



## Supporting Information

for

### Intermediates and shunt products of massiliachelin biosynthesis in *Massilia* sp. NR 4-1

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### UV and total ion chromatograms of culture extracts from *Massilia* sp. NR 4-1. Copies of MS/MS and NMR spectra for new compounds

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Table S1: Inhibition zone diameters of **1-6** as well as the reference antibiotics ampicillin (amp), tetracycline (tet) and ciprofloxacin (cip) against the tested bacteria.

	<b>Diameter of Inhibition Zone (mm) in 10 yL/disk</b>			
	<i>B. subtilis</i> (DSM 168)	<i>E. coli</i> (DSM 18039)	<i>P. fluorescens</i> (DSM 11532)	<i>A. tumefaciens</i> (C58)
<b>1</b>	2	-	-	1
<b>2</b>	-	-	-	-
<b>3</b>	4	-	-	2
<b>4</b>	3	-	-	-
<b>5</b>	3	-	-	-
<b>6</b>	0.5	-	-	0.5
<b>ampicillin</b>	14	22	-	22
<b>tetracycline</b>	22	20	16	11
<b>ciprofloxacin</b>	37	38	24	31

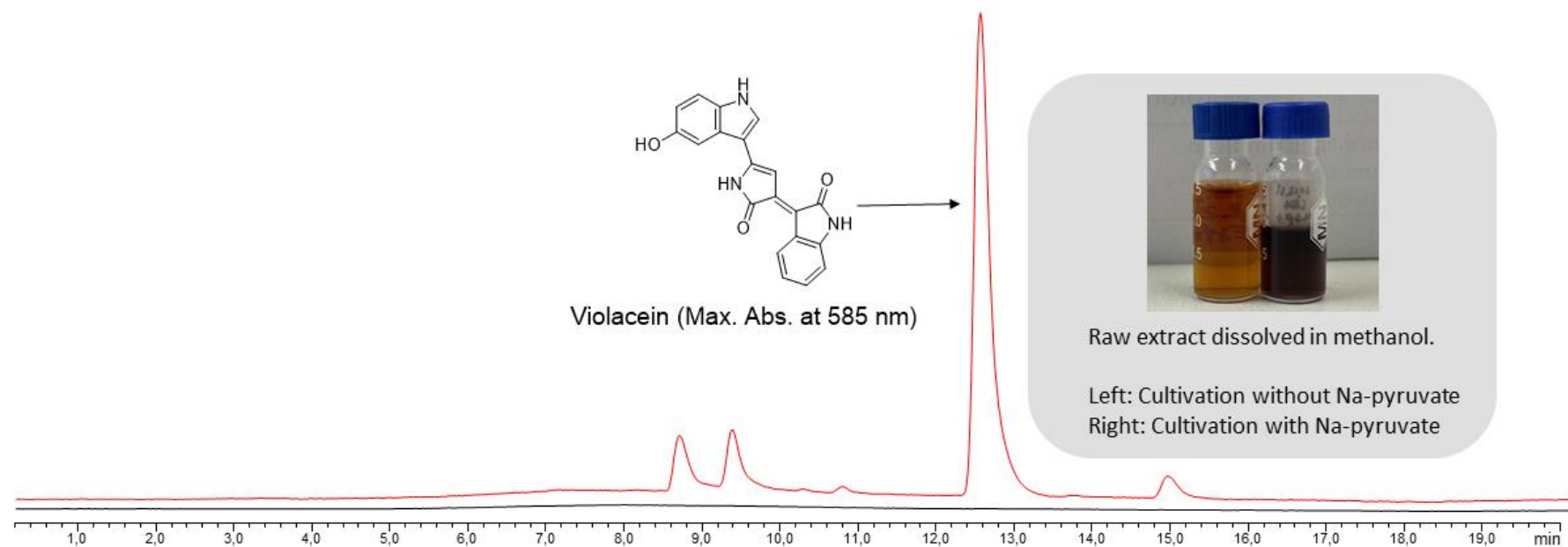


Figure S1: UV chromatogram (585 nm) of crude culture extract from *Massilia* sp. NR 4-1 grown with sodium pyruvate (red) and without sodium pyruvate (black). The darker coloring of the raw extract is due to a higher concentration of violacein.

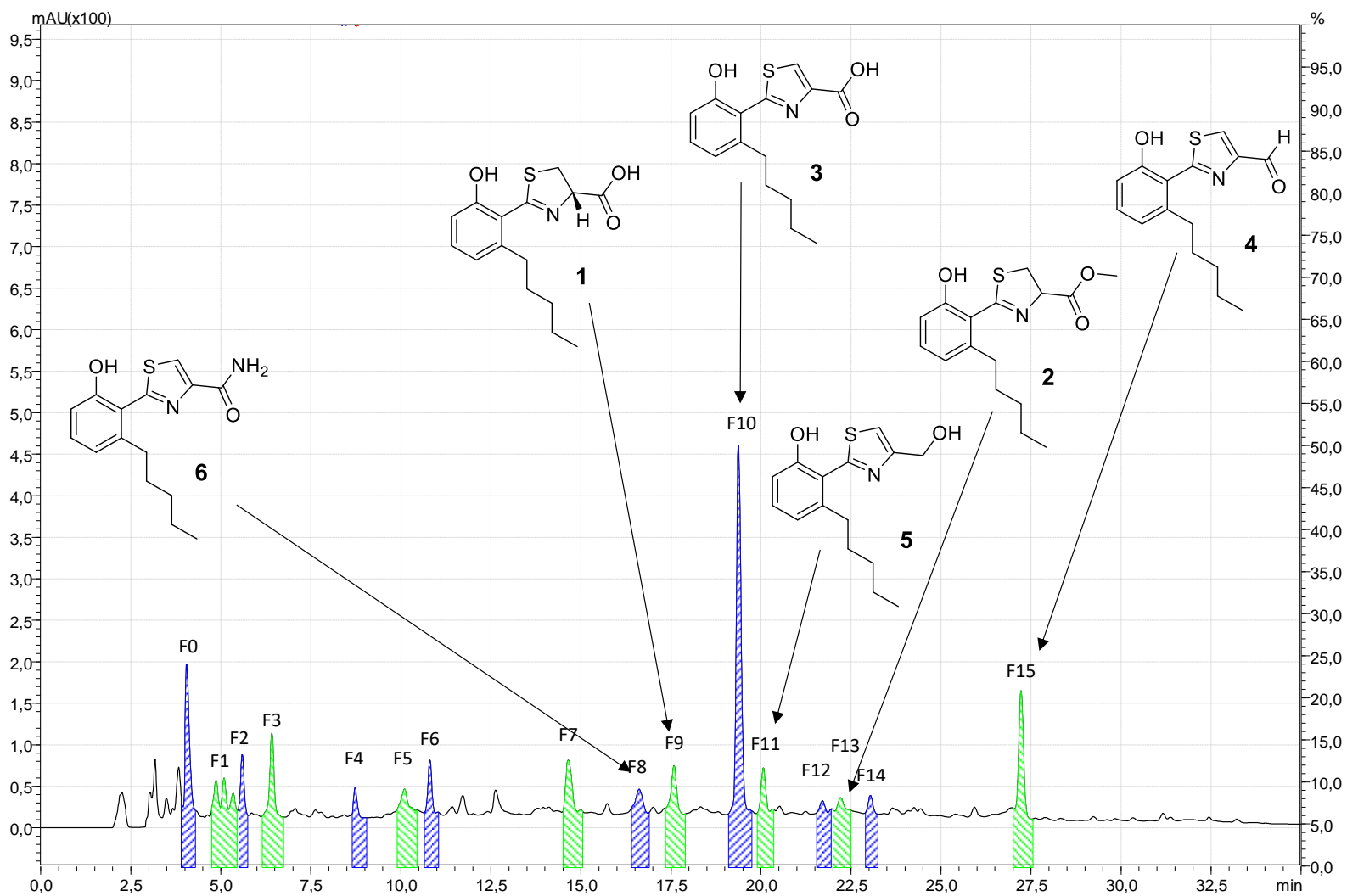


Figure S2: UV chromatogram (280 nm) of the crude culture extract from *Massilia* sp. NR 4-1. Fractions 8, 9, 10, 11, 13, and 15 showed a visible color change with the CAS assay from blue to yellow.

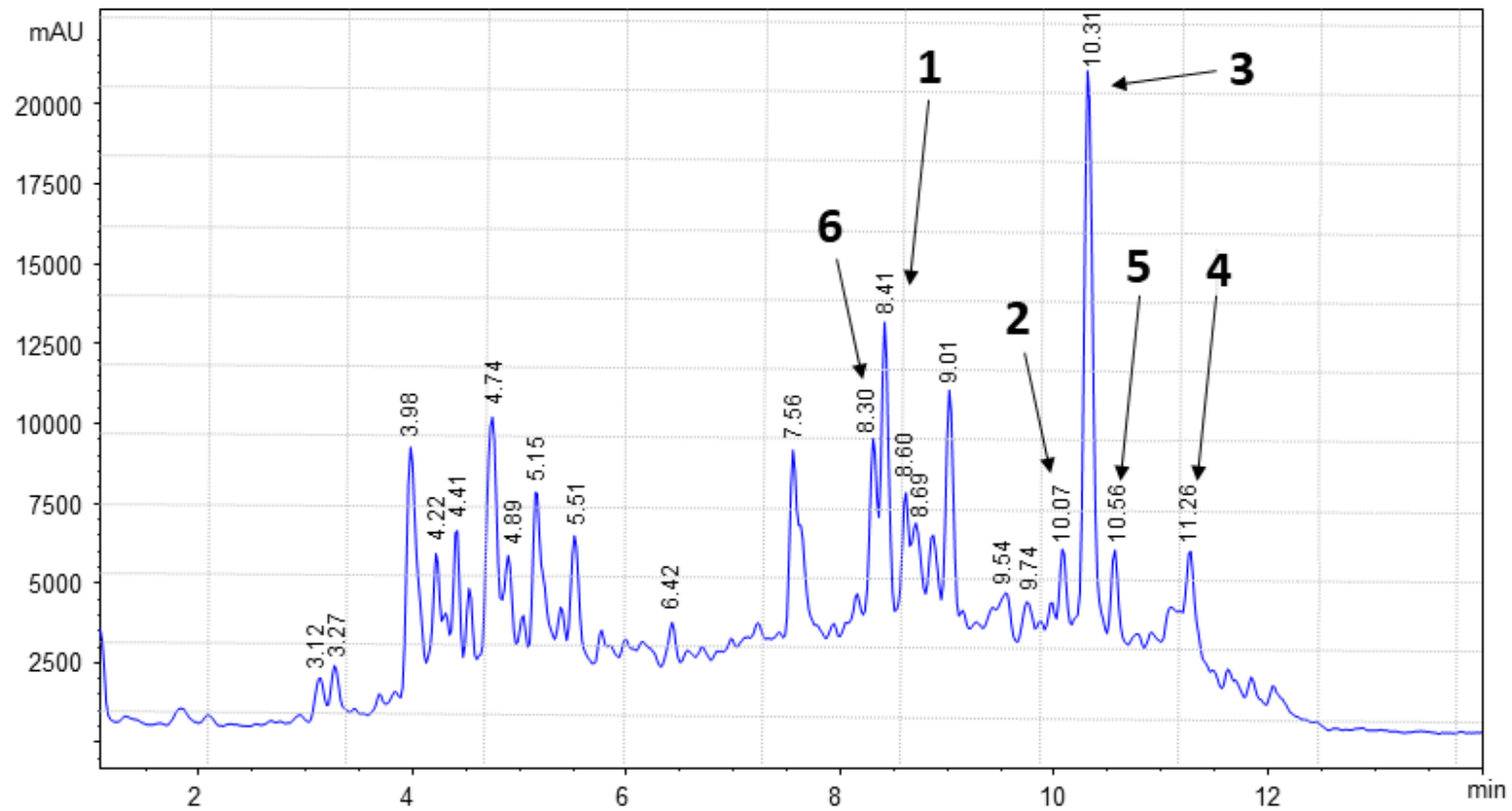


Figure S3: Total ion chromatogram of the crude culture extract from *Massilia sp.* NR 4-1.

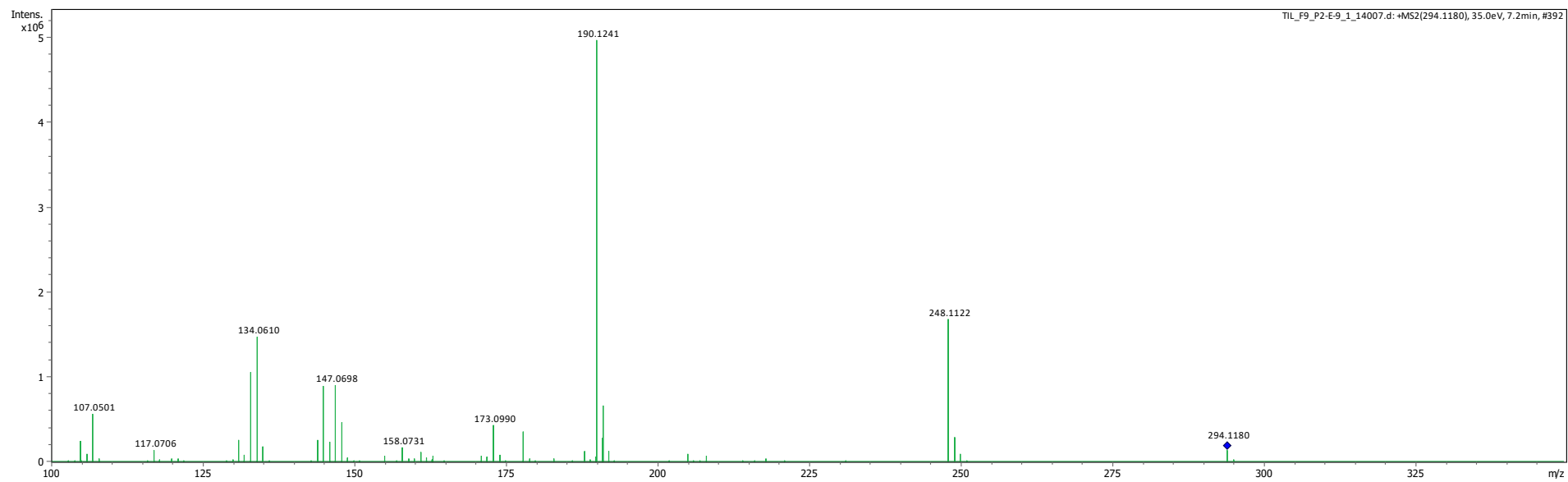


Figure S1: MS/MS spectrum of **1**

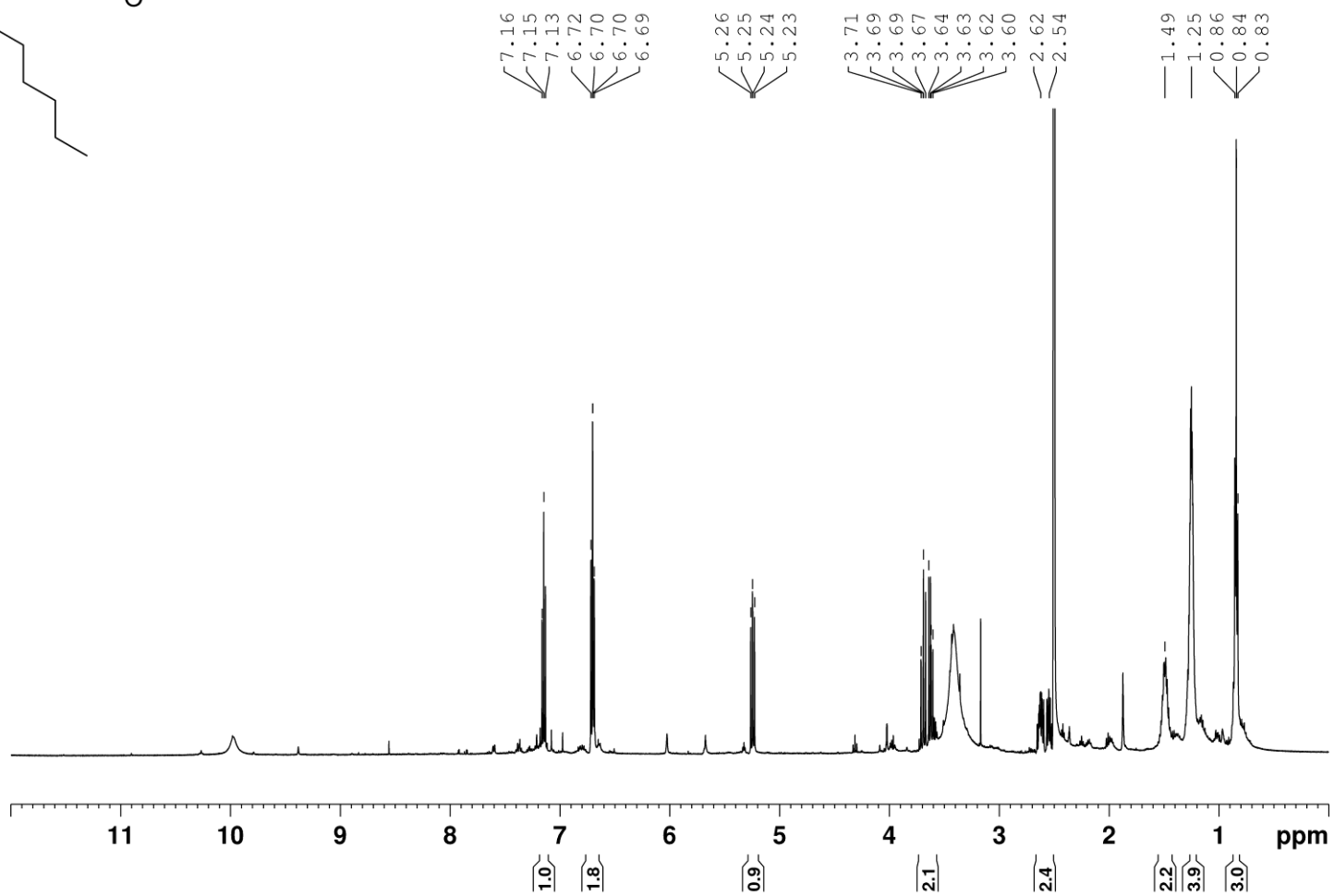
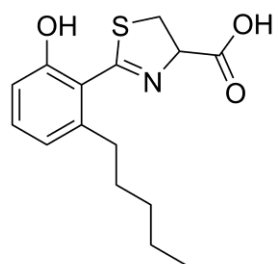


Figure S2: <sup>1</sup>H NMR spectrum of **1** (600 MHz, DMSO-*d*<sub>6</sub>, 25 °C)



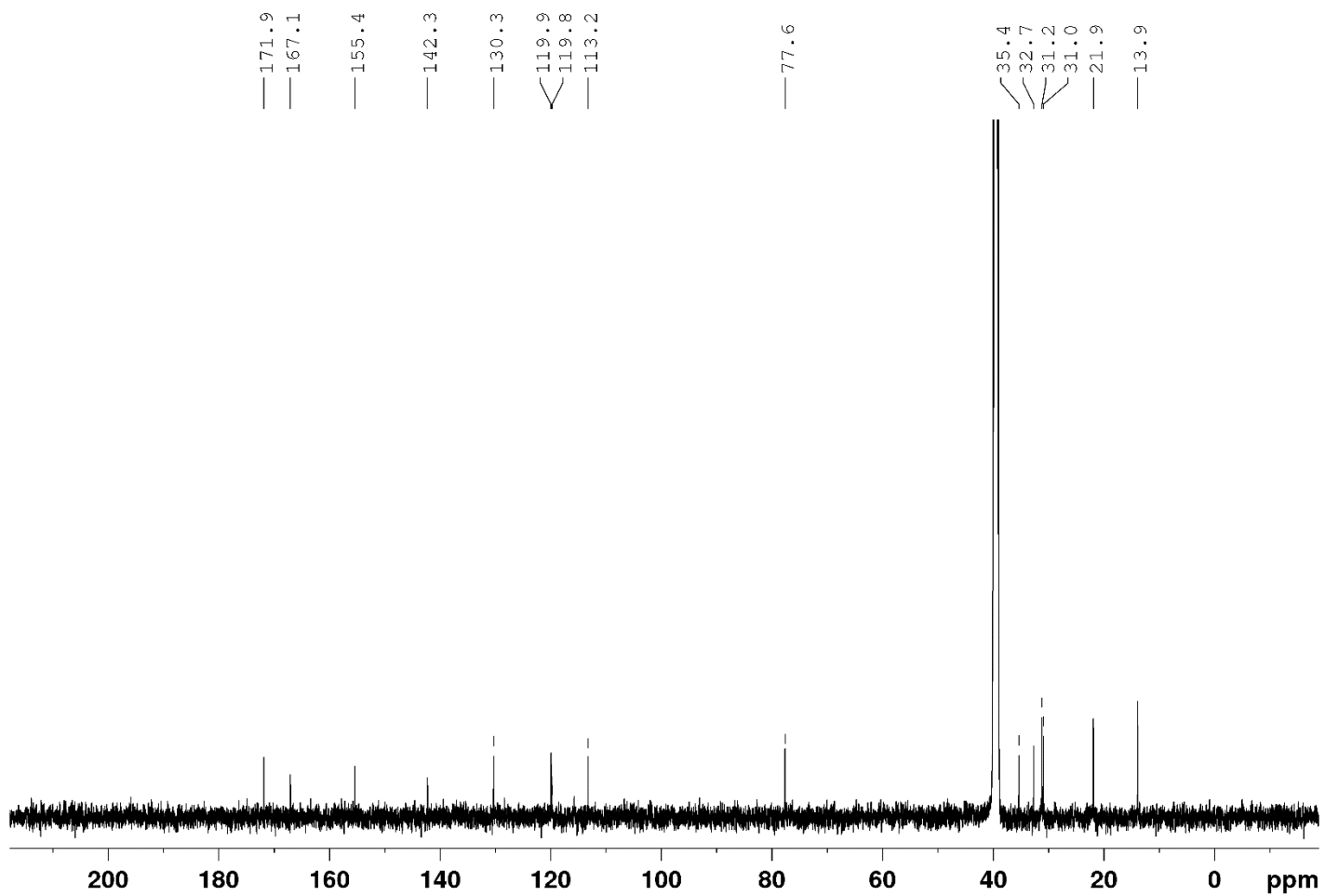


Figure S3:  $^{13}\text{C}$  NMR spectrum of **1** (150 MHz,  $\text{DMSO-}d_6$ , 25 °C)

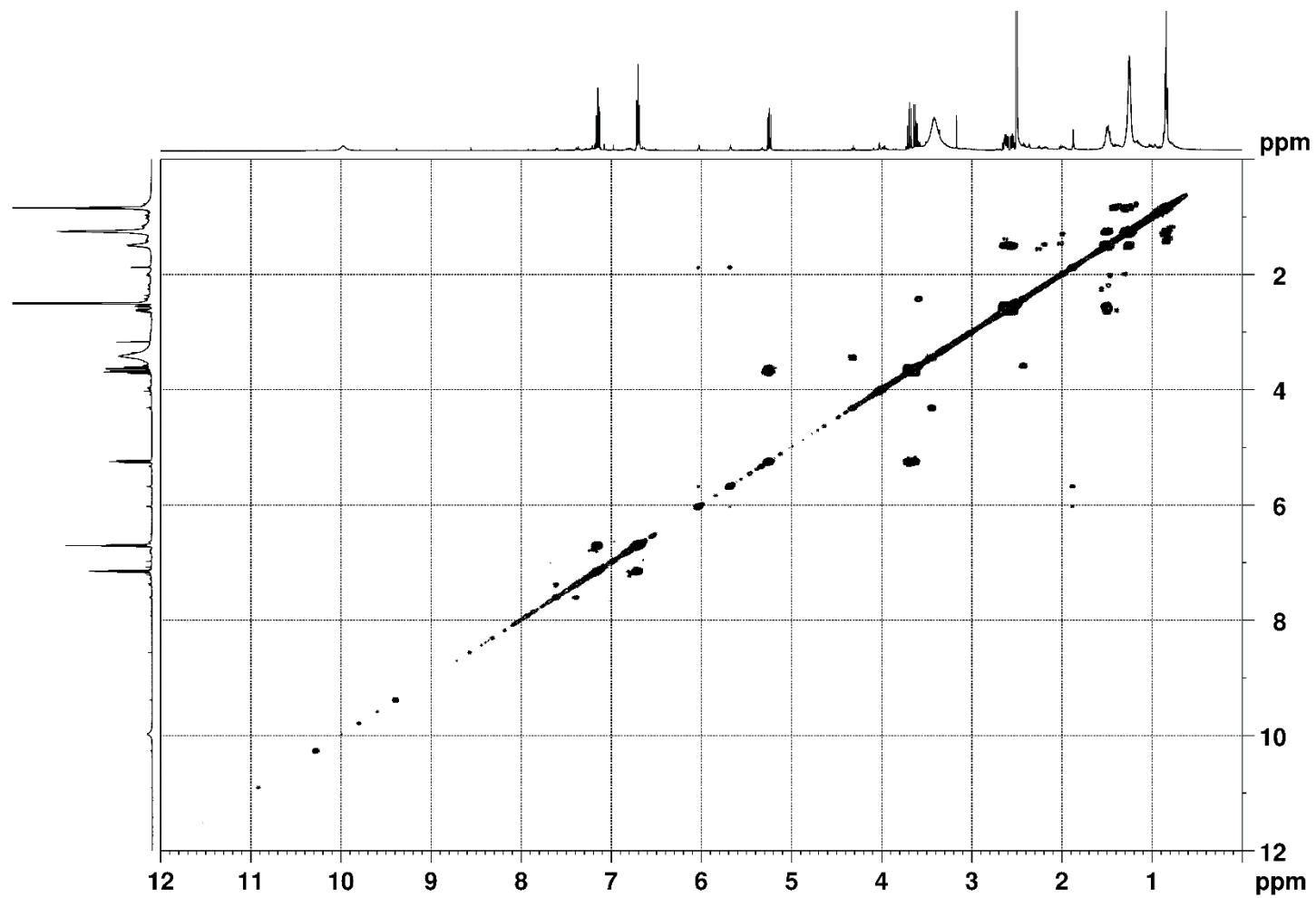


Figure S4: COSY spectrum of **1** (600 MHz, DMSO-*d*<sub>6</sub>, 25 °C)

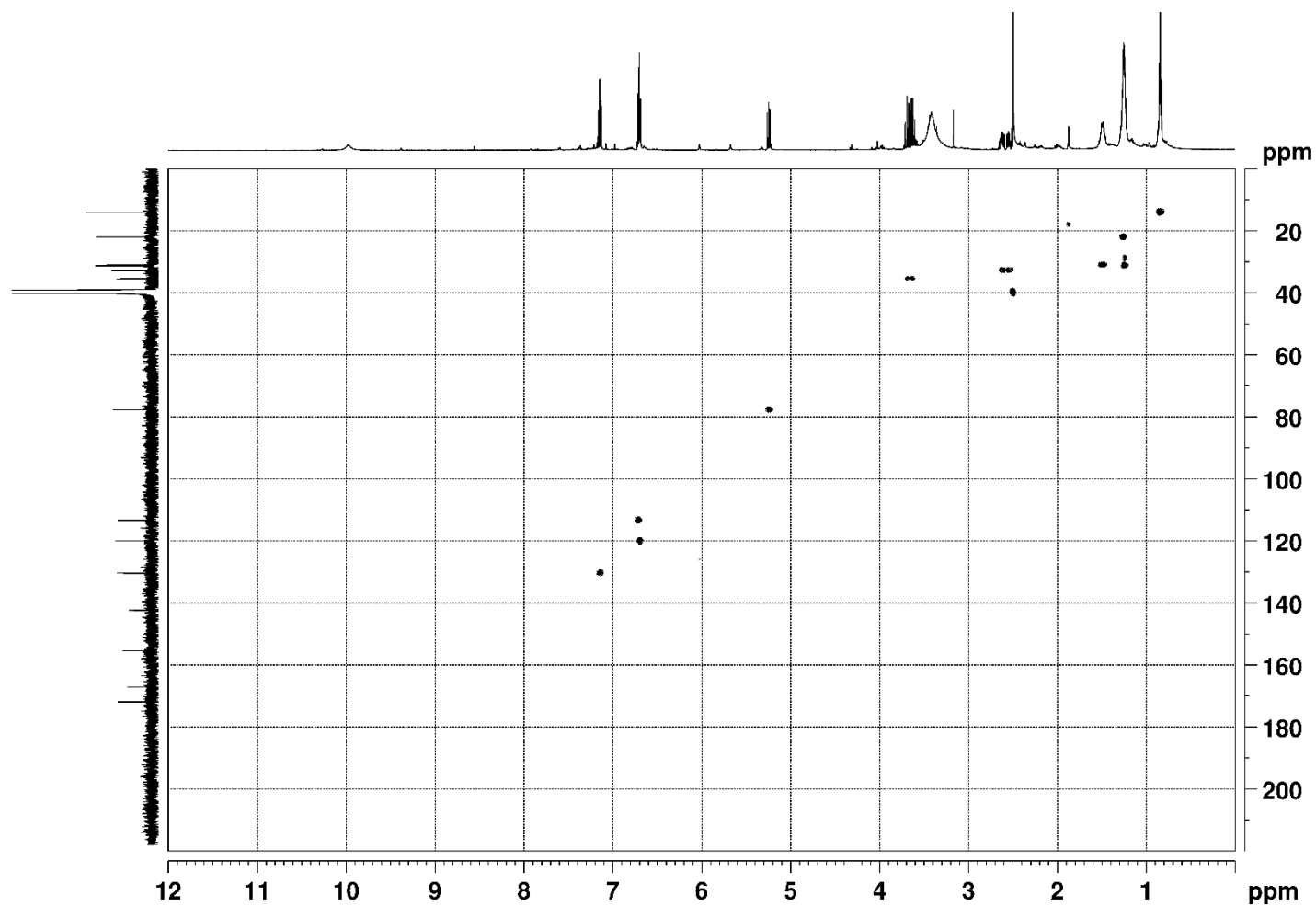


Figure S5: HSQC spectrum of **1** (600 MHz, DMSO- $d_6$ , 25 °C)

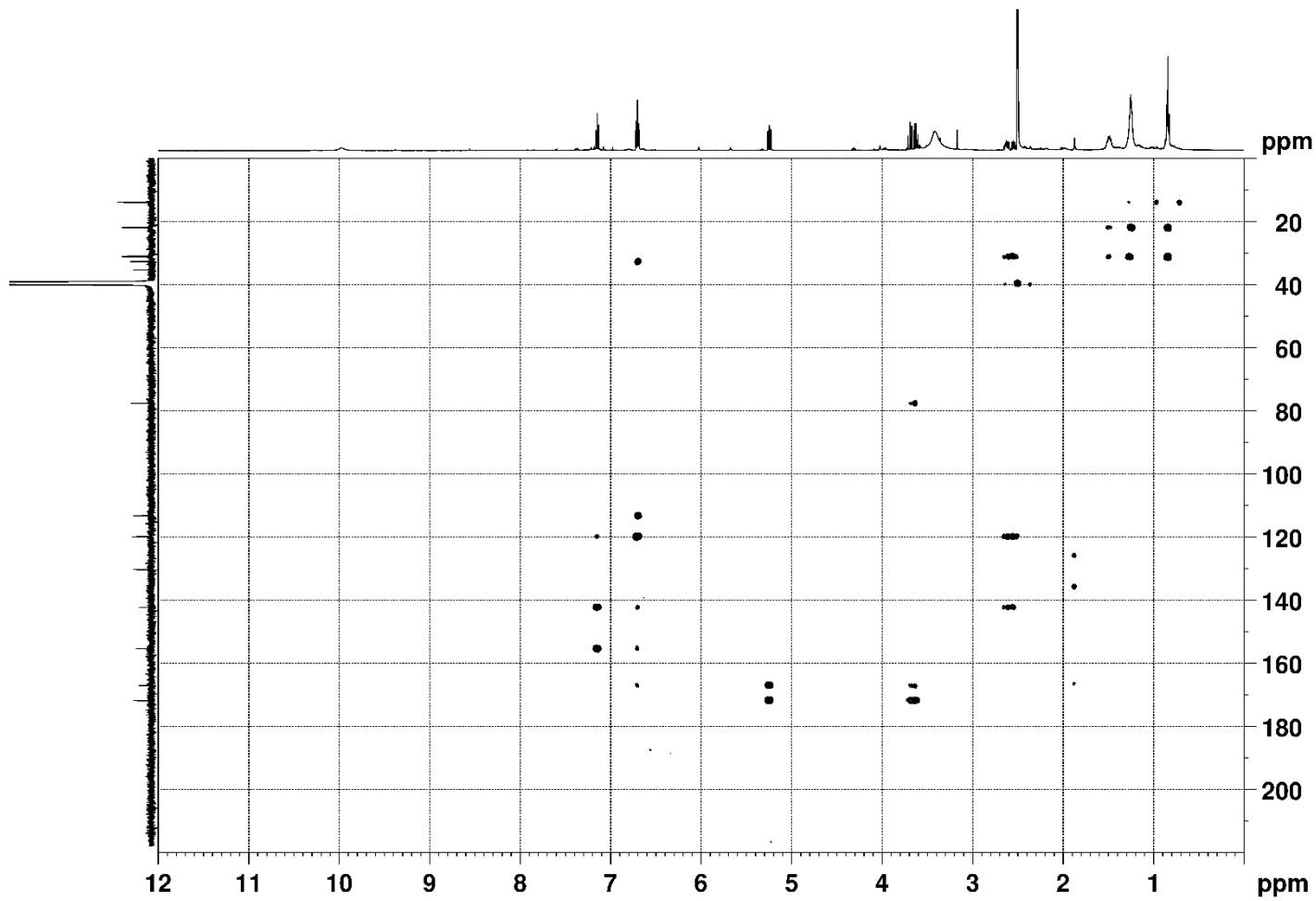


Figure S6: HMBC spectrum of **1** (600 MHz,  $\text{DMSO}-d_6$ , 25 °C)

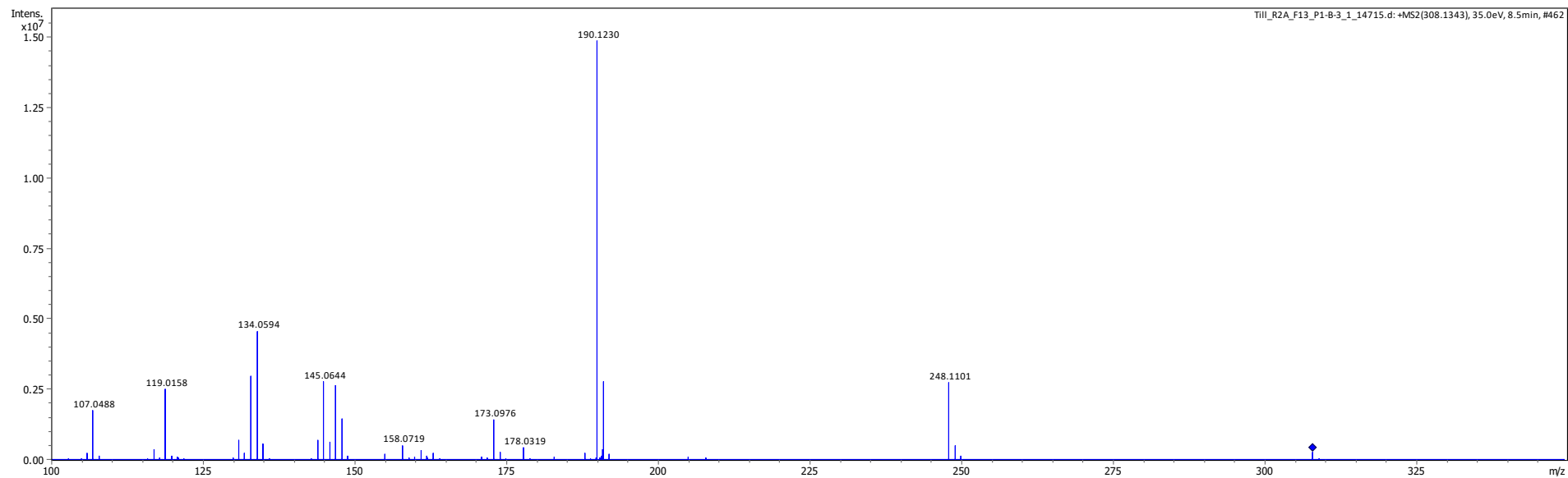


Figure S7: MS/MS spectrum of **2**

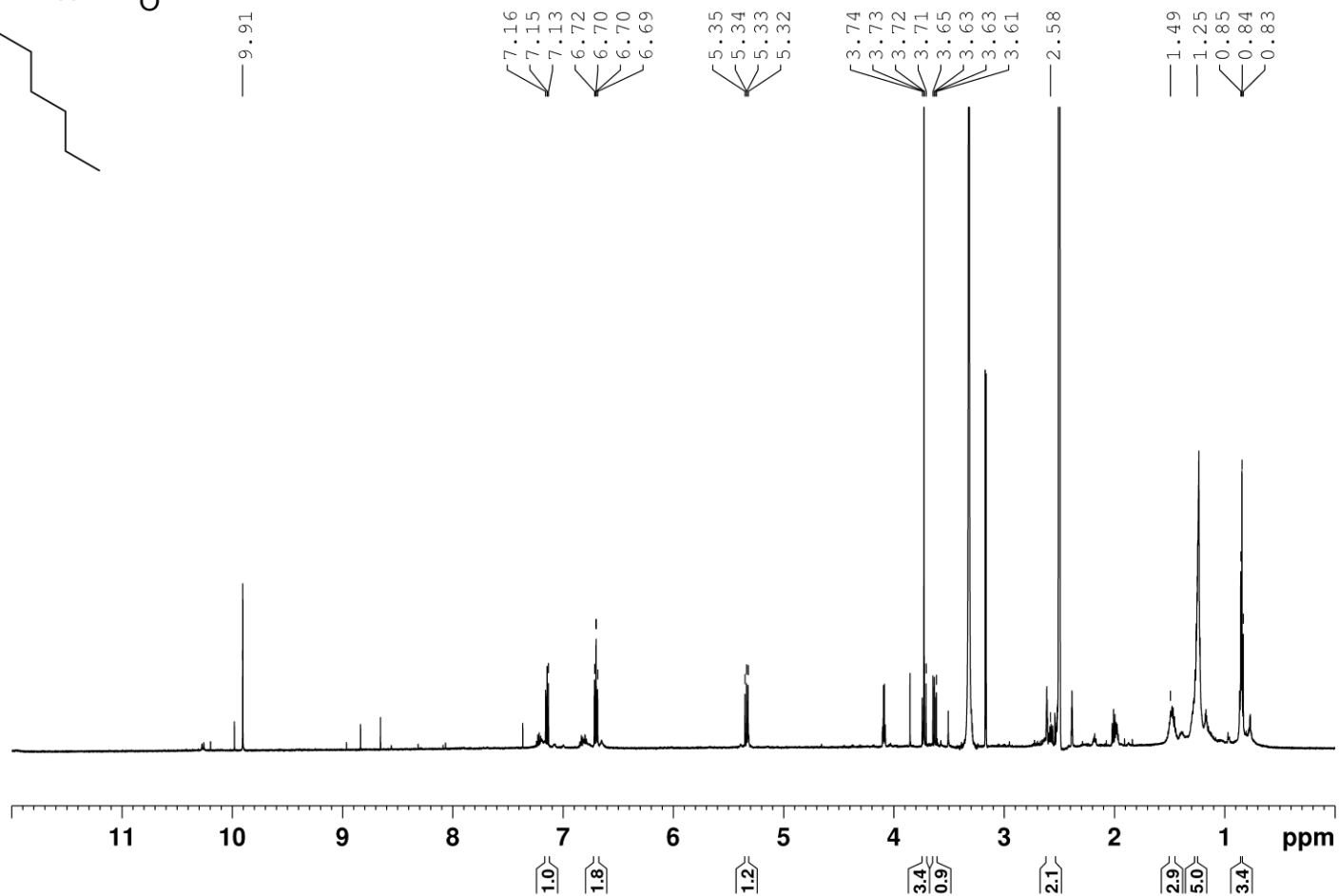
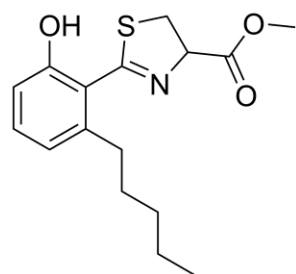


Figure S8:  $^1\text{H}$  NMR spectrum of **2** (600 MHz,  $\text{DMSO-}d_6$ , 25 °C)

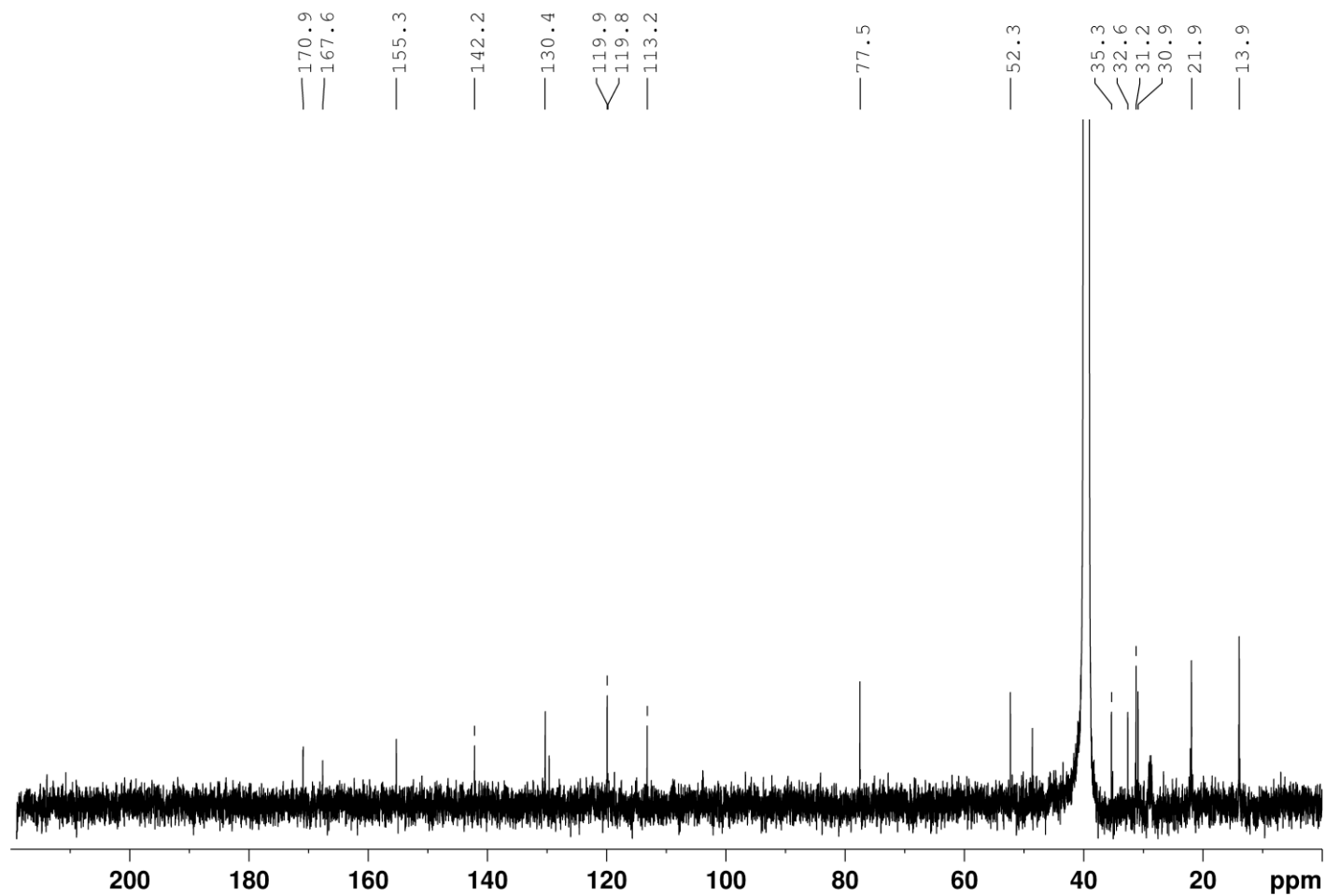


Figure S9:  $^{13}\text{C}$  NMR spectrum of **2** (150 MHz,  $\text{DMSO-}d_6$ ,  $25\text{ }^\circ\text{C}$ )

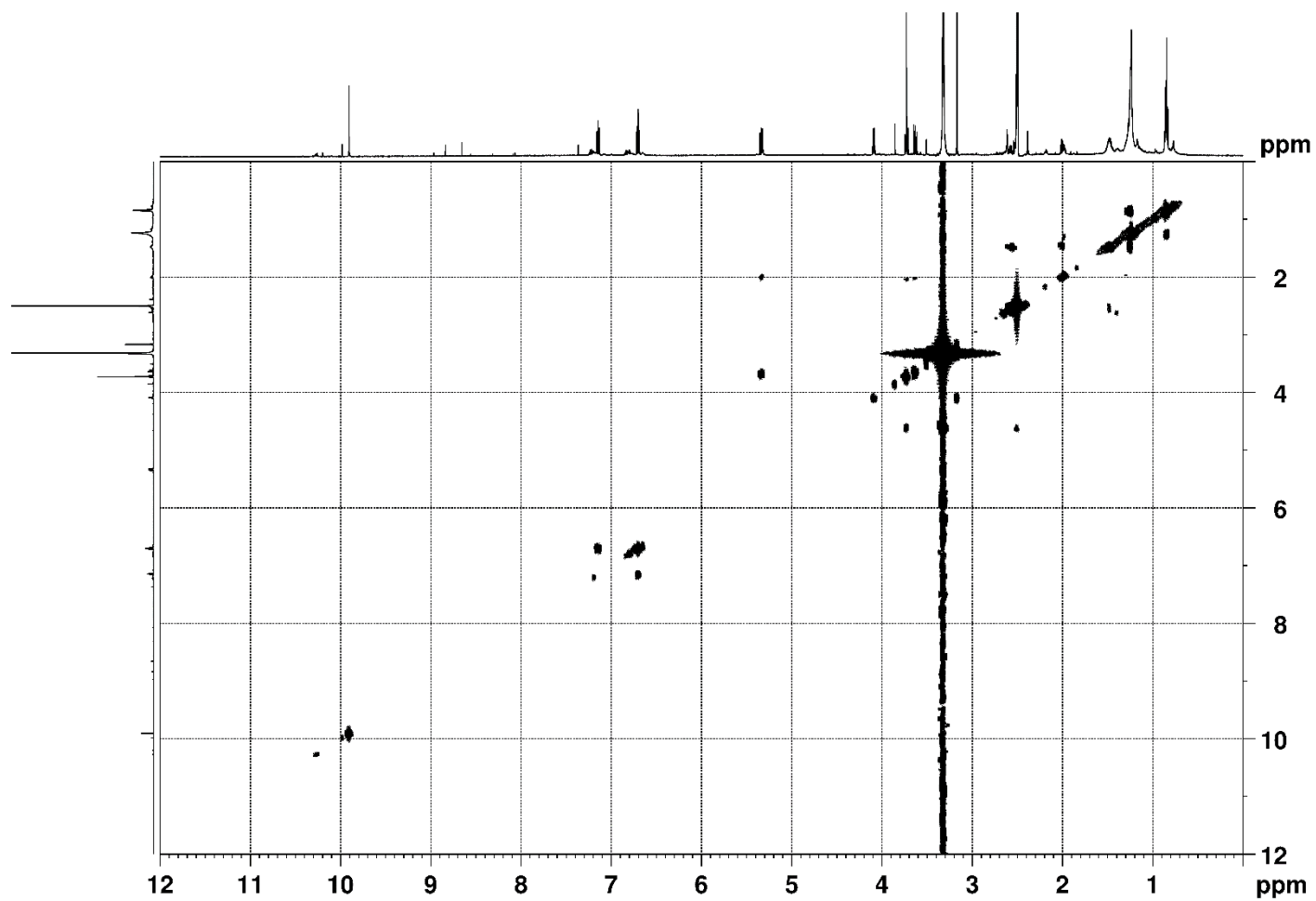


Figure S10: COSY spectrum of **2** (600 MHz, DMSO- $d_6$ , 25 °C)



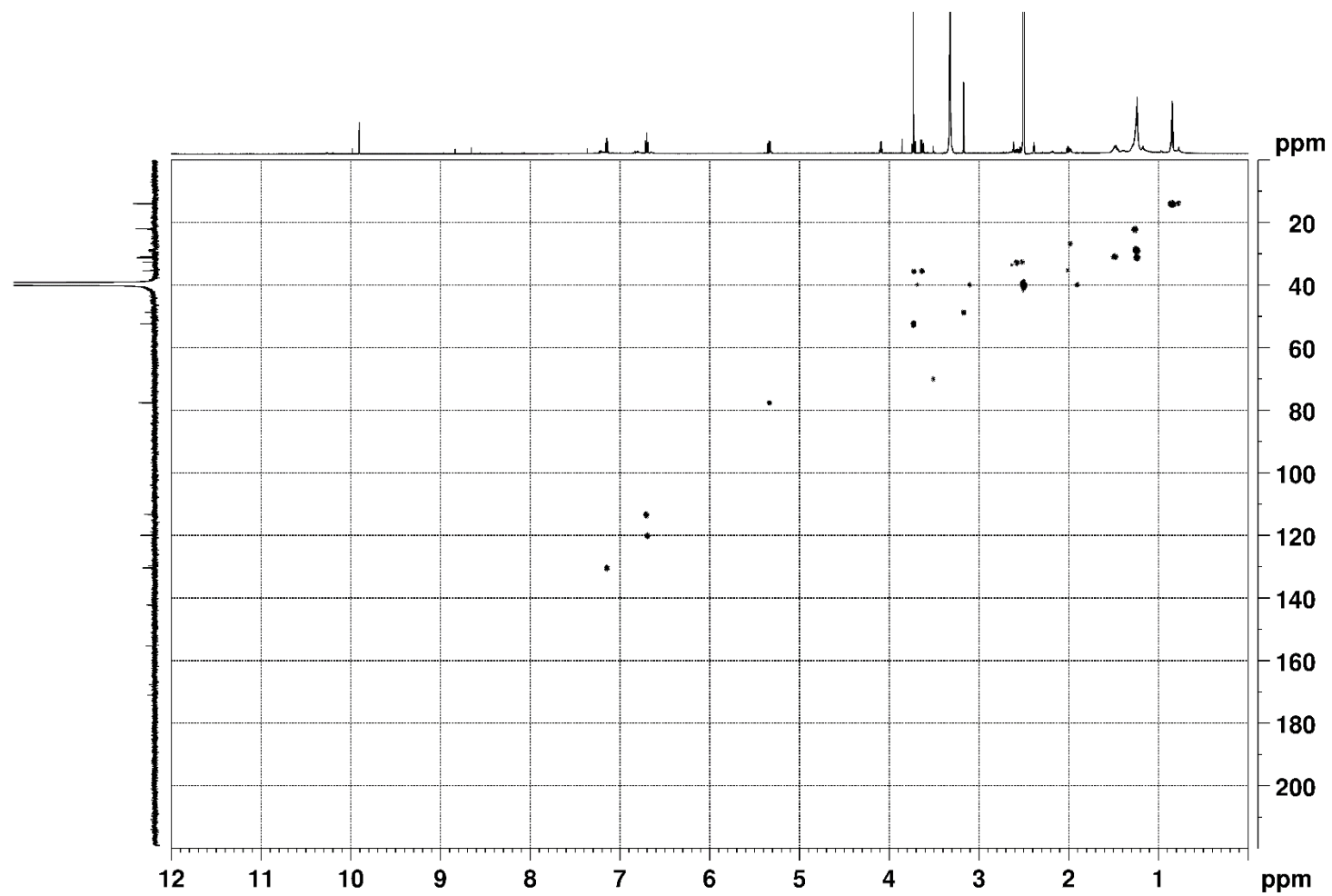


Figure S11: HSQC spectrum of **2** (600 MHz,  $\text{DMSO}-d_6$ , 25 °C)

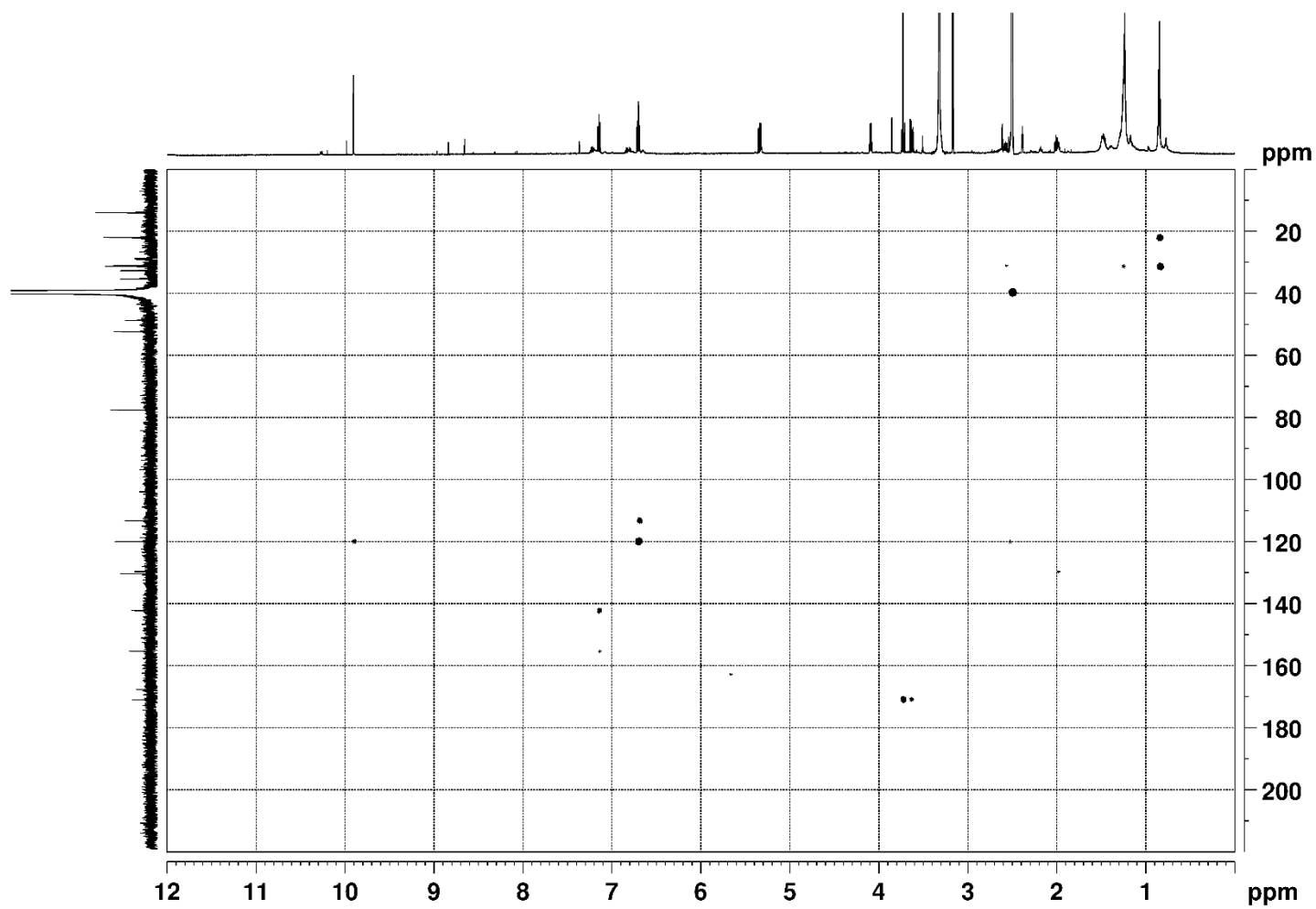


Figure S12: HMBC spectrum of **2** (600 MHz, DMSO-*d*<sub>6</sub>, 25 °C)

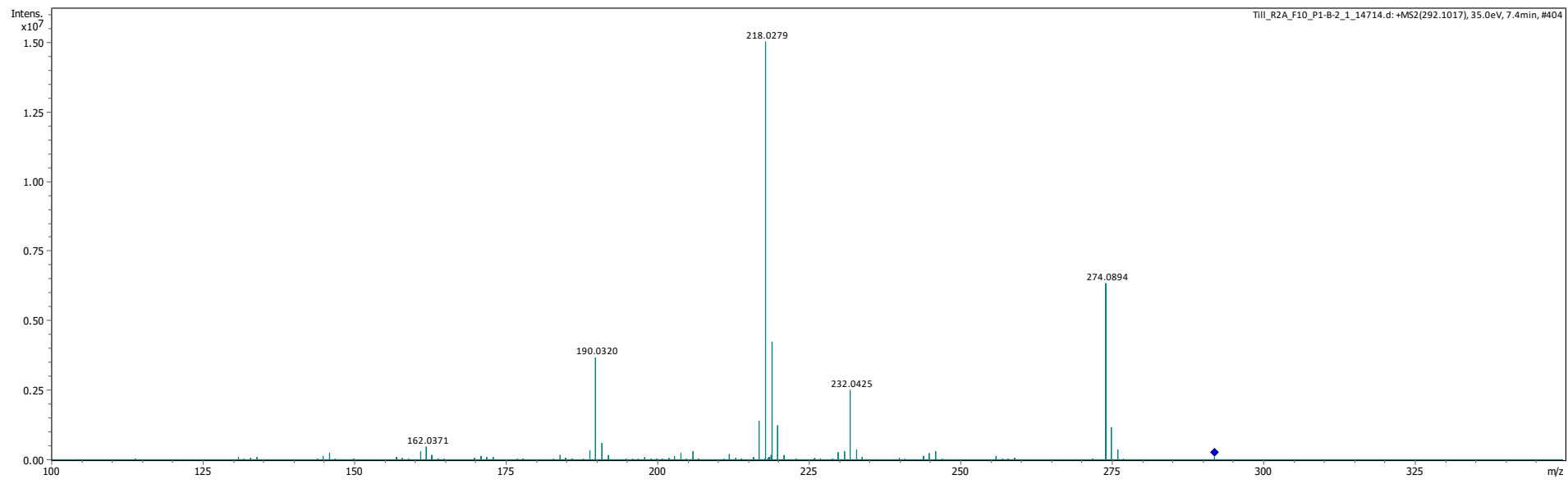


Figure S13: MS/MS spectrum of **3**

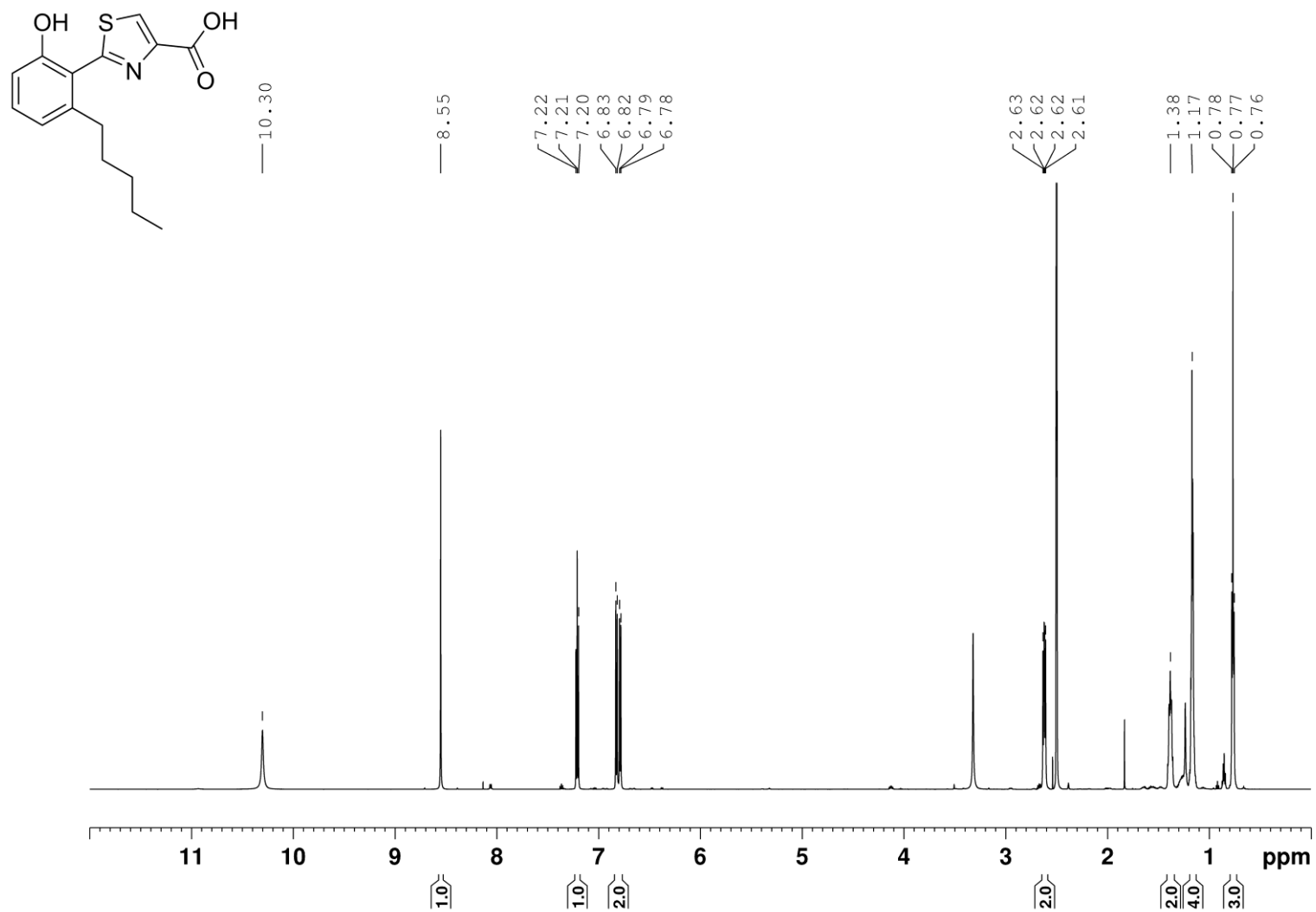


Figure S14: <sup>1</sup>H NMR spectrum of **3** (600 MHz, DMSO-*d*<sub>6</sub>, 25 °C)

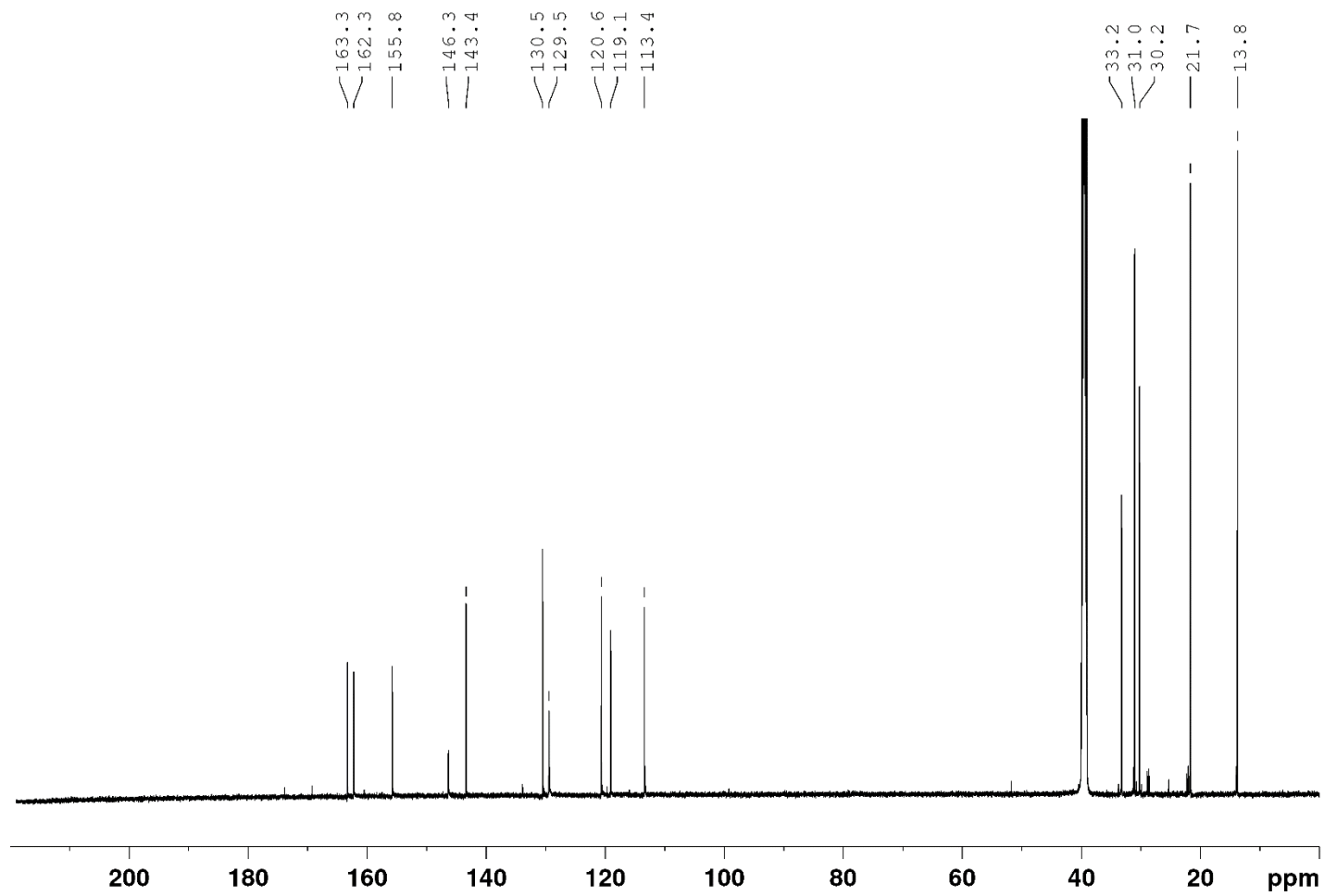


Figure S15:  $^{13}\text{C}$  NMR spectrum of **3** (150 MHz, DMSO- $d_6$ , 25 °C)

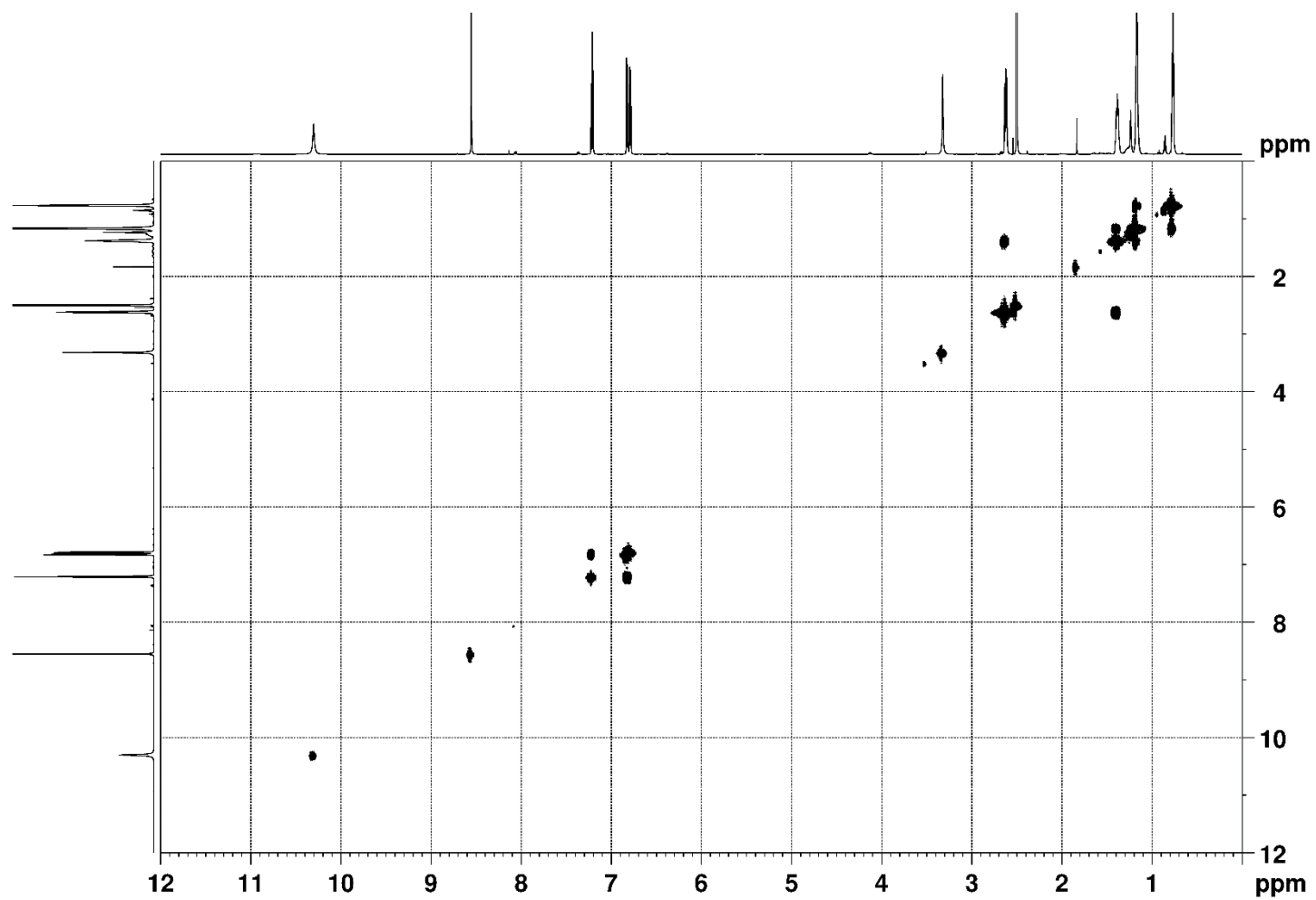


Figure S16: COSY spectrum of **3** (600 MHz, DMSO-*d*<sub>6</sub>, 25 °C)

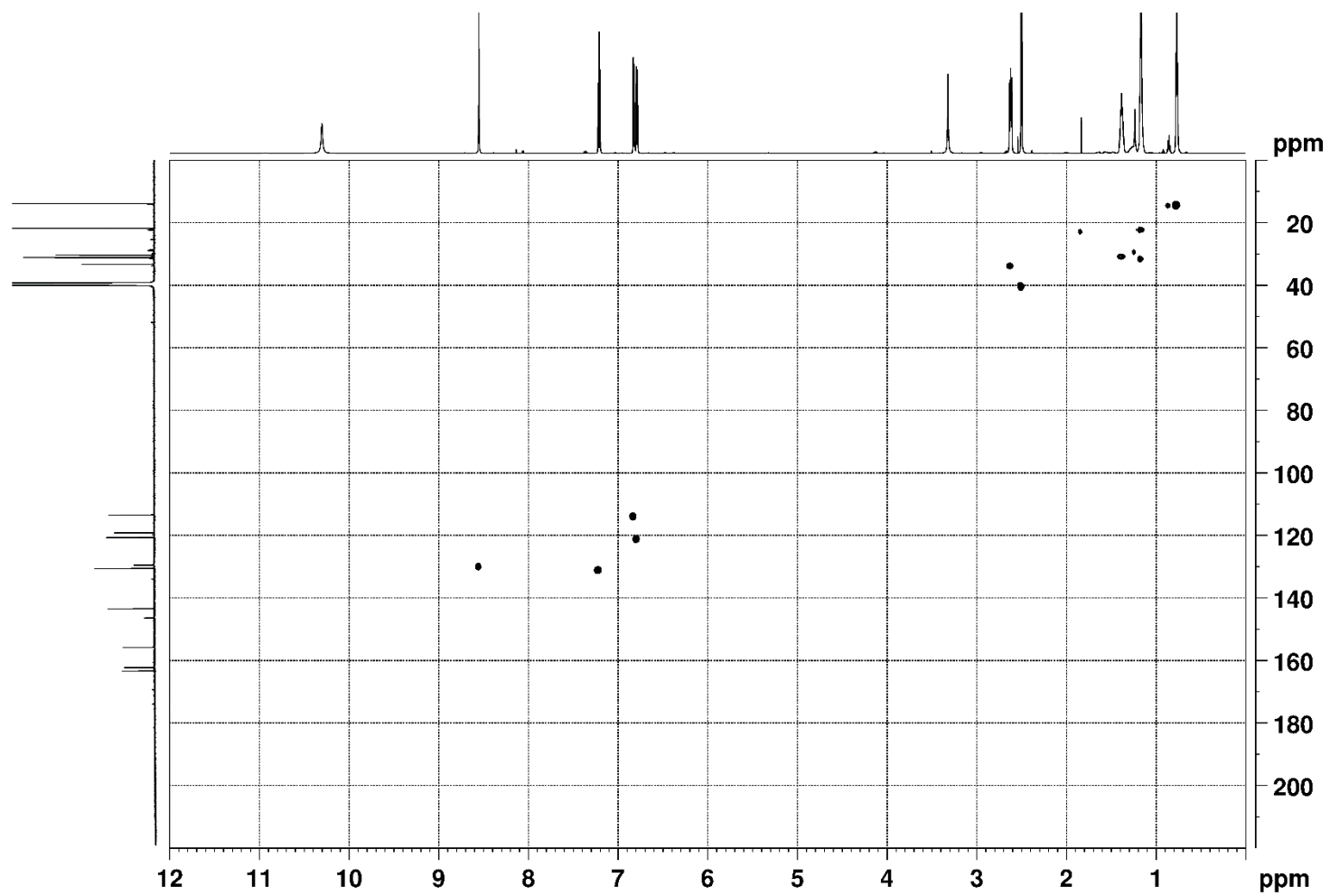


Figure S17: HSQC spectrum of **3** (600 MHz,  $\text{DMSO-}d_6$ , 25 °C)

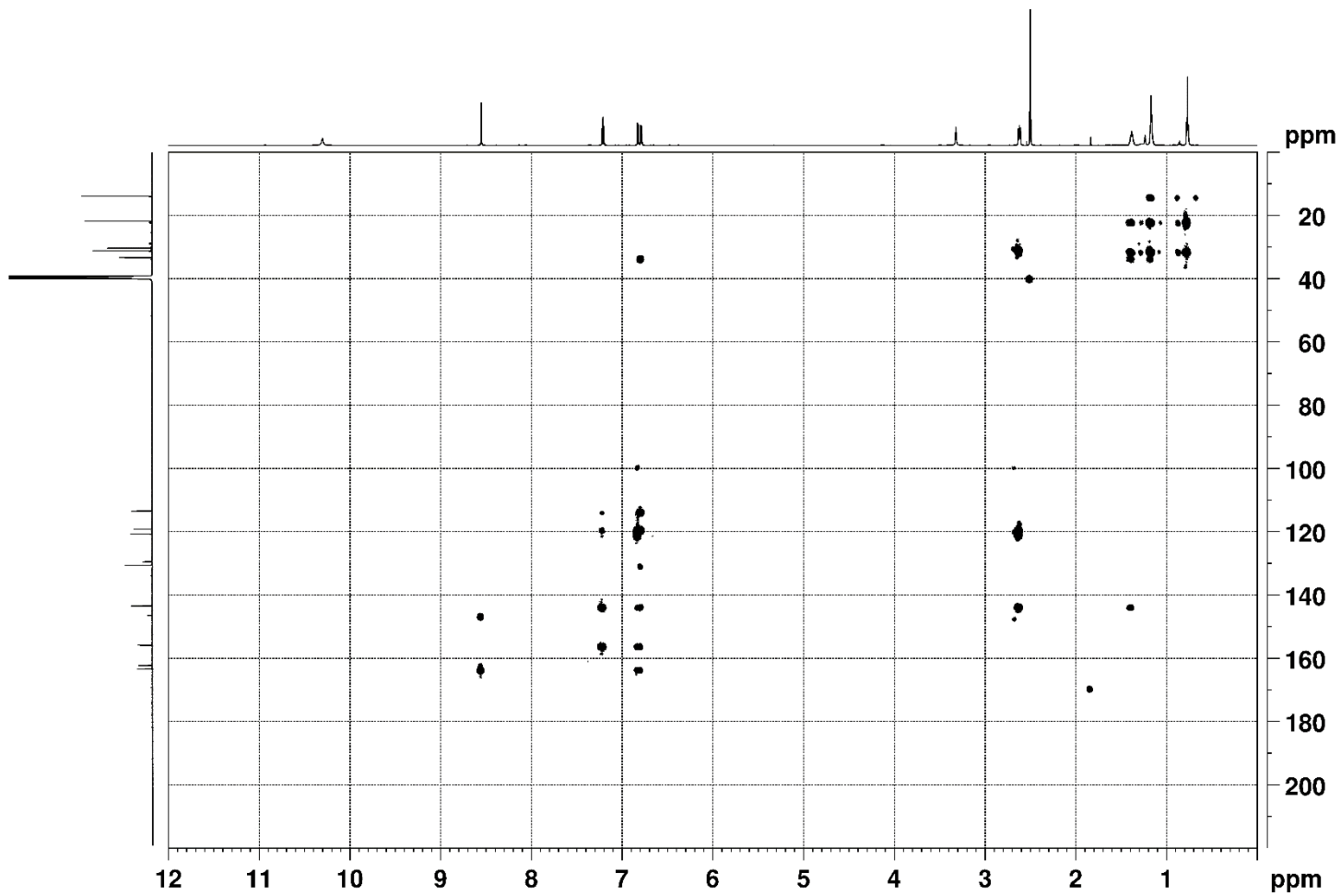


Figure S18: HMBC spectrum of **3** (600 MHz, DMSO- $d_6$ , 25 °C)



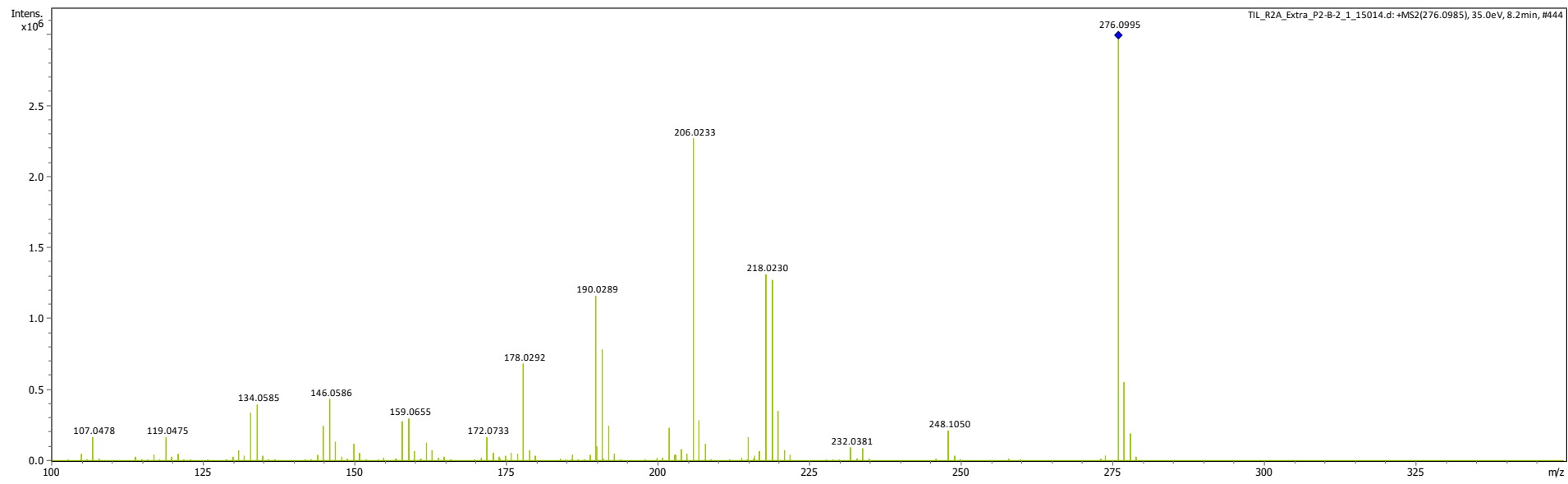


Figure S19: MS/MS spectrum of **4**

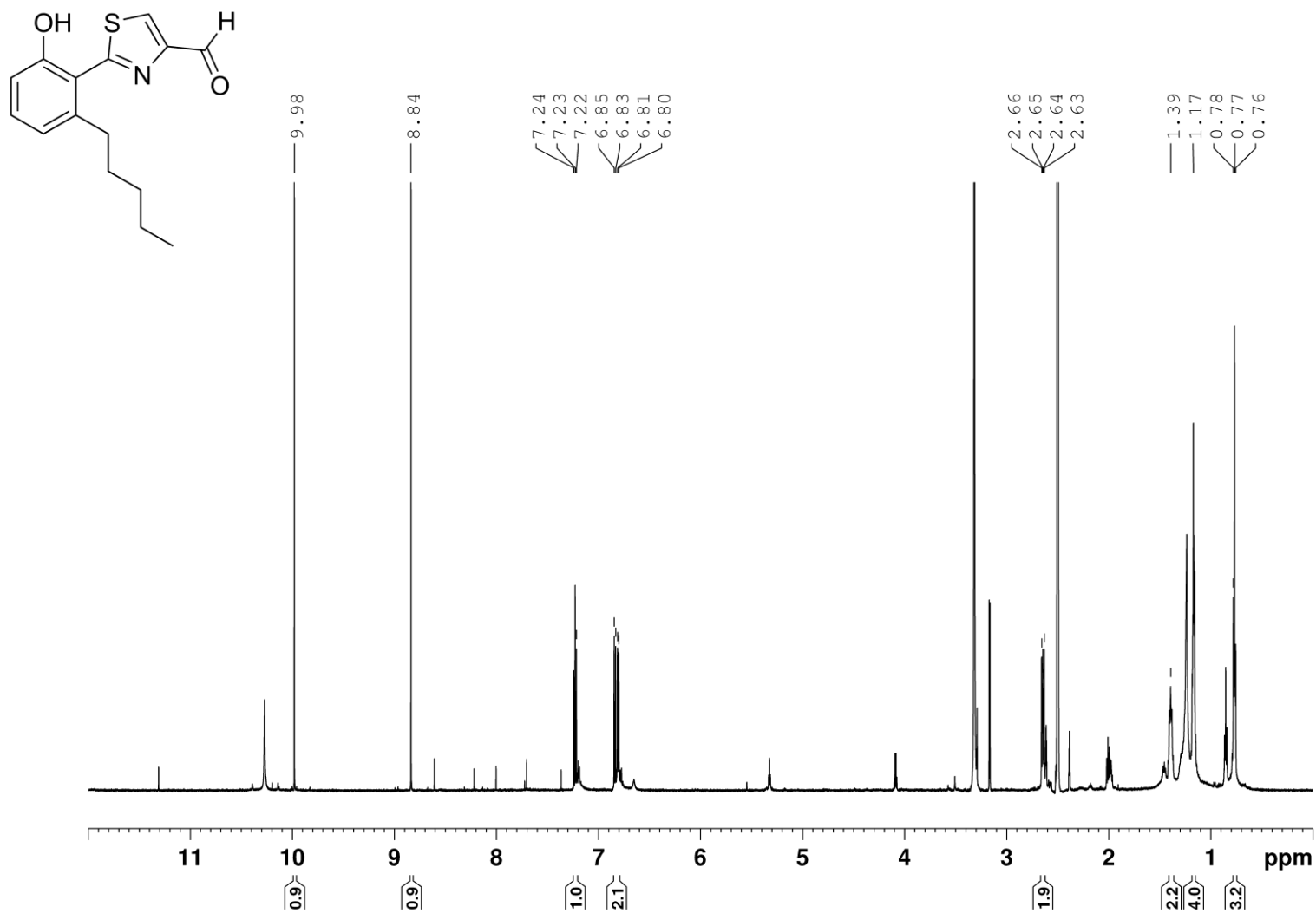


Figure S20:  $^1\text{H}$  NMR spectrum of 4 (600 MHz,  $\text{DMSO}-d_6$ , 25 °C)

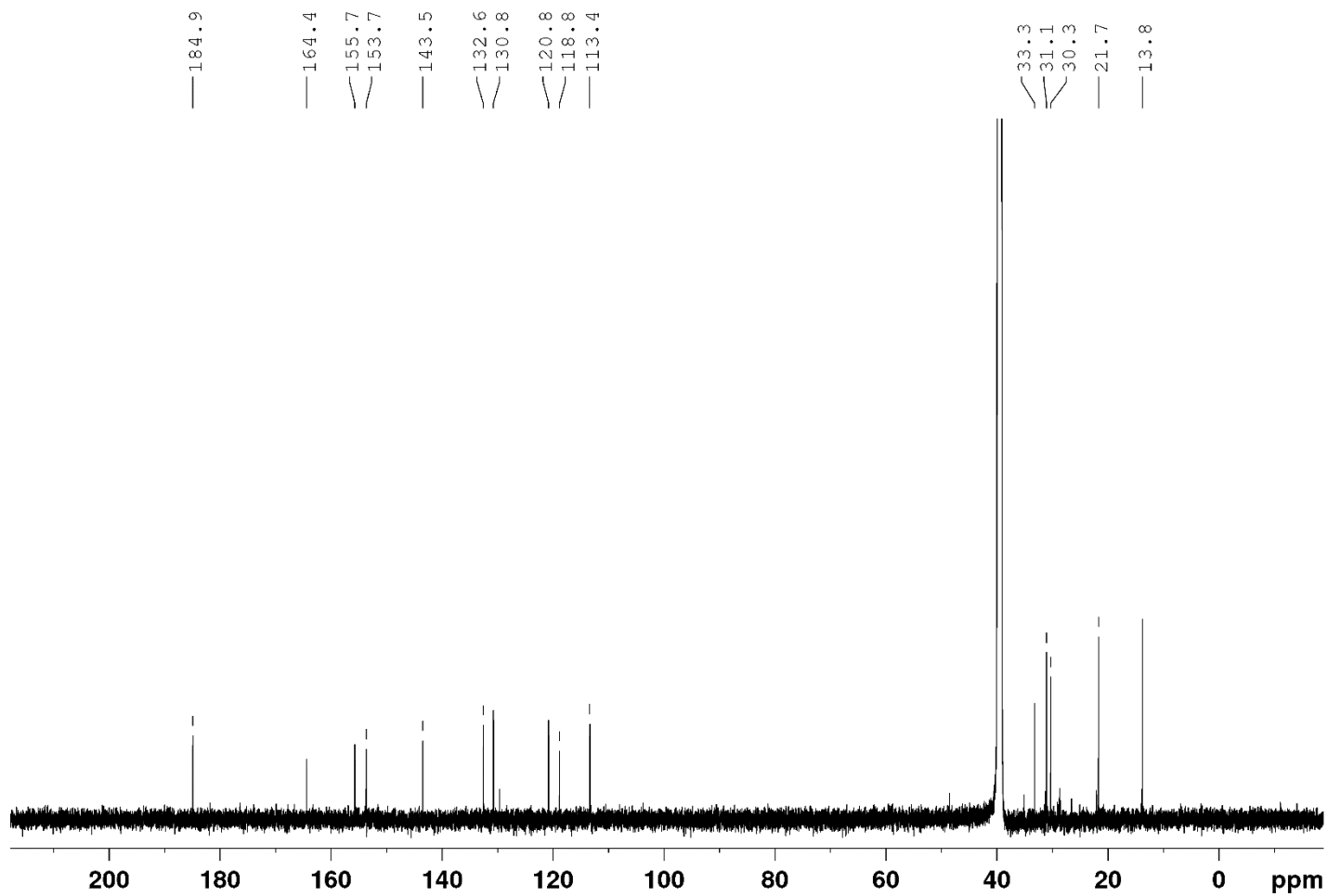


Figure S21:  $^{13}\text{C}$  NMR spectrum of **4** (150 MHz,  $\text{DMSO-}d_6$ , 25 °C)

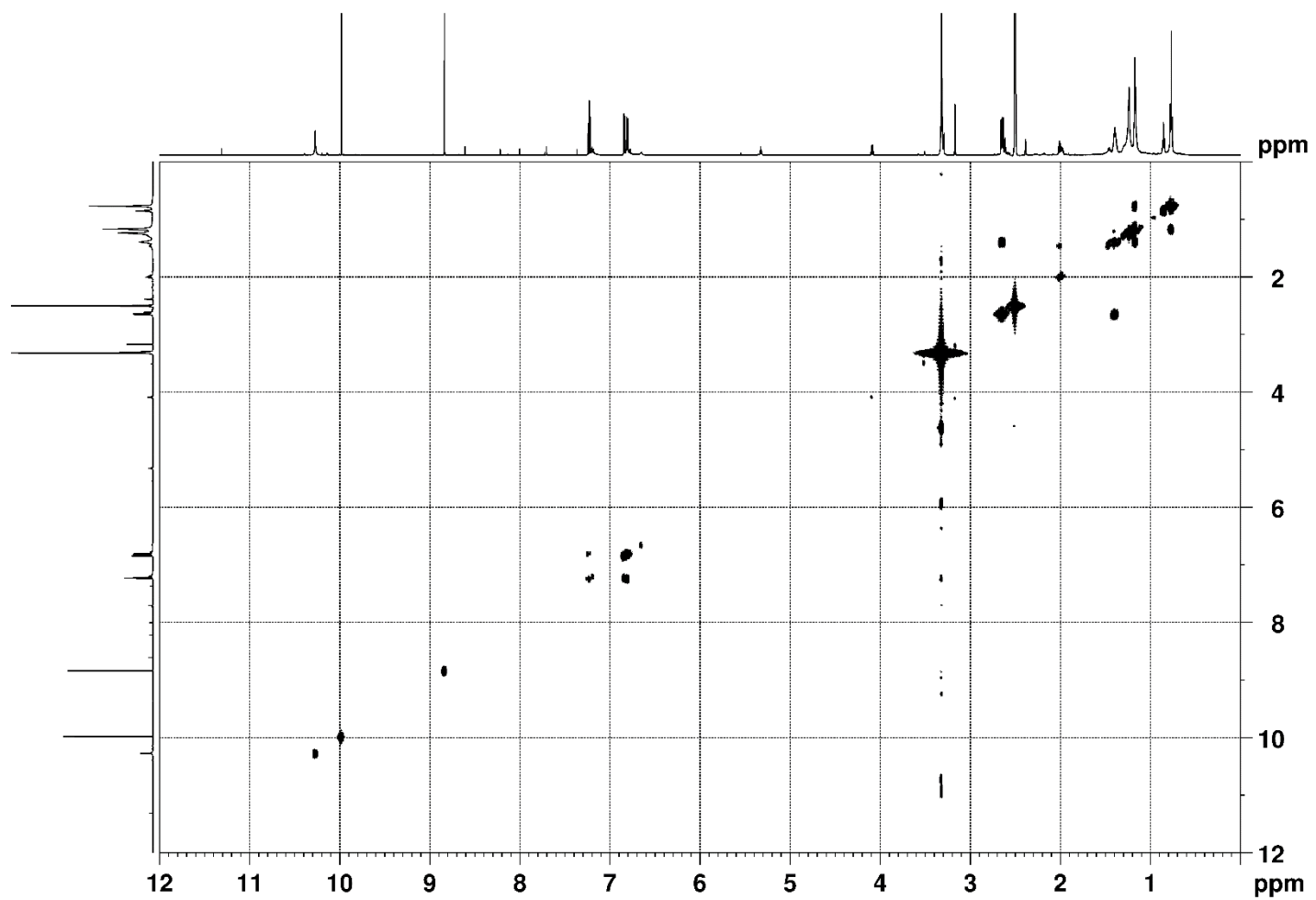


Figure S22: COSY spectrum of **4** (600 MHz, DMSO-*d*<sub>6</sub>, 25 °C)

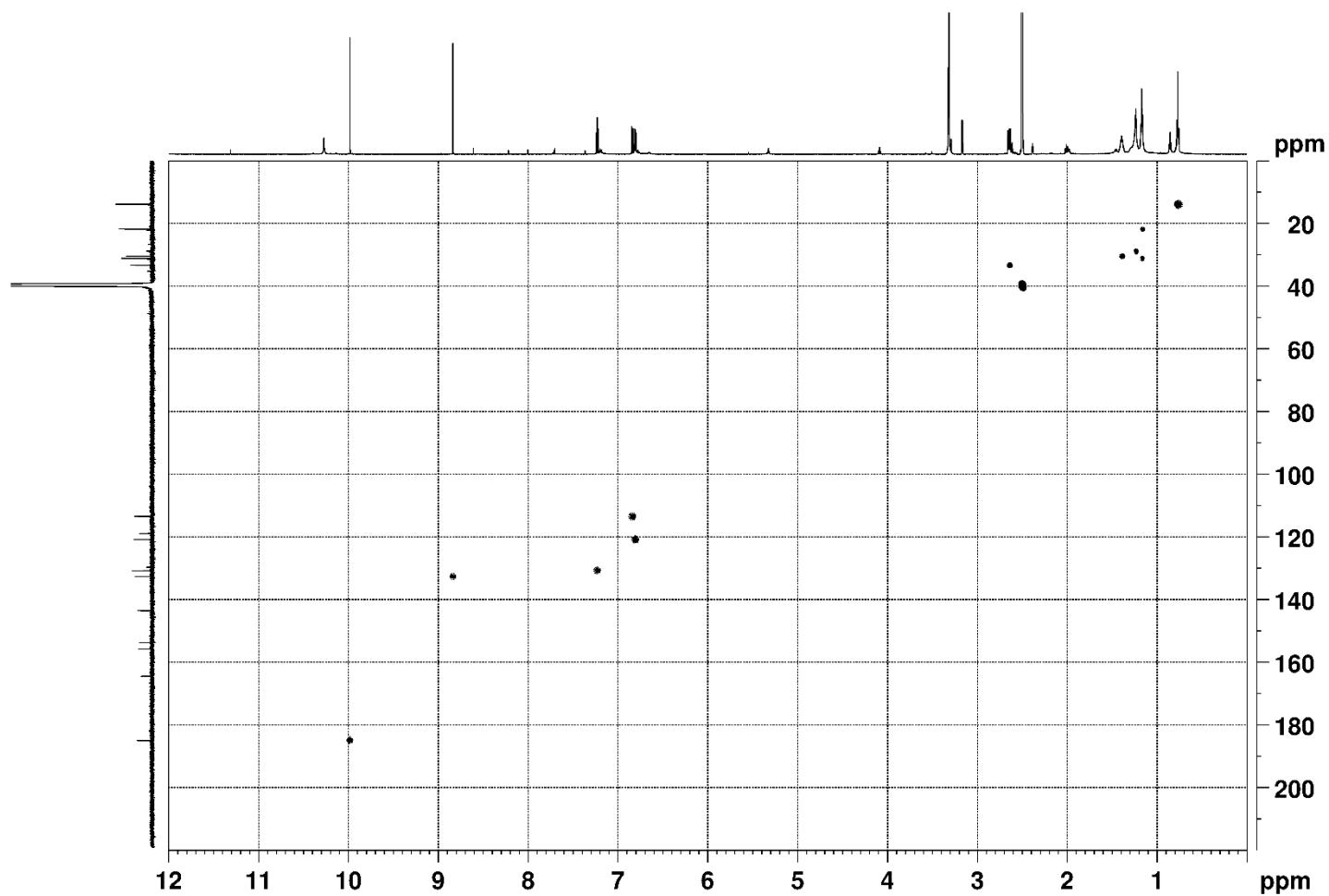


Figure S23: HSQC spectrum of **4** (600 MHz,  $\text{DMSO}-d_6$ , 25 °C)

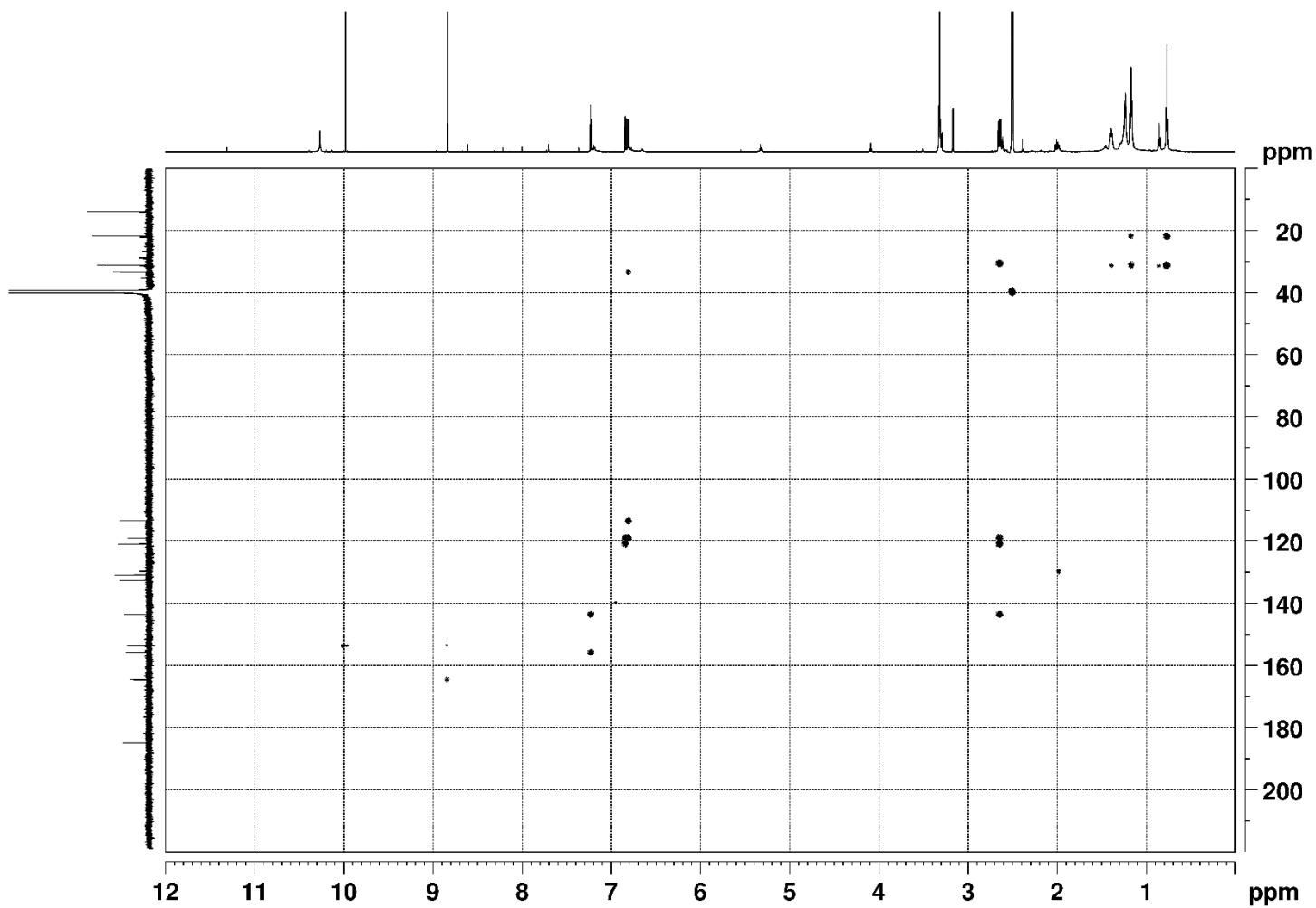


Figure S24: HMBC spectrum of 4 (600 MHz, DMSO-*d*<sub>6</sub>, 25 °C)

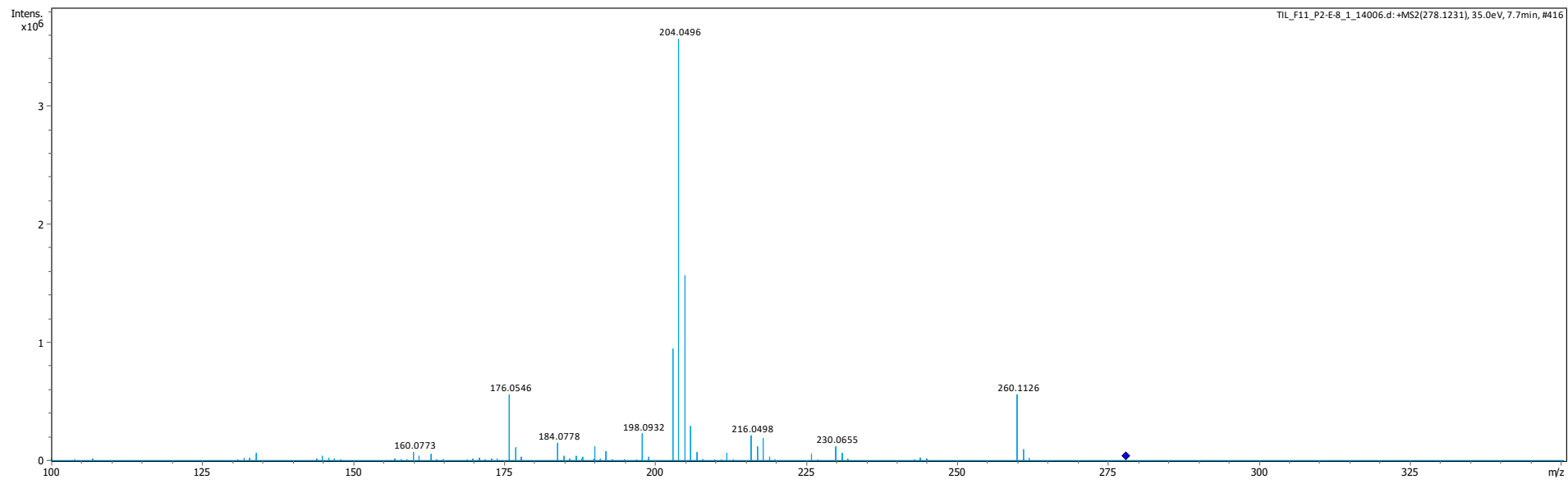


Figure S25: MS/MS spectrum of 5

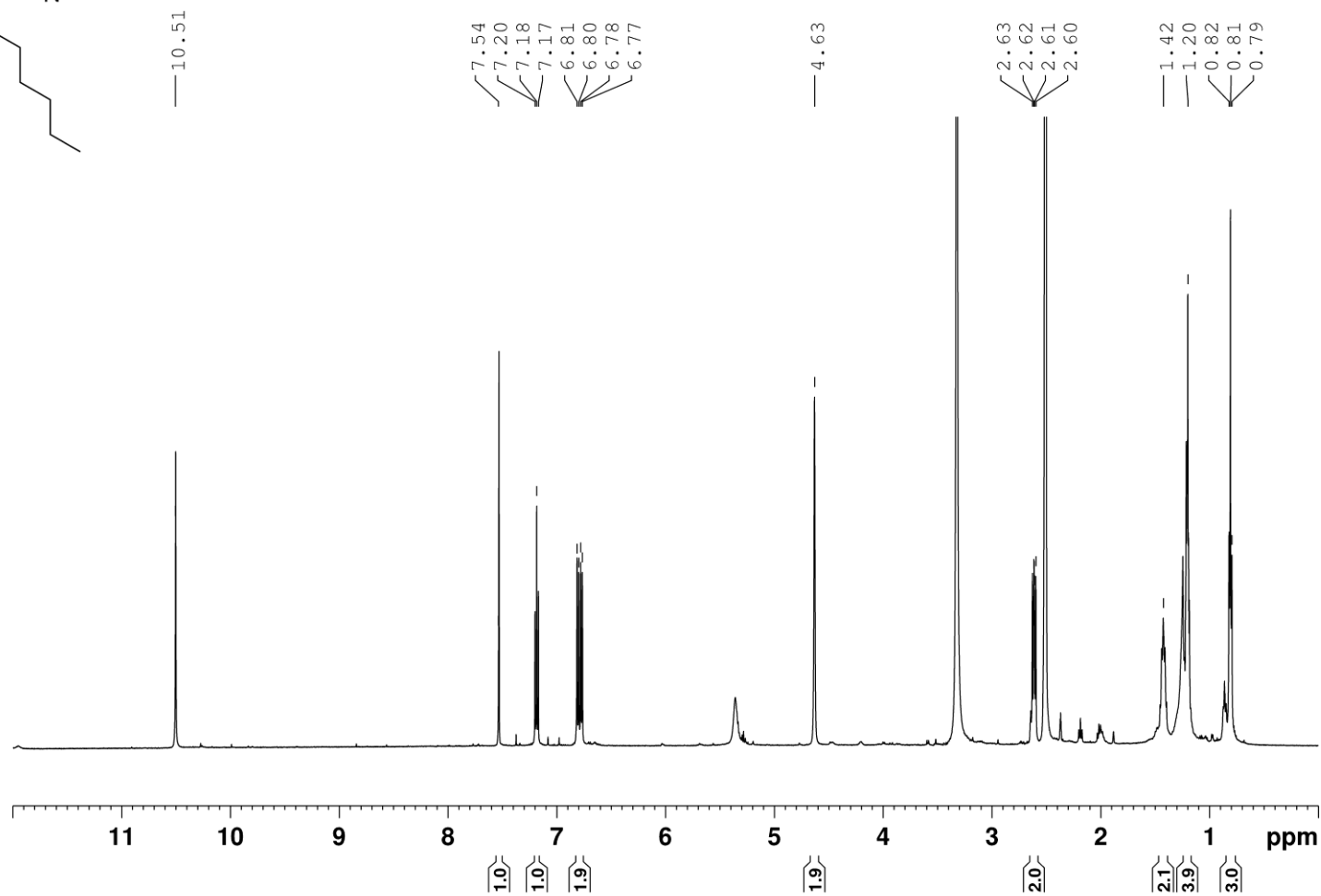
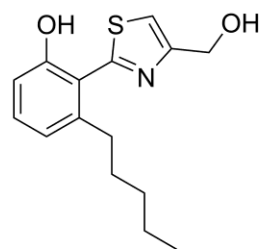


Figure S26:  $^1\text{H}$  NMR spectrum of **5** (600 MHz,  $\text{DMSO-}d_6$ , 25 °C)



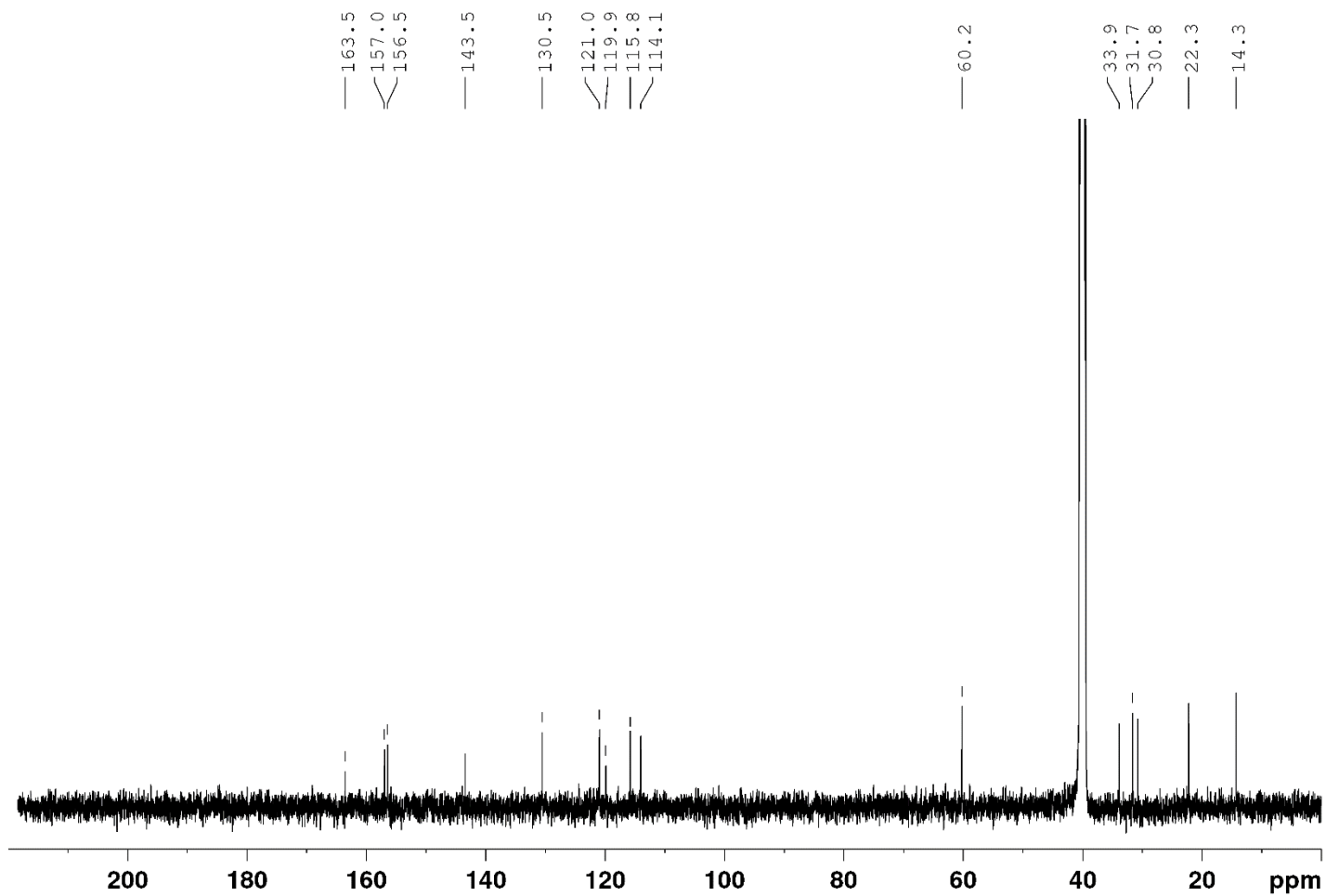


Figure S27:  $^{13}\text{C}$  NMR spectrum of **5** (150 MHz,  $\text{DMSO-}d_6$ , 25 °C)

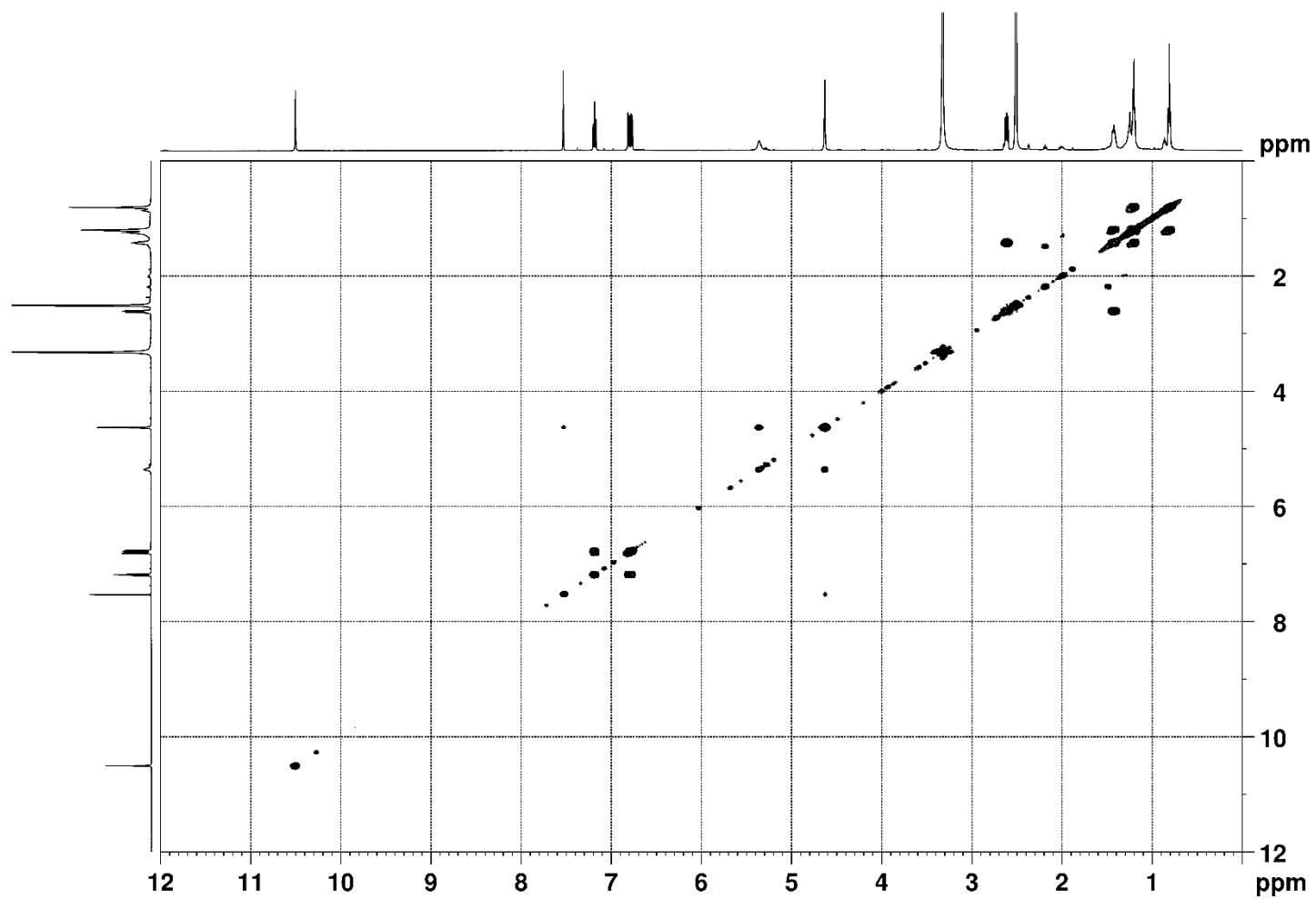


Figure S28: COSY spectrum of **5** (600 MHz, DMSO-*d*<sub>6</sub>, 25 °C)

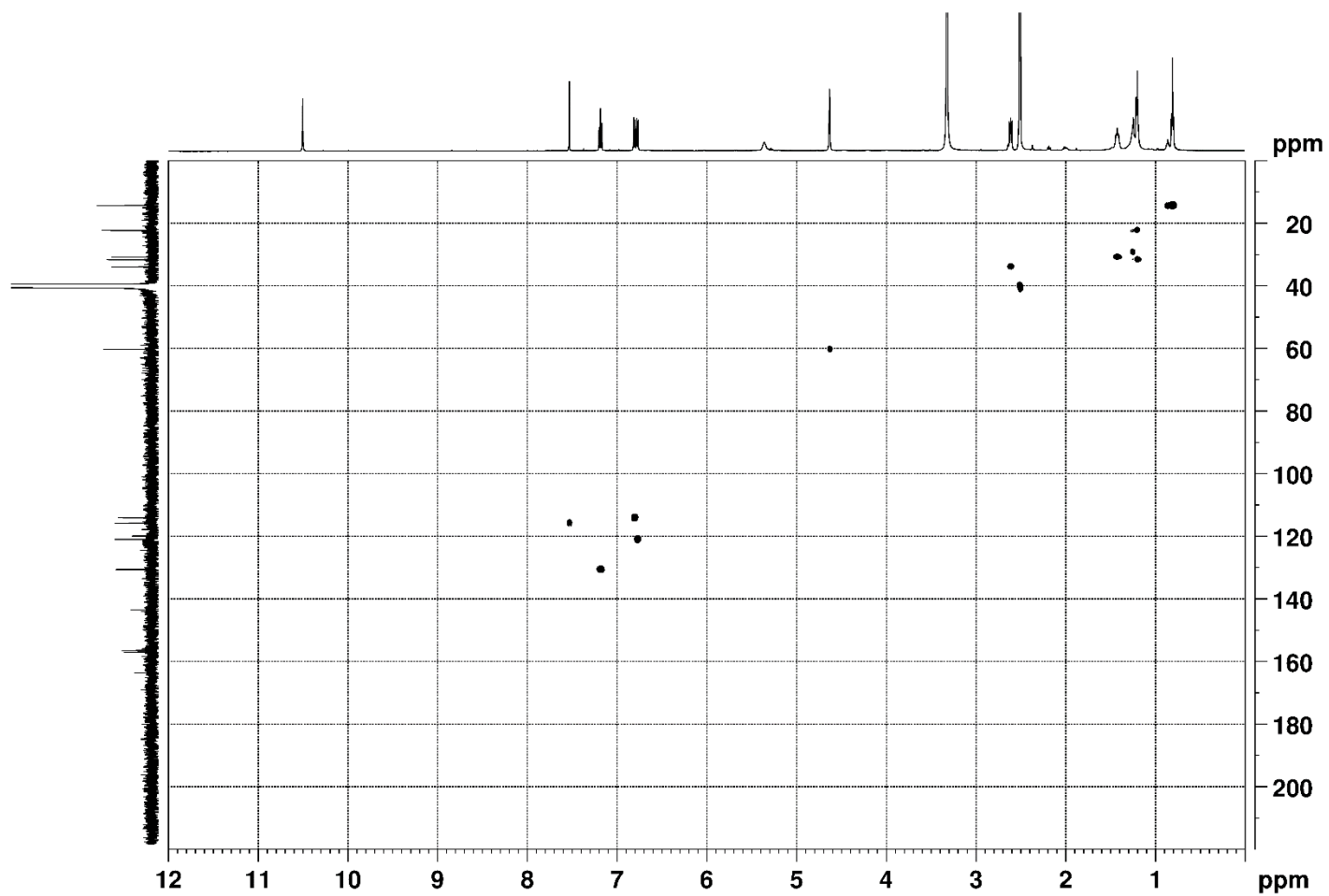


Figure S29: HSQC spectrum of **5** (600 MHz,  $\text{DMSO}-d_6$ , 25 °C)

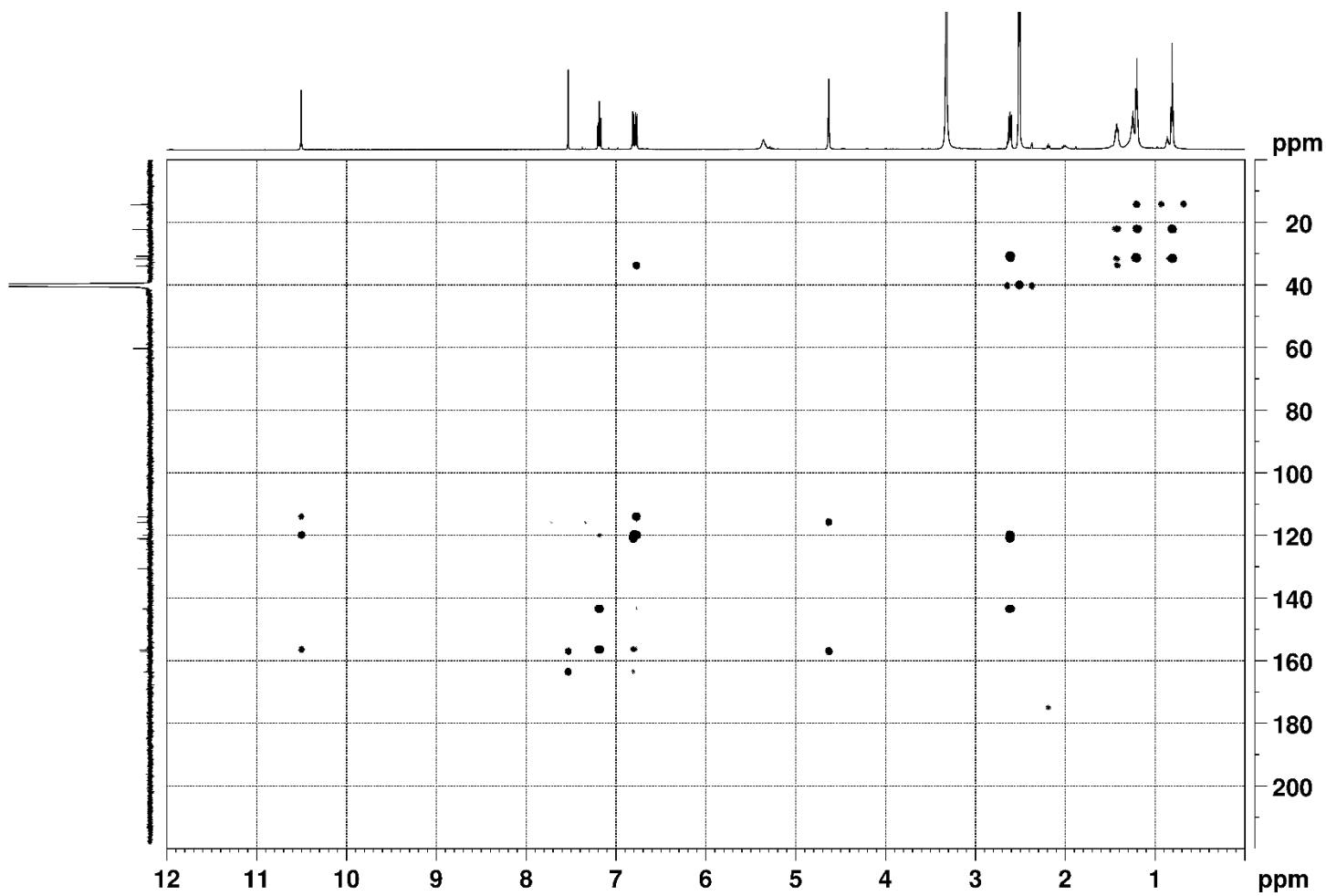


Figure S30: HMBC spectrum of **5** (600 MHz, DMSO-*d*<sub>6</sub>, 25 °C)

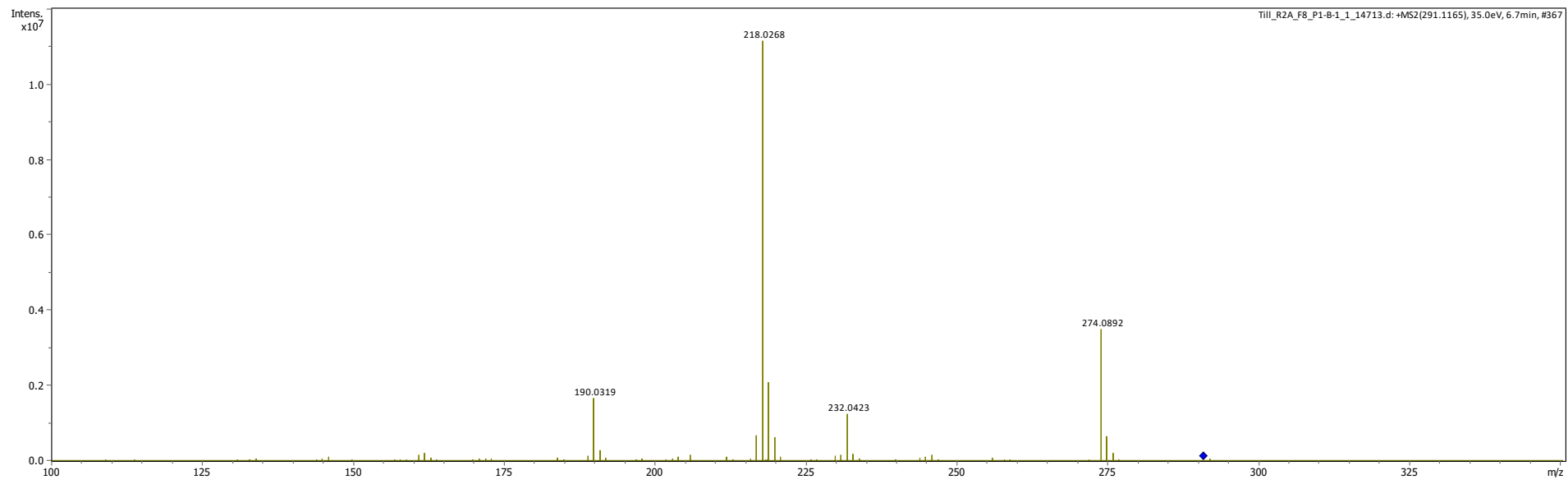


Figure S31: MS/MS spectrum of 6

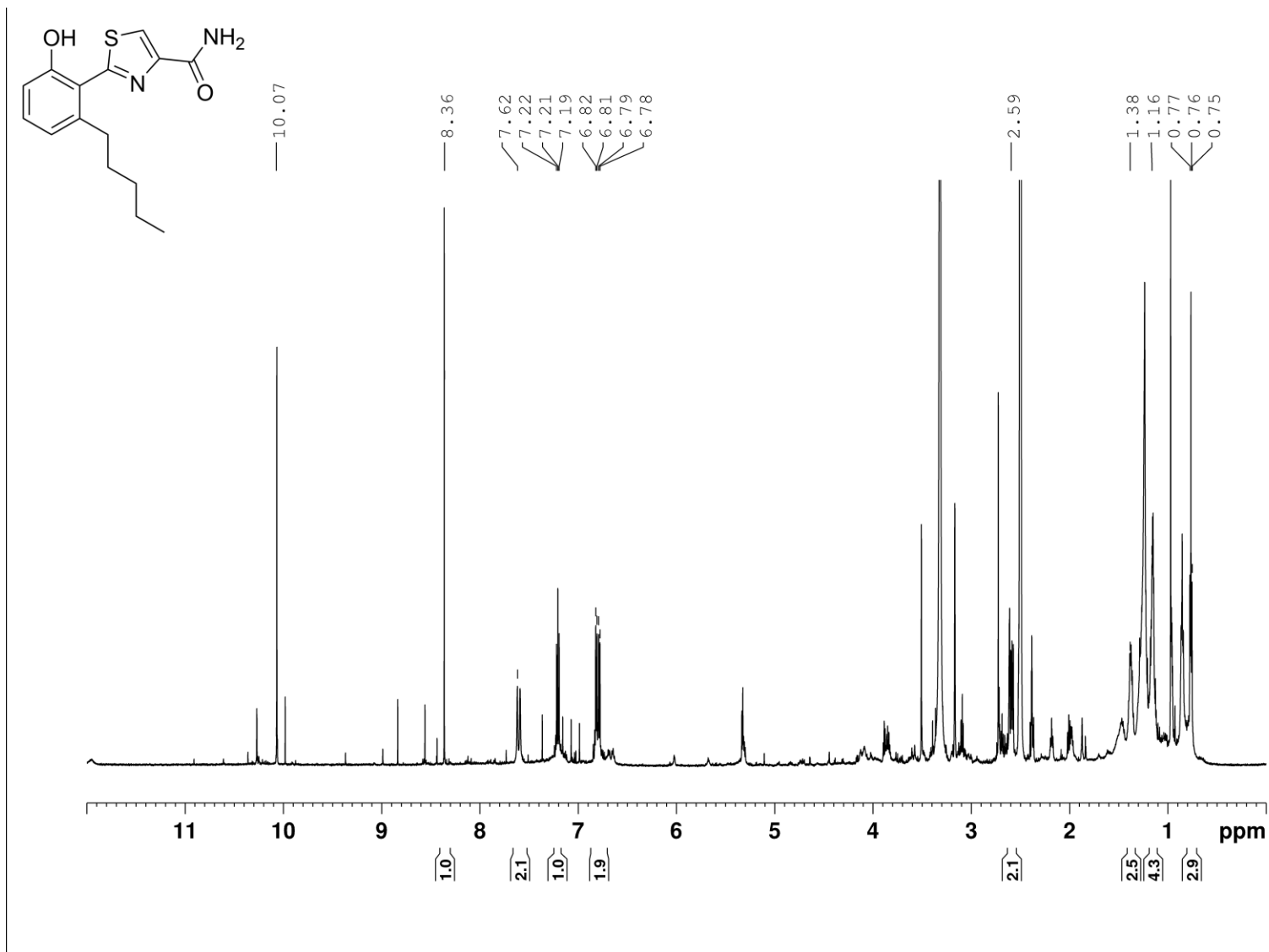


Figure S32: <sup>1</sup>H NMR spectrum of **6** (600 MHz, DMSO-*d*<sub>6</sub>, 25 °C)

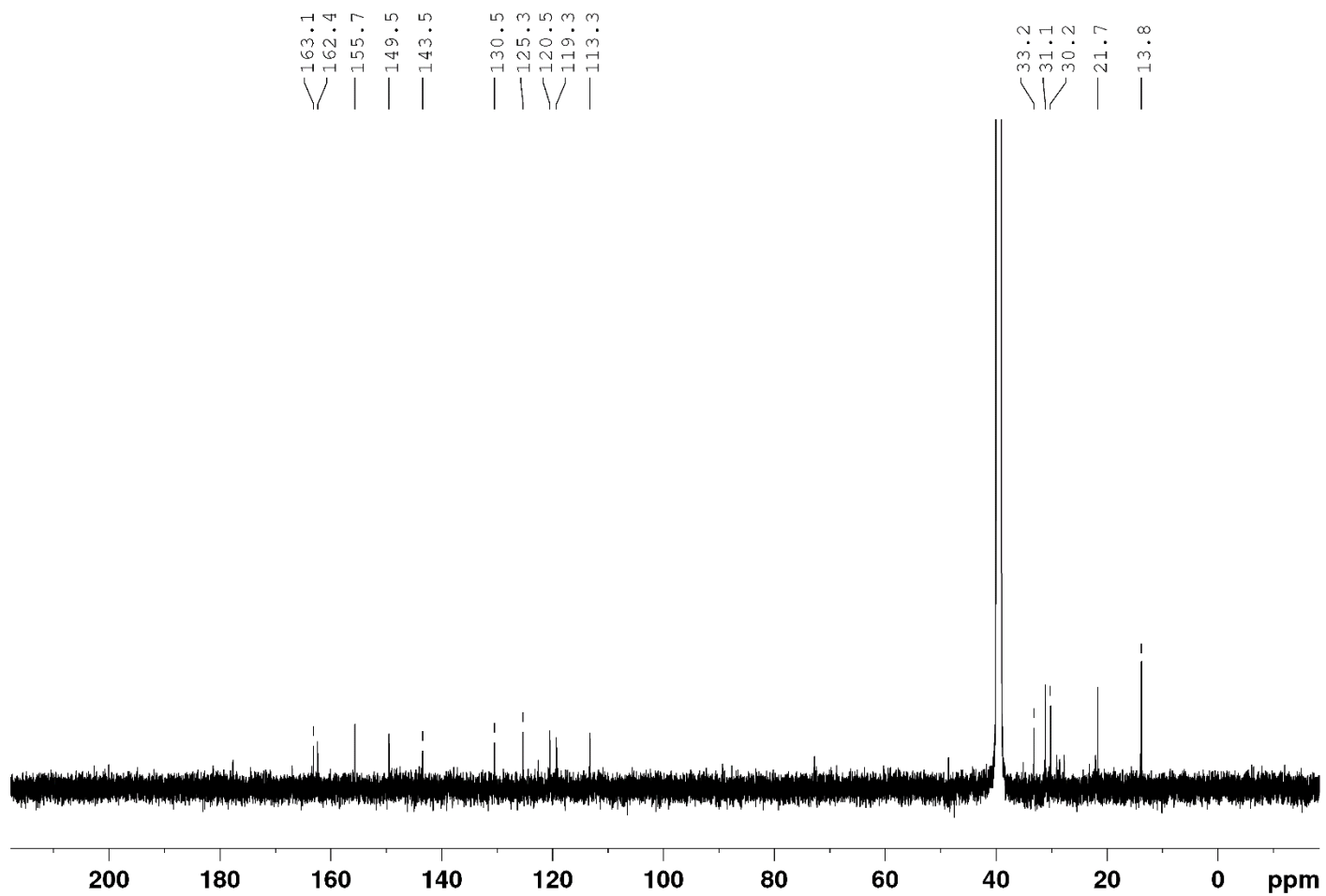


Figure S33:  $^{13}\text{C}$  NMR spectrum of **6** (150 MHz,  $\text{DMSO}-d_6$ , 25 °C)

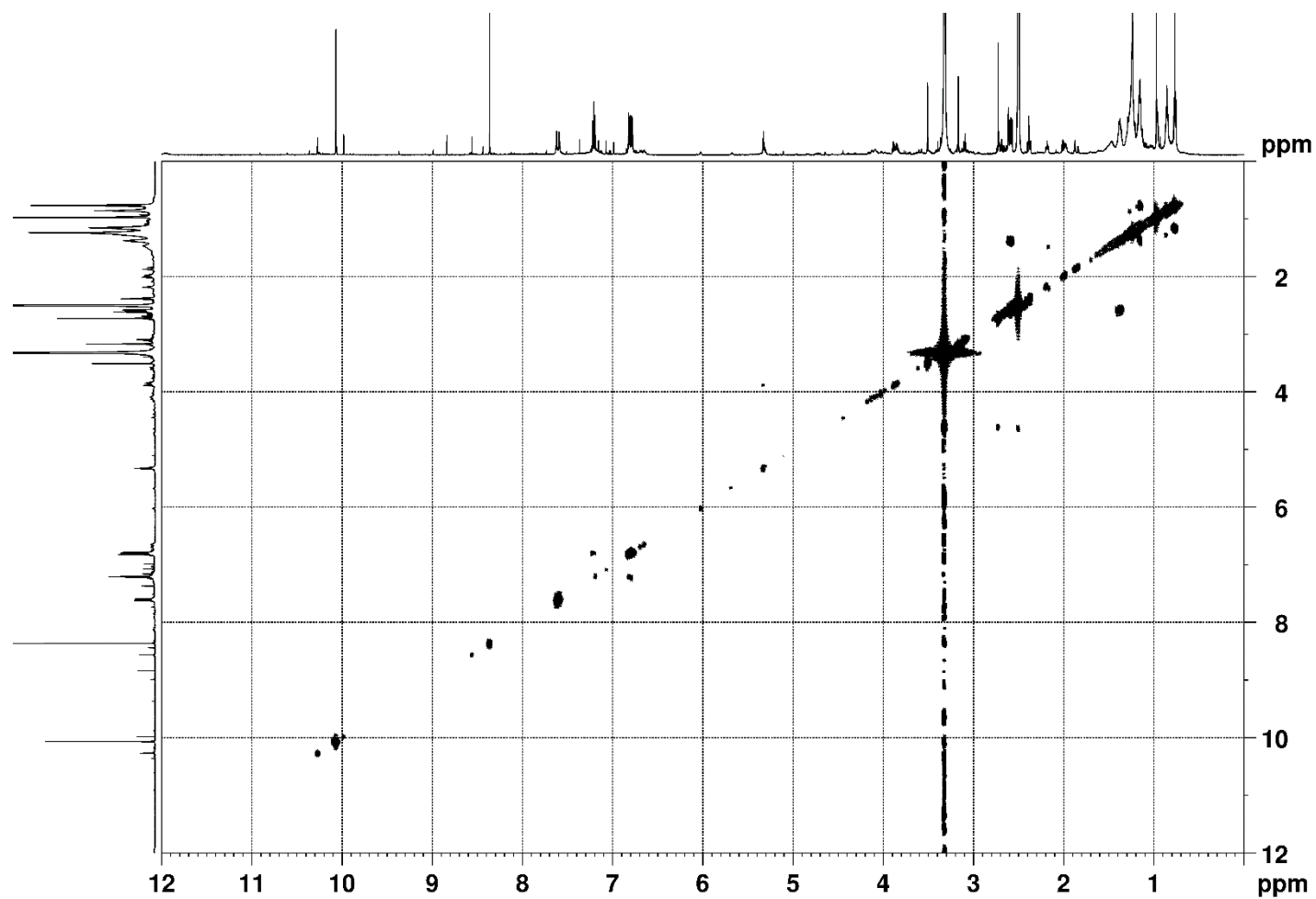


Figure S34: COSY spectrum of **6** (600 MHz, DMSO-*d*<sub>6</sub>, 25 °C)



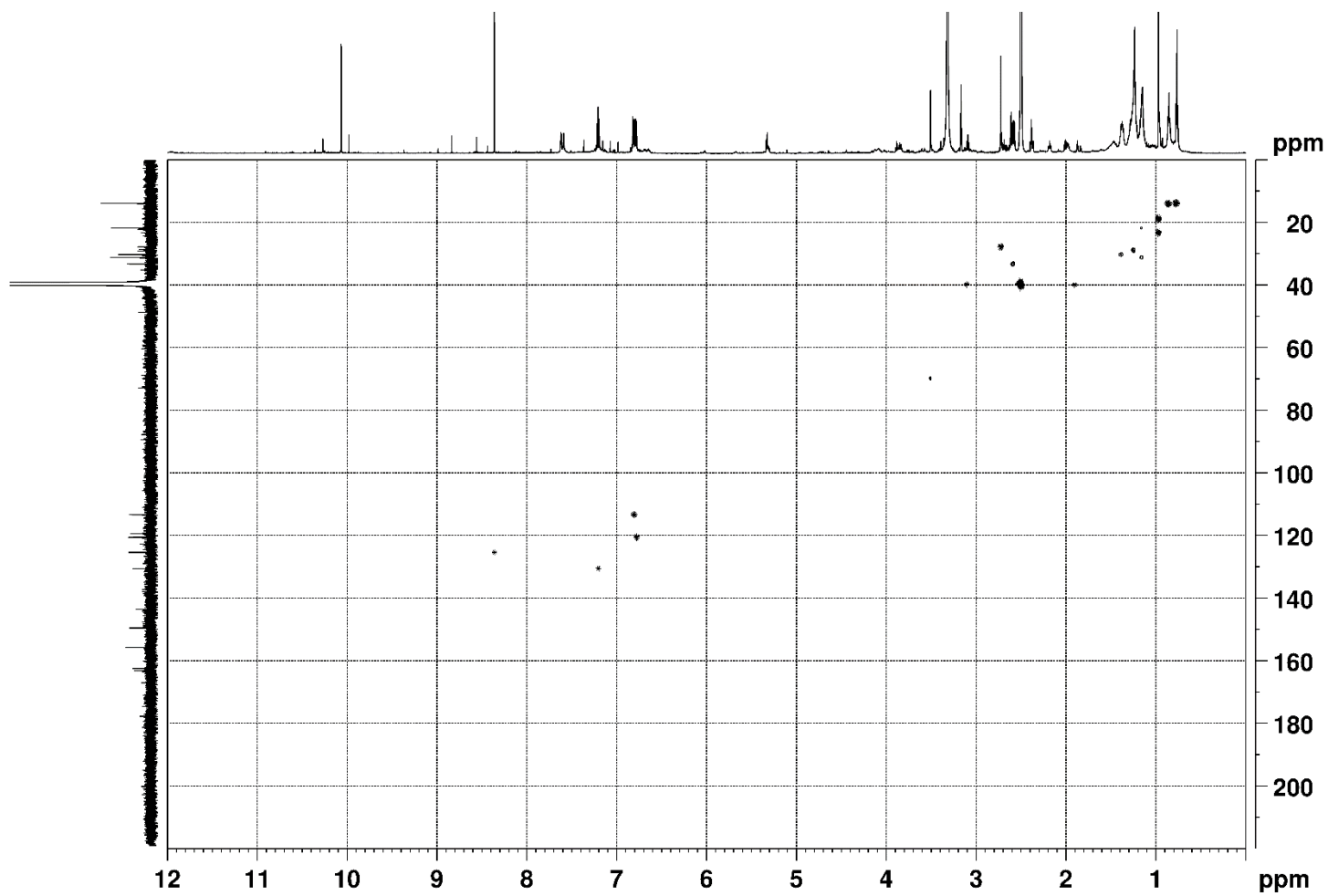


Figure S35: HSQC spectrum of **6** (600 MHz, DMSO- $d_6$ , 25 °C)

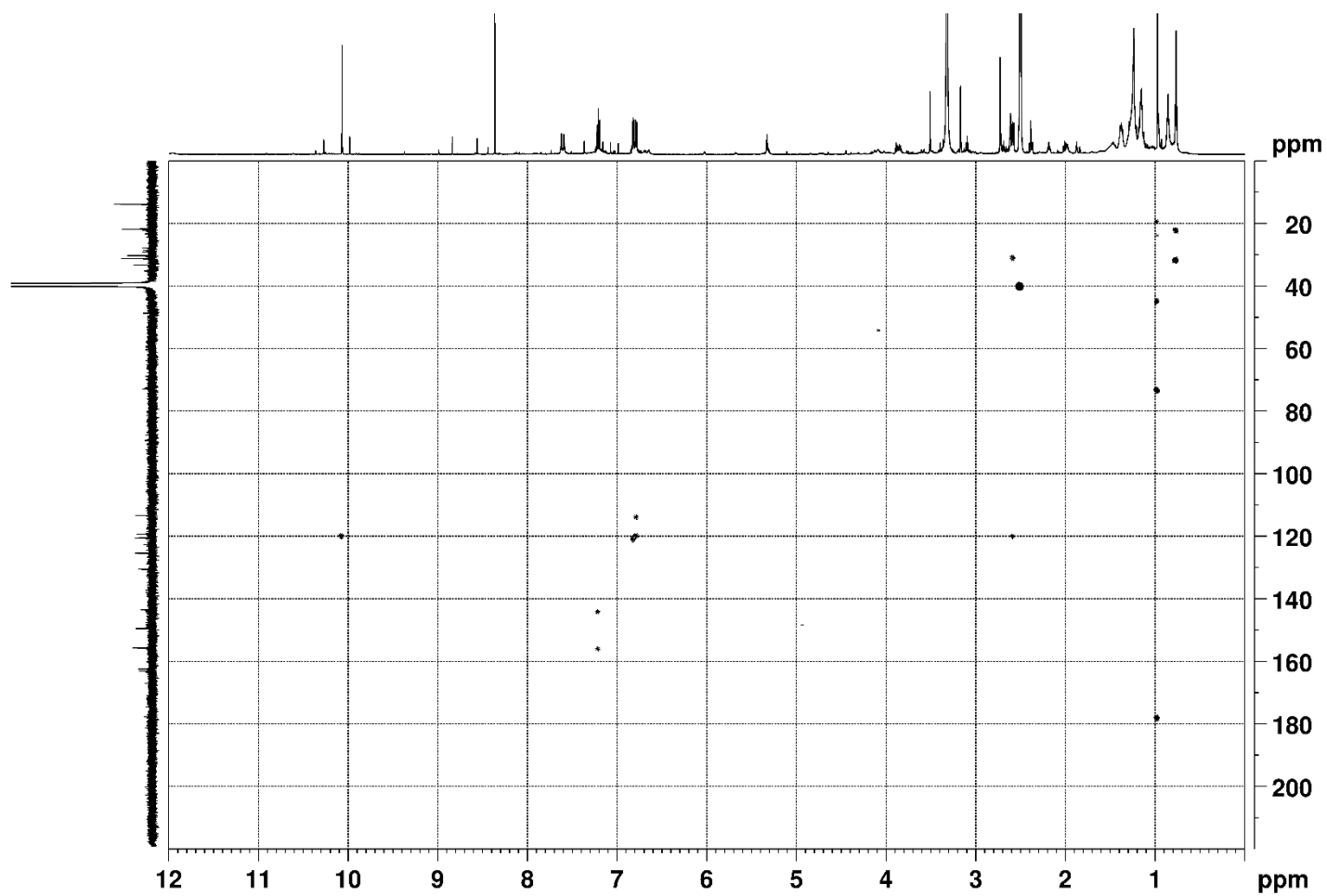


Figure S36: HMBC spectrum of **6** (600 MHz,  $\text{DMSO}-d_6$ , 25 °C)