

**Supplementary Material for:**

# **New Pregnane Glycosides from *Mandevilla dardanoi* and Their Anti-inflammatory Activity**

**Francisca S. V. Lins<sup>1</sup>, Thalisson A. de Souza<sup>1</sup>, Luiza C. F. Opretzka<sup>2</sup>, Joanda P. R. e Silva<sup>1</sup>, Laiane C. O. Pereira<sup>1</sup>, Lucas S. Abreu<sup>2</sup>, Anderson A. V. Pinheiro<sup>1</sup>, George Luís Dias dos Santos<sup>1</sup>, Yuri M. do Nascimento<sup>1</sup>, José I. M. de Melo<sup>3</sup>, Raimundo Braz-Filho<sup>4</sup>, Cristiane Flora Villarreal<sup>2</sup>, Marcelo S. da Silva<sup>1</sup> and Josean F. Tavares<sup>1,\*</sup>**

<sup>1</sup> Postgraduate Program in Natural and Synthetic Bioactive Products, Federal University of Paraíba, João Pessoa, Brazil

<sup>2</sup> School of Pharmacy, Federal University of Bahia, Salvador, Brazil

<sup>3</sup> Department of Chemistry, Institute of Chemistry, Fluminense Federal University, Niterói, Brazil

<sup>4</sup> Department of Biological Sciences, State University of Paraíba, 58429-500 Campina Grande-PB, Brazil

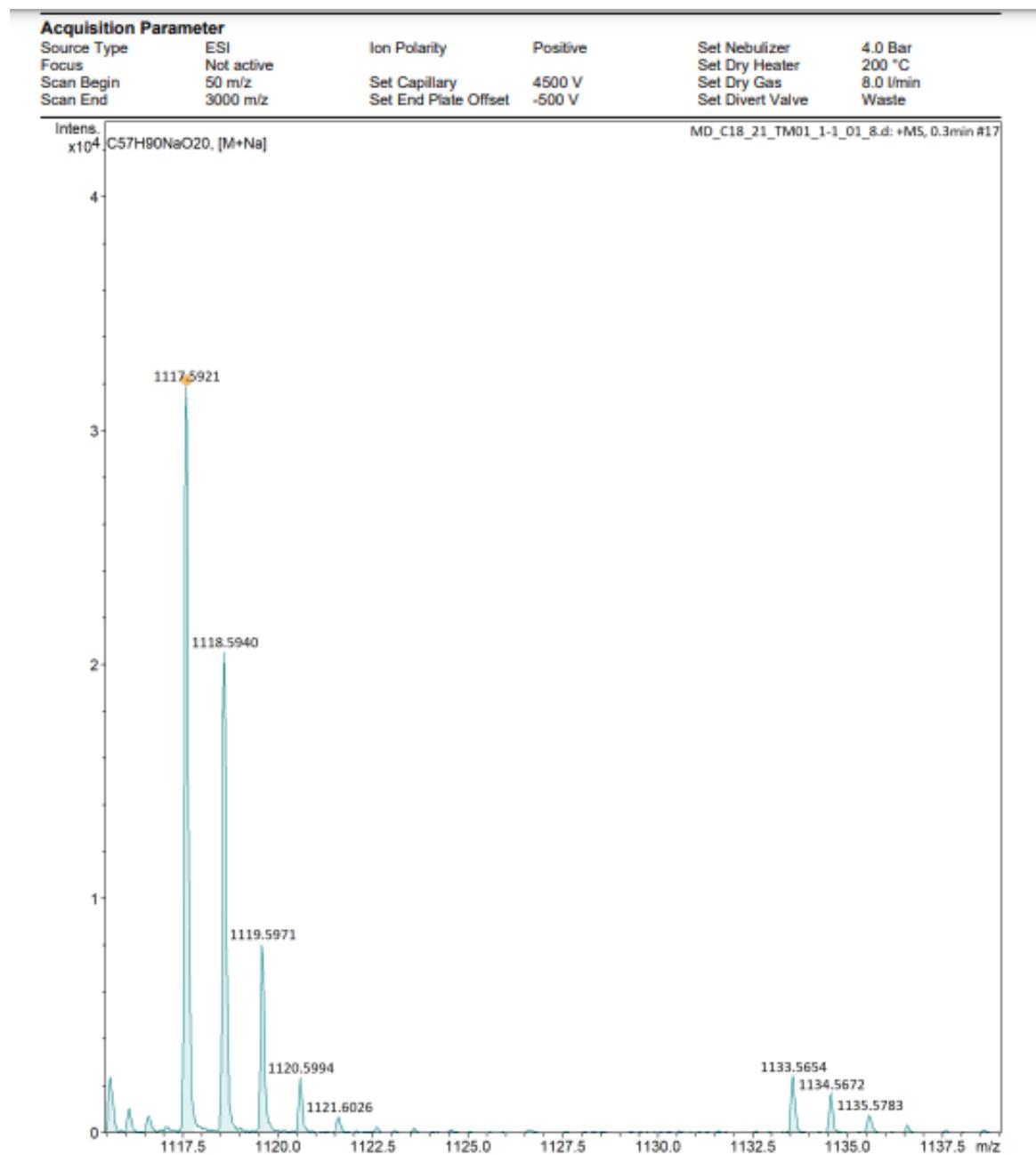
<sup>5</sup> Department of Chemistry, Institute of Chemistry, Federal Rural University of Rio de Janeiro, Seropédica, Brazil

\*Corresponding author: Josean Fechine Tavares; Instituto de Pesquisa em Fármacos e Medicamentos - Programa de Pós-Graduação em Produtos Naturais e Sintéticos Bioativos, Universidade Federal da Paraíba, 58051-900 João Pessoa-PB, Brazil. Tel.: + 55 83 988027809; E-mail address: josean@ltf.ufpb.br; ORCID ID: 6009412640611523.

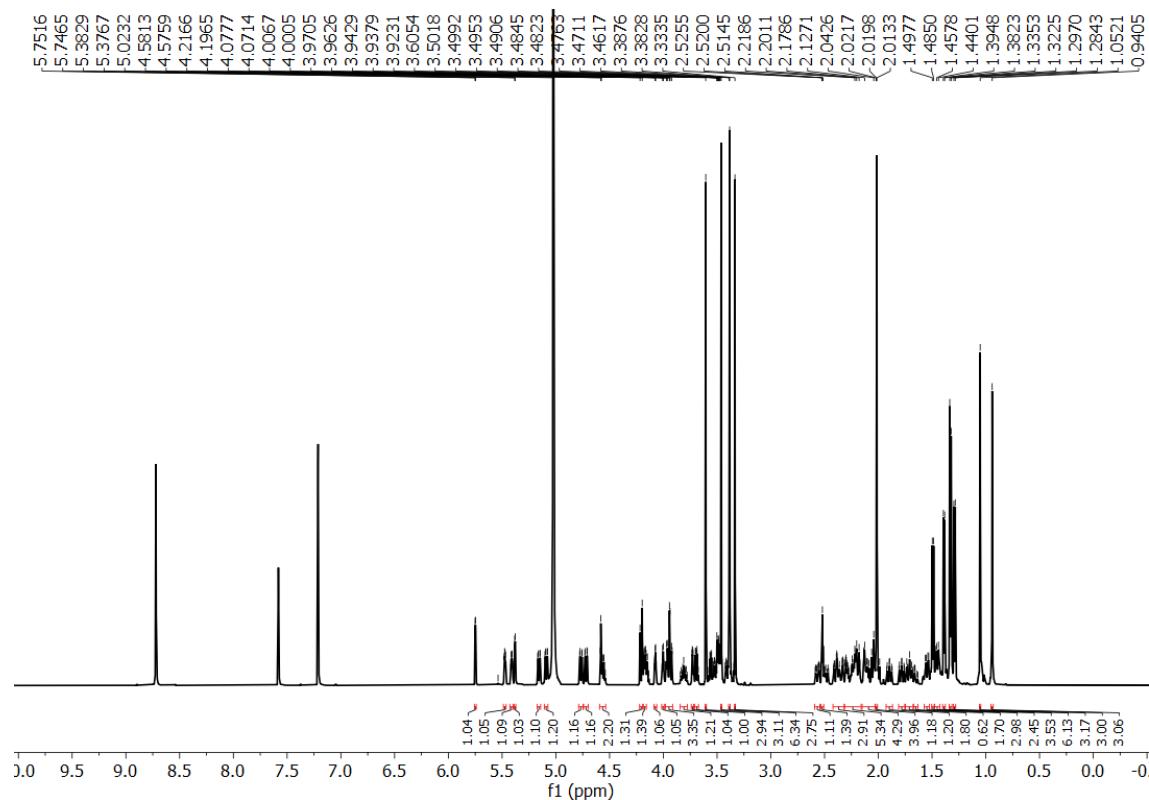
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- Figure S85** COSY spectrum (400 MHz, pyridine-d<sub>5</sub>) of compound **5**
- Figure S86** Effect of 1, 2, 3 and 5 on cell viability of stimulated J774 macrophages

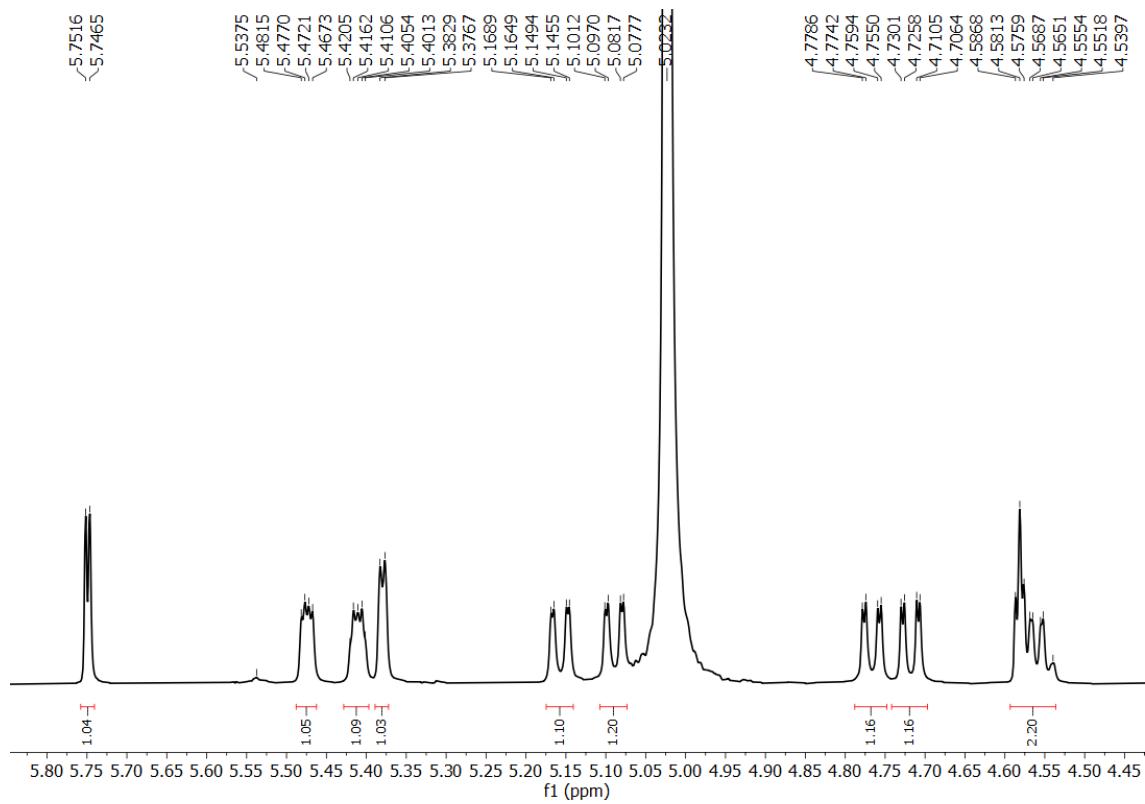
**Figure S1:** ESI-HRMS spectrum of compound 1



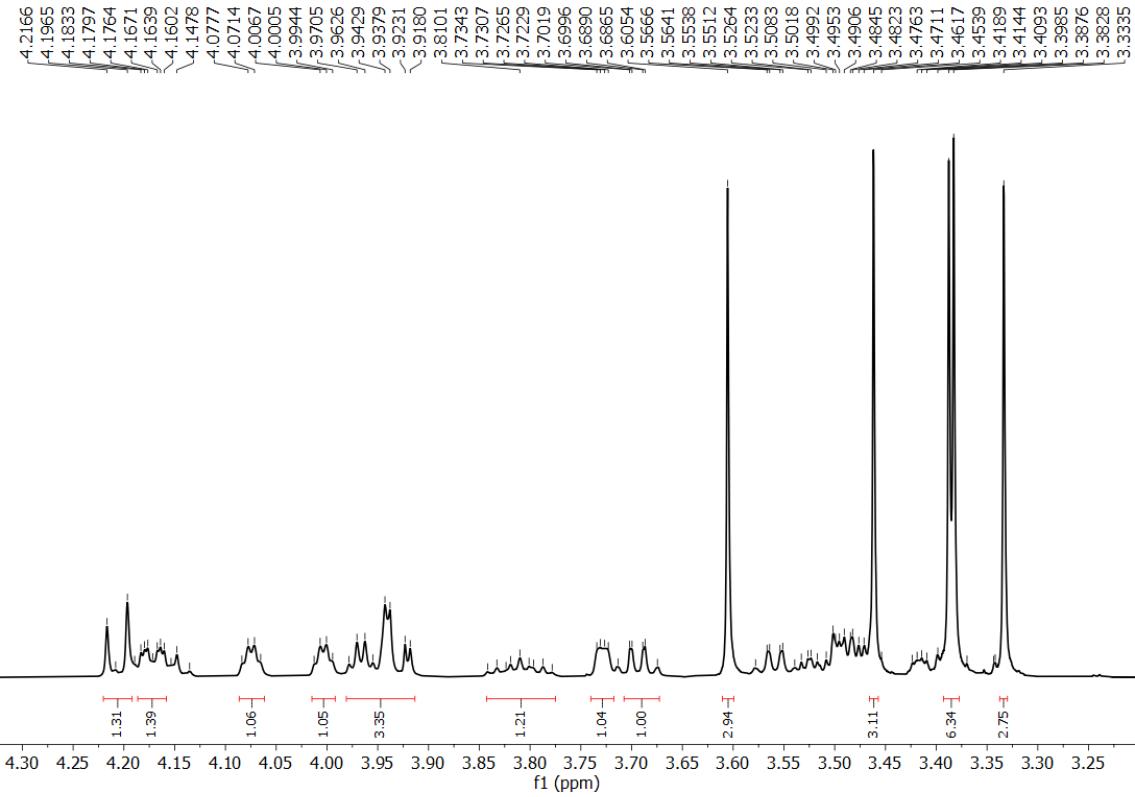
**Figure S2:**  $^1\text{H}$  NMR spectrum (pyridine-d<sub>5</sub>, 500 MHz) of compound **1**



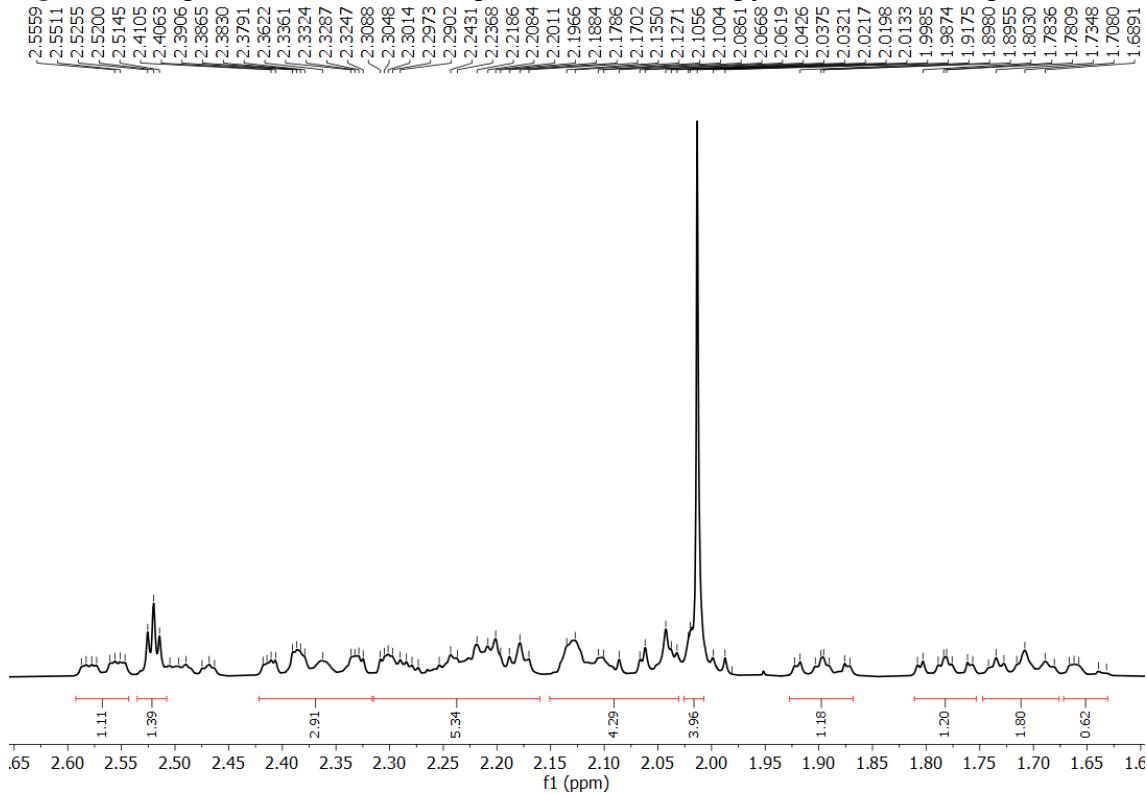
**Figure S3:** Expansion of  $^1\text{H}$  NMR spectrum (500 MHz, pyridine- $d_5$ ) of compound 1.



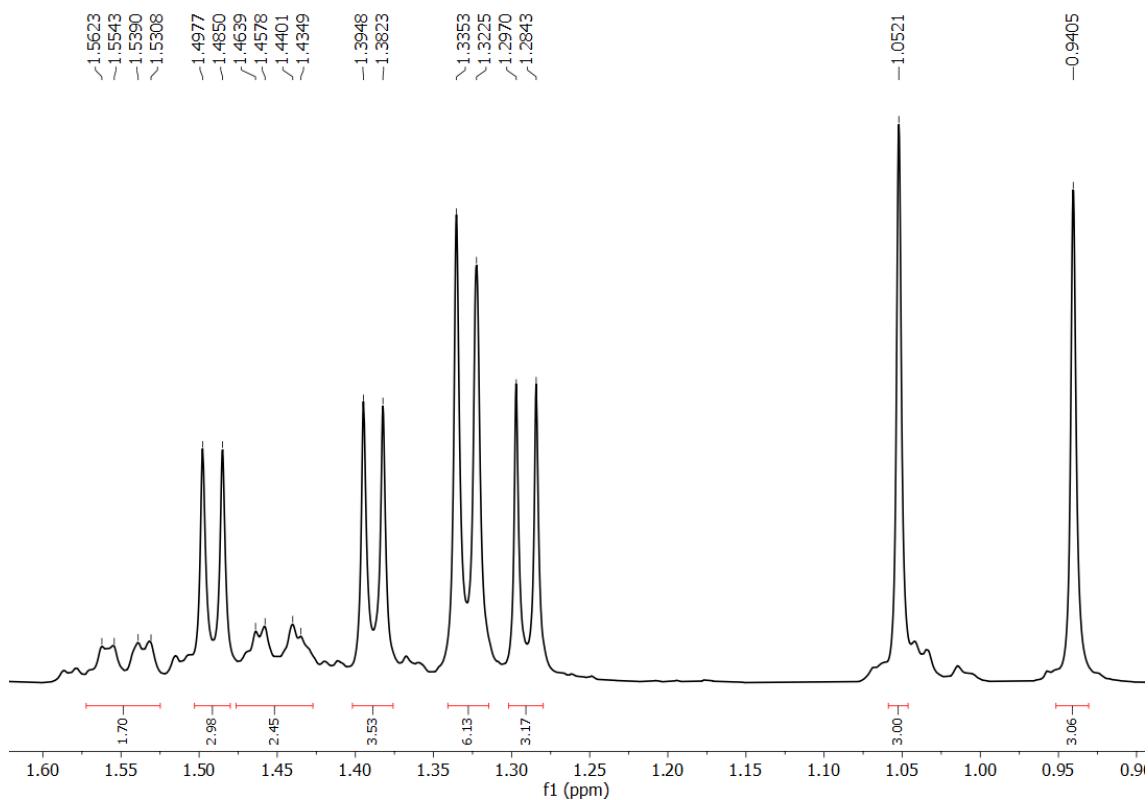
**Figure S4:** Expansion of  $^1\text{H}$  NMR spectrum (500 MHz, pyridine-d<sub>5</sub>) of compound 1.



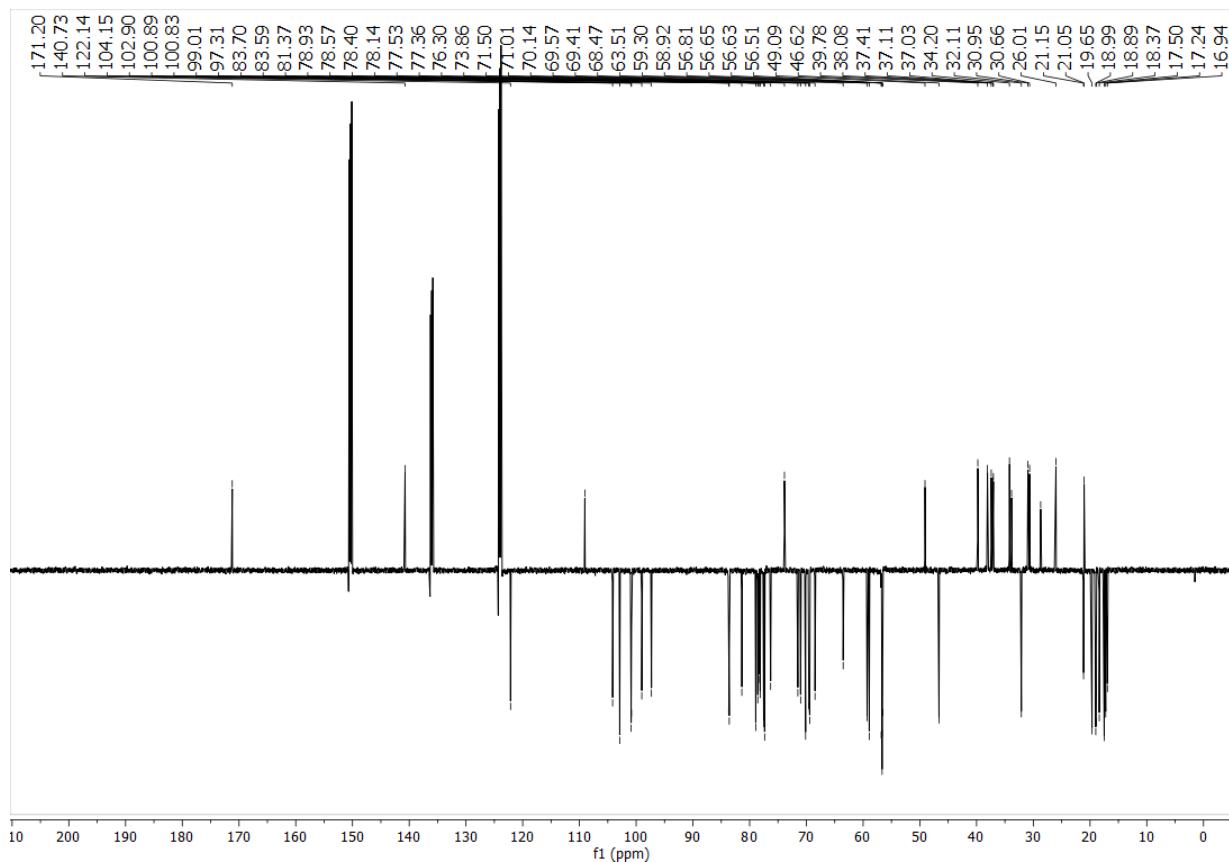
**Figure S5:** Expansion of  $^1\text{H}$  NMR spectrum (500 MHz, pyridine-d<sub>5</sub>) of compound 1.



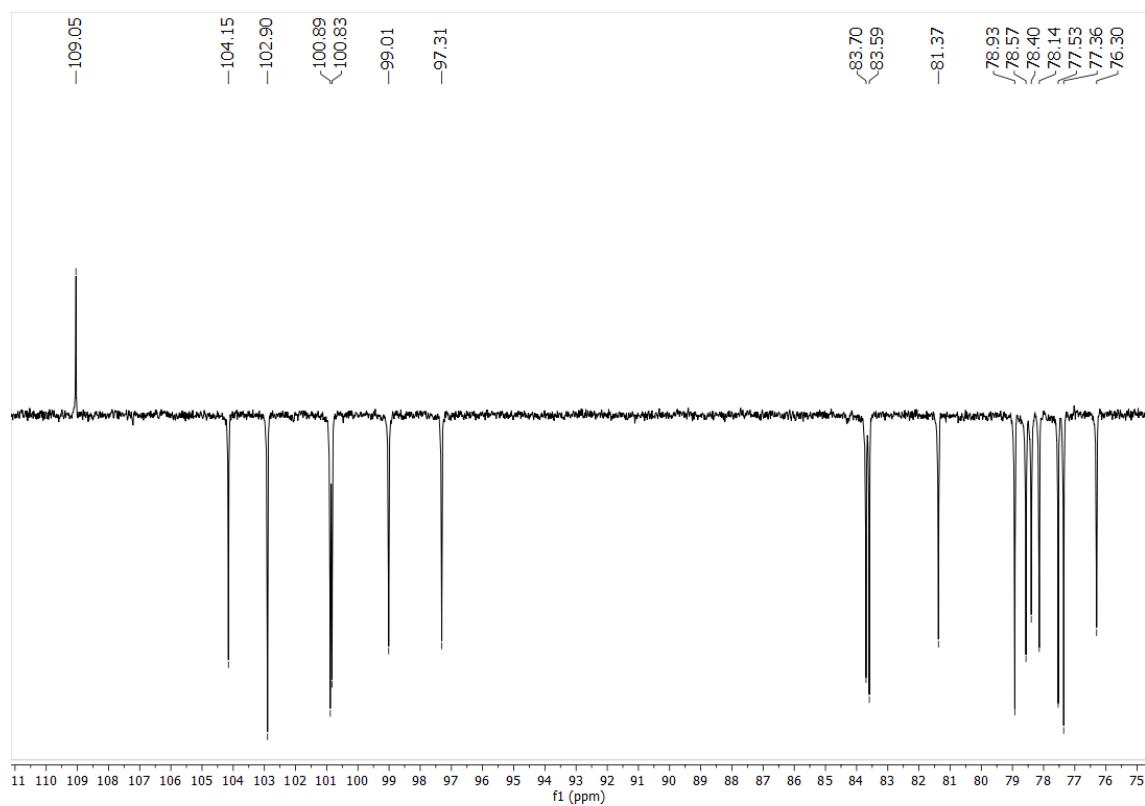
**Figure S6:** Expansion of  $^1\text{H}$  NMR spectrum (500 MHz, pyridine-d<sub>5</sub>) of compound **1**.



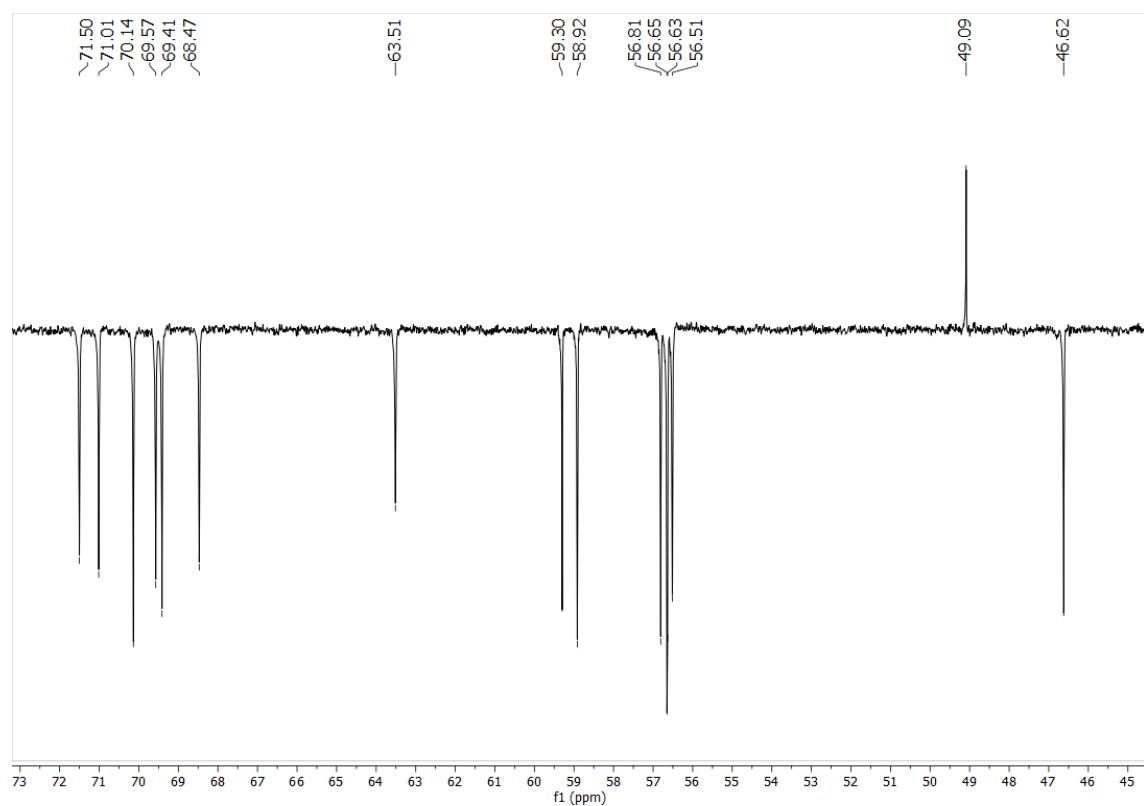
**Figure S7:** APT NMR spectrum (pyridine-d<sub>5</sub>, 125 MHz) of compound **1**.



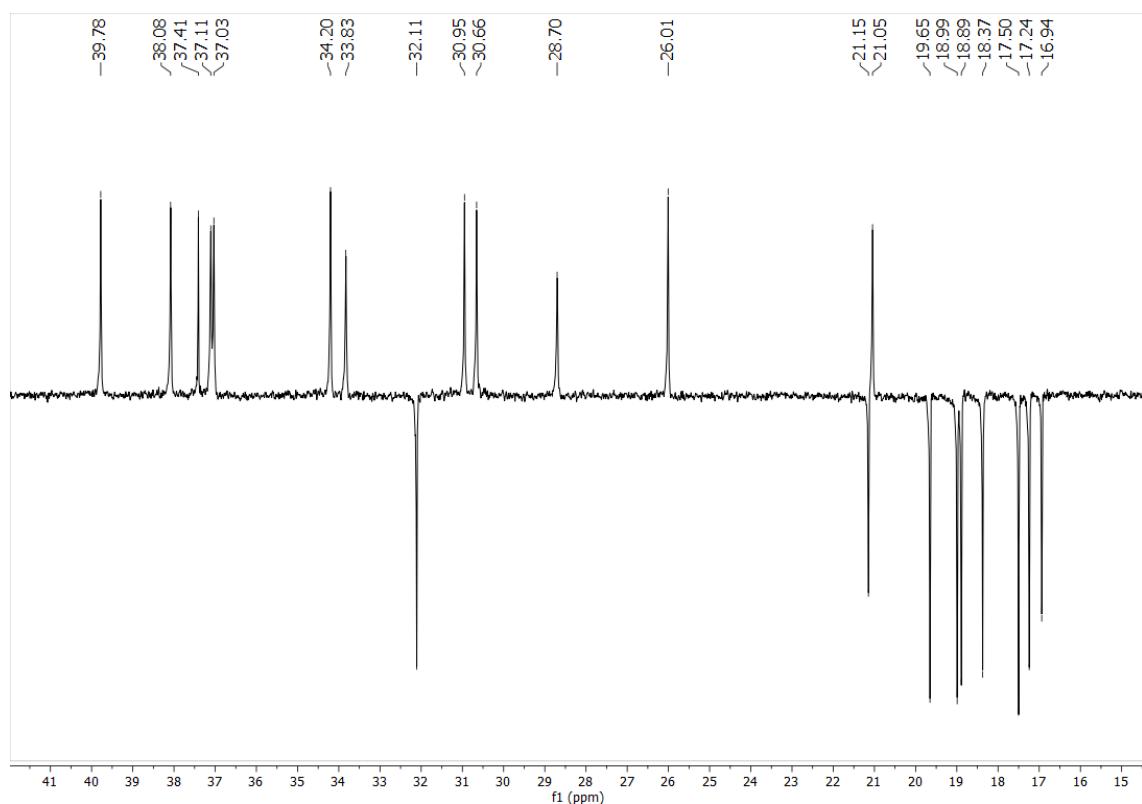
**Figure S8:** Expansion of APT NMR spectrum (pyridine-d<sub>5</sub>, 125 MHz) of compound **1**.



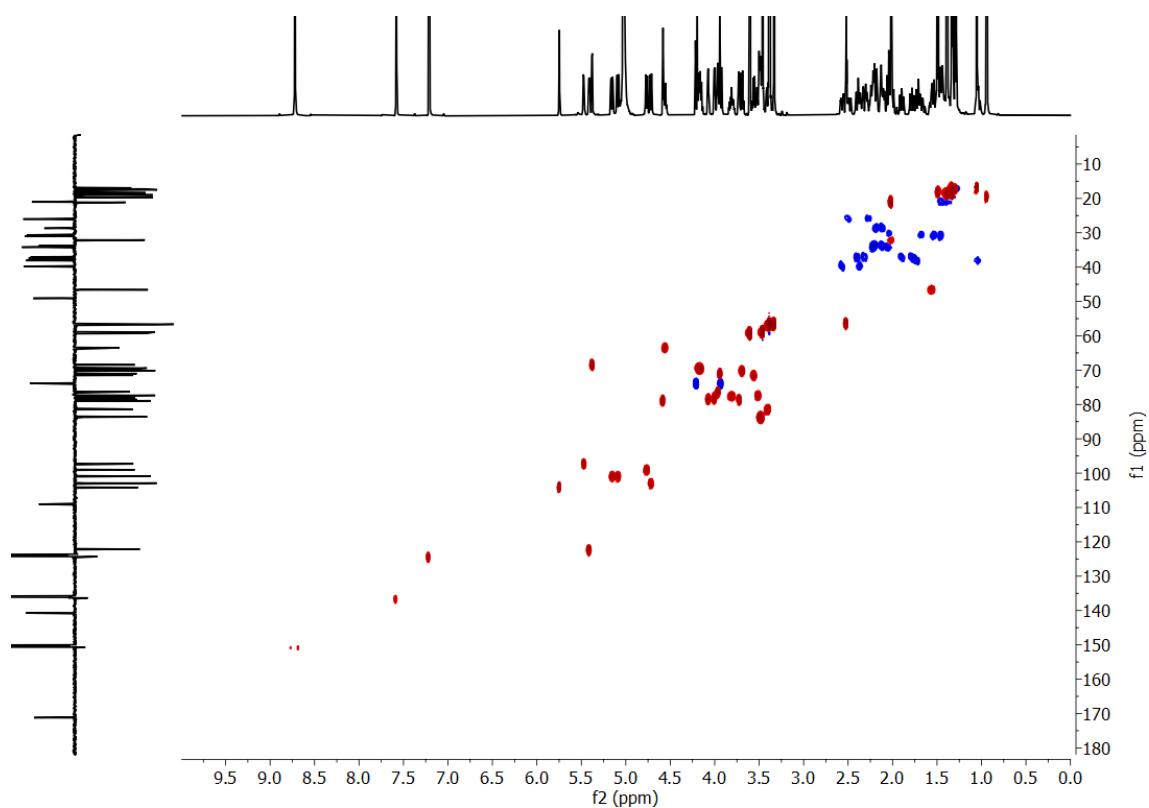
**Figure S9:** Expansion of APT NMR spectrum (pyridine-d<sub>5</sub>, 125 MHz) of compound **1**.



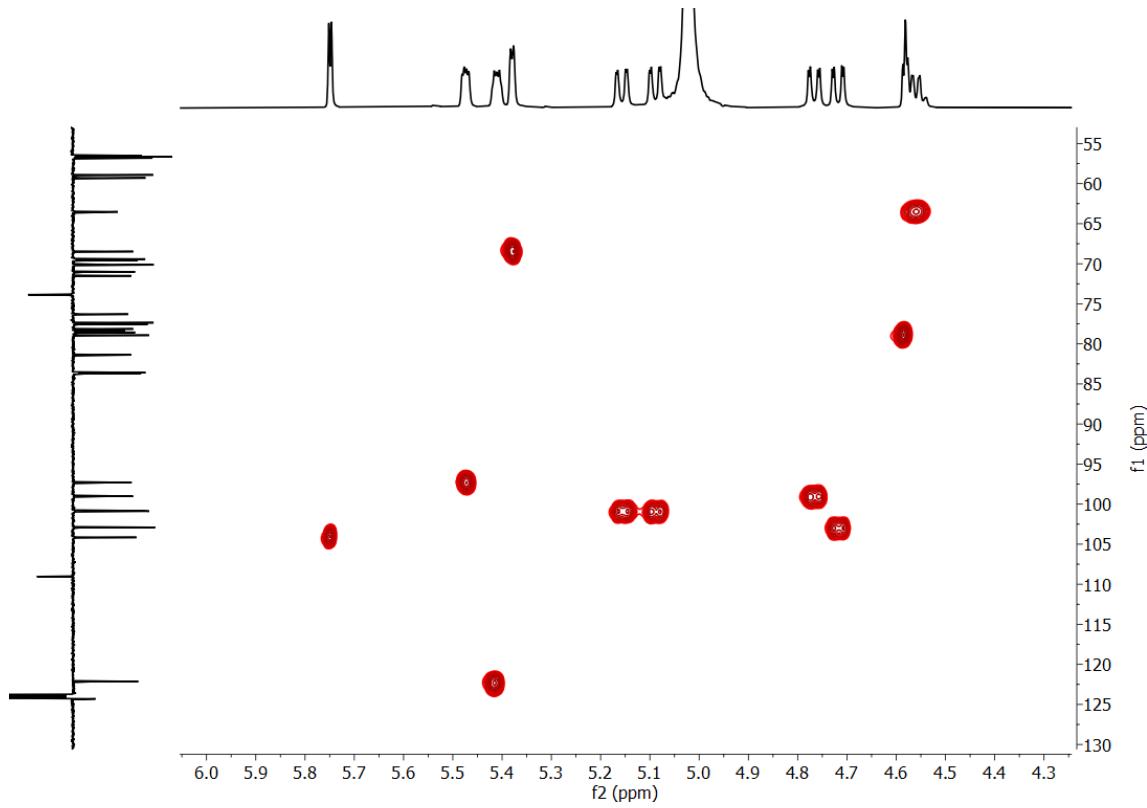
**Figure S10:** Expansion of APT NMR spectrum (pyridine-d<sub>5</sub>, 125 MHz) of compound **1**.



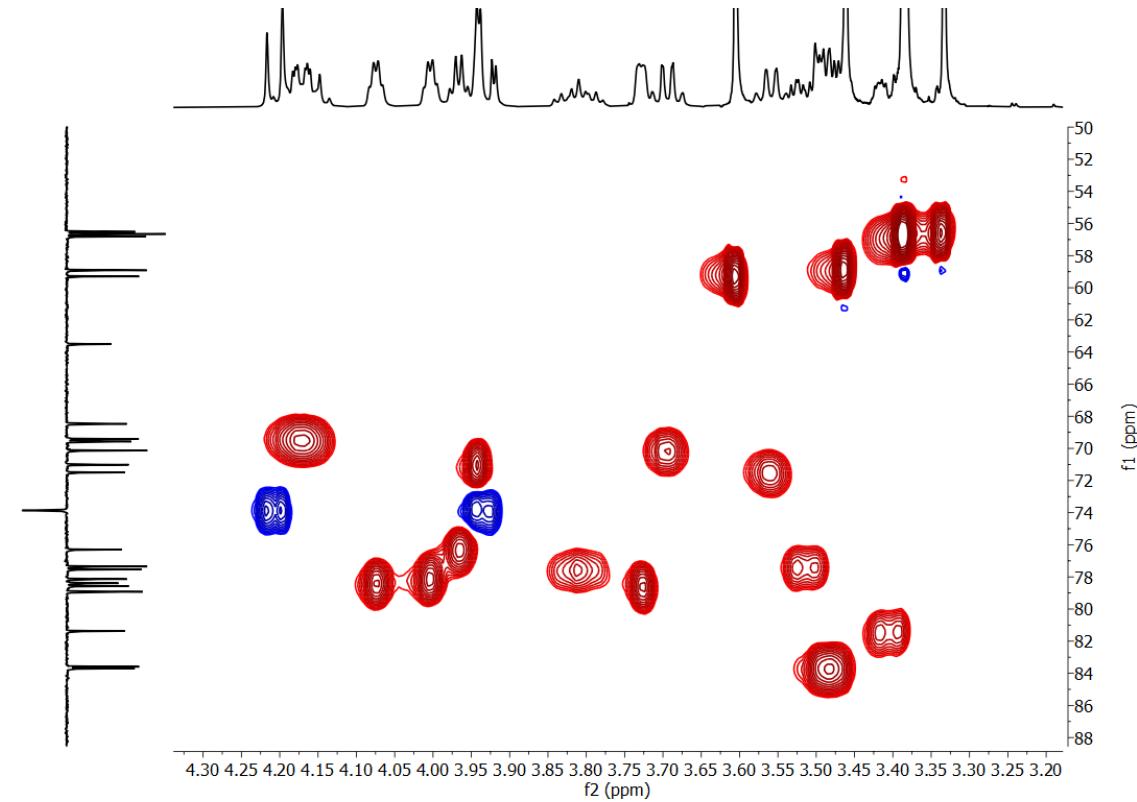
**Figure S11:** HSQC spectrum(500 and 125 MHz, pyridine-d<sub>5</sub>) of compound **1**.



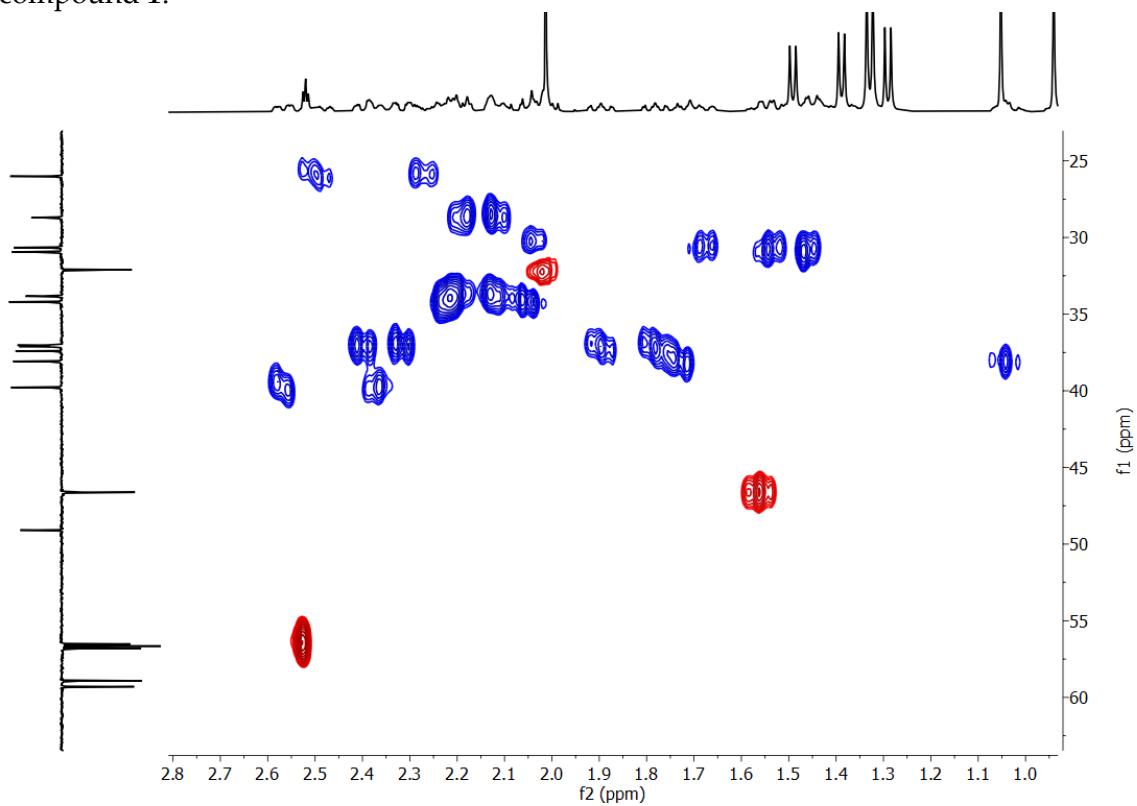
**Figure S12:** Expansion of HSQC spectrum (500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 1.



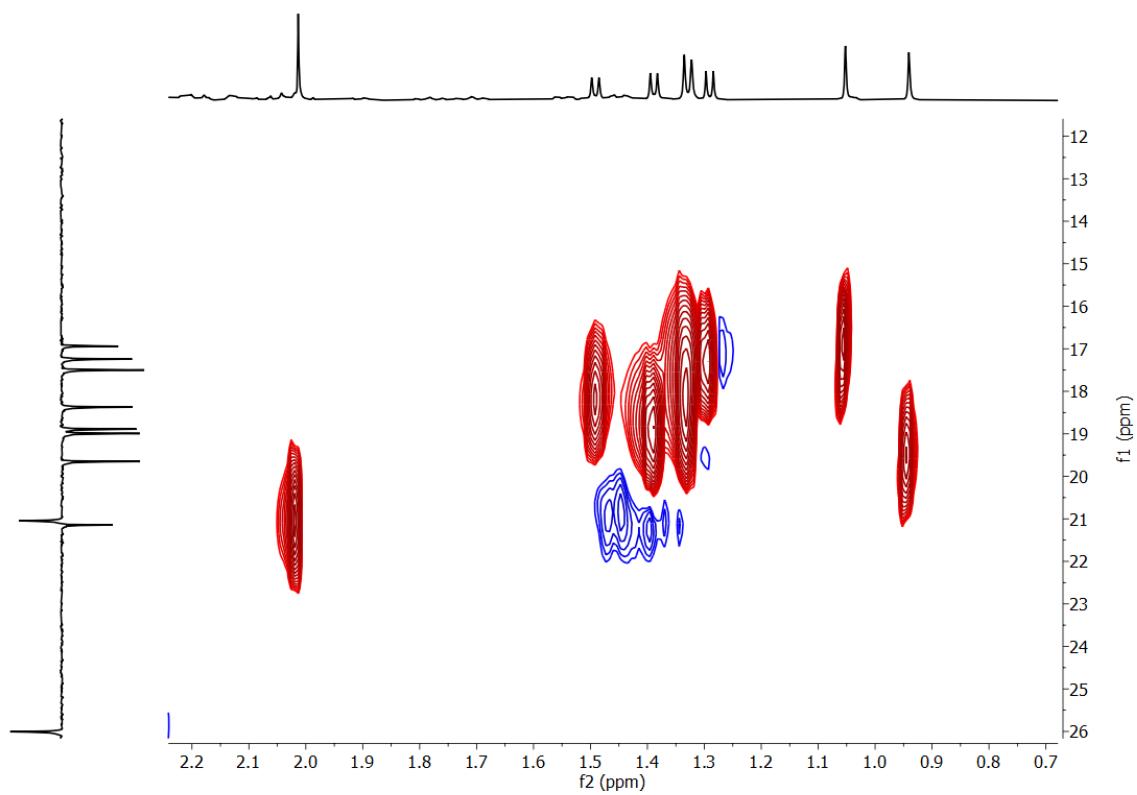
**Figure S13:** Expansion of HSQC spectrum (500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 1.



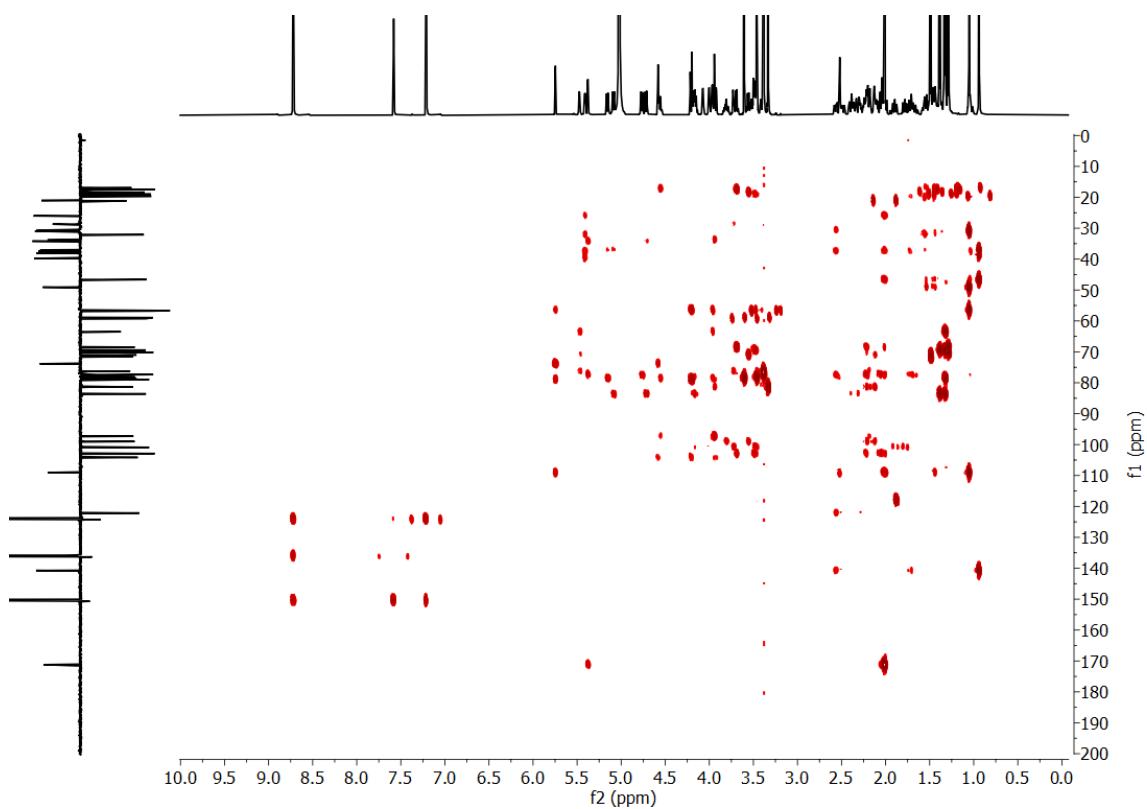
**Figure S14:** Expansion of HSQC spectrum(500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 1.



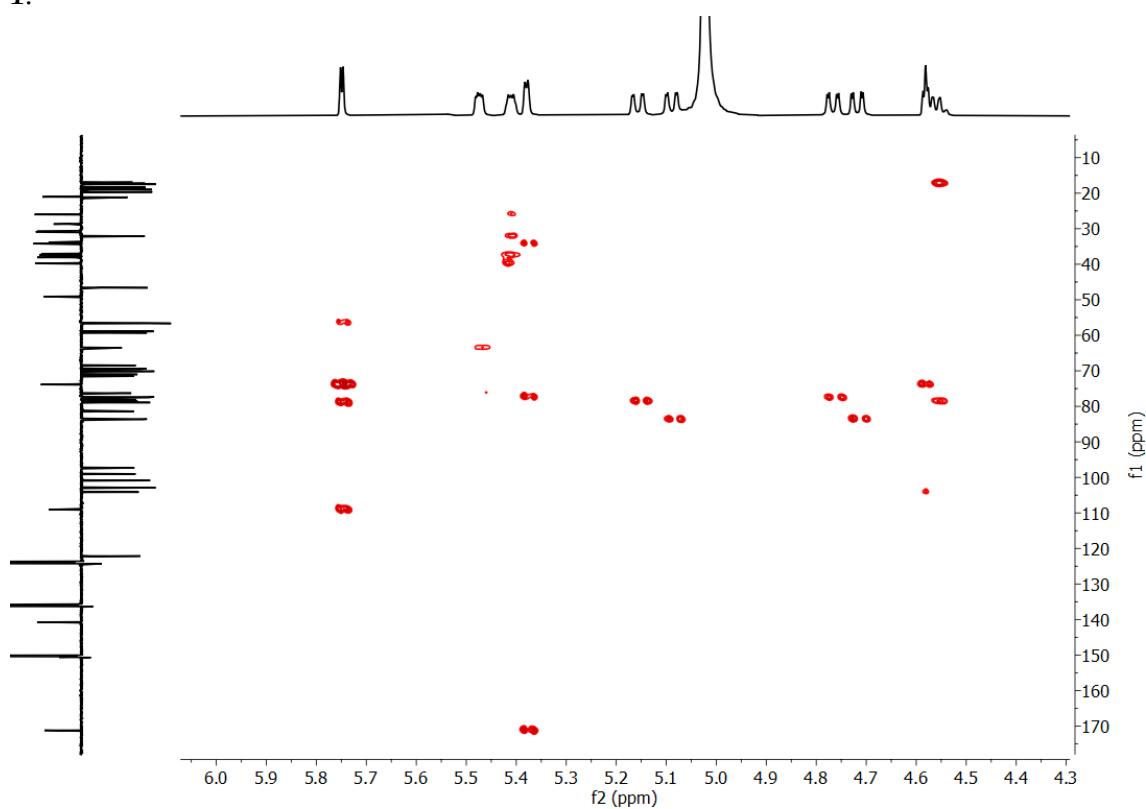
**Figure S15:** Expansion of HSQC spectrum(500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 1.



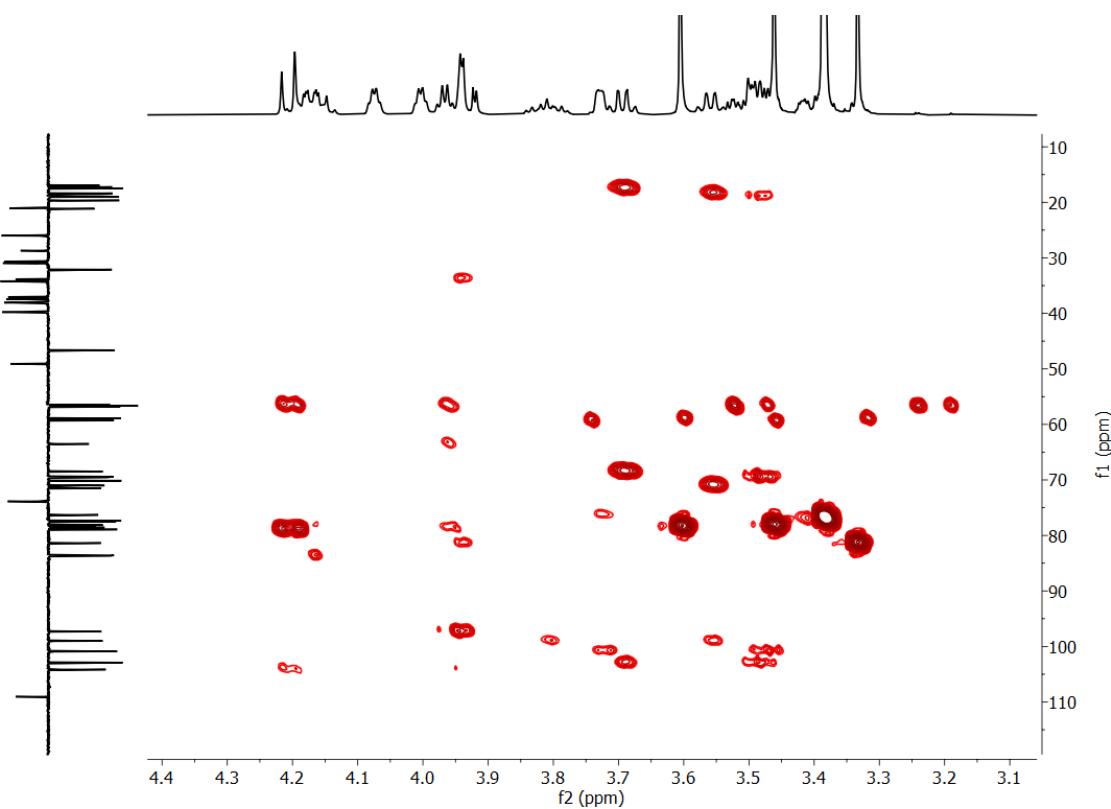
**Figure S16:** Expansion of HMBC spectrum(500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 1.



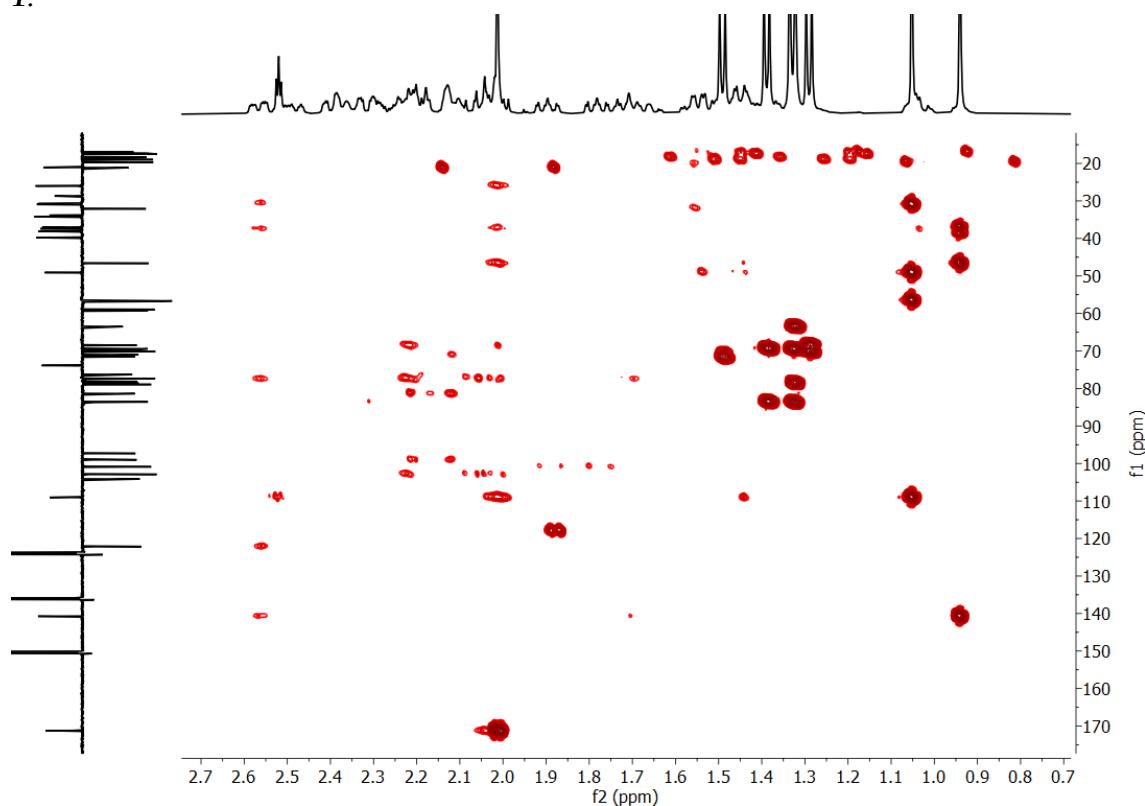
**Figure S17:** Expansion of HMBC spectrum(500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 1.



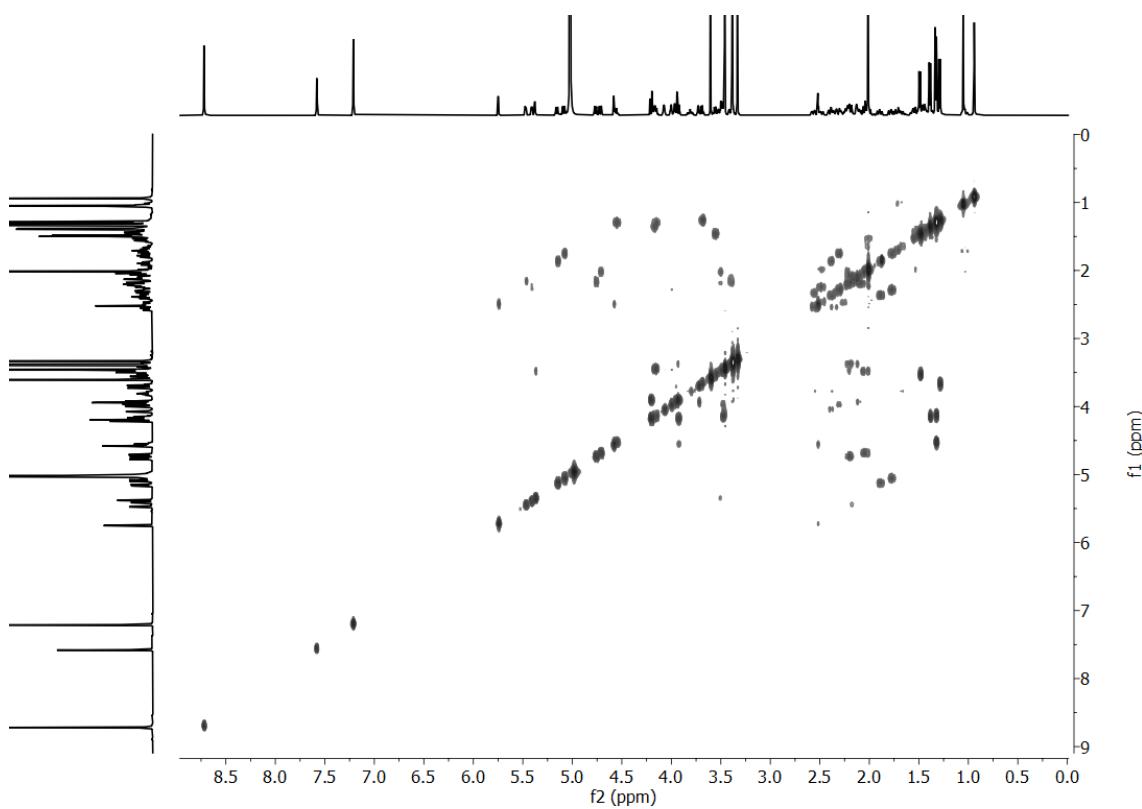
**Figure S18:** Expansion of HMBC spectrum(500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 1.



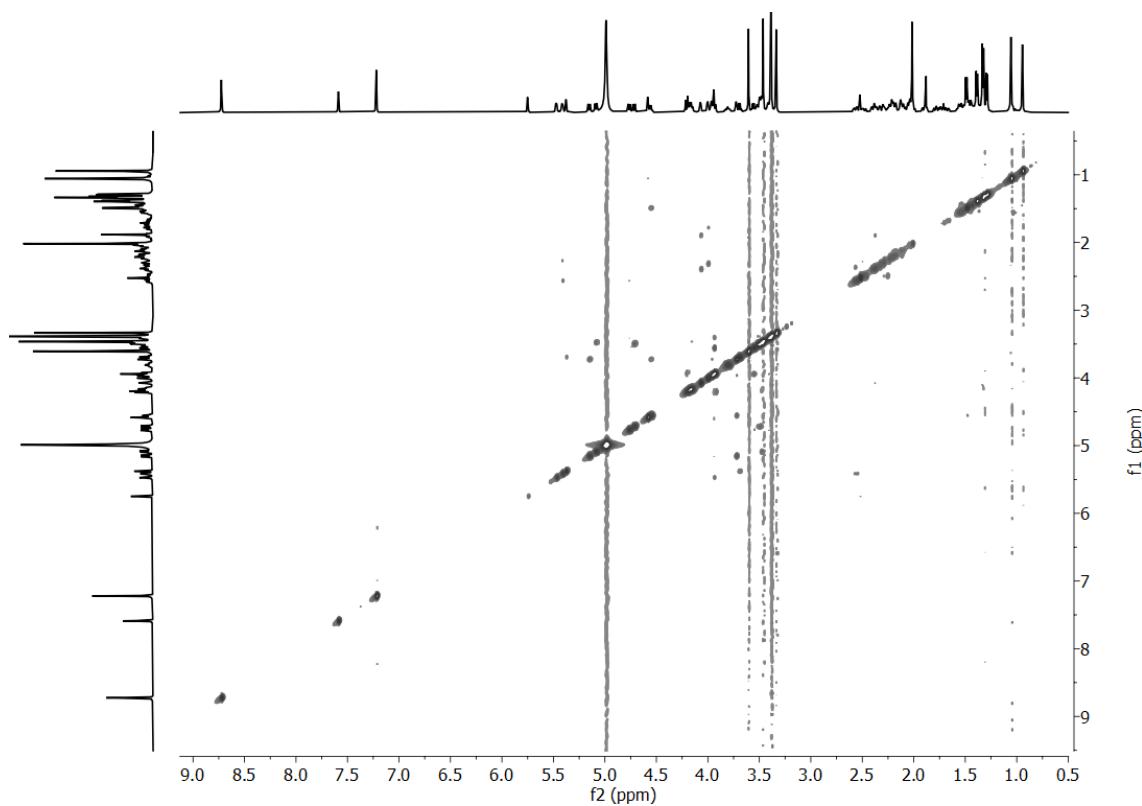
**Figure S19:** Expansion of HMBC spectrum(500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 1.



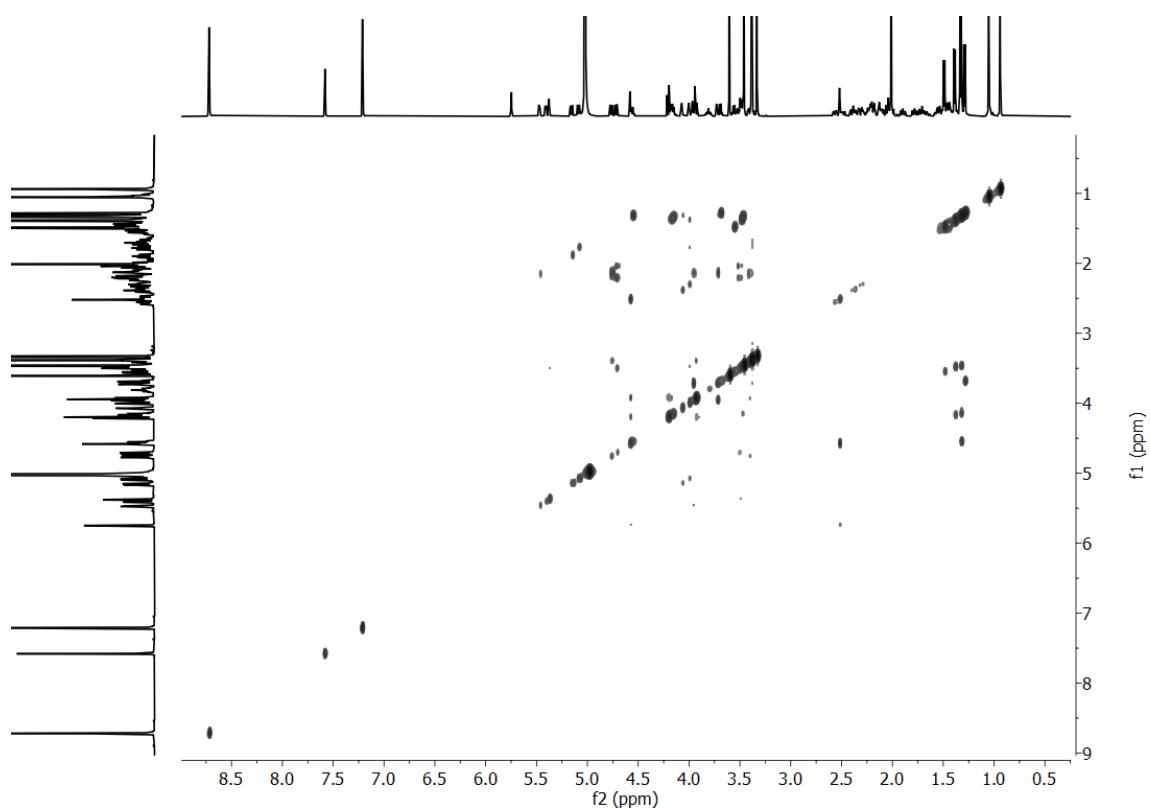
**Figure S20:** COSY spectrum (pyridine-d<sub>5</sub>, 500 MHz) of compound **1**.



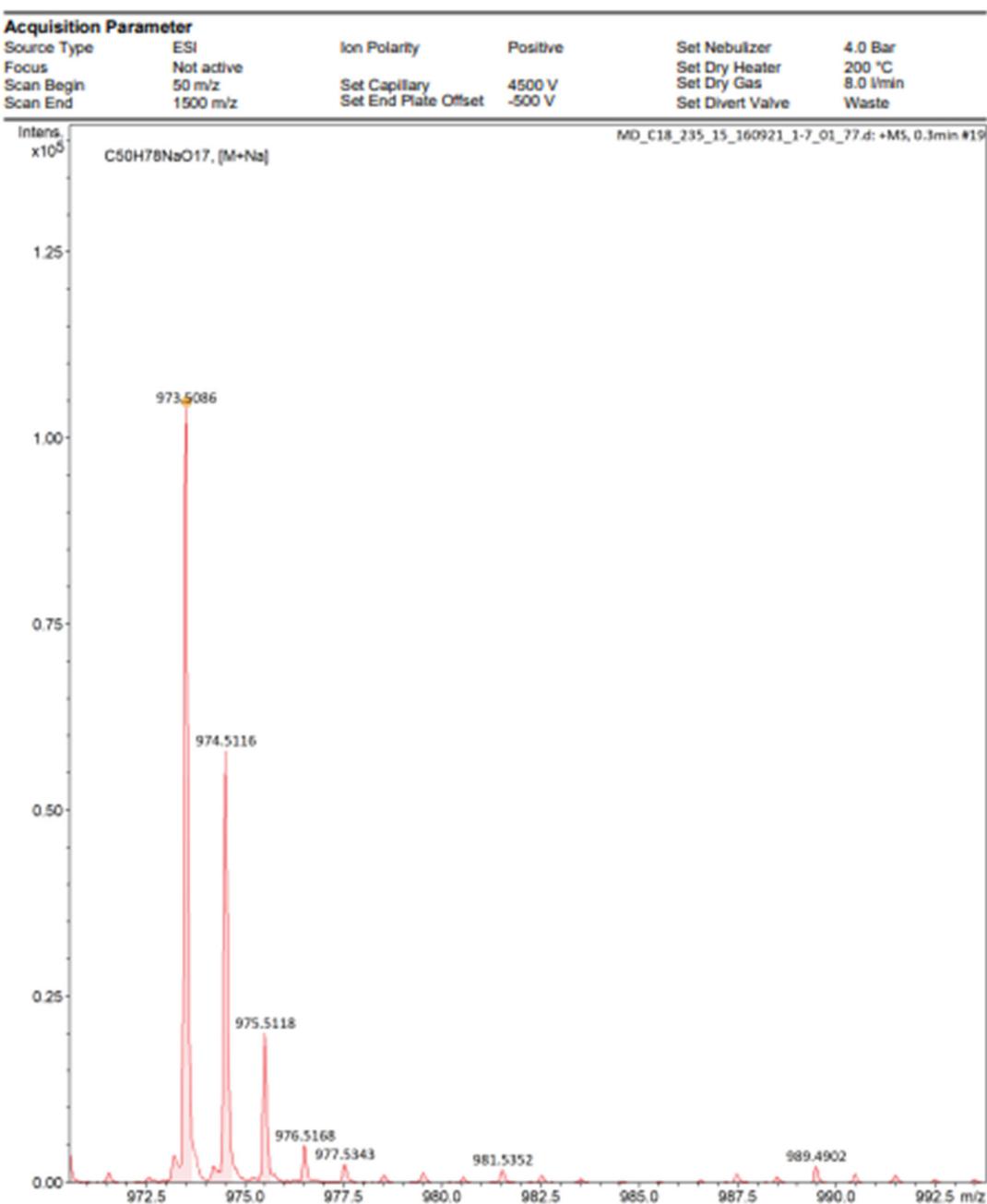
**Figure S21:** NOESY spectrum (pyridine-d<sub>5</sub>, 500 MHz) of compound **1**.



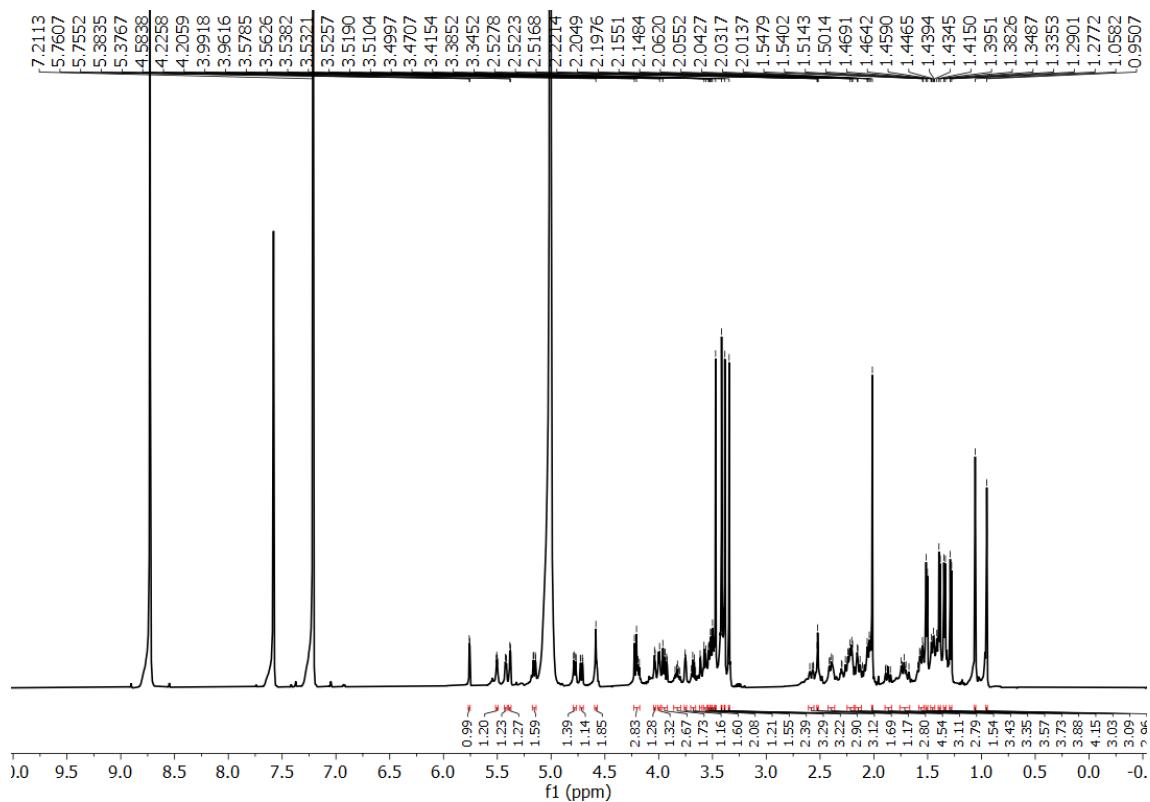
**Figure S22:** TOCSY spectrum (pyridine-d<sub>5</sub>, 500 MHz) of compound 1.



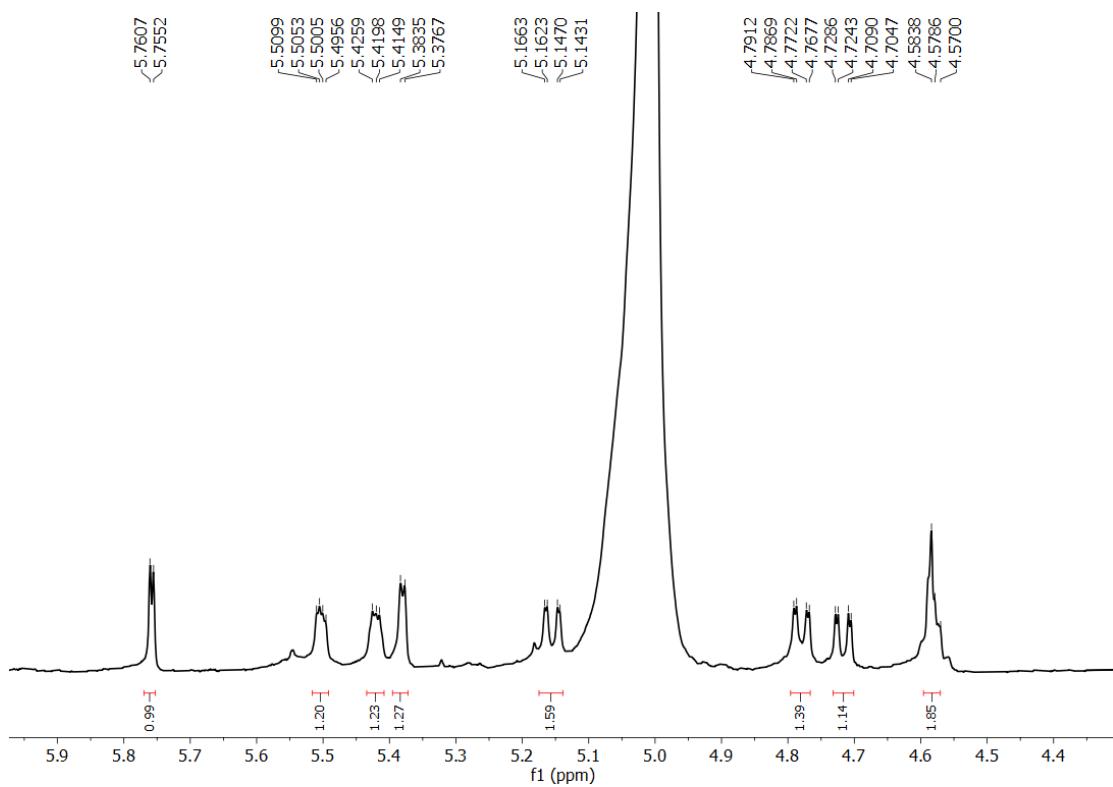
**Figure S23:** ESI-HRMS spectrum of compound 2



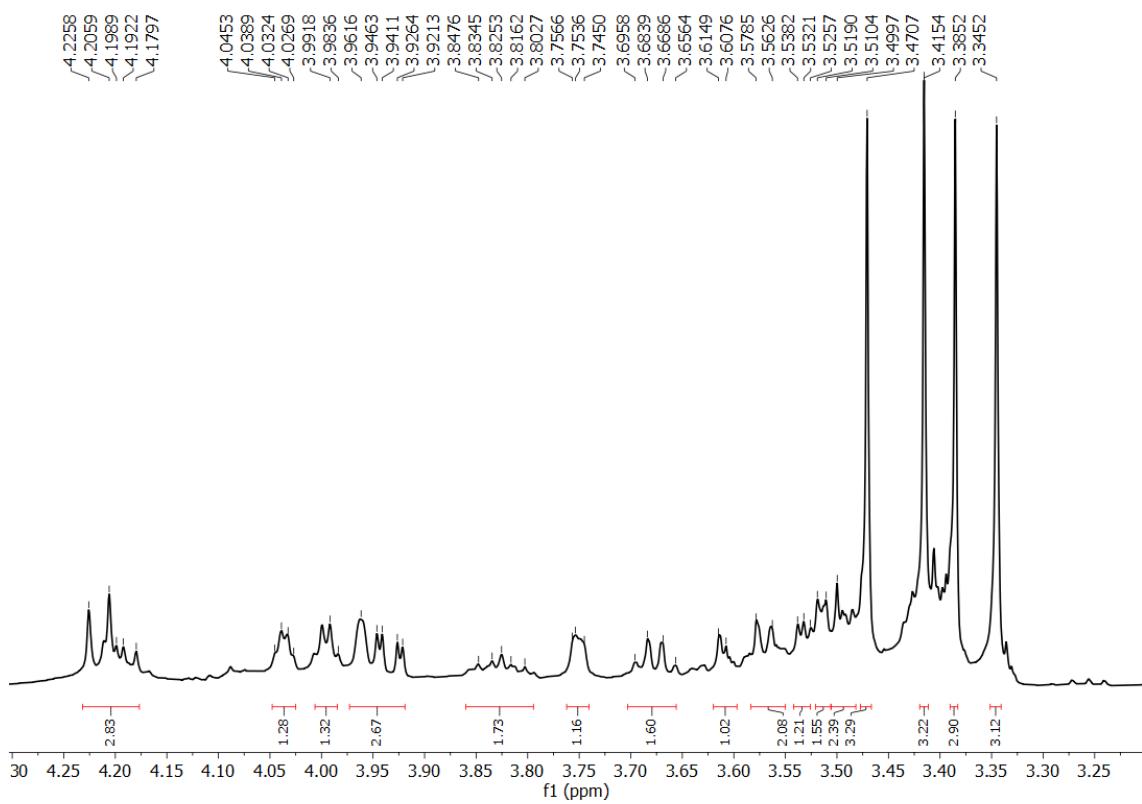
**Figure S24:**  $^1\text{H}$  NMR spectrum (pyridine-d<sub>5</sub>, 500 MHz) of compound 2.



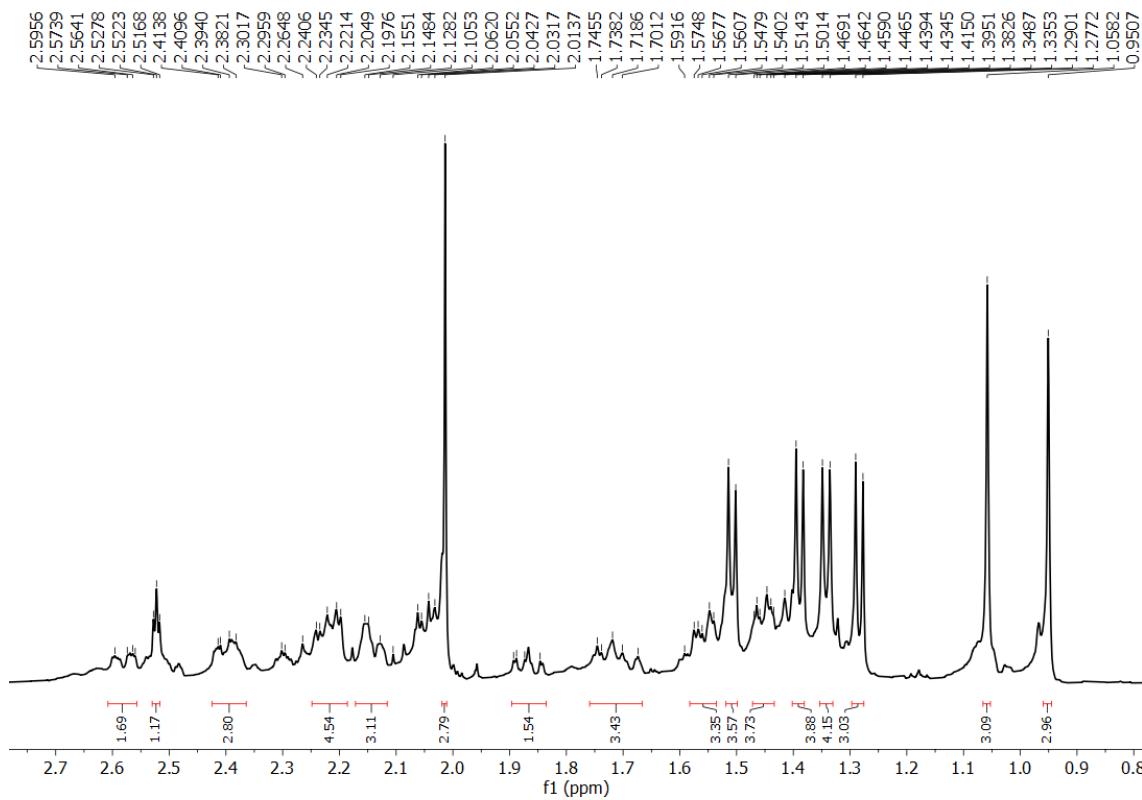
**Figure S25:** Expansion of  $^1\text{H}$  NMR spectrum (pyridine-d<sub>5</sub>, 500 MHz) of compound 2.



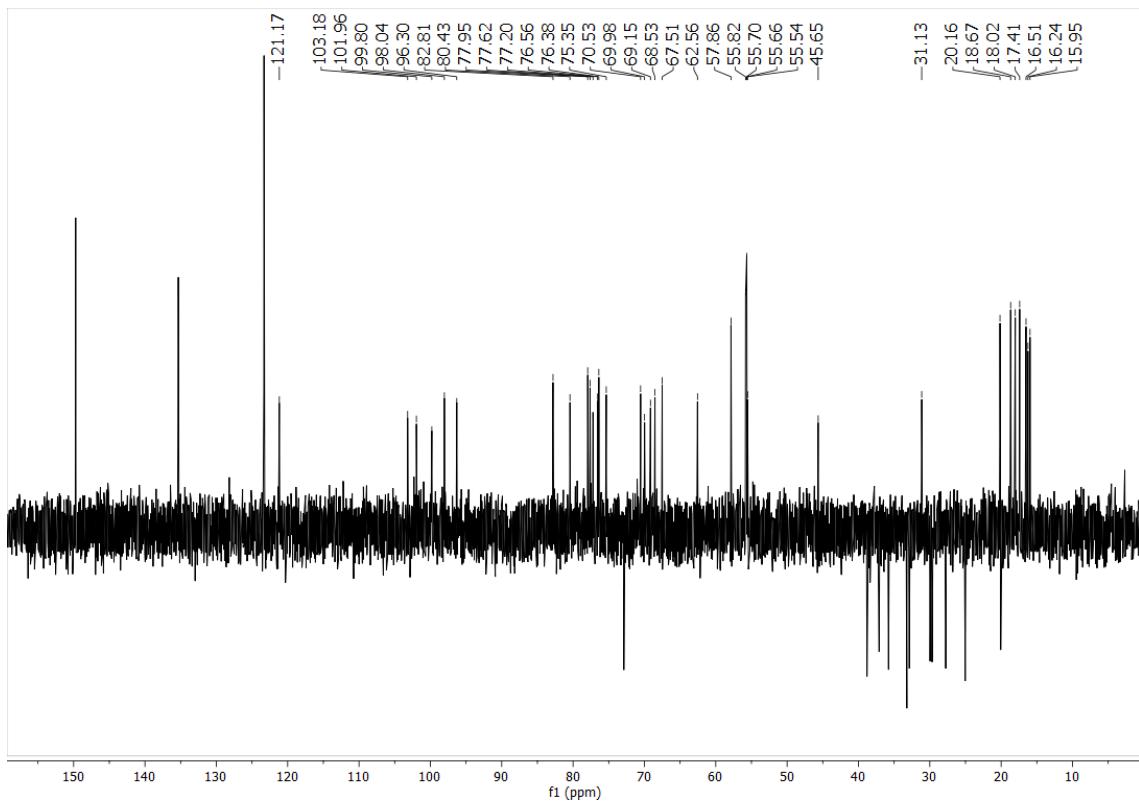
**Figure S26:** Expansion of  $^1\text{H}$  NMR spectrum (pyridine-d<sub>5</sub>, 500 MHz) of compound 2.



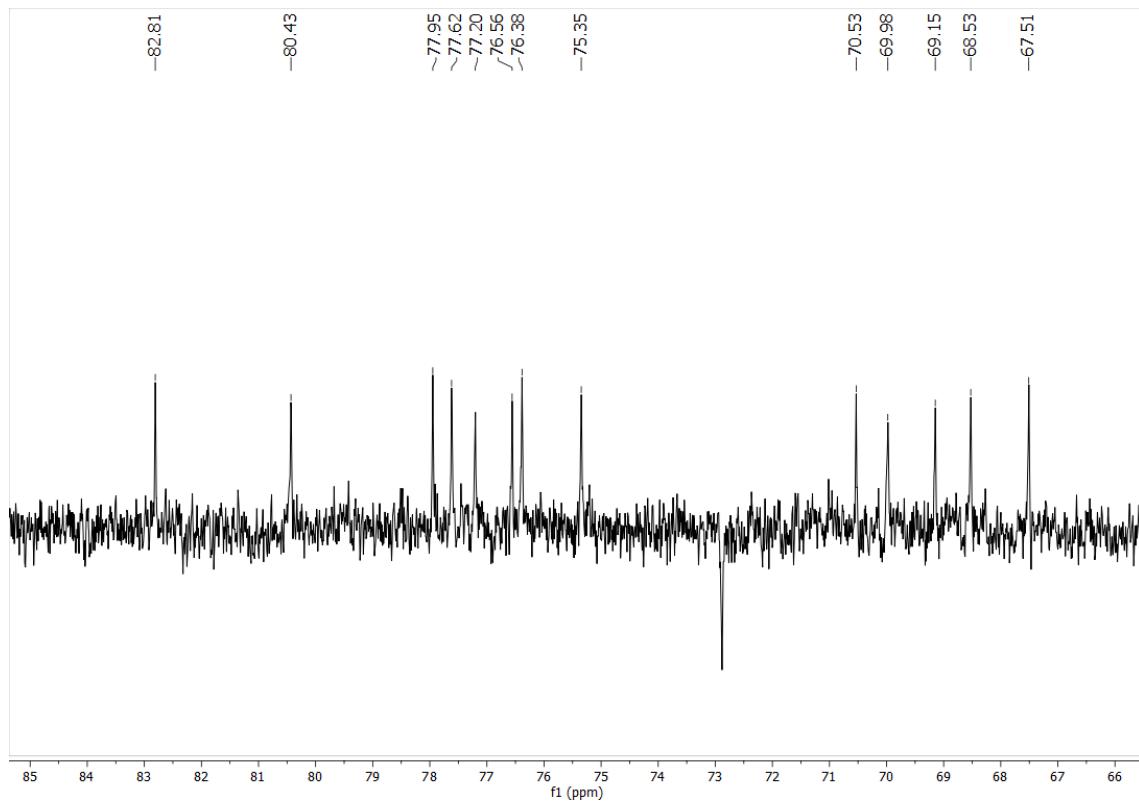
**Figure S27:** Expansion of  $^1\text{H}$  NMR spectrum (pyridine-d<sub>5</sub>, 500 MHz) of compound 2.



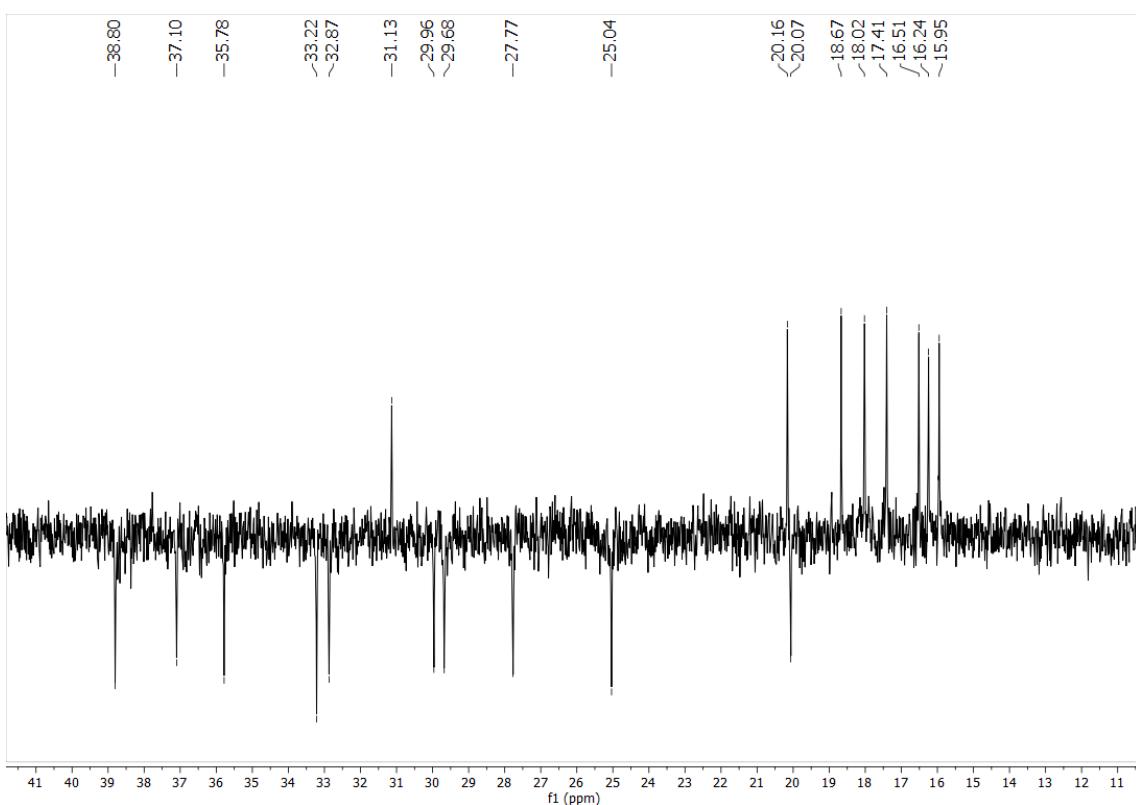
**Figure S28:** Dept 135 NMR spectrum (pyridine-d<sub>5</sub>, 500 MHz) of compound 2.



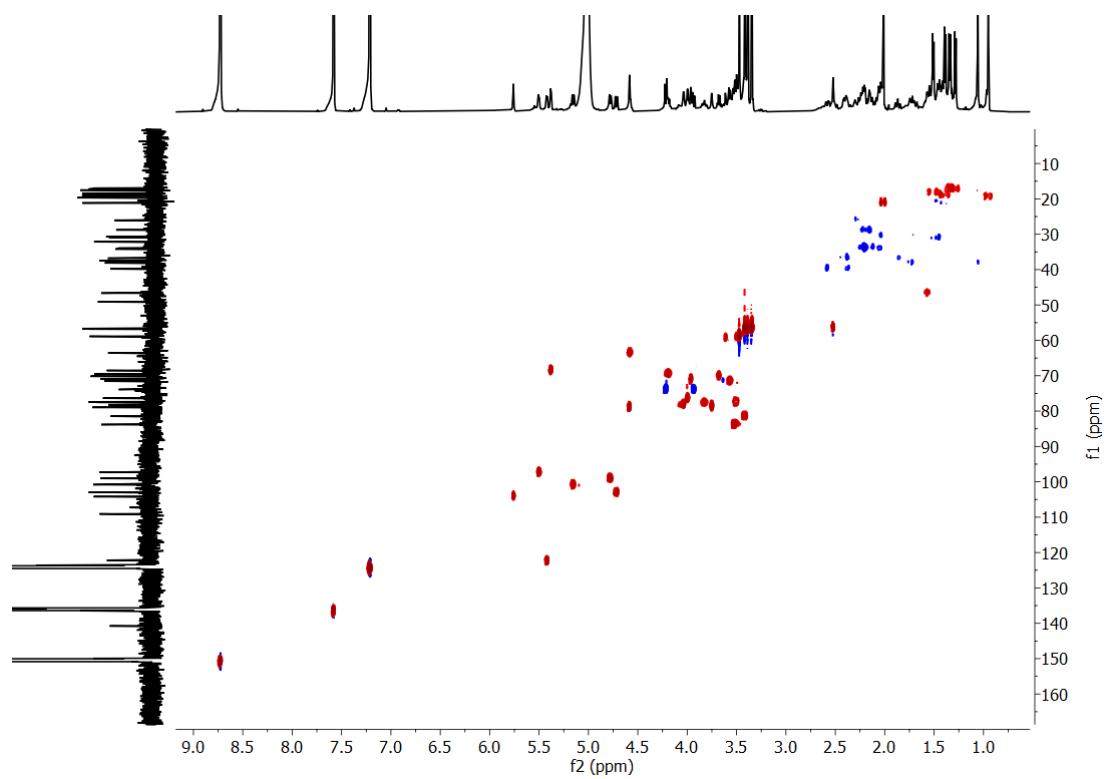
**Figure S29:** Expansion of Dept 135 NMR spectrum (pyridine-d<sub>5</sub>, 500 MHz) of compound 2.



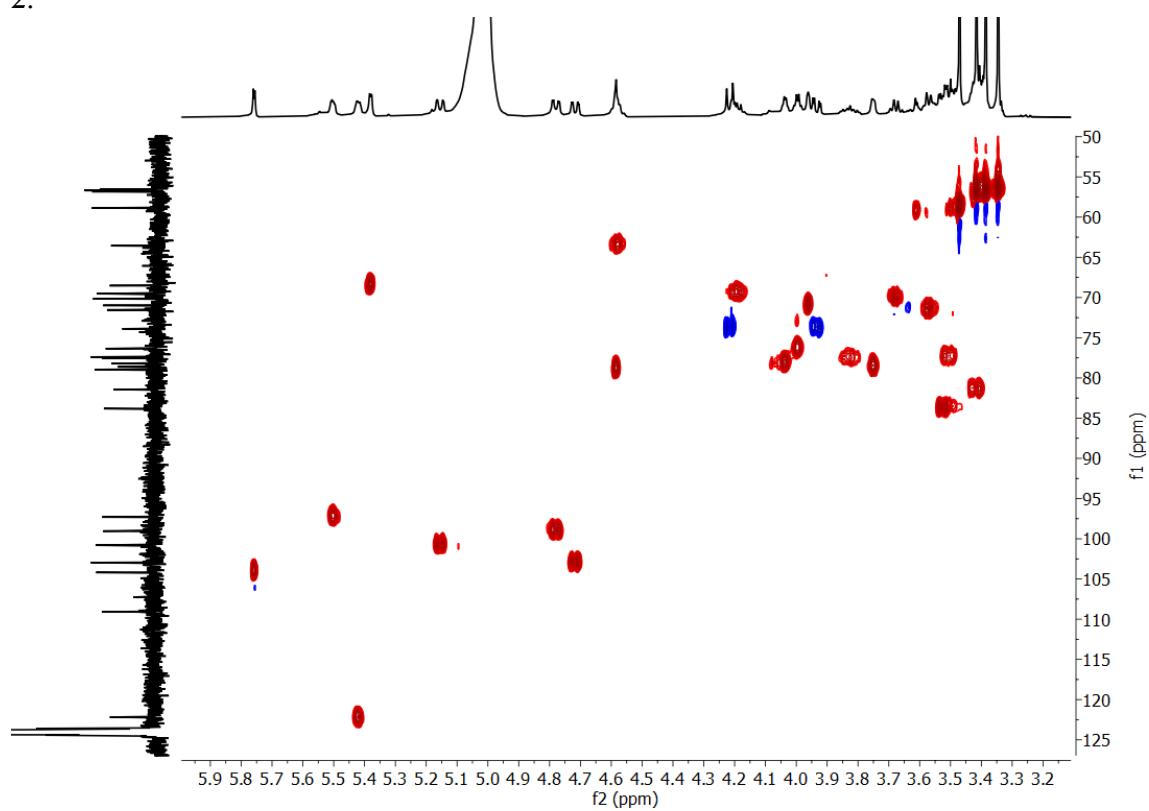
**Figure S30:** Expansion of Dept 135 NMR spectrum (pyridine-d<sub>5</sub>, 500 MHz) of compound 2.



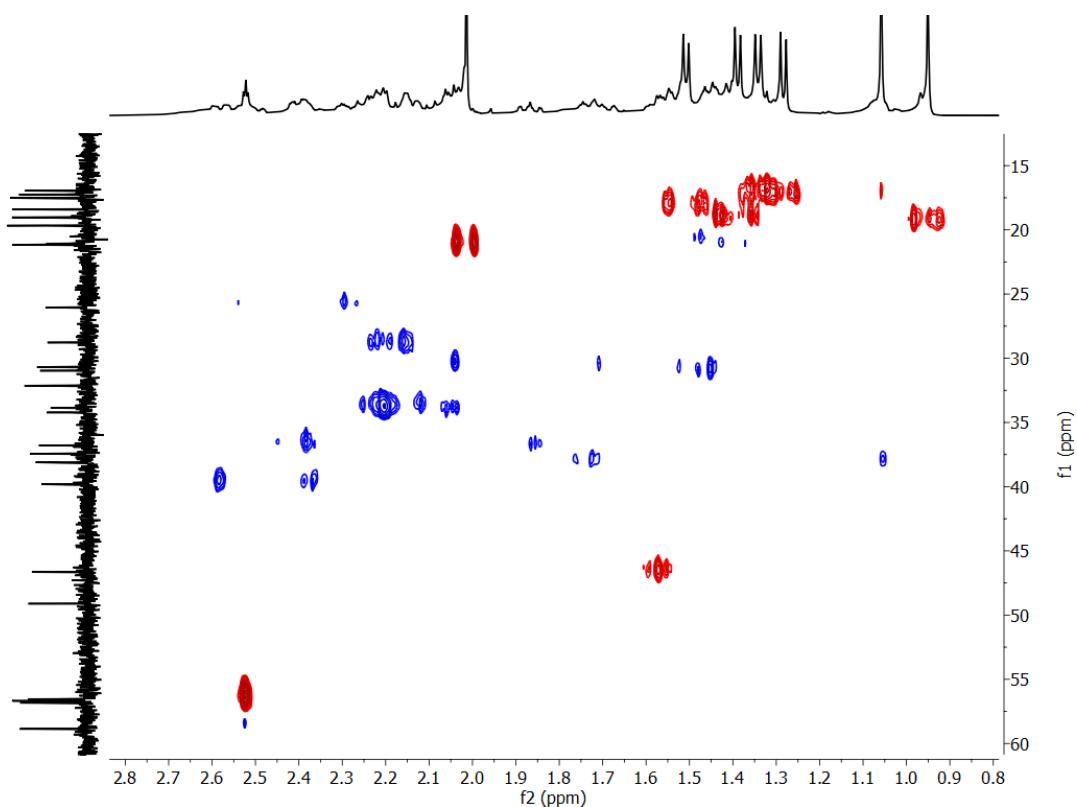
**Figure S31:** HSQC spectrum(500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 2.



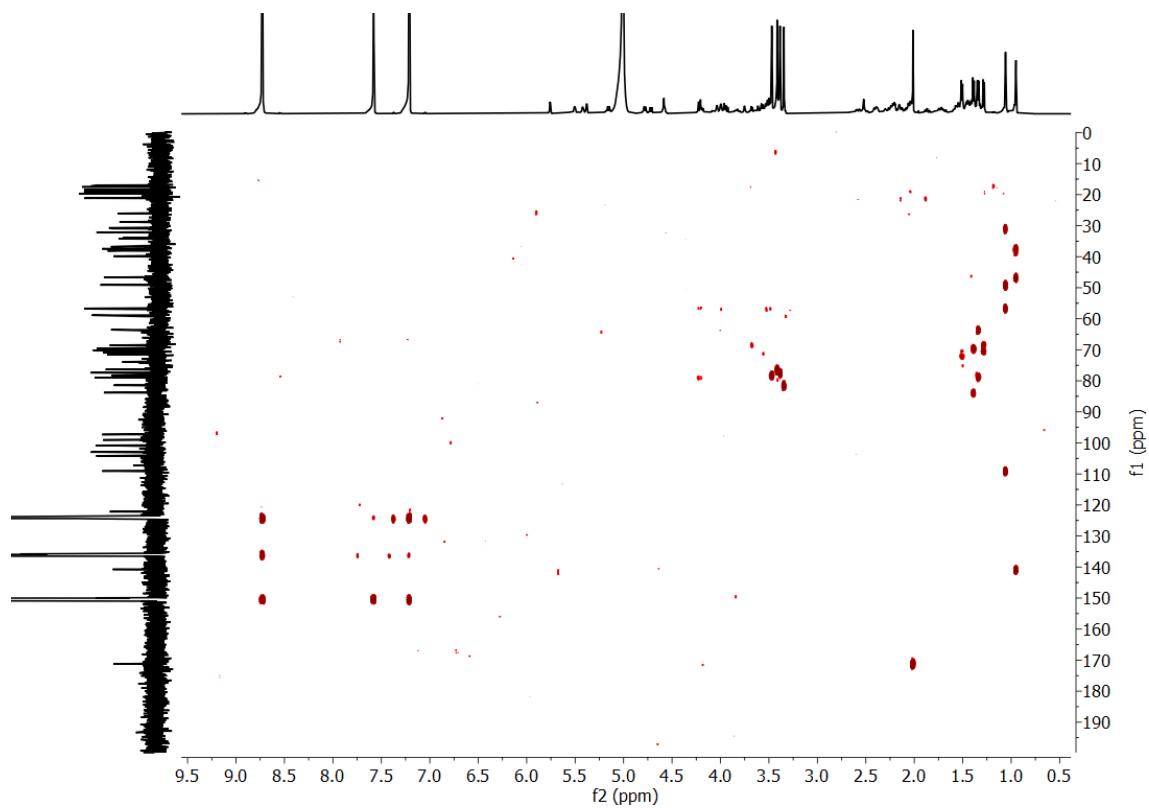
**Figure S32:** Expansion of HSQC spectrum(500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 2.



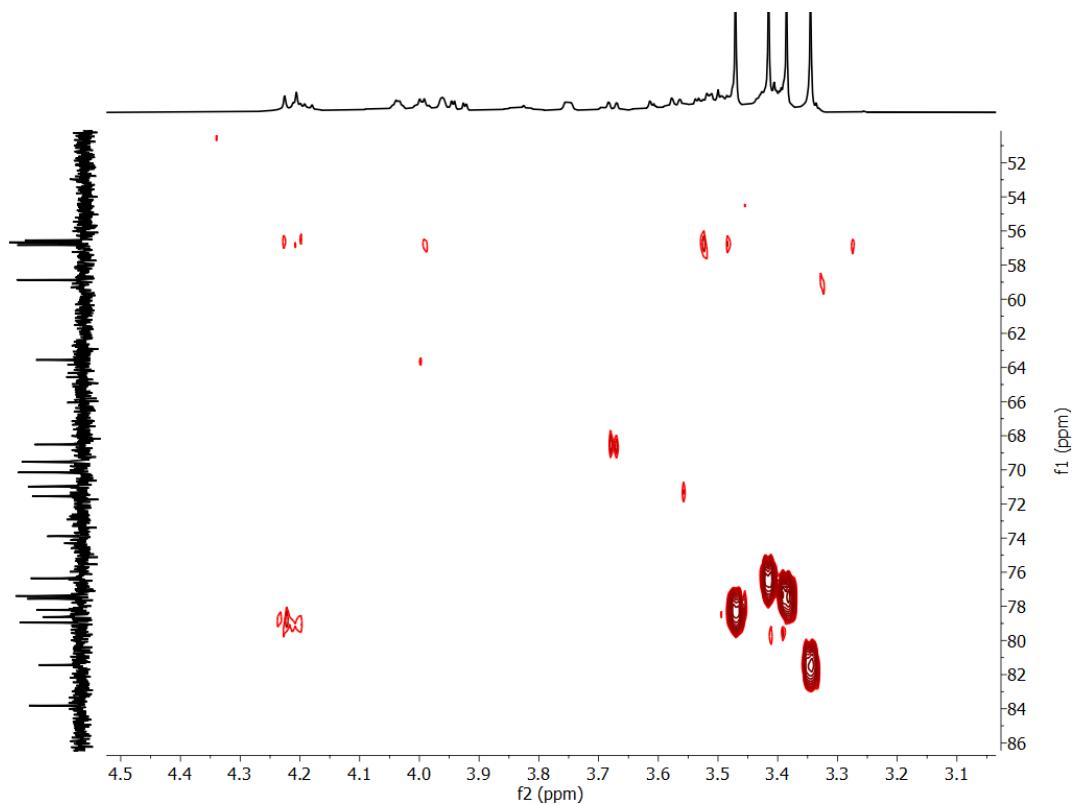
**Figure S33:** Expansion of HSQC spectrum(500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 2.



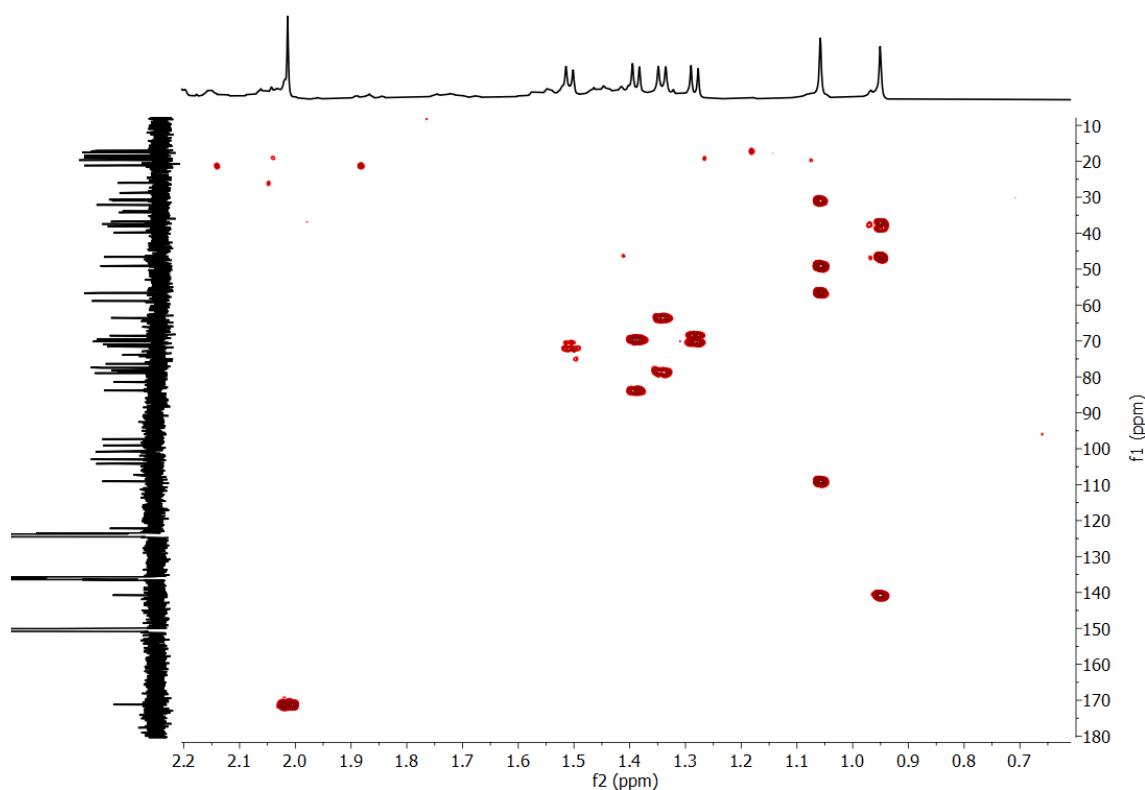
**Figure S34:** HMBC spectrum(500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 2.



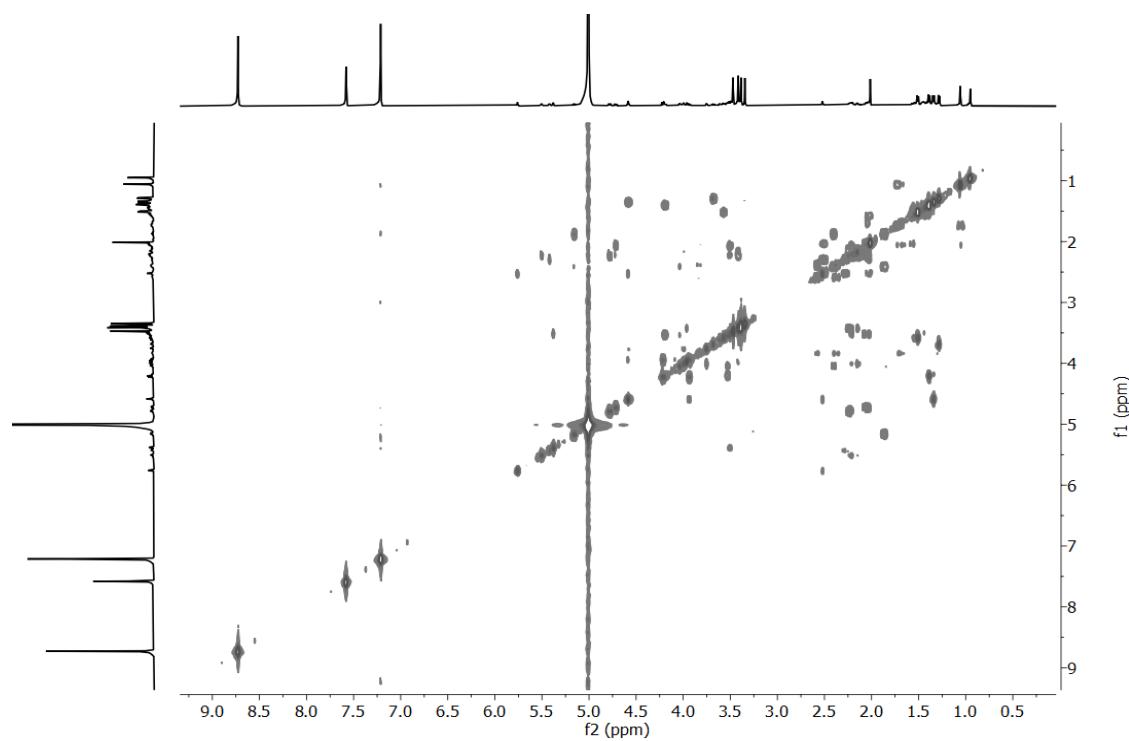
**Figure S35:** Expansion of HMBC spectrum(500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 2.



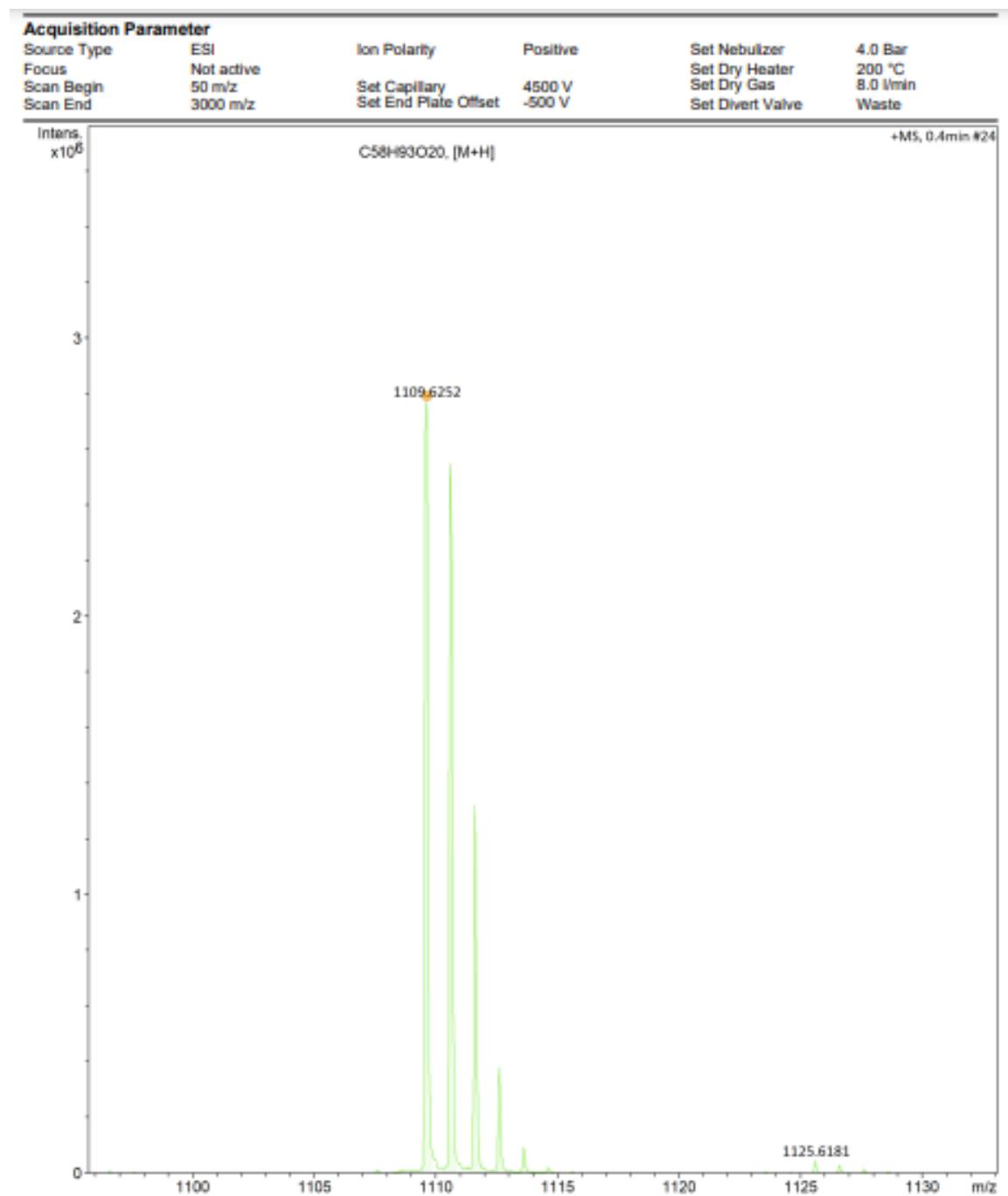
**Figure S36:** Expansion of HMBC spectrum (500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 2.



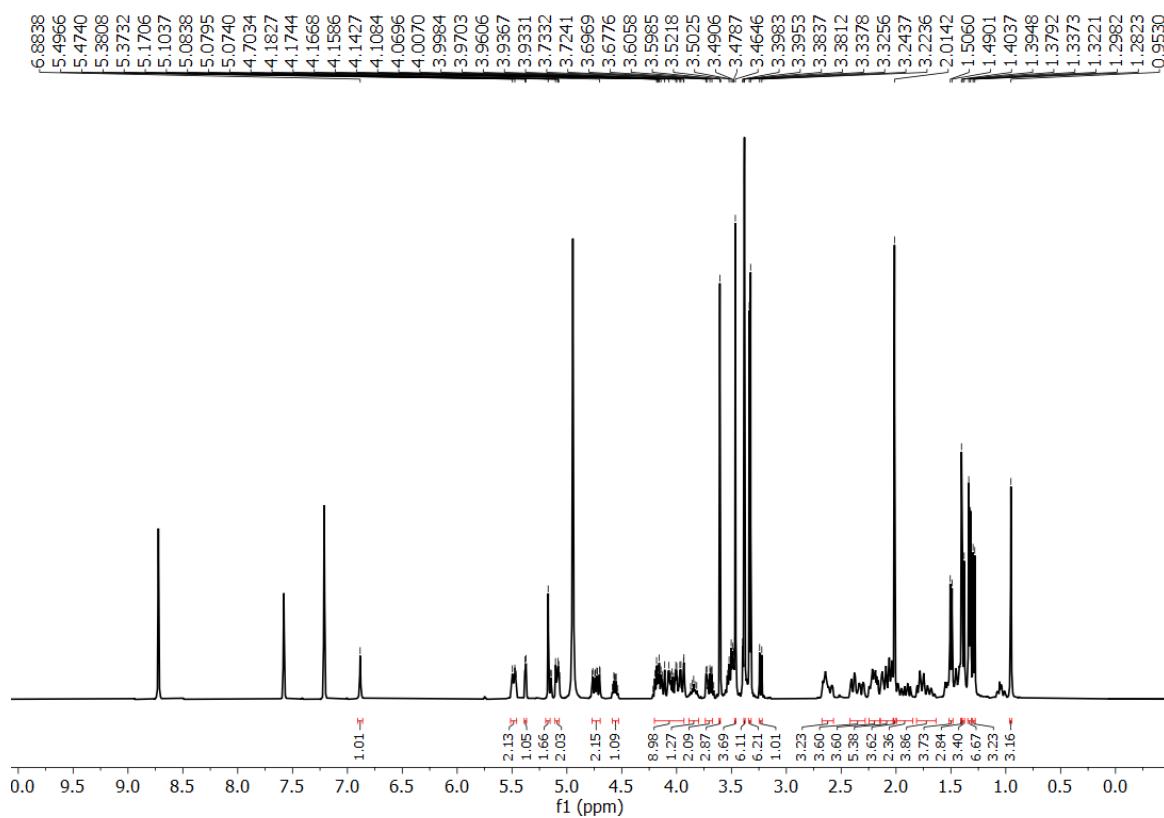
**Figure S37:** COSY spectrum (500 and 125 MHz, pyridine-d<sub>5</sub>) of compound 2.



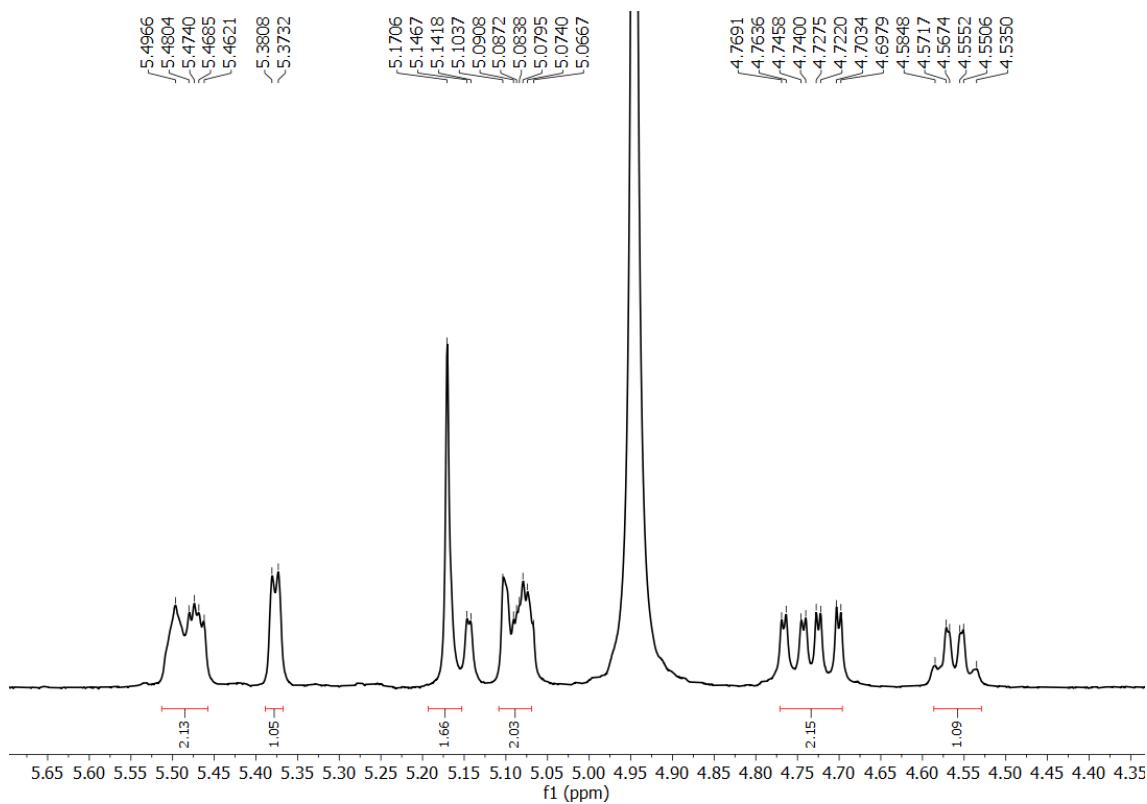
**Figure S38:** ESI-HRMS spectrum of compound 3



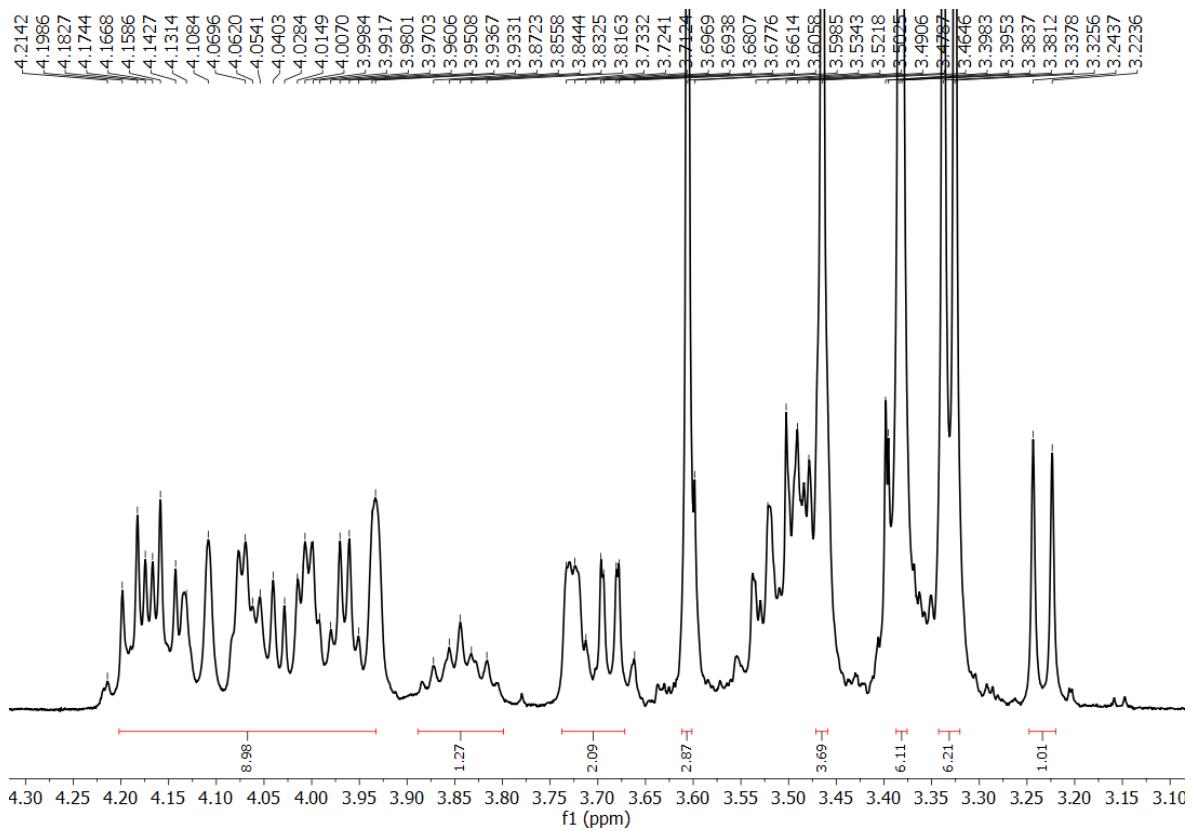
**Figure S39:**  $^1\text{H}$  NMR spectrum (400 MHz, pyridine-d5) of compound 3.



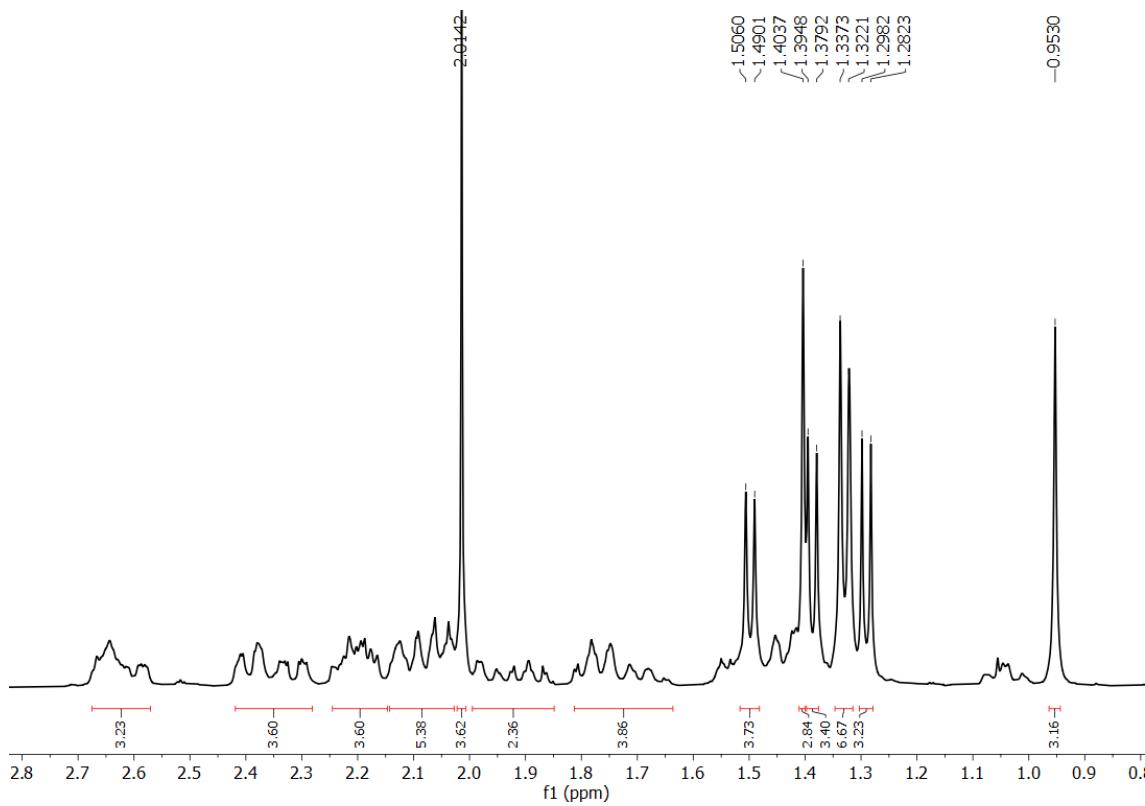
**Figure S40:** Expansion of  $^1\text{H}$  NMR spectrum (400 MHz, pyridine-d5) of compound 3.



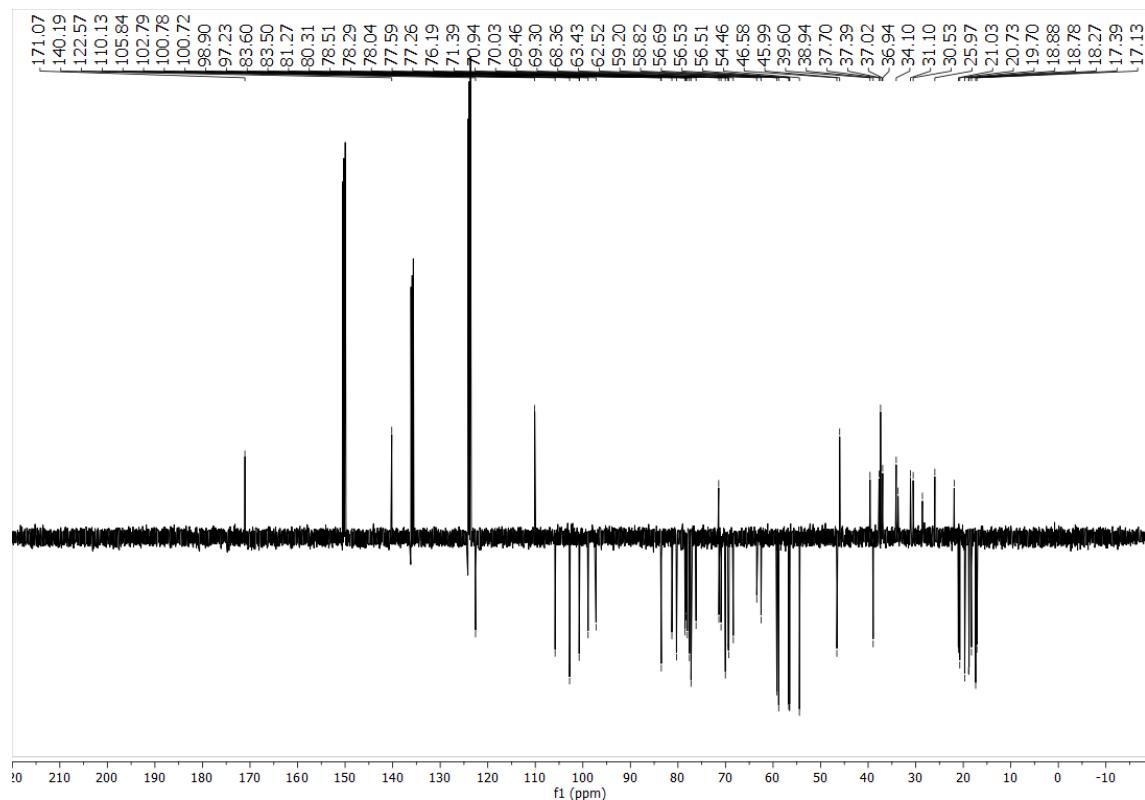
**Figure S41:** Expansion of  $^1\text{H}$  NMR spectrum (400 MHz, pyridine-d5) of compound 3.



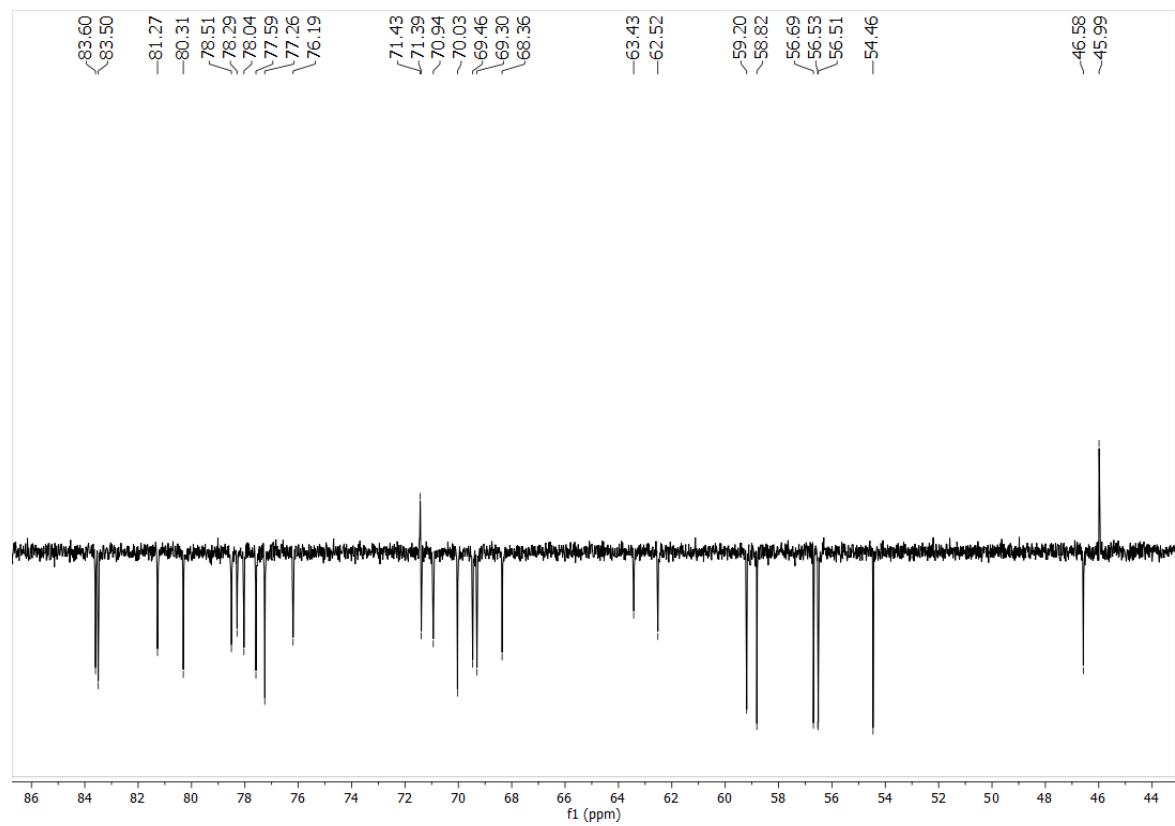
**Figure S42:** Expansion of  $^1\text{H}$  NMR spectrum (400 MHz, pyridine-d5) of compound 3.



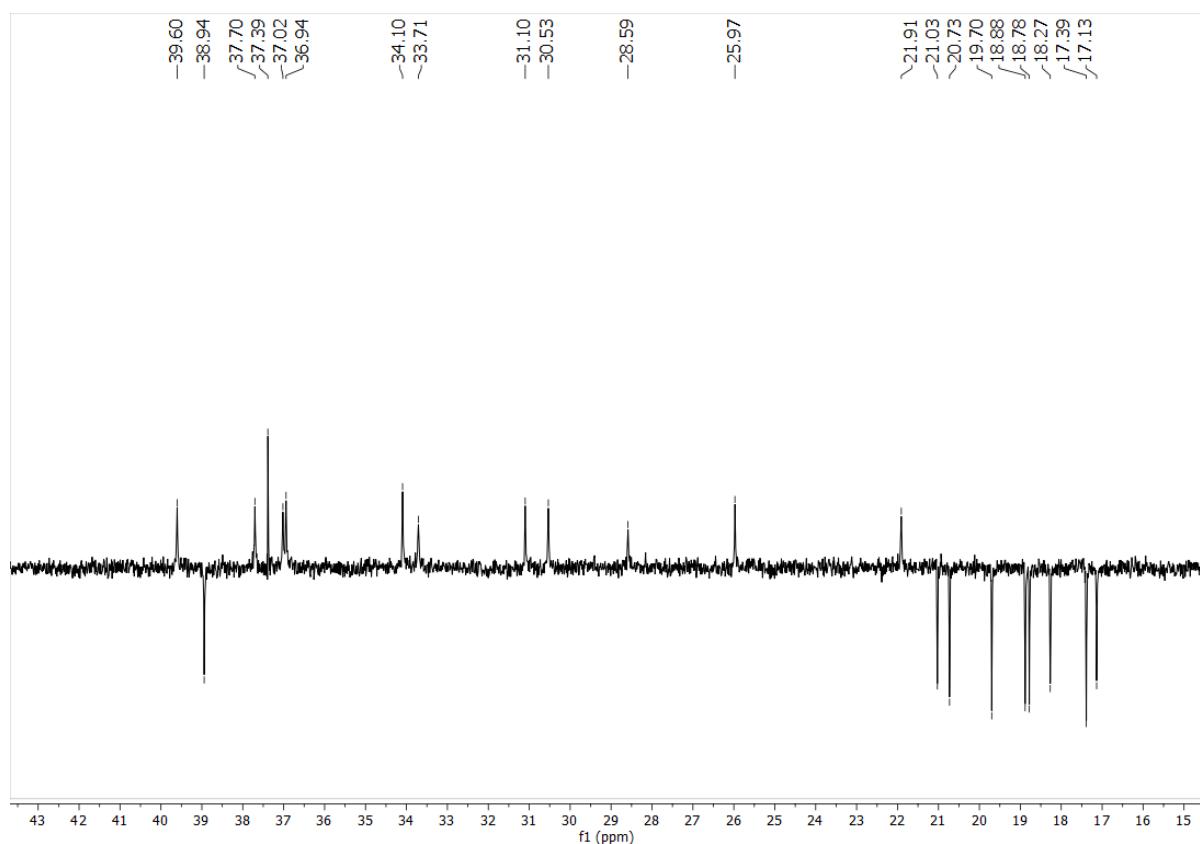
**Figure S43:** APT NMR spectrum (400 MHz, pyridine-d<sub>5</sub>) of compound 3.



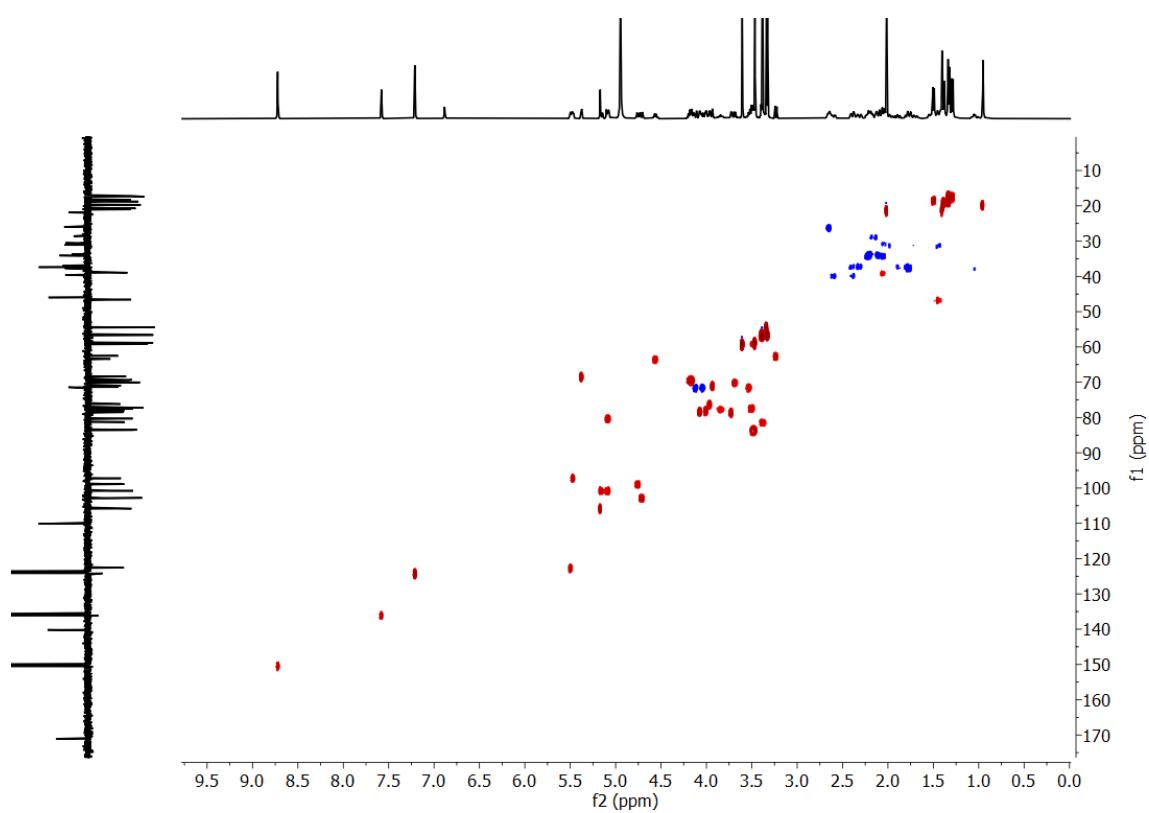
**Figure S44:** Expansion of APT NMR spectrum (400 MHz, pyridine-d<sub>5</sub>) of compound 3.



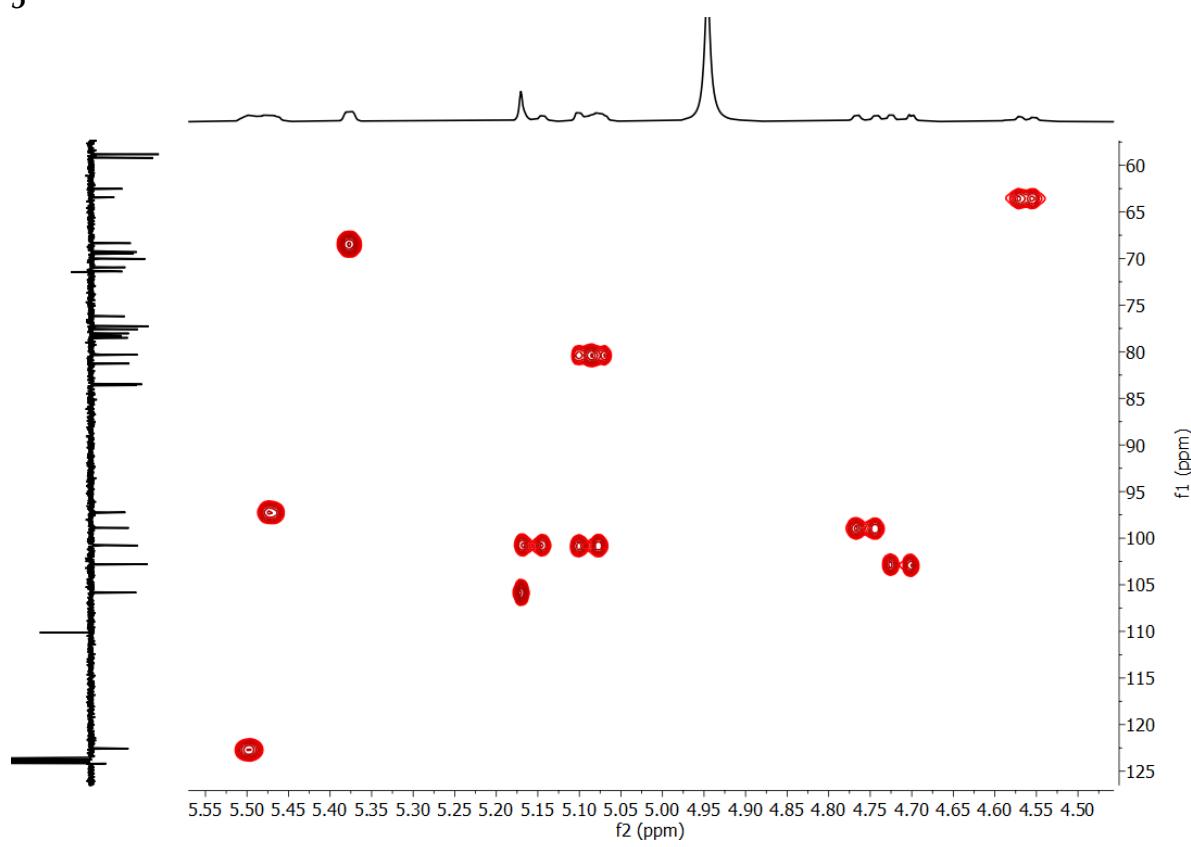
**Figure S45:** Expansion of APT NMR spectrum (400 MHz, pyridine-d<sub>5</sub>) of compound 3.



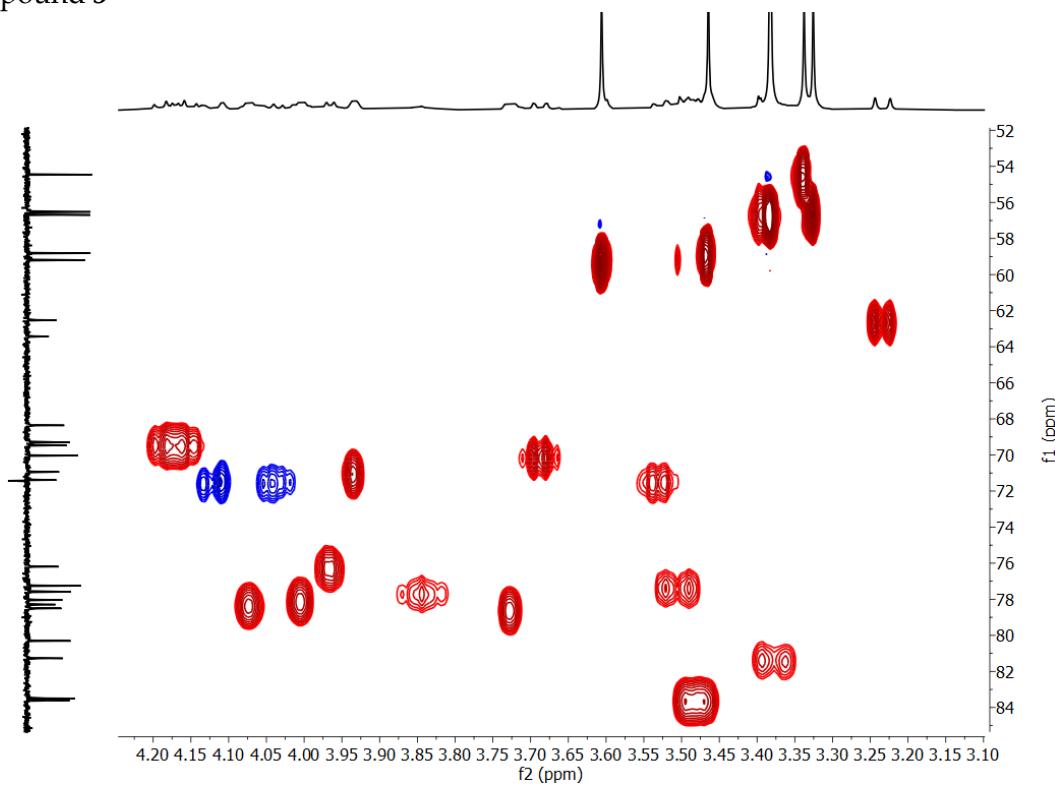
**Figure S46:** HSQC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 3



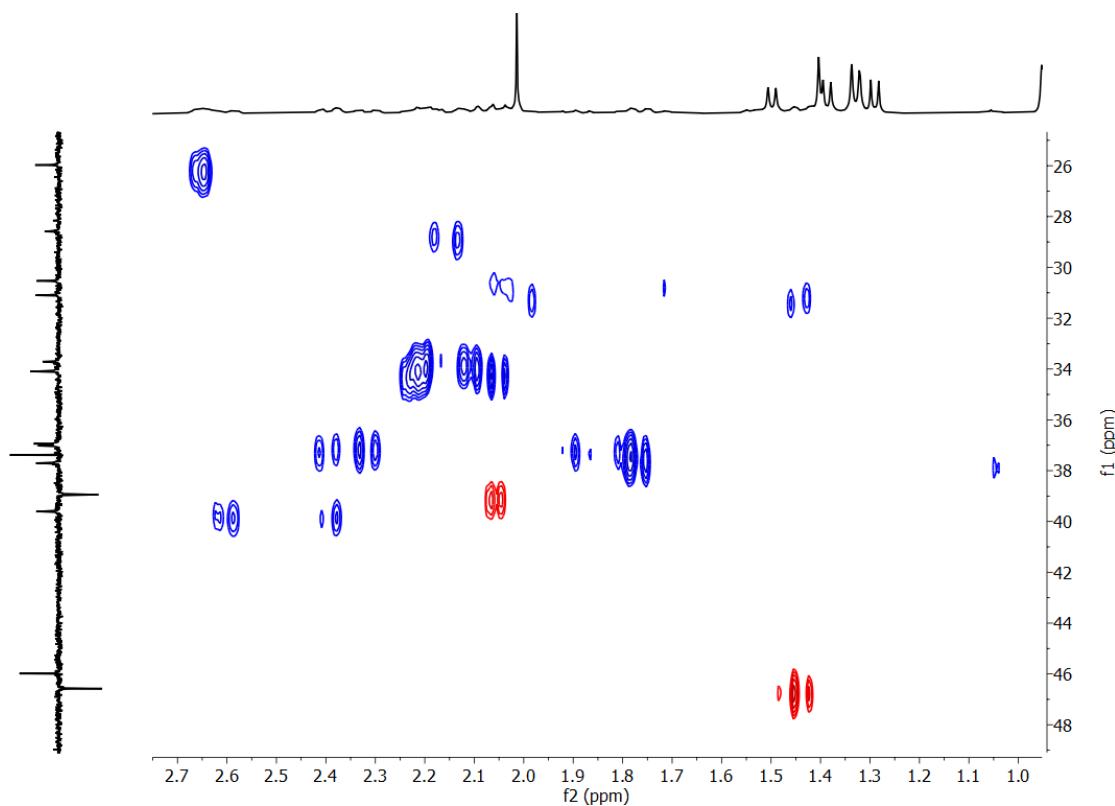
**Figure S47:** Expansion of HSQC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 3



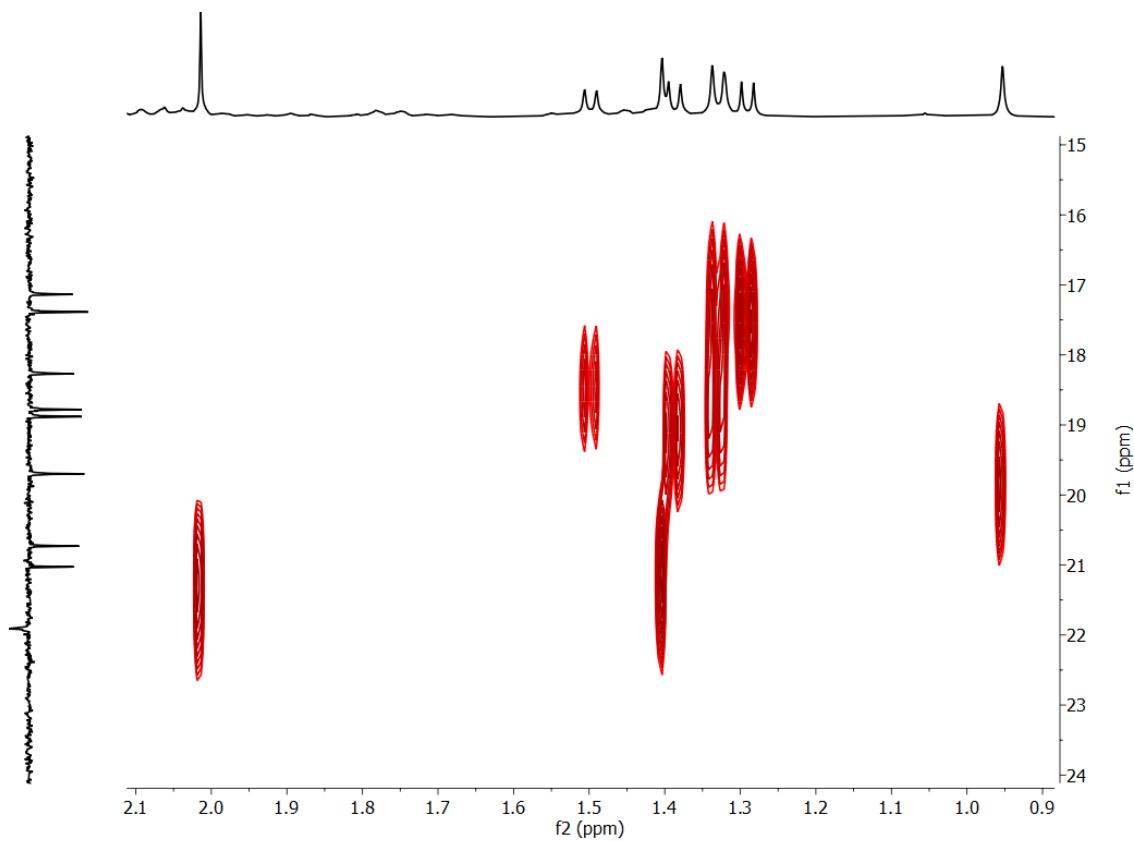
**Figure S48:** Expansion of HSQC spectra (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 3



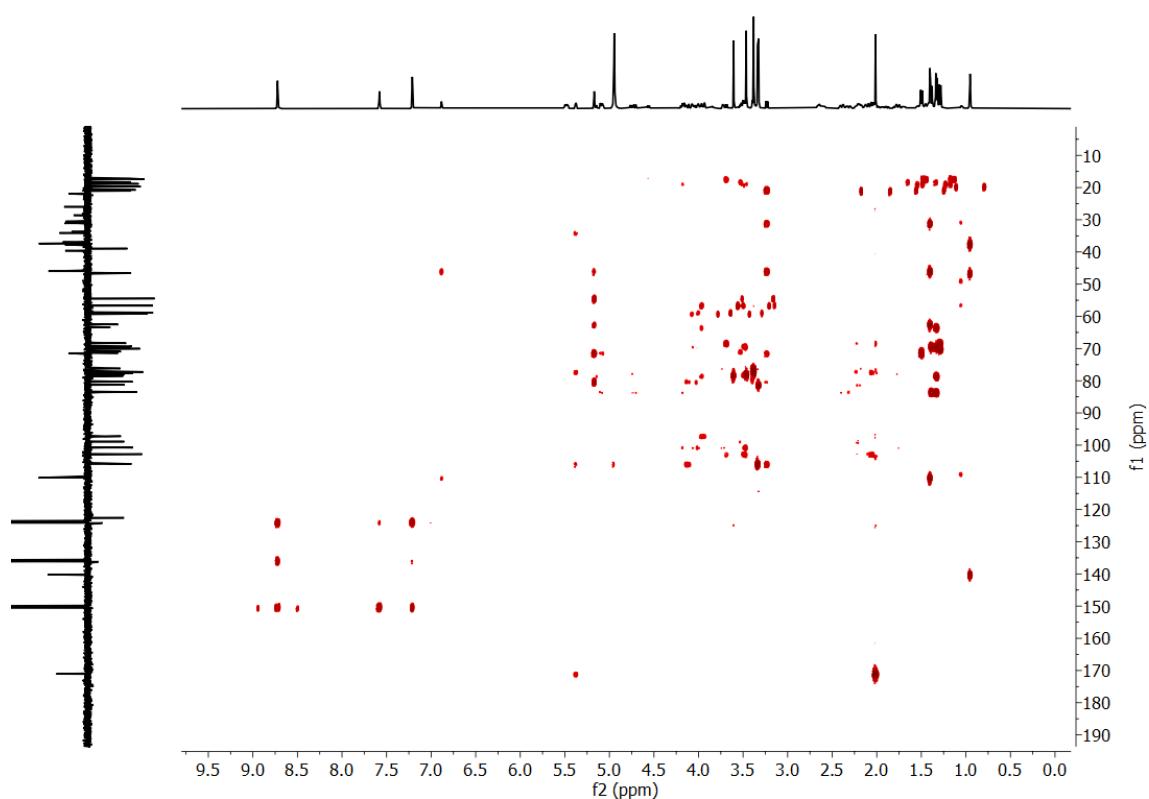
**Figure S49:** Expansion of HSQC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 3



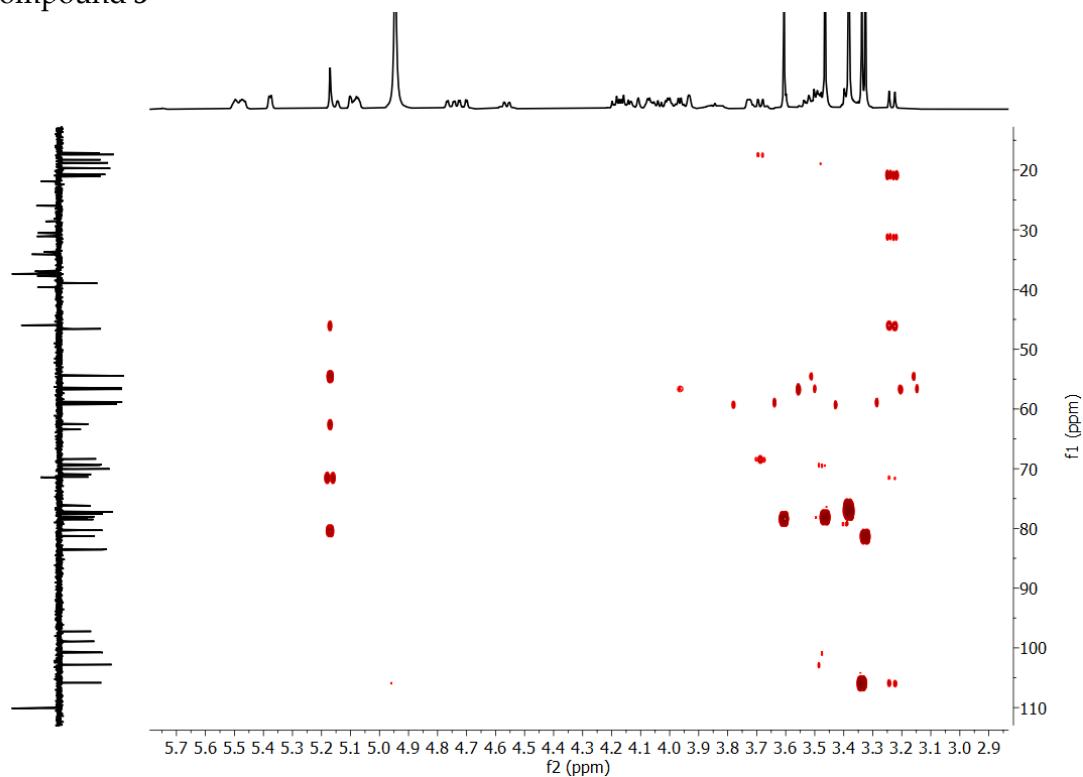
**Figure S50:** Expansion of HSQC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 3



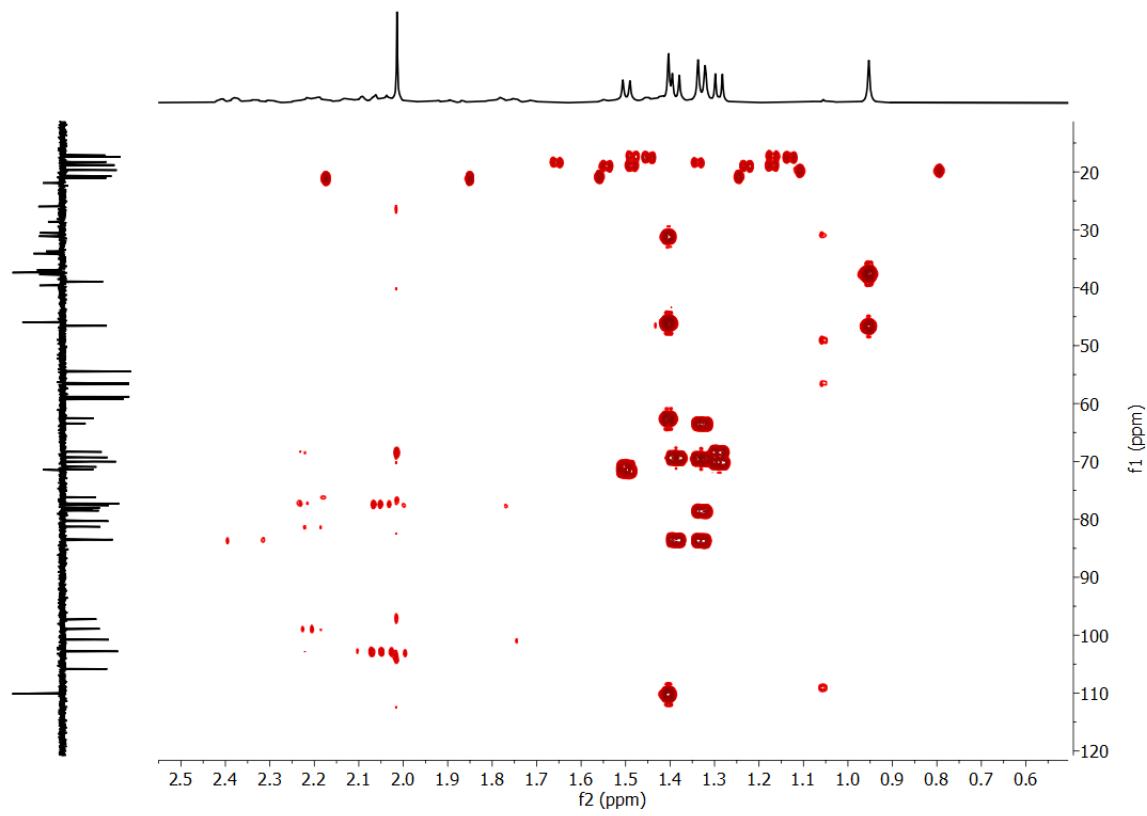
**Figure S51:** HMBC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 3



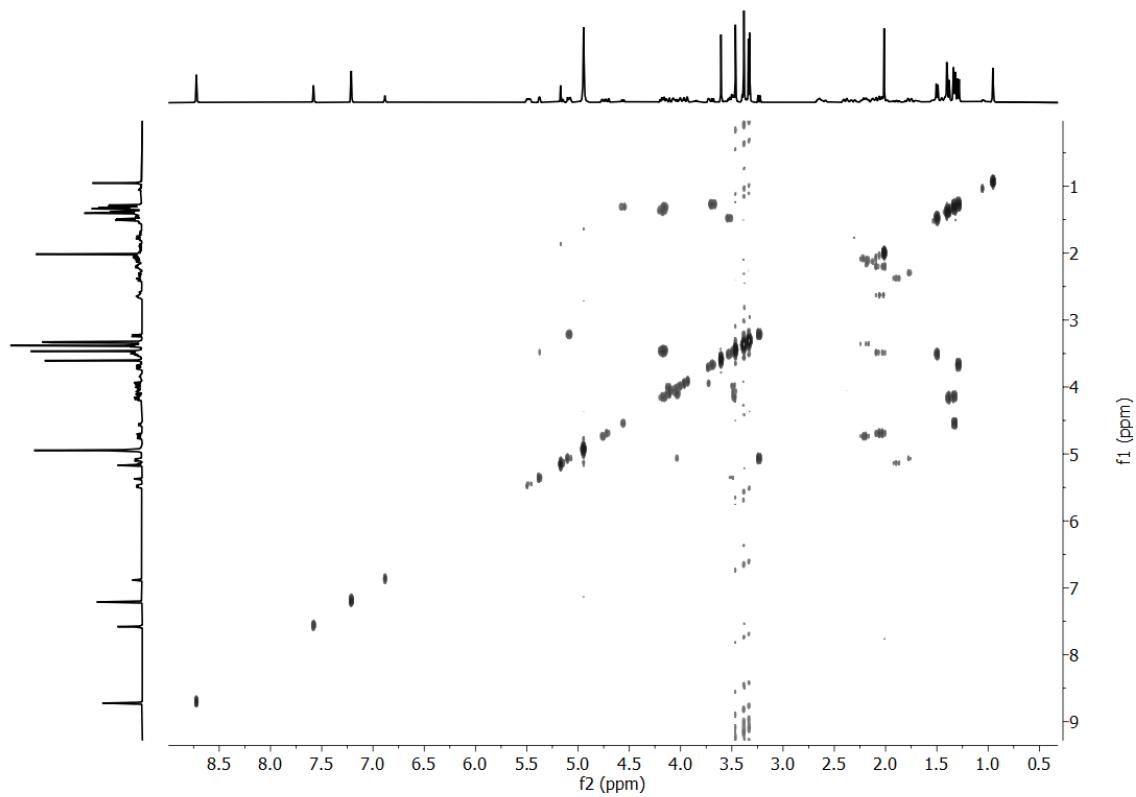
**Figure S52:** Expansion of HMBC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 3



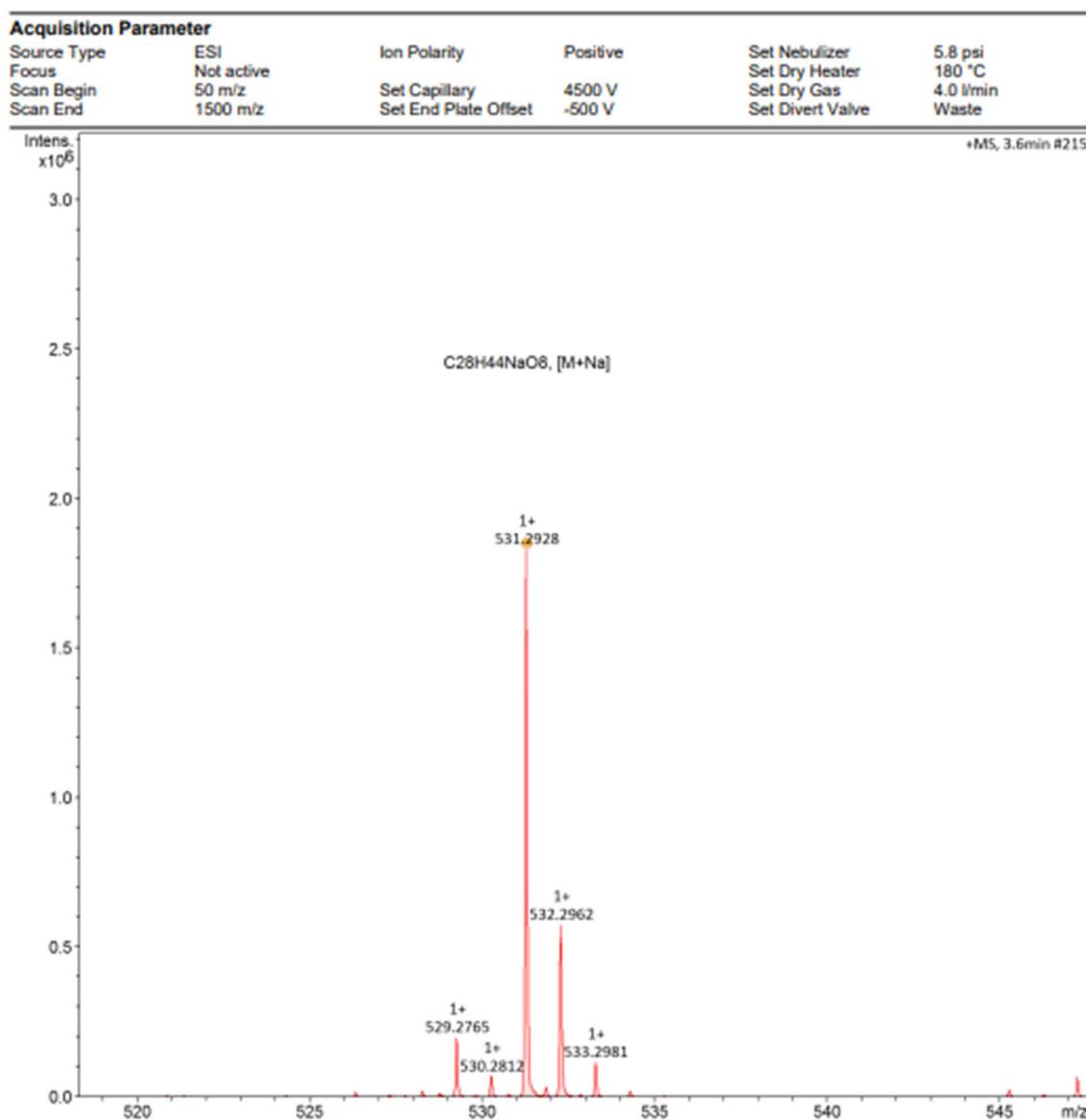
**Figure S53:** Expansion of HMBC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 3



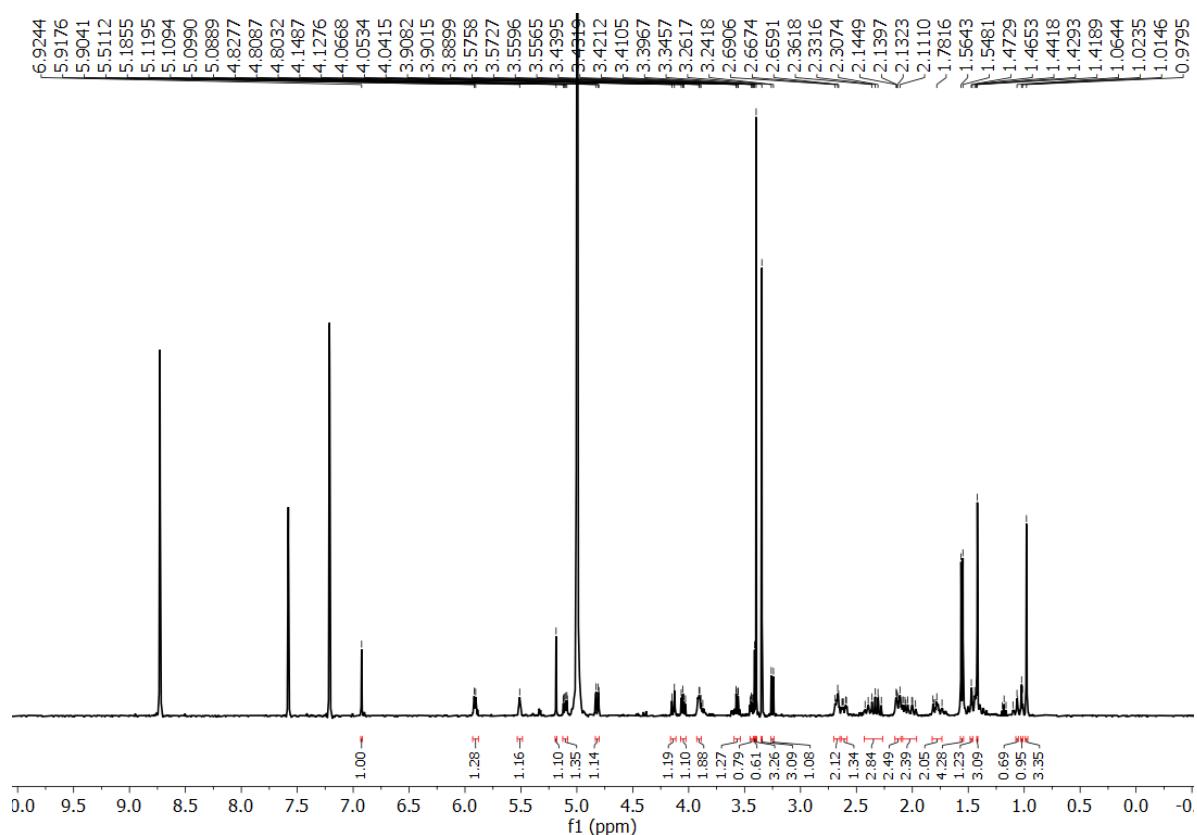
**Figure S54:** COSY spectrum (400 MHz, pyridine-d<sub>5</sub>) of compound 3



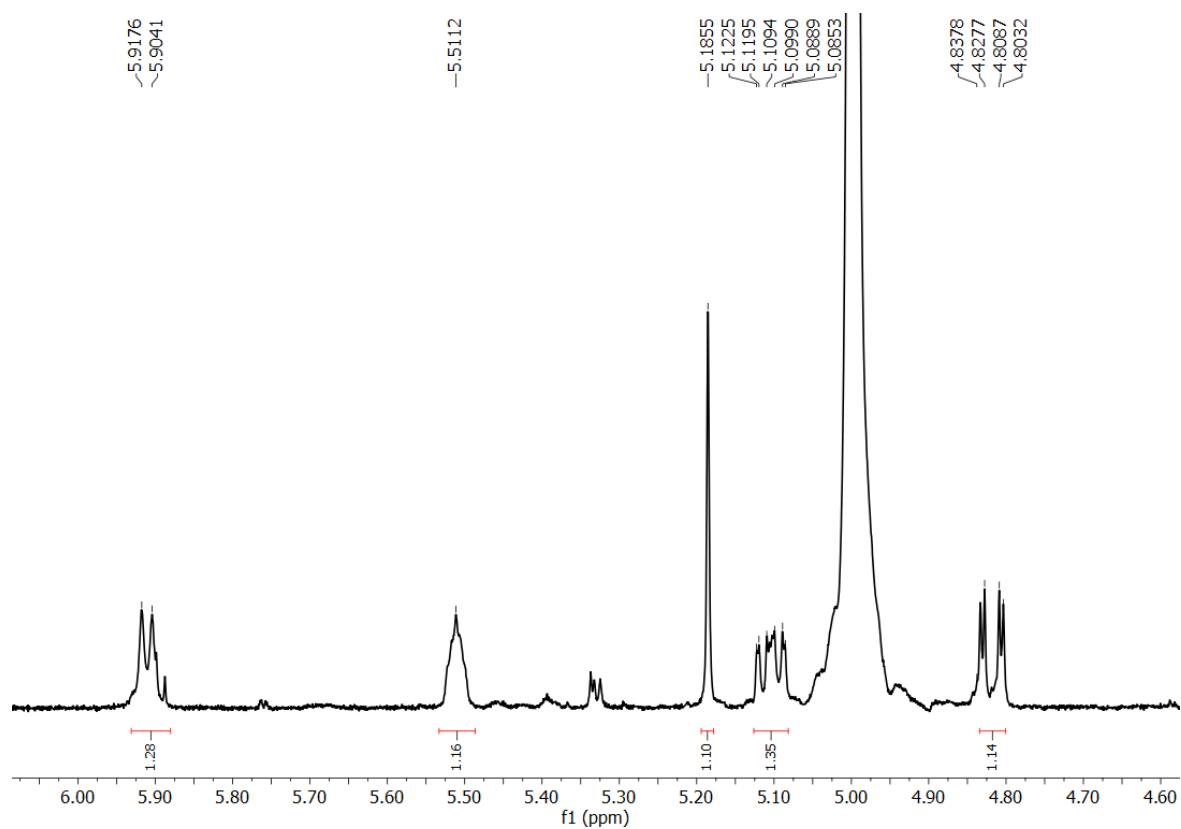
**Figure S55:** ESI-HRMS spectrum of compound 4



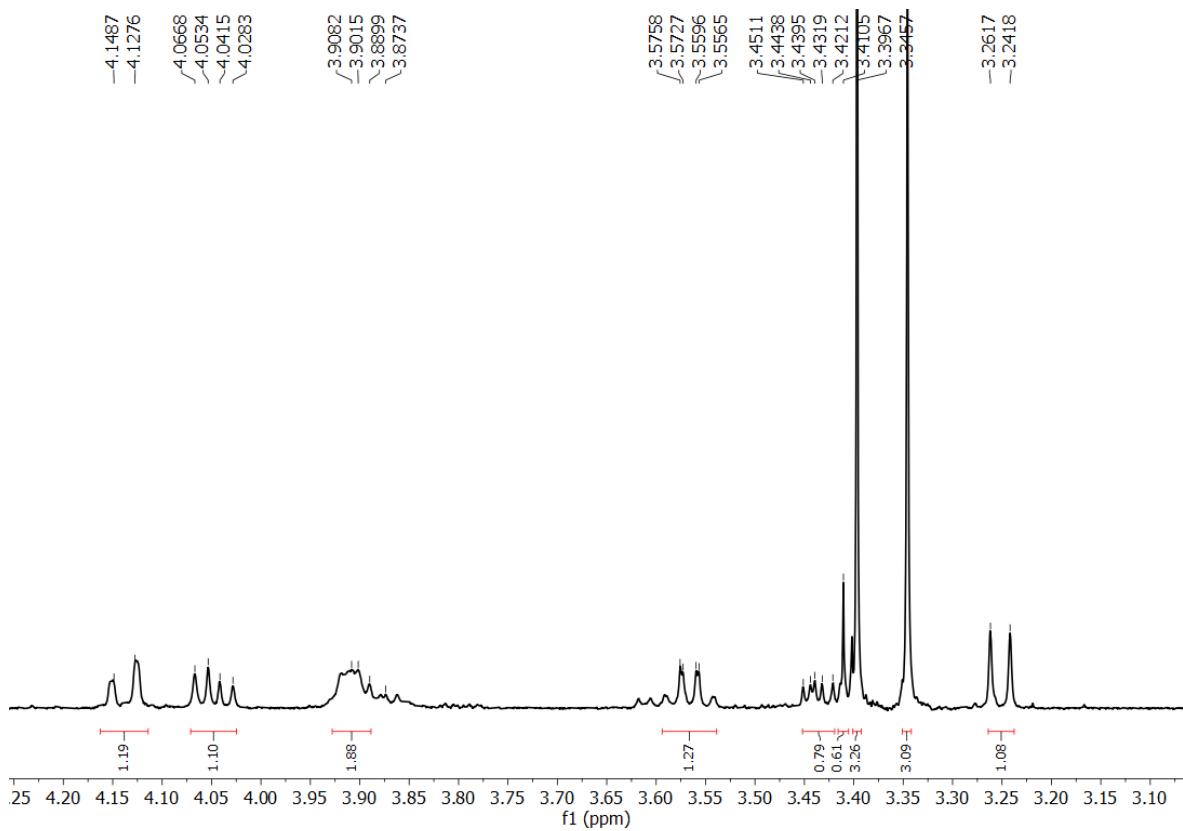
**Figure S56:**  $^1\text{H}$  NMR spectrum (400 MHz, pyridine-d<sub>5</sub>) of compound 4



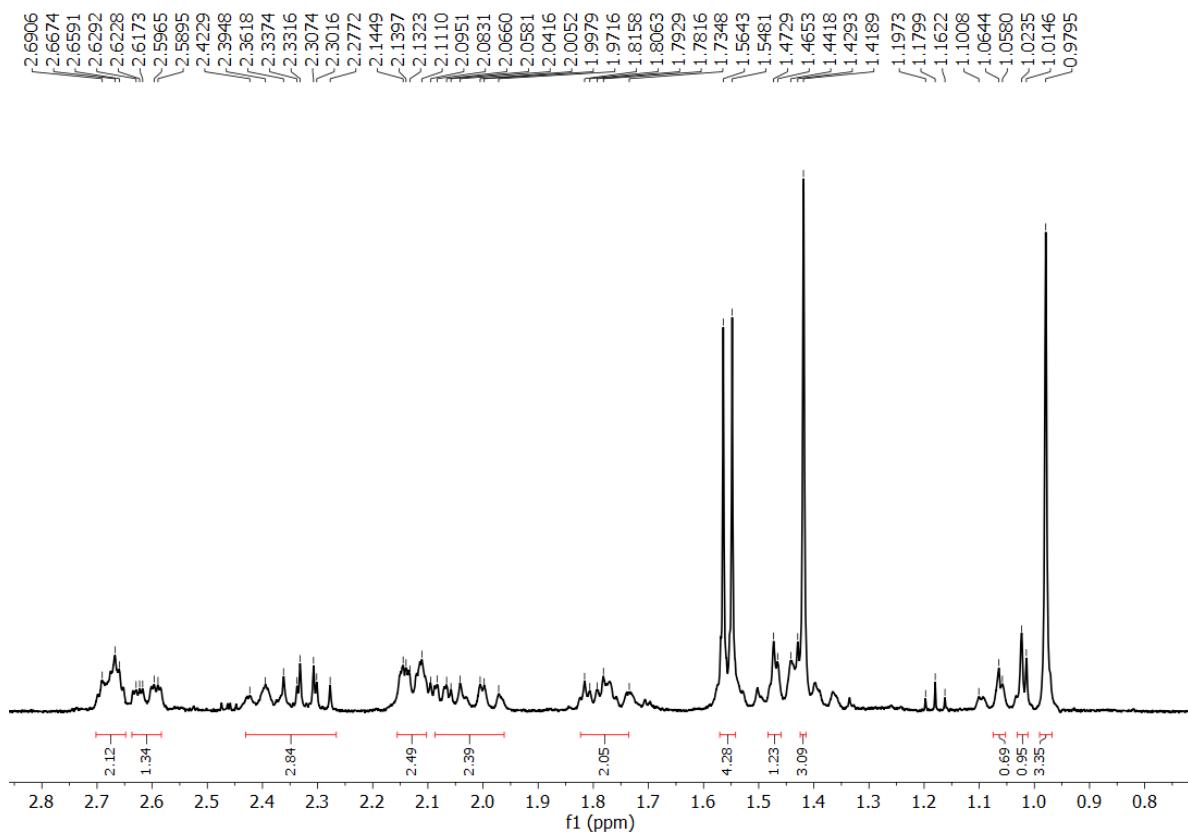
**Figure S57:** Expansion of  $^1\text{H}$  NMR spectrum (400 MHz, pyridine-d<sub>5</sub>) of compound 4



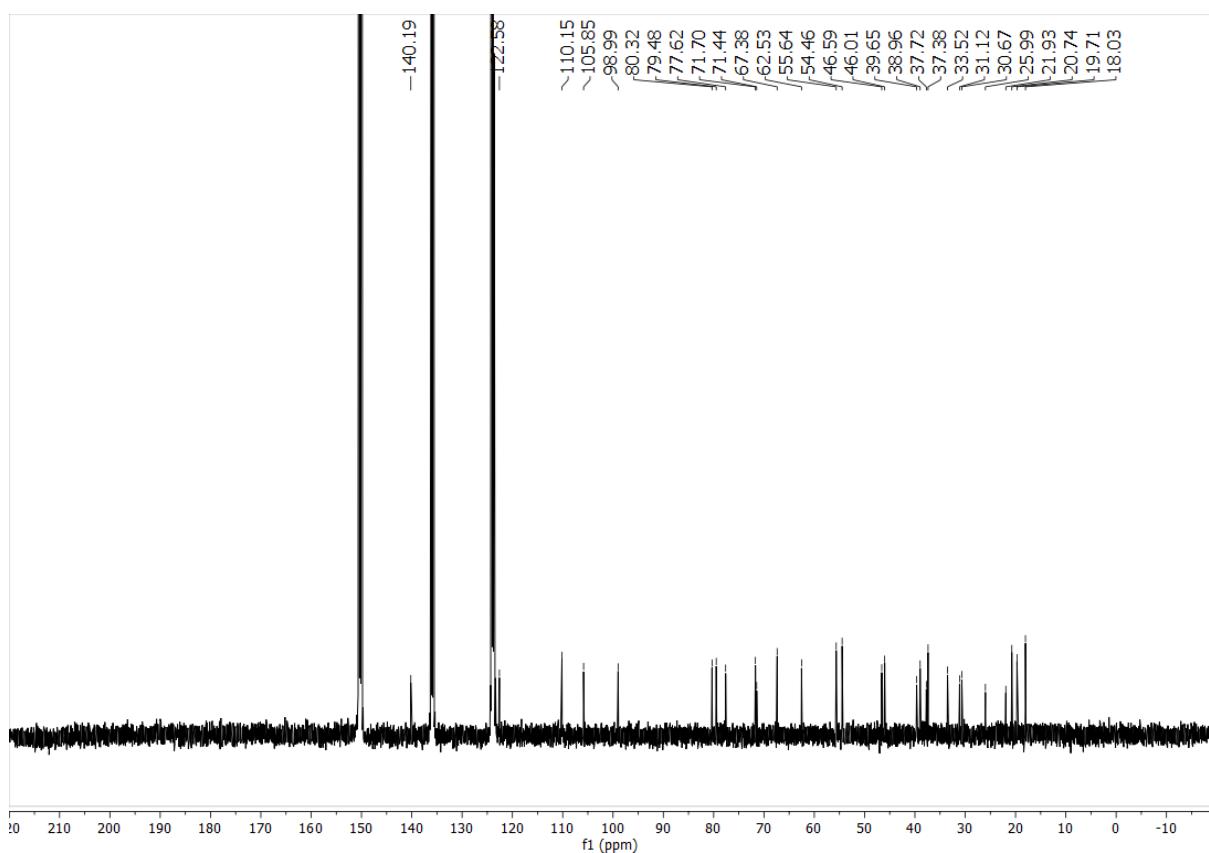
**Figure S58:** Expansion of  $^1\text{H}$  NMR spectrum (400 MHz, pyridine-d<sub>5</sub>) of compound 4



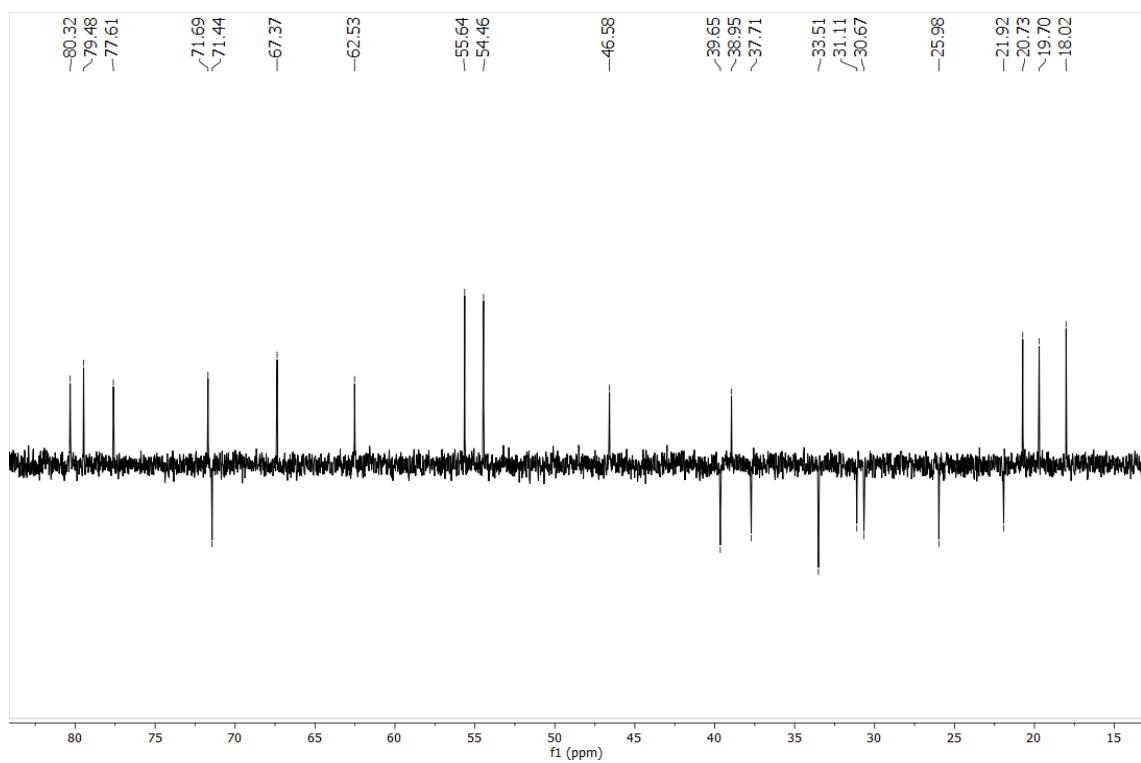
**Figure S59:** Expansion of  $^1\text{H}$  NMR spectrum (400 MHz, pyridine-d<sub>5</sub>) of compound 4



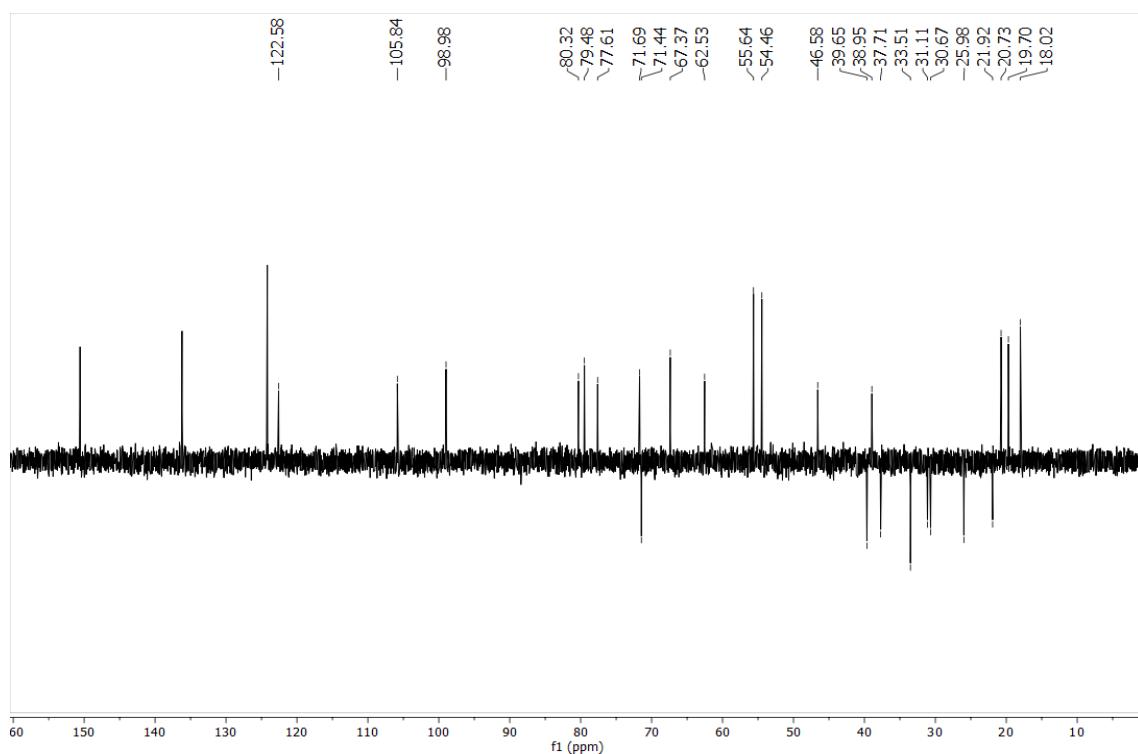
**Figure S60:** Broadband  $^{13}\text{C}$  NMR (100 MHz, pyridine-d<sub>5</sub>) of compound 4



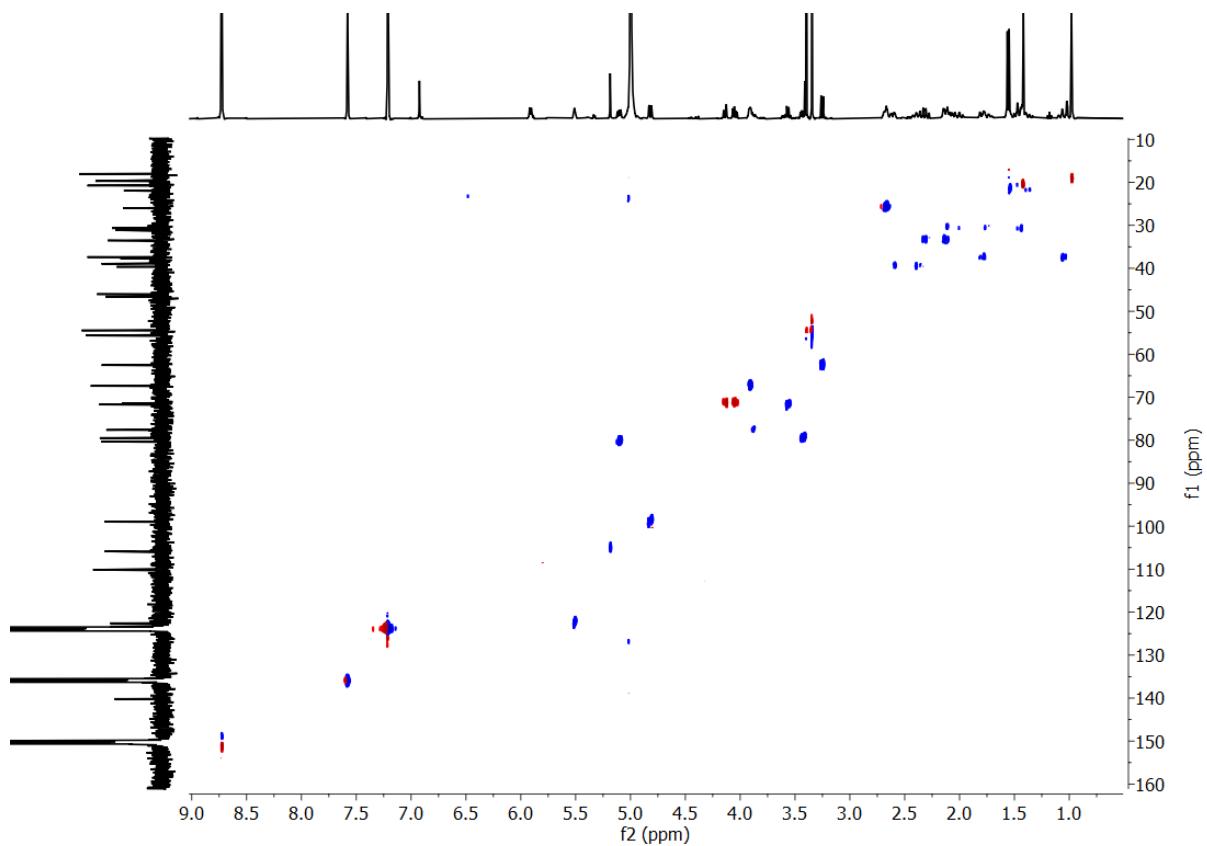
**Figure S61:** DEPT 135 spectrum (100 MHz, pyridine-d<sub>5</sub>) of compound 4



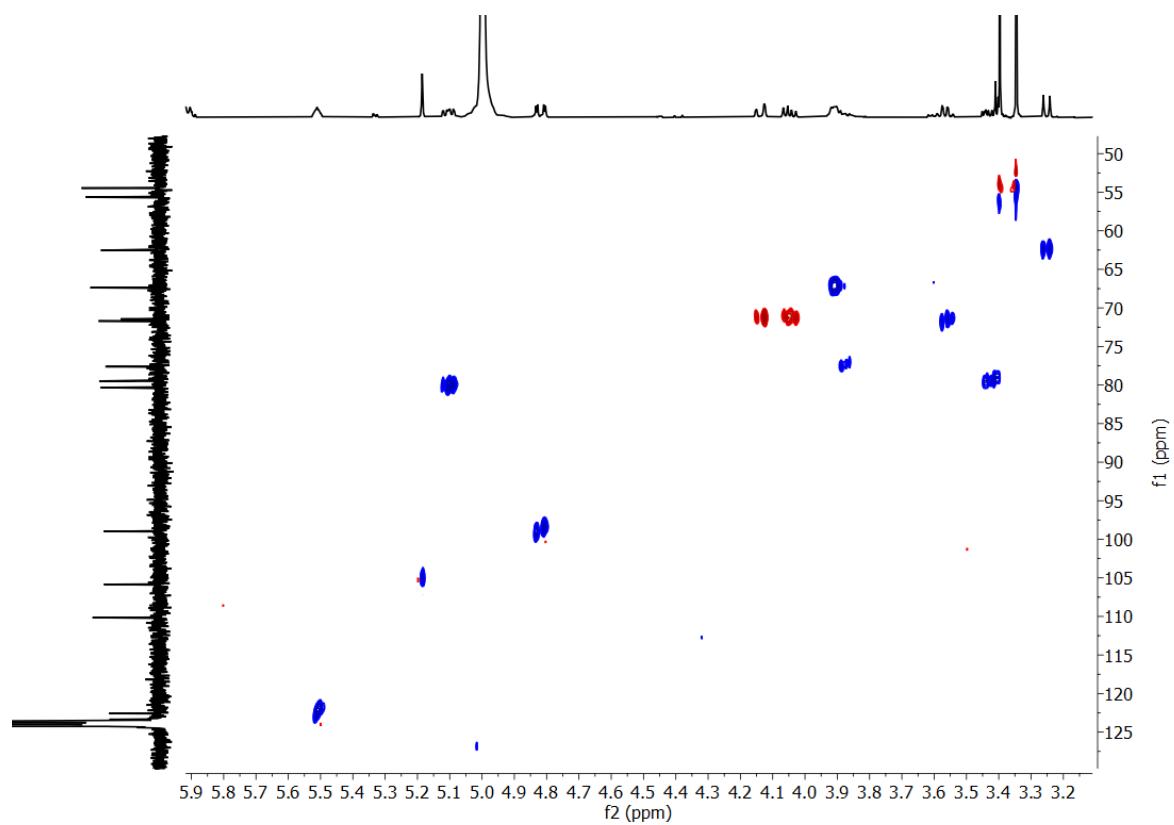
**Figure S62:** Expansion of DEPT 135 spectrum (100 MHz, pyridine-d<sub>5</sub>) of compound 4



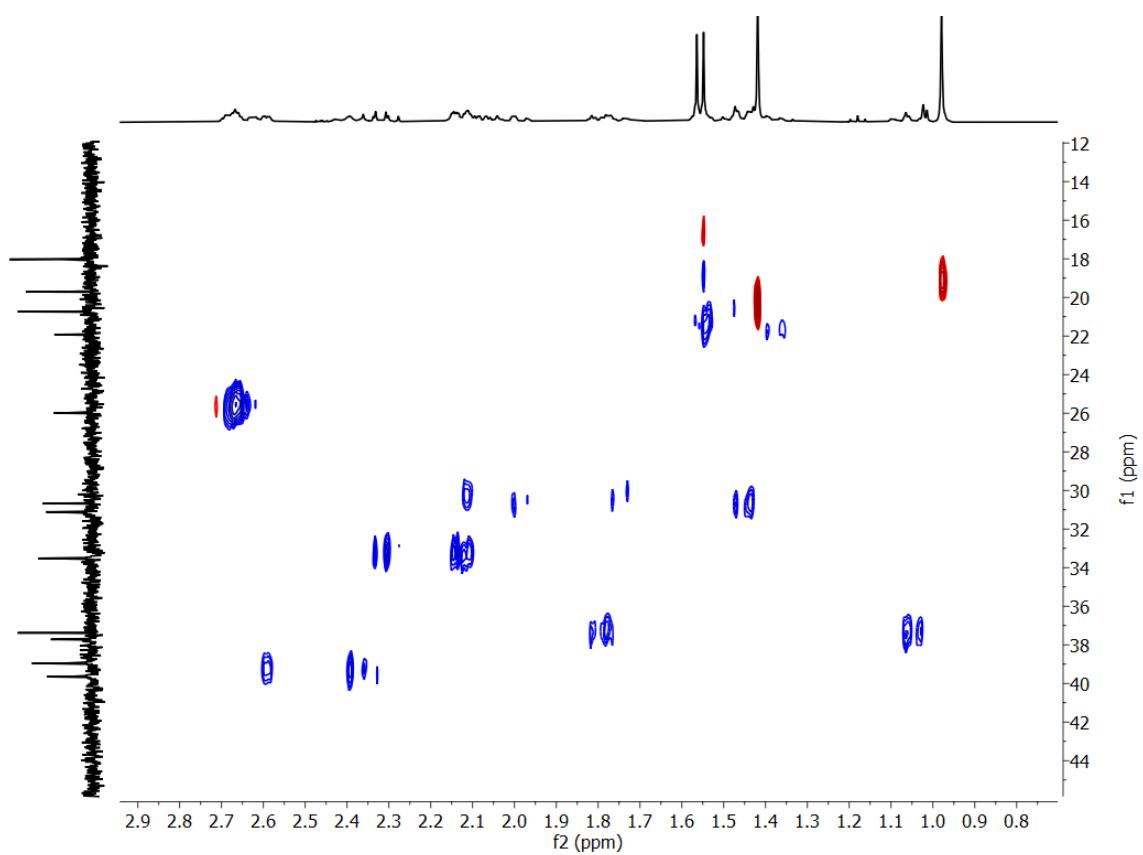
**Figure S63:** HSQC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 4



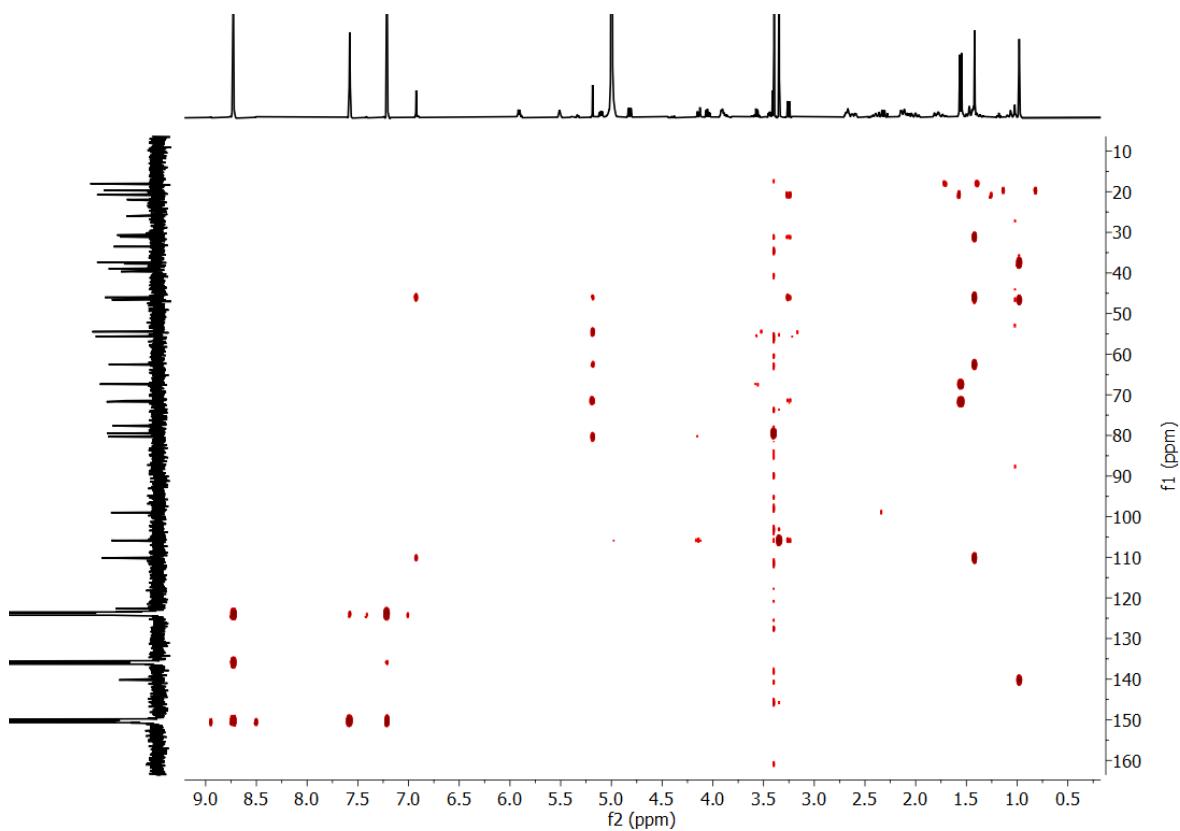
**Figure S64:** Expansion of HSQC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 4



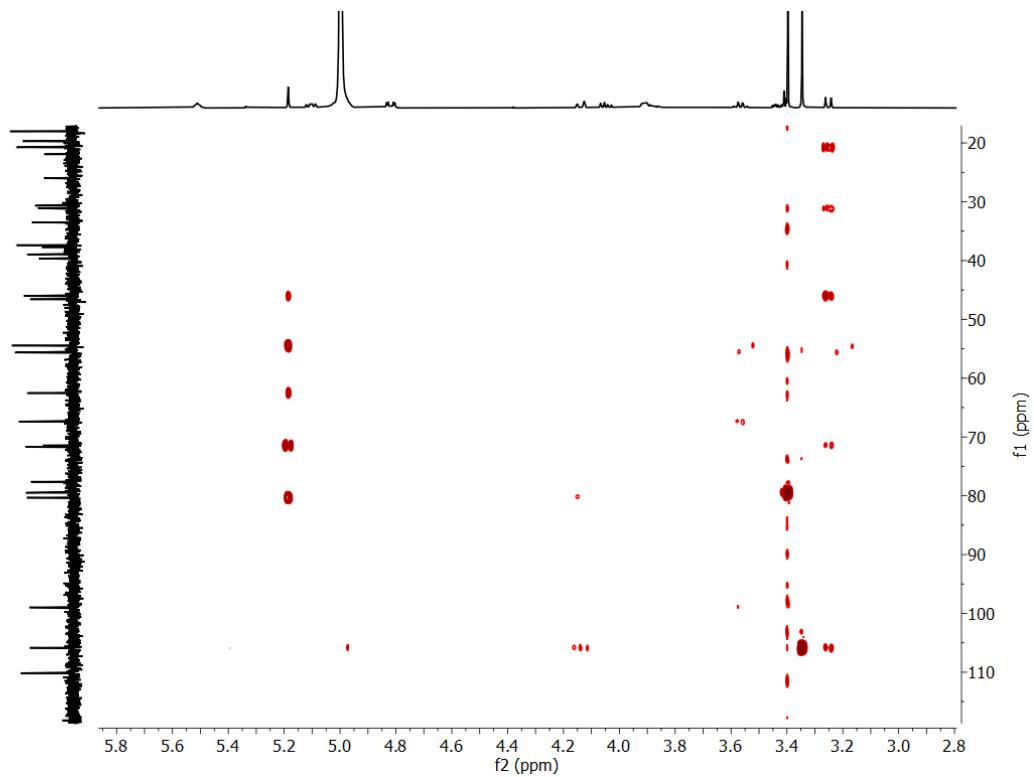
**Figure S65:** Expansion of HSQC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 4



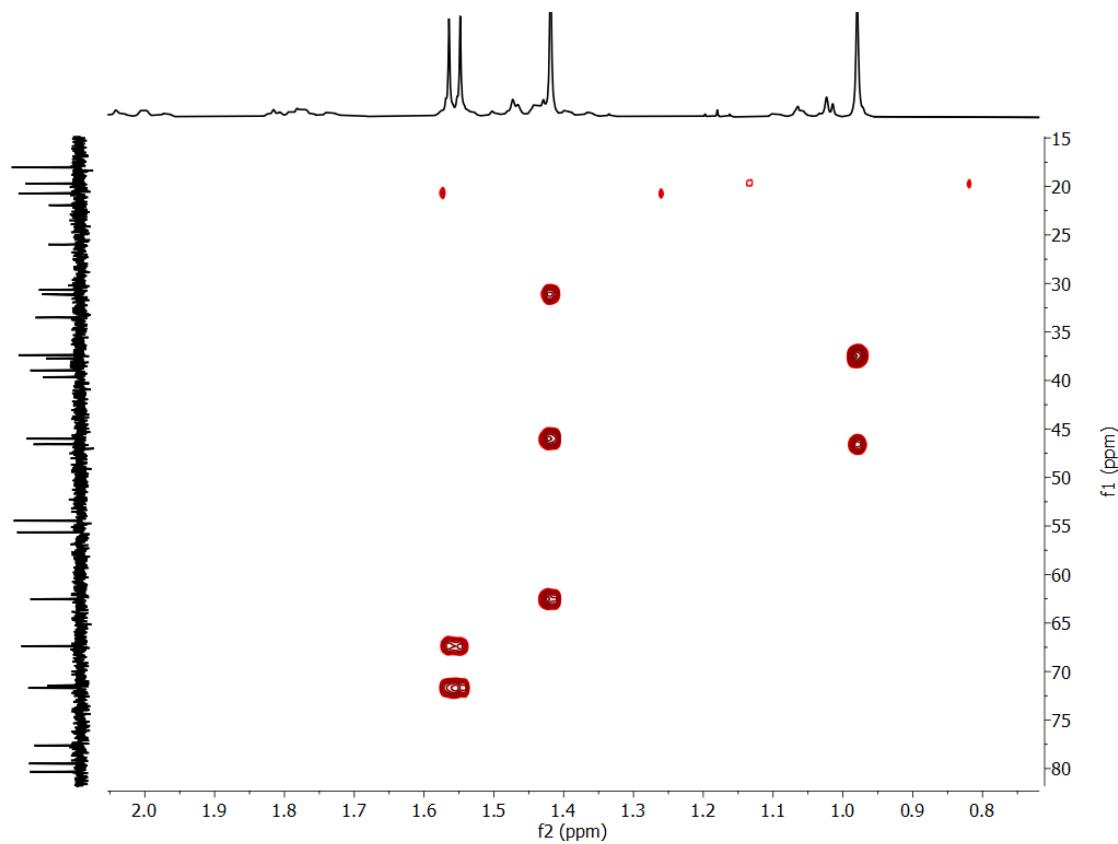
**Figure S66:** HMBC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 4



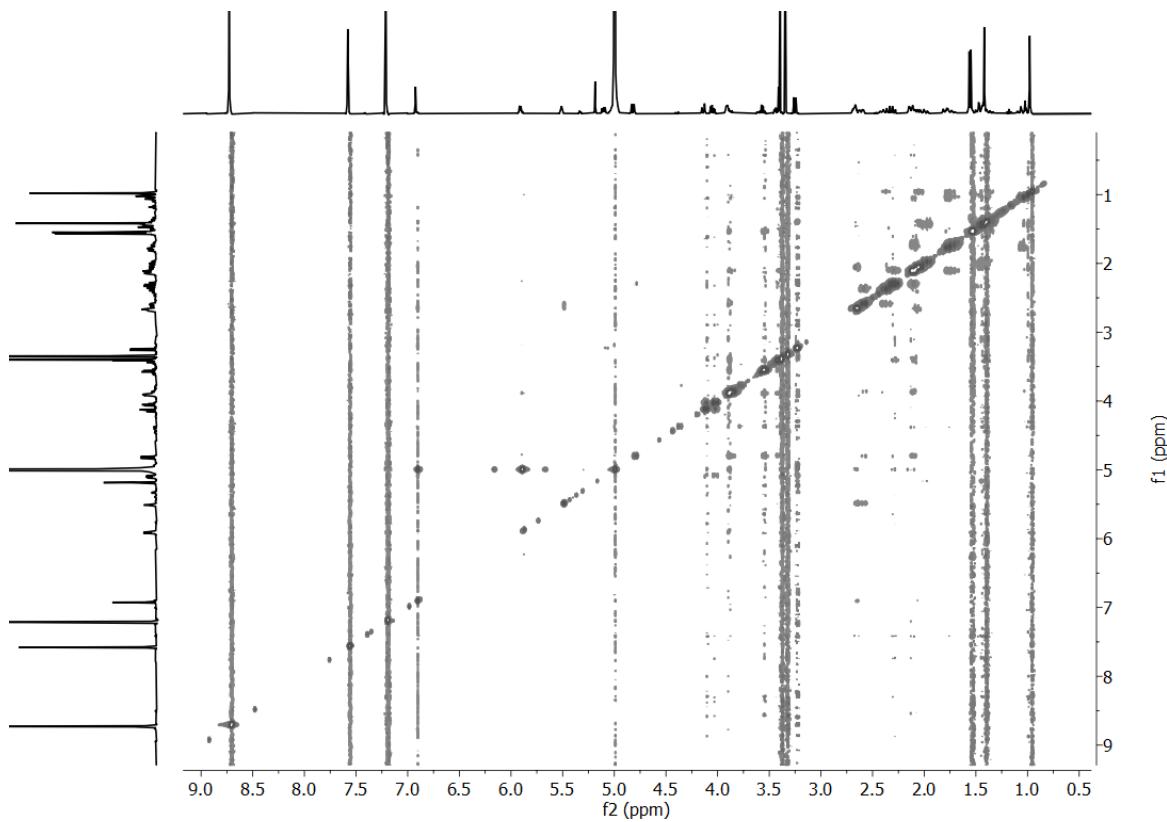
**Figure S67:** Expansion of HMBC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 4



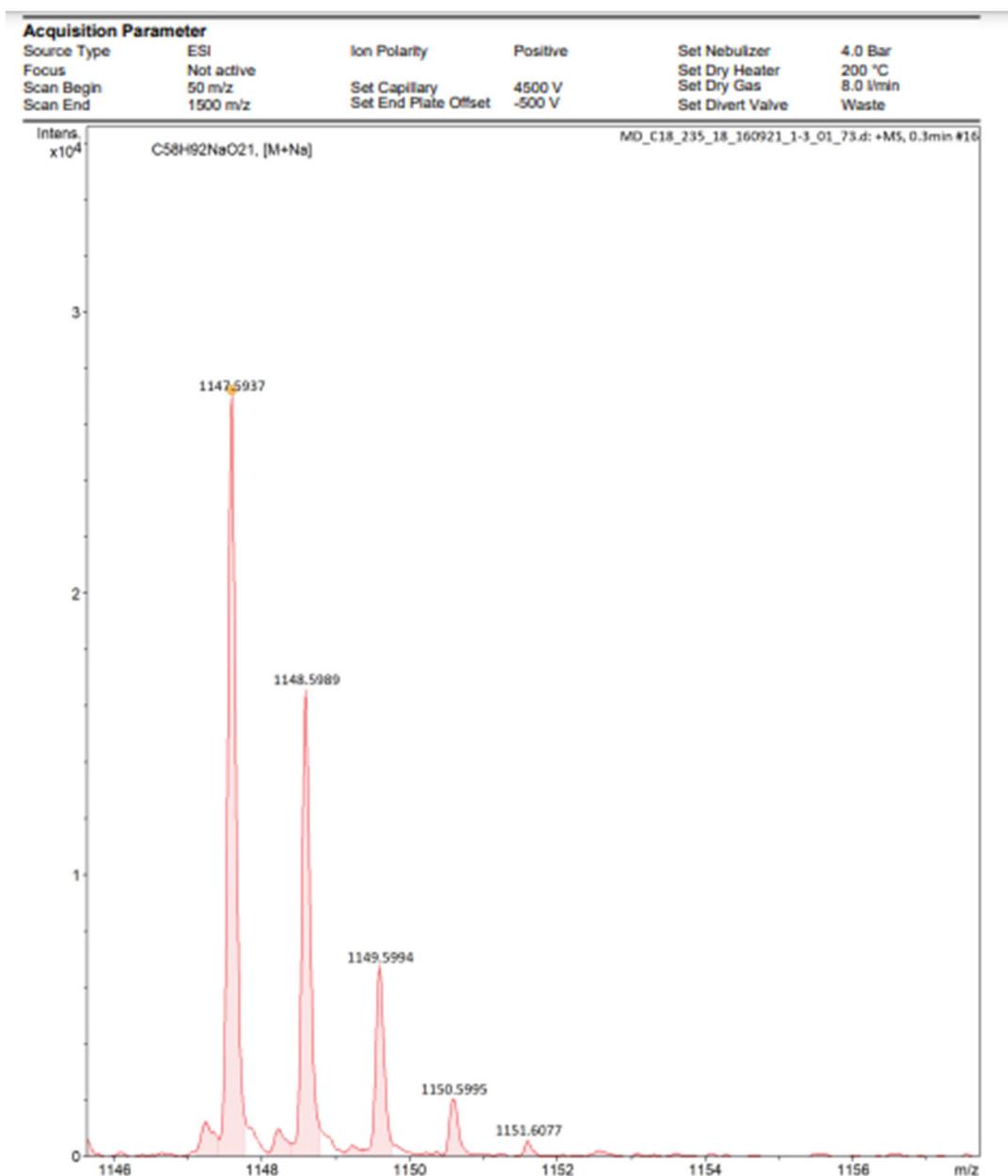
**Figure S68:** HMBC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 4



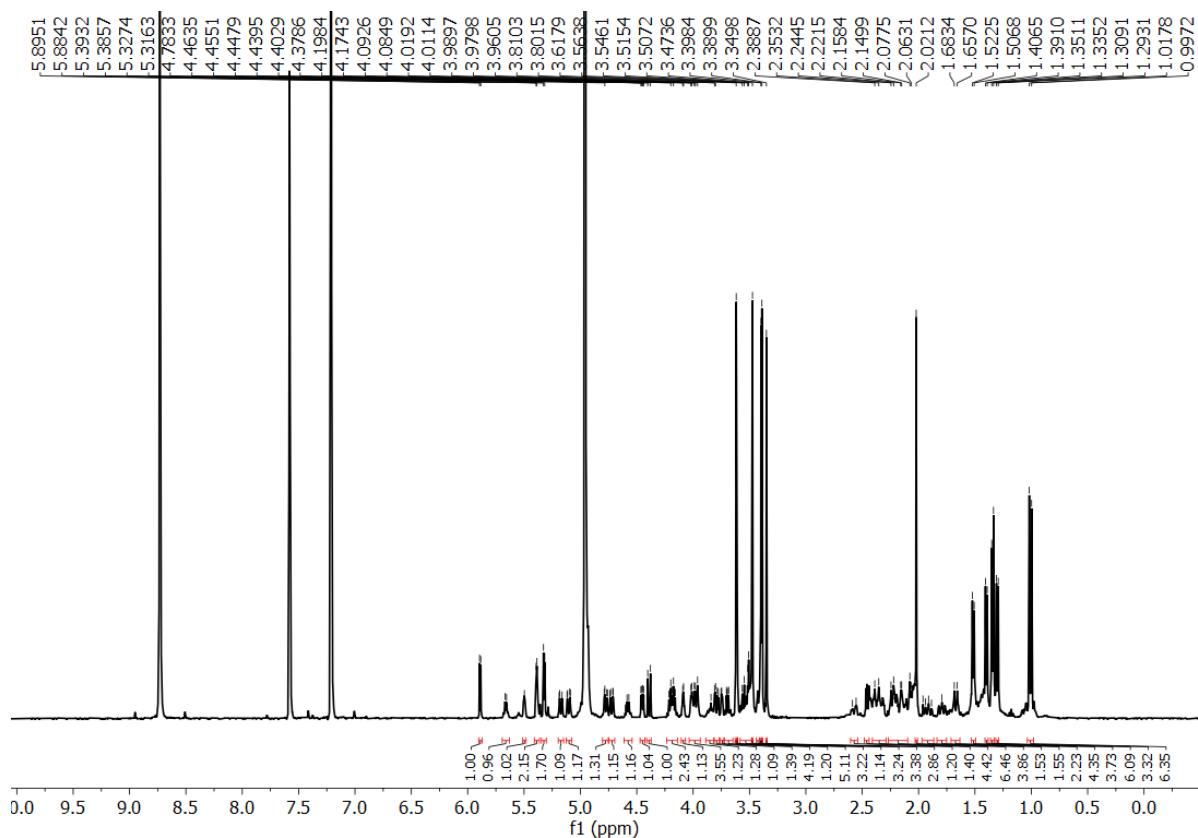
**Figure S69:** COSY spectrum (400 MHz, pyridine-d<sub>5</sub>) of compound 4



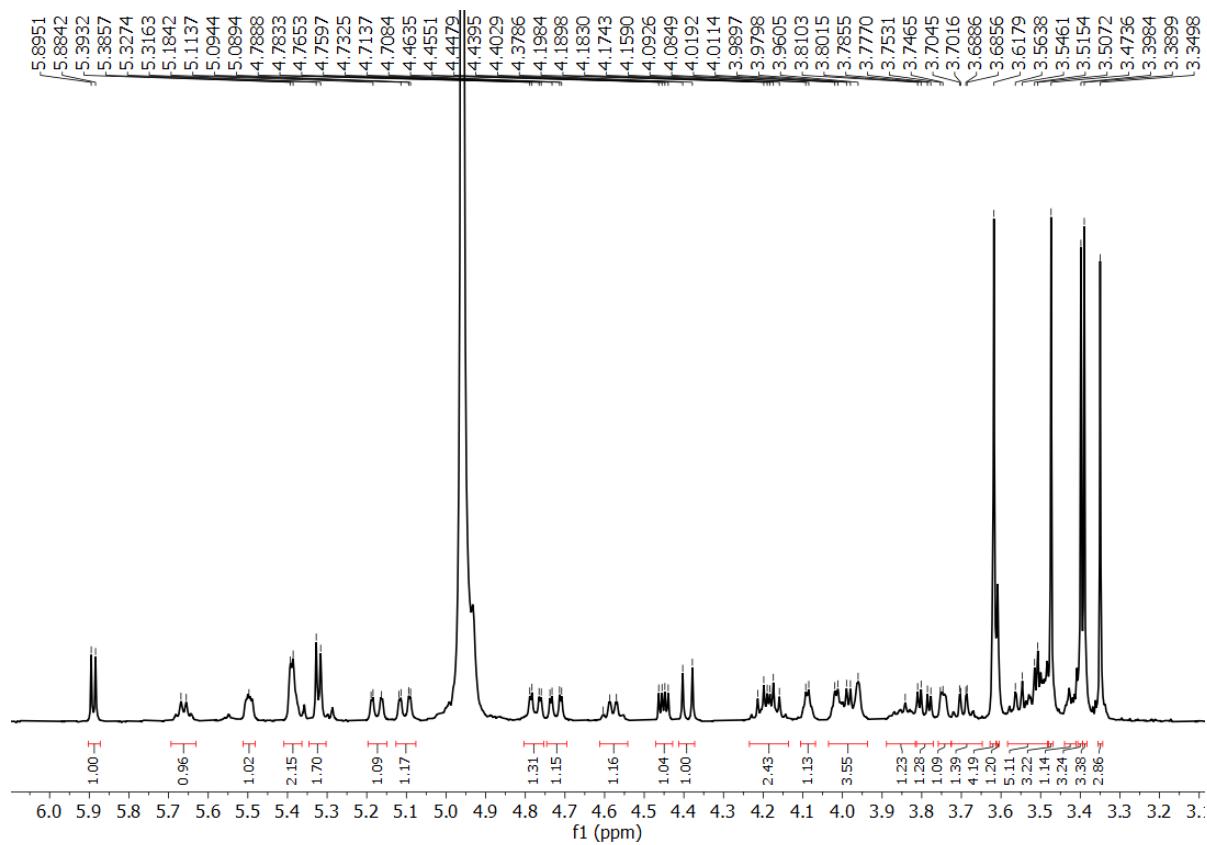
**Figure S70:** ESI-HRMS spectrum of compound 5



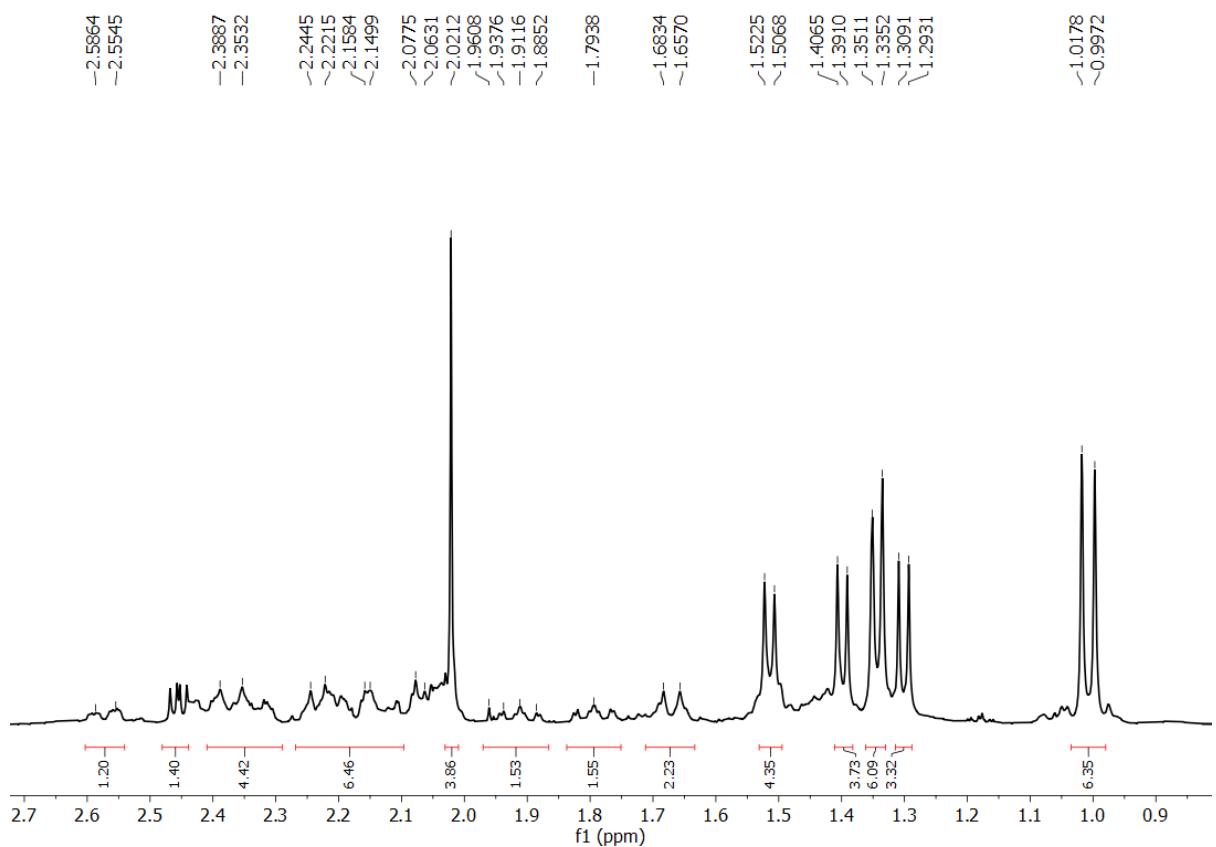
**Figure S71:**  $^1\text{H}$  NMR spectrum (400 MHz, pyridine-d<sub>5</sub>) of compound 5



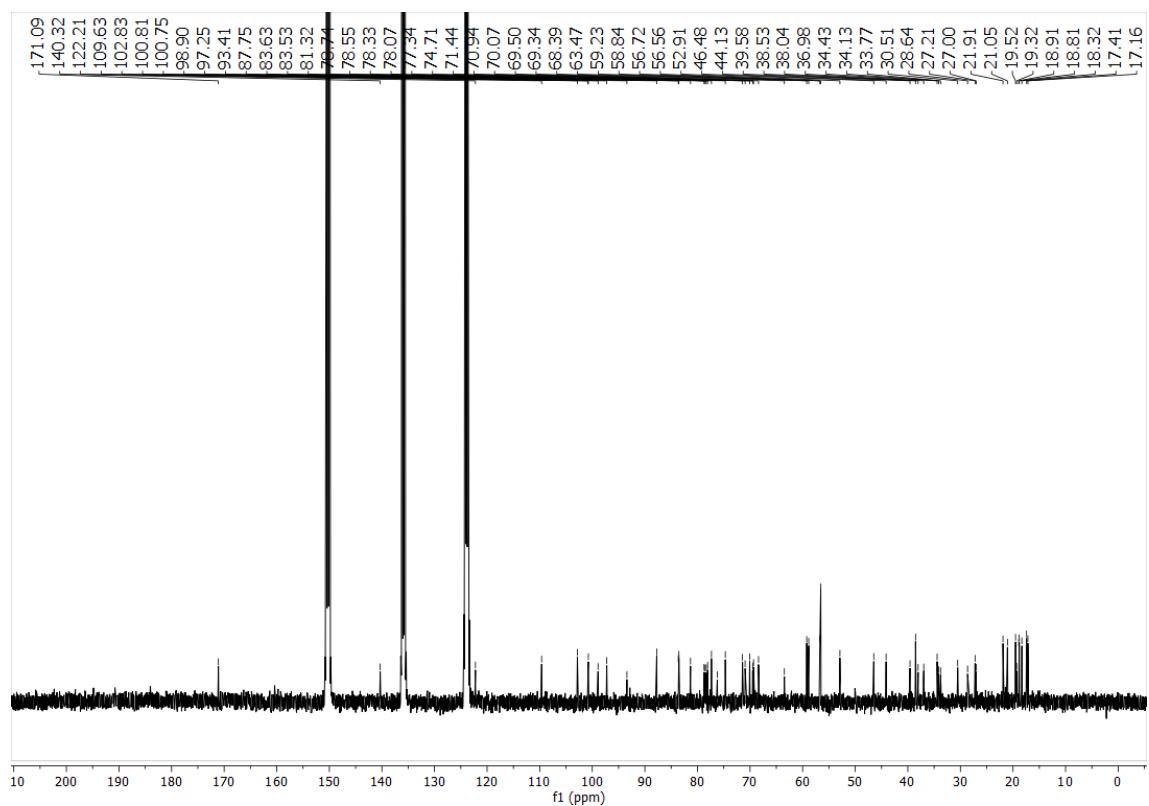
**Figure S72:** Expansion of  $^1\text{H}$  NMR spectrum (400 MHz, pyridine-d<sub>5</sub>) of compound 5



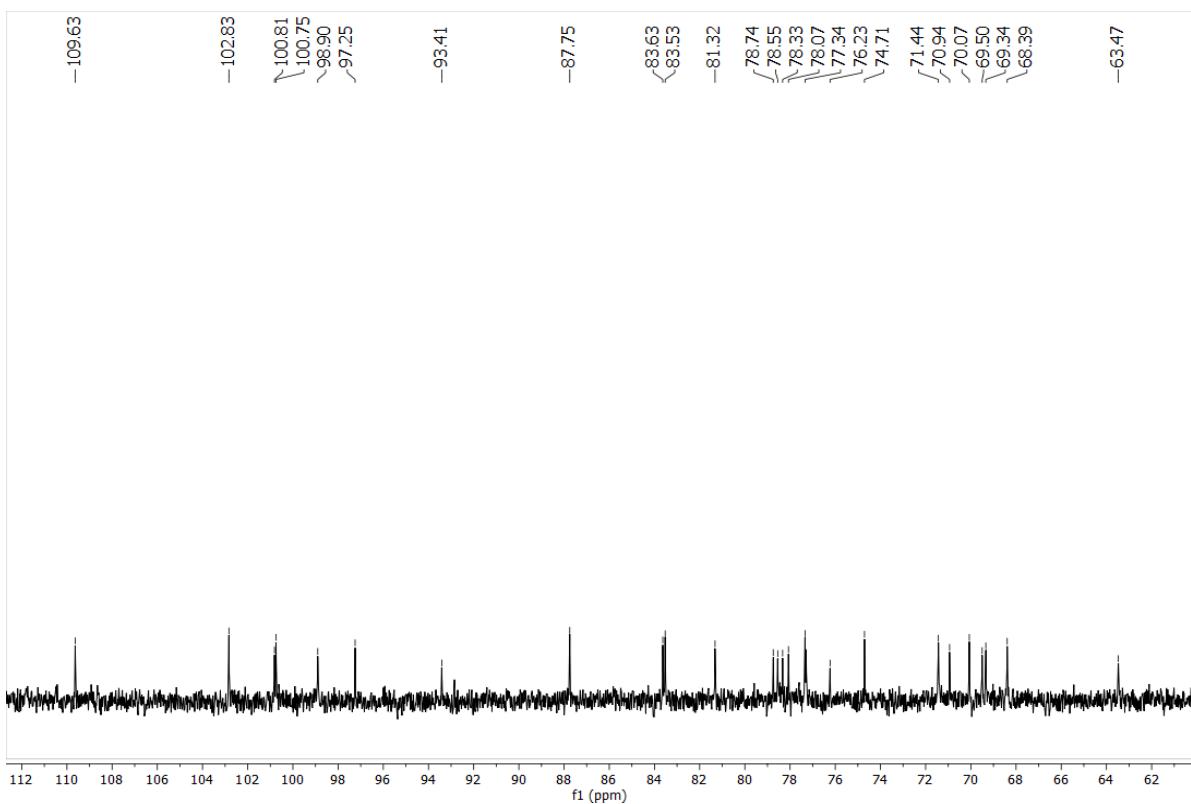
**Figure S73:** Expansion of  $^1\text{H}$  NMR spectrum (400 MHz, pyridine-d<sub>5</sub>) of compound 5



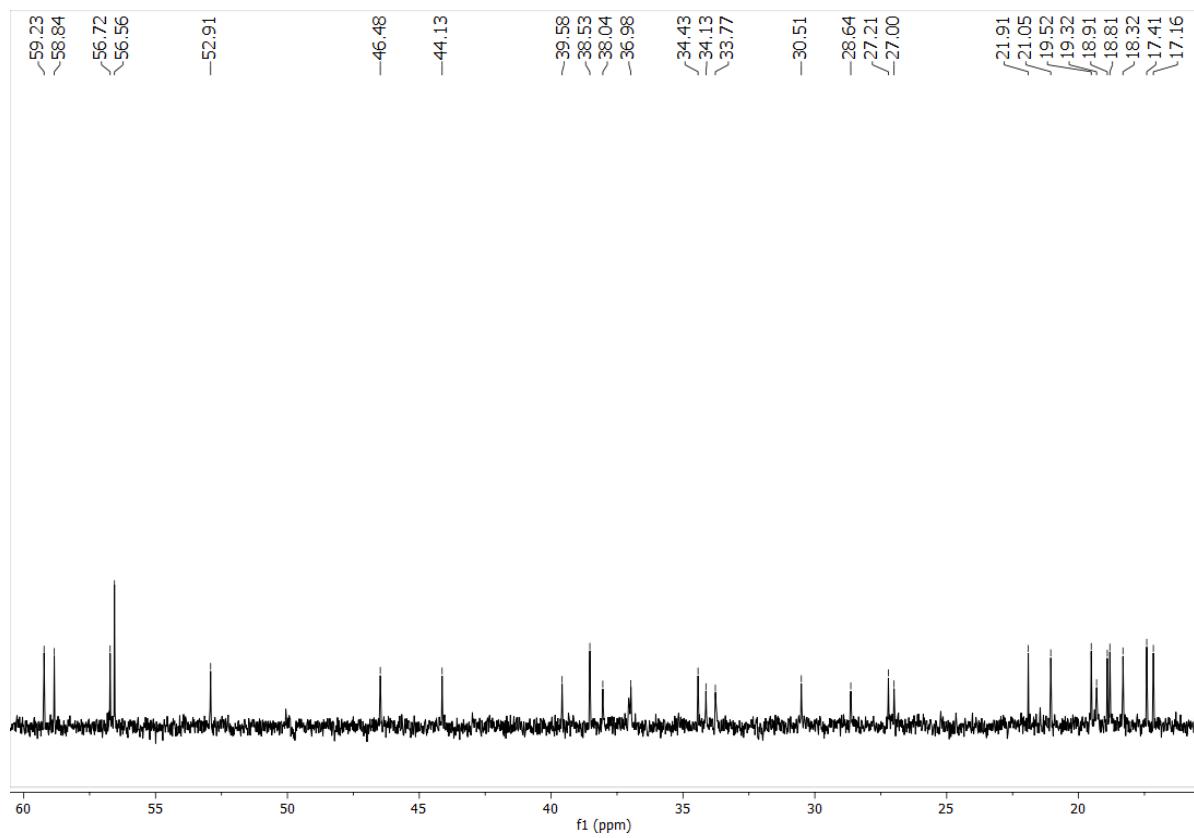
**Figure S74:**  $^{13}\text{C}$  NMR spectrum (100 MHz, pyridine-d<sub>5</sub>) of compound 5



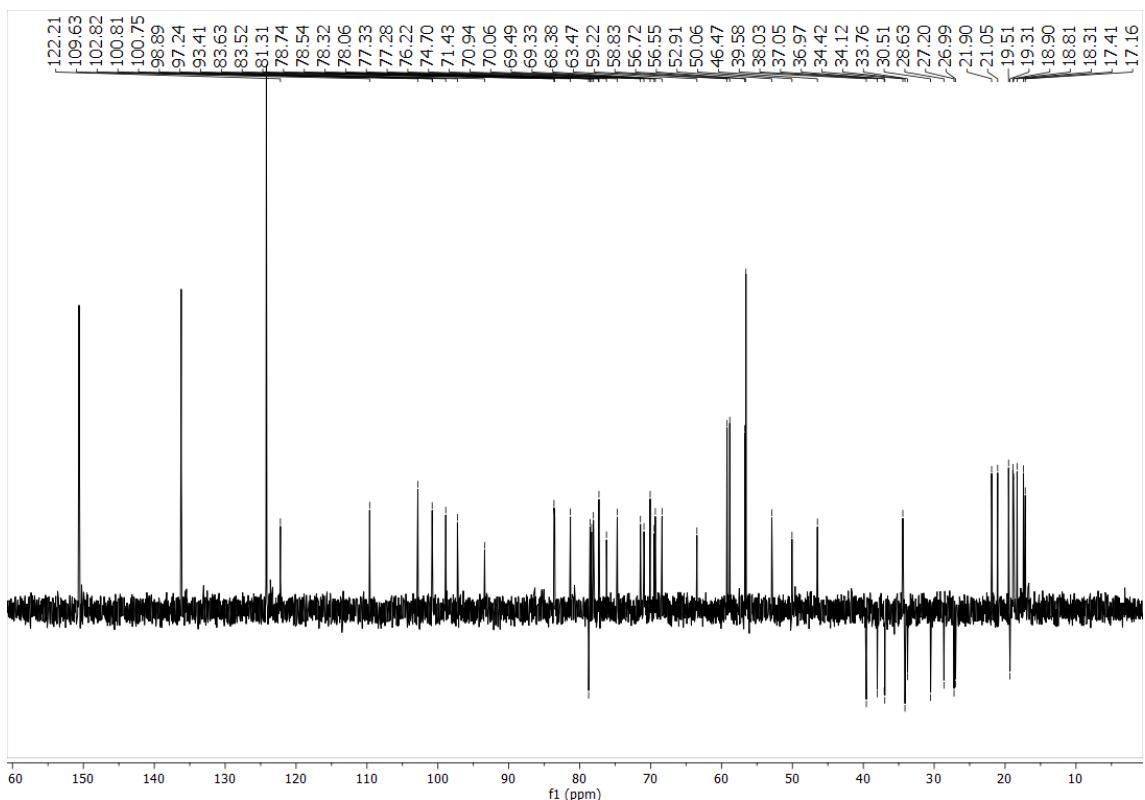
**Figure S75:** Expansion of  $^{13}\text{C}$  NMR spectrum (100 MHz, pyridine-d<sub>5</sub>) of compound 5



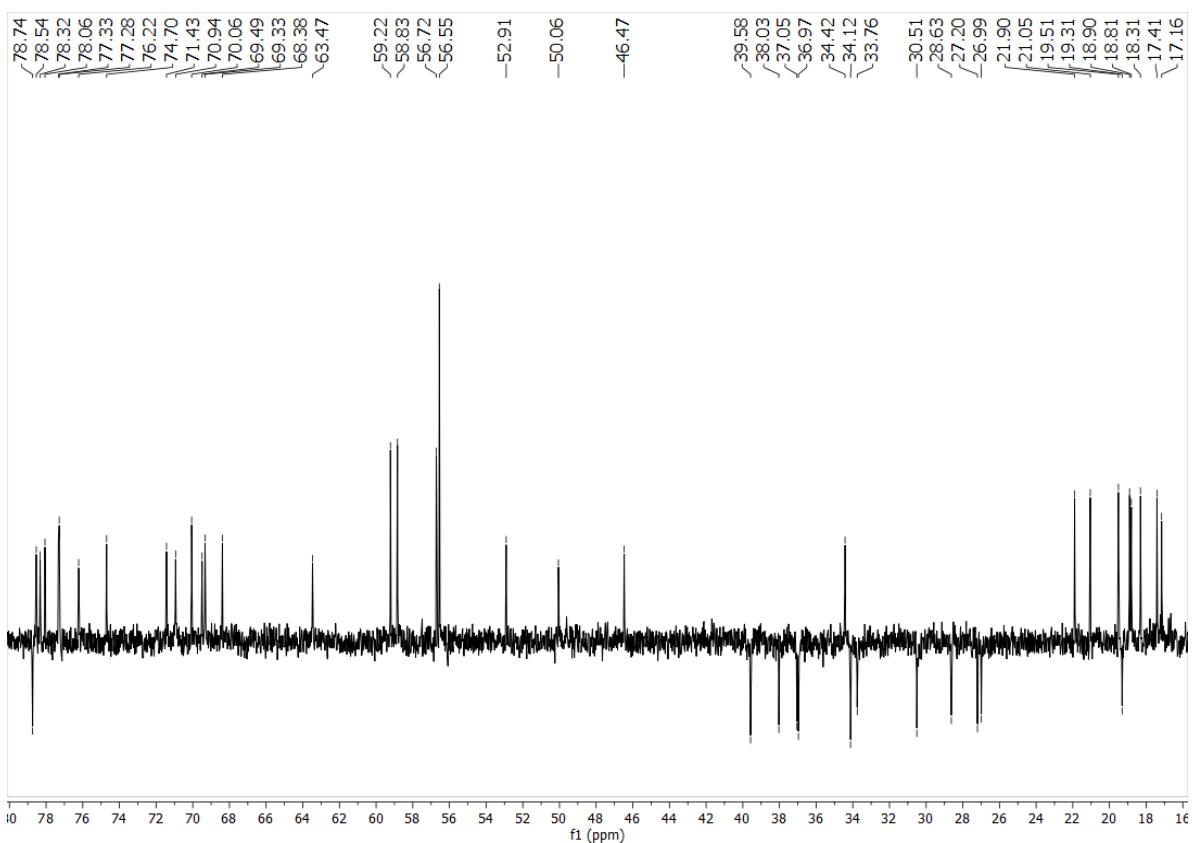
**Figure S76:** Expansion of  $^{13}\text{C}$  NMR spectrum (100 MHz, pyridine-d<sub>5</sub>) of compound 5



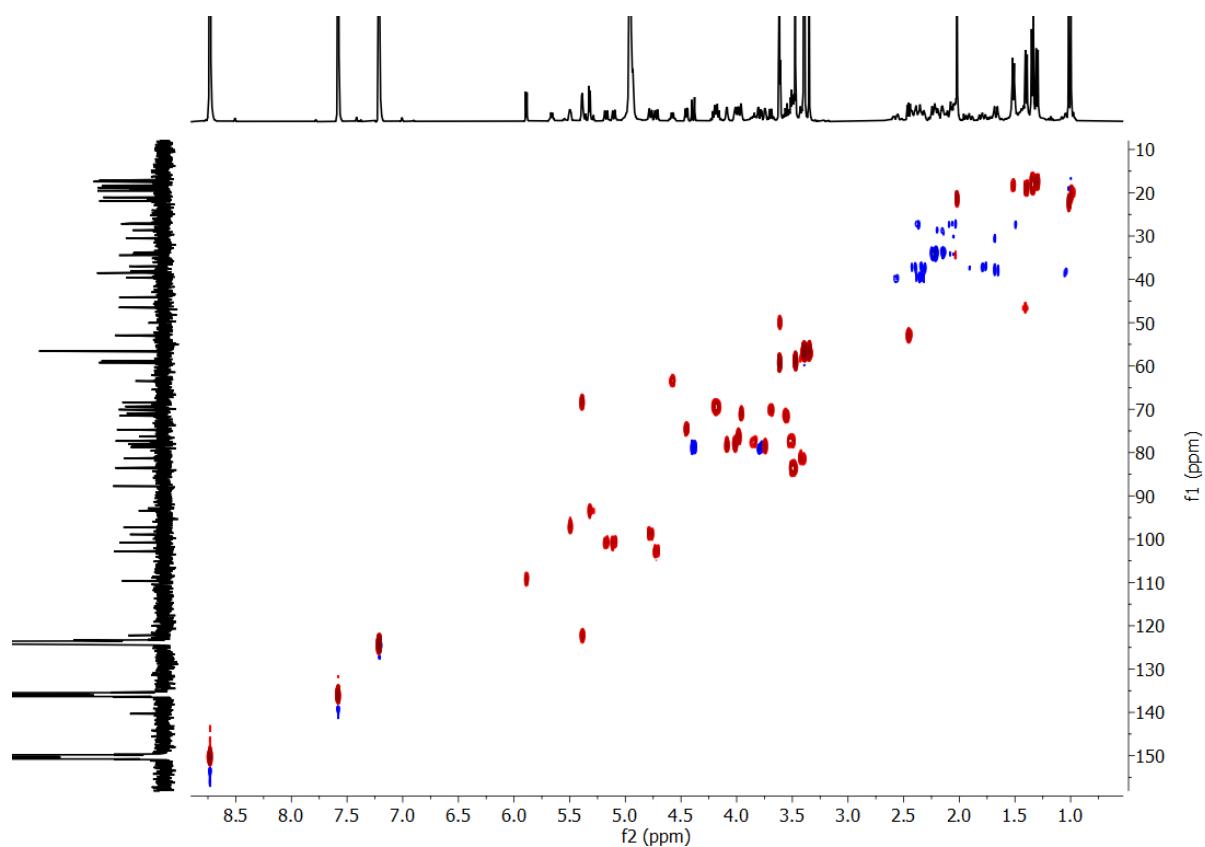
**Figure S77:** DEPT spectrum (100 MHz, pyridine-d<sub>5</sub>) of compound 5



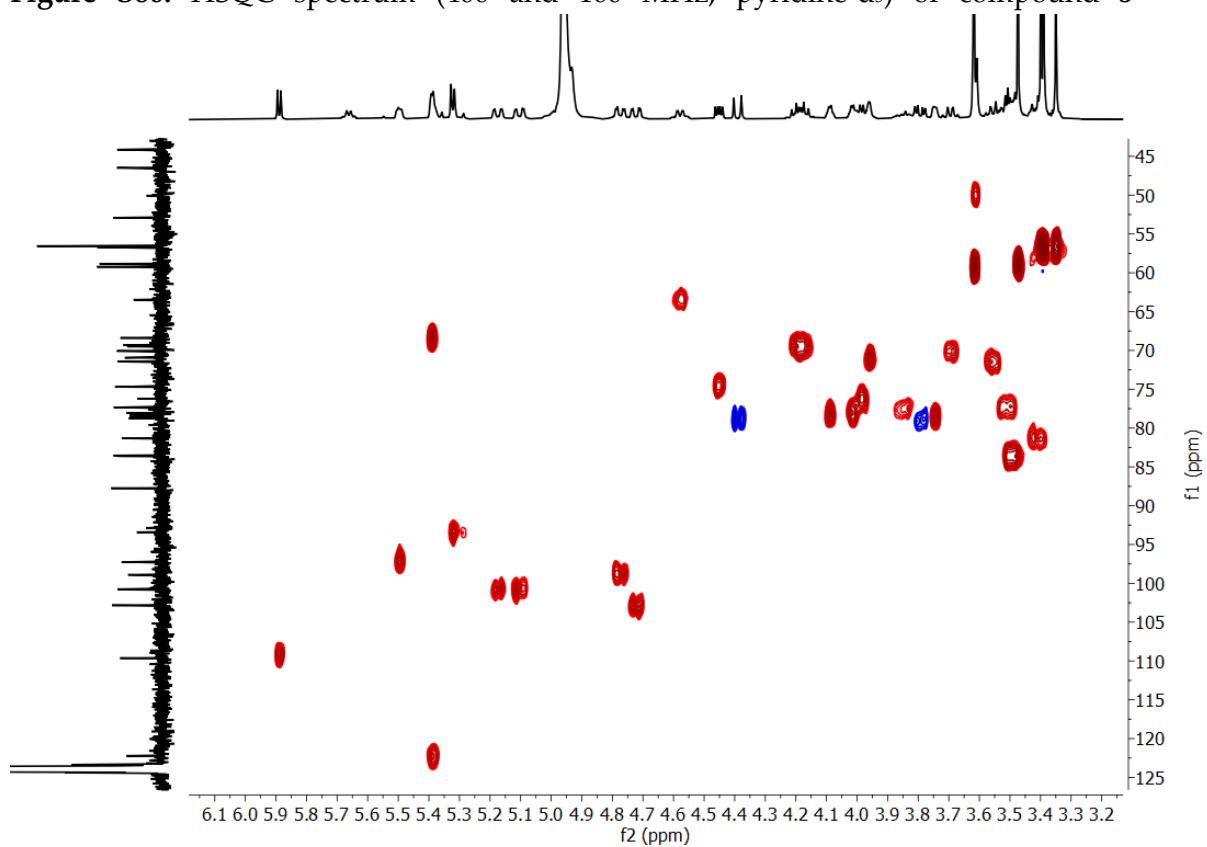
**Figure S78:** Expansion of DEPT spectrum (100 MHz, pyridine-d<sub>5</sub>) of compound 5



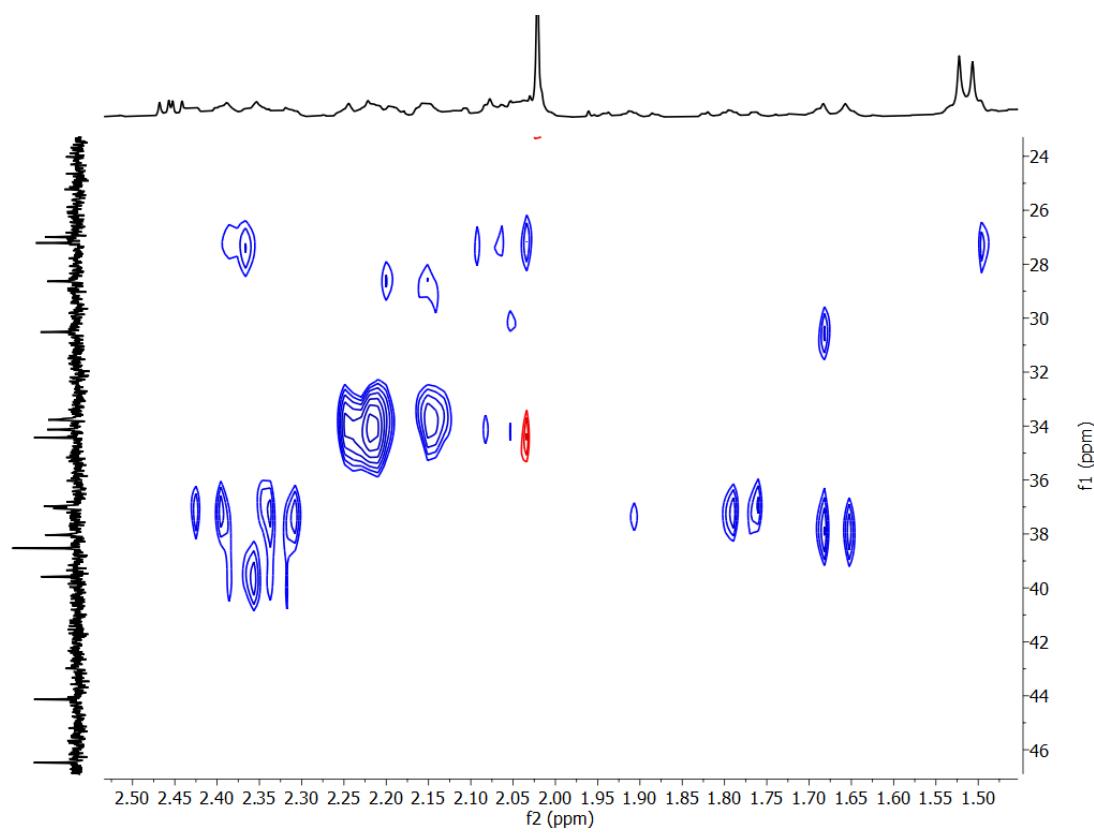
**Figure S79:** HSQC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 5



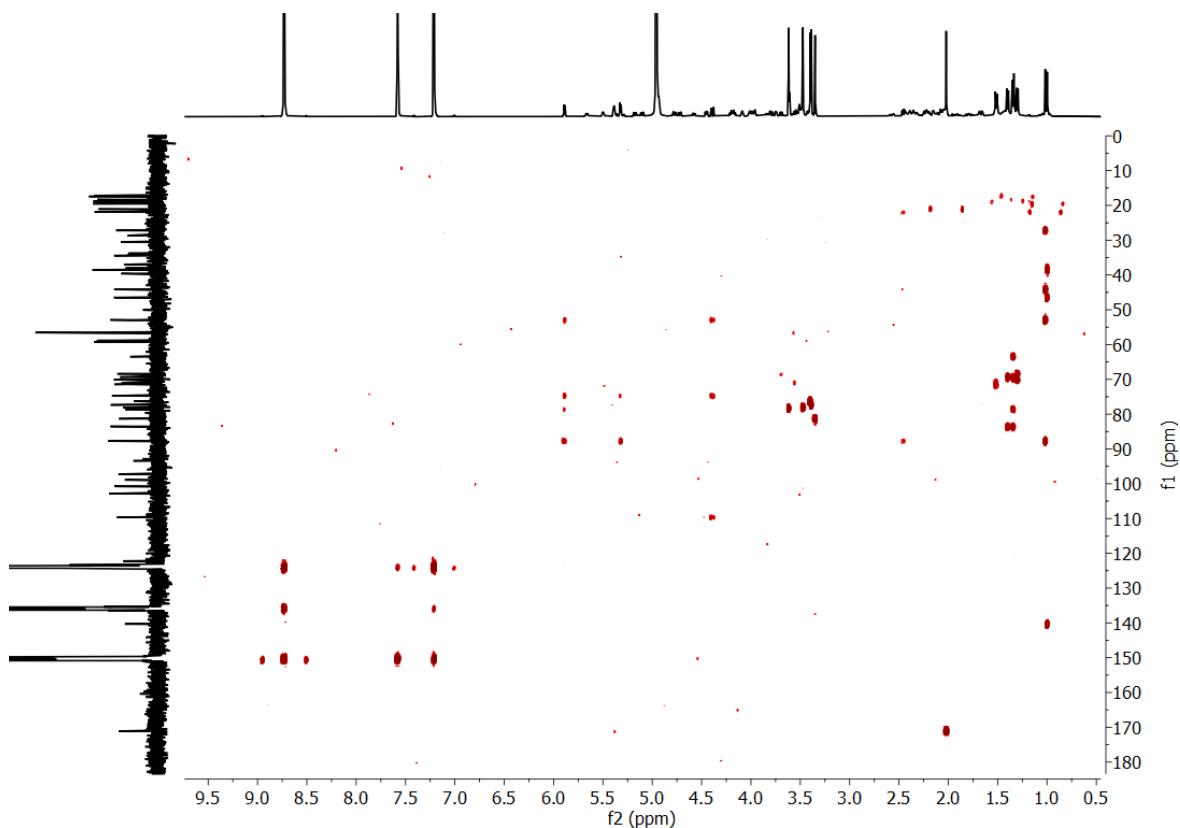
**Figure S80:** HSQC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 5



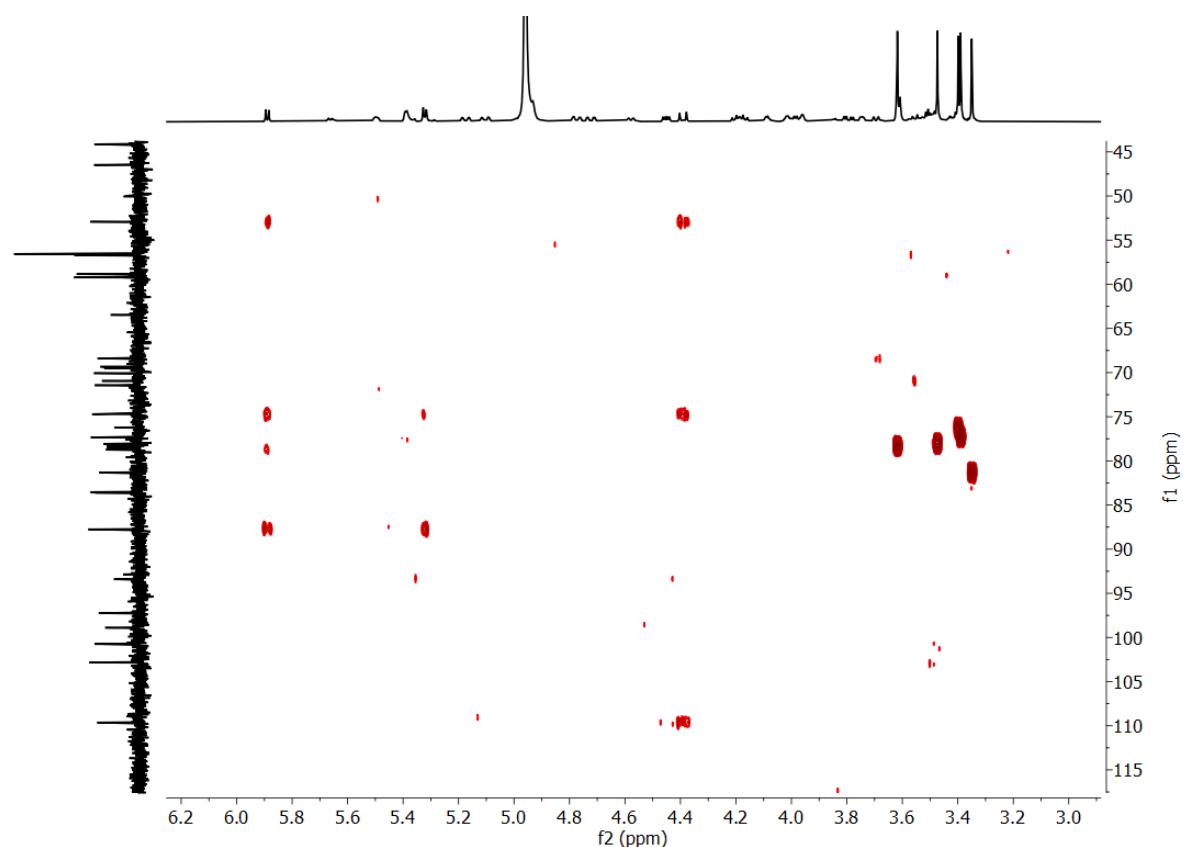
**Figure S81:** HSQC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 5



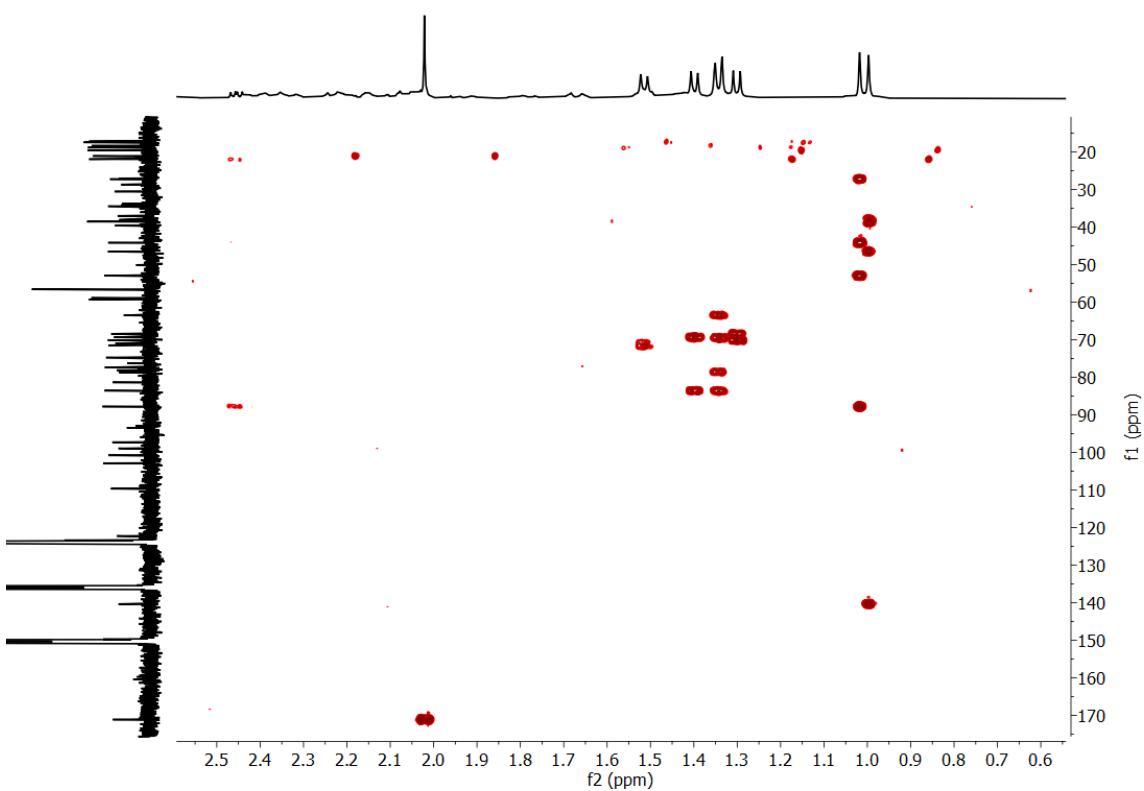
**Figure S82:** HMBC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 5 in pyridine-d<sub>5</sub>, 400 MHz



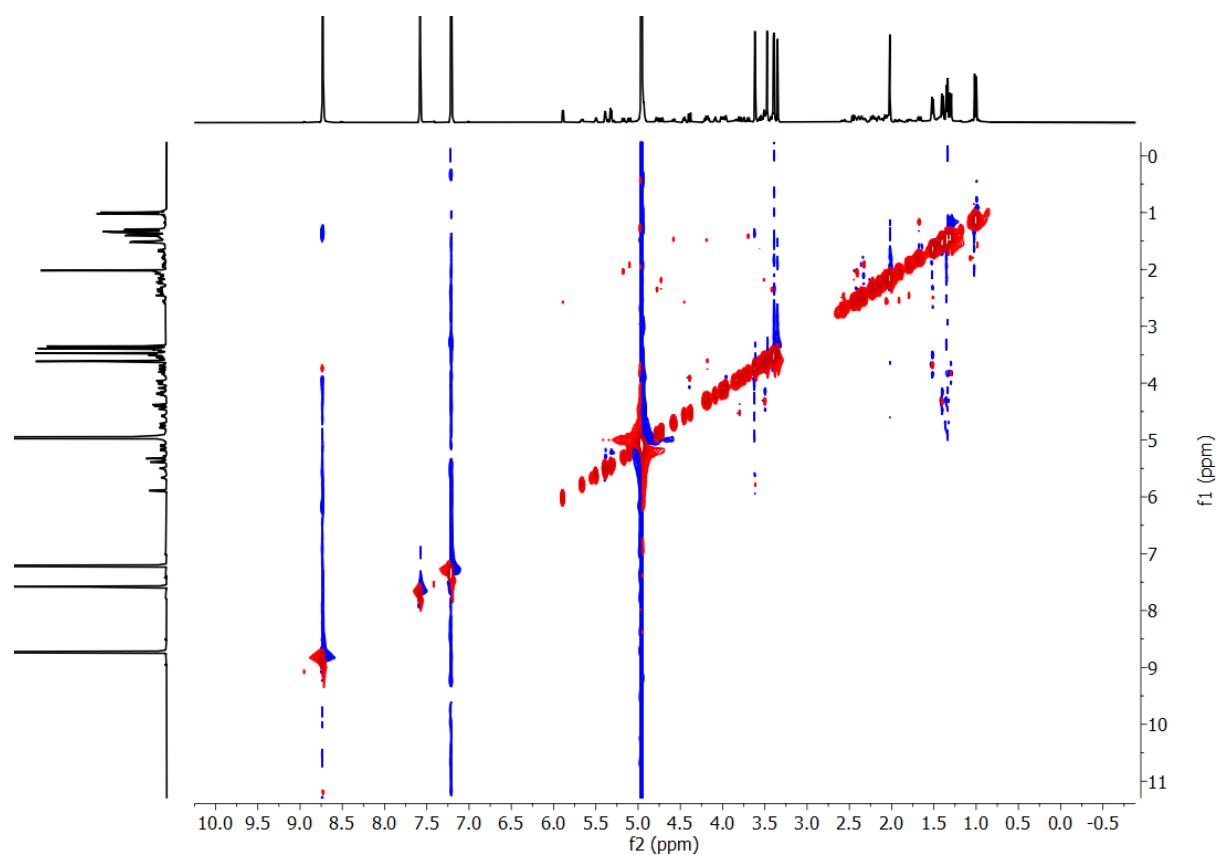
**Figure S83:** HMBC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 5



**Figure S84:** HMBC spectrum (400 and 100 MHz, pyridine-d<sub>5</sub>) of compound 5



**Figure S85:** COSY spectrum (400 MHz, pyridine-d<sub>5</sub>) of compound 5



**Figure S86. Effect of 1, 2, 3 and 5 on cell viability of stimulated J774 macrophages.** Different concentrations of the compounds (50 - 200  $\mu$ M) or gentian violet (GV; 10  $\mu$ M, positive control) were added to the macrophage culture and incubated for 72 h. Control group (Ctrl) represents untreated cells stimulated with LPS (500 ng/mL) and IFN- $\gamma$  (5 ng/mL). \*Different from the control (Ctrl) group ( $p < 0.0001$ ).

