

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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C.C.: column chromatography
H: *n*-hexane
D: Dichloromethane
E: ethyl acetate
A: acetone
M: MeOH
W: H₂O
ACN: acetonitrile

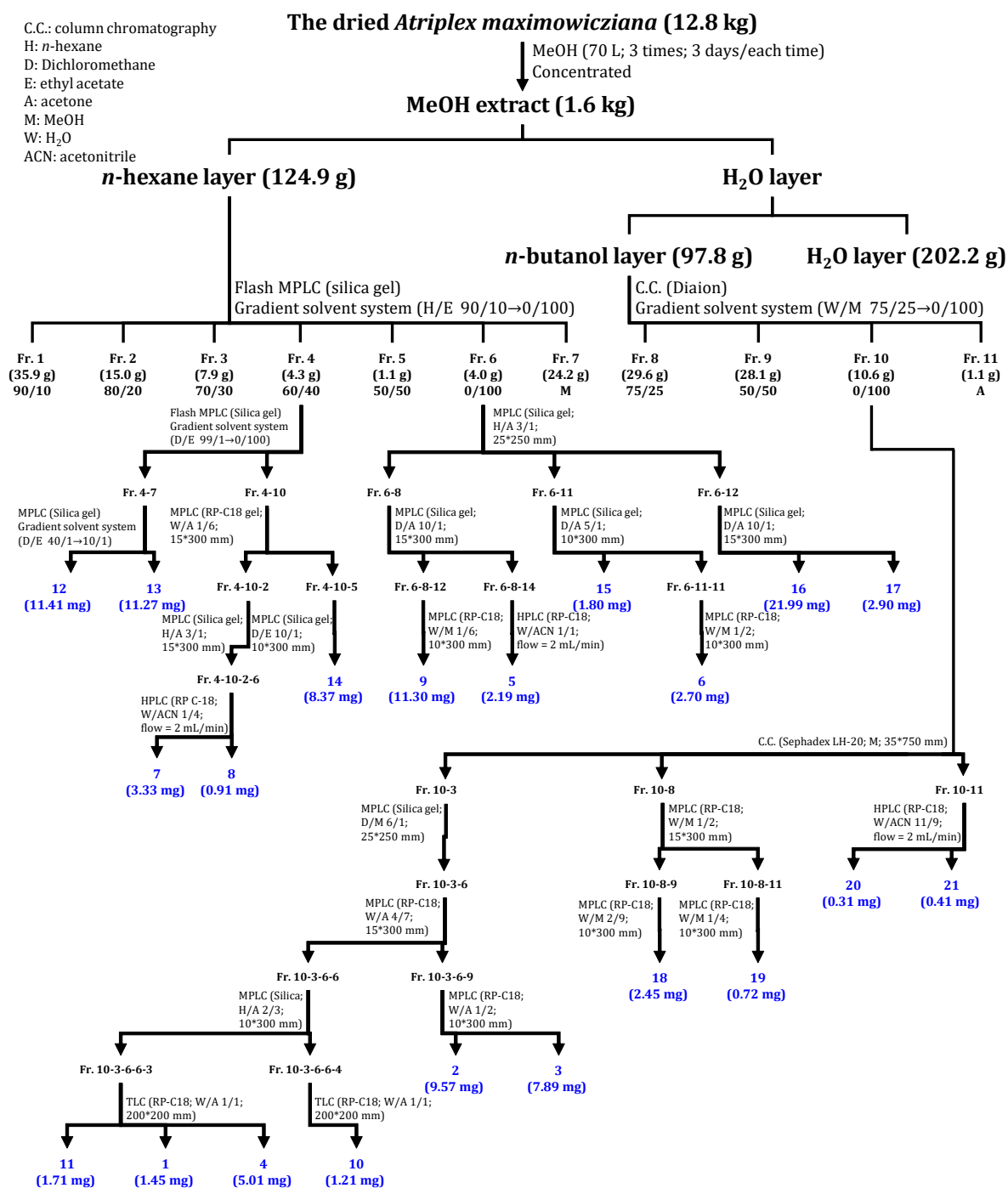


Fig. S1 The isolation flow chart of compounds **1–21** from *Atriplex maximowicziana*.

— 800MHz ^1H 1D/ ^1H
AMWMB-4-3-6-6-3-2

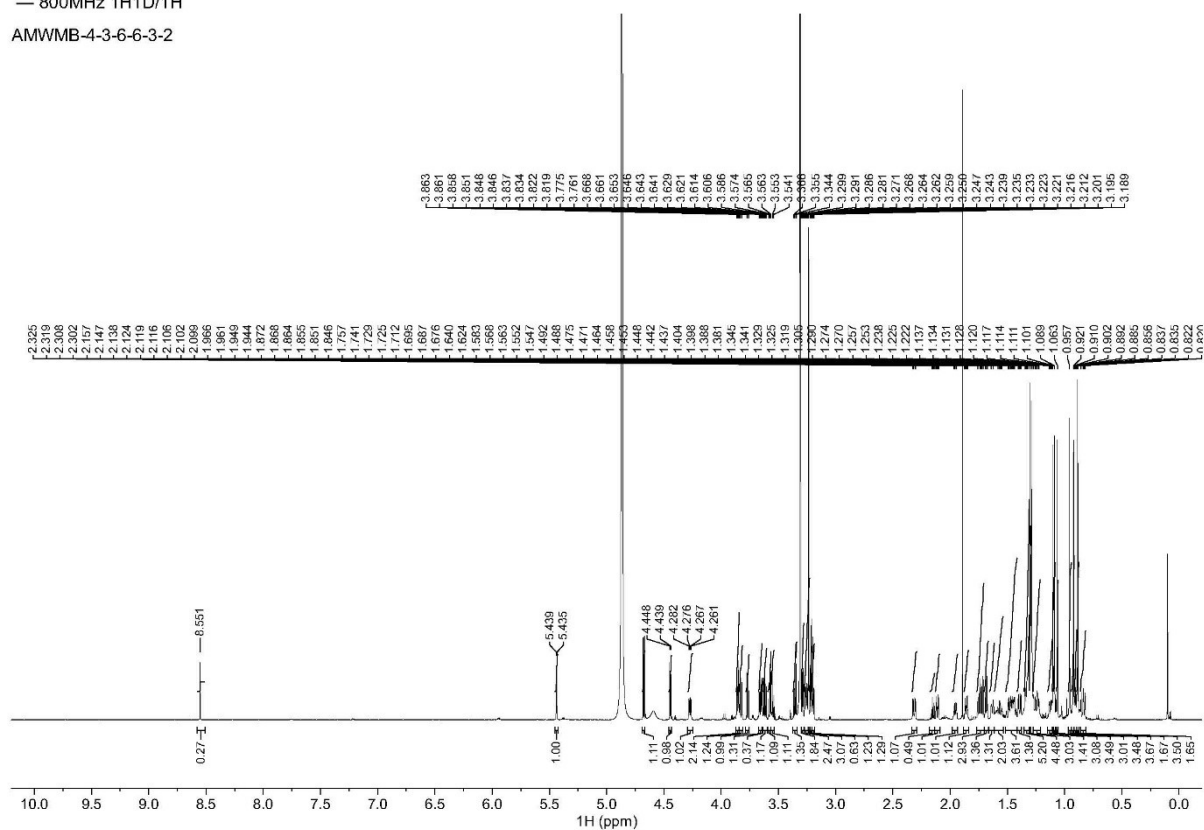


Fig. S2 ^1H NMR spectrum (800 MHz, CD_3OD) of **1**.

— 800MHz ^{13}C 1D/ ^{13}C
AMWMB-4-3-6-6-3-2

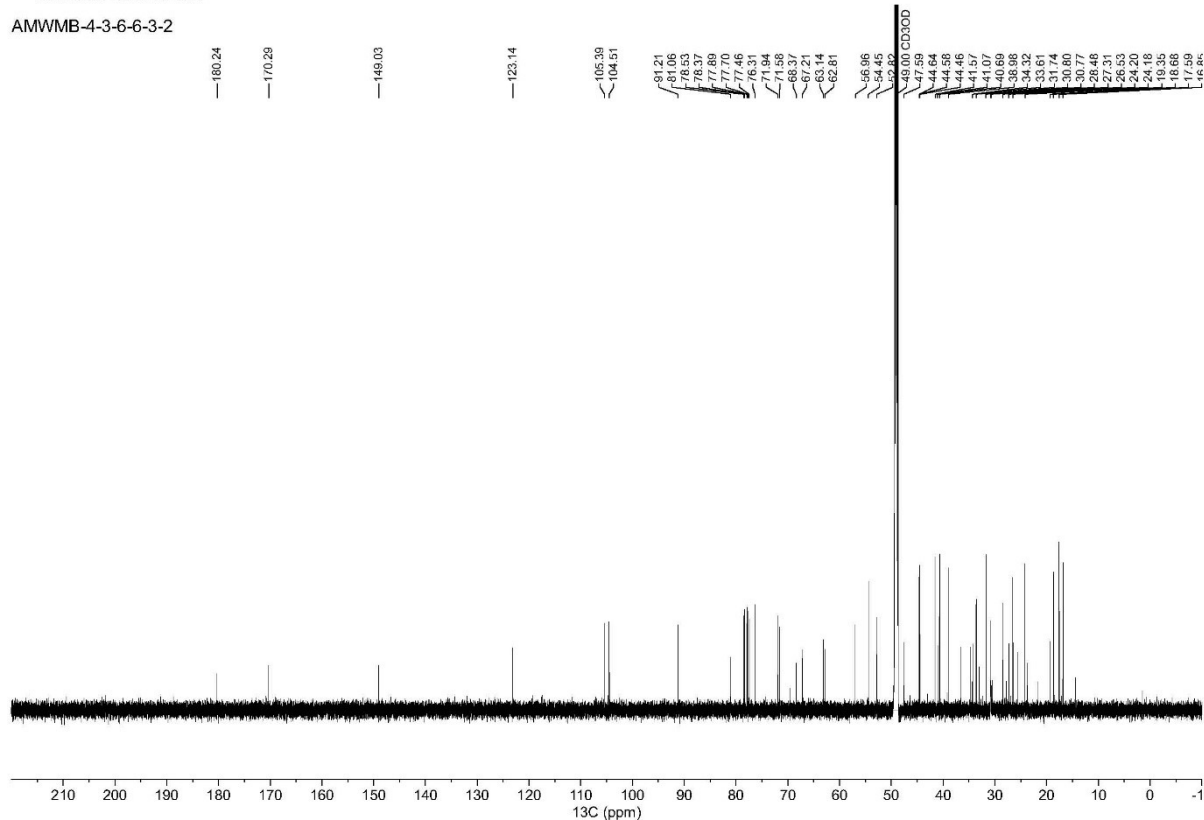


Fig. S3 ^{13}C NMR spectrum (200 MHz, CD_3OD) of **1**.

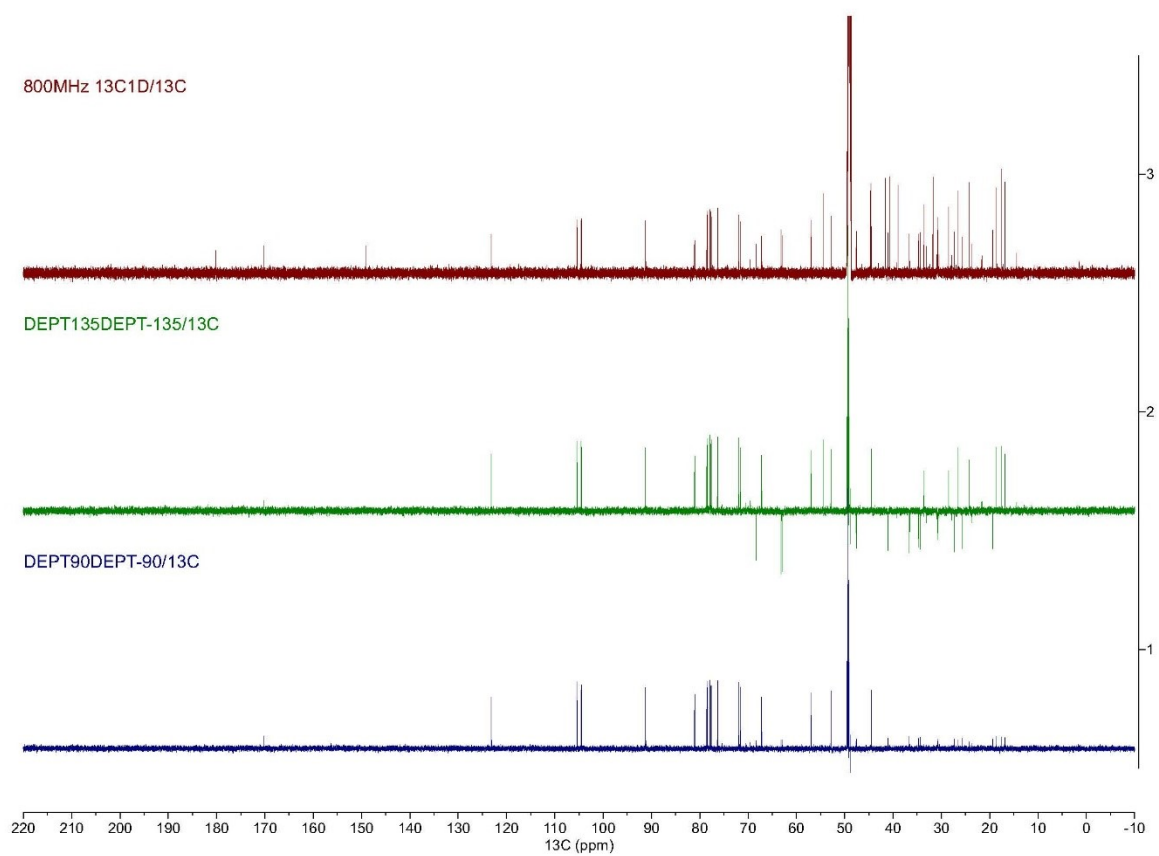


Fig. S4 DEPT spectrum of **1**.

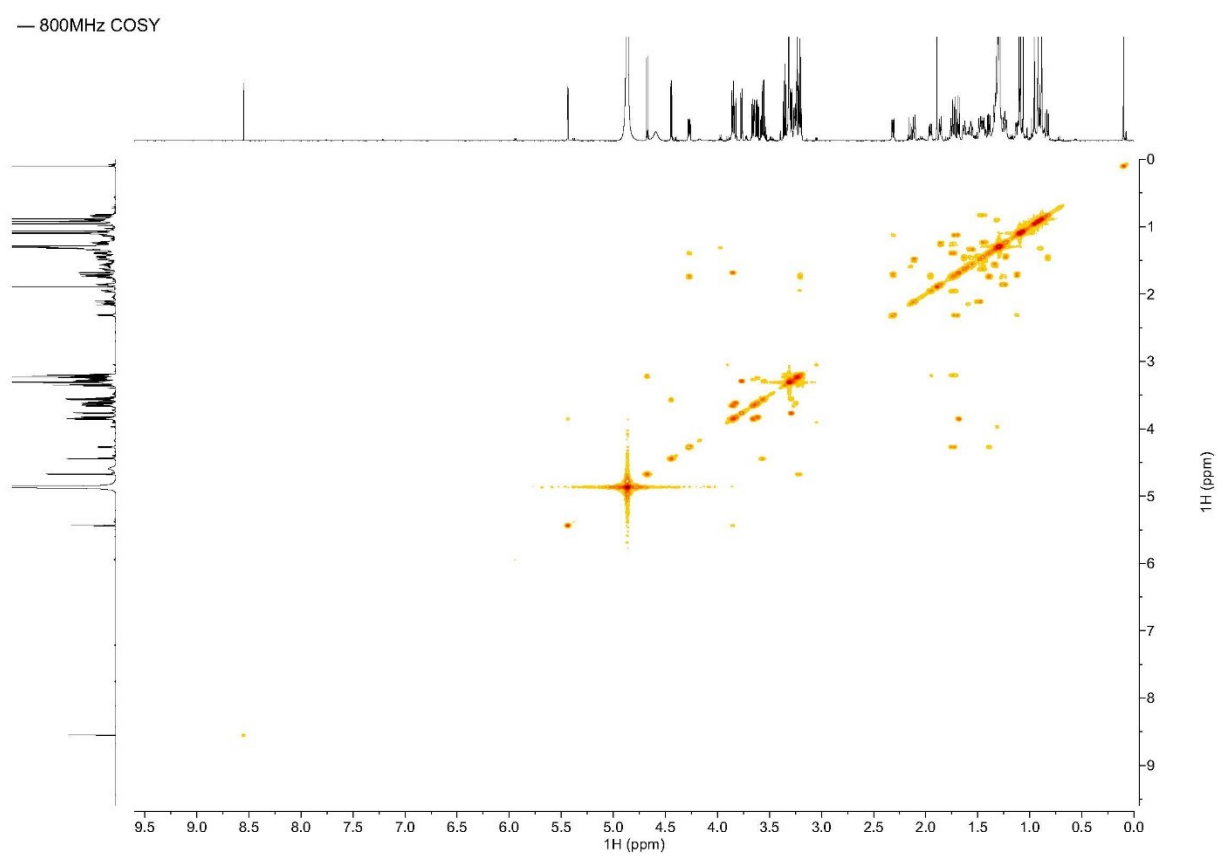


Fig. S5 COSY spectrum of **1**.

— 800MHz HSQC

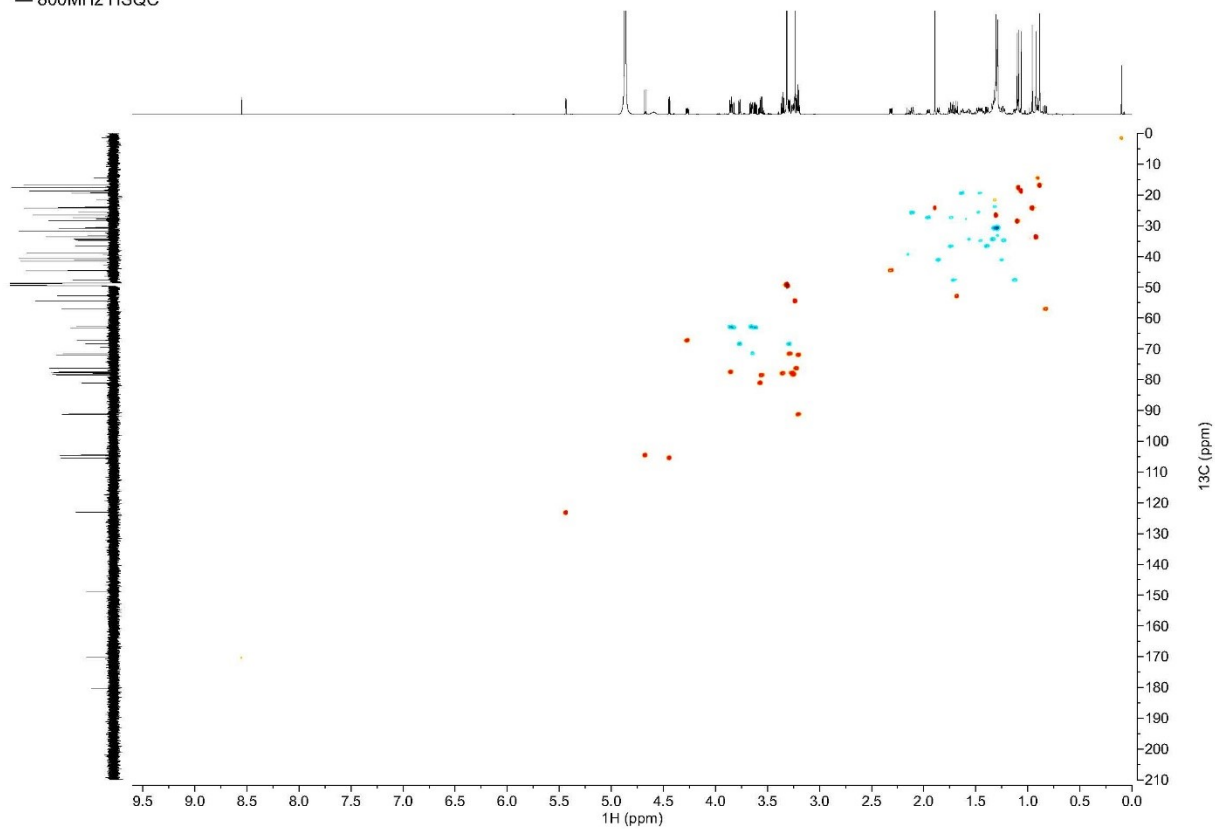


Fig. S6 HSQC spectrum of **1**.

— 800MHz HMBC

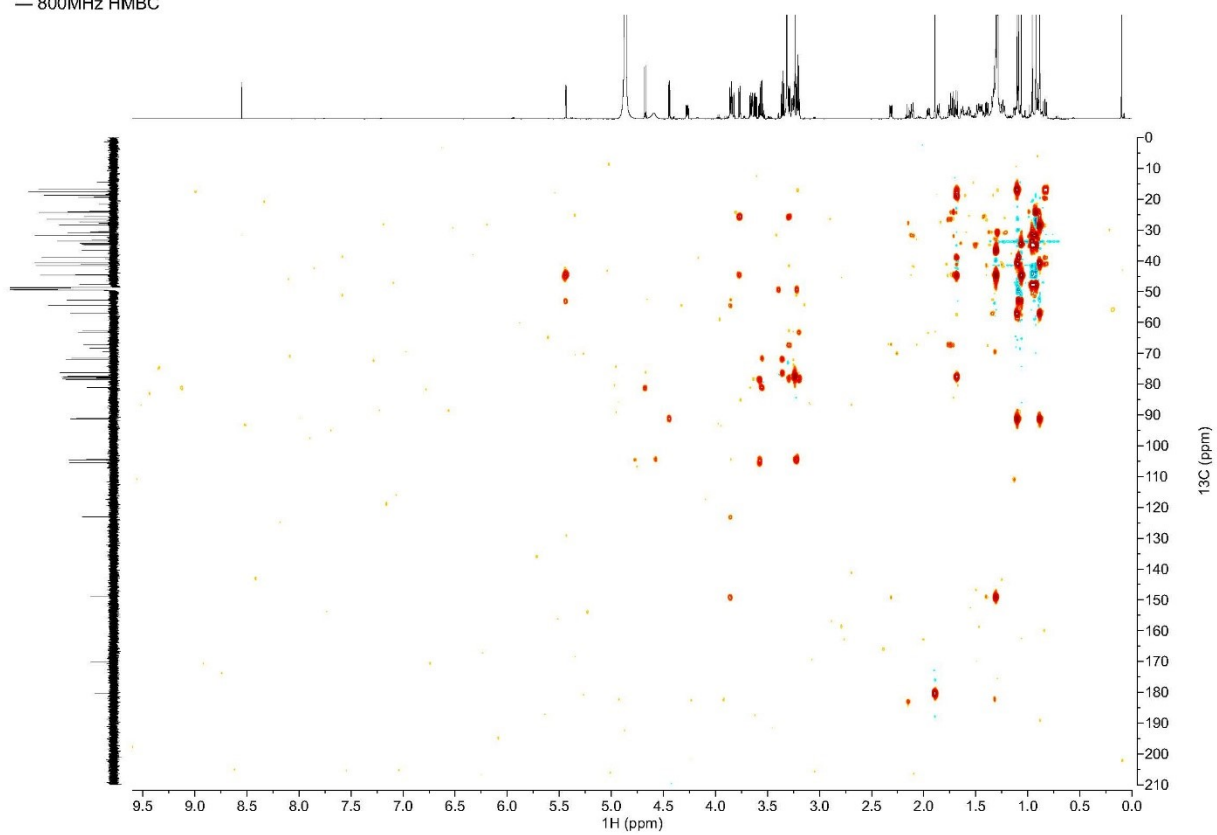


Fig. S7 HMBC spectrum of **1**.

— NOESY24Jun05_AMWMB-4-3-6-6-3-2.733.ser

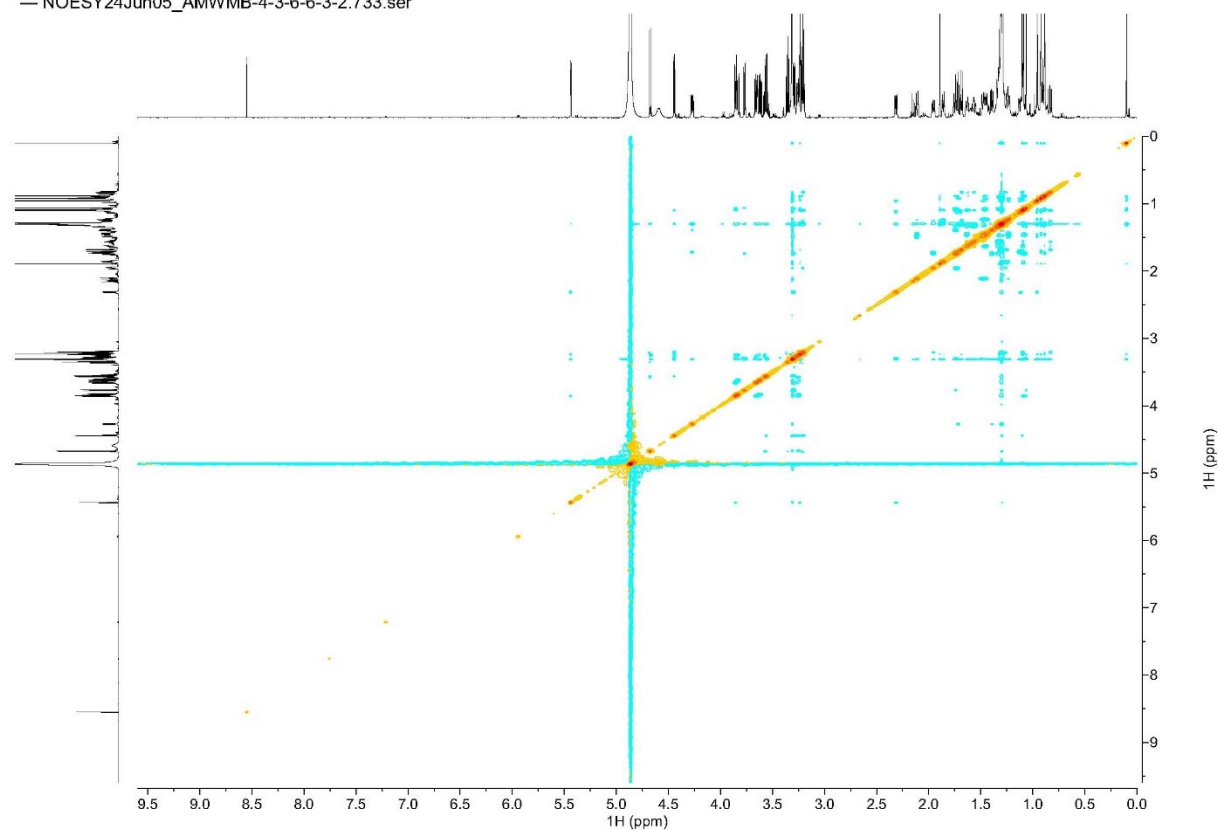


Fig. S8 NOESY spectrum of **1**.

C:\Users\...\20241015\AMWMB-4-3-6-6-3-2

10/15/24 16:07:26

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F: FTMS + p ESI Full ms [100.0000-1200.0000]

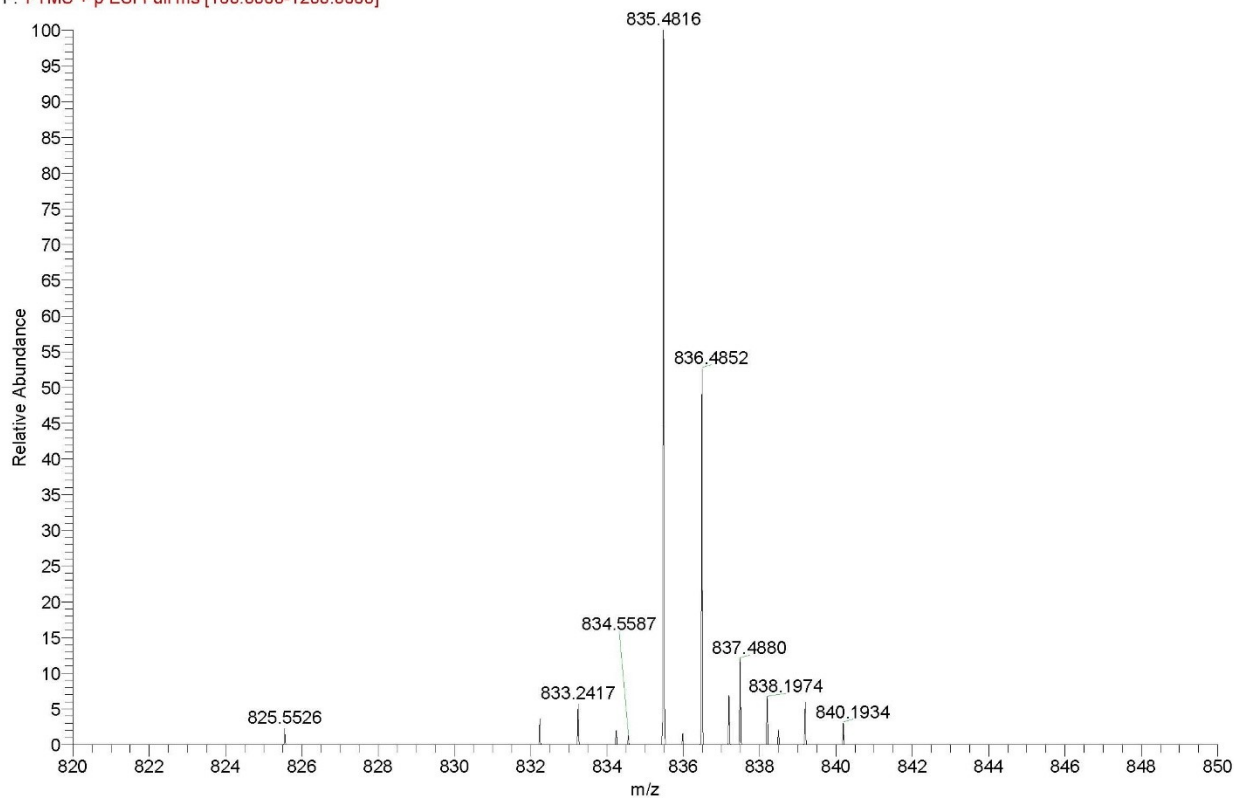


Fig. S9 HRESIMS spectrum of **1**.

— 800MHz ¹H — AMWMB-4-3-6-9-31D/1H

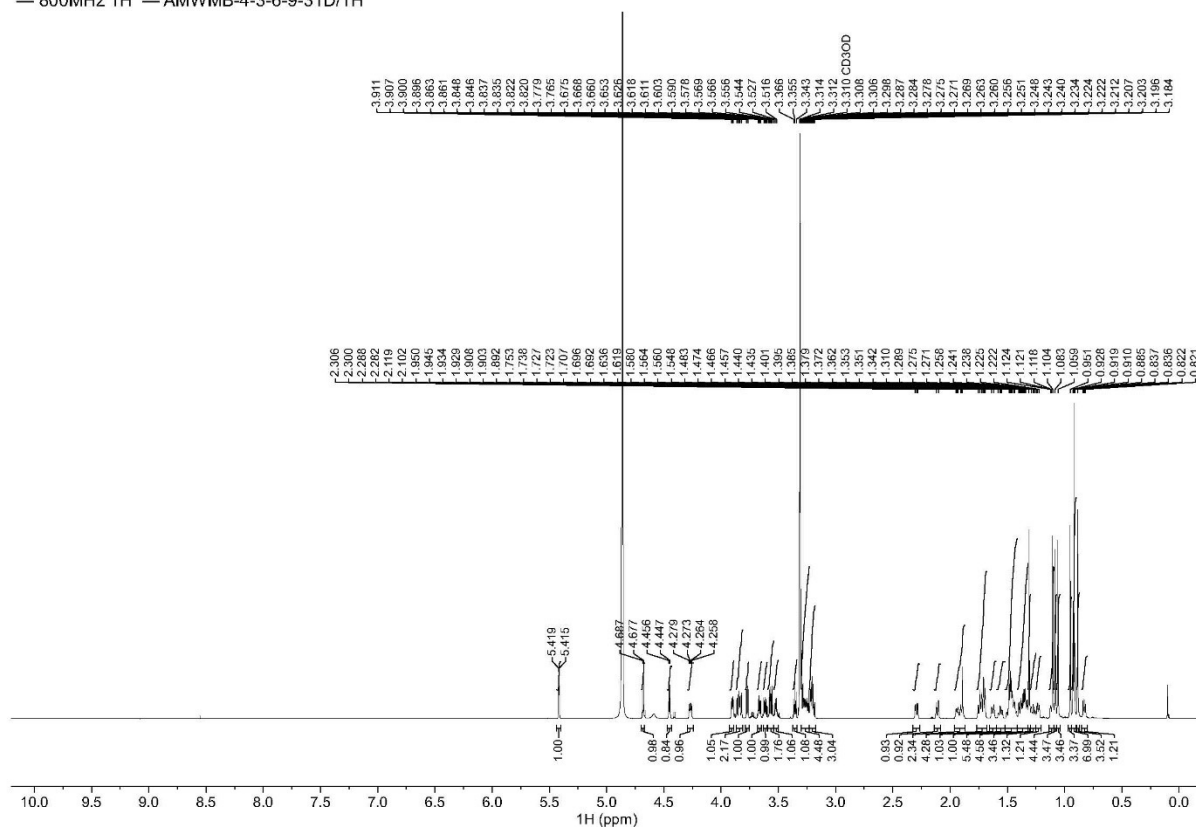


Fig. S10 ¹H NMR spectrum (800 MHz, CD₃OD) of 2.

— 800MHz ¹³C — 13C1D/13C

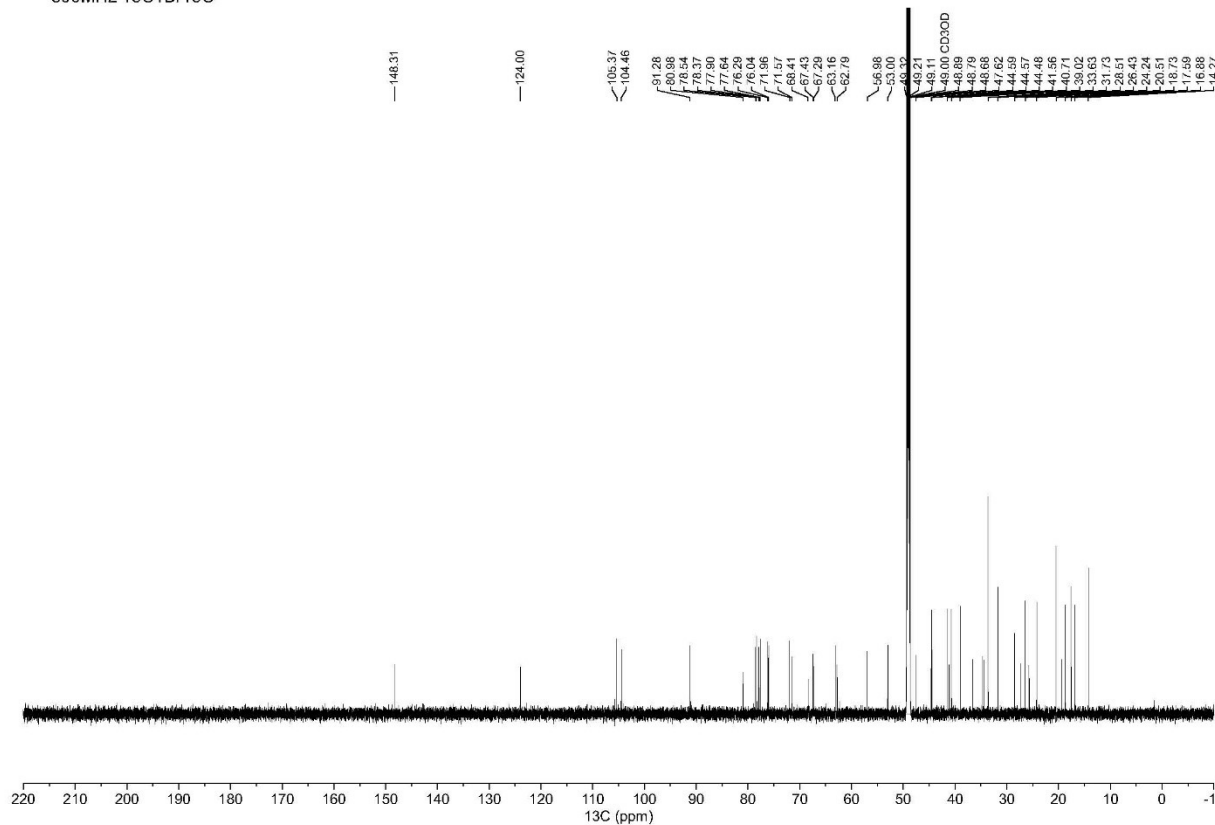


Fig. S11 ¹³C NMR spectrum (200 MHz, CD₃OD) of 2.

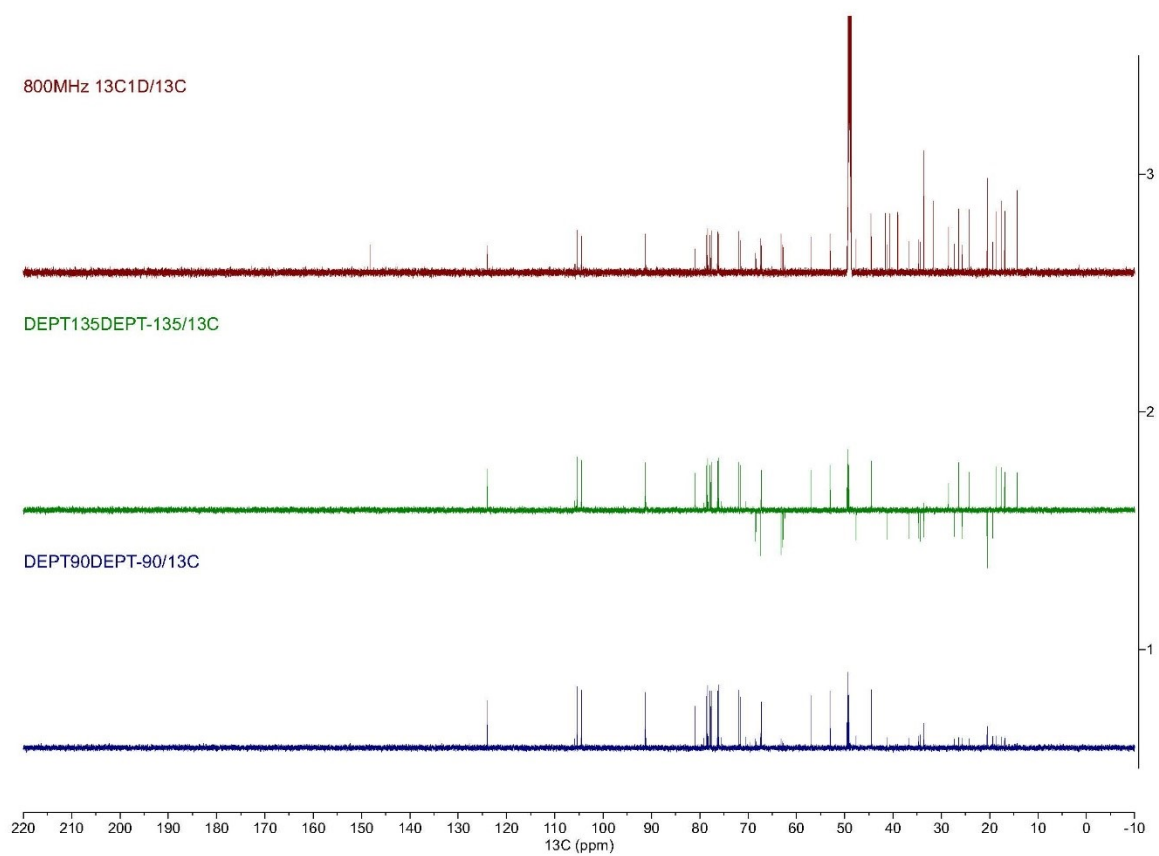


Fig. S12 DEPT spectrum of **2**.

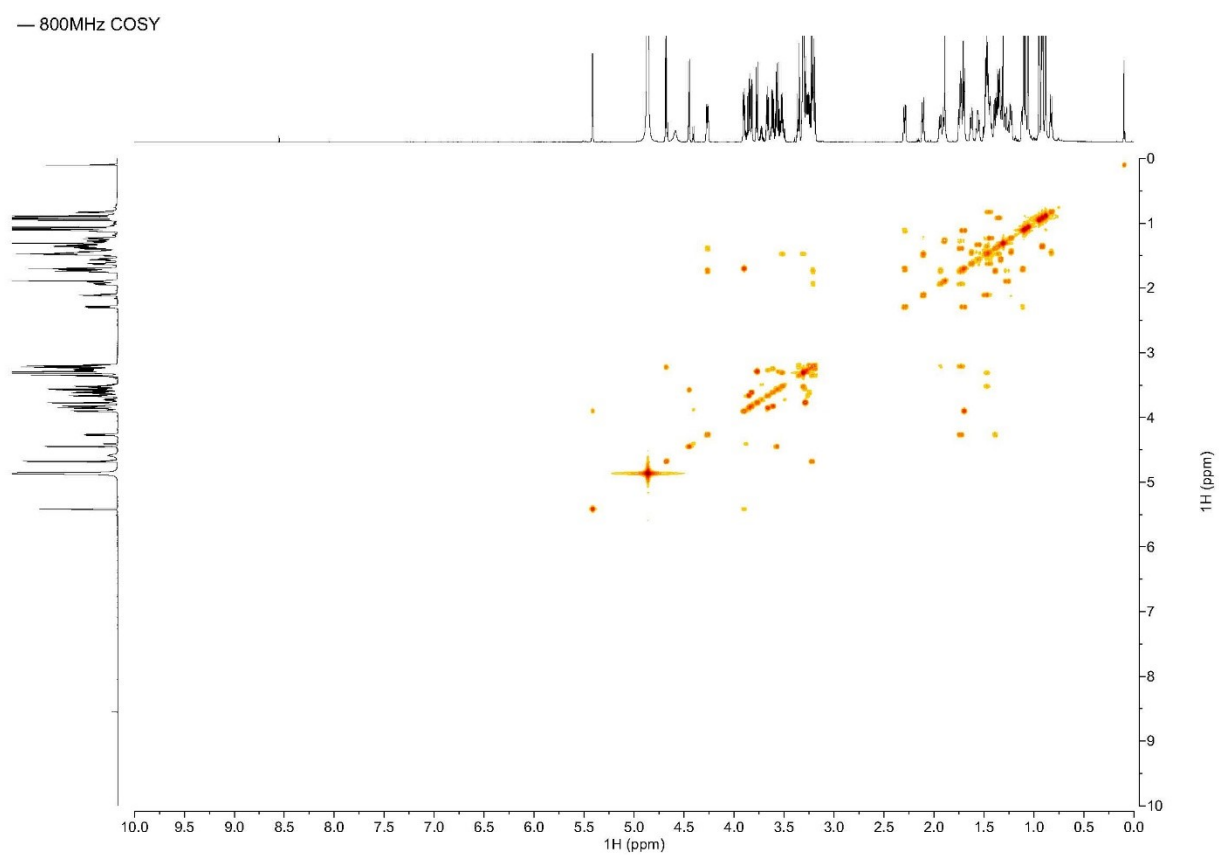


Fig. S13 COSY spectrum of **2**.

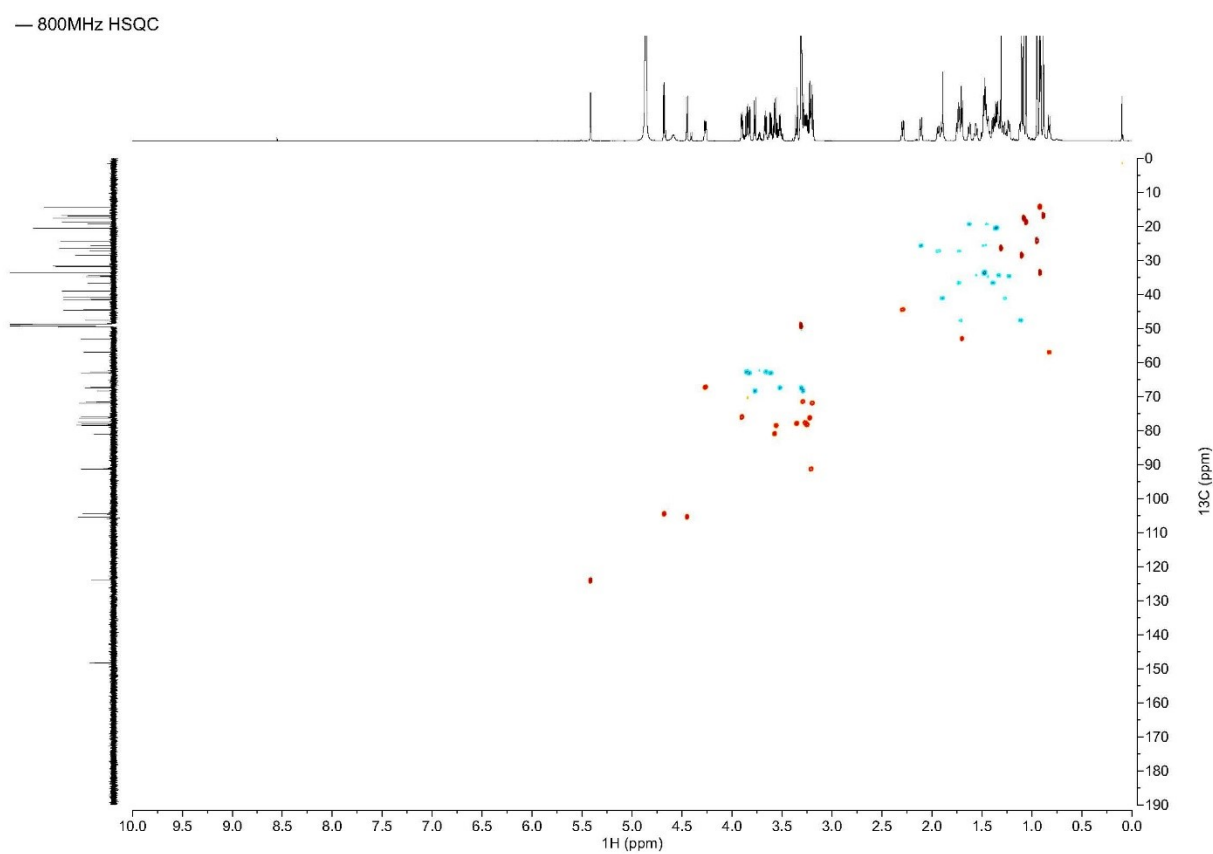


Fig. S14 HSQC spectrum of **2**.

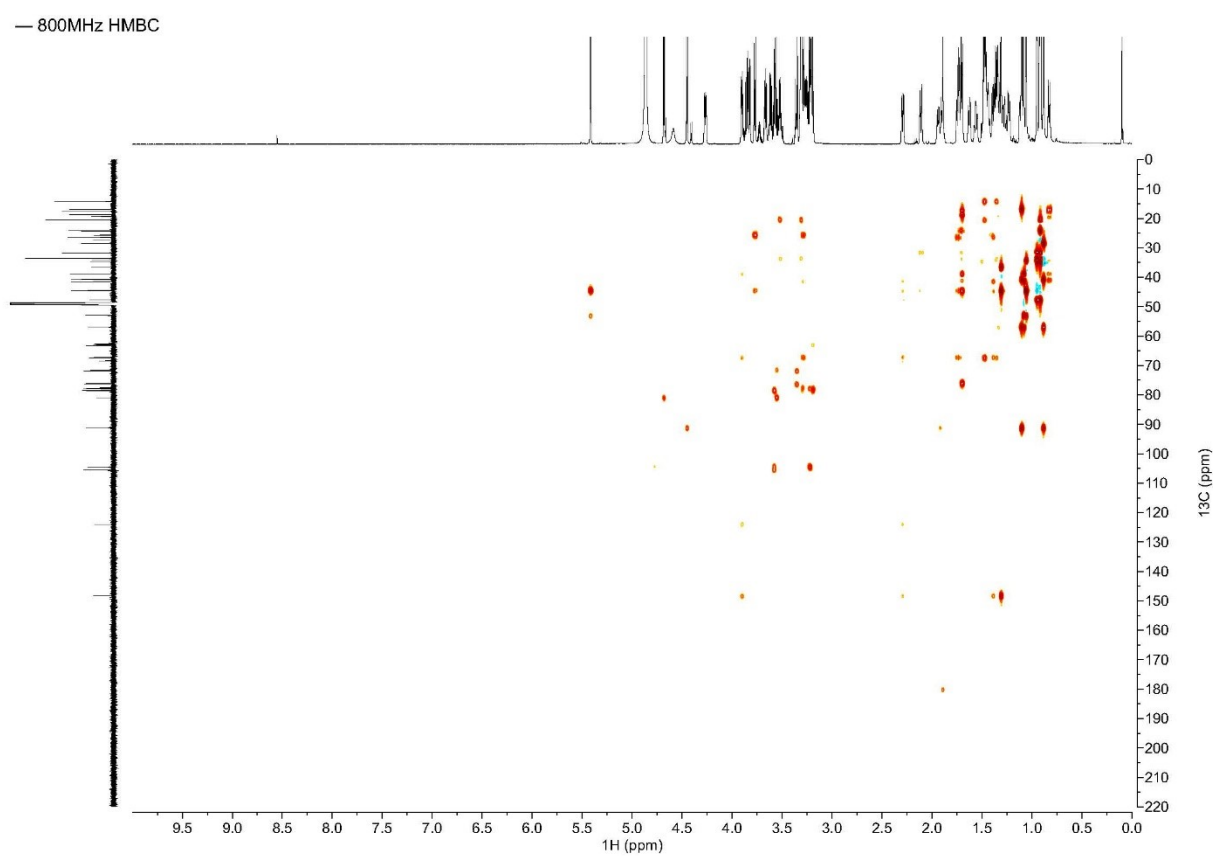


Fig. S15 HMBC spectrum of **2**.

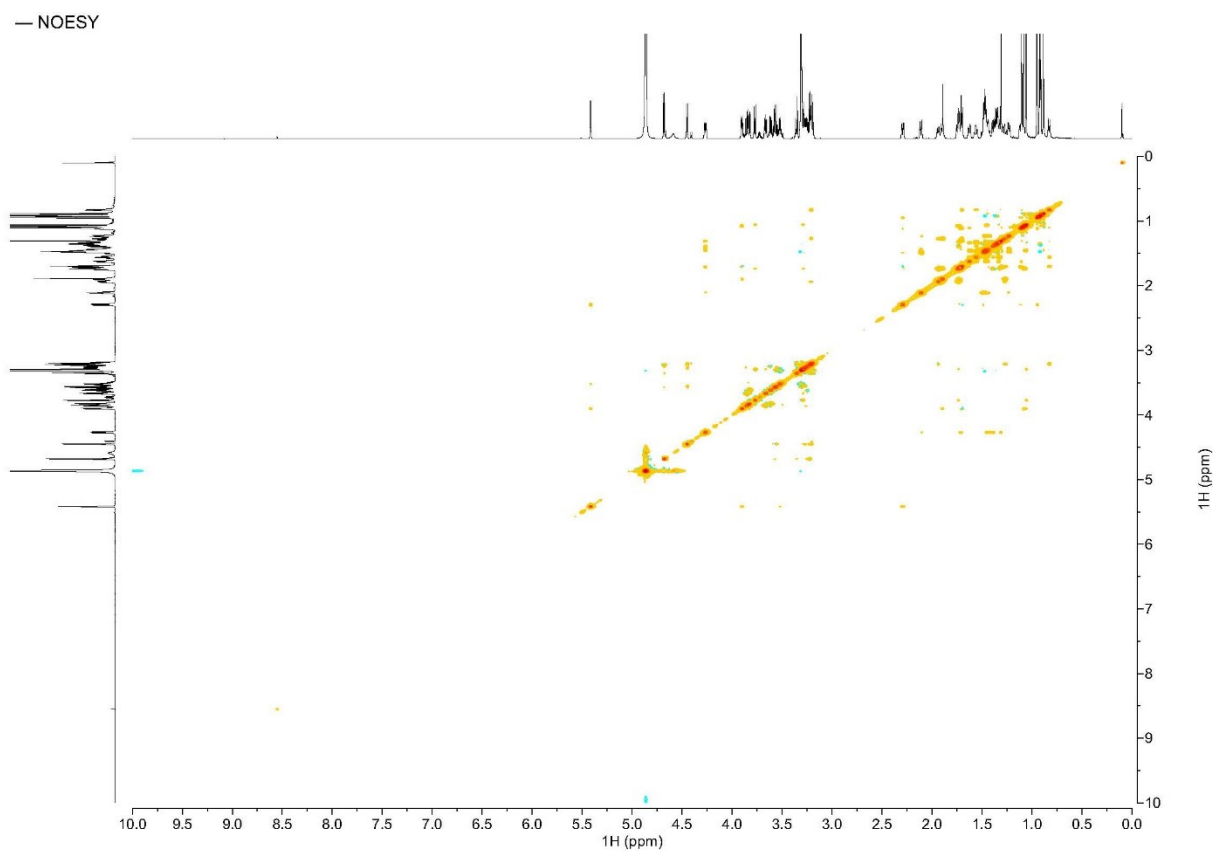


Fig. S16 NOESY spectrum of **2**.

C:\Users\...\20241015\AMWMB-4-3-6-9-3

10/15/24 16:11:04

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F: FTMS + p ESI Full ms [100.0000-1200.0000]

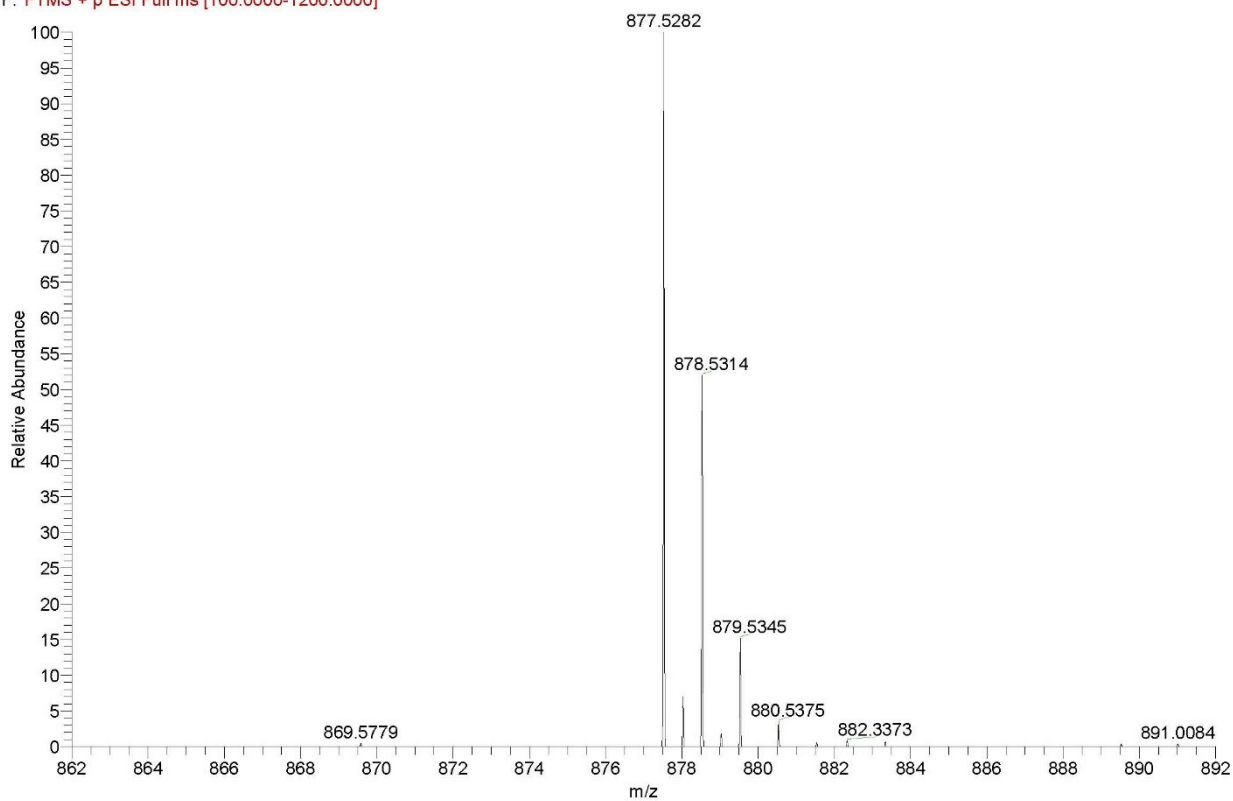


Fig. S17 HRESIMS spectrum of **2**.

Chemical shifts (ppm): 4.685, 4.676, 4.453, 4.444, 4.435, 4.086, 4.052, 3.972, 3.958, 3.889, 3.886, 3.883, 3.884, 3.863, 3.860, 3.848, 3.845, 3.836, 3.833, 3.821, 3.818, 3.675, 3.668, 3.660, 3.653, 3.646, 3.618, 3.611, 3.603, 3.578, 3.568, 3.565, 3.555, 3.543, 3.532, 3.521, 3.355, 3.348, 3.345, 3.314, 3.312, 3.308, 3.306, 3.287, 3.267, 3.274, 3.270, 3.267, 3.262, 3.259, 3.256, 3.253, 3.247, 3.242, 3.239, 3.233, 3.223, 3.221, 3.217, 3.206, 3.205, 3.197, 3.185, 1.893, 1.749, 1.698, 1.687, 1.617, 1.484, 1.476, 1.467, 1.468, 1.455, 1.365, 1.363, 1.355, 1.321, 1.321, 1.115, 1.078, 1.043, 1.056, 1.056, 1.031, 1.024, 1.022, 0.992, 0.892.

Integration values: 1.00, 1.05, 0.96, 0.96, 0.94, 0.97, 1.11, 2.41, 1.21, 1.18, 1.71, 1.16, 1.36, 0.66, 2.26, 3.42, 0.98, 2.89, 0.99, 1.83, 1.12, 2.00, 1.10, 1.83, 1.41, 4.44, 3.34, 4.86, 1.54, 1.30, 3.47, 3.67, 3.28, 3.65, 2.16, 1.38.

— 800MHz 13C1D/13C

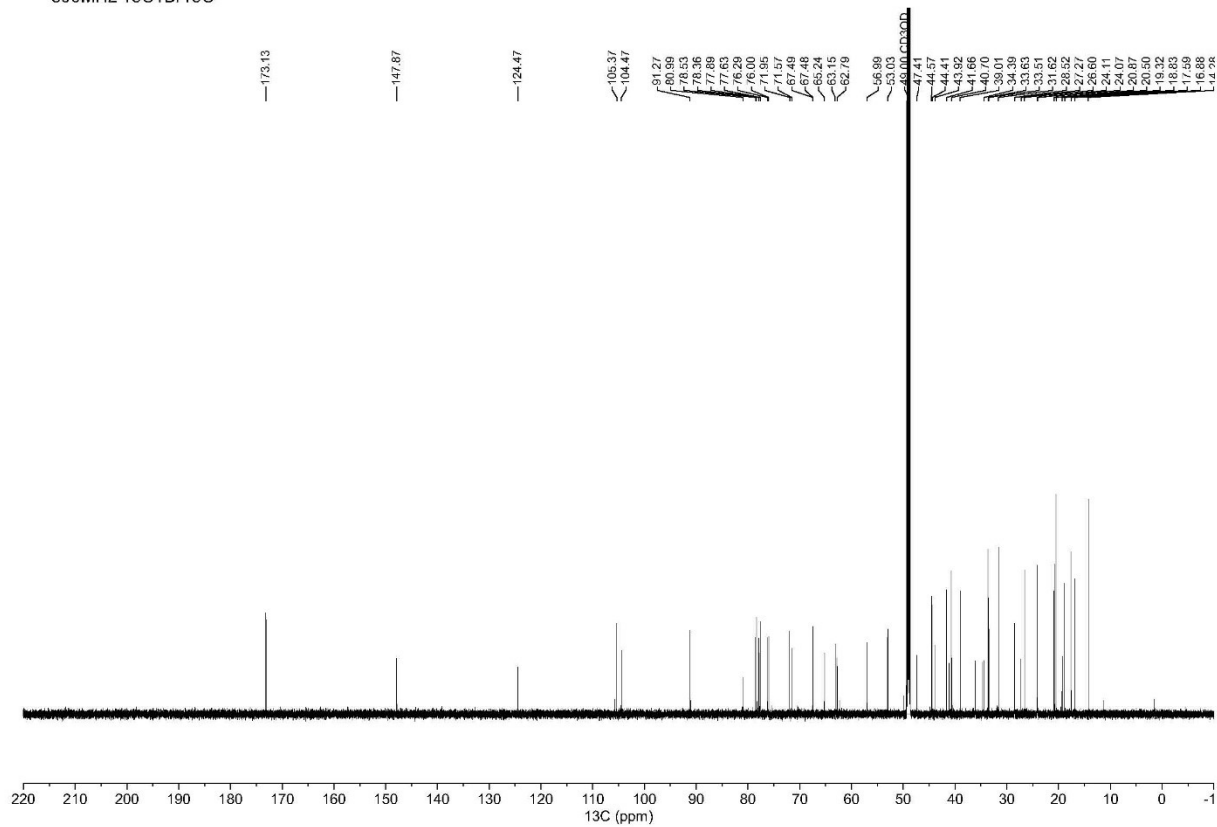


Fig. S19 ^{13}C NMR spectrum (200 MHz, CD_3OD) of **3**.

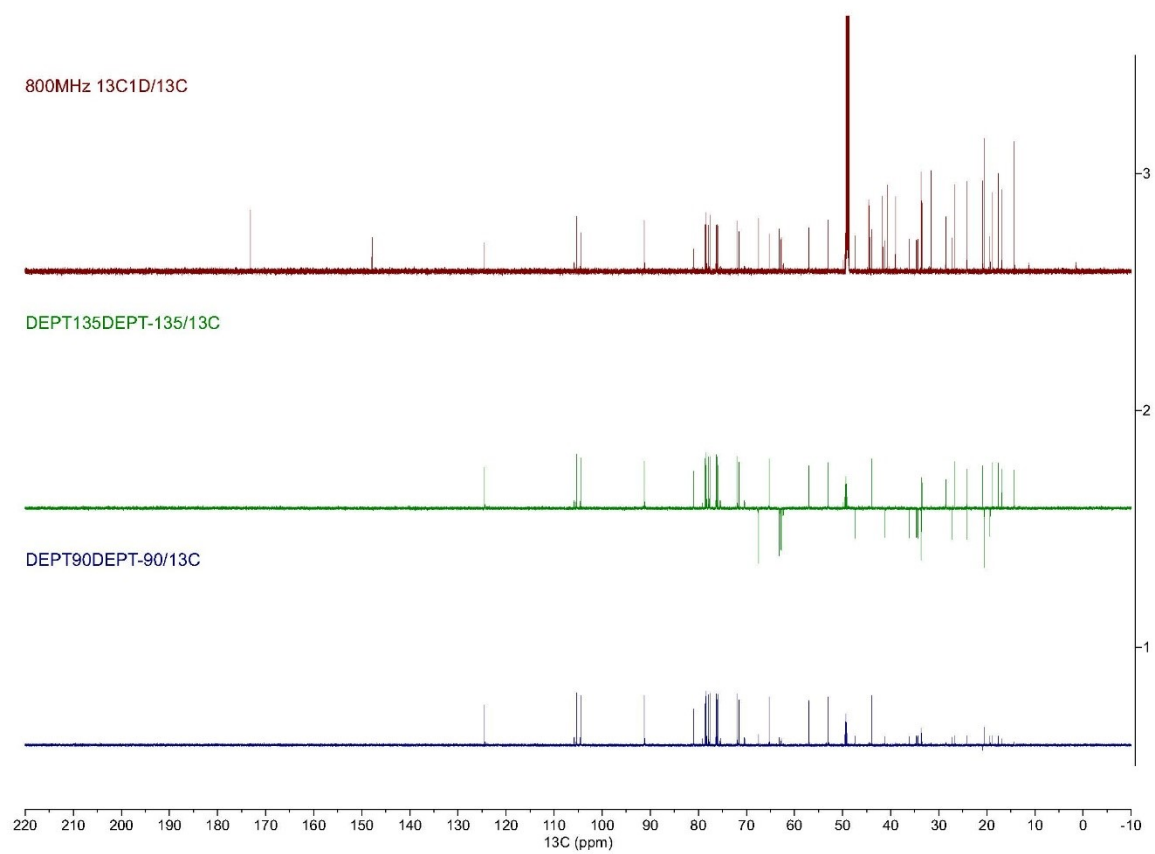


Fig. S20 DEPT spectrum of **3**.

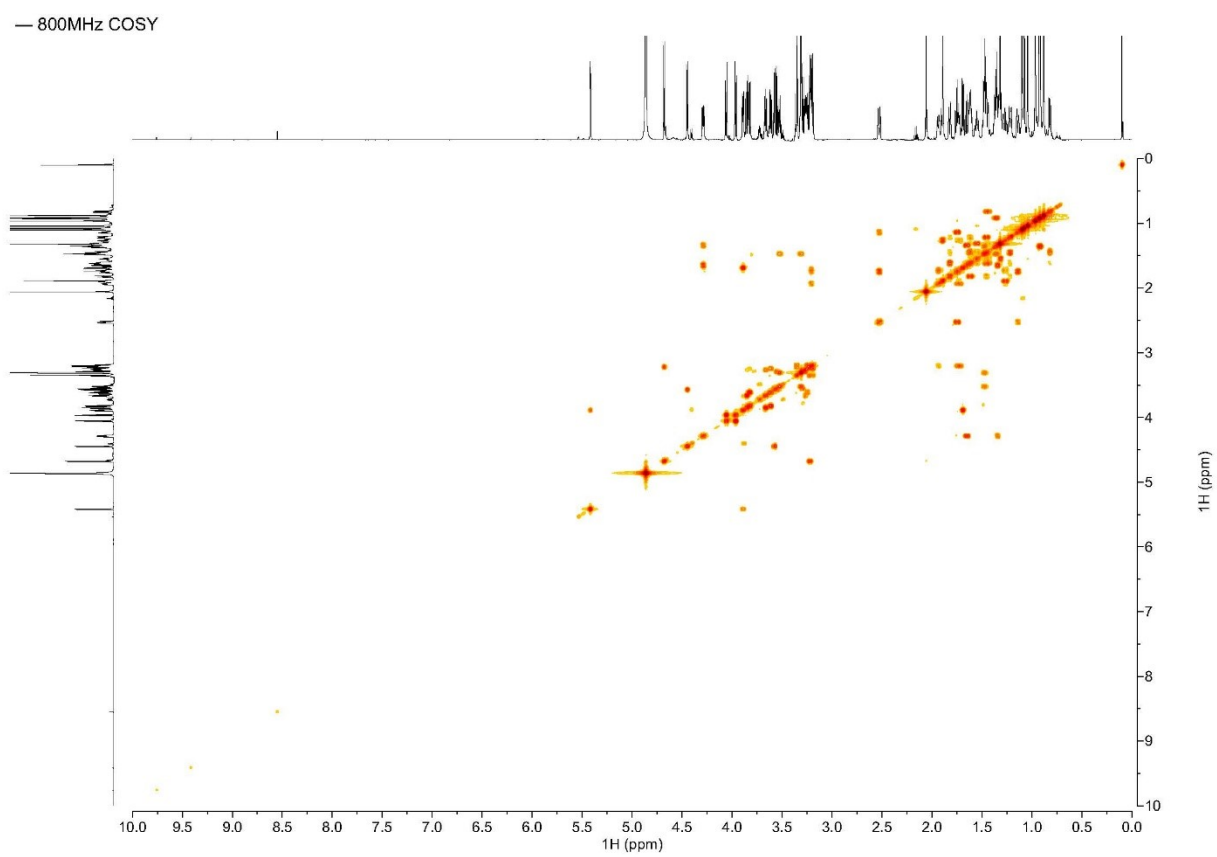


Fig. S21 COSY spectrum of **3**.

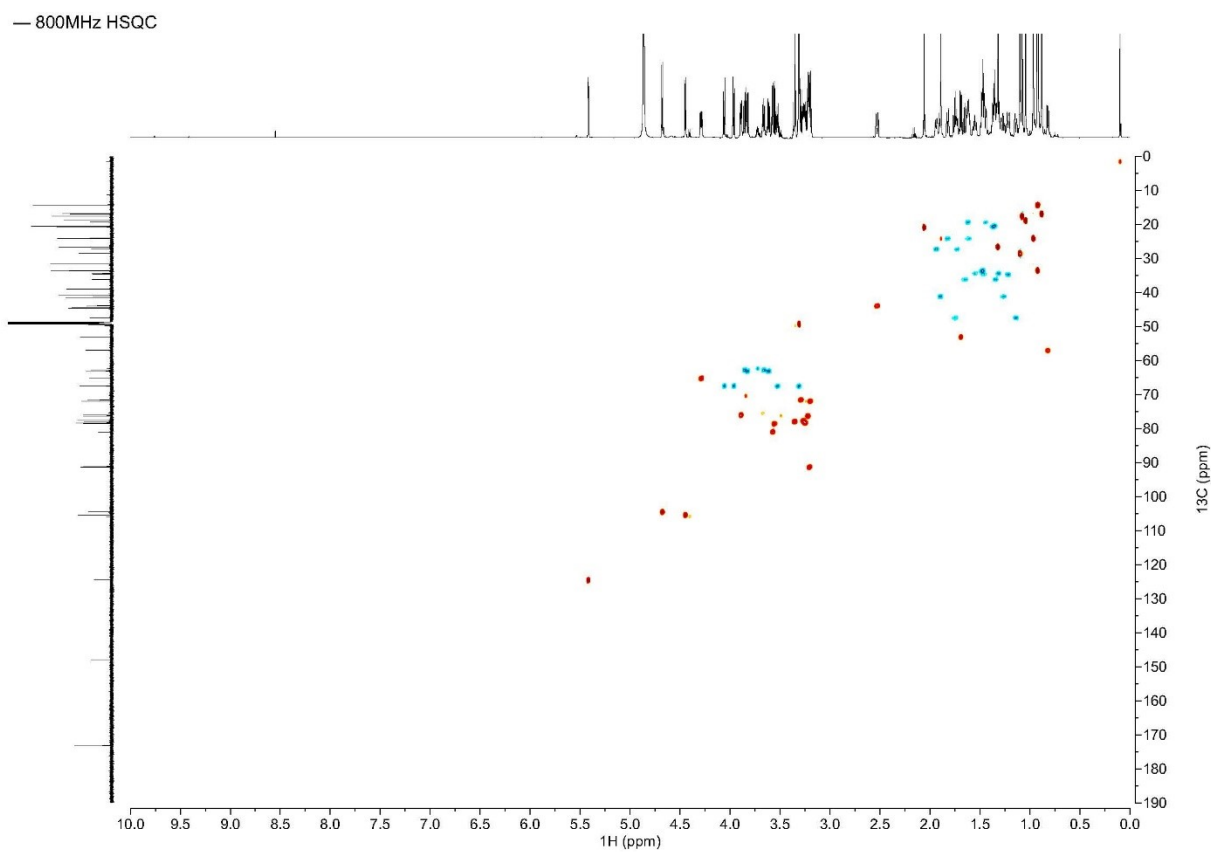


Fig. S22 HSQC spectrum of **3**.

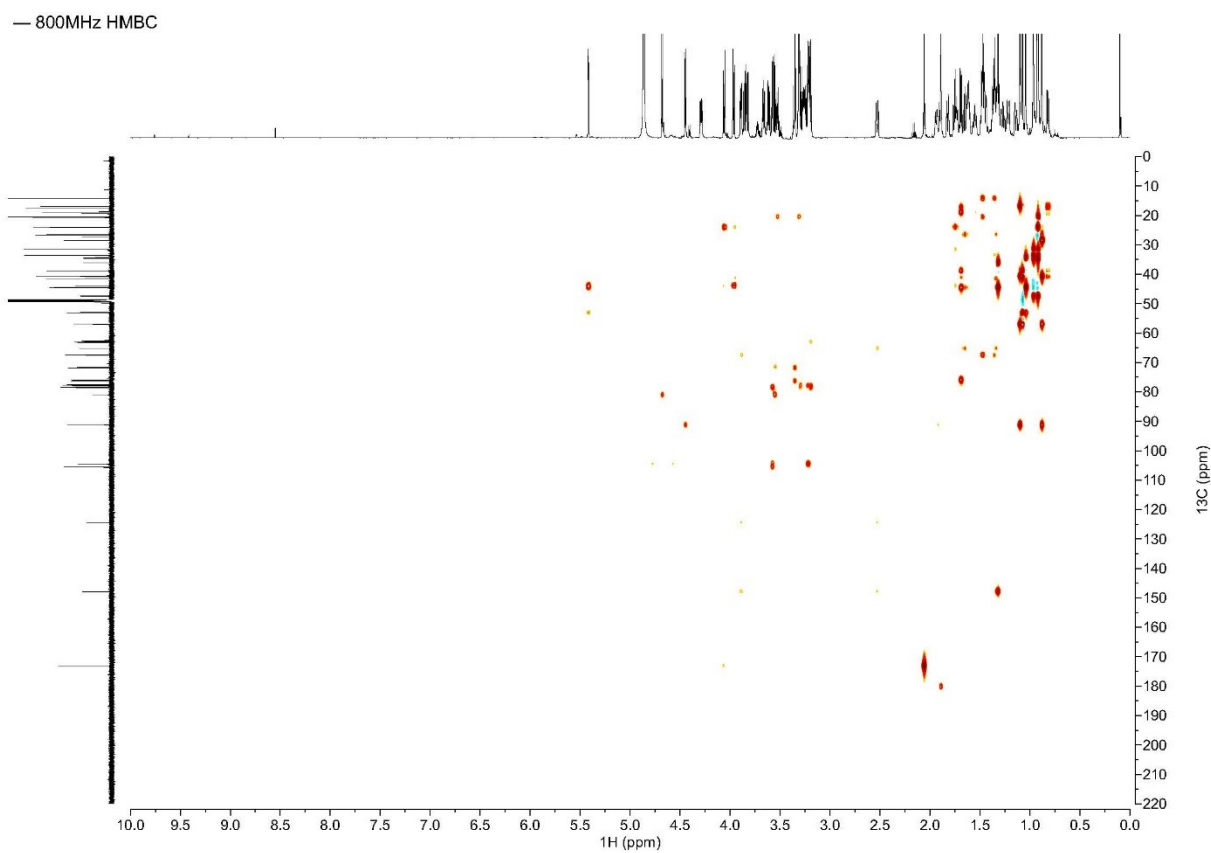


Fig. S23 HMBC spectrum of **3**.

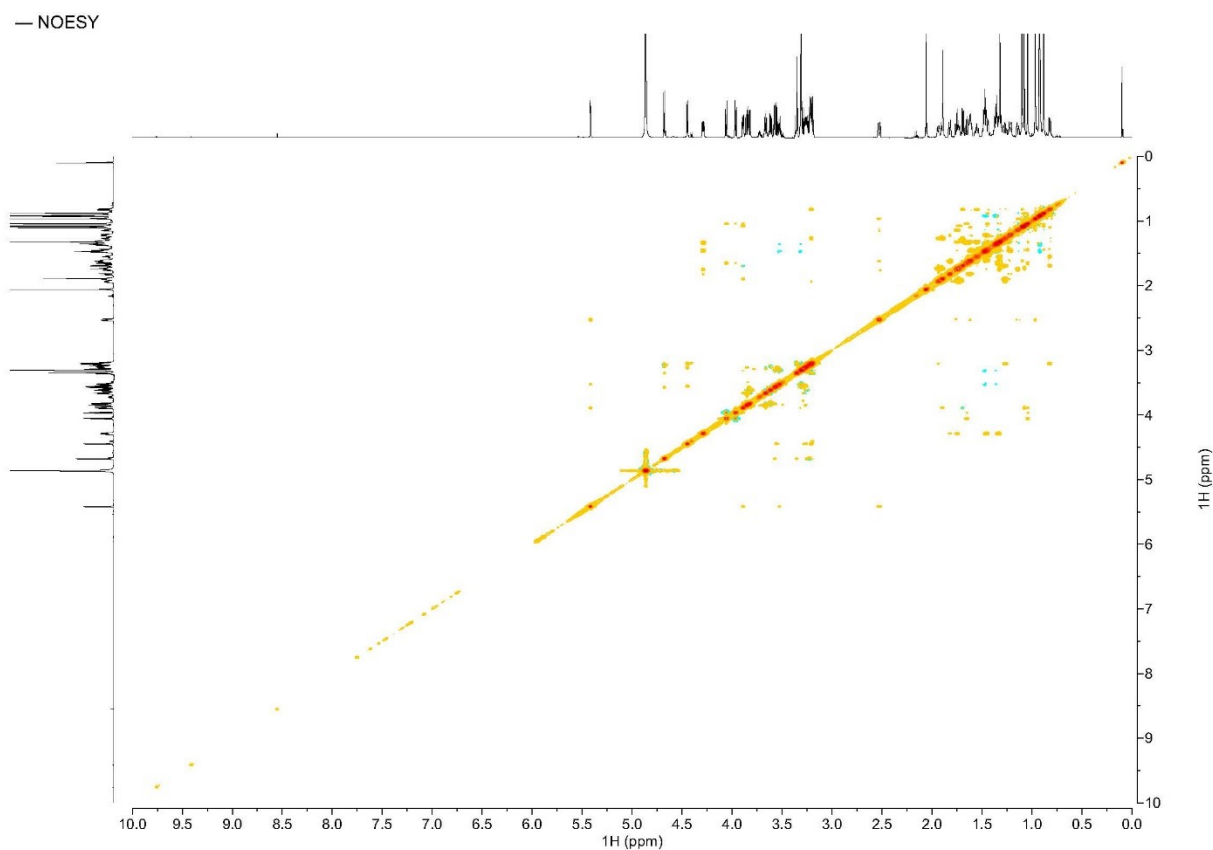


Fig. S24 NOESY spectrum of **3**.

C:\Users\...\20241015\AMWMB-4-3-6-9-7

10/15/24 16:14:42

AMWMB-4-3-6-9-7 #47 RT: 0.15 AV: 1 NL: 3.34E5

F: FTMS + p ESI Full ms [100.0000-1200.0000]

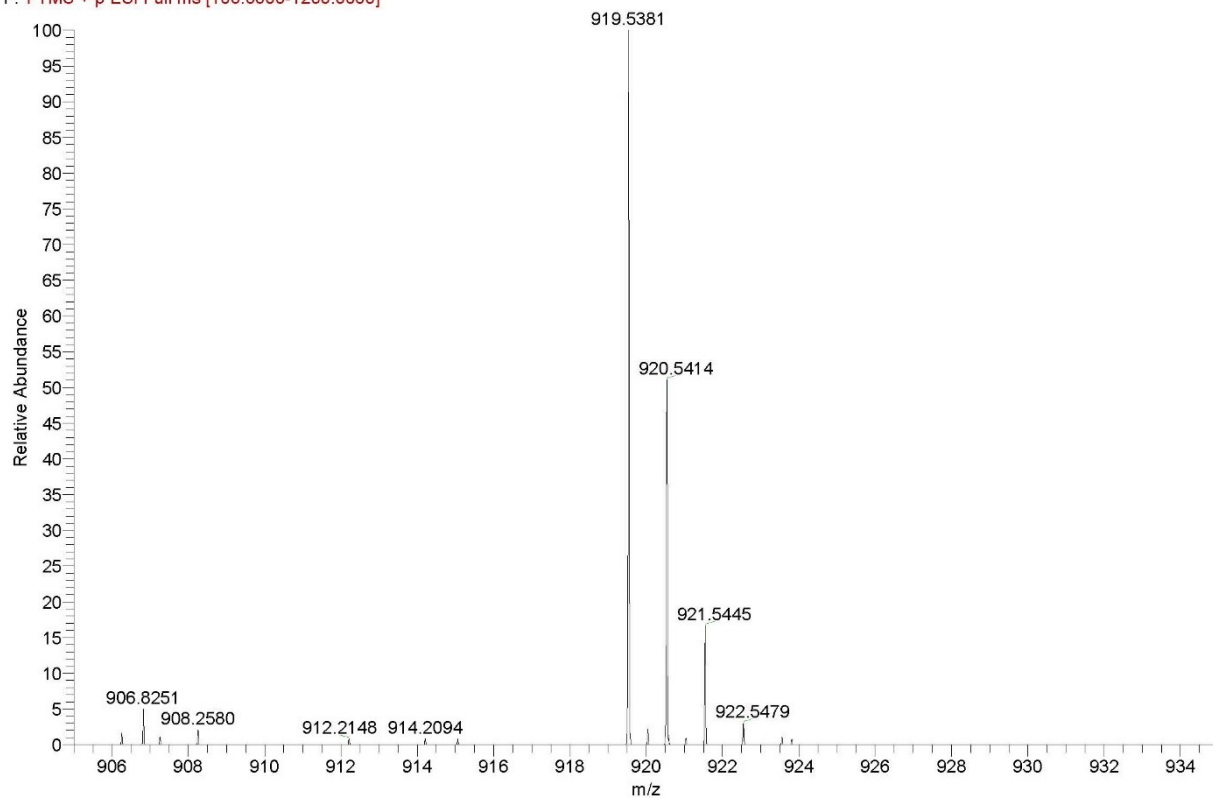


Fig. S25 HRESIMS spectrum of **3**.

— 0422-AMWMB-4-3-6-6-3-6 — 300K/CD3OD — 1D/1H

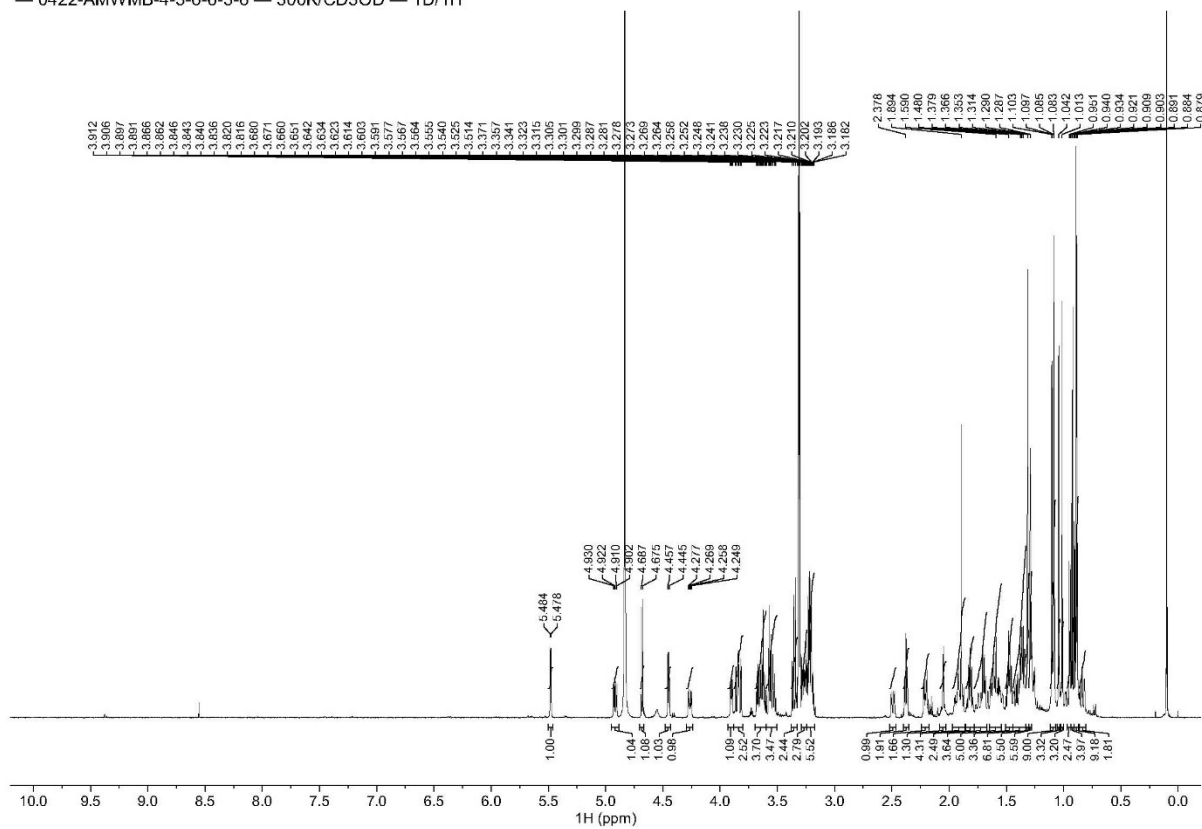


Fig. S26 ^1H NMR spectrum (600 MHz, CD_3OD) of **4**.

— 0422-AMWMB-4-3-6-6-3-6 — 300K/CD3OD — 1D/13C

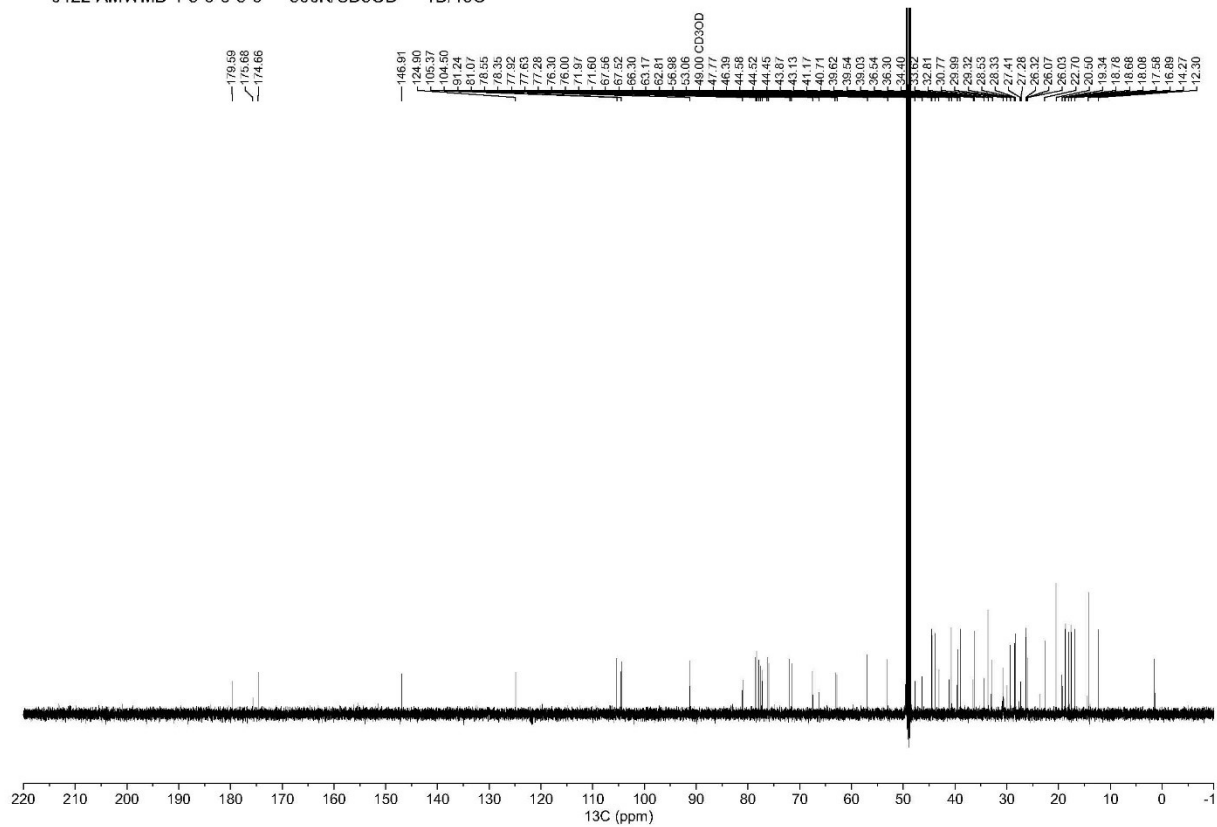


Fig. S27 ^{13}C NMR spectrum (150 MHz, CD_3OD) of **4**.

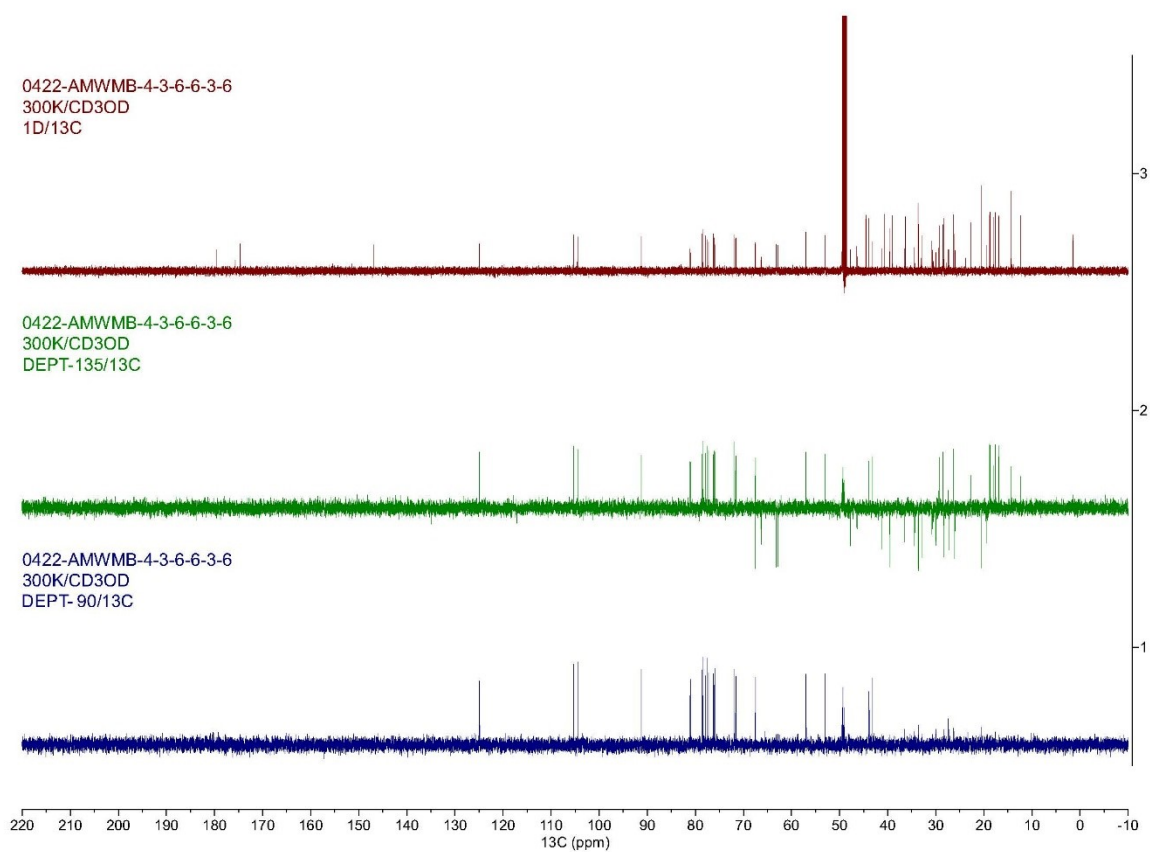


Fig. S28 DEPT spectrum of **4**.

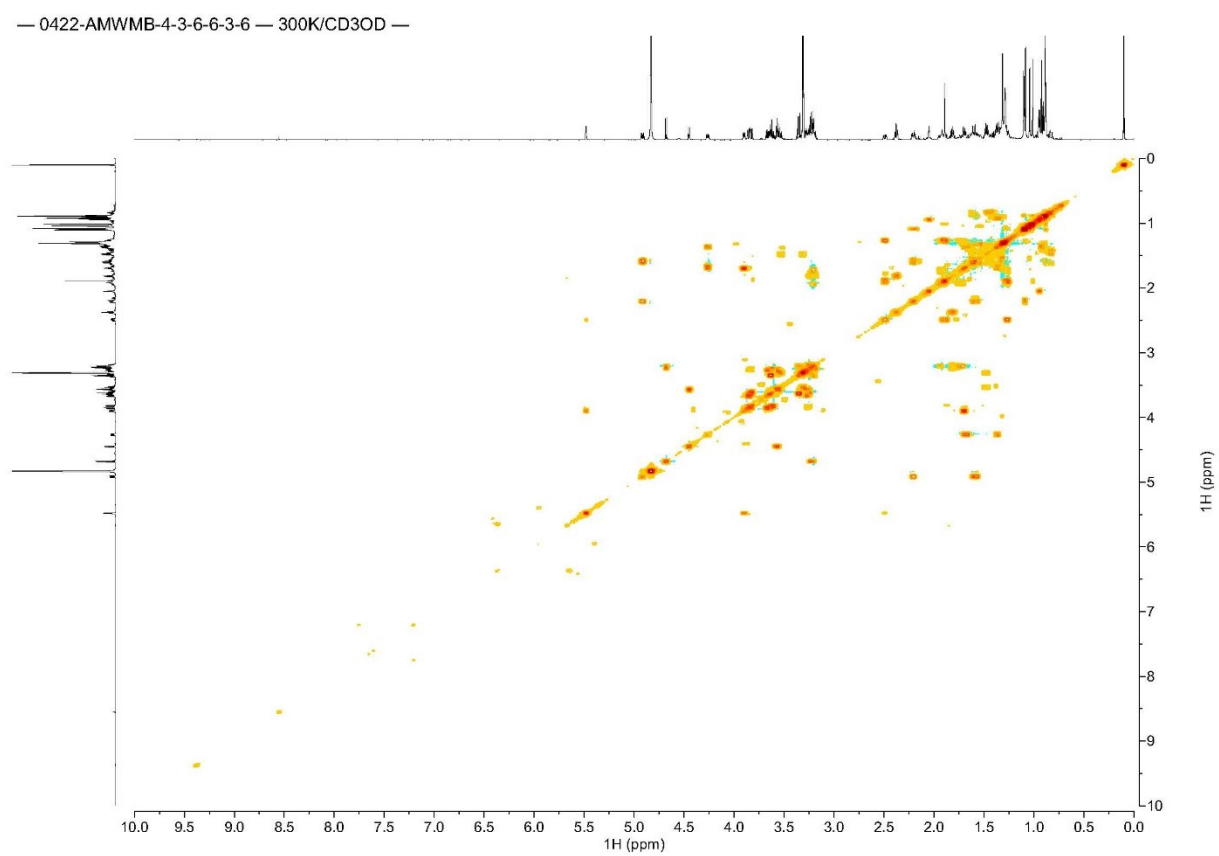


Fig. S29 COSY spectrum of **4**.

— 0422-AMWMB-4-3-6-6-3-6 — 300K/CD3OD —

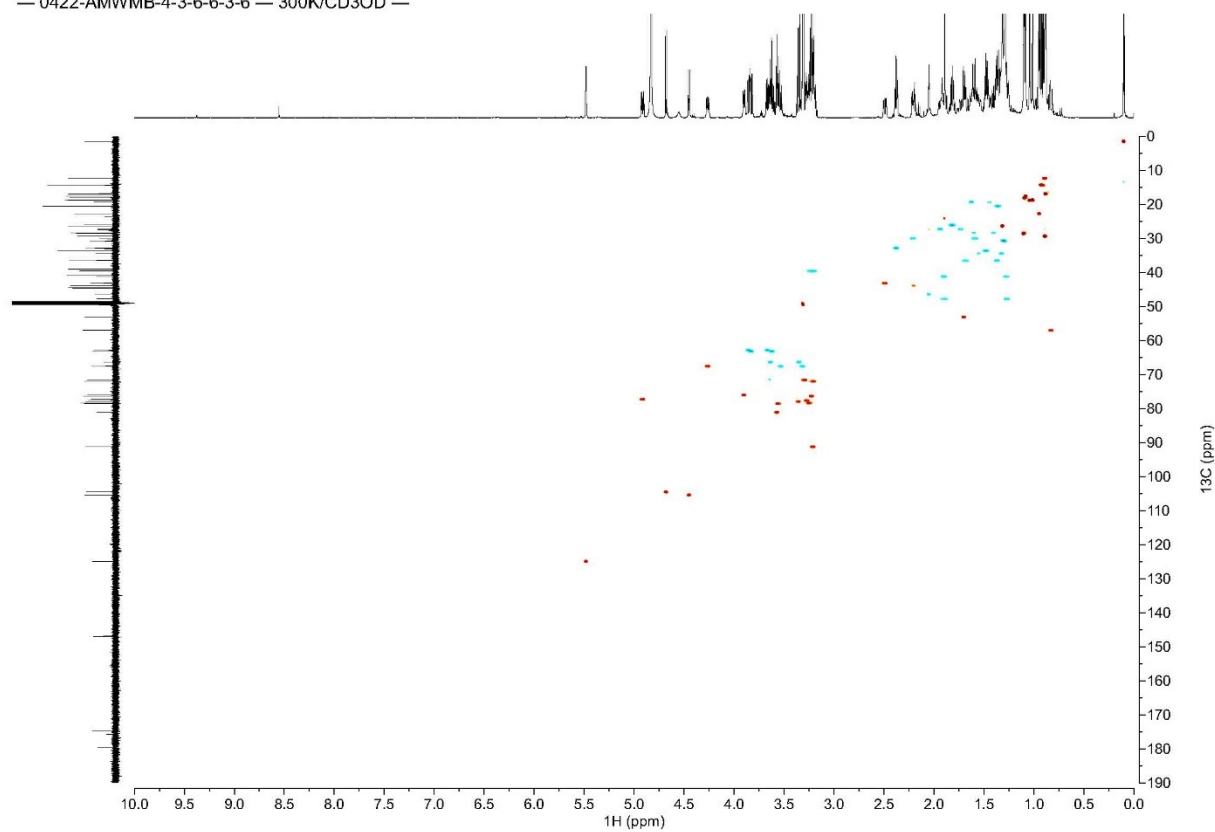


Fig. S30 HSQC spectrum of **4**.

— 0422-AMWMB-4-3-6-6-3-6 — 300K/CD3OD —

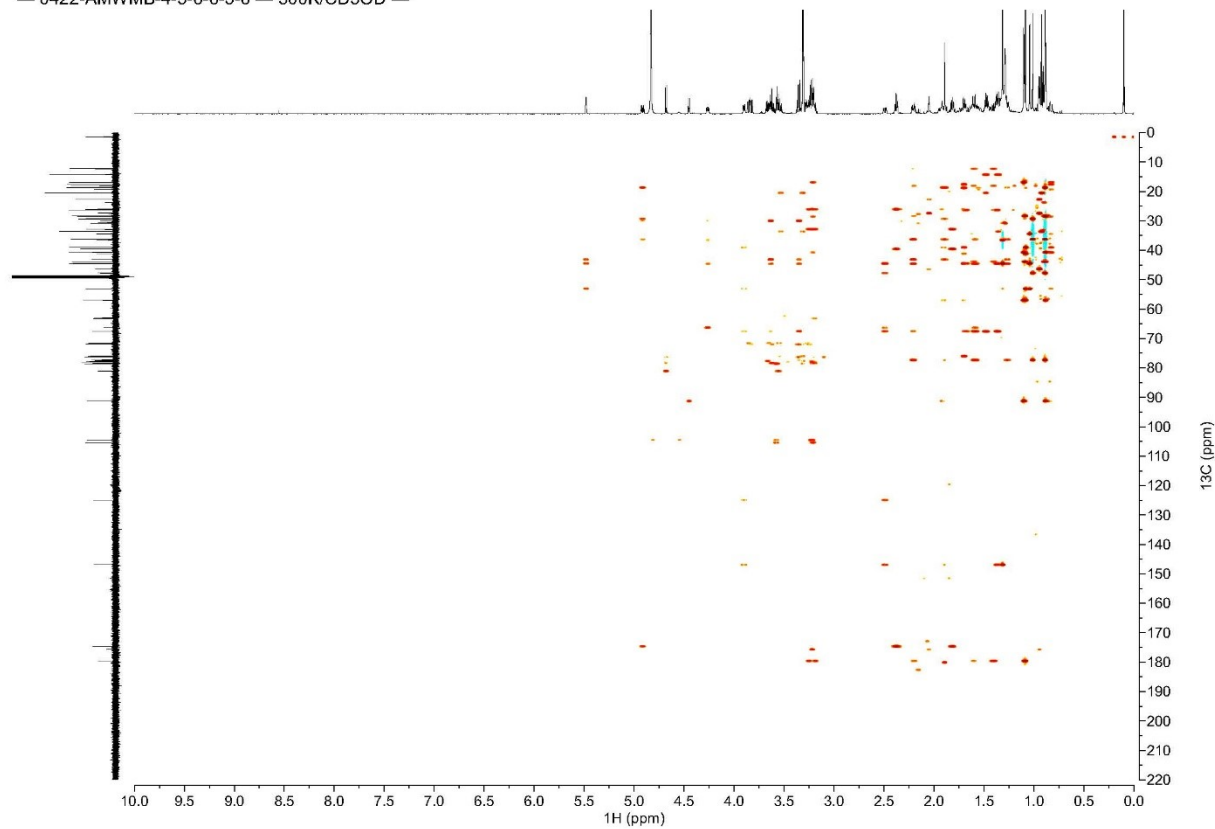


Fig. S31 HMBC spectrum of **4**.

— 0427-AMWMB-4-3-6-6-3-6 — 300K/CD3OD —

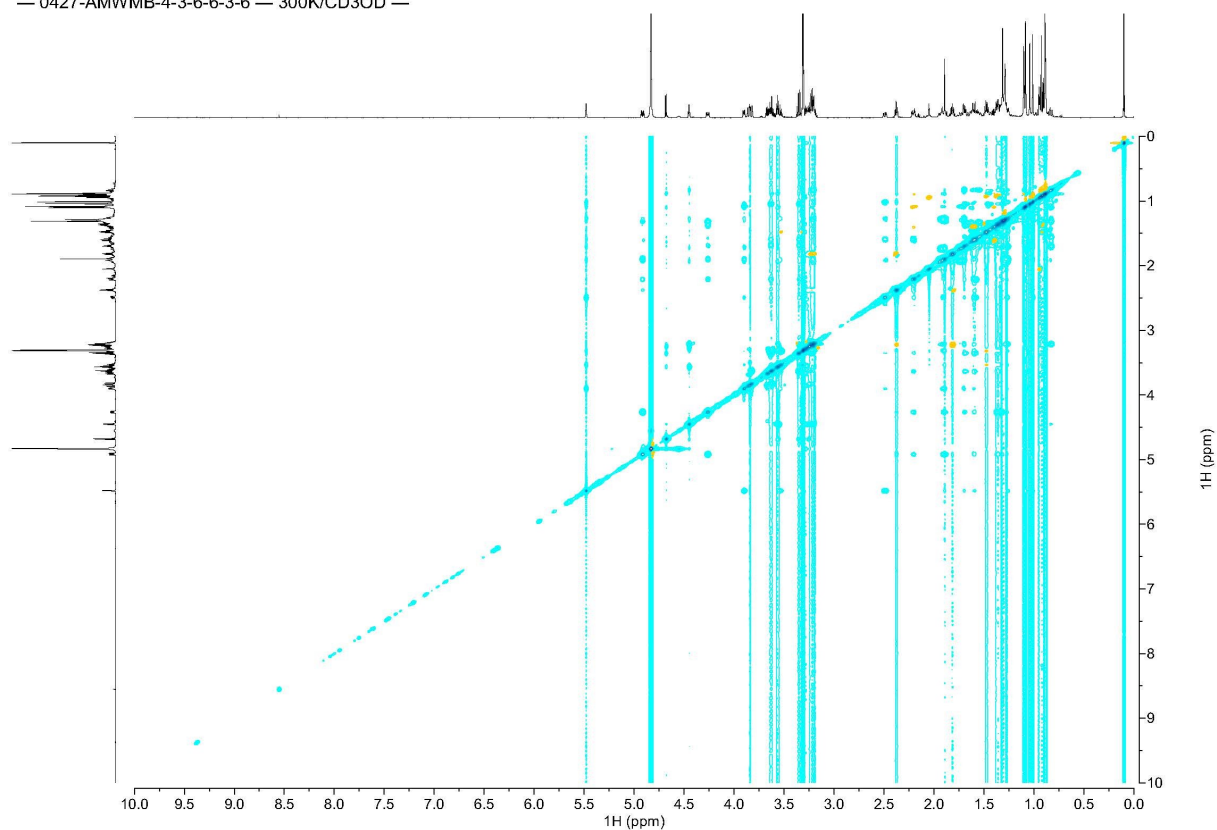


Fig. S32 NOESY spectrum of **4**.

AMWMB_4_3_6_6_3_6_P

06/17/24 22:17:46

Leu

AMWMB_4_3_6_6_3_6_P#2198 RT: 6.68 AV: 1 NL: 3.62E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]

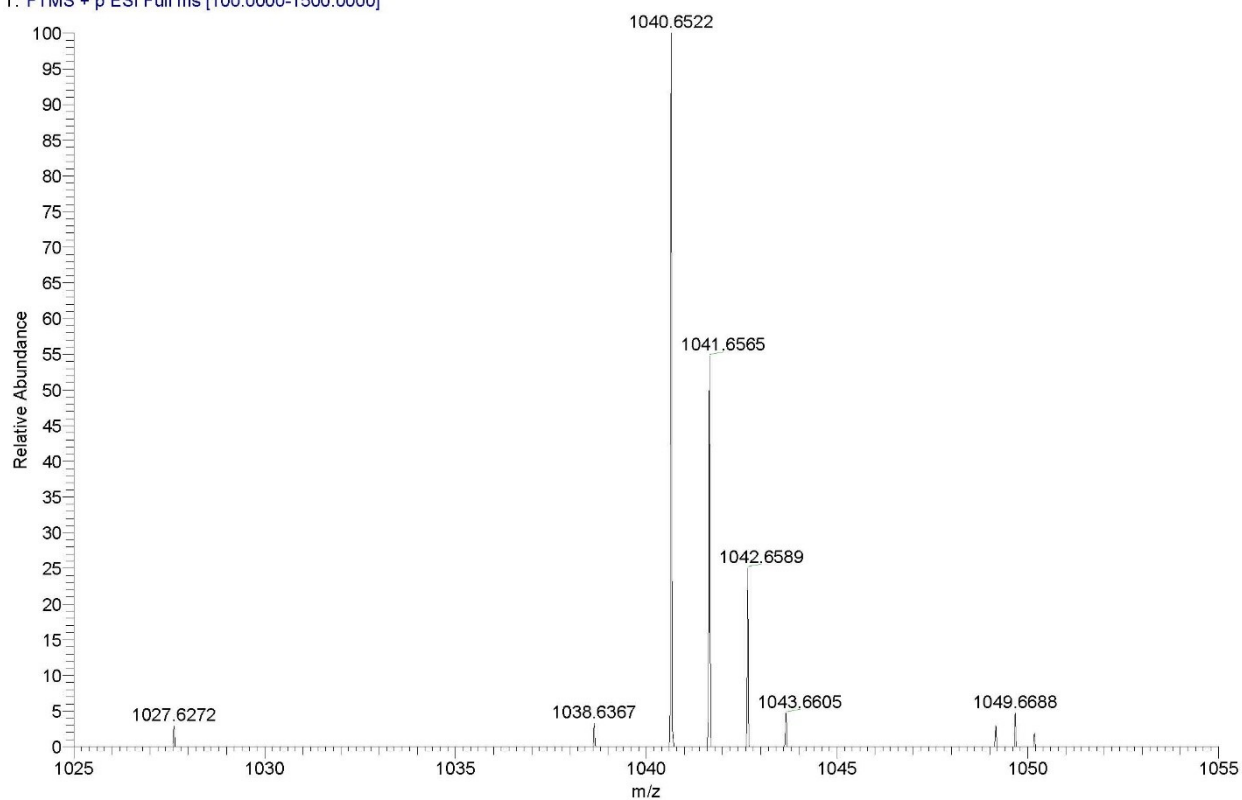


Fig. S33 HRESIMS spectrum of **4**.

— 800MHz ^1H D/ ^1H

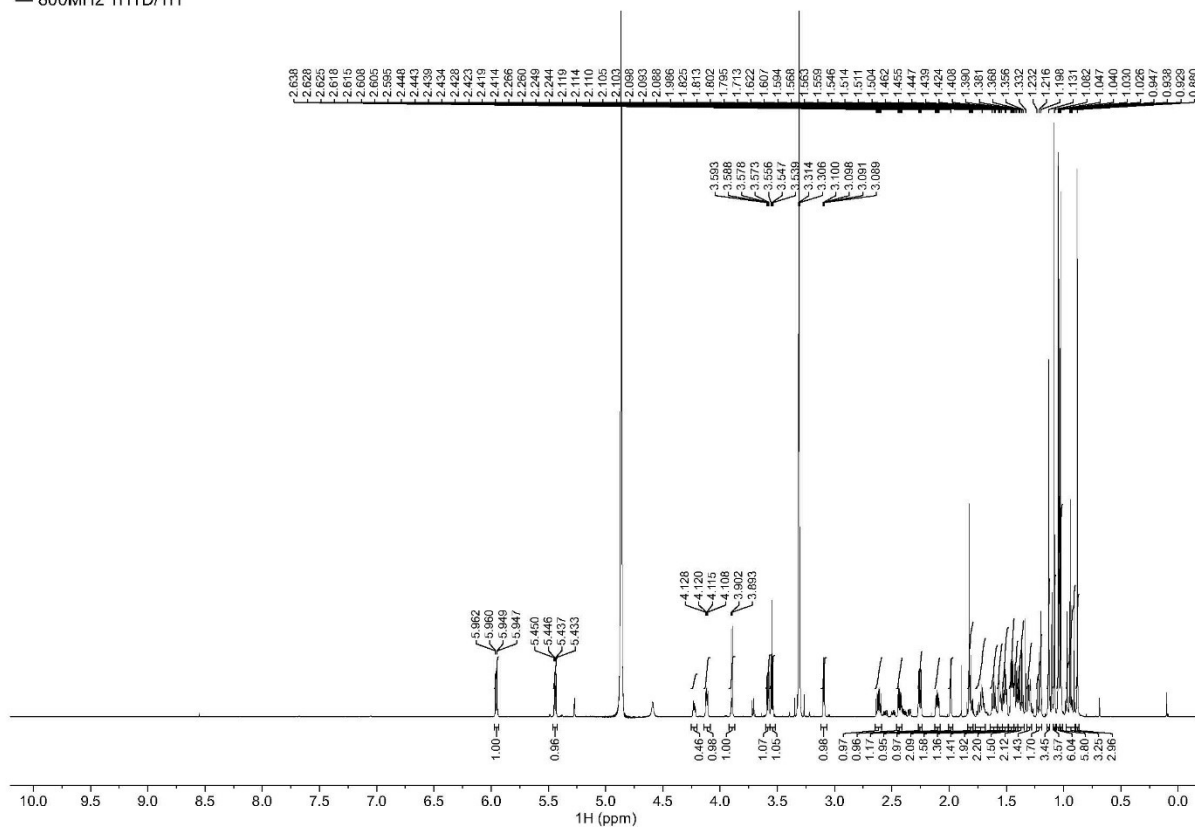


Fig. S34 ^1H NMR spectrum (800 MHz, CD_3OD) of **5**.

— 800MHz ^{13}C D/ ^{13}C

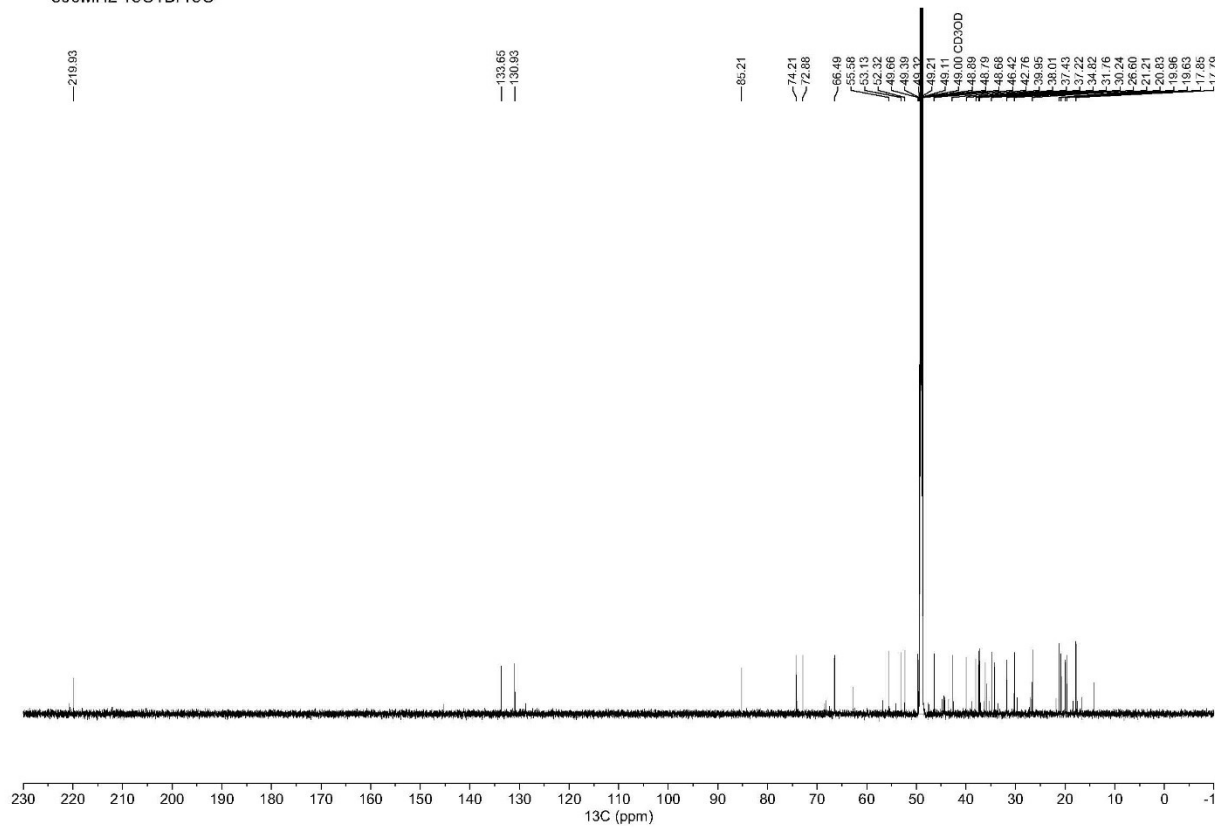


Fig. S35 ^{13}C NMR spectrum (200 MHz, CD_3OD) of **5**.

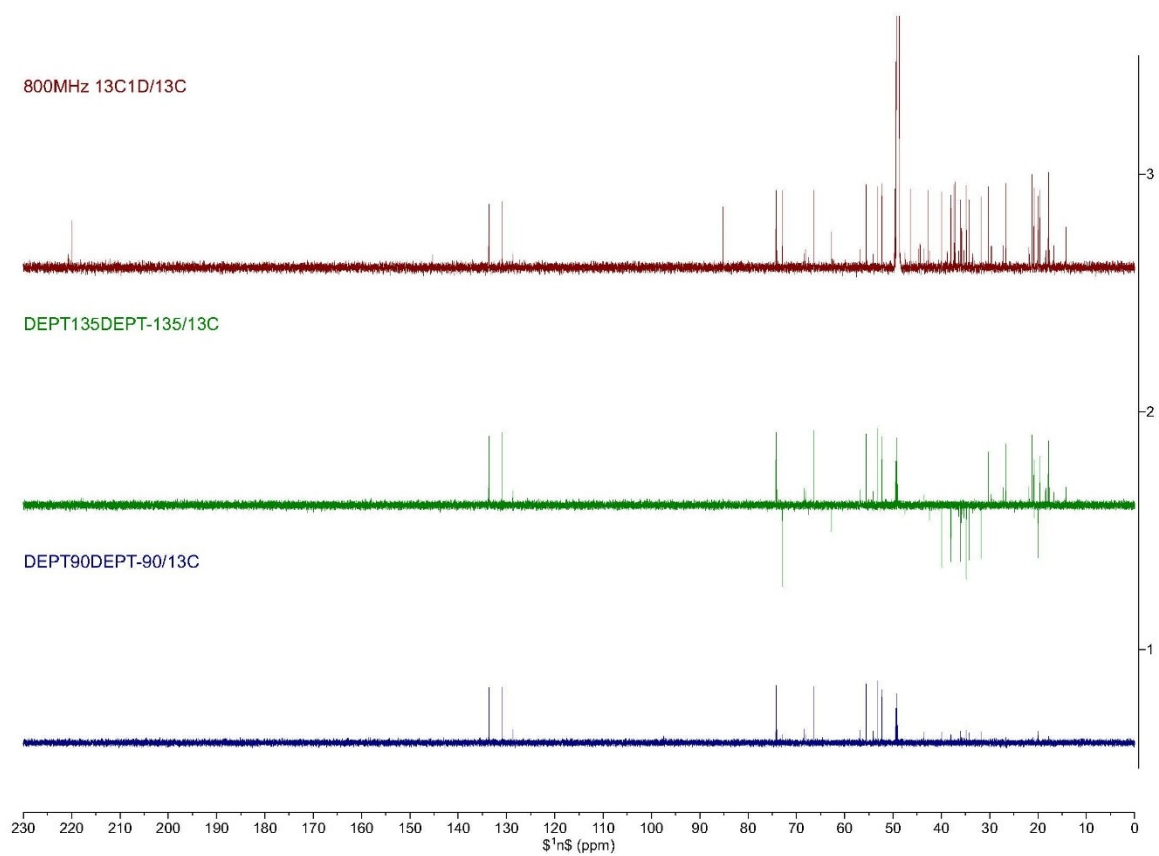


Fig. S36 DEPT spectrum of **5**.

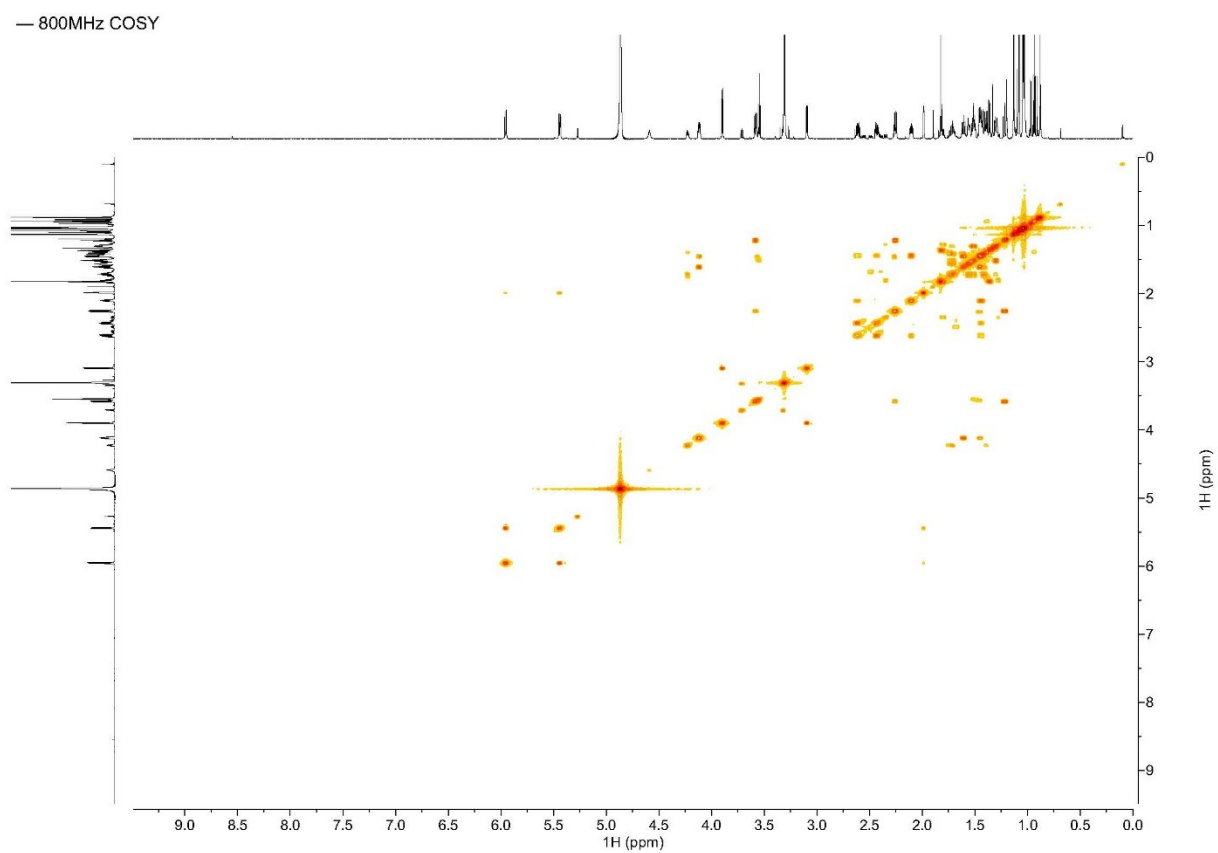


Fig. S37 COSY spectrum of **5**.

— 800MHz HSQC

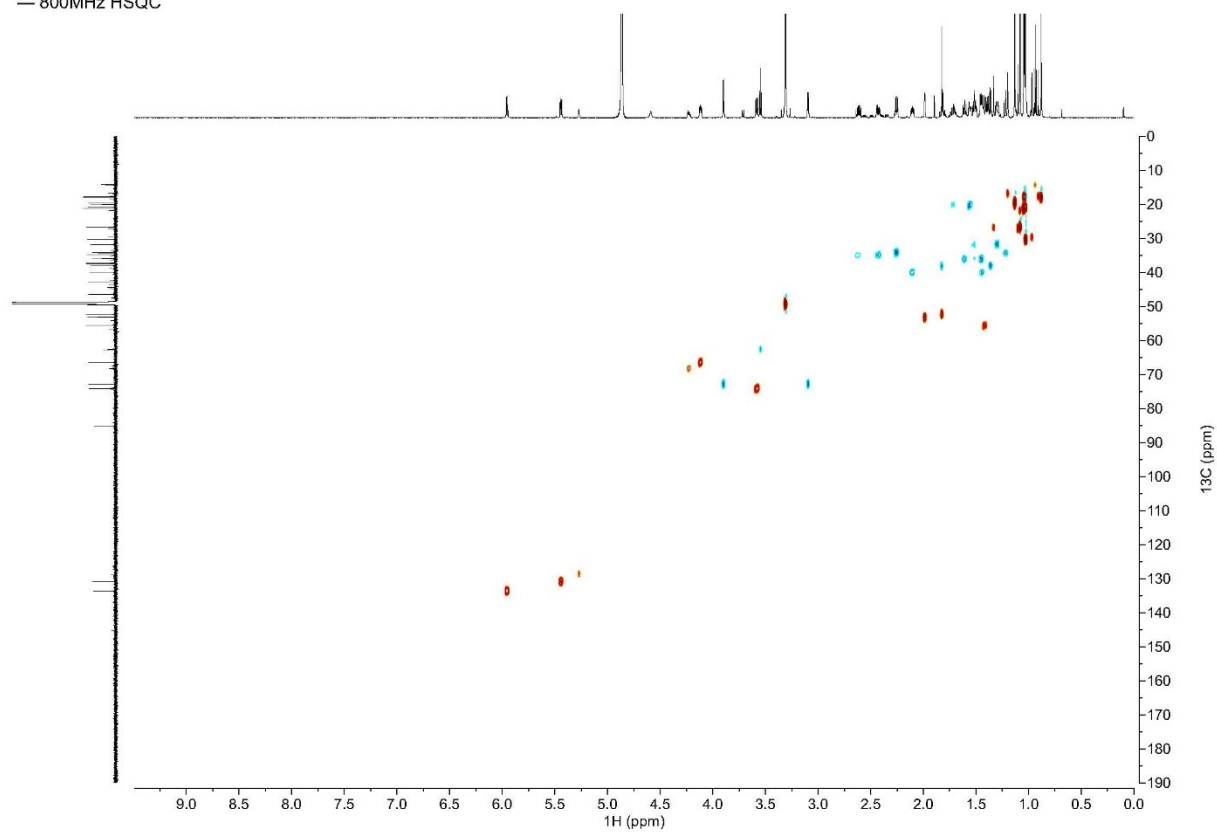


Fig. S38 HSQC spectrum of **5**.

— 800MHz HMBC

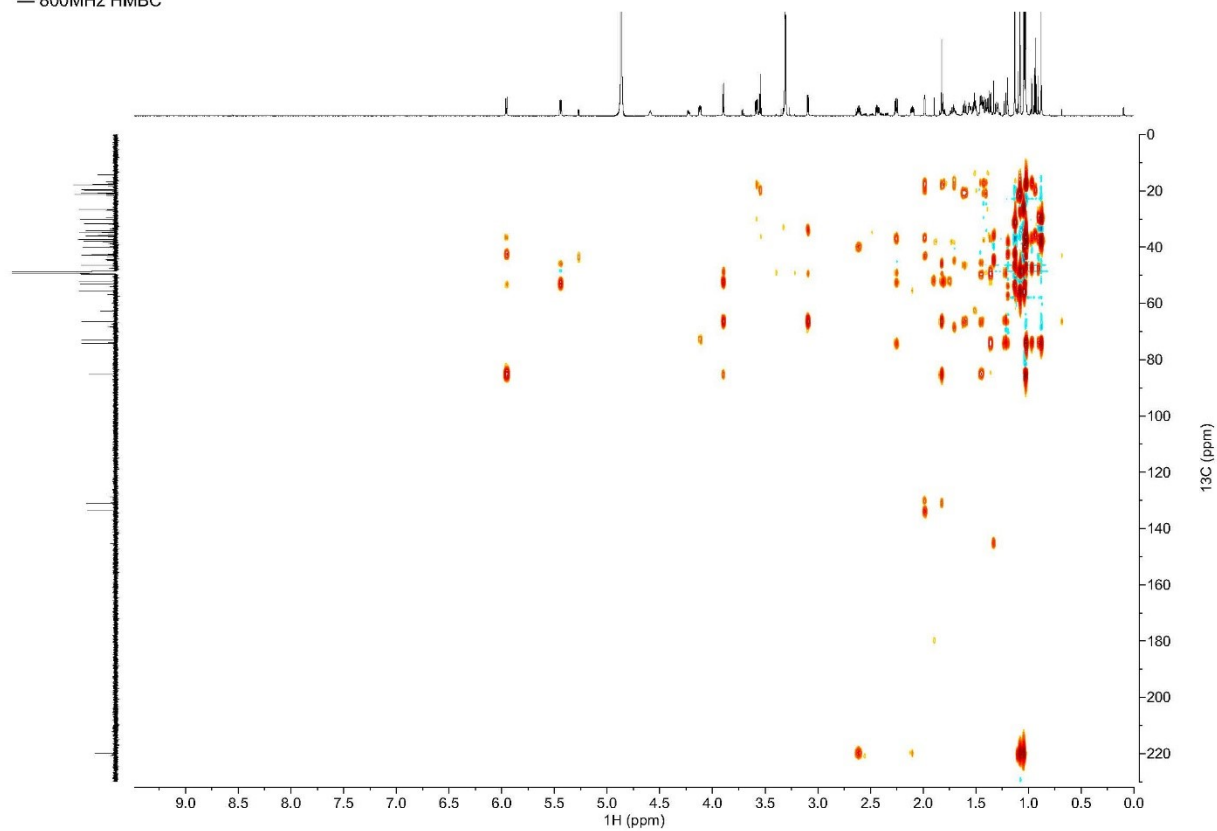


Fig. S39 HMBC spectrum of **5**.

— 0421-AMWMH-6-8-14-3 — 300K/CD₃OD —

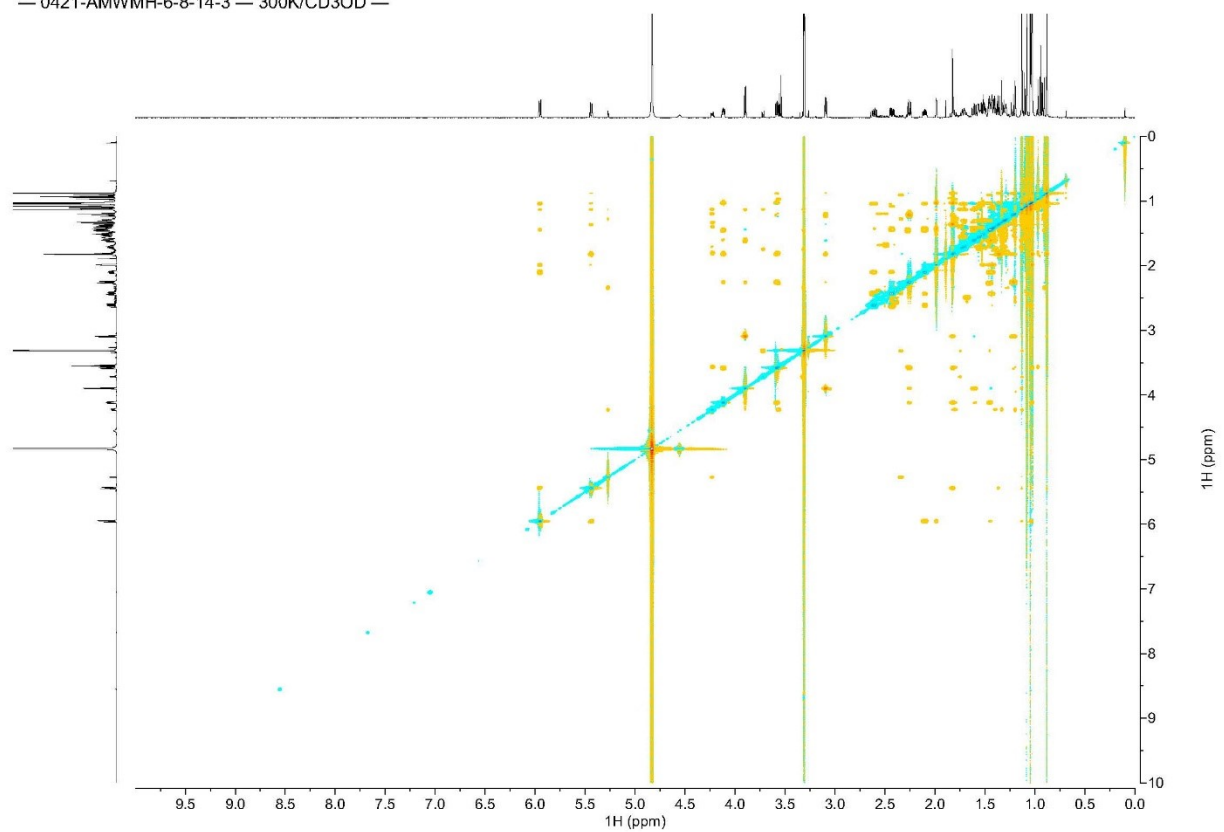


Fig. S40 NOESY spectrum (600 MHz, CD₃OD) of **5**.

D:\000-MS_Ori_work\...AMWMH_6_8_14_3_P

06/17/24 19:24:00

Leu

AMWMH_6_8_14_3_P #2125 RT: 6.01 AV: 1 NL: 1.12E5

T: FTMS + p ESI Full ms [100.0000-1500.0000]

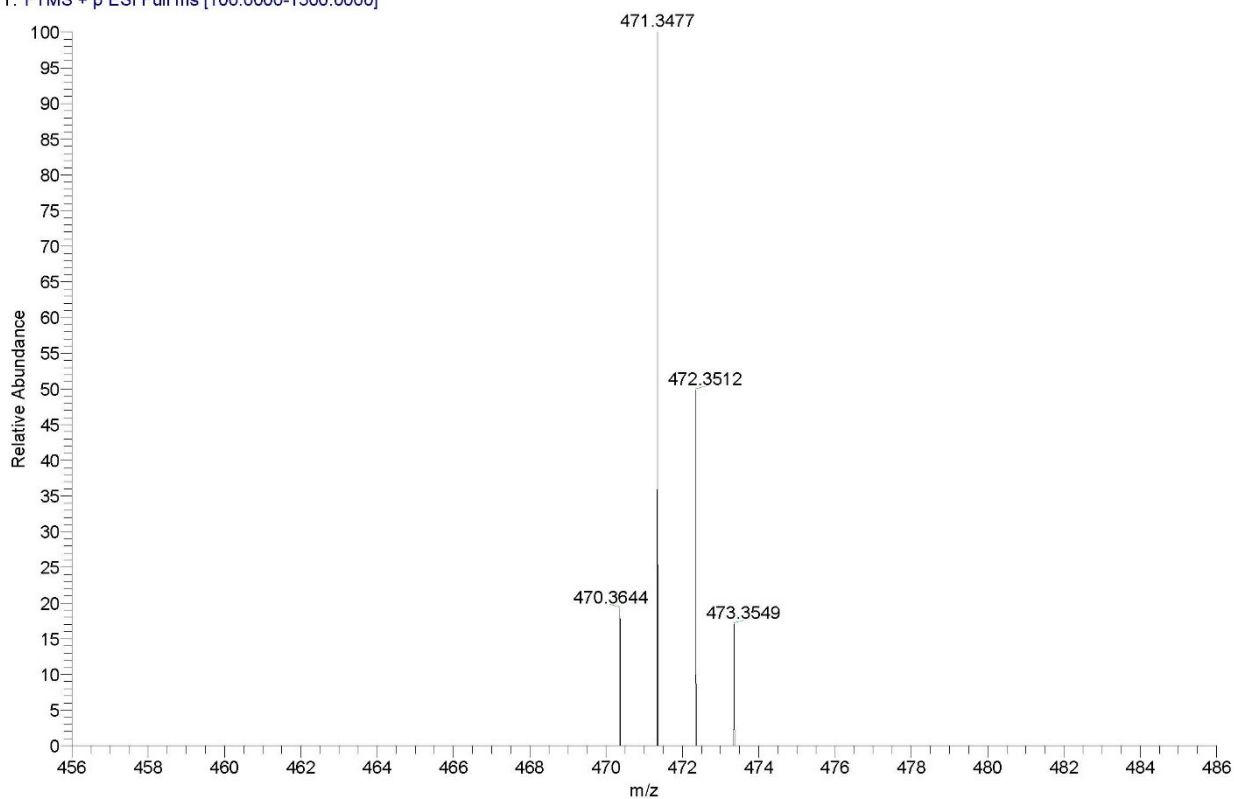


Fig. S41 HRESIMS spectrum of **5**.

— 800MHz ¹H — AMWMH-6-11-11-51D/1H

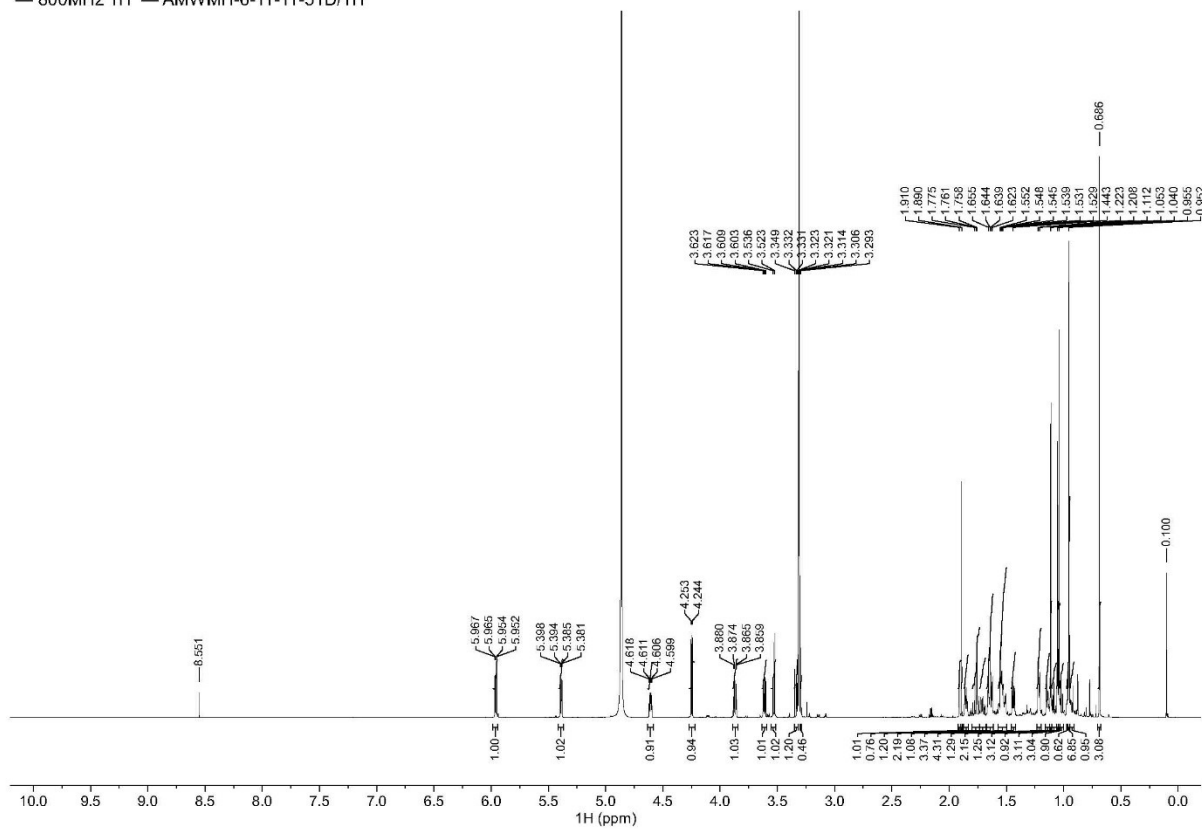


Fig. S42 ¹H NMR spectrum (800 MHz, CD₃OD) of **6**.

— 800MHz ¹³C1D/13C

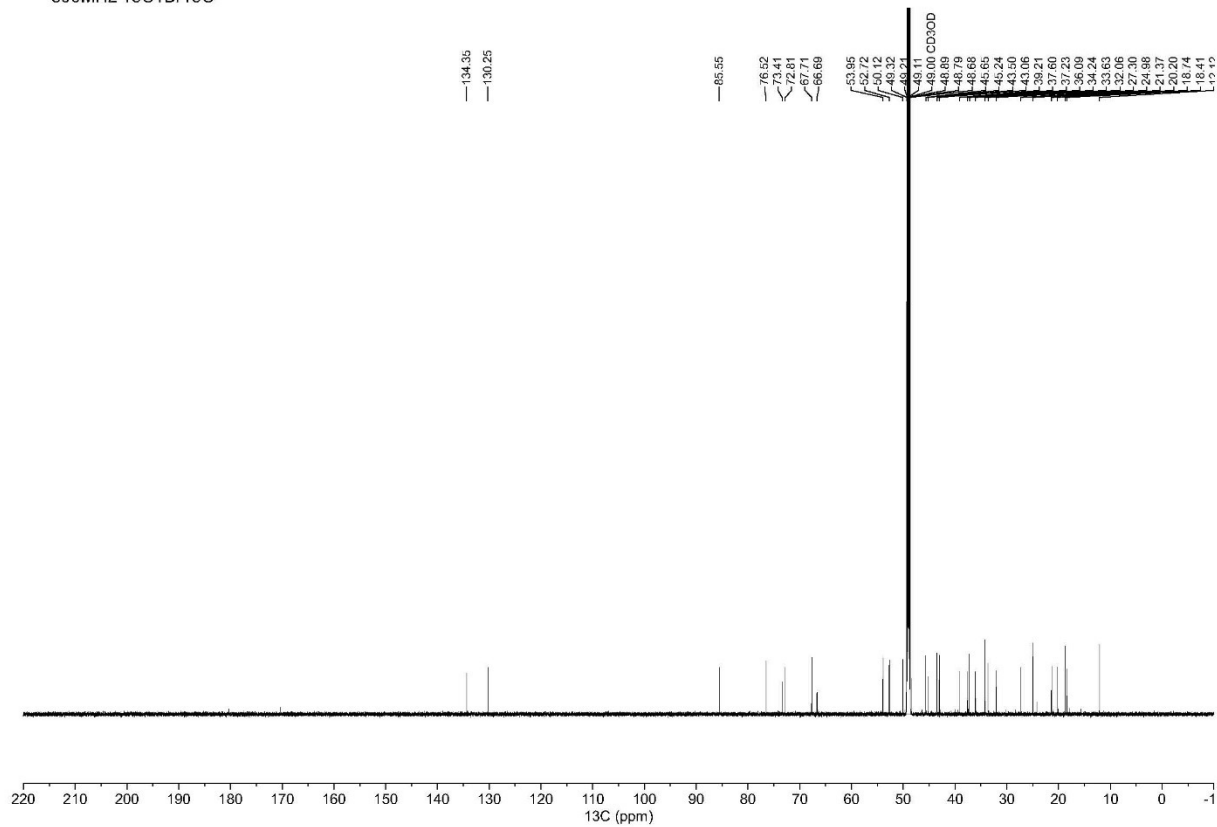


Fig. S43 ¹³C NMR spectrum (200 MHz, CD₃OD) of **6**.

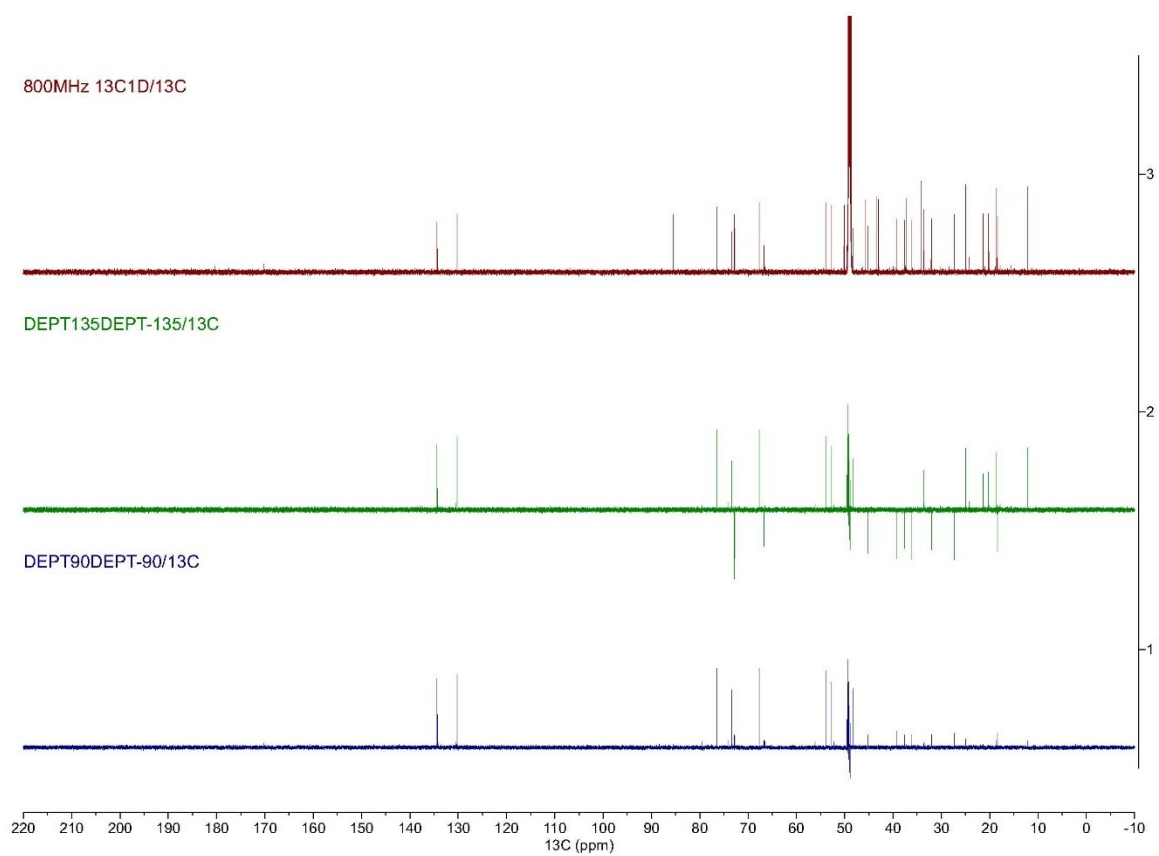


Fig. S44 DEPT spectrum of **6**.

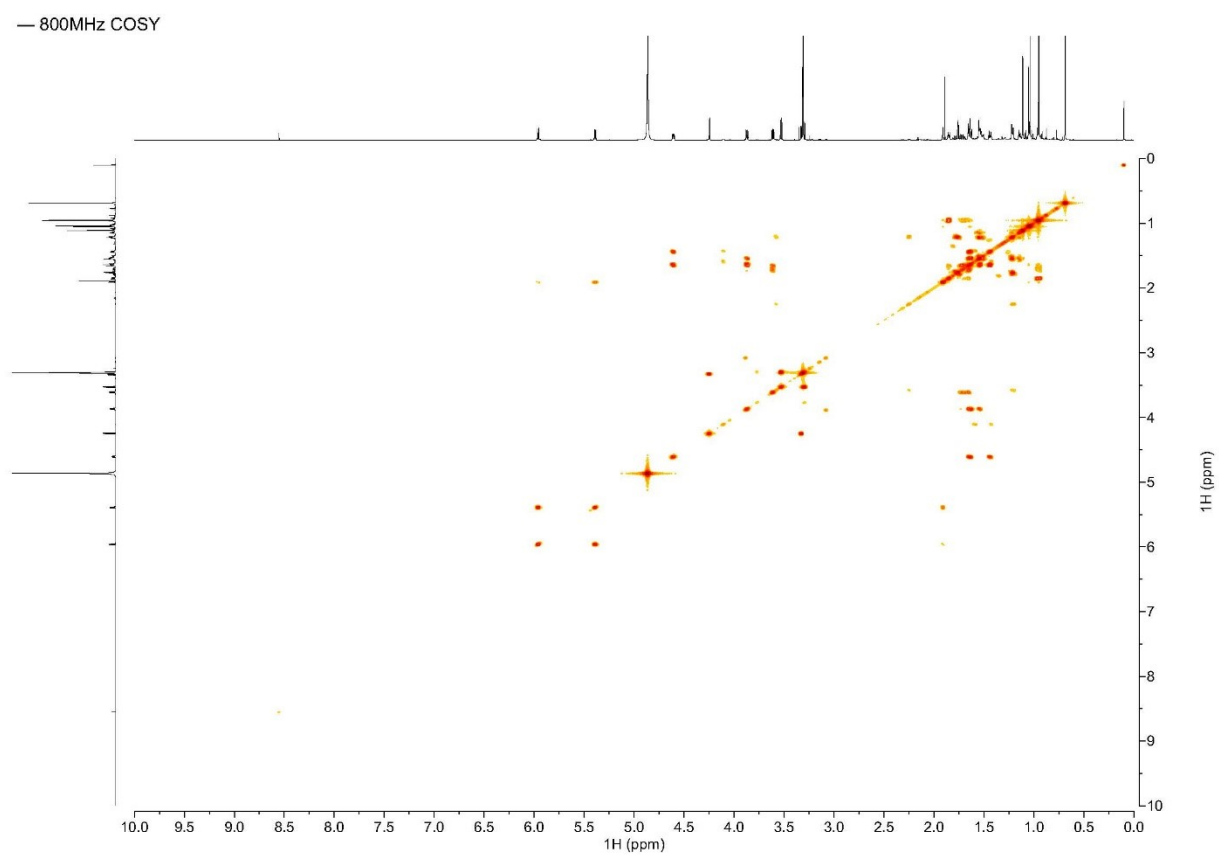


Fig. S45 COSY spectrum of **6**.

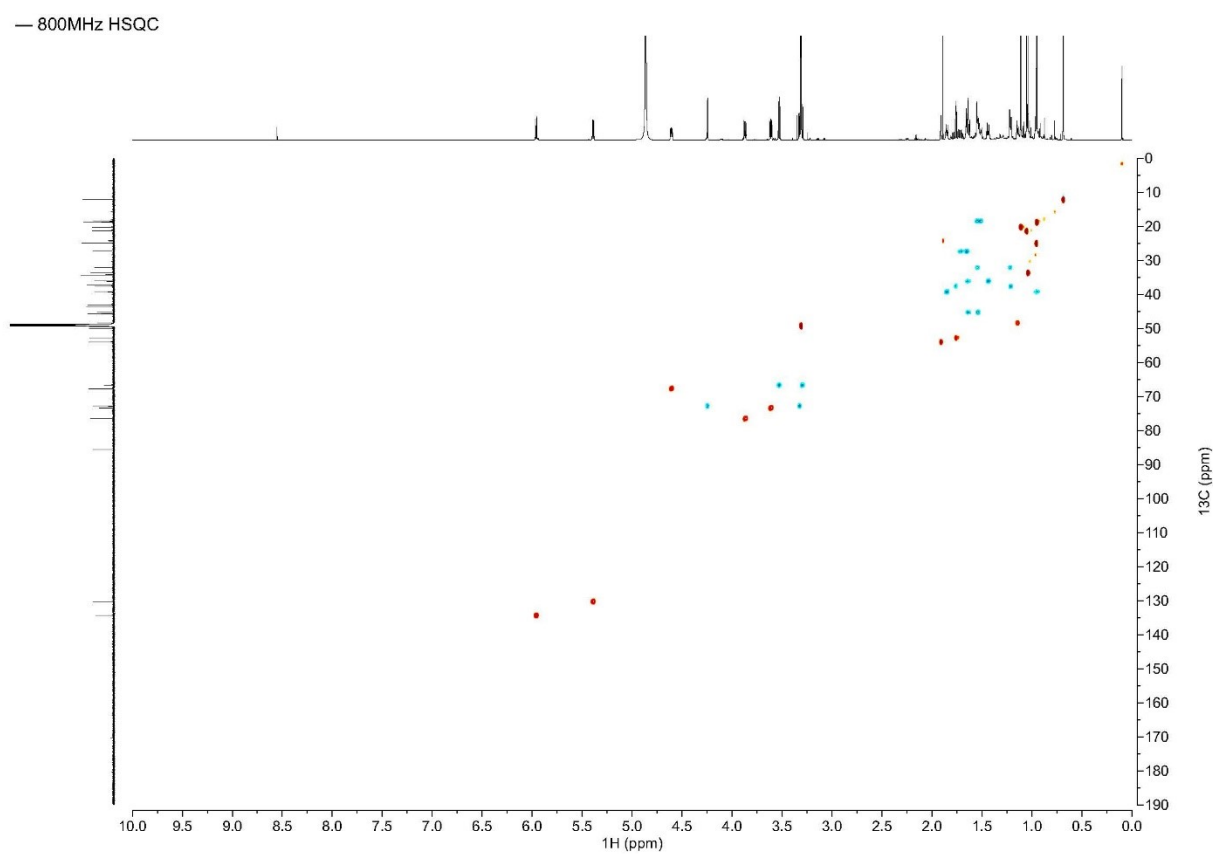


Fig. S46 HSQC spectrum of **6**.

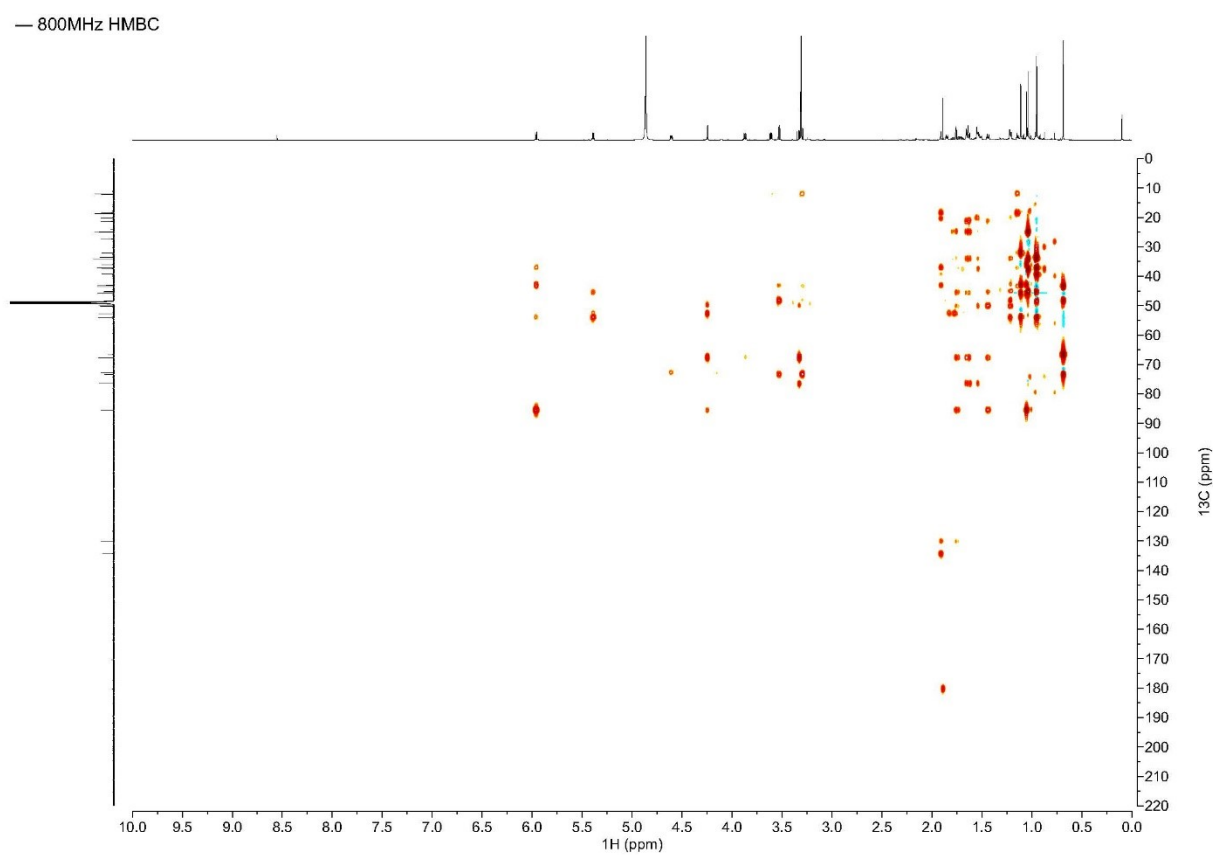


Fig. S47 HMBC spectrum of **6**.

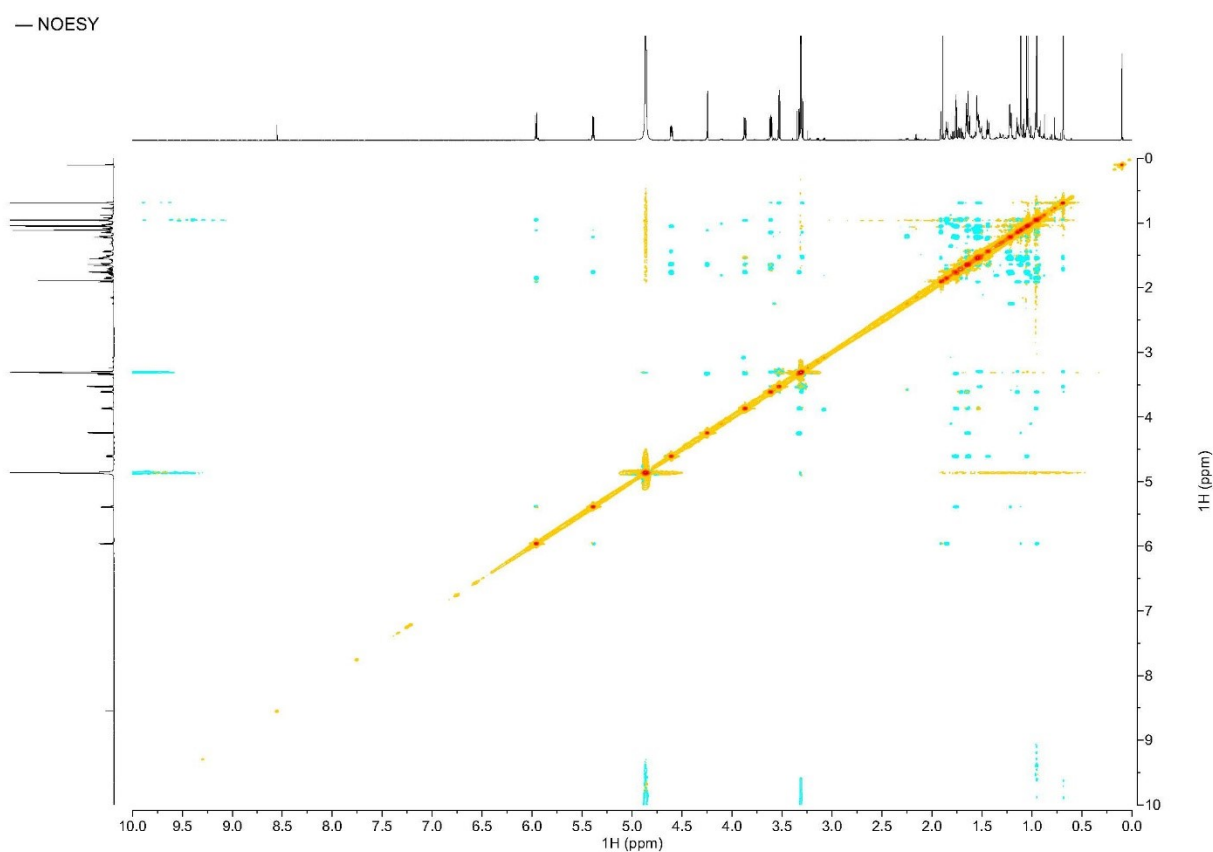


Fig. S48 NOESY spectrum of **6**.

D:\000-MS_Ori_work\...AMWMH_6_11_11_5_P

06/17/24 21:40:21

Leu

AMWMH_6_11_11_5_P #2161 RT: 6.54 AV: 1 NL: 9.43E6

T: FTMS + p ESI Full ms [100.0000-1500.0000]

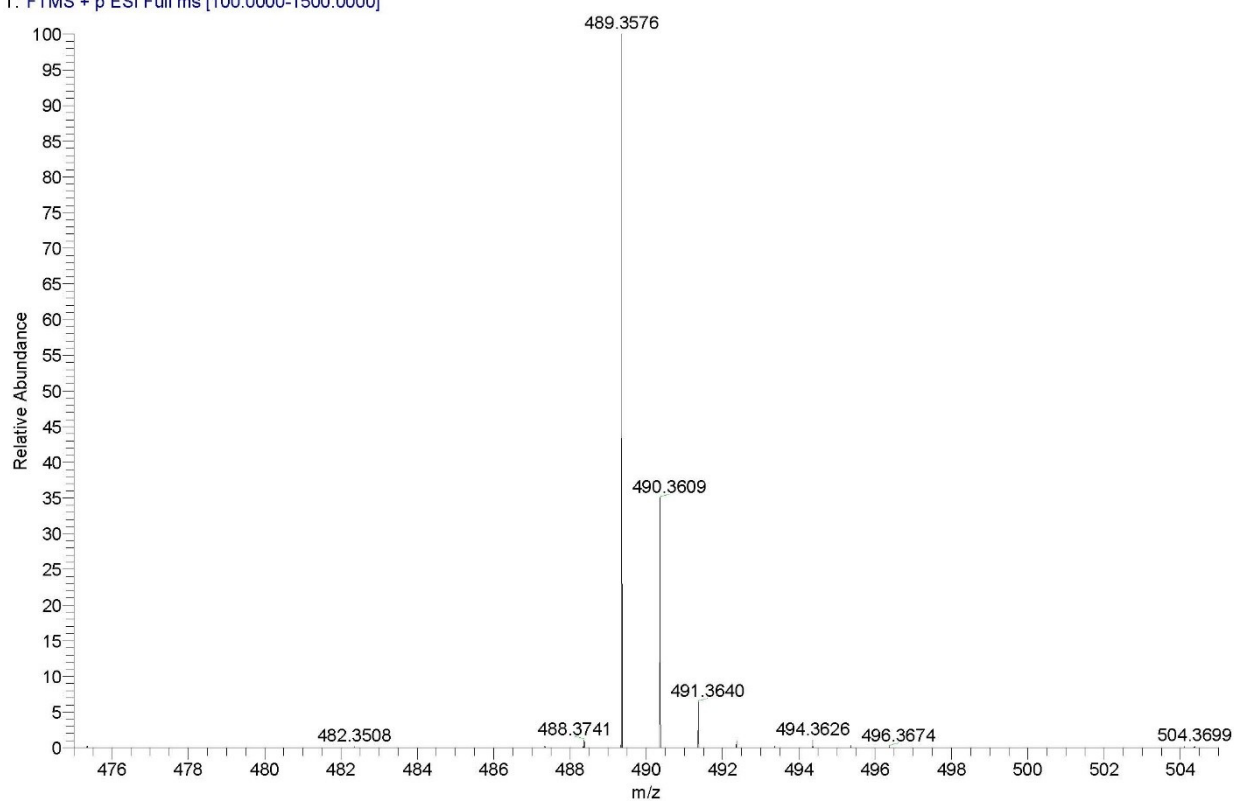


Fig. S49 HRESIMS spectrum of **6**.

— 0419-AMWMH-4-10-6-2 — 300K/CD₃OD — 1D/¹H

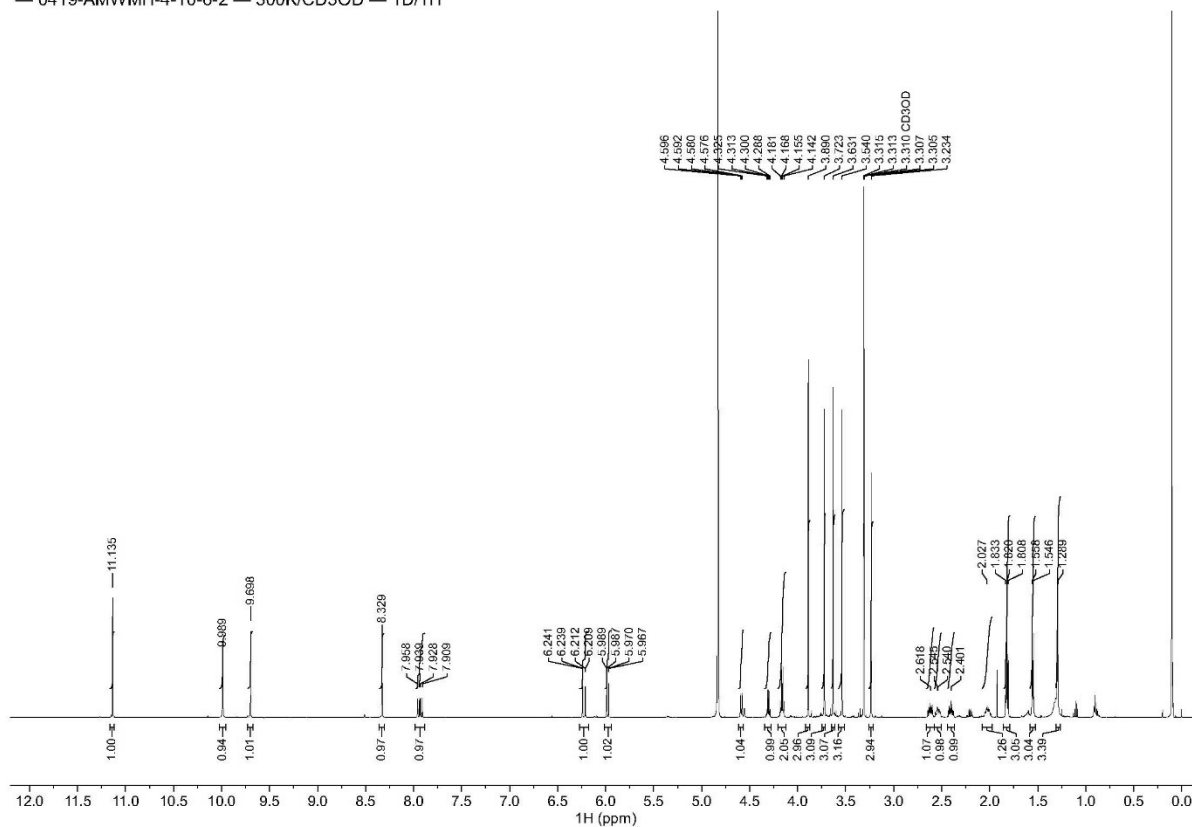


Fig. S50 ¹H NMR spectrum (600 MHz, CD₃OD) of **7**.

— 0419-AMWMH-4-10-6-2 — 300K/CD₃OD — 1D/¹³C

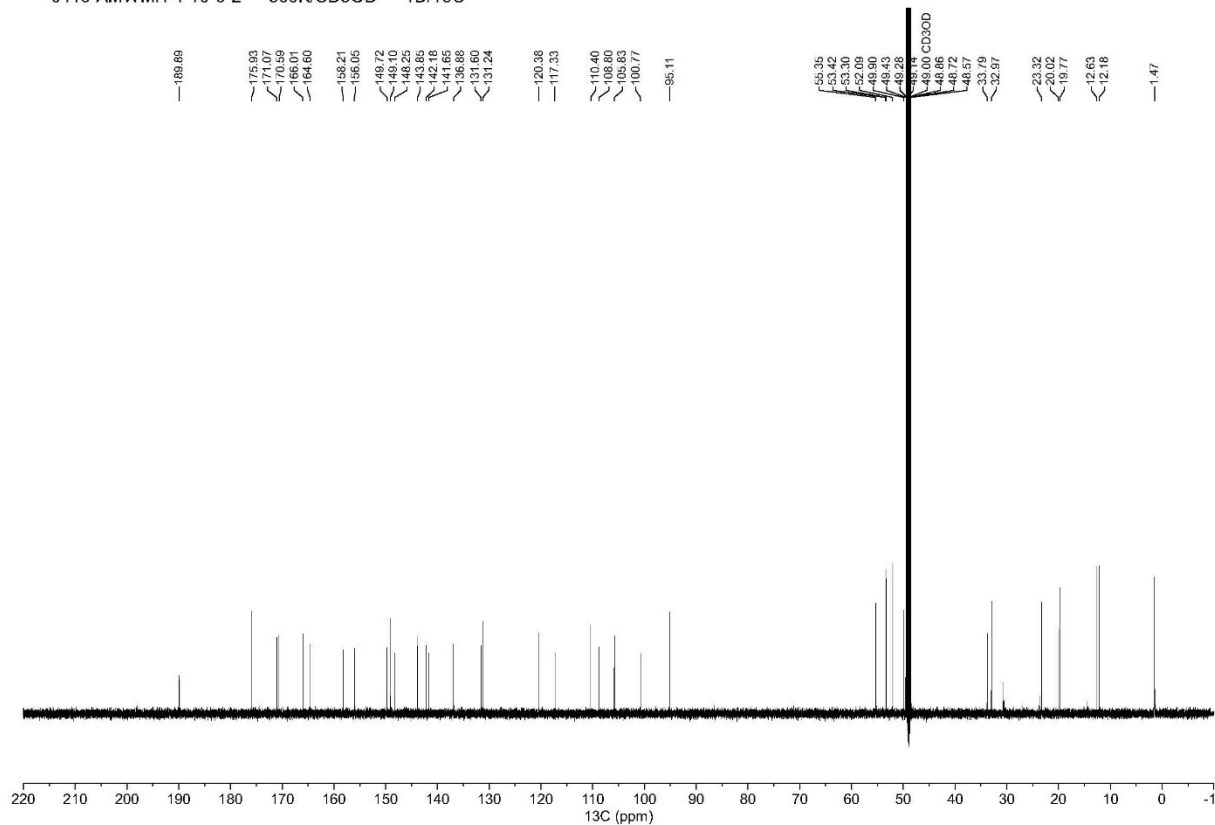


Fig. S51 ¹³C NMR spectrum (150 MHz, CD₃OD) of **7**.

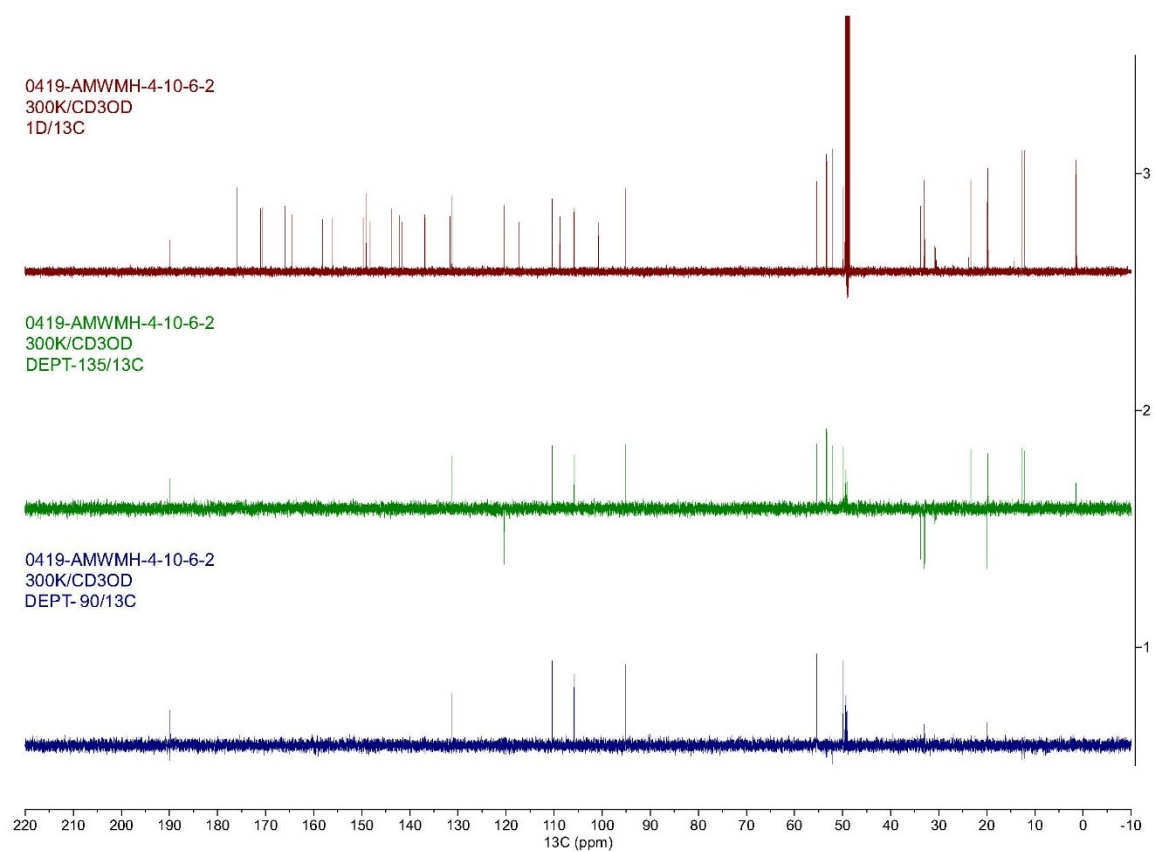


Fig. S52 DEPT spectrum of 7.

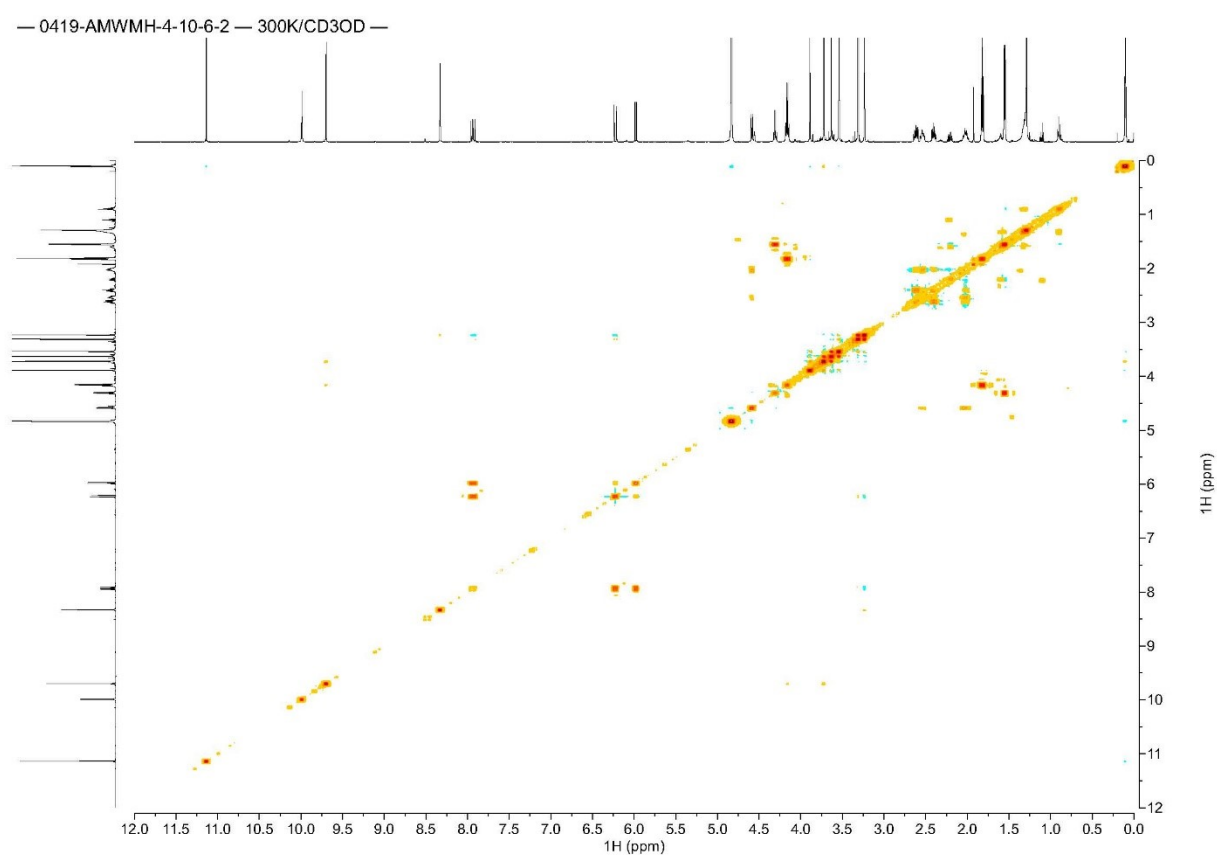


Fig. S53 COSY spectrum of 7.

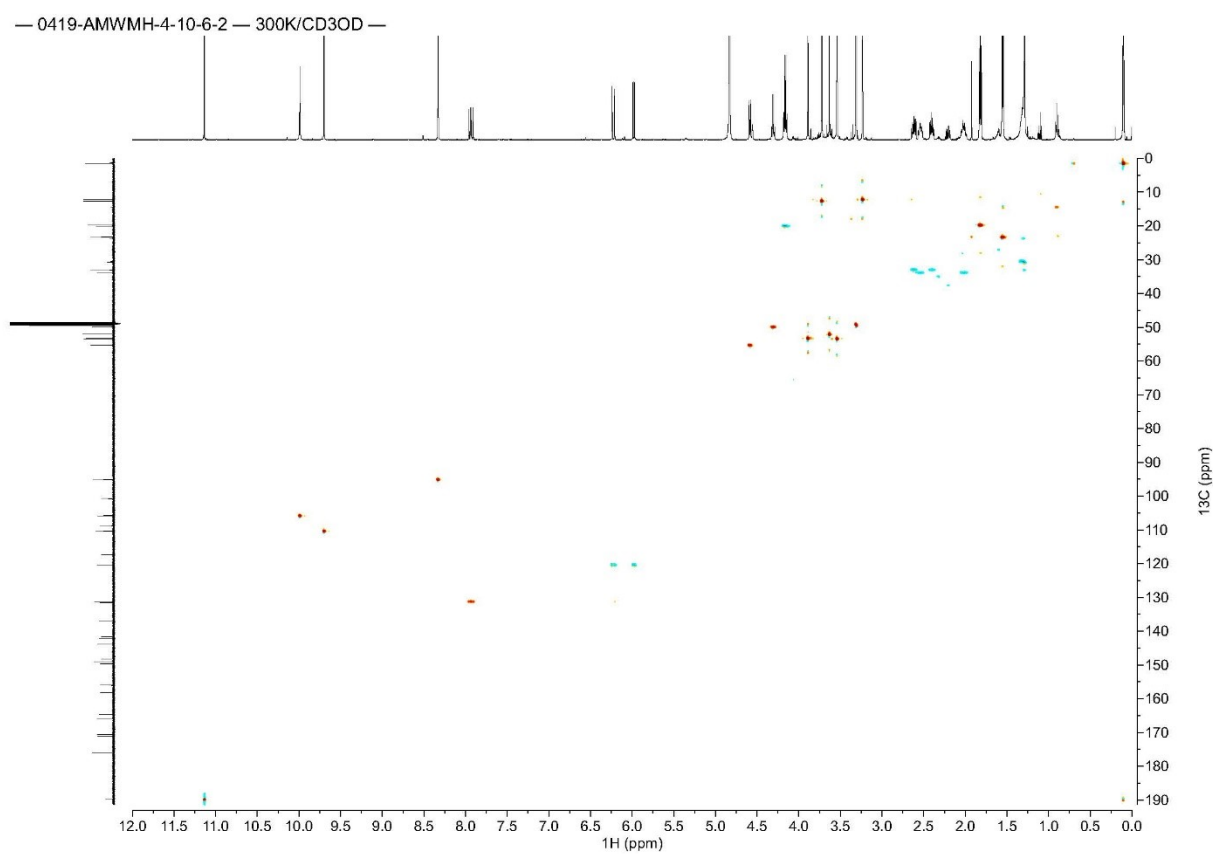


Fig. S54 HSQC spectrum of **7**.

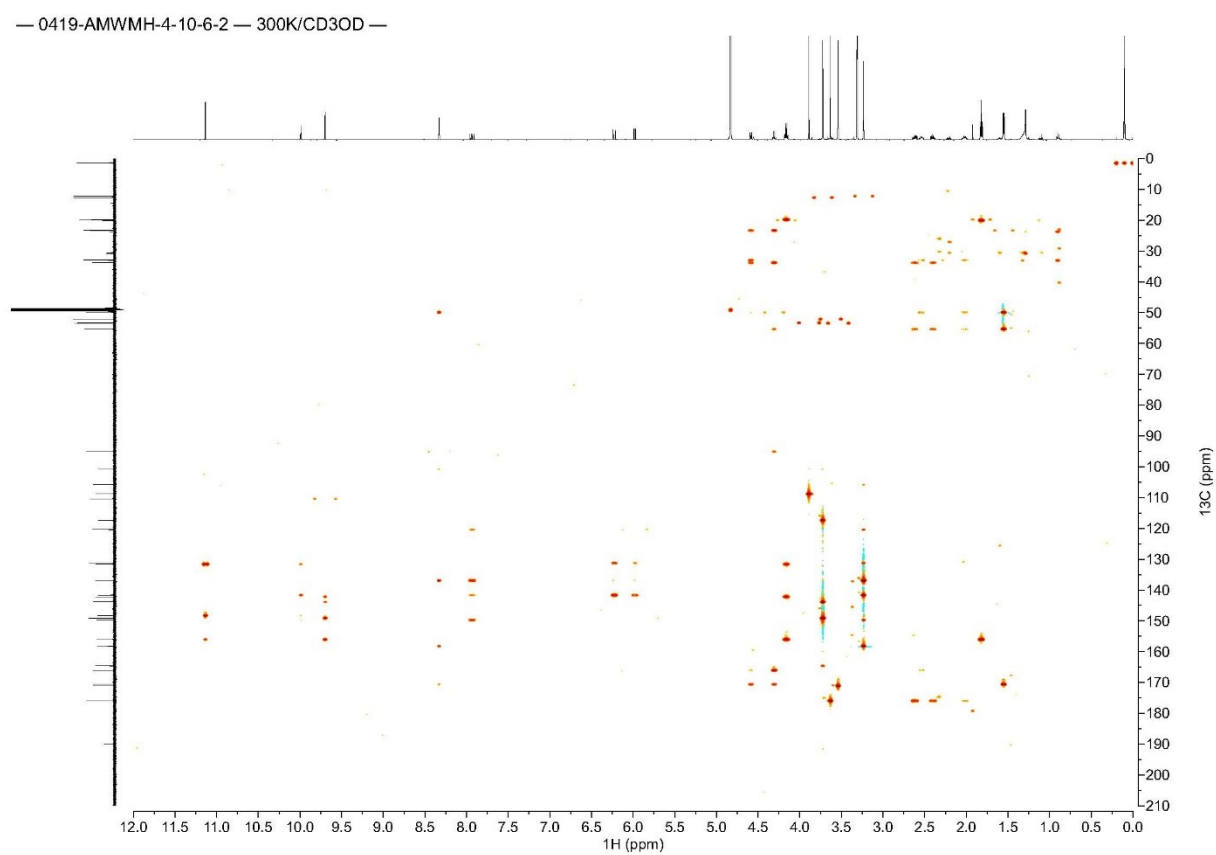


Fig. S55 HMBC spectrum of **7**.

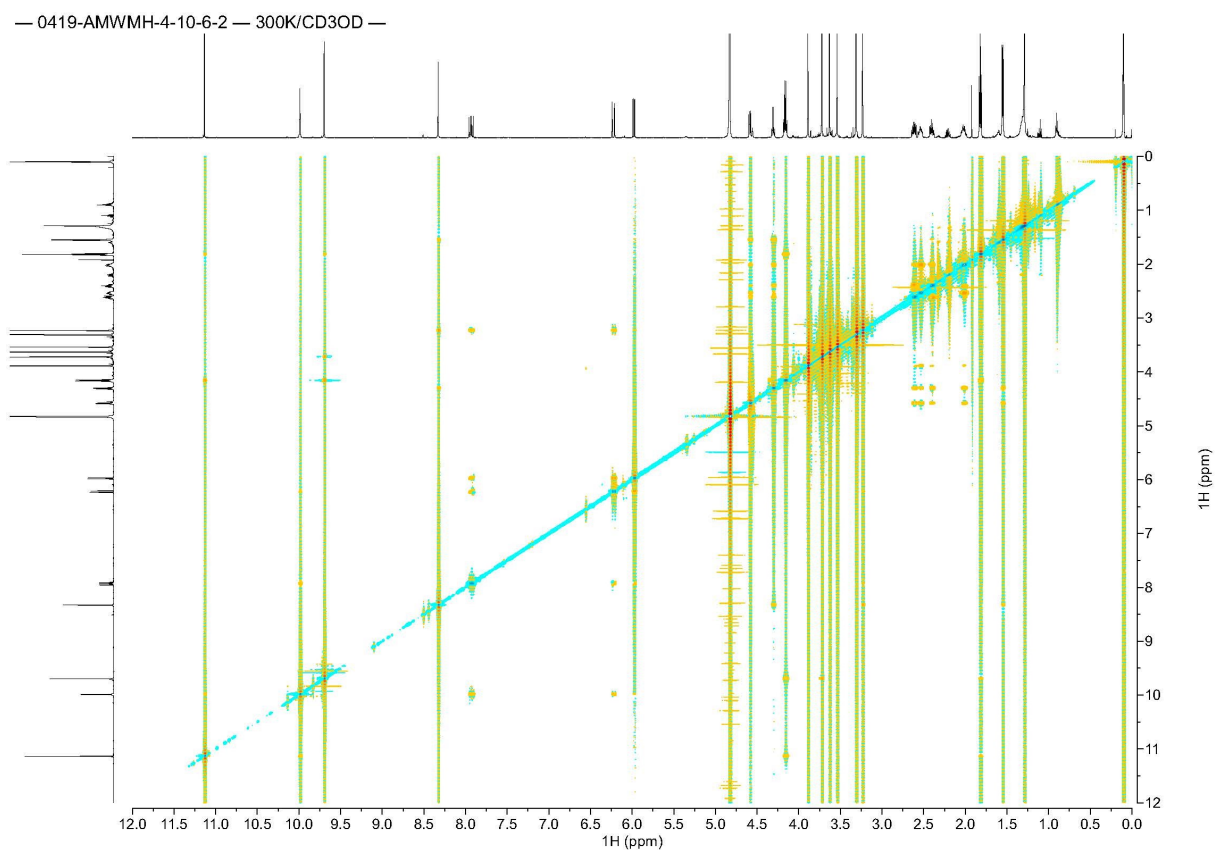


Fig. S56 NOESY spectrum of **7**.

D:\000-MS_Ori_work\...AMWMH_4_10_2_6_2

11/14/24 03:27:56

AMWMH_4_10_2_6_2 #6616 RT: 11.40 AV: 1 NL: 3.56E8

F: FTMS + p ESI Full ms [100.0000-1500.0000]

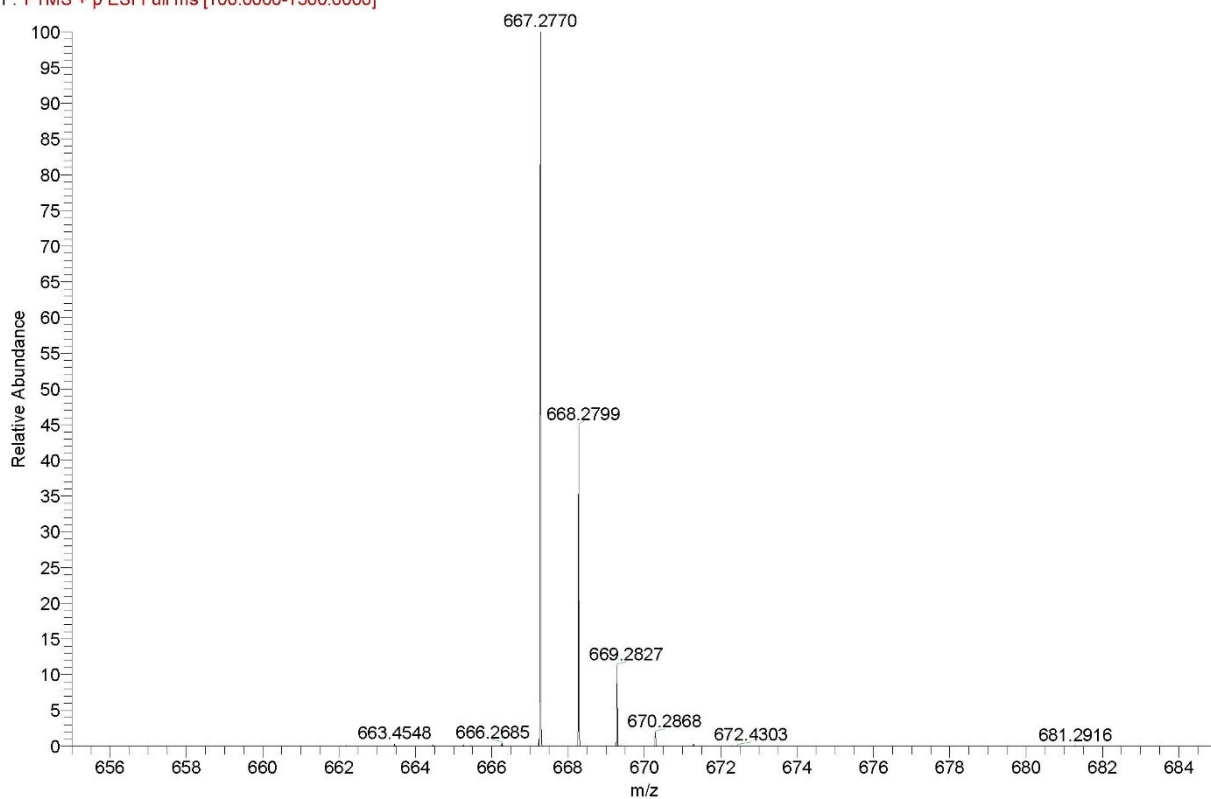


Fig. S57 HRESIMS spectrum of **7**.

¹H NMR spectrum (CDCl₃) of compound 1d. The x-axis represents the chemical shift in ppm, ranging from 12.0 to 0.0. The spectrum shows several peaks with their corresponding chemical shifts and integrations.

Chemical shifts (ppm): 11.163, 10.028, 9.727, 8.359, 7.921, 7.670, 7.561, 7.440, 6.251, 6.249, 6.222, 6.219, 5.986, 5.985, 5.979, 5.976, 4.659, 4.653, 4.649, 4.291, 4.279, 4.201, 4.191, 4.181, 4.176, 4.175, 4.164, 3.718, 3.675, 3.541, 3.536, 3.239, 2.428, 2.361, 1.849, 1.836, 1.823, 1.722, 1.694, 1.682.

Integrations: 1.00, 0.99, 1.01, 0.96, 0.96, 0.97, 1.00, 0.97, 0.98, 1.98, 3.01, 3.04, 5.98, 2.95, 1.06, 1.06, 3.03, 1.42, 3.54.

— 800MHz 13C1D/13C

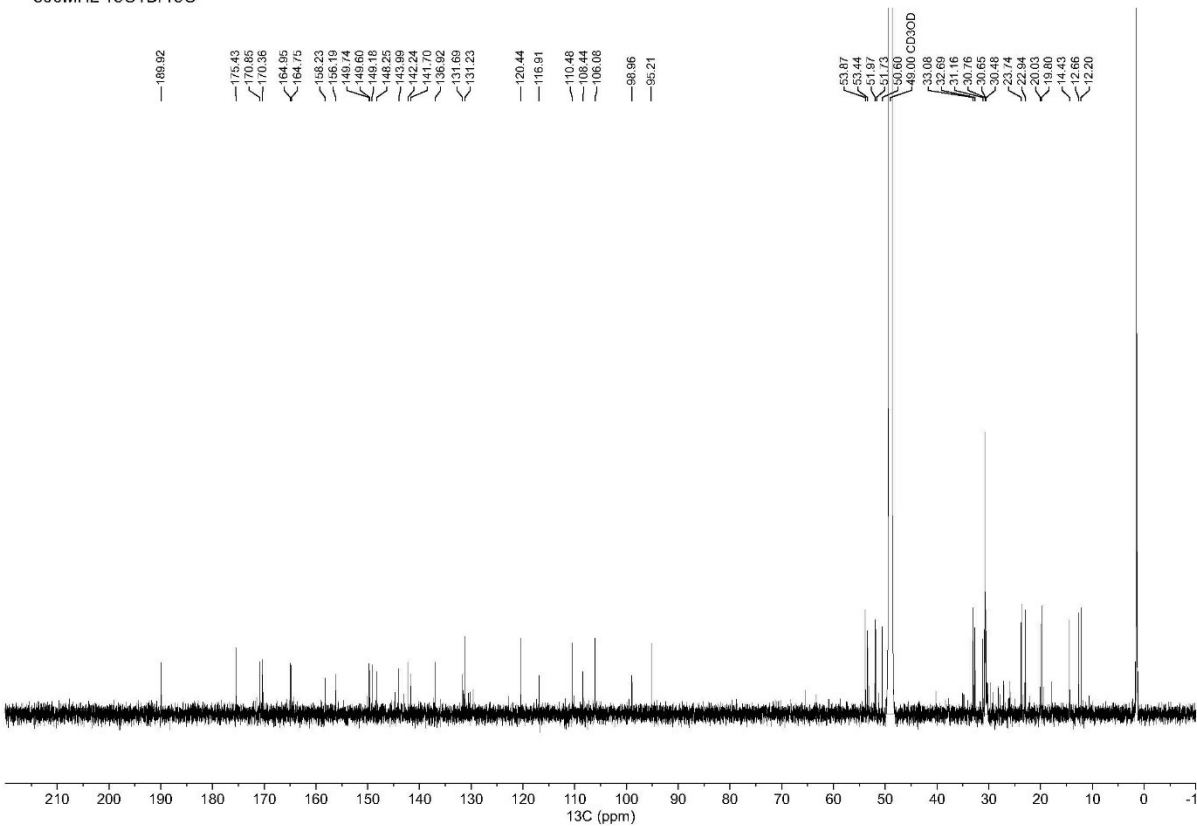


Fig. S59 ^{13}C NMR spectrum (200 MHz, CD_3OD) of **8**.

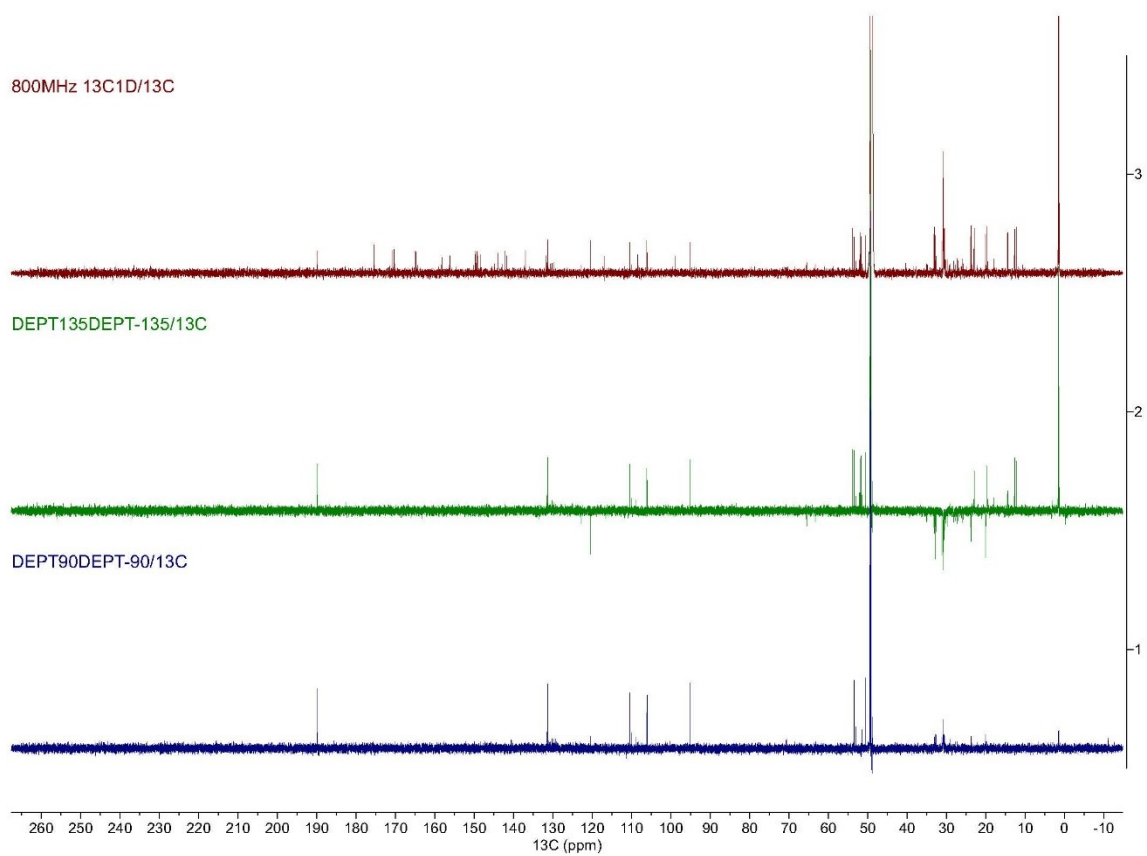


Fig. S60 DEPT spectrum of **8**.

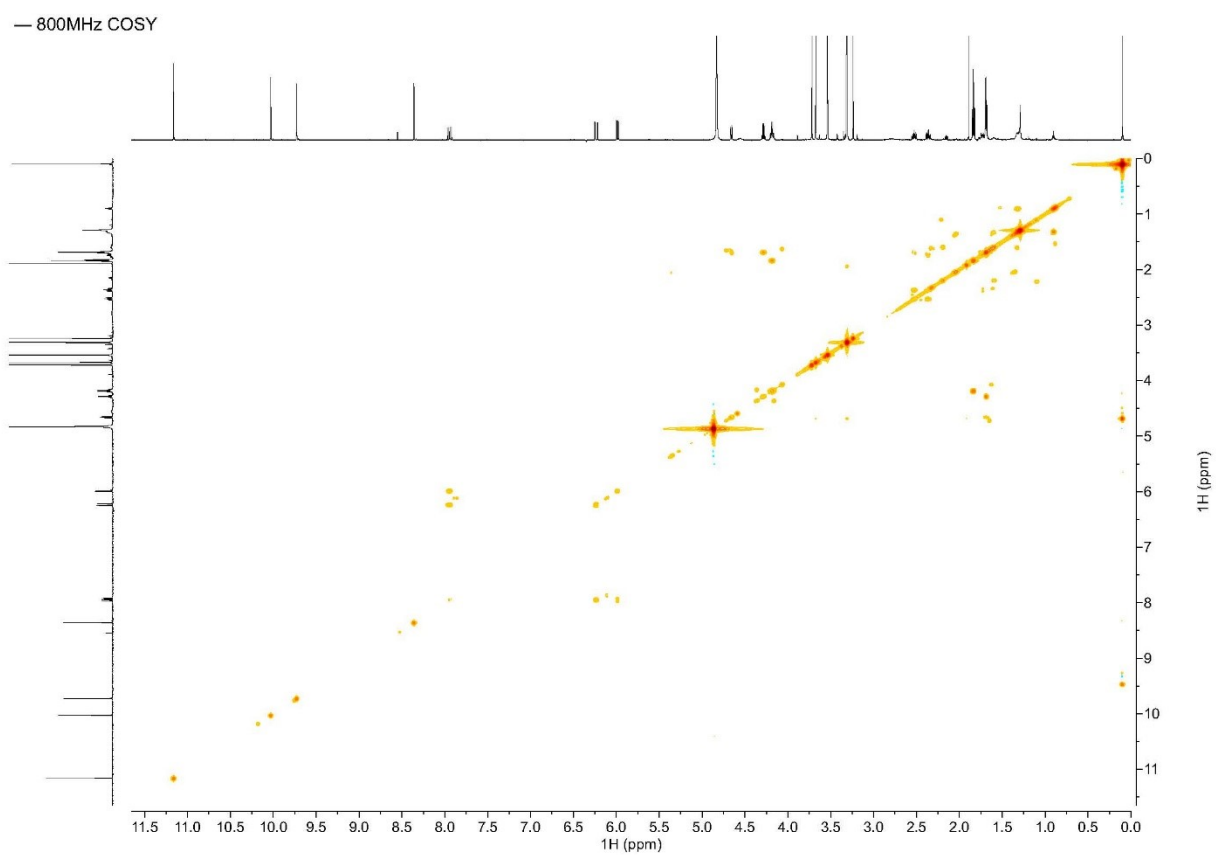


Fig. S61 COSY spectrum of **8**.

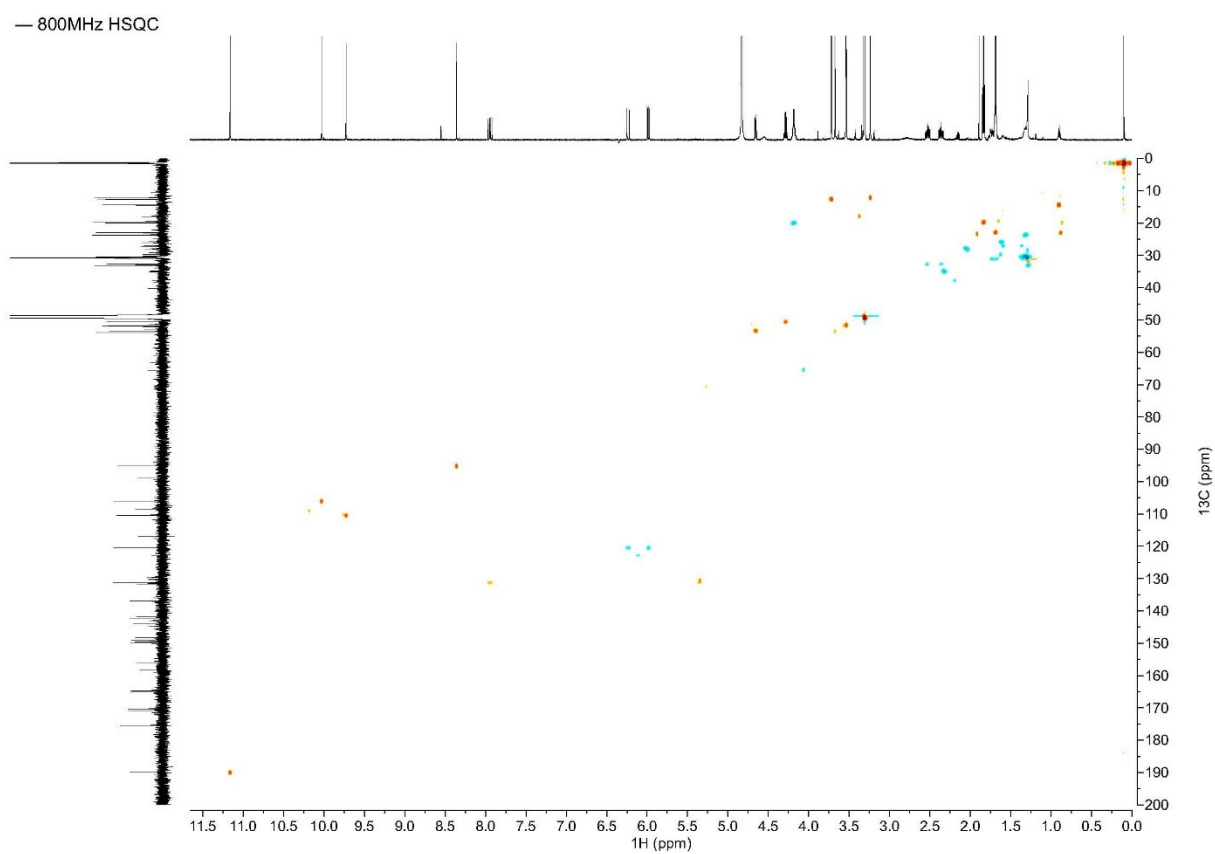


Fig. S62 HSQC spectrum of **8**.

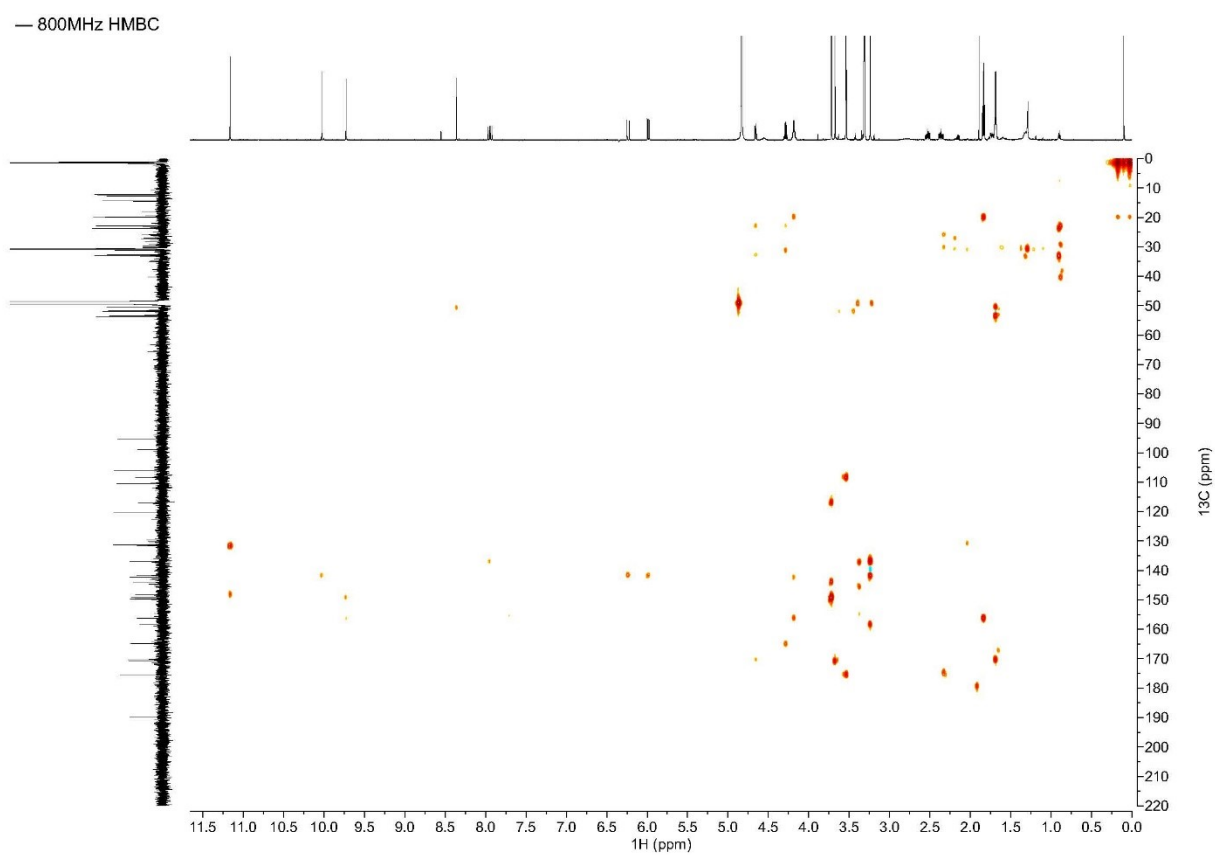


Fig. S63 HMBC spectrum of **8**.

— NOESY

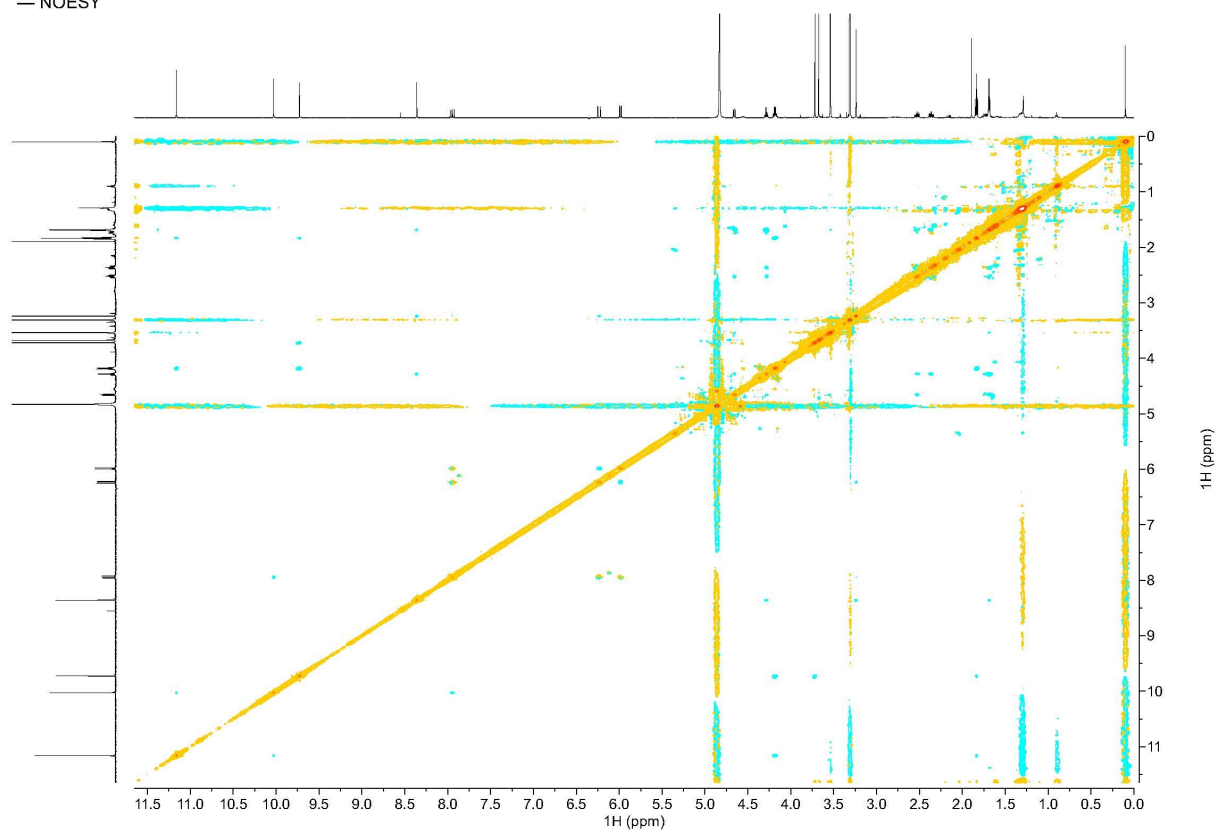


Fig. S64 NOESY spectrum of **8**.

D:\000-MS_Ori_work\...AMVMH_4_10_2_6_3

11/14/24 03:47:42

AMVMH_4_10_2_6_3 #6607 RT: 11.34 AV: 1 NL: 2.32E8
F: FTMS + p ESI Full ms [100.0000-1500.0000]

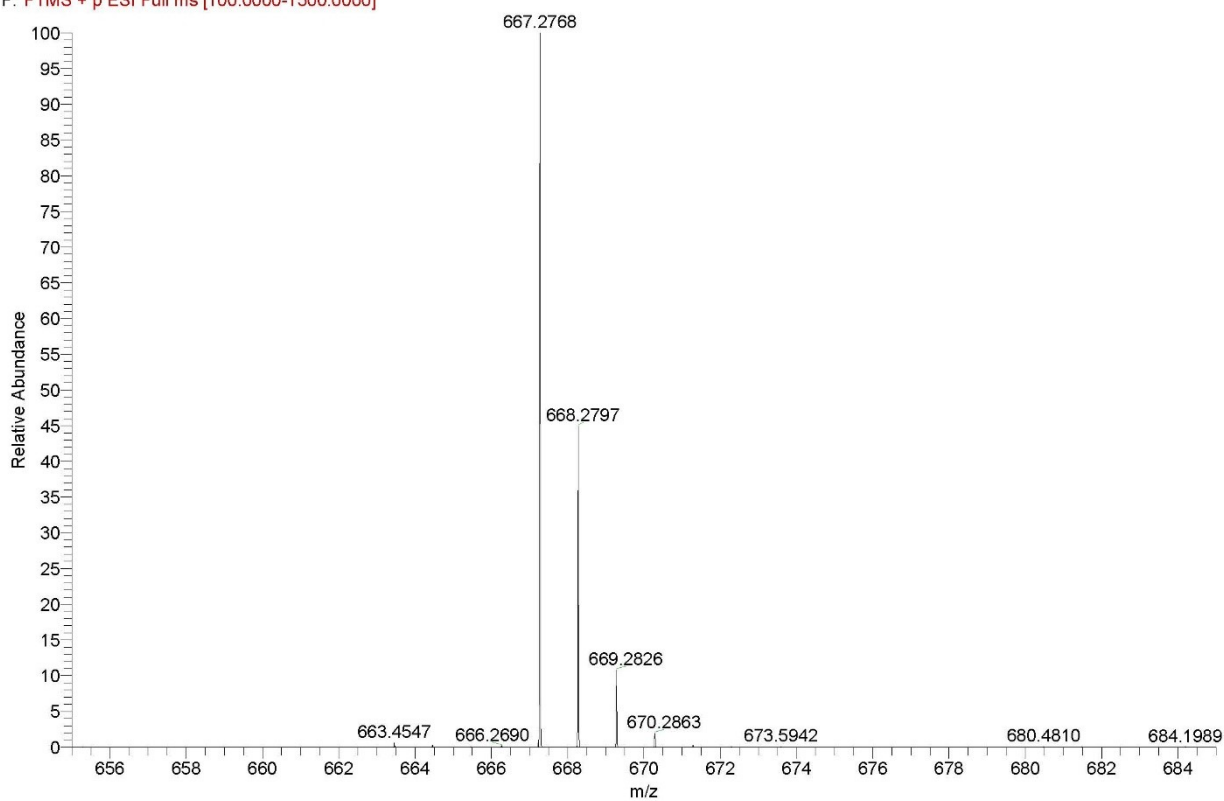


Fig. S65 HRESIMS spectrum of **8**.

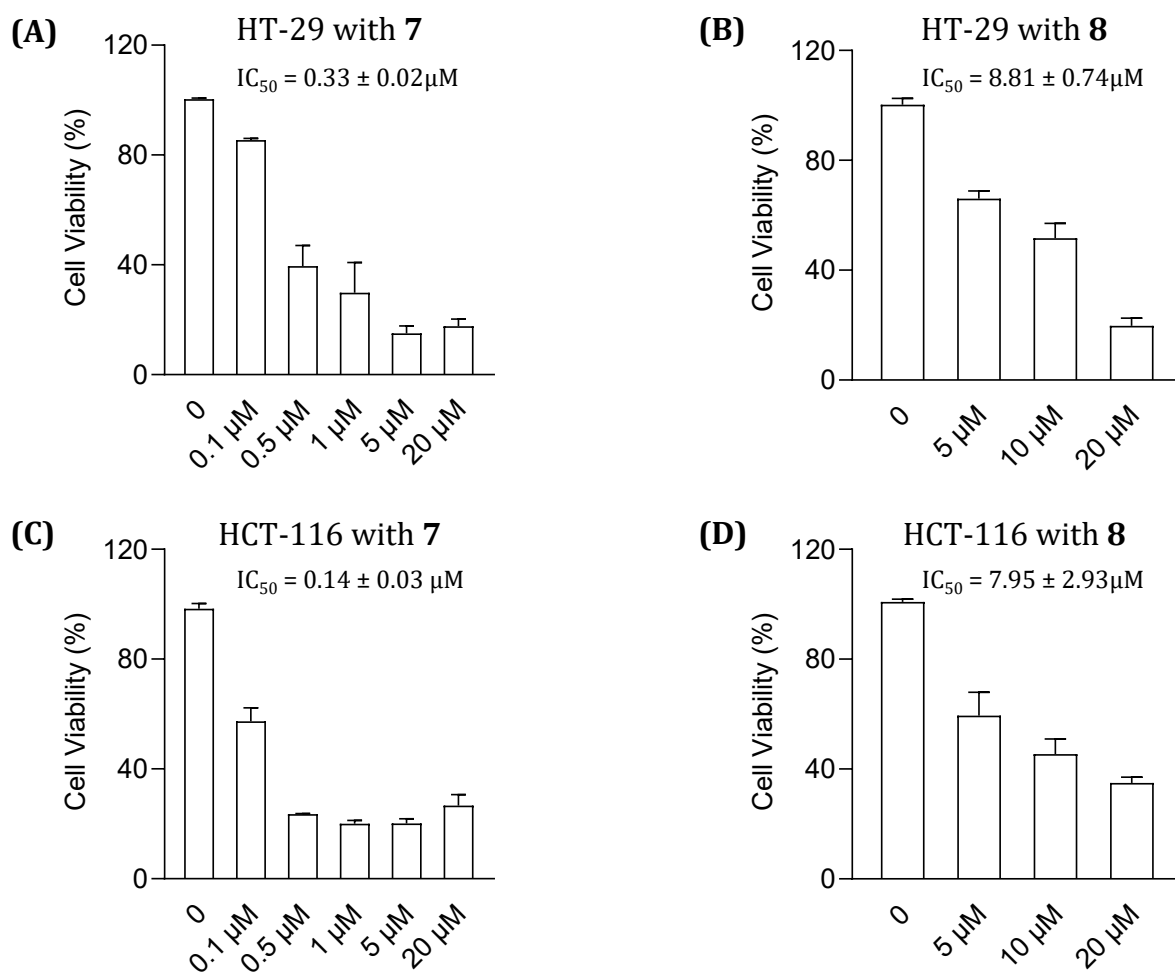


Fig. S66 Cell viability at different concentrations of compounds **7** and **8** in HT-29 and HCT-116 cells for IC_{50} calculation.

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 $\pm$ 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**.