

## Supporting Information

### Synthesis of an Ethylenediaminetetraacetic Acid-like Ligand Based on Sucrose Scaffold and Complexation and Proton Relaxivity Studies of Its Gadolinium (III) Complex in Solution

Ping Zhang,<sup>1</sup> Cécile Barbot,<sup>2</sup> Ramakrishna Gandikota,<sup>2</sup> Cenxiao Li,<sup>1</sup> Laura Gouriou,<sup>2</sup> Géraldine Gouhier,<sup>2,\*</sup> Chang-Chun Ling<sup>1,\*</sup>

<sup>1</sup>Department of Chemistry, University of Calgary, 2500 University Drive NW, Calgary, Alberta T2N 1N4, Canada

<sup>2</sup>Univ Rouen Normandie, INSA Rouen Normandie, CNRS, Normandie Univ, COBRA UMR 6014, INC3M FR 3038, F-76000 Rouen, France

E-mail: [ccling@ucalgary.ca](mailto:ccling@ucalgary.ca), Fax: +1-403-289-9488; [geraldine.gouhier@univ-rouen.fr](mailto:geraldine.gouhier@univ-rouen.fr); Fax: +33-235522959

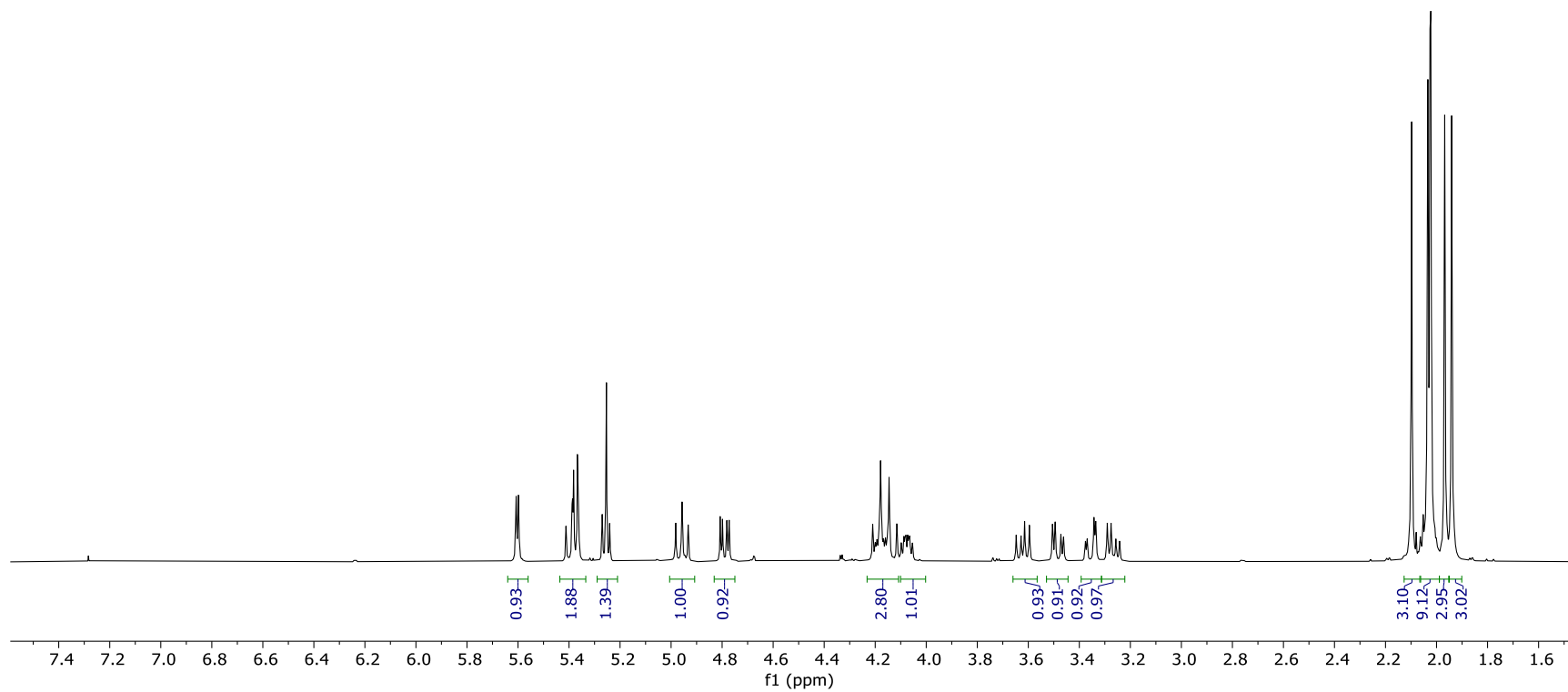
## Contents

|   |    |
|---|----|
| NMR Spectra .....   | 3  |
| <b>Figure S1:</b> $^1\text{H}$ NMR spectrum of compound <b>5</b> in $\text{CDCl}_3$ , 400 MHz, 298 K. ....                                  | 3  |
| <b>Figure S2:</b> $^{13}\text{C}$ NMR spectrum of compound <b>5</b> in $\text{CDCl}_3$ , 100 MHz, 298 K. ....                               | 4  |
| <b>Figure S3:</b> $^1\text{H}$ - $^1\text{H}$ 2D GCOSY NMR spectrum of compound <b>5</b> in $\text{CDCl}_3$ , 400 MHz, 298 K. ....          | 5  |
| <b>Figure S4:</b> $^1\text{H}$ - $^{13}\text{C}$ 2D GHSQC NMR spectrum of compound <b>5</b> in $\text{CDCl}_3$ , 400 MHz, 298 K. ....       | 6  |
| <b>Figure S5:</b> $^1\text{H}$ NMR spectrum of compound <b>7</b> in $\text{CDCl}_3$ , 400 MHz, 298 K. ....                                  | 7  |
| <b>Figure S6:</b> $^{13}\text{C}$ NMR spectrum of compound <b>7</b> in $\text{CDCl}_3$ , 100 MHz, 298 K. ....                               | 8  |
| <b>Figure S7:</b> $^1\text{H}$ - $^1\text{H}$ 2D GCOSY NMR spectrum of compound <b>7</b> in $\text{CDCl}_3$ , 400 MHz, 298 K. ....          | 9  |
| <b>Figure S8:</b> $^1\text{H}$ - $^{13}\text{C}$ 2D GHSQC NMR spectrum of compound <b>7</b> in $\text{CDCl}_3$ , 400 MHz, 298 K. ....       | 10 |
| <b>Figure S9:</b> $^1\text{H}$ NMR spectrum of compound <b>2</b> in $\text{D}_2\text{O}$ , 400 MHz, 298 K. ....                             | 11 |
| <b>Figure S10:</b> $^{13}\text{C}$ NMR spectrum of compound <b>2</b> in $\text{D}_2\text{O}$ , 100 MHz, 298 K. ....                         | 12 |
| <b>Figure S11:</b> $^1\text{H}$ - $^1\text{H}$ 2D GCOSY NMR spectrum of compound <b>2</b> in $\text{D}_2\text{O}$ , 400 MHz, 298 K. ....    | 13 |
| <b>Figure S12:</b> $^1\text{H}$ - $^{13}\text{C}$ 2D GHSQC NMR spectrum of compound <b>2</b> in $\text{D}_2\text{O}$ , 400 MHz, 298 K. .... | 14 |

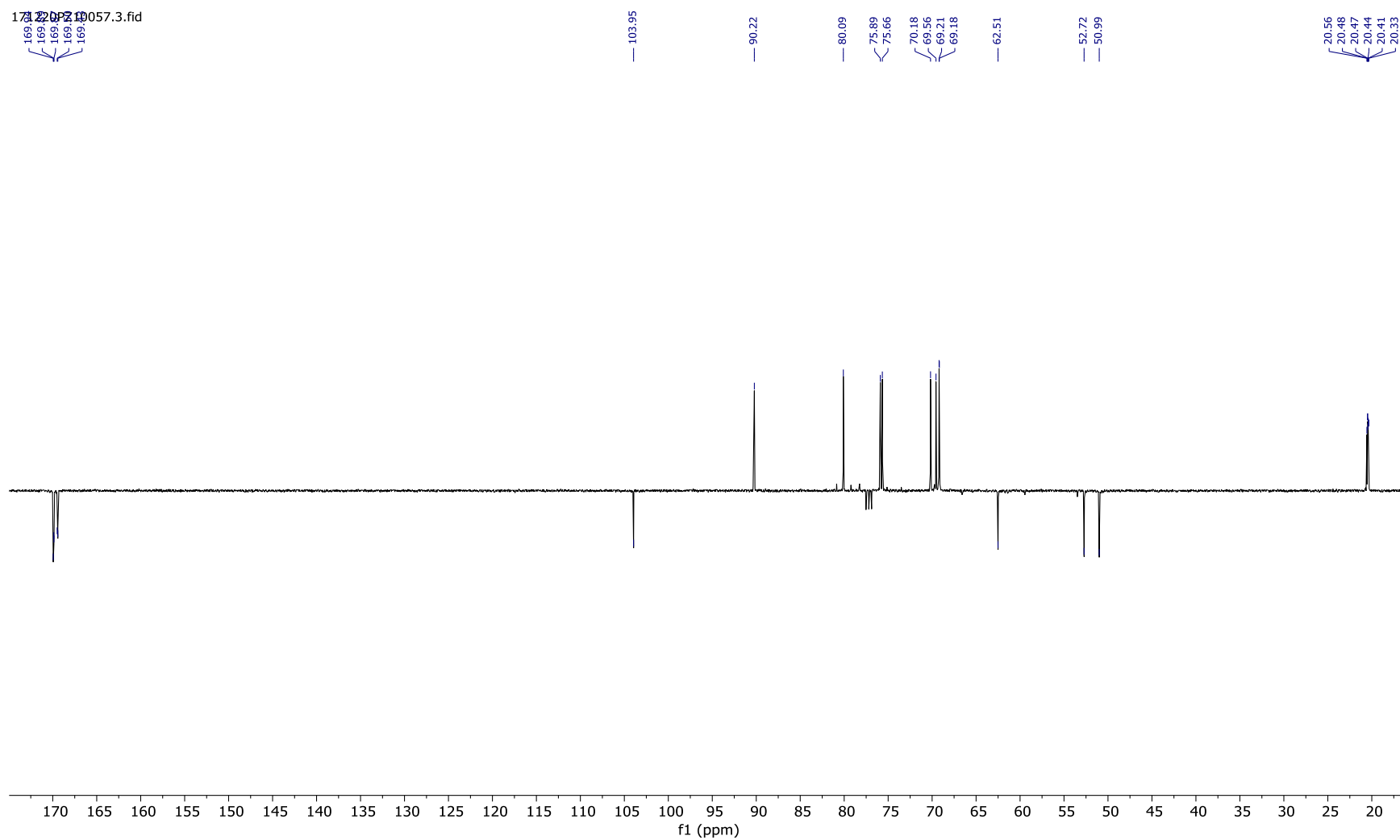
## NMR Spectra

**Figure S1:**  $^1\text{H}$  NMR spectrum of compound **5** in  $\text{CDCl}_3$ , 400 MHz, 298 K.

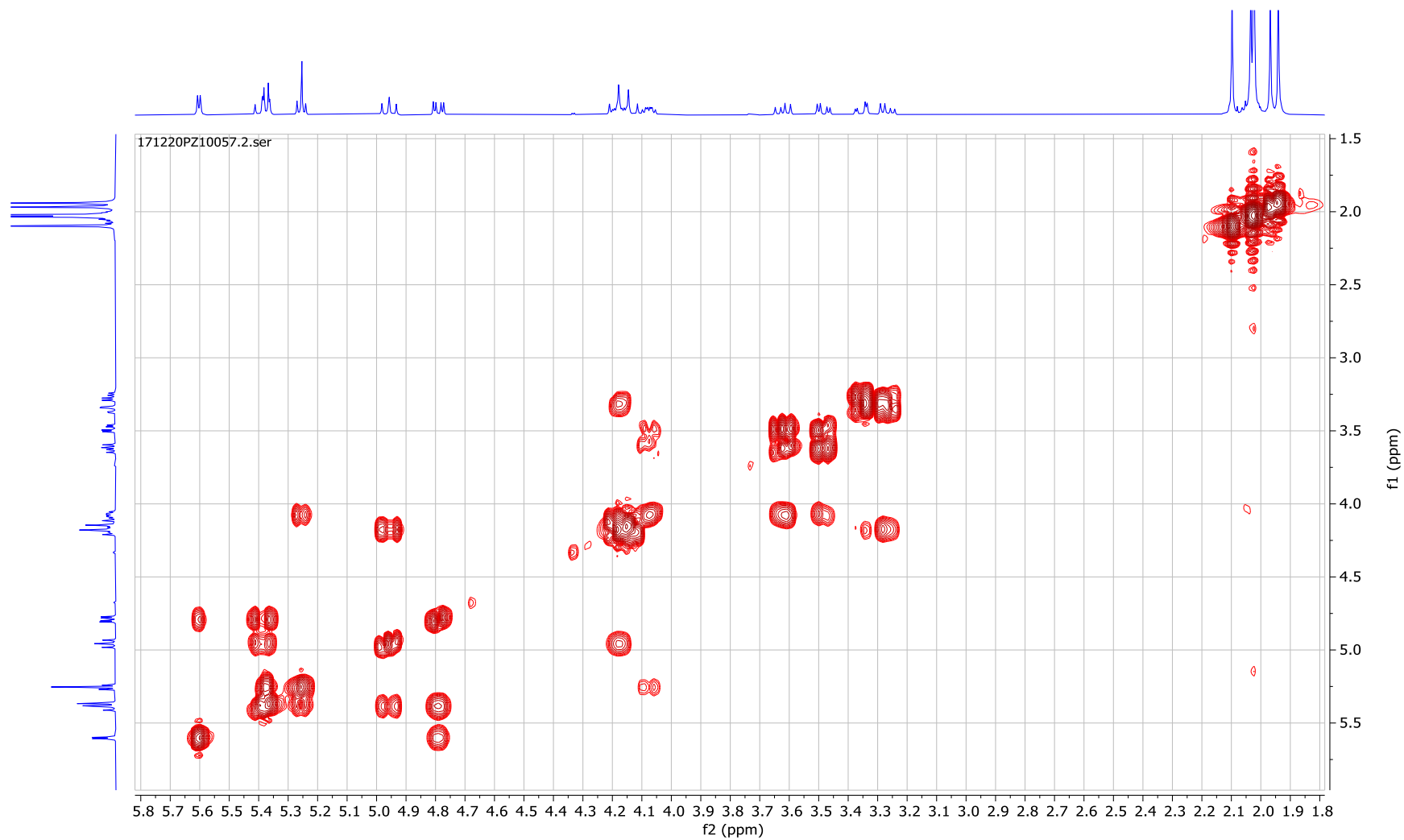
171220PZ10057.1.fid



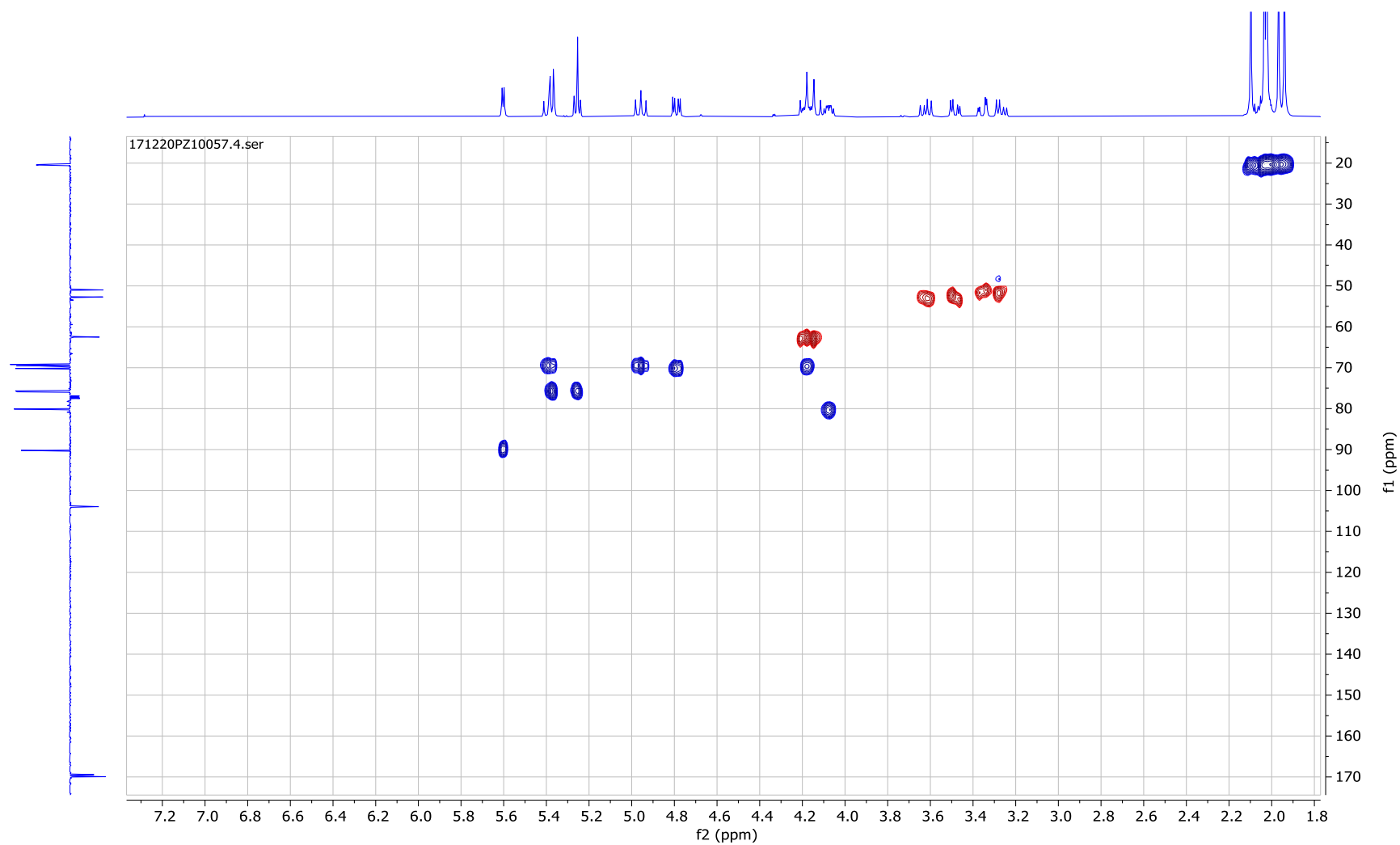
**Figure S2:**  $^{13}\text{C}$  NMR spectrum of compound **5** in  $\text{CDCl}_3$ , 100 MHz, 298 K.



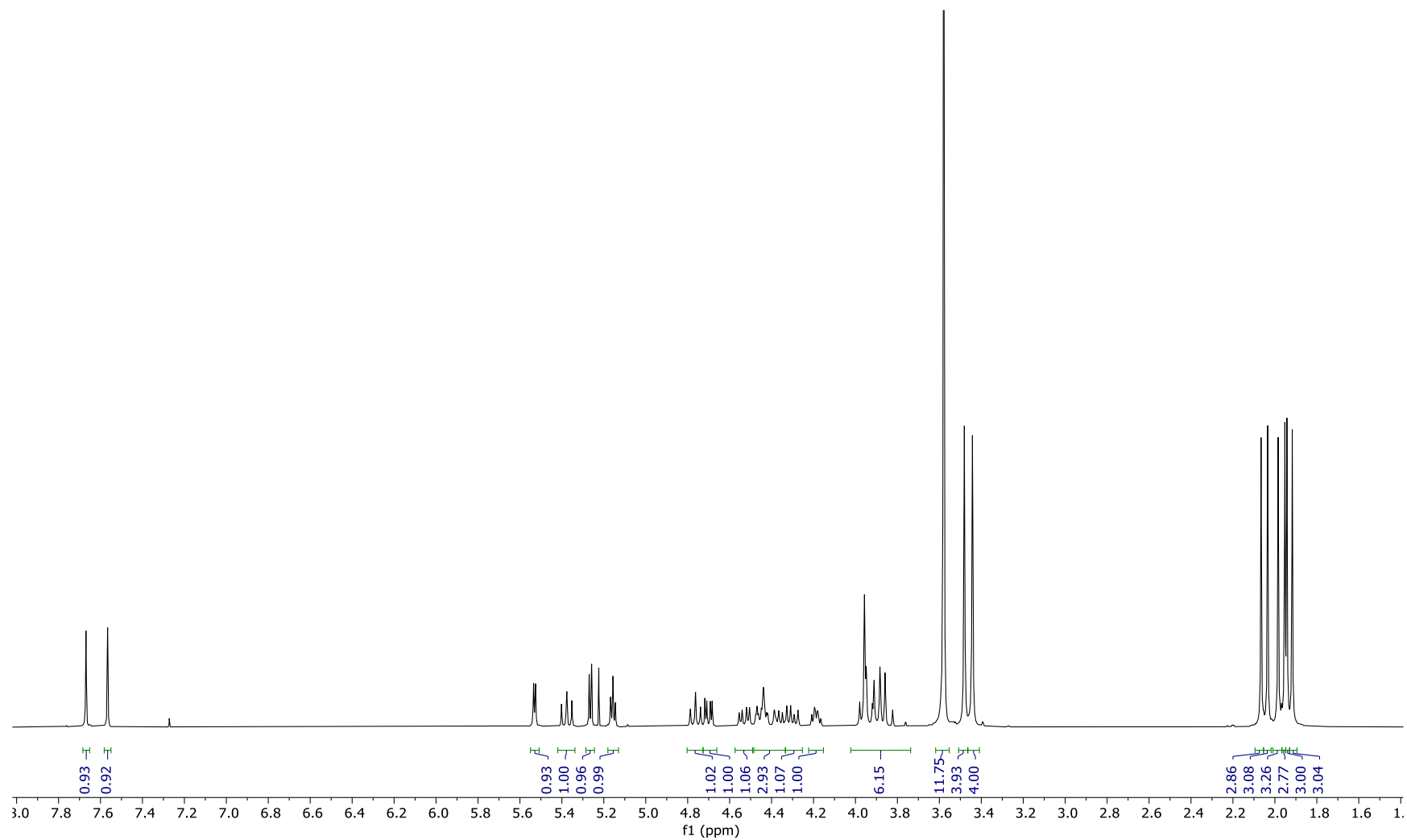
**Figure S3:**  $^1\text{H}$ - $^1\text{H}$  2D GCOSY NMR spectrum of compound **5** in  $\text{CDCl}_3$ , 400 MHz, 298 K.



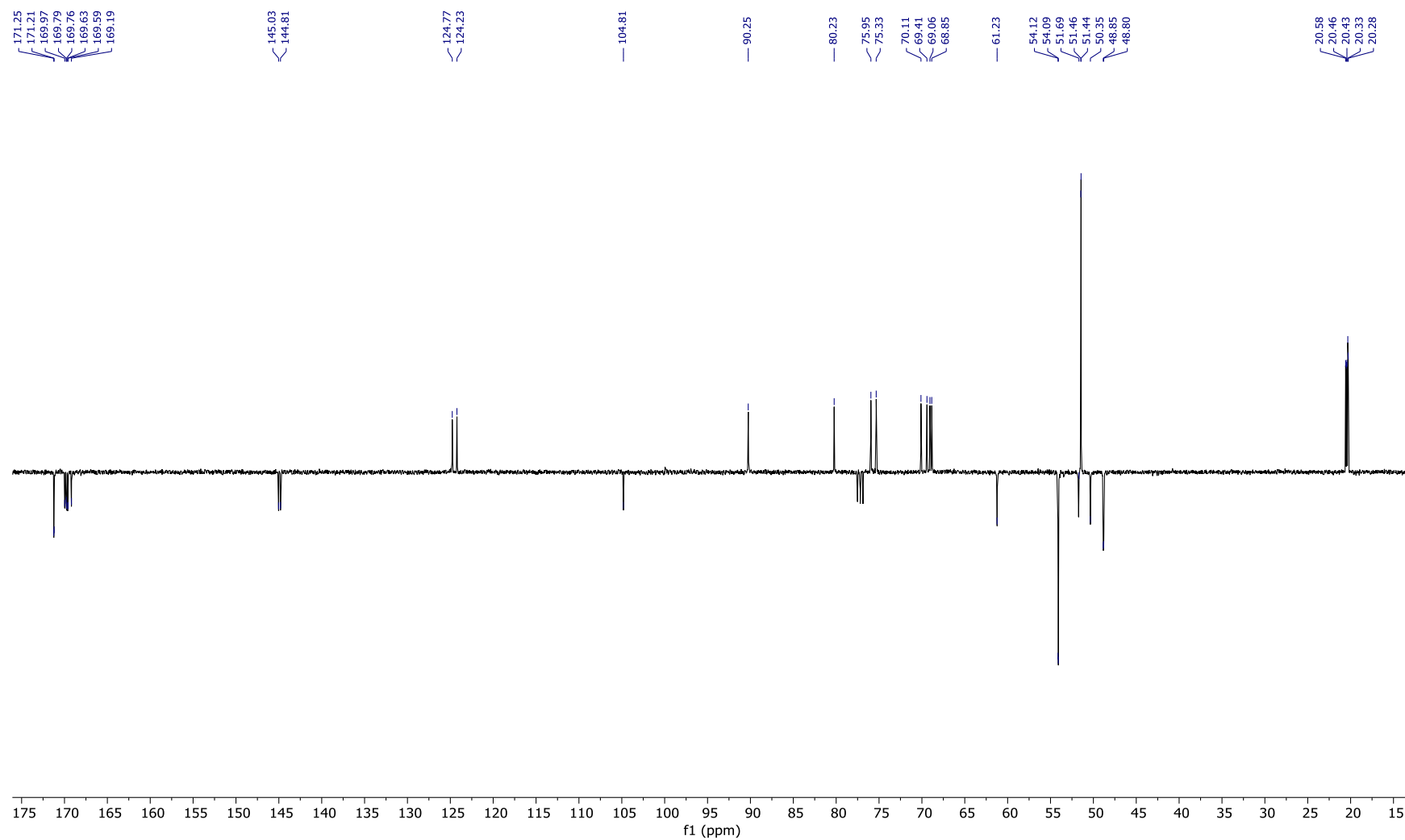
**Figure S4:**  $^1\text{H}$ - $^{13}\text{C}$  2D GHSQC NMR spectrum of compound **5** in  $\text{CDCl}_3$ , 400 MHz, 298 K.



**Figure S5:**  $^1\text{H}$  NMR spectrum of compound **7** in  $\text{CDCl}_3$ , 400 MHz, 298 K.

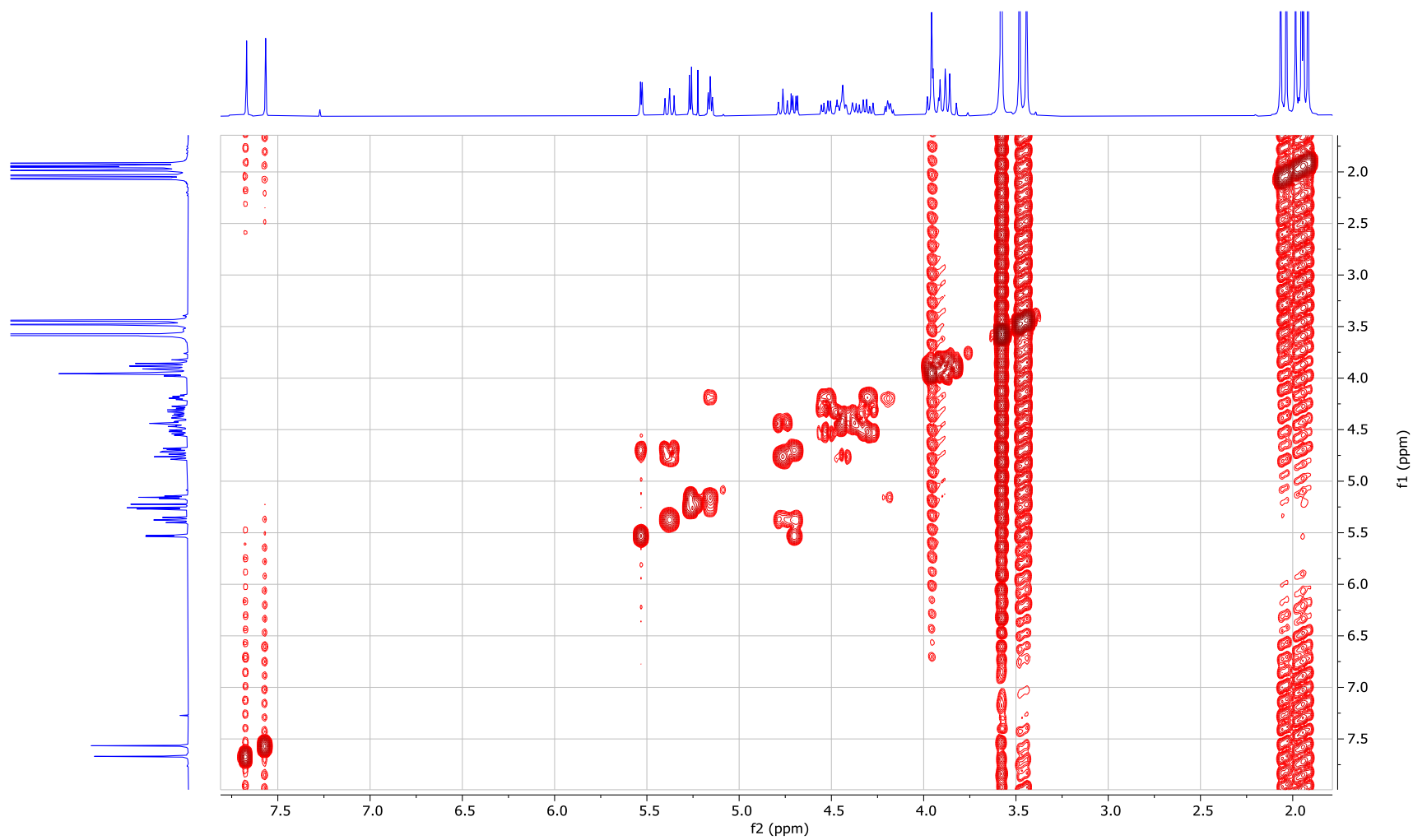


**Figure S6:**  $^{13}\text{C}$  NMR spectrum of compound **7** in  $\text{CDCl}_3$ , 100 MHz, 298 K.

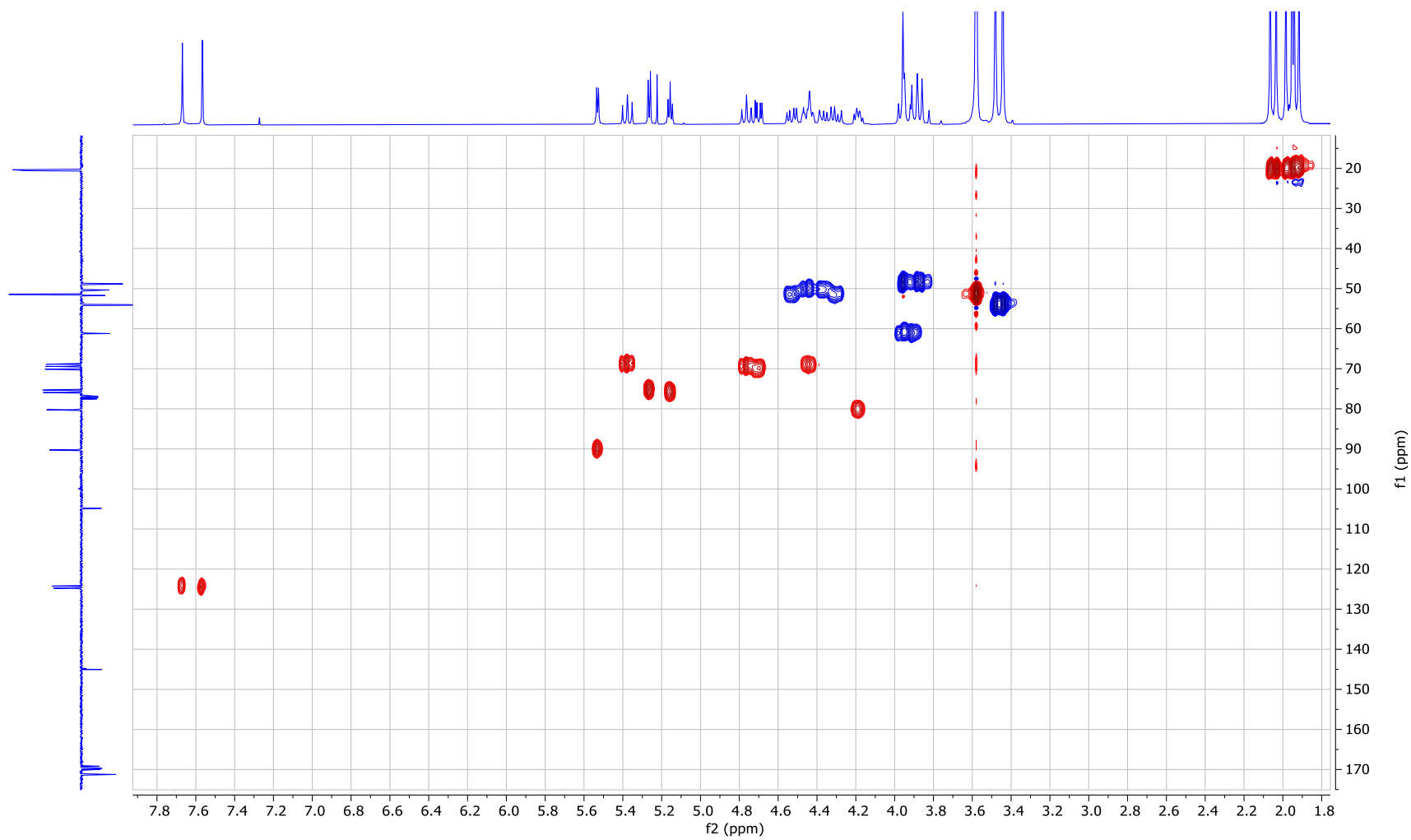




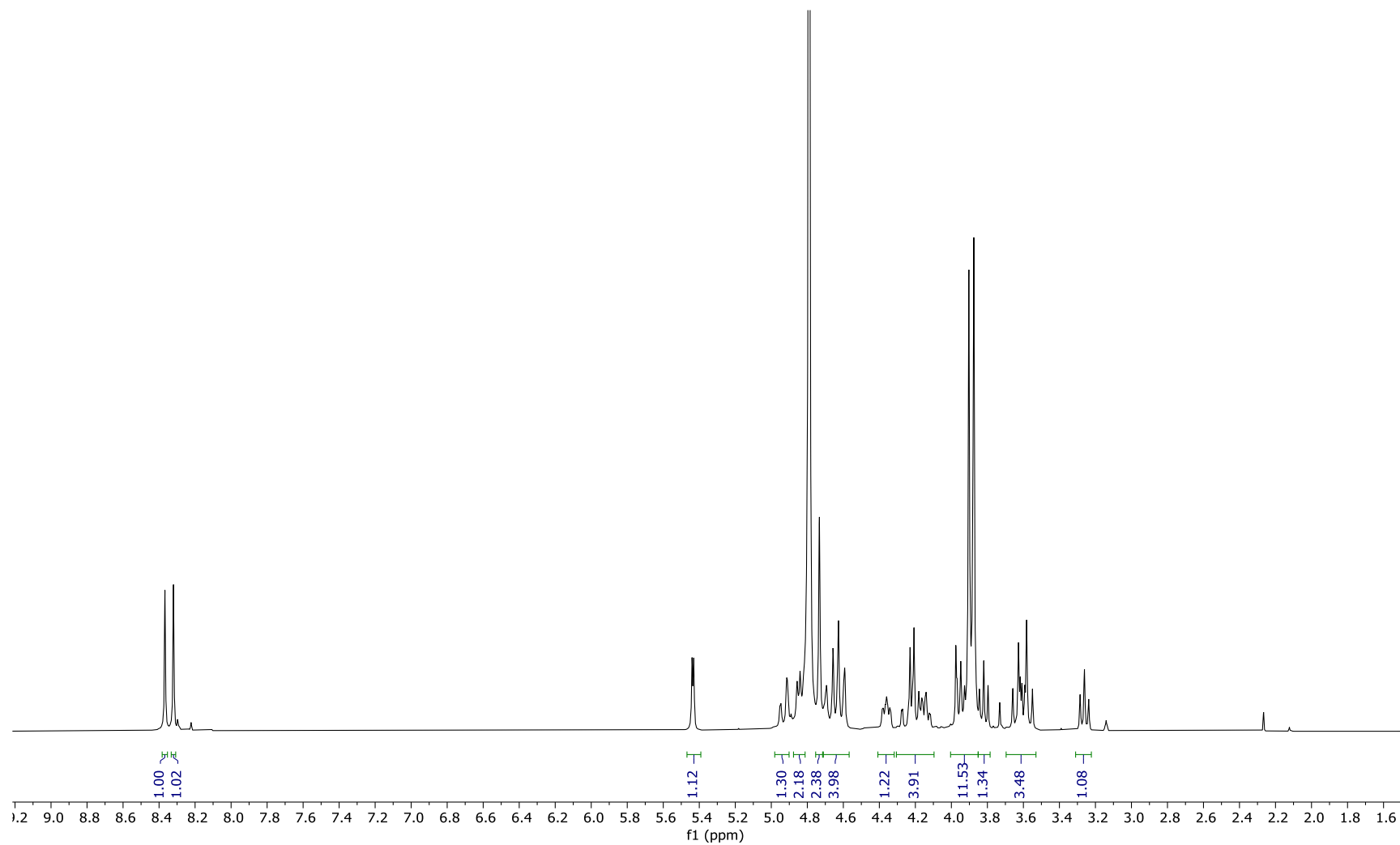
**Figure S7:**  $^1\text{H}$ - $^1\text{H}$  2D GCOSY NMR spectrum of compound **7** in  $\text{CDCl}_3$ , 400 MHz, 298 K.



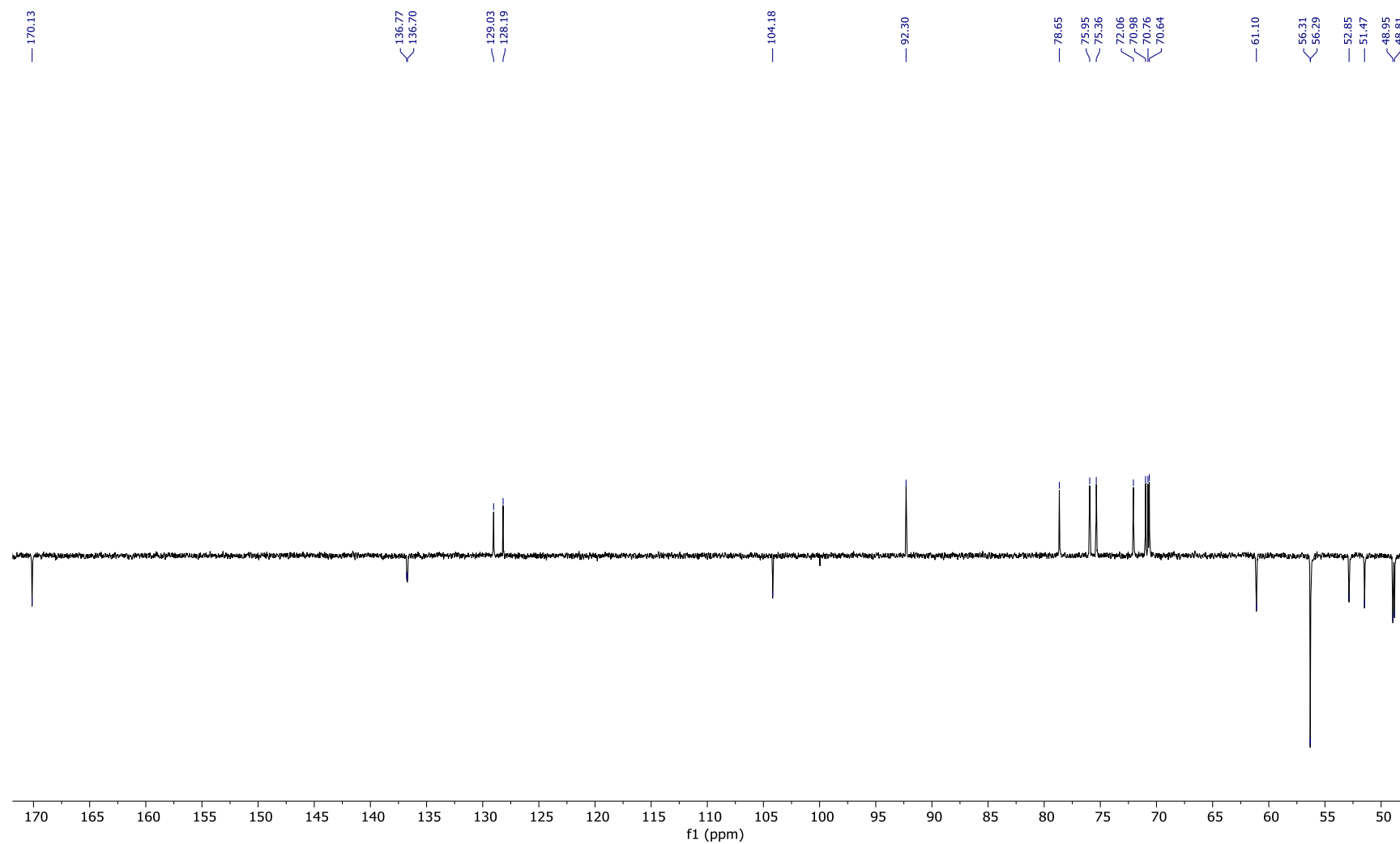
**Figure S8:**  $^1\text{H}$ - $^{13}\text{C}$  2D GHSQC NMR spectrum of compound **7** in  $\text{CDCl}_3$ , 400 MHz, 298 K.



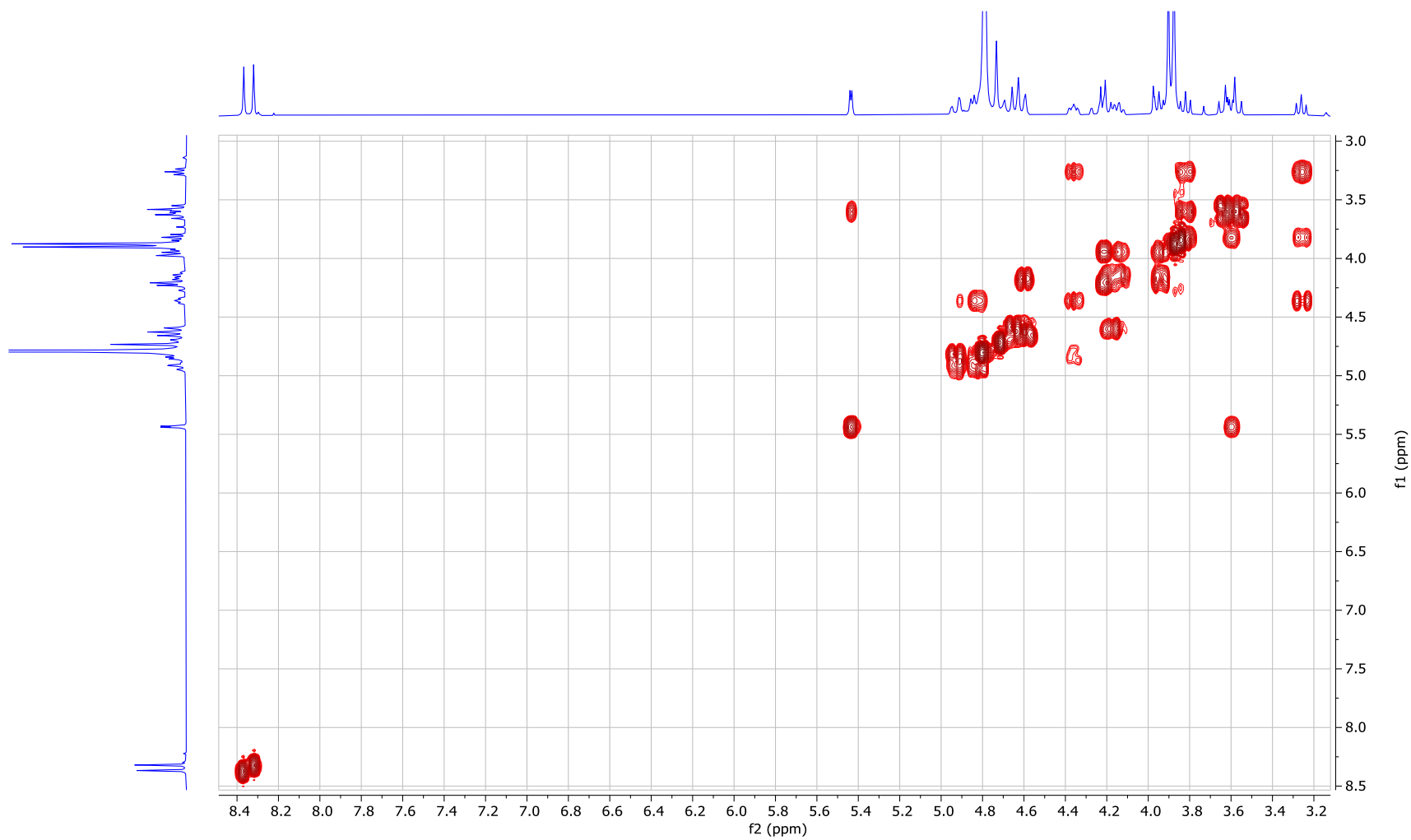
**Figure S9:**  $^1\text{H}$  NMR spectrum of compound **2** in  $\text{D}_2\text{O}$ , 400 MHz, 298 K.



**Figure S10:**  $^{13}\text{C}$  NMR spectrum of compound **2** in  $\text{D}_2\text{O}$ , 100 MHz, 298 K.



**Figure S11:**  $^1\text{H}$ - $^1\text{H}$  2D GCOSY NMR spectrum of compound **2** in  $\text{D}_2\text{O}$ , 400 MHz, 298 K.



**Figure S12:**  $^1\text{H}$ - $^{13}\text{C}$  2D GHSQC NMR spectrum of compound **2** in  $\text{D}_2\text{O}$ , 400 MHz, 298 K.

