

Supplementary Material for

Teratopyrones A–C, Dimeric Naphtho- γ -pyrones and Other Metabolites from *Teratosphaeria* sp. AK1128, a Fungal Endophyte of *Equisetum arvense*

Ya-ming Xu ¹, A. Elizabeth Arnold ², Jana M. U'Ren ², Li-Jiang Xuan³, Wen-qiong Wang³, A. A. Leslie Gunatilaka ^{1,*}

¹ Natural Products Center, School of Natural Resources and the Environment,
College of Agriculture and Life Sciences, University of Arizona, 250 E. Valencia Road, Tucson, Arizona 85706, United States; yamingx@arizona.edu;
leslieg1@email.arizona.edu

² School of Plant Sciences, College of Agriculture and Life Sciences, University of Arizona, Tucson, Arizona 85721, United States; juren@arizona.edu;
barnoldaz@gmail.com

³ State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 501 Haike Road, Zhangjiang Hi-Tech Park,
Shanghai 201203, P. R. China; ljxuan@sim.ac.cn; wenqiong1019@126.com

* Correspondence: leslieg@cals.arizona.edu; Tel.: + (520) 621-9932

Table of Contents

Figure S1. ^1H NMR Spectrum (400 MHz) of Teratopyrone A (1) in CDCl_3	S3
Figure S2. ^{13}C NMR Spectrum (100 MHz) of Teratopyrone A (1) in CDCl_3	S4
Figure S3. HSQC Spectra (400 MHz) of Teratopyrone A (1) in CDCl_3	S5
Figure S4. HMBC Spectra (400 MHz) of Teratopyrone A (1) in CDCl_3	S6
Figure S5. ^1H NMR Spectrum (400 MHz) of Teratopyrone B (2) in DMSO-d_6	S7
Figure S6. ^{13}C NMR Spectrum (100 MHz) of Teratopyrone B (2) in DMSO-d_6	S8
Figure S7. HSQC Spectrum (400 MHz) of Teratopyrone B (2) in DMSO-d_6	S9
Figure S8. HMBC Spectrum (400 MHz) of Teratopyrone B (2) in DMSO-d_6	S10
Figure S9. ^1H NMR Spectrum (400 MHz) of Teratopyrone C (3) in DMSO-d_6	S11
Figure S10. ^{13}C NMR Spectrum (100 MHz) of Teratopyrone C (3) in DMSO-d_6	S12
Figure S11. HSQC Spectrum (400 MHz) of Teratopyrone C (3) in DMSO-d_6	S13
Figure S12. HMBC Spectrum (400 MHz) of Teratopyrone C (3) in DMSO-d_6	S14
Figure S13. Results of maximum likelihood analysis placing strain AK1128 within <i>Teratosphaeria</i> with high support. Numbers in association with nodes indicate bootstrap values (values ≥ 70 are shown).	S15

Figure S1. ^1H NMR Spectrum (400 MHz) of Teratopyrone A (**1**) in CDCl_3

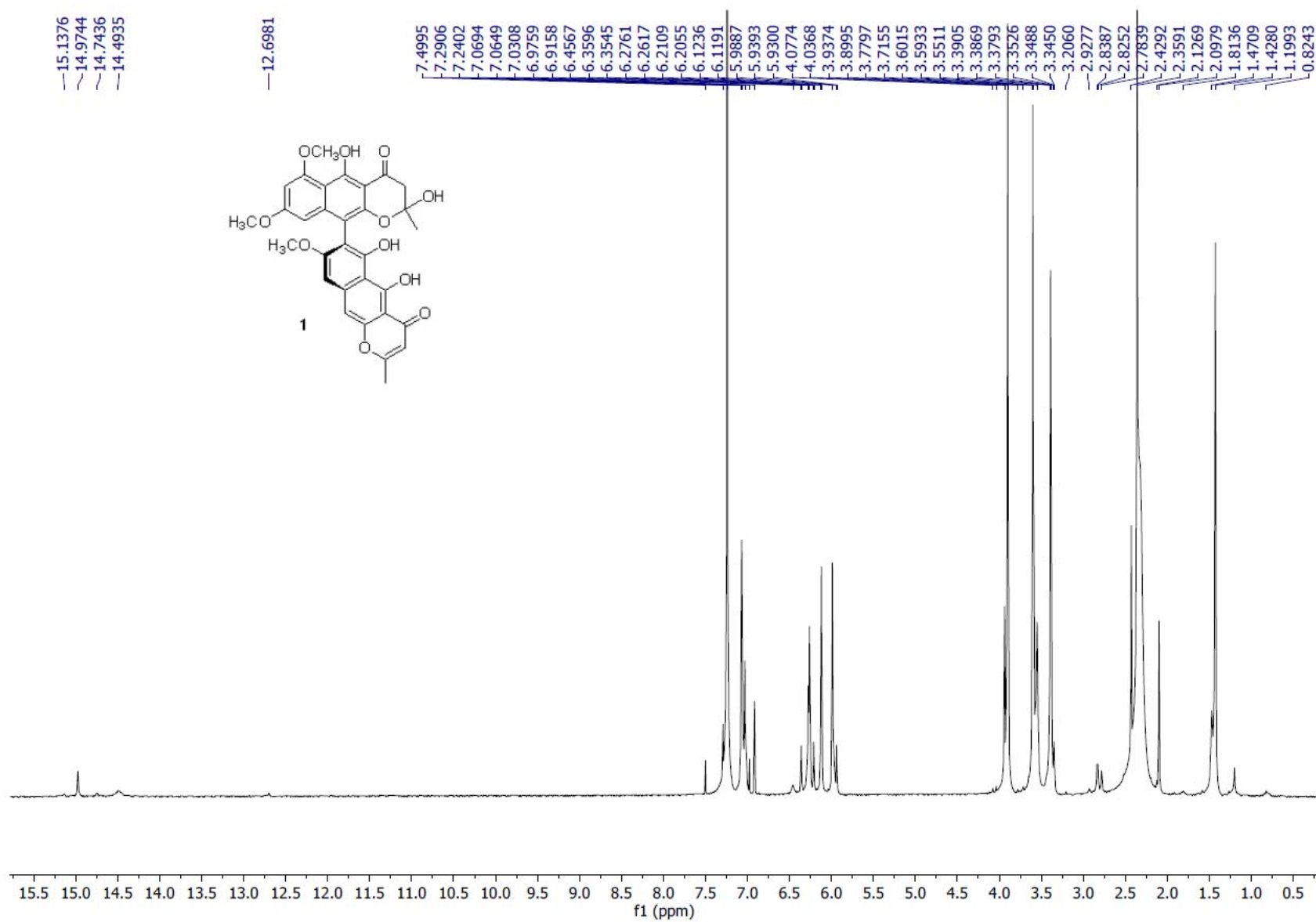


Figure S2. ^{13}C NMR Spectrum (100 MHz) of Teratopyrone A (**1**) in CDCl_3

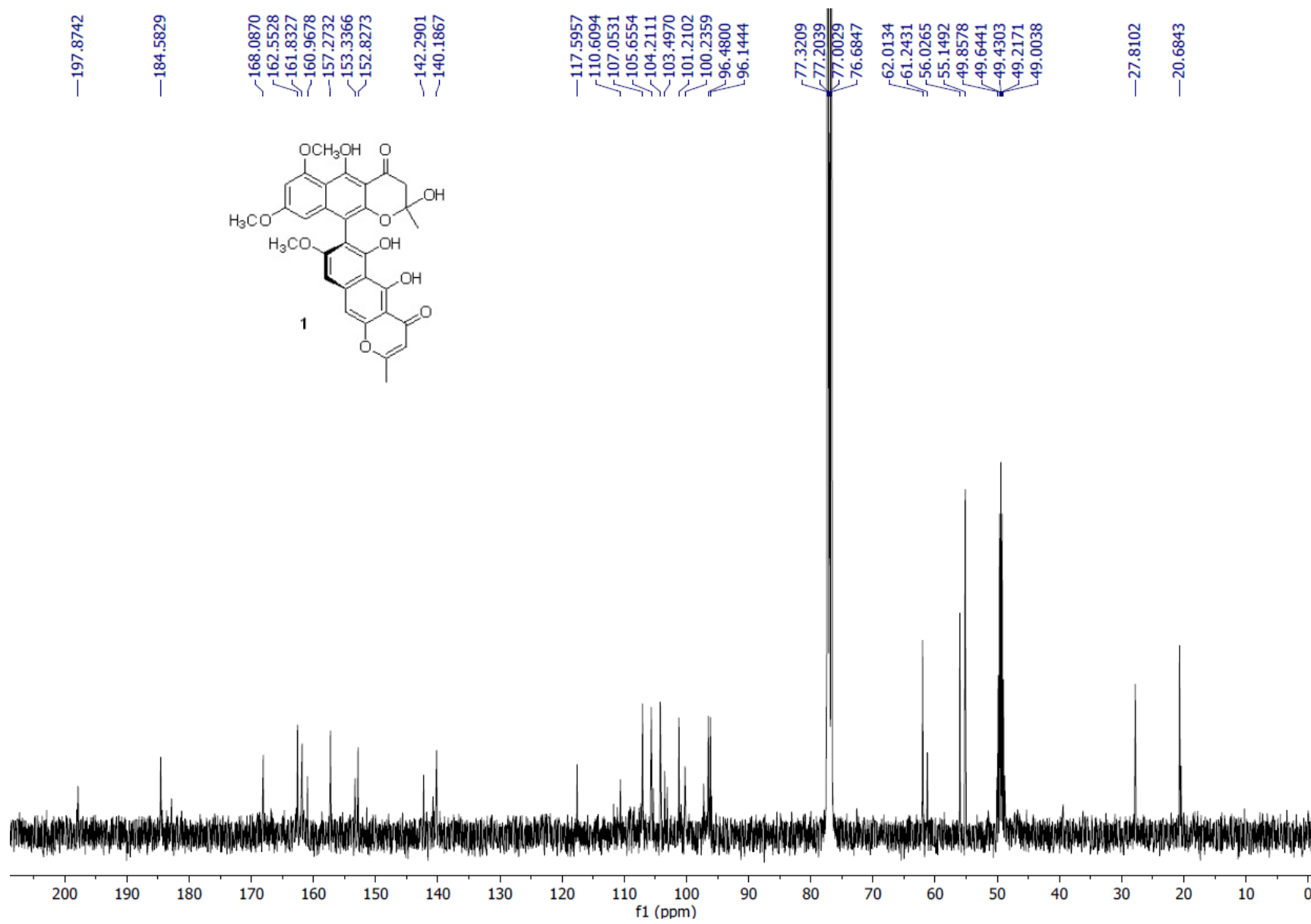


Figure S3. HSQC Spectra (400 MHz) of Teratopyrone A (**1**) in CDCl₃

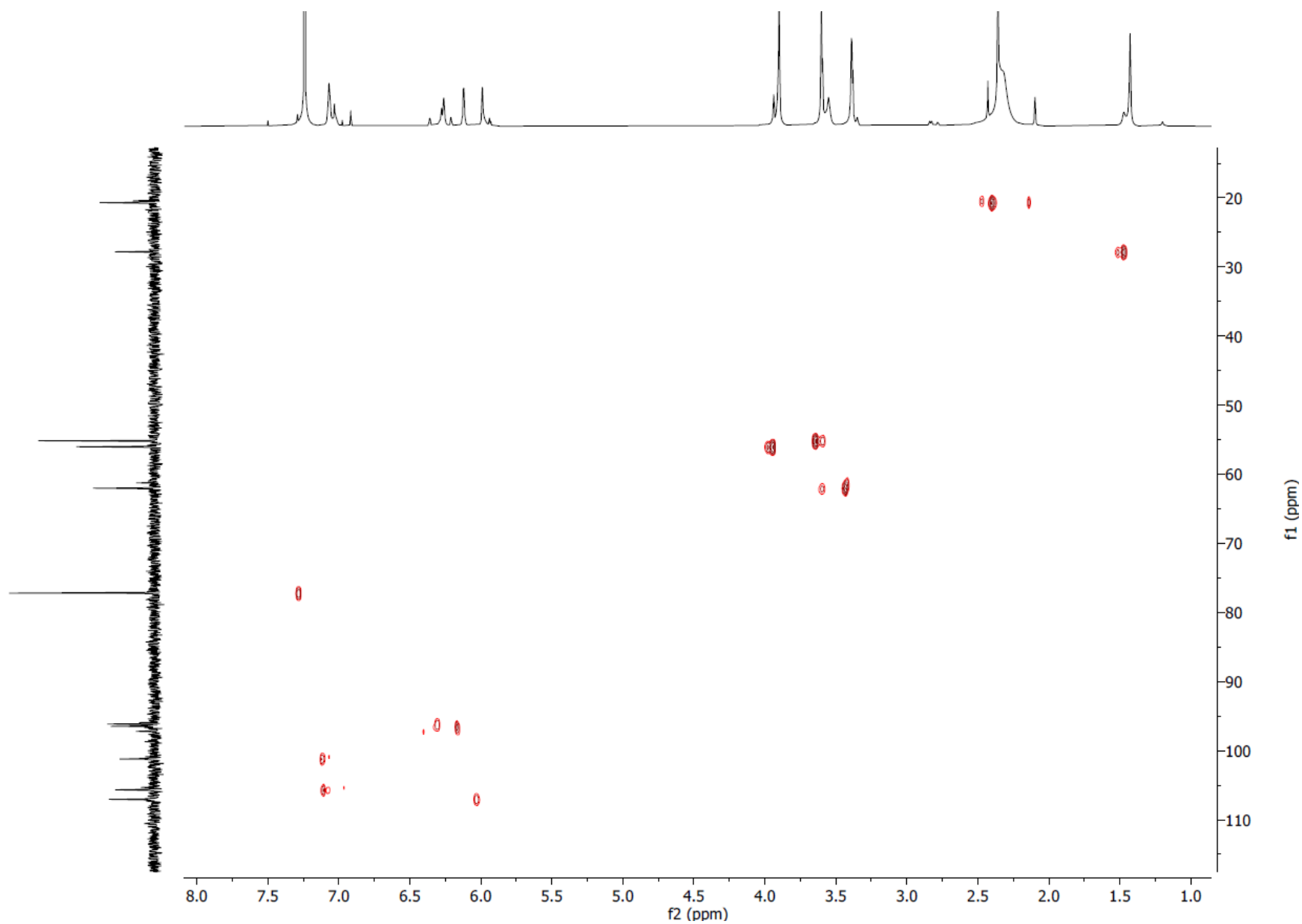


Figure S4. HMBC Spectra (400 MHz) of Teratopyrone A (**1**) in CDCl₃

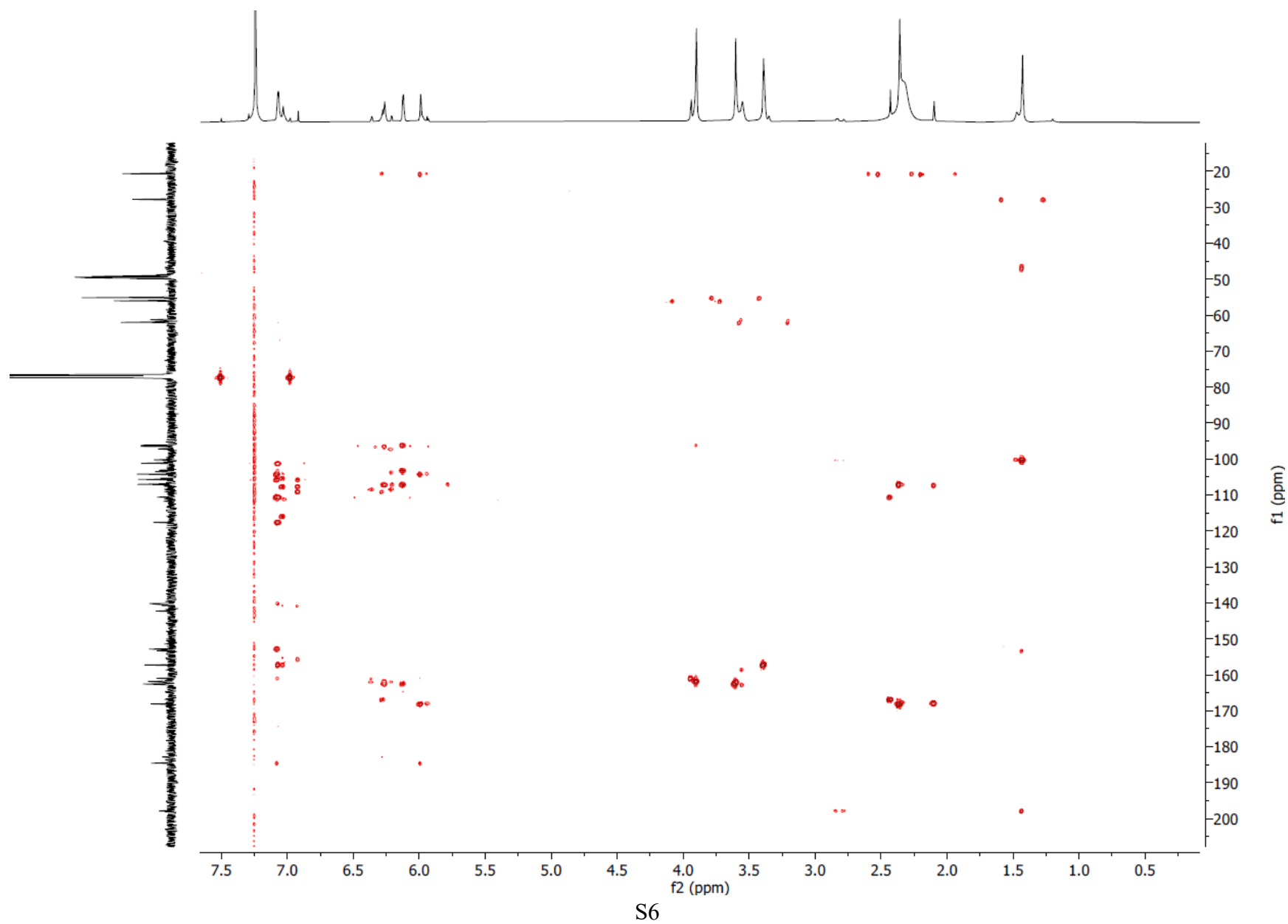


Figure S5. ^1H NMR Spectrum (400 MHz) of Teratopyrone B (**2**) in DMSO-d_6

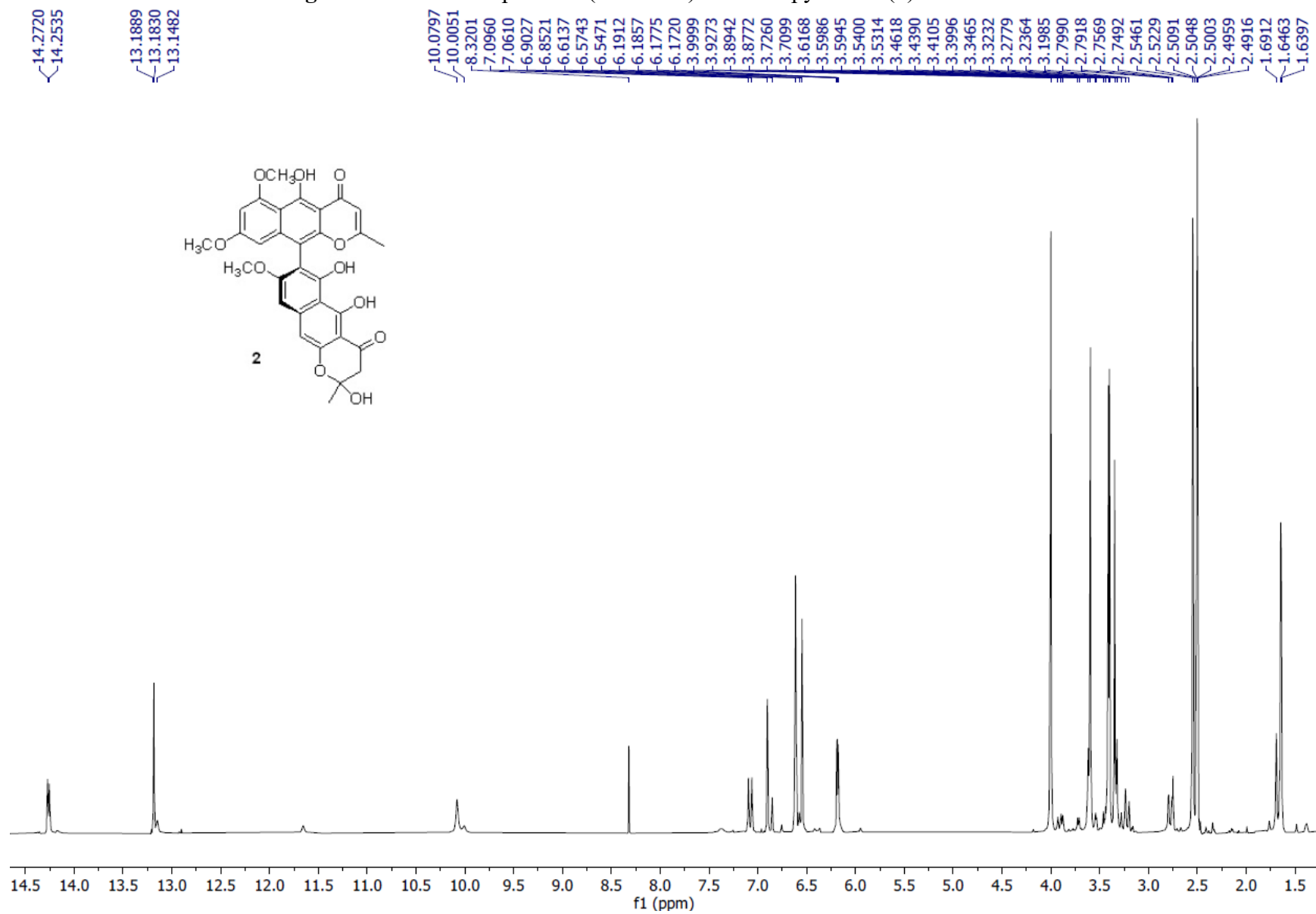


Figure S6. ^{13}C NMR Spectrum (400 MHz) of Teratopyrone B (**2**) in DMSO- d_6

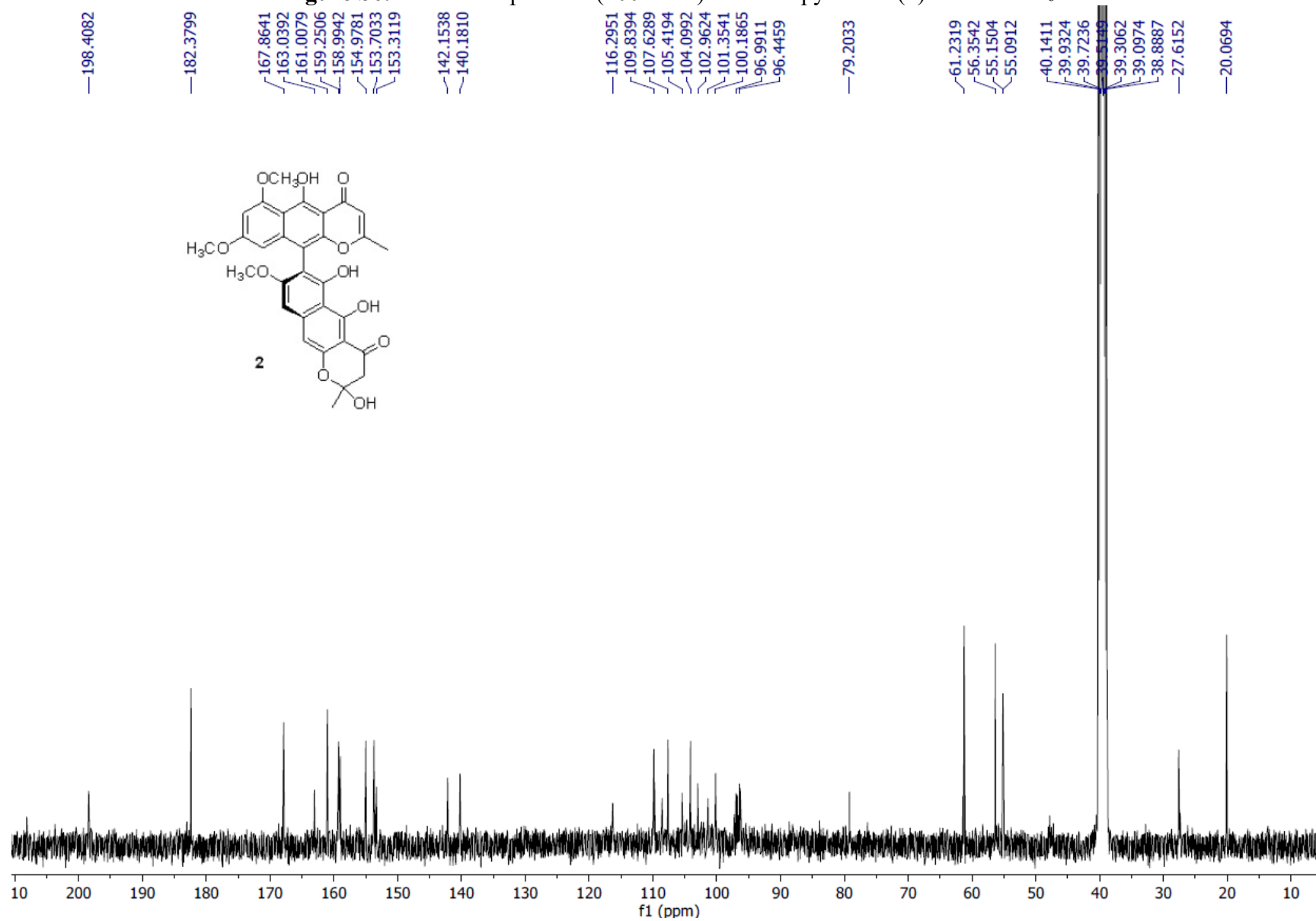


Figure S7. HSQC Spectrum (400 MHz) of Teratopyrone B (**2**) in DMSO-d₆

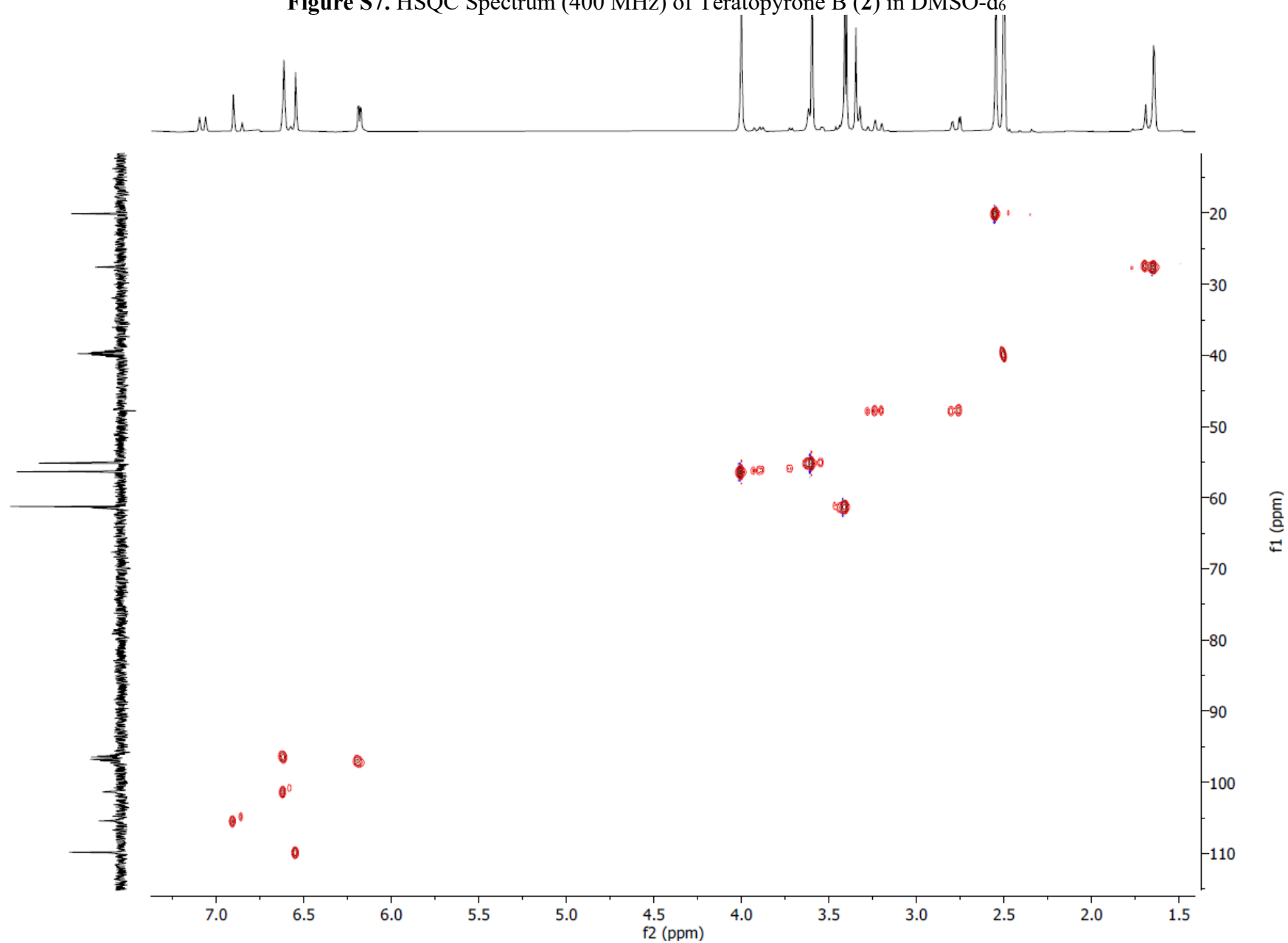


Figure S8. HMBC Spectrum (400 MHz) of Teratopyrone B (**2**) in DMSO-d₆

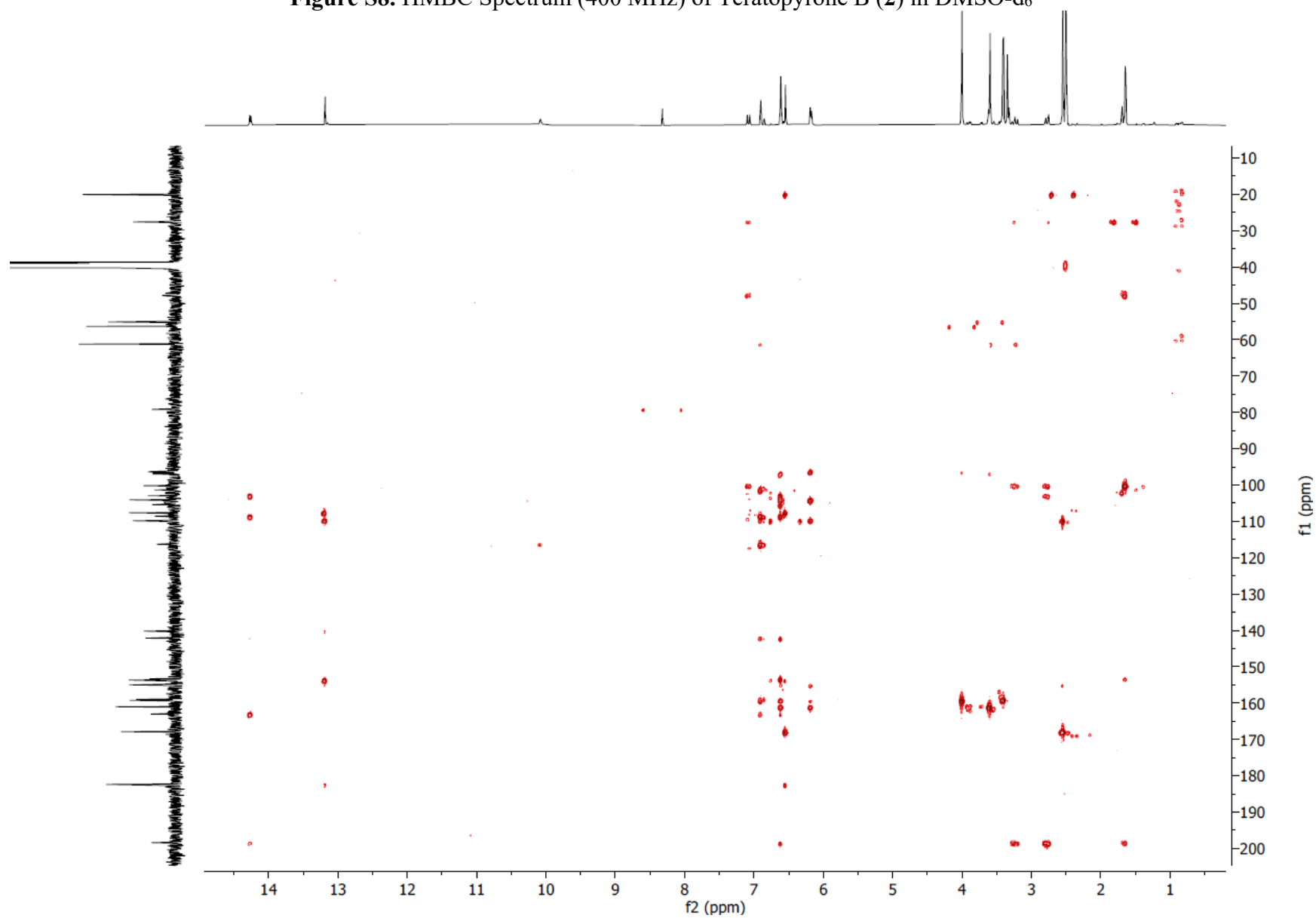


Figure S9. ^1H NMR Spectrum (400 MHz) of Teratopyrone C (**3**) in DMSO-d_6

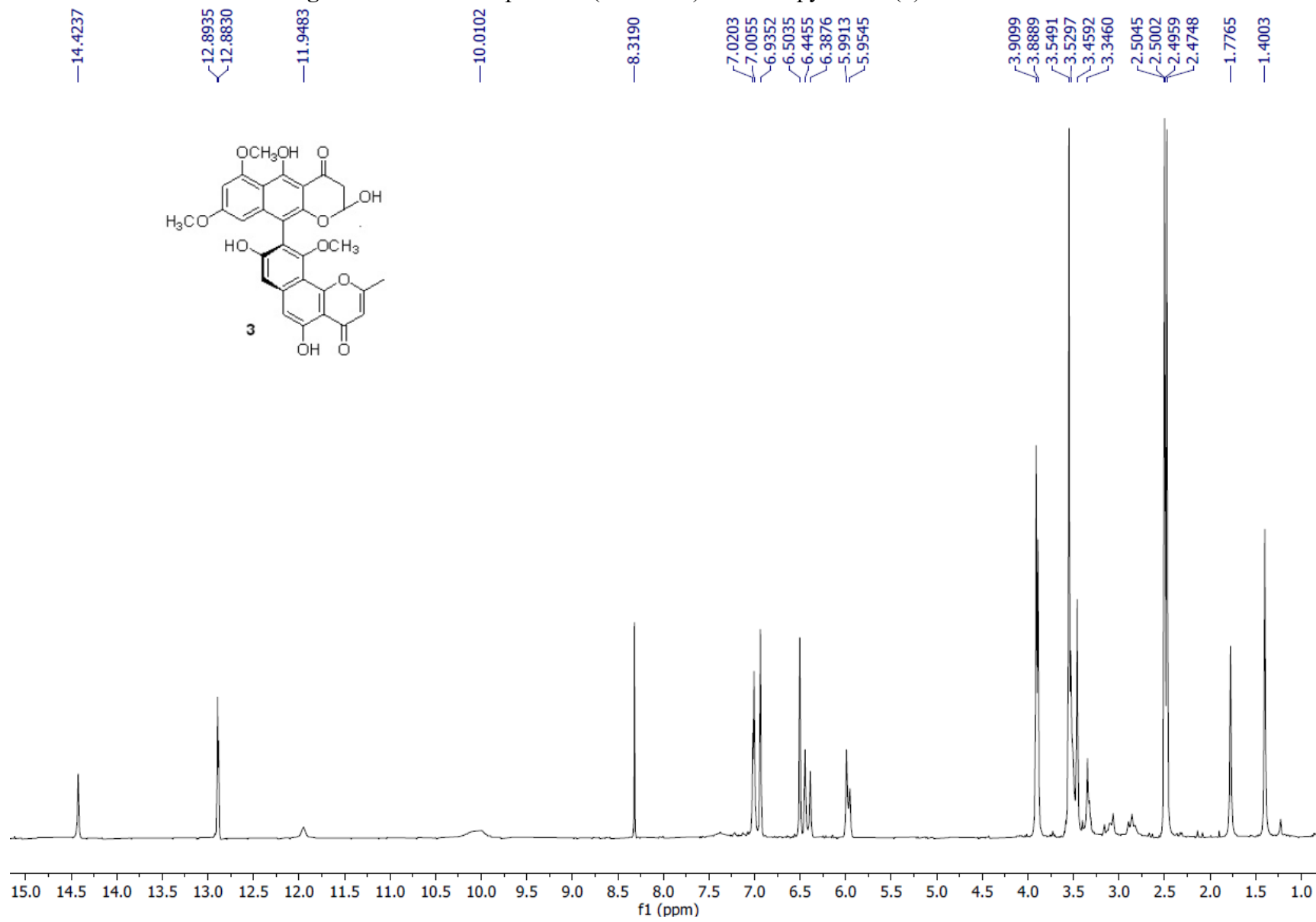


Figure S10. ^{13}C NMR Spectrum (400 MHz) of Teratopyrone C (**3**) in DMSO-d_6

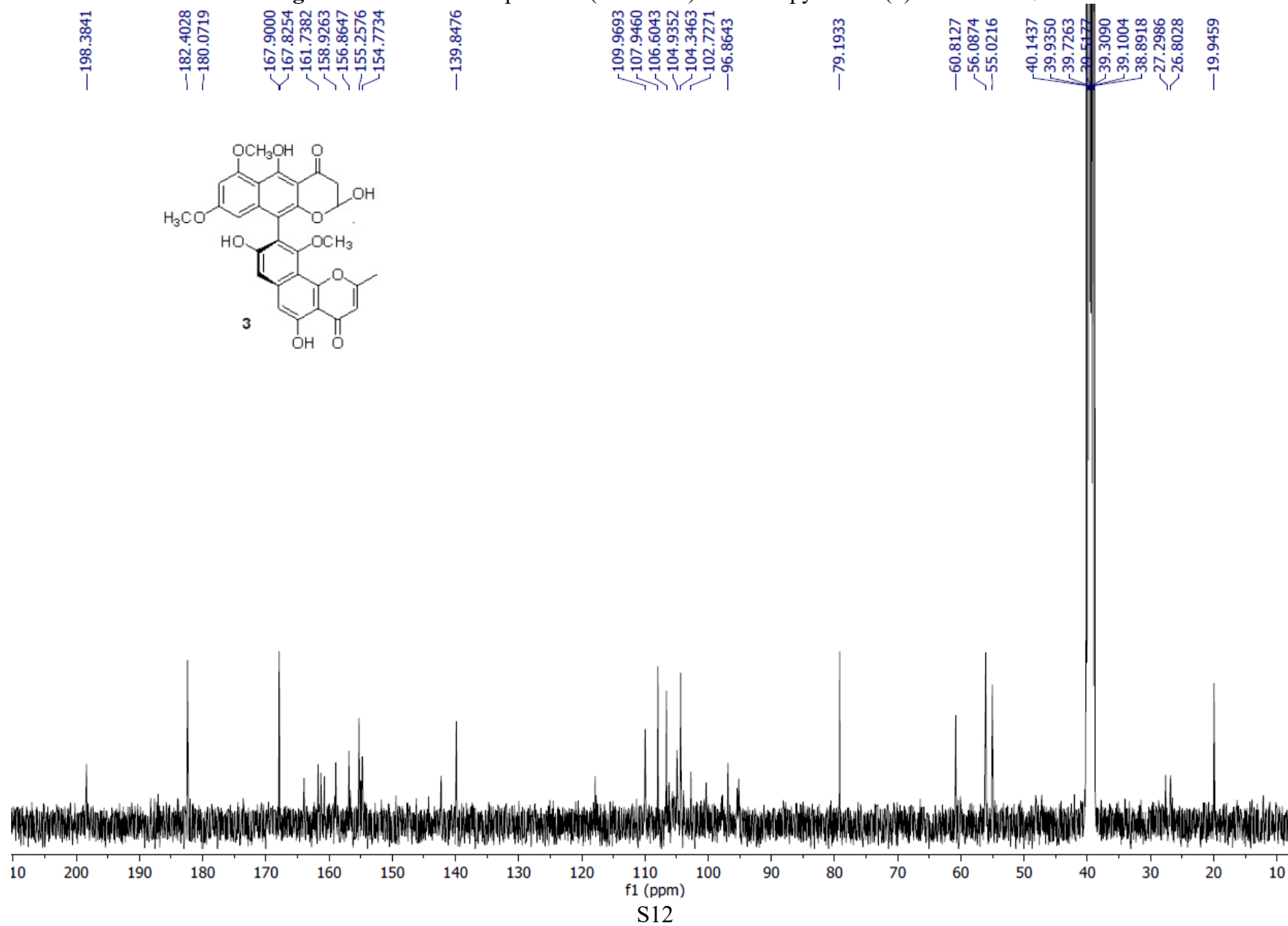


Figure S11. HSQC Spectrum (400 MHz) of Teratopyrone C (**3**) in DMSO-d₆

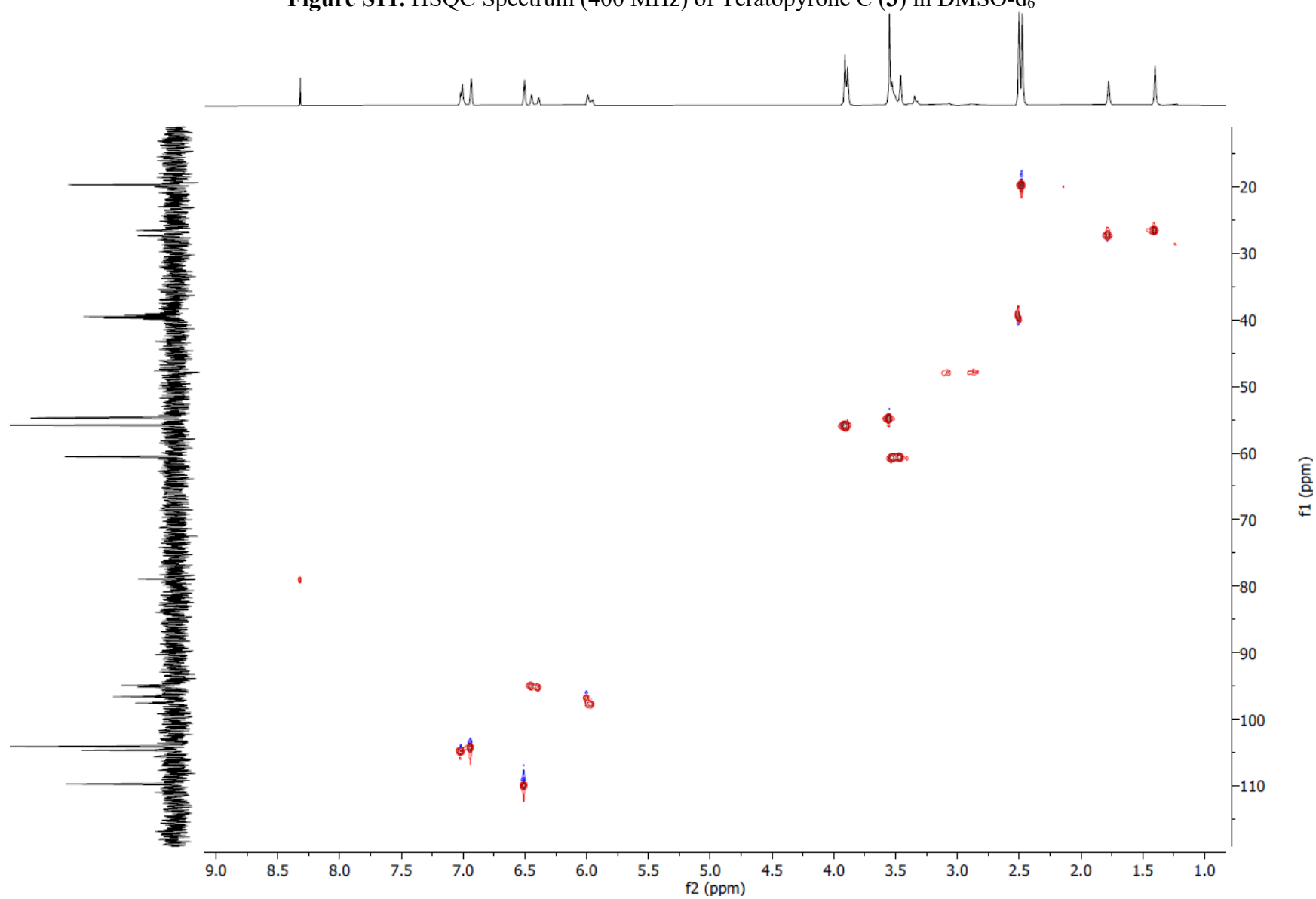


Figure S12. HMBC Spectrum (400 MHz) of Teratopyrone C (**3**) in DMSO-d₆

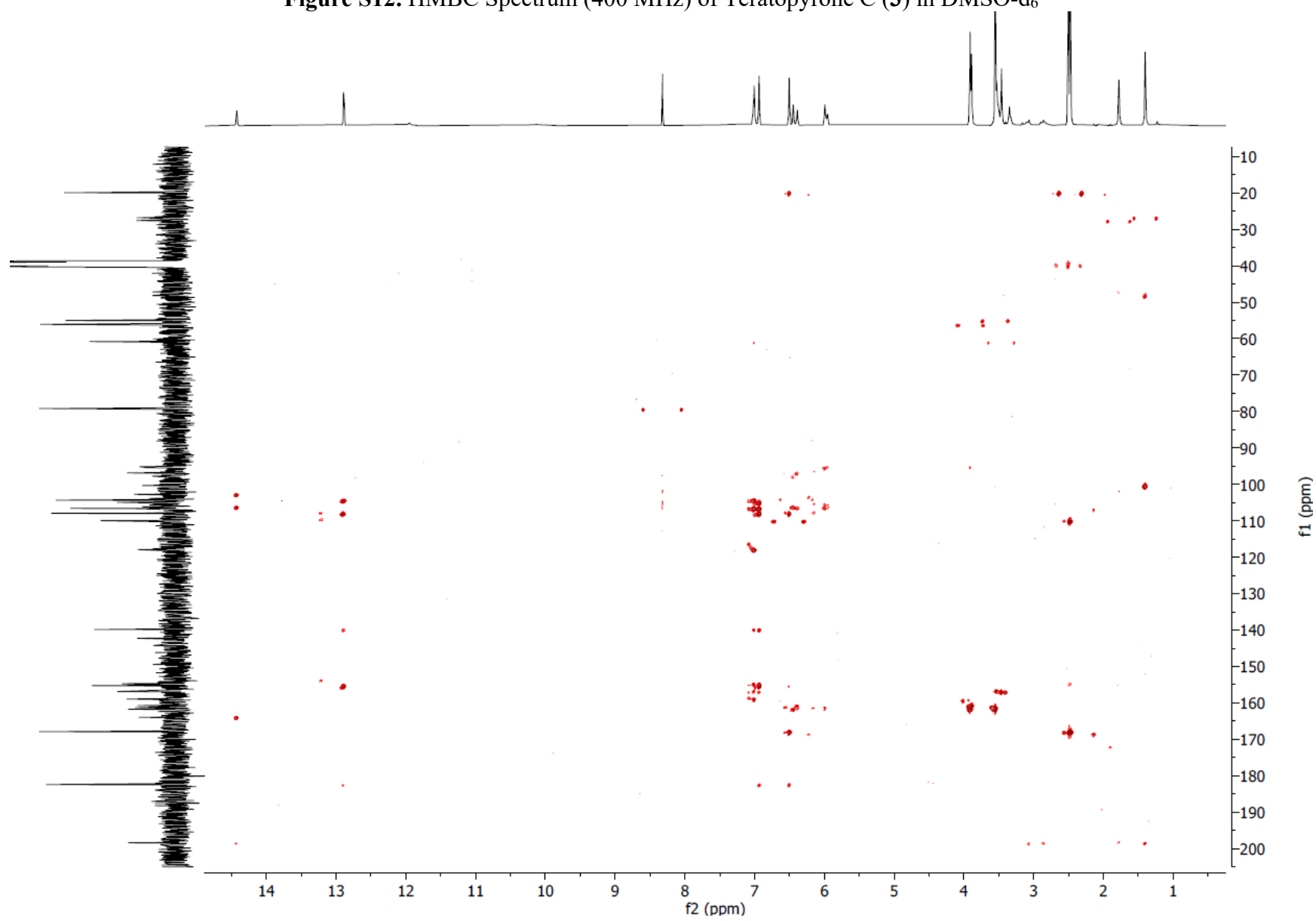


Figure S13. Results of maximum likelihood analysis placing strain AK1128 within *Teratosphaeria* with high support. Numbers in association with nodes indicate bootstrap values (values ≥ 70 are shown).

