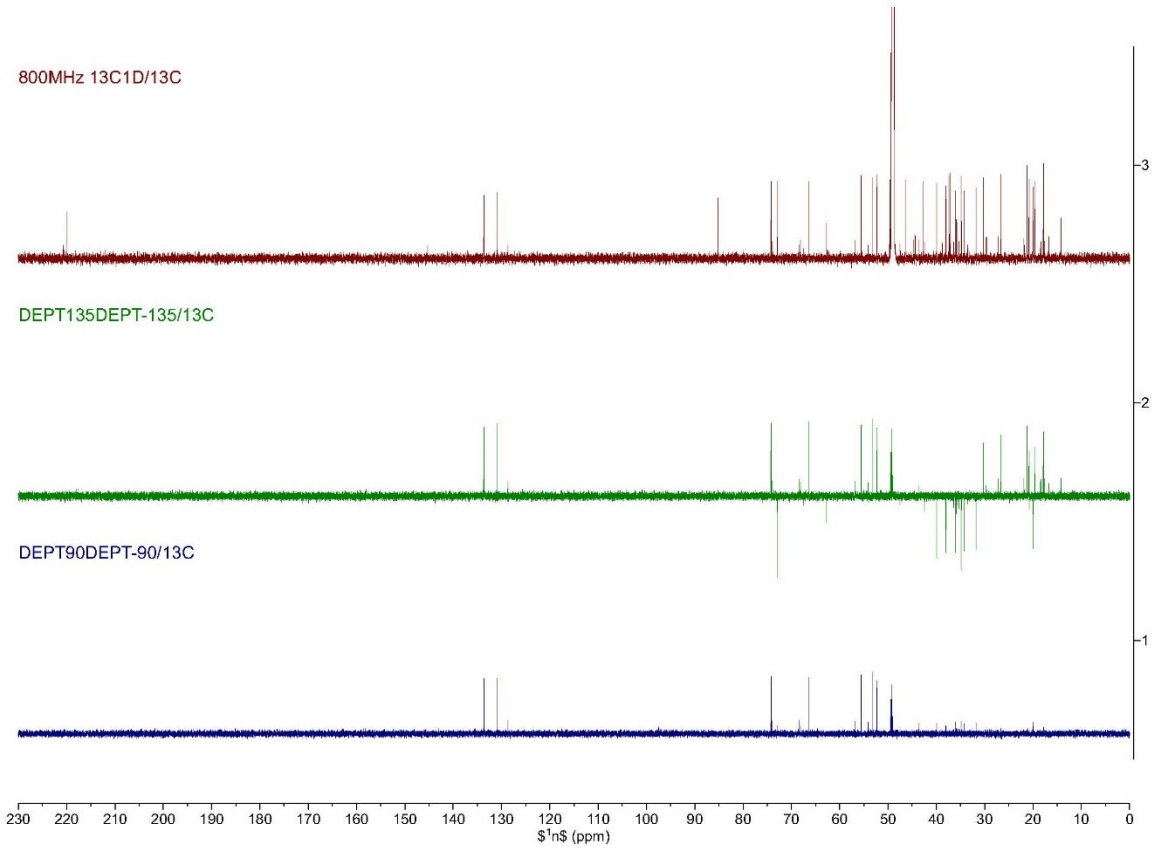

Fig. S36 DEPT spectrum of **5**.

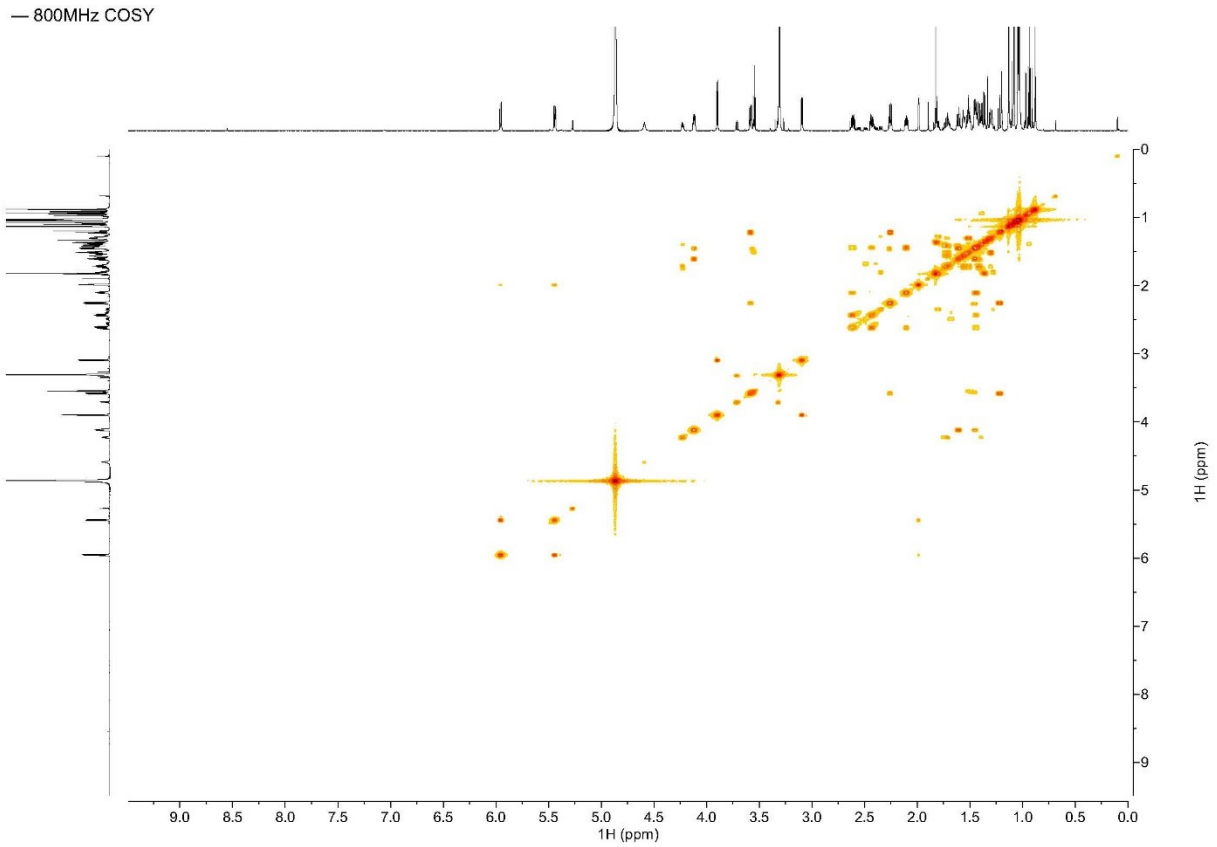

Fig. S37 COSY spectrum of **5**.

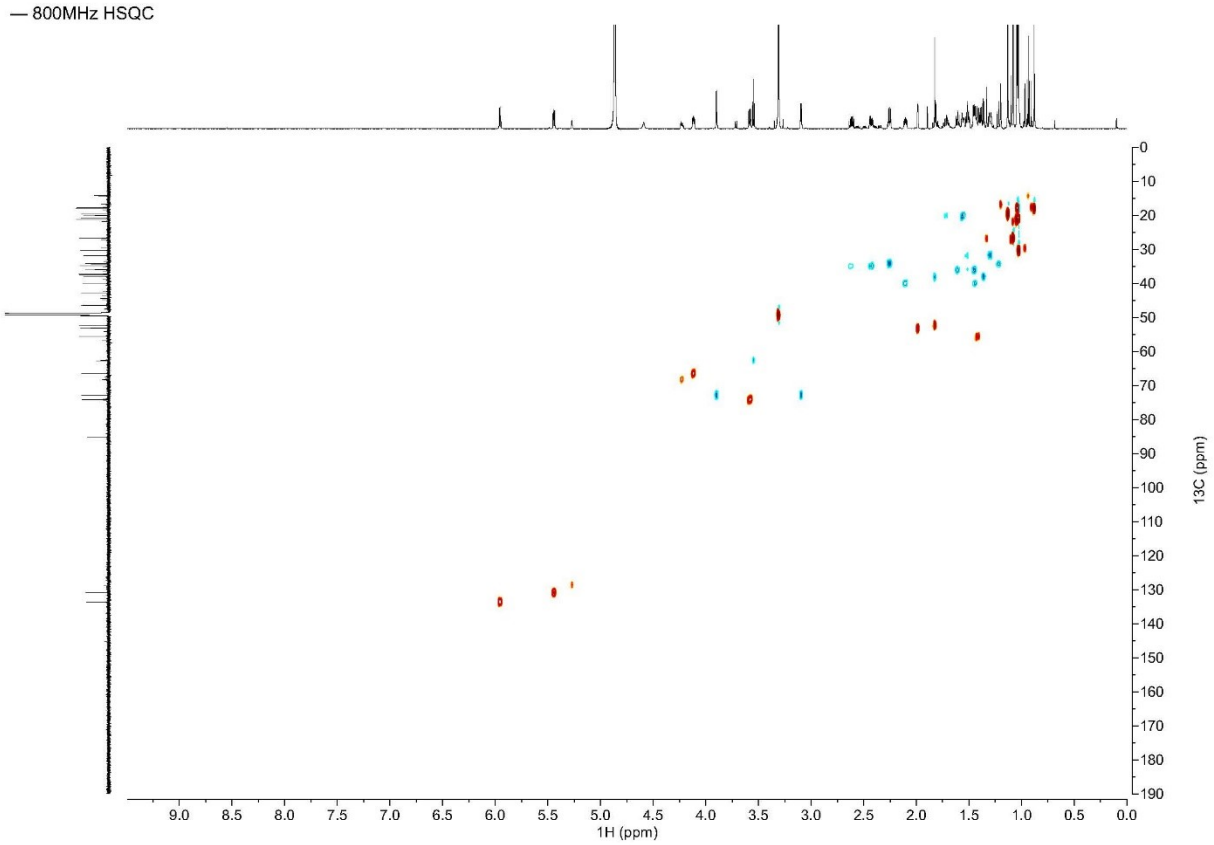

Fig. S38 HSQC spectrum of **5**.

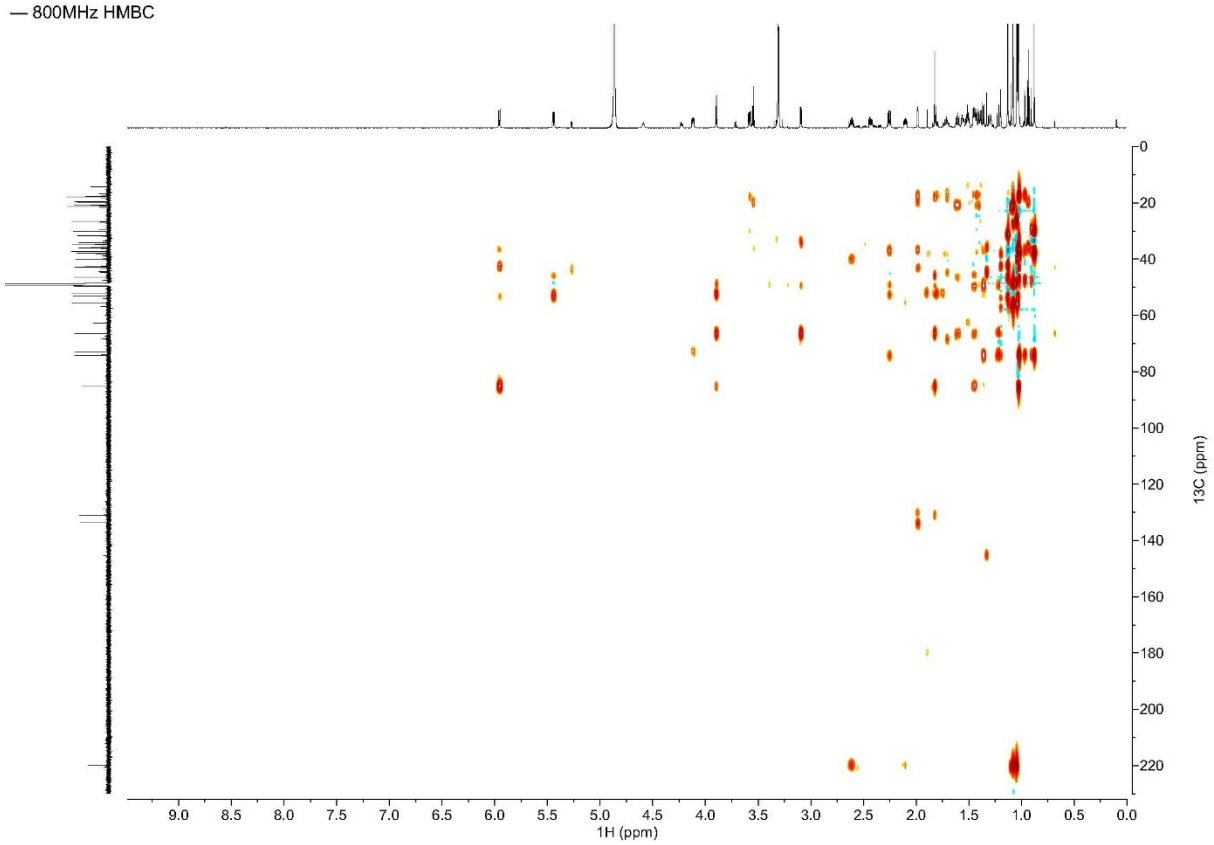

Fig. S39 HMBC spectrum of **5**.

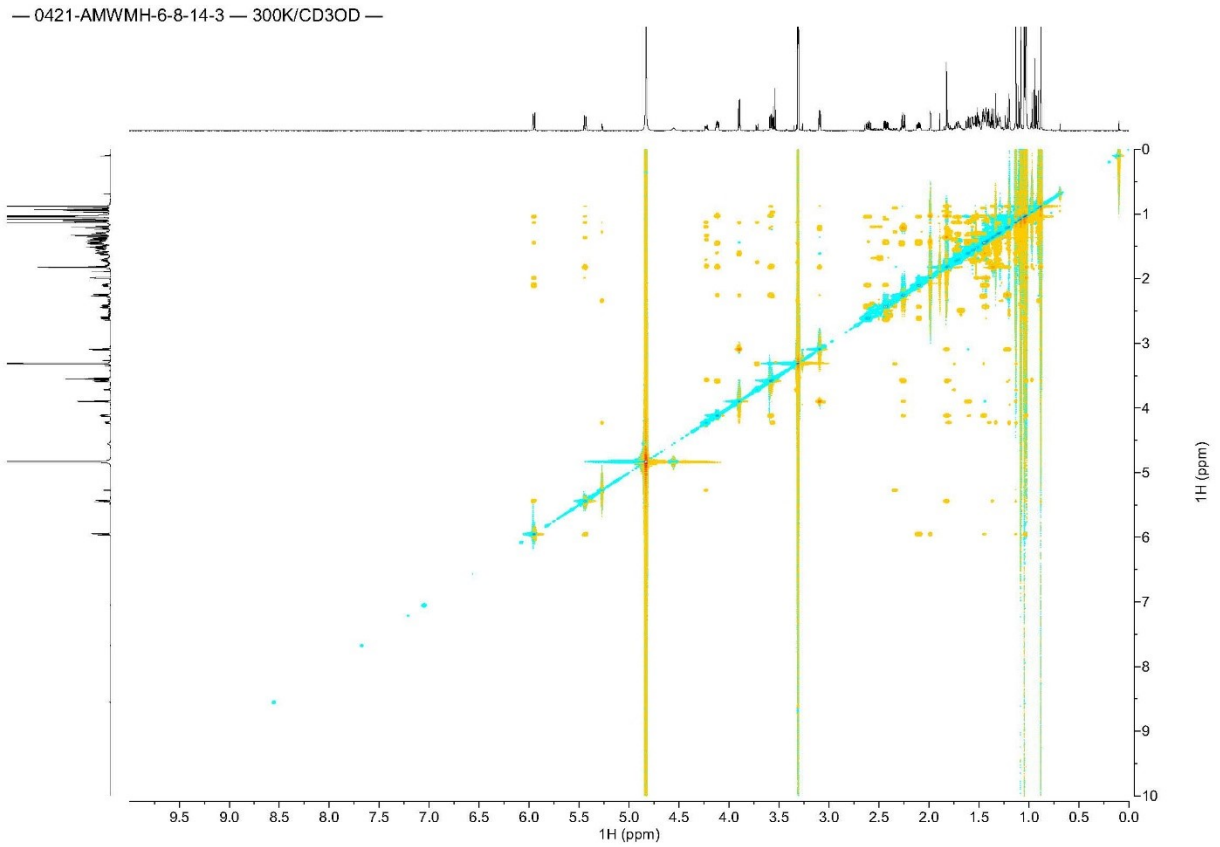

Fig. S40 NOESY spectrum (600 MHz, CD_3OD) of **5**.

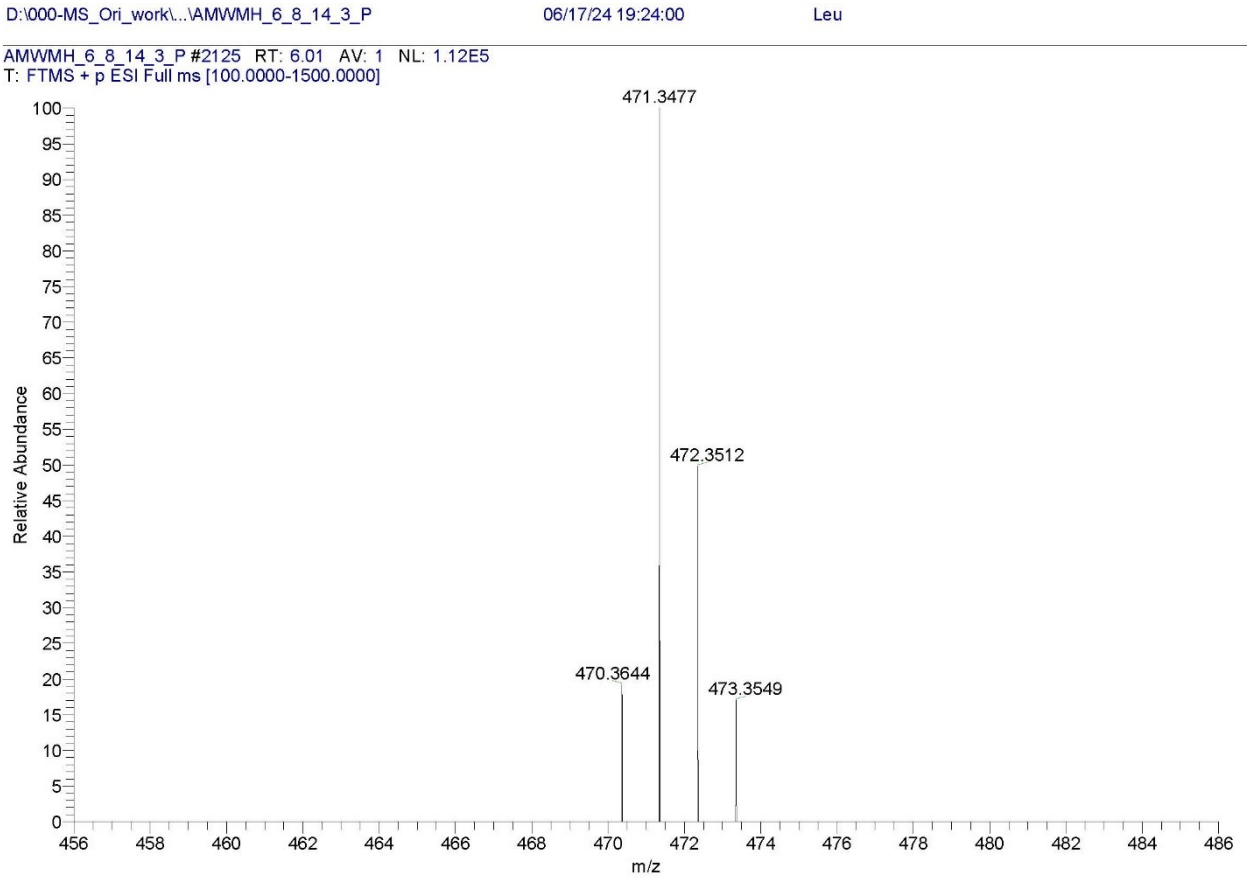

Fig. S41 HRESIMS spectrum of **5**.

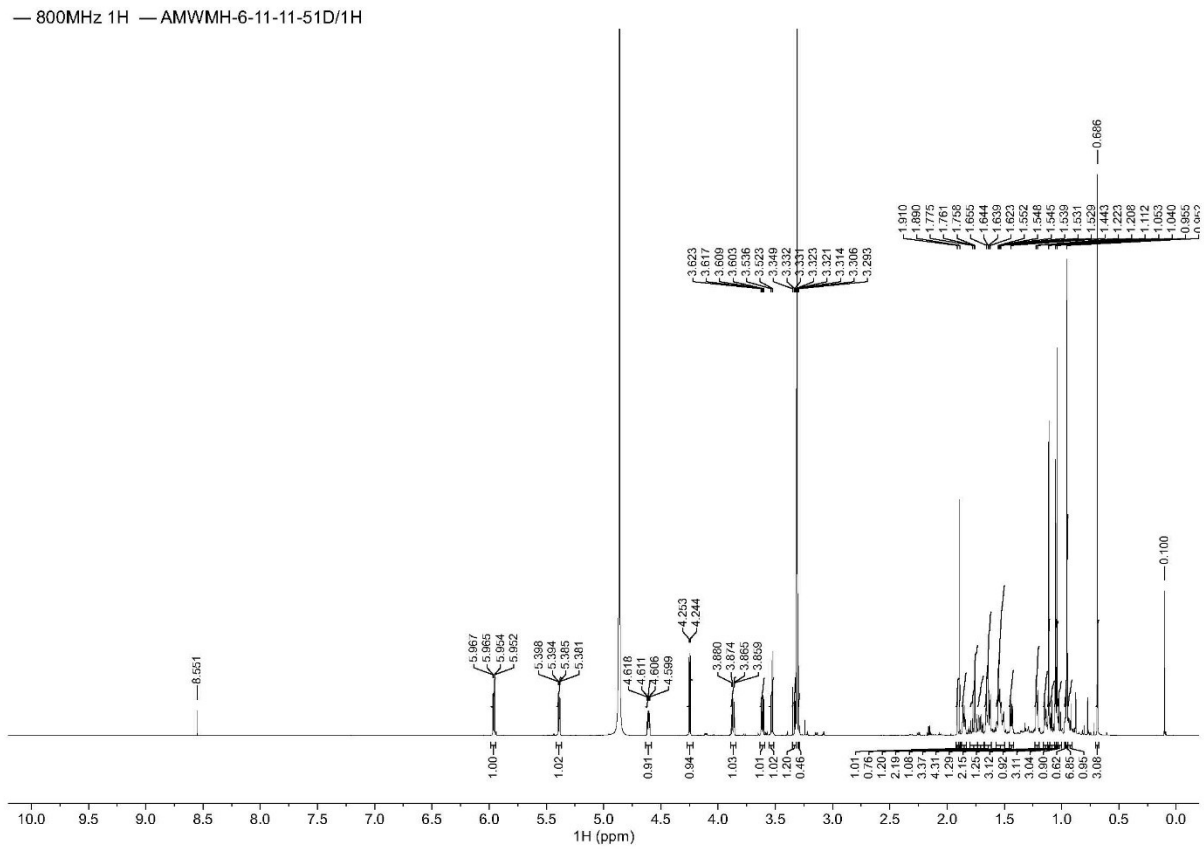

Fig. S42 ^{1}H NMR spectrum (800 MHz, CD_3OD) of **6**.

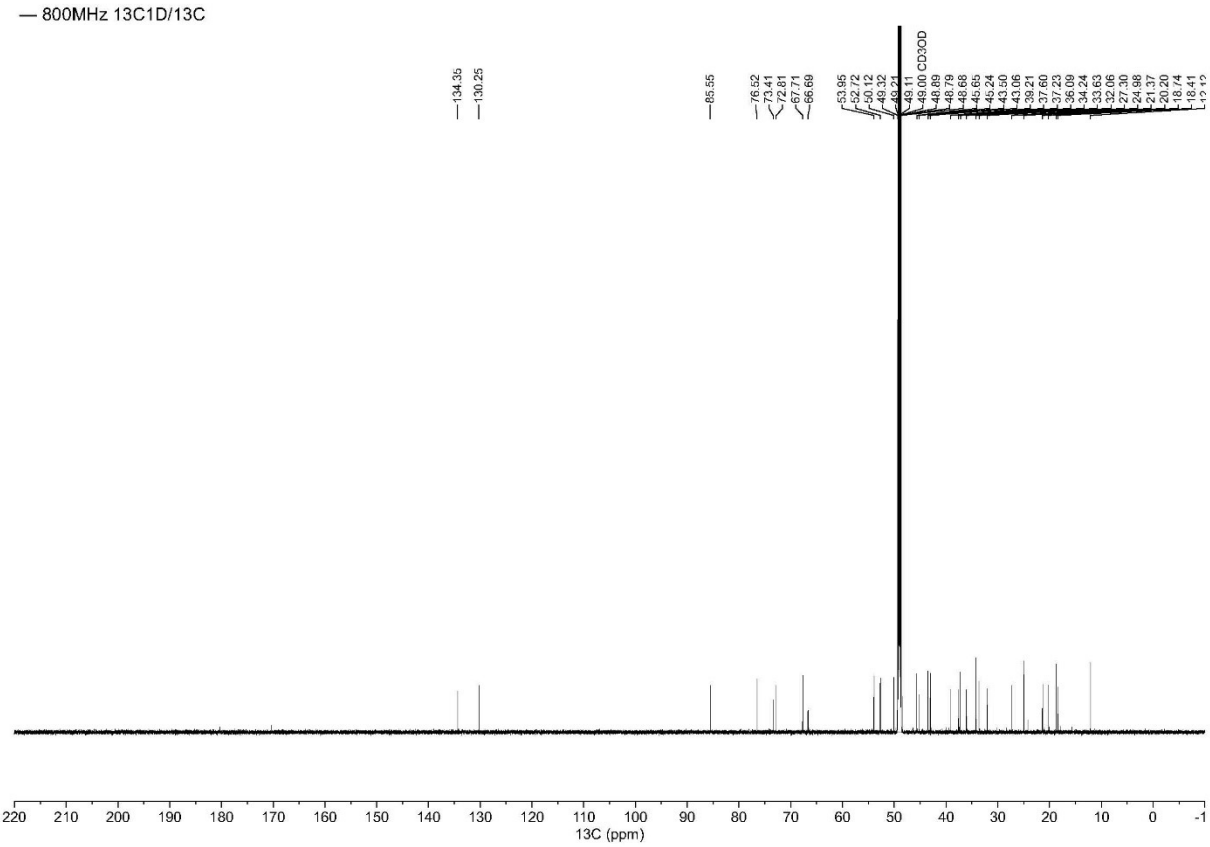

Fig. S43 ^{13}C NMR spectrum (200 MHz, CD_3OD) of **6**.

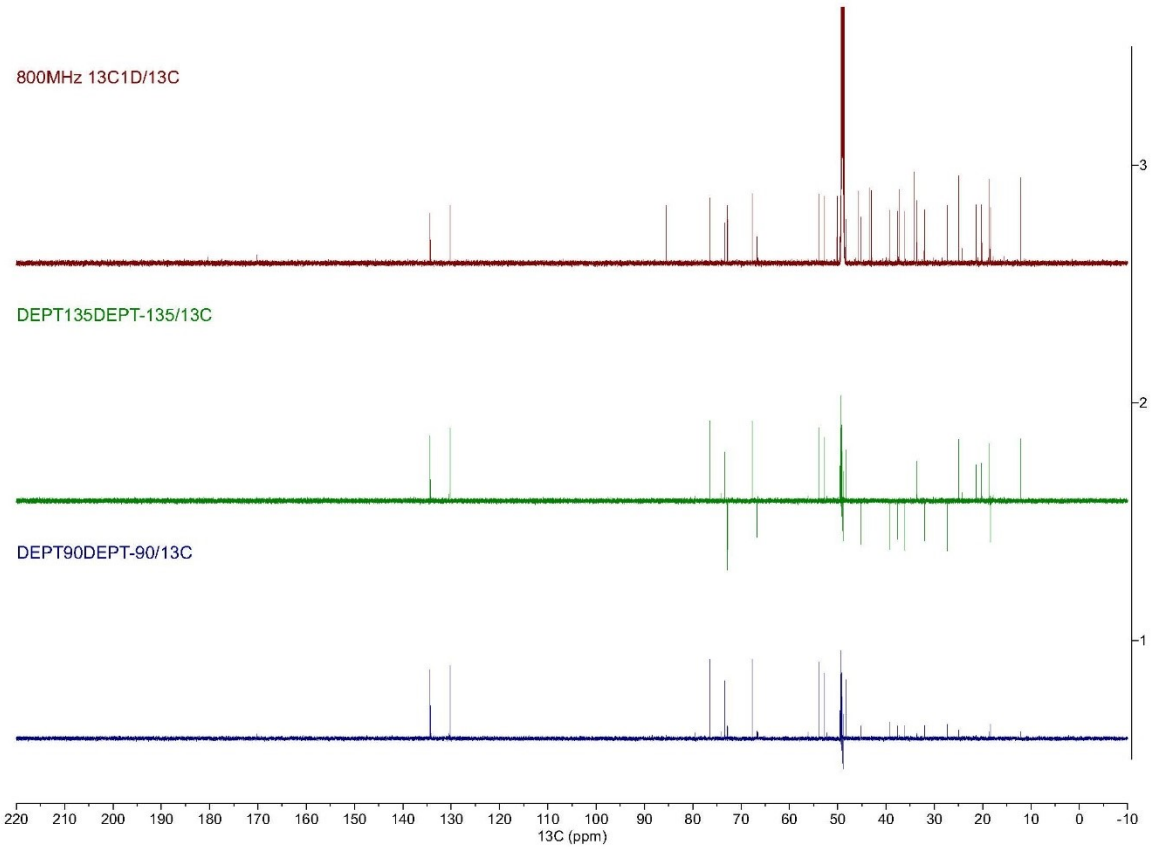

Fig. S44 DEPT spectrum of **6**.

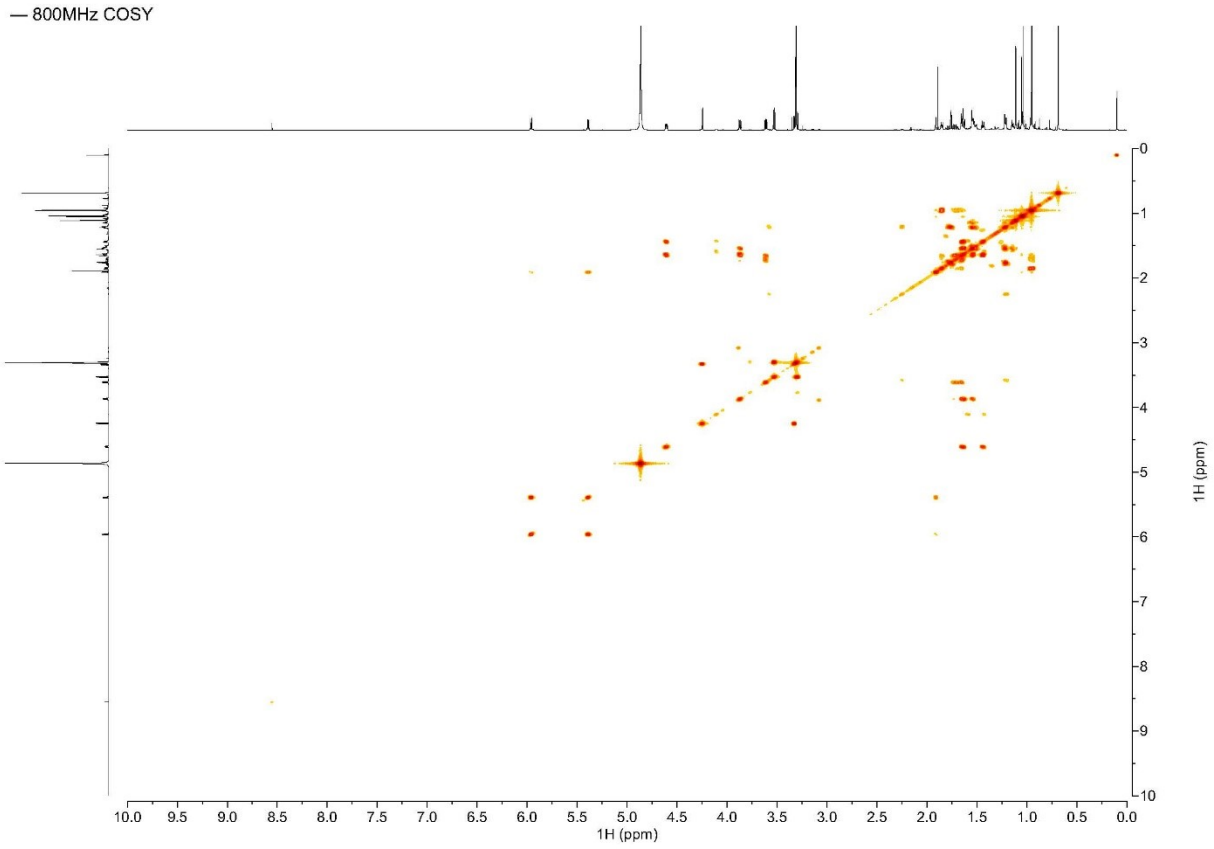

Fig. S45 COSY spectrum of **6**.

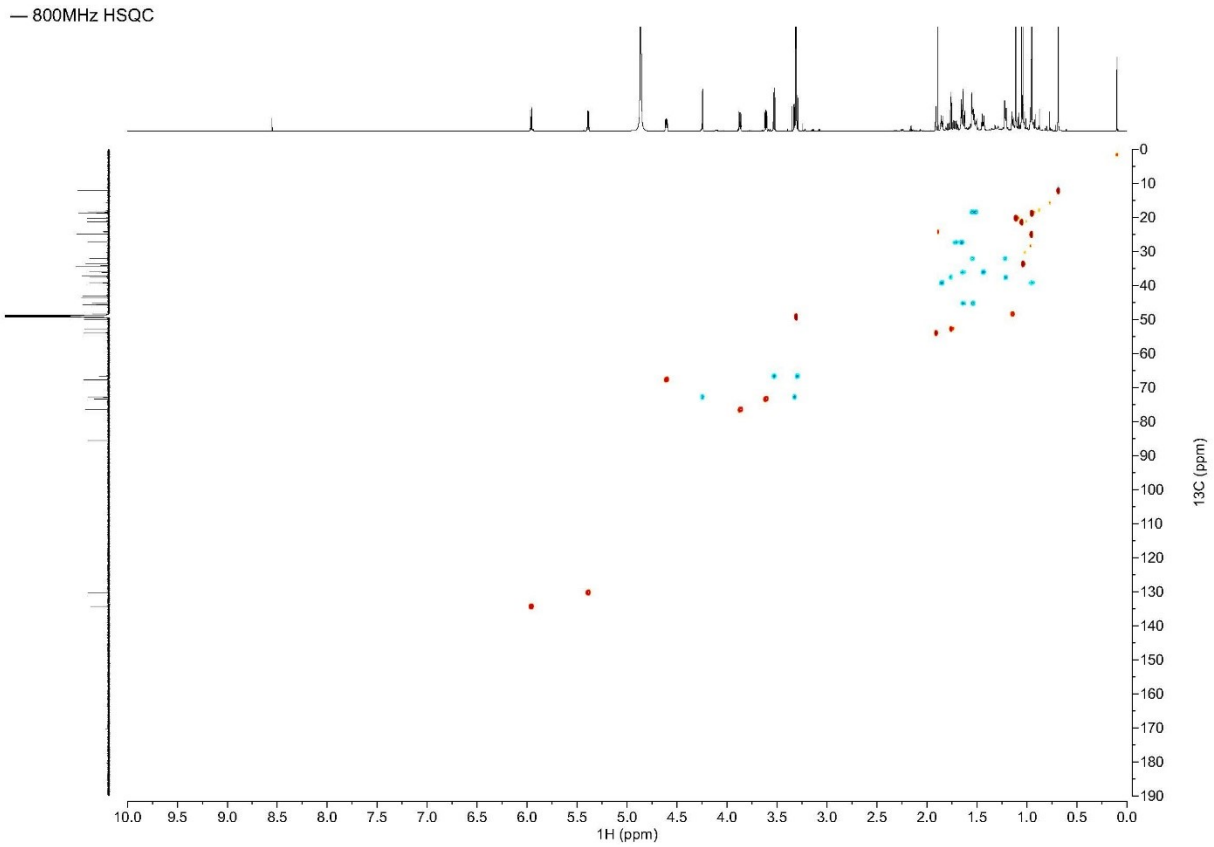

Fig. S46 HSQC spectrum of **6**.

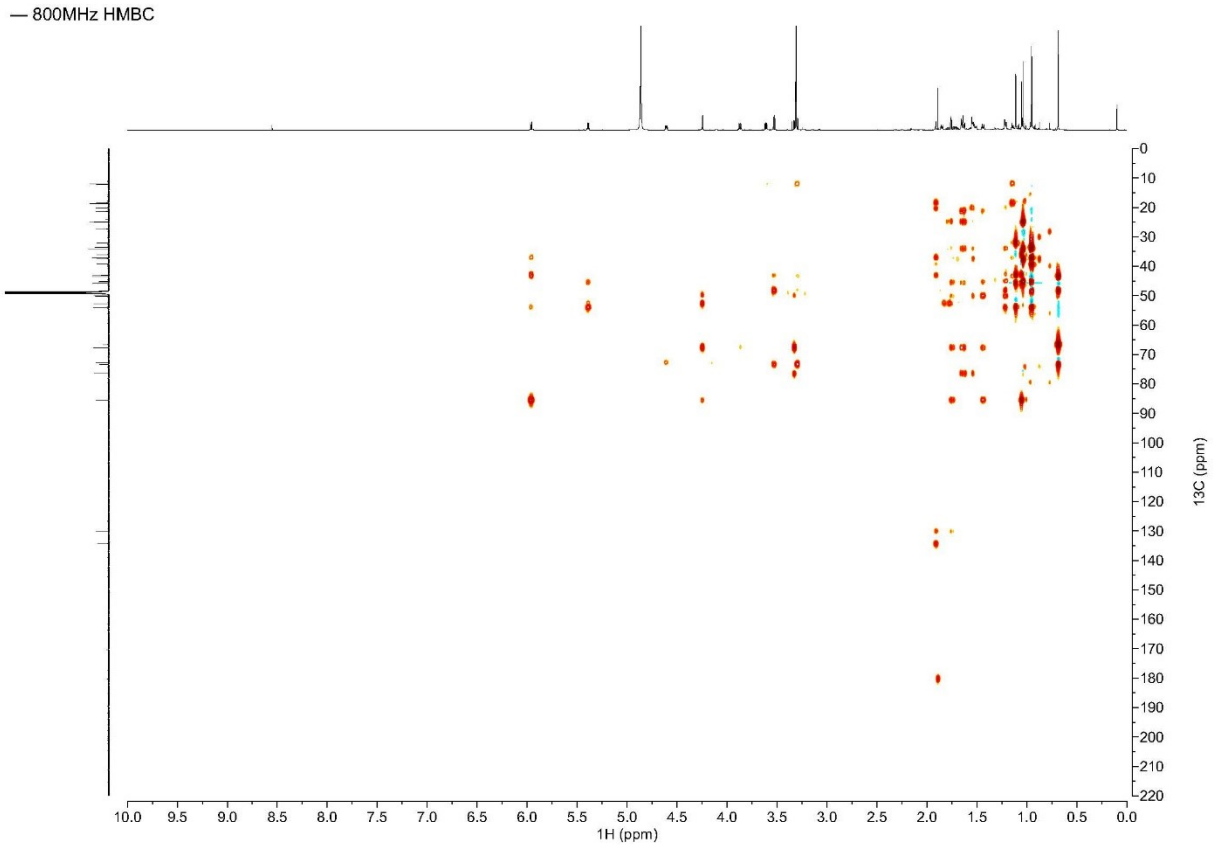

Fig. S47 HMBC spectrum of **6**.

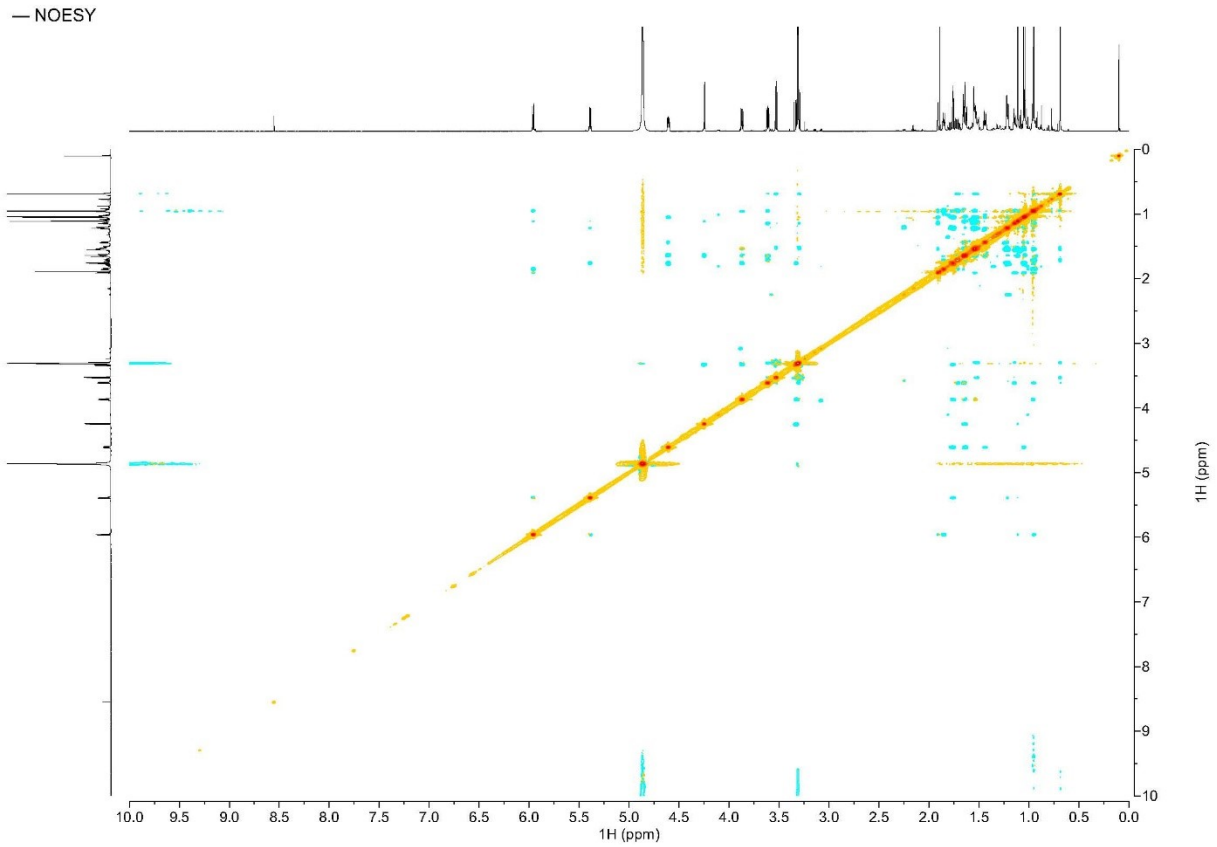

Fig. S48 NOESY spectrum of **6**.

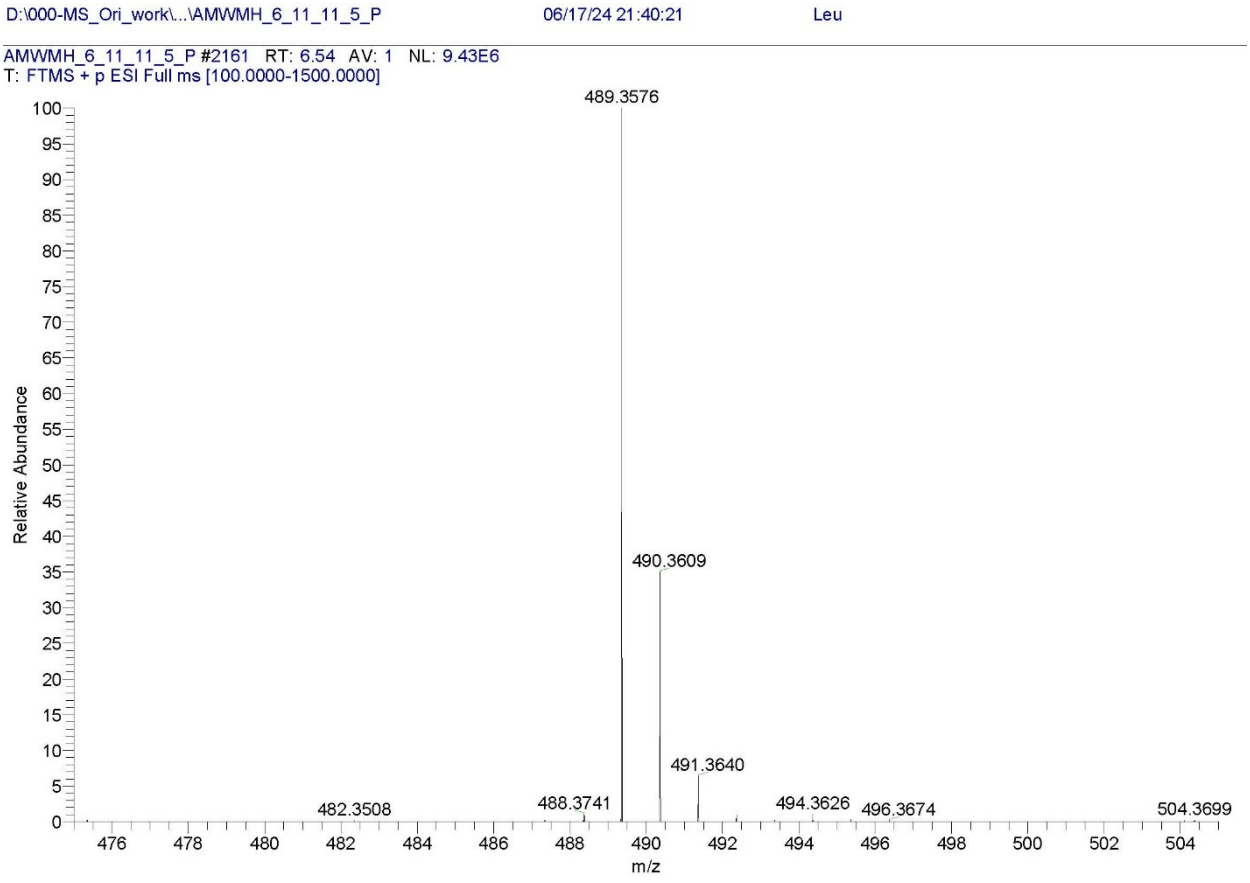

Fig. S49 HRESIMS spectrum of **6**.

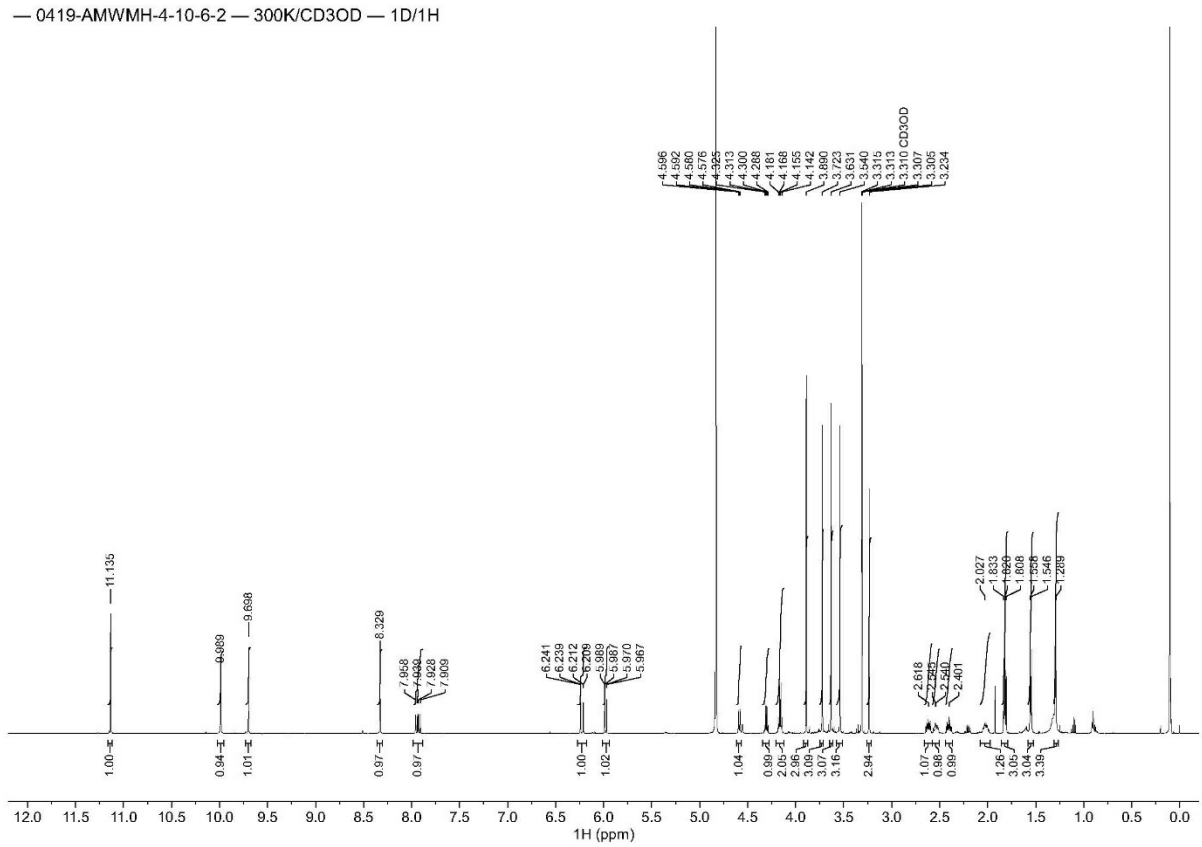

Fig. S50 ^{1}H NMR spectrum (600 MHz, CD_3OD) of **7**.

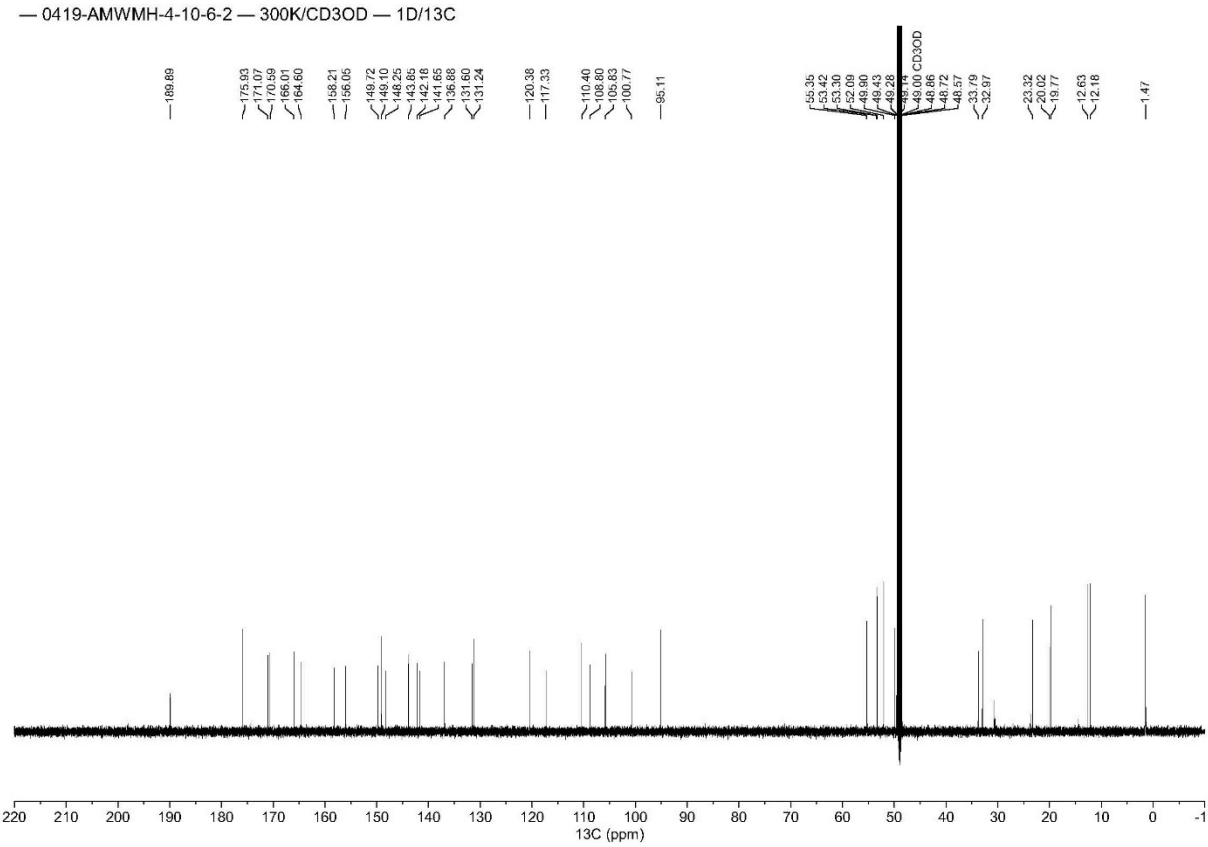

Fig. S51 ^{13}C NMR spectrum (150 MHz, CD_3OD) of **7**.

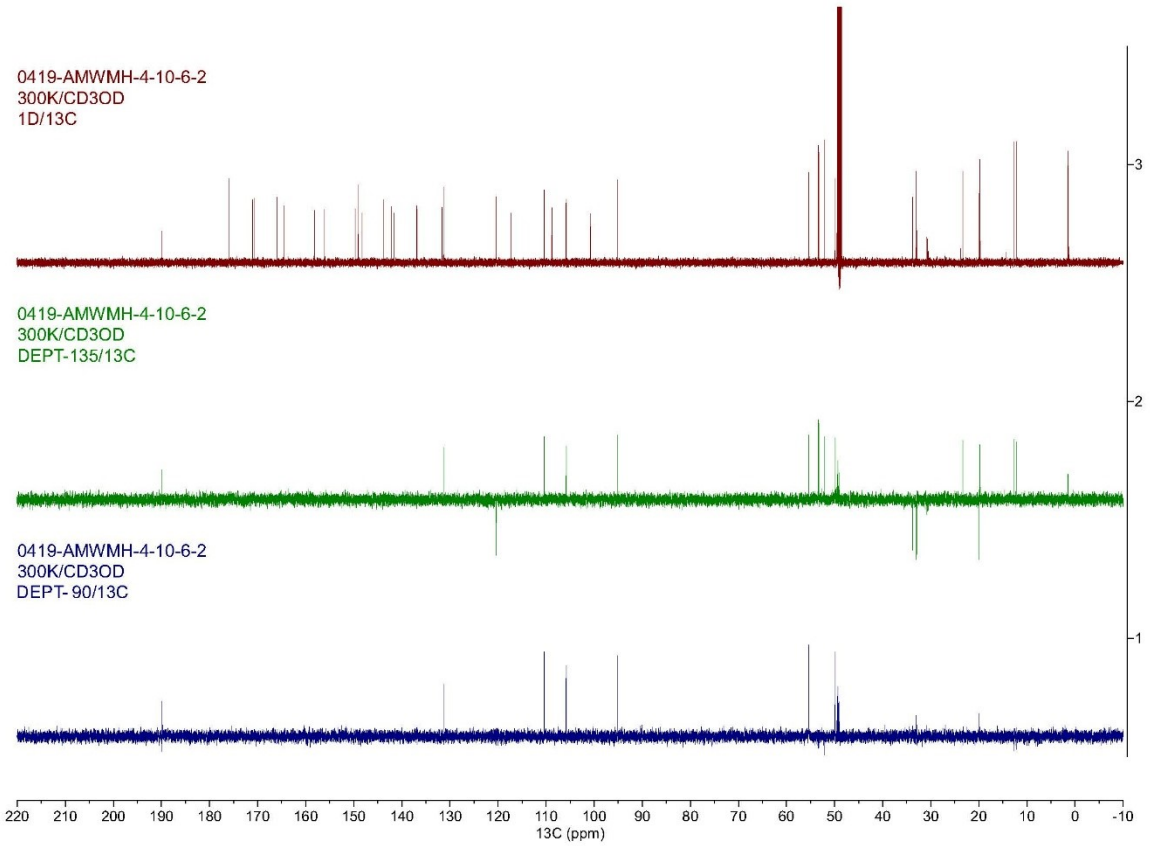

Fig. S52 DEPT spectrum of **7**.

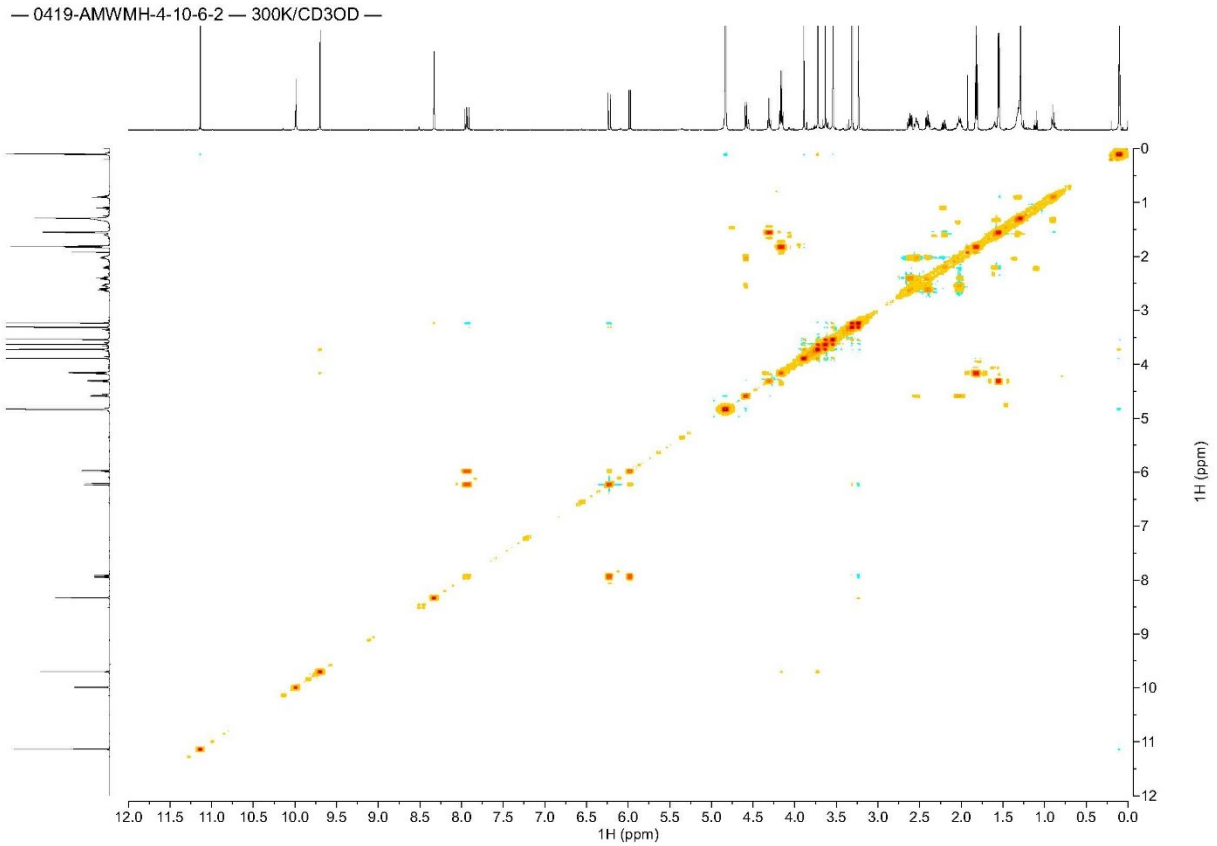

Fig. S53 COSY spectrum of **7**.

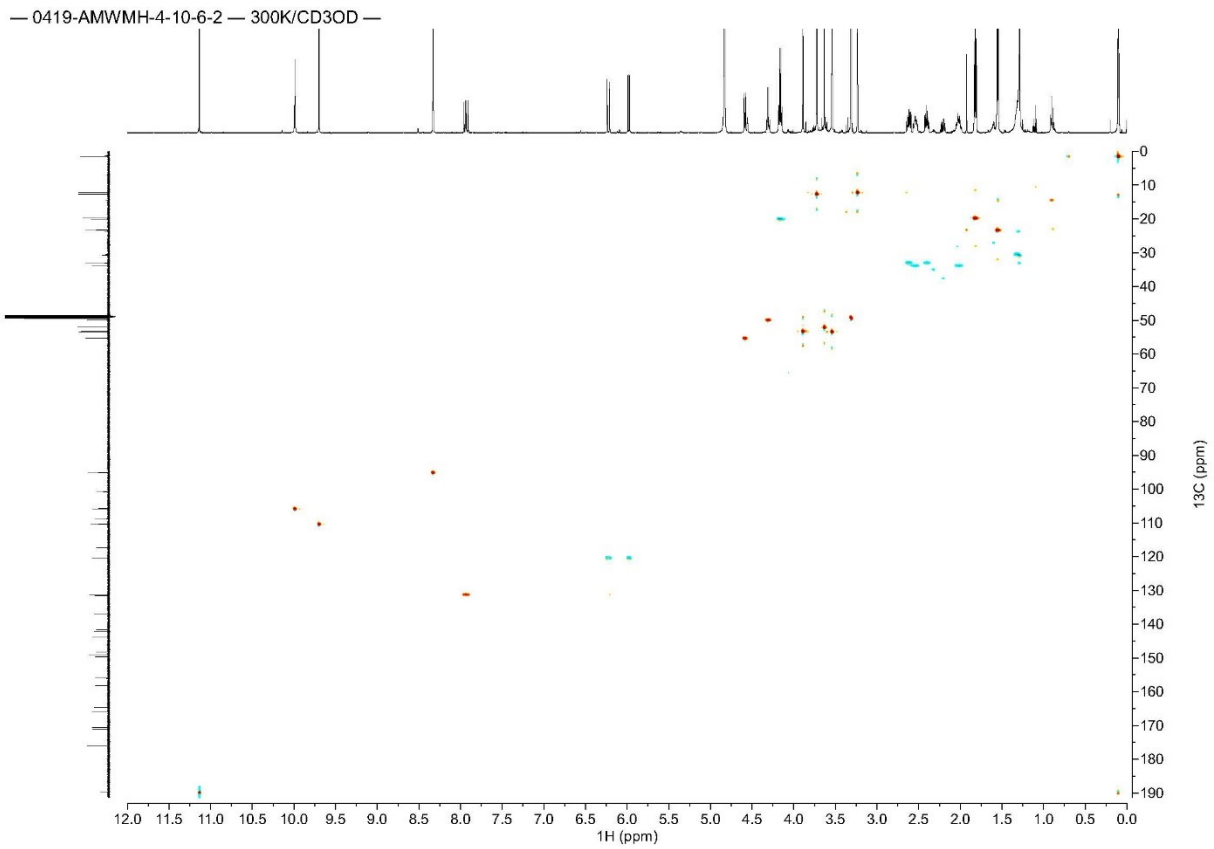

Fig. S54 HSQC spectrum of **7**.

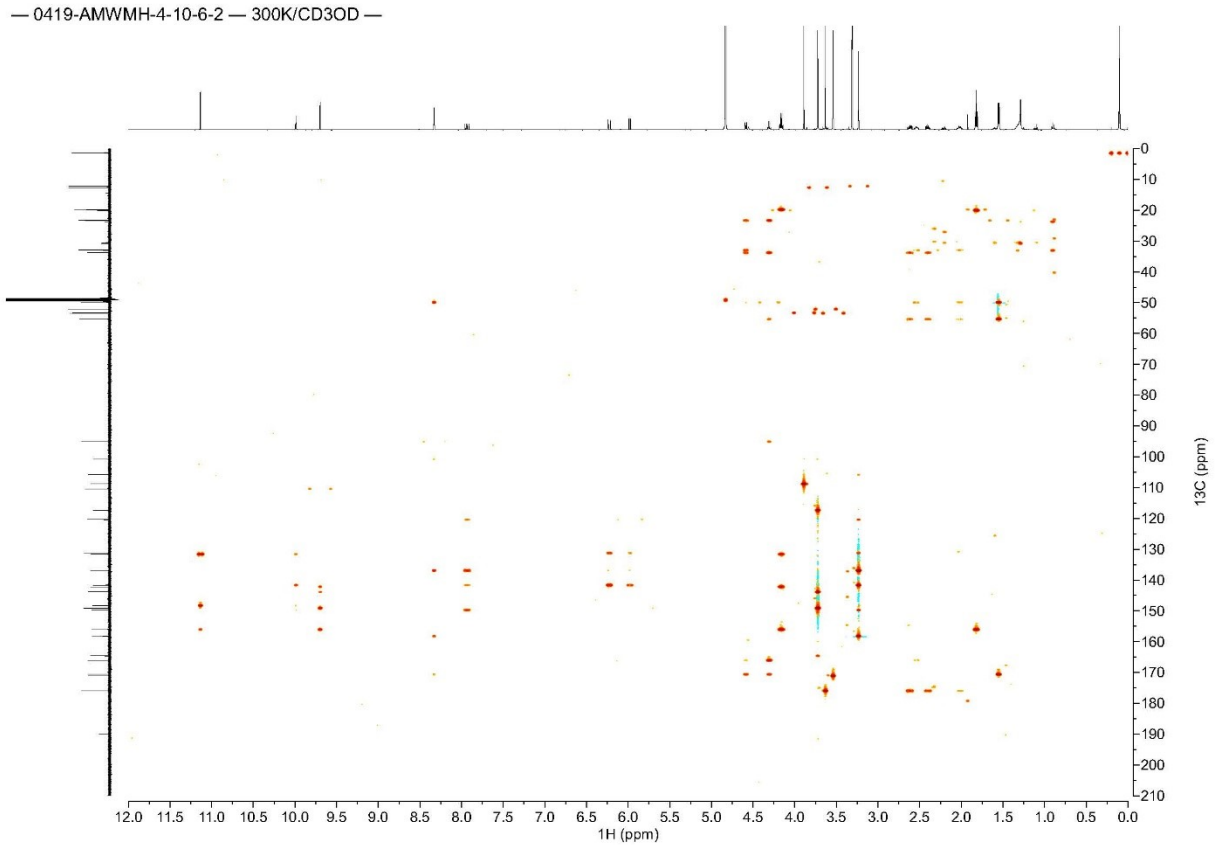

Fig. S55 HMBC spectrum of **7**.

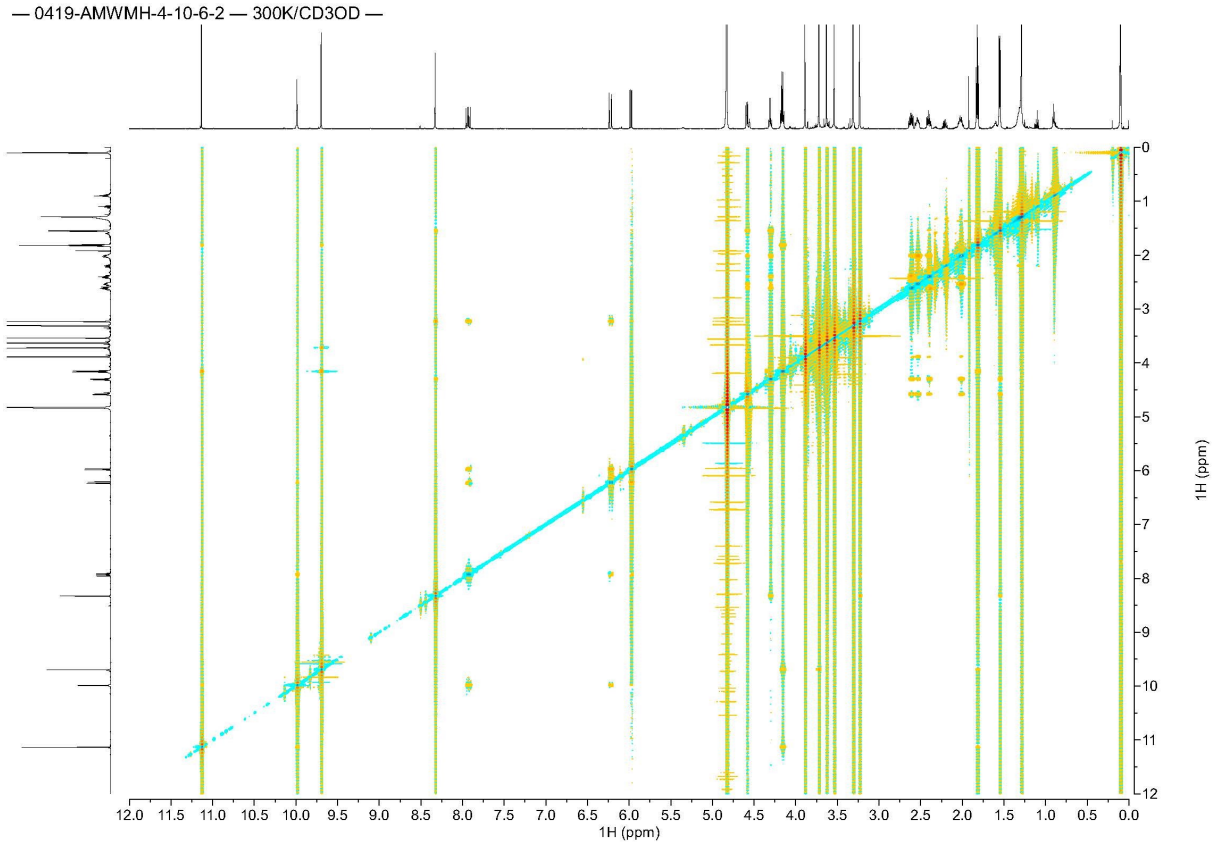

Fig. S56 NOESY spectrum of **7**.

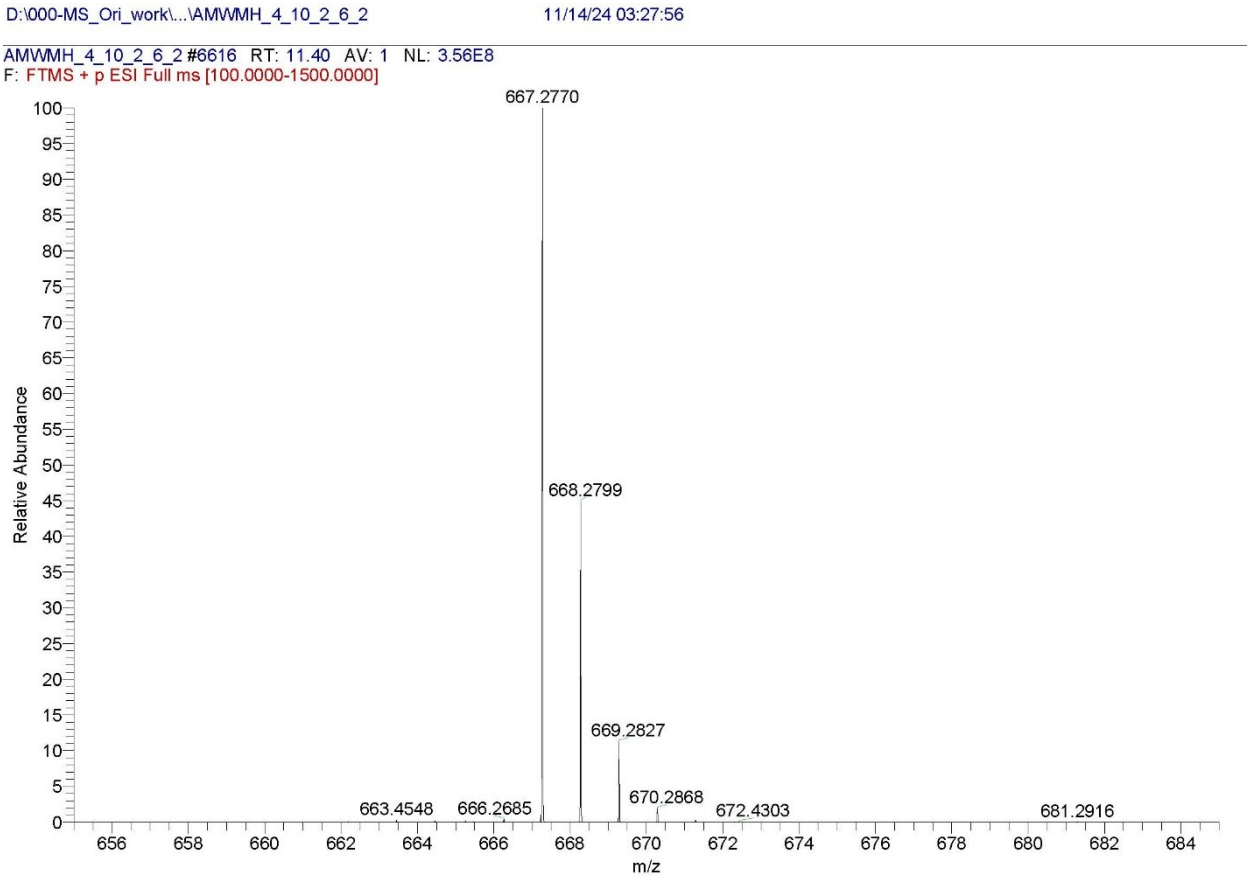

Fig. S57 HRESIMS spectrum of **7**.

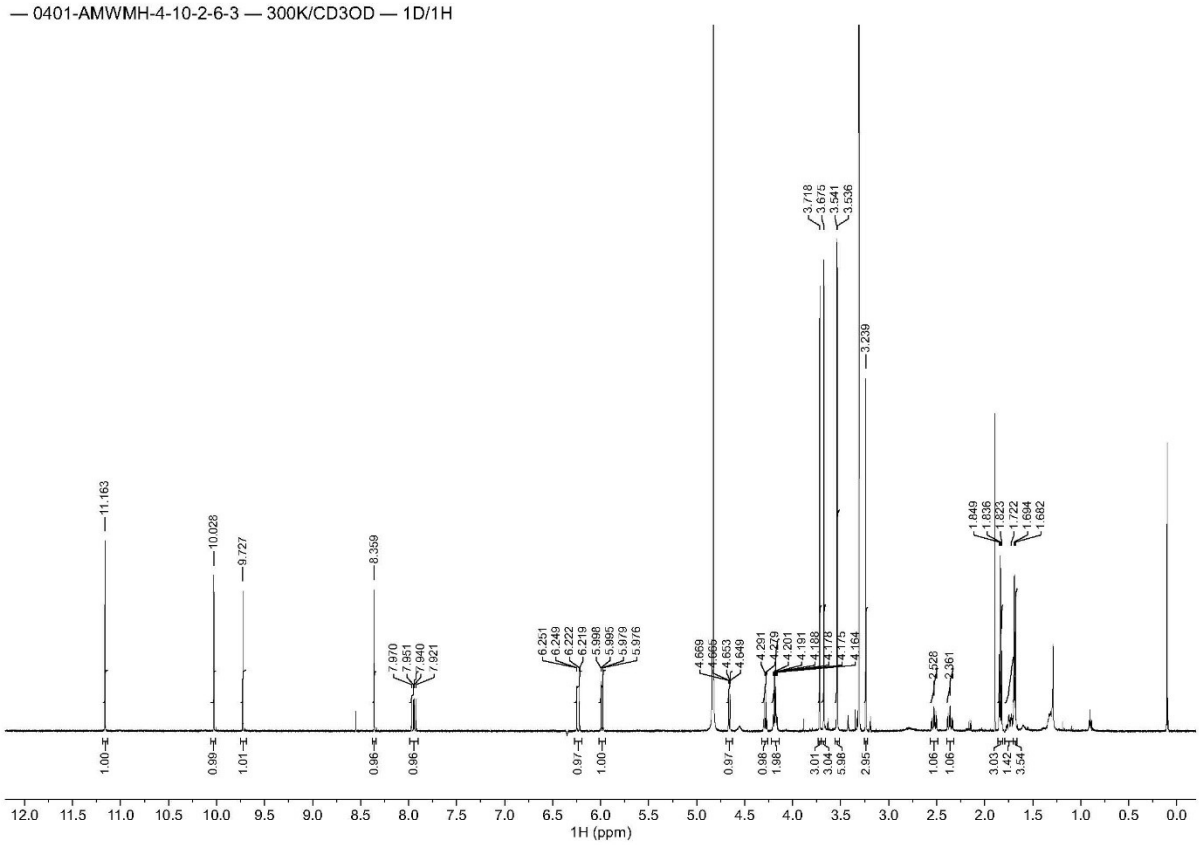

Fig. S58 ^{1}H NMR spectrum (600 MHz, CD_3OD) of **8**.

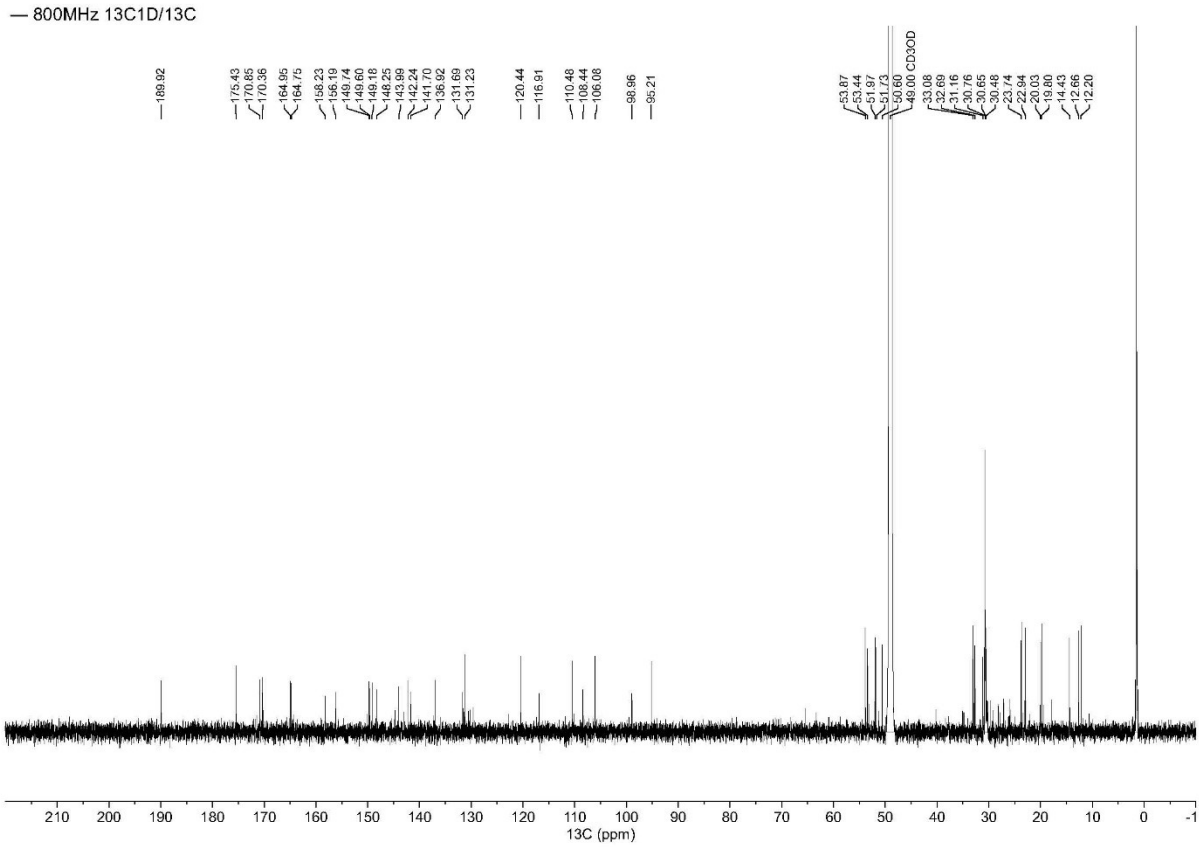

Fig. S59 ^{13}C NMR spectrum (200 MHz, CD_3OD) of **8**.

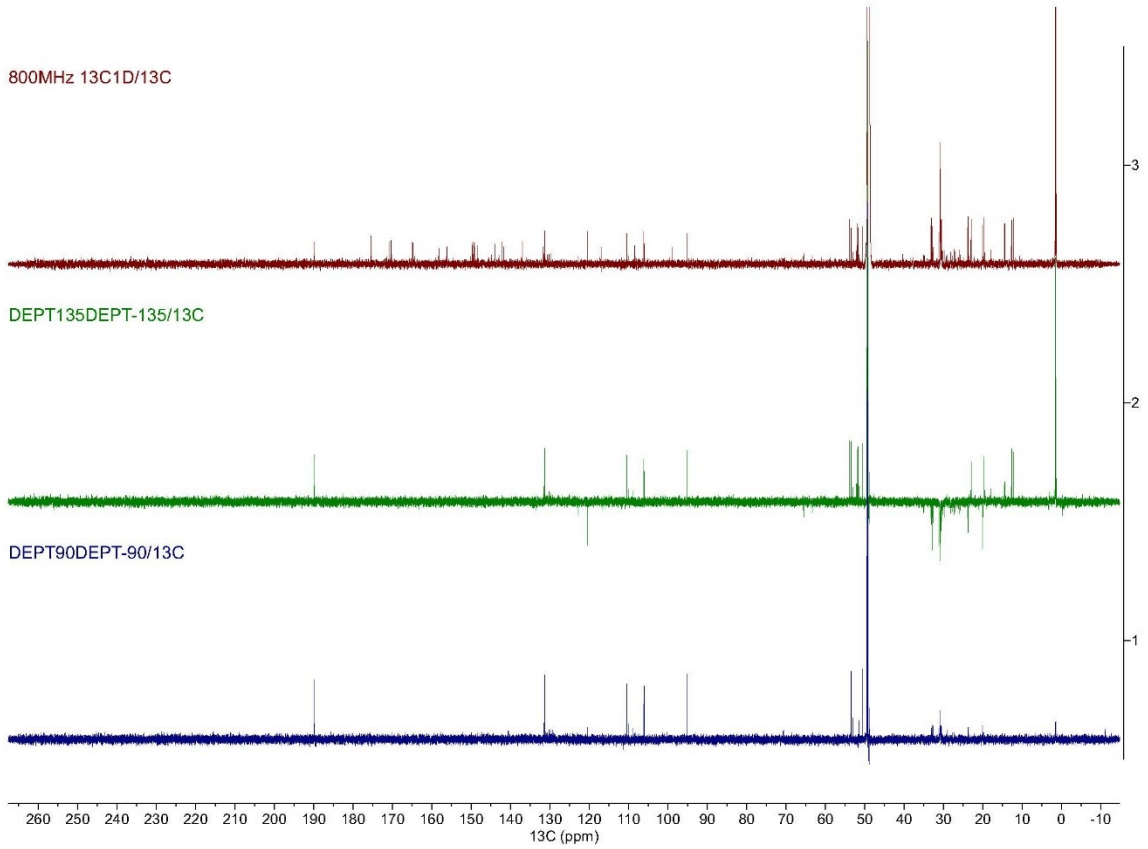

Fig. S60 DEPT spectrum of **8**.

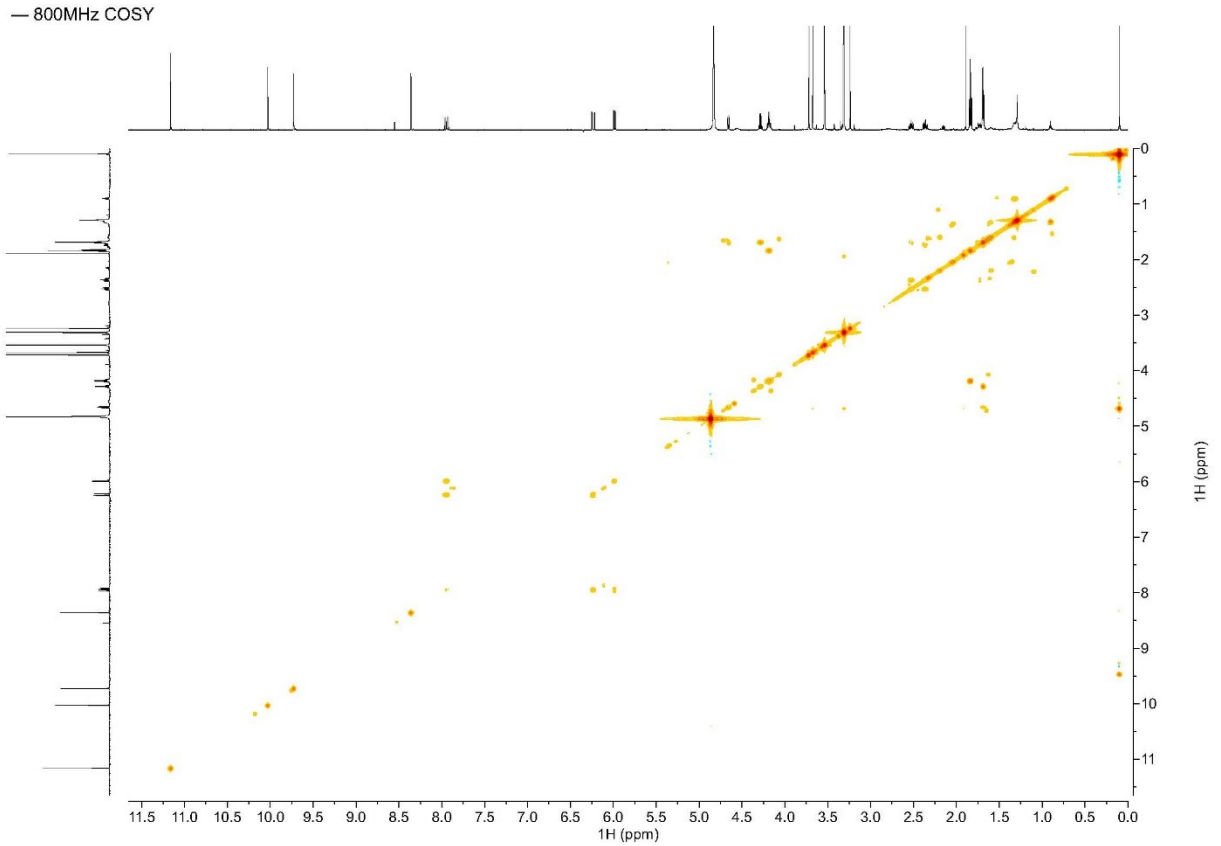

Fig. S61 COSY spectrum of **8**.

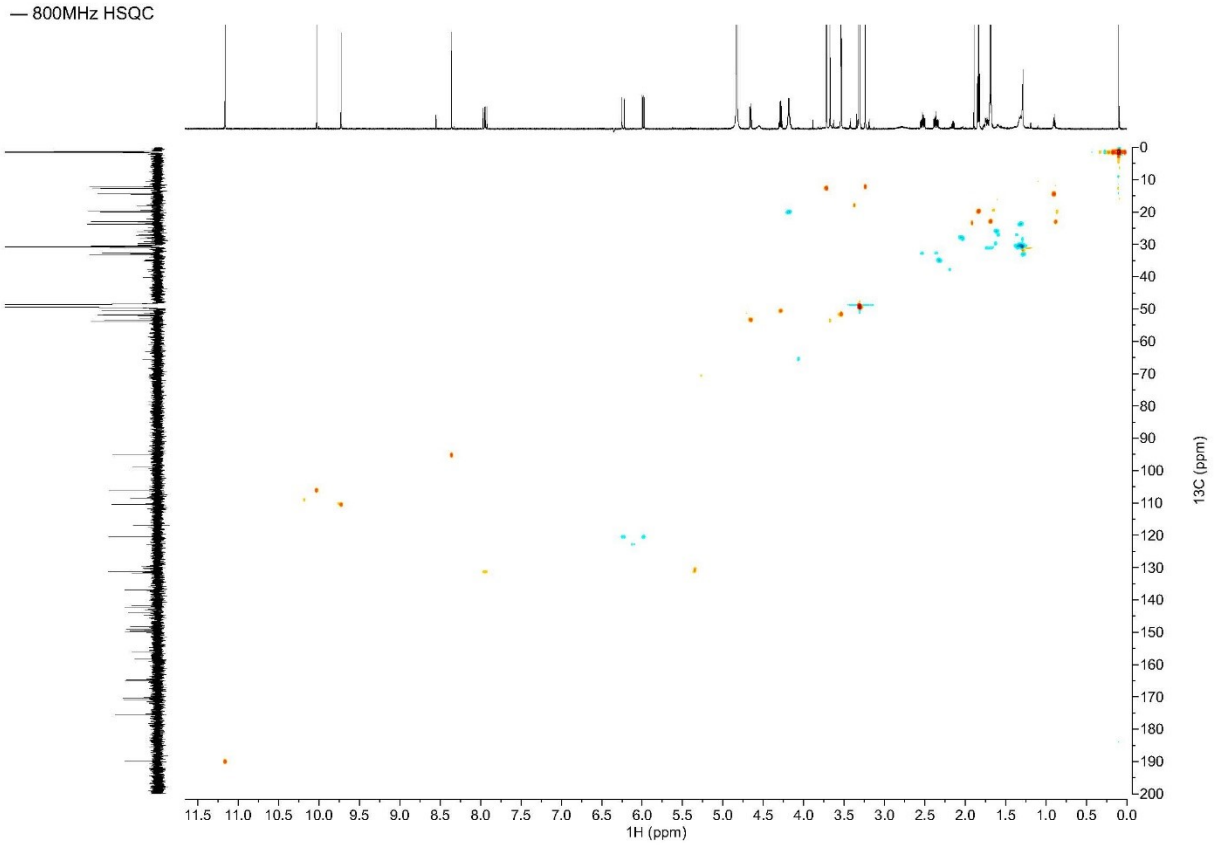

Fig. S62 HSQC spectrum of **8**.

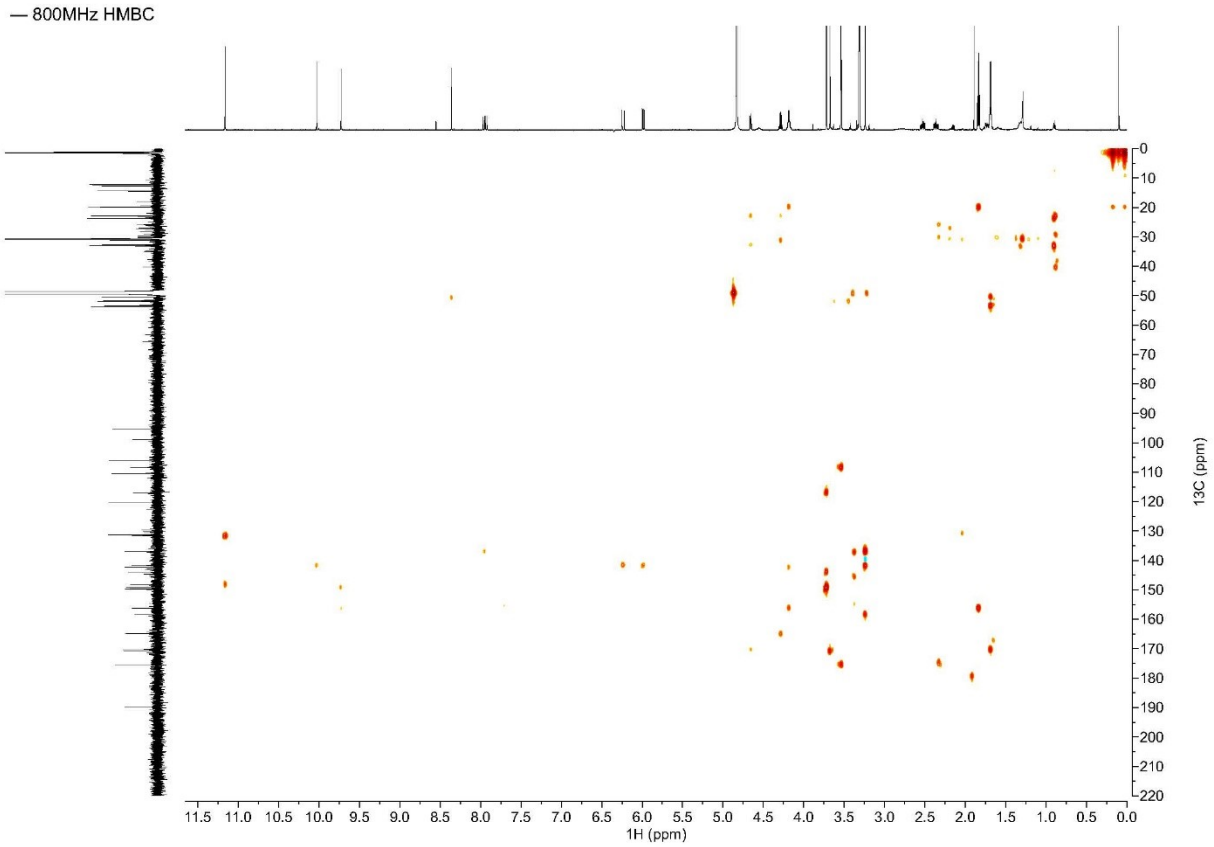

Fig. S63 HMBC spectrum of **8**.

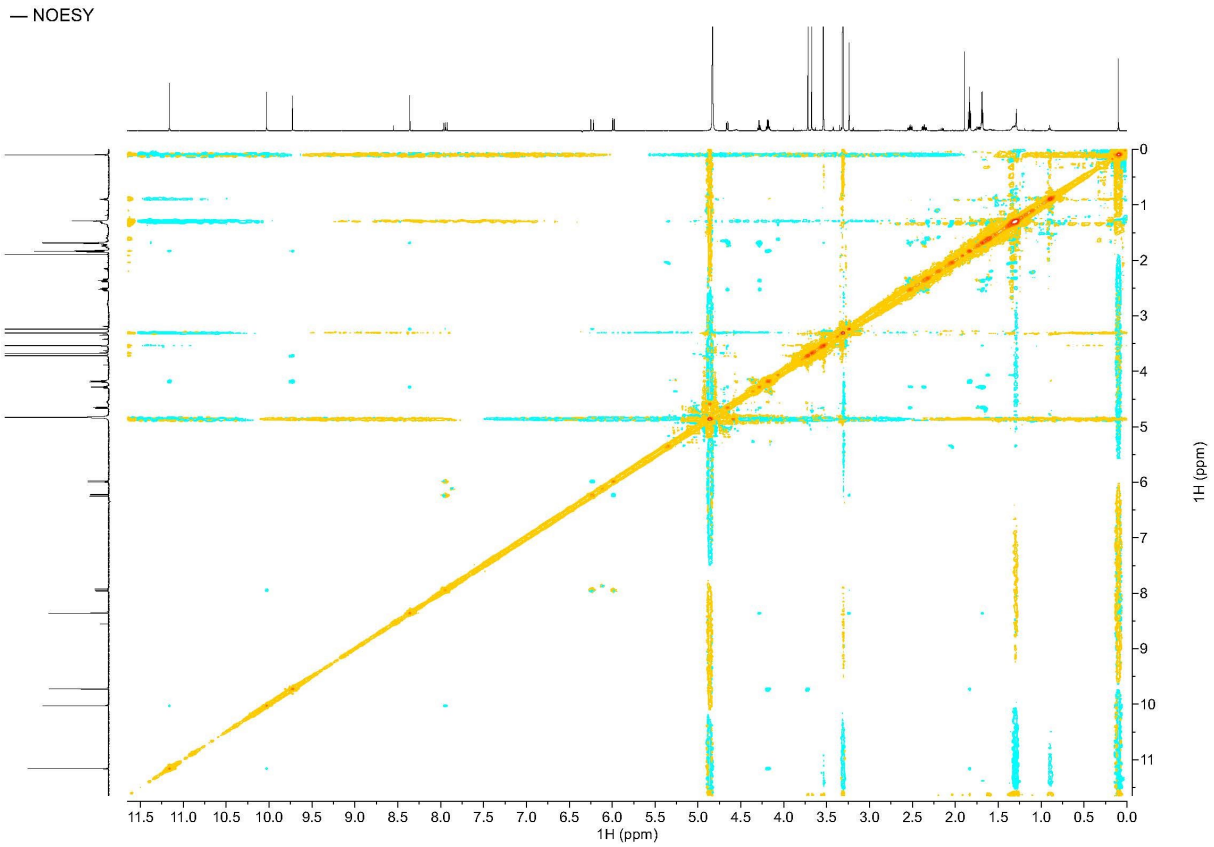

Fig. S64 NOESY spectrum of **8**.

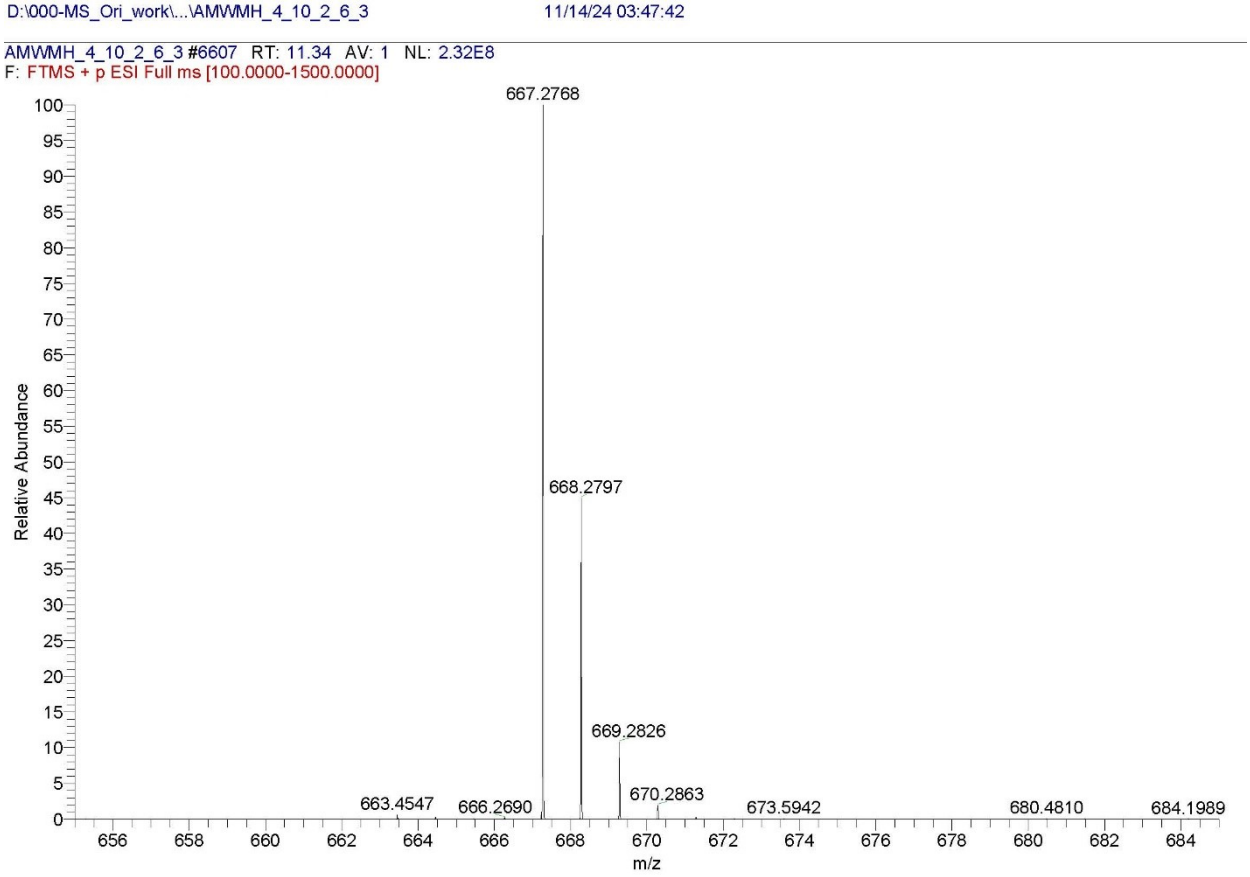

Fig. S65 HRESIMS spectrum of **8**.

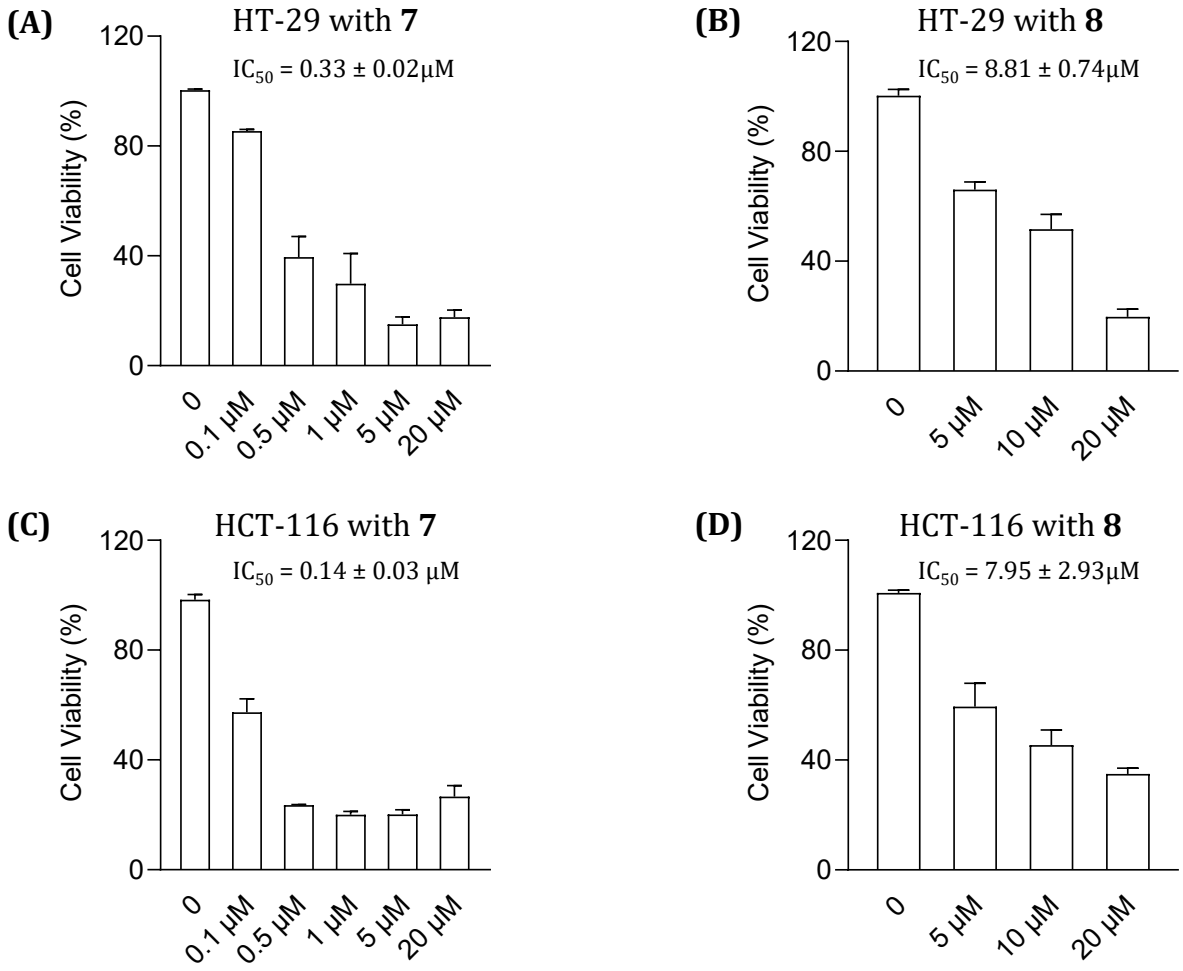

Fig. S66 Cell viability at different concentrations of compounds **7** and **8** in HT-29 and HCT-116 cells for IC_{50} calculation.

Cell viability of human colorectal cancer cell lines HT-29 and HCT-116 with different concentrations of compounds **7** and **8** for 48h. Results are presented as mean ± S.E.M. (n = 3) and used to calculate IC_{50} values. (A) HT-29 cells with compound **7**. (B) HT-29 cells with compound **8**. (C) HCT-116 cells with compound **7**. (D) HCT-116 cells with compound **8**.