

Supplementary Material

Discovery of Brominated Alboflavusins With Anti-MRSA Activities

Chao Li^{1,2†}, Wuyundalai Bao^{3†}, Haoyue Zhang⁴, Zhitang Lyu⁴, Yihua Chen^{1,2}, Zhengyan Guo^{1,2*}

¹State Key Laboratory of Microbial Resources & CAS Key Laboratory of Microbial Physiological and Metabolic Engineering, Institute of Microbiology, Chinese Academy of Sciences, 100101 Beijing, China

²College of Life Sciences, University of Chinese Academy of Sciences, 100049 Beijing, China

³College of Food Science and Engineering, Inner Mongolia Agricultural University, 010018 Hohhot, Inner Mongolia, China

⁴Key Laboratory of Microbial Diversity Research and Application of Hebei Province, Institute of Life Science and Green Development, College of Life Sciences, Hebei University, 071002 Baoding, Hebei, China

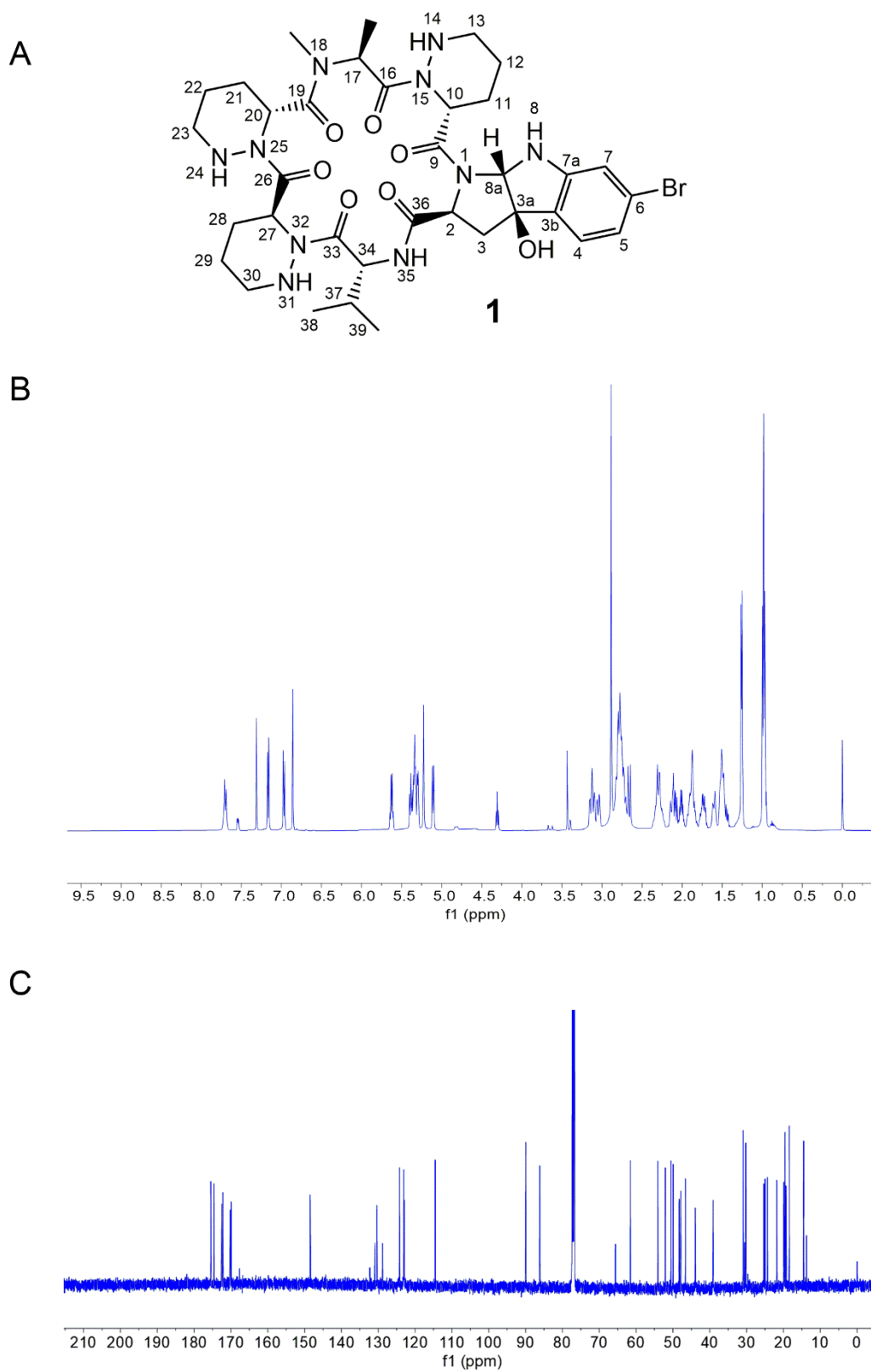
*** Correspondence:**

Corresponding Author: Zhengyan Guo guozhengyan@im.ac.cn

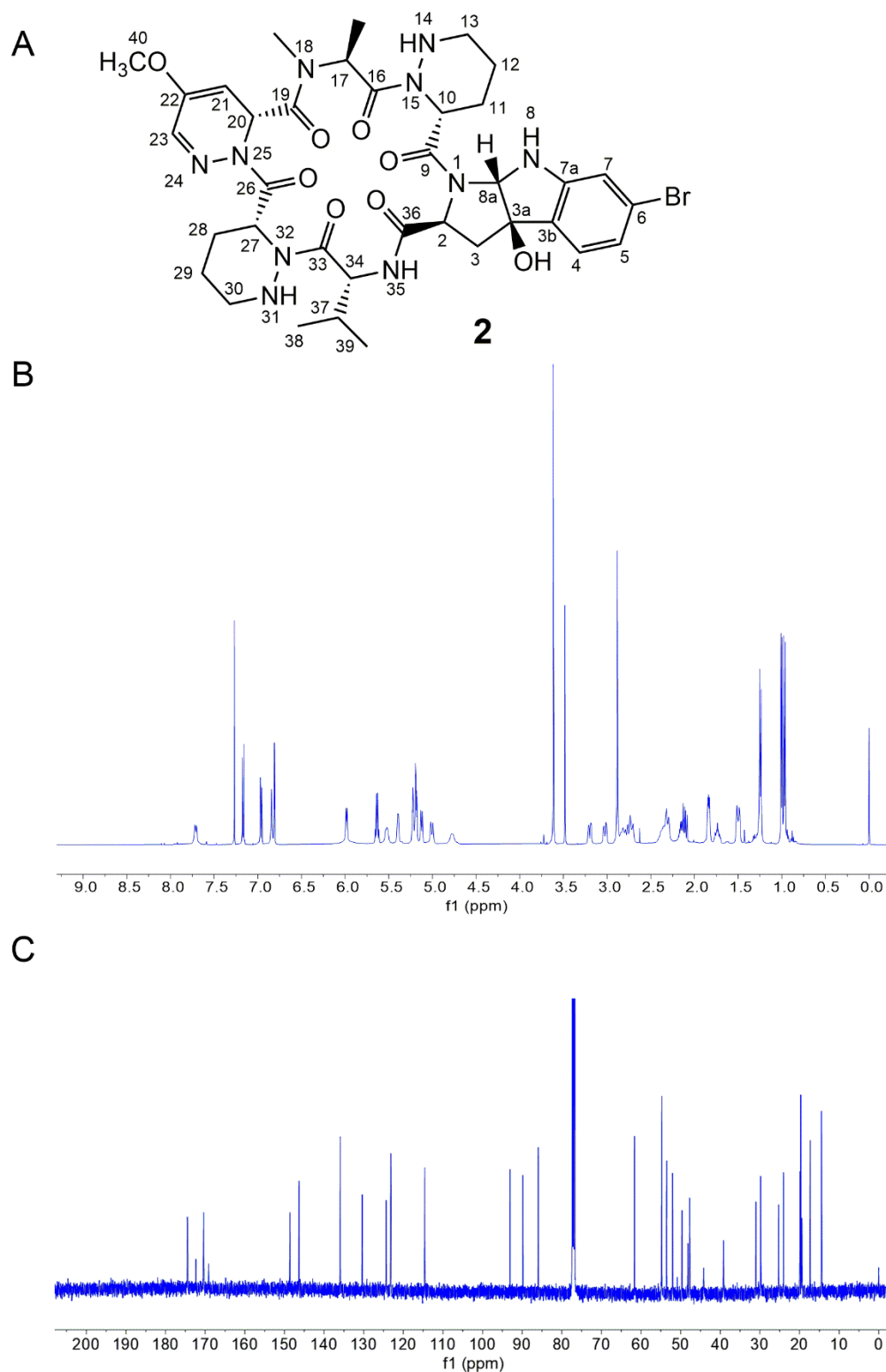
[†]These authors have contributed equally to this work

Contents

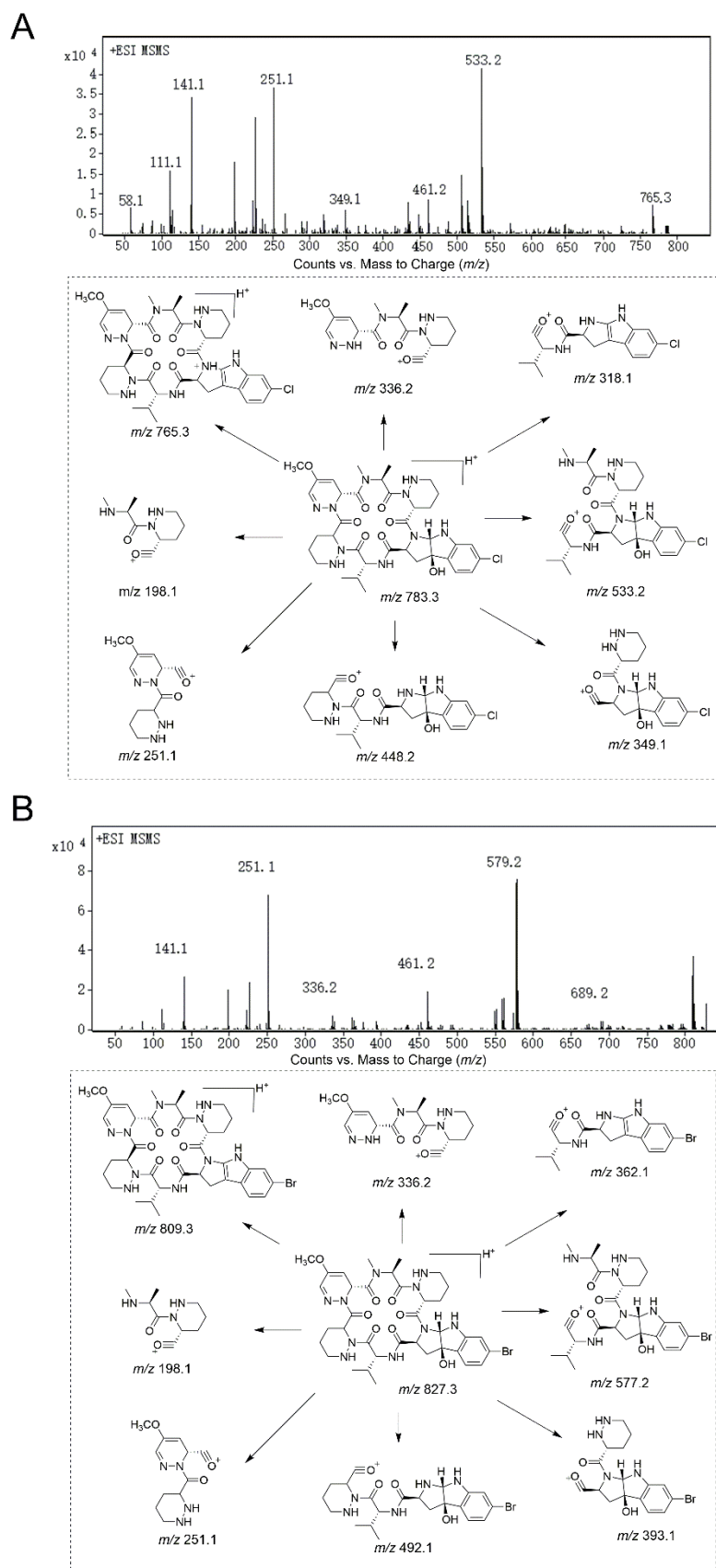
Supplementary Figure S1. Spectral data of 1 .	S3
Supplementary Figure S2. Spectral data of 2 .	S4
Supplementary Figure S3. The MS/MS spectra of AFN B ₁ (A) and 2 (B).	S5
Supplementary Figure S4. Spectral data of 3 .	S6
Supplementary Figure S5. The MS/MS spectra of 3 (A) and 5 (B).	S7
Supplementary Figure S6. Spectral data of 5 .	S8
Supplementary Figure S6. Spectral data of 5 .	S9
Supplementary Figure S6. Spectral data of 5 .	S10
Supplementary Figure S6. Spectral data of 5 .	S11



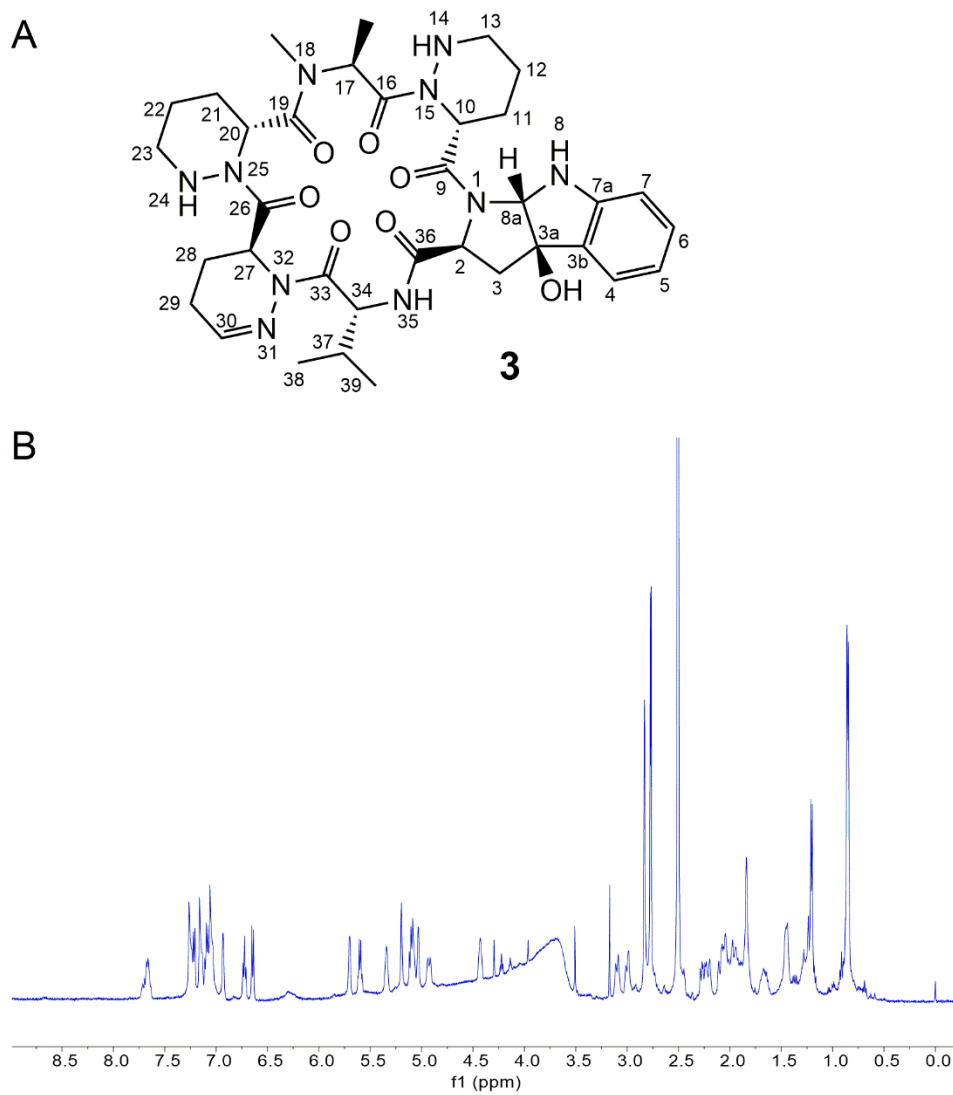
Supplementary Figure S1. Spectral data of **1**. (A) Structure of **1**. (B) ^1H NMR spectrum of **1** in CDCl_3 . (C) ^{13}C NMR spectrum of **1** in CDCl_3 .



Supplementary Figure S2. Spectral data of **2**. (A) Structure of **2**. (B) ^1H NMR spectrum of **2** in CDCl_3 . (C) ^{13}C NMR spectrum of **2** in CDCl_3 .

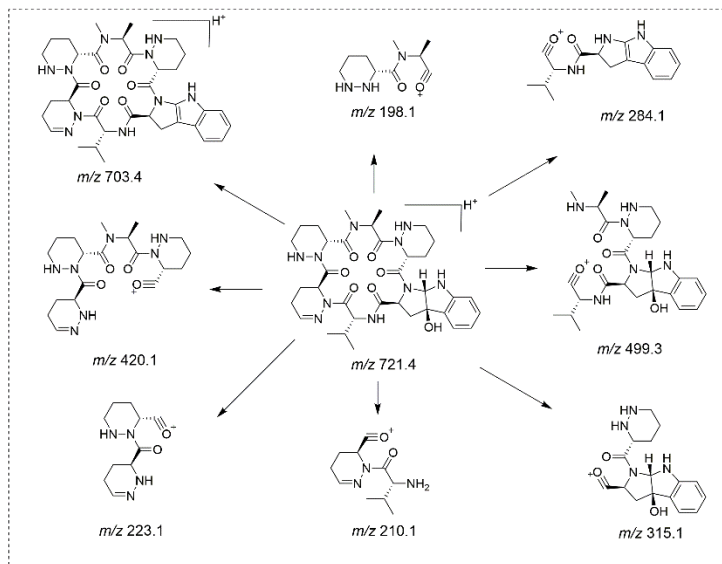
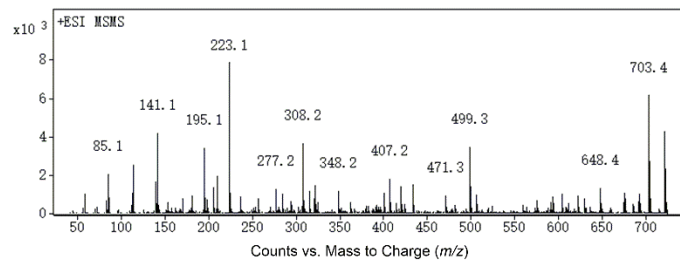


Supplementary Figure S3. The MS/MS spectra of AFN B₁ (A) and 2 (B).

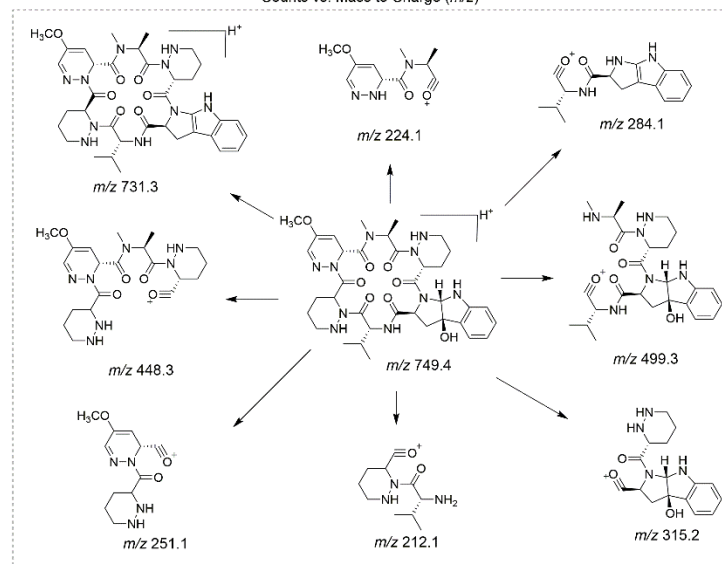
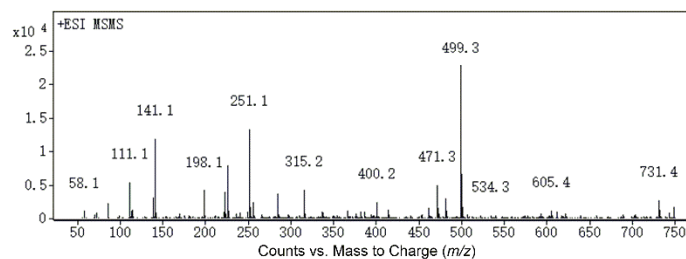


Supplementary Figure S4. Spectral data of **3**. (A) Structure of **3**. (B) ^1H NMR spectrum of **3** in $\text{DMSO-}d_6$.

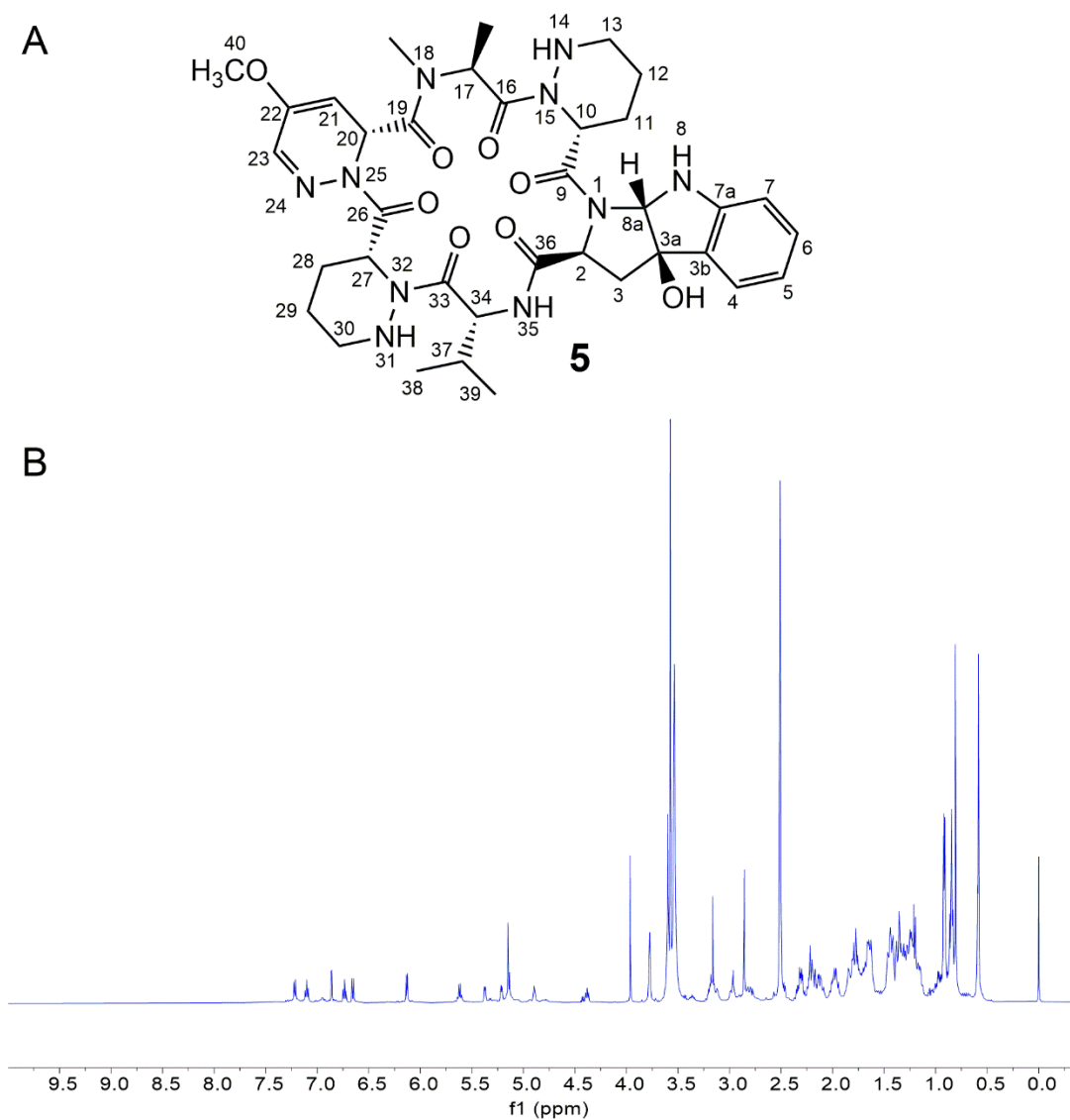
A



B

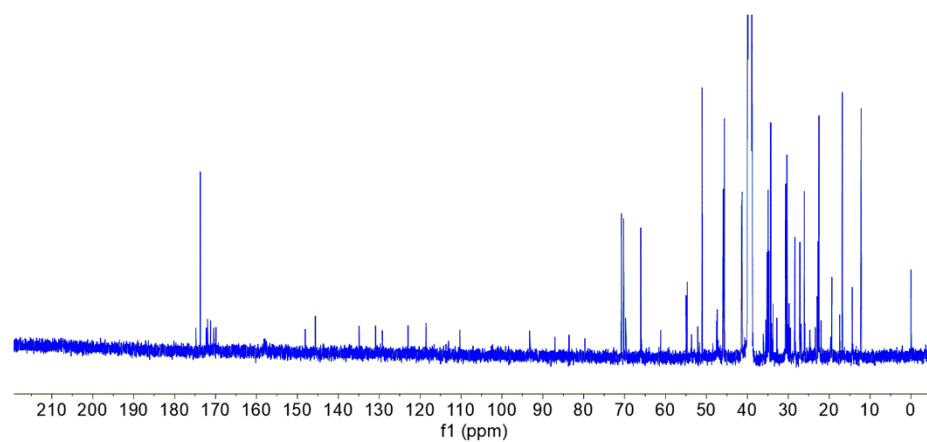


Supplementary Figure S5. The MS/MS spectra of **3** (A) and **5** (B).

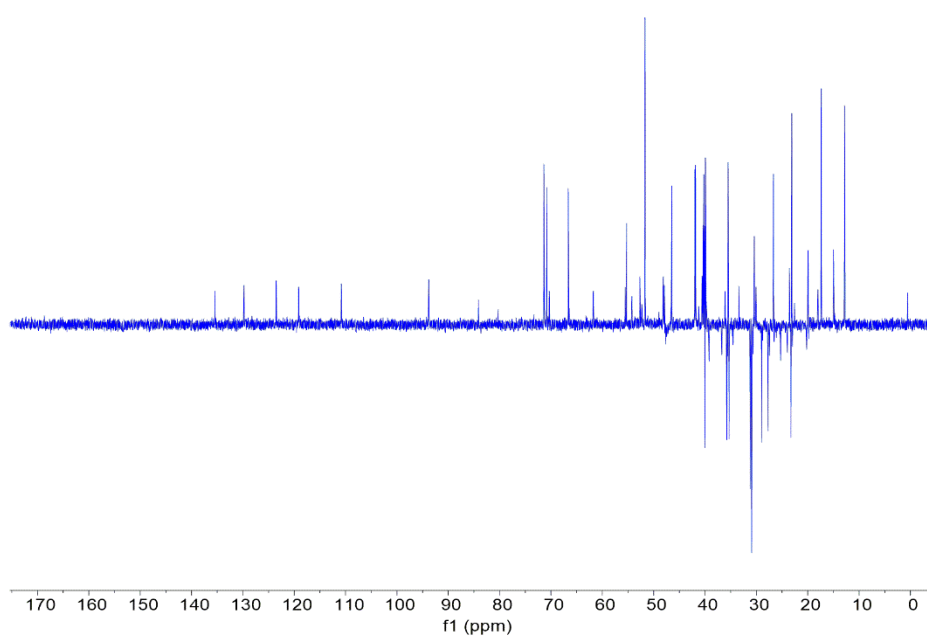


Supplementary Figure S6. Spectral data of **5**. (A) Structure of **5**. (B) ^1H NMR spectrum of **5** in $\text{DMSO-}d_6$.

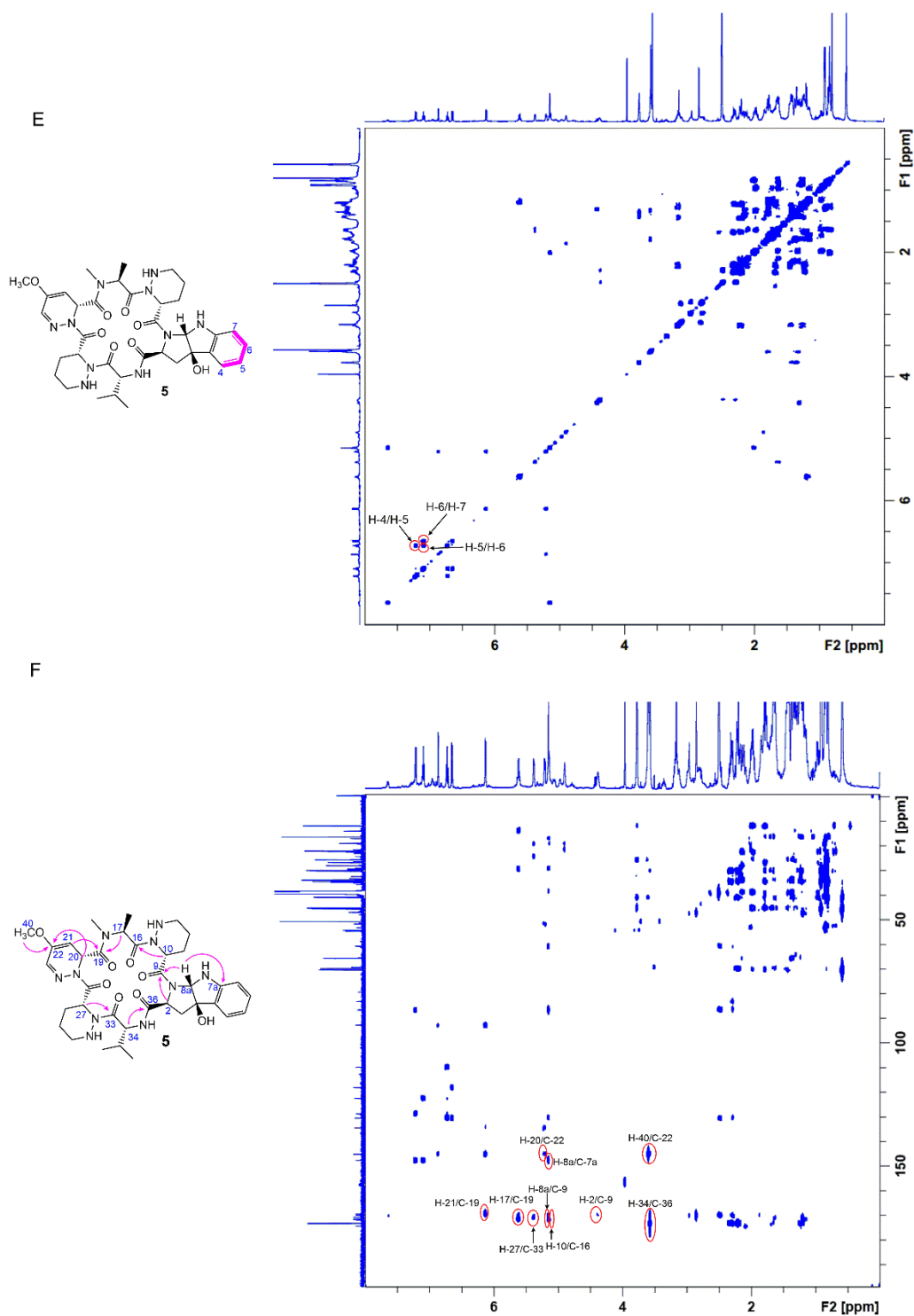
C



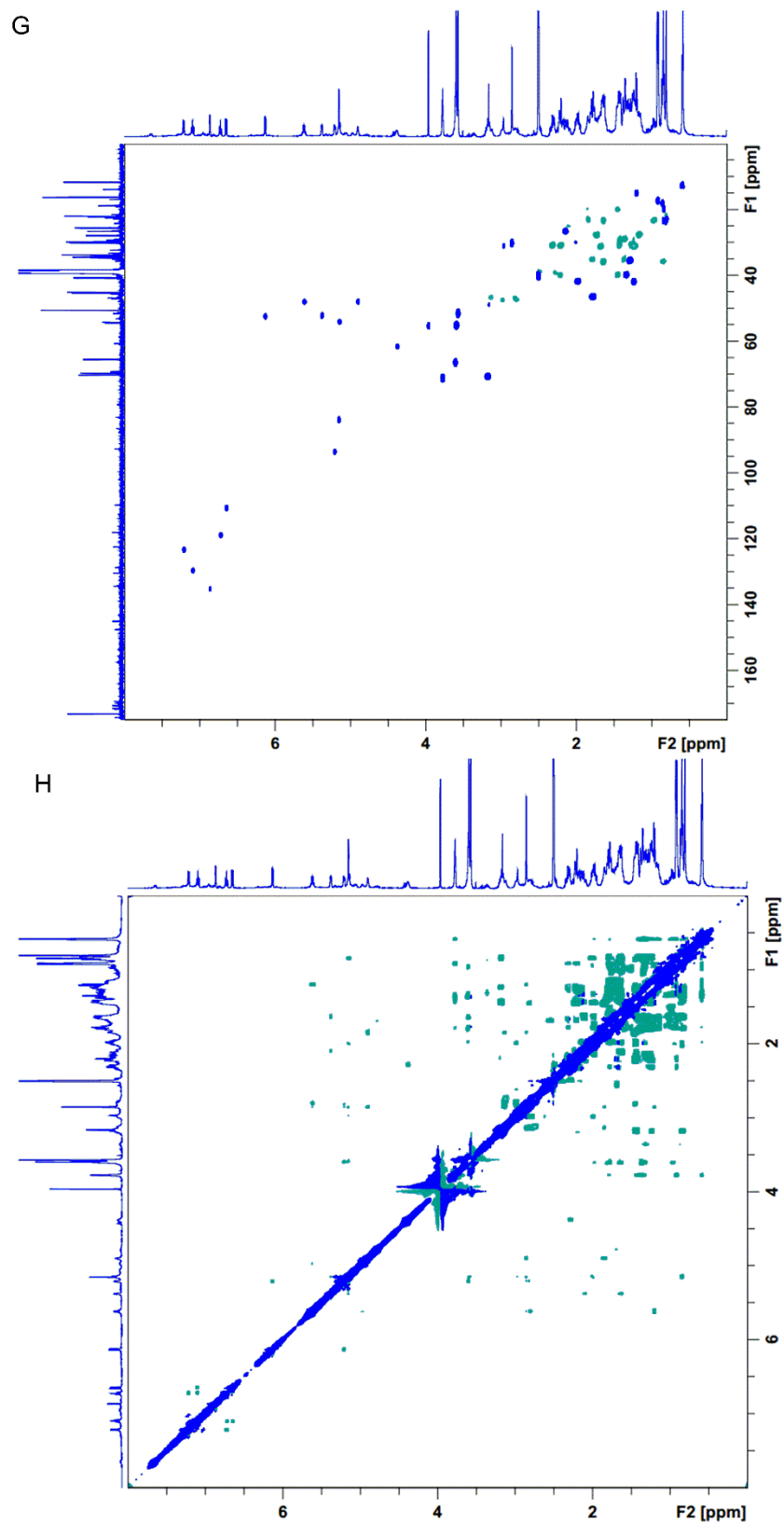
D



Supplementary Figure S6. Spectral data of **5**. (C) ^{13}C NMR spectrum of **5** in $\text{DMSO-}d_6$. (D) DEPT- 135 spectrum of **5** in $\text{DMSO-}d_6$.



Supplementary Figure S6. Spectral data of **5**. (E) ^1H - ^1H COSY spectrum of **5** in $\text{DMSO-}d_6$. The key ^1H - ^1H COSY correlation are marked on the structure of **5** with pink bold bonds and at the spectrum with red circles. (F) HMBC spectrum of **5** in $\text{DMSO-}d_6$. The key HMBC correlations are marked on the structure of **5** with pink arrows and at the spectrum with red circles.



Supplementary Figure S6. Spectral data of **5**. (G) HSQC spectrum of **5** in DMSO- d_6 . (H) ROESY spectrum of **5** in DMSO- d_6 .