

Supplementary Information for

Zoanthamine alkaloids from the Zoantharian *Zoanthus* cf. *pulchellus* and their effect in neuroinflammation

Paul O. Guillen ^{1,2}, Sandra Gegunde ³, Karla B. Jaramillo ^{1,4}, Amparo Alfonso ³, Kevin Calabro ², Eva Alonso ³, Jenny Rodriguez ¹, Luis M. Botana ^{3,*}, and Olivier P. Thomas ^{2,*}

¹ ESPOL Escuela Superior Politécnica del Litoral, ESPOL, Centro Nacional de Acuicultura e Investigaciones Marinas, Campus Gustavo Galindo km. 30.5 vía Perimetral, P.O.Box 09-01-5863, Guayaquil, Ecuador.; P.GUILLENMENA1@nuigalway.ie, K.JARAMILLOAGUILAR1@nuigalway.ie, jenrodri@espol.edu.ec

² Marine Biodiscovery, School of Chemistry and Ryan Institute, National University of Ireland Galway (NUI Galway), University Road, H91 TK33 Galway, Ireland; kevin.calabro@nuigalway.ie, olivier.thomas@nuigalway.ie

³ Departamento de Farmacología, Facultad de Veterinaria, Universidade de Santiago de Compostela, 27002 Lugo, Spain; sandra.gegunde@rai.usc.es, amparo.alfonso@usc.es, eva.alonso@usc.es, luis.botana@usc.es

⁴ Zoology, School of Natural Sciences and Ryan Institute, National University of Ireland Galway (NUI Galway), University Road, H91 TK33 Galway, Ireland

* Correspondence: luis.botana@usc.es and olivier.thomas@nuigalway.ie; Tel.: +353-91-493563

P **Figure S1.** (+)-HRESIMS analysis of **1**

P **Figure S2.** ¹H NMR spectrum of **1** at 500 MHz in CDCl₃

P **Figure S3.** COSY NMR spectrum of **1** at 500 MHz in CDCl₃

P **Figure S4.** ¹³C NMR spectrum of **1** at 125 MHz in CDCl₃

P **Figure S5.** HSQC NMR spectrum of **1** at 500MHz in CDCl₃

P **Figure S6.** HMBC NMR spectrum of **1** at 500MHz in CDCl₃

P **Figure S7.** HMBC NMR spectrum of **1** at 500MHz in CDCl₃

P **Figure S8.** (+)-HRESIMS analysis of **2**

P **Figure S9.** ¹H NMR spectrum of **2** at 500 MHz in CDCl₃

P **Figure S10.** COSY NMR spectrum of **2** at 500 MHz in CDCl₃

P **Figure S11.** ¹³C NMR spectrum of **2** at 125 MHz in CDCl₃

P **Figure S12.** HSQC NMR spectrum of **2** at 500 MHz in CDCl₃

P **Figure S13.** HMBC NMR spectrum of **2** at 500 MHz in CDCl₃

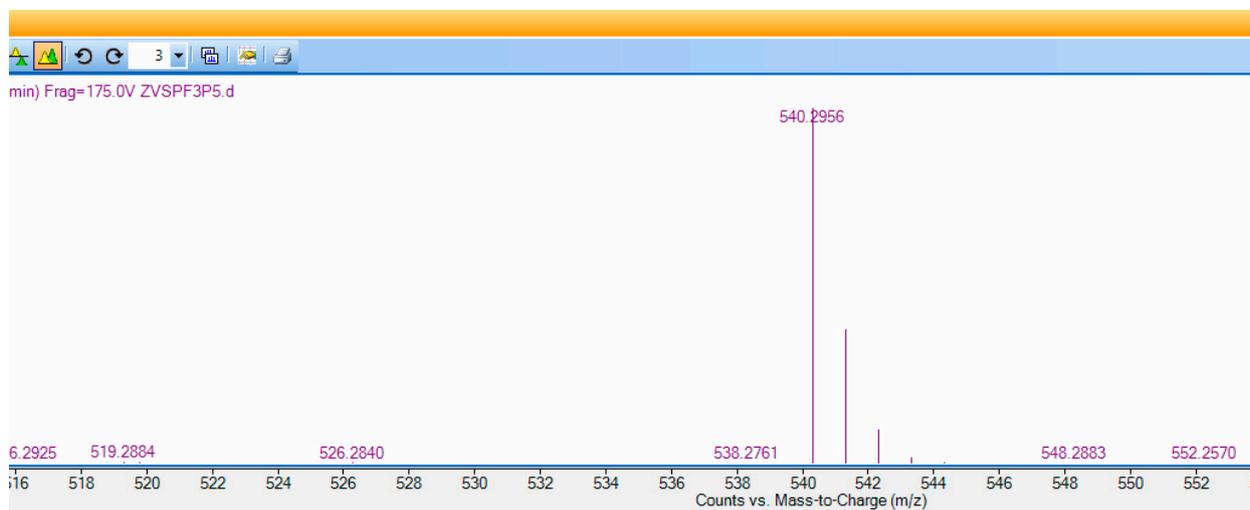


Figure S1. (+)-HRESIMS analysis of **1**.

PROTON01

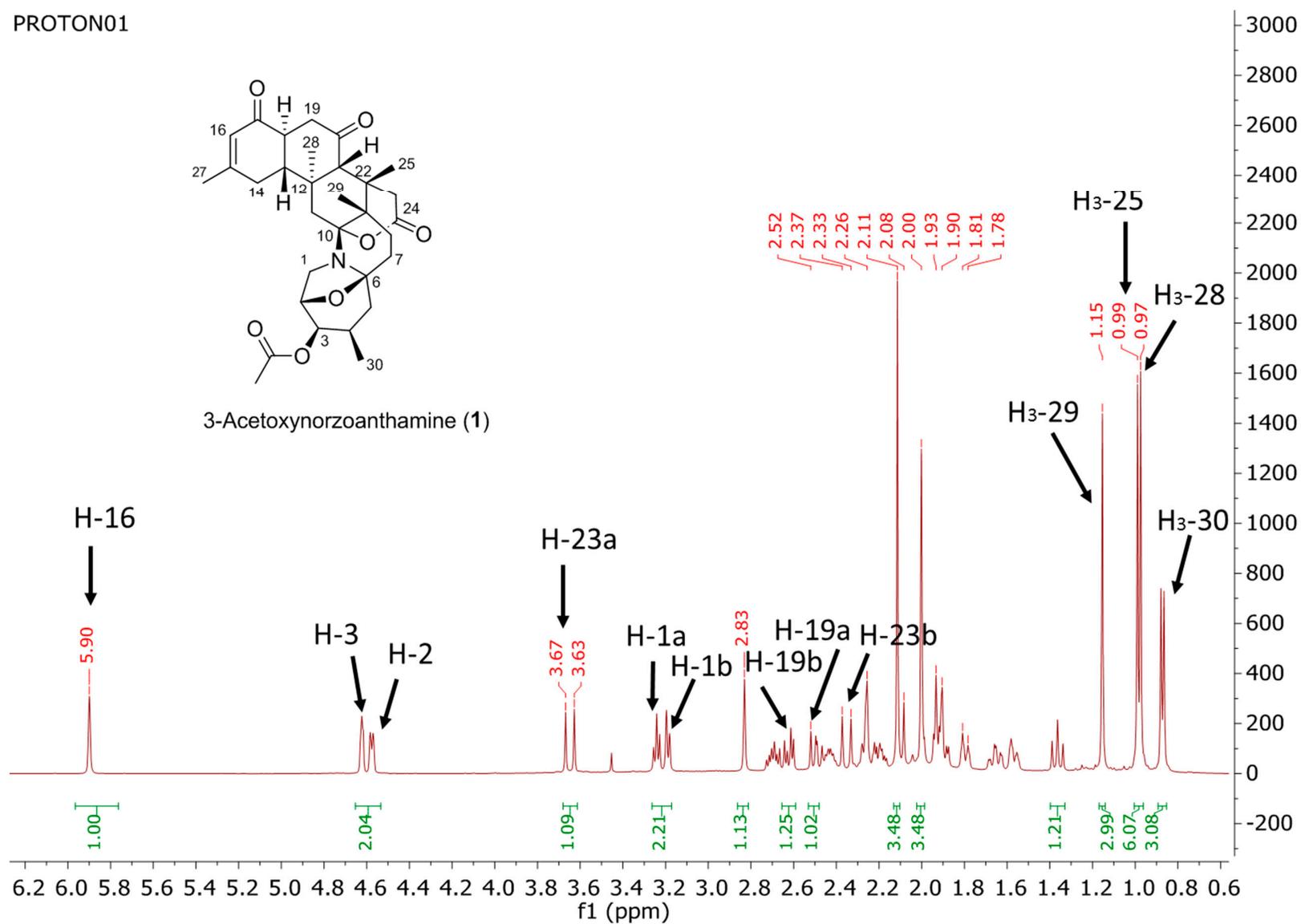


Figure S2. ¹H NMR spectrum of 1 at 500 MHz in CDCl₃

CARBON01

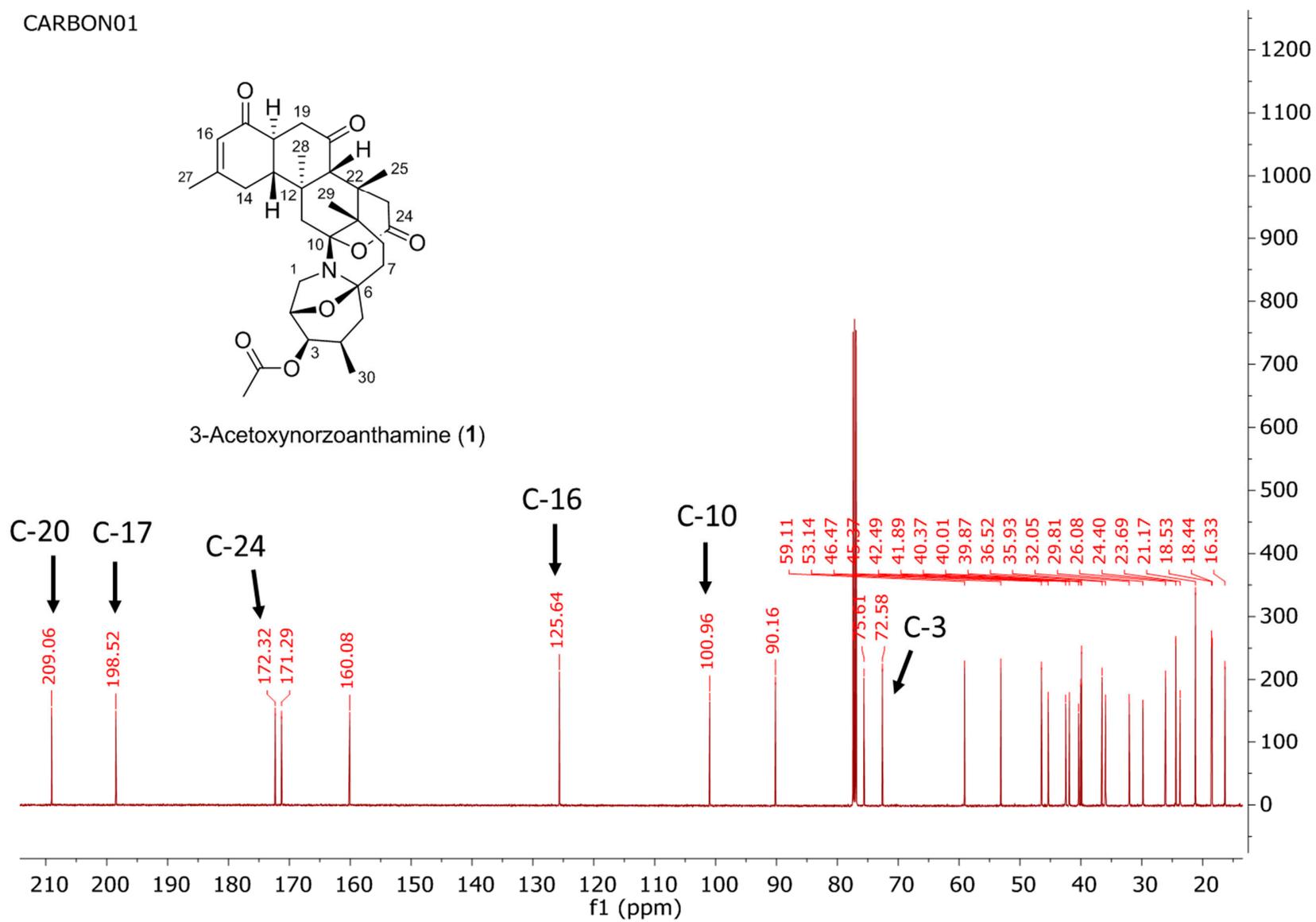


Figure S3. ^{13}C NMR spectrum of **1** at 125 MHz in CDCl_3

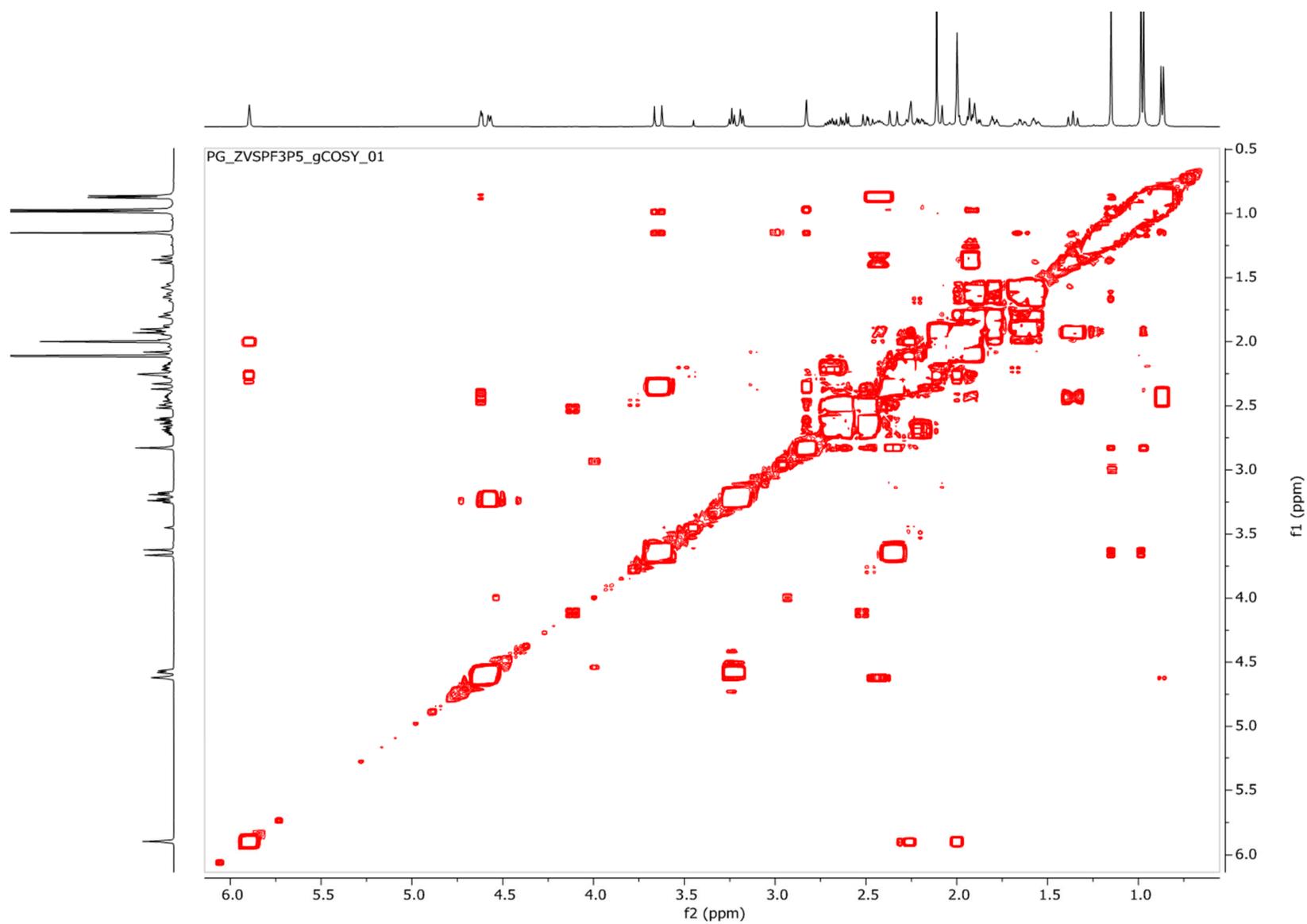


Figure S4. COSY NMR spectrum of **1** at 500 MHz in CDCl_3

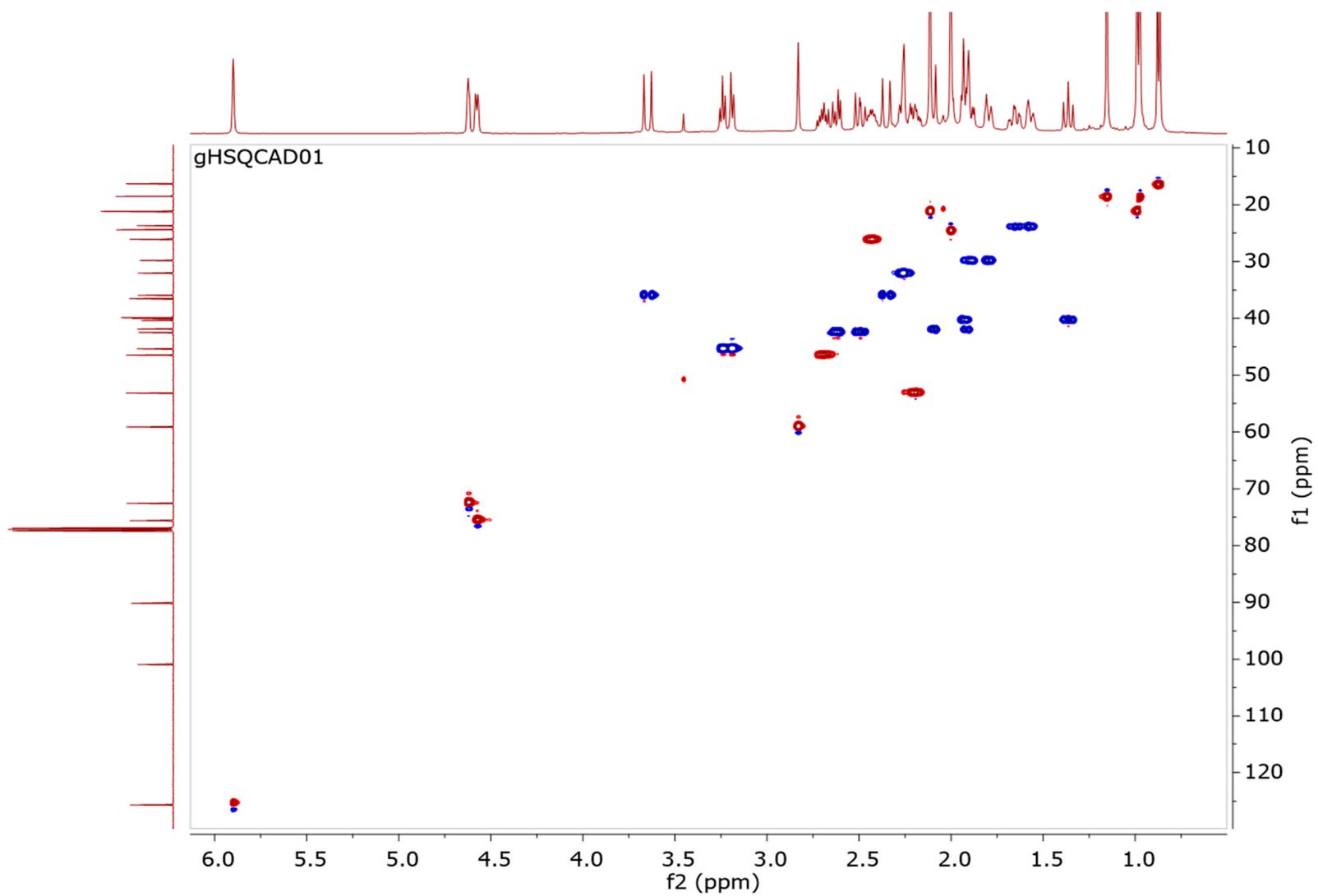


Figure S3. HSQC NMR spectrum of **1** at 500MHz in CDCl_3

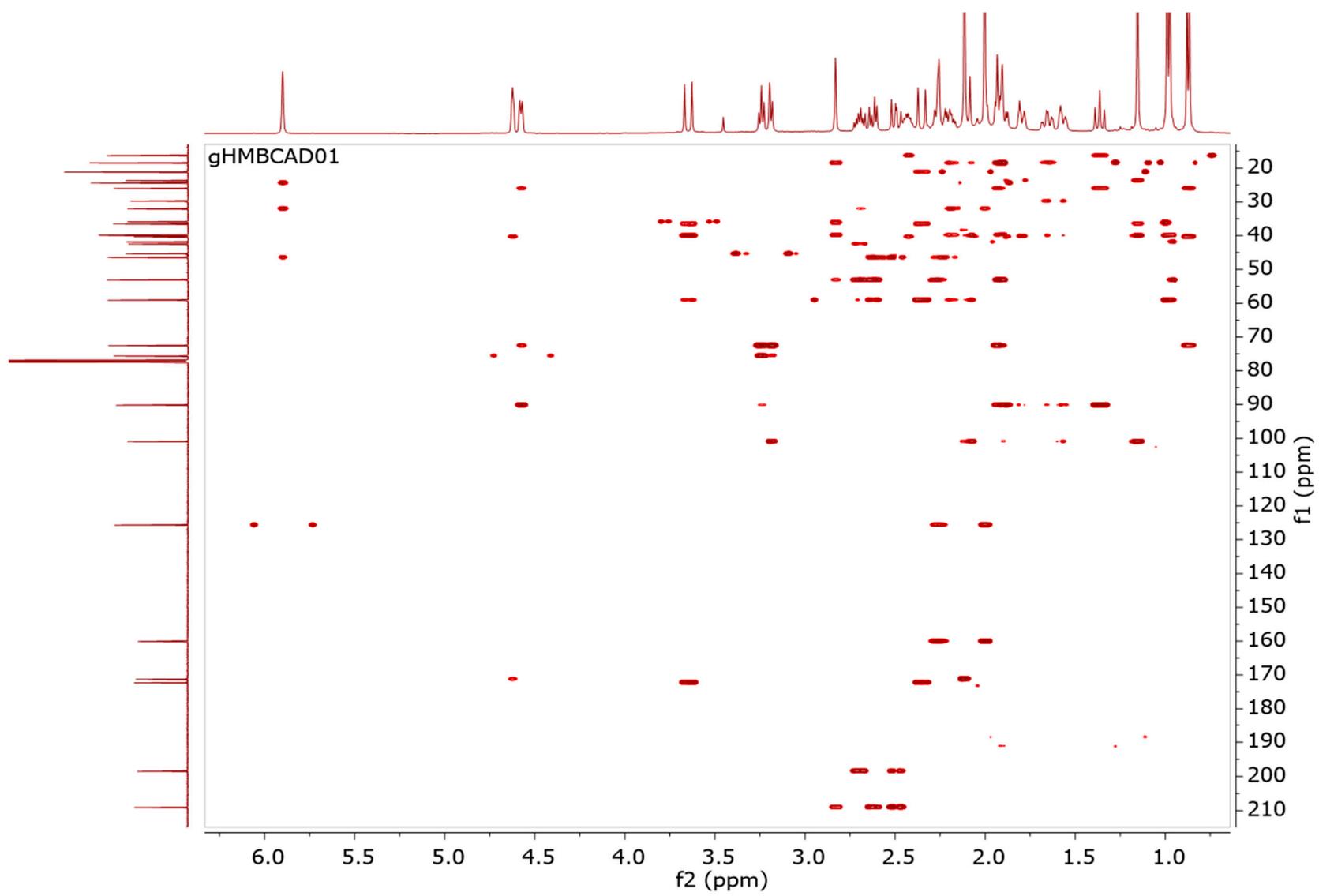


Figure S4. HMBC NMR spectrum of **1** at 500MHz in CDCl₃

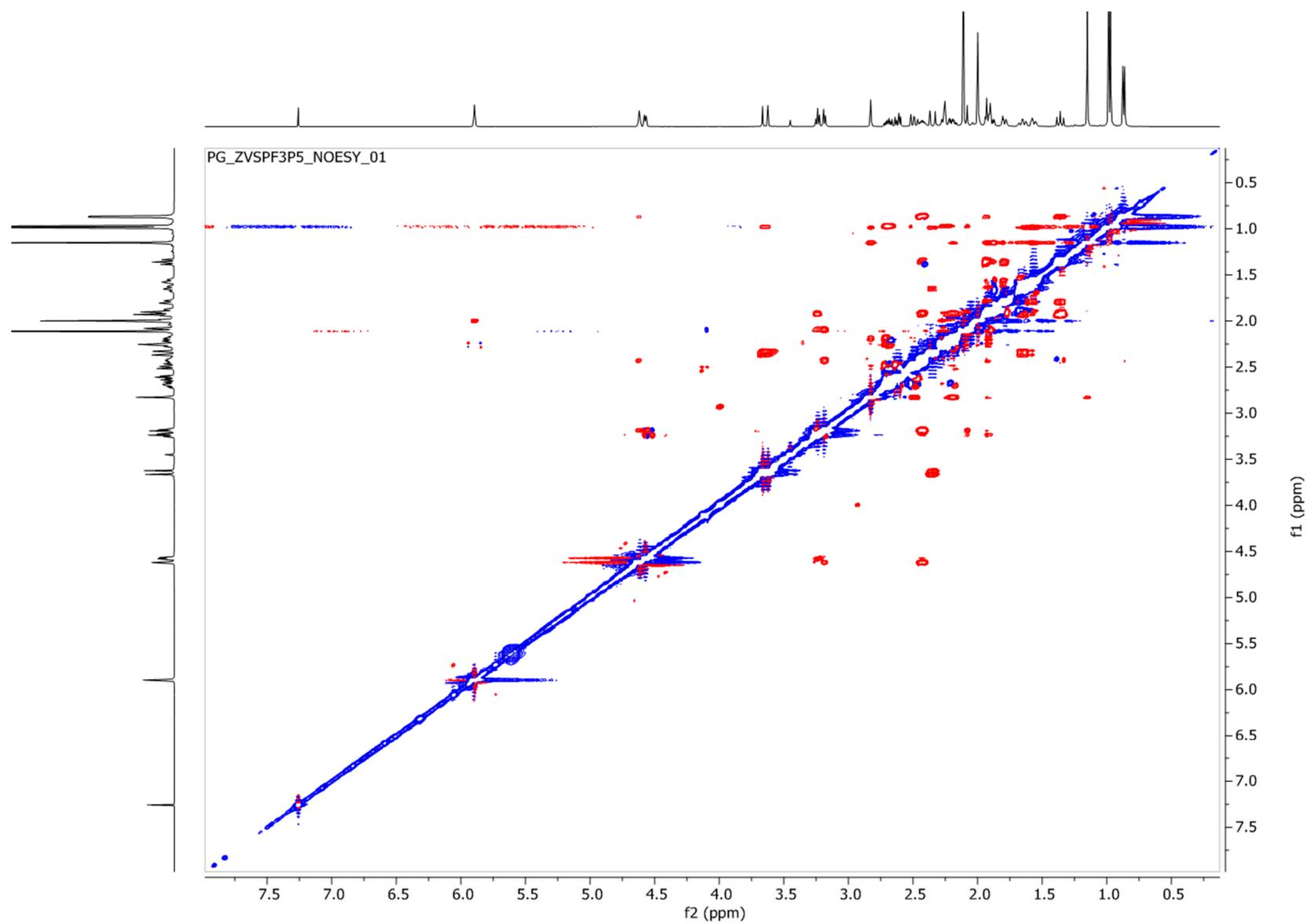


Figure S7. NOESY NMR spectrum of **1** at 500 MHz in CDCl₃

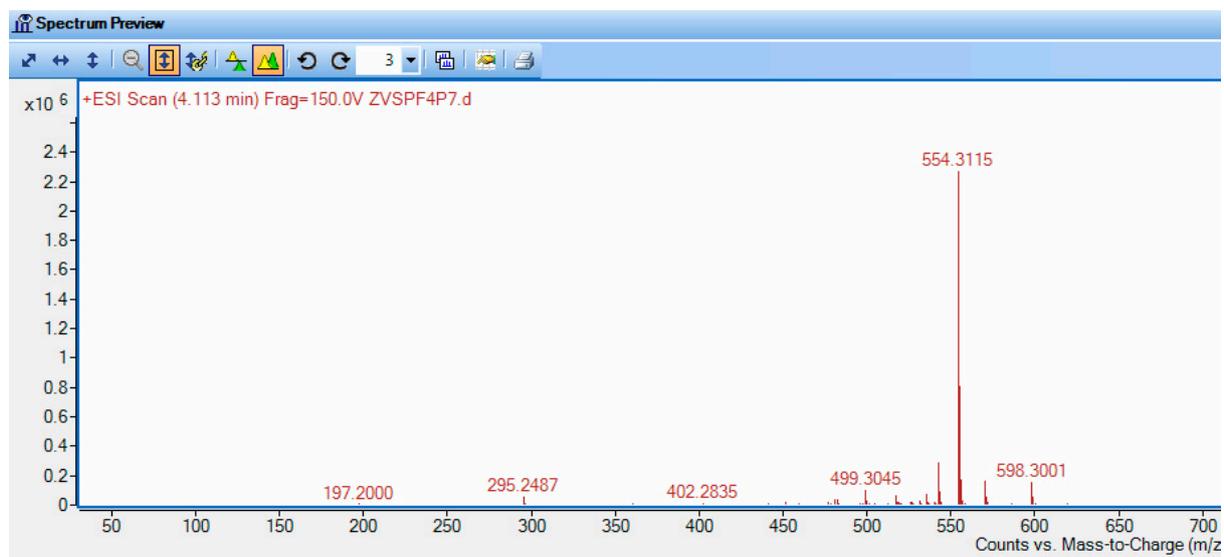


Figure S8. UHPLC-qToF analysis of **2** in (+)-ESI

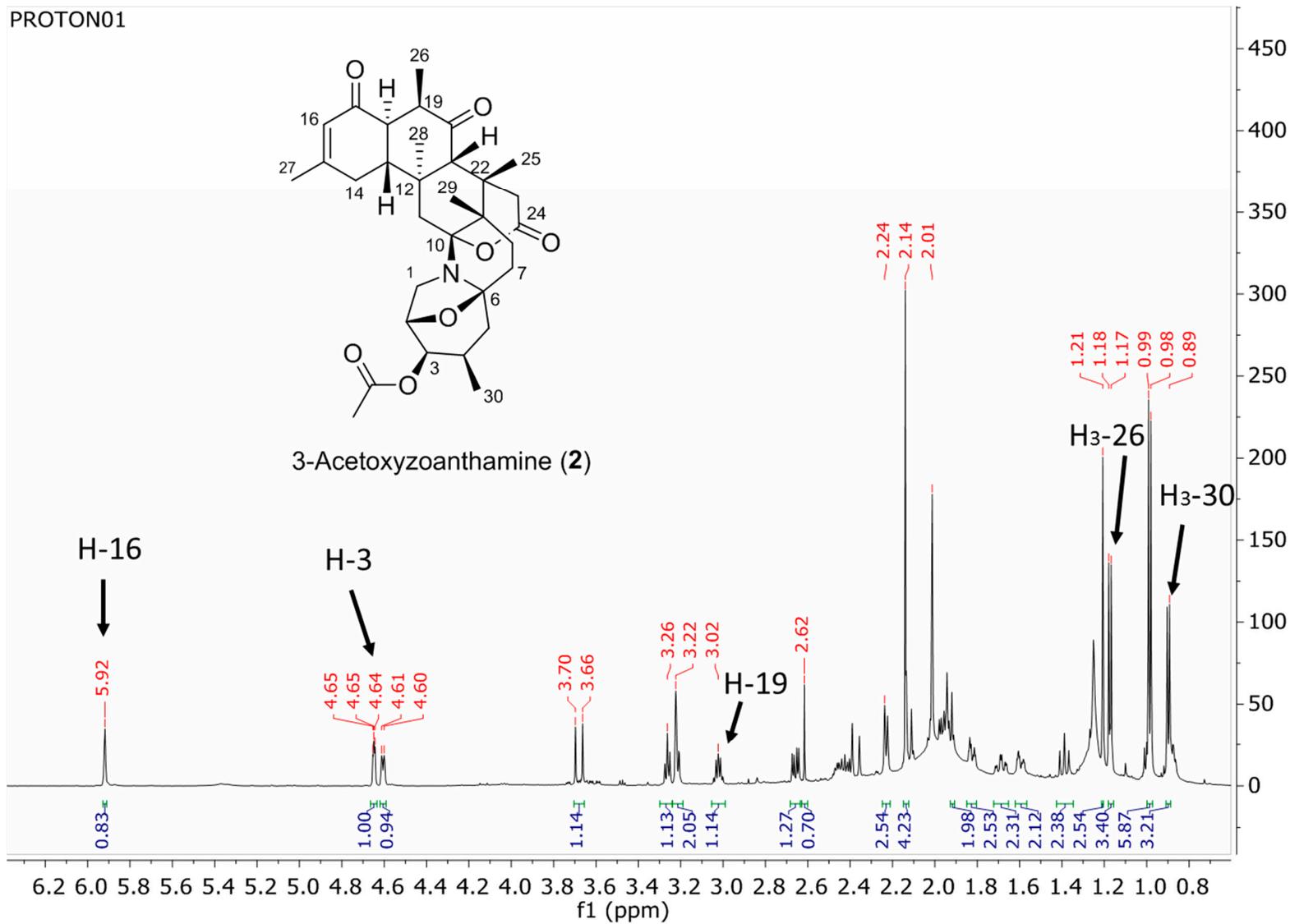


Figure S5. ¹H NMR spectrum of **2** at 500 MHz in CDCl₃

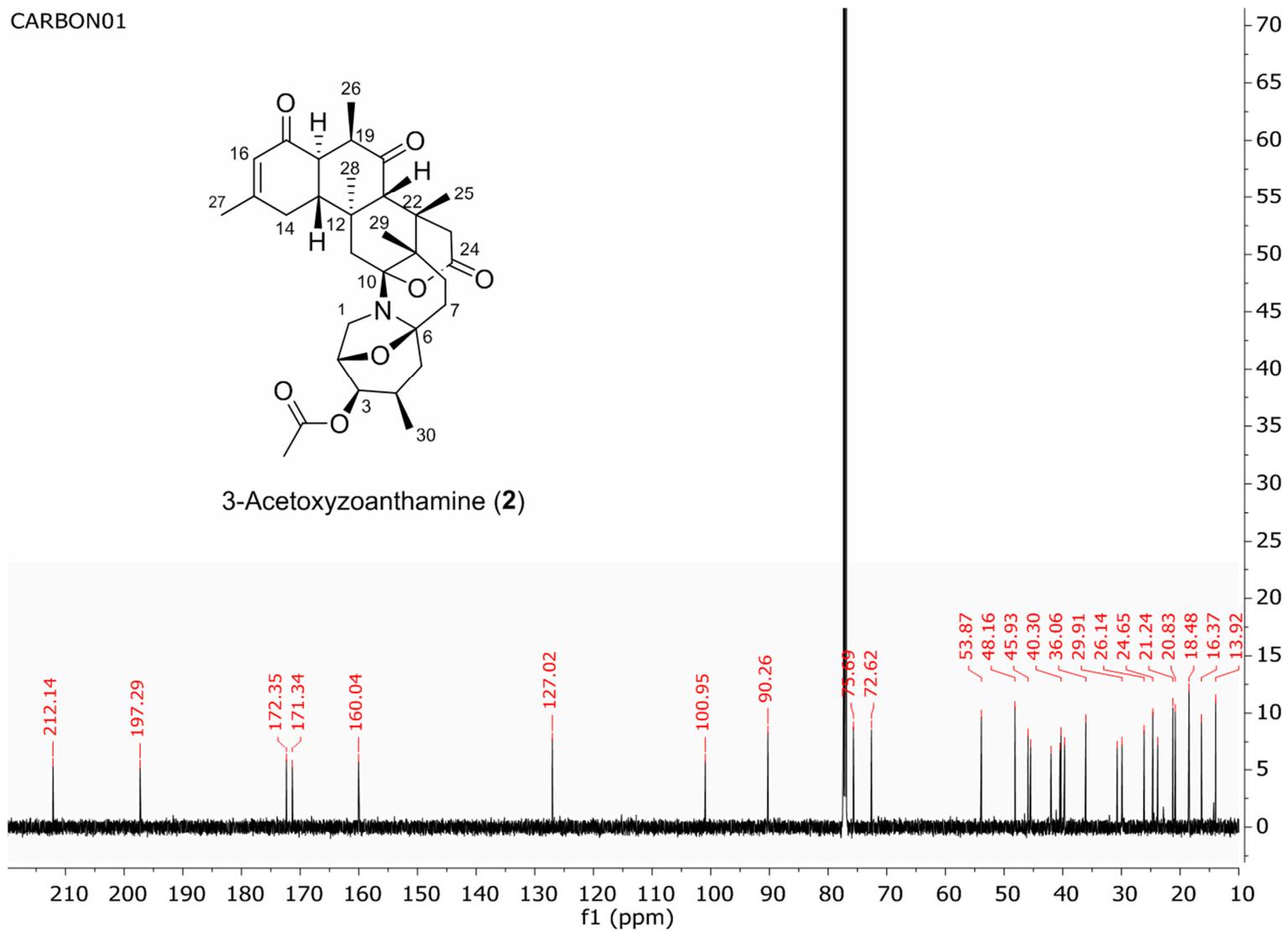


Figure S9. ¹³C NMR spectrum of **2** at 125 MHz in CDCl₃

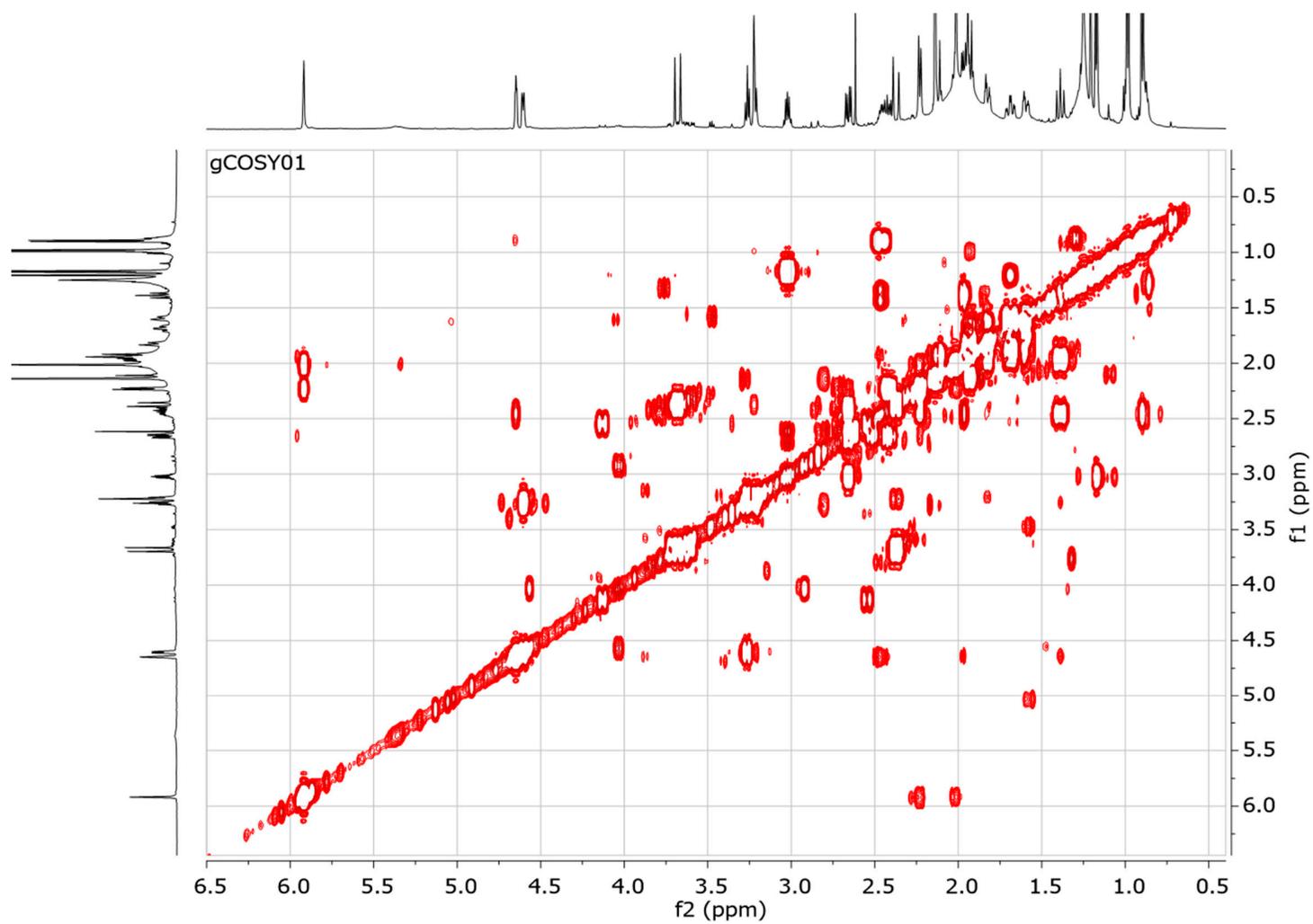


Figure S10. COSY NMR spectrum of **2** at 500 MHz in CDCl₃

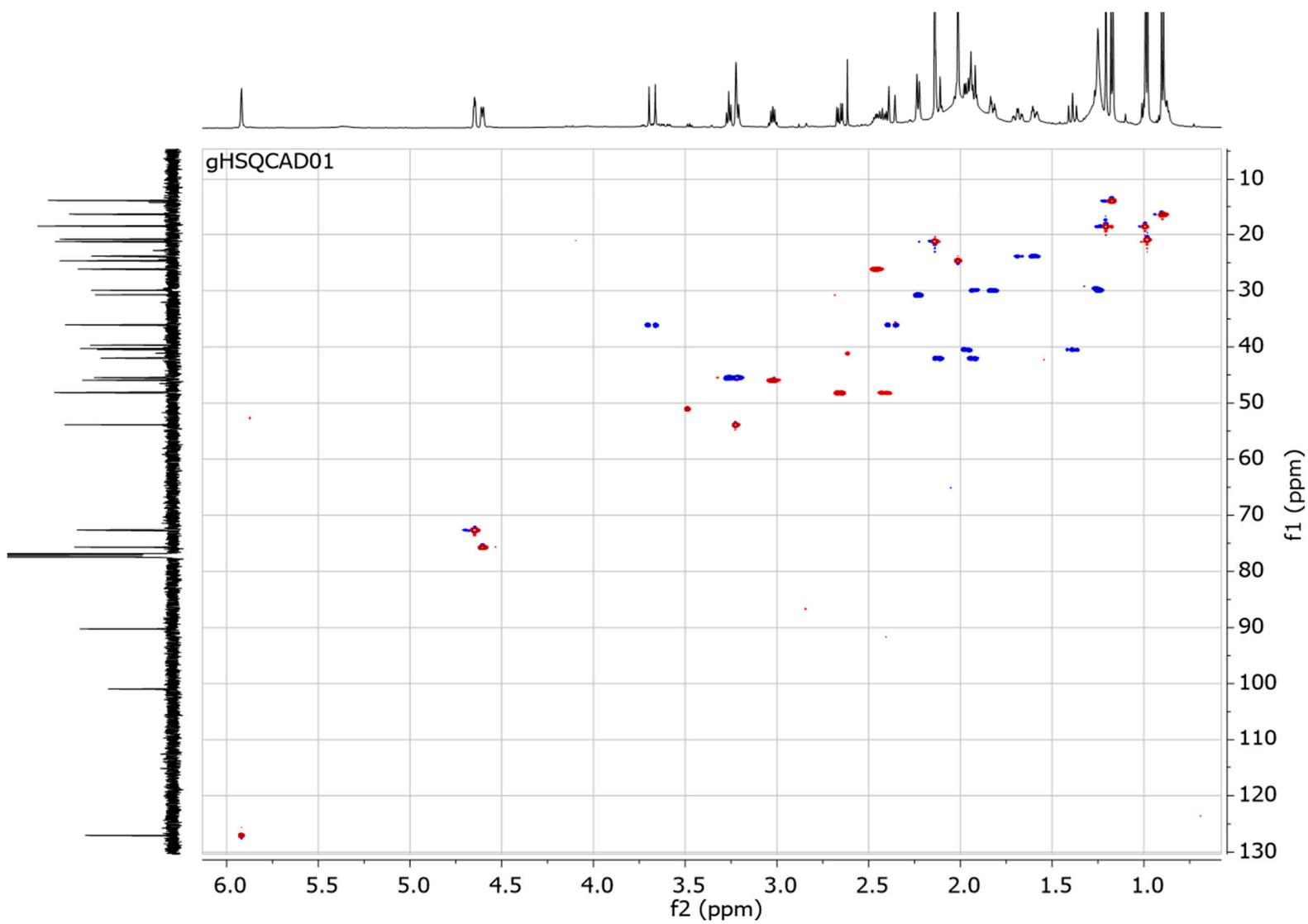


Figure S6. HSQC NMR spectrum of 2 at 500 MHz in CDCl_3

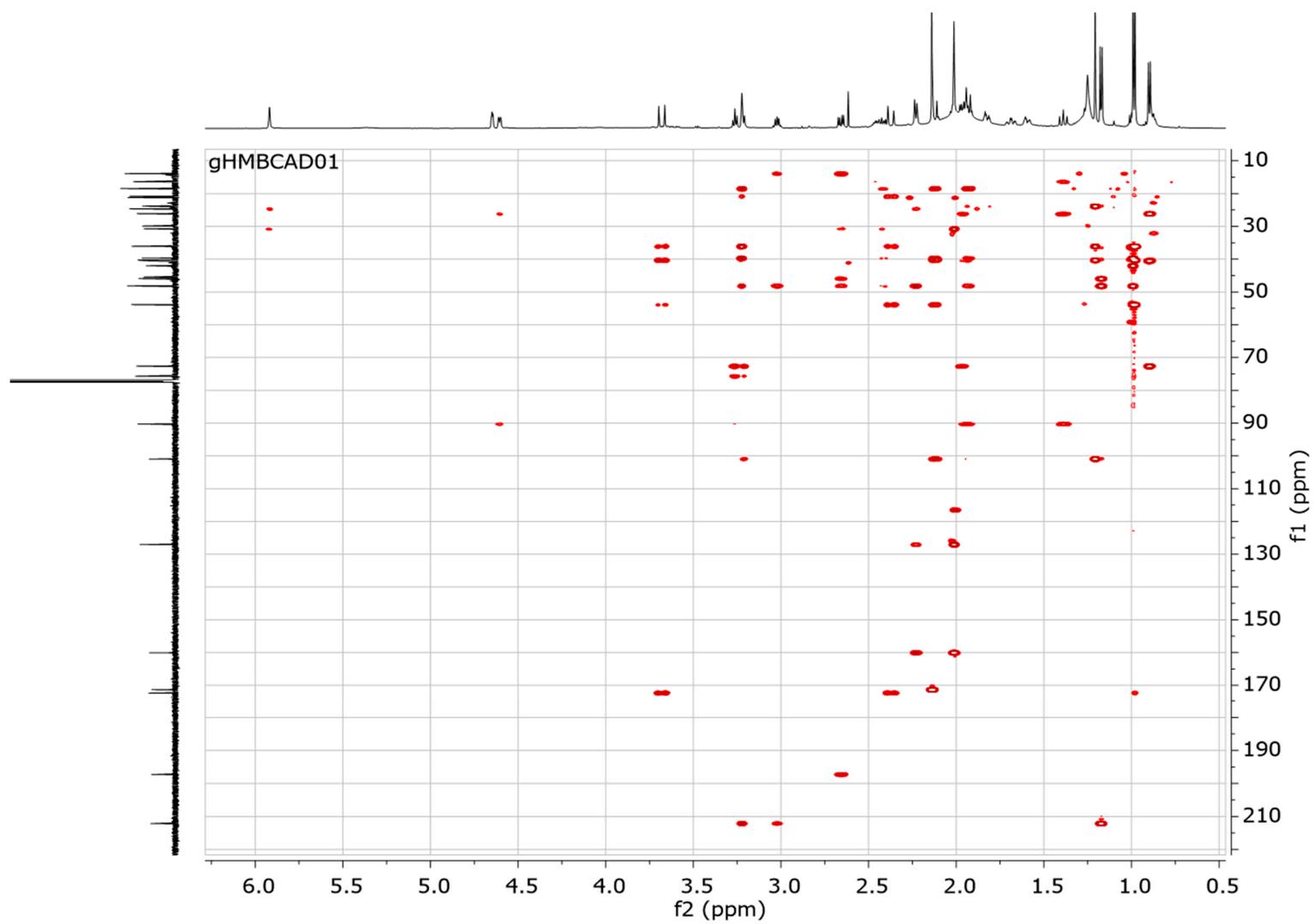


Figure S7. HMBC NMR spectrum of **2** at 500 MHz in CDCl₃