

# SUPPORTING INFORMATION

## 3,3,3',3'-Tetramethyl-2,2'-diphenyl-3*H*,3'*H*-5,5'-biindole

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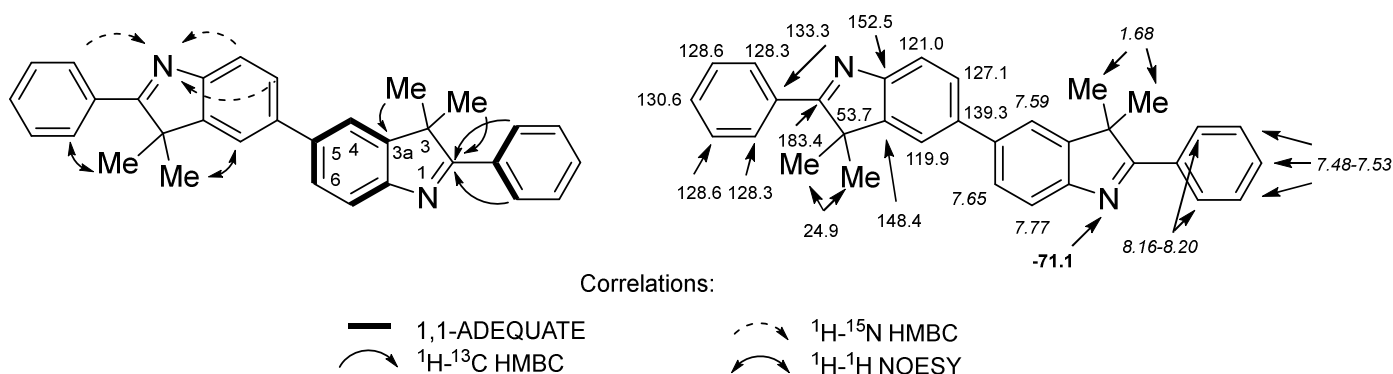
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### Table of Contents

1. <sup>1</sup> H NMR spectrum of compound 2	S1
2. <sup>1</sup> H 1D Selective Gradient NOESY spectrum of compound 2	S2
3. <sup>13</sup> C NMR spectrum of compound 2	S3
4. <sup>13</sup> C NMR and DEPT-135 <sup>13</sup> C NMR spectrum of compound 2	S4
5. <sup>1</sup> H- <sup>15</sup> N HMBC NMR spectrum of compound 2	S5
6. The overlaid <sup>1</sup> H- <sup>13</sup> C gs-HSQC and 60 Hz 1,1-ADEQUATE NMR spectra of compound 2	S6
7. The overlaid <sup>1</sup> H- <sup>13</sup> C gs-HSQC and gs-HMBC NMR spectra of compound 2	S7
8. <sup>1</sup> H- <sup>1</sup> H TOCSY NMR spectrum of compound 2	S8
9. <sup>1</sup> H- <sup>1</sup> H COSY NMR spectrum of compound 2	S9
10. HRMS spectrum of compound 2	S10



Relevant 1,1-ADEQUATE, <sup>1</sup>H-<sup>13</sup>C HMBC, <sup>1</sup>H-<sup>15</sup>N HMBC, <sup>1</sup>H-<sup>1</sup>H NOESY correlations and <sup>1</sup>H NMR (in italics), <sup>15</sup>N NMR (in bold) and <sup>13</sup>C NMR chemical shifts of compound 2.

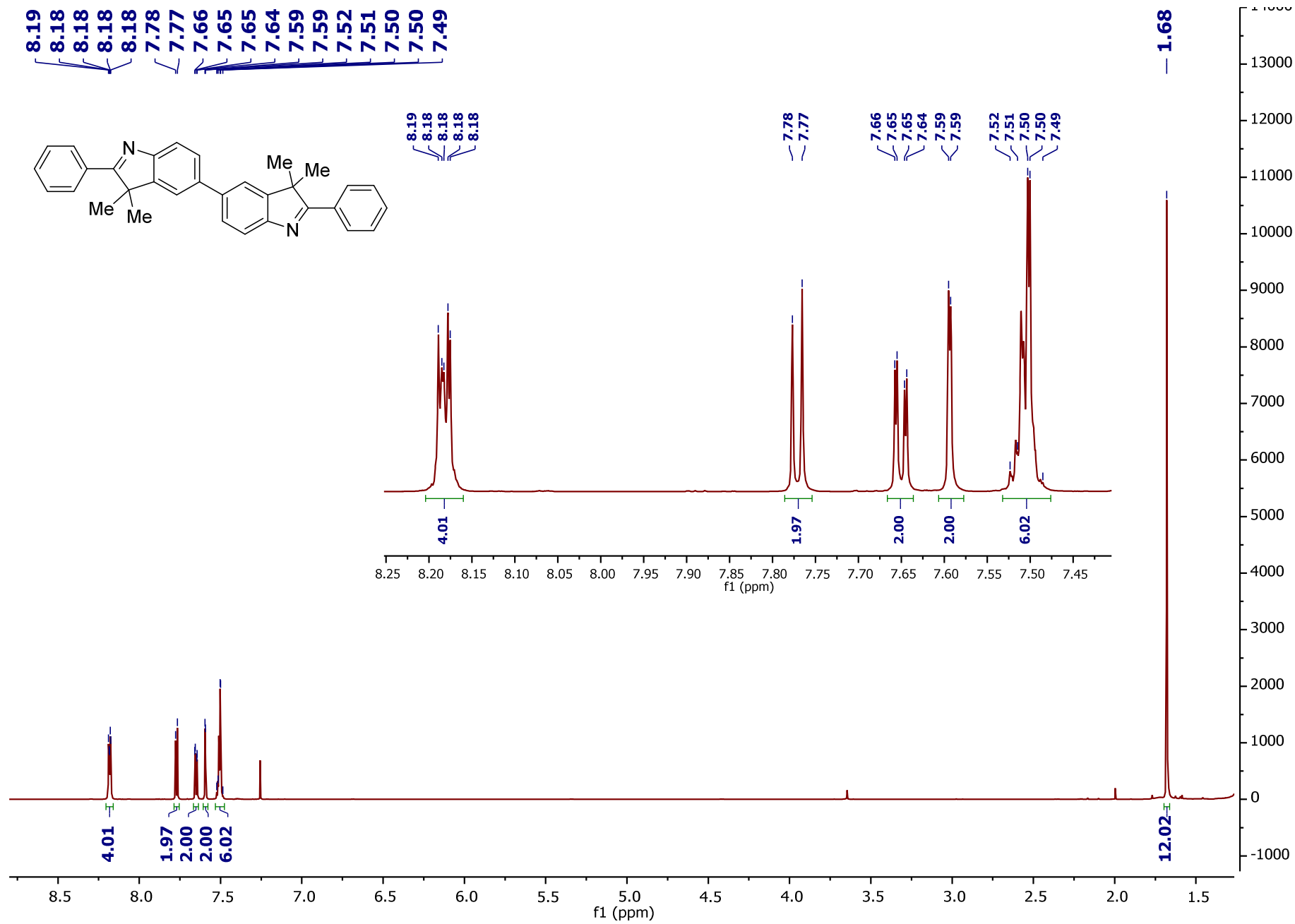
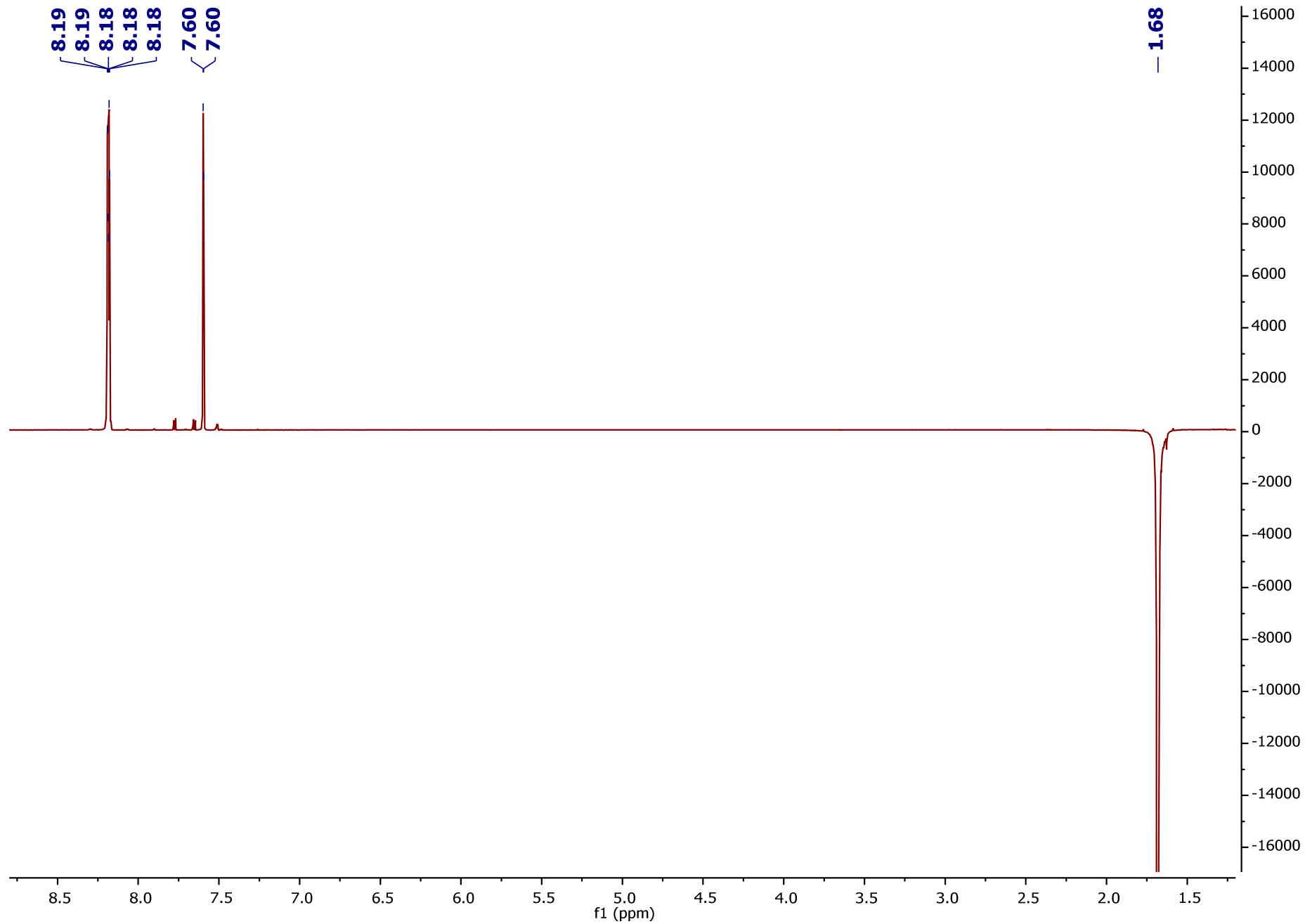


Figure S1. <sup>1</sup>H-NMR spectrum of Compound 2.



**Figure S2.**  $^1\text{H}$  1D Selective Gradient NOESY spectrum of Compound 2.

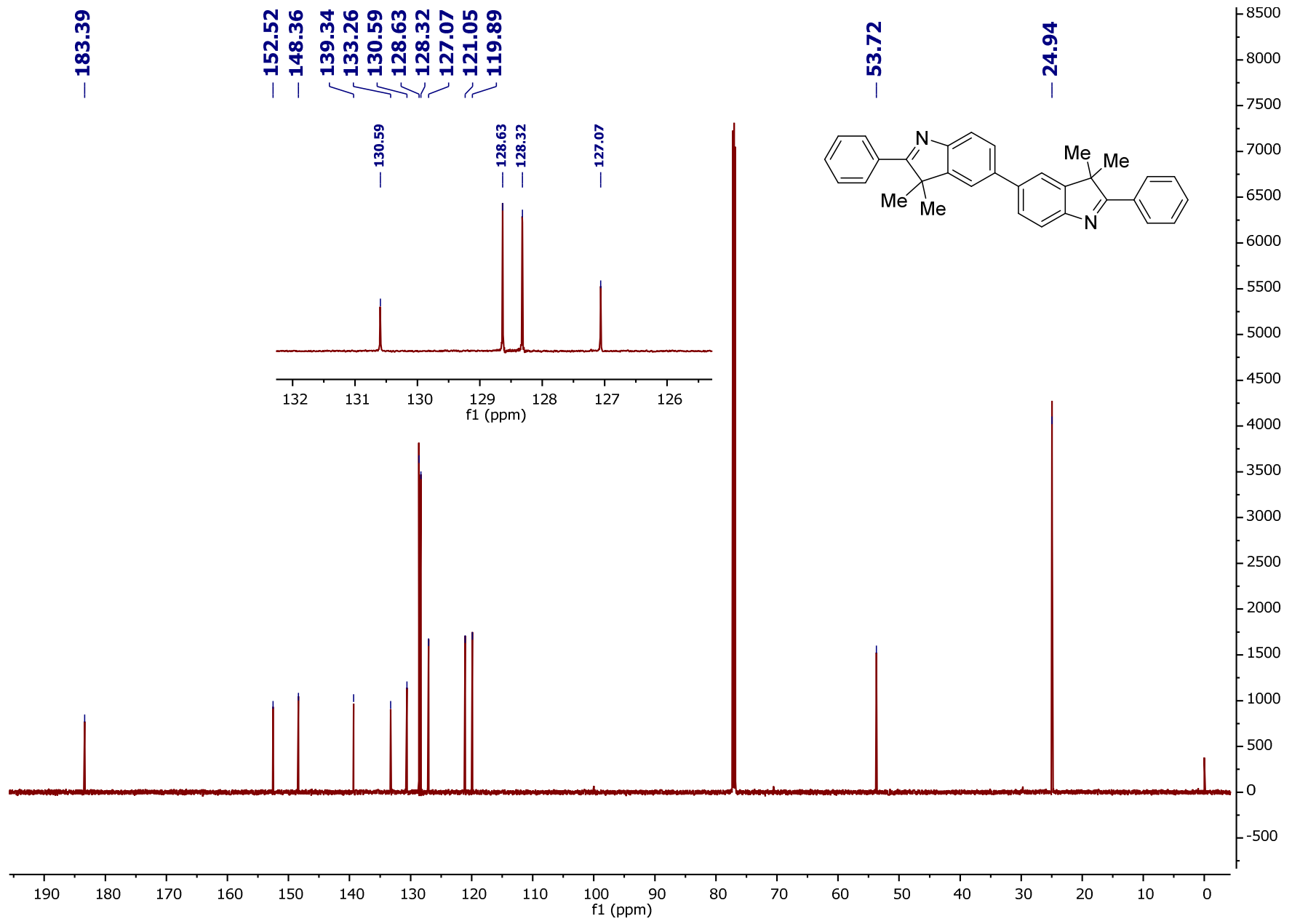


Figure S3. <sup>13</sup>C-NMR spectrum of Compound 2.

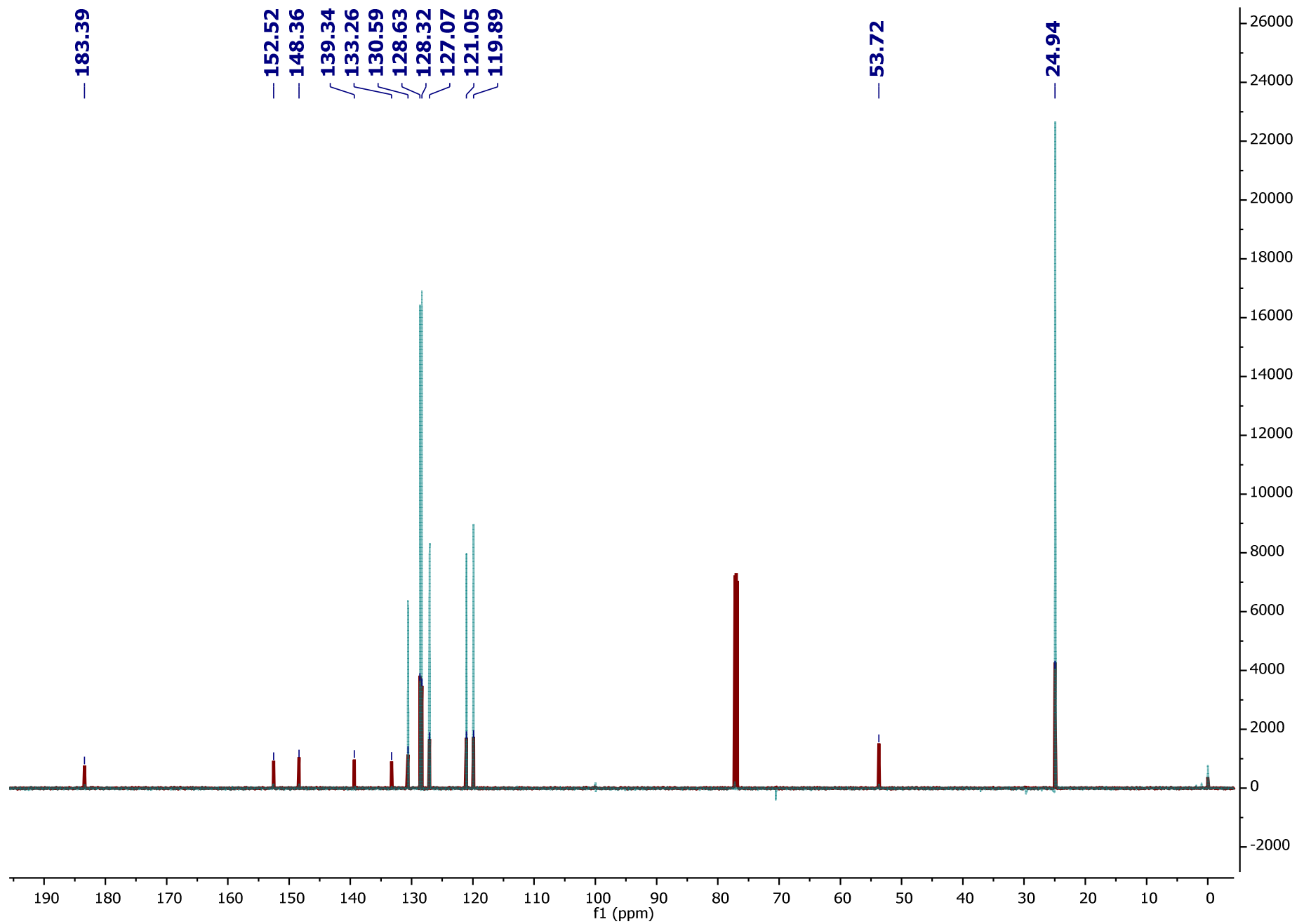


Figure S4.  $^{13}\text{C}$ -NMR and DEPT-135  $^{13}\text{C}$ -NMR spectrum of Compound 2.

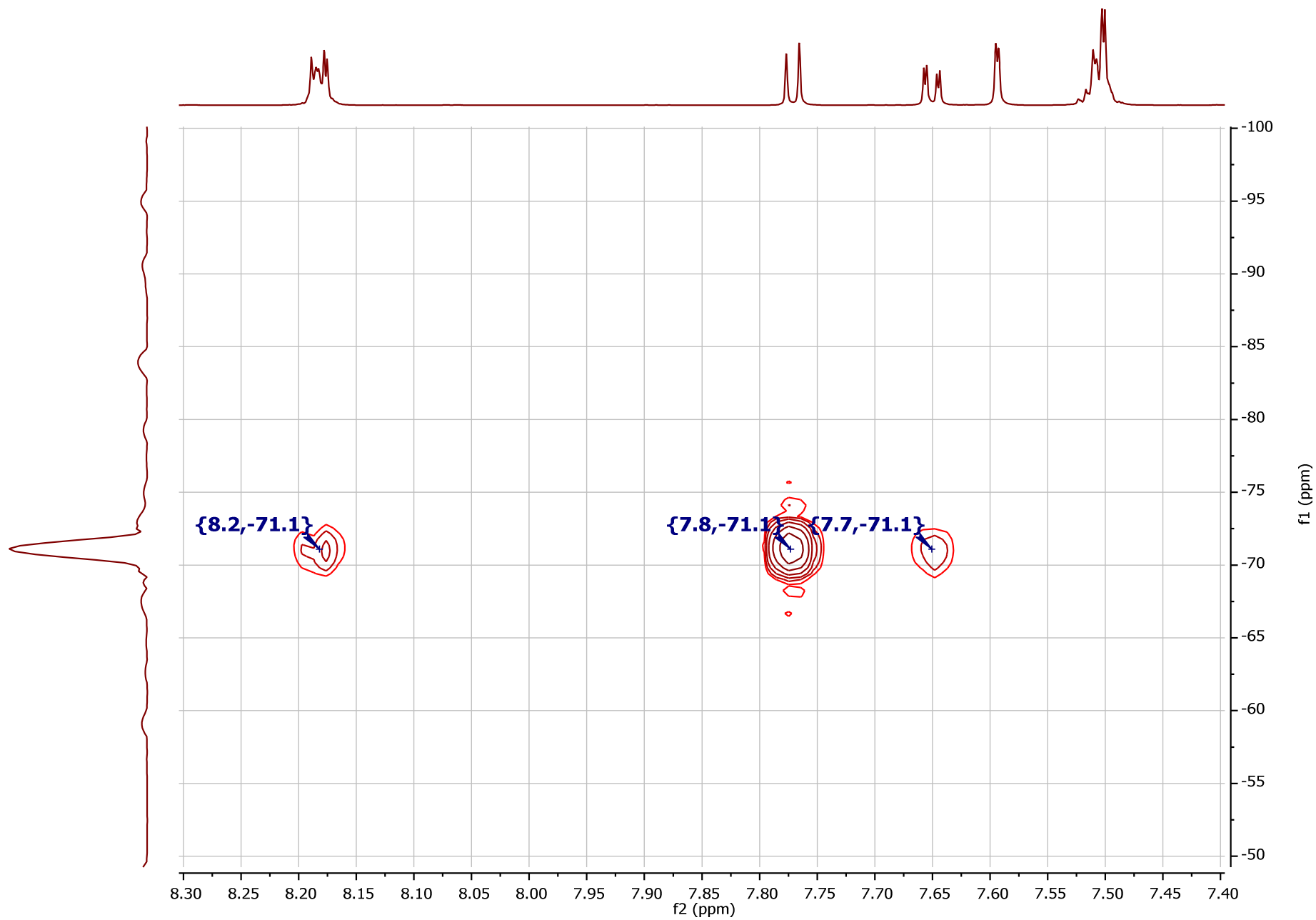


Figure S5.  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum of Compound 2.

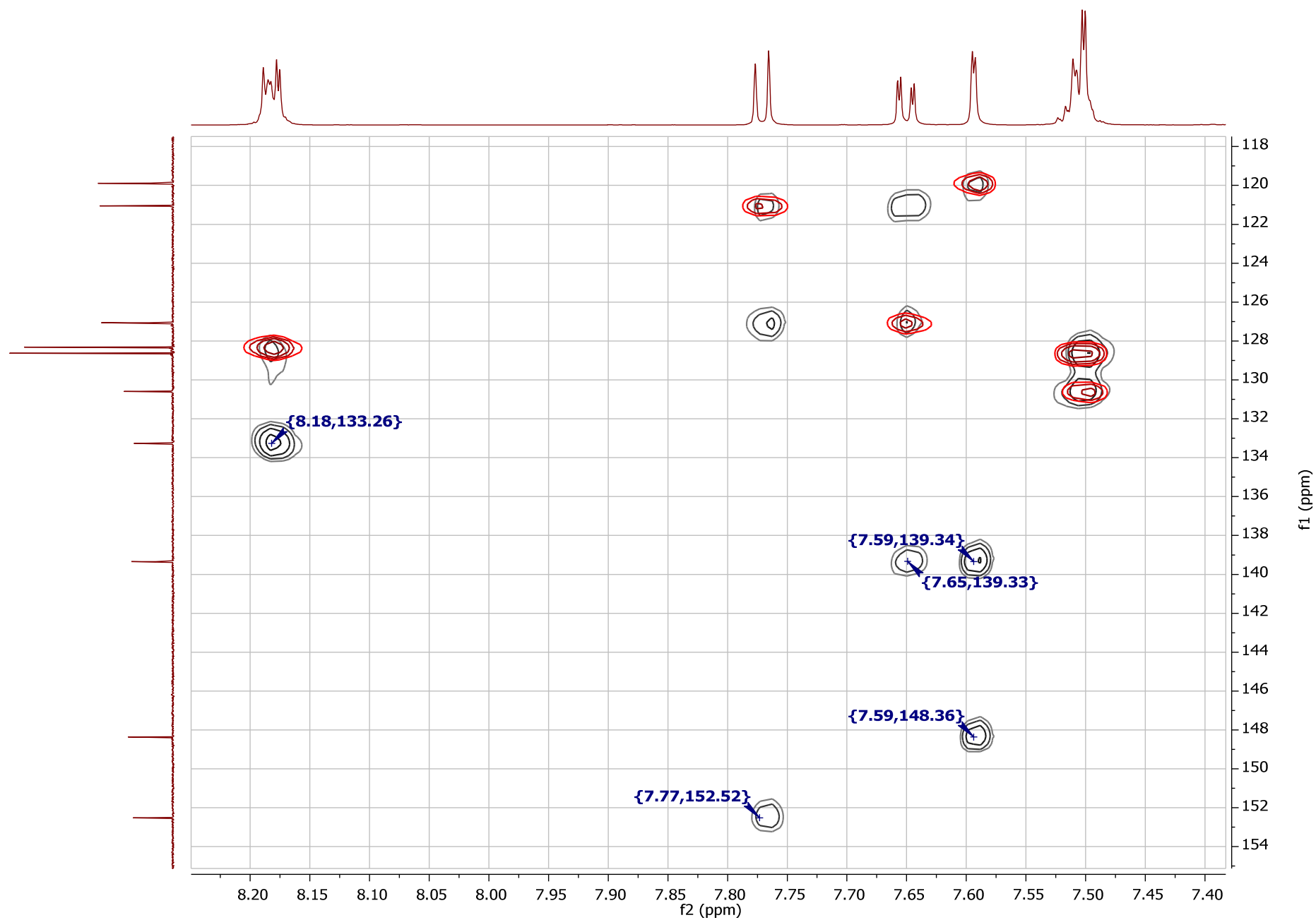


Figure S6. The overlaid  $^1\text{H}$ - $^{13}\text{C}$  gs-HSQC (red) and 60 Hz 1,1-ADEQUATE (black) NMR spectra of Compound 2.

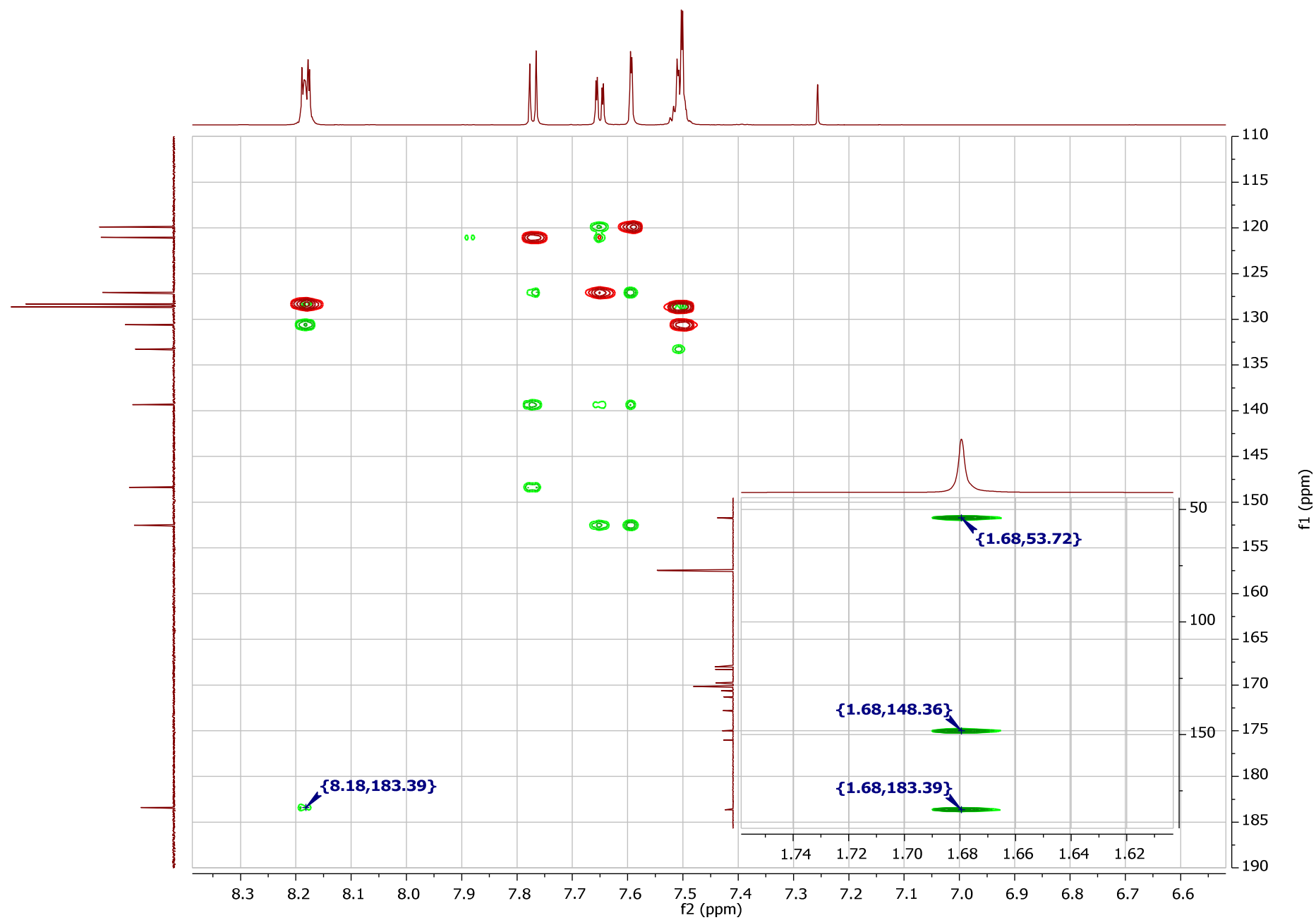
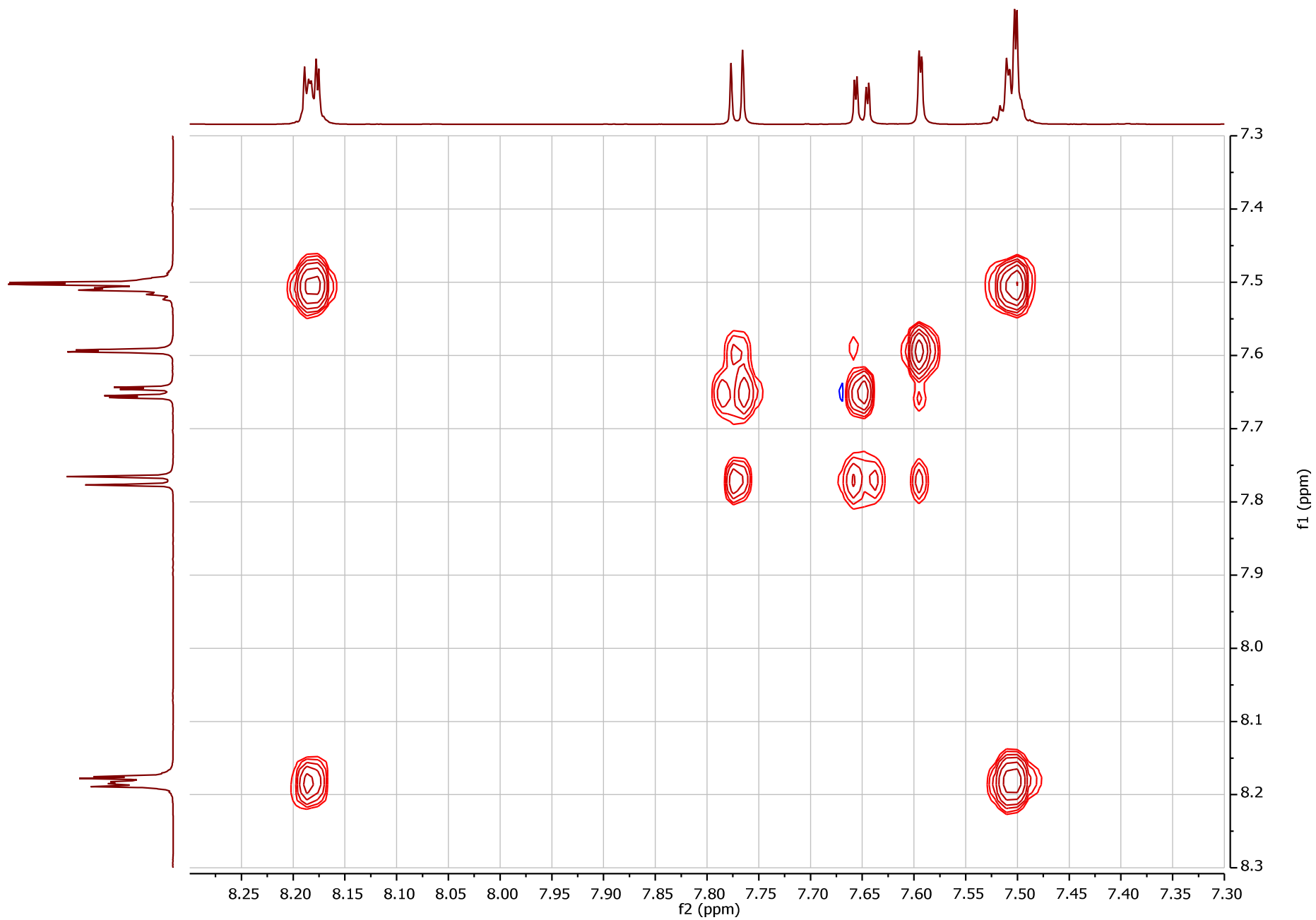


Figure S7. The overlaid  $^1\text{H}$ - $^{13}\text{C}$  gs-HSQC and gs-HMBC NMR spectra of Compound 2.





**Figure S8.**  $^1\text{H}$ - $^1\text{H}$  TOCSY NMR spectrum of Compound 2.

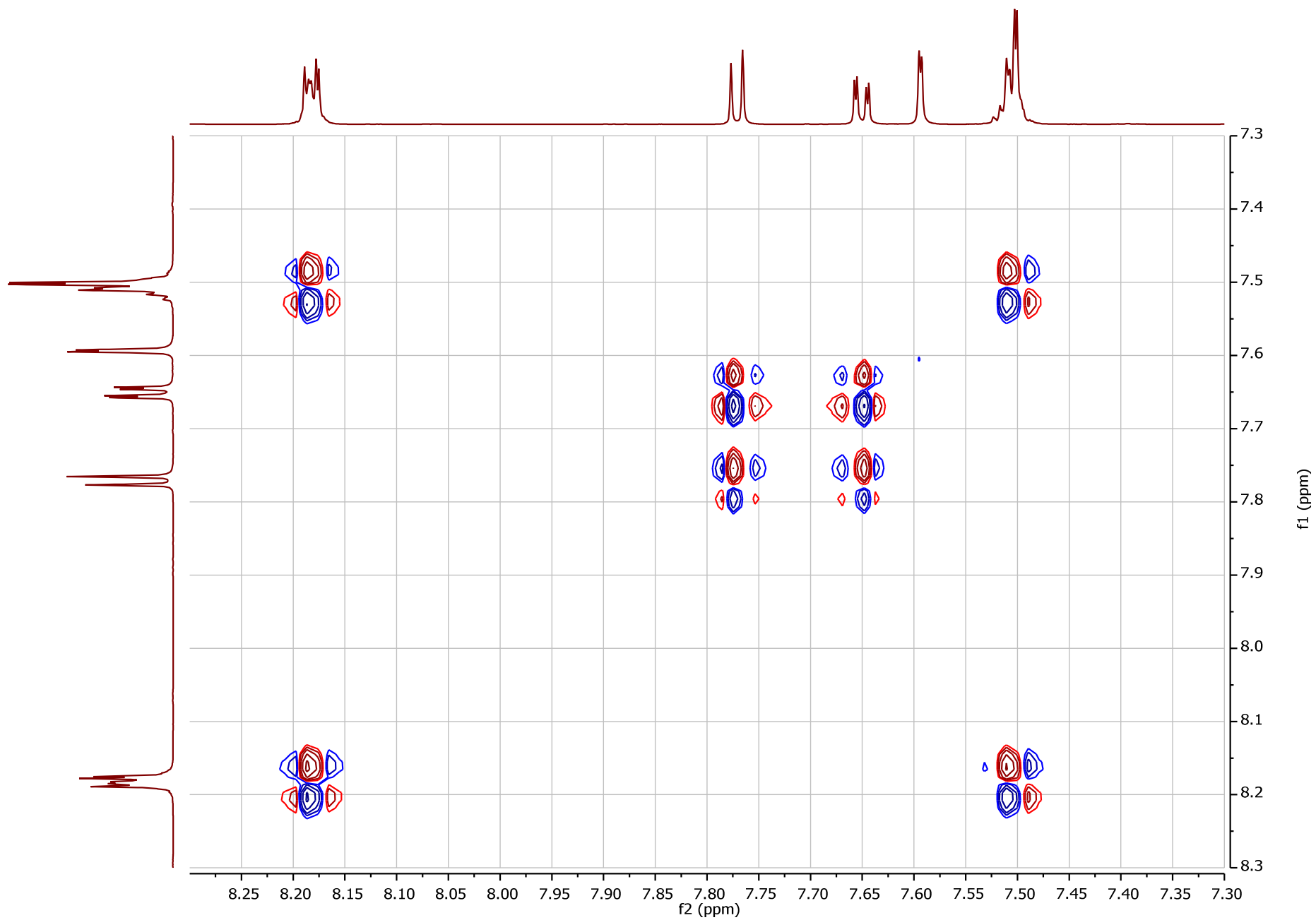


Figure S9.  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of Compound 2.

# Compound Spectrum SmartFormula Report

## Analysis Info

Analysis Name D:\Data\GV-37\_apatinis.d  
Method DirectInfusion\_TuneLow\_pos.m  
Sample Name GV-37\_apatinis  
Comment AB

Acquisition Date 5/11/2018 11:09:19 PM  
Operator hplc  
Instrument micrOTOF-Q III 8228888.20448

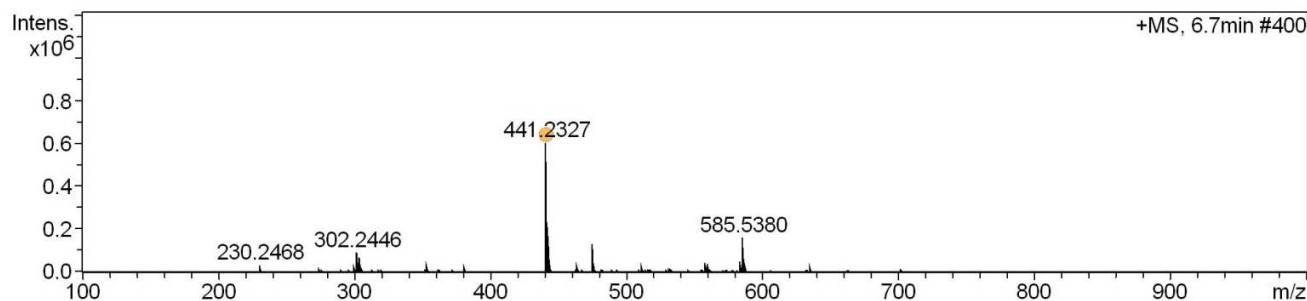
## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	6.7	n.a.	Single spectrum	n.a.	n.a.	n.a.	441.2327	n.a.

## +MS, 6.7min #400



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
441.2327	1	C32H29N2	441.2325	-0.5	7.0	1	100.00	19.5	even	ok

Figure S10. HRMS spectrum of Compound 2.