

# SUPPORTING INFORMATION

## Isoflavones and Rotenoids from the Leaves of *Millettia oblata* ssp. *teitensis*

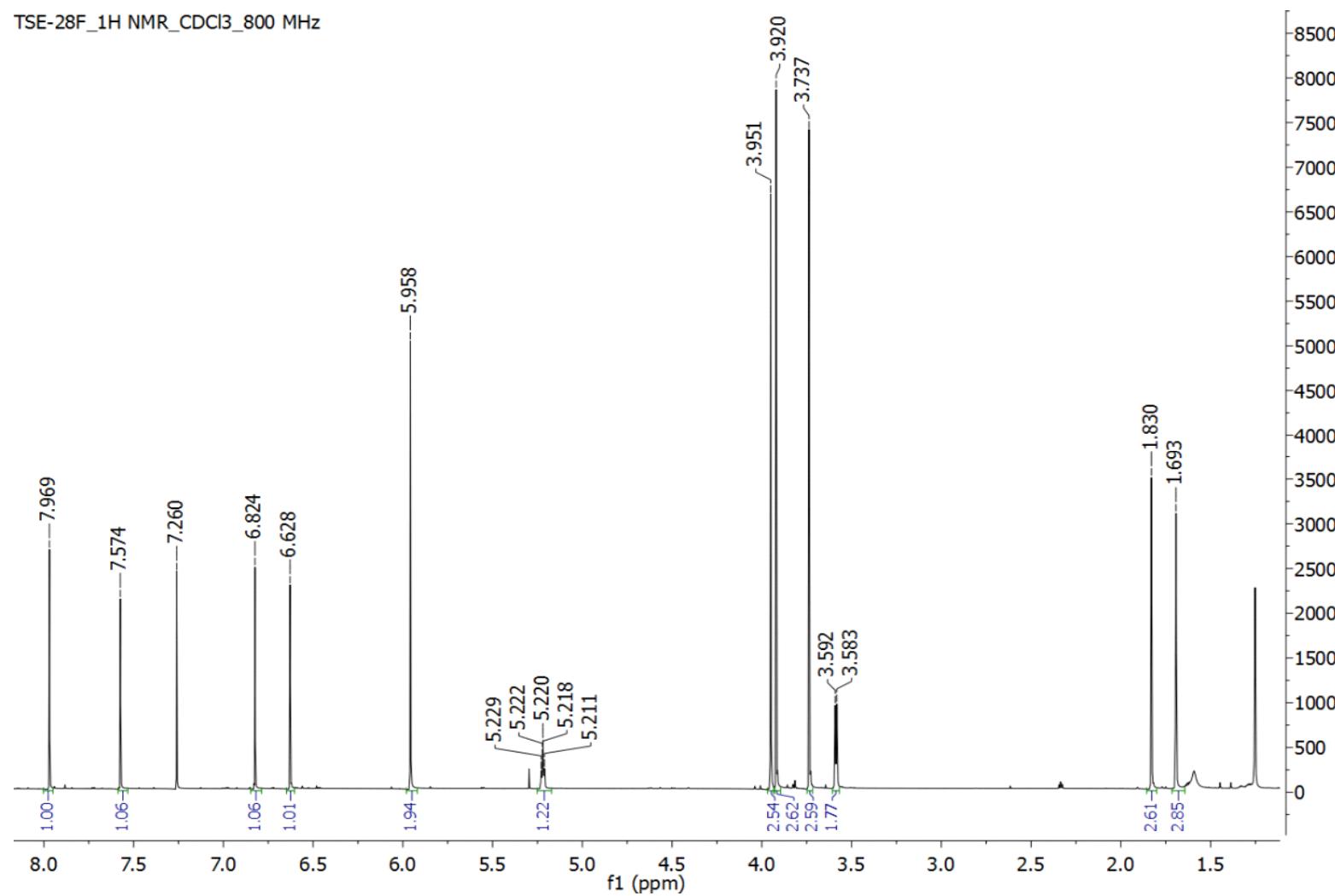
Tsegaye Deyou, Marco Makungu, Matthias Heydenreich, Fangfang Pan, Amra Gruhonjic, Paul A. Fitzpatrick,  
Andreas Koch, Solomon Derese, Jerry Pelletier, Kari Rissanen, Abiy Yenesew, and Máté Erdélyi

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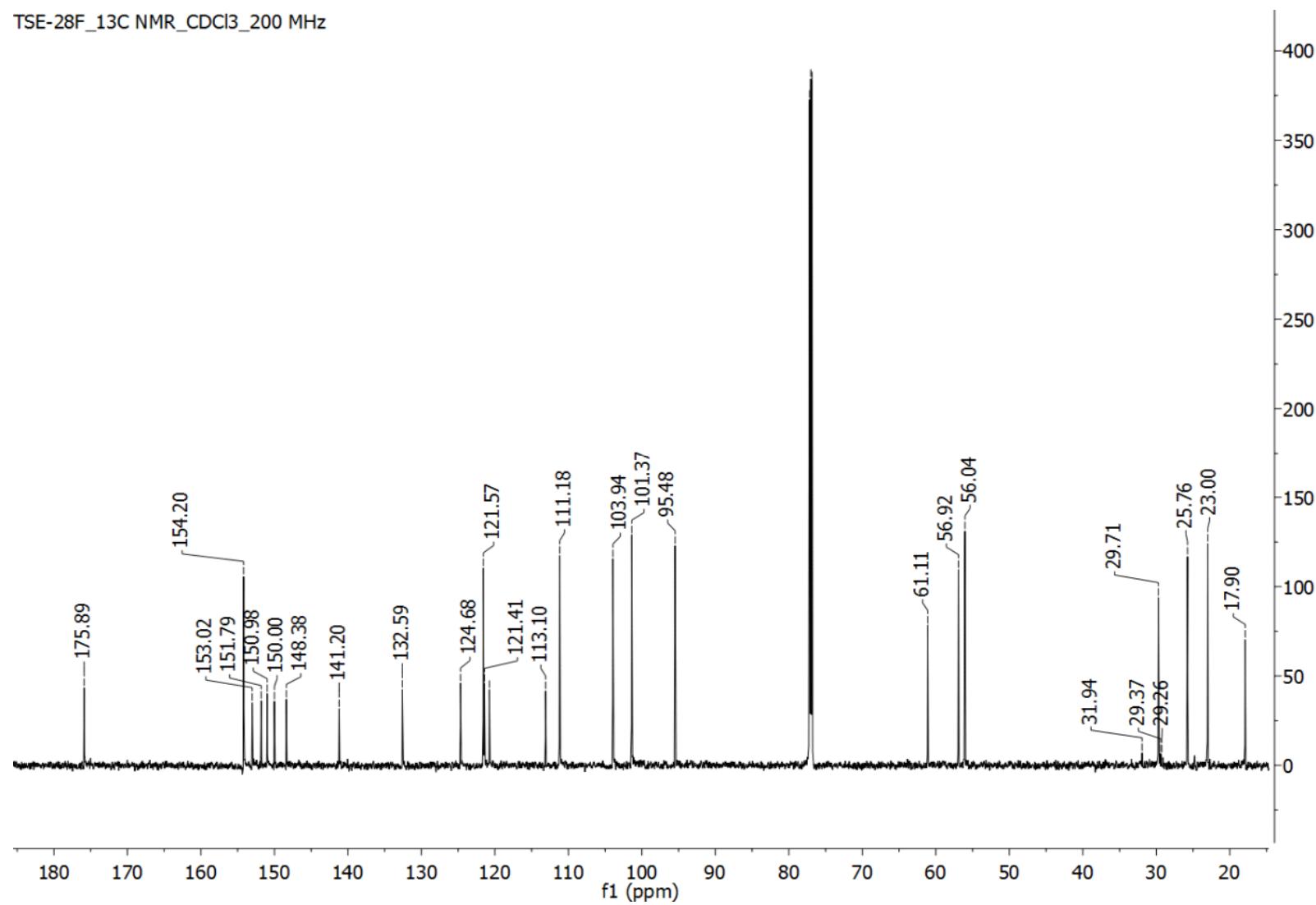
**Figure S1A:**  $^1\text{H}$  NMR (799.87 MHz) spectrum of compound 1

TSE-28F\_1H NMR\_CDCI3\_800 MHz

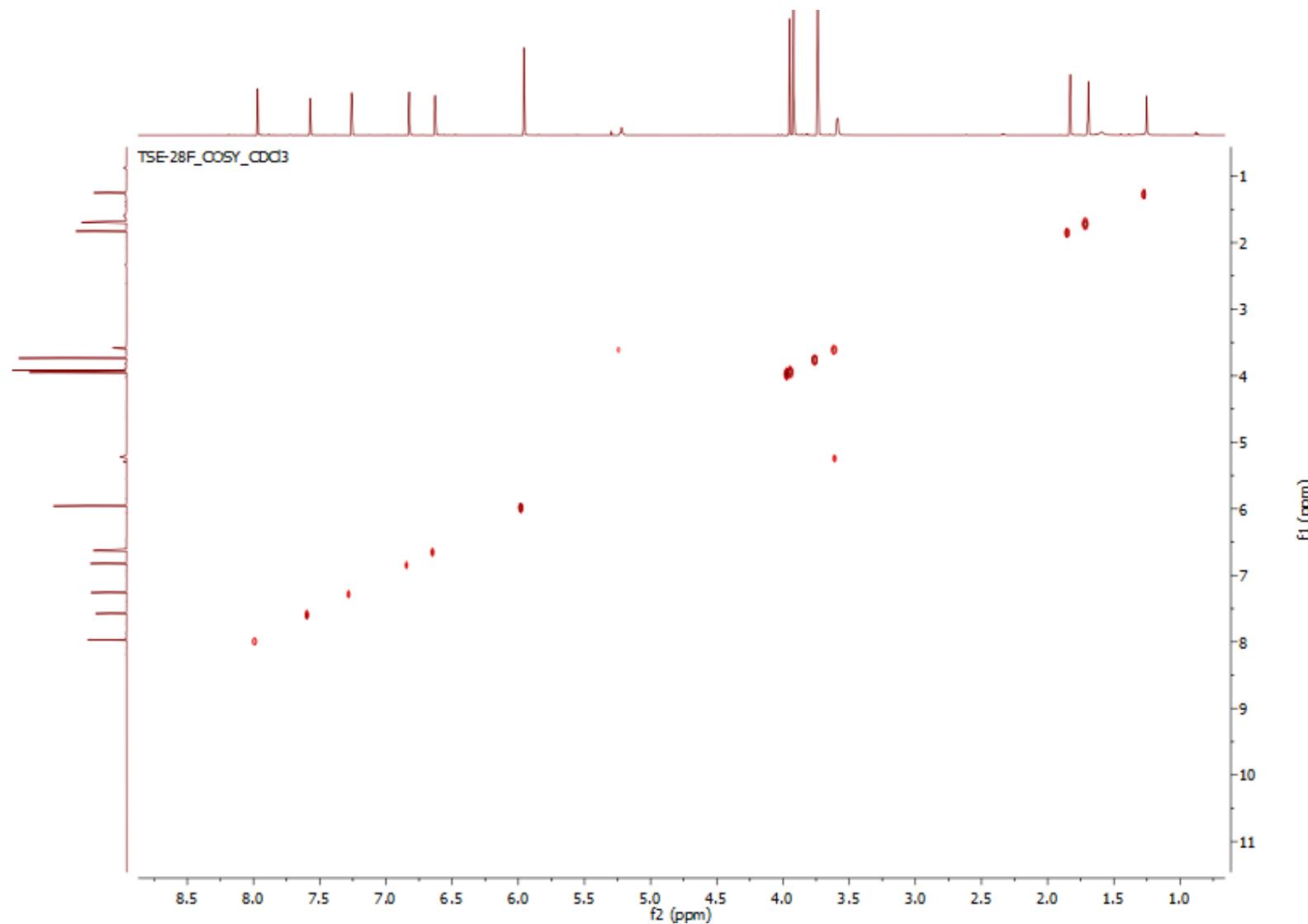


**Figure S1B:**  $^{13}\text{C}$  NMR (201.15 MHz) spectrum of compound 1

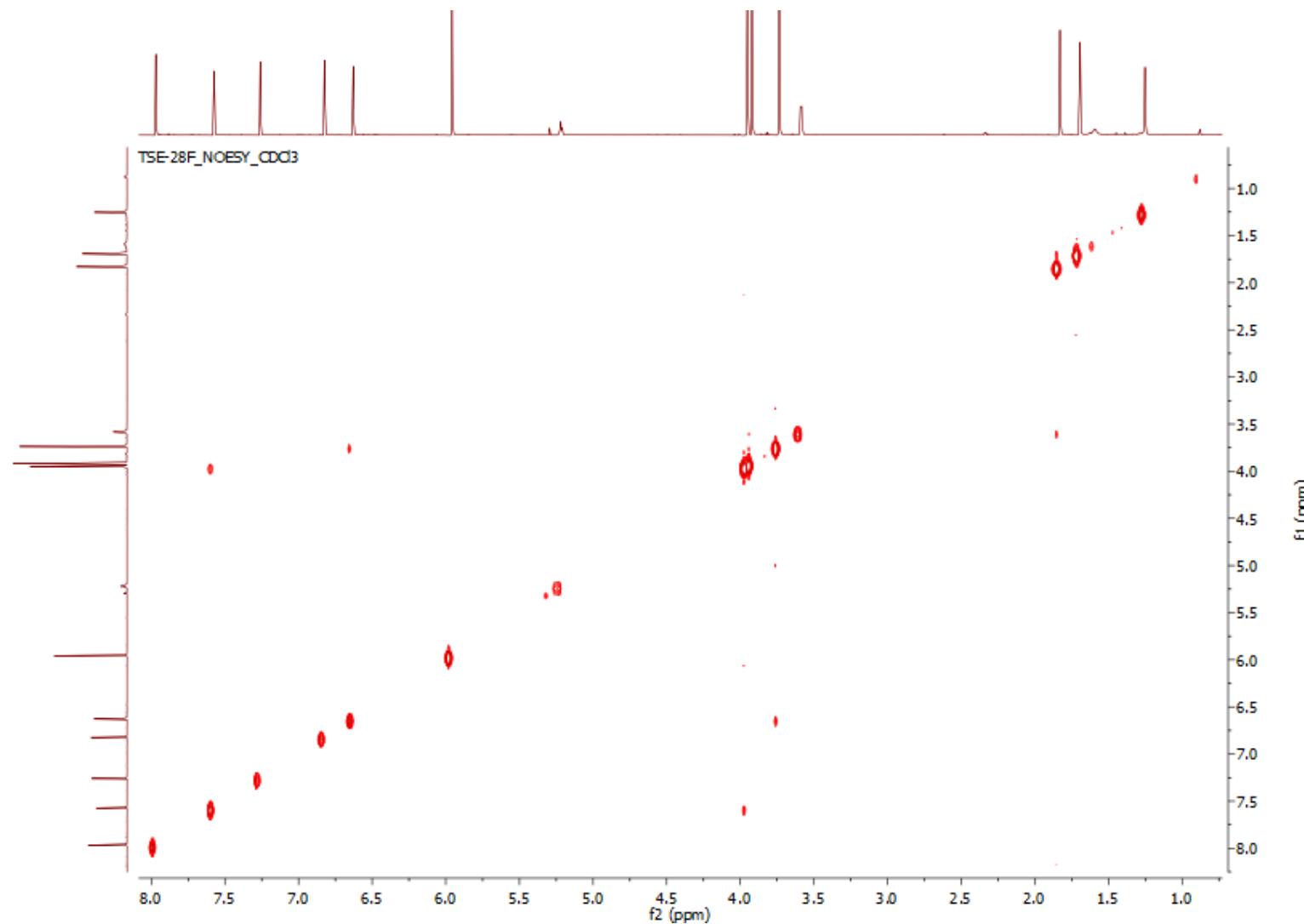
TSE-28F\_13C NMR\_CDCl<sub>3</sub>\_200 MHz



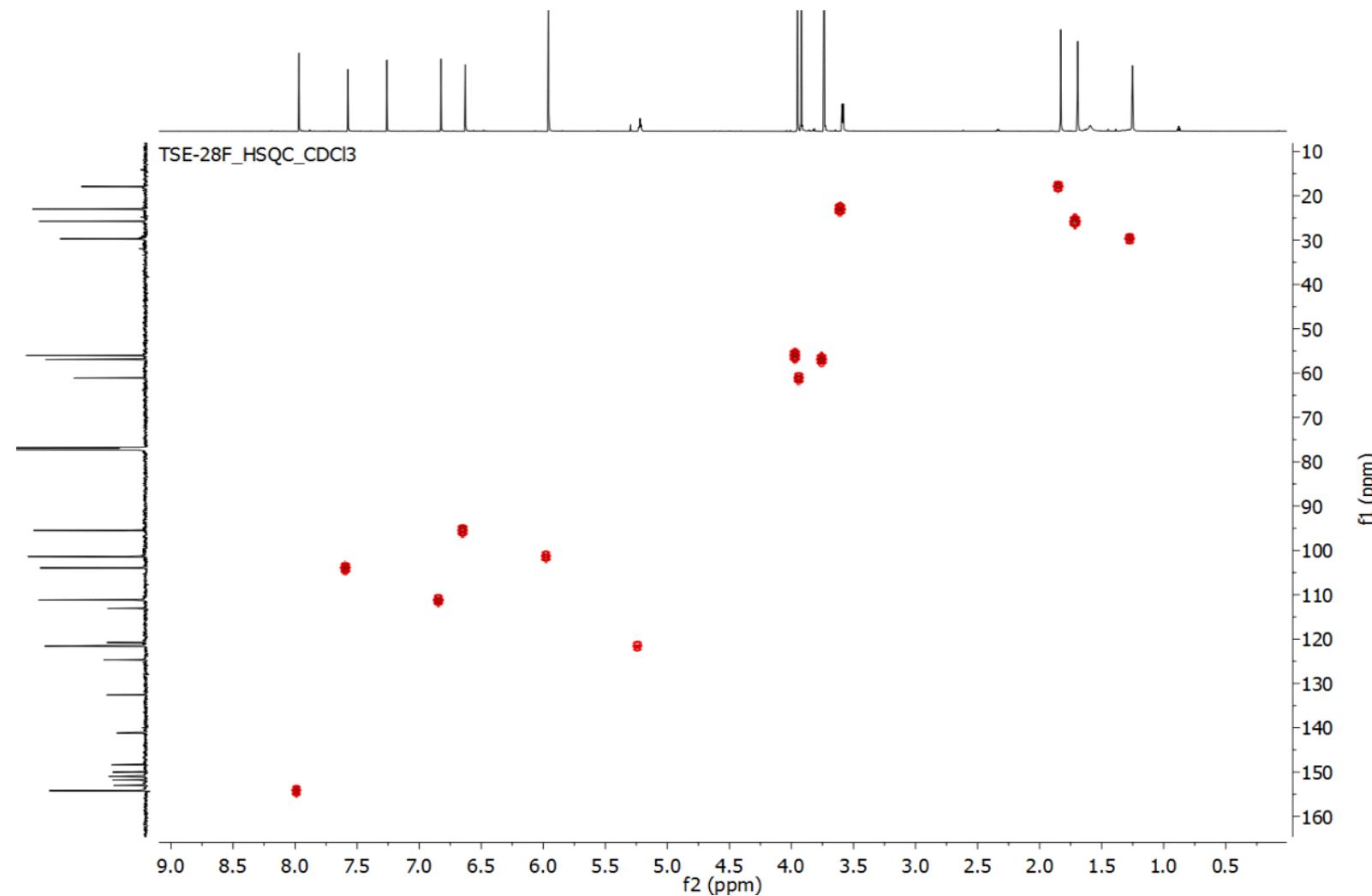
**Figure S1C:** COSY (799.87 MHz) spectrum of compound 1



**Figure S1D:** NOESY (799.87 MHz) spectrum of compound 1



**Figure S1E:** HSQC (799.87/201.15 MHz) spectrum of compound 1



**Figure S1F:** HMBC (799.87/201.15 MHz) spectrum of compound 1

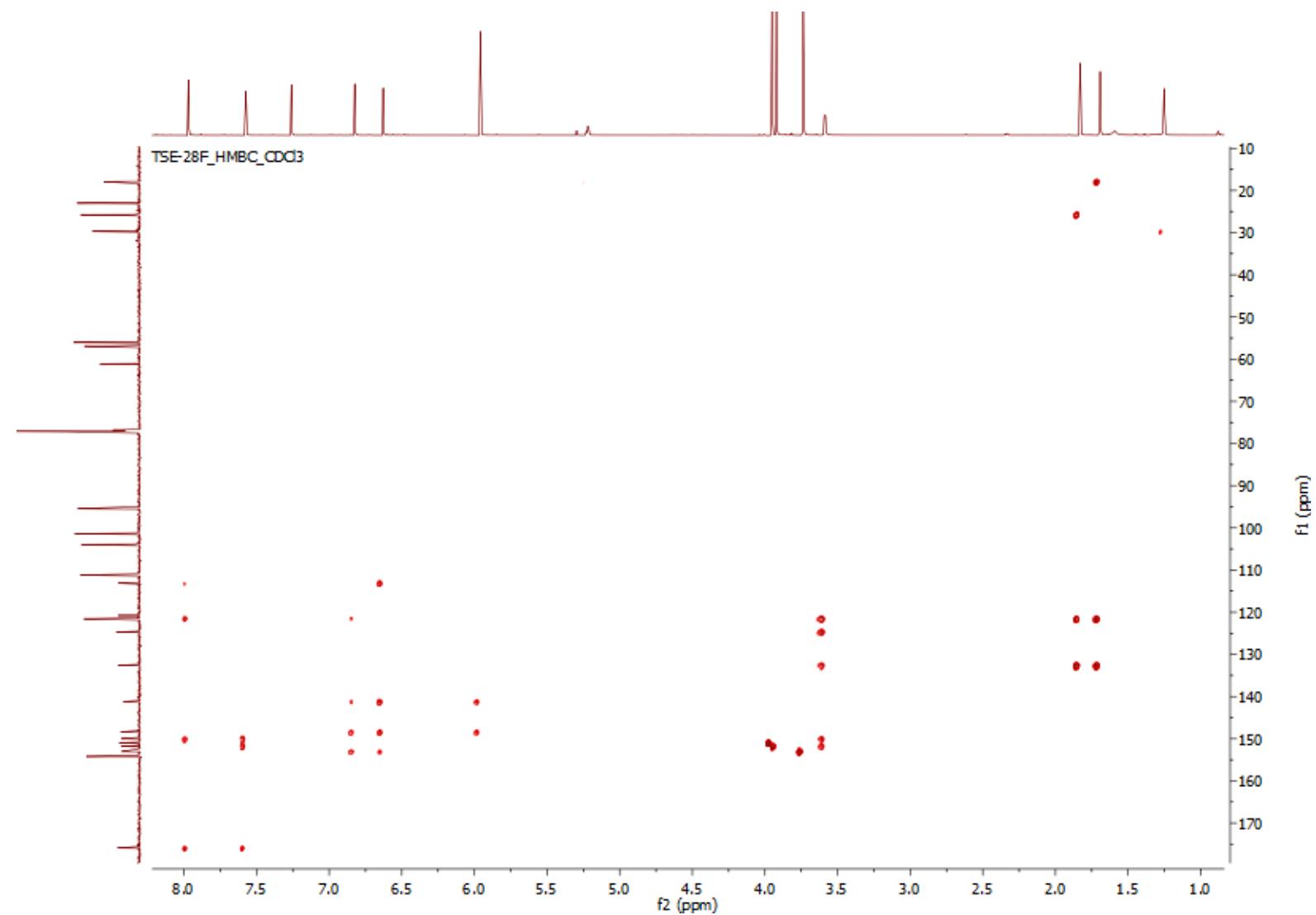
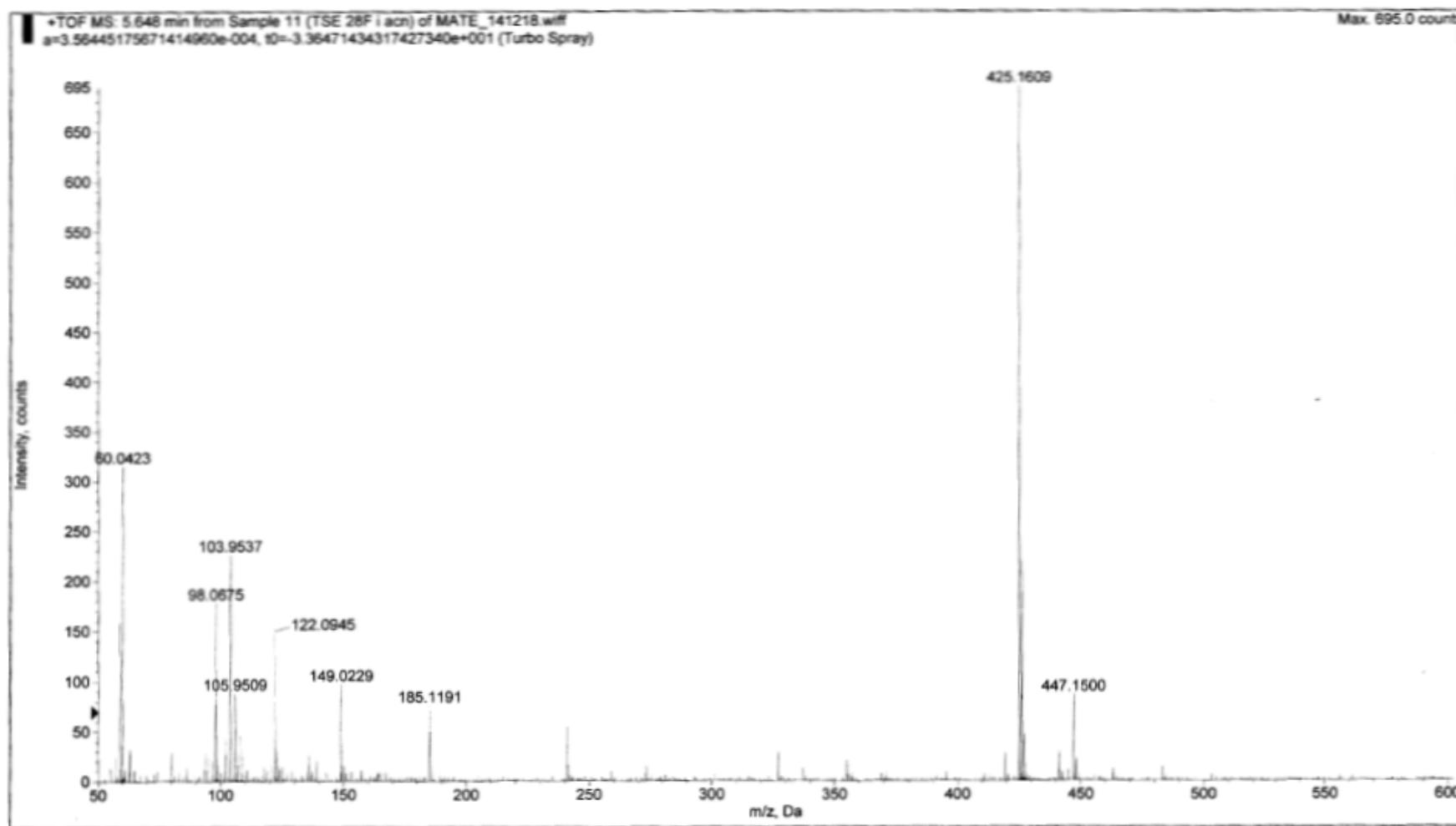
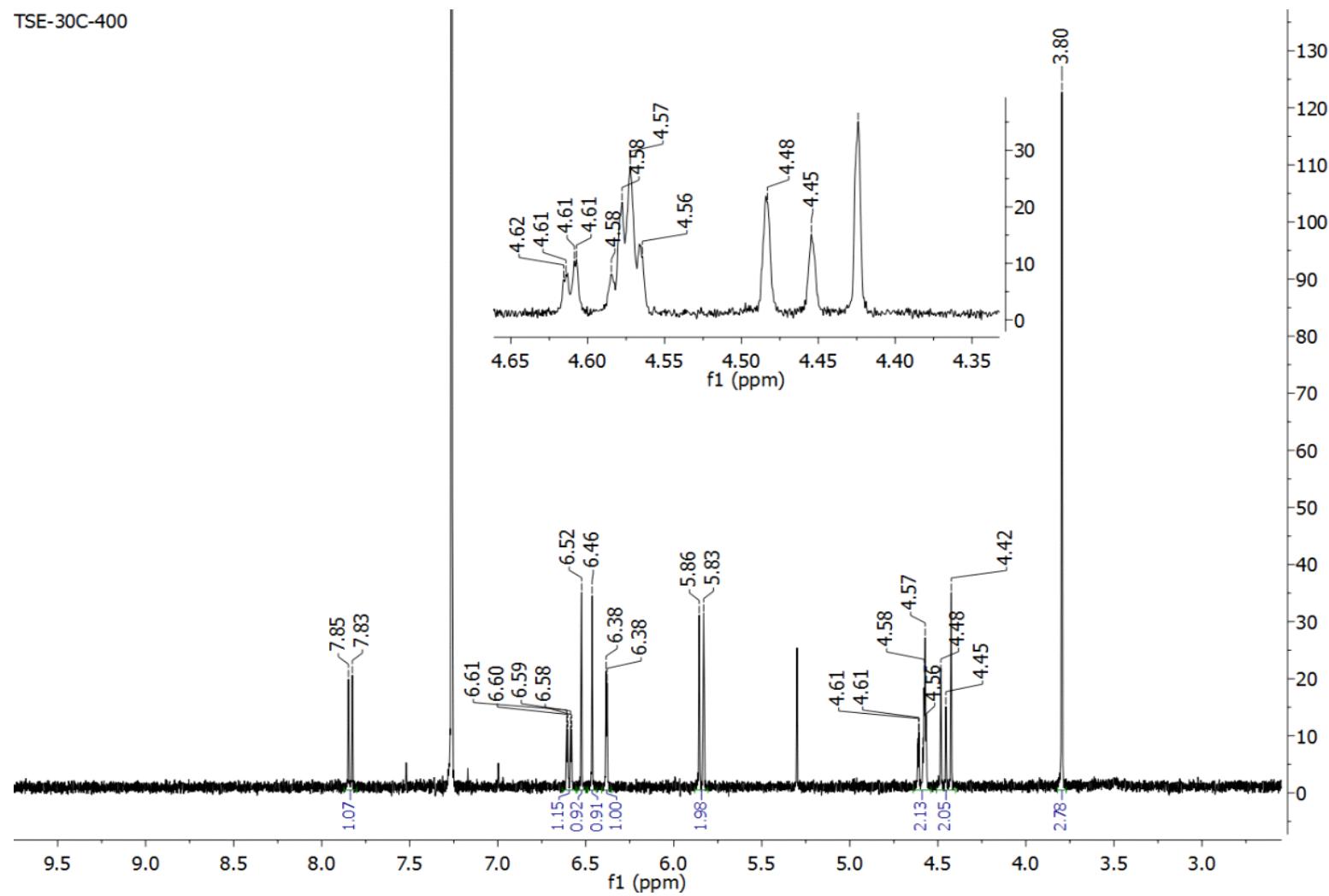


Figure S1G: HREIMS spectrum of compound 1

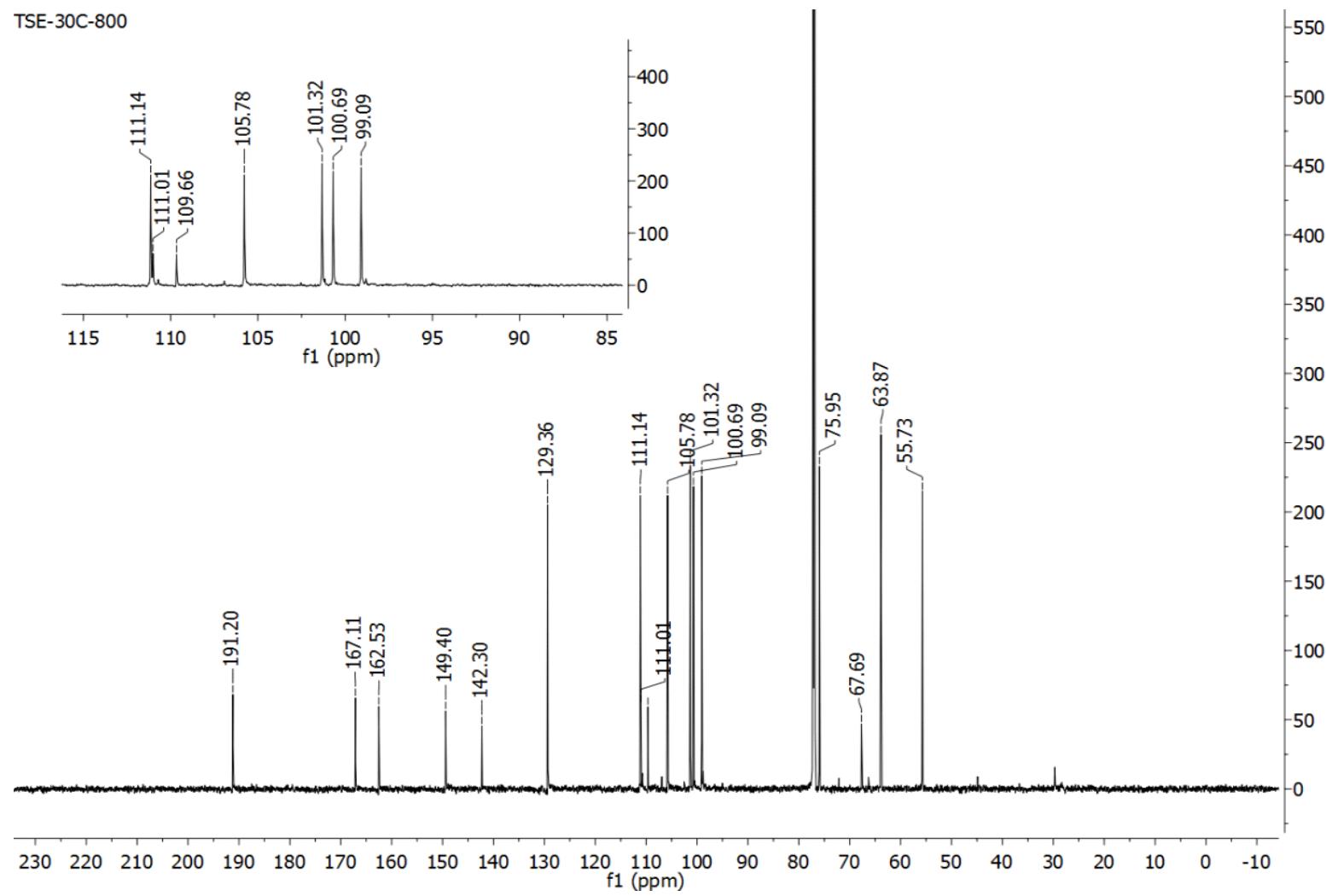


**Figure S2A:**  $^1\text{H}$  NMR (399.97 MHz) spectrum of compound 2

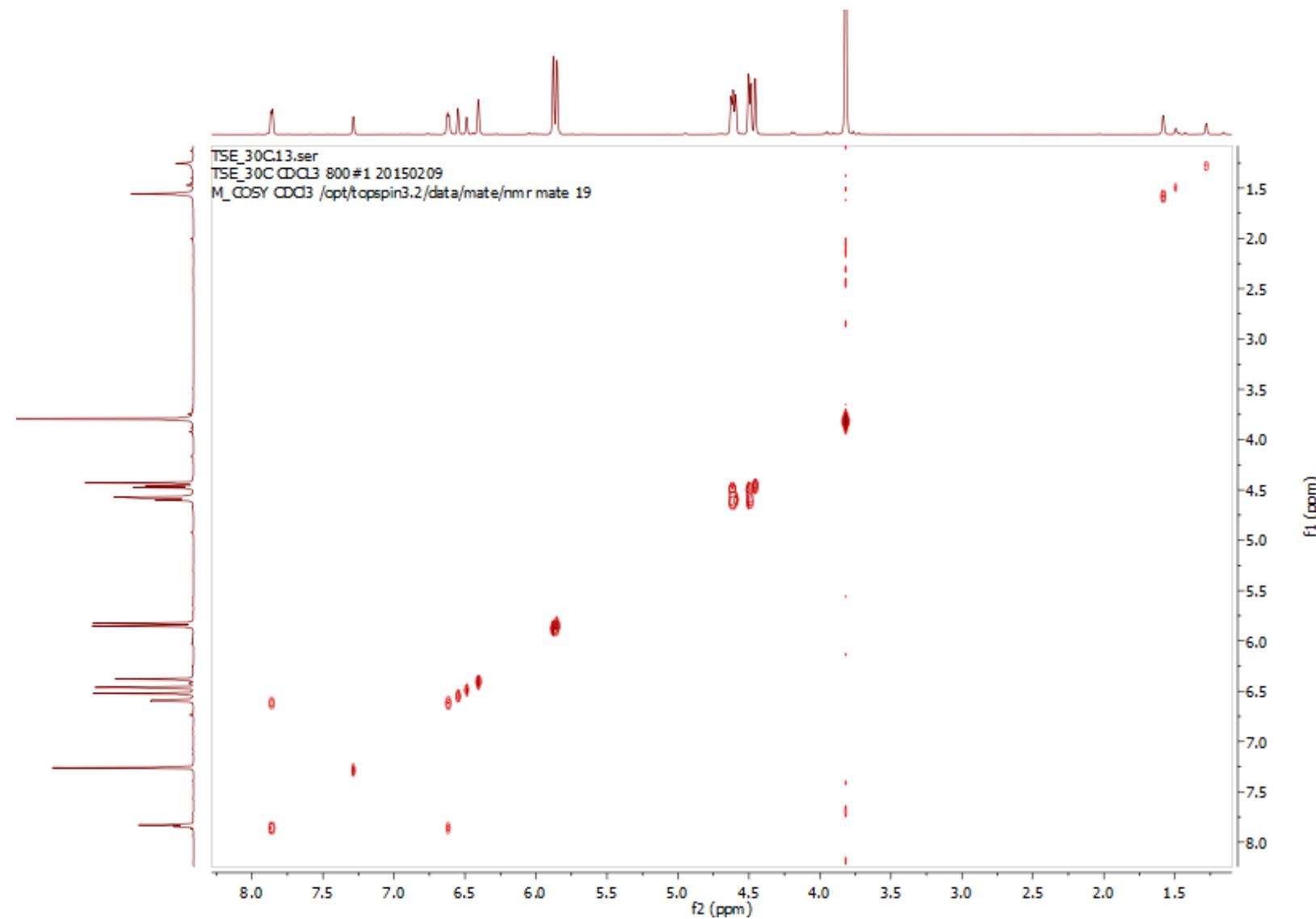
TSE-30C-400



**Figure S2B:**  $^{13}\text{C}$  NMR (201.15 MHz) spectrum of compound 2



**Figure S2C: COSY (799.87 MHz) spectrum of compound 2**



**Figure S2D:** NOESY (799.87 MHz) spectrum of compound 2

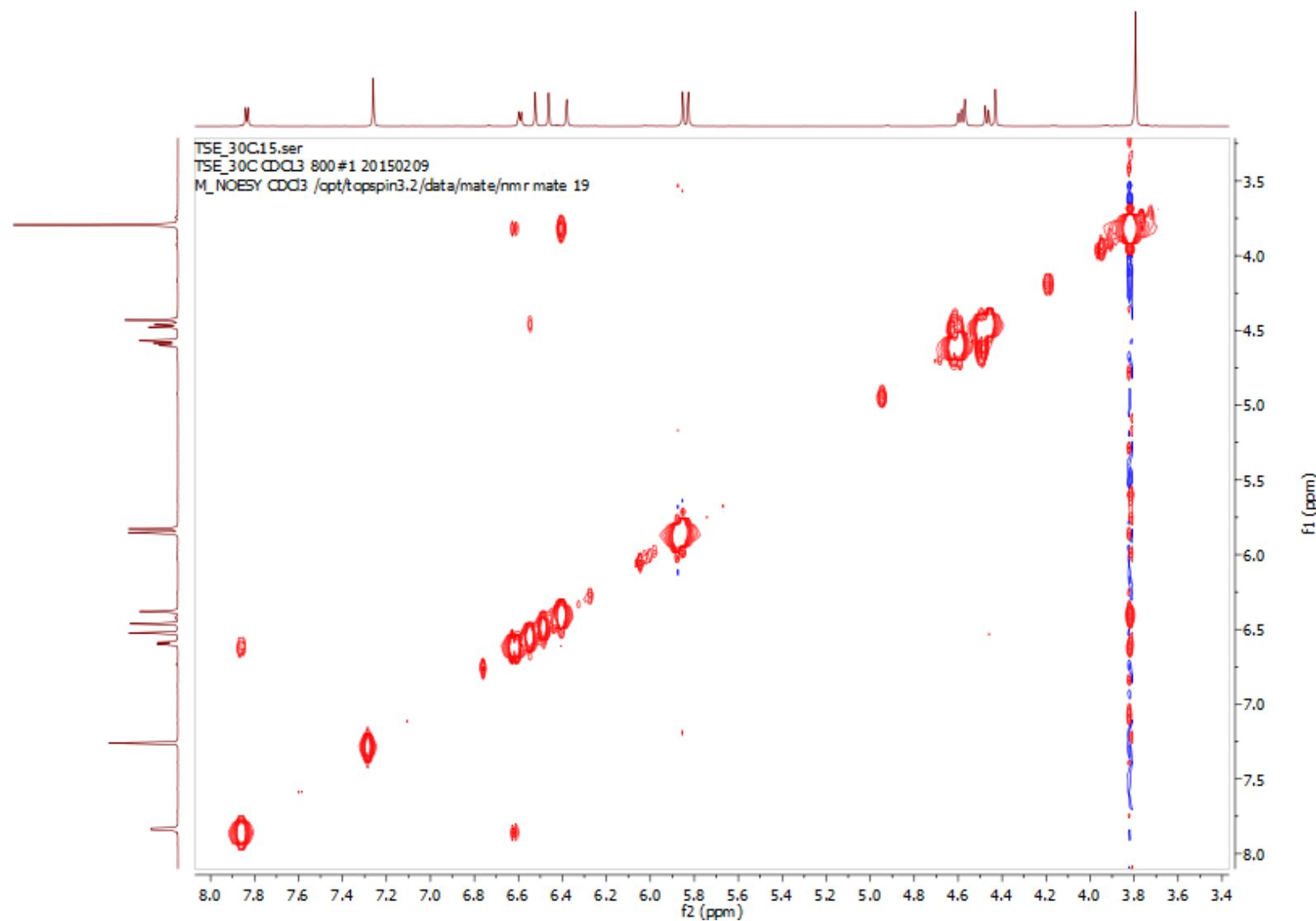
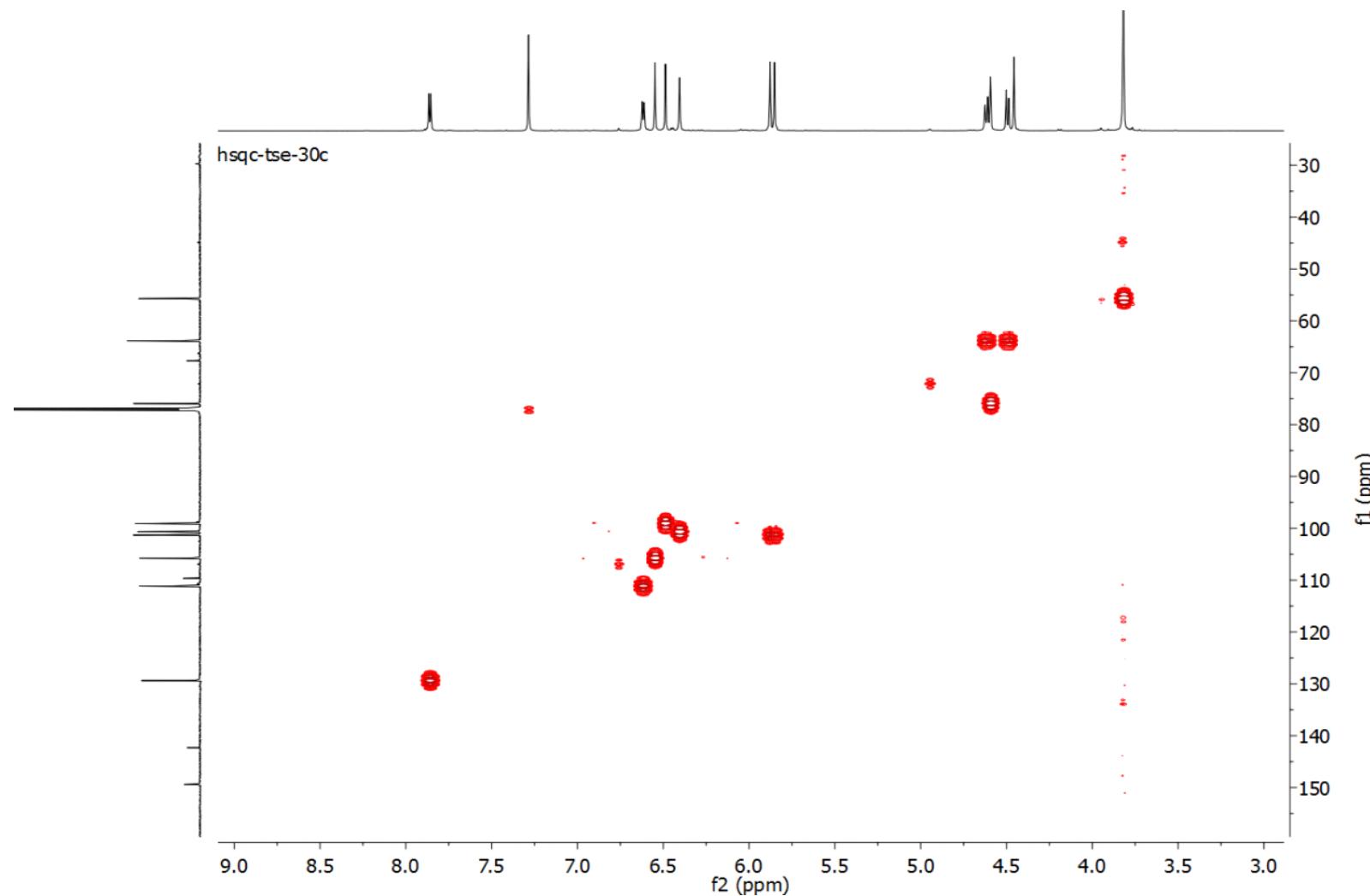
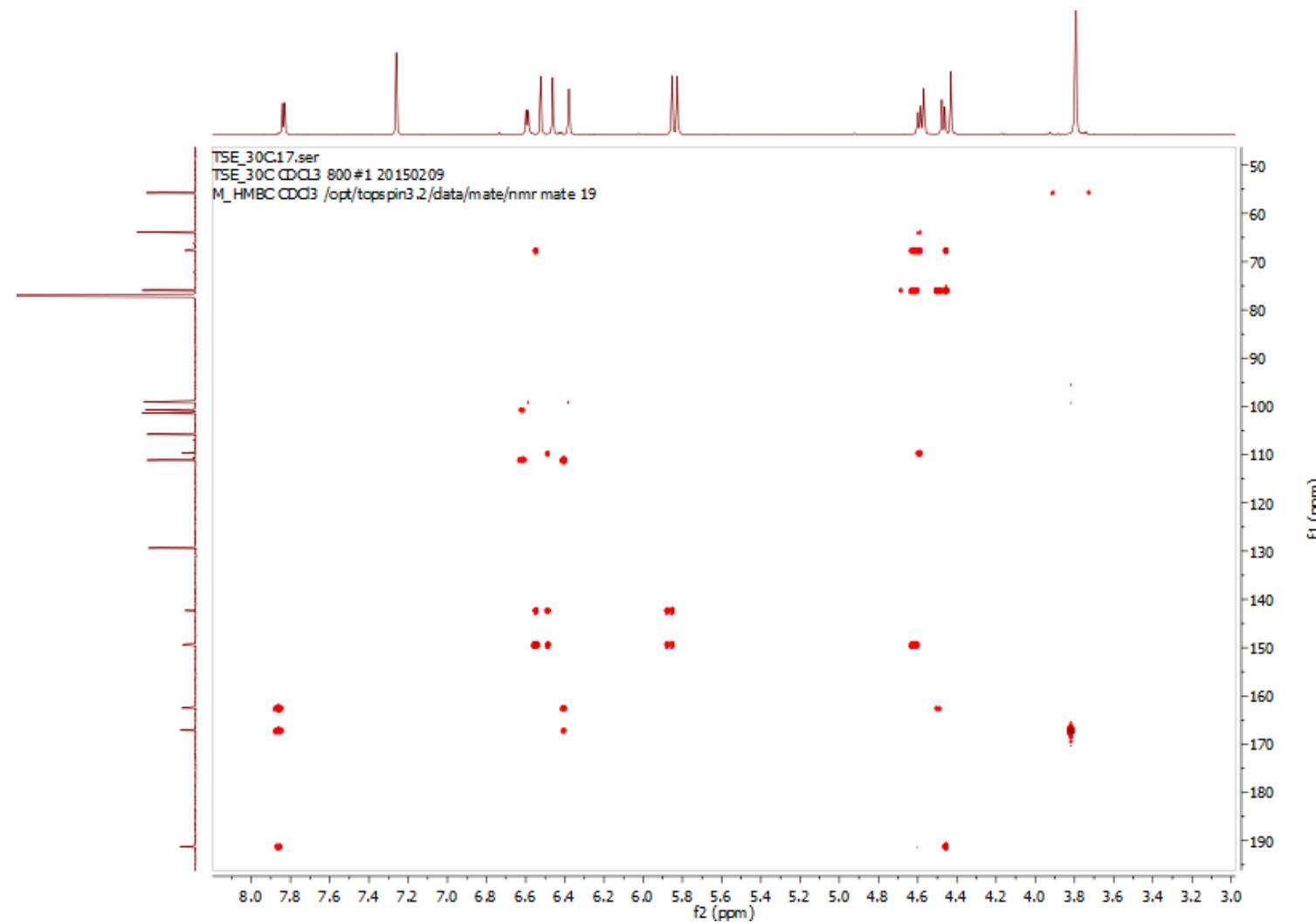


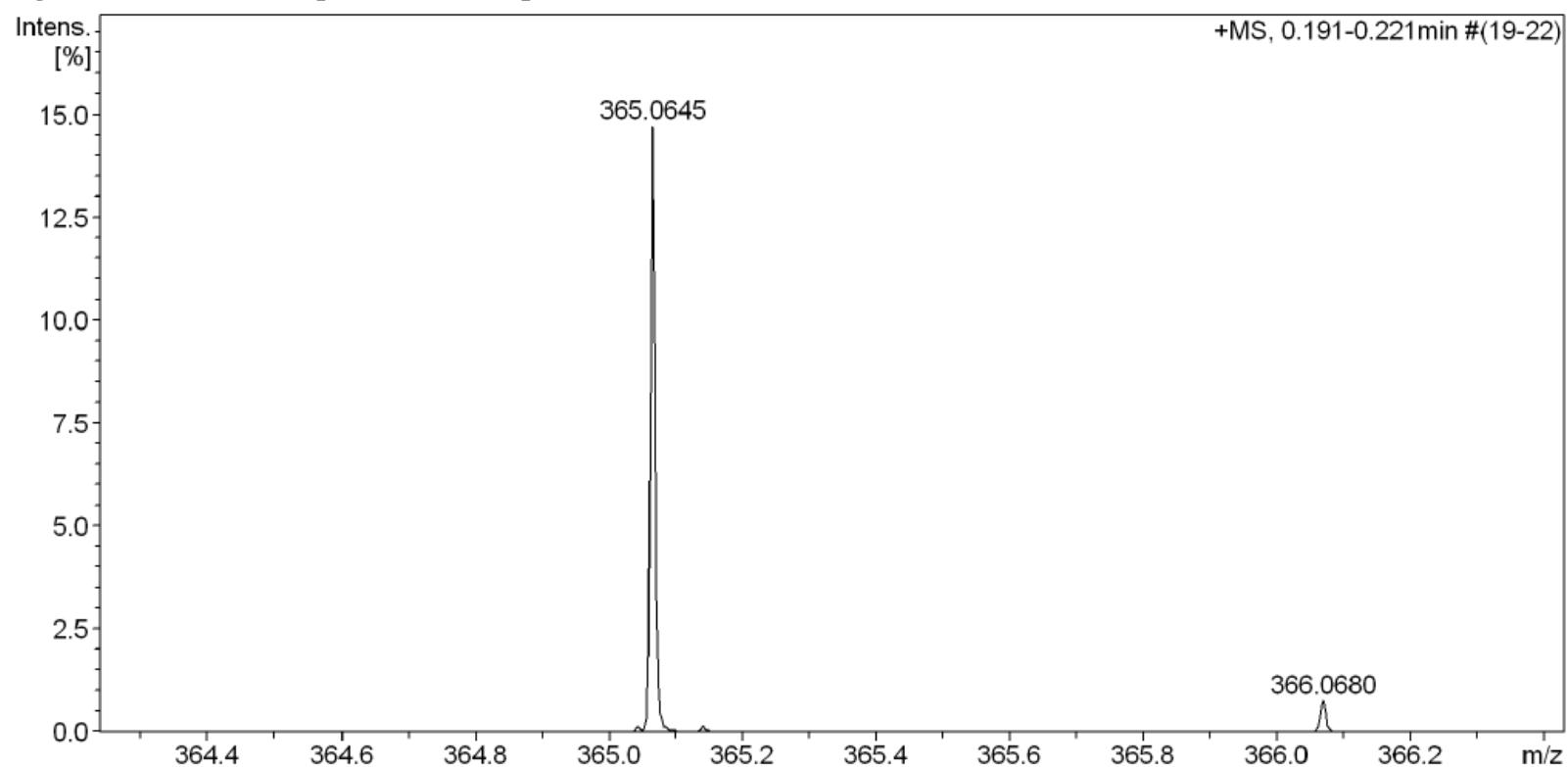
Figure S2E: HSQC (799.87 MHz/201.15 MHz) spectrum of compound 2



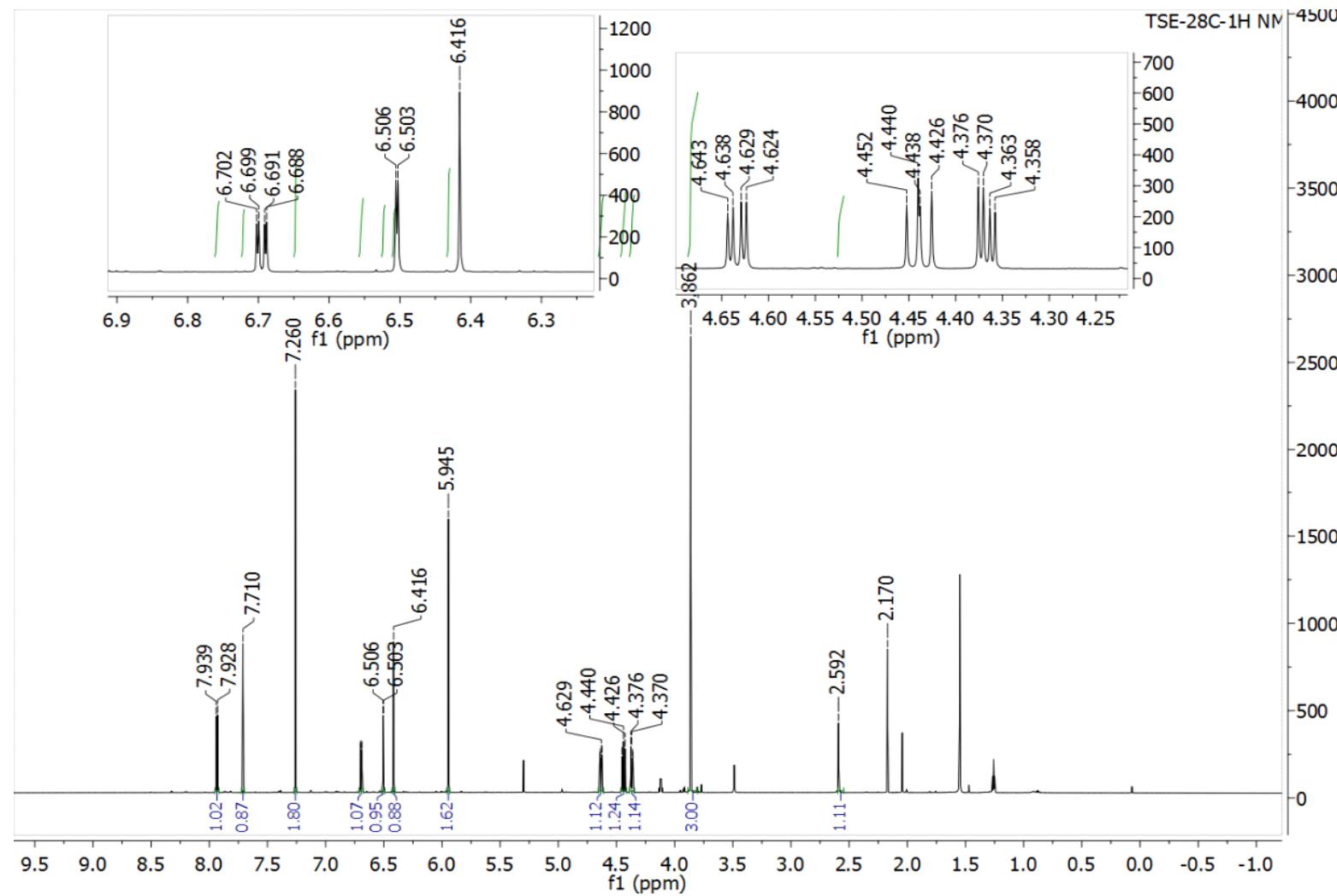
**Figure S2F: HMBC (799.87 MHz/201.15 MHz) spectrum of compound 2**



**Figure S1G: HREIMS spectrum of compound 2**



**Figure S3A:**  $^1\text{H}$  NMR (799.78 MHz) spectrum of compound 3



**Figure S3B:**  $^{13}\text{C}$  NMR (201.15 MHz) spectrum of compound 3

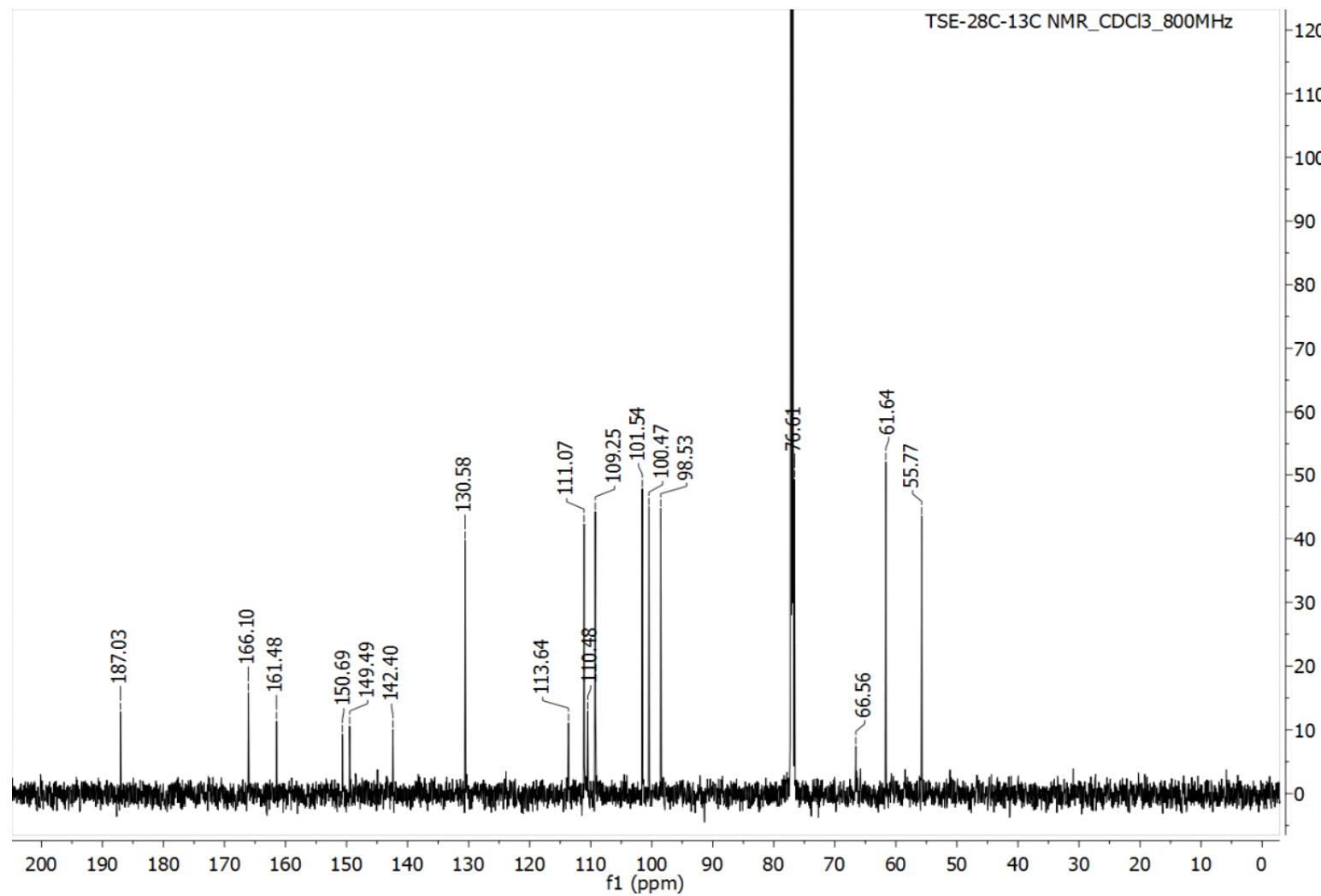
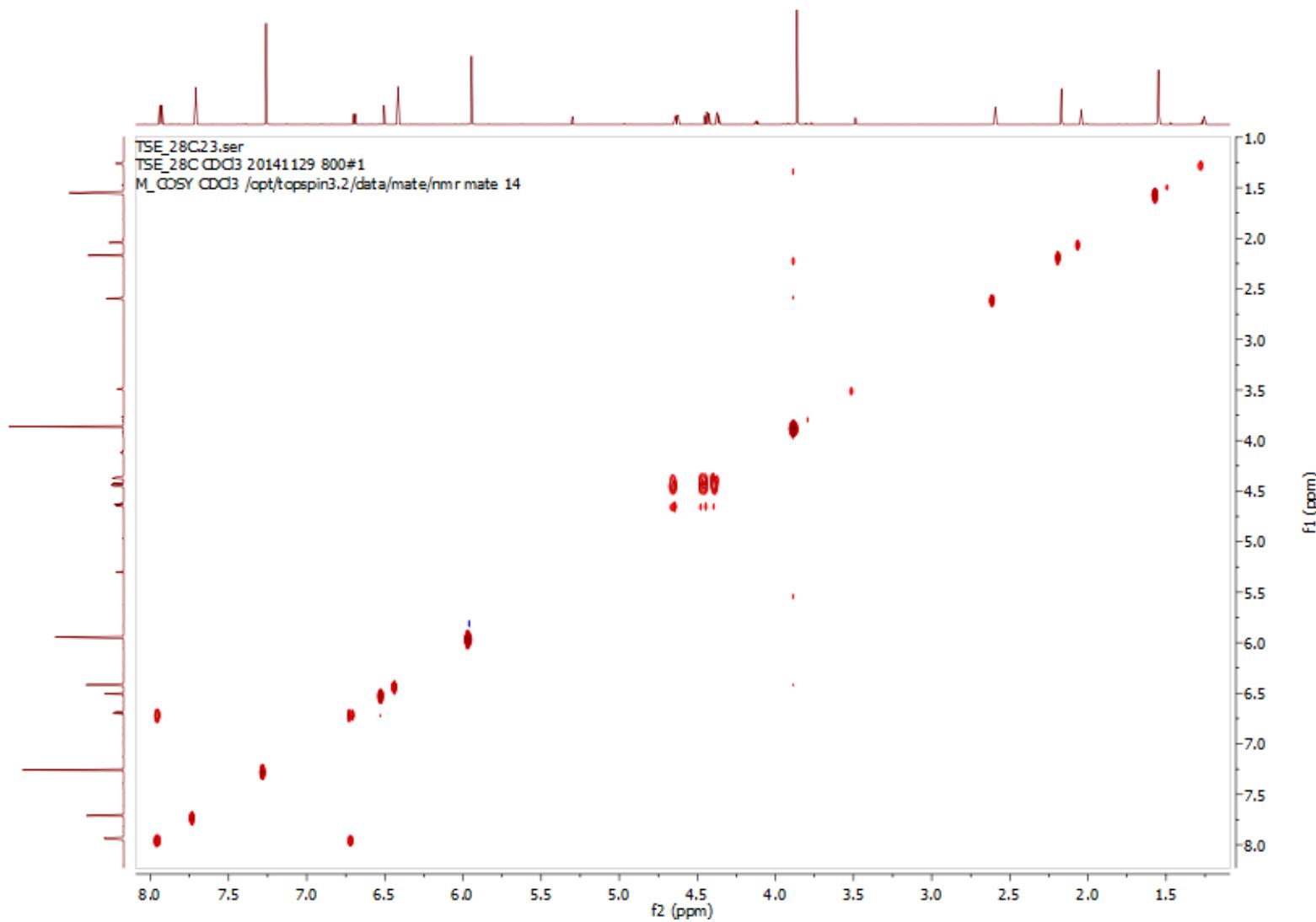
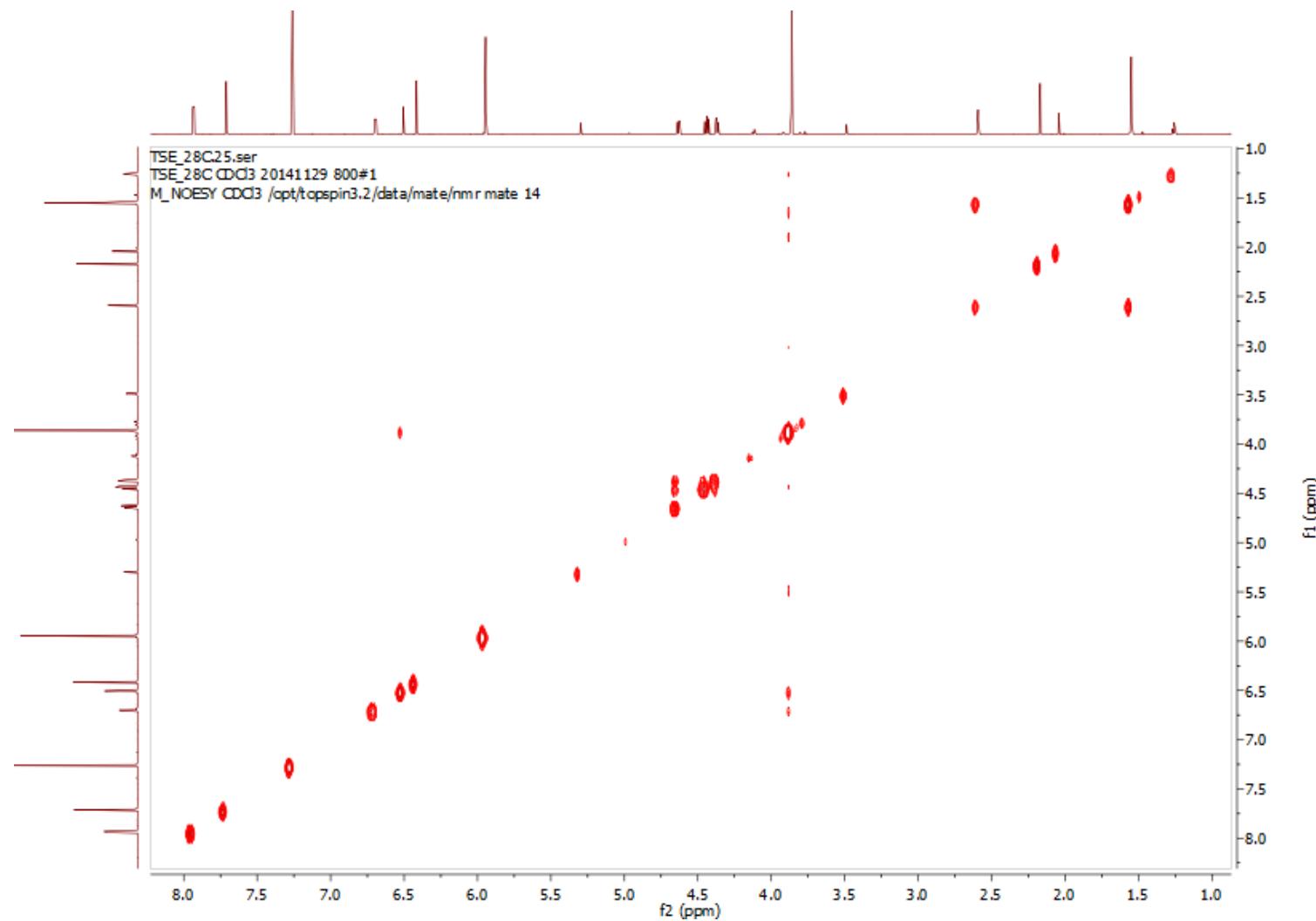


Figure S3C: COSY (799.87 MHz) spectrum of compound 3



**Figure S3D:** NOESY (799.87 MHz) spectrum of compound 3



**Figure S3E:** HSQC (799.87/201.15 MHz) spectrum of compound 3

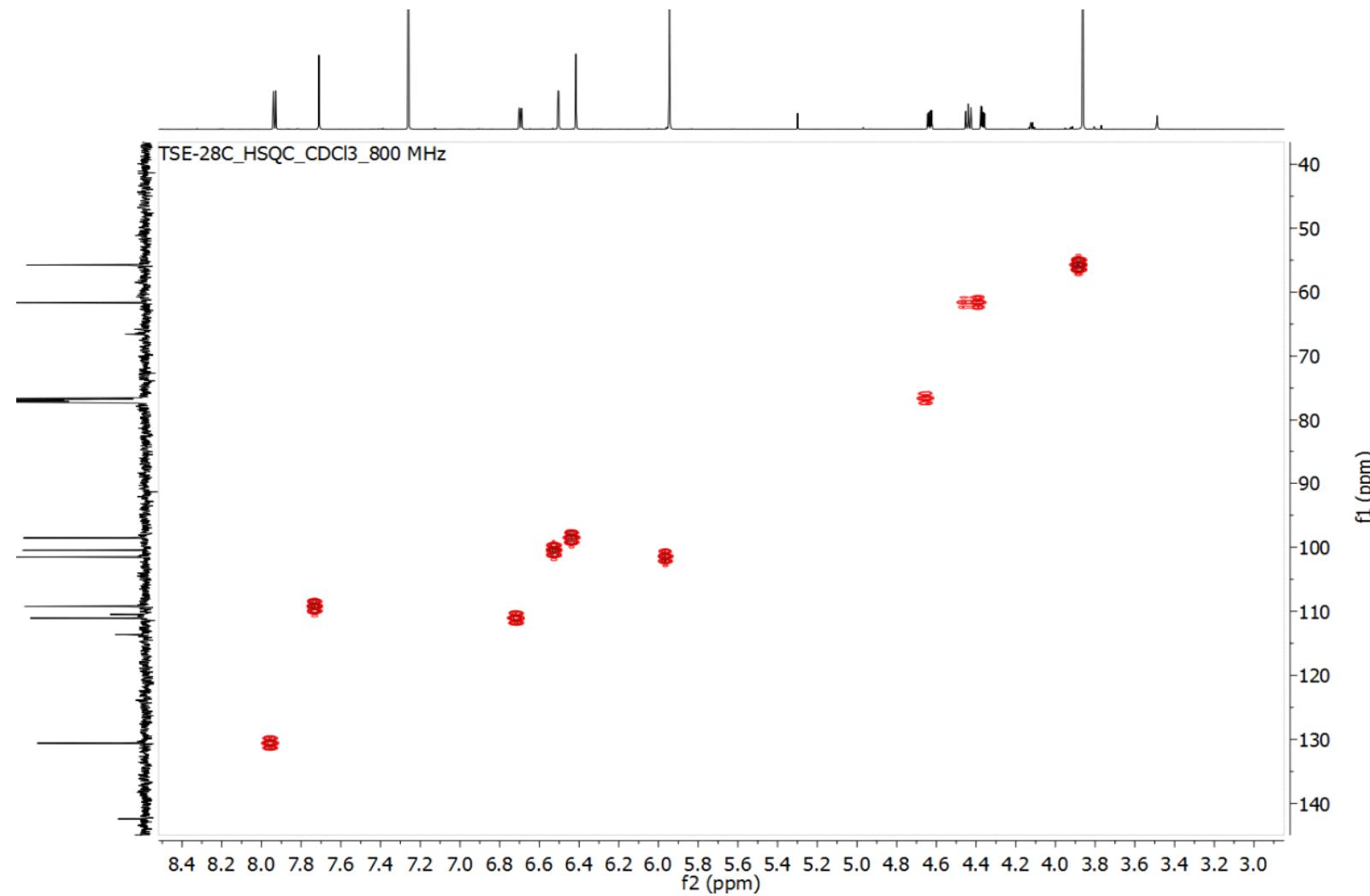


Figure S3F: HMBC (799.87/201.15 MHz) spectrum of compound 3

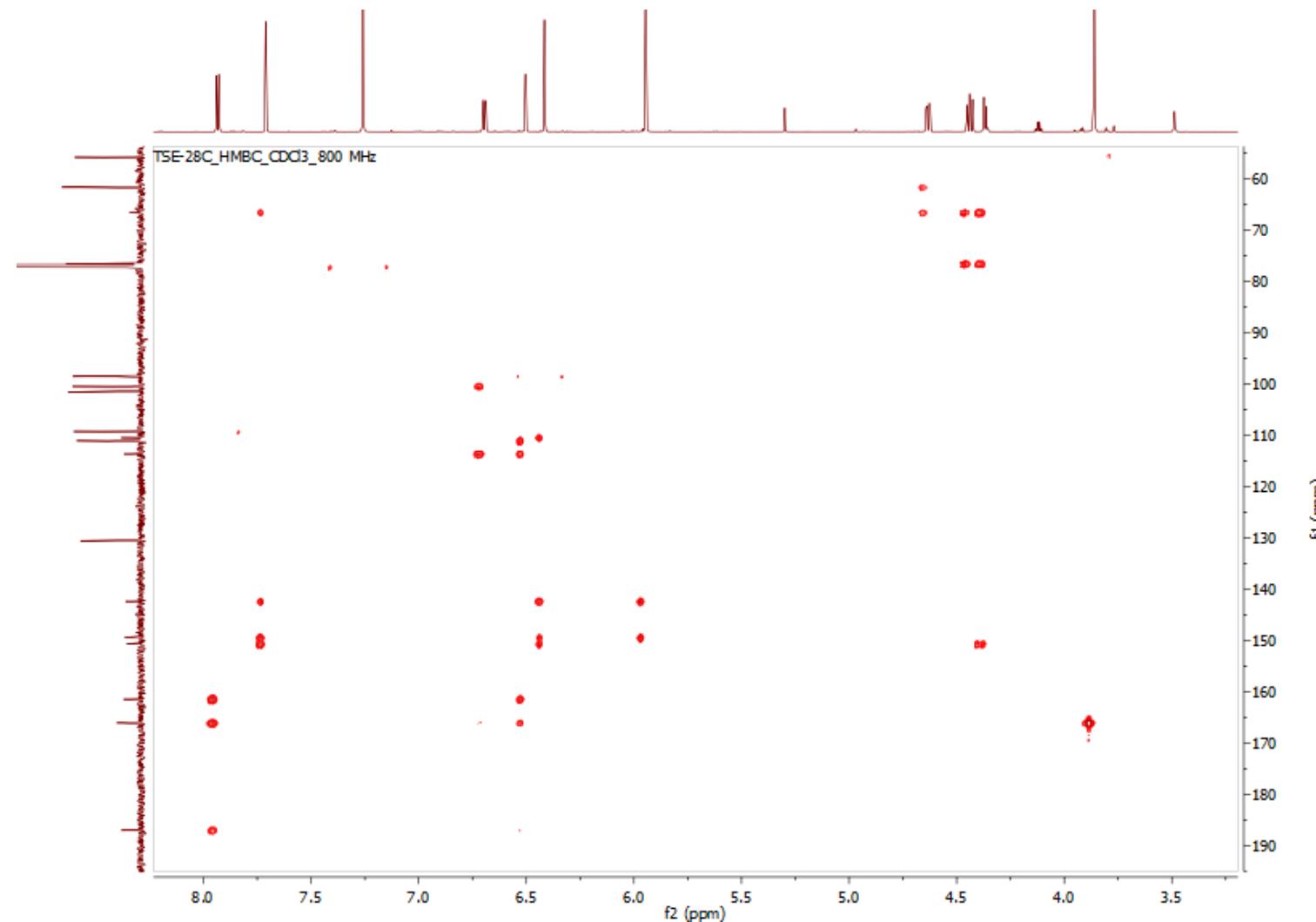
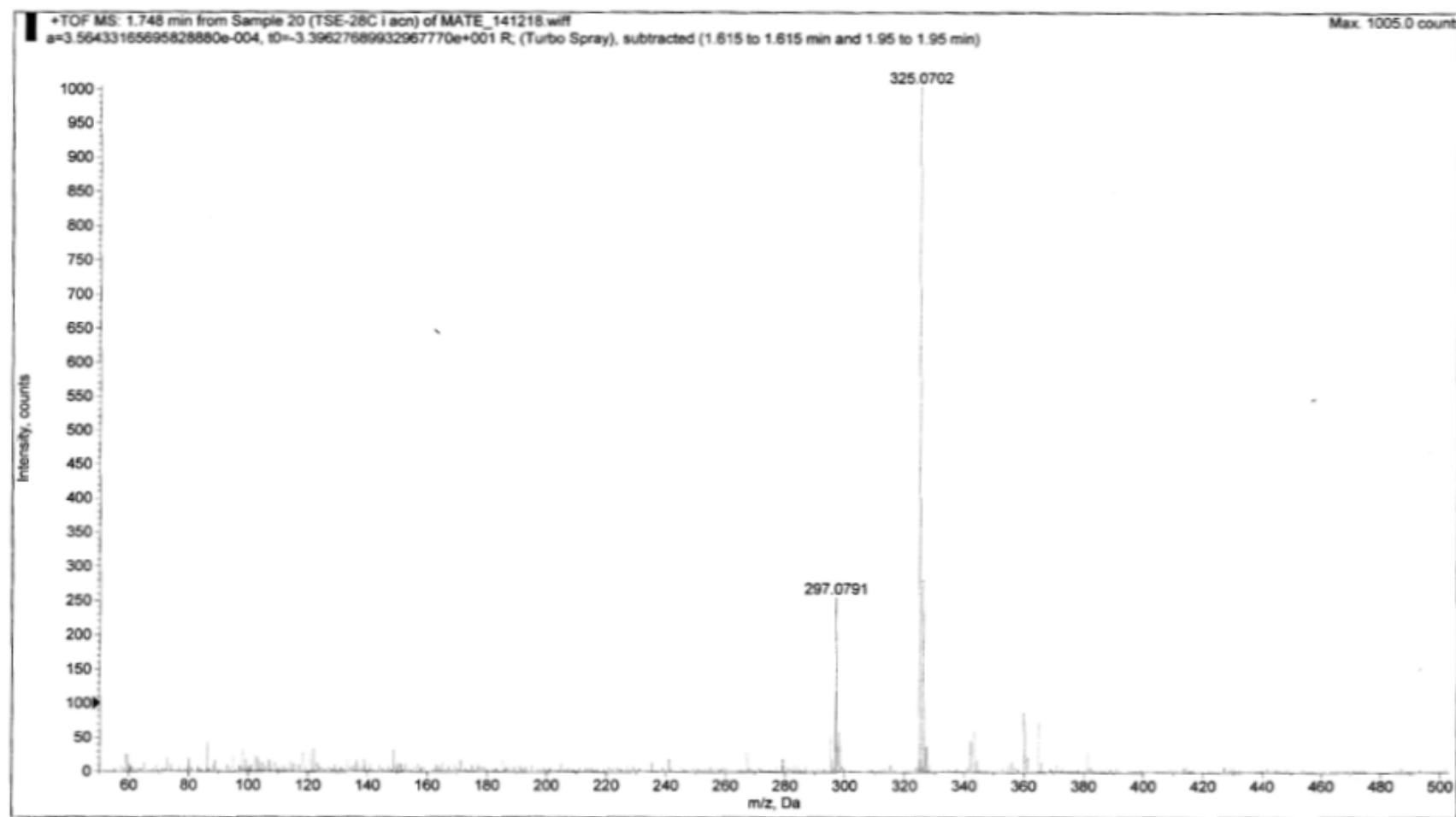
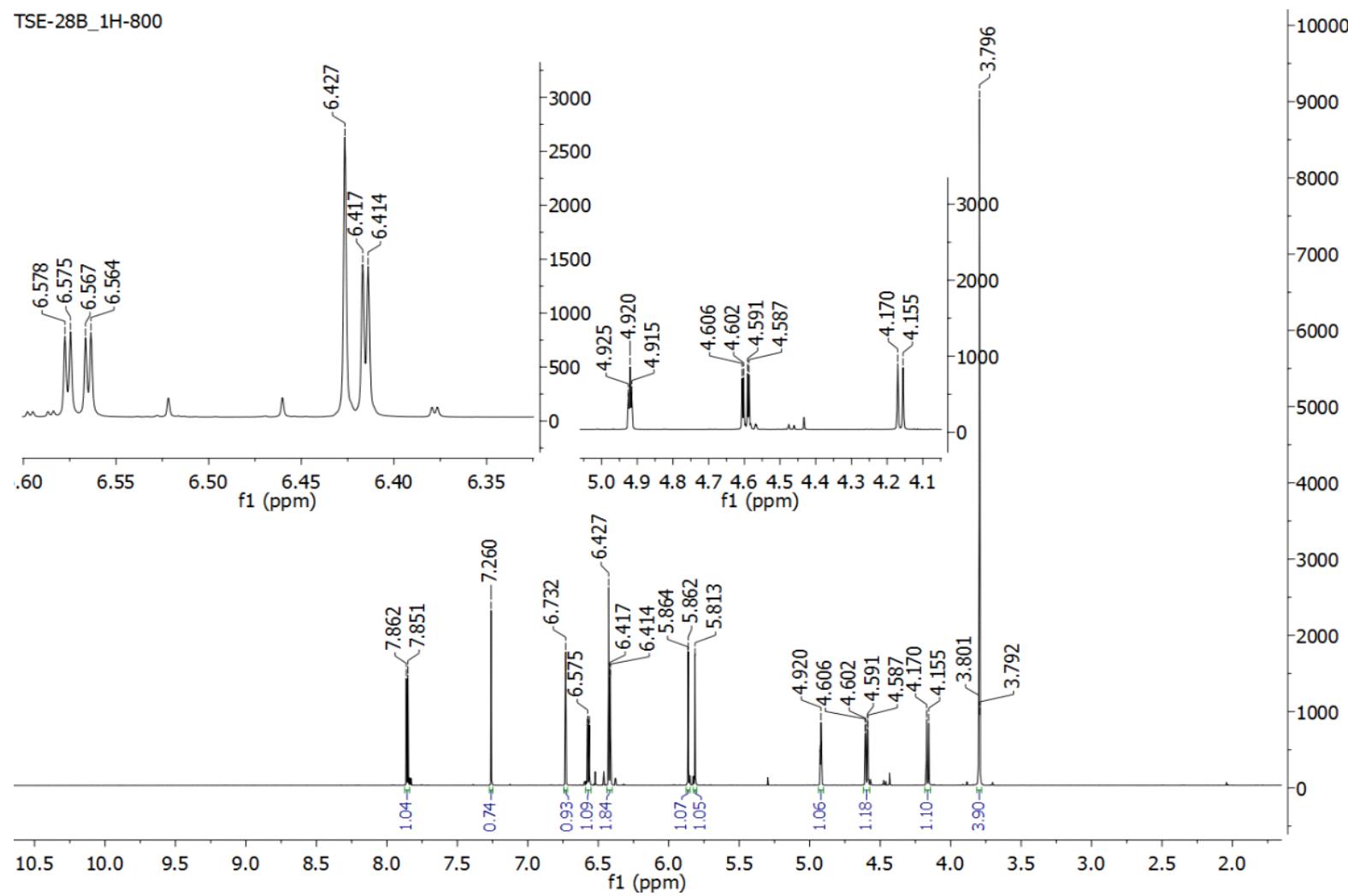


Figure S3G: HREIMS spectrum of compound 3



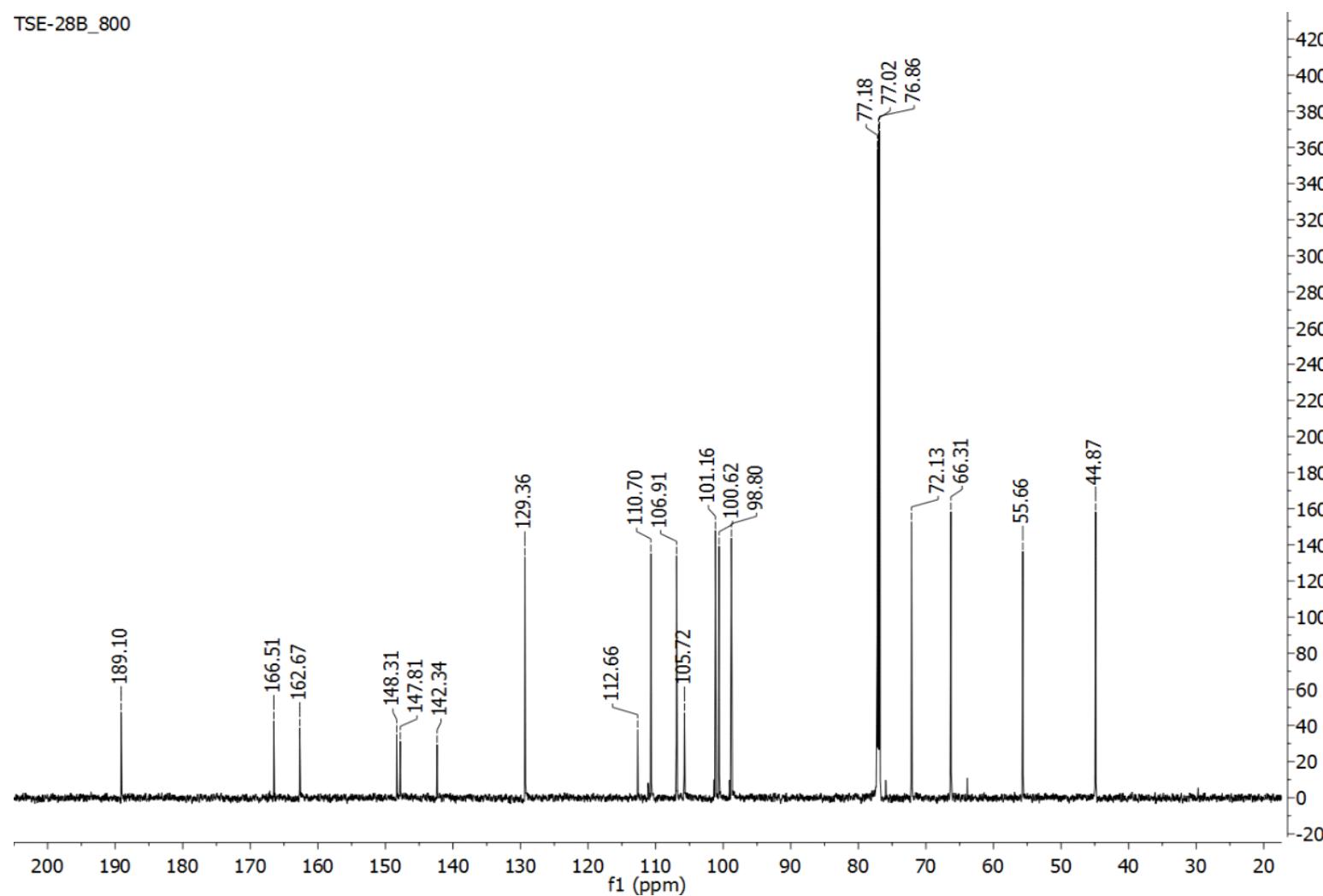
**Figure S4A:**  $^1\text{H}$  NMR (799.87 MHz) spectrum of compound 4

TSE-28B\_1H-800

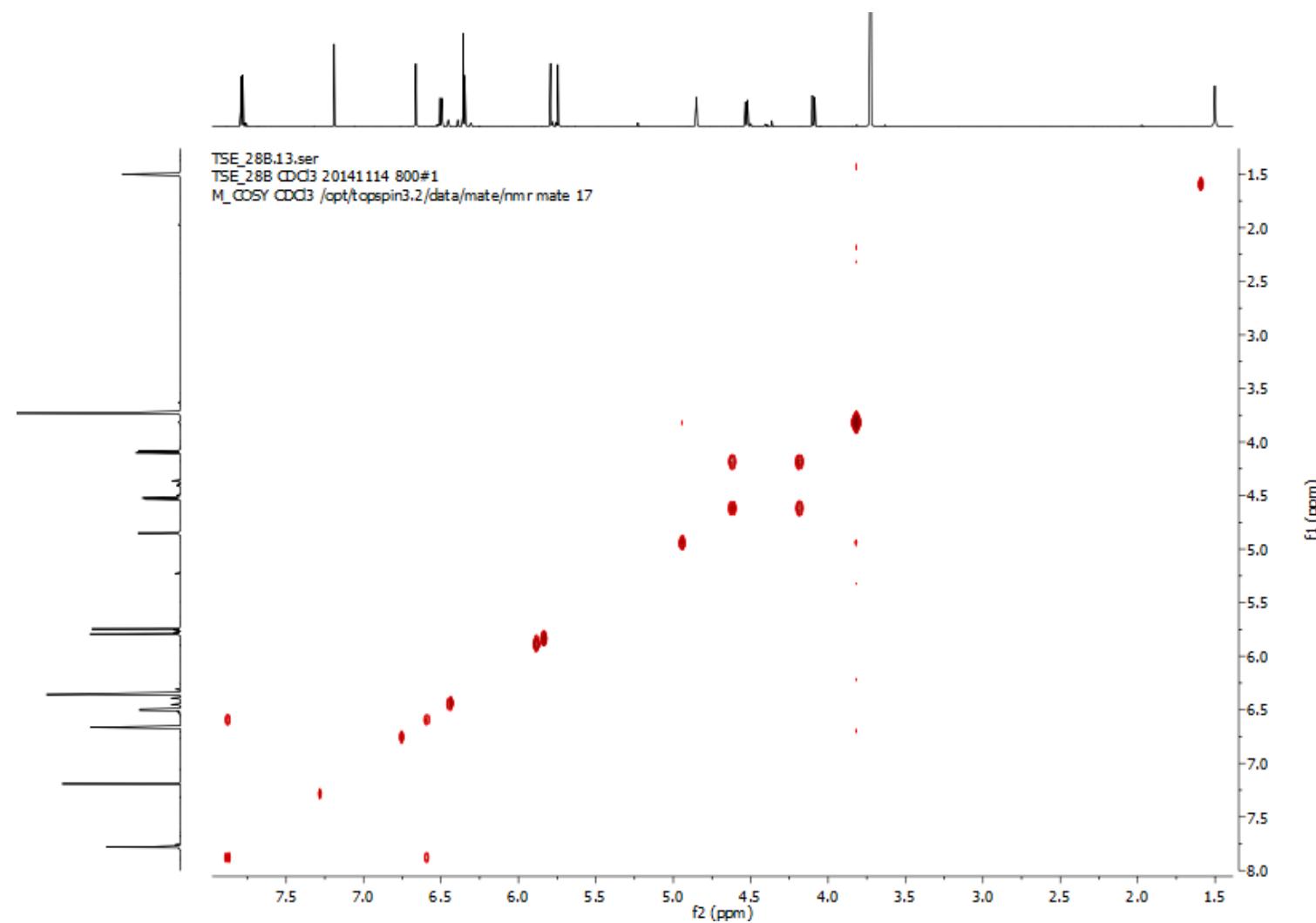


**Figure S4B:**  $^{13}\text{C}$  NMR (799.87 MHz) spectrum of compound 4

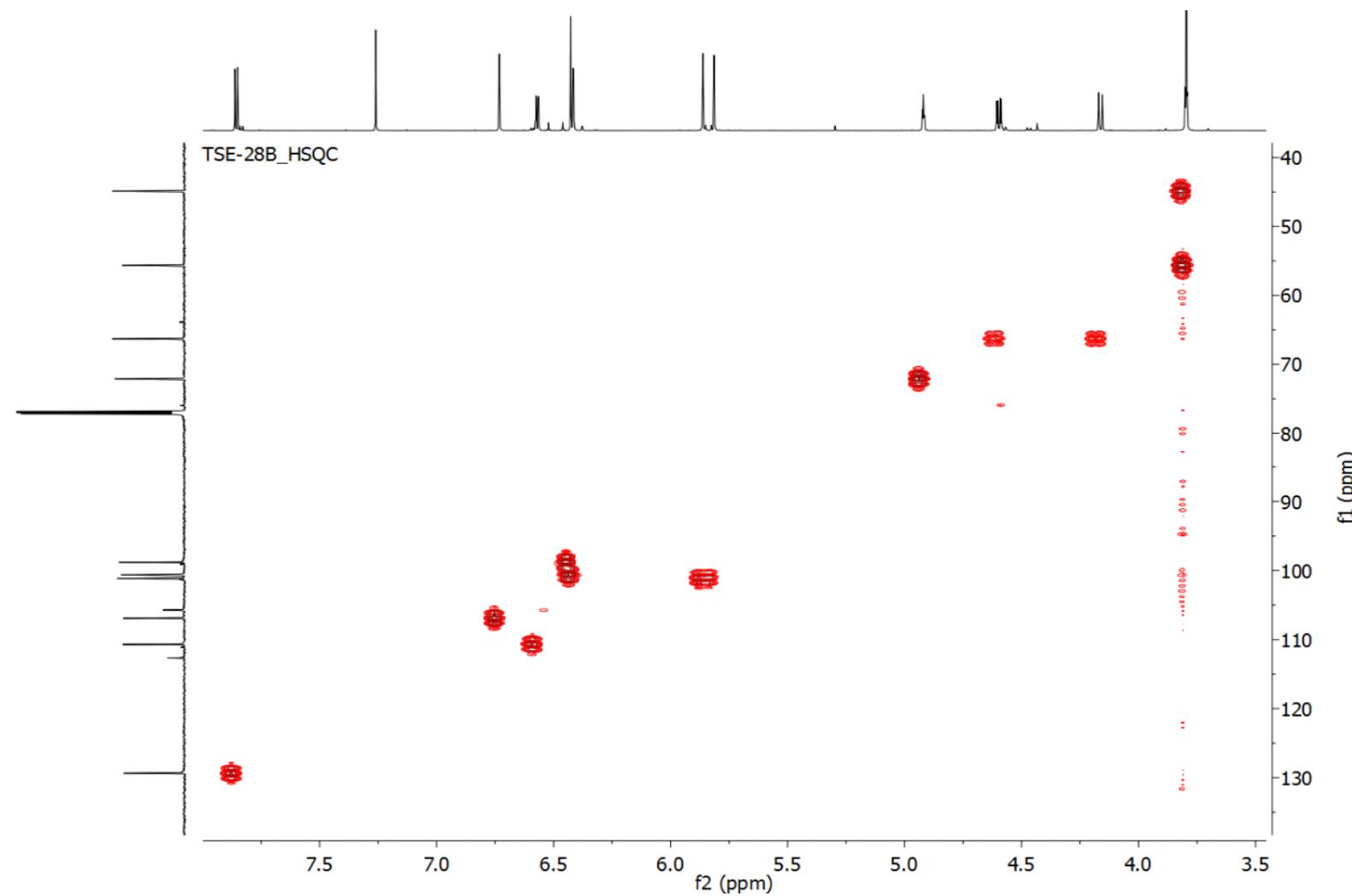
TSE-28B\_800



Appendix 4C: COSY (799.87 MHz) spectrum of compound 4



**Figure S4D:** HSQC (799.87/201.15 MHz) spectrum of compound 4



**Figure S4E:** HMBC (799.87/201.15 MHz) spectrum of compound 4

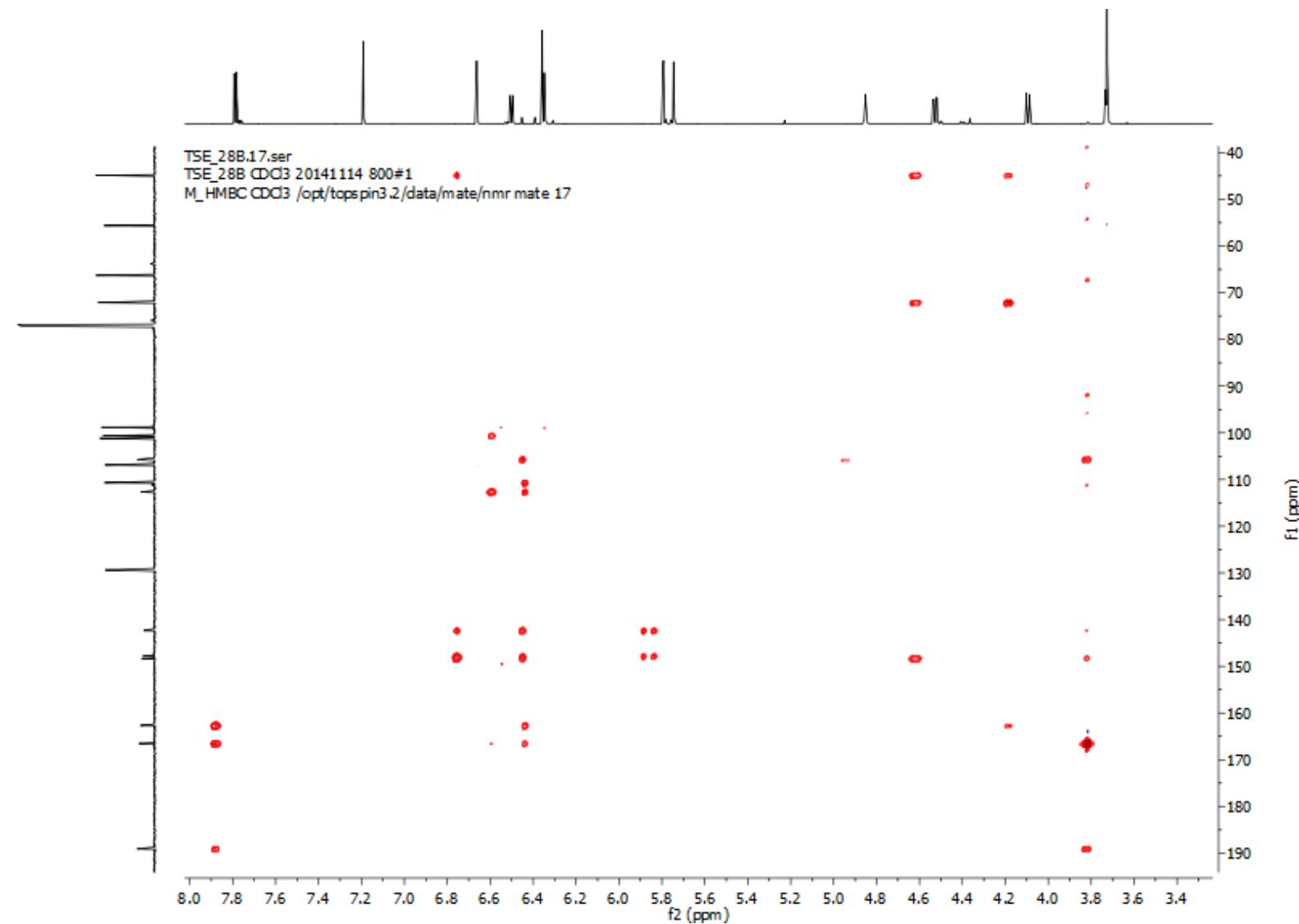
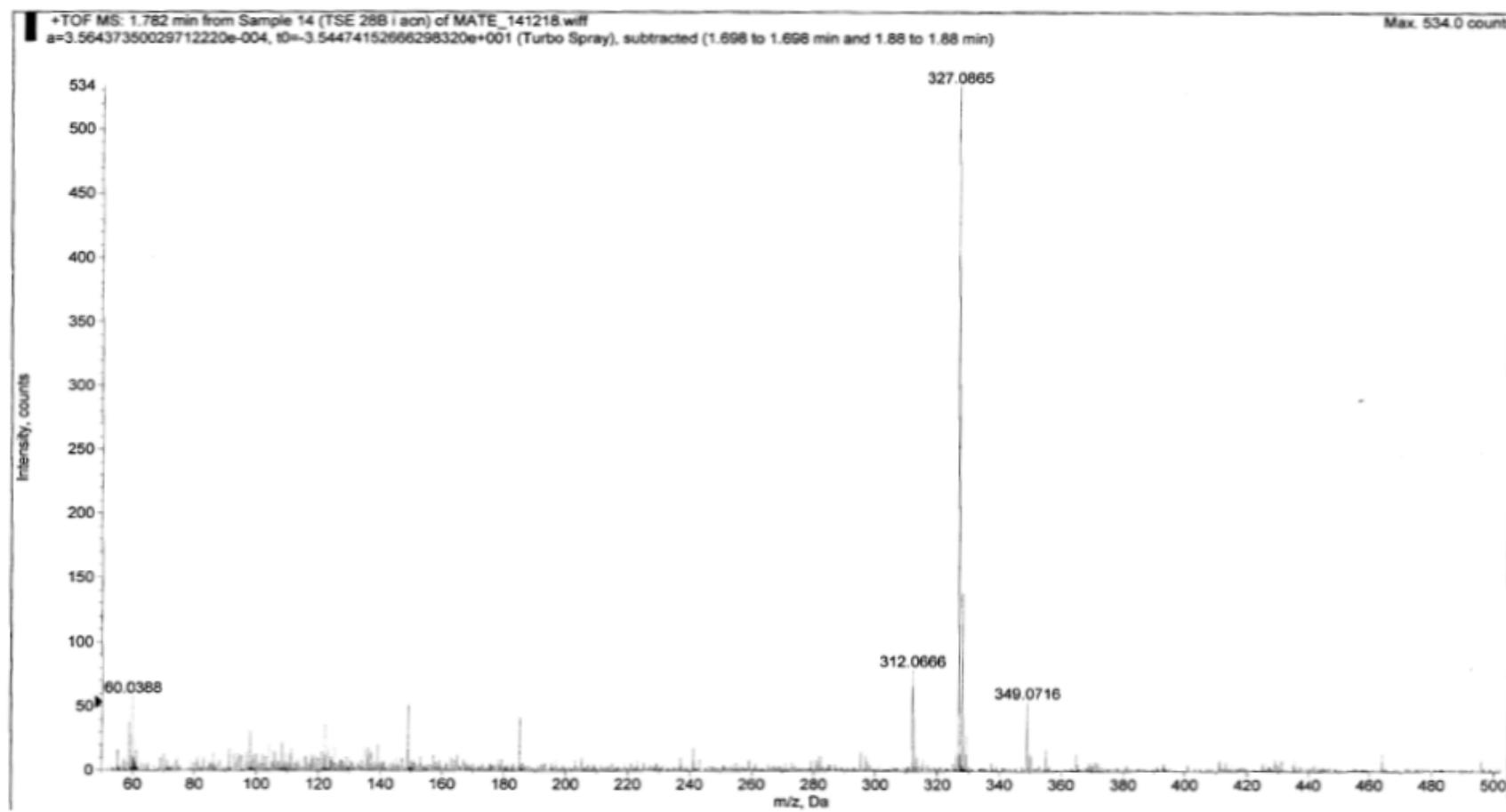
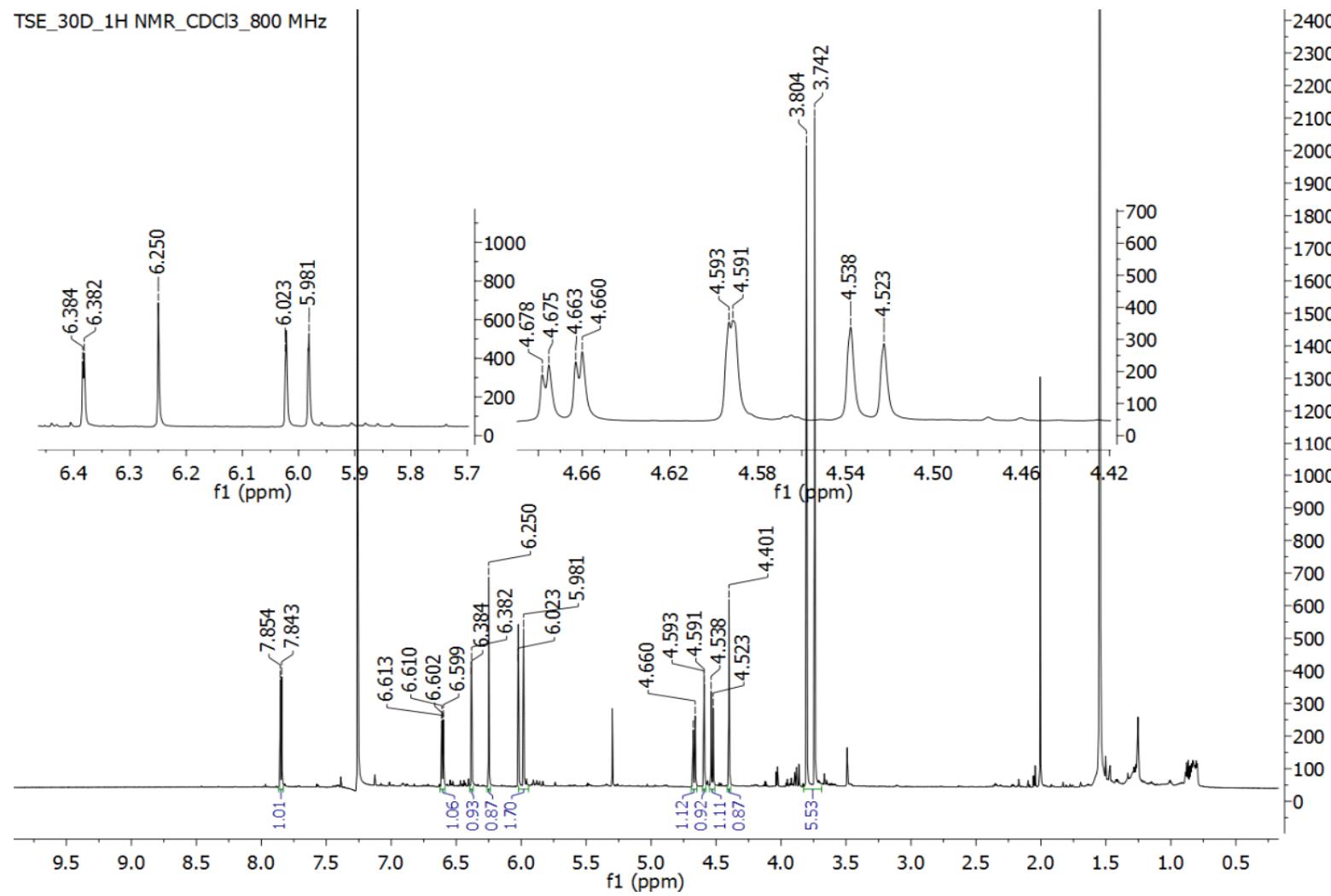


Figure S4F: HRESMS spectrum of compound 4

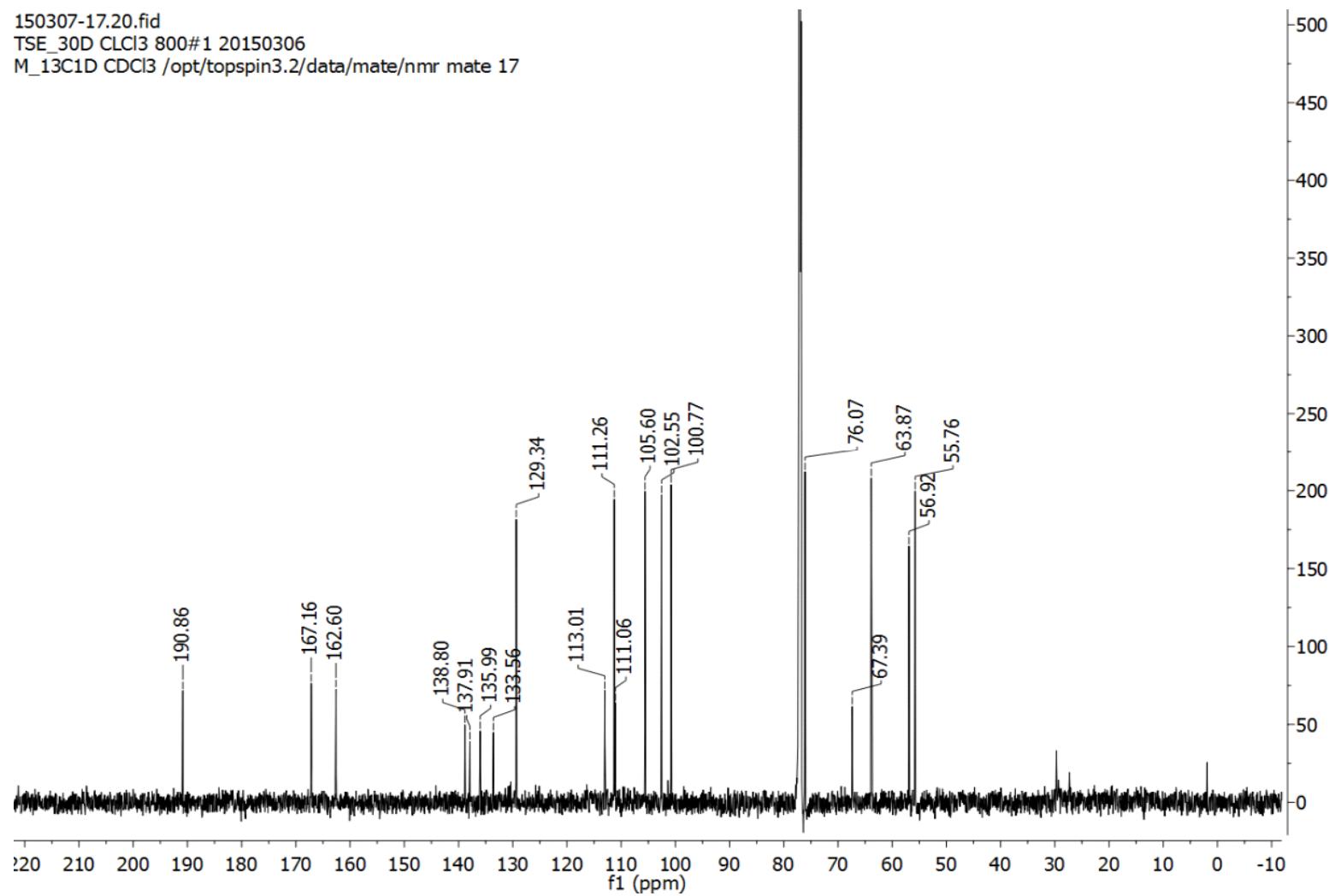


**Figure S5A:**  $^1\text{H}$  NMR (799.87 MHz) spectrum of compound 5

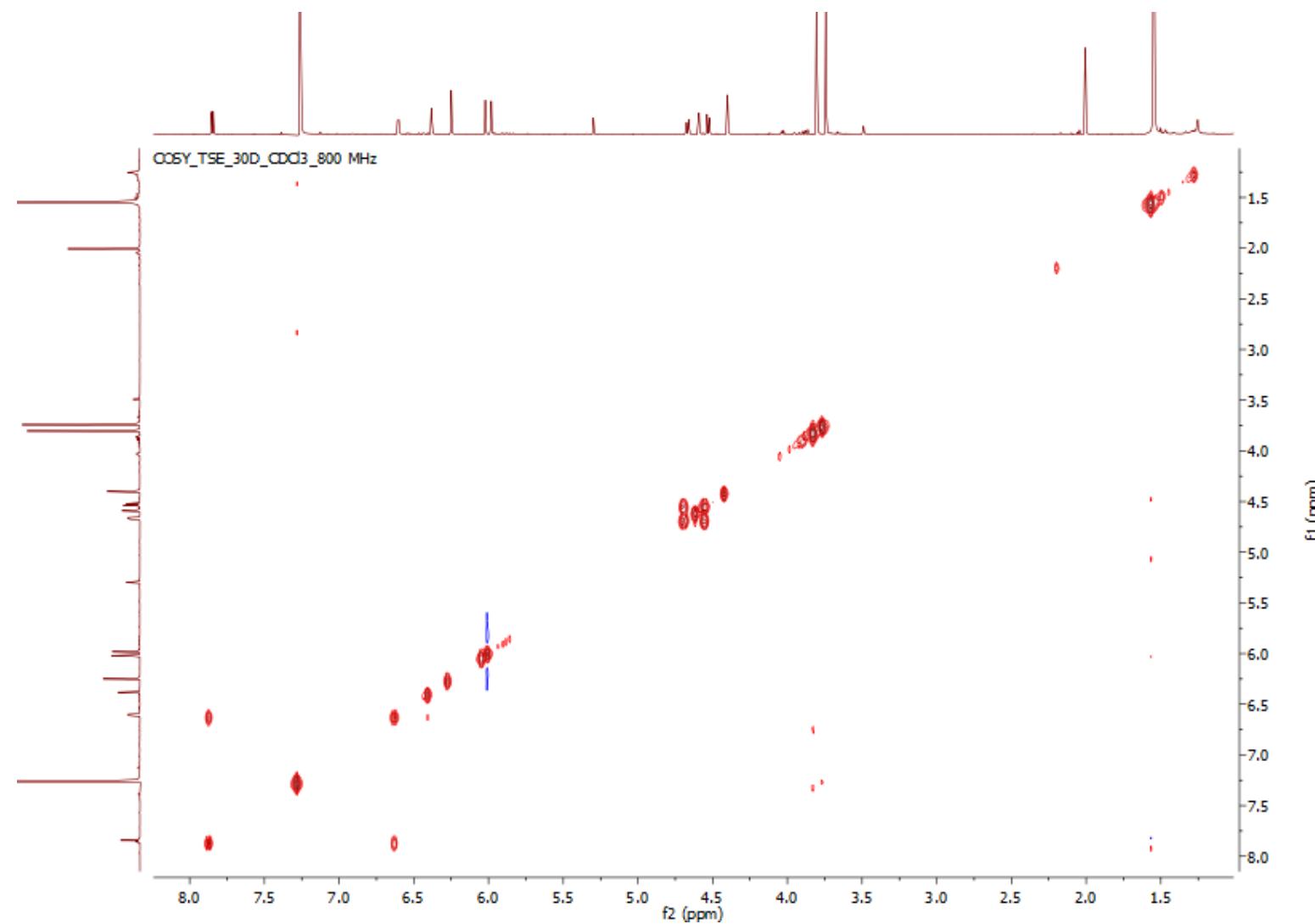


**Figure S5B:**  $^{13}\text{C}$  NMR (201.15 MHz) spectrum of compound 5

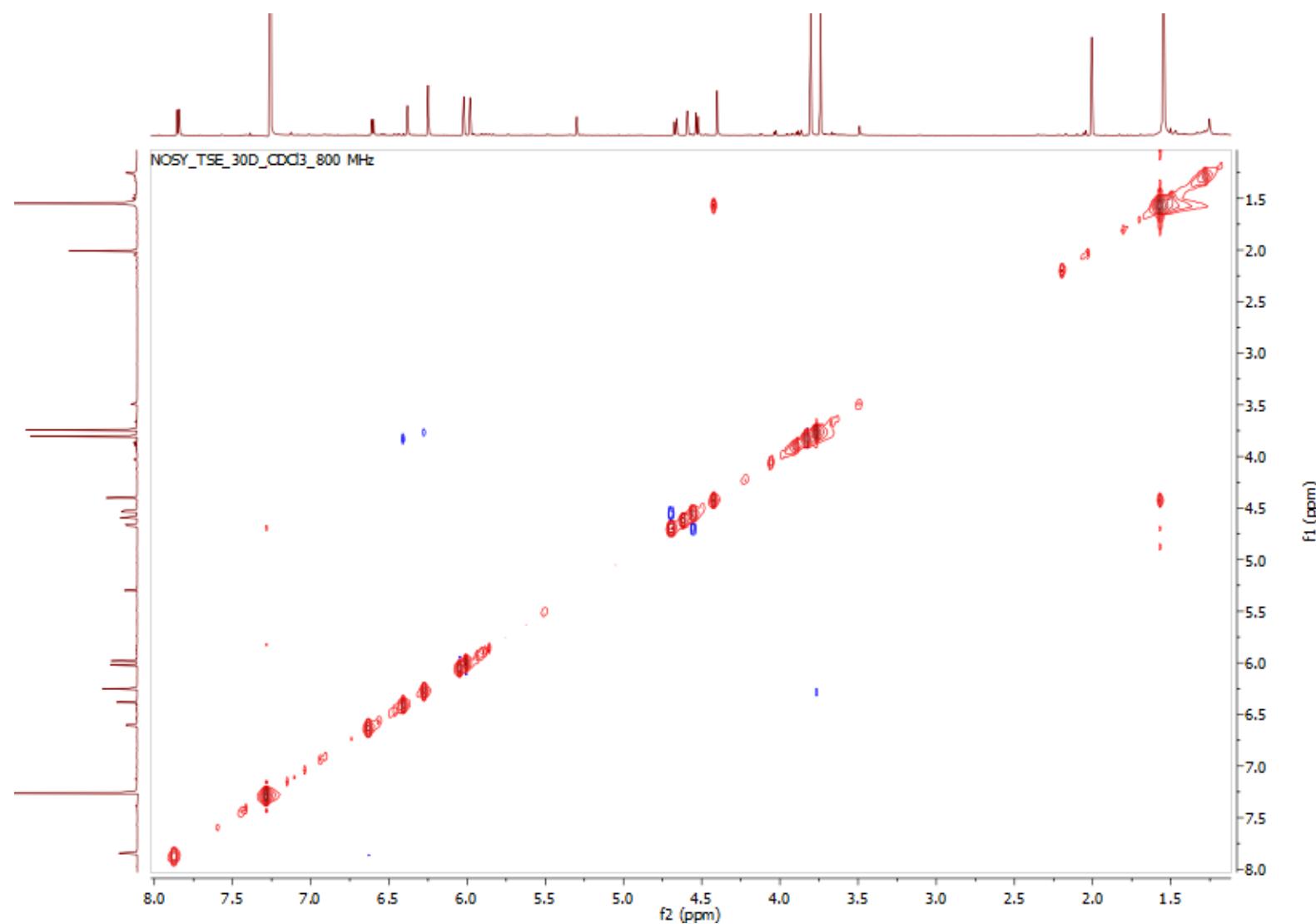
150307-17.20.fid  
TSE\_30D CLC<sub>3</sub> 800#1 20150306  
M\_13C1D CDCl<sub>3</sub> /opt/topspin3.2/data/mate/nmr mate 17



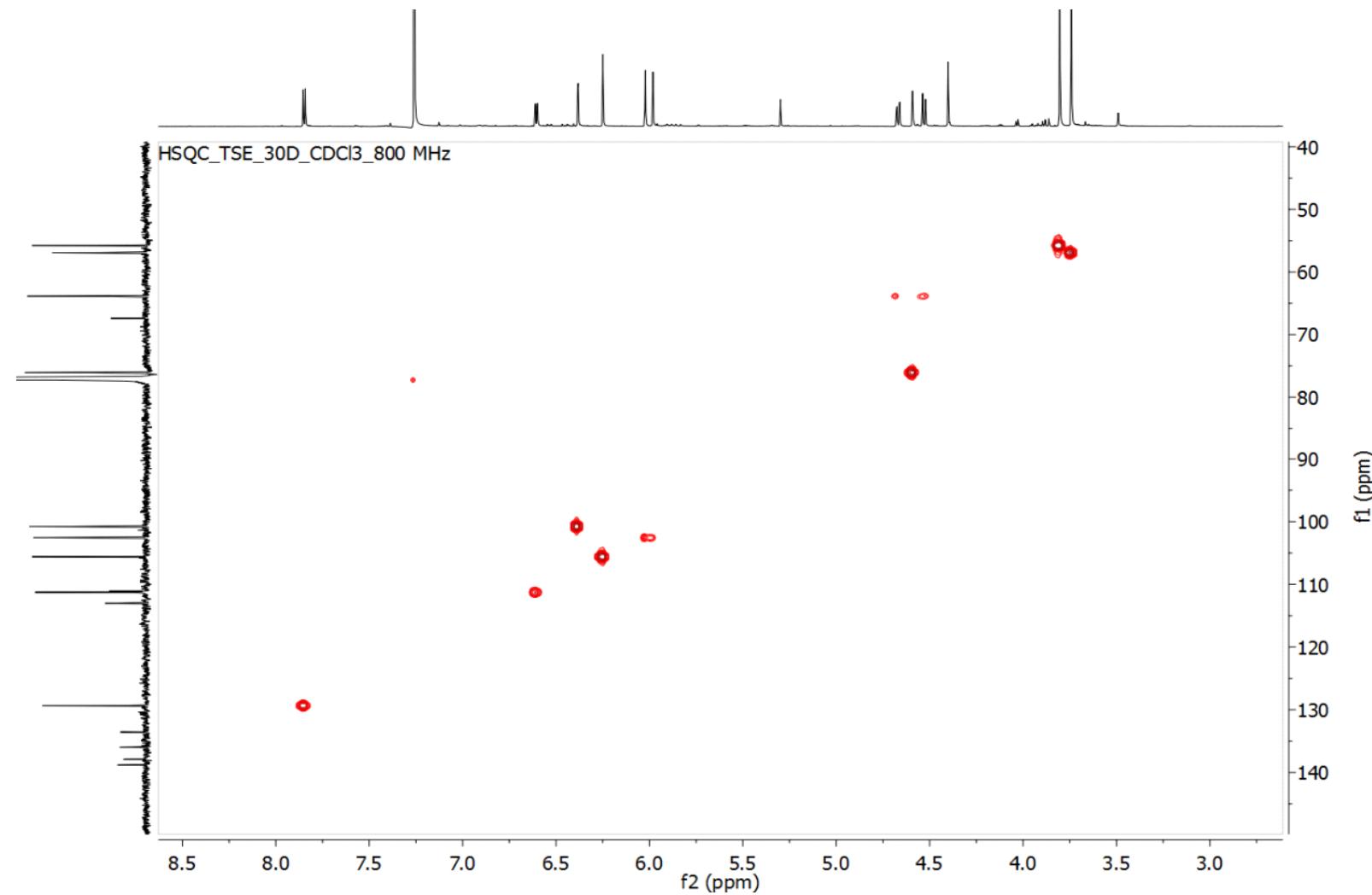
**Figure S5C:** COSY (799.87 MHz) spectrum of compound 5



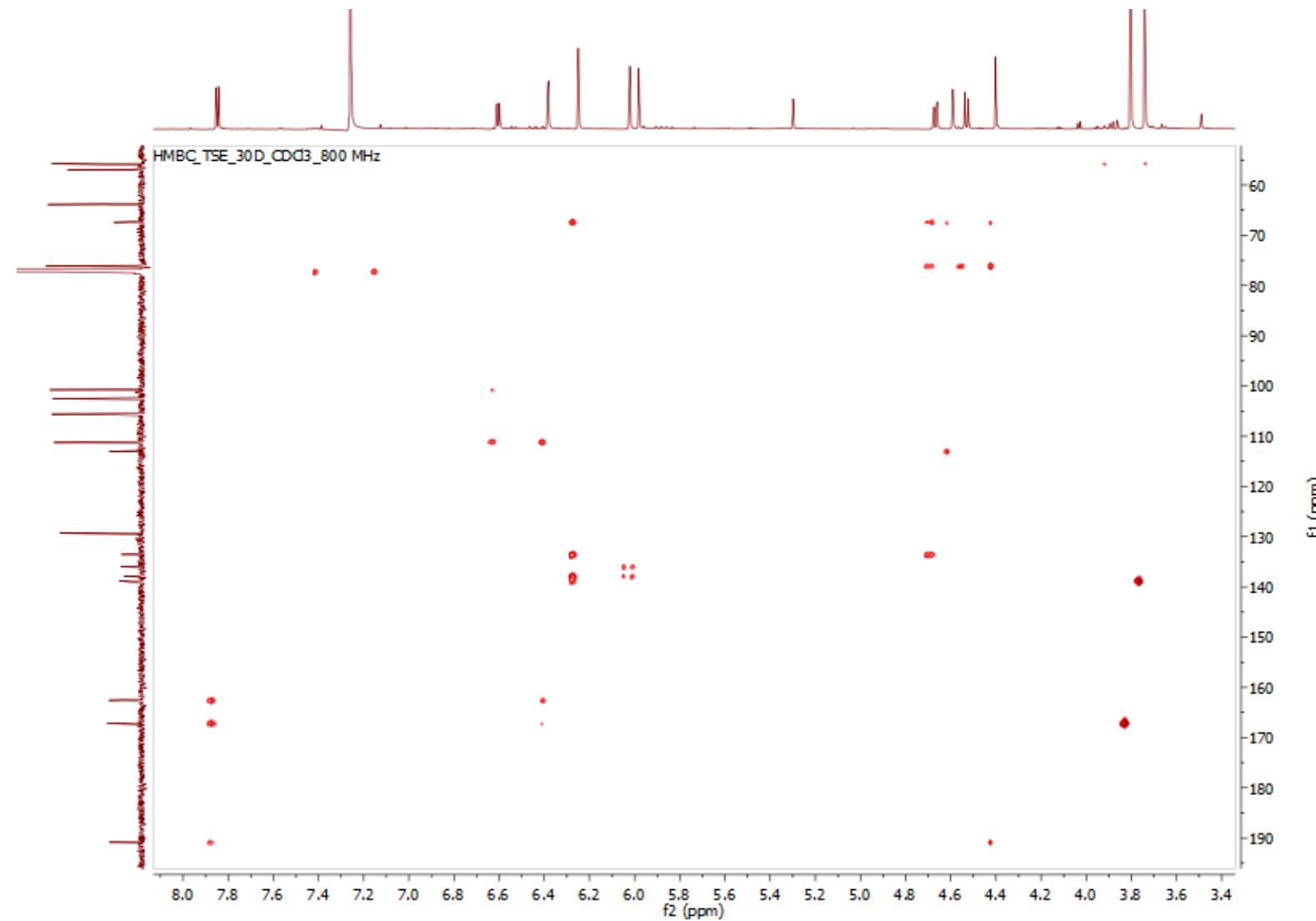
**Figure S5D:** NOESY (799.87 MHz) spectrum of compound 5



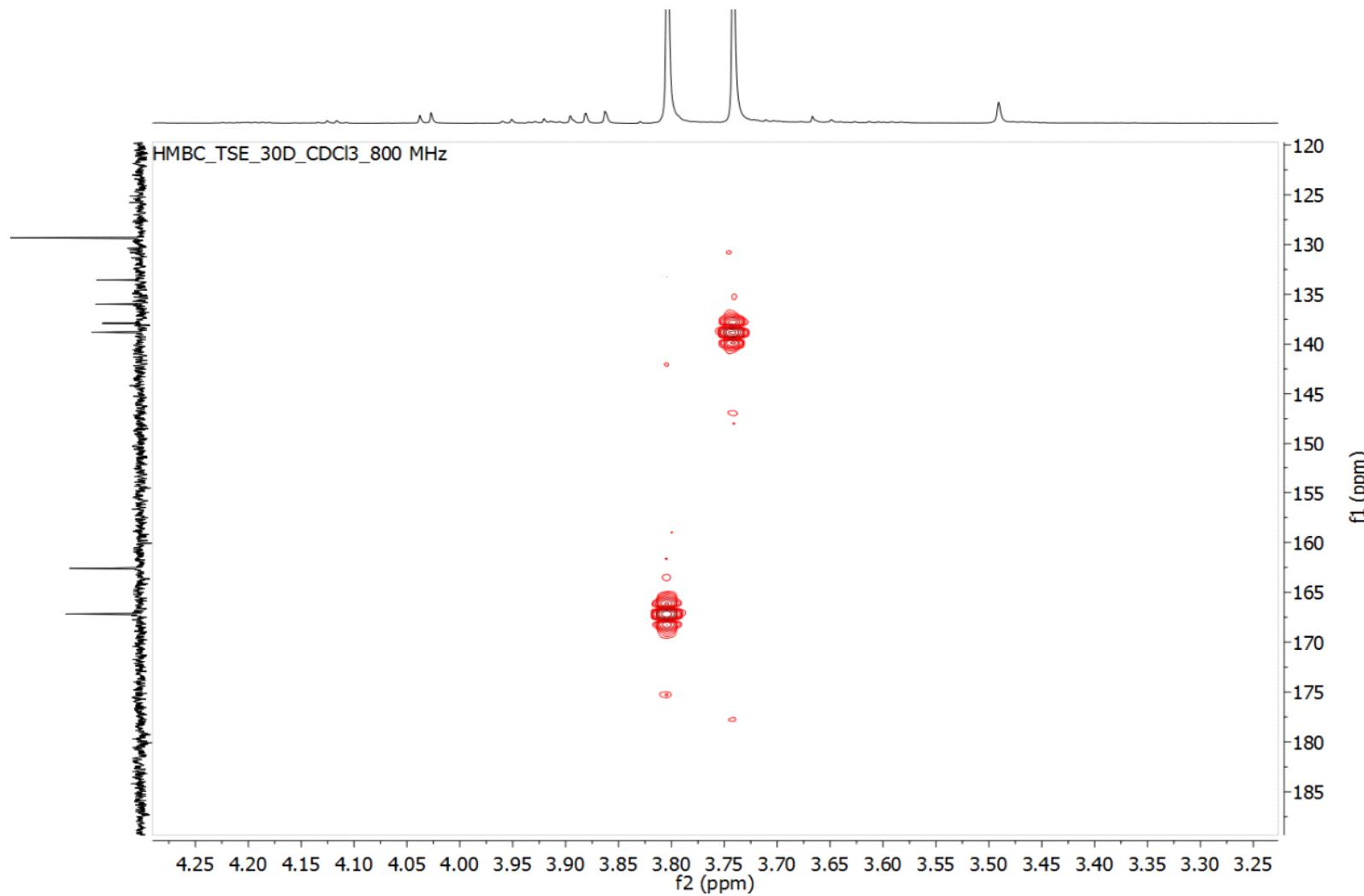
**Figure S5E:** HSQC (799.87/201.15 MHz) spectrum of compound 5



**Figure S5F:** HMBC (799.87/201.15 MHz) spectrum of compound 5



**Figure S5G:** HMBC expanded (799.87/201.15 MHz) spectrum of compound 5



**Figure S5H: HMBC expanded-1 (799.87/201.15 MHz) spectrum of compound 5**

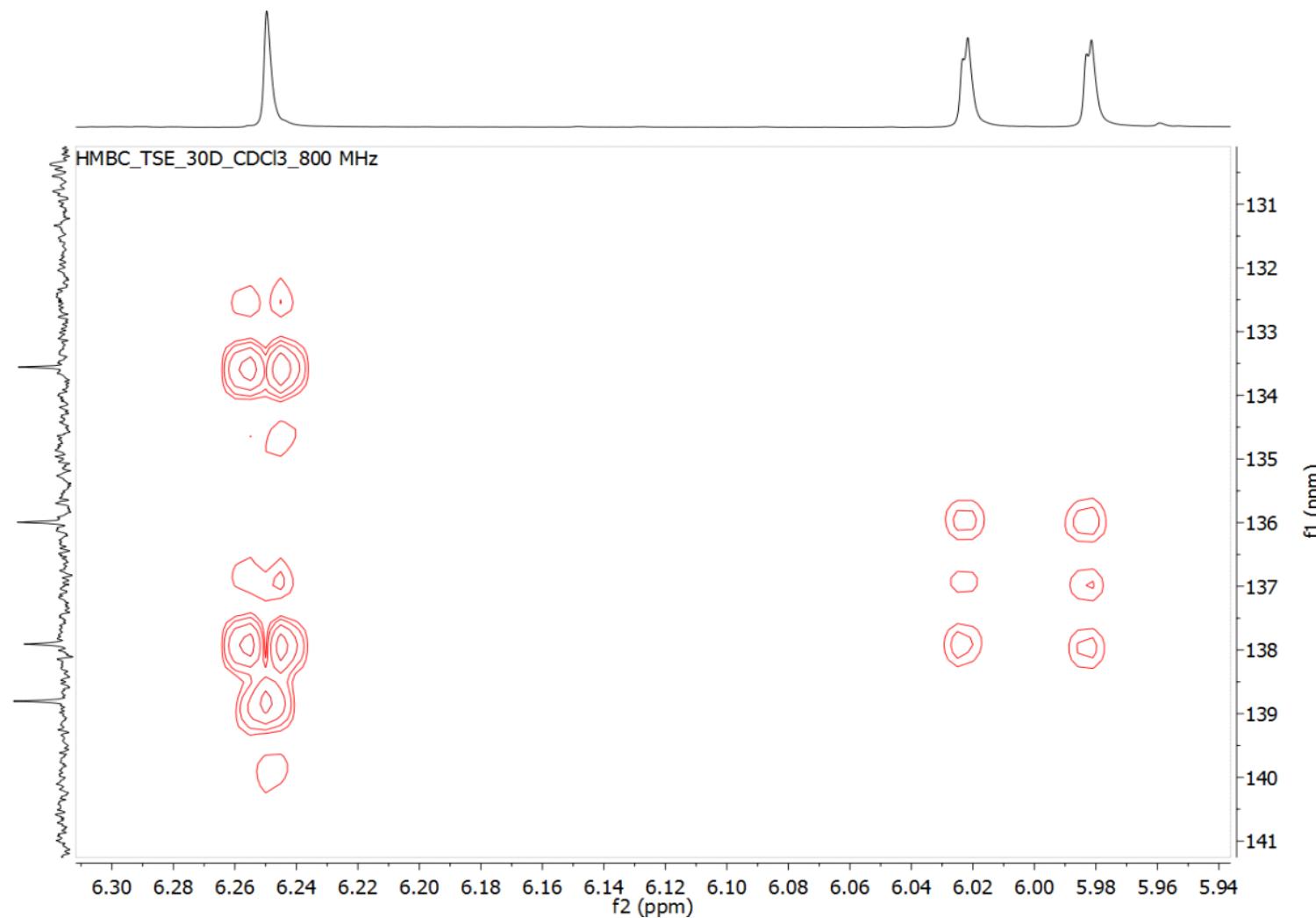
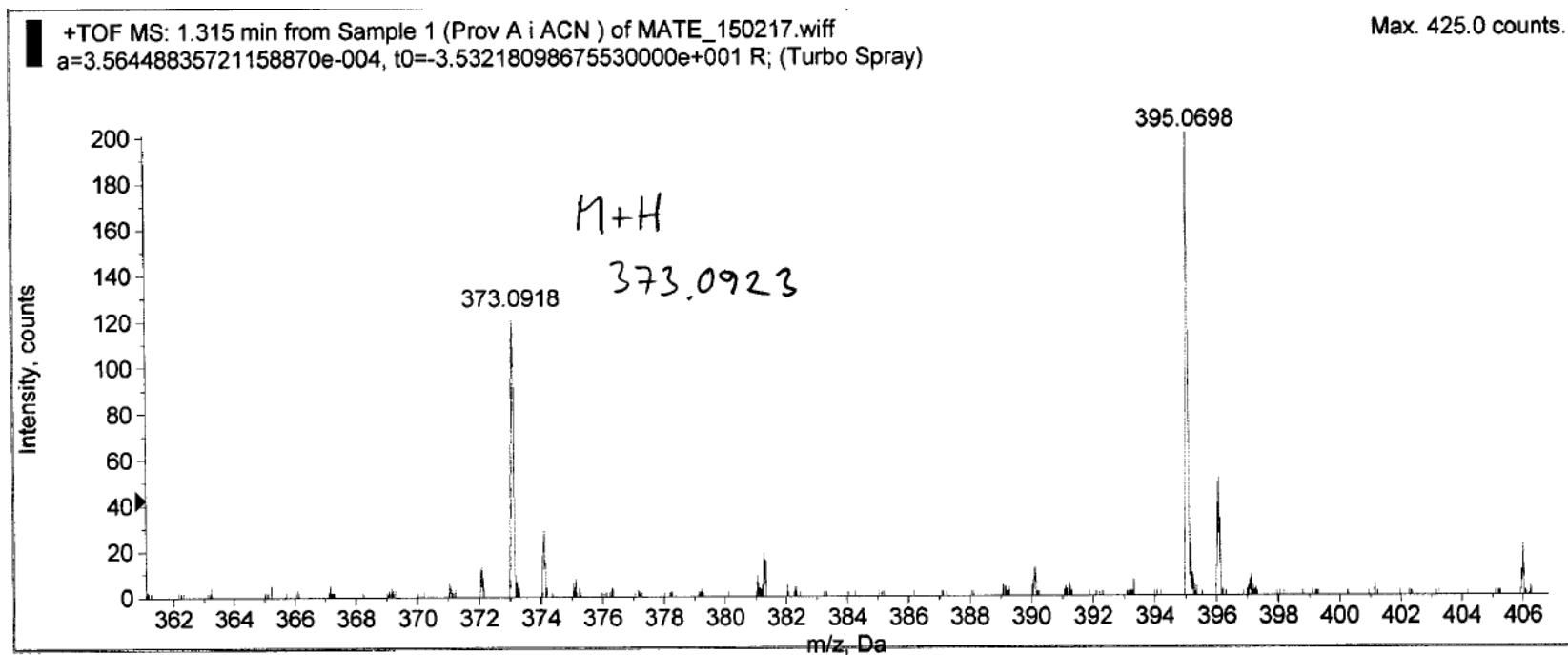
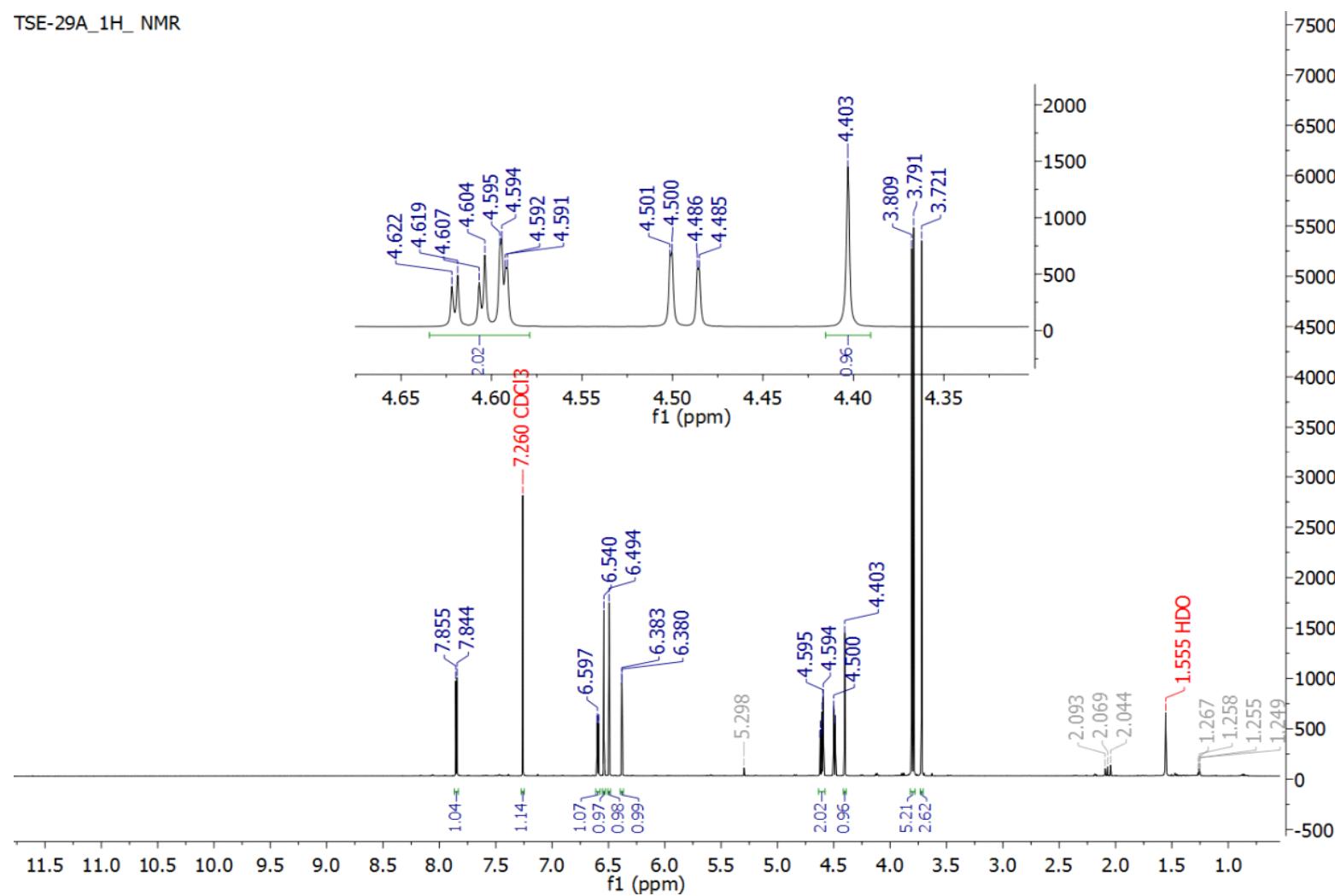


Figure S5I: HREIMS spectrum of compound 5



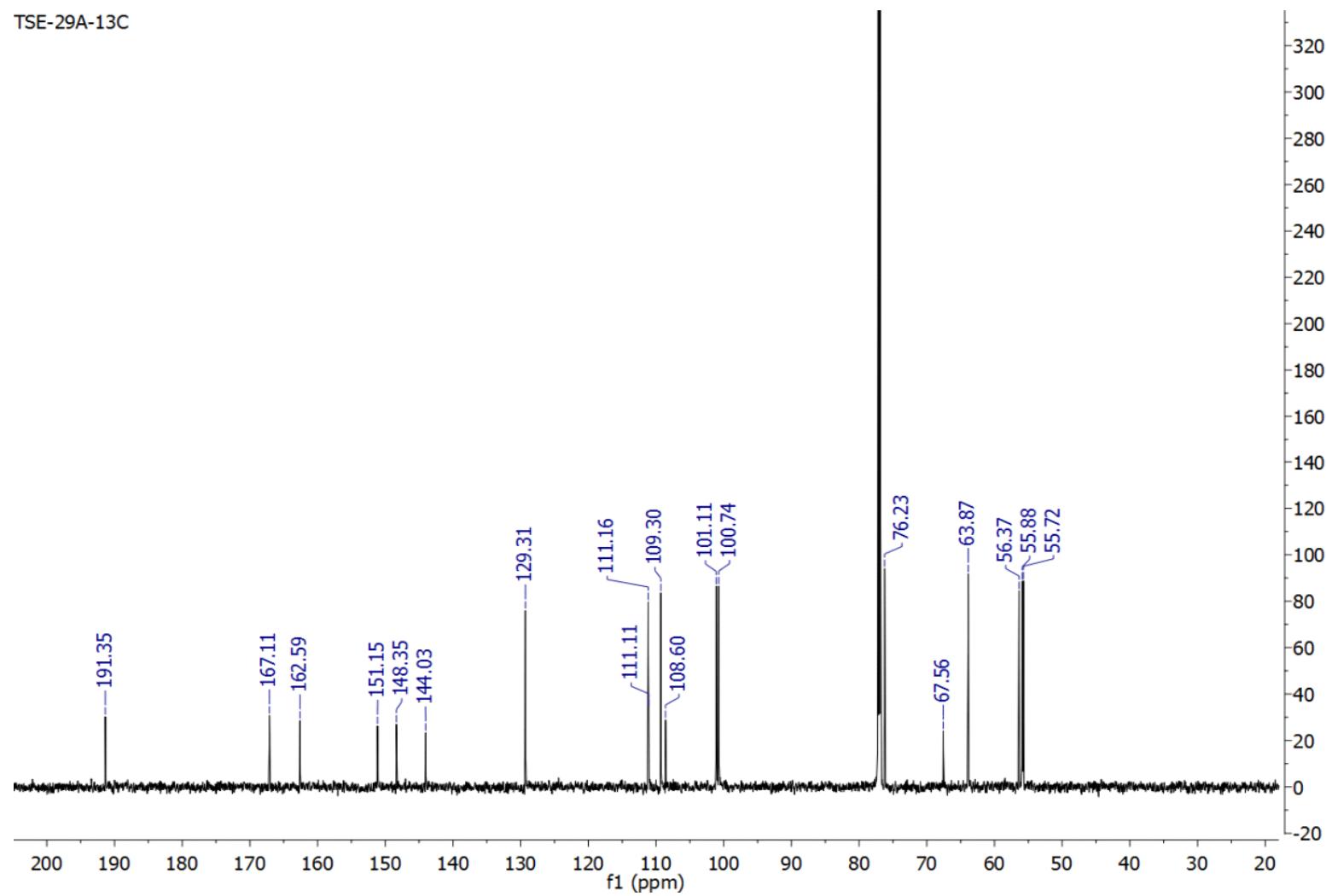
**Figure S6A:**  $^1\text{H}$ NMR (799.87 MHz) spectrum of compound 6

TSE-29A\_1H\_NMR

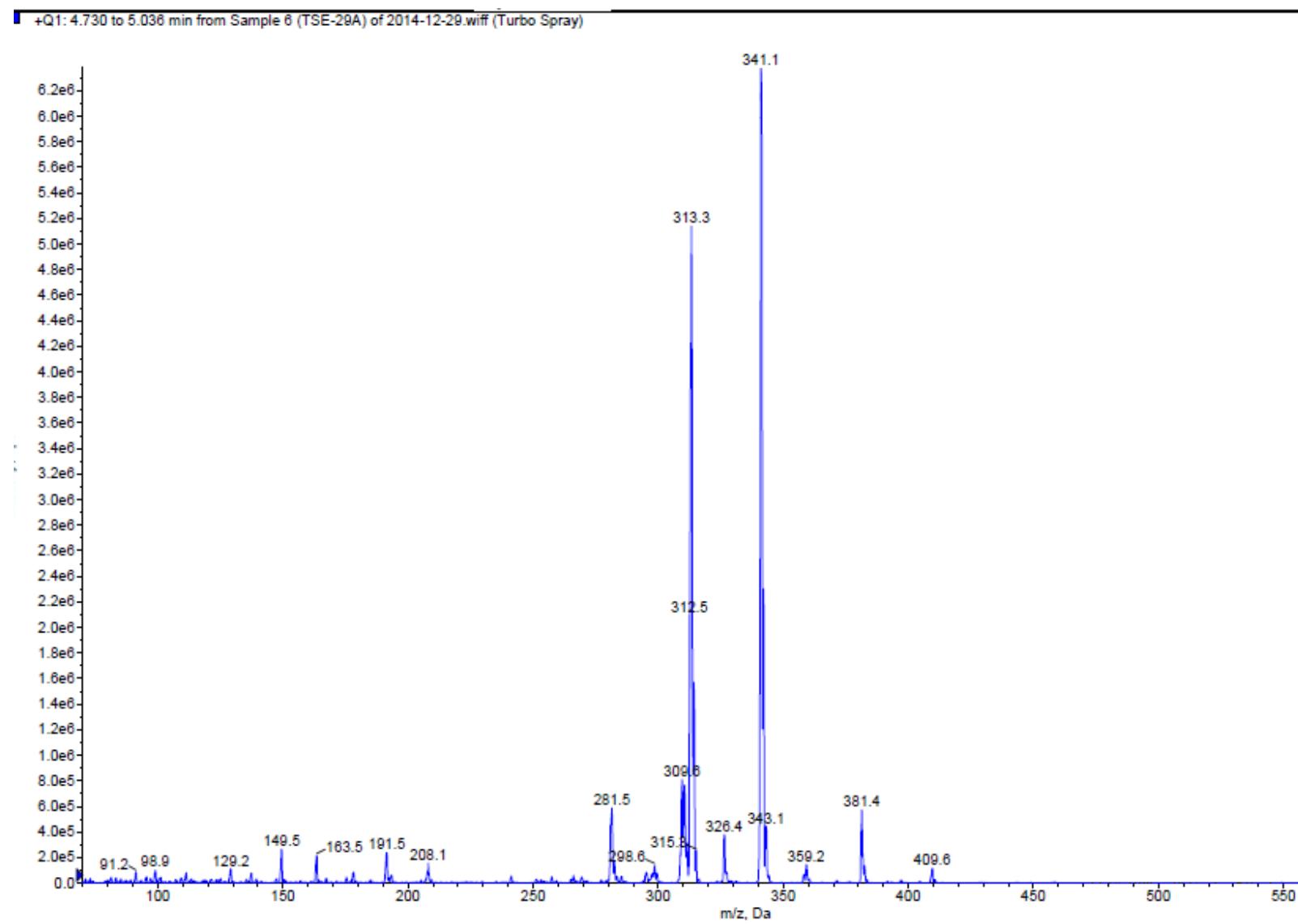


**Figure S6B:**  $^{13}\text{C}$  NMR (201.15 MHz) spectrum of compound 6

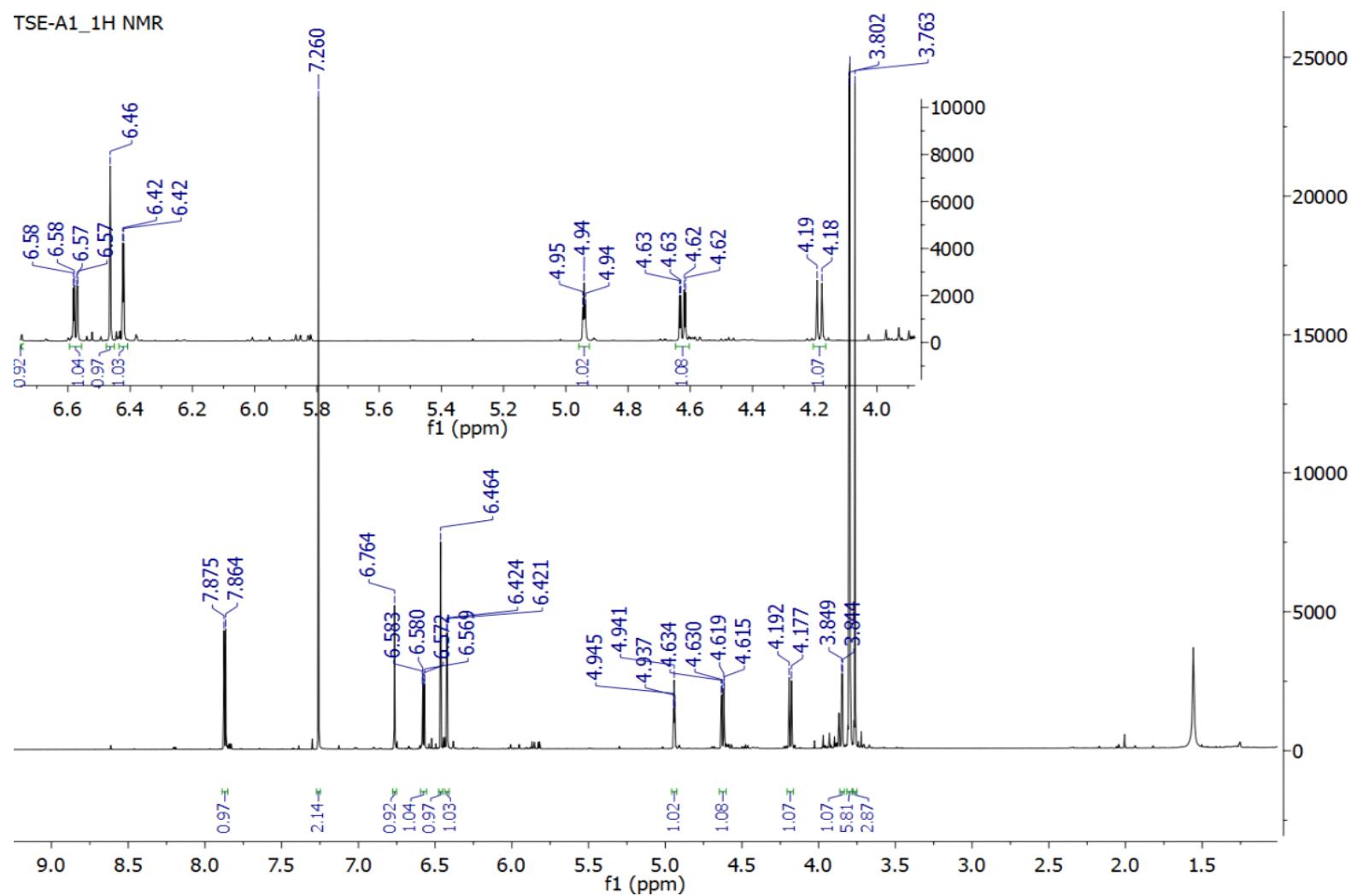
TSE-29A-13C



**Figure S6C:** ESIMS spectrum of compound 6

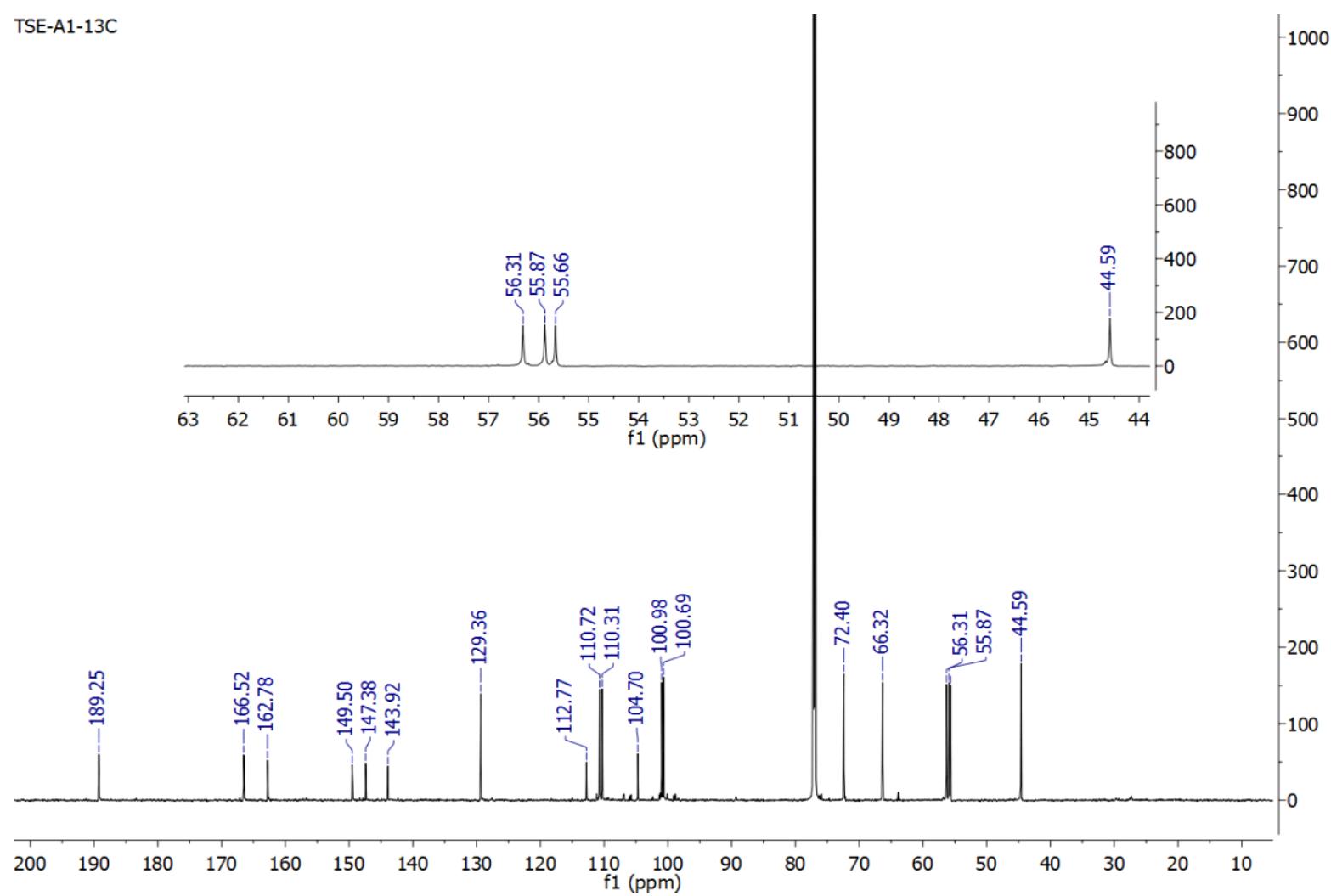


**Figure S7A:**  $^1\text{H}$  NMR (799.87 MHz) spectrum of compound 7



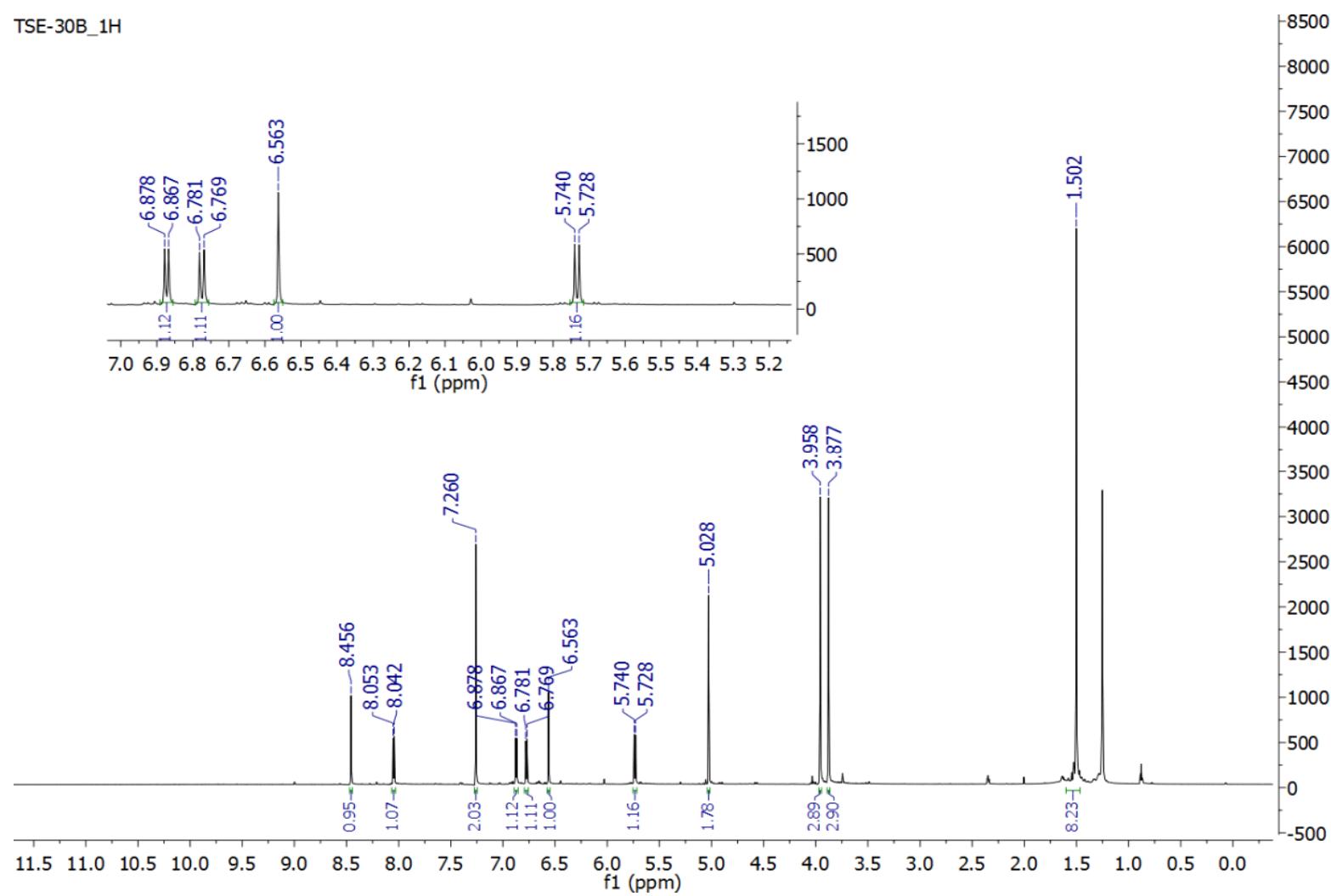
**Figure S7B:**  $^{13}\text{C}$  NMR (201.15 MHz) spectrum of compound 7

TSE-A1-13C



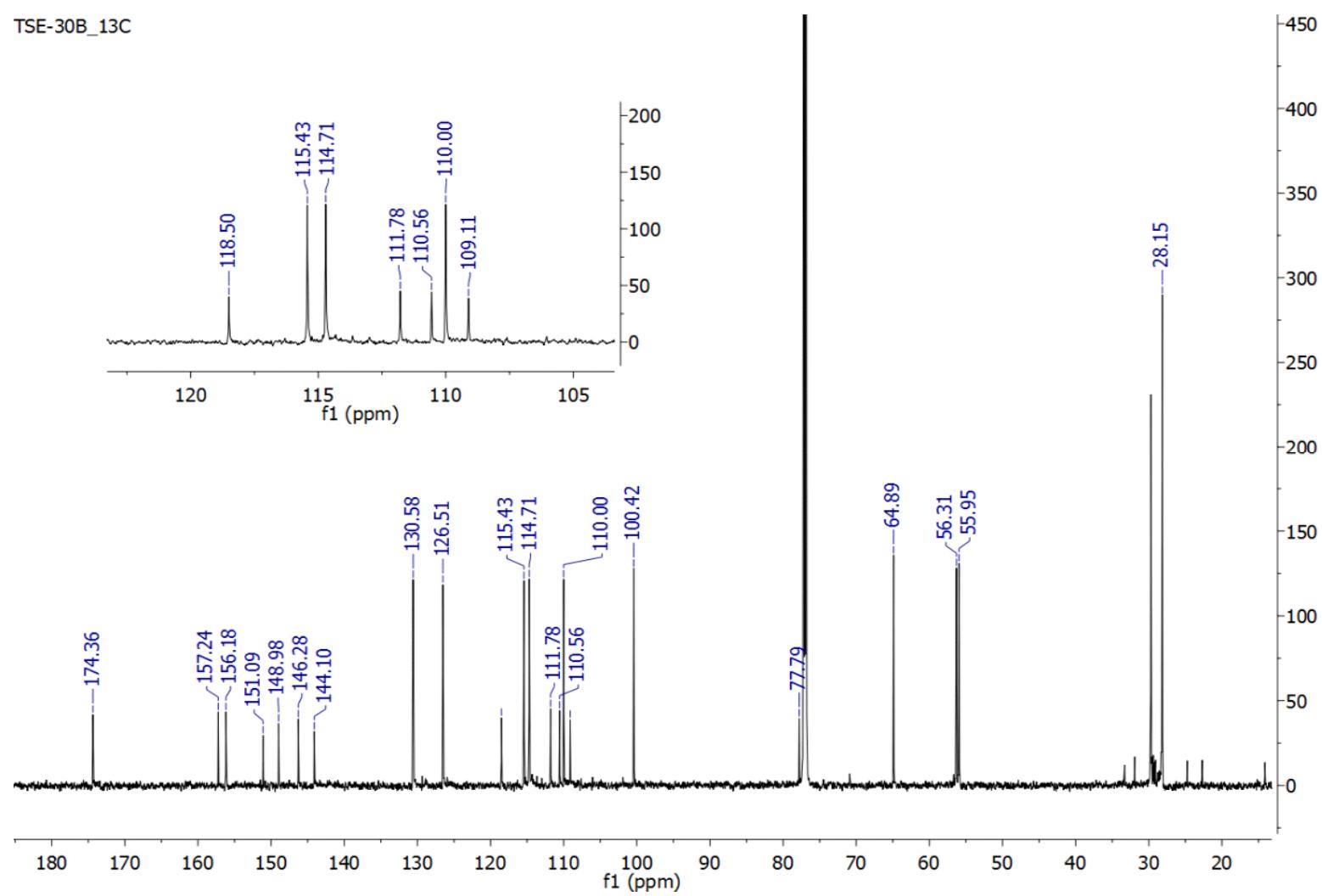
**Figure S8A:**  $^1\text{H}$  NMR (799.87 MHz) spectrum of compound 8

TSE-30B\_1H

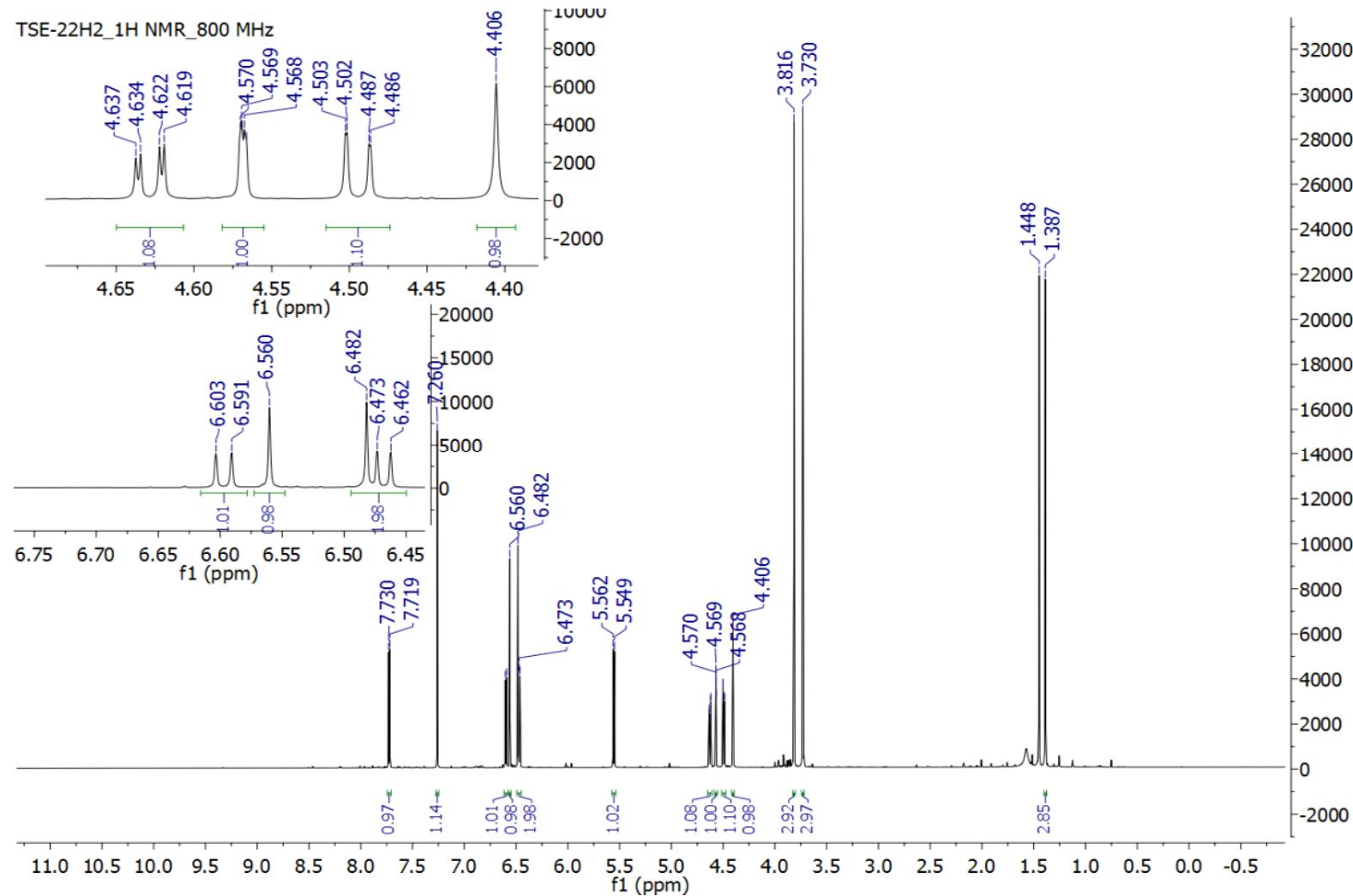


**Figure S8B:**  $^{13}\text{C}$  NMR (201.15 MHz) spectrum of compound 8

TSE-30B\_13C

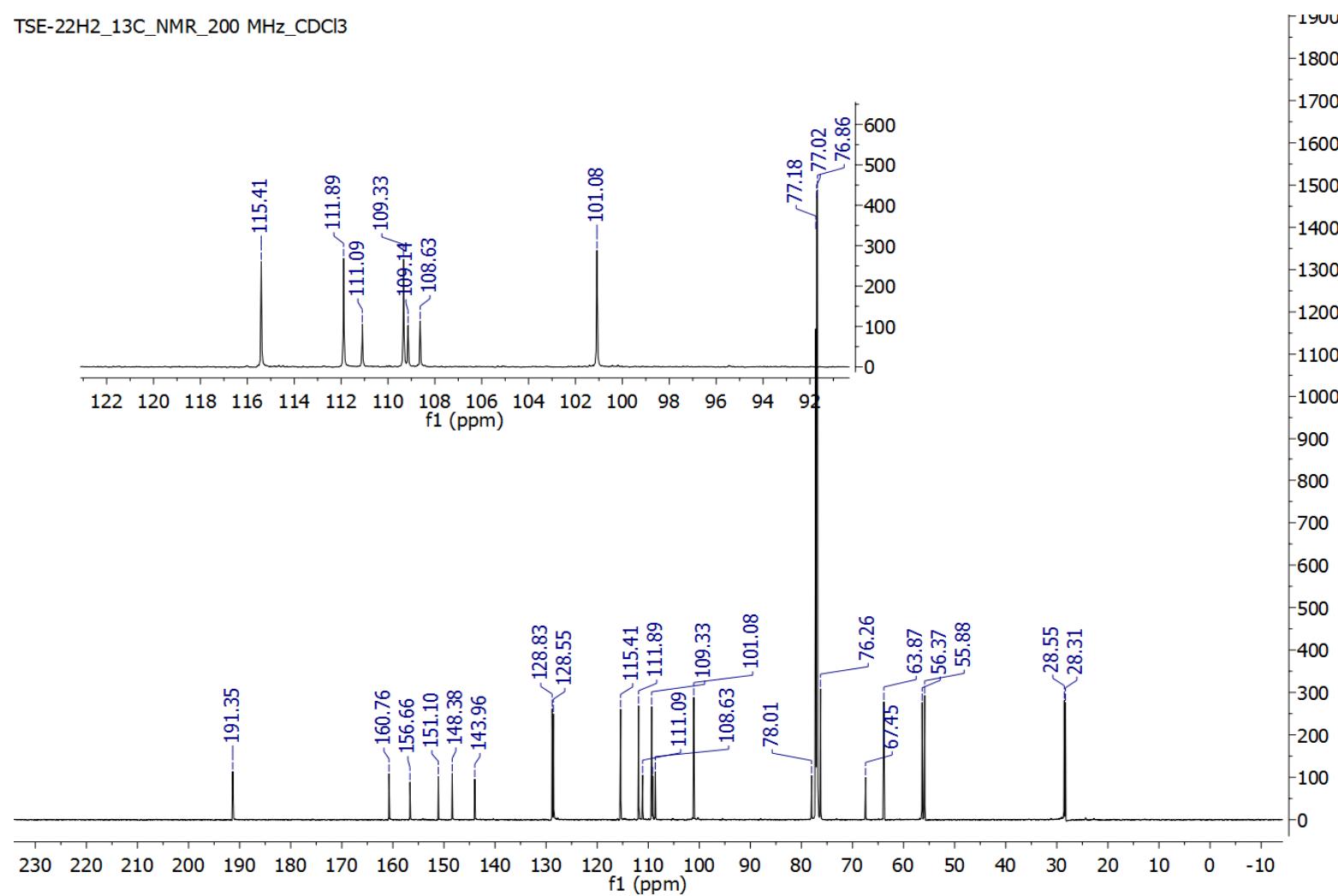


**Figure S9A:**  $^1\text{H}$  NMR (799.87 MHz) spectrum of compound 9



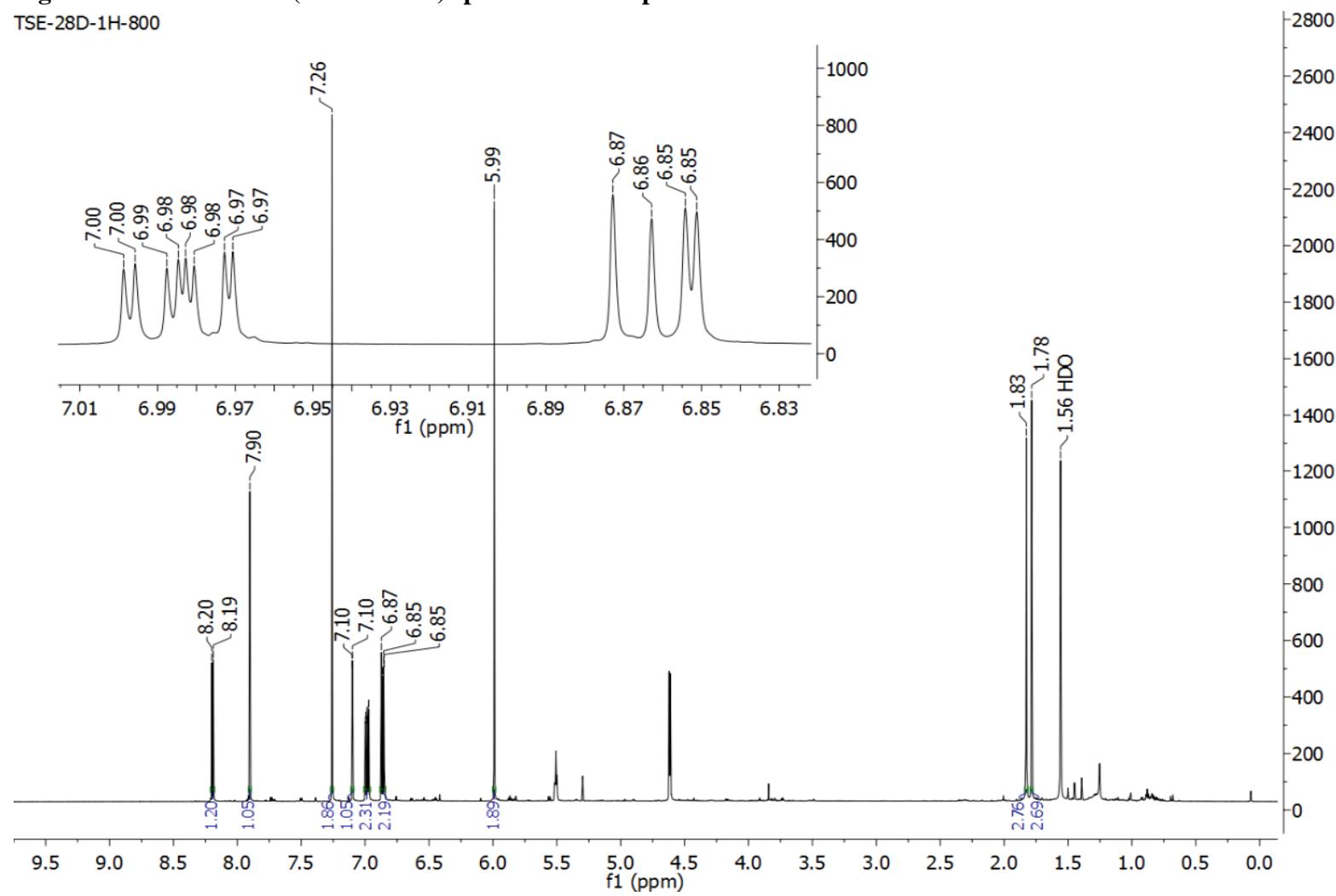
**Figure S9B:**  $^{13}\text{C}$  NMR (201.15 MHz) spectrum of compound 9

TSE-22H2\_13C\_NMR\_200 MHz\_CDCl<sub>3</sub>



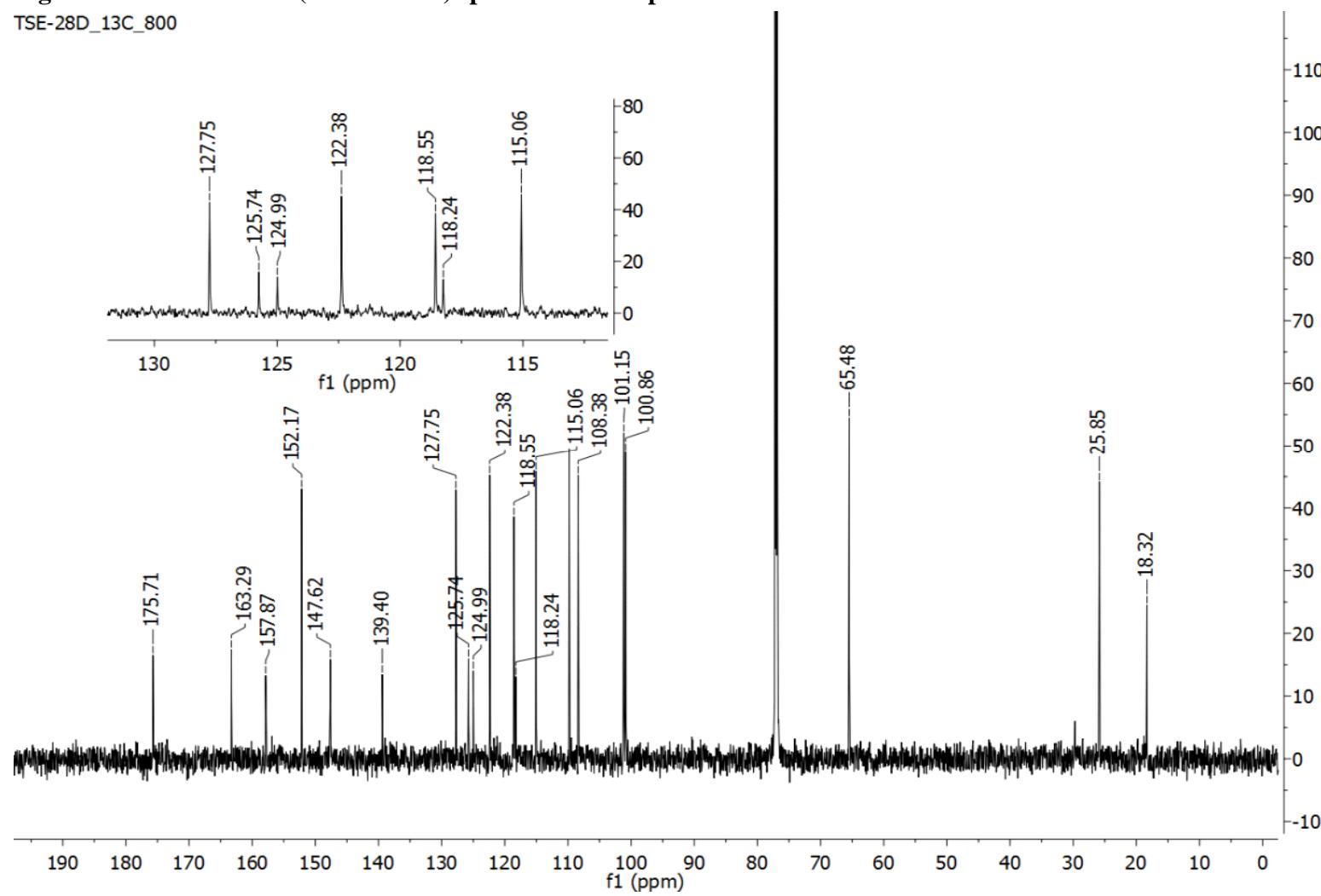
**Figure S10A:**  $^1\text{H}$  NMR (799.87 MHz) spectrum of compound 10

TSE-28D-1H-800



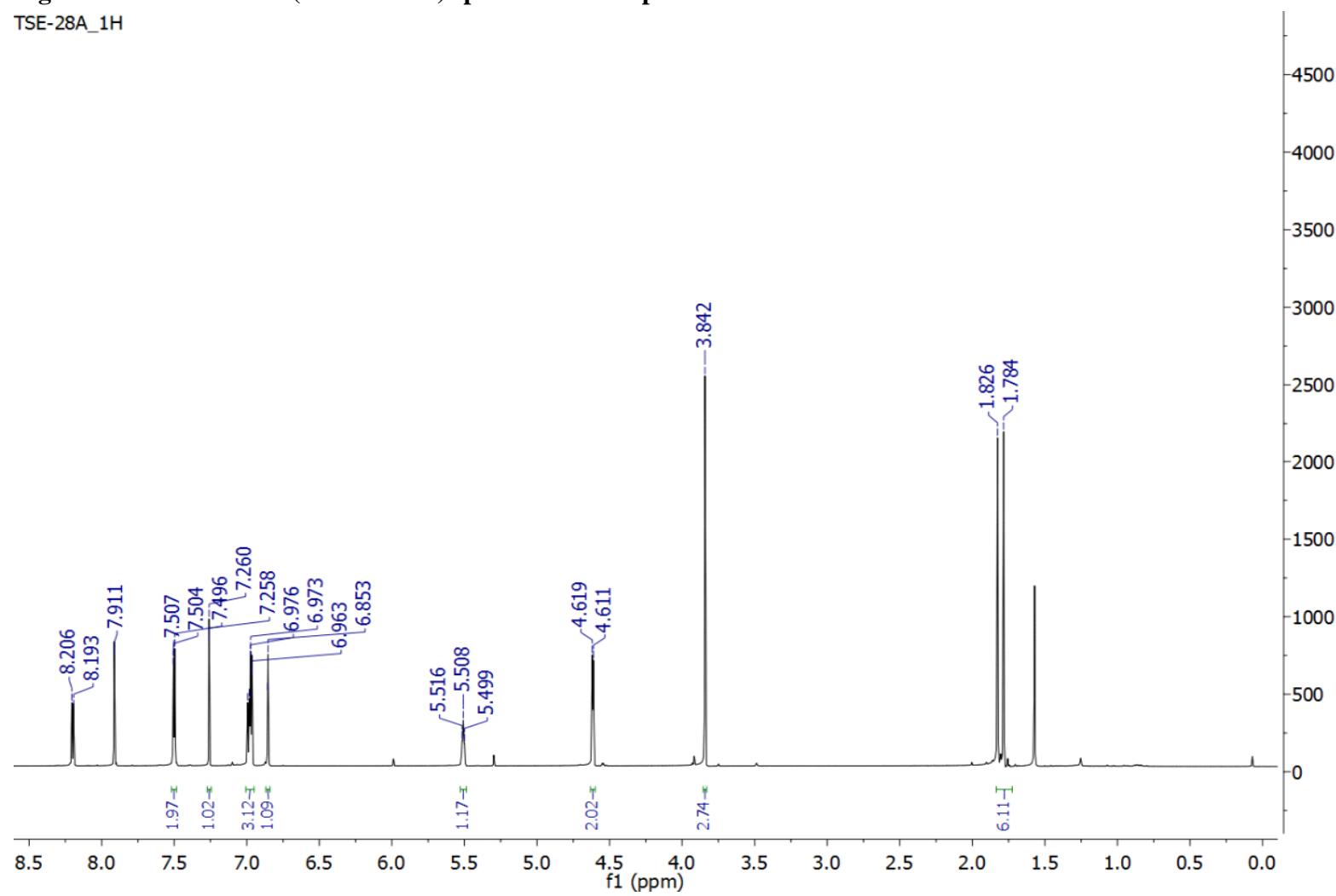
**Figure S10B:**  $^{13}\text{C}$  NMR (201.15 MHz) spectrum of compound 10

TSE-28D\_13C\_800



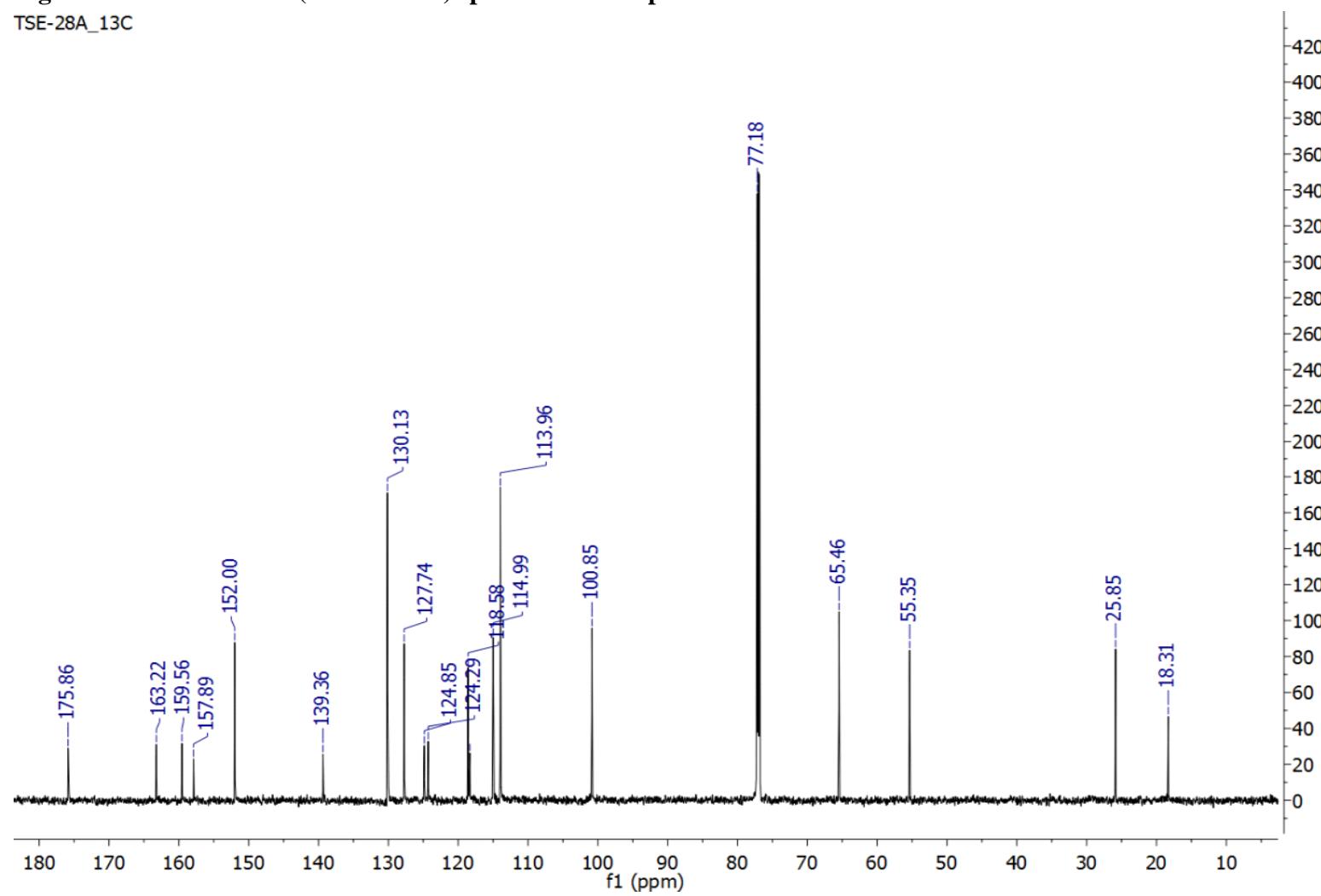
**Figure S11A:**  $^1\text{H}$  NMR (799.87 MHz) spectrum of compound 11

TSE-28A\_1H



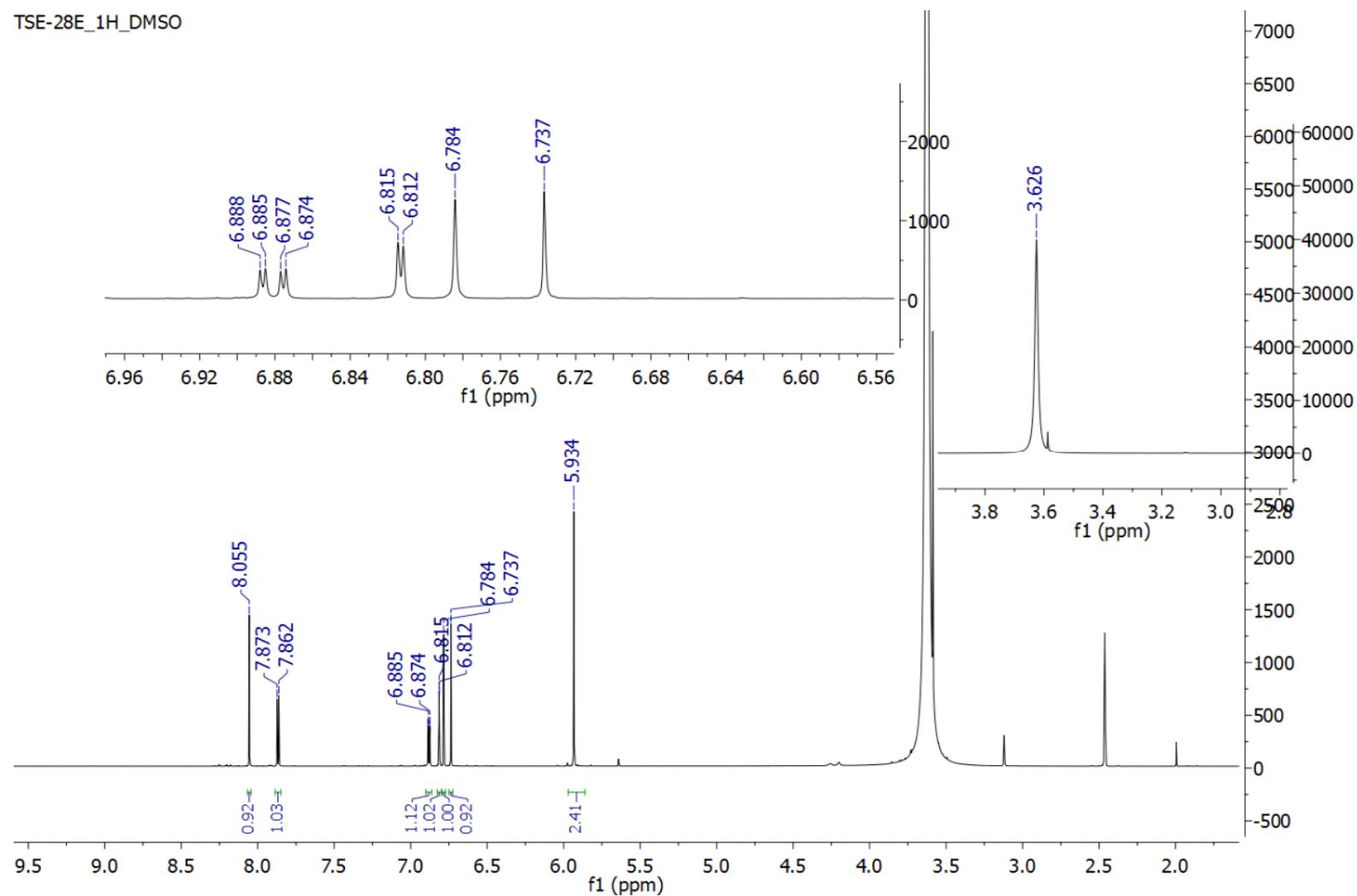
**Figure S11B:**  $^{13}\text{C}$  NMR (201.15 MHz) spectrum of compound 11

TSE-28A\_13C



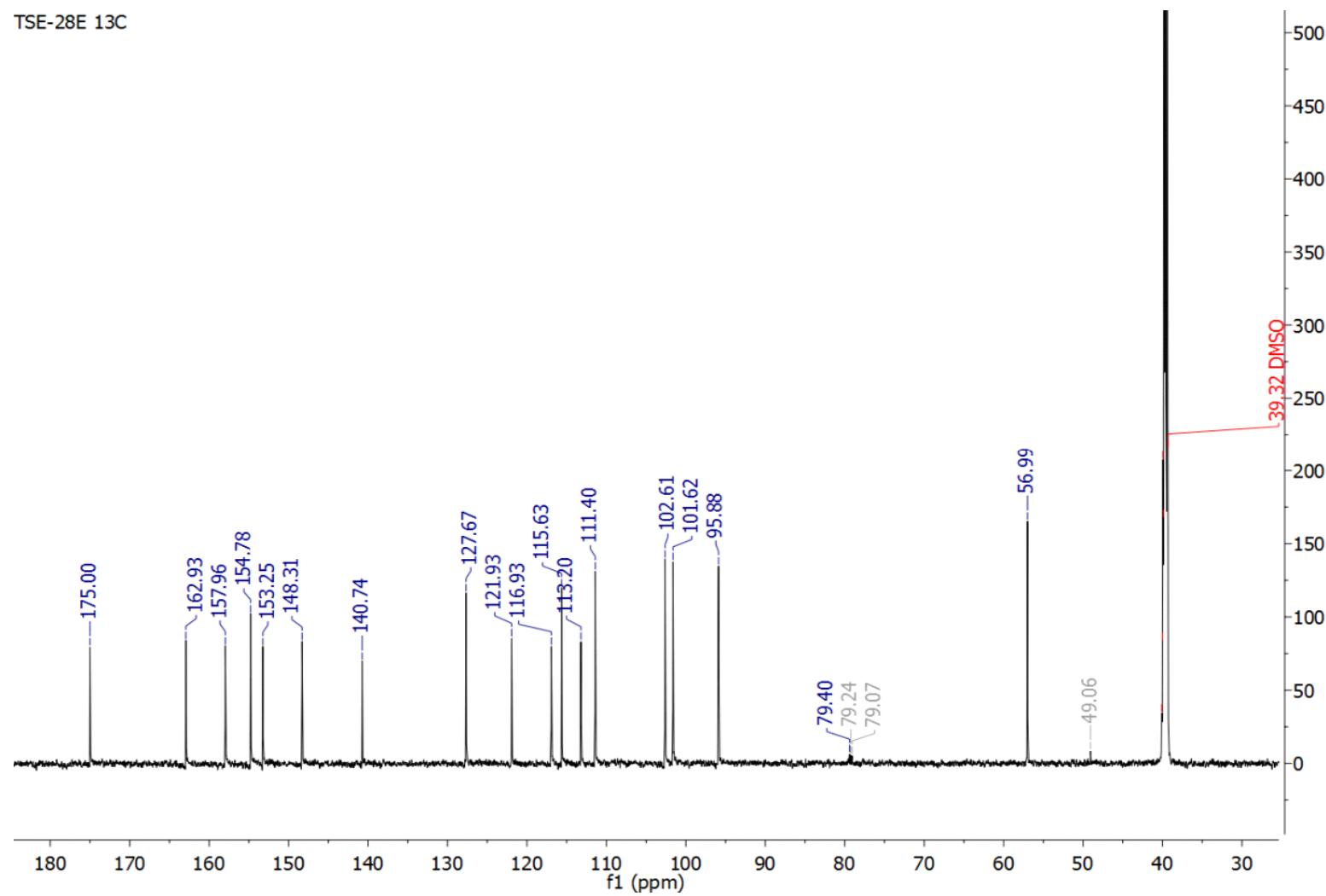
**Figure S12A:**  $^1\text{H}$  NMR (799.87 MHz) spectrum of compound 12

TSE-28E\_1H\_DMSO



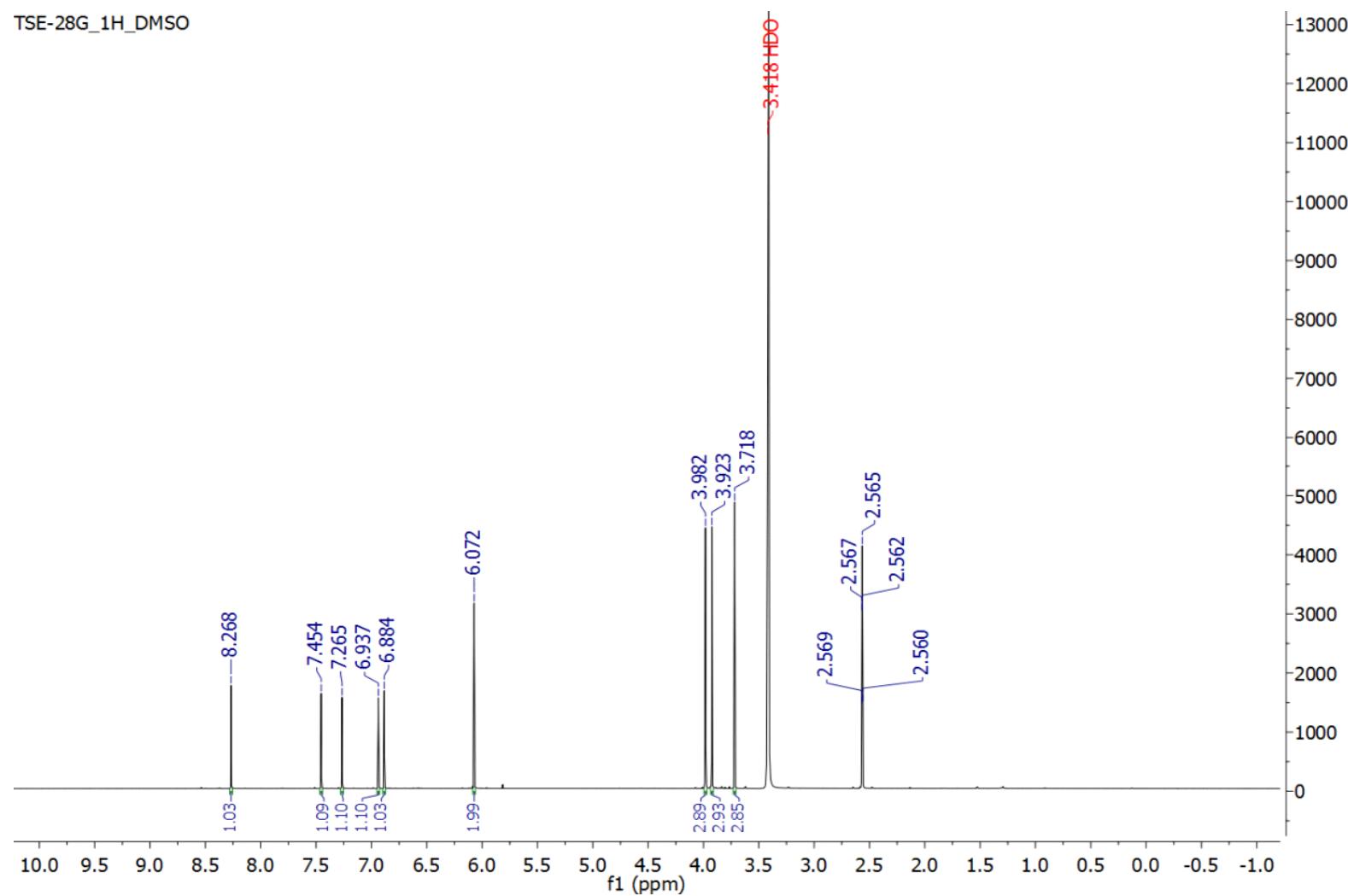
**Figure S12B:**  $^{13}\text{C}$  NMR (201.15 MHz) spectrum of compound 12

TSE-28E 13C



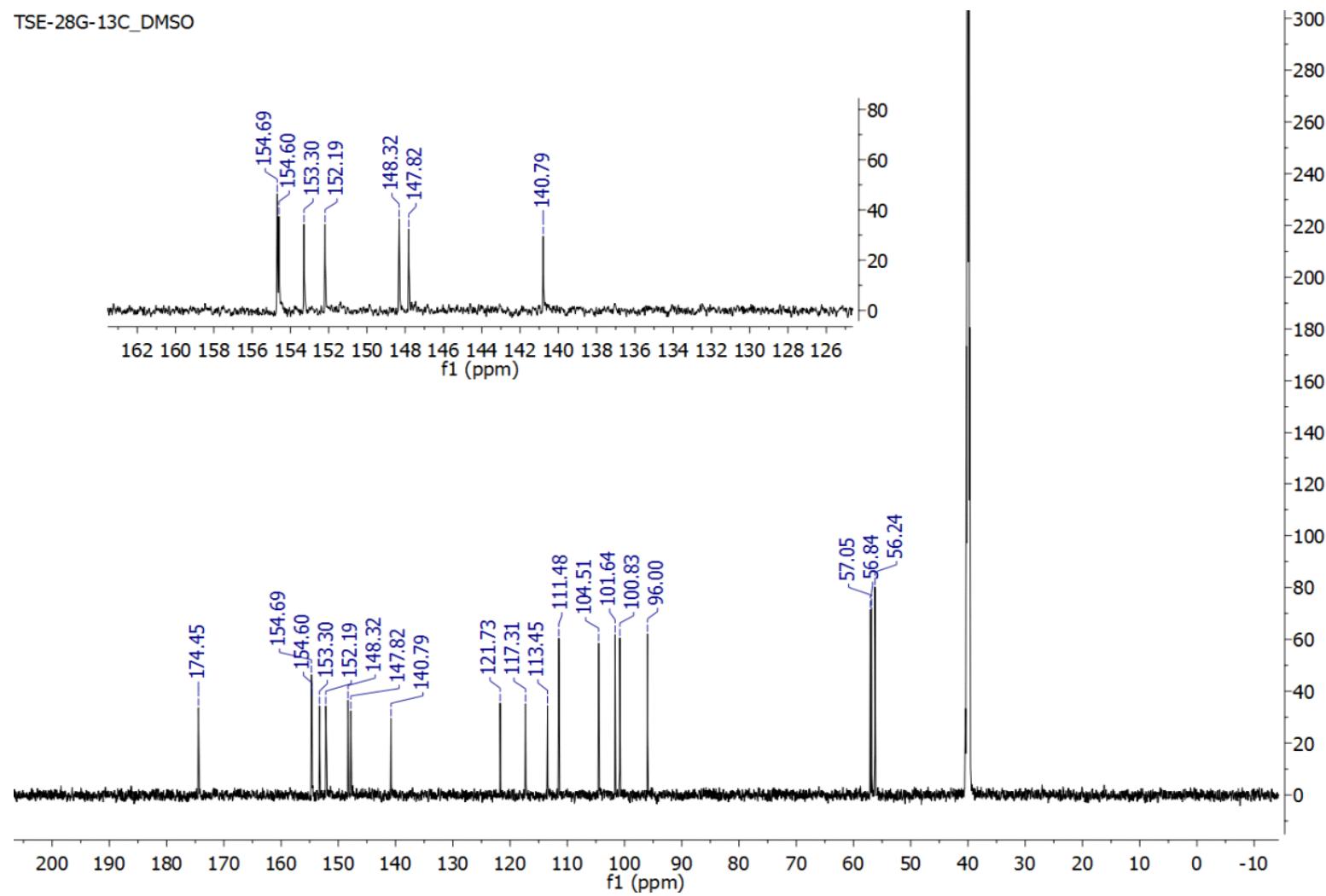
**Figure S13A:**  $^1\text{H}$  NMR (799.87 MHz) spectrum of compound 13

TSE-28G\_1H\_DMSO

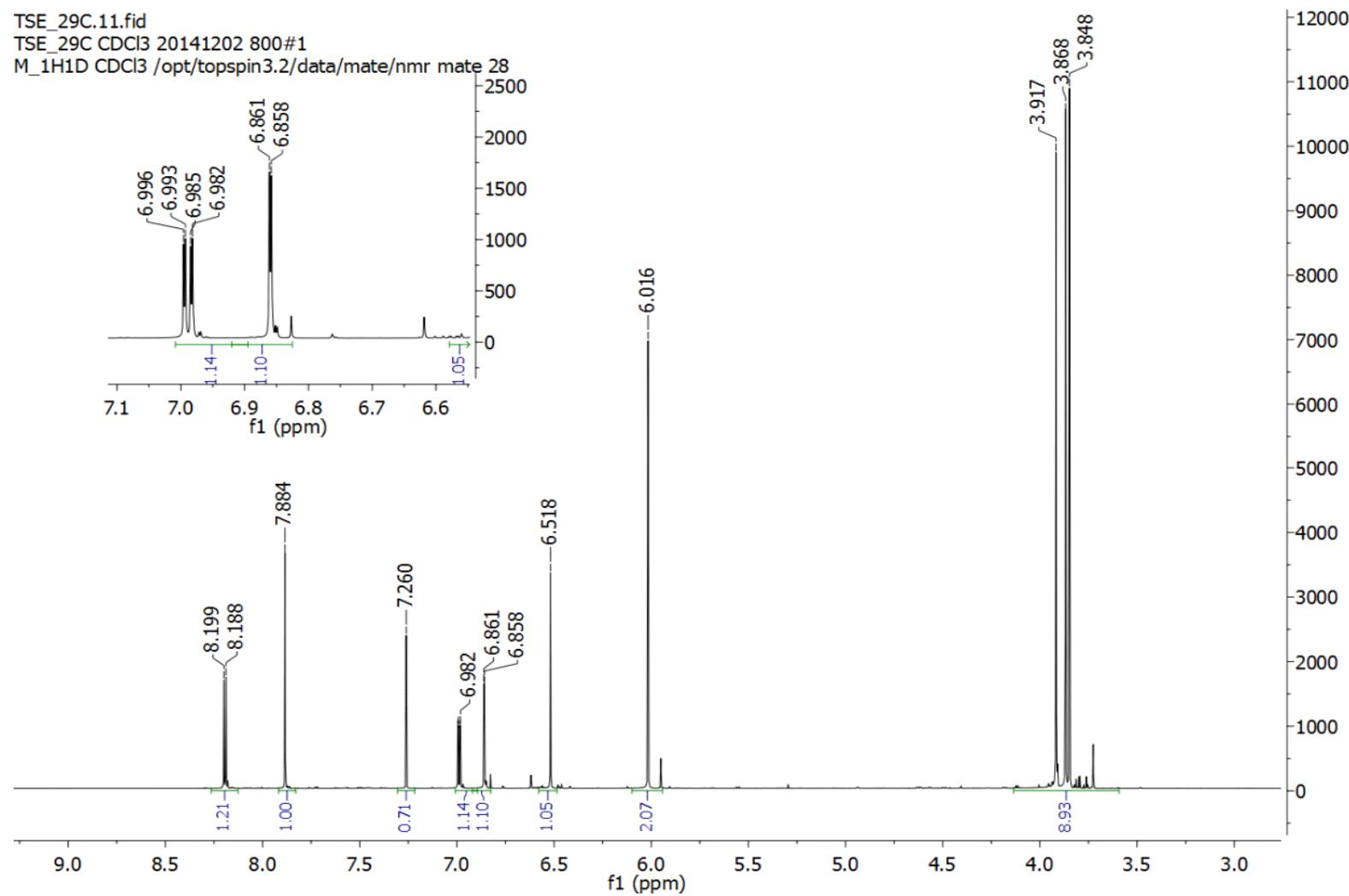


**Figure S13B:**  $^{13}\text{C}$  NMR (201.15 MHz) spectrum of compound 13

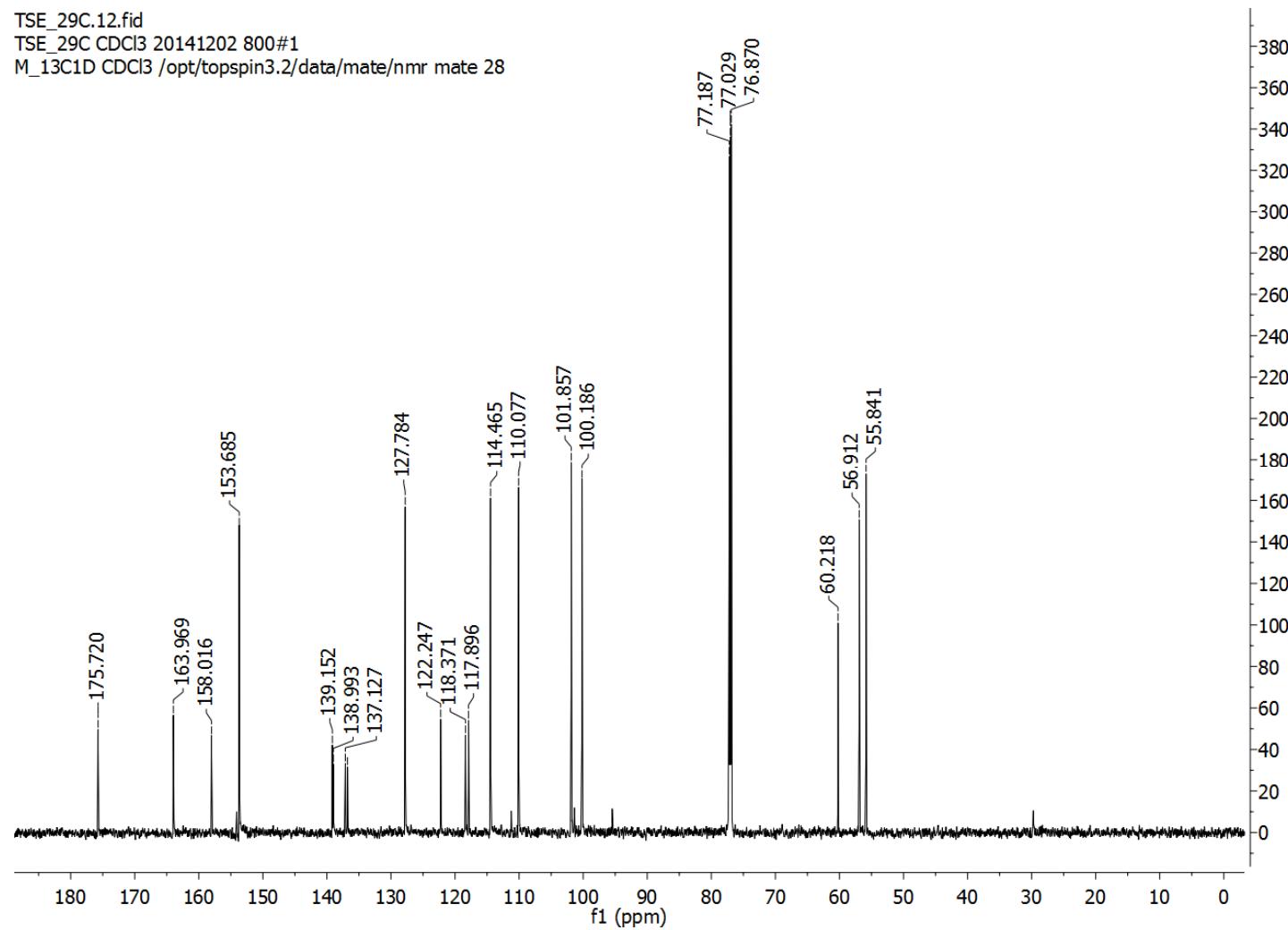
TSE-28G-13C\_DMSO



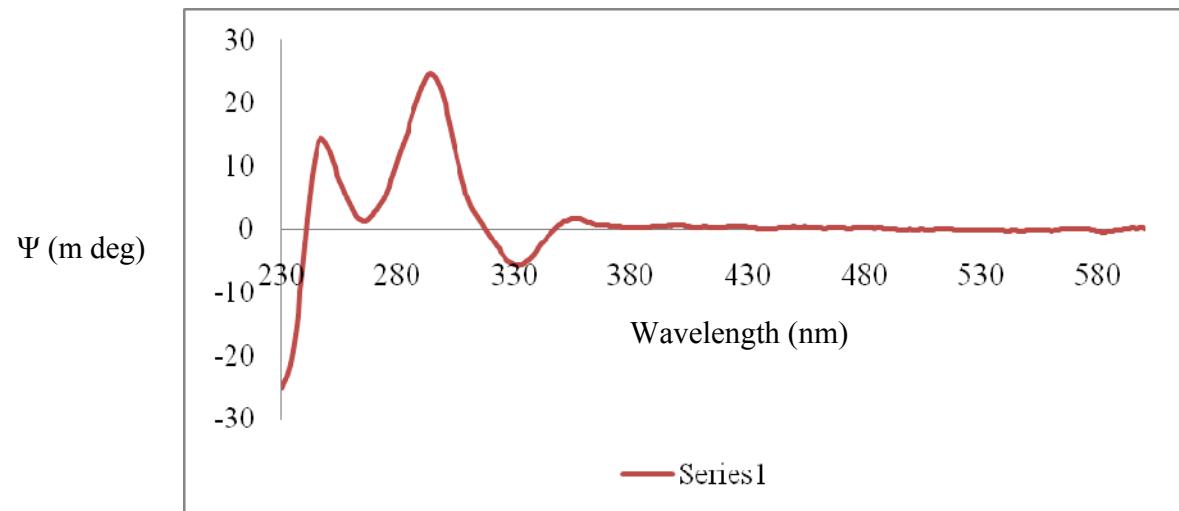
**Figure S14A:**  $^1\text{H}$  NMR (799.87 MHz) spectrum of compound 14



**Figure S14B:**  $^{13}\text{C}$  NMR (201.15 MHz) spectrum of compound 14



**Figure S15A: CD spectrum of compound 6**



**Computed energies for various conformations of compound oblarotenoid A (2)**

	<b>B3LYP/6-311G**</b>	<b>ΔE (kcal/mol)</b>	
3-cis1	-1221,16509470	7,31	SS
3-cis2	-1221,16583640	6,85	SS
3-cis3	-1221,17685860	0,00	SS
3-cis4	-1221,17685860	0,00	SS
3-cis5	-1221,17580060	0,66	RR
3-cis6	-1221,17685860	0,00	RR
3-trans1	-1221,16695720	6,15	RS
3-trans2	-1221,16526320	7,21	RS
3-trans3	-1221,16695717	6,15	RS
3-trans4	-1221,16695720	6,15	RS
3-trans5	-1221,16526310	7,21	RS
3-cis1	-1148,33070150	0,00	RR
3-cis2	-1148,33011720	0,36	SS
3-trans1	-1148,31584030	9,24	RS
3-trans2	-1148,31584030	9,24	SR

### X-ray diffraction analysis of oblarotenoid C (**4**)

Single crystals were obtained from methanol. X-ray data were collected on an Agilent SuperNova Dual diffractometer with Atlas detector at  $T = 123.0\text{ K}$  using mirror-monochromatized Cu- $K\alpha$  radiation ( $\lambda = 1.54184\text{ \AA}$ ). CrysAlisPro<sup>[1]</sup> software was used for data collection, integration and reduction as well as applying the Analytical numeric absorption correction using a multifaceted crystal model<sup>[2]</sup>. The structure was solved by Direct method with SHELXS<sup>[3]</sup> and refined by full-matrix least-squares using SHELXL-2013<sup>[3]</sup> within OLEX2<sup>[4]</sup> package. All non-hydrogen atoms were refined anisotropically. All the hydrogen atoms were refined using riding models with  $U_{eq}(\text{H})$  of  $1.5U_{eq}(\text{parent})$  for terminal groups and  $1.2U_{eq}(\text{parent})$  for non-terminal groups.

**5**:  $0.565 \times 0.090 \times 0.056\text{ mm}$ ,  $2 \times \text{C}_{18}\text{H}_{14}\text{O}_6$ ,  $M = 652.58$ , orthorhombic, space group  $P2_12_12_1$ ,  $a = 5.19667(5)\text{ \AA}$ ,  $b = 13.40708(9)\text{ \AA}$ ,  $c = 42.3221(3)\text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 90^\circ$ ,  $V = 2948.67(4)\text{ \AA}^3$ ,  $Z = 4$ ,  $\rho = 1.470\text{ g cm}^{-3}$ ,  $\mu = 0.936\text{ mm}^{-1}$ ,  $F(000) = 1360$ , 74051 reflections ( $\theta_{max} = 76.883^\circ$ ) measured (6232 unique,  $R_{\text{int}} = 0.030$ , completeness = 99.9%), Final  $R$  indices ( $I > 2\sigma(I)$ ):  $R_1 = 0.0297$ ,  $wR_2 = 0.0746$ ,  $R$  indices (all data):  $R_1 = 0.0441$ ,  $wR_2 = 0.0753$ .  $GOF = 1.061$  for 435 parameters and 0 restraints, largest diff. peak and hole  $0.213/-0.193\text{ e\AA}^{-3}$ . Absolute structure parameter  $x = 0.0(4)$ . CCDC-1061111 contains the supplementary data for this structure. An ORTEP image of both crystallographically independent molecules of **4** is shown below.

<sup>[1]</sup> CrysAlisPro, 1.171.36.32 ed., Agilent Technologies, Ltd., Yarnton, UK, **2009–2013**.

<sup>[2]</sup> R. C. Clark, J. S. Reid, *Acta Crystallogr. Sect. A: Found. Crystallogr.* **1995**, *51*, 887-891.

<sup>[3]</sup> G. M. Sheldrick, *Acta Crystallogr. Sect. A: Found. Crystallogr.* **2008**, *64*, 112.

<sup>[4]</sup> O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann *J. Appl. Cryst.* **2009**, *42*, 339-341.