

## ***Supporting Information***

### **Isolation, Structure Elucidation, and Biological Evaluation of 16,23-Epoxycucurbitacin Constituents from *Eleaocarpus chinensis*<sup>#</sup>**

Li Pan,<sup>†</sup> Yeonjoong Yong,<sup>‡</sup> Ye Deng,<sup>†</sup> Daniel D. Lantvit,<sup>§</sup> Tran Ngoc Ninh,<sup>⊥</sup> Heebyung Chai,<sup>†</sup> Esperanza J. Carcache de Blanco,<sup>‡</sup> Djaja D. Soejarto,<sup>§,||</sup> Steven M. Swanson,<sup>§</sup> and A. Douglas Kinghorn<sup>\*,†</sup>

<sup>#</sup> Dedicated to Dr. Gordon M. Cragg, formerly of the National Cancer Institute, Frederick, Maryland, for his pioneering work on the development of natural product anticancer agents.

<sup>†</sup> Division of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, The Ohio State University, Columbus, Ohio 43210, United States

<sup>‡</sup> Division of Pharmacy Practice and Administration, College of Pharmacy, The Ohio State University, Columbus, Ohio 43210, United States

<sup>§</sup> Program for Collaborative Research in the Pharmaceutical Science and Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, University of Illinois at Chicago, Chicago, Illinois 60612, United States

<sup>⊥</sup> Institute of Ecology and Biological Resources, Vietnamese Academy of Science and Technology, Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam

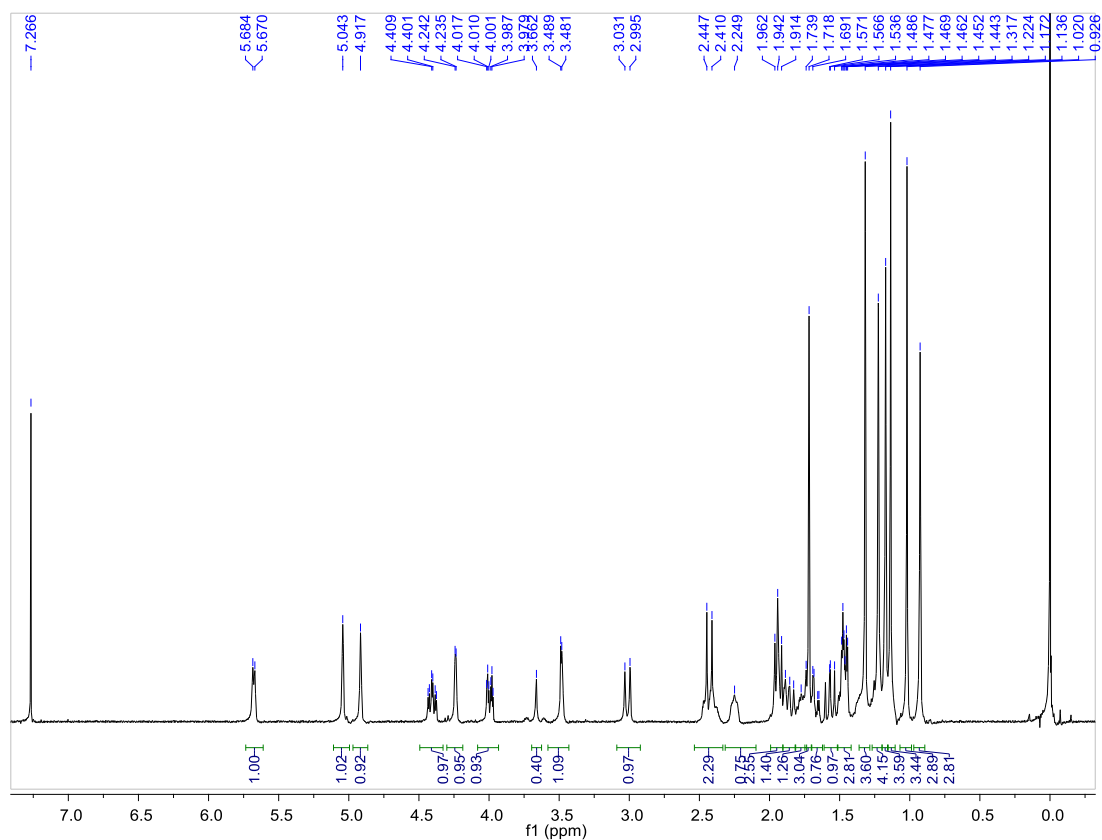
<sup>||</sup> Department of Botany, Field Museum of Natural History, 1400 S. Lake Shore Drive, Chicago, Illinois 60605, United States

### Supporting information list.

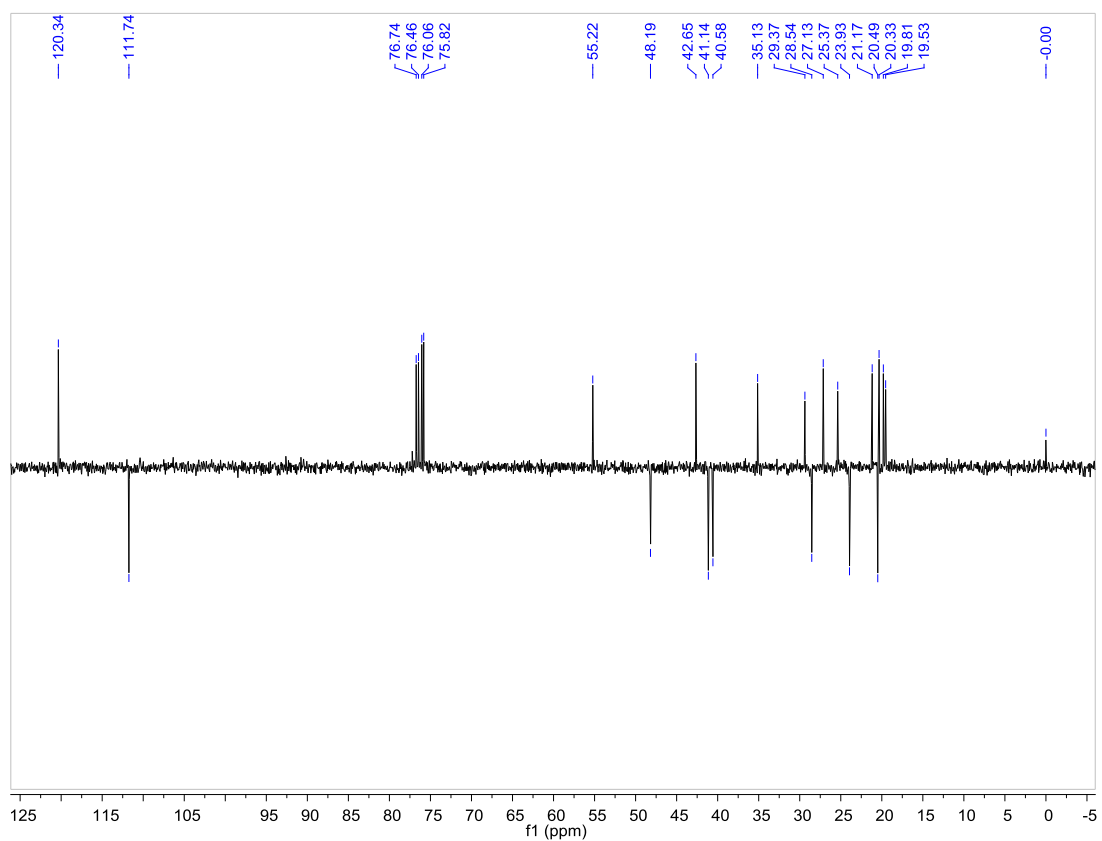
- Figure S1.**  $^1\text{H}$  NMR spectrum of compound **1** ( $\text{CDCl}_3$ , 400 MHz).
- Figure S2.**  $^{13}\text{C}$  DEPT 135 spectrum of compound **1** ( $\text{CDCl}_3$ , 100 MHz).
- Figure S3.**  $^{13}\text{C}$  NMR spectrum of compound **1** ( $\text{CDCl}_3$ , 100 MHz).
- Figure S4.** HSQC spectrum of compound **1** ( $\text{CDCl}_3$ , 400 MHz).
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- Figure S8.**  $^1\text{H}$  NMR spectrum of compound **2** ( $\text{CDCl}_3$ , 400 MHz).
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- Figure S15.**  $^1\text{H}$  NMR spectrum of compound **3** ( $\text{CDCl}_3$ , 400 MHz).
- Figure S16.**  $^{13}\text{C}$  DEPT 135 spectrum of compound **3** ( $\text{CDCl}_3$ , 100 MHz).
- Figure S17.**  $^{13}\text{C}$  NMR spectrum of compound **3** ( $\text{CDCl}_3$ , 100 MHz).
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- Figure S22.**  $^1\text{H}$  NMR spectrum of compound **4** ( $\text{CDCl}_3$ , 400 MHz).
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- Figure S24.**  $^{13}\text{C}$  NMR spectrum of compound **4** ( $\text{CDCl}_3$ , 100 MHz).
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- Figure S26.** HMBC spectrum of compound **4** ( $\text{CDCl}_3$ , 400 MHz).
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- Figure S29.**  $^1\text{H}$  NMR spectrum of compound **5** ( $\text{CDCl}_3$ , 400 MHz).
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- Figure S31.** HSQC spectrum of compound **5** ( $\text{CDCl}_3$ , 400 MHz).
- Figure S32.** HMBC spectrum of compound **5** ( $\text{CDCl}_3$ , 400 MHz).
- Figure S33.**  $^1\text{H}$  NMR spectrum of compound **6** ( $\text{CDCl}_3$ , 400 MHz).
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- Figure S37.**  $^1\text{H}$  NMR spectrum of compound **7** ( $\text{CDCl}_3$ , 400 MHz).
- Figure S38.**  $^{13}\text{C}$  NMR spectrum of compound **7** ( $\text{CDCl}_3$ , 100 MHz).
- Figure S39.** HSQC spectrum of compound **7** ( $\text{CDCl}_3$ , 400 MHz).
- Figure S40.** HMBC spectrum of compound **7** ( $\text{CDCl}_3$ , 400 MHz).
- Figure S41.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7** ( $\text{CDCl}_3$ , 400 MHz).

- Figure S42.**  $^1\text{H}$  NMR spectrum of compound **8** ( $\text{CDCl}_3$ , 400 MHz).
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- Figure S46.**  $^1\text{H}$  NMR spectrum of (*R*)-MTPA ester of compound **1** (pyridine-*d*<sub>5</sub>, 400 MHz).
- Figure S47.**  $^1\text{H}$  NMR spectrum of (*S*)-MTPA ester of compound **1** (pyridine-*d*<sub>5</sub>, 400 MHz).
- Figure S48.**  $^1\text{H}$  NMR spectrum of (*R*)-MTPA ester of compound **2** (pyridine-*d*<sub>5</sub>, 400 MHz).
- Figure S49.**  $^1\text{H}$  NMR spectrum of (*S*)-MTPA ester of compound **2** (pyridine-*d*<sub>5</sub>, 400 MHz).
- Figure S50.** Hollow fiber assay testing result for elaeocarpucin C (**3**).

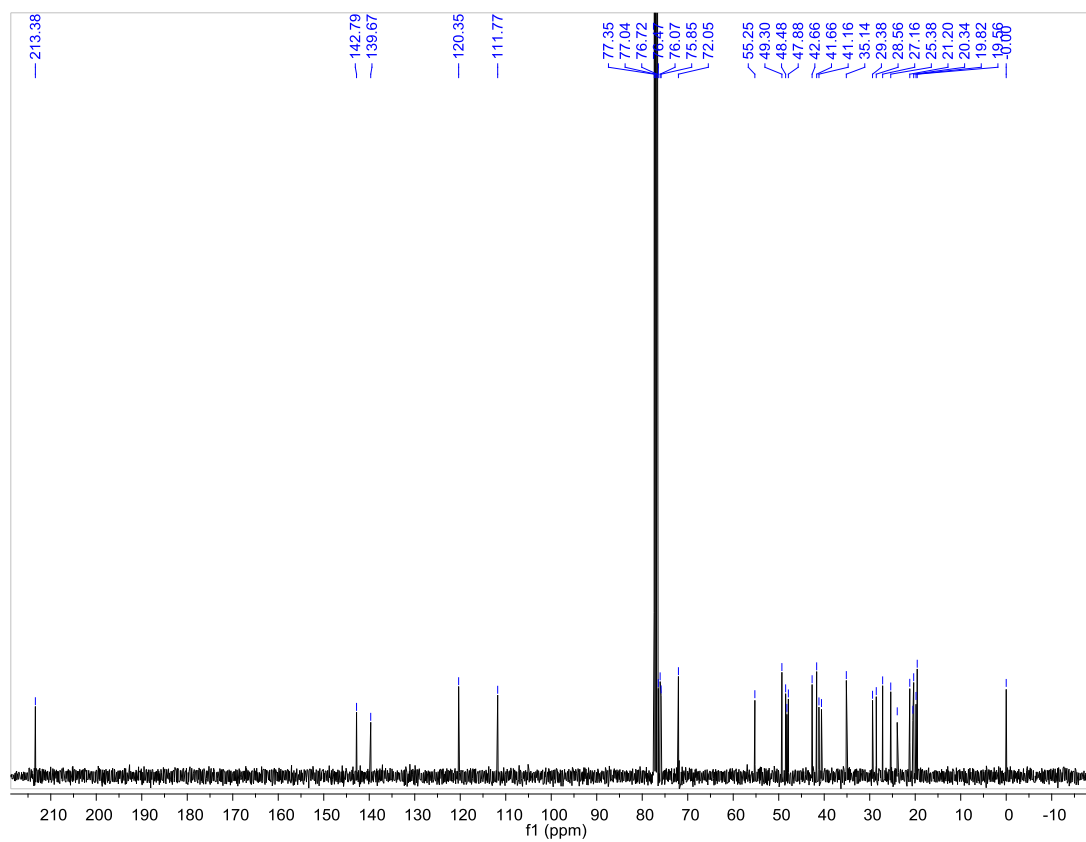
**Figure S1.**  $^1\text{H}$  NMR spectrum of compound **1** ( $\text{CDCl}_3$ , 400 MHz).



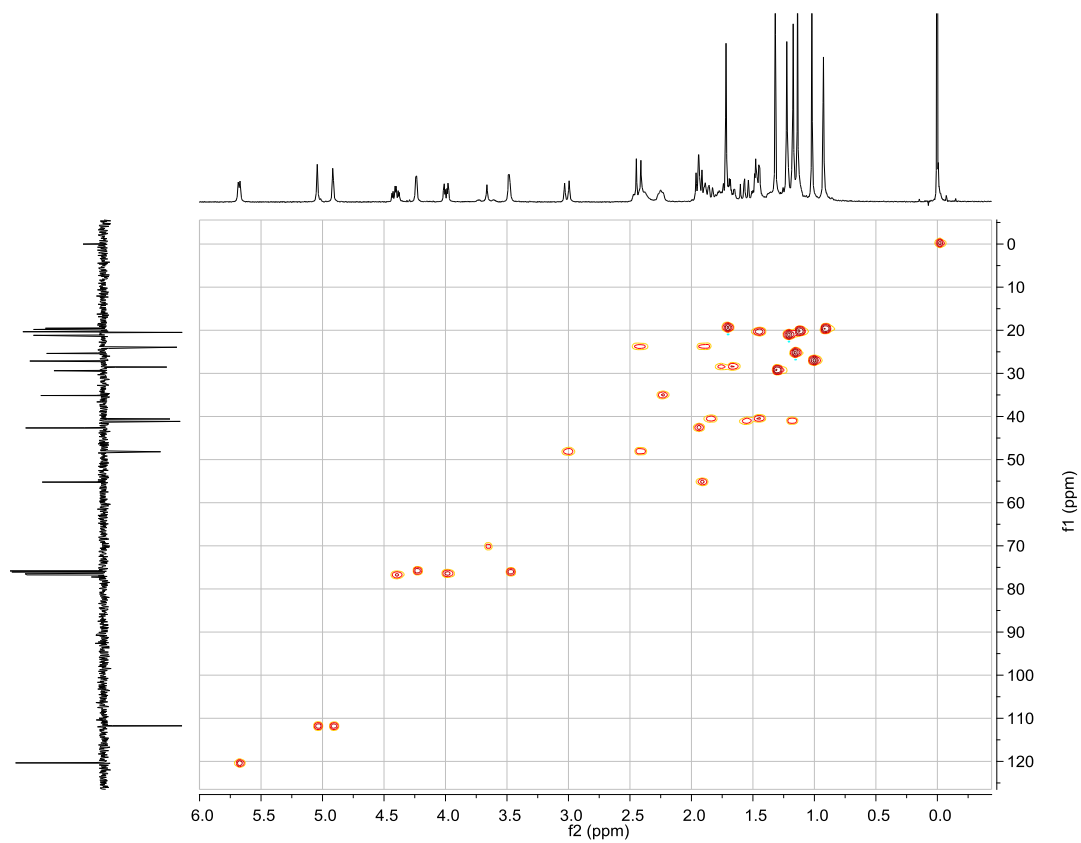
**Figure S2.**  $^{13}\text{C}$  DEPT135 NMR spectrum of compound **1** ( $\text{CDCl}_3$ , 100 MHz).



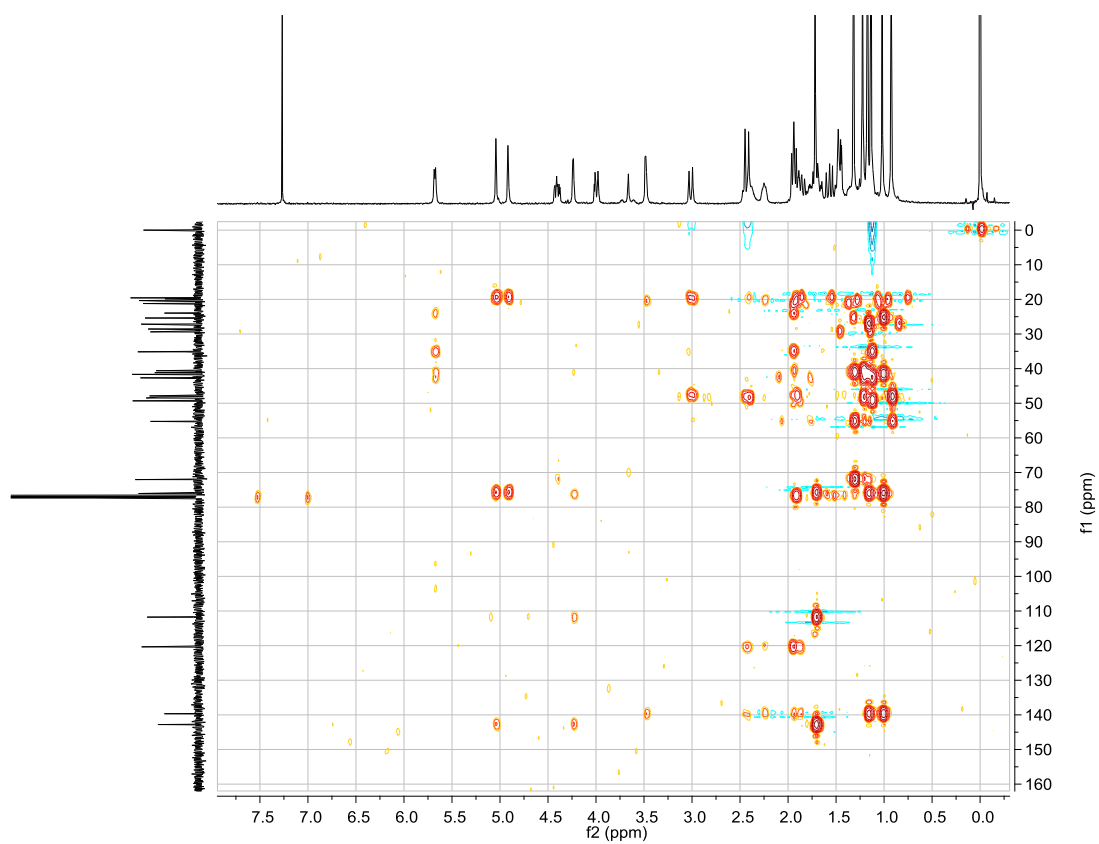
**Figure S3.**  $^{13}\text{C}$  NMR spectrum of compound **1** ( $\text{CDCl}_3$ , 100 MHz).



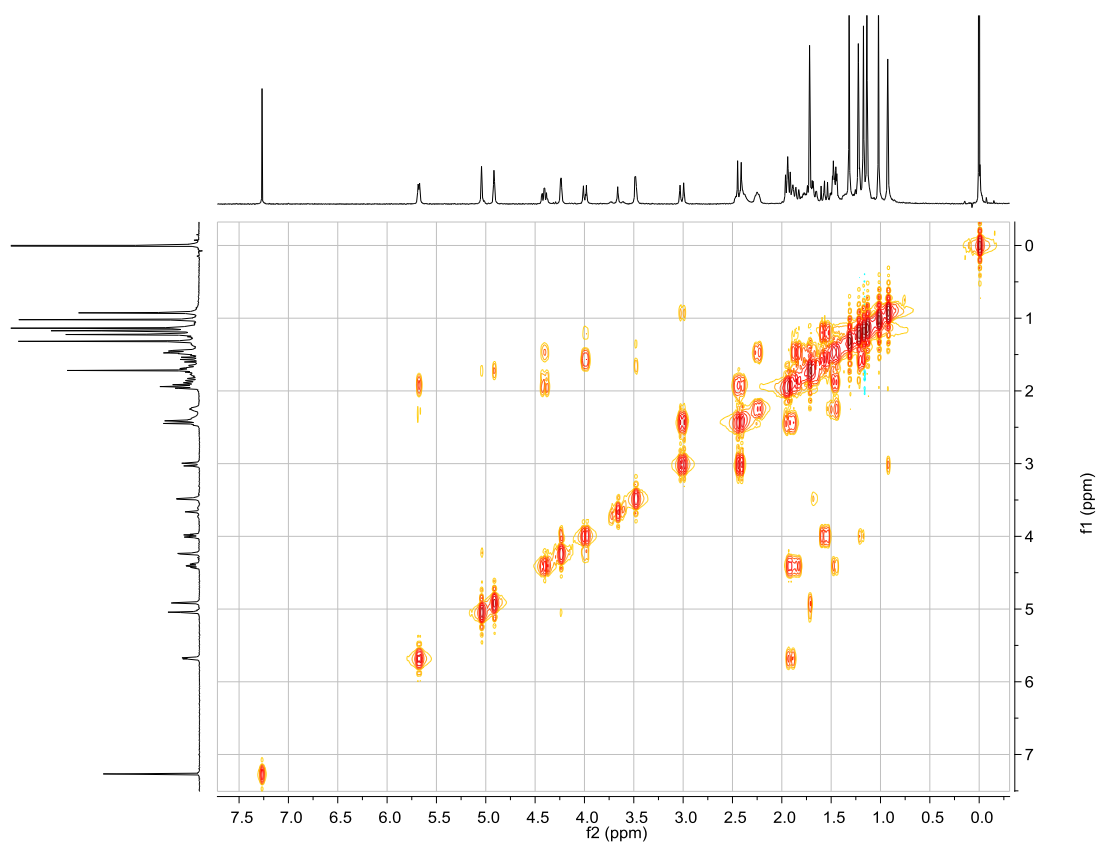
**Figure S4.** HSQC spectrum of compound **1** ( $\text{CDCl}_3$ , 400 MHz).



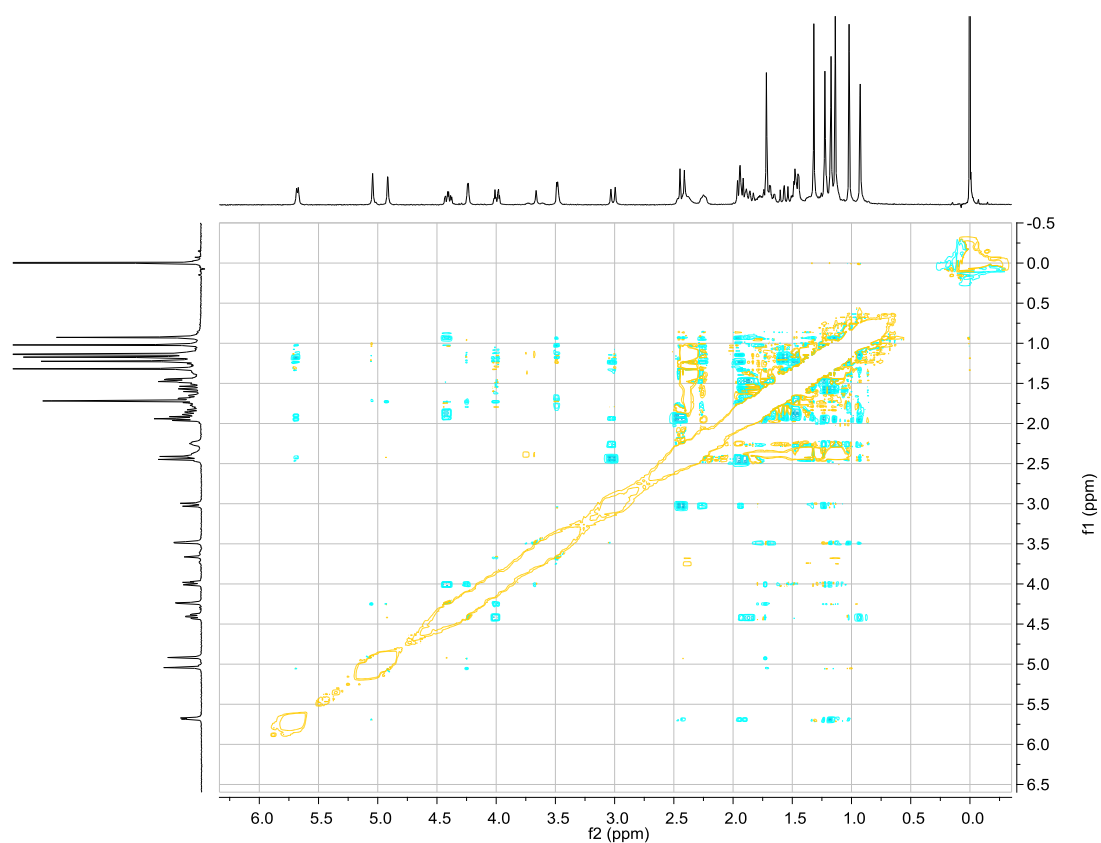
**Figure S5.** HMBC spectrum of compound **1** (CDCl<sub>3</sub>, 400 MHz).



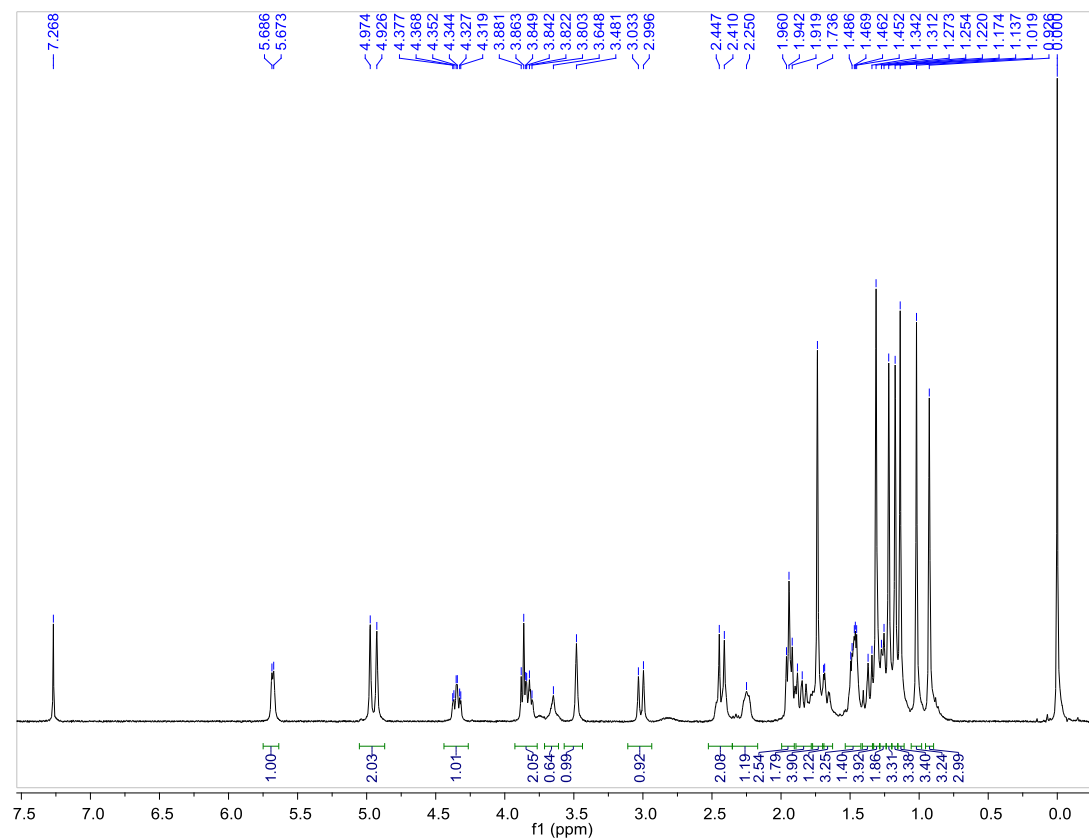
**Figure S6.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **1** (CDCl<sub>3</sub>, 400 MHz).



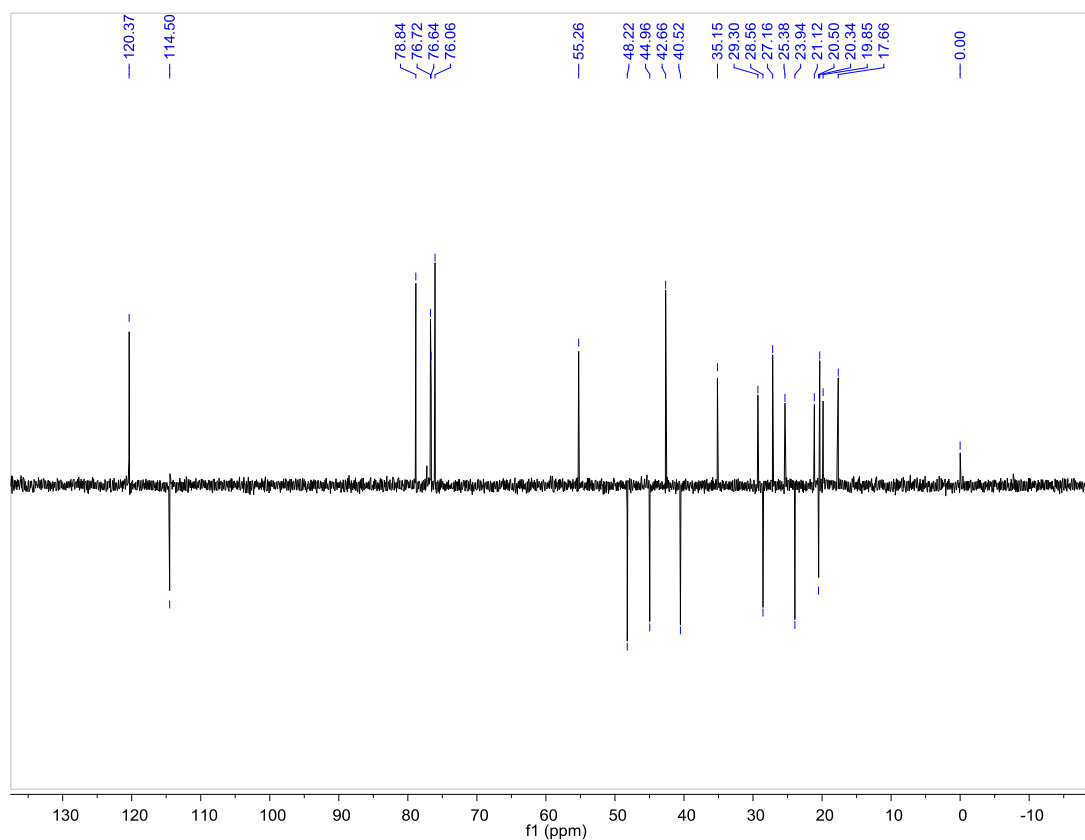
**Figure S7.** NOESY spectrum of compound **1** (CDCl<sub>3</sub>, 400 MHz).



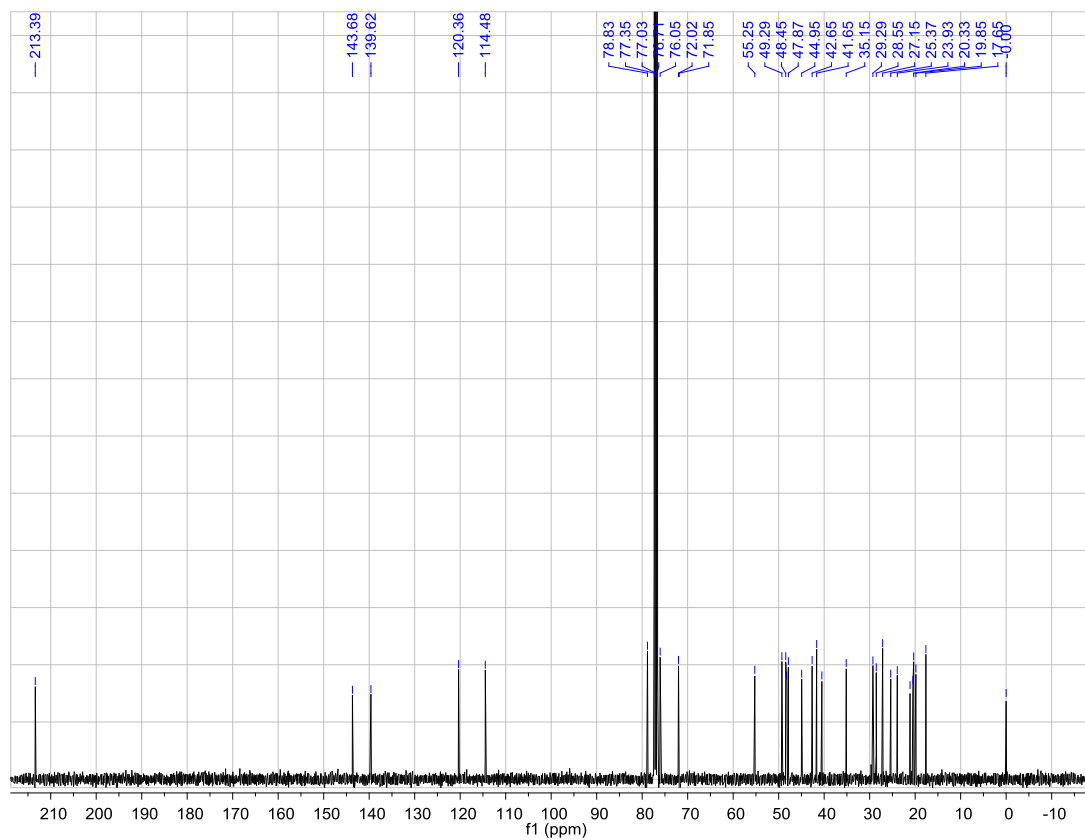
**Figure S8.** <sup>1</sup>H NMR spectrum of compound **2** (CDCl<sub>3</sub>, 400 MHz).



**Figure S9.**  $^{13}\text{C}$  DEPT135 NMR spectrum of compound **2** ( $\text{CDCl}_3$ , 100 MHz).

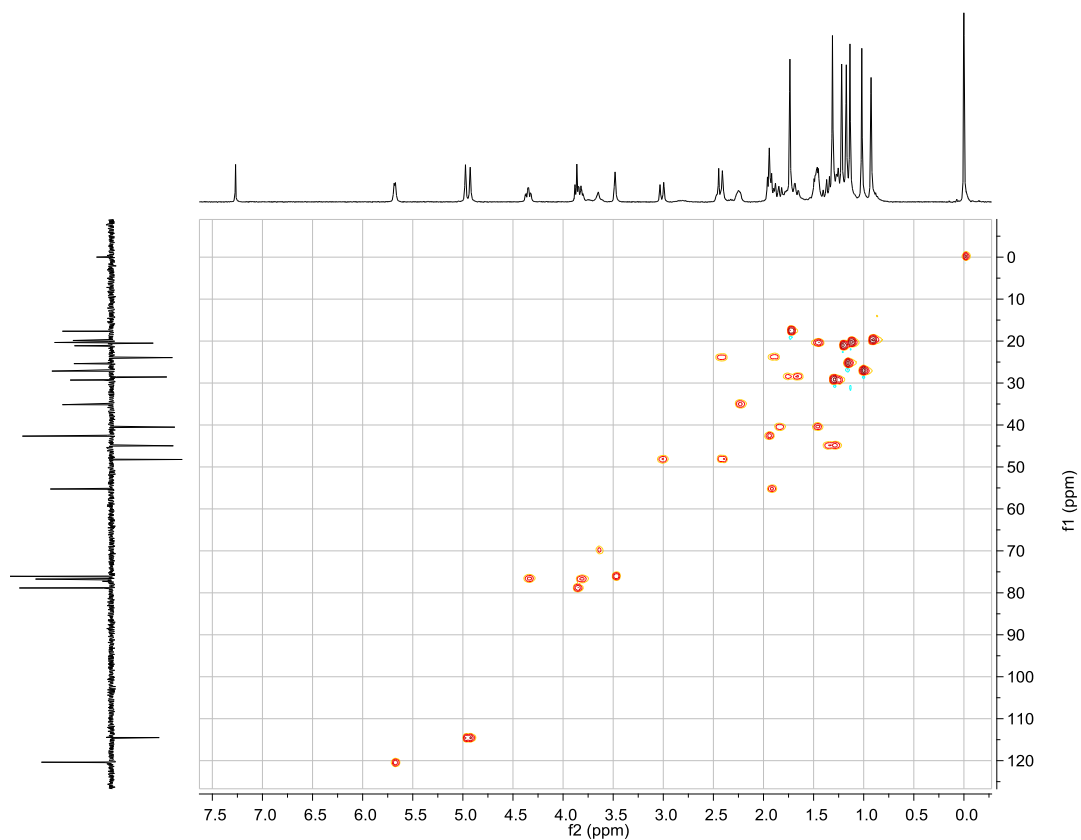


**Figure S10.**  $^{13}\text{C}$  NMR spectrum of compound **2** ( $\text{CDCl}_3$ , 100 MHz).

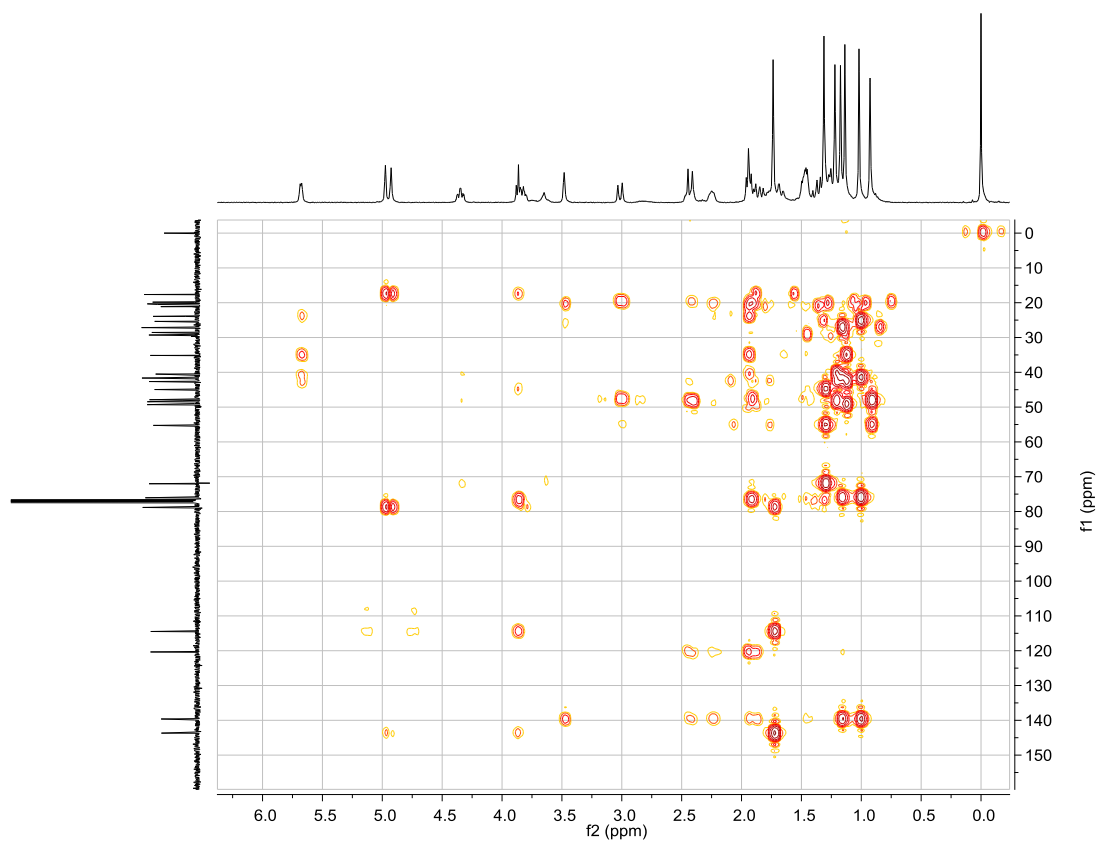




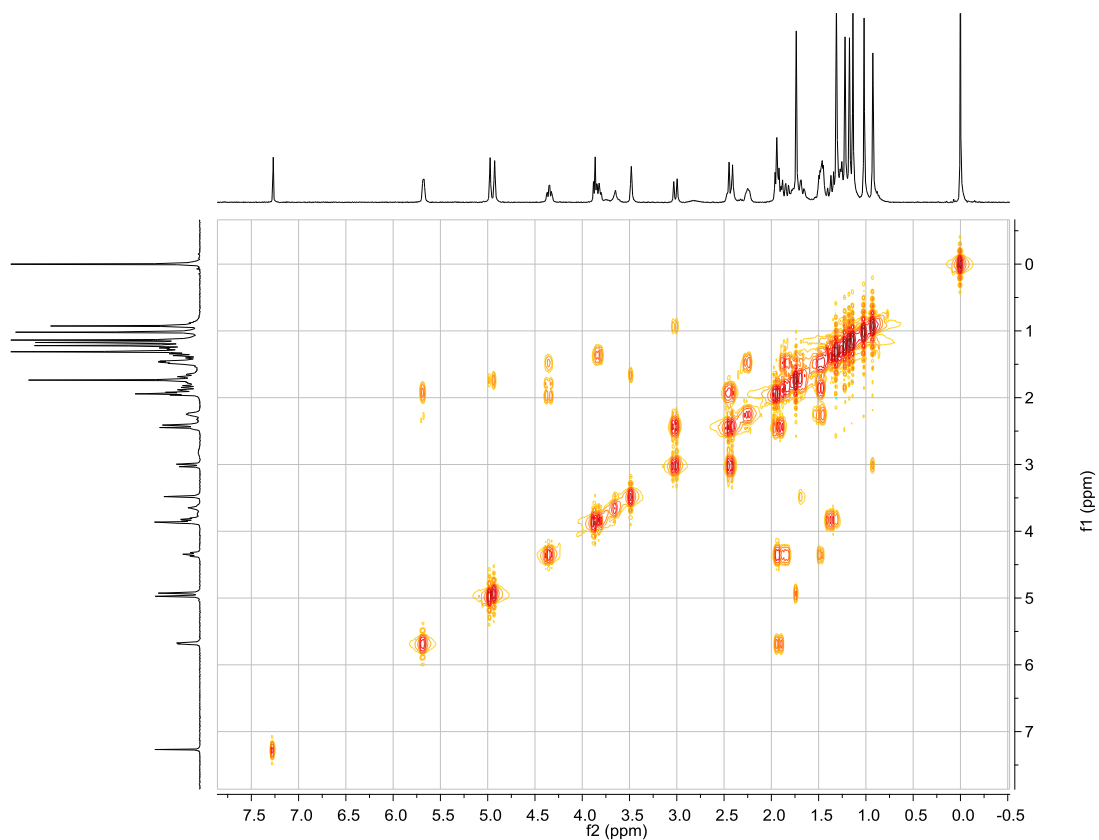
**Figure S11.** HSQC spectrum of compound **2** (CDCl<sub>3</sub>, 400 MHz).



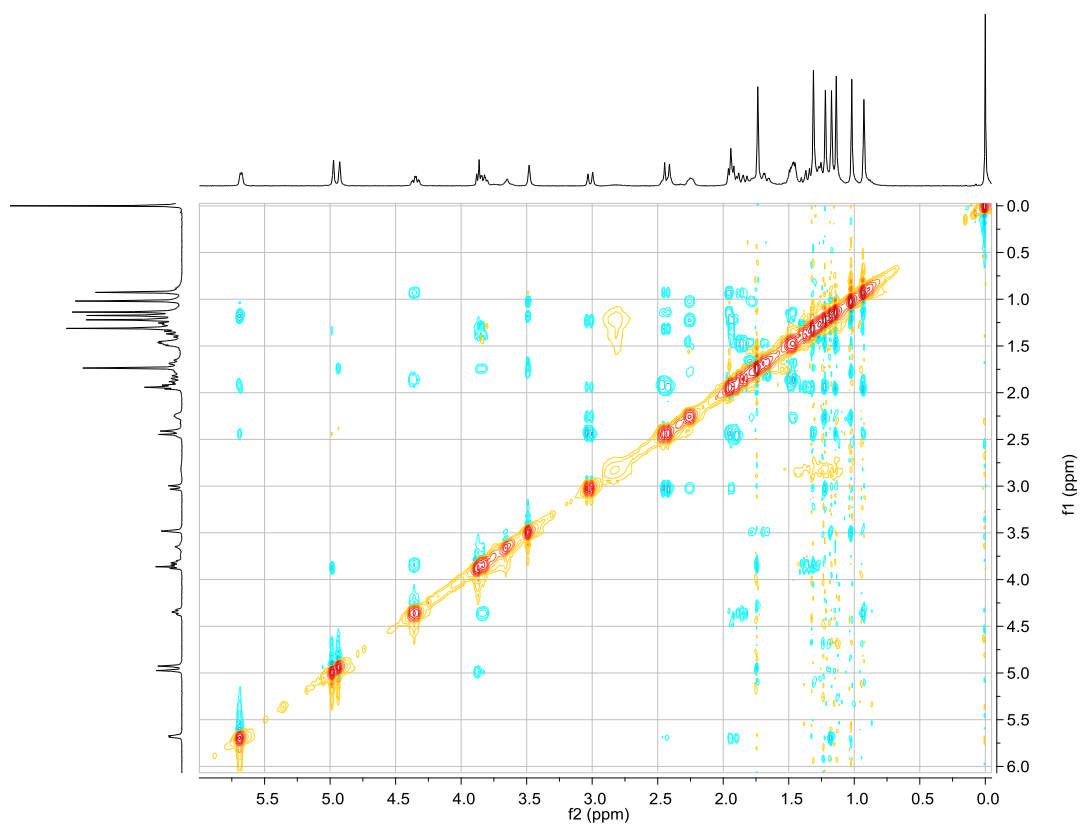
**Figure S12.** HMBC spectrum of compound **2** (CDCl<sub>3</sub>, 400 MHz).



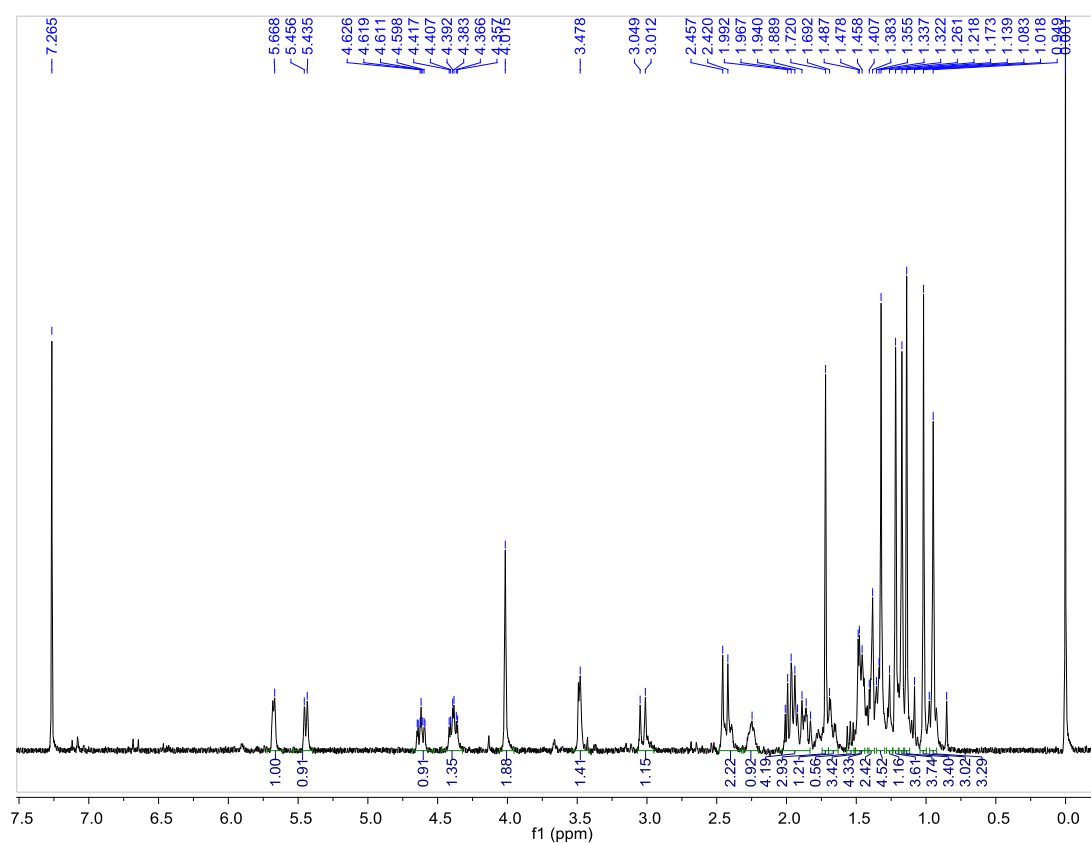
**Figure S13.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2** ( $\text{CDCl}_3$ , 400 MHz).



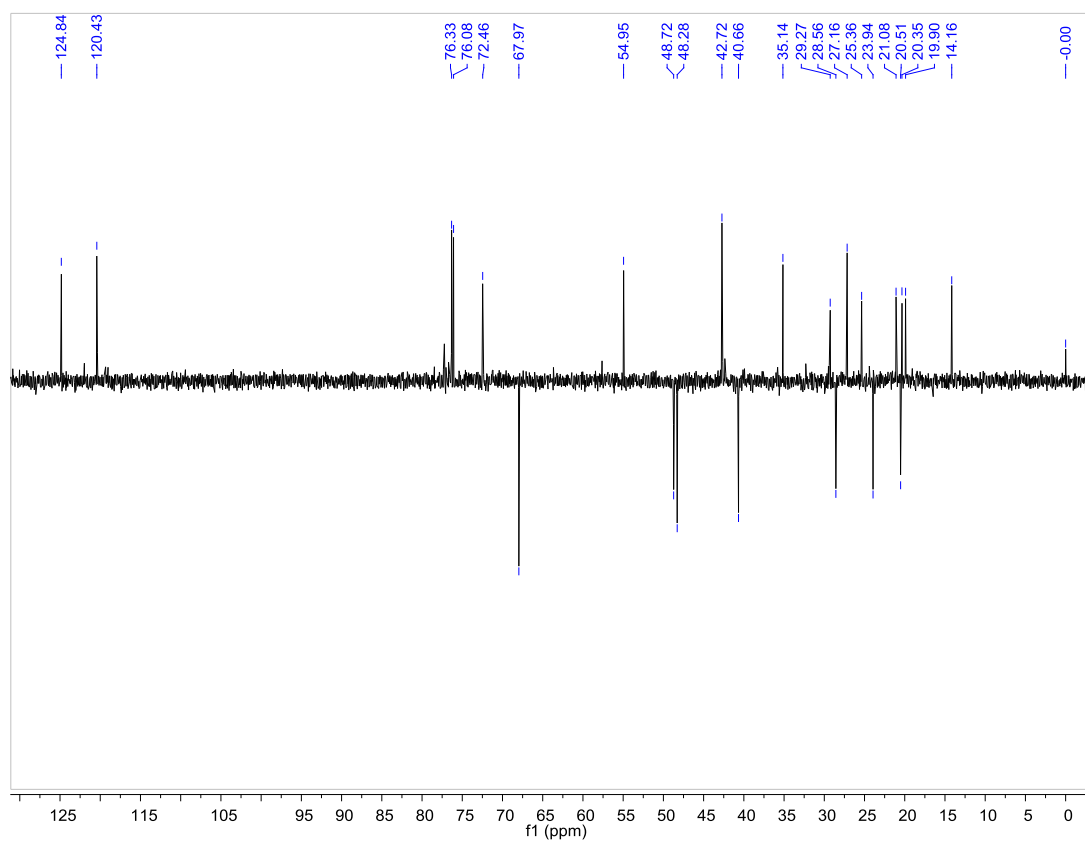
**Figure S14.** NOESY spectrum of compound **2** ( $\text{CDCl}_3$ , 400 MHz).



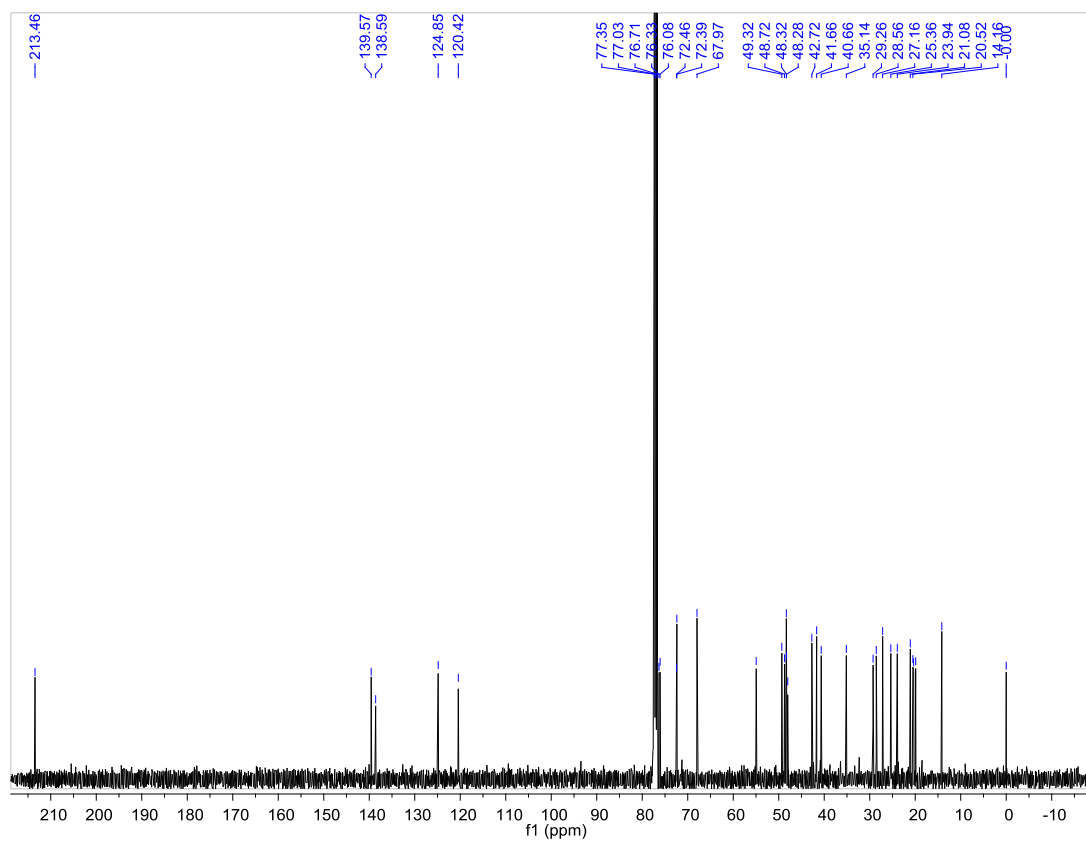
**Figure S15.**  $^1\text{H}$  NMR spectrum of compound **3** ( $\text{CDCl}_3$ , 400 MHz).



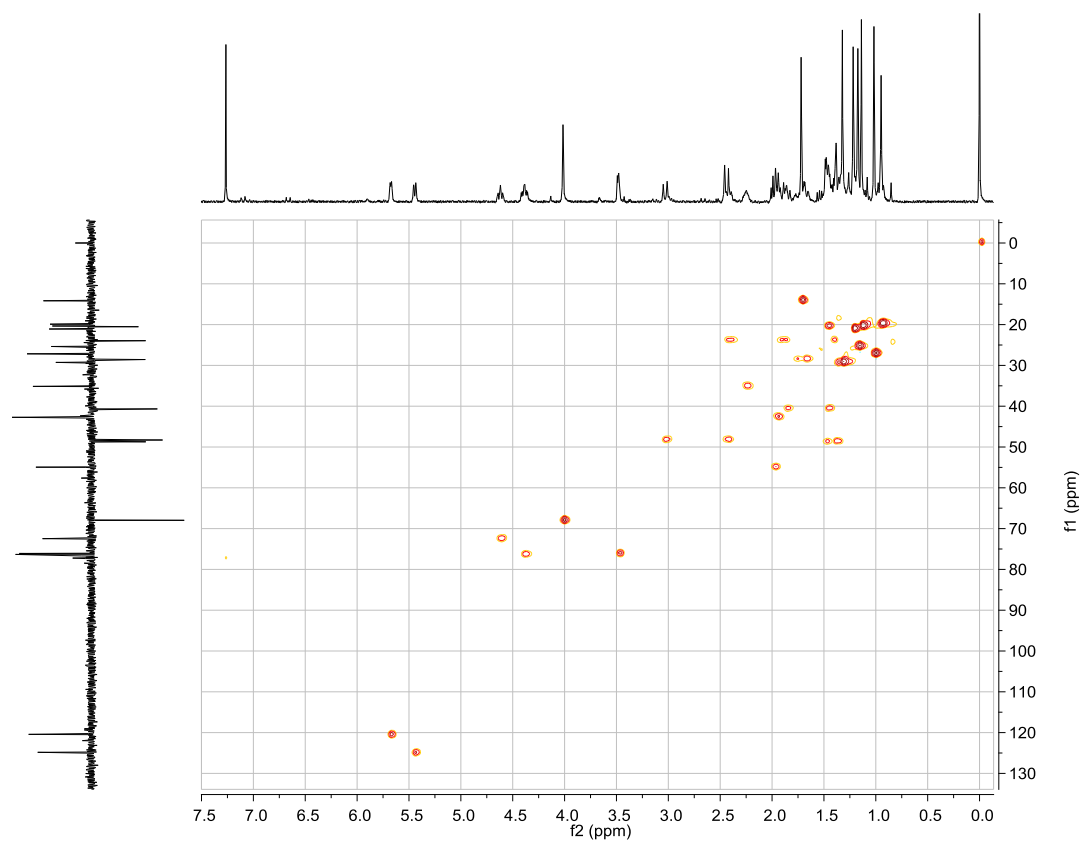
**Figure S16.**  $^{13}\text{C}$  DEPT 135 NMR spectrum of compound **3** ( $\text{CDCl}_3$ , 100 MHz).



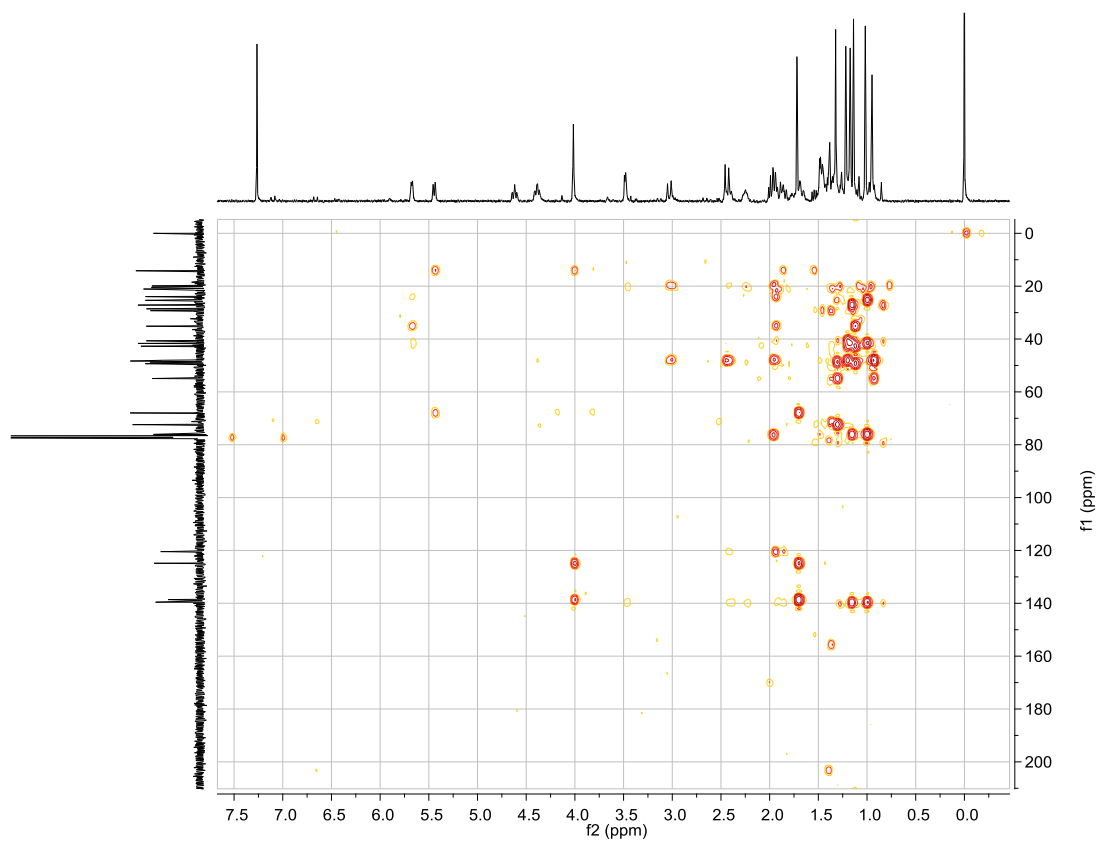
**Figure S17.**  $^{13}\text{C}$  NMR spectrum of compound **3** ( $\text{CDCl}_3$ , 100 MHz).



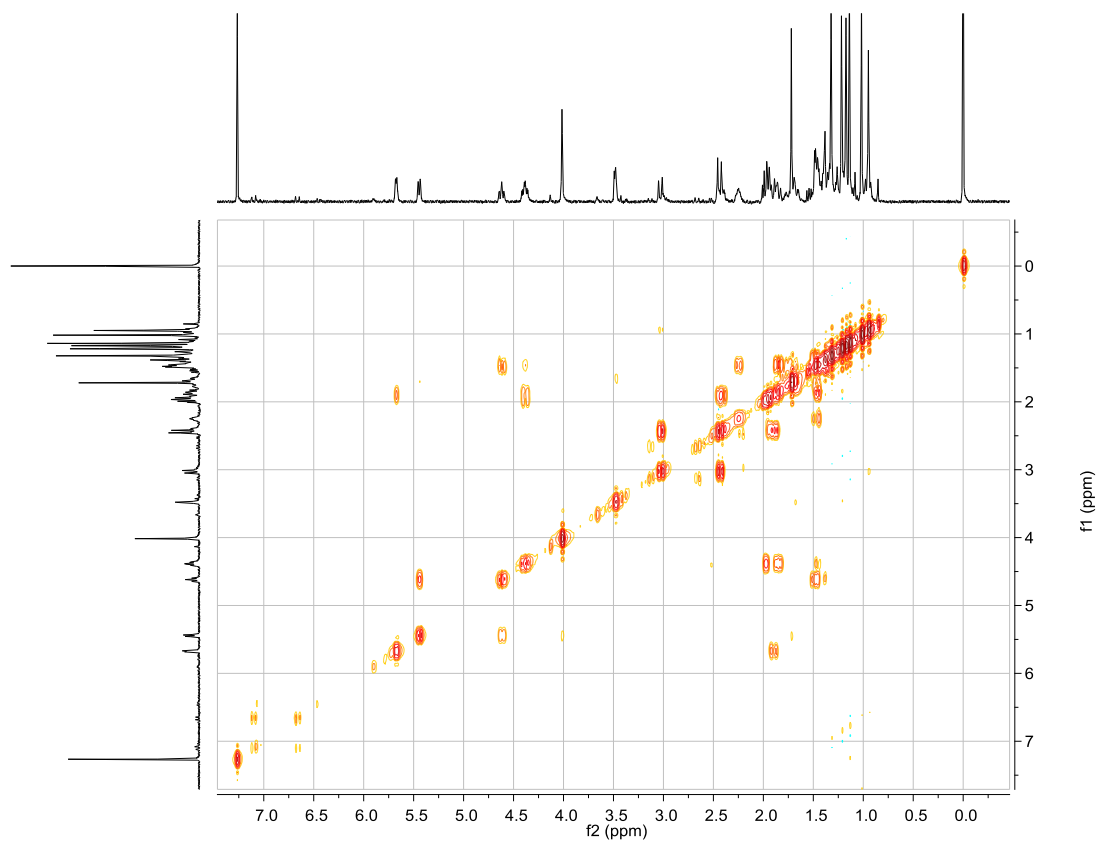
**Figure S18.** HSQC spectrum of compound **3** ( $\text{CDCl}_3$ , 400 MHz).



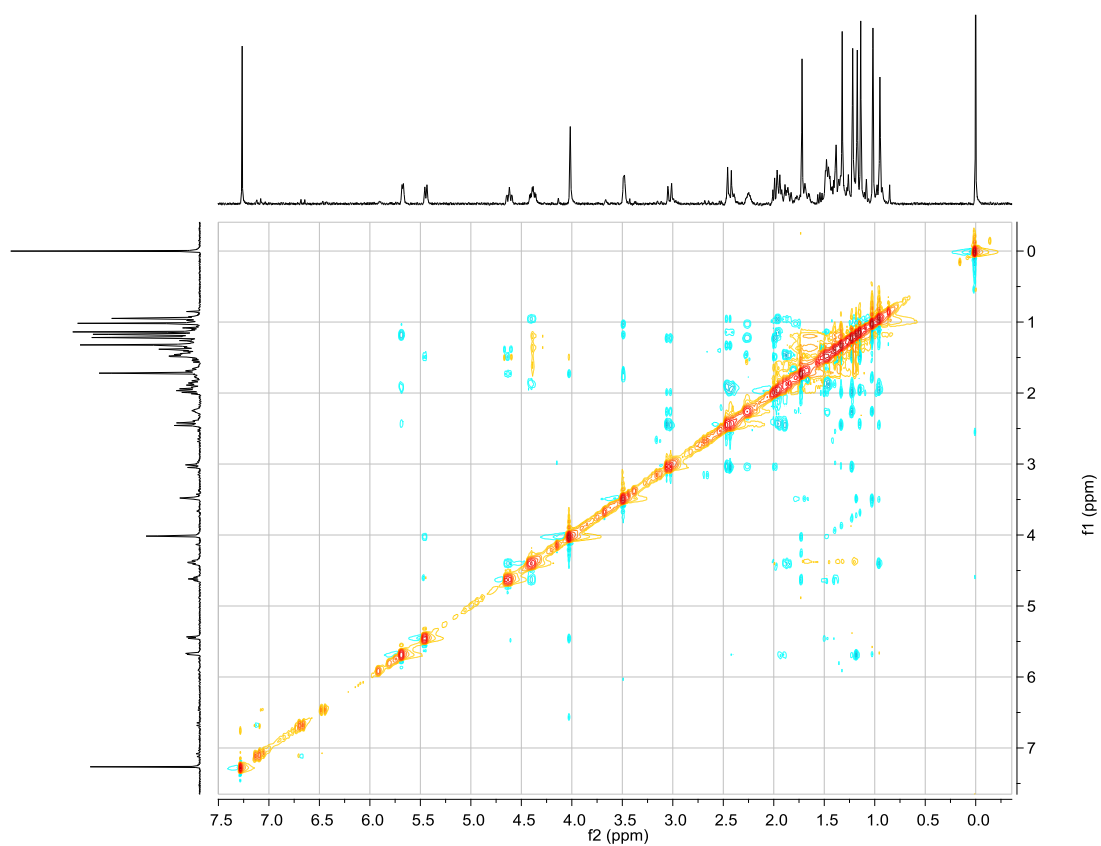
**Figure S19.** HMBC spectrum of compound **3** (CDCl<sub>3</sub>, 400 MHz).



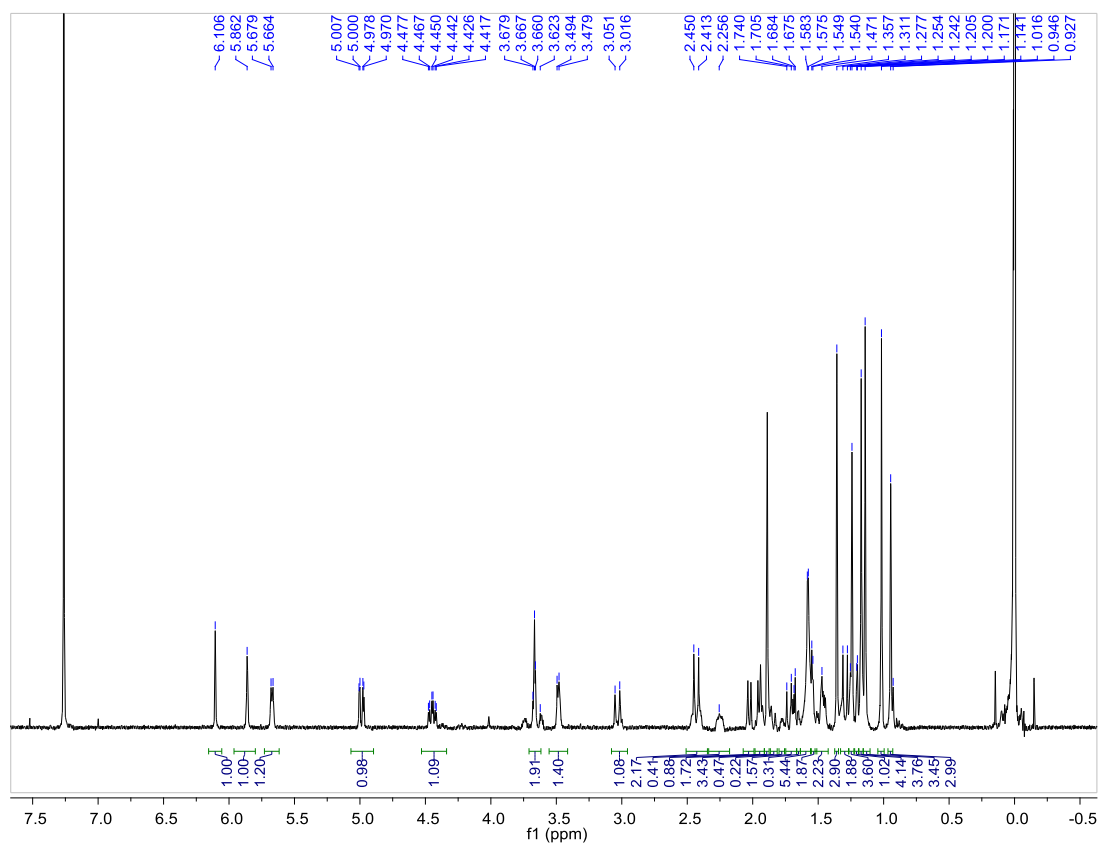
**Figure S20.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **3** (CDCl<sub>3</sub>, 400 MHz).



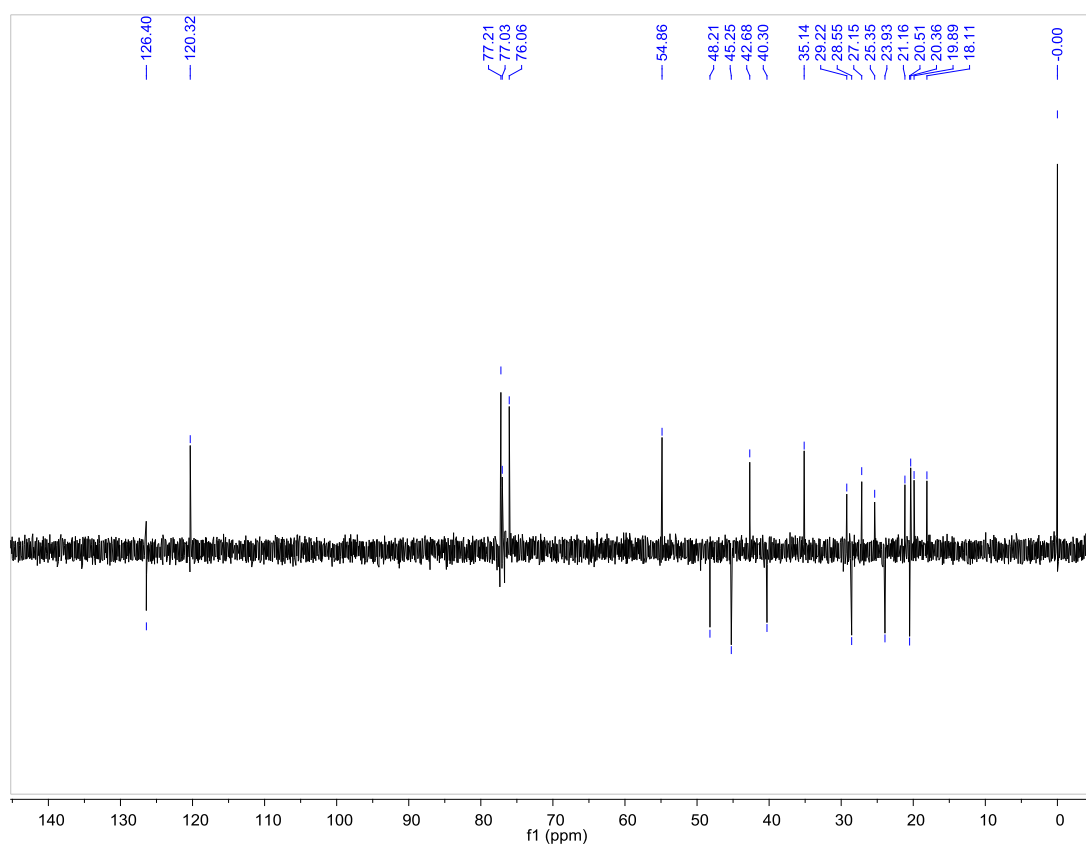
**Figure S21.** NOESY spectrum of compound **3** (CDCl<sub>3</sub>, 400 MHz).



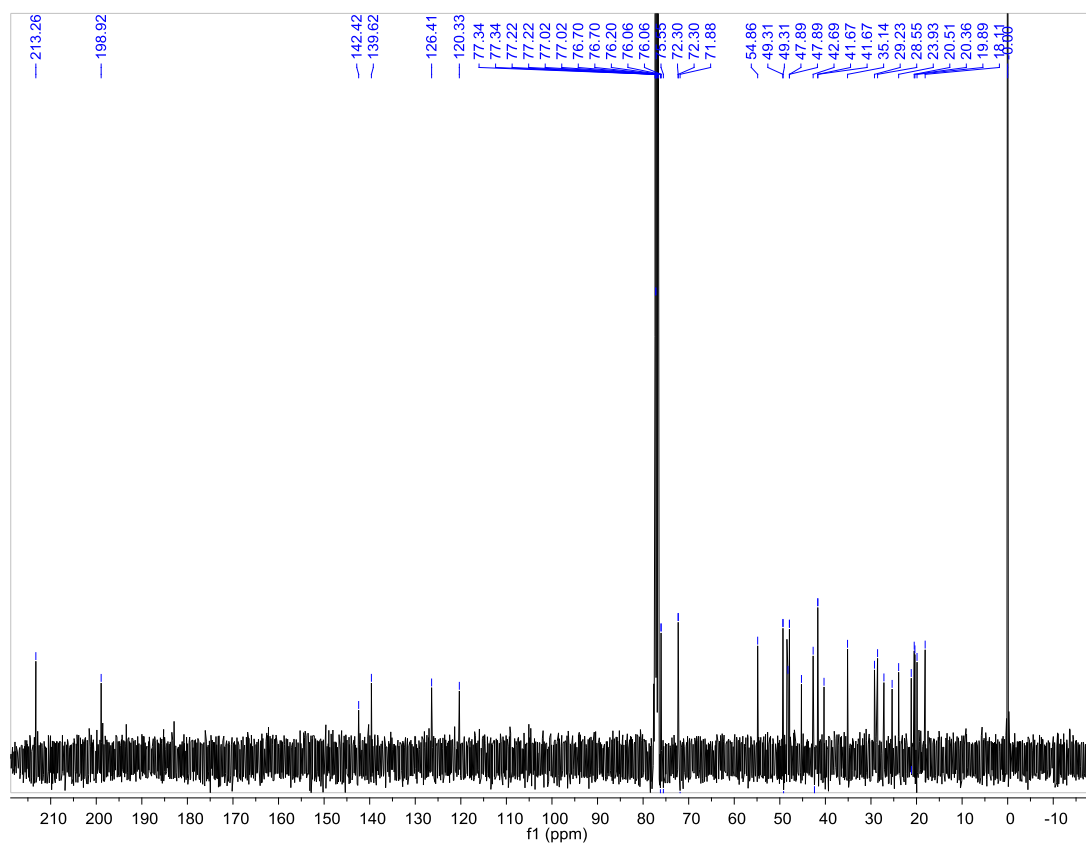
**Figure S22.** <sup>1</sup>H NMR spectrum of compound **4** (CDCl<sub>3</sub>, 400 MHz).



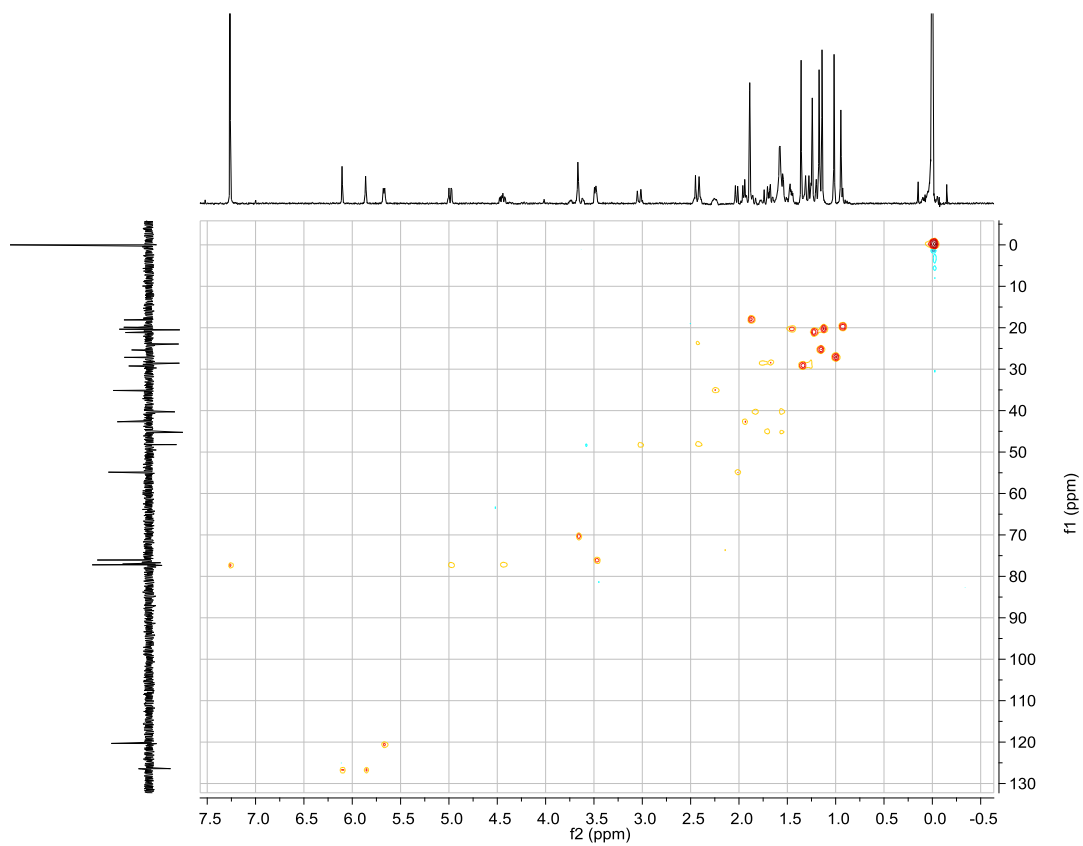
**Figure S23.**  $^{13}\text{C}$  DEPT135 NMR spectrum of compound **4** ( $\text{CDCl}_3$ , 100 MHz).



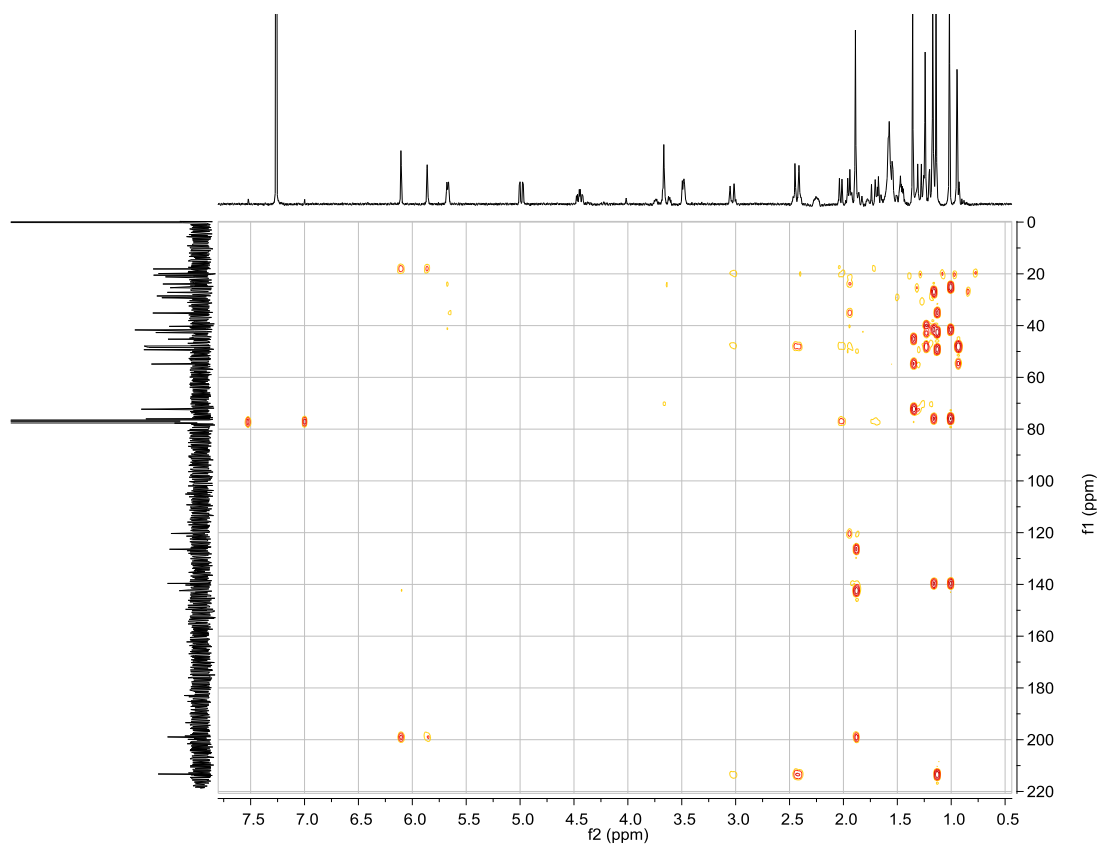
**Figure S24.**  $^{13}\text{C}$  NMR spectrum of compound **4** ( $\text{CDCl}_3$ , 100 MHz).



**Figure S25.** HSQC spectrum of compound **4** (CDCl<sub>3</sub>, 400 MHz).

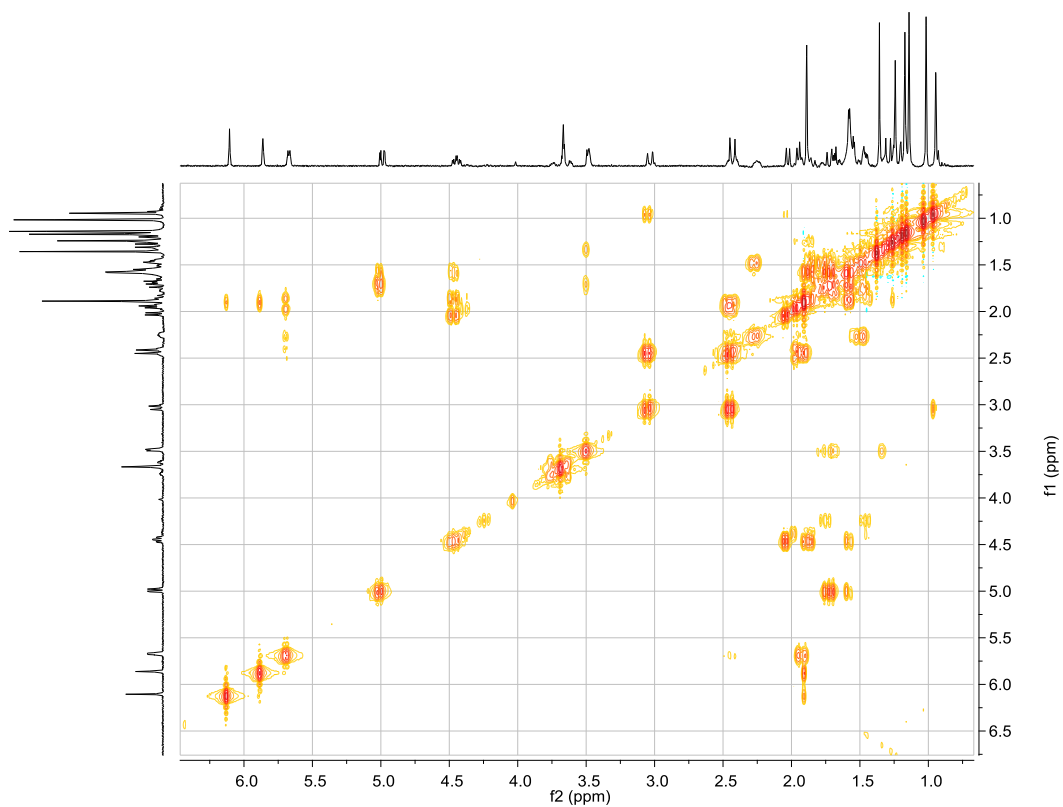


**Figure S26.** HMBC spectrum of compound **4** (CDCl<sub>3</sub>, 400 MHz).

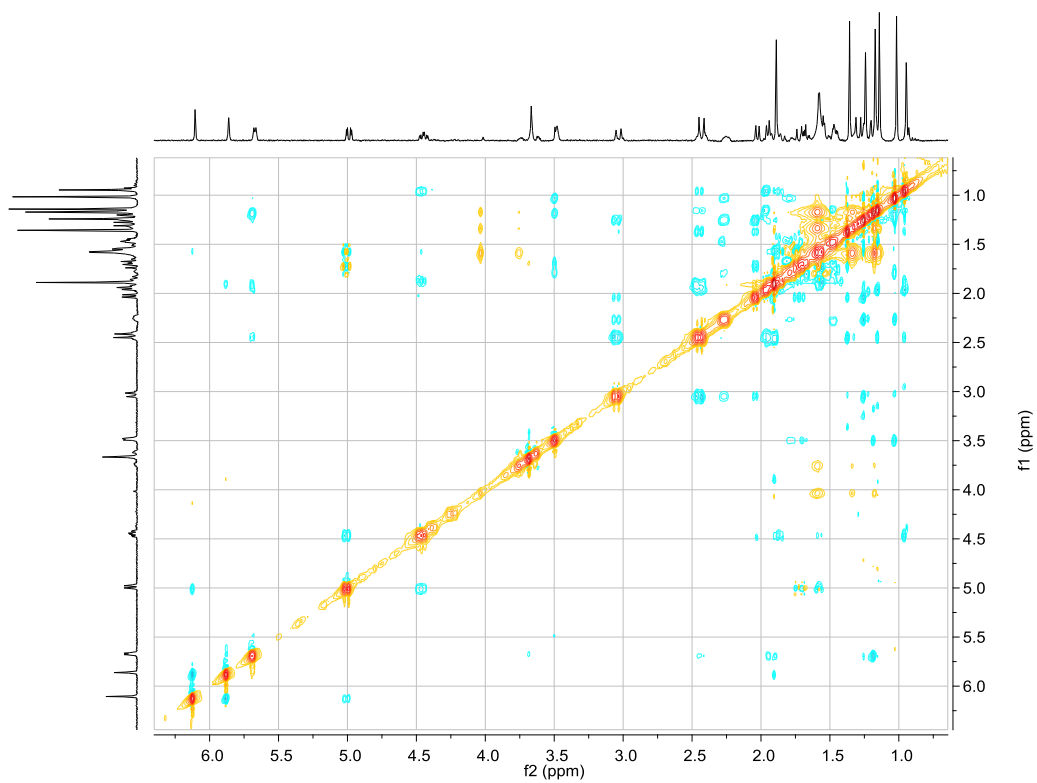




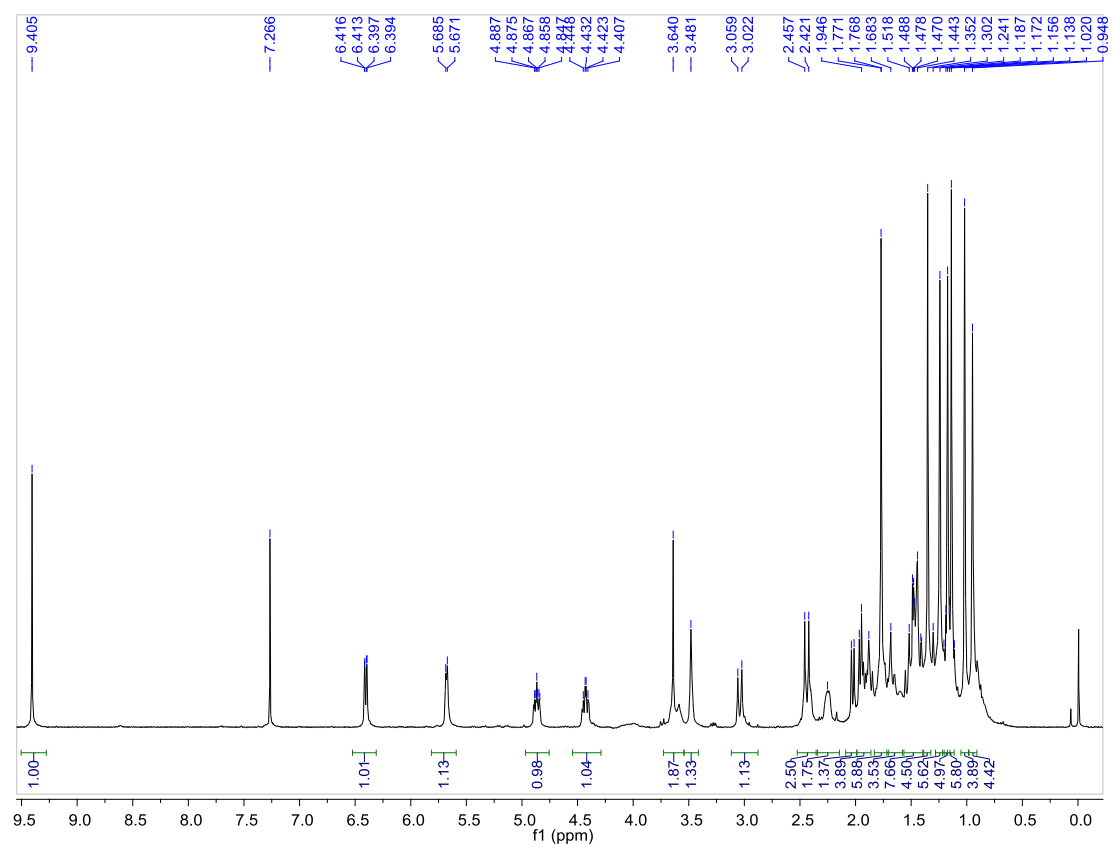
**Figure S27.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **4** ( $\text{CDCl}_3$ , 400 MHz).



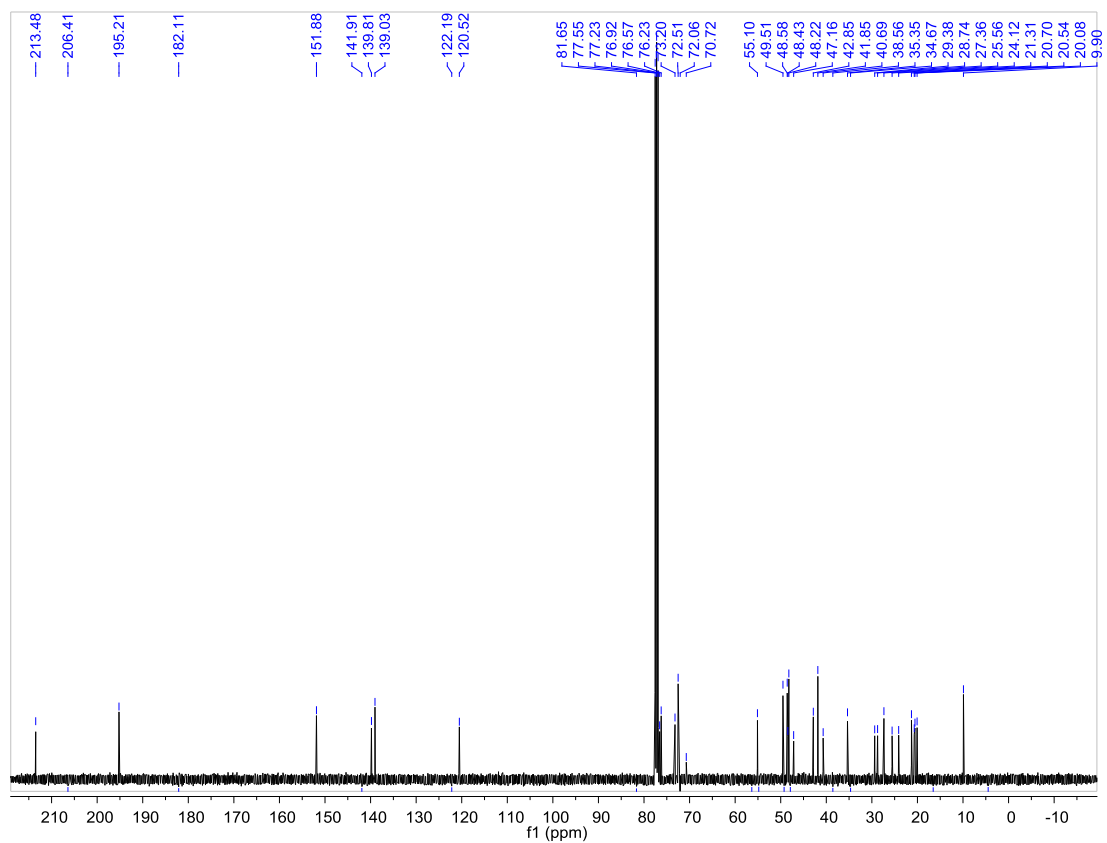
**Figure S28.** NOESY spectrum of compound **4** ( $\text{CDCl}_3$ , 400 MHz).



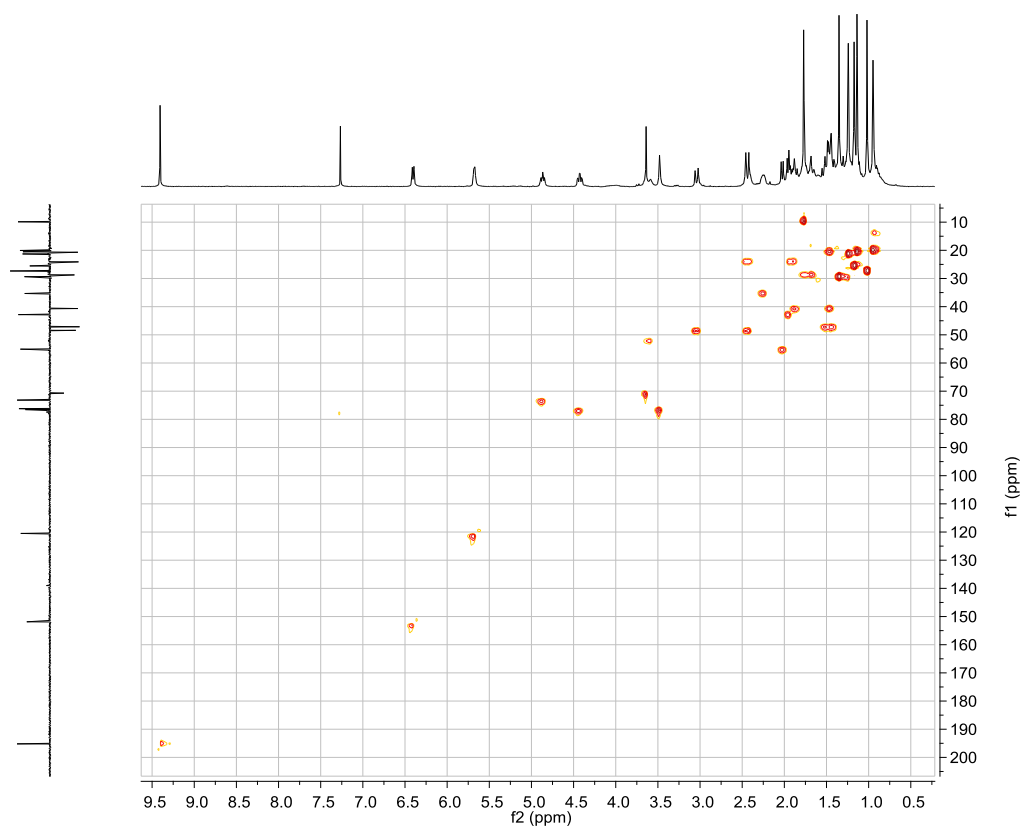
**Figure S29.**  $^1\text{H}$  NMR spectrum of compound **5** ( $\text{CDCl}_3$ , 400 MHz).



**Figure S30.**  $^{13}\text{C}$  NMR spectrum of compound **5** ( $\text{CDCl}_3$ , 100 MHz).



**Figure S31.** HSQC spectrum of compound **5** (CDCl<sub>3</sub>, 400 MHz).



**Figure S32.** HMBC spectrum of compound **5** (CDCl<sub>3</sub>, 400 MHz).

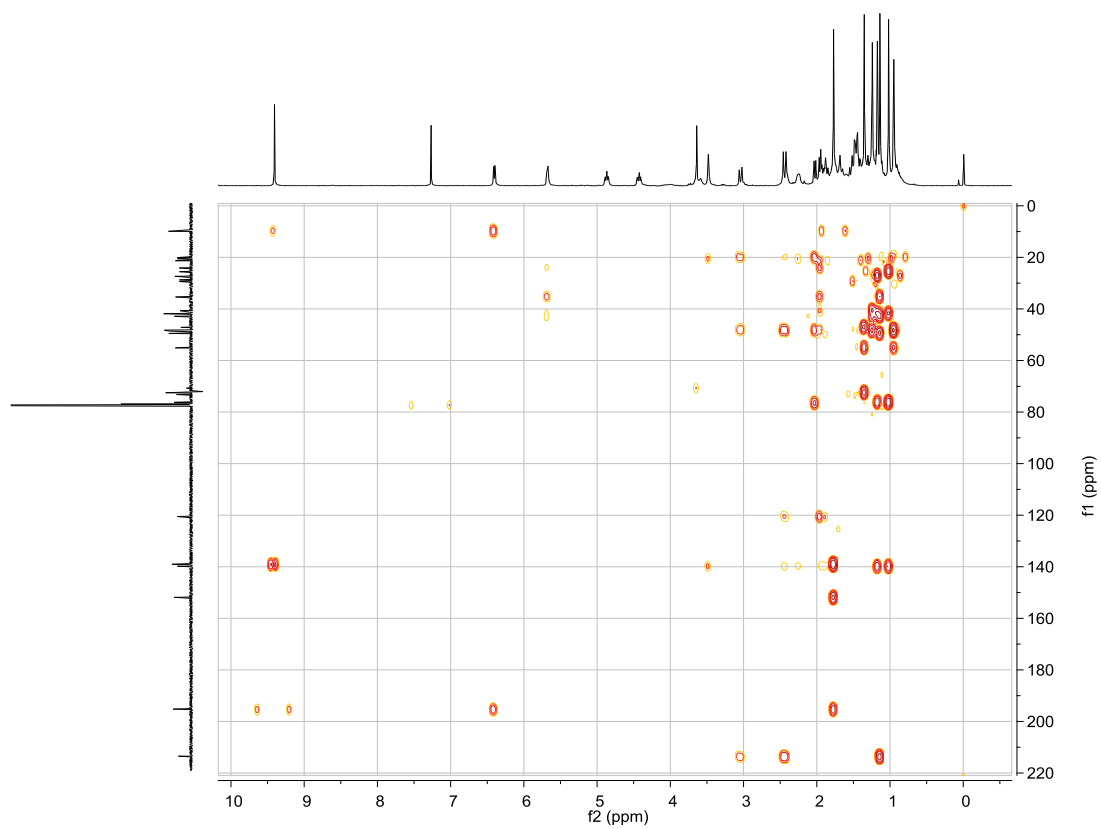


Figure S33.  $^1\text{H}$  NMR spectrum of compound **6** ( $\text{CDCl}_3$ , 400 MHz).

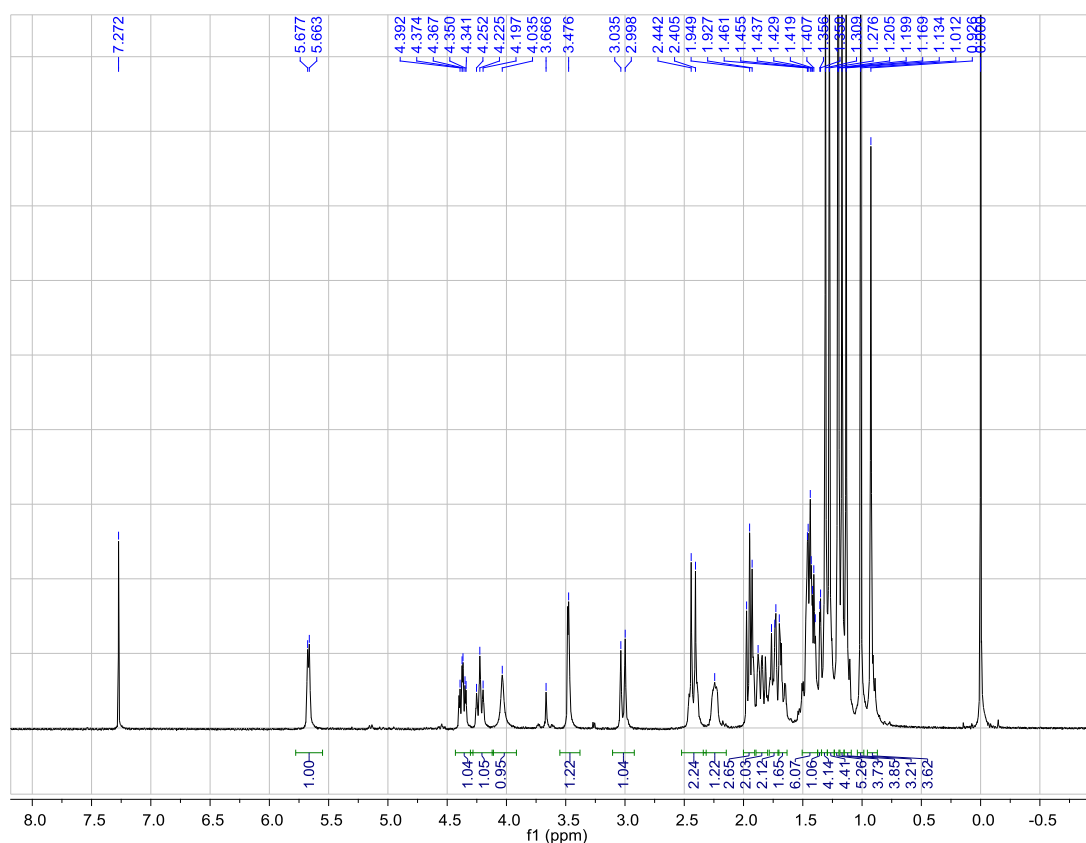
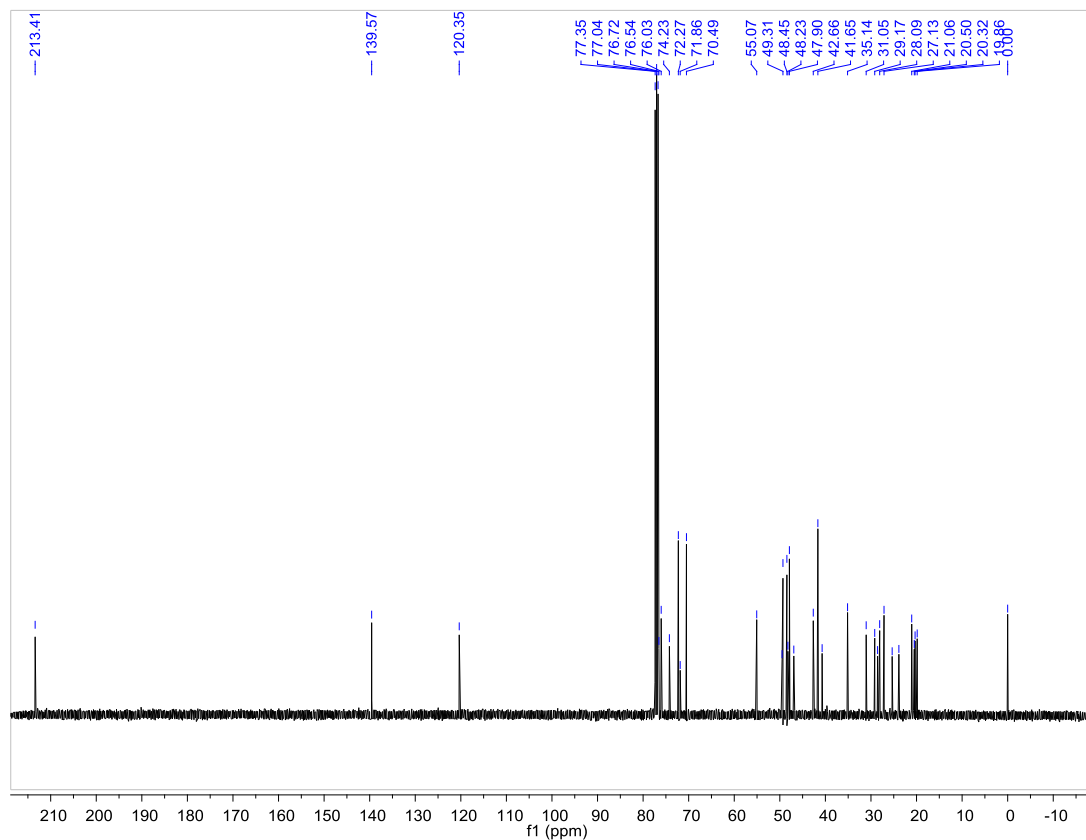
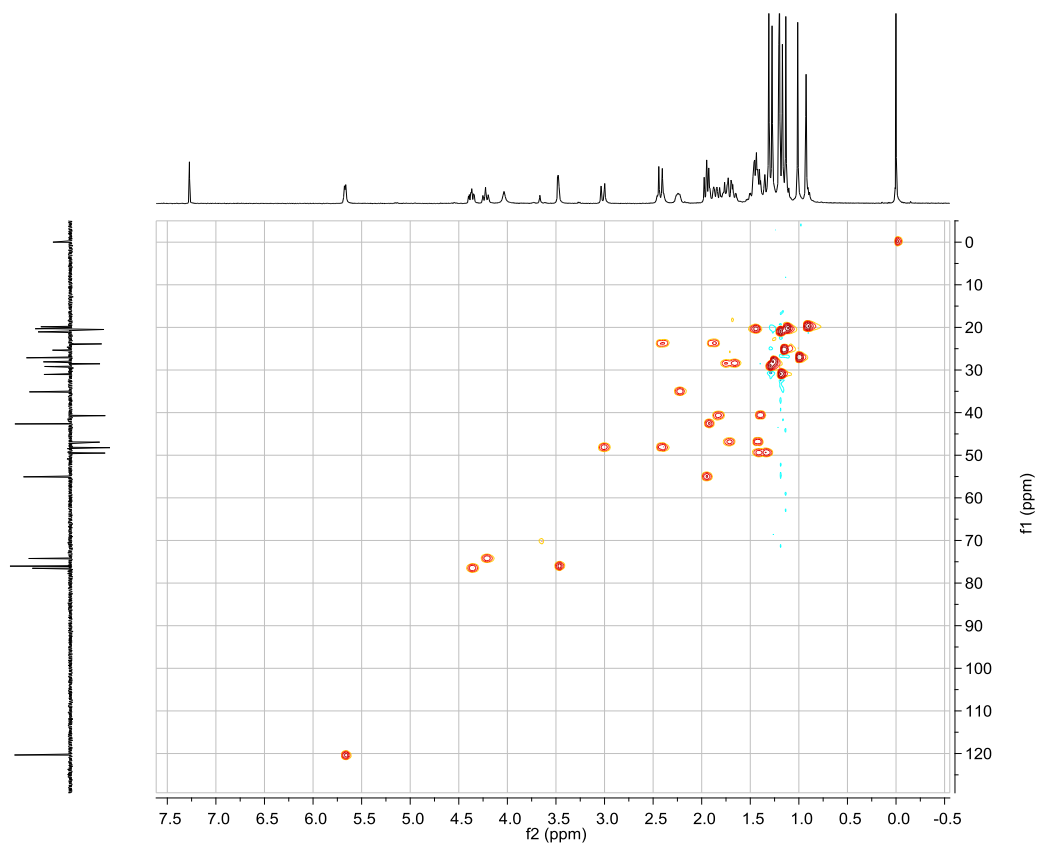


Figure S34.  $^{13}\text{C}$  NMR spectrum of compound **6** ( $\text{CDCl}_3$ , 100 MHz).



**Figure S35.** HSQC spectrum of compound **6** (CDCl<sub>3</sub>, 400 MHz).



**Figure S36.** HMBC spectrum of compound **6** (CDCl<sub>3</sub>, 400 MHz).

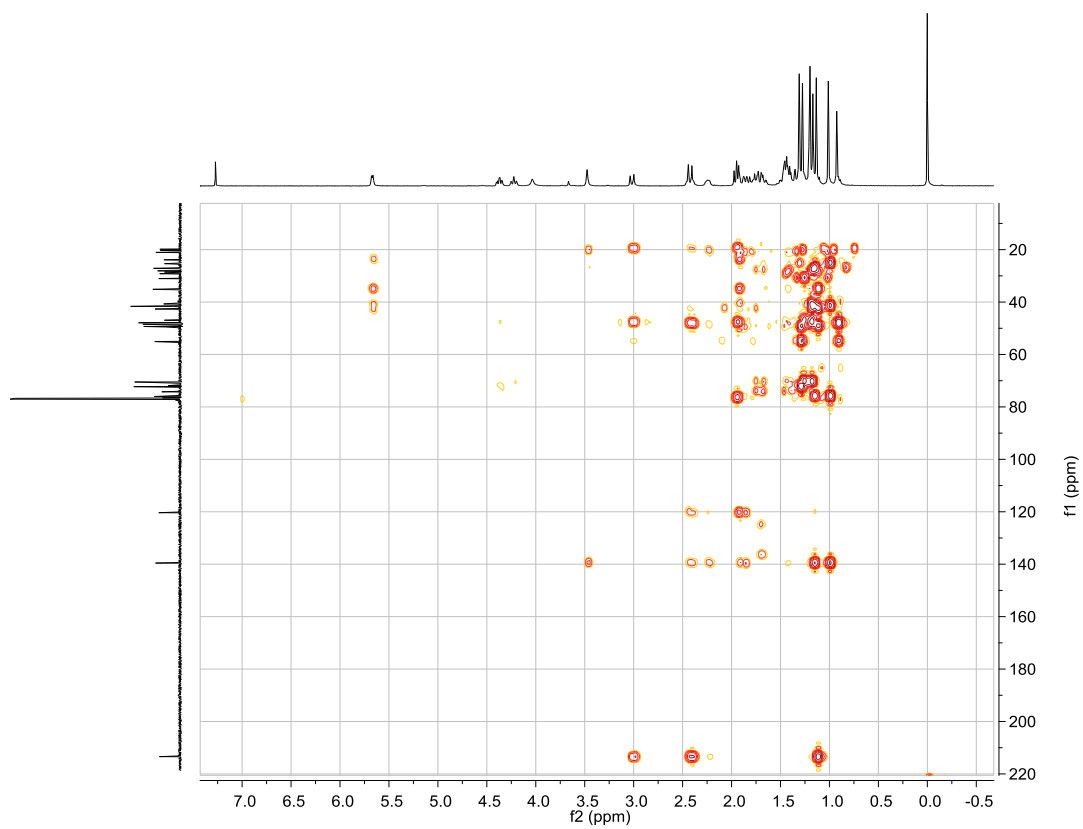


Figure S37.  $^1\text{H}$  NMR spectrum of compound 7 ( $\text{CDCl}_3$ , 400 MHz).

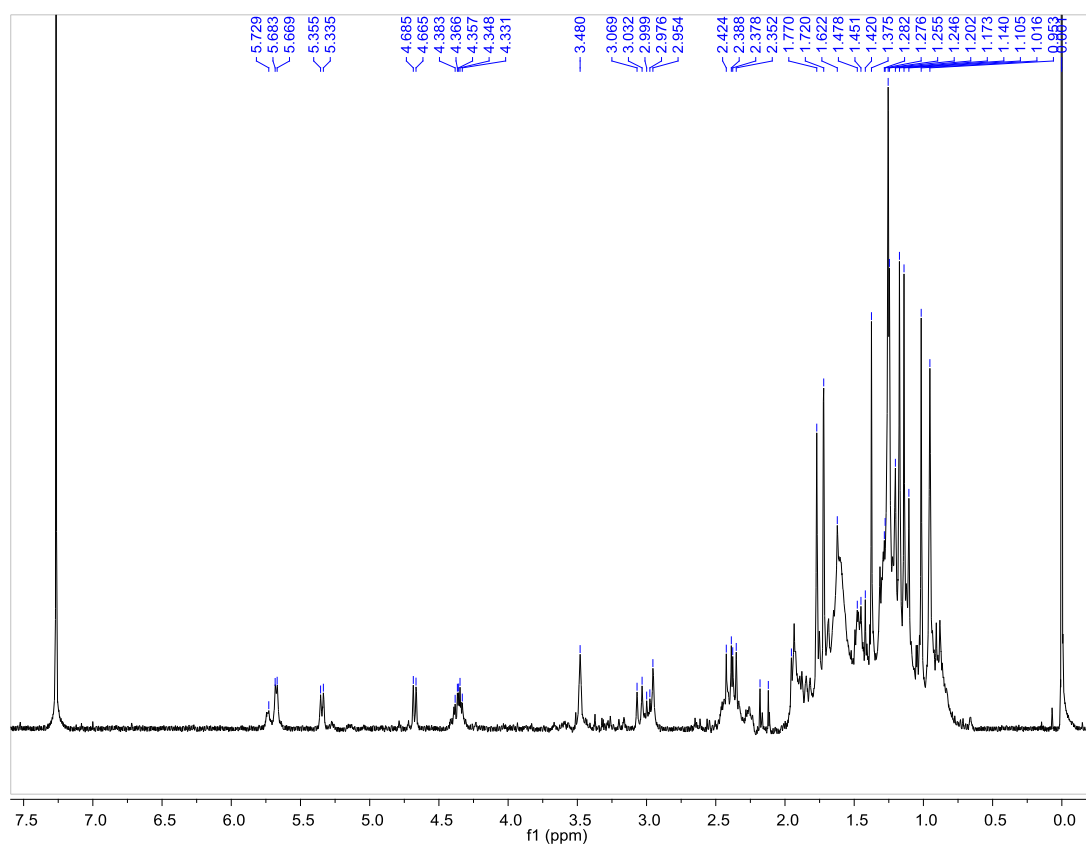
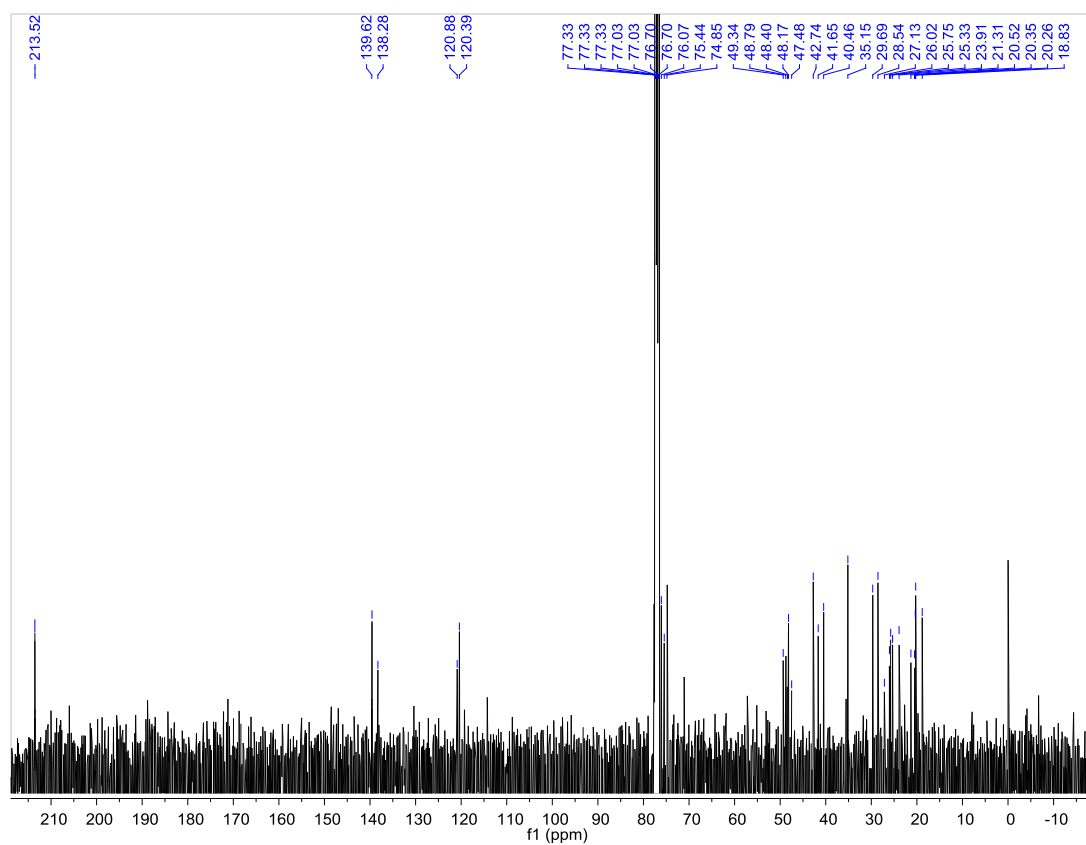
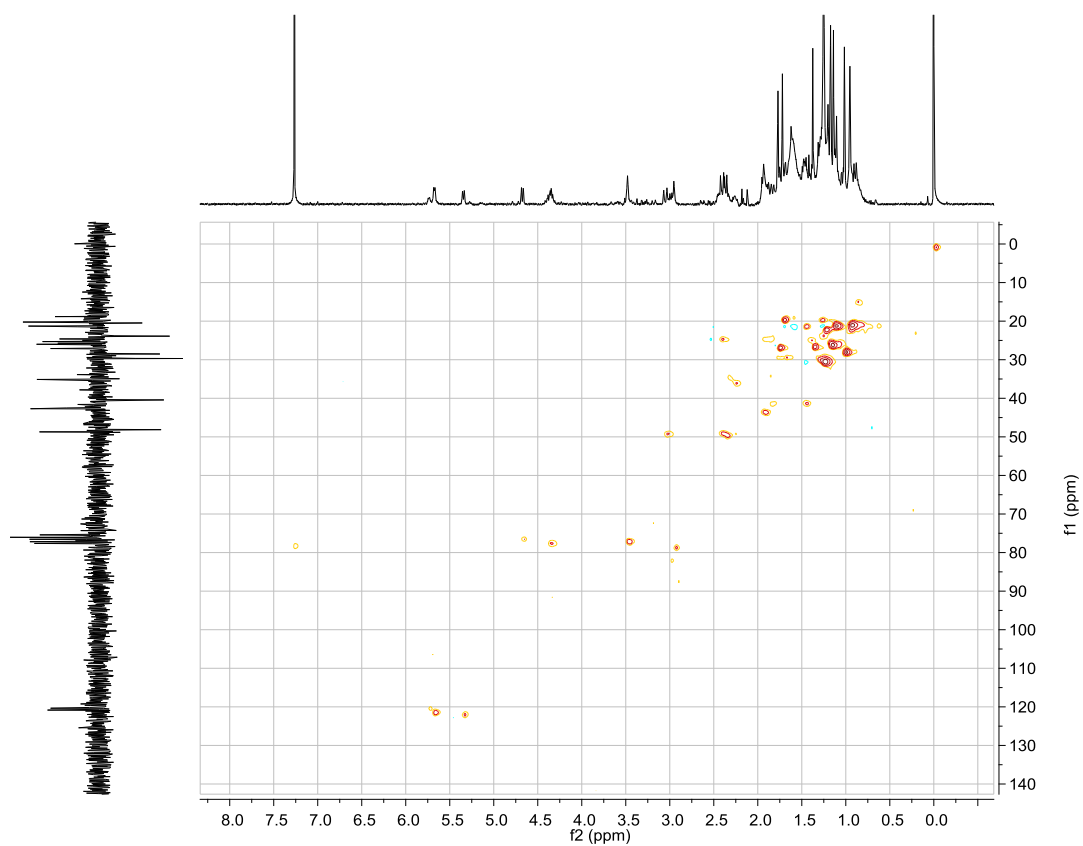


Figure S38.  $^{13}\text{C}$  NMR spectrum of compound 7 ( $\text{CDCl}_3$ , 100 MHz).



**Figure S39.** HSQC spectrum of compound **7** (CDCl<sub>3</sub>, 400 MHz).



**Figure S40.** HMBC spectrum of compound **7** (CDCl<sub>3</sub>, 400 MHz).

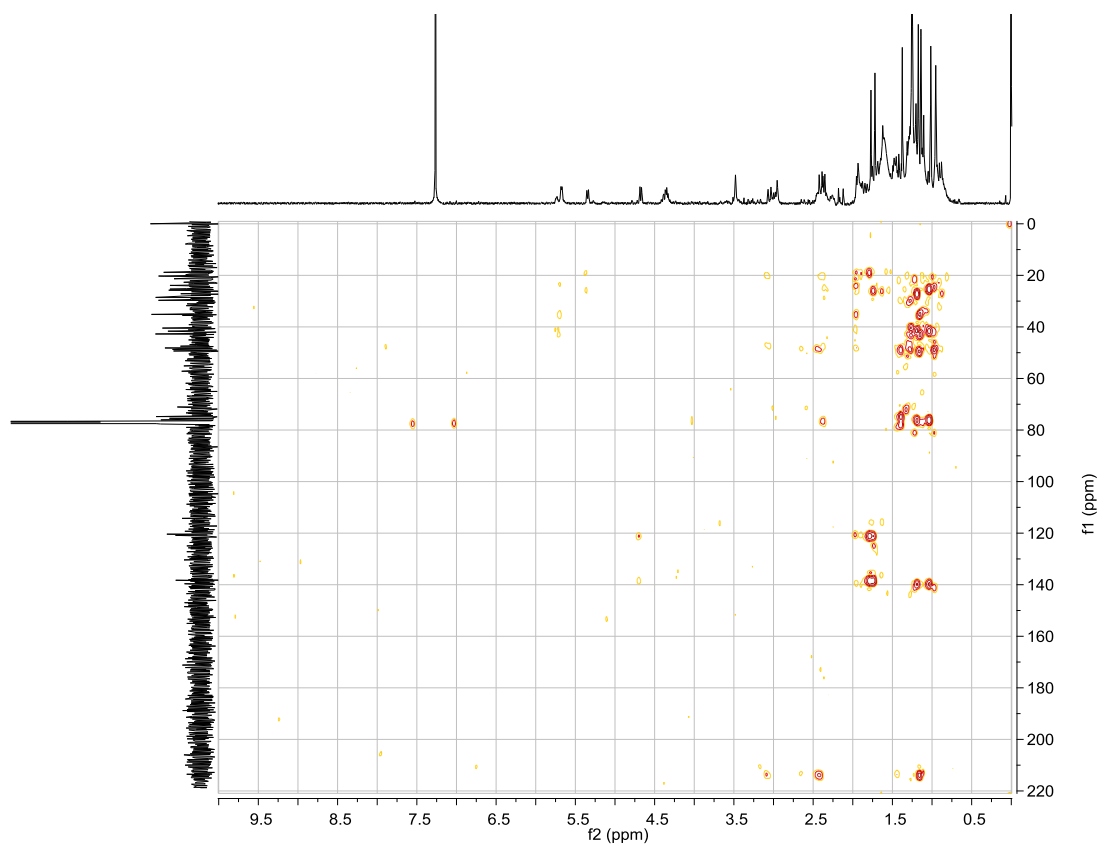


Figure S41.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7** ( $\text{CDCl}_3$ , 400 MHz).

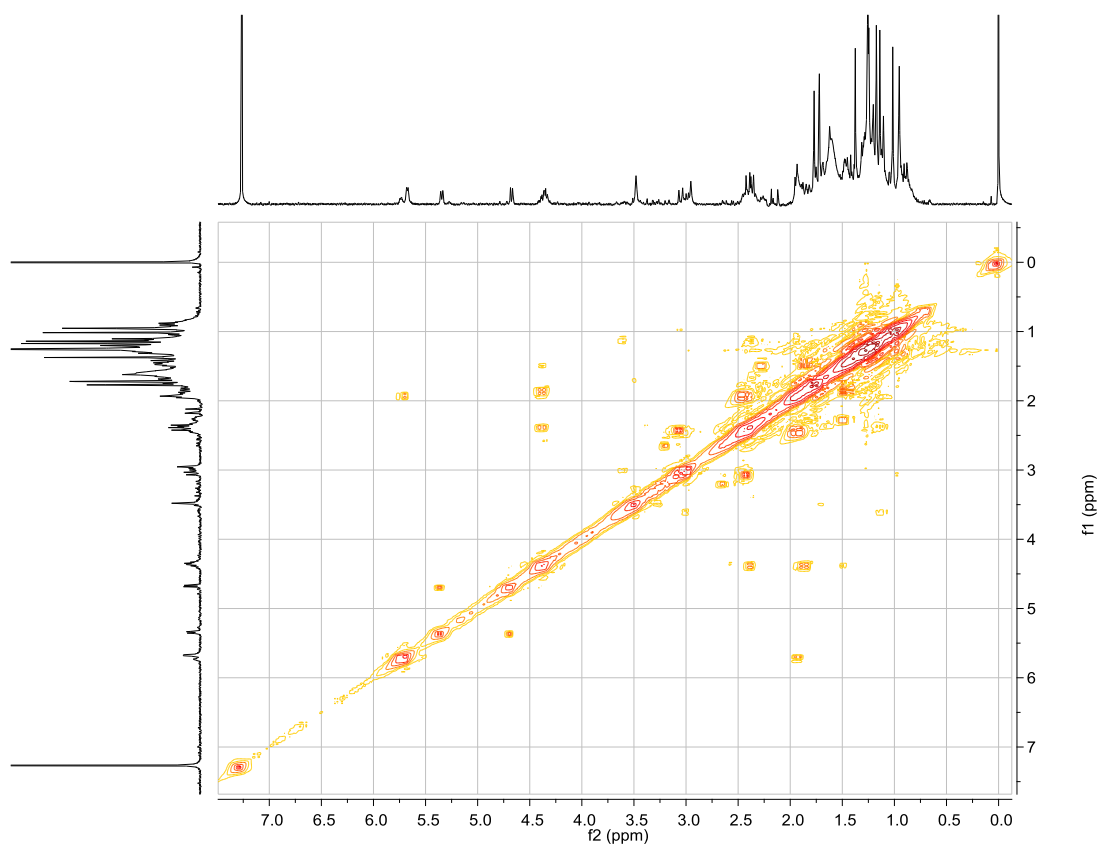
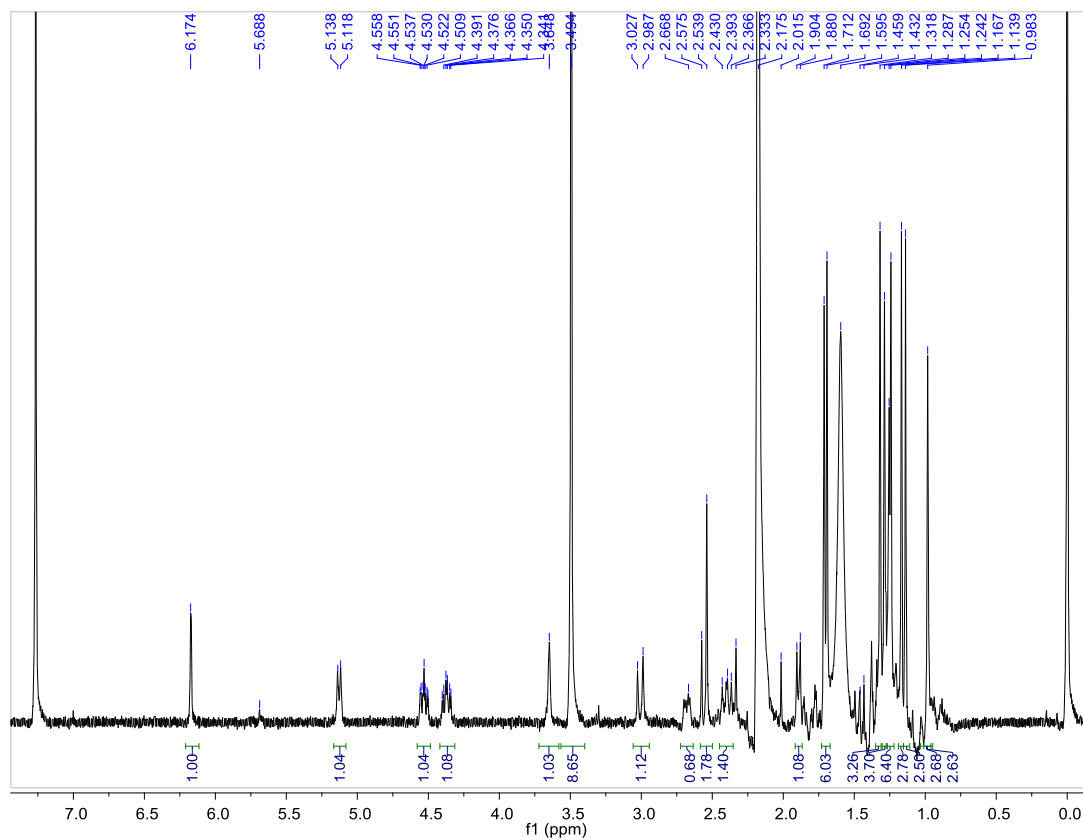
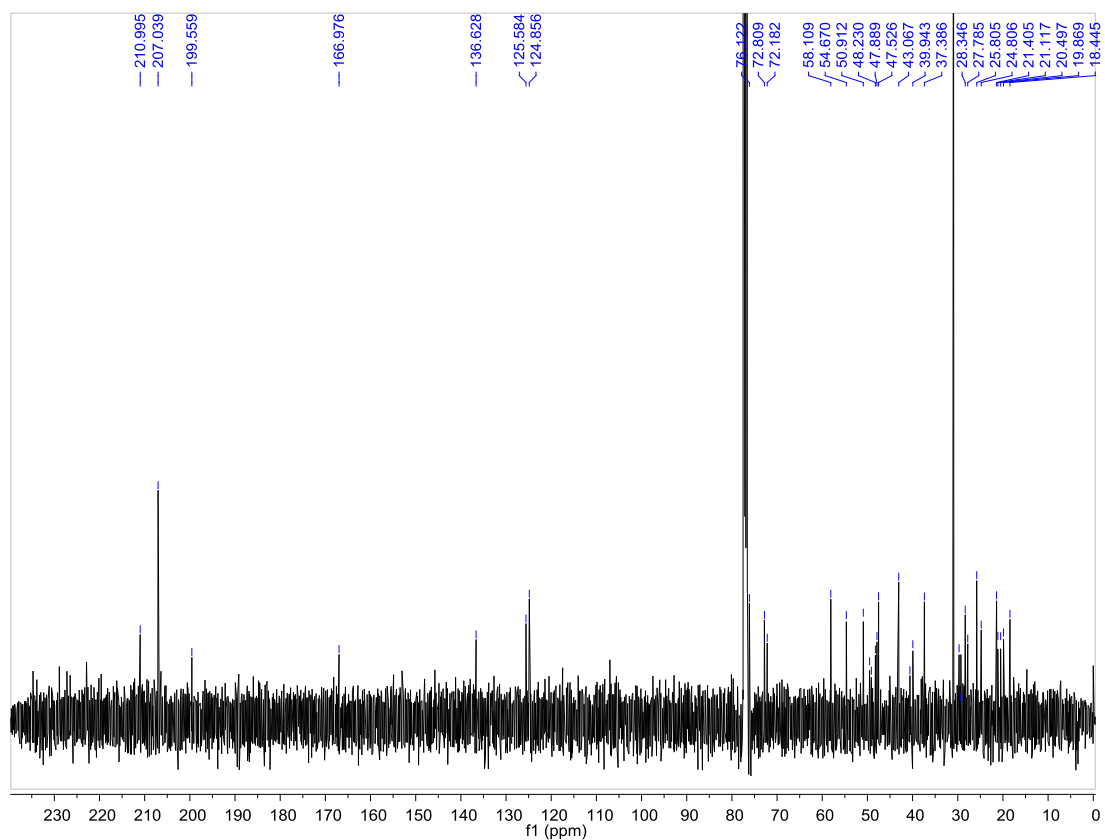


Figure S42.  $^1\text{H}$  NMR spectrum of compound **8** ( $\text{CDCl}_3$ , 400 MHz).

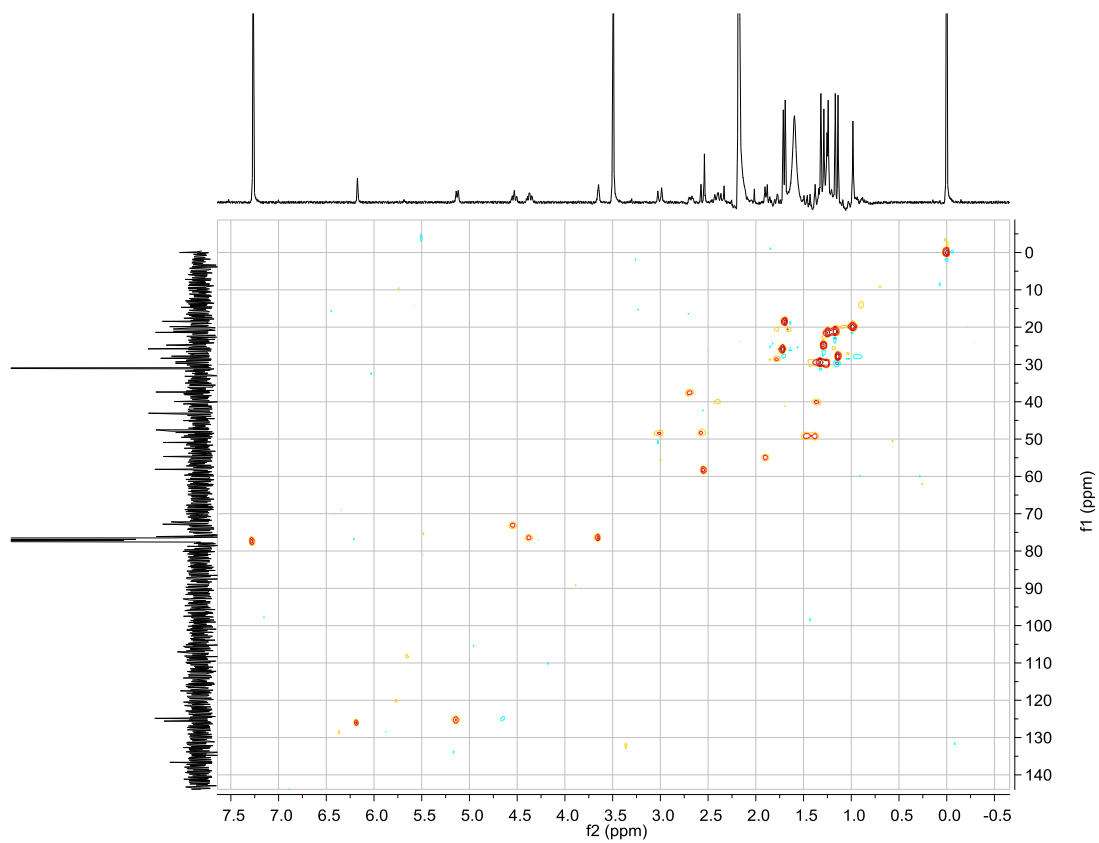




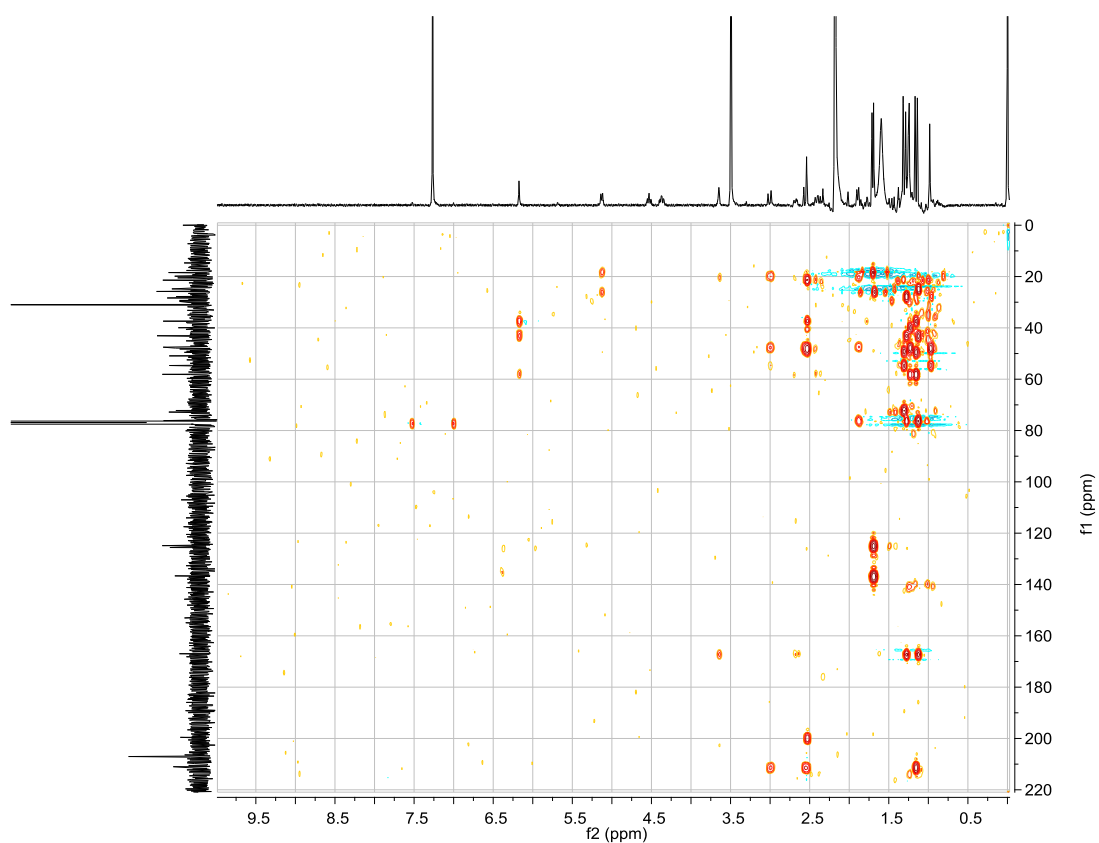
**Figure S43.**  $^{13}\text{C}$  NMR spectrum of compound **8** ( $\text{CDCl}_3$ , 100 MHz).



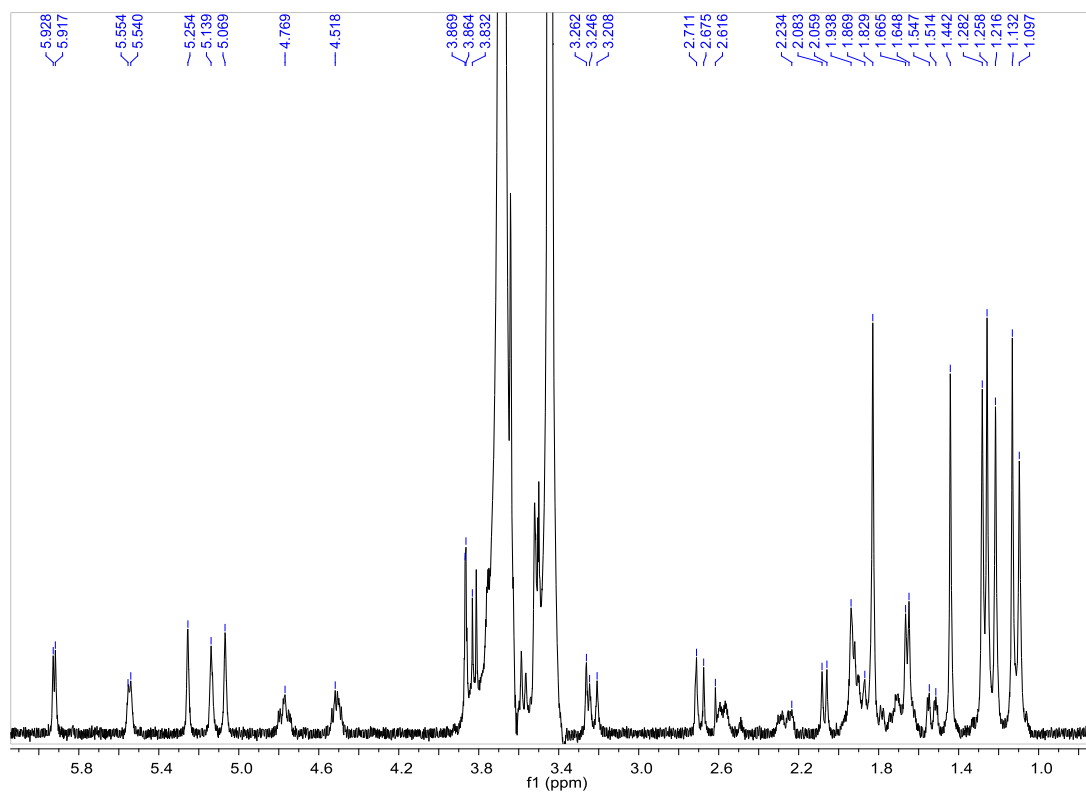
**Figure S44.** HSQC spectrum of compound **8** ( $\text{CDCl}_3$ , 400 MHz).



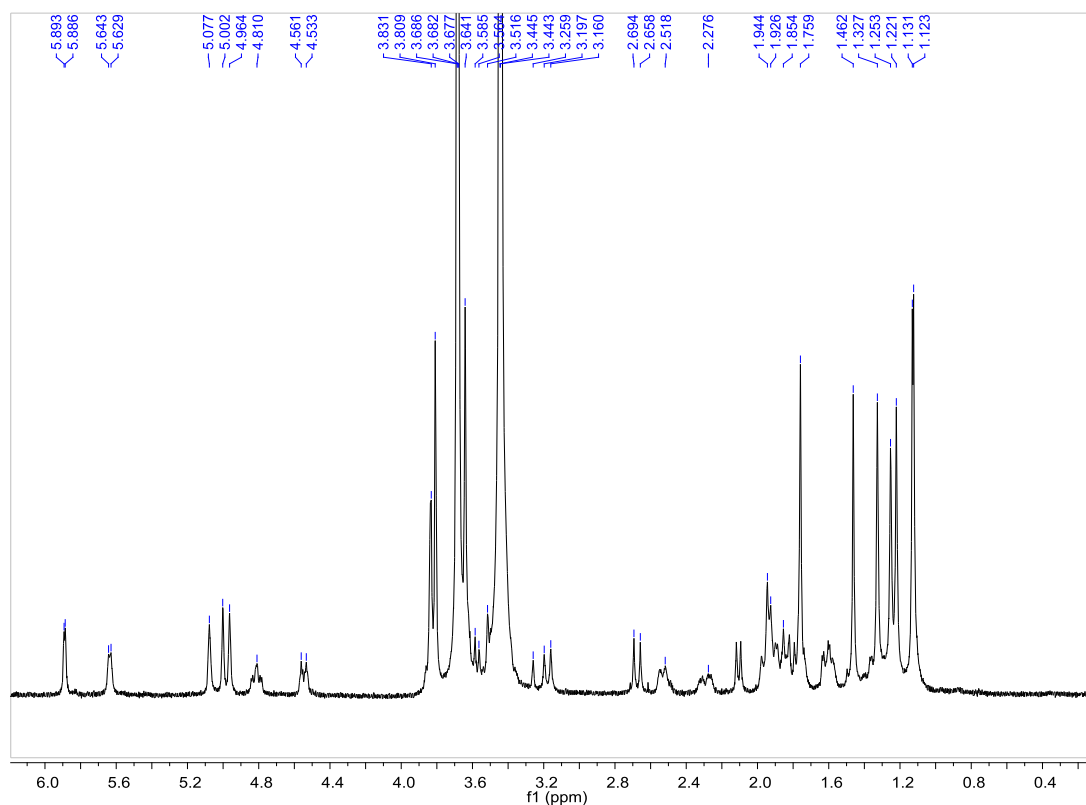
**Figure S45.** HMBC spectrum of compound **8** (CDCl<sub>3</sub>, 400 MHz).



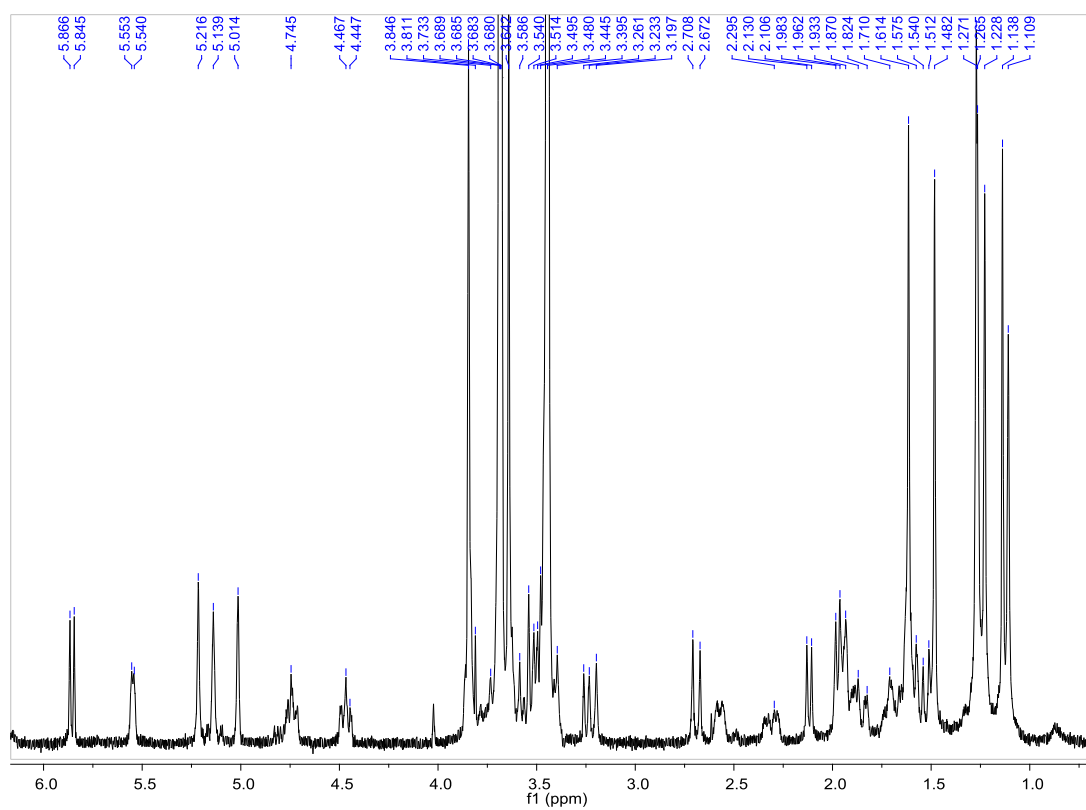
**Figure S46.** <sup>1</sup>H NMR spectrum of (*R*)-MTPA ester of compound **1** (pyridine-*d*<sub>5</sub>, 400 MHz).



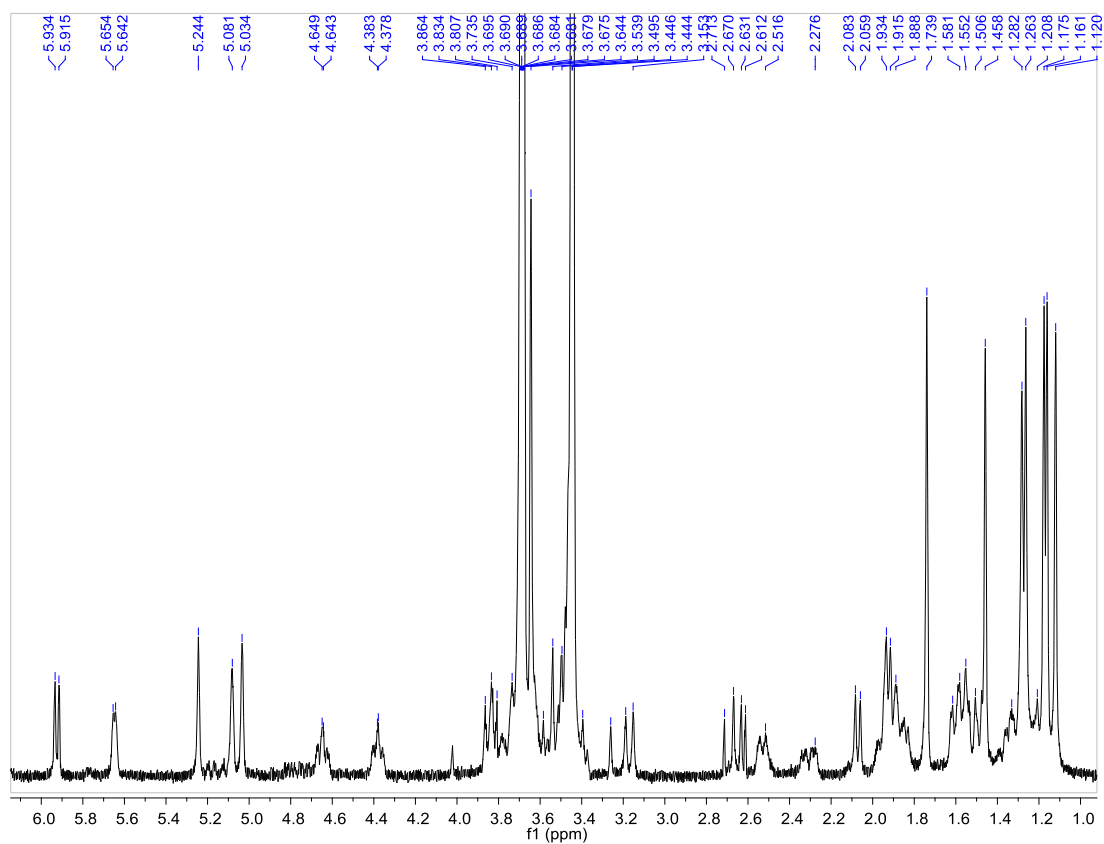
**Figure S47.**  $^1\text{H}$  NMR spectrum of (*S*)-MTPA ester of compound **1** (pyridine- $d_5$ , 400 MHz).



**Figure S48.**  $^1\text{H}$  NMR spectrum of (*R*)-MTPA ester of compound **2** (pyridine- $d_5$ , 400 MHz).



**Figure S49.**  $^1\text{H}$  NMR spectrum of (*S*)-MTPA ester of compound **2** (pyridine- $d_5$ , 400 MHz).



**Figure S50.** Hollow fiber assay testing result for elaeocarpucin C (**3**).

