

## Supporting Information

In this ‘Supporting Information’ file for the manuscript entitled “**Thymol Derivatives with Antibacterial and Cytotoxic Activity from the Aerial Parts of *Ageratina adenophora***”, the MS, IR, 1D and 2D NMR spectra of new compounds **1**, **2** and **3** are listed below.

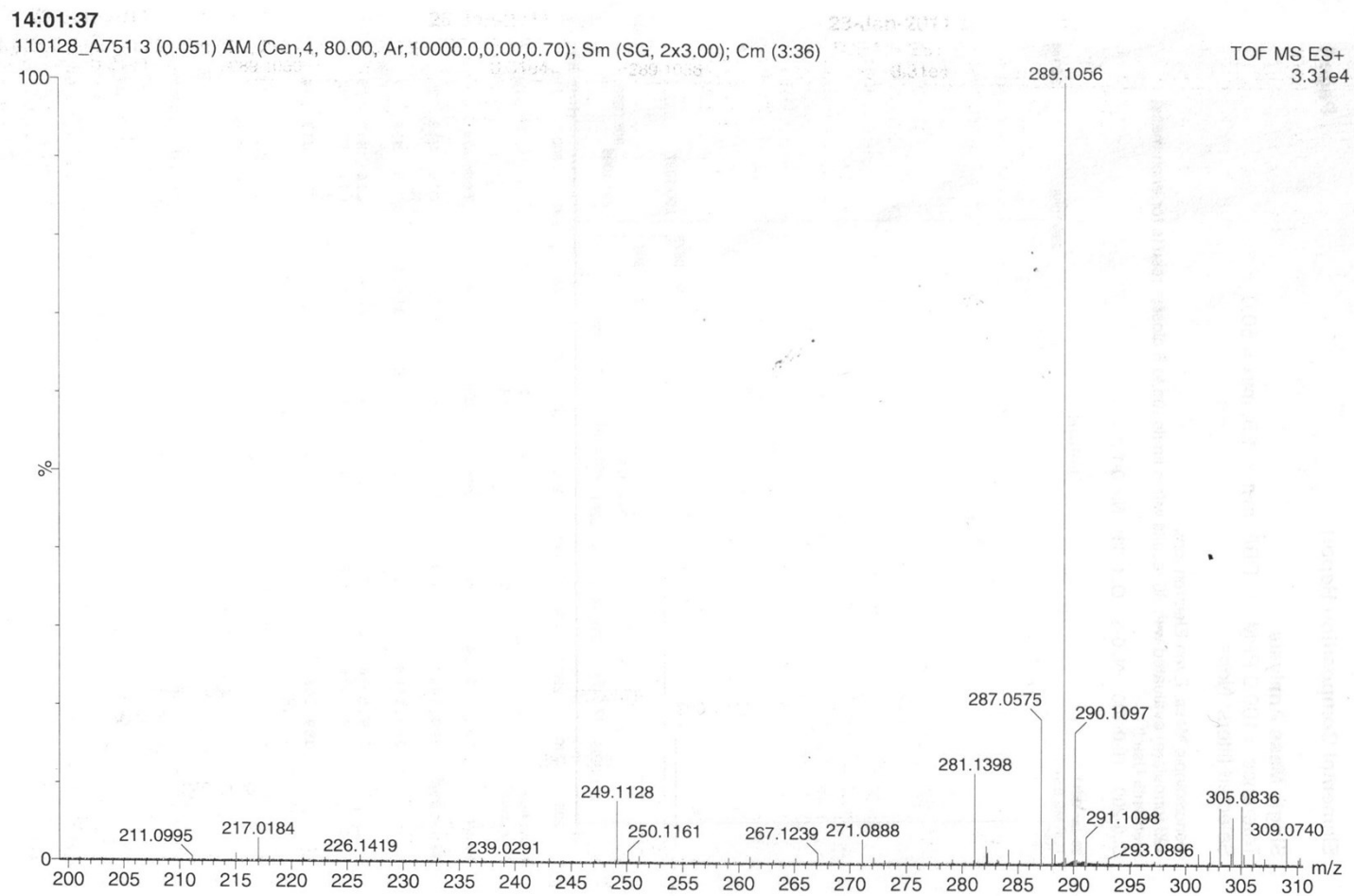
### Contents:

Page 2–9: HR-ESI-MS, IR, <sup>1</sup>H and <sup>13</sup>C (DEPT) NMR, HSQC, HMBC and NOESY spectra of **1**.

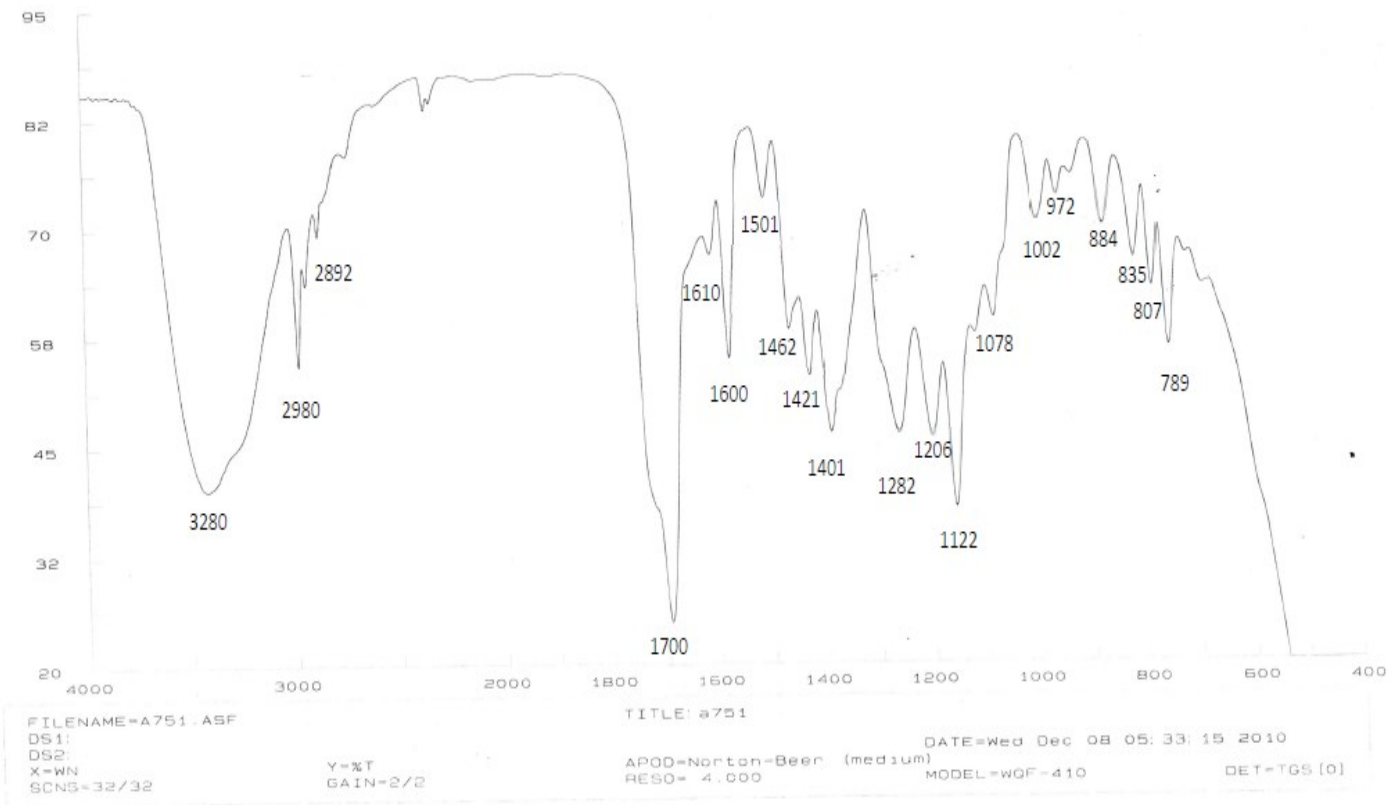
Page 10–17: HR-ESI-MS, IR, <sup>1</sup>H and <sup>13</sup>C (DEPT) NMR, HSQC, HMBC and NOESY spectra of **2**.

Page 18–25: HR-EI-MS, IR, <sup>1</sup>H and <sup>13</sup>C (DEPT) NMR, HSQC, HMBC and NOESY spectra of **3**.

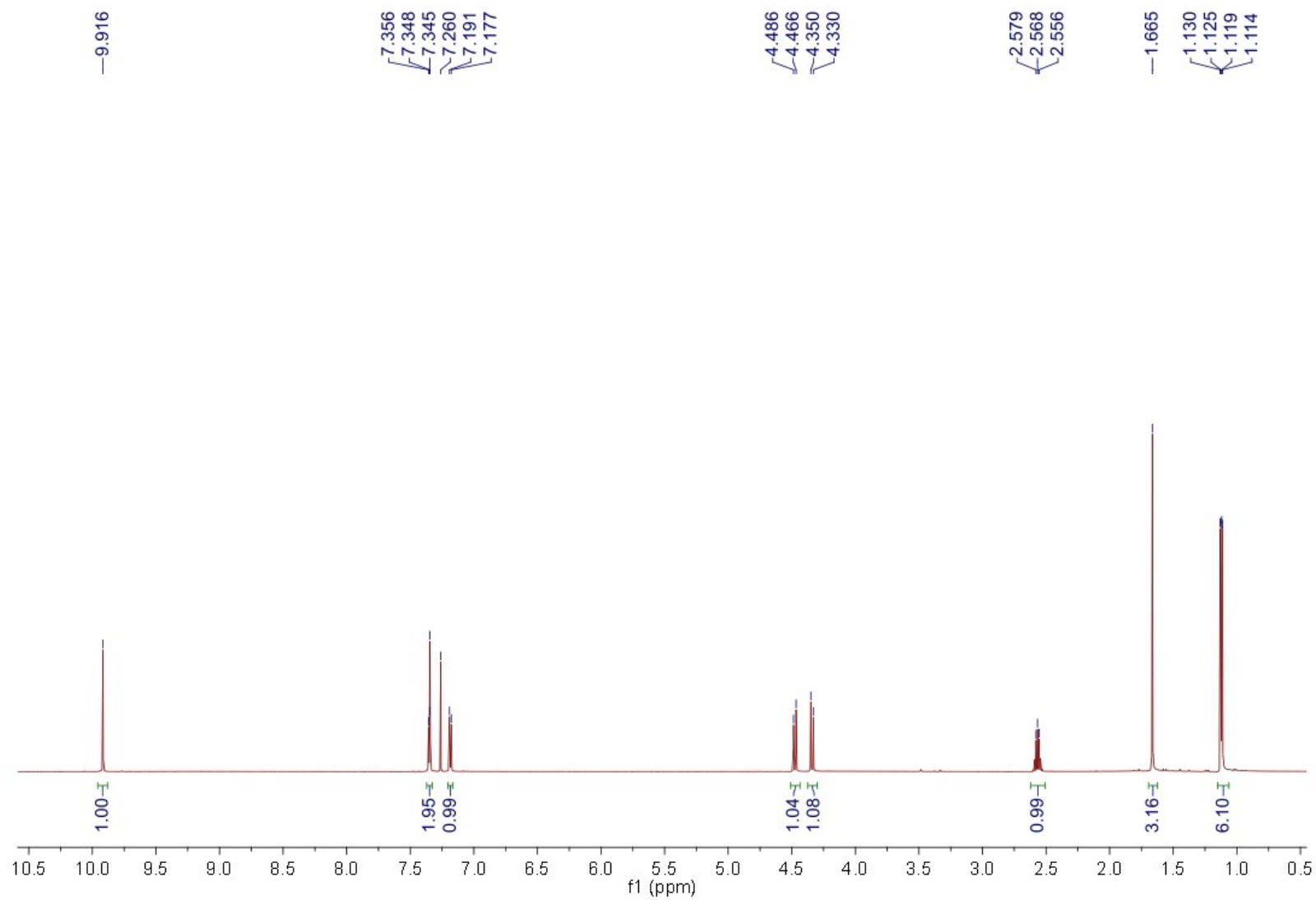
# HR-ESI-MS spectrum of compound 1



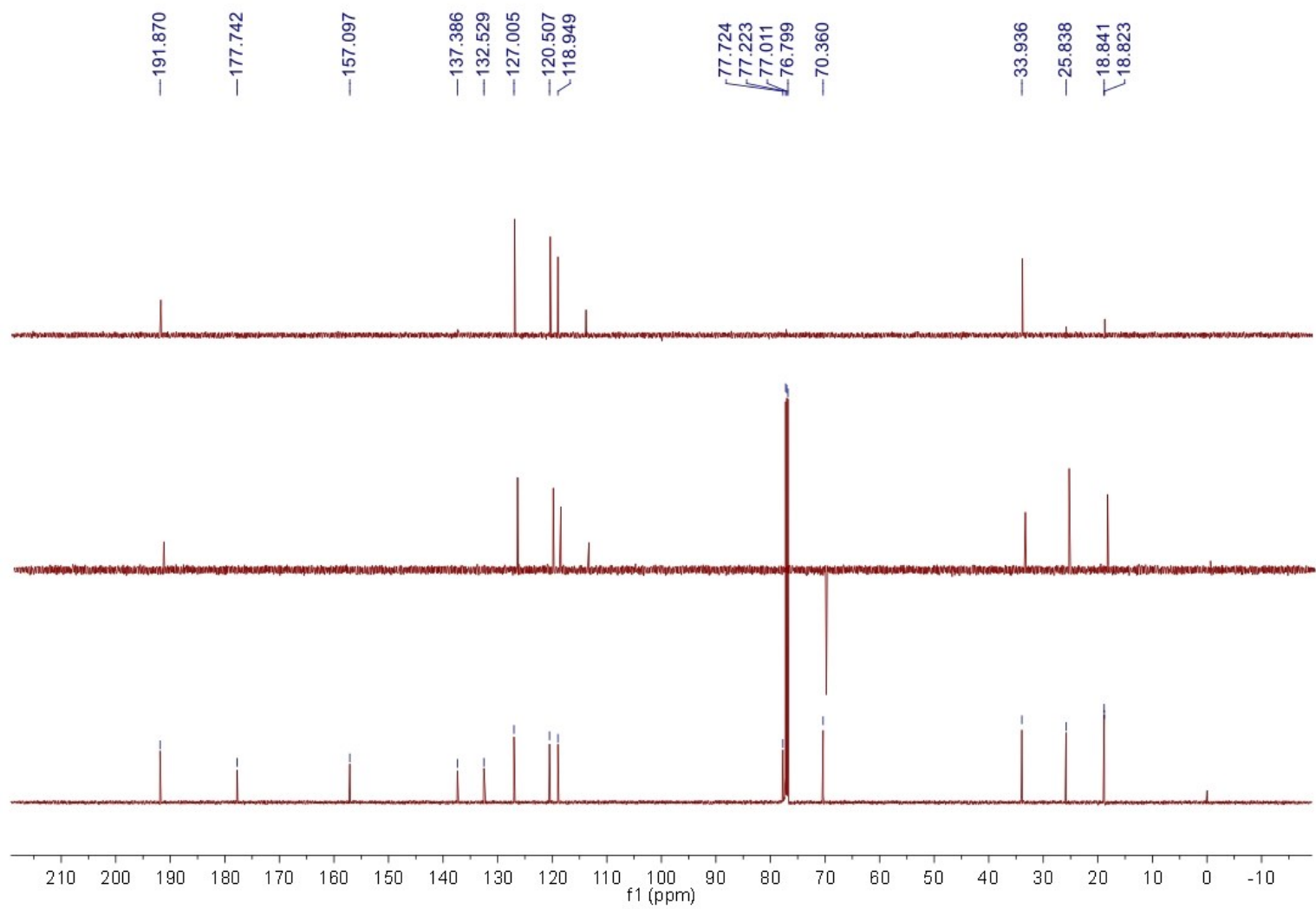
# IR spectrum of compound 1



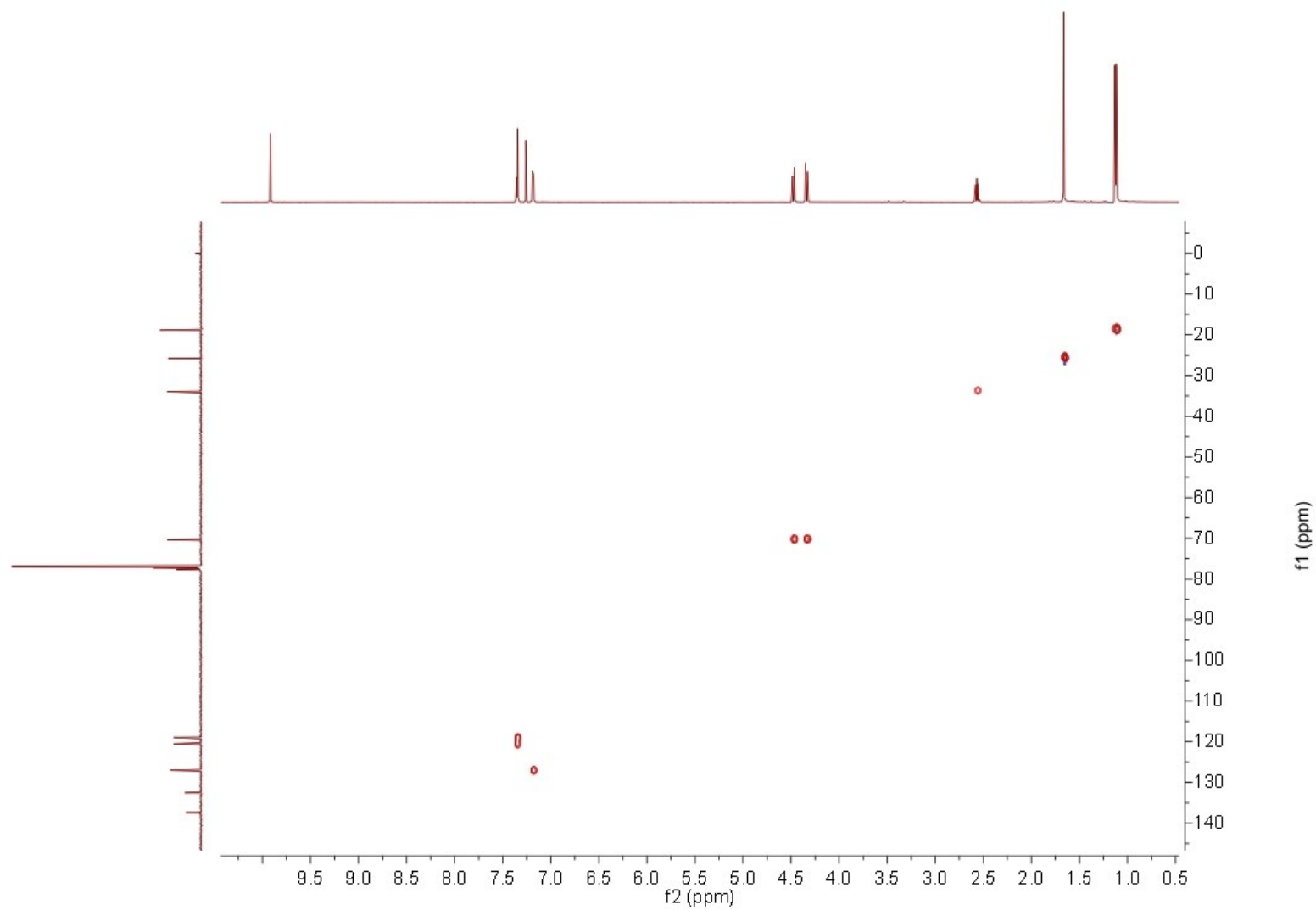
# $^1\text{H}$ -NMR spectrum of compound **1**



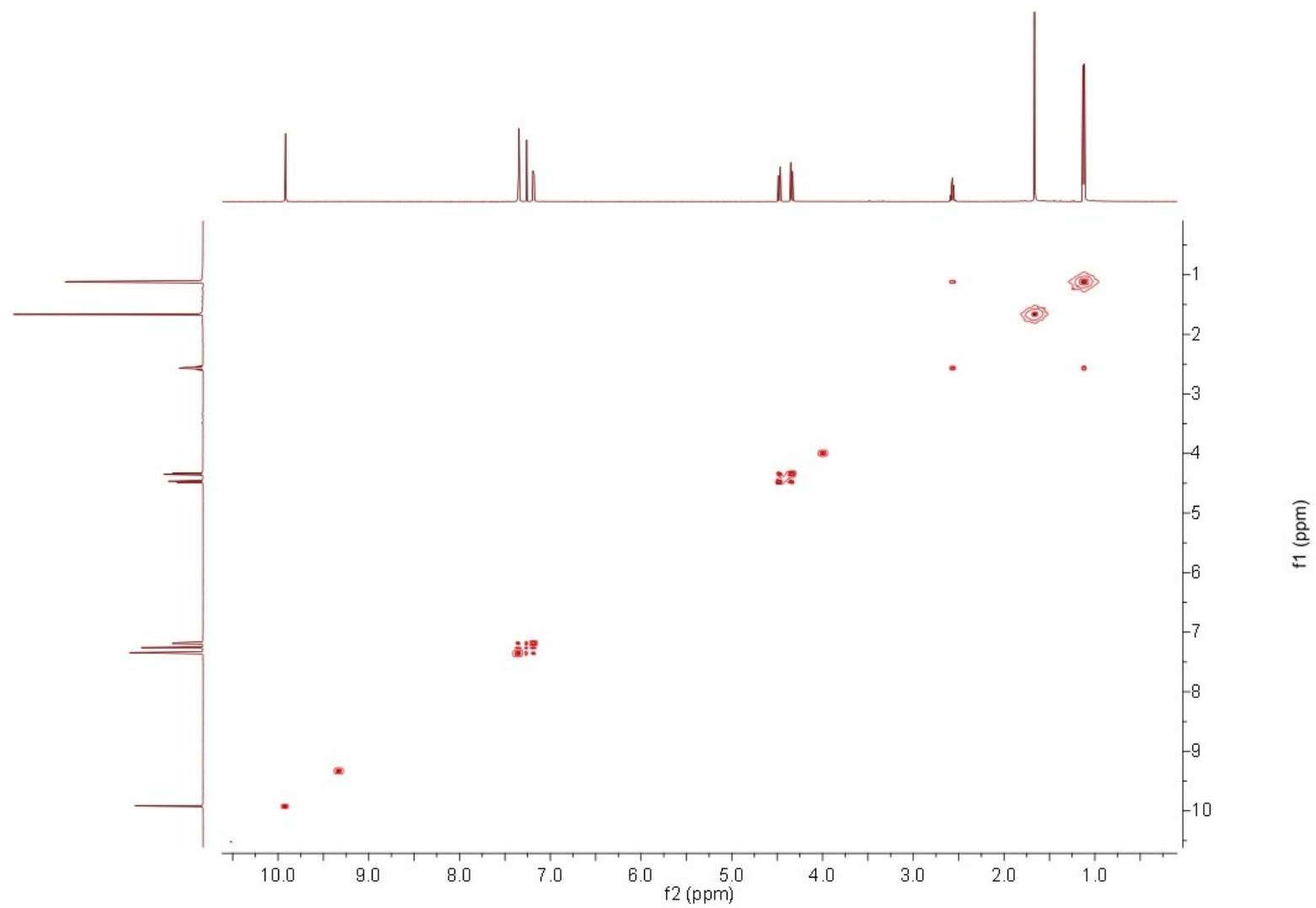
$^{13}\text{C}$ -NMR (DEPT) spectra of compound **1**



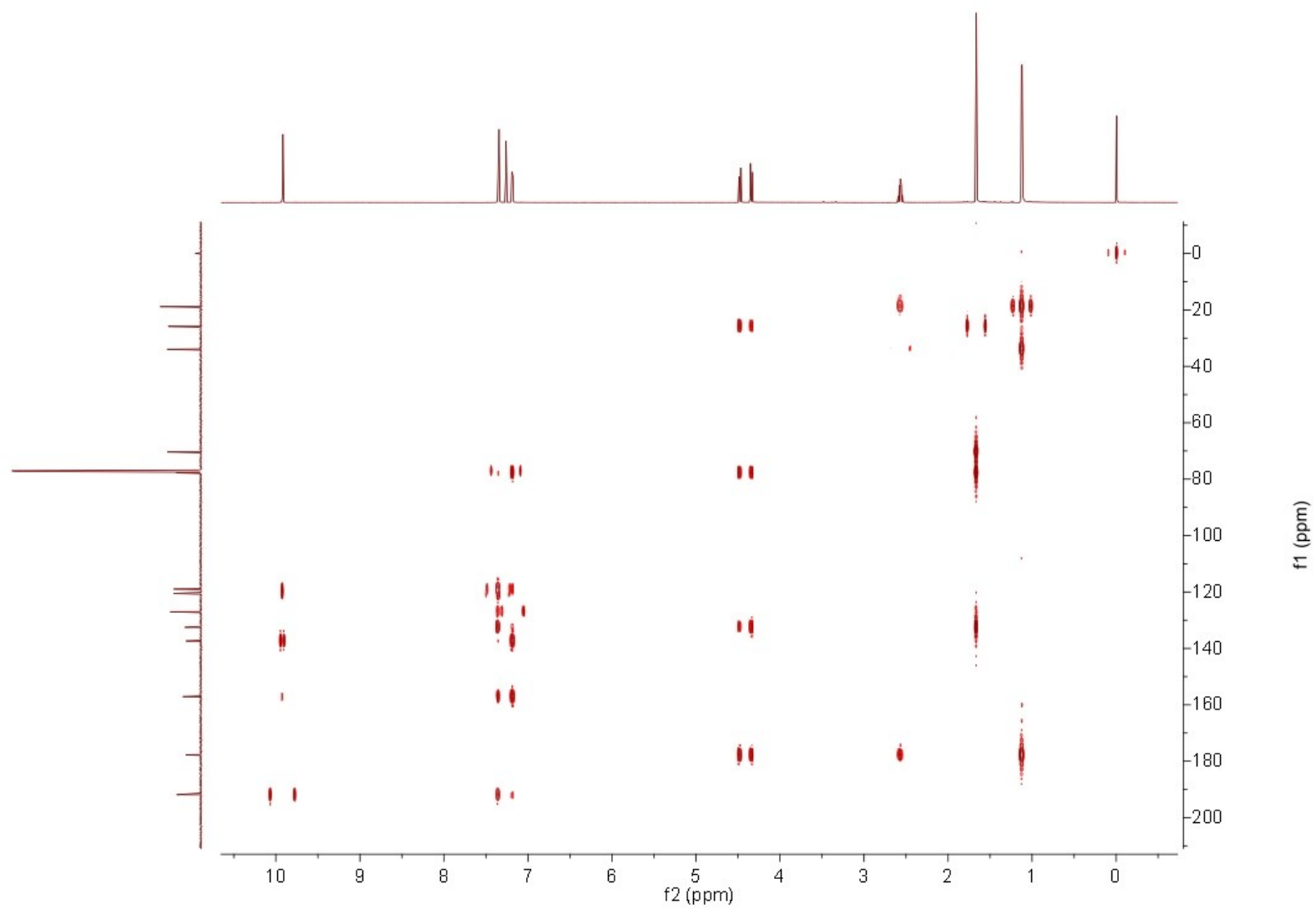
# HSQC spectrum of compound 1



$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1**

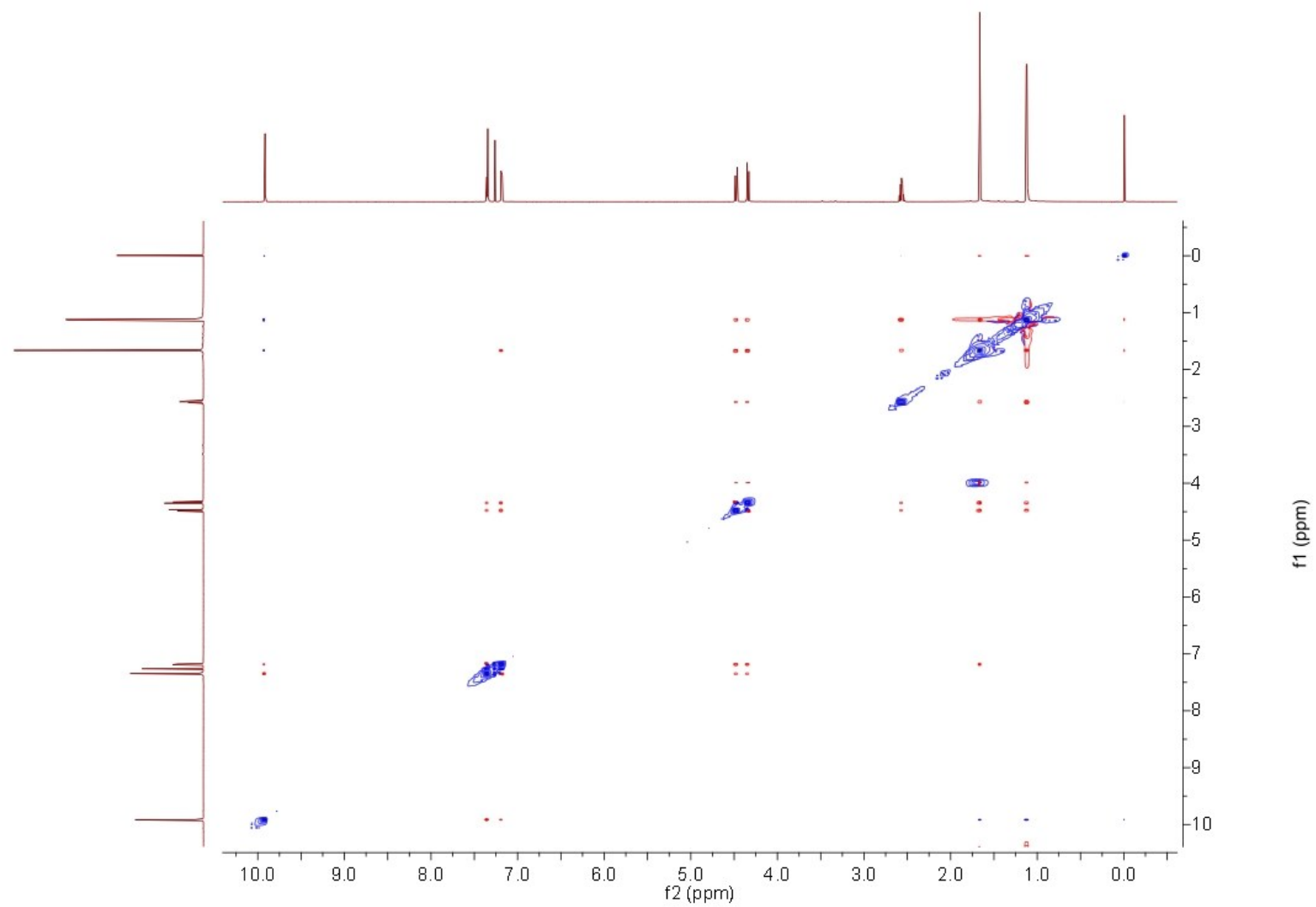


# HMBC spectrum of compound **1**

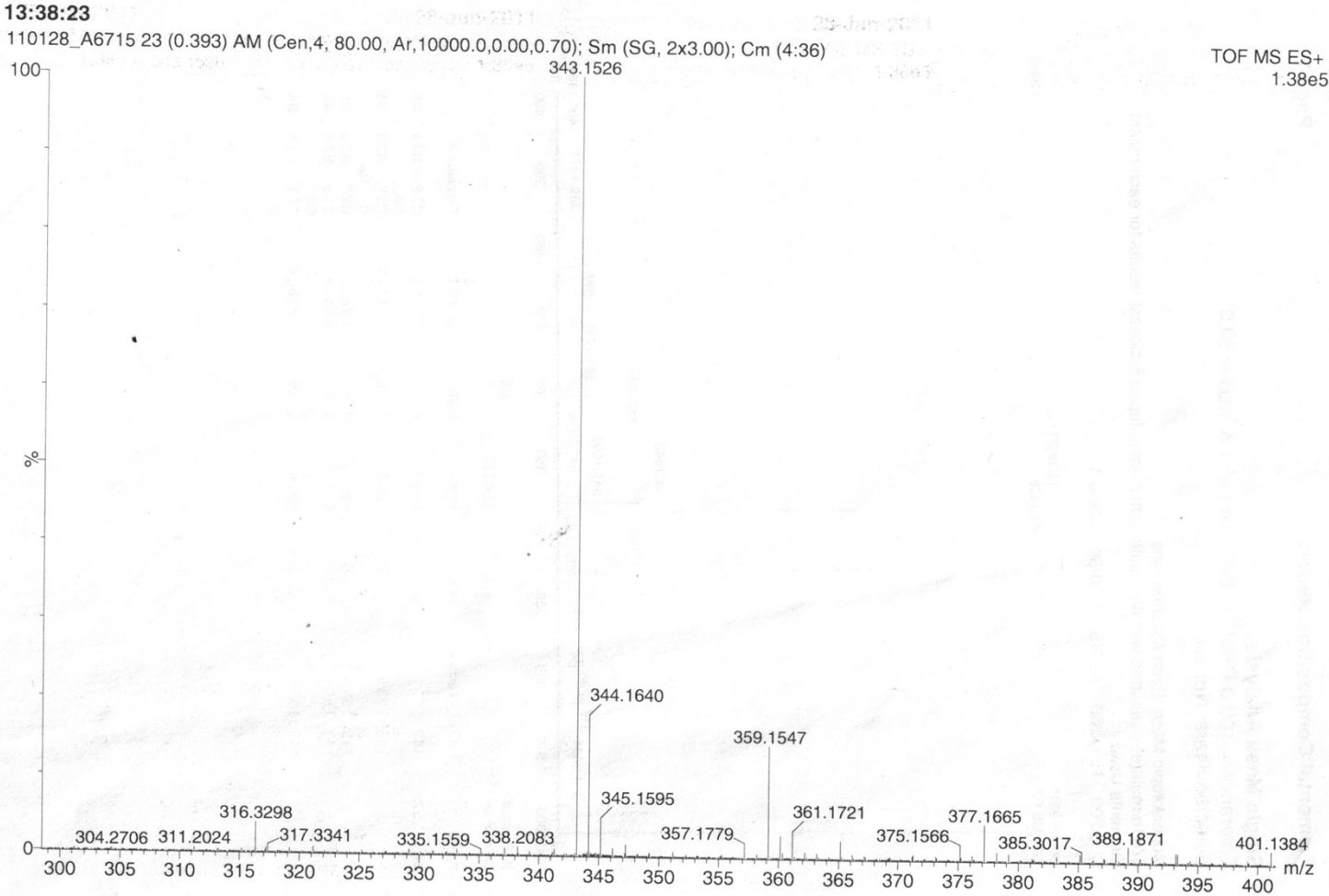




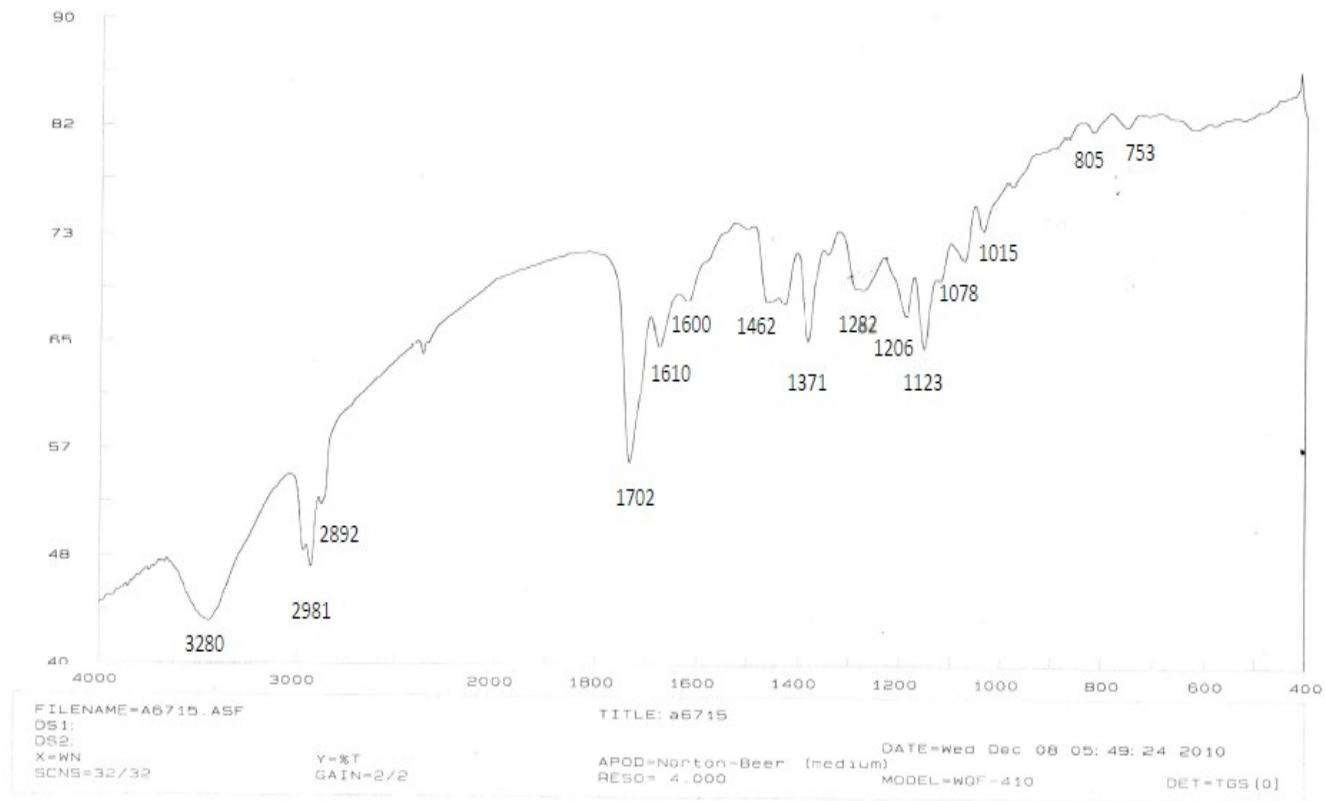
# NOESY spectrum of compound 1



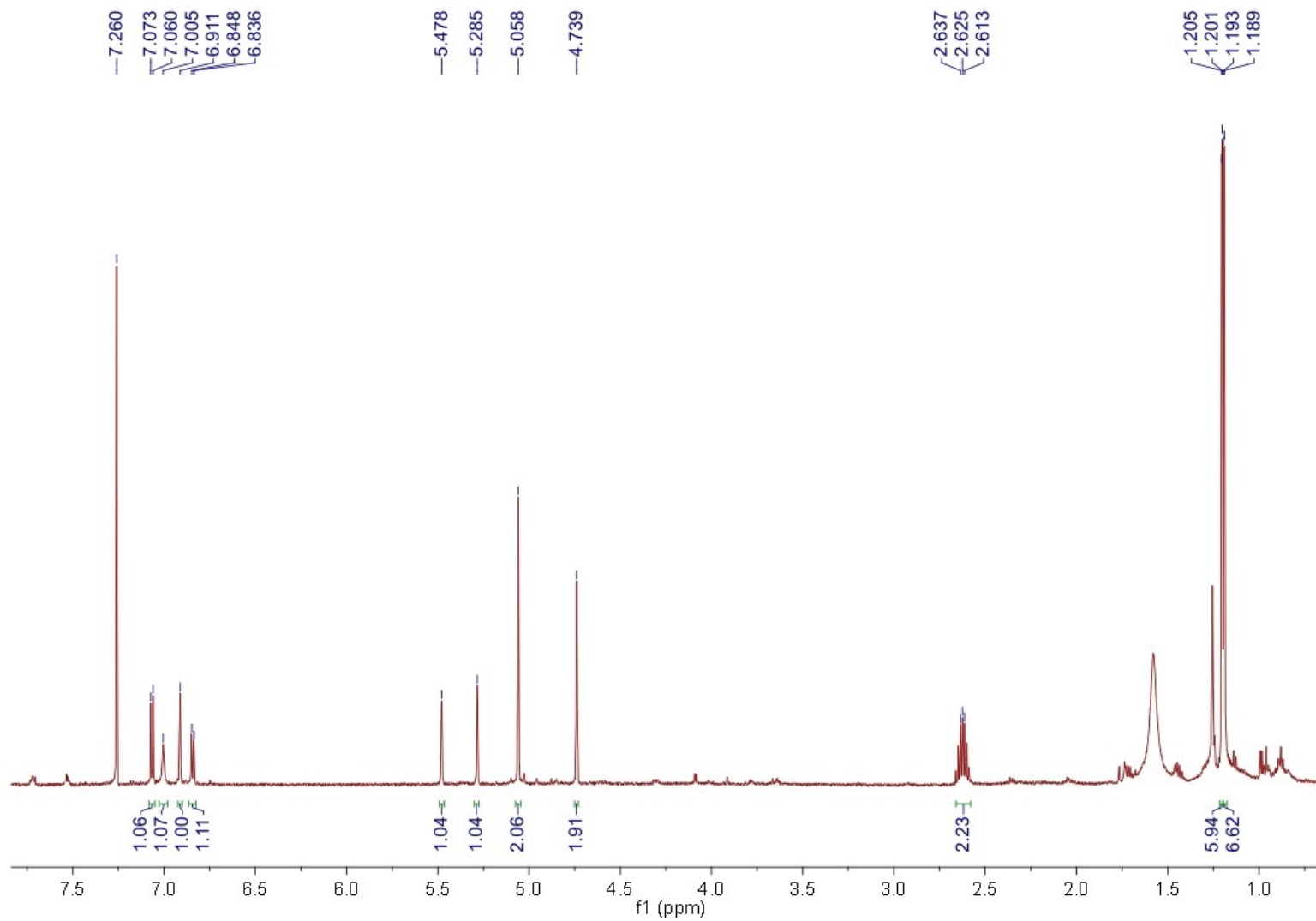
# HR-ESI-MS spectrum of compound 2



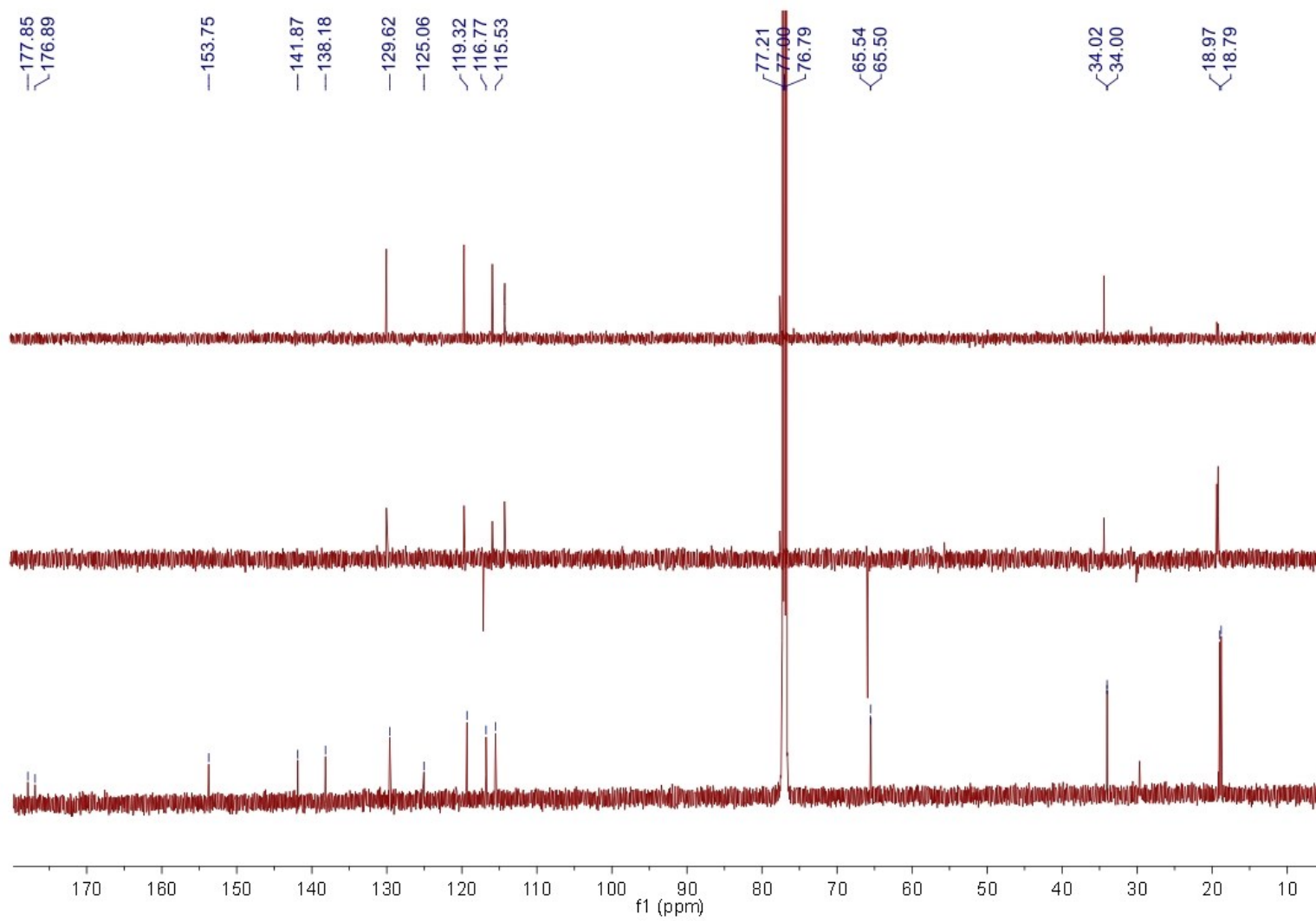
# IR spectrum of compound 2



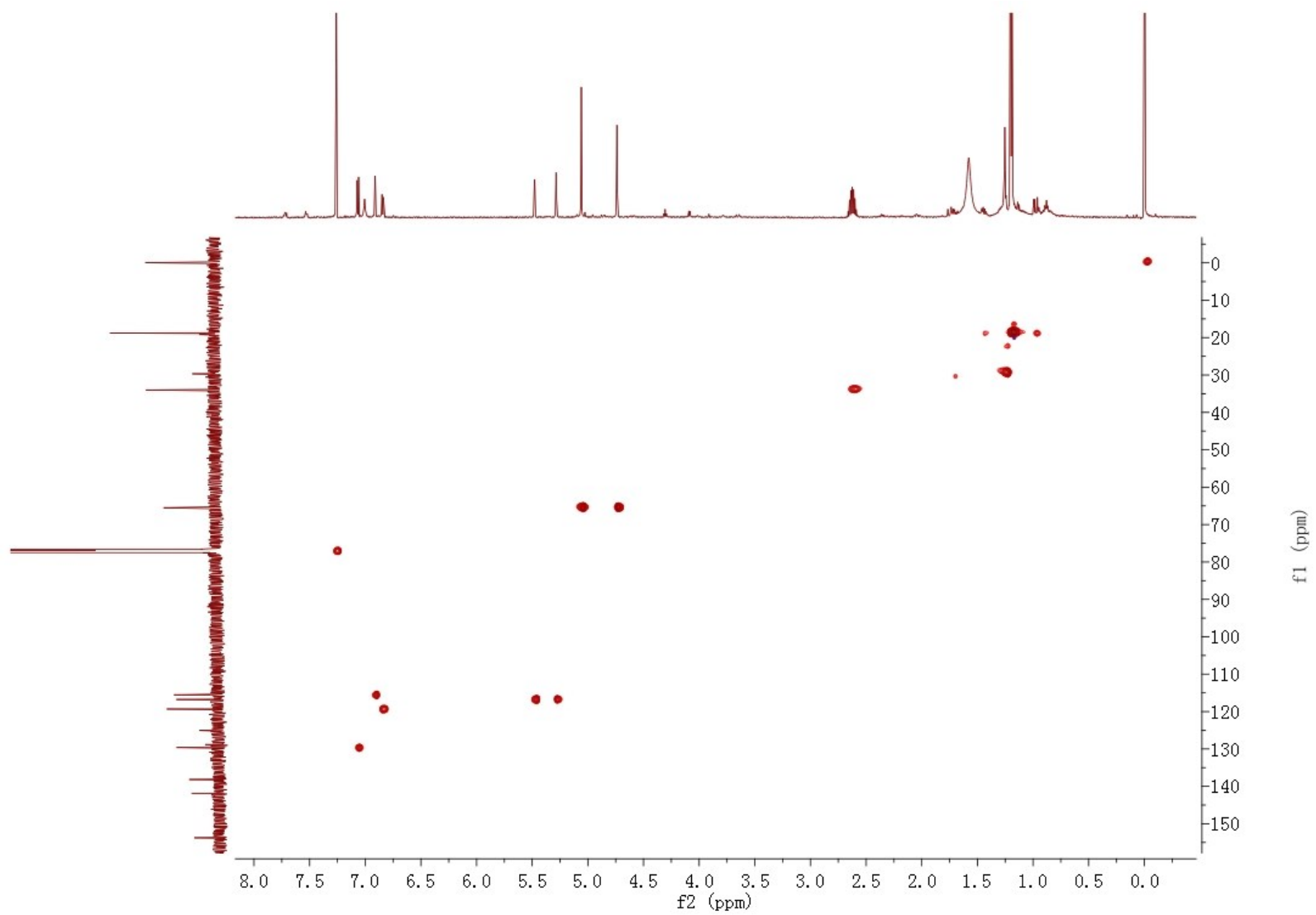
# $^1\text{H-NMR}$ spectrum of compound **2**



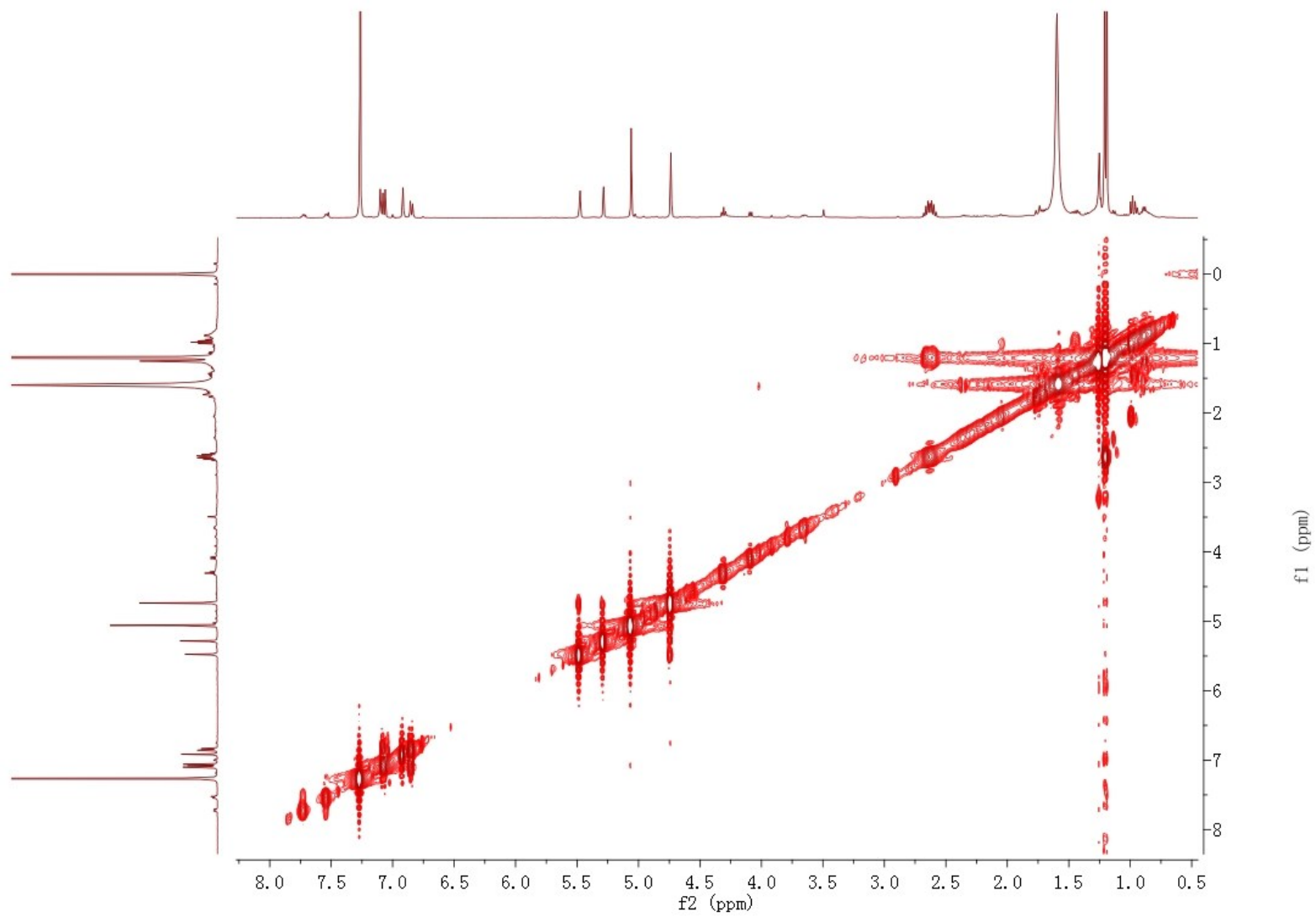
$^{13}\text{C}$ -NMR (DEPT) spectra of compound **2**



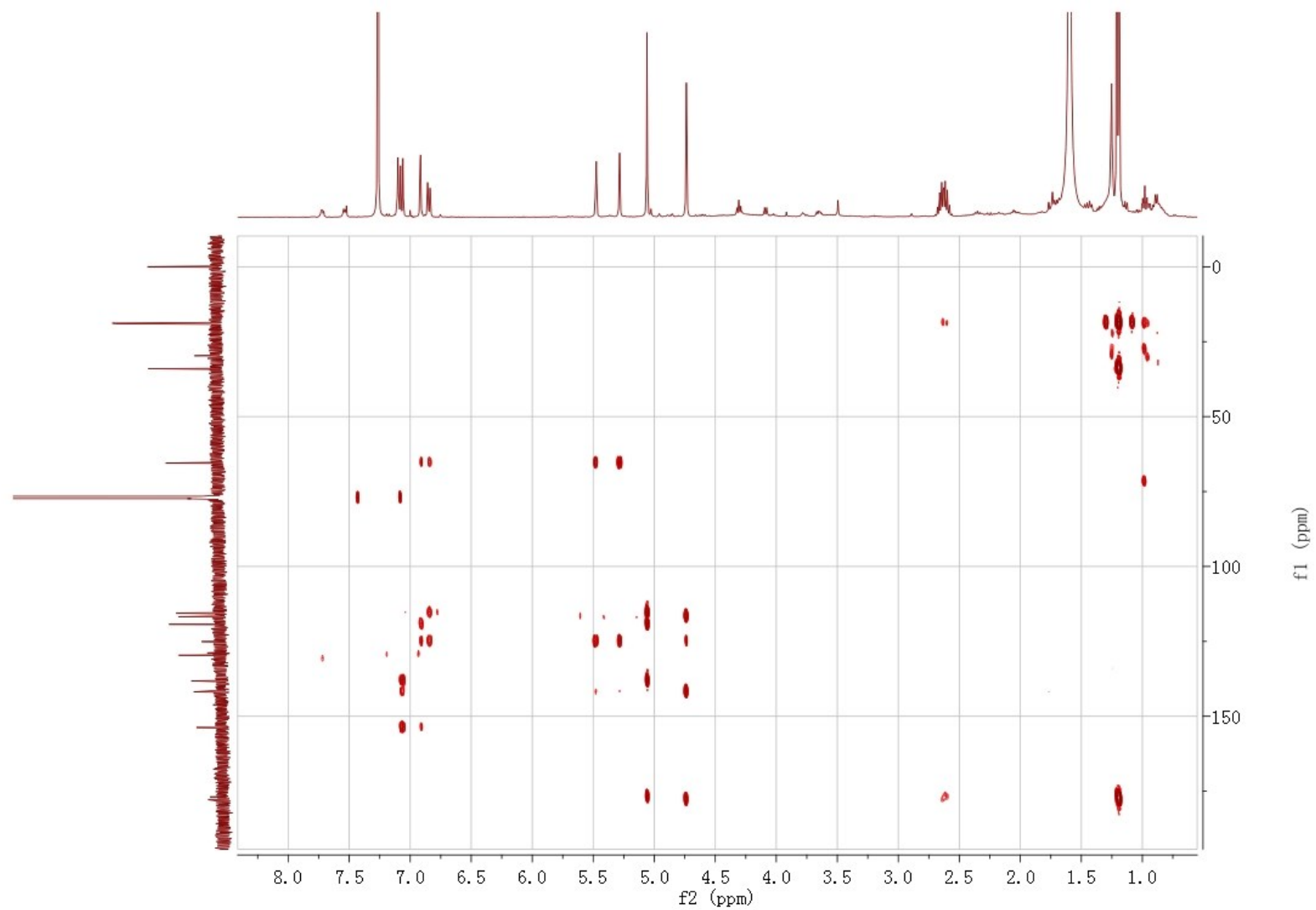
# HSQC spectrum of compound 2



$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2**

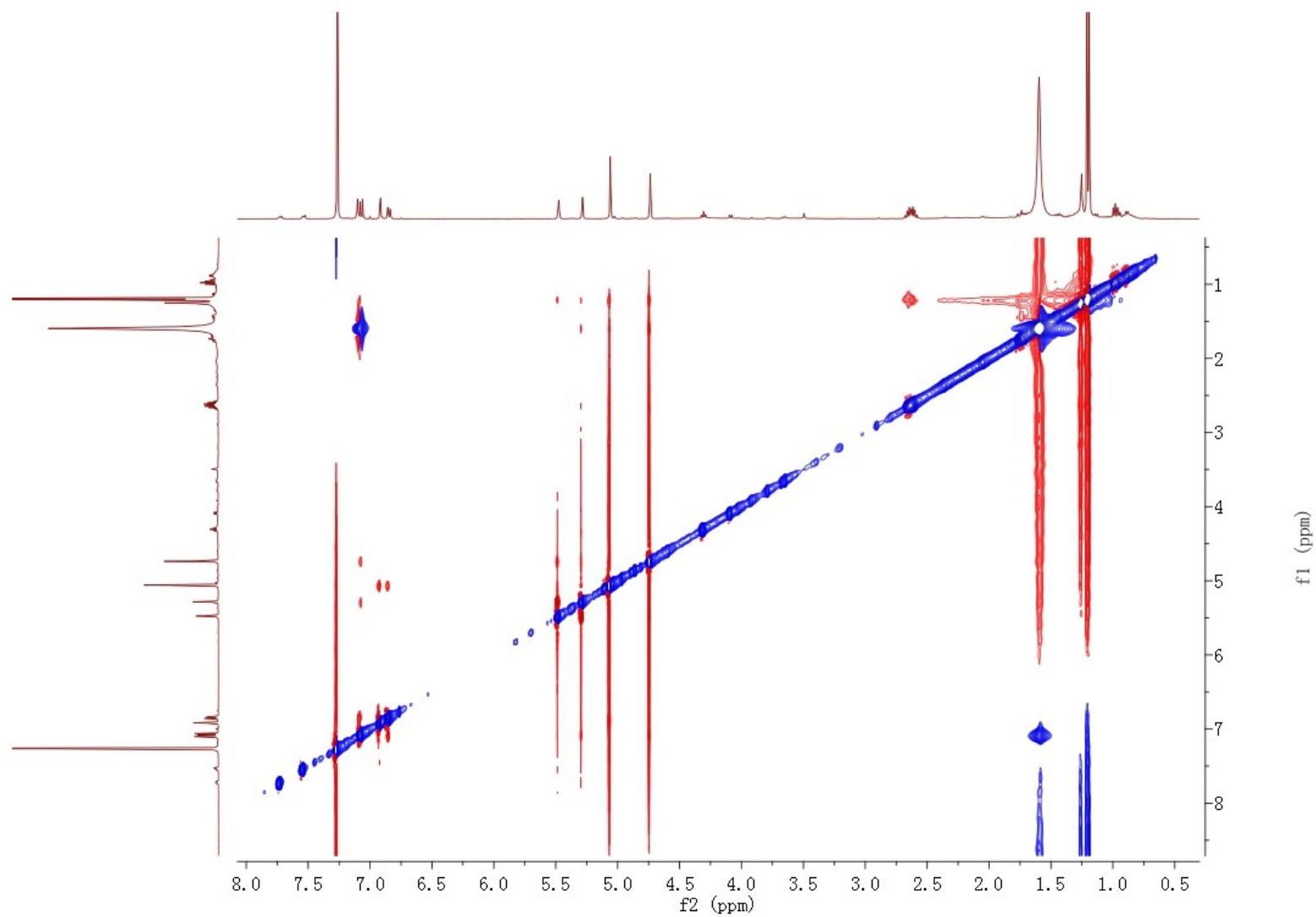


# HMBC spectrum of compound 2

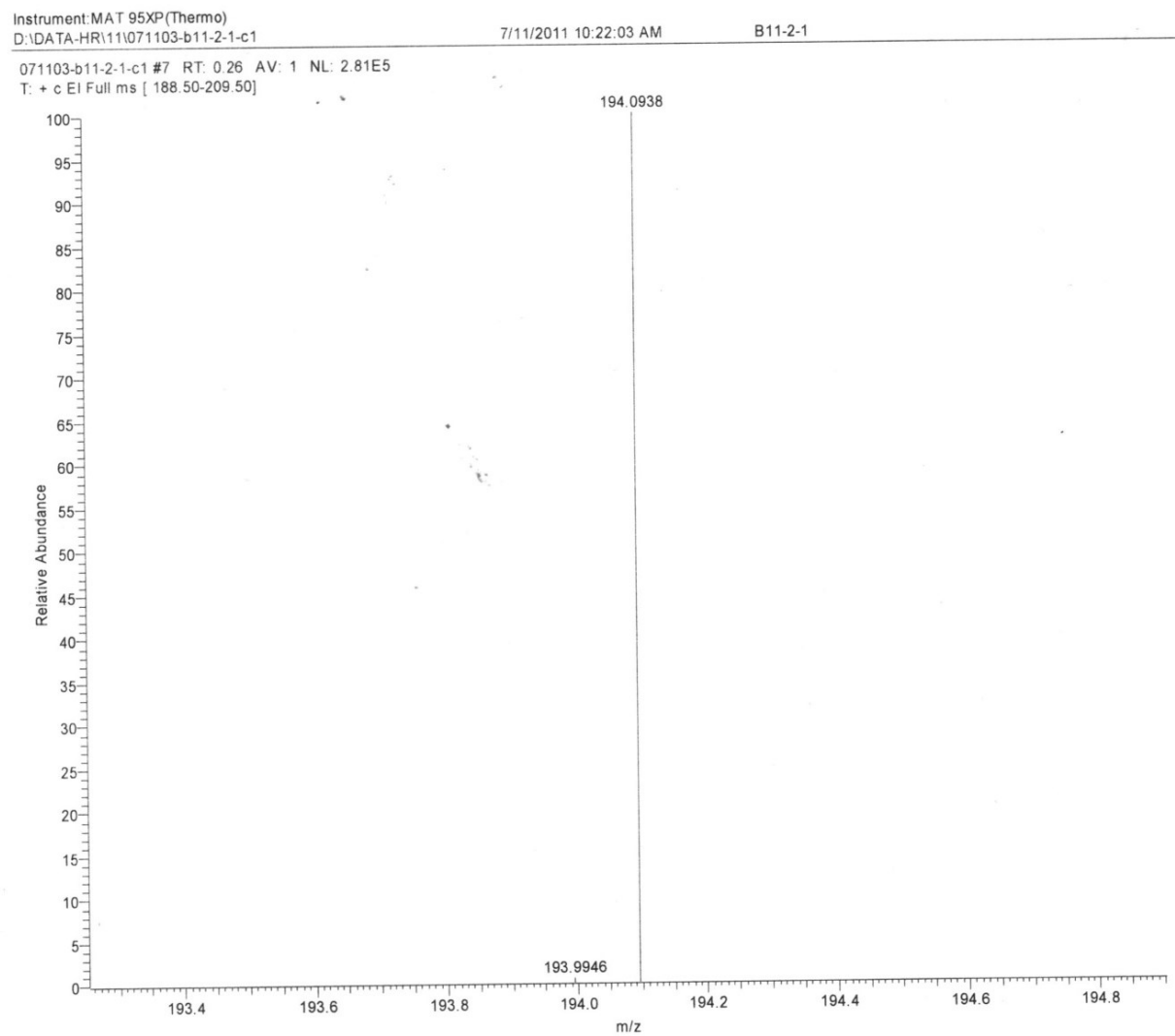




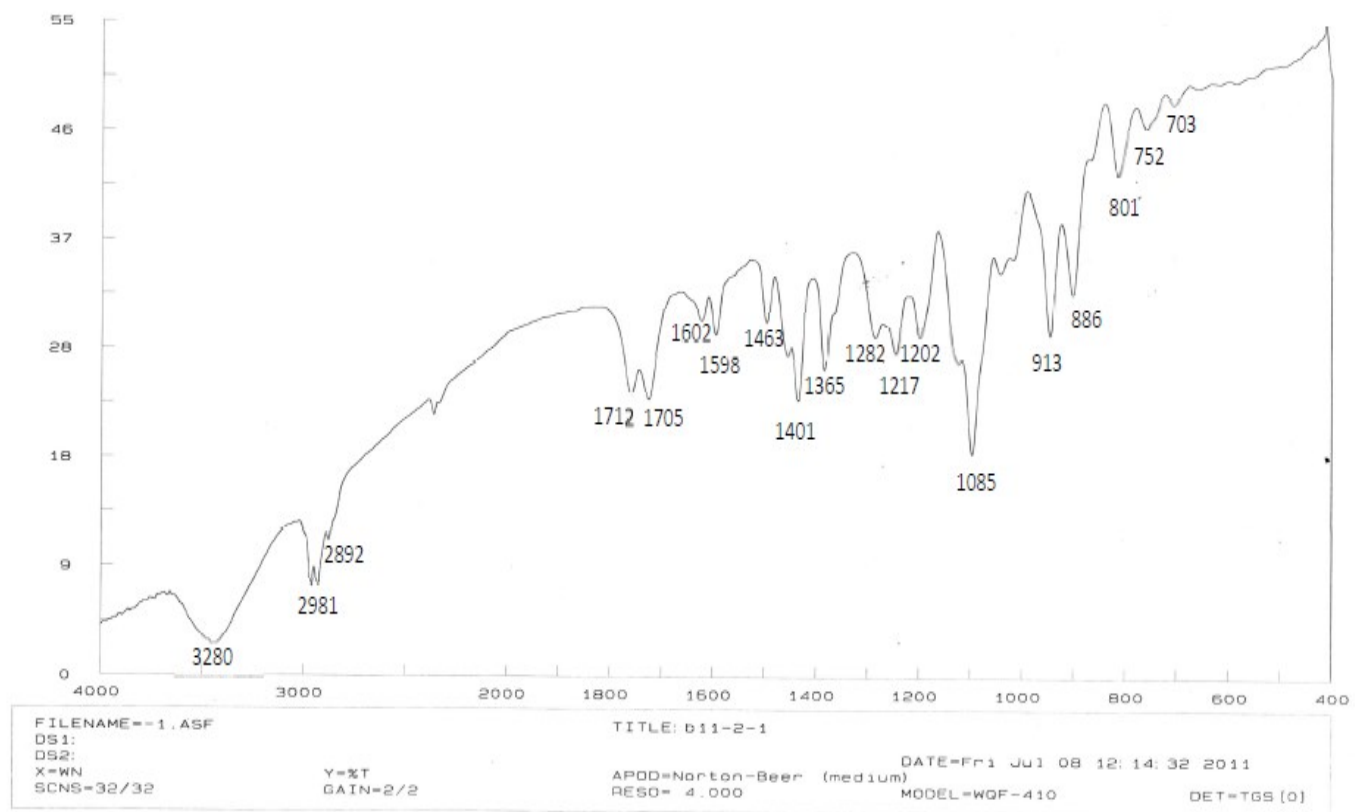
# NOESY spectrum of compound 2



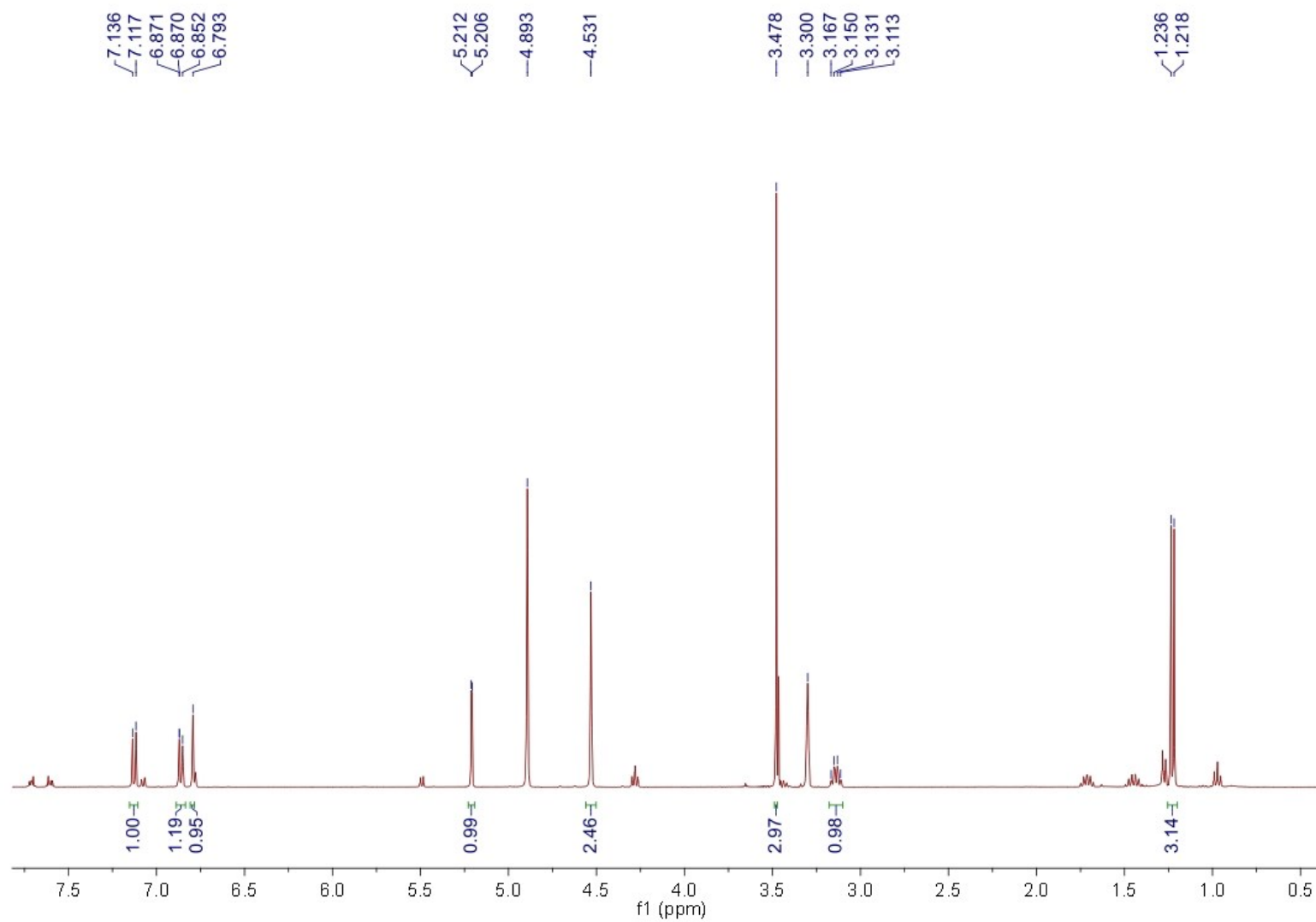
# HR-EI-MS spectrum of compound 3



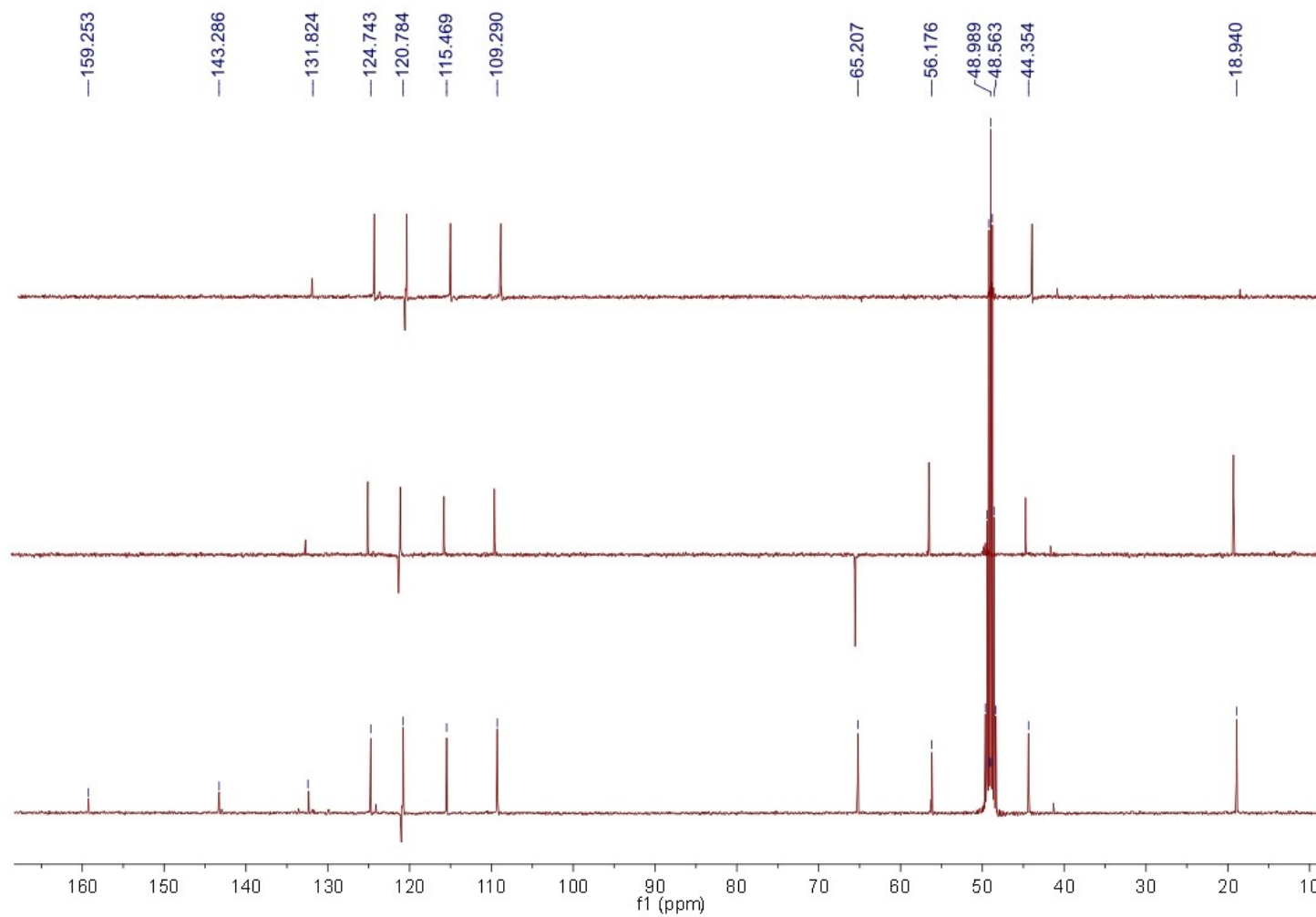
# IR spectrum of compound 3



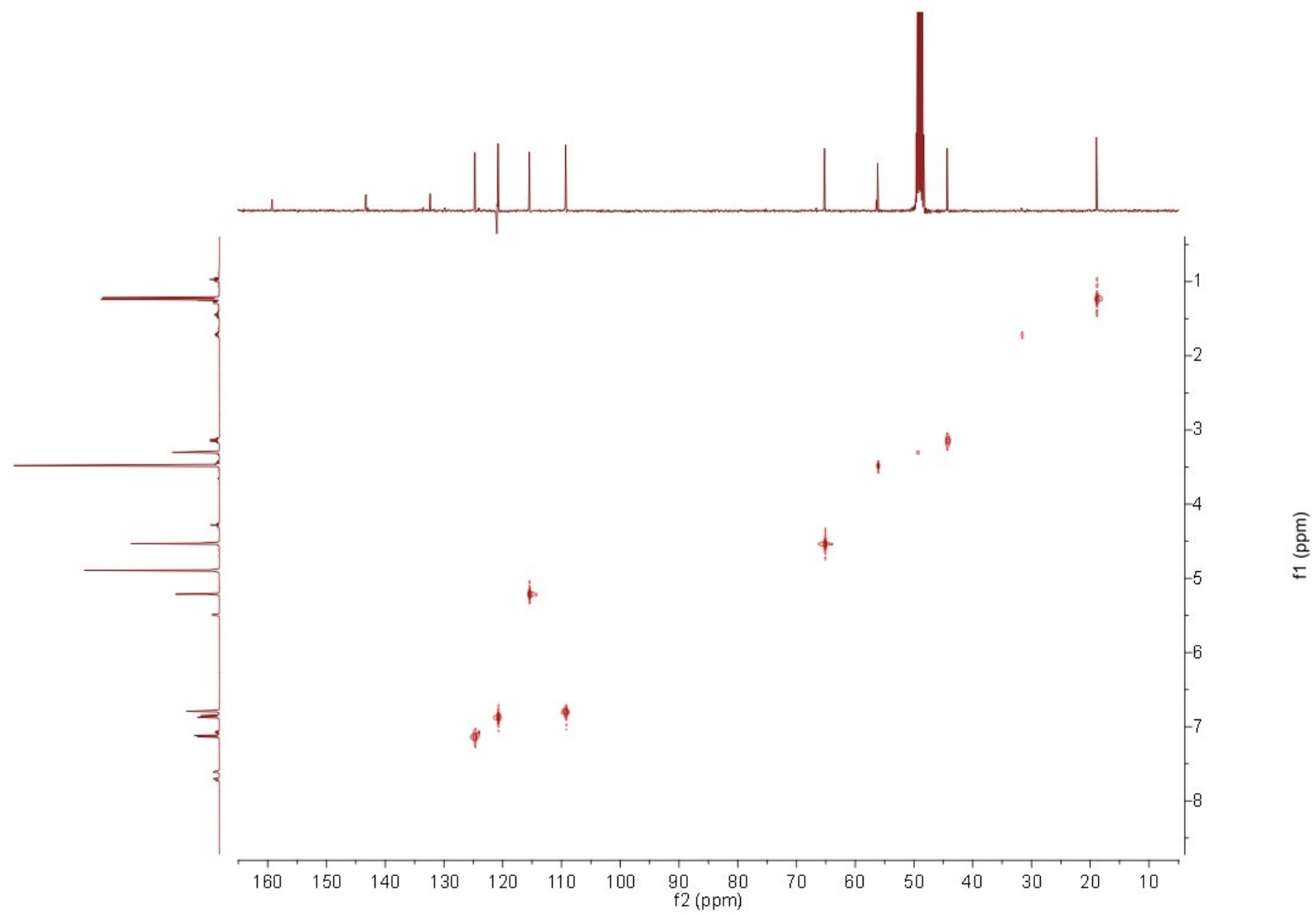
# $^1\text{H-NMR}$ spectrum of compound **3**



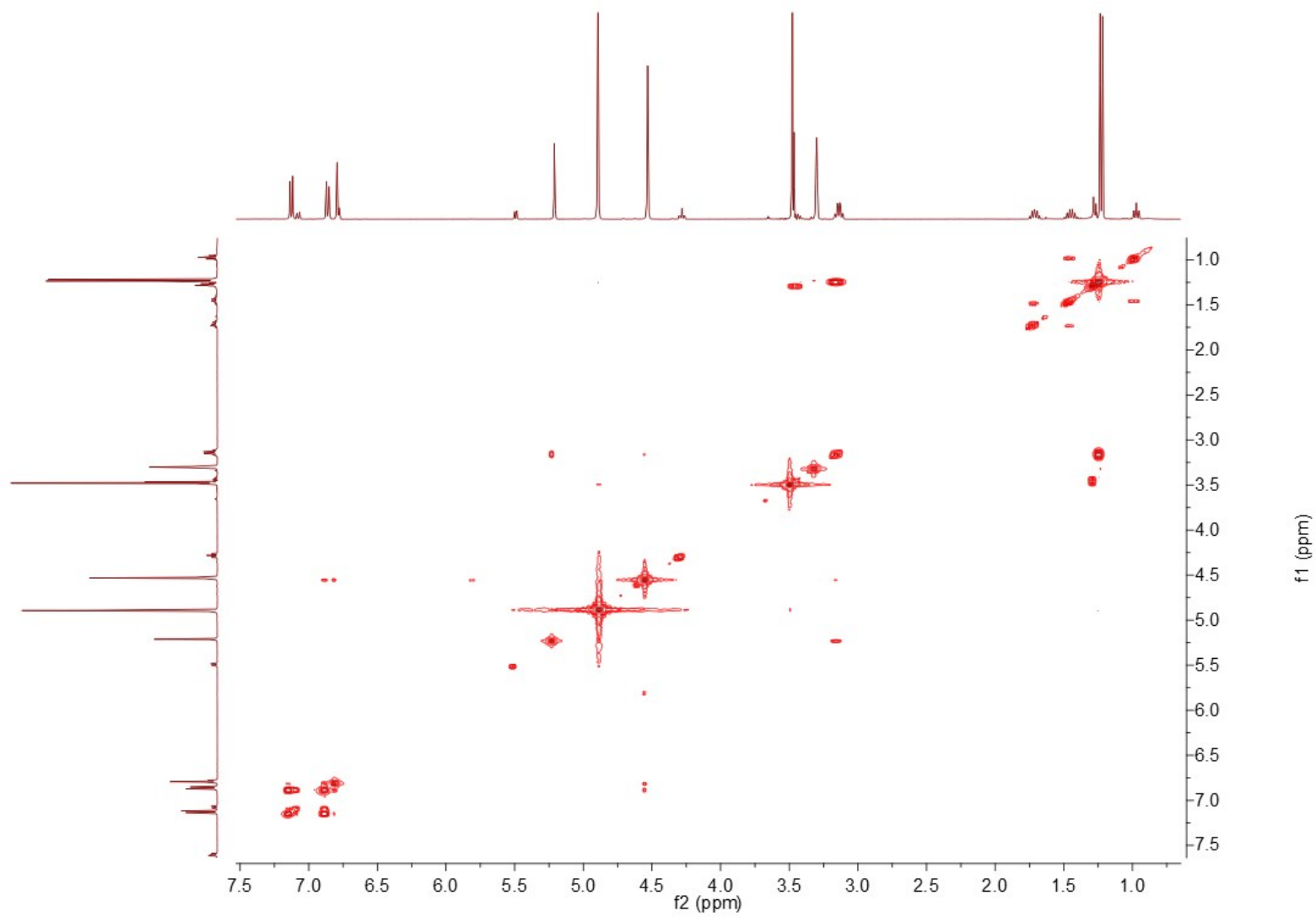
$^{13}\text{C}$ -NMR (DEPT) spectra of compound **3**



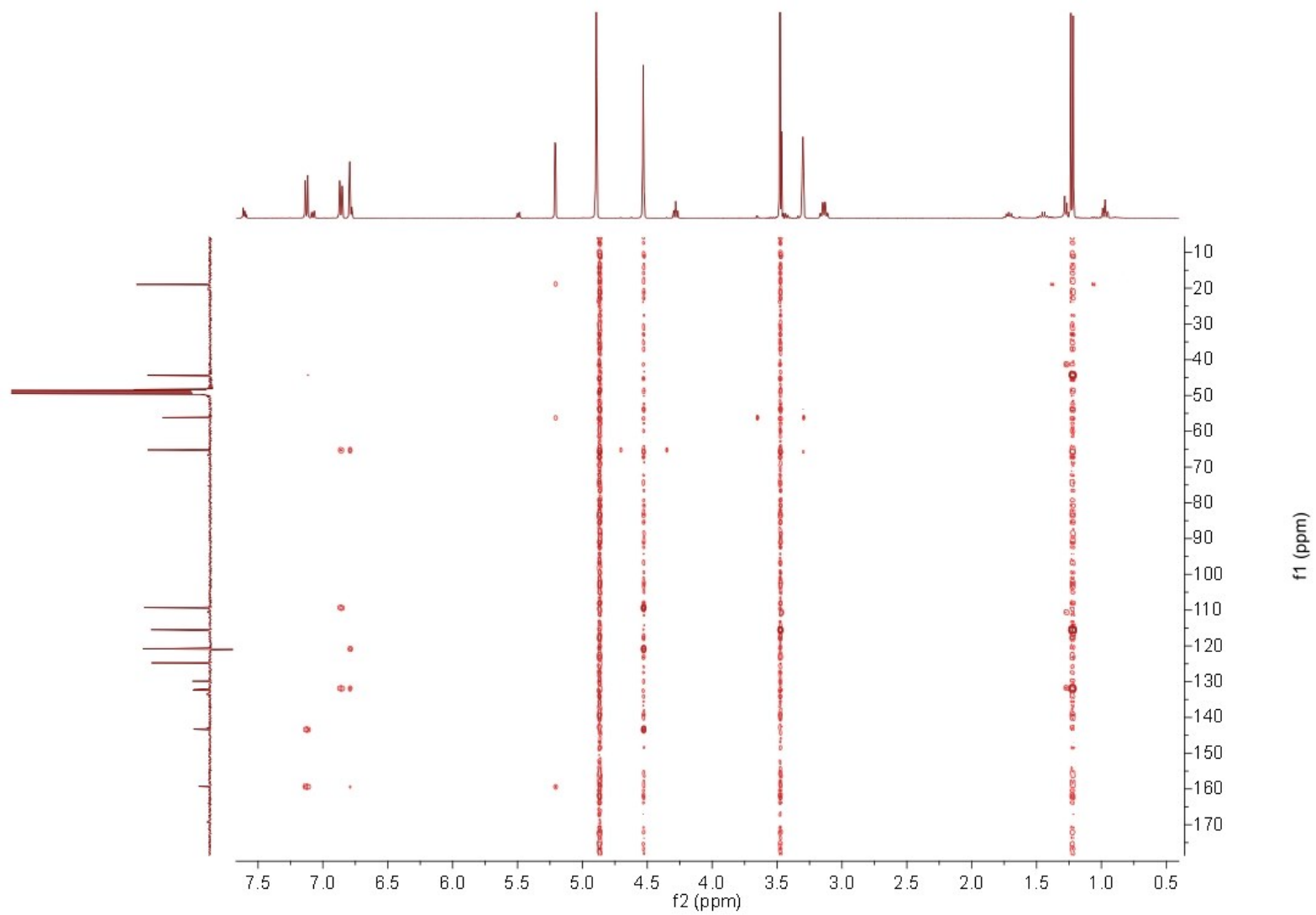
# HSQC spectrum of compound 3



$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **3**



# HMBC spectrum of compound 3





# NOESY spectrum of compound 3

