

## Supporting Information

### Site-selective iron-catalyzed C-H alkylation of pyrazinone, azauracils and quinoxalinones

Vaibhav Ramchandra Pansare, Sreelakshmi. N and Nagaraju Barsu\*  
CSIR-National Chemical Laboratory  
*n.barsu@ncl.res.in*

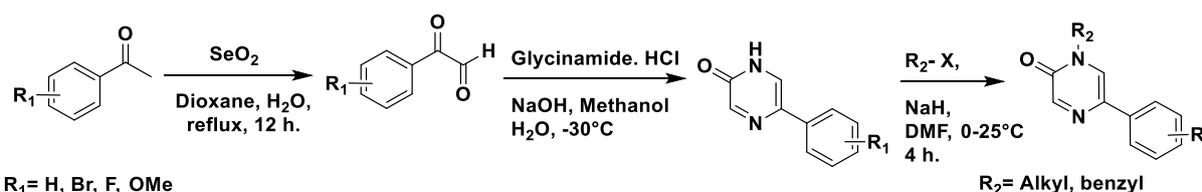
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## 1. General Information

Unless stated otherwise, all reactions were carried out under Argon in a 25 mL Schlenk tube. Dry distilled solvents were prepared by using fractional distillation and vacuum distillation. All the reactions were monitored by analytical thin layer chromatography (TLC) using commercial aluminium sheets precoated with silica gel. Column Chromatography was conducted on silica gel (Merck, 100-200 mesh and 230-400 mesh). All other chemicals were received and used as such from the commercial sources. Iron precursor was purchased from the sigma Aldrich (Purity 97%). NMR spectra were recorded on Bruker Advance 200, 400, 500 MHz instruments. NMR data have been reported as follows: chemical shift ( $\delta$ ) in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q =quartet, and m = multiplet), coupling constant ( $J$ ) in Hz, and integration. Mass spectra were recorded ion Thermo Scientific Q Exactive mass spectrometer, the column specification is Hypersil gold C18 column 150  $\times$  4.6 mm diameter 8  $\mu$ m particle size mobile phase used is acetonitrile and methanol.

## 2. Preparation for pyrazinone derivatives<sup>1,2</sup>

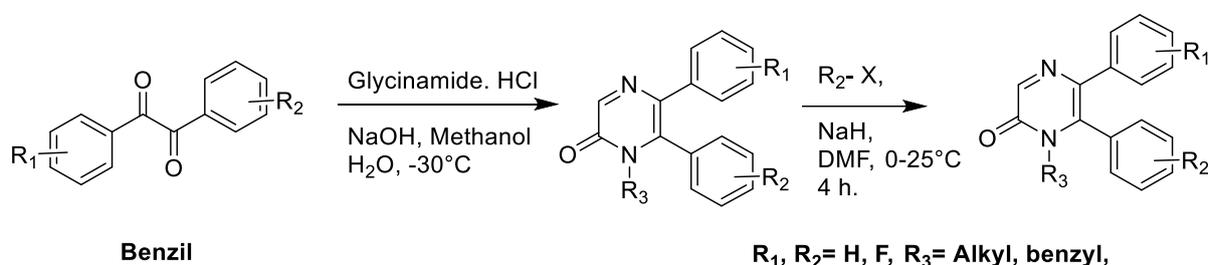


An oven-dried round-bottom flask was charged with substituted acetophenones (1.0 equiv.), dioxane (24 volumes), and water (1.1 volumes). Selenium dioxide ( $\text{SeO}_2$ , 1.0 equiv.) was added in one portion under a nitrogen atmosphere. The reaction mixture was stirred at 115  $^\circ\text{C}$  for 12 hours. After cooling to room temperature, the mixture was filtered through a celite pad. The filtrate was concentrated under reduced pressure, and the residue was purified by flash chromatography on silica gel using a n-hexanes/ethyl acetate (4:1) solvent system to afford the corresponding aryl glyoxal compounds.

An oven-dried round-bottom flask was charged with glycinamide hydrochloride (1.0 equiv.) and methanol (9 volumes). water (2 volumes) was added to form a suspension. At 30 $^\circ\text{C}$ , 12.5 M aqueous sodium hydroxide solution (2.2 volumes, 1.4 equiv.) was added, followed by a solution of sodium hydroxide (1.0 equiv.) in methanol (4 volumes). Substituted phenyl glyoxal monohydrate (1.0 equiv.) was added at 30 $^\circ\text{C}$ , and the reaction mixture was stirred at this temperature for 2 hours. It was then warmed to room temperature and stirred for an additional hour. The mixture was cooled in an ice bath and acidified with acetic acid. The precipitate formed was collected by filtration and dried to afford the substituted 5-phenyl pyrazinone (1a) as a pale red solid in 70% yield.

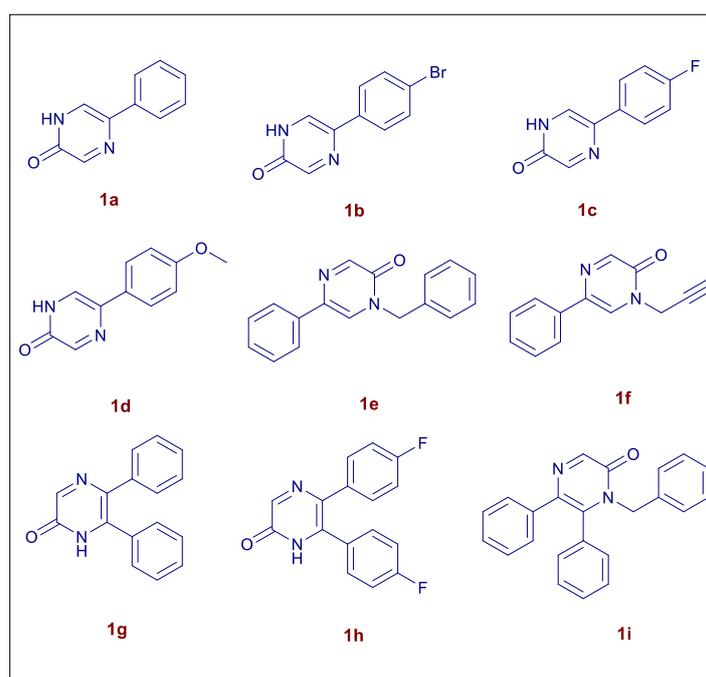
An oven-dried round-bottom flask was charged with sodium hydride (1.5 equiv., 60% dispersion in mineral oil) and dimethylformamide (DMF, 2 mL) under nitrogen atmosphere. A solution of 1a (3.5 mmol, 1.0 equiv.) in DMF (2 mL) and tetrahydrofuran (THF, 2 mL) was added dropwise at 0 °C. After 15 minutes, a solution of the corresponding alkyl halide (1.3 equiv.) in THF (1 mL) was added dropwise. Tetra-*n*-butylammonium iodide (0.1 equiv.) was added as a phase-transfer catalyst. The reaction mixture was stirred at room temperature for 3 hours, then quenched with ice water and extracted with ethyl acetate. The combined organic layers were washed with brine, dried over sodium sulfate (Na<sub>2</sub>SO<sub>4</sub>), and concentrated under reduced pressure. The crude product was purified by flash chromatography using a *n*-hexanes/ethyl acetate solvent system to afford the corresponding *N*-alkyl 5-phenyl pyrazinones

### 3. Synthesis of *N*-substituted 5,6-diphenyl pyrazinones (1g-i)

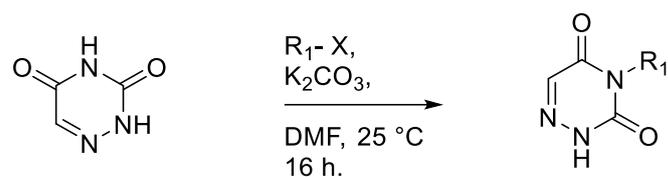


*N*-Substituted 5,6-diphenyl pyrazinone was prepared from according to the protocol described for 1a.

### 4. List of pyrazinone substrates



## 5. General procedure for the synthesis of *N*-alkyl azauracils.

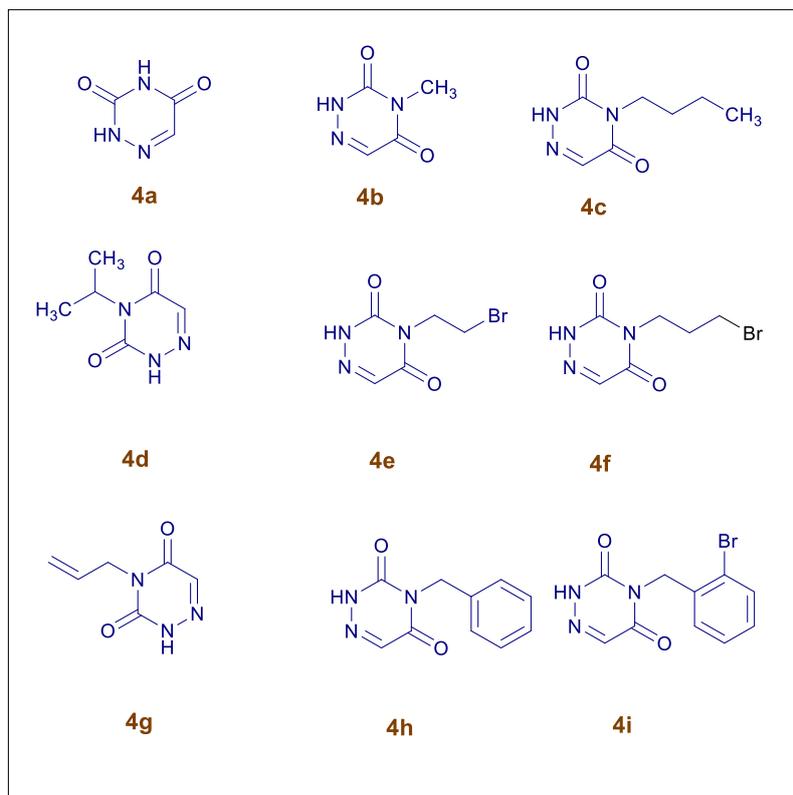


**6-azauracil**

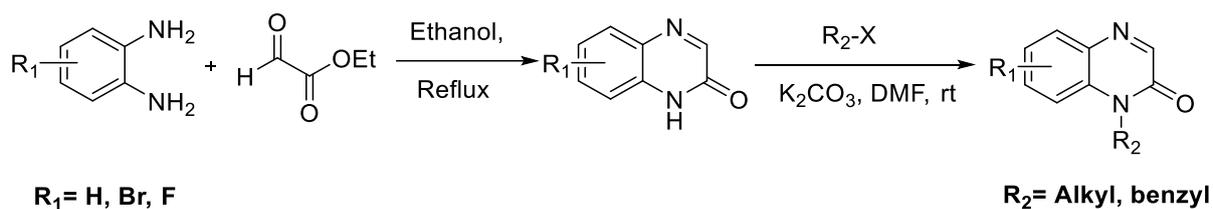
**R<sub>1</sub> = Alkyl, benzyle**

In an oven-dried 100 mL round-bottom flask equipped with a magnetic stir bar, 6-azauracil (4.0 mmol, 1.0 equiv.) and potassium carbonate (K<sub>2</sub>CO<sub>3</sub>; 0.5 equiv.) were suspended in anhydrous *N,N*-dimethylformamide (DMF; 40 mL) under ambient atmosphere. To this suspension, the appropriate alkyl halide (0.9 equiv.) was added dropwise over 5 minutes. The reaction mixture was stirred at room temperature (~25 °C) for 16 hours. Upon completion, the reaction mixture was concentrated under reduced pressure using a rotary evaporator. The resulting crude residue was subjected to purification by flash column chromatography (*n*-hexanes/EtOAc) to afford the desired *N*-1-alkyl-6-azauracil derivative as a purified product (**4a-4i**).

## 6. List of azauracil substrates.

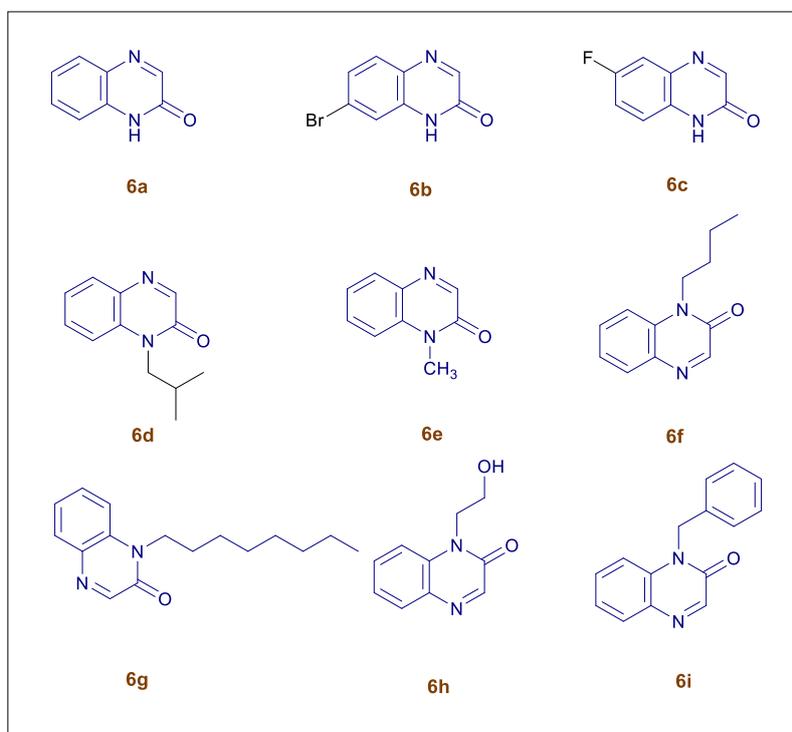


## 7. Preparation for quinoxalinone derivatives<sup>3</sup>

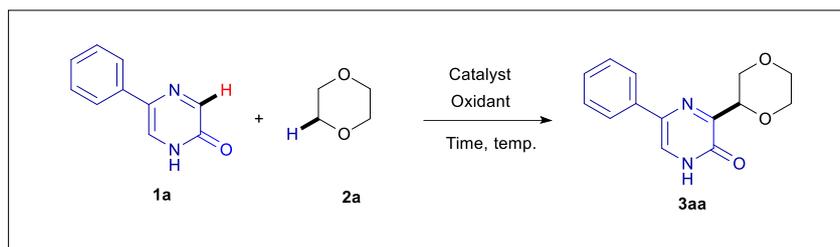


Quinoxalin-2(1*H*)-one was prepared from 1,2-phenylenediamines following the procedure of Cui and co-workers on 5 mmol scale. To a solution of 1,2-phenylenediamines (5 mmol, 1.0 equiv.) in ethanol (40 mL) was added ethyl glyoxalate (6 mmol, 1.2 equiv.). The resultant reaction mixture was stirred at reflux until the raw material disappears. Then, the mixture was filtered and washed by ethanol. The solid was dried in vacuo. For alkylation, the corresponding halogenoalkane (1.6 equiv.) was added to a suspension of quinoxalinone (1.0 equiv.) and potassium carbonate (1.2 equiv.) in DMF (16 mL). The mixture was stirred at room temperature overnight. After complete reaction, brine was added, and then extracted three times with EtOAc, dried over anhydrous  $\text{Na}_2\text{SO}_4$ , filtered and evaporated in vacuo. The residue was purified by column chromatography on silica gel to afford the desired product. The compound (**6a-6i**) was synthesized according to previously reported literature.<sup>2</sup>

## 8. List of quinoxalinone derivatives (**6a-6i**)



## 9. Table S1: Optimization of the reaction conditions for the alkylation of pyrazin-2(1H)-one with dioxane.<sup>a</sup>



Entry	Catalyst (mol%)	Oxidant (equiv.)	Temp.(°C)	Yield <sup>b</sup> (%)
1	Fe(acac) <sub>3</sub> (20)	TBHP (4.0)	100	75
2	Fe(acac) <sub>3</sub> (20)	TBHP (50mol%)	100	24
3	Fe(acac) <sub>3</sub> (20)	TBHP (1.0)	100	41
4	Fe(acac) <sub>3</sub> (20)	TBHP (2.0)	100	81
5	Fe(acac) <sub>3</sub> (10)	TBHP (4.0)	80	84
<b>5</b>	<b>Fe(acac)<sub>3</sub>(10)</b>	<b>TBHP (2.0)</b>	<b>80</b>	<b>86</b>
6	Fe(acac) <sub>3</sub> (10)	TBHP (2.0)	60	65
7	Fe(acac) <sub>3</sub> (10)	TBHP (2.0)	40	15
8 <sup>c</sup>	Fe(acac) <sub>3</sub> (10)	TBHP (2.0)	80	76
9 <sup>d</sup>	Fe(acac) <sub>3</sub> (10)	TBHP (2.0)	80	81
10 <sup>e</sup>	Fe(acac) <sub>3</sub> (10)	TBHP (2.0)	80	65
11	-	TBHP (2.0)	80	NR
12	Fe(acac) <sub>3</sub> (10)	-	80	NR
13	Fe(acac) <sub>3</sub> (10)	DTBP (2.0)	80	NR
14	Fe(acac) <sub>3</sub> (10)	H <sub>2</sub> O <sub>2</sub> (2.0)	80	NR
15	Cu(OAc) <sub>2</sub> (10)	TBHP (2.0)	80	55

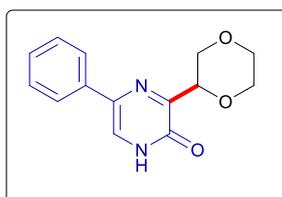
<sup>a</sup>Reaction conditions: Phenylpyrazin-2(1H)-one (1a) (0.3 mmol), Dioxane (2a) (2 mL), Fe(acac)<sub>3</sub>- (10mol%), TBHP (2.0 equiv), for 24 h under argon at 80°C. <sup>b</sup>Isolated yield, <sup>c</sup>48h, <sup>d</sup>dioxane (1mL), <sup>e</sup>in air, NR: no reaction.

## 10. General procedure alkylation of pyrazinones, azauracils and quinoxalinones

An oven dried Schlenk tube was charged with Teflon coated magnetic stir bar under inert atmosphere added substituted *N*-heterocycles (0.3 mmol, 1 equiv.), Fe(acac)<sub>3</sub> (10 mol%) and 1,4 dioxane (2 mL). Followed by TBHP (0.6 mmol, 2 equiv.). The resultant reaction mixture was stirred and heated in a closed system at 80 °C for 24 h. Solvent was evaporated under reduced pressure and the crude mixture was purified by flash column chromatography (60% EtOAc: Hexane) on silica gel afforded alkylated *N*-heterocycles.

## 11. Analytical data of the products

### 3-(1,4-dioxan-2-yl)-5-phenylpyrazin-2(1H)-one (3aa)



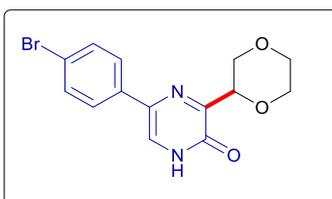
Compound **3aa** prepared according to the general procedure and purified by flash column chromatography (65% EtOAc:pet ether) yield 86% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.61 (s, 1H), 8.00 (s, 1H), 7.86 (d, *J* = 7.6 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.2 Hz, 1H), 4.92 (d, *J* = 7.8 Hz, 1H), 3.91 (t, *J* = 9.8 Hz, 2H), 3.75 (dd, *J* = 16.6, 10.4 Hz, 3H), 3.62 (d, *J* = 11.8 Hz, 1H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  154.39, 152.38, 135.73, 131.30, 128.67, 127.44, 124.59, 124.27, 72.28, 68.17, 66.35, 65.82.

**HRMS:** *m/z* (ESI) Calculated for C<sub>14</sub>H<sub>15</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 259.1083; found: 259.1077.

### 5-(4-bromophenyl)-3-(1,4-dioxan-2-yl)pyrazin-2(1H)-one(3ba)



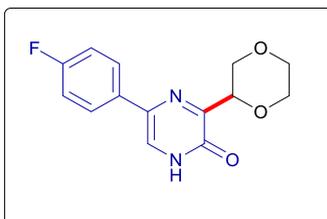
Compound **3ba** prepared according to the general procedure and purified by flash column chromatography (65% EtOAc:pet ether) yield 75% as pale yellow solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.70 (s, 1H), 8.06 (s, 1H), 7.83 (d, 2H), 7.62 (d, 2H), 4.91 (t, 1H), 3.92 (d, 2H), 3.73 (m, 3H), 3.60 (t, *J* = 11.8, 2.7 Hz, 1H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  154.36, 152.72, 135.05, 131.60, 130.09, 126.62, 124.64, 120.63, 72.35, 68.20, 66.39, 65.83.

**HRMS:** *m/z* (ESI) Calculated for C<sub>14</sub>H<sub>13</sub>BrN<sub>2</sub>O<sub>3</sub> [M]<sup>+</sup> 336.0110; found: 336.0375.

### 3-(1,4-dioxan-2-yl)-5-(4-fluorophenyl)pyrazin-2(1H)-one (3ca)



Compound **3ca** prepared according to the general procedure and purified by flash column chromatography (65% EtOAc:pet ether) yield 83% as white solid.

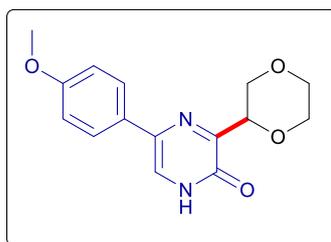
**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.64 (s, 1H), 8.00 (s, 1H), 7.95 – 7.84 (m, 2H), 7.25 (t, *J* = 8.9 Hz, 2H), 4.91 (dd, *J* = 9.6, 2.6 Hz, 1H), 3.95 – 3.84 (m, 2H), 3.73 (ddd, *J* = 11.4, 8.4, 3.3 Hz, 3H), 3.62 (dd, *J* = 11.8, 2.7 Hz, 1H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  161.80 (d, *J* = 244.4 Hz), 154.34, 152.42, 132.31 (d, *J* = 2.9 Hz), 130.61, 126.71 (d, *J* = 8.2 Hz), 124.23, 115.54 (d, *J* = 21.5 Hz), 72.33, 68.22, 66.40, 65.86.

**<sup>19</sup>F NMR (376 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  -115.06.

**HRMS:** *m/z* (ESI) Calculated for C<sub>14</sub>H<sub>14</sub>FN<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 277.0988; found: 277.0983.

### 3-(1,4-dioxan-2-yl)-5-(4-methoxyphenyl)pyrazin-2(1H)-one (3da)



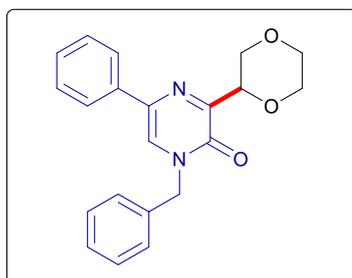
Compound **3da** prepared according to the general procedure and purified by flash column chromatography (65% EtOAc:pet ether) yield 81% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.51 (s, 1H), 7.90 (s, 1H), 7.79 (d, *J* = 8.6 Hz, 2H), 6.98 (d, *J* = 8.6 Hz, 2H), 4.91 (d, *J* = 9.5 Hz, 1H), 3.90 (dd, *J* = 9.2, 7.1 Hz, 2H), 3.78 (s, 3H), 3.73 (dd, *J* = 9.6, 4.7 Hz, 3H), 3.65 – 3.57 (m, 1H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  158.88, 154.22, 151.90, 131.72, 128.32, 125.97, 123.33, 114.06, 72.28, 68.17, 66.33, 65.80, 55.15.

**HRMS:** *m/z* (ESI) Calculated for C<sub>15</sub>H<sub>17</sub>N<sub>2</sub>O<sub>4</sub> [M+H]<sup>+</sup> 289.1188; found: 289.1183.

### 1-benzyl-3-(1,4-dioxan-2-yl)-5-phenylpyrazin-2(1H)-one (3ea)



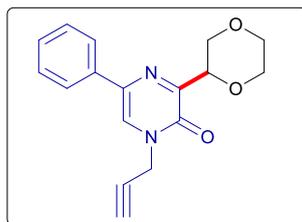
Compound **3ea** prepared according to the general procedure and purified by flash column chromatography (40% EtOAc:pet ether) yield 70% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  8.51 (s, 1H), 7.86 (d, *J* = 7.7 Hz, 2H), 7.47 – 7.40 (m, 4H), 7.38 – 7.29 (m, 4H), 5.17 (q, *J* = 14.1 Hz, 2H), 5.02 – 4.91 (m, 1H), 3.97 – 3.85 (m, 2H), 3.75 (dd, *J* = 22.5, 11.0 Hz, 3H), 3.61 (d, *J* = 11.8 Hz, 1H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  153.54, 152.66, 135.99, 135.42, 130.68, 128.75, 128.68, 128.12, 127.94, 127.66, 126.93, 124.58, 72.51, 68.16, 66.36, 65.81, 52.22.

**HRMS:** *m/z* (ESI) Calculated for C<sub>21</sub>H<sub>21</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 349.1552; found: 349.1547.

### 3-(1,4-dioxan-2-yl)-5-phenyl-1-(prop-2-yn-1-yl)pyrazin-2(1H)-one (3fa)



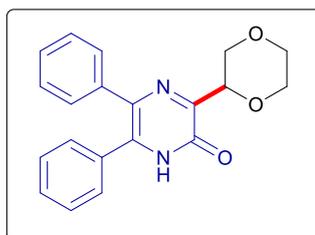
Compound **3fa** prepared according to the general procedure and purified by flash column chromatography (45% EtOAc:pet ether) yield 60% as white solid.

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  7.73 (s, 1H), 7.60 (d,  $J$  = 7.8 Hz, 2H), 7.26 (t,  $J$  = 7.4 Hz, 2H), 7.18 (d,  $J$  = 7.0 Hz, 1H), 5.01 (d,  $J$  = 9.3 Hz, 1H), 4.63 (s, 2H), 3.94 (d,  $J$  = 11.6 Hz, 1H), 3.81 (ddd,  $J$  = 17.6, 15.4, 8.7 Hz, 3H), 3.64 (d,  $J$  = 5.7 Hz, 2H), 2.45 (s, 1H).

**<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)**  $\delta$  153.63, 153.38, 135.56, 133.37, 128.98, 128.32, 125.39, 122.88, 77.20, 75.49, 73.51, 68.90, 67.35, 66.56, 38.27.

**HRMS:**  $m/z$  (ESI) Calculated for C<sub>17</sub>H<sub>17</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 297.1239; found 297.1197.

### 3-(1,4-dioxan-2-yl)-5,6-diphenylpyrazin-2(1H)-one (**3ga**)



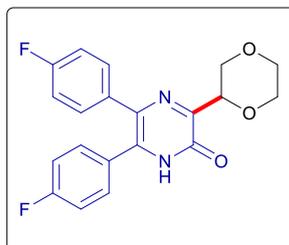
Compound **3ga** prepared according to the general procedure and purified by flash column chromatography (65% EtOAc:pet ether) yield 76% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.53 (s, 1H), 7.39 – 7.29 (m, 5H), 7.21 (d,  $J$  = 5.0 Hz, 5H), 4.95 (d,  $J$  = 9.5 Hz, 1H), 3.91 (dd,  $J$  = 19.9, 11.6 Hz, 2H), 3.81 – 3.71 (m, 3H), 3.61 (d,  $J$  = 11.2 Hz, 1H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  154.97, 137.63, 131.22, 129.68, 129.28, 128.34, 128.21, 127.87, 127.47, 127.17, 72.32, 68.28, 66.43, 65.80.

**HRMS:**  $m/z$  (ESI) Calculated for C<sub>20</sub>H<sub>19</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 335.1396; found 335.1390.

### 3-(1,4-dioxan-2-yl)-5,6-bis(4-fluorophenyl)pyrazin-2(1H)-one (**3ha**)



Compound **3ha** prepared according to the general procedure and purified by flash column chromatography (65% EtOAc:pet ether) yield 80% as white solid.

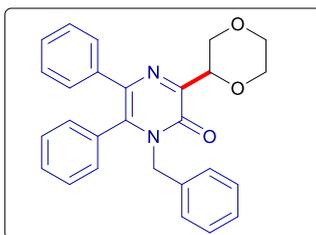
**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)** δ 7.45 – 7.31 (m, 2H), 7.22 (dt, *J* = 14.3, 5.5 Hz, 4H), 7.09 (t, *J* = 8.9 Hz, 2H), 4.94 (dd, *J* = 9.7, 2.6 Hz, 1H), 3.98 – 3.84 (m, 2H), 3.81 – 3.68 (m, 3H), 3.59 (td, *J* = 11.5, 2.7 Hz, 1H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)** δ 162.48 (d, *J* = 247.0 Hz), 161.39 (d, *J* = 244.7 Hz), 155.11, 155.03, 134.01, 133.98, 132.09 (d, *J* = 8.6 Hz), 131.31 (d, *J* = 8.3 Hz), 115.46 (d, *J* = 21.9 Hz), 114.91 (d, *J* = 21.5 Hz), 72.31, 68.25, 66.42, 65.78.

**<sup>19</sup>F NMR (376 MHz, DMSO-*d*<sub>6</sub>)** δ -111.69, -114.79.

**HRMS:** *m/z* (ESI) Calculated for C<sub>20</sub>H<sub>17</sub>F<sub>2</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 371.1207; found 371.1201.

### 1-benzyl-3-(1,4-dioxan-2-yl)-5,6-diphenylpyrazin-2(1H)-one(3ia)



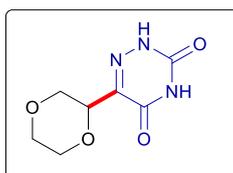
Compound **3ia** prepared according to the general procedure and purified by flash column chromatography (65% EtOAc:pet ether) yield 65% as white solid.

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)** δ 7.36 – 7.31 (m, 1H), 7.15 – 7.07 (m, 5H), 7.00 (d, *J* = 7.7 Hz, 1H), 6.93 (d, *J* = 7.6 Hz, 1H), 6.85 (dd, *J* = 6.4, 3.1 Hz, 2H), 5.30 (dd, *J* = 9.6, 2.7 Hz, 1H), 5.14 (dd, *J* = 35.1, 14.7 Hz, 2H), 4.20 (dd, *J* = 11.4, 2.6 Hz, 1H), 4.08 – 3.93 (m, 3H), 3.84 – 3.79 (m, 2H).

**<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)** δ 154.73, 152.71, 138.55, 137.57, 135.94, 133.56, 131.85, 130.62, 130.42, 129.64, 128.67, 128.61, 127.80, 127.70, 127.38, 127.18, 73.90, 69.14, 67.48, 66.54, 49.25.

**HRMS:** *m/z* (ESI) Calculated for C<sub>27</sub>H<sub>25</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 425.1865; found 425.1901.

### 6-(1,4-dioxan-2-yl)-1,2,4-triazine-3,5(2H,4H)-dione (5aa)



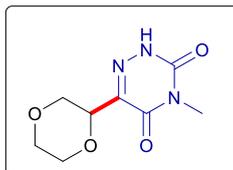
Compound **5aa** prepared according to the general procedure and purified by flash column chromatography (65% EtOAc:pet ether) yield 78% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)** δ 12.34 (s, 1H), 12.03 (s, 1H), 4.59 (dd, *J* = 9.9, 2.5 Hz, 1H), 3.83 – 3.73 (m, 2H), 3.68 (dd, *J* = 9.7, 2.2 Hz, 2H), 3.53 (ddd, *J* = 14.6, 11.6, 7.0 Hz, 2H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)** δ 156.36, 149.18, 141.03, 70.58, 67.84, 66.47, 65.76.

**HRMS:** *m/z* (ESI) Calculated for C<sub>7</sub>H<sub>10</sub>N<sub>3</sub>O<sub>4</sub> [M+H]<sup>+</sup> 200.0671; found 200.0666.

### 6-(1,4-dioxan-2-yl)-4-methyl-1,2,4-triazine-3,5(2H,4H)-dione (5ba)



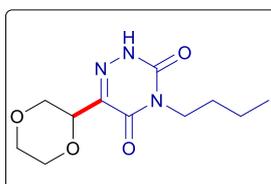
Compound **5ba** prepared according to the general procedure and purified by flash column chromatography (60% EtOAc:pet ether) yield 65% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.59 (s, 1H), 4.63 (dd, *J* = 9.9, 2.6 Hz, 1H), 3.84 – 3.75 (m, 2H), 3.68 (dd, *J* = 16.6, 6.5 Hz, 2H), 3.60 – 3.49 (m, 2H), 3.11 (s, 3H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  155.65, 149.37, 139.96, 71.12, 67.94, 66.51, 65.81, 26.10.

**HRMS:** *m/z* (ESI) Calculated for C<sub>8</sub>H<sub>12</sub>N<sub>3</sub>O<sub>4</sub> [M+H]<sup>+</sup> 214.0828; found 214.0828.

#### 4-butyl-6-(1,4-dioxan-2-yl)-1,2,4-triazine-3,5(2H,4H)-dione (**5ca**)



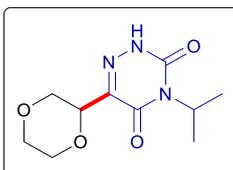
Compound **5ca** prepared according to the general procedure and purified by flash column chromatography (55% EtOAc:pet ether) yield 77% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.58 (s, 1H), 4.62 (dd, *J* = 9.9, 2.5 Hz, 1H), 3.79 (dd, *J* = 11.2, 2.5 Hz, 2H), 3.76 – 3.64 (m, 4H), 3.62 – 3.49 (m, 2H), 1.55 – 1.44 (m, 2H), 1.33 – 1.20 (m, 2H), 0.88 (t, *J* = 7.3 Hz, 3H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  155.31, 149.09, 140.24, 71.03, 67.85, 66.49, 65.78, 39.52, 39.21, 28.80, 19.66, 13.65.

**HRMS:** *m/z* (ESI) Calculated for C<sub>11</sub>H<sub>18</sub>N<sub>3</sub>O<sub>4</sub> [M+H]<sup>+</sup> 256.1297; found 256.1292.

#### 6-(1,4-dioxan-2-yl)-4-isopropyl-1,2,4-triazine-3,5(2H,4H)-dione (**5da**)



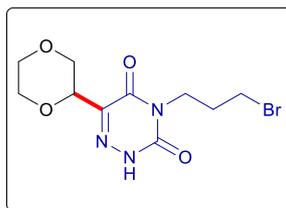
Compound **5da** prepared according to the general procedure and purified by flash column chromatography (55% EtOAc:pet ether) yield 70% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.44 (s, 1H), 4.89 (dt, *J* = 13.8, 6.9 Hz, 1H), 4.62 (dd, *J* = 9.8, 2.1 Hz, 1H), 3.79 (d, *J* = 11.3 Hz, 2H), 3.66 (dd, *J* = 18.9, 7.0 Hz, 2H), 3.61 – 3.49 (m, 2H), 1.36 (d, *J* = 6.9 Hz, 6H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  155.54, 148.97, 140.54, 70.88, 67.85, 66.48, 65.76, 44.47, 18.70, 18.62.

**HRMS:** *m/z* (ESI) Calculated for C<sub>10</sub>H<sub>16</sub>N<sub>3</sub>O<sub>4</sub> [M+H]<sup>+</sup> 242.1141; found 242.1141.

#### 4-(3-bromopropyl)-6-(1,4-dioxan-2-yl)-1,2,4-triazine-3,5(2H,4H)-dione (**5ea**)



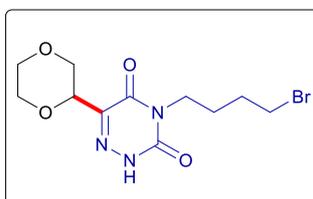
Compound **5ea** prepared according to the general procedure and purified by flash column chromatography (50% EtOAc:petether) yield 75% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.57 (s, 1H), 4.62 (dd, *J* = 9.8, 2.1 Hz, 1H), 3.84 (dd, *J* = 15.0, 8.2 Hz, 3H), 3.78 (s, 2H), 3.53 (dd, *J* = 16.0, 8.7 Hz, 4H), 2.08 (p, *J* = 6.7 Hz, 2H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  155.51, 149.18, 140.25, 71.07, 67.95, 66.48, 65.78, 38.47, 32.05, 30.13.

**HRMS:** *m/z* (ESI) Calculated for C<sub>10</sub>H<sub>15</sub>BrN<sub>3</sub>O<sub>4</sub> [M+H]<sup>+</sup> 320.0246; found: 320.0240.

#### 4-(4-bromobutyl)-6-(1,4-dioxan-2-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione(5fa)



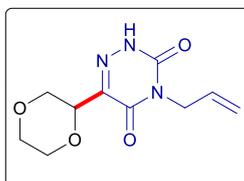
Compound **5fa** prepared according to the general procedure and purified by flash column chromatography (50% EtOAc:pet ether) yield 76% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.59 (s, 1H), 4.75 – 4.53 (m, 1H), 3.77 (dd, *J* = 17.1, 9.5 Hz, 4H), 3.68 (d, *J* = 10.5 Hz, 2H), 3.59 (d, *J* = 10.7 Hz, 1H), 3.57 – 3.51 (m, 3H), 1.85 – 1.74 (m, 2H), 1.71 – 1.61 (m, 2H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  155.36, 149.12, 140.25, 71.03, 67.86, 66.47, 65.77, 38.65, 34.63, 29.68, 25.52.

**HRMS:** *m/z* (ESI) Calculated for C<sub>11</sub>H<sub>17</sub>BrN<sub>3</sub>O<sub>4</sub> [M+H]<sup>+</sup> 334.0402; found: 334.0401

#### 4-allyl-6-(1,4-dioxan-2-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (5ga)



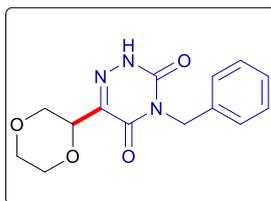
Compound **5ga** prepared according to the general procedure and purified by flash column chromatography (50% EtOAc:pet ether) yield 67% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.64 (s, 1H), 5.86 – 5.74 (m, 1H), 5.14 (s, 1H), 5.11 (dd, *J* = 6.4, 1.3 Hz, 1H), 4.63 (dd, *J* = 9.9, 2.6 Hz, 1H), 4.34 (d, *J* = 5.4 Hz, 2H), 3.84 – 3.75 (m, 2H), 3.68 (d, *J* = 9.2 Hz, 2H), 3.63 – 3.51 (m, 2H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  155.02, 148.83, 140.29, 131.35, 117.37, 71.05, 67.82, 66.50, 65.79, 41.49.

**HRMS:** *m/z* (ESI) Calculated for C<sub>10</sub>H<sub>14</sub>N<sub>3</sub>O<sub>4</sub> [M+H]<sup>+</sup> 240.0984; found 240.0979.

#### 4-benzyl-6-(1,4-dioxan-2-yl)-1,2,4-triazine-3,5(2H,4H)-dione (5ha)



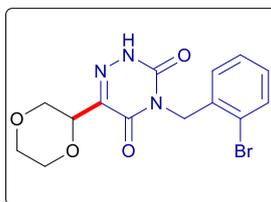
Compound **5ha** prepared according to the general procedure and purified by flash column chromatography (50% EtOAc:petether) yield 70% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.71 (s, 1H), 7.33 – 7.25 (m, 5H), 4.92 (s, 2H), 4.64 (dd, *J* = 9.8, 1.8 Hz, 1H), 3.80 (t, *J* = 10.6 Hz, 2H), 3.68 (d, *J* = 11.3 Hz, 2H), 3.65 – 3.51 (m, 2H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  155.70, 149.55, 140.83, 136.37, 128.90, 128.34, 127.94, 71.44, 68.14, 66.89, 66.16, 43.13.

**HRMS:** *m/z* (ESI) Calculated for C<sub>14</sub>H<sub>16</sub>N<sub>3</sub>O<sub>4</sub> [M+H]<sup>+</sup> 290.1141; found 290.1135.

#### 4-(2-bromobenzyl)-6-(1,4-dioxan-2-yl)-1,2,4-triazine-3,5(2H,4H)-dione (5ia)



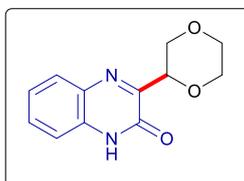
Compound **5ia** prepared according to the general procedure and purified by flash column chromatography (50% EtOAc:petether) yield 67% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.78 (s, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.31 (t, *J* = 7.5 Hz, 1H), 7.23 (t, *J* = 7.2 Hz, 1H), 7.07 (d, *J* = 7.7 Hz, 1H), 4.93 (s, 2H), 4.68 – 4.62 (m, 1H), 3.83 (dd, *J* = 18.7, 7.0 Hz, 2H), 3.68 (t, *J* = 10.3 Hz, 3H), 3.59 – 3.52 (m, 1H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  155.39, 149.10, 140.39, 134.19, 132.59, 129.21, 127.99, 127.12, 121.79, 71.11, 67.85, 66.47, 65.77, 43.26, 39.52.

**HRMS:** *m/z* (ESI) Calculated for C<sub>14</sub>H<sub>15</sub>BrN<sub>3</sub>O<sub>4</sub> [M+H]<sup>+</sup> 368.0246; found 368.0240

#### 3-(1,4-dioxan-2-yl)quinoxalin-2(1H)-one (7aa)



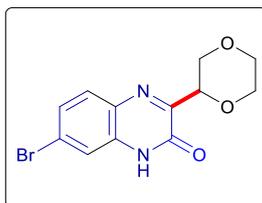
Compound **7aa** prepared according to the general procedure and purified by flash column chromatography (50% EtOAc:petether) yield 92% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.49 (s, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.53 (t, *J* = 7.7 Hz, 1H), 7.30 (t, *J* = 6.9 Hz, 2H), 5.01 (t, 1H), 3.95 (d, 2H), 3.75 (t, 2H), 3.60 (t, 2H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  156.26, 153.75, 131.90, 131.42, 130.60, 128.75, 123.39, 115.42, 72.72, 68.54, 66.32, 65.79.

**HRMS:** *m/z* (ESI) Calculated for C<sub>12</sub>H<sub>13</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 233.0926; found: 233.0921

### 7-bromo-3-(1,4-dioxan-2-yl) quinoxalin-2(1H)-one(7ba)



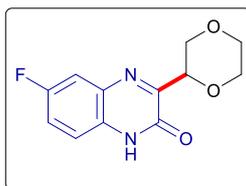
Compound **7ba** prepared according to the general procedure and purified by flash column chromatography (50% EtOAc:petether) yield 79% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.60 (s, 1H), 7.98 (d, *J* = 2.2 Hz, 1H), 7.69 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.24 (d, *J* = 8.7 Hz, 1H), 5.02 (dd, *J* = 9.5, 2.6 Hz, 1H), 3.99 (dd, *J* = 11.4, 2.6 Hz, 1H), 3.92 (dd, *J* = 11.4, 2.3 Hz, 1H), 3.79 – 3.71 (m, 2H), 3.63 – 3.55 (m, 2H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  157.77, 153.53, 133.17, 132.38, 131.28, 130.73, 117.40, 114.68, 72.85, 68.53, 66.28, 65.79.

**HRMS:** *m/z* (ESI) Calculated for C<sub>12</sub>H<sub>12</sub>BrN<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 311.0031; found: 311.0042.

### 3-(1,4-dioxan-2-yl)-6-fluoroquinoxalin-2(1H)-one (7ca)



Compound **7ca** prepared according to the general procedure and purified by flash column chromatography (50% EtOAc:petether) yield 82% as white solid.

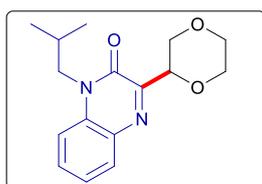
**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.57 (s, 1H), 7.64 (dd, *J* = 9.3, 2.8 Hz, 1H), 7.46 (td, *J* = 8.8, 2.9 Hz, 1H), 7.32 (dd, *J* = 9.0, 5.2 Hz, 1H), 5.03 (dd, *J* = 9.5, 2.6 Hz, 1H), 4.00 (dd, *J* = 11.4, 2.4 Hz, 1H), 3.92 (dd, *J* = 11.4, 2.4 Hz, 1H), 3.74 (dt, *J* = 6.2, 5.7 Hz, 2H), 3.58 (ddd, *J* = 20.9, 11.6, 6.2 Hz, 2H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  157.82 (d, *J* = 239.8 Hz), 157.80, 153.45, 131.79 (d, *J* = 11.6 Hz), 128.79, 118.65 (d, *J* = 24.4 Hz), 116.87 (d, *J* = 8.9 Hz), 113.87 (d, *J* = 22.7 Hz), 72.88, 68.56, 66.27, 65.79.

**<sup>19</sup>F NMR (376 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  -119.04.

**HRMS:** *m/z* (ESI) Calculated for C<sub>12</sub>H<sub>12</sub>FN<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 251.0832; found: 251.0826.

### 3-(1,4-dioxan-2-yl)-1-isobutylquinoxalin-2(1H)-one(7da)



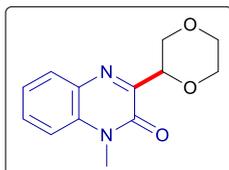
Compound **7da** prepared according to the general procedure and purified by flash column chromatography (50% EtOAc:petether) yield 74% as white solid.

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)** δ 7.97 (d, *J* = 8.0 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 1H), 7.26 (dd, *J* = 14.5, 7.8 Hz, 2H), 5.24 (d, *J* = 9.4 Hz, 1H), 4.19 (d, *J* = 11.1 Hz, 1H), 4.15 – 3.98 (m, 3H), 3.92 (d, *J* = 6.5 Hz, 1H), 3.76 (d, *J* = 6.9 Hz, 2H), 3.57 (t, *J* = 10.3 Hz, 1H), 2.18 (dt, *J* = 13.8, 6.9 Hz, 1H), 0.92 (d, *J* = 6.7 Hz, 6H).

**<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)** δ 155.31, 153.98, 132.97, 132.72, 131.08, 130.68, 123.76, 114.17, 74.79, 69.59, 67.65, 66.45, 49.05, 27.36, 20.31, 20.26.

**HRMS:** *m/z* (ESI) Calculated for C<sub>16</sub>H<sub>21</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 289.1552; found: 289.1547.

### 3-(1,4-dioxan-2-yl)-1-methylquinoxalin-2(1H)-one (7ea)



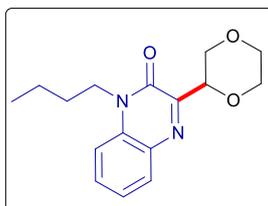
Compound **7ea** prepared according to the general procedure and purified by flash column chromatography (20% EtOAc:petether) yield 79% as white solid

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)** δ 7.84 (d, *J* = 7.9 Hz, 1H), 7.64 (d, *J* = 7.3 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 1H), 5.06 (dd, *J* = 9.4, 2.1 Hz, 1H), 4.00 (d, *J* = 11.3 Hz, 1H), 3.93 (d, *J* = 11.5 Hz, 1H), 3.76 (t, *J* = 10.5 Hz, 2H), 3.63 (s, 3H), 3.61 – 3.50 (m, 2H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)** δ 154.76, 153.17, 133.09, 131.74, 130.85, 129.51, 123.60, 114.80, 73.25, 68.59, 66.29, 65.79, 28.95.

**HRMS:** *m/z* (ESI) Calculated for C<sub>13</sub>H<sub>15</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 247.1083; found: 247.1077.

### 1-butyl-3-(1,4-dioxan-2-yl) quinoxalin-2(1H)-one(7fa)



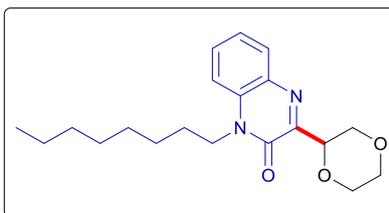
Compound **7fa** prepared according to the general procedure and purified by flash column chromatography (20% EtOAc:petether) yield 77% as thick liquid

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)** δ 8.03 (d, *J* = 8.0 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 1H), 7.33 (dd, *J* = 14.2, 8.0 Hz, 2H), 5.30 (dd, *J* = 9.5, 2.2 Hz, 1H), 4.24 (dd, *J* = 16.9, 8.2 Hz, 3H), 4.11 (d, *J* = 11.7 Hz, 1H), 3.99 (d, *J* = 7.3 Hz, 1H), 3.83 (d, *J* = 6.0 Hz, 2H), 3.65 (t, *J* = 10.4 Hz, 1H), 1.77 – 1.68 (m, 2H), 1.47 (dd, *J* = 15.0, 7.5 Hz, 2H), 0.99 (t, *J* = 7.3 Hz, 3H).

**<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)** δ 155.22, 153.55, 133.02, 132.44, 131.09, 130.86, 123.78, 113.76, 74.73, 69.60, 67.66, 66.46, 42.27, 29.40, 20.39, 13.87.

**HRMS:** *m/z* (ESI) Calculated for C<sub>16</sub>H<sub>21</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 289.1552; found: 289.1547.

### 3-(1,4-dioxan-2-yl)-1-octylquinoxalin-2(1H)-one(7ga)



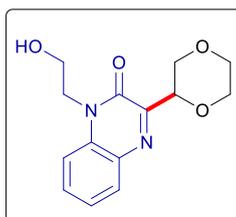
Compound **7ga** prepared according to the general procedure and purified by flash column chromatography (20% EtOAc:pet ether) yield 76% as thick liquid

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**  $\delta$  8.03 (d,  $J$  = 8.0 Hz, 1H), 7.56 (t,  $J$  = 7.8 Hz, 1H), 7.33 (dd,  $J$  = 16.2, 8.2 Hz, 2H), 5.30 (dd,  $J$  = 9.5, 2.4 Hz, 1H), 4.29 – 4.17 (m, 3H), 4.10 (d,  $J$  = 11.7 Hz, 1H), 3.99 (d,  $J$  = 7.5 Hz, 1H), 3.82 (d,  $J$  = 6.0 Hz, 2H), 3.69 – 3.61 (m, 1H), 1.72 (d,  $J$  = 7.8 Hz, 2H), 1.44 (s, 2H), 1.30 (dt,  $J$  = 18.5, 8.7 Hz, 9H), 0.87 (t,  $J$  = 6.6 Hz, 3H).

**<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)**  $\delta$  155.22, 153.52, 133.01, 132.44, 131.07, 130.84, 123.75, 113.75, 74.72, 69.59, 67.65, 66.45, 42.50, 31.85, 29.33, 29.27, 27.37, 27.11, 22.71, 14.18.

**HRMS:**  $m/z$  (ESI) Calculated for C<sub>20</sub>H<sub>29</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 345.2178; found: 345.2201.

### 3-(1,4-dioxan-2-yl)-1-(2-hydroxyethyl) quinoxalin-2(1H)-one(7ha)



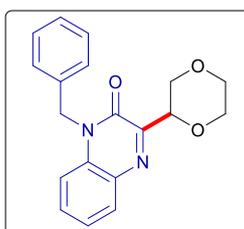
Compound **7ha** prepared according to the general procedure and purified by flash column chromatography (25% EtOAc:petether) yield 75% as viscous liquid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  7.83 (d,  $J$  = 7.6 Hz, 1H), 7.67 (d,  $J$  = 8.3 Hz, 1H), 7.61 (t,  $J$  = 7.6 Hz, 1H), 7.37 (t,  $J$  = 7.4 Hz, 1H), 5.06 (dd,  $J$  = 9.5, 2.4 Hz, 1H), 4.94 (t,  $J$  = 5.8 Hz, 1H), 4.31 (dd,  $J$  = 12.5, 6.2 Hz, 2H), 3.99 (dd,  $J$  = 11.4, 2.1 Hz, 1H), 3.91 (s, 1H), 3.80 – 3.66 (m, 4H), 3.65 – 3.55 (m, 2H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  154.81, 153.38, 133.13, 132.06, 130.78, 129.72, 123.60, 115.36, 73.25, 68.72, 66.43, 65.91, 57.92, 44.36.

**HRMS:**  $m/z$  (ESI) Calculated for C<sub>14</sub>H<sub>17</sub>N<sub>2</sub>O<sub>4</sub> [M+H]<sup>+</sup> 277.1188; found: 277.1183.

### 1-benzyl-3-(1,4-dioxan-2-yl) quinoxalin-2(1H)-one(7ia)



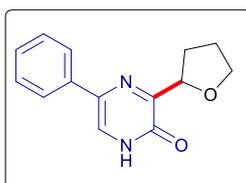
Compound **7ia** prepared according to the general procedure and purified by flash column chromatography (15% EtOAc:petether) yield 71% as viscous liquid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  8.04 (d, *J* = 8.0 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.26 (s, 2H), 7.22 (d, *J* = 7.4 Hz, 2H), 5.56 (d, *J* = 15.6 Hz, 1H), 5.41 (dd, *J* = 27.2, 12.5 Hz, 2H), 4.31 (d, *J* = 11.1 Hz, 1H), 4.14 (d, *J* = 11.7 Hz, 1H), 4.07 – 3.95 (m, 1H), 3.85 (d, *J* = 5.8 Hz, 2H), 3.71 (t, *J* = 10.3 Hz, 1H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  155.42, 153.96, 135.06, 133.03, 132.62, 130.99, 129.14, 127.97, 126.98, 124.09, 114.60, 74.77, 69.64, 67.71, 66.50, 46.03.

**HRMS:** *m/z* (ESI) Calculated for C<sub>19</sub>H<sub>19</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 323.1396; found: 323.1390.

### 5-phenyl-3-(tetrahydrofuran-2-yl) pyrazin-2(1H)-one(3ab)



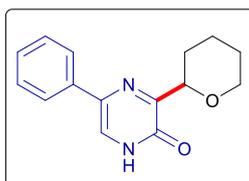
Compound **3ab** prepared according to the general procedure and purified by flash column chromatography (65% EtOAc:petether) yield 90% as white solid

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.43 (s, 1H), 7.94 (s, 1H), 7.89 – 7.84 (m, 2H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.29 (t, *J* = 7.3 Hz, 1H), 5.18 (dd, *J* = 7.5, 5.6 Hz, 1H), 4.01 (d, *J* = 7.1 Hz, 1H), 3.84 (d, *J* = 5.8 Hz, 1H), 2.18 – 2.09 (m, 2H), 2.05 – 1.92 (m, 2H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  156.95, 154.41, 135.96, 130.73, 128.67, 127.30, 124.44, 123.32, 75.77, 68.13, 29.24, 25.43.

**HRMS:** *m/z* (ESI) Calculated for C<sub>14</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> 243.1134; found: 243.1128.

### 5-phenyl-3-(tetrahydro-2H-pyran-2-yl) pyrazin-2(1H)-one(3ac)



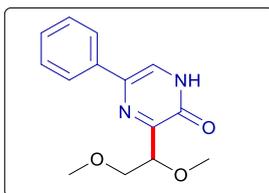
Compound **3ac** prepared according to the general procedure and purified by flash column chromatography (55% EtOAc:pet ether) yield 70% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.47 (s, 1H), 7.96 (s, 1H), 7.90 – 7.83 (m, 2H), 7.47 – 7.37 (m, 2H), 7.32 – 7.25 (m, 1H), 4.73 (dd, *J* = 10.6, 2.3 Hz, 1H), 3.98 (d, *J* = 11.1 Hz, 1H), 3.52 (dd, *J* = 12.3, 9.3 Hz, 1H), 1.94 – 1.87 (m, 1H), 1.86 – 1.77 (m, 1H), 1.73 (dd, *J* = 16.6, 4.8 Hz, 1H), 1.66 – 1.49 (m, 3H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  155.33, 154.36, 135.94, 131.04, 128.65, 127.34, 124.57, 123.64, 74.16, 68.09, 28.37, 25.57, 22.97.

**HRMS:** *m/z* (ESI) Calculated for C<sub>15</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> 257.1290; found: 257.1297.

### 3-(1,2-dimethoxyethyl)-5-phenylpyrazin-2(1H)-one(3ad)



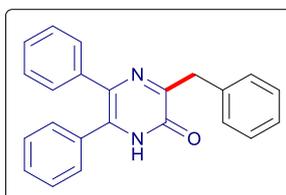
Compound **3ad** prepared according to the general procedure and purified by flash column chromatography (55% EtOAc:petether) yield 66% as white solid

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.57 (s, 1H), 7.98 (s, 1H), 7.87 (d, *J* = 7.5 Hz, 2H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 4.83 – 4.75 (m, 1H), 3.74 – 3.65 (m, 2H), 3.32 (s, 3H), 3.28 (s, 3H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  154.92, 153.12, 135.85, 131.33, 128.66, 127.39, 124.56, 123.87, 76.89, 72.80, 58.37, 57.25.

**HRMS:** *m/z* (ESI) Calculated for C<sub>14</sub>H<sub>17</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 261.1239; found: 261.1234.

### 3-benzyl-5,6-diphenylpyrazin-2(1H)-one(3ge)



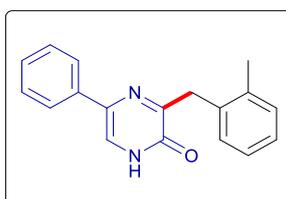
Compound **3ge** prepared according to the general procedure and purified by flash column chromatography (65% EtOAc:petether) yield 70% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.36 (s, 1H), 7.39 – 7.27 (m, 9H), 7.20 (d, *J* = 13.8 Hz, 6H), 4.09 (s, 2H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  155.41, 138.09, 137.74, 131.31, 129.70, 129.22, 129.07, 128.30, 127.79, 126.98, 126.23, 38.47.

**HRMS:** *m/z* (ESI) Calculated for C<sub>23</sub>H<sub>19</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 339.1497; found: 339.1492

### 3-(2-methylbenzyl)-5-phenylpyrazin-2(1H)-one(3af)



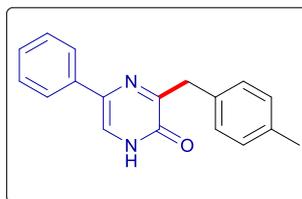
Compound **3af** prepared according to the general procedure and purified by flash column chromatography (35% EtOAc:petether) yield 60% as pale-yellow solid

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.44 (s, 1H), 7.88 (s, 1H), 7.76 (d, *J* = 7.8 Hz, 2H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.28 – 7.20 (m, 2H), 7.16 (d, *J* = 5.7 Hz, 1H), 7.12 – 7.07 (m, 2H), 4.07 (s, 2H), 2.36 (s, 3H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  156.86, 154.98, 136.62, 136.39, 135.98, 130.78, 129.90, 129.76, 128.63, 127.23, 126.35, 125.64, 124.33, 122.20, 36.13, 19.55.

**HRMS:** *m/z* (ESI) Calculated for C<sub>18</sub>H<sub>17</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 277.1341; found: 277.1335.

### 3-(4-methylbenzyl)-5-phenylpyrazin-2(1H)-one(3ag)



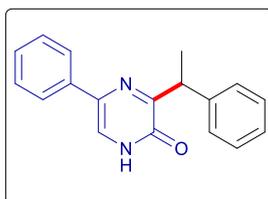
Compound **3ag** prepared according to the general procedure and purified by flash column chromatography (65% EtOAc:petether) yield 55% as pale yellow solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.40 (s, 1H), 7.85 (dd,  $J$  = 8.8, 7.6 Hz, 3H), 7.39 (t,  $J$  = 7.7 Hz, 2H), 7.29 (d,  $J$  = 7.3 Hz, 1H), 7.22 (d,  $J$  = 8.0 Hz, 2H), 7.08 (d,  $J$  = 7.9 Hz, 2H), 4.01 (s, 2H), 2.24 (s, 3H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  157.21, 154.98, 135.99, 135.21, 134.82, 130.95, 128.98, 128.85, 128.66, 127.28, 124.51, 122.40, 38.46, 20.66.

**HRMS:**  $m/z$  (ESI) Calculated for C<sub>18</sub>H<sub>17</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 277.1341; found: 277.1335.

### 5-phenyl-3-(1-phenylethyl) pyrazin-2(1H)-one(3ah)



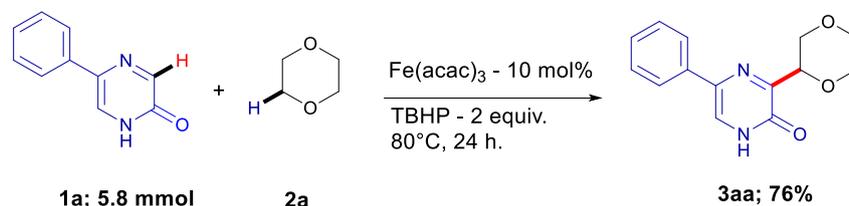
Compound **3ah** prepared according to the general procedure and purified by flash column chromatography (65% EtOAc:petether) yield 64% as white solid.

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.35 (s, 1H), 7.92 (d,  $J$  = 7.7 Hz, 2H), 7.86 (s, 1H), 7.43 (t,  $J$  = 7.6 Hz, 2H), 7.35 – 7.23 (m, 5H), 7.17 (d,  $J$  = 7.1 Hz, 1H), 4.61 (q,  $J$  = 7.0 Hz, 1H), 1.56 (d,  $J$  = 7.1 Hz, 3H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  159.72, 154.53, 143.62, 136.21, 130.53, 128.75, 128.30, 127.74, 127.31, 126.27, 124.50, 121.98, 40.12, 19.87.

**HRMS:**  $m/z$  (ESI) Calculated for C<sub>18</sub>H<sub>17</sub>N<sub>2</sub>O [M+H]<sup>+</sup> 277.1341; found: 277.1335.

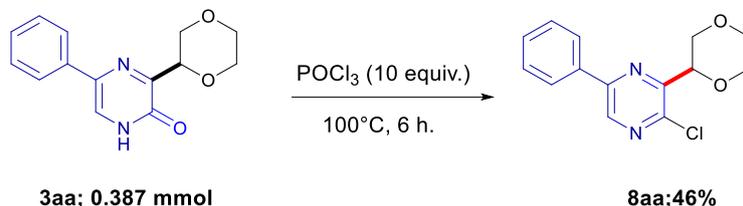
## 12. Gram scale reaction



An oven dried Schlenk tube was charged with Teflon coated magnetic stir bar under inert atmosphere added 5-phenylpyrazin-2(1H)-one (5.8 mmol, 1equiv.), Fe(acac)<sub>3</sub> (10mol%) and 1,4 dioxane (12ml), followed by TBHP (11.6 mmol, 2 equiv.). The resultant reaction mixture was stirred and heated in a closed system at 80°C for 24h. Solvent was evaporated under

reduced pressure and the crude mixture was purified by flash column chromatography (60% EtOAc:Hexane) on silica gel afforded **3aa** in 76% yield.

### 13. Downstream functionalization of C3-alkylated pyrazine-2(1H)-one 2-chloro-3-(1,4-dioxan-2-yl)-5-phenylpyrazine (**8aa**):



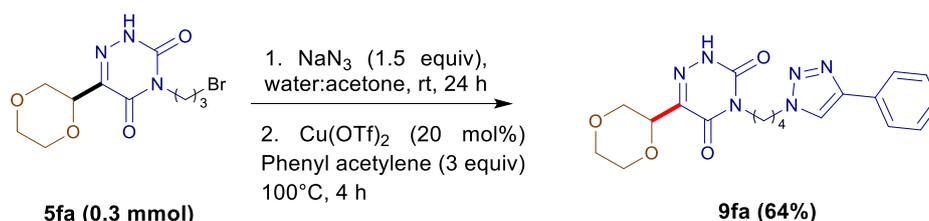
**Procedure:** An oven dried Schlenk tube was charged with Teflon coated magnetic stir bar under inert atmosphere, added mixture of compound 3-(1,4-dioxan-2-yl)-5-phenylpyrazin-2(1H)-one (**3aa**), (0.387 mmol, 1.0 equiv) and POCl<sub>3</sub> (10 equiv) was heated (100 °C) for 6 h. Later the reaction mixture was cooled to room temperature, quench into ice cold water. Finally, reaction mixture was extracted with dichloromethane and evaporated to obtain a residue, which was purified by flash column chromatography (10% EtOAc:petether) yield 48% of **8aa** as a white solid

**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  9.06 (s, 1H), 8.12 (d, *J* = 6.2 Hz, 2H), 7.54 (d, *J* = 6.6 Hz, 3H), 4.96 (dd, *J* = 8.0, 4.1 Hz, 1H), 4.00 (d, *J* = 8.3 Hz, 2H), 3.90 (d, *J* = 11.2 Hz, 1H), 3.80 (dd, *J* = 23.7, 11.9 Hz, 3H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  149.59, 149.20, 146.52, 141.02, 134.60, 130.62, 129.36, 127.07, 73.85, 68.00, 66.93, 65.91.

**HRMS:** *m/z* (ESI) Calculated for C<sub>14</sub>H<sub>14</sub>ClN<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> 277.0744; found: 277.0738.

### 6-(1,4-dioxan-2-yl)-4-(4-(4-phenyl-1H-1,2,3-triazol-1-yl)butyl)-1,2,4-triazine-3,5(2H,4H)-dione



**Procedure:** An oven-dried Schlenk tube equipped with a Teflon-coated magnetic stir bar was charged under an inert atmosphere with a mixture of 4-(4-bromobutyl)-6-(1,4-dioxan-2-yl)-1,2,4-triazine-3,5(2H,4H)-dione (**5fa**) (0.387 mmol, 1.0 equiv) and sodium azide (NaN<sub>3</sub>, 1.5 equiv) in a solvent mixture of water:acetone (1:4). The reaction mixture was stirred at room temperature for 24 h. After completion, the mixture was extracted with ethyl acetate, and the organic layer was concentrated under reduced pressure. The crude product was carried forward without further purification. In a separate oven-dried Schlenk tube under an inert atmosphere, the crude azide intermediate was combined with copper (II) triflate (CuOTf)<sub>2</sub> (20 mol%) and phenylacetylene (3.0 equiv). The mixture was heated at 100 °C for 3 h. Upon completion, the reaction mixture was cooled to room temperature and purified by flash

column chromatography (70% EtOAc in petroleum ether) to afford the desired triazole product as a white solid in 62% (**9fa**) yield.

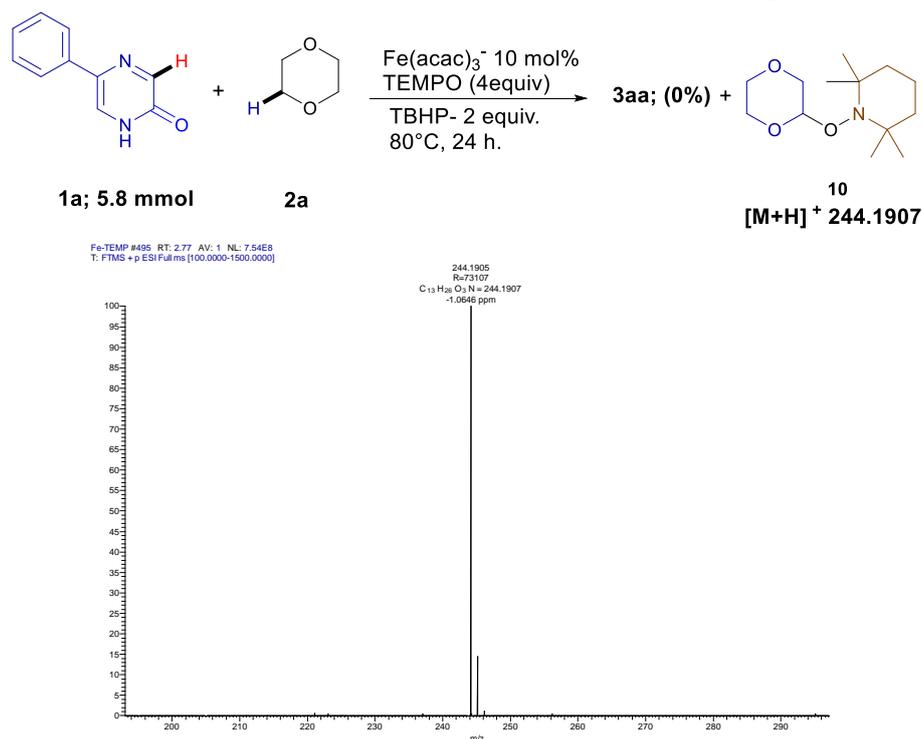
**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  12.59 (s, 1H), 8.55 (s, 1H), 7.84 – 7.79 (m, 2H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.33 (d, *J* = 7.4 Hz, 1H), 4.62 (dd, *J* = 9.9, 2.6 Hz, 1H), 4.42 (t, *J* = 6.9 Hz, 2H), 3.79 (dd, *J* = 11.3, 3.1 Hz, 4H), 3.71 – 3.65 (m, 2H), 3.58 – 3.50 (m, 2H), 1.90 – 1.83 (m, 2H), 1.59 – 1.50 (m, 2H).

**<sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)**  $\delta$  155.39, 149.14, 146.33, 140.25, 130.87, 128.95, 127.86, 125.16, 121.42, 71.04, 67.86, 66.47, 65.76, 49.13, 38.83, 27.11, 23.79.

**HRMS:** *m/z* (ESI) Calculated for C<sub>19</sub>H<sub>23</sub>N<sub>6</sub>O<sub>4</sub> [M+H]<sup>+</sup> 399.1781; found: 399.1775.

#### 14. Control experiments

**Reaction with (TEMPO):** An oven dried Schlenk tube was charged with Teflon coated magnetic stir bar under inert atmosphere, added pyrazin-2(1*H*)-one (0.3 mmol, 1equiv), Dioxane (2 ml), Fe(acac)<sub>3</sub> (10 mol%), TBHP (0.6 mmol, 2equiv) and Tempo (1.2 mmol, 4equiv). The resultant reaction mixture was stirred and heated in a closed system at 80°C for 24 h. Solvent was evaporated under reduced pressure and the reaction mixture was submitted to HRMS. The formation of tempo and dioxane adduct was confirmed as shown in fig.S1

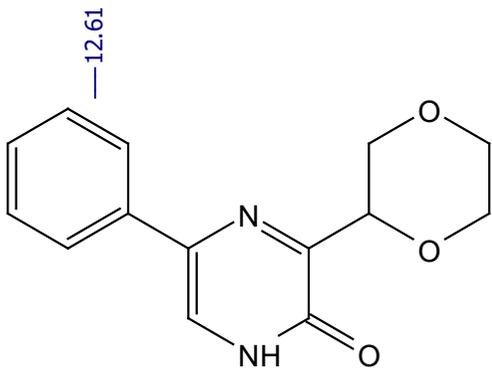


**Figure S1:** HRMS of compound (**10**).

#### 15. References

1. J. Ackrell, E. Galeazzi, J. M. Muchowski and L. Tökés, *Can J Chem*, 1979, **57**, 2696–2702
2. P. Ghosh, N. Y. Kwon, S. Kim, S. Han, S. H. Lee, W. An, N. K. Mishra, S. B. Han and I. S. Kim, *Angew. Chem. Int. Ed.* 2021, **60**, 191–196.
3. V. R. Pansare and N. Barsu, *Org Biomol Chem*, 2025, **23**, 303–307

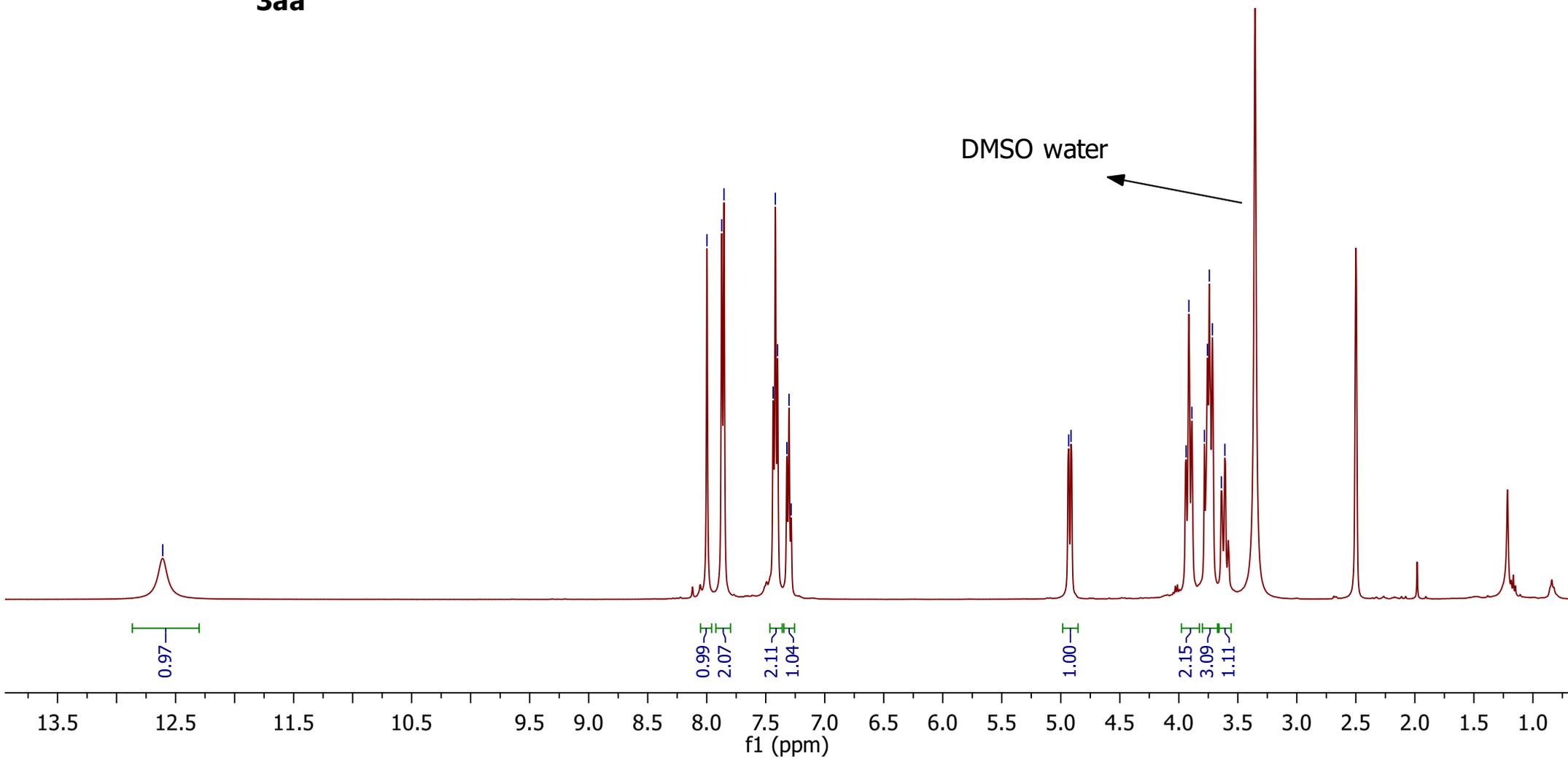
#### 16. NMR spectra

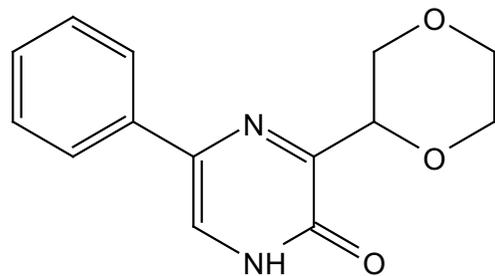


**3aa**

8.00  
7.87  
7.85  
7.44  
7.42  
7.40  
7.32  
7.30  
7.28

4.93  
4.91  
3.94  
3.91  
3.89  
3.78  
3.76  
3.74  
3.72  
3.64  
3.61



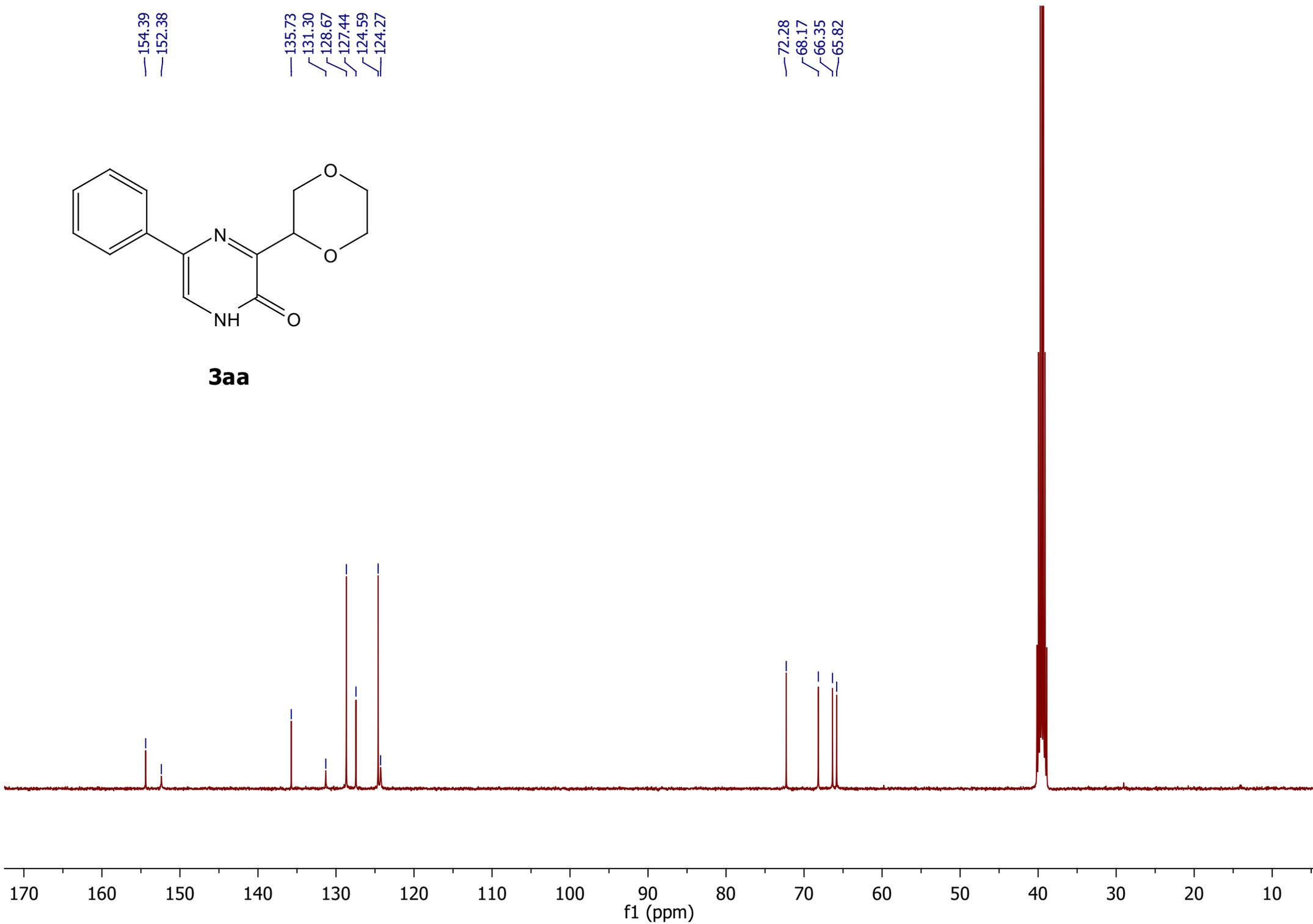


**3a**

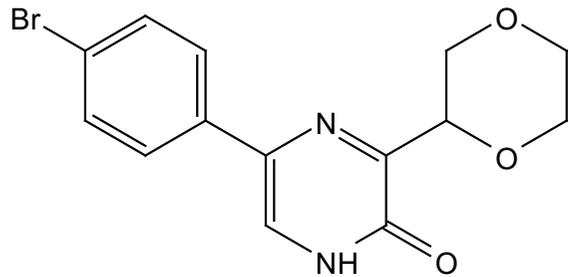
154.39  
152.38

135.73  
131.30  
128.67  
127.44  
124.59  
124.27

72.28  
68.17  
66.35  
65.82



12.70



**3ba**

8.06  
7.84  
7.84  
7.83  
7.82  
7.62  
7.62  
7.60

4.93  
4.92  
4.90  
4.90  
3.94  
3.94  
3.91  
3.91  
3.89  
3.88  
3.76  
3.74  
3.73  
3.72  
3.71  
3.70  
3.69  
3.64  
3.63  
3.61  
3.60  
3.35

DMSO water

13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5

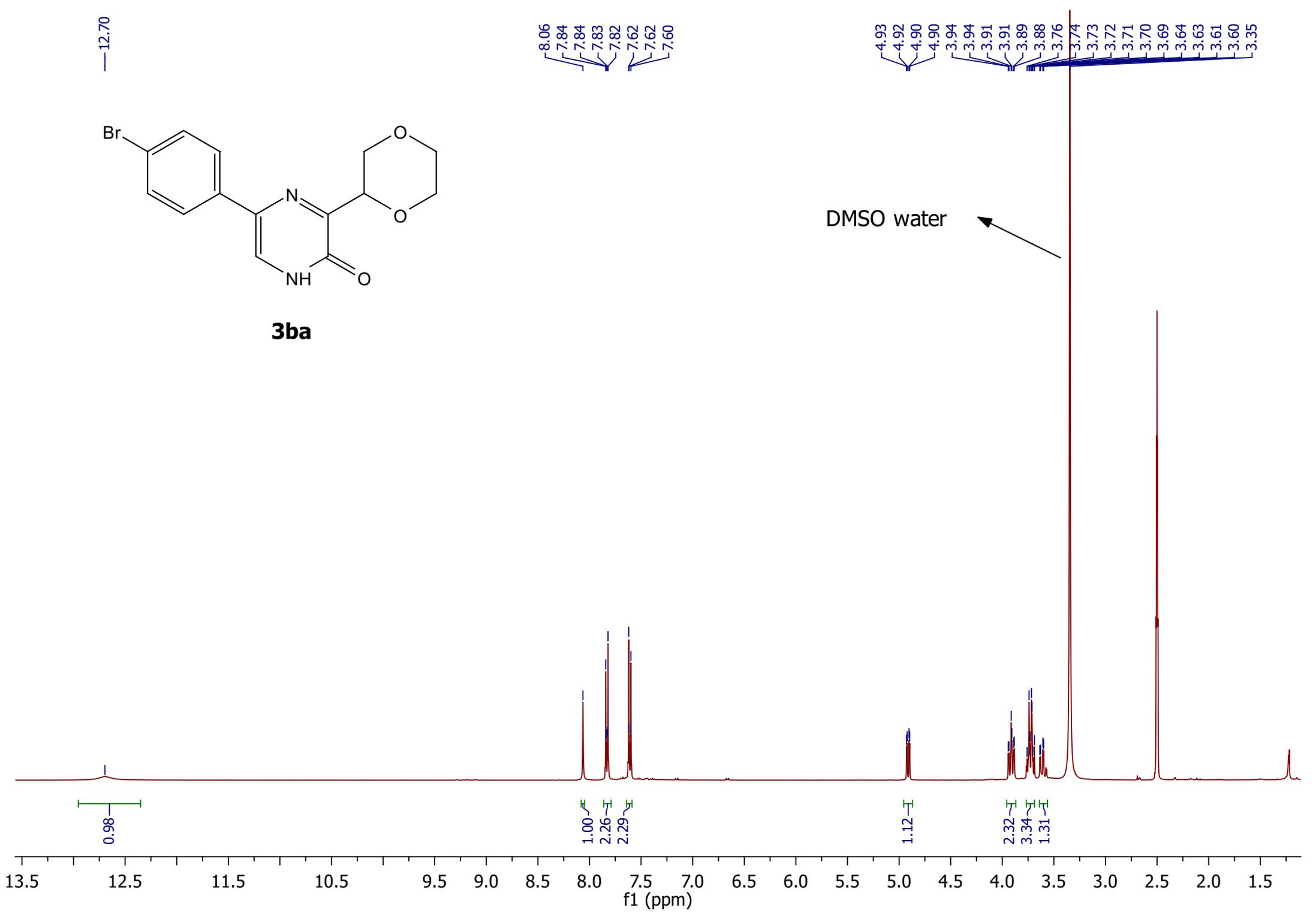
f1 (ppm)

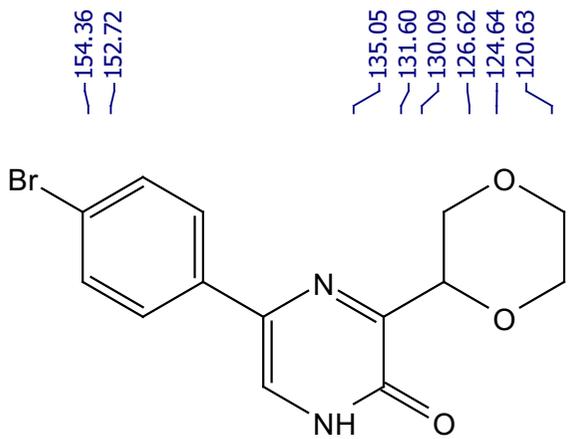
0.98

1.00  
2.26  
2.29

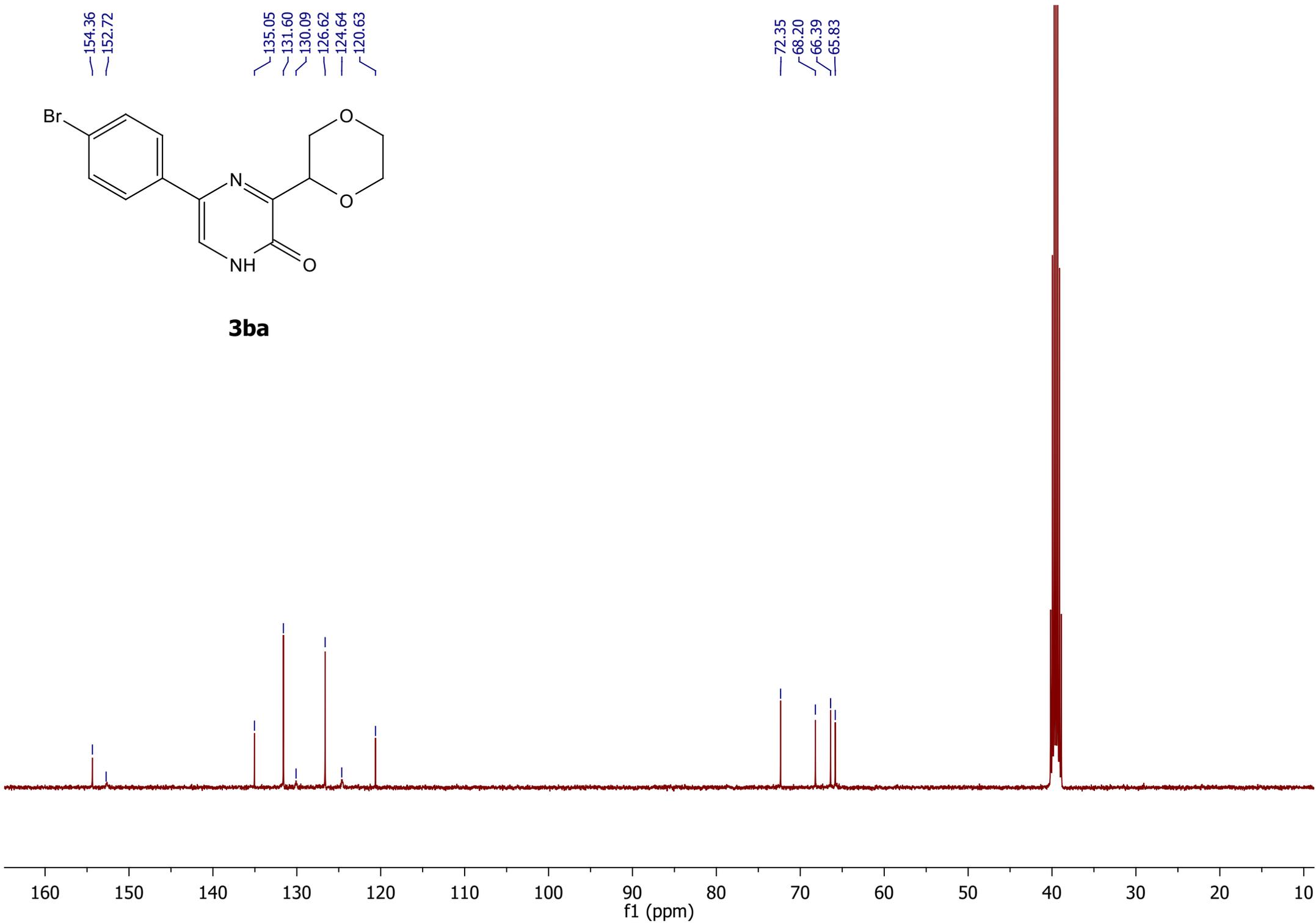
1.12

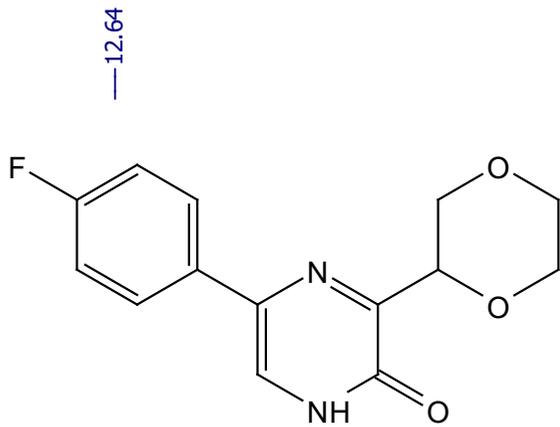
2.32  
3.34  
1.31



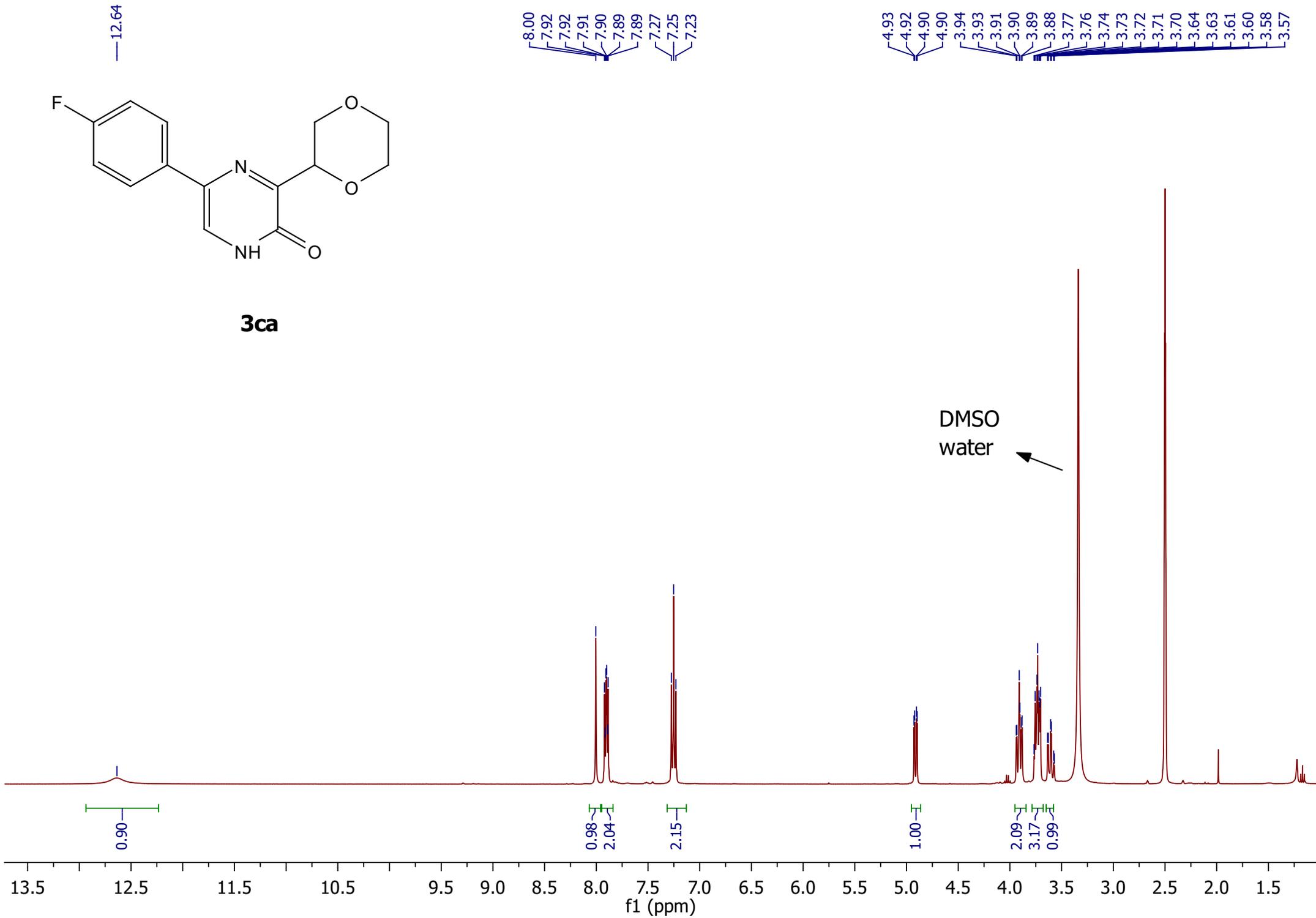


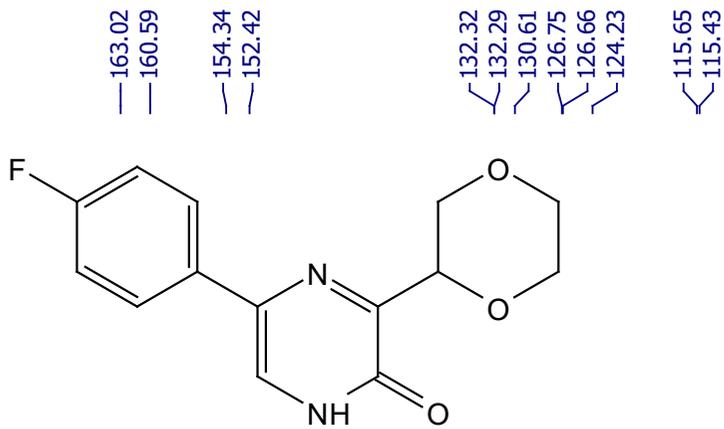
**3ba**





**3ca**

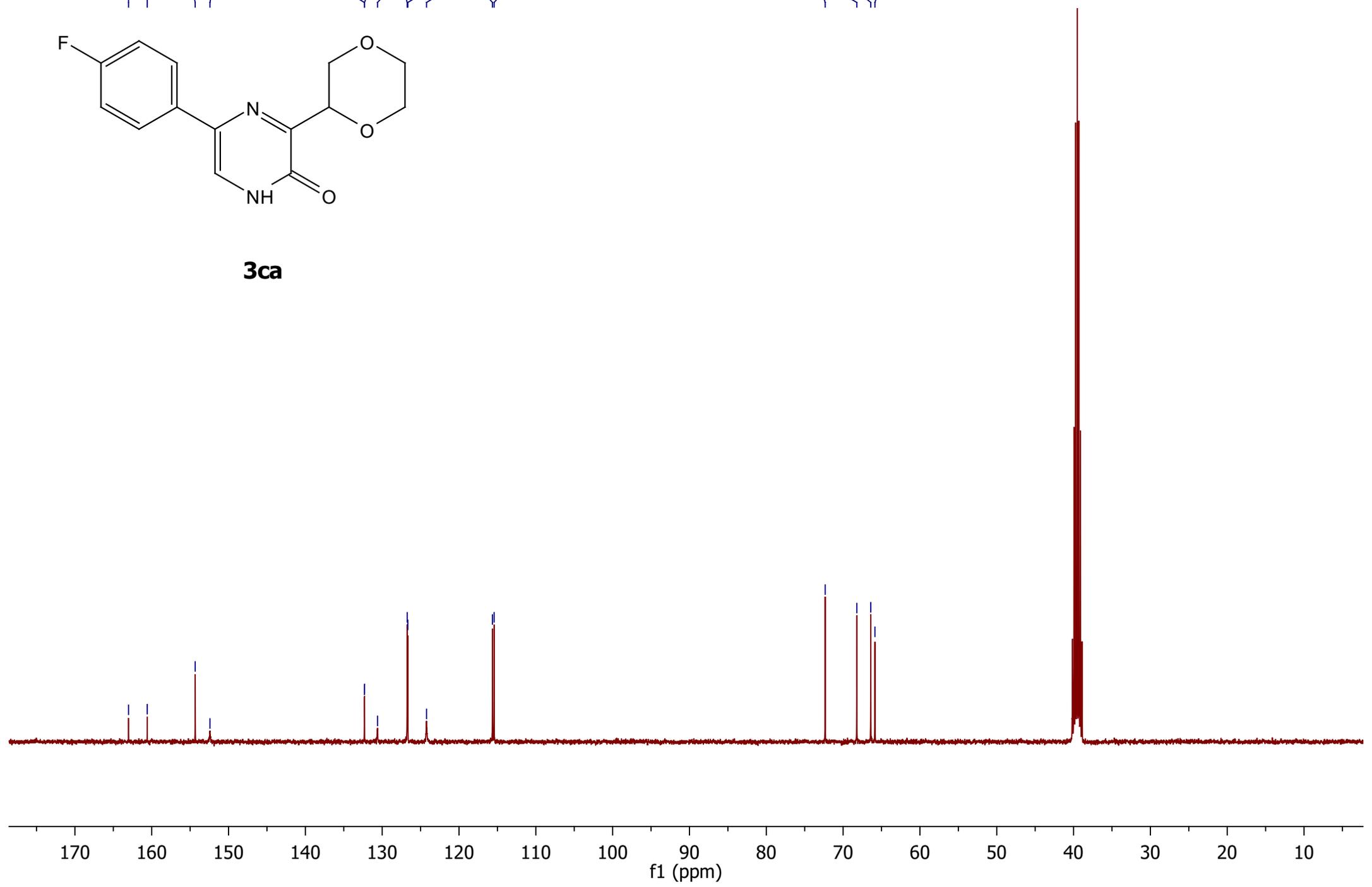


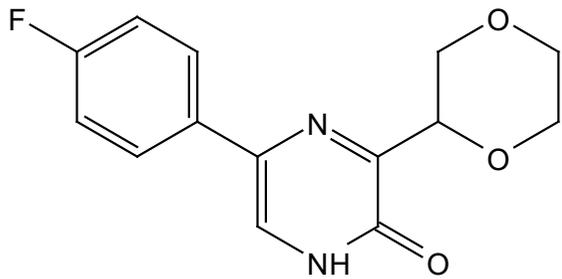


**3ca**

163.02  
160.59  
154.34  
152.42  
132.32  
132.29  
130.61  
126.75  
126.66  
124.23  
115.65  
115.43

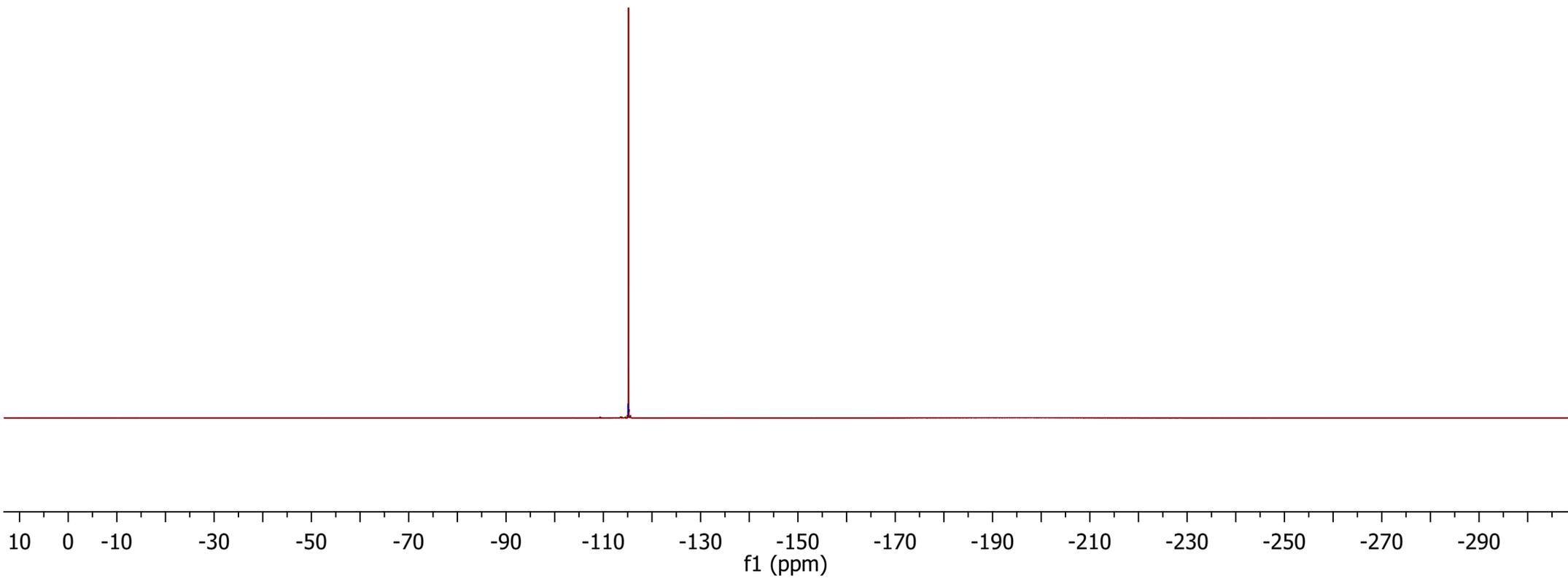
72.33  
68.22  
66.40  
65.86

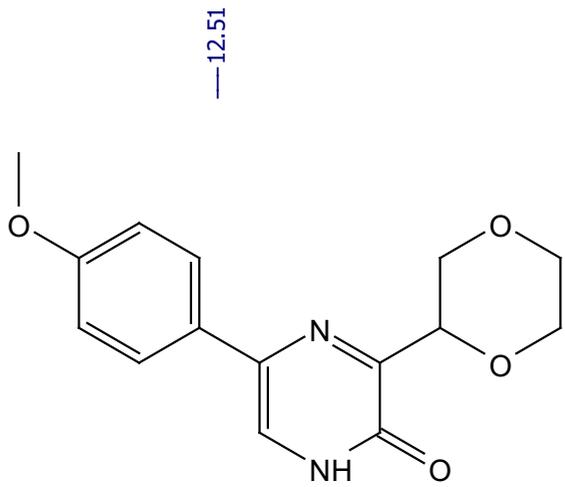




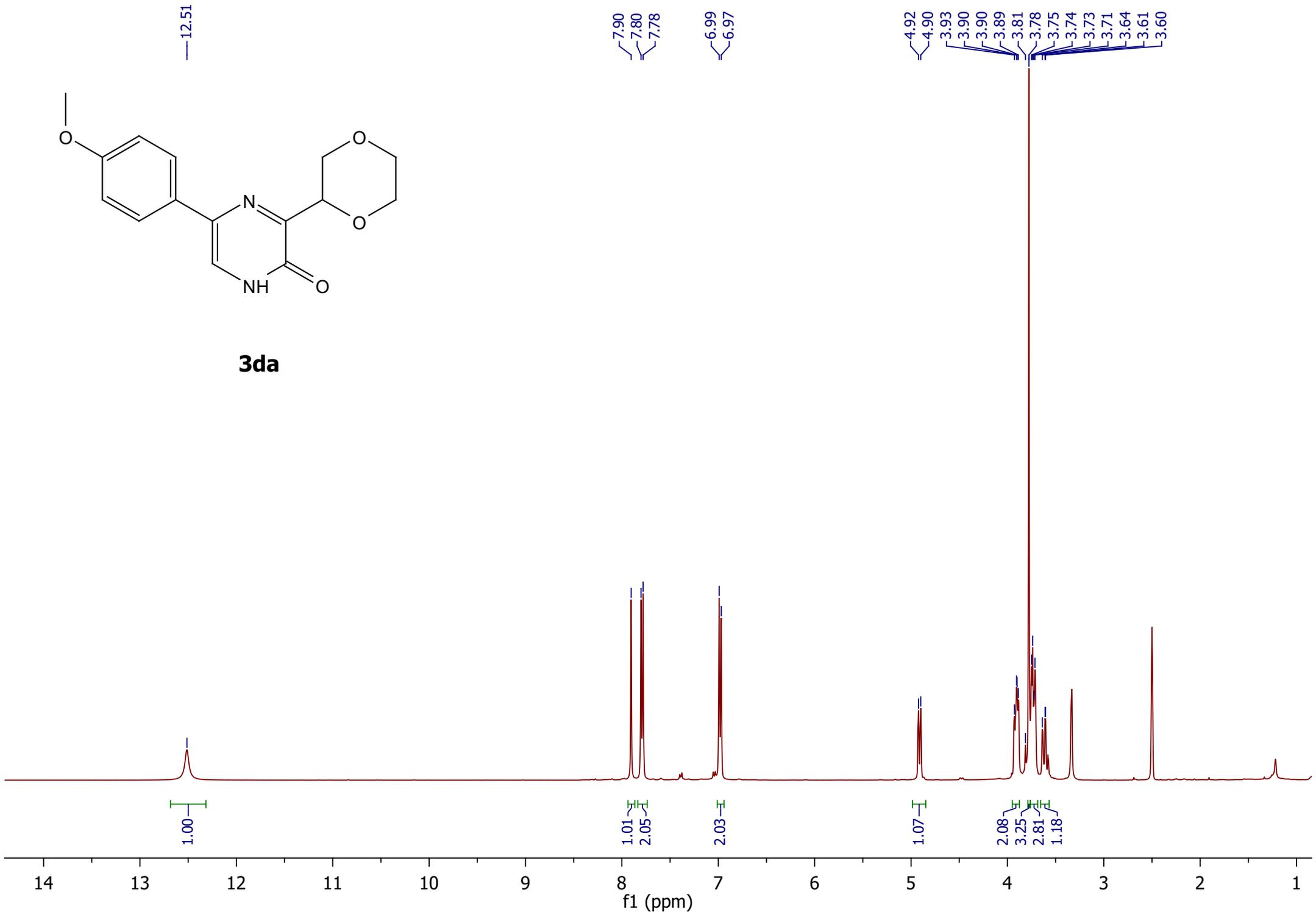
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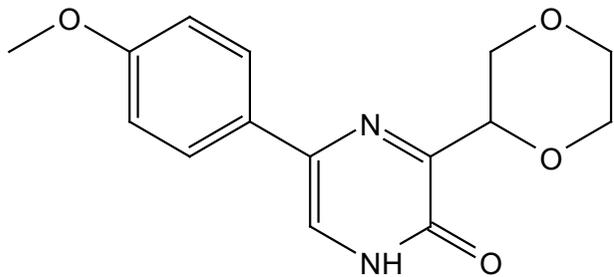
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**3da**





**3da**

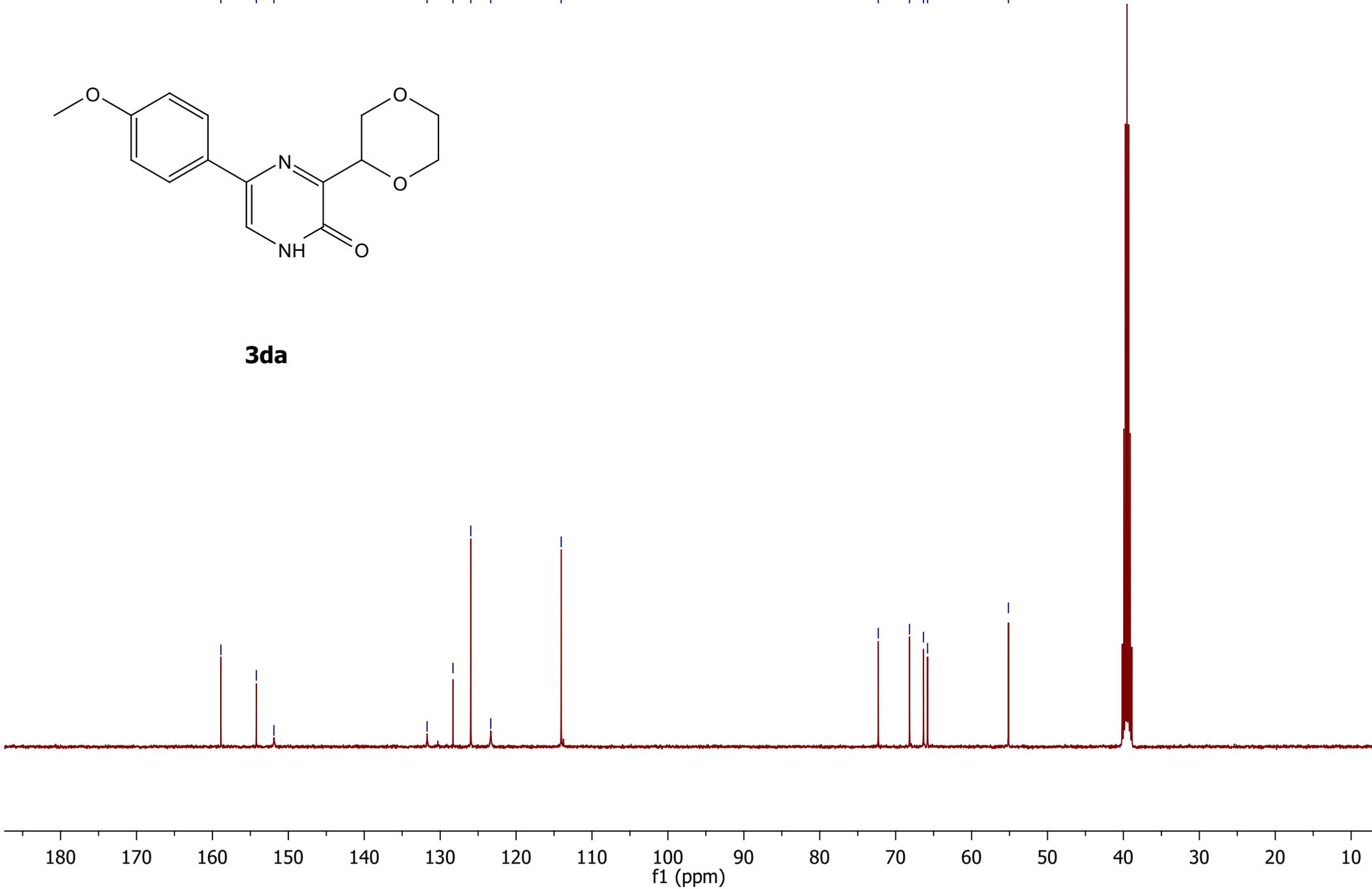
158.88  
154.22  
151.90

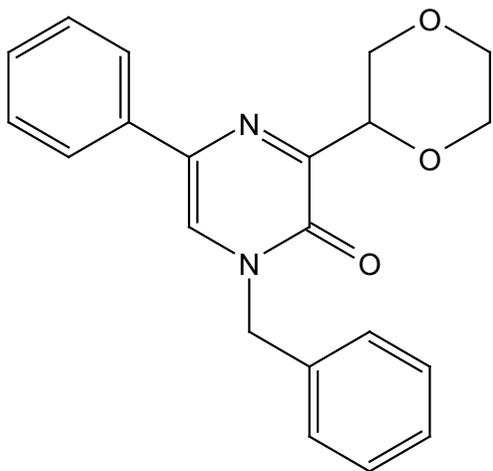
131.72  
128.32  
125.97  
123.33

114.06

72.28  
68.17  
66.33  
65.80

55.15





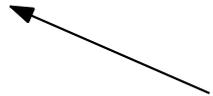
**3ea**

8.51  
7.87  
7.85  
7.44  
7.43  
7.41  
7.38  
7.36  
7.34  
7.32  
7.30

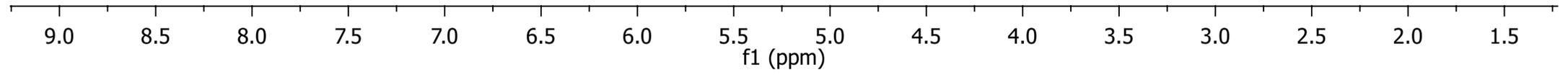
5.22  
5.19  
5.16  
5.12  
4.97  
4.95  
4.95

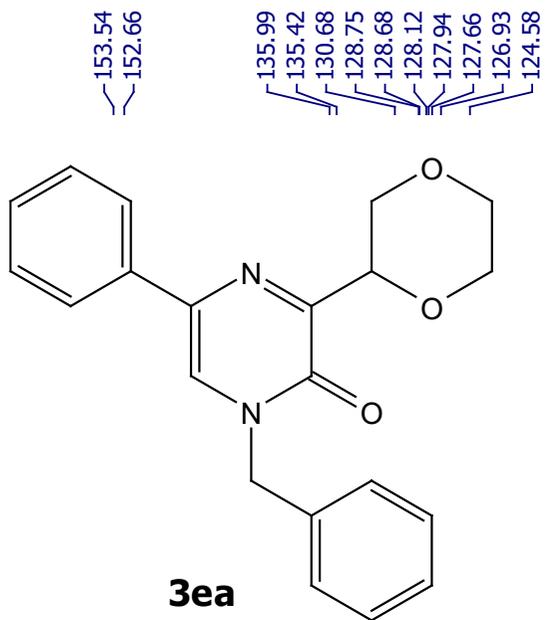
3.94  
3.91  
3.88  
3.79  
3.76  
3.74  
3.71  
3.63  
3.60  
3.37

DMSO  
Water



1.00  
2.08  
4.09  
4.14  
2.07  
1.07  
2.11  
3.22  
1.20



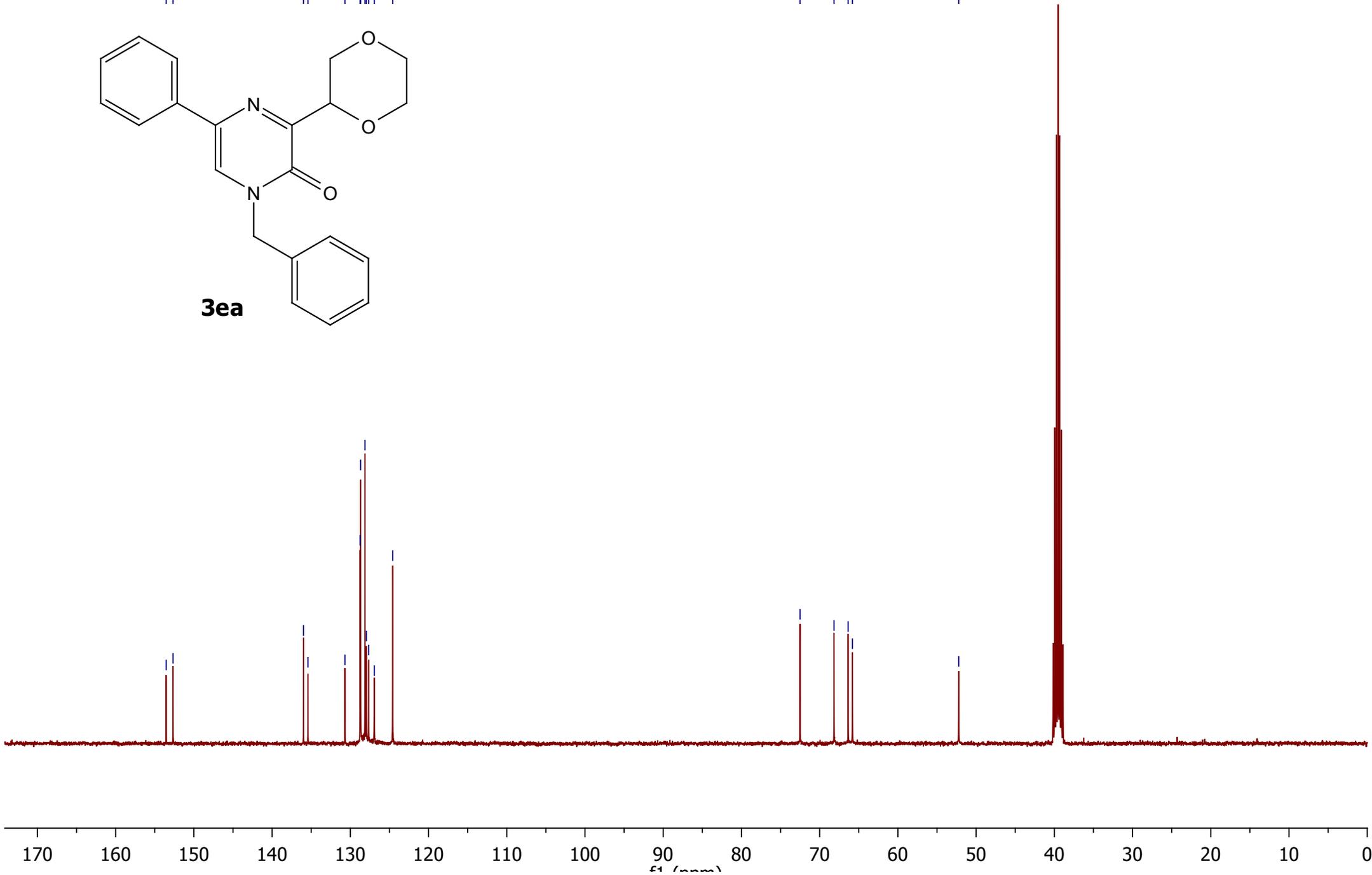


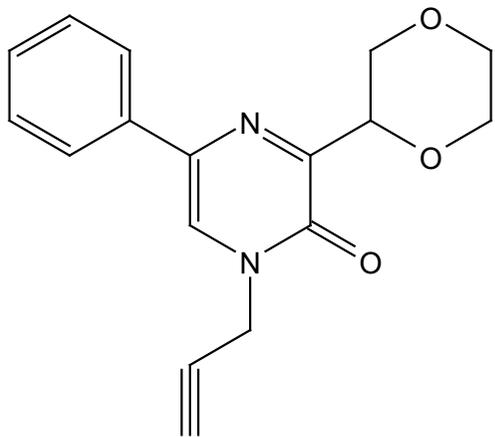
153.54  
152.66

135.99  
135.42  
130.68  
128.75  
128.68  
128.12  
127.94  
127.66  
126.93  
124.58

72.51  
68.16  
66.36  
65.81

52.22





**3fa**

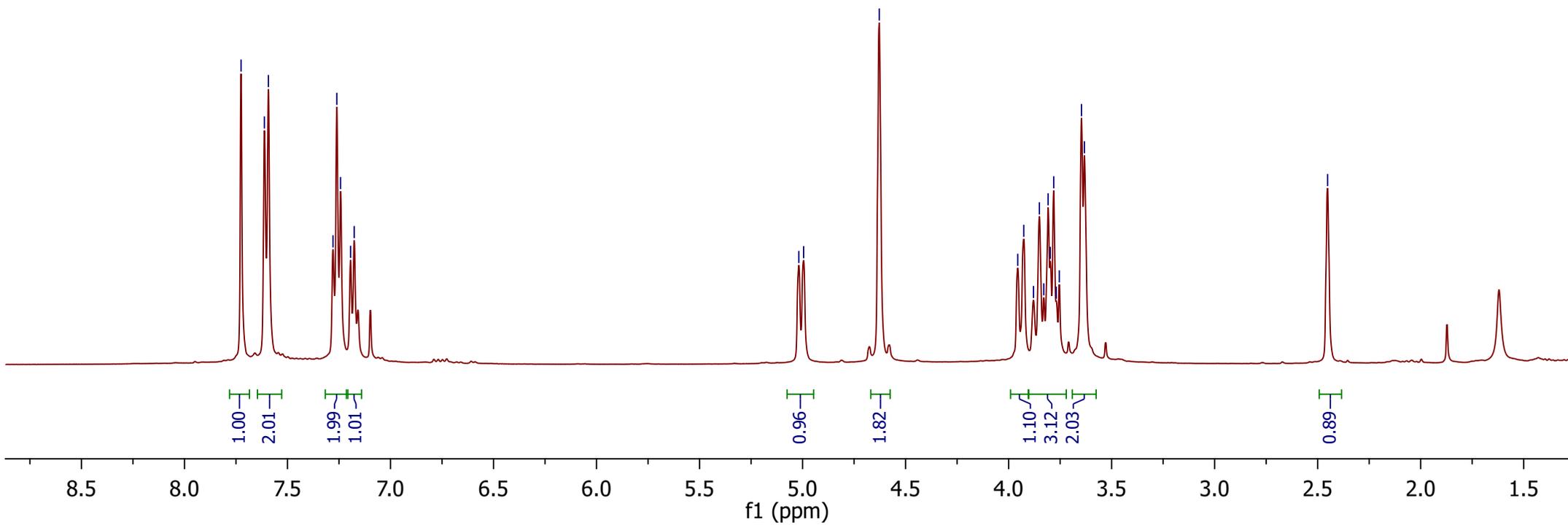
7.73  
7.61  
7.59  
7.28  
7.26  
7.24  
7.19  
7.18

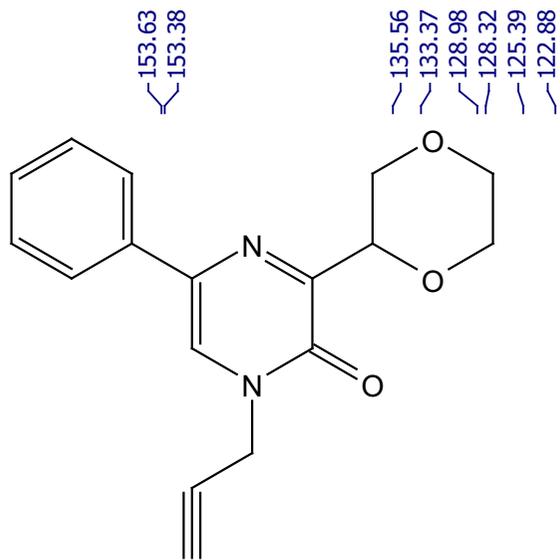
5.02  
4.99

4.63

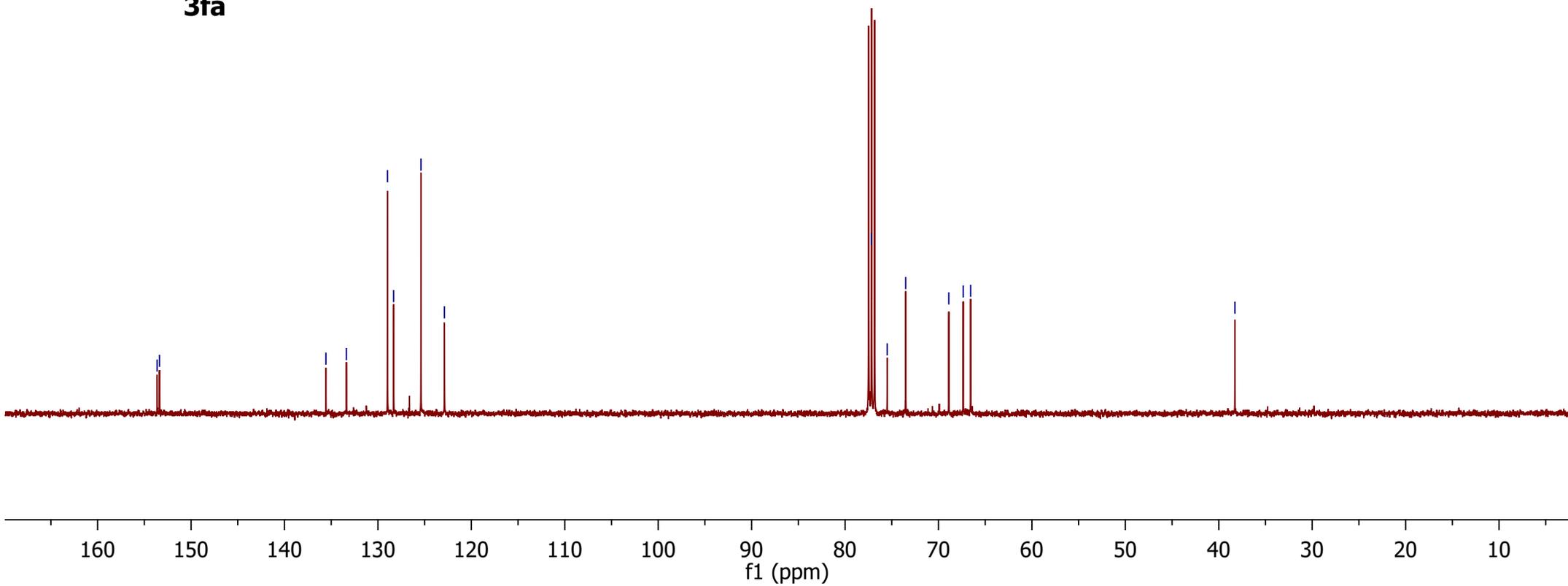
3.96  
3.93  
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3.83  
3.81  
3.80  
3.78  
3.77  
3.75  
3.65  
3.63

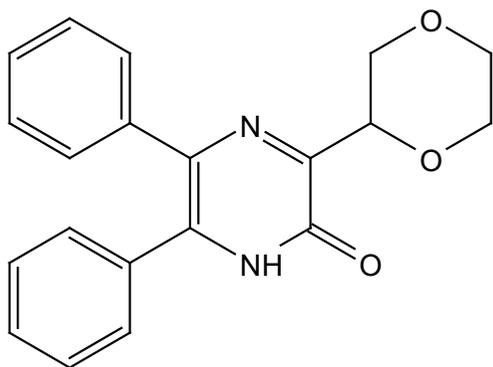
2.45





**3fa**





**3ga**

12.53

7.39  
7.36  
7.34  
7.32  
7.30  
7.22  
7.20

4.96  
4.94  
3.95  
3.92  
3.90  
3.87  
3.79  
3.75  
3.72  
3.62  
3.60

DMSO  
water

1.00

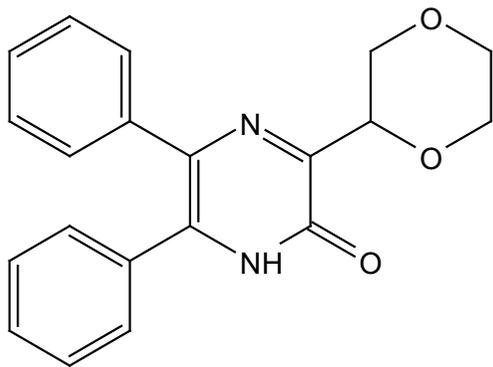
5.33  
5.15

1.11

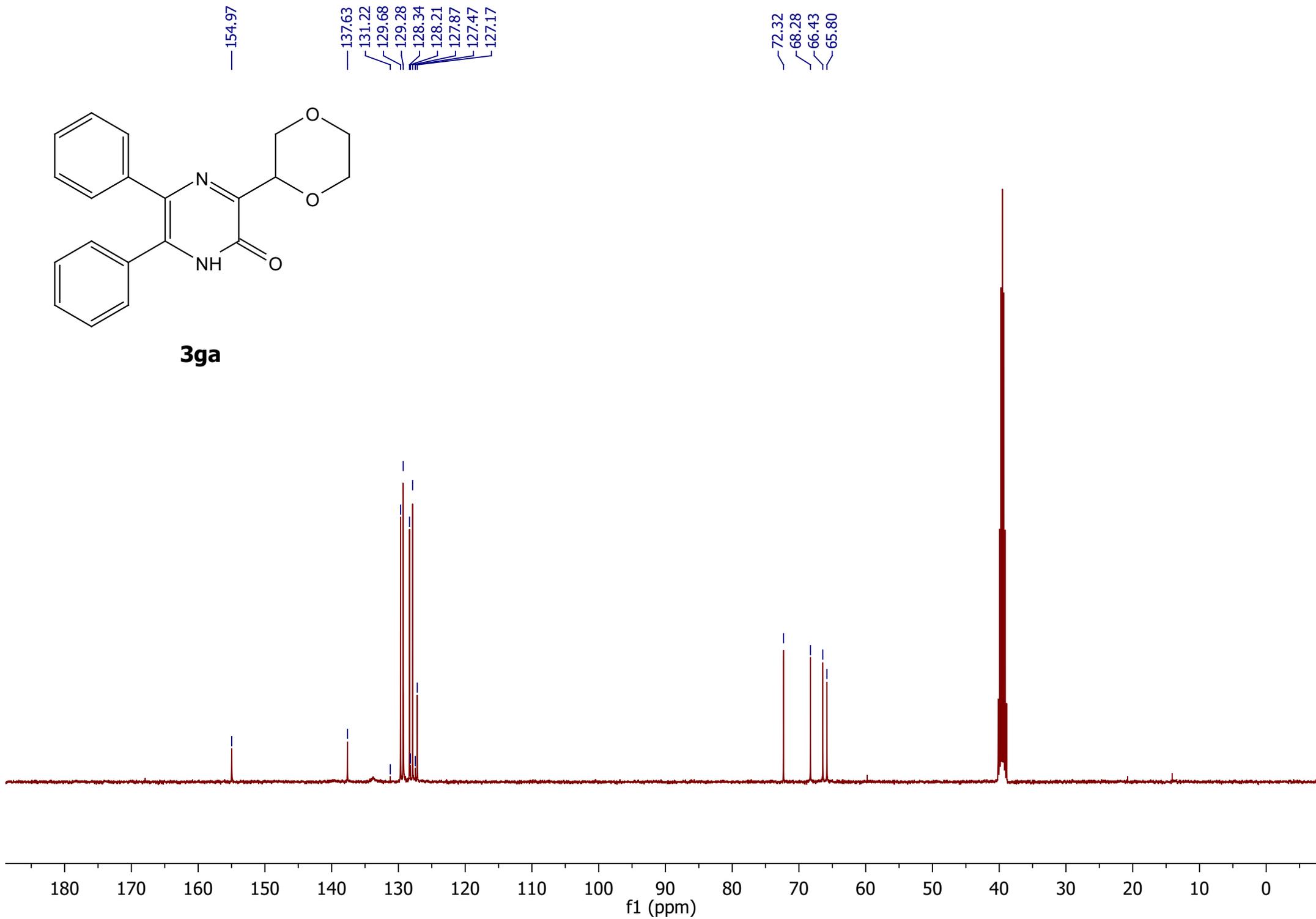
2.34  
3.29  
1.24

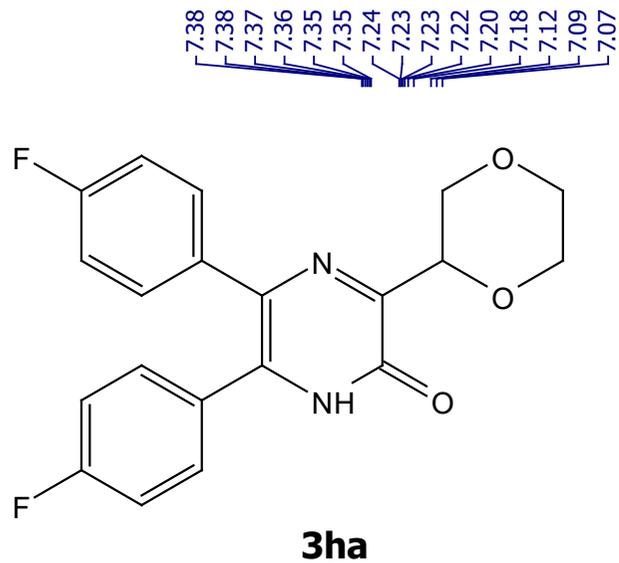
13 12 11 10 9 8 7 6 5 4 3 2 1

f1 (ppm)



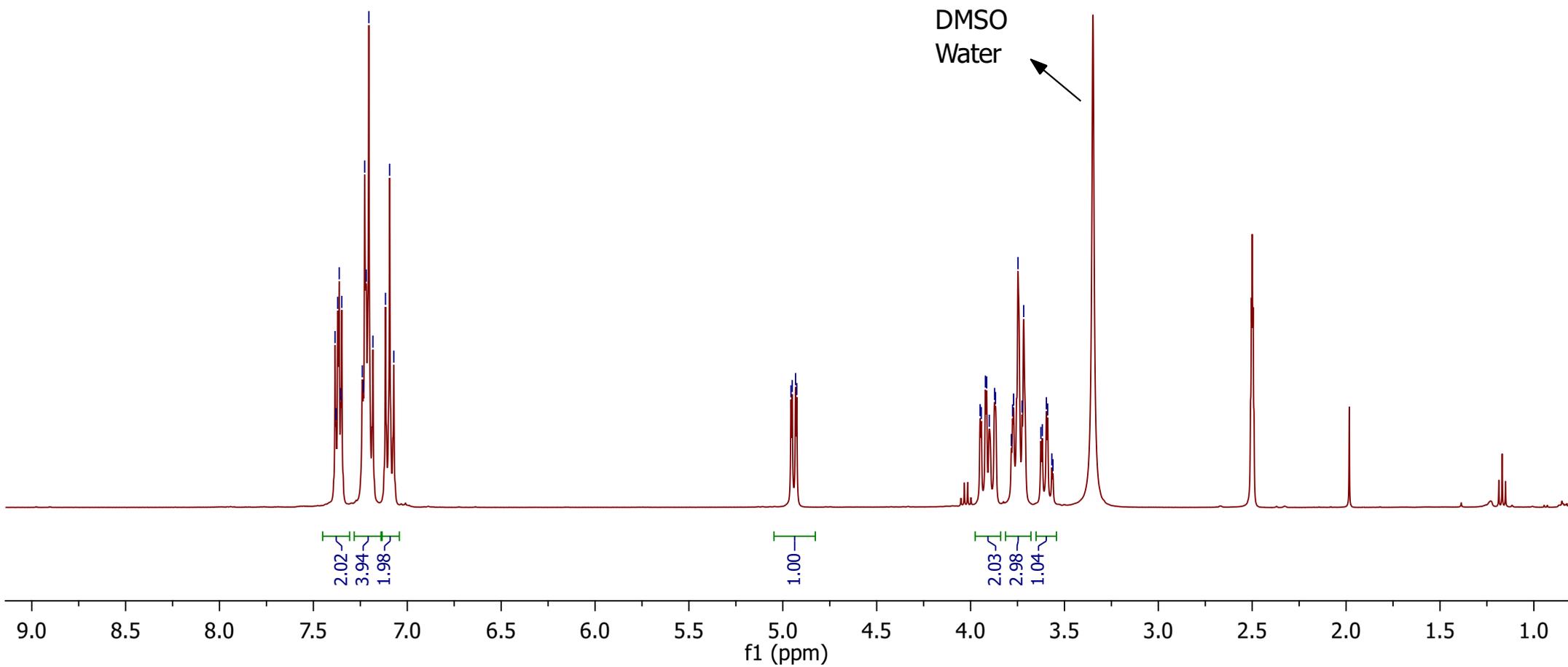
**3ga**

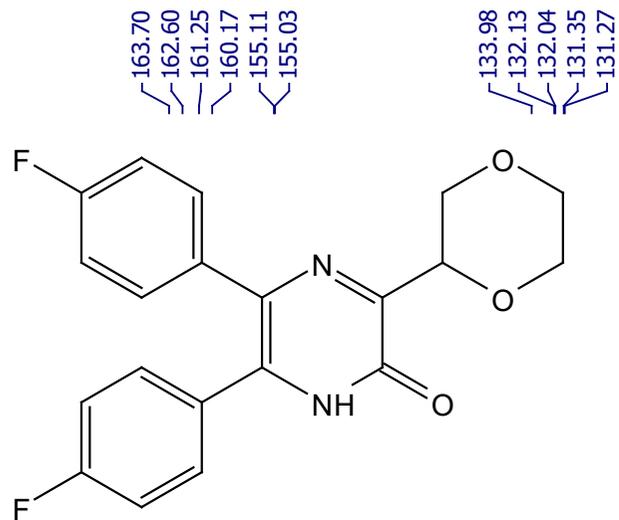




7.38  
7.38  
7.37  
7.36  
7.35  
7.35  
7.24  
7.23  
7.23  
7.22  
7.20  
7.18  
7.12  
7.09  
7.07

4.96  
4.95  
4.93  
4.93  
3.95  
3.94  
3.92  
3.91  
3.90  
3.87  
3.87  
3.78  
3.78  
3.77  
3.75  
3.73  
3.72  
3.63  
3.62  
3.60  
3.59  
3.57  
3.56





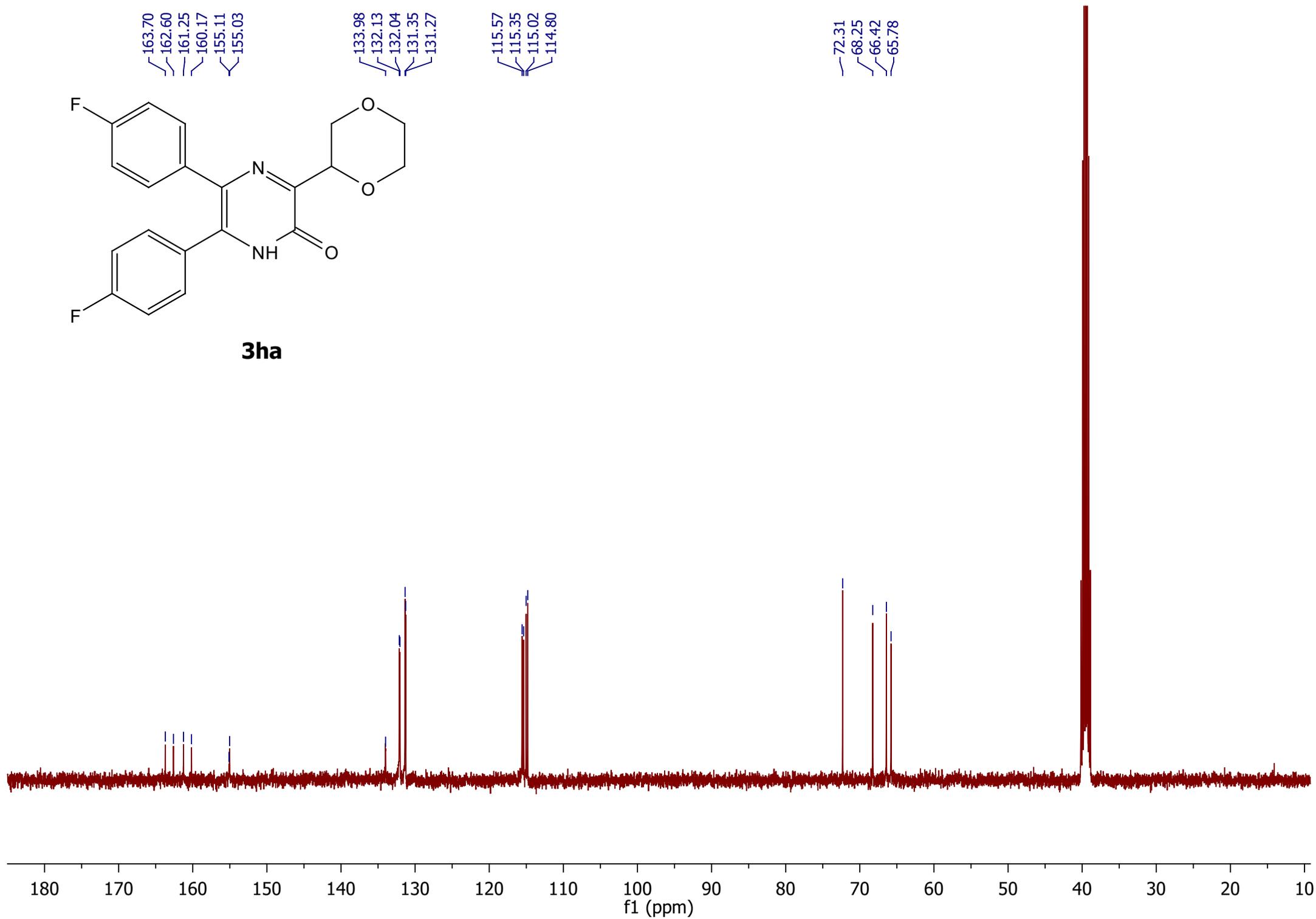
3ha

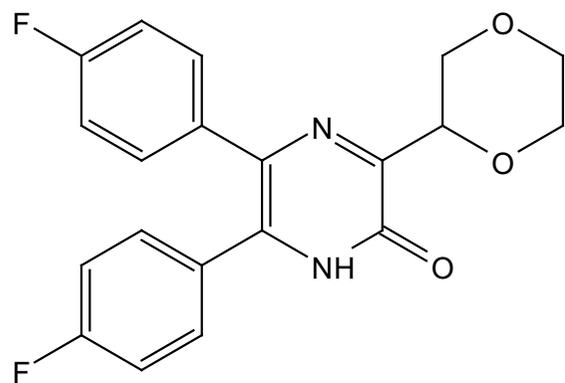
163.70  
162.60  
161.25  
160.17  
155.11  
155.03

133.98  
132.13  
132.04  
131.35  
131.27

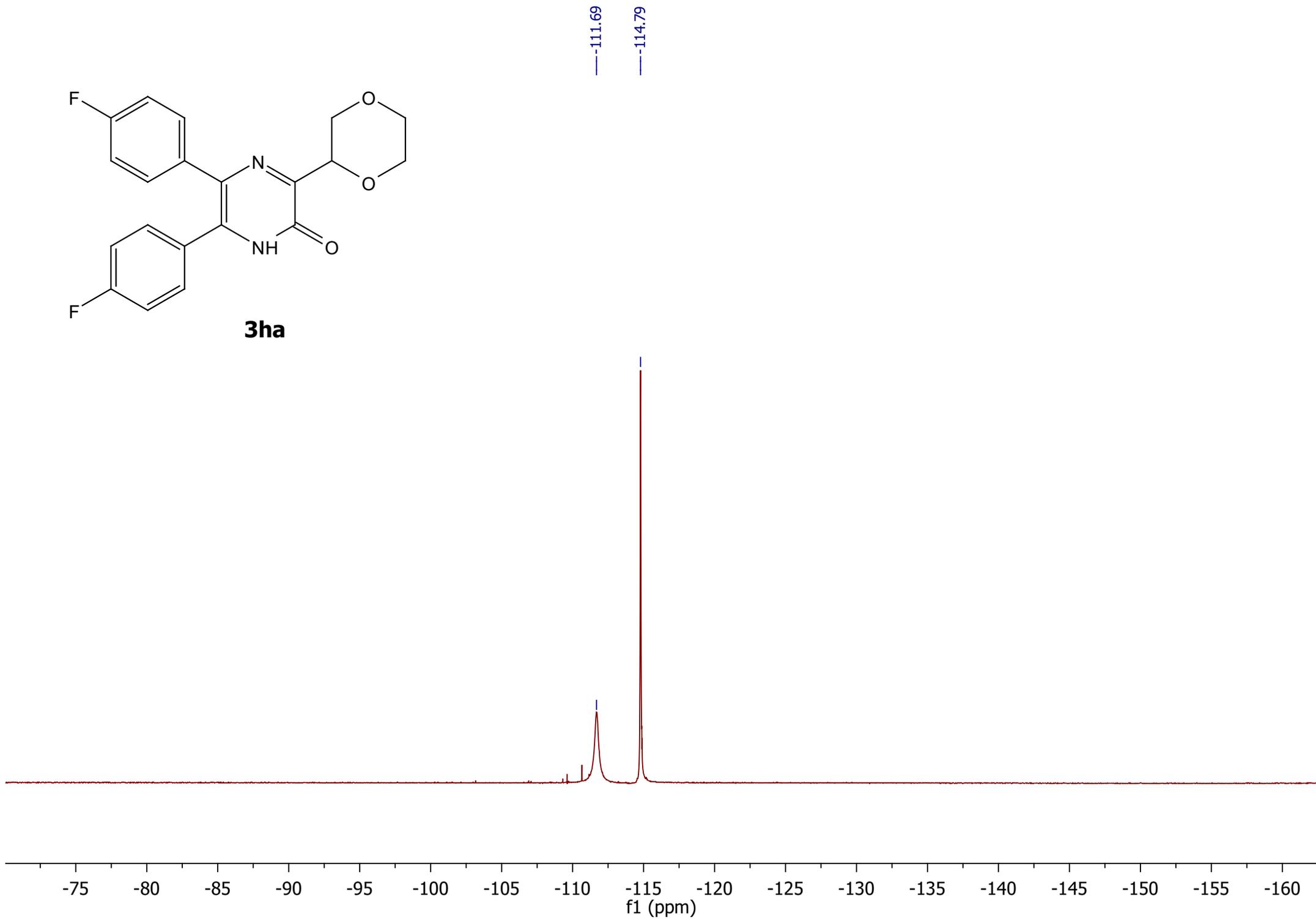
115.57  
115.35  
115.02  
114.80

72.31  
68.25  
66.42  
65.78

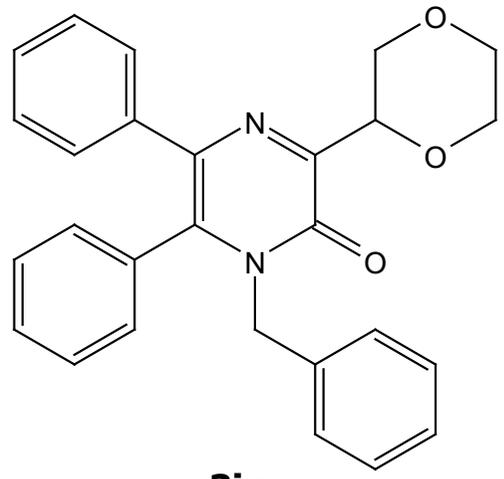




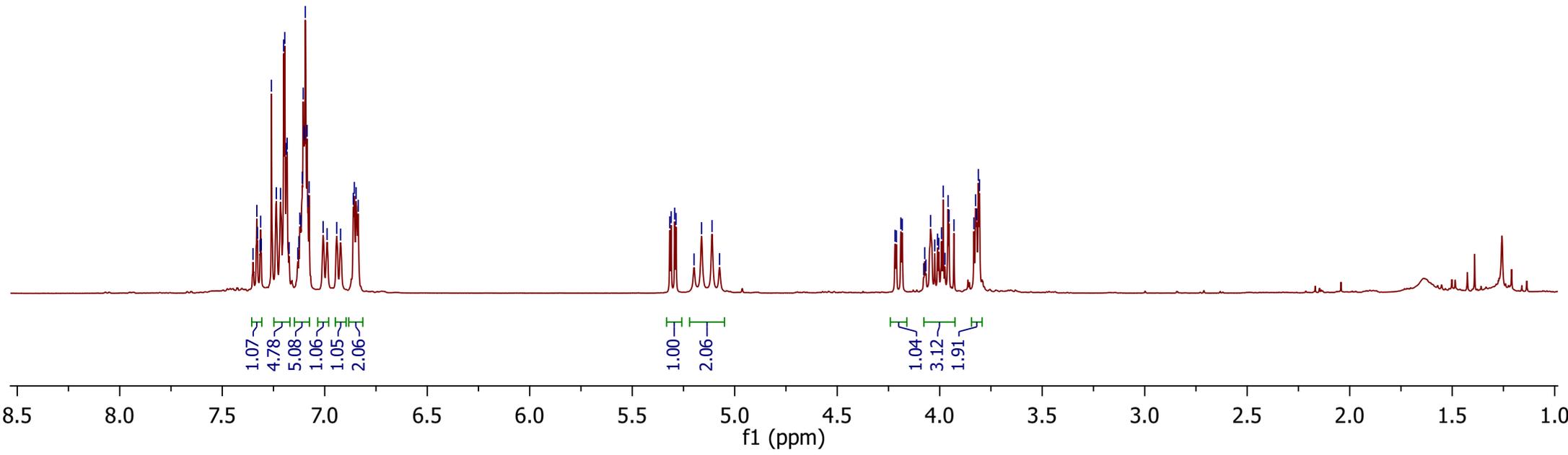
**3ha**

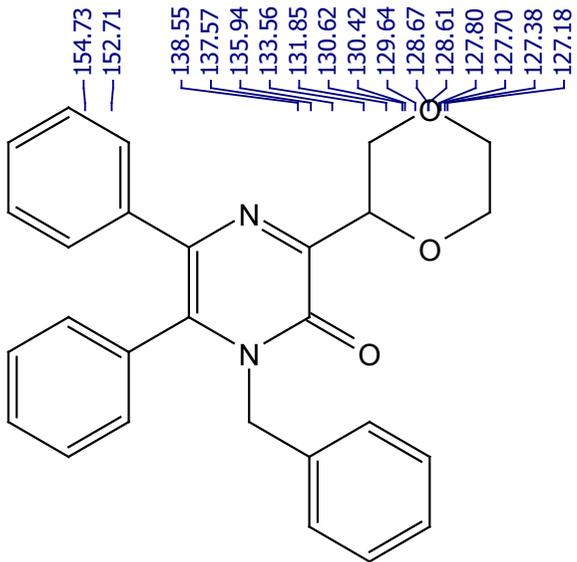


7.33  
7.33  
7.31  
7.26  
7.24  
7.22  
7.20  
7.20  
7.19  
7.18  
7.12  
7.12  
7.11  
7.11  
7.10  
7.10  
7.09  
7.09  
7.08  
7.08  
7.01  
7.01  
6.99  
6.94  
6.94  
6.92  
6.86  
6.86  
6.85  
6.84  
6.84  
5.31  
5.29  
5.29  
5.20  
5.16  
5.11  
5.07  
4.22  
4.21  
4.21  
4.19  
4.18  
4.08  
4.07  
4.07  
4.04  
4.02  
4.01  
4.00  
3.99  
3.98  
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3.96  
3.95  
3.93  
3.83  
3.83  
3.82  
3.81  
3.81

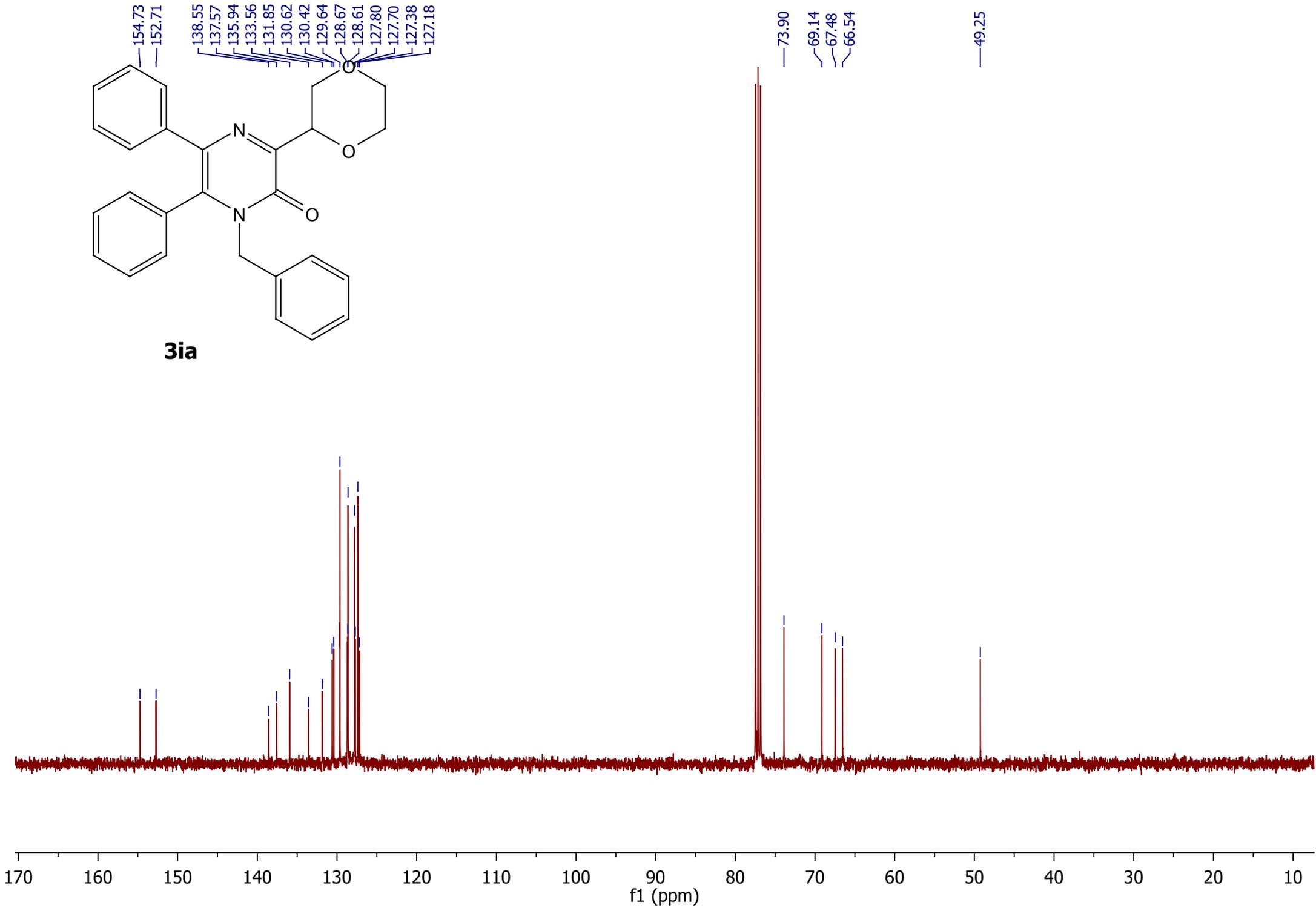


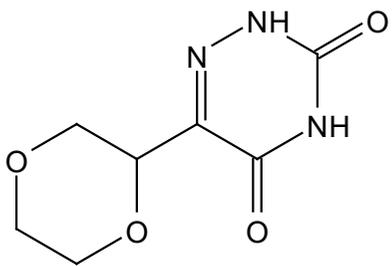
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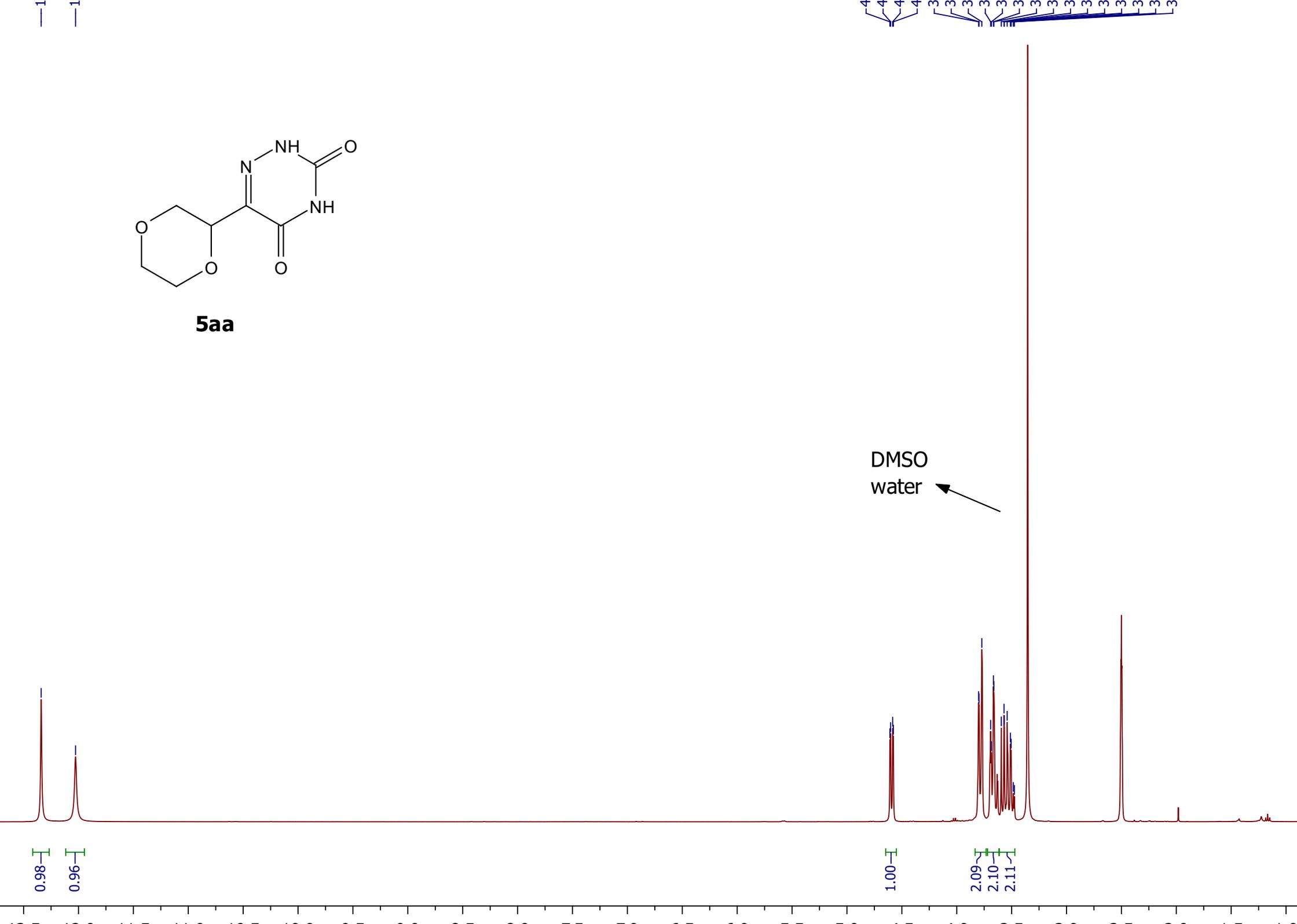


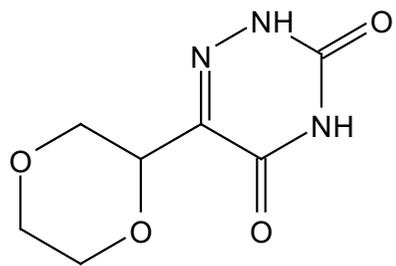
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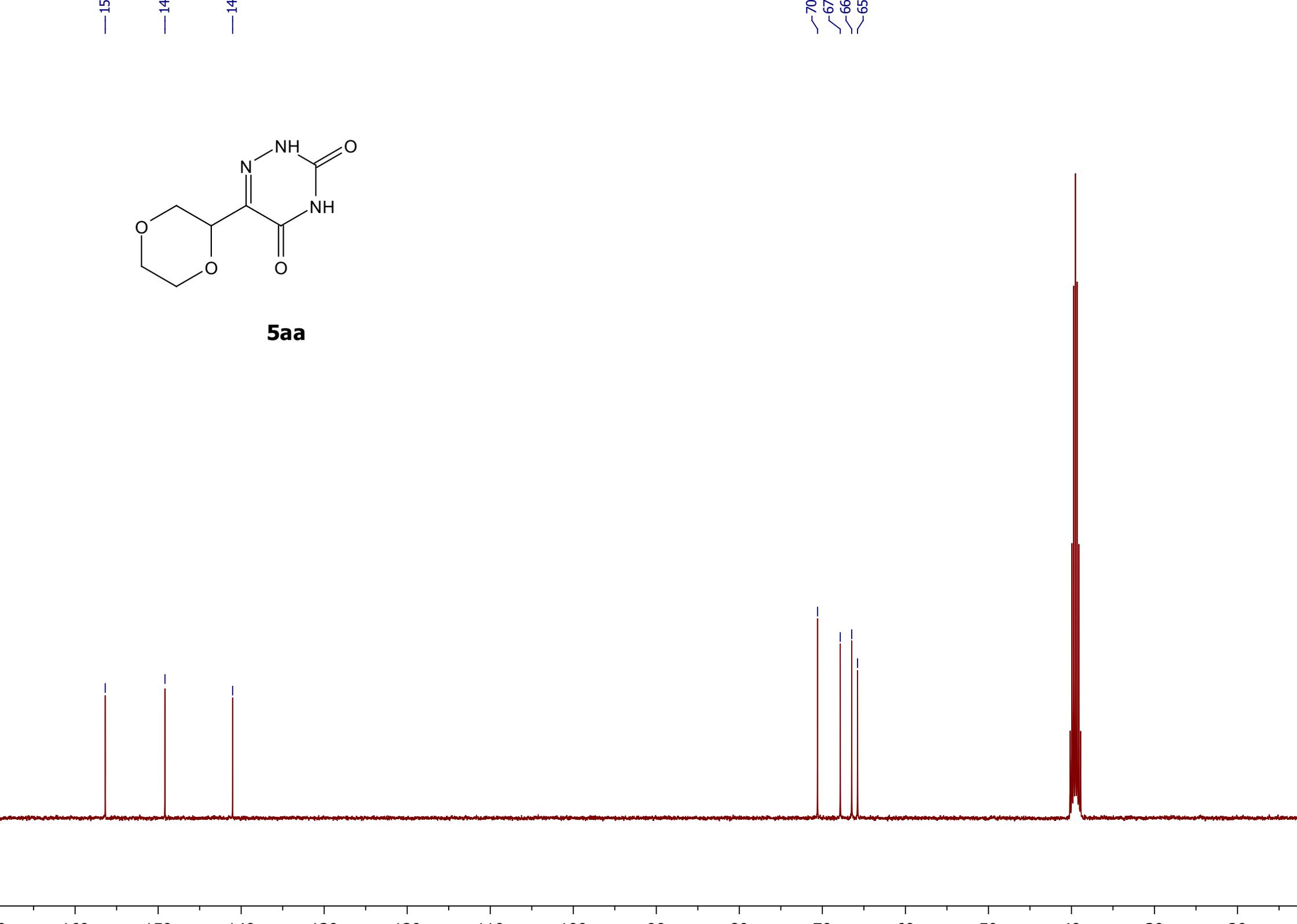


**5aa**

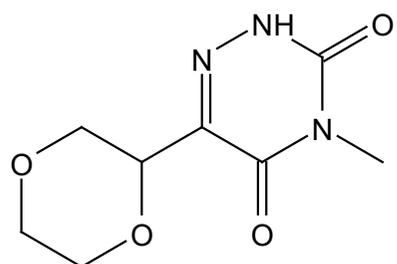




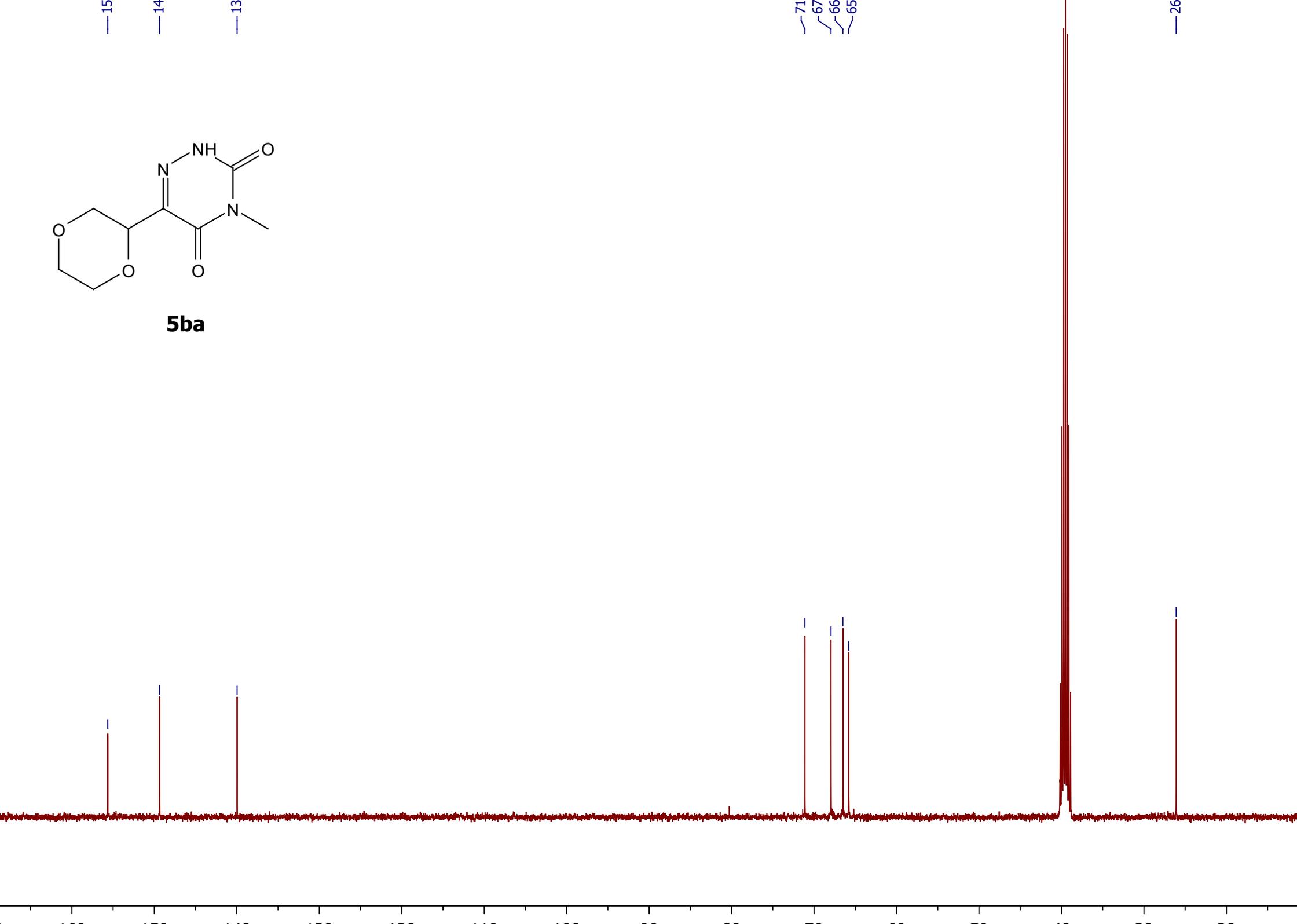
**5aa**

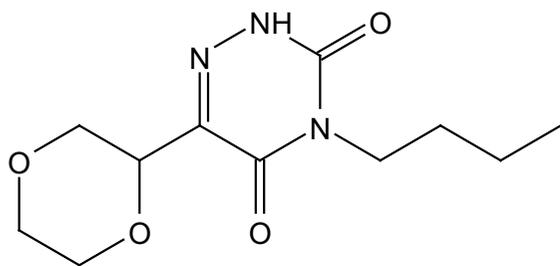




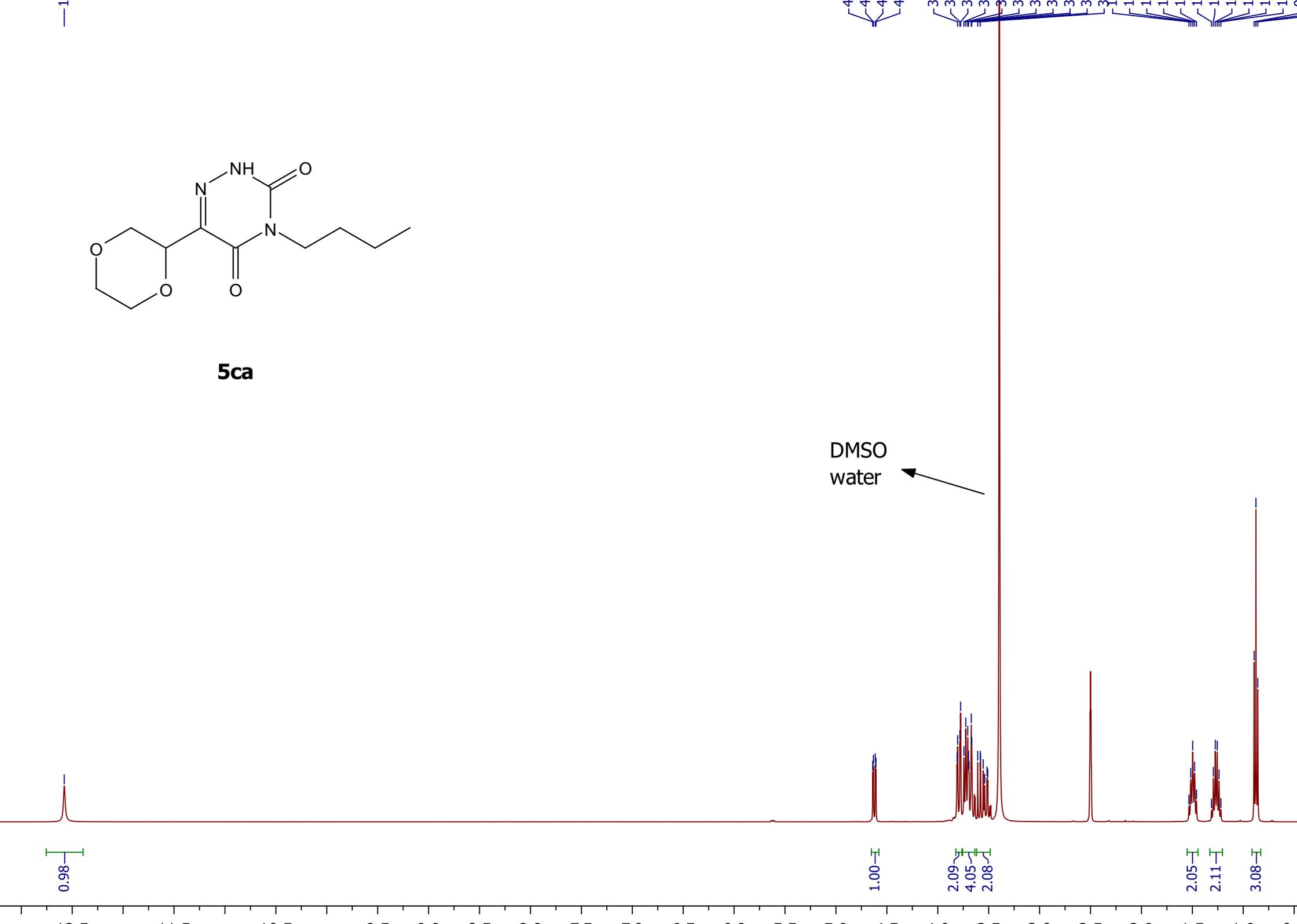


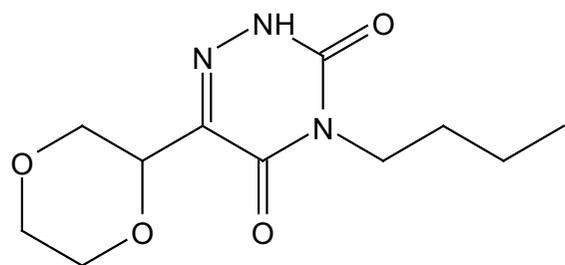
**5ba**



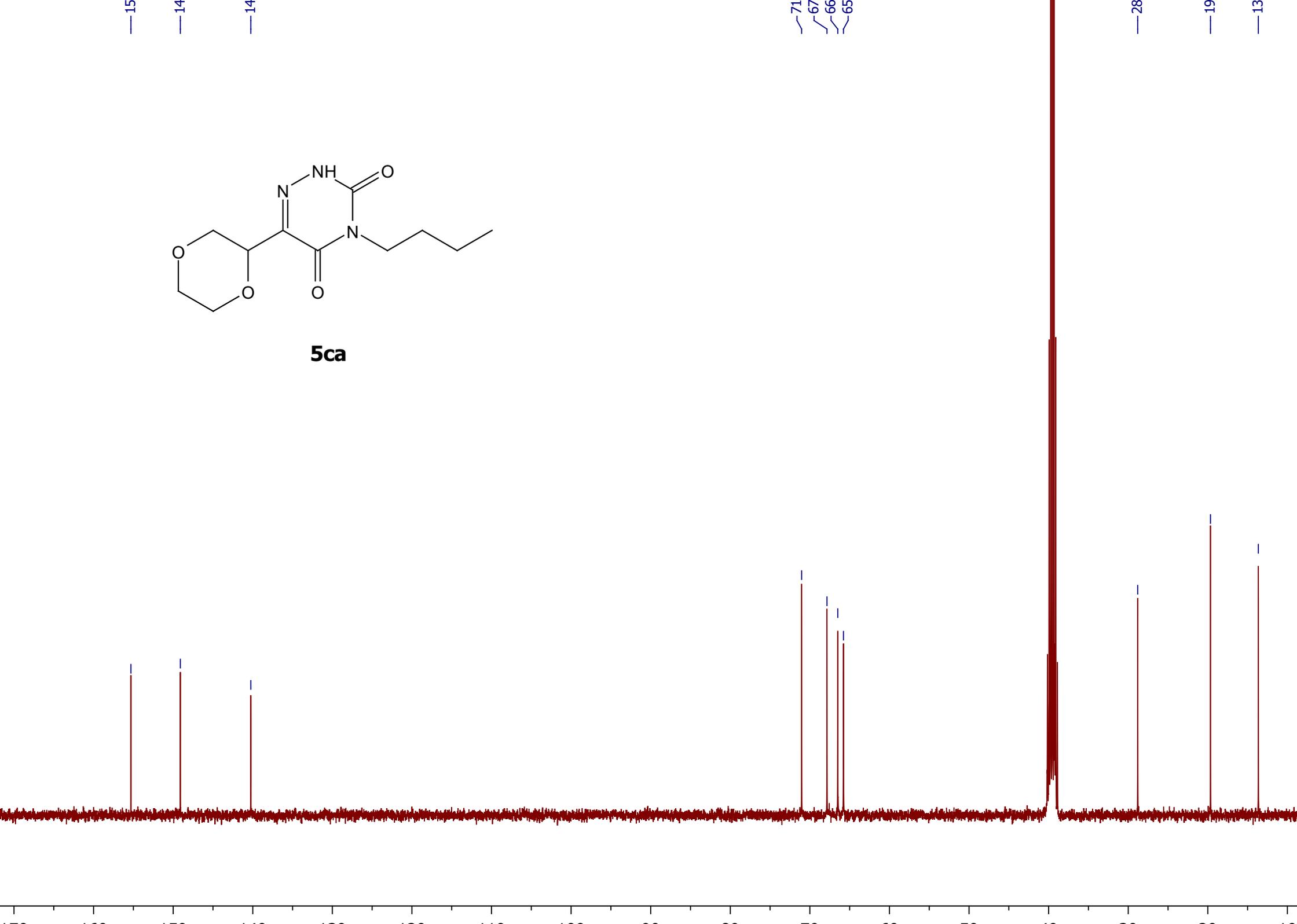


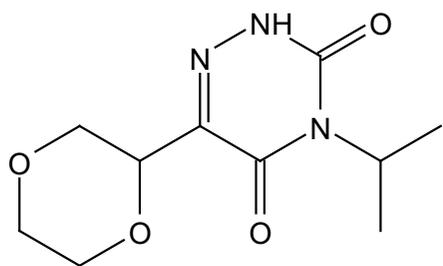
**5ca**



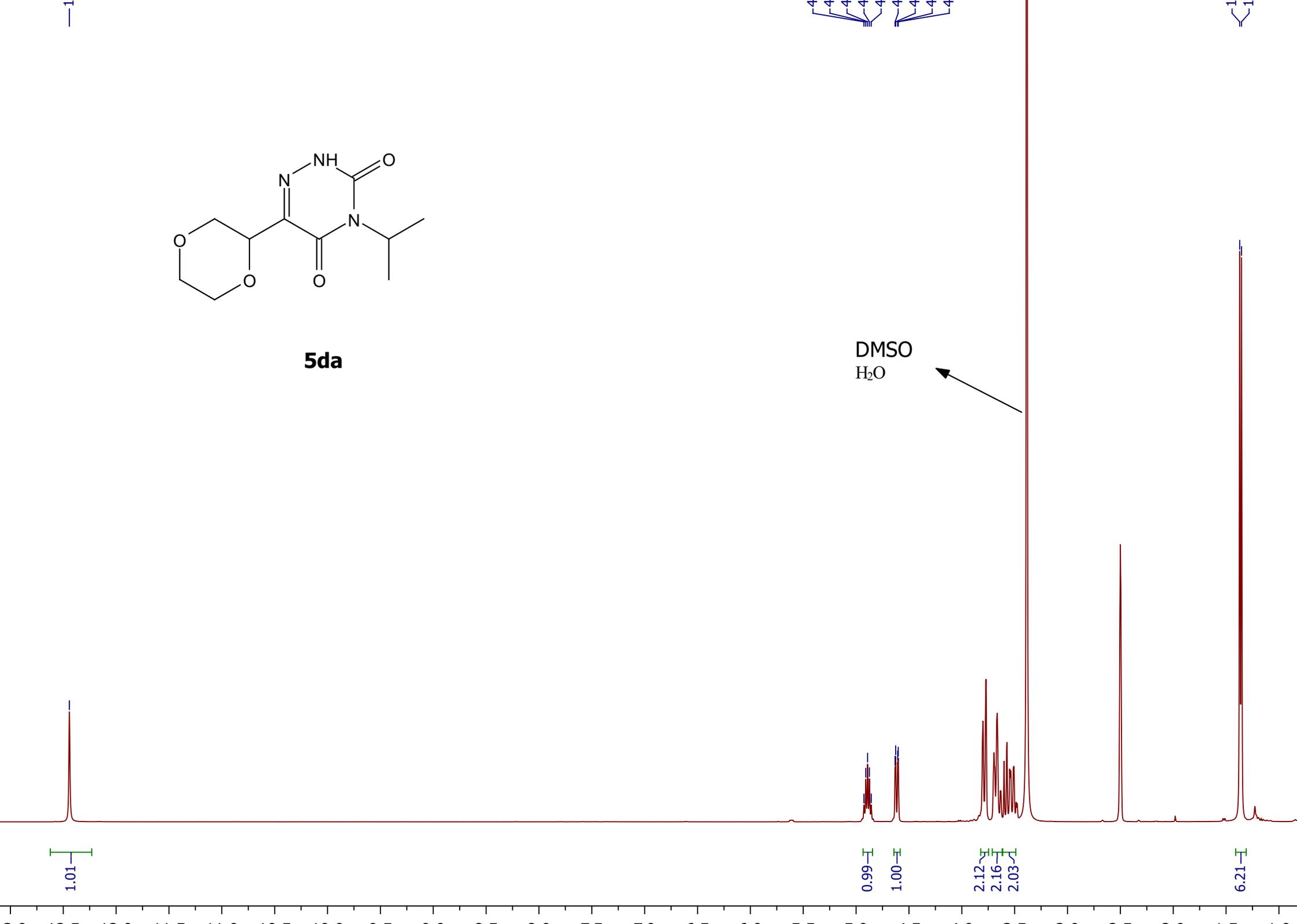


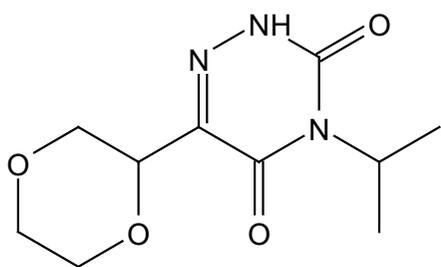
**5ca**



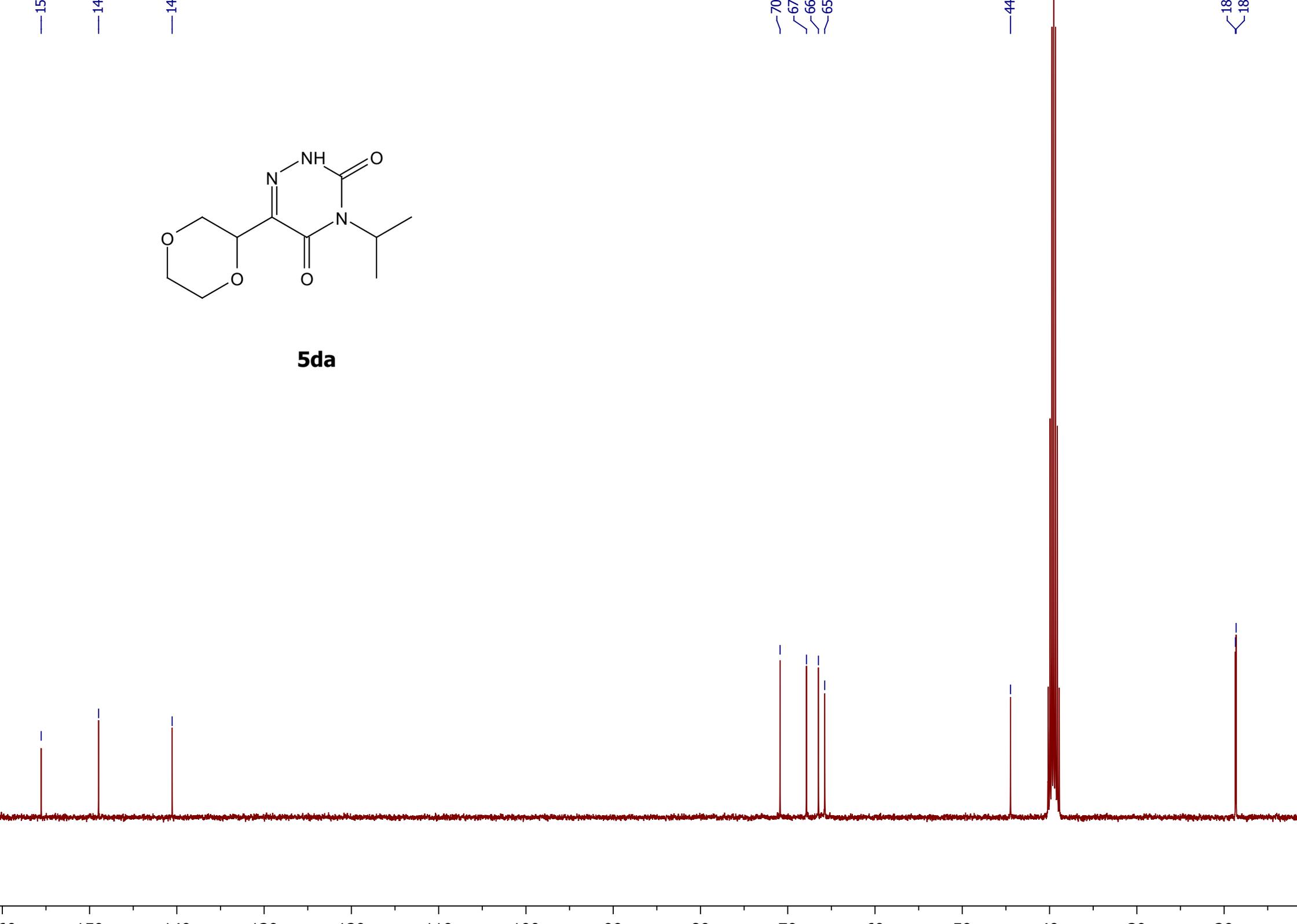


**5da**

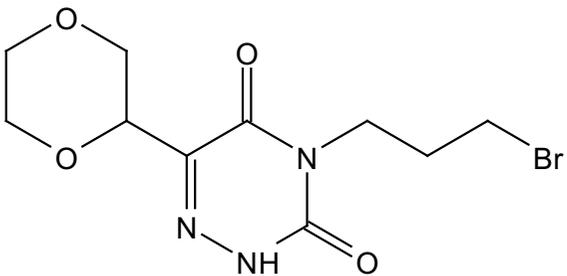




**5da**



12.57



**5ea**

4.64  
4.63  
4.61  
4.61

3.86  
3.85  
3.83  
3.81  
3.78  
3.57  
3.54  
3.52  
2.51  
2.11  
2.10  
2.08  
2.06  
2.04

1.00

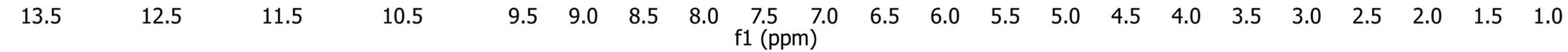
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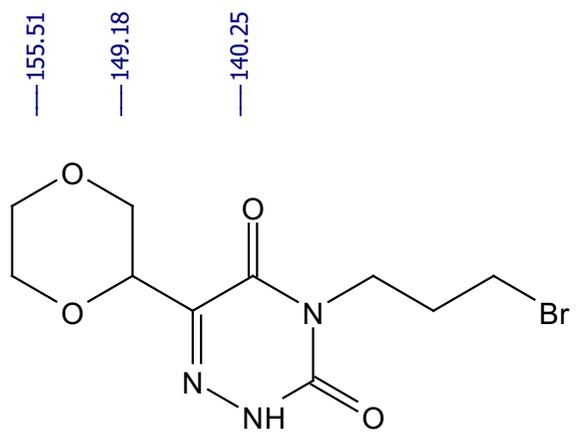
4.81

0.92

4.26

2.02



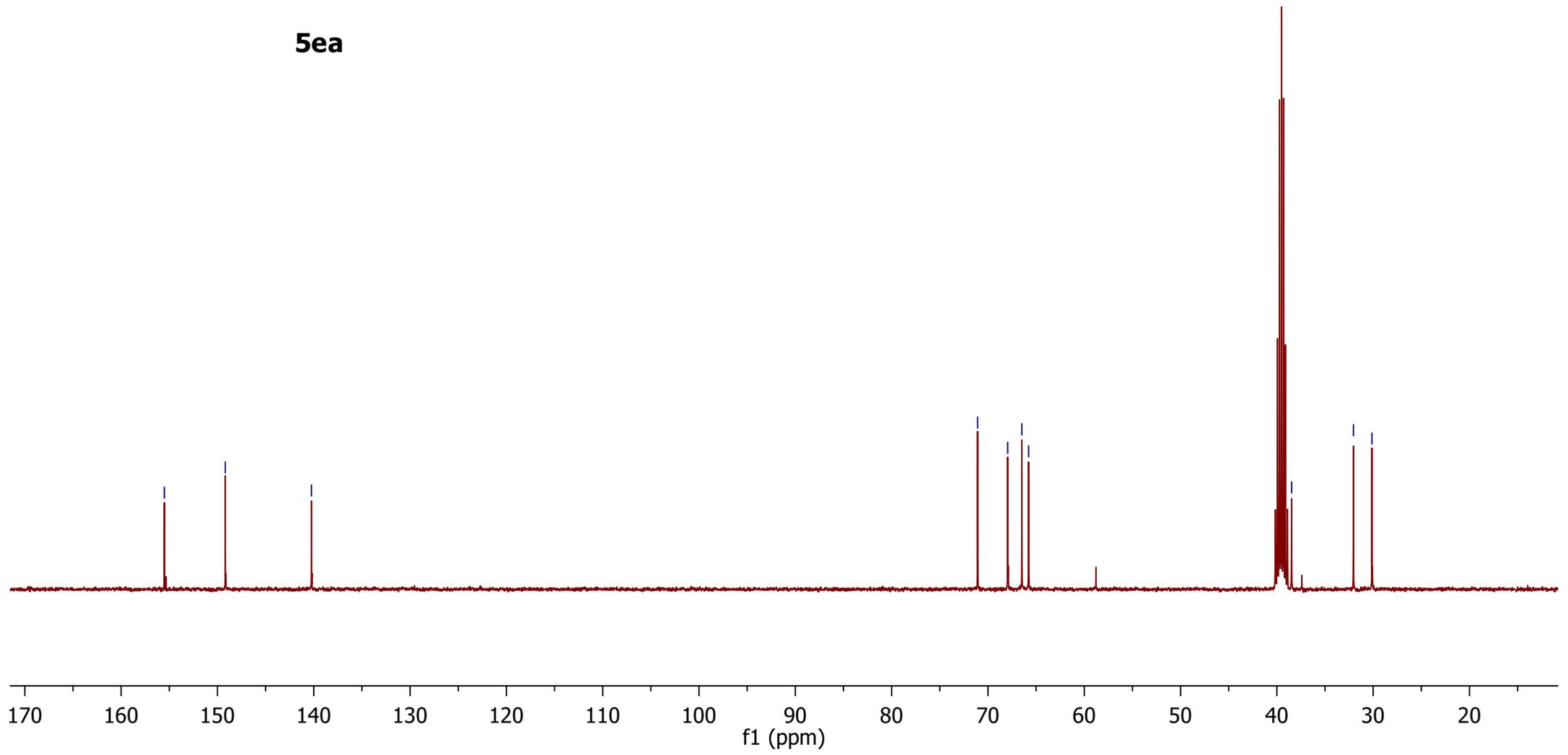


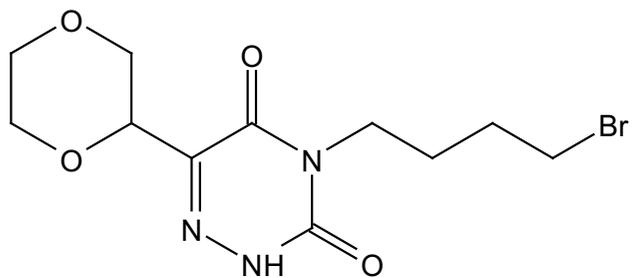
**5ea**

— 155.51  
— 149.18  
— 140.25

— 71.07  
— 67.95  
— 66.48  
— 65.78

— 38.47  
— 32.05  
— 30.13





**5fa**

12.59

4.64  
4.62  
4.61

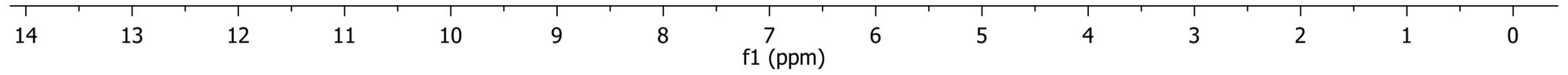
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3.78  
3.76  
3.70  
3.67  
3.55  
3.53  
3.51  
3.46  
1.81  
1.79  
1.78  
1.68  
1.66  
1.64

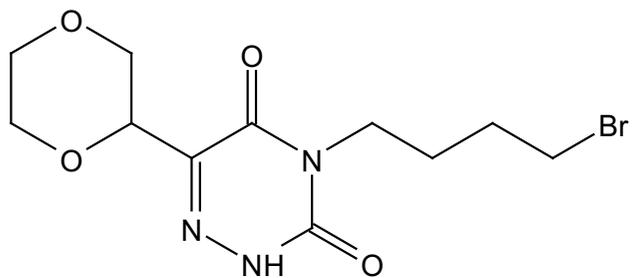
1.00

1.05

4.16  
1.94  
0.93  
3.19

1.99  
2.07



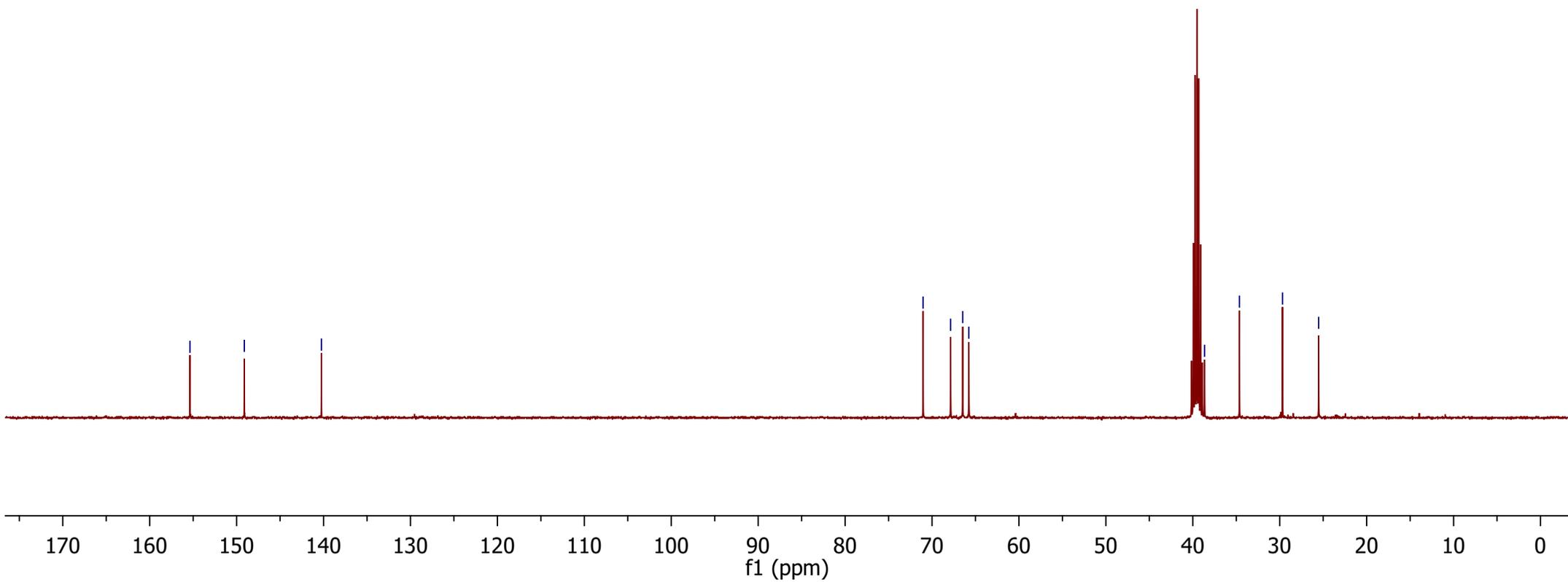


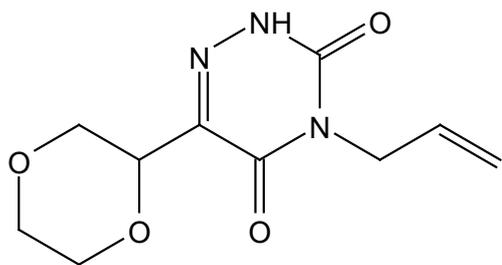
**5fa**

— 155.36  
— 149.12  
— 140.25

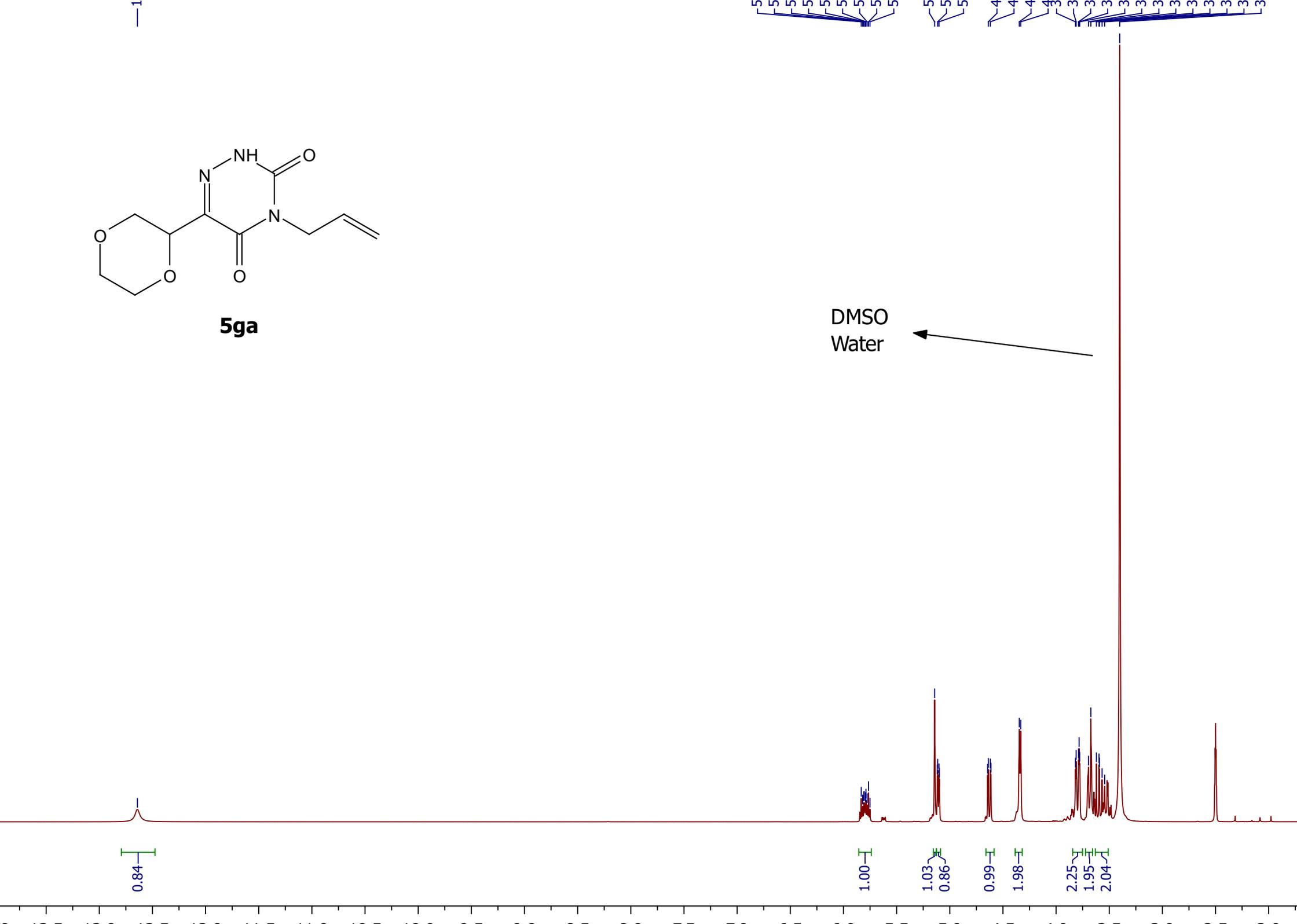
71.03  
67.86  
66.47  
65.77

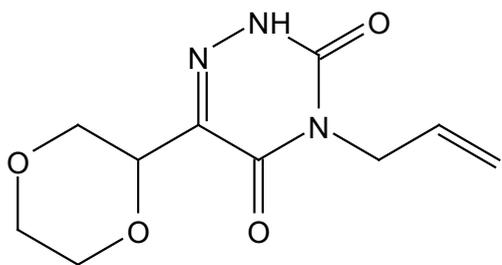
— 38.65  
— 34.63  
— 29.68  
— 25.52



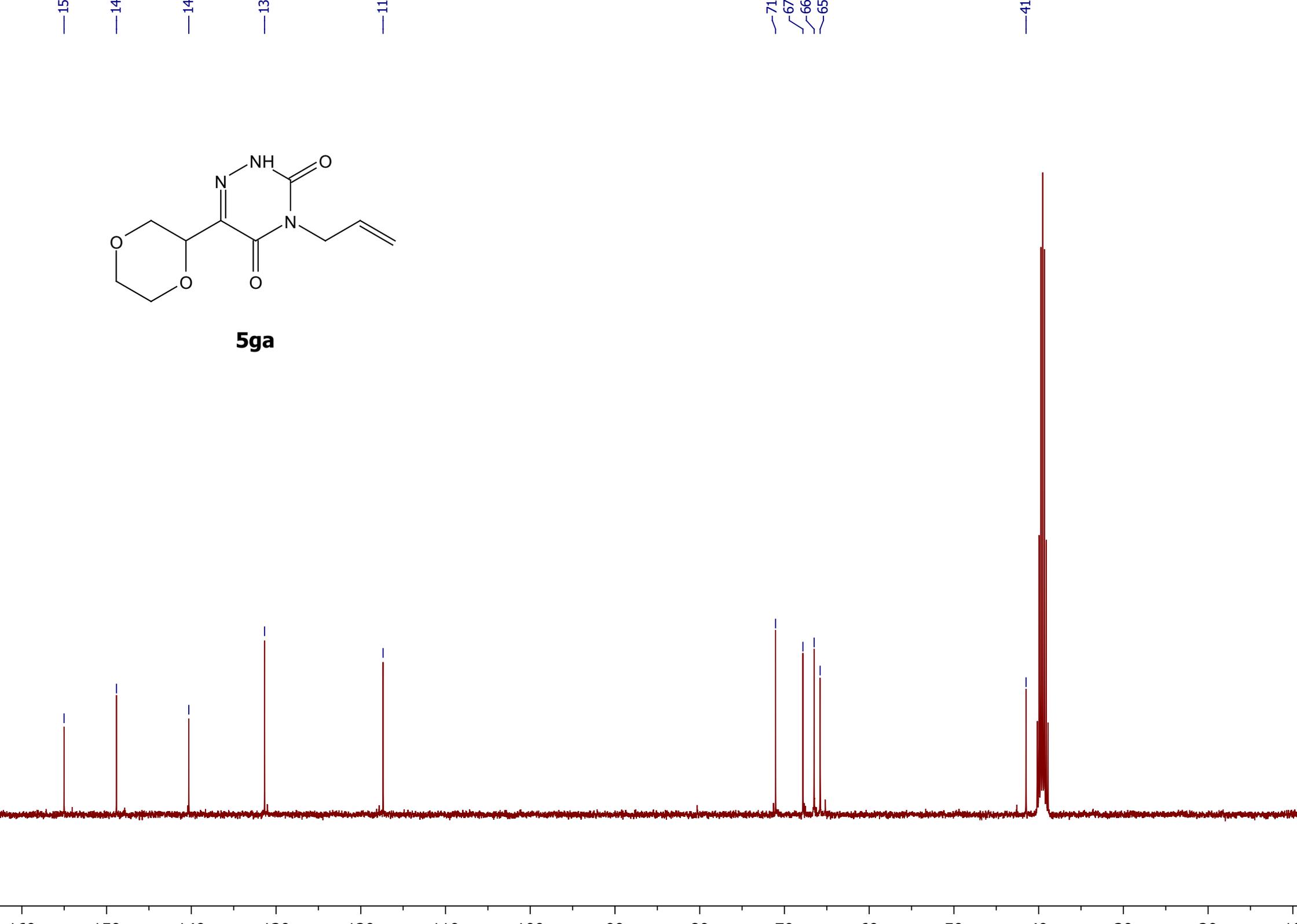


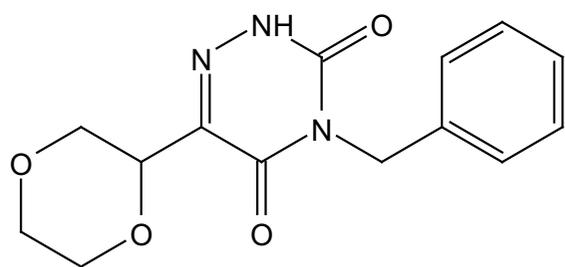
**5ga**



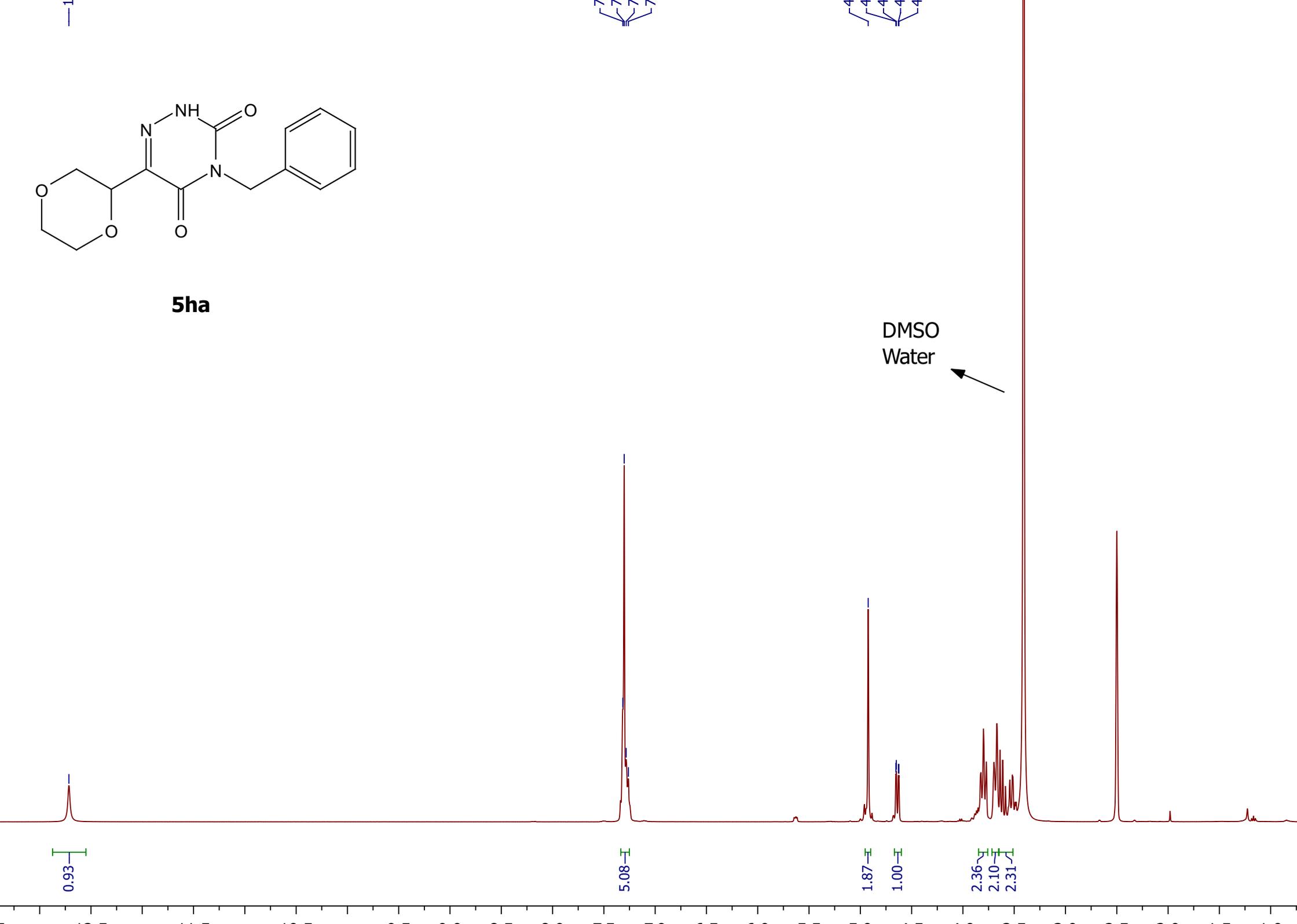


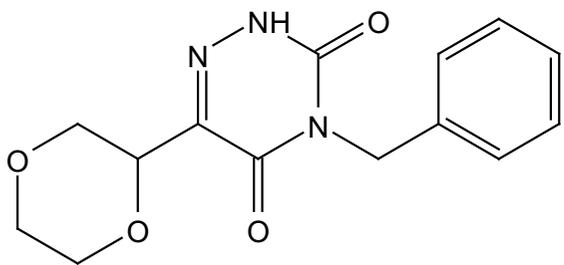
**5ga**



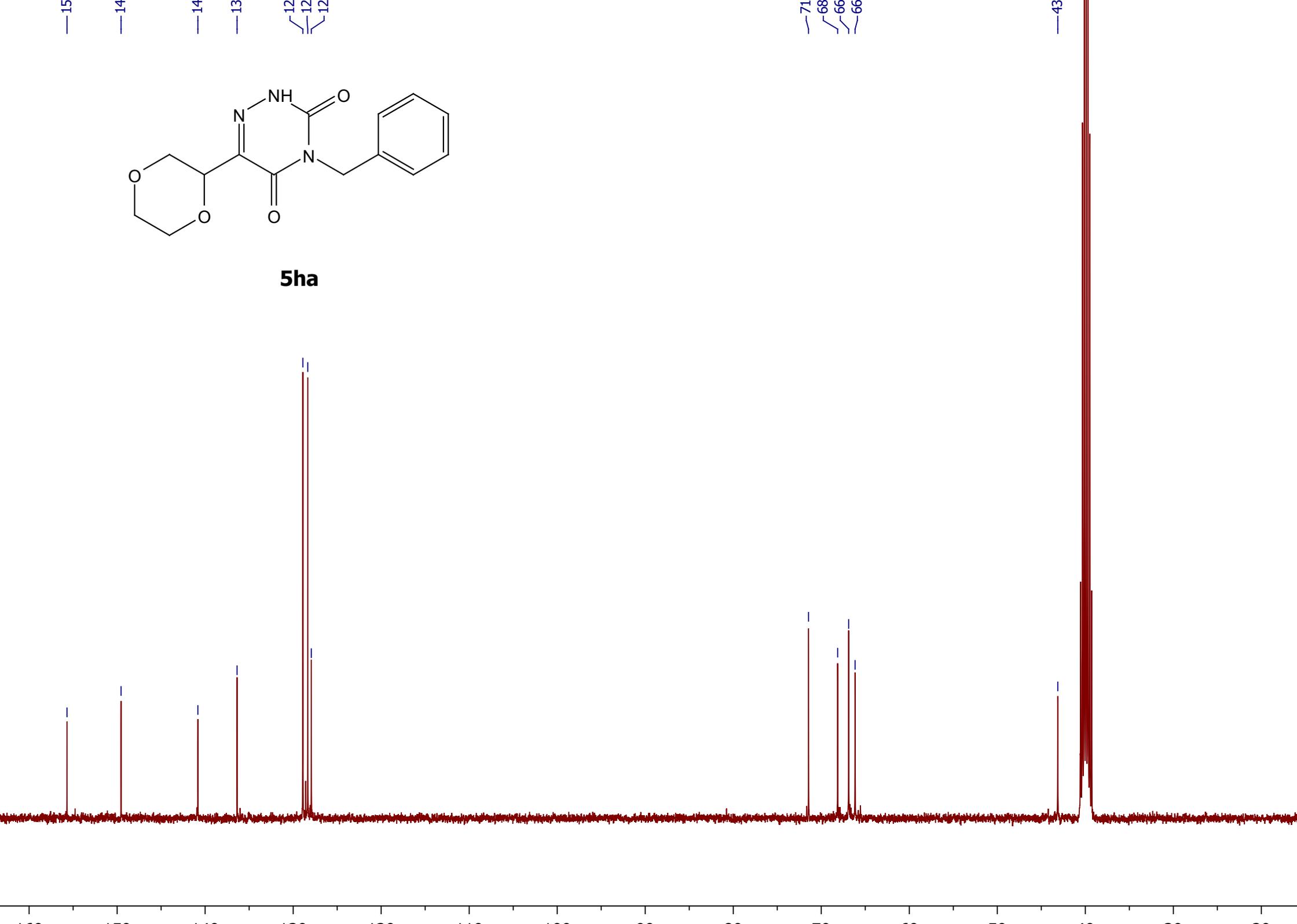


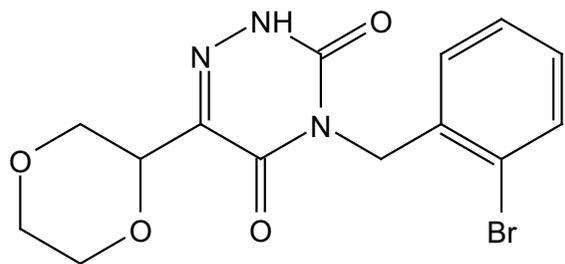
**5ha**



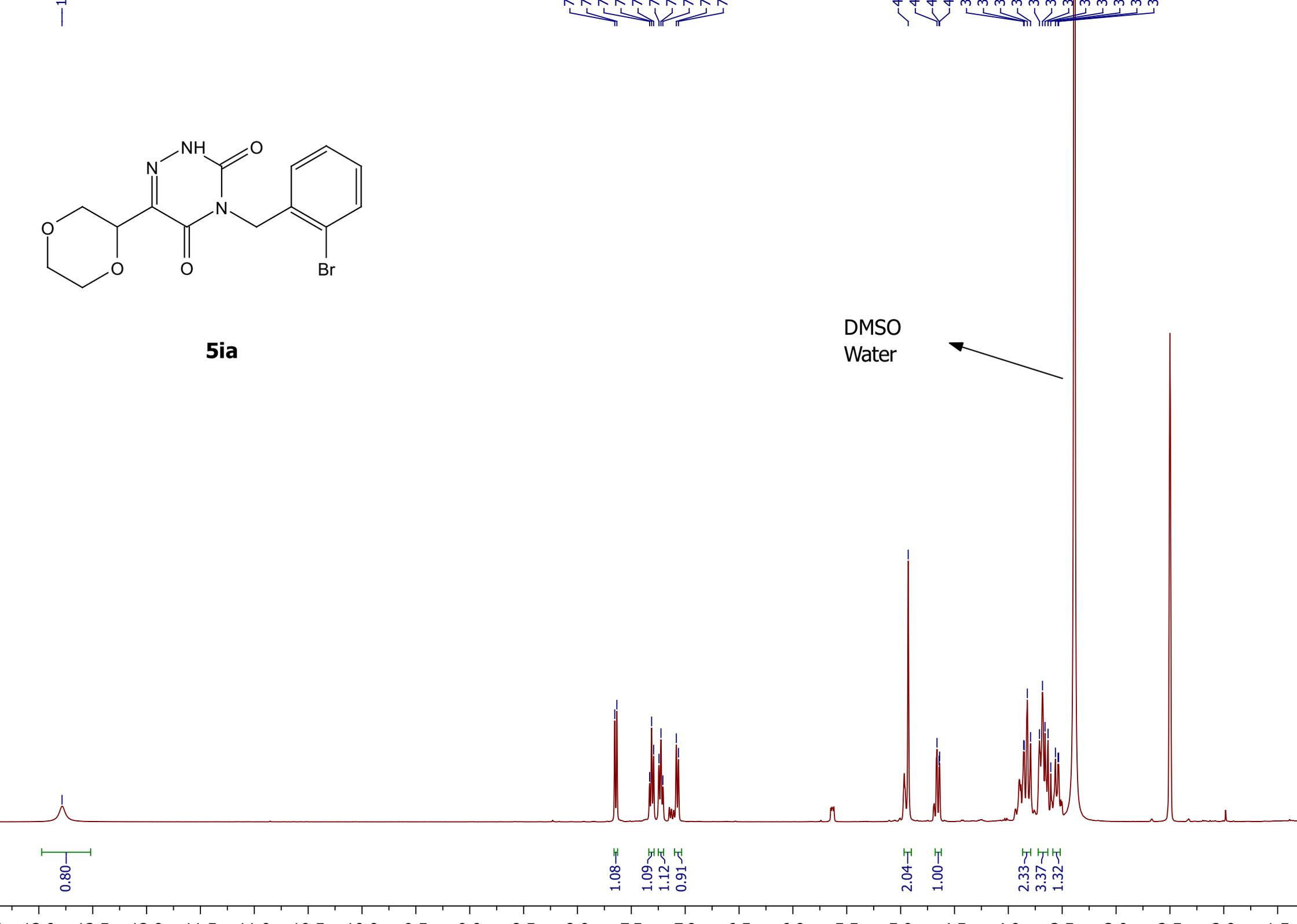


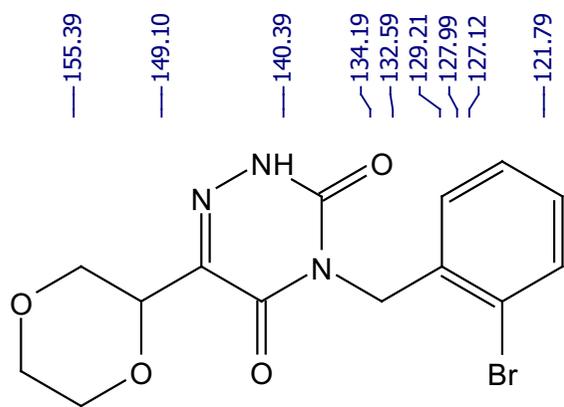
**5ha**



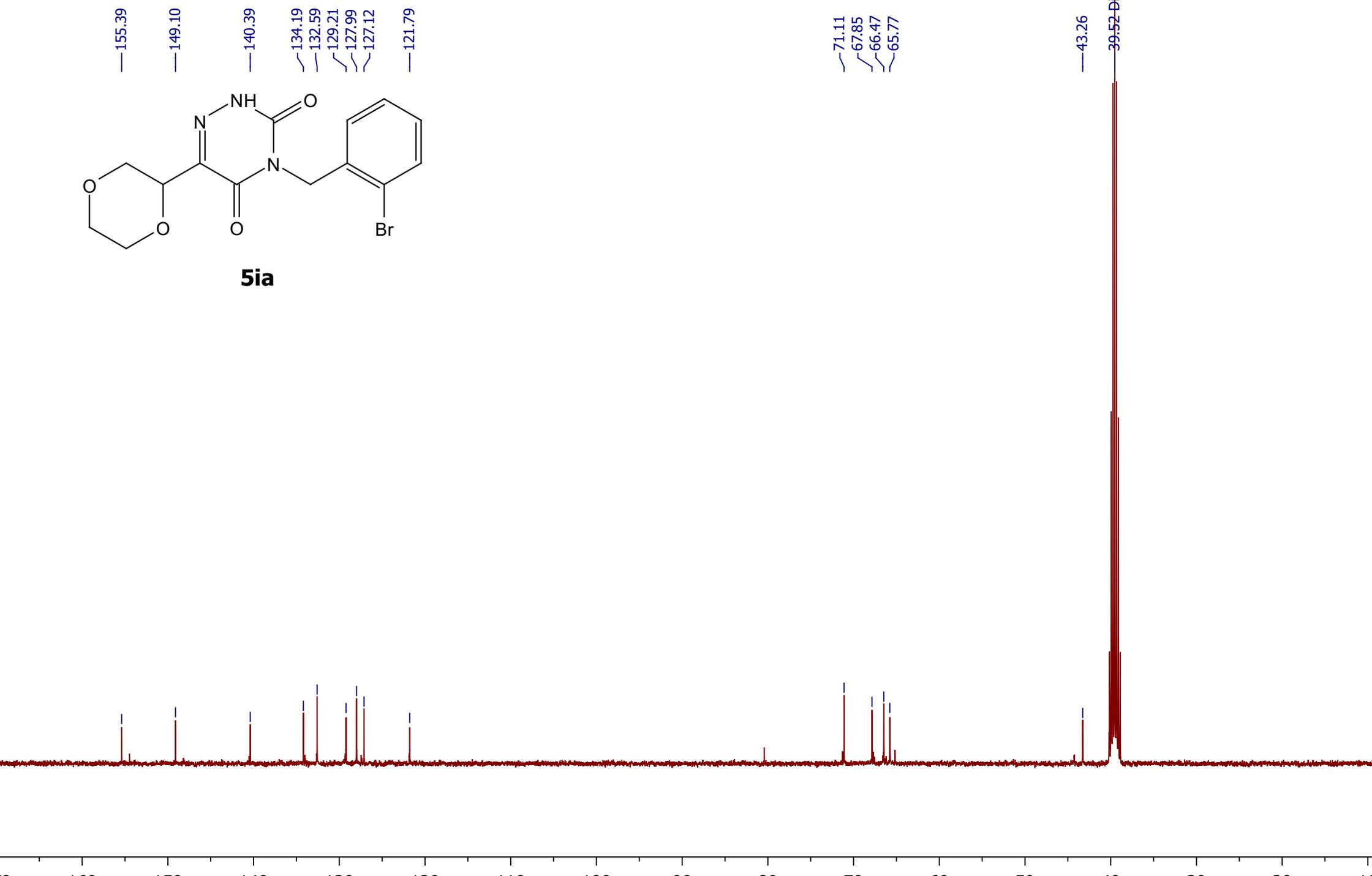


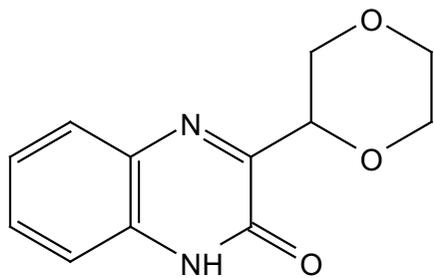
**5ia**





**5ia**



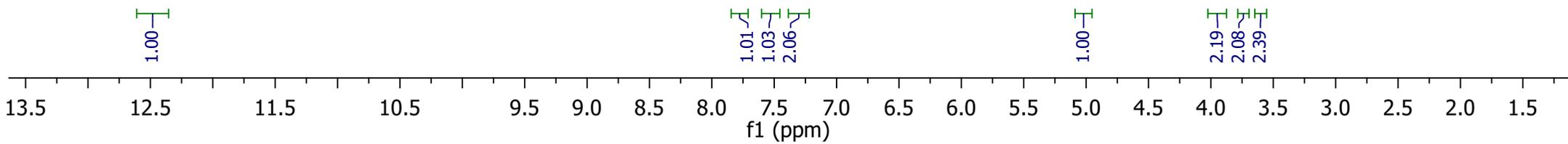


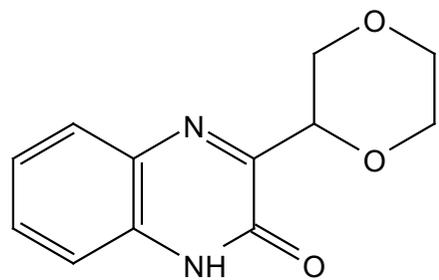
**7aa**

—12.49

7.80  
7.78  
7.55  
7.53  
7.51  
7.32  
7.30  
7.29

5.04  
5.02  
5.02  
4.00  
3.97  
3.93  
3.90  
3.78  
3.75  
3.73  
3.63  
3.62  
3.59  
3.57





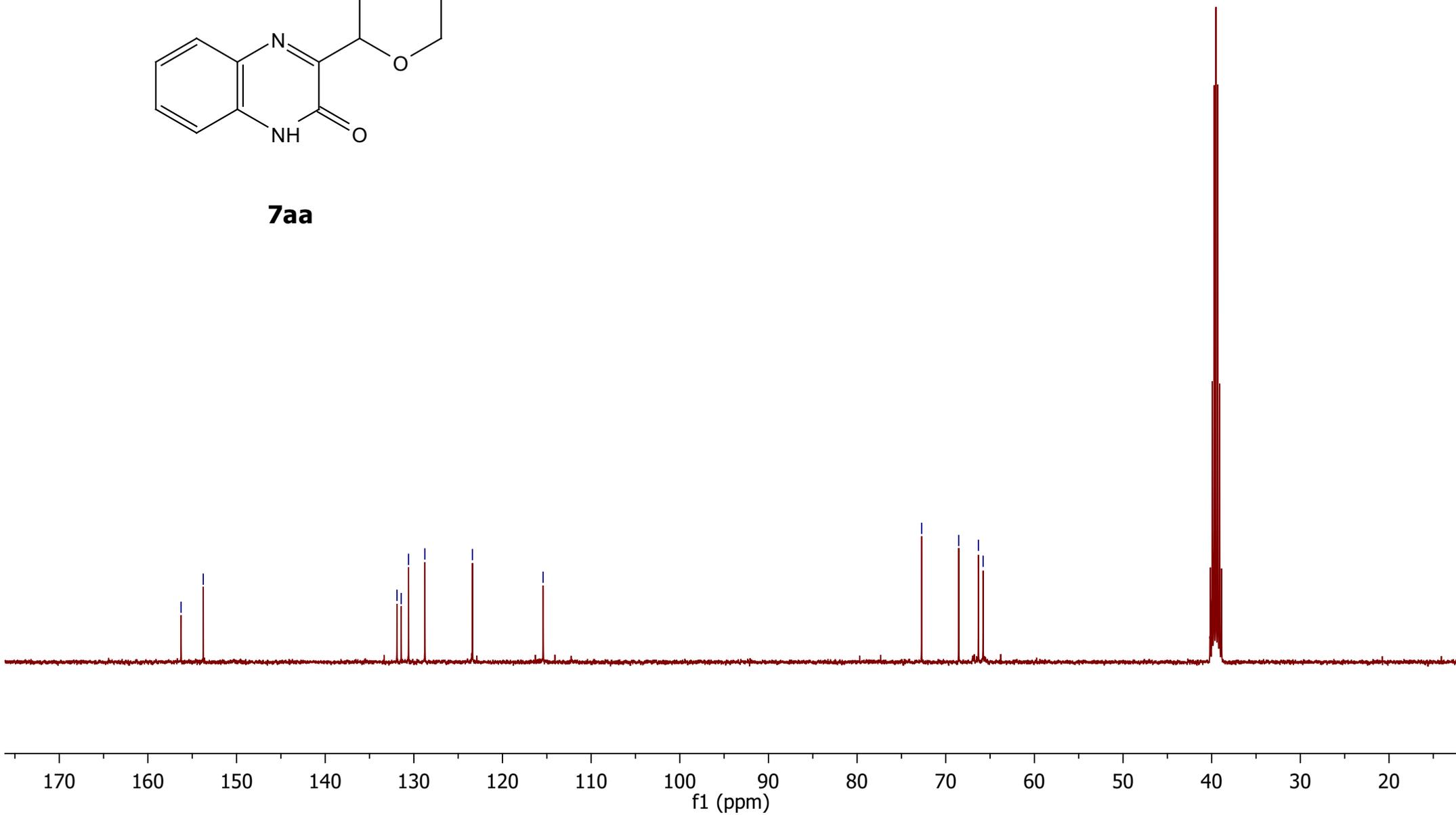
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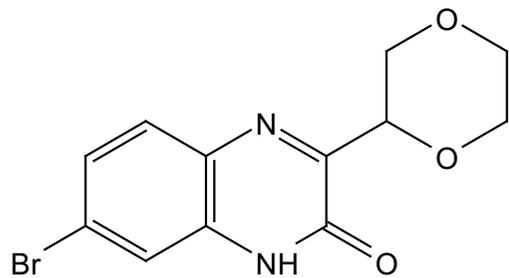
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— 153.75

— 131.90  
— 131.42  
— 130.60  
— 128.75  
— 123.39

— 115.42

— 72.72  
— 68.54  
— 66.32  
— 65.79





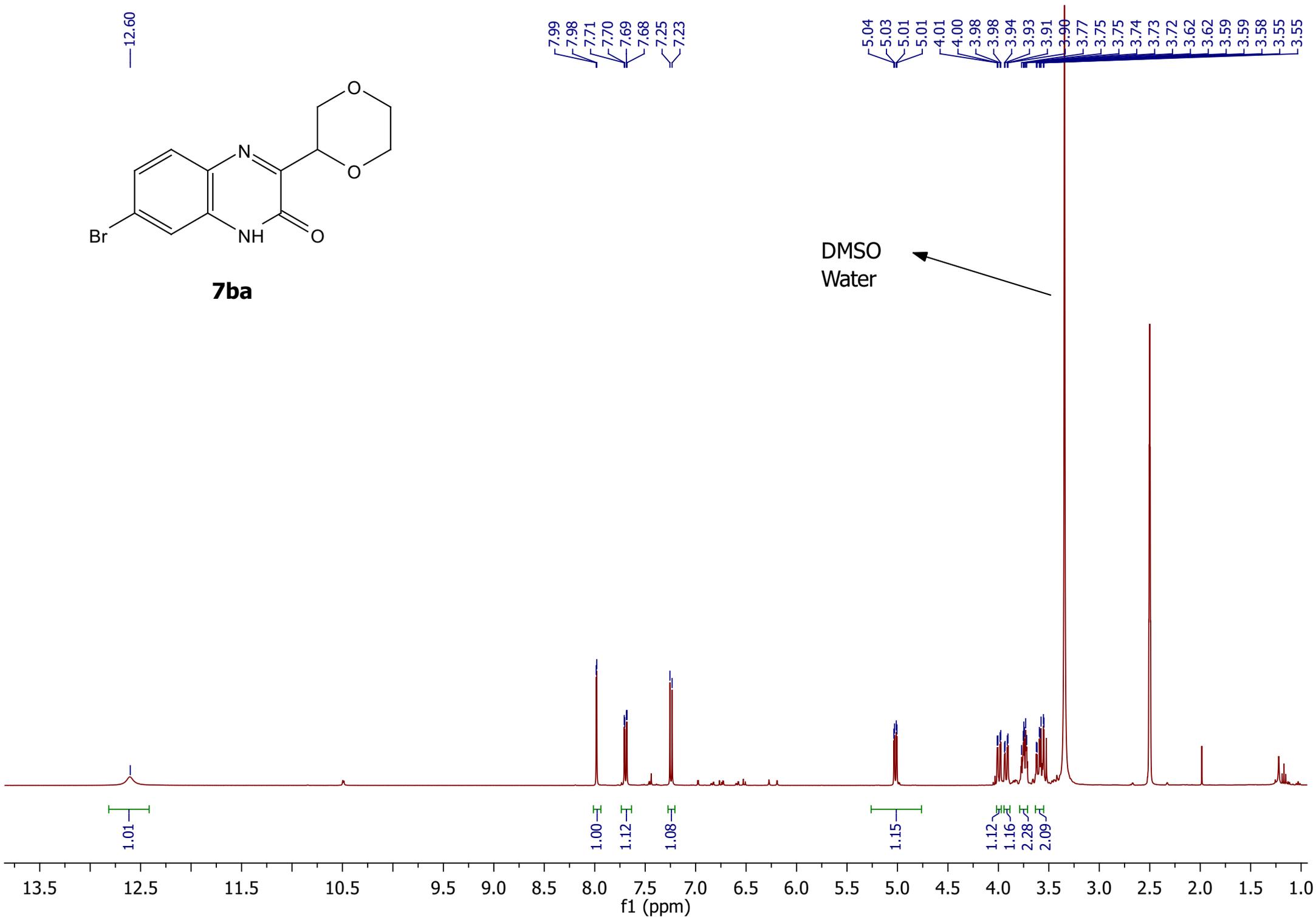
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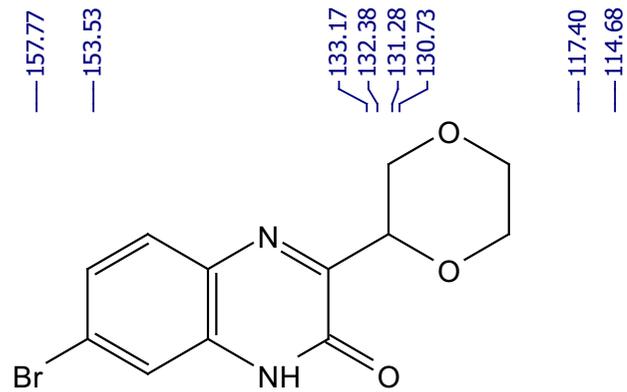
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7.98  
7.71  
7.70  
7.69  
7.68  
7.25  
7.23

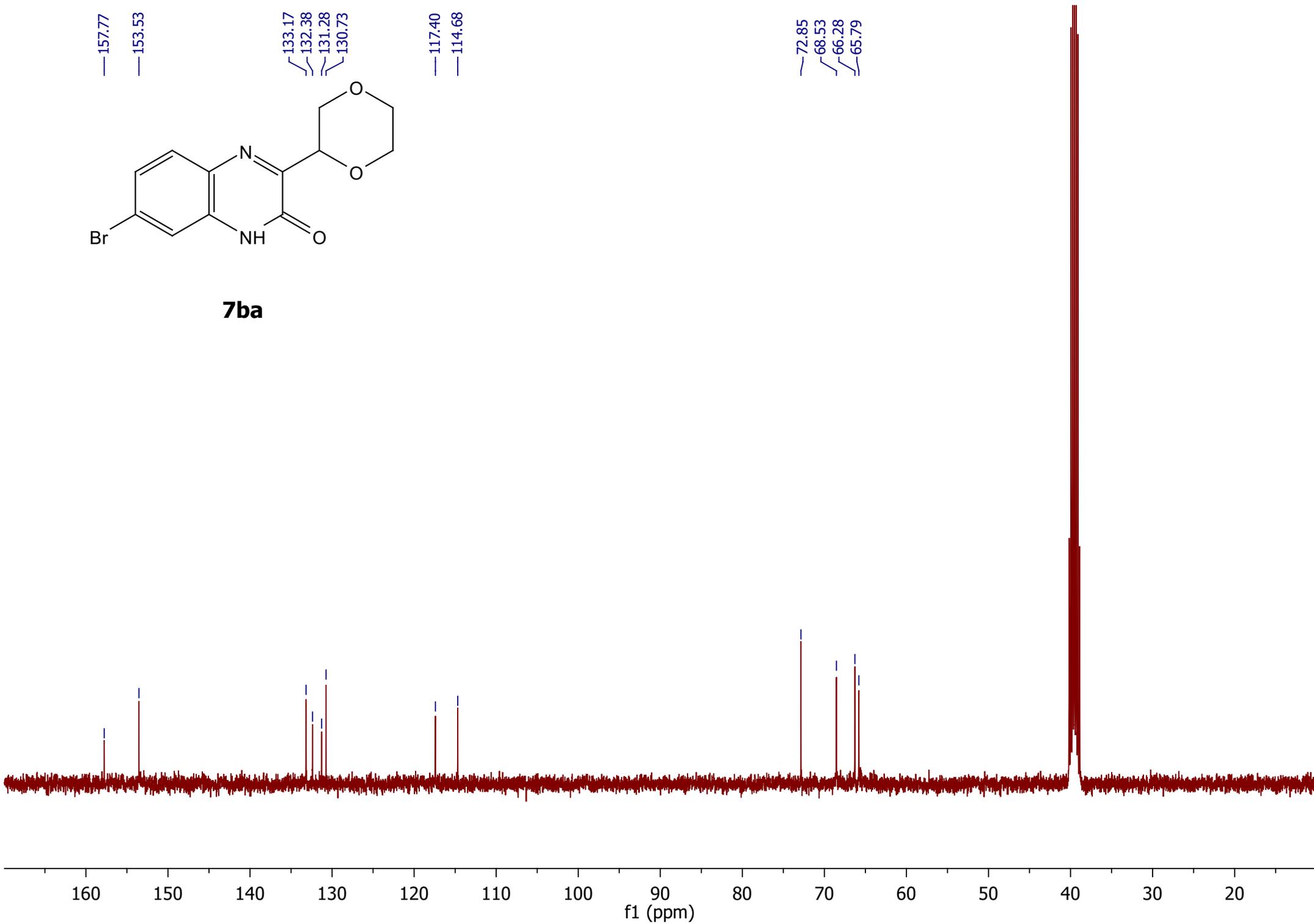
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5.01  
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4.01  
4.00  
3.98  
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3.94  
3.93  
3.91  
3.90  
3.77  
3.75  
3.75  
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3.72  
3.62  
3.62  
3.59  
3.59  
3.58  
3.55  
3.55

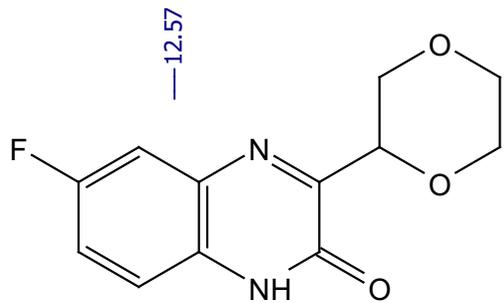
DMSO  
Water



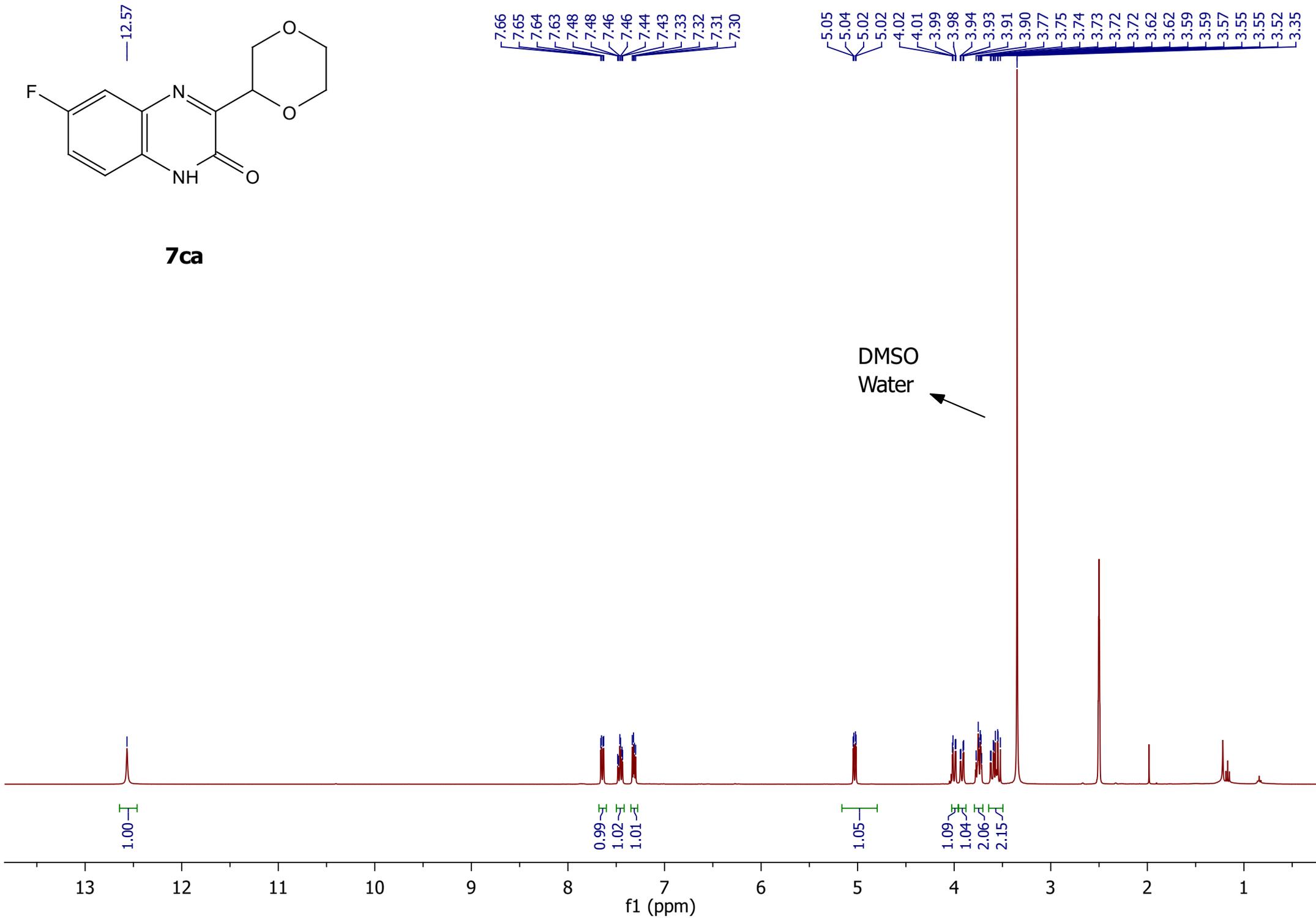


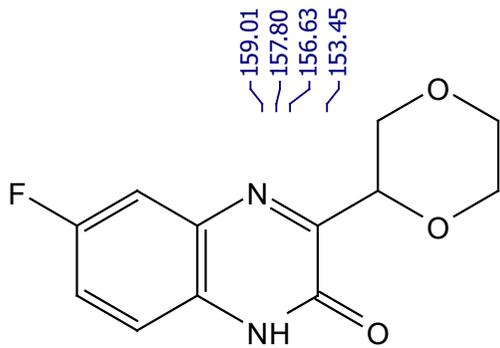
**7ba**





**7ca**





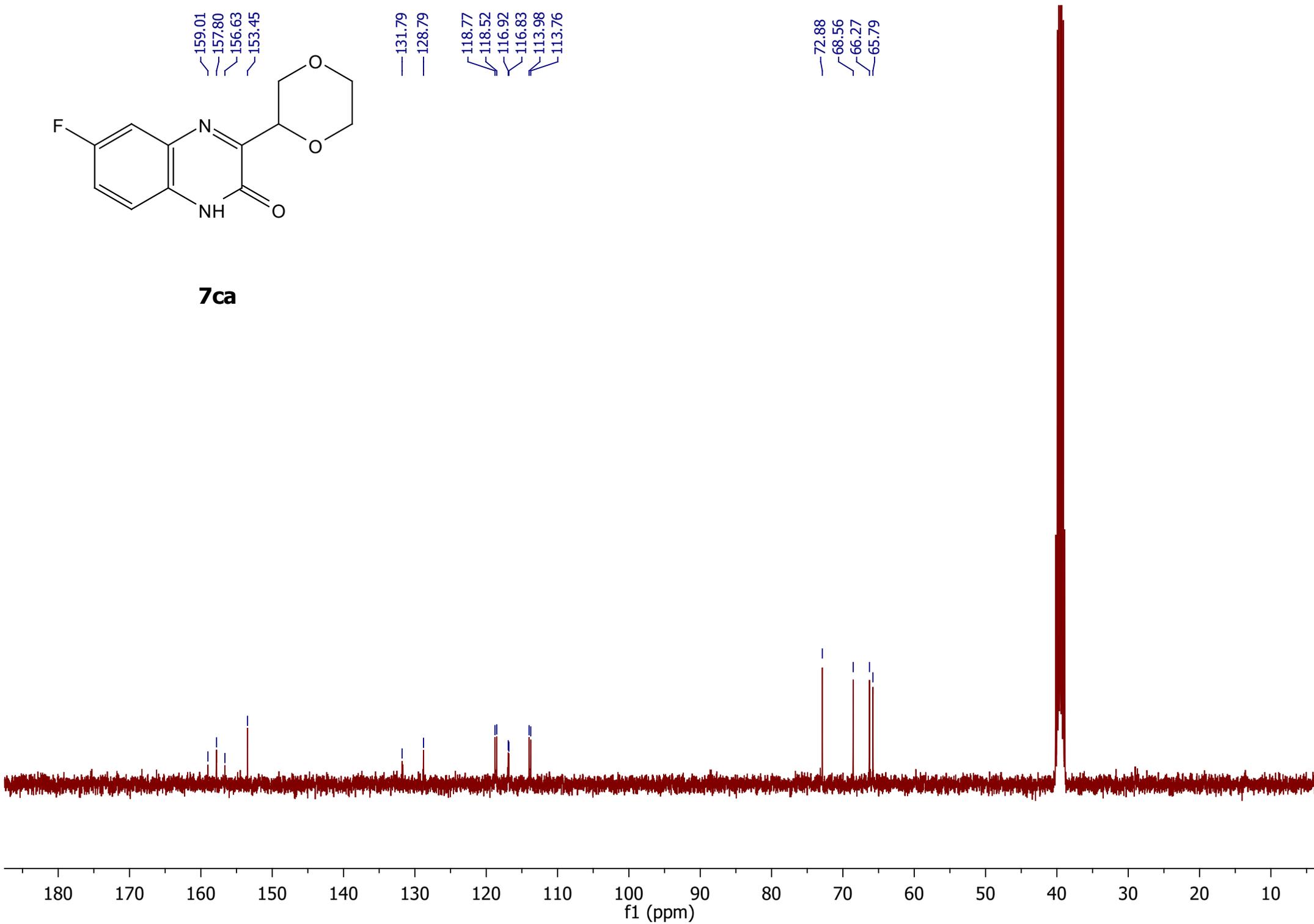
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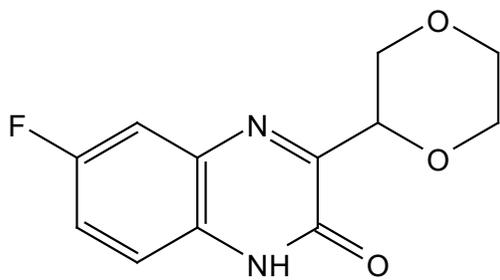
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156.63  
153.45

131.79  
128.79

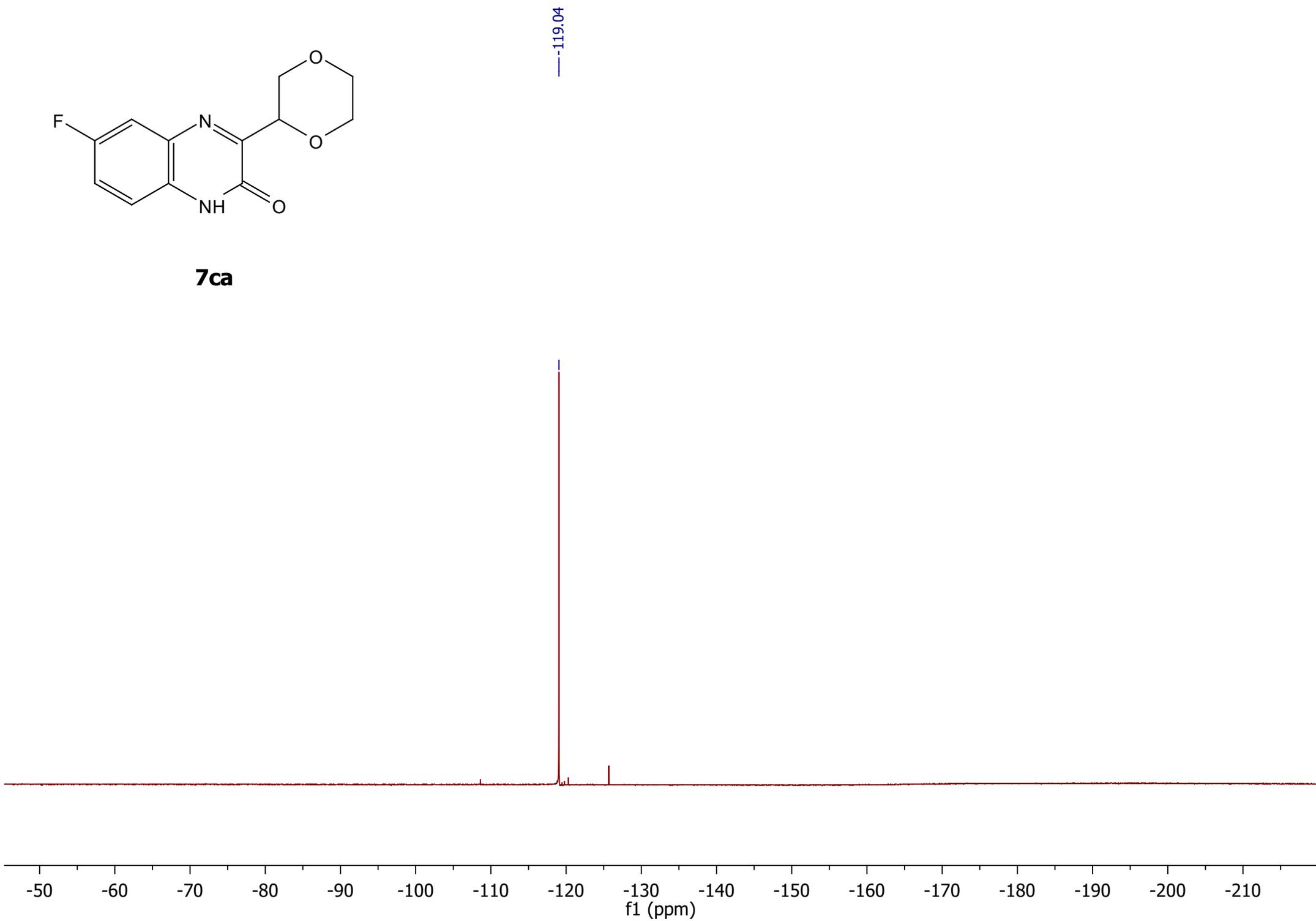
118.77  
118.52  
116.92  
116.83  
113.98  
113.76

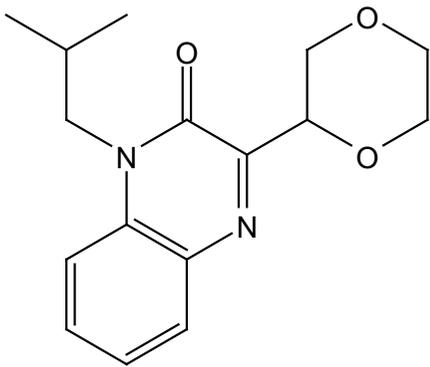
72.88  
68.56  
66.27  
65.79





**7ca**





**7da**

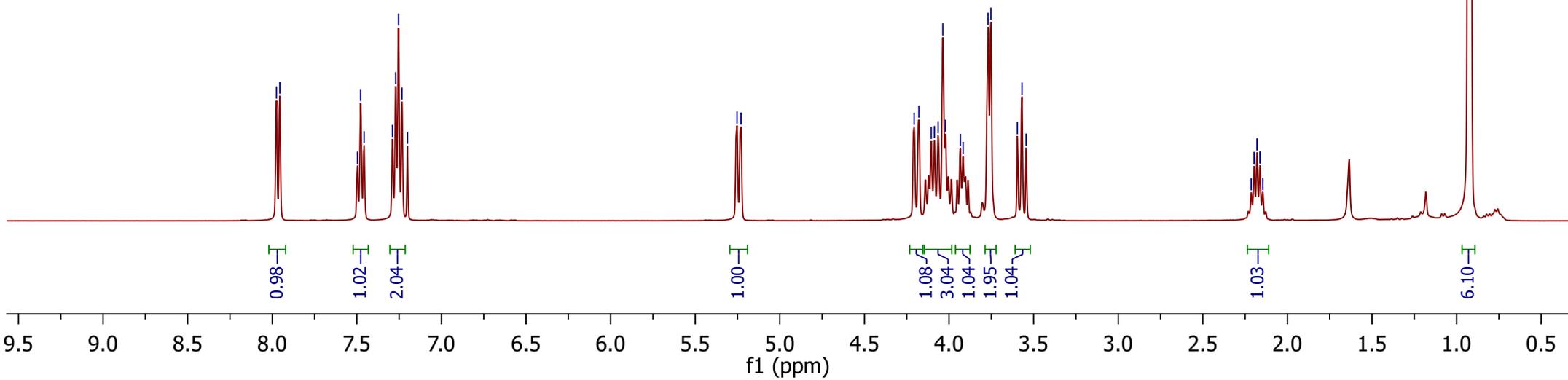
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7.50  
7.48  
7.46  
7.29  
7.27  
7.25  
7.23  
7.20

5.25  
5.23

4.21  
4.18  
4.11  
4.09  
4.06  
4.04  
4.02  
3.93  
3.92  
3.77  
3.75  
3.60  
3.57  
3.54

2.21  
2.20  
2.18  
2.16  
2.15

0.93  
0.92



155.31  
153.98

132.97  
132.72  
131.08  
130.68

123.76

114.17

74.79

69.59

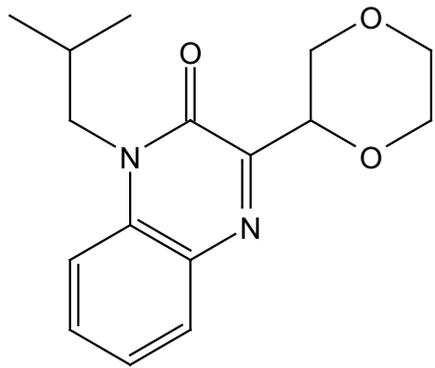
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66.45

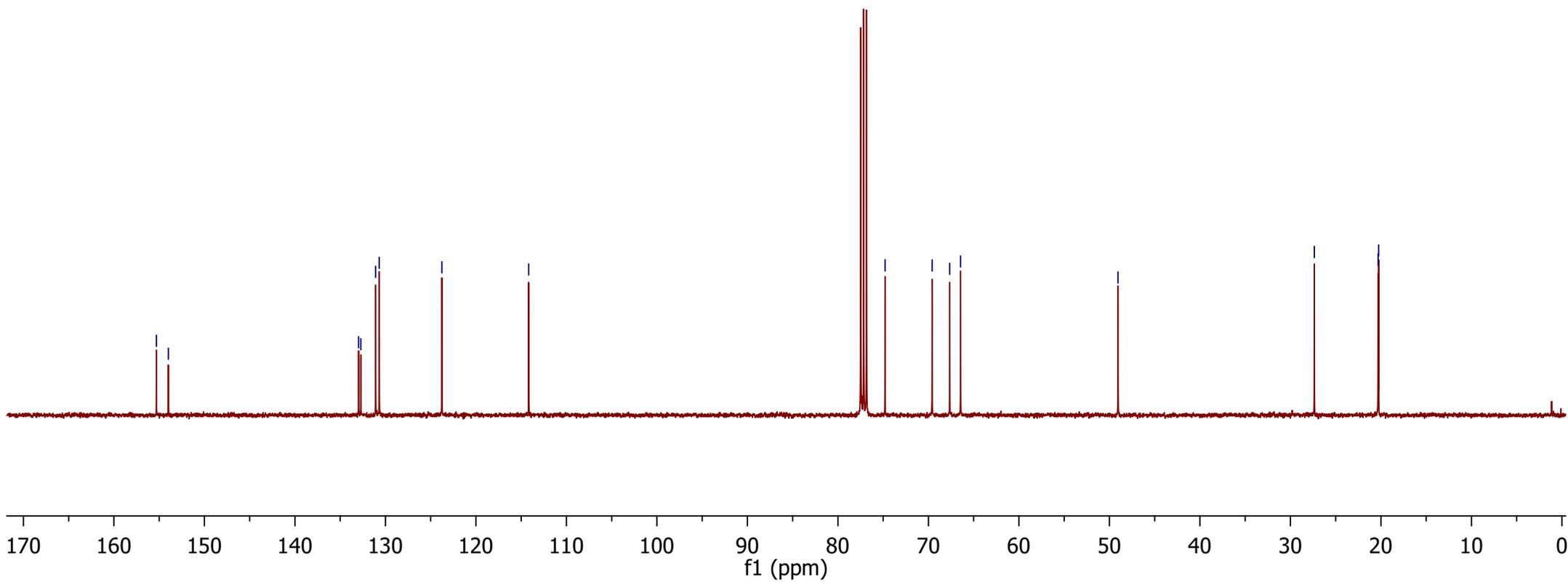
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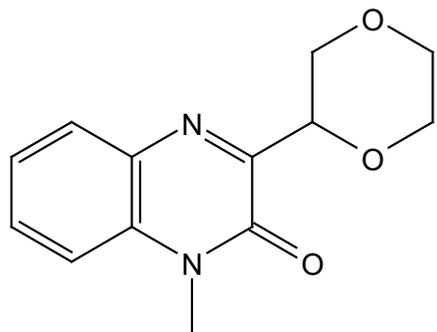
27.36

20.31  
20.26



**7da**





**7ea**

7.85  
7.83  
7.65  
7.63  
7.57  
7.55  
7.41  
7.39  
7.37

5.07  
5.07  
5.05  
5.04

4.02  
3.99  
3.94  
3.91  
3.79  
3.76  
3.74  
3.64  
3.61  
3.60  
3.57  
3.55

0.99  
1.02  
1.01  
1.04

1.00

1.03  
1.01  
2.13  
2.97  
2.02

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0

f1 (ppm)

154.76  
153.17

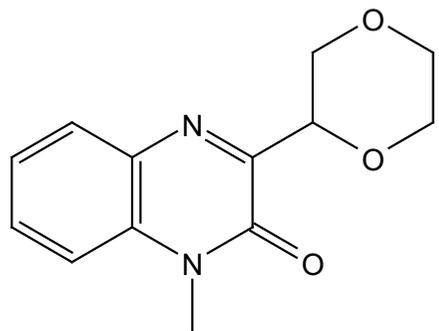
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123.60

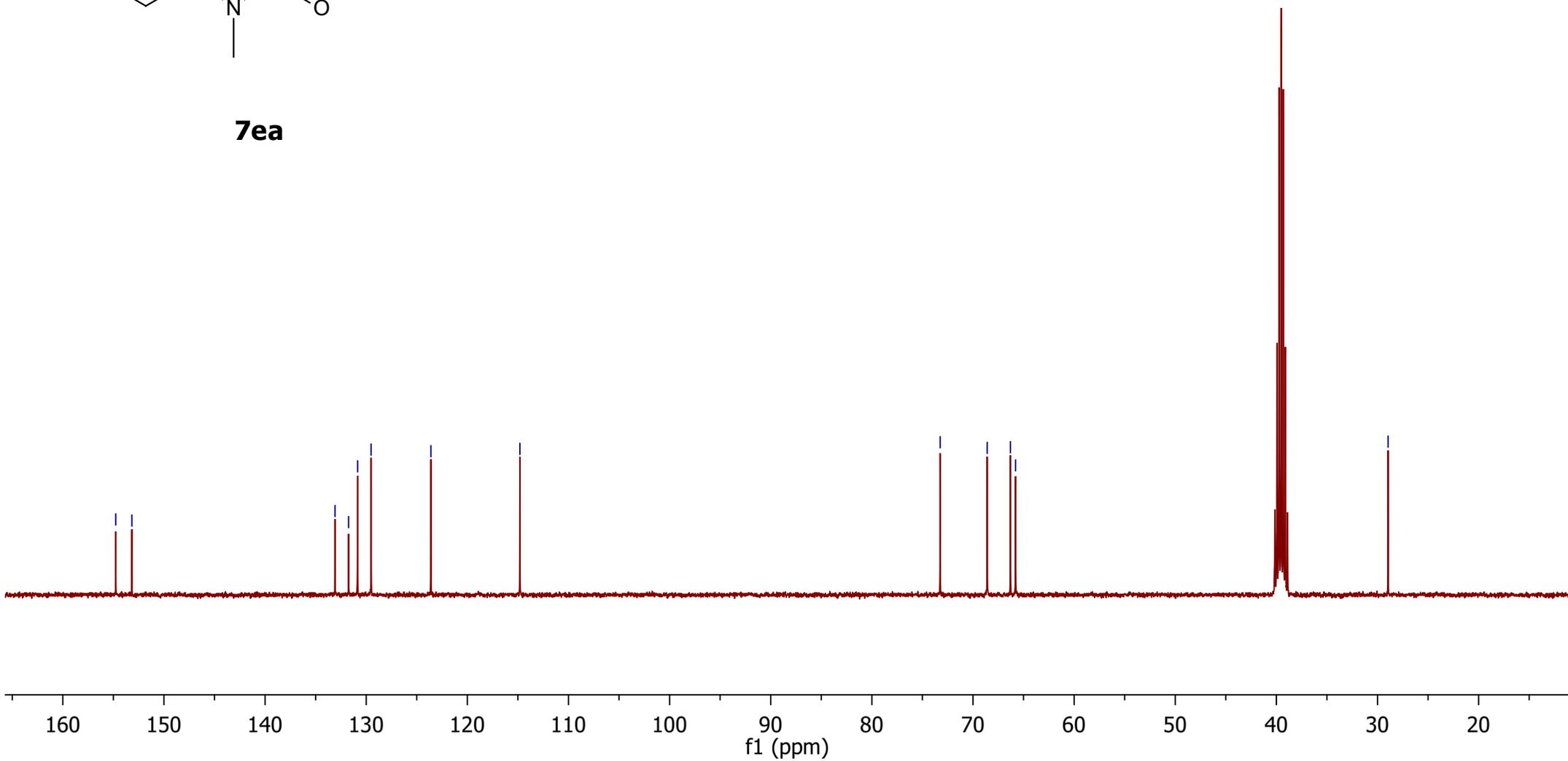
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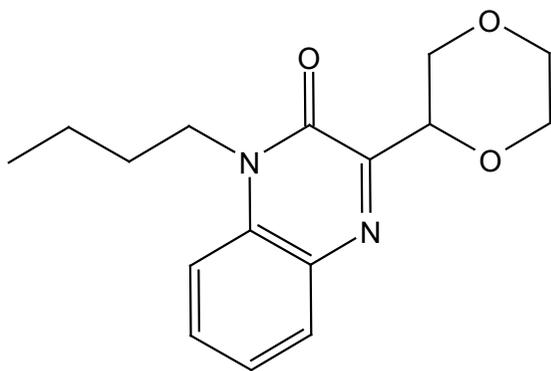
73.25  
68.59  
66.29  
65.79

28.95



**7ea**





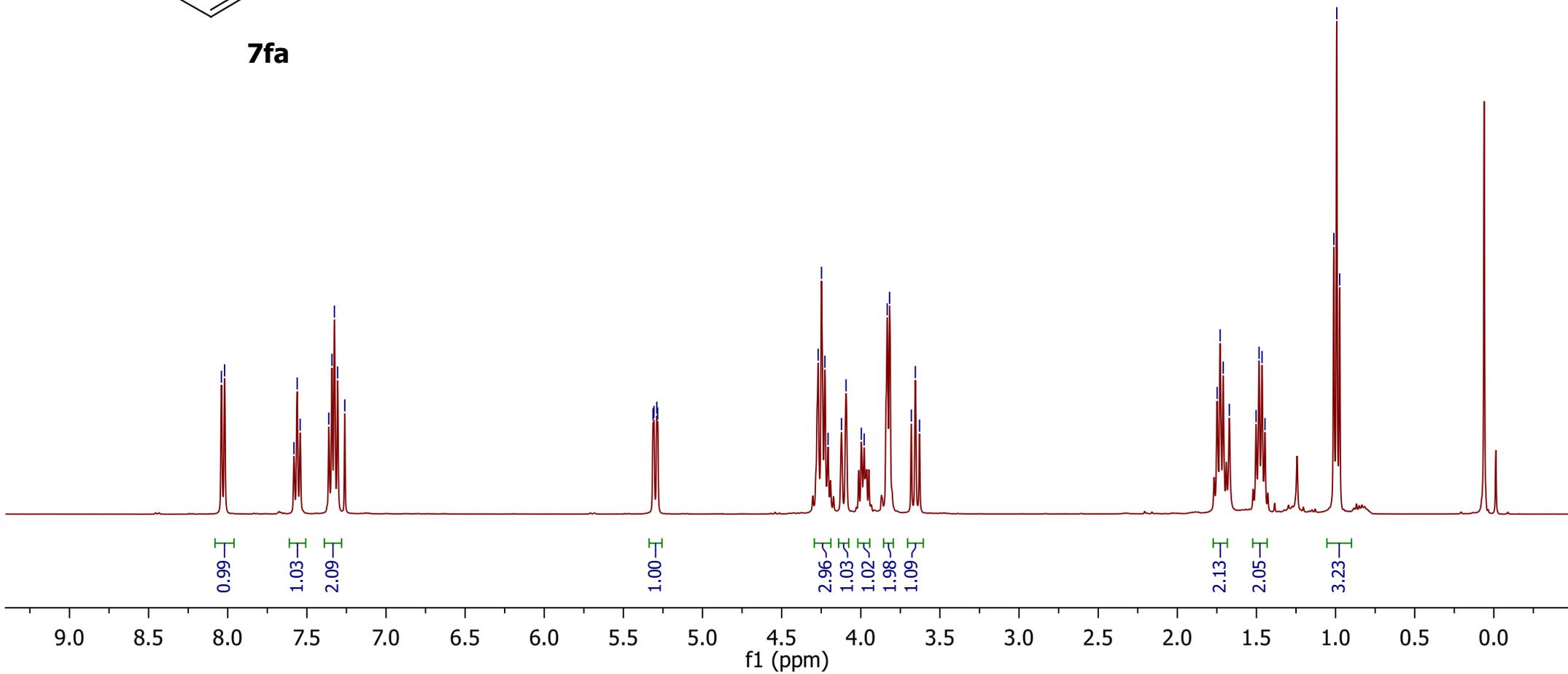
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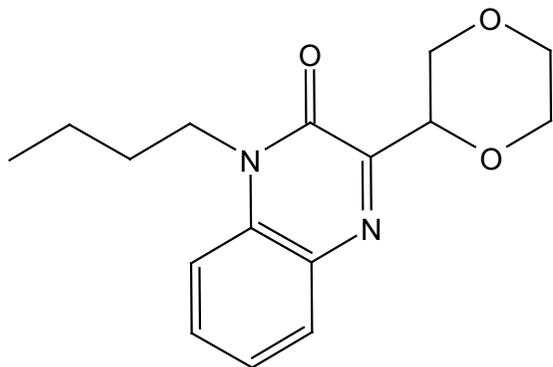
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7.58  
7.56  
7.54  
7.36  
7.34  
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7.31  
7.26

5.31  
5.31  
5.29  
5.28

4.27  
4.25  
4.23  
4.21  
4.12  
4.09  
4.00  
3.98  
3.83  
3.82  
3.68  
3.66  
3.63

1.75  
1.73  
1.71  
1.67  
1.50  
1.48  
1.46  
1.45  
1.01  
0.99  
0.97





**7fa**

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133.02  
132.44  
131.09  
130.86

123.78

113.76

74.73

69.60

67.66

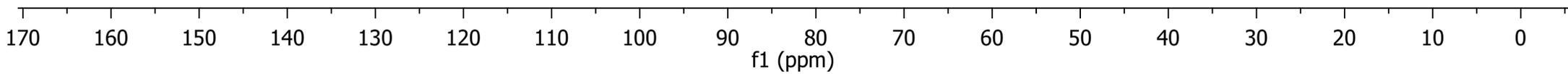
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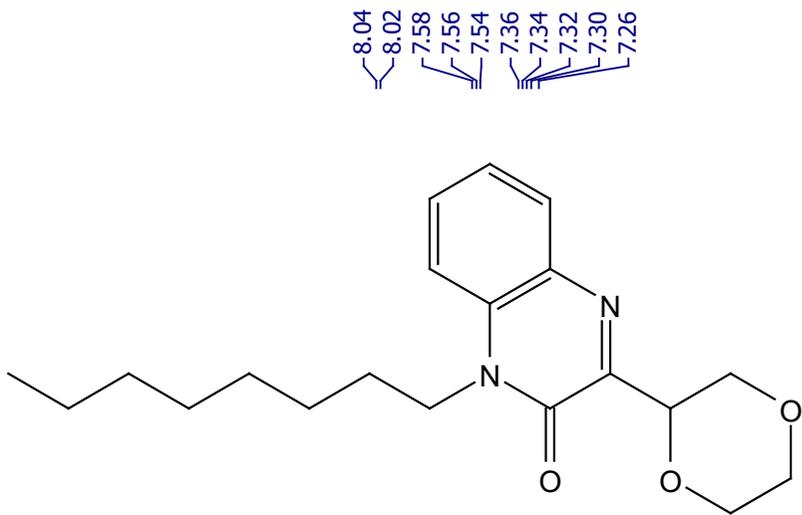
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29.40

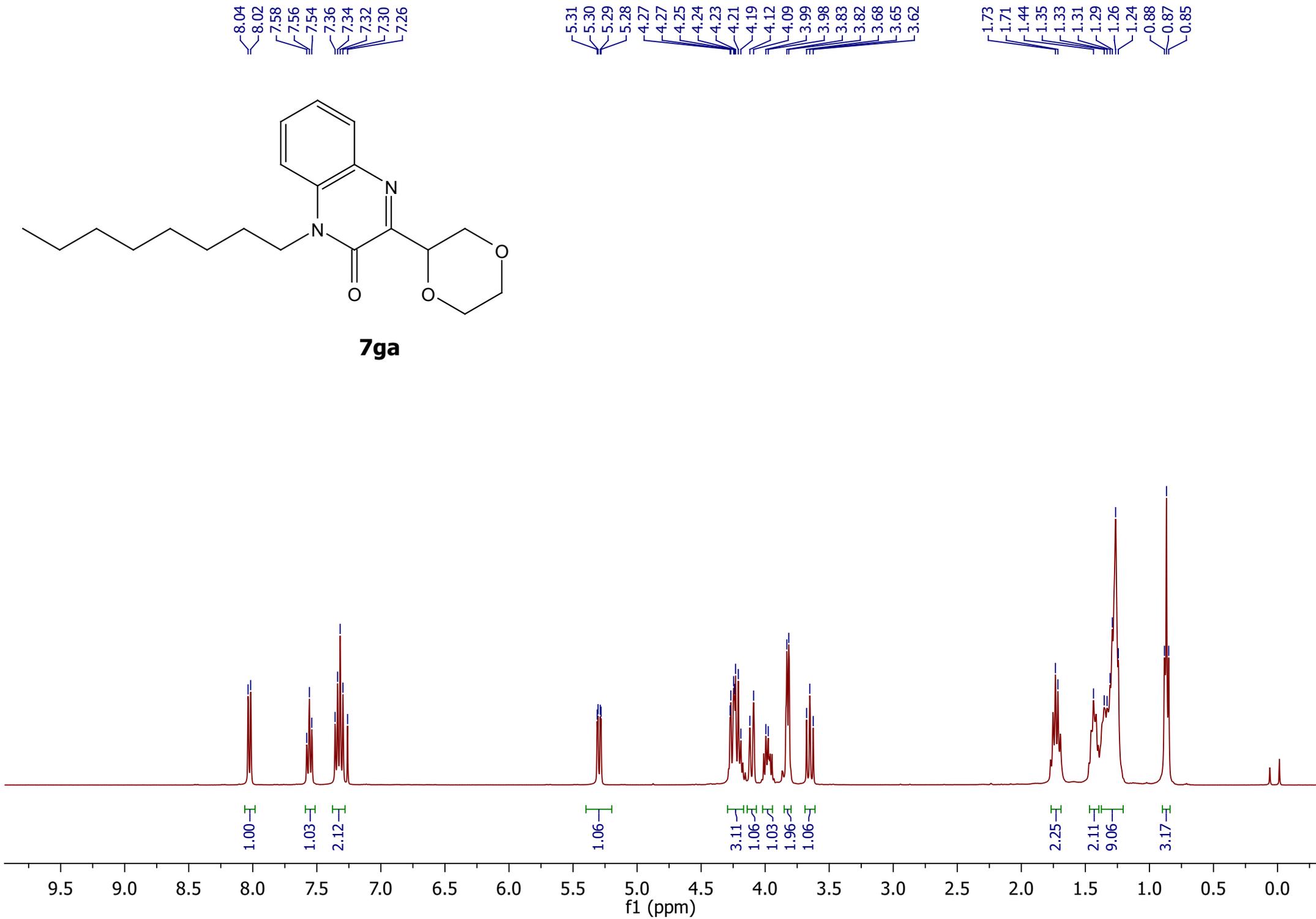
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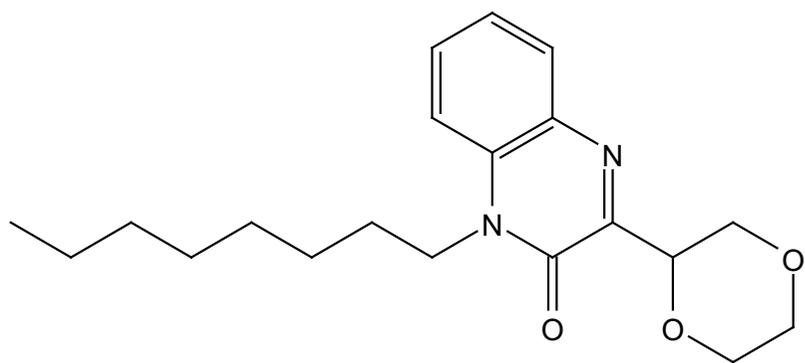
13.87





**7ga**





**7ga**

155.22  
153.52

133.01  
132.44  
131.07  
130.84

123.75

113.75

74.72

69.59

67.65

66.45

42.50

31.85

29.33

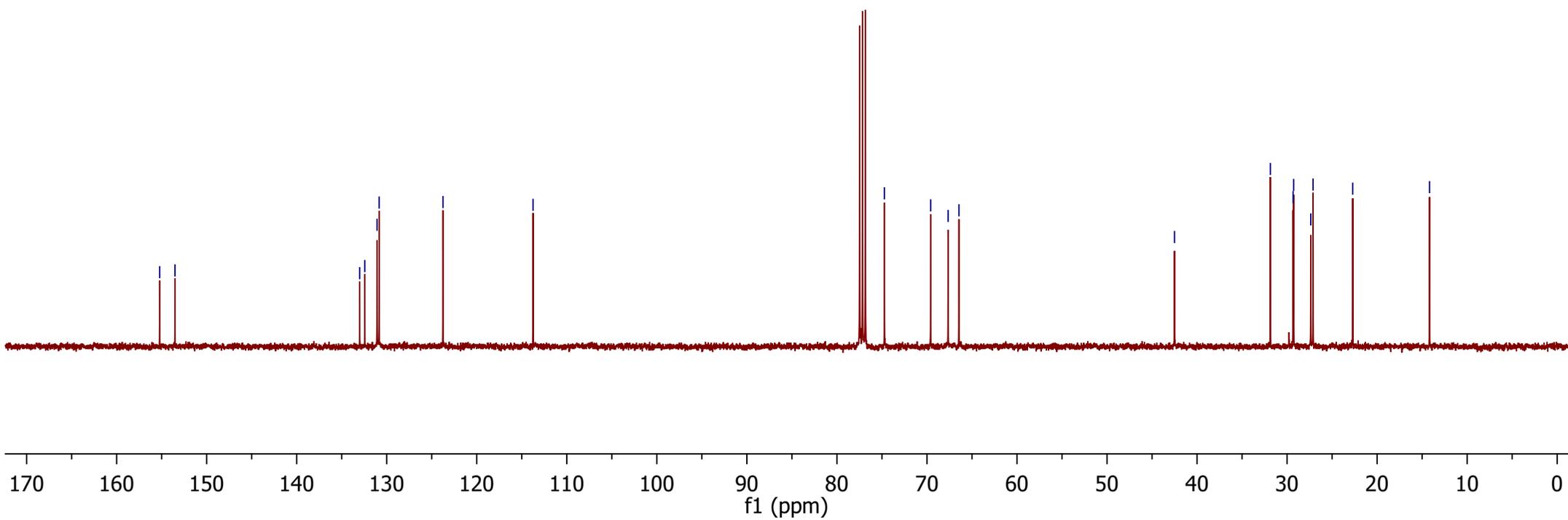
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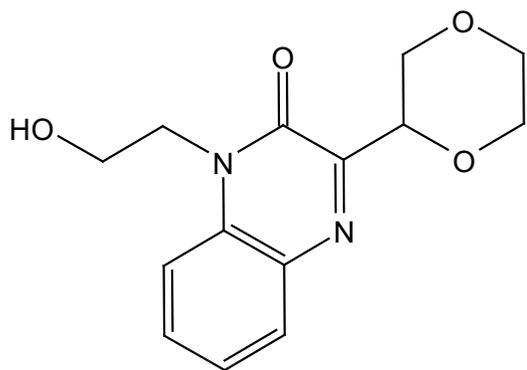
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27.11

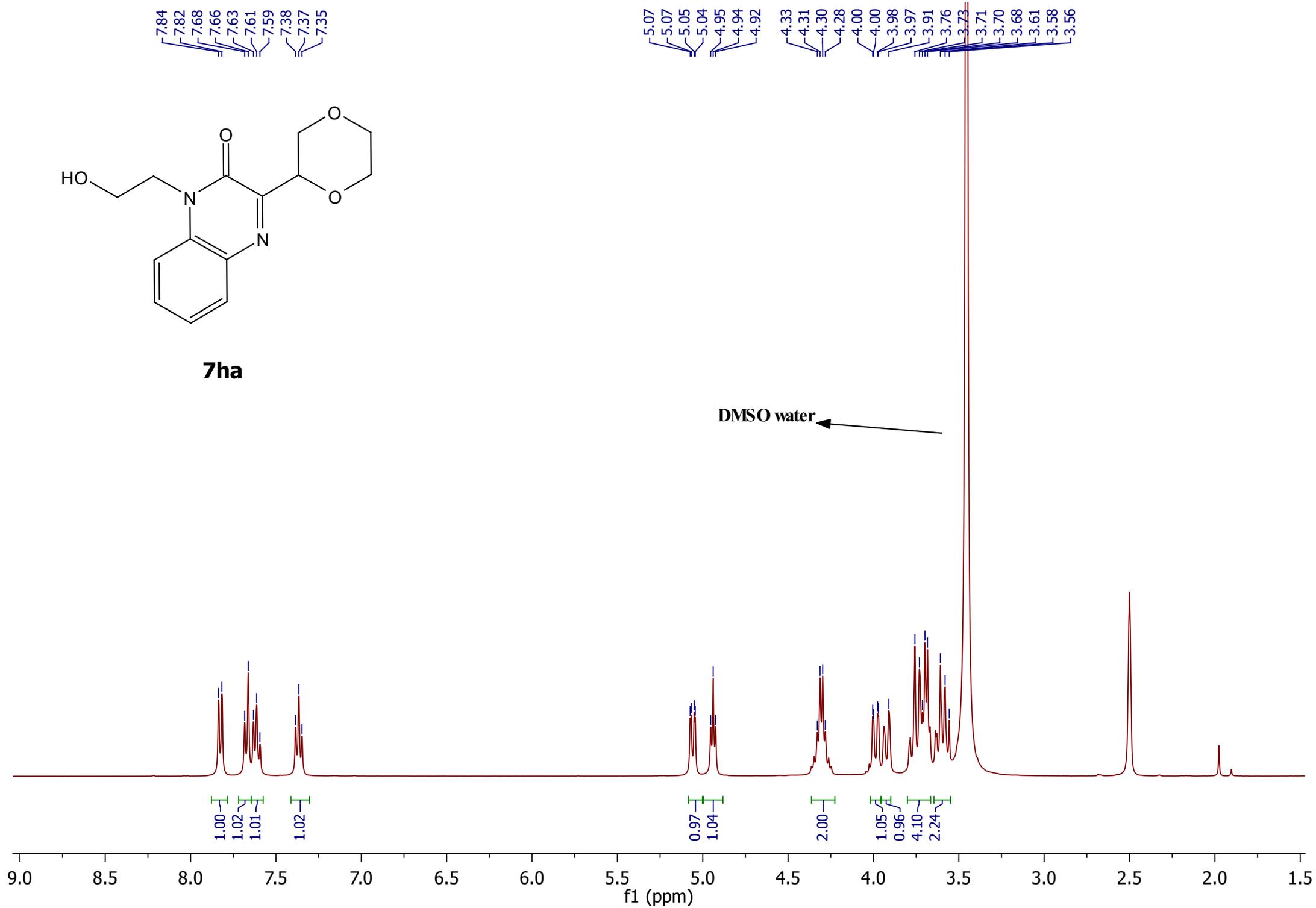
22.71

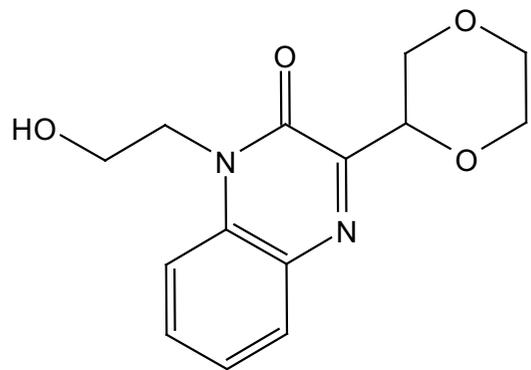
14.18





**7ha**





**7ha**

154.81  
153.38

133.13  
132.06  
130.78  
129.72

123.60

115.36

73.25

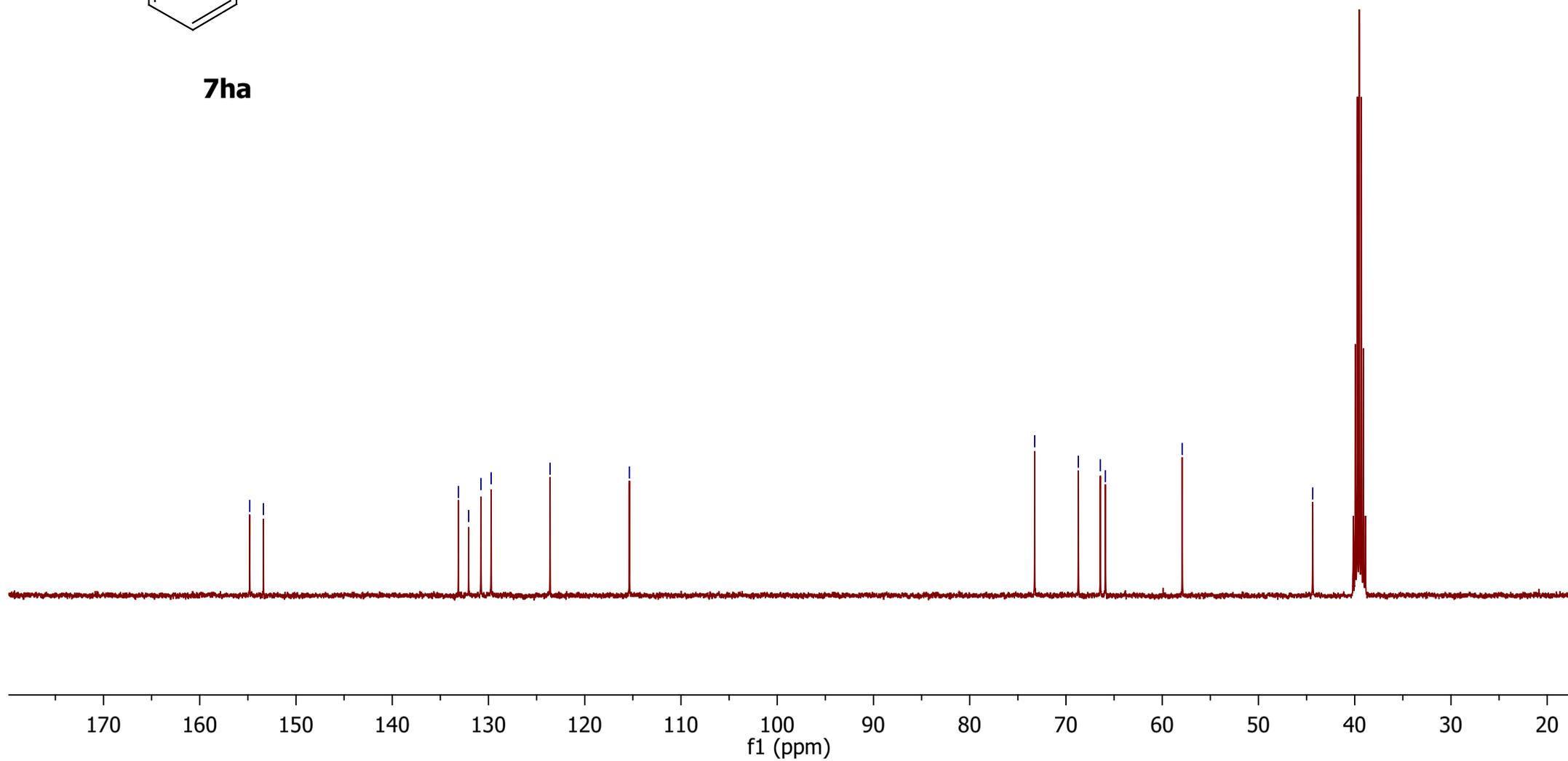
68.72

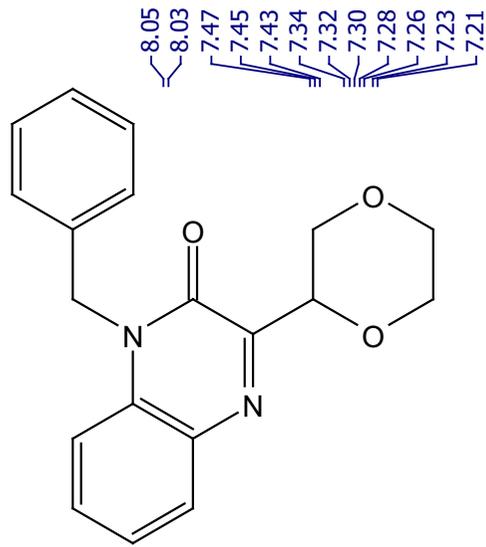
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65.91

57.92

44.36



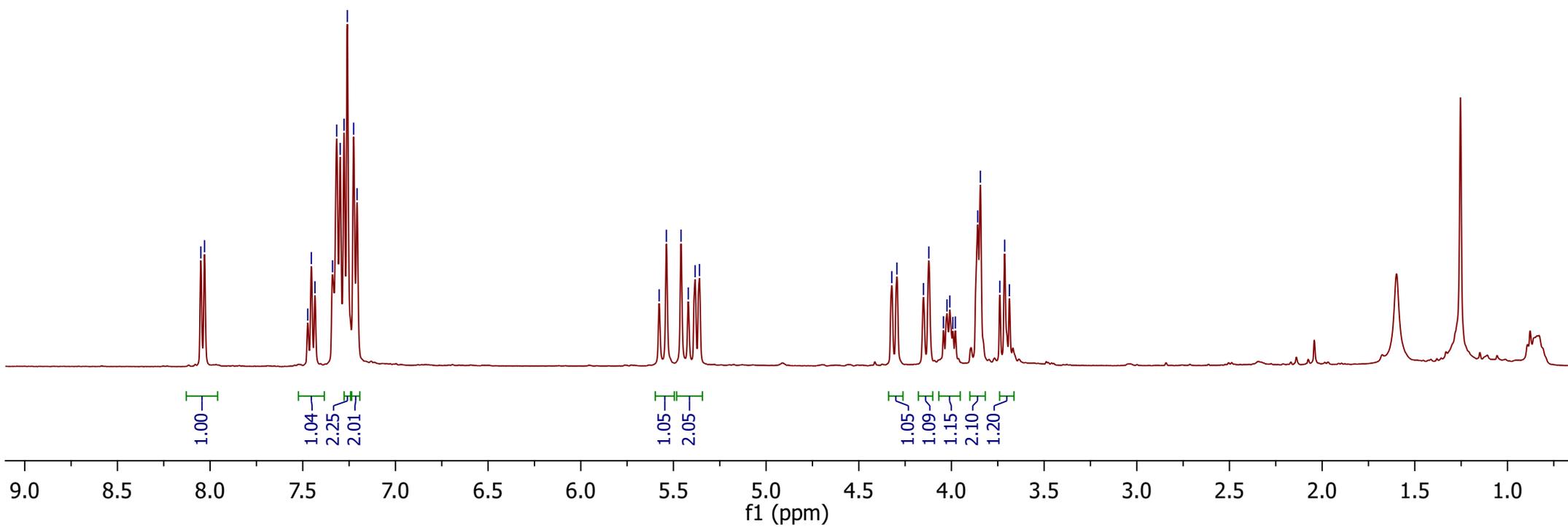


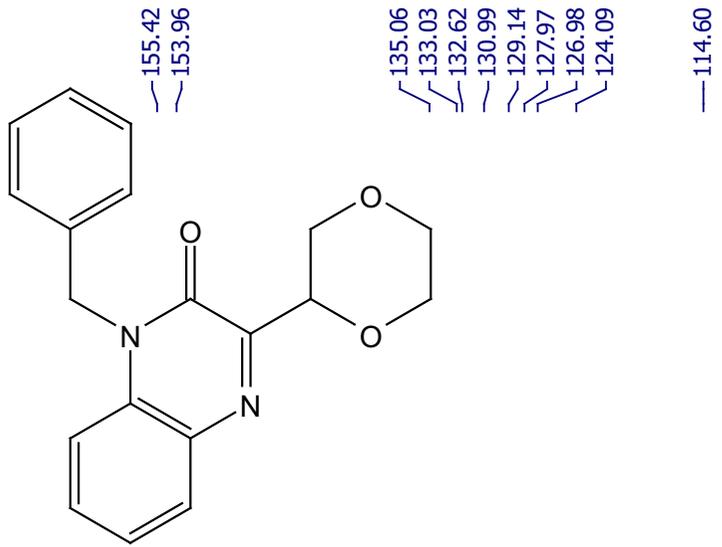
**7ia**

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8.03  
7.47  
7.45  
7.43  
7.34  
7.32  
7.30  
7.28  
7.26  
7.23  
7.21

5.58  
5.54  
5.46  
5.42  
5.38  
5.36

4.32  
4.29  
4.15  
4.12  
4.04  
4.02  
4.01  
3.99  
3.98  
3.86  
3.84  
3.74  
3.71  
3.69





**7ia**

155.42  
153.96

135.06  
133.03  
132.62  
130.99  
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127.97  
126.98  
124.09

114.60

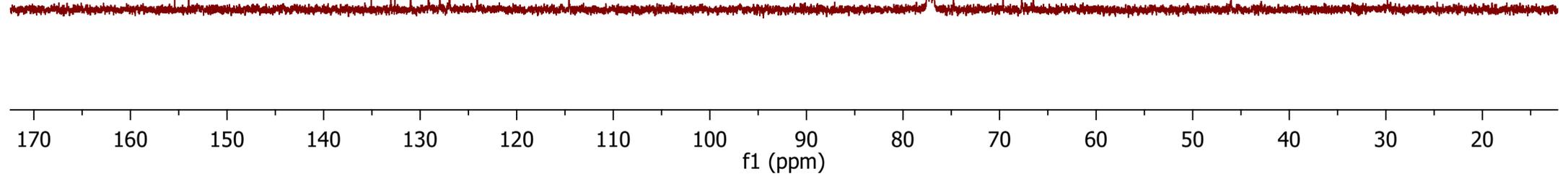
74.77

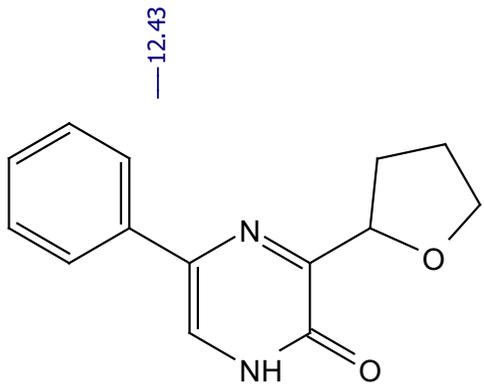
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67.71

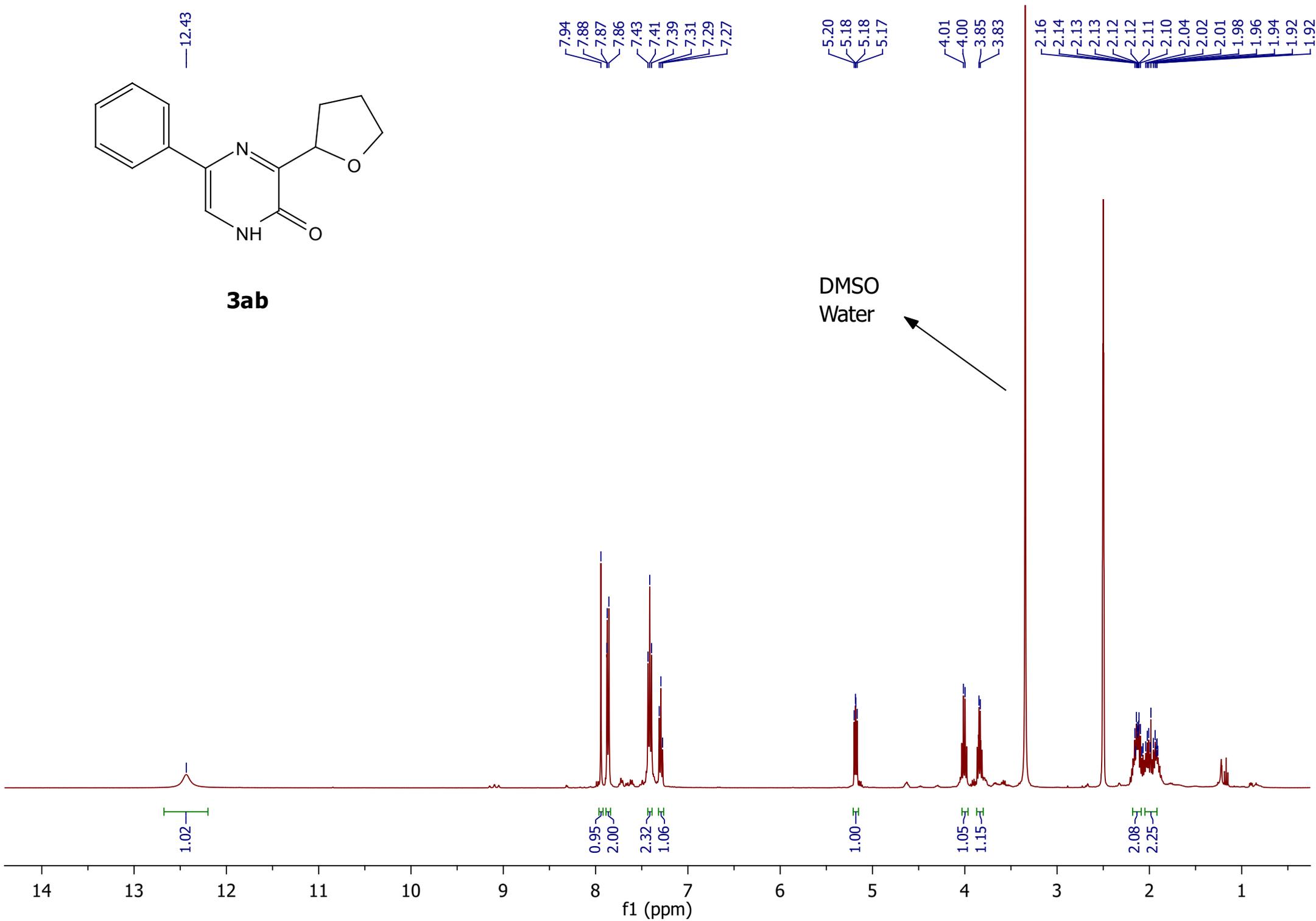
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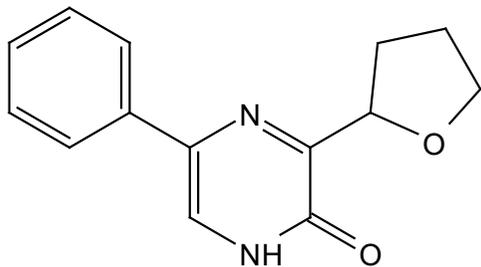
46.03



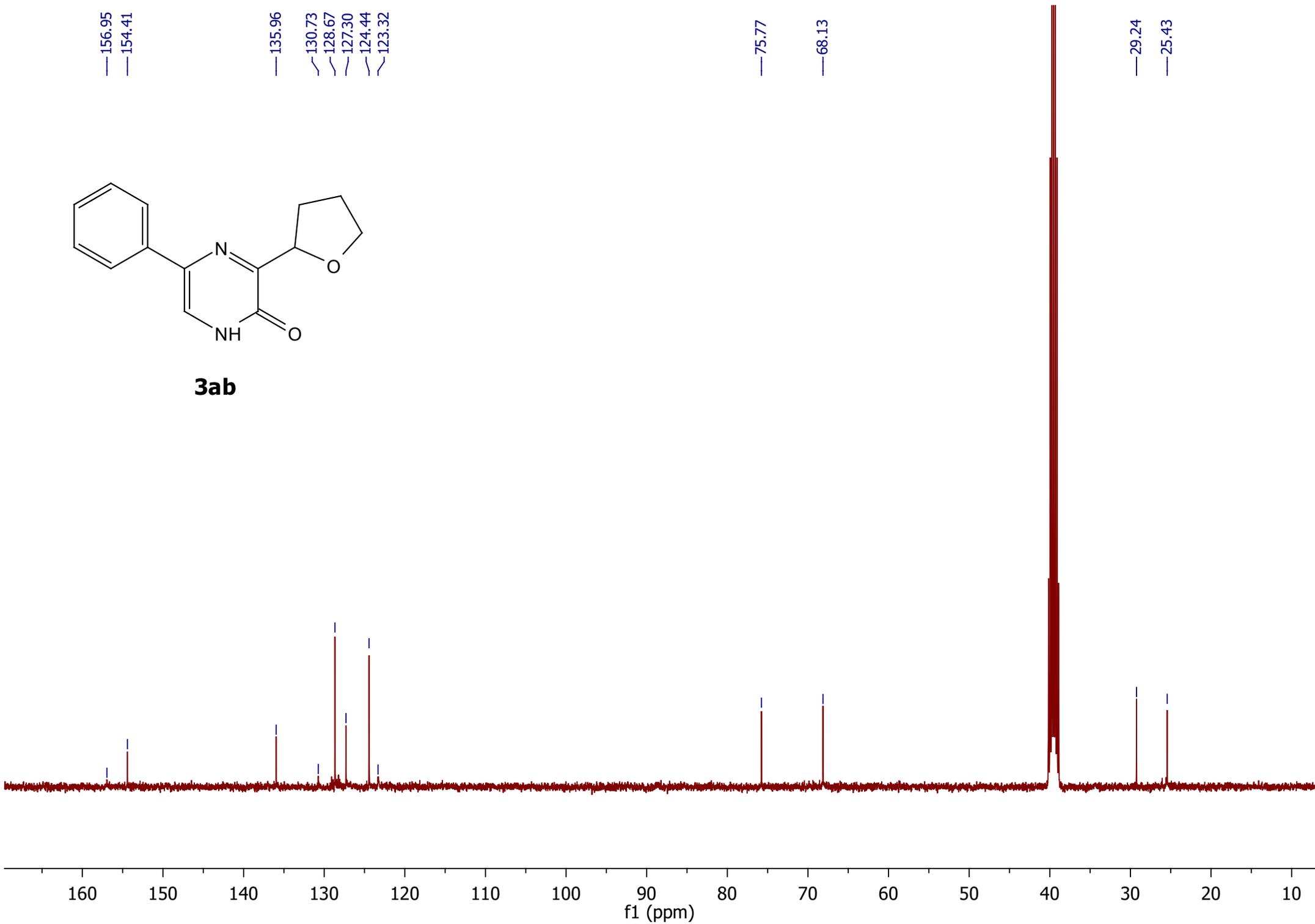


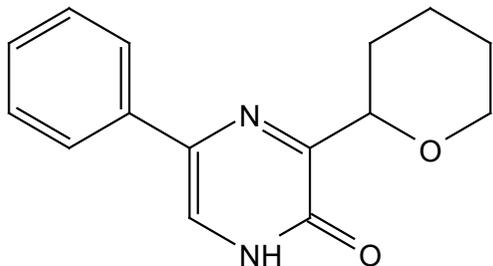
**3ab**





**3ab**





**3ac**

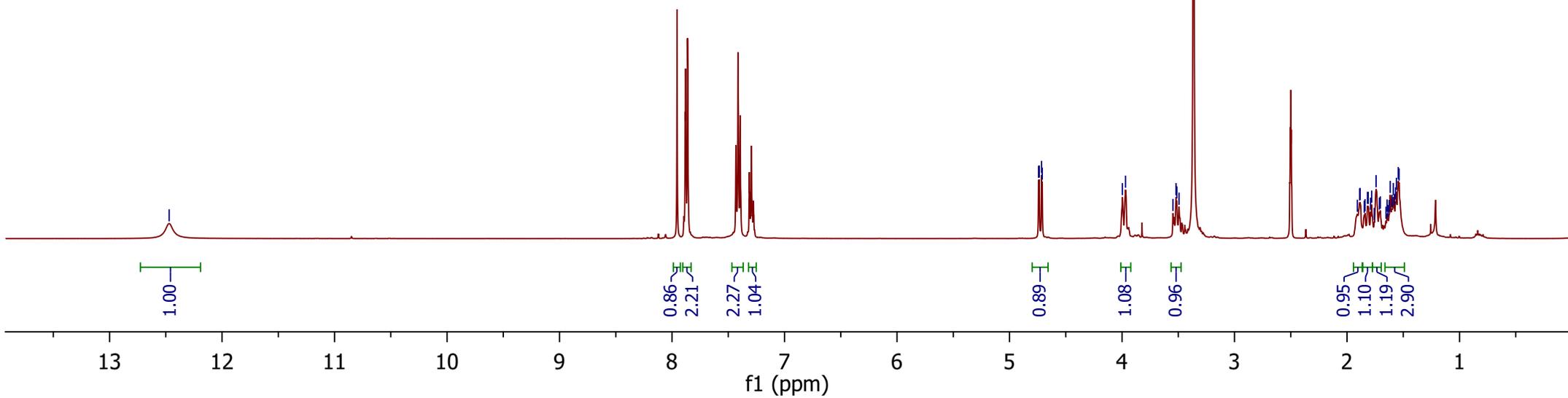
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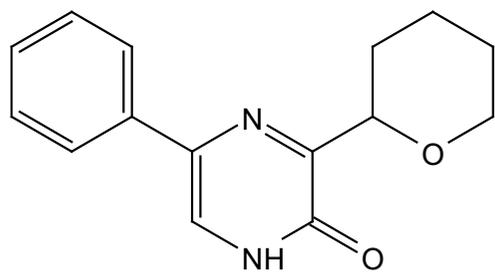
4.74  
4.74  
4.72  
4.71

4.00  
3.97  
3.55  
3.52  
3.51  
3.49  
3.36

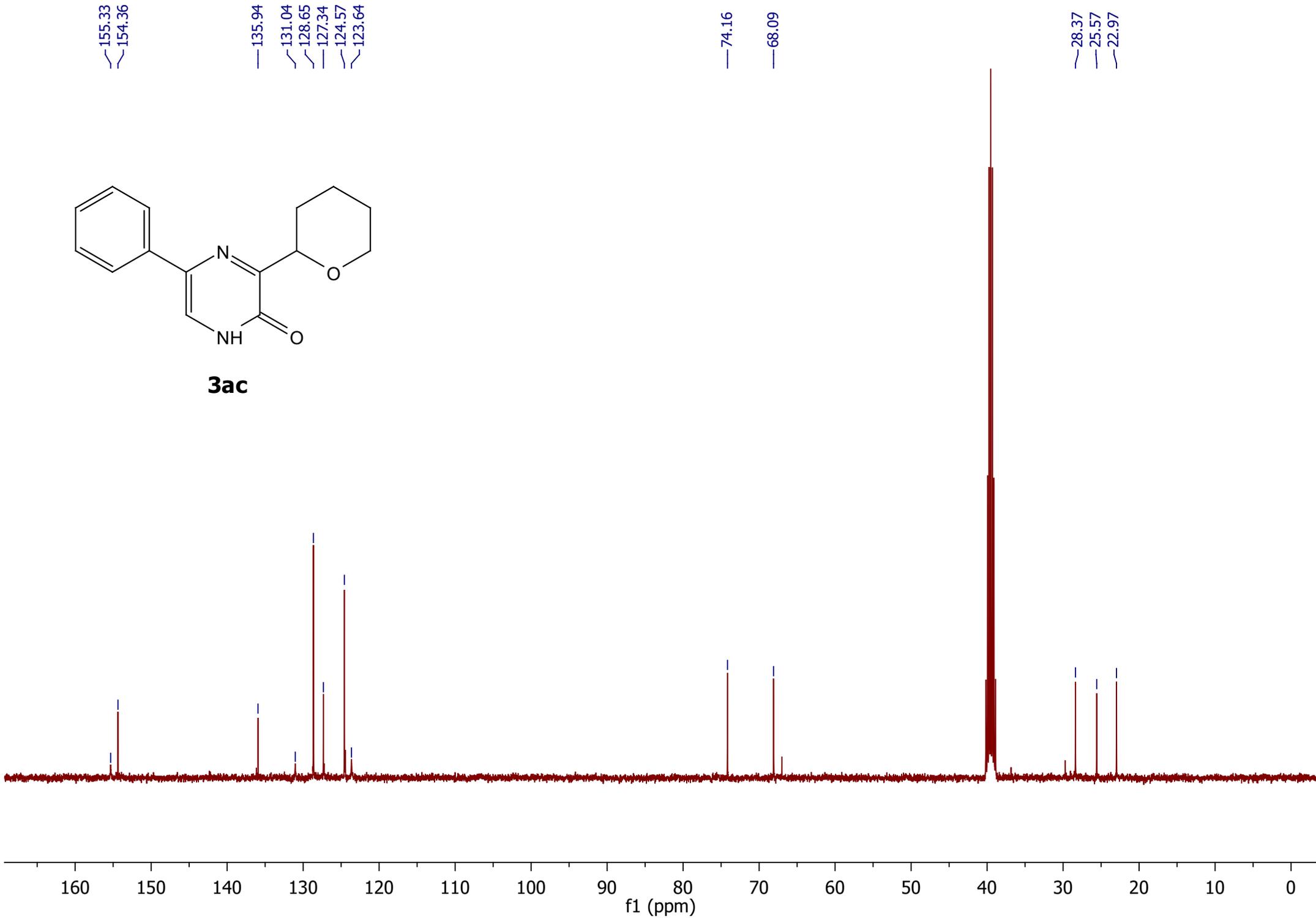
1.89  
1.88  
1.82  
1.81  
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1.62  
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1.59  
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1.57  
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1.54  
1.54

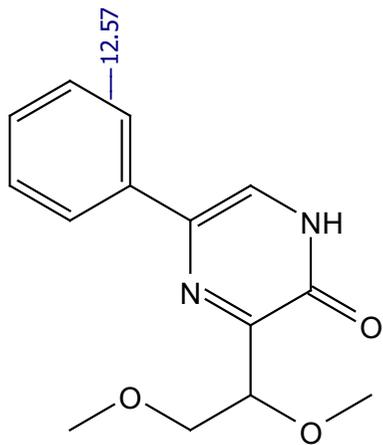
DMSO water



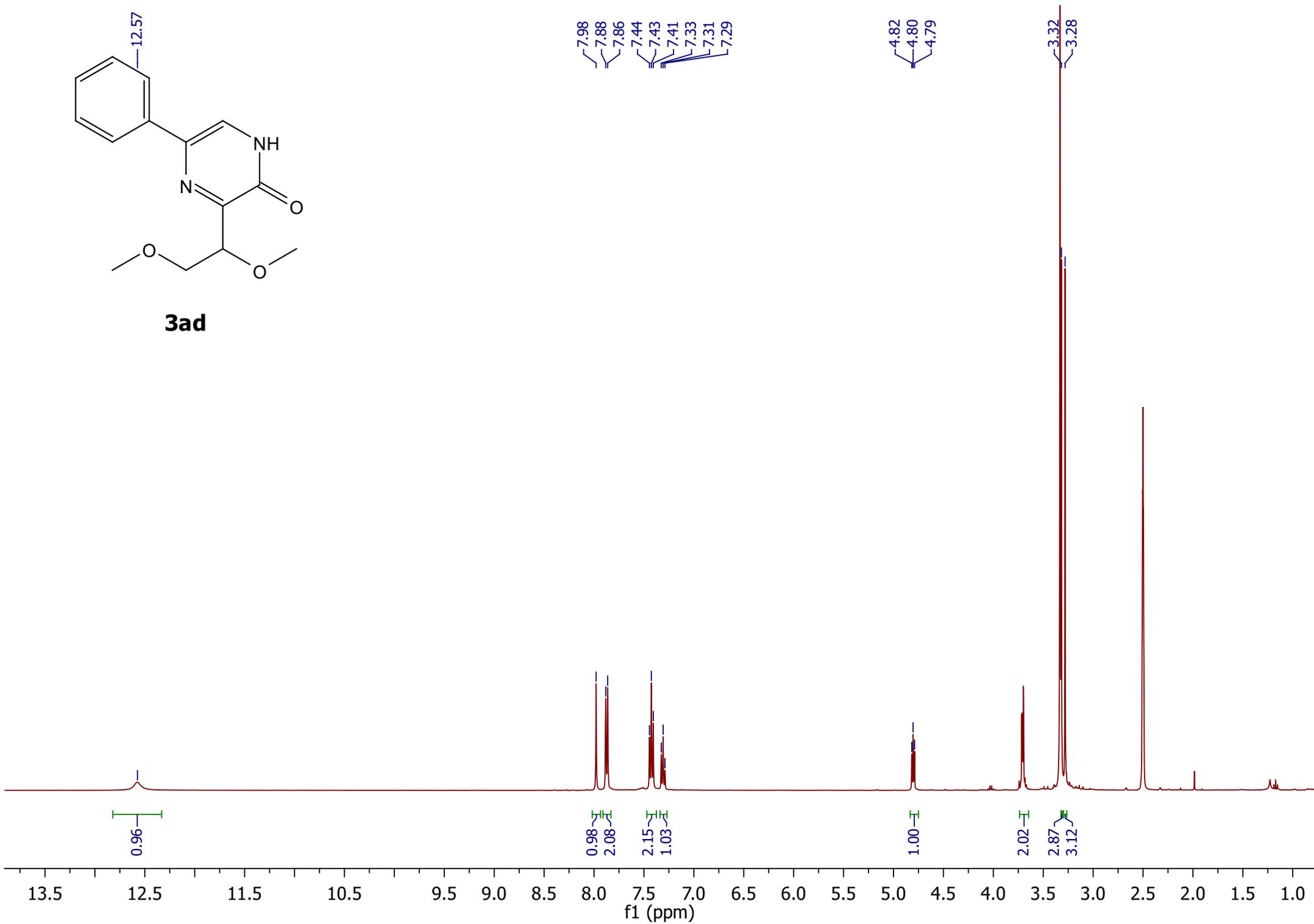


**3ac**





**3ad**

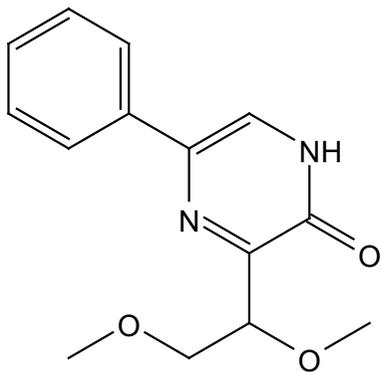


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153.12

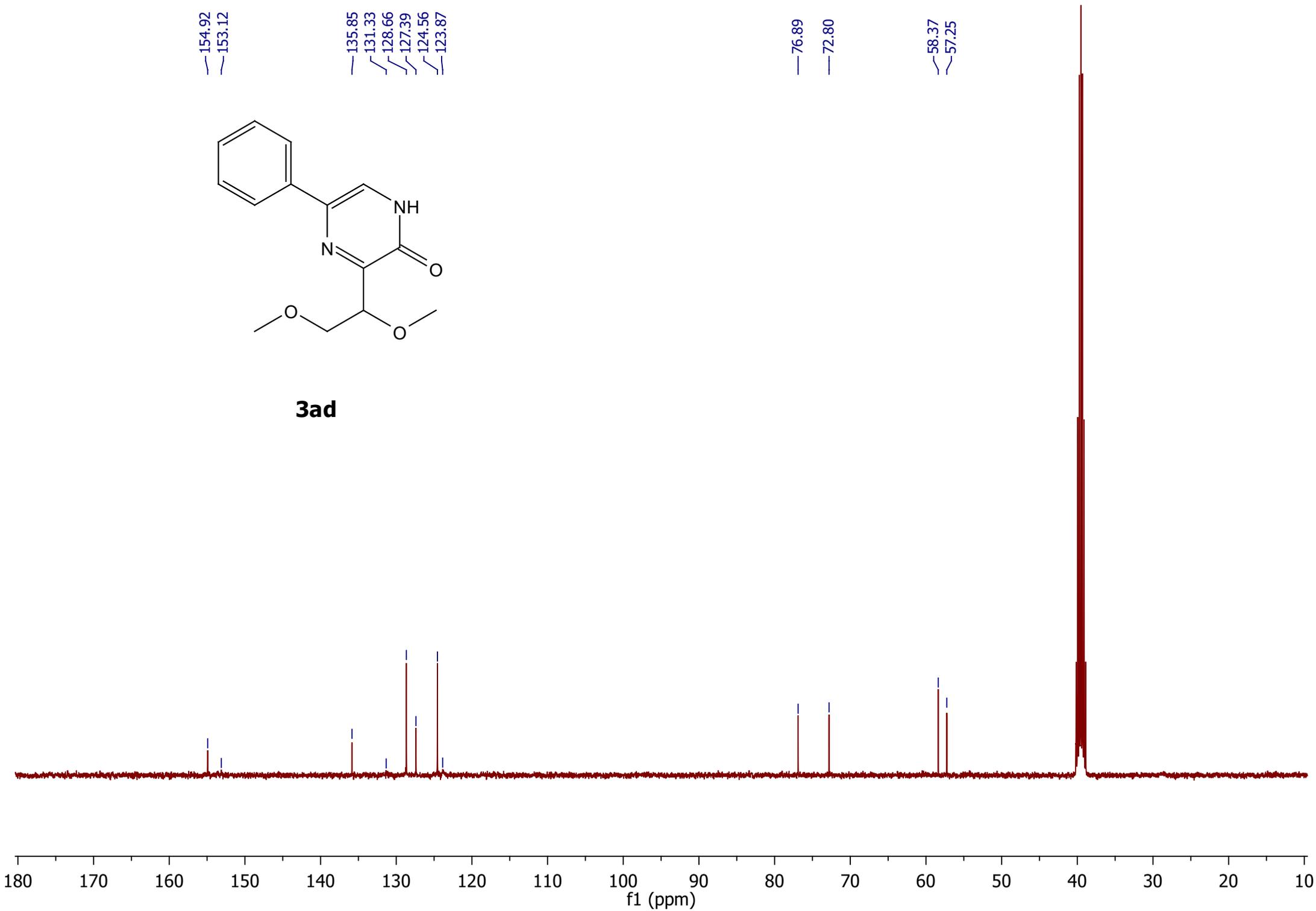
135.85  
131.33  
128.66  
127.39  
124.56  
123.87

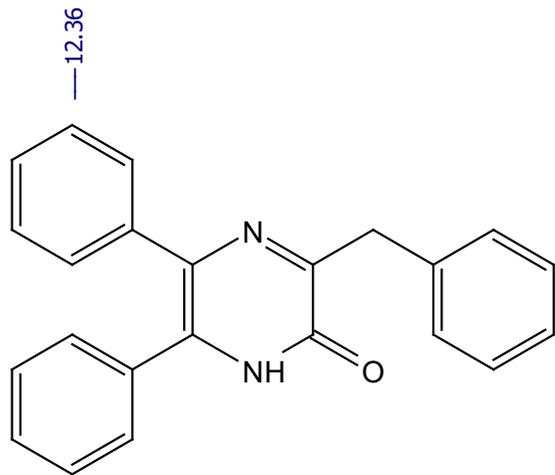
76.89  
72.80

58.37  
57.25



**3ad**



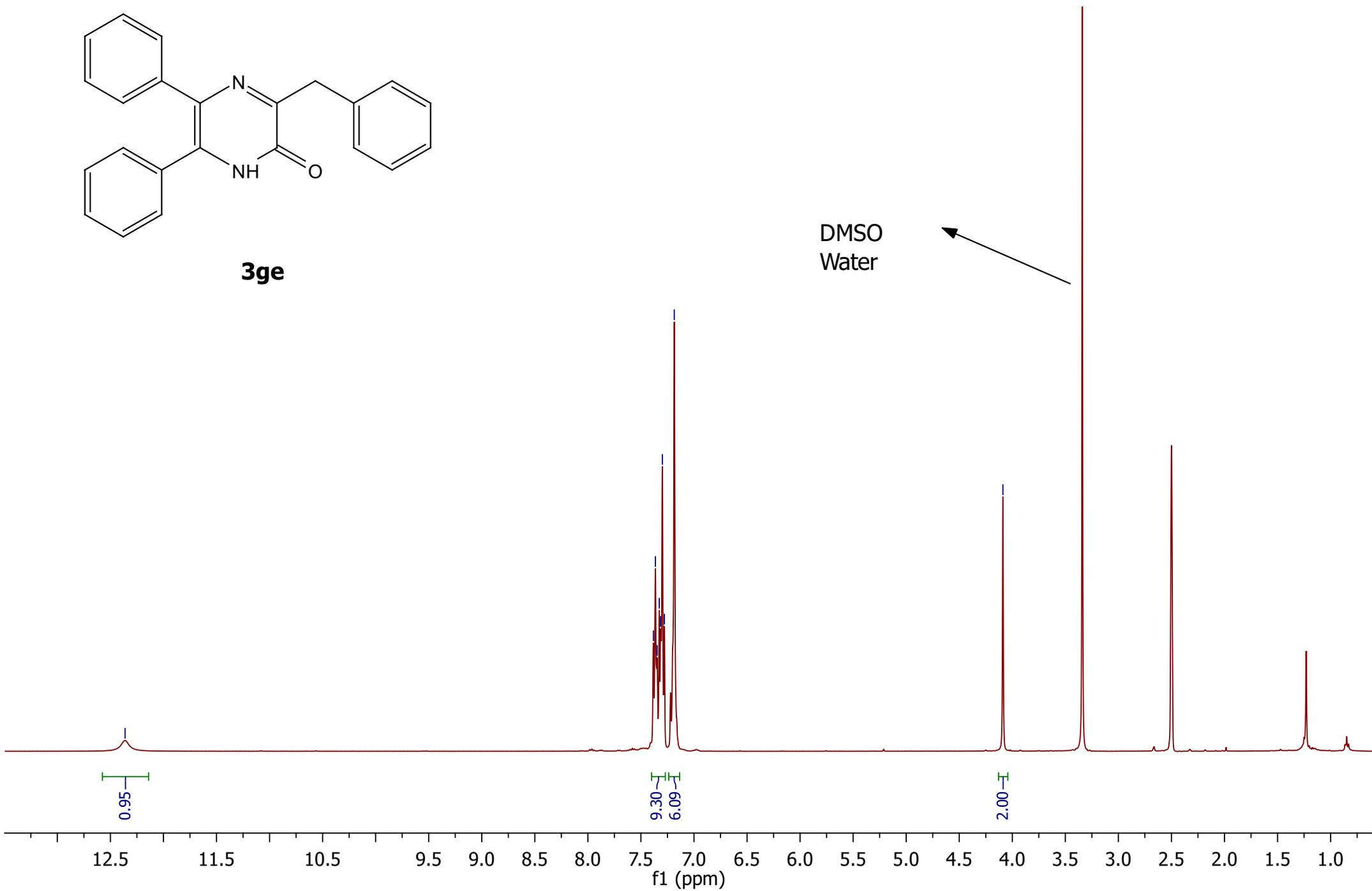


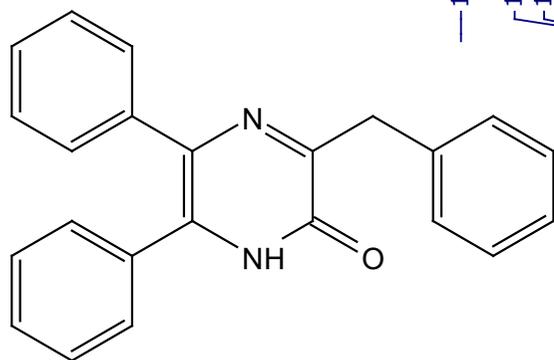
**3ge**

7.38  
7.36  
7.35  
7.33  
7.31  
7.30  
7.28  
7.19

4.09

DMSO  
Water

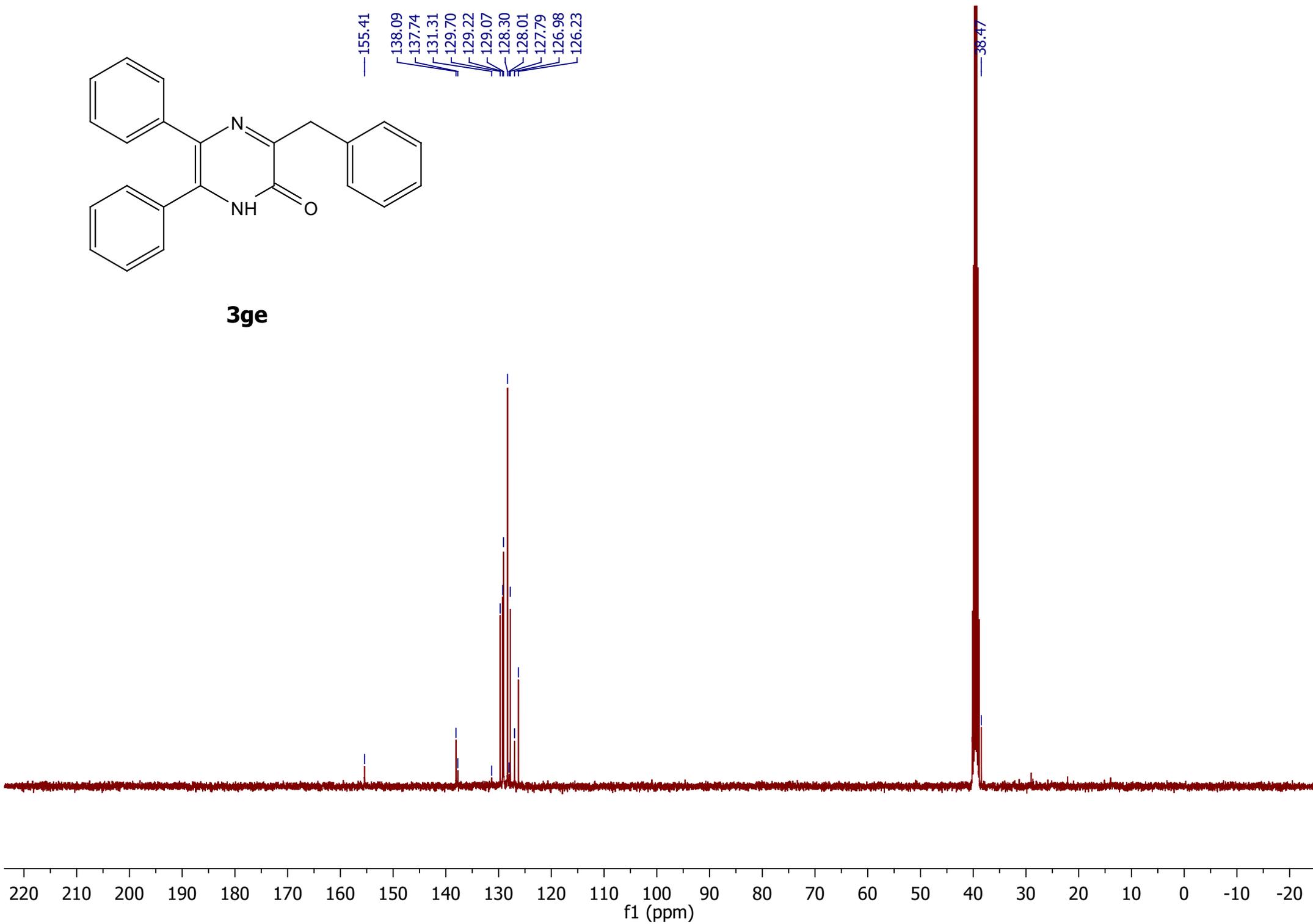


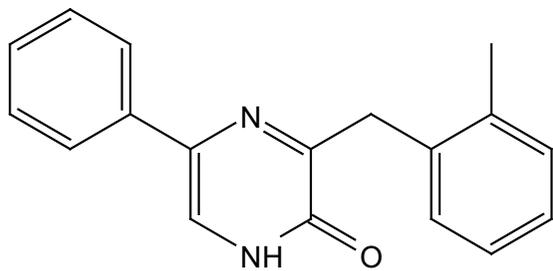


**3ge**

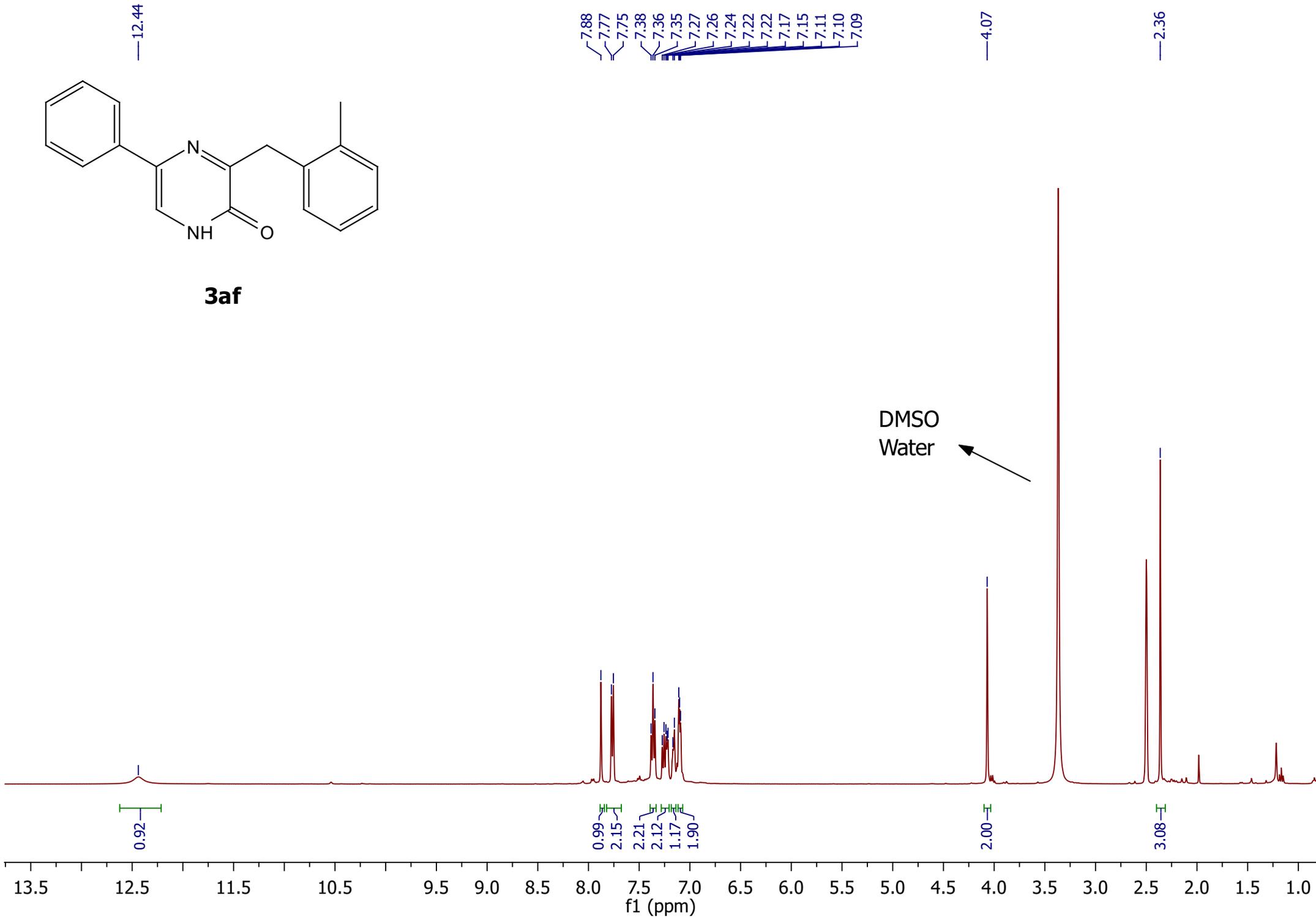
— 155.41  
138.09  
137.74  
131.31  
129.70  
129.22  
129.07  
128.30  
128.01  
127.79  
126.98  
126.23

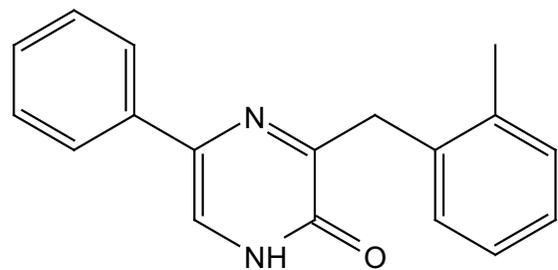
— 38.47





**3af**





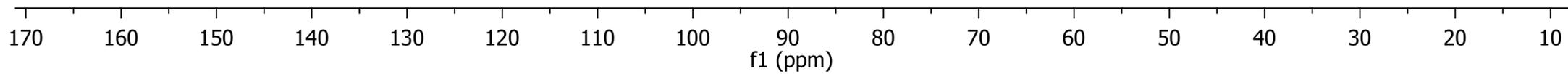
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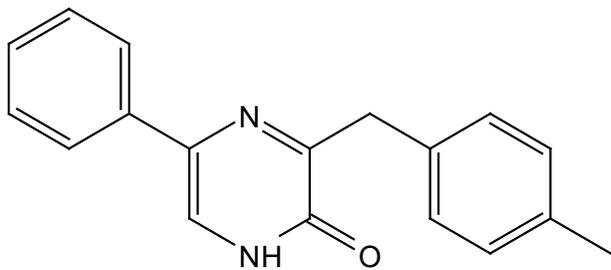
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154.98

136.62  
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130.78  
129.90  
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128.63  
127.23  
126.35  
125.64  
124.33  
122.20

36.13

19.55





**3ag**

12.40

7.87  
7.85  
7.84  
7.83  
7.41  
7.39  
7.37  
7.30  
7.28  
7.23  
7.21  
7.09  
7.07

4.01

2.24

DMSO  
Water

1.01

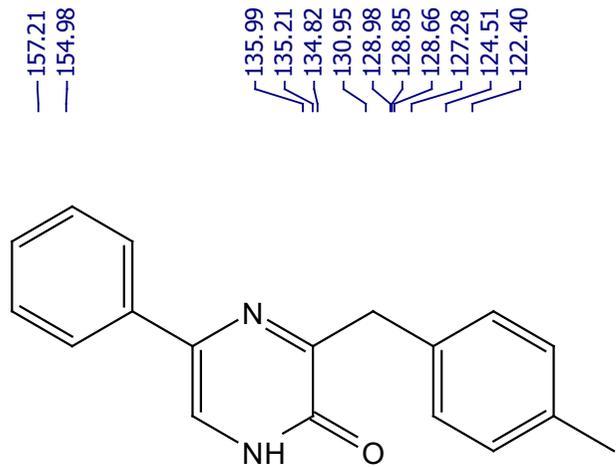
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1.03  
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1.97

1.94

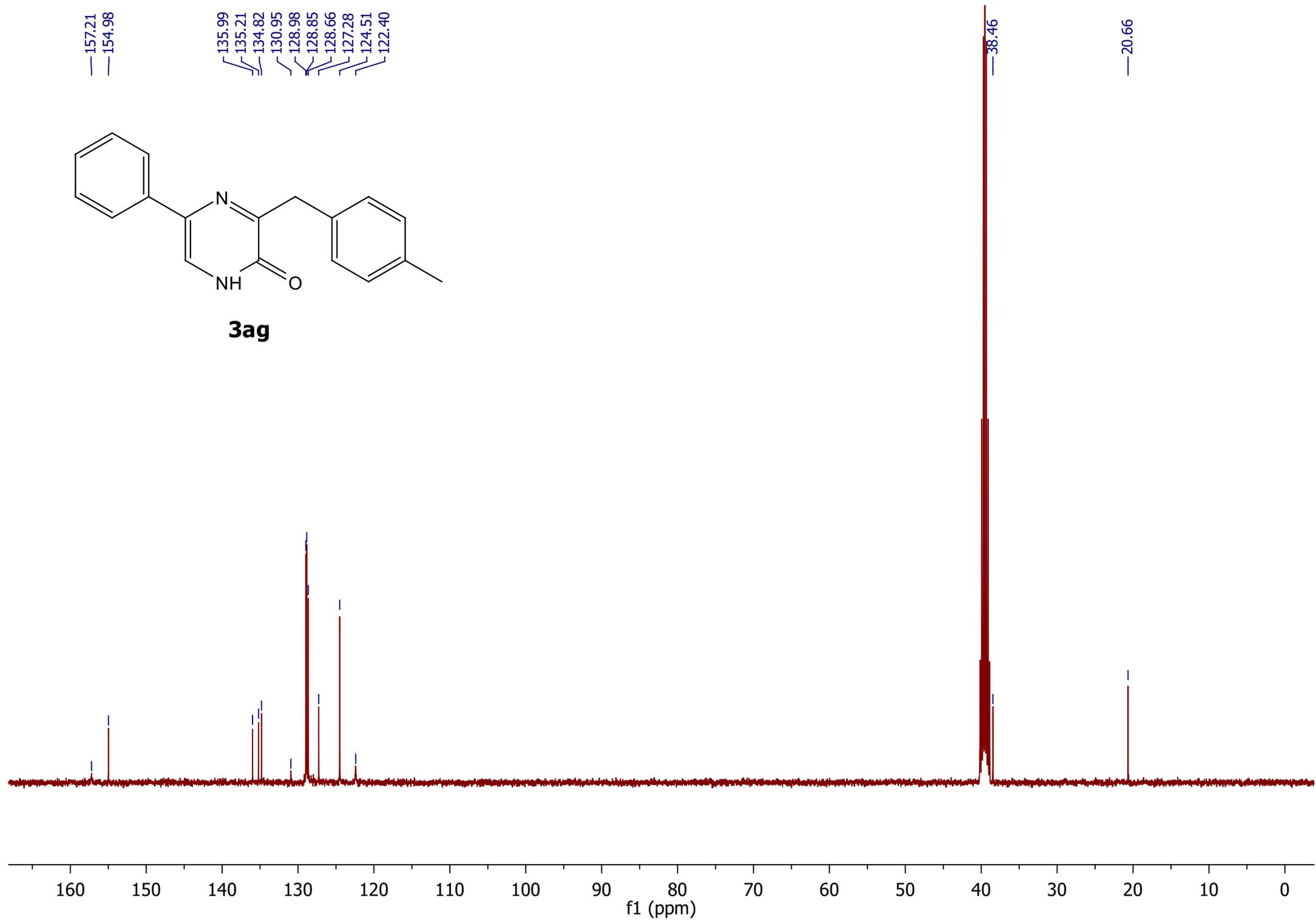
3.00

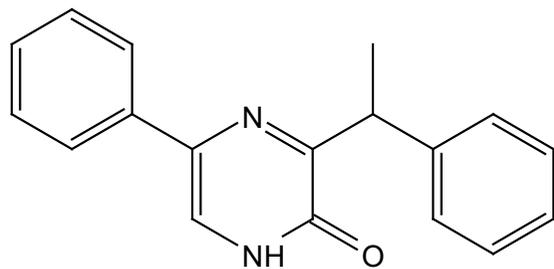
14 13 12 11 10 9 8 7 6 5 4 3 2 1

f1 (ppm)

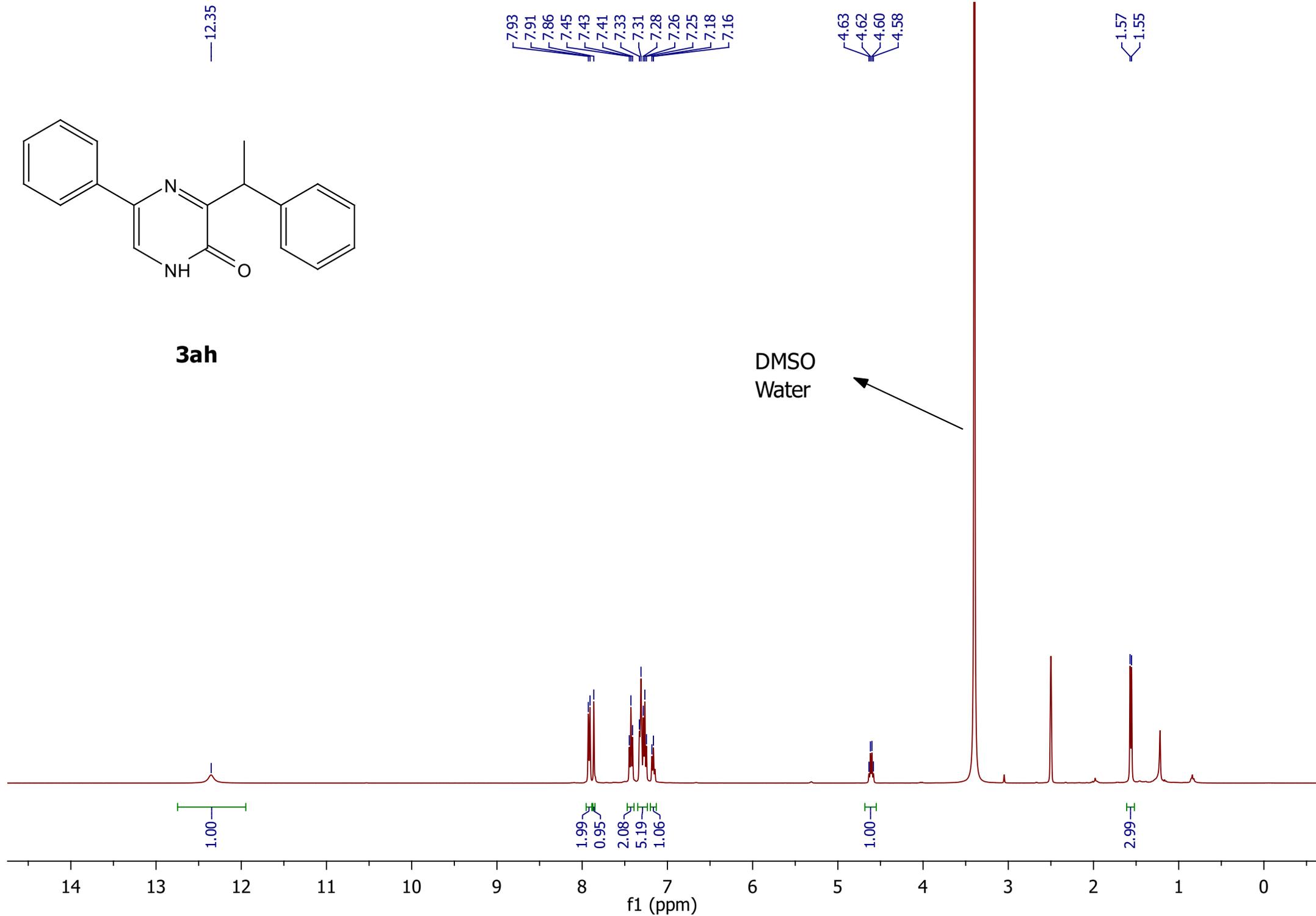


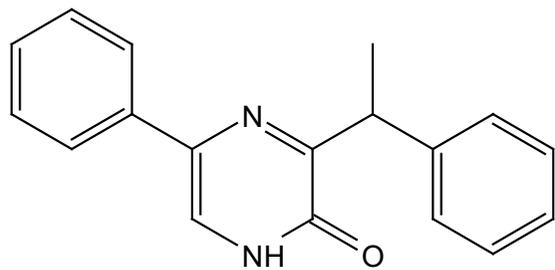
**3ag**





**3ah**



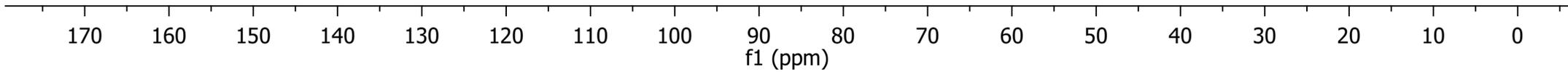


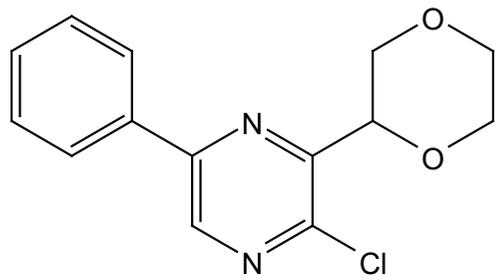
**3ah**

— 159.72  
— 154.53  
— 143.62  
— 136.21  
— 130.53  
— 128.75  
— 128.30  
— 127.74  
— 127.31  
— 126.27  
— 124.50  
— 121.98

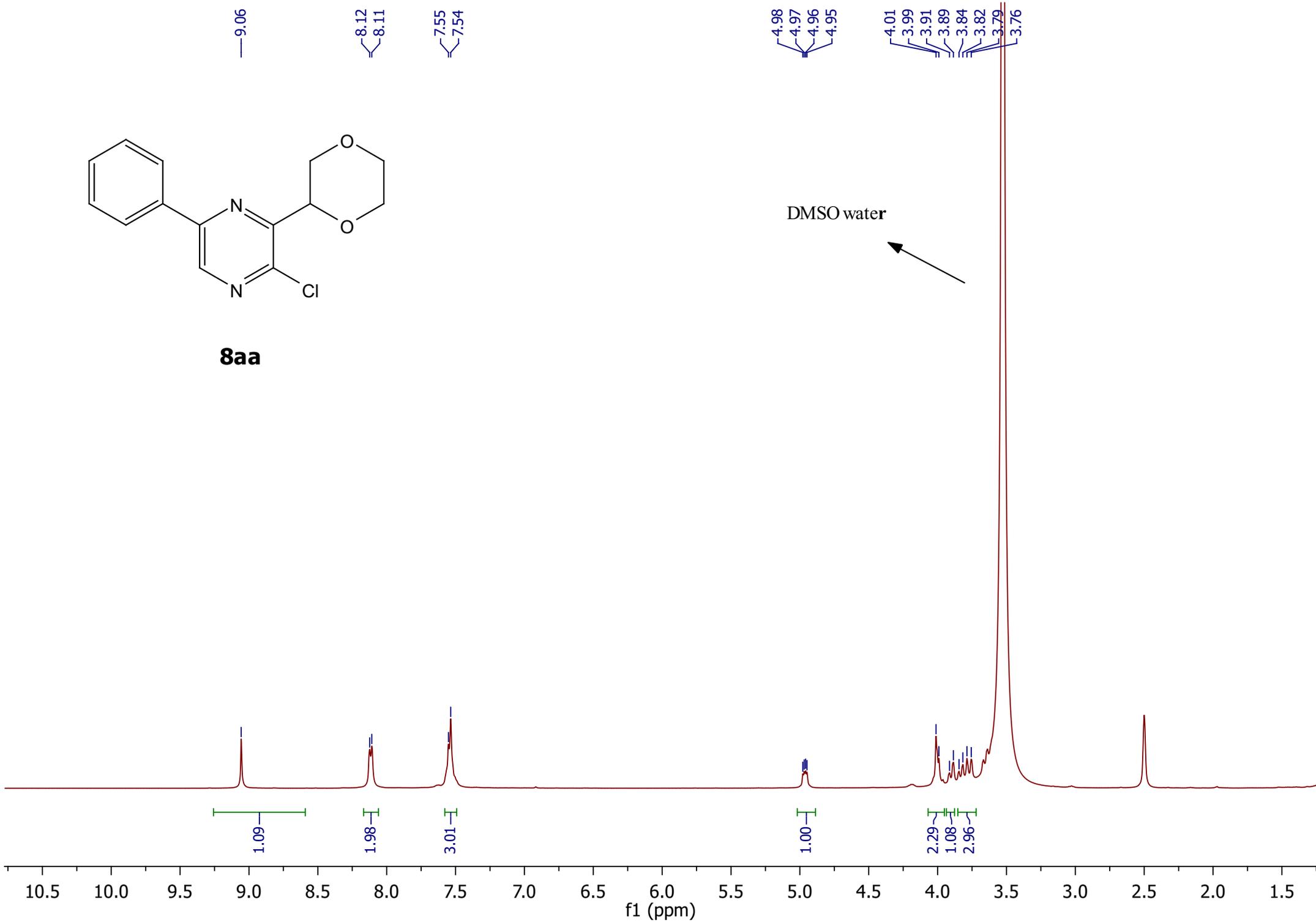
— 40.12

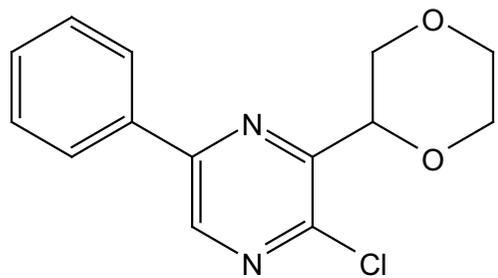
— 19.87





**8aa**

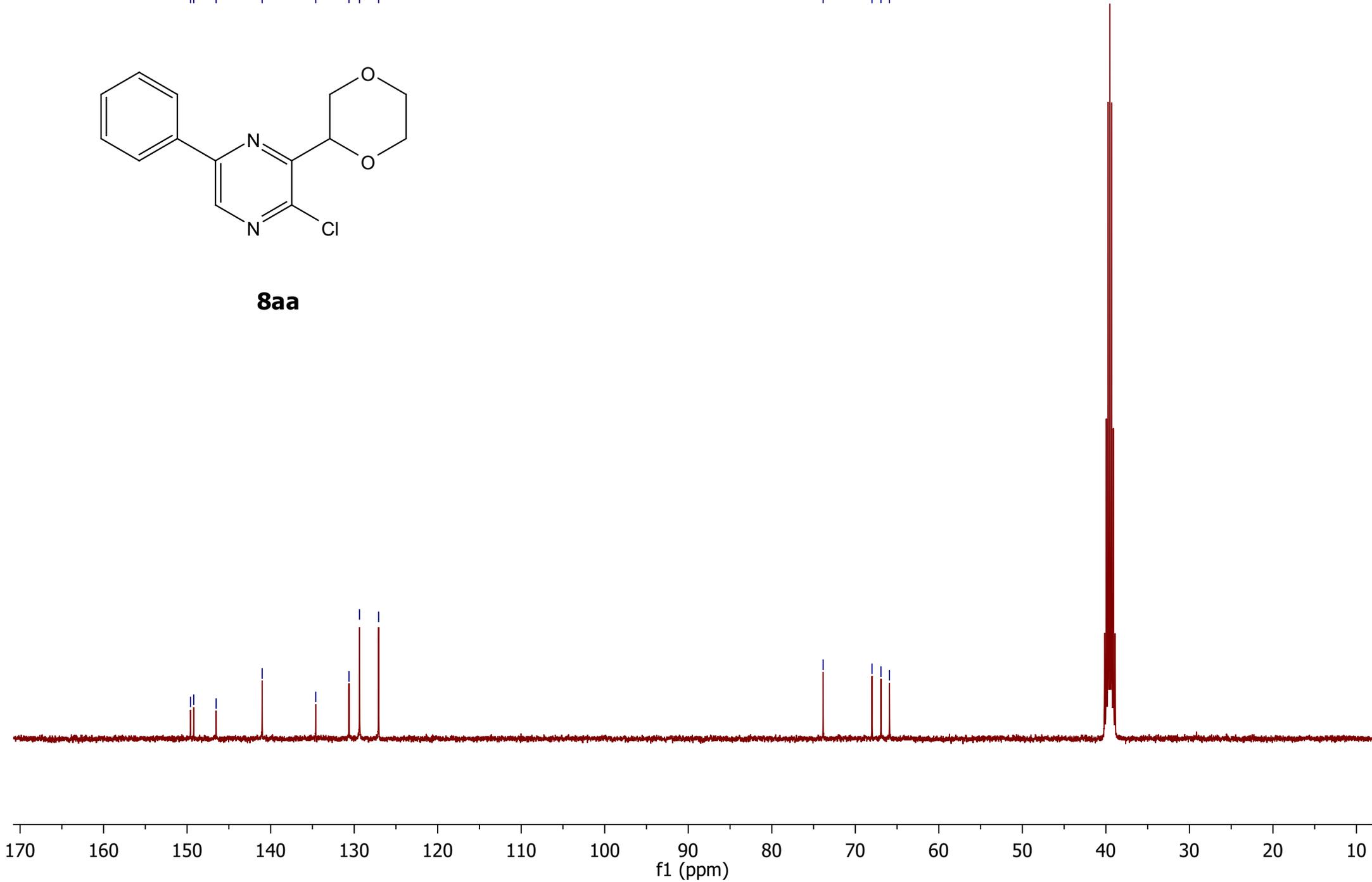


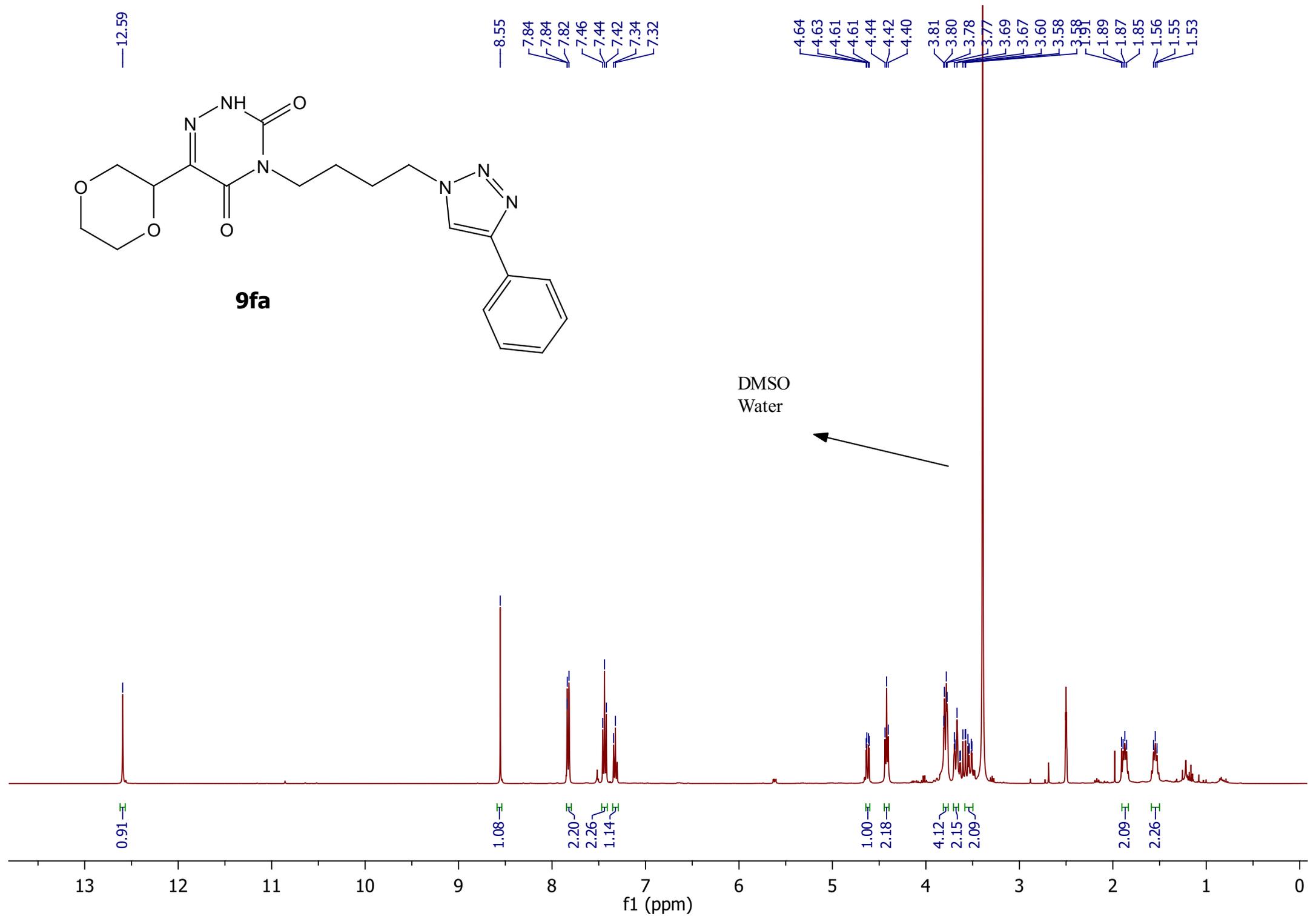
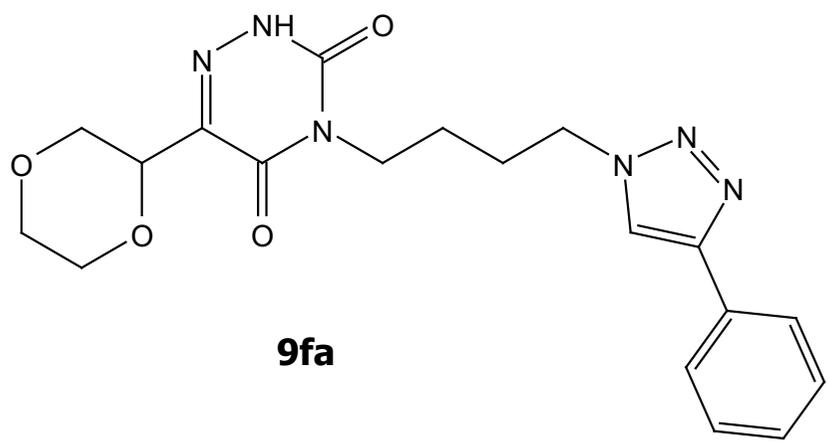


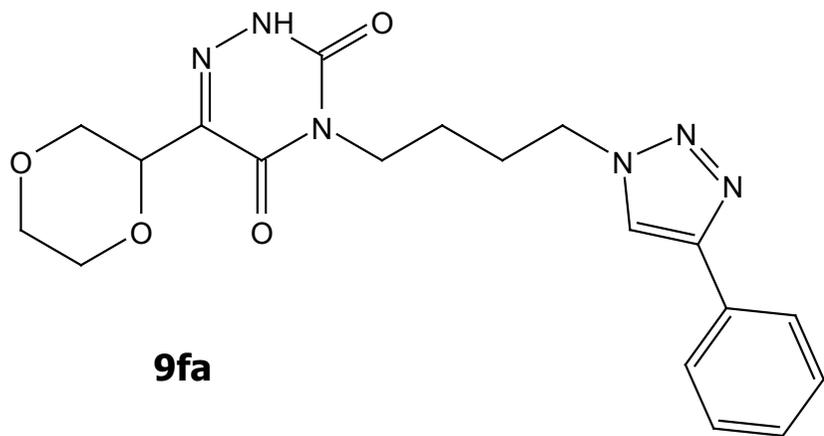
**8aa**

149.59  
149.20  
146.52  
141.02  
134.60  
130.62  
129.36  
127.07

73.85  
68.00  
66.93  
65.91







—155.39  
—149.14  
—146.33  
—140.25  
—130.87  
—128.95  
—127.86  
—125.16  
—121.42

—71.04  
—67.86  
—66.47  
—65.76

—49.13

—38.83

—27.11  
—23.79

