

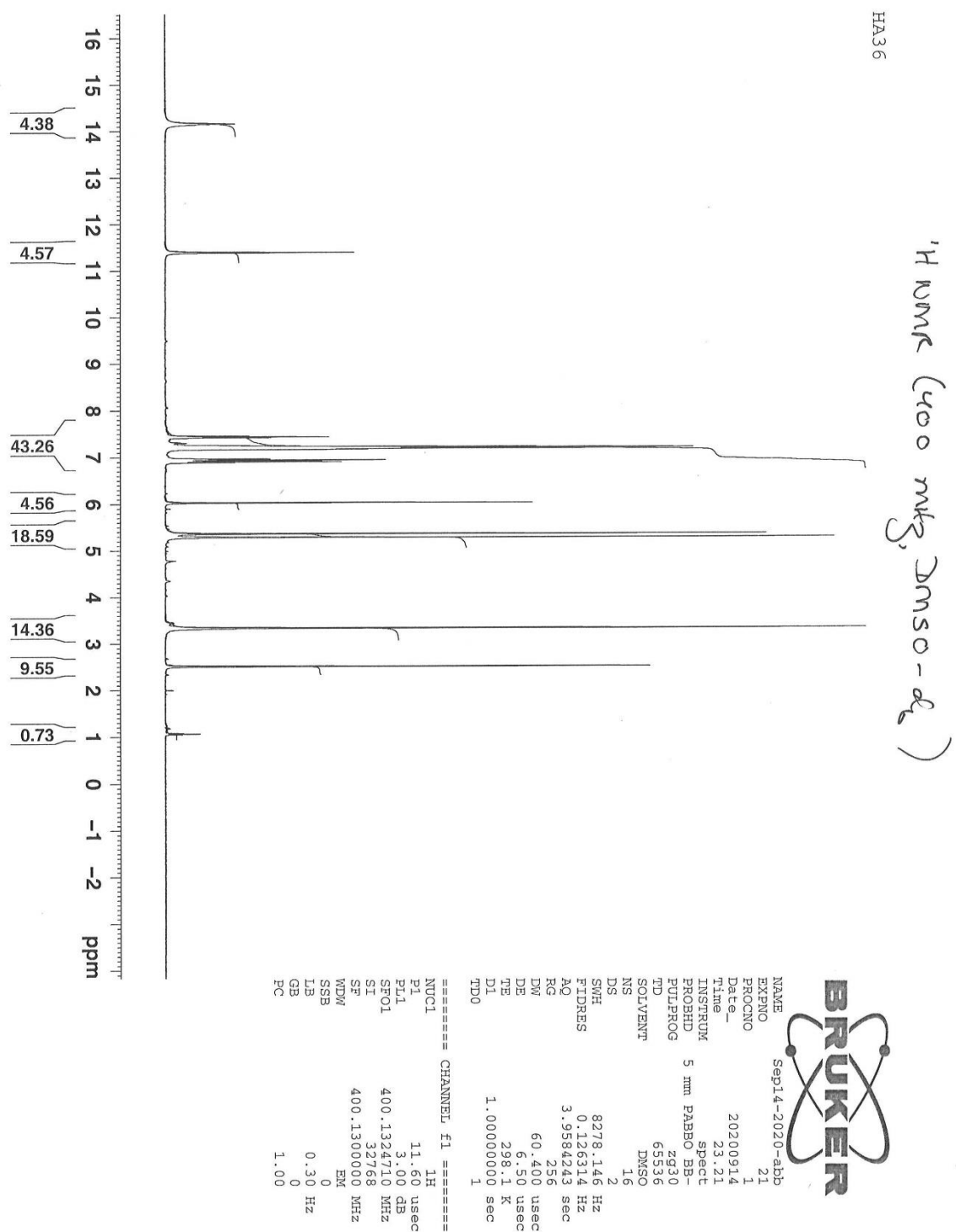
## Supplementary Material, part 1

Y.A.M.M. Elshaier, A.A. Aly,\* M. Abd El-Aziz, H.M. Fathy, A.B. Brown, S. Bräse, and M. Ramadan

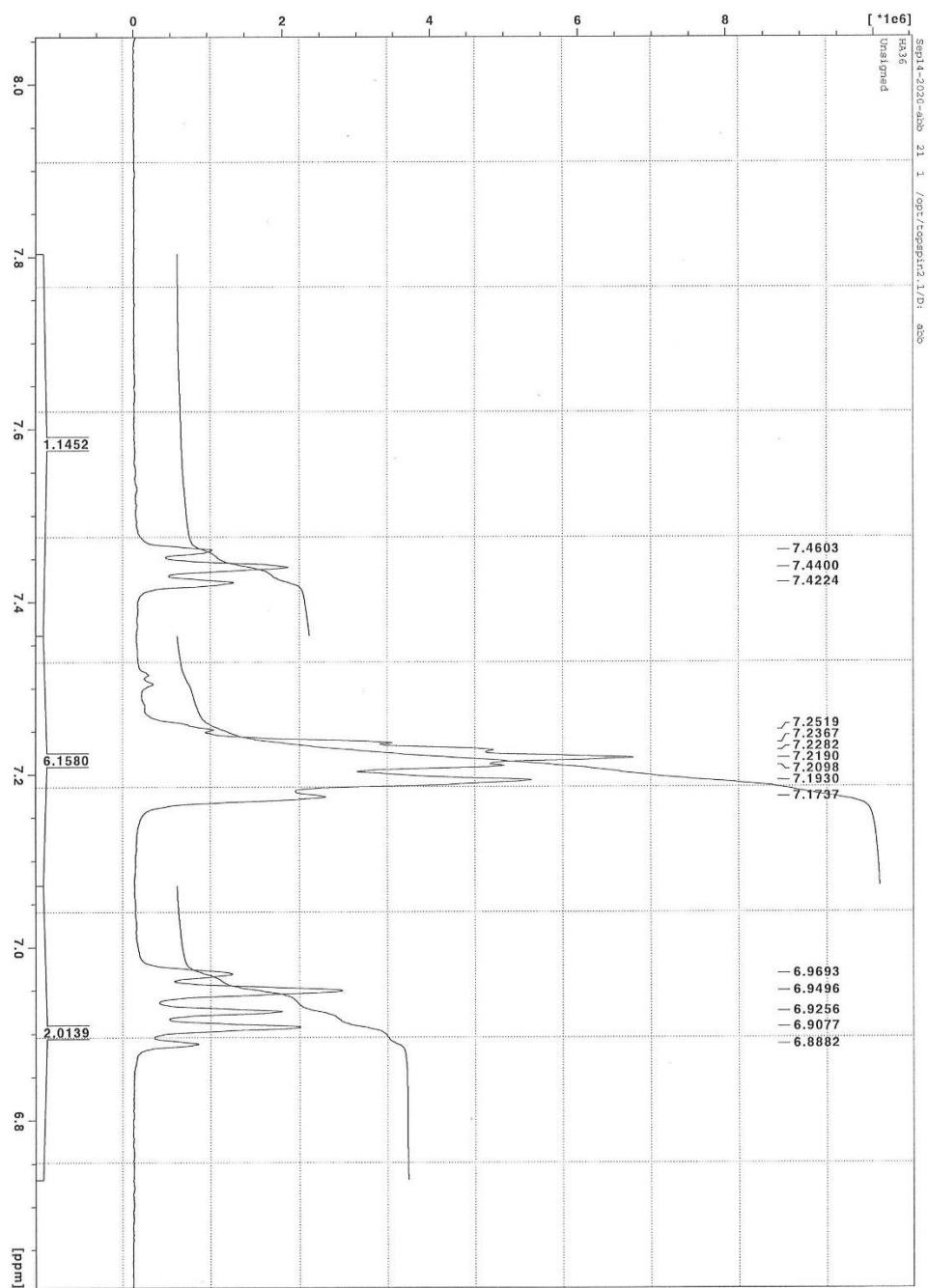
“Synthesis and identification of new *N,N*-disubstituted thiourea and thiazolidinone scaffolds based on quinolone moiety as urease inhibitors”

### Contents

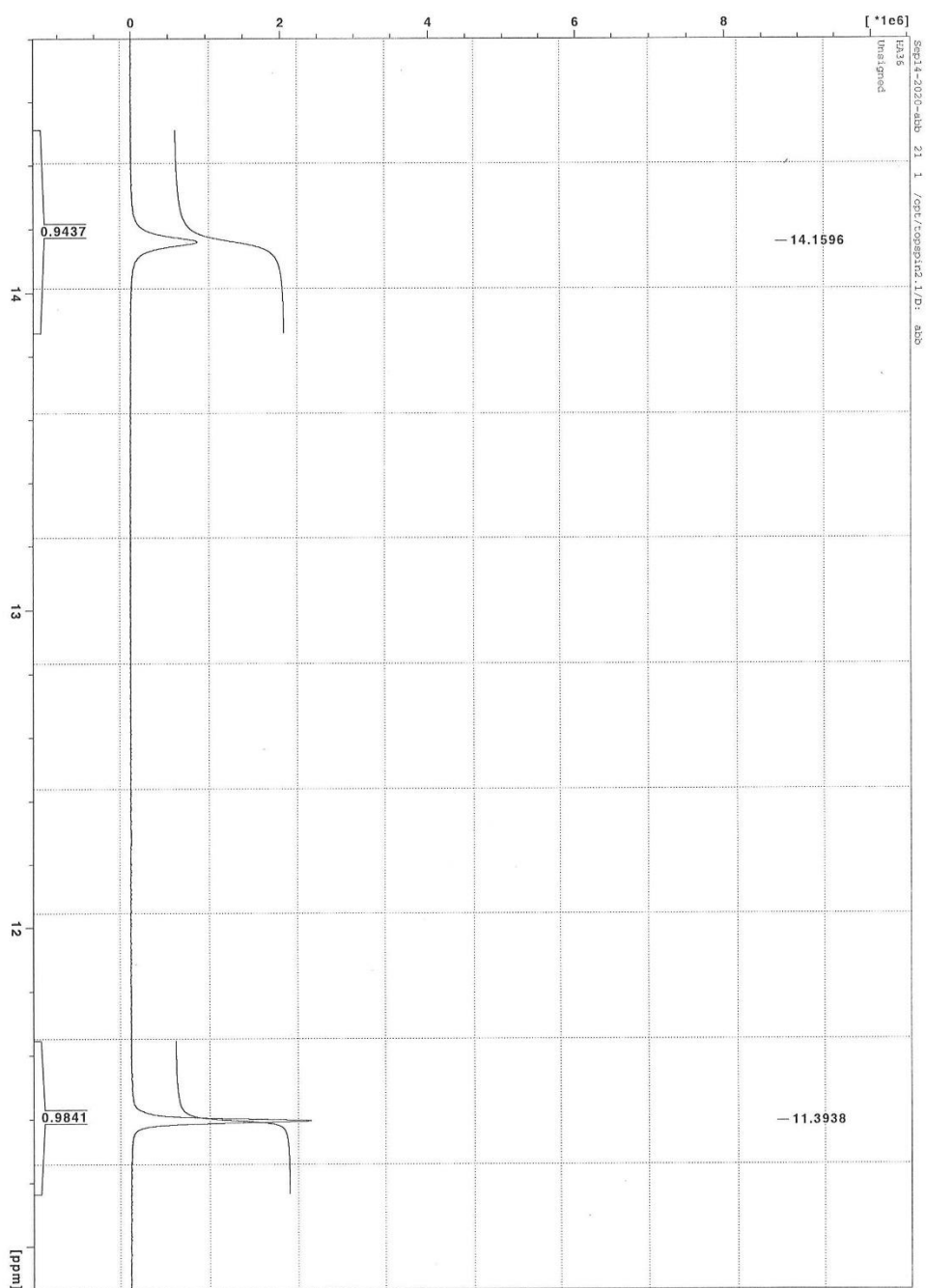
|                    |                 |
|--------------------|-----------------|
| Compound <b>5g</b> | <b>S1-S19</b>   |
| Compound <b>7b</b> | <b>S20-S39</b>  |
| Compound <b>7a</b> | <b>S40-S57</b>  |
| Compound <b>7c</b> | <b>S58-S75</b>  |
| Compound <b>7d</b> | <b>S76-S92</b>  |
| Compound <b>7e</b> | <b>S93-S116</b> |



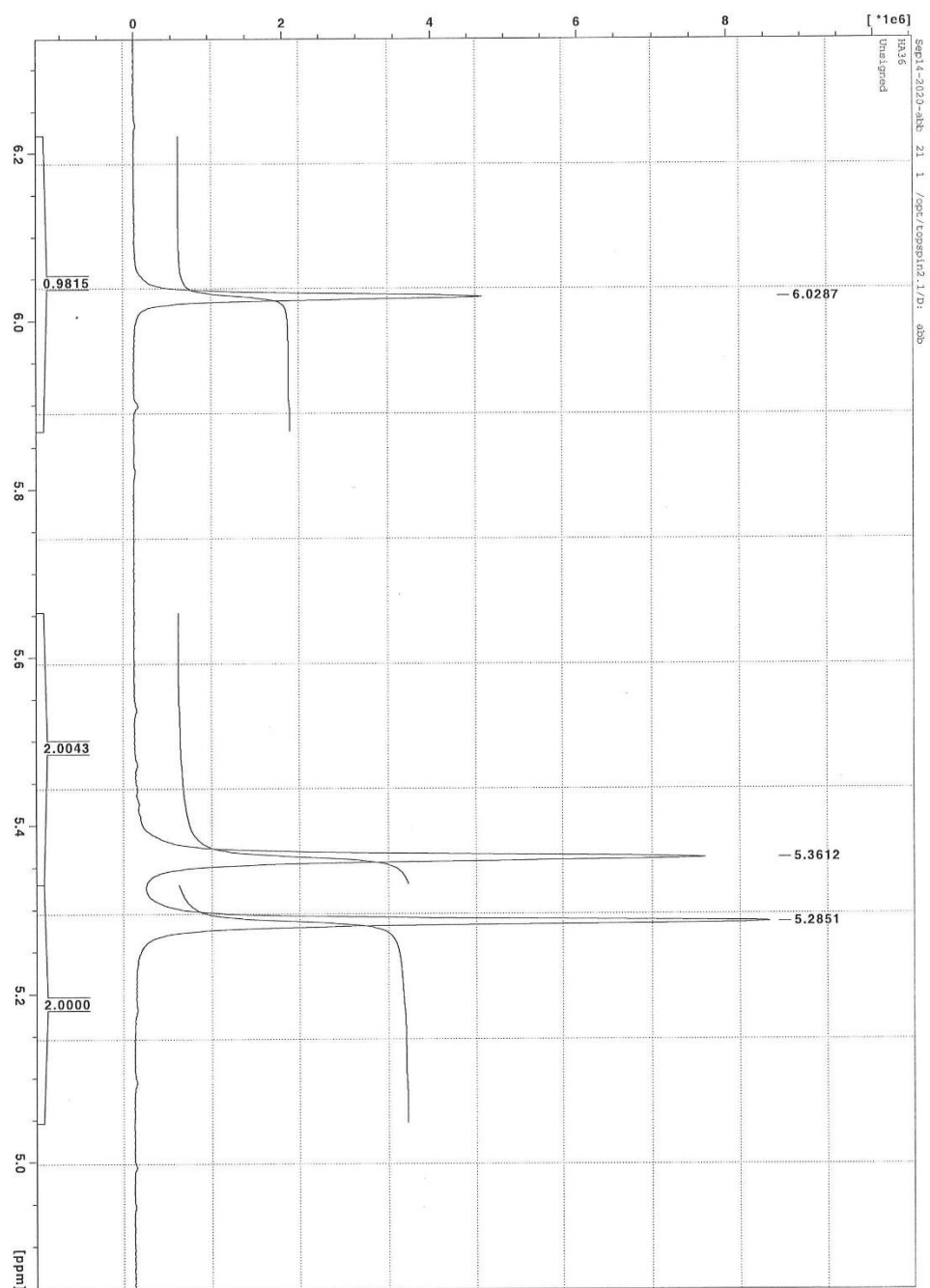
**Figure S1.** <sup>1</sup>H NMR spectrum of compound **5g** (400 MHz, DMSO-d<sub>6</sub>).



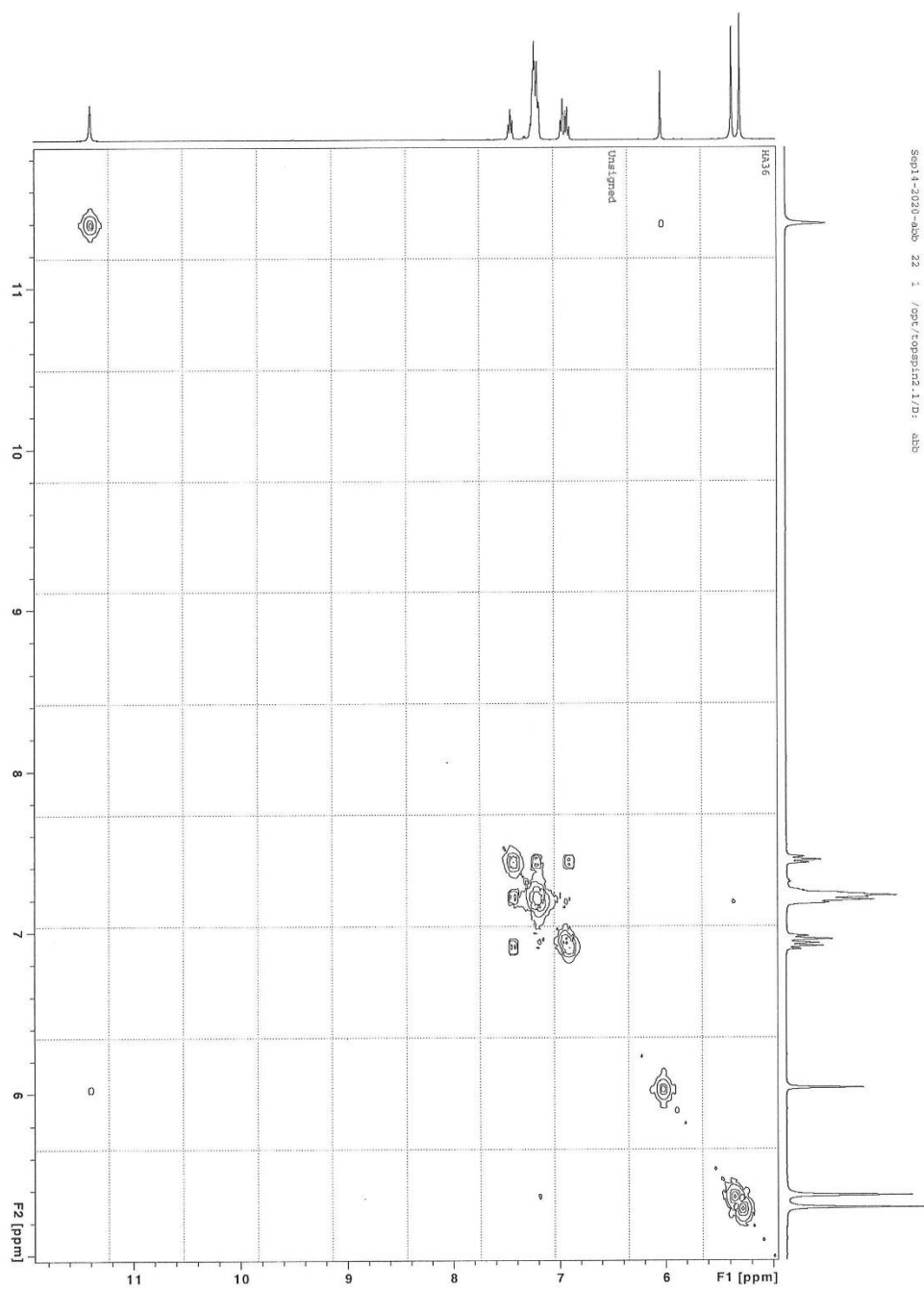
**Figure S2.** Detail of  $^1\text{H}$  NMR spectrum of compound **5g**.

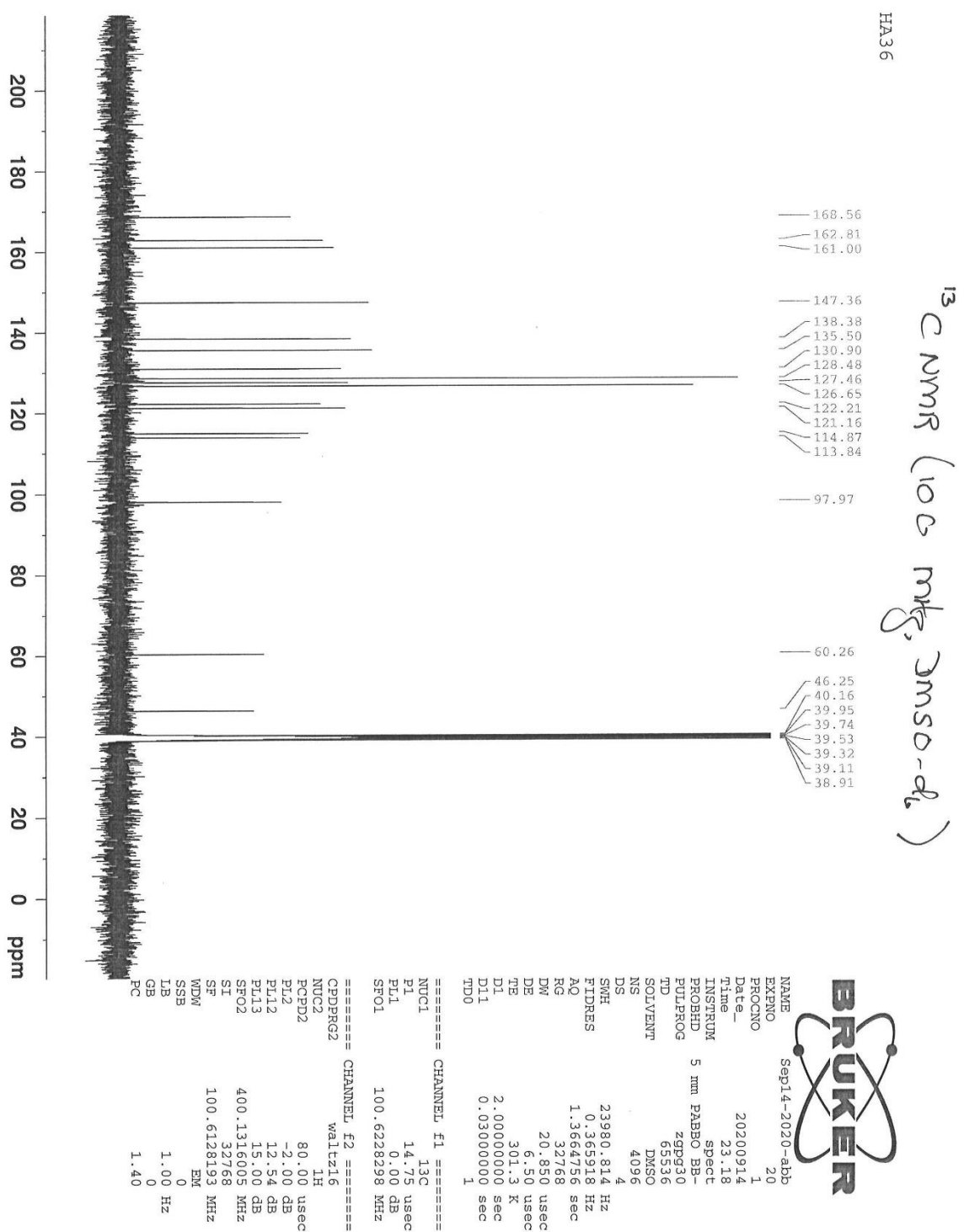


**Figure S3.** Detail of  $^1\text{H}$  NMR spectrum of compound **5g**.

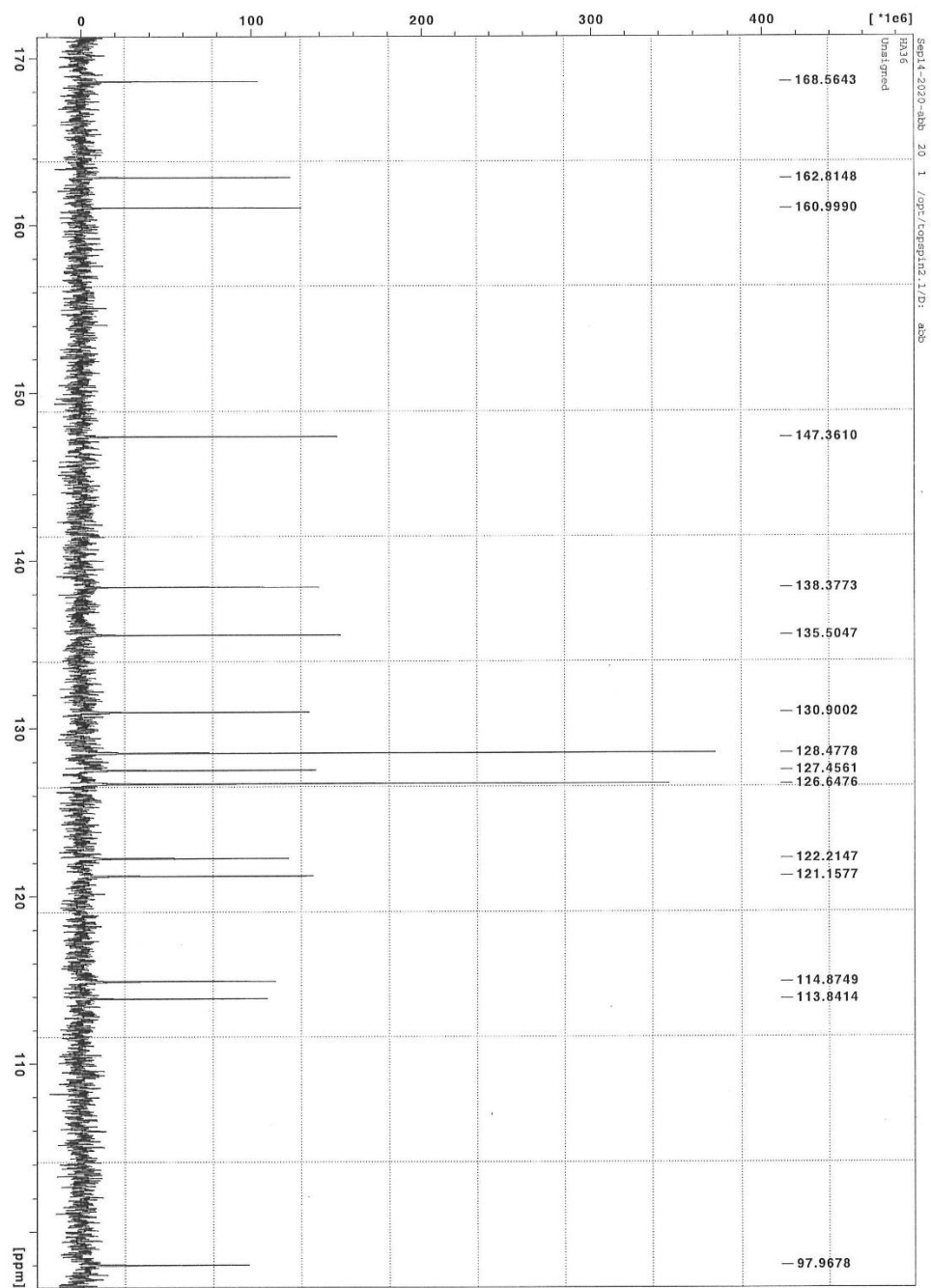


**Figure S4.** Detail of  $^1\text{H}$  spectrum of compound **5g**.

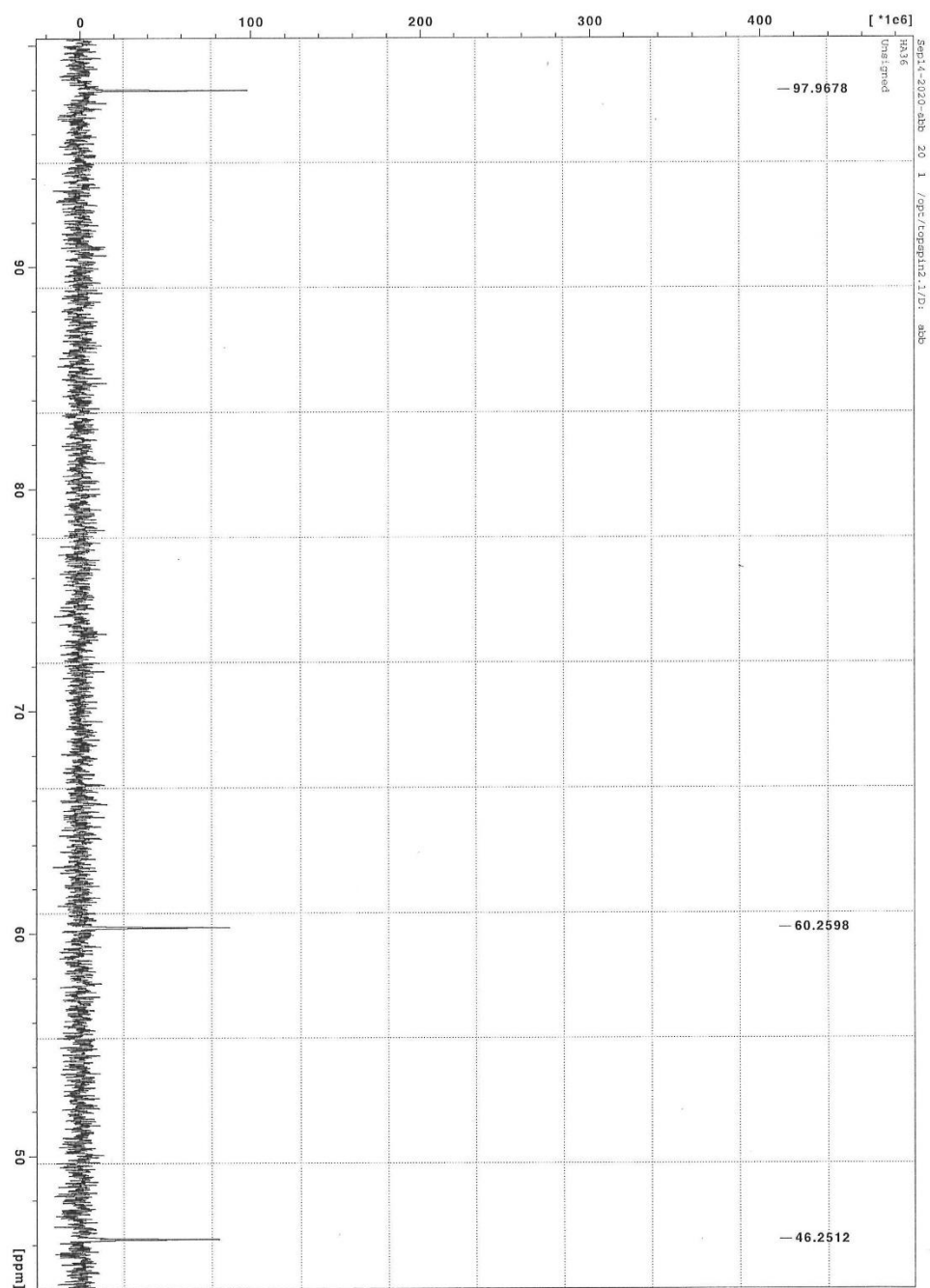




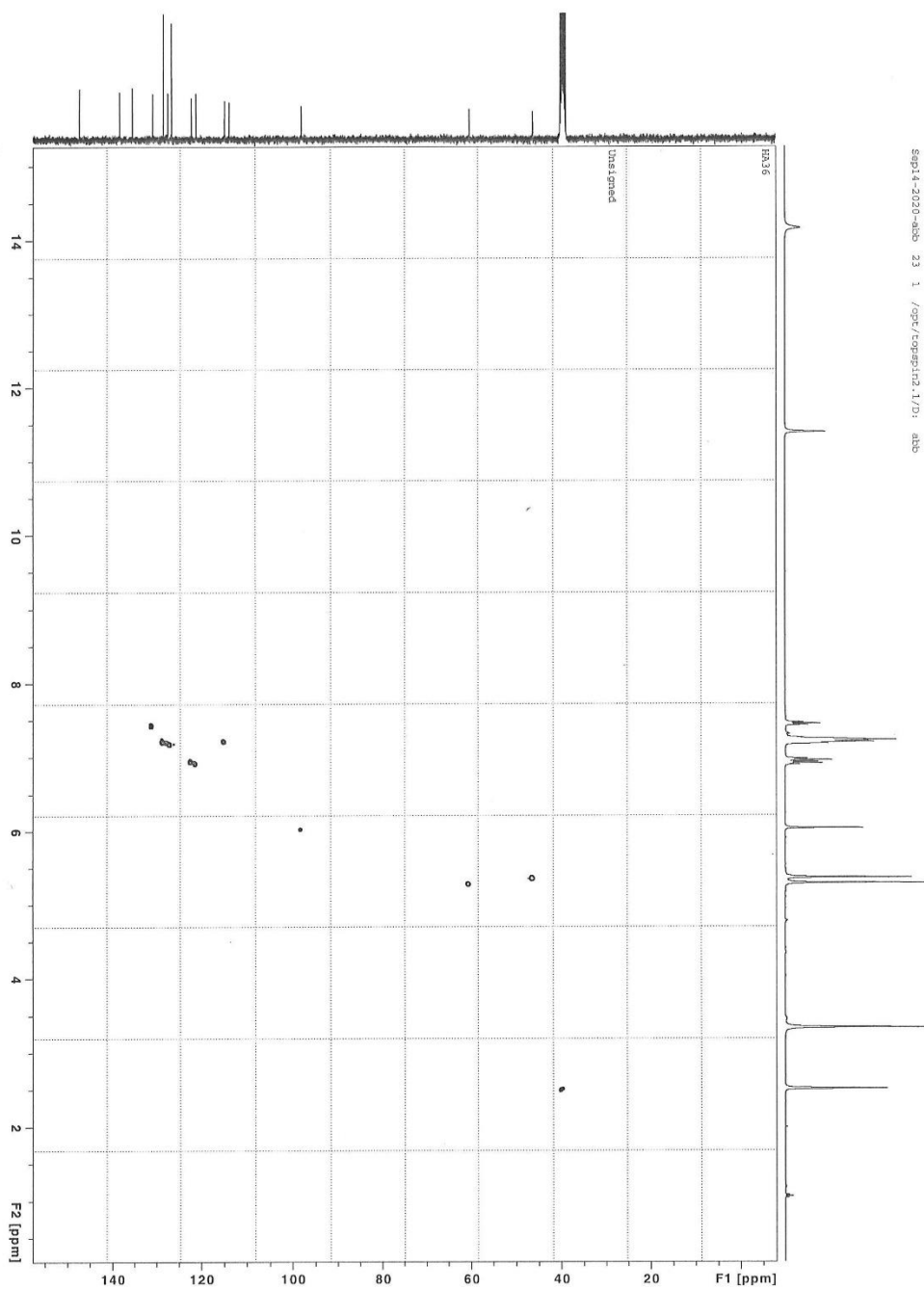
**Figure S6.** <sup>13</sup>C NMR spectrum of compound **5g** (100 MHz, DMSO-*d*<sub>6</sub>).



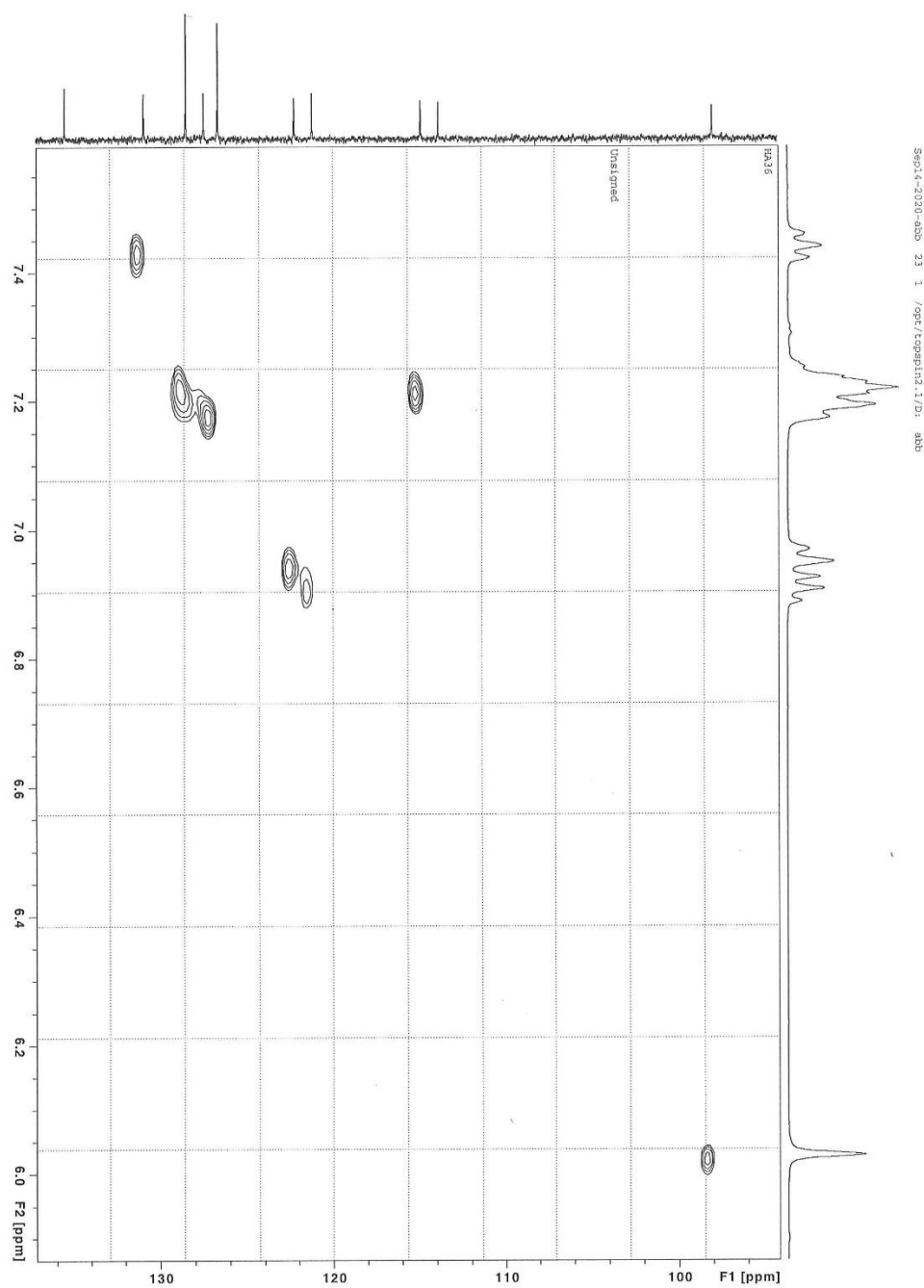
**Figure S7.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **5g**.



**Figure S8.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **5g**.

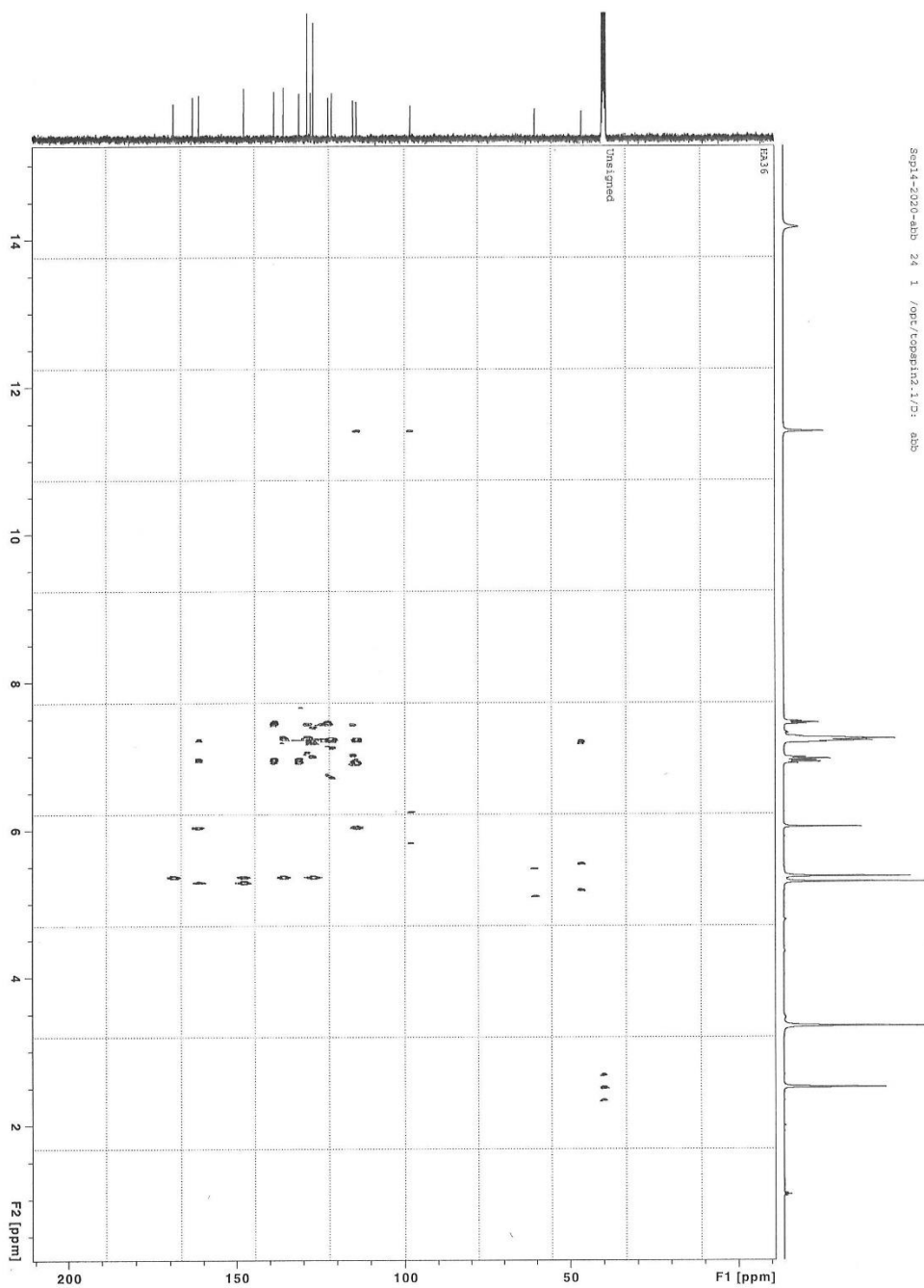


**Figure S9.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7a**.

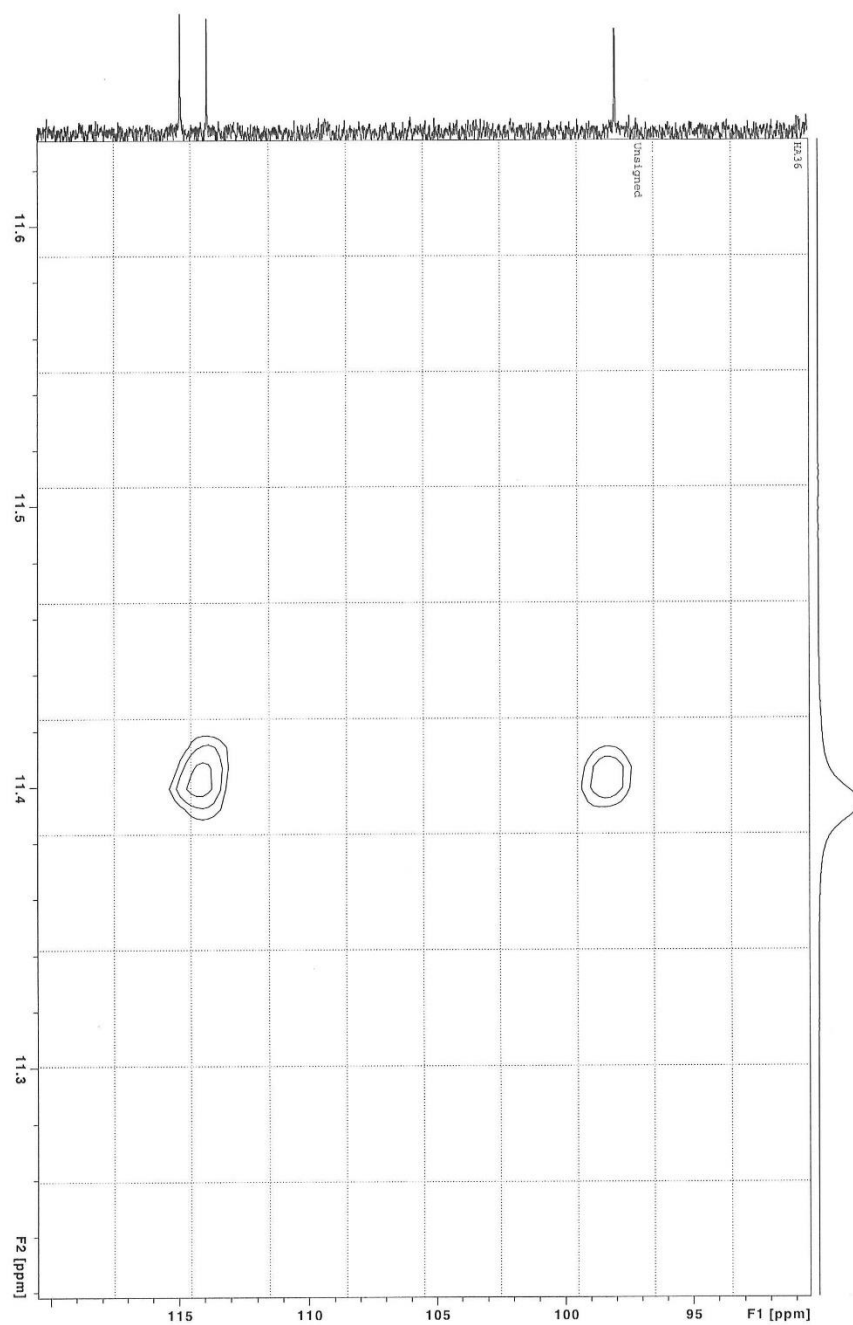


**Figure S10.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **5g**.

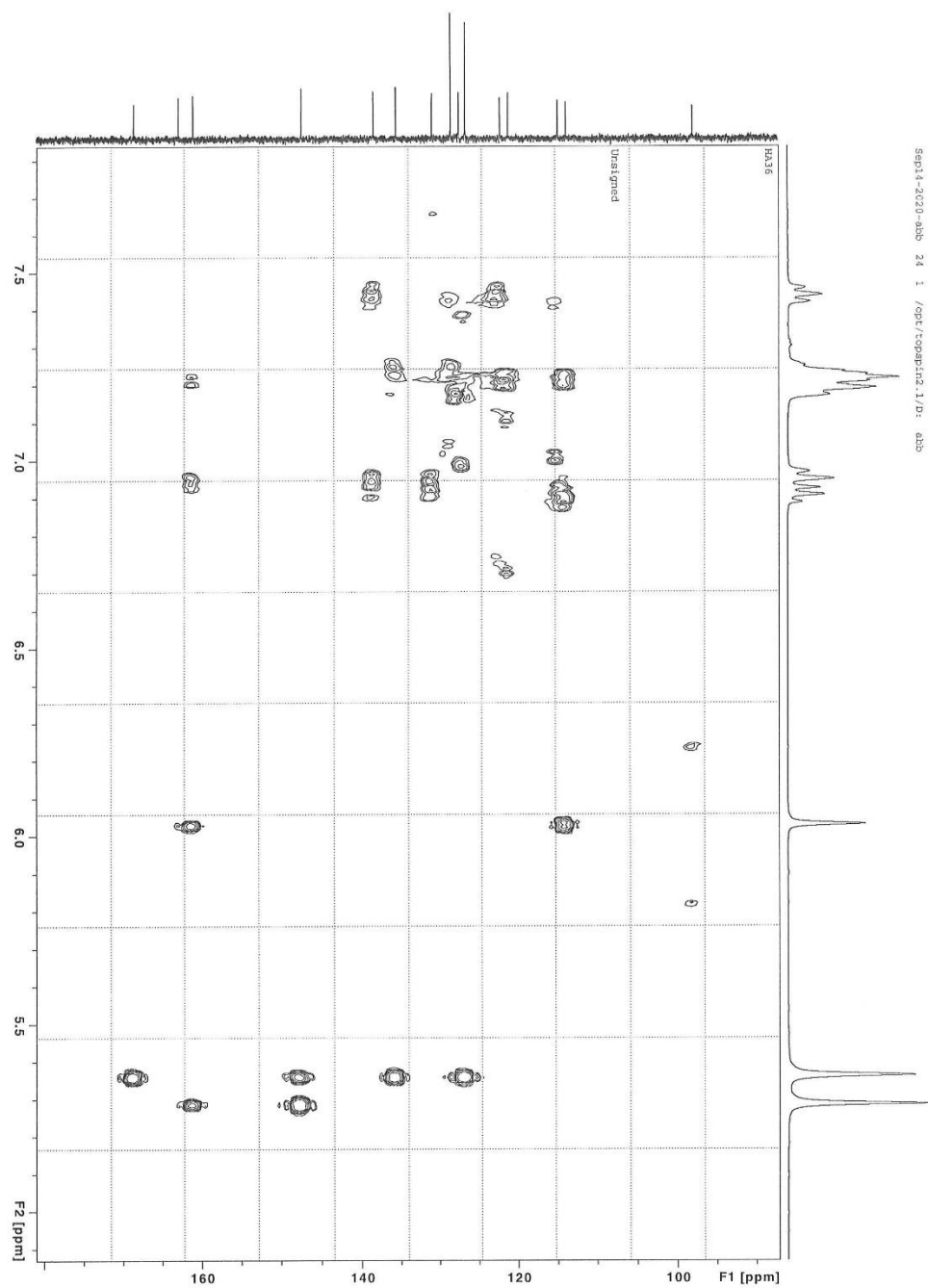




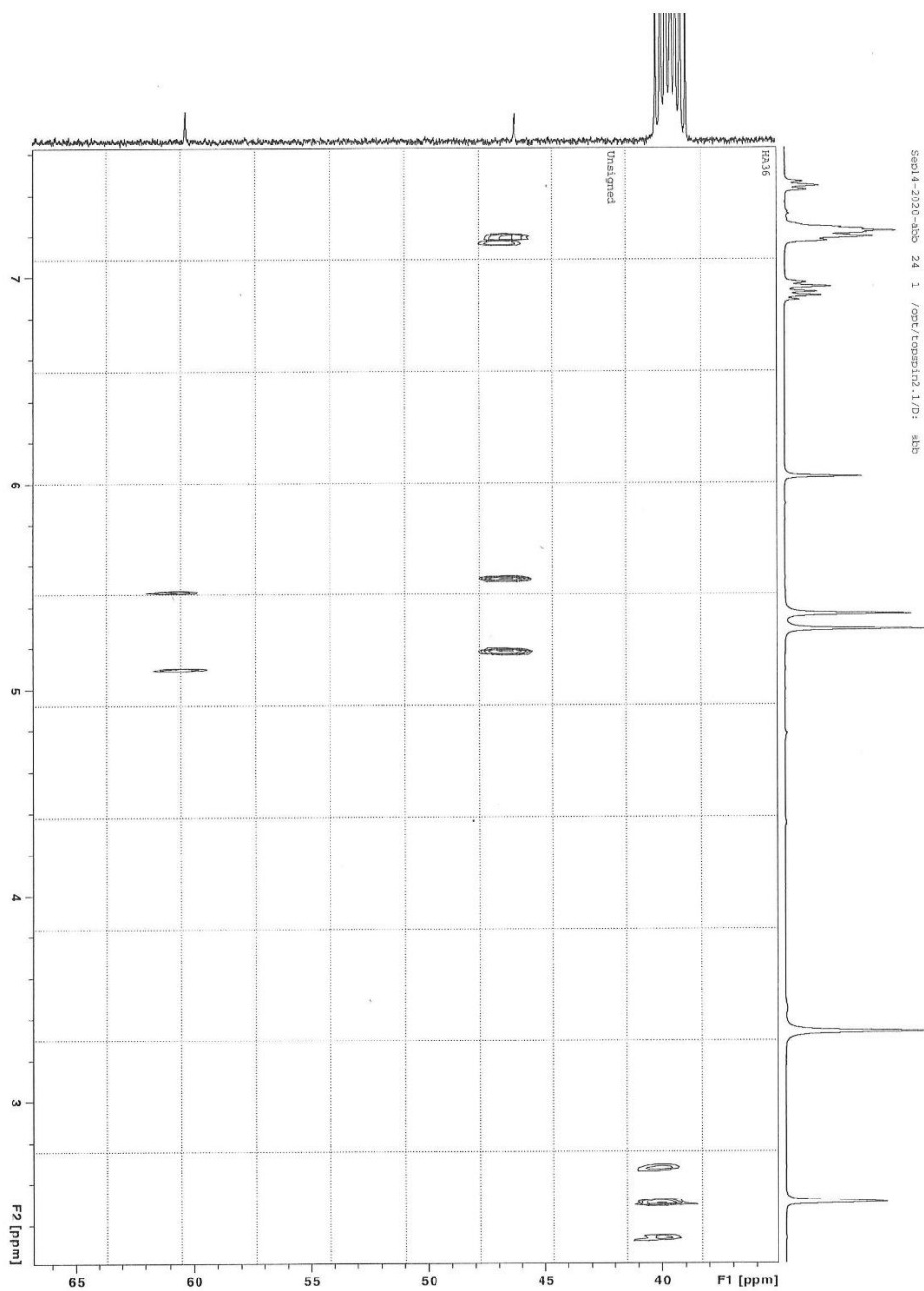
**Figure S12.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **5g**.



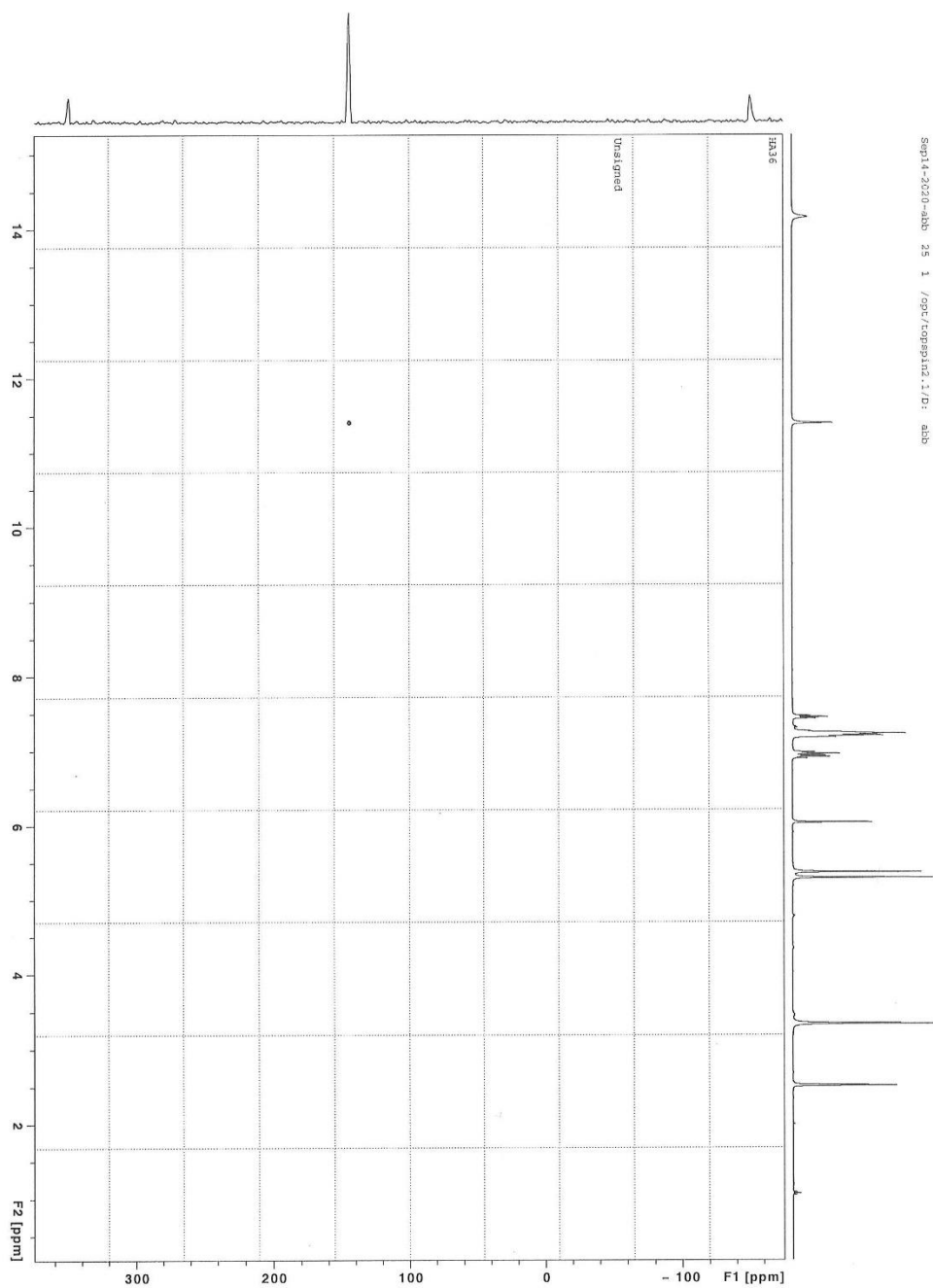
**Figure S13.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **5g**,



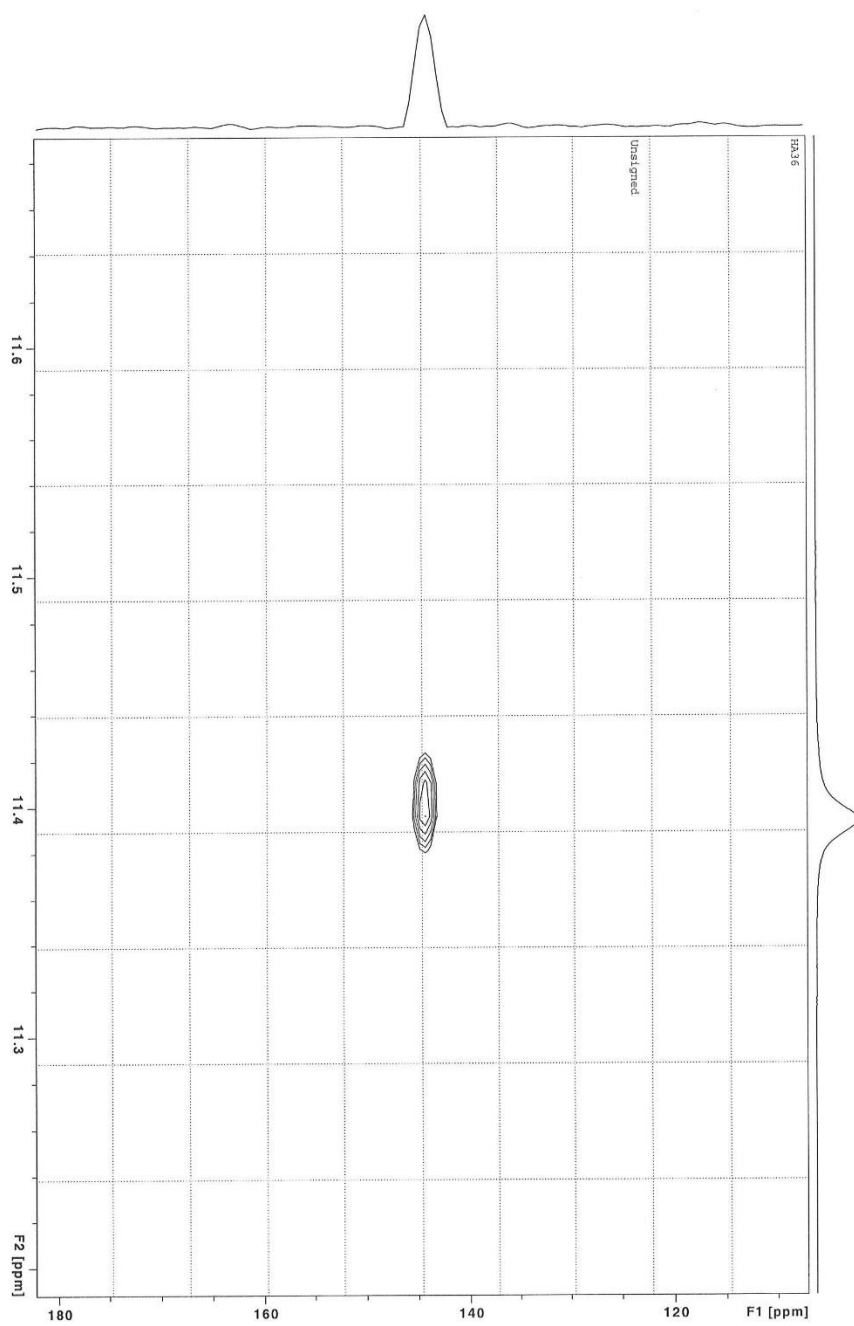
**Figure S14.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **5g**.



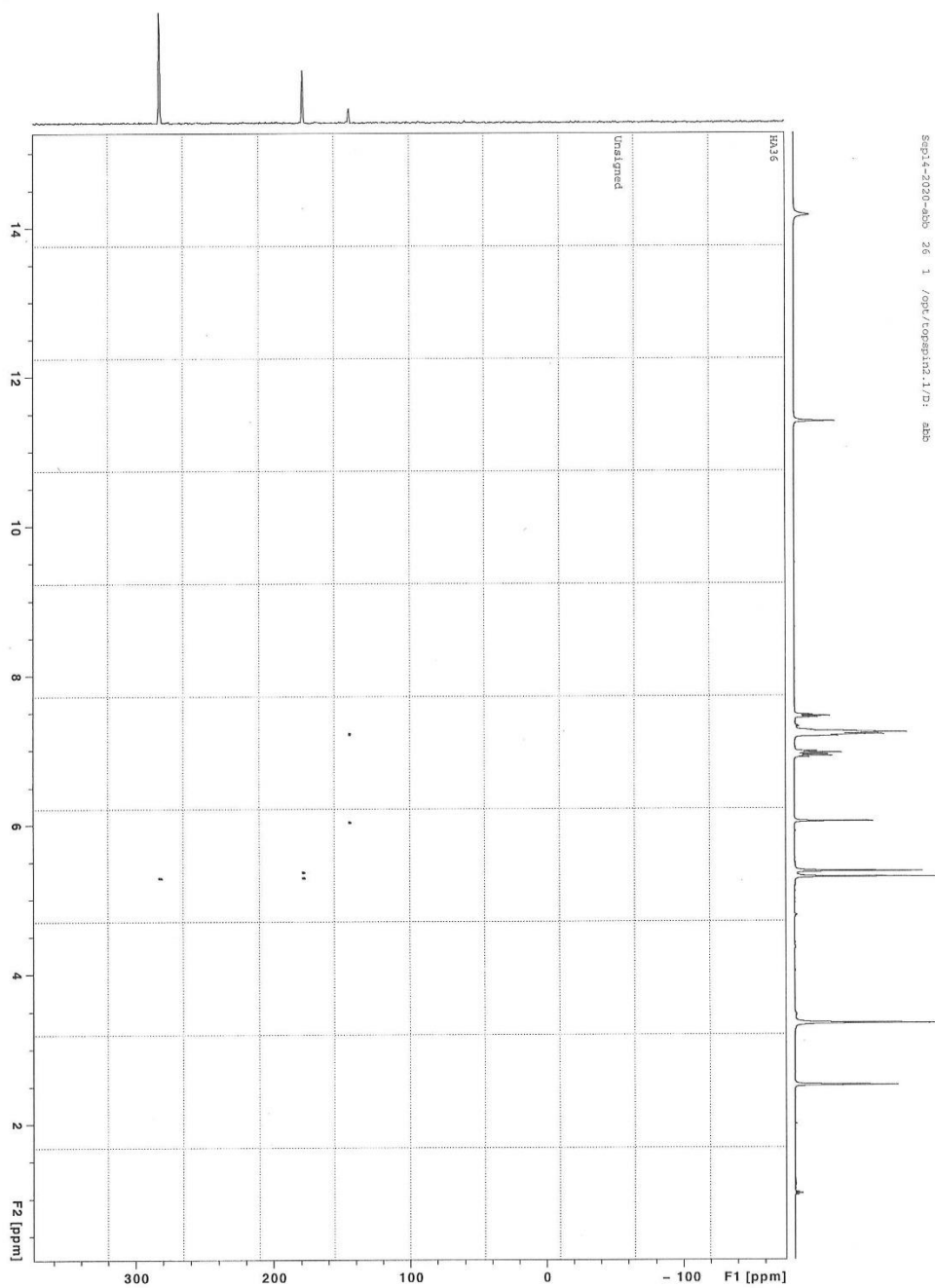
**Figure S15.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **5g**.



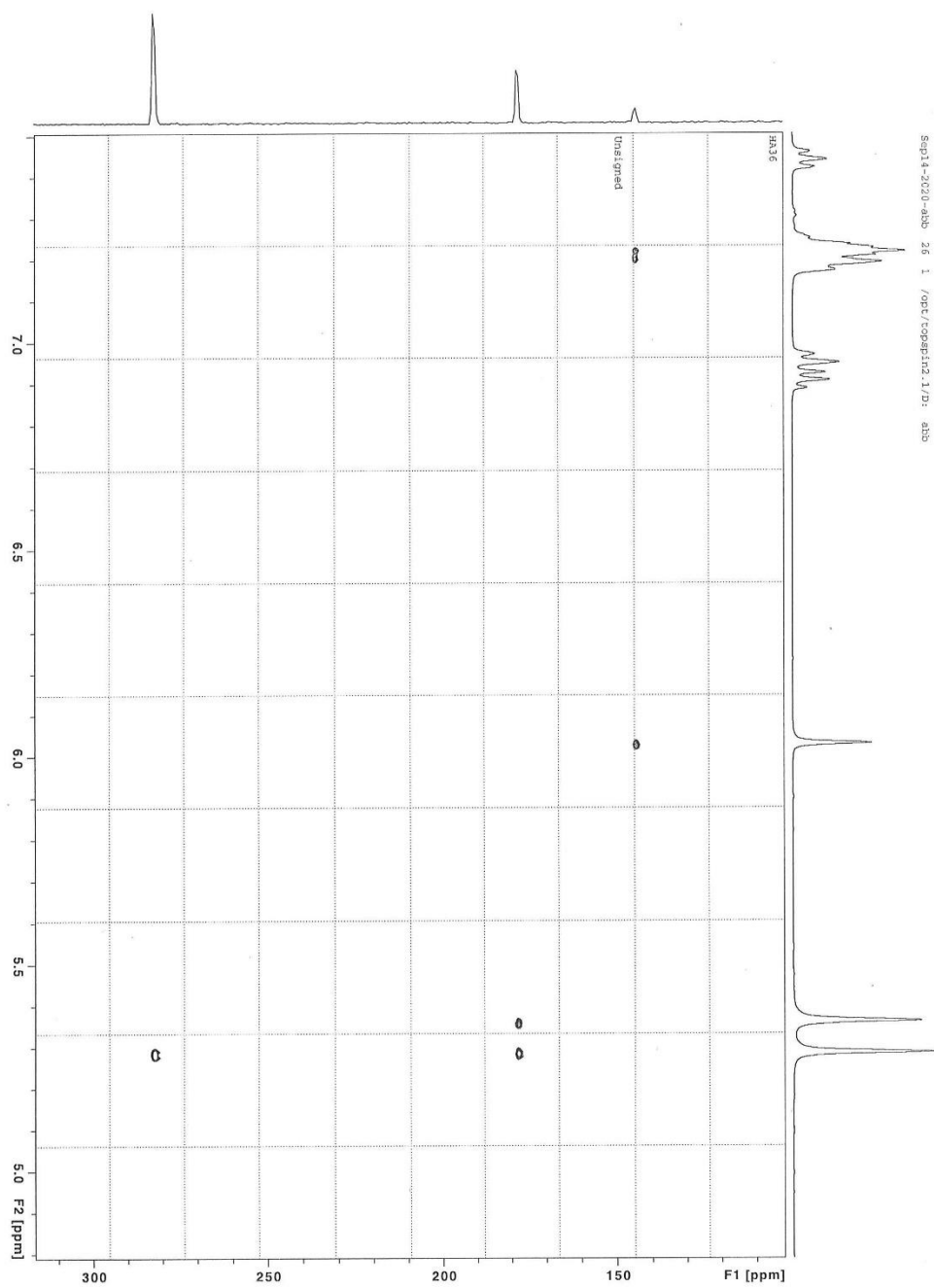
**Figure S16.**  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **5g**.



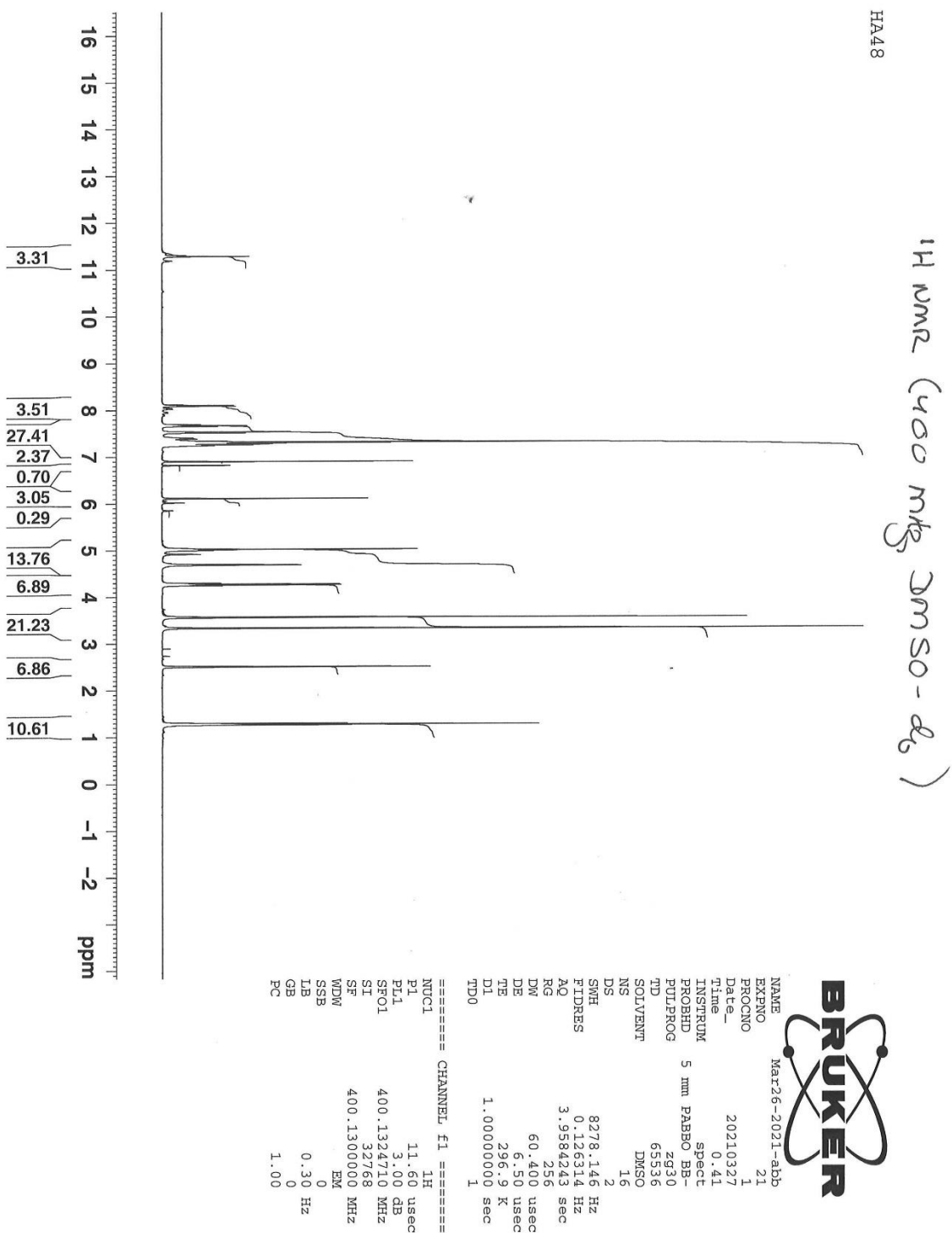
**Figure S17.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **5g**.



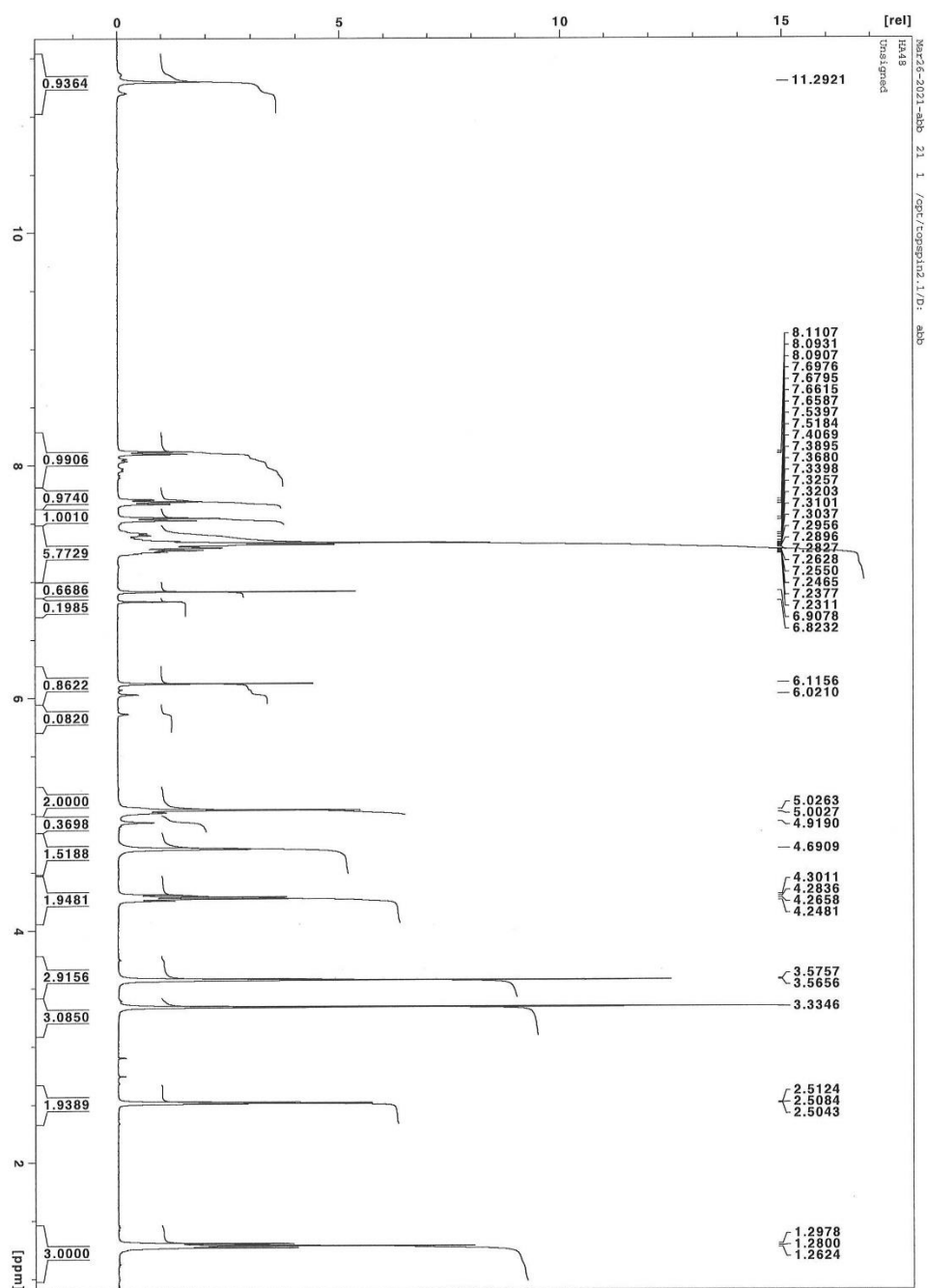
**Figure S18.**  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **5g**.



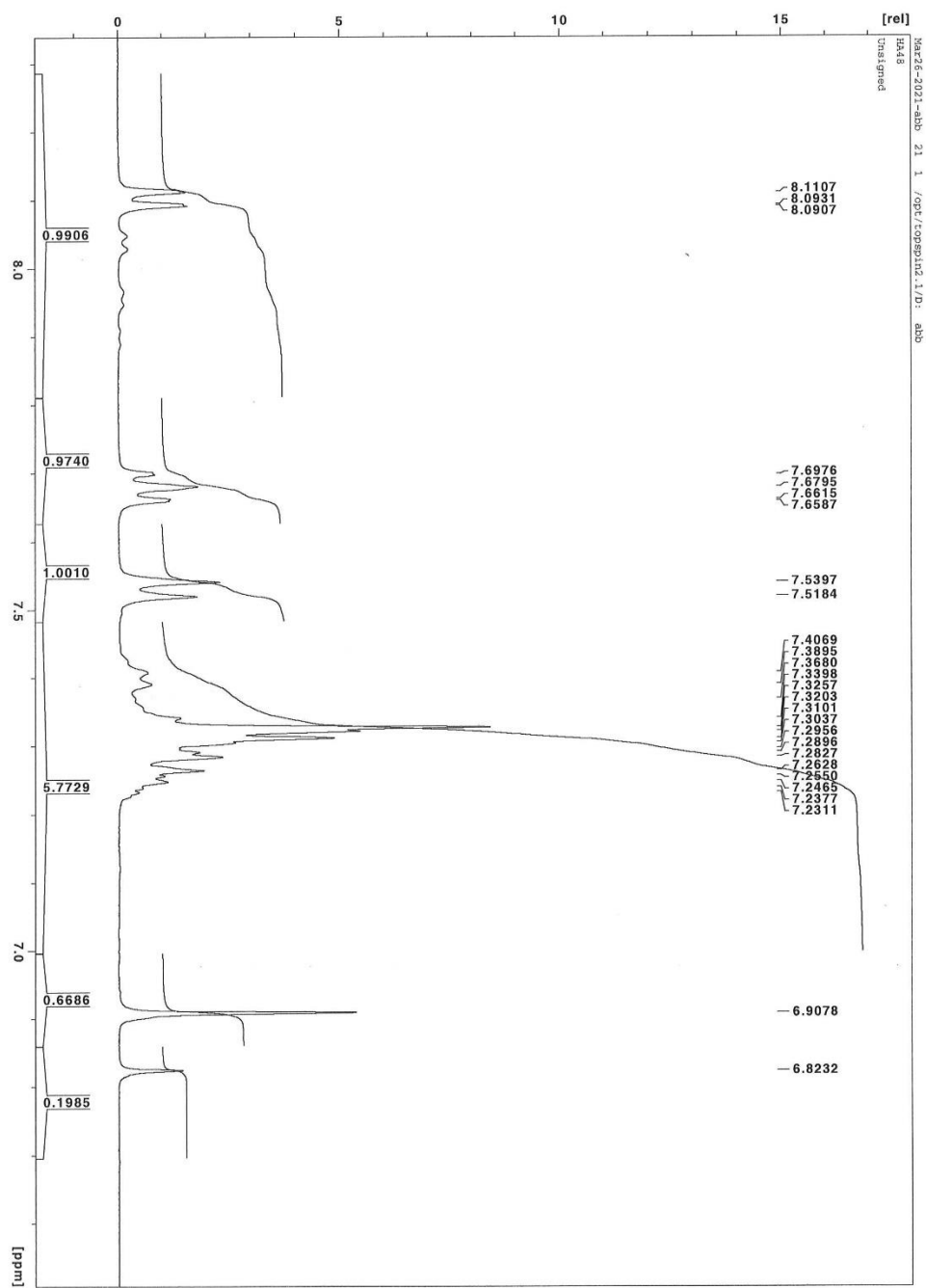
**Figure S19.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **5g**.



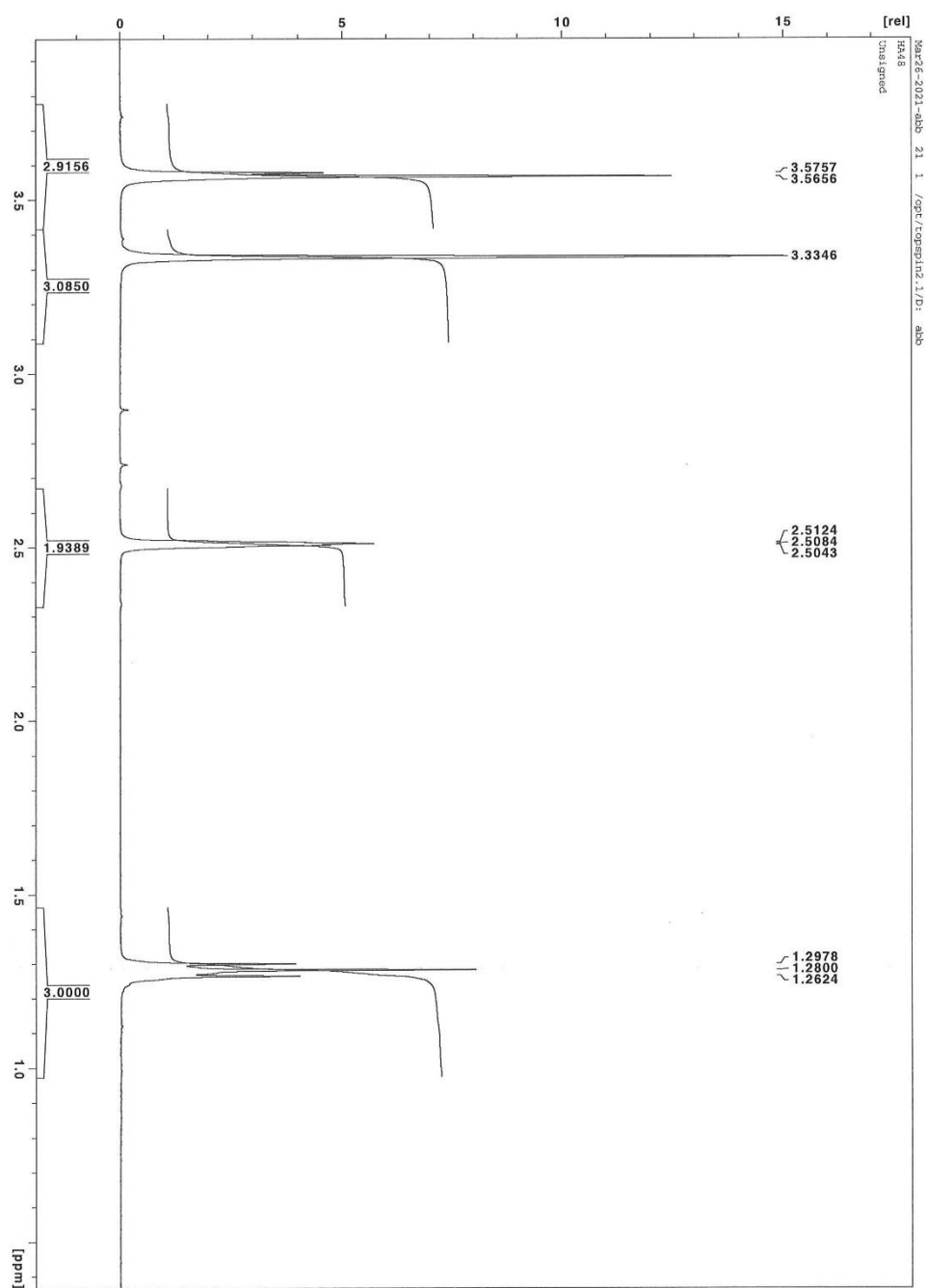
**Figure S20.** <sup>1</sup>H NMR spectrum of compound **7b** (400 MHz, DMSO-d<sub>6</sub>).



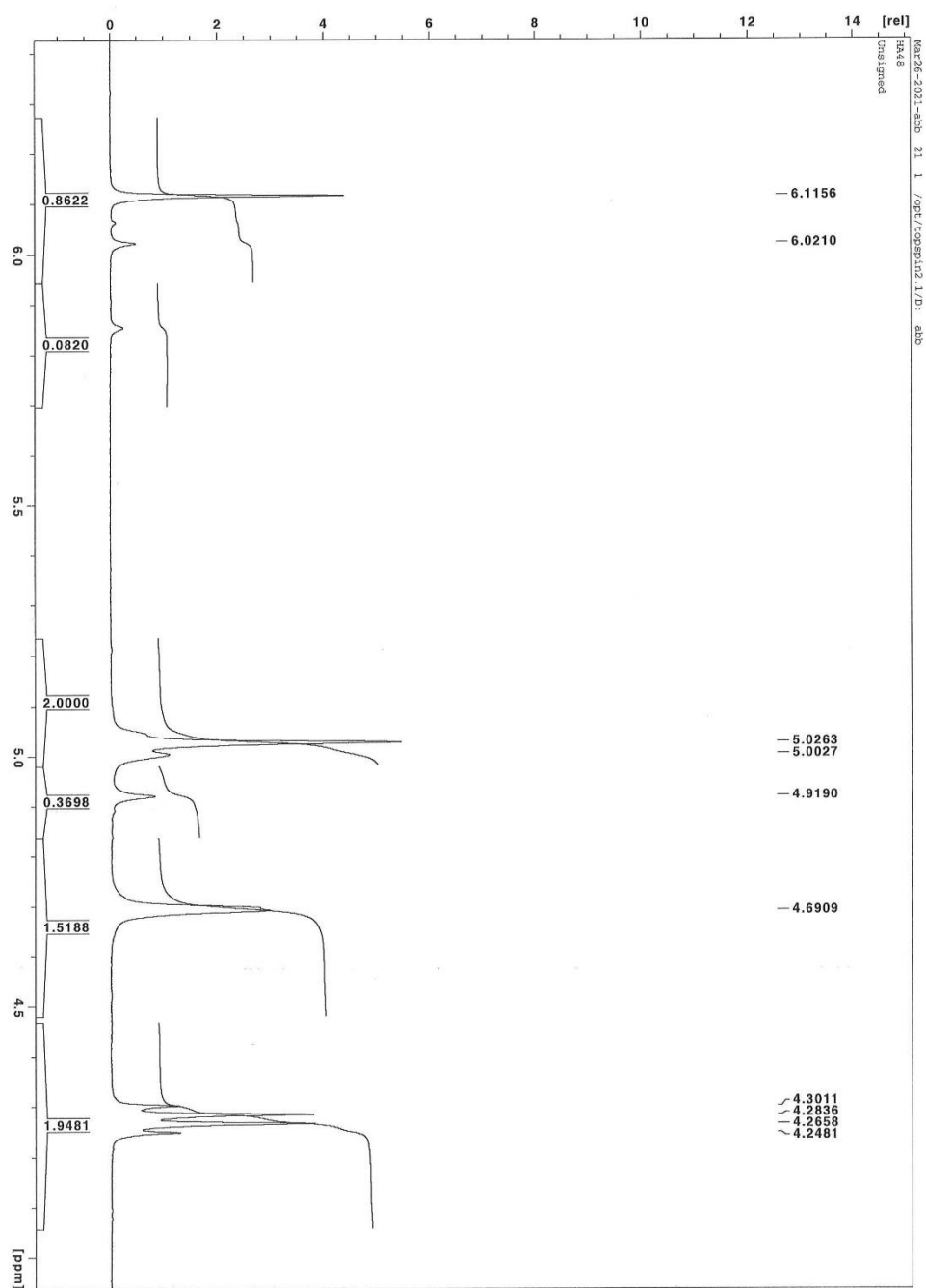
**Figure S21.** Detail of  $^1\text{H}$  NMR spectrum of compound **7b**.



**Figure S22.** Detail of  $^1\text{H}$  NMR spectrum of compound **7b**.



**Figure S23.** Detail of  $^1\text{H}$  NMR spectrum of compound **7b**.



**Figure S24.** Detail of  $^1\text{H}$  NMR spectrum of compound **7b**.

HA48

$^1\text{H}$ - $^1\text{H}$  cosy

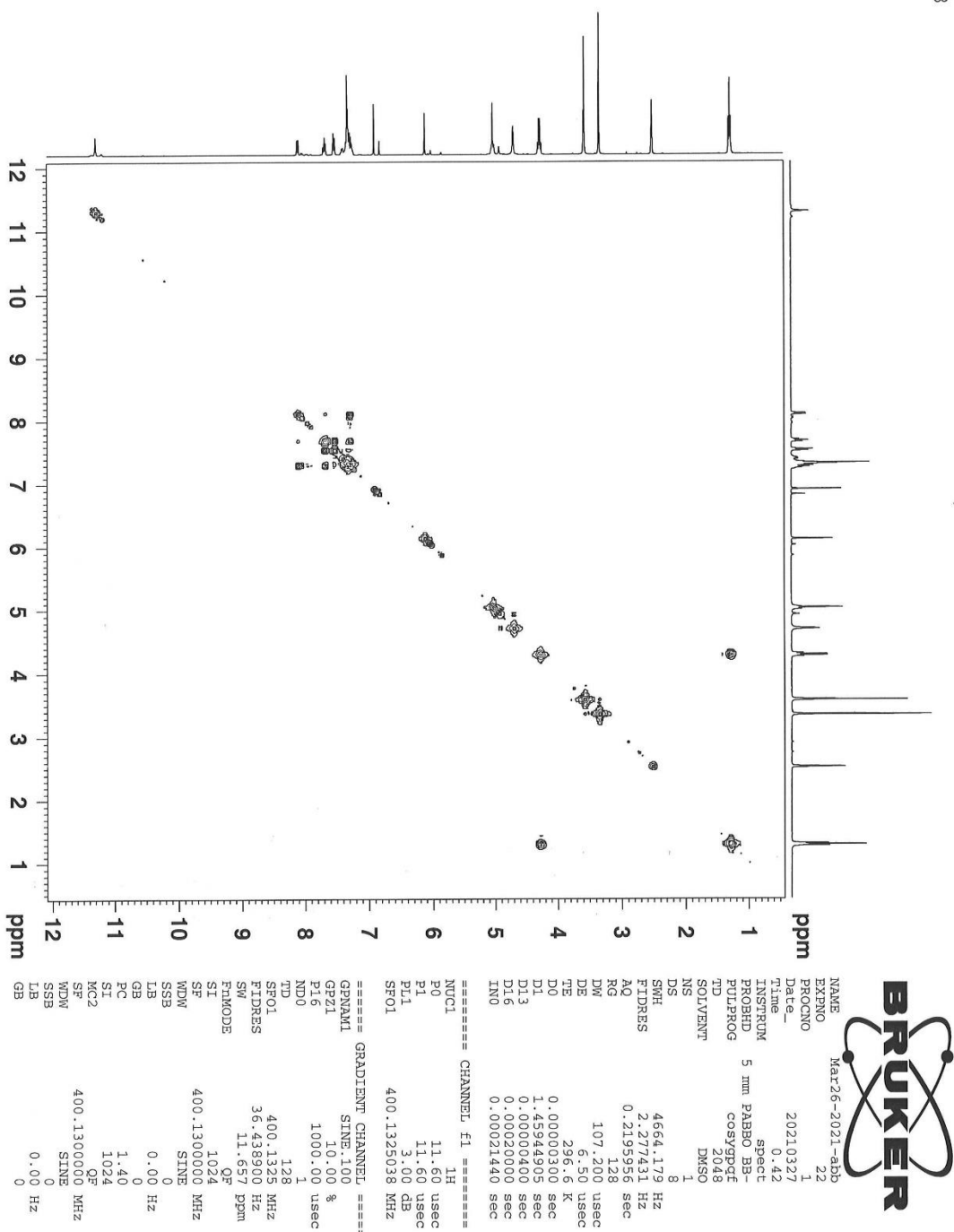
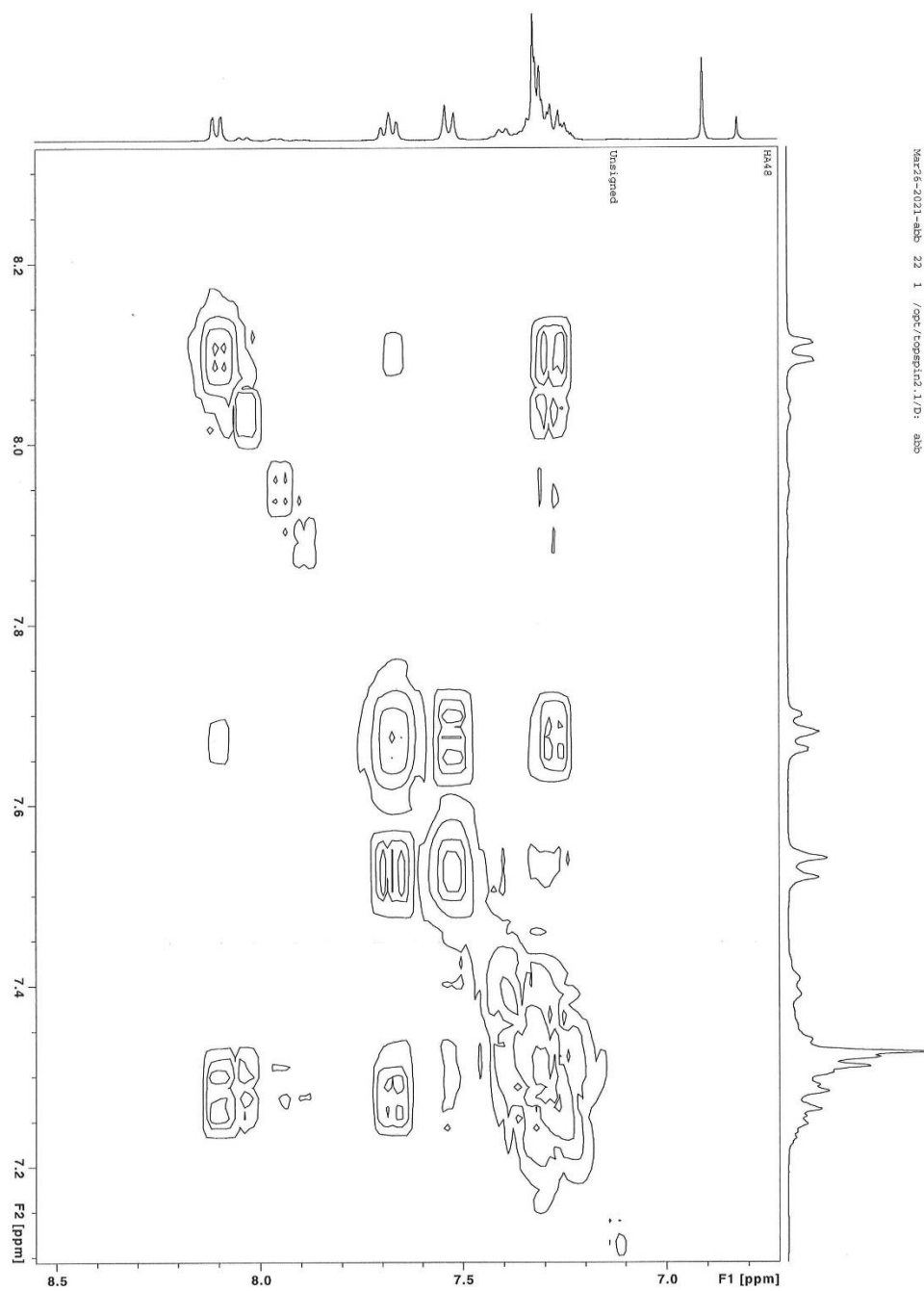
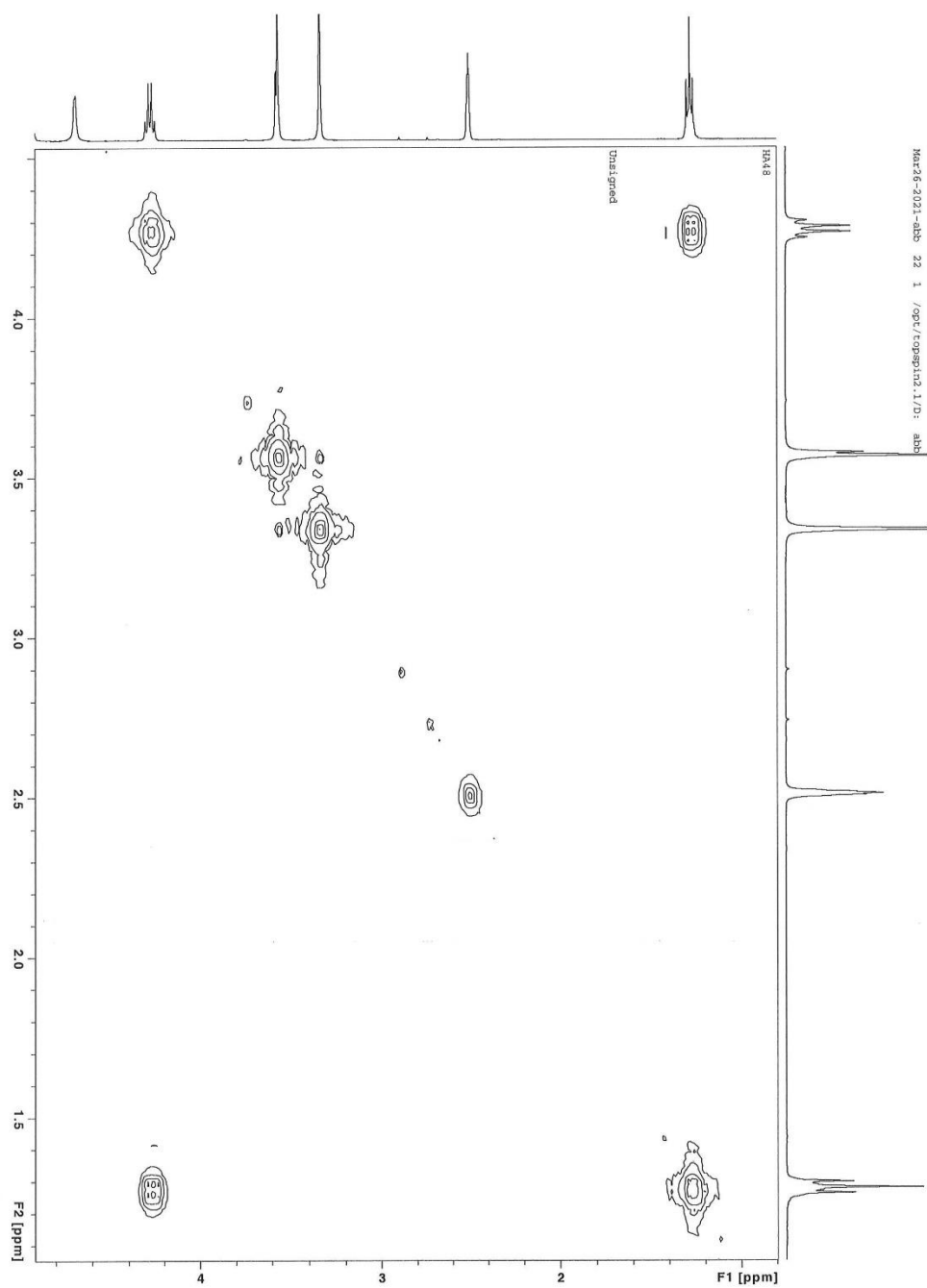


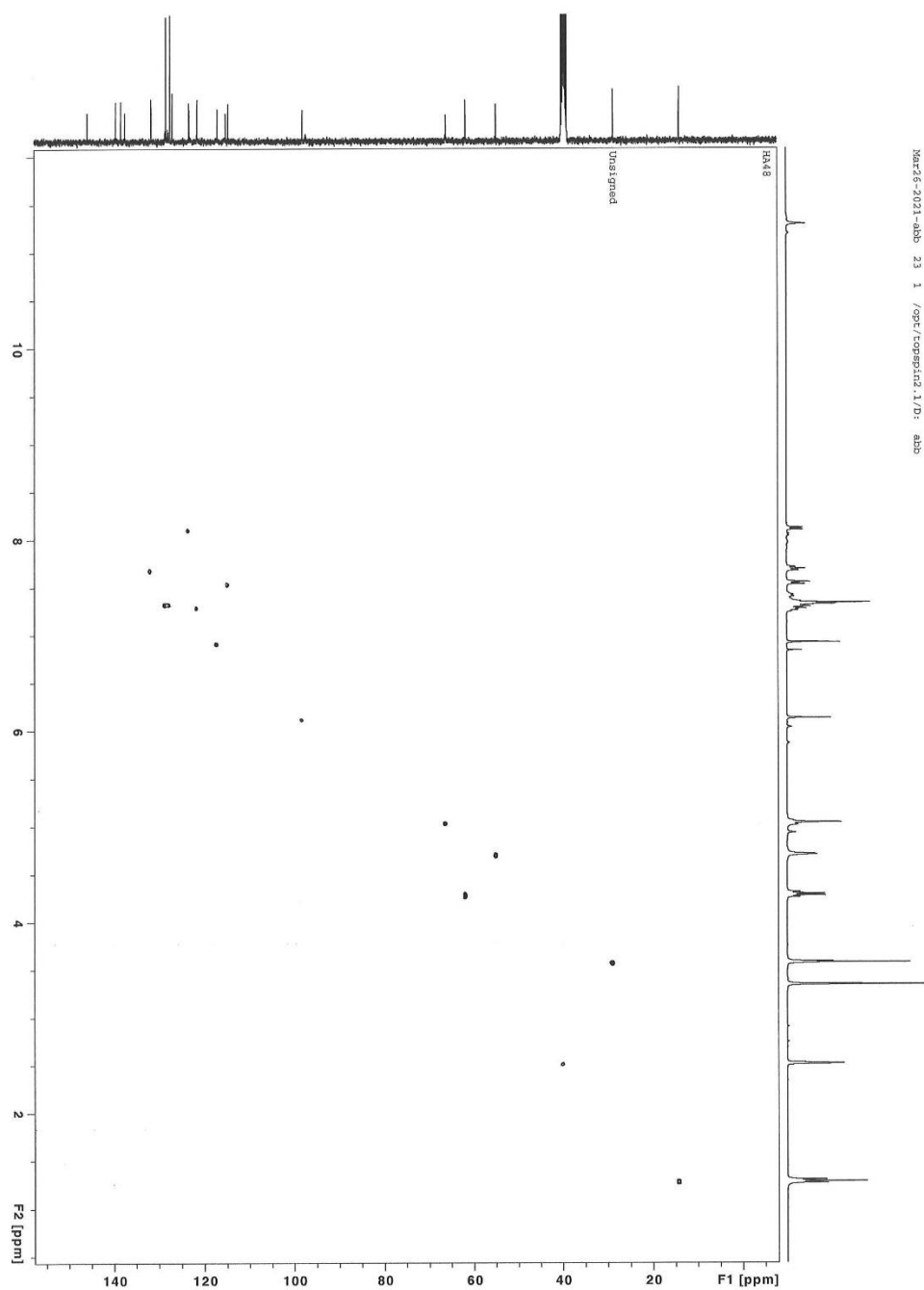
Figure S25.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7b**.



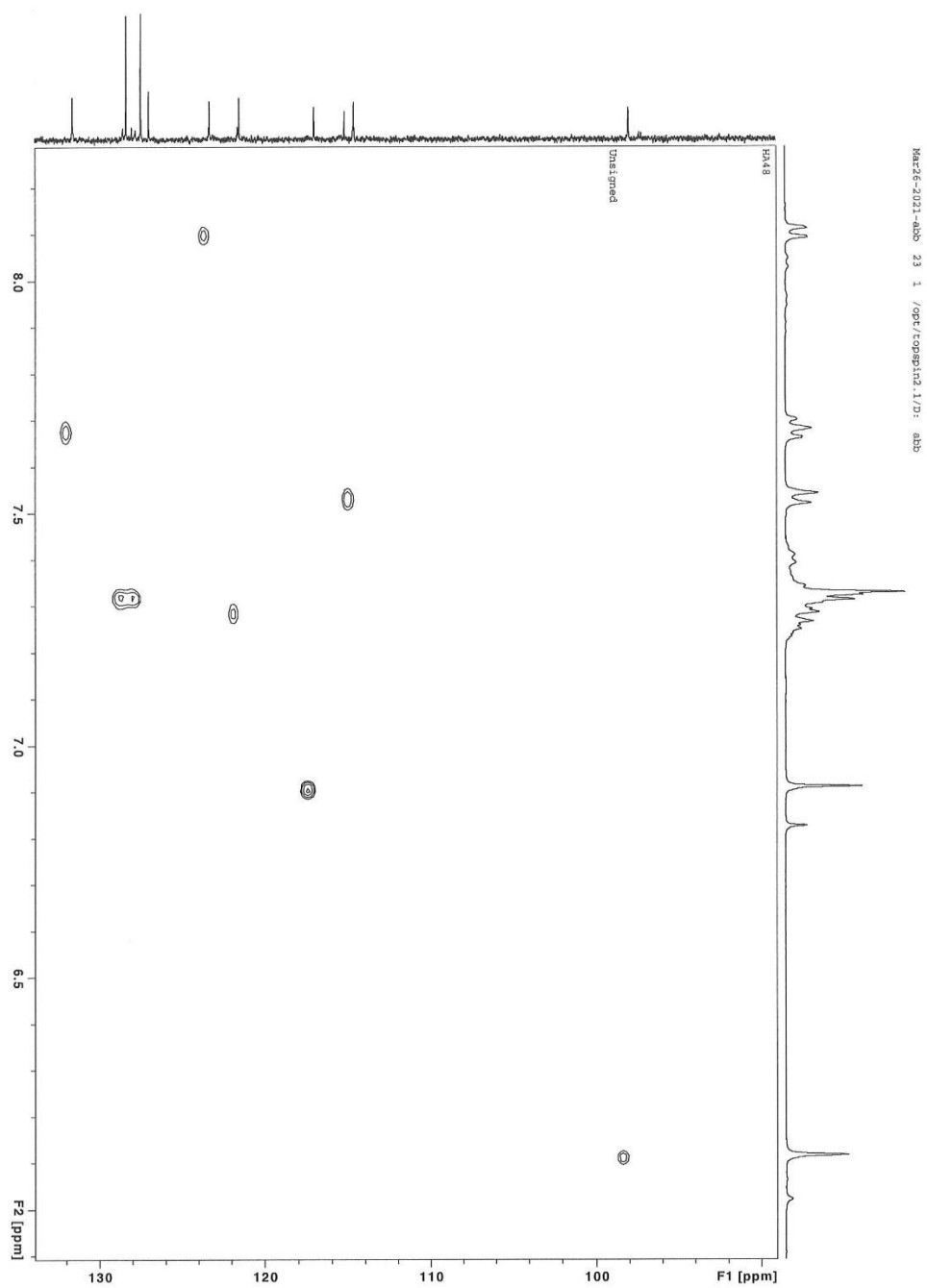
**Figure S26.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7b**.



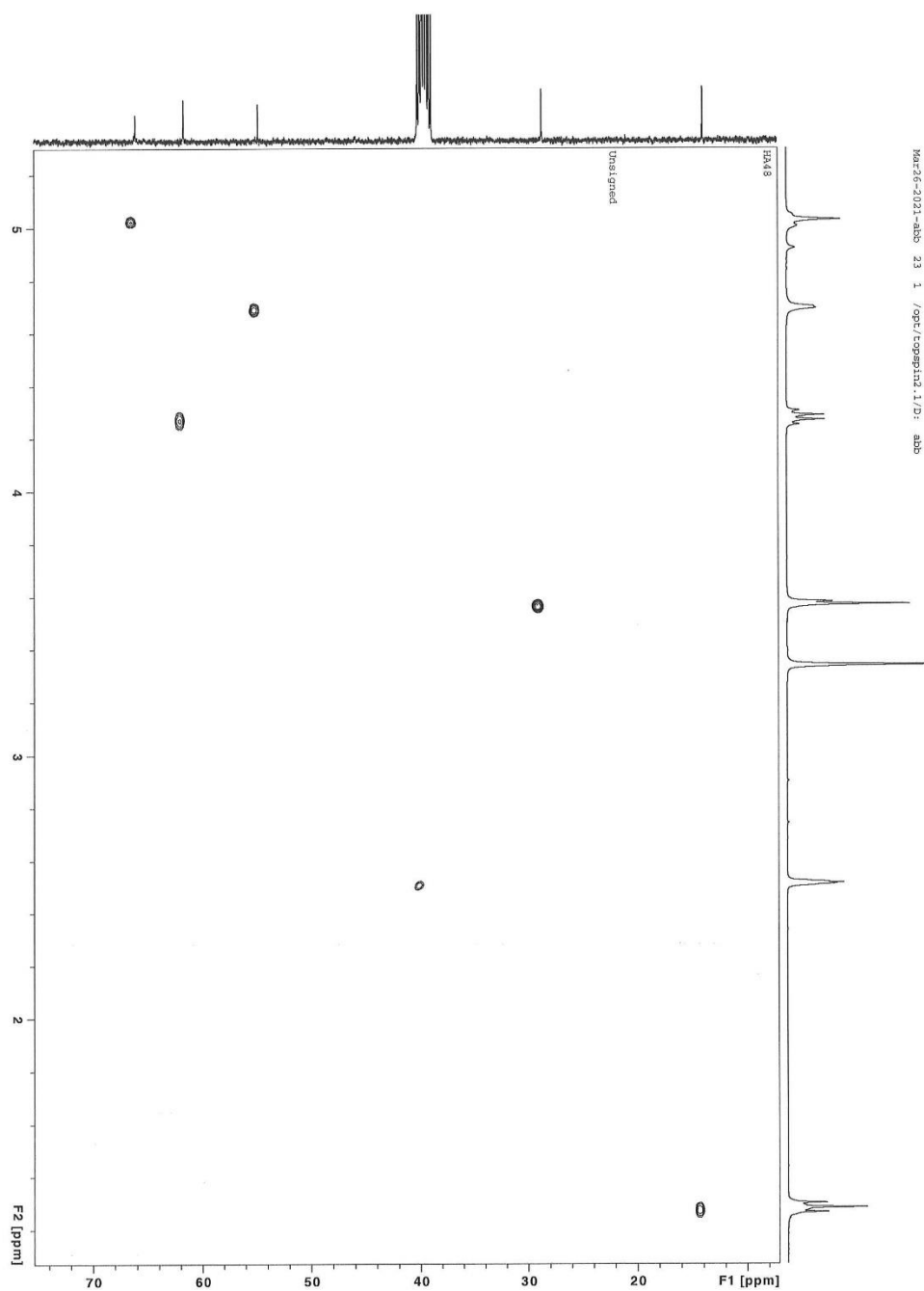
**Figure S27.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7b**.



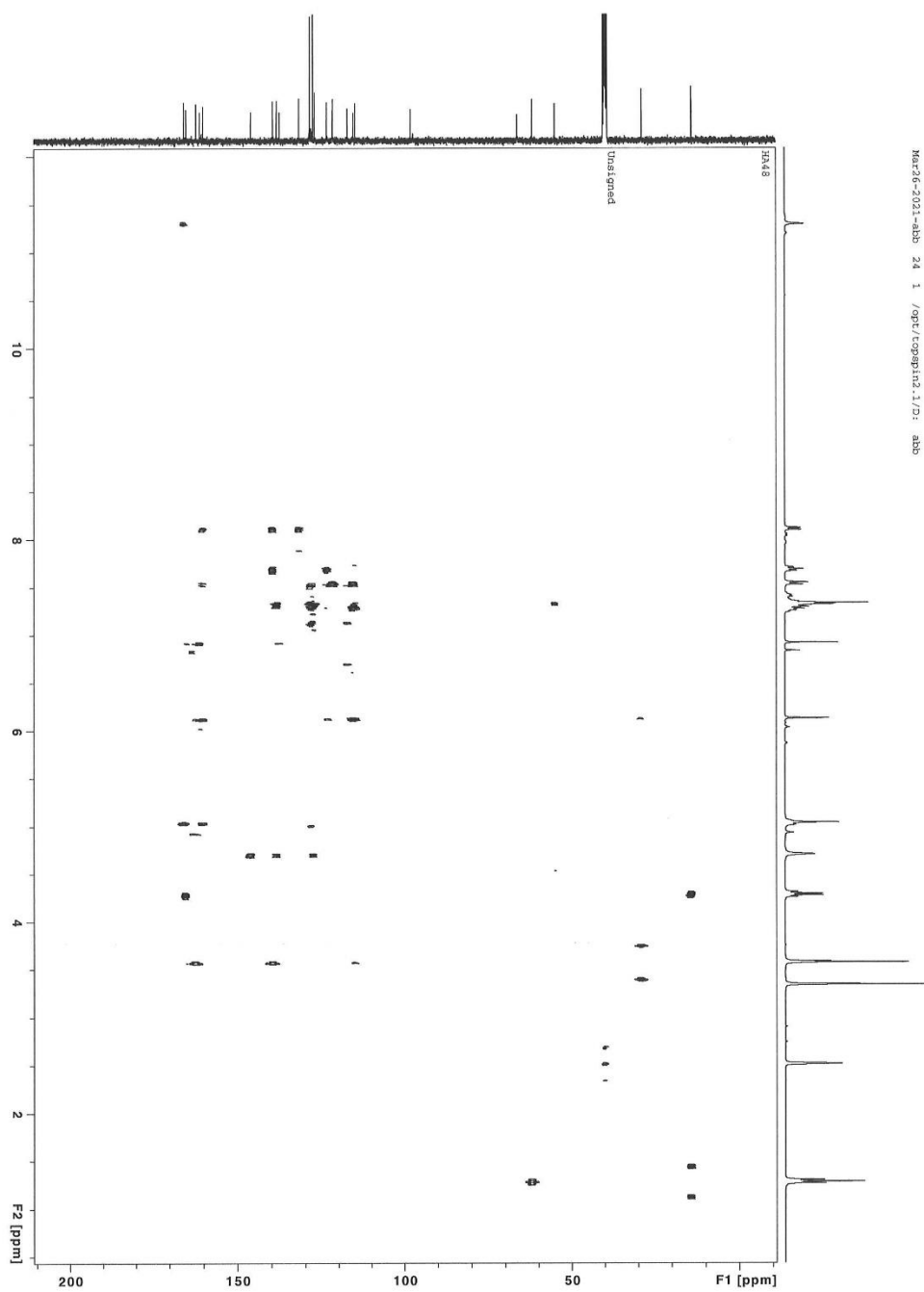
**Figure S28.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7b**.



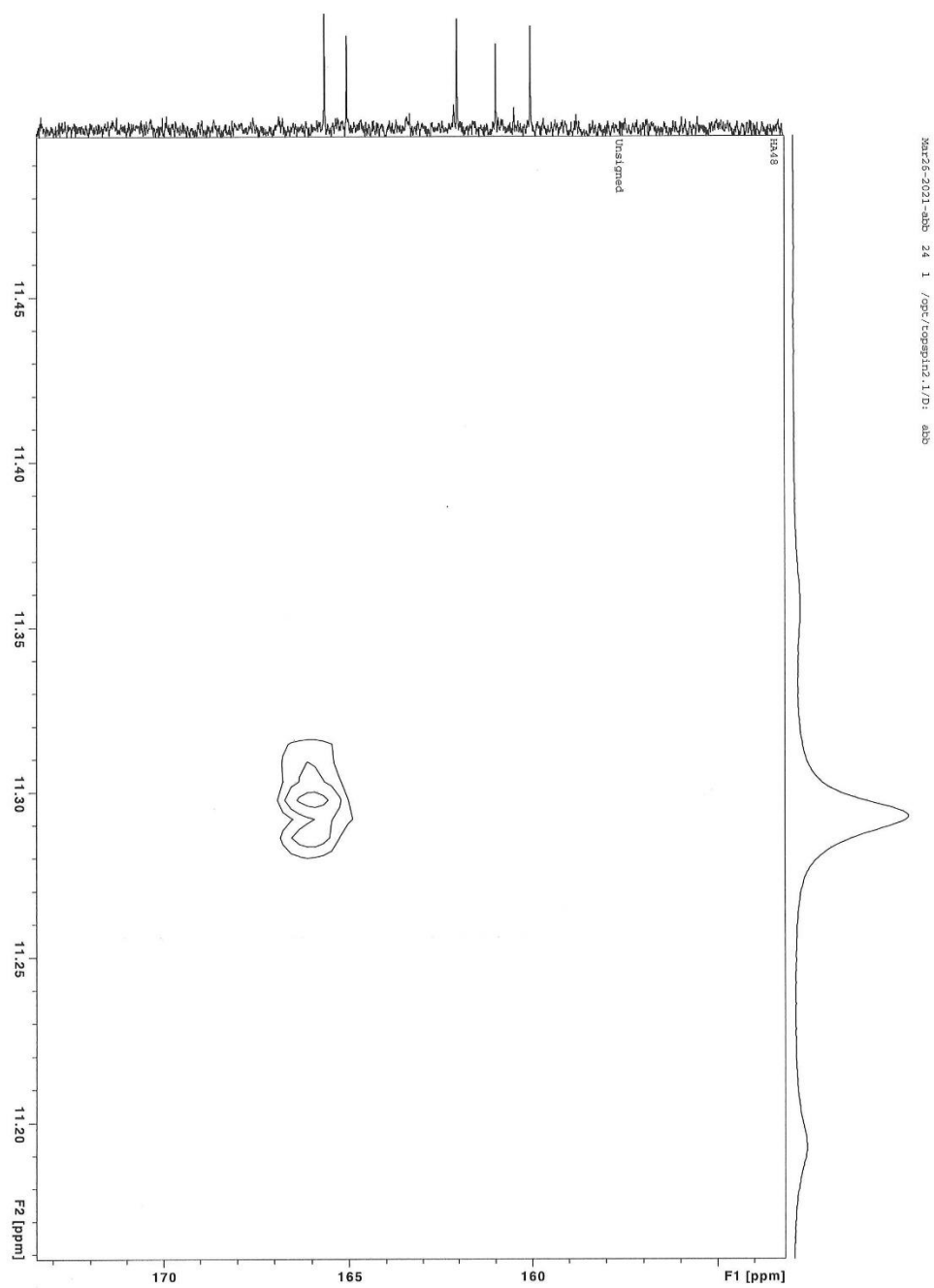
**Figure S29.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7b**.



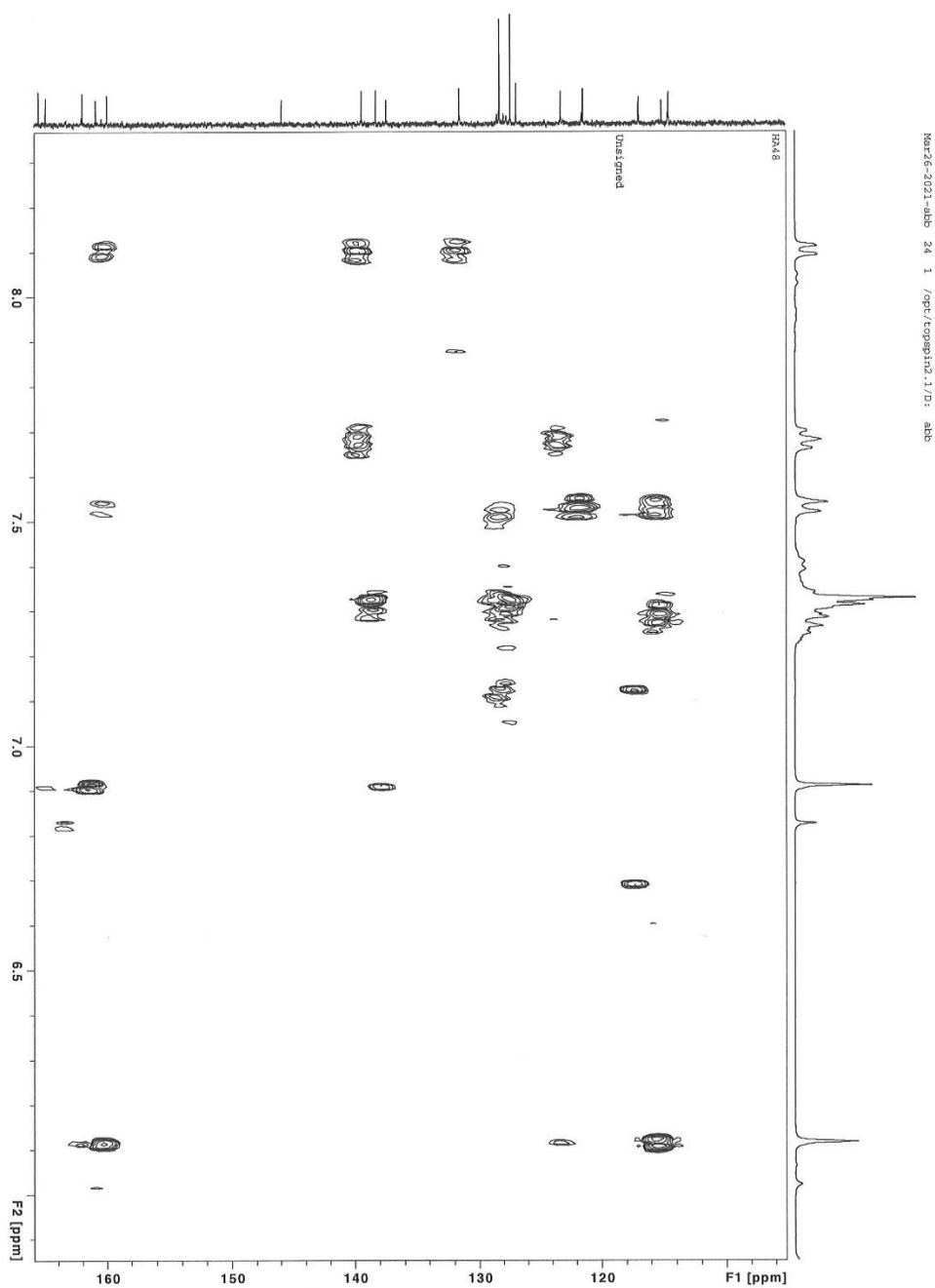
**Figure S30.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7b**.



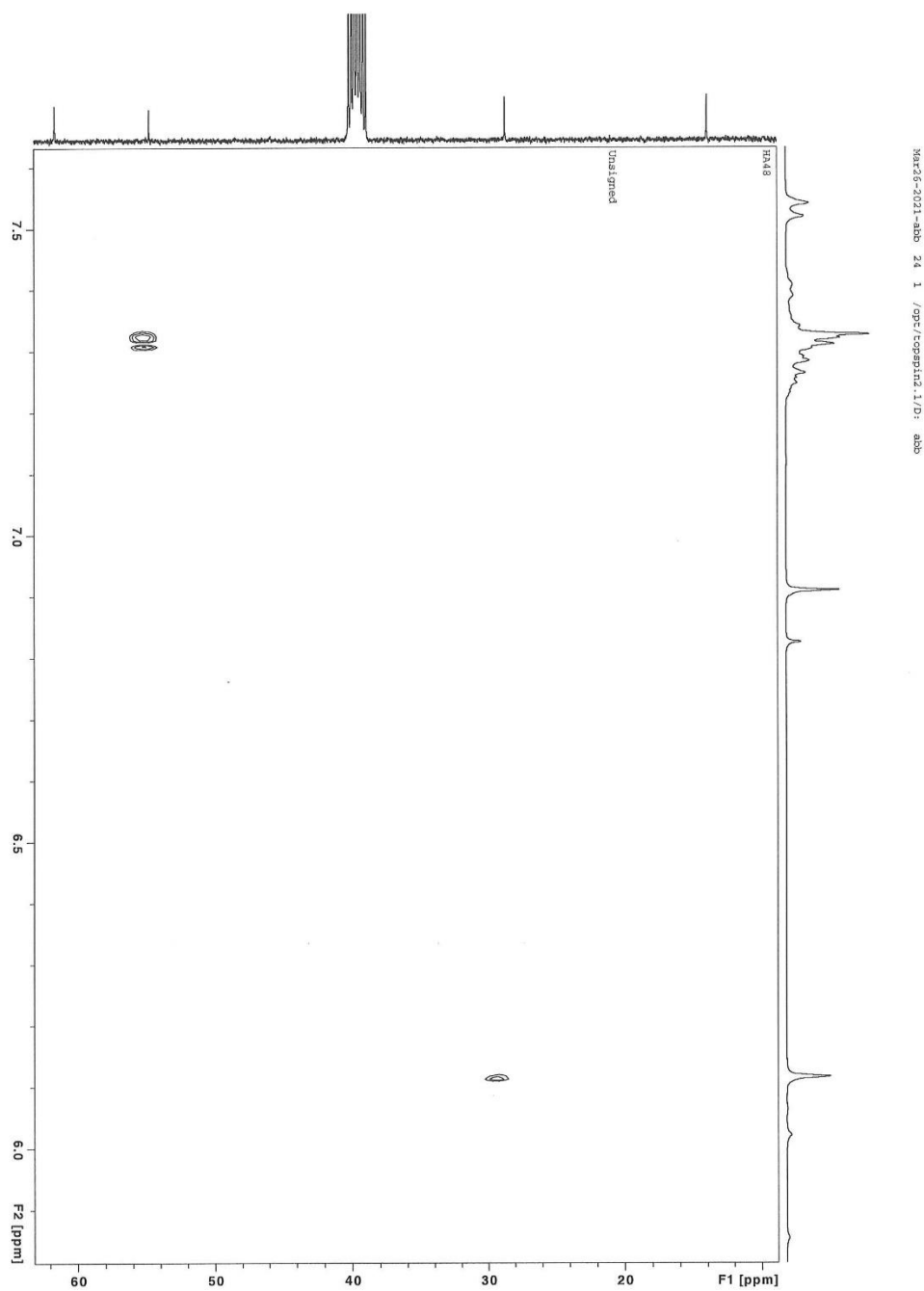
**Figure S31.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7b**.



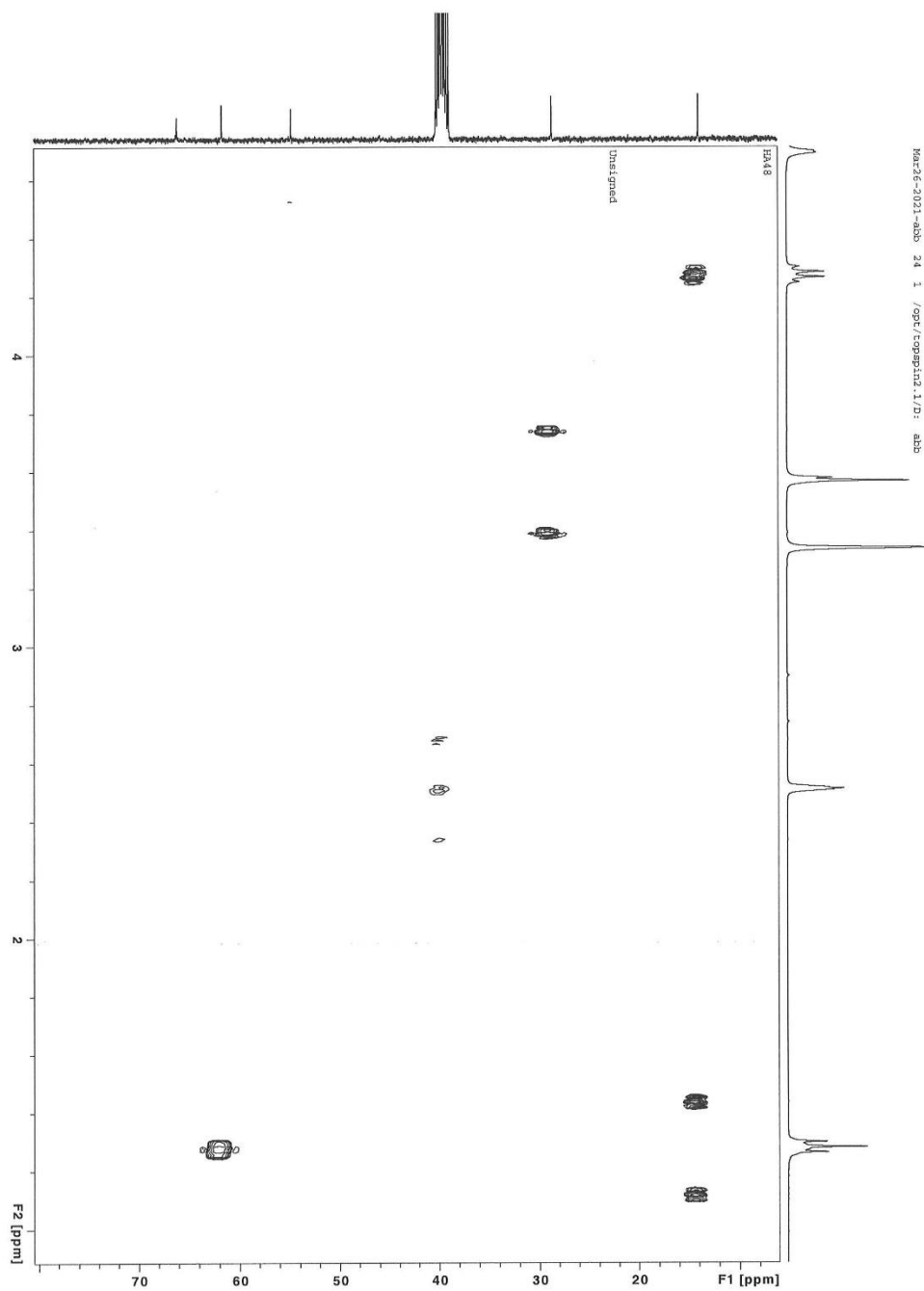
**Figure S32.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7b**.



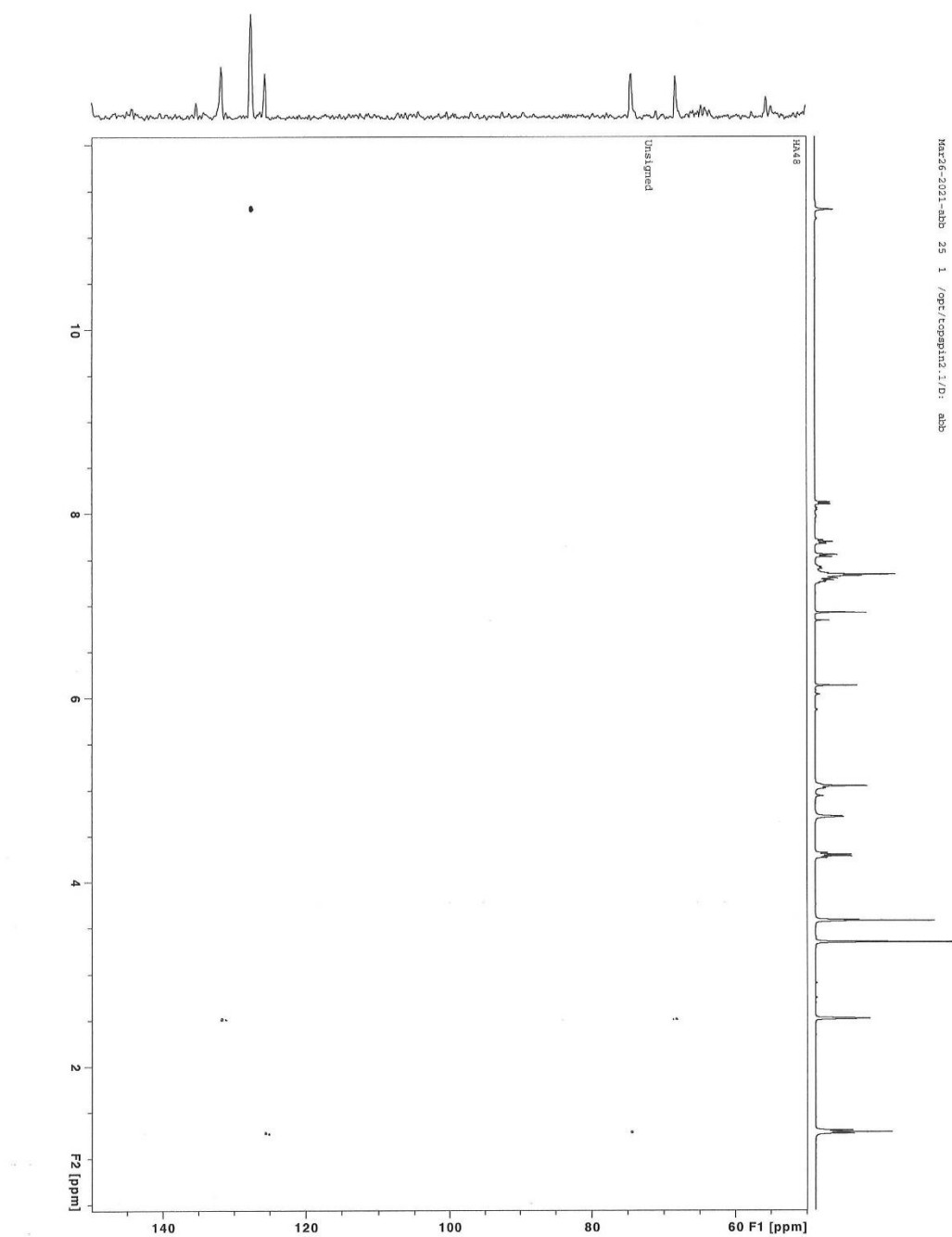
**Figure S33.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7b**.



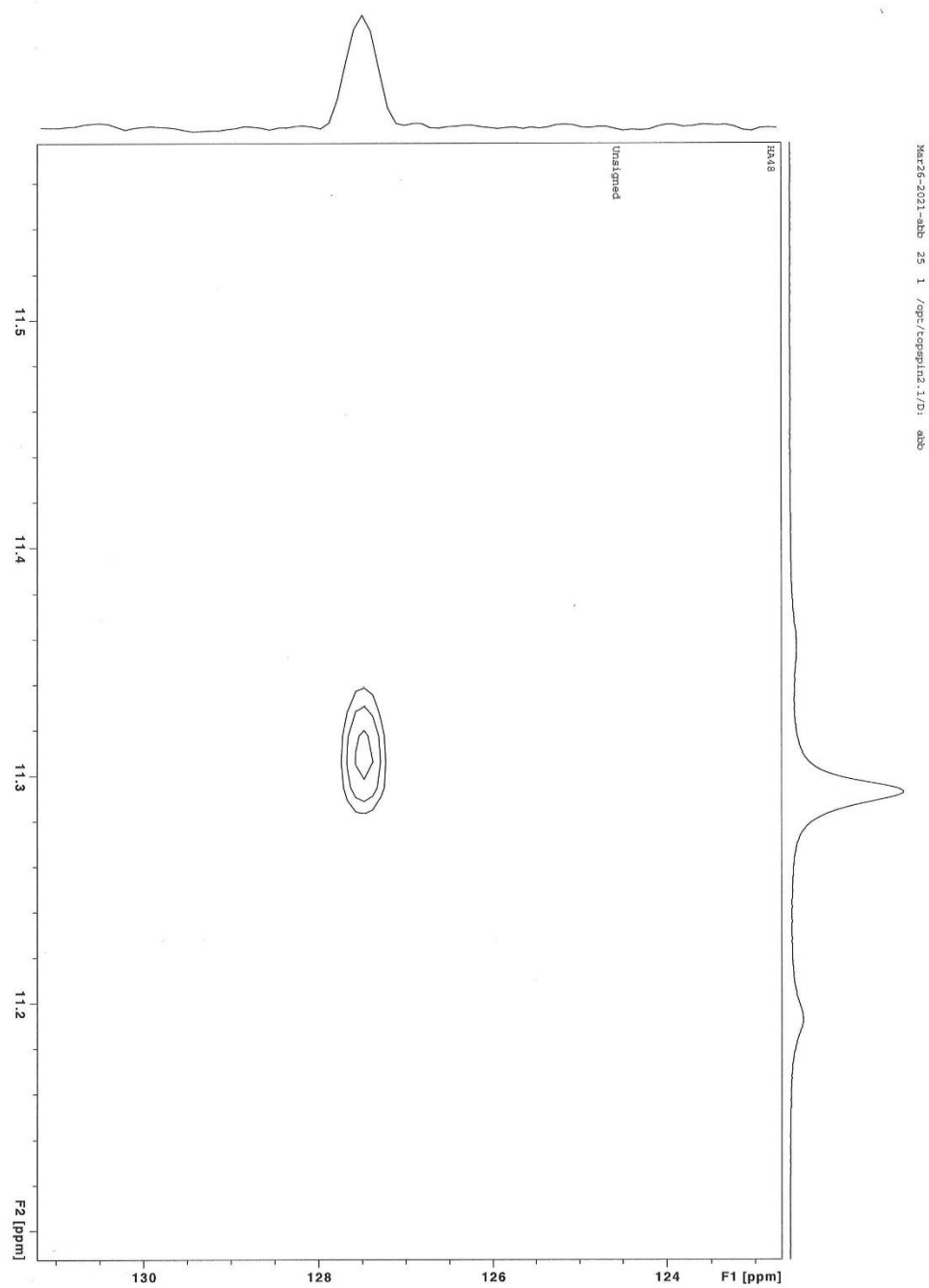
**Figure S34.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7b**.



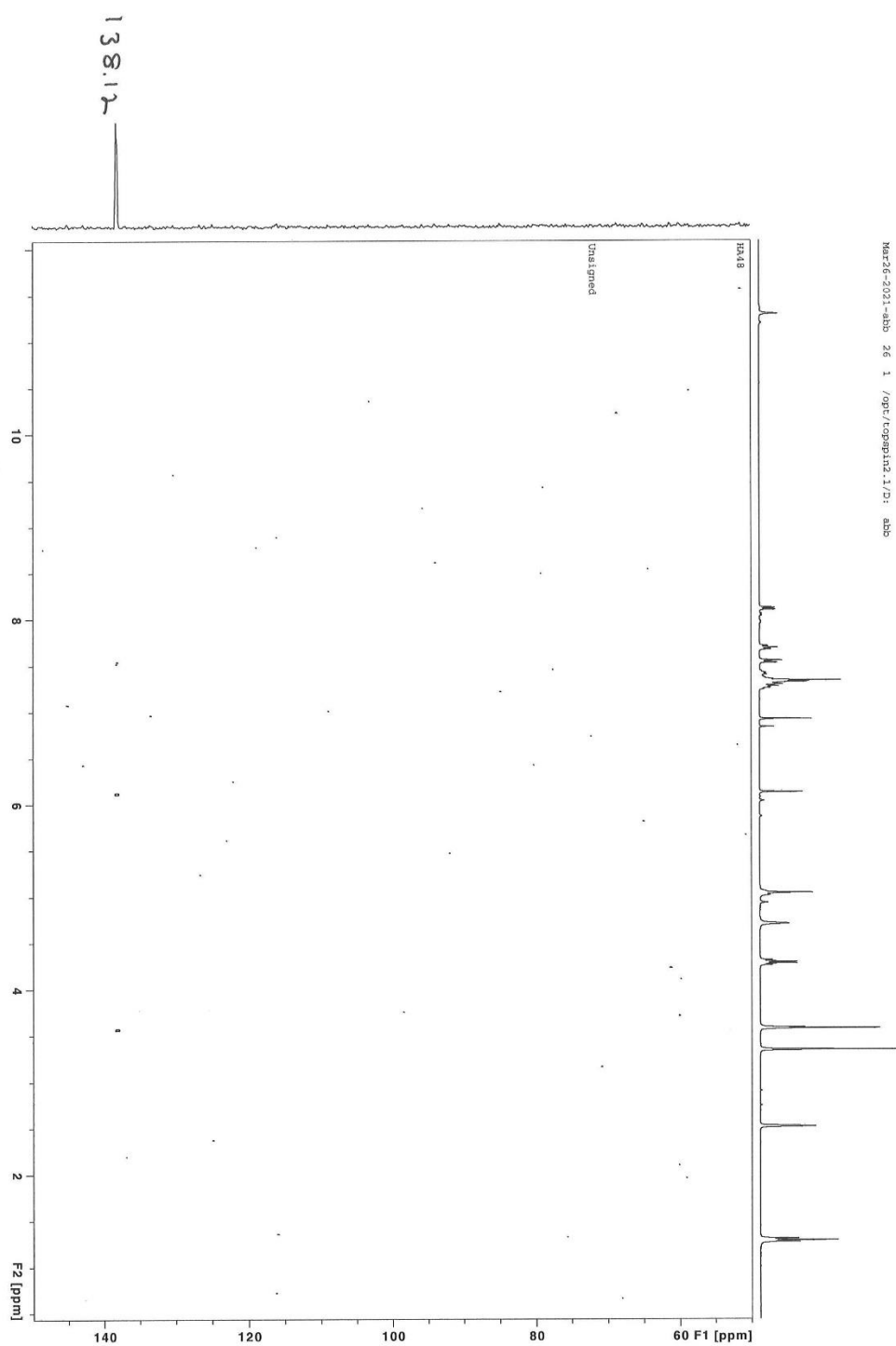
**Figure S35.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7b**.



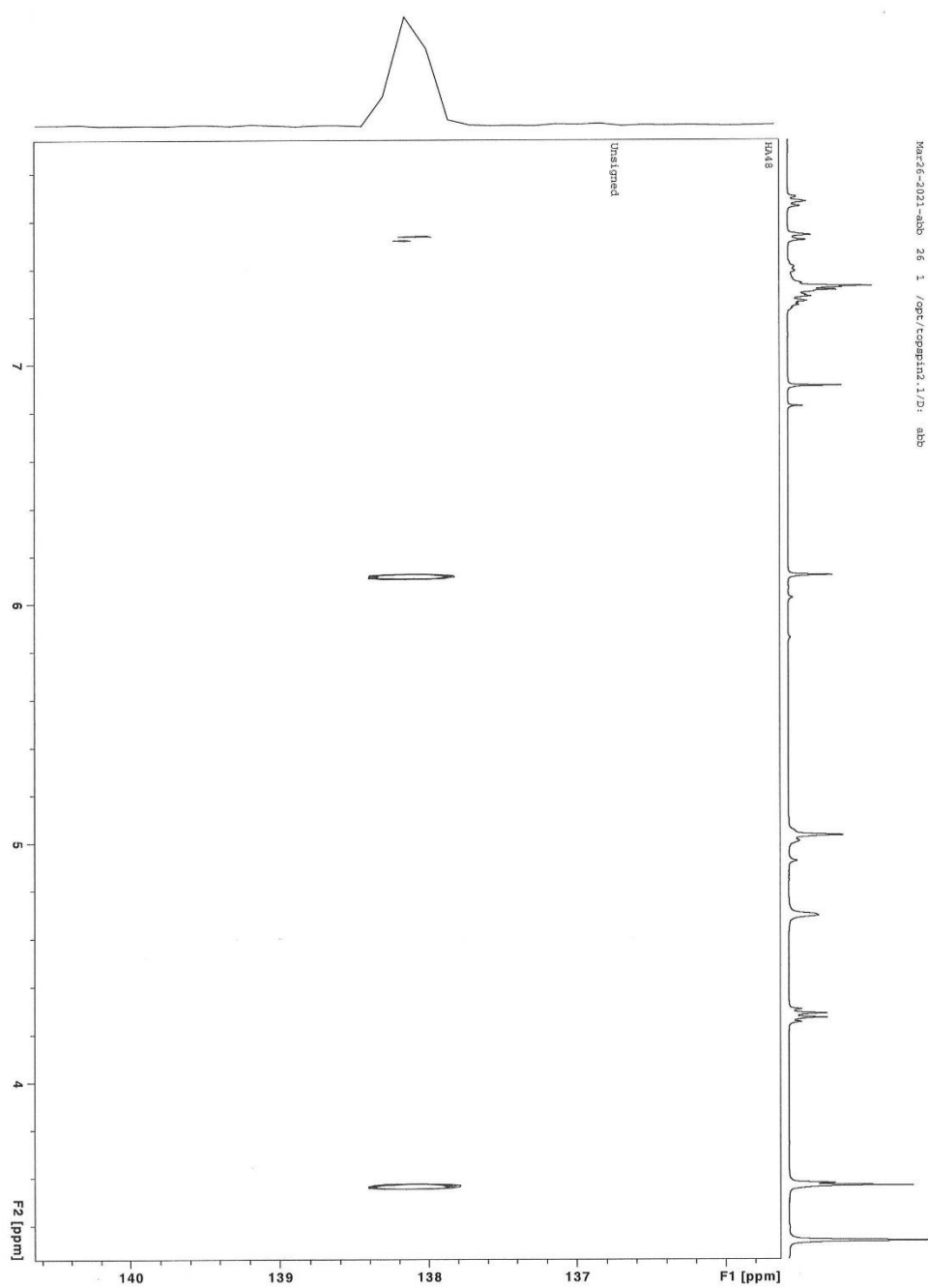
**Figure S36.**  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **7b**.



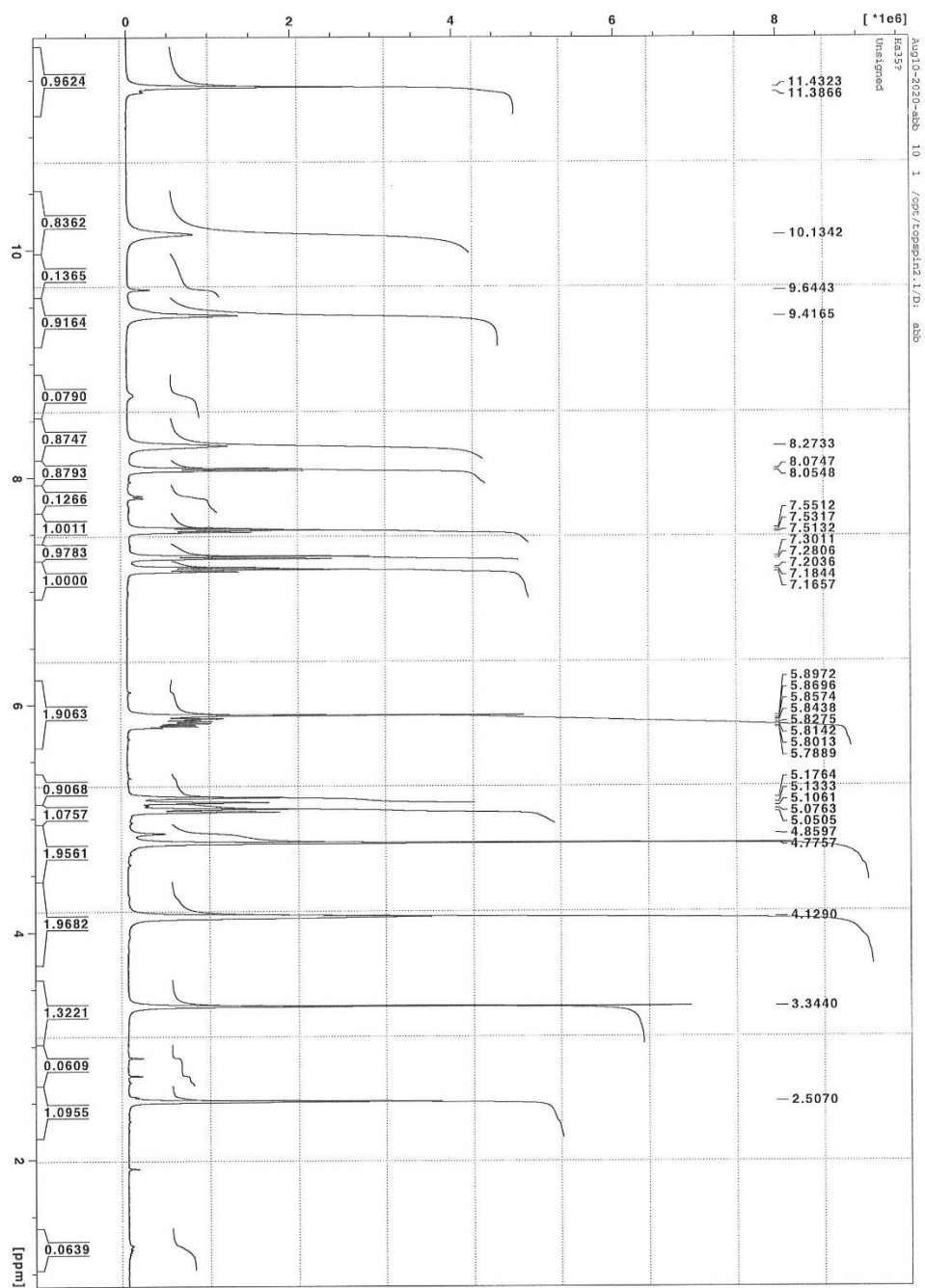
**Figure S37.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **7b**.



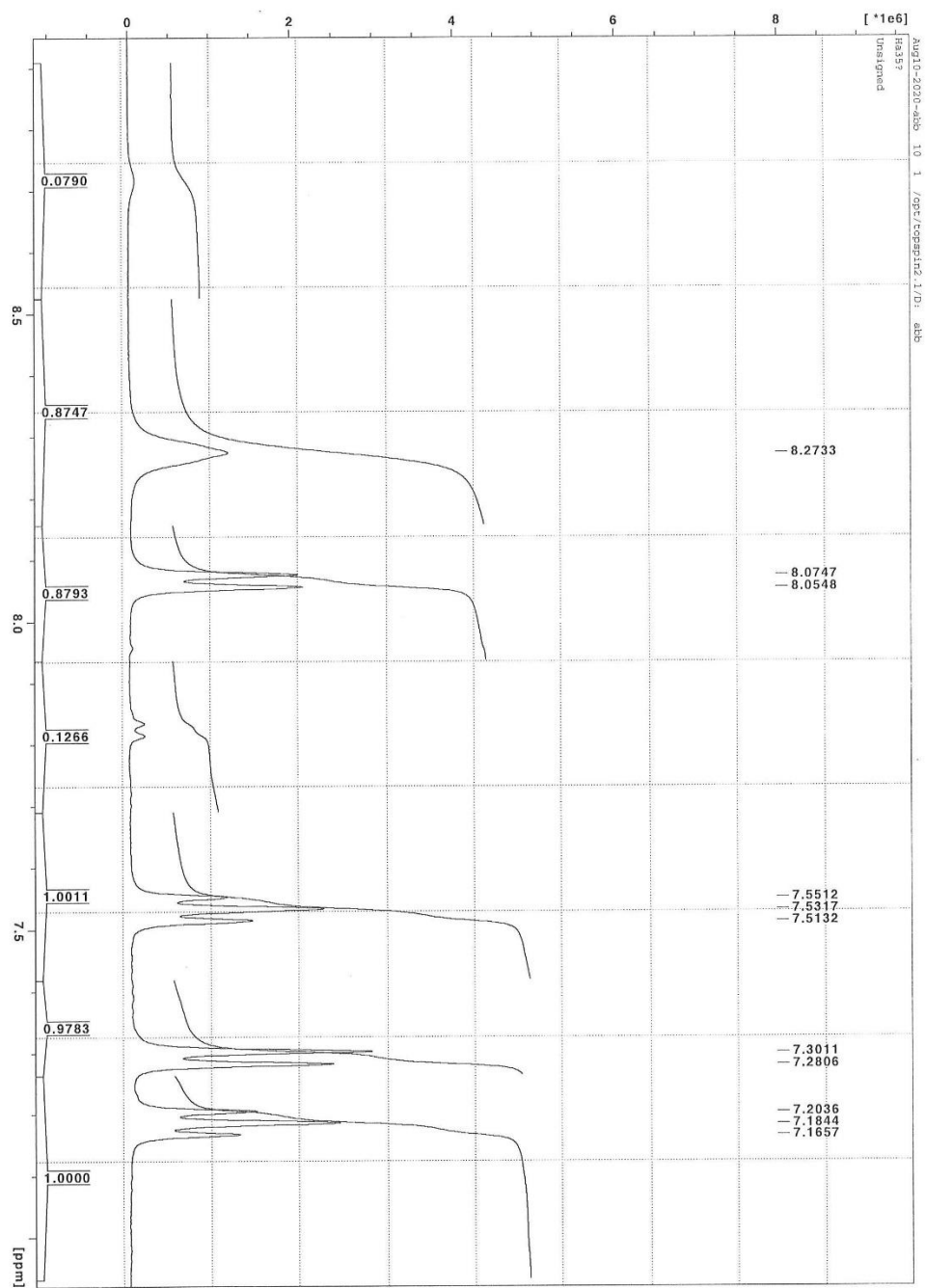
**Figure S38.**  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **7b**.



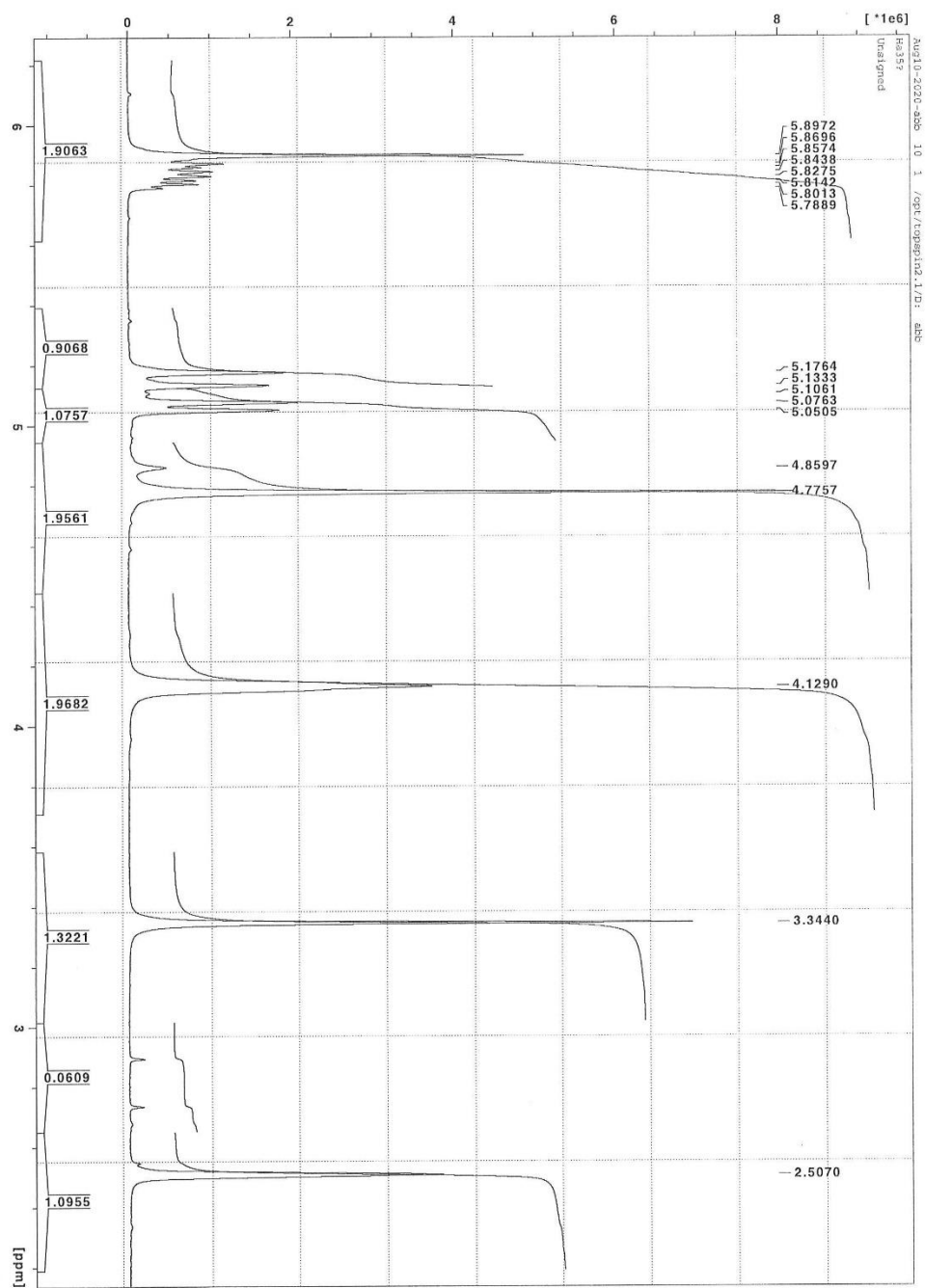
**Figure S39.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **7b**.



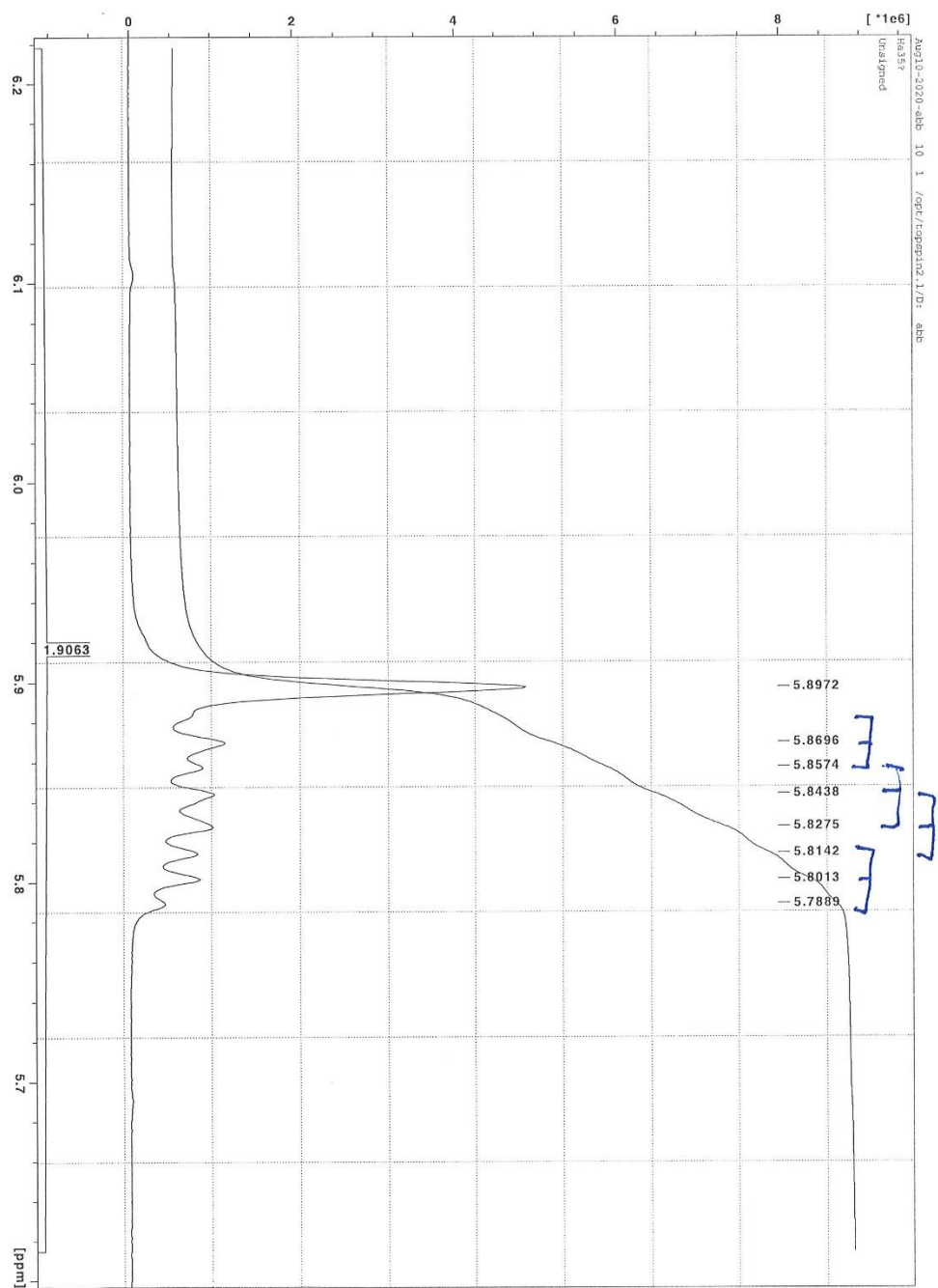
**Figure S40.**  $^1\text{H}$  spectrum of compound **7a** (400 MHz,  $\text{DMSO-}d_6$ ).



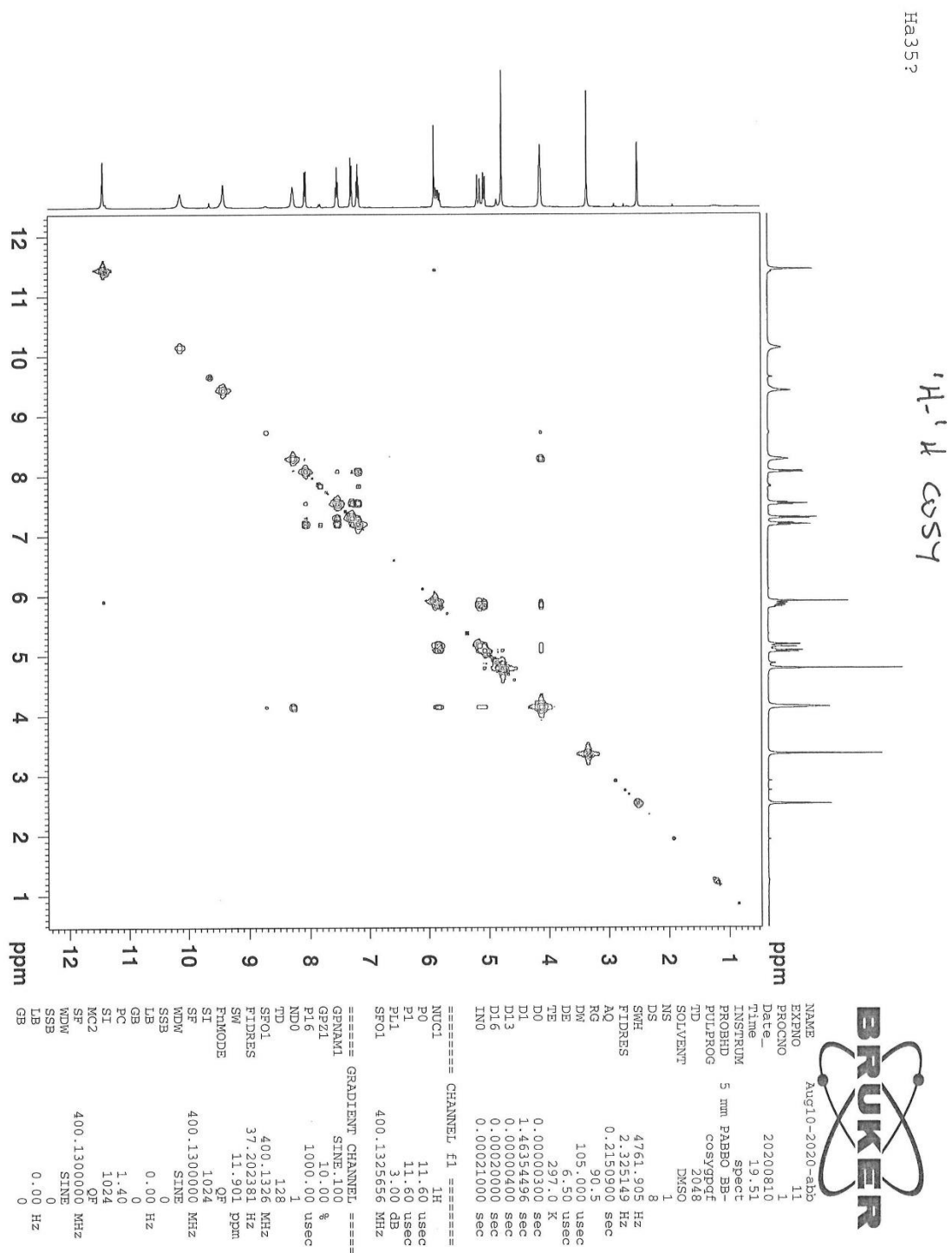
**Figure S41.** Detail of  $^1\text{H}$  spectrum of compound **7a**.



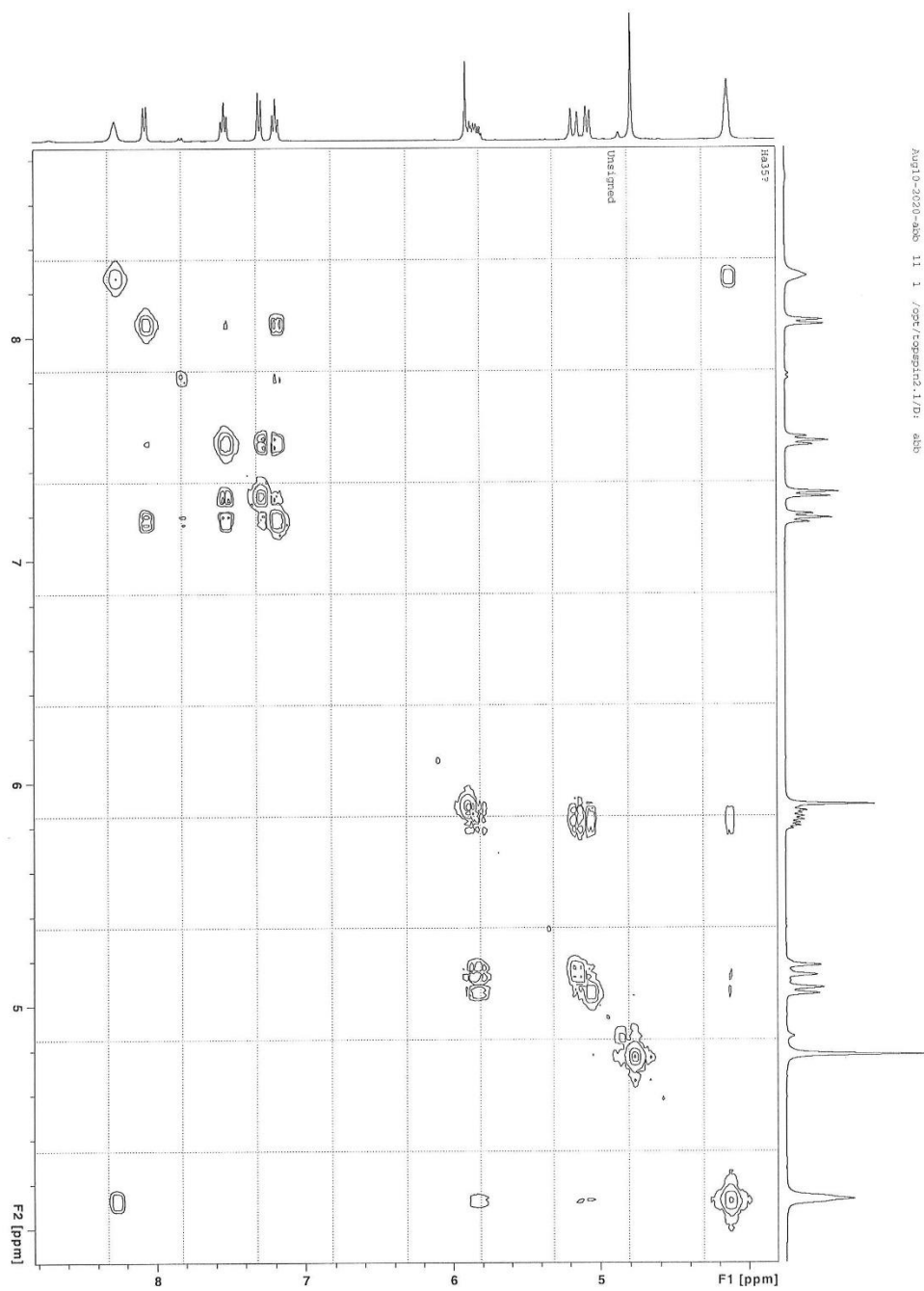
**Figure S42.** Detail of <sup>1</sup>H spectrum of compound **7a**.



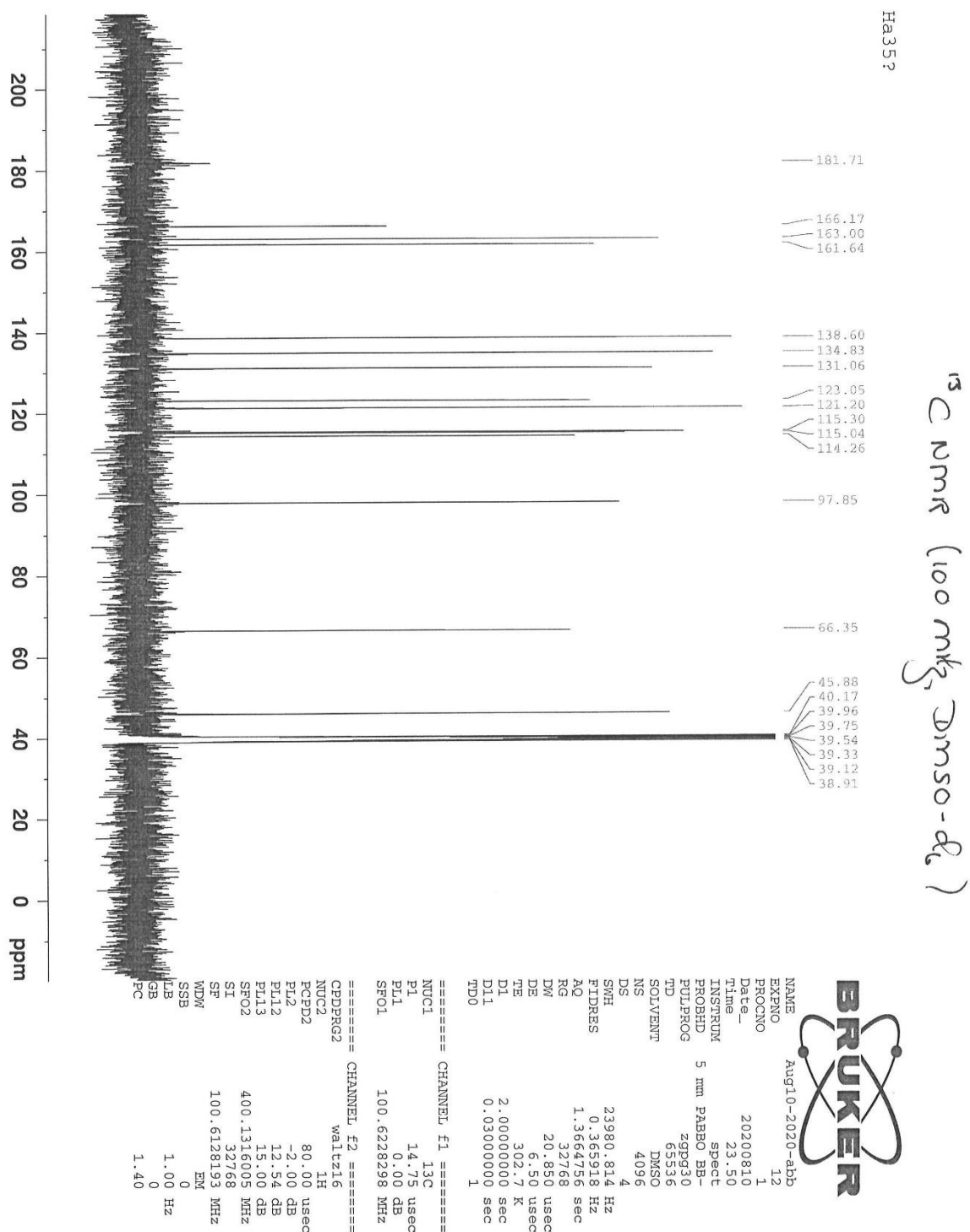
**Figure S43.** Detail of  $^1\text{H}$  spectrum of compound **7a**.



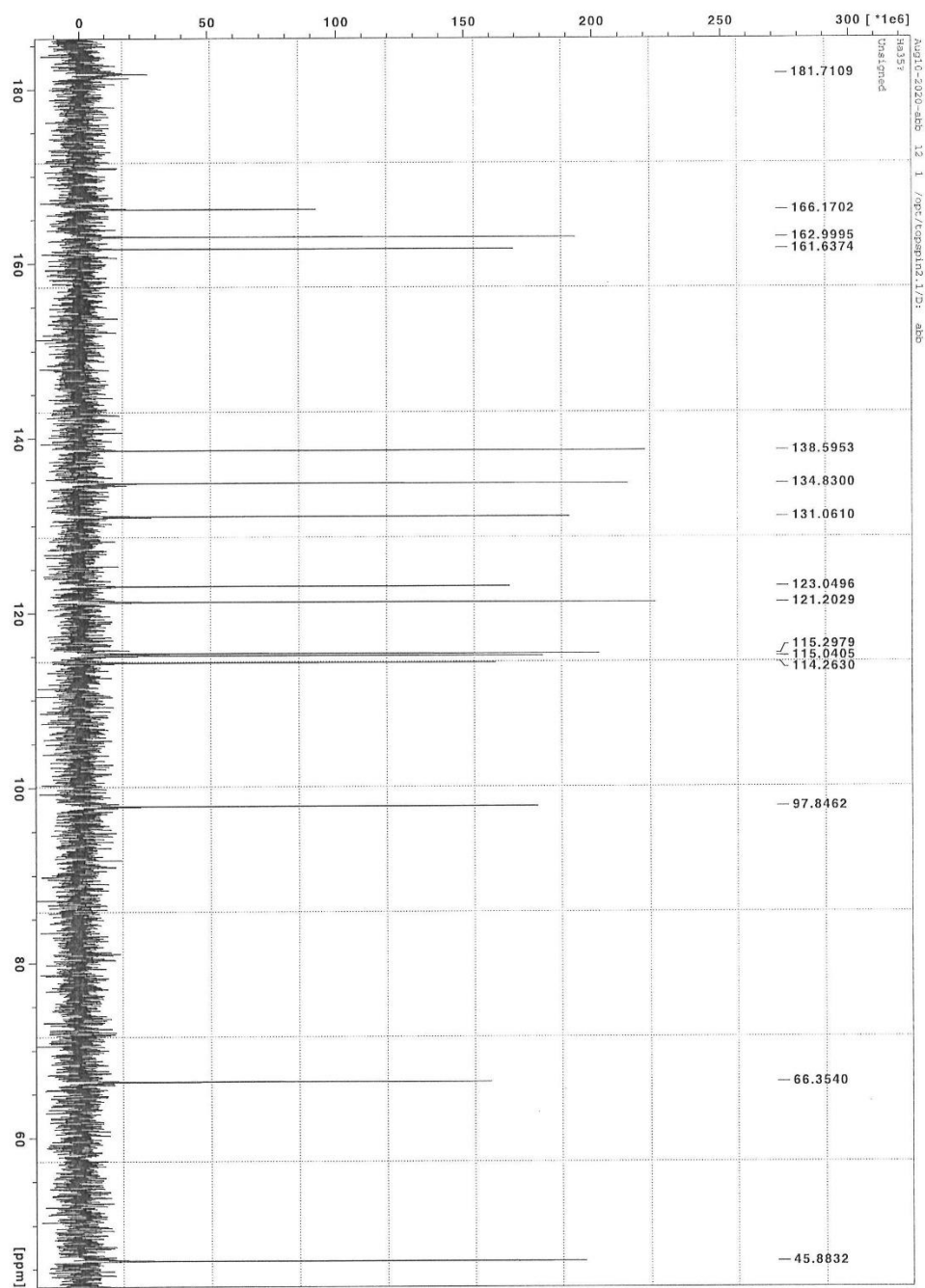
**Figure S44.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7a**.



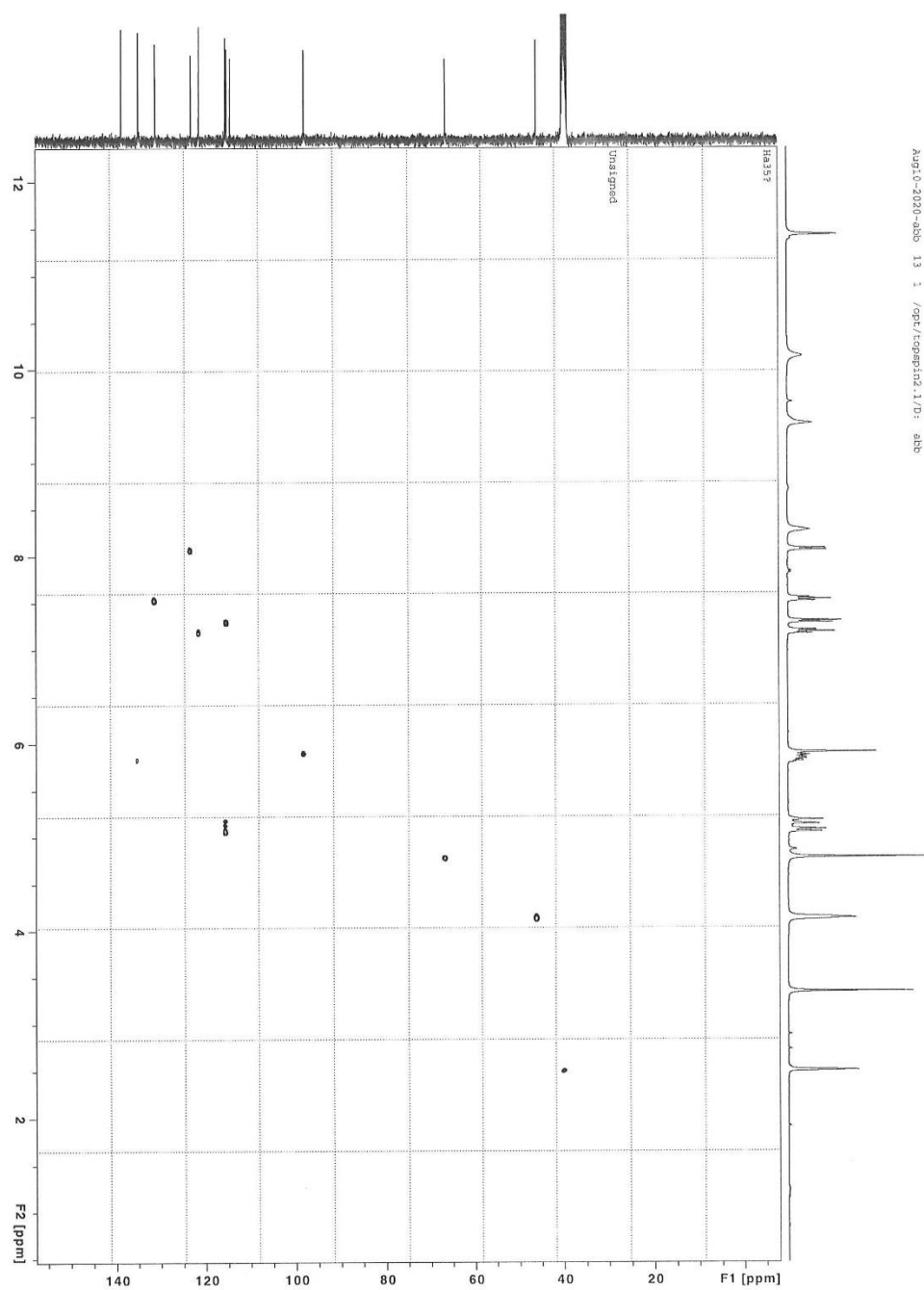
**Figure S45.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7a**.



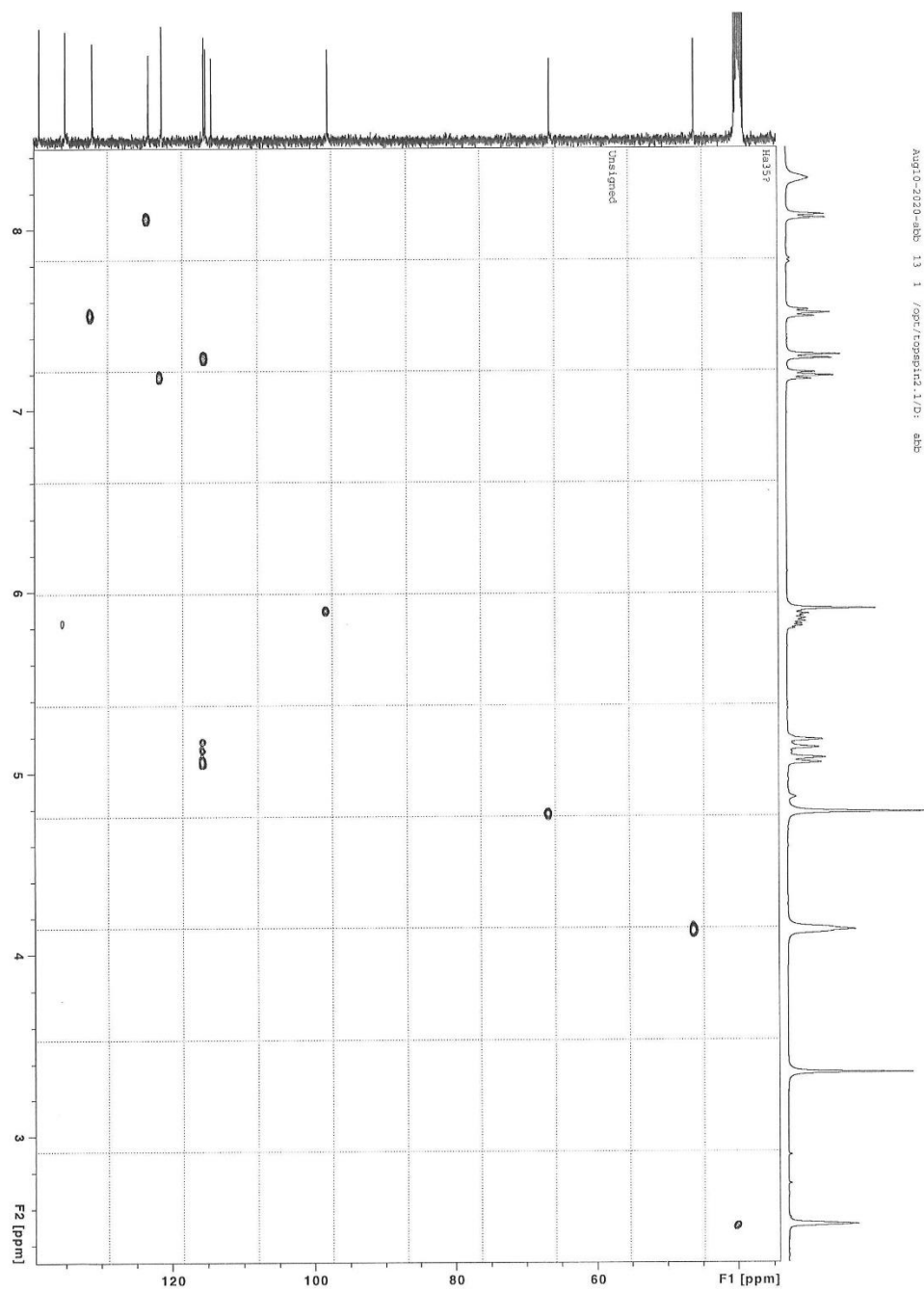
**Figure S46.** <sup>13</sup>C spectrum of compound **7a** (100 MHz, DMSO-d<sub>6</sub>).



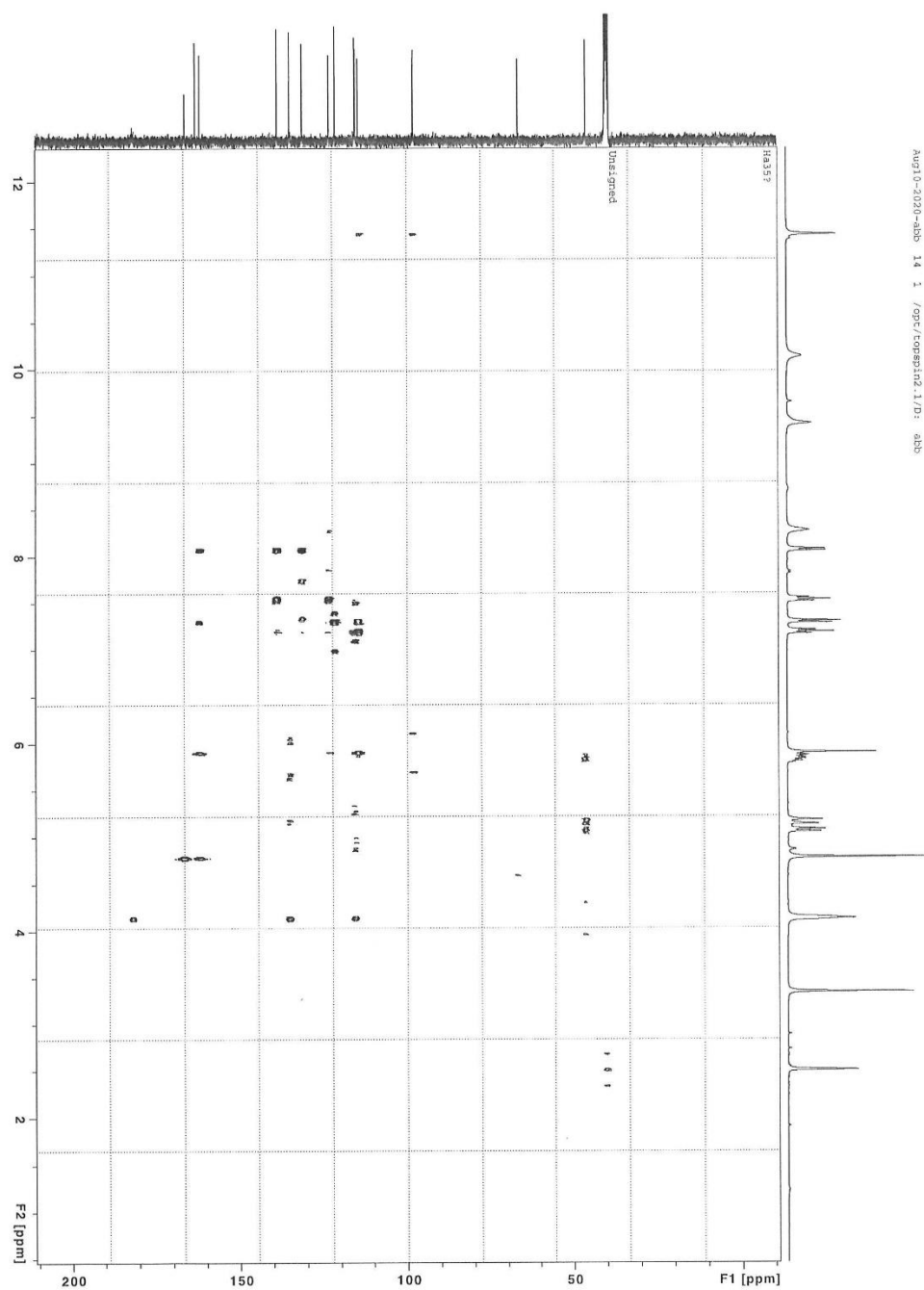
**Figure S47.** Detail of  $^{13}\text{C}$  spectrum of compound **7a**.



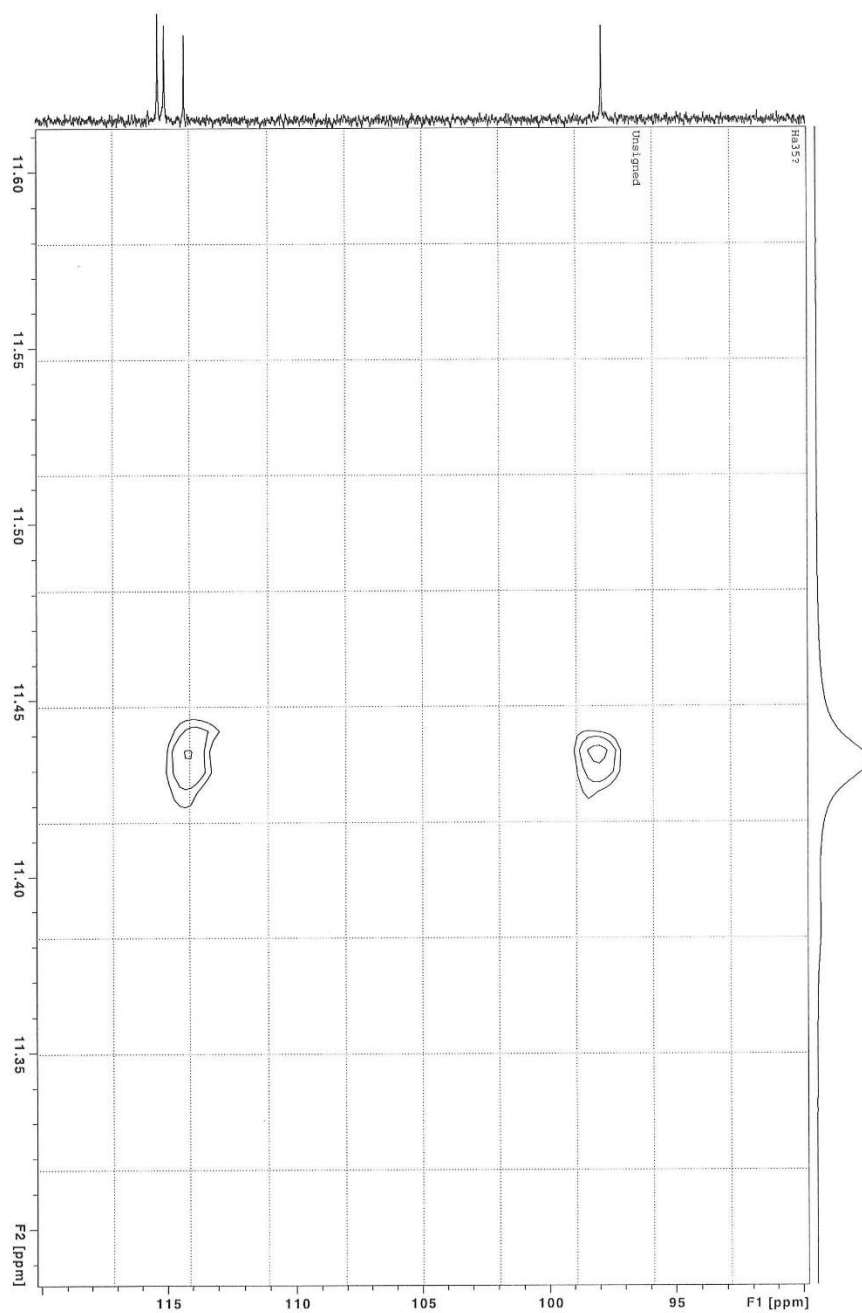
**Figure S48.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7a**.



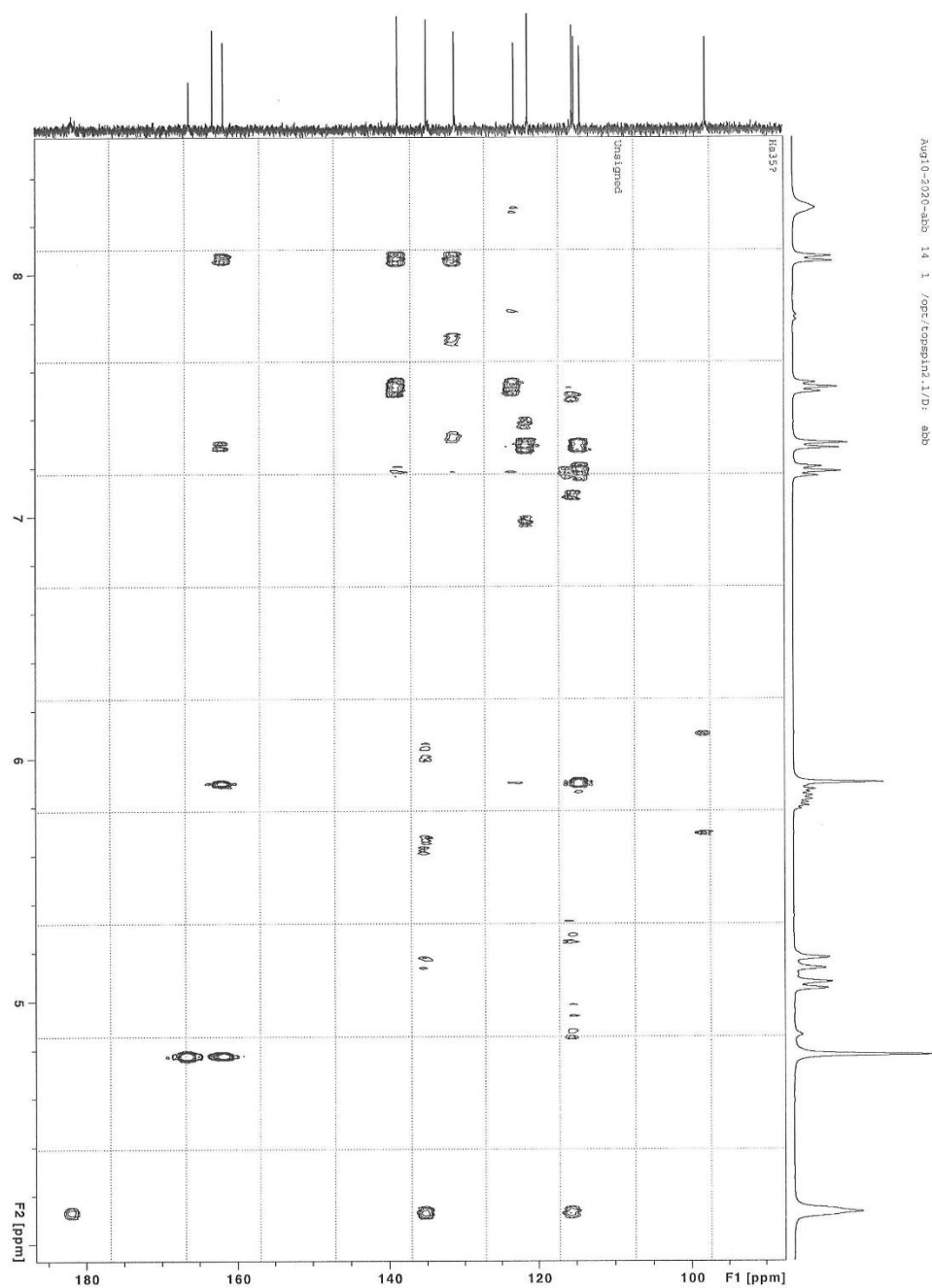
**Figure S49.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7a**.



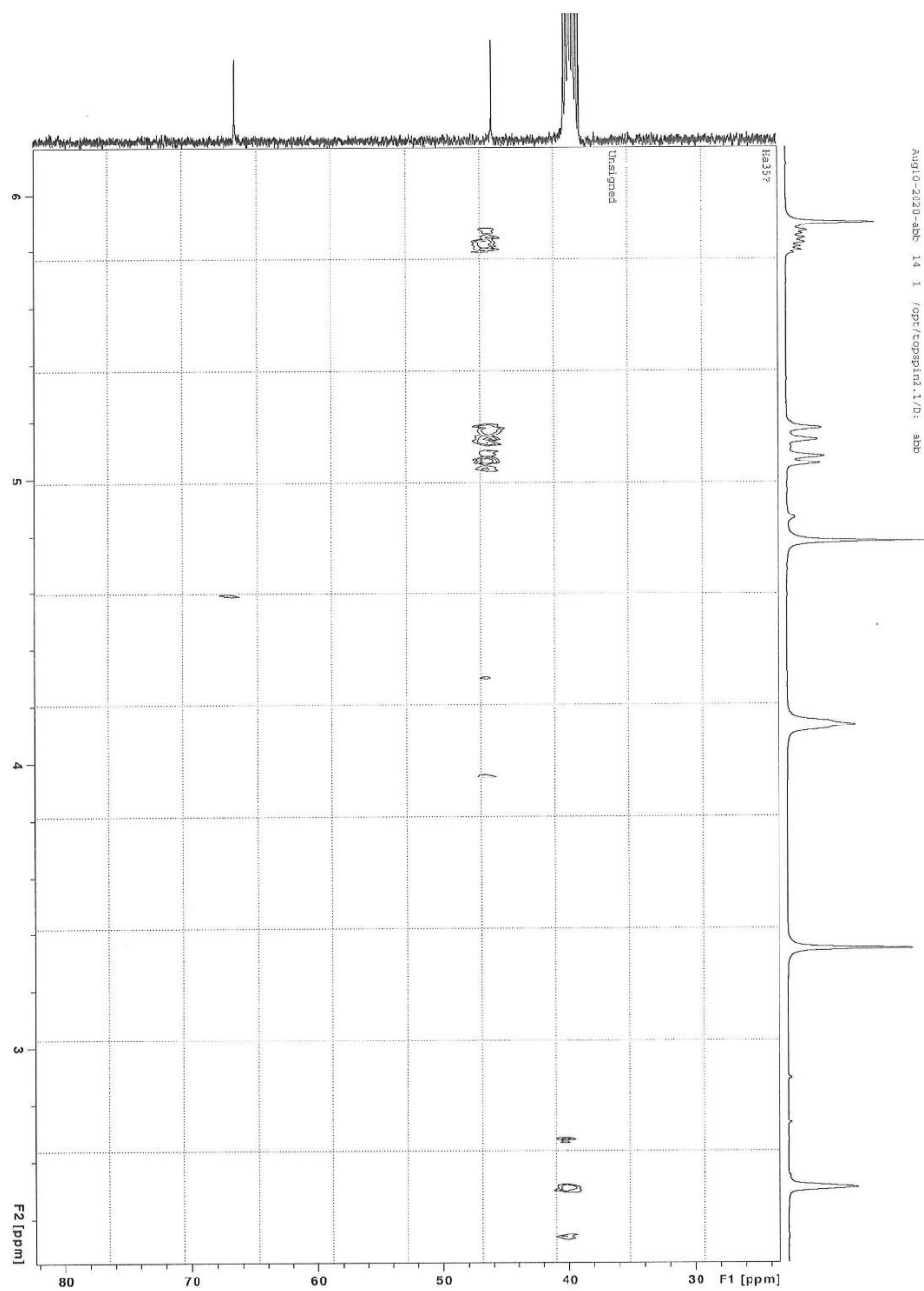
**Figure S50.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7a**.



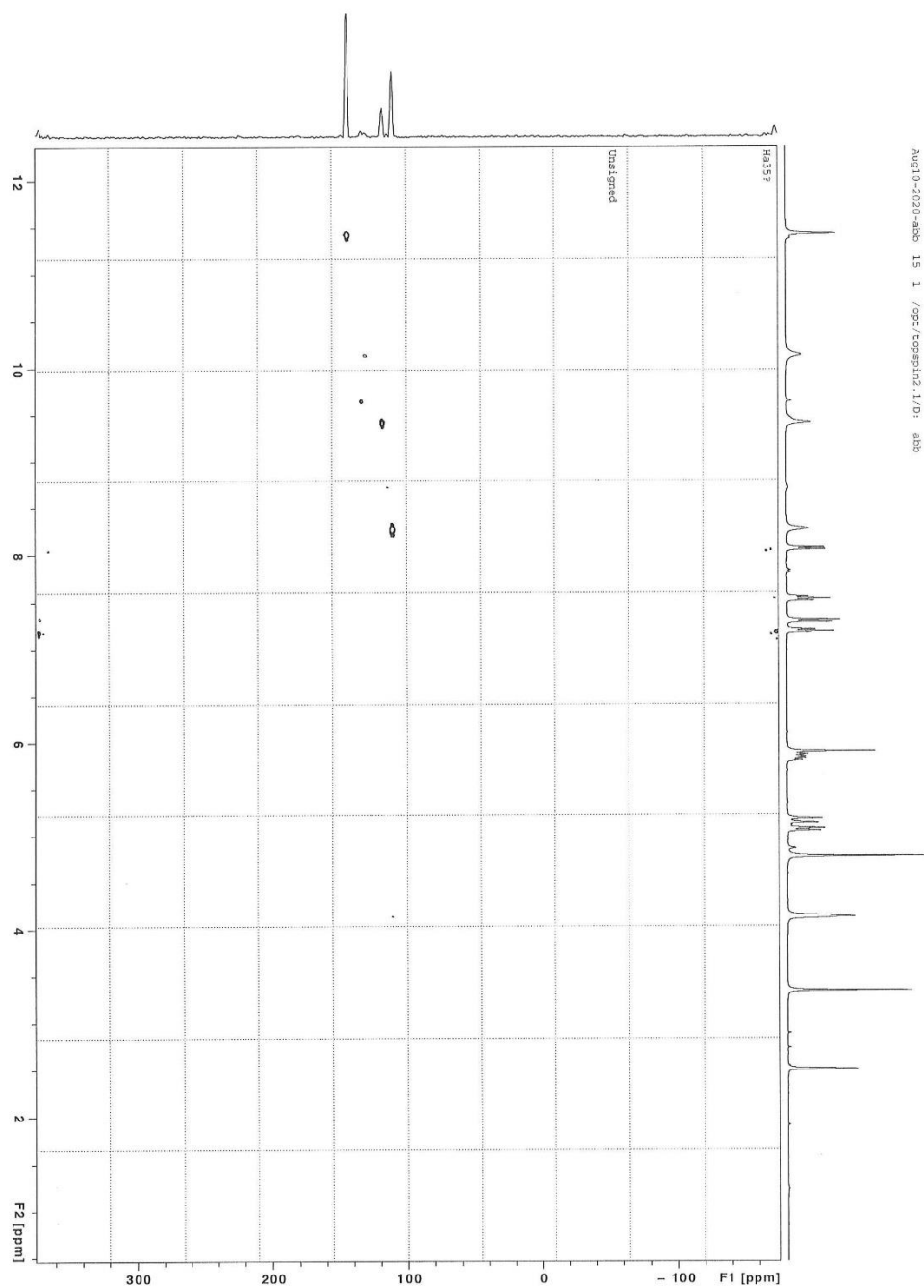
**Figure S51.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7a**.



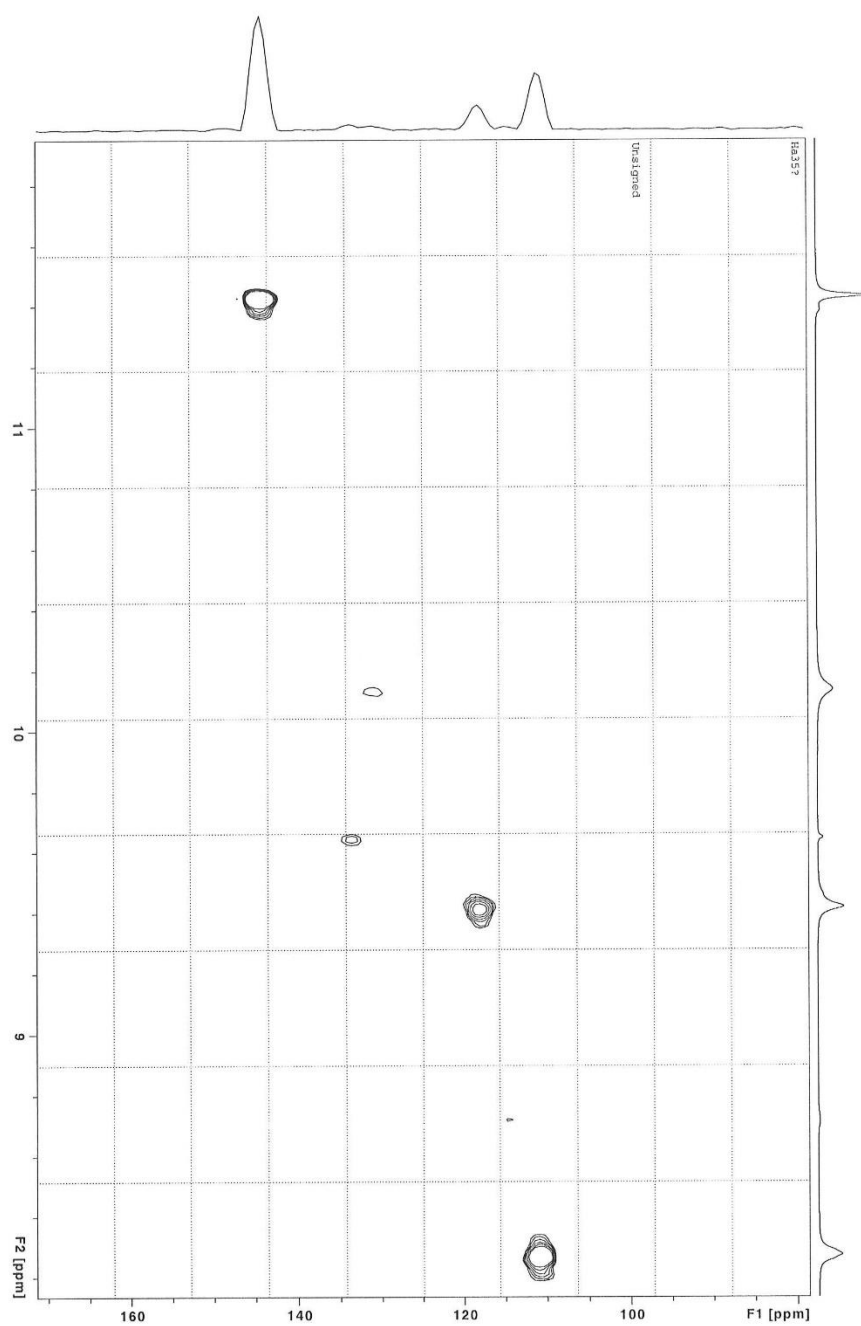
**Figure S52.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7a**



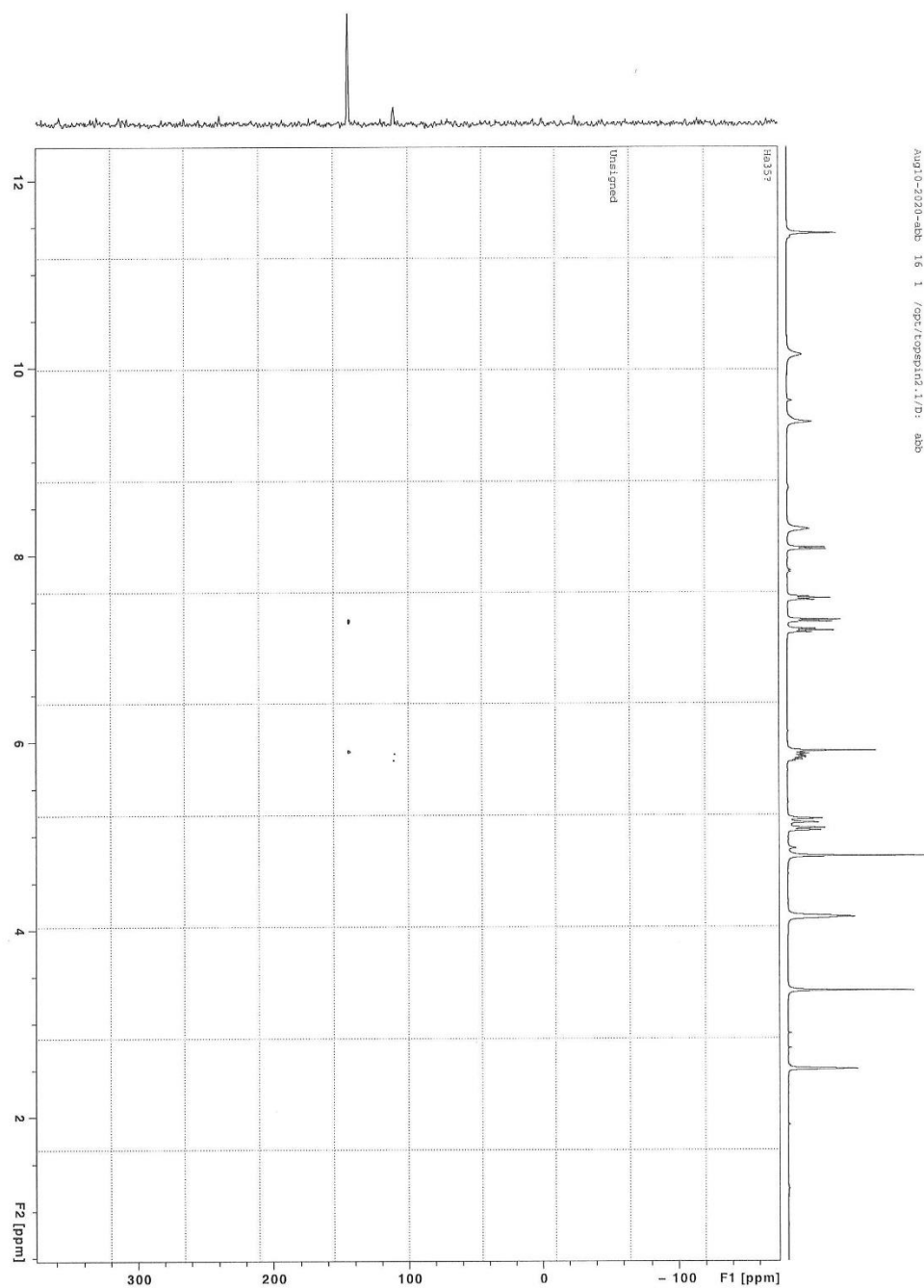
**Figure S53.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7a**.



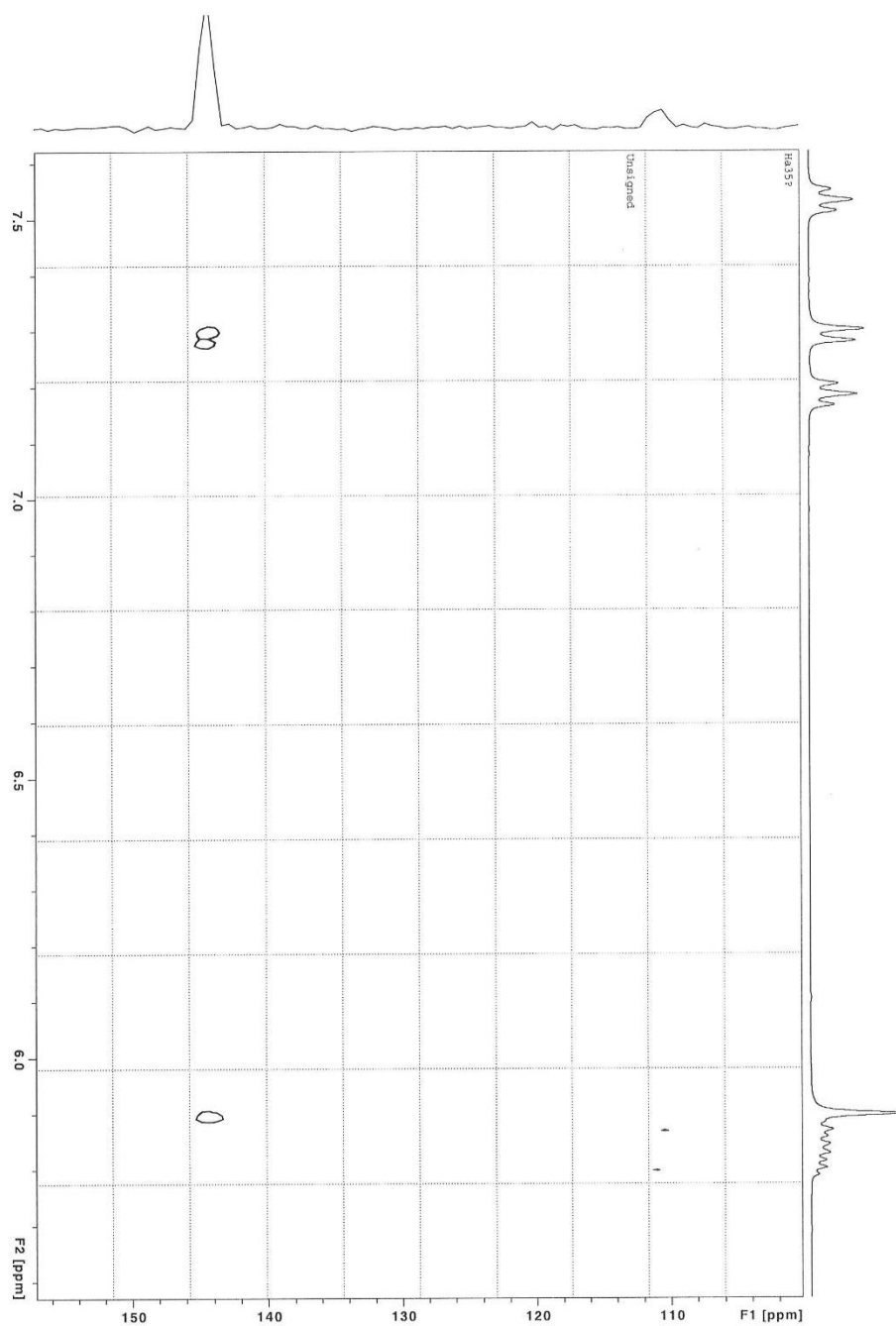
**Figure S54.**  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **7a**.



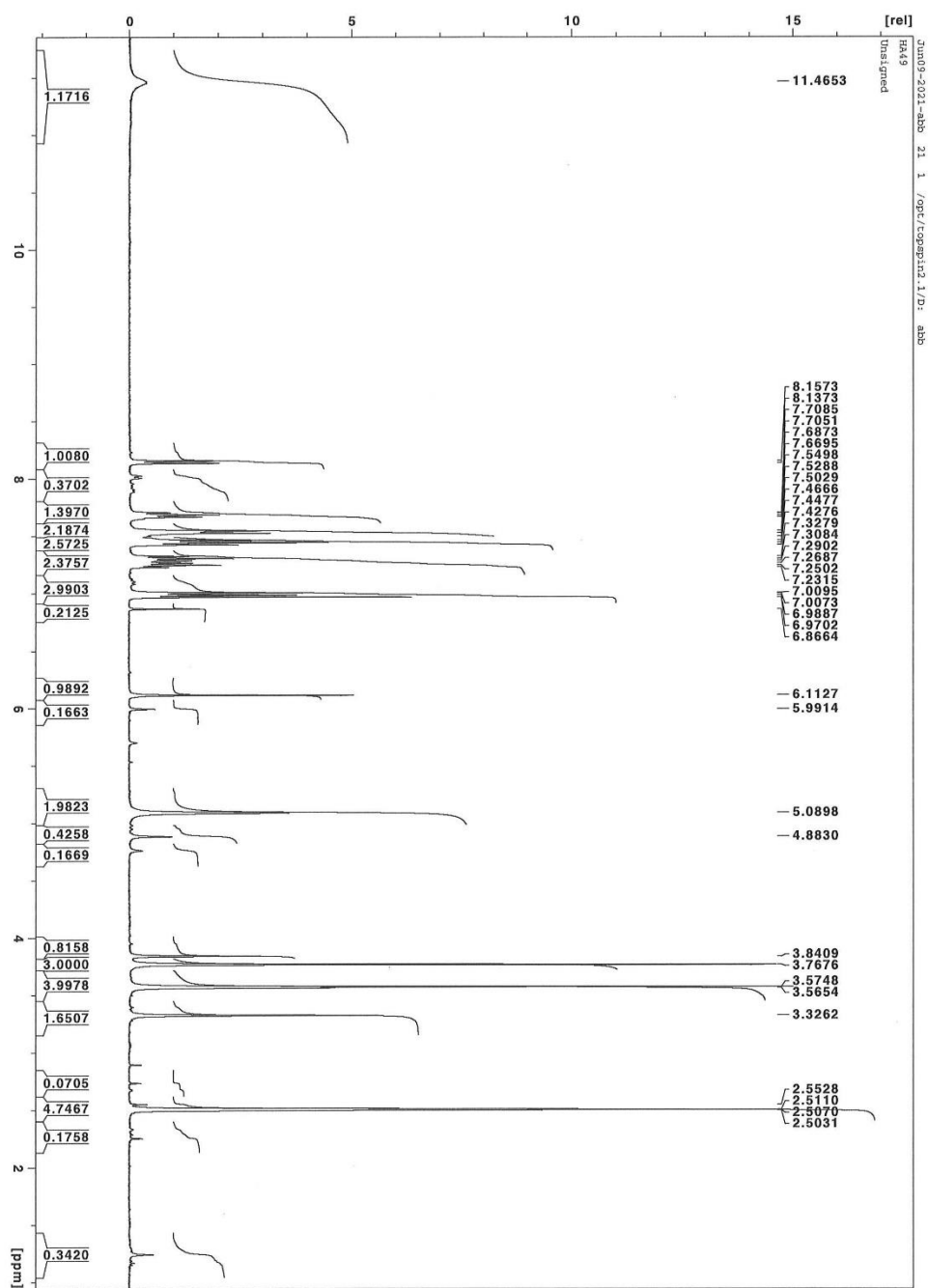
**Figure S55.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **7a**.



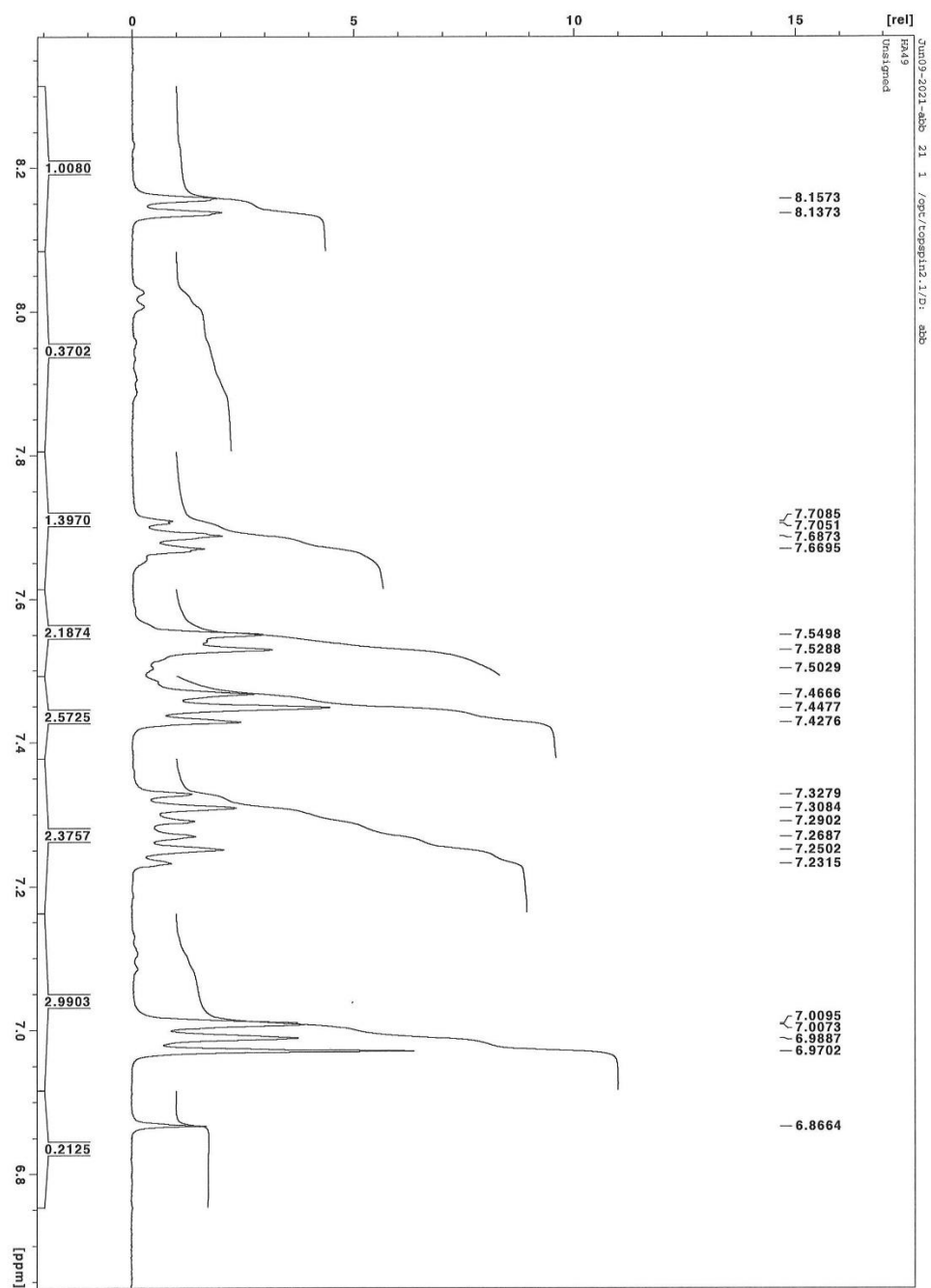
**Figure S56.**  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **7a**.



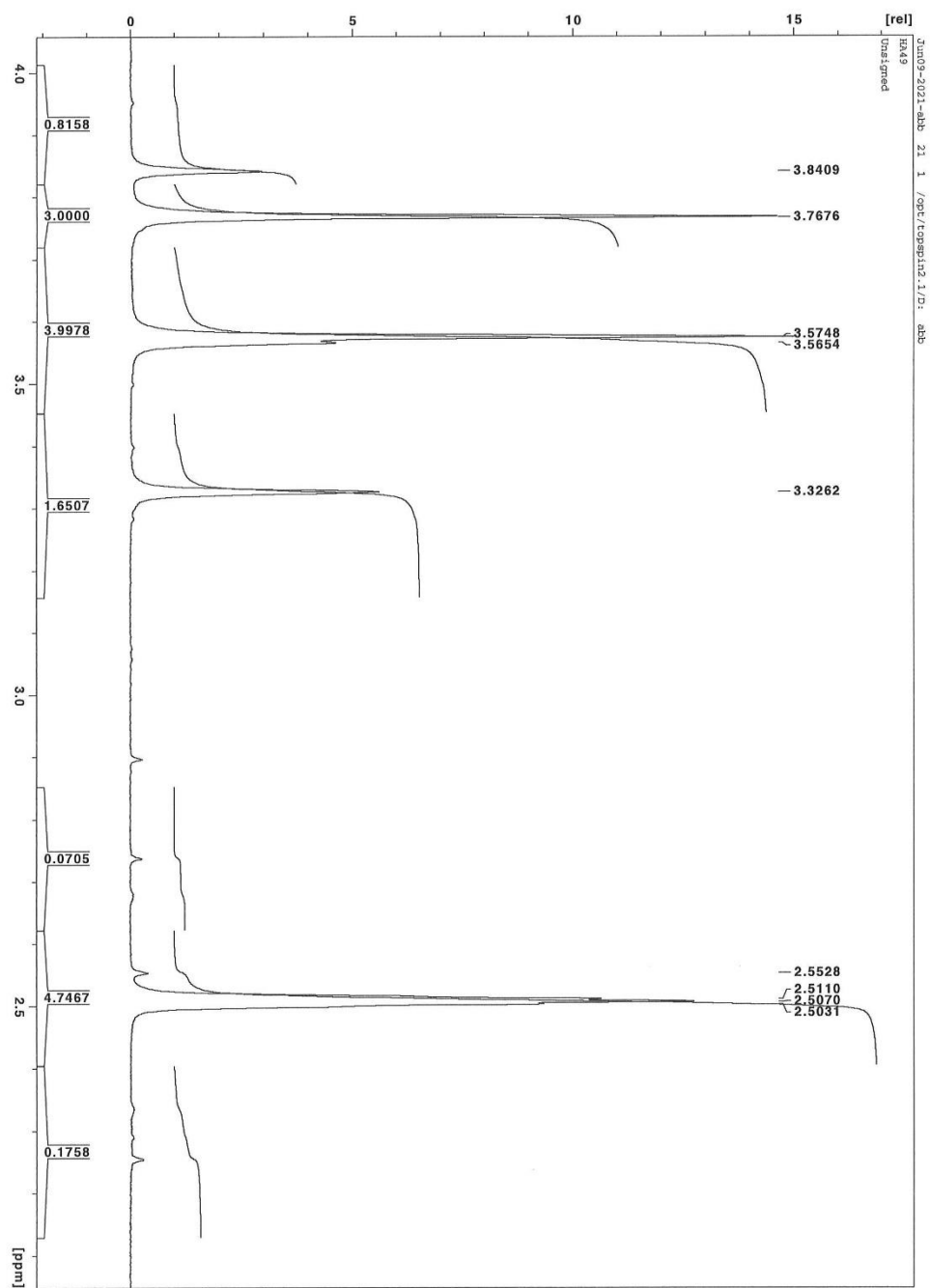
**Figure S57.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **7a**.



**Figure S58.**  $^1\text{H}$  spectrum of compound **7c** (400 MHz,  $\text{DMSO-}d_6$ ).

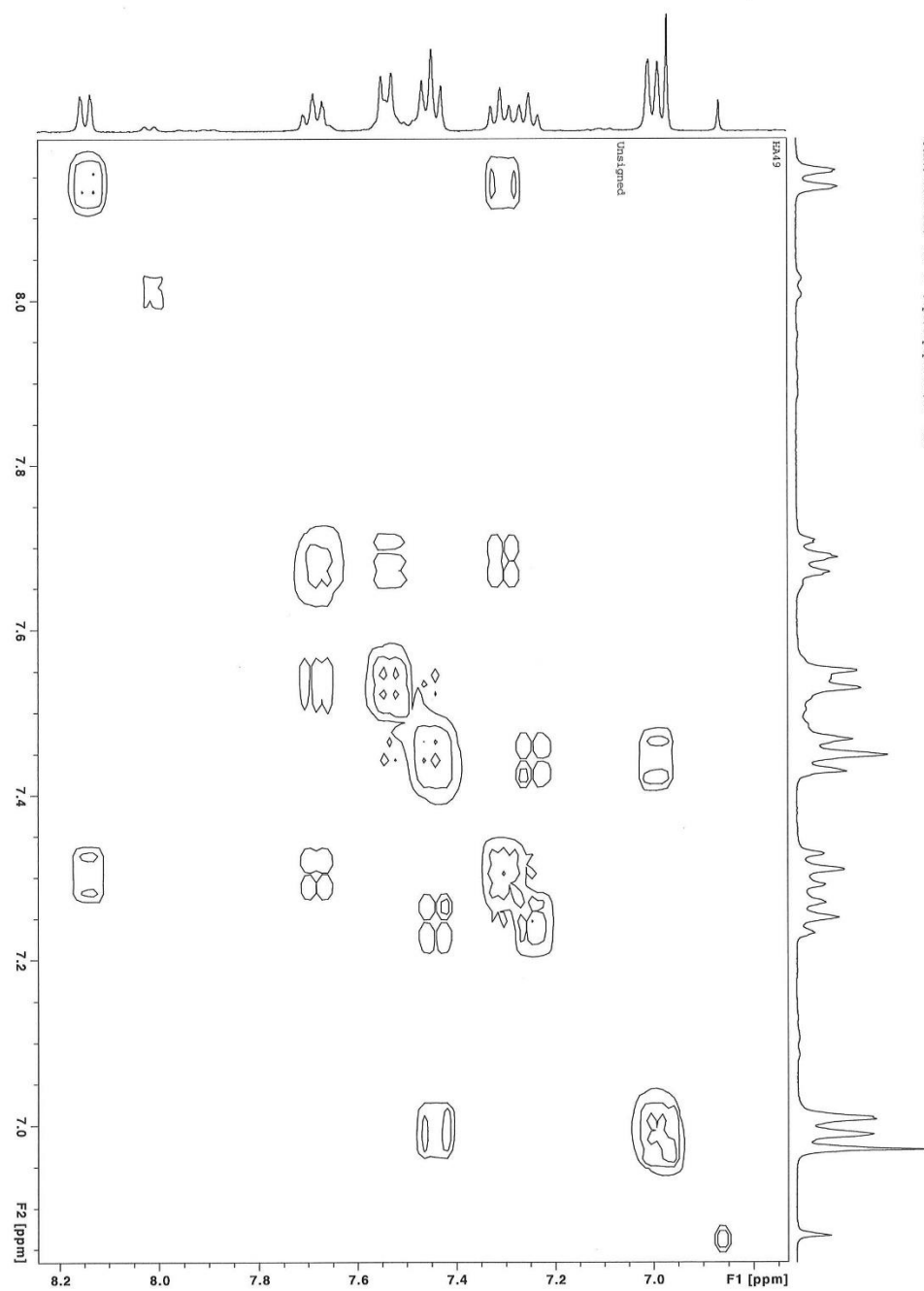


**Figure S59.** Detail of  $^1\text{H}$  NMR spectrum of compound **7c**.



**Figure S60.** Detail of  $^1\text{H}$  NMR spectrum of compound **7c**.

$$\cos \theta = \frac{H_1 - H_2}{H_1 + H_2}$$

**Figure S62.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7c**.

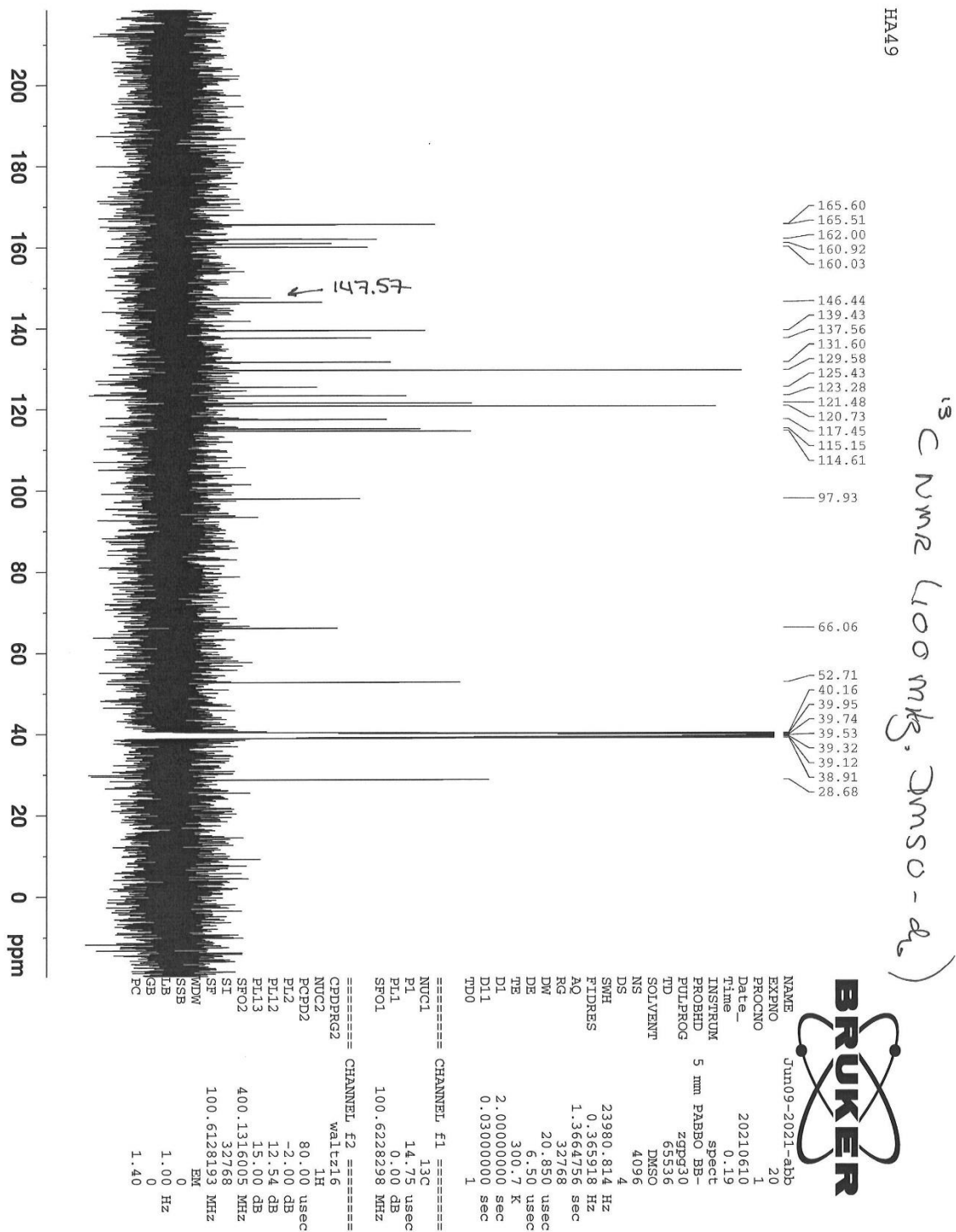
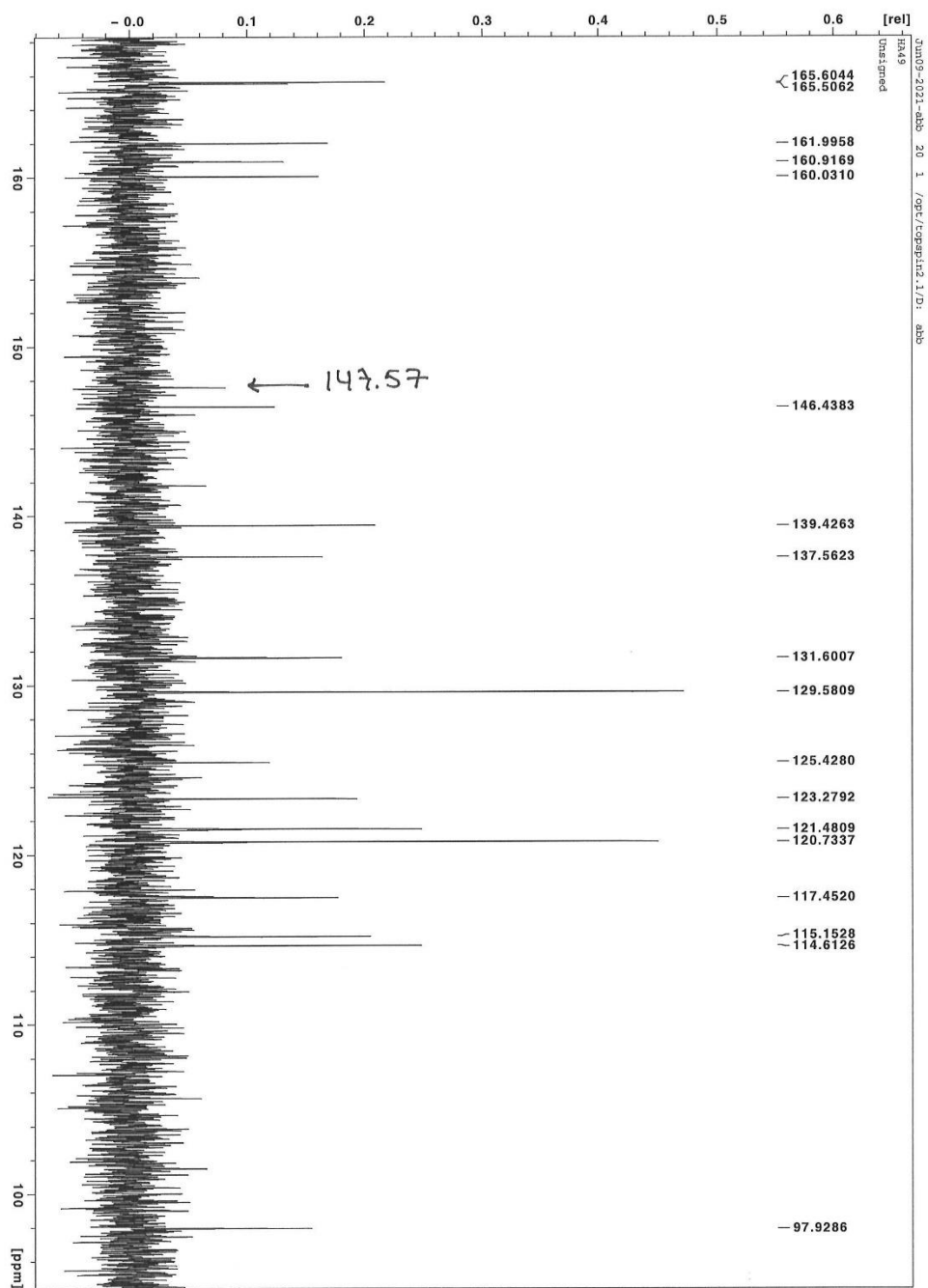
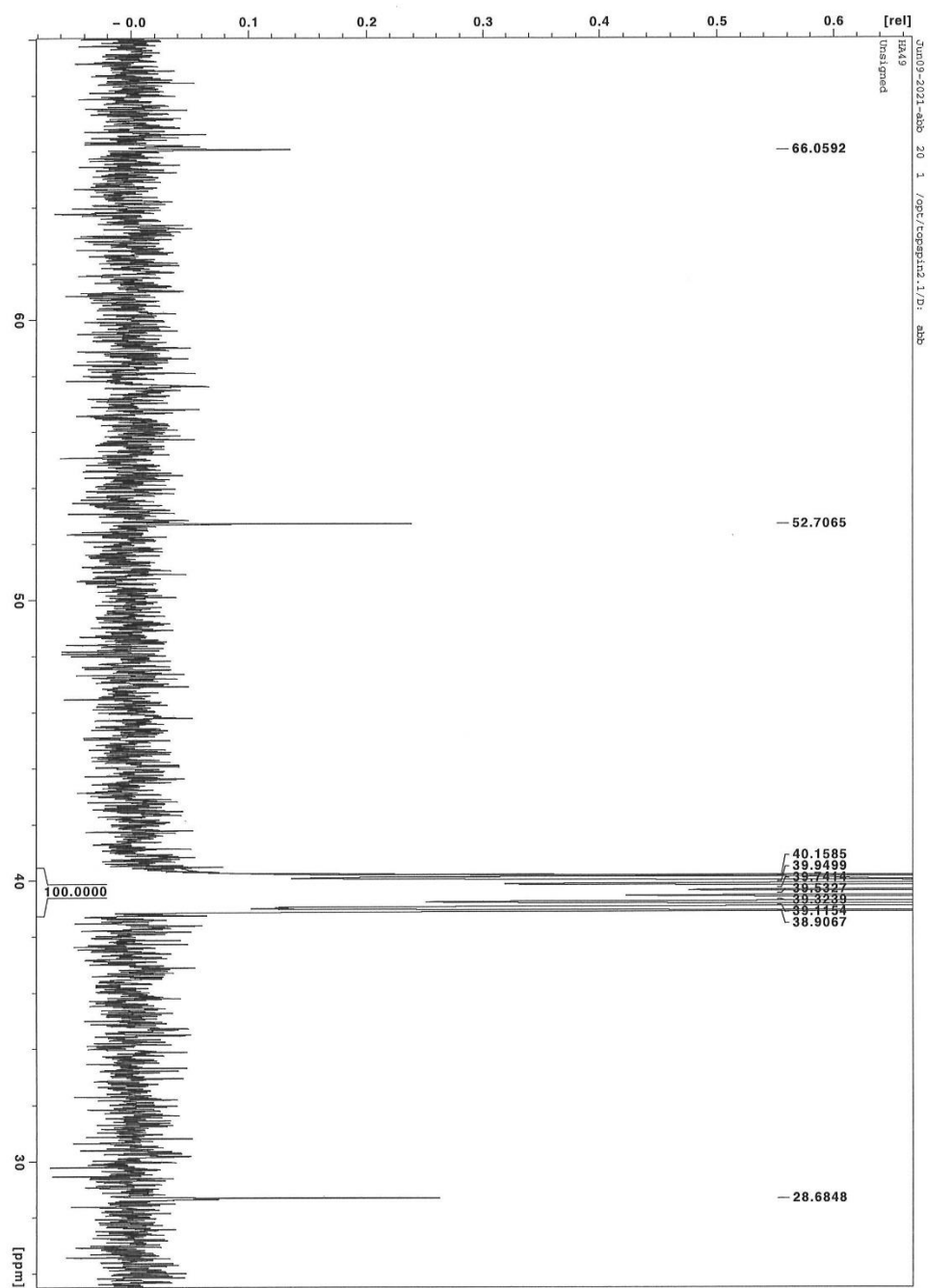


Figure S63. <sup>13</sup>C NMR spectrum of compound **7c** (100 MHz, DMSO-d<sub>6</sub>).

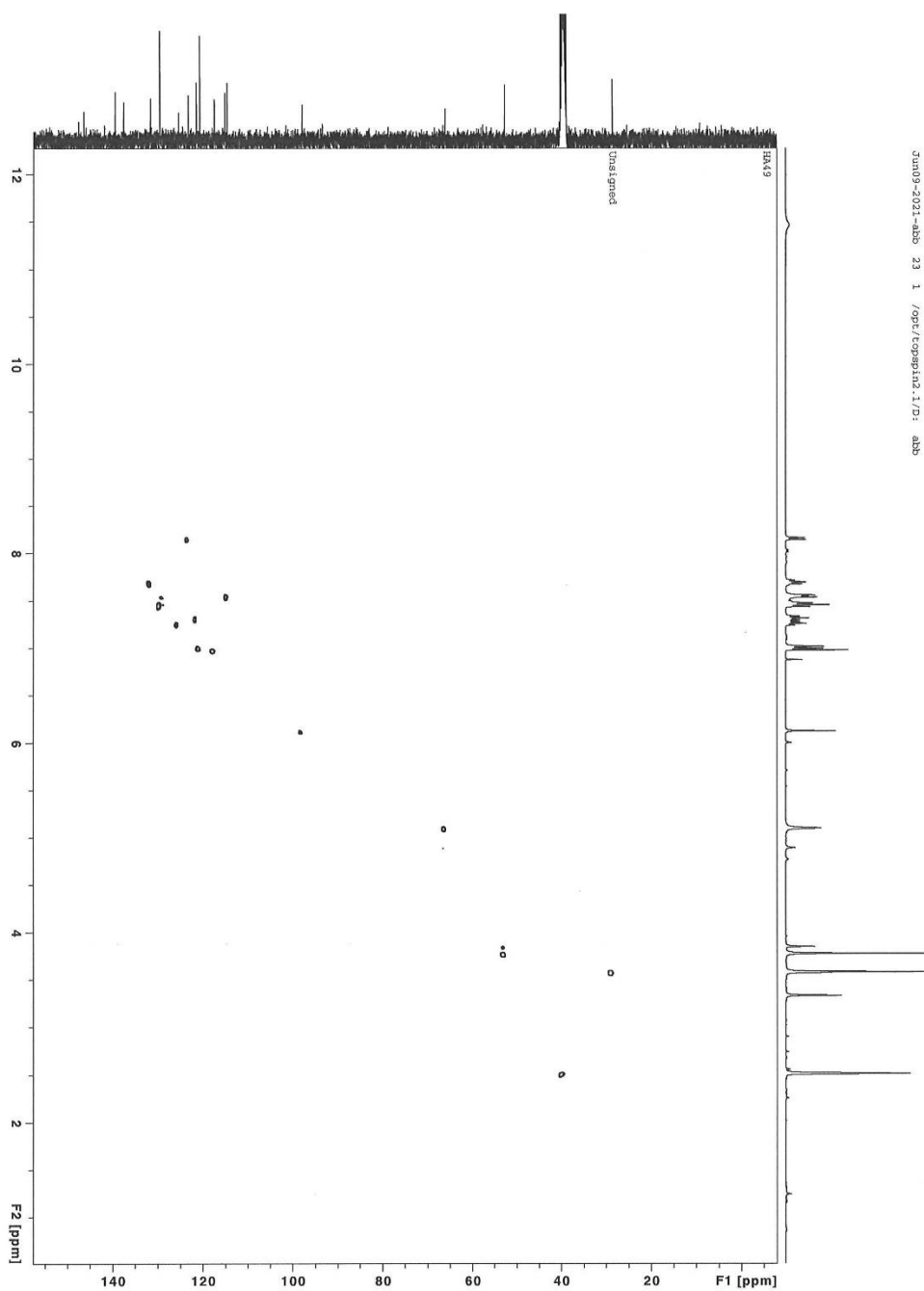


**Figure S64.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **7c**.

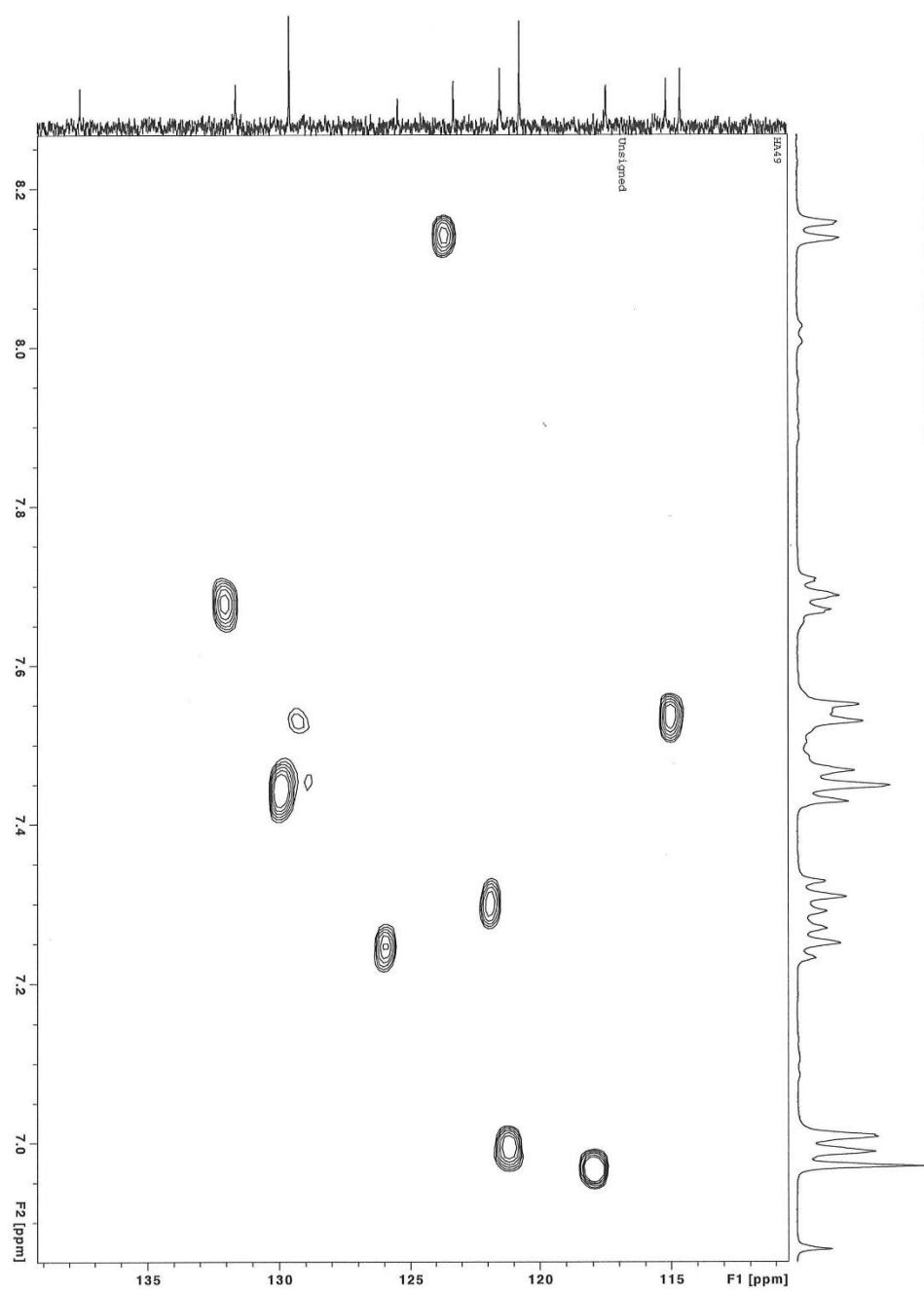




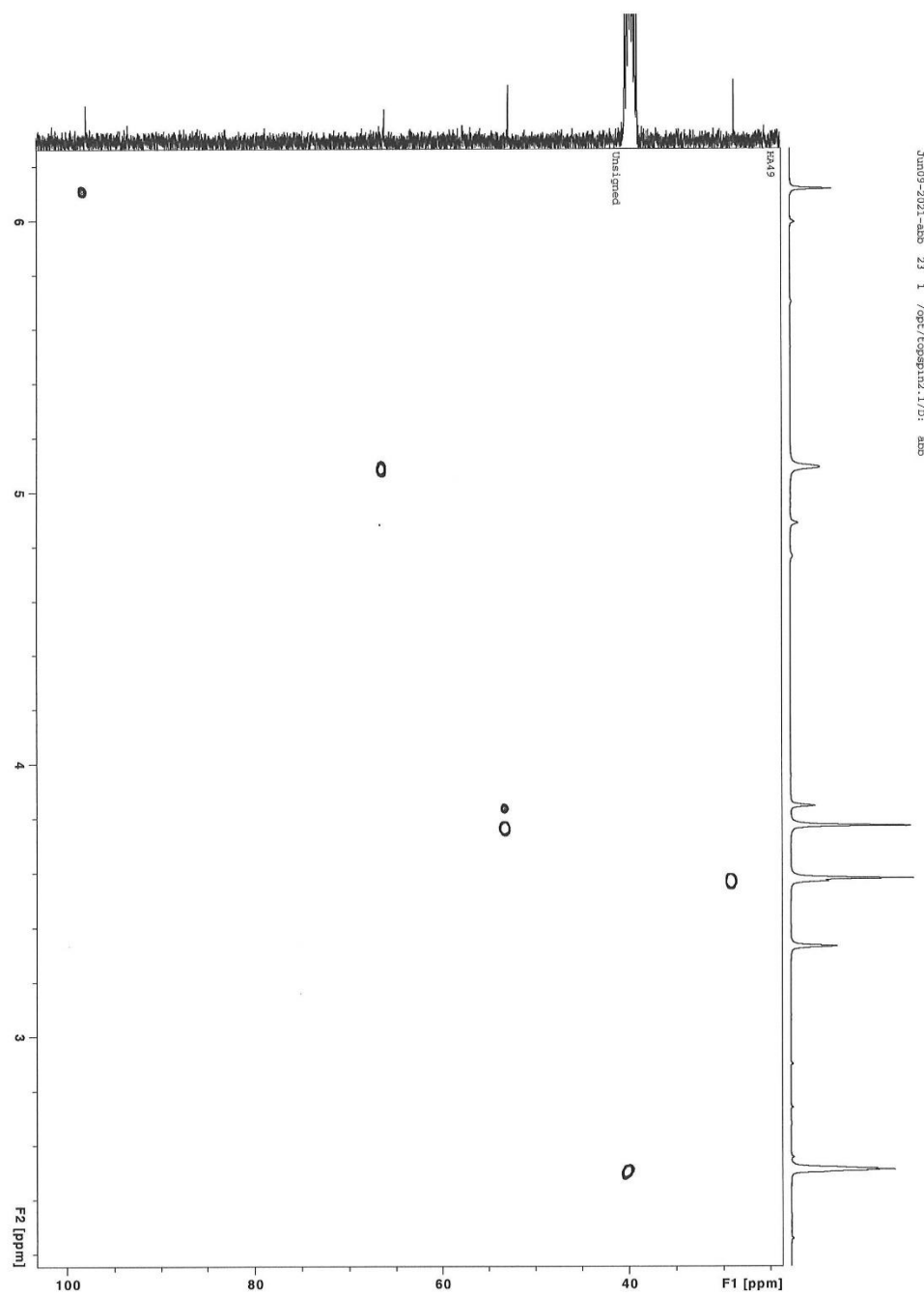
**Figure S66.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **7c**.



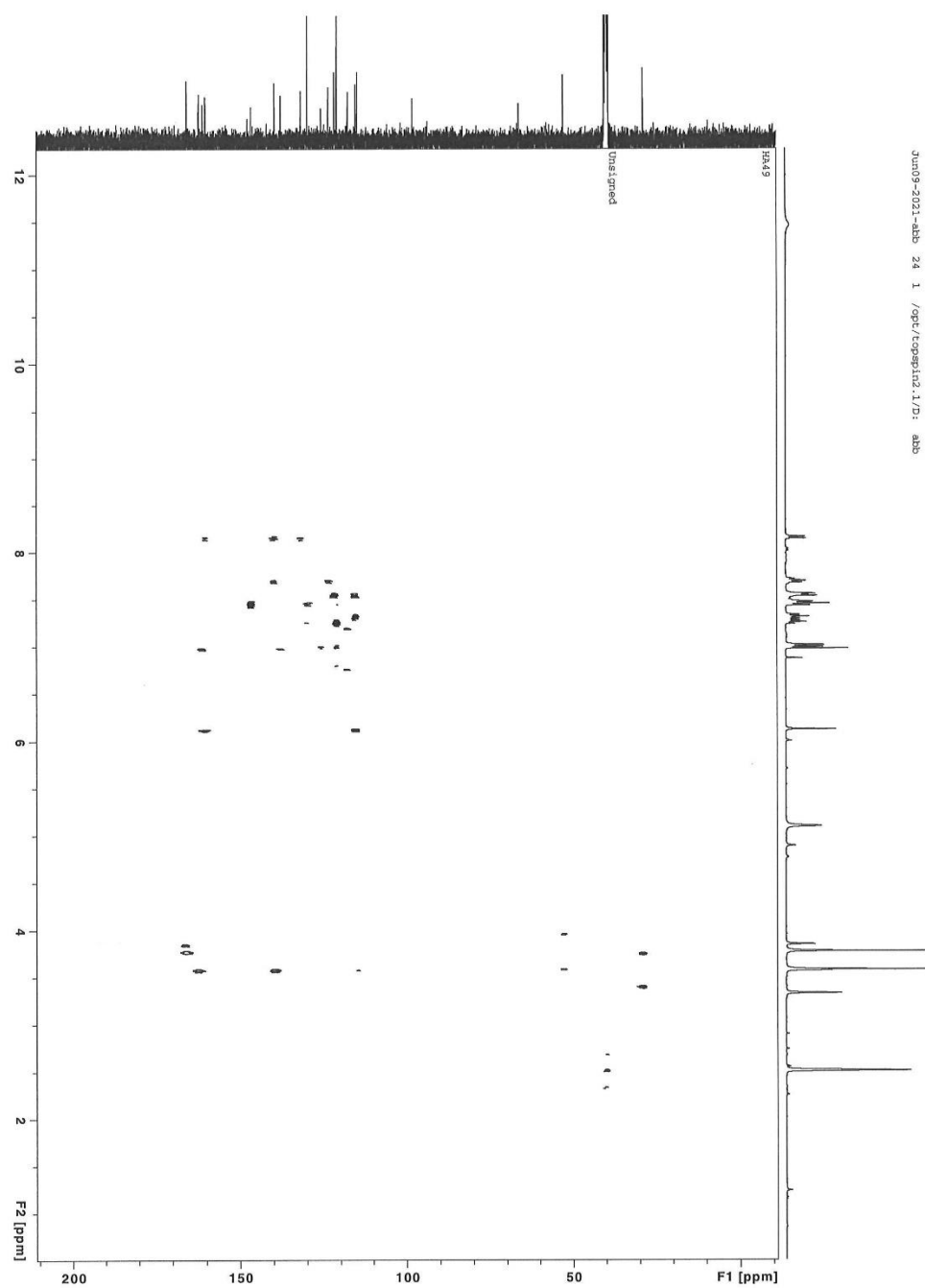
**Figure S67.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7c**.



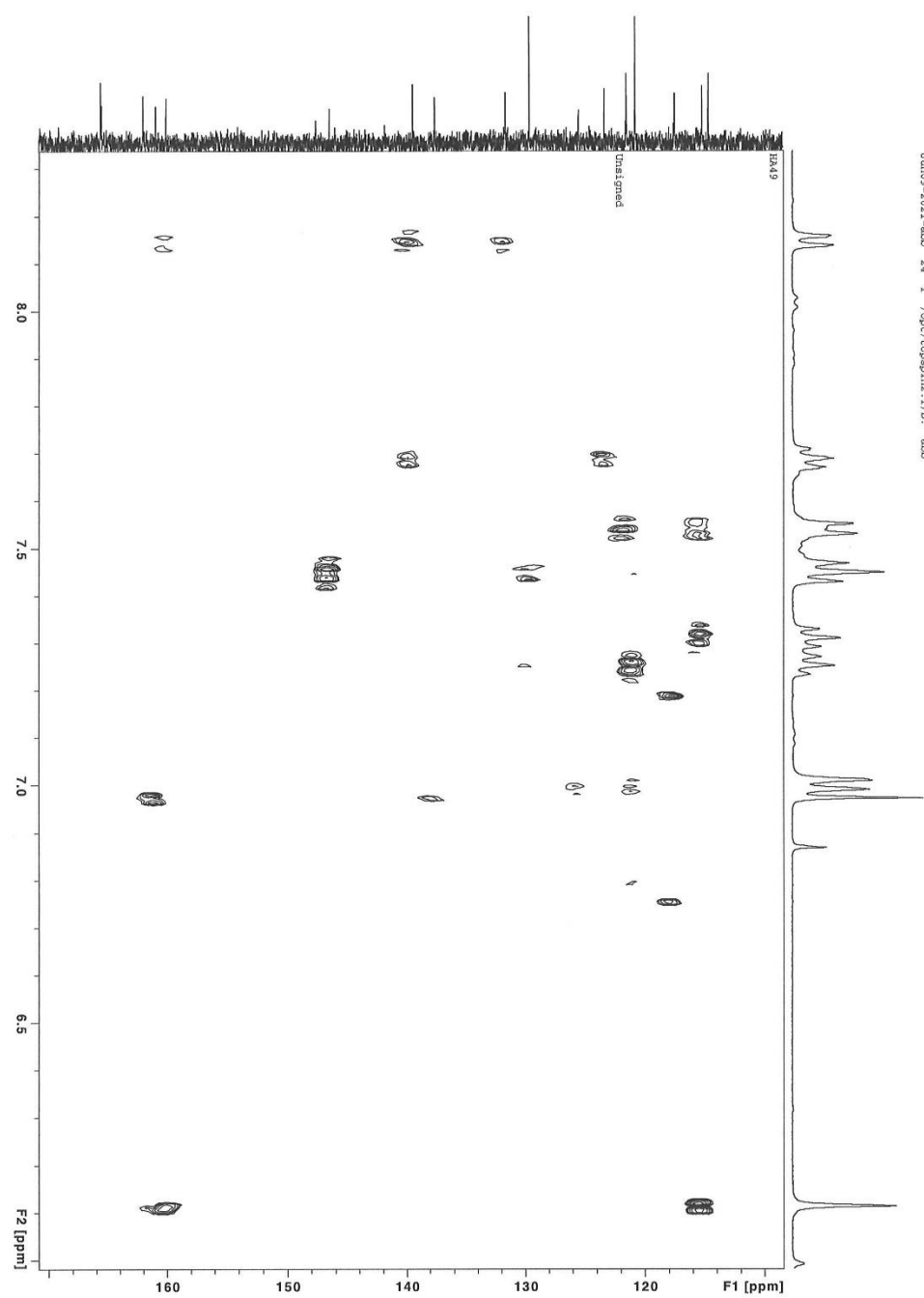
**Figure S68.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7c**.



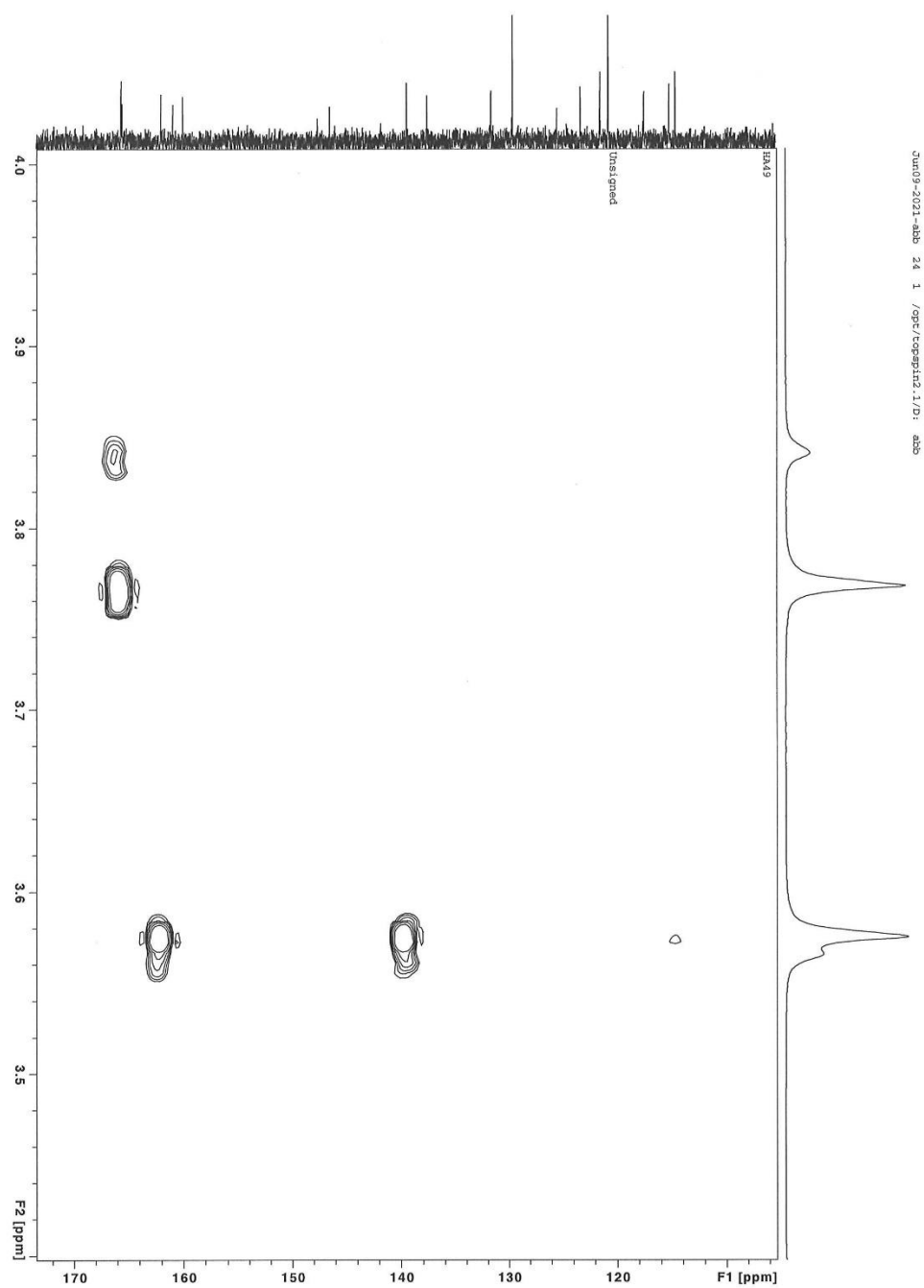
**Figure S69.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7c**.



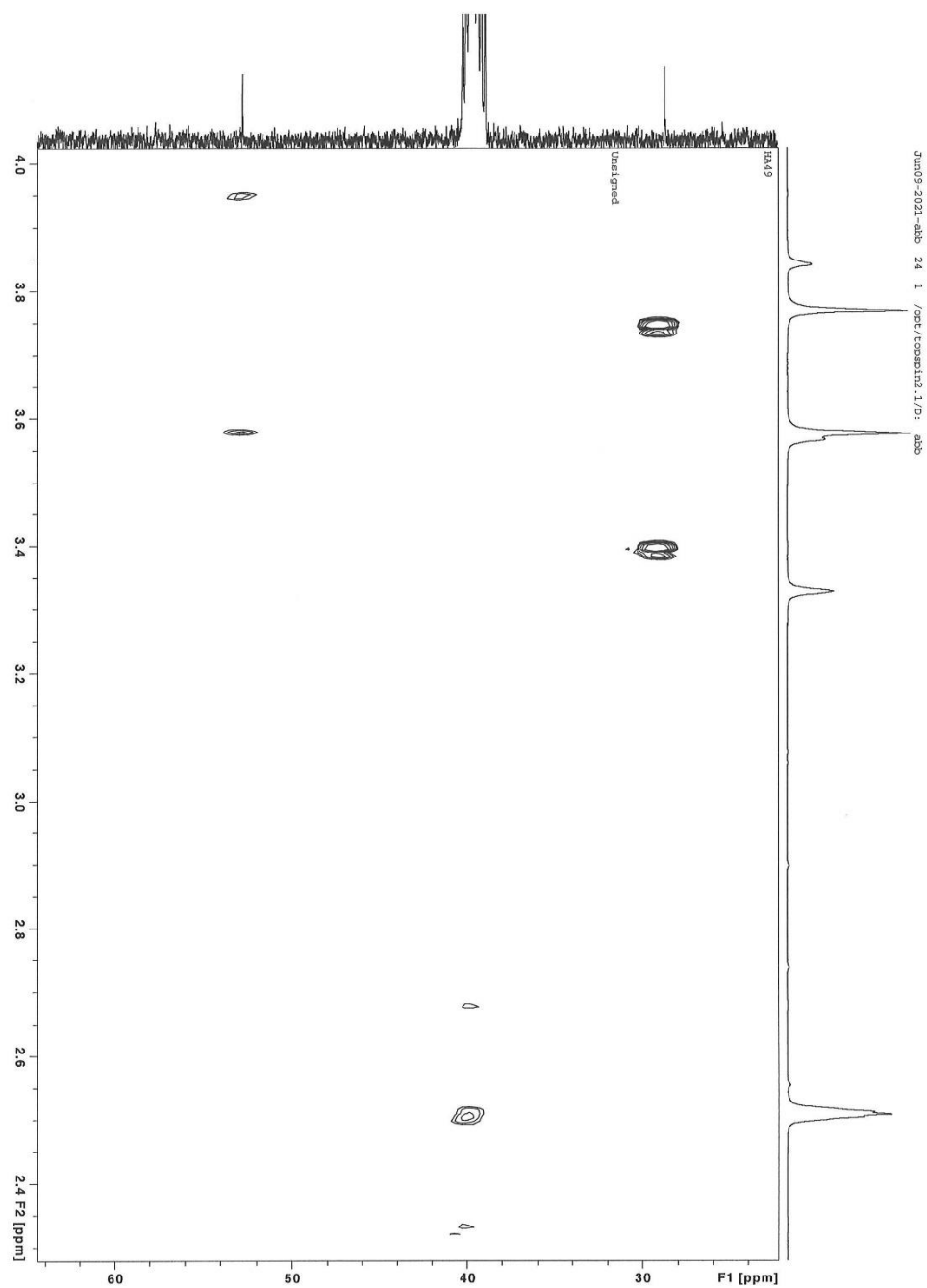
**Figure S70.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7c**.



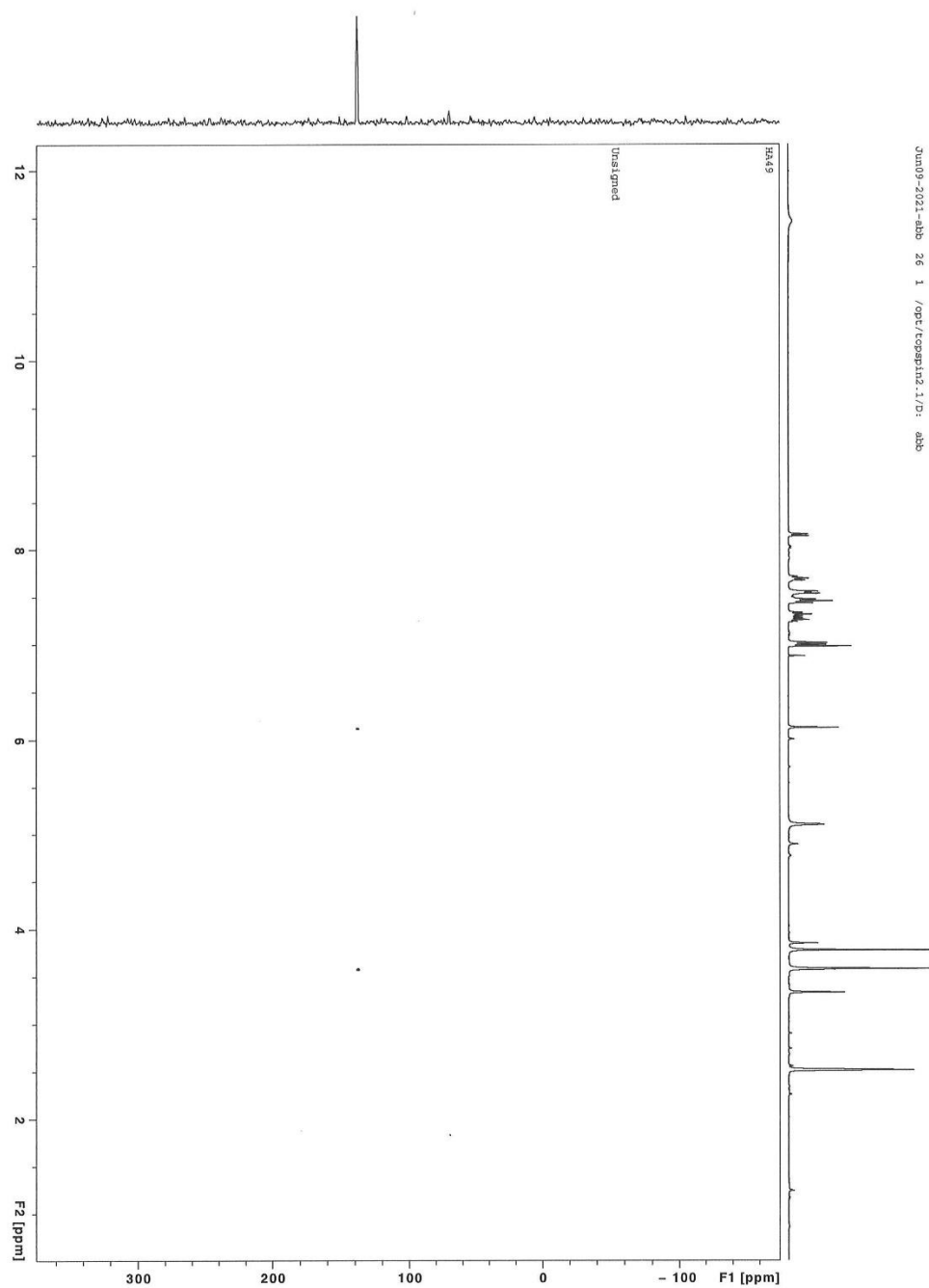
**Figure S71.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7c**.



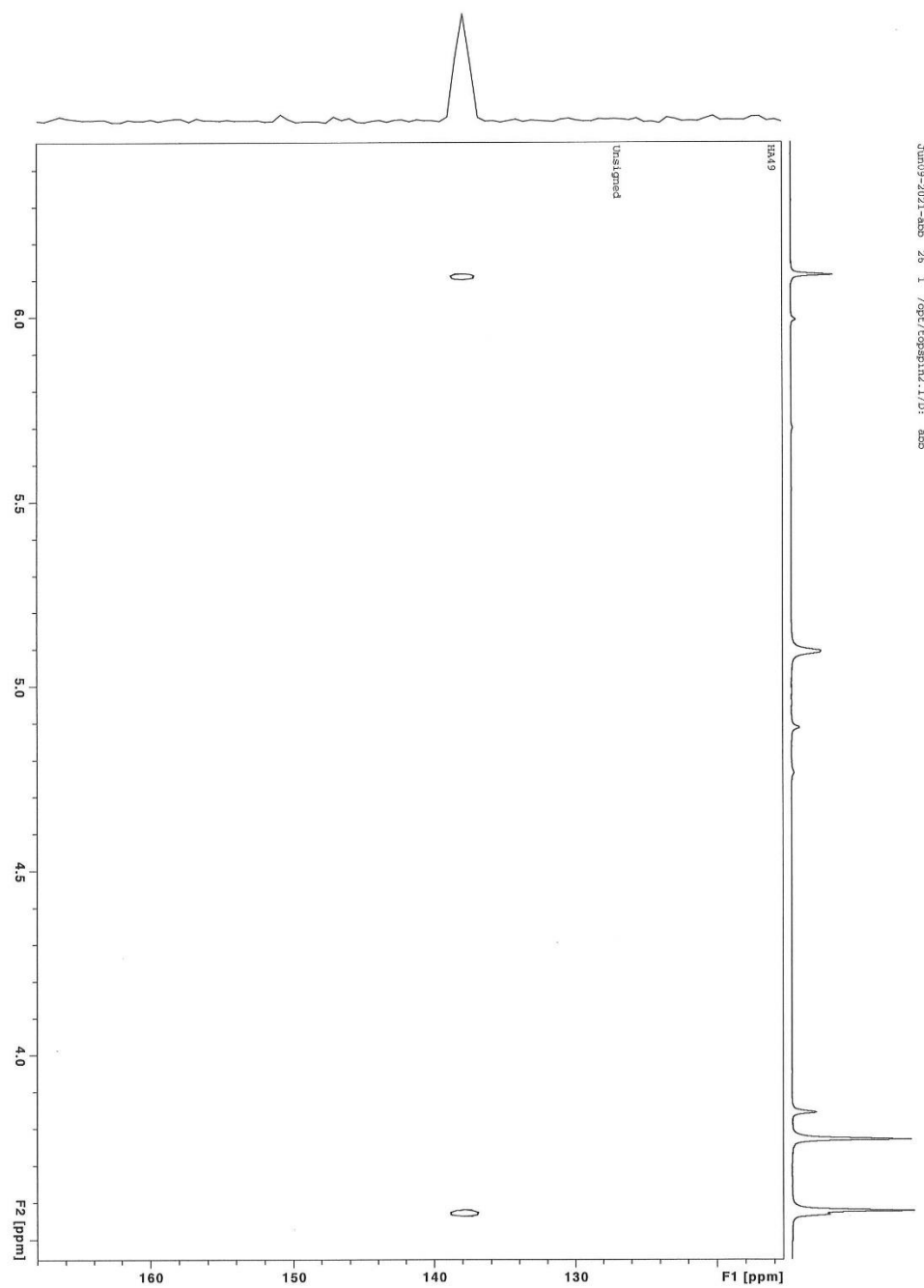
**Figure S72.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7c**.



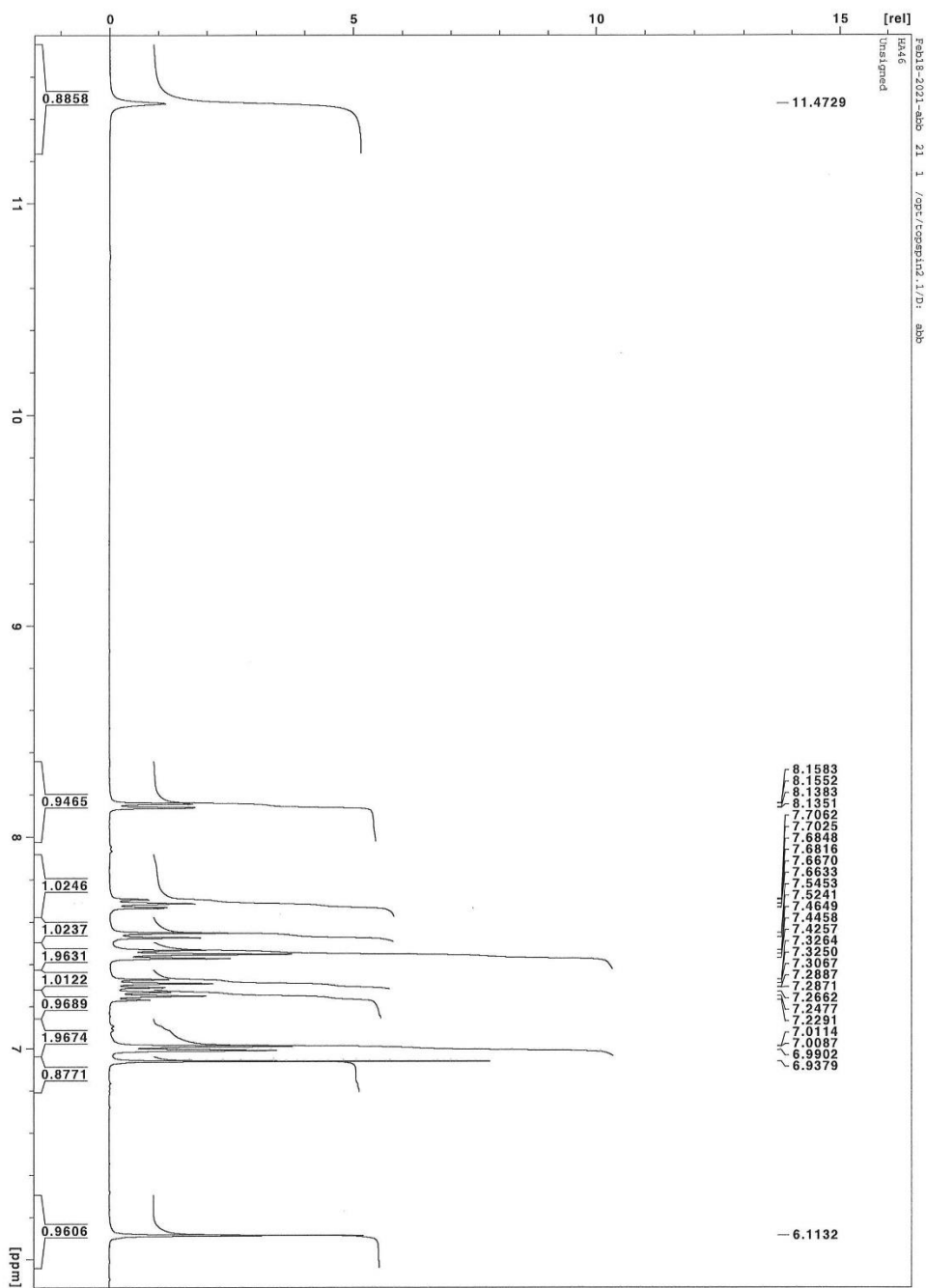
**Figure S73.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7c**.



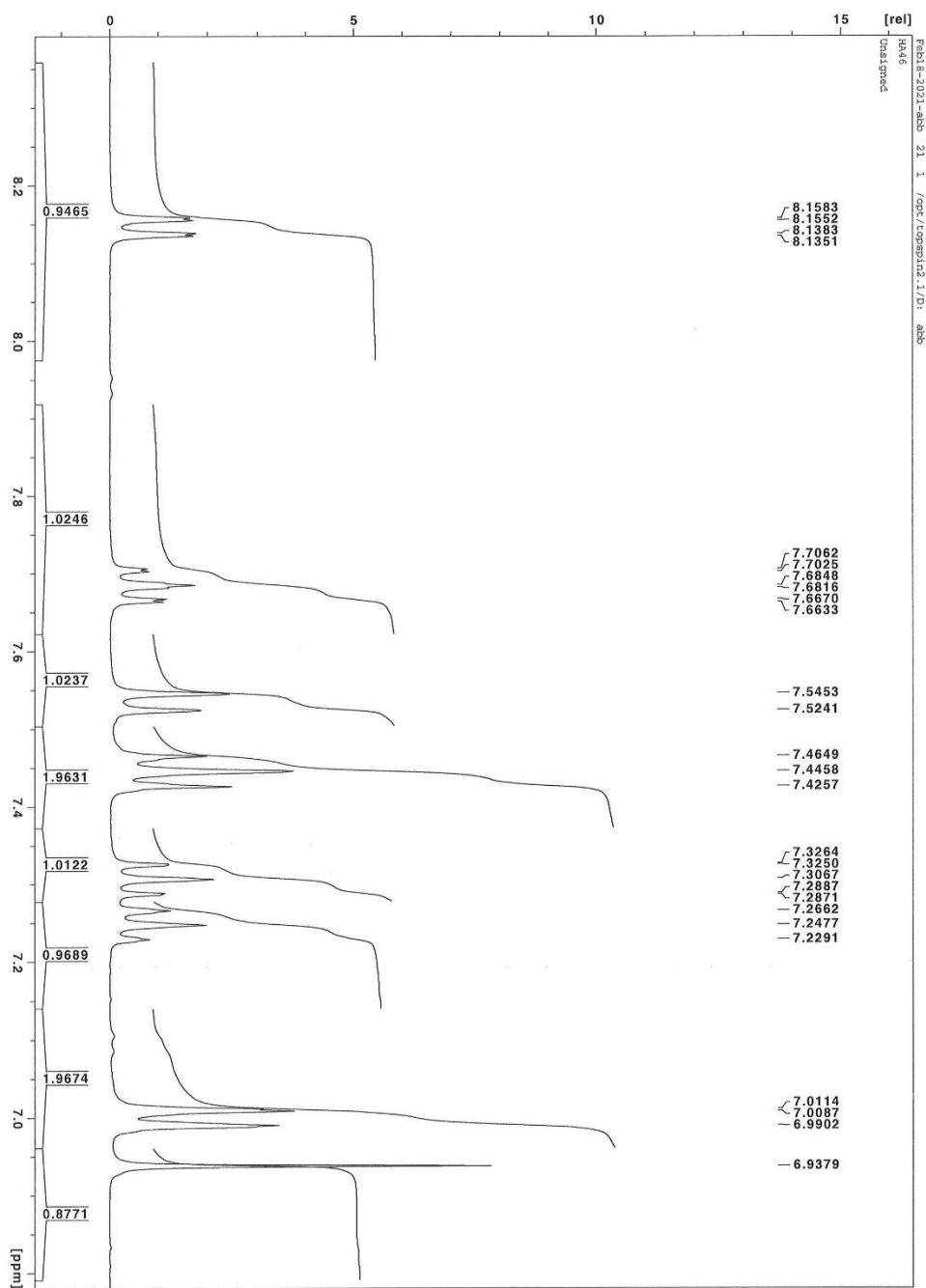
**Figure S74.**  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **7c** ( $^1\text{H}$ - $^{15}\text{N}$  experiment gave no cross peaks).



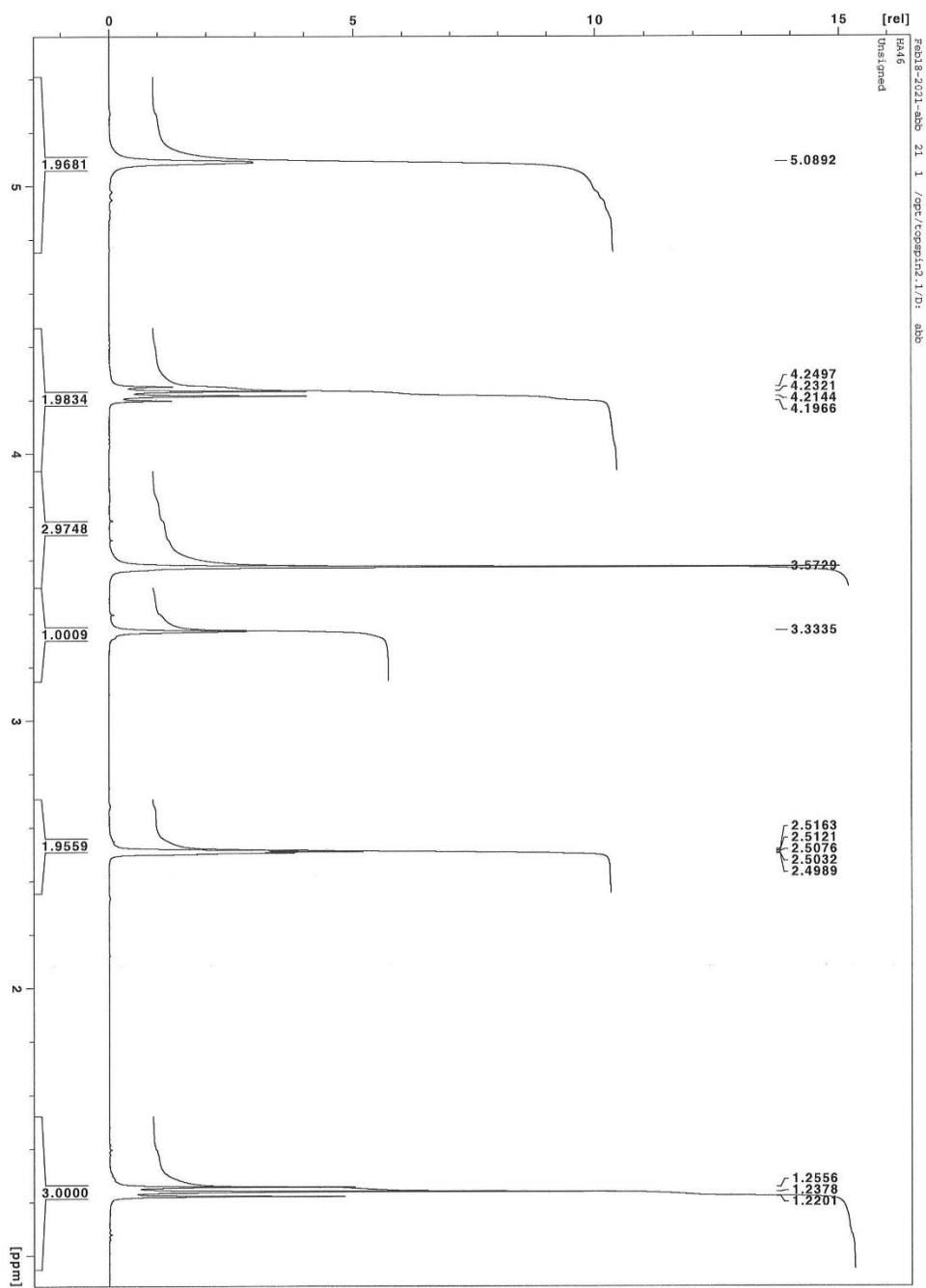
**Figure S75.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **7c**.



**Figure S76.**  $^1\text{H}$  spectrum of compound **7d** (400 MHz,  $\text{DMSO-}d_6$ ).



**Figure S77.** Detail of <sup>1</sup>H spectrum of compound **7d**.



**Figure S78.** Detail of  $^1\text{H}$  spectrum of compound **7d**.

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<sup>1</sup>H-<sup>1</sup>H COSY

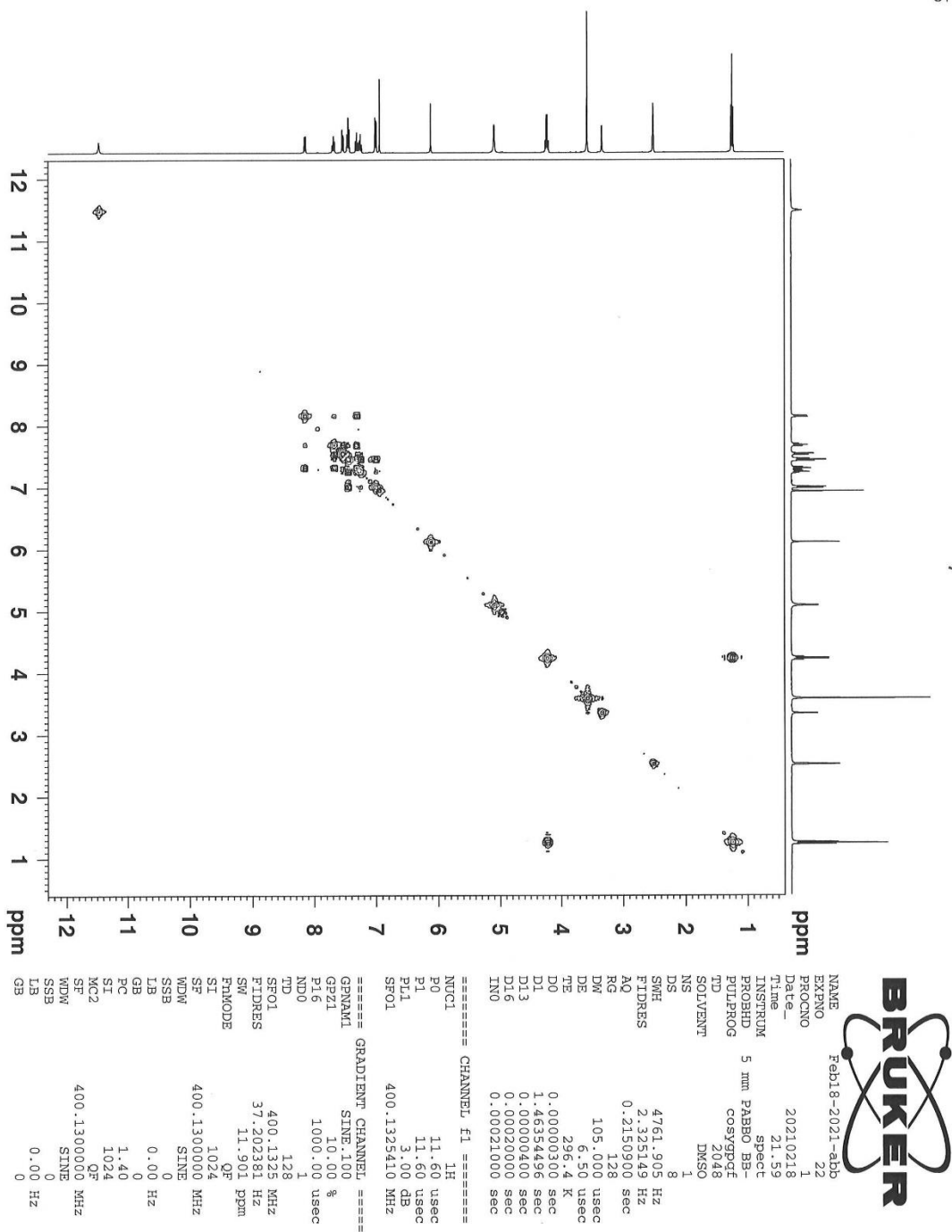
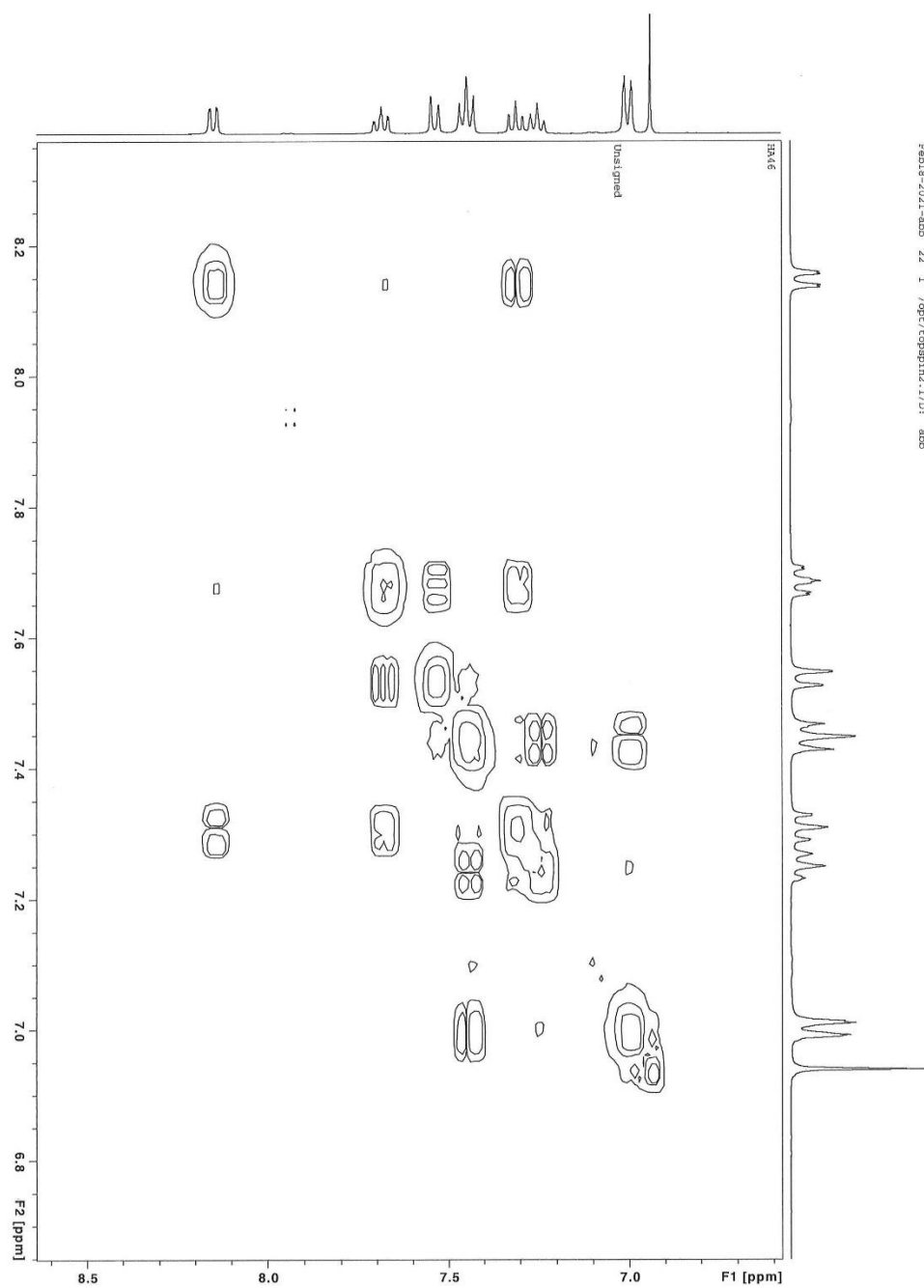
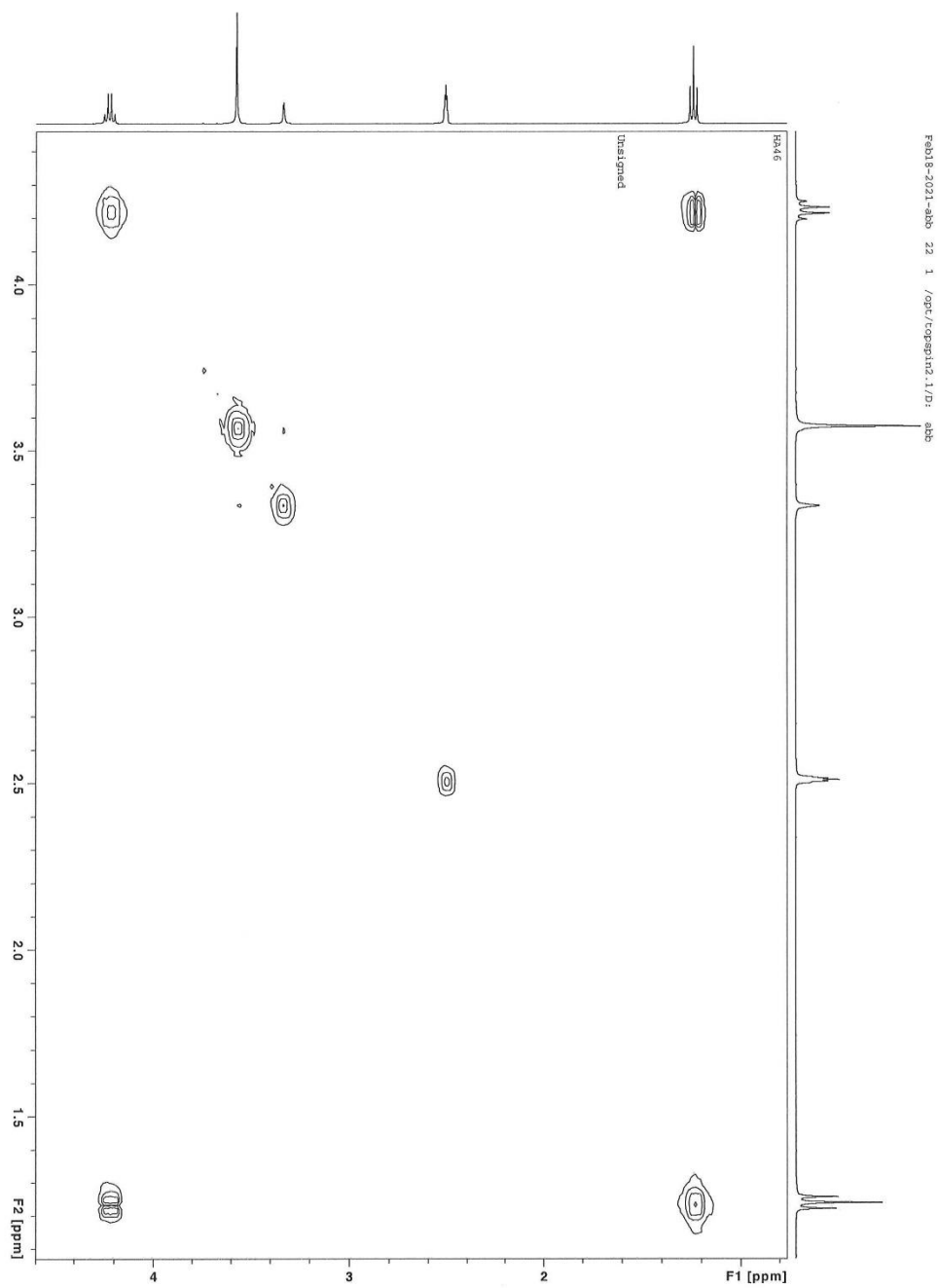


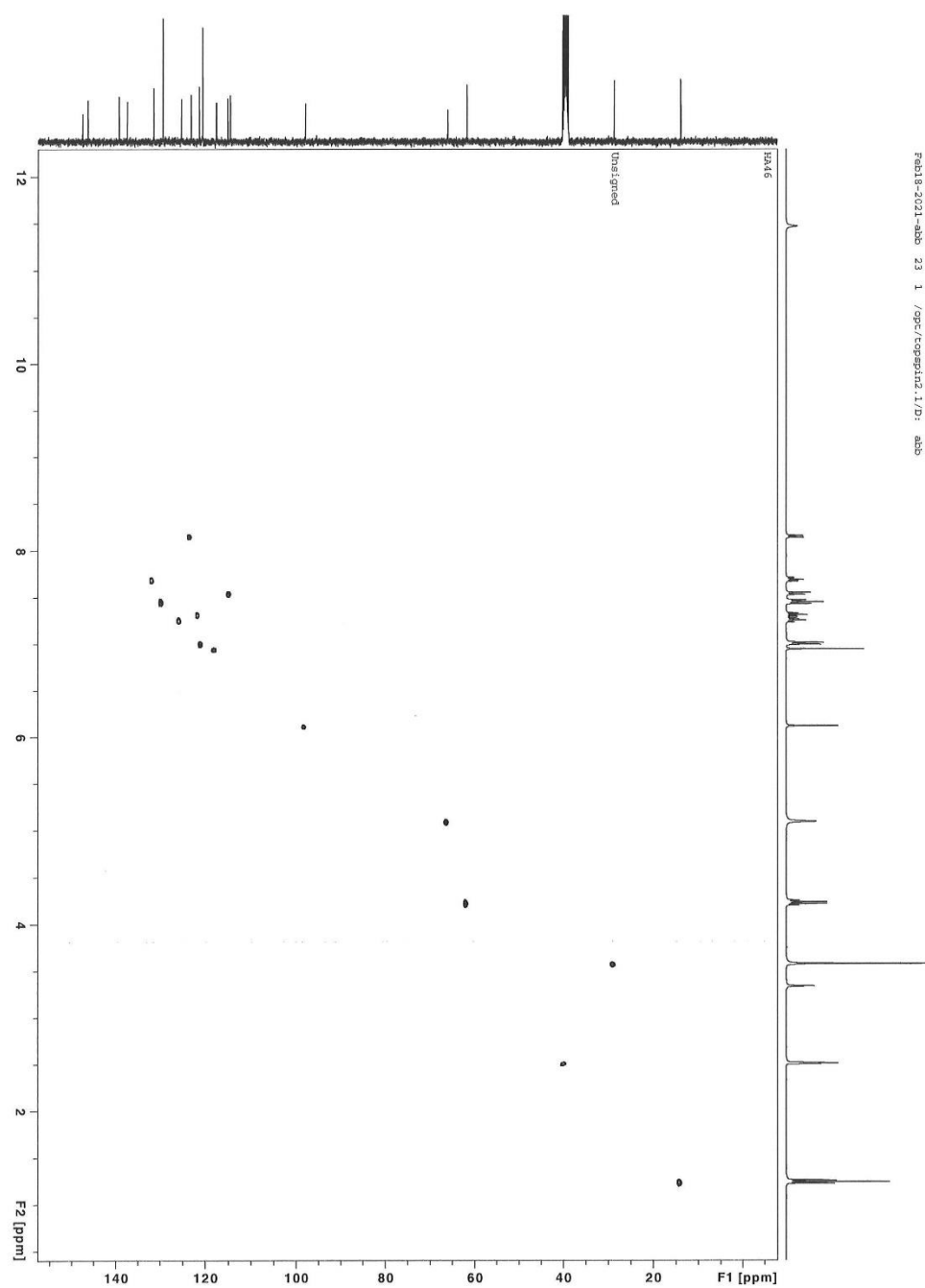
Figure S79. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **7d**.



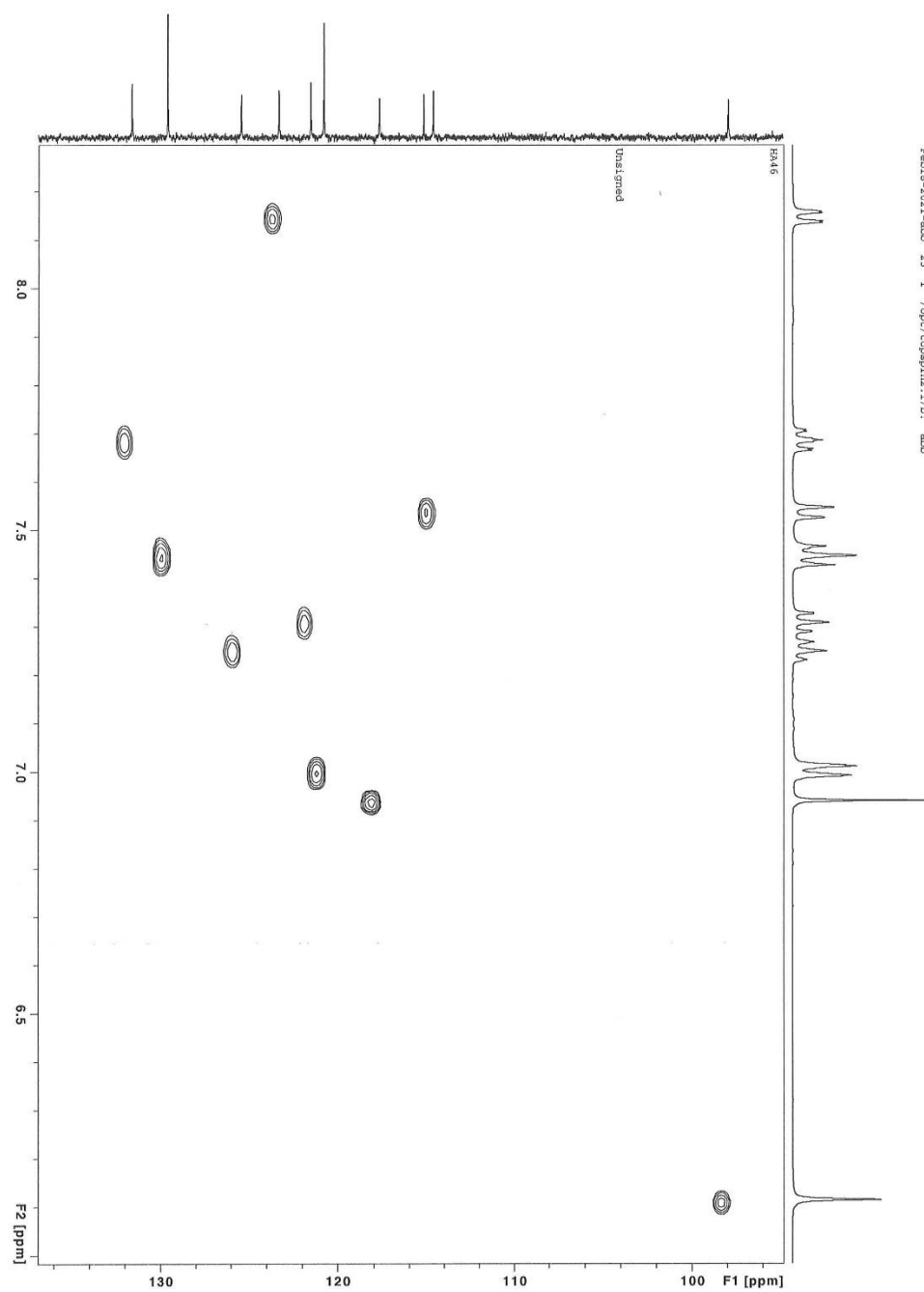
**Figure S80.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7d**.



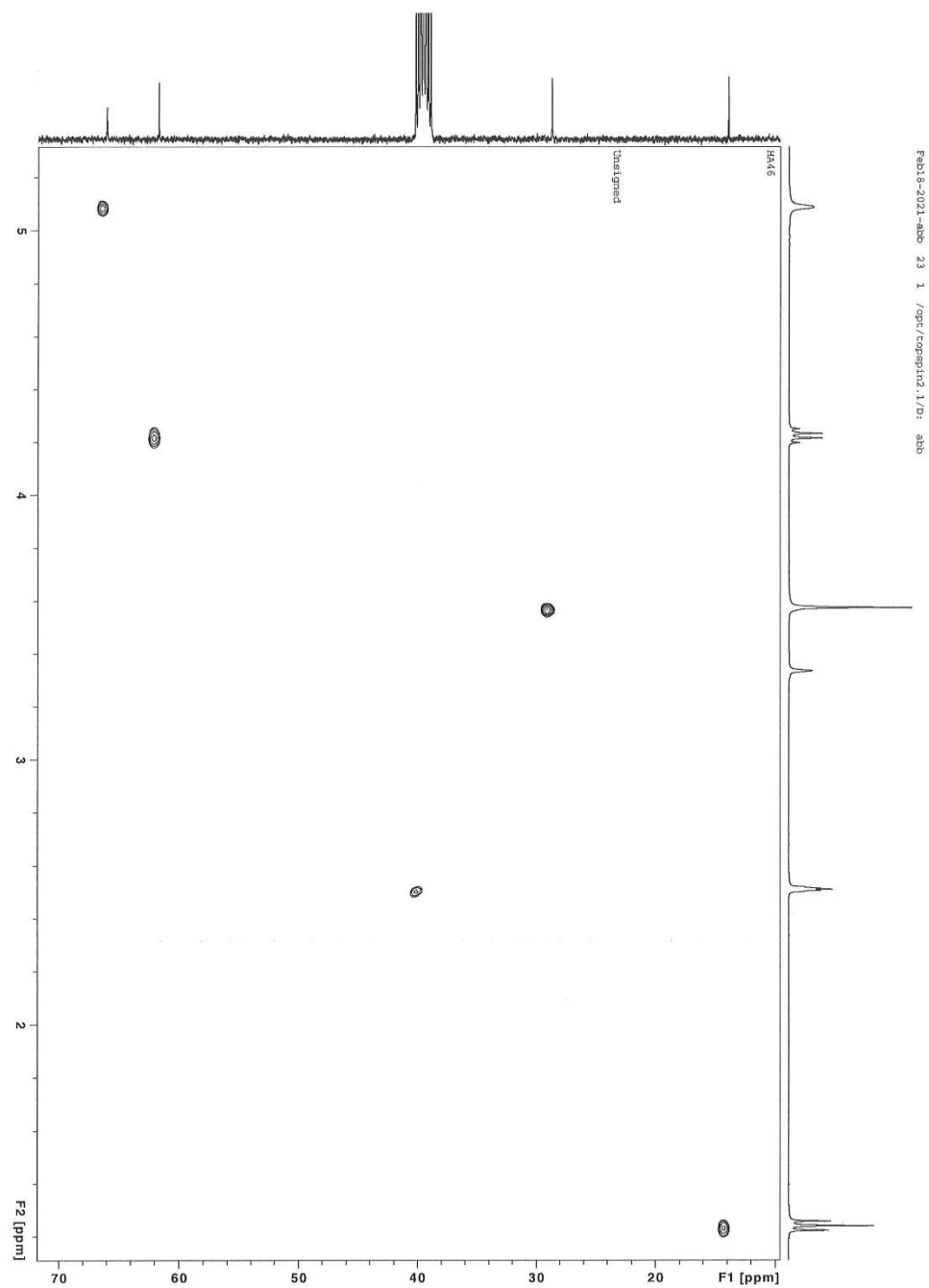
**Figure S81.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7d**.



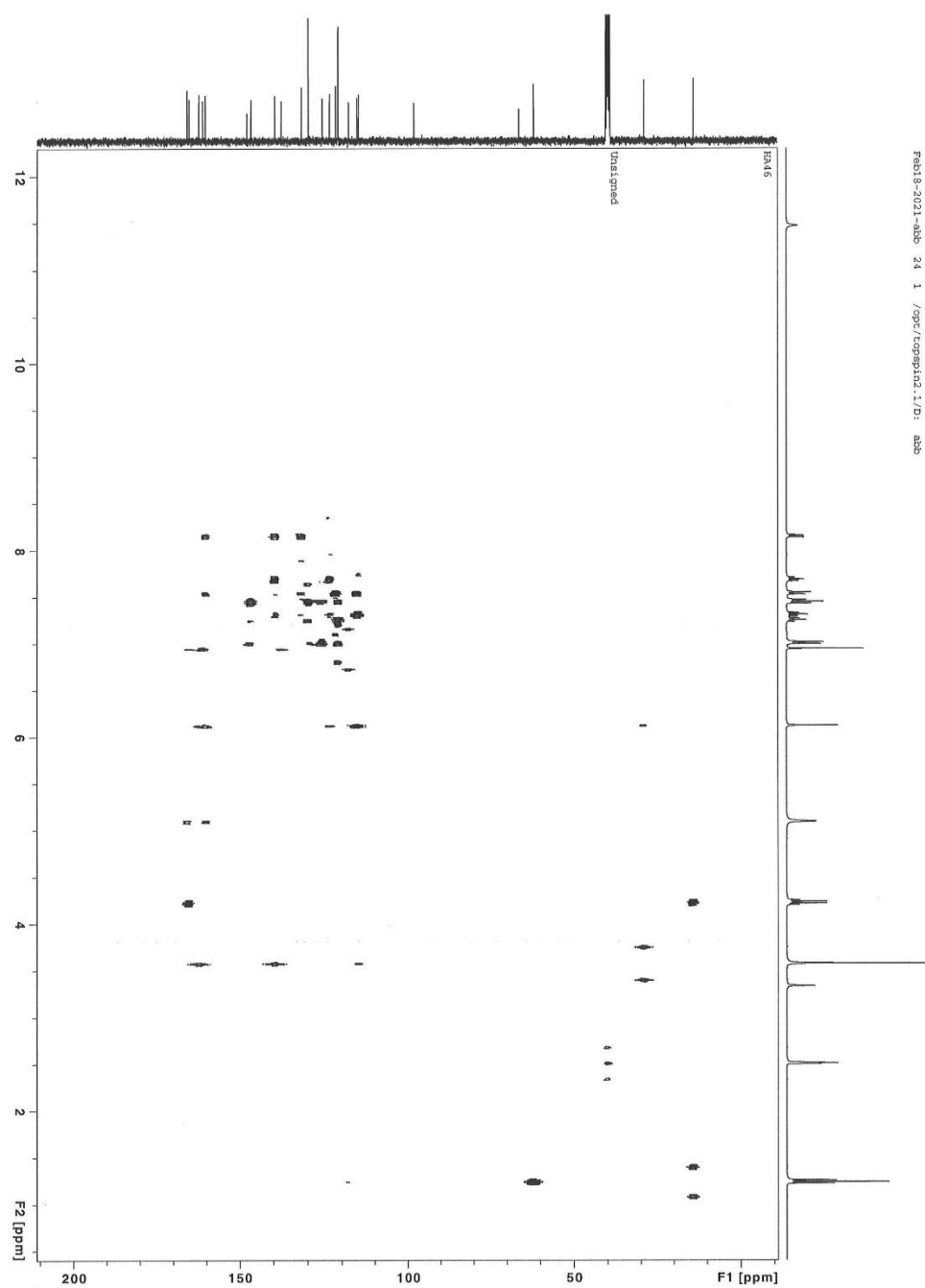
**Figure S82.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7d**.



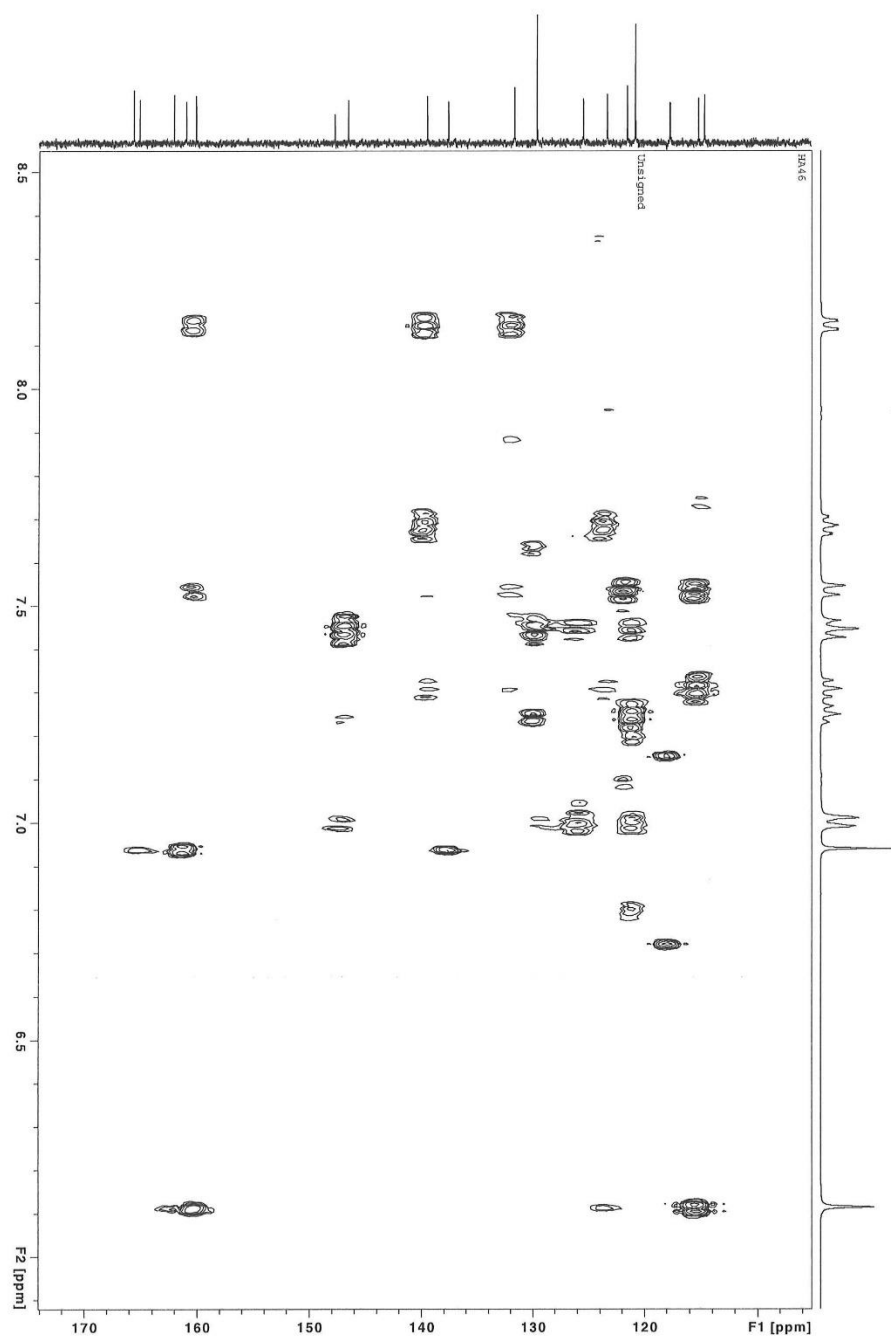
**Figure S83.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7d**.



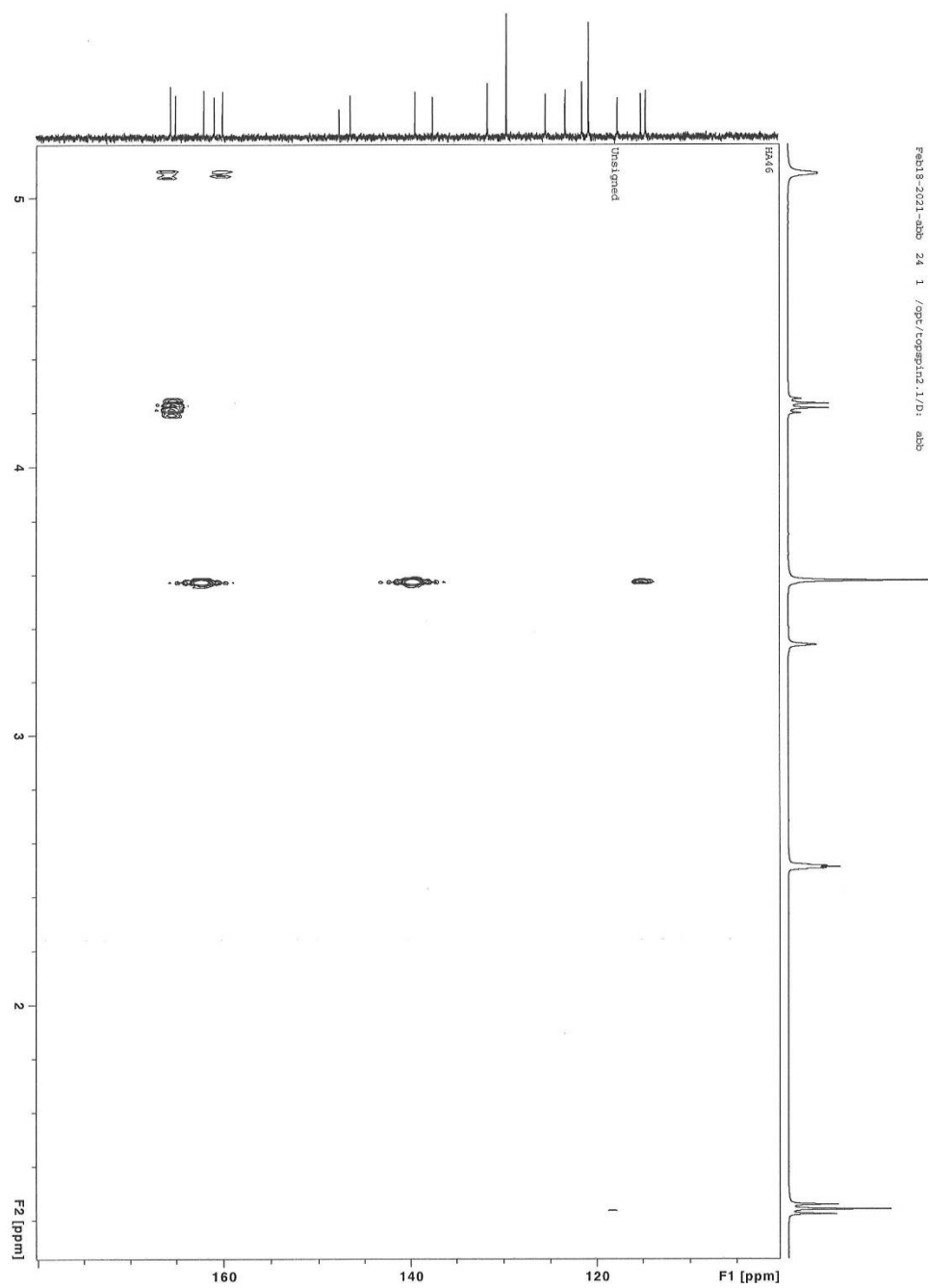
**Figure S84.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7d**.



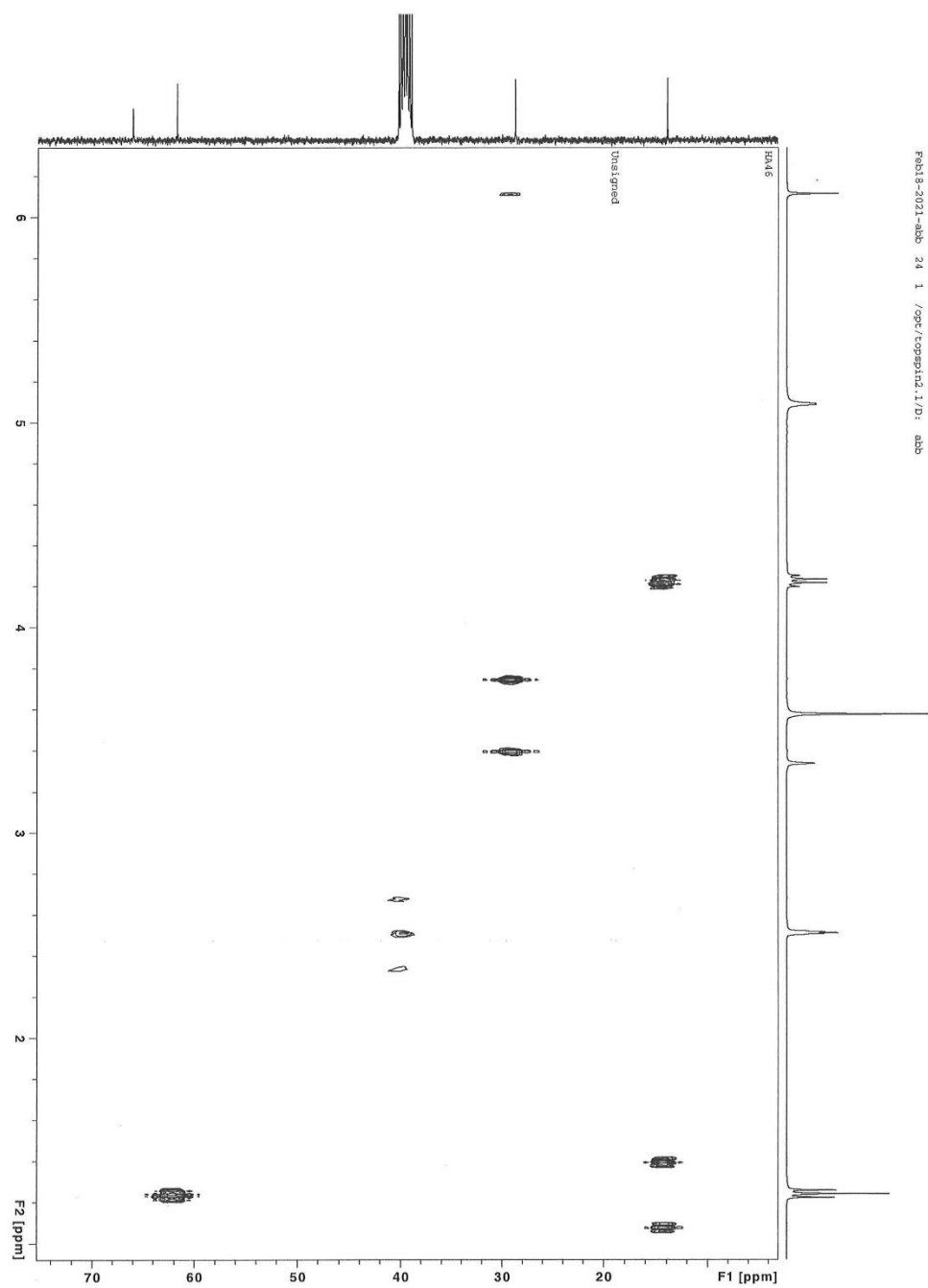
**Figure S85.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7d**.



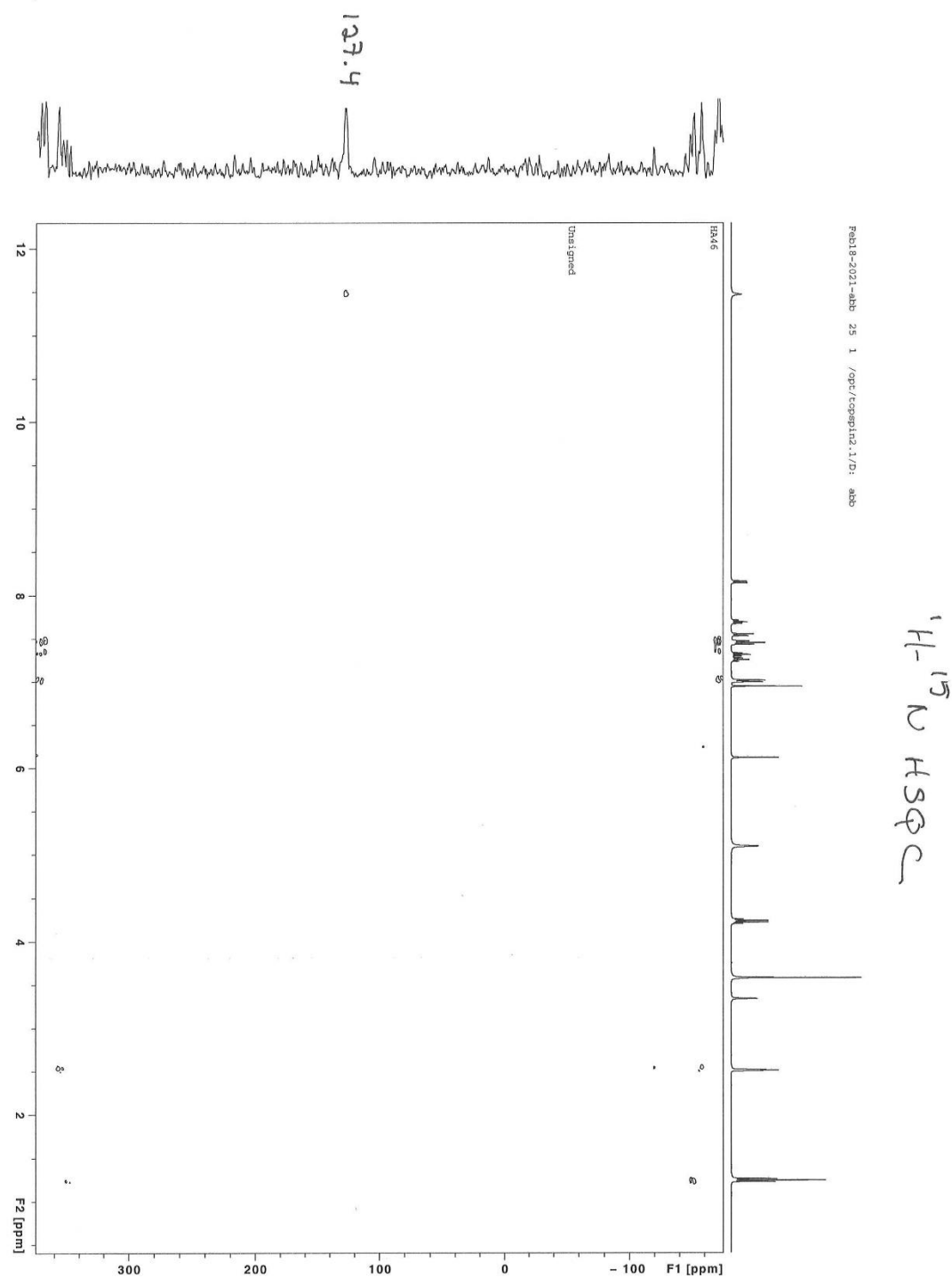
**Figure S86.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7d**.



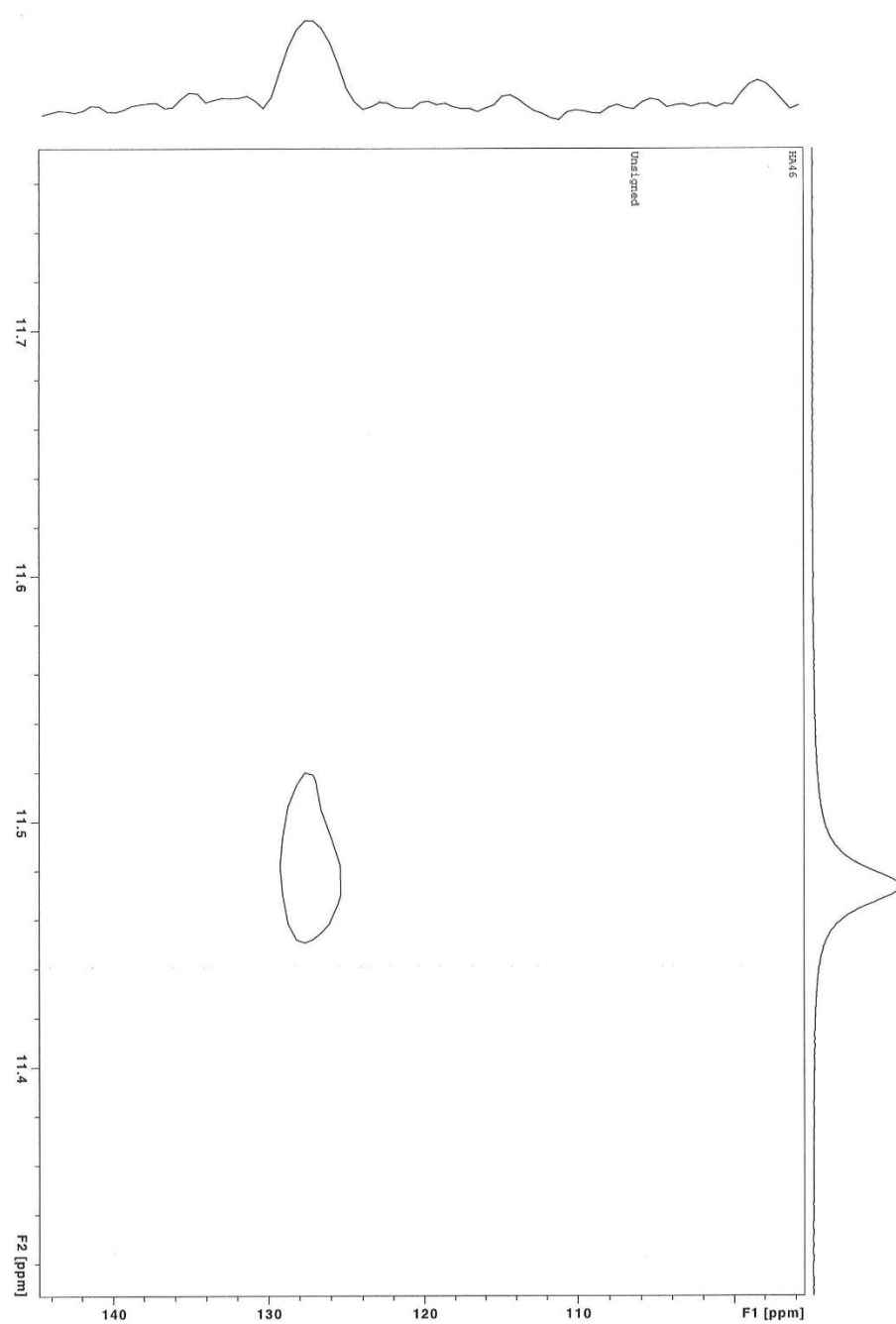
**Figure S87.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7d**.



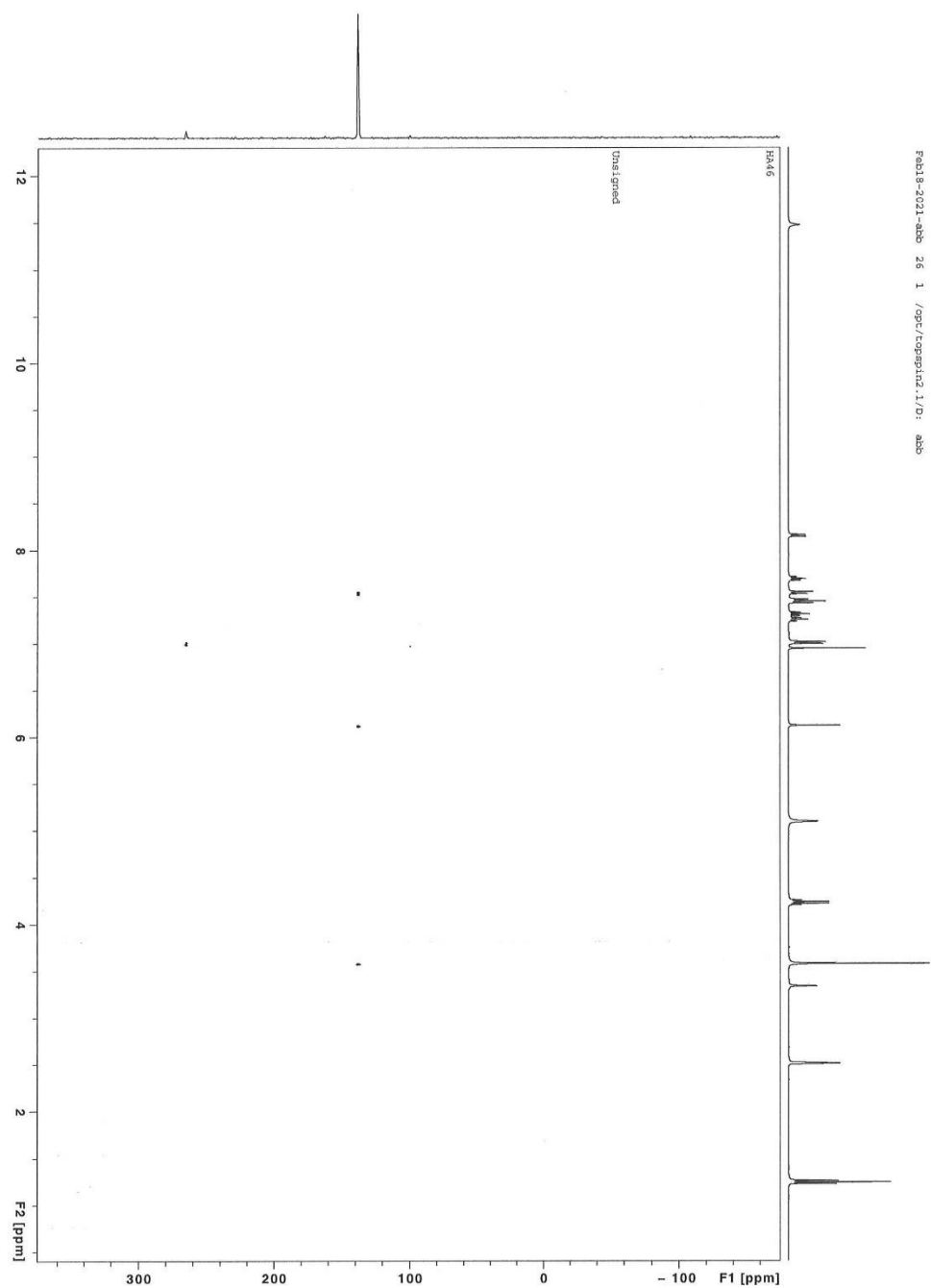
**Figure S88.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7d**.



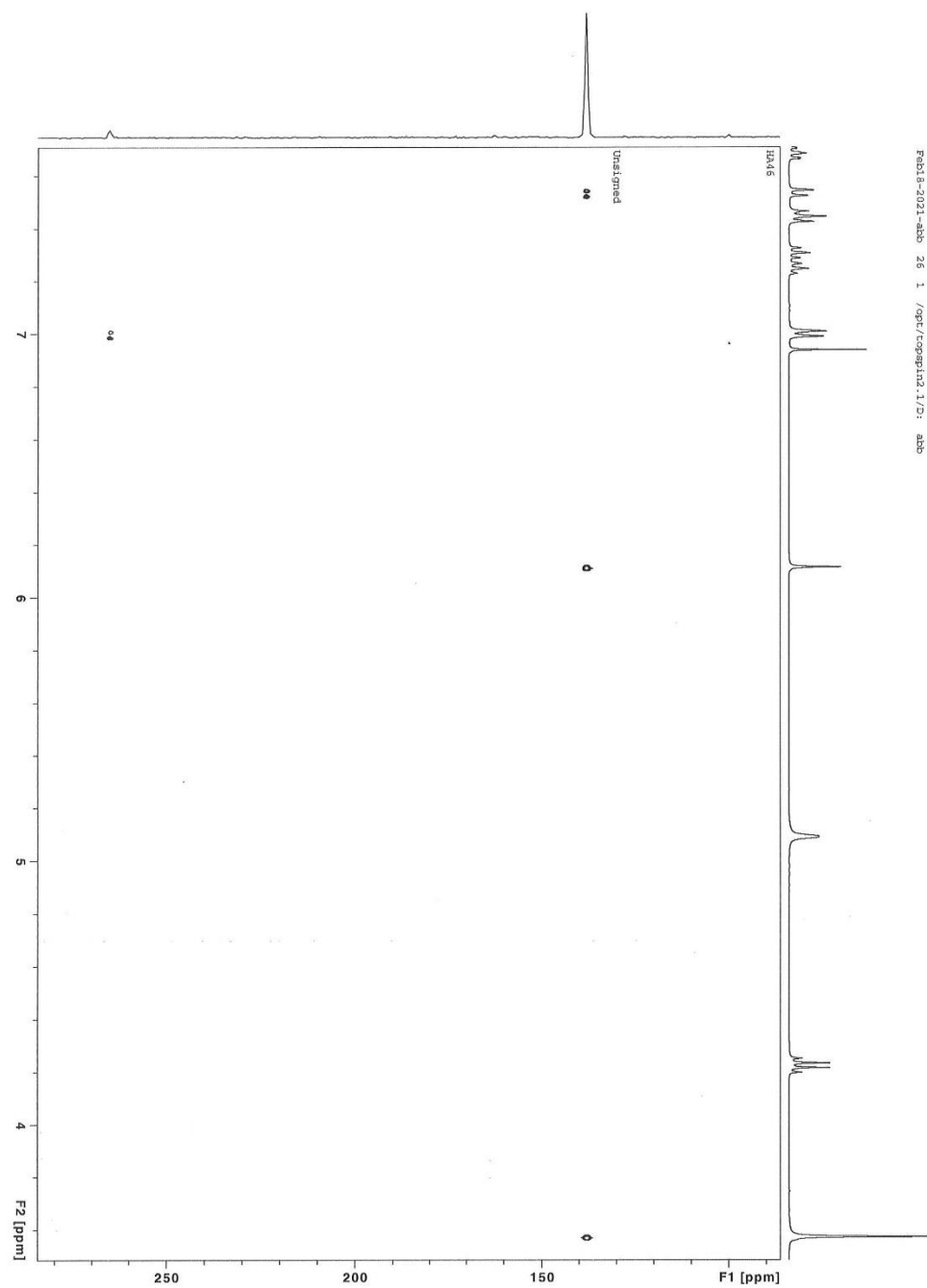
**Figure S89.**  $^1\text{H}-^{15}\text{N}$  HSQC spectrum of compound **7d**.



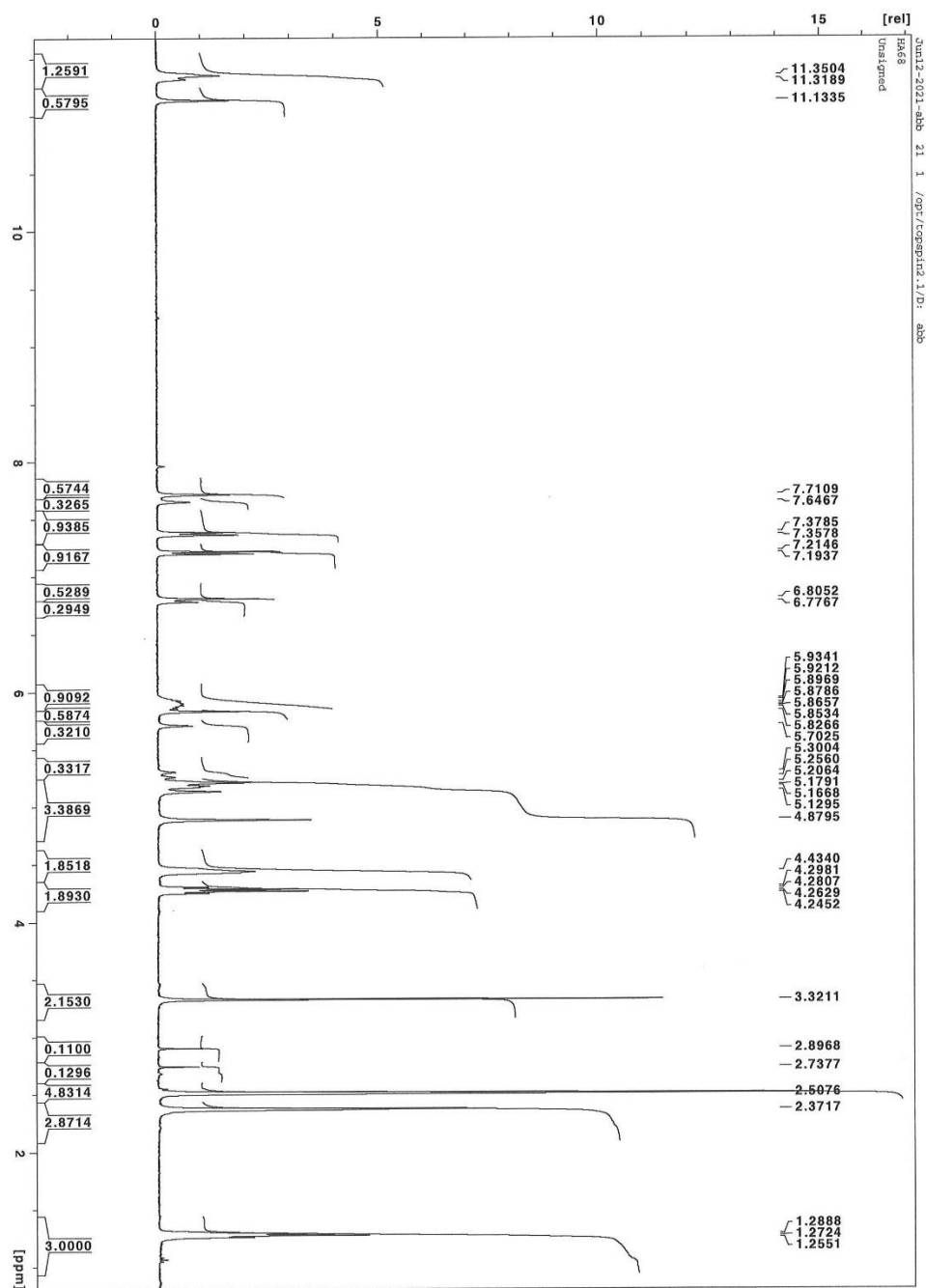
**Figure S90.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **7d**.



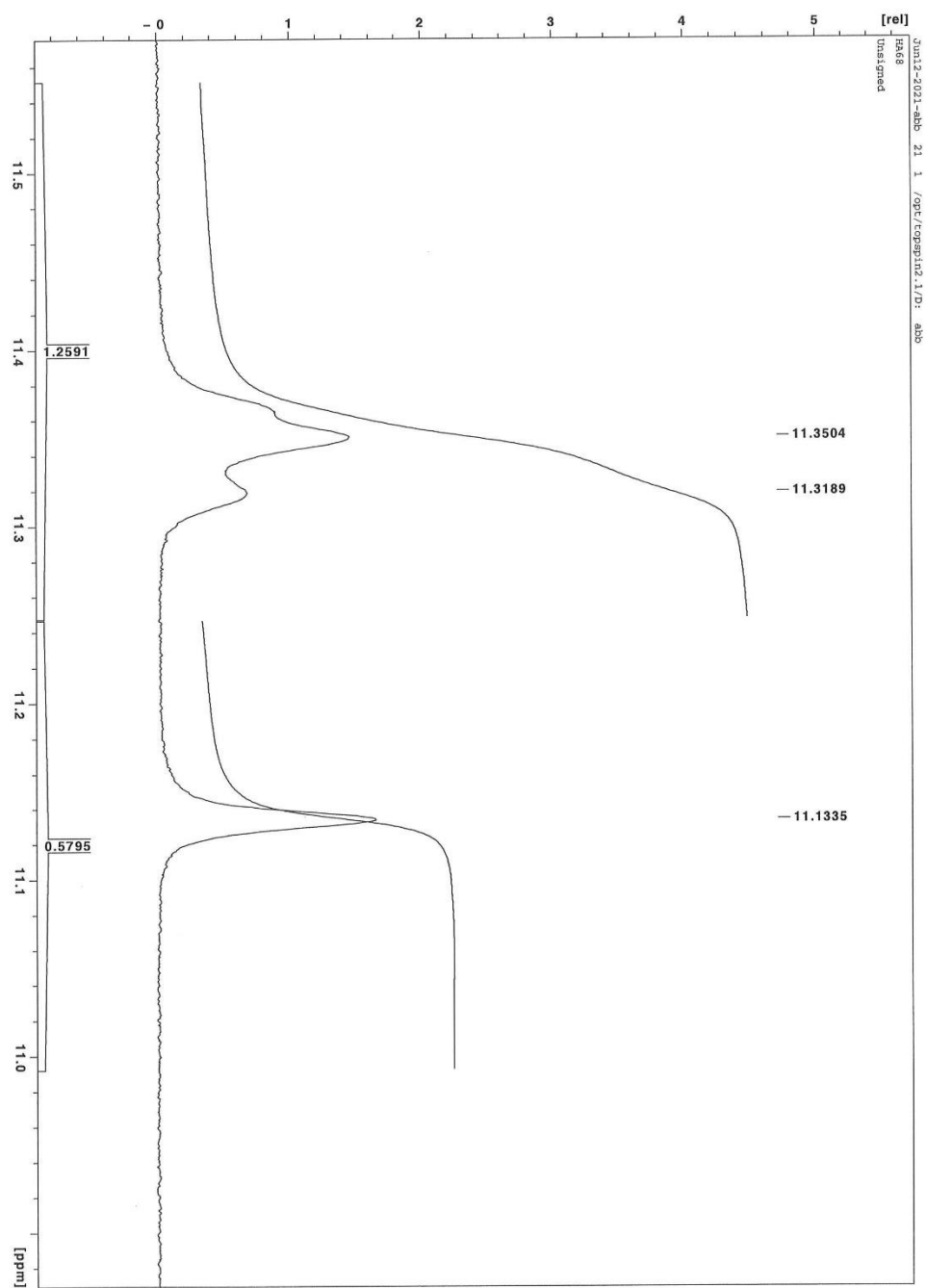
**Figure S91.**  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **7d**.



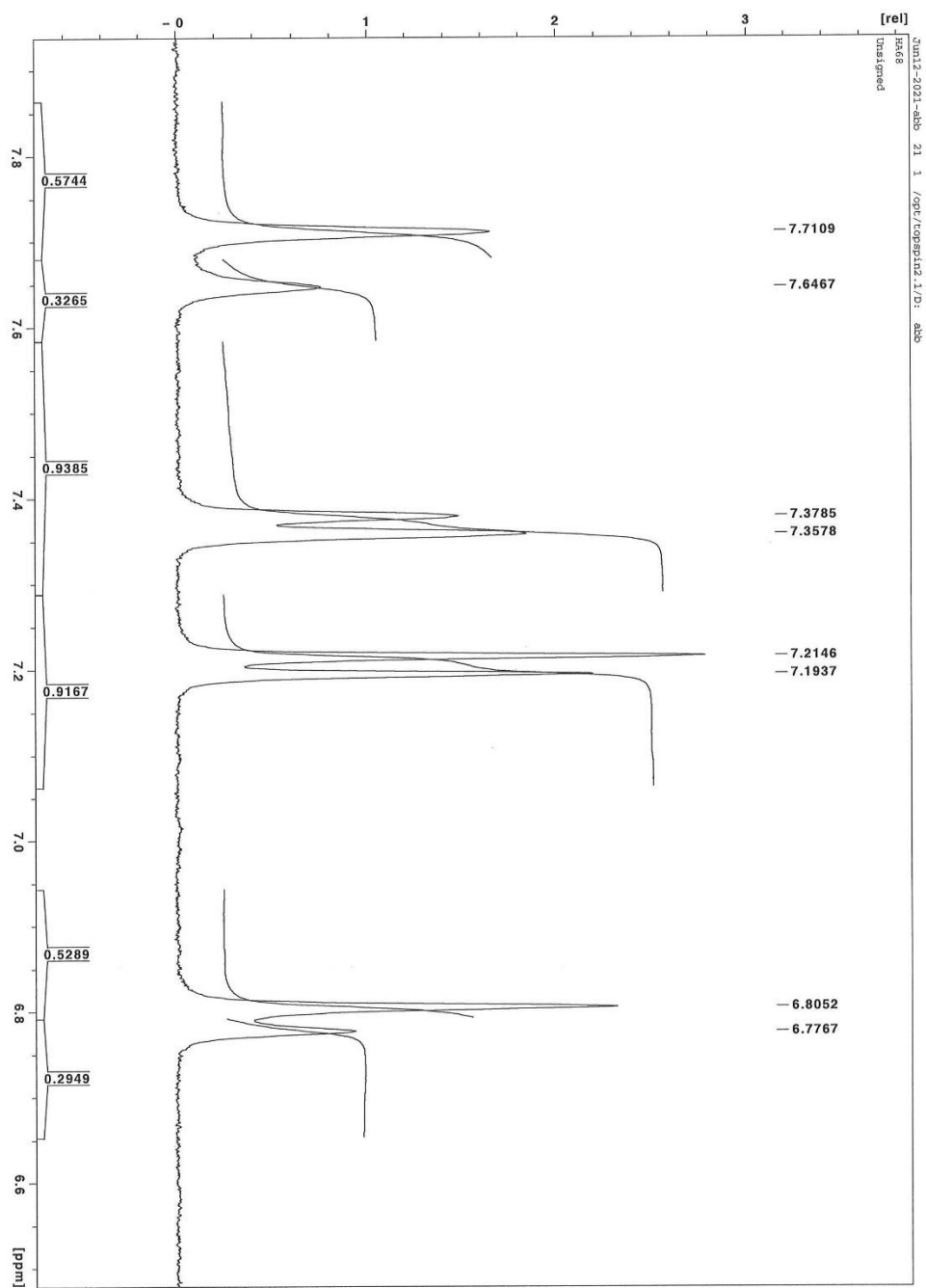
**Figure S92.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **7d**.



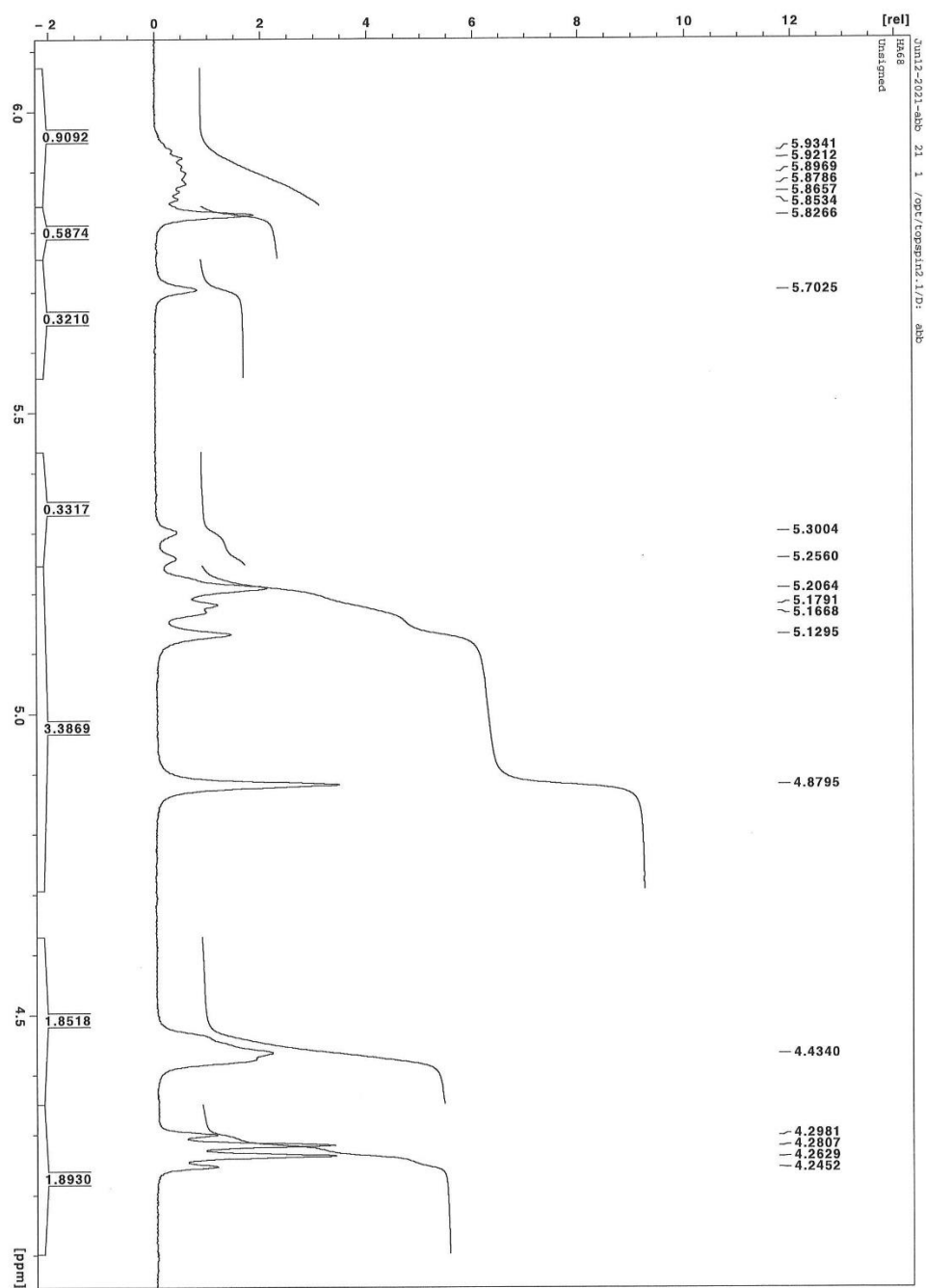
**Figure S93.**  $^1\text{H}$  spectrum of compound **7e** (400 MHz,  $\text{DMSO-}d_6$ ). Solubility was low, and sample contains a small amount of DMF.



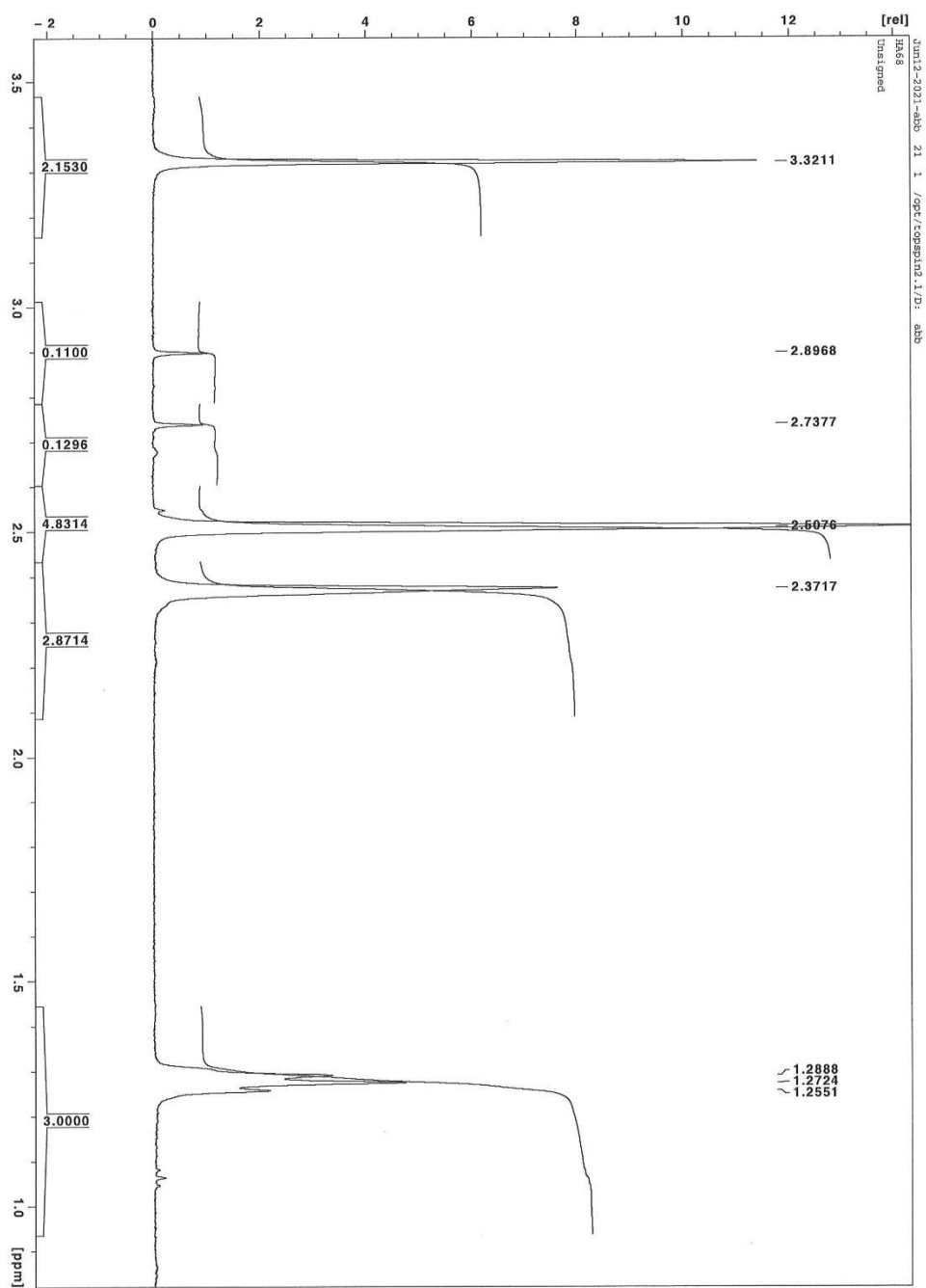
**Figure S94.** Detail of  $^1\text{H}$  spectrum of compound **7e**.



**Figure S95.** Detail of  $^1\text{H}$  spectrum of compound **7e**.



**Figure S96.** Detail of  $^1\text{H}$  spectrum of compound **7e**.



**Figure S97.** Detail of  $^1\text{H}$  spectrum of compound **7e**.

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<sup>1</sup>H-<sup>1</sup>H COSY

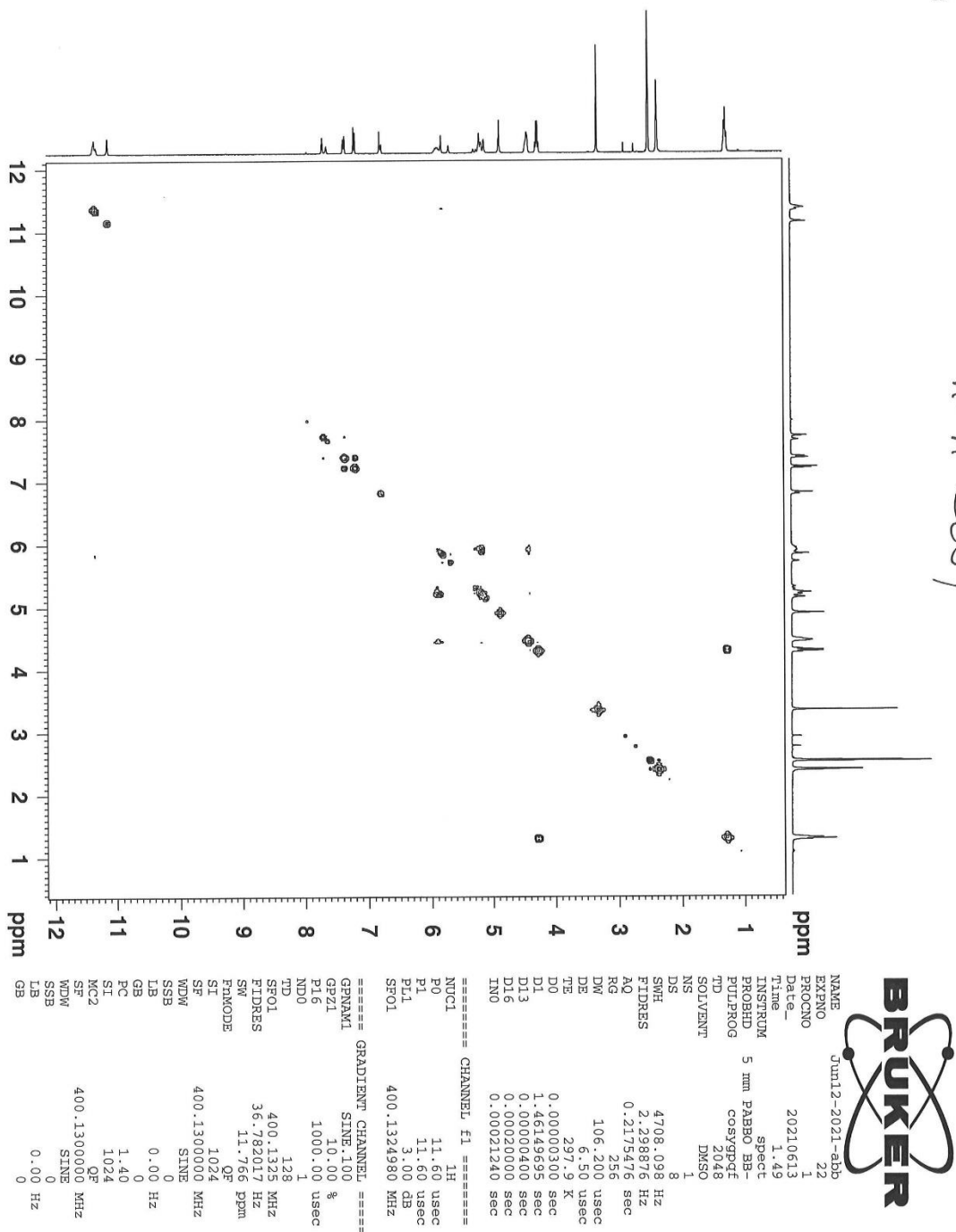
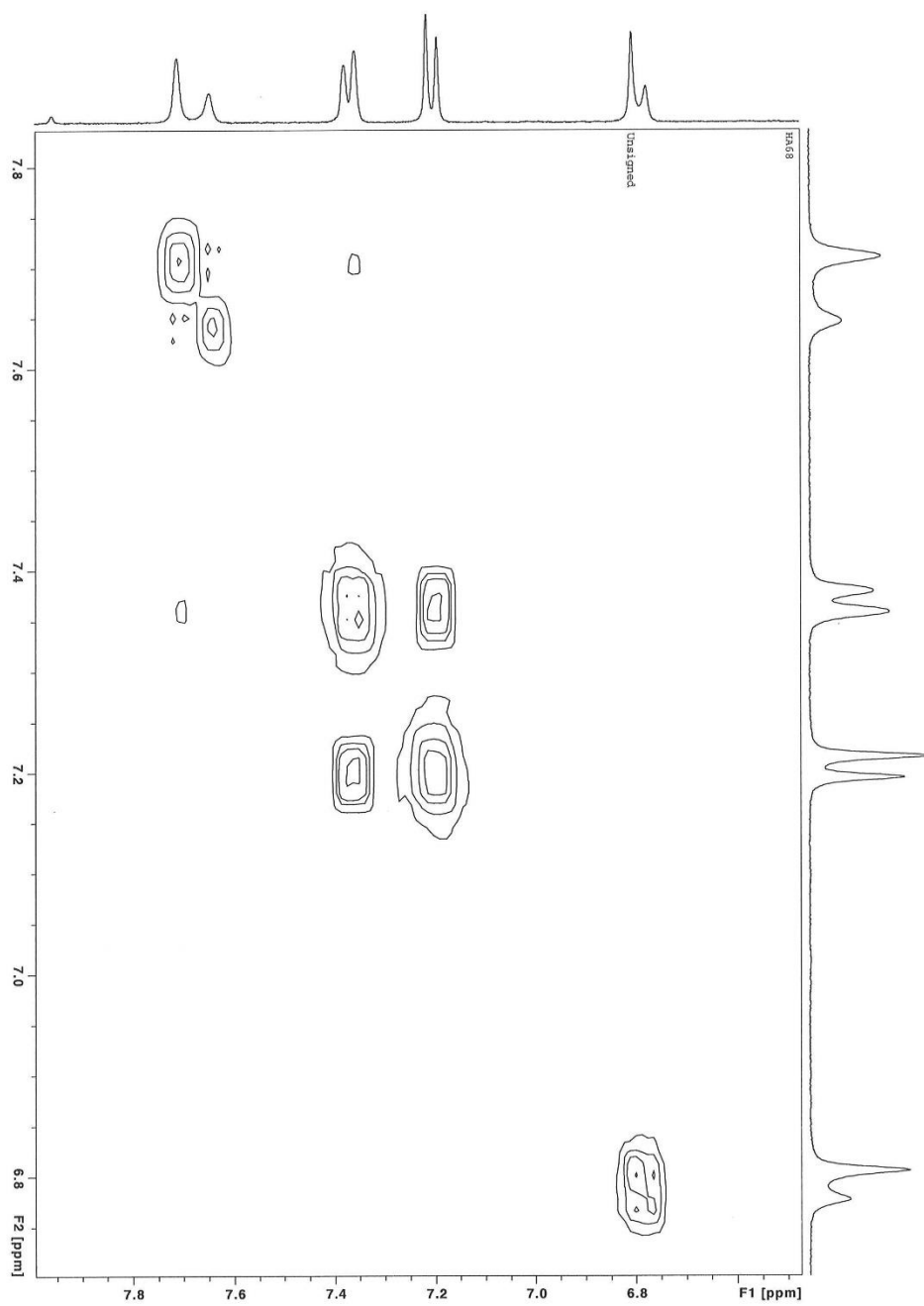
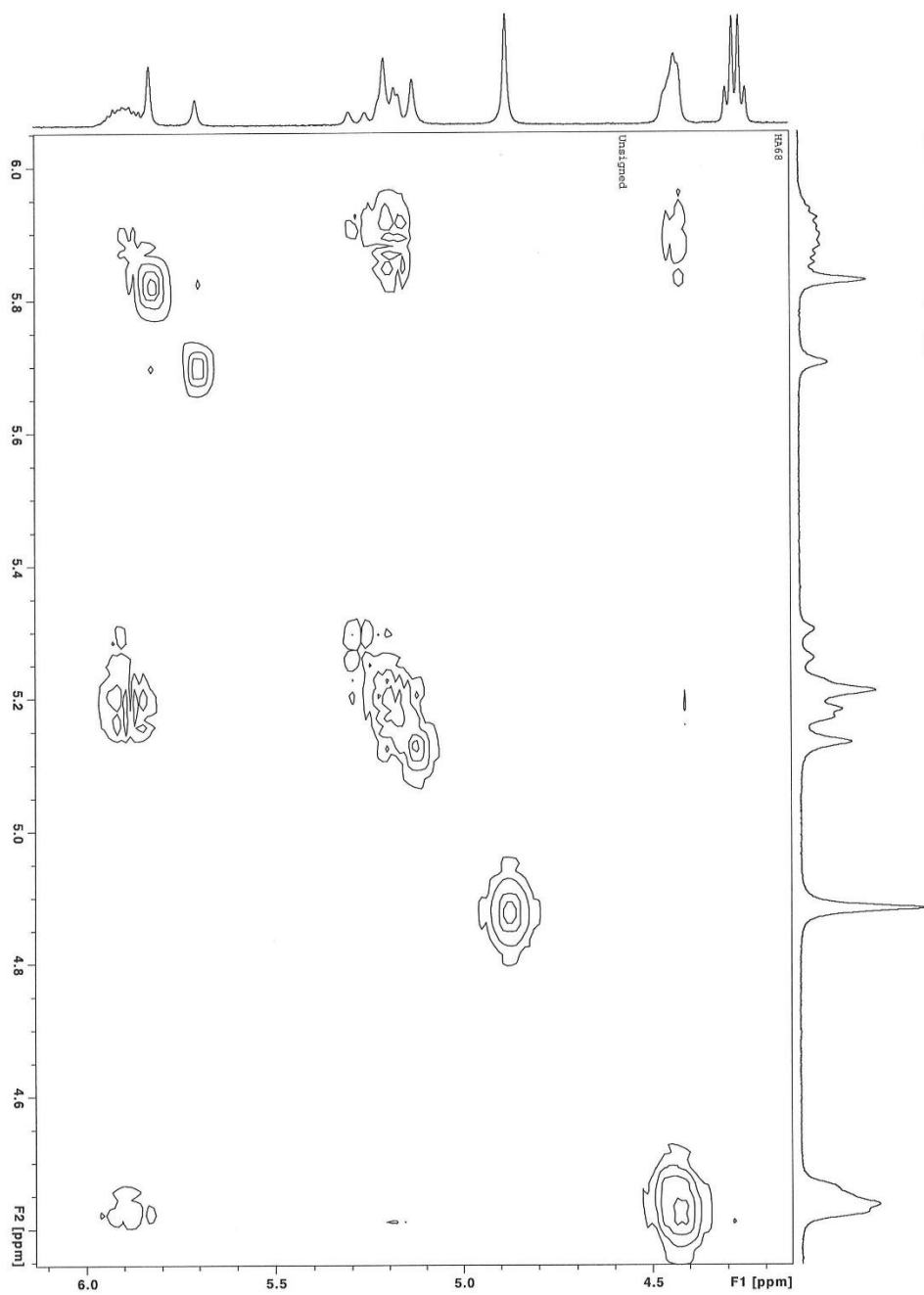


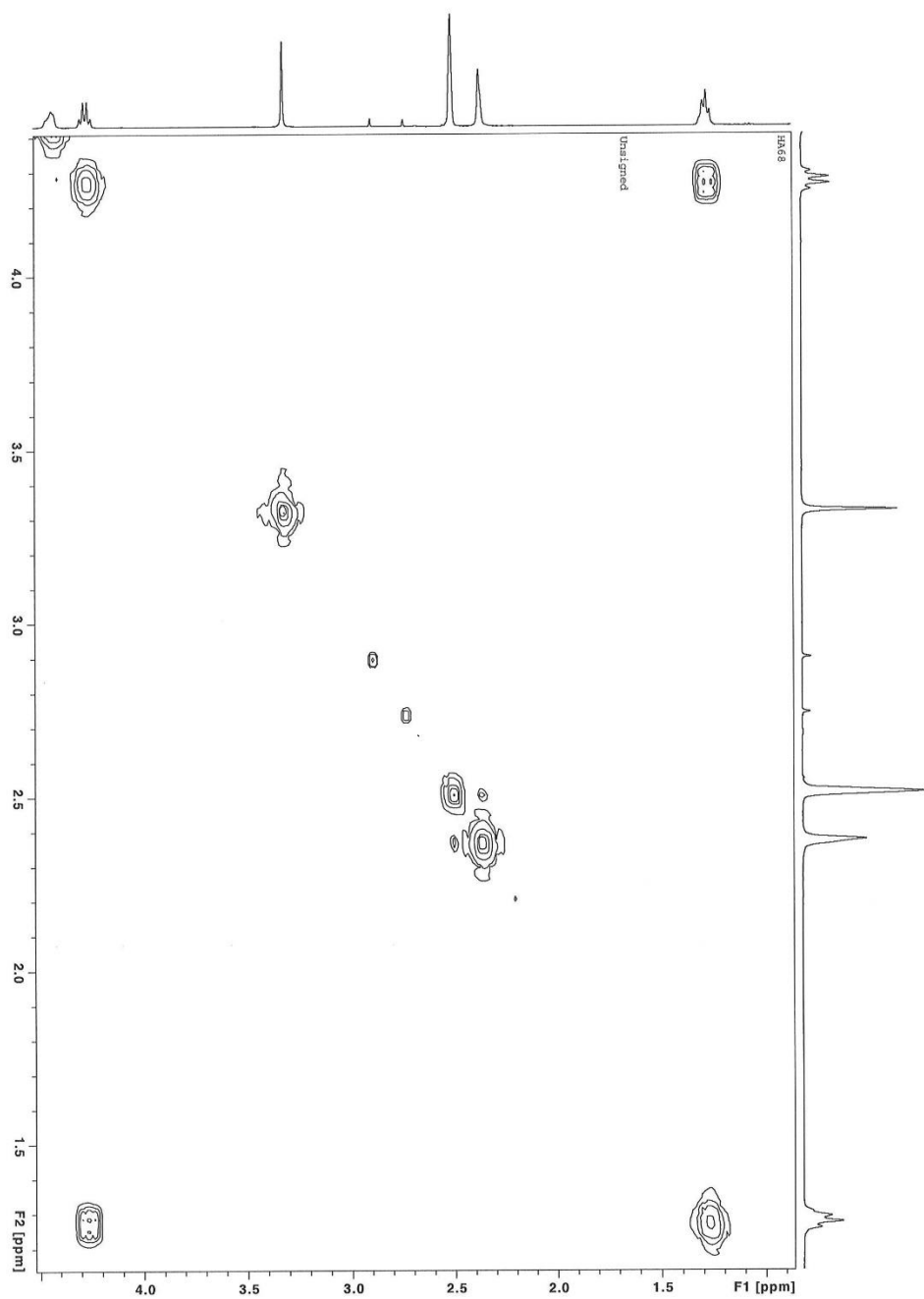
Figure S98. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **7e**.



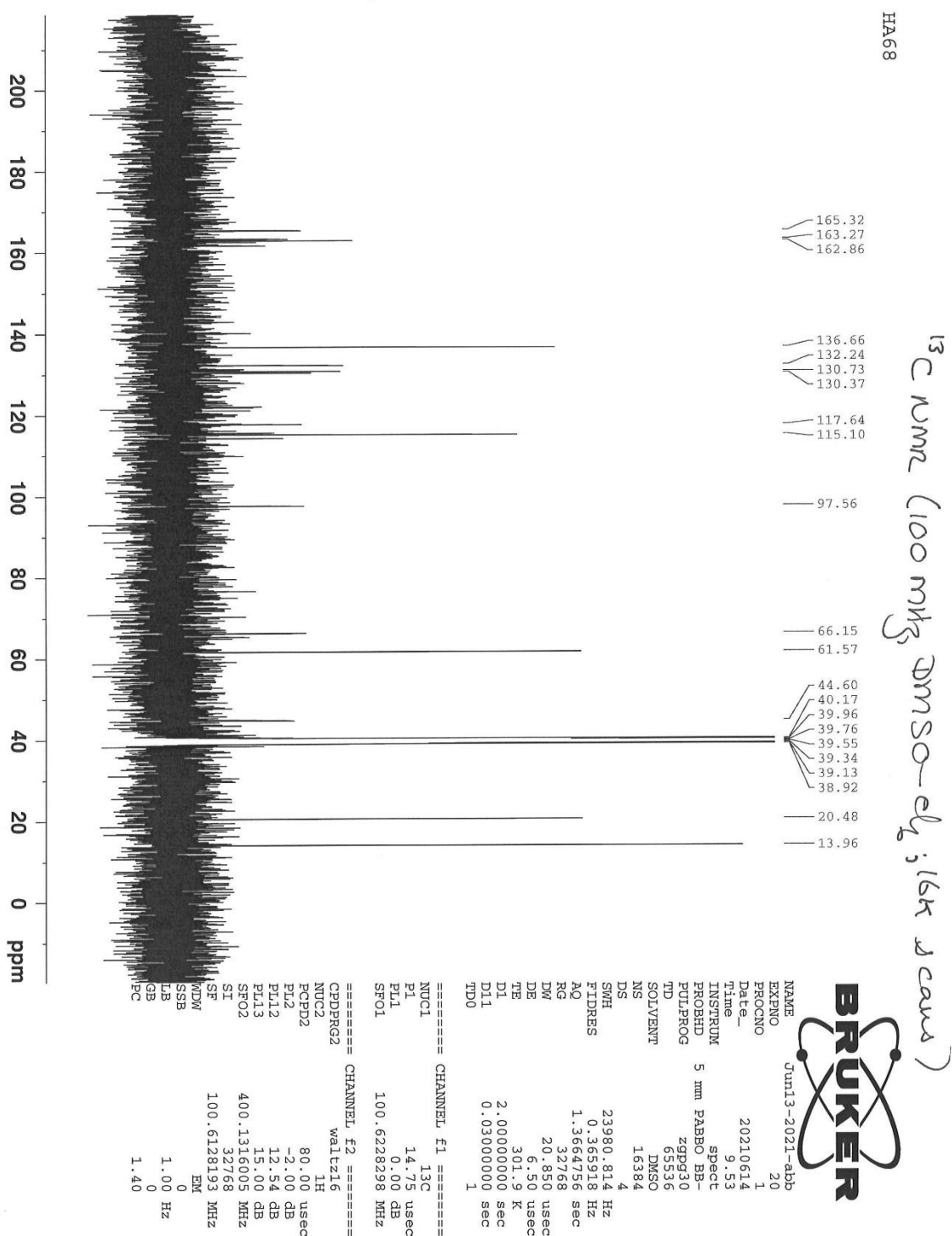
**Figure S99.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7e**.



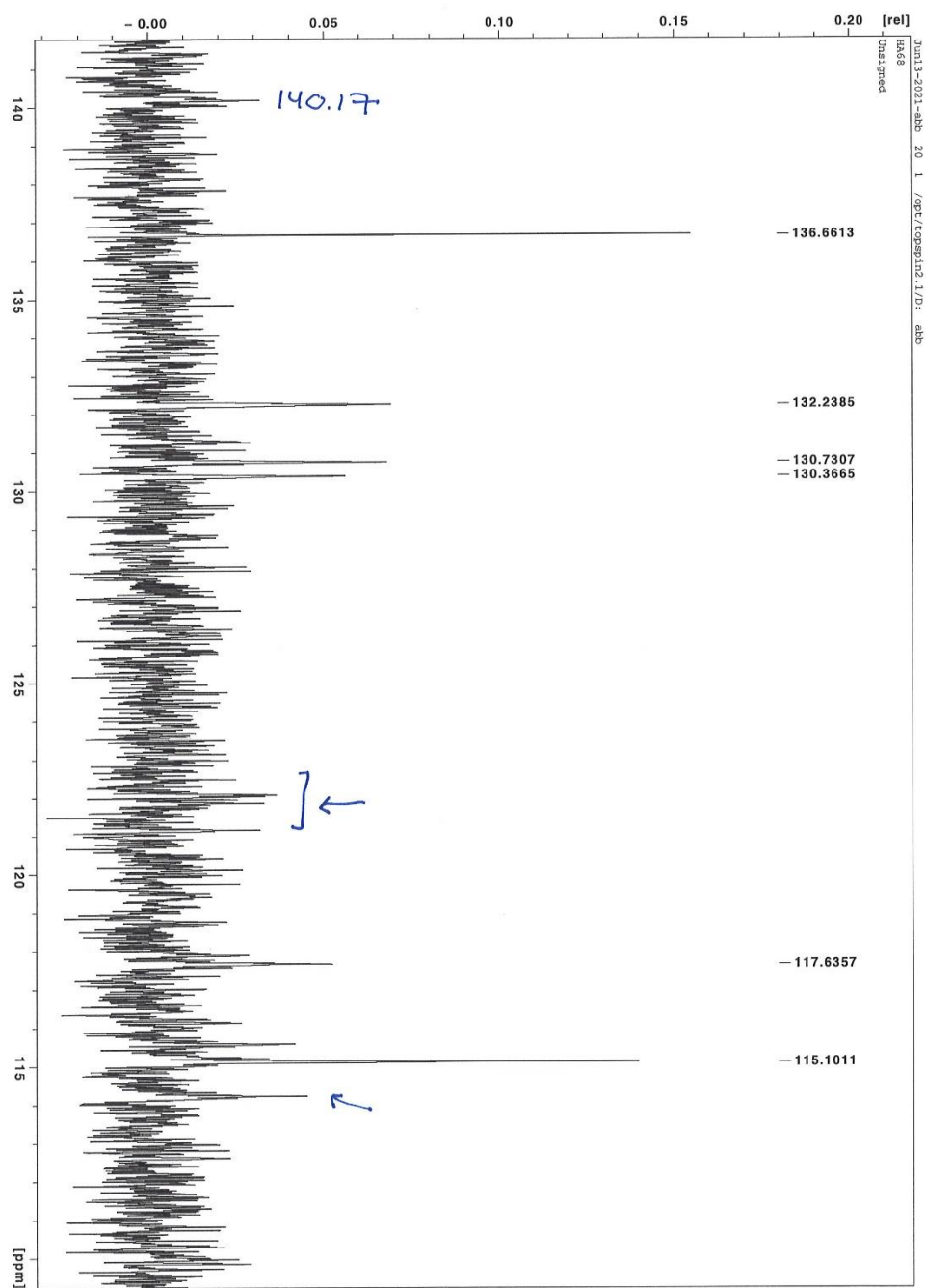
**Figure S100.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7e**.



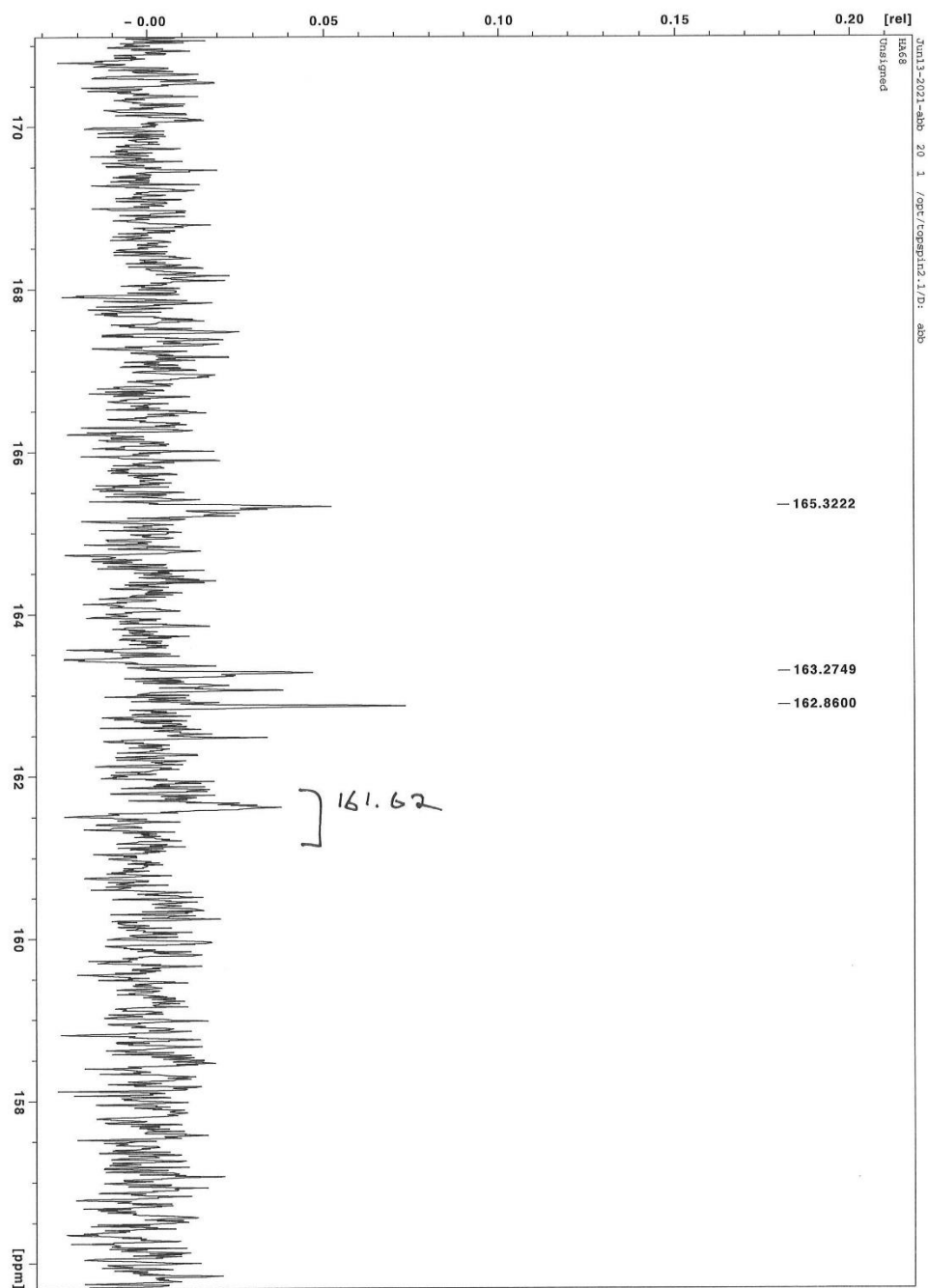
**Figure S101.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7e**.



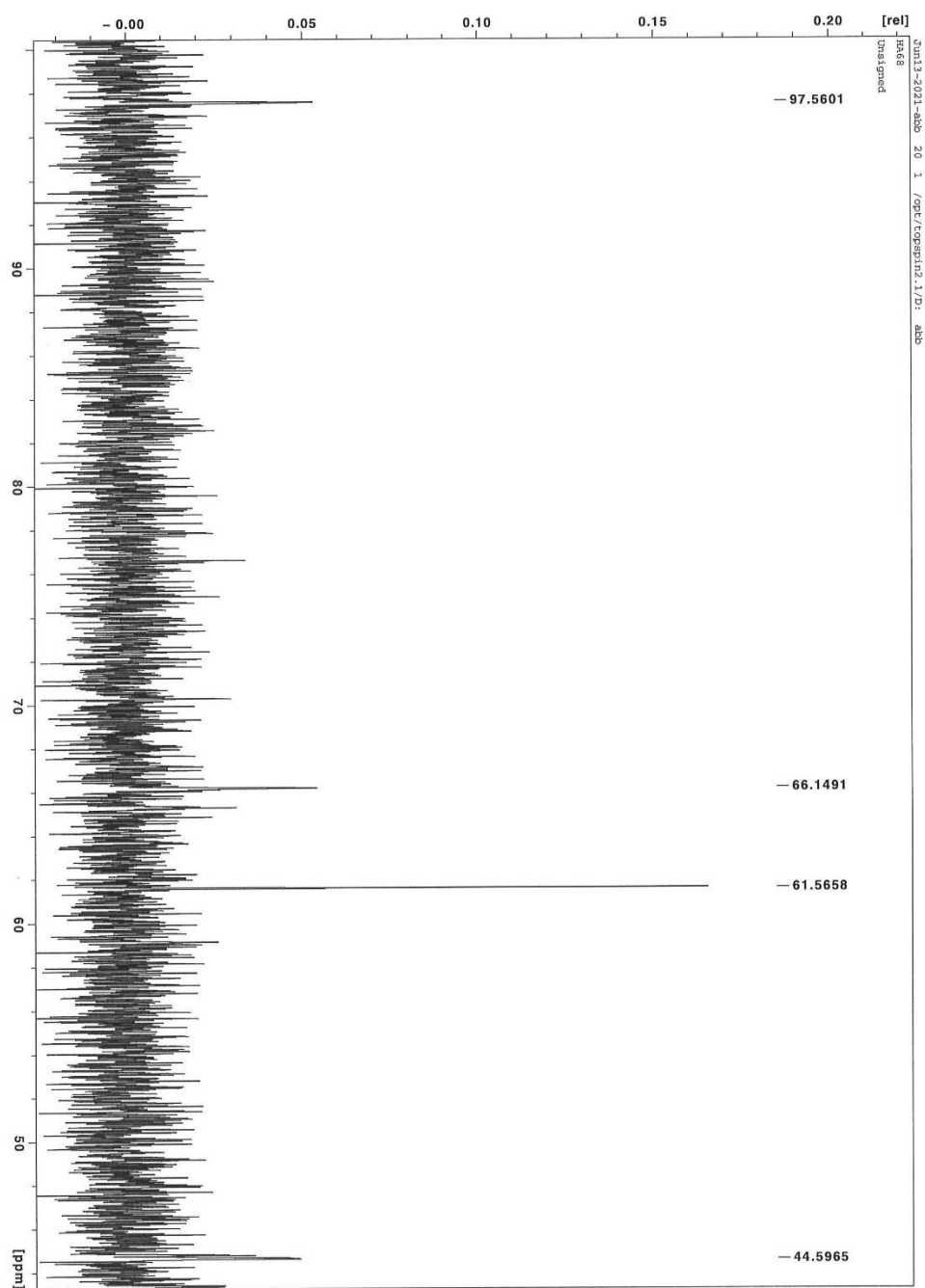
**Figure S102.**  $^{13}\text{C}$  spectrum of compound **7e** (100 MHz, DMSO- $d_6$ ).



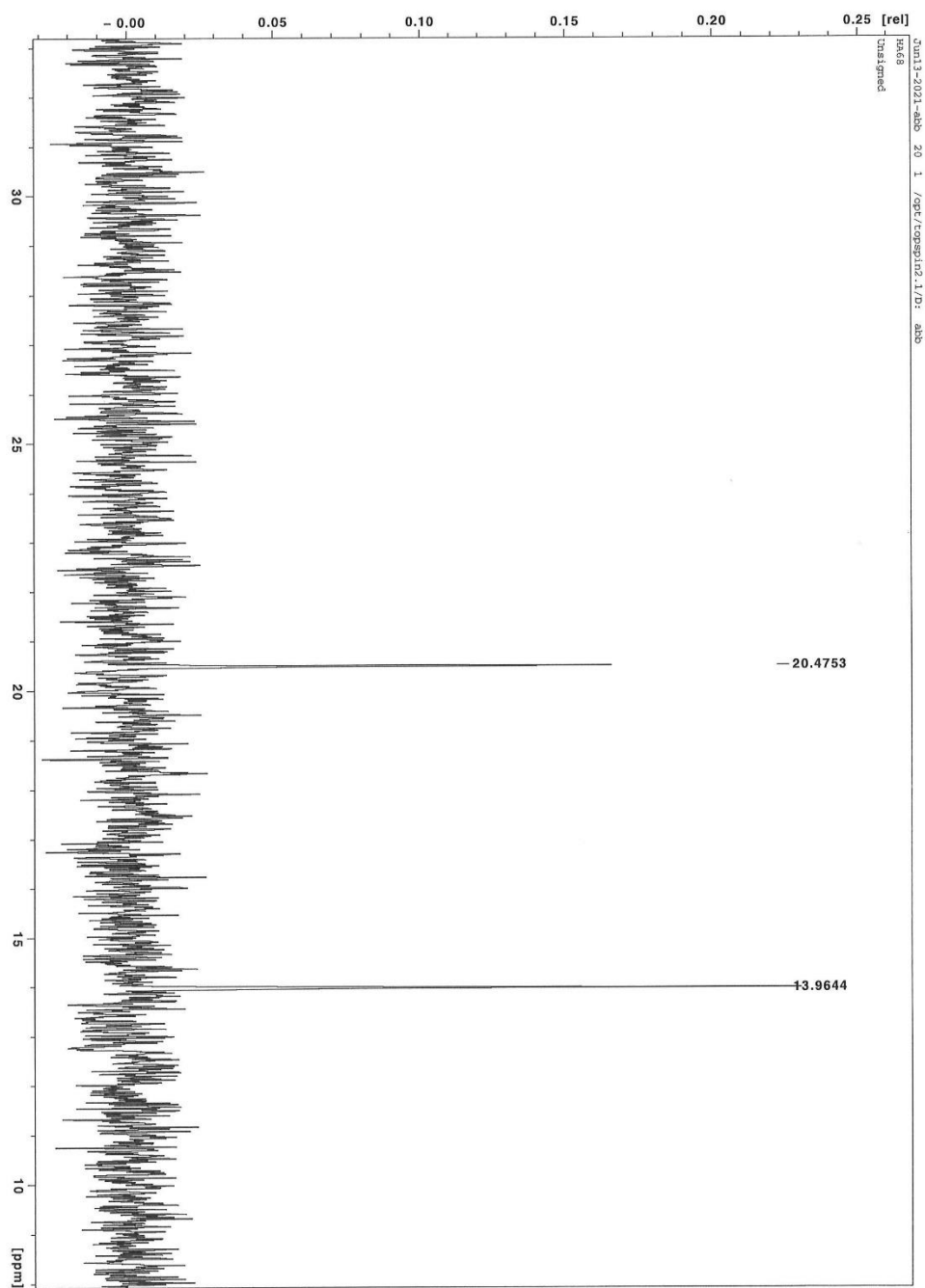
**Figure S103.** Detail of  $^{13}\text{C}$  spectrum of compound **7e**.



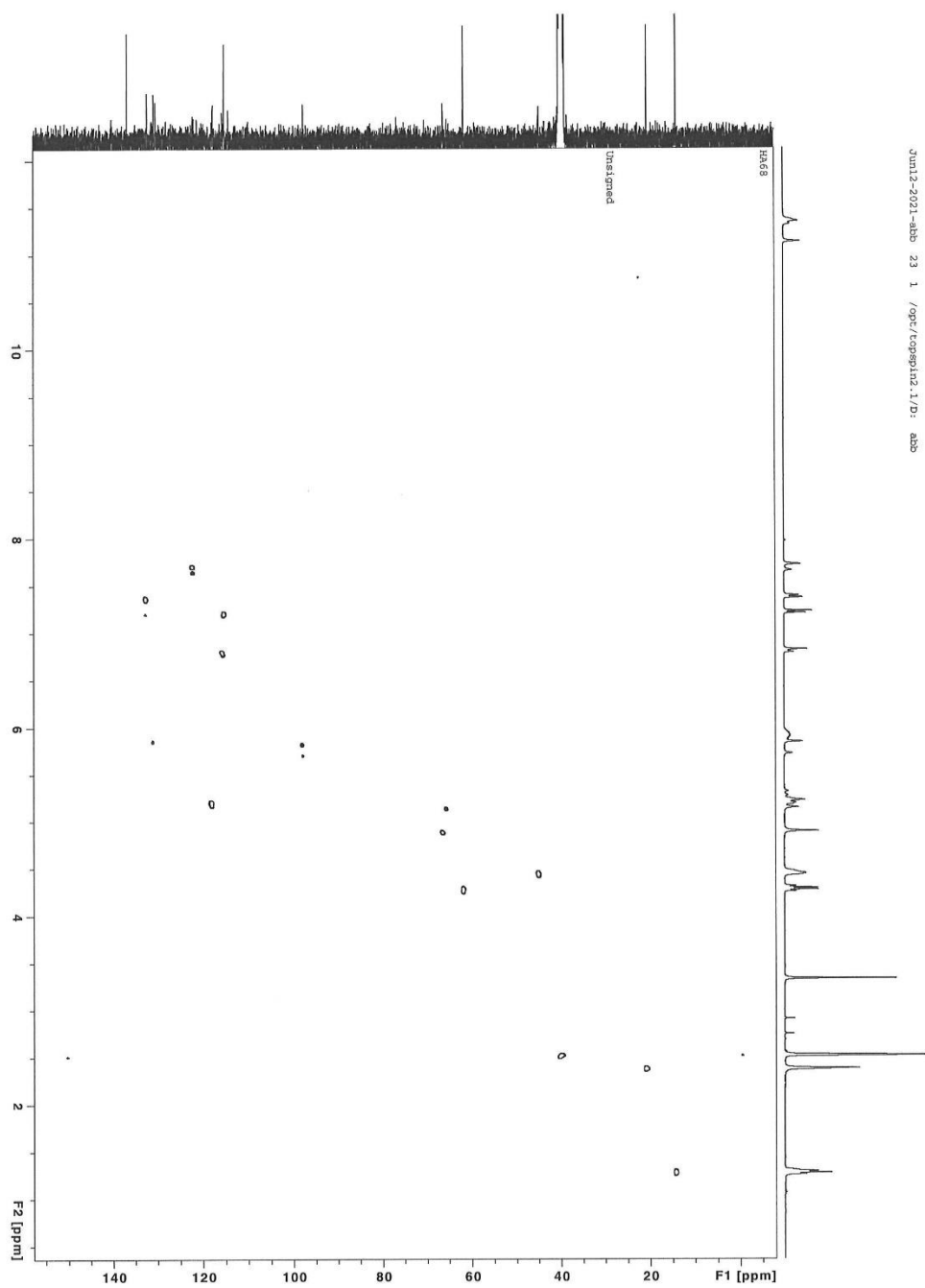
**Figure S104.** Detail of  $^{13}\text{C}$  spectrum of compound **7e**.



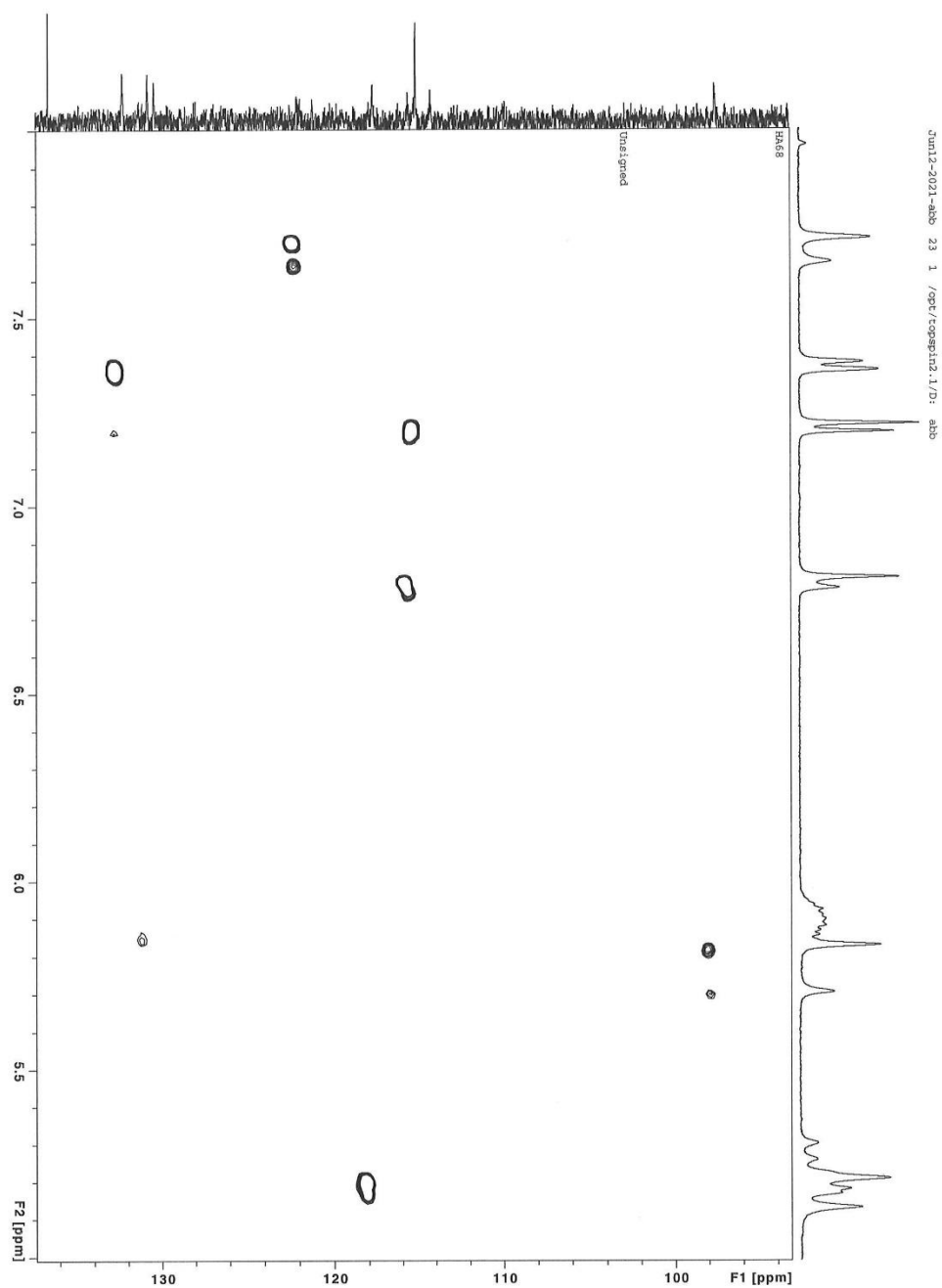
**Figure S105.** Detail of  $^{13}\text{C}$  spectrum of compound **7e**.



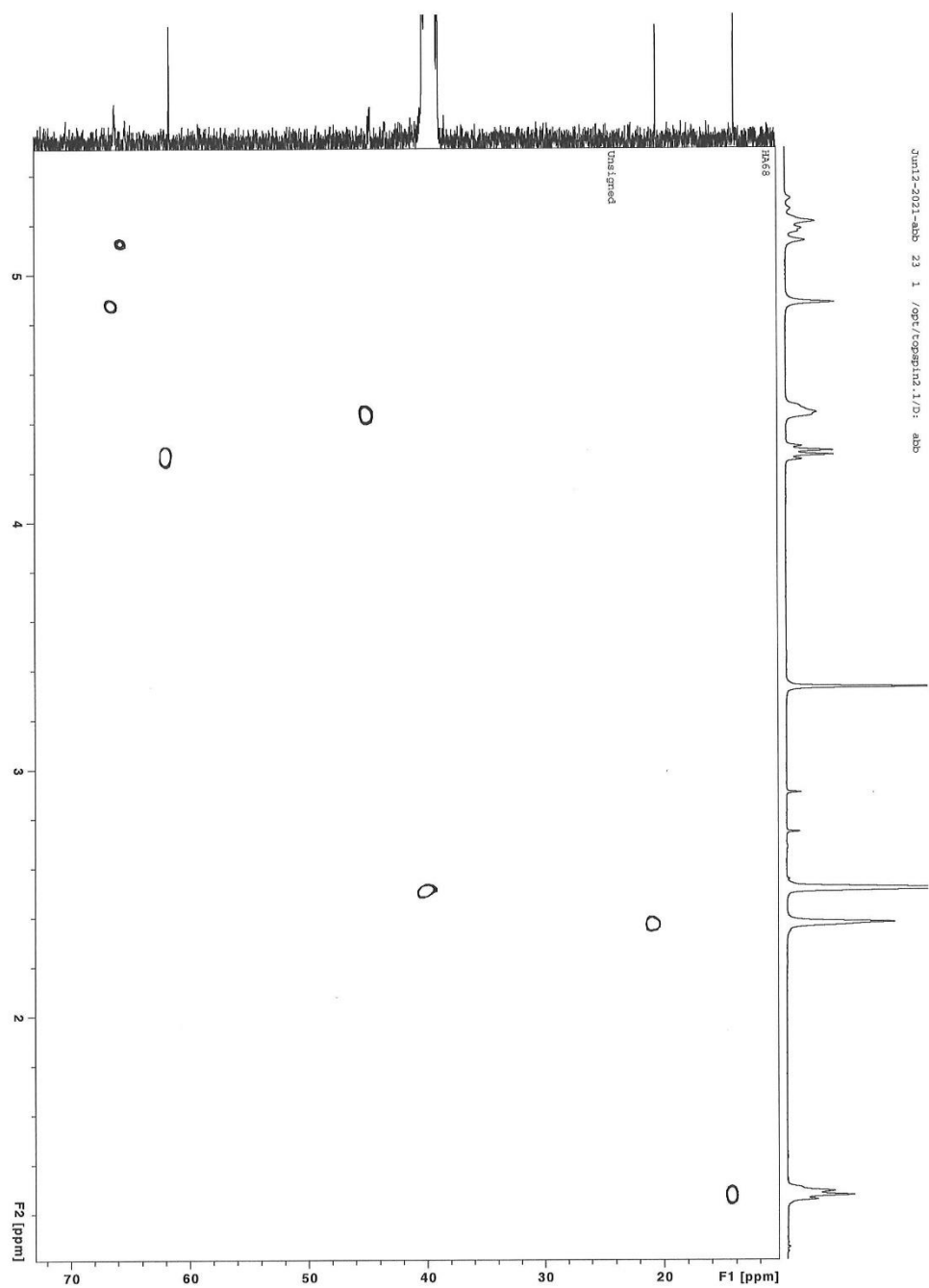
**Figure S106.** Detail of  $^{13}\text{C}$  spectrum of compound **7e**.



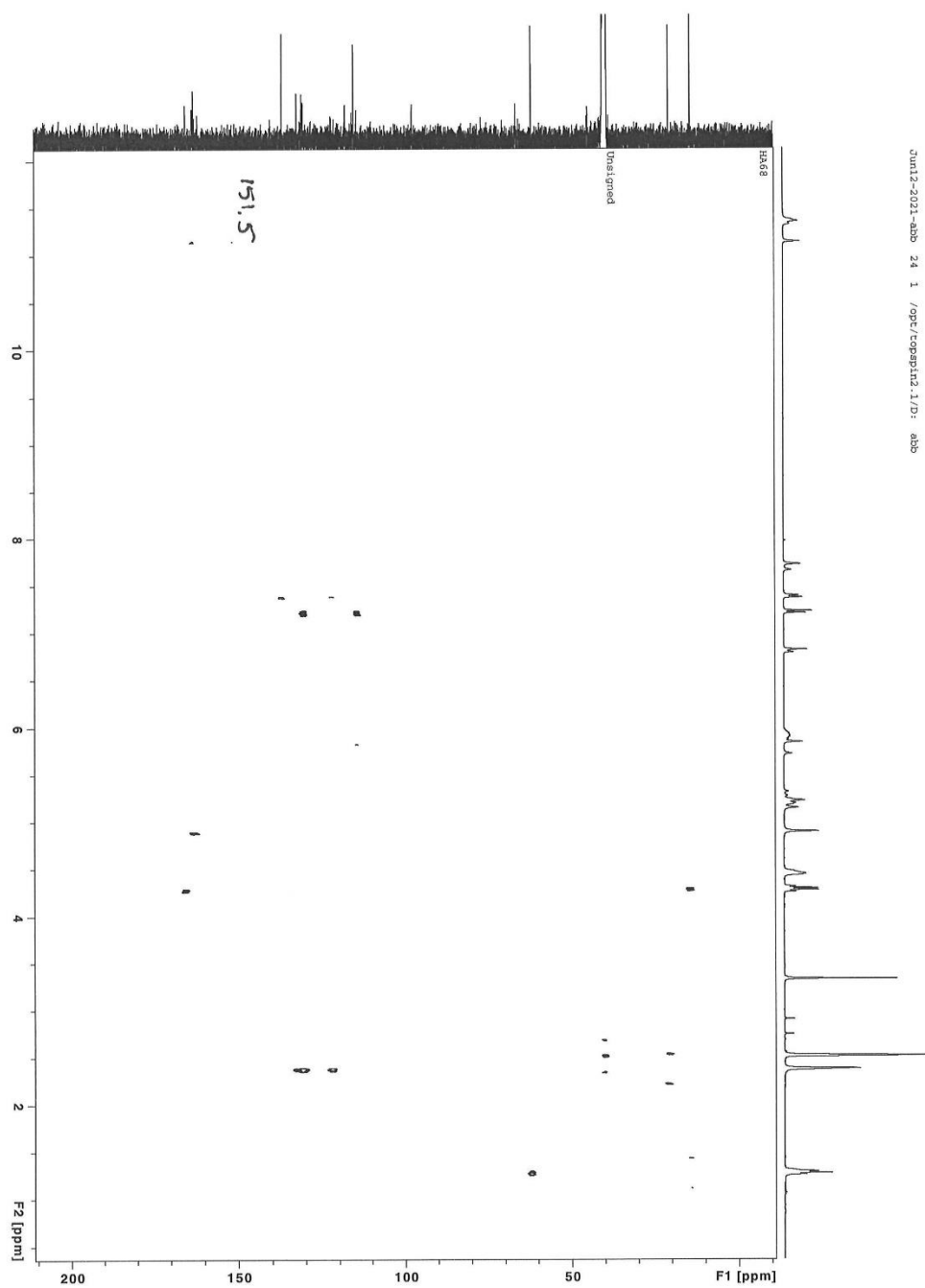
**Figure S107.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7e**.



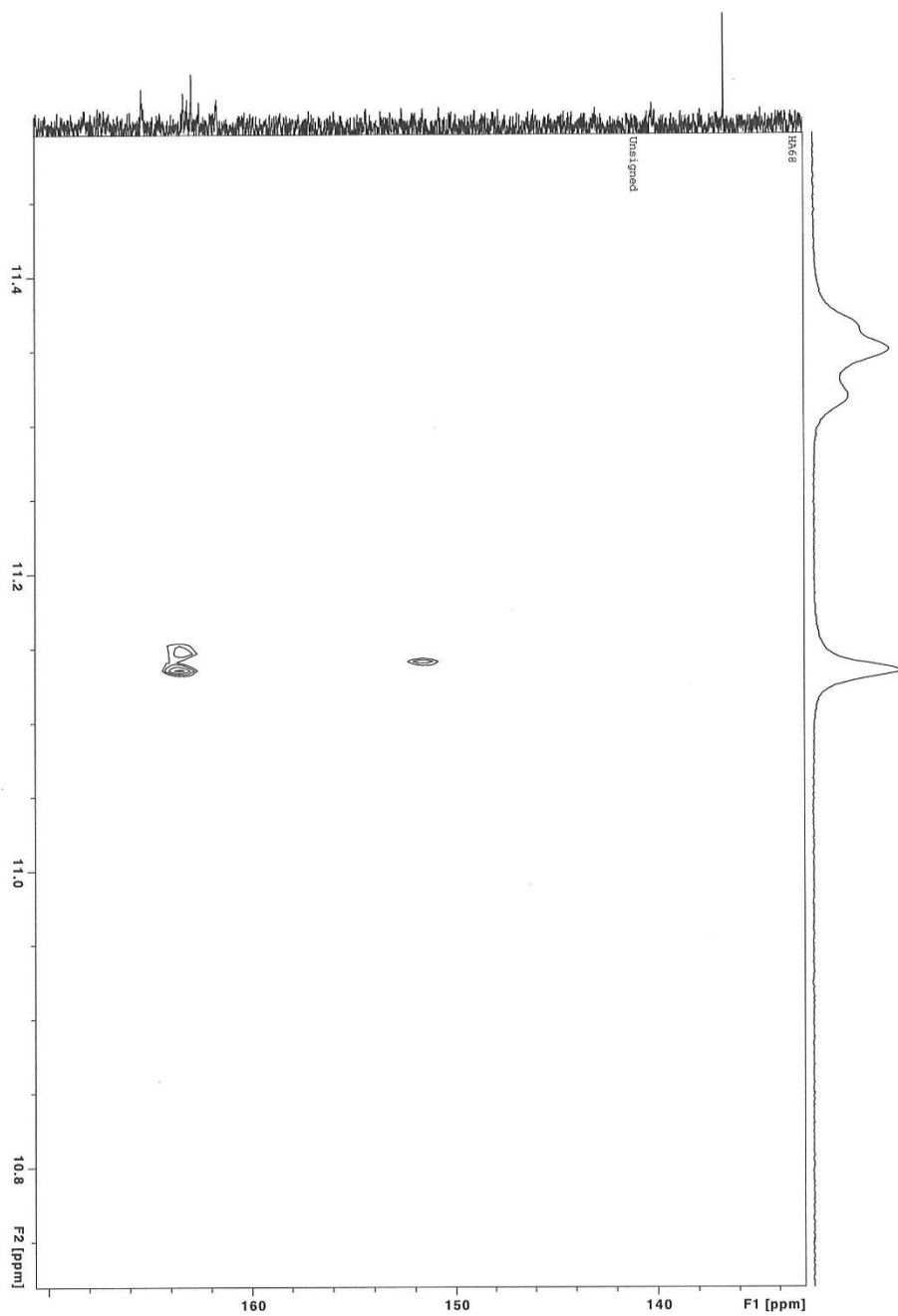
**Figure S108.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7e**.



**Figure S109.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7e**.

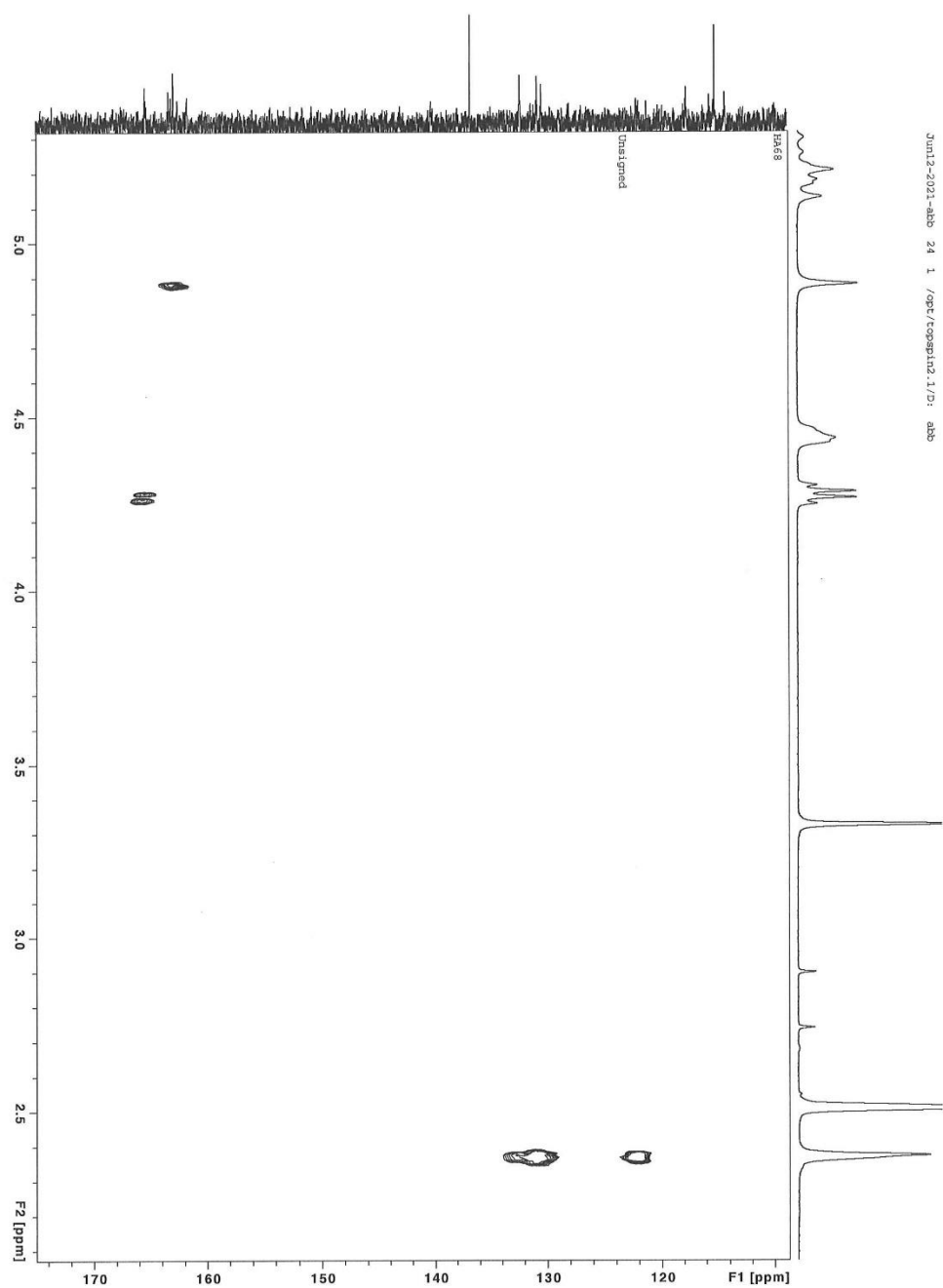


**Figure S110.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7e**.

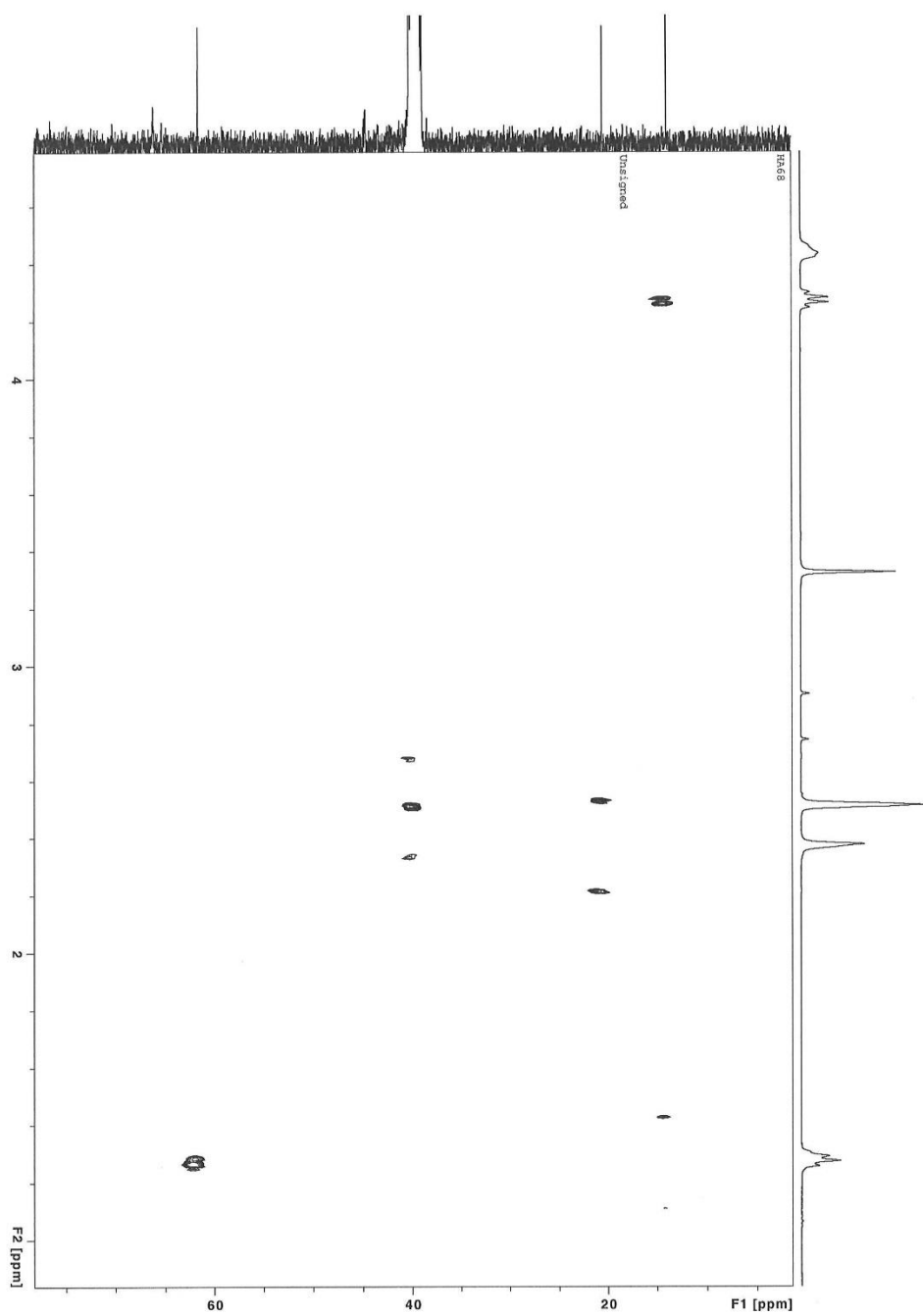


**Figure S111.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7e**.

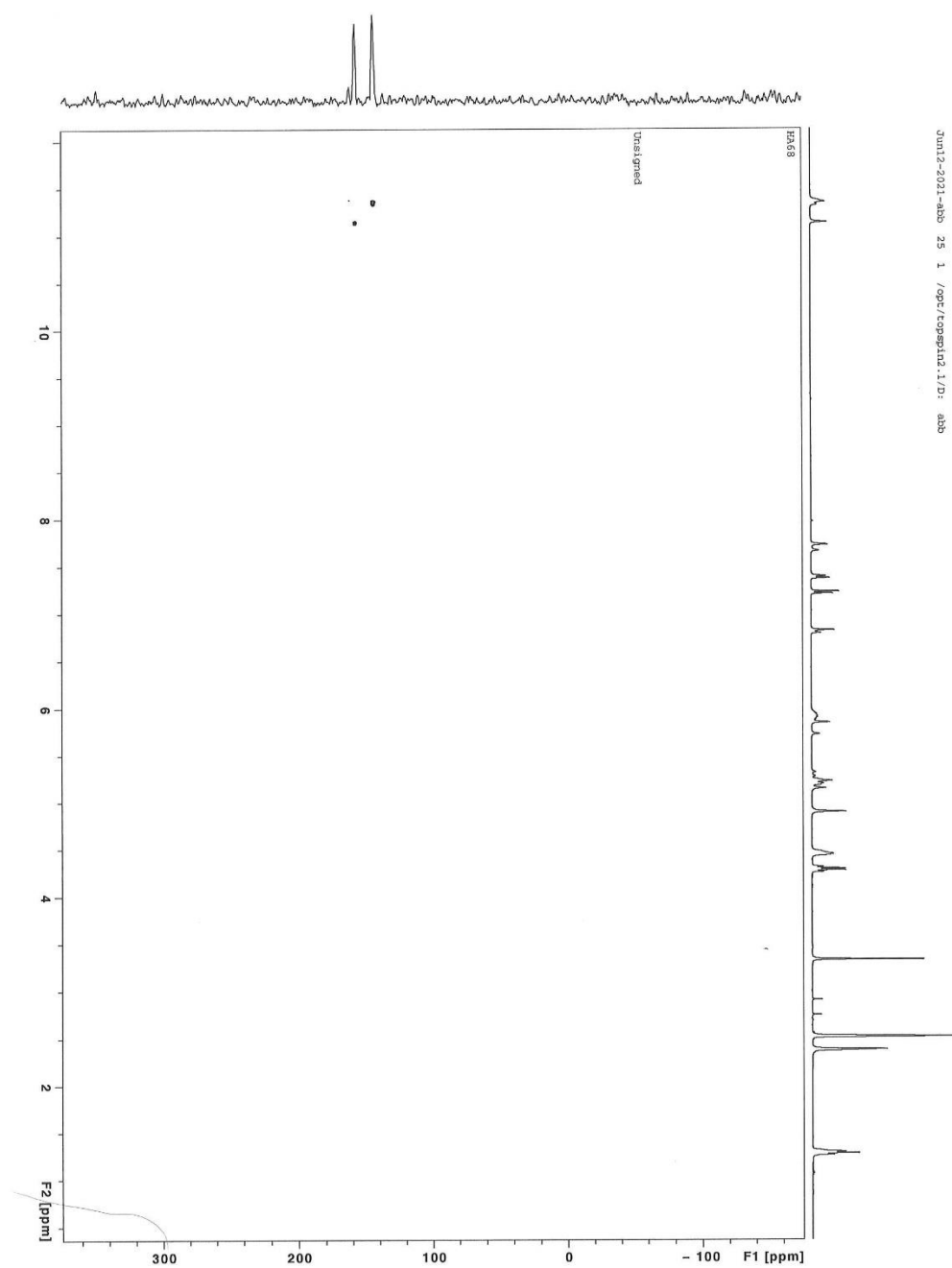




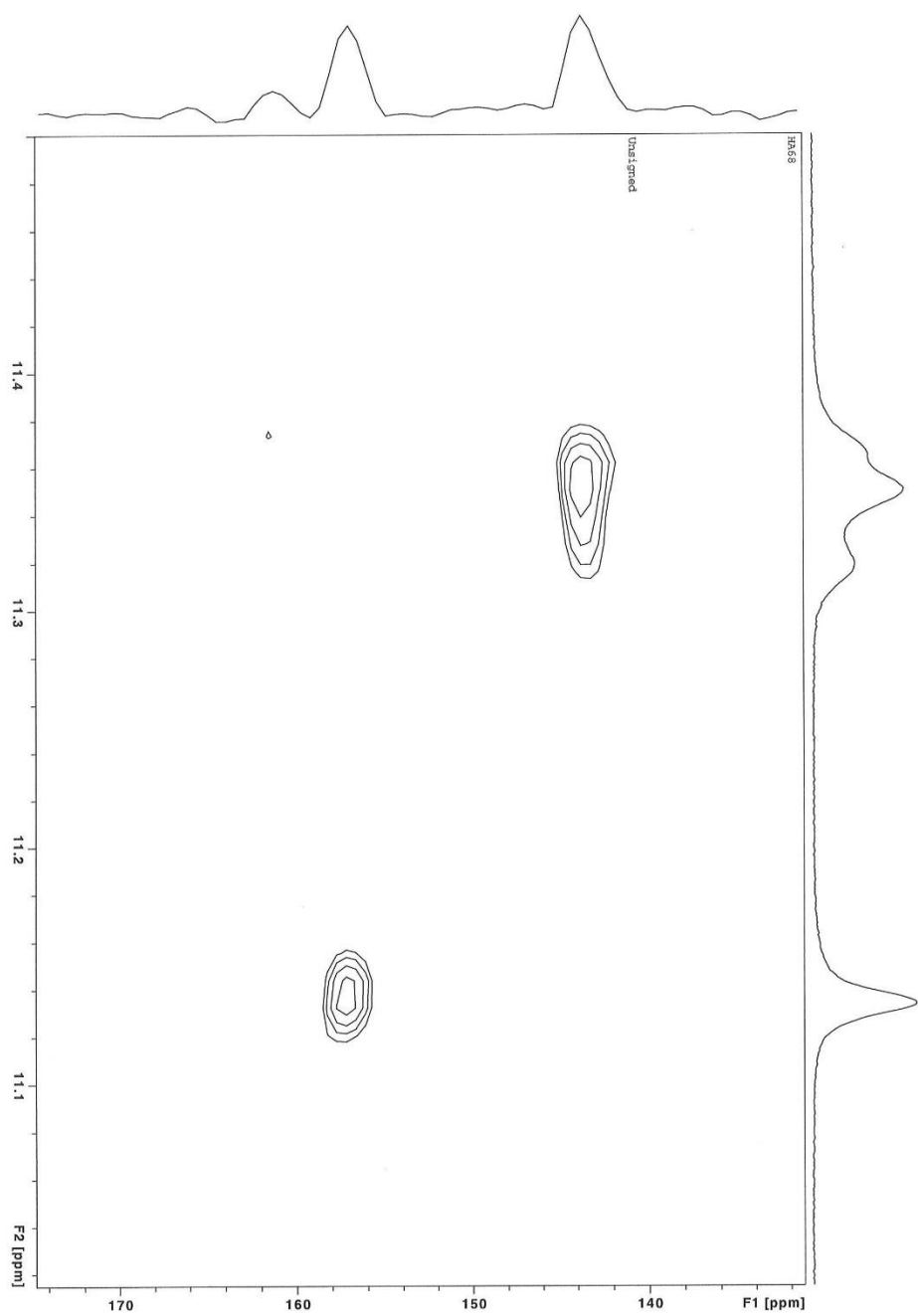
**Figure S113.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7e**.



**Figure S114.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7e**.



**Figure S115.**  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **7e** ( $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum gave no cross peaks).



**Figure S116.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **7e**.

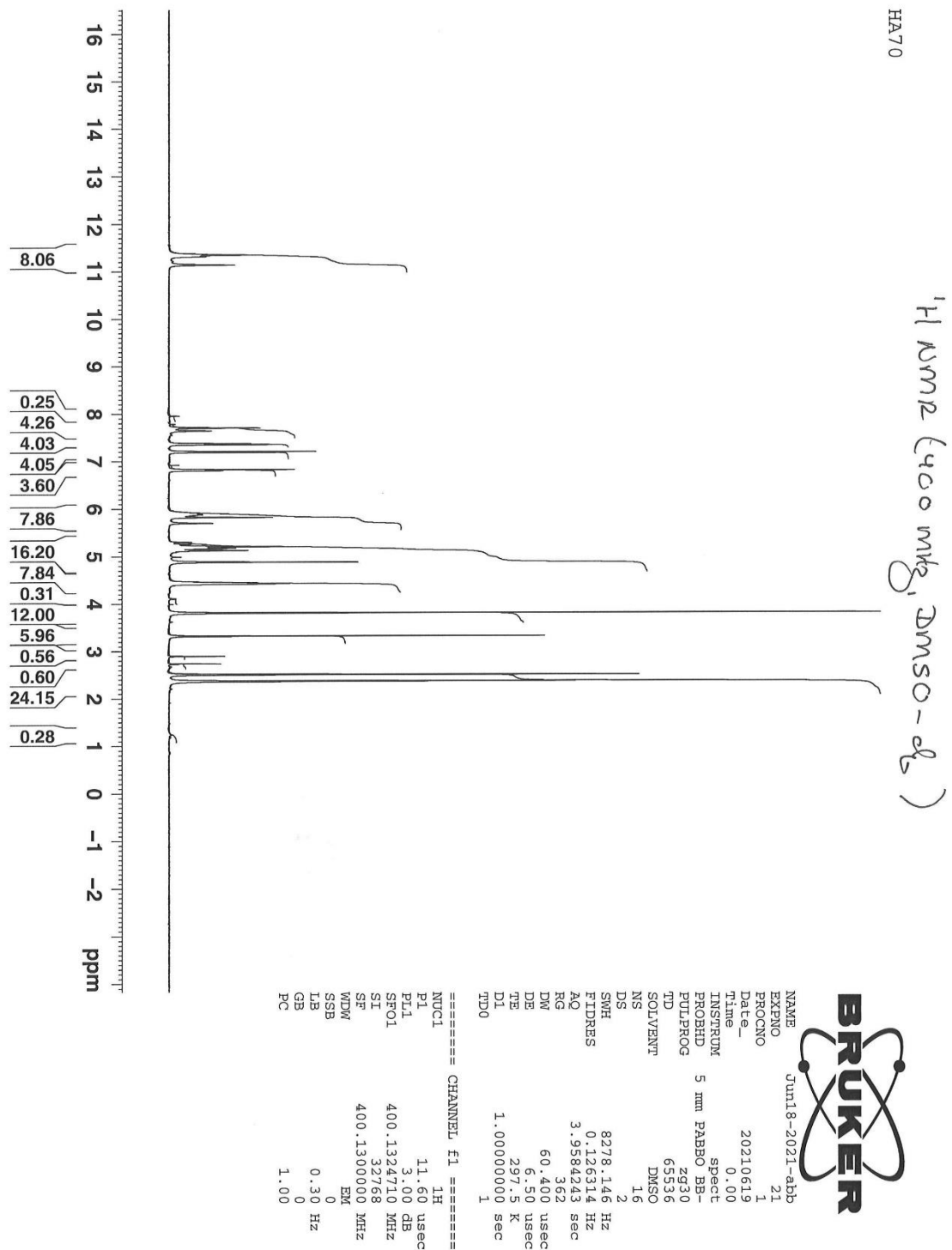
## Supplementary Material, part 2

Y.A.M.M. Elshaier, A.A. Aly,\* M. Abd El-Aziz, H.M. Fathy, A.B. Brown, S. Bräse, and M. Ramadan

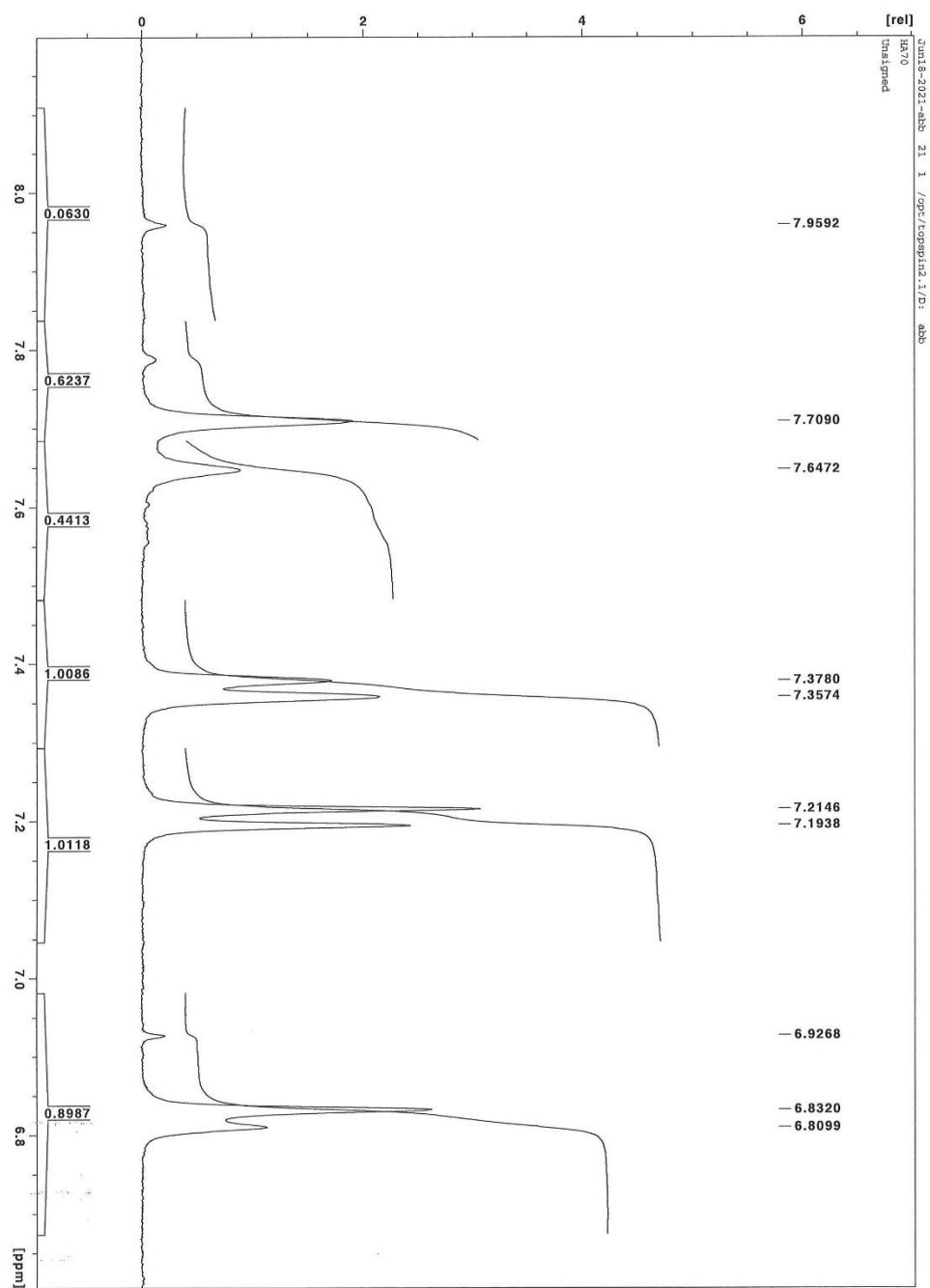
“Synthesis and identification of new *N,N*-disubstituted thiourea and thiazolidinone scaffolds based on quinolone moiety as urease inhibitors”

### Contents

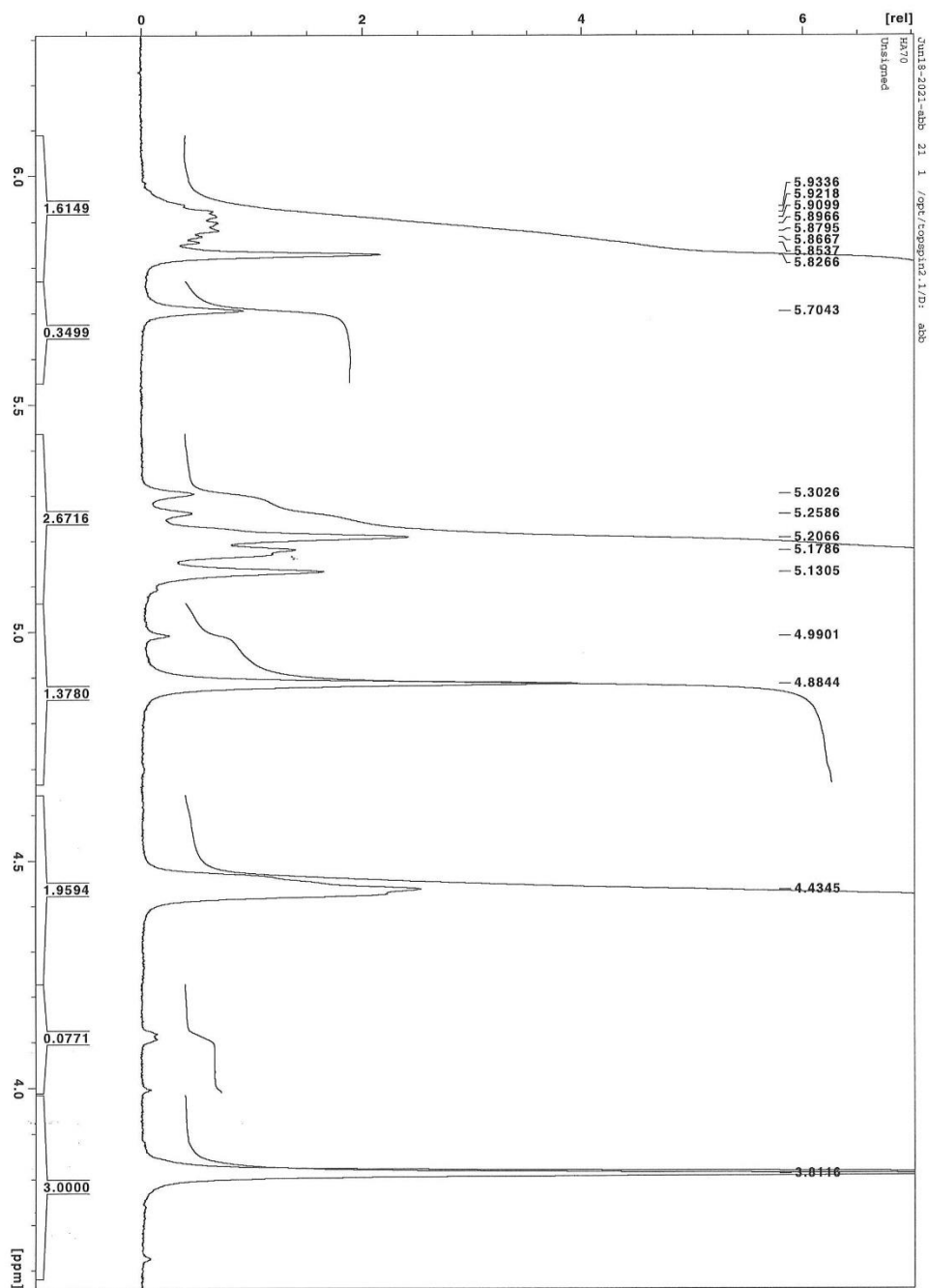
|                    |                  |
|--------------------|------------------|
| Compound <b>7f</b> | <b>S117-S139</b> |
| Compound <b>7g</b> | <b>S140-S159</b> |
| Compound <b>7h</b> | <b>S160-S171</b> |
| Compound <b>7j</b> | <b>S172-S189</b> |
| Compound <b>7k</b> | <b>S190-S205</b> |
| Compound <b>7l</b> | <b>S206-S228</b> |



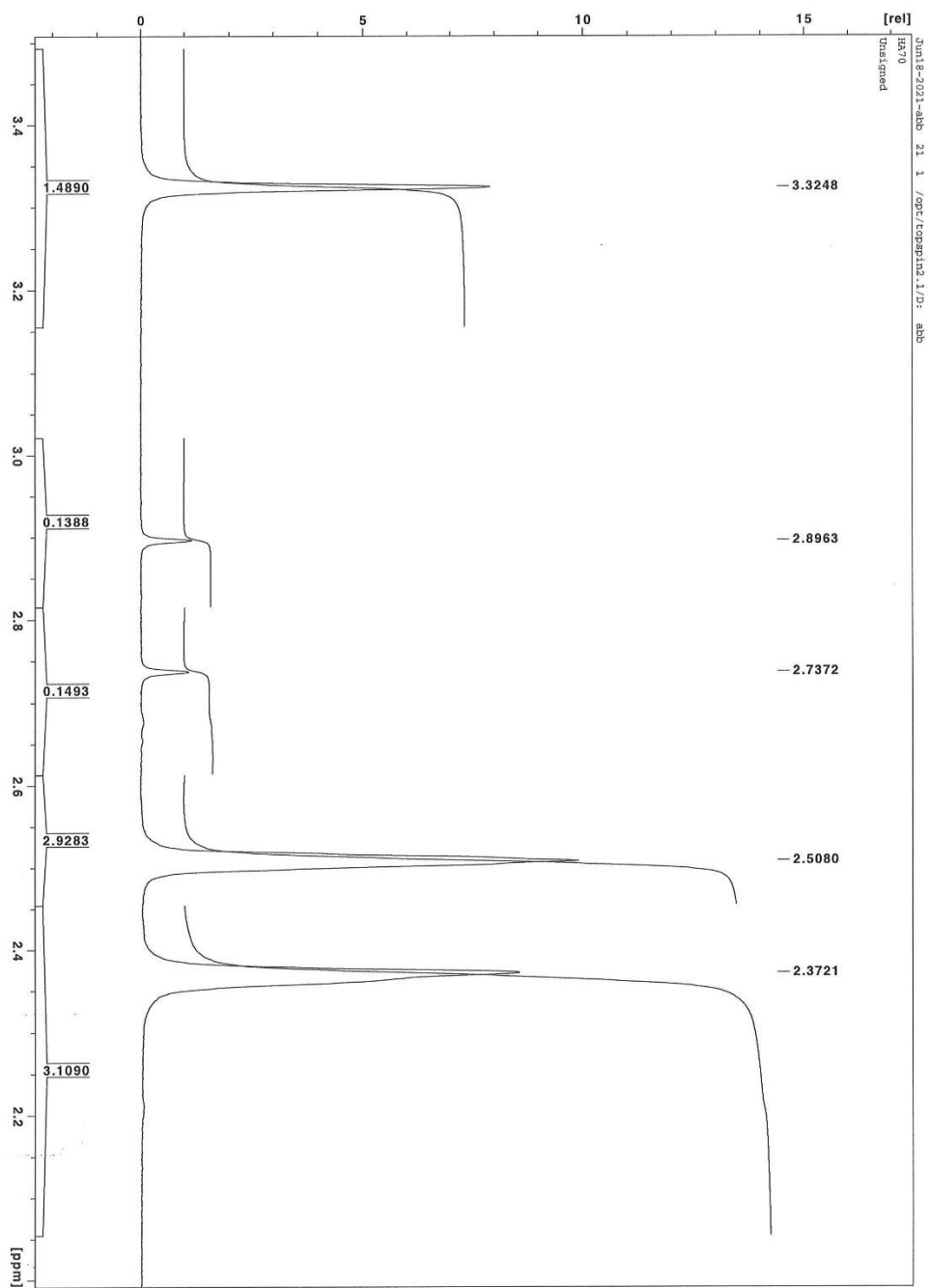
**Figure S117.** <sup>1</sup>H NMR spectrum of compound **7f** (400 MHz, DMSO-d<sub>6</sub>).



**Figure S118.** Detail of  $^1\text{H}$  NMR spectrum of compound **7f**.

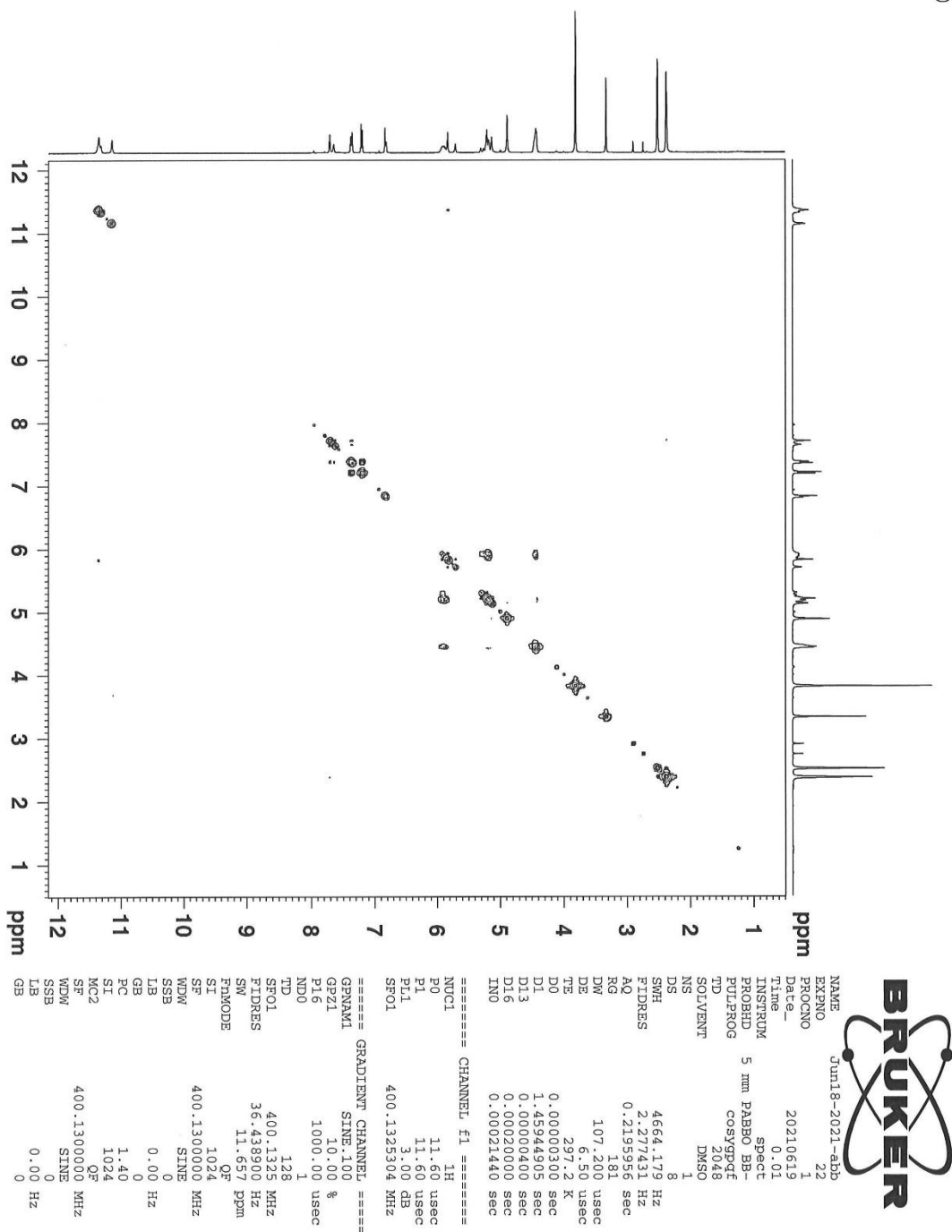


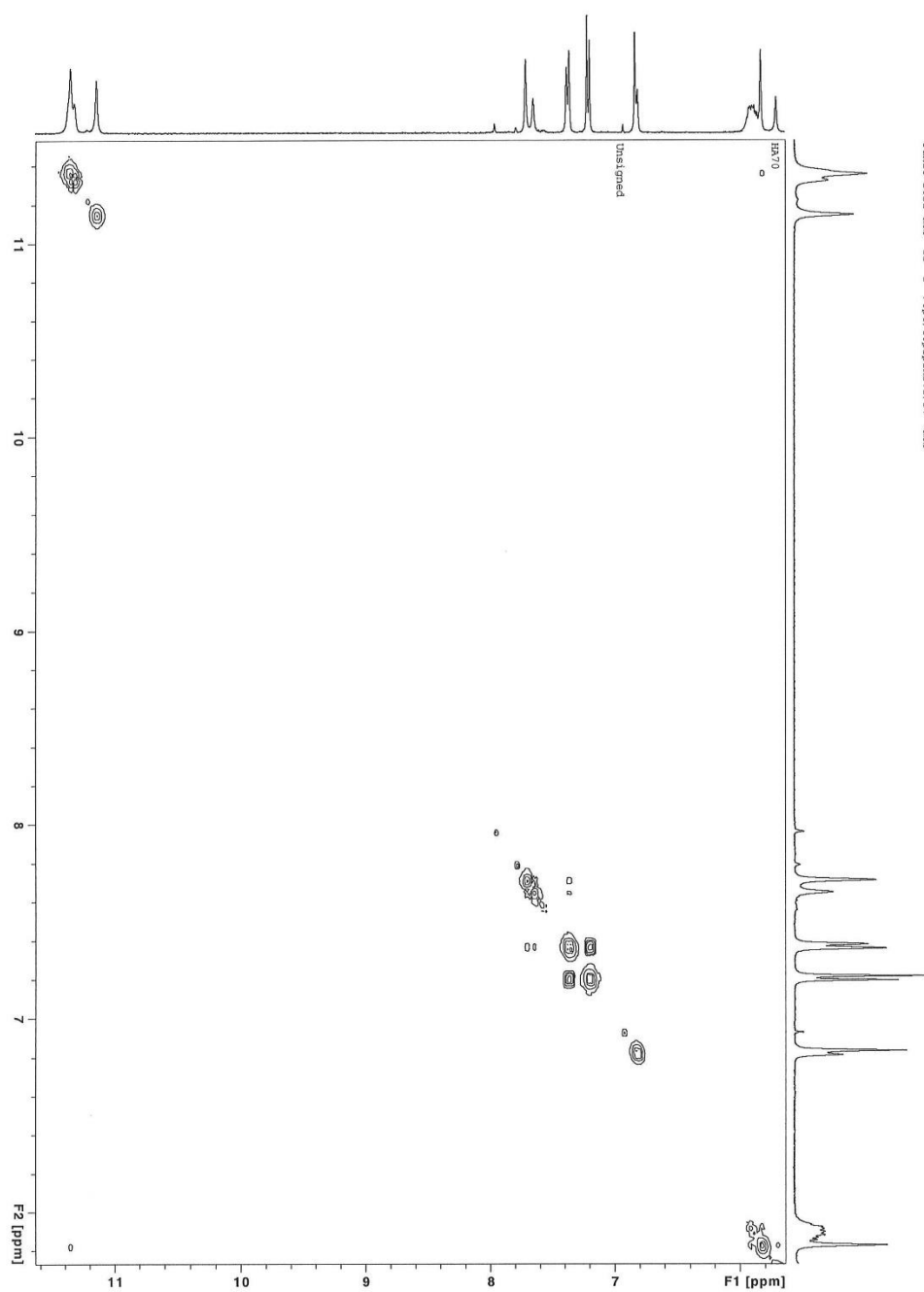
**Figure S119.** Detail of  $^1\text{H}$  NMR spectrum of compound **7f**.



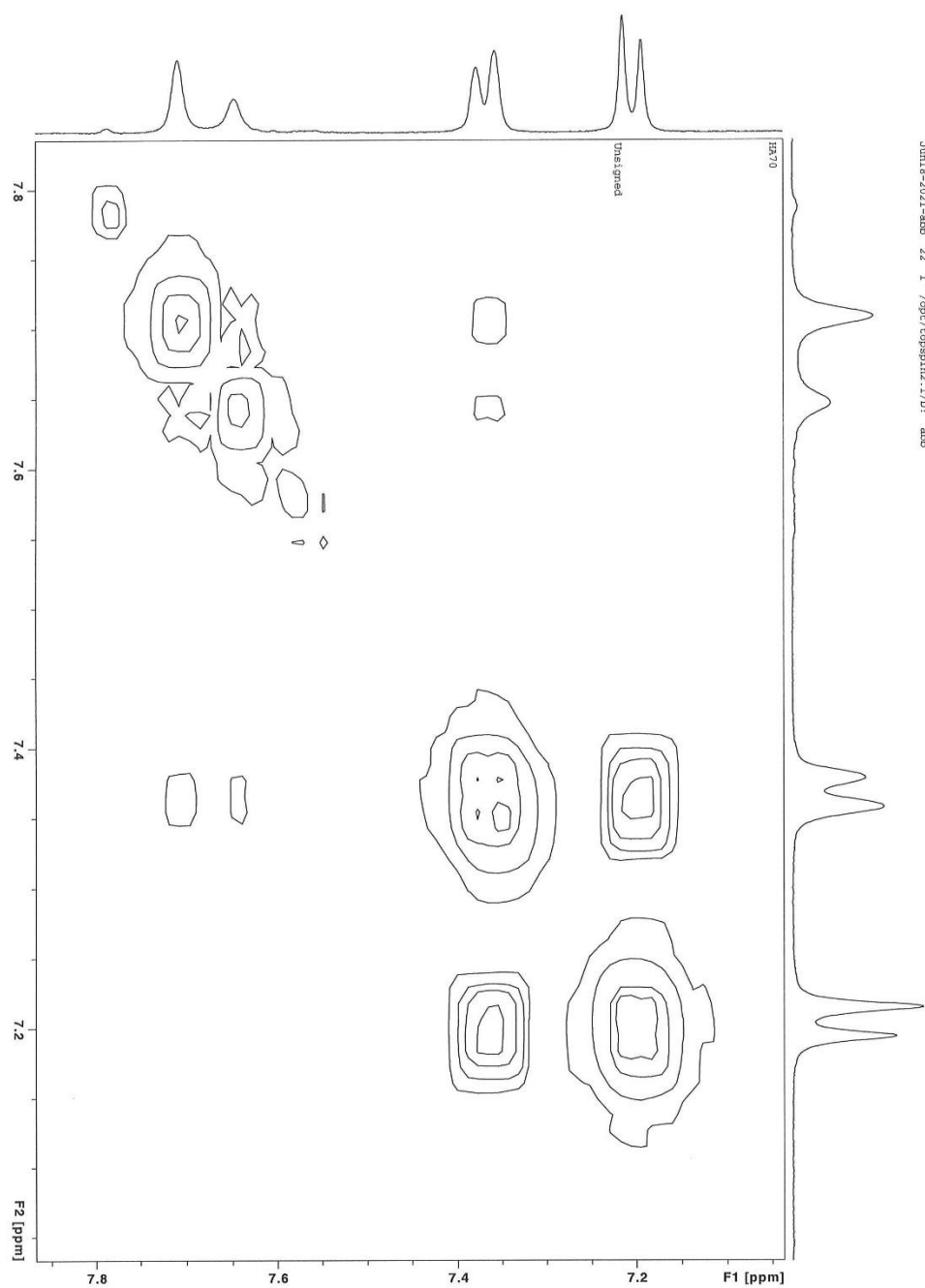
**Figure S120.** Detail of  $^1\text{H}$  NMR spectrum of compound **7f**.

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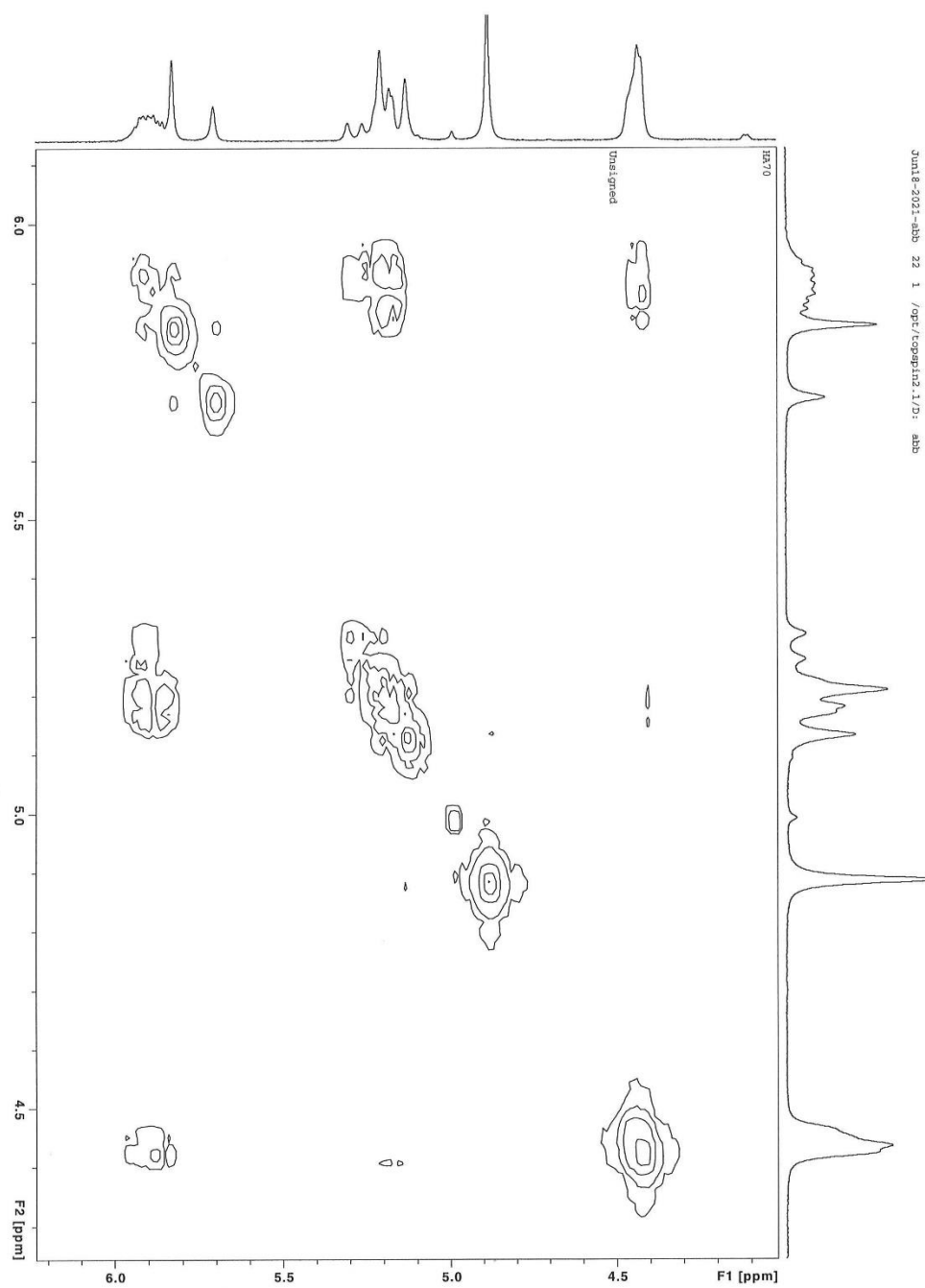
 $^1\text{H}$ - $^1\text{H}$  COSYFigure S121.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7f**.



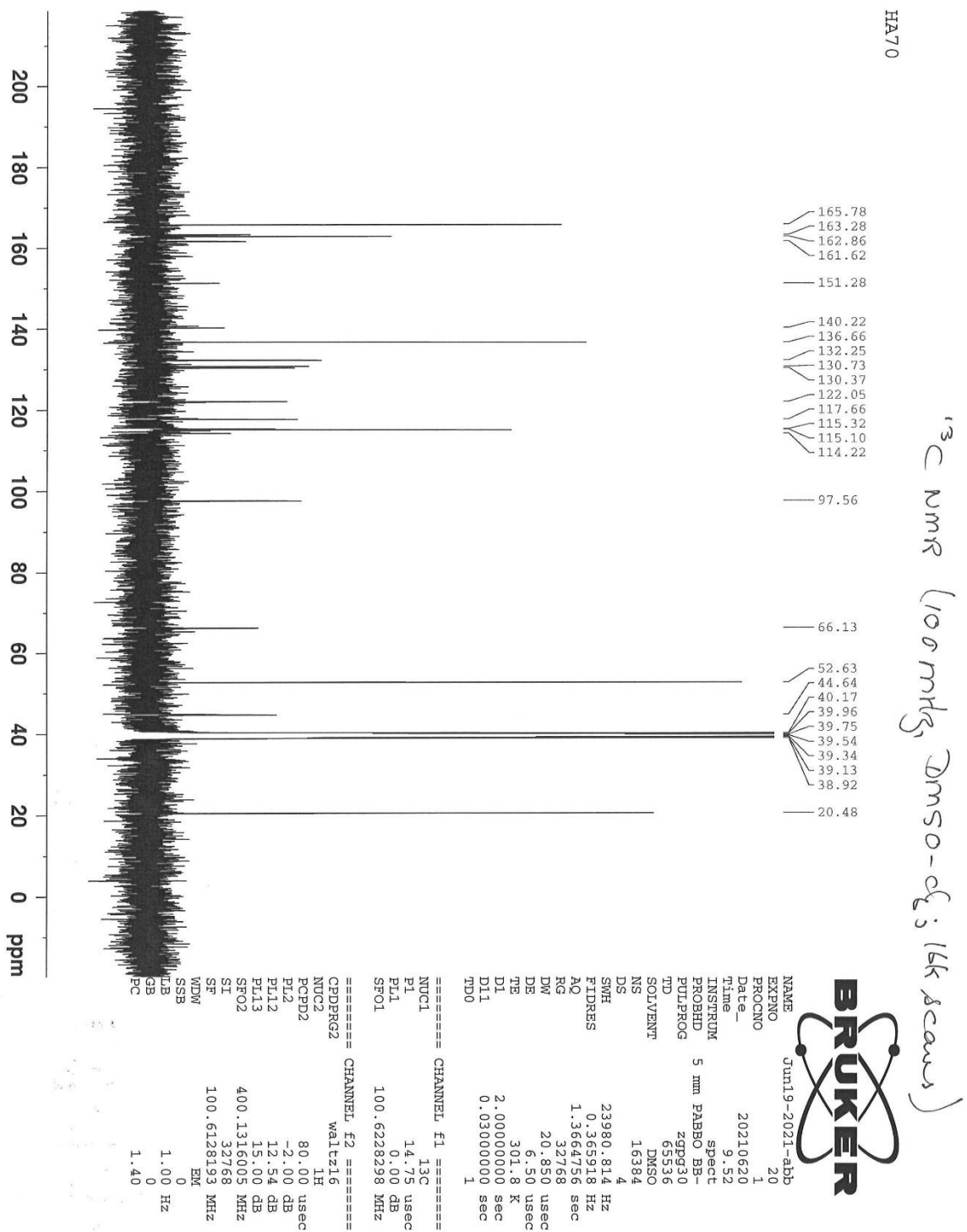
**Figure S122.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7f**.



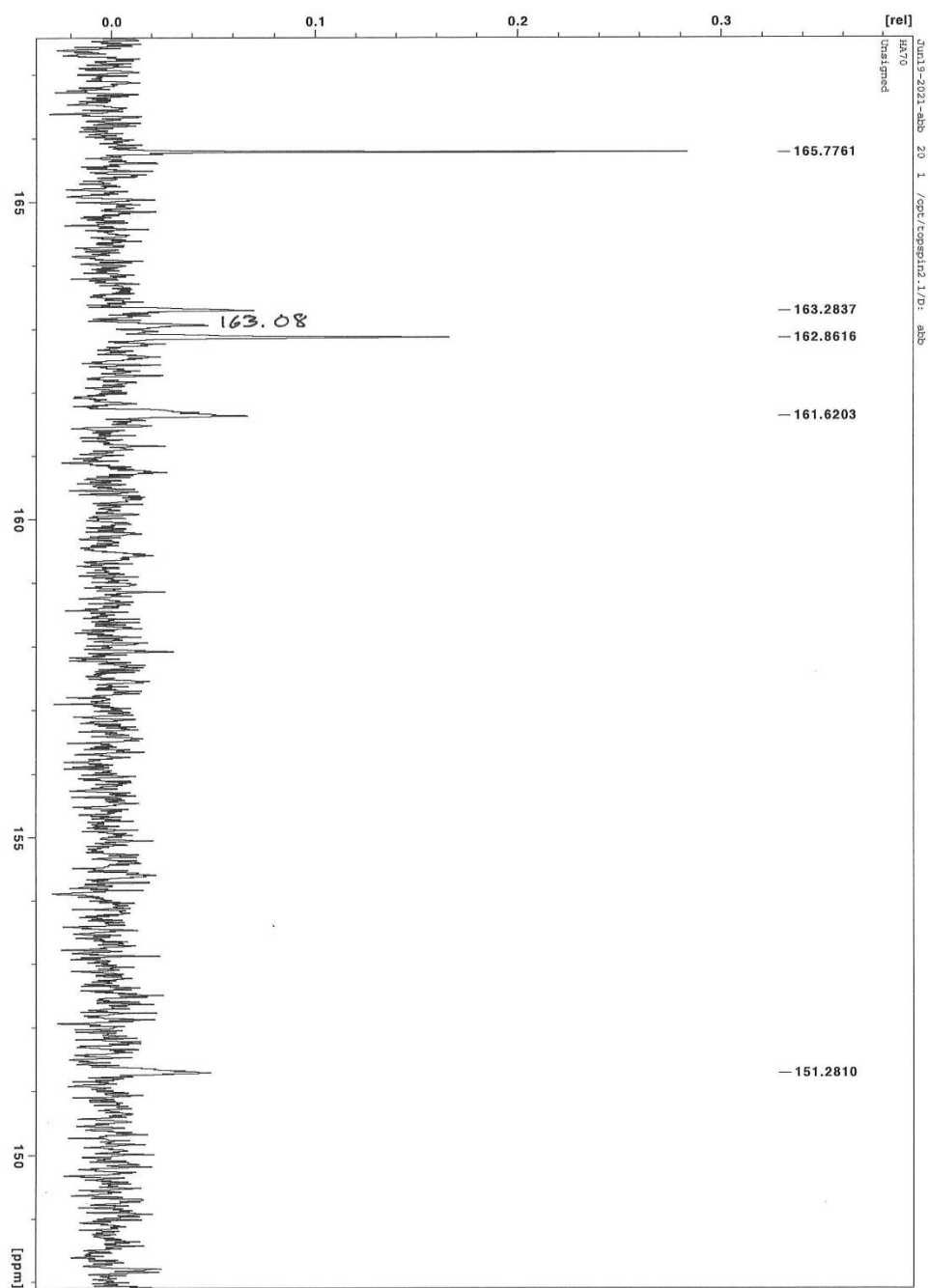
**Figure S123.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7f**.



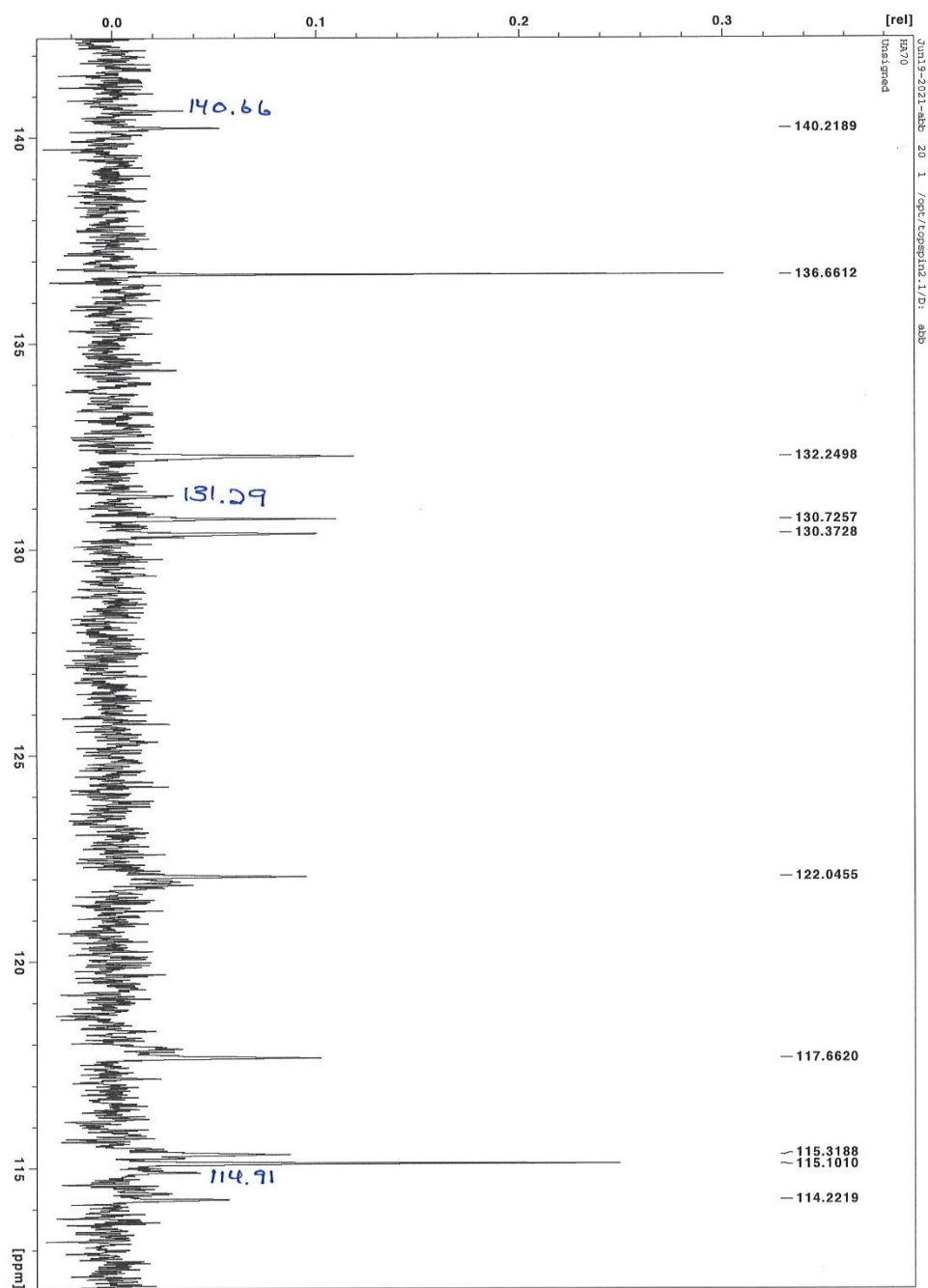
**Figure S124.** Detail of  $^1\text{H}$ - $^1\text{H}$  spectrum of compound **7f**.



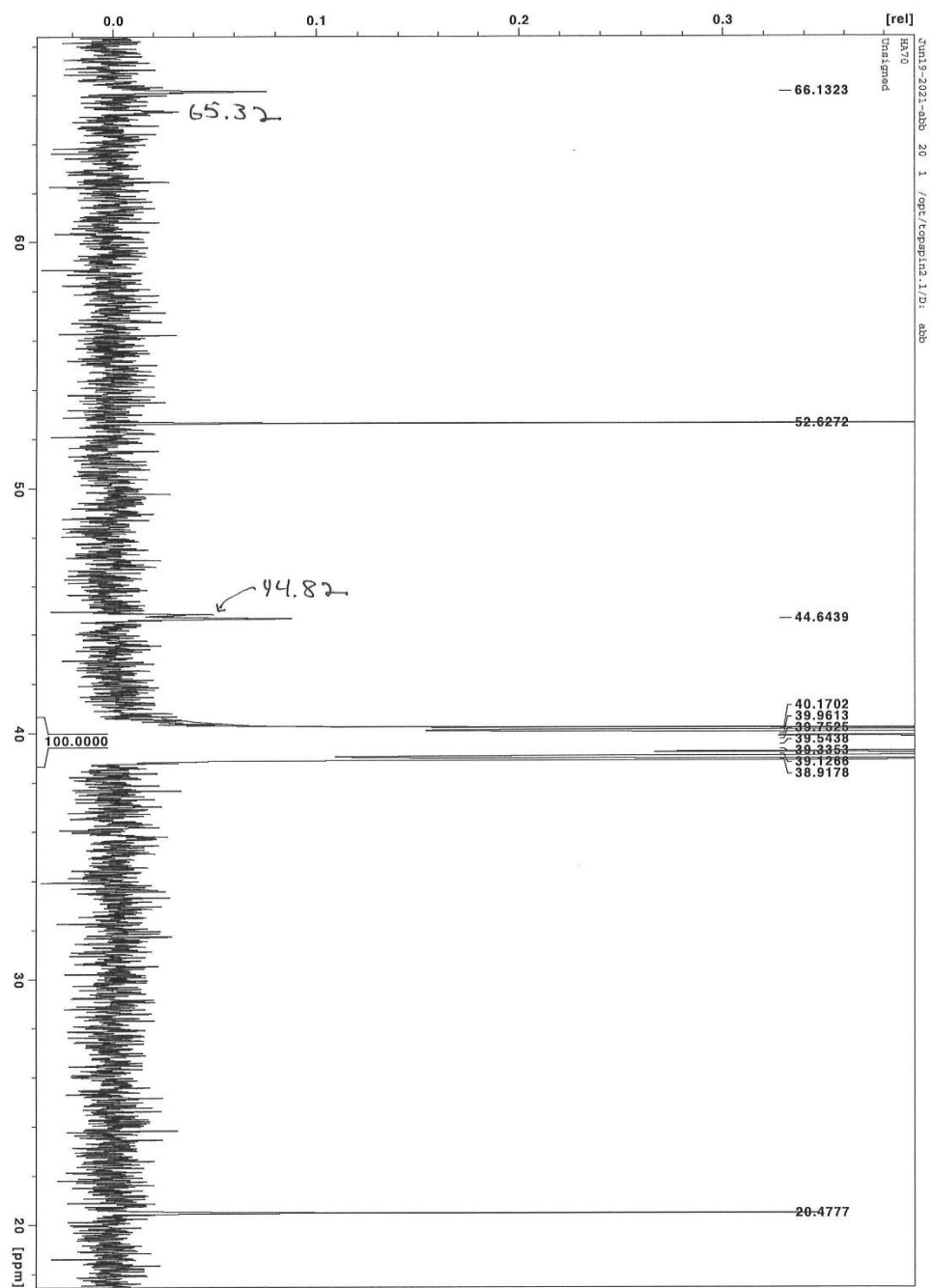
**Figure S125.** <sup>13</sup>C NMR spectrum of compound **7f** (100 MHz, DMSO-d<sub>6</sub>).



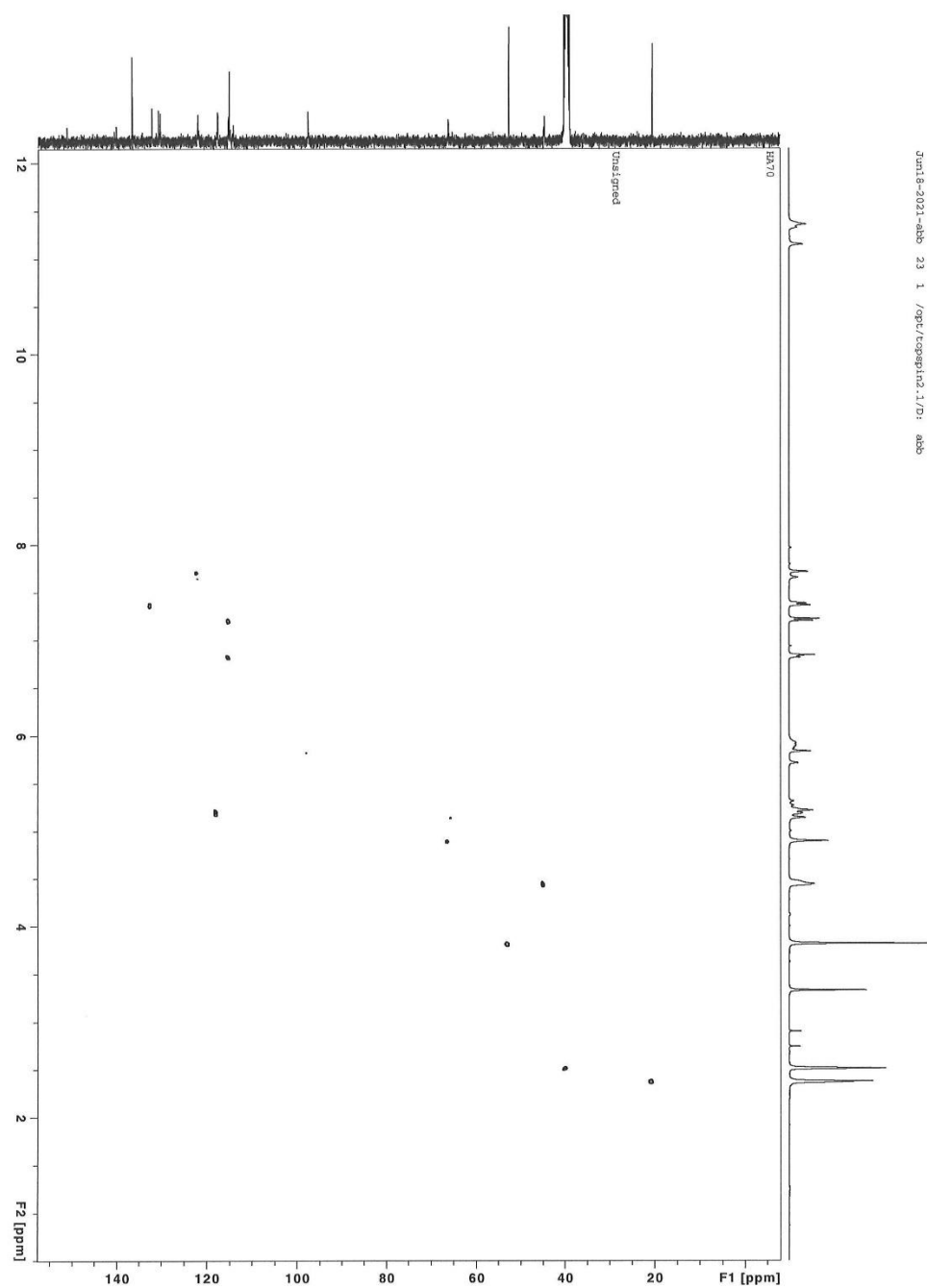
**Figure S126.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **7f**.



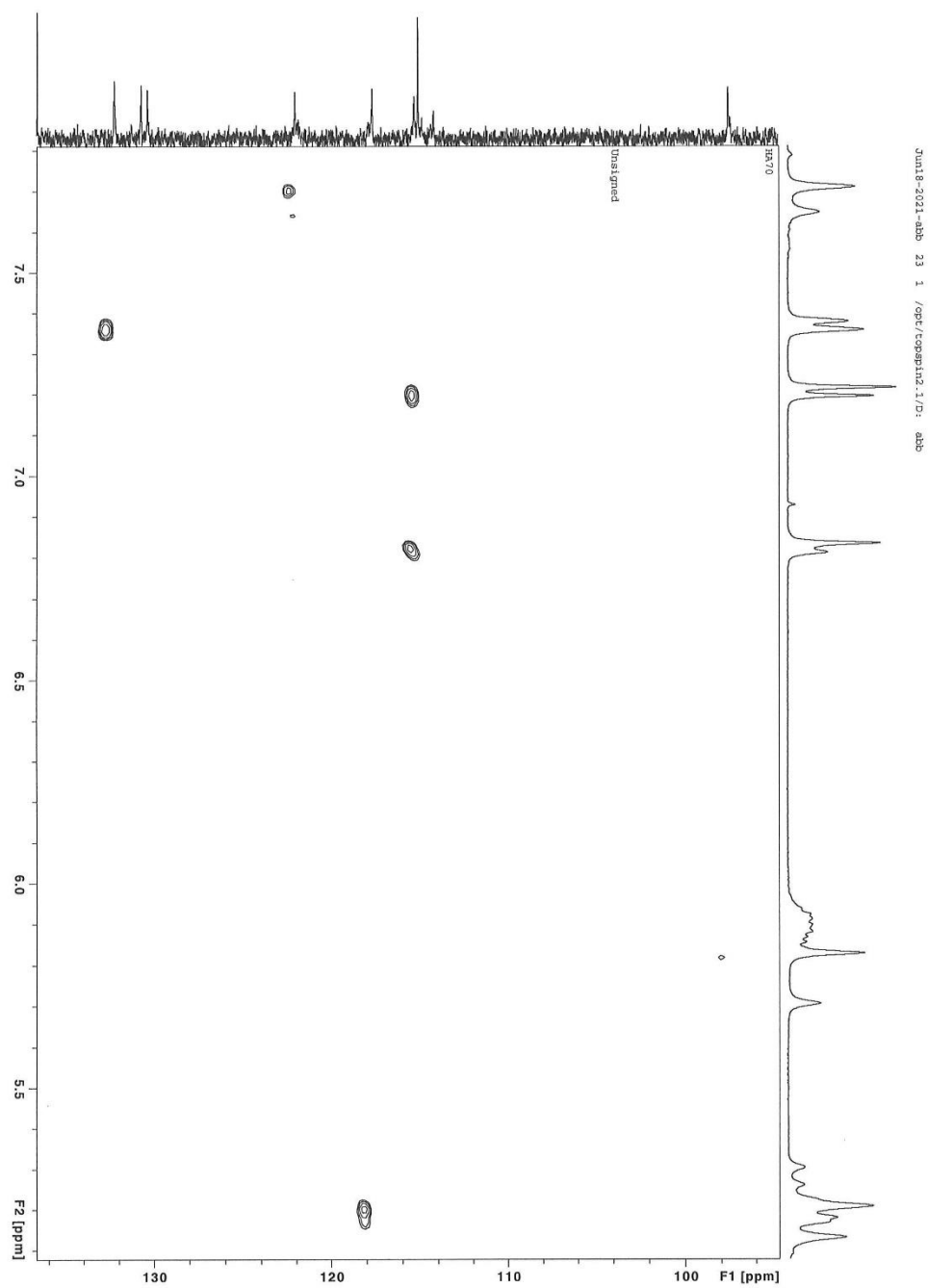
**Figure S127.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **7f**.



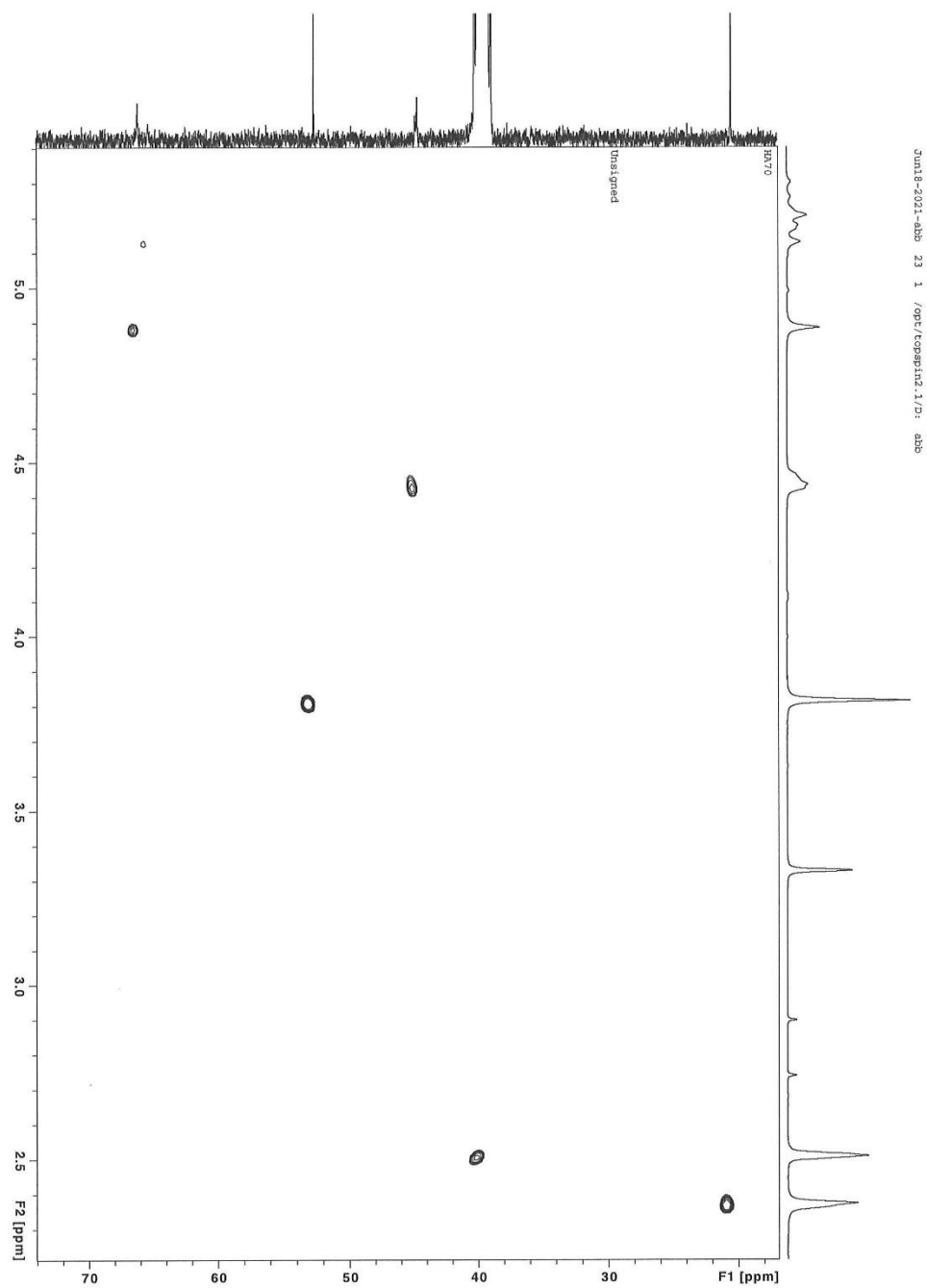
**Figure S128.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **7f**.



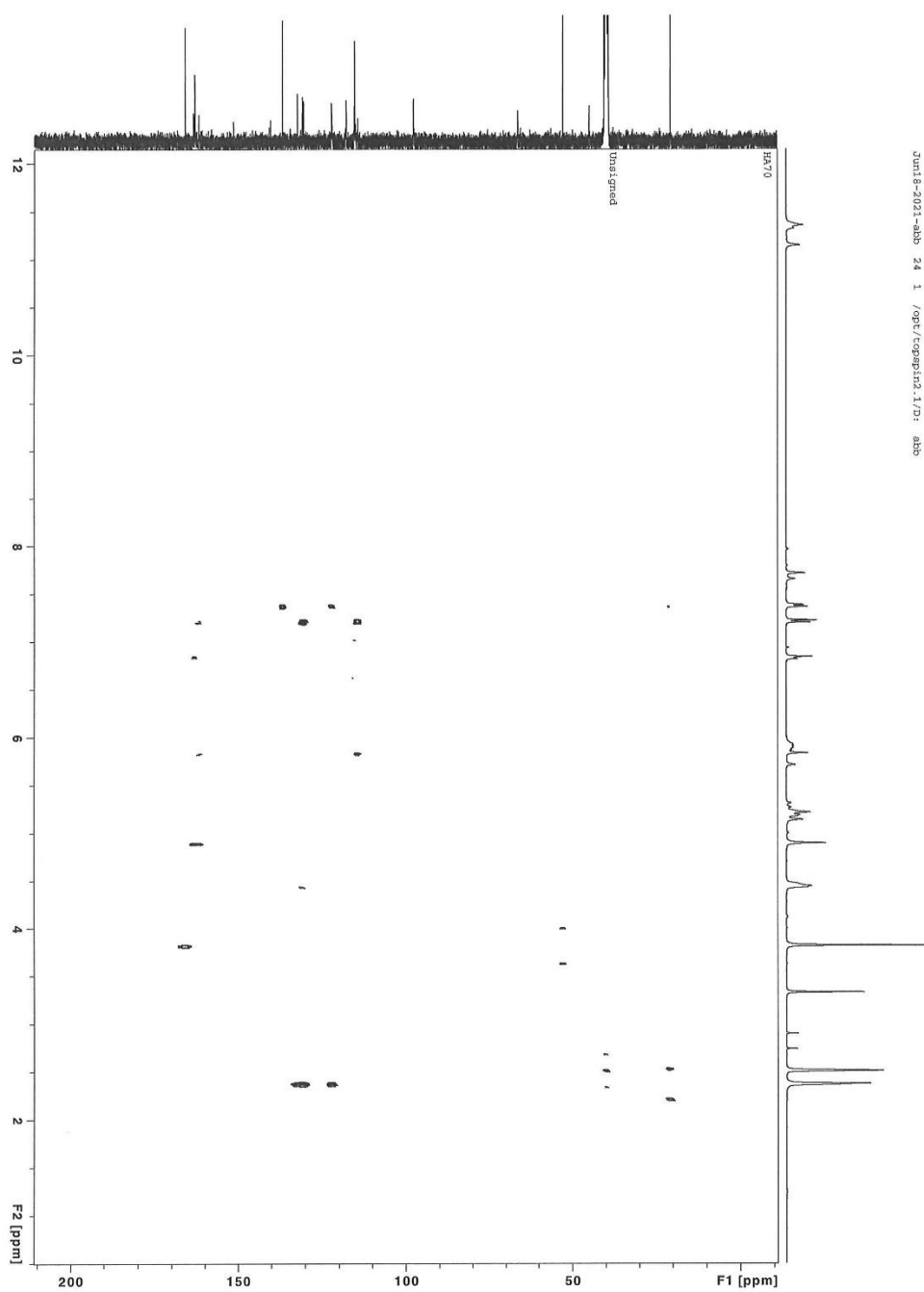
**Figure S129.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7f**.



**Figure S130.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7f**.

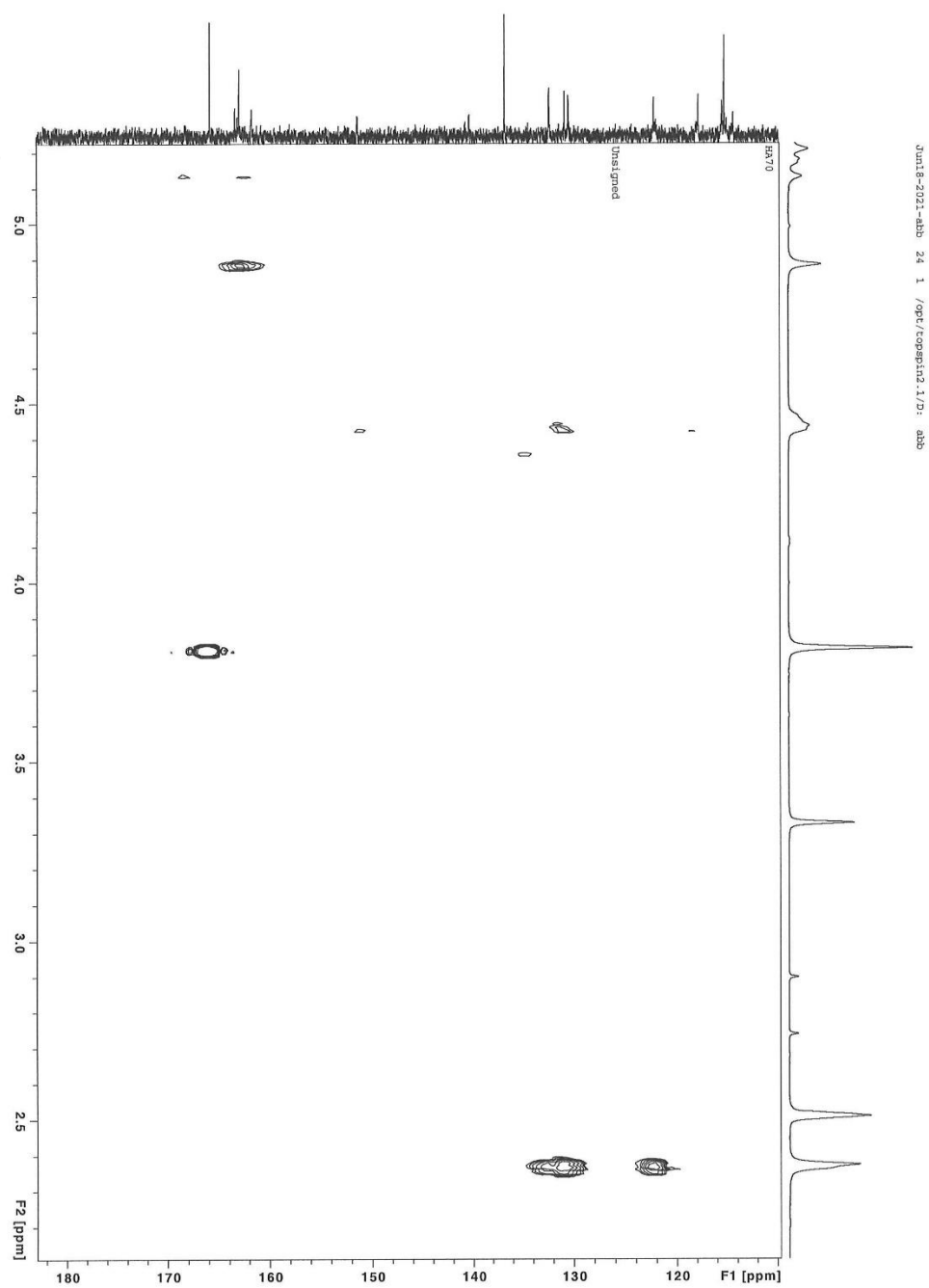


**Figure S131.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7f**.

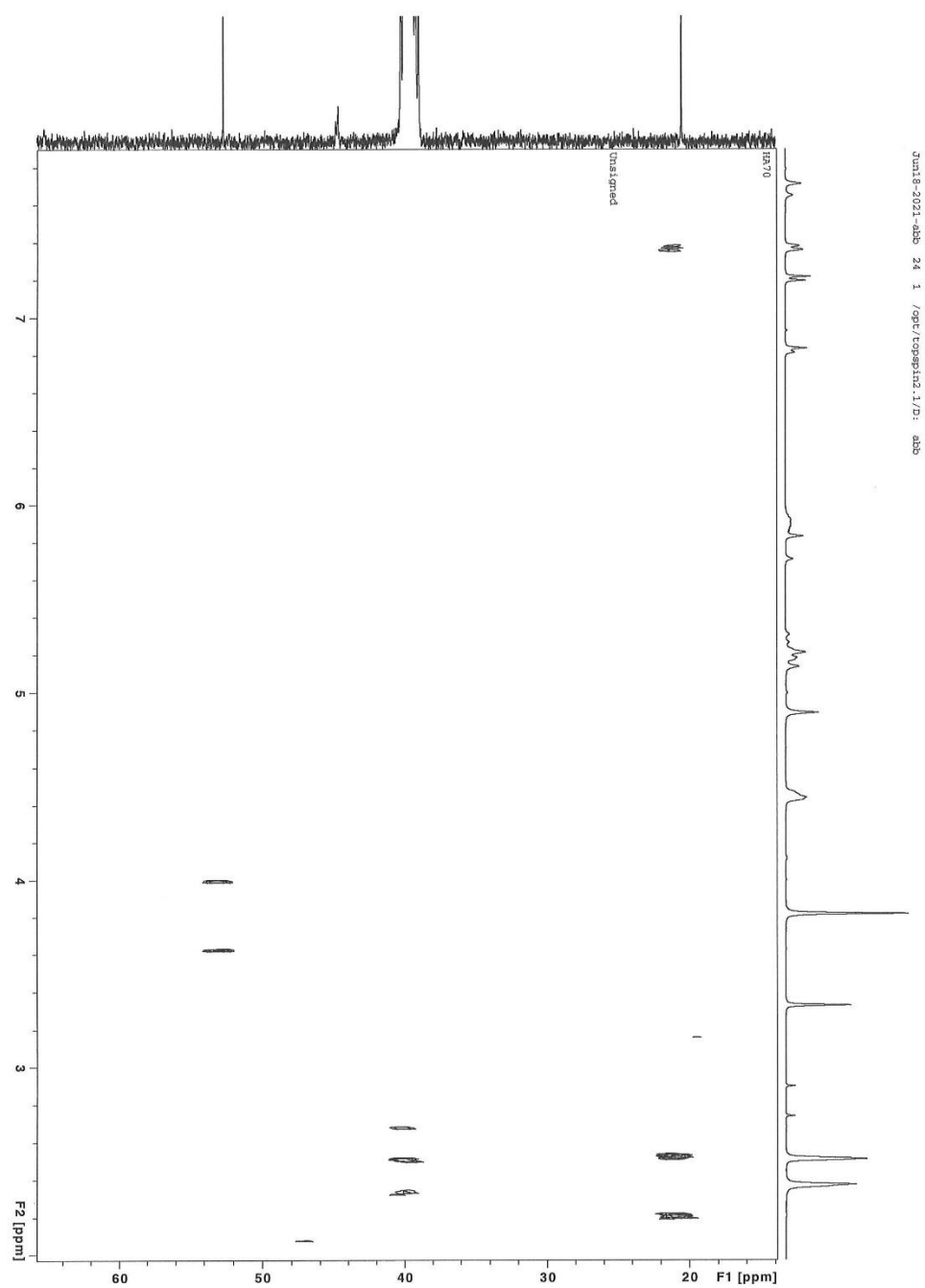


**Figure S132.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7f**.

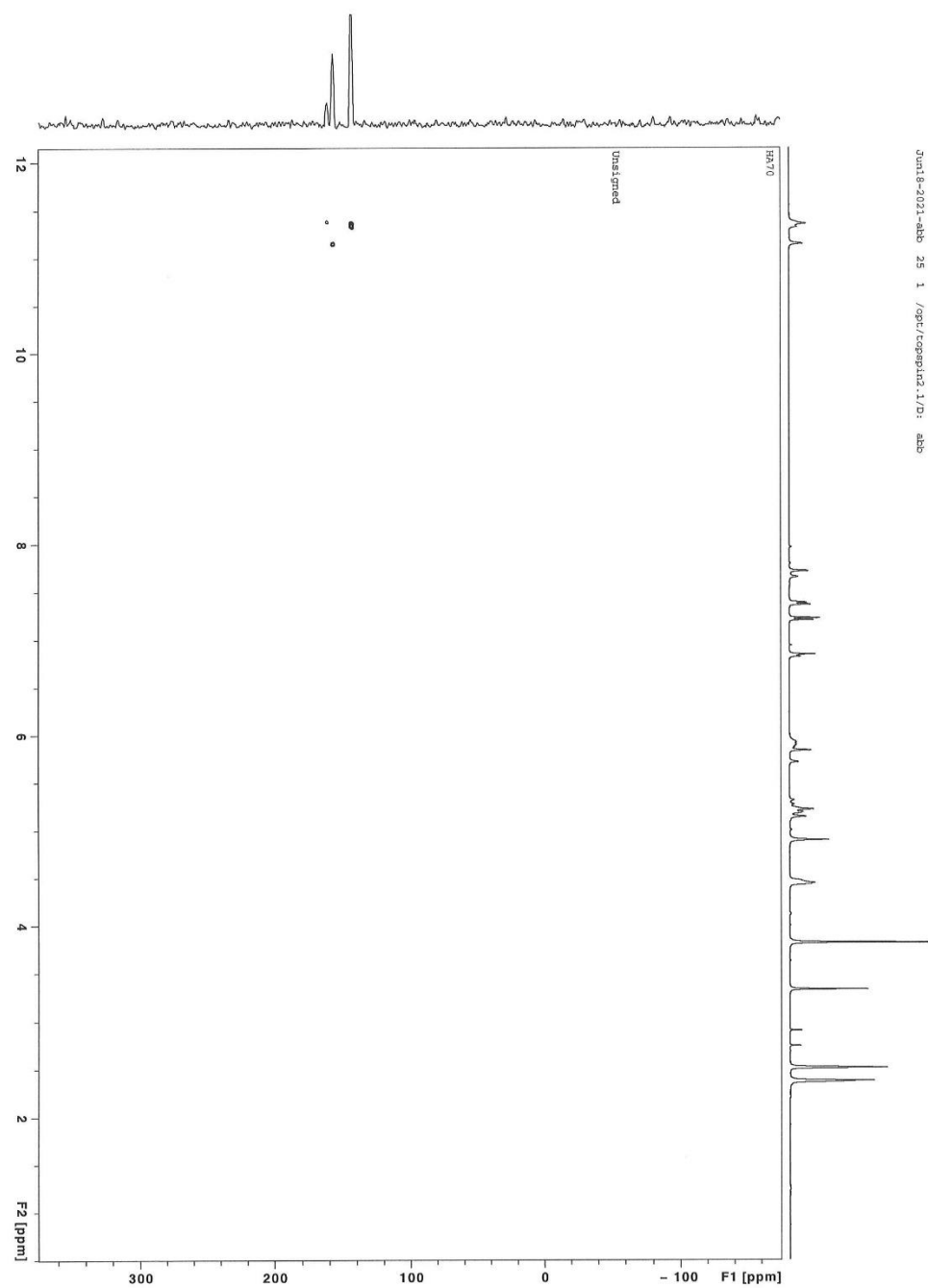




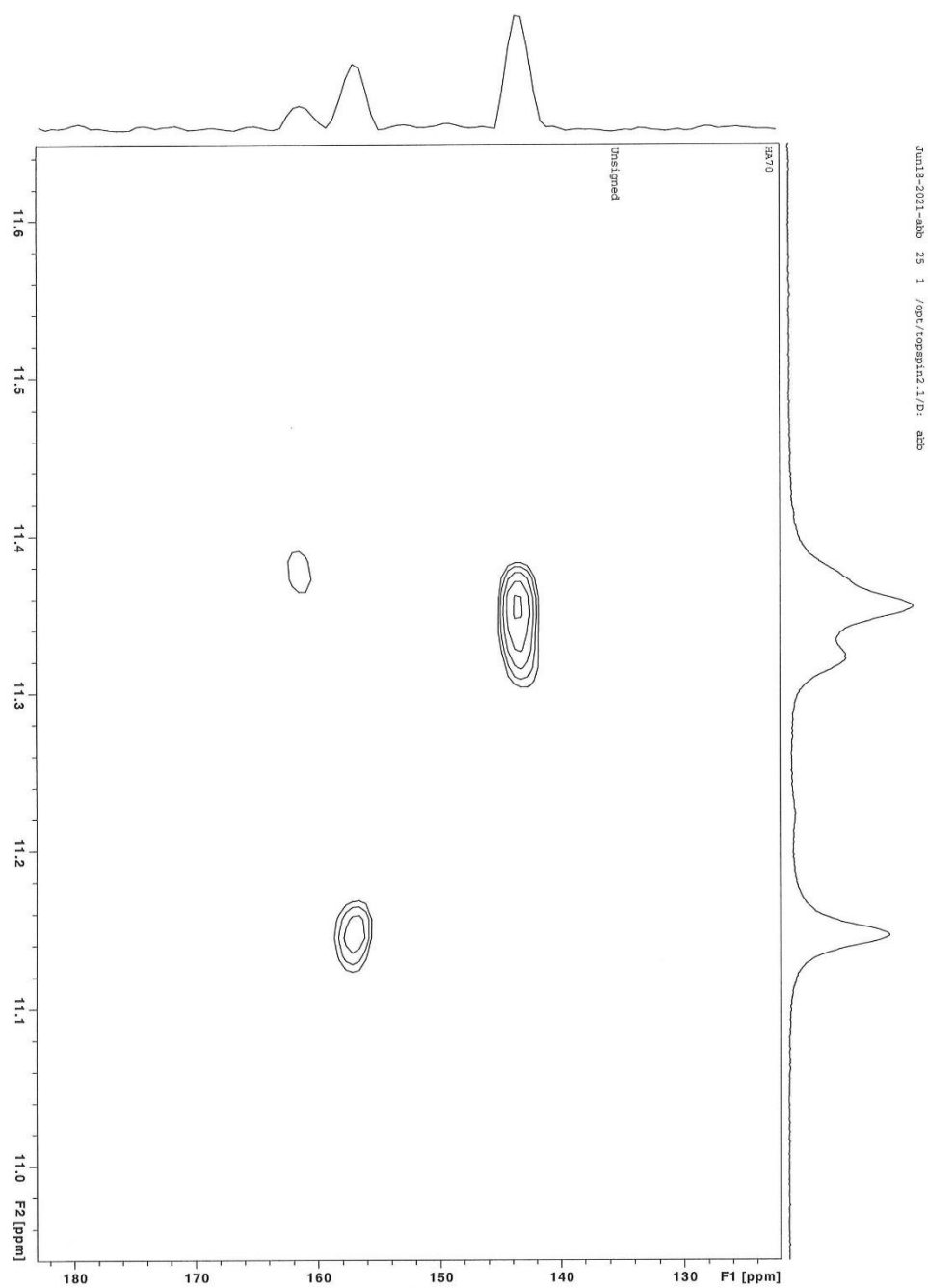
**Figure S134.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7f**.



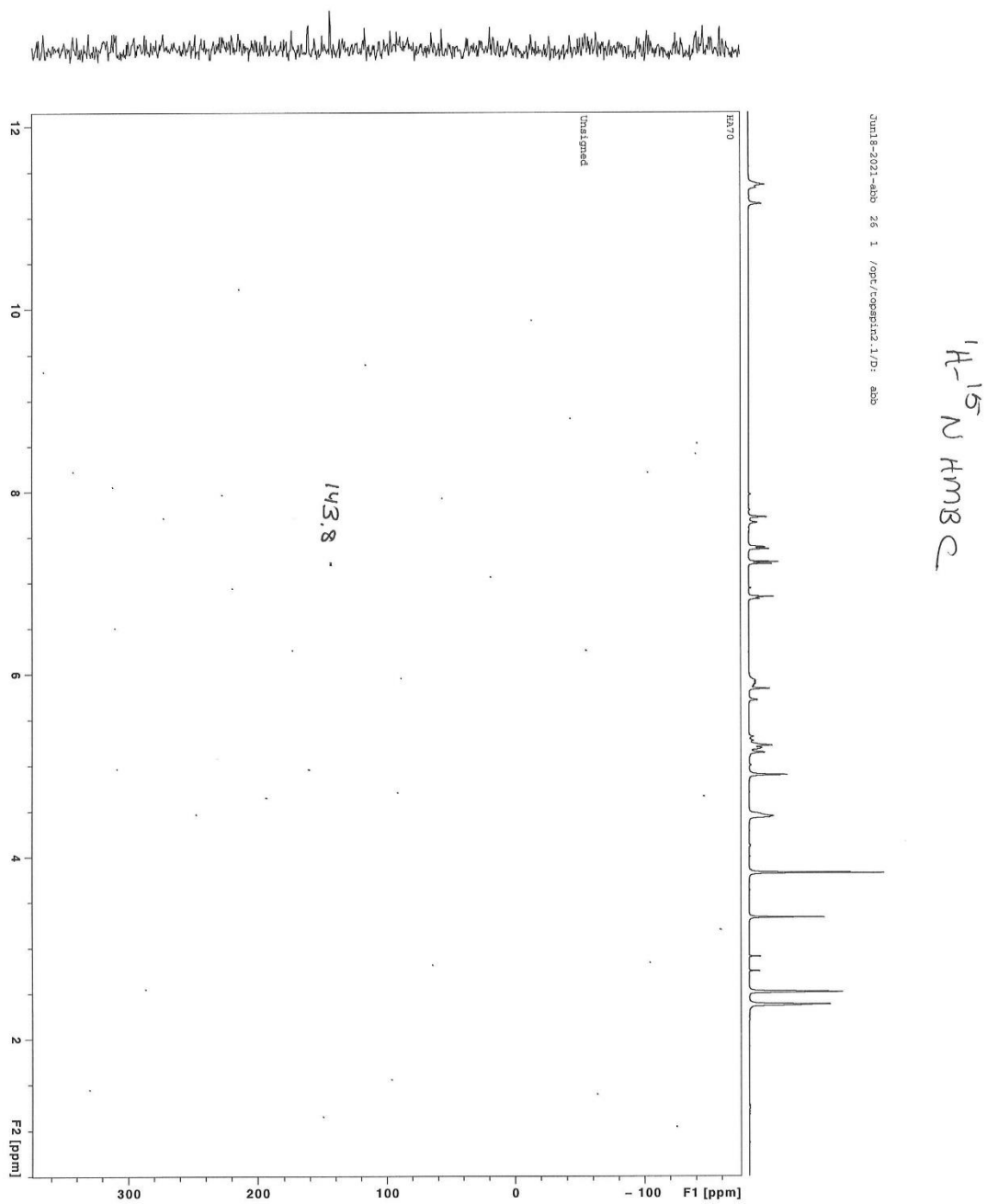
**Figure S135.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7f**.



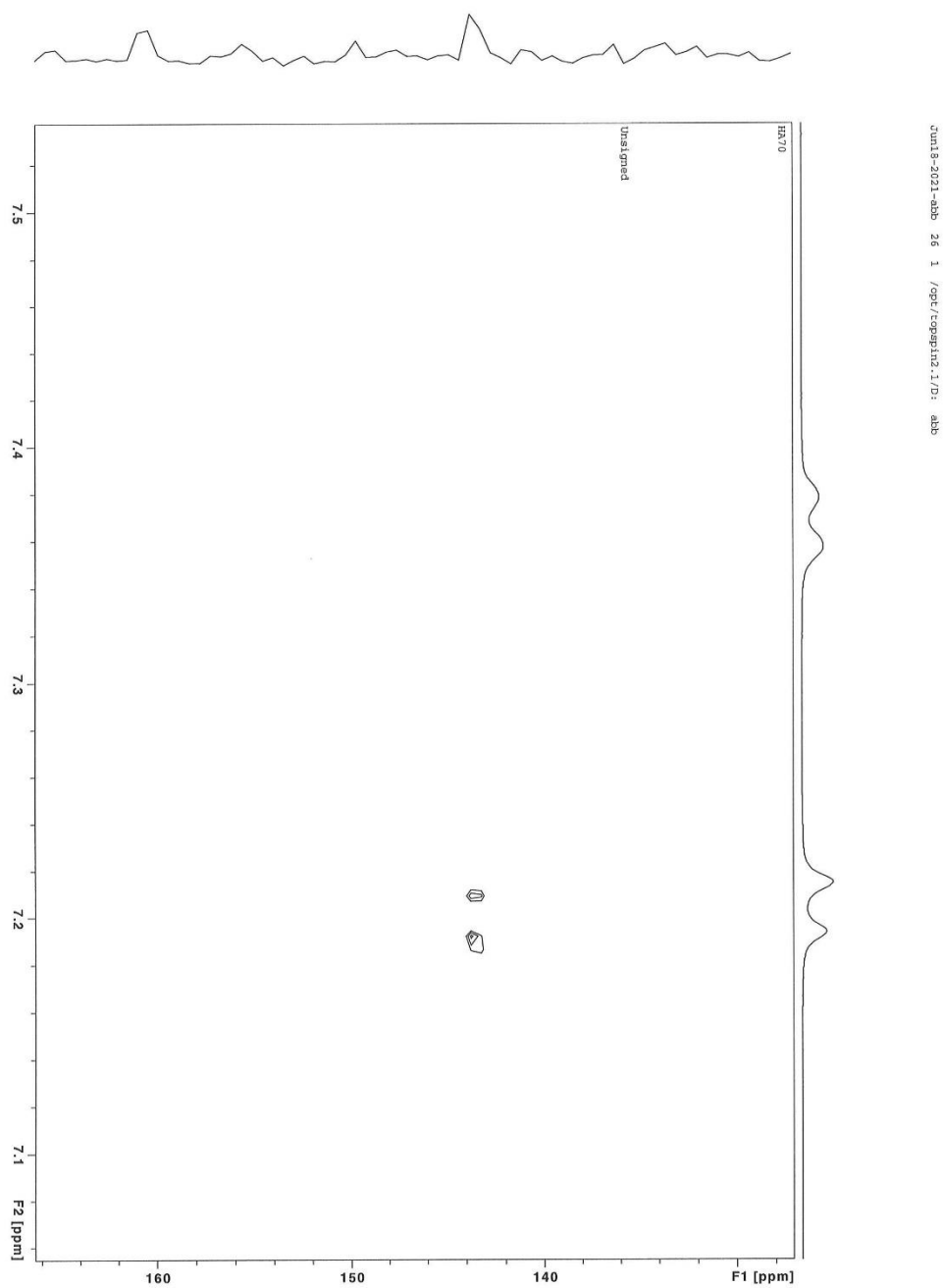
**Figure S136.**  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **7f**.



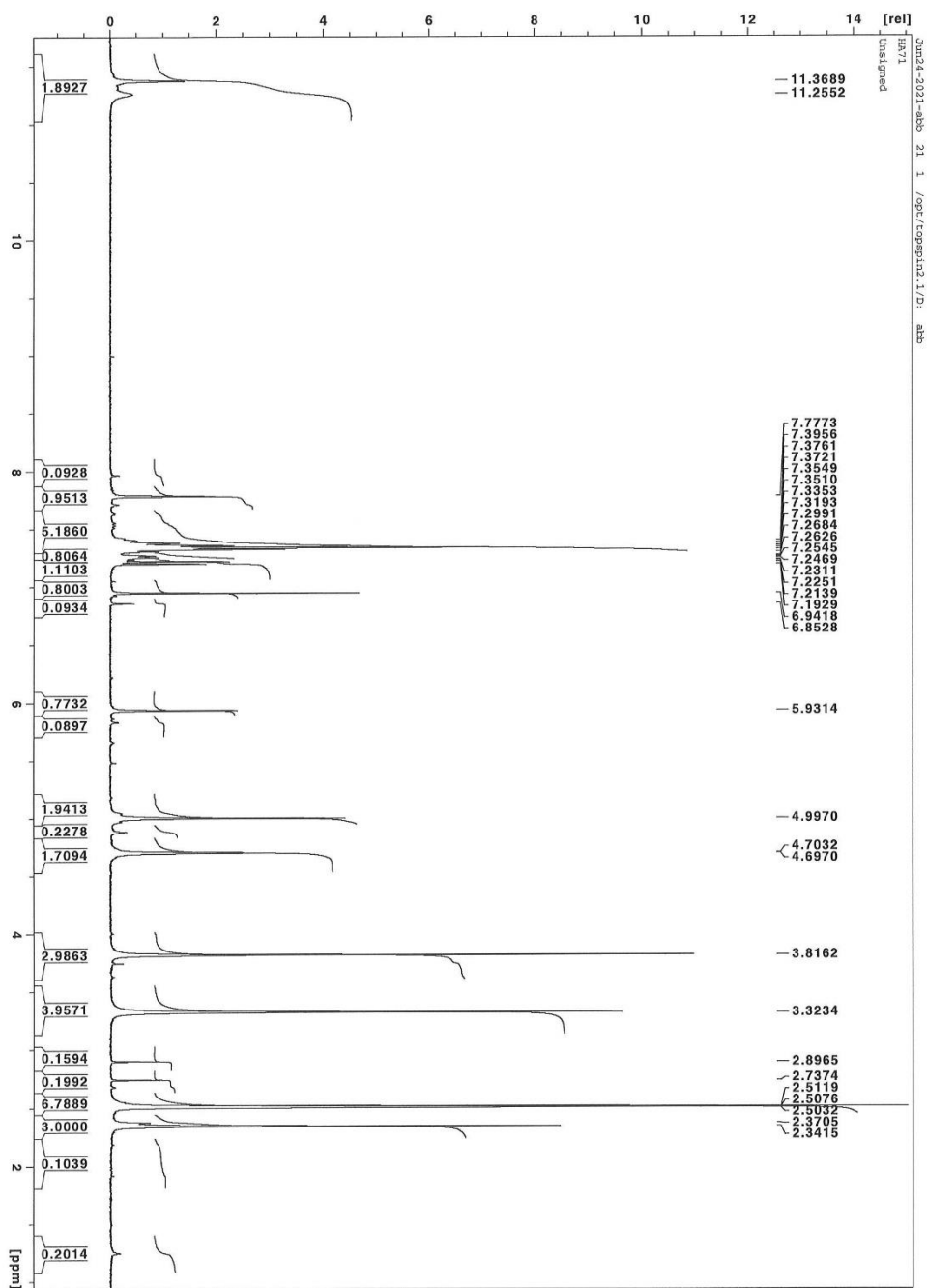
**Figure S137.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **7f**.



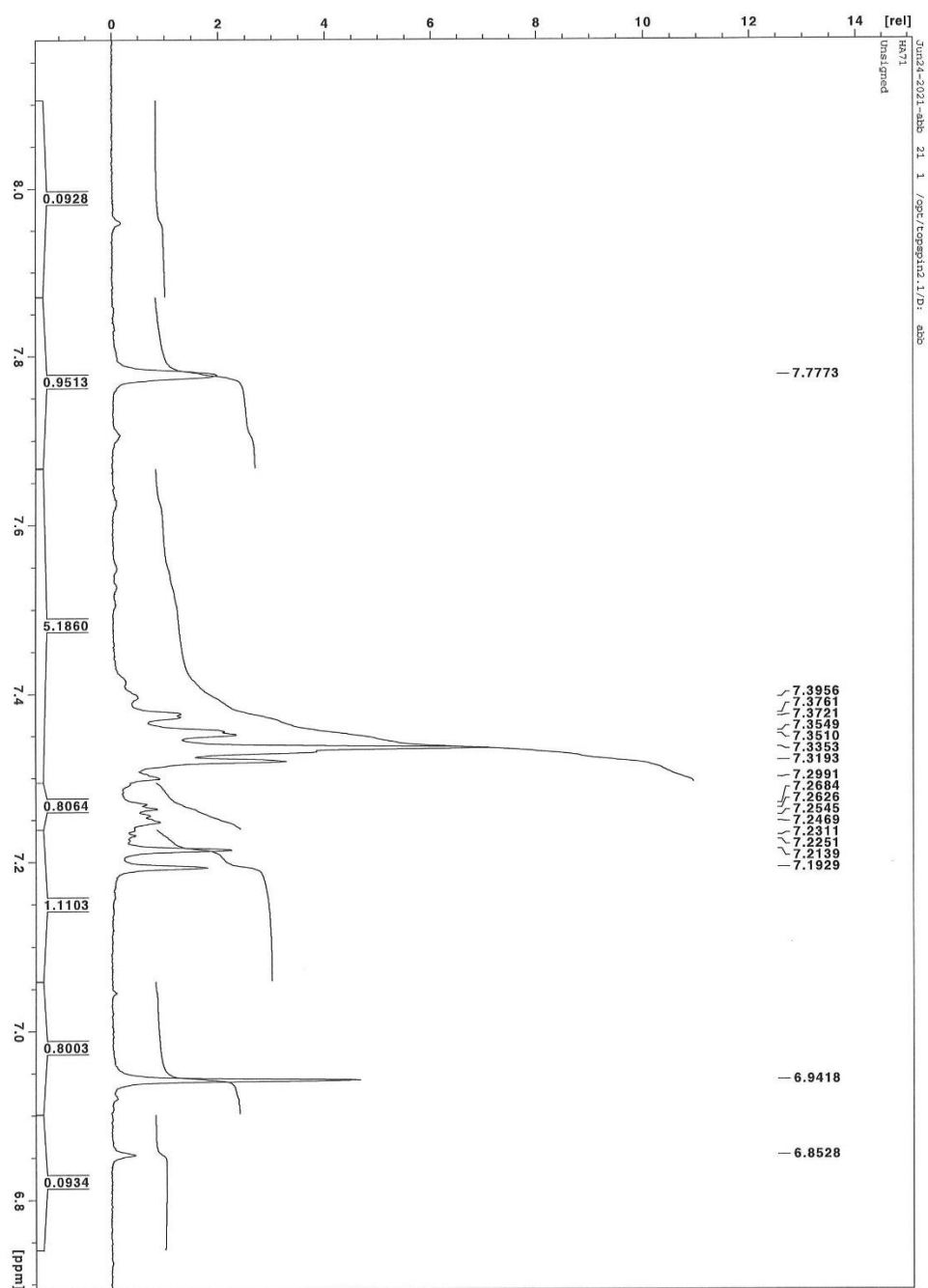
**Figure S138.**  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **7f**.



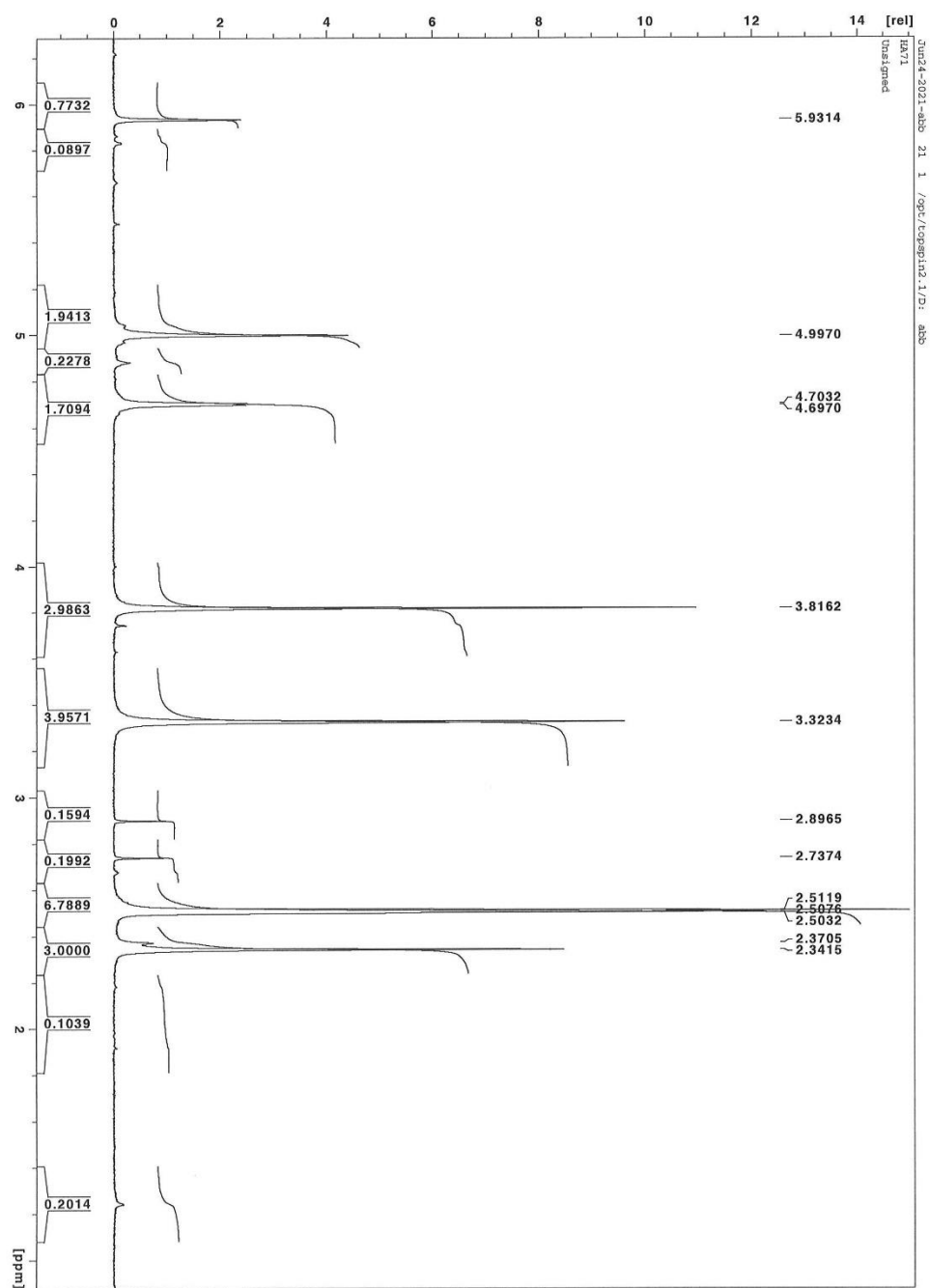
**Figure S139.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **7f**.



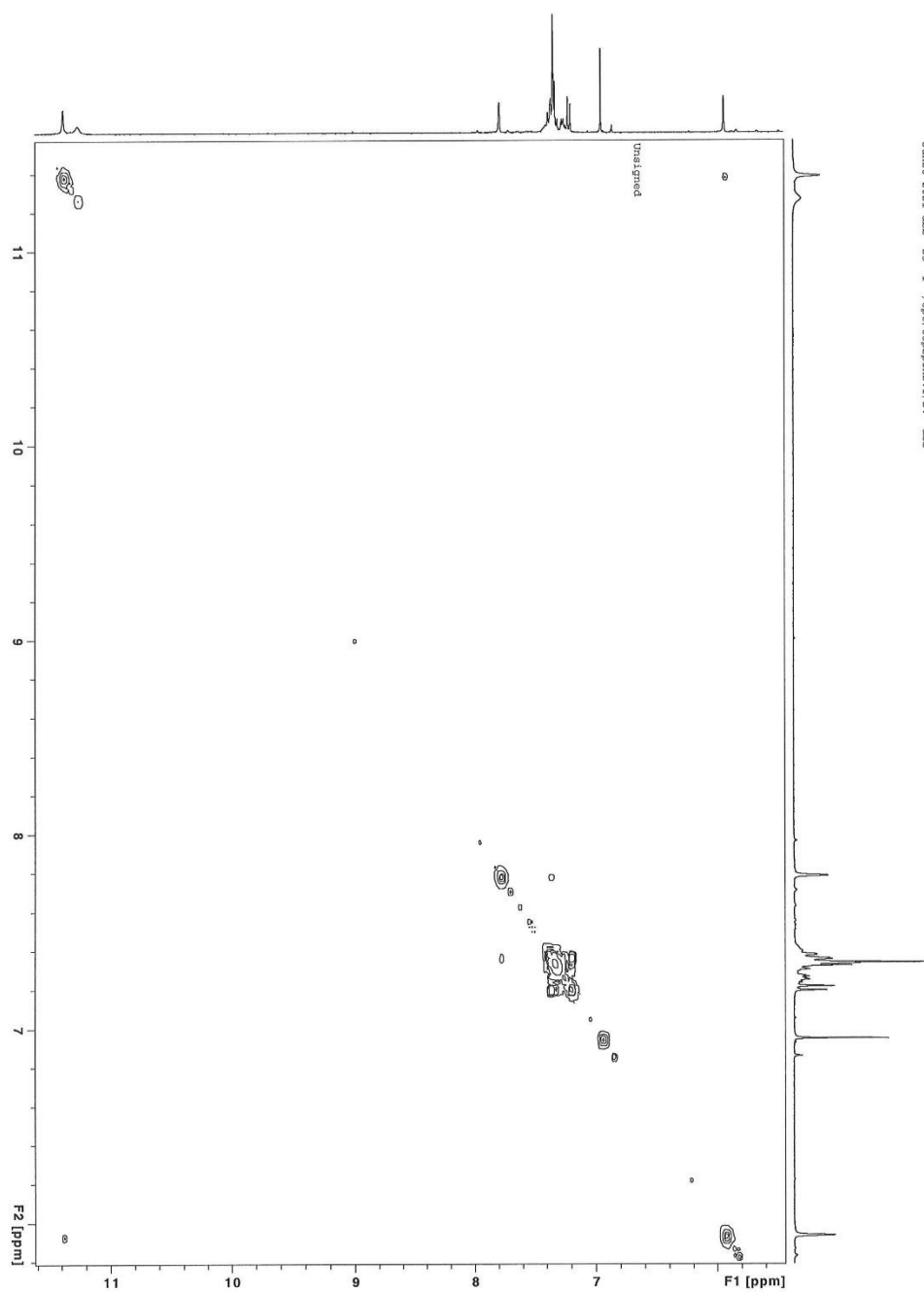
**Figure S140.**  $^1\text{H}$  NMR spectrum of compound **7g** (400 MHz,  $\text{DMSO}-d_6$ ).



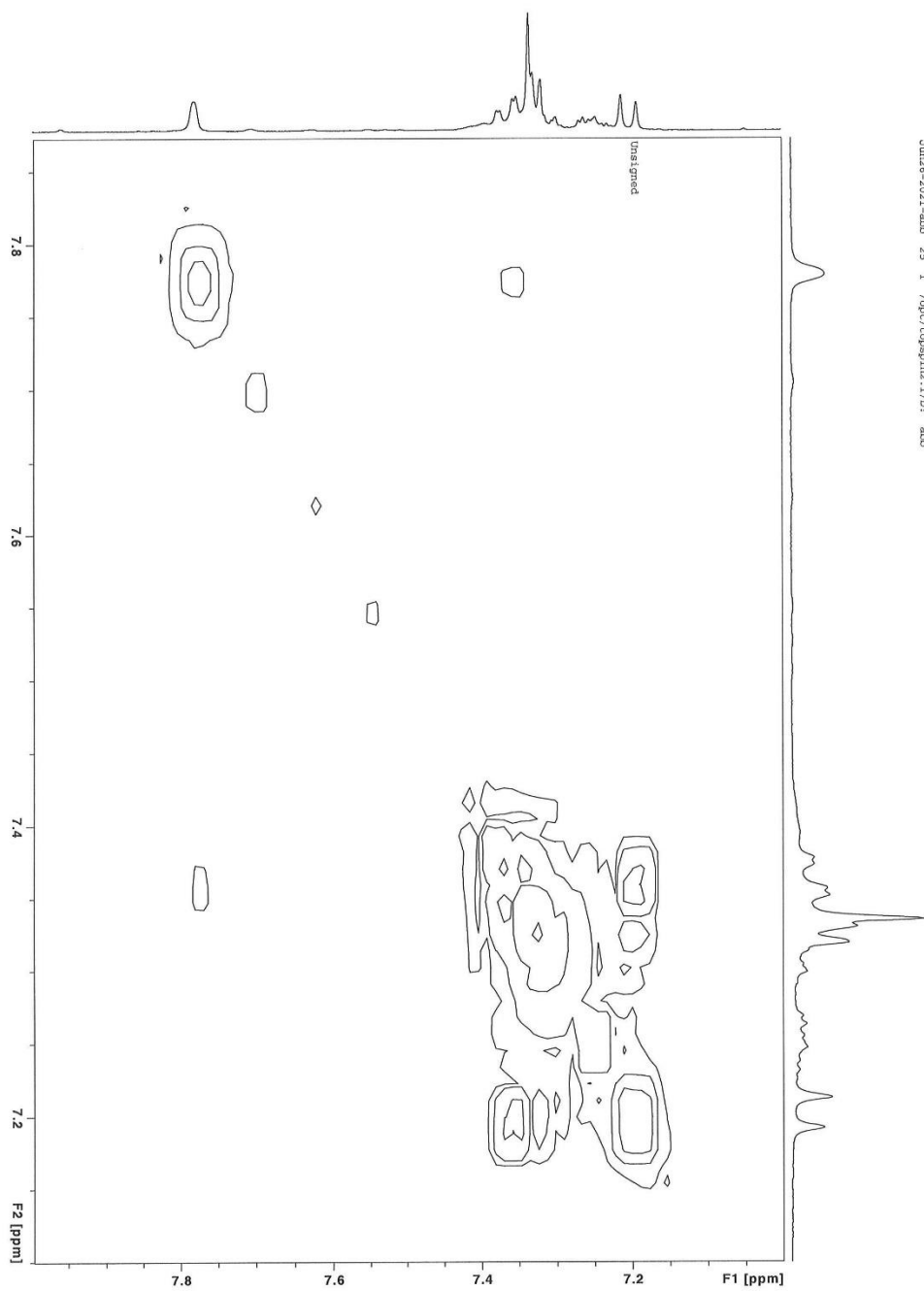
**Figure S141.** Detail of  $^1\text{H}$  NMR spectrum of compound **7g**.



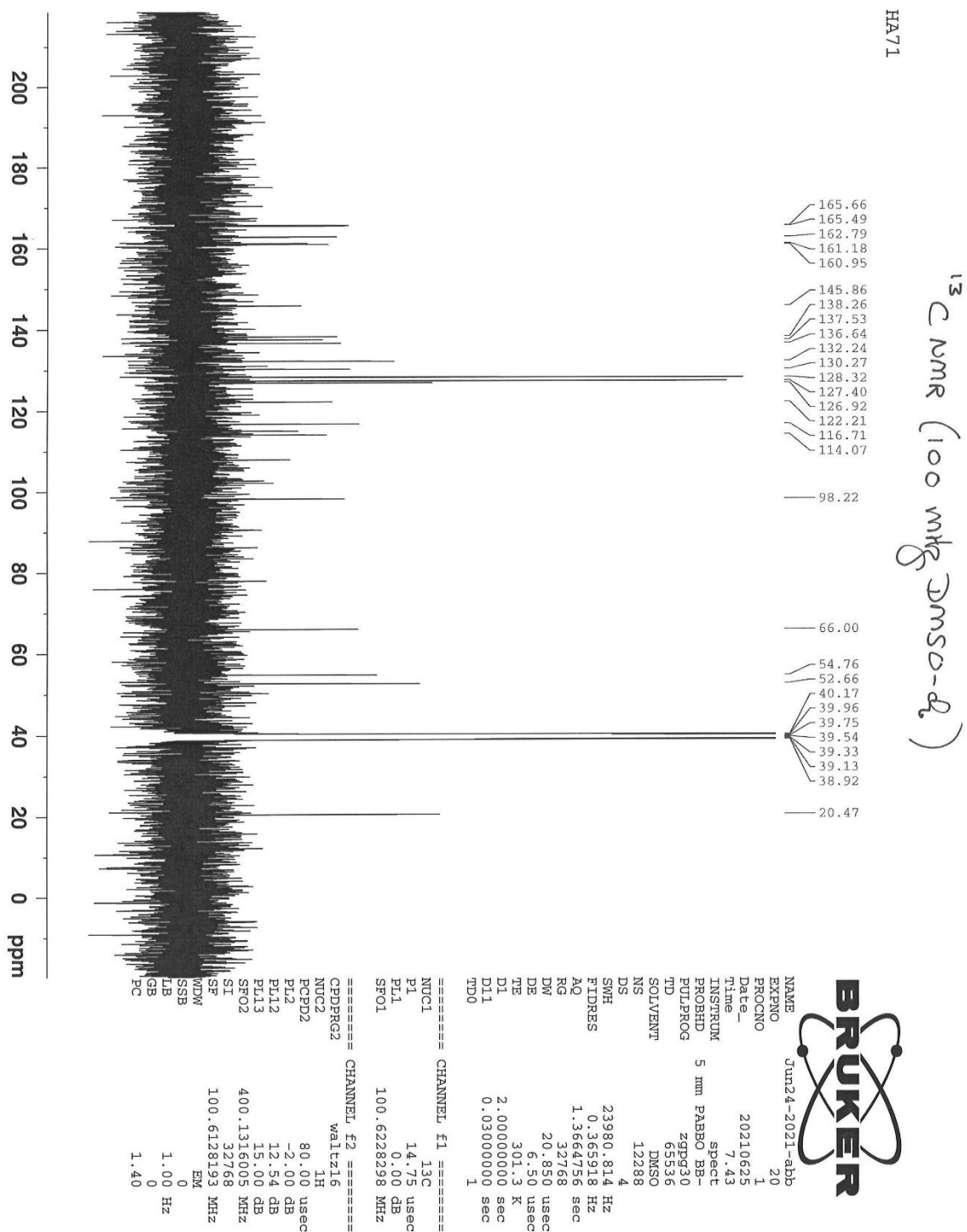
**Figure S142.** Detail of  $^1\text{H}$  NMR spectrum of compound **7g**.



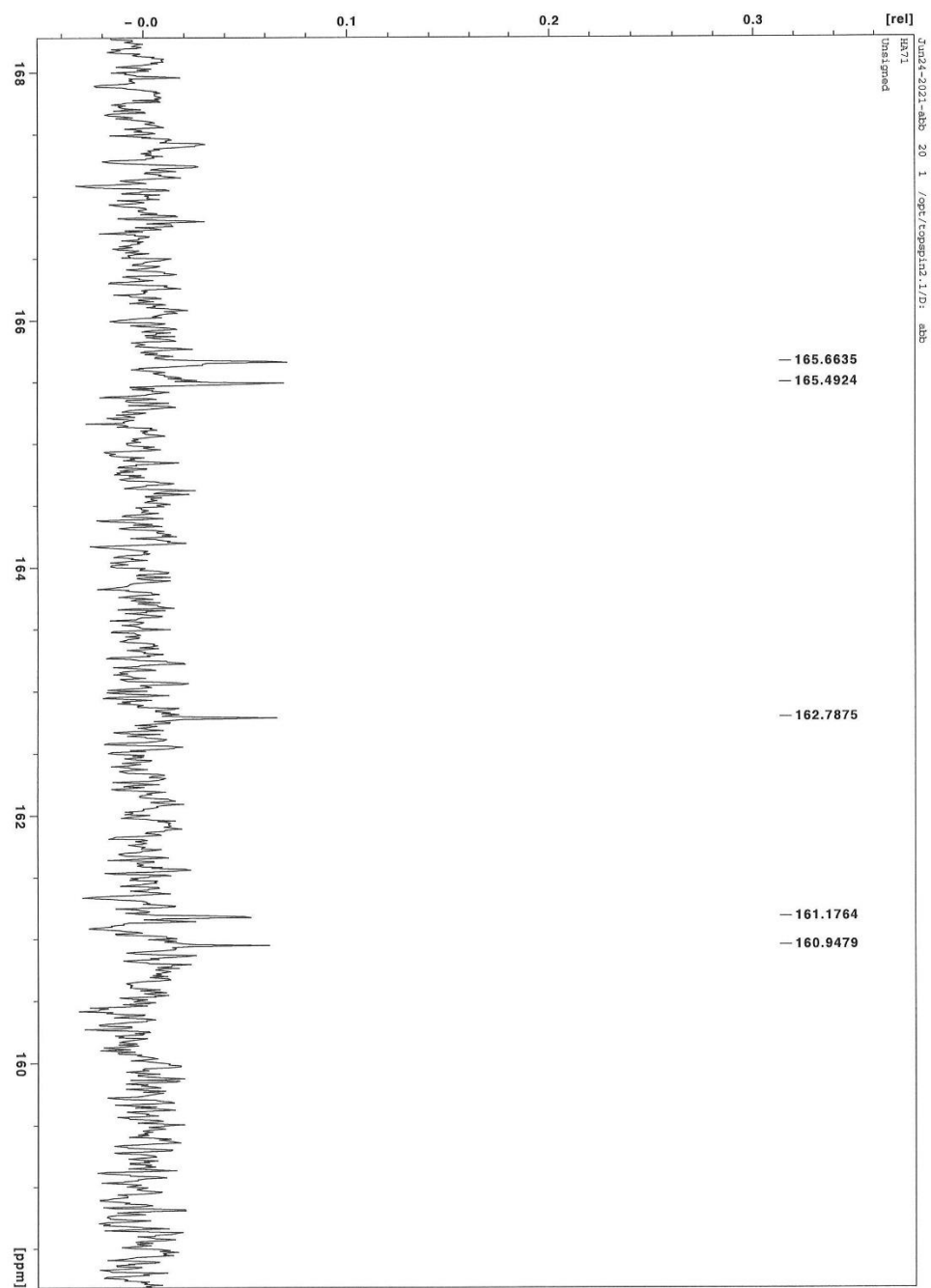
**Figure S143.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7g**.



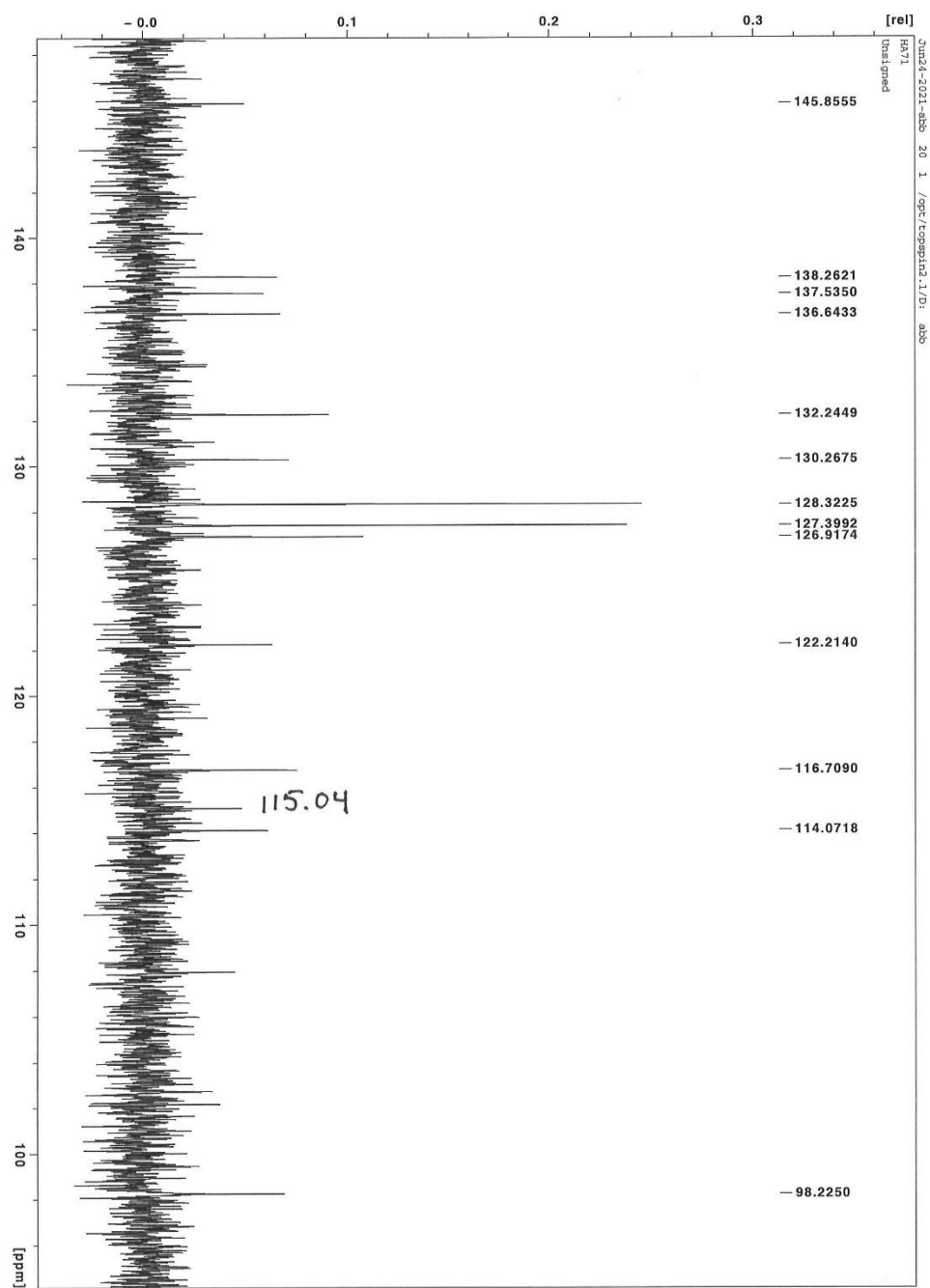
**Figure S144.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7g**.



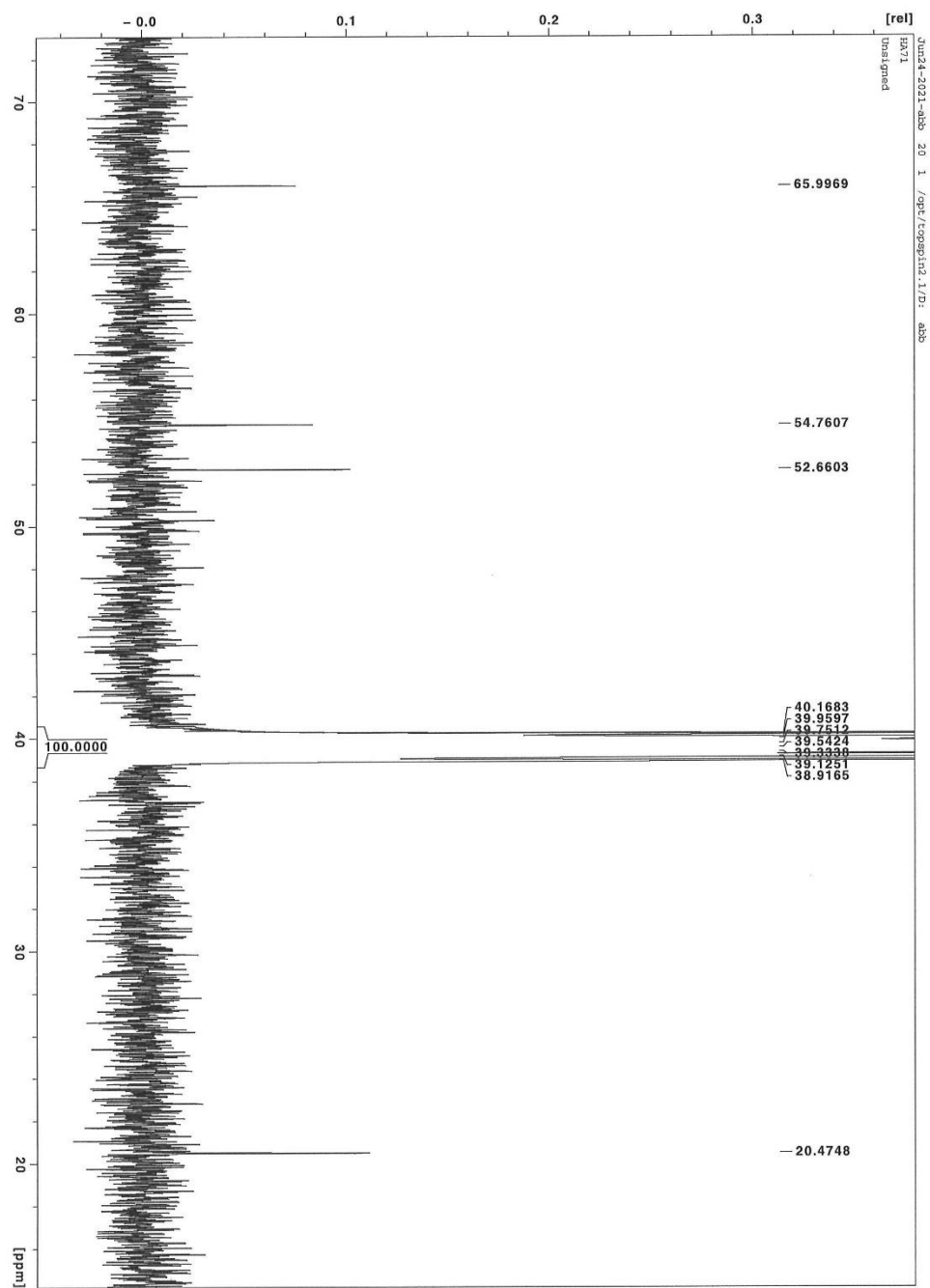
**Figure S145.** <sup>13</sup>C NMR spectrum of compound **7g** (100 MHz, DMSO-d<sub>6</sub>).



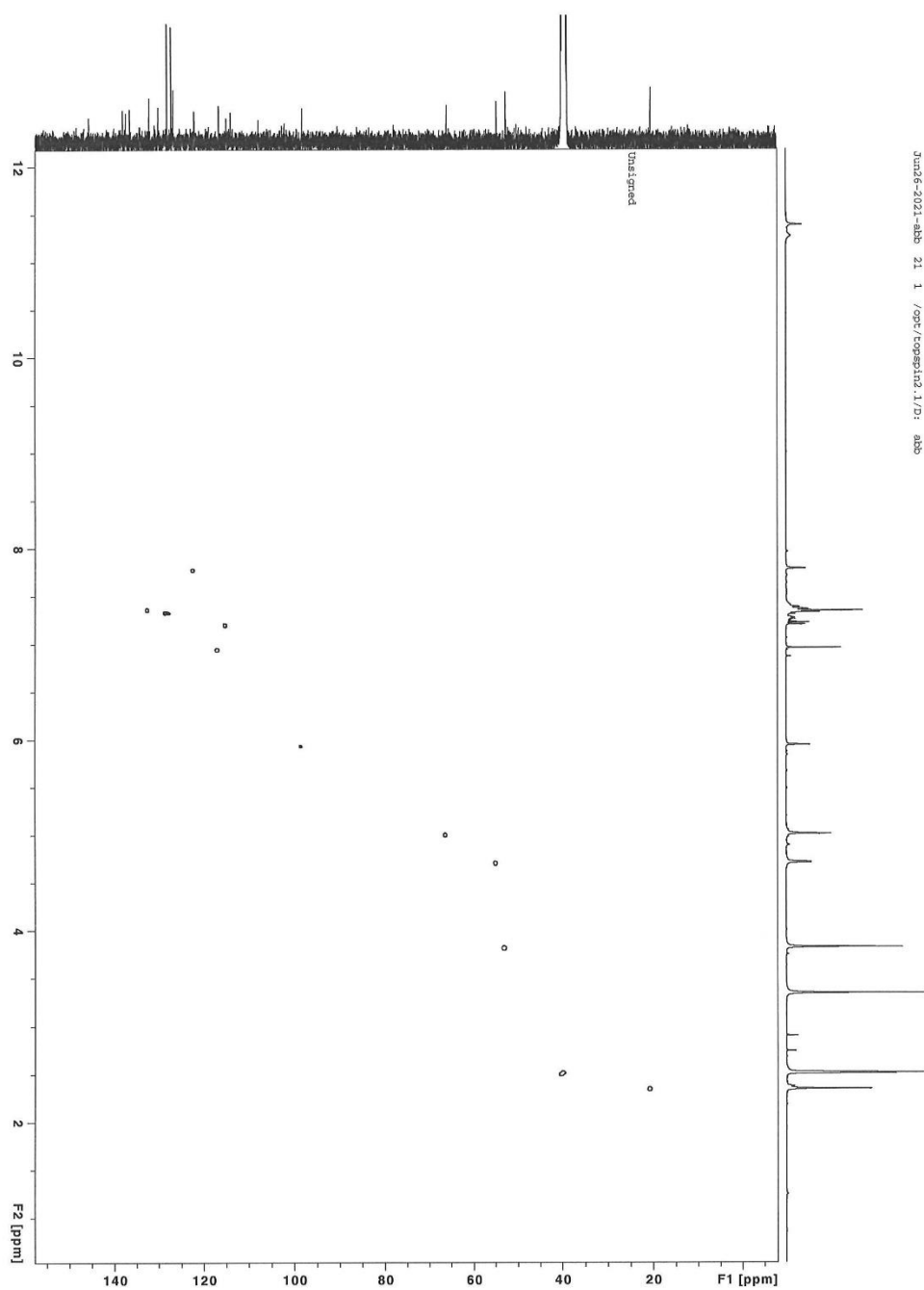
**Figure S146.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **7g**.



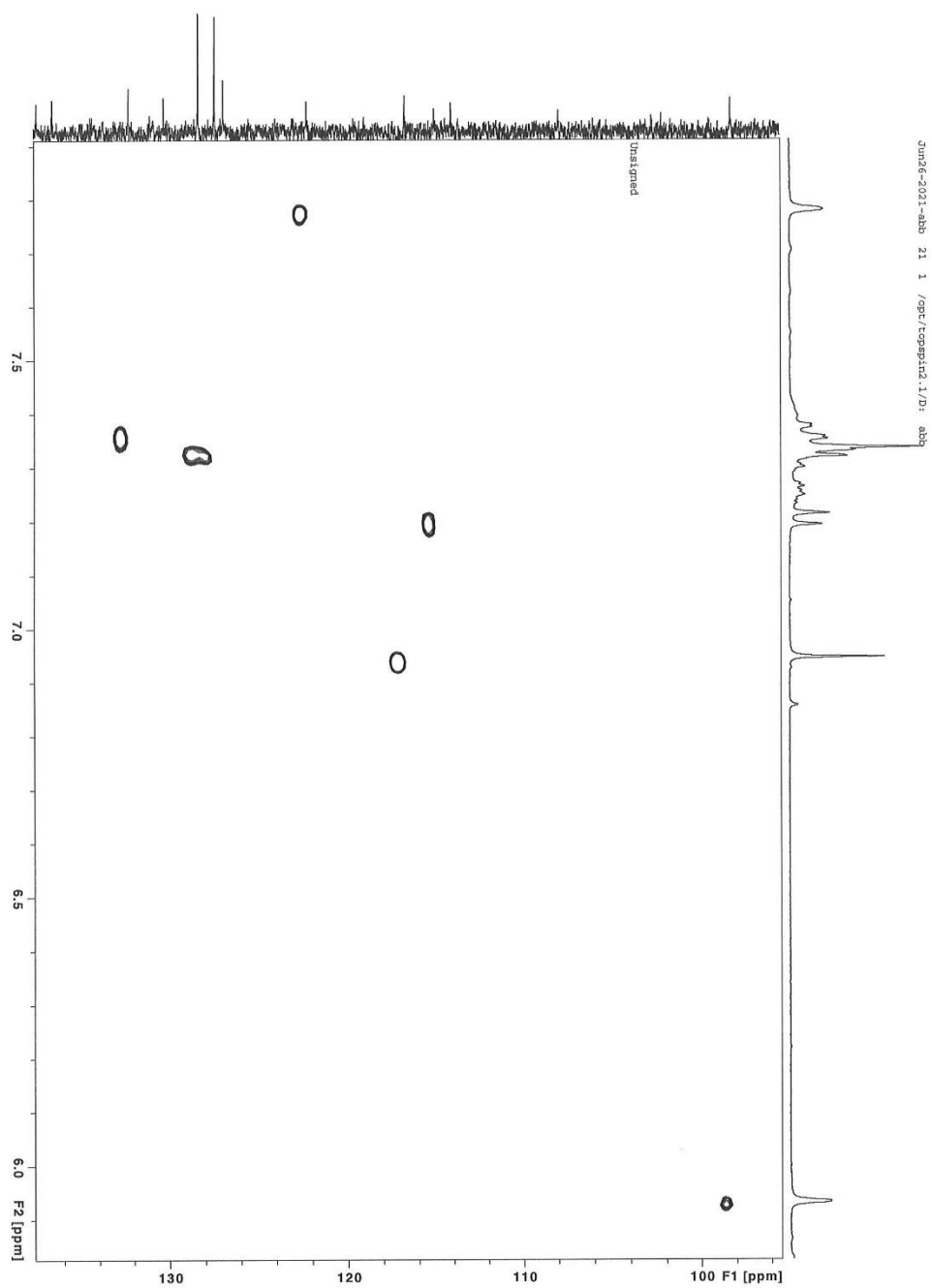
**Figure S147.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **7g**.



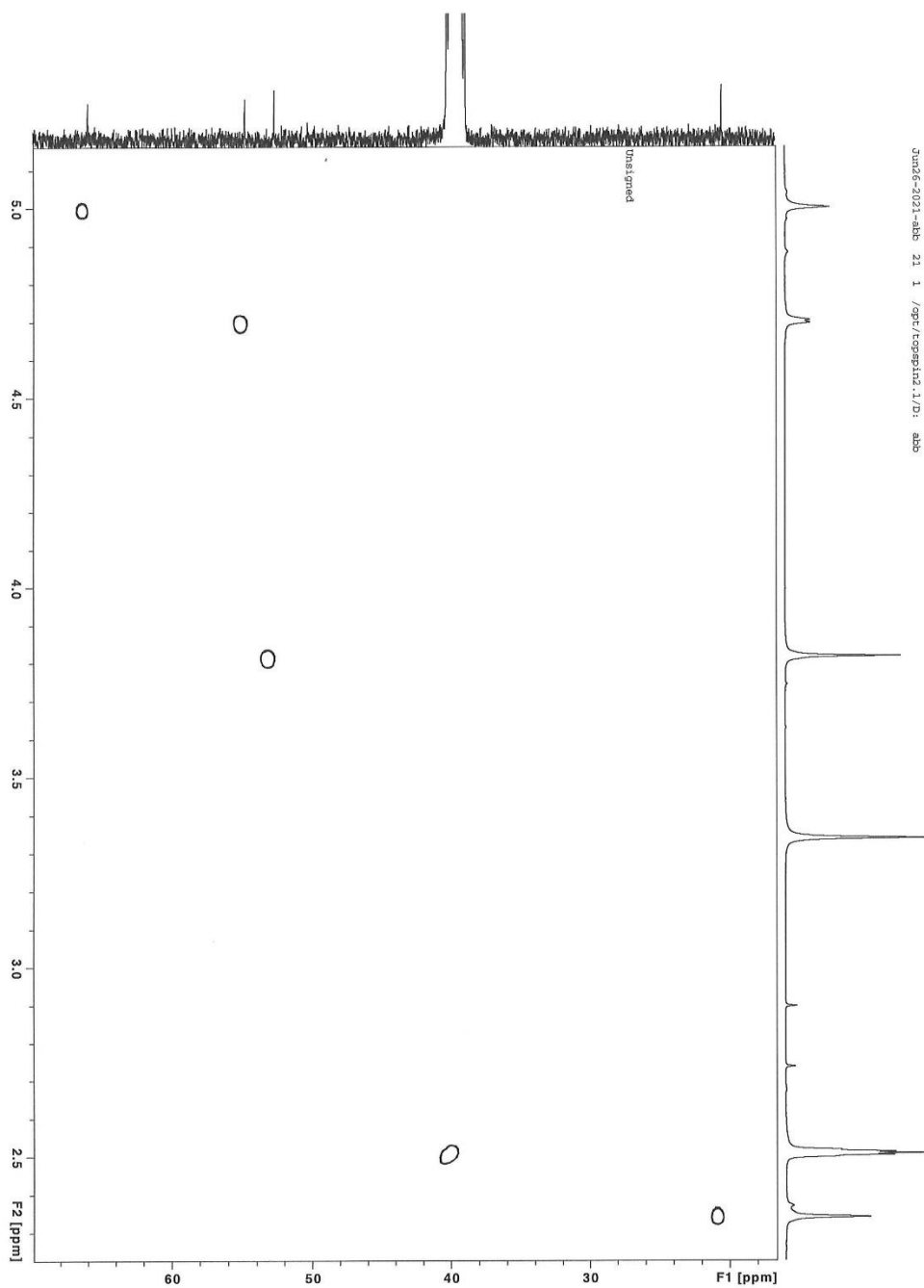
**Figure S148.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **7g**.



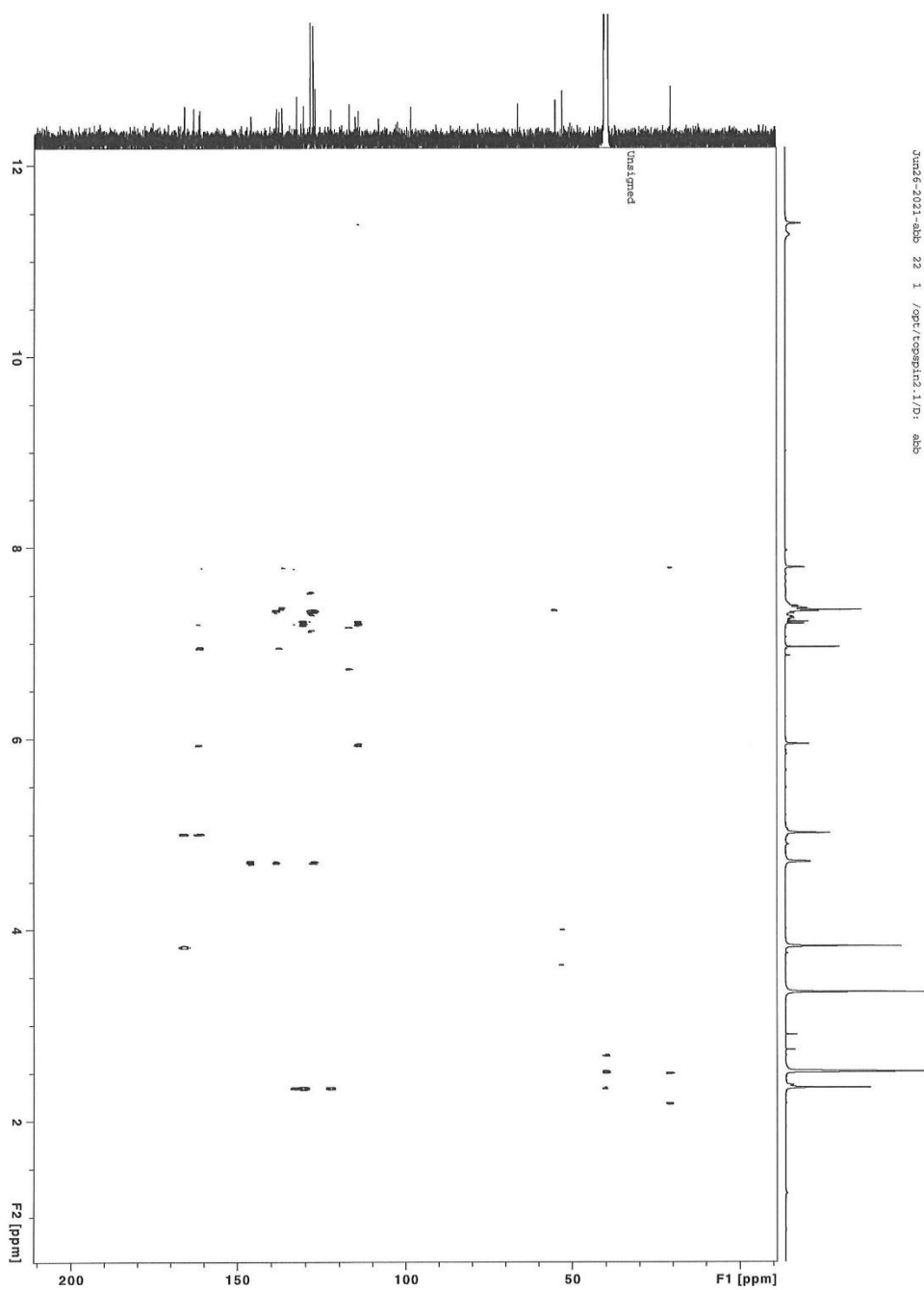
**Figure S149.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7g**.



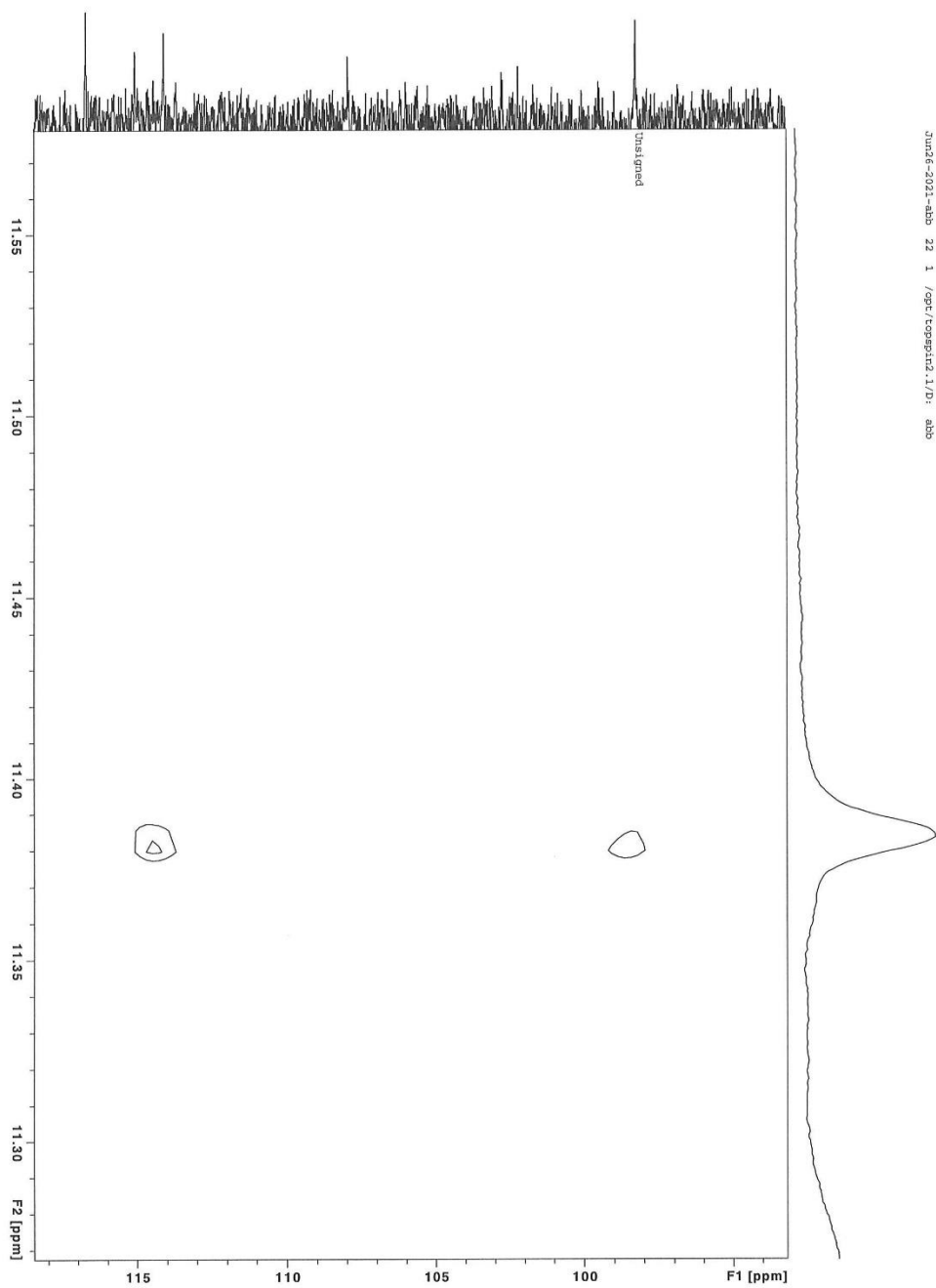
**Figure S150.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7g**.



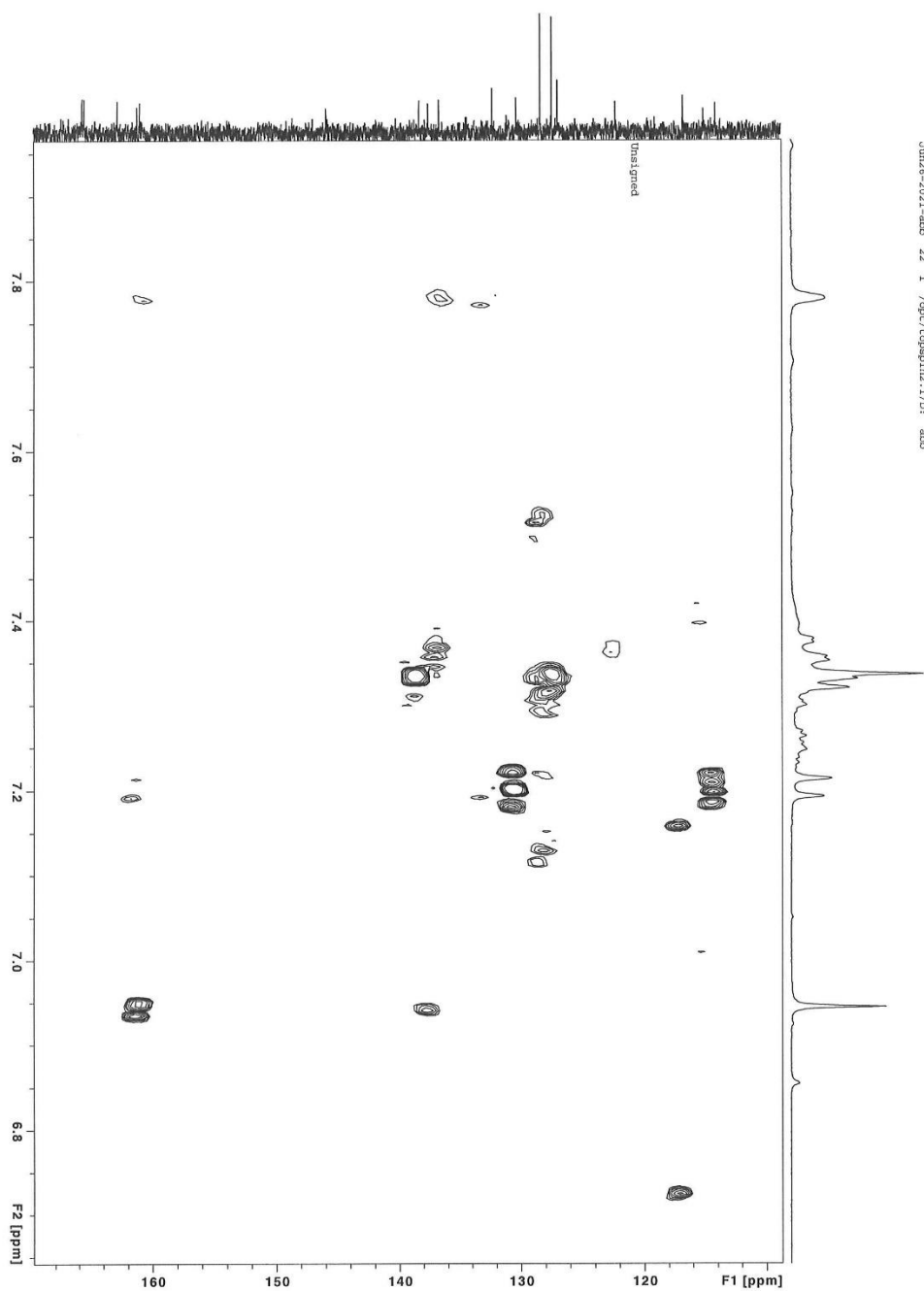
**Figure S151.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7g**.



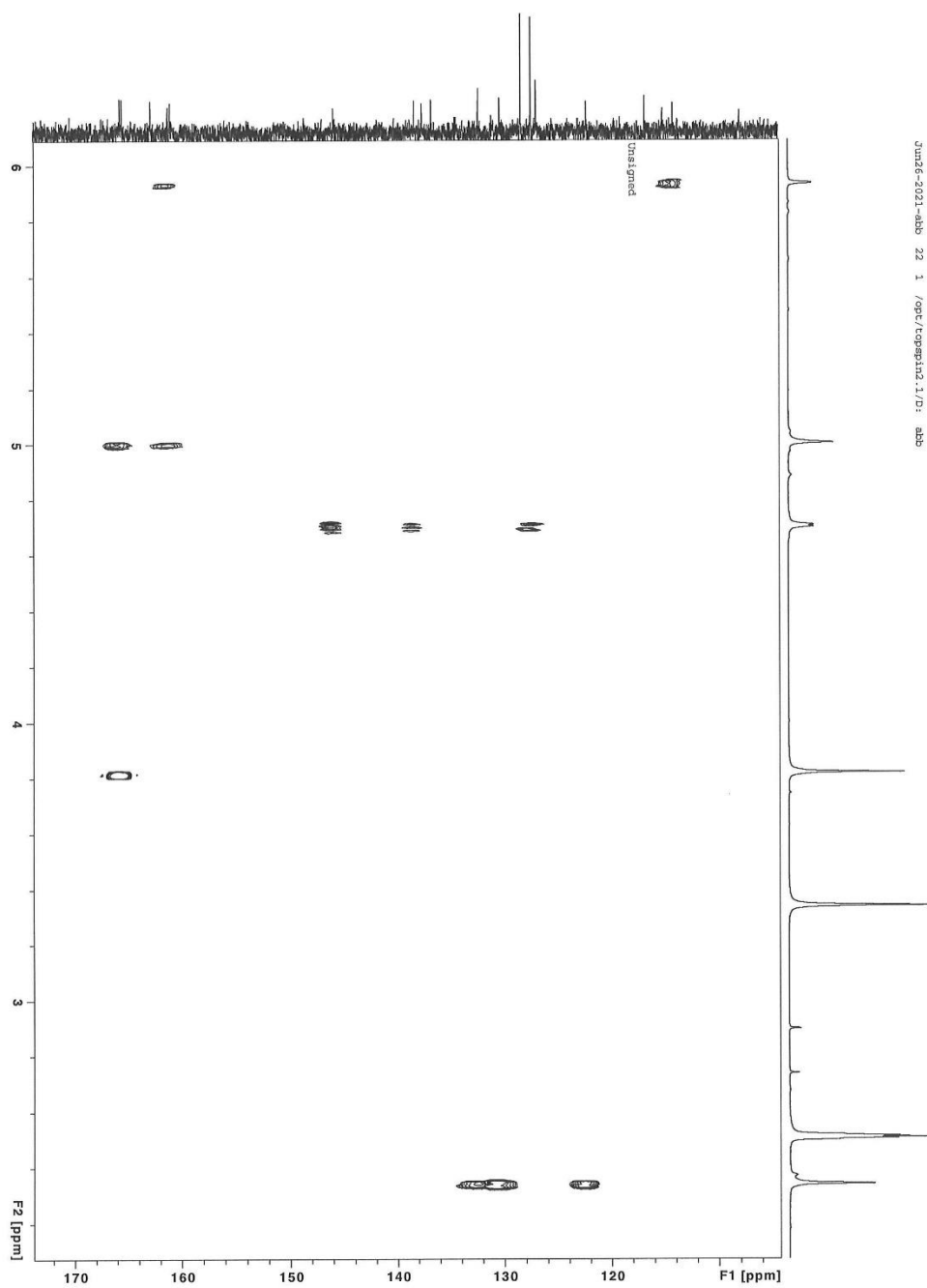
**Figure S152.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7g**.



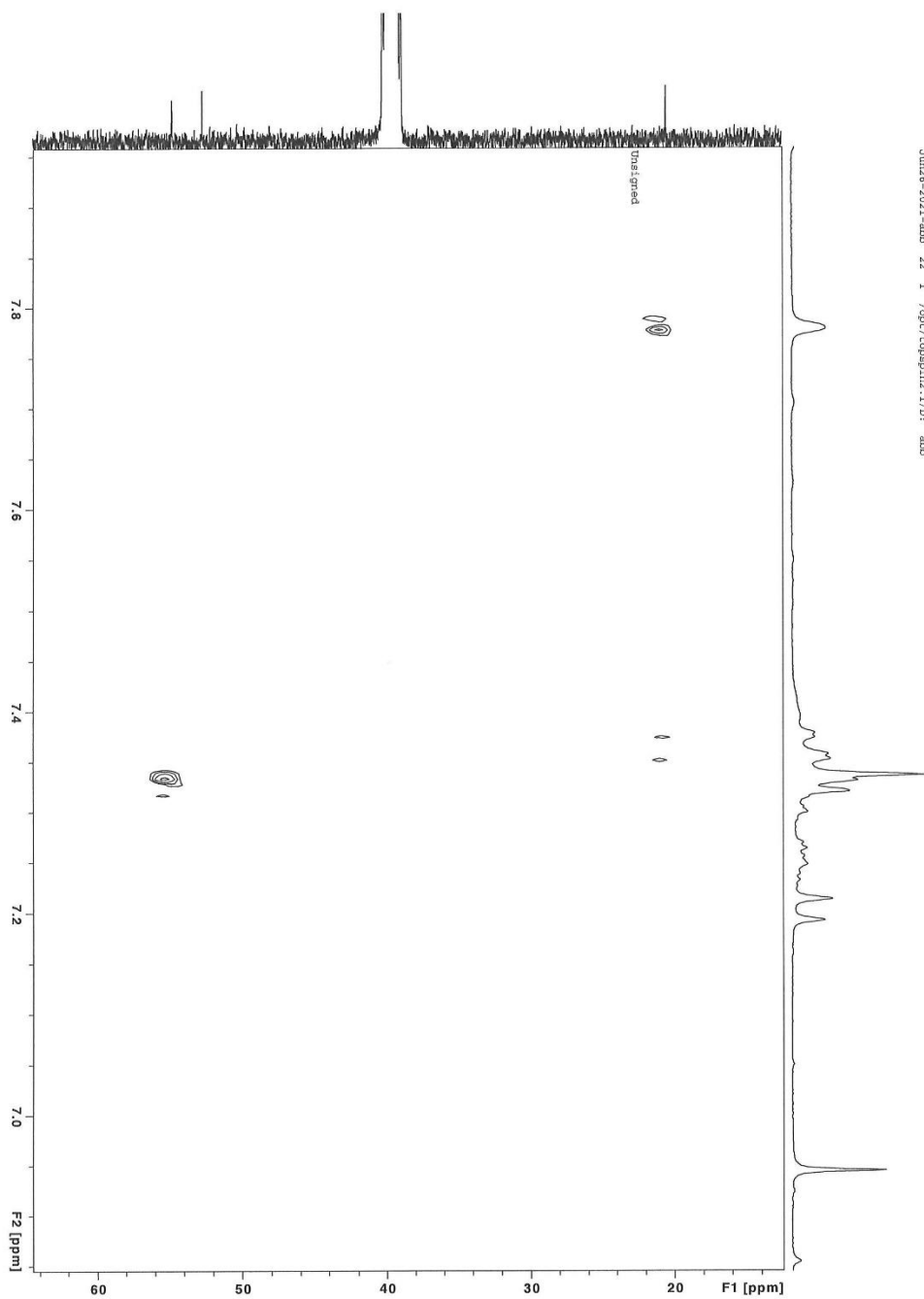
**Figure S153.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7g**.



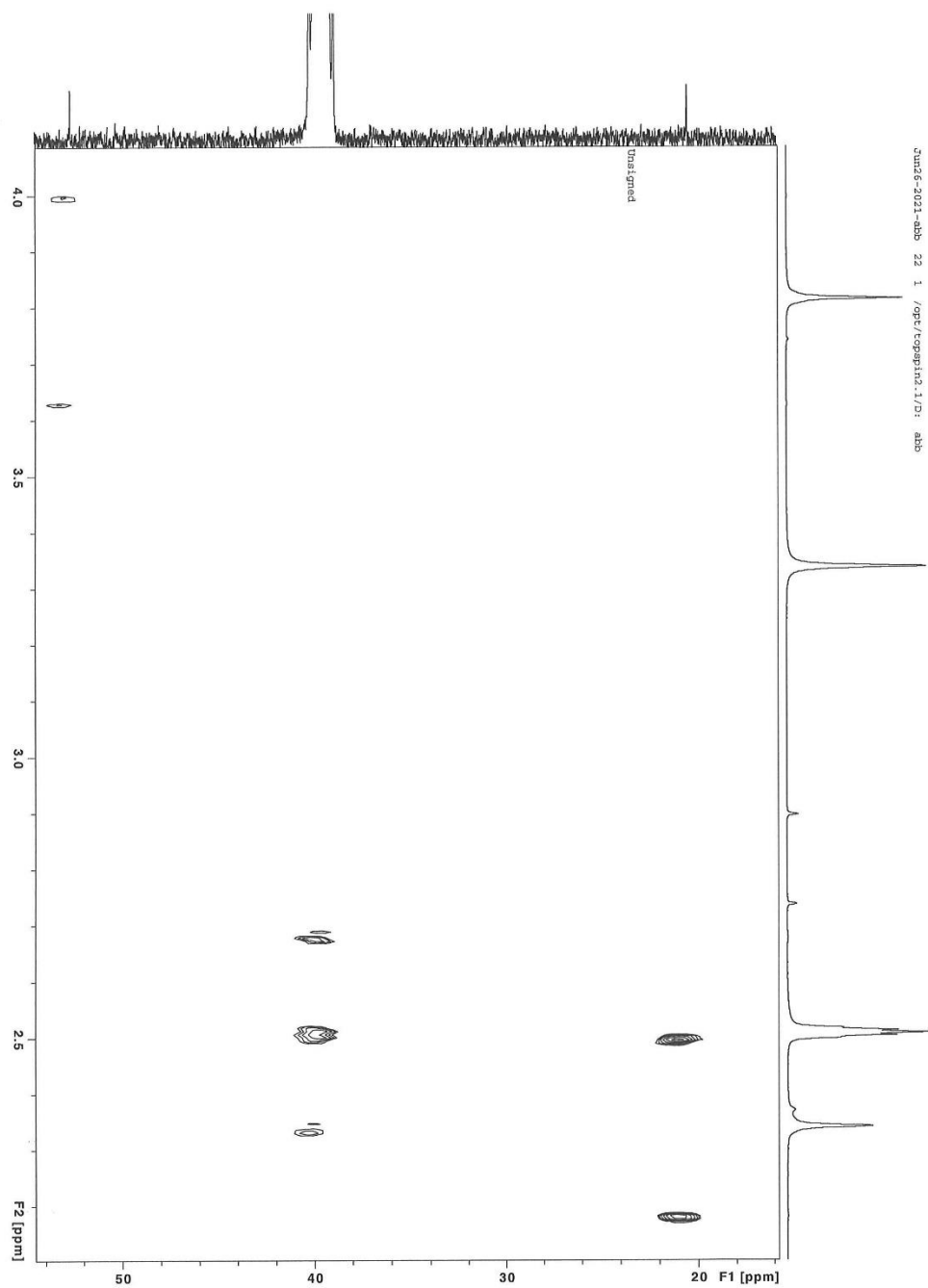
**Figure S154.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7g**.



**Figure S155.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7g**.



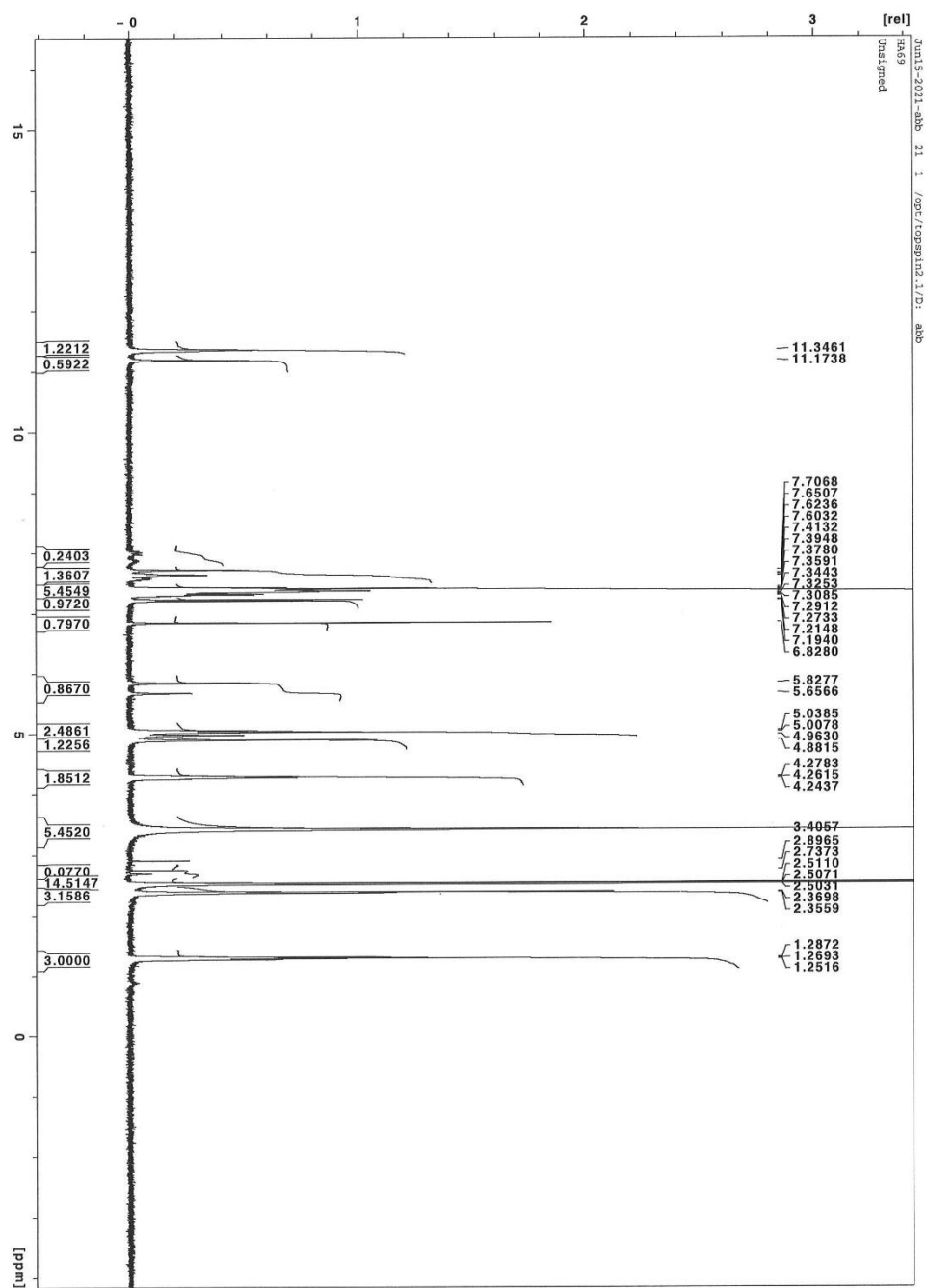
**Figure S156.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7g**.



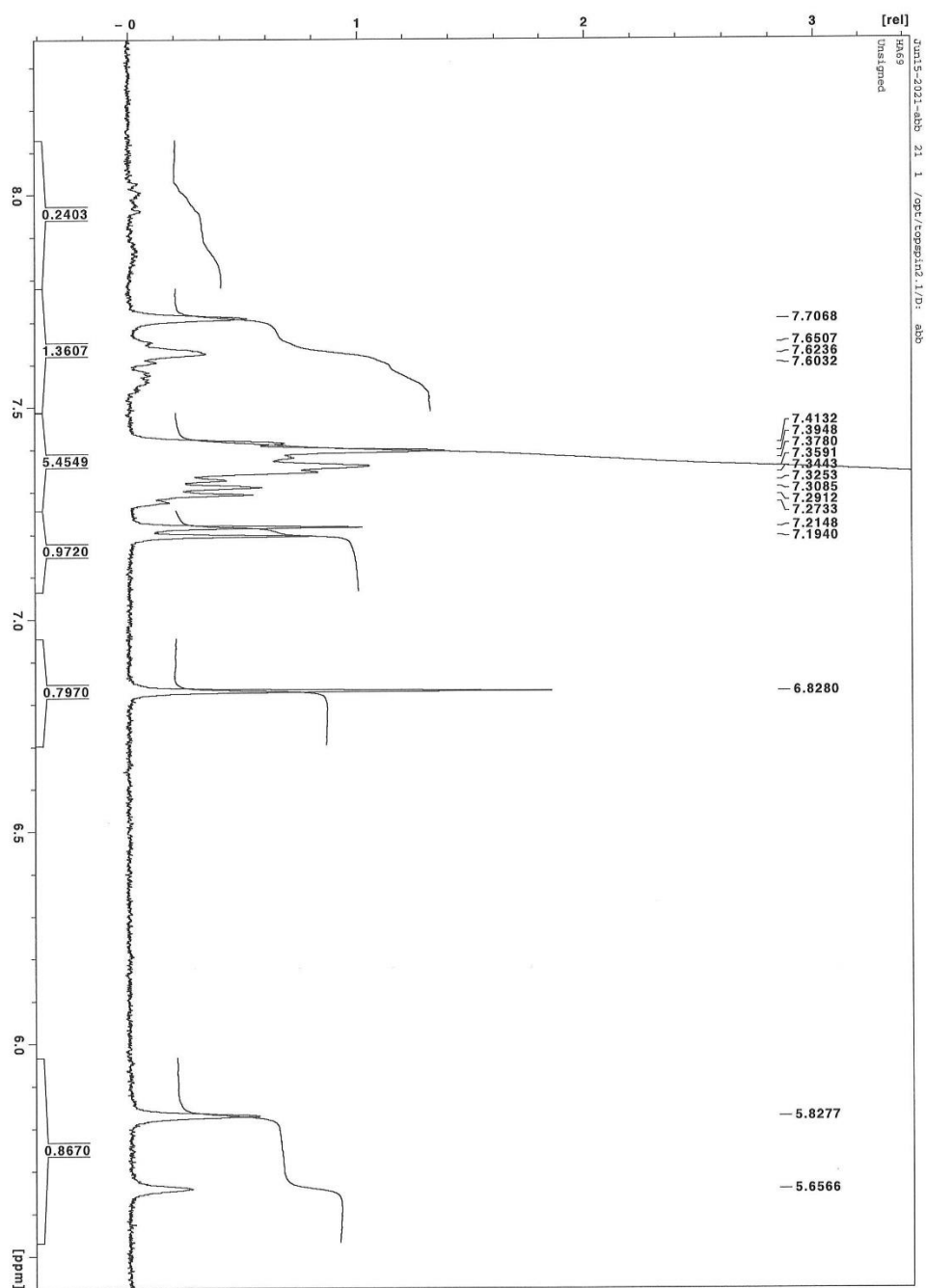
**Figure S157.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7g**.



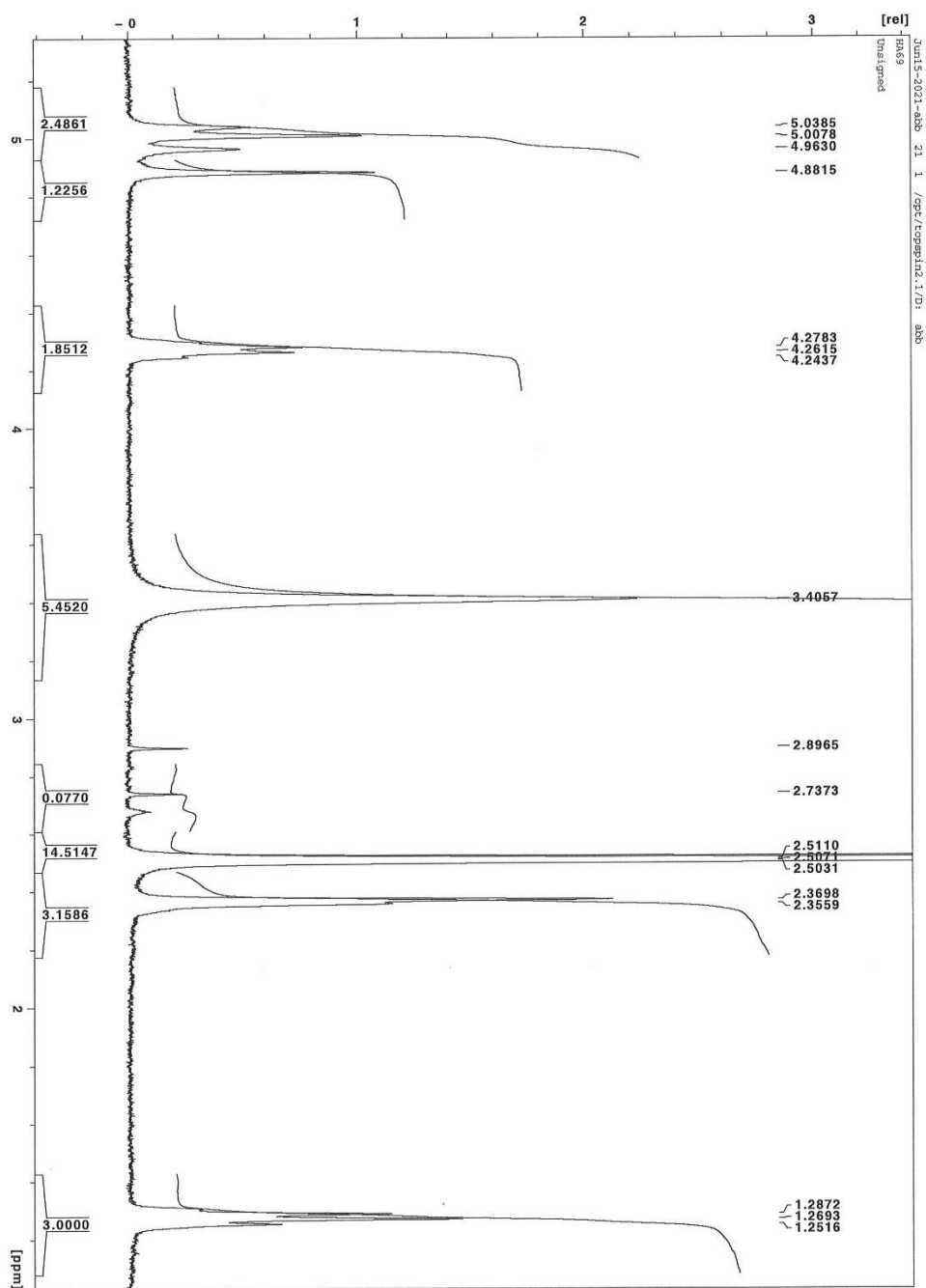




**Figure S160.**  $^1\text{H}$  NMR spectrum of compound **7h** (400 MHz,  $\text{DMSO}-d_6$ ).



**Figure S161.** Detail of  $^1\text{H}$  NMR spectrum of compound **7h**.



**Figure S162.** Detail of  $^1\text{H}$  NMR spectrum of compound **7h**.

HA69

$^1\text{H}-^1\text{H}$  COSY

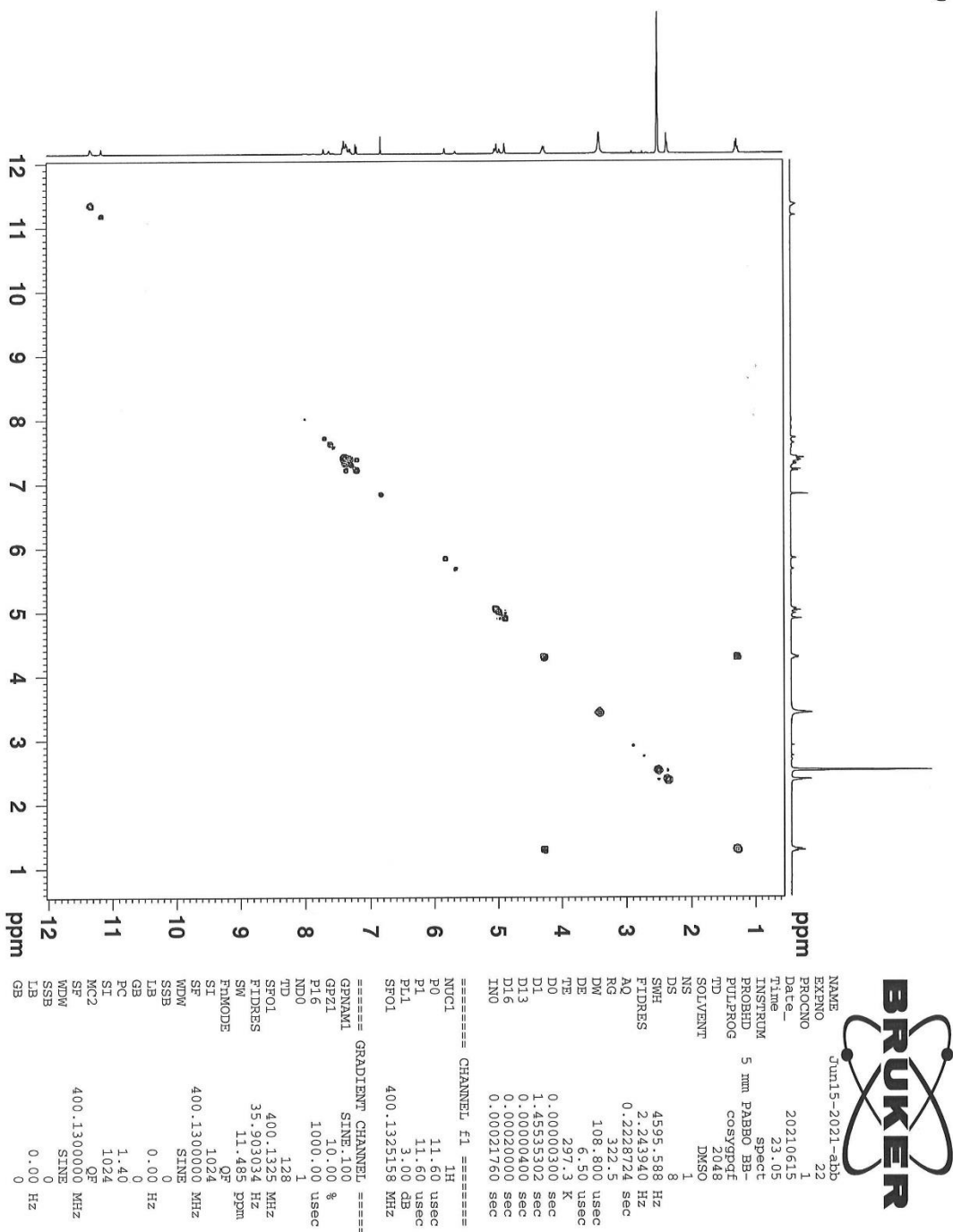
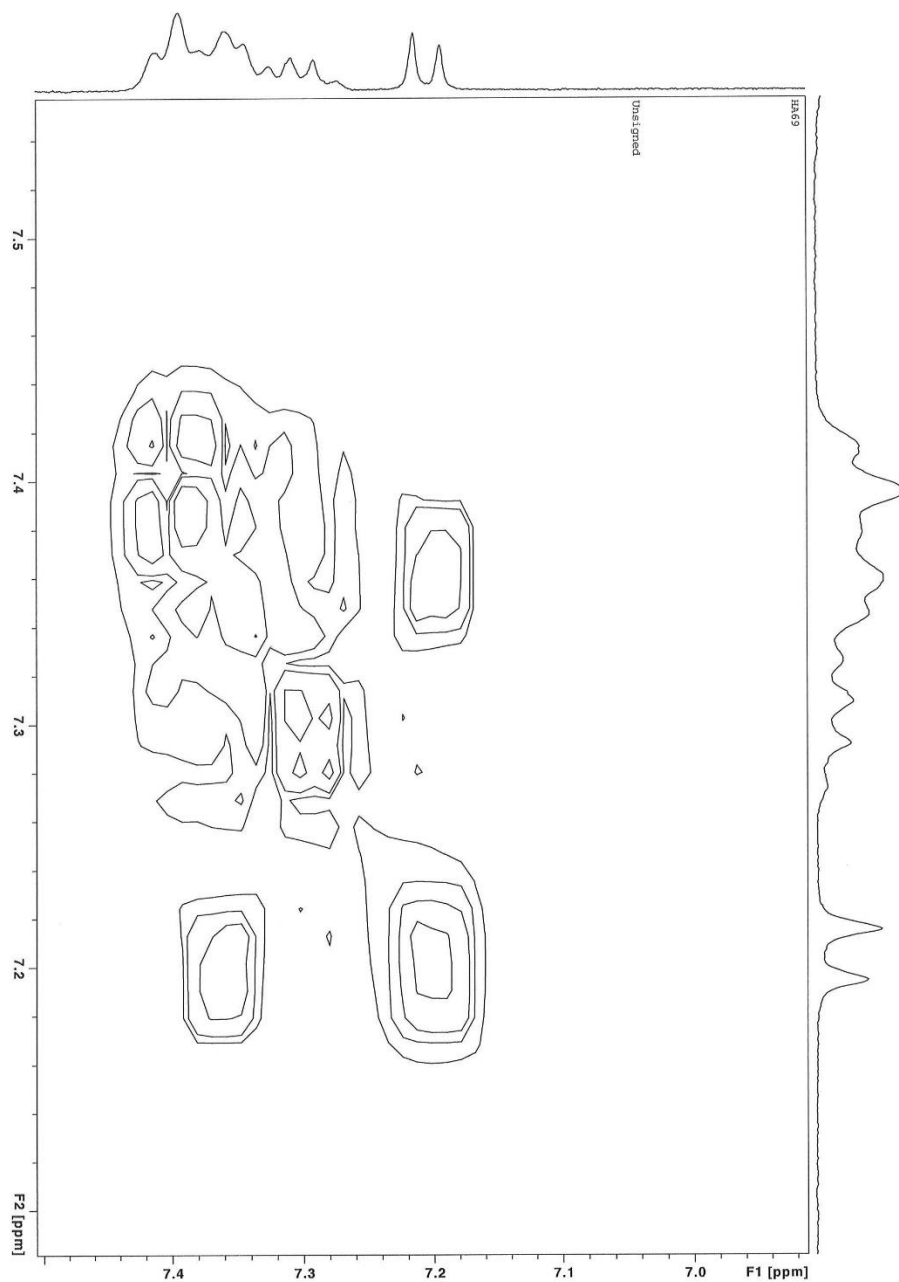
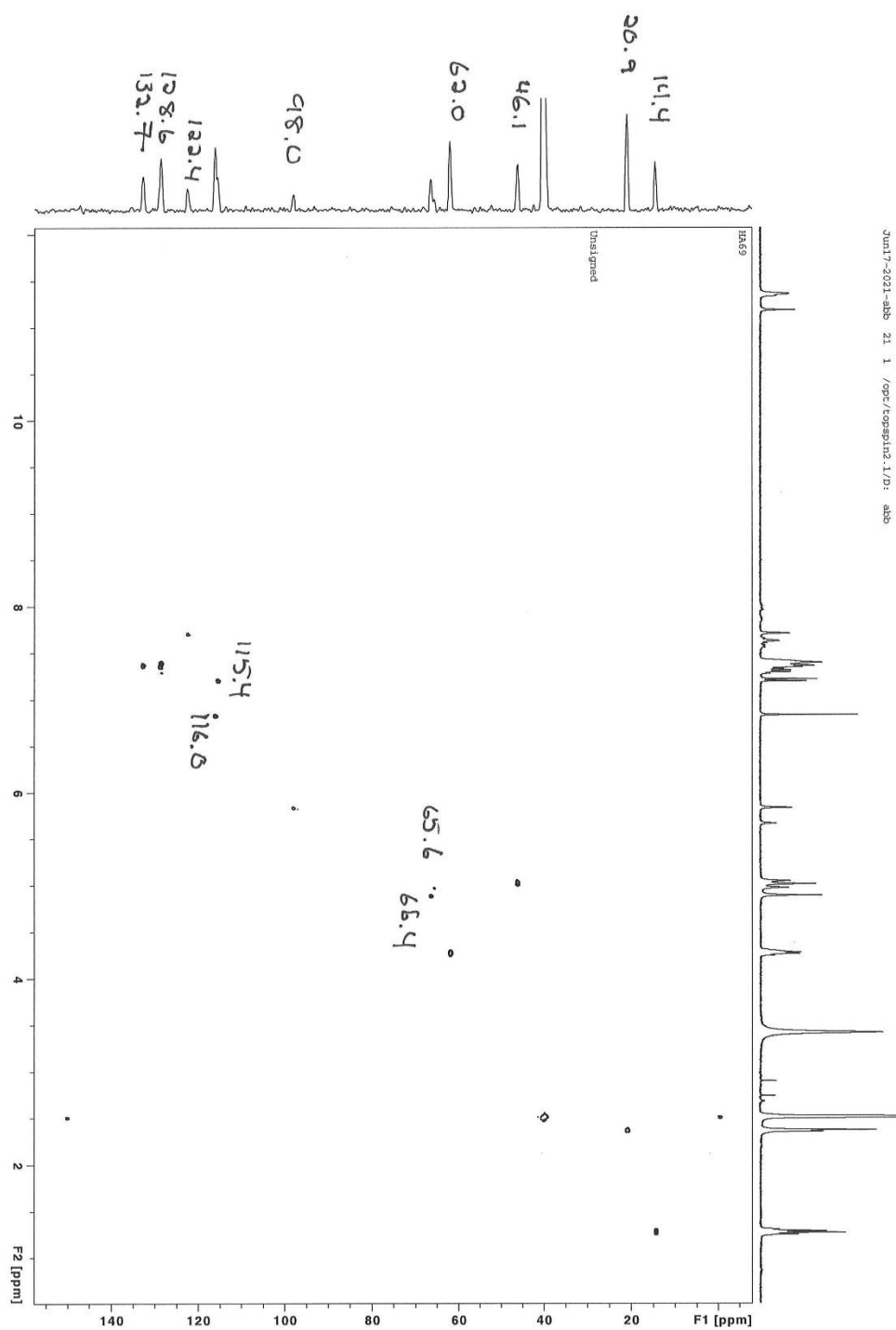


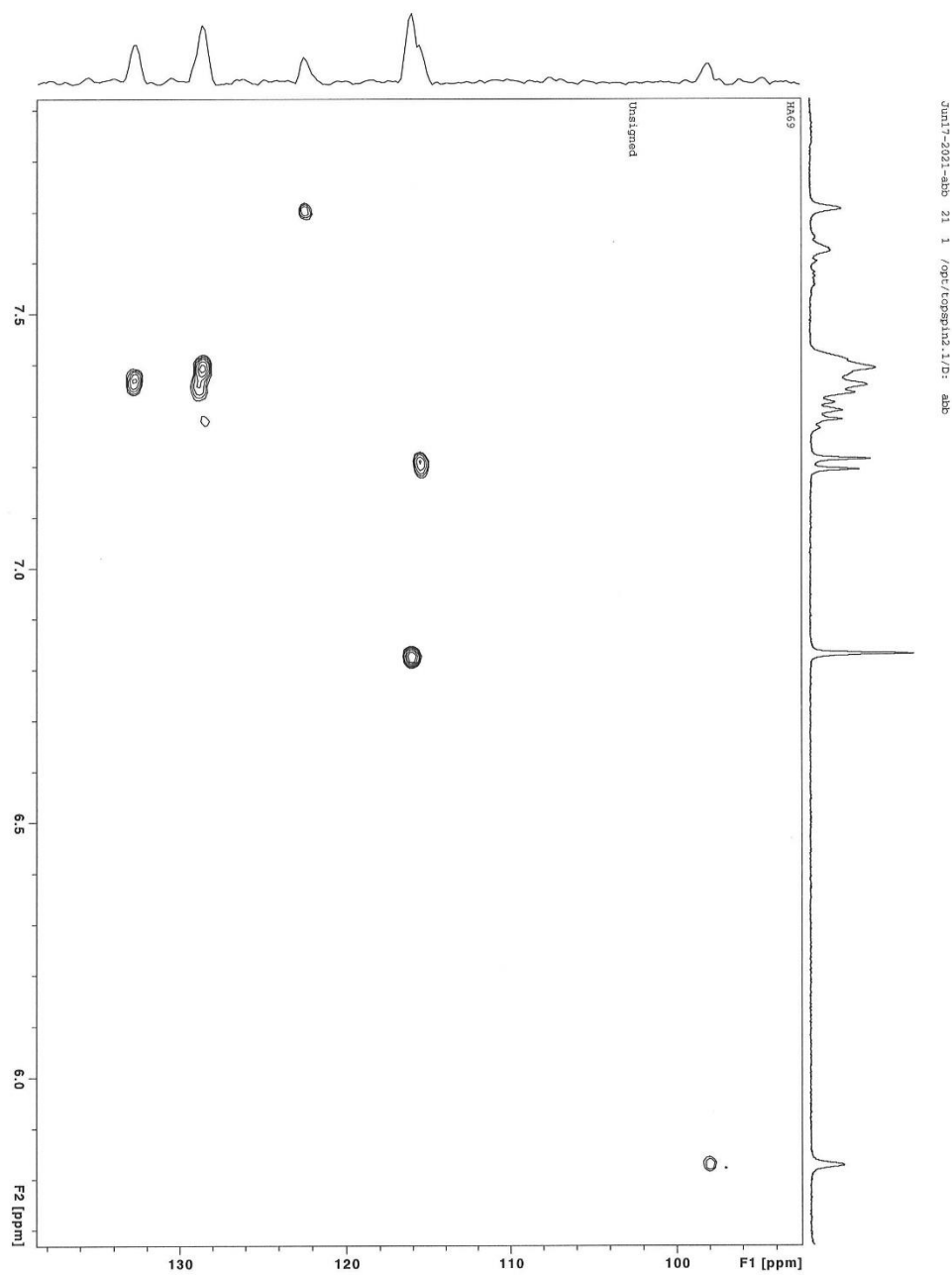
Figure S163.  $^1\text{H}-^1\text{H}$  COSY spectrum of compound **7h**.



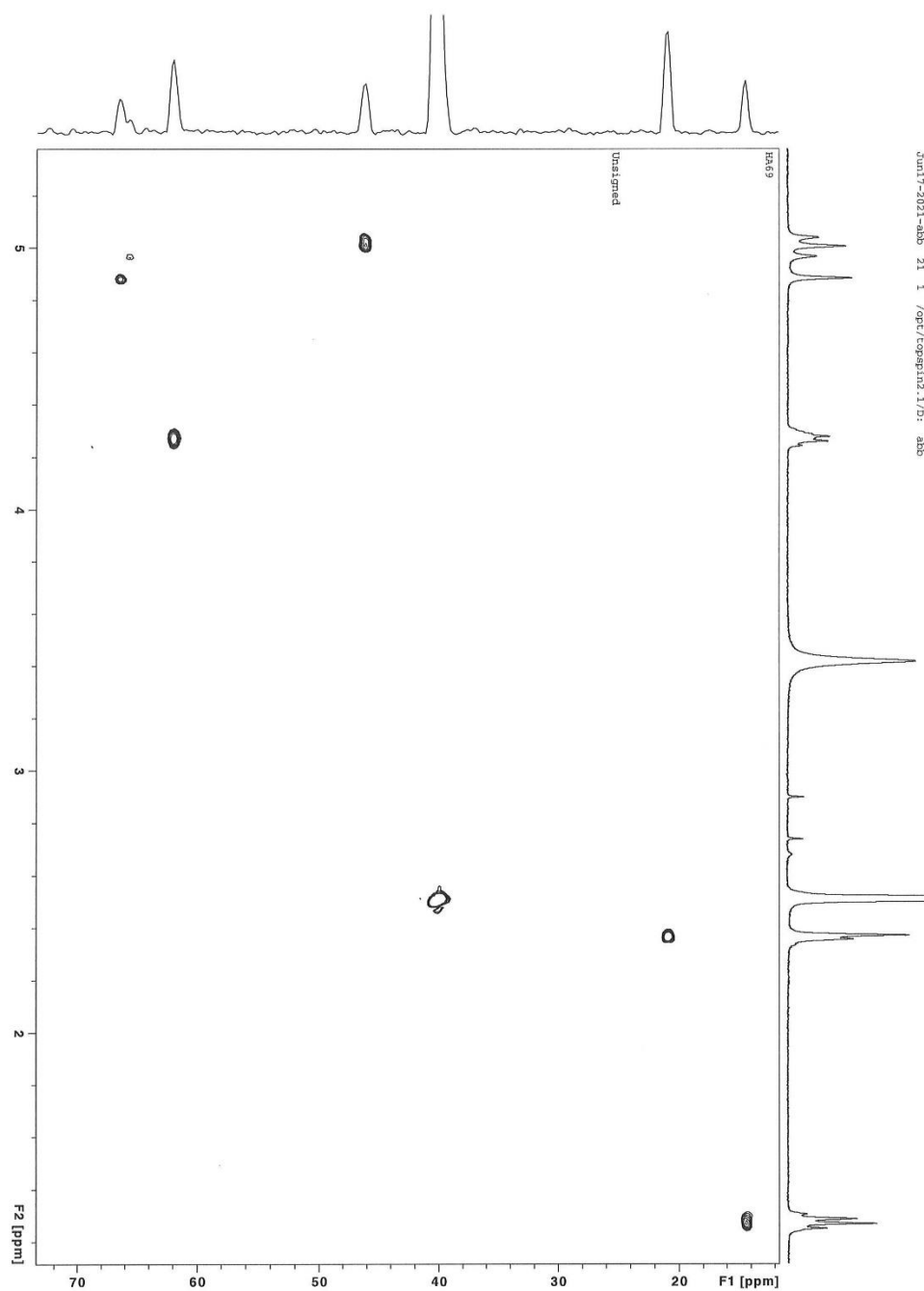
**Figure S164.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7h**.



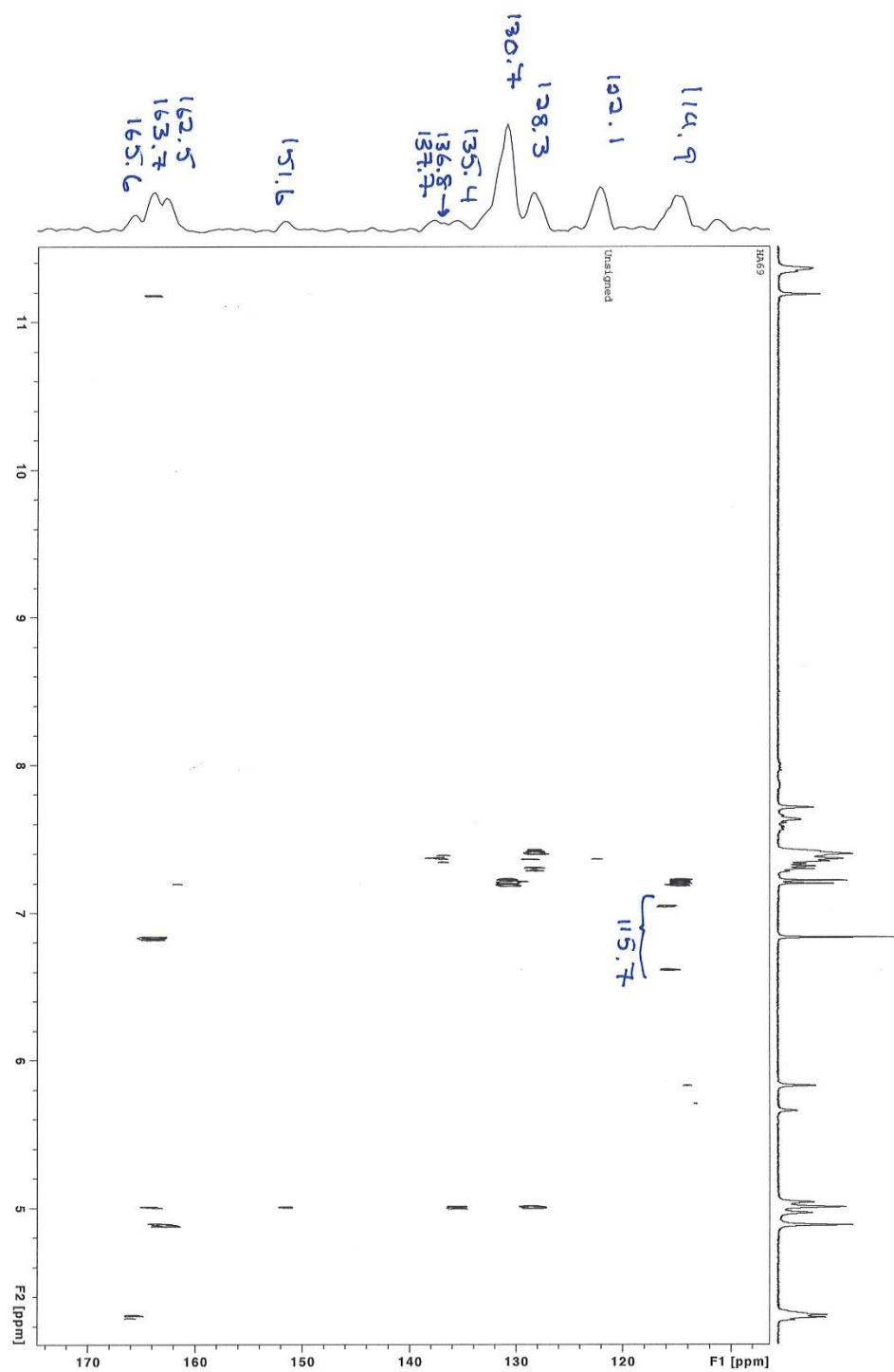
**Figure S165.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7h**. (Solubility was low:  $^{13}\text{C}$  signals were detected indirectly, *via* HSQC and HMBC spectra.)



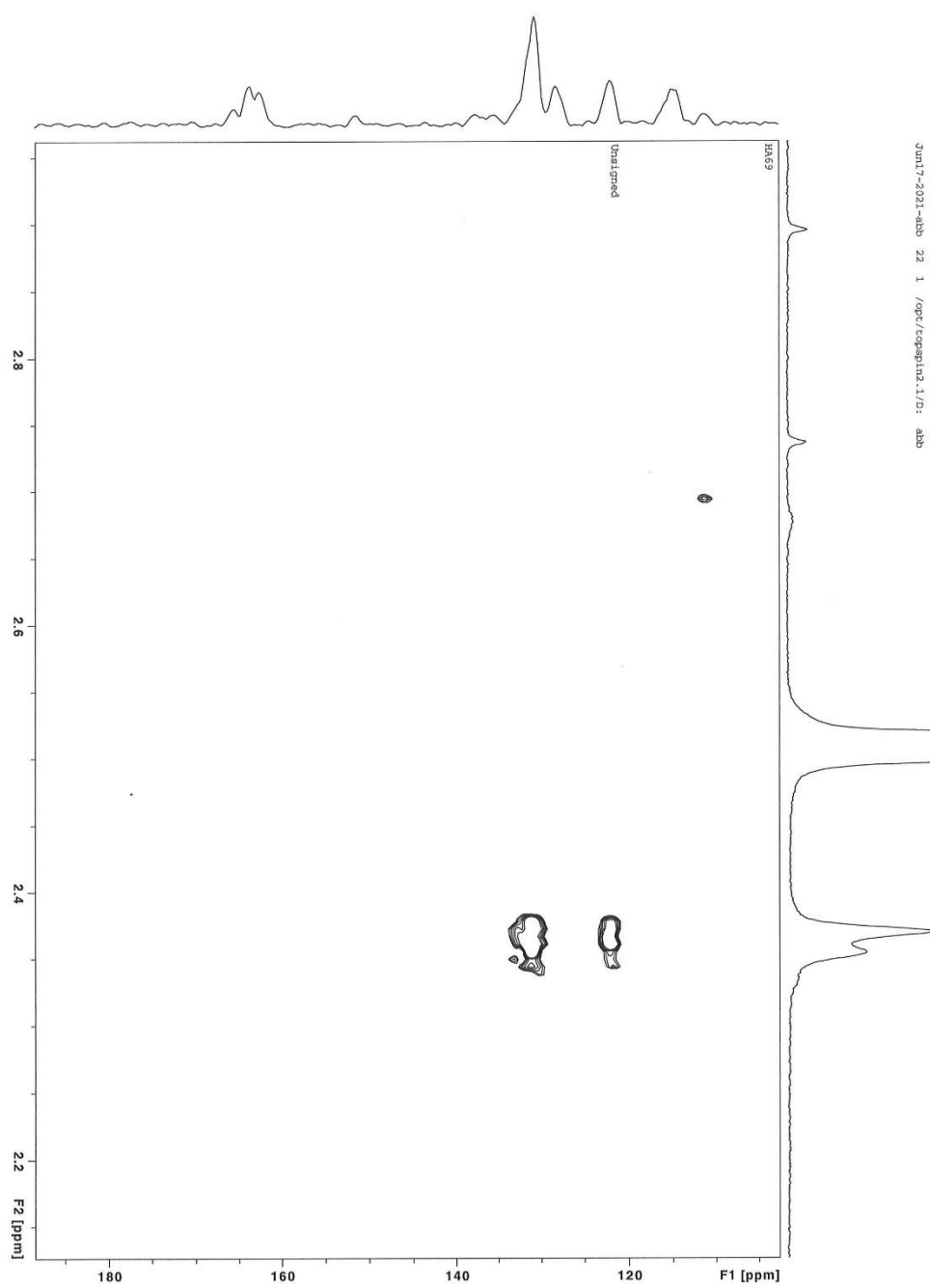
**Figure S166.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7h**.



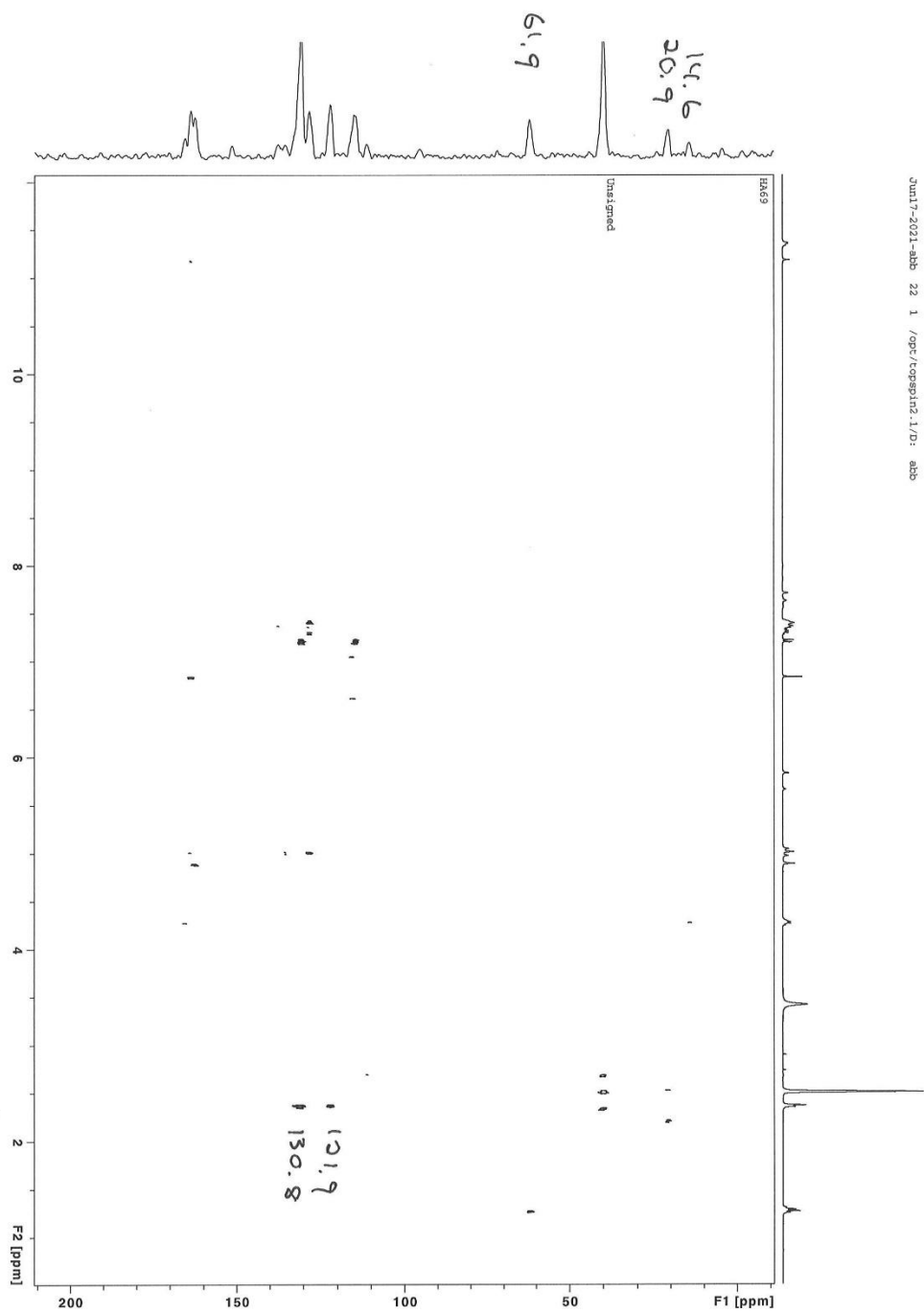
**Figure S167.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7h**.



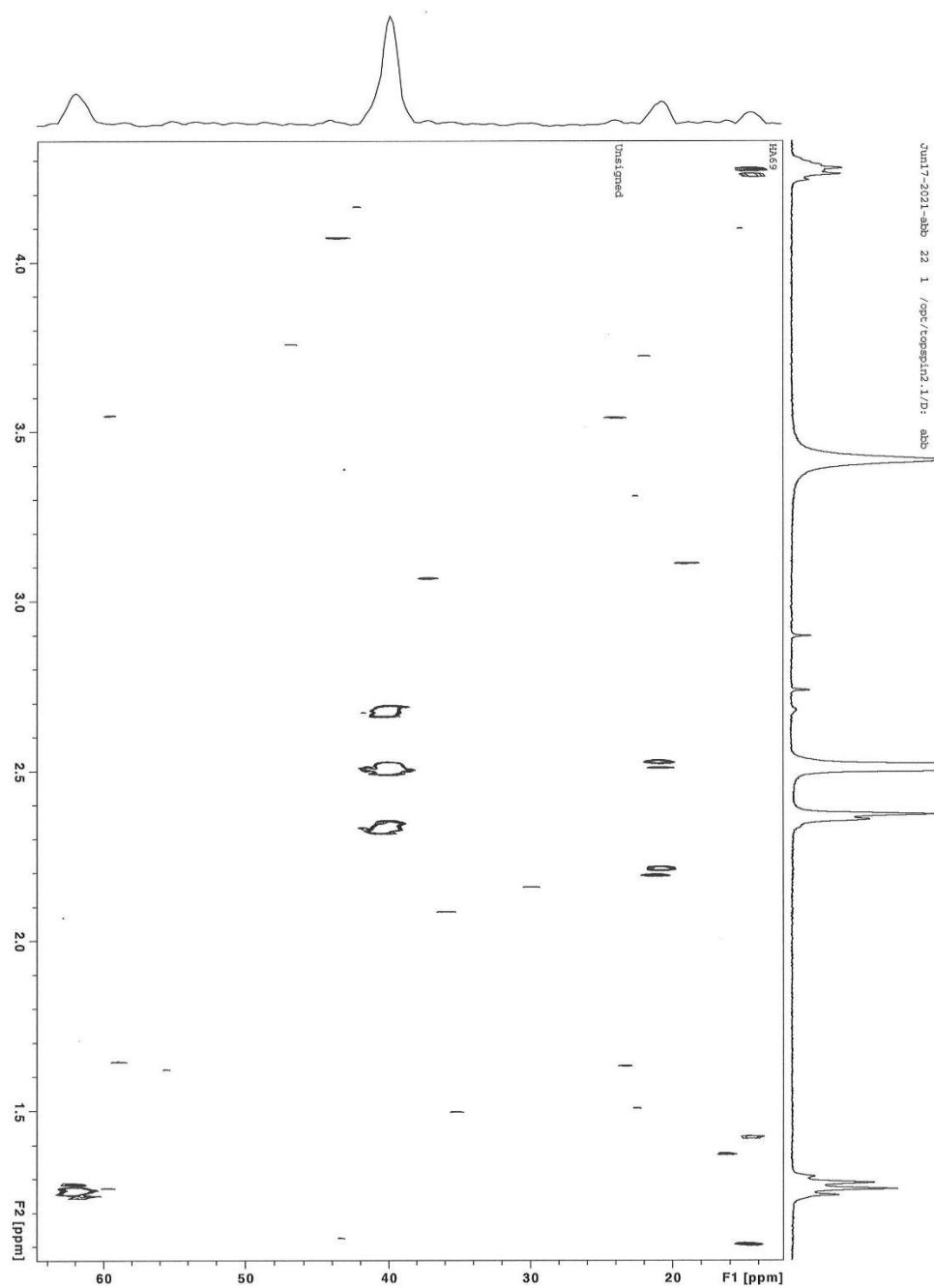
**Figure S168.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7h**.



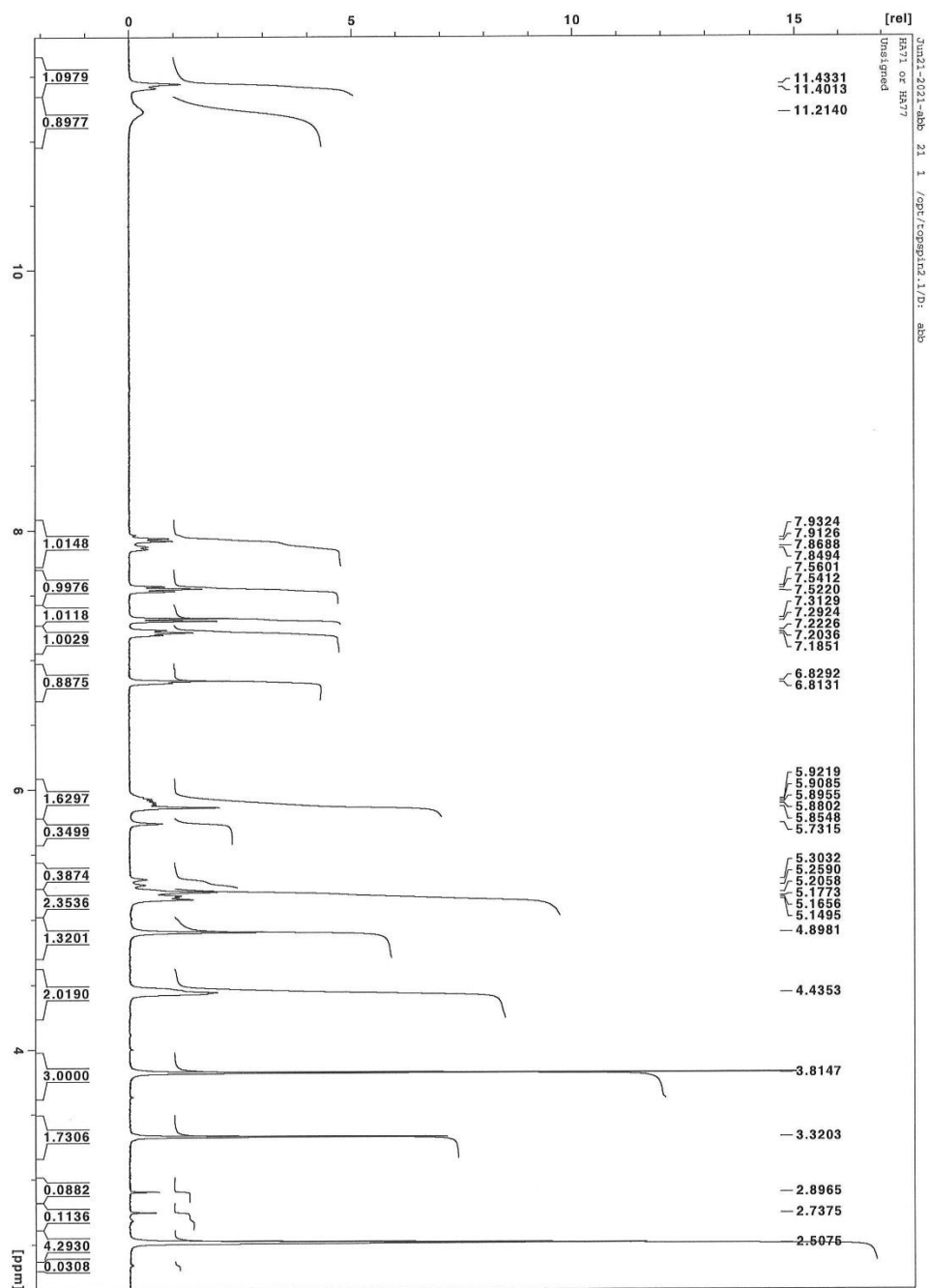
**Figure S169.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7h**.



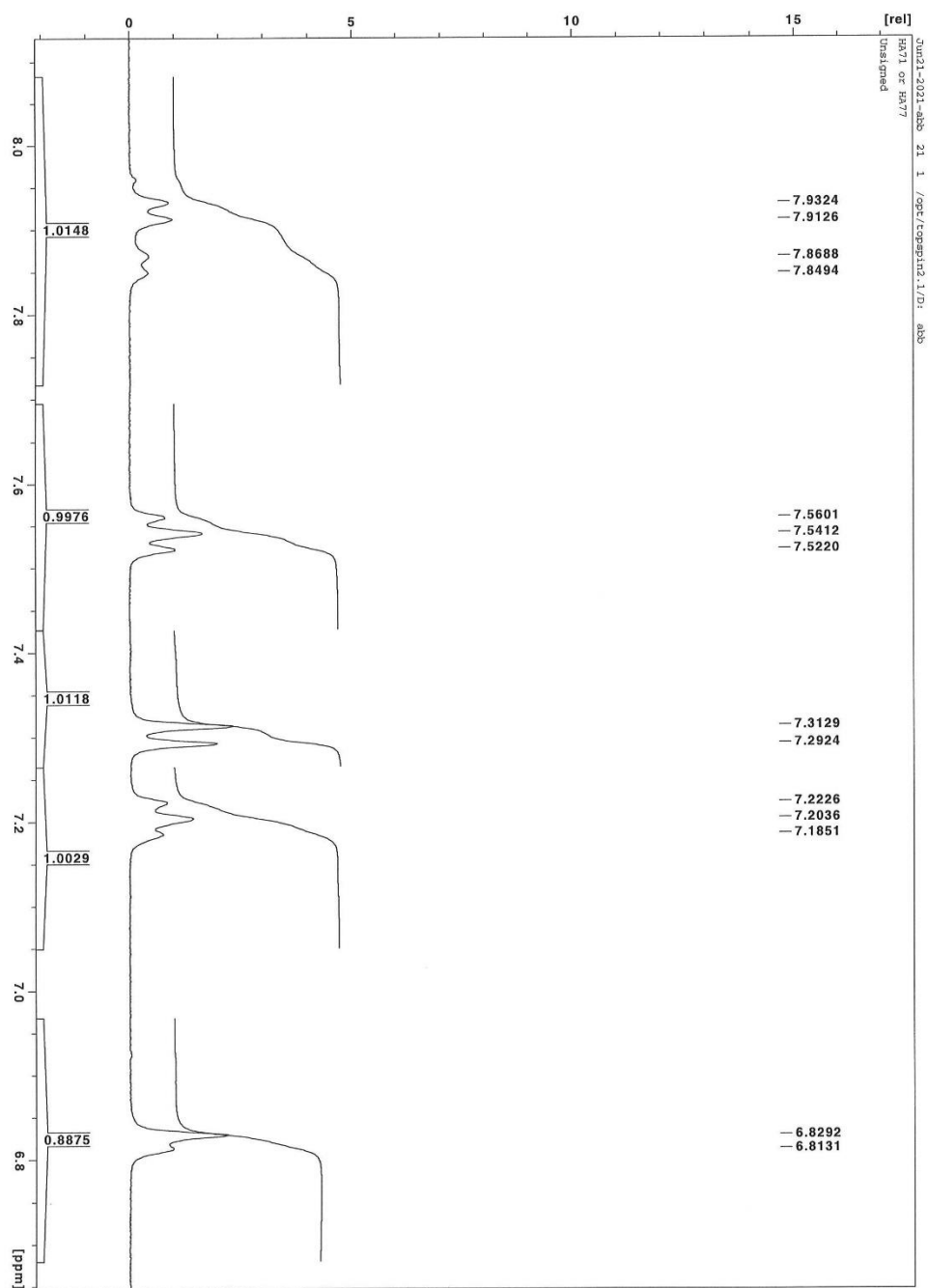
**Figure S170.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7h**.



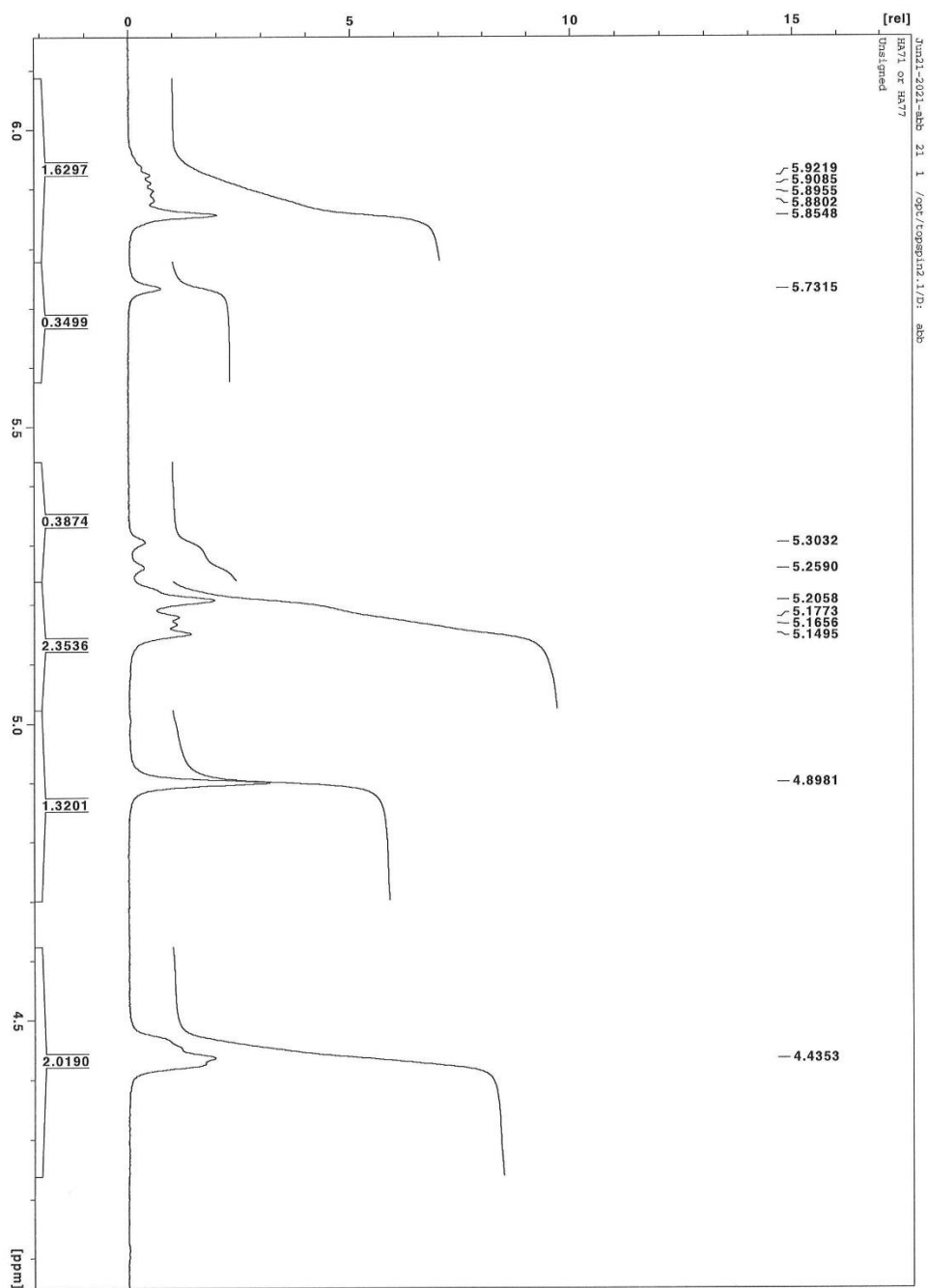
**Figure S171.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7h**. ( $^1\text{H}$ - $^{15}\text{N}$  HSQC and HMBC experiments gave no cross peaks.)



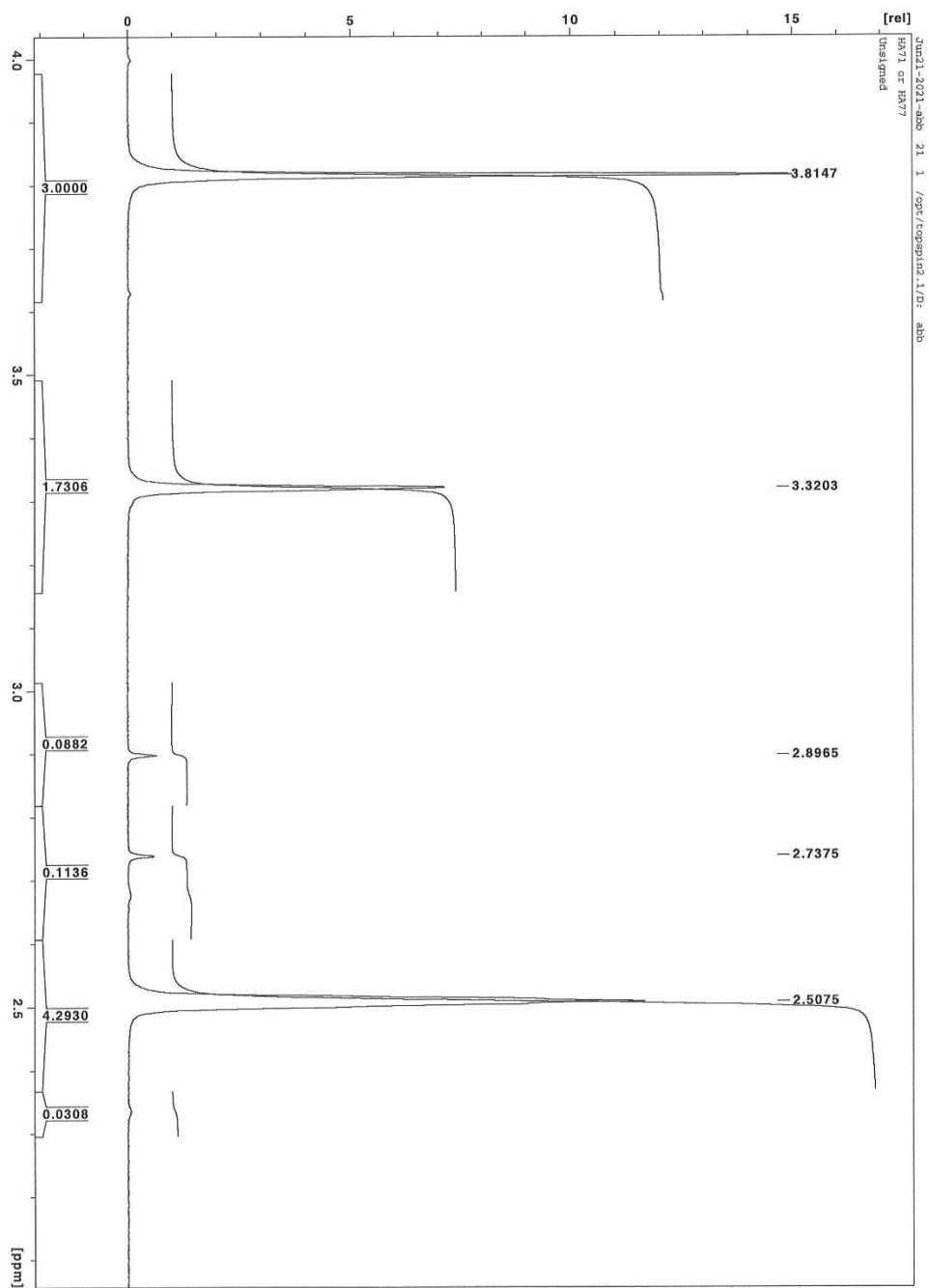
**Figure S172.**  $^1\text{H}$  NMR spectrum of compound **7j** (400 MHz,  $\text{DMSO}-d_6$ ).



**Figure S173.** Detail of  $^1\text{H}$  NMR spectrum of compound **7j**.



**Figure S174.** Detail of  $^1\text{H}$  NMR spectrum of compound **7j**.



**Figure S175.** Detail of  $^1\text{H}$  NMR spectrum of compound **7j**.

HA71 or HA77

$^1\text{H}$ - $^1\text{H}$  COSY

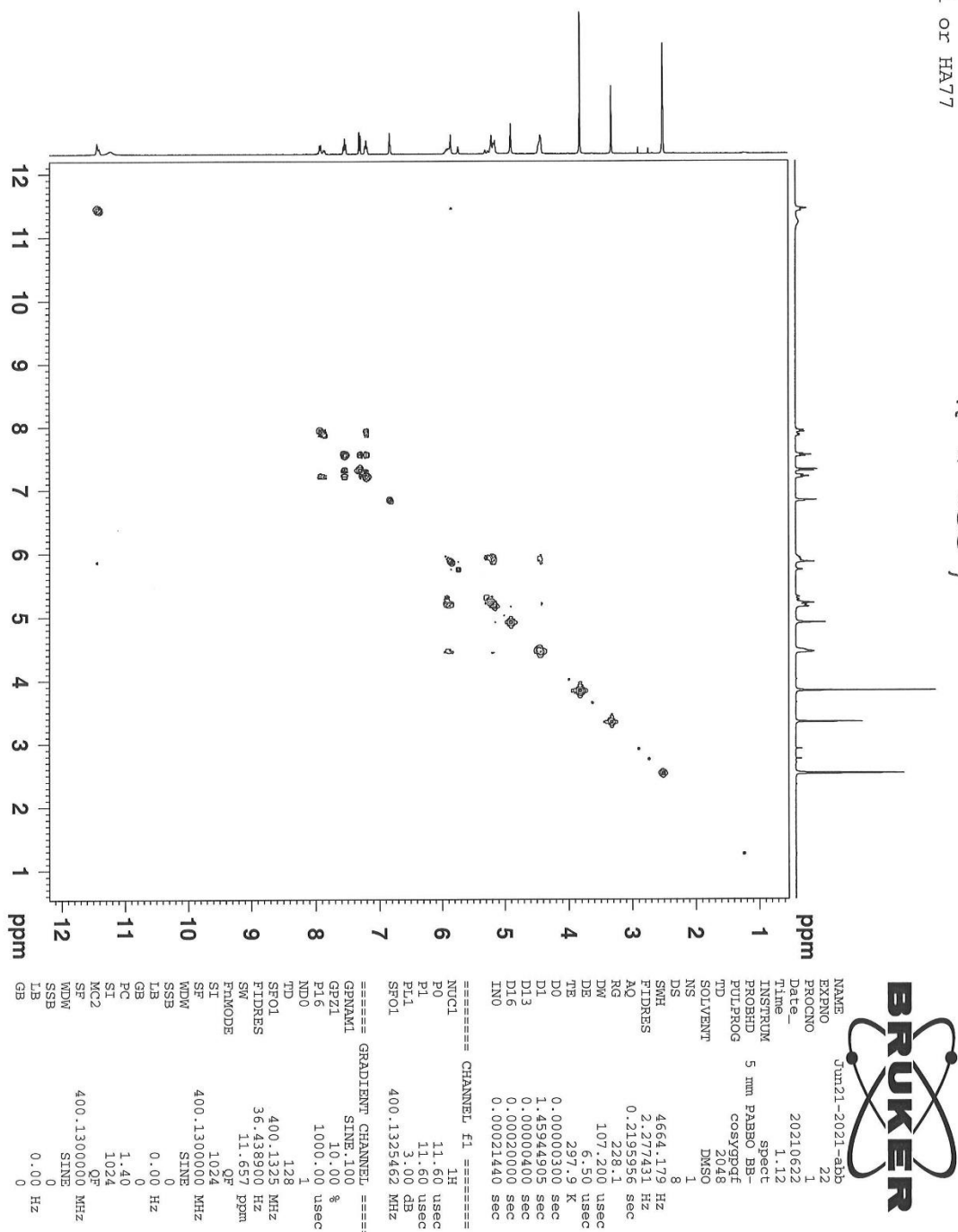
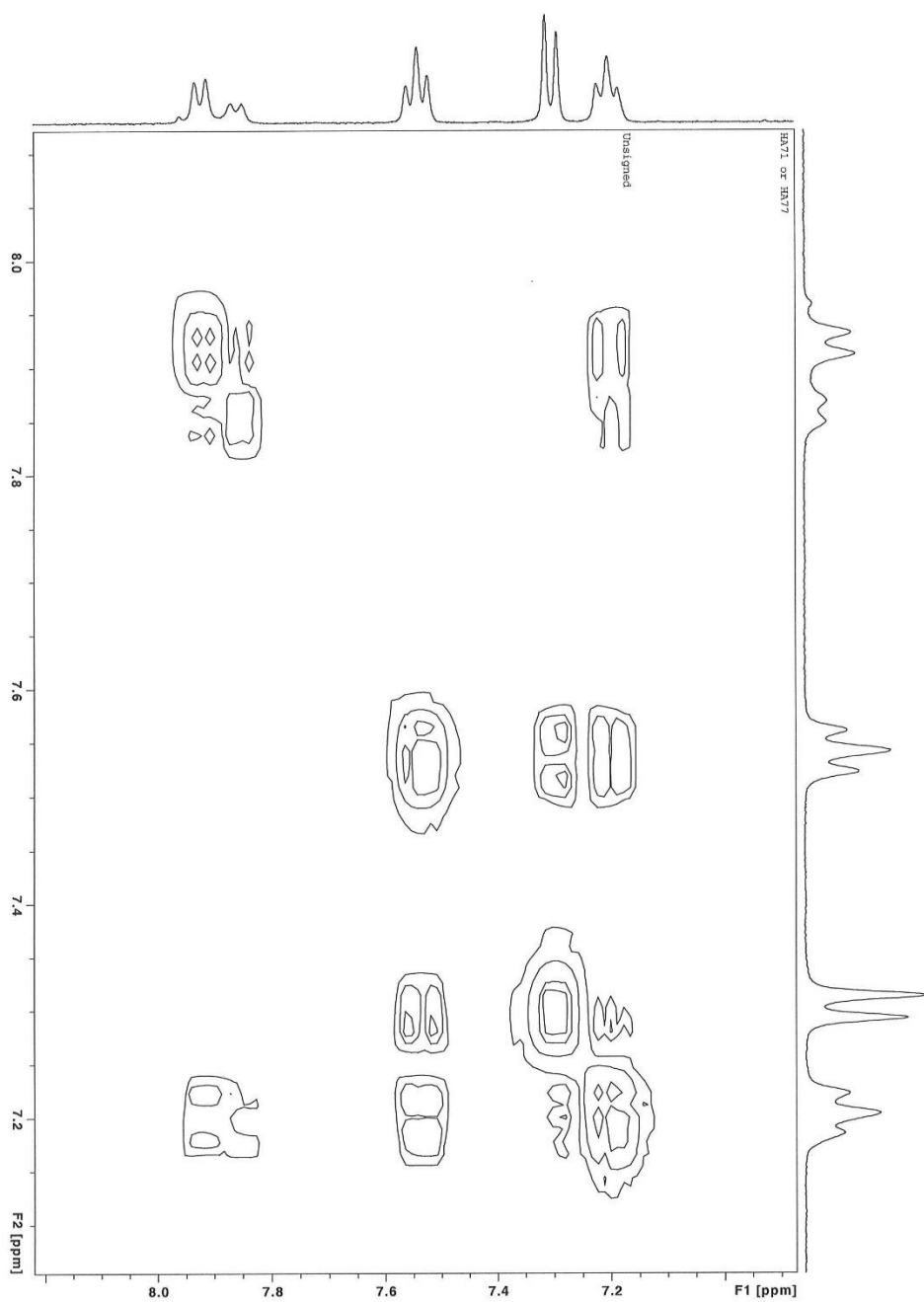
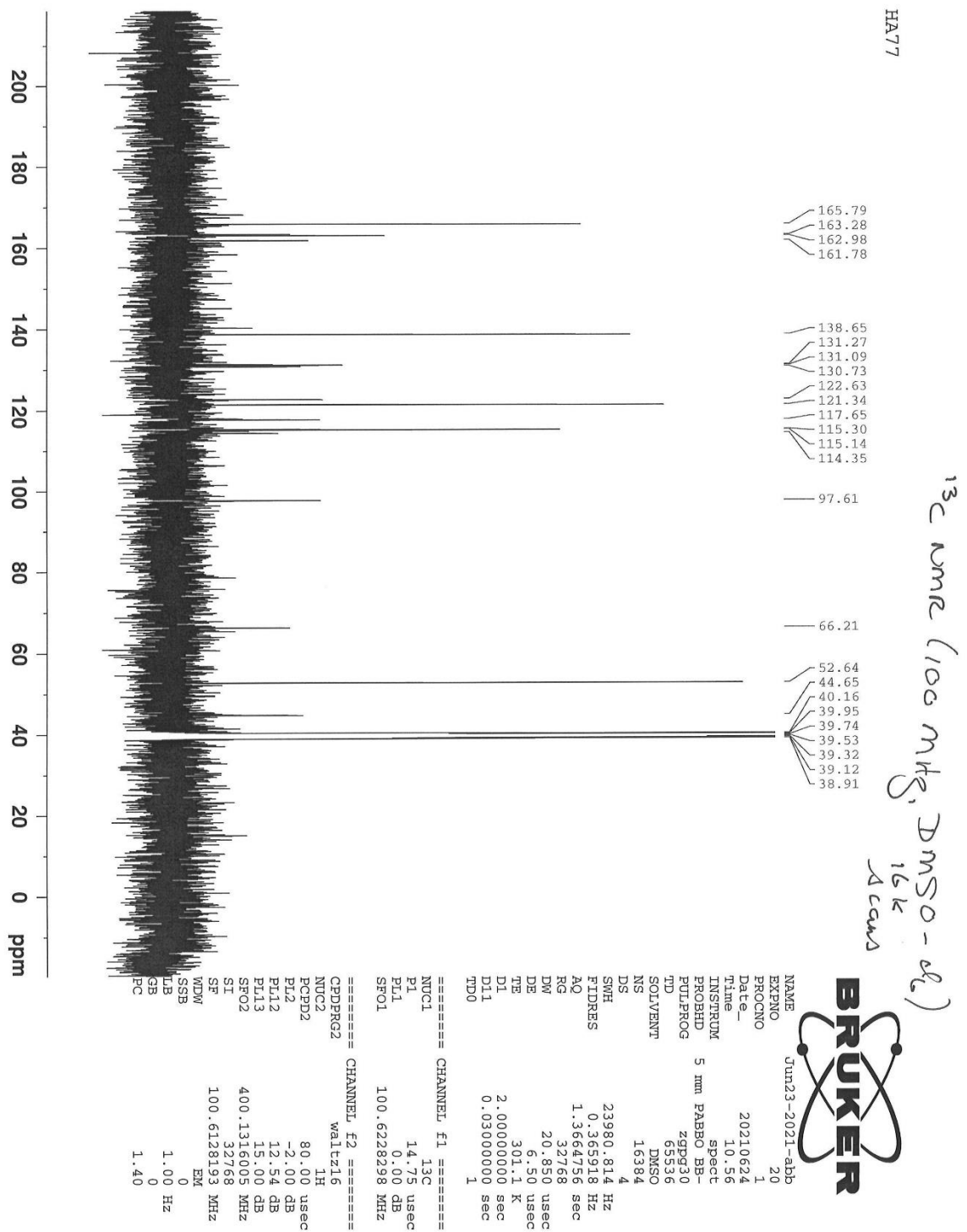


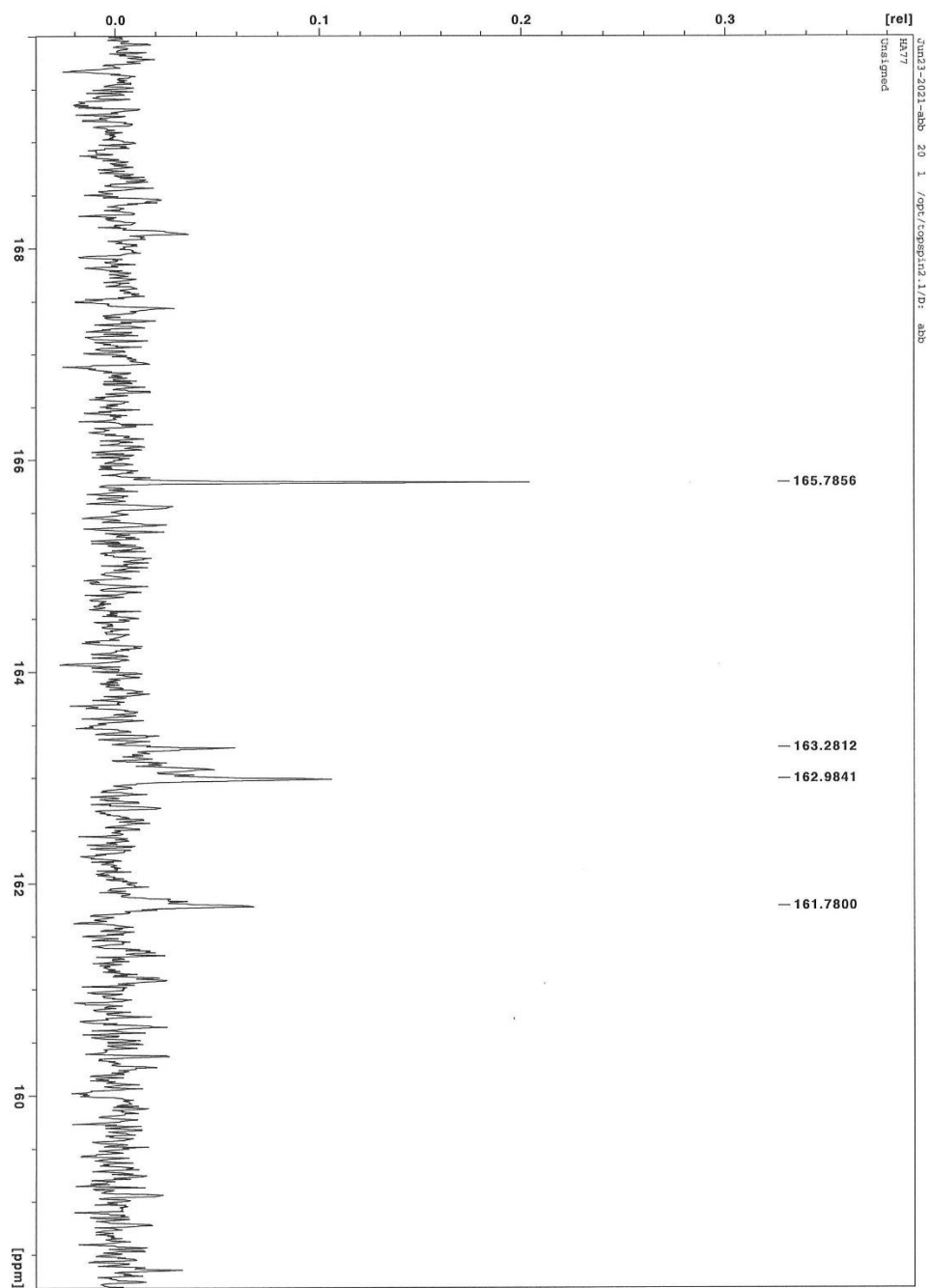
Figure S176.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7j**.



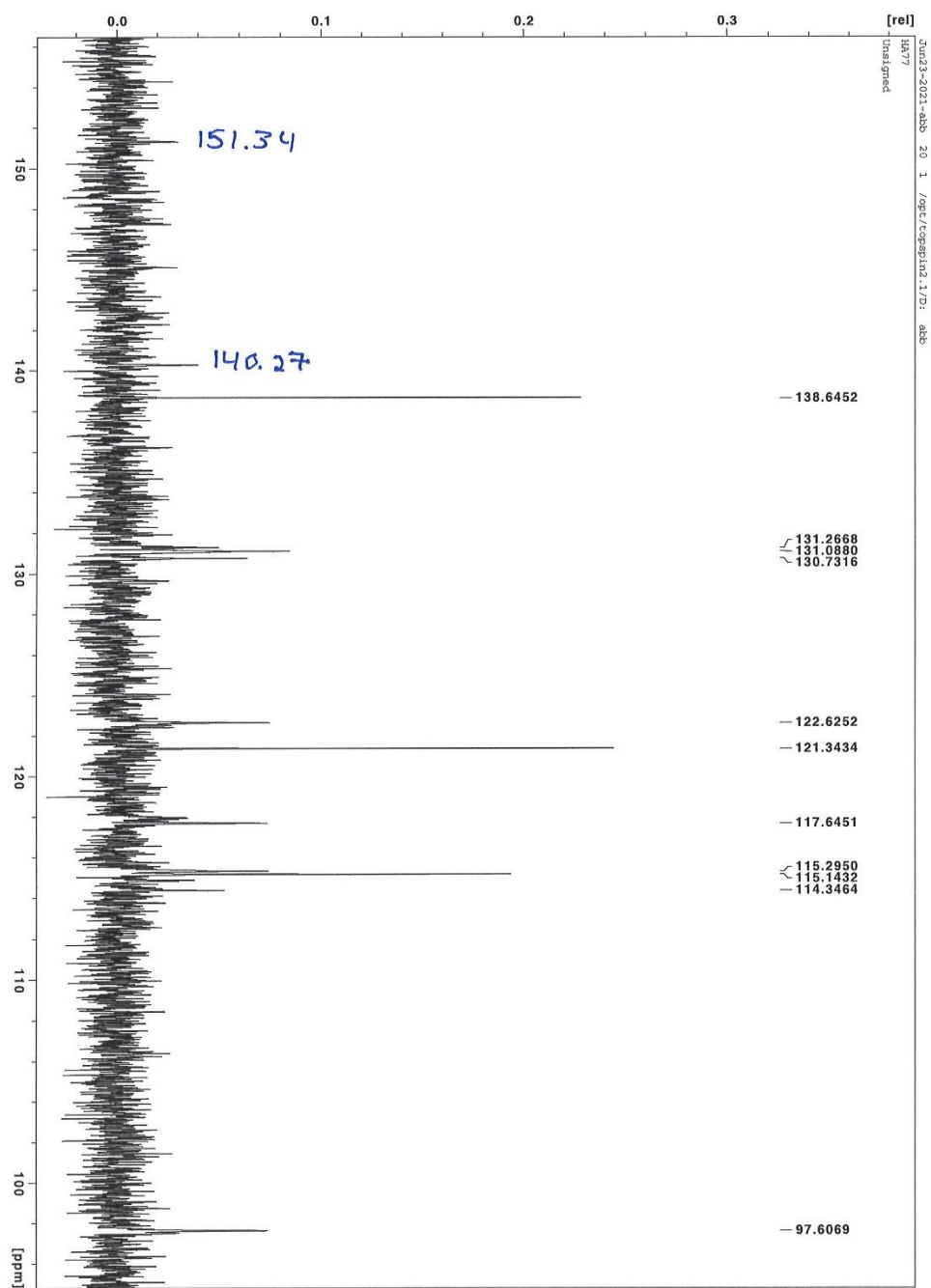
**Figure S177.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7j**.



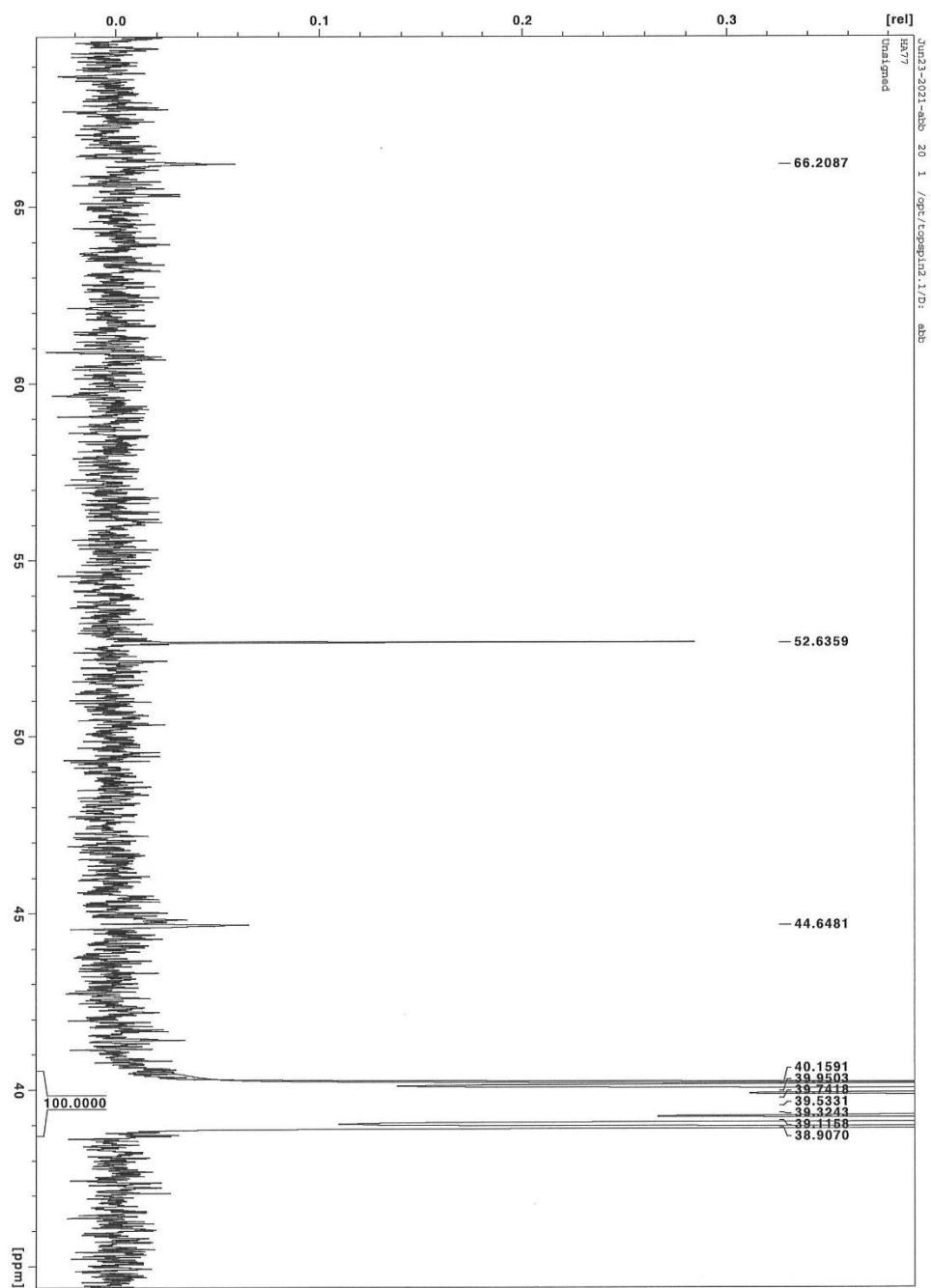
**Figure S178.** <sup>13</sup>C NMR spectrum of compound **7j** (100 MHz, DMSO-*d*<sub>6</sub>).



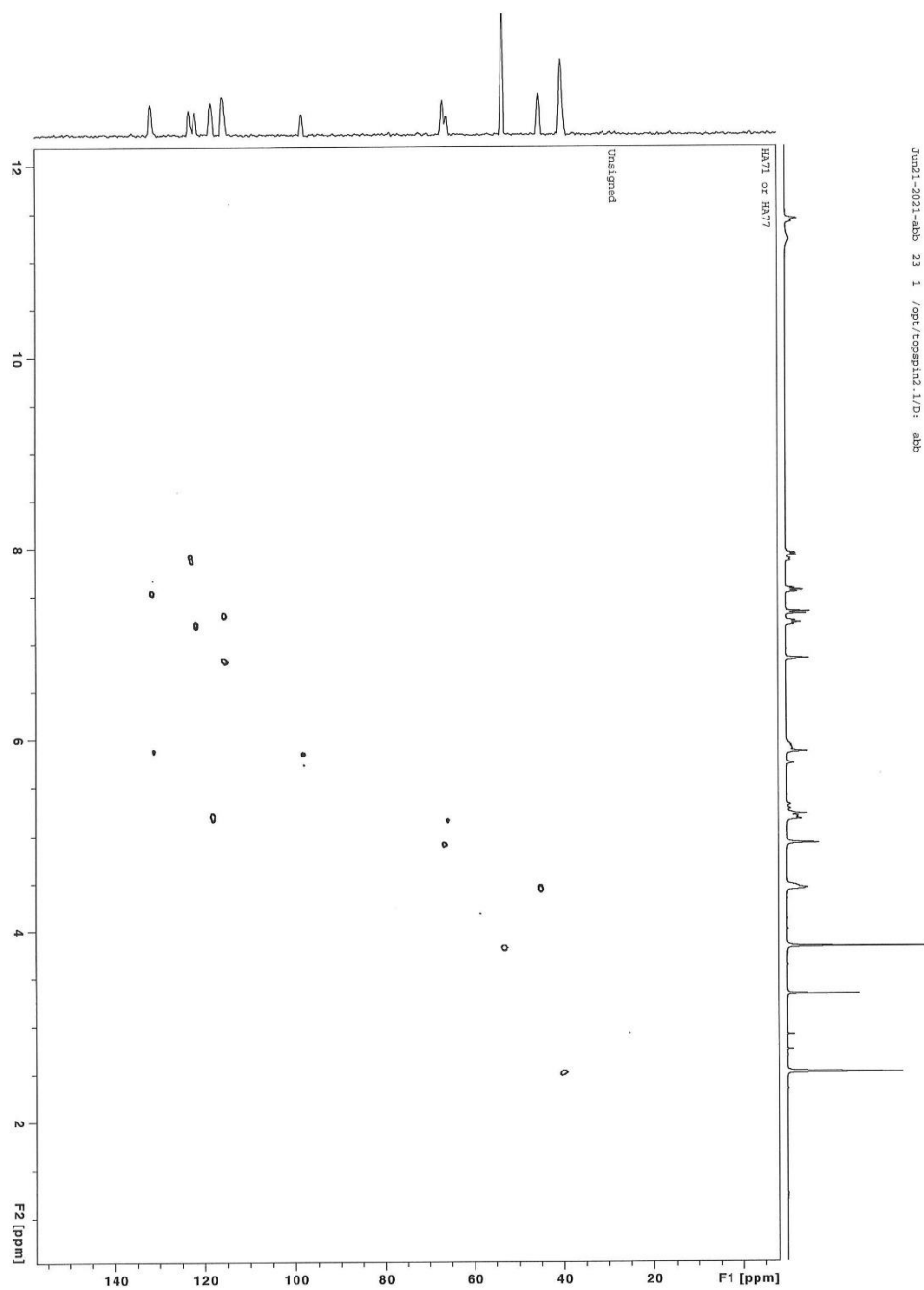
**Figure S179.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **7j**.



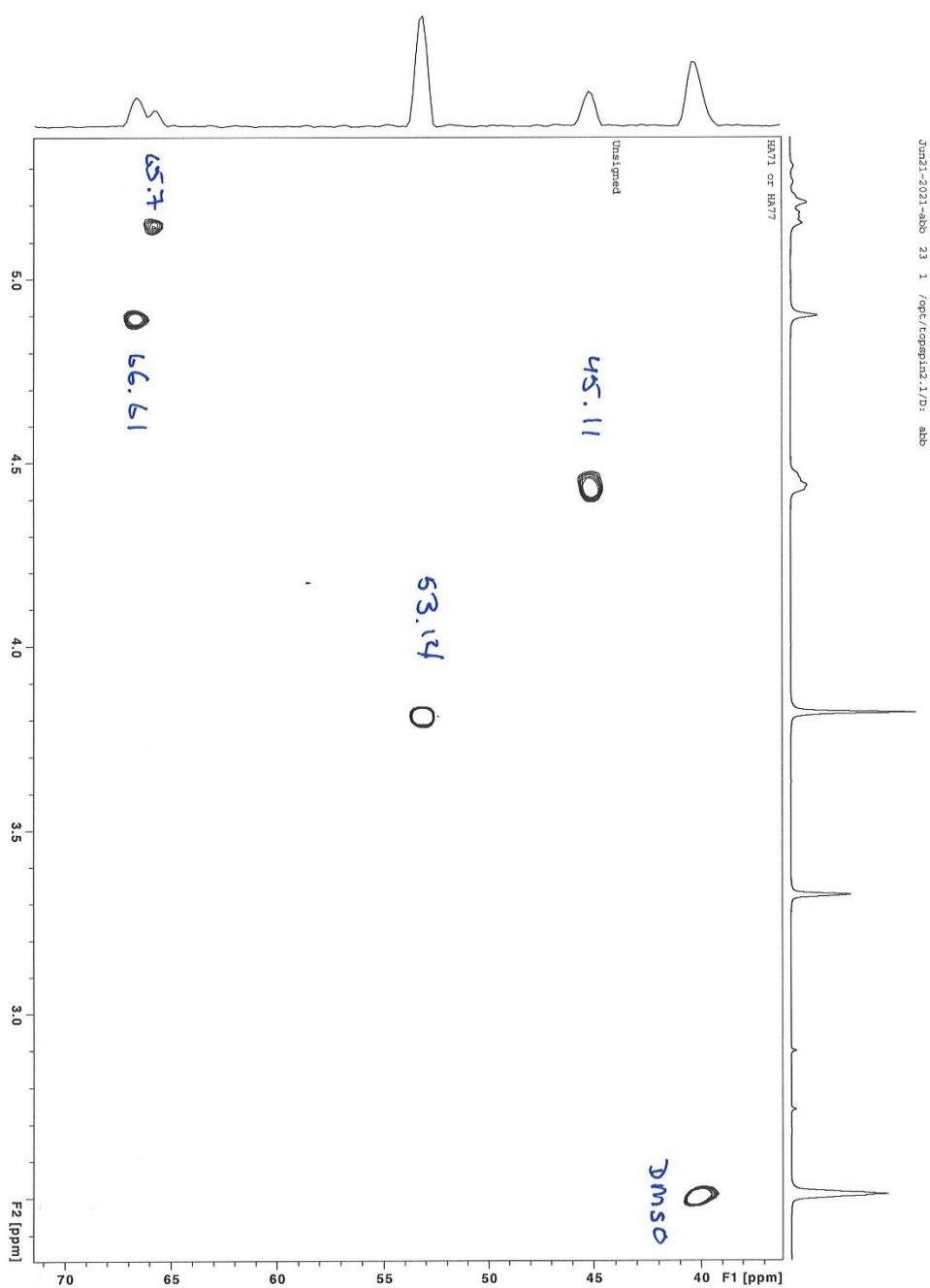
**Figure S180.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **7j**.



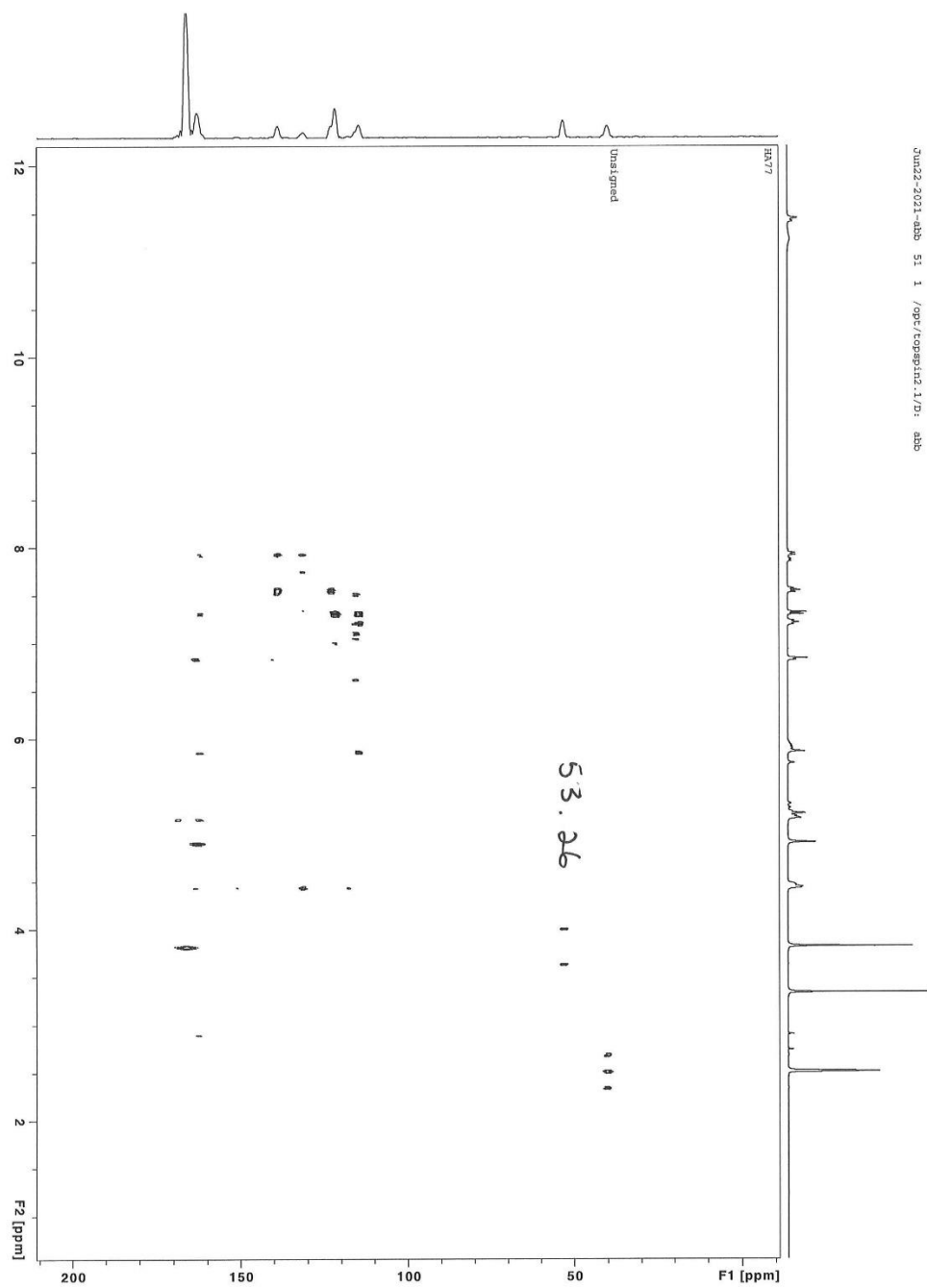
**Figure S181.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **7j**.



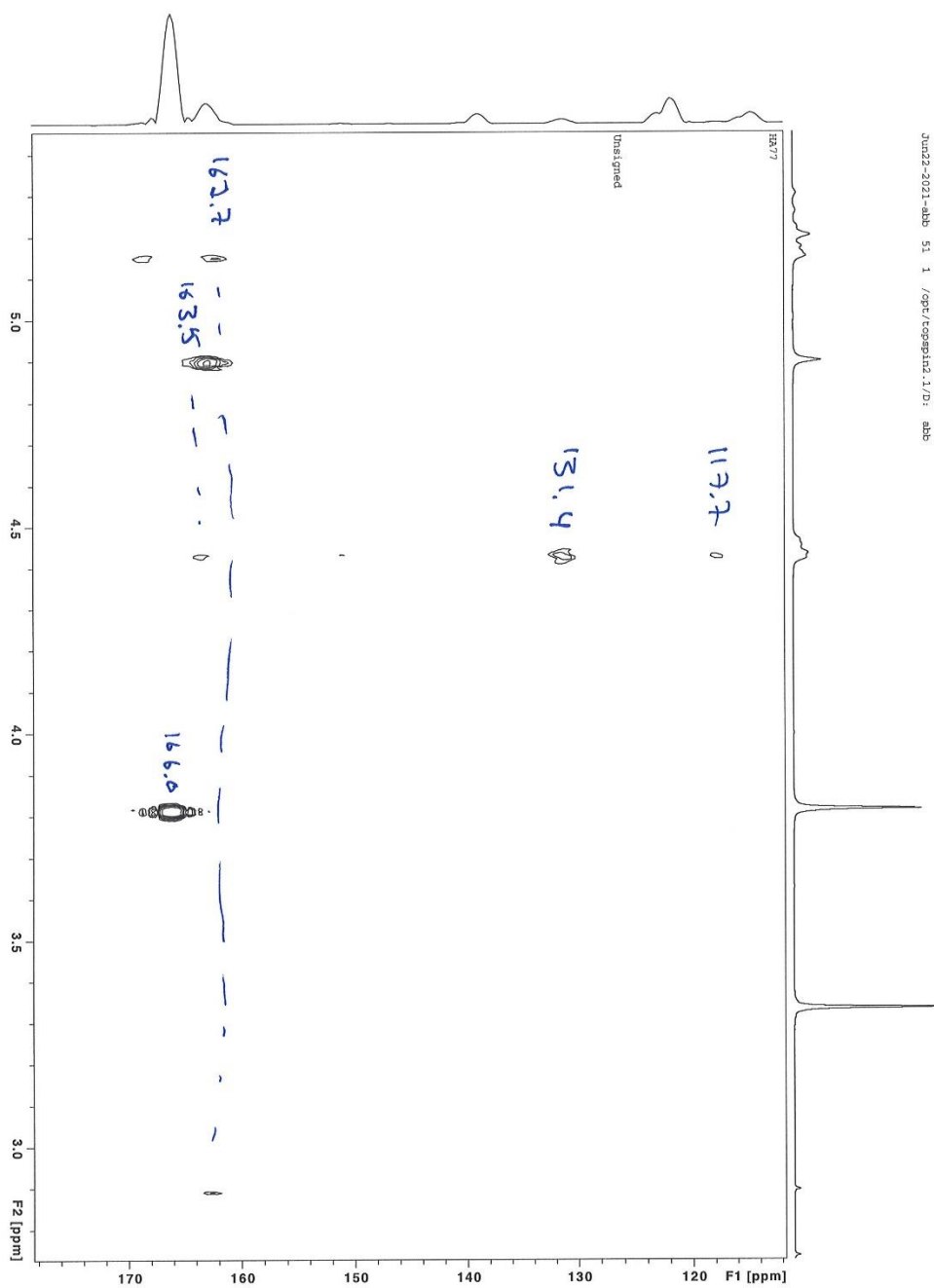
**Figure S182.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7j**.



**Figure S183.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7j**.



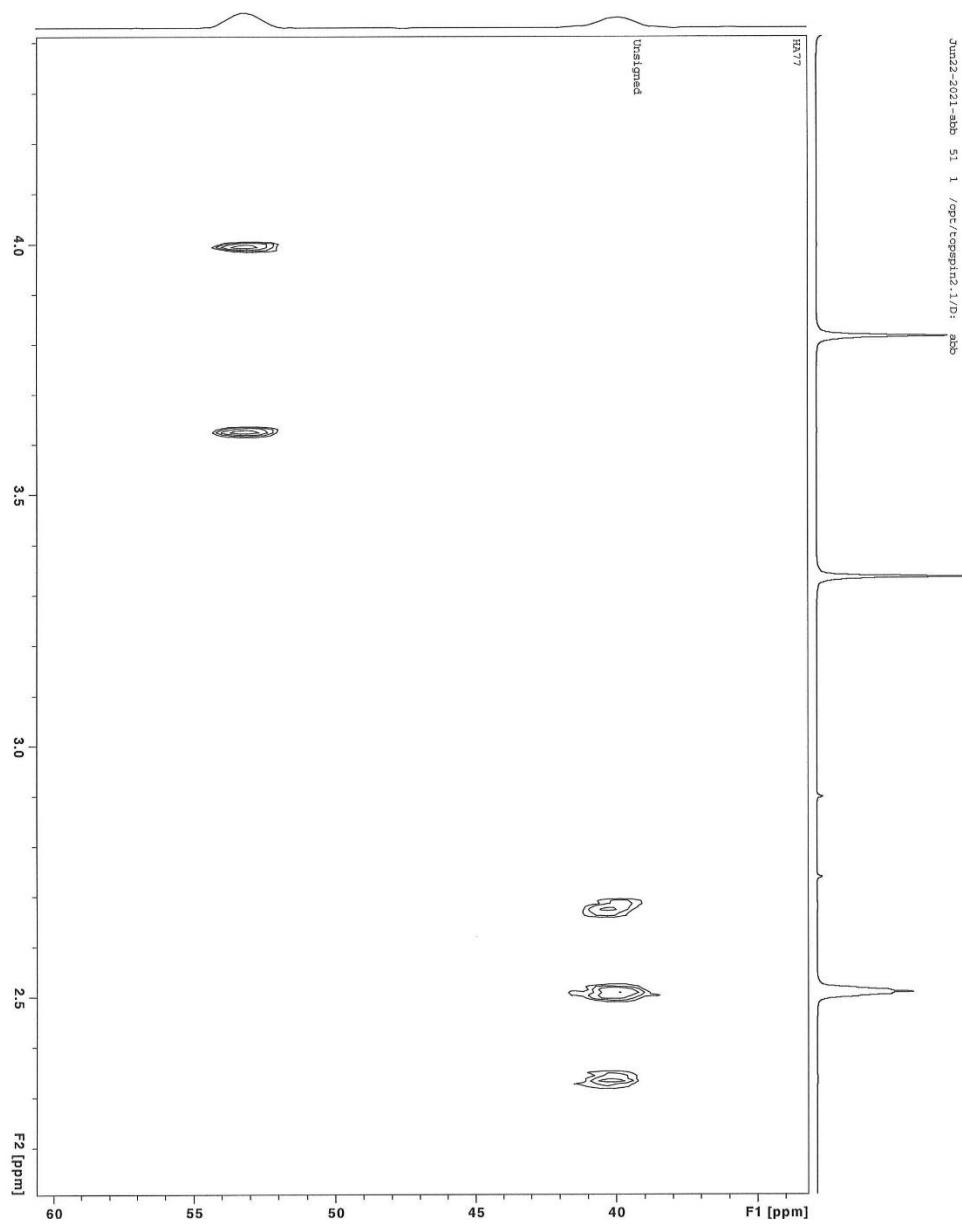
**Figure S184.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7j**.



**Figure S185.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7j**.

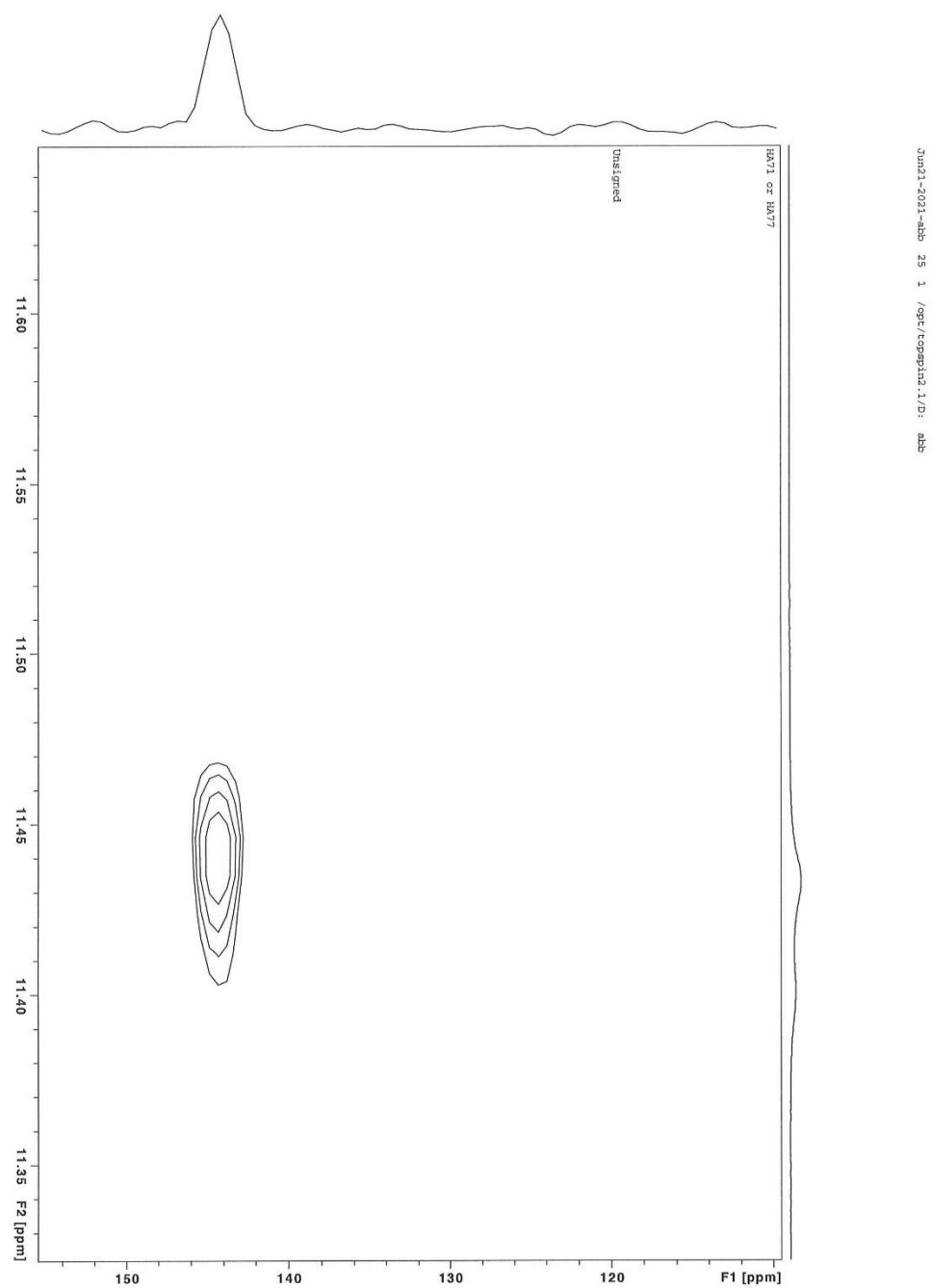


**Figure S186.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7j**.

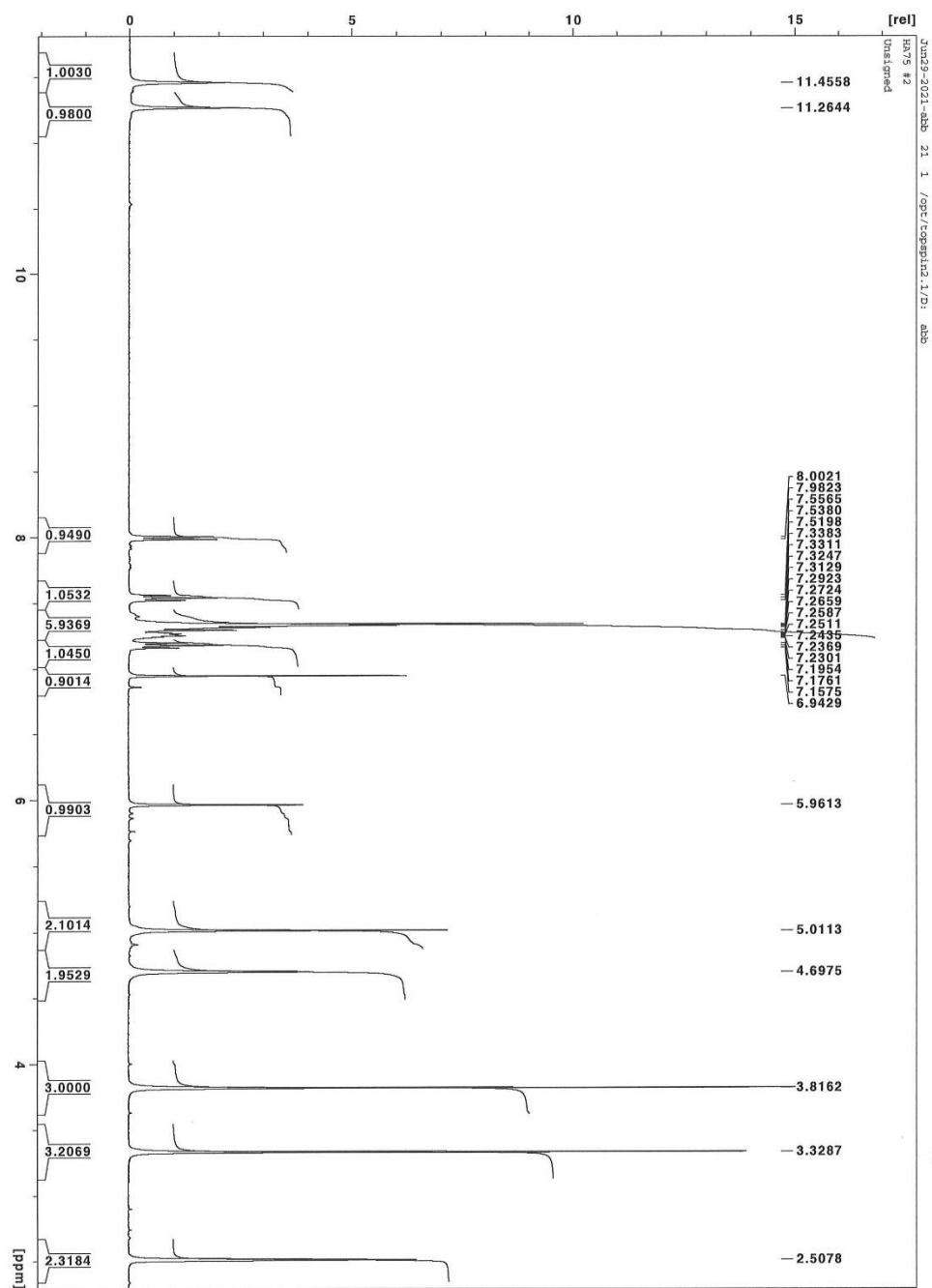


**Figure S187.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7j**.

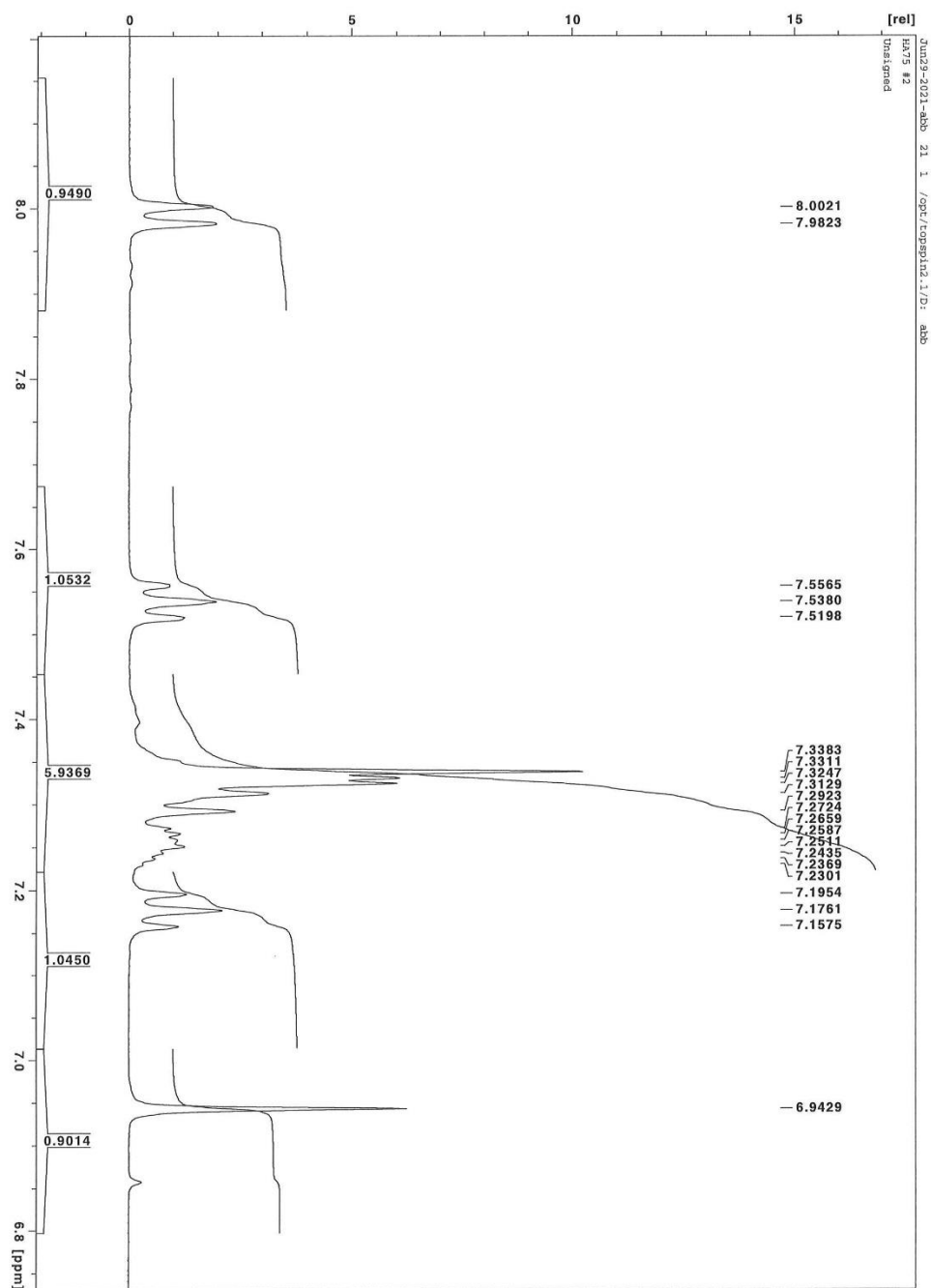




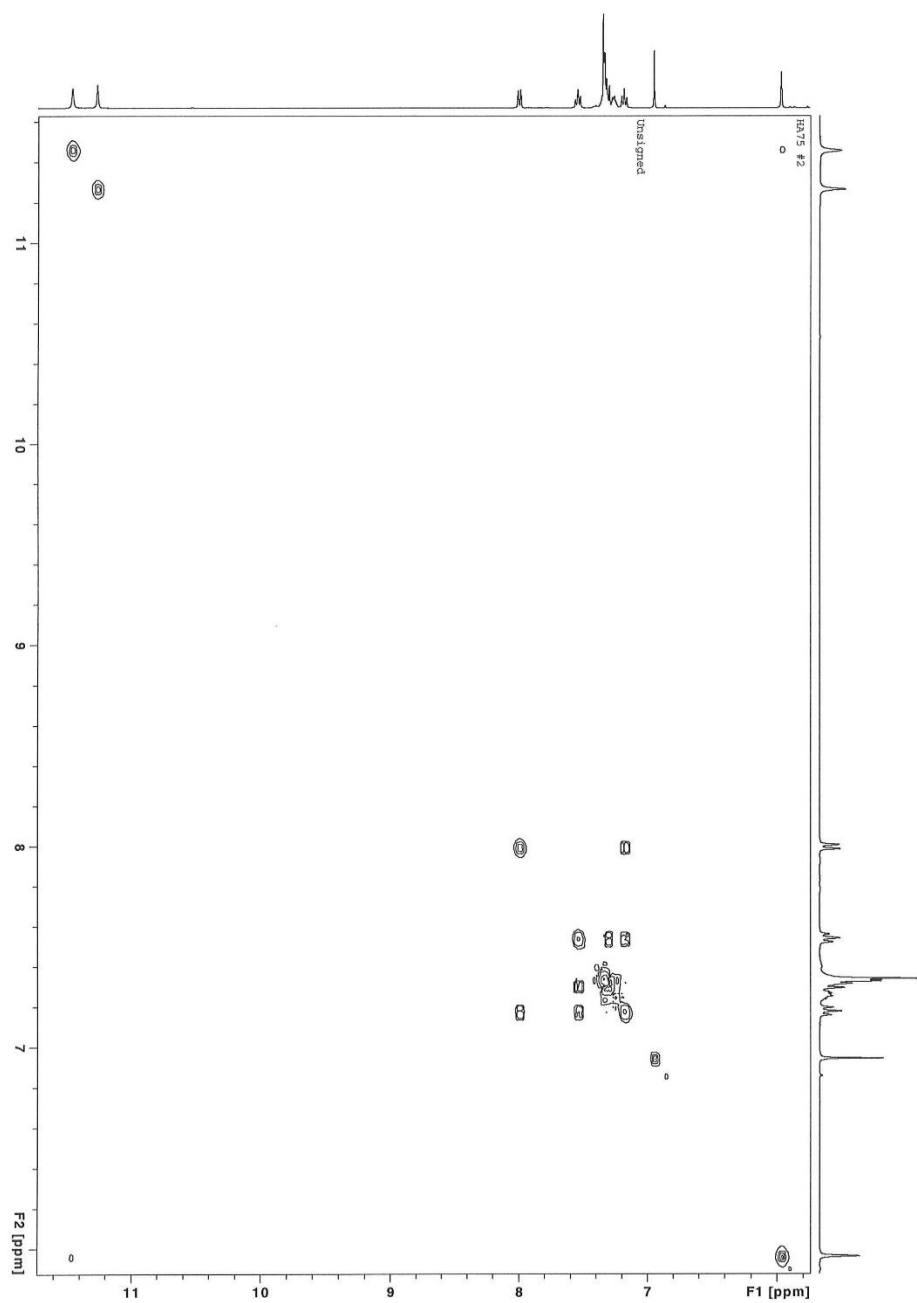
**Figure S189.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **7j** (HMBC spectrum gave no cross peaks).



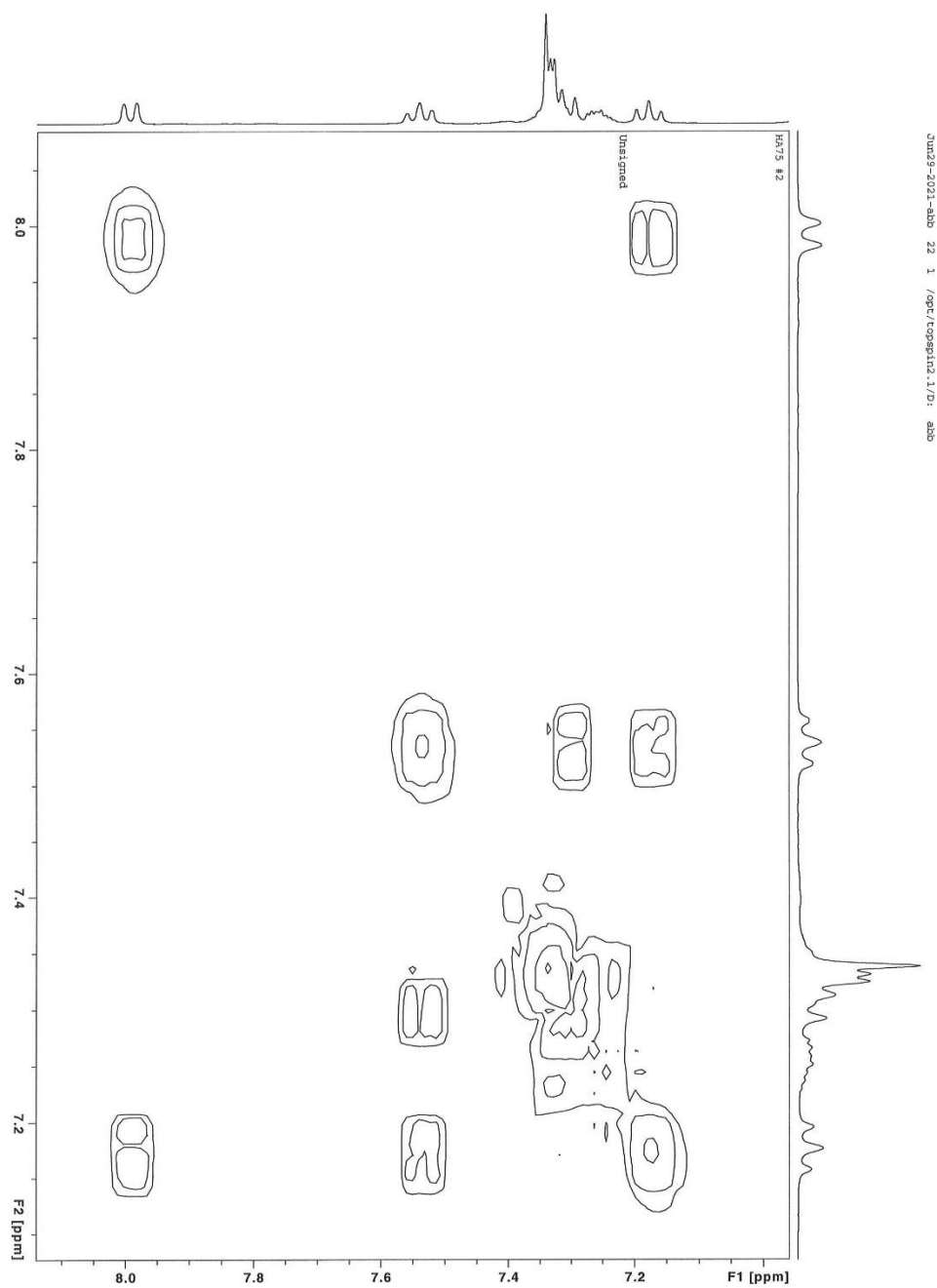
**Figure S190.**  $^1\text{H}$  spectrum of compound **7k** (400 MHz,  $\text{DMSO}-d_6$ ).



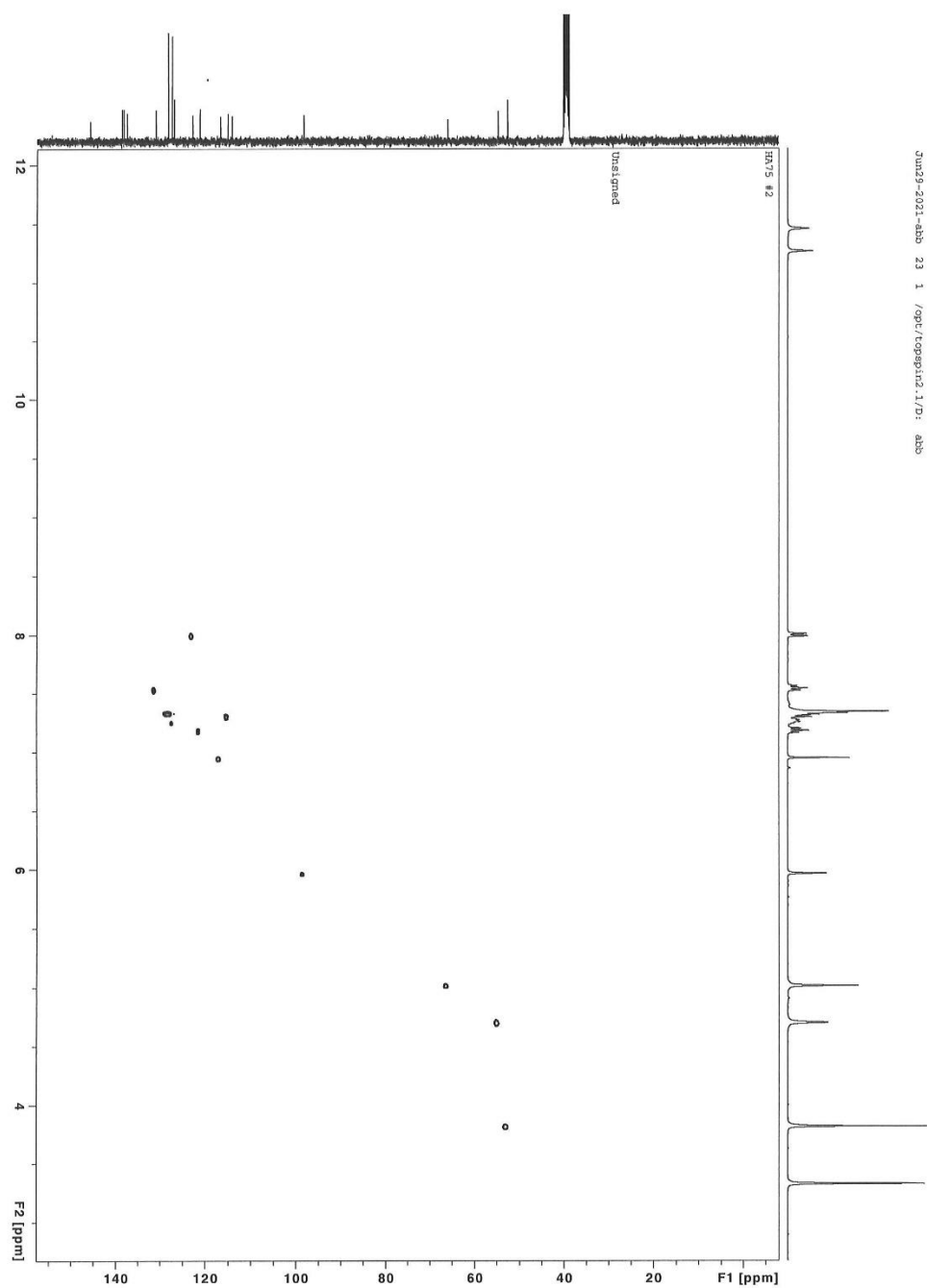
**Figure S191.** Detail of  $^1\text{H}$  NMR spectrum of compound **7k**.



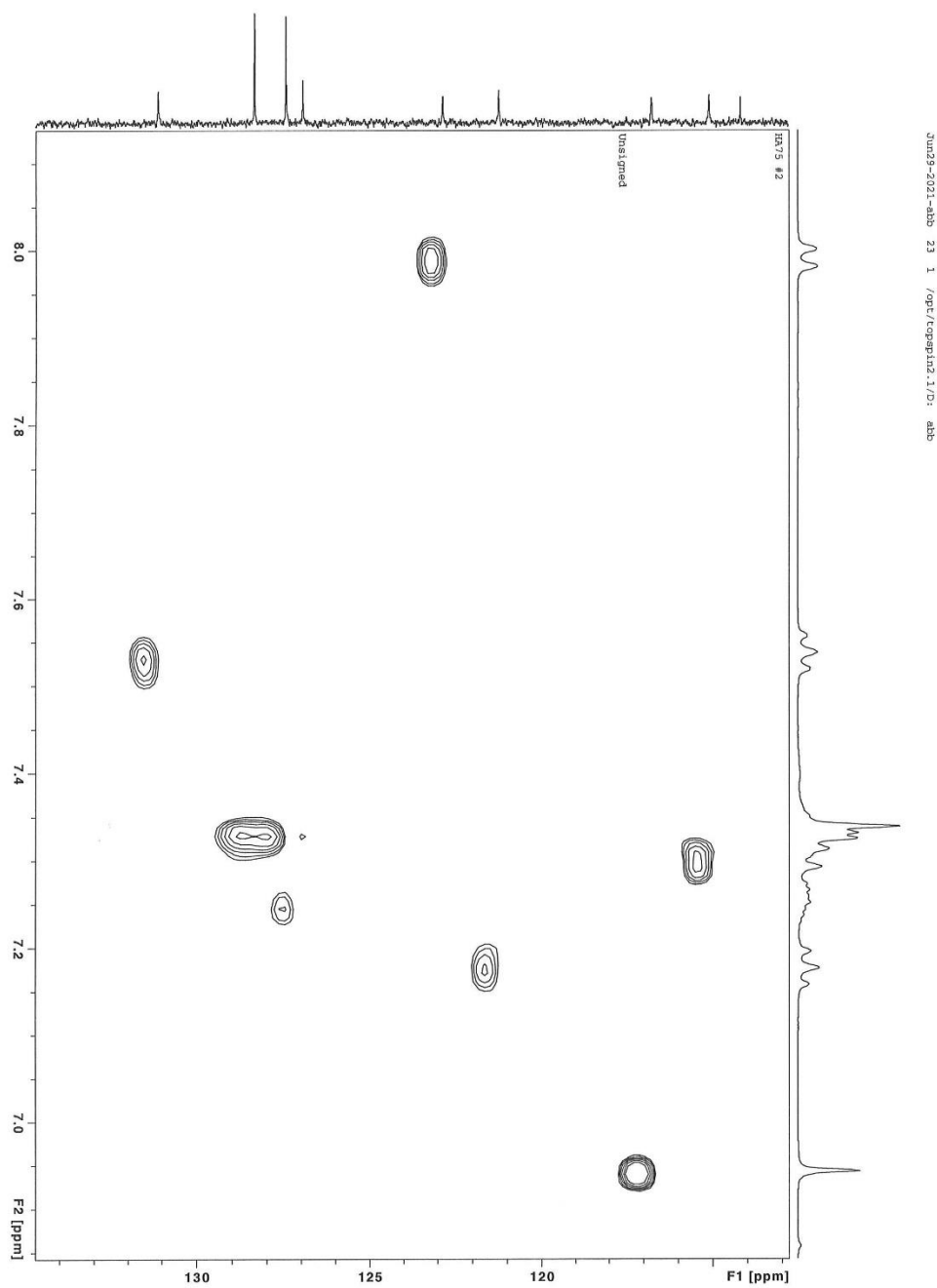
**Figure S192.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7k**.



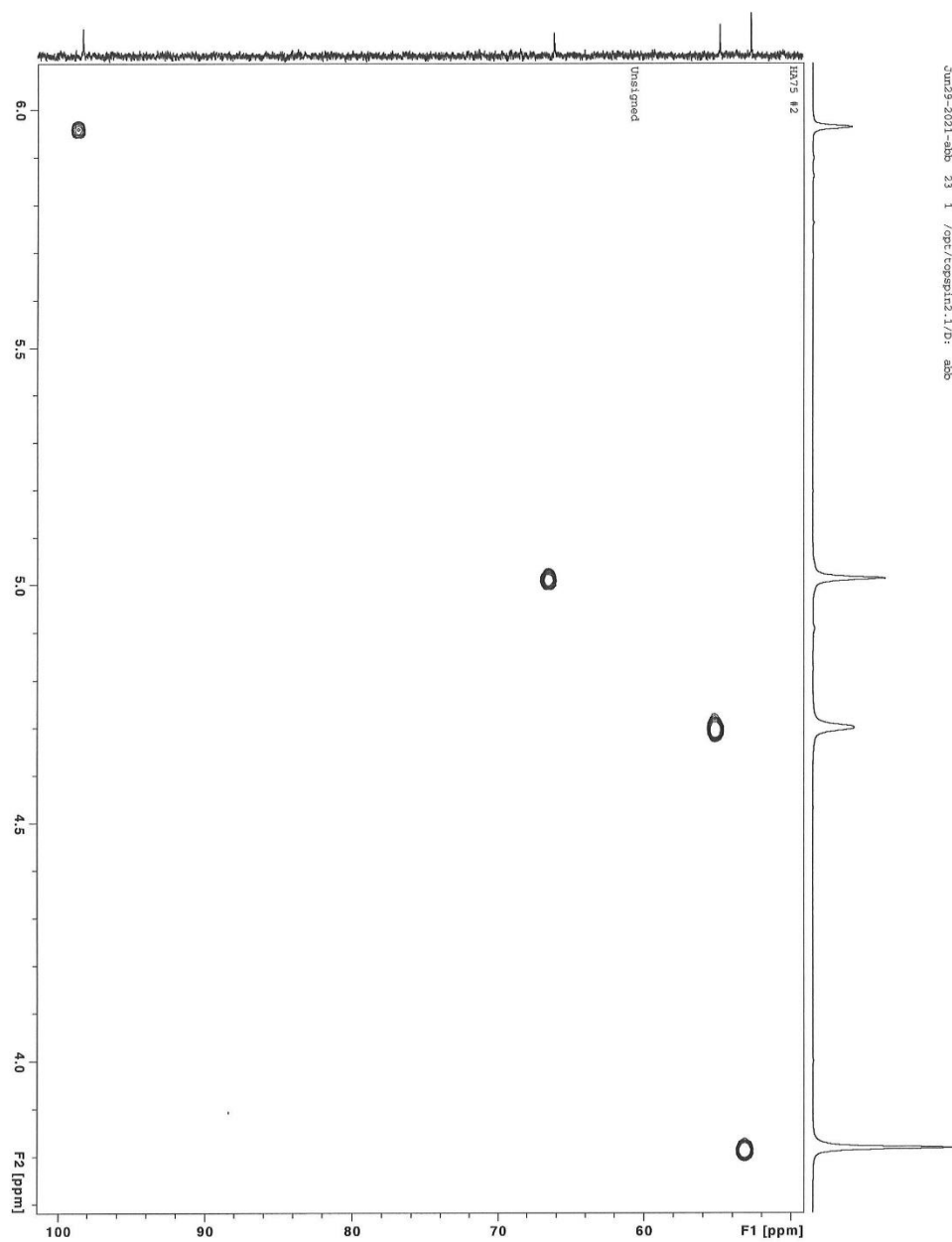
**Figure S193.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7k**.



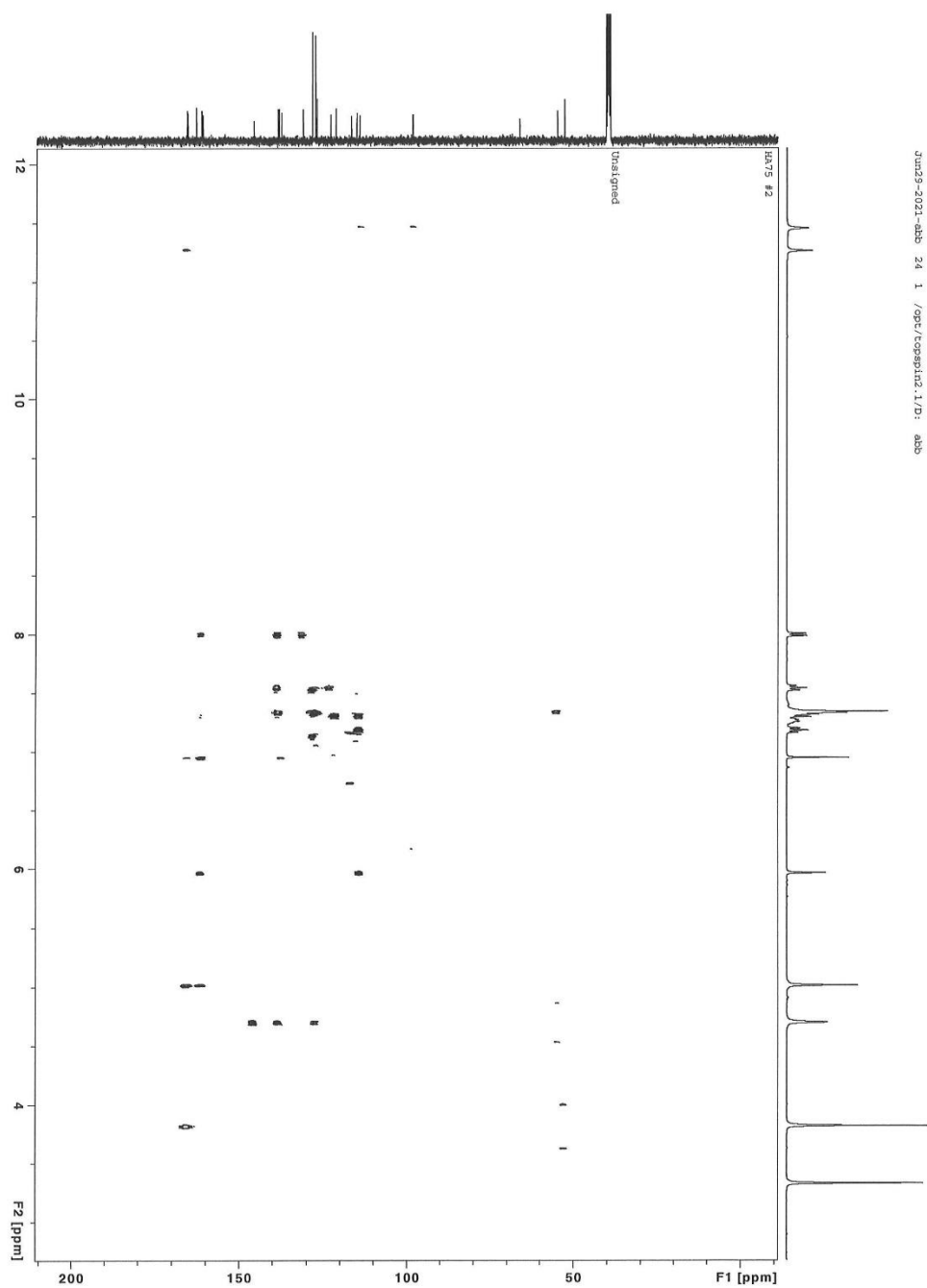
**Figure S194.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7k**.



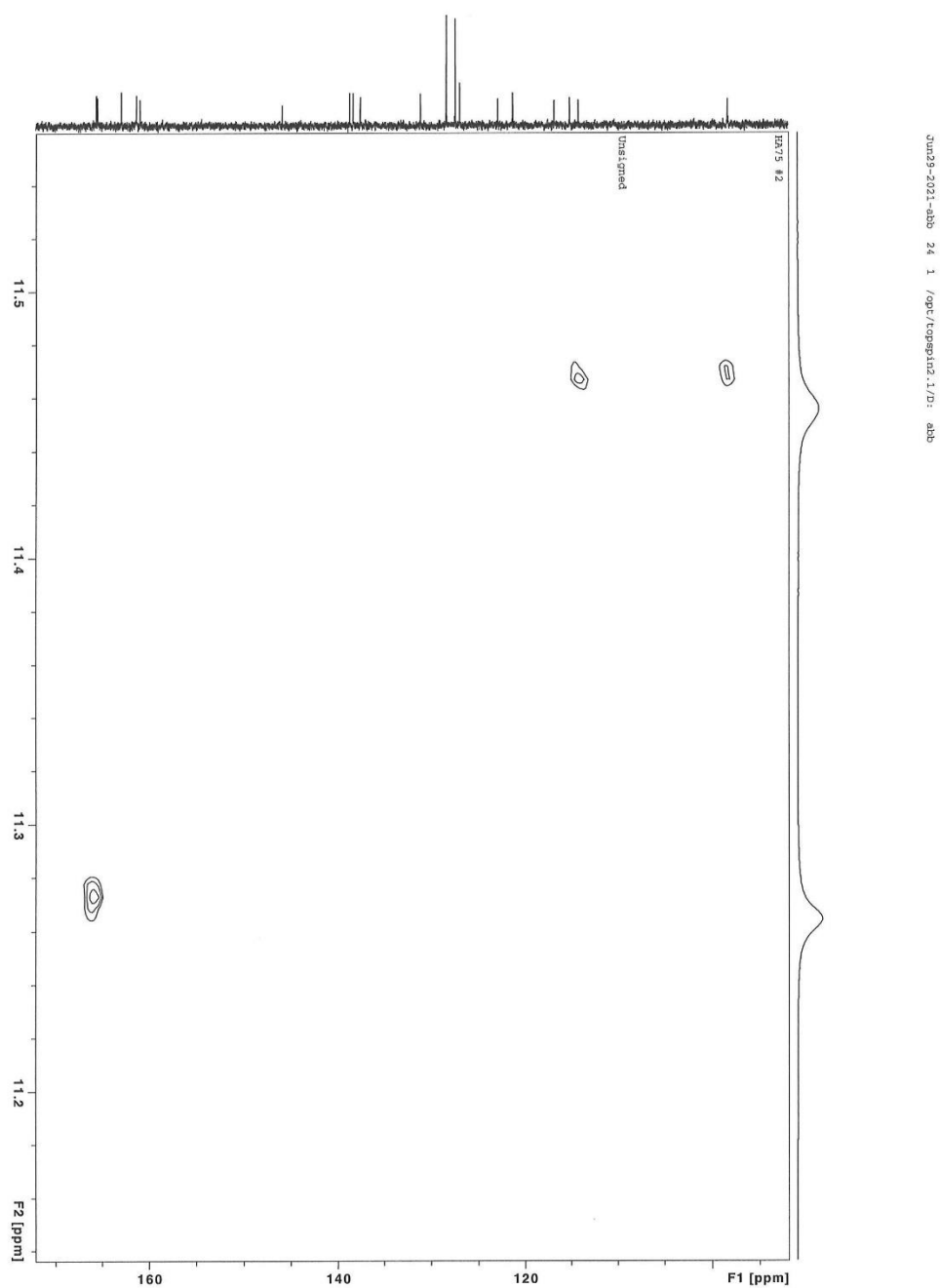
**Figure S195.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7k**.



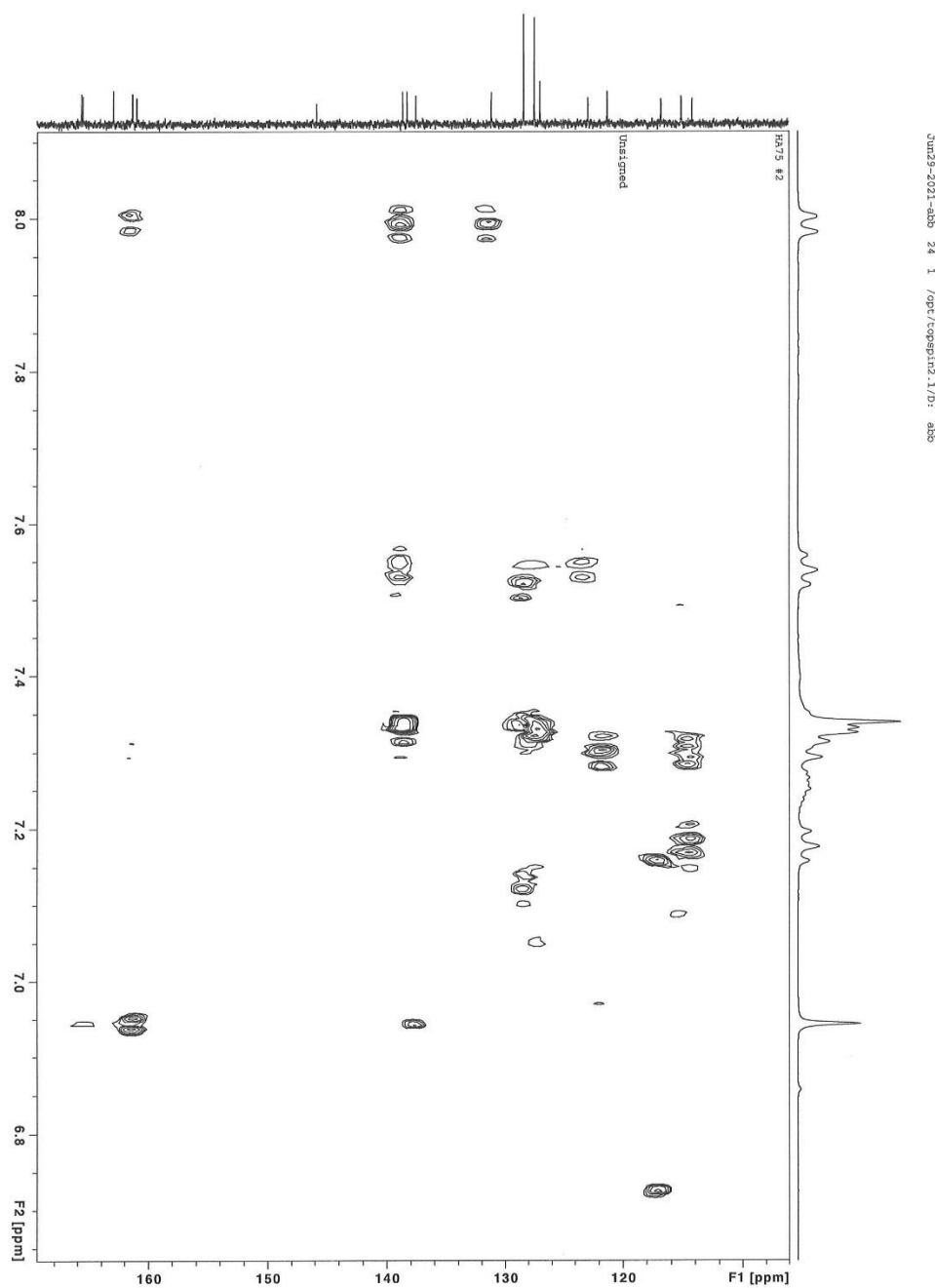
**Figure S196.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7k**.



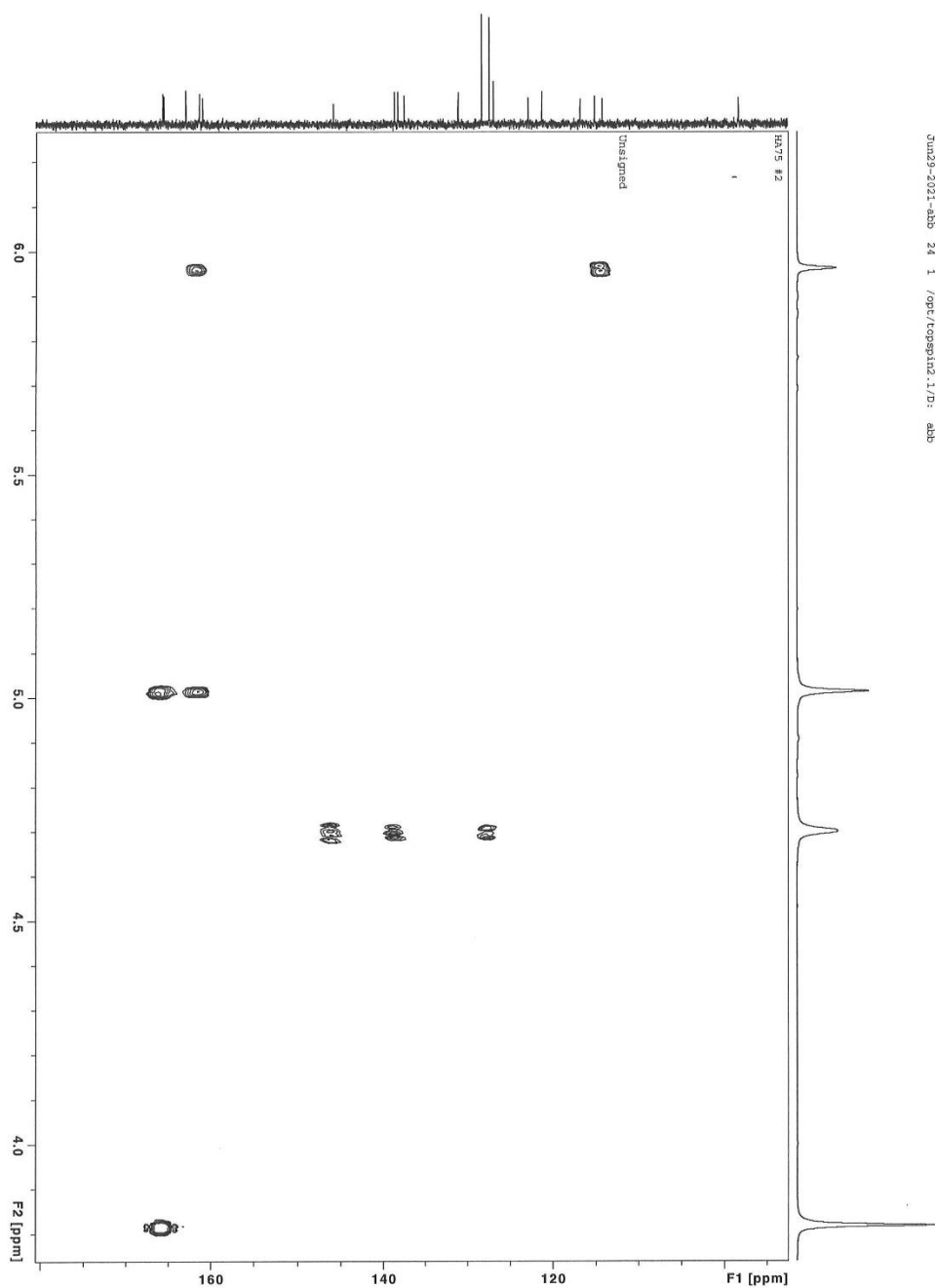
**Figure S197.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of sample **7k**.



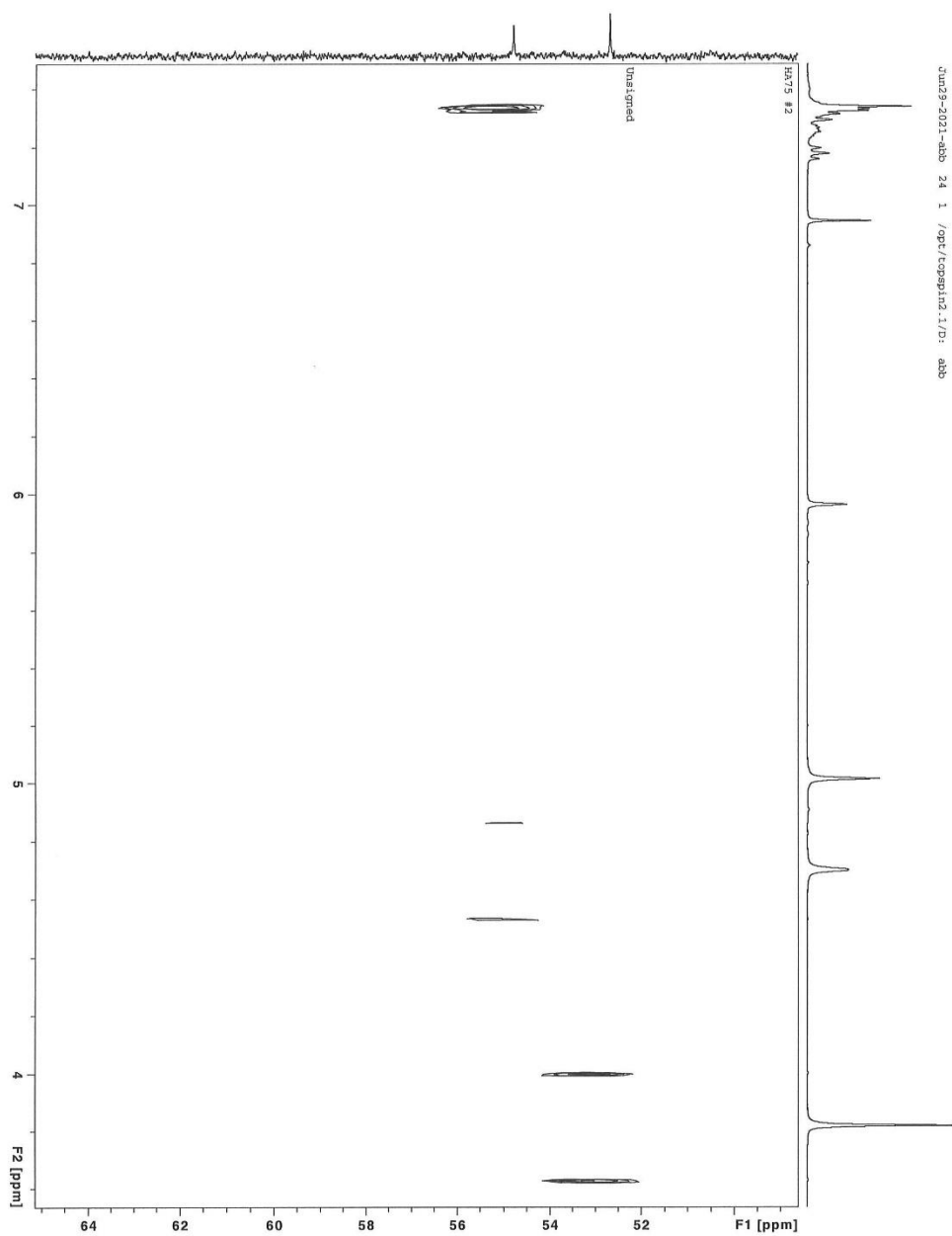
**Figure S198.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7k**.



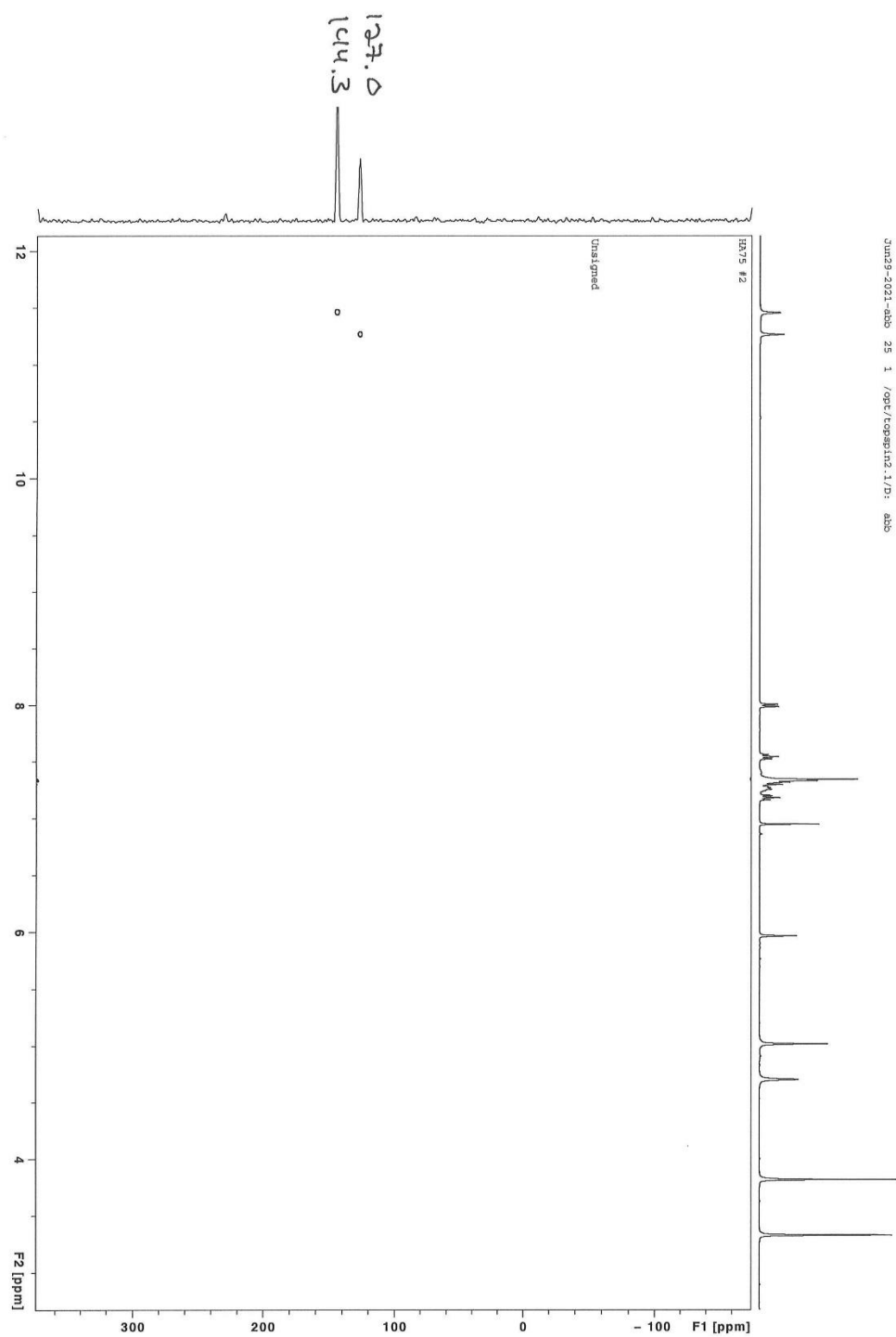
**Figure S199.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7k**.



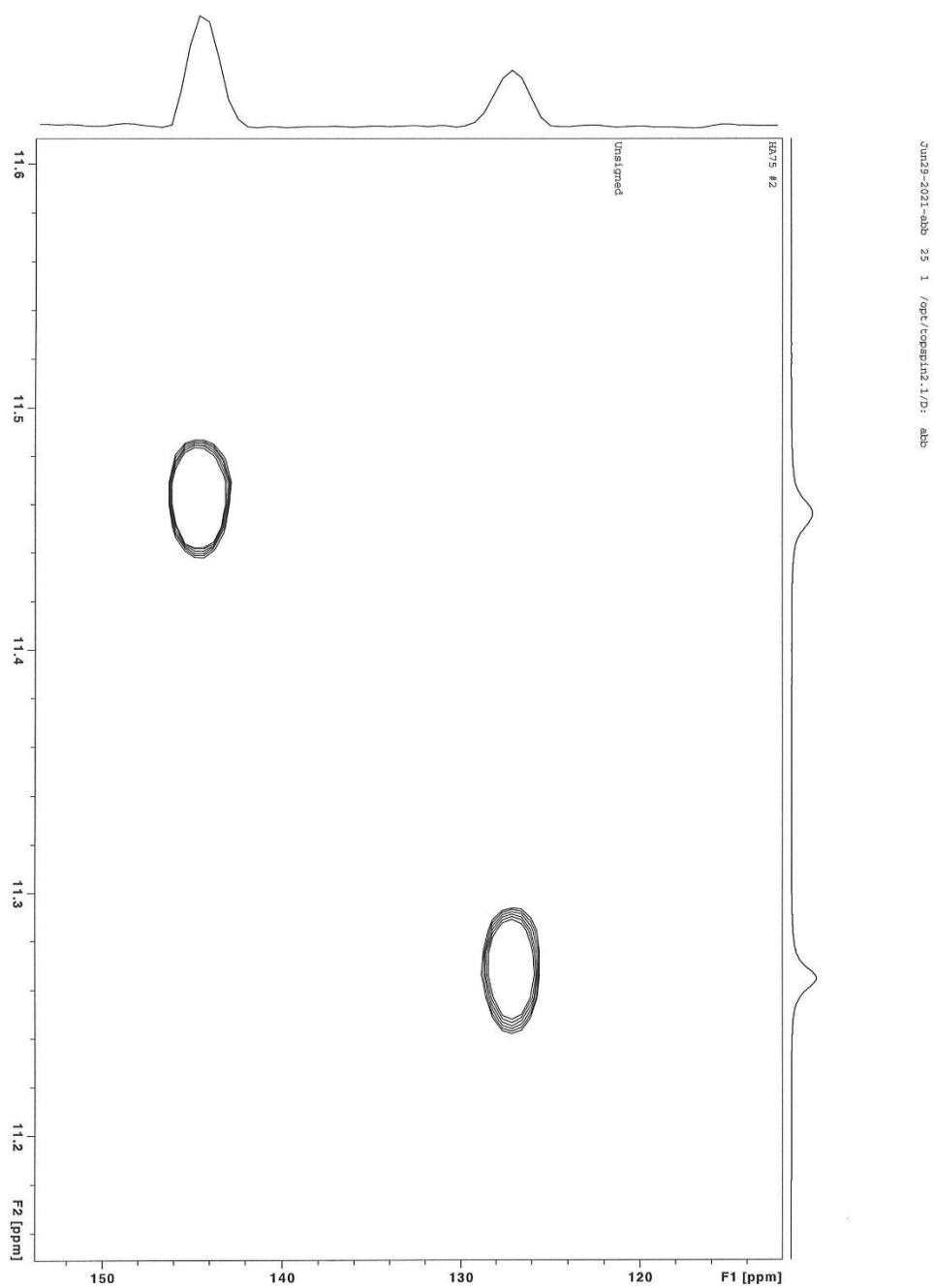
**Figure S200.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7k**.



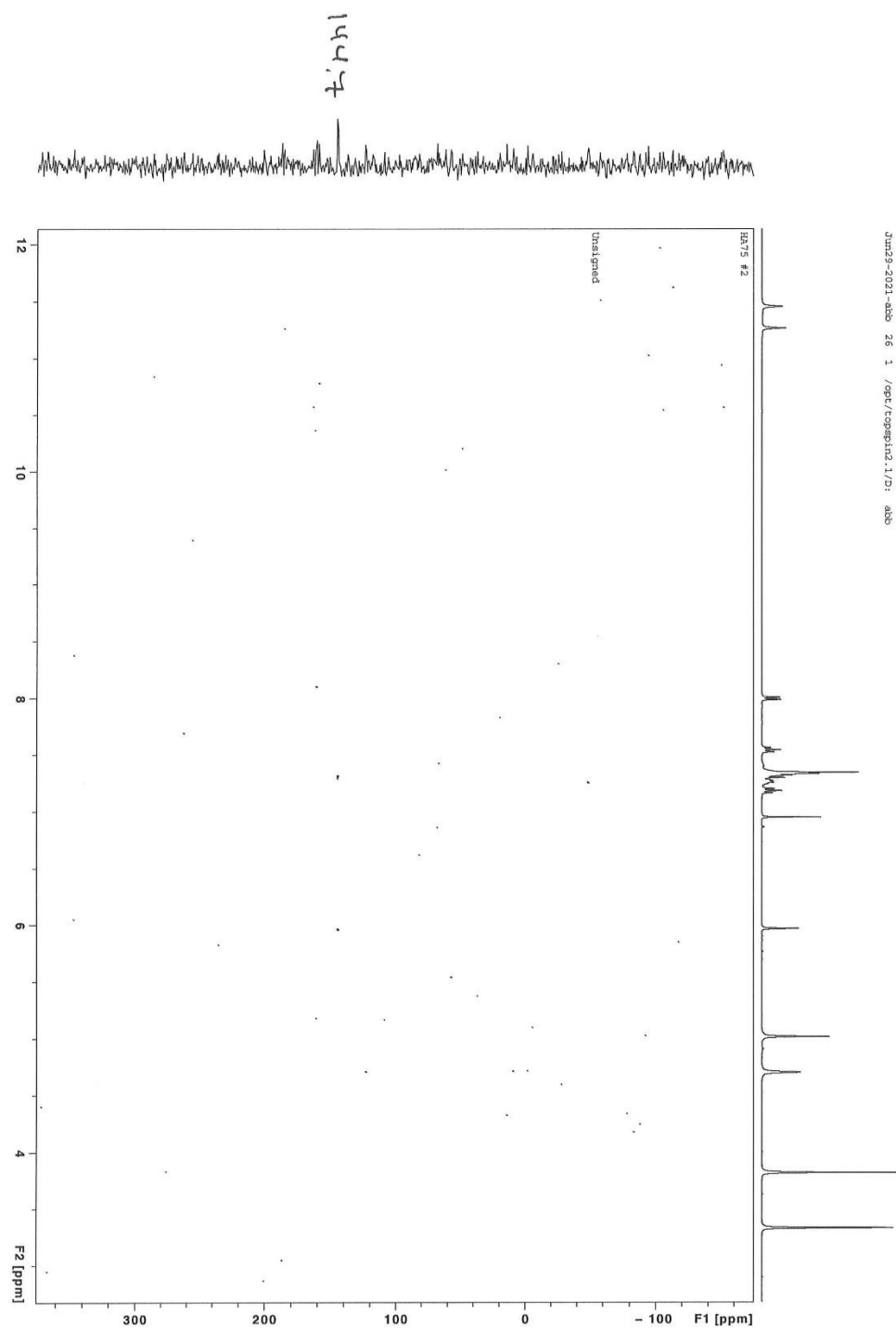
**Figure S201.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7k**.



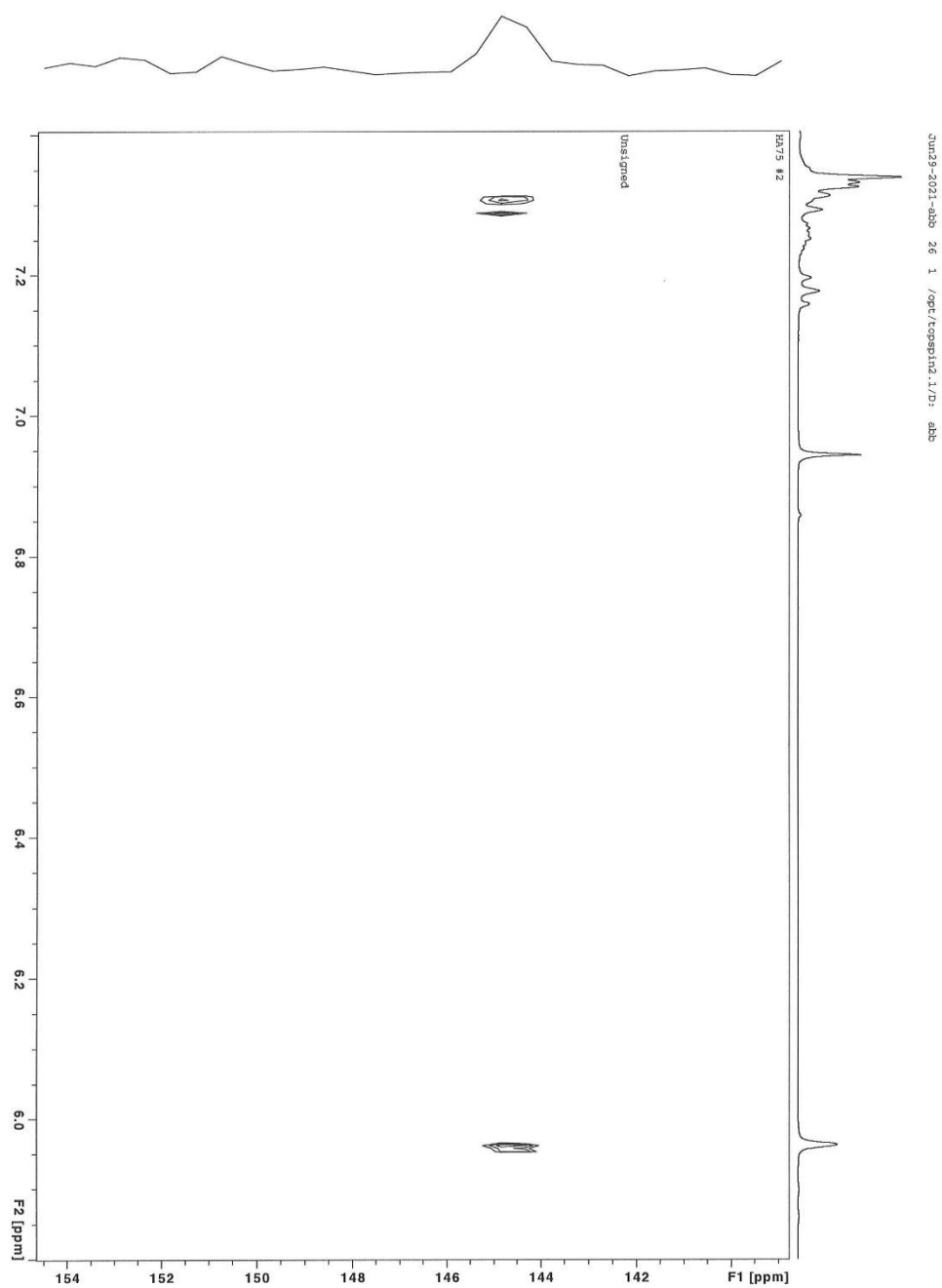
**Figure S202.**  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **7k**.



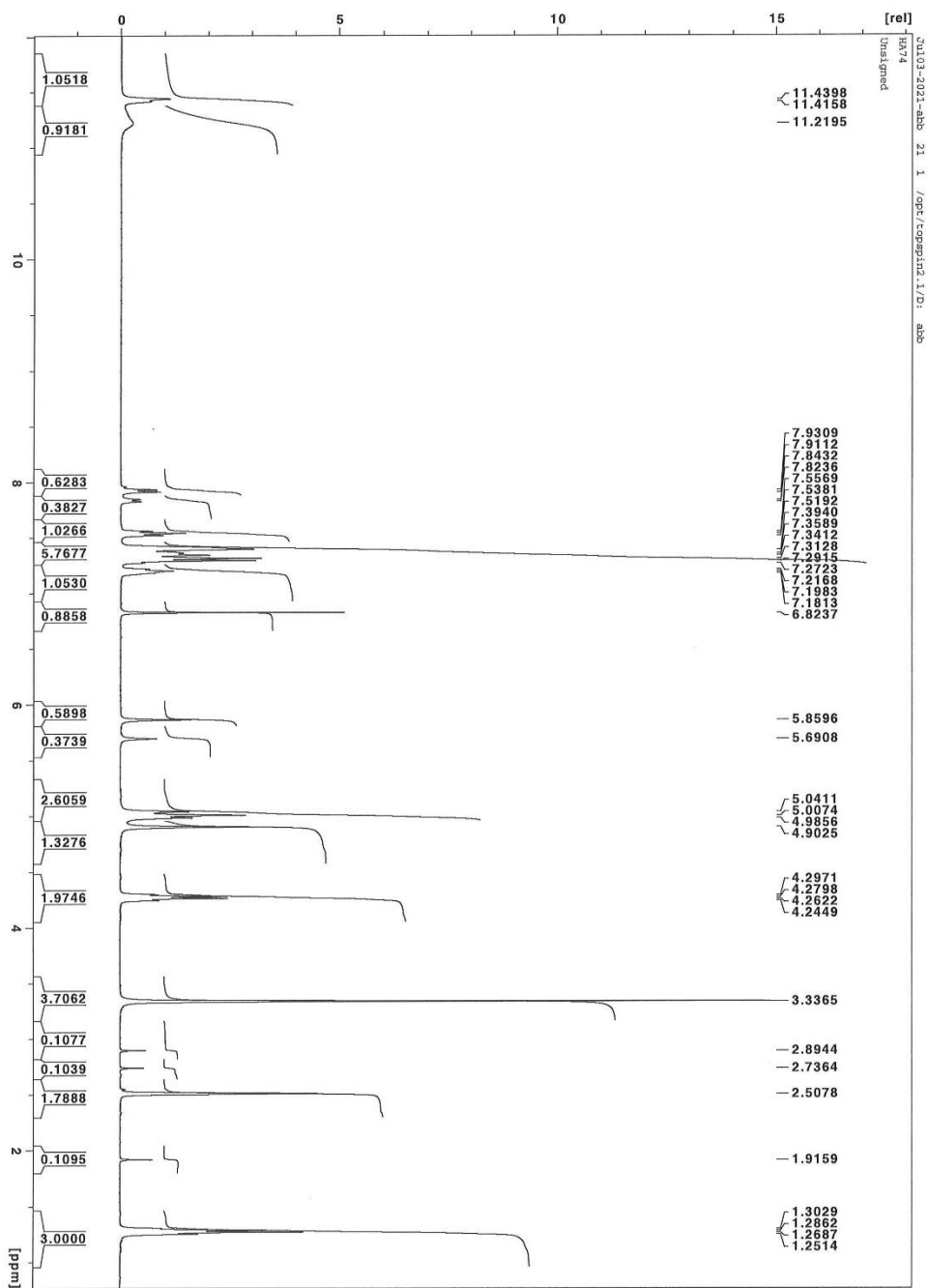
**Figure S203.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **7k**.



**Figure S204.**  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **7k**.

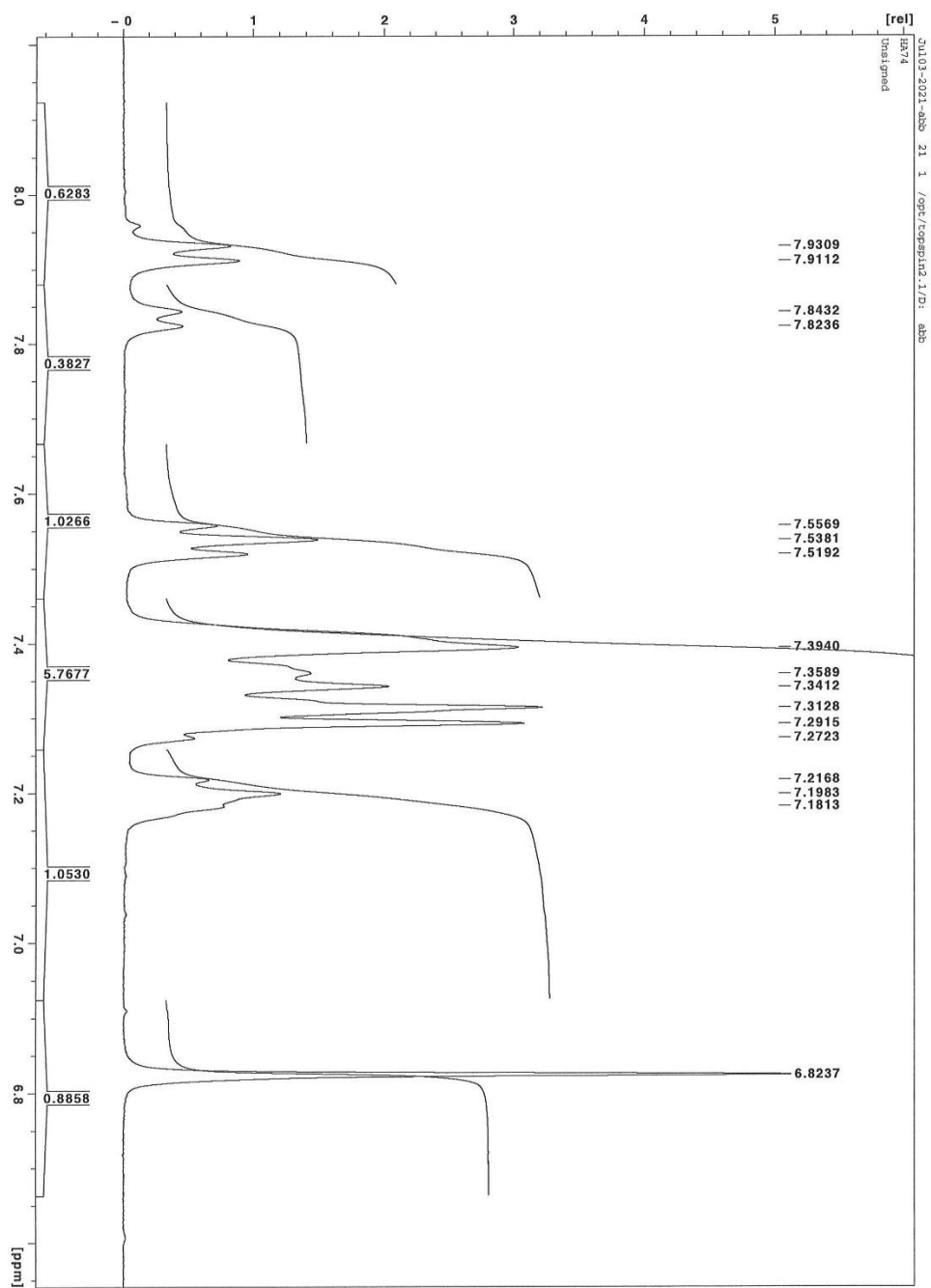


**Figure S205.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **7k**.

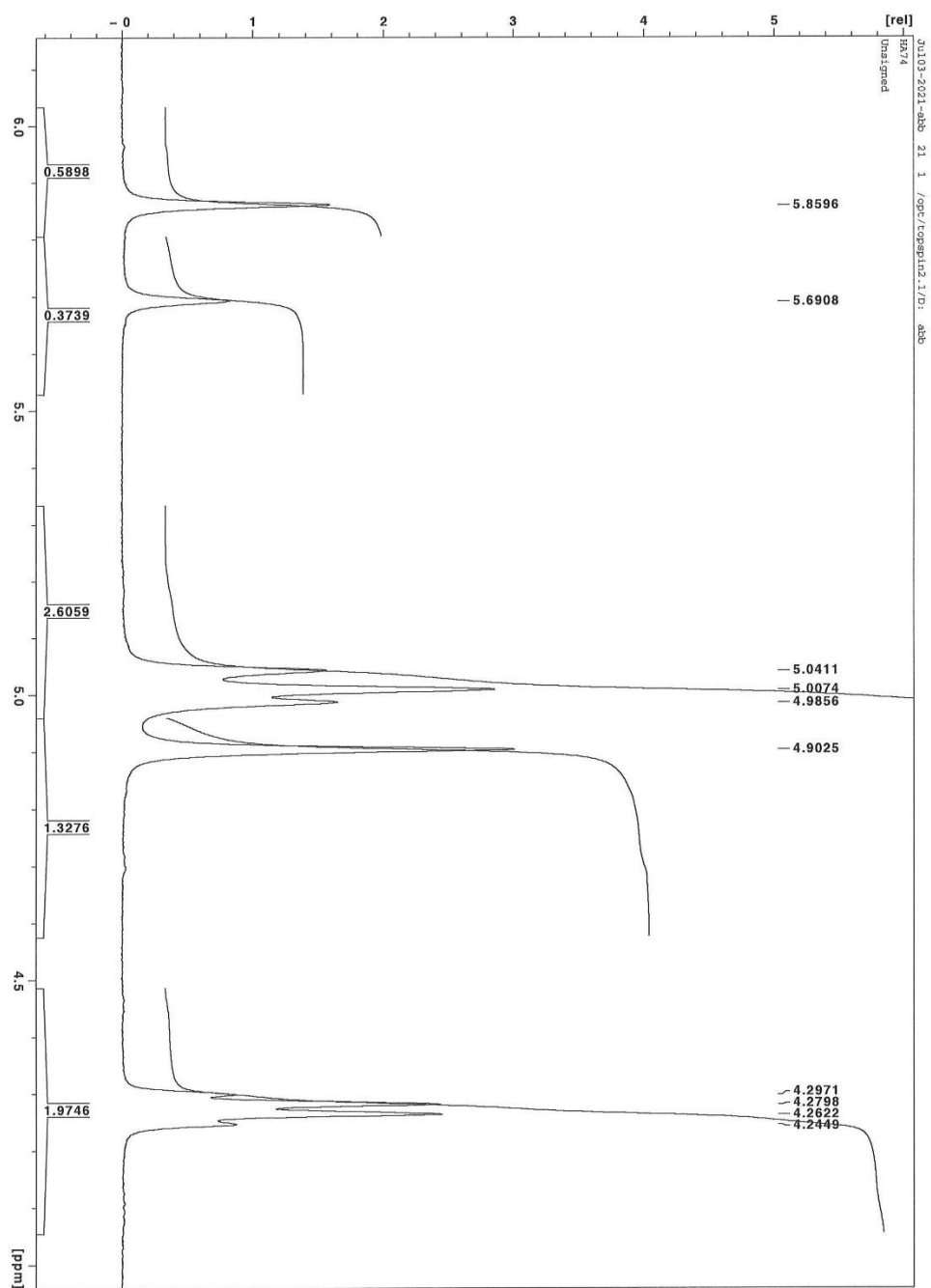


**Figure S206.**  $^1\text{H}$  NMR spectrum of compound **7I** (400 MHz,  $\text{DMSO}-d_6$ ).

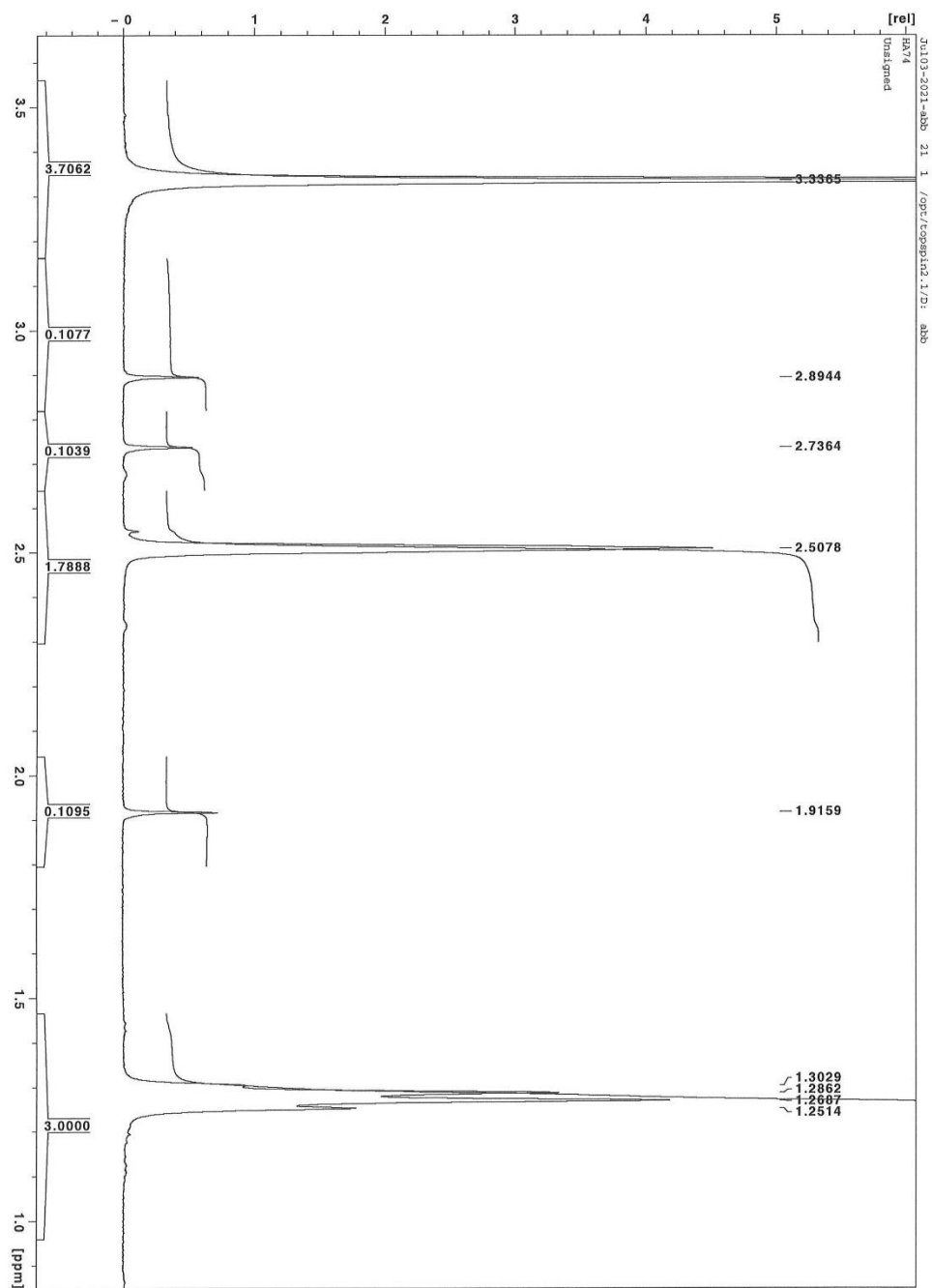




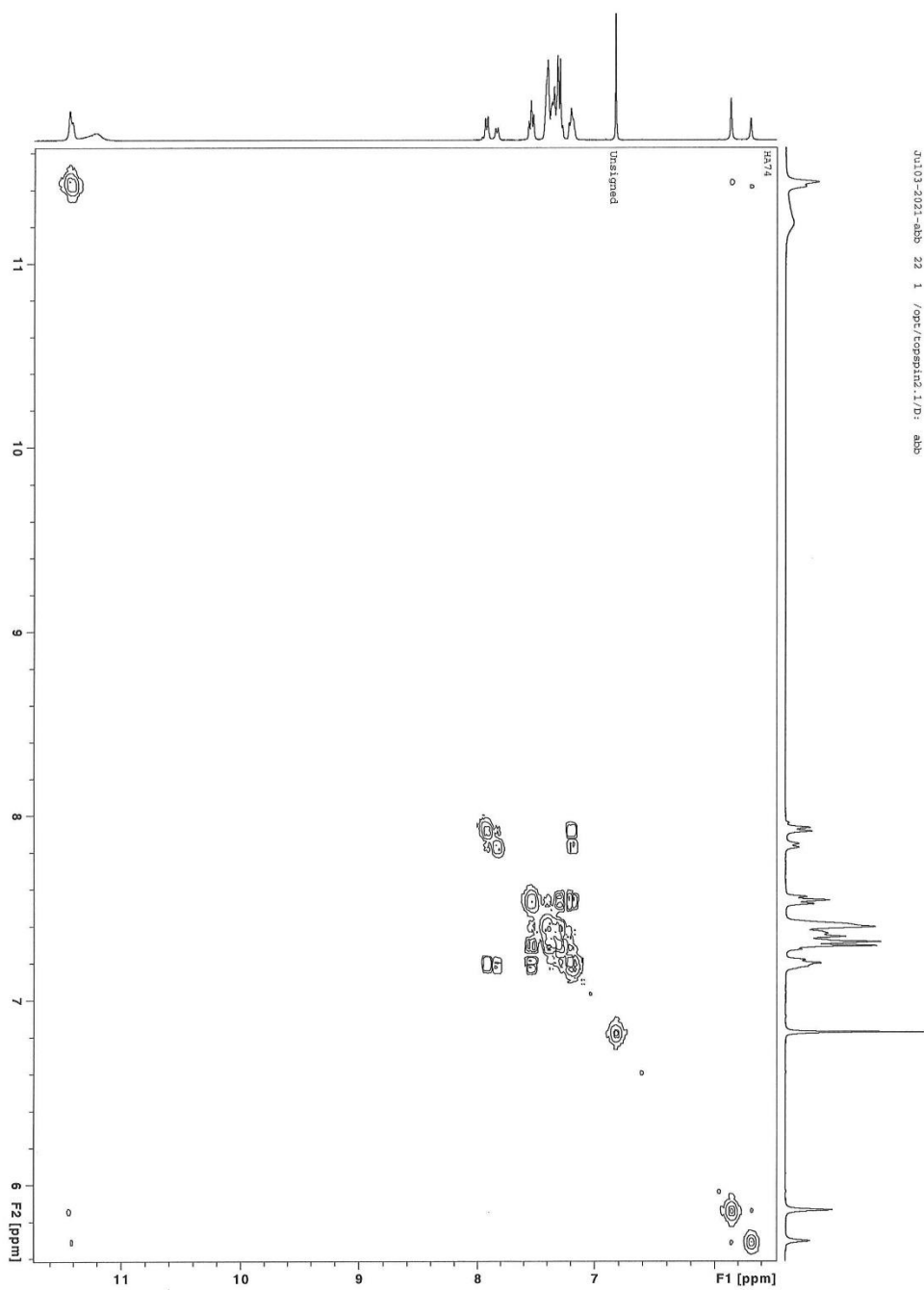
**Figure S208.** Detail of  $^1\text{H}$  NMR spectrum of compound **7l**.



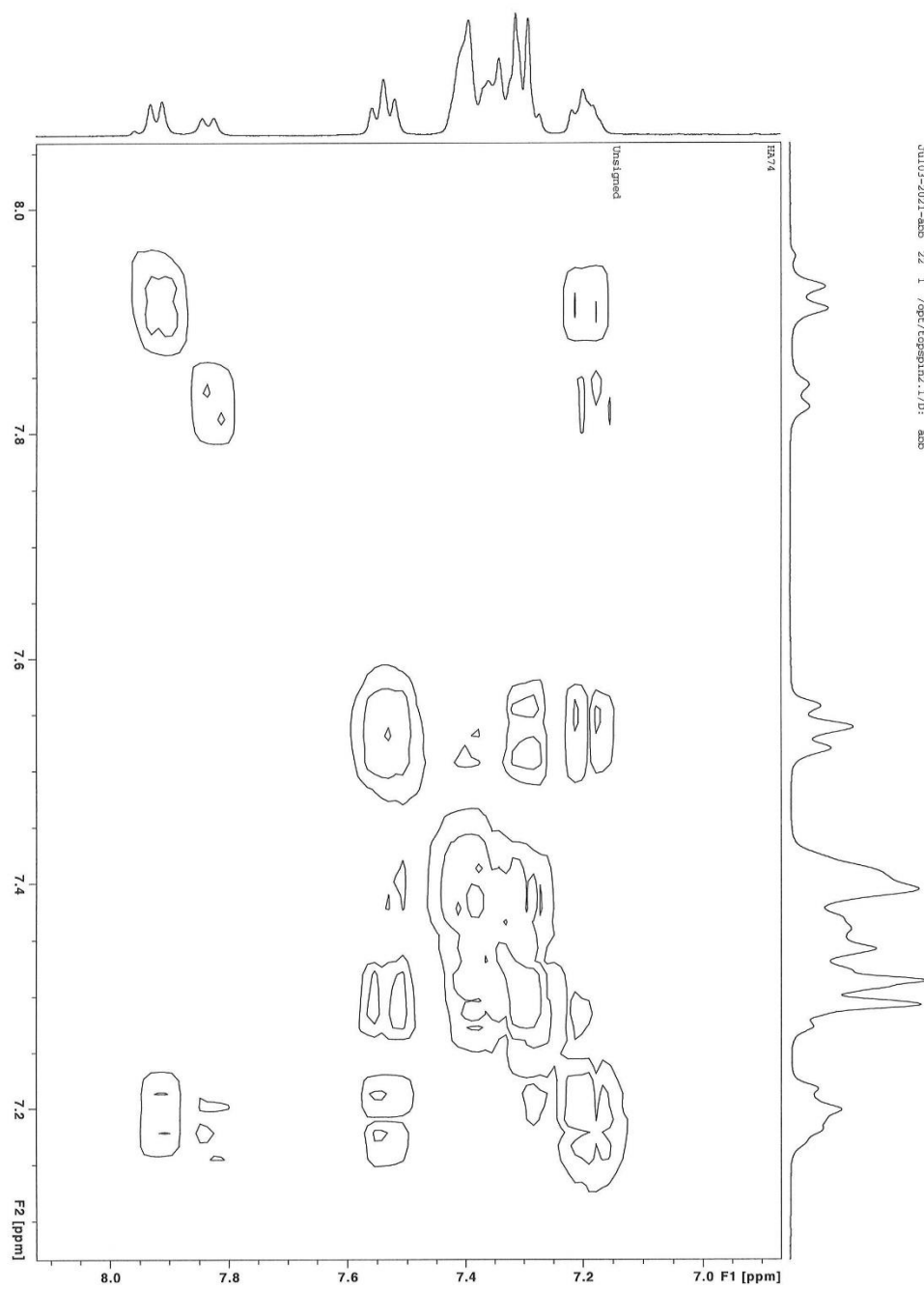
**Figure S209.** Detail of  $^1\text{H}$  NMR spectrum of compound **7l**.



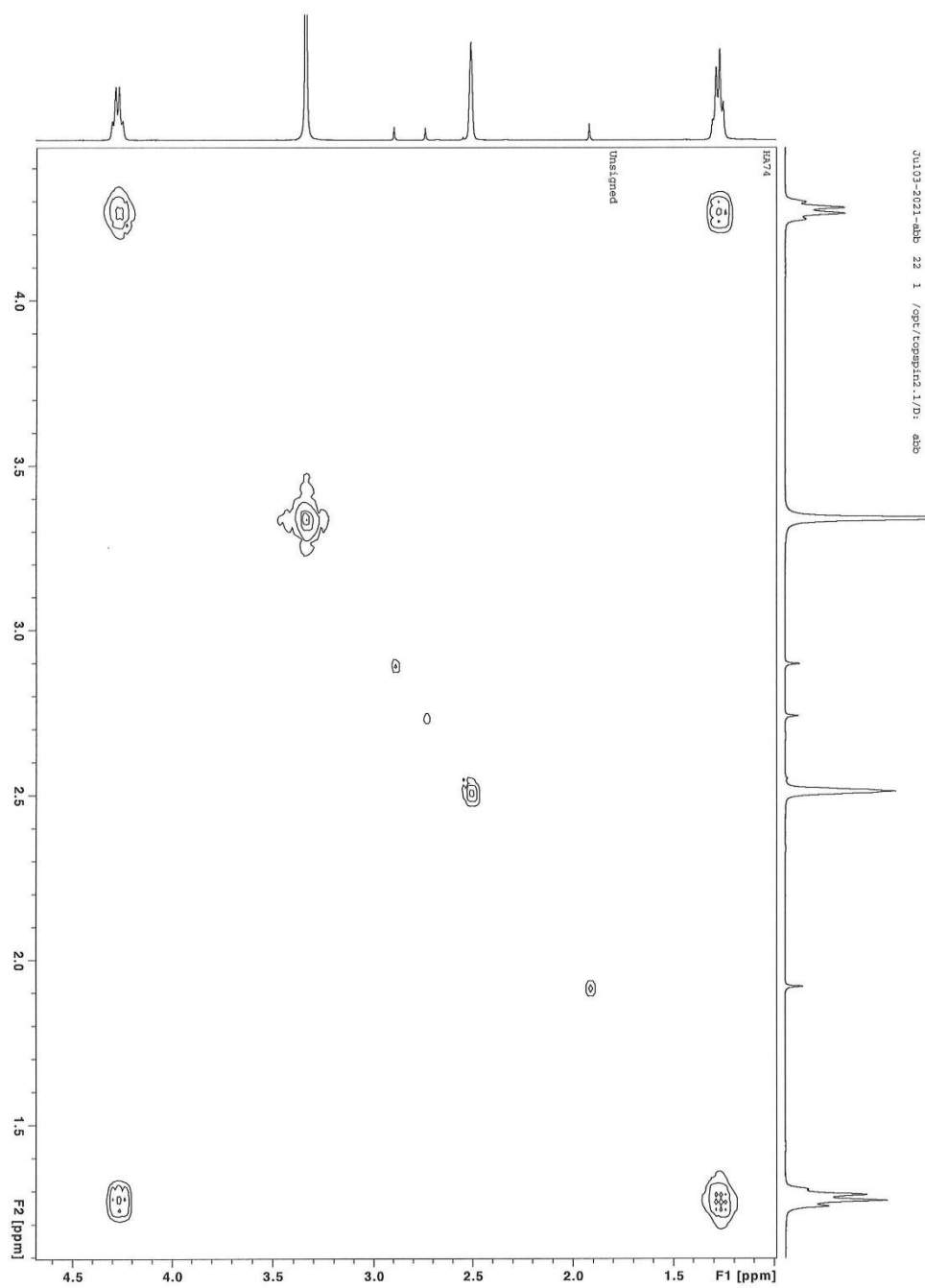
**Figure S210.** Detail of  $^1\text{H}$  NMR spectrum of compound **7l**.



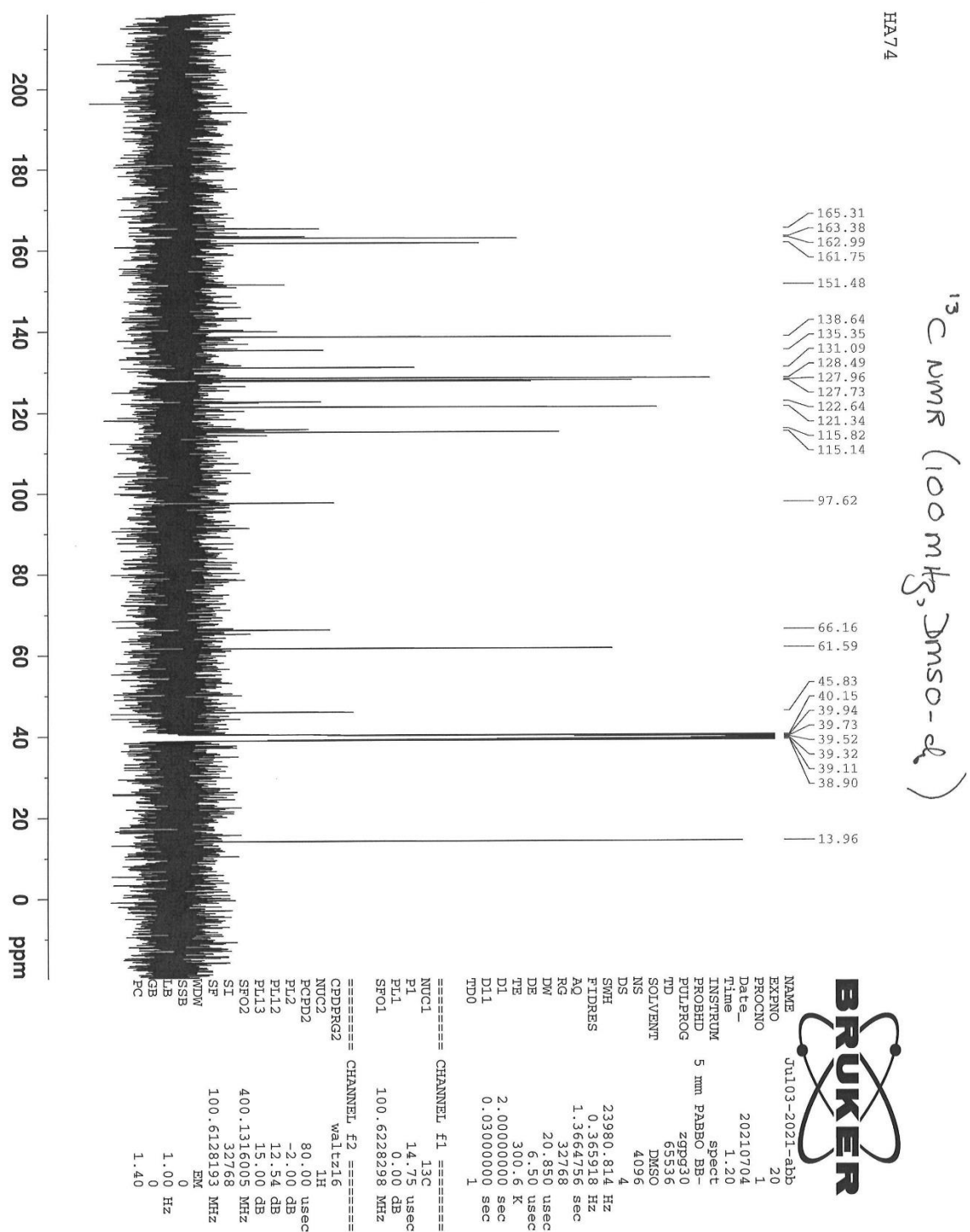
**Figure S211.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7l**.



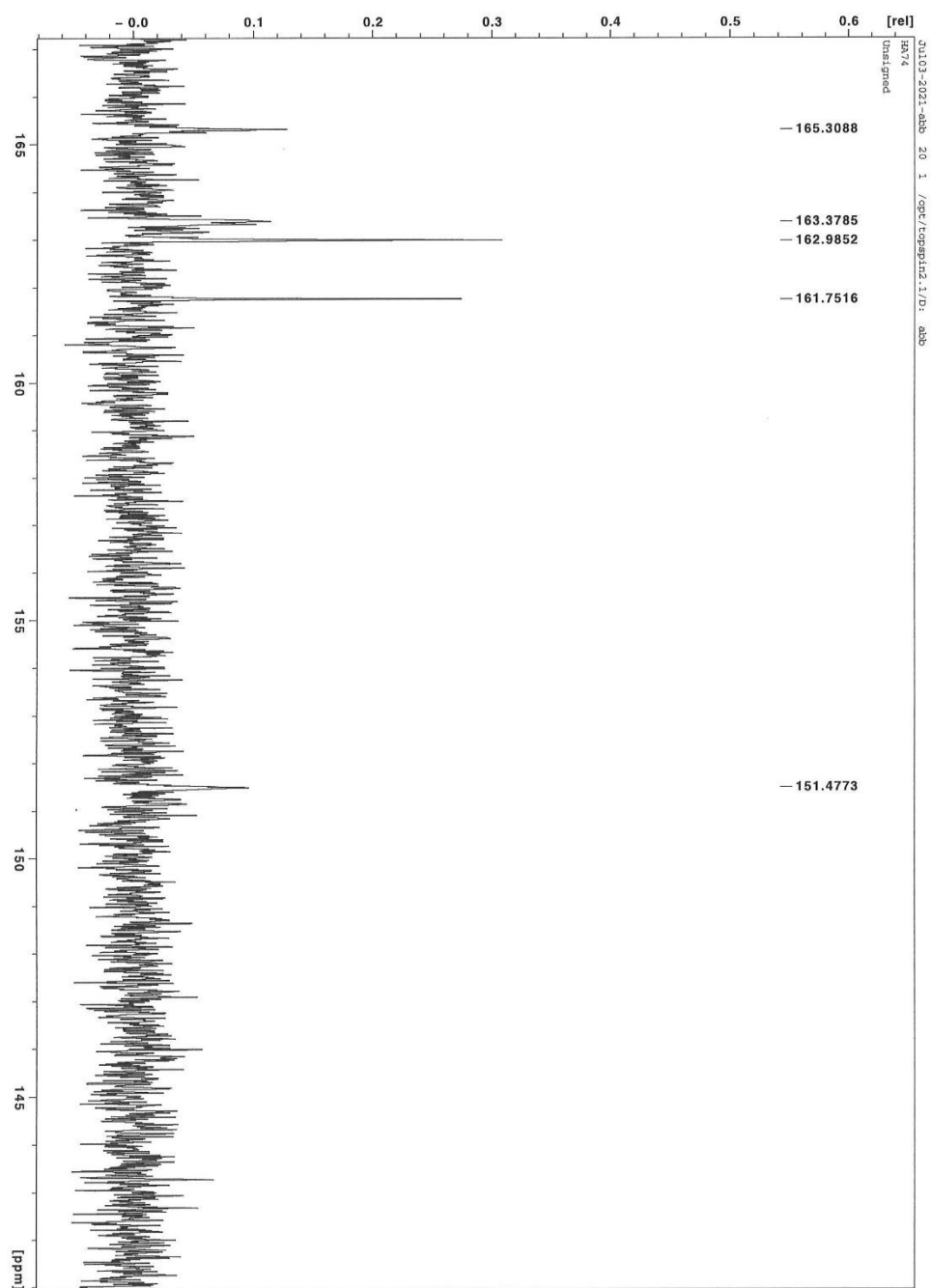
**Figure S212.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **7l**.



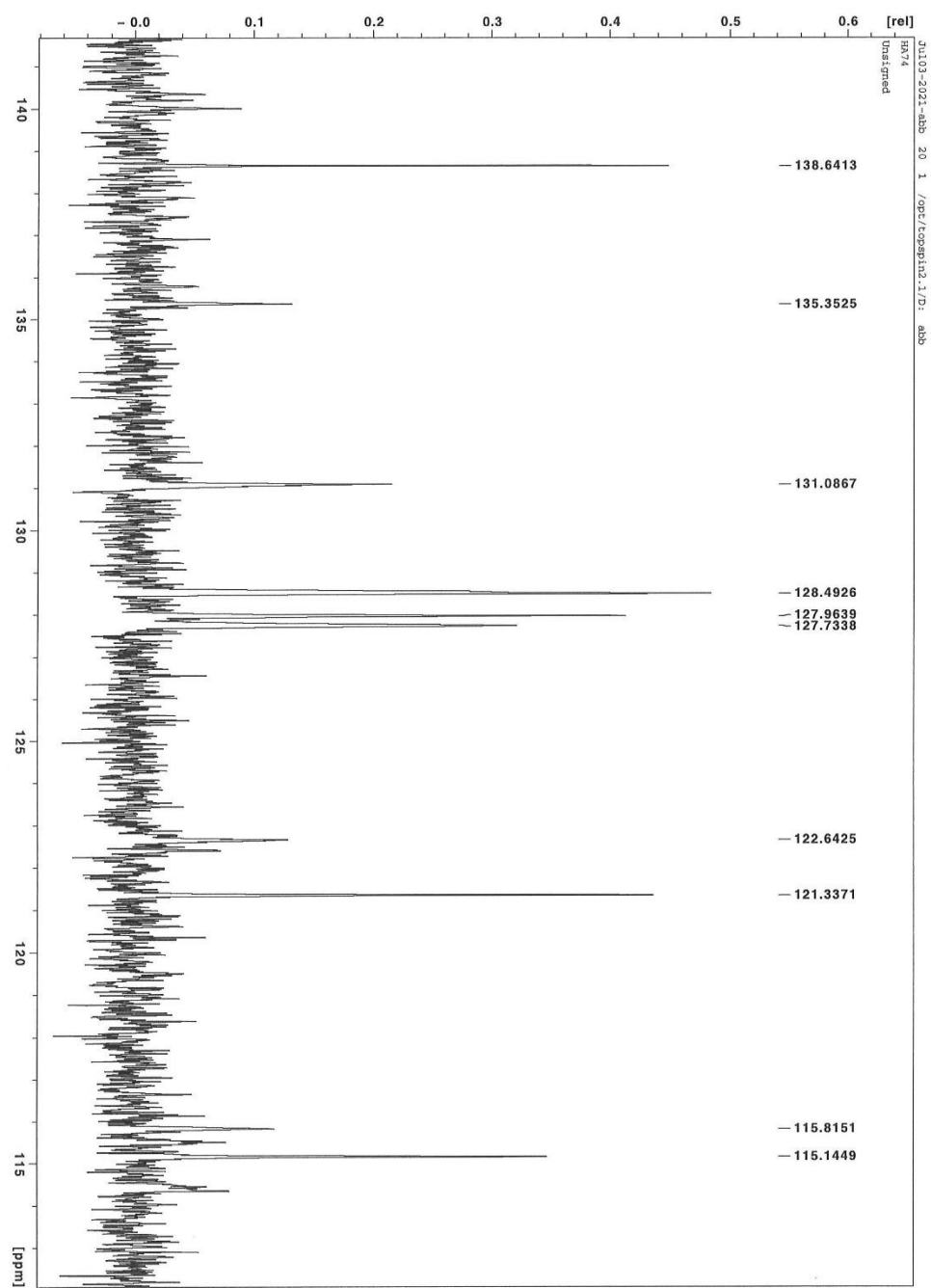
**Figure S213.** Detail of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **71**.



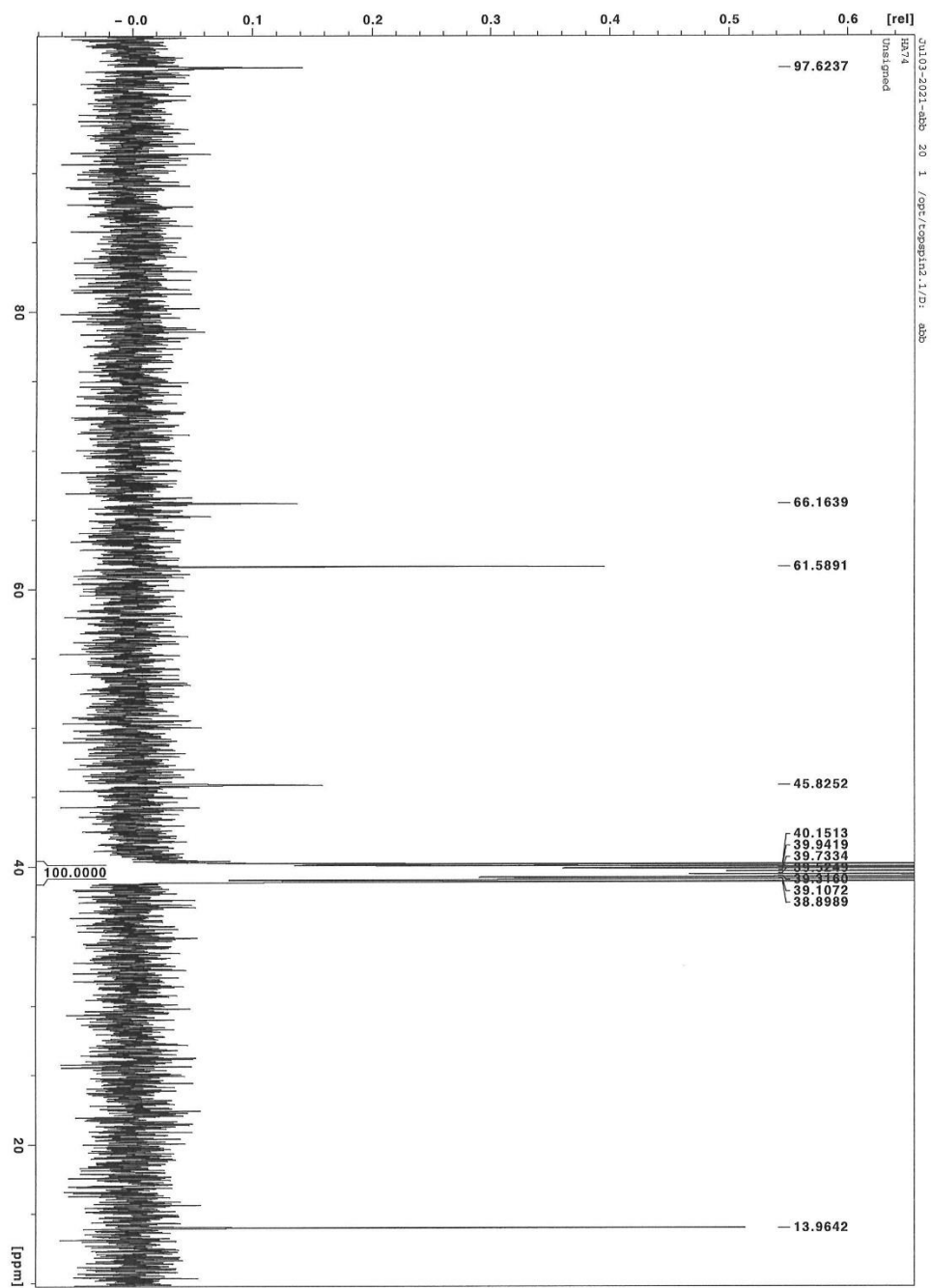
**Figure S214.** <sup>13</sup>C NMR spectrum of compound **71** (100 MHz, DMSO-d<sub>6</sub>)



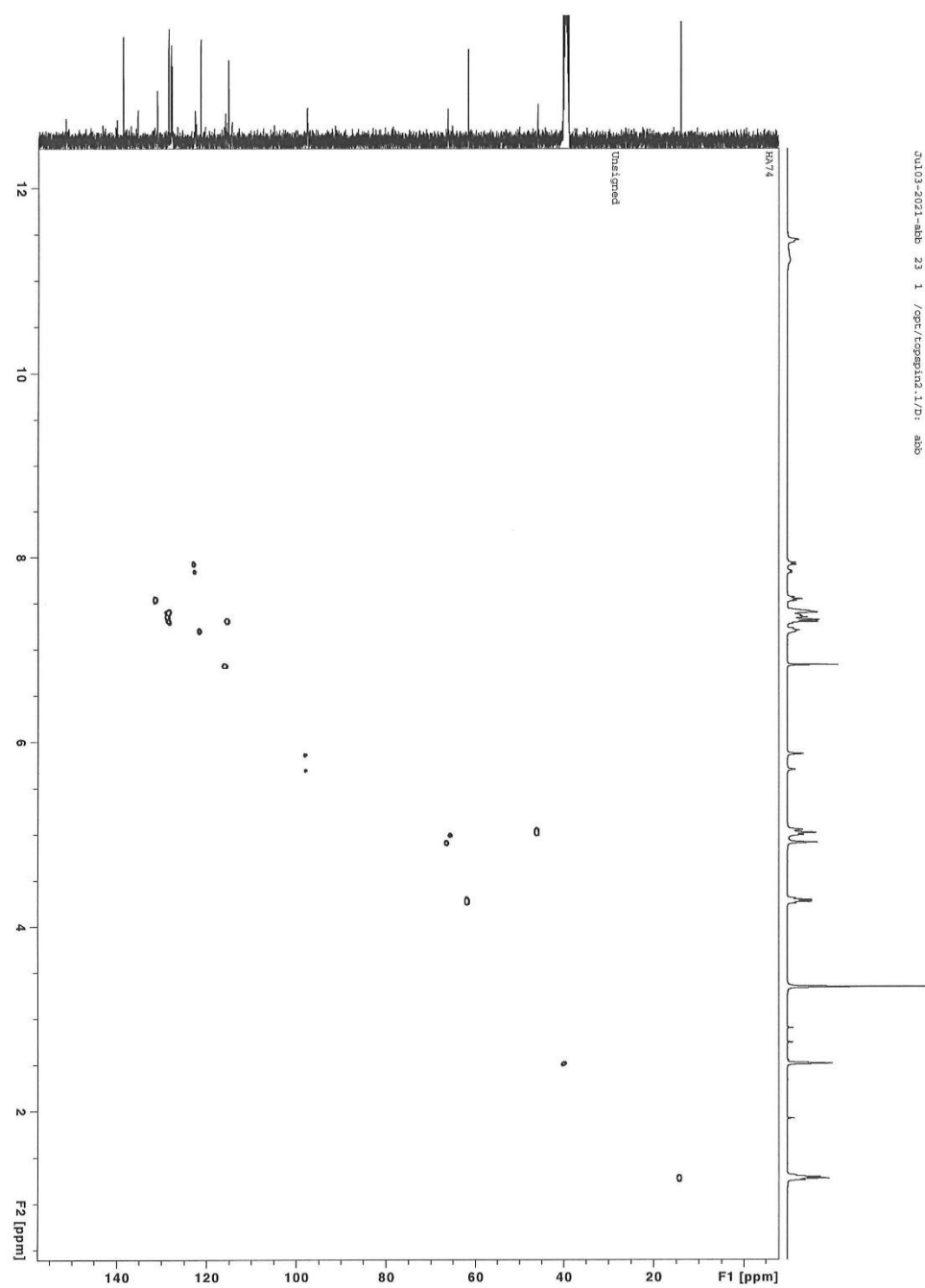
**Figure S215.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **7l**.



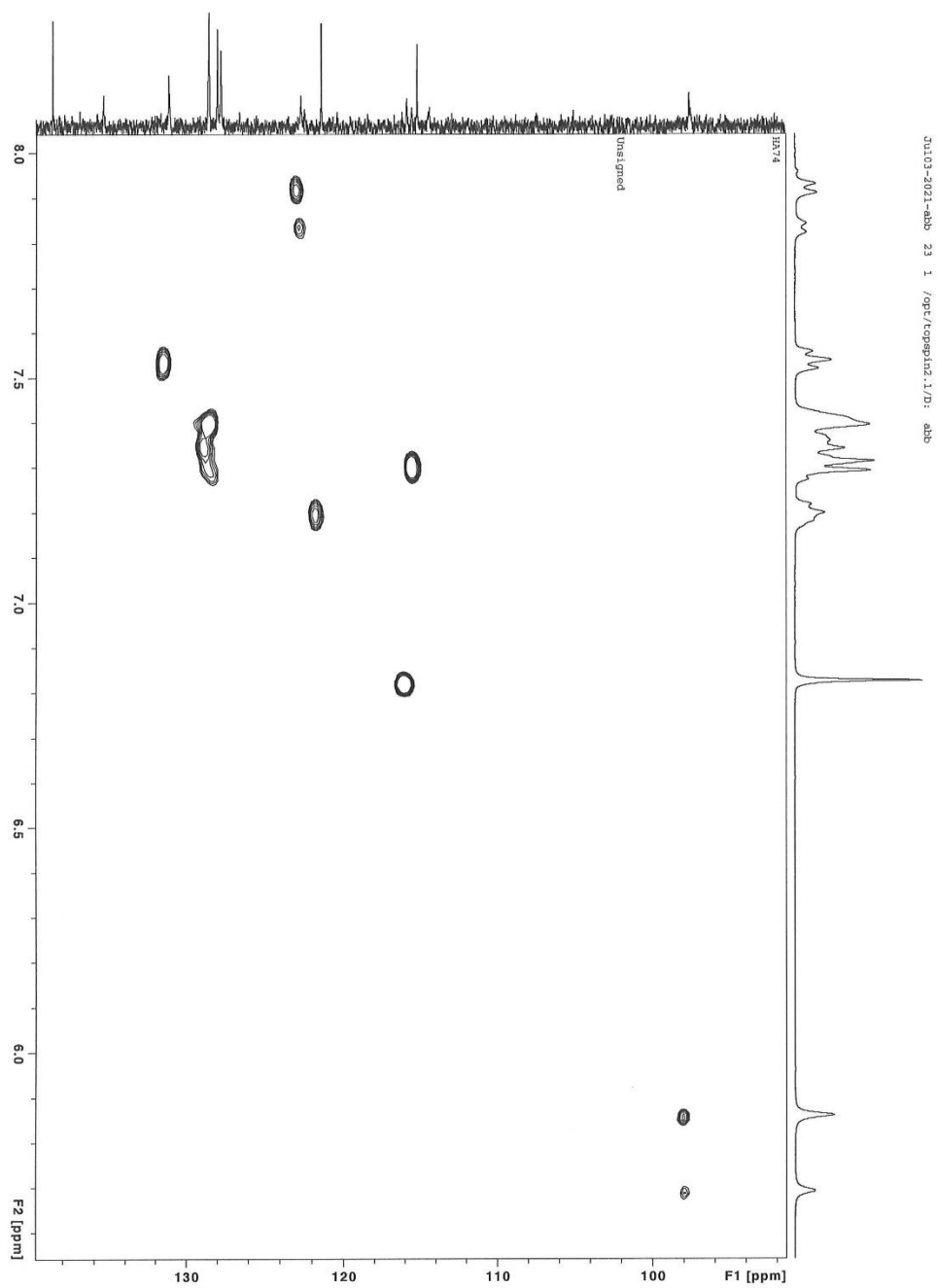
**Figure S216.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **7l**.



**Figure S217.** Detail of  $^{13}\text{C}$  NMR spectrum of compound **7l**.



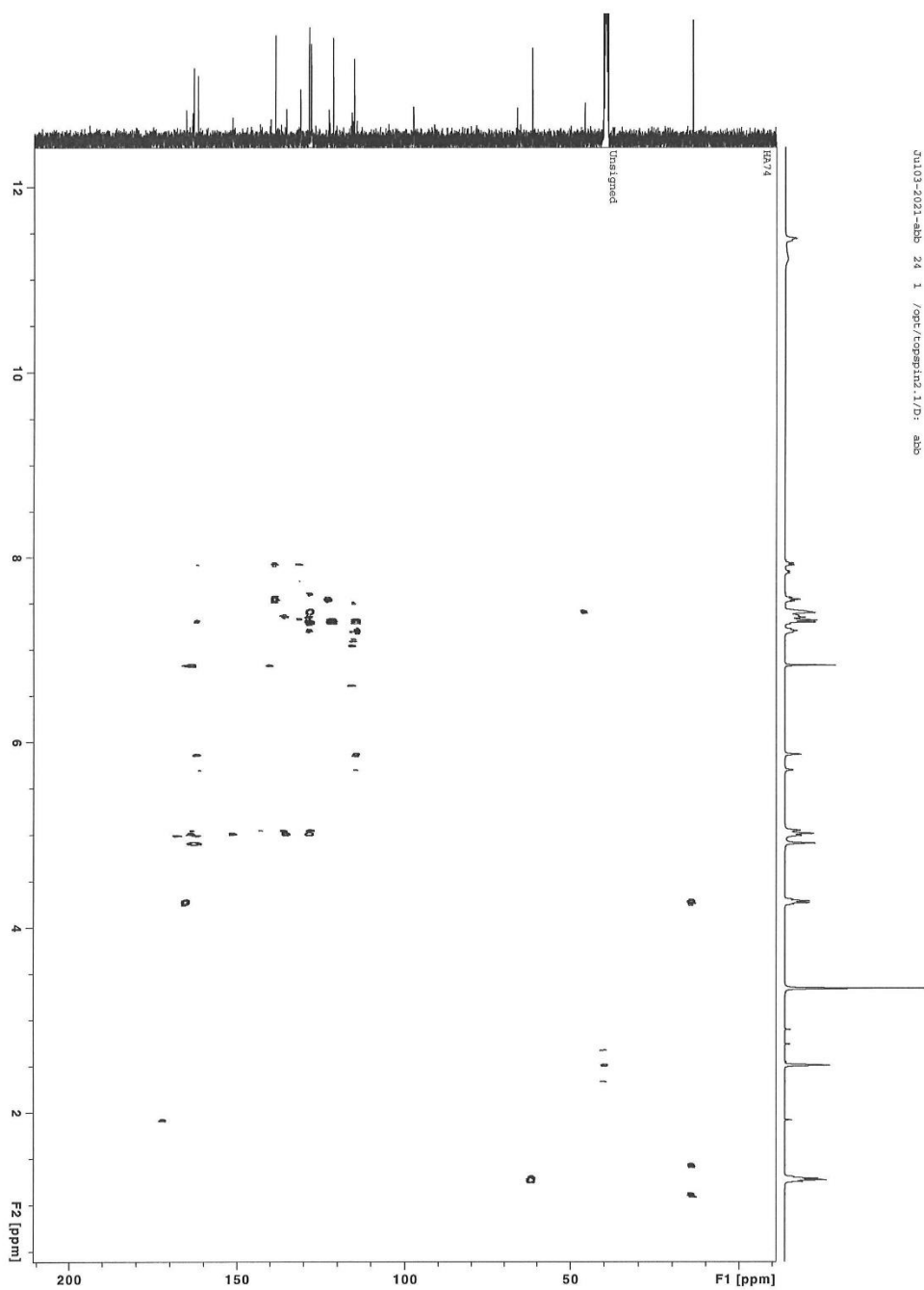
**Figure S218.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7l**.



**Figure S219.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **71**.

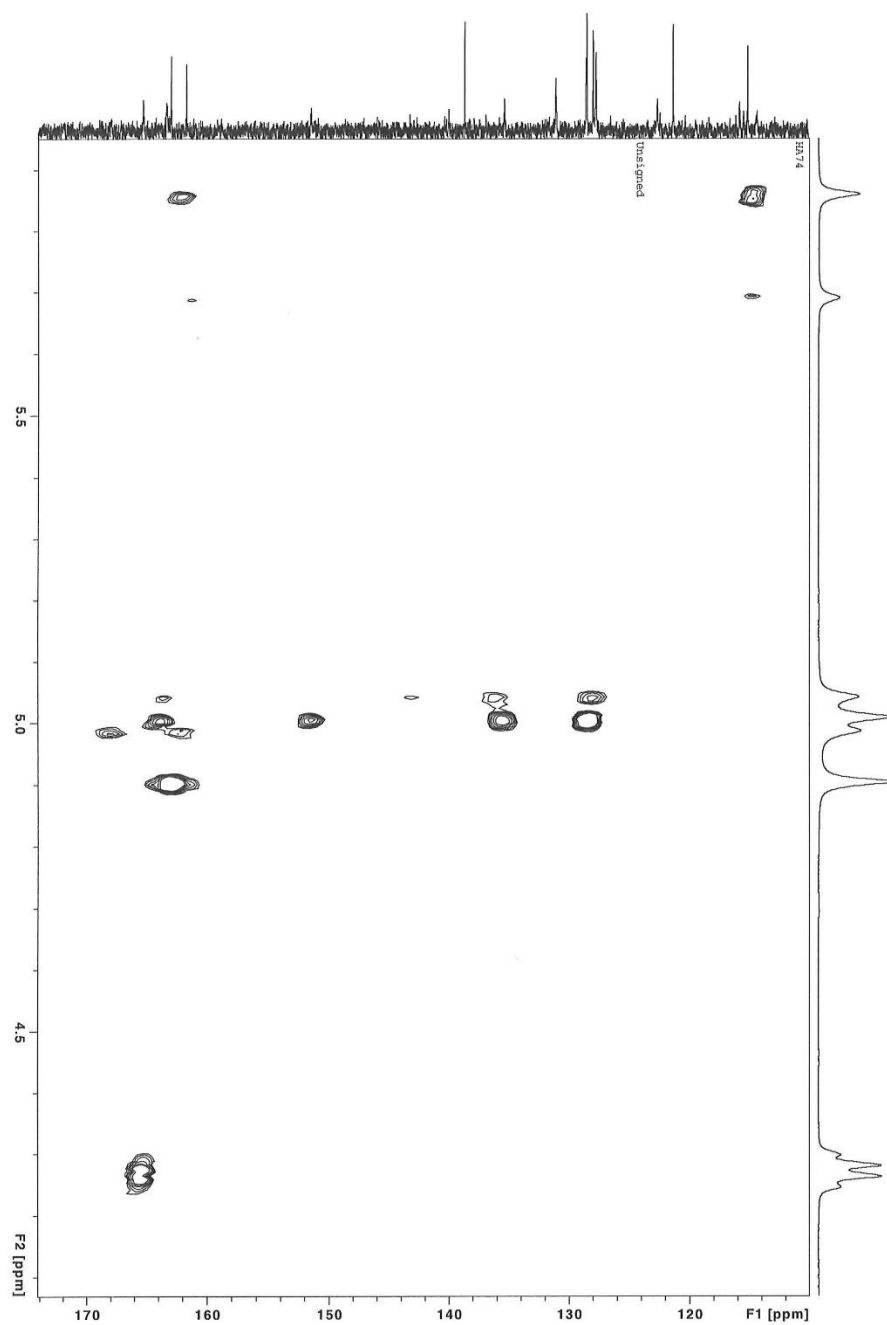


**Figure S220.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **7l**.

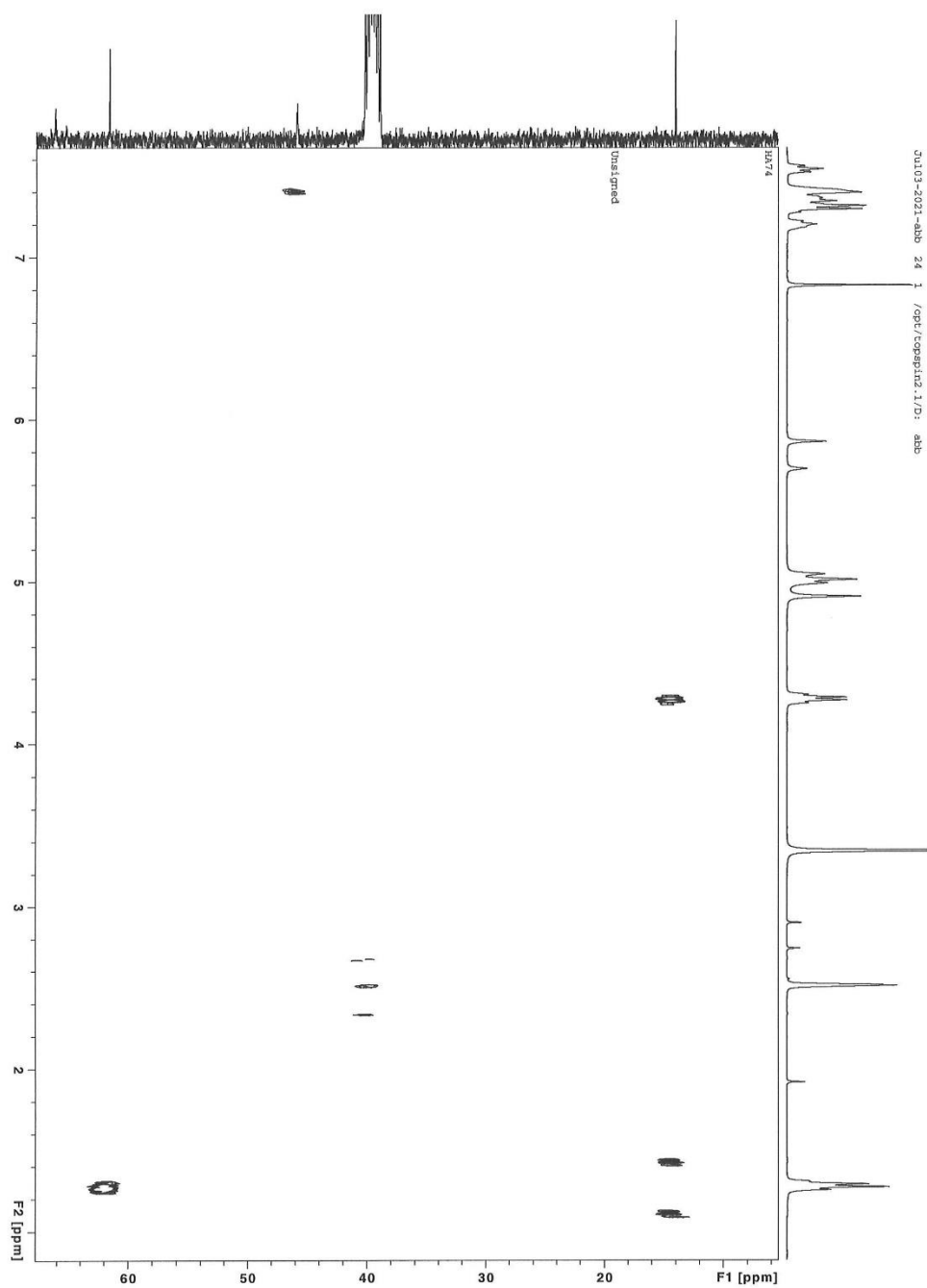


**Figure S221.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7l**.



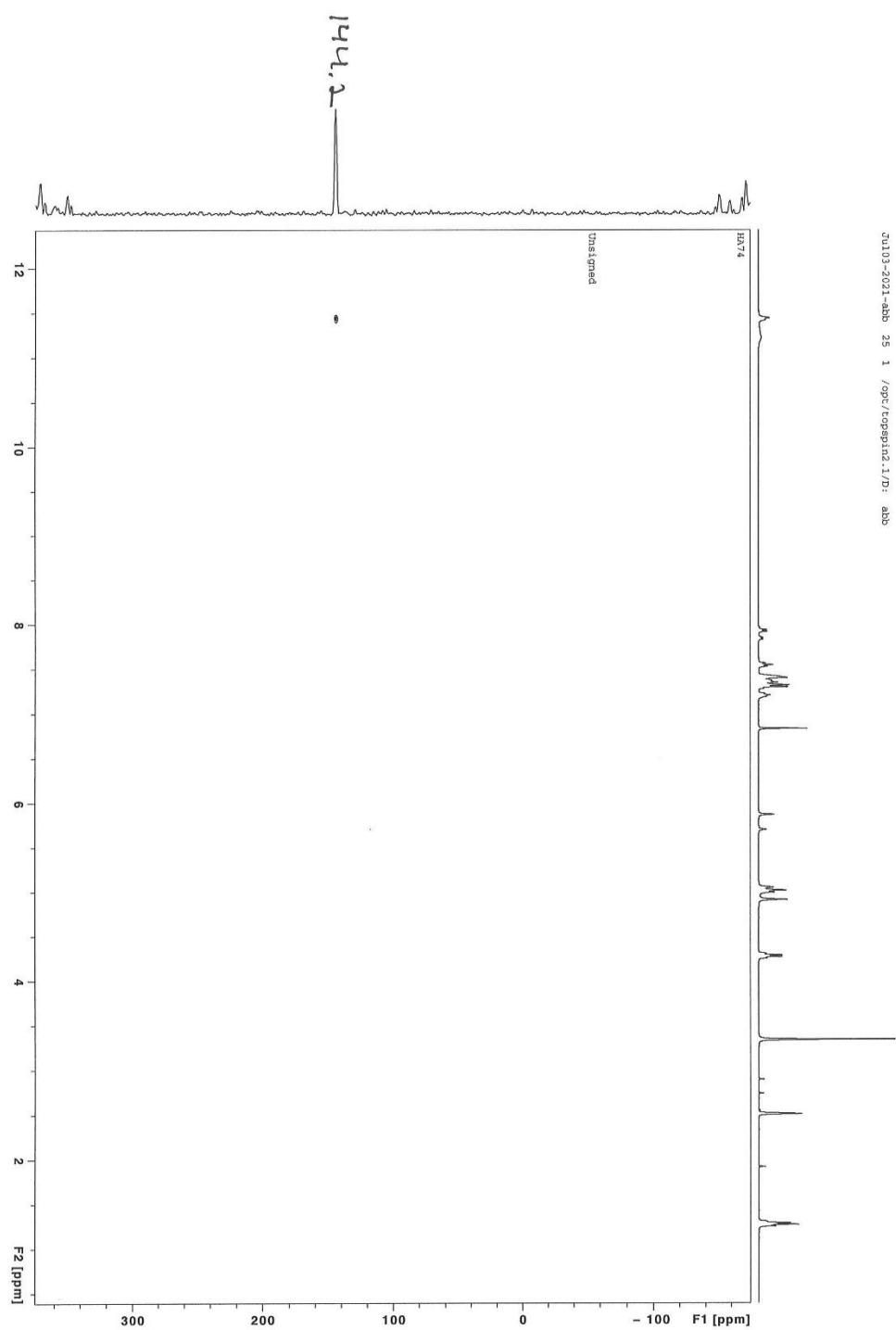


**Figure S223.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7l**.

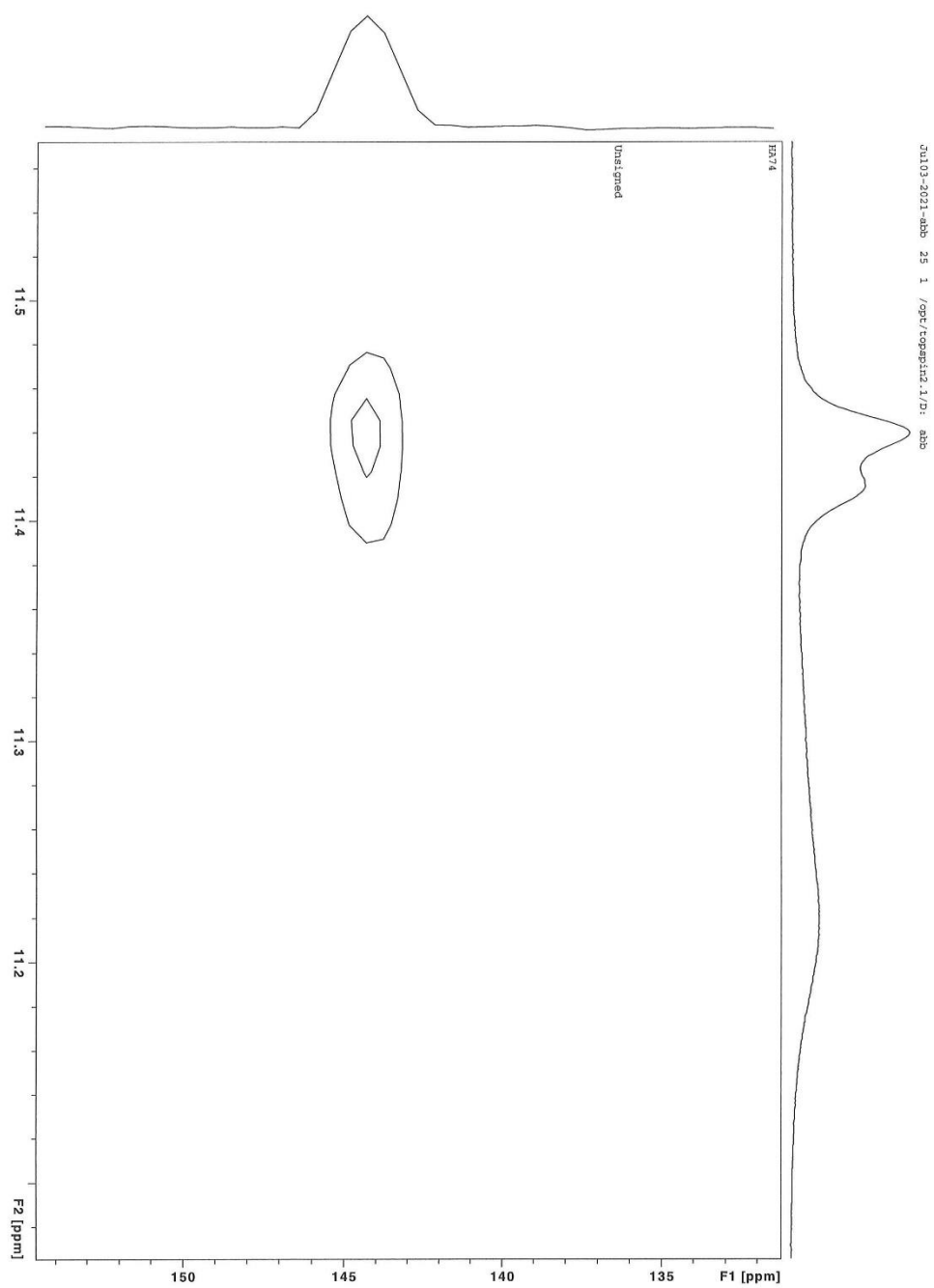


**Figure S224.** Detail of  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **7l**.

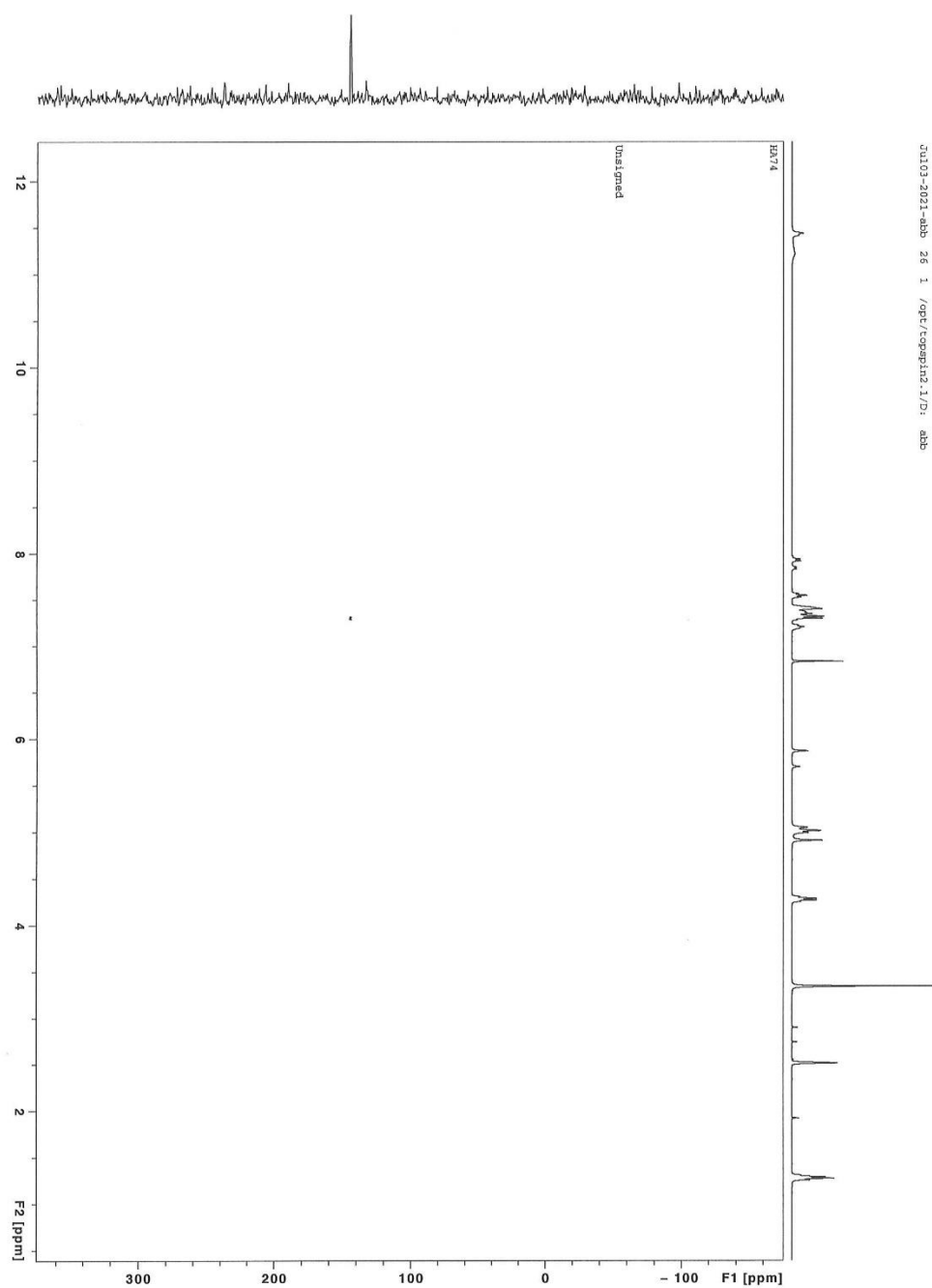
15-11-19



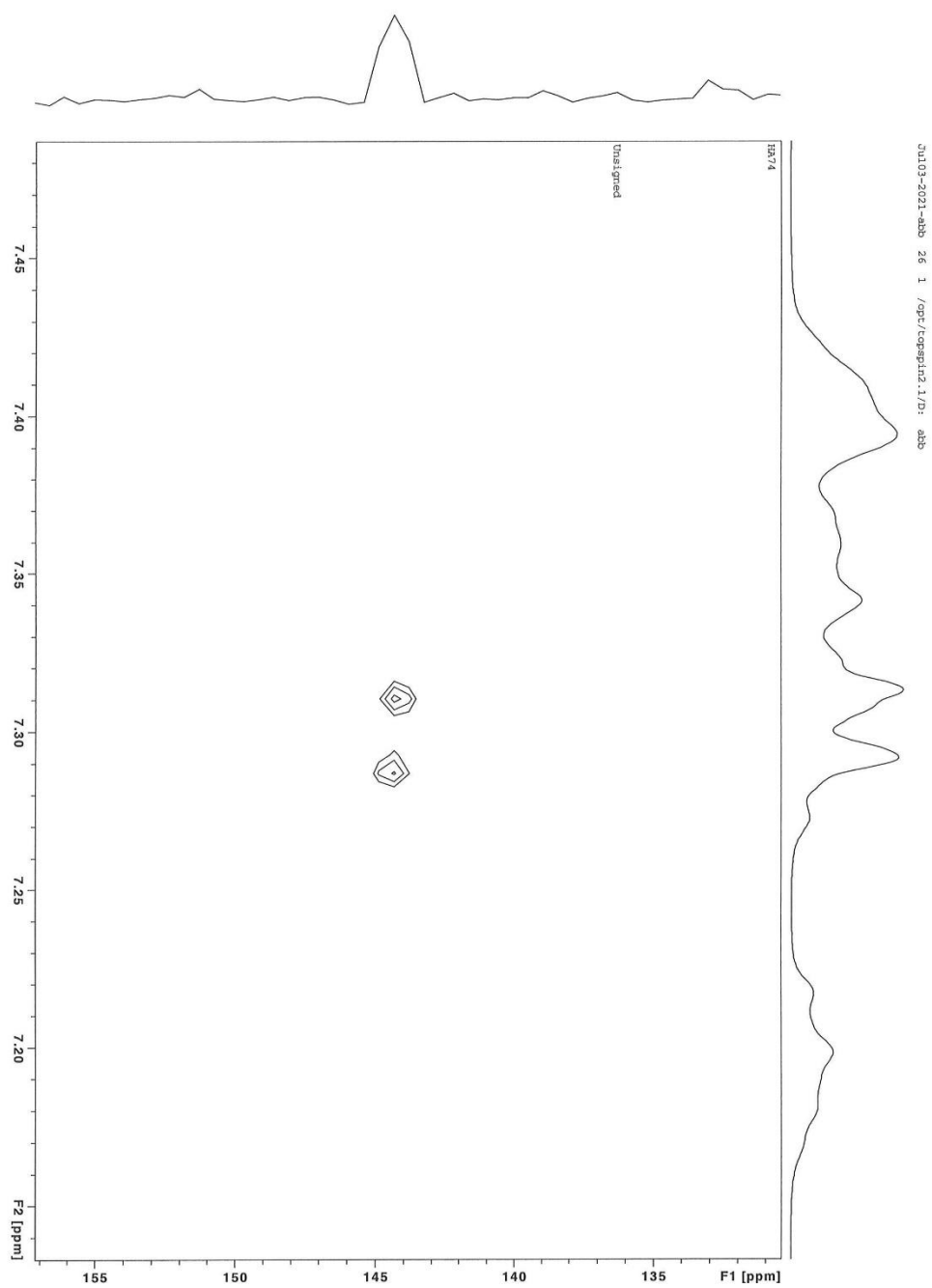
**Figure S225.**  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **7l**.



**Figure S226.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **7l**.



**Figure S227.**  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **7l**.



**Figure S228.** Detail of  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of compound **7l**.