

## SUPPORTING INFORMATION FOR

The potential of achiral sponge-derived and synthetic bromoindoles as selective cytotoxins against PANC-1 tumor cells

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	Page Number
<b>Figure S1.</b> <sup>1</sup> H NMR spectrum of <b>(2)</b> , (600 MHz, DMSO-d <sub>6</sub> )	3
<b>Figure S2.</b> <sup>13</sup> C NMR spectrum of <b>(2)</b> , (150 MHz, DMSO-d <sub>6</sub> )	4
<b>Figure S3.</b> gHSQC NMR spectrum of <b>(2)</b> , (600 MHz, DMSO-d <sub>6</sub> )	5
<b>Figure S4.</b> gHMBCAD NMR spectrum of <b>(2)</b> , (600 MHz, DMSO-d <sub>6</sub> )	6
<b>Figure S5.</b> <sup>1</sup> H spectrum of <b>(2a)</b> (600 MHz-DMSO-d <sub>6</sub> )	7
<b>Figure S6.</b> <sup>13</sup> C spectrum of <b>(2a)</b> (150 MHz)	8
<b>Figure S7.</b> <sup>1</sup> H spectrum of <b>(3)</b> (600 MHz, DMSO-d <sub>6</sub> )	9
<b>Figure S8.</b> <sup>13</sup> C spectrum of <b>(3)</b> (150 MHz, DMSO-d <sub>6</sub> )	10
<b>Figure S9.</b> Stacked <sup>1</sup> H NMR spectra of the natural product <b>(2)</b> and synthetic <b>2a</b> and <b>3</b> ; (600MHz, DMSO-d <sub>6</sub> )	11
<b>Figure S10.</b> Stacked <sup>13</sup> C NMR spectra of the natural product <b>(2)</b> and synthetic <b>2a</b> and <b>3</b> ; (150MHz, DMSO-d <sub>6</sub> )	12
<b>Figure S11.</b> <sup>1</sup> H spectrum of 5uL formic acid (600 MHz, DMSO-d <sub>6</sub> )	13
<b>Figure S12.</b> <sup>13</sup> C spectrum of 5uL formic acid (150 MHz)	14
<b>Figure S13.</b> <sup>1</sup> H spectrum of <b>(7)</b> (600 MHz, DMSO-d <sub>6</sub> )	15
<b>Figure S14.</b> <sup>13</sup> C spectrum of <b>(7)</b> (150 MHz, DMSO-d <sub>6</sub> )	16
<b>Figure S15.</b> <sup>1</sup> H spectrum of 6-bromo-1H-indol-3-carbonyl cyanide <b>(9)</b> in (600 MHz, DMSO-d <sub>6</sub> ).	17
<b>Figure S16.</b> <sup>13</sup> C spectrum of 6-bromo-1H-indol-3-carbonyl cyanide <b>(9)</b> in (150 MHz, DMSO-d <sub>6</sub> ).	18
<b>Figure S17.</b> <sup>1</sup> H spectrum of <b>(10)</b> (600 MHz, DMSO-d <sub>6</sub> )	19
<b>Figure S18.</b> <sup>13</sup> C spectrum of <b>(10)</b> (150 MHz, DMSO-d <sub>6</sub> )	20
<b>Figure S19.</b> <sup>1</sup> H spectrum of <b>(11)</b> (500 MHz, DMSO-d <sub>6</sub> )	21
<b>Figure S20.</b> <sup>13</sup> C spectrum of <b>(11)</b> (125 MHz, DMSO-d <sub>6</sub> )	22
<b>Figure S21.</b> <sup>1</sup> H spectrum of <b>(12)</b> (500 MHz, DMSO-d <sub>6</sub> )	23
<b>Figure S22.</b> <sup>13</sup> C spectrum of <b>(12)</b> (125 MHz, DMSO-d <sub>6</sub> )	24
<b>Figure S23.</b> <sup>1</sup> H spectrum of <b>(13)</b> (600 MHz, DMSO-d <sub>6</sub> )	25
<b>Figure S24.</b> <sup>13</sup> C spectrum of <b>(13)</b> (150 MHz, DMSO-d <sub>6</sub> )	26
<b>Figure S25.</b> <sup>1</sup> H spectrum of <b>(14)</b> (600 MHz, DMSO-d <sub>6</sub> )	27
<b>Figure S26.</b> gHMBCAD spectrum of <b>(14)</b> (600 MHz, DMSO-d <sub>6</sub> )	28
<b>Figure S27.</b> gHMBCAD spectrum expansion of <b>(14)</b> (600 MHz, DMSI-d <sub>6</sub> )	29
<b>Figure S28.</b> <sup>1</sup> H spectrum of <b>(15)</b> (600 MHz, DMSO-d <sub>6</sub> )	30
<b>Figure S29.</b> gHMBCAD spectrum of <b>(15)</b> (600 MHz, DMSO-d <sub>6</sub> )	31
<b>Figure S30.</b> gHMBCAD spectrum expansion of <b>(15)</b> (600 MHz, DMSI-d <sub>6</sub> )	32
<b>Figure S31.</b> <sup>1</sup> H spectrum of <b>(16)</b> (600 MHz, DMSO-d <sub>6</sub> )	33
<b>Figure S32.</b> gHMBCAD spectrum of <b>(16)</b> (600 MHz, DMSO-d <sub>6</sub> )	34
<b>Figure S33.</b> gHMBCAD spectrum expansion of <b>(16)</b> (600 MHz, DMSI-d <sub>6</sub> )	35

<b>Figure S34.</b> $^1\text{H}$ spectrum (600 MHz) of 6-bromo-1H-indol-3-yl-carboxaldehyde ( <b>5</b> ) in DMSO-d <sub>6</sub> .	36
<b>Figure S35.</b> $^1\text{H}$ spectrum expansion (600 MHz) of 6-bromo-1H-indol-3-yl-carboxaldehyde ( <b>5</b> ) in DMSO-d <sub>6</sub> .	37
<b>Figure S36.</b> $^{13}\text{C}$ spectrum (150 MHz) of 6-bromo-1H-indol-3-yl-carboxaldehyde ( <b>5</b> ) in DMSO-d <sub>6</sub> .	38
<b>Figure S37.</b> gHSQCAD spectrum (600 MHz) of ( <b>5</b> ) in DMSO-d <sub>6</sub> .	39
<b>Figure S38.</b> NOESY spectrum (600 MHz, 600ms mixing time) of ( <b>5</b> ) in DMSO-d <sub>6</sub> .	40

Figure S1.  $^1\text{H}$  NMR spectrum (600 MHz) of 6-Br-8-keto-conicamin A (**2**) in DMSO- $d_6$ .

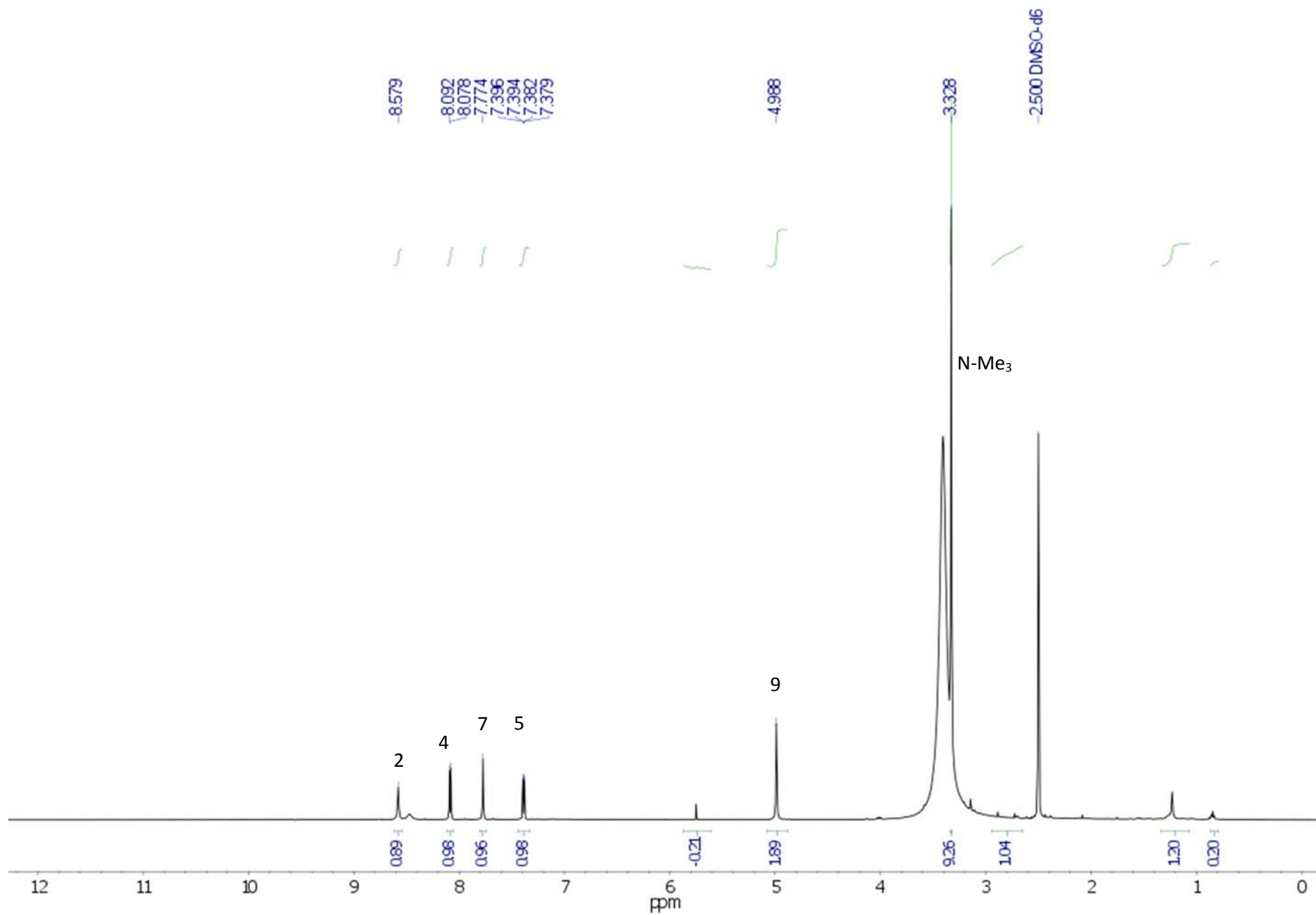


Figure S2.  $^{13}\text{C}$  NMR spectrum (150 MHz) of in DMSO-d<sub>6</sub>.

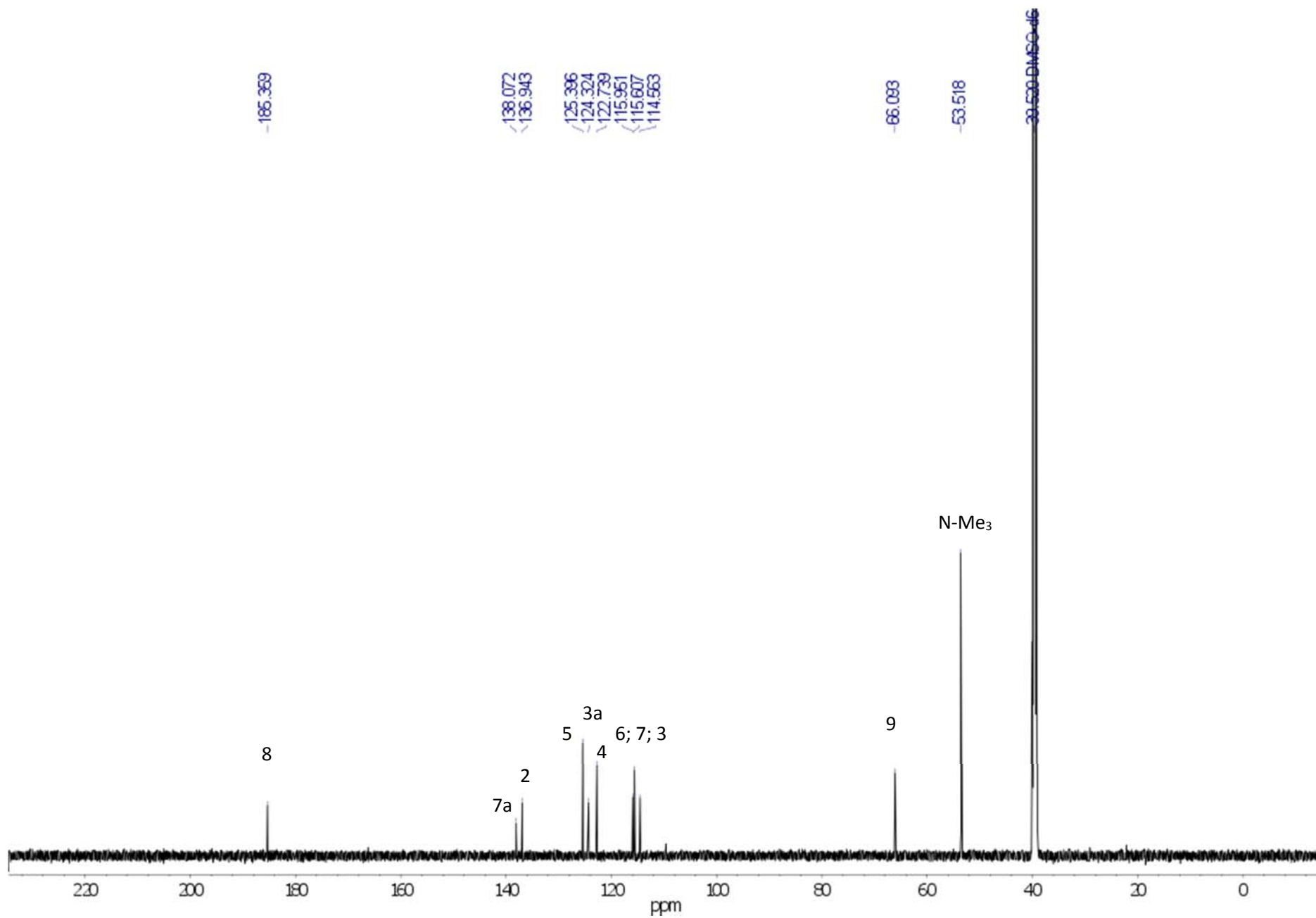


Figure S3. gHSQCAD spectrum (600MHz) of 6-Br-8-keto-conicamin A (**2**) in DMSO-d6.

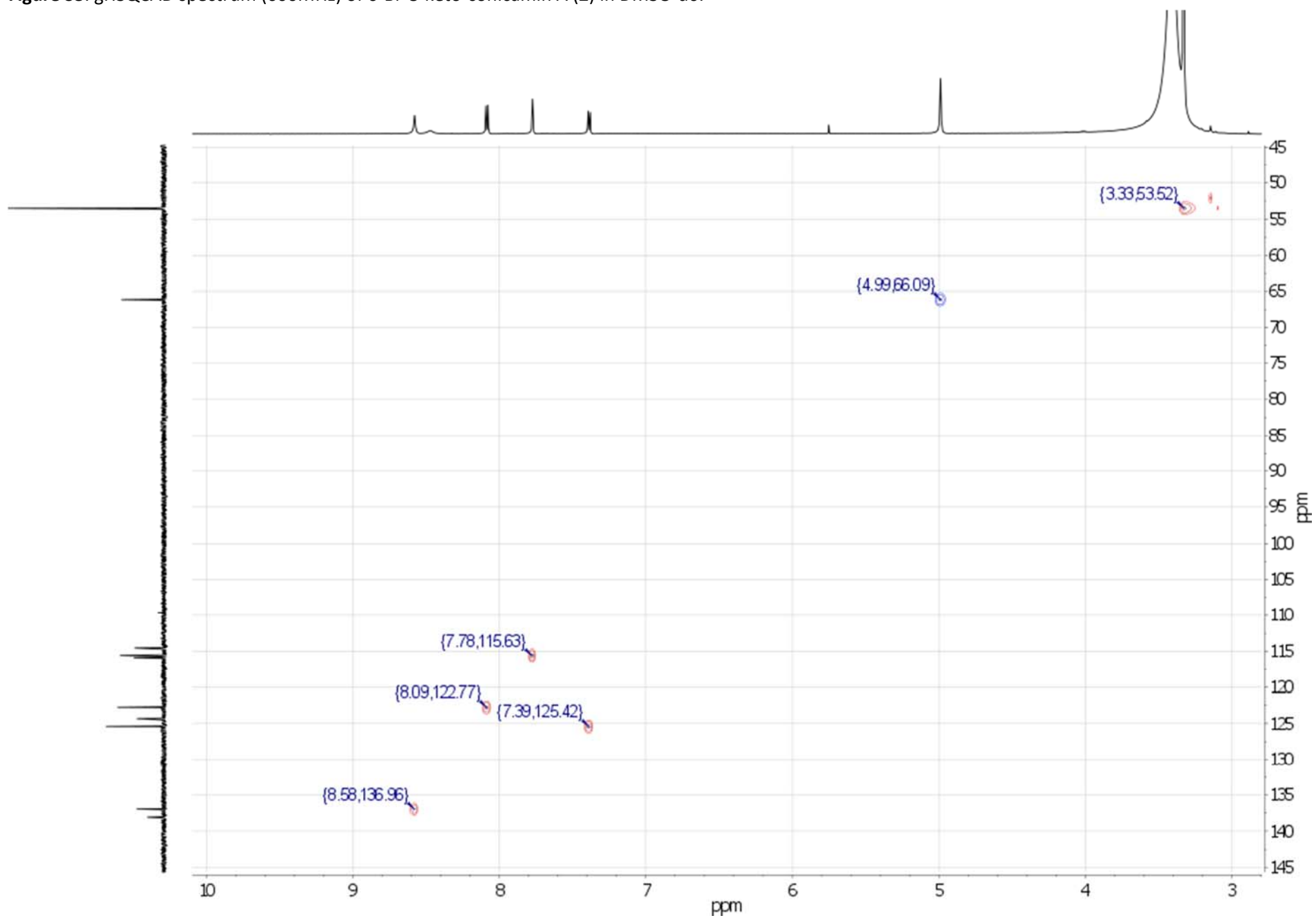


Figure S4. gHMBCAD spectrum (600MHz) of 6-Br-8-keto-conicamin A (**2**) in DMSO-d<sub>6</sub>.

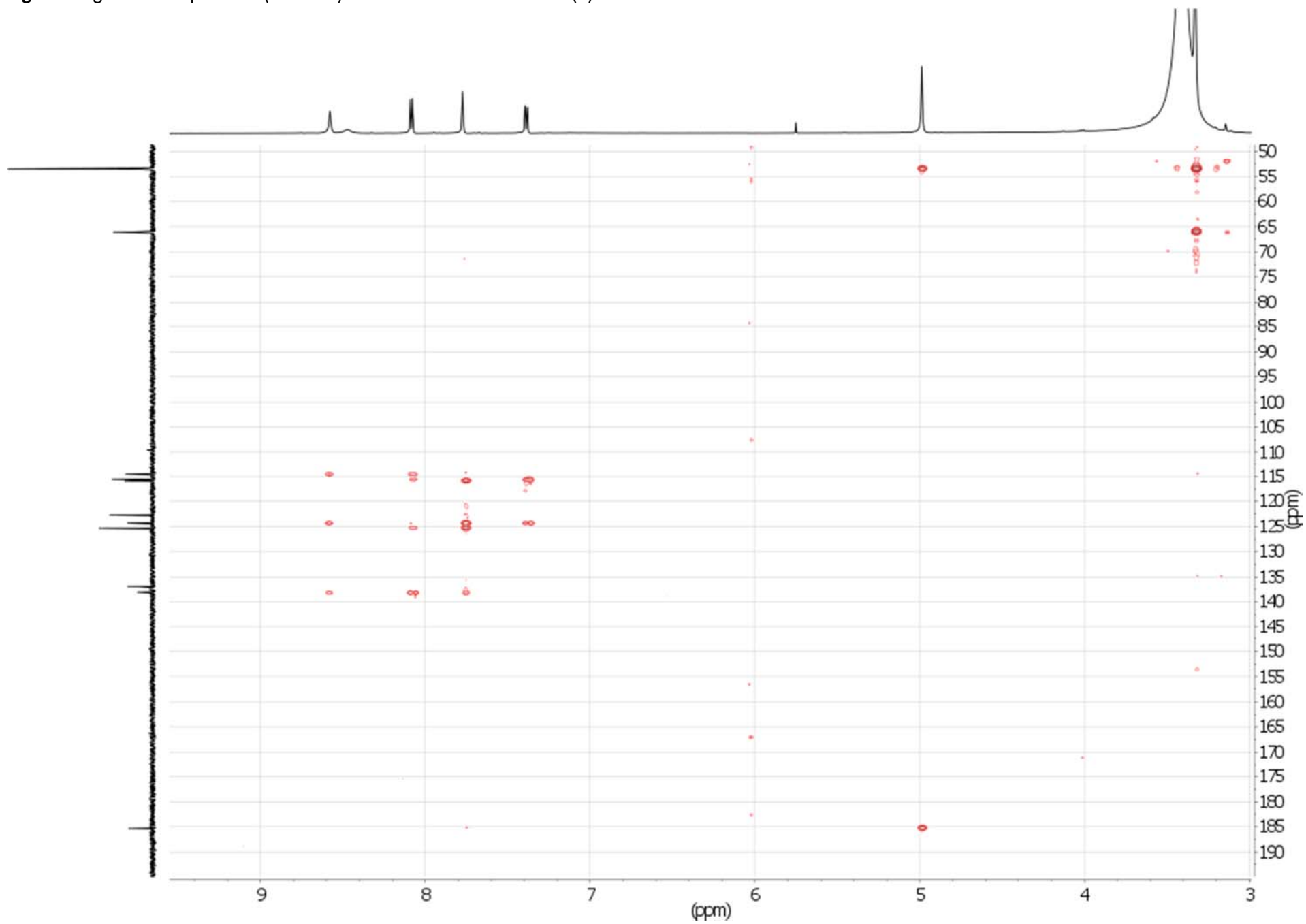


Figure S5.  $^1\text{H}$  spectrum (600 MHz) of 6-bromo- $\beta$ -oxo-*N,N,N*-trimethyl-tryptamine (formate salt) in DMSO- $d_6$ .

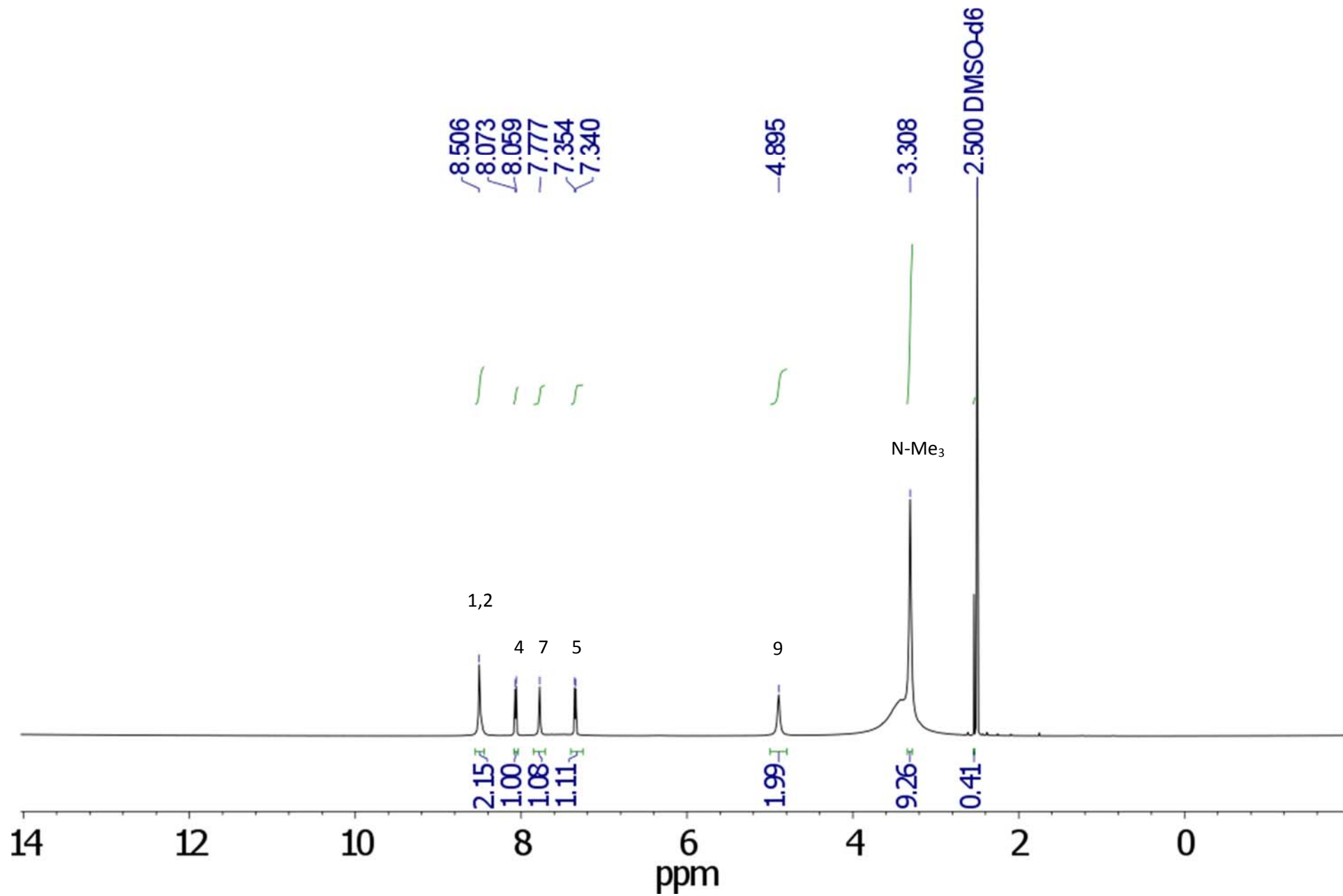


Figure S6.  $^{13}\text{C}$  spectrum (150 MHz) of 6-bromo-8-keto-*N,N,N*-trimethyl-tryptamine (**2s**) (formate salt) in DMSO- $d_6$ .

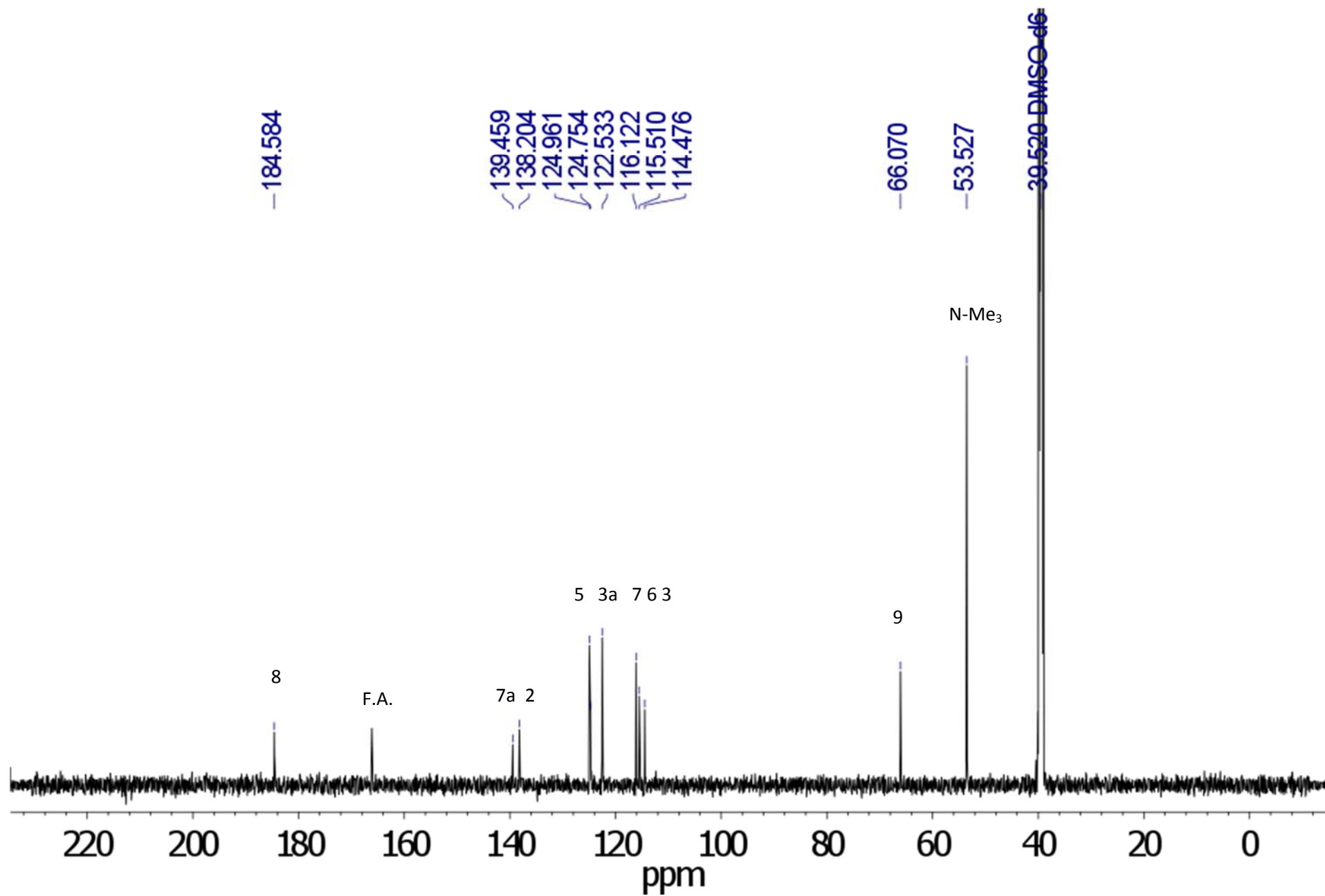




Figure S7.  $^1\text{H}$  spectrum (600 MHz) of 5-bromo-8-keto-*N,N,N*-trimethyl-tryptamine (**3**) (formate salt) in DMSO- $d_6$ .

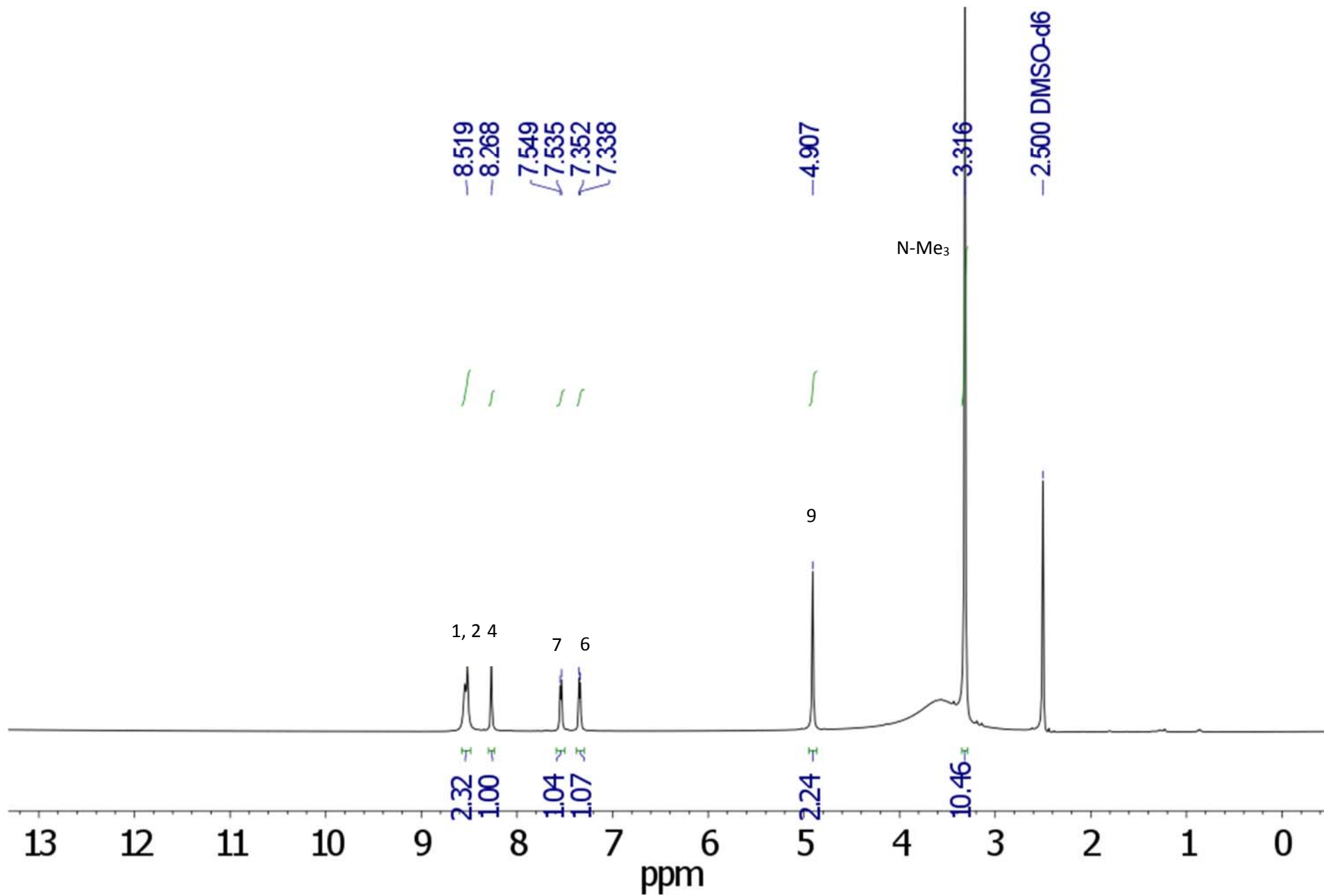
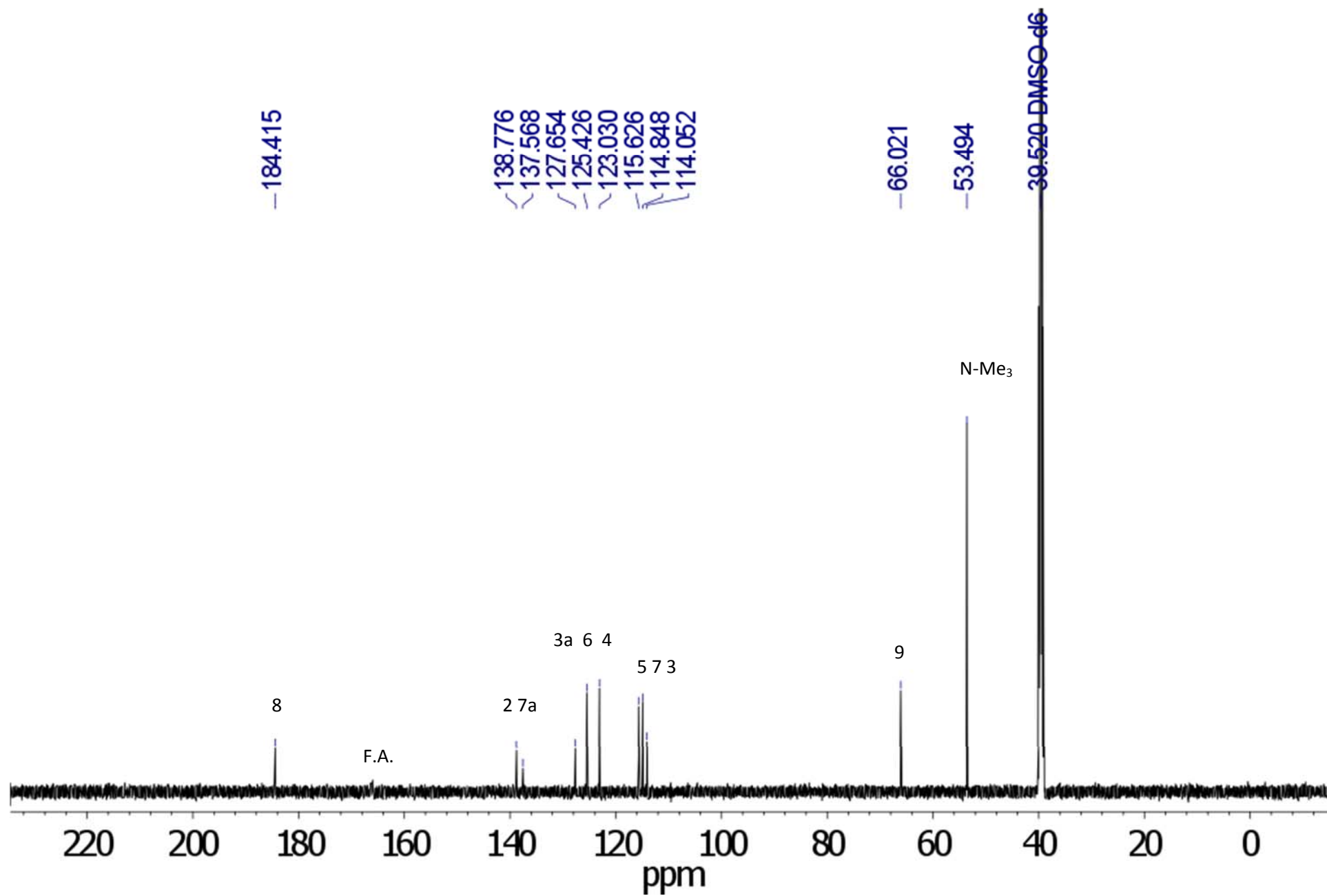


Figure S8.  $^{13}\text{C}$  spectrum (150 MHz) of 5-bromo-8-keto-*N,N,N*-trimethyl-tryptamine (**3**) (formate salt) in DMSO- $d_6$ .

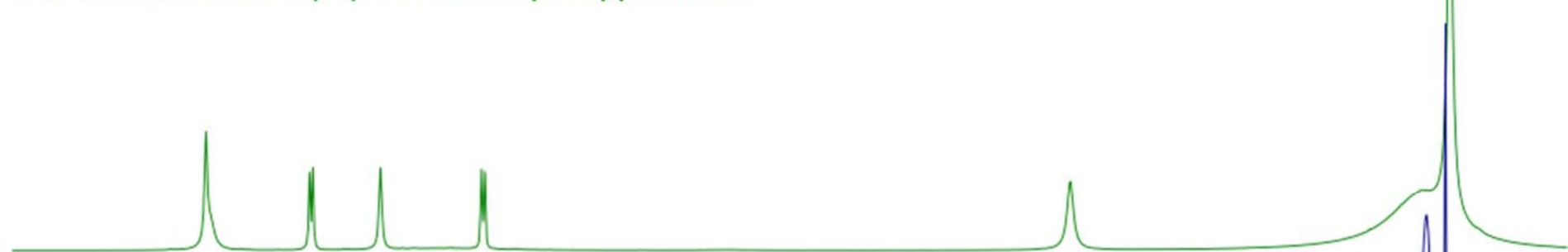


**Figure S9.** Stacked  $^{13}\text{C}$  NMR spectra of the natural product and 5- and 6-bromo isomers of beta-keto-N,N,N-trimethyl-tryptamine (150MHz, DMSO-d6)

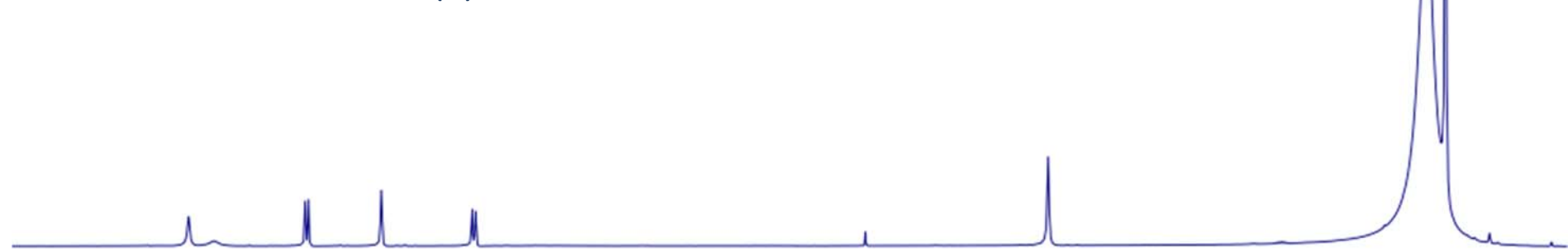
5-bromo-b-oxo-N,N,N-trimethyl tryptamine



6-bromo-b-oxo-N,N,N-trimethyl tryptamine

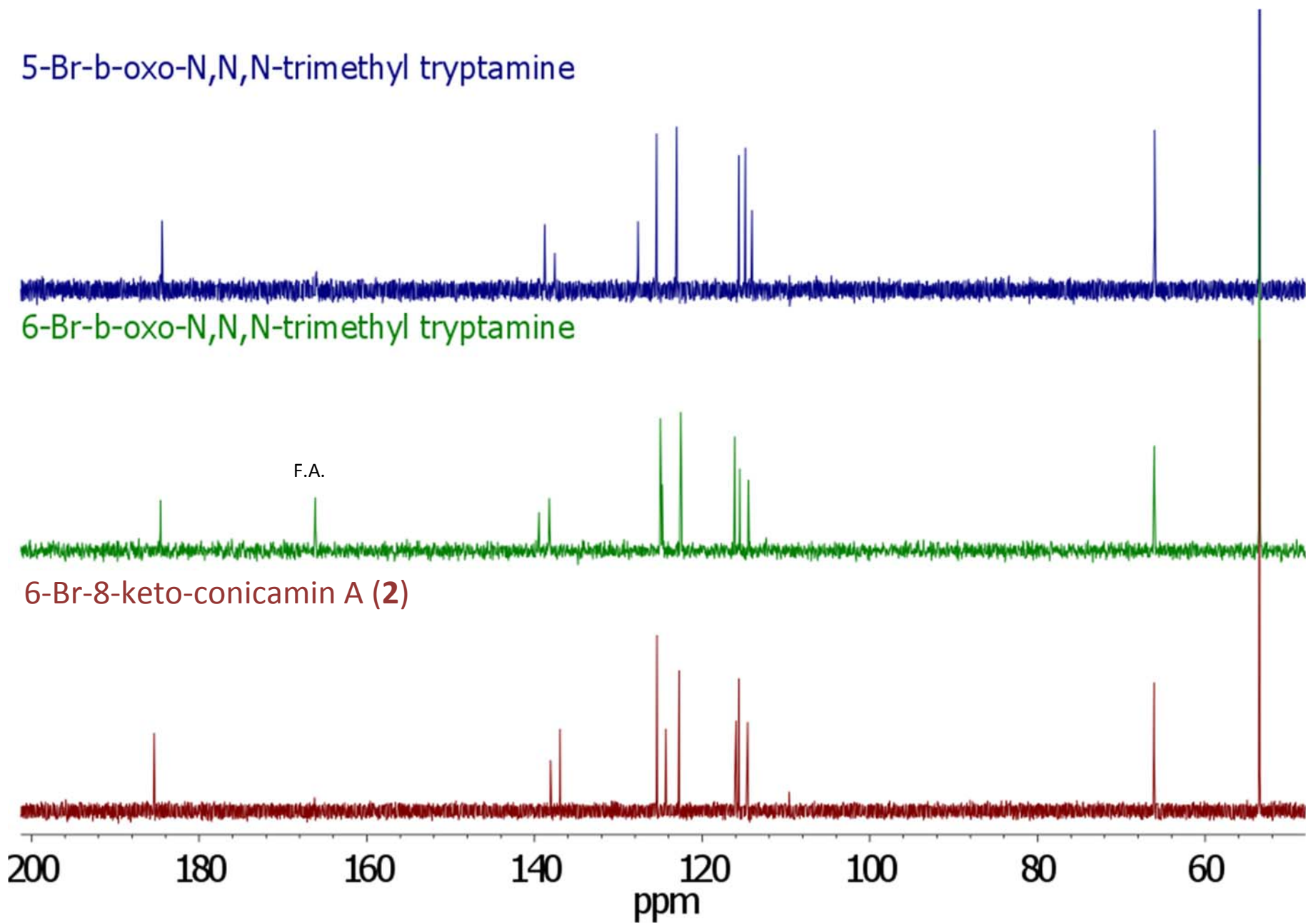


6-Br-8-keto-conicamin A (2)

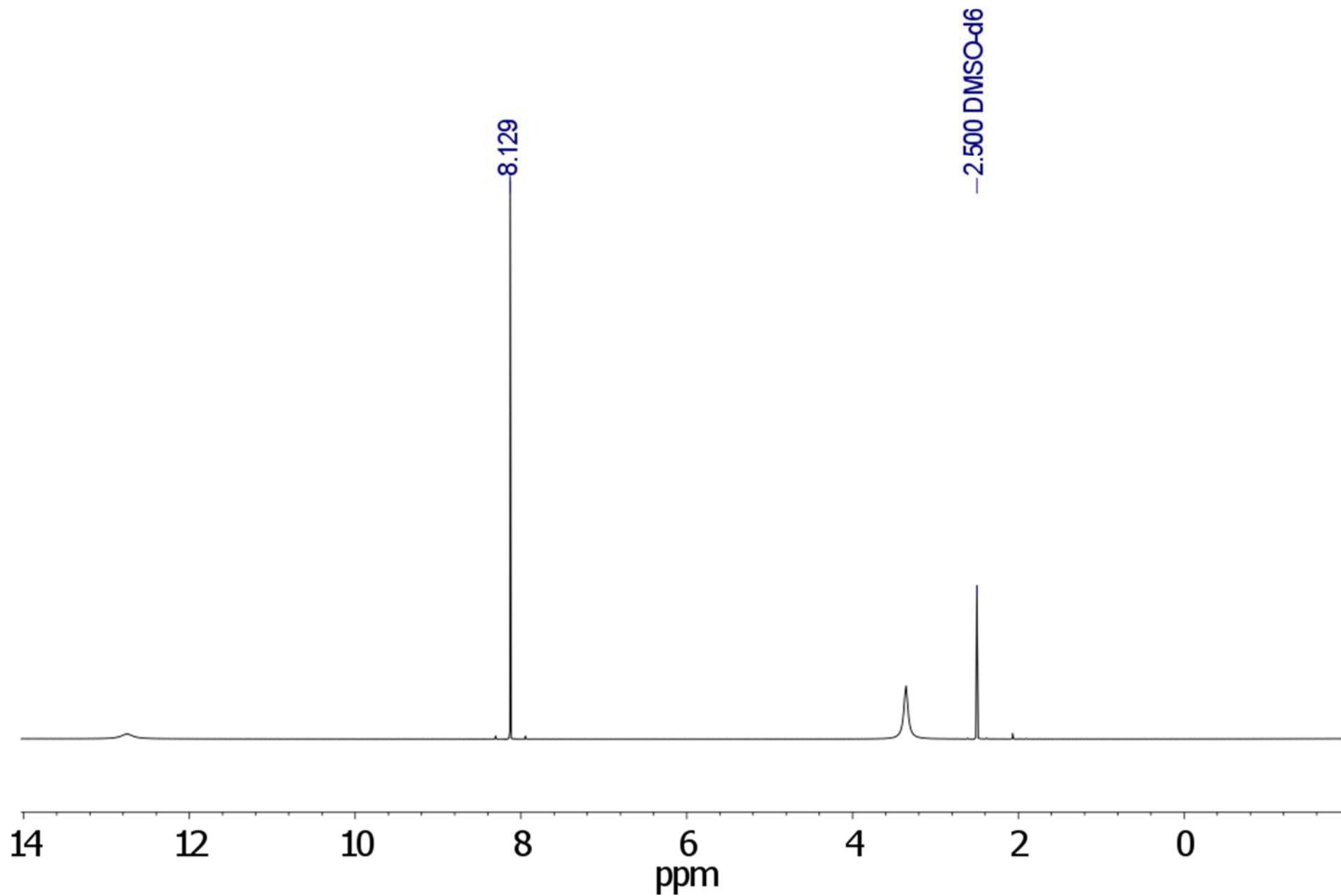


9 8 7 6 5 4 3  
ppm

Figure S10. Stacked  $^{13}\text{C}$  NMR spectra of the natural product and 5- and 6-bromo isomers of beta-oxo-tryptamine (150MHz, DMSO-d6)



**Figure S11.**  $^1\text{H}$  spectrum (600 MHz) of 5 $\mu\text{L}$  formic acid in DMSO- $d_6$ . Note that chemical shift varies with presence of other compounds.



**Figure S12.**  $^{13}\text{C}$  spectrum (150 MHz) of 5 $\mu\text{L}$  formic acid in DMSO- $d_6$ . Note that chemical shift varies with presence of other compounds.

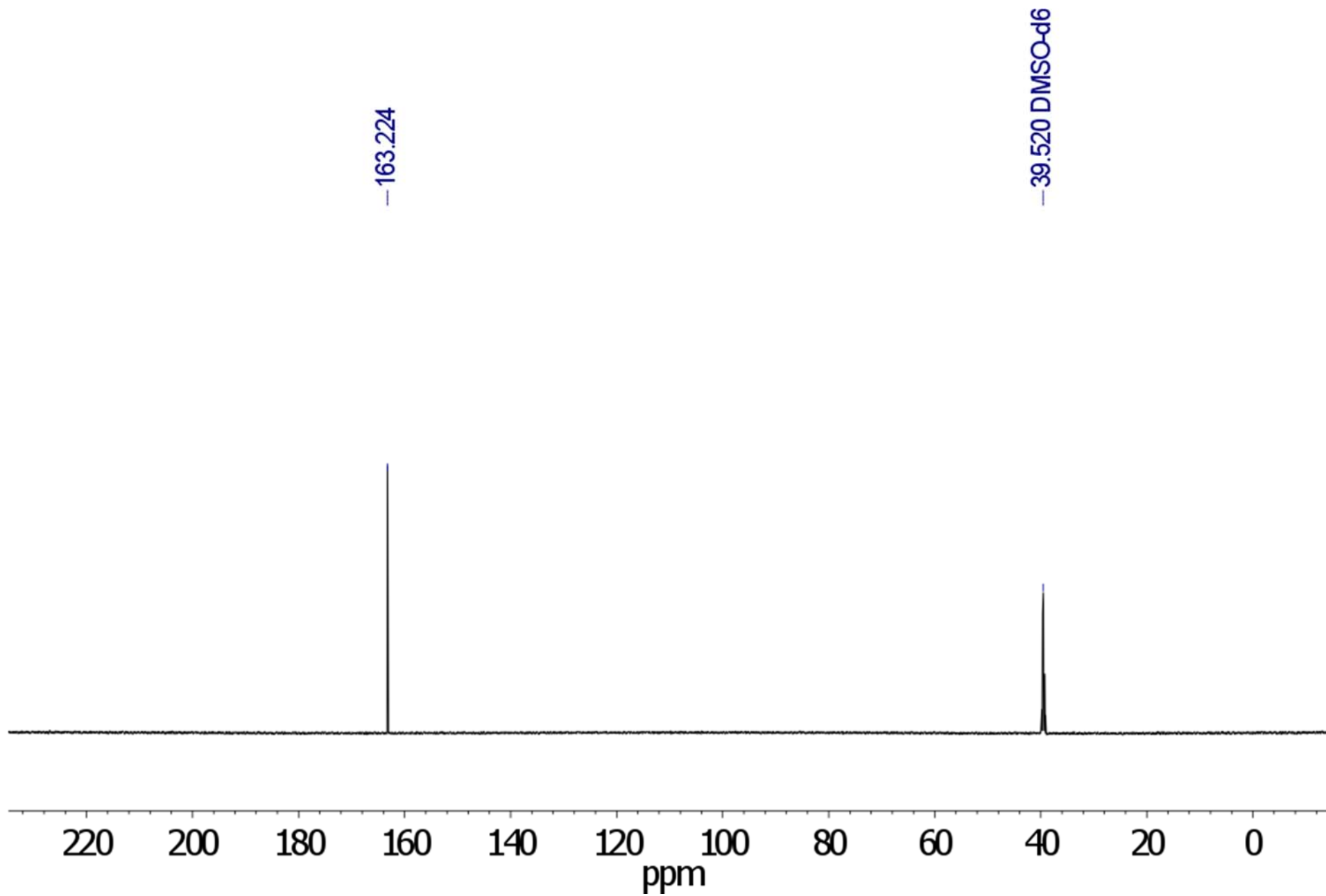


Figure S13.  $^1\text{H}$  spectrum (600 MHz) of 2-(6-Bromo-1H-indol-3-yl)-2-(trimethylsiloxy)acetonitrile (**7**) in DMSO- $d_6$ .

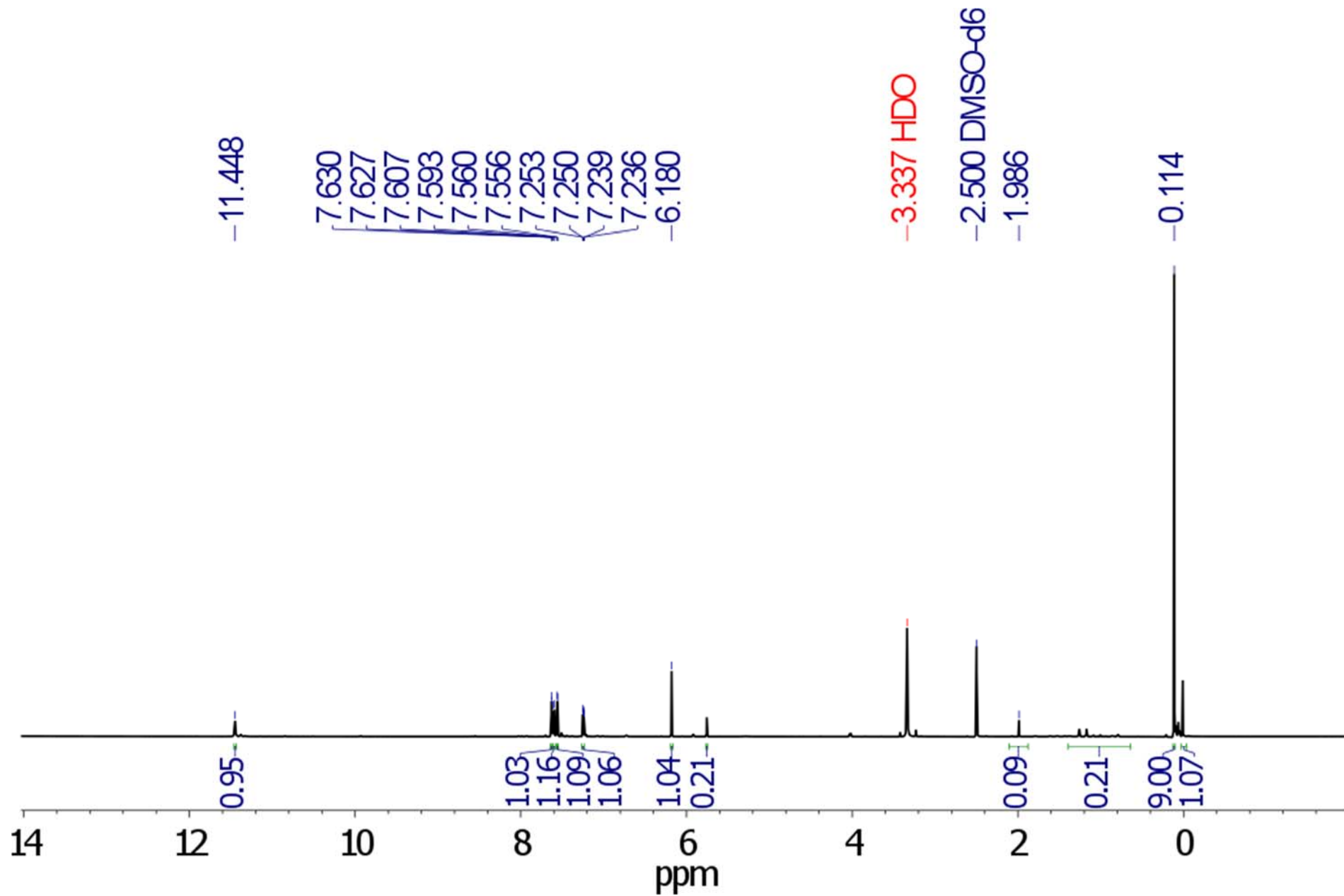


Figure S14.  $^{13}\text{C}$  spectrum (150 MHz) of (6-Bromo-1H-indol-3yl)-(trimethylsiloxy)acetonitrile (**7**) in DMSO- $d_6$ .

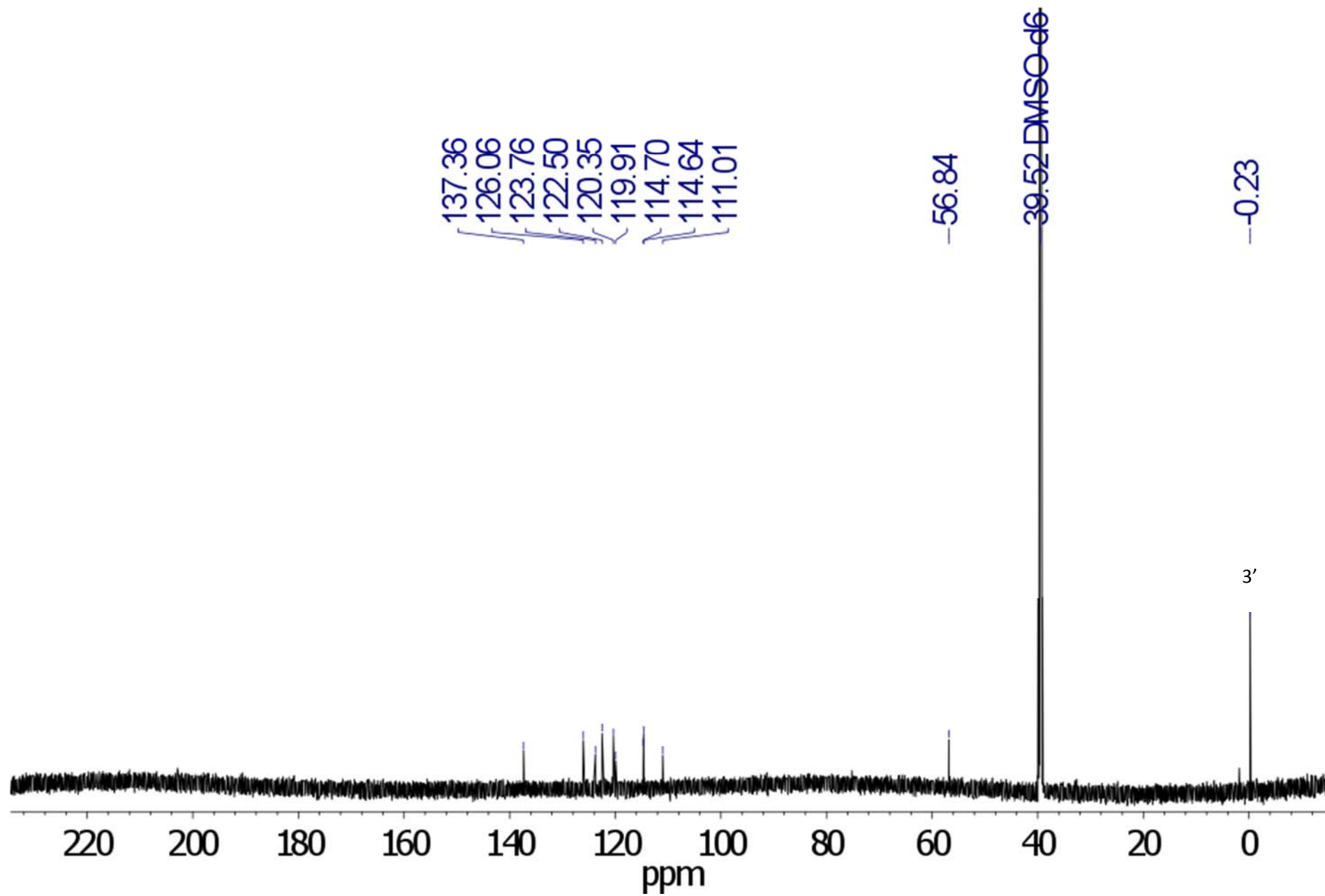
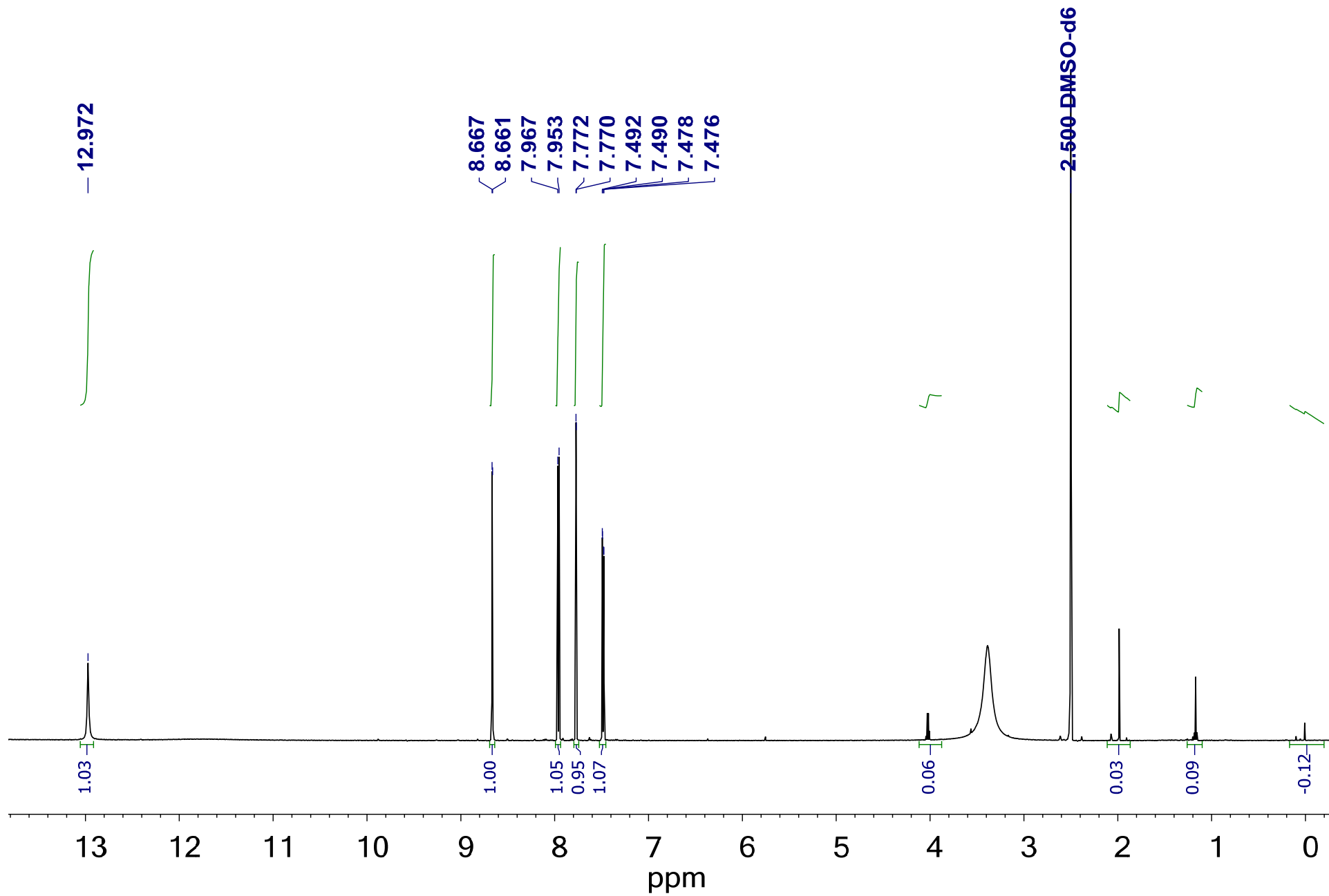




Figure S15. <sup>1</sup>H spectrum (600 MHz) of 6-bromo-1H-indol-3-carbonyl cyanide (**9**) in DMSO-d<sub>6</sub>.



**Figure S16.**  $^{13}\text{C}$  spectrum (150 MHz) of 6-bromo-1H-indol-3-carbonyl cyanide (**9**) in DMSO- $d_6$ . Unmarked peaks are putatively of reduced DDQ (predicted  $^{13}\text{C}$  NMR: 151.5, 129.0, 113.5, 102.8 via nmrdb.org) or other aprotic contaminants as there are no associated proton signals (see above). However rigorous assignment was not done at this stage.

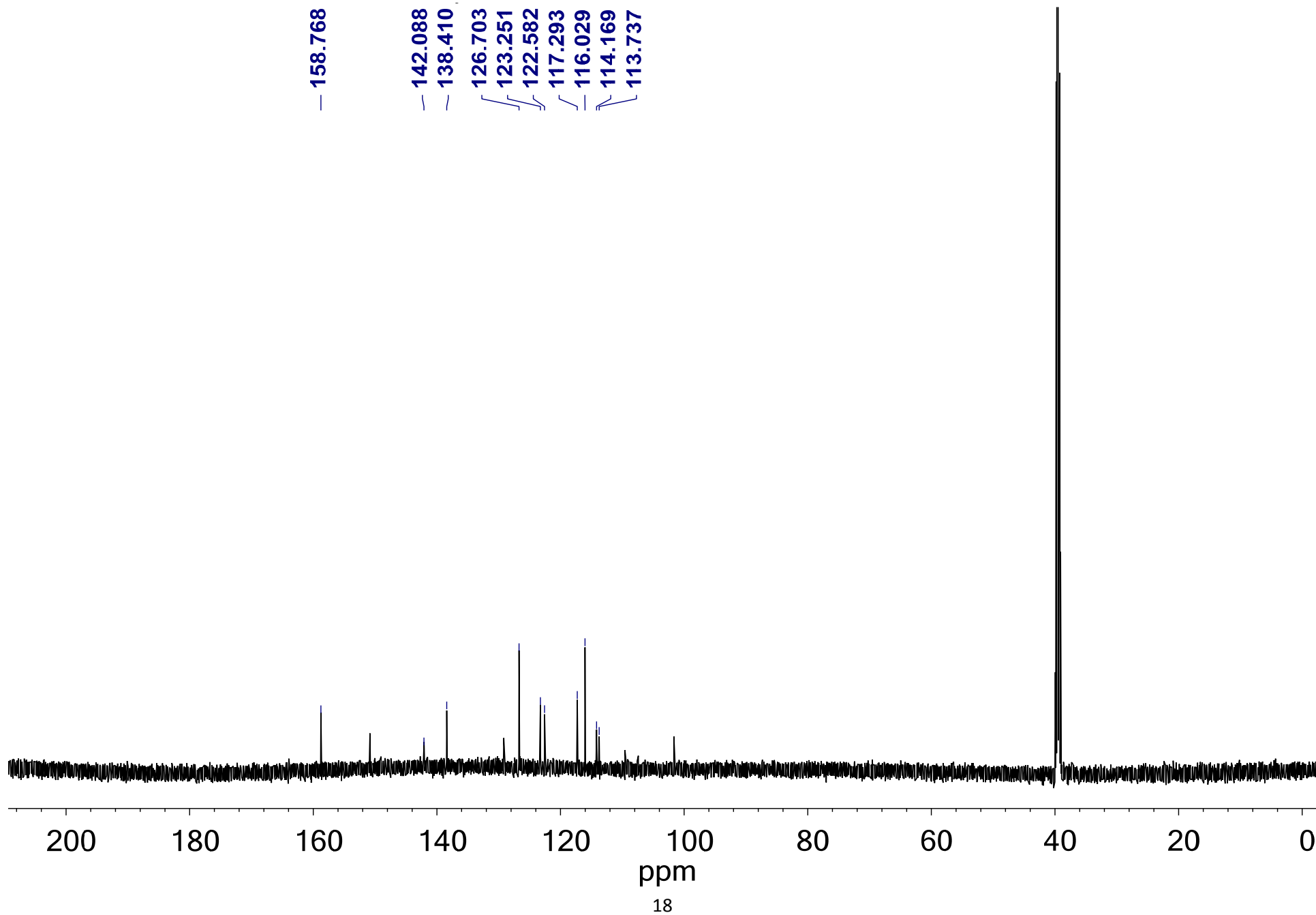


Figure S17.  $^1\text{H}$  spectrum (600 MHz) of 8-keto-tryptamine (**10**) in DMSO- $d_6$ .

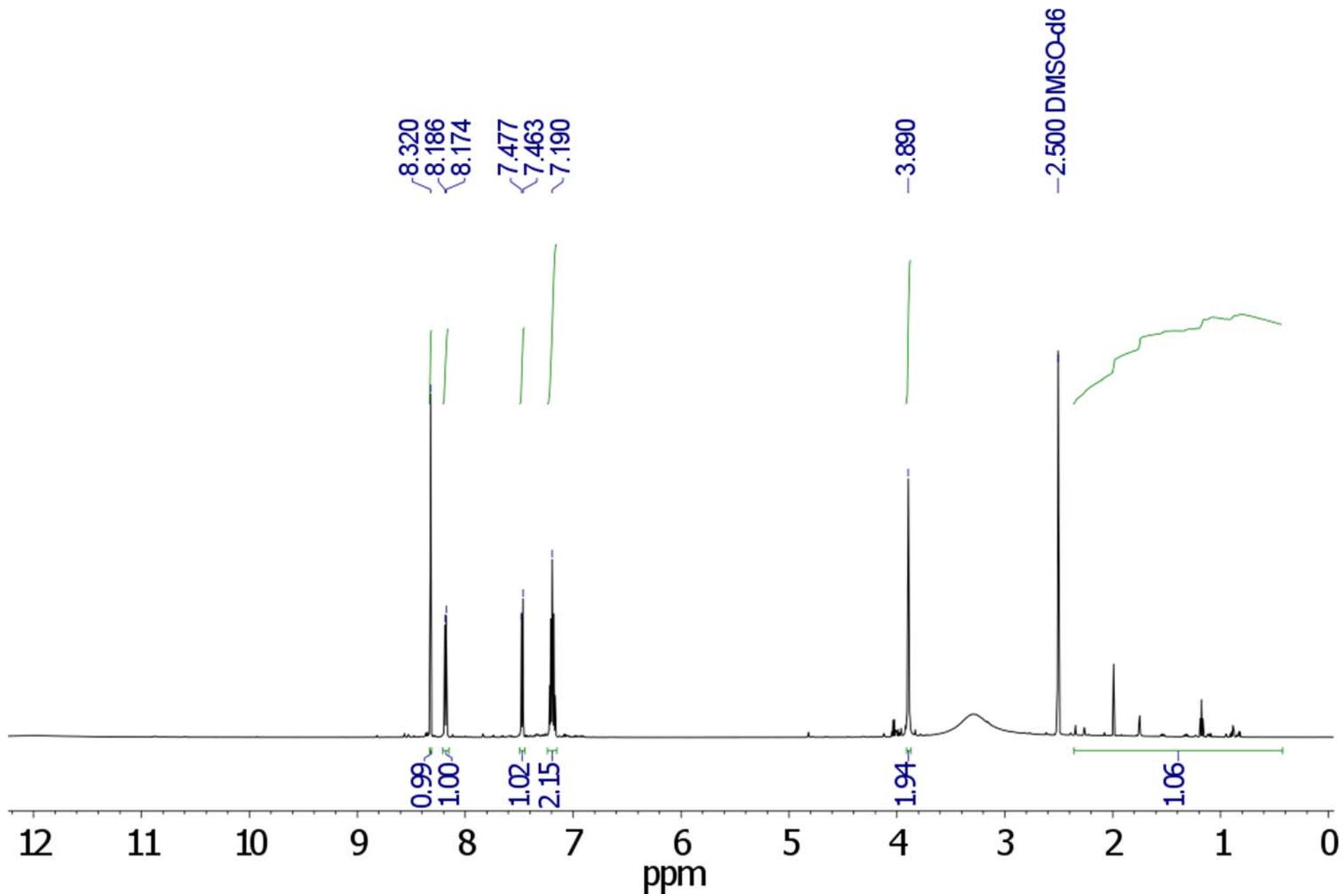


Figure S18.  $^{13}\text{C}$  spectrum (150 MHz) of 8-keto-tryptamine (**10**) in DMSO- $d_6$ .

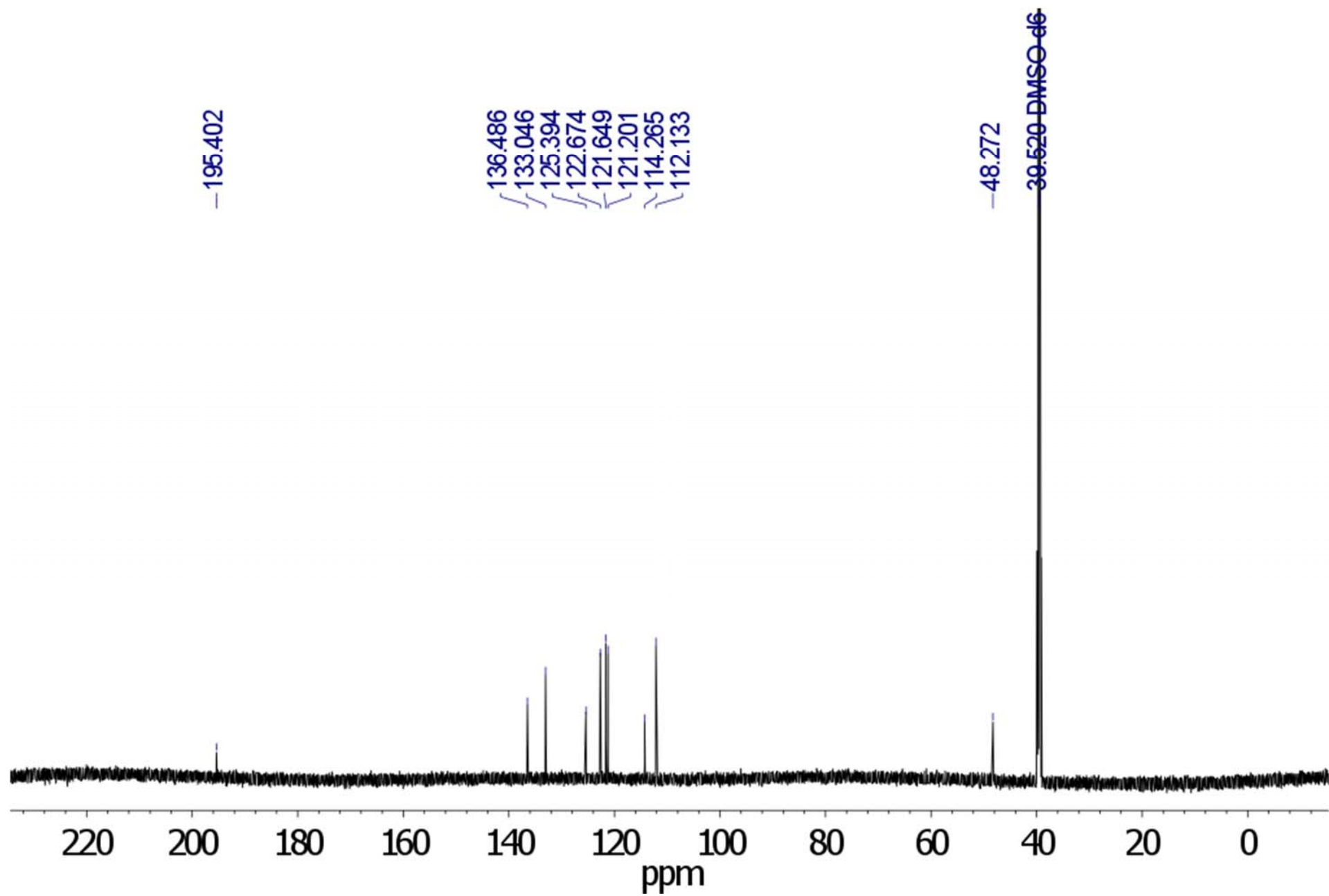


Figure S19.  $^1\text{H}$  spectrum (500 MHz) of 6-Br-8-keto-tryptamine (**11**) (formate salt) in DMSO- $d_6$ .

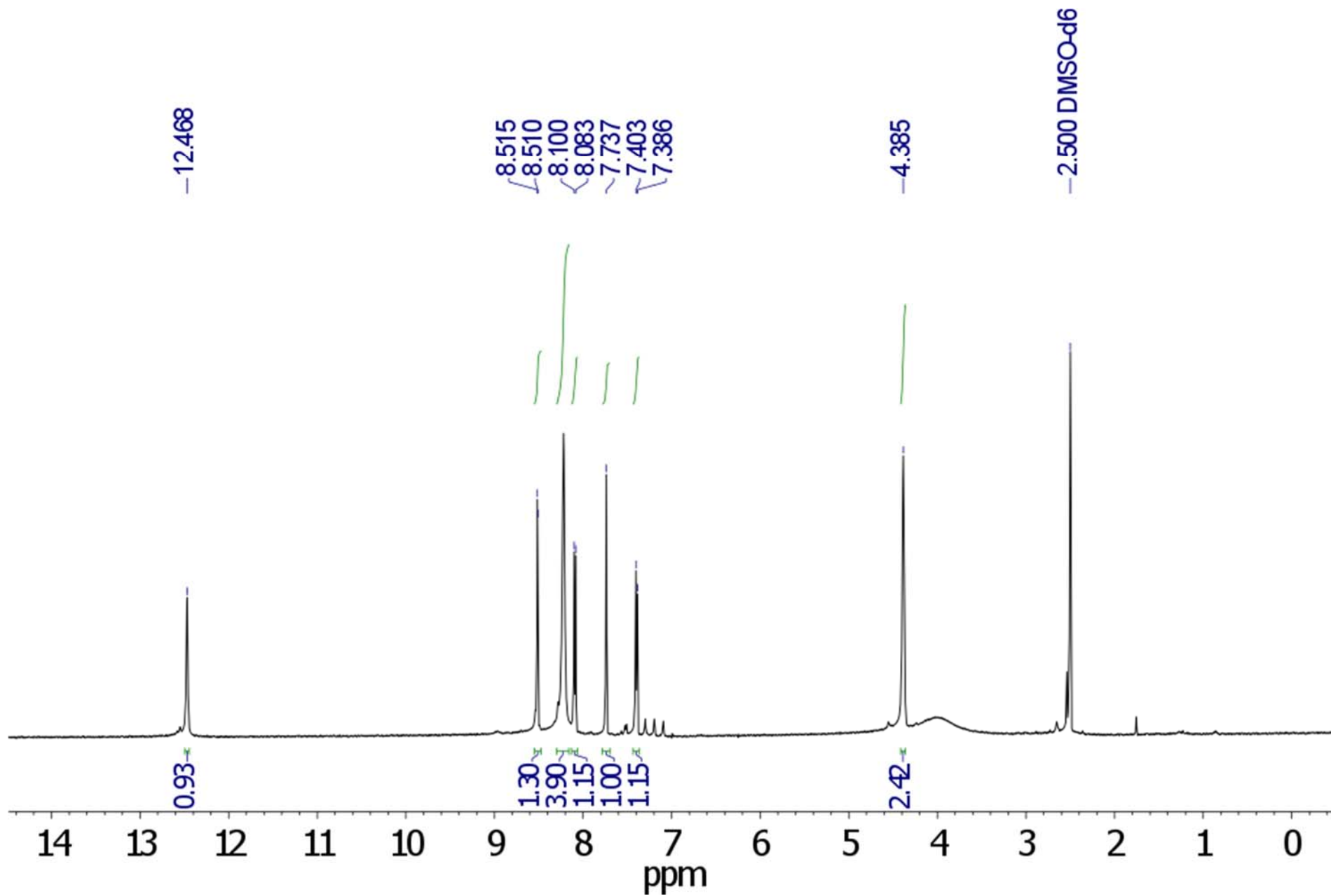


Figure S20.  $^{13}\text{C}$  spectrum (125 MHz) of 6-Br-8-keto-tryptamine (**11**) in DMSO- $d_6$ .

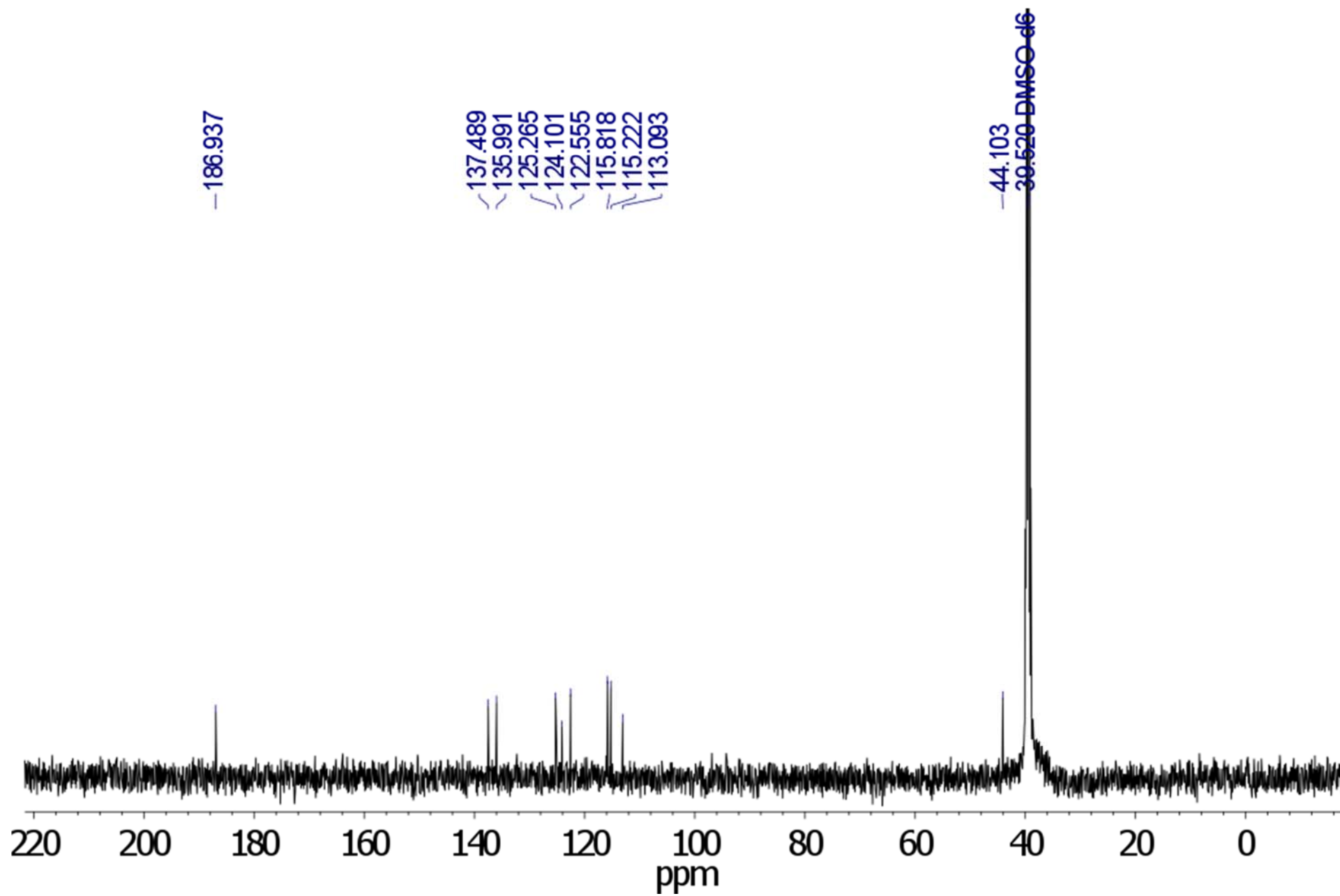


Figure S21.  $^1\text{H}$  spectrum (500 MHz) of 5-Br-8-keto-tryptamine (**12**) (formate salt) in DMSO- $d_6$ .

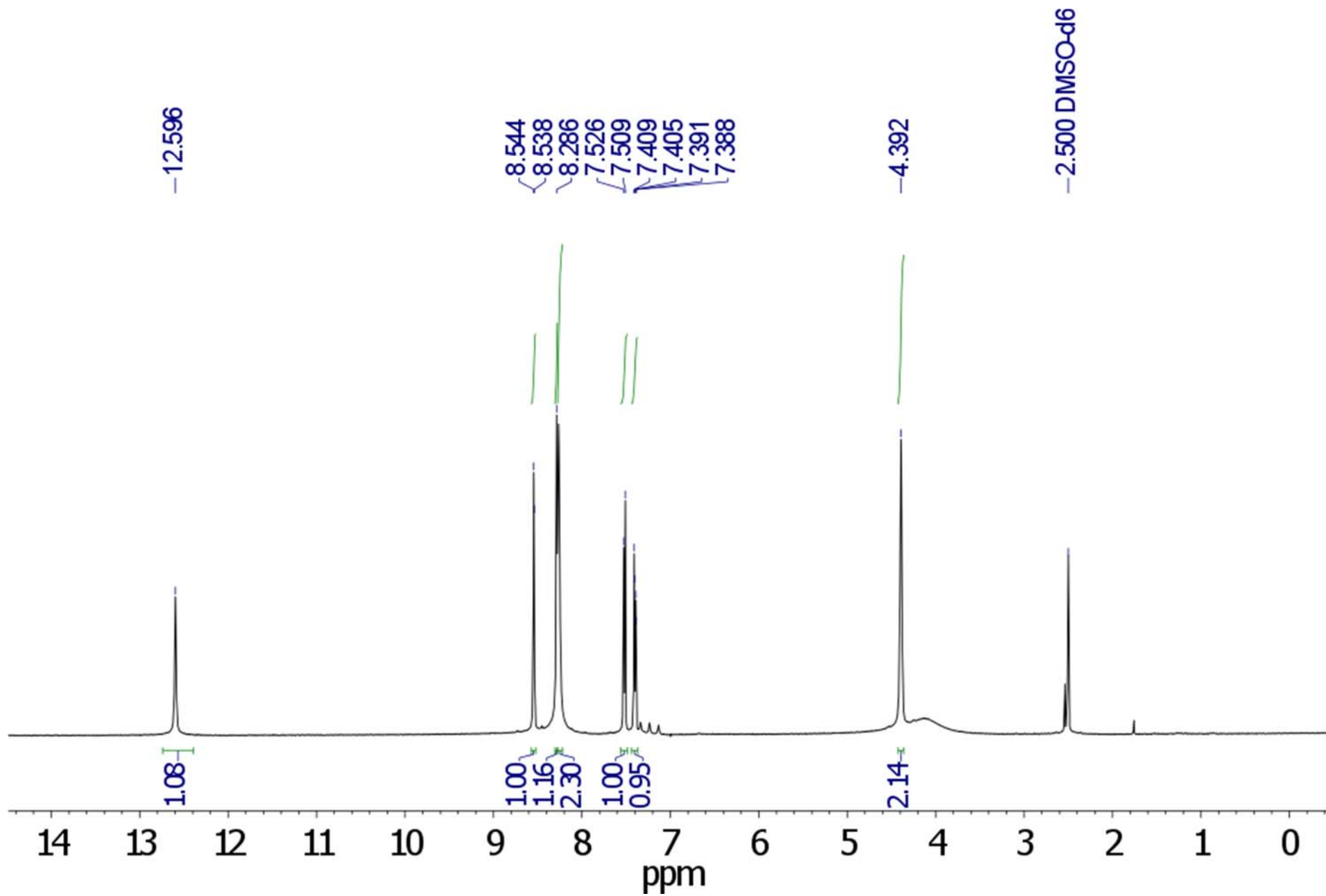


Figure S22.  $^{13}\text{C}$  spectrum (125 MHz) of 5-Br-8-keto-tryptamine (**12**) in DMSO- $d_6$ .

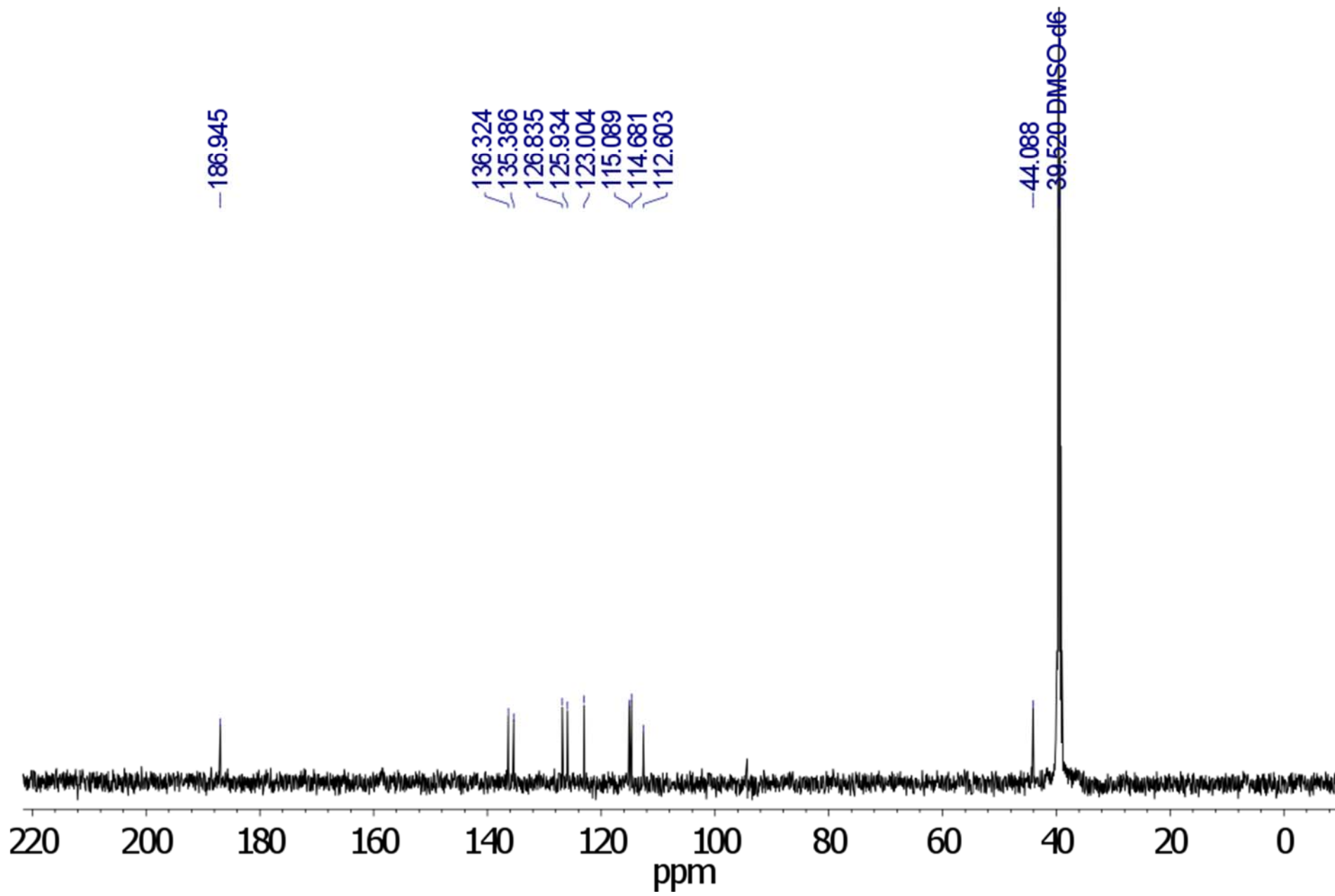




Figure S23. <sup>1</sup>H spectrum (600 MHz) of 8-keto-N,N,N-trimethyl-tryptamine (**13**) (formate salt) in DMSO-d<sub>6</sub>.

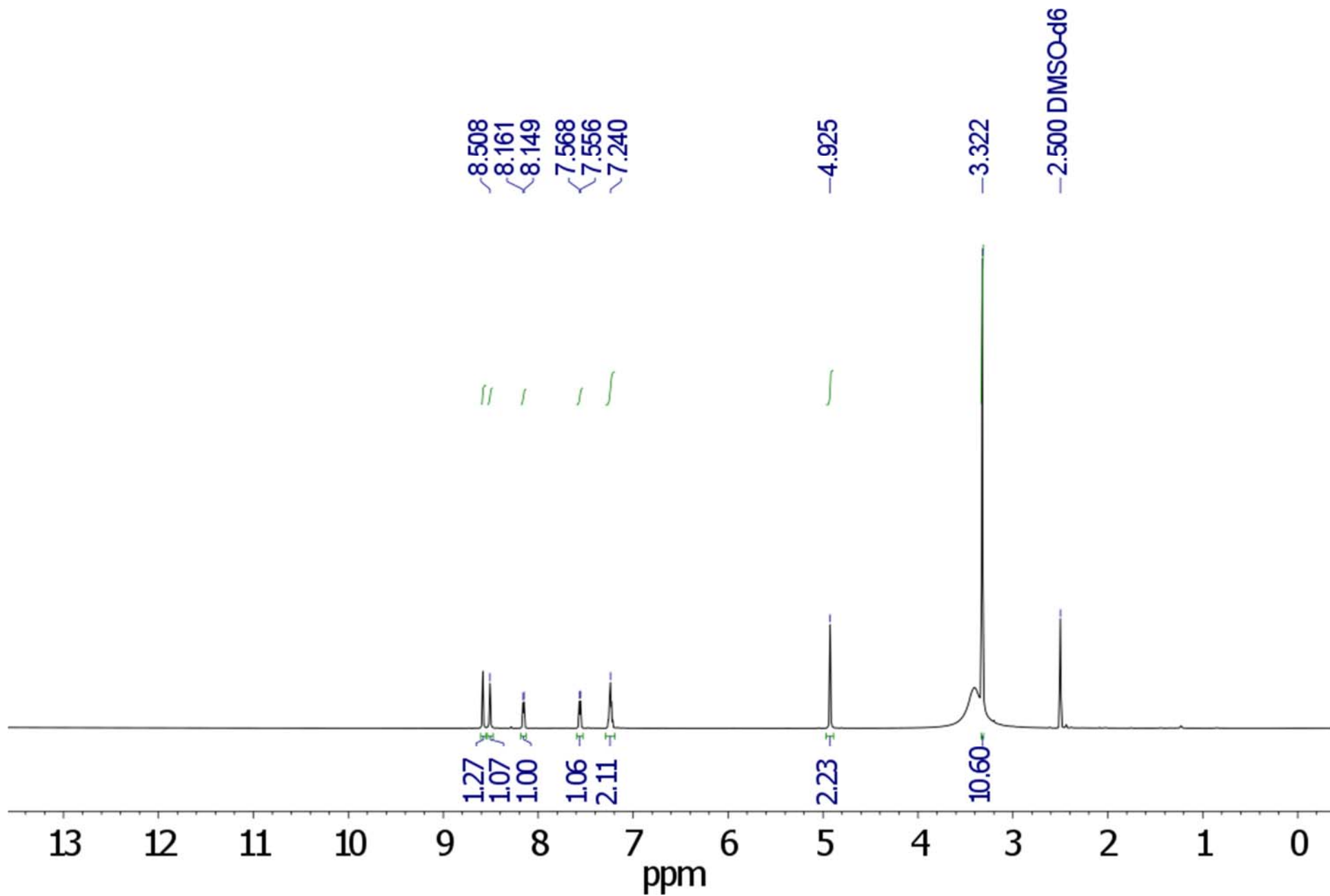


Figure S24.  $^{13}\text{C}$  spectrum (150 MHz) of  $\beta$ -oxo-*N,N,N*-trimethyl-tryptamine (**13**) (formate salt) in DMSO- $d_6$ .

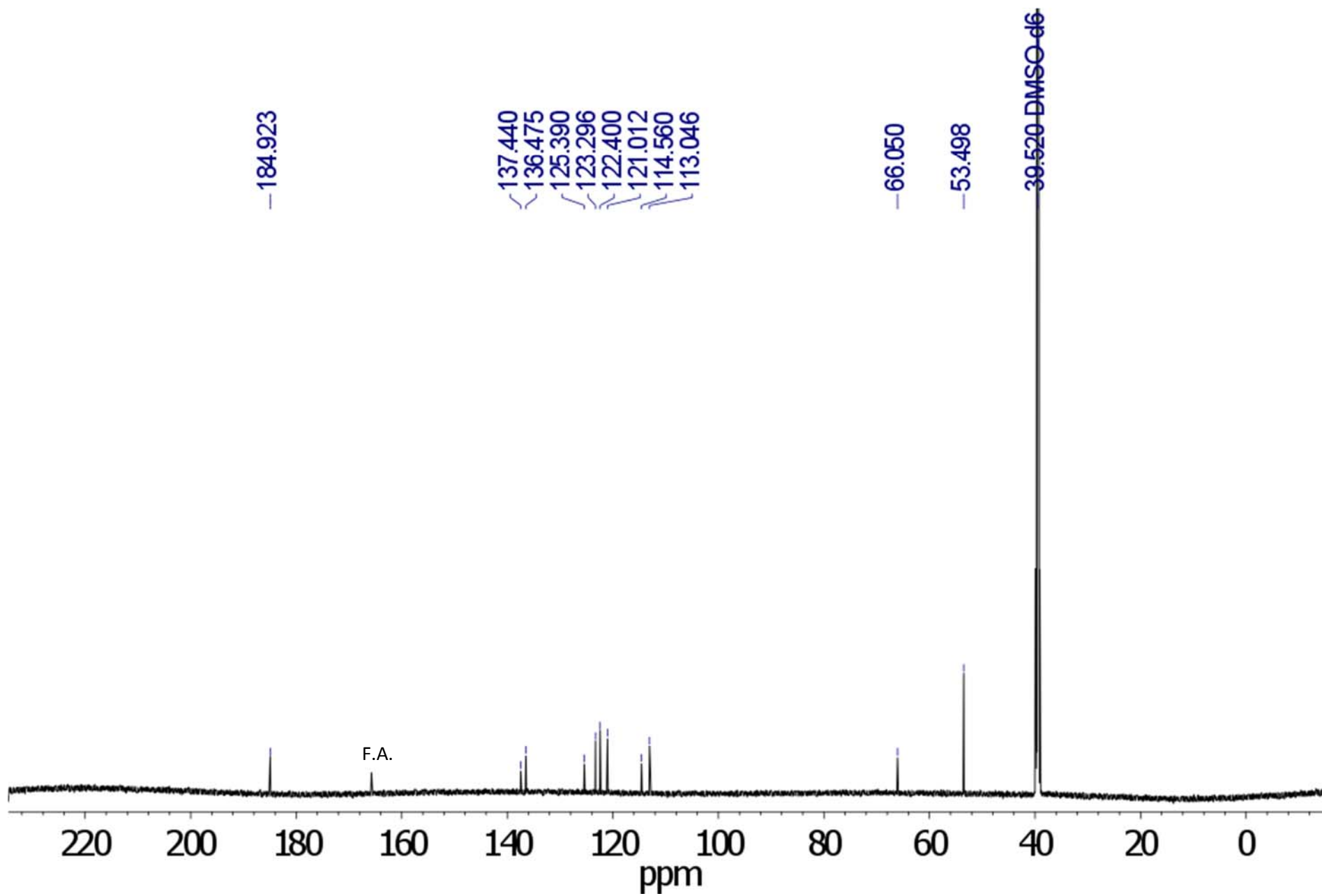


Figure S25. <sup>1</sup>H spectrum (600 MHz) of 6-Br-8-keto-*N,N*-dimethyl-tryptamine (**14**) in DMSO-d<sub>6</sub>.

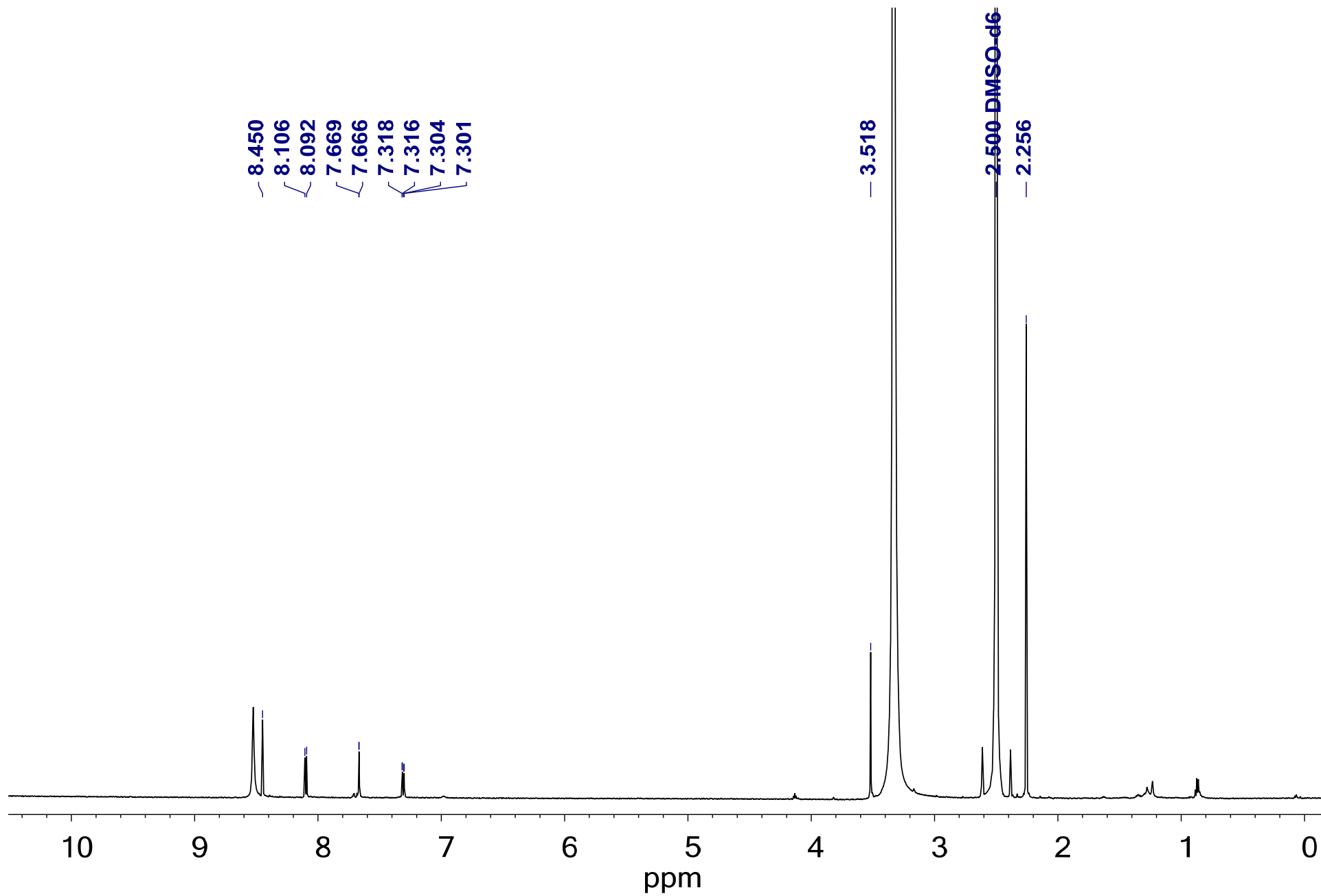


Figure S26. gHMBCAD spectrum (600 MHz) of 6-Br-8-keto-*N,N*-dimethyl-tryptamine (**14**) in DMSO-d<sub>6</sub>.

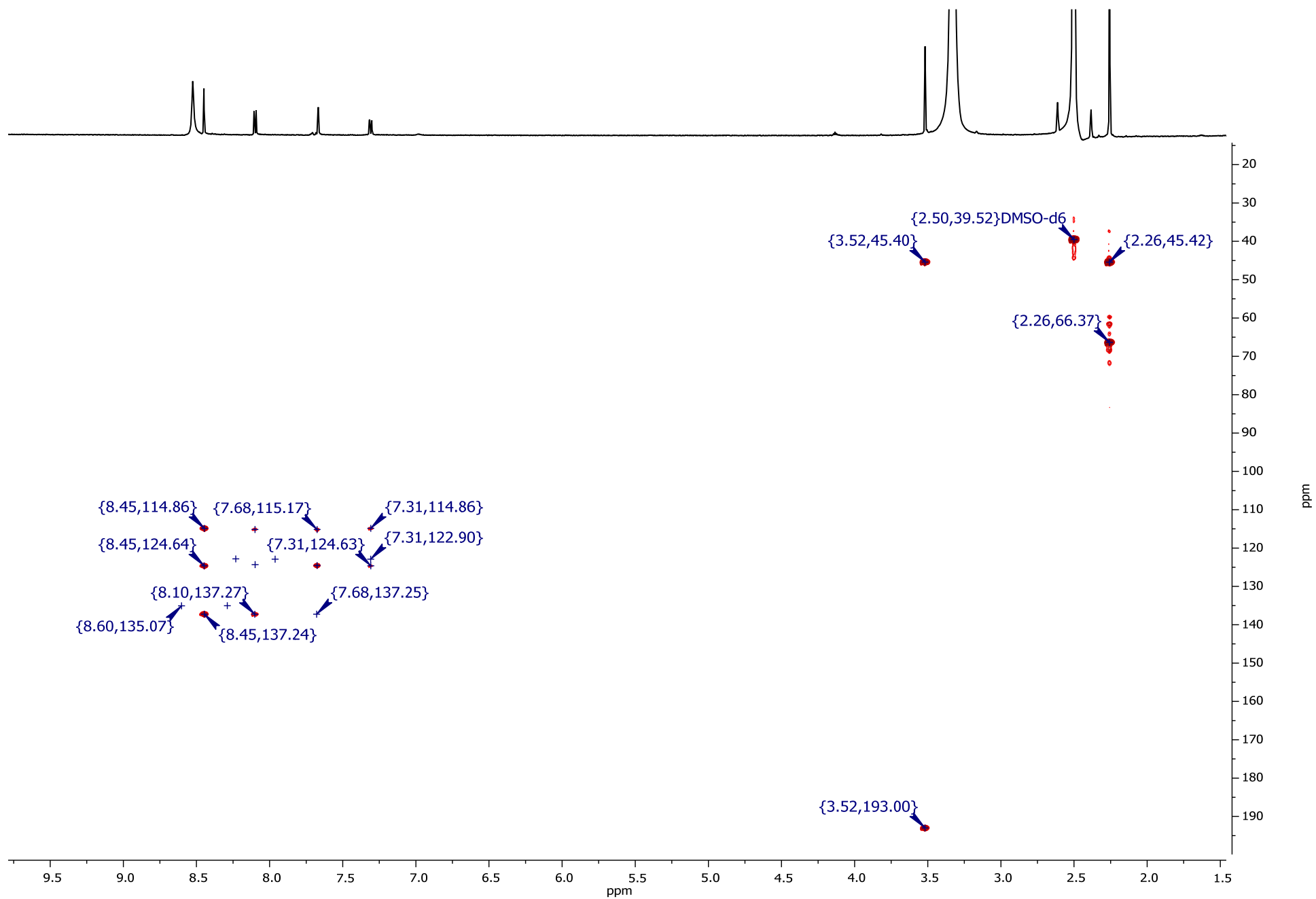


Figure S27. gHMBCAD spectrum (600 MHz) expansion of 6-Br-8-keto-*N,N*-dimethyl-tryptamine (**14**) in DMSO-*d*<sub>6</sub>.

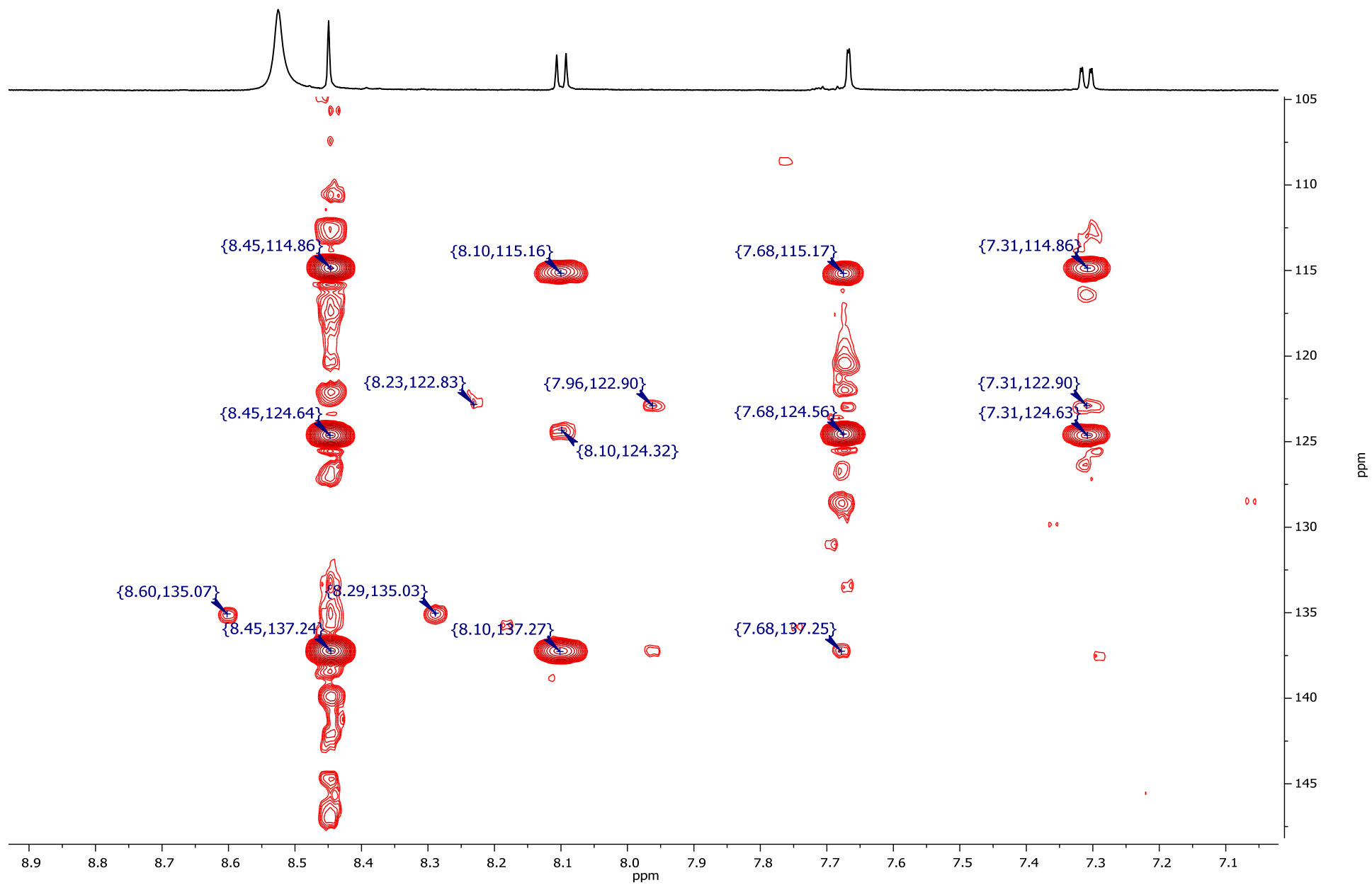


Figure S28. <sup>1</sup>H spectrum (600 MHz) of 5-Br-8-keto-*N,N*-dimethyl-tryptamine (**15**) in DMSO-d<sub>6</sub>.

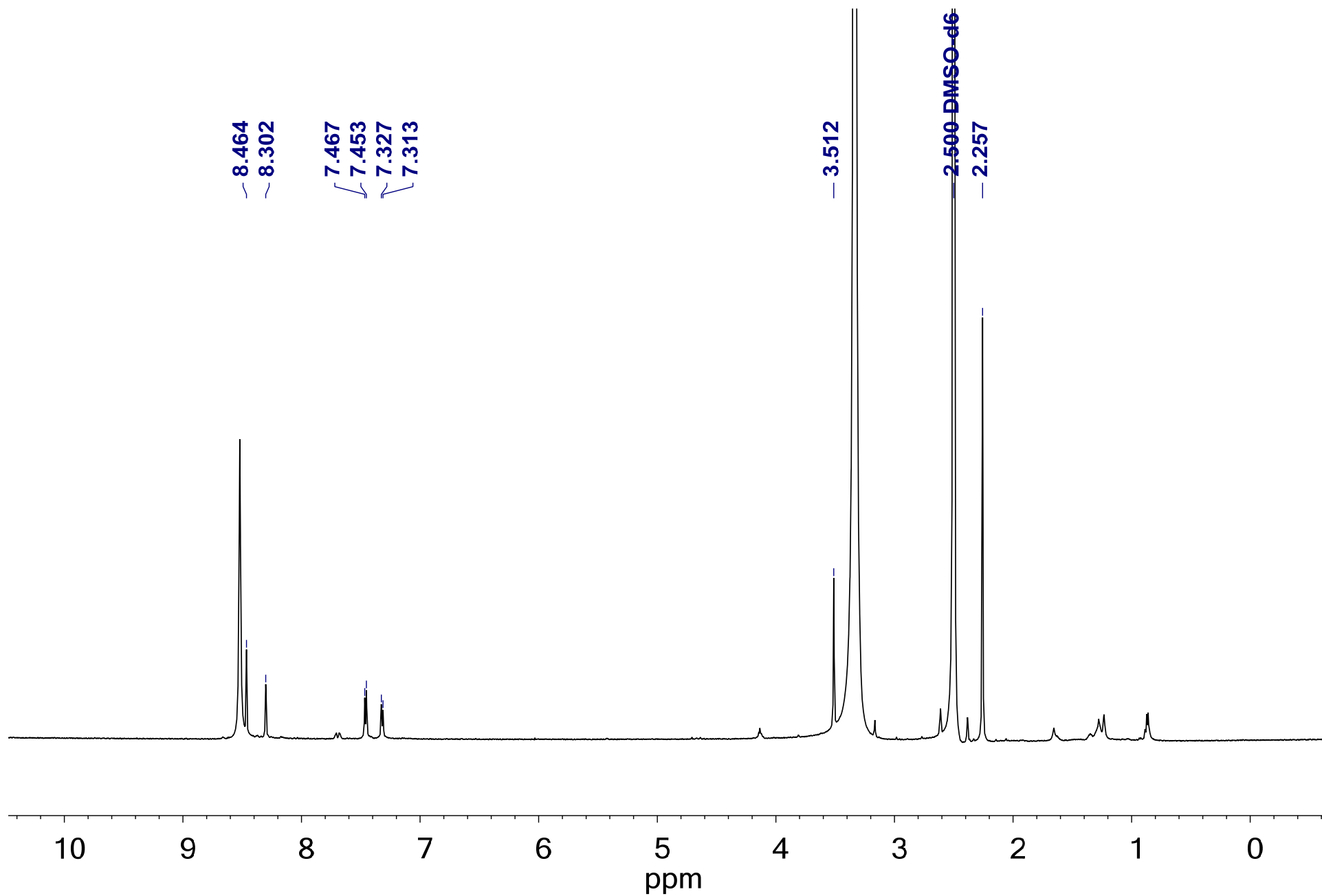


Figure S29. gHMBCAD spectrum (600 MHz) of 5-Br-8-keto-*N,N*-dimethyl-tryptamine (**15**) in DMSO-d<sub>6</sub>.

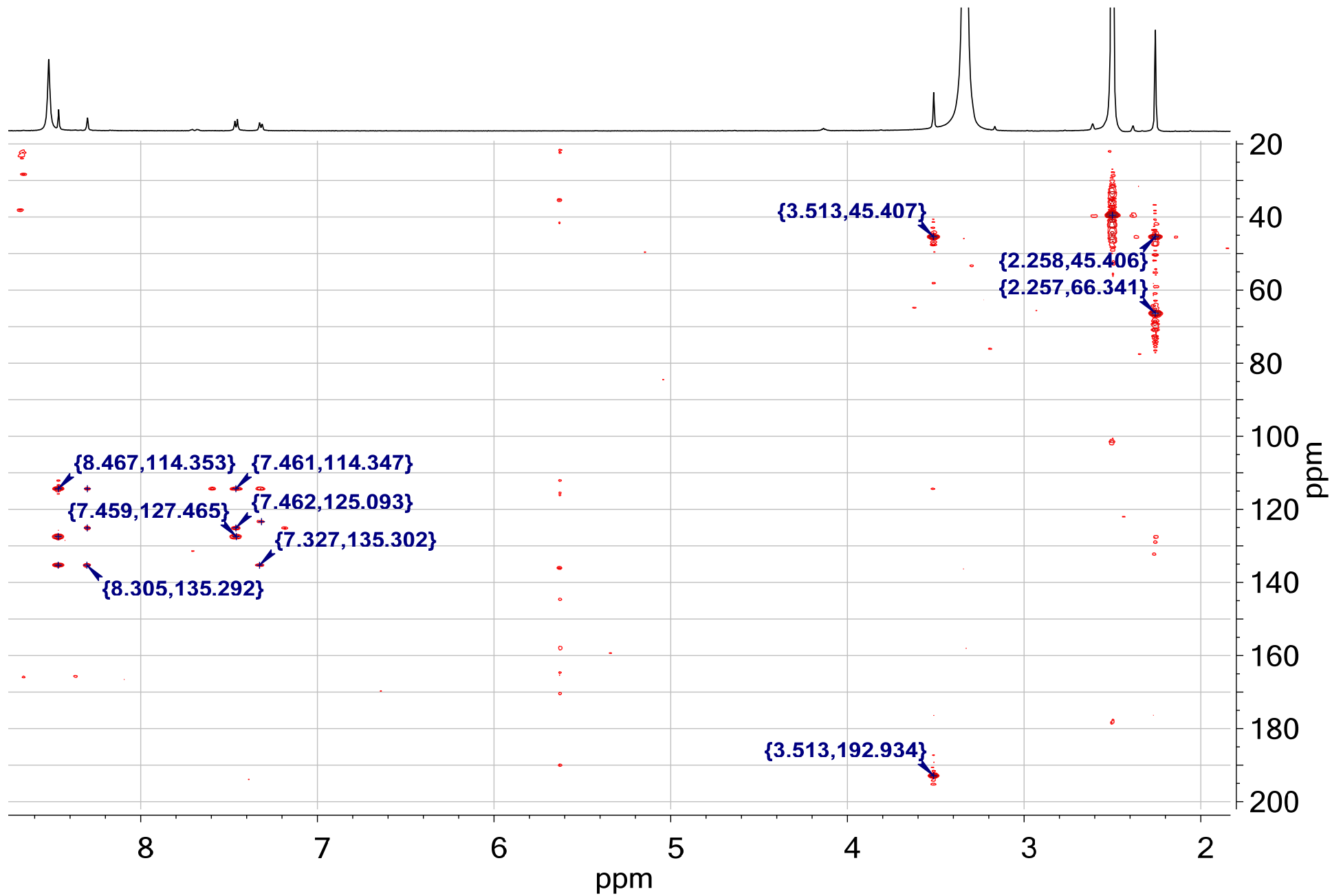


Figure S30. gHMBCAD spectrum (600 MHz) expansion of 5-Br-8-keto-*N,N*-dimethyl-tryptamine (**15**) in DMSO-*d*<sub>6</sub>.

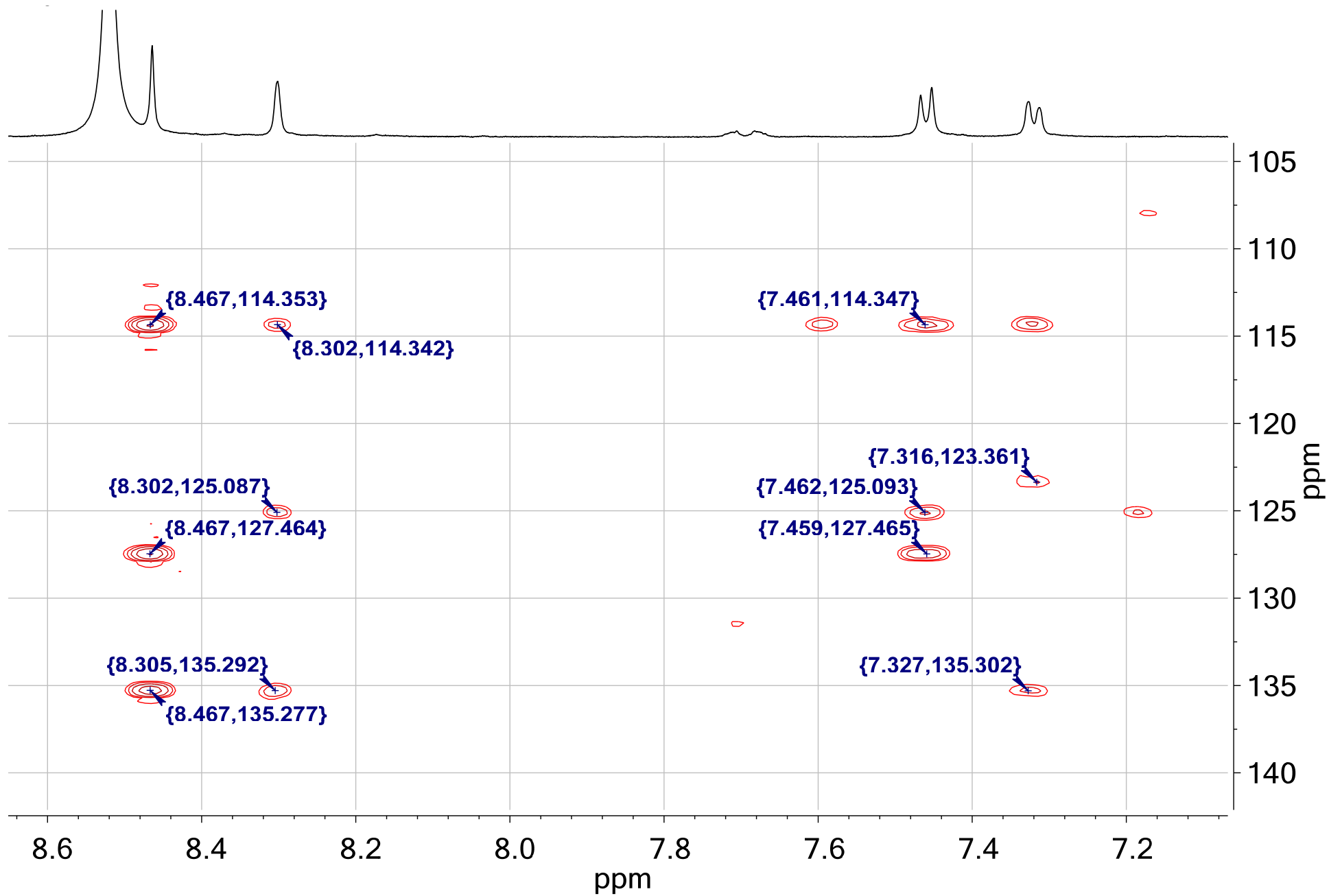




Figure S31.  $^1\text{H}$  spectrum (600 MHz) of 8-keto-*N,N*-dimethyl-tryptamine (**16**) in DMSO- $d_6$ .

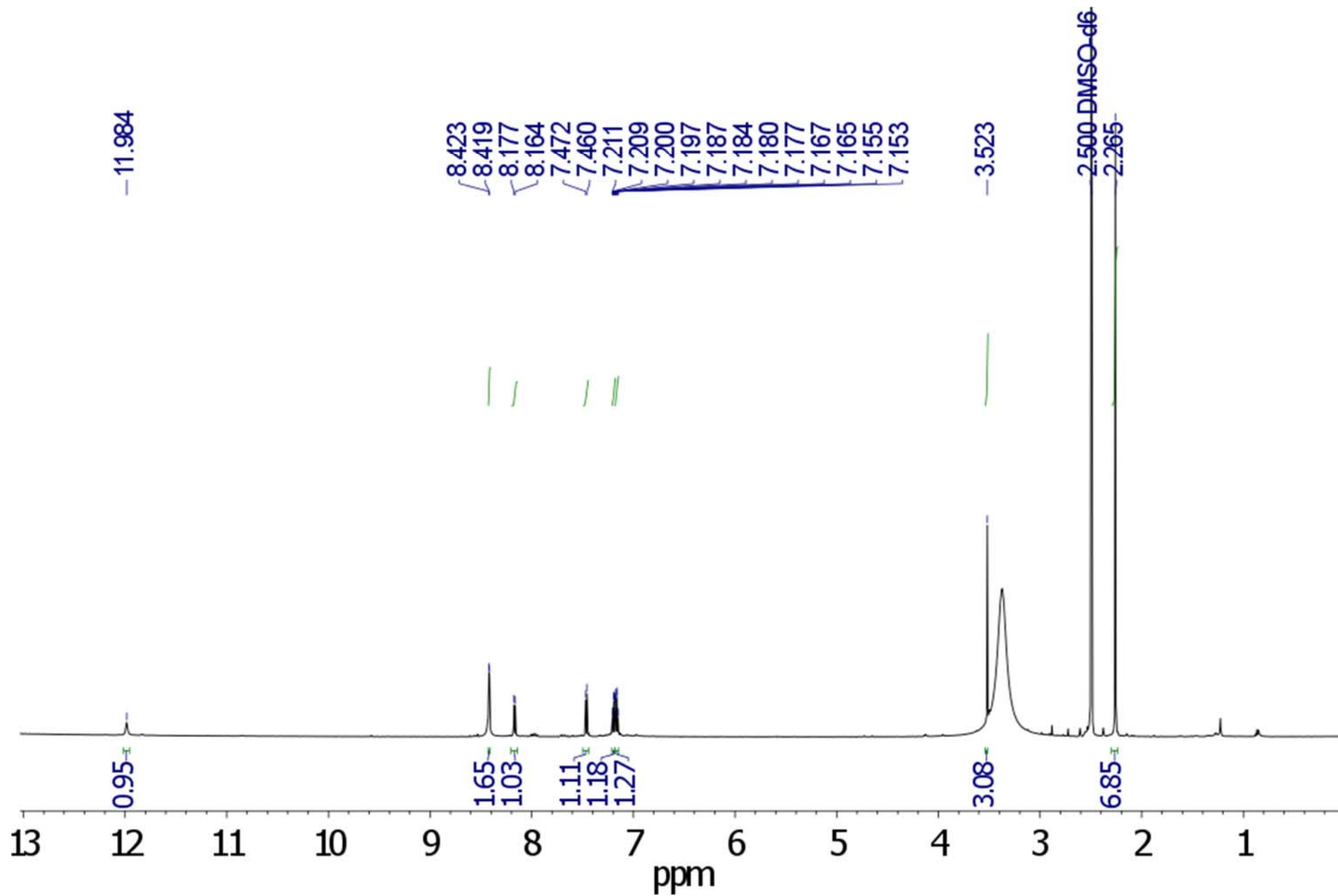


Figure S32. gHMBCAD spectrum (600 MHz) of 8-keto-*N,N*-dimethyl-tryptamine (**16**) in DMSO-d<sub>6</sub>.

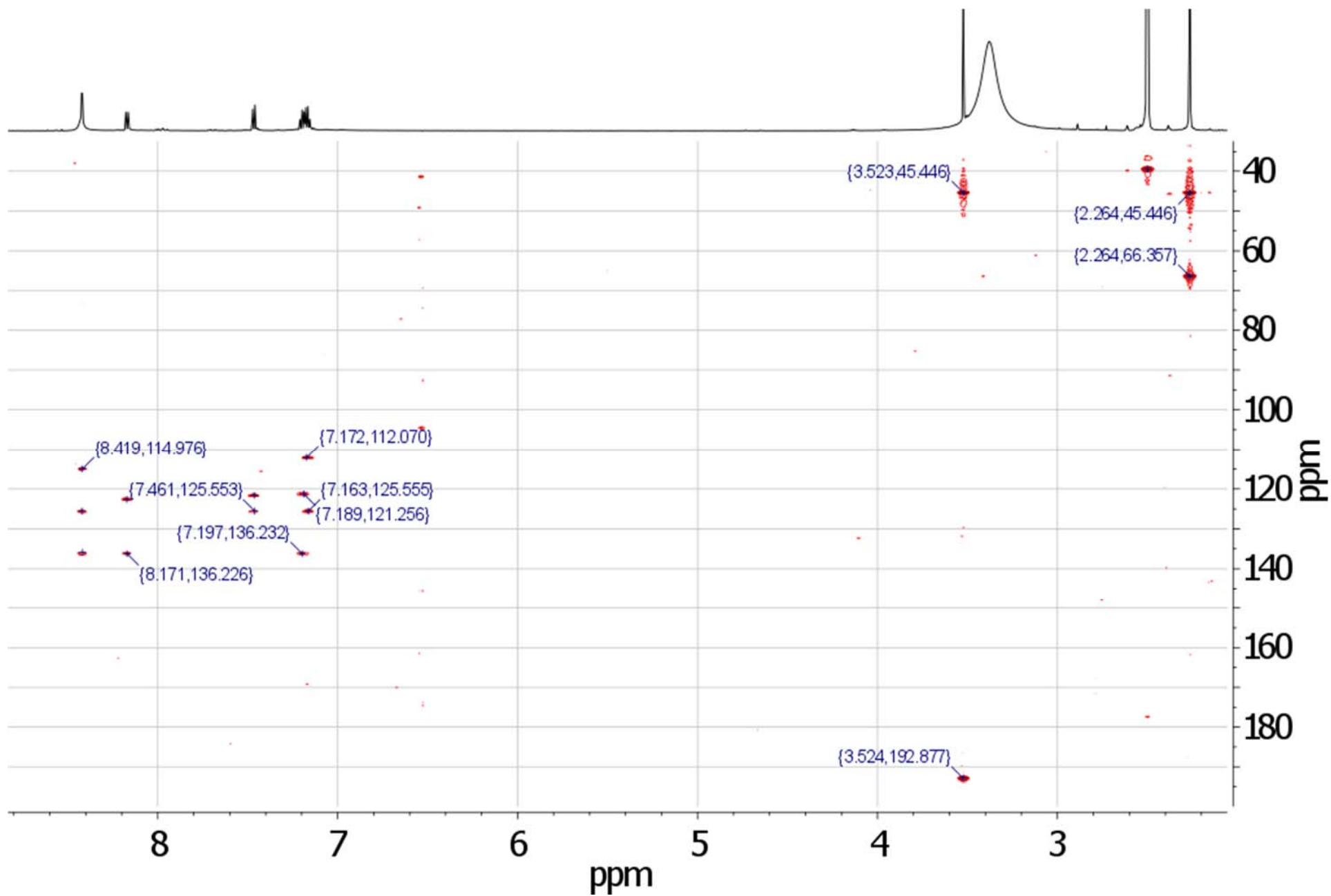
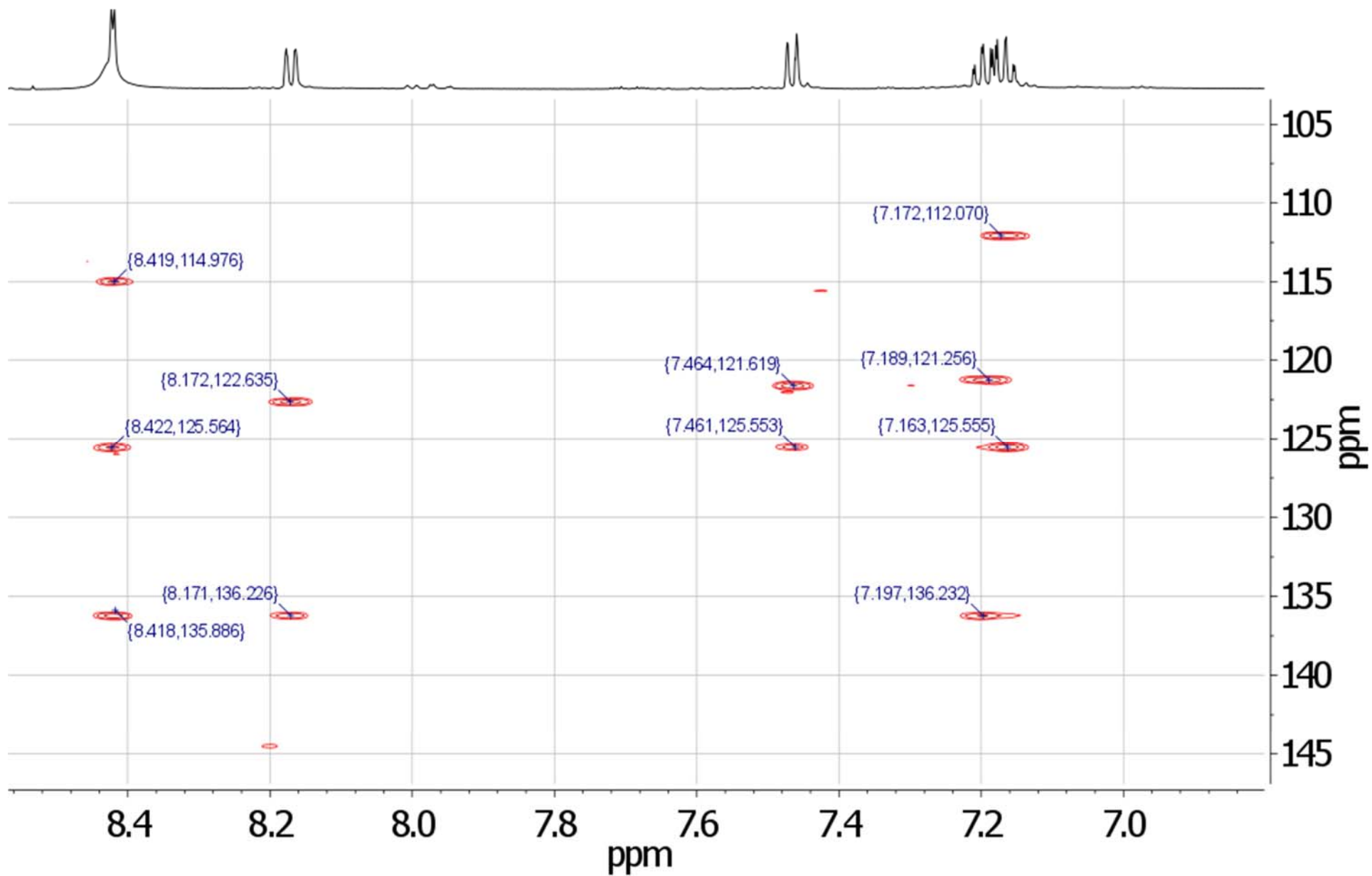
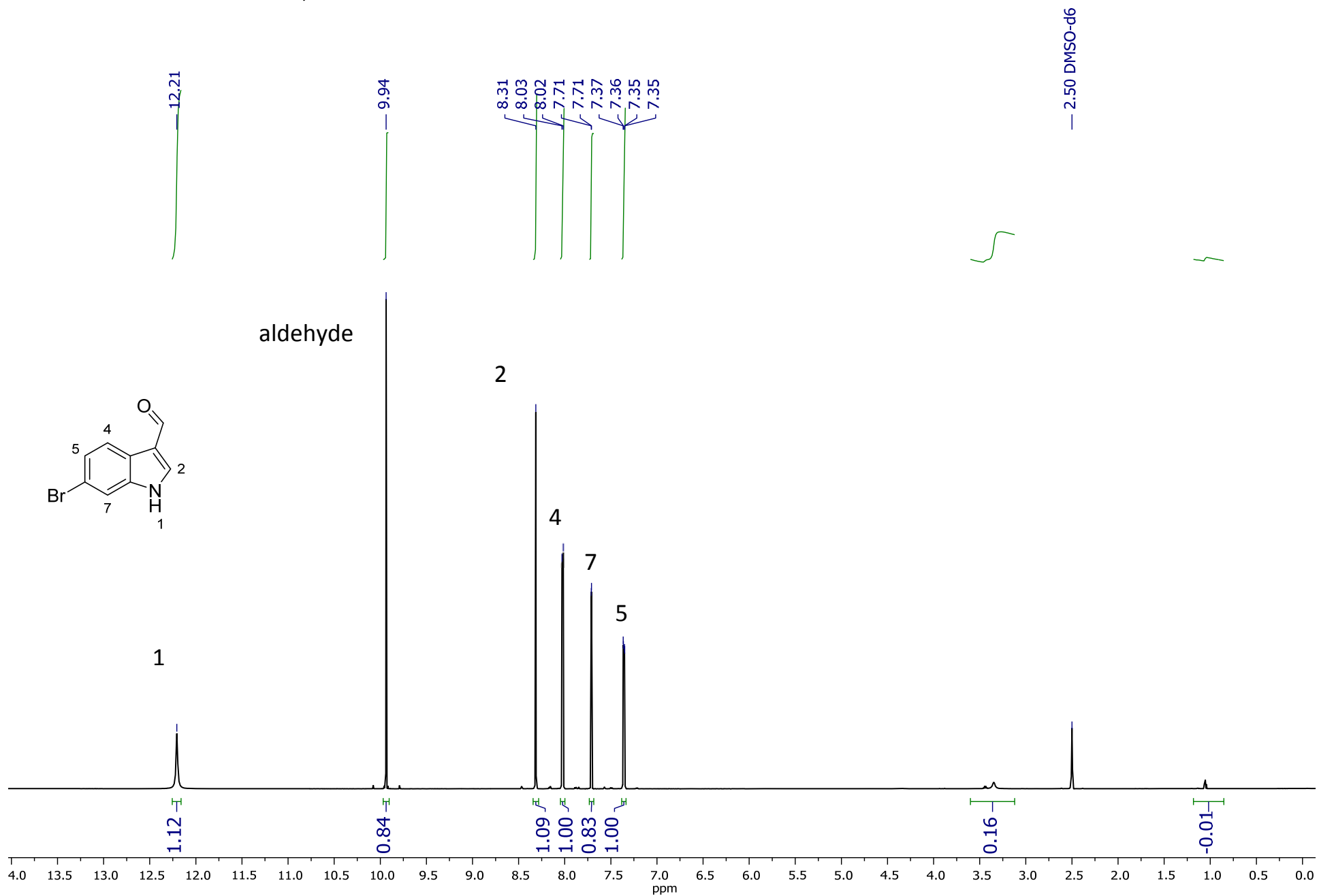


Figure S33. gHMBCAD spectrum expansion (600 MHz) of 8-keto-*N,N*-dimethyl-tryptamine (**16**) in DMSO-d<sub>6</sub>.



**Figure S34.**  $^1\text{H}$  spectrum (600 MHz) of 6-bromo-1H-indol-3-yl-carboxaldehyde (Tokyo Chemical Industry, Tokyo, Japan) (**5**) in DMSO-d<sub>6</sub>.



**Figure S35.**  $^1\text{H}$  spectrum expansion (600 MHz) of 6-bromo-1H-indol-3-yl-carboxaldehyde (Tokyo Chemical Industry, Tokyo, Japan) (**5**) in DMSO-d<sub>6</sub>.

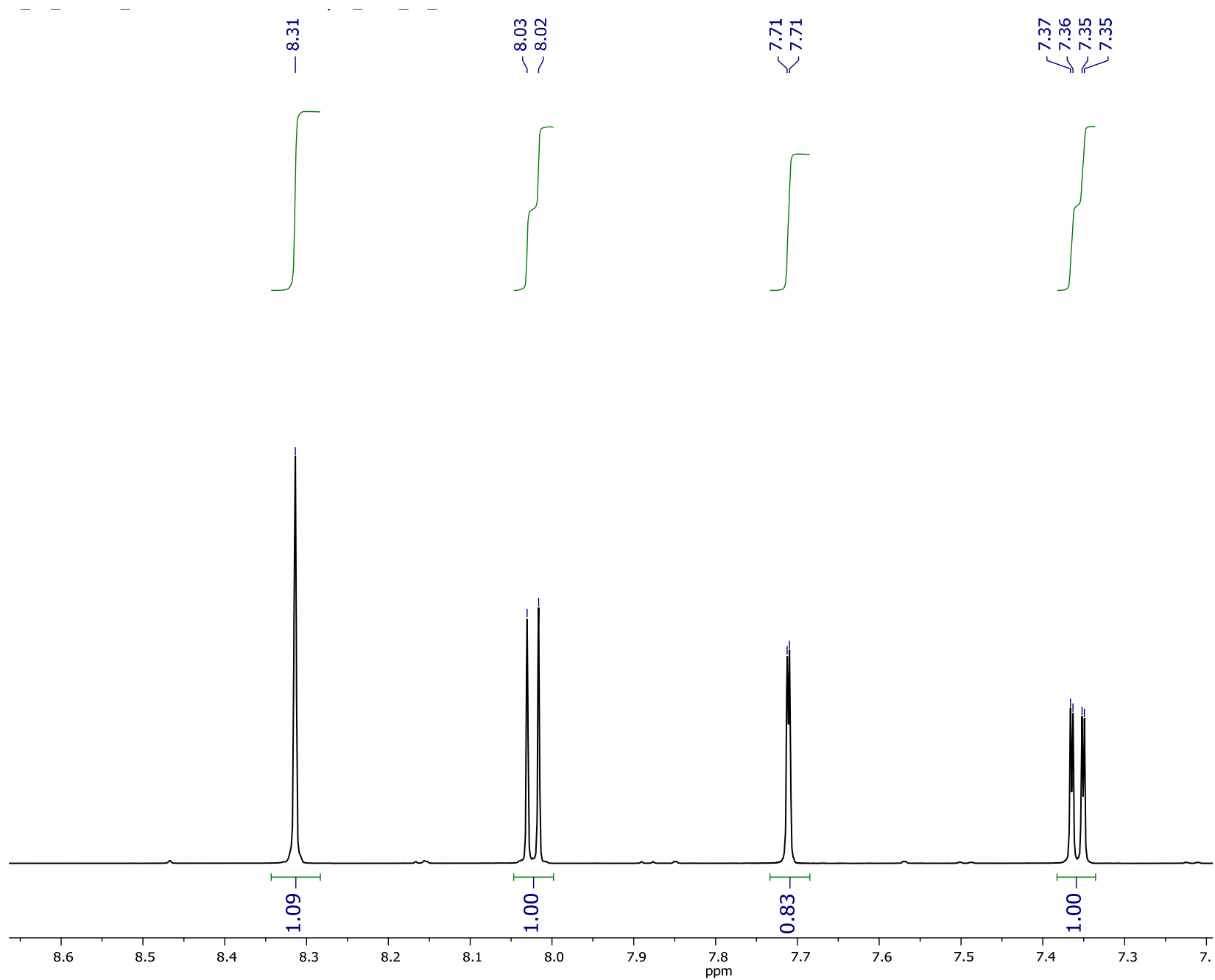


Figure S36.  $^{13}\text{C}$  spectrum (150 MHz) of 6-bromo-1H-indol-3-yl-carboxaldehyde (Tokyo Chemical Industry, Tokyo, Japan) (5) in DMSO-d<sub>6</sub>.

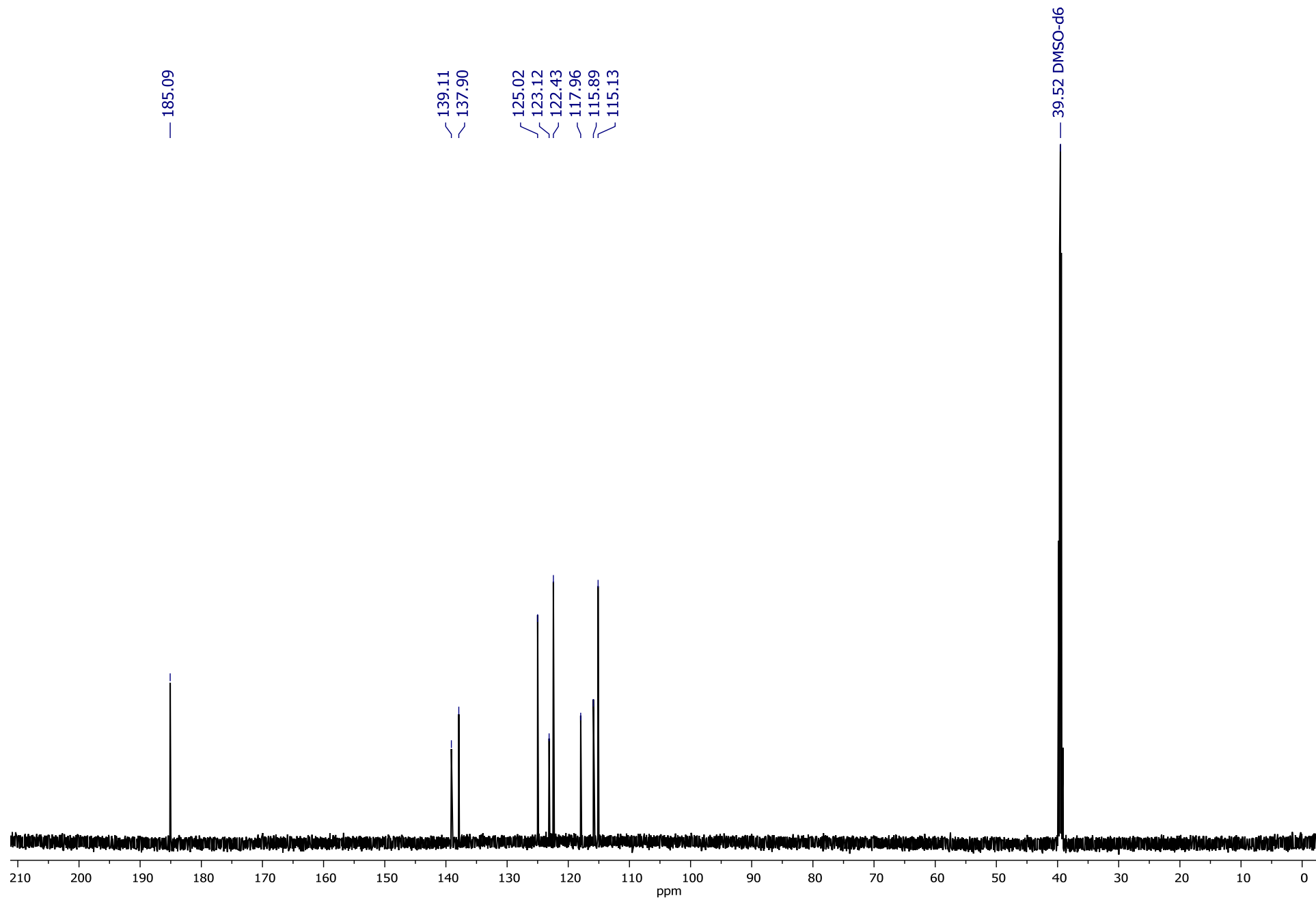
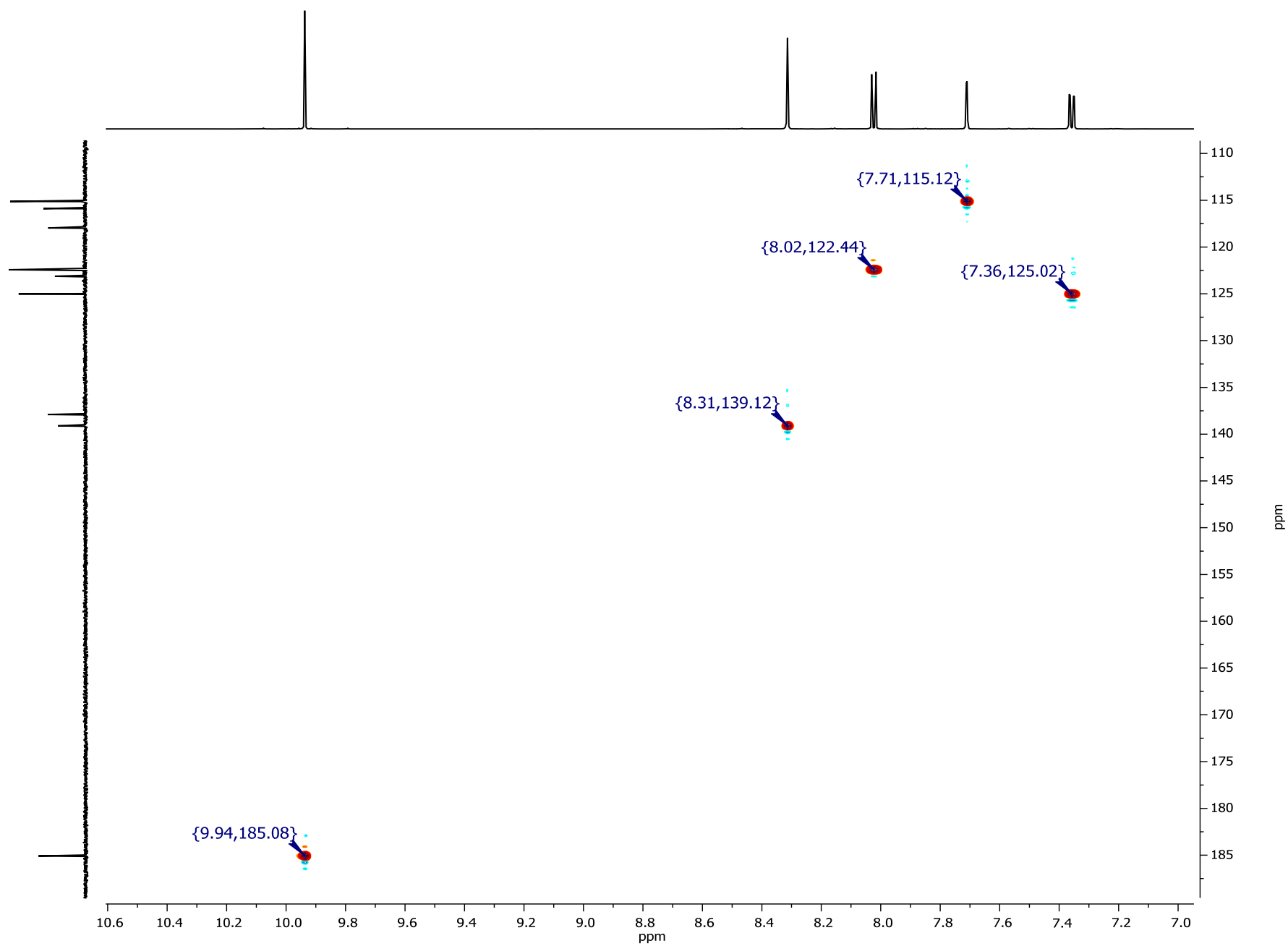


Figure S37. gHSQCAD spectrum (600 MHz) of 6-bromo-1H-indol-3-yl-carboxaldehyde (Tokyo Chemical Industry, Tokyo, Japan) (5) in DMSO-d6.



**Figure S38.** NOESY spectrum (600 MHz, 600ms mixing time) of 6-bromo-1H-indol-3-yl-carboxaldehyde (Tokyo Chemical Industry, Tokyo, Japan) (**5**) in DMSO-d<sub>6</sub>.

