

**Synthesis of diversely substituted pyridin-2(1H)-ones and *in vivo* evaluation of their anti-allodynic effect on cutaneous inflammatory mechanical allodynia**

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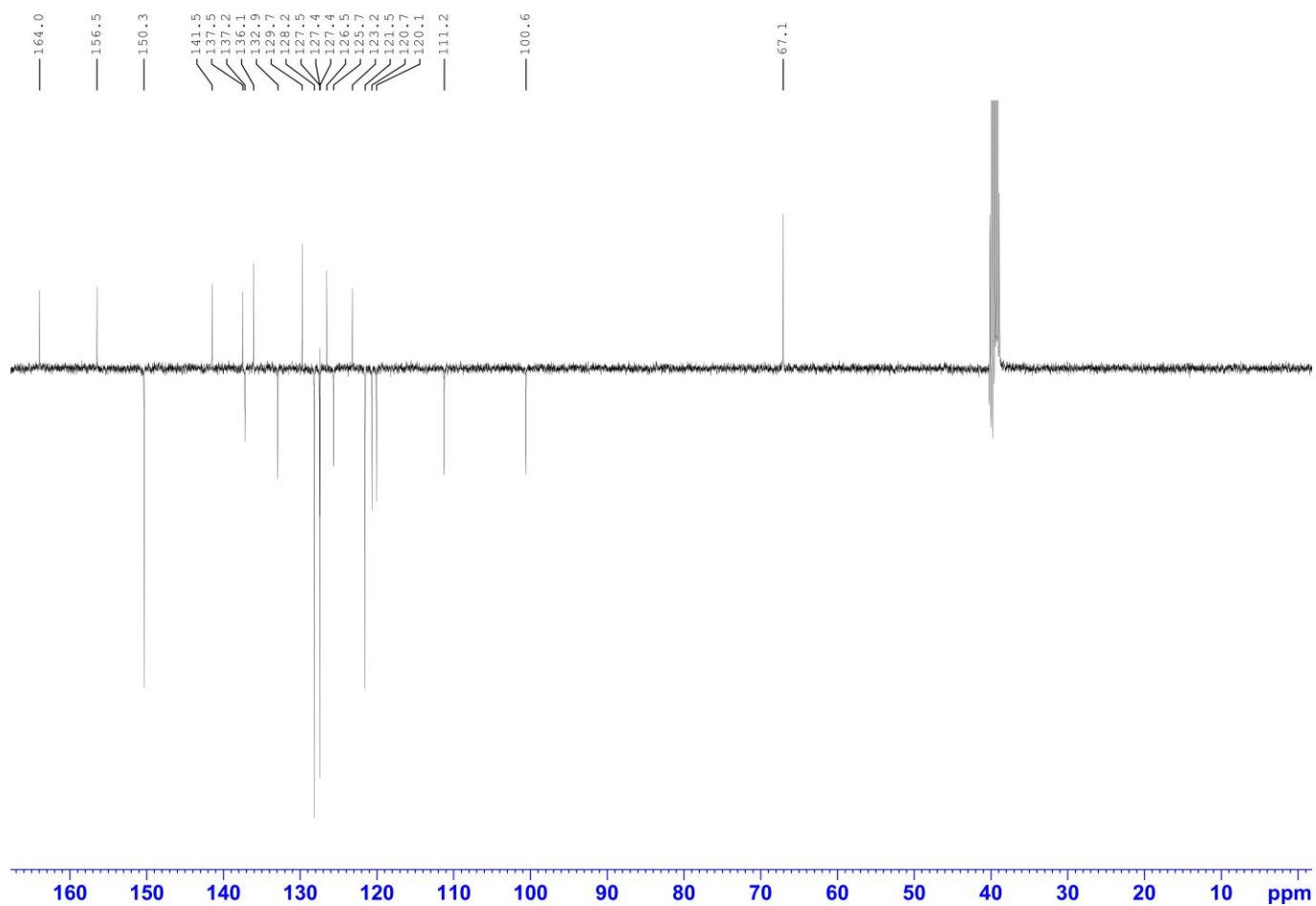
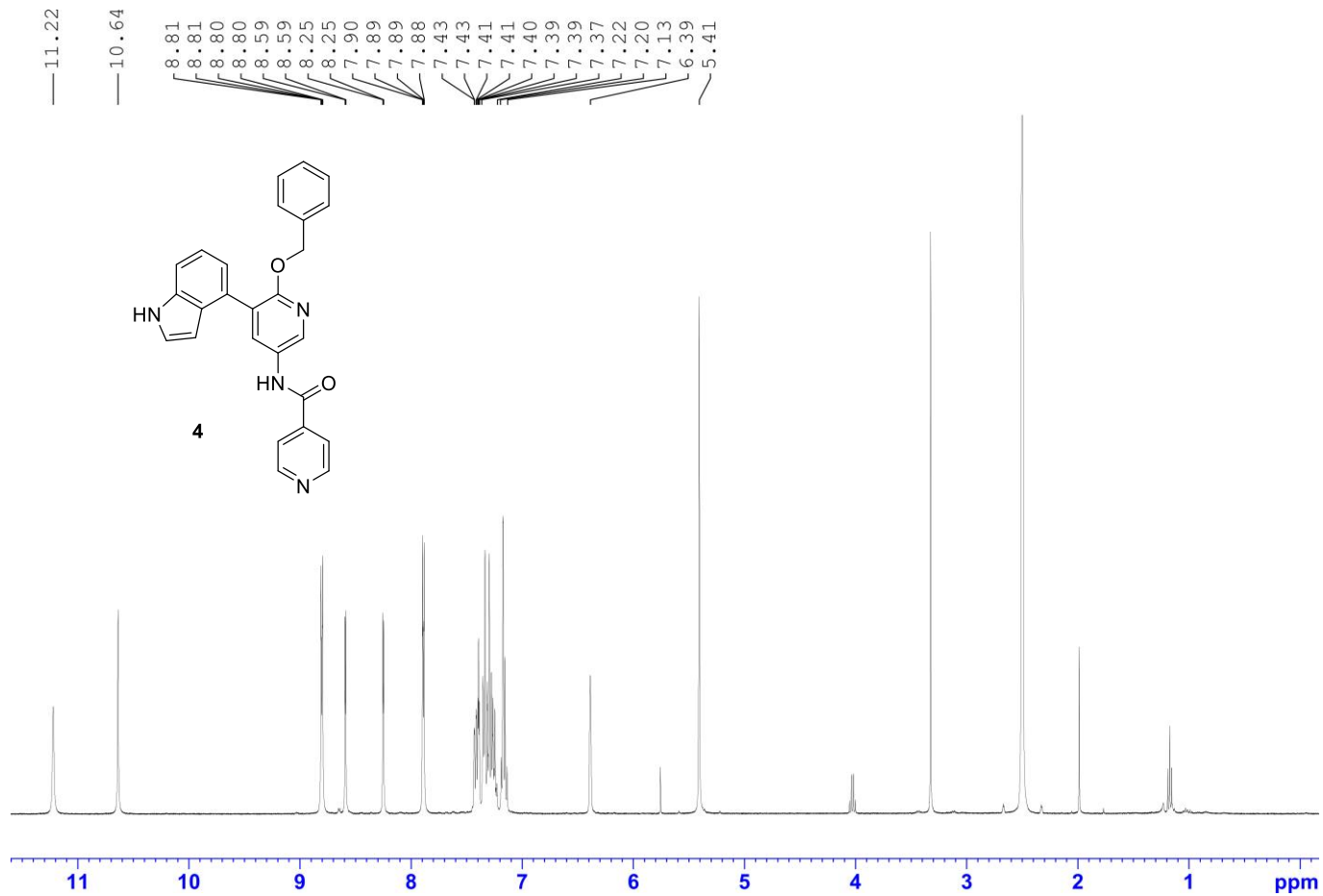
<sup>a</sup> Université Clermont Auvergne, CNRS, Clermont Auvergne INP, ICCF, F-63000 Clermont-Ferrand, France.

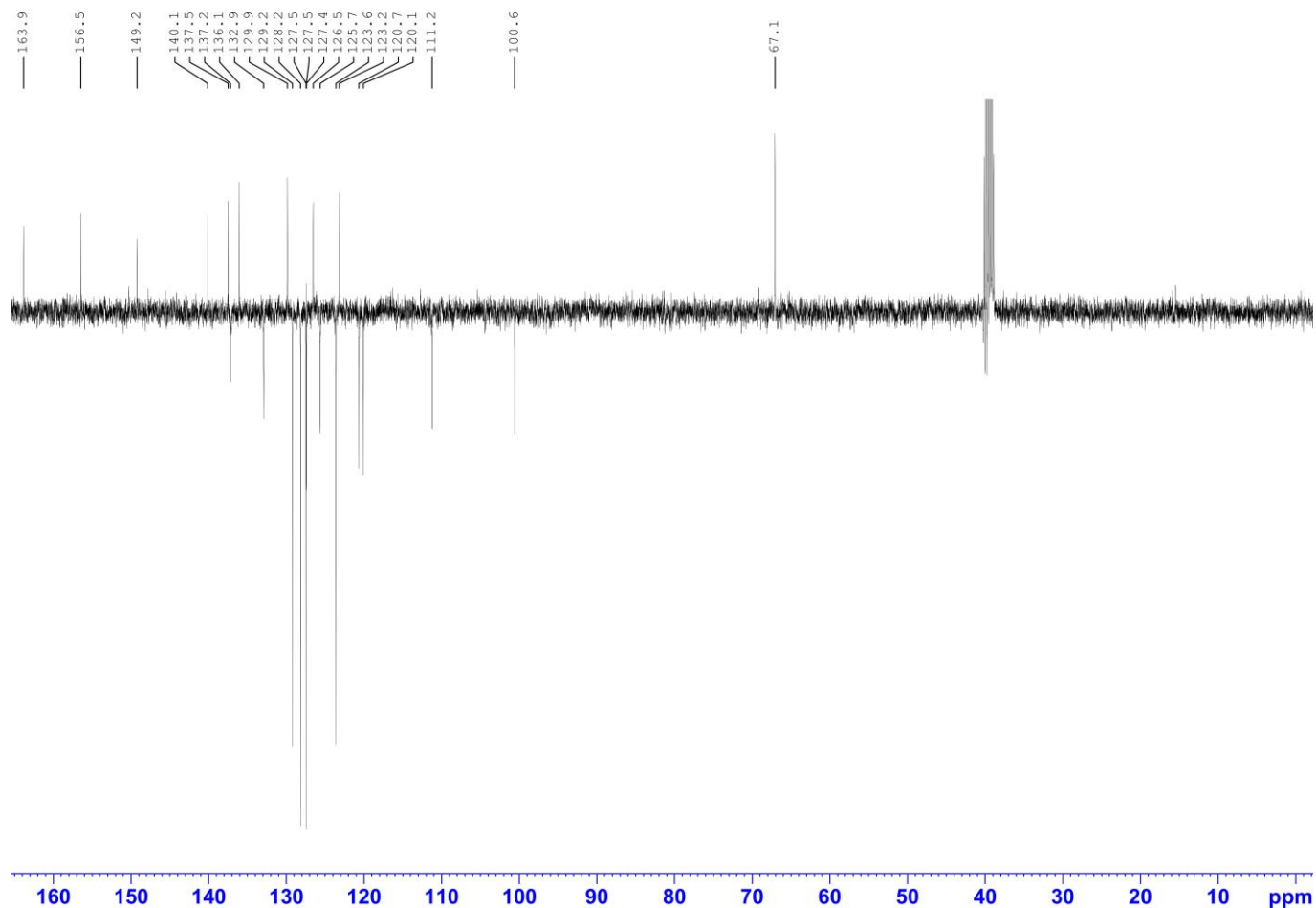
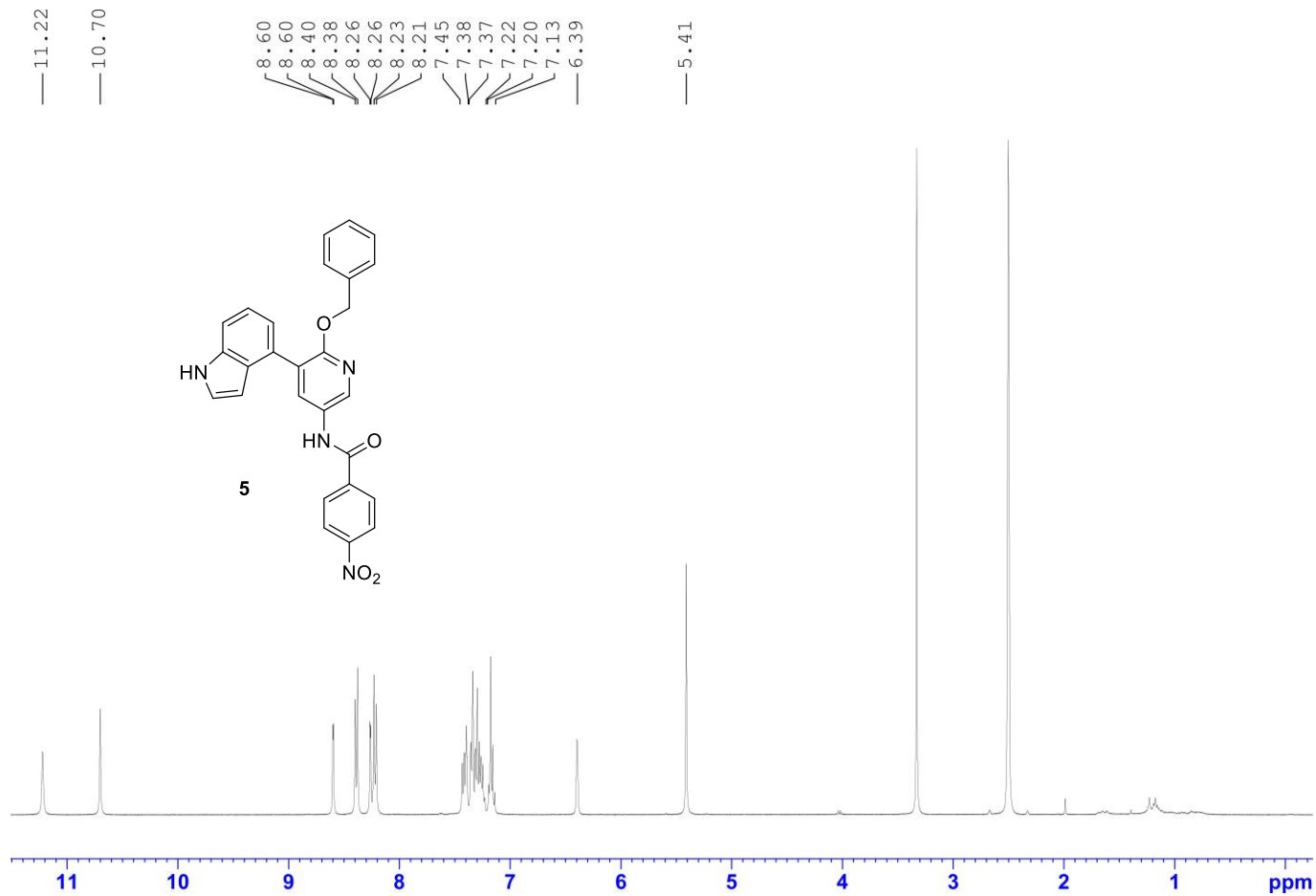
<sup>b</sup> Université Clermont Auvergne, CHU Clermont-Ferrand, Inserm, Neuro-Dol, F-63000 Clermont-Ferrand, France.

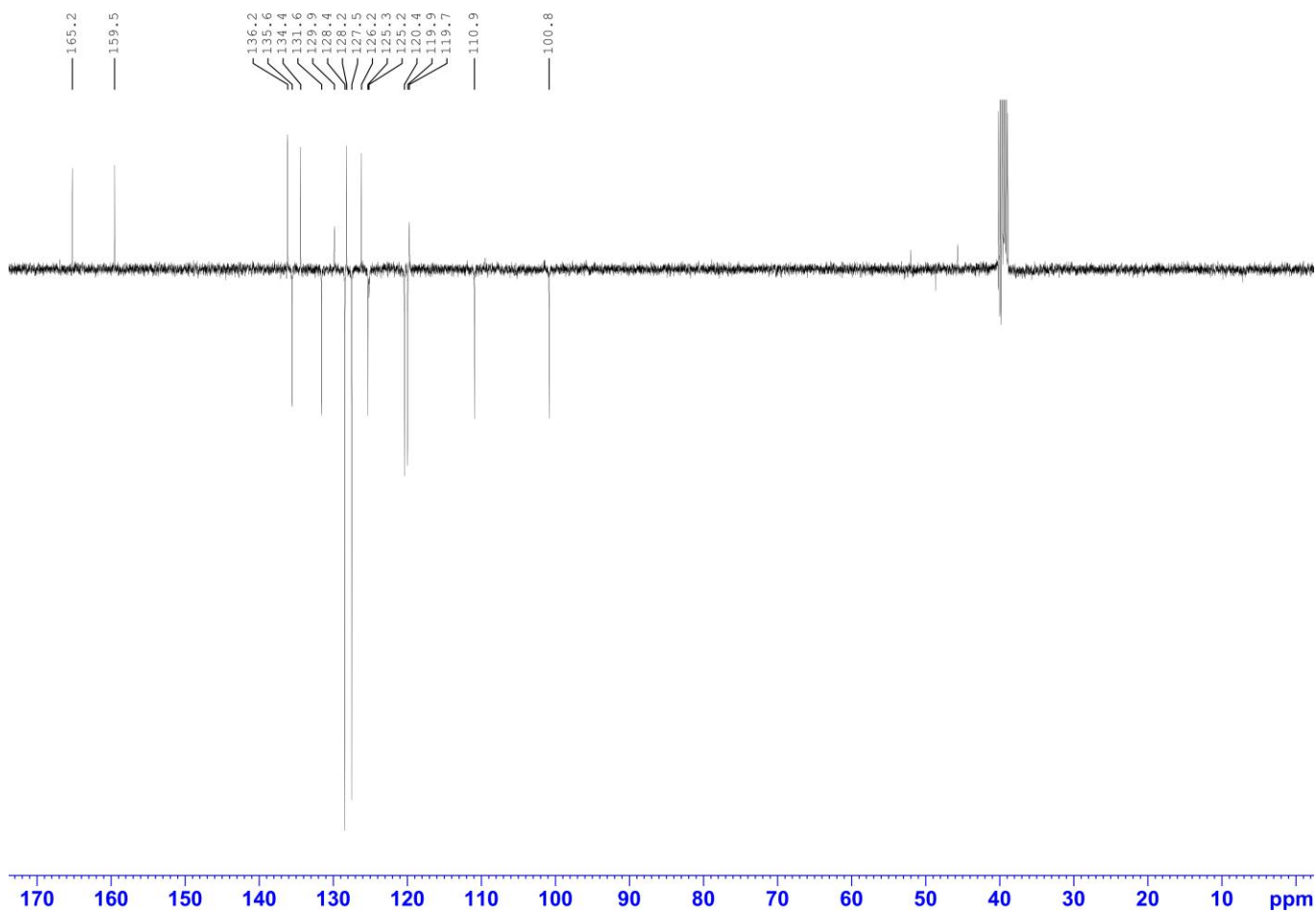
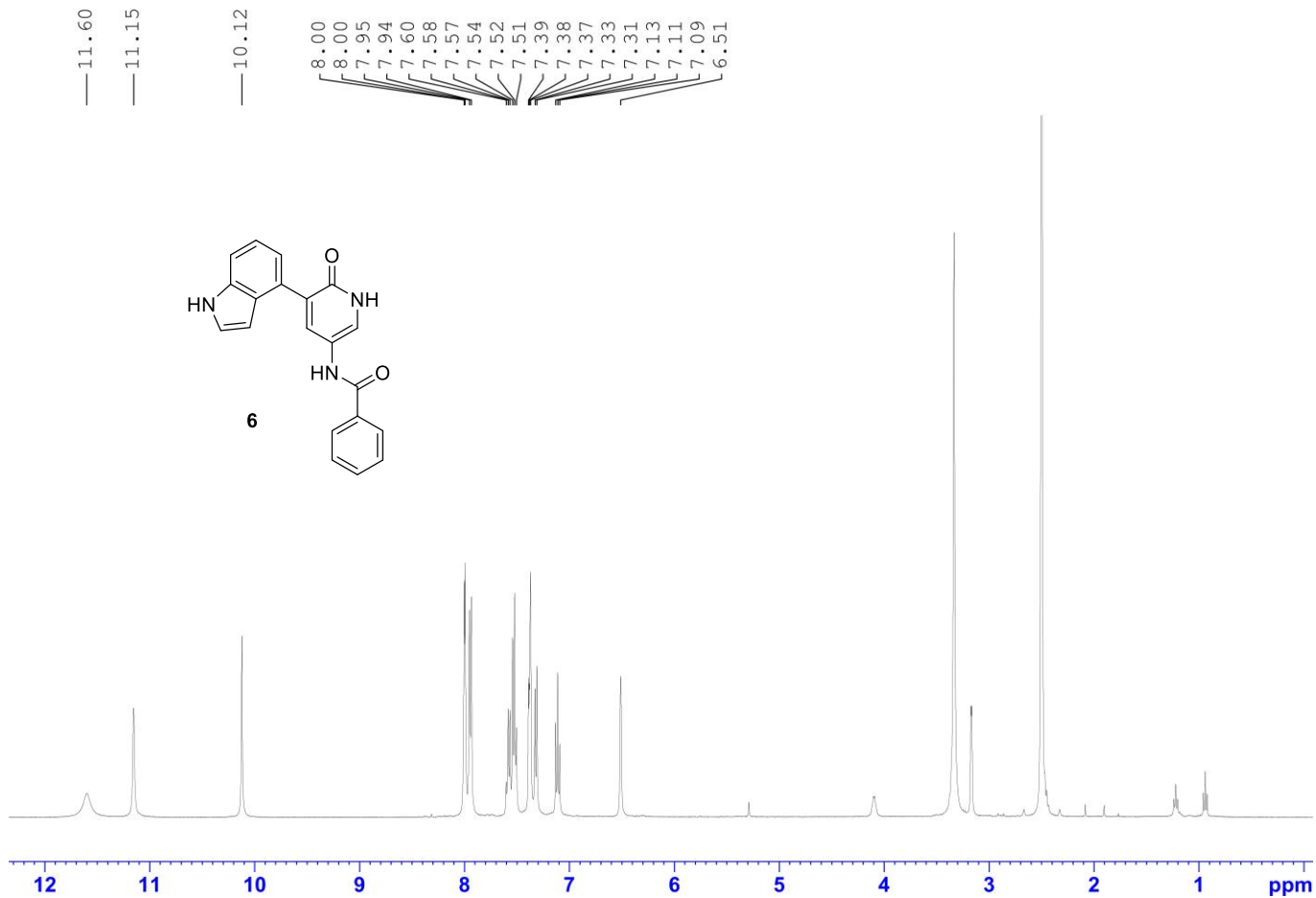
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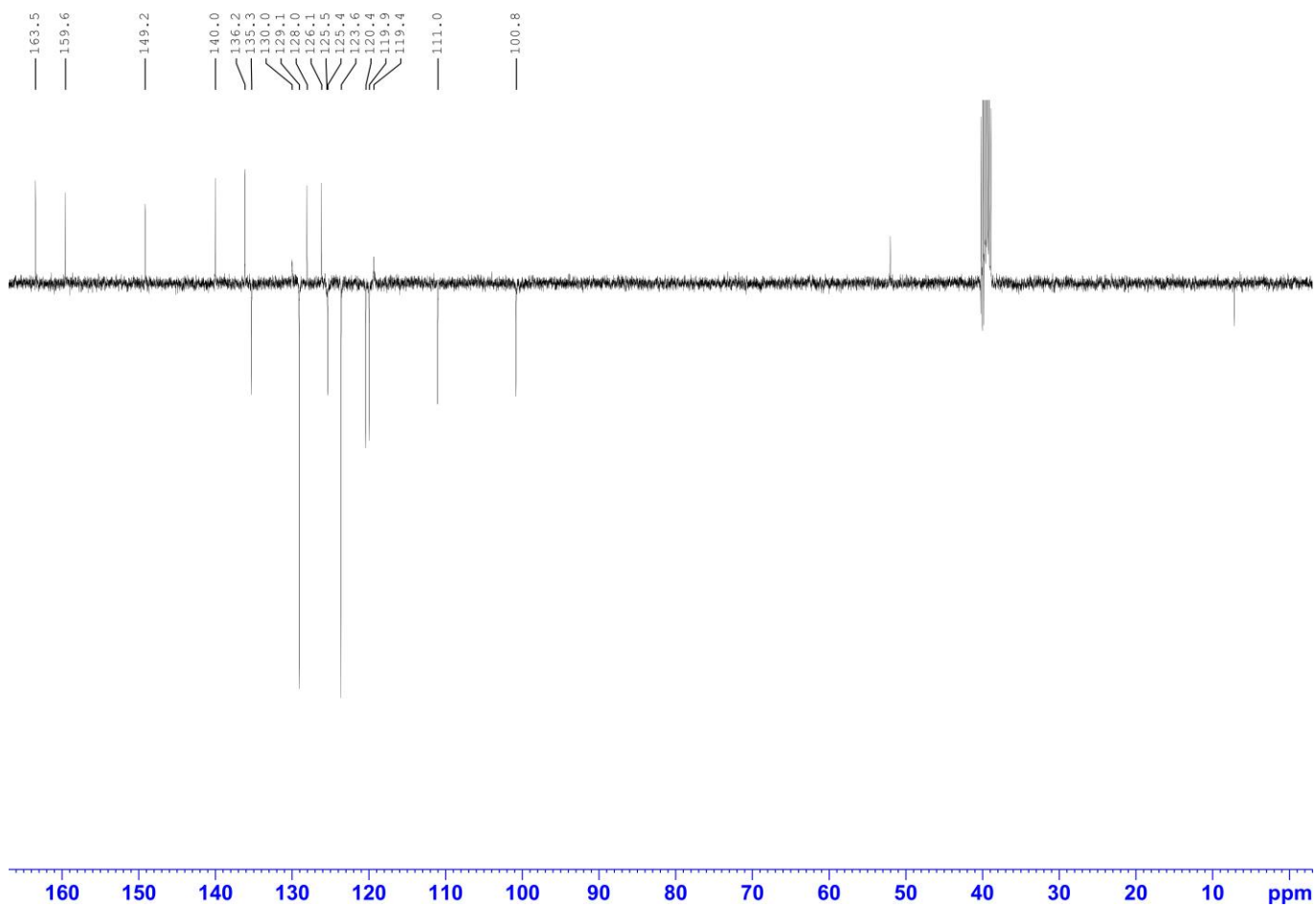
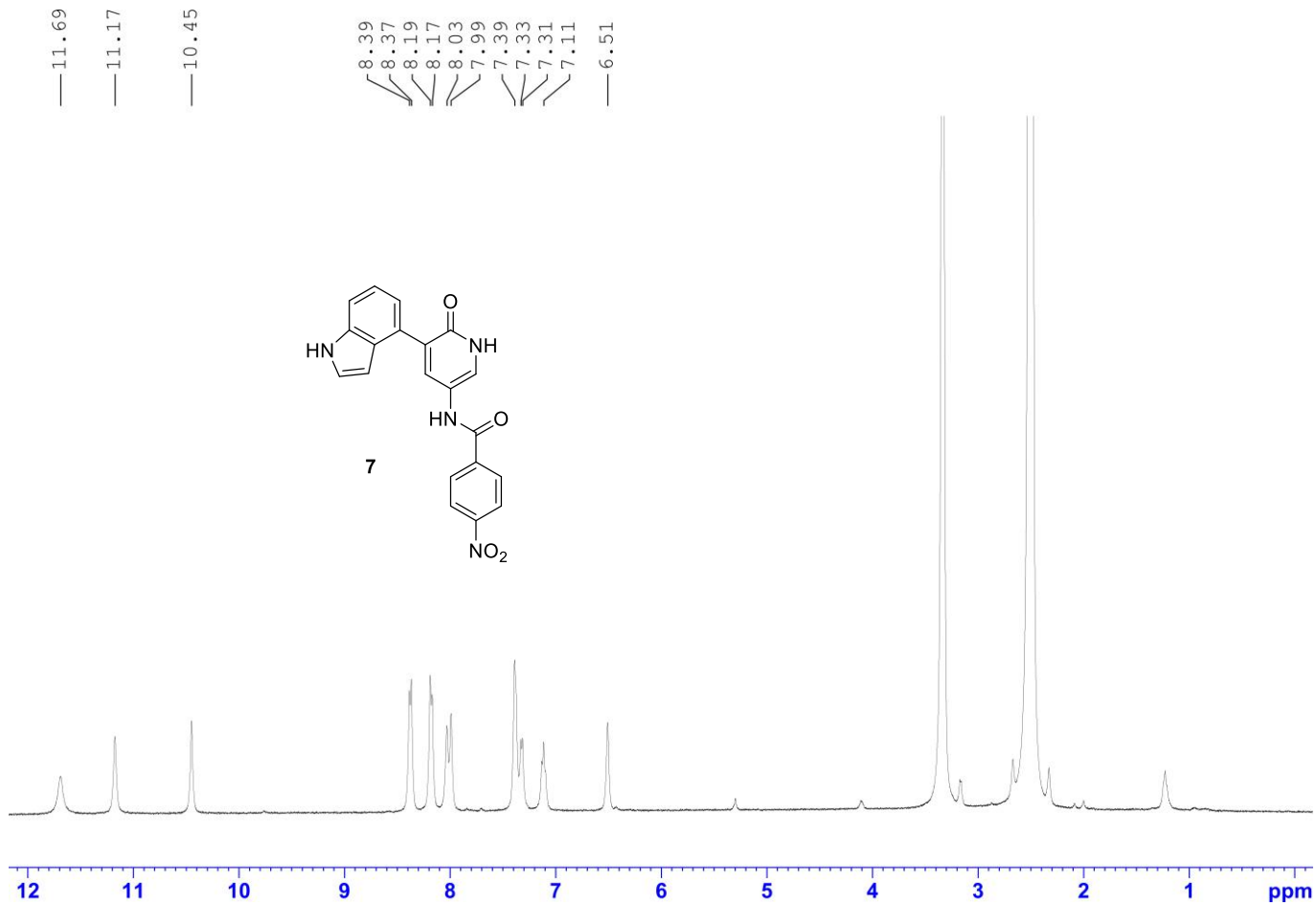
*<sup>1</sup>H and <sup>13</sup>C NMR spectra of compounds 4–10, 12–27, 31–40, 44, 45, 49–58, 69–88.....S2 to S68*

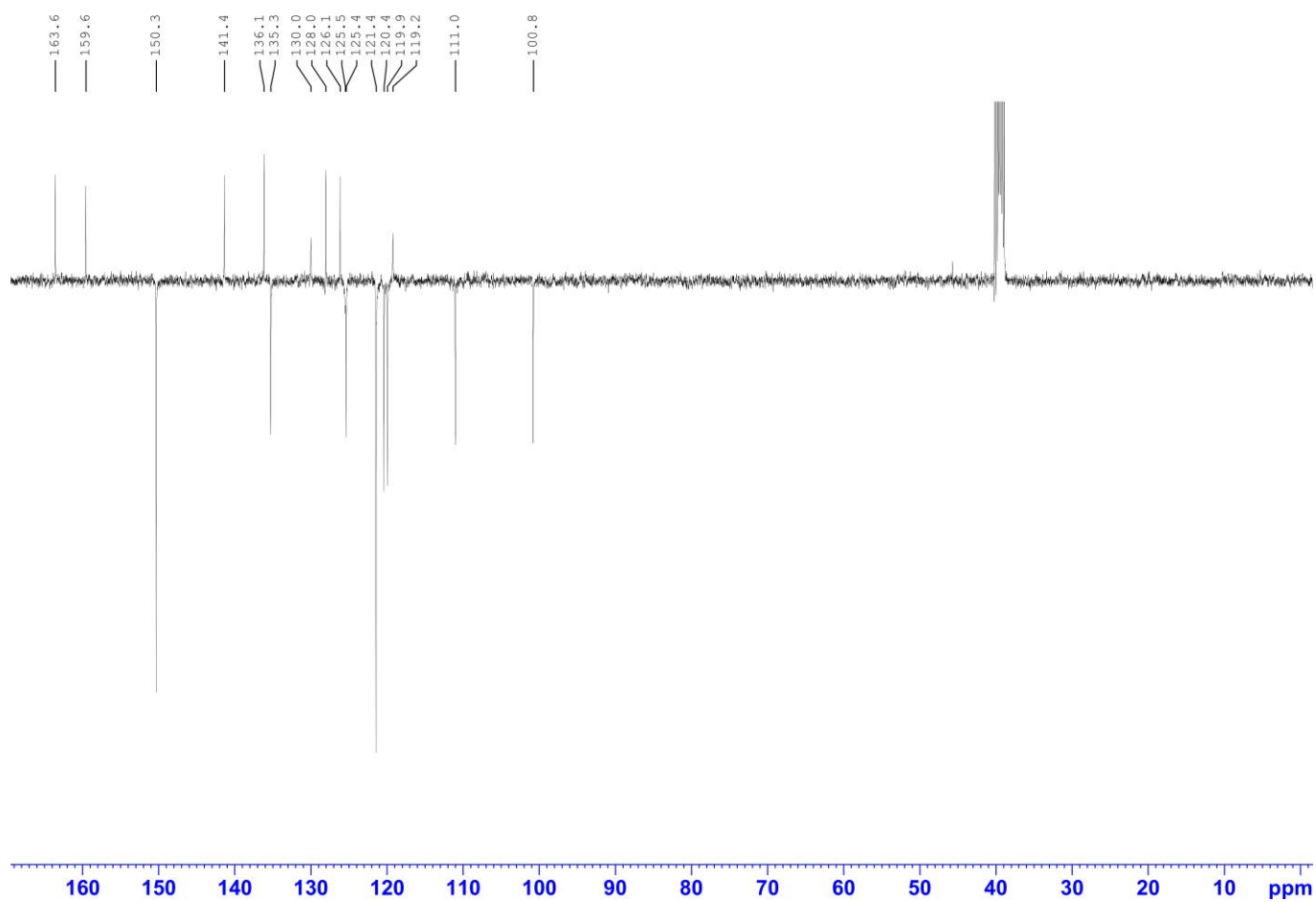
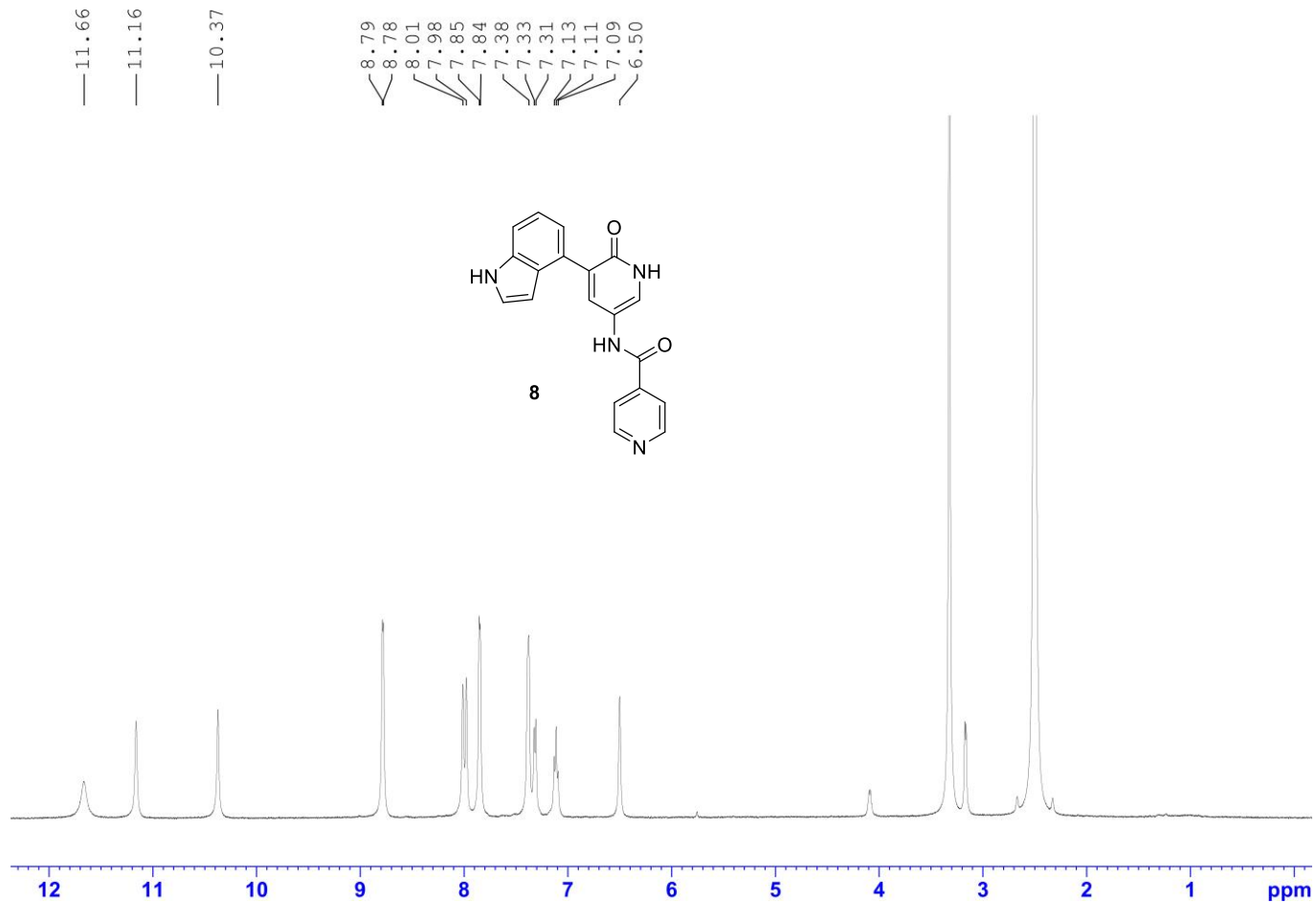
*HRMS spectra of compounds 4–10, 12–27, 31–40, 44, 45, 49–58, 69–88.....S69 to S102*

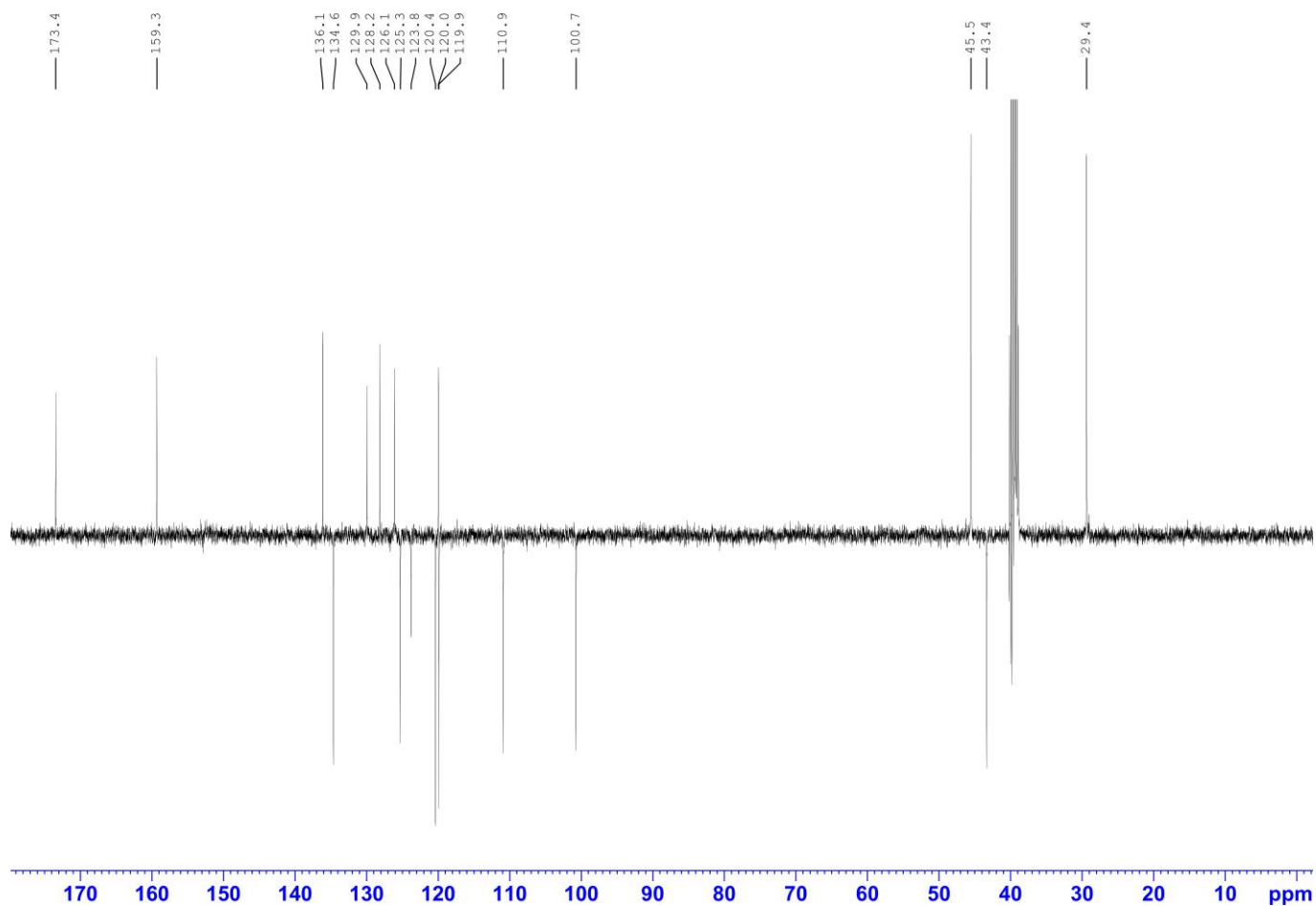
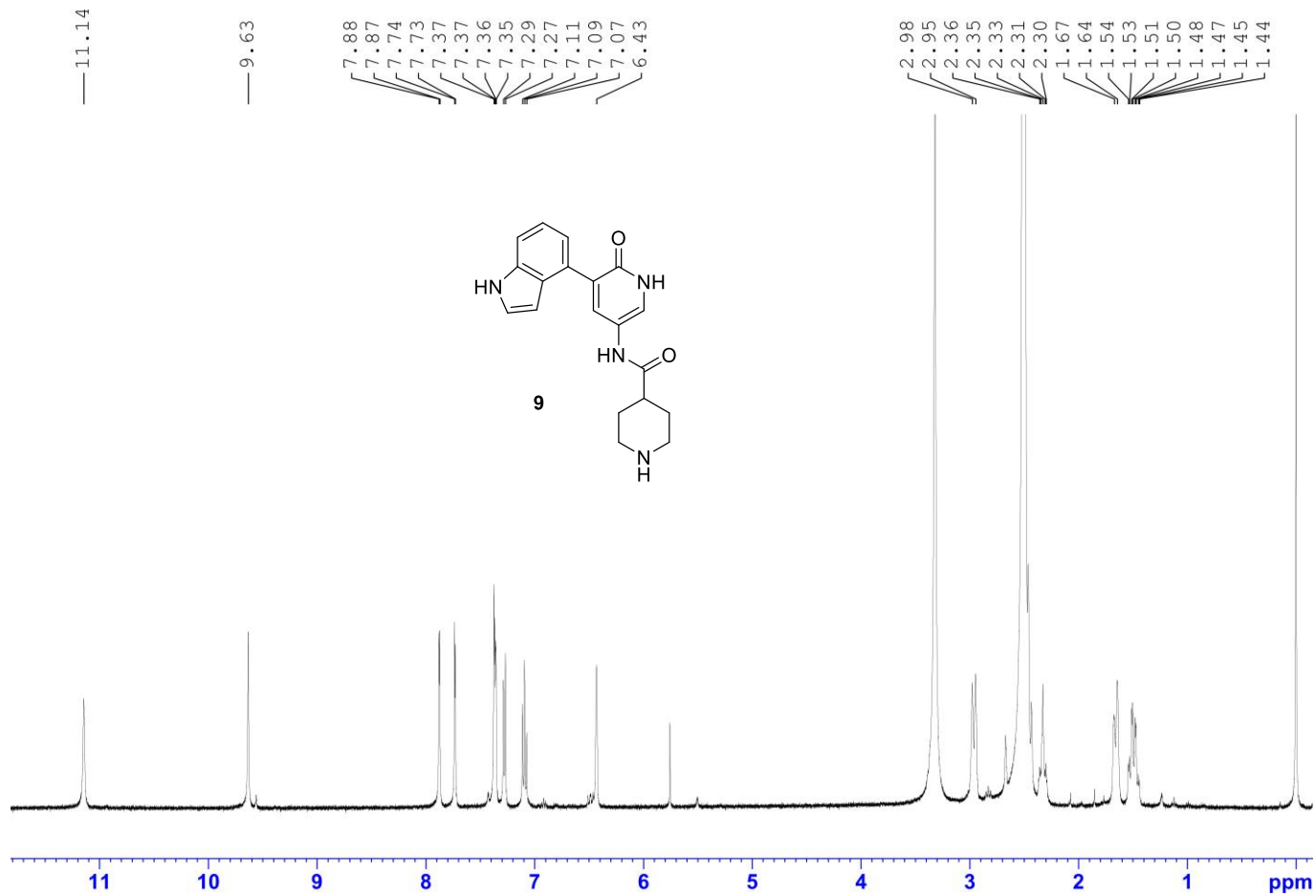


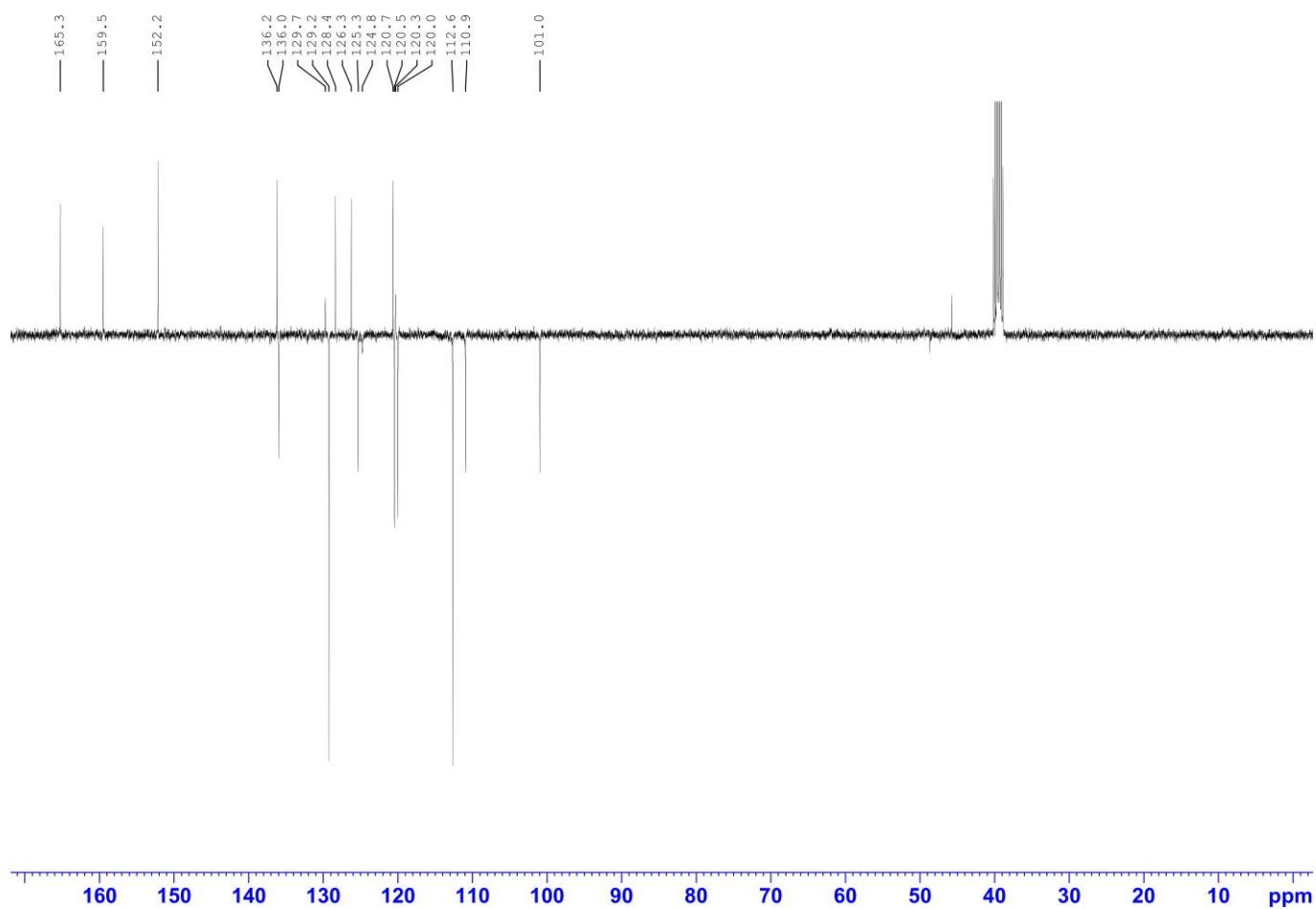
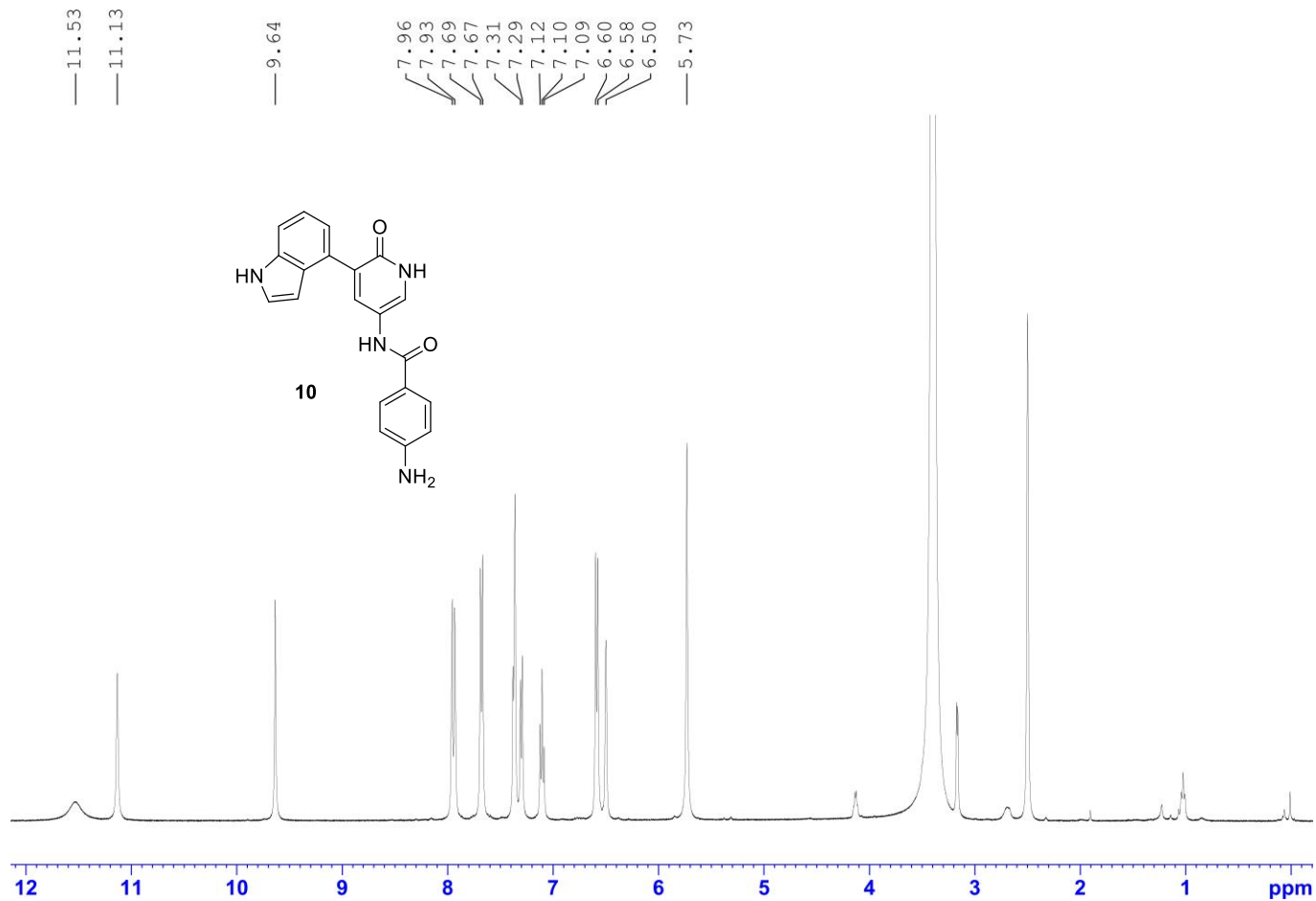




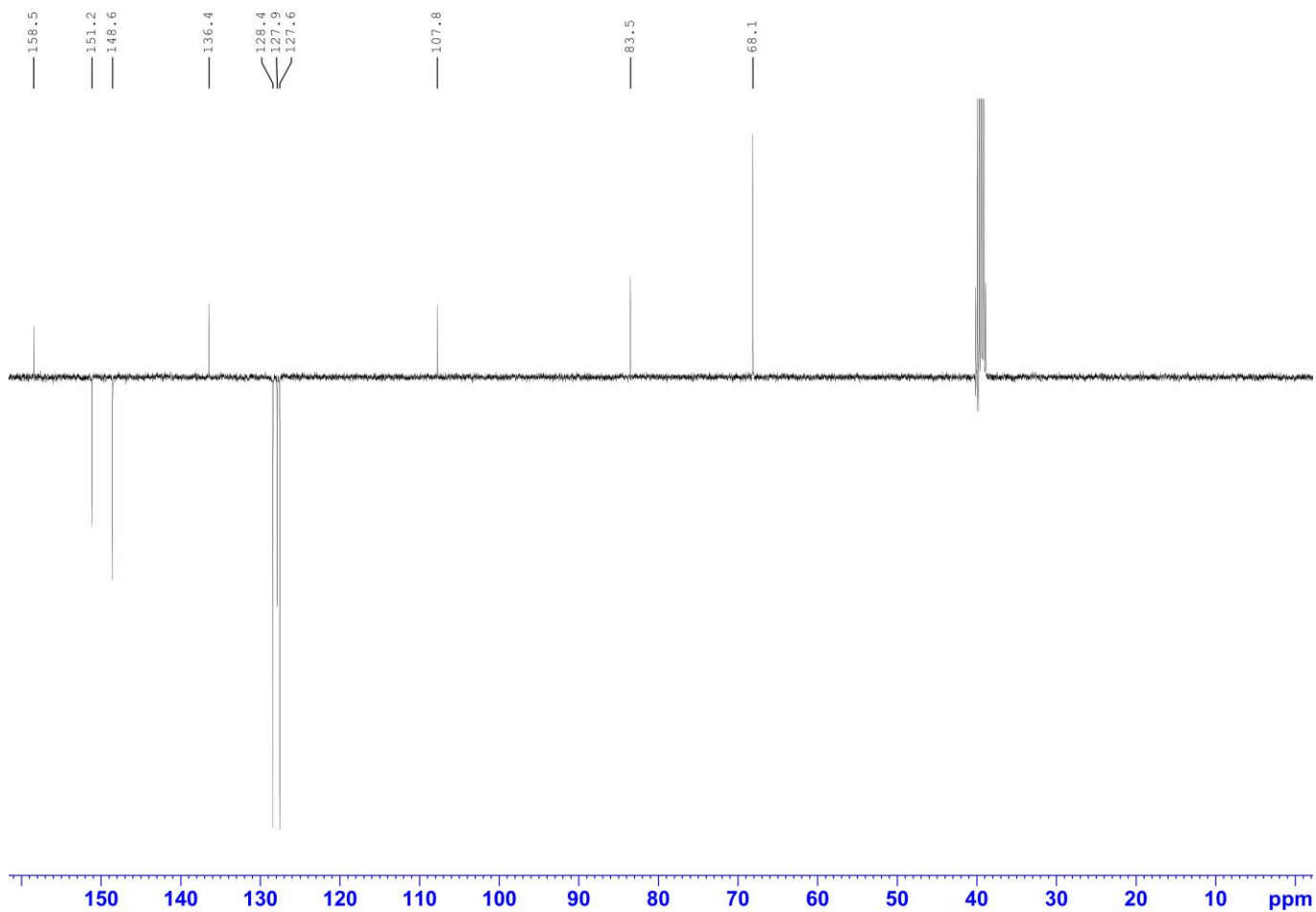
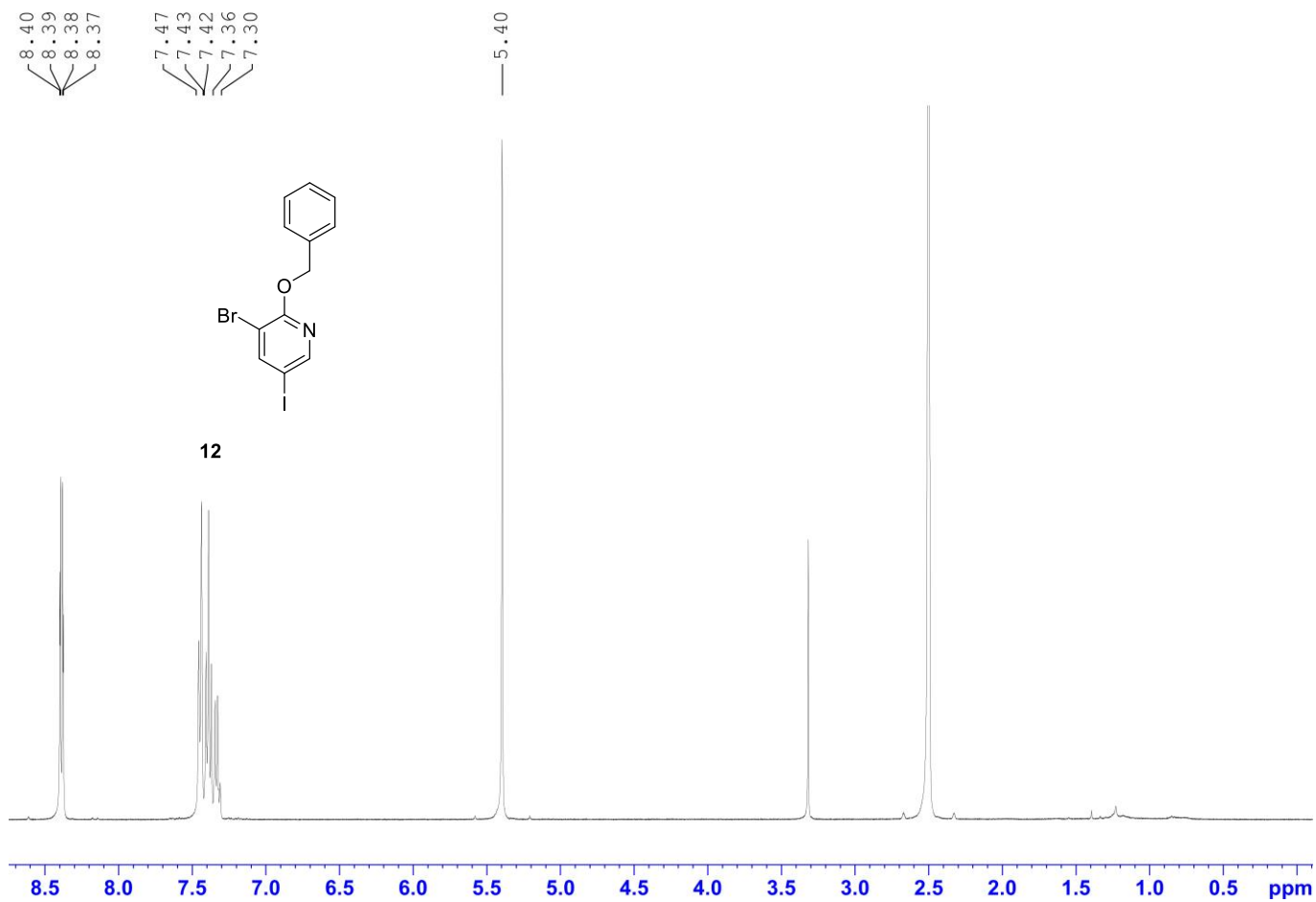


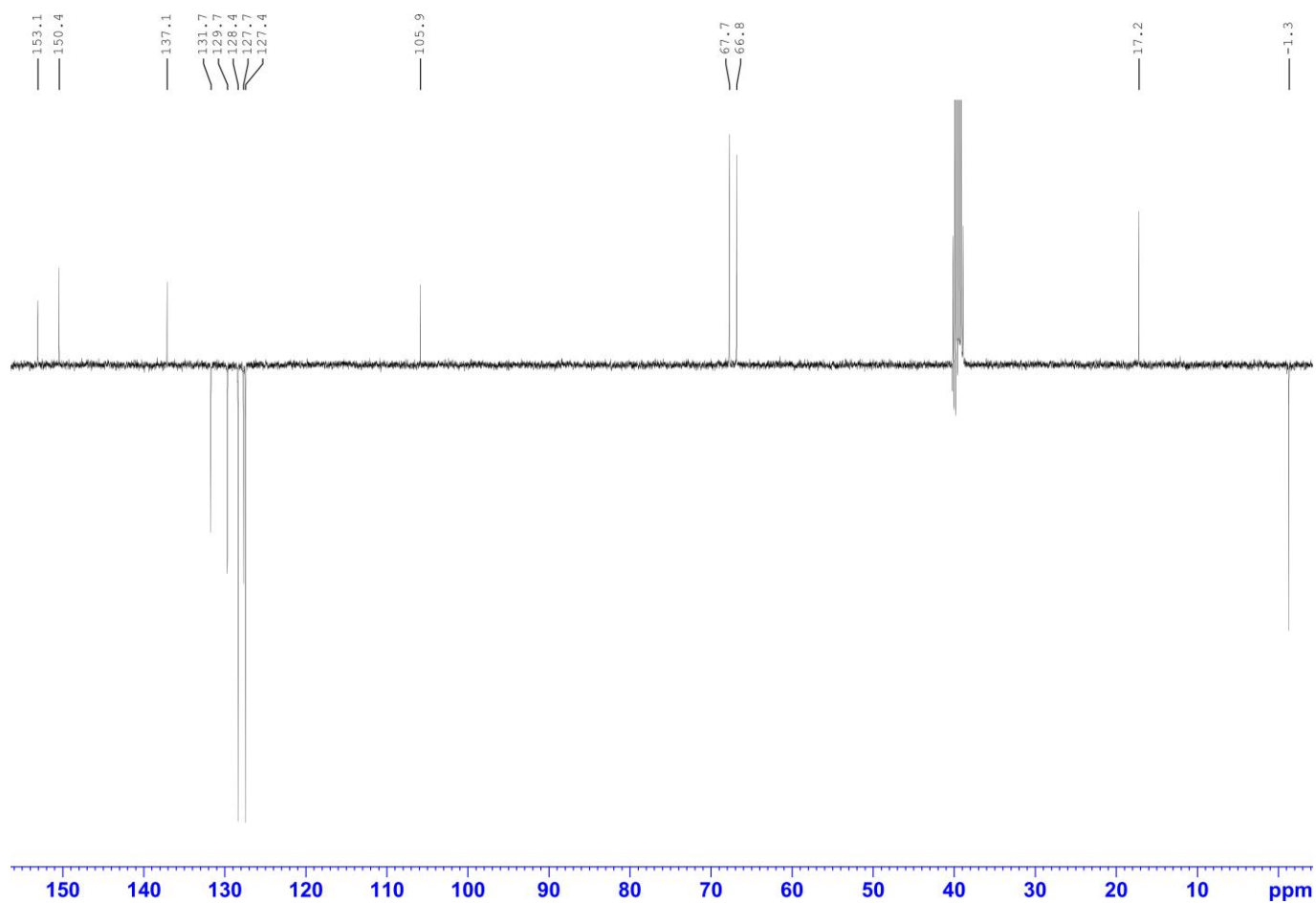
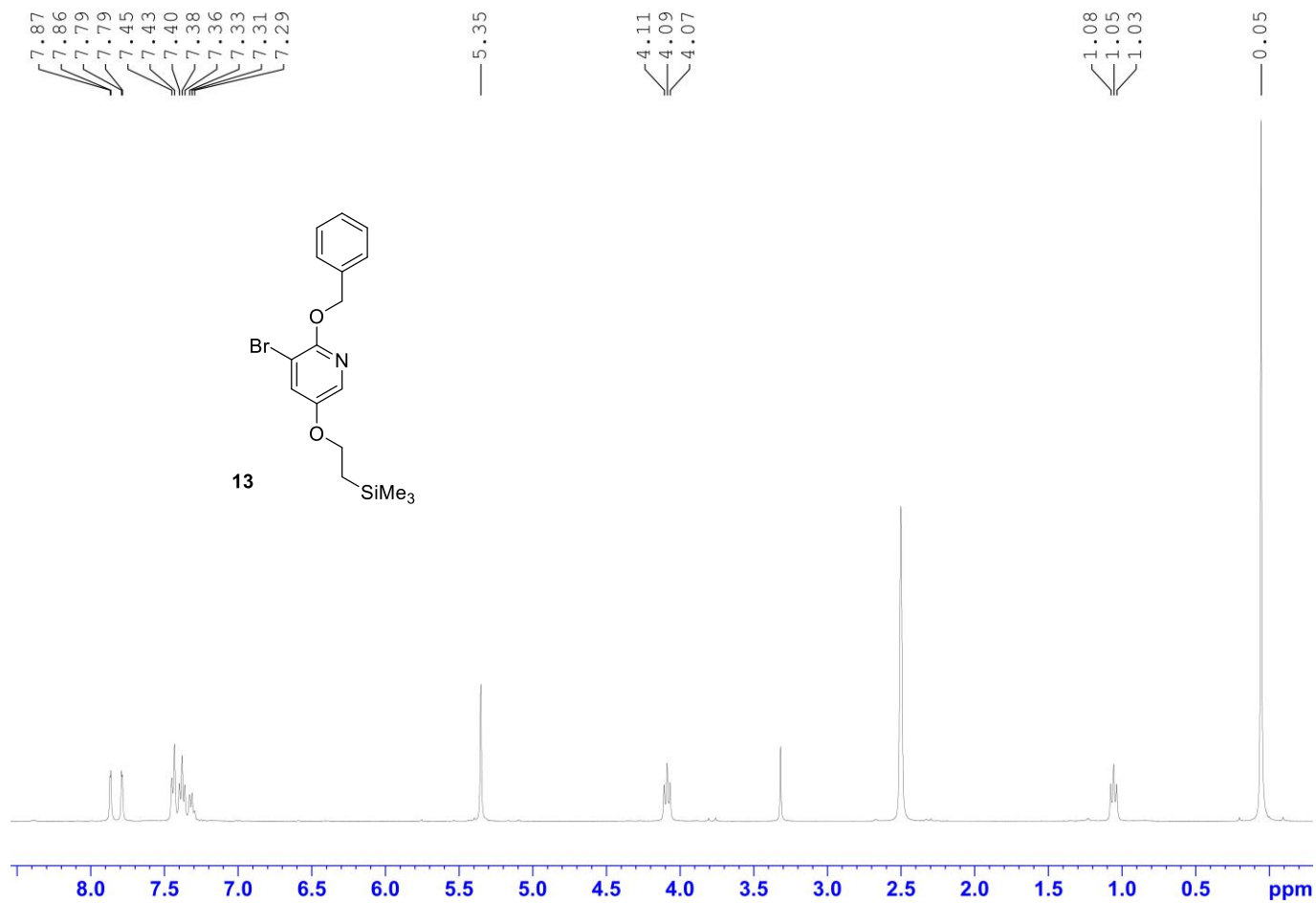


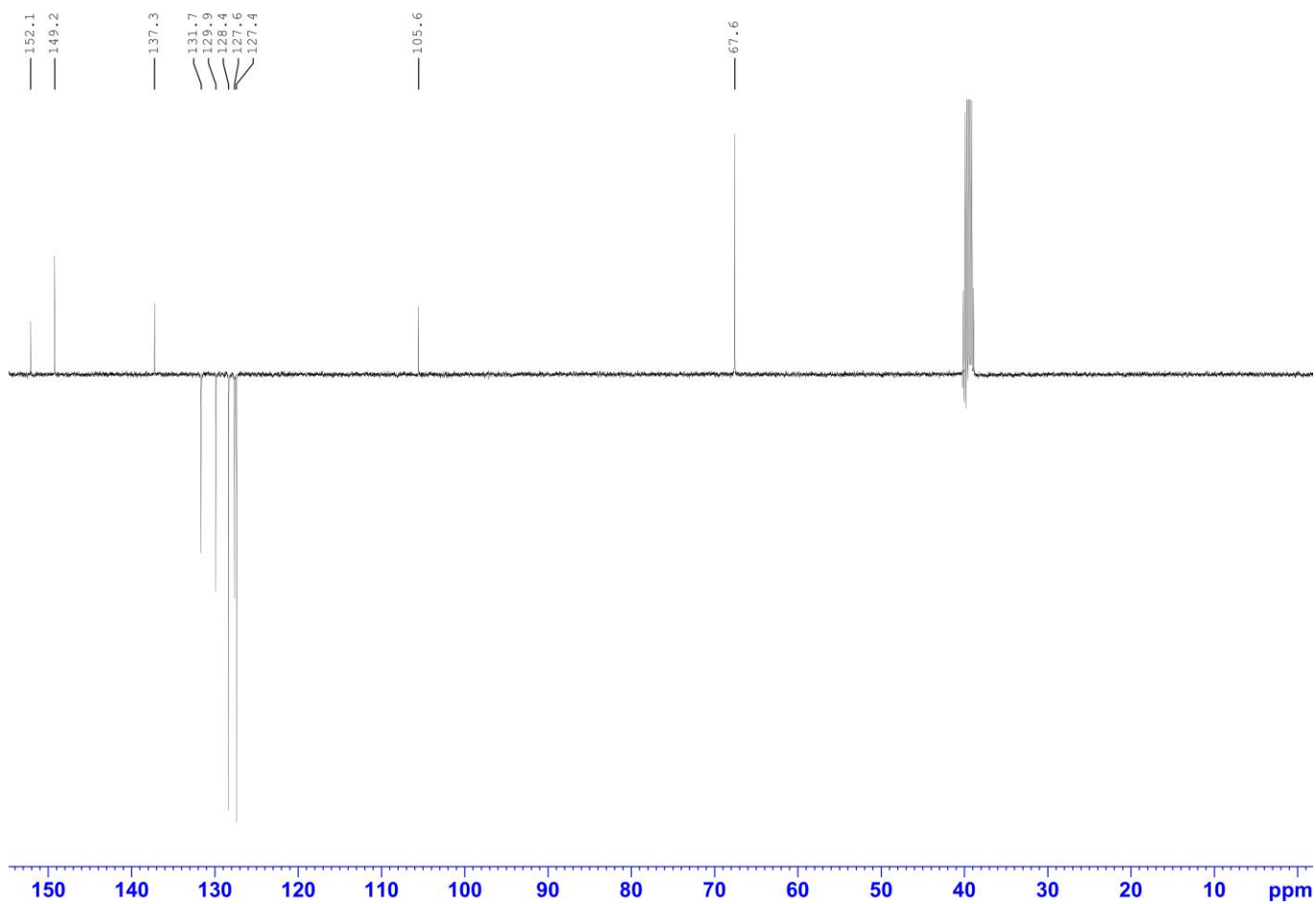
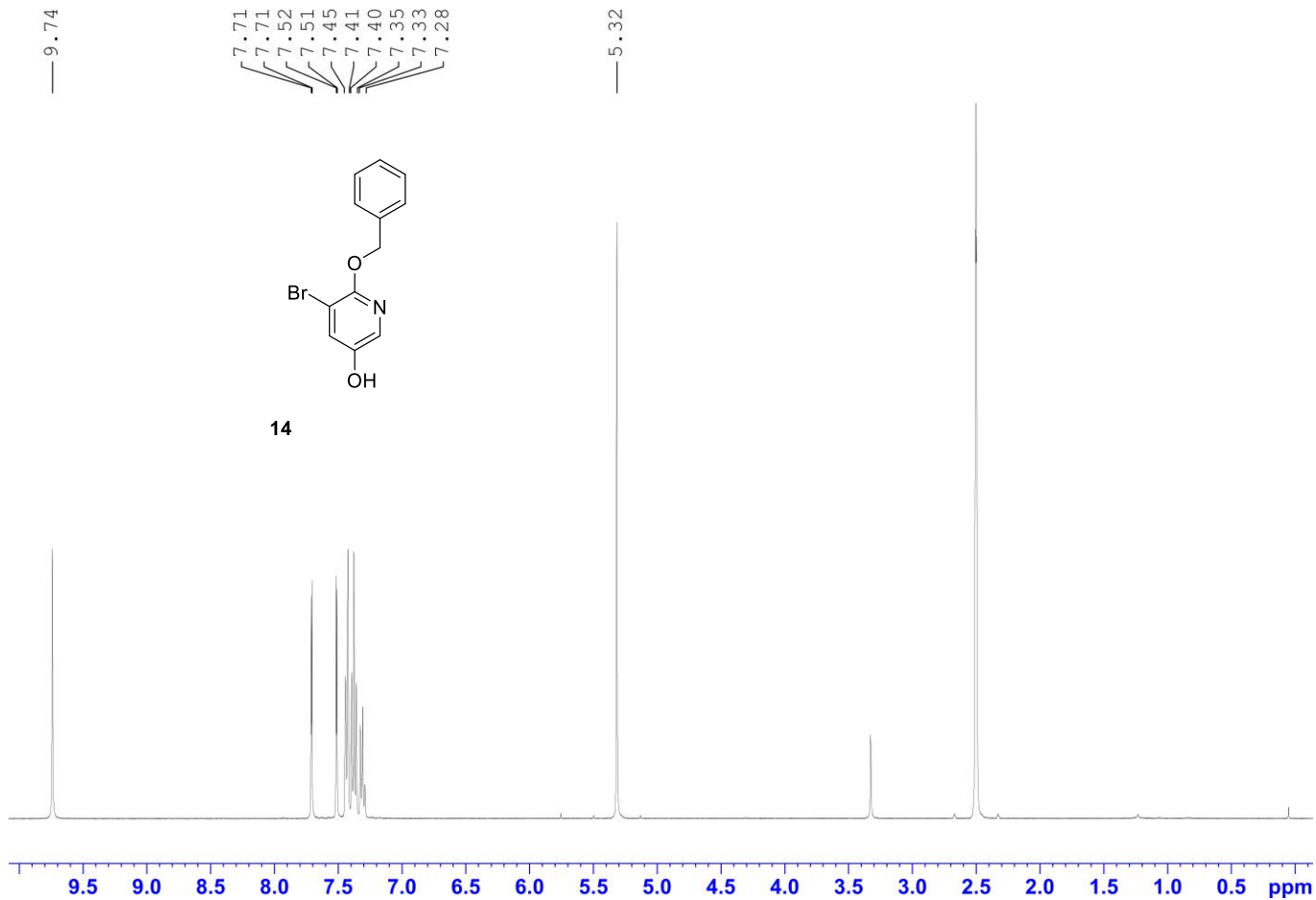


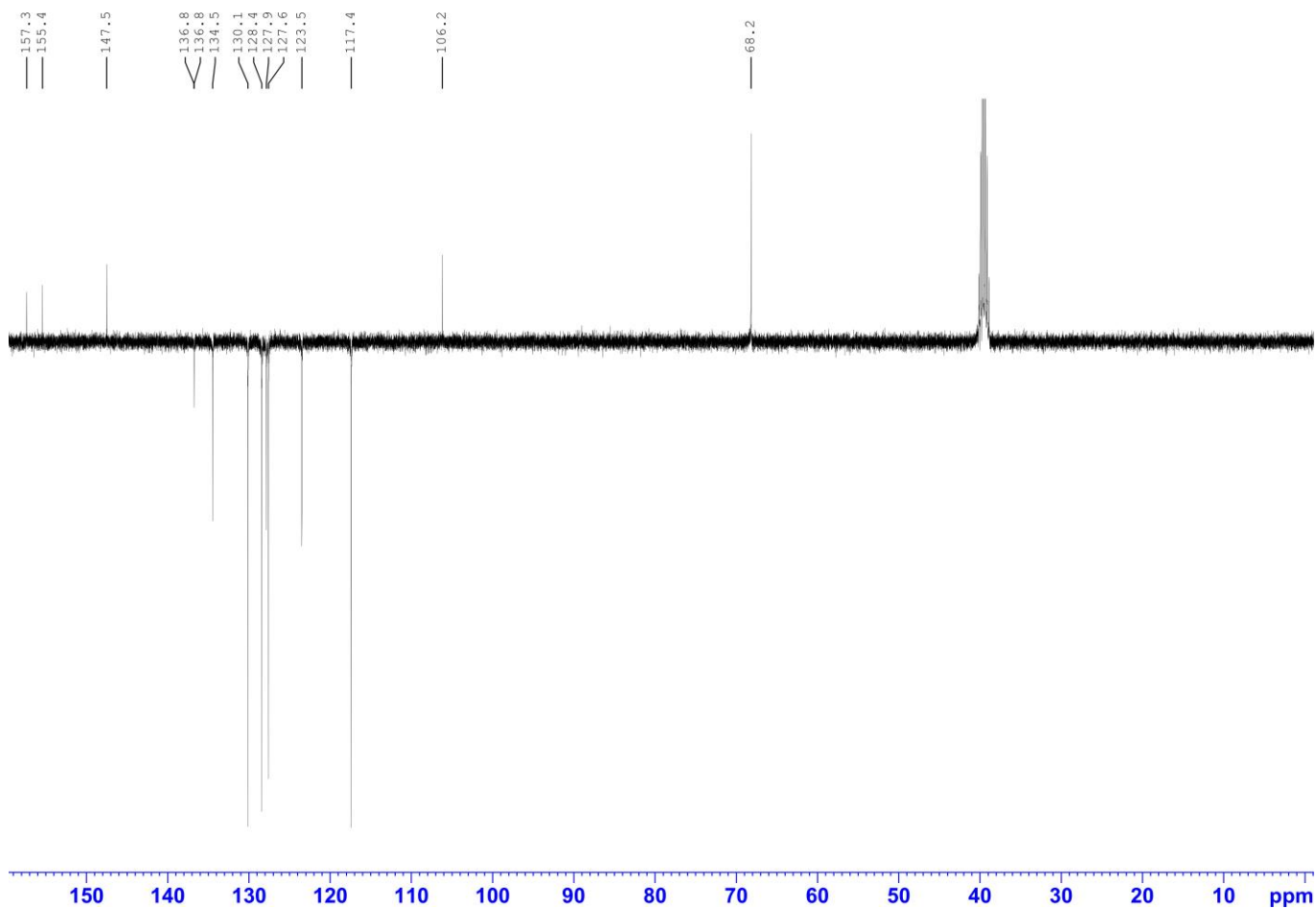
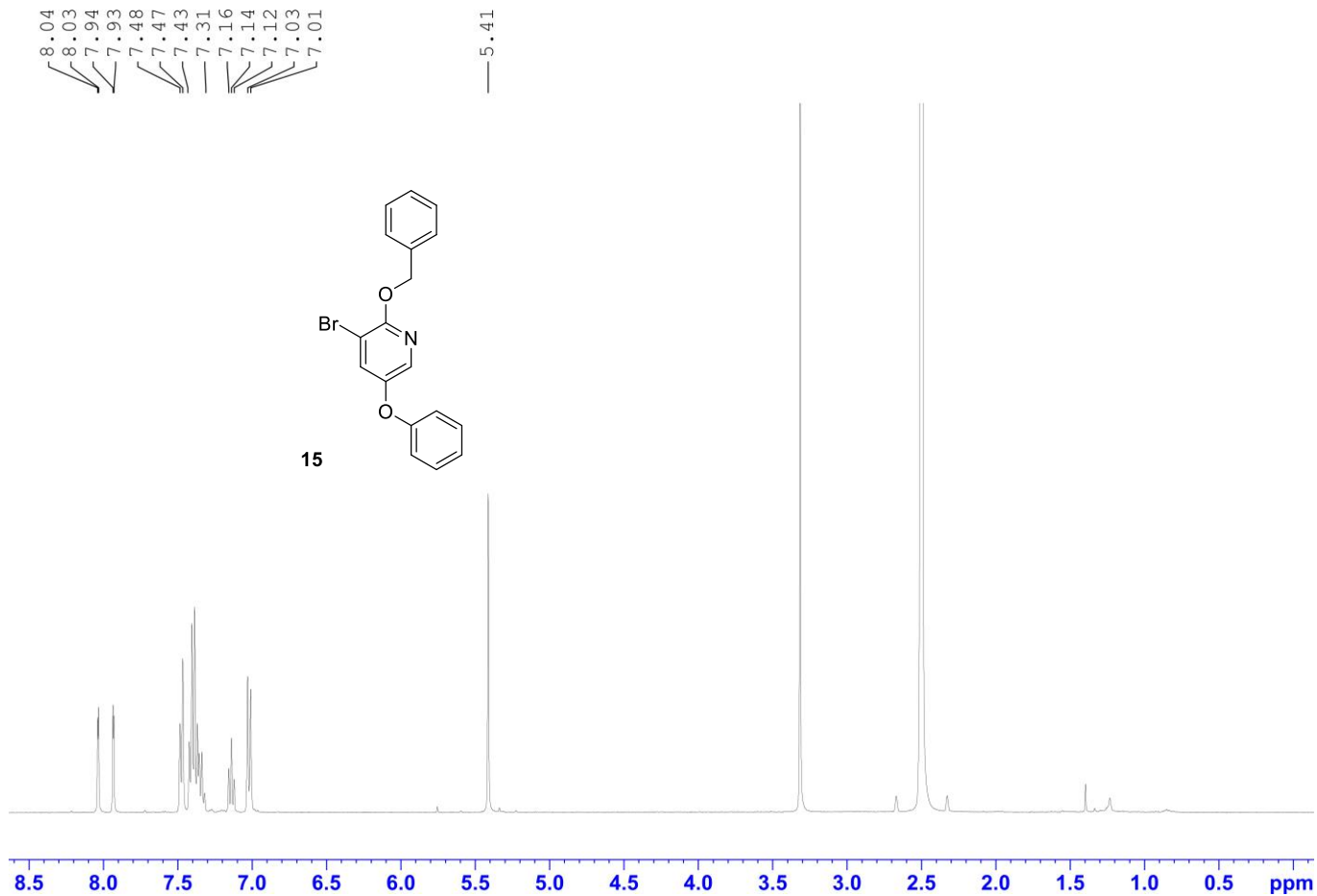


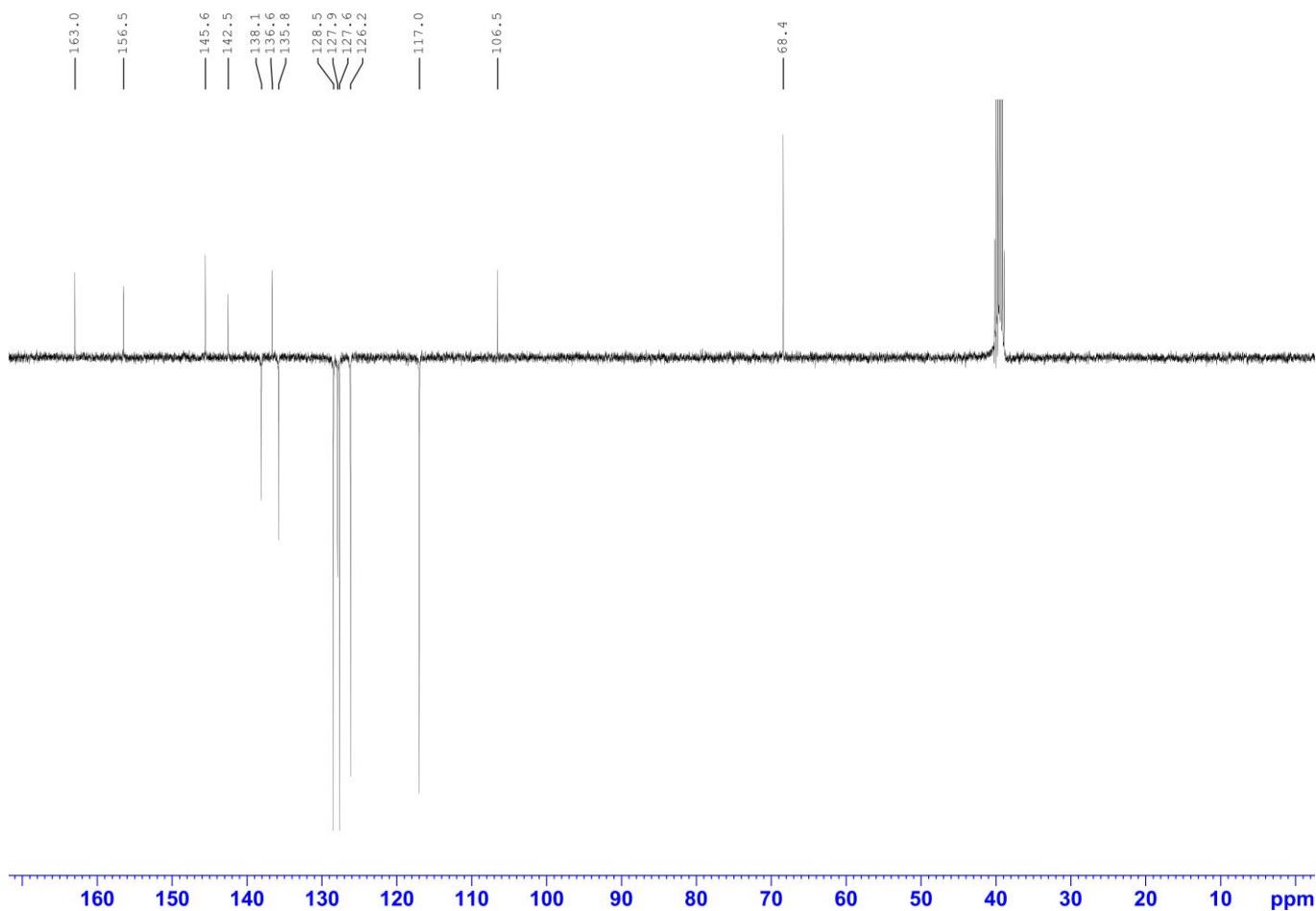
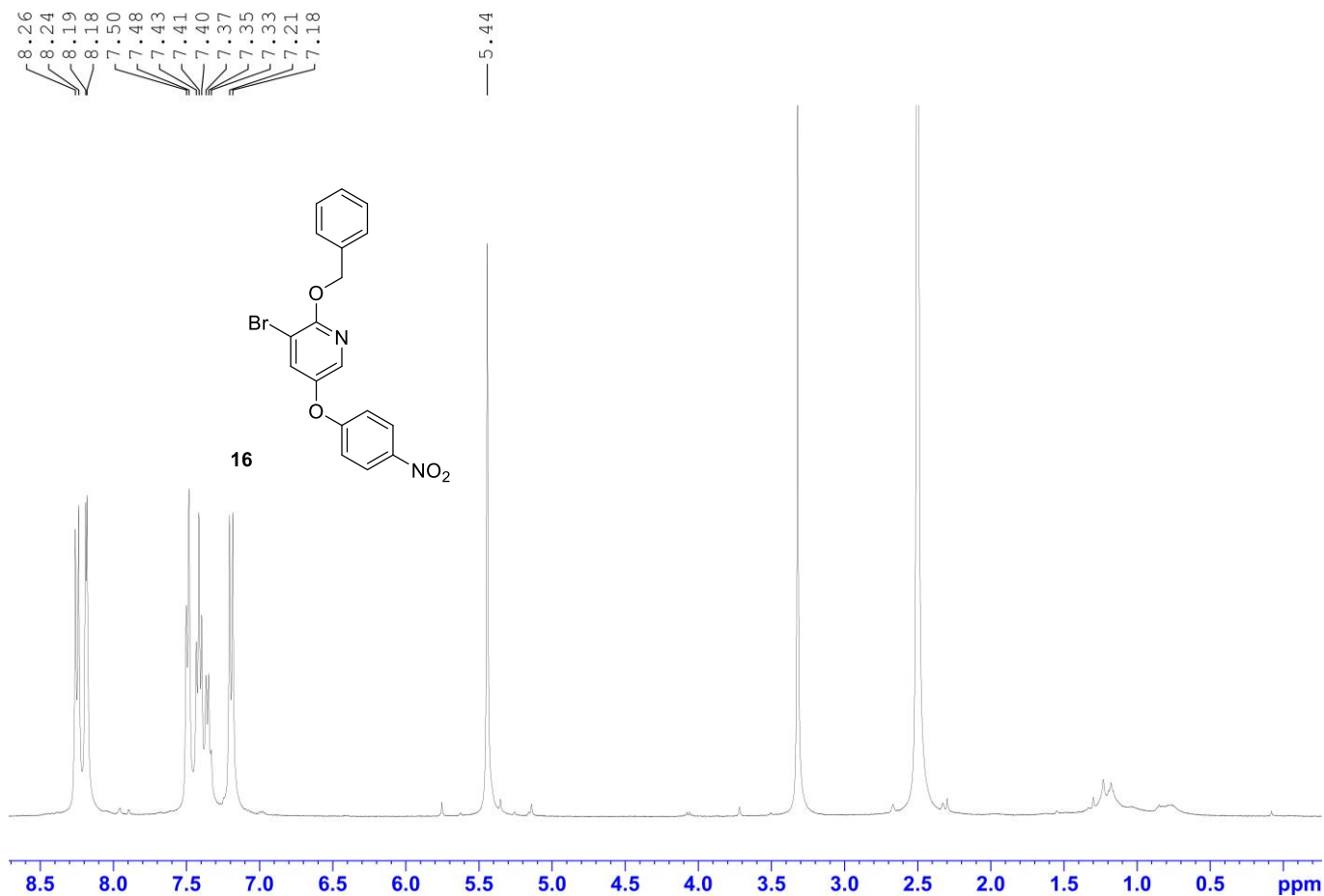


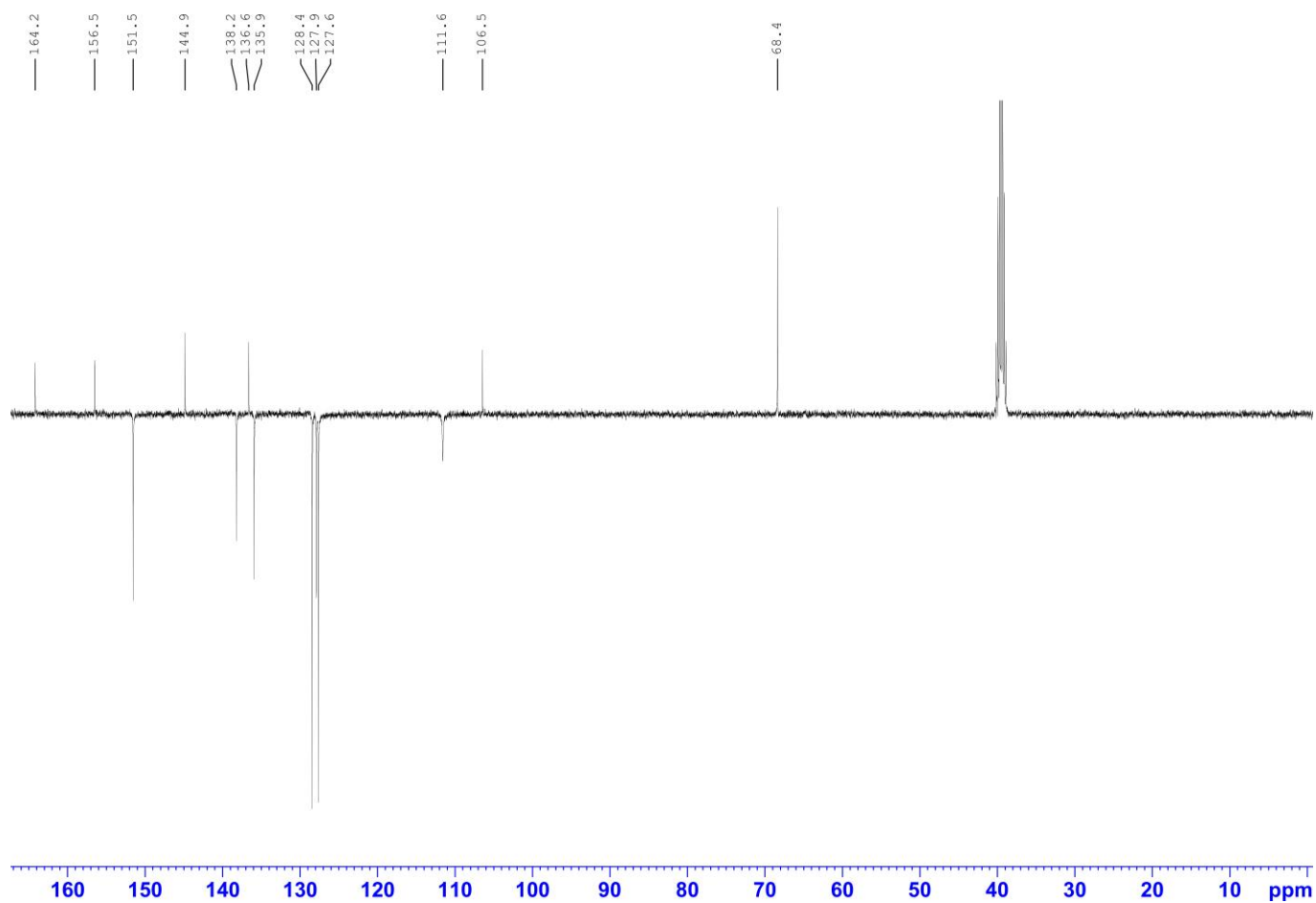
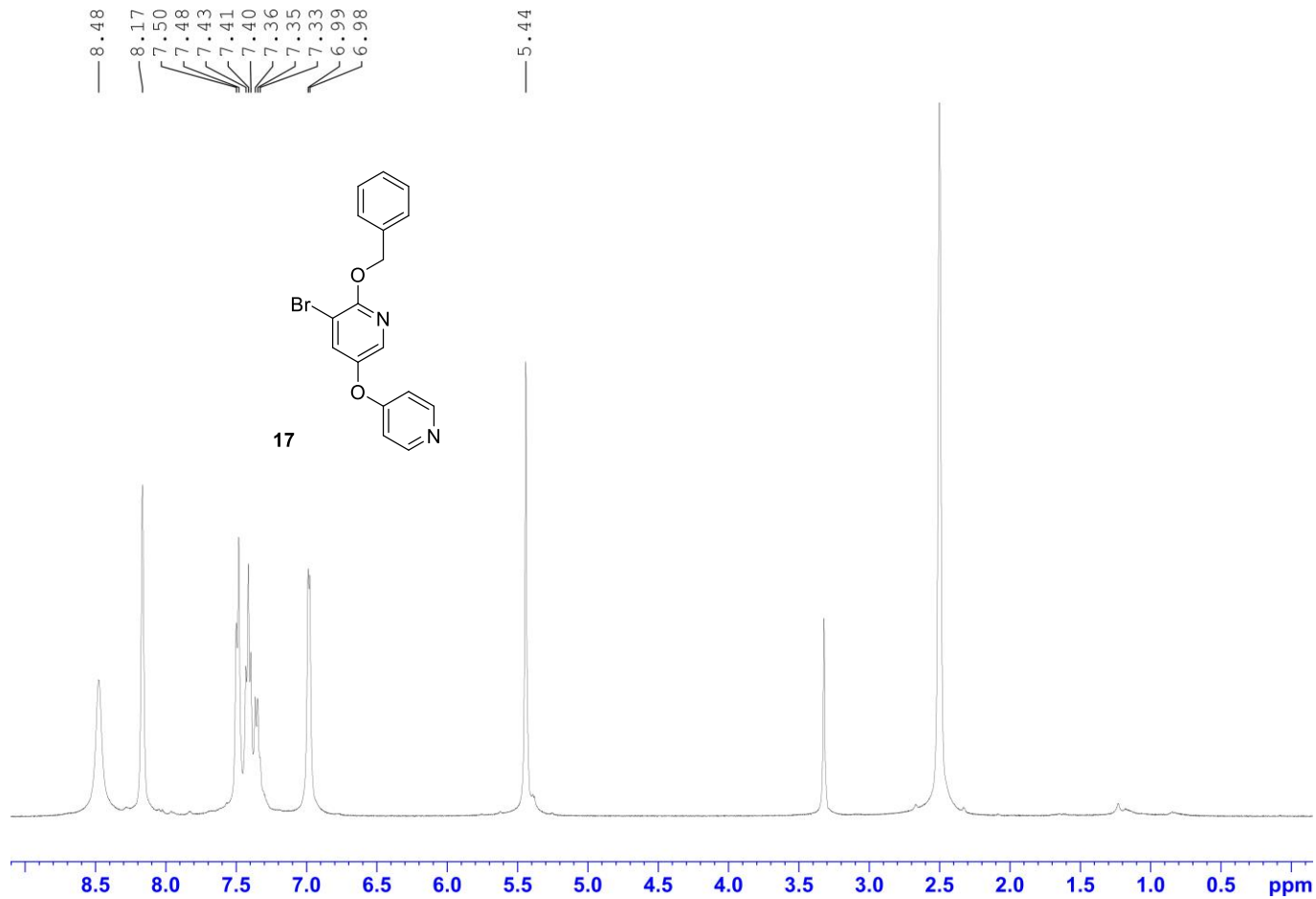


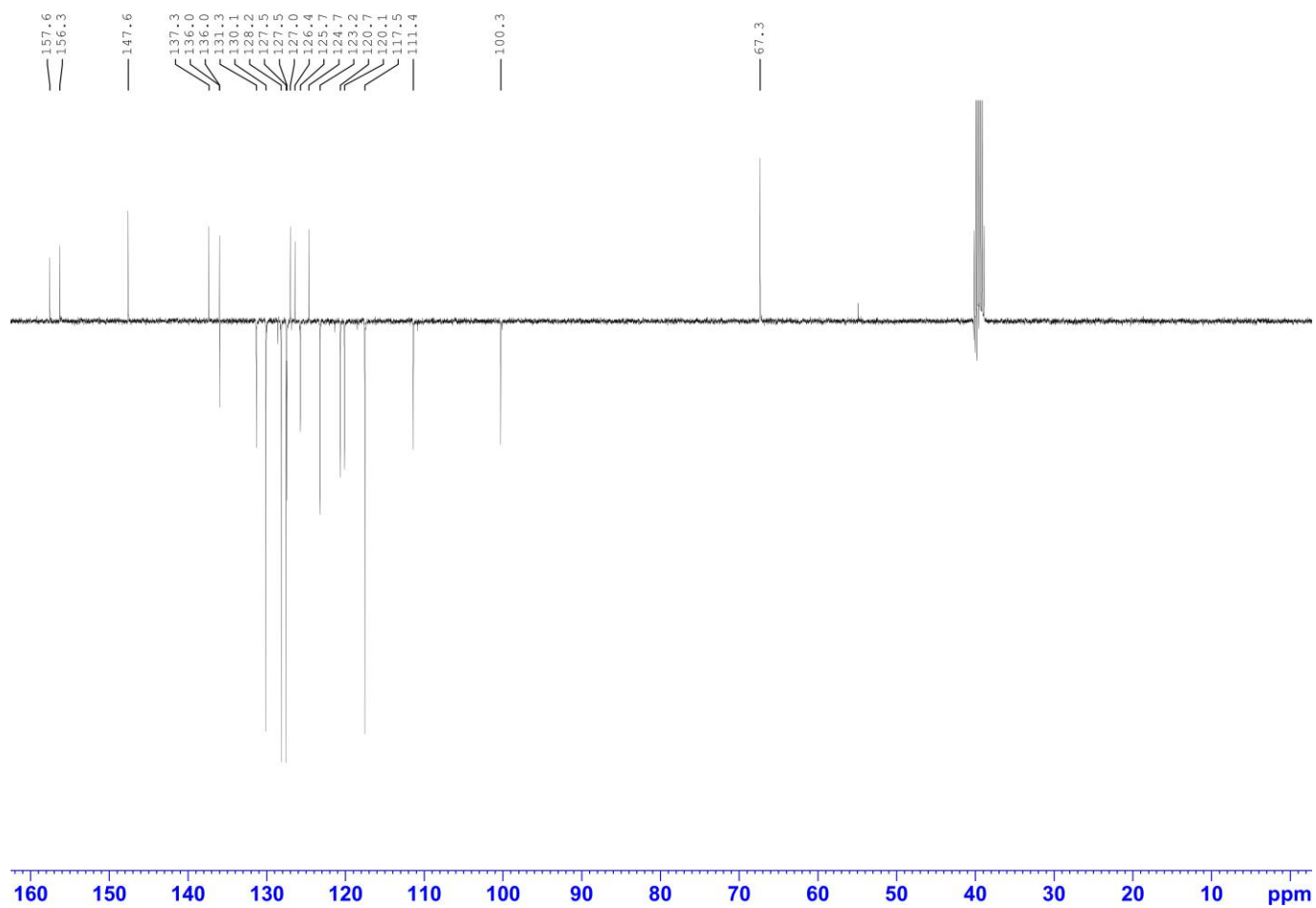
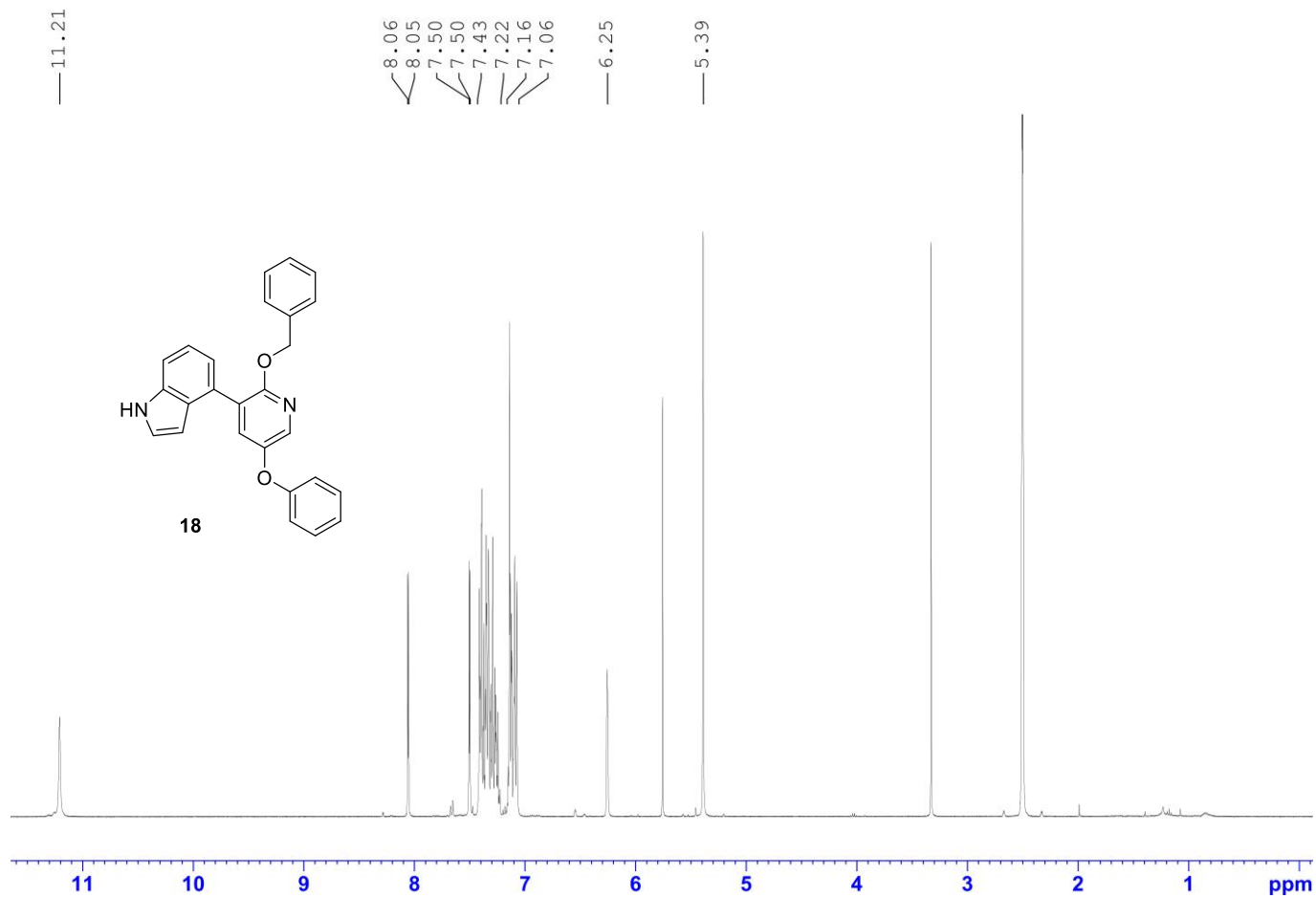


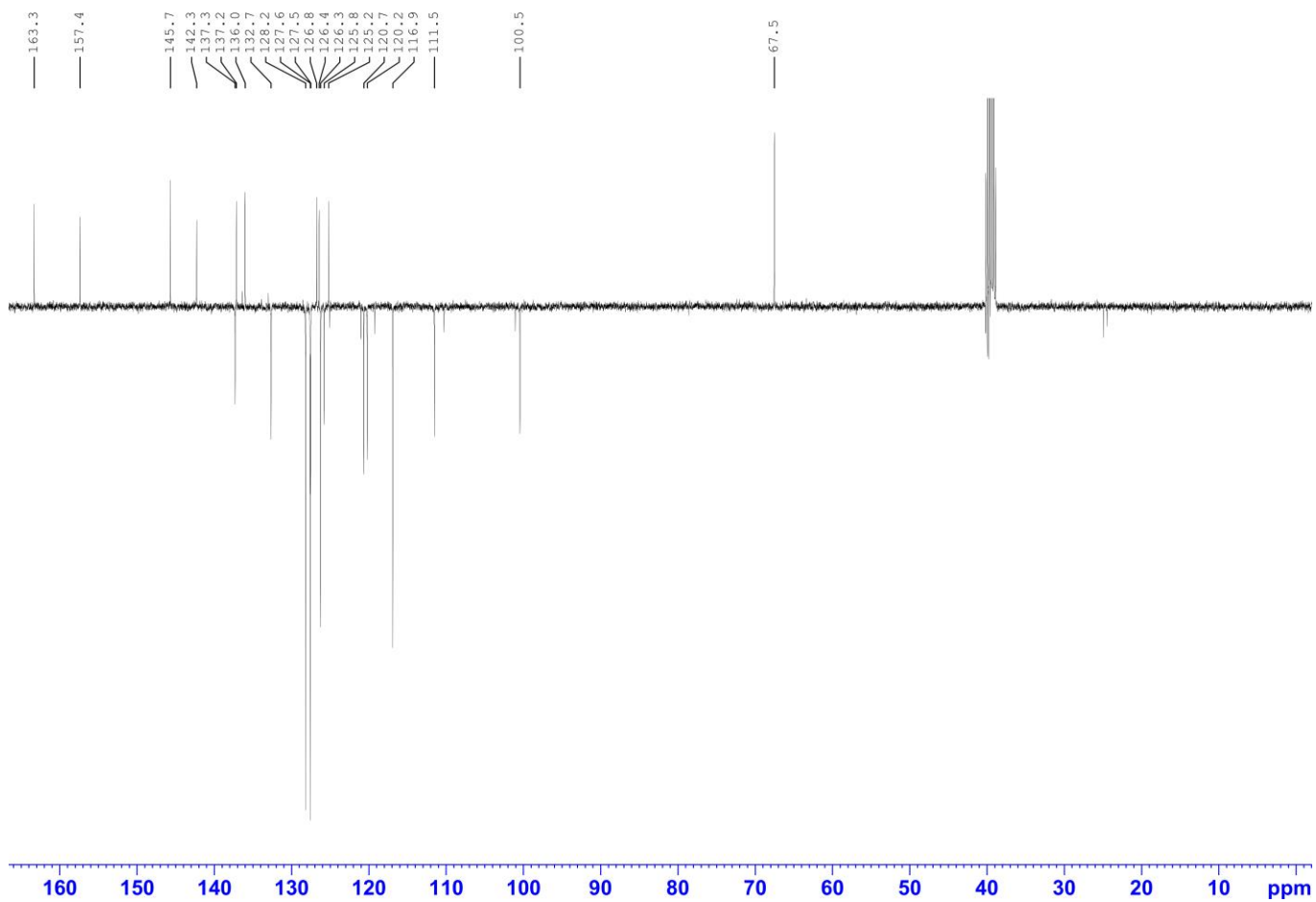
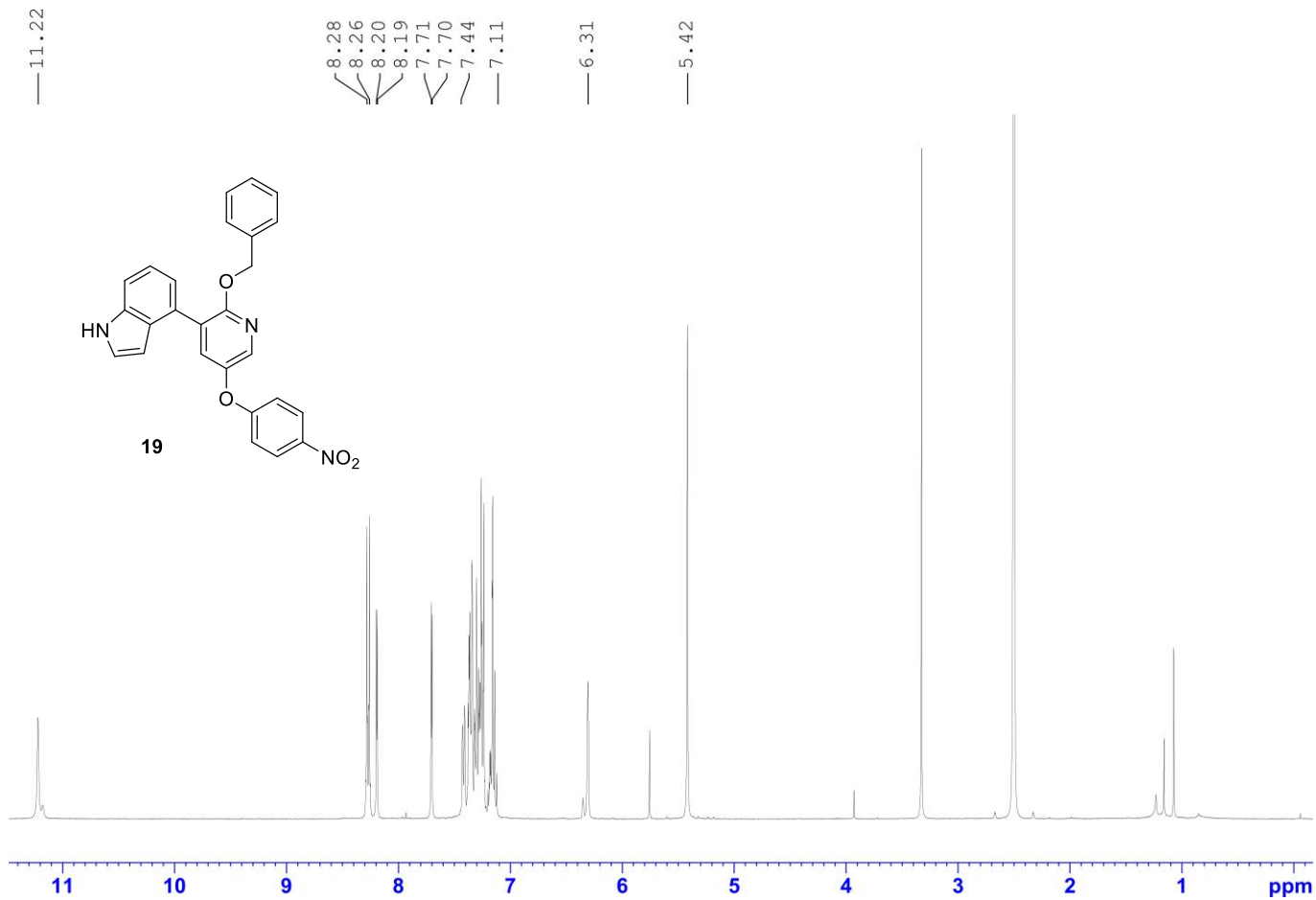




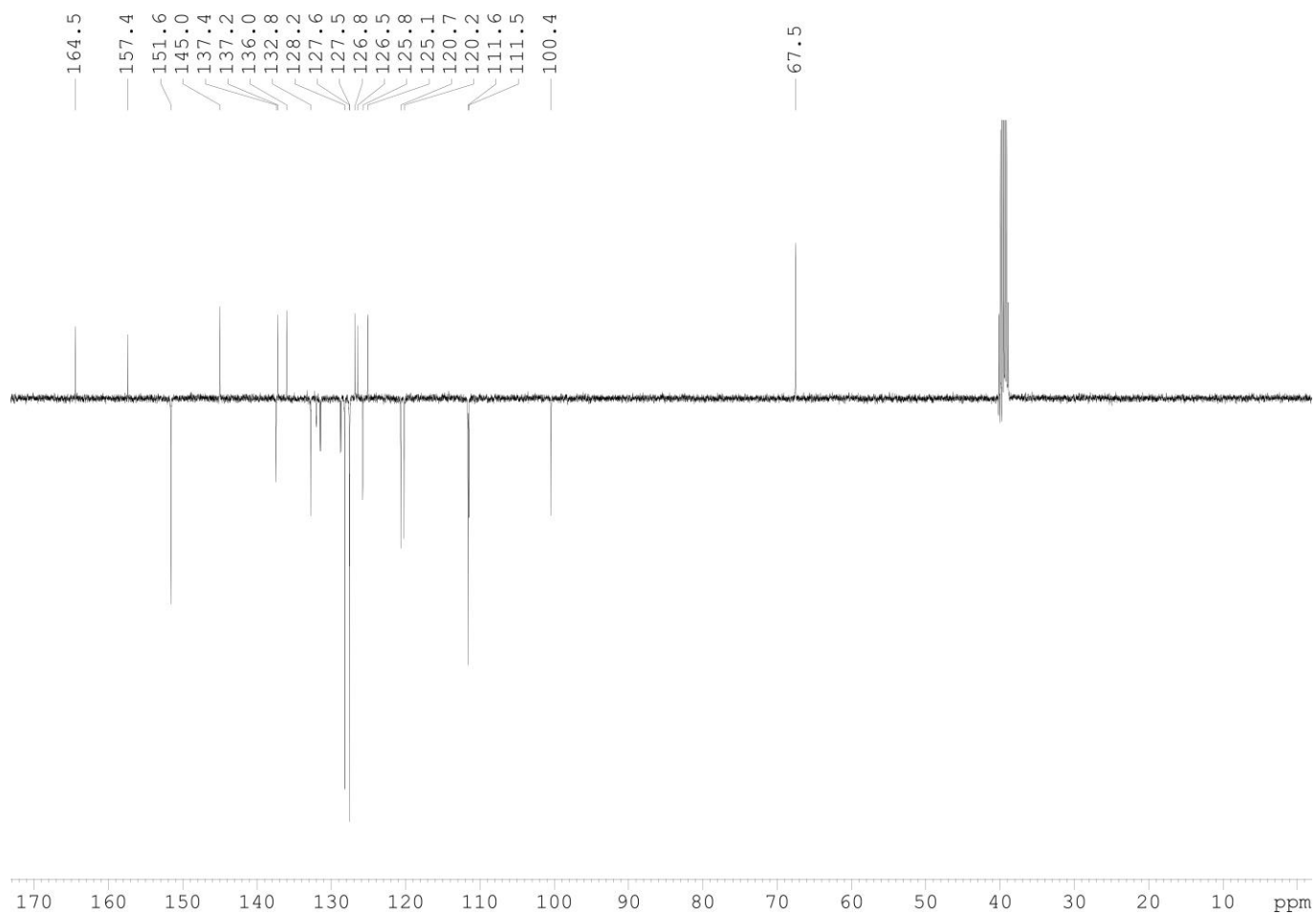
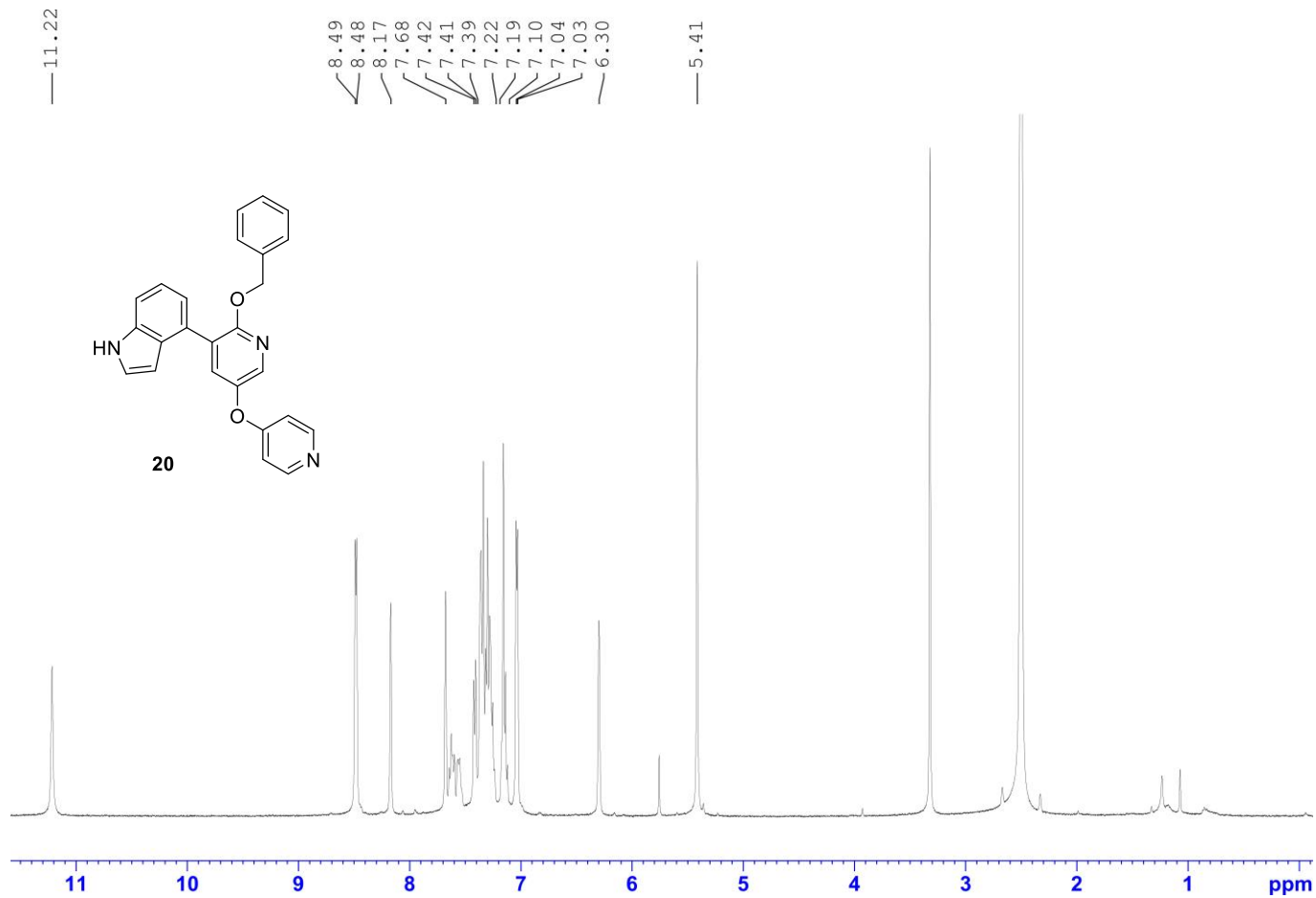


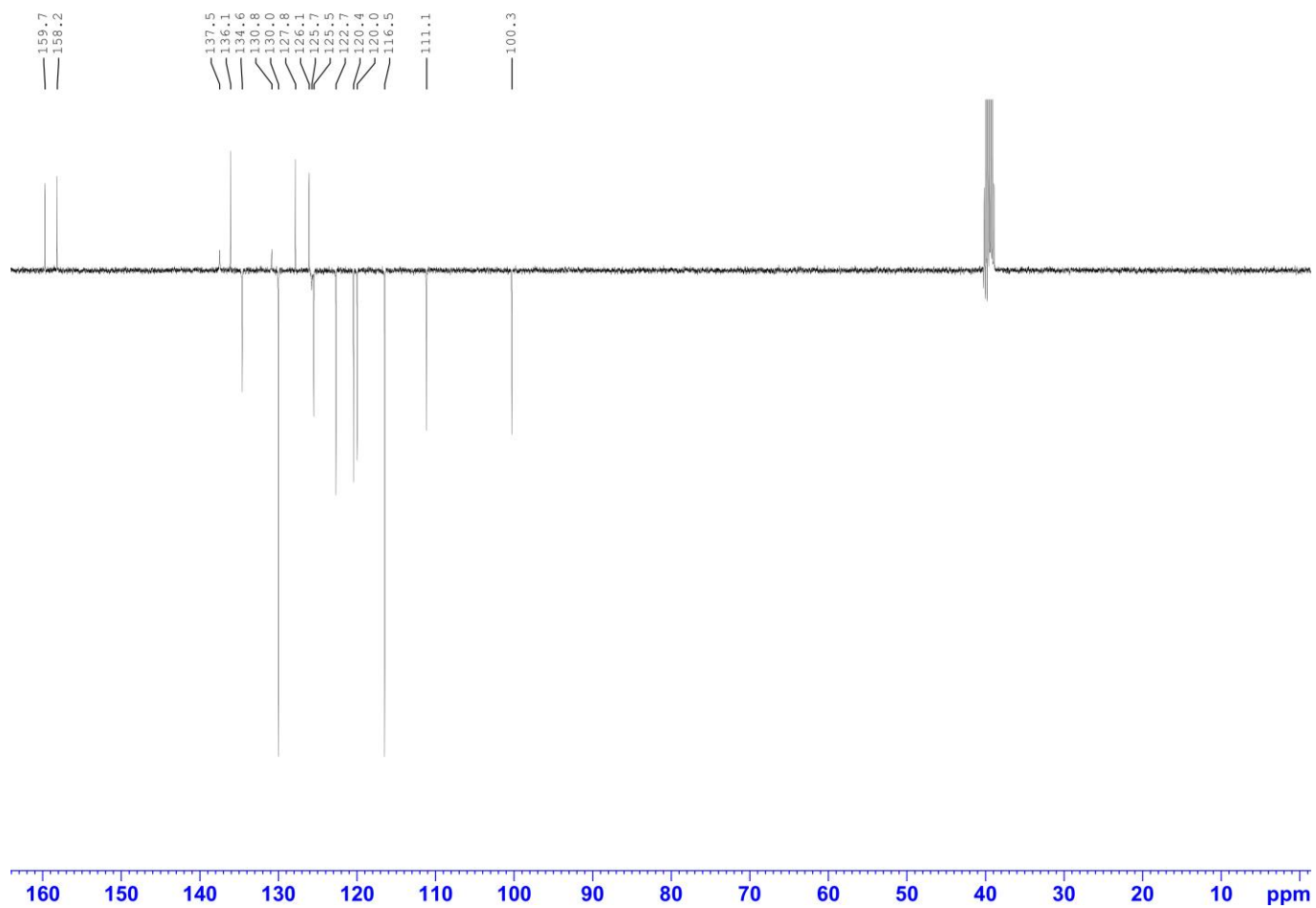
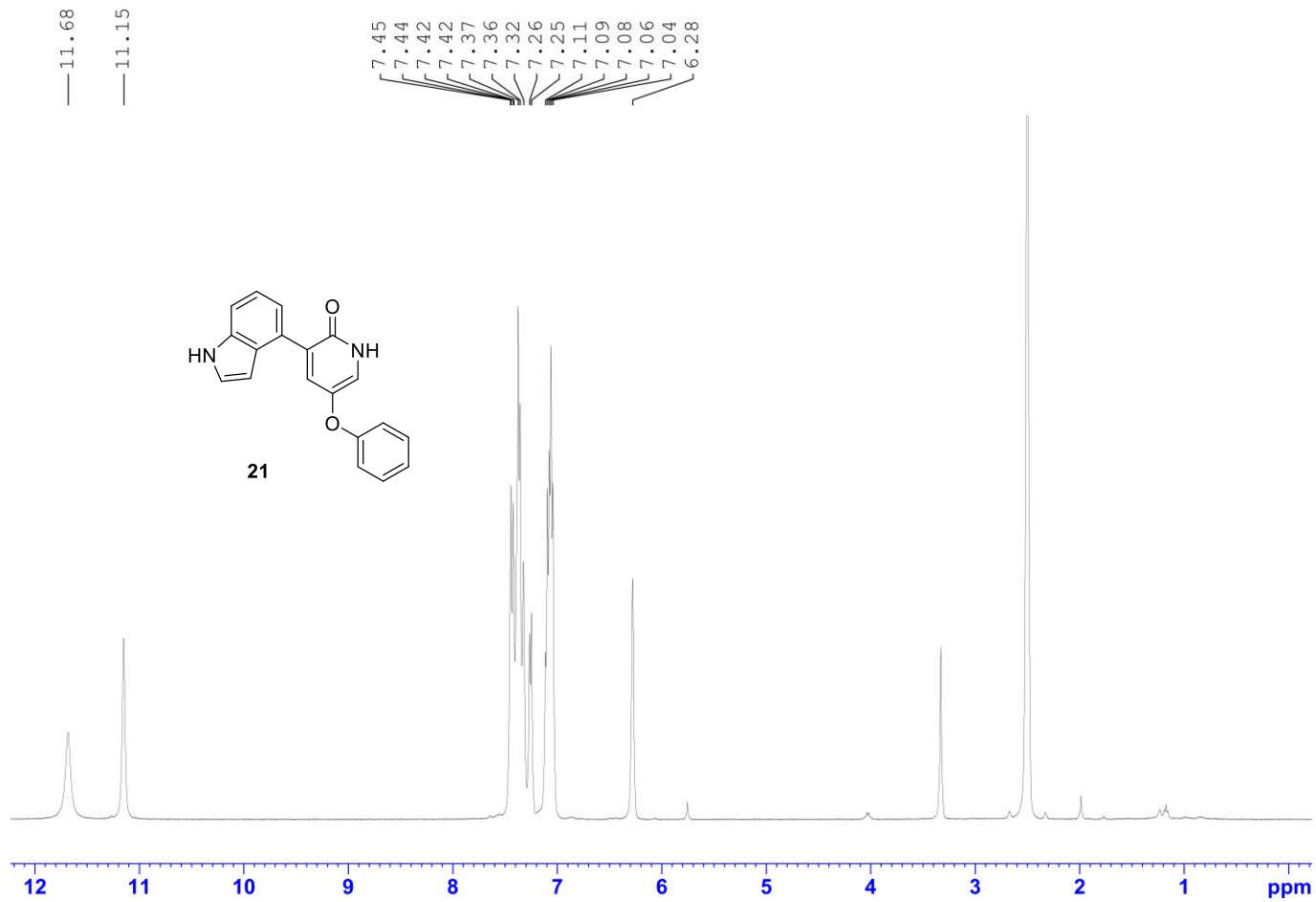


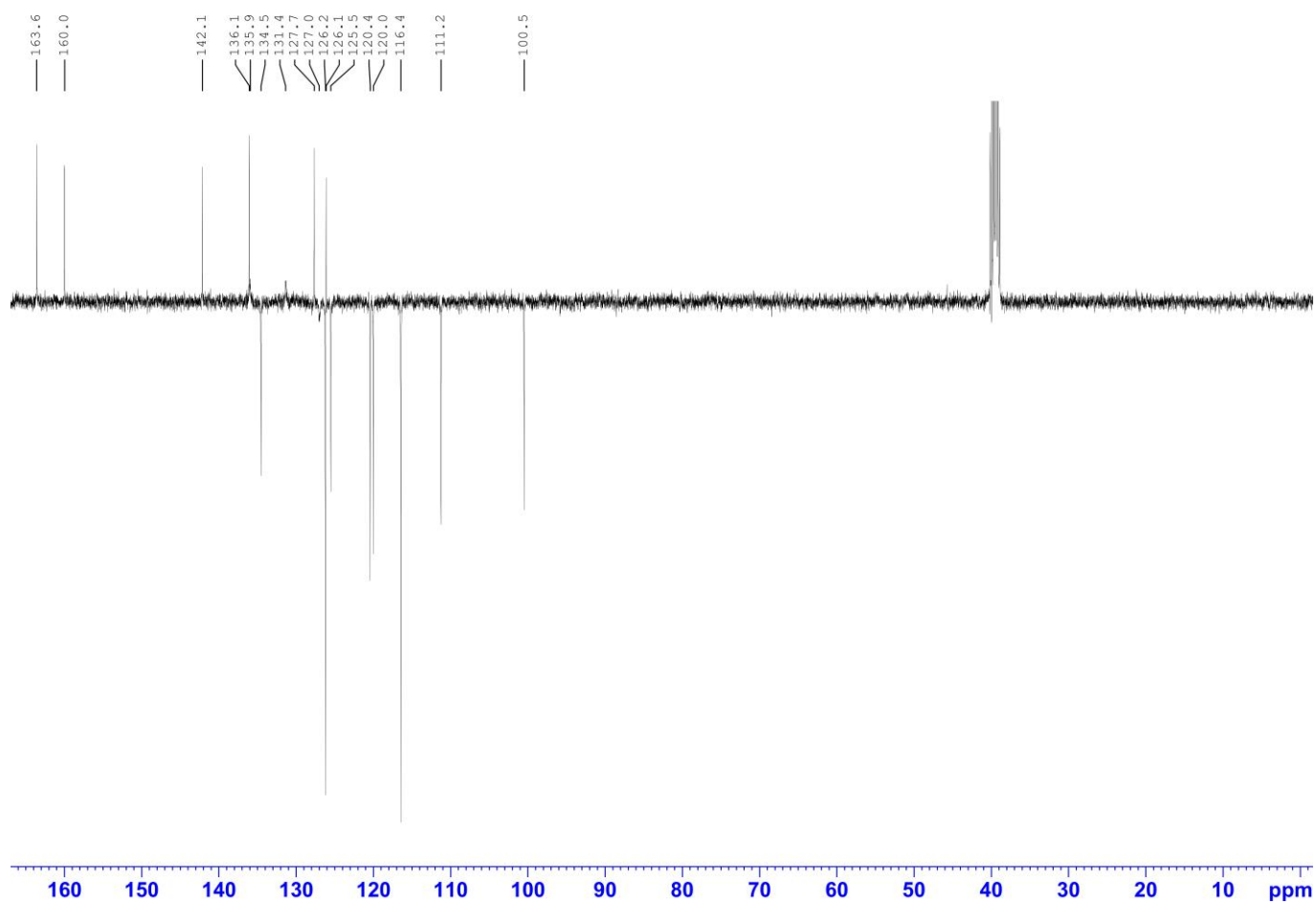
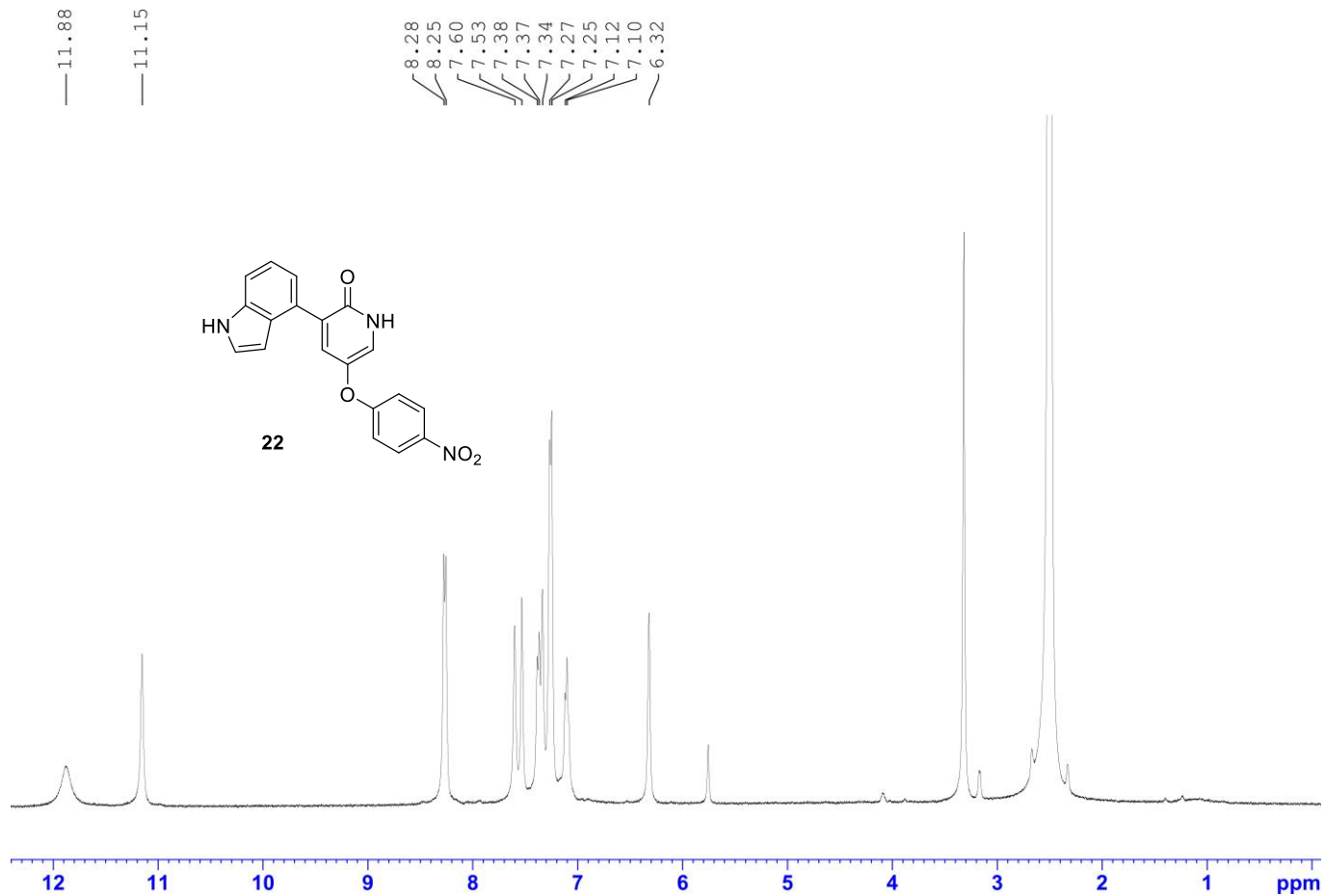








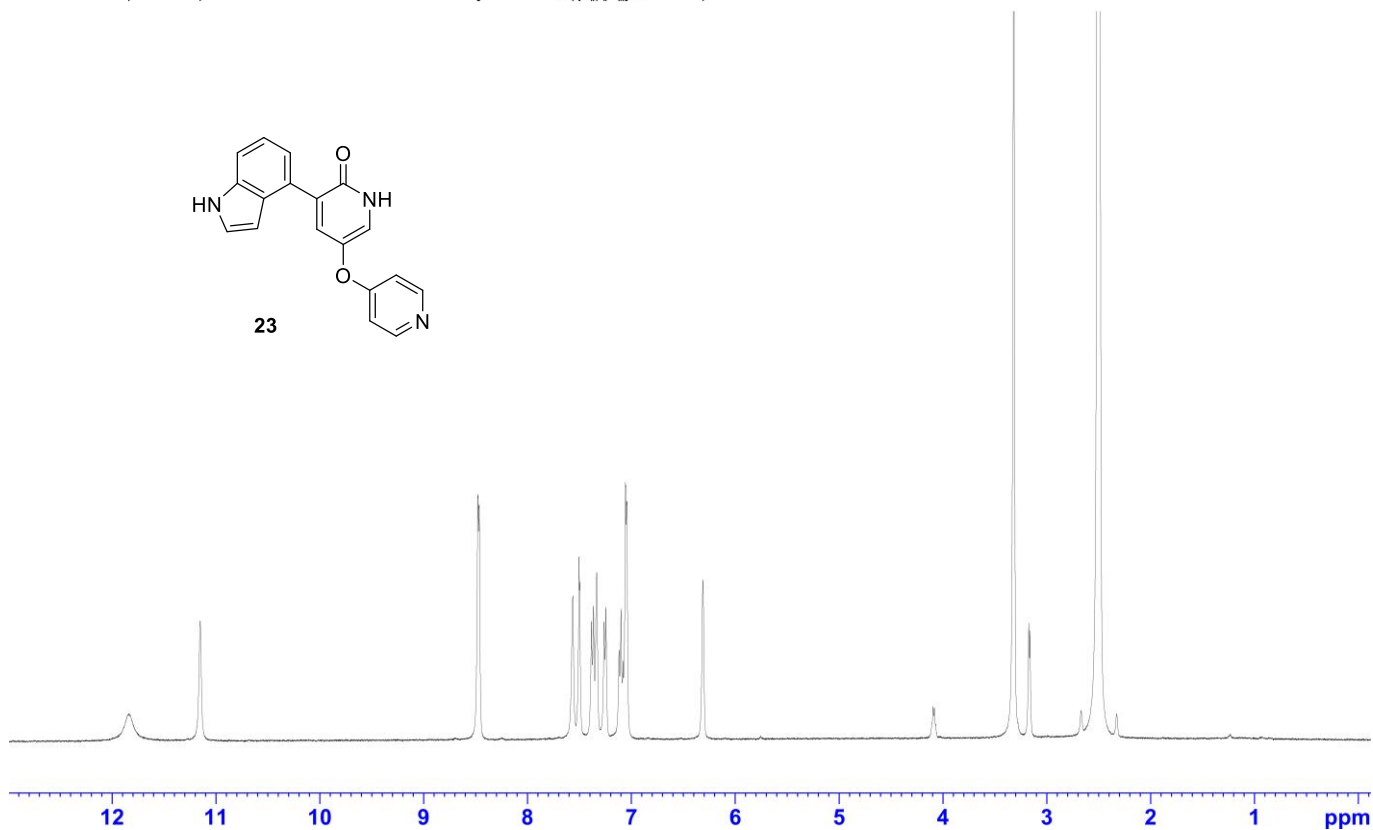
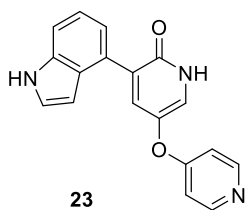




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— 11.15

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7.37  
7.33  
7.26  
7.25  
7.12  
7.10  
7.08  
7.06  
7.05  
7.04  
6.31



— 164.7

— 160.0

— 151.5

136.1

135.3

134.6

131.2

127.7

126.1

125.5

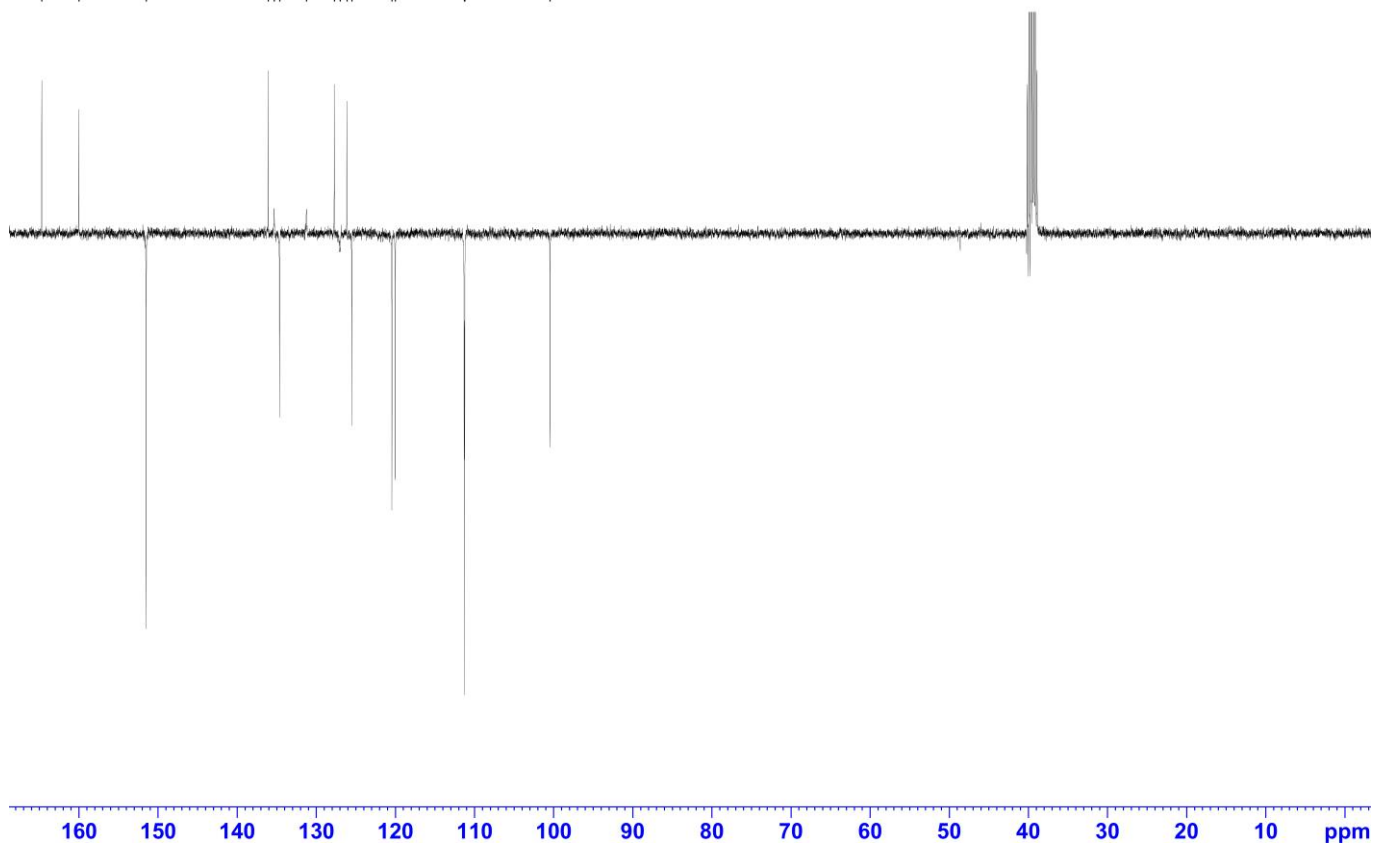
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120.0

111.3

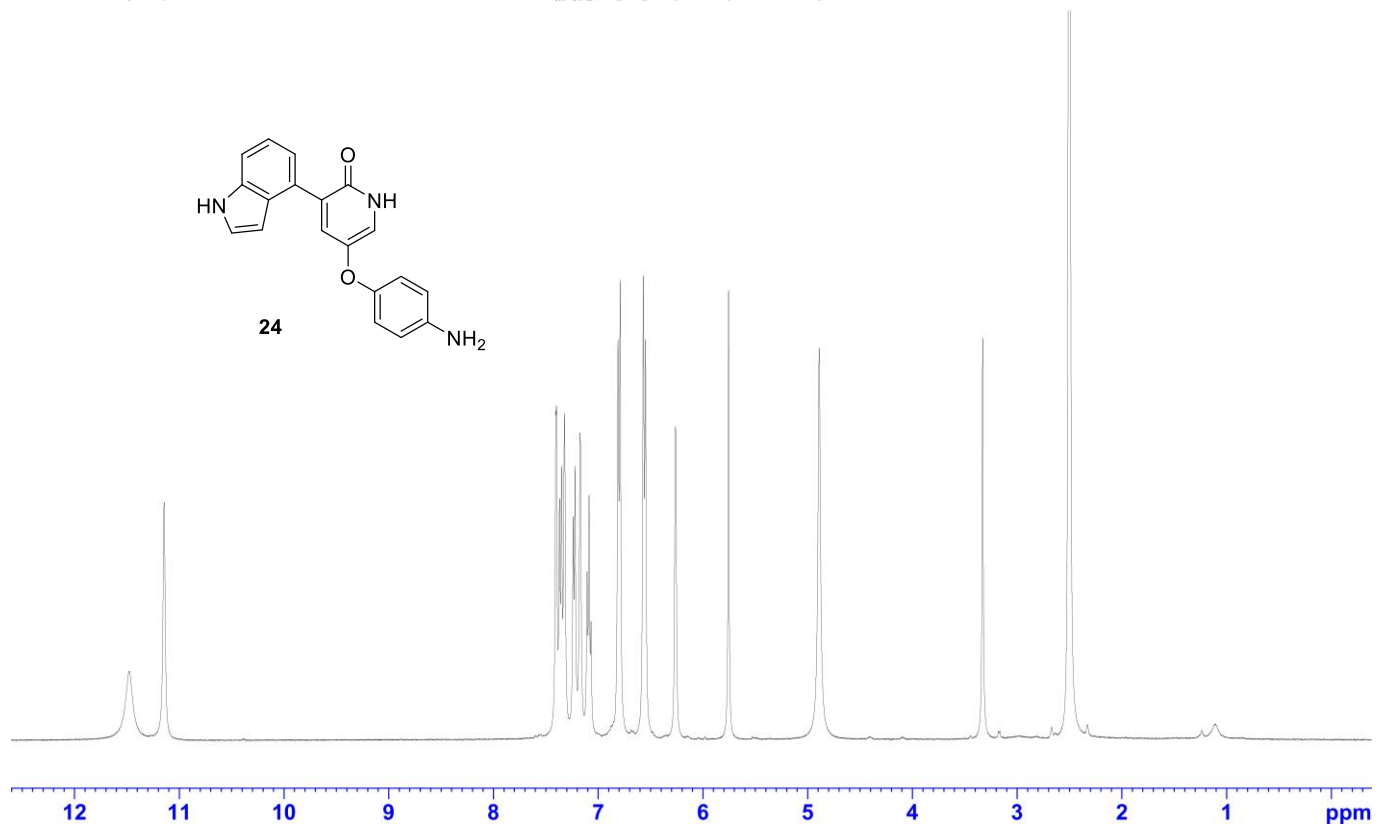
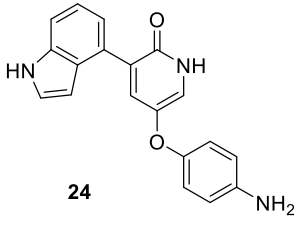
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— 100.4

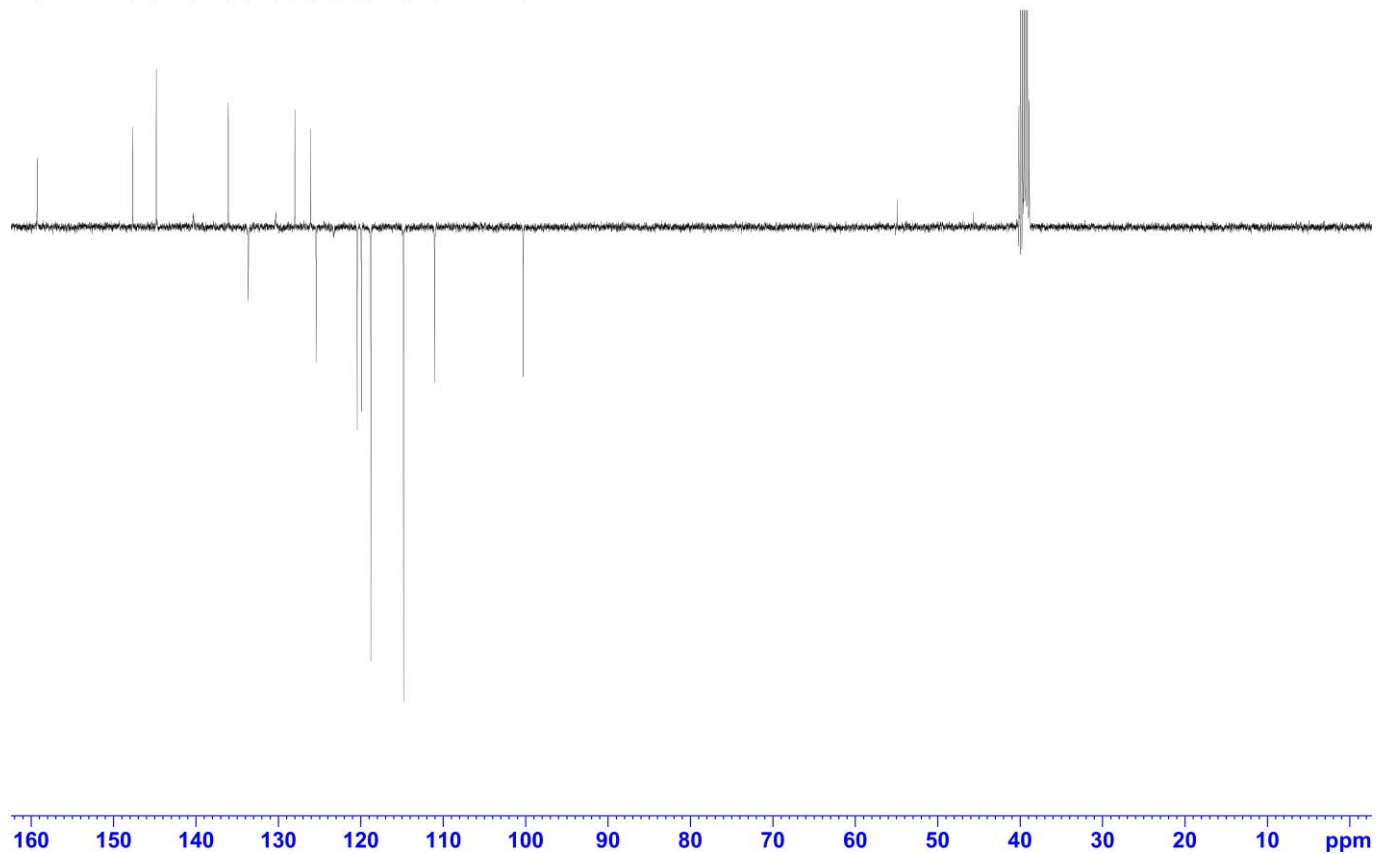


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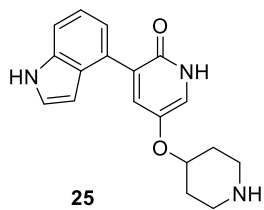
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6.81  
6.79  
6.57  
6.55  
6.26  
5.75  
— 4.89



159.3  
147.7  
144.8  
140.3  
136.1  
133.6  
130.3  
128.0  
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100.3



— 11.13

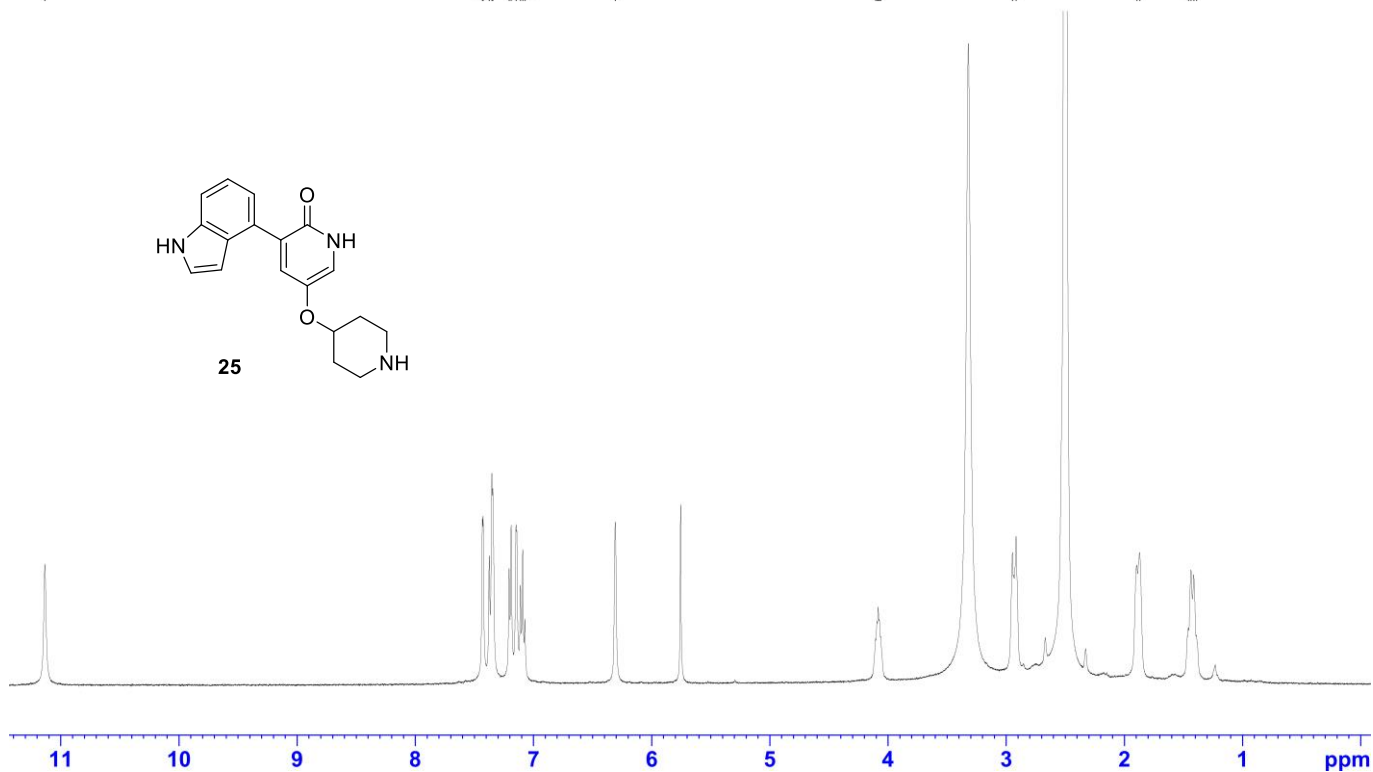


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7.21  
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7.11  
7.09  
7.07  
6.31

4.10  
4.09  
4.08  
4.07  
4.06

2.95  
2.92

1.90  
1.87  
1.46  
1.44  
1.41  
1.39



— 159.0

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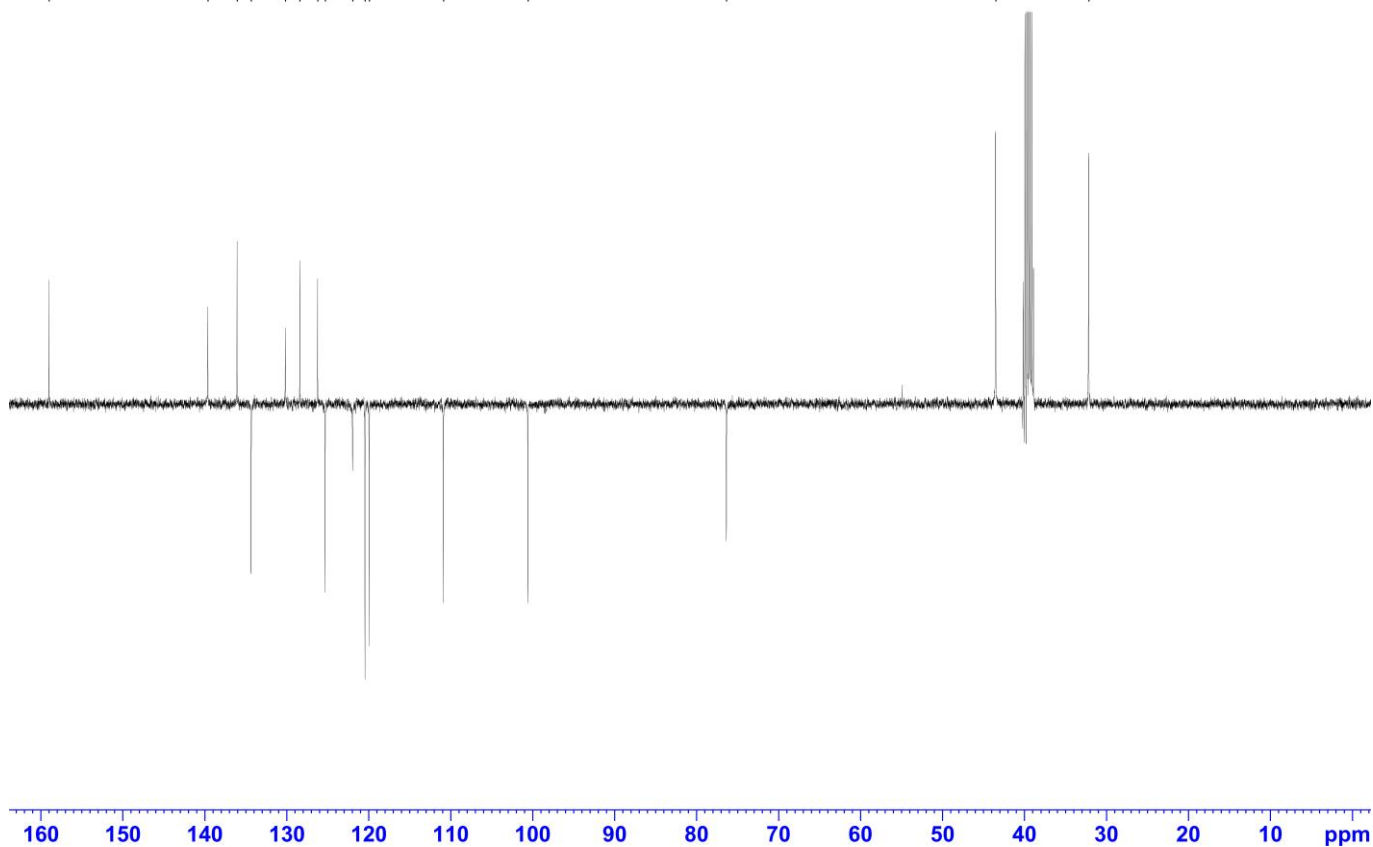
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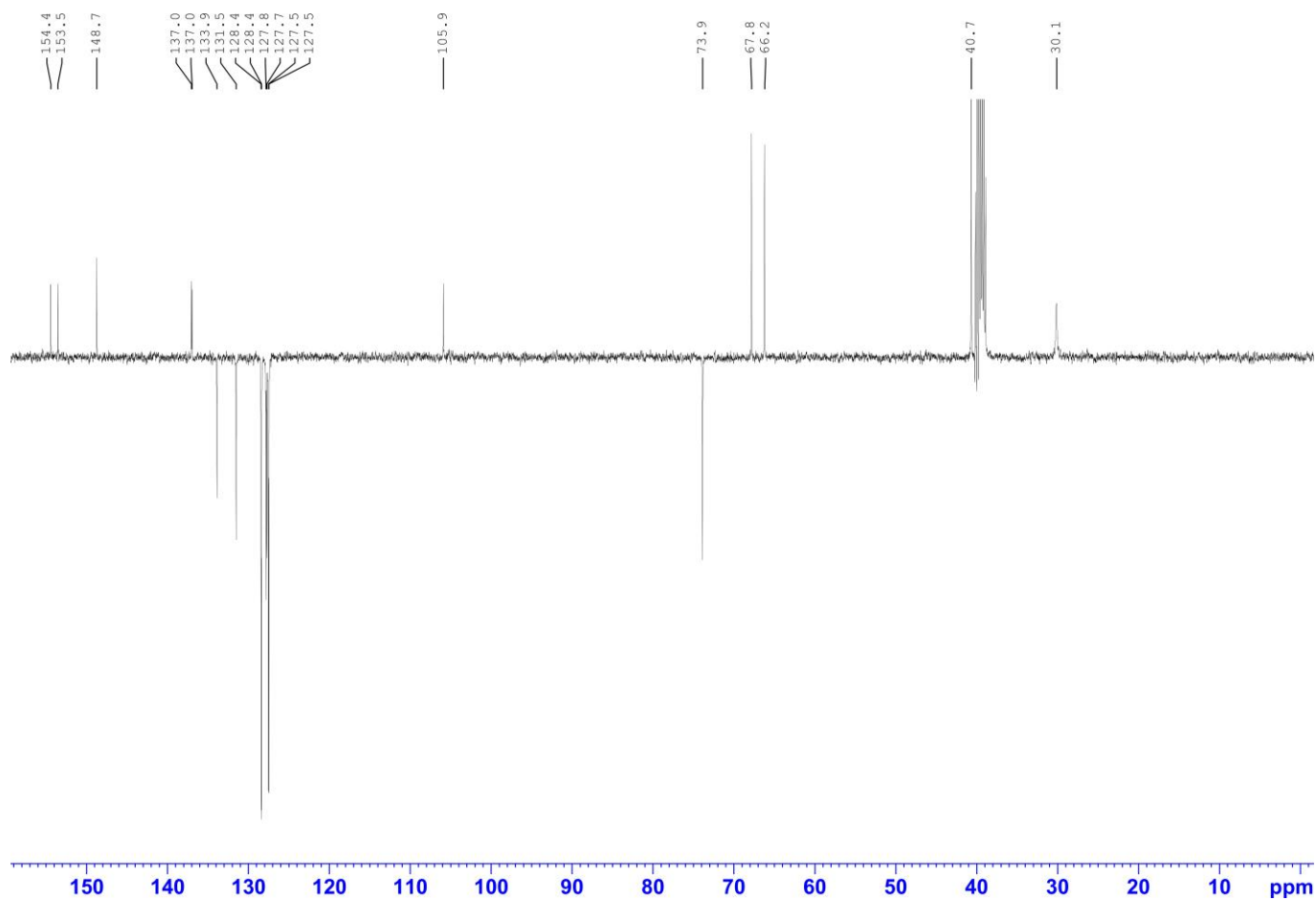
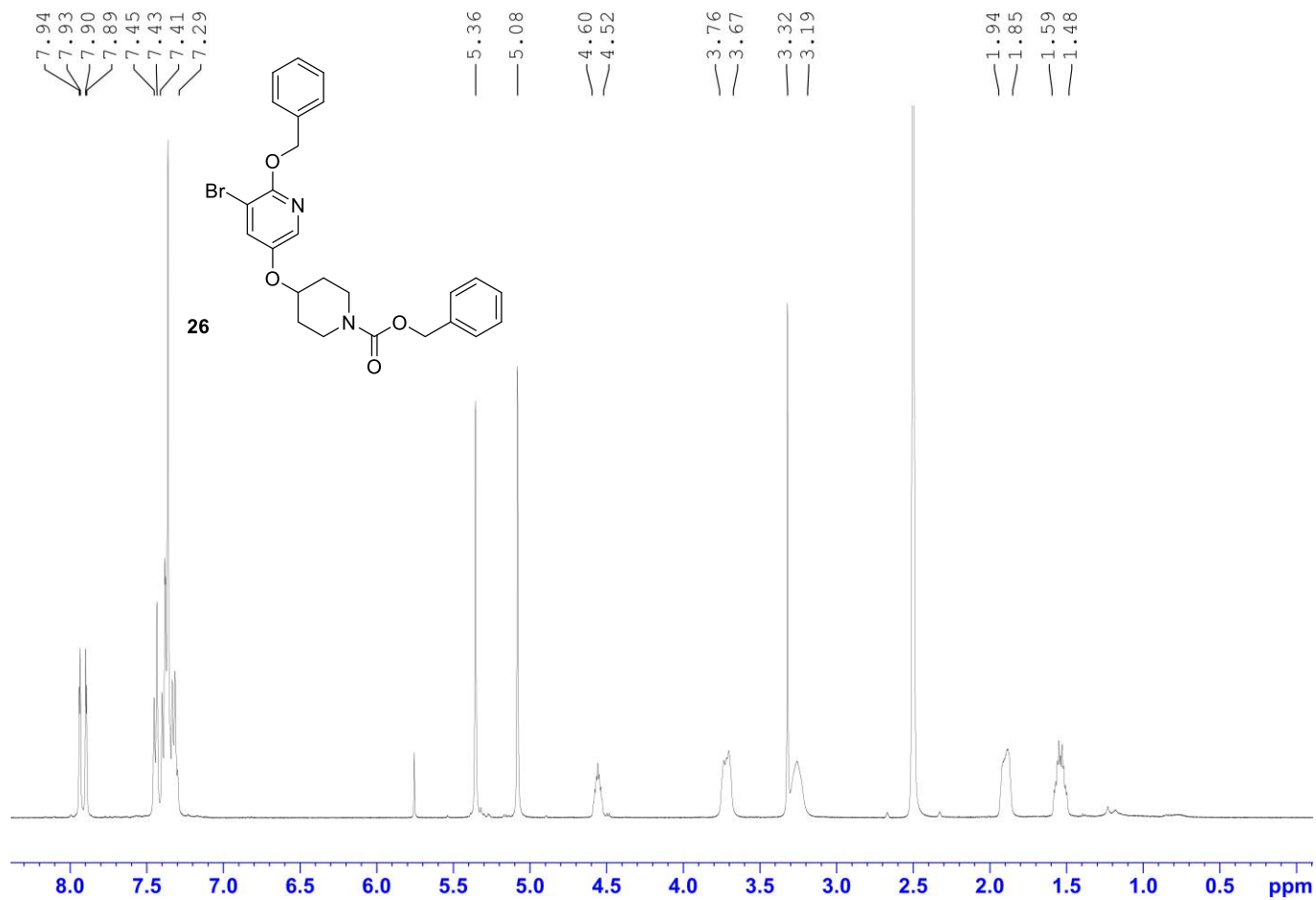
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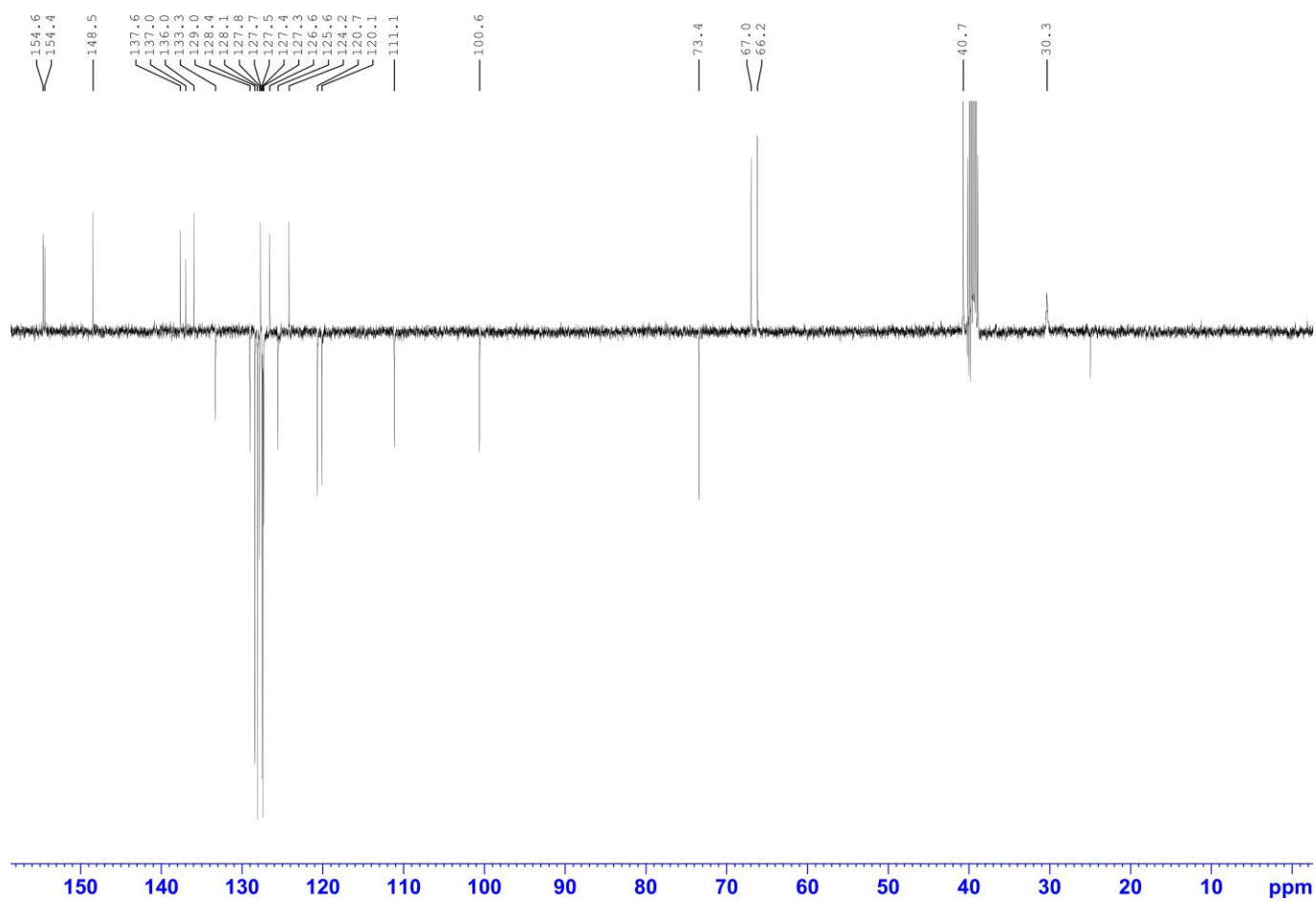
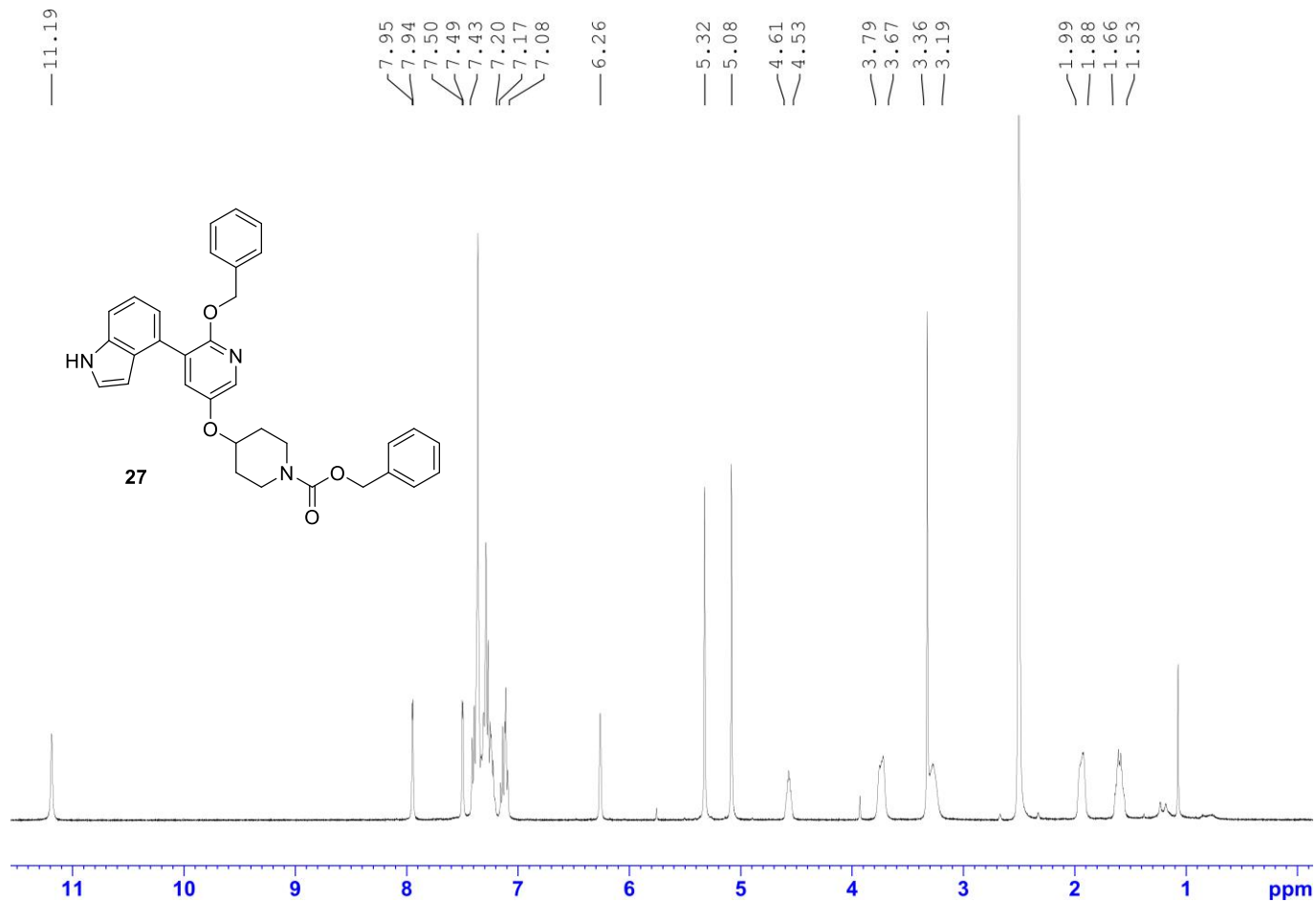
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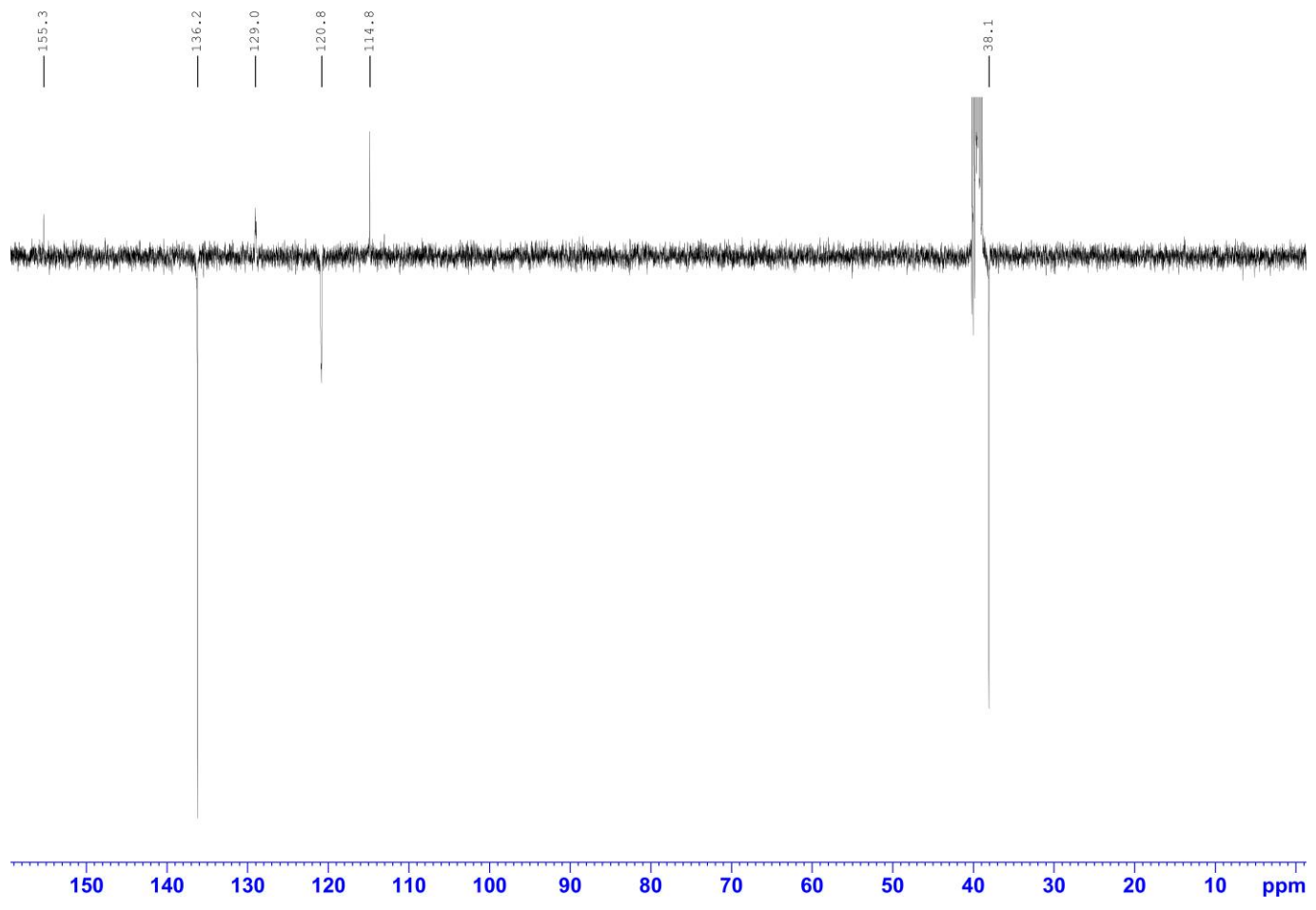
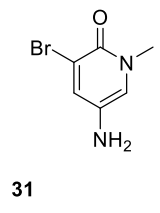
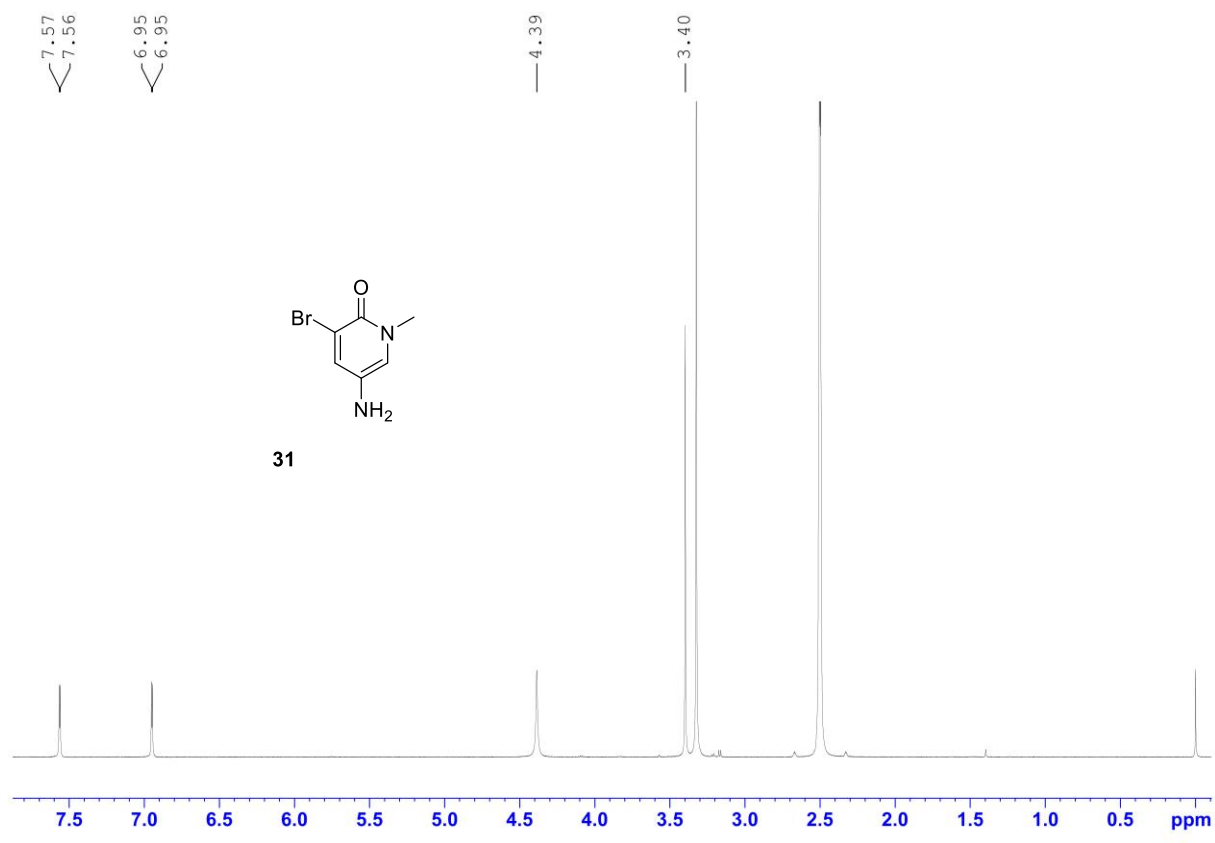
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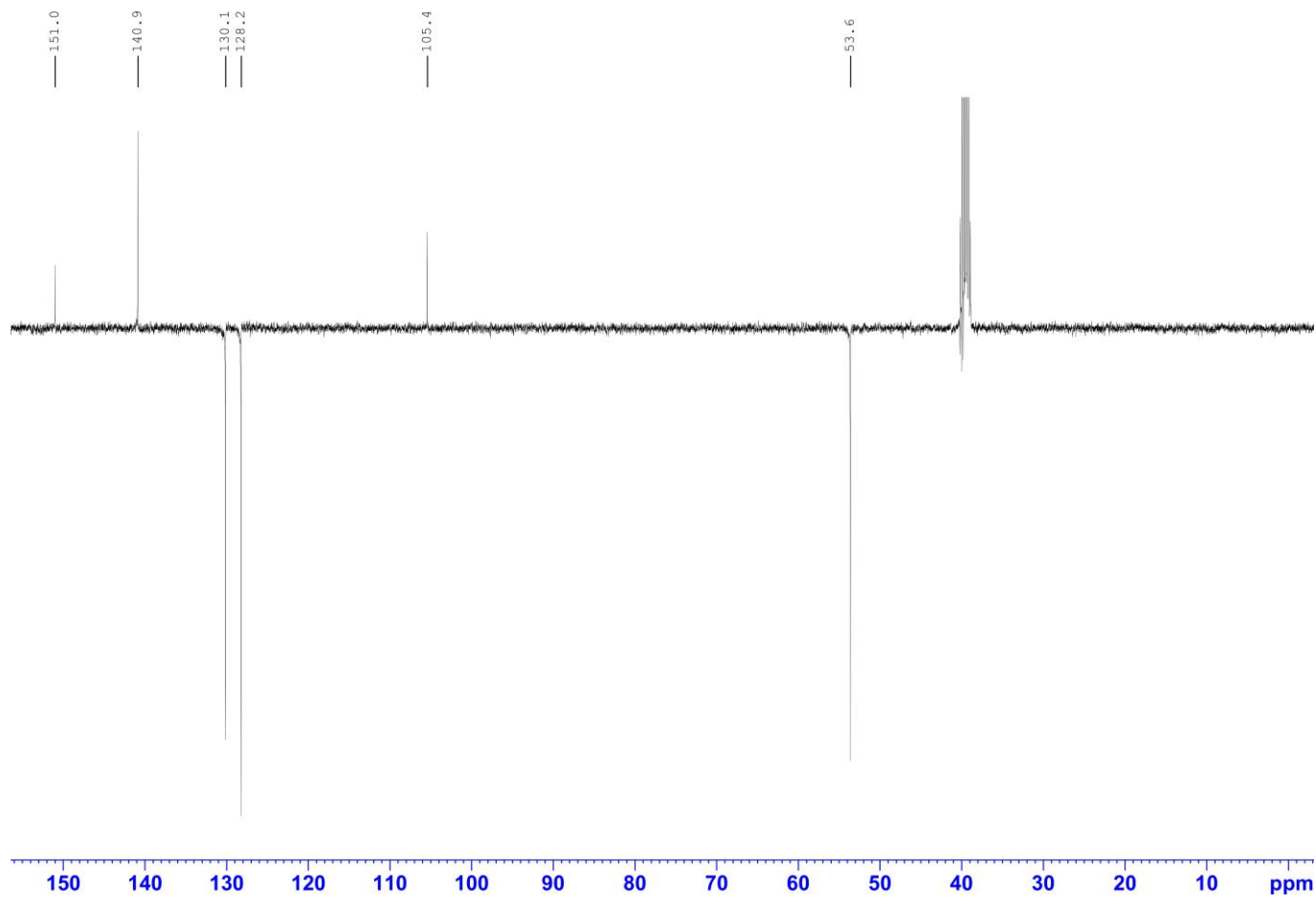
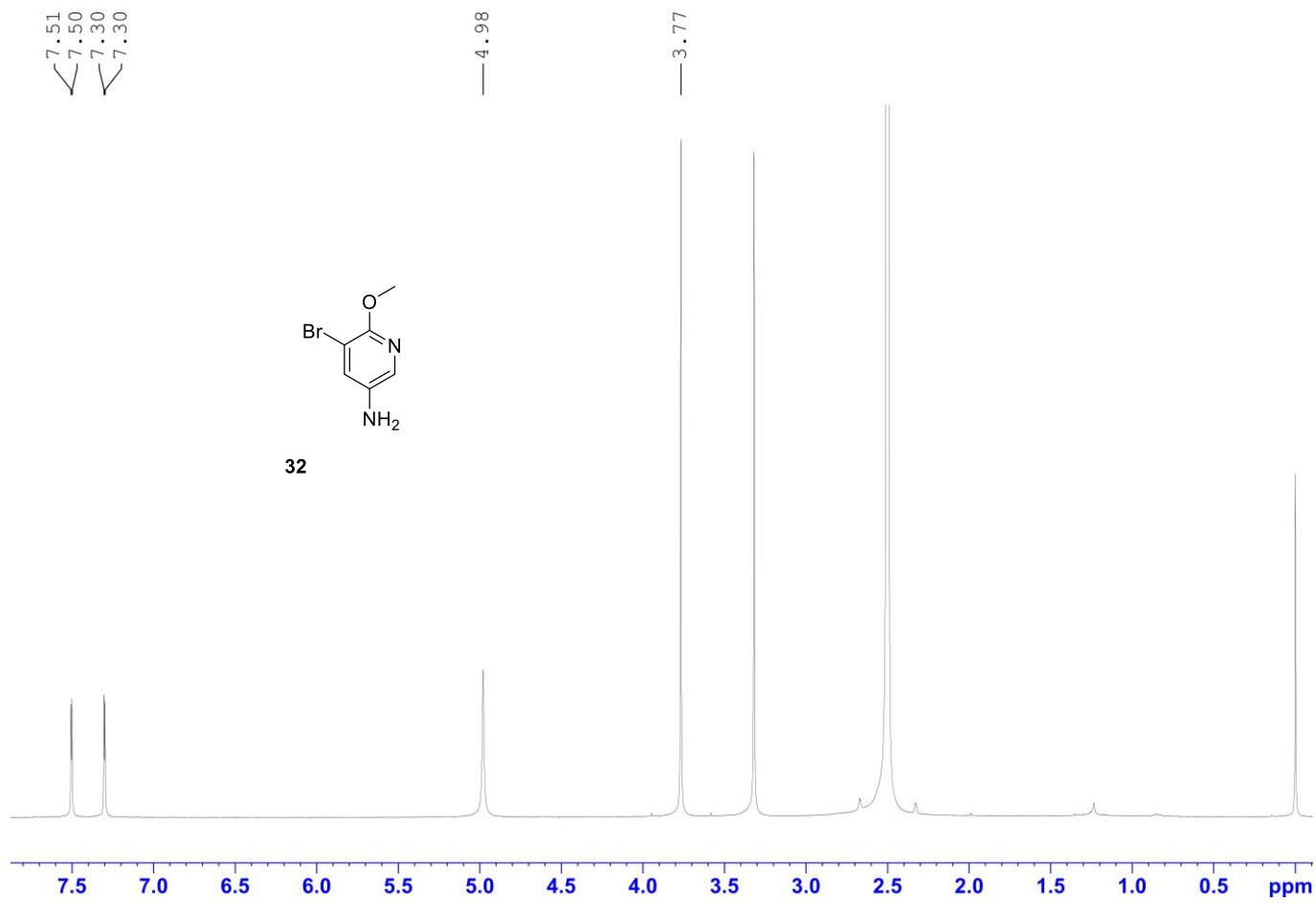


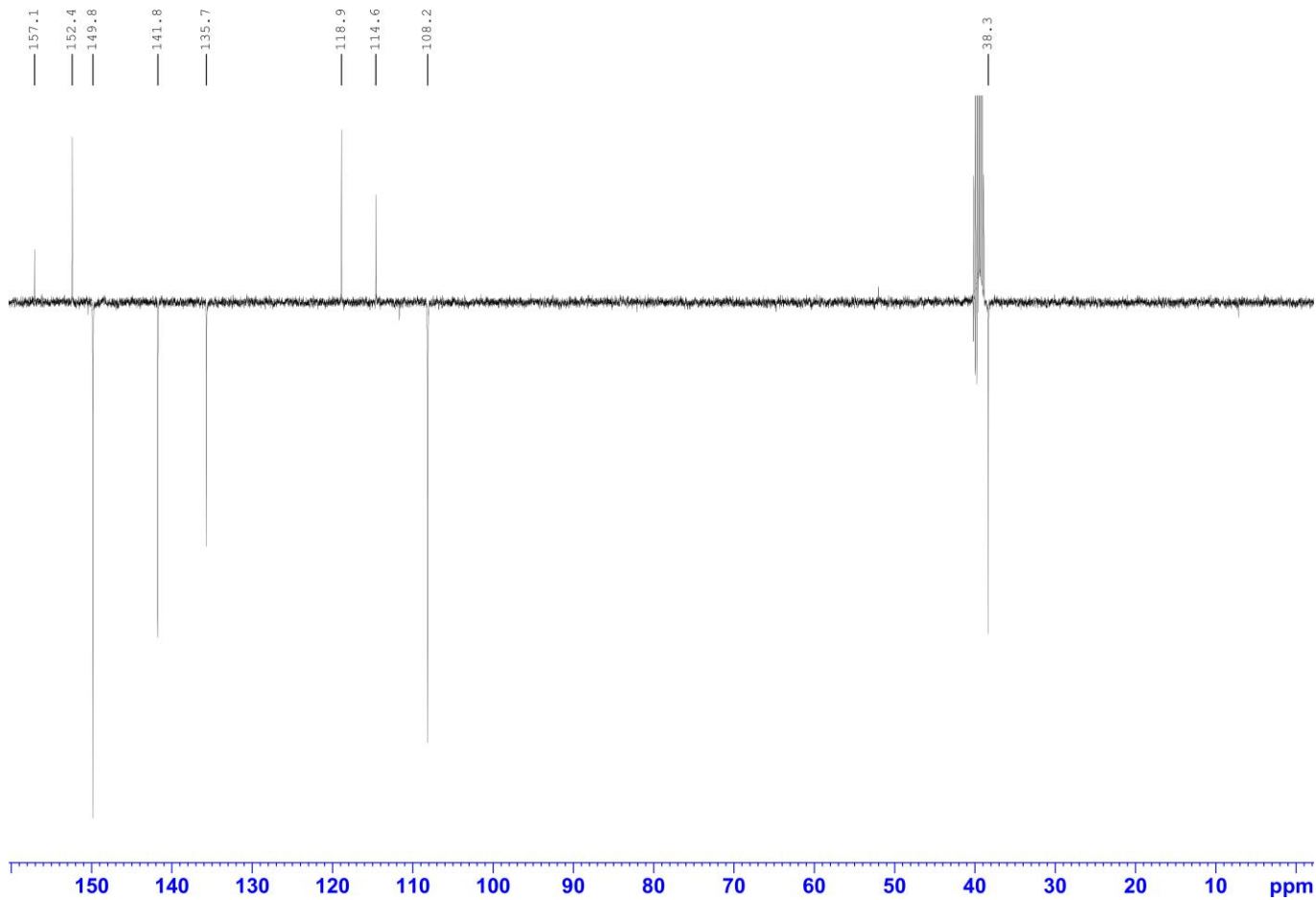
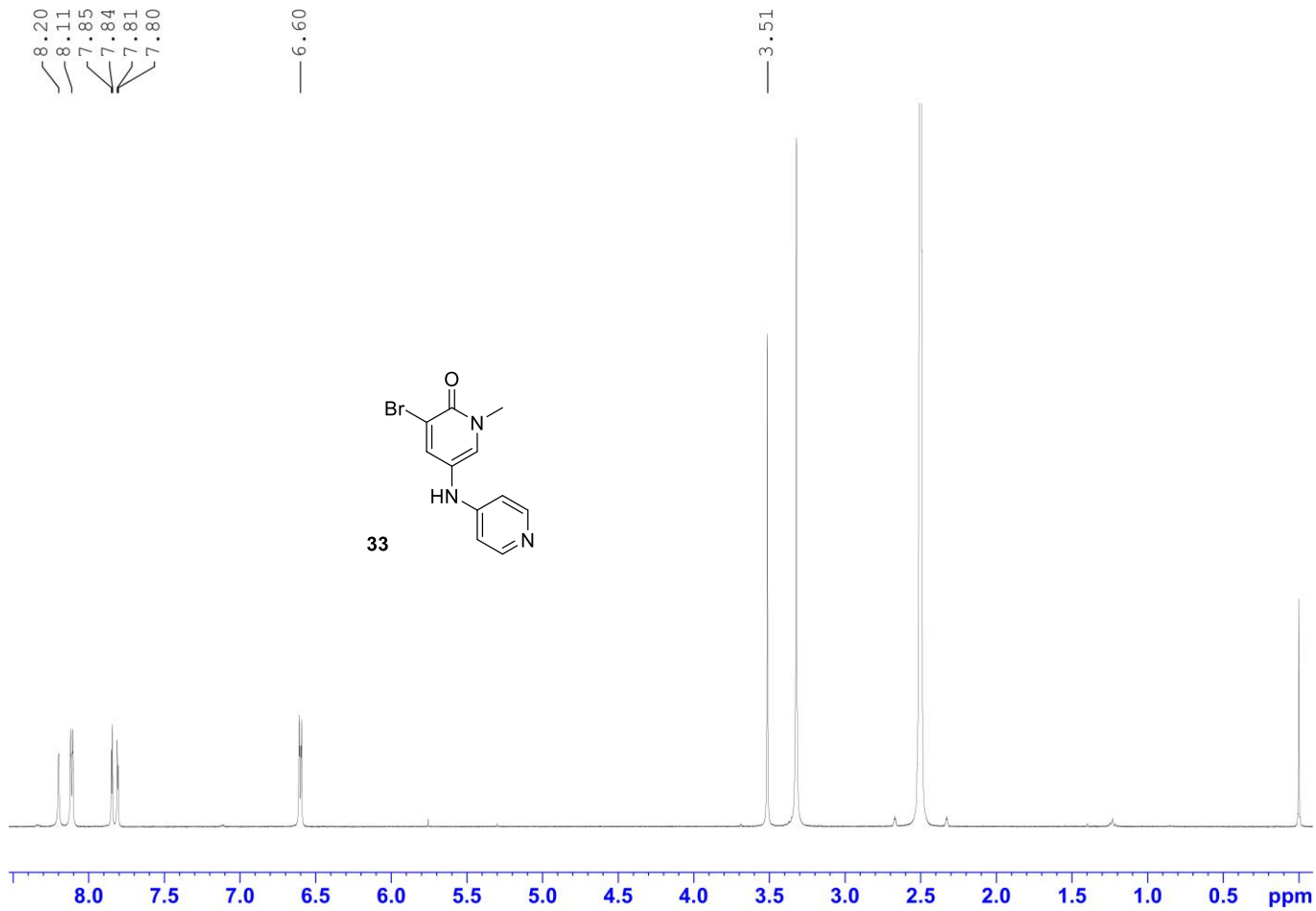


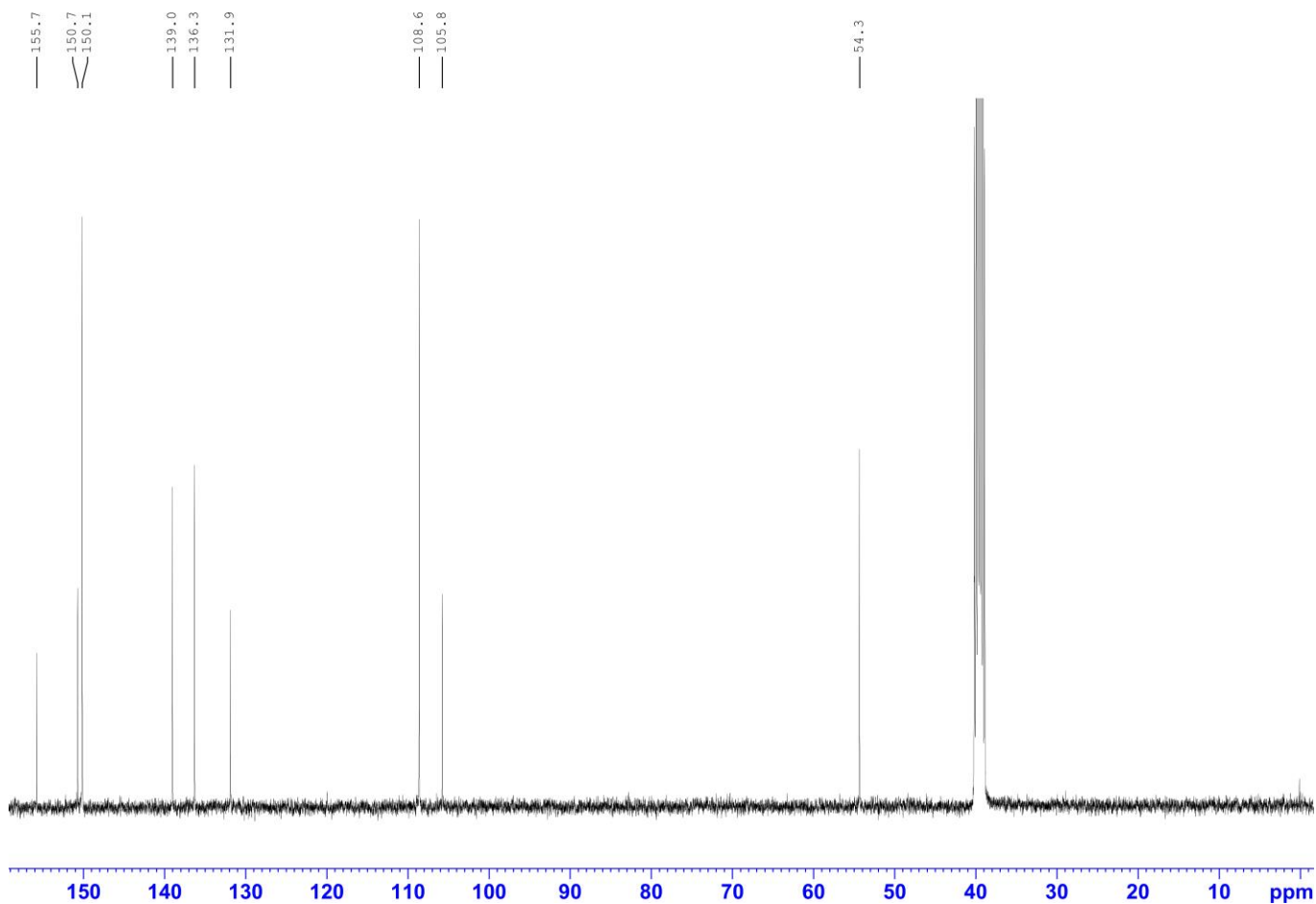
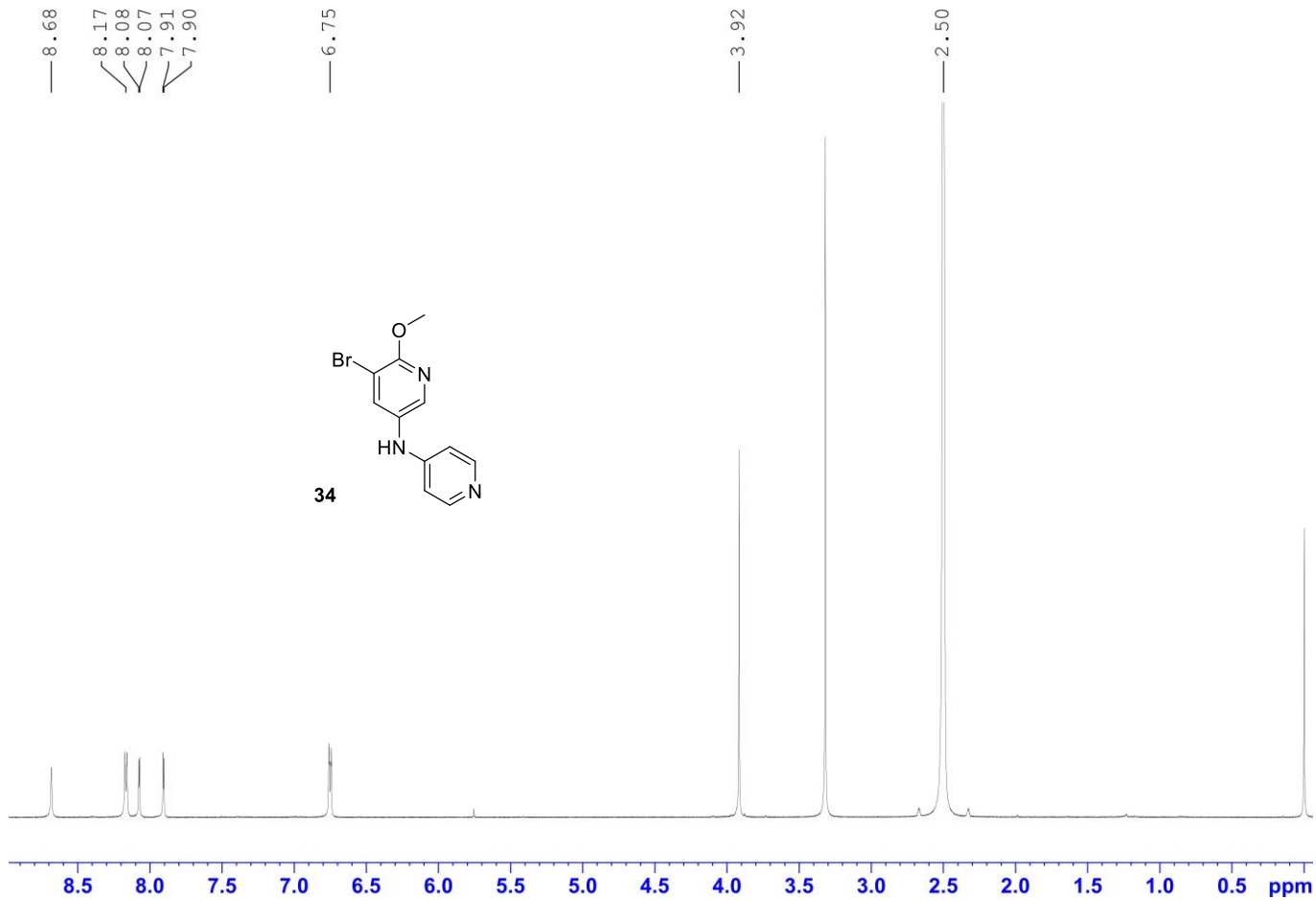


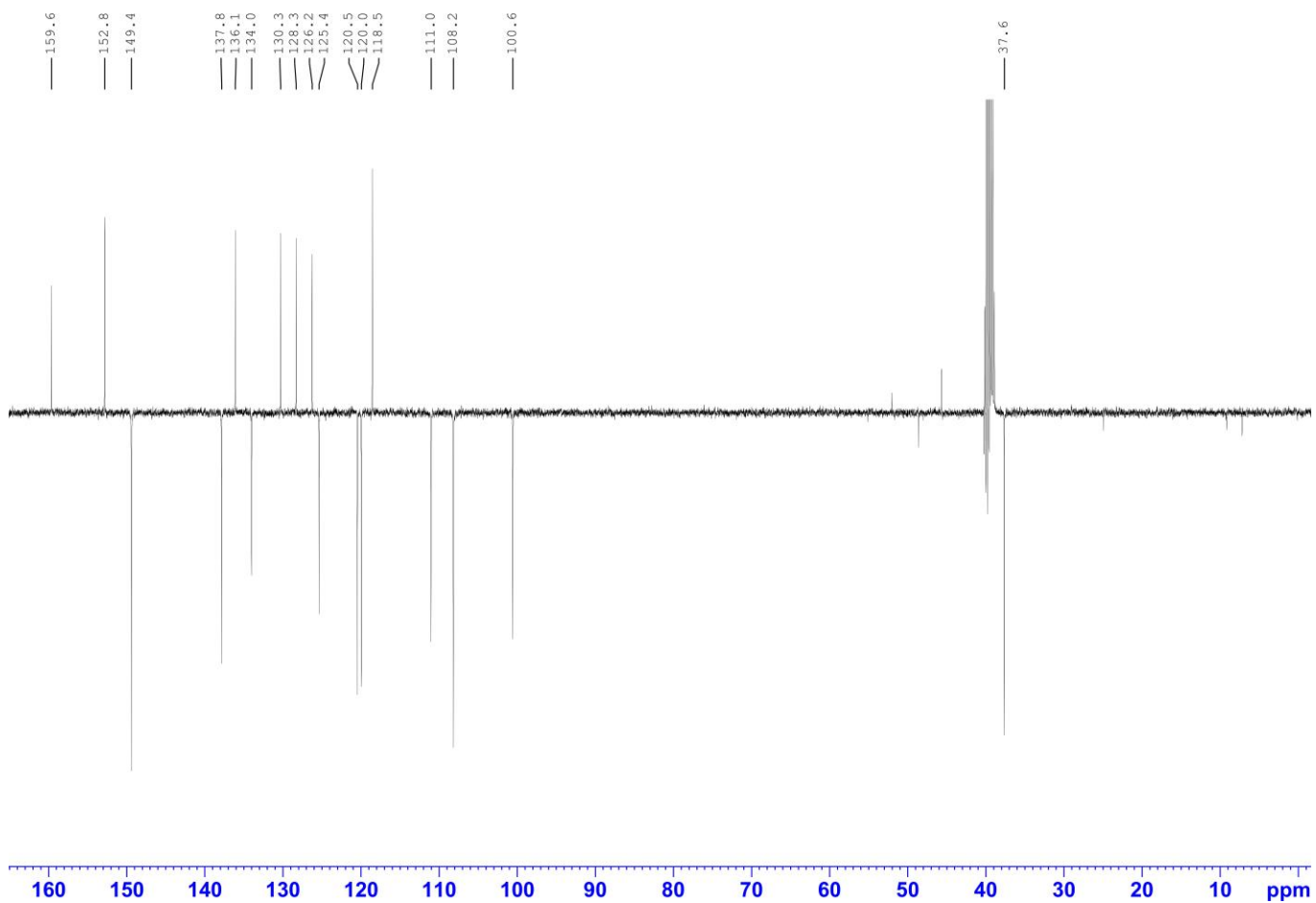
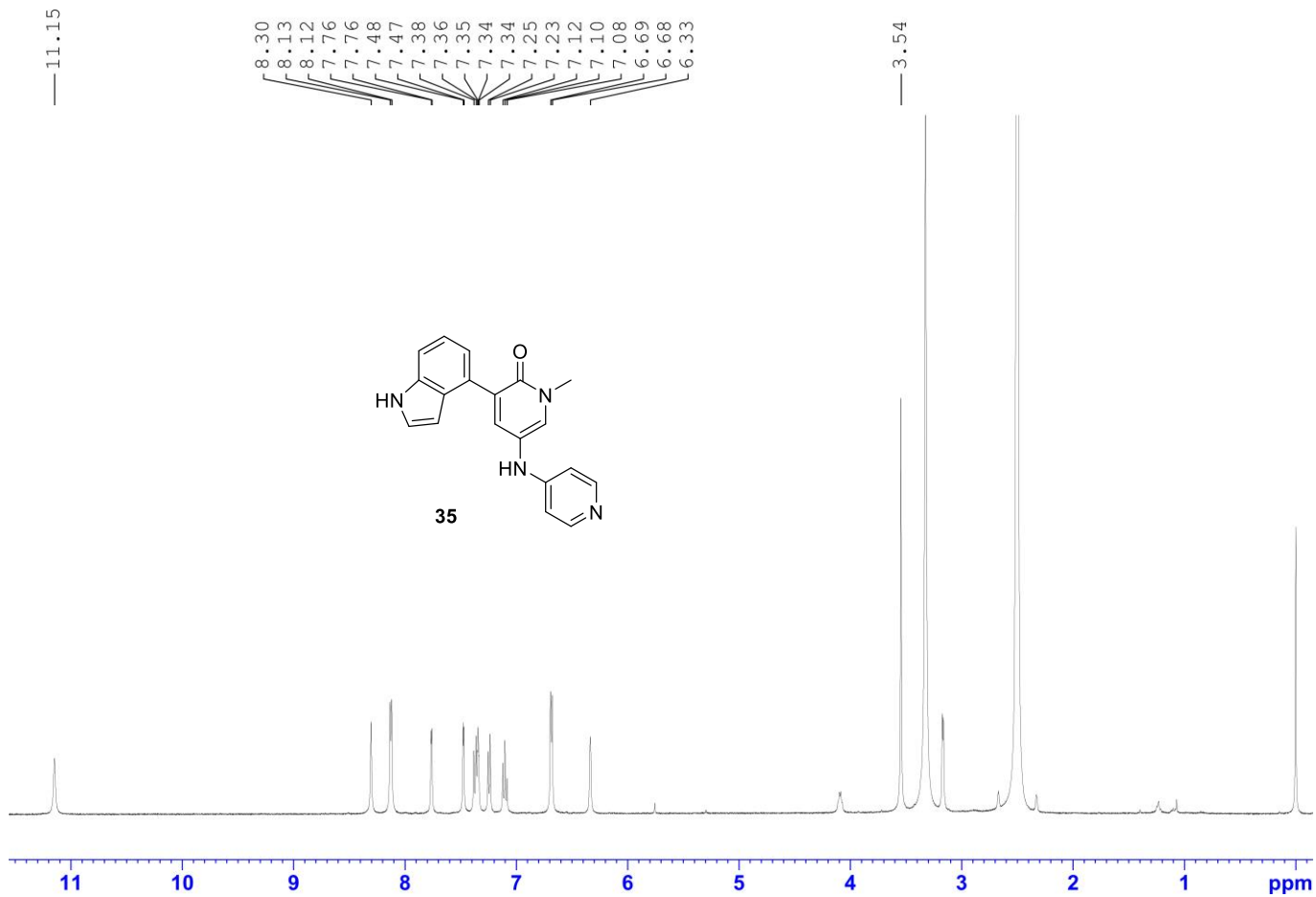


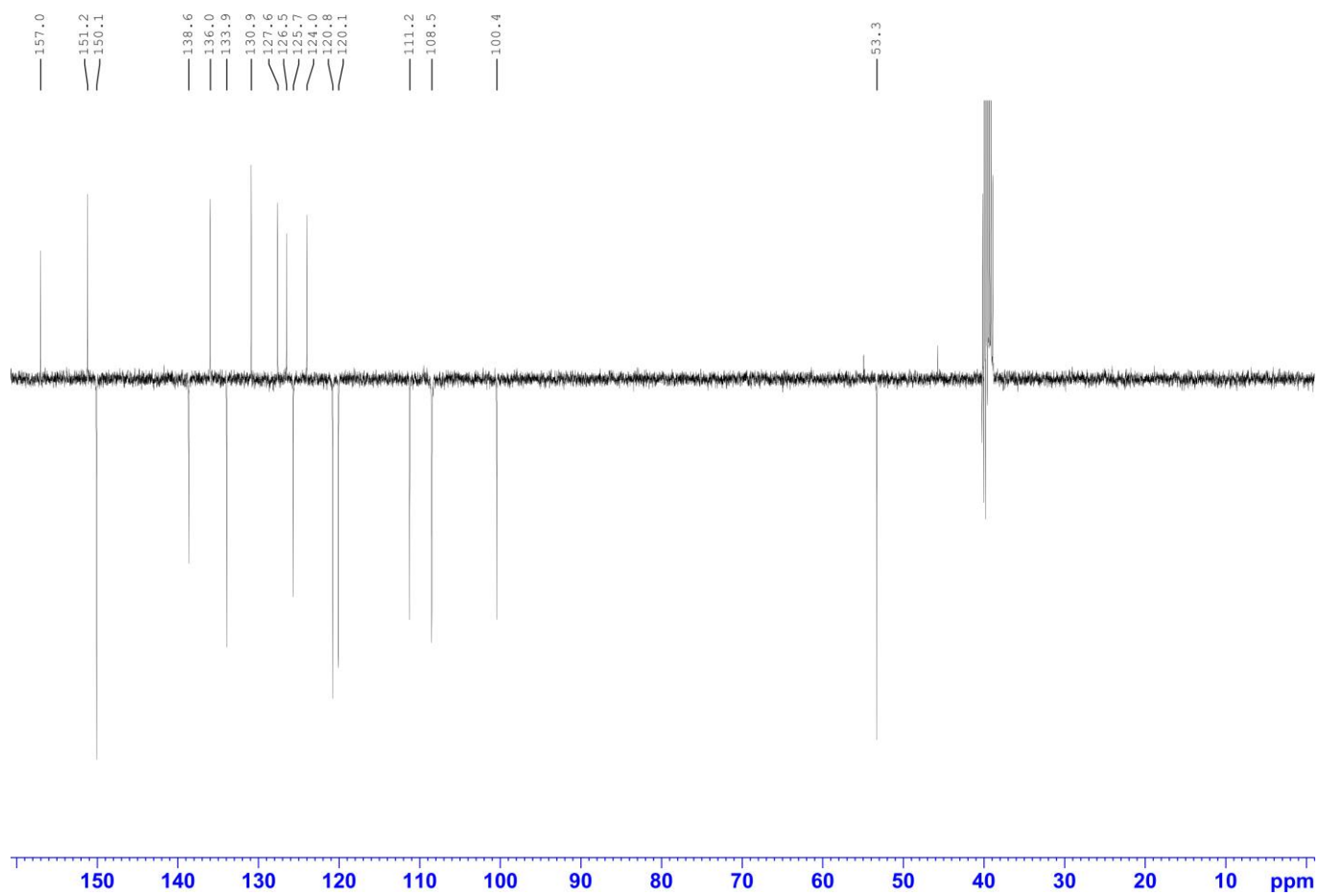
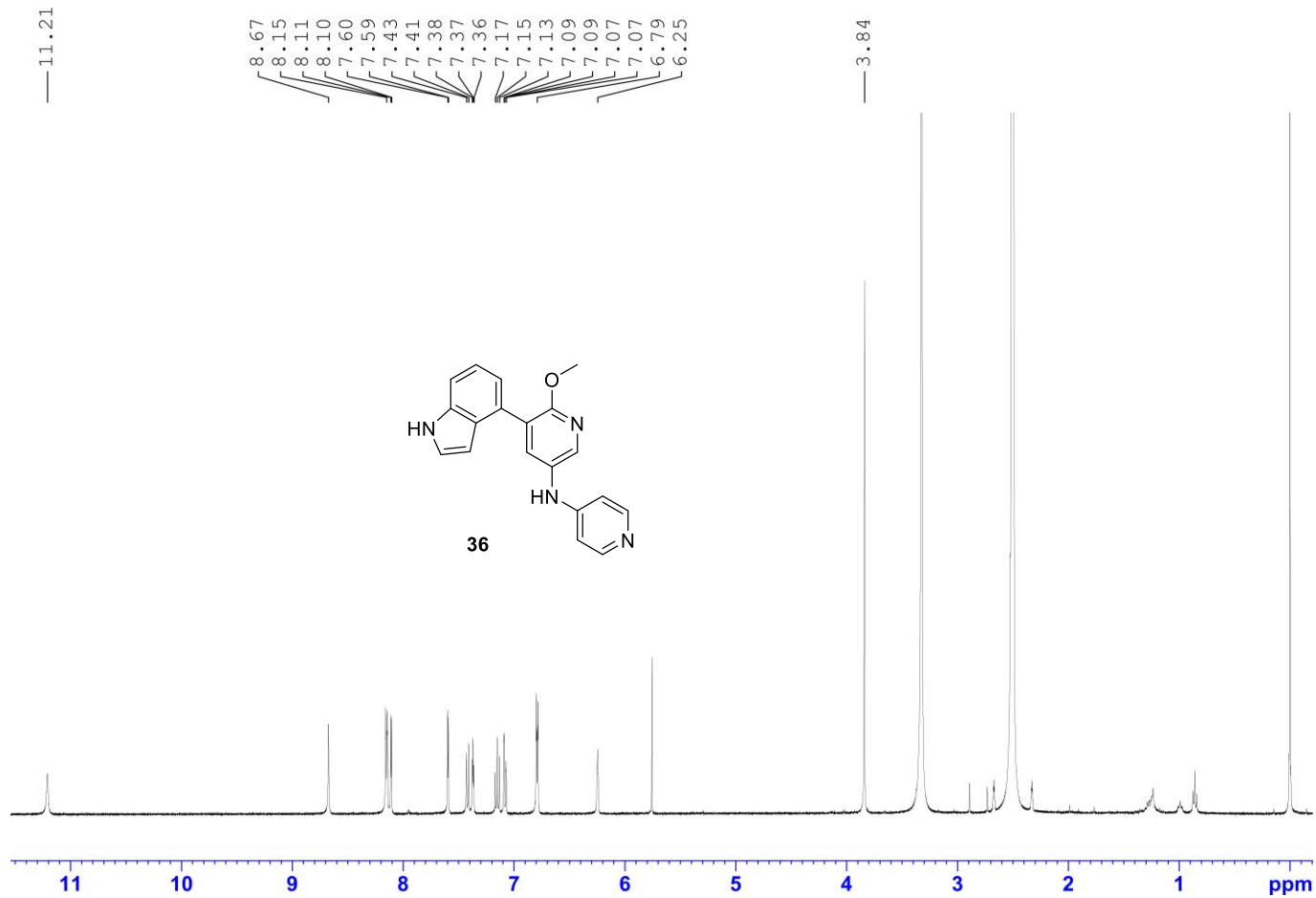


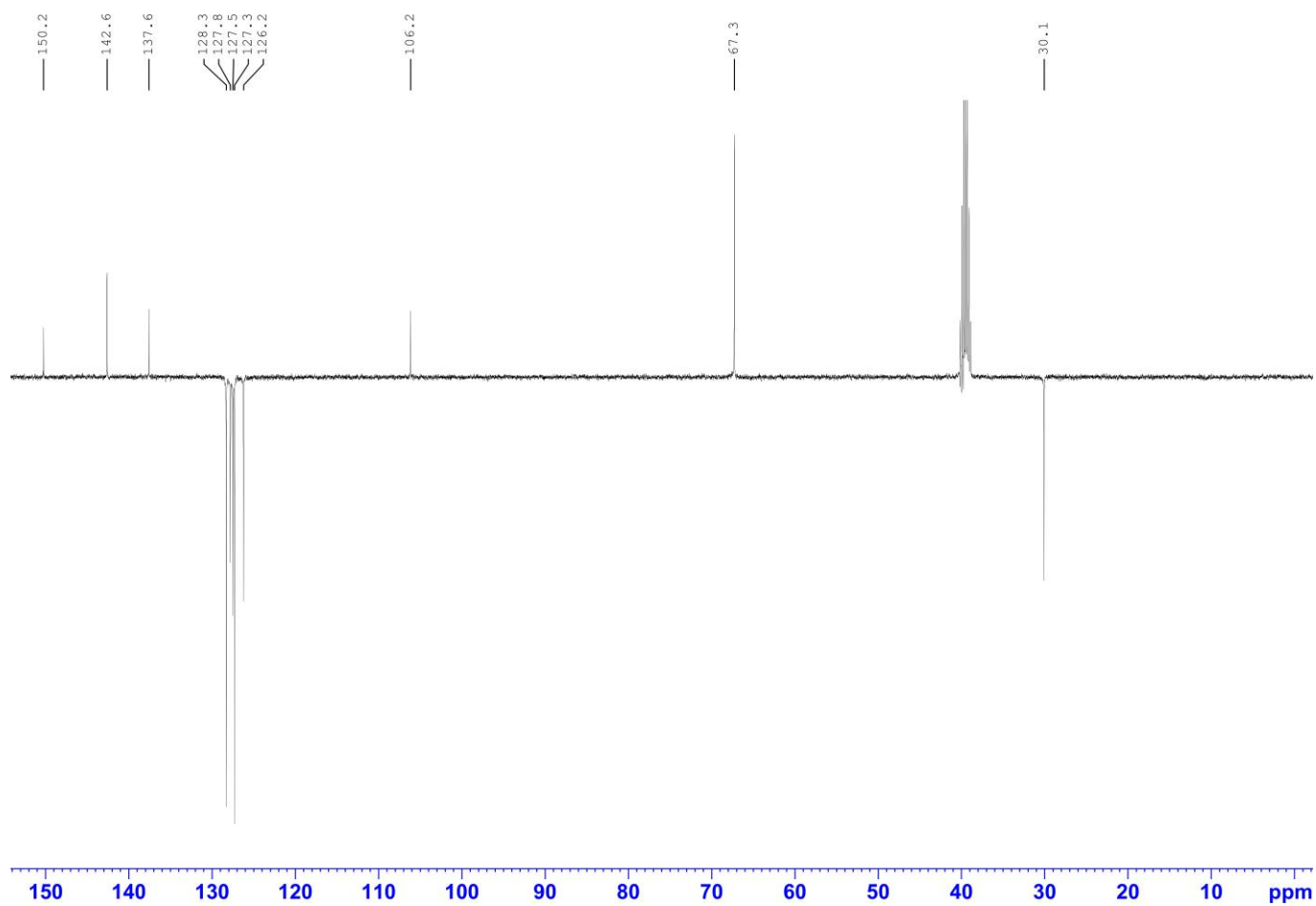
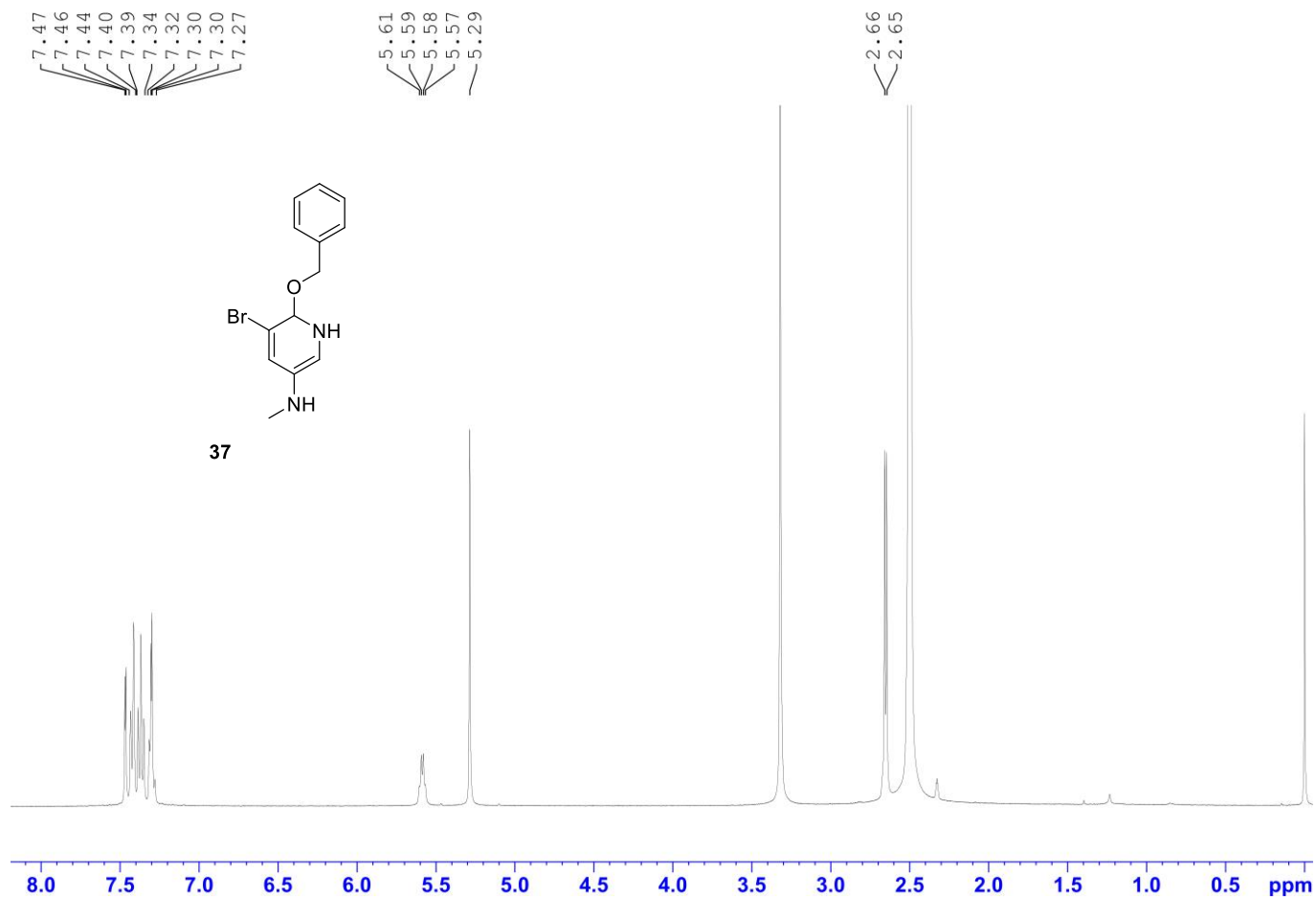


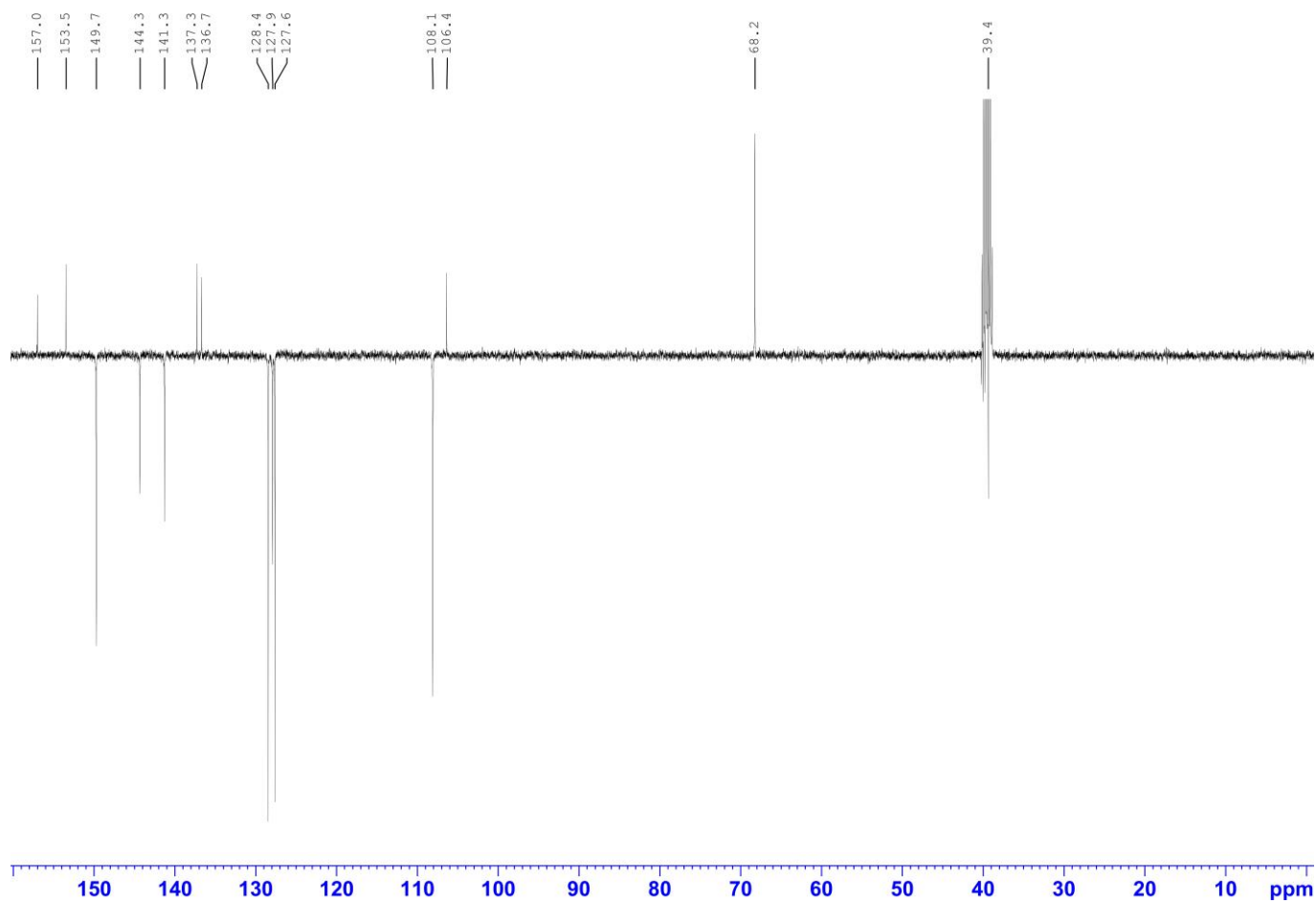
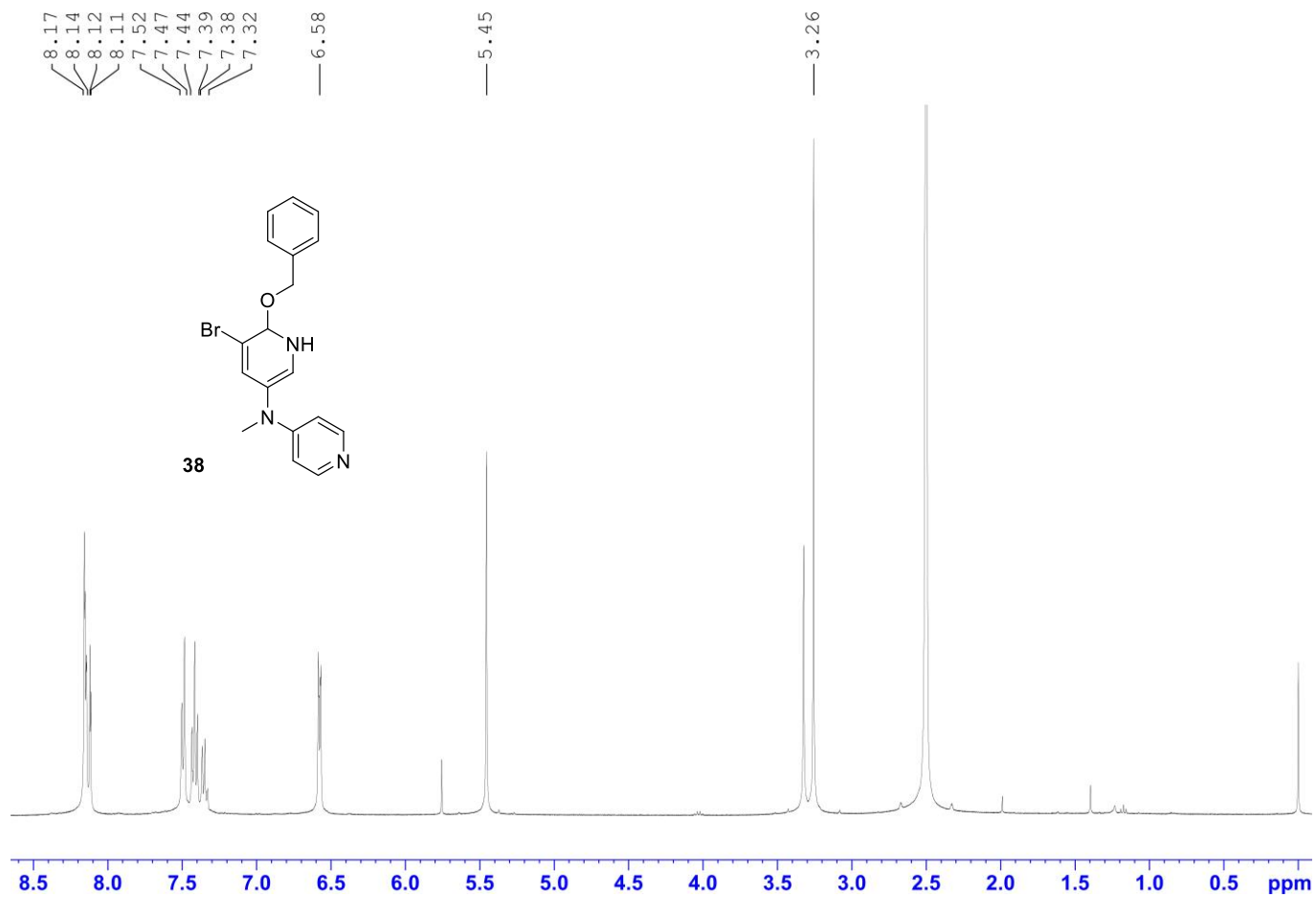




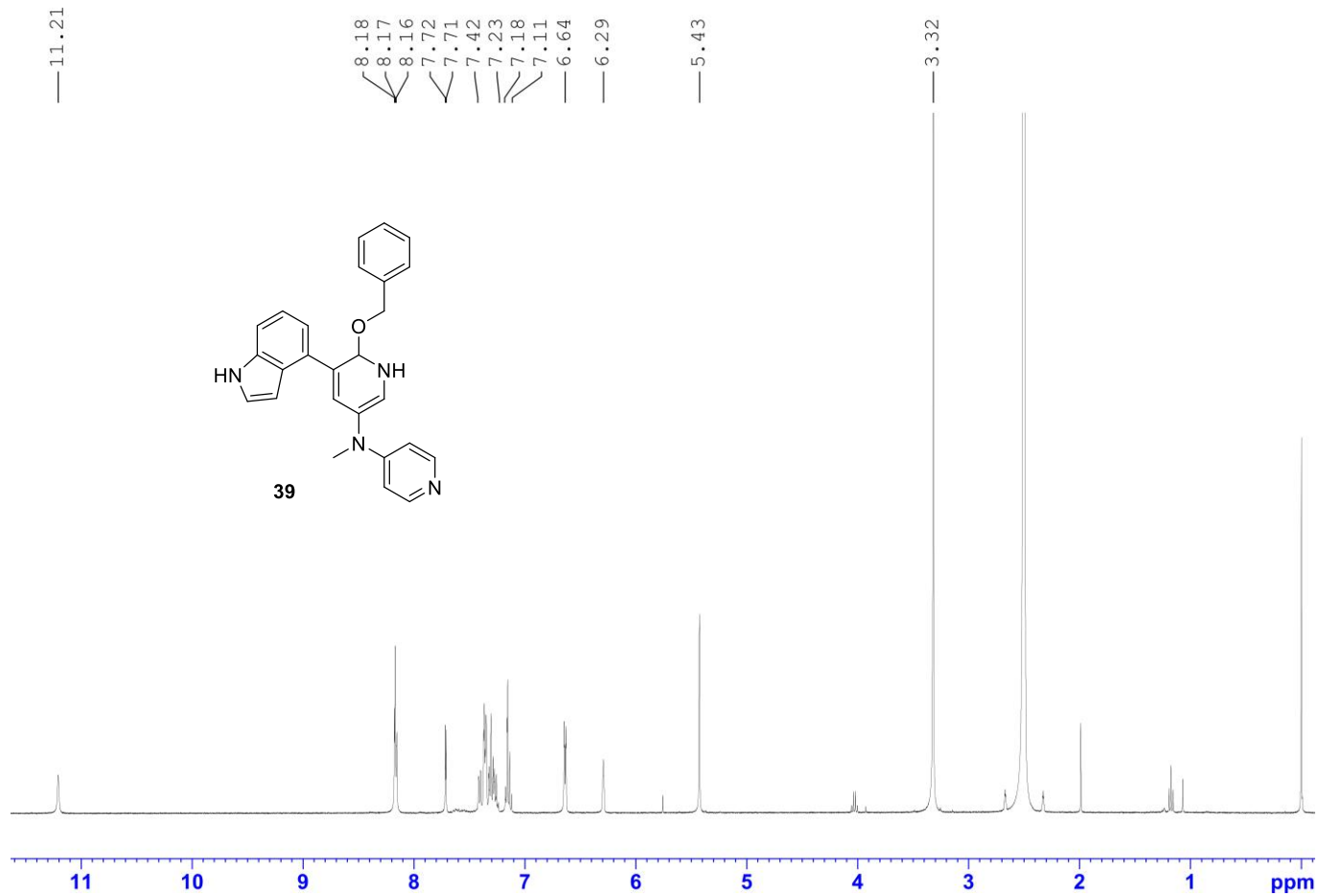


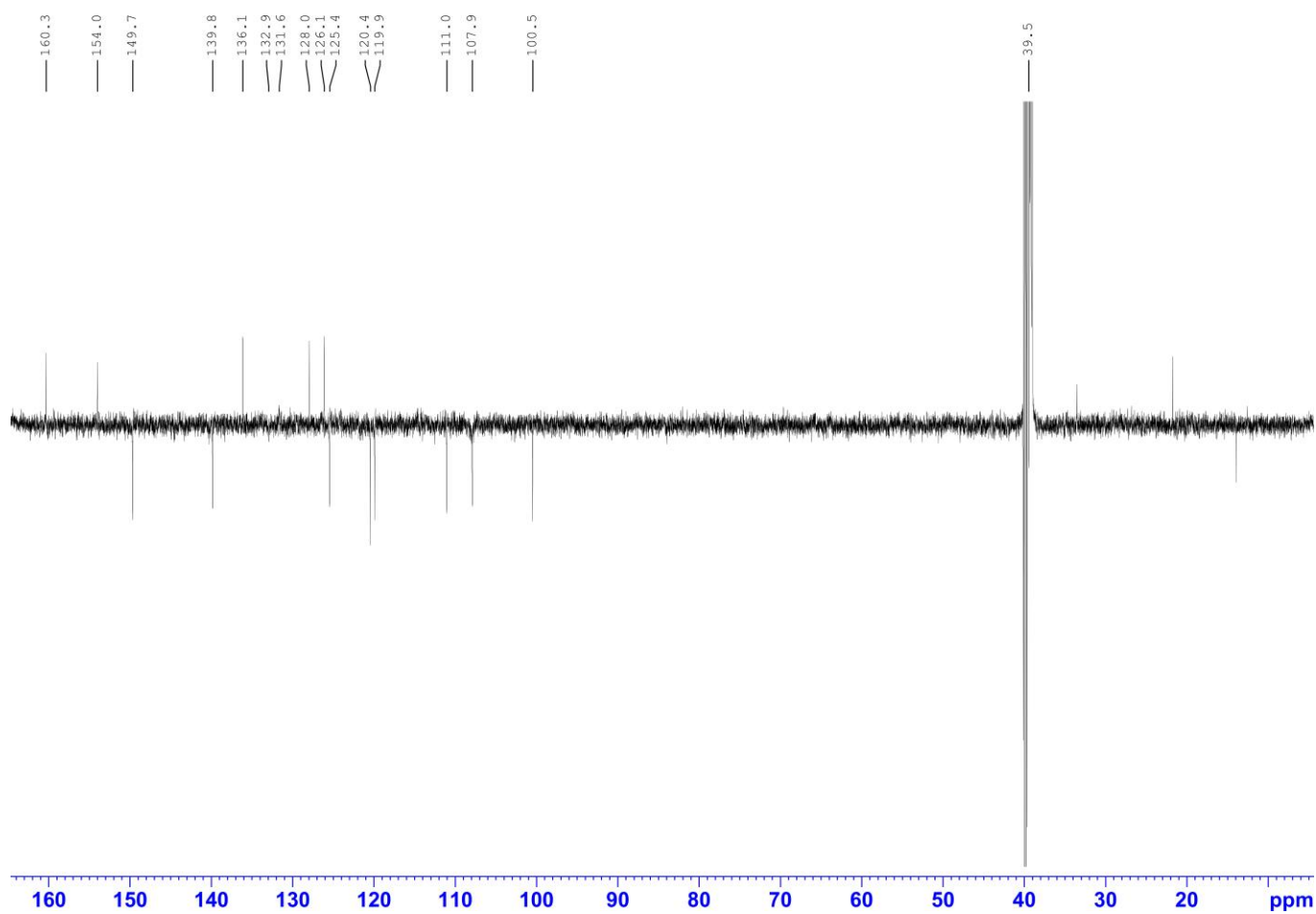
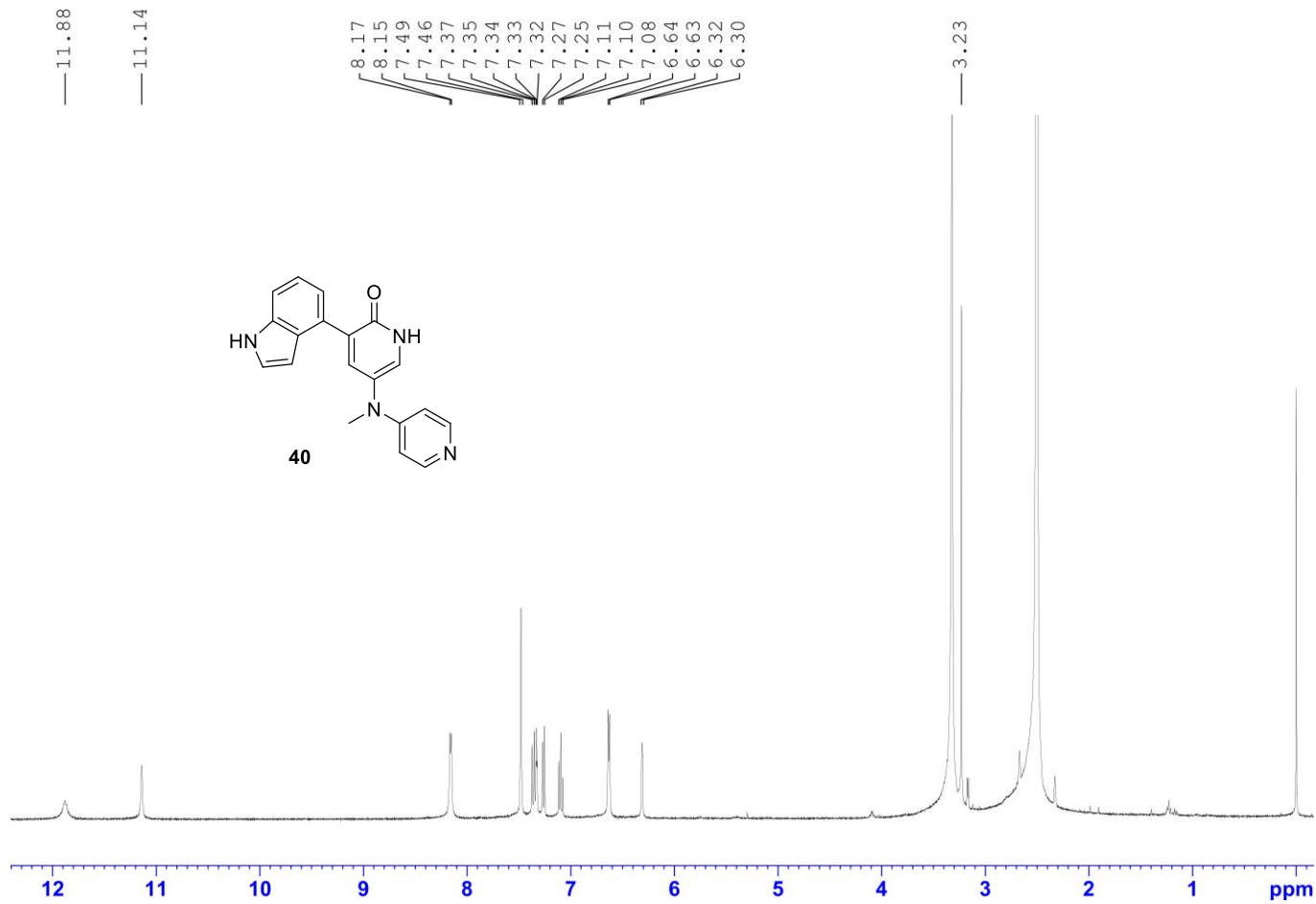


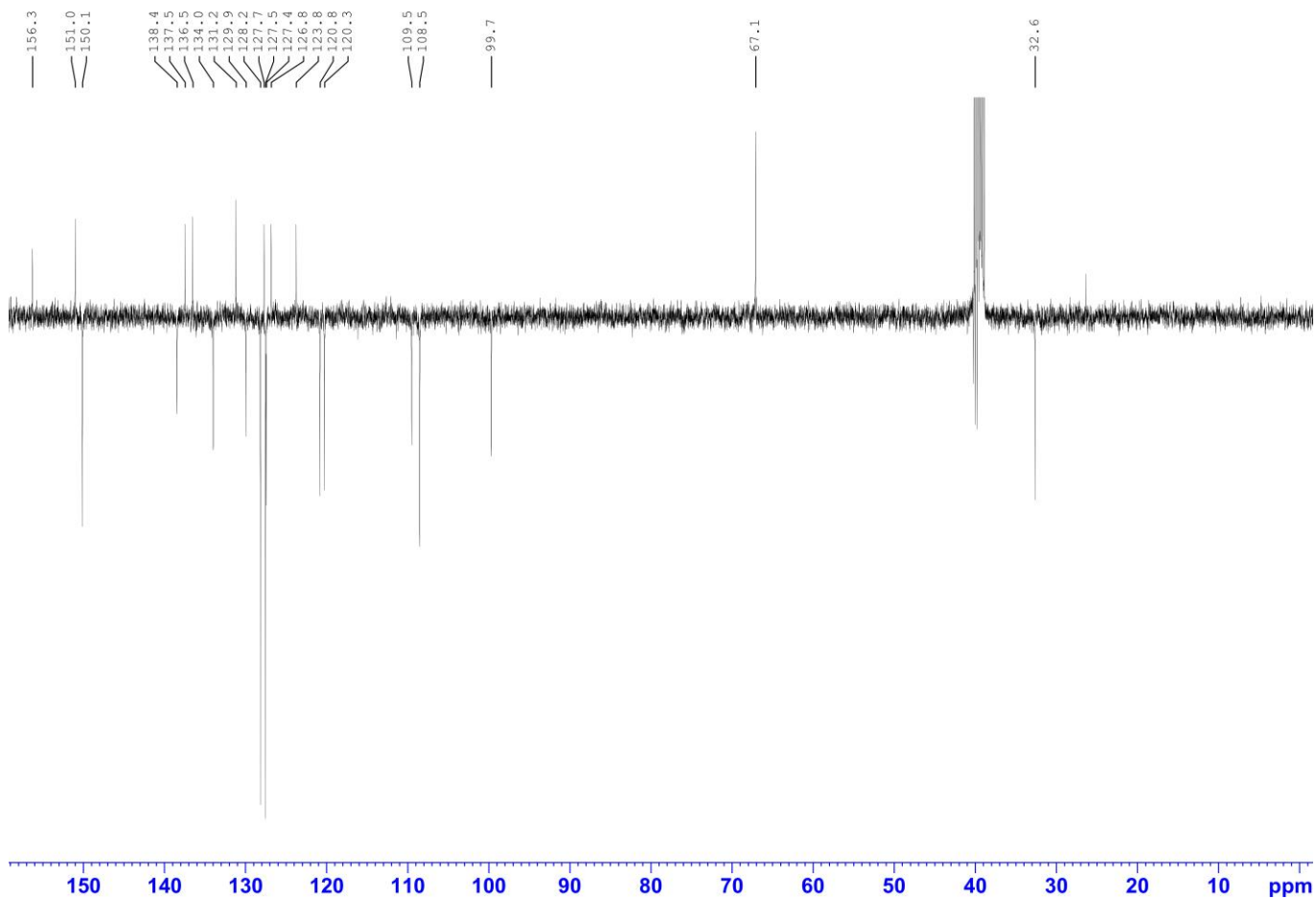
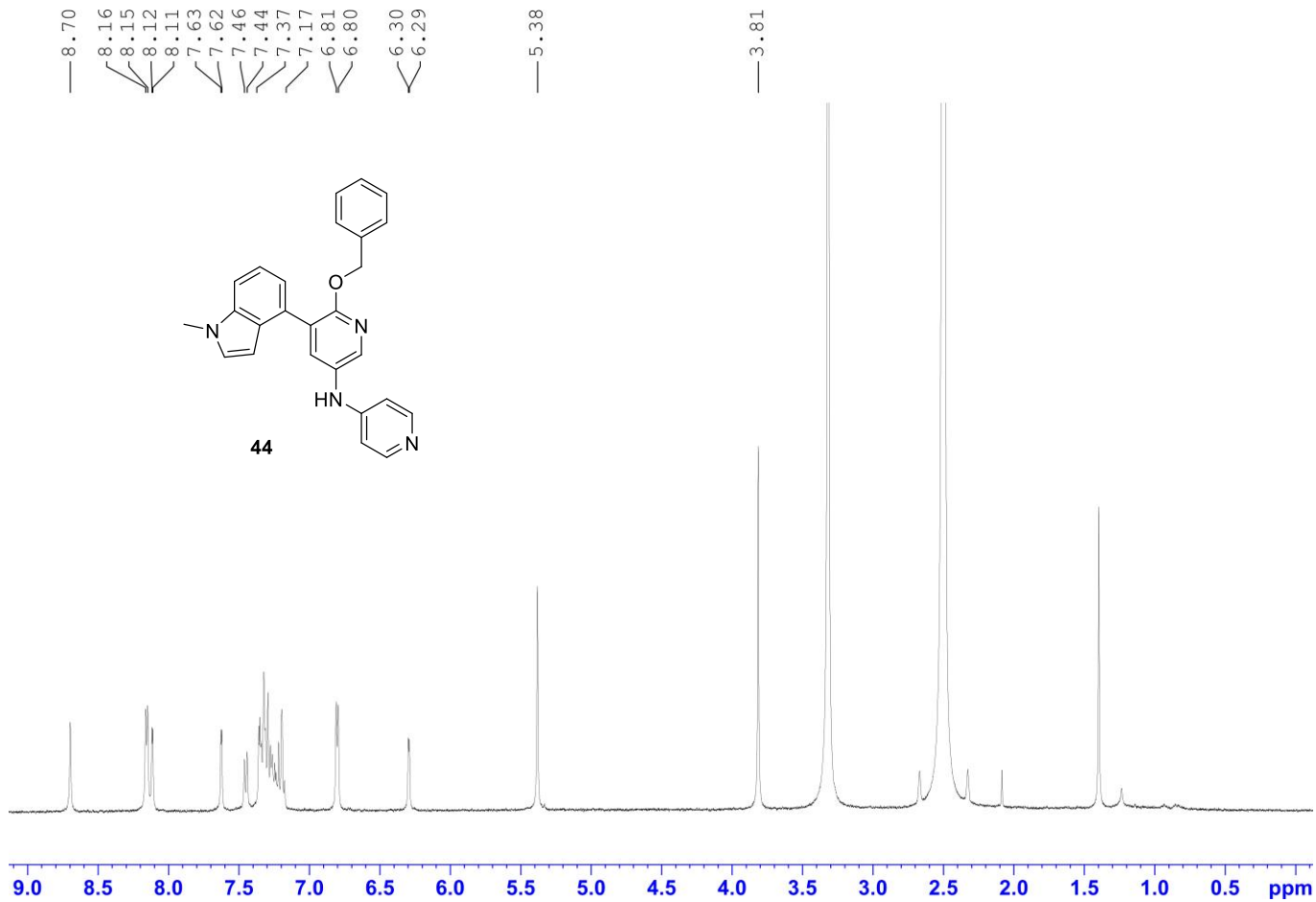


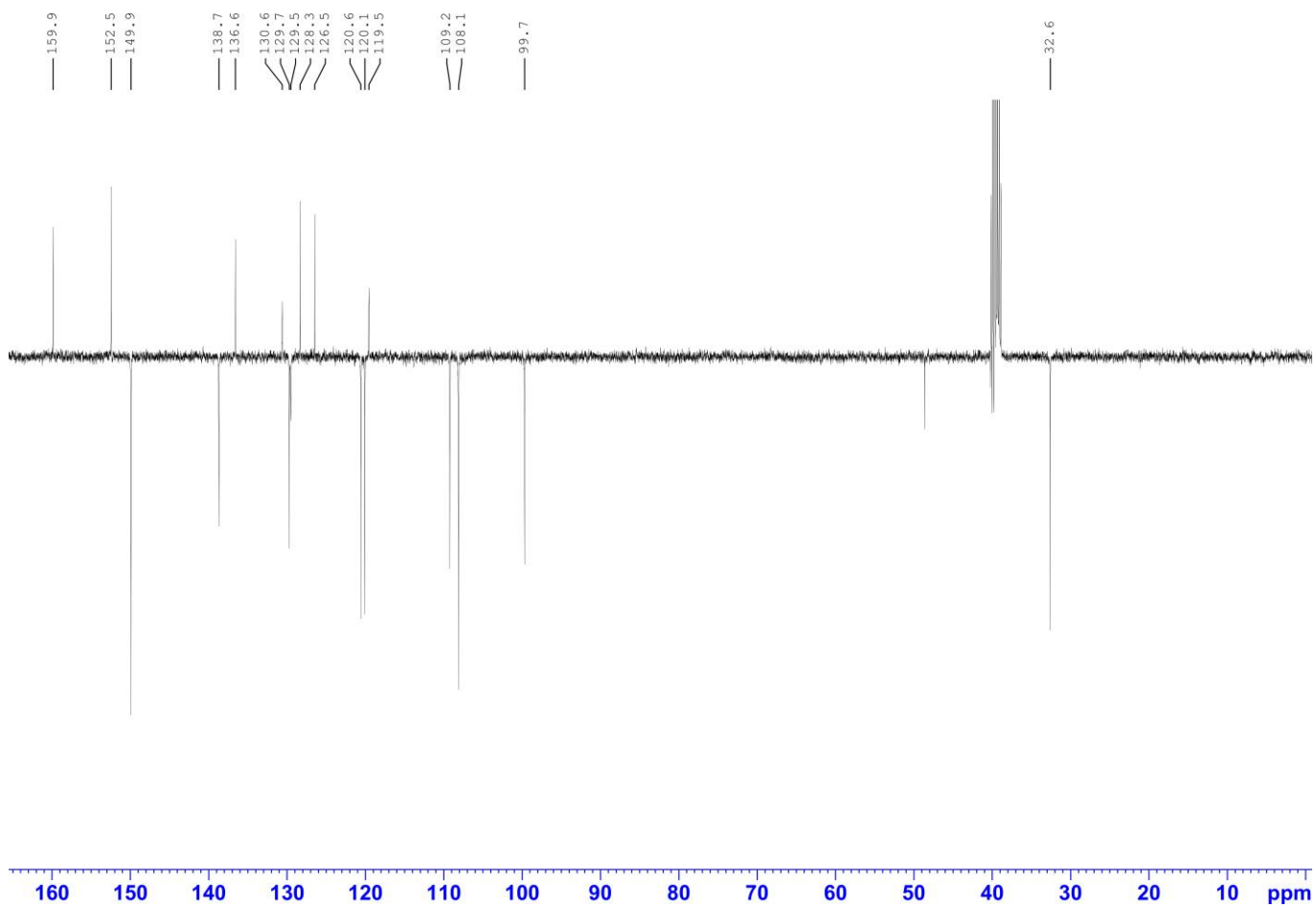
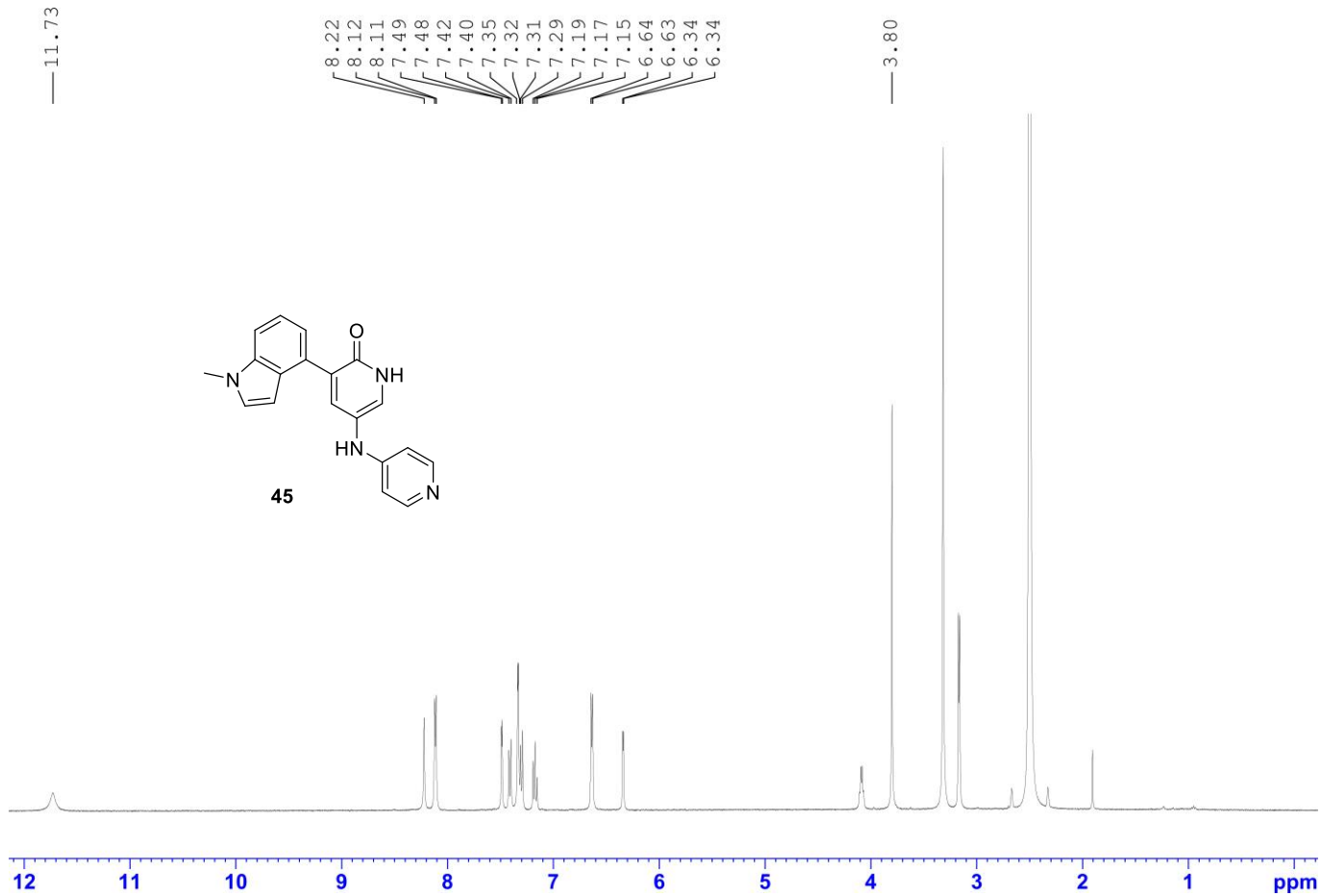


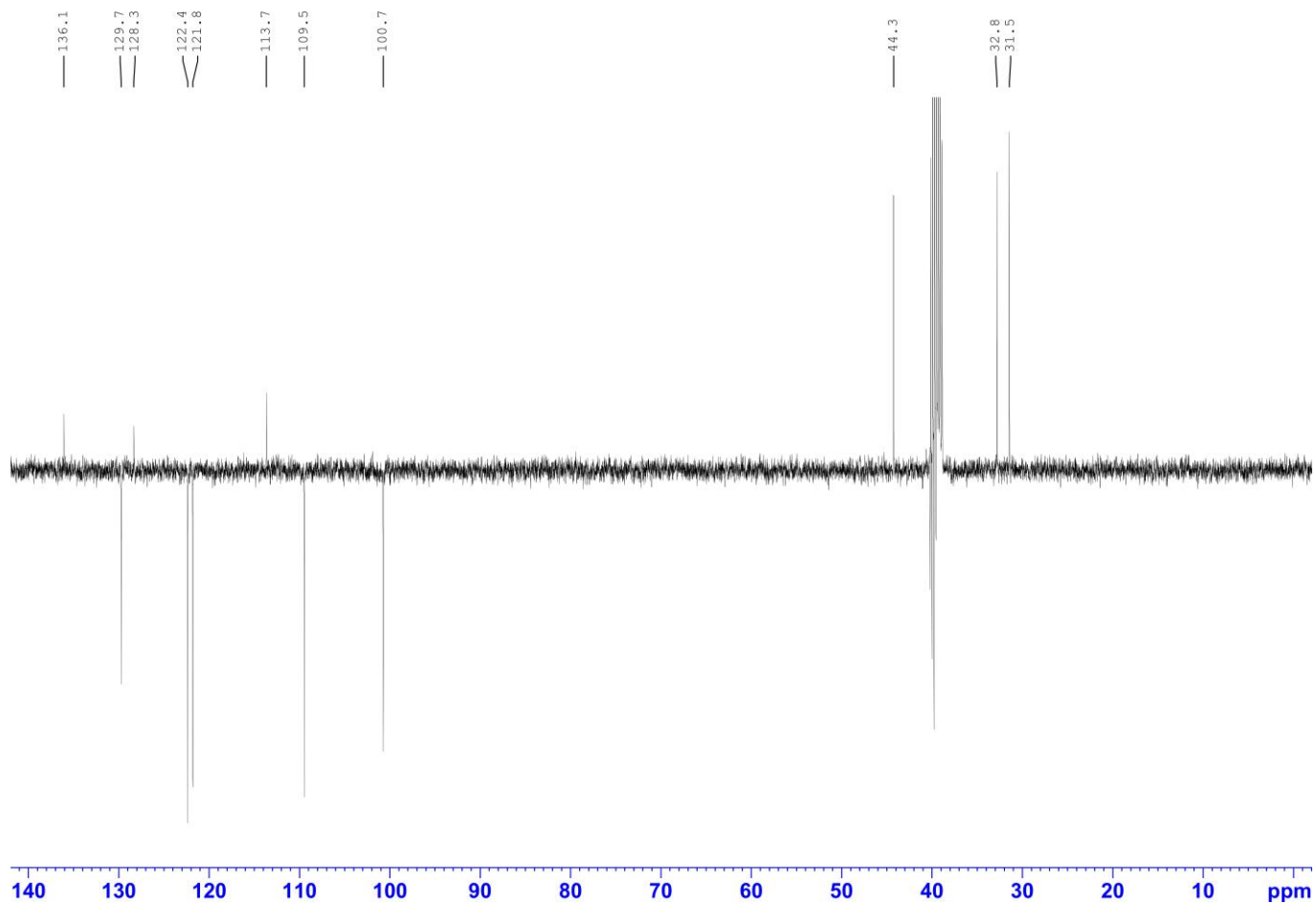
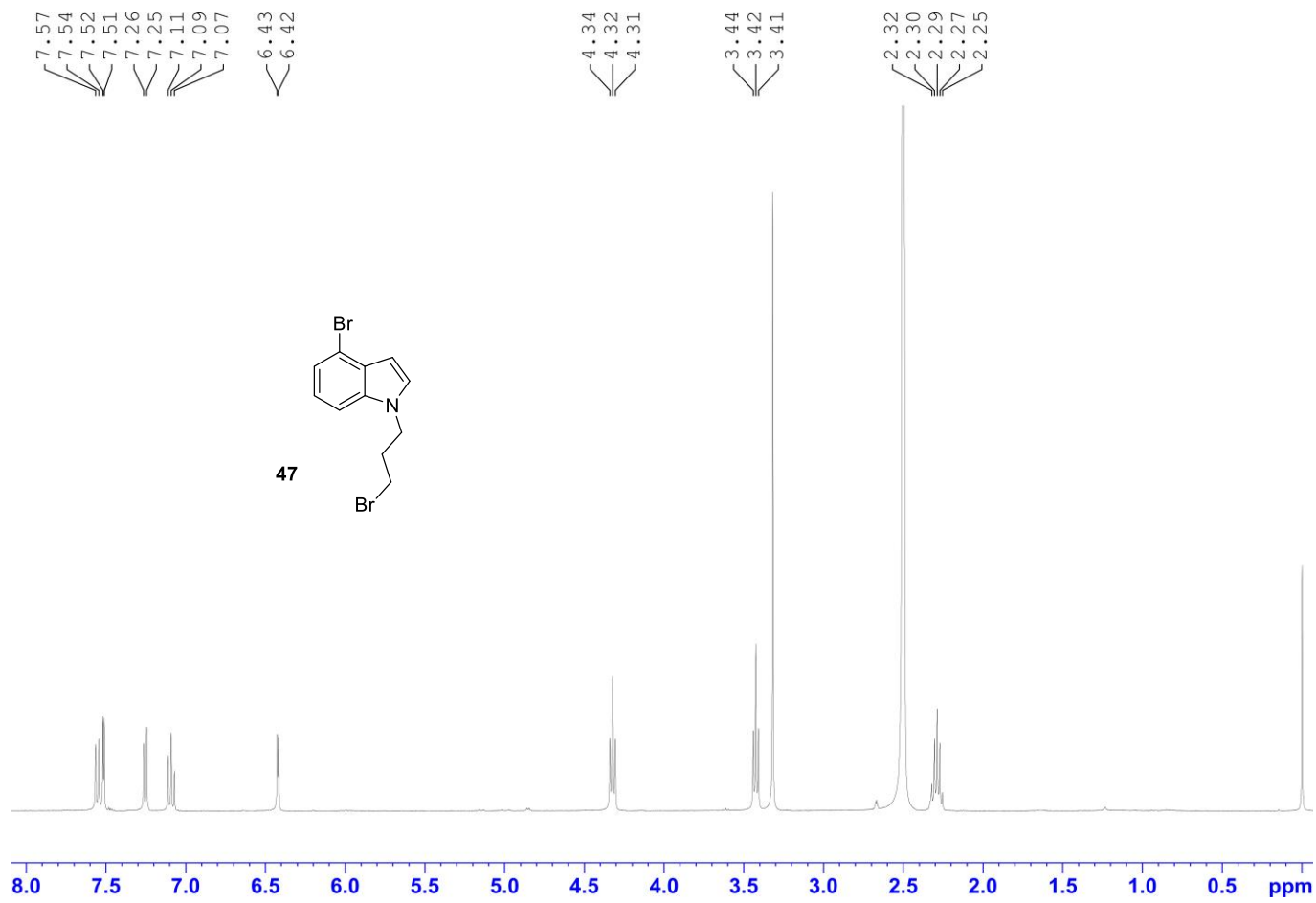


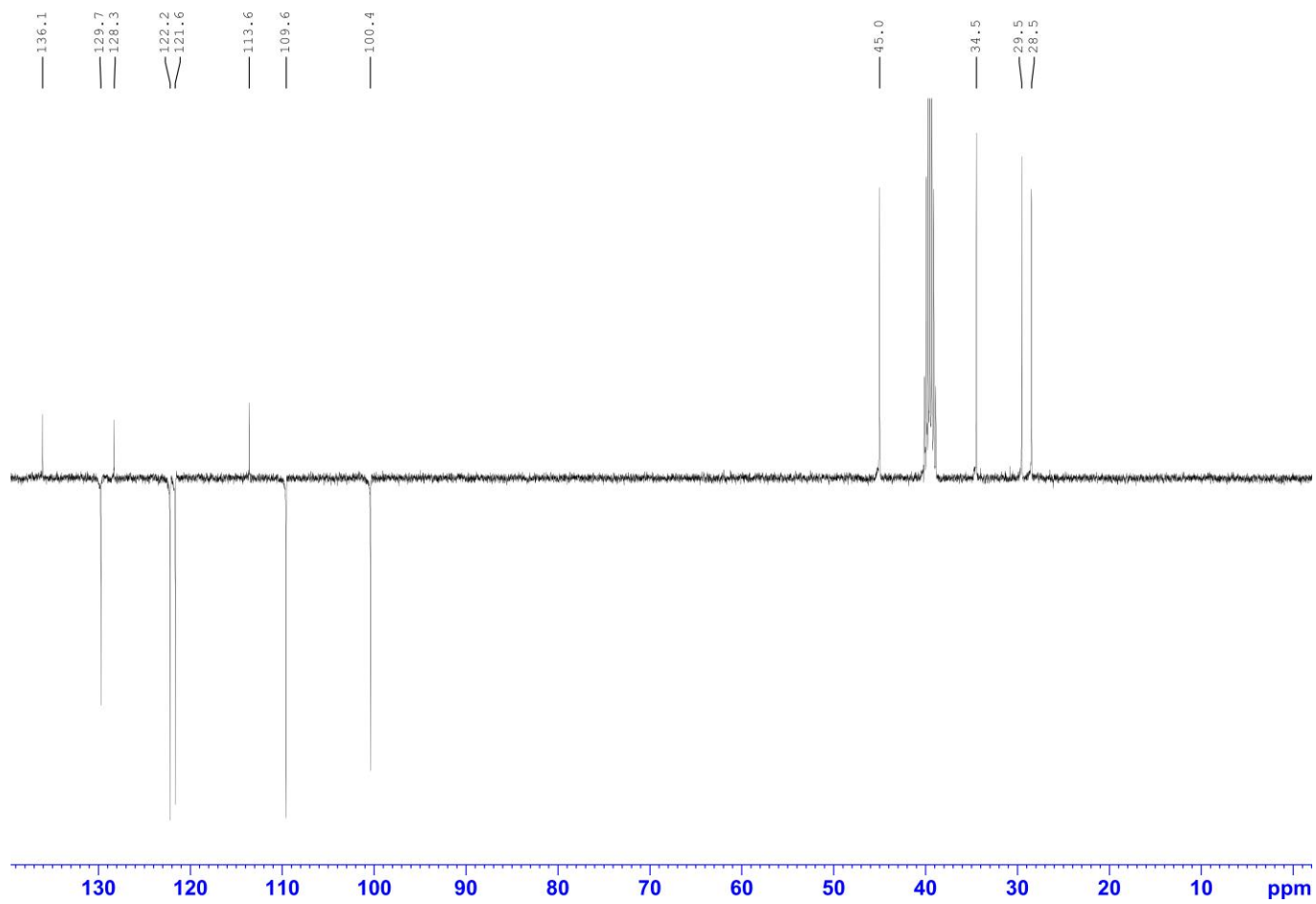
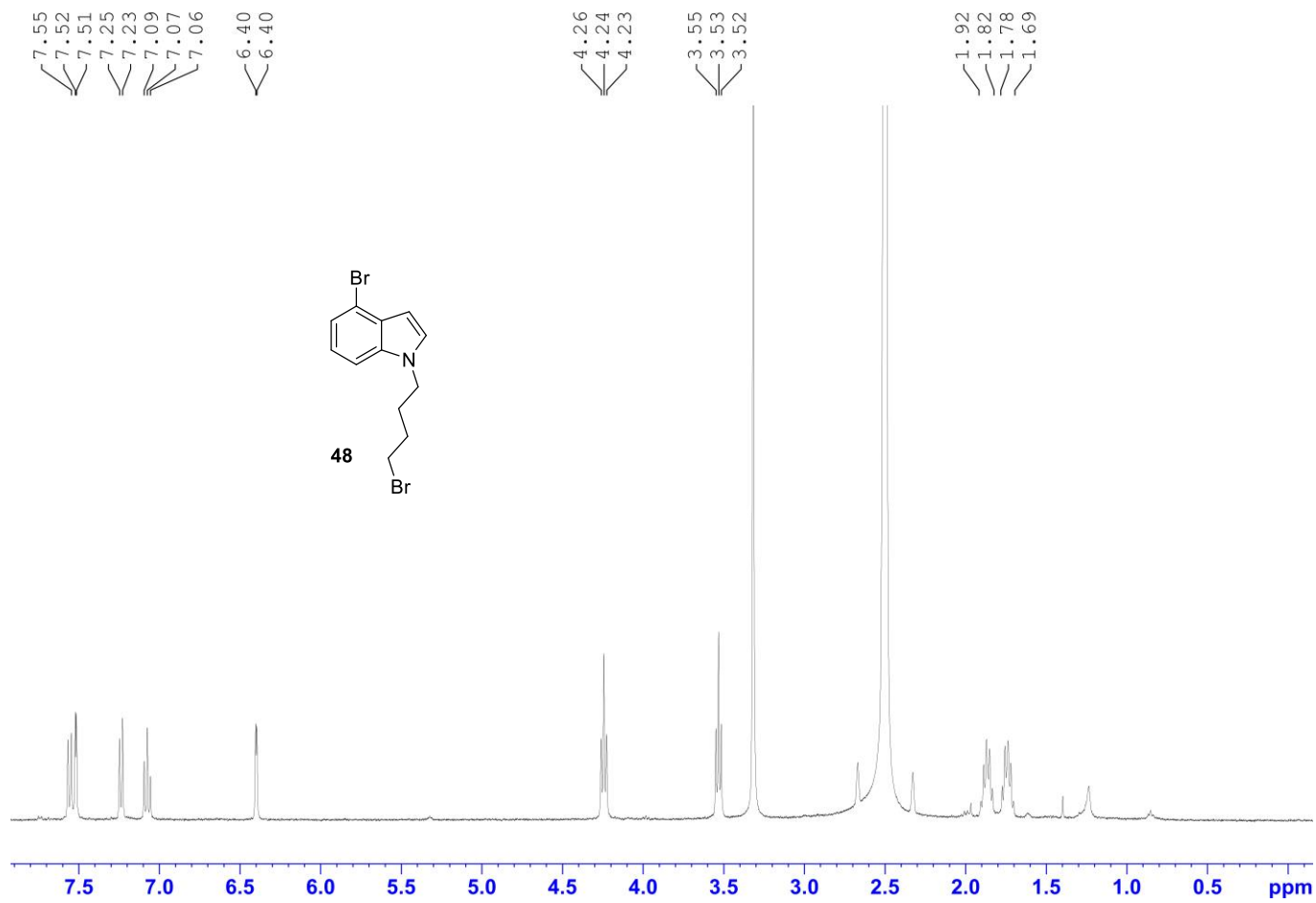


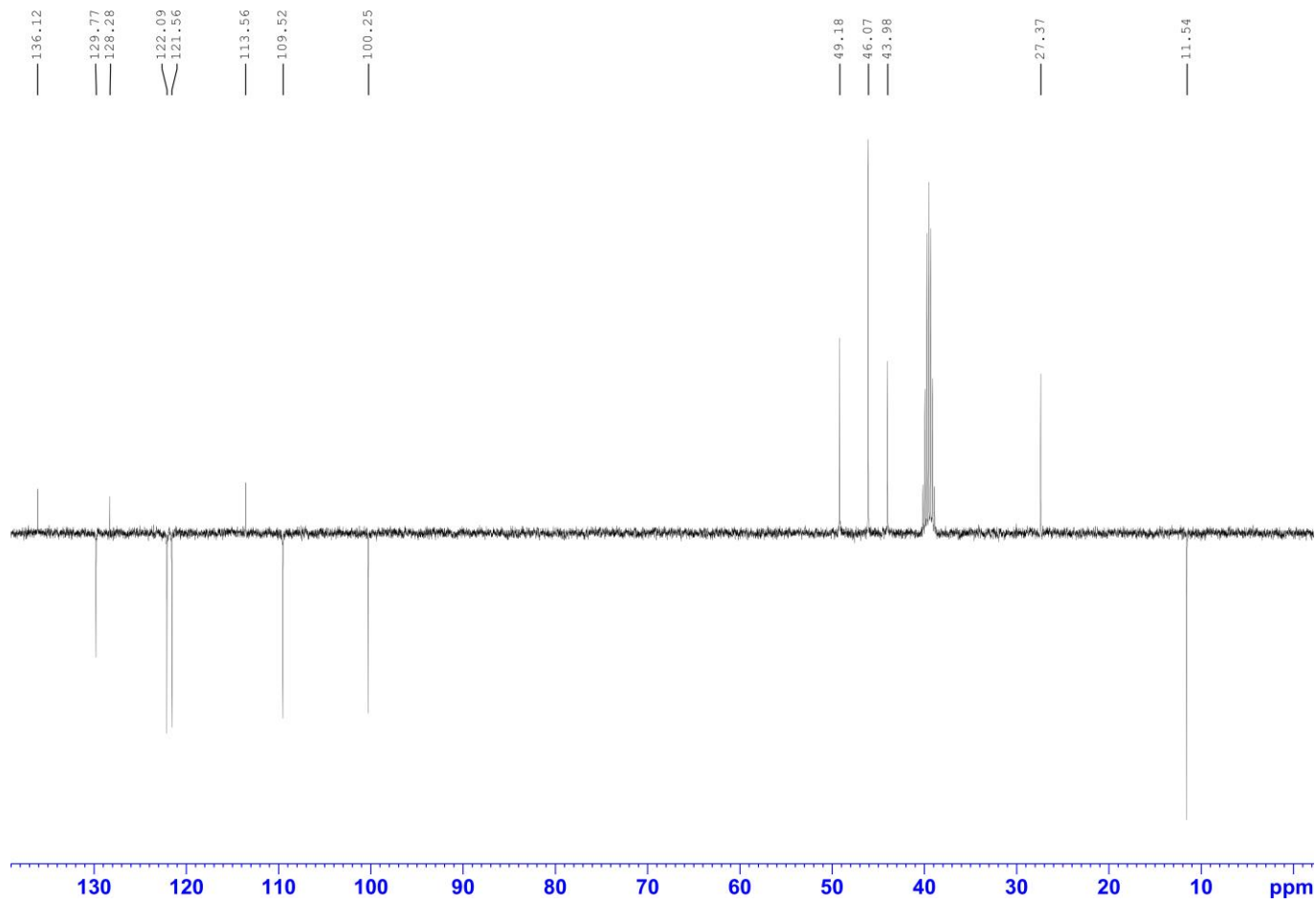
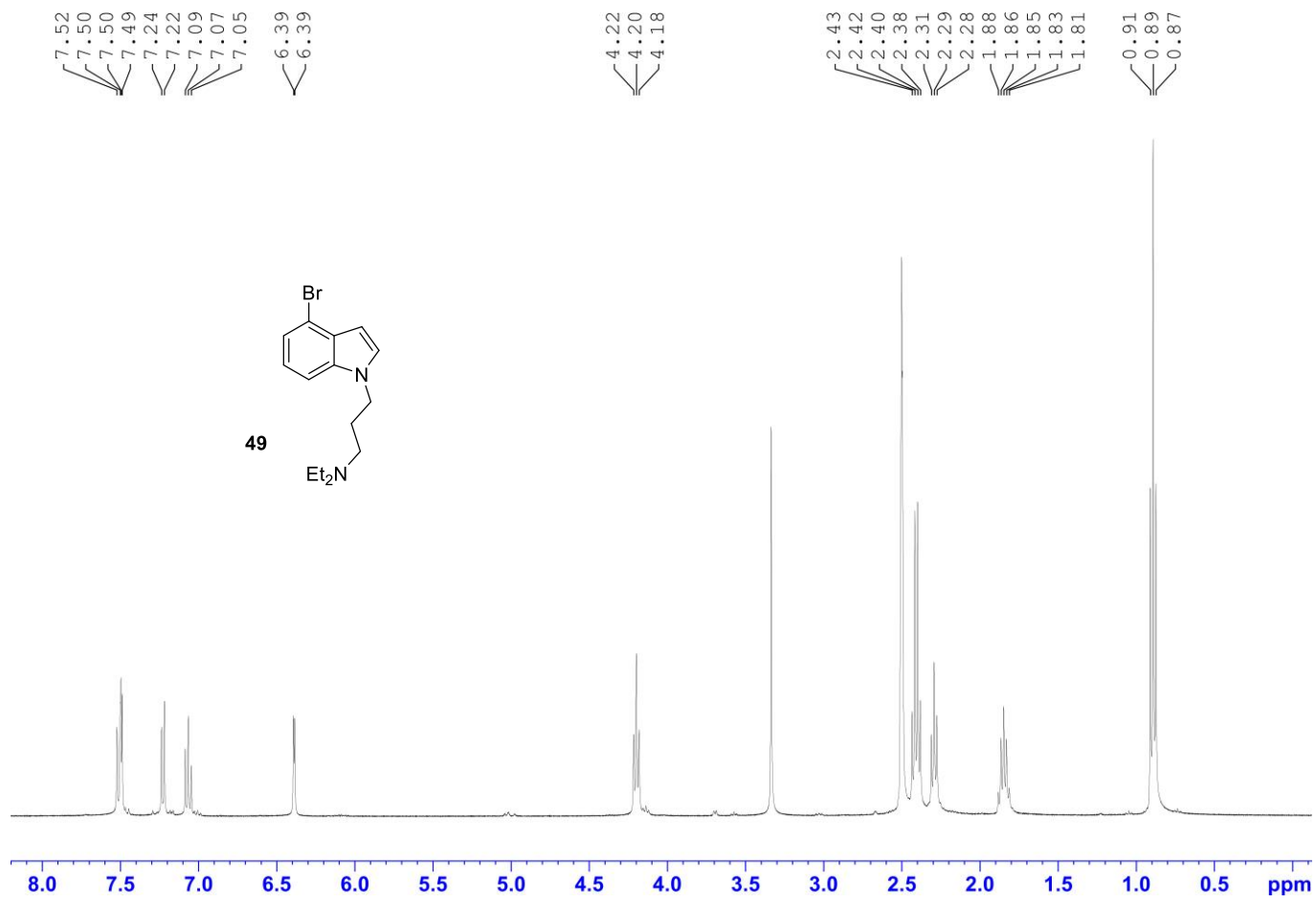


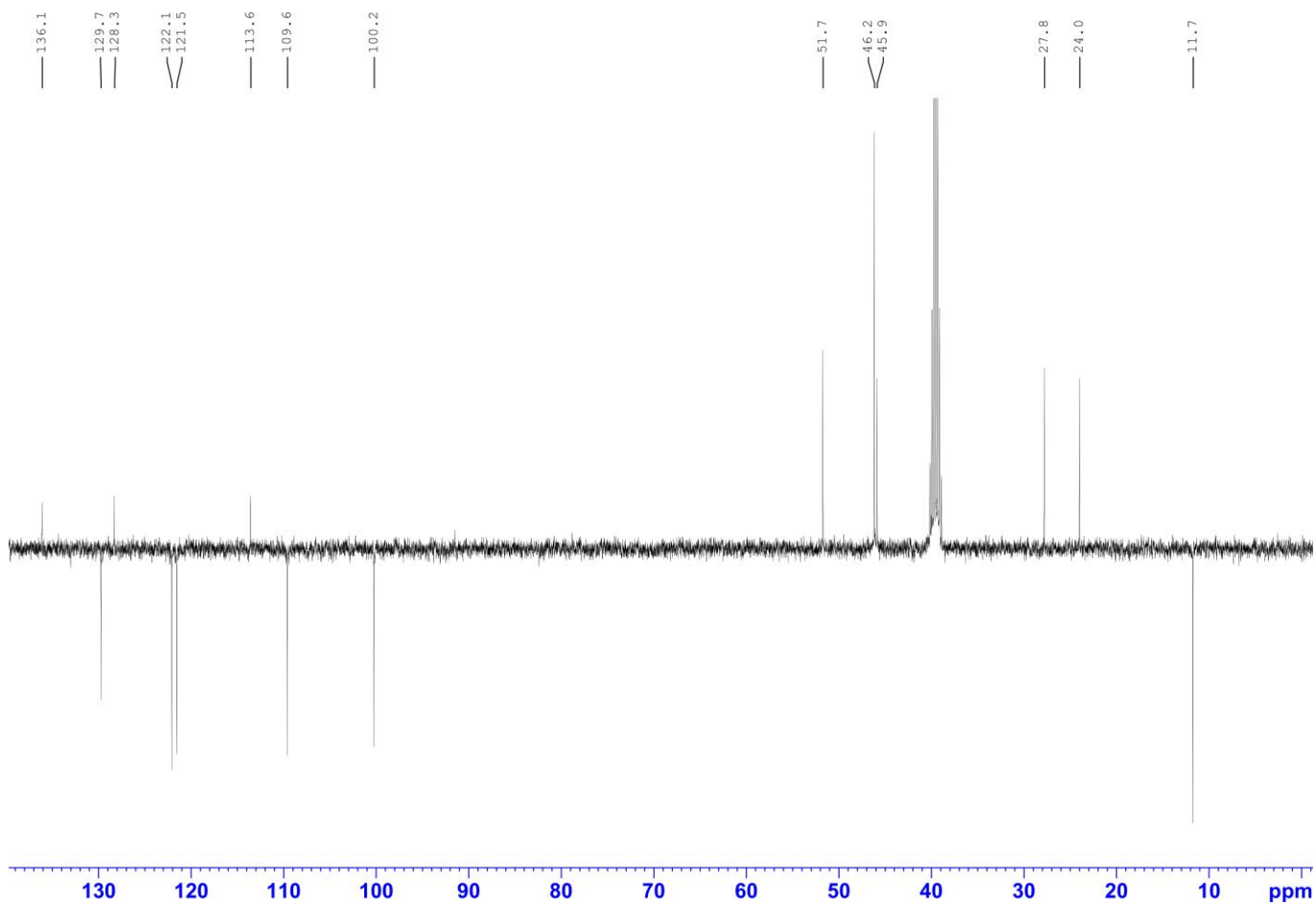
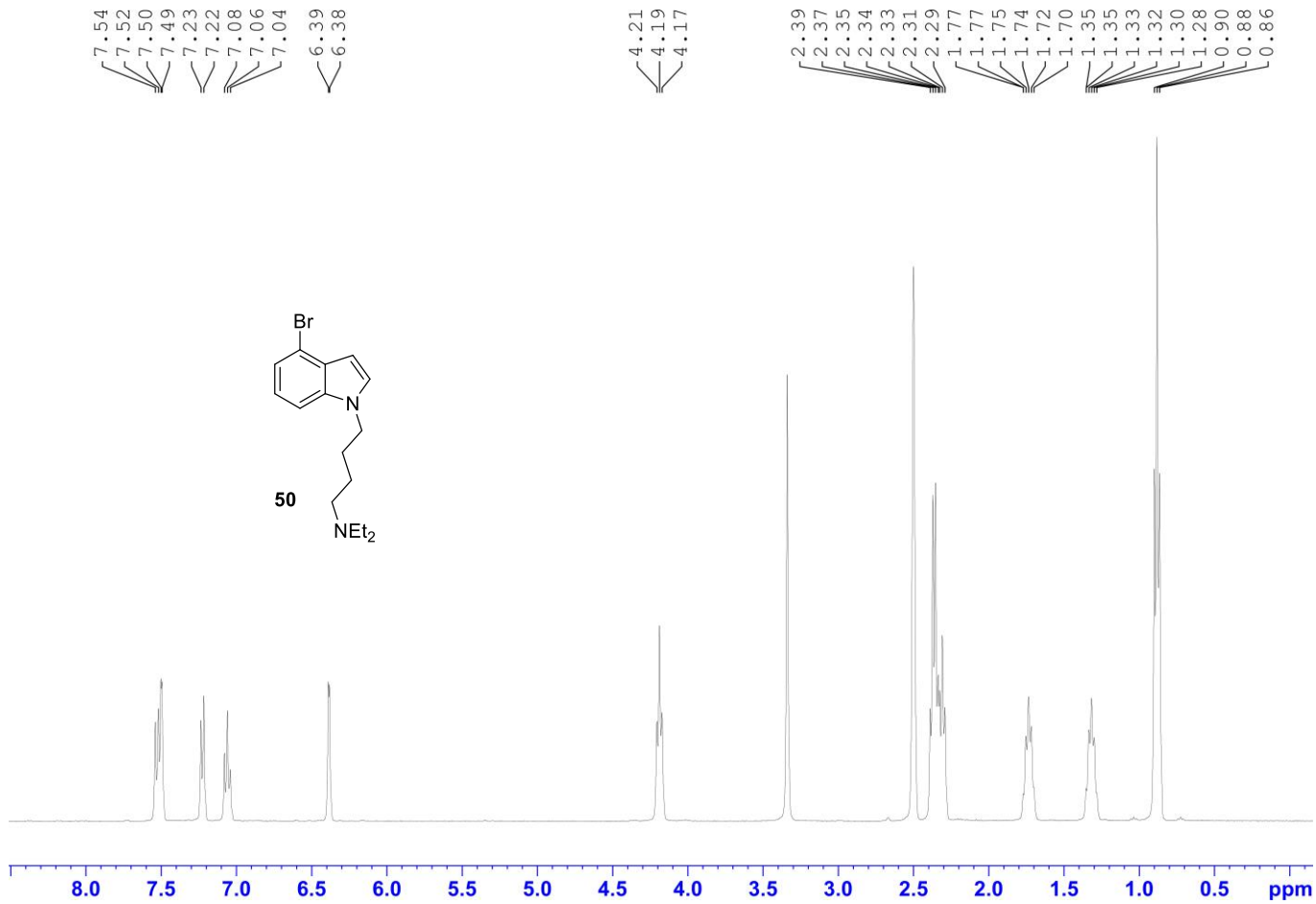




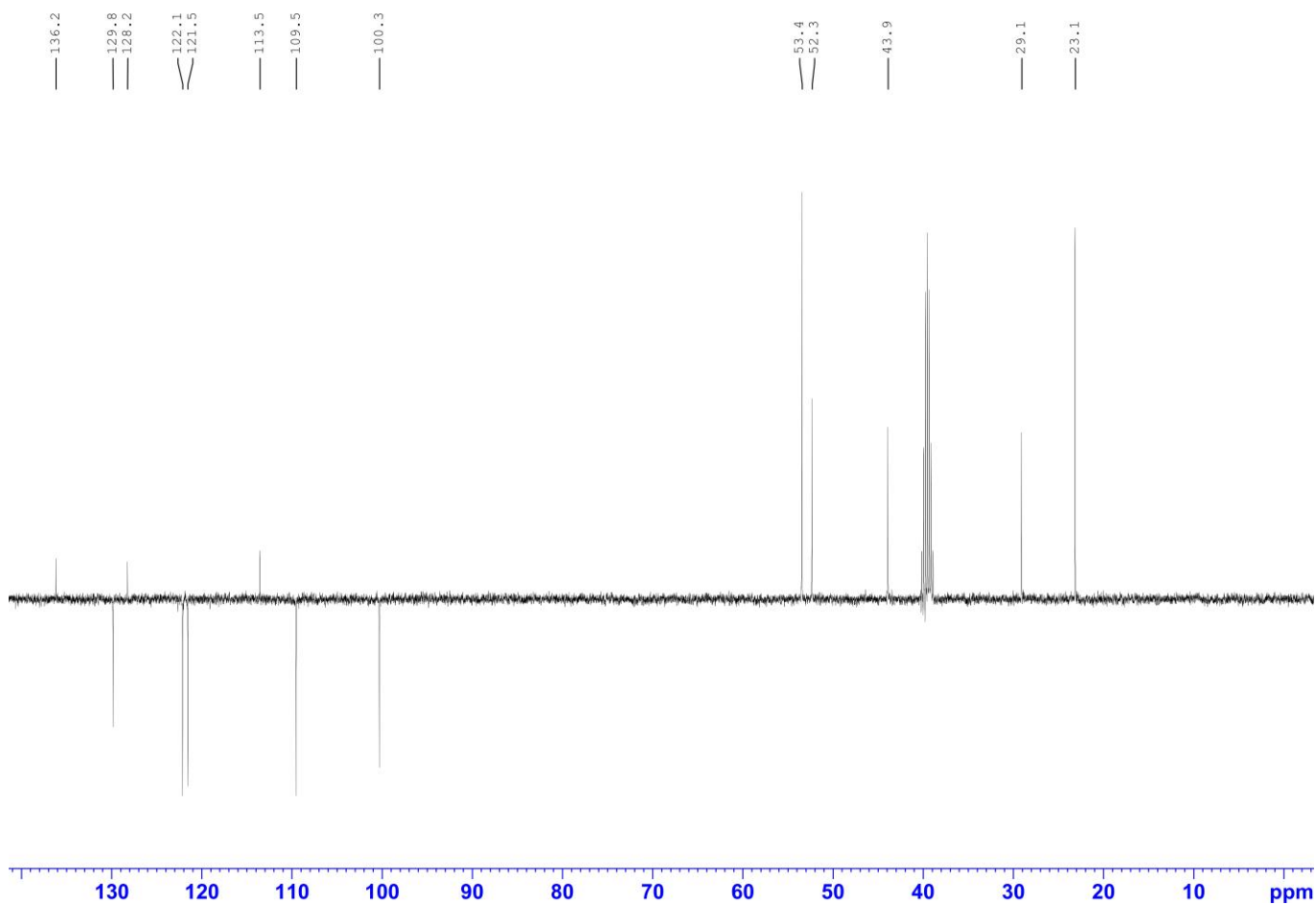
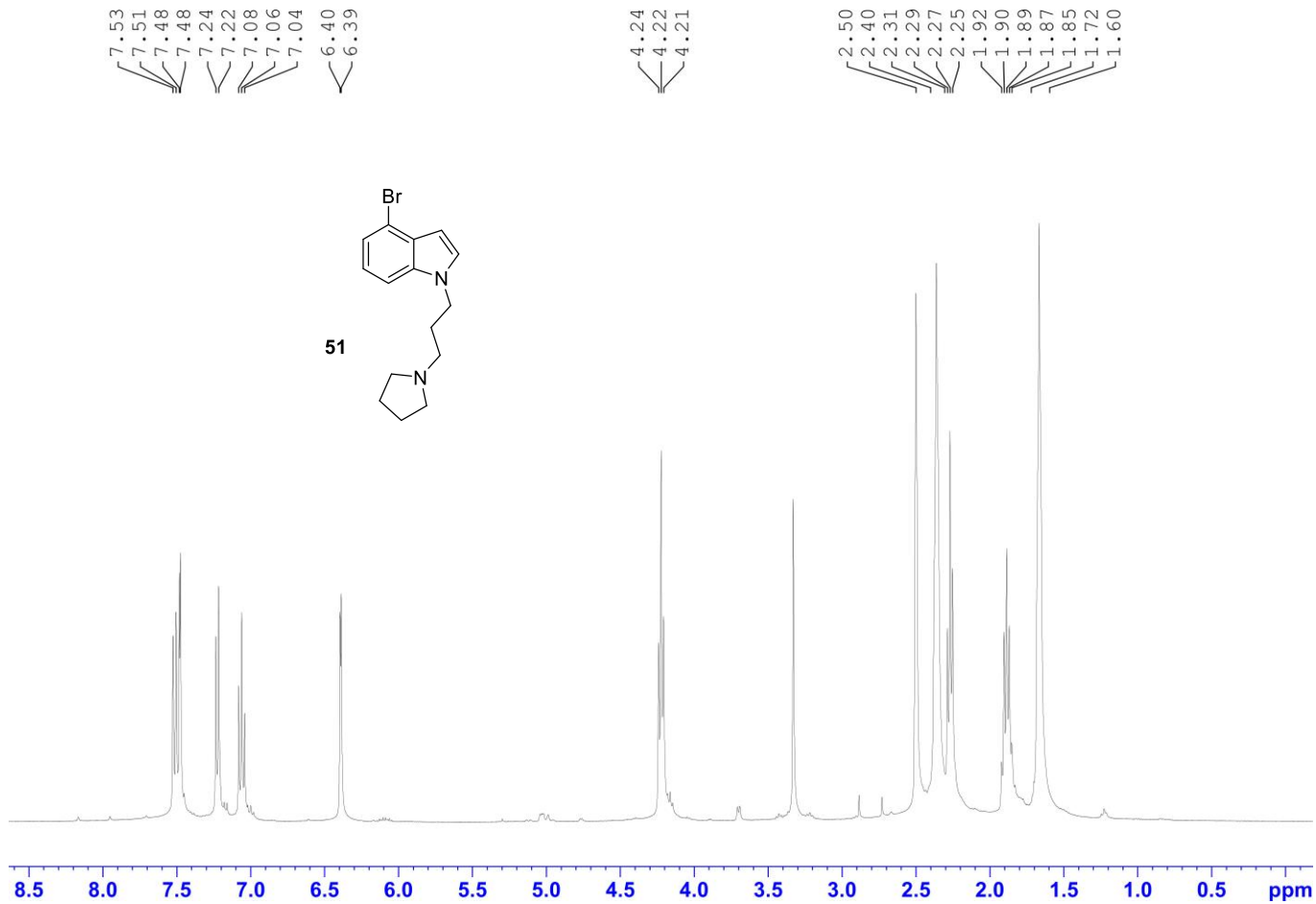


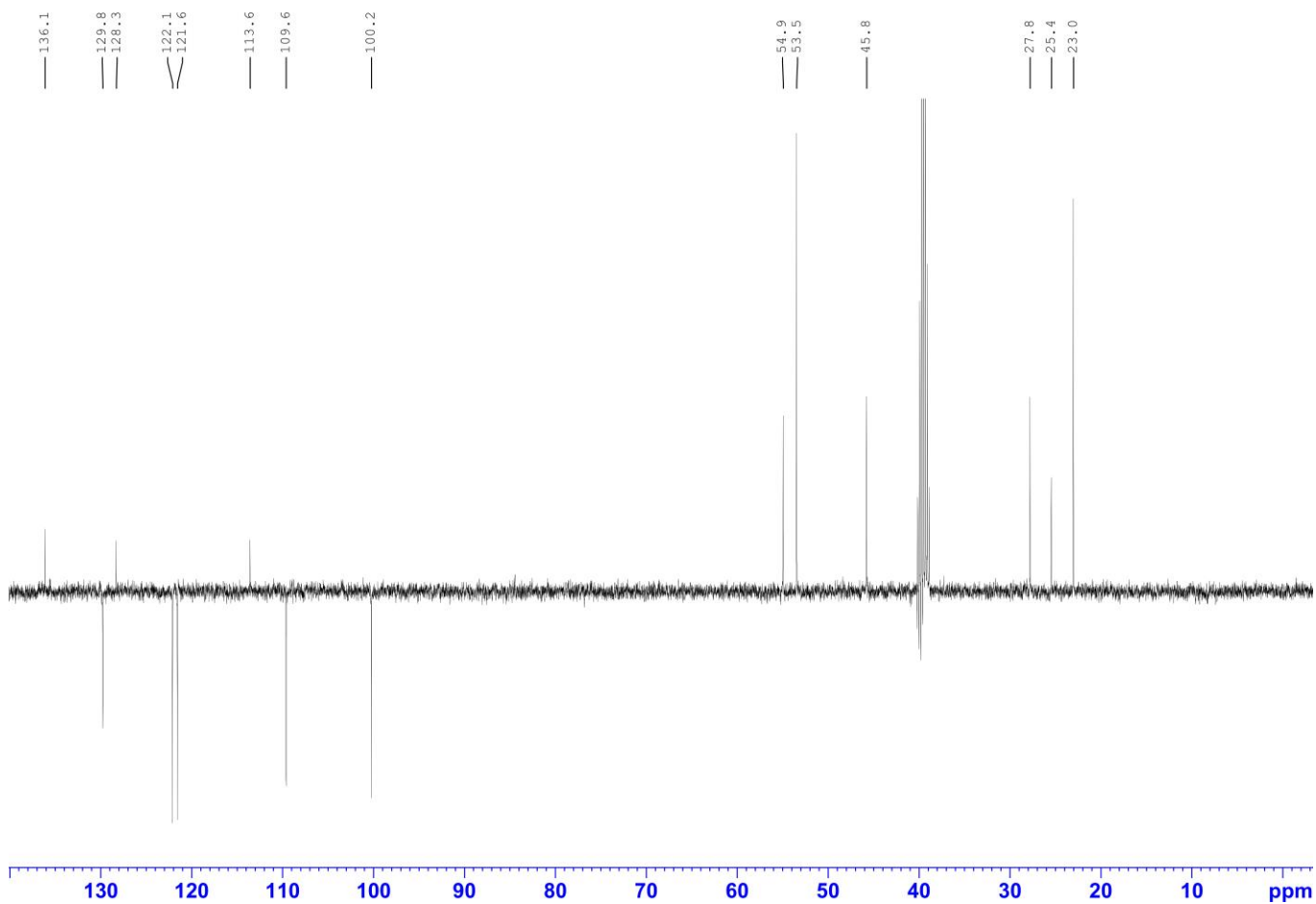
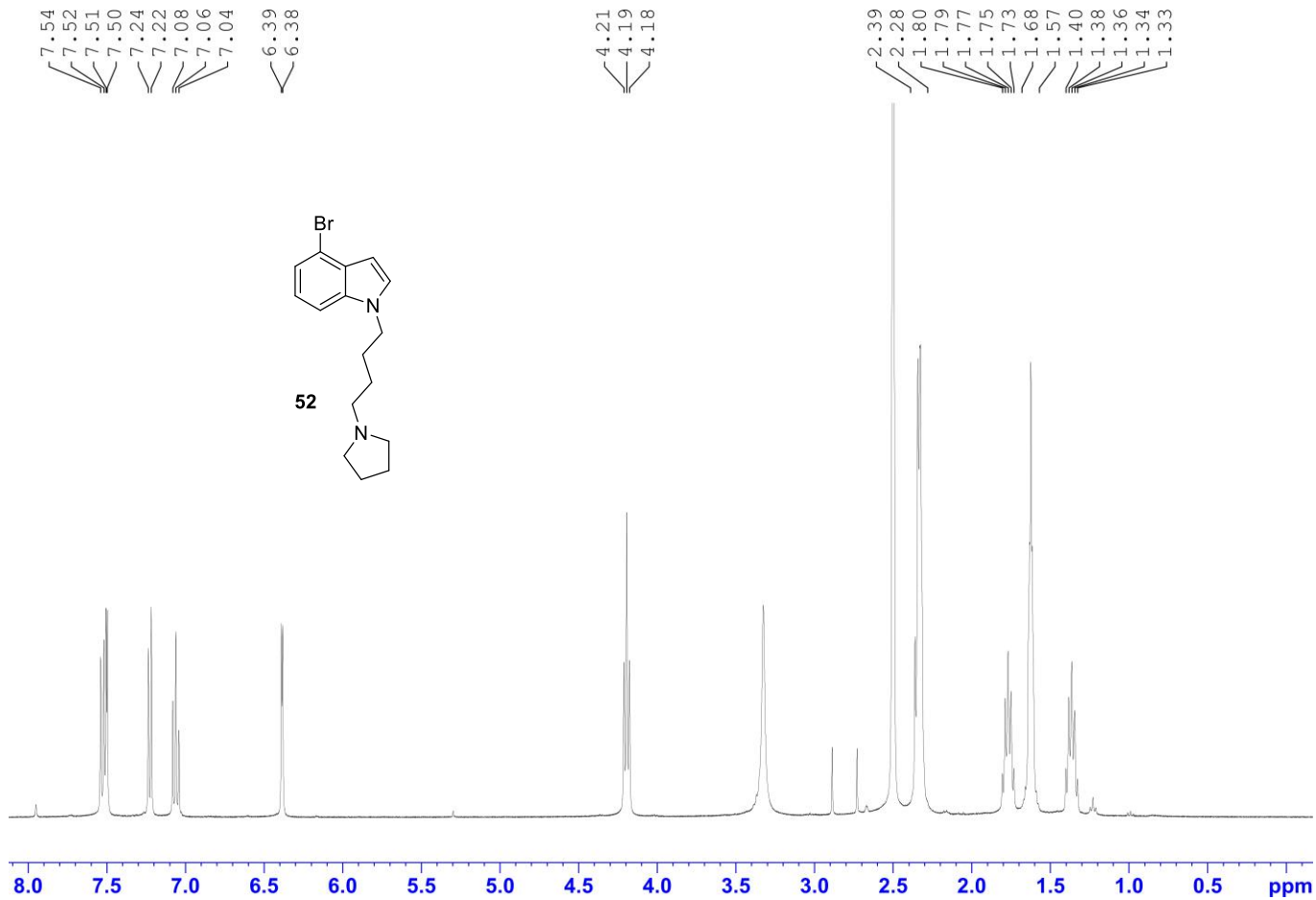


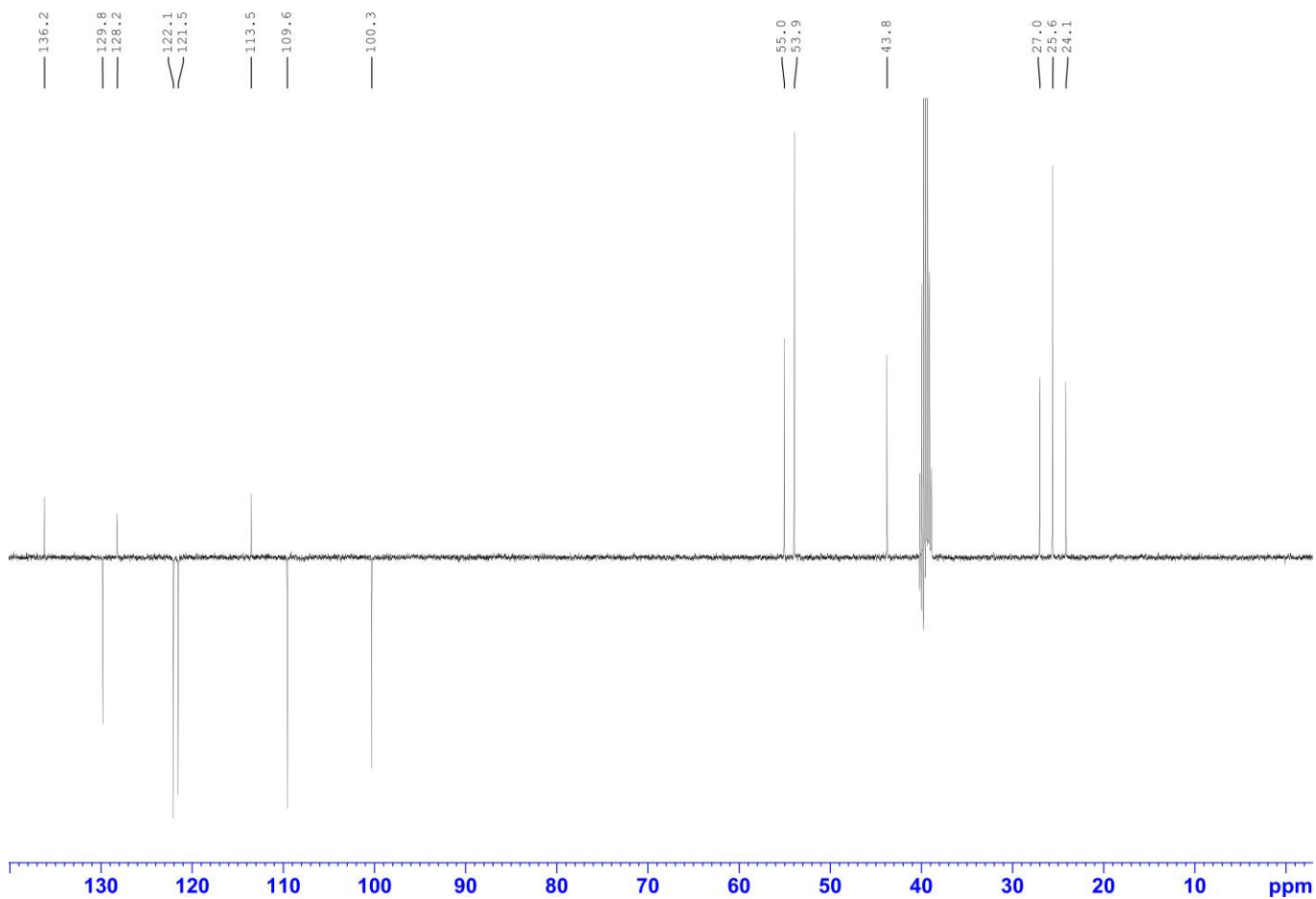
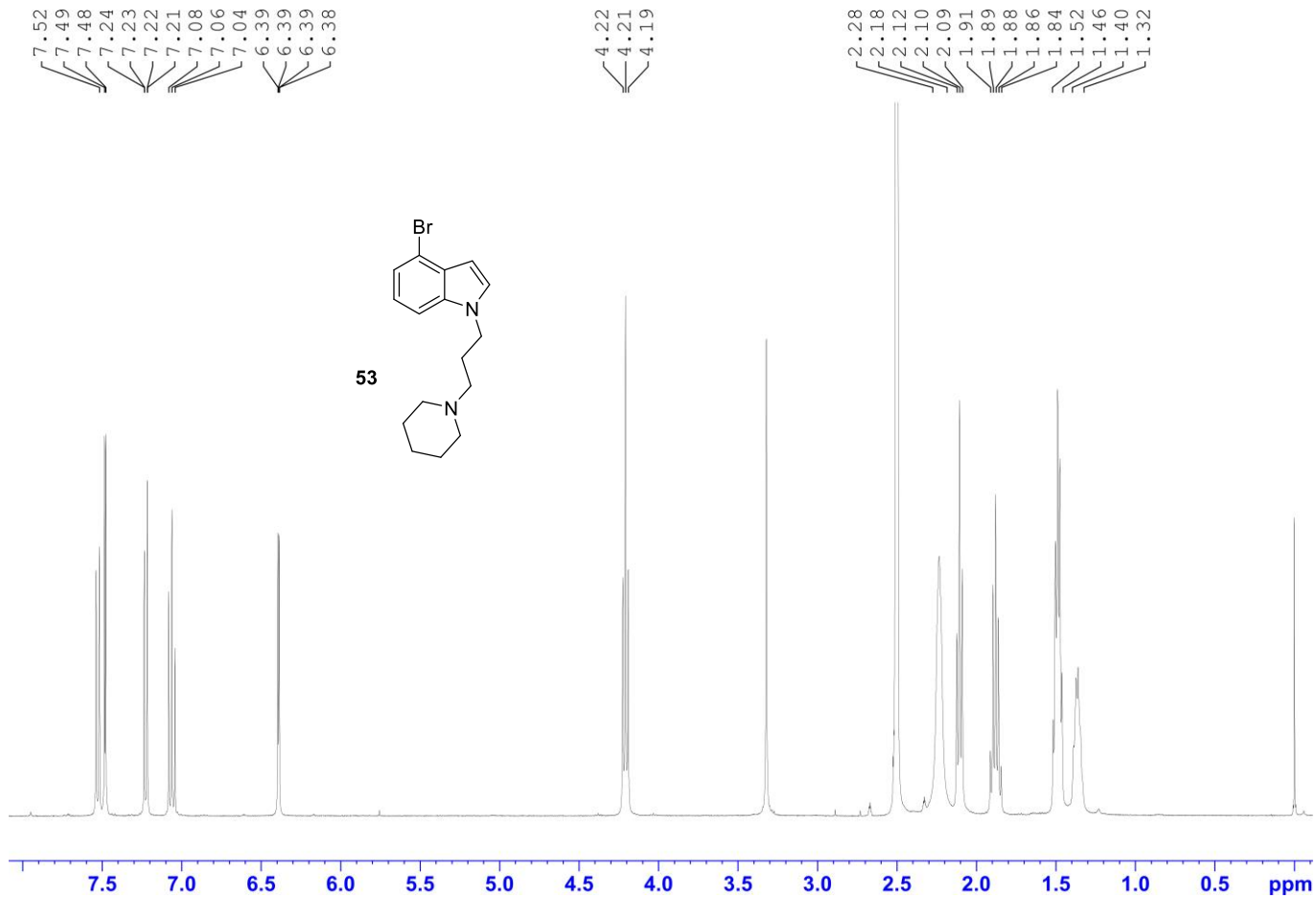


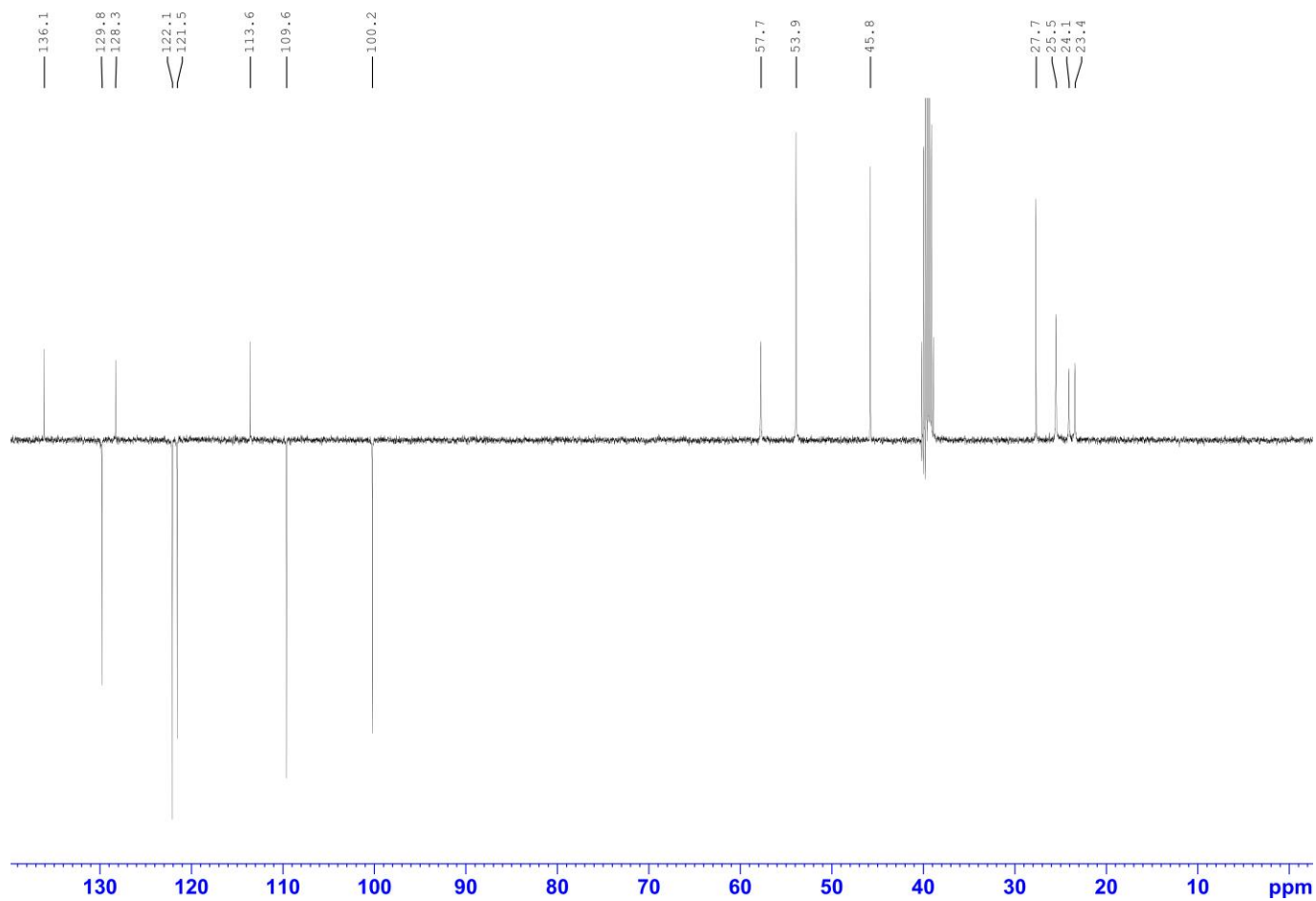
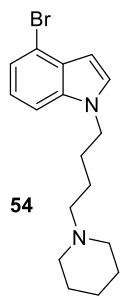
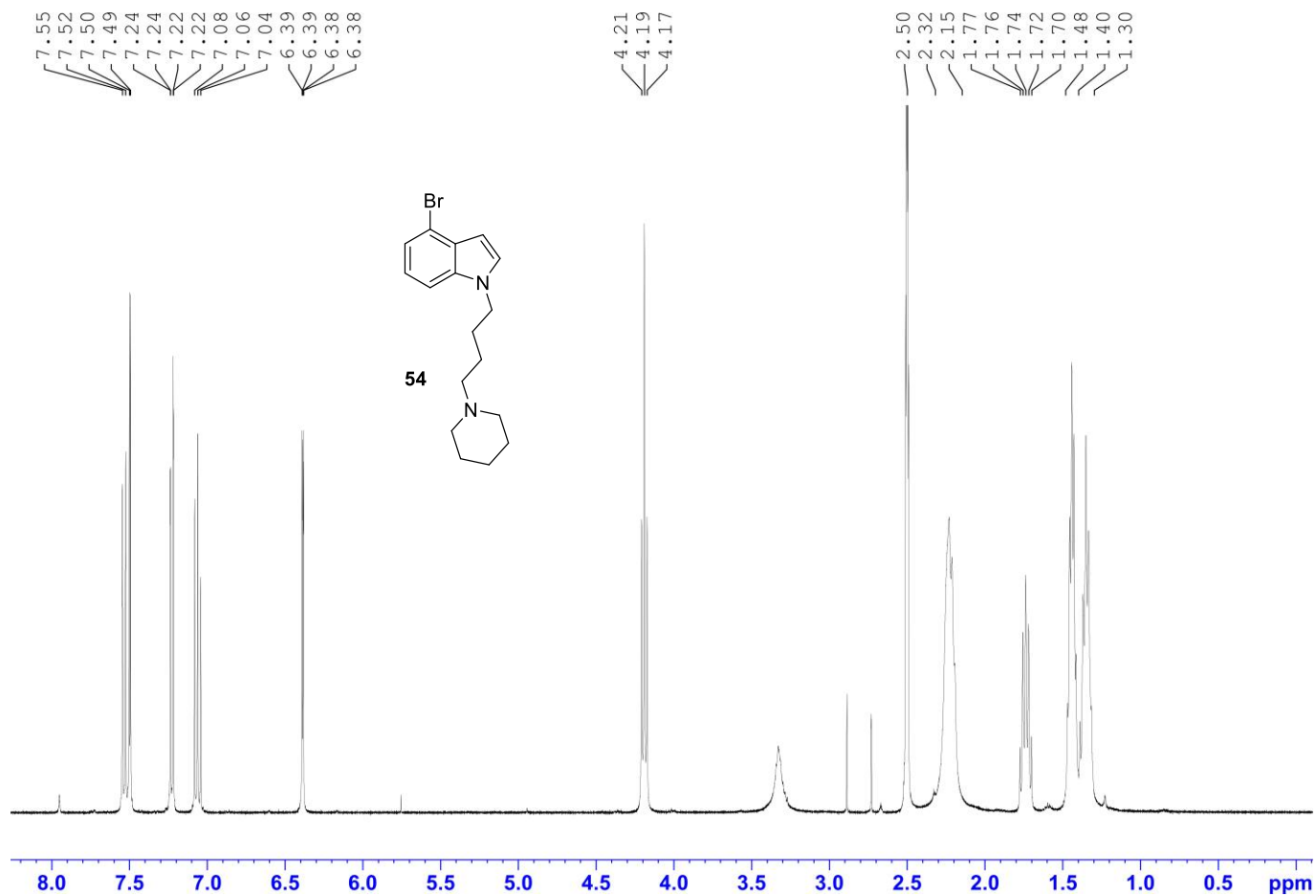


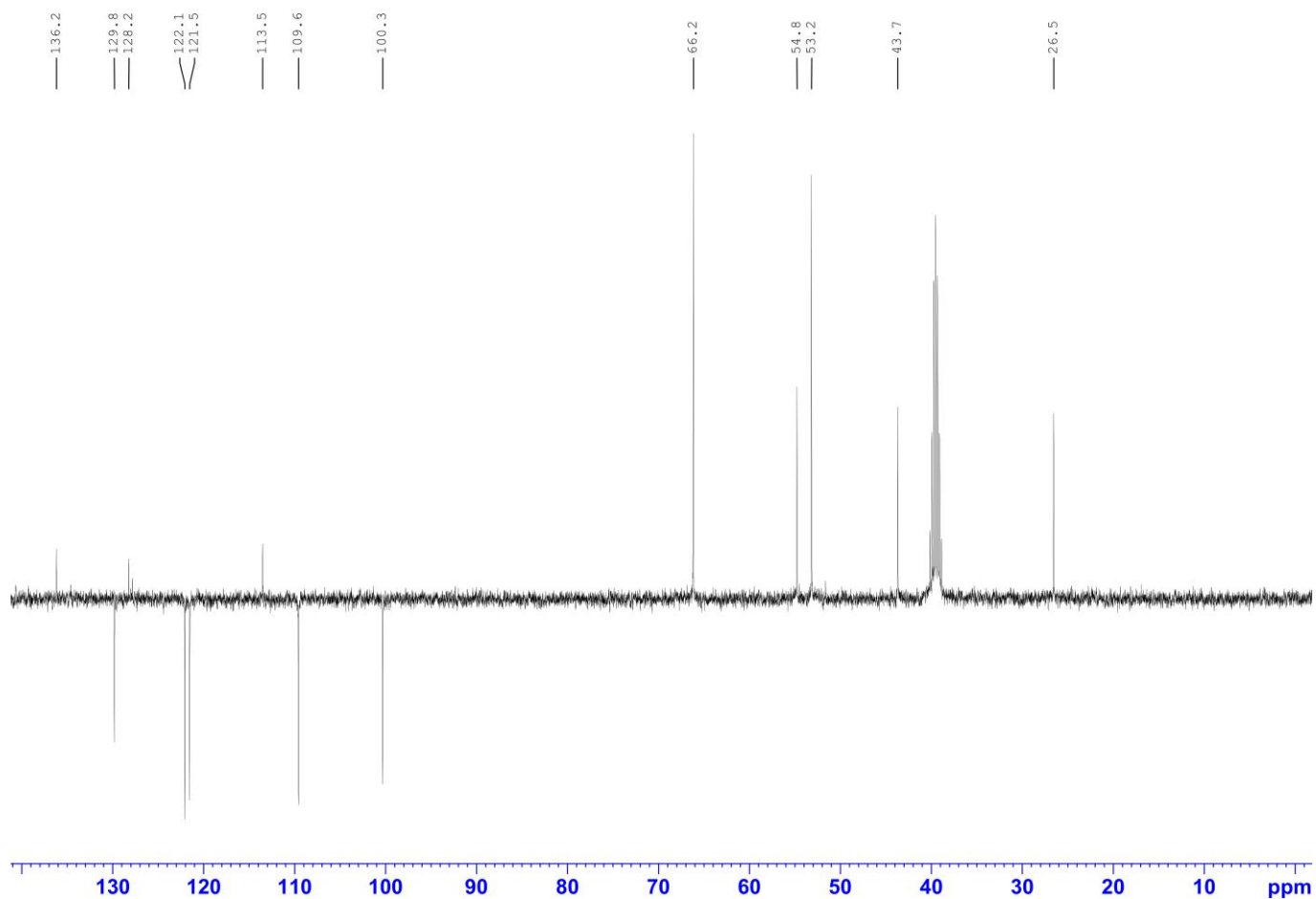
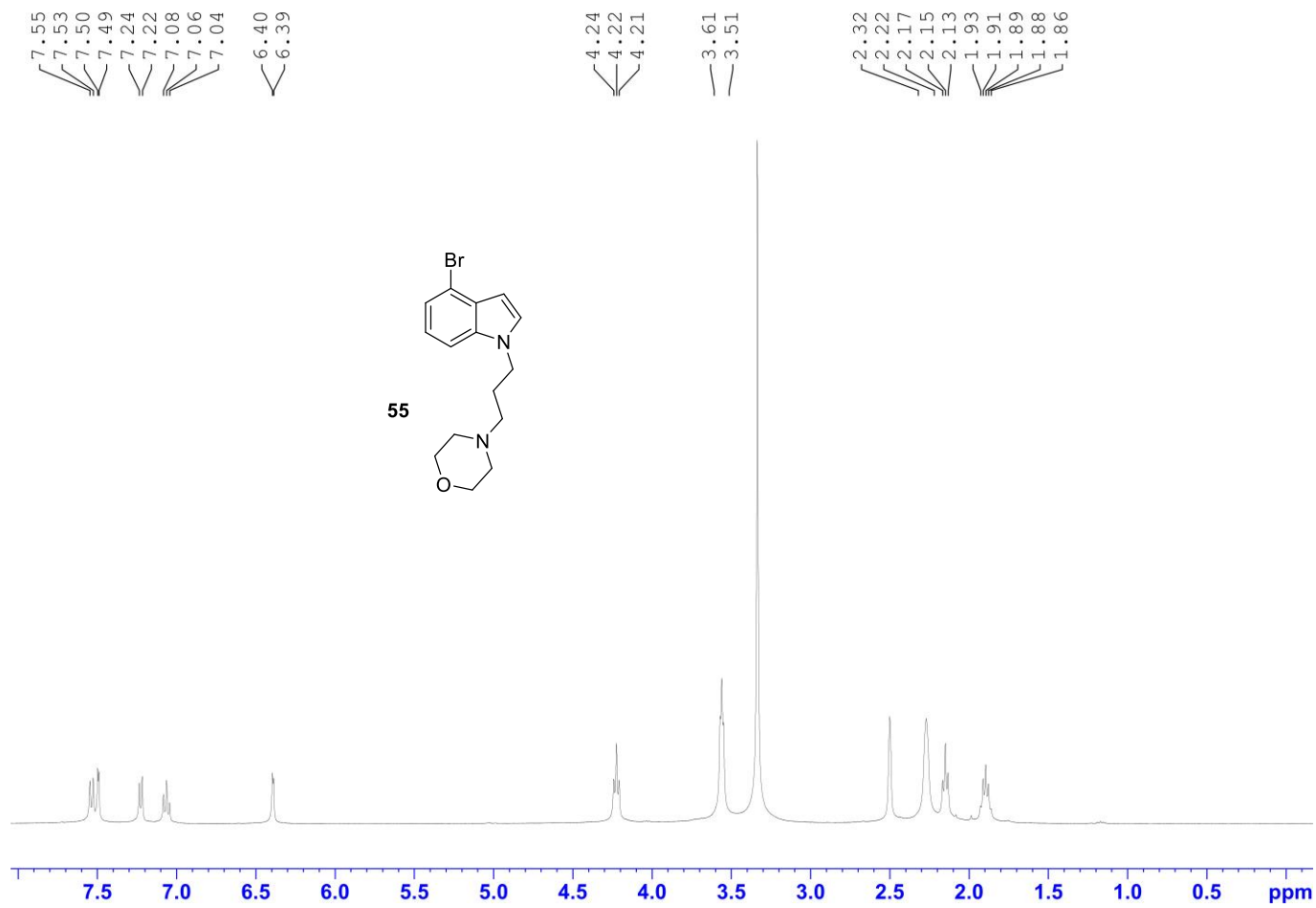


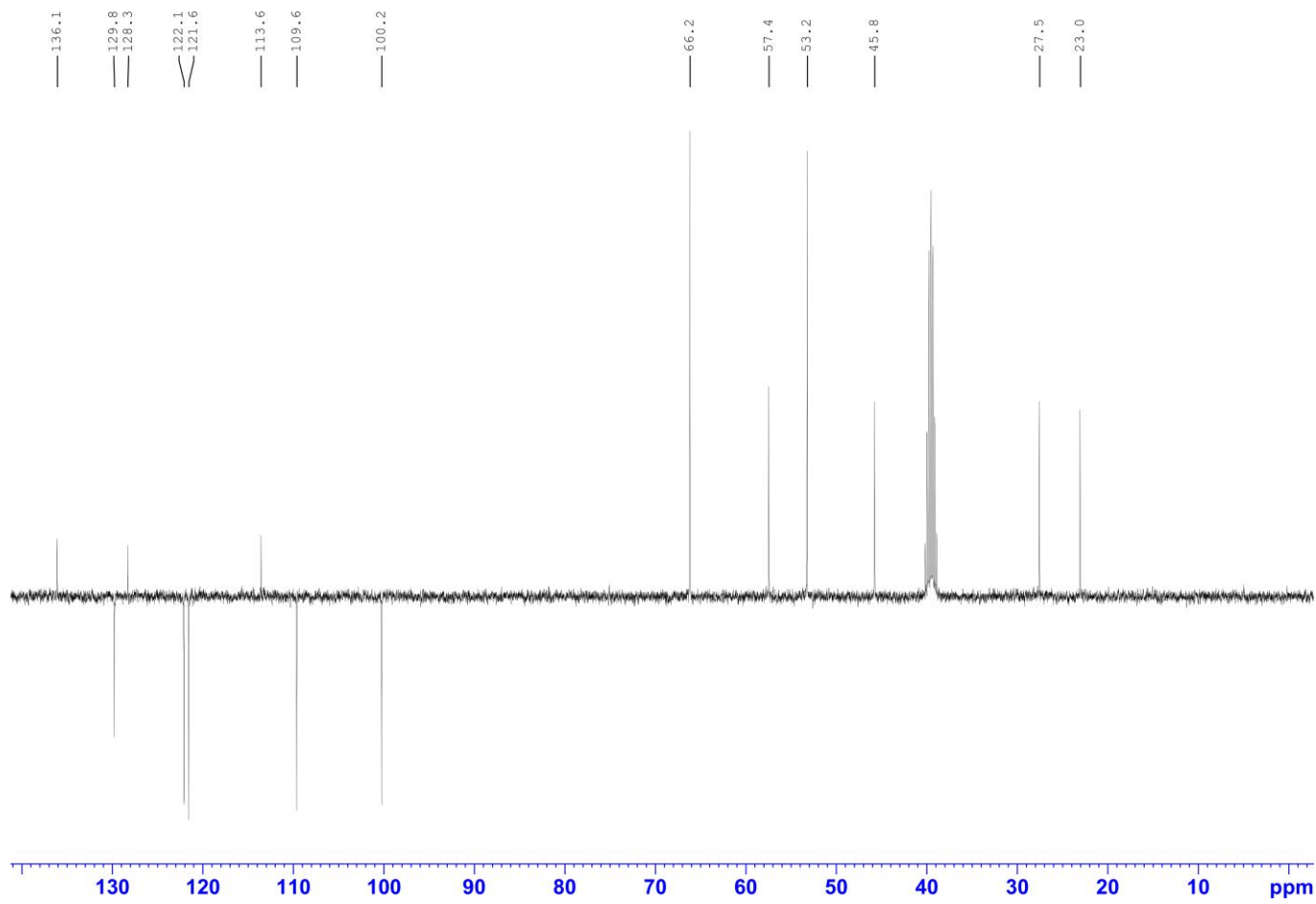
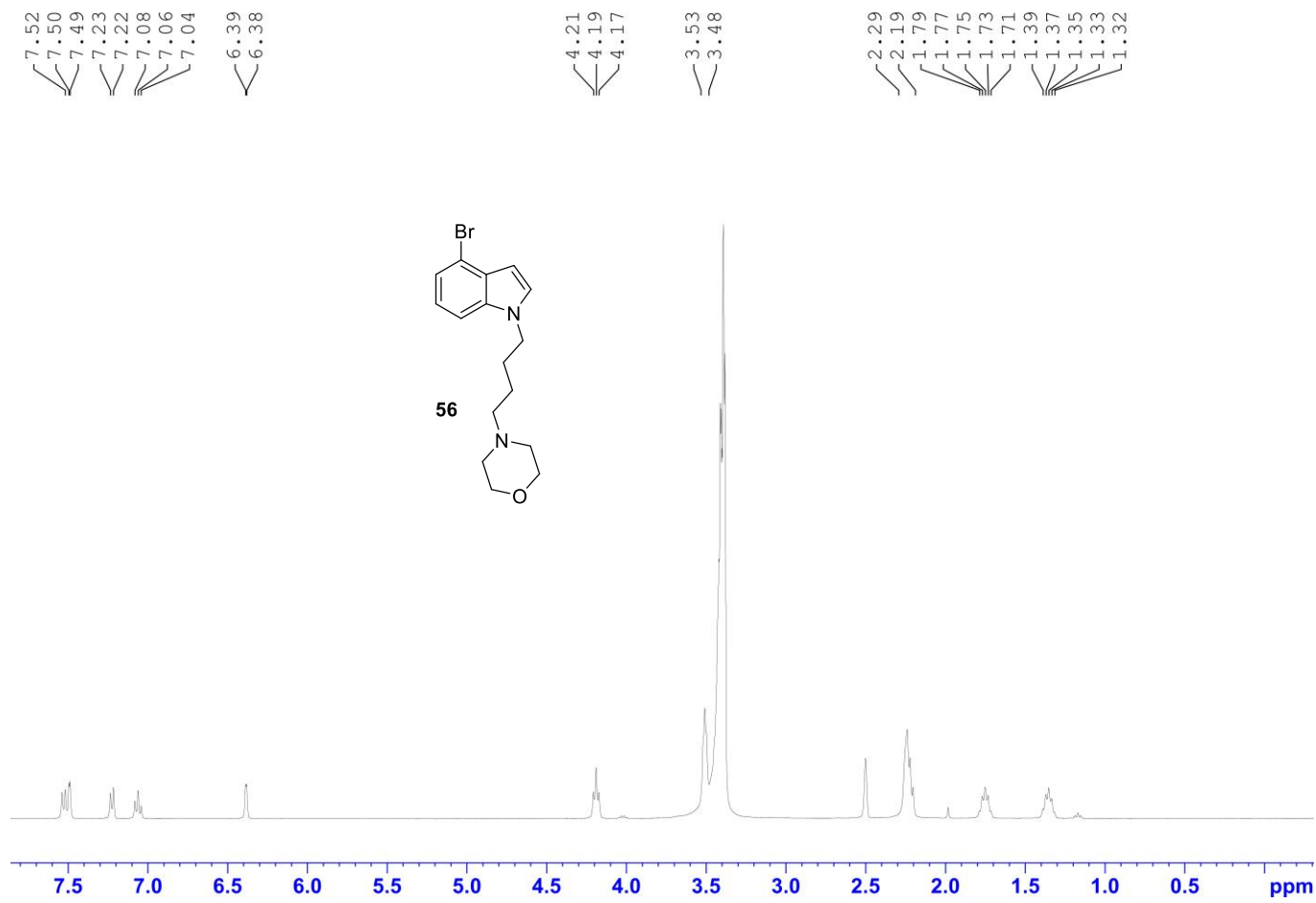


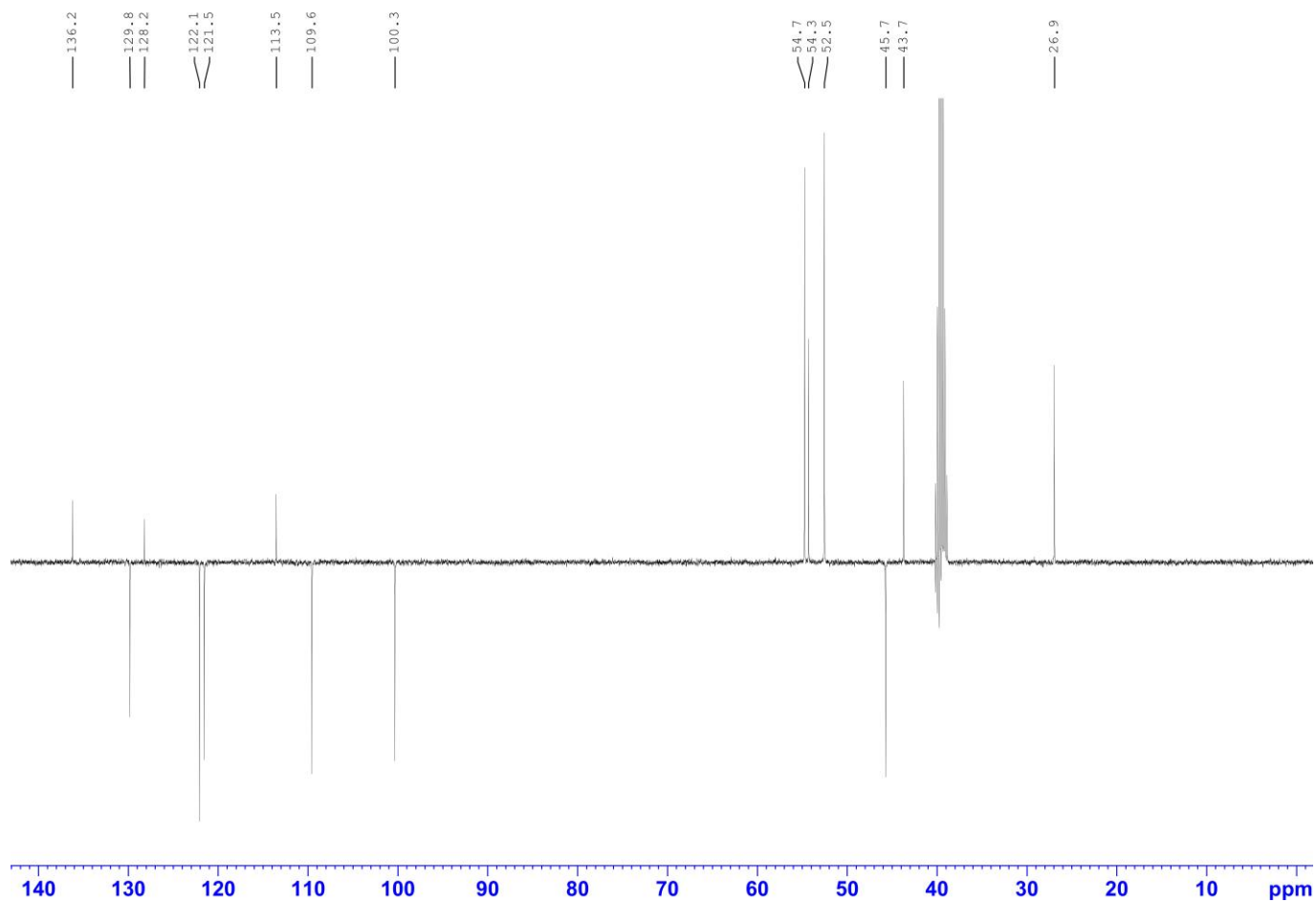
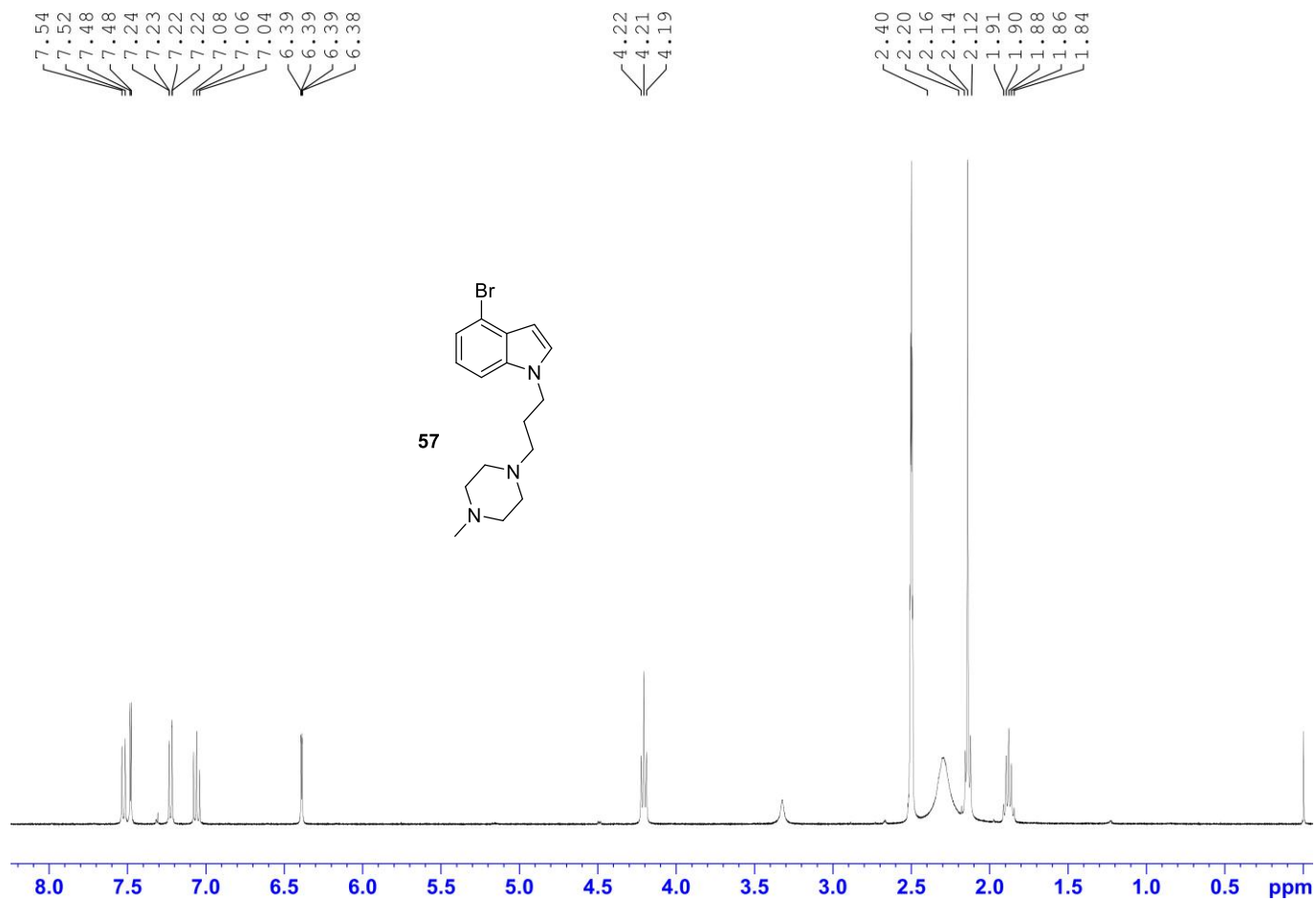


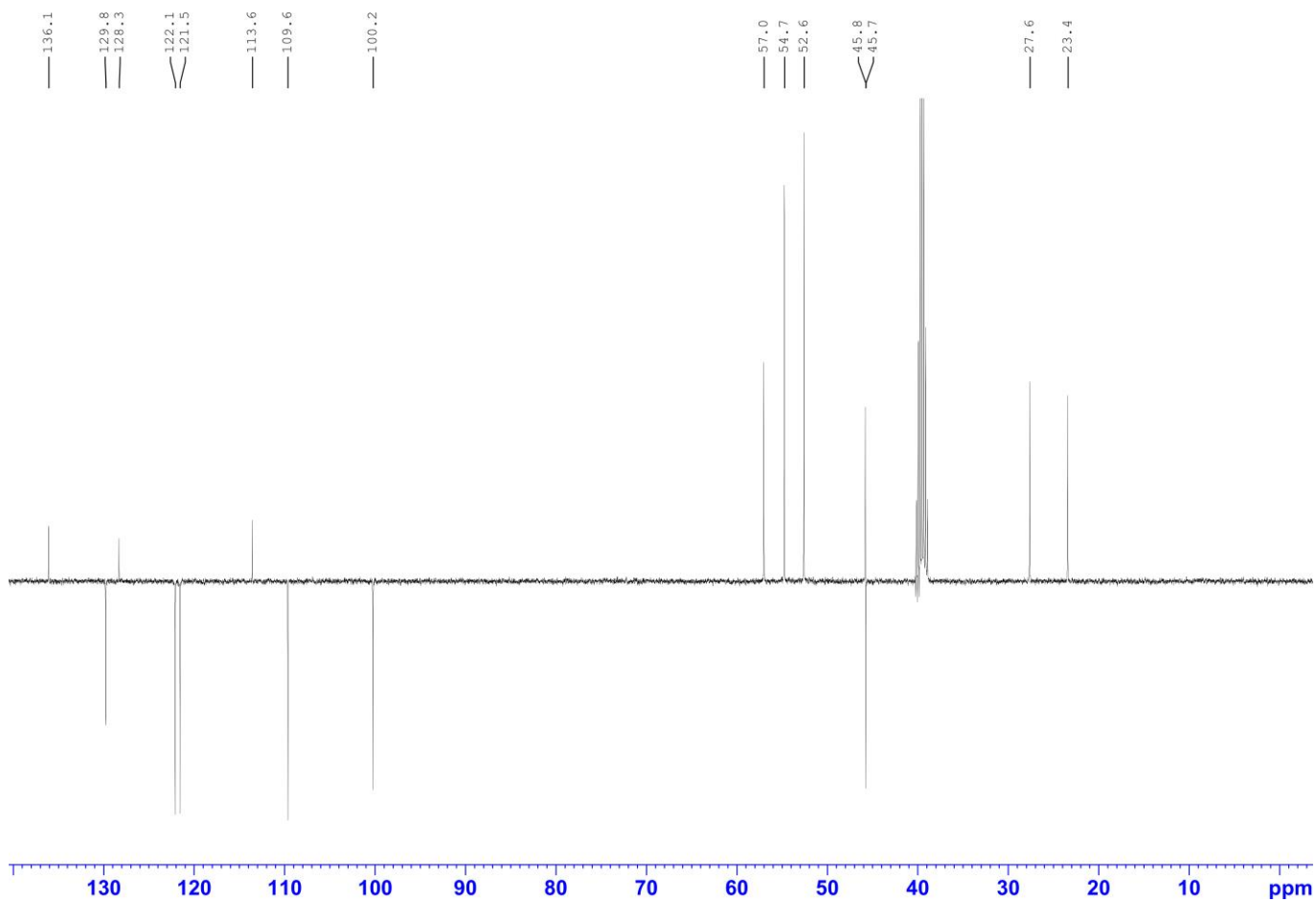
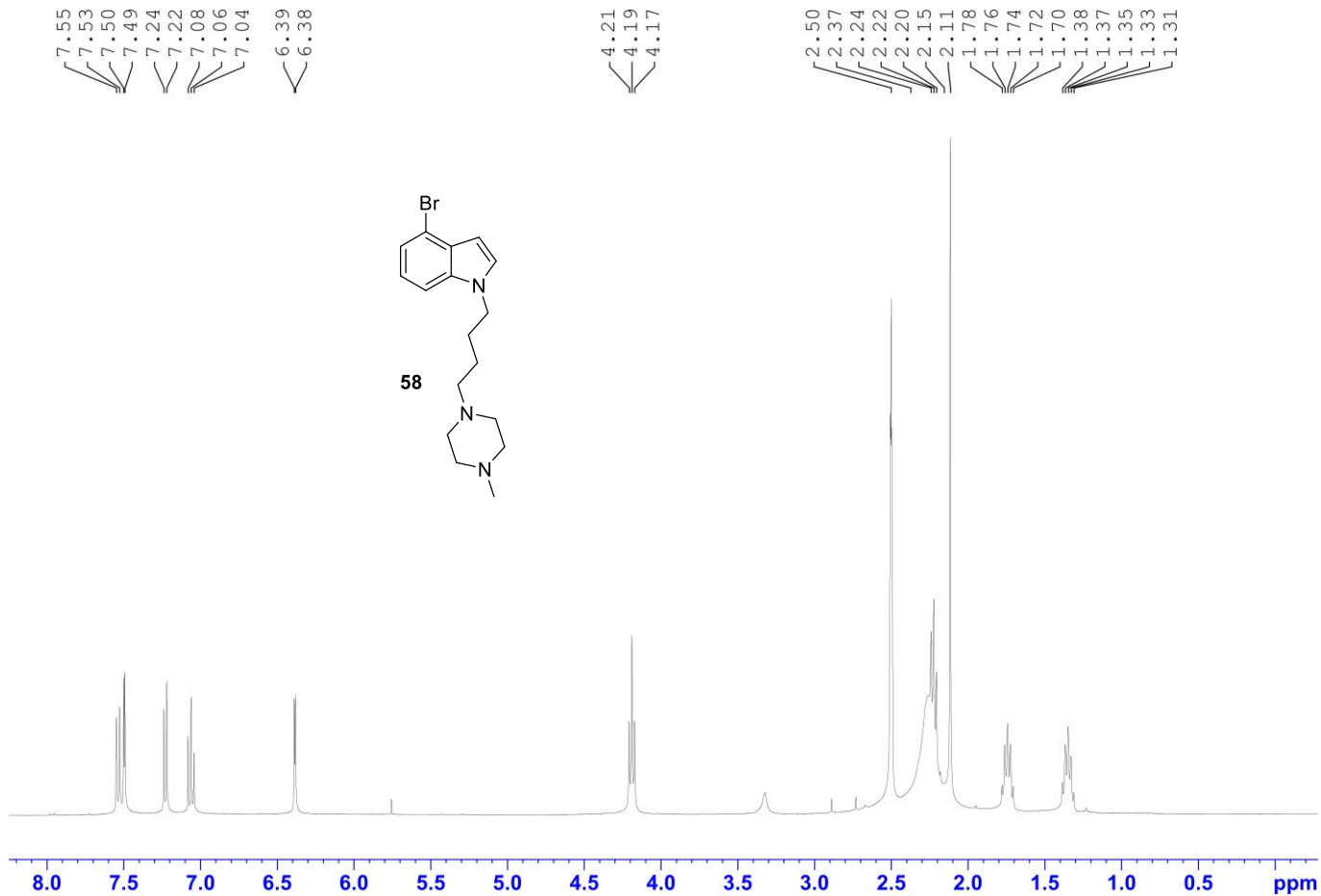




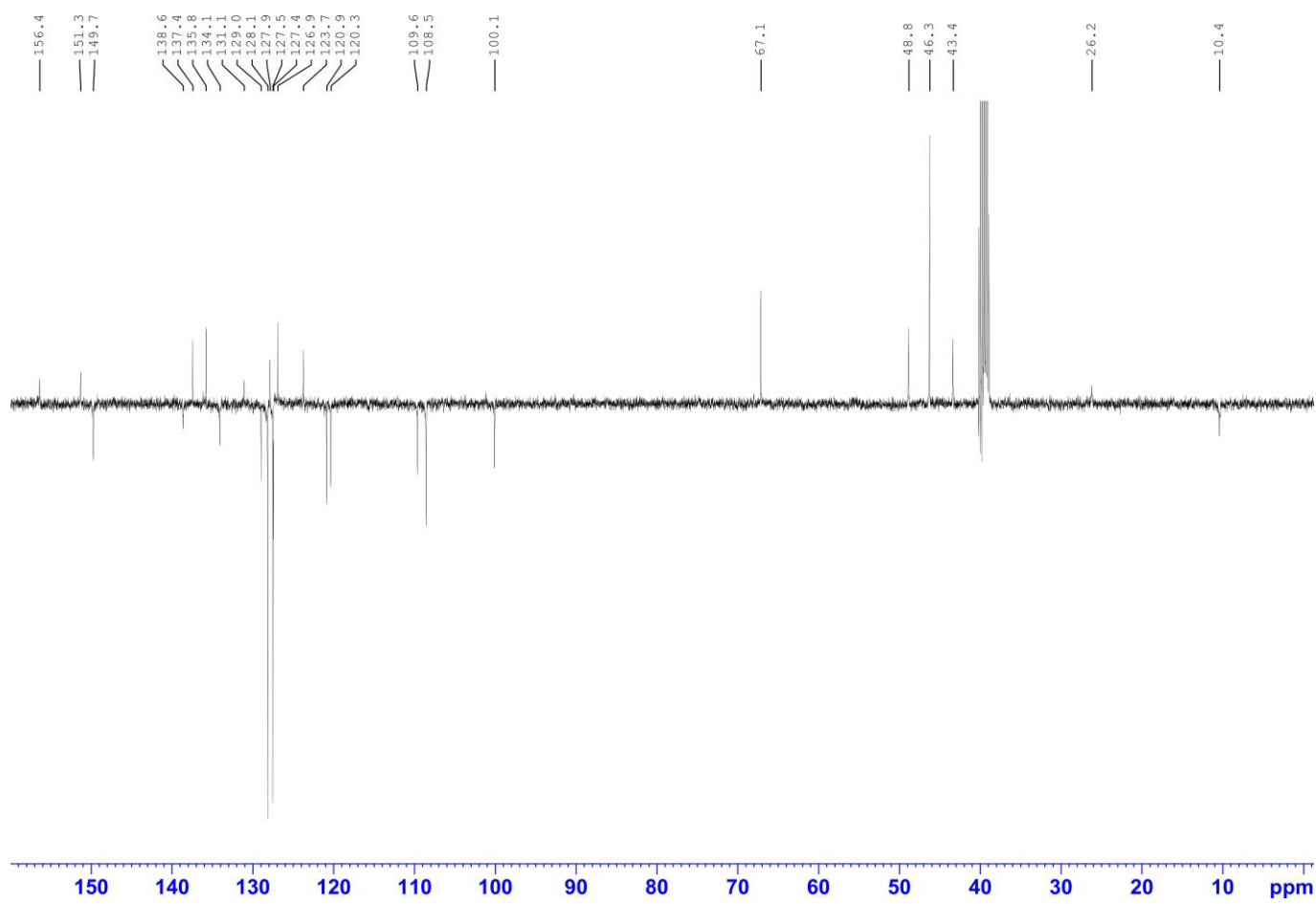
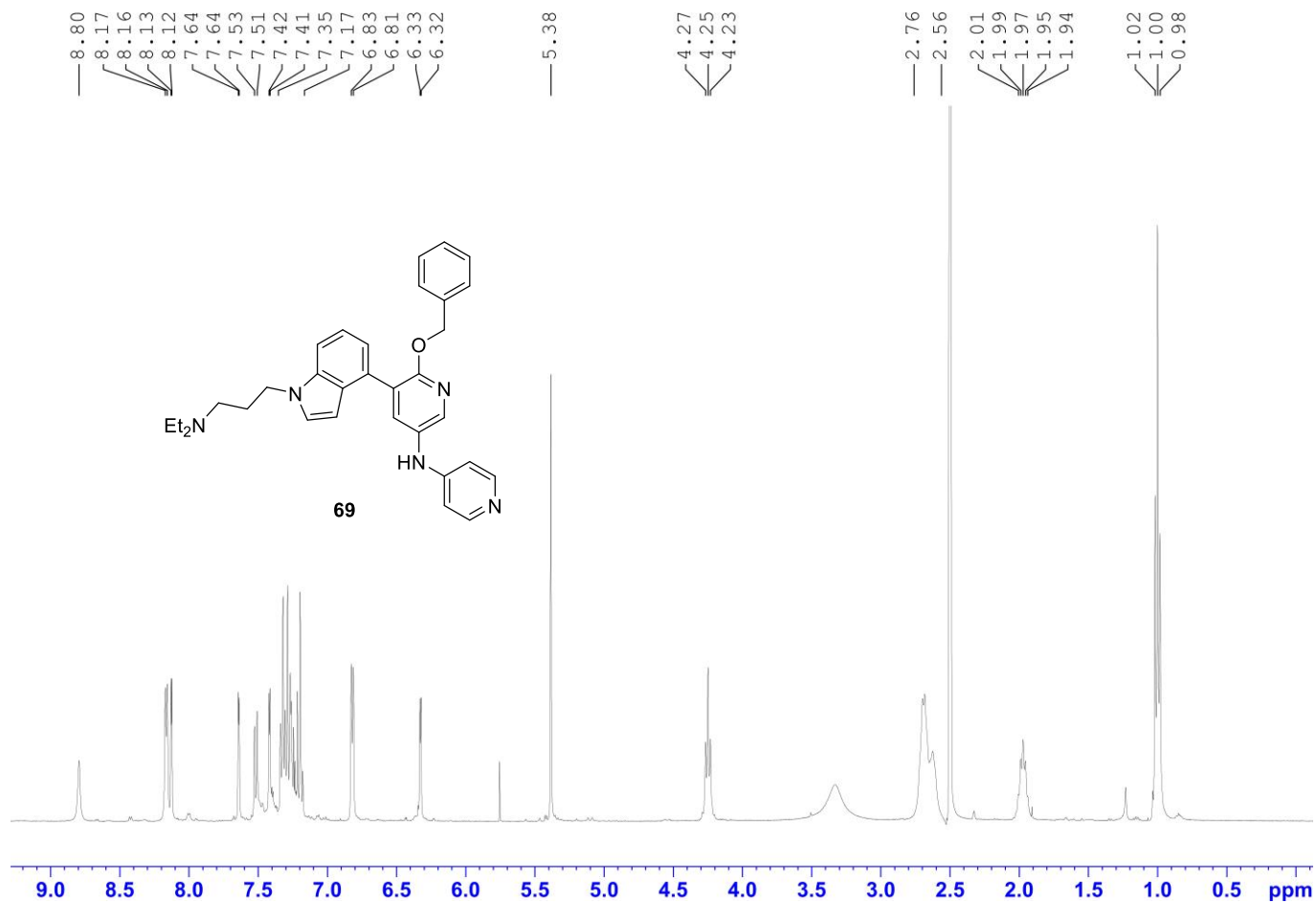


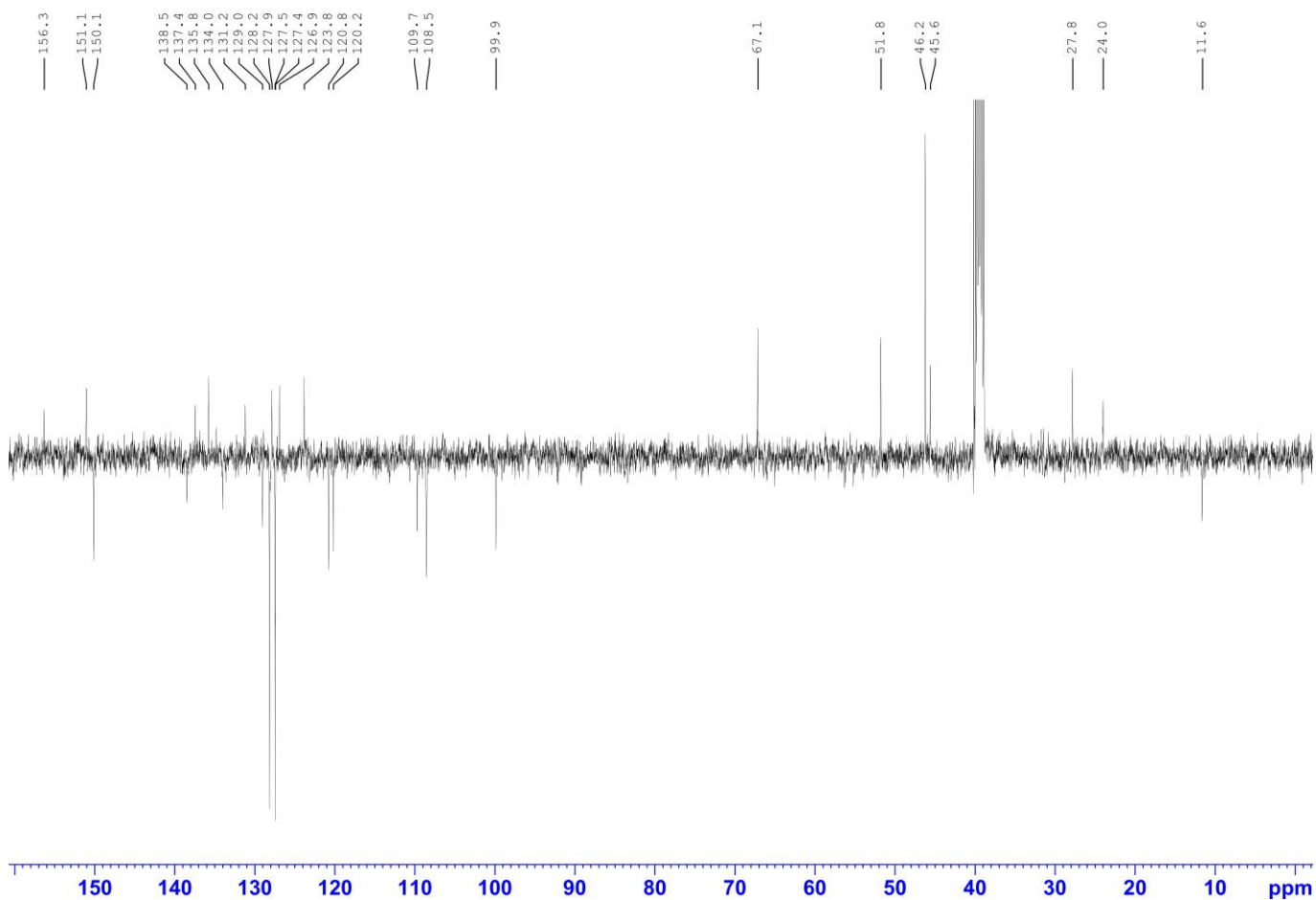
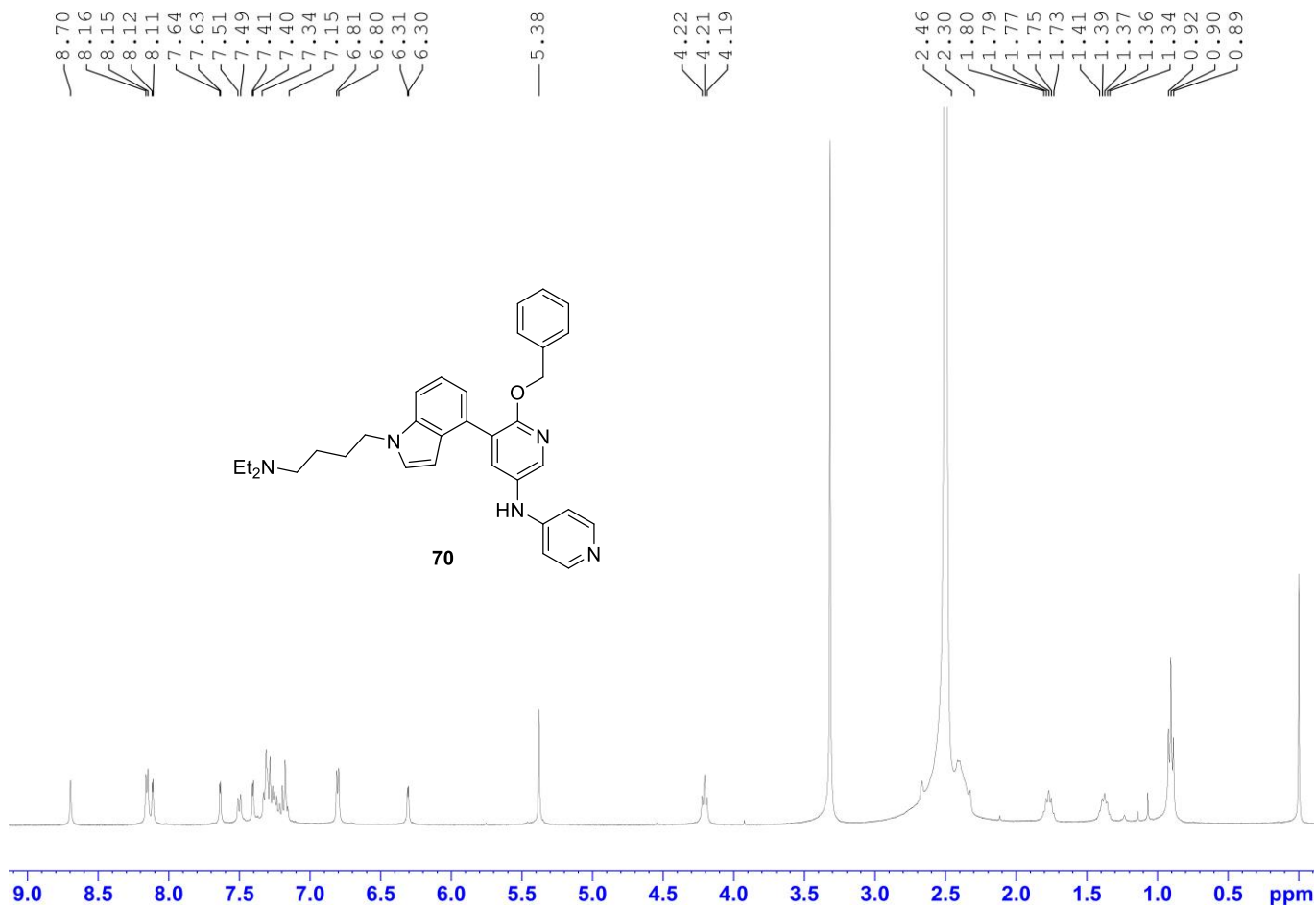


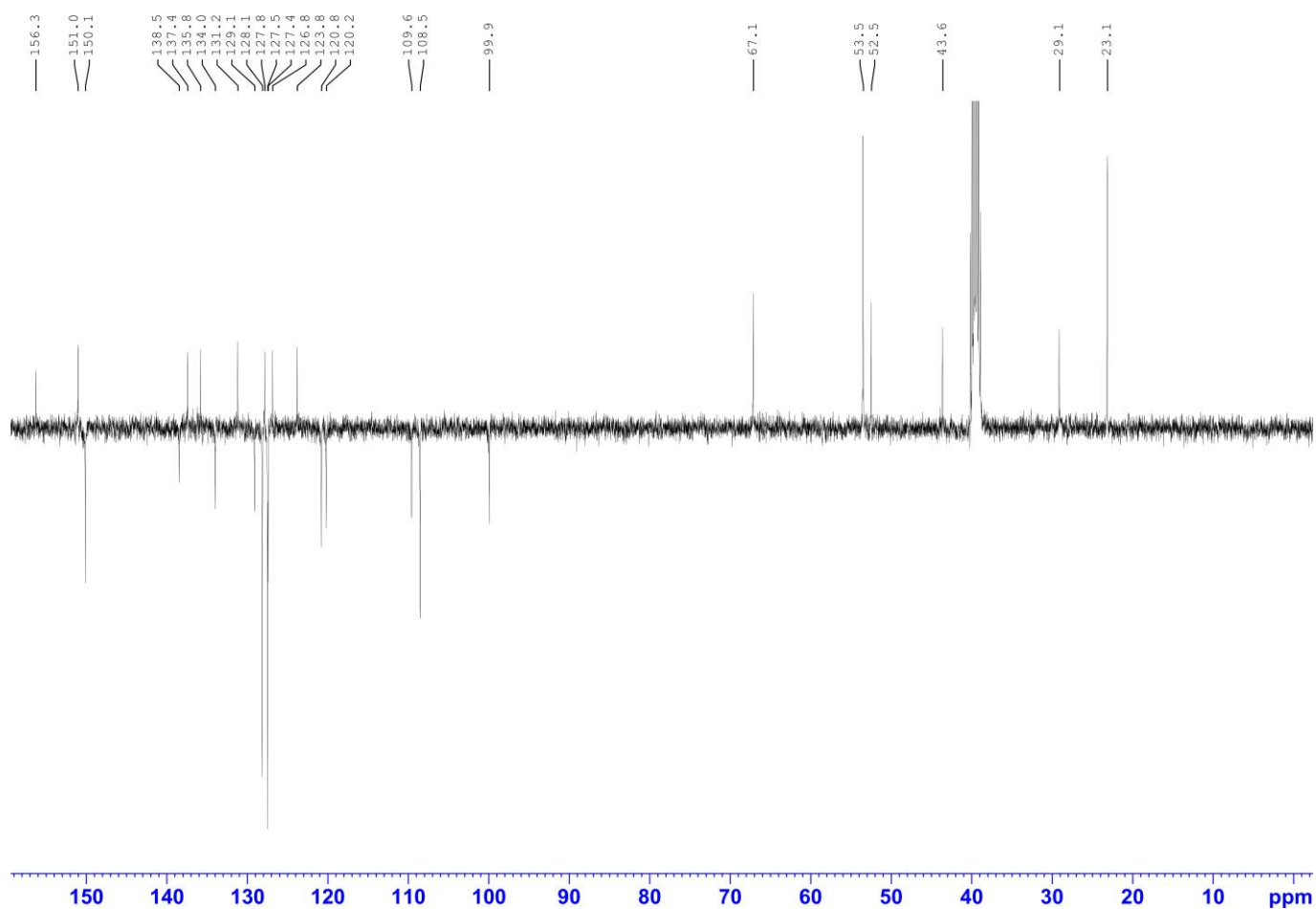
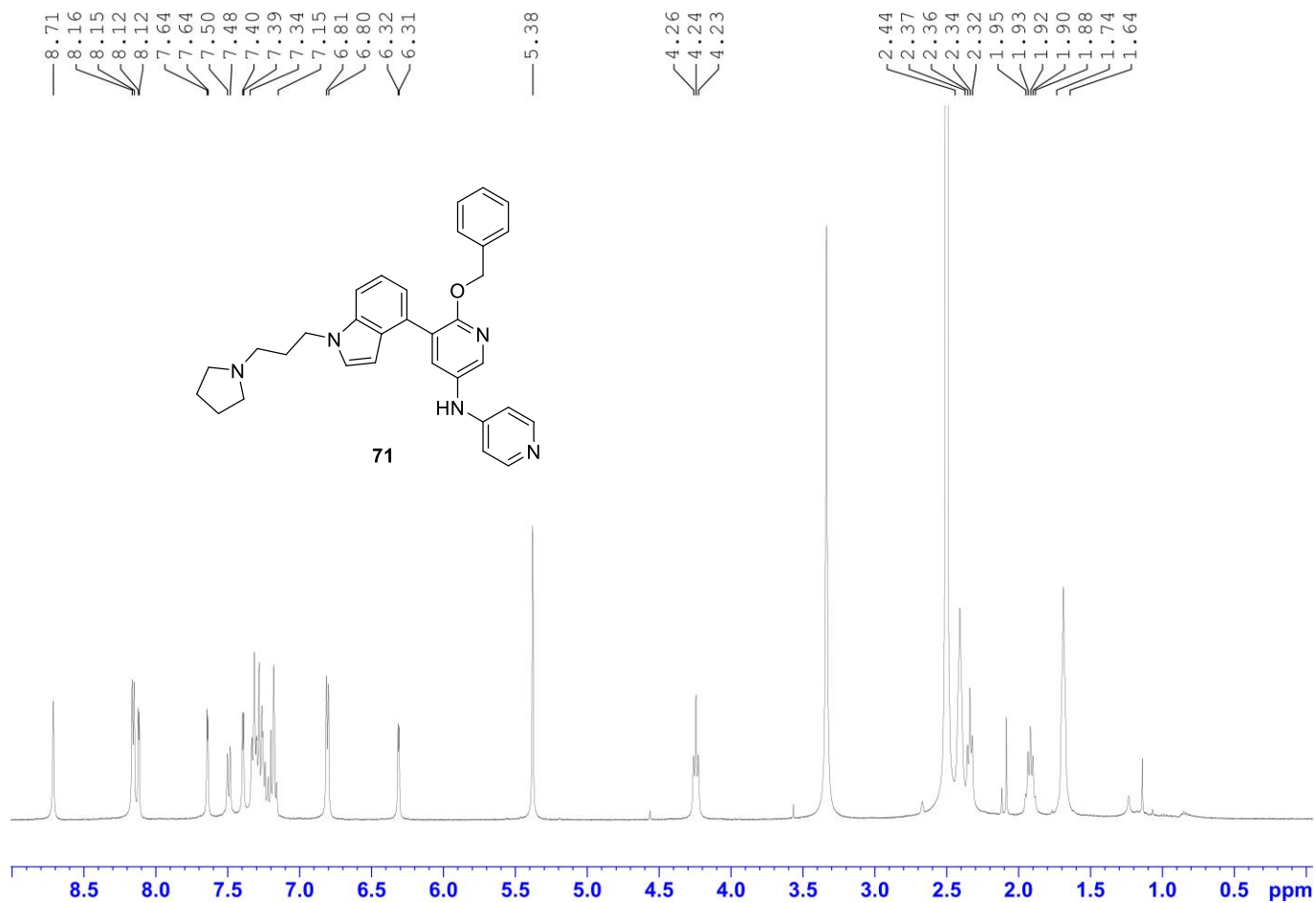


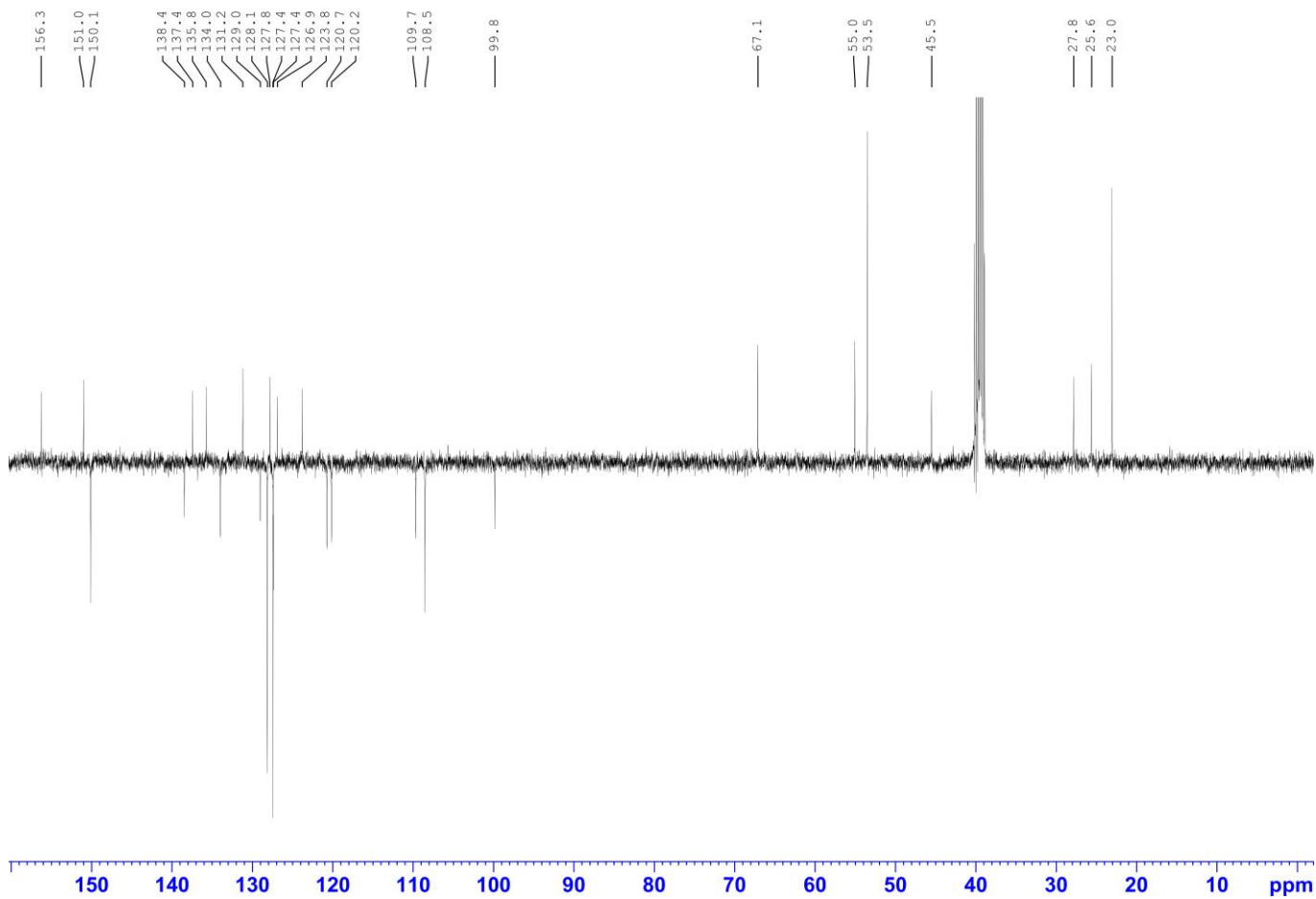
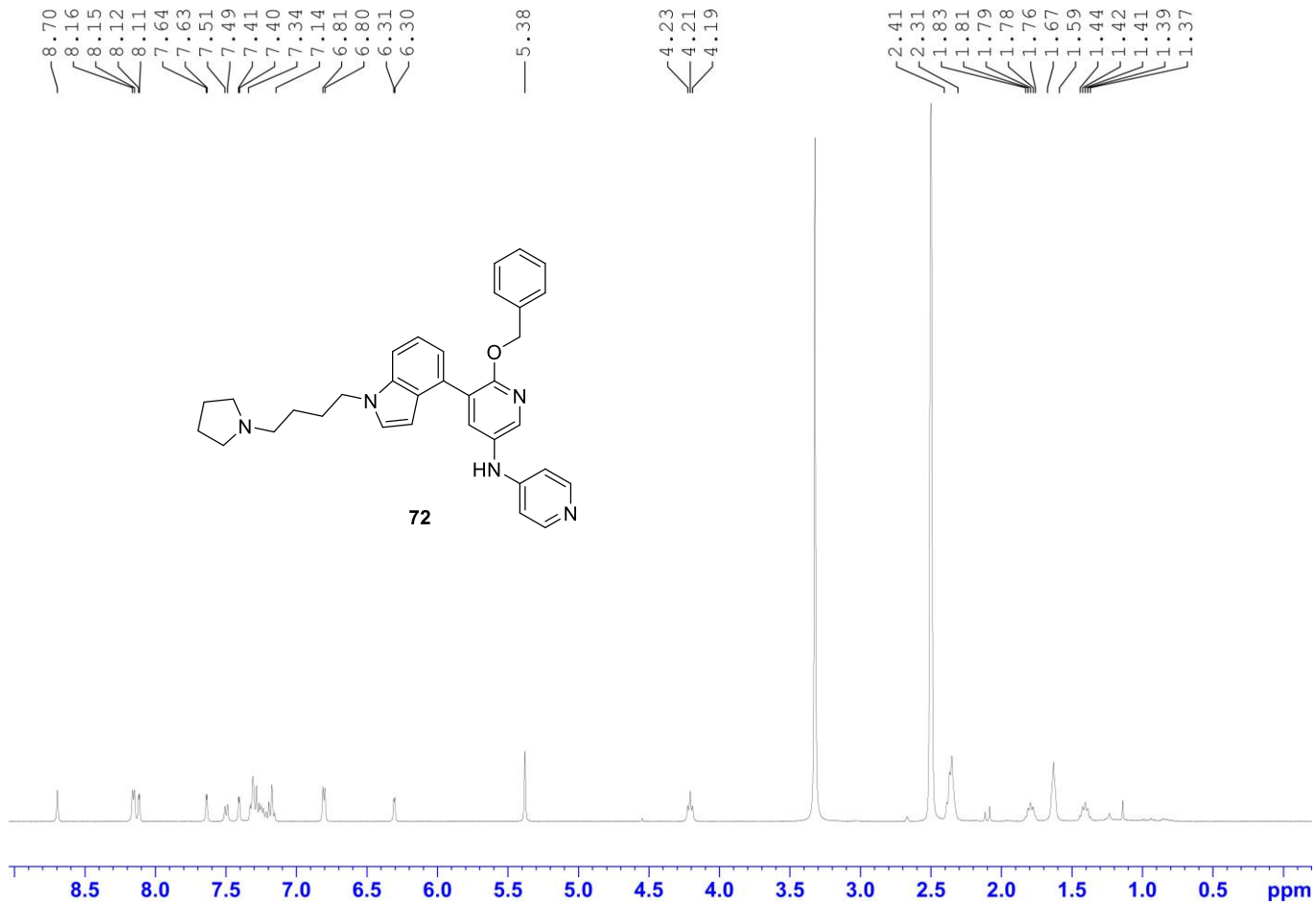


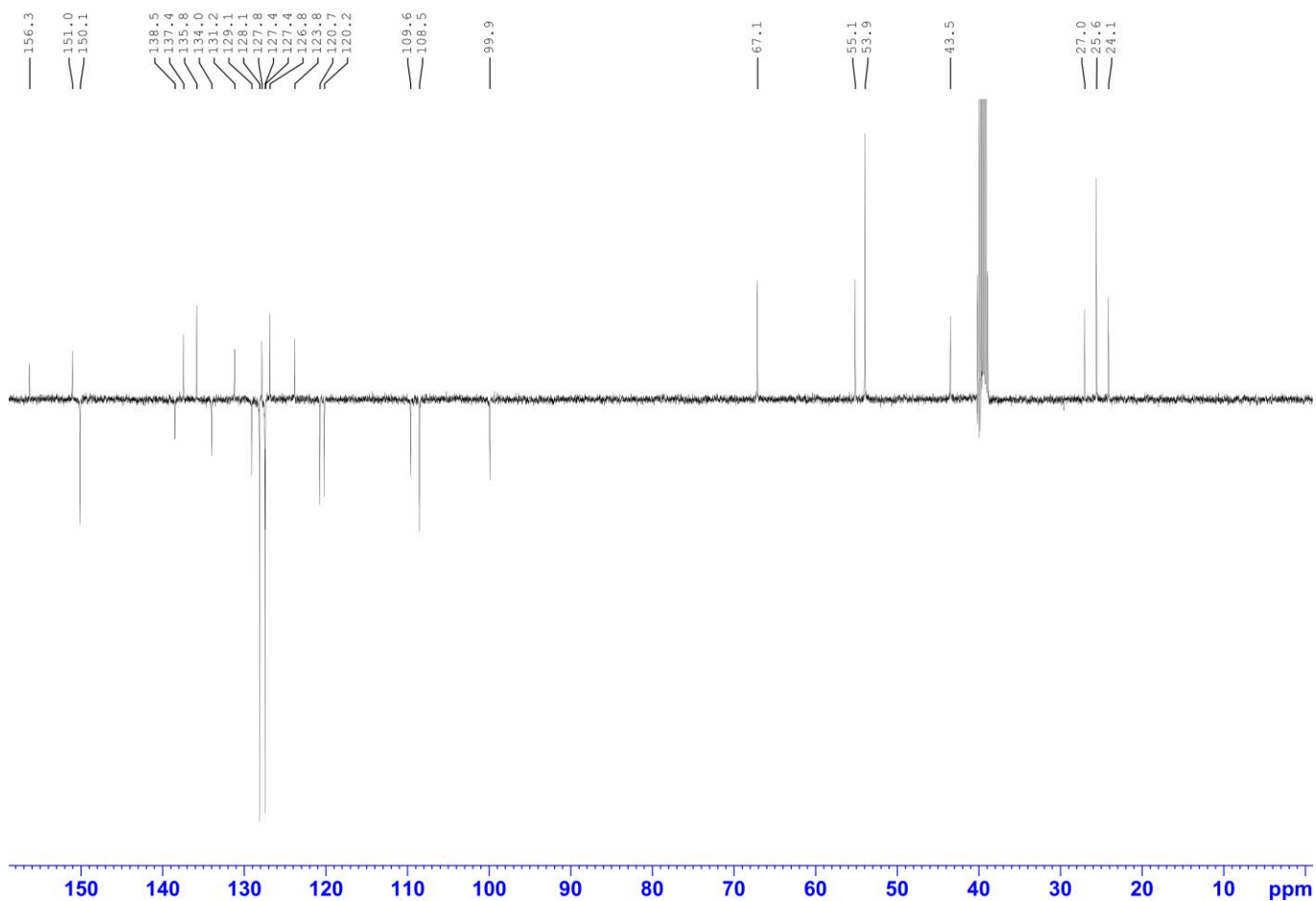
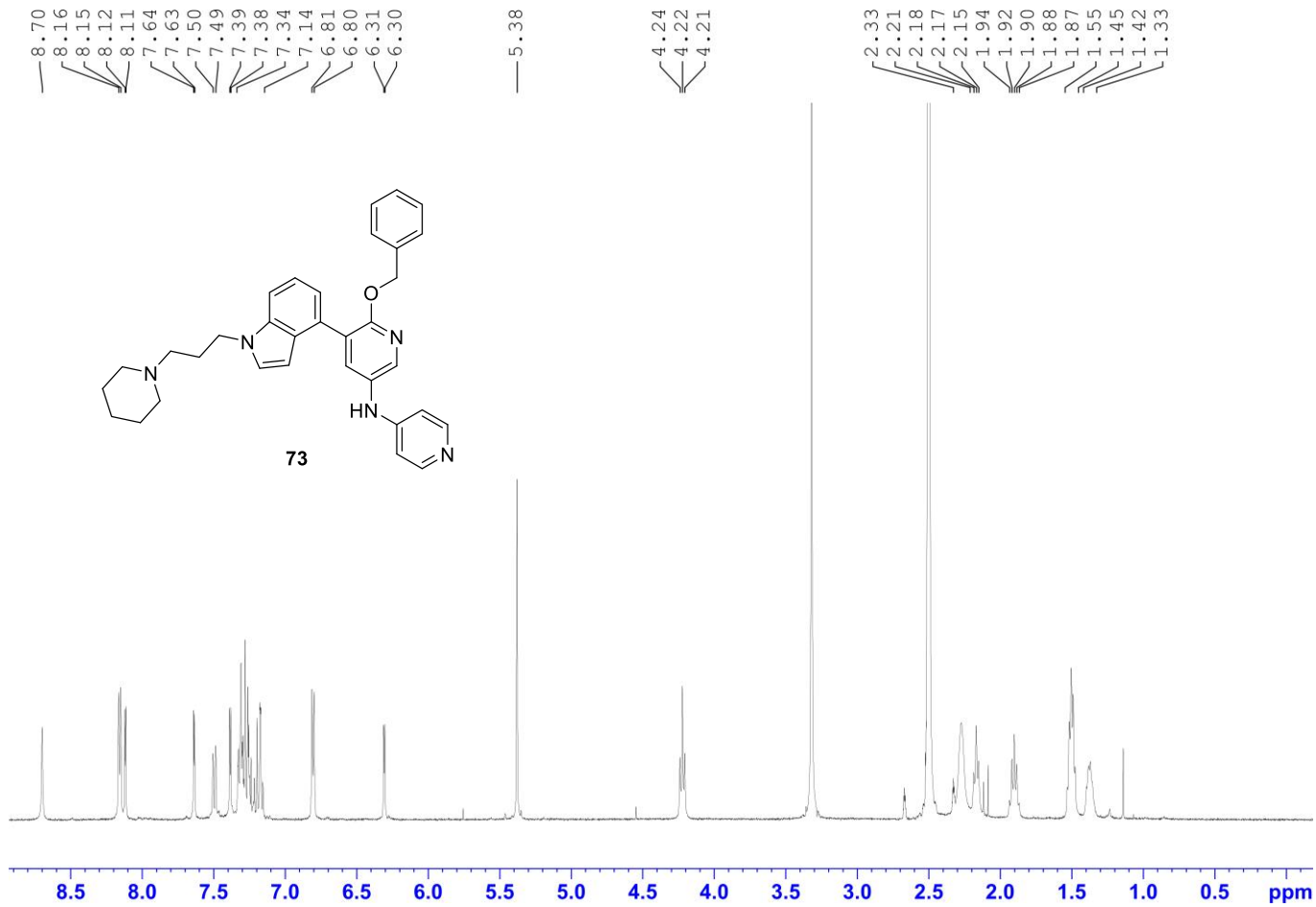


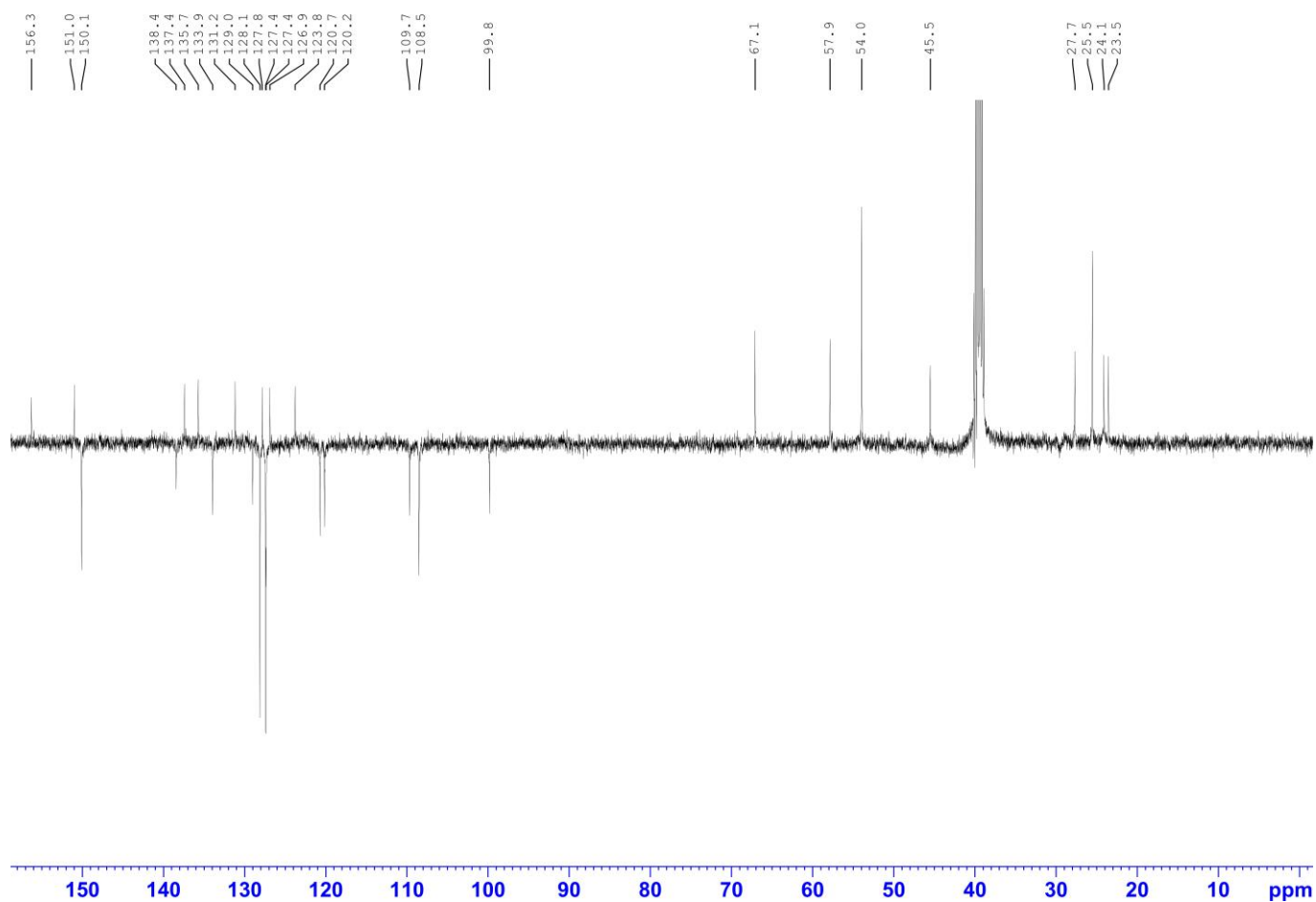
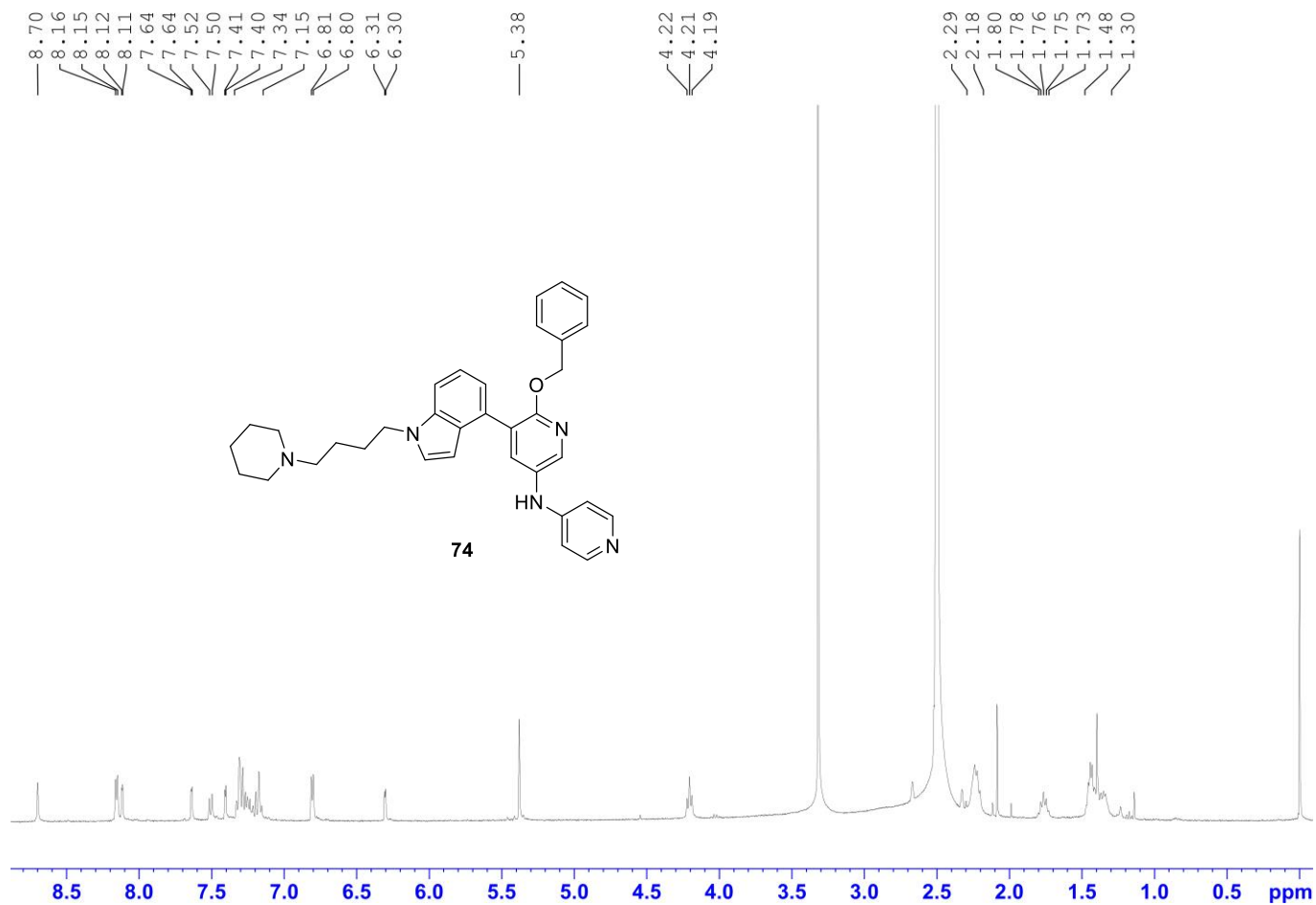


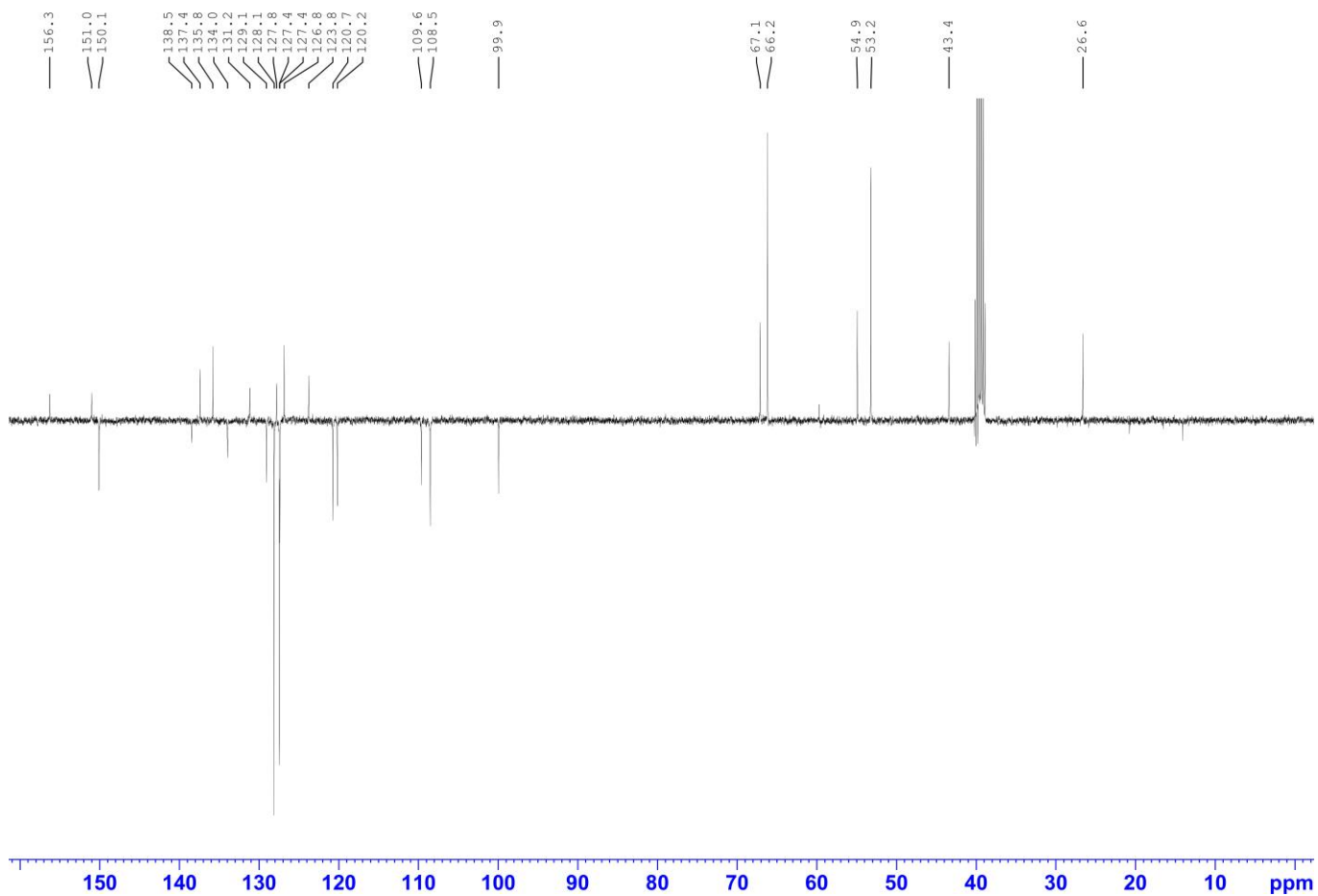
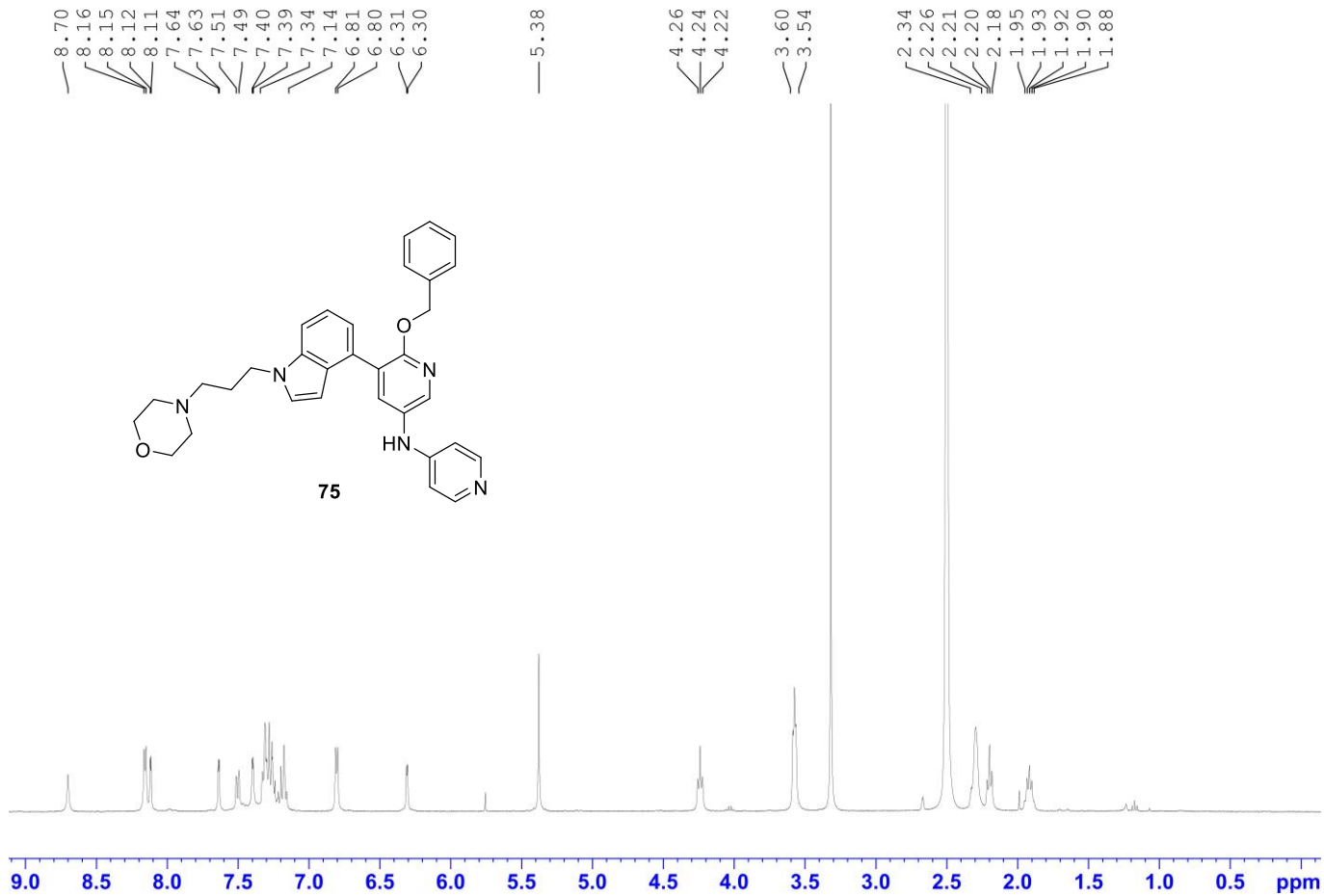


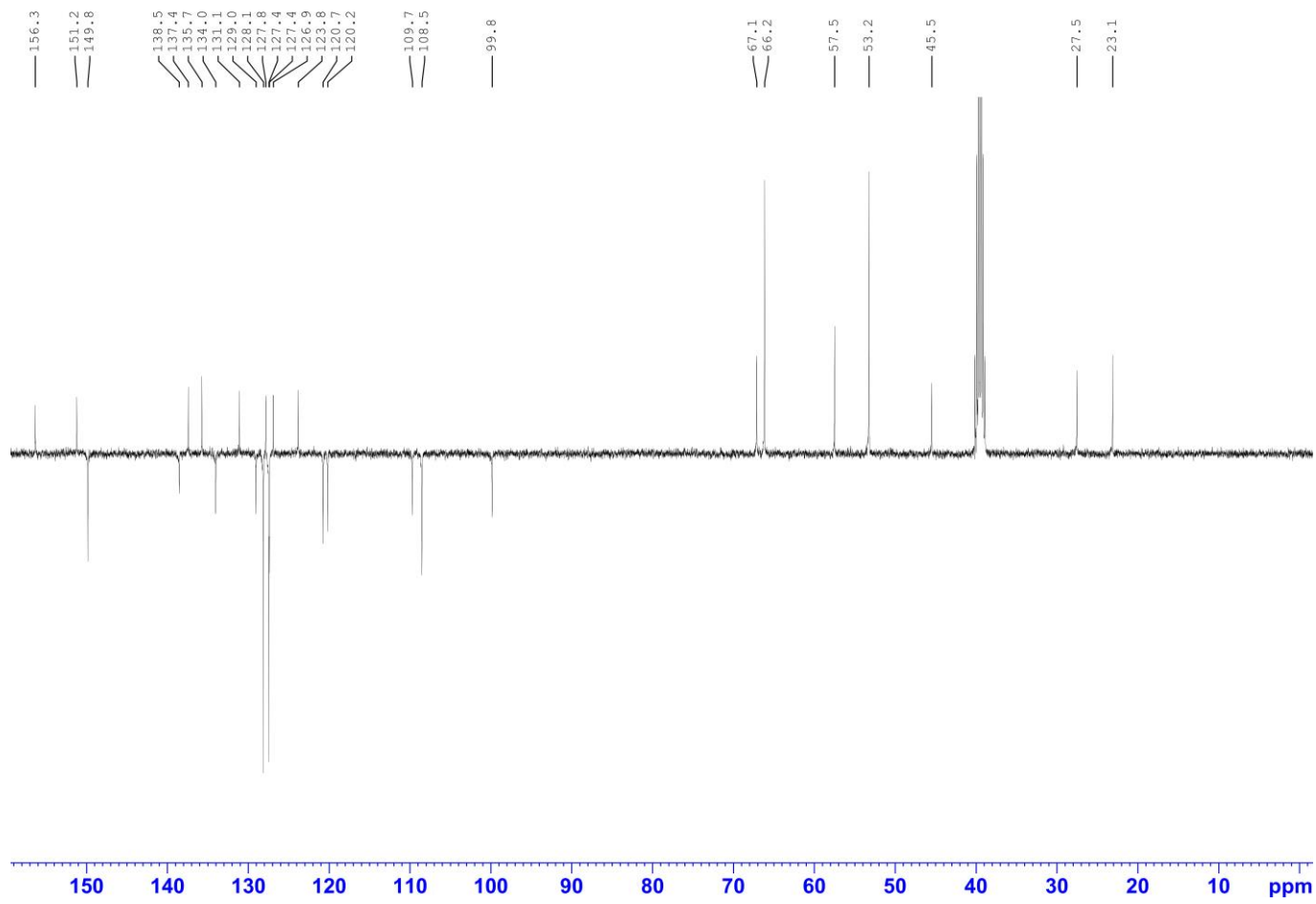
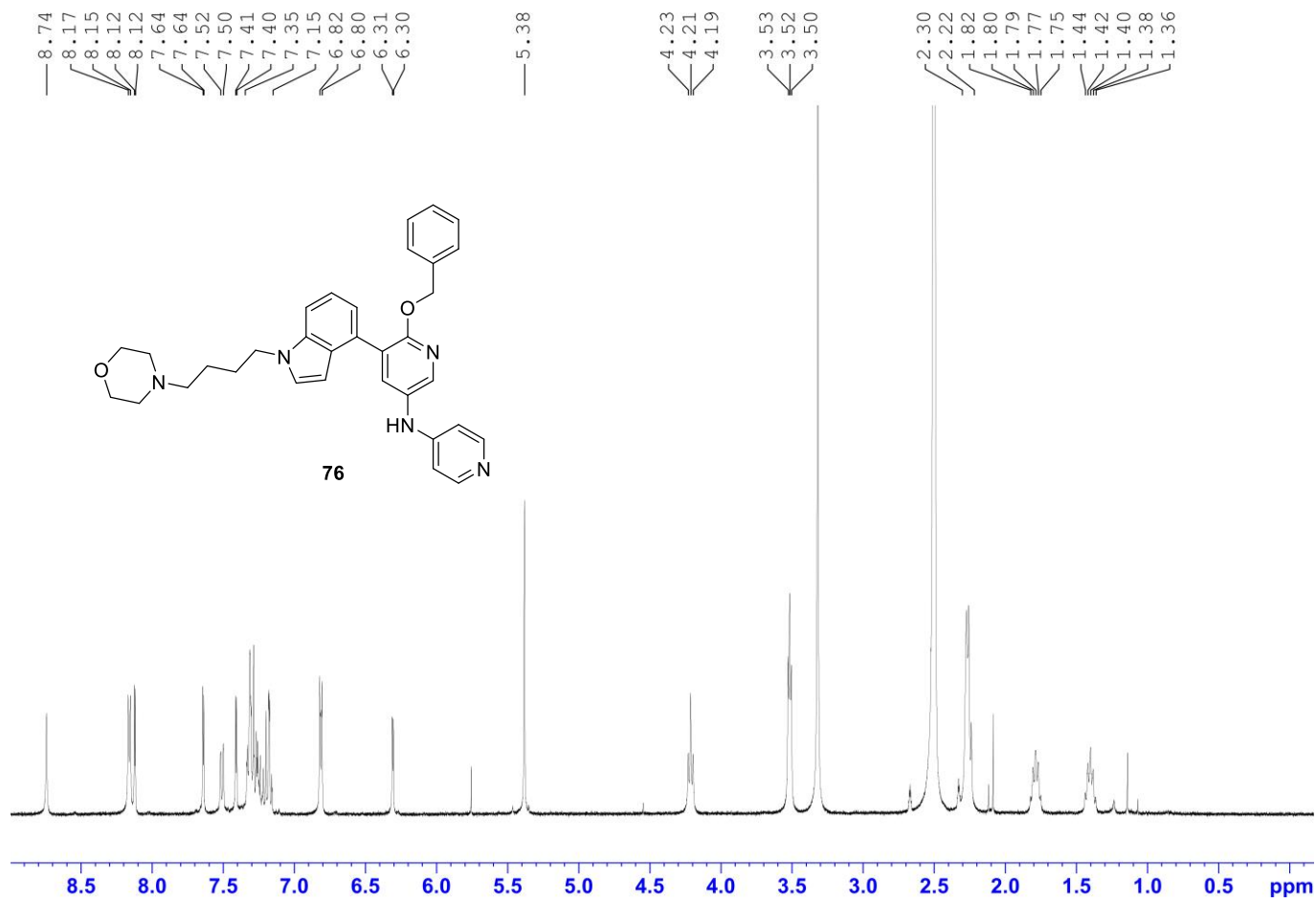




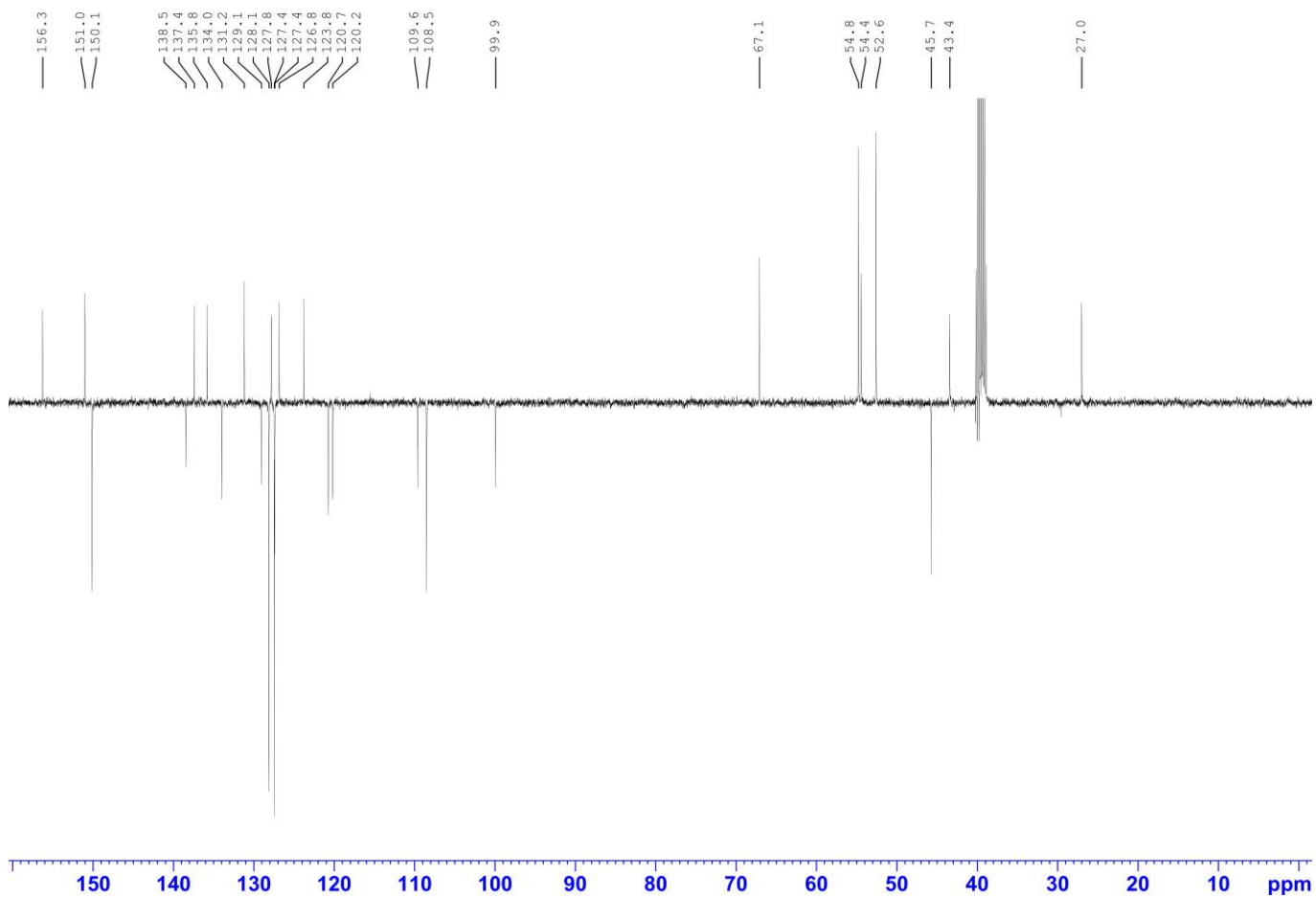
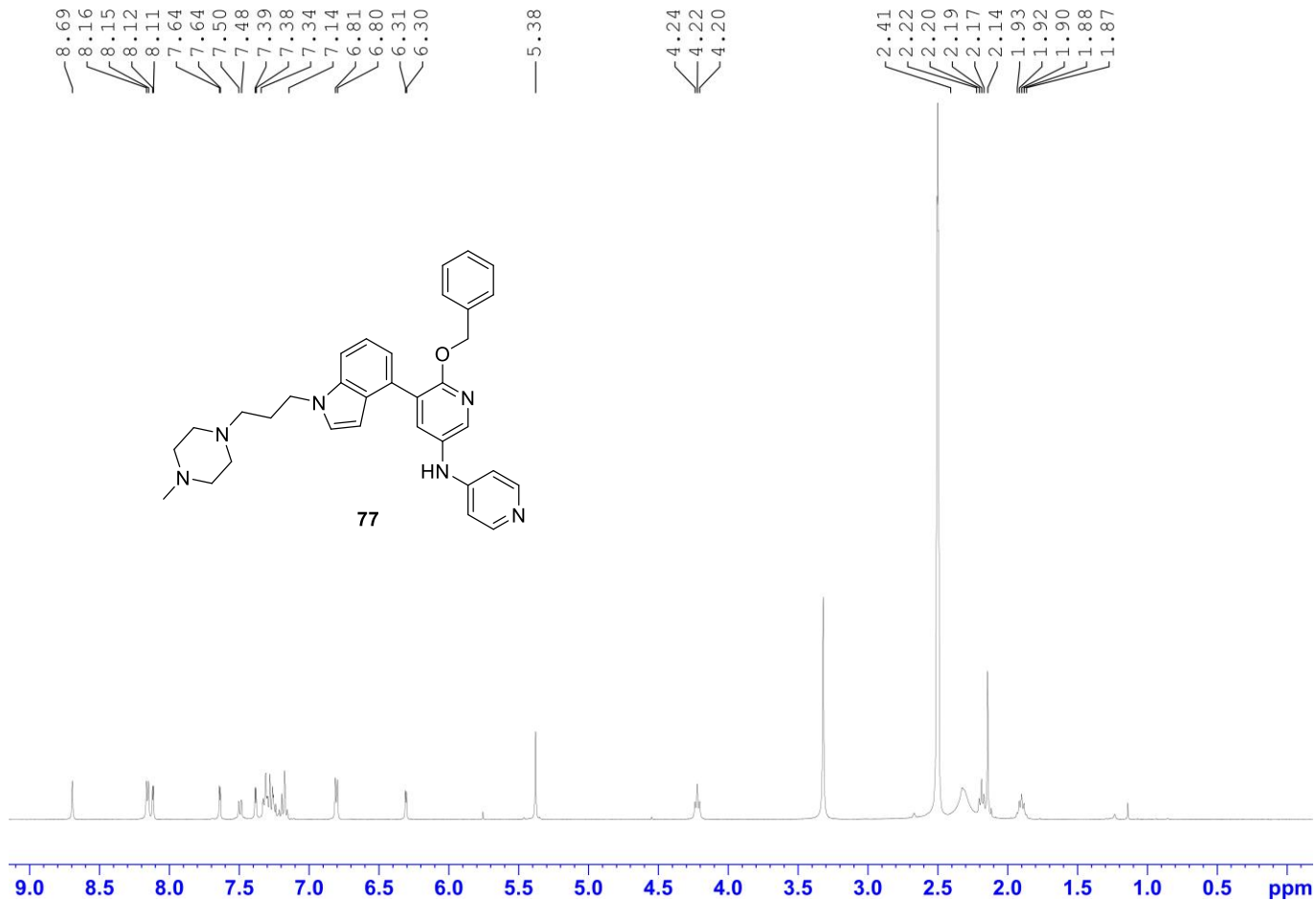


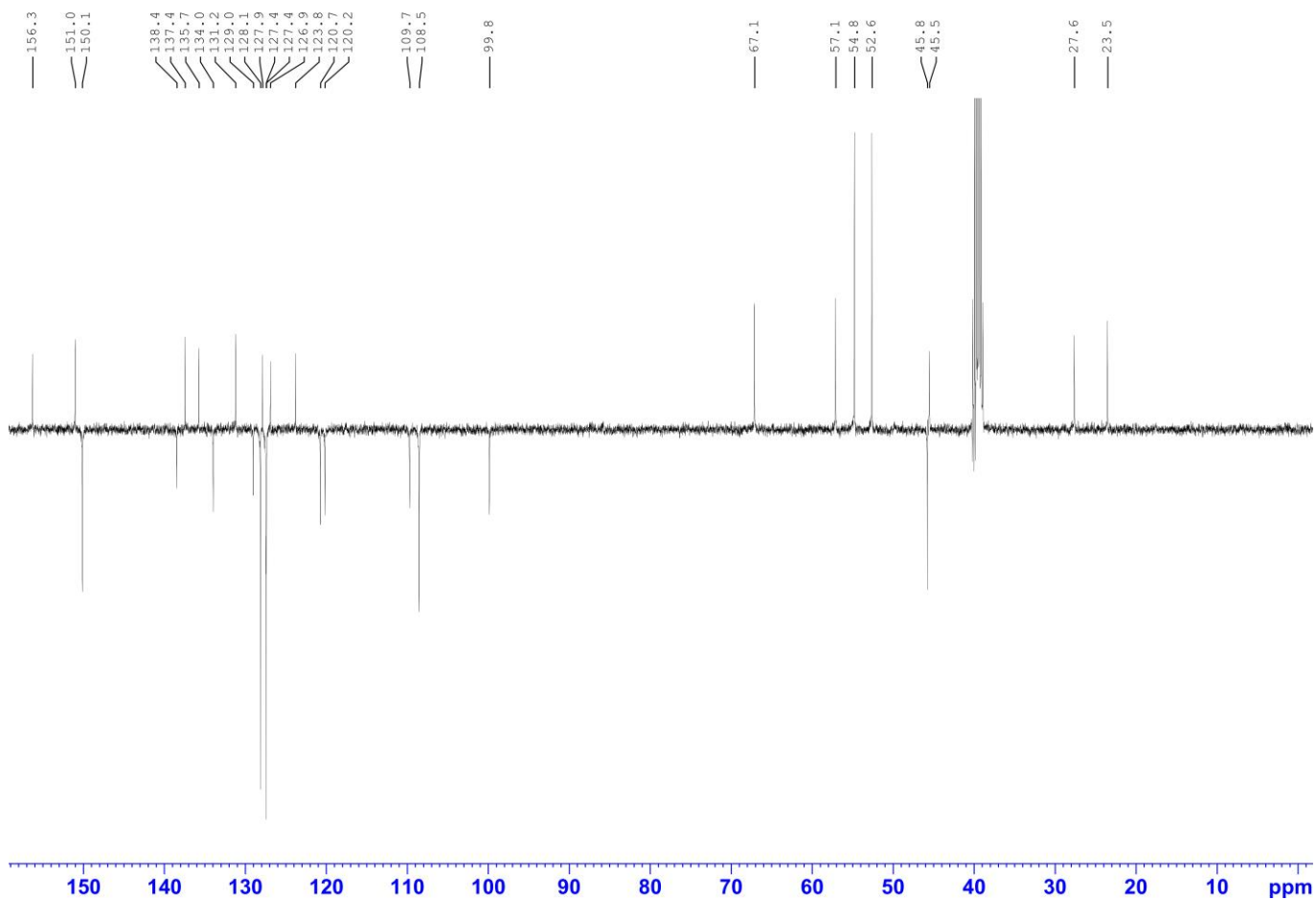
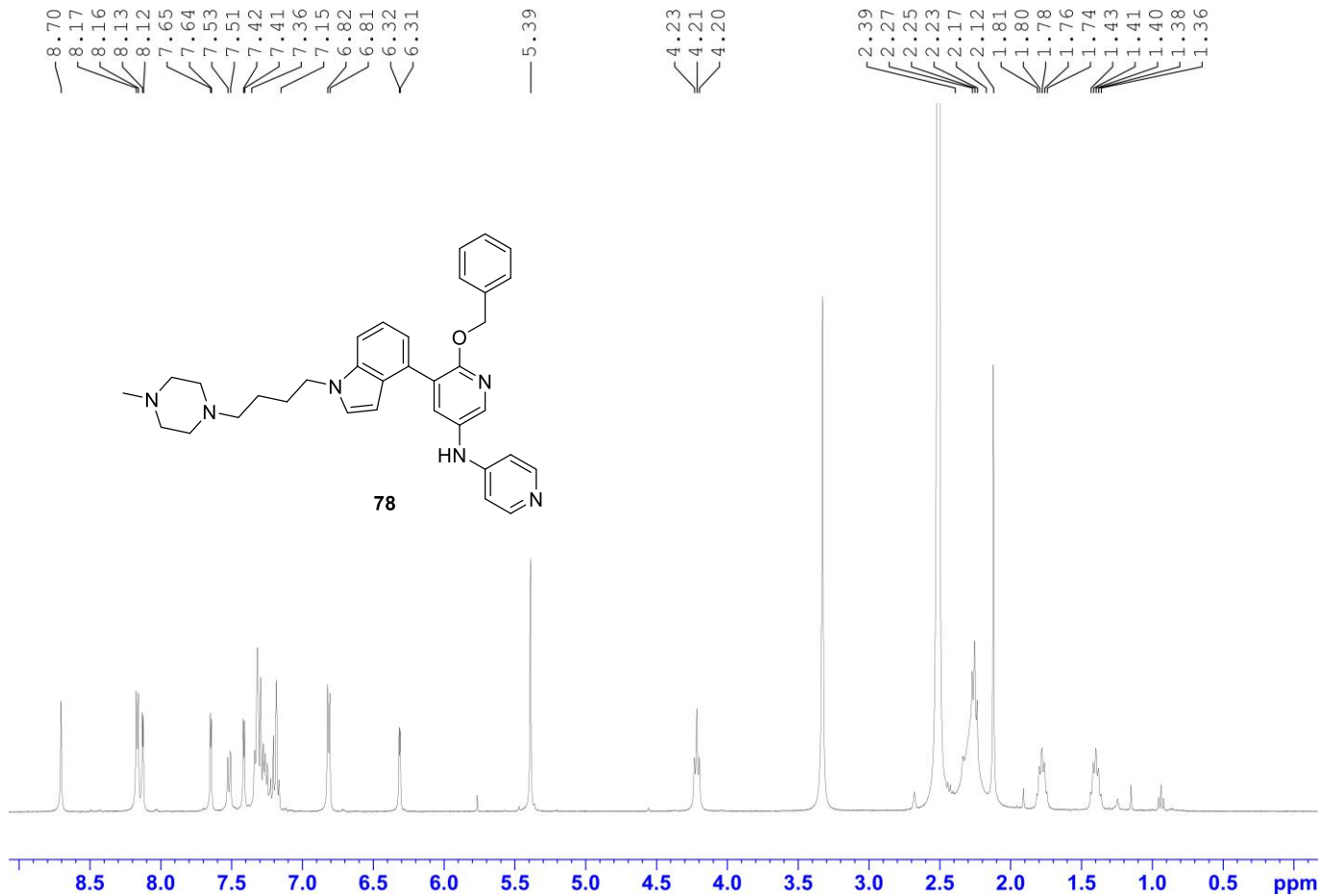










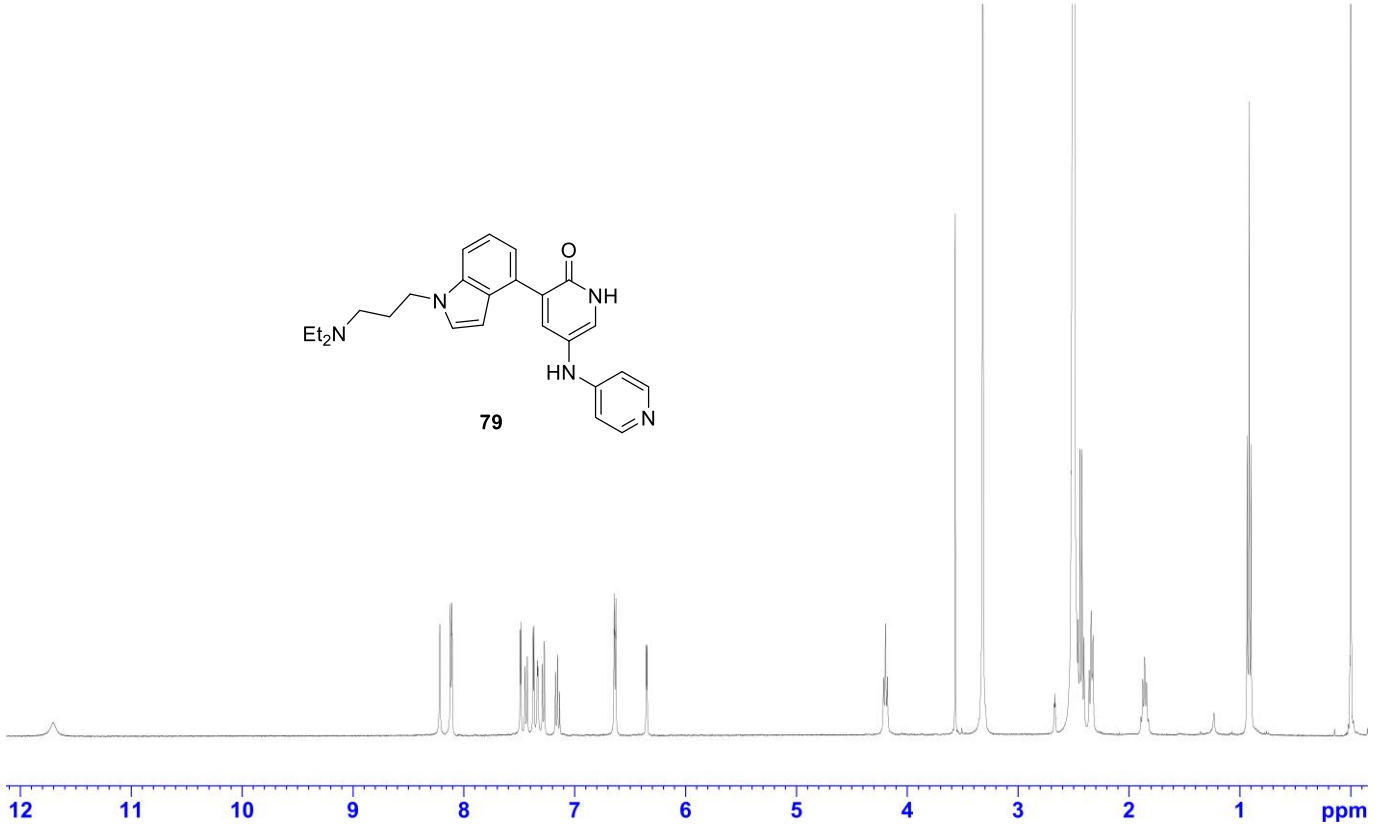
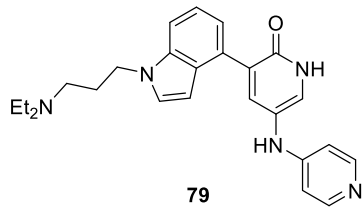


—11.70

8.22  
8.12  
8.12  
8.11  
8.11  
7.49  
7.48  
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7.43  
7.37  
7.37  
7.34  
7.33  
7.29  
7.27  
7.17  
7.15  
7.13  
6.64  
6.64  
6.63  
6.63  
6.35  
6.35

4.21  
4.20  
4.18

2.46  
2.44  
2.42  
2.40  
2.36  
2.34  
2.32  
1.89  
1.87  
1.86  
1.84  
0.93  
0.92  
0.90



159.9  
152.4  
149.9  
138.7  
135.9  
130.6  
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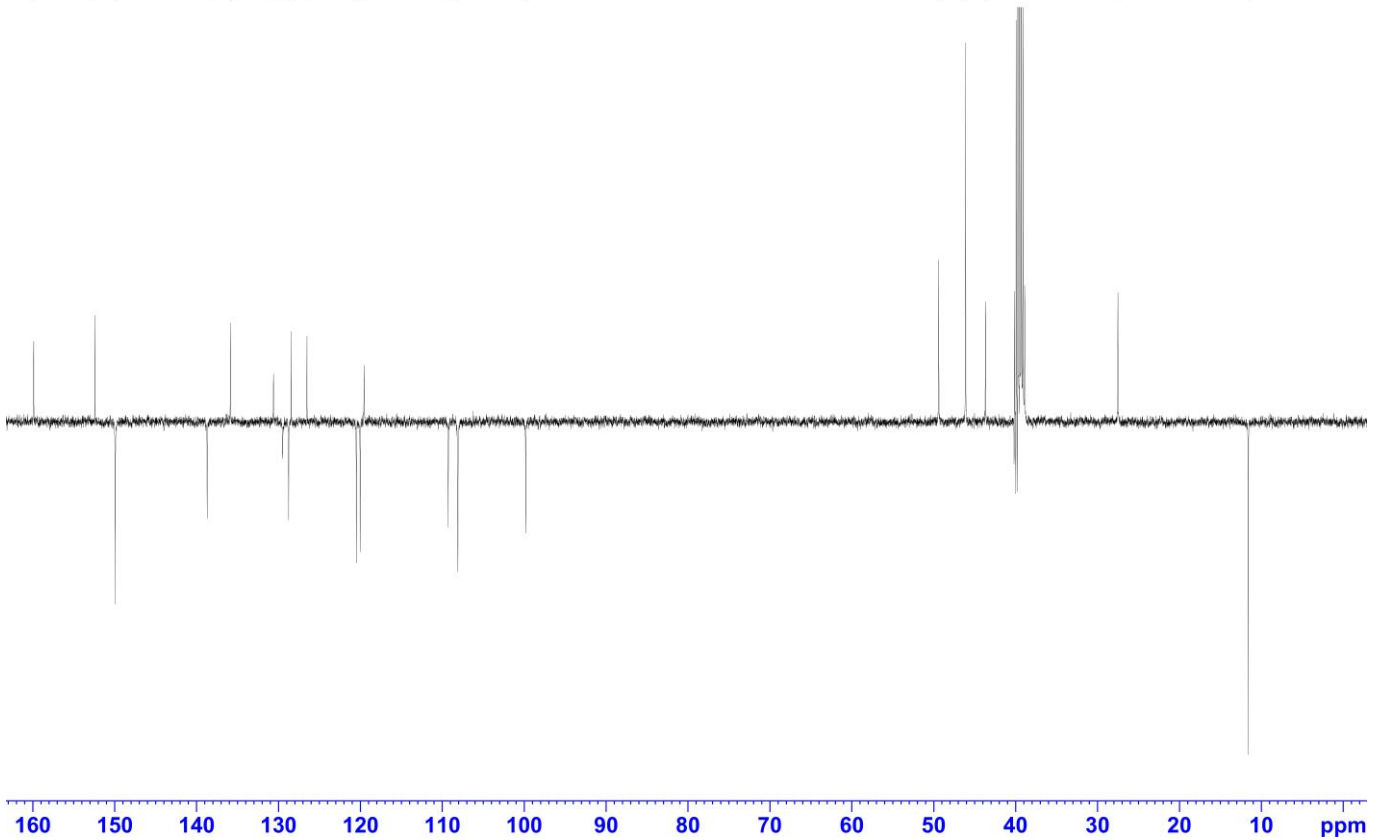
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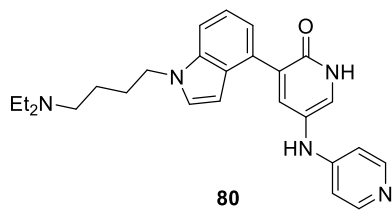
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7.13  
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6.63  
6.35  
6.34

4.20  
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4.17  
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2.33  
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1.77  
1.75  
1.73  
1.72  
1.39  
1.38  
1.36  
1.34  
1.32  
0.91  
0.90  
0.88



11 10 9 8 7 6 5 4 3 2 1 0 ppm

160.0

152.4

149.9

138.6

135.9

130.5

128.7

128.5

126.5

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119.5

109.3

108.1

99.8

51.8

46.2

45.5

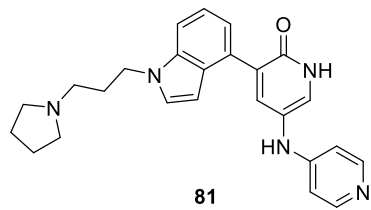
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24.1

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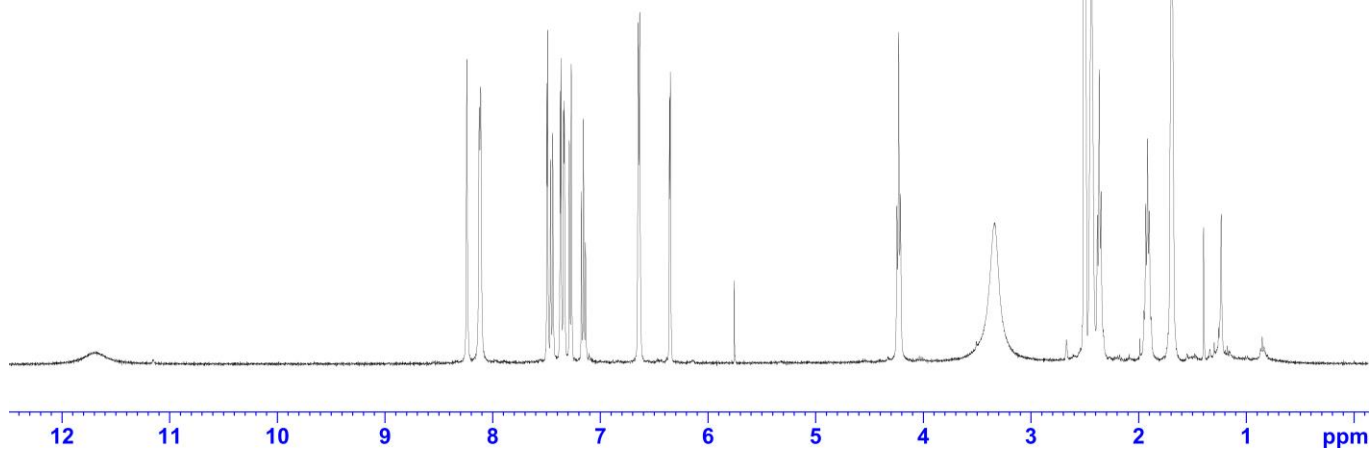
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7.33  
7.29  
7.27  
7.17  
7.15  
7.14  
6.65  
6.63  
6.36  
6.35

4.24  
4.23  
4.21

2.44  
2.38  
2.36  
2.35  
1.95  
1.93  
1.92  
1.90  
1.88  
1.69



159.9

152.5

149.9

138.7

135.9

130.6

129.5

128.8

128.4

126.5

120.5

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119.5

109.3

108.1

99.9

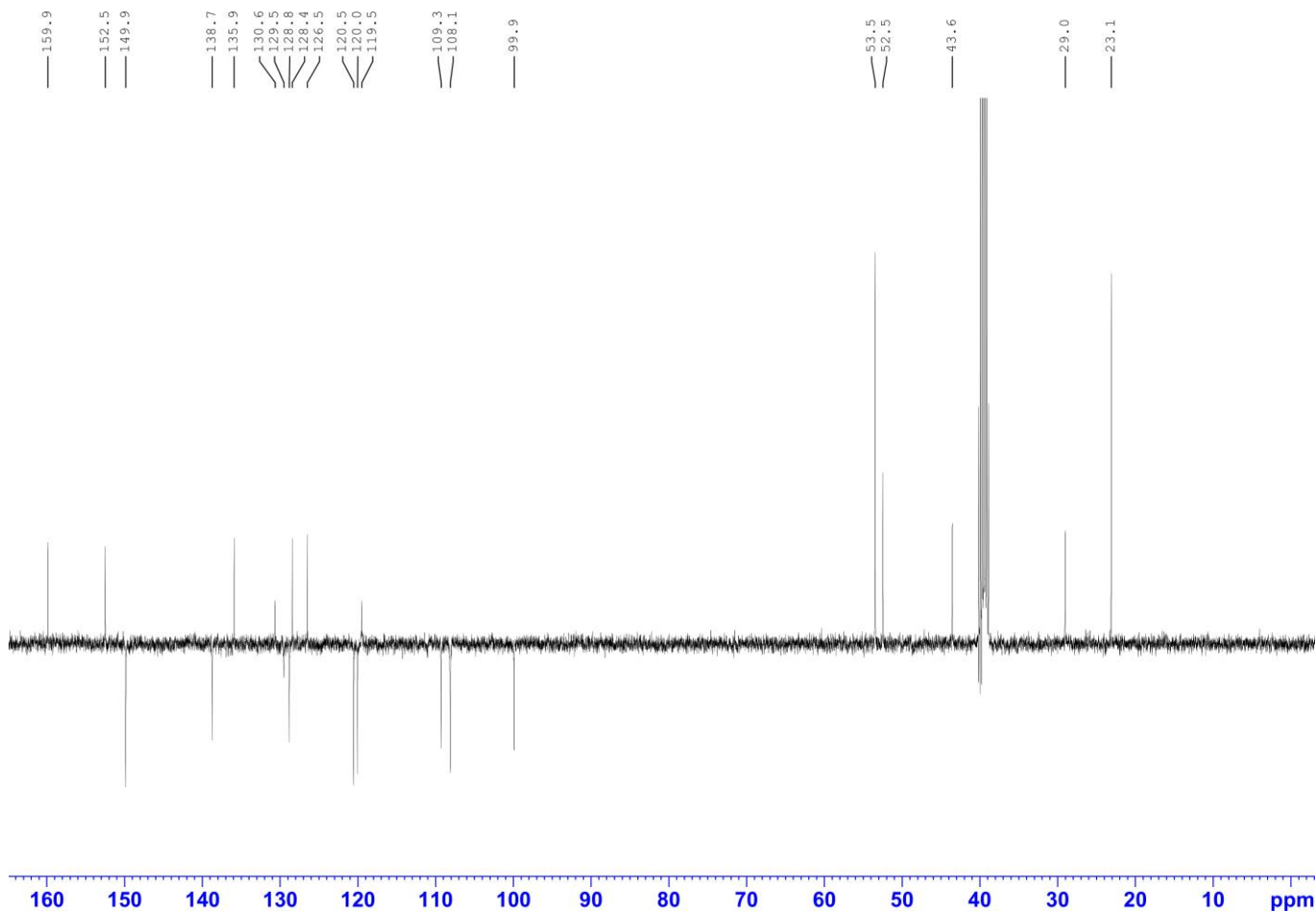
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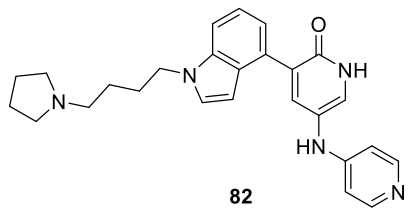
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23.1



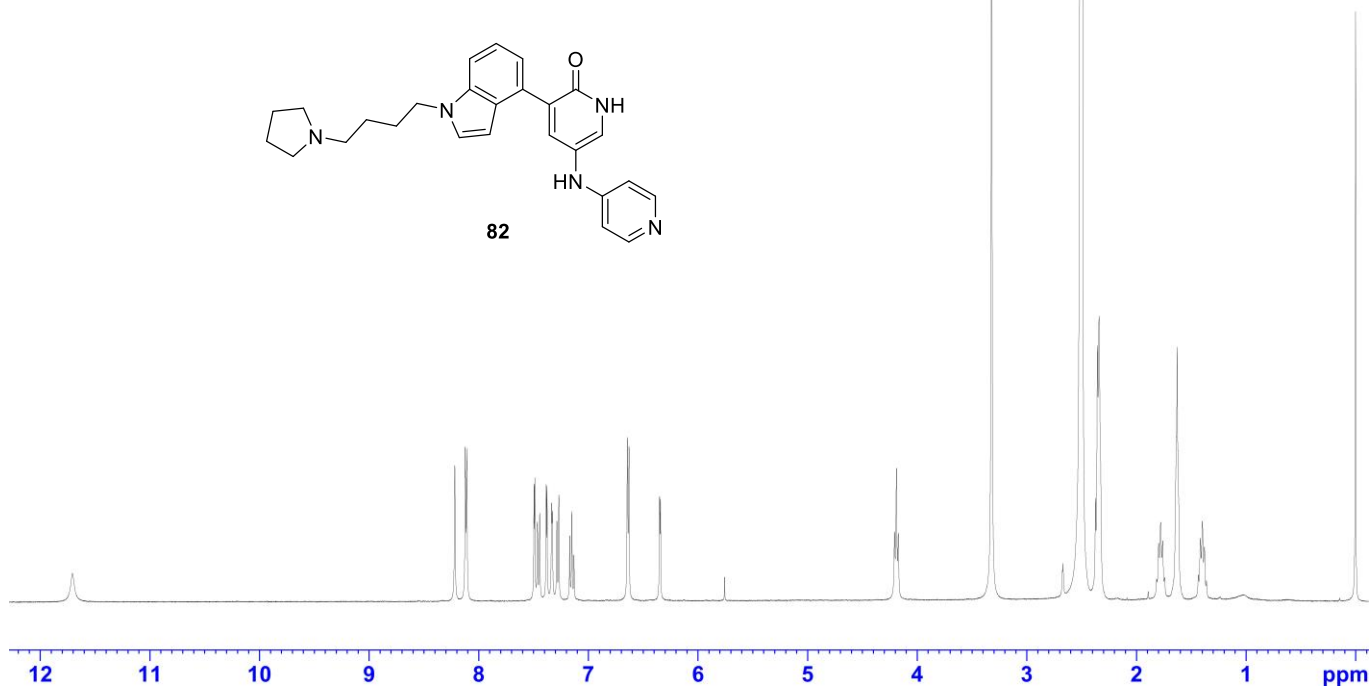
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7.27  
7.17  
7.15  
7.13  
6.64  
6.63  
6.63  
6.35  
6.34

4.21  
4.19  
4.17

2.37  
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2.34  
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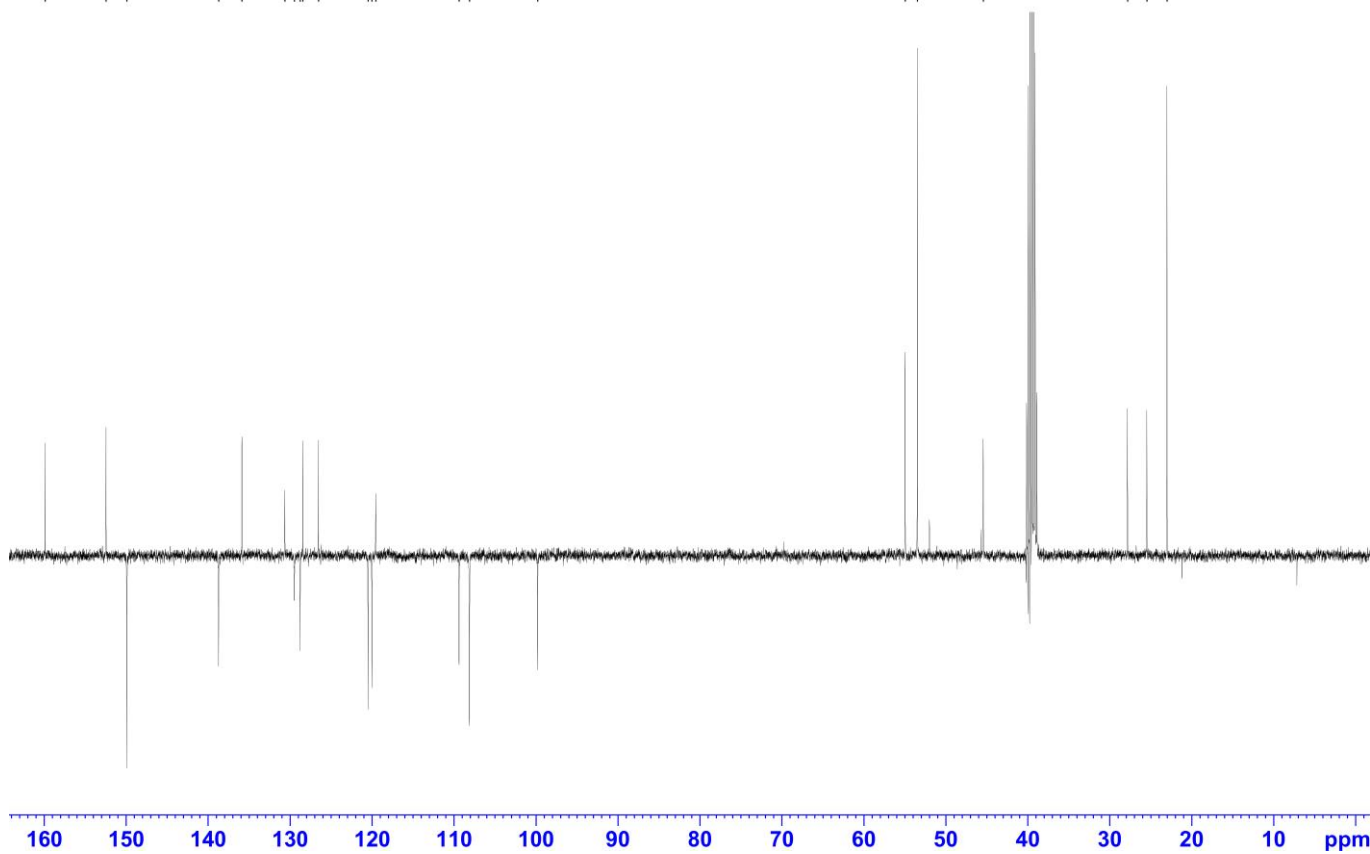


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152.5  
149.9  
138.7  
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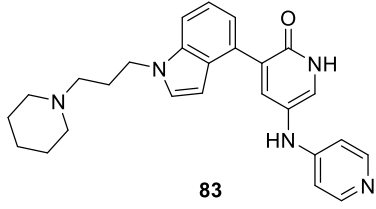
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55.0  
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45.4

27.8  
25.5  
23.0



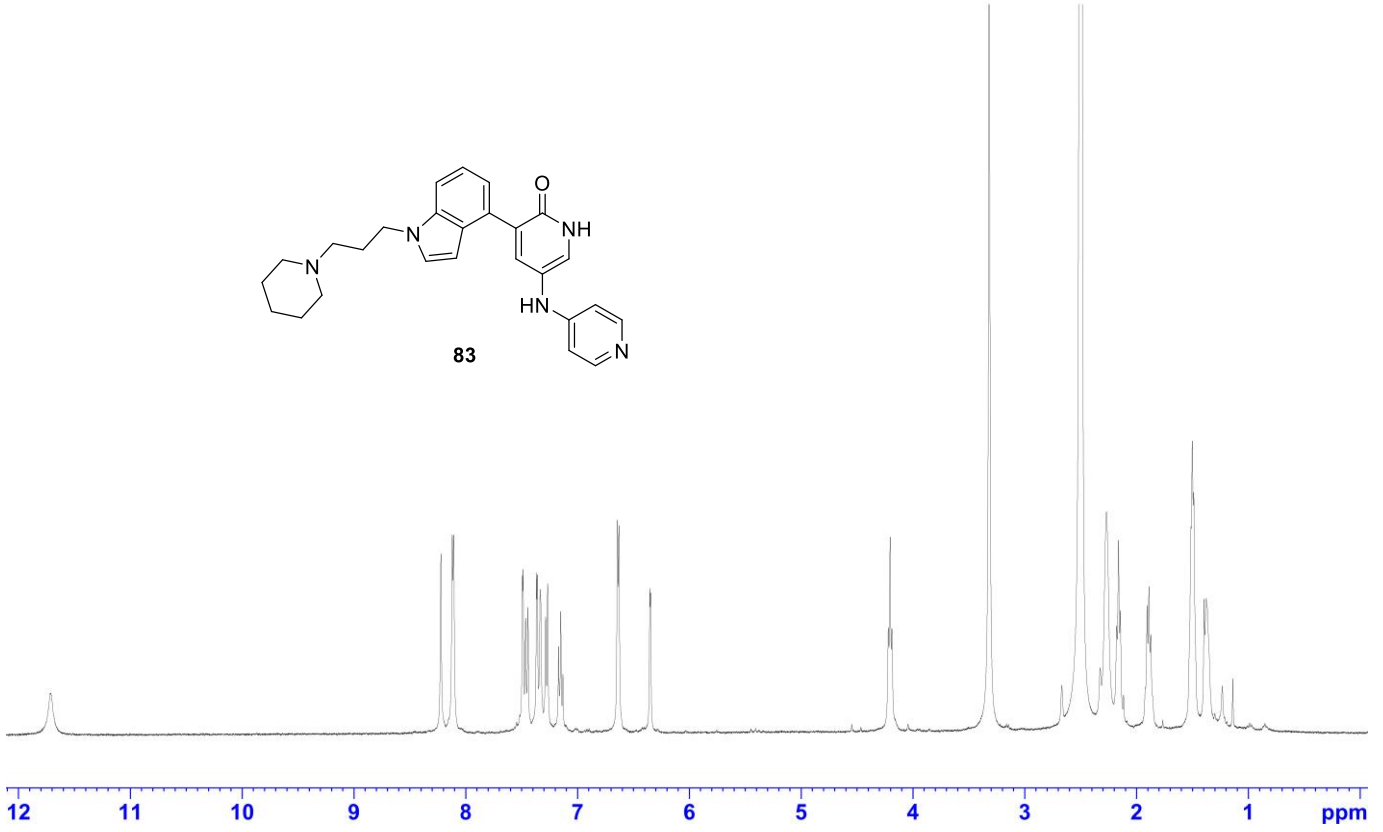
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7.17  
7.15  
7.13  
6.64  
6.63  
6.35  
6.35

4.22  
4.20  
4.19

2.32  
2.21  
2.18  
2.16  
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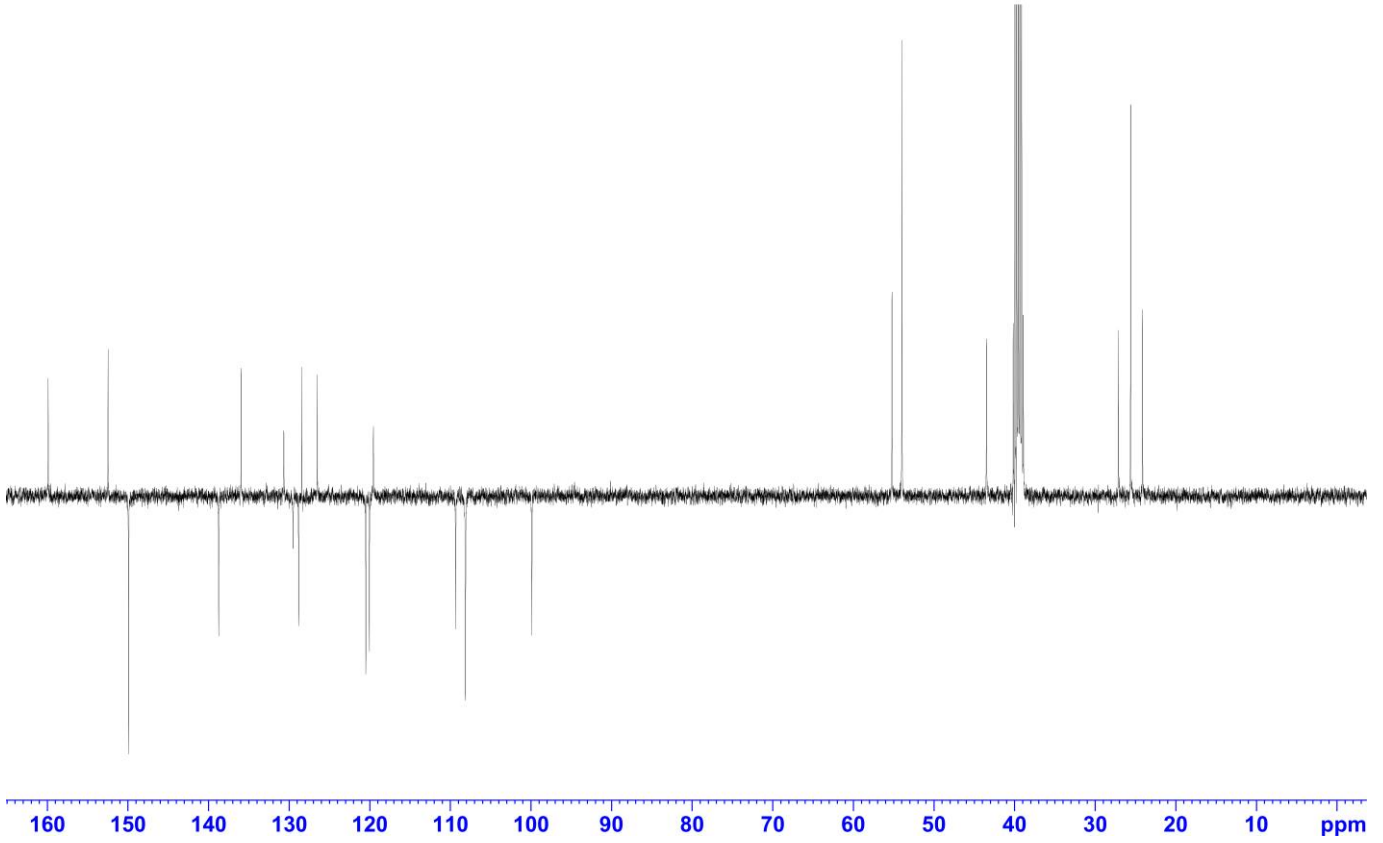
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109.3  
108.1  
99.9

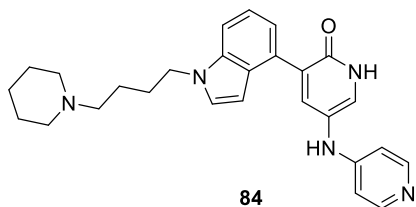
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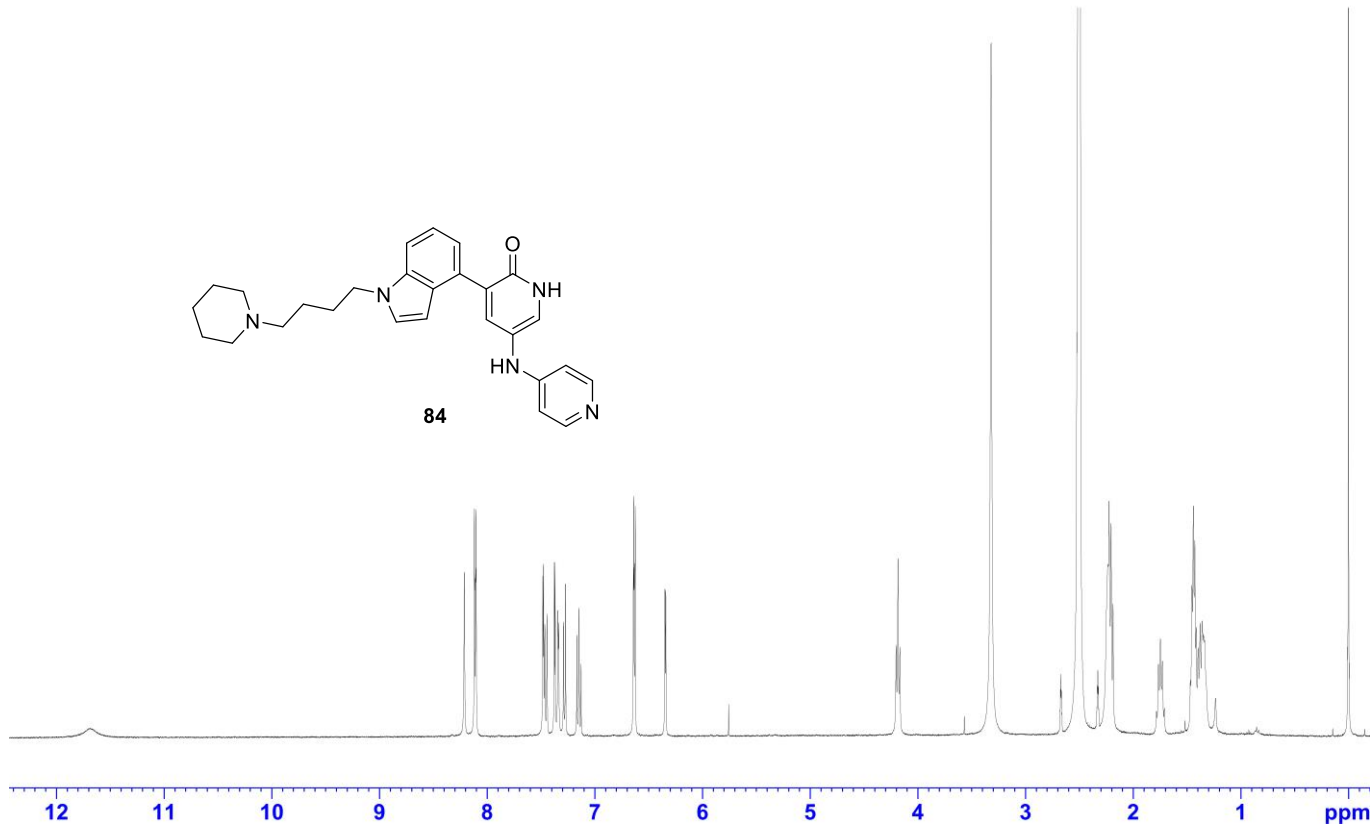
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7.13  
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6.35  
6.34

4.20  
4.18  
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2.27  
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2.22  
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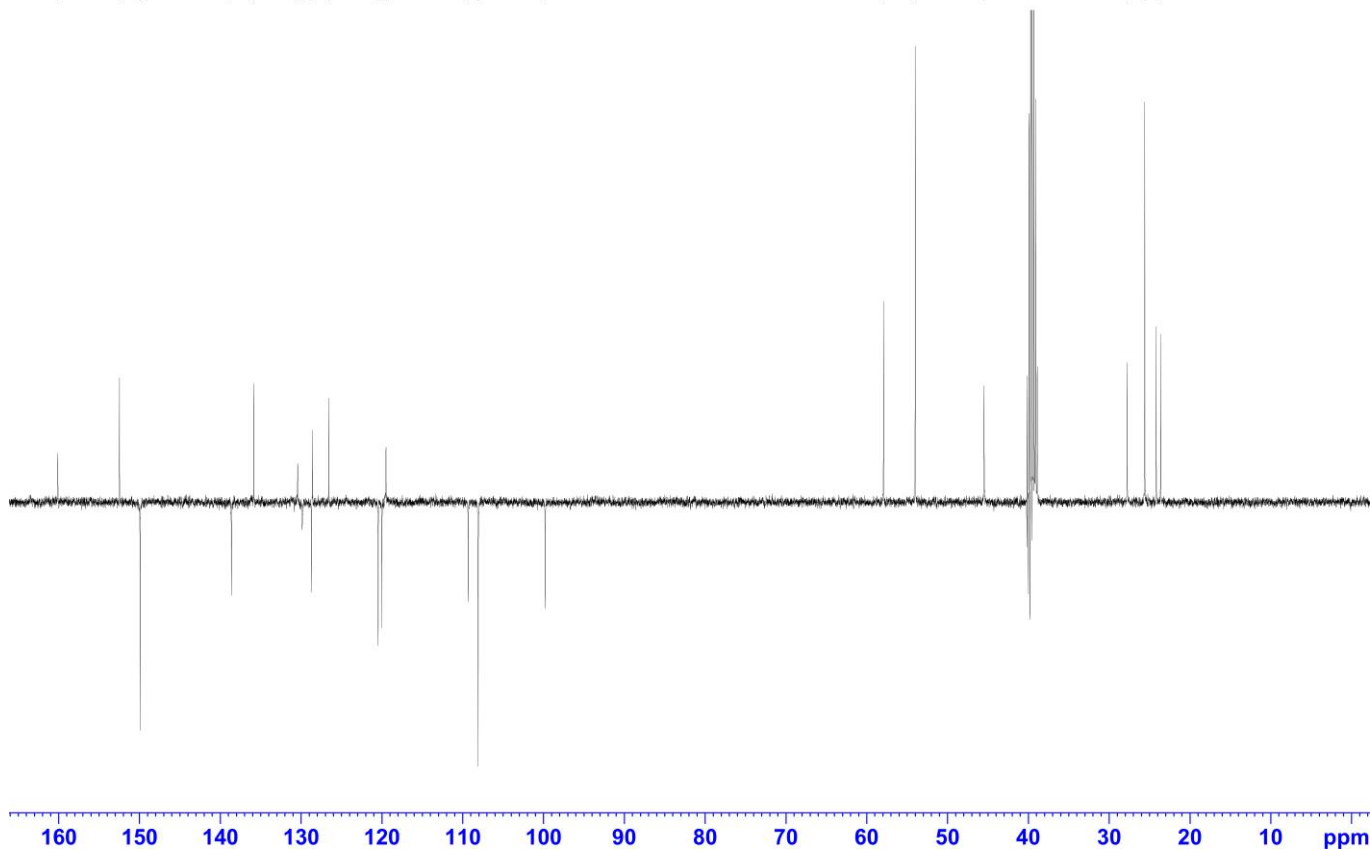
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138.6  
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120.5  
120.0  
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109.3  
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57.9  
54.0

45.5

27.8  
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24.2  
23.6



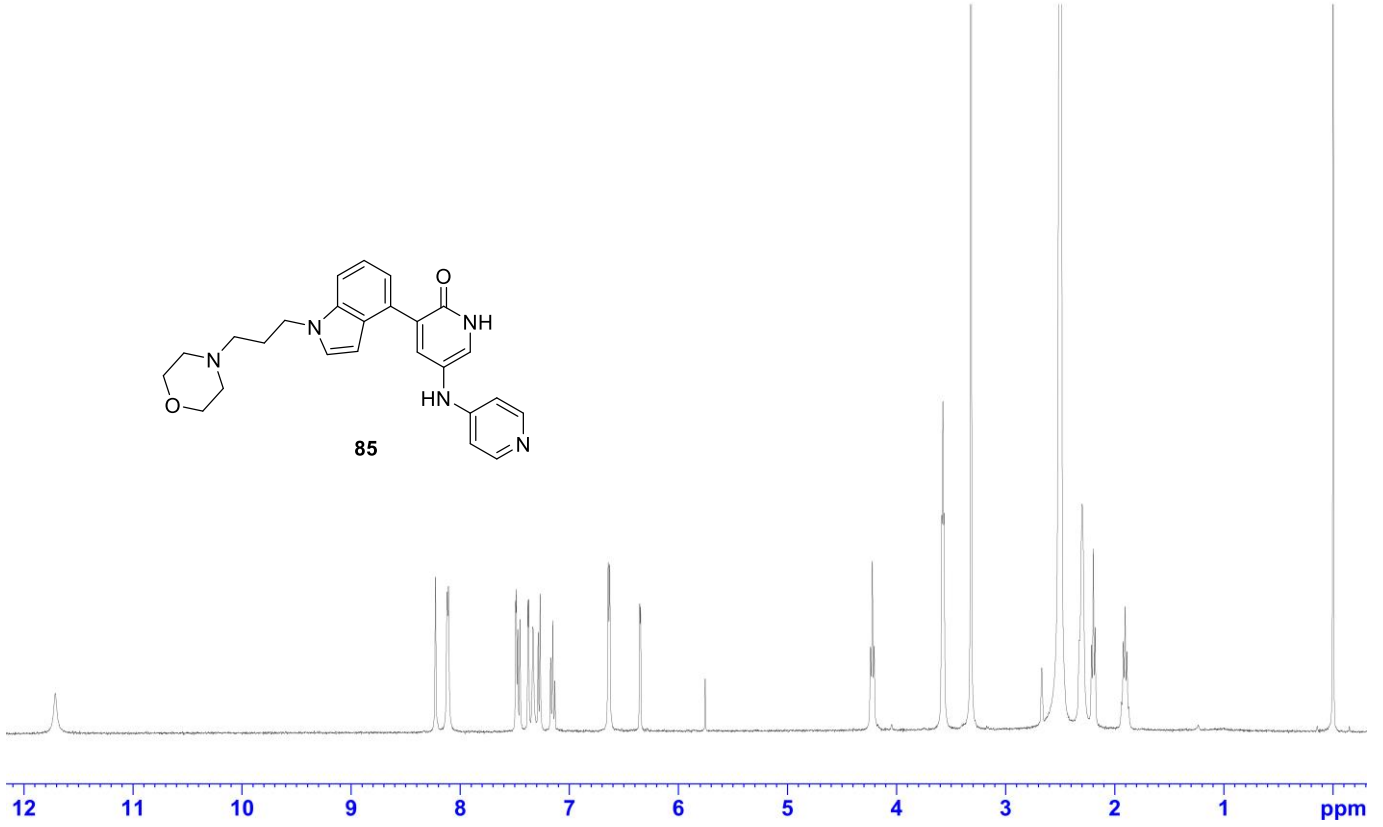
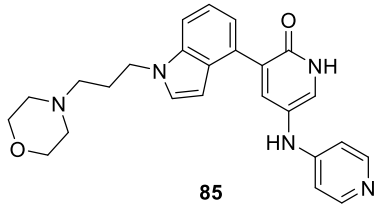


—11.71

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7.15  
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6.64  
6.63  
6.35  
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4.24  
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4.21  
3.60  
3.55

2.34  
2.25  
2.21  
2.20  
2.18  
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1.92  
1.91  
1.89  
1.87



—159.9

—152.5

—149.9

—138.7

—135.9

—130.6

—129.5

—128.6

—126.5

—120.5

—120.0

—119.5

—109.3

—108.1

—99.9

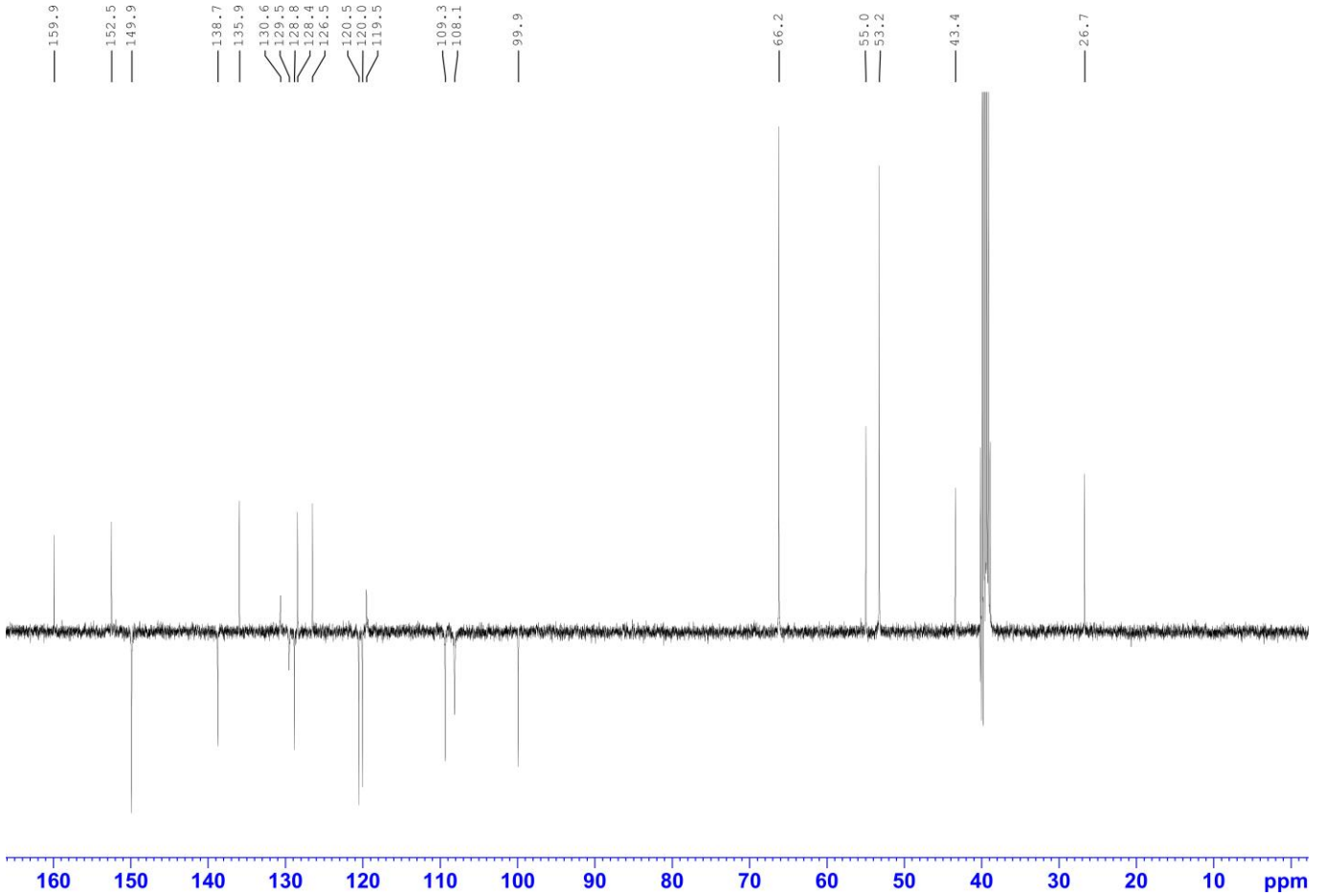
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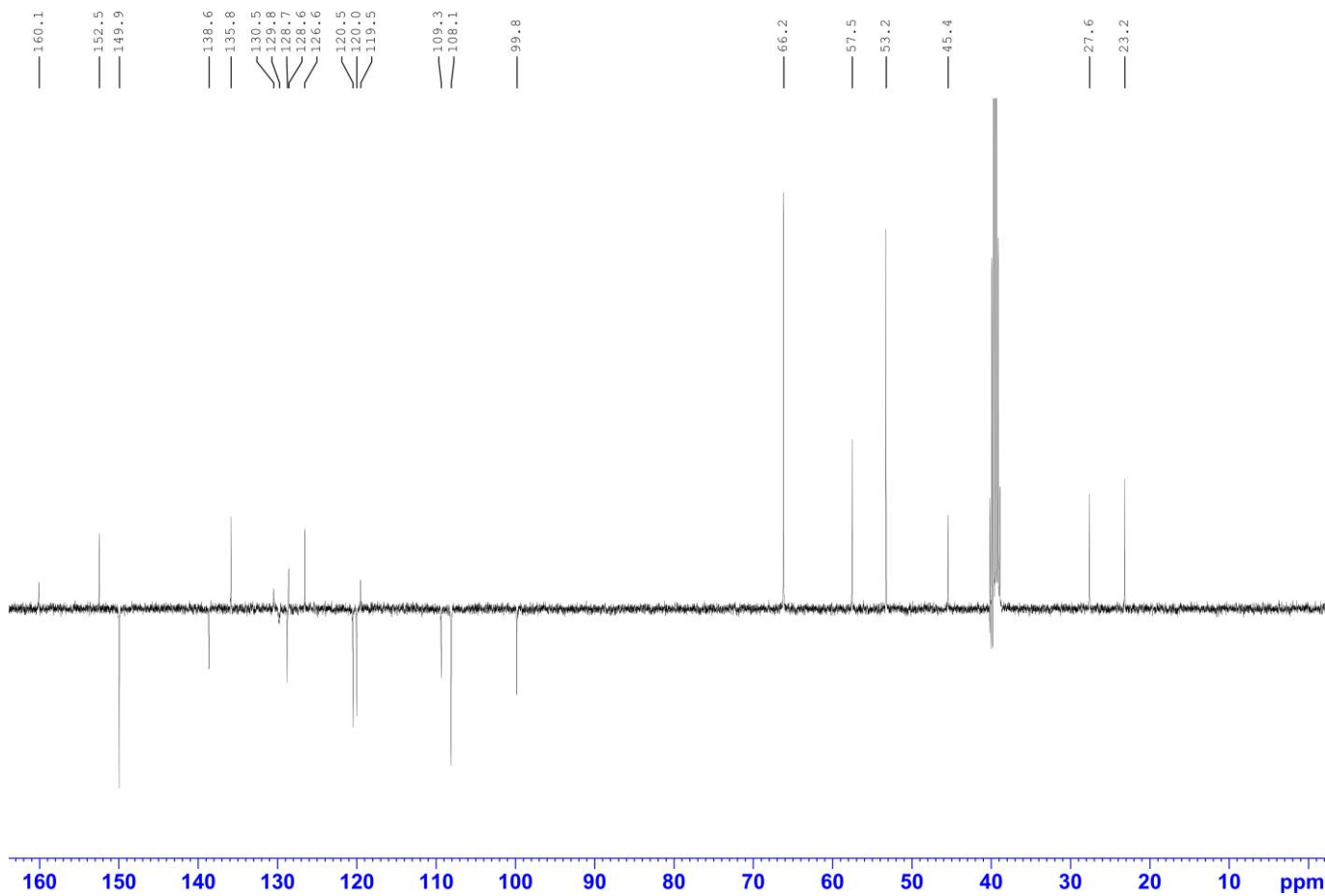
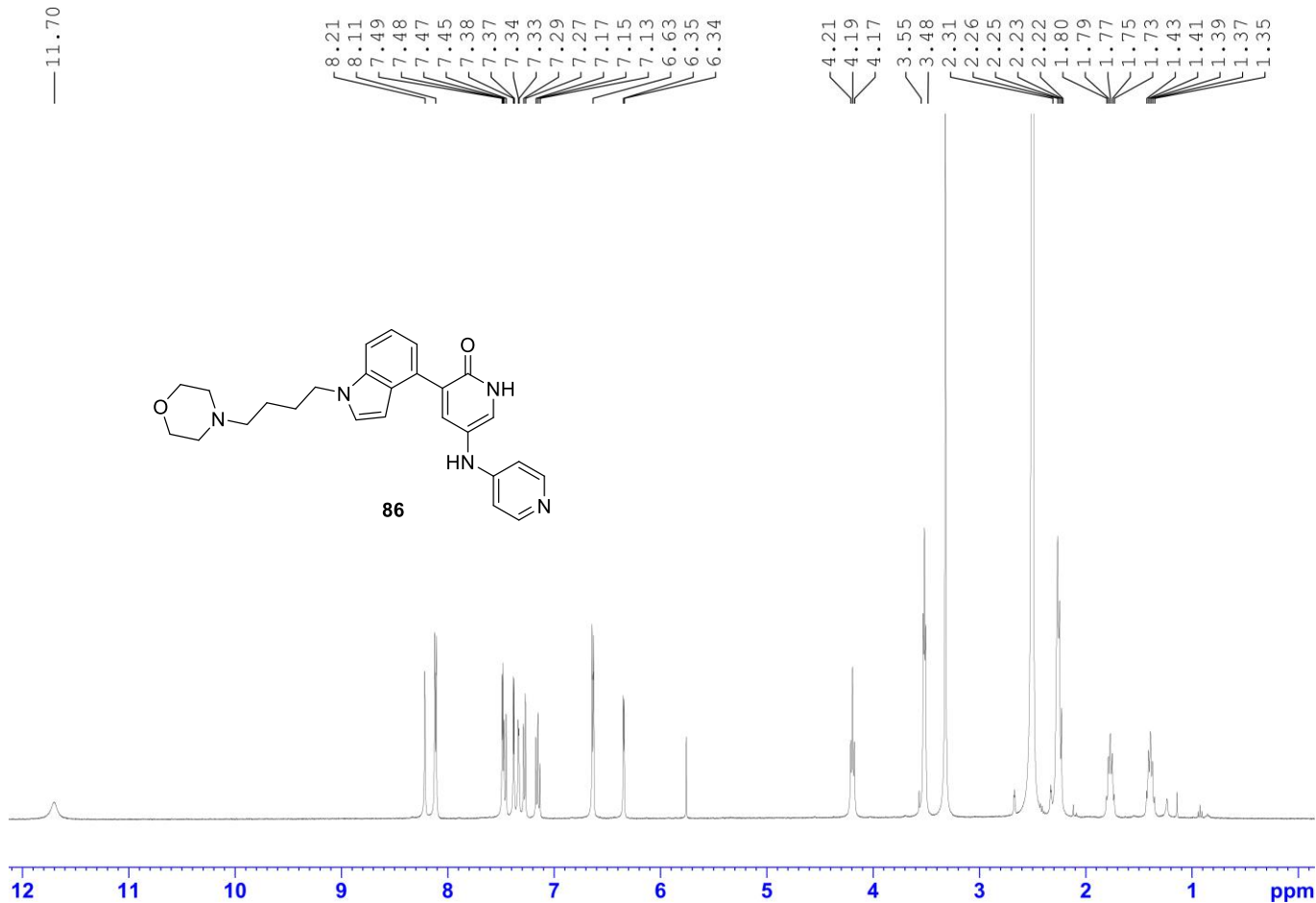
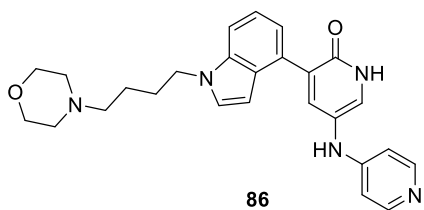
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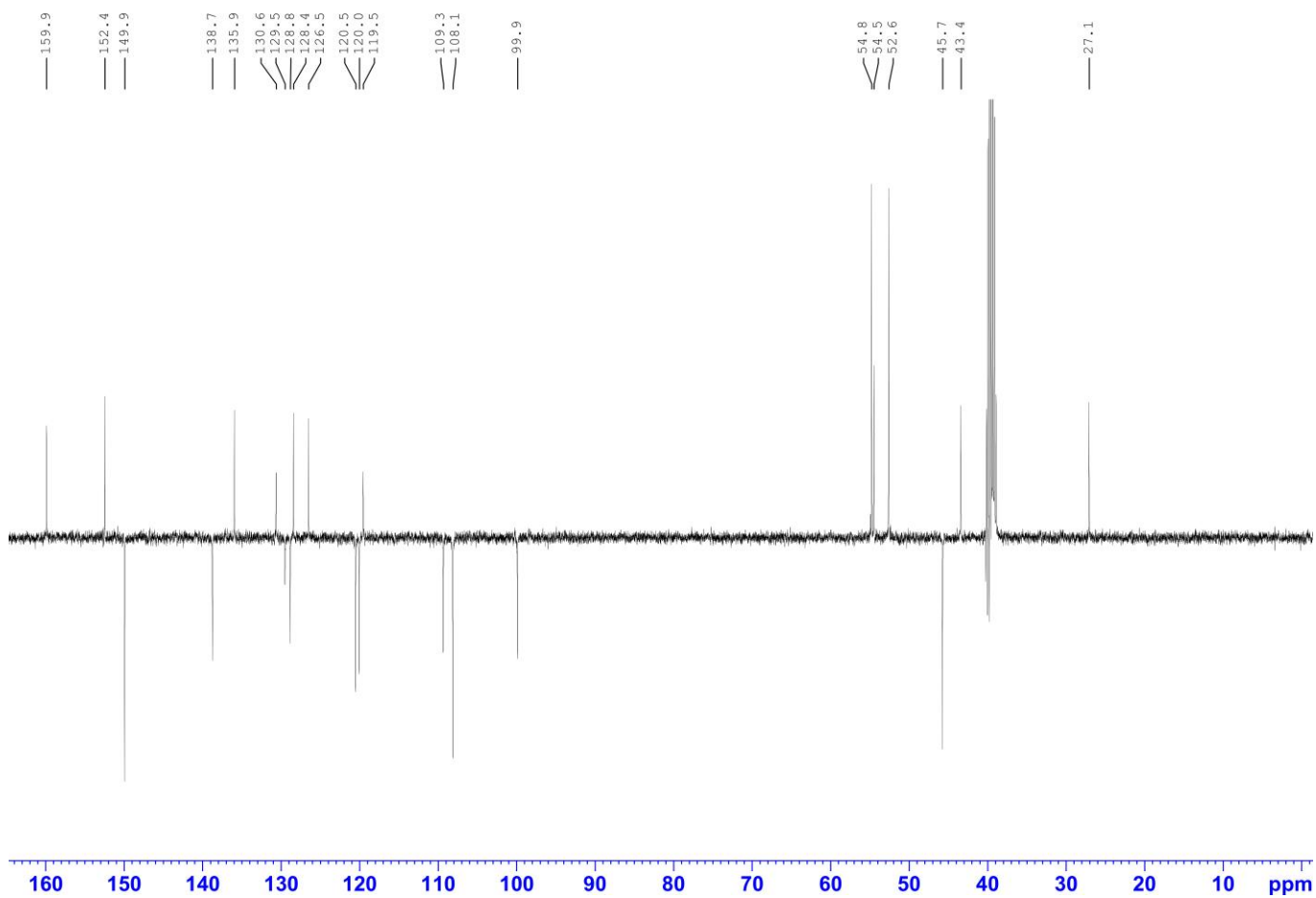
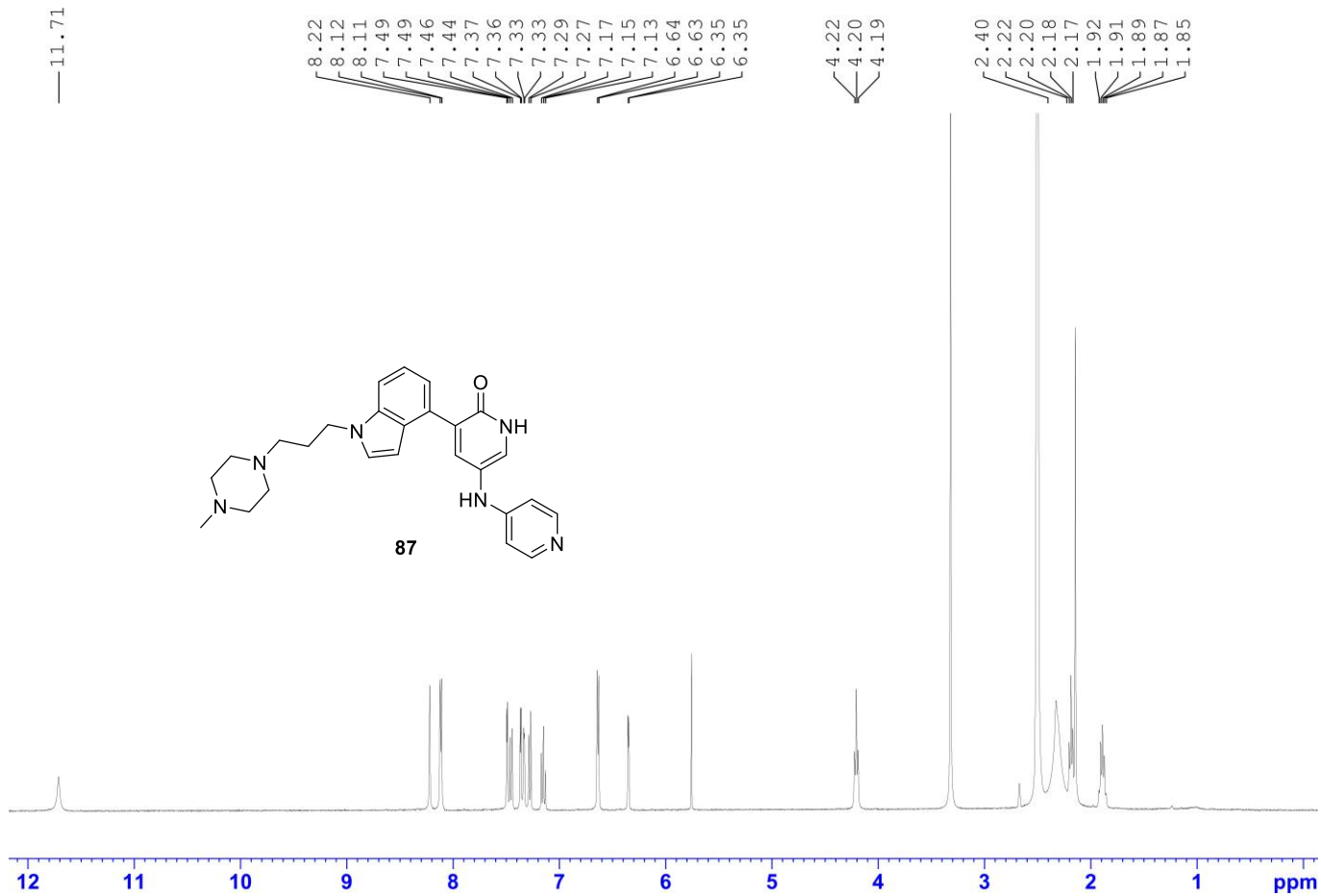
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—26.7



—11.70



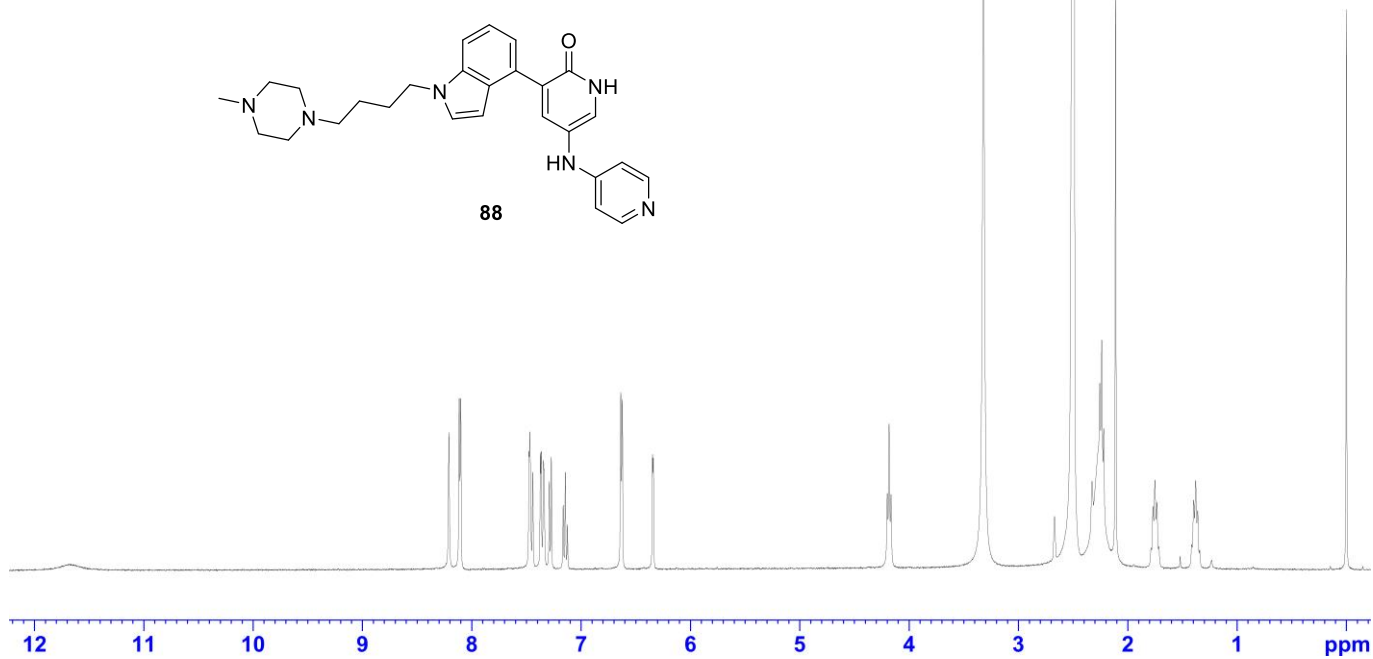
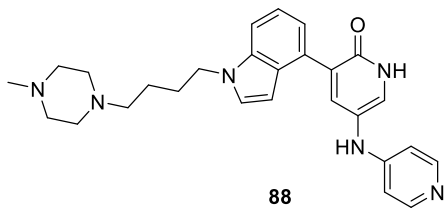


—11.67

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7.14  
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6.35  
6.34

4.20  
4.18  
4.16

2.38  
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2.24  
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160.0  
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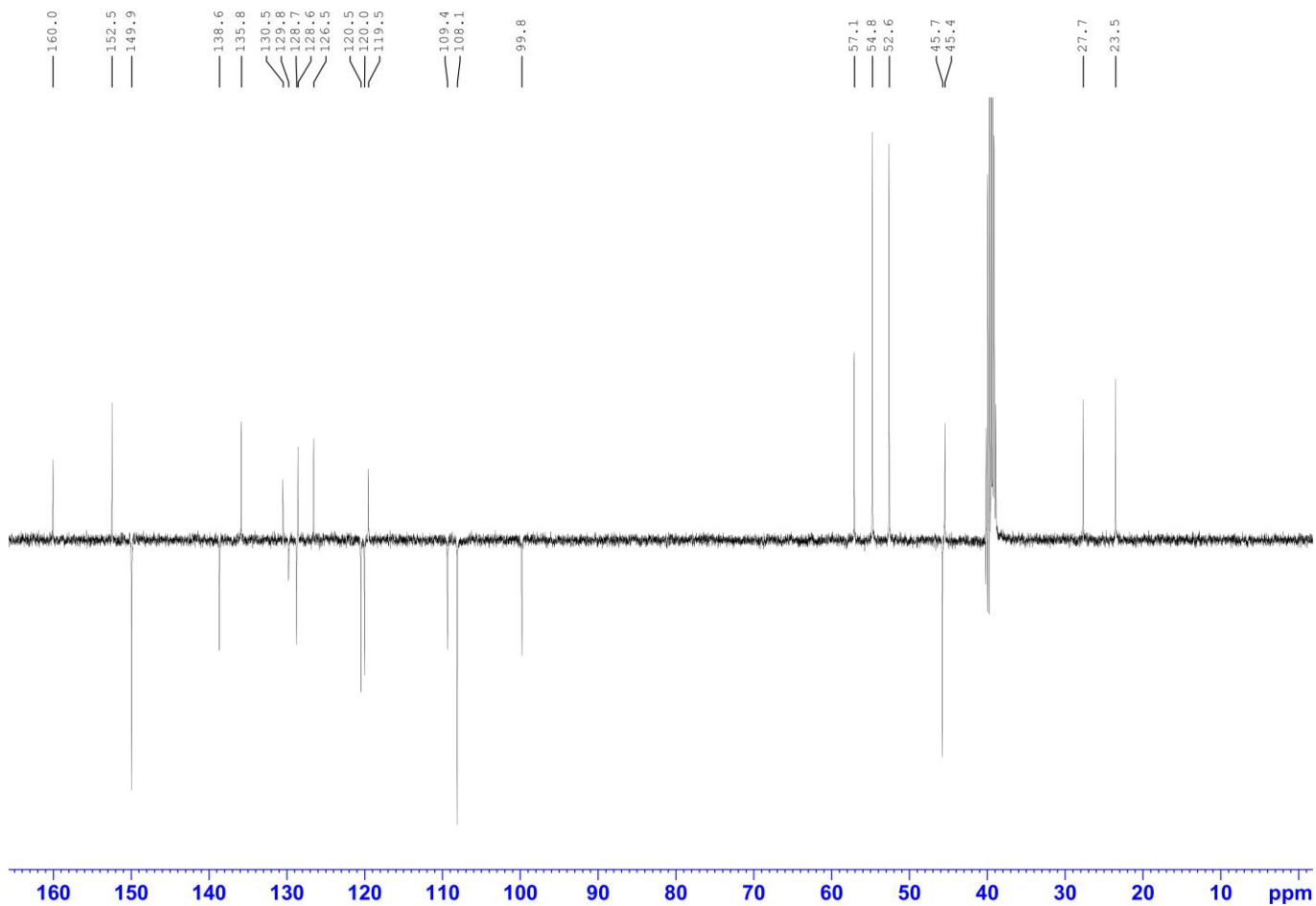
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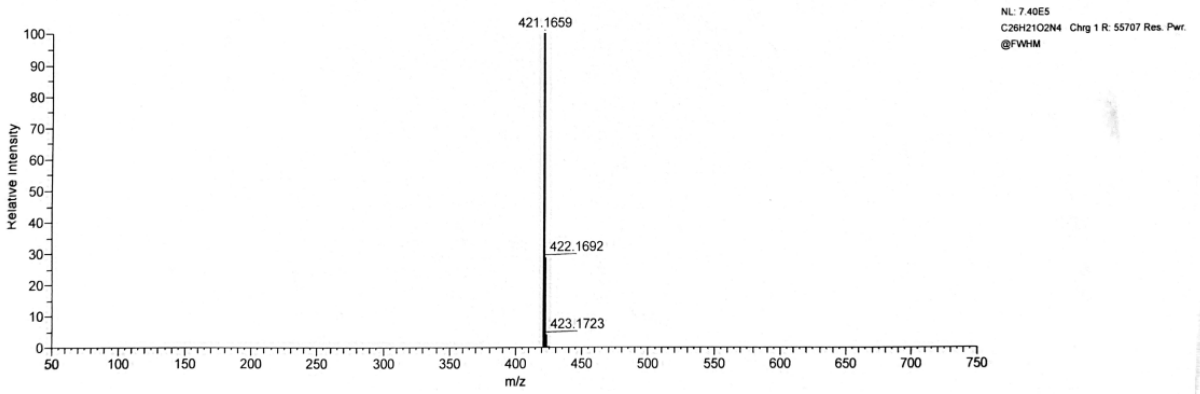
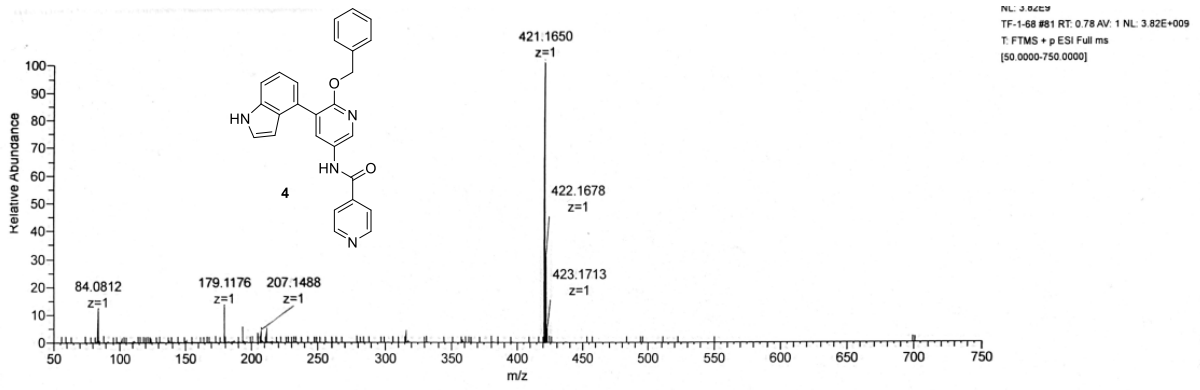
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54.8  
52.6

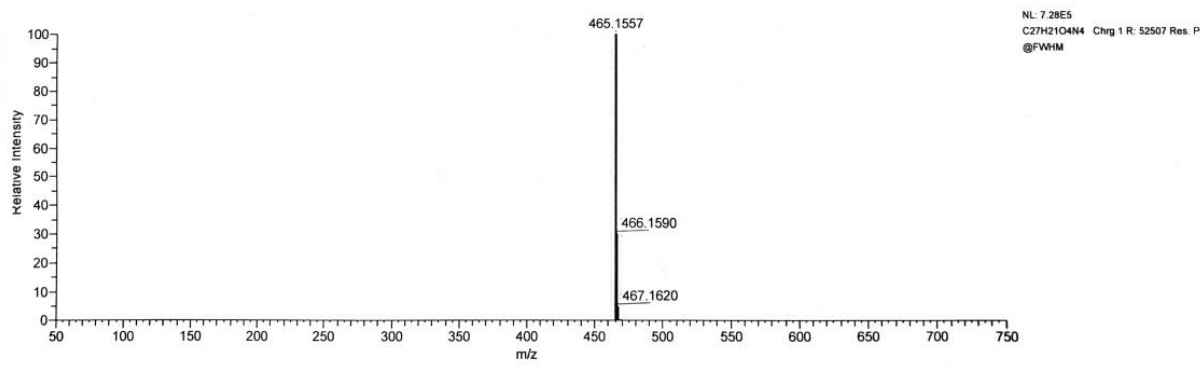
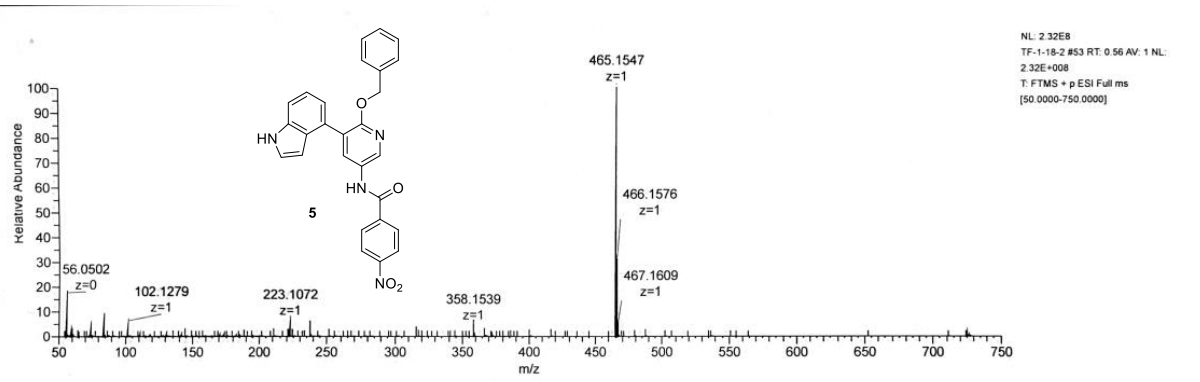
45.7  
45.4

27.7  
23.5

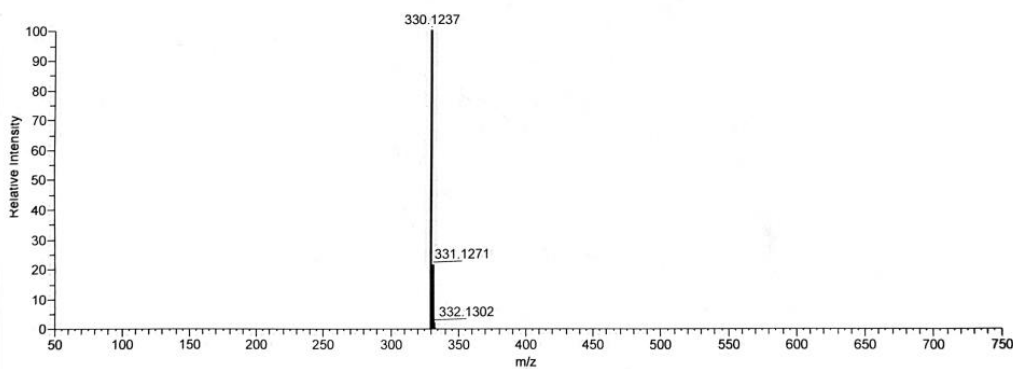
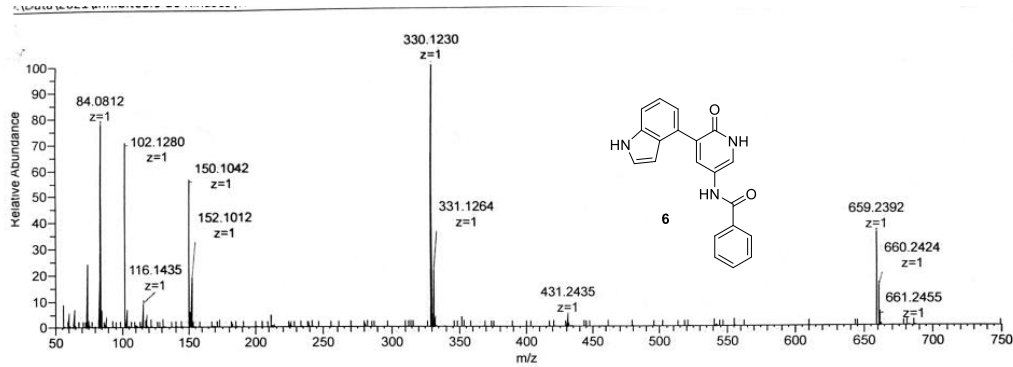




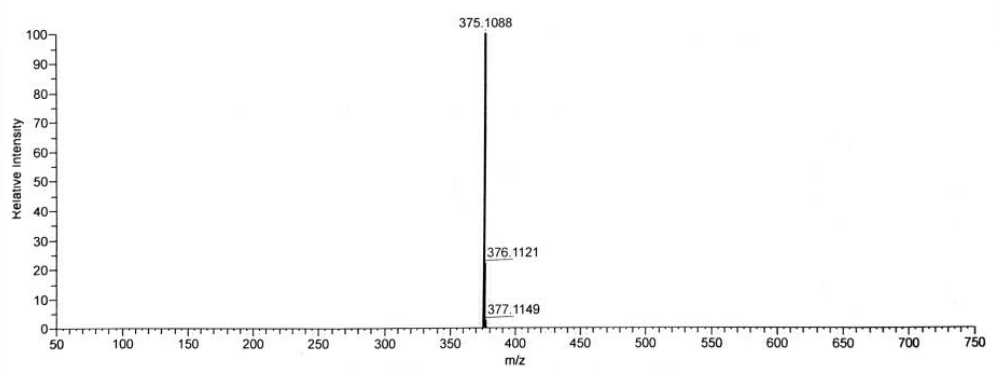
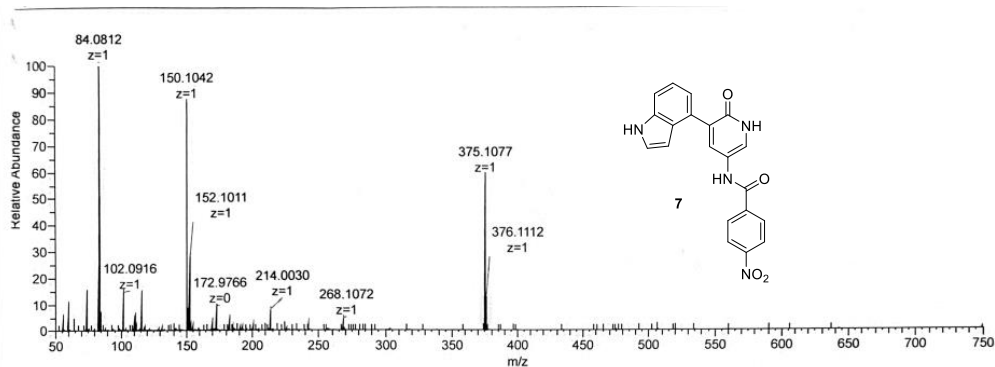
index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	421.1650	C <sub>26</sub> H <sub>21</sub> O <sub>2</sub> N <sub>4</sub>	100	18.5	-2.12	C26H21O2N4	421.16590



index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	465.1547	C <sub>27</sub> H <sub>21</sub> O <sub>4</sub> N <sub>4</sub>	100	19.5	-2.3	C27H21O4N4	465.15573

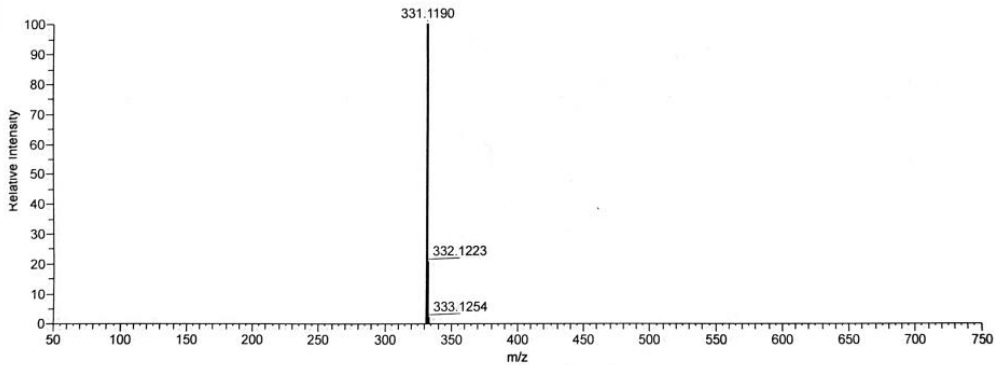
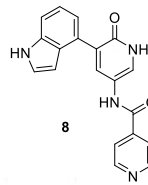
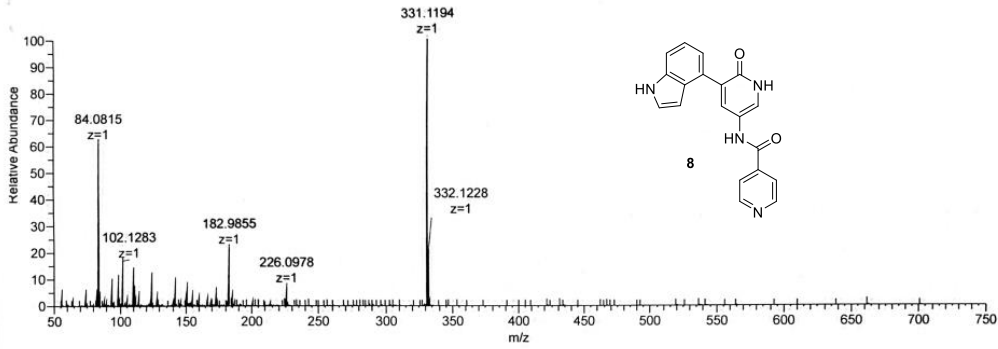


index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	330.1230	C <sub>20</sub> H <sub>16</sub> O <sub>2</sub> N <sub>3</sub>	100	14.5	-2.08	C20H16O2N3	330.12370



index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	375.1077	C <sub>20</sub> H <sub>15</sub> O <sub>4</sub> N <sub>4</sub>	100	15.5	-2.89	C20H15O4N4	375.10878

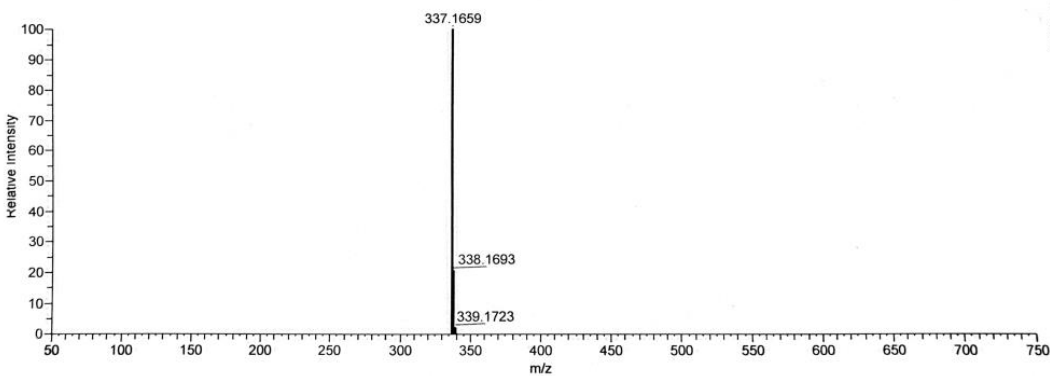
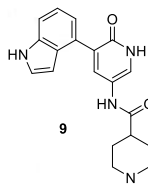
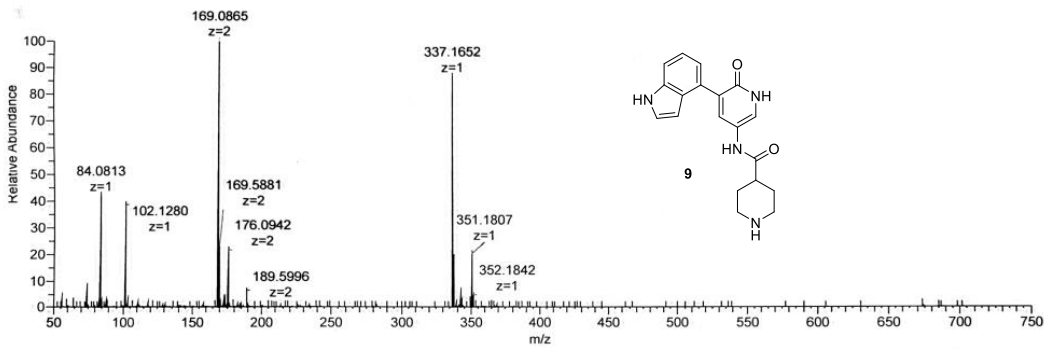
NL: 5.80E8  
 TF-1 #87 RT: 0.85 AV: 1 NL: 5.80E+008  
 T: FTMS + p ESI Full ms  
 [50 0000-750 0000]



NL: 7.98E5  
 C19H15O2N4 Chrg 1 R: 63007 Res. Pwr:  
 @FWHM

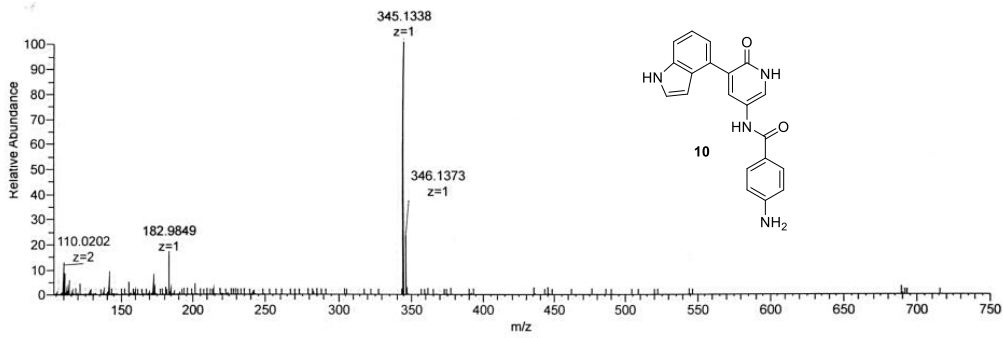
index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	331.1194	C <sub>19</sub> H <sub>15</sub> O <sub>2</sub> N <sub>4</sub>	100	14.5	1.21	C19H15O2N4	331.11895

NL: 7.89E8  
 TF-1-70 #91 RT: 0.88 AV: 1 NL: 7.8  
 T: FTMS + p ESI Full ms  
 [50 0000-750 0000]

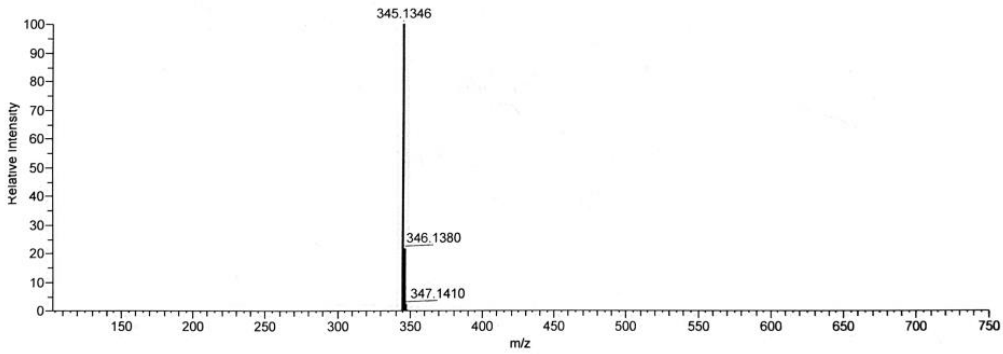


NL: 7.97E5  
 C19H21O2N4 Chrg 1 R: 62307  
 @FWHM

index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	337.1652	C <sub>19</sub> H <sub>21</sub> O <sub>2</sub> N <sub>4</sub>	100	11.5	-2.02	C19H21O2N4	337.16590

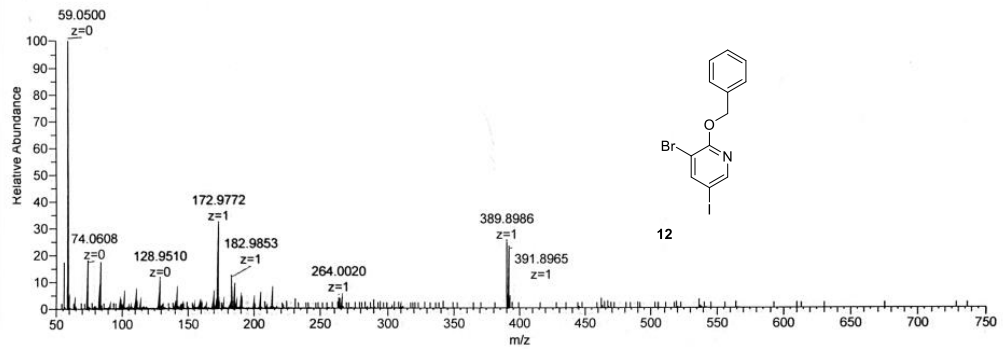


NL: 1.96E8  
 TF-1-46 #191 RT: 1.88 AV: 1 NL:  
 5.37E+008  
 T: FTMS + p ESI Full ms  
 [50.0000-750.0000]

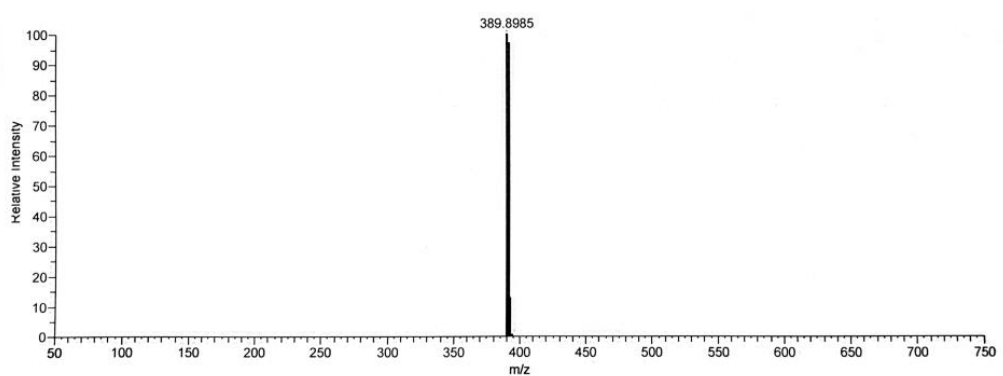


NL: 7.89E5  
 C20H17O2N4 Chrg 1 R: 61807 Res. Pwr.  
 @FWHM

Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	345.1338	C <sub>20</sub> H <sub>17</sub> O <sub>2</sub> N <sub>4</sub>	100	14.5	-2.27	C <sub>20</sub> H <sub>17</sub> O <sub>2</sub> N <sub>4</sub>	345.13460



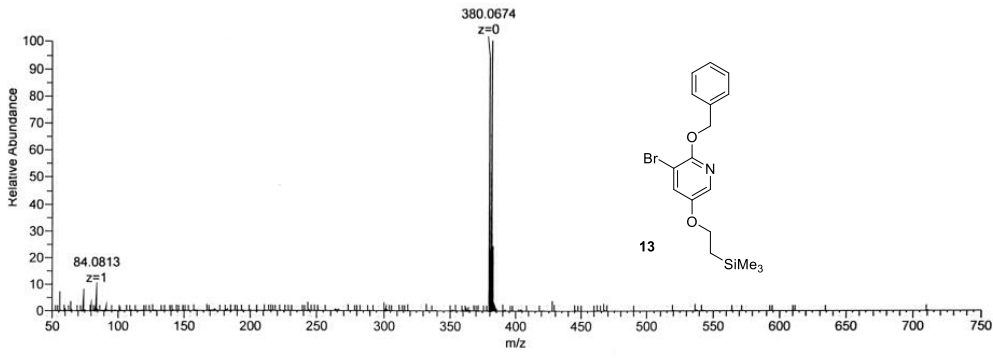
NL: 3.01E8  
 TF-1-60 #97 RT: 0.93 AV: 1 NL: 3.01E+008  
 T: FTMS + p ESI Full ms  
 [50.0000-750.0000]



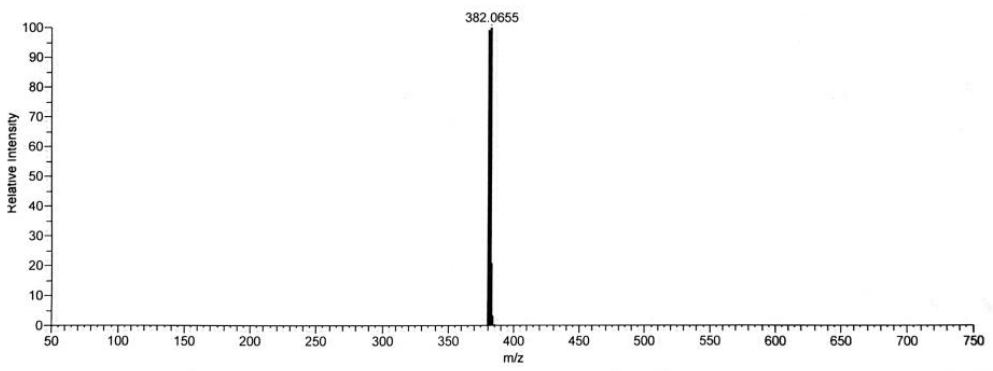
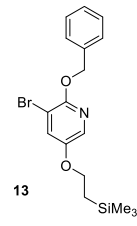
NL: 4.42E5  
 C12H10O1N1Br1I1 Chrg 1 R: 57906 Res.  
 Pwr. @FWHM

Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	389.8986	C <sub>12</sub> H <sub>10</sub> ON <sup>19</sup> Br <sup>127</sup> I	100	7.5	0.24	C <sub>12</sub> H <sub>10</sub> ON[79]Br[127]I	389.89850



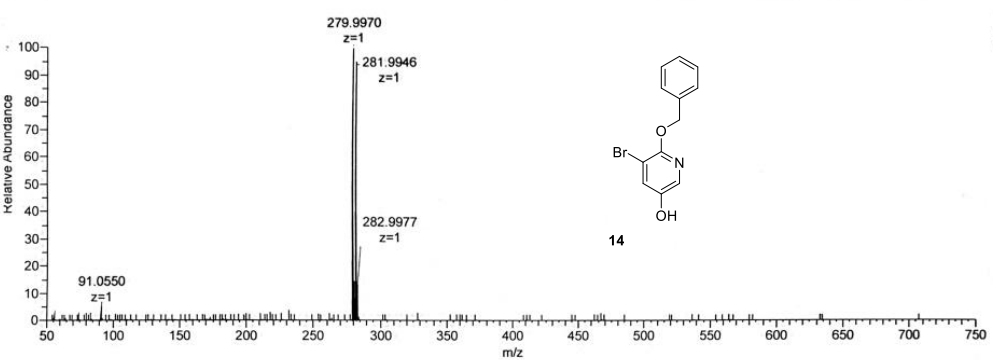


NL: 8.69E8  
 TF-1-110 #93 RT: 0.92 AV: 1 NL:  
 8.69E+008  
 T: FTMS + p ESI Full ms  
 [50.0000-750.0000]

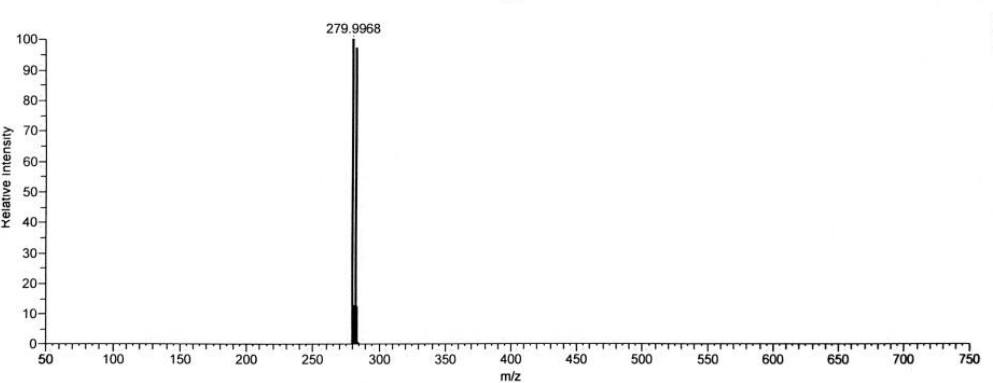
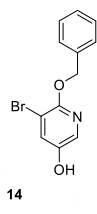


NL: 3.88E5  
 C17H23O2N1Br1Si1 Chrg 1 R: 58502  
 Res. Pwr. @FWHM

Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	380.0674	C <sub>17</sub> H <sub>23</sub> O <sub>2</sub> N <sup>79</sup> Br <sup>78</sup> Si	100	7.5	-0.56	C17H23O2N(79)Br[28...	380.06759



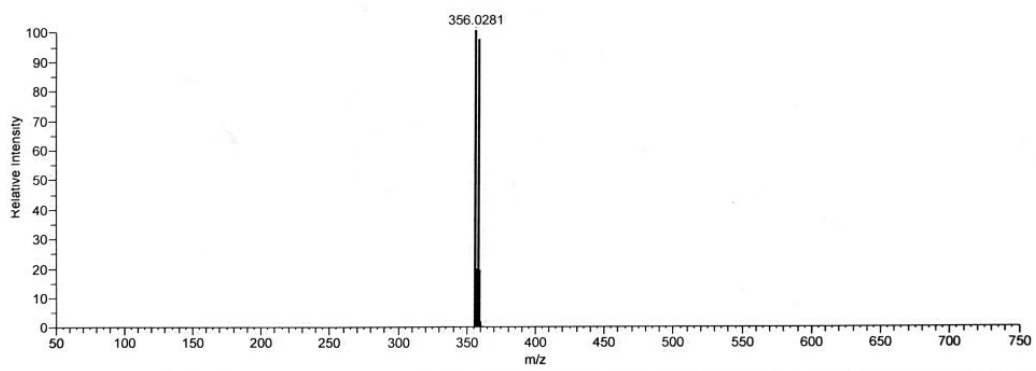
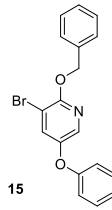
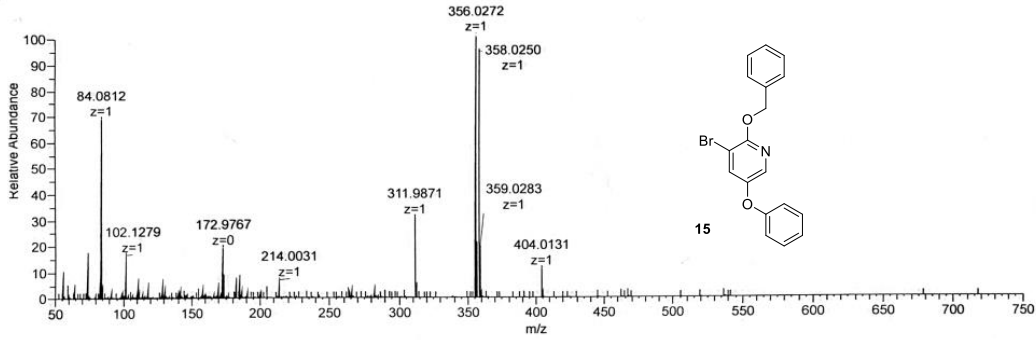
NL: 1.90E9  
 TF-1-111 #93 RT: 0.92 AV: 1 NL: 1.90E+009  
 T: FTMS + p ESI Full ms  
 [50.0000-750.0000]



NL: 4.41E5  
 C12H11O2N1Br1 Chrg 1 R: 68306 Res.  
 Pwr. @FWHM

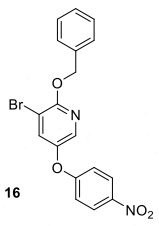
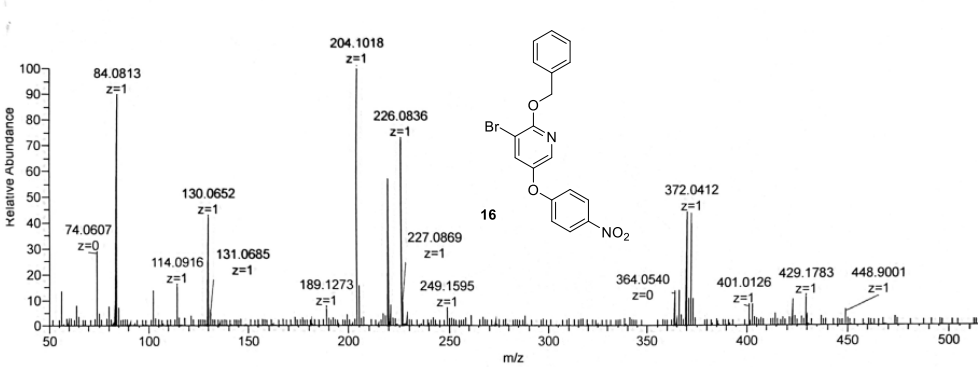
Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	279.9970	C <sub>12</sub> H <sub>11</sub> O <sub>2</sub> N <sup>79</sup> Br	100	7.5	0.97	C12H11O2N(79)Br	279.99677

NL: 3.62E8  
 TF-1-77 #89 RT: 0.87 AV: 1 NL: 3.6  
 T: FTMS + p ESI Full ms  
 [50.0000-750.0000]

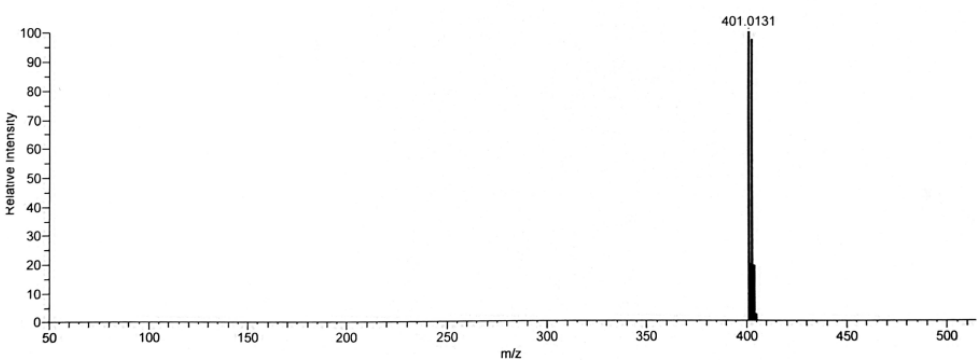


NL: 4.13E5  
 C18H15O2N1Br1 Chrg 1 R: 604  
 Pwr: @FWHM

Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	356.0272	C <sub>18</sub> H <sub>15</sub> O <sub>2</sub> N <sup>1</sup> Br	100	11.5	-2.46	C18H15O2N[79]Br	356.02807

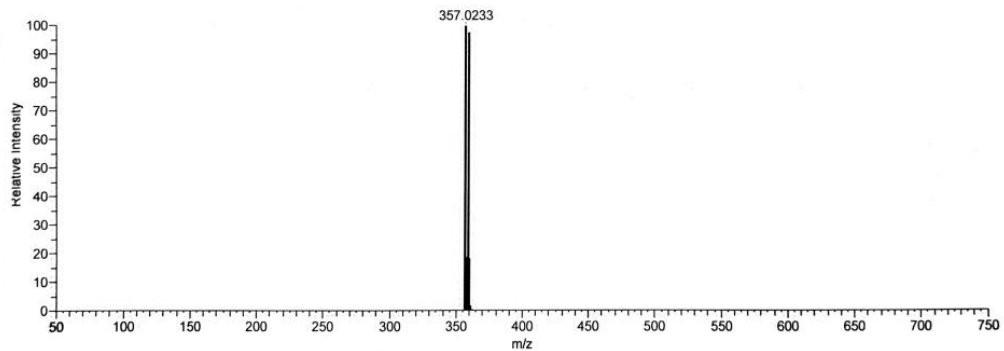
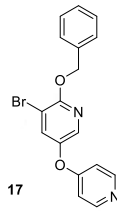
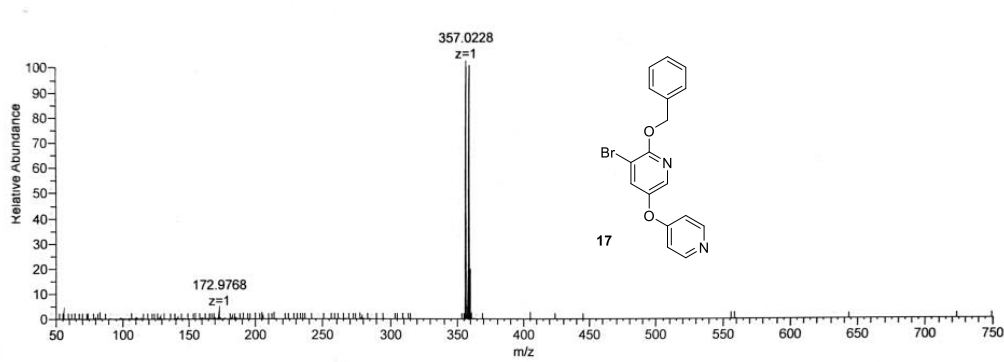


NL: 3.34E8  
 TF-1-117-40 #91 RT: 0.92 AV: 1 NL:  
 3.34E+008  
 T: FTMS + p ESI Full ms  
 [50.0000-750.0000]

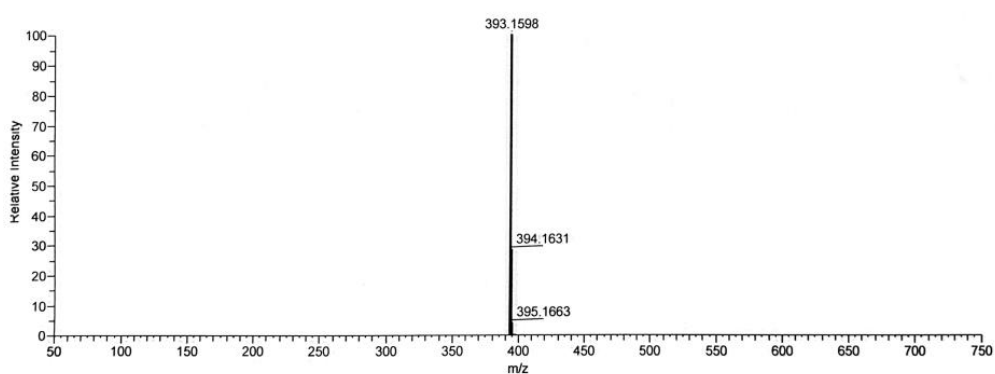
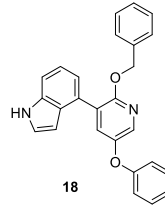
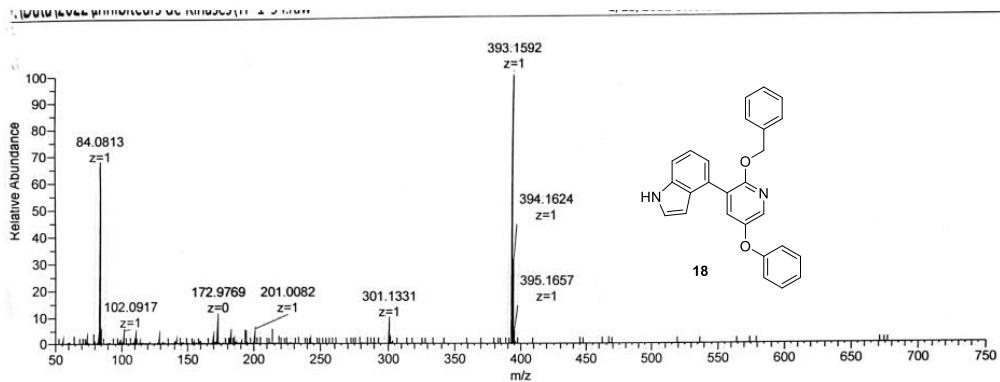


NL: 4.10E5  
 C18H14O4N21Br1 Chrg 1 R: 55406 Res.  
 Pwr: @FWHM

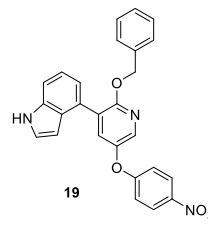
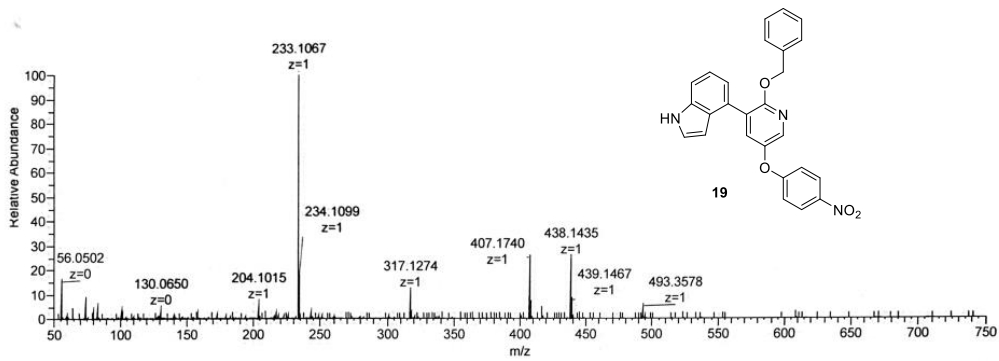
Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	401.0126	C <sub>18</sub> H <sub>14</sub> O <sub>4</sub> N <sub>2</sub> <sup>1</sup> Br	100	12.5	-1.28	C18H14O4N2[79]Br	401.01315



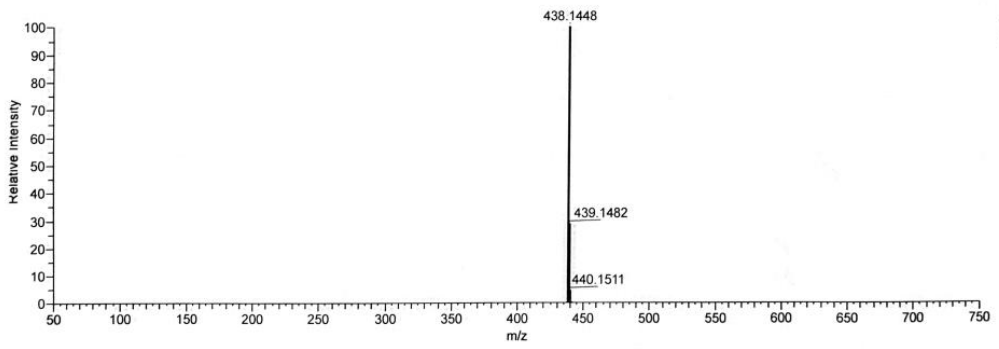
Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	357.0228	C <sub>17</sub> H <sub>14</sub> O <sub>2</sub> N <sub>2</sub> <sup>79</sup> Br	100	11.5	-1.46	C17H14O2N2[79]Br	357.02332



Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	393.1592	C <sub>26</sub> H <sub>21</sub> O <sub>2</sub> N <sub>2</sub>	100	17.5	-1.31	C26H21O2N2	393.15975

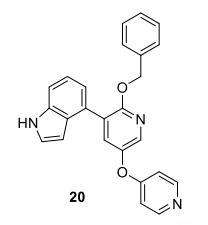
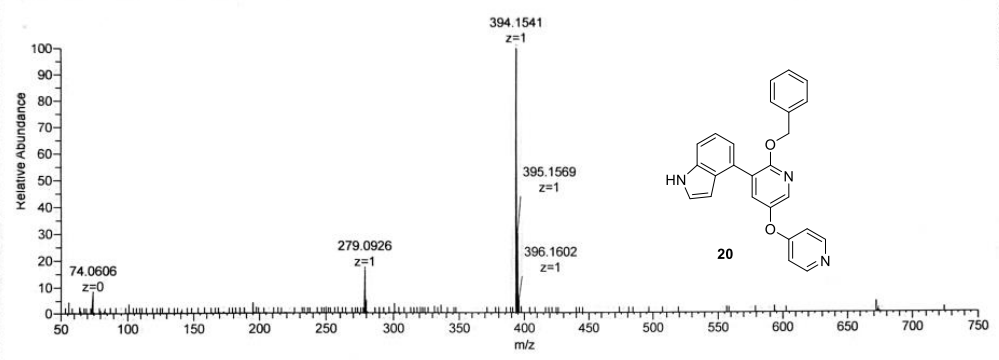


NL: 3.48E8  
 TF-1-12S #95 RT: 0.95 AV: 1 NL:  
 3.48E+008  
 T: FTMS + p ESI Full ms  
 [50.0000-750.0000]

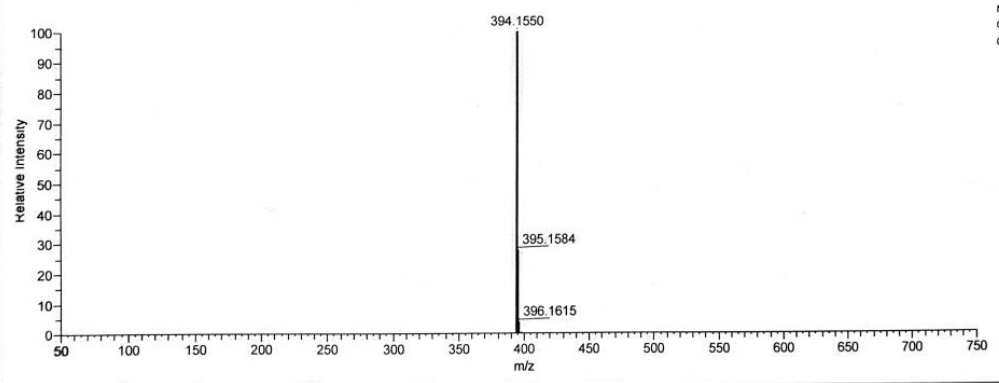


NL: 7.39E5  
 C26H20O4N3 Chrg 1 R: 54107 Res. Pwr.  
 @FWHM

index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	438.1435	C <sub>26</sub> H <sub>20</sub> O <sub>4</sub> N <sub>3</sub>	92.0940585297288	18.5	-3.13	C26H20O4N3	438.14483

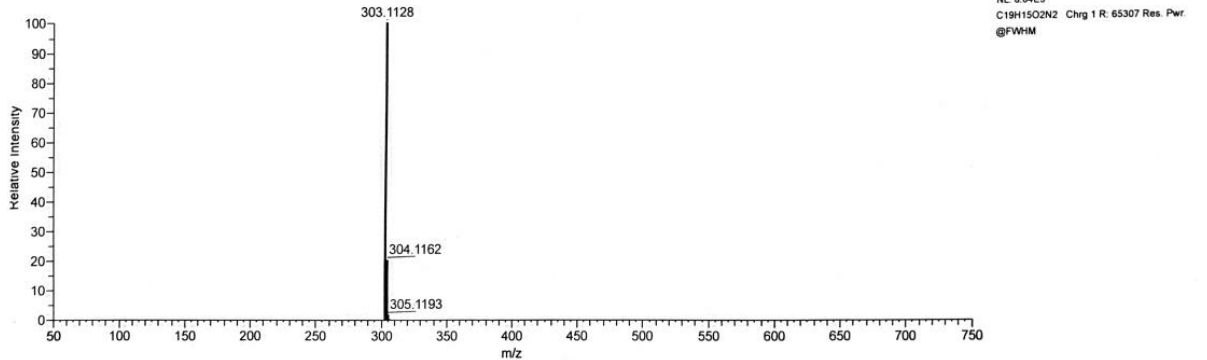
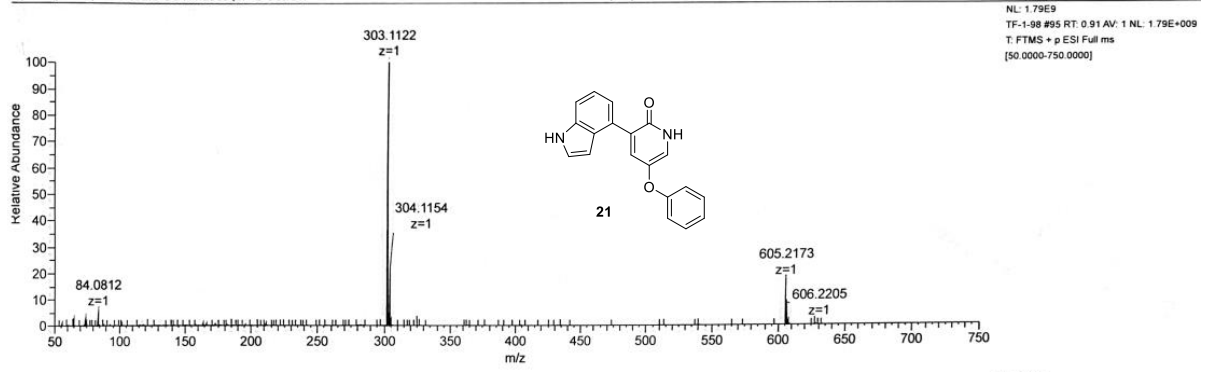


NL: 2.48E9  
 TF-1-131 #105 RT: 1.04 AV: 1 NL:  
 2.48E+009  
 T: FTMS + p ESI Full ms  
 [50.0000-750.0000]

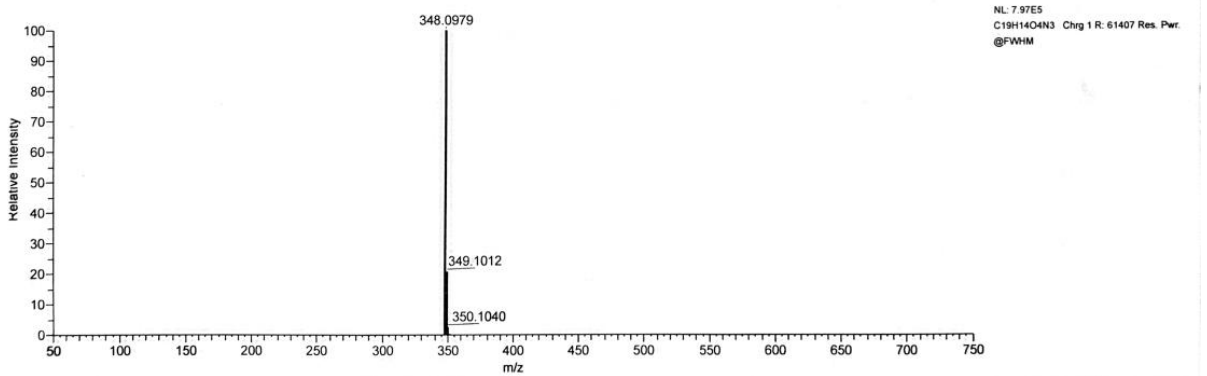
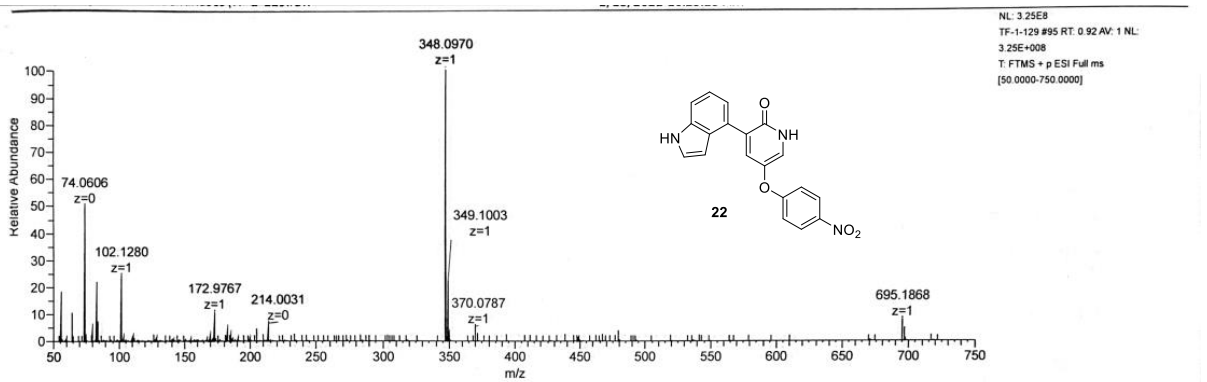


NL: 7.50E5  
 C25H20O2N3 Chrg 1 R: 57707 Res. Pwr.  
 @FWHM

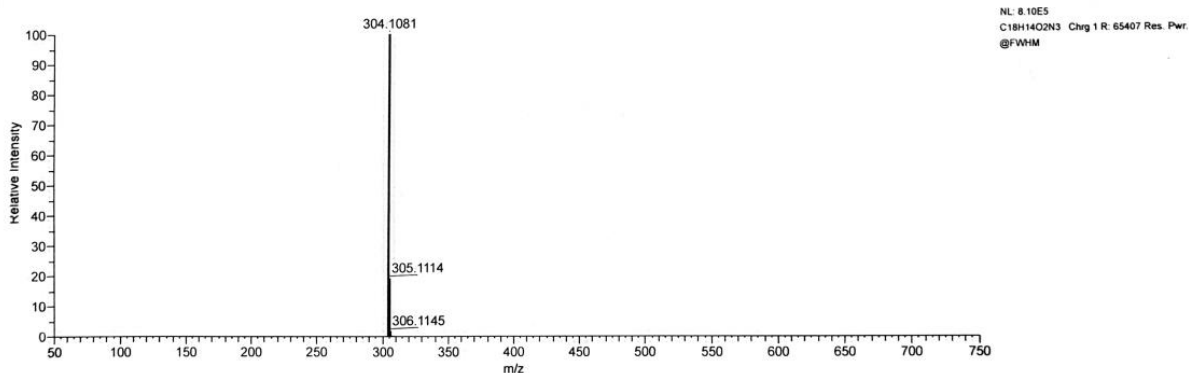
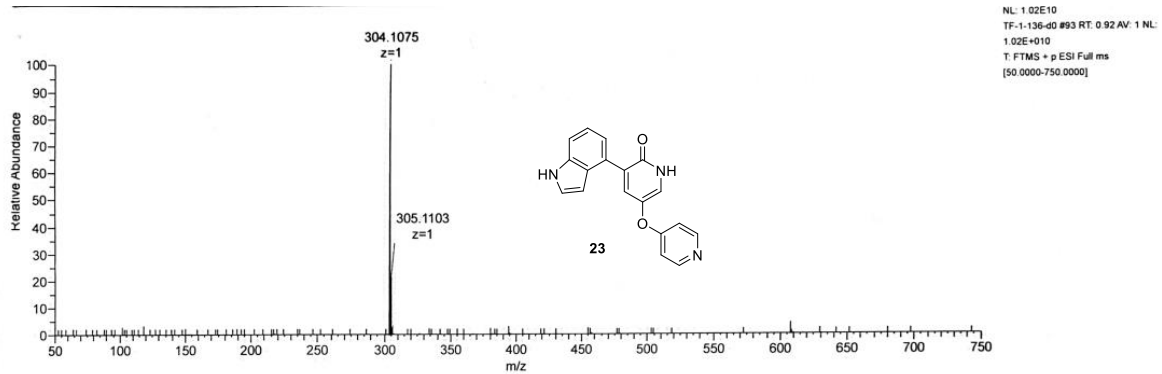
index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	394.1541	C <sub>25</sub> H <sub>20</sub> O <sub>2</sub> N <sub>3</sub>	100	17.5	-2.41	C25H20O2N3	394.15500



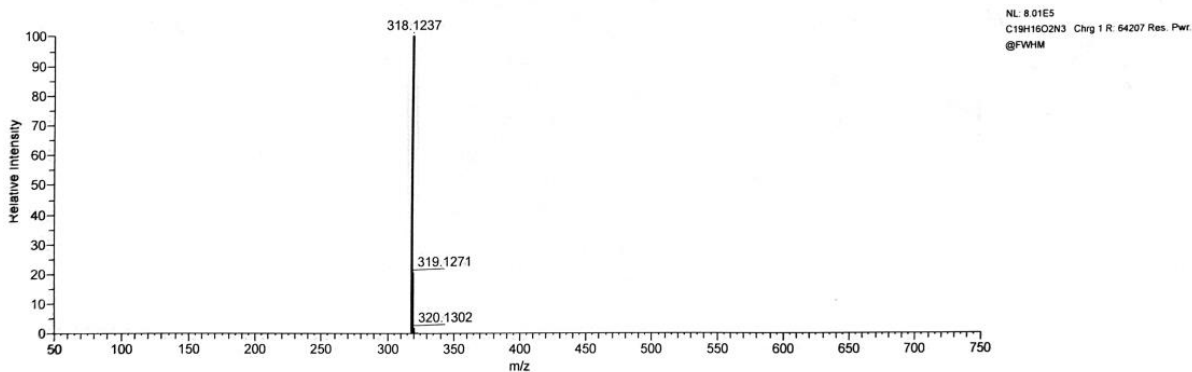
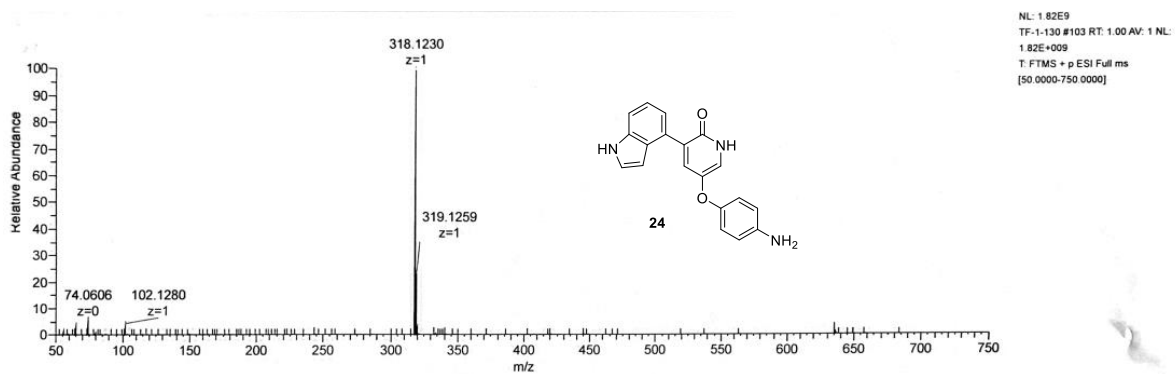
Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	303.1122	C <sub>19</sub> H <sub>15</sub> O <sub>2</sub> N <sub>2</sub>	100	13.5	-2.05	C19H15O2N2	303.11280



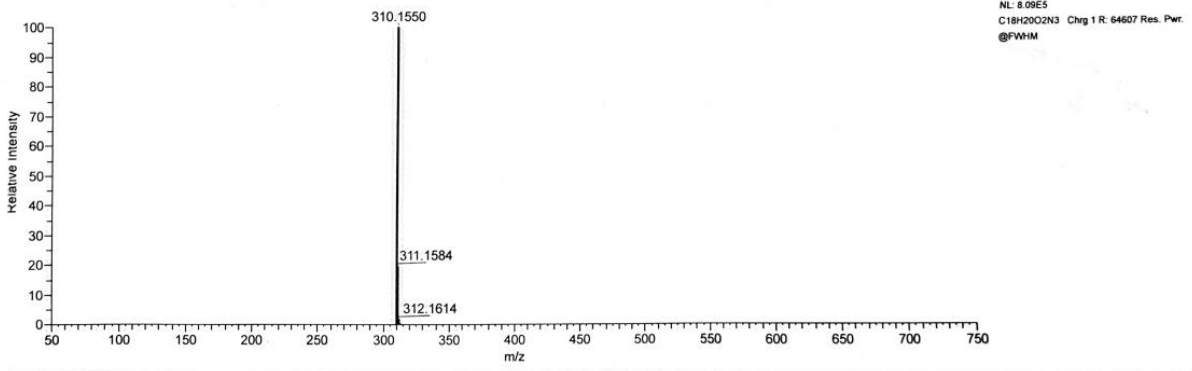
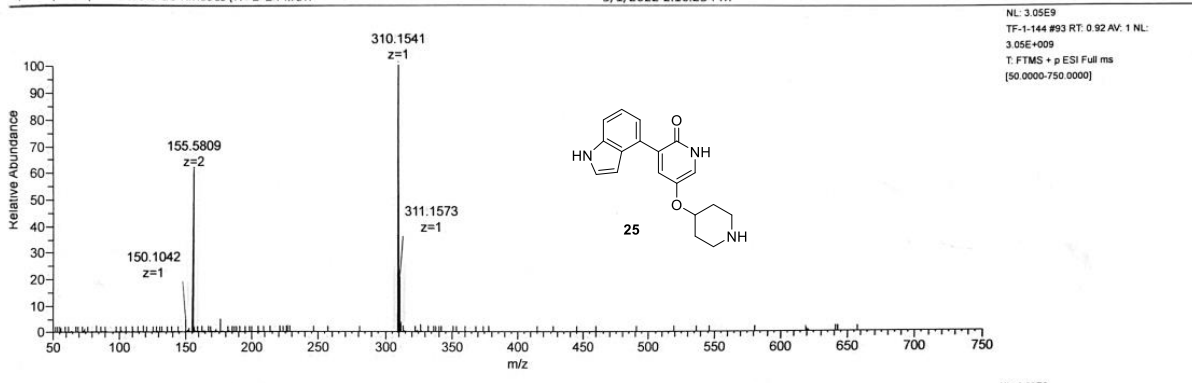
Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	348.0970	C <sub>19</sub> H <sub>14</sub> O <sub>4</sub> N <sub>3</sub>	100	14.5	-2.49	C19H14O4N3	348.09788



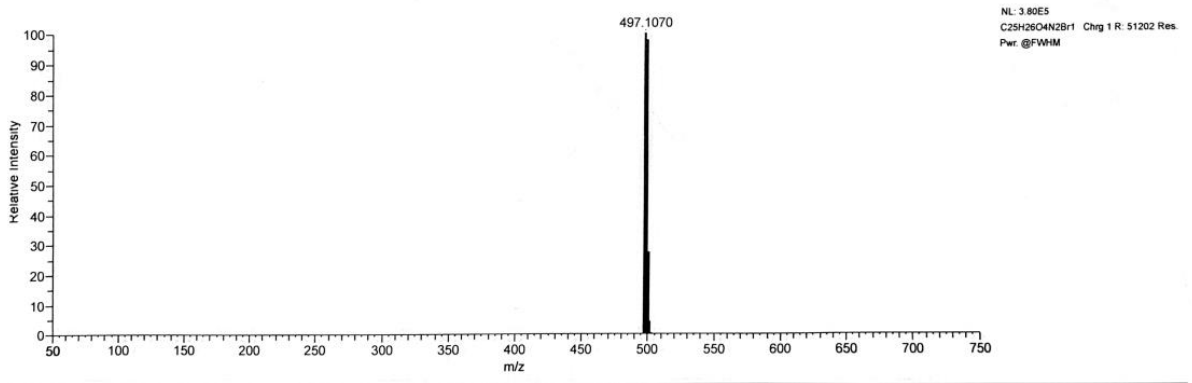
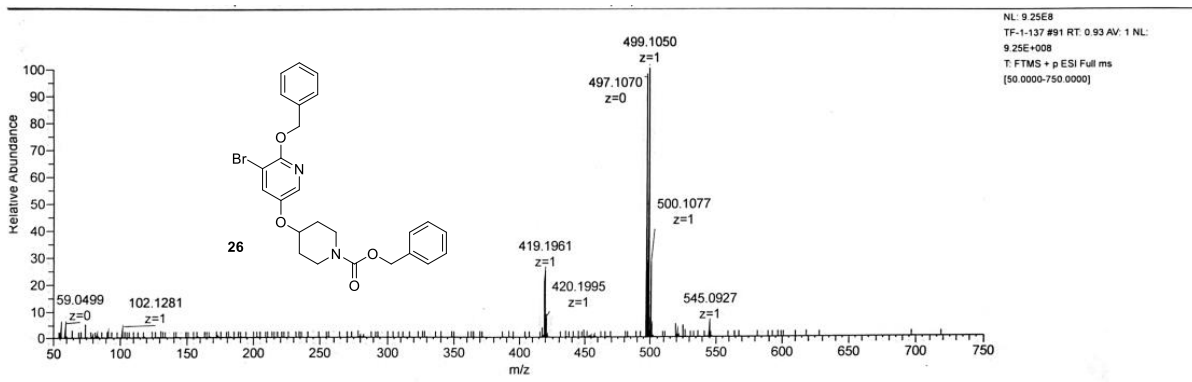
Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	304.1075	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> N <sub>3</sub>	100	13.5	-1.98	C18H14O2N3	304.10805



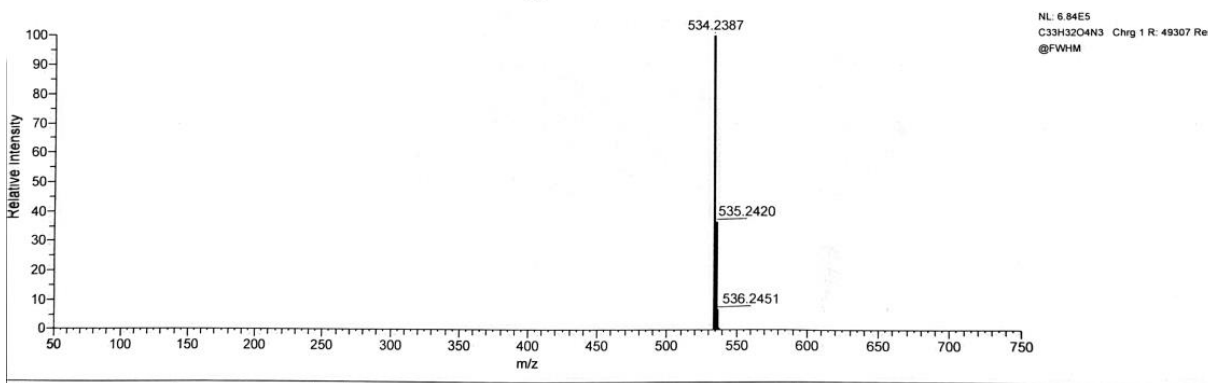
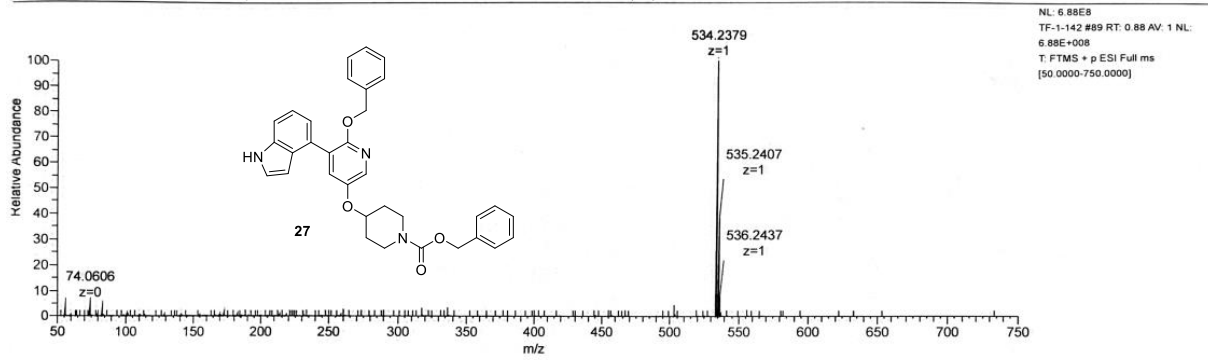
Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	318.1230	C <sub>19</sub> H <sub>16</sub> O <sub>2</sub> N <sub>3</sub>	100	13.5	-2.16	C19H16O2N3	318.12370



Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	310.1541	C <sub>18</sub> H <sub>20</sub> O <sub>2</sub> N <sub>3</sub>	92.4016783285469	10.5	-3.07	C18H20O2N3	310.15500

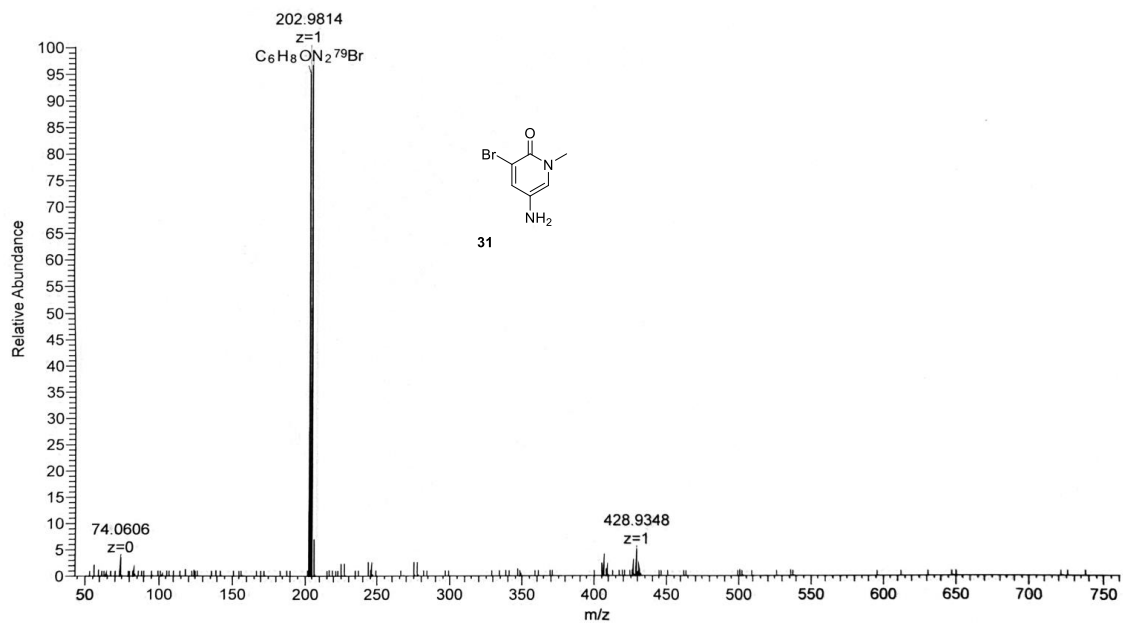


Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	497.1070	C <sub>25</sub> H <sub>26</sub> O <sub>4</sub> N <sub>2</sub> <sup>79</sup> Br	100	13.5	-0.17	C25H26O4N2[79]Br	497.10705



Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	534.2379	C <sub>33</sub> H <sub>32</sub> O <sub>4</sub> N <sub>3</sub>	100	19.5	-1.65	C33H32O4N3	534.23873

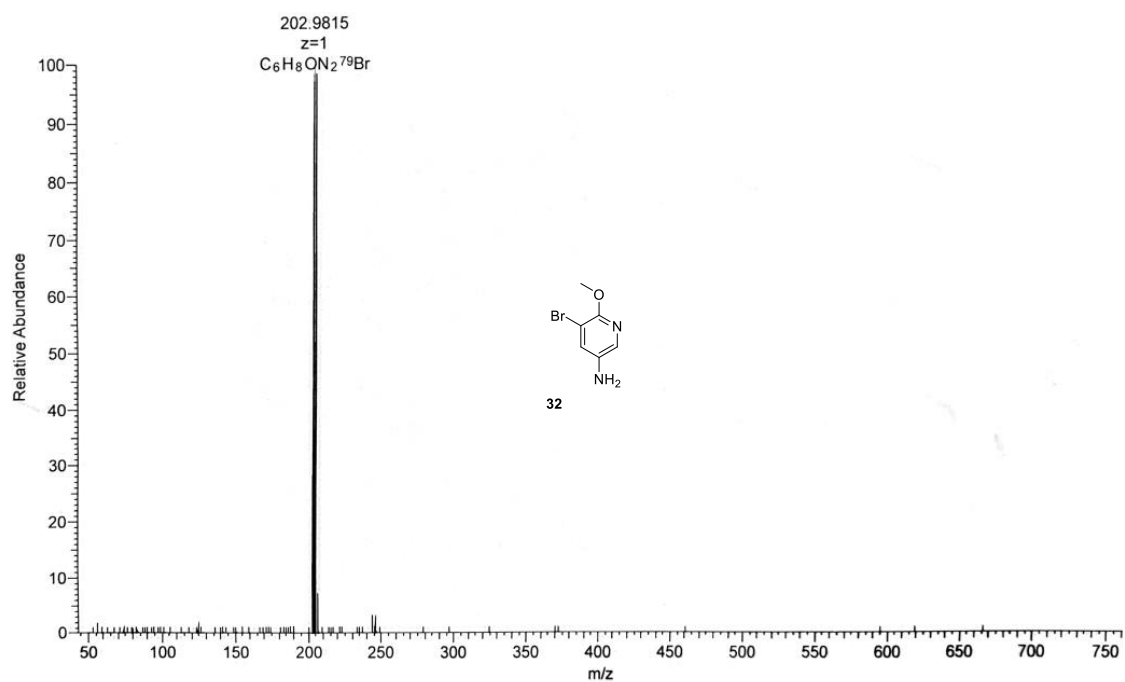
NC-016 #89 RT: 0.88 AV: 1 NL: 2.89E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]



Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments
202.9814	C <sub>6</sub> H <sub>8</sub> ON <sub>2</sub> <sup>79</sup> Br	-0.48	202.98145	96.54	99.7	(Collection)

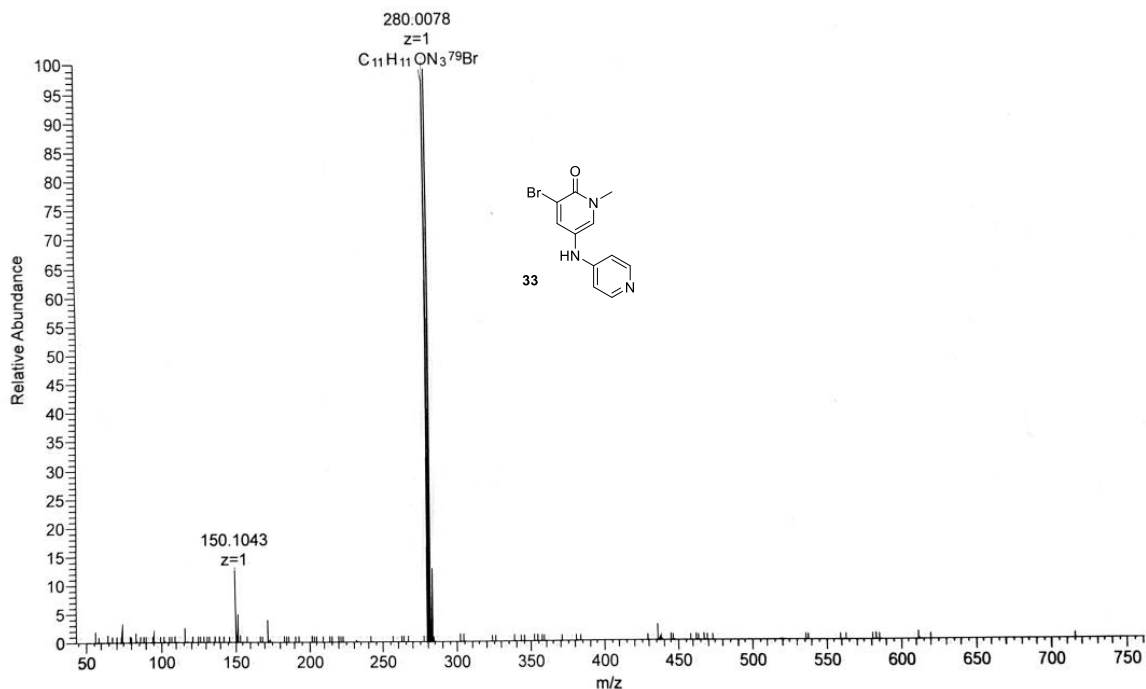


NC-023 #131 RT: 1.32 AV: 1 NL: 3.24E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]



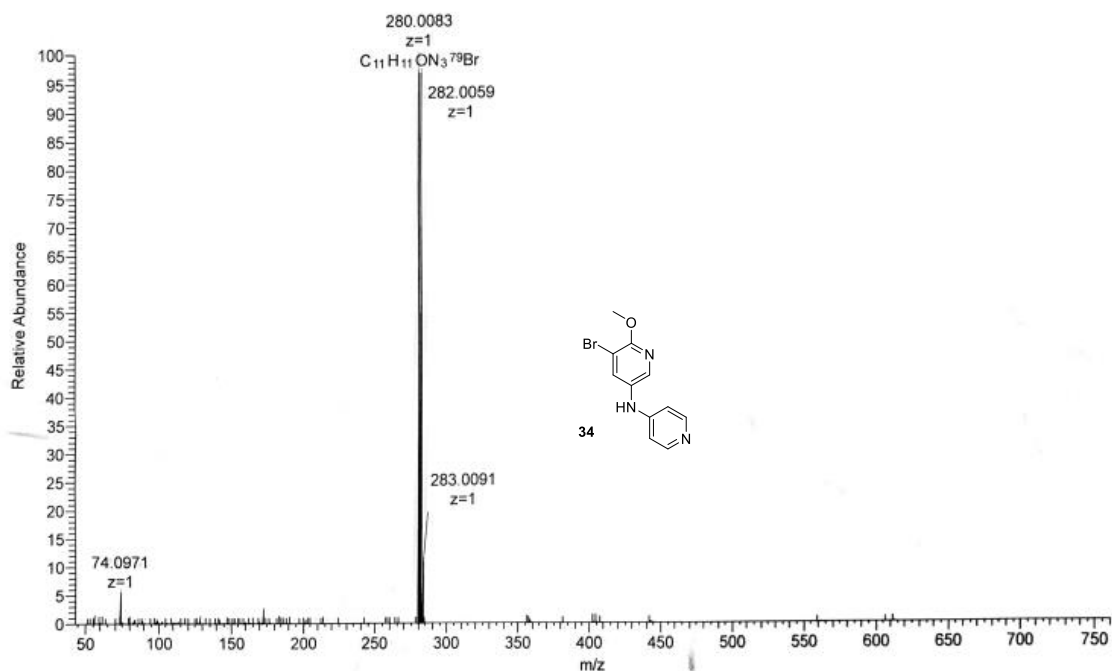
Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments (Collection)
202.9815	C <sub>6</sub> H <sub>8</sub> ON <sub>2</sub> <sup>79</sup> Br	0.12	202.98145	96.11	99.61	

NC-020 #89 RT: 0.87 AV: 1 NL: 3.19E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]



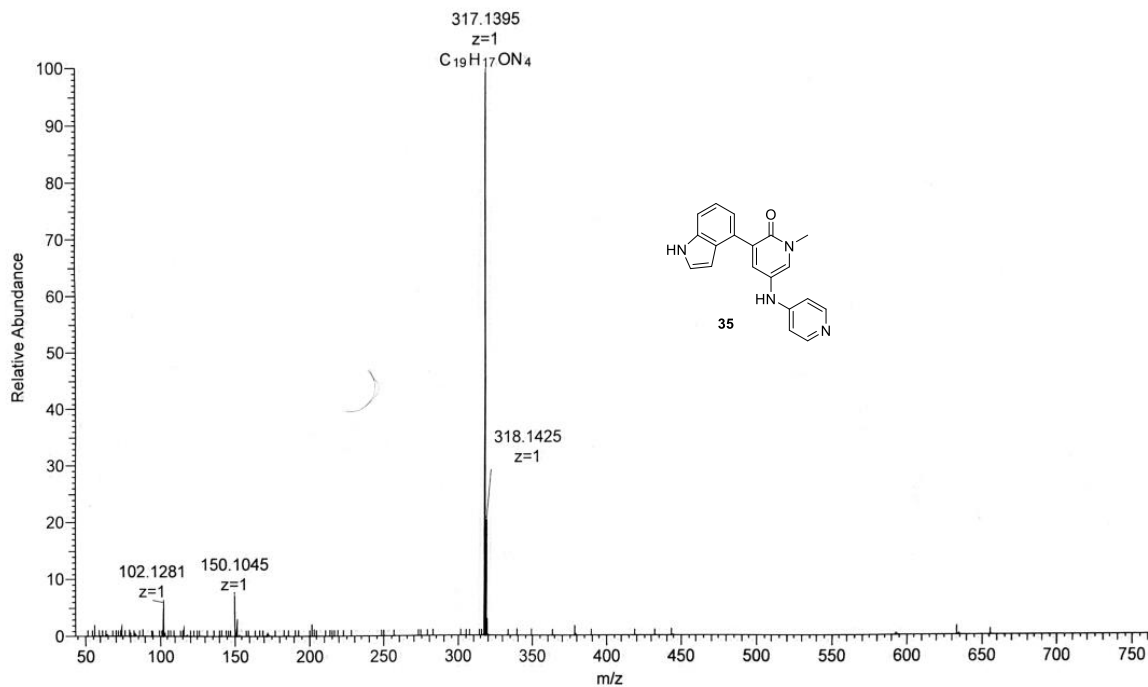
Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragment
280.0078	C <sub>11</sub> H <sub>11</sub> ON <sub>3</sub> <sup>79</sup> Br	-0.56	280.00800	96.15	98.68	(Collection)

NC-024 #175 RT: 1.73 AV: 1 NL: 2.05E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]



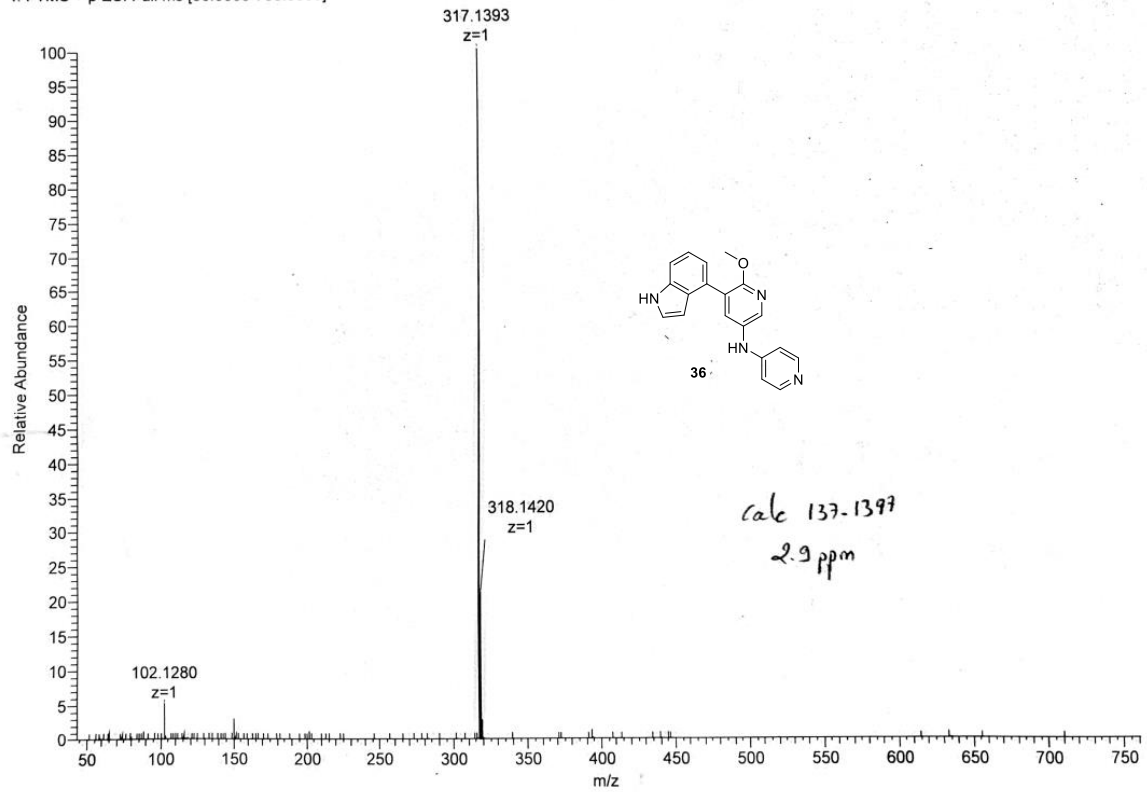
Peak Mass	Display Formula	Delta (ppm)	Theo. mass	Combined Score	Pattern Cov. (%)	MSMS Matched Fragments (Collection)
280.0083	C <sub>11</sub> H <sub>11</sub> ON <sub>3</sub> <sup>79</sup> Br	1.07	280.00800	96.57	98.68	

NC-021 #93 RT: 0.92 AV: 1 NL: 4.25E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

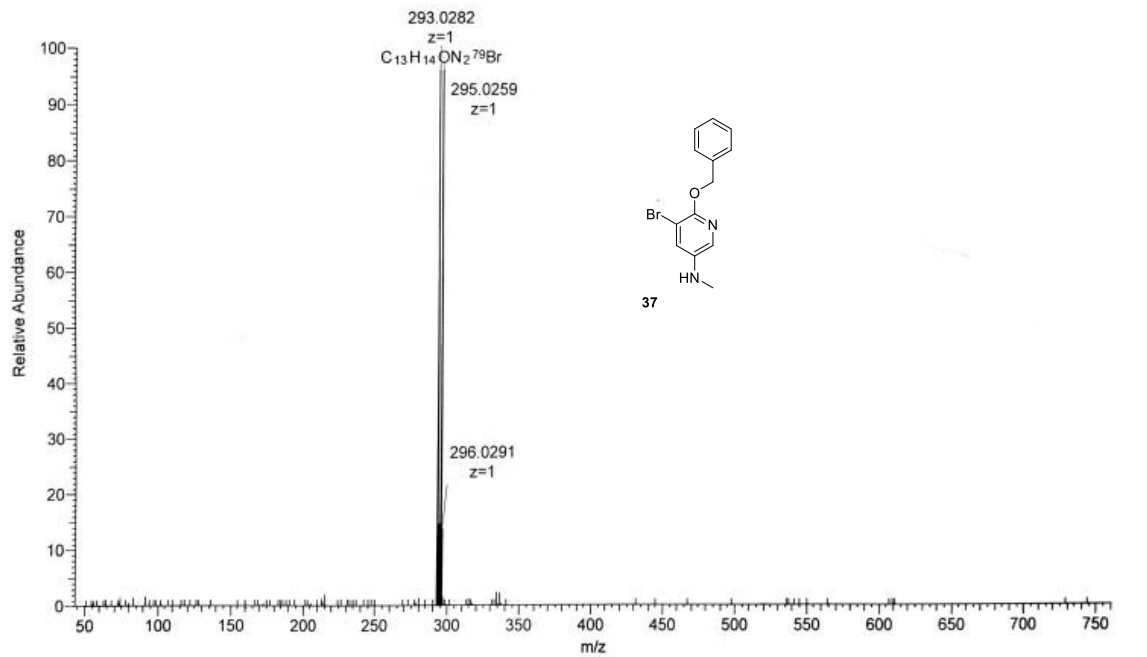


Peak Mass	Display Formula	Delta (ppm)	Theo. mass	Combined Score	Pattern Cov. (%)	MSMS Matched Fragments (Collection)
317.1395	C <sub>19</sub> H <sub>17</sub> ON <sub>4</sub>	-0.51	317.13969	98.37	100	

NC-027 #93 RT: 0.91 AV: 1 NL: 5.37E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

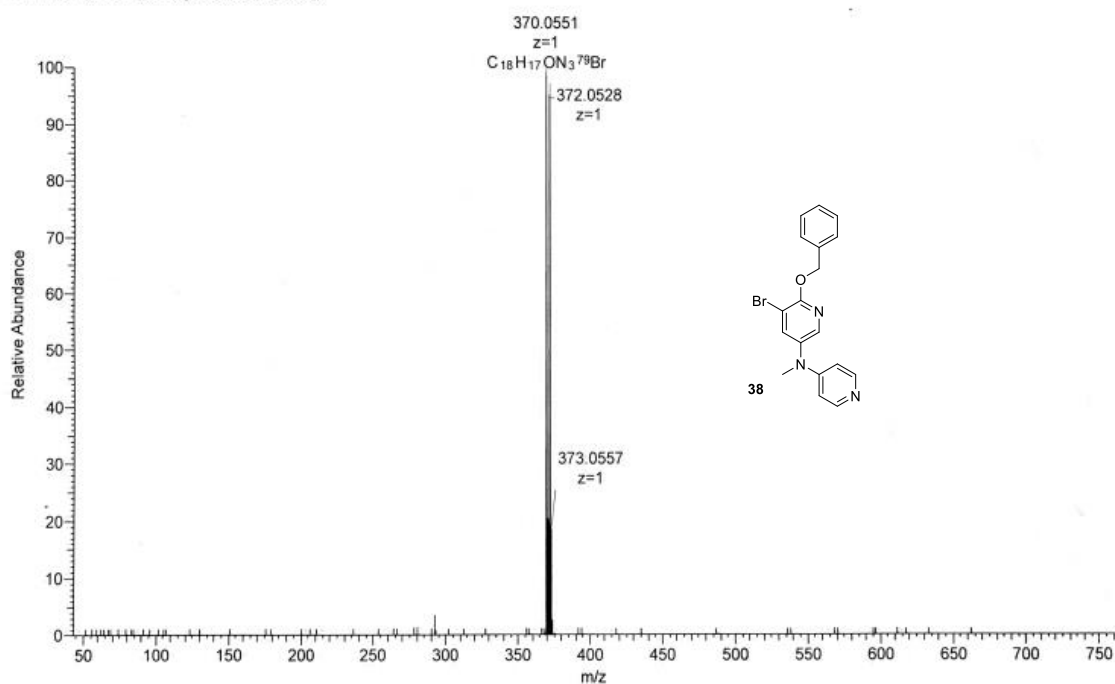


TF-2-202 #93 RT: 0.91 AV: 1 NL: 4.14E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]



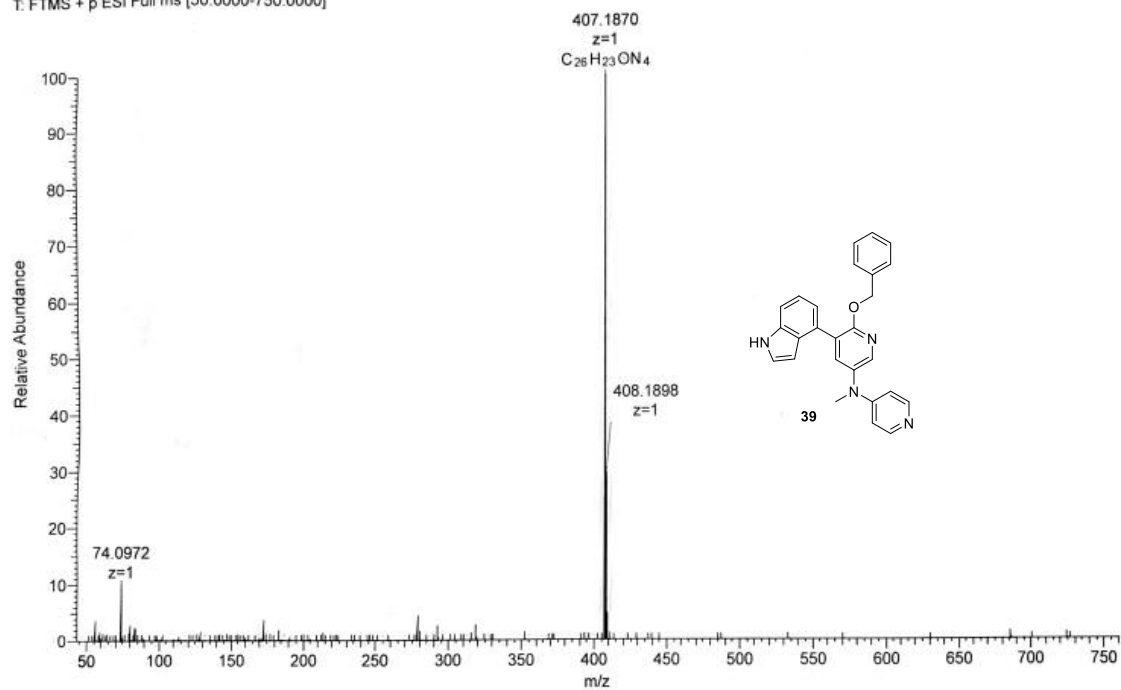
Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments
293.0282	C <sub>13</sub> H <sub>14</sub> ON <sub>2</sub> <sup>79</sup> Br	-0.59	293.02840	97.49	99.55	(Collection)

TF-2-204 #91 RT: 0.90 AV: 1 NL: 6.30E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]



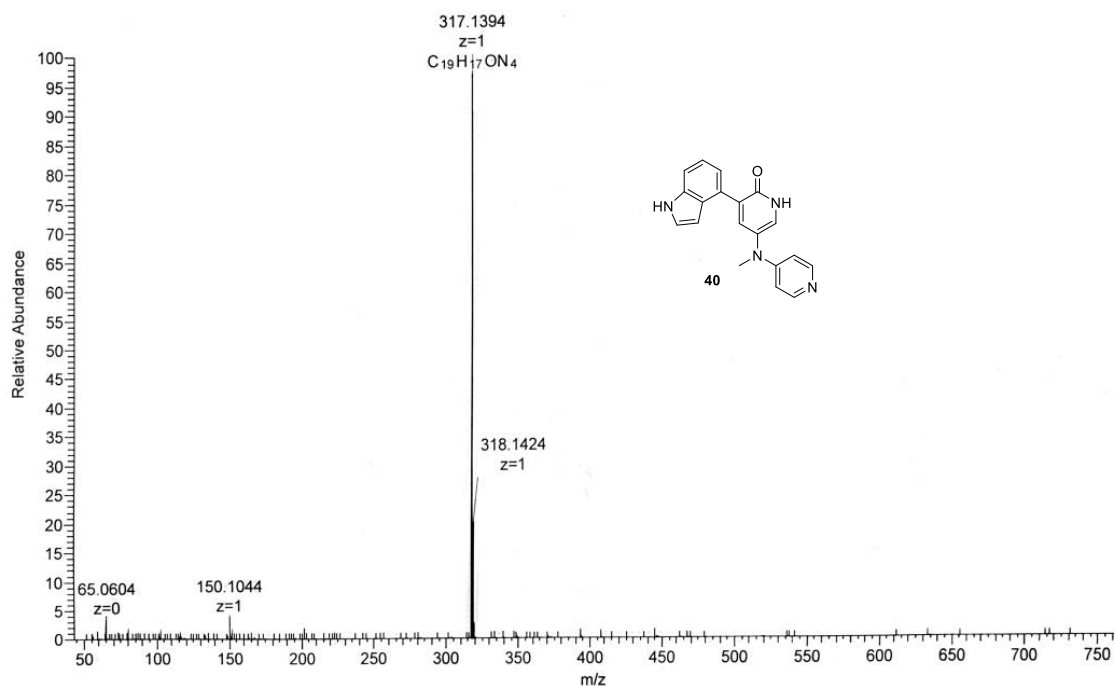
Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments (Collection)
370.0551	C <sub>18</sub> H <sub>17</sub> ON <sub>3</sub> <sup>79</sup> Br	0.28	370.05495	98.81	100	

TF-2-205 #199 RT: 1.97 AV: 1 NL: 8.45E8  
 T: FTMS + p ESI Full ms [50.0000-750.0000]



Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments (Collection)
407.1870	C <sub>26</sub> H <sub>23</sub> ON <sub>4</sub>	0.92	407.18664	98.41	100	

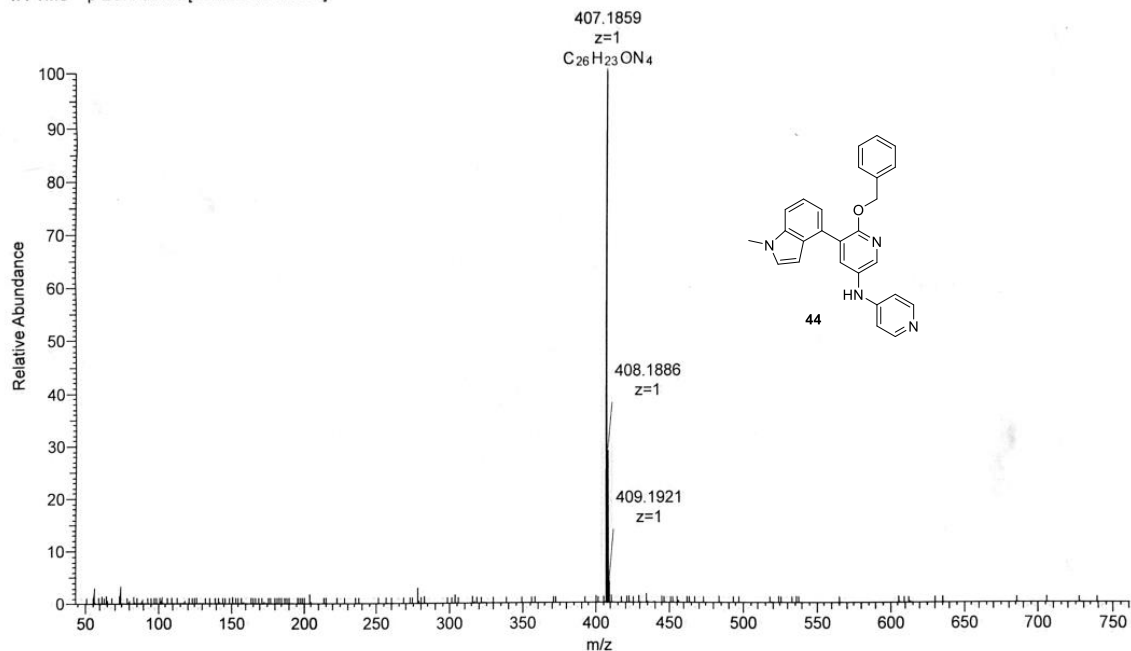
NC-026 #93 RT: 0.91 AV: 1 NL: 1.91E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]



Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments (Collection)
317.1394	C <sub>19</sub> H <sub>17</sub> ON <sub>4</sub>	-0.89	317.13969	98.68	100	

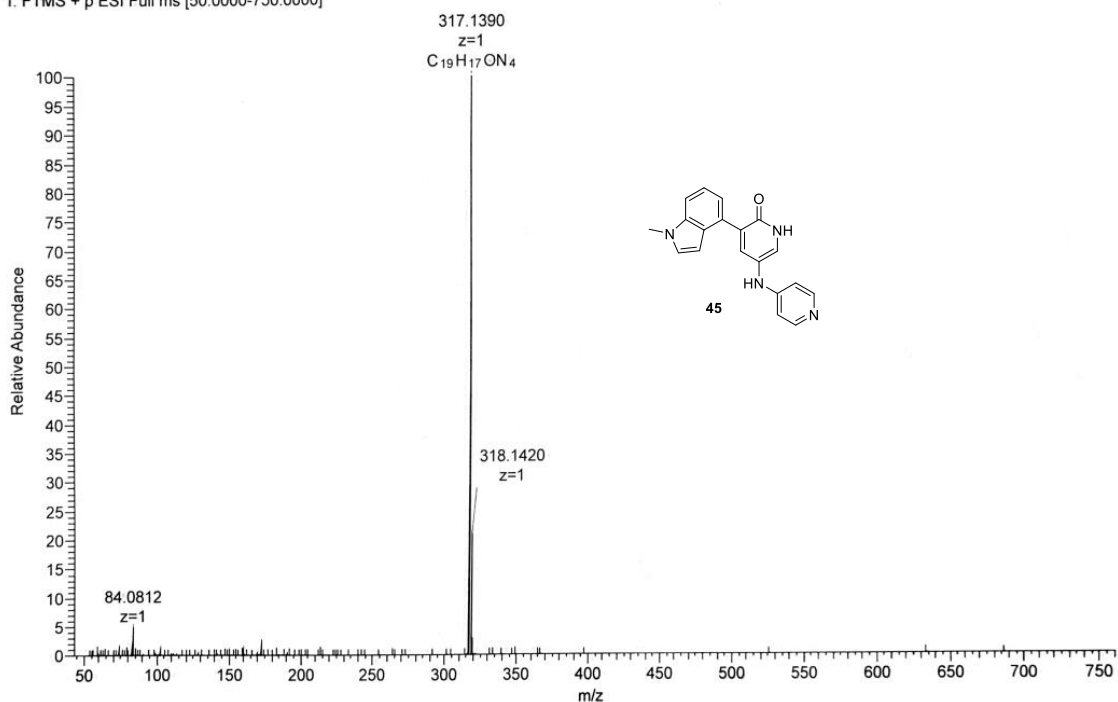
2

AB-1-158 #93 RT: 0.90 AV: 1 NL: 2.19E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]



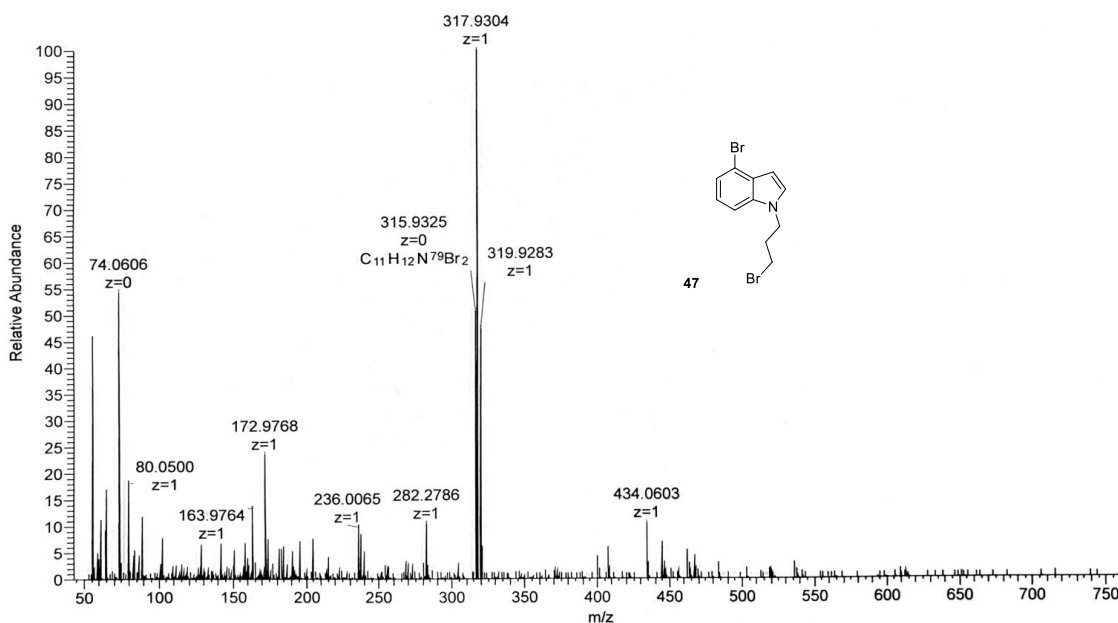
Rank	Peak Mass	Display Formula	RDB	Combined Score	Delta [ppm]	Theo. mass	MSMS Matched Fragm...
1	407.1859	C <sub>26</sub> H <sub>23</sub> ON <sub>4</sub>	17.50	98.07	-1.93	407.18664	(Collection)

TF-1-184 #95 RT: 0.92 AV: 1 NL: 1.70E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]



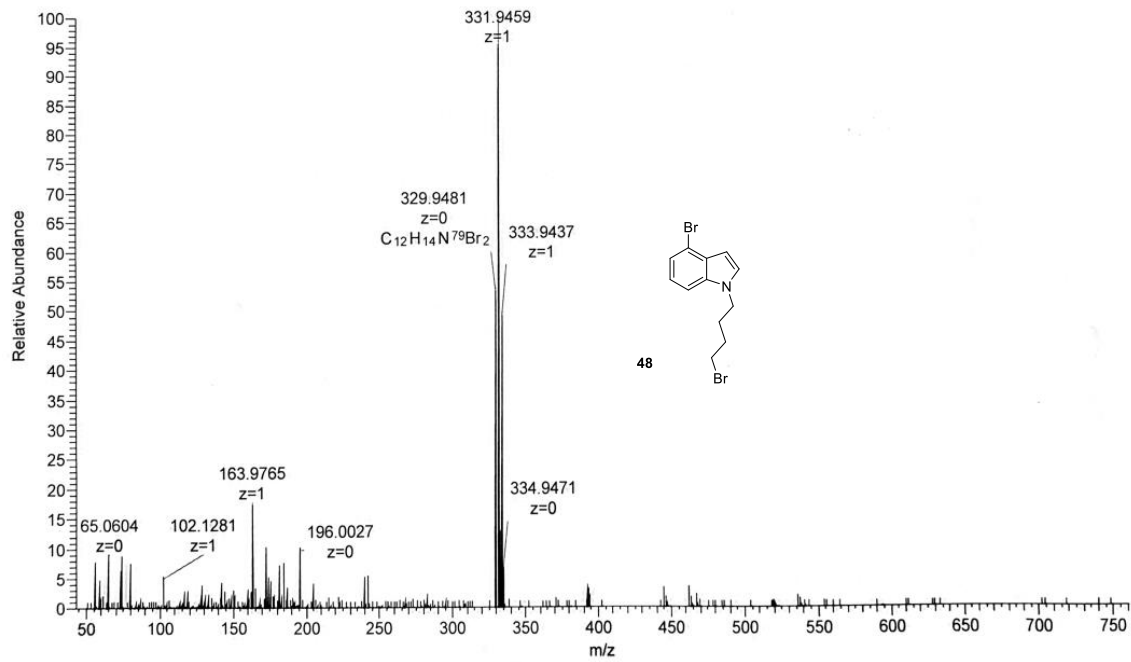
Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments (Collection)
317.1390	C <sub>19</sub> H <sub>17</sub> ON <sub>4</sub>	-2.24	317.13969	97.53	100	

TF-1-161 #85 RT: 0.83 AV: 1 NL: 7.37E7  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

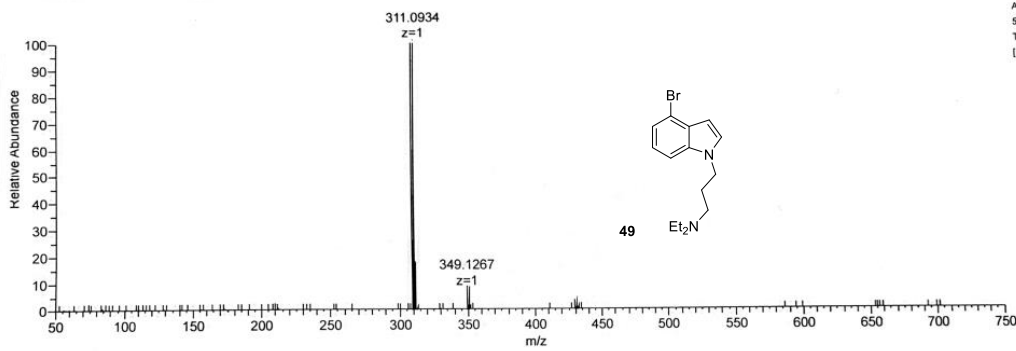


Rank	Peak Mass	Display Formula	RDB	Combined Score	Delta [ppm]	Theo. mass	MSMS Matched Fragments (Collection)
1	315.9325	C <sub>11</sub> H <sub>12</sub> N <sup>79</sup> Br <sub>2</sub>	5.50	95.53	-1.92	315.93310	

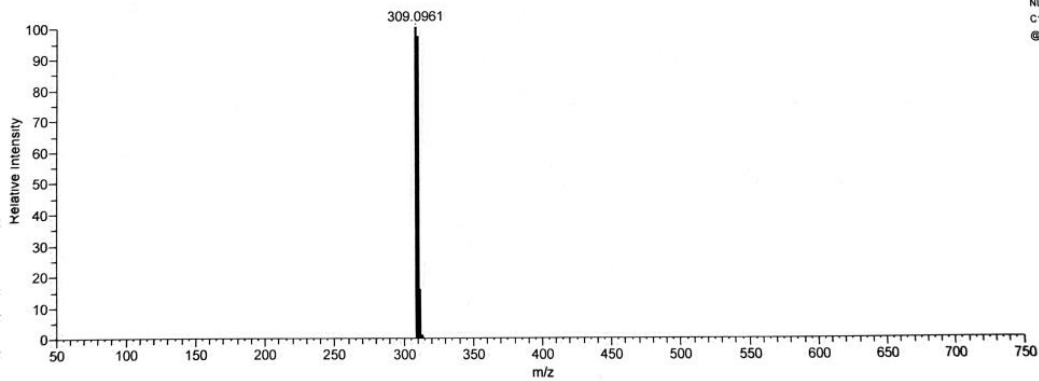
TF-1-179 #91 RT: 0.88 AV: 1 NL: 2.76E8  
 T: FTMS + p ESI Full ms [50.0000-750.0000]



Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments (Collection)
329.9481	C <sub>12</sub> H <sub>14</sub> N <sup>79</sup> Br <sub>2</sub>	-2.01	329.94875	96.33	100	

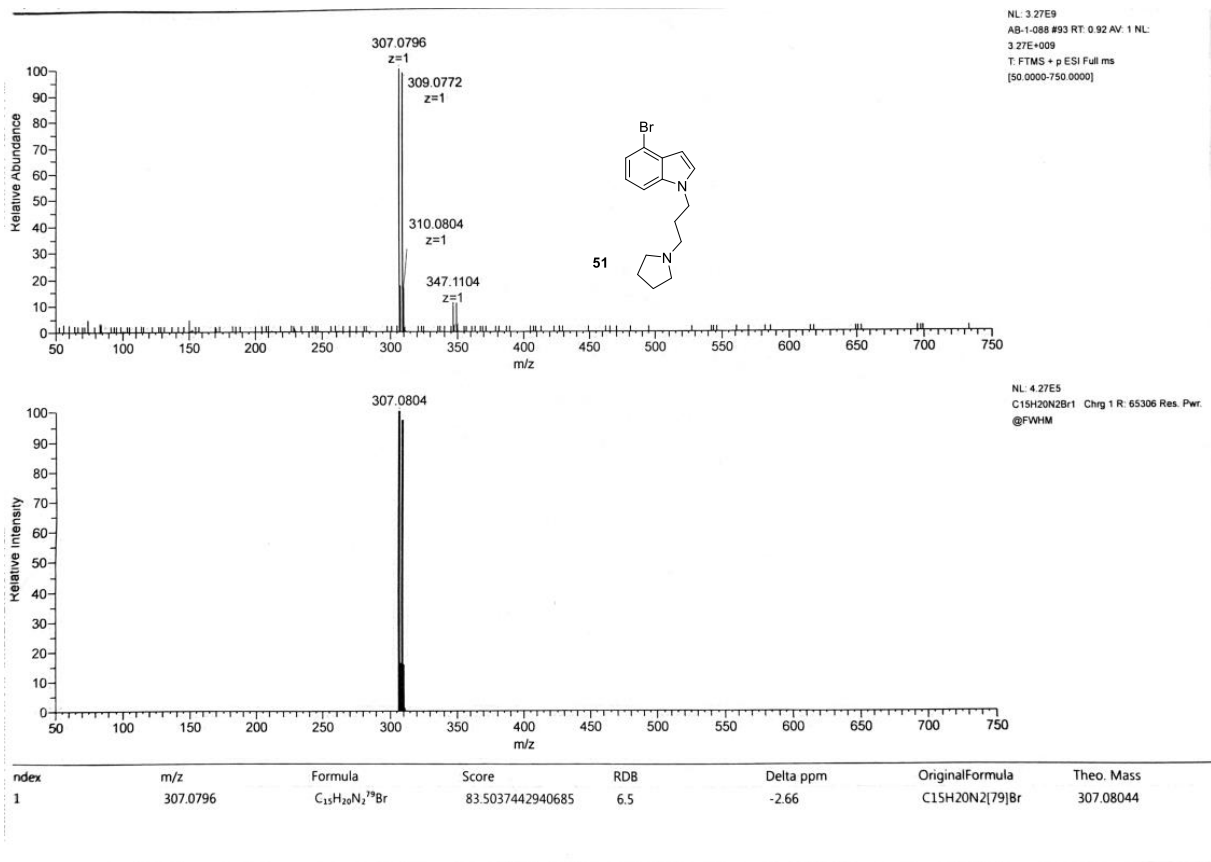
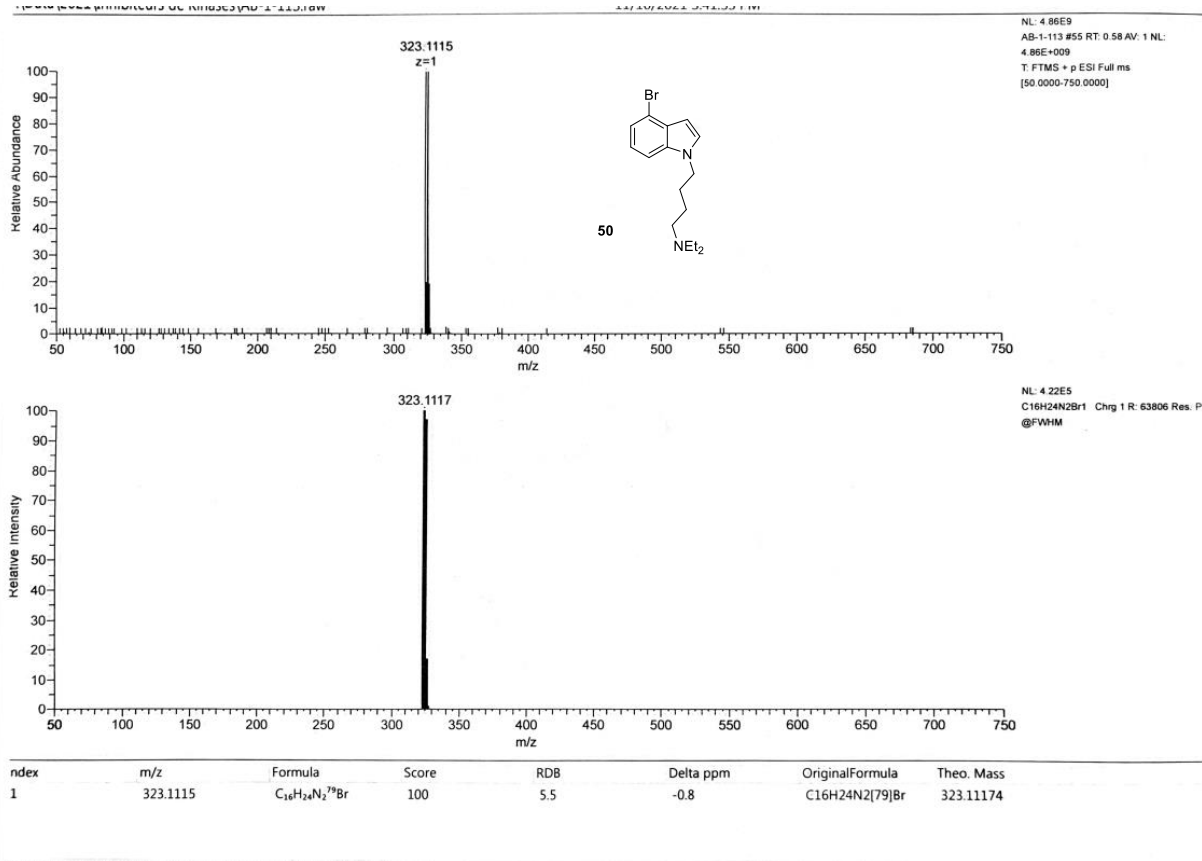


NL: 5.20E9  
 AB-1-112 #55 RT: 0.57 AV: 1 NL:  
 5.20E+009  
 T: FTMS + p ESI Full ms  
 [50.0000-750.0000]

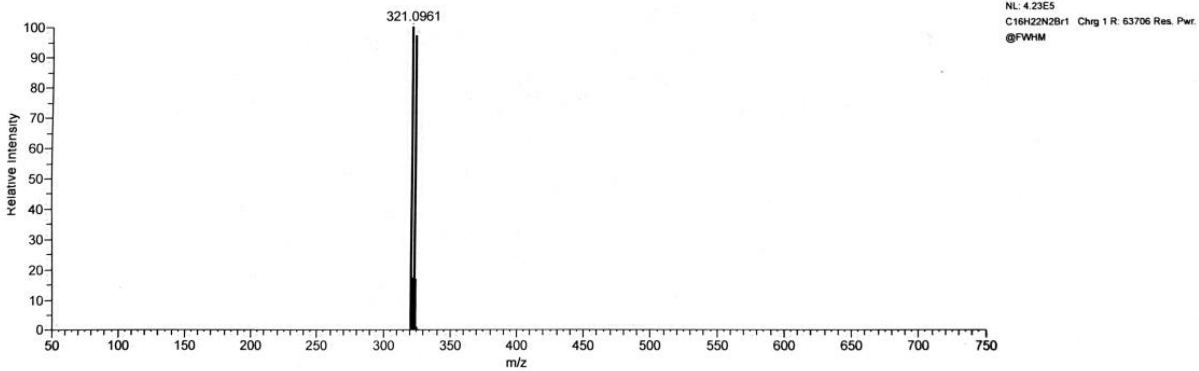
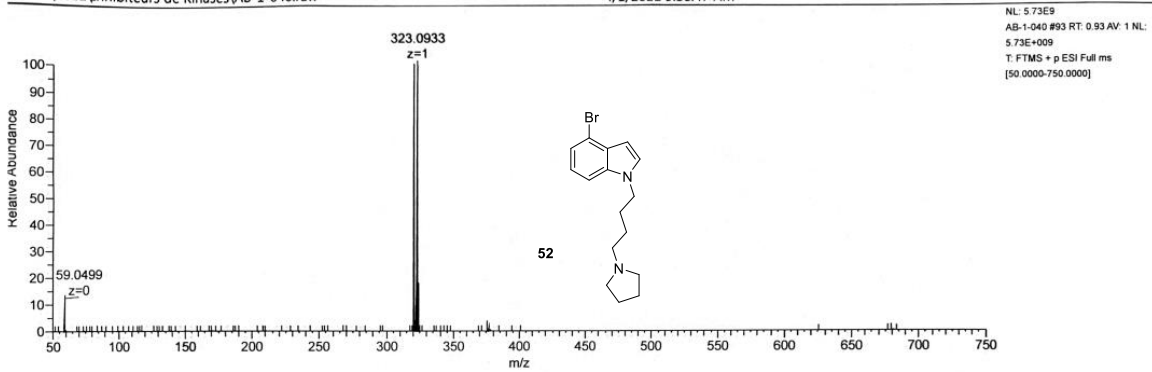


NL: 4.27E5  
 C15H22N2Br1 Chrg 1 R: 65206 Res. P1  
 @FWHM

index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	309.0958	C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> <sup>79</sup> Br	100	5.5	-0.85	C15H22N2[79]Br	309.09609

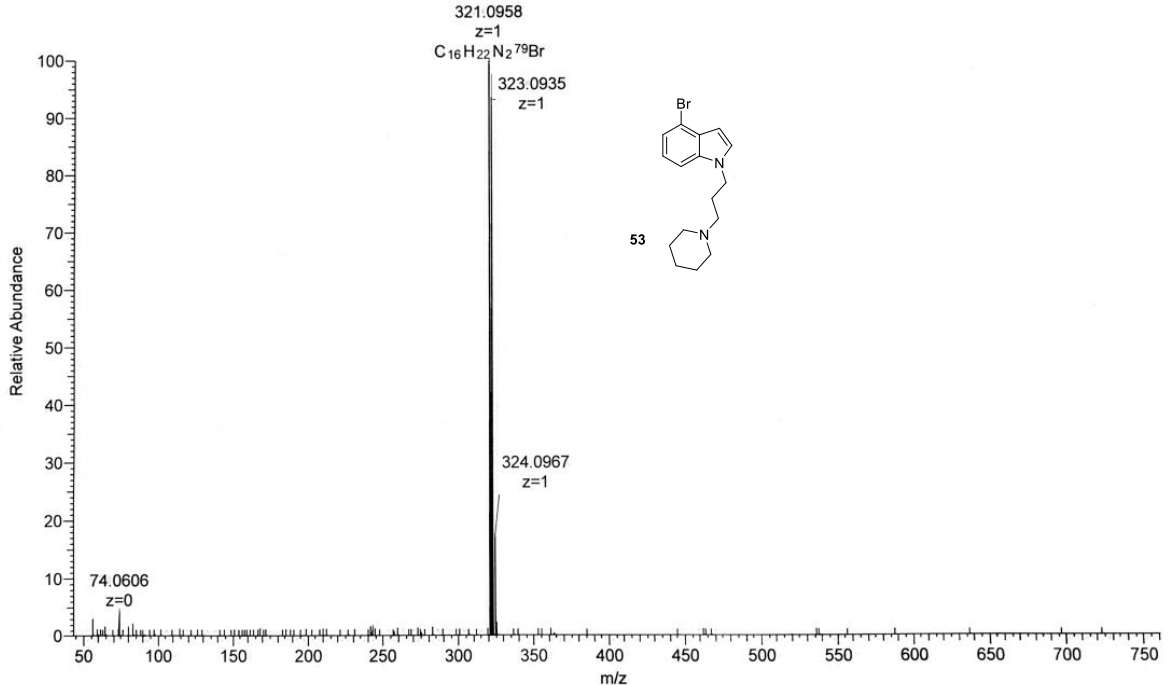






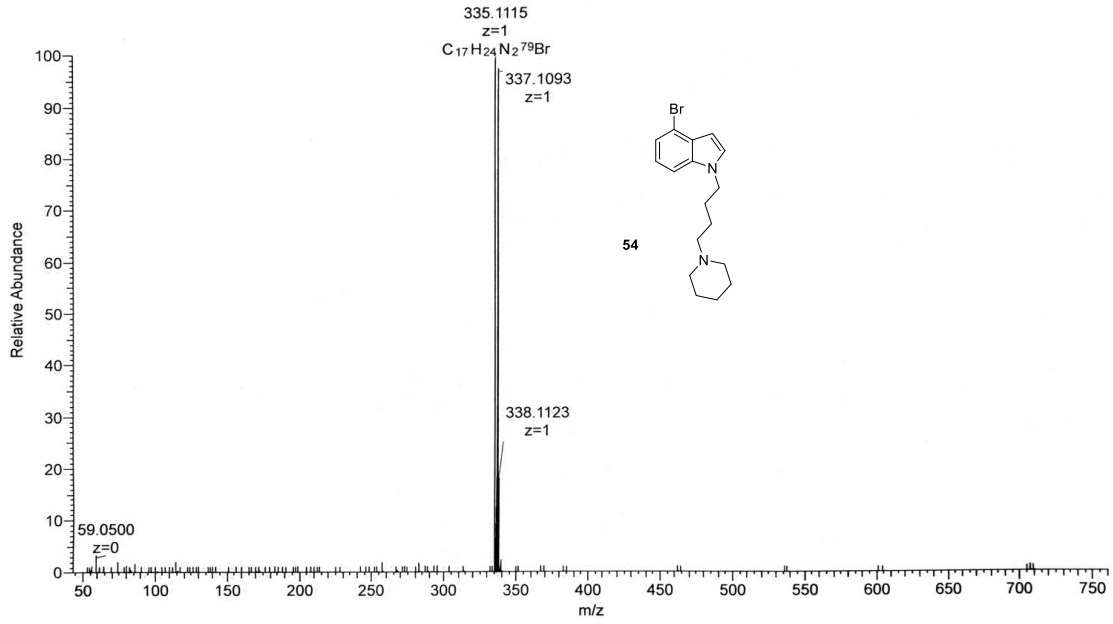
index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	321.0957	C <sub>16</sub> H <sub>22</sub> N <sub>2</sub> <sup>79</sup> Br	100	6.5	-1.29	C <sub>16</sub> H <sub>22</sub> N <sub>2</sub> [79]Br	321.09609

TF-1-162 #91 RT: 0.91 AV: 1 NL: 2.13E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

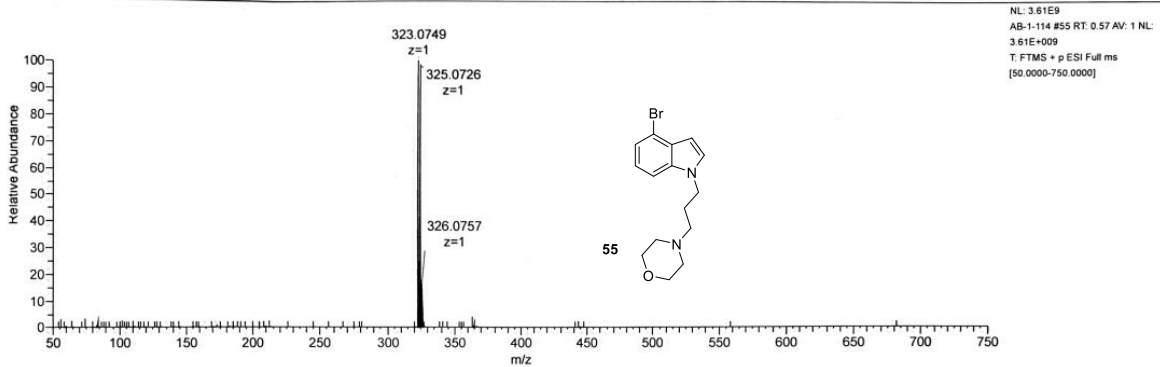


Rank	Peak Mass	Display Formula	RDB	Combined Score	Delta [ppm]	Theo. mass	MSMS Matched Fr
1	321.0958	C <sub>16</sub> H <sub>22</sub> N <sub>2</sub> <sup>79</sup> Br	6.50	97.52	-0.82	321.09609 (Collection)	

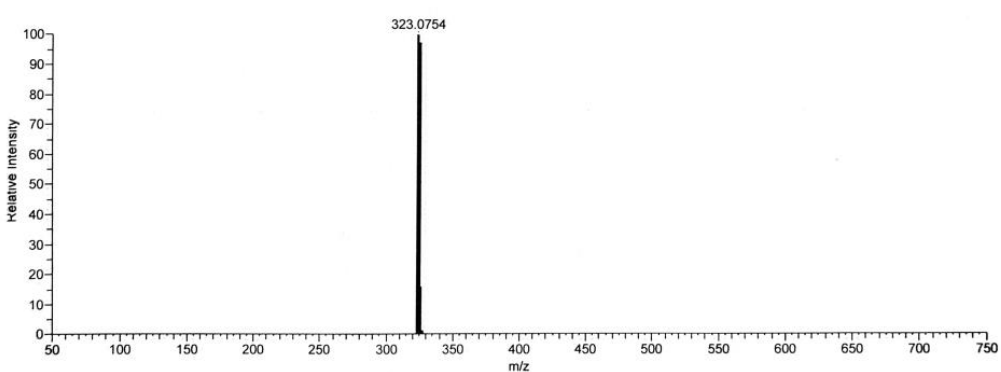
AB-1-180 #93 RT: 0.91 AV: 1 NL: 3.39E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]



Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments
335.1115	C <sub>17</sub> H <sub>24</sub> N <sub>2</sub> <sup>79</sup> Br	-0.59	335.11174	98.5	100	(Collection)

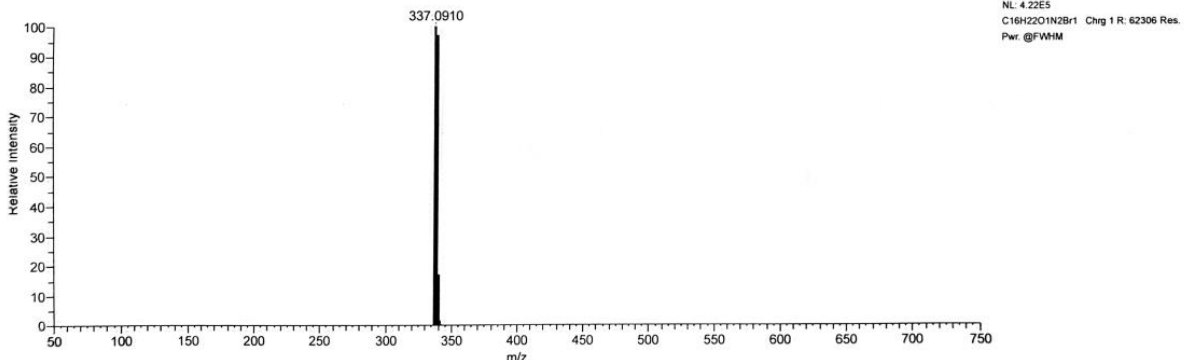
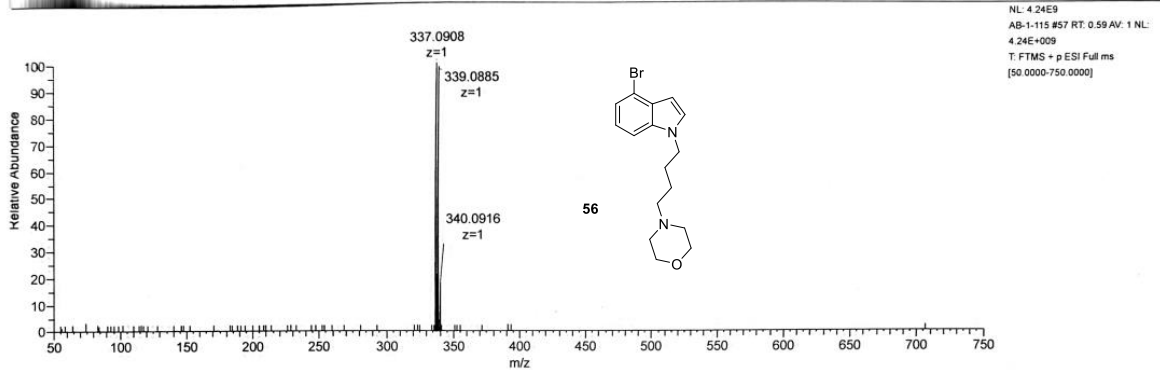


NL: 3.61E9  
 AB-1-114 #55 RT: 0.57 AV: 1 NL:  
 3.61E+009  
 T: FTMS + p ESI Full ms  
 [50.0000-750.0000]



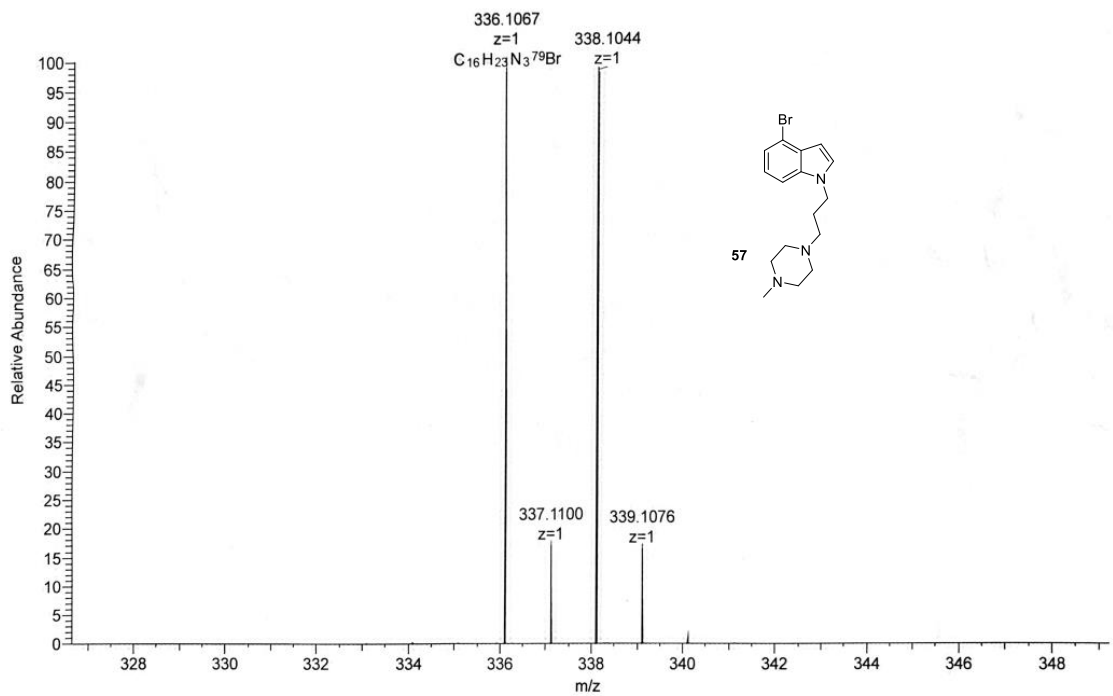
NL: 4.26E5  
 C15H20O1N2Br1 Chrg 1 R: 63606 Res.  
 Pwr. @FWHM

ndex	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	323.0749	C <sub>15</sub> H <sub>20</sub> ON <sub>2</sub> <sup>79</sup> Br	100	6.5	-1.34	C15H20ON2[79]Br	323.07535



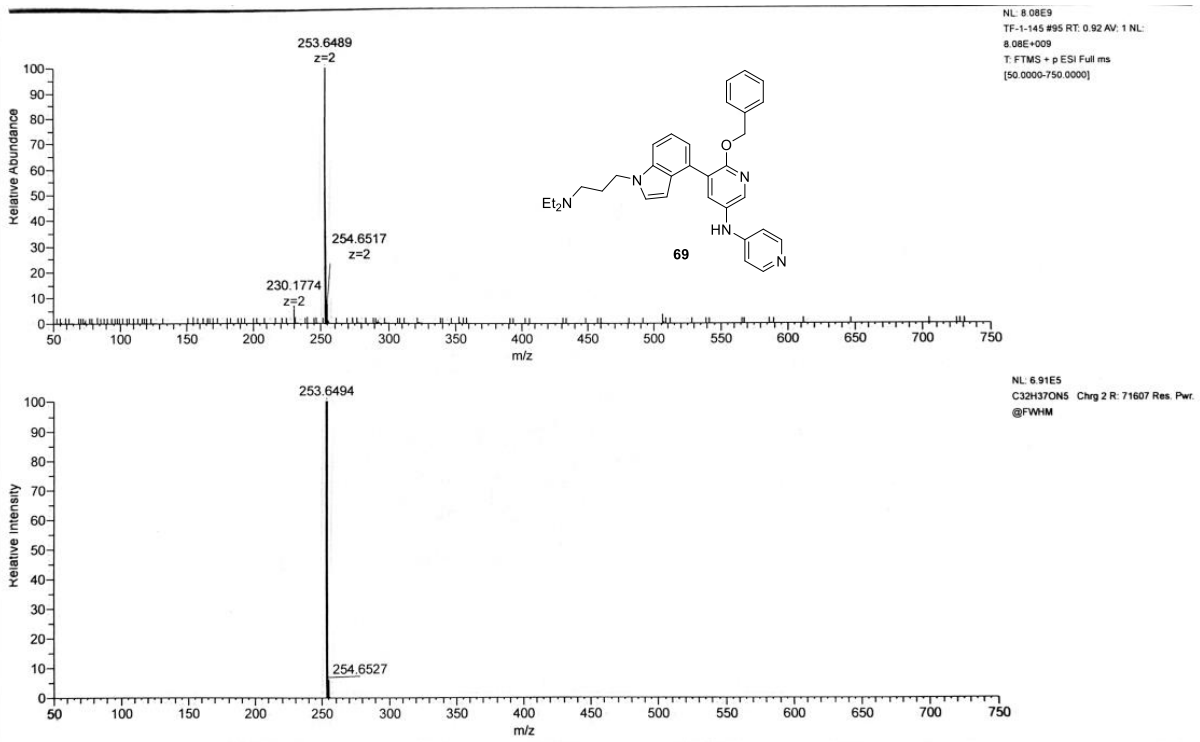
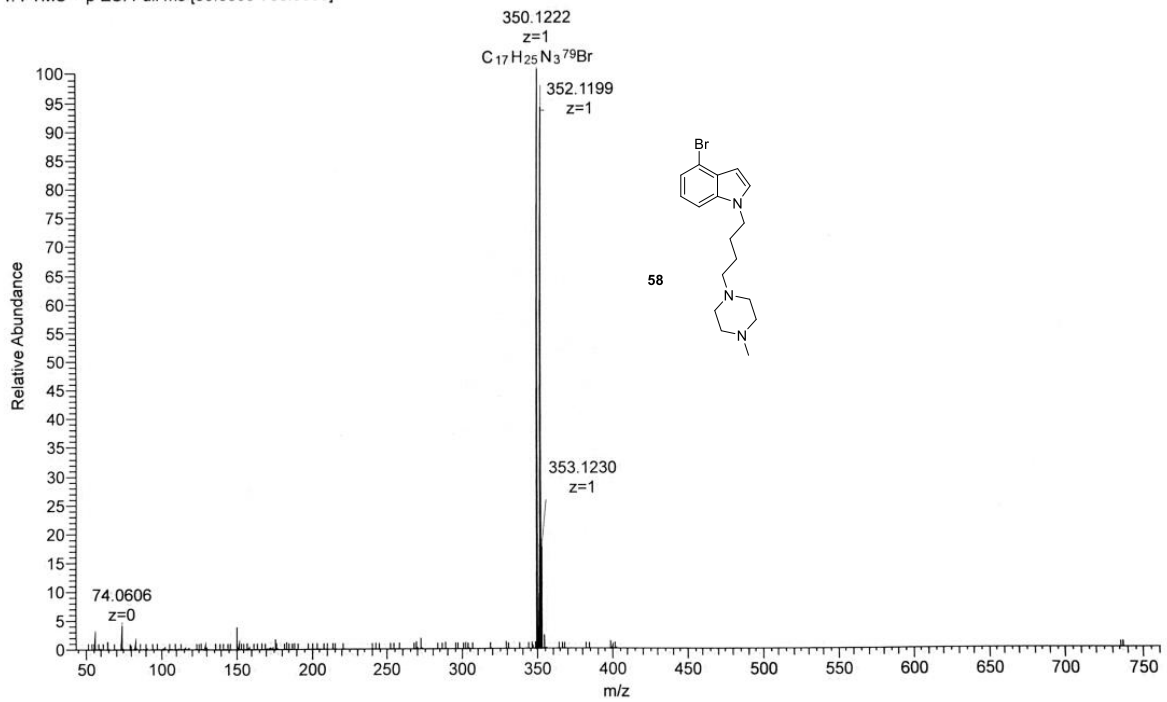
Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	337.0908	C <sub>16</sub> H <sub>22</sub> ON <sub>2</sub> <sup>79</sup> Br	100	6.5	-0.72	C16H22ON2[79]Br	337.09100

TF-1-163 #91 RT: 0.91 AV: 1 NL: 2.29E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

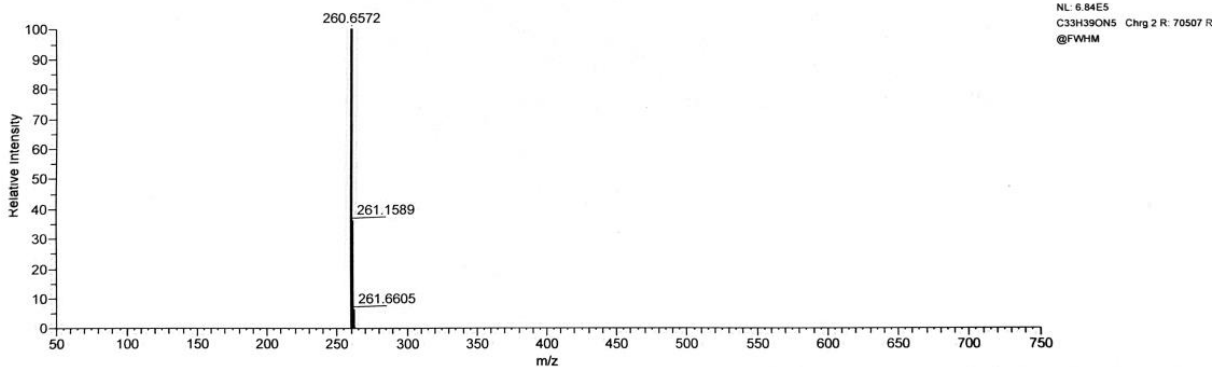
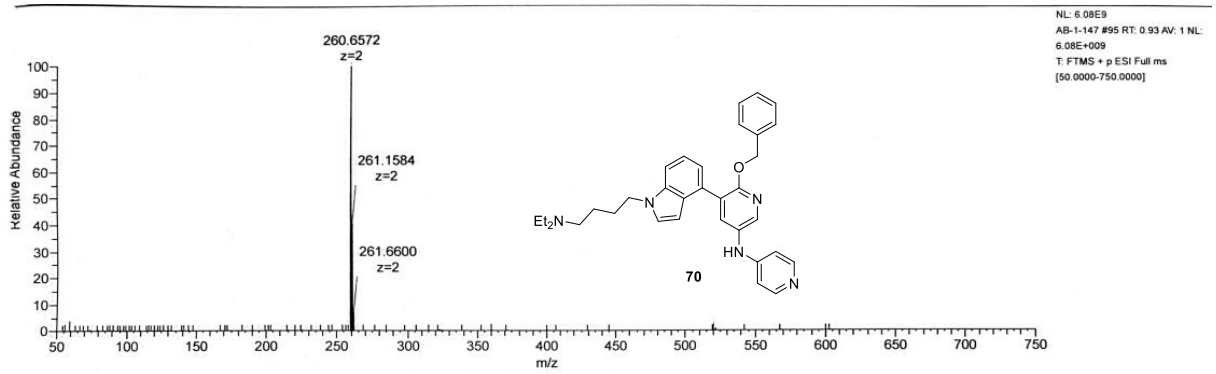


Rank	Peak Mass	Display Formula	RDB	Combined Score	Delta [ppm]	Theo. mass	MSMS Matched Fragm...
1	336.1067	C <sub>16</sub> H <sub>23</sub> N <sub>3</sub> <sup>79</sup> Br	6.50	98.63	-0.79	336.10699	(Collection)

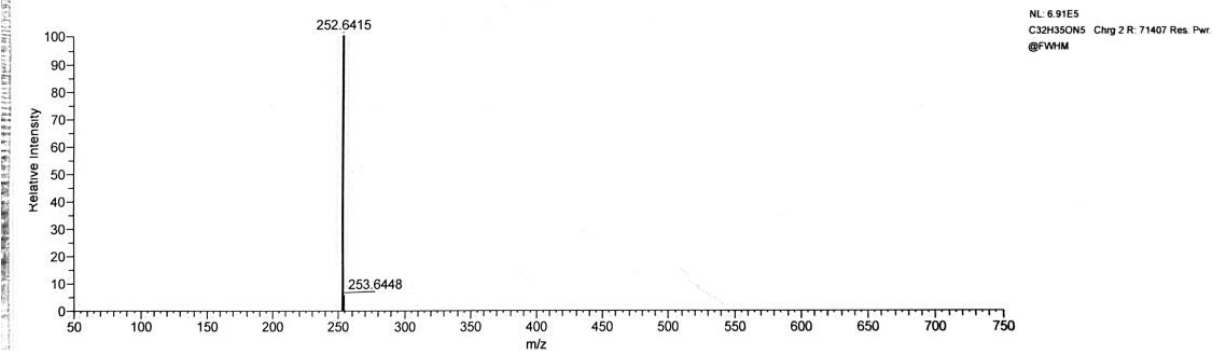
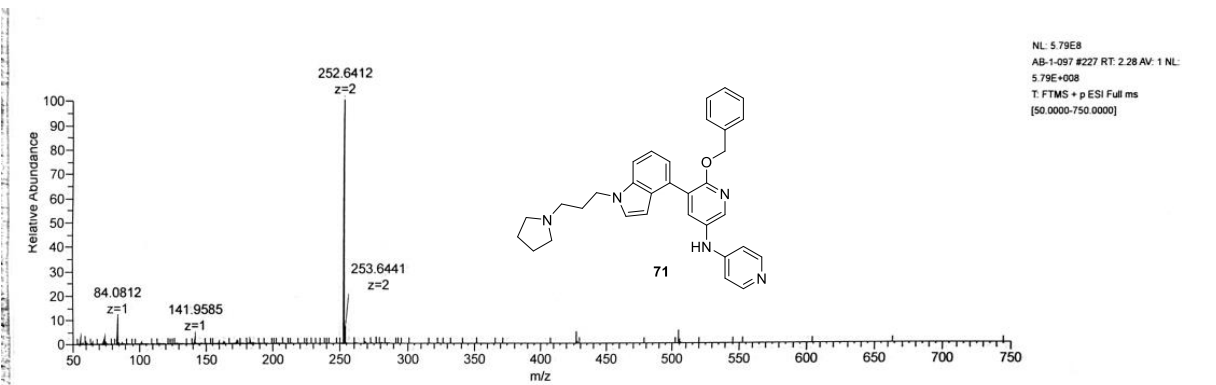
TF-1-181 #95 RT: 0.97 AV: 1 NL: 1.99E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]



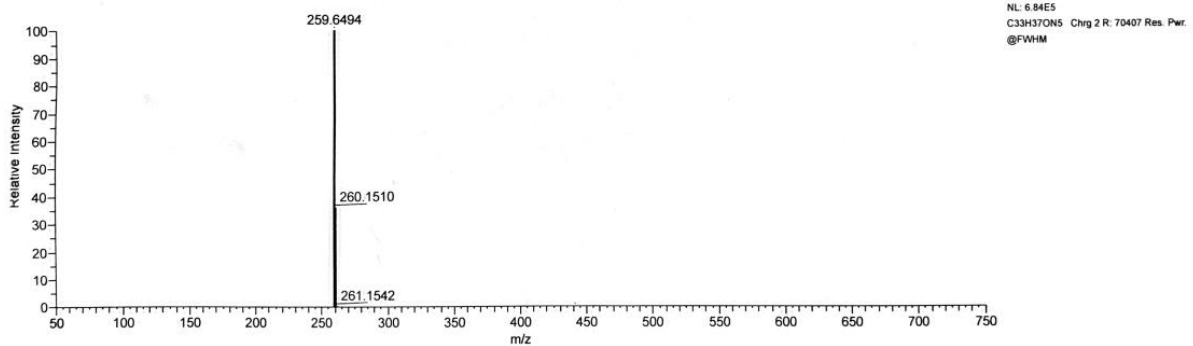
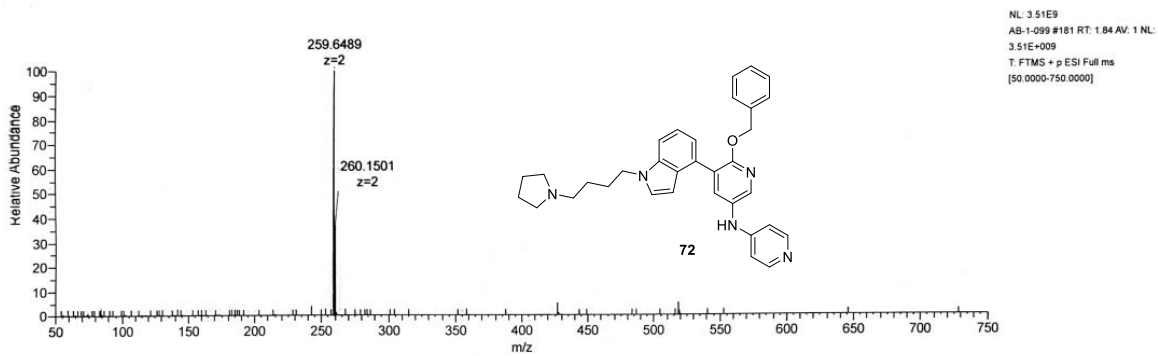
Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	253.6489	C <sub>32</sub> H <sub>37</sub> ON <sub>5</sub>	100	17	-1.64	C32H37ON5	253.64936



ndex	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	260.6572	C <sub>33</sub> H <sub>39</sub> ON <sub>5</sub>	100	17	-0.06	C33H39ON5	260.65718

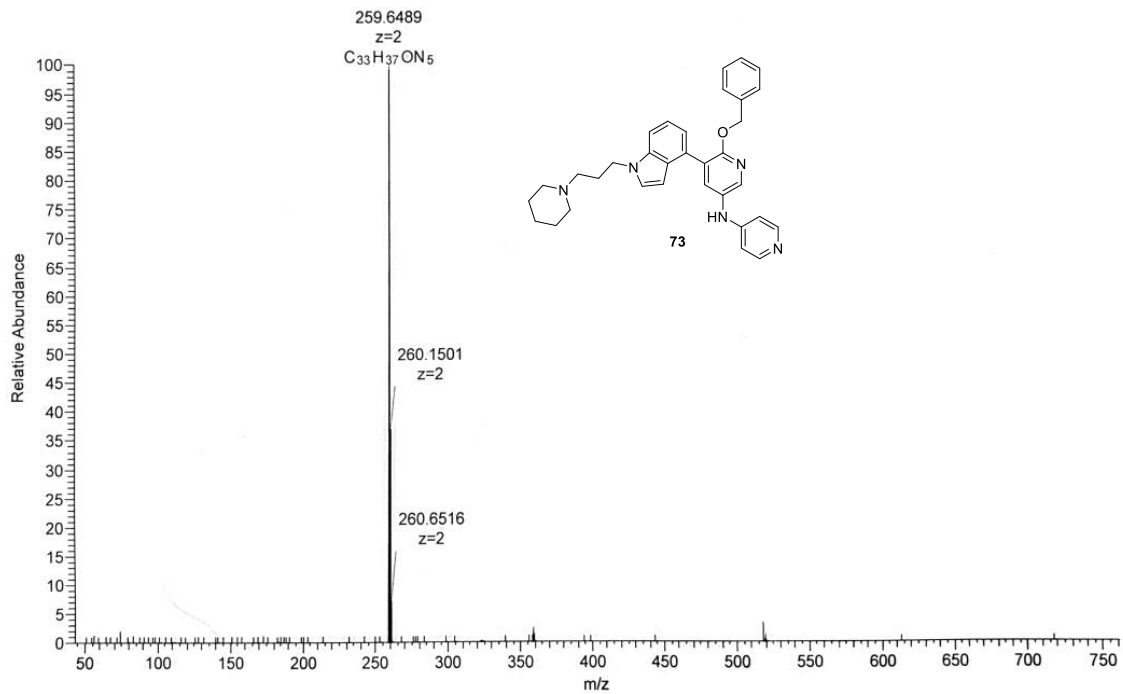


ndex	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	252.6412	C <sub>32</sub> H <sub>35</sub> ON <sub>5</sub>	100	18	-1.42	C32H35ON5	252.64153



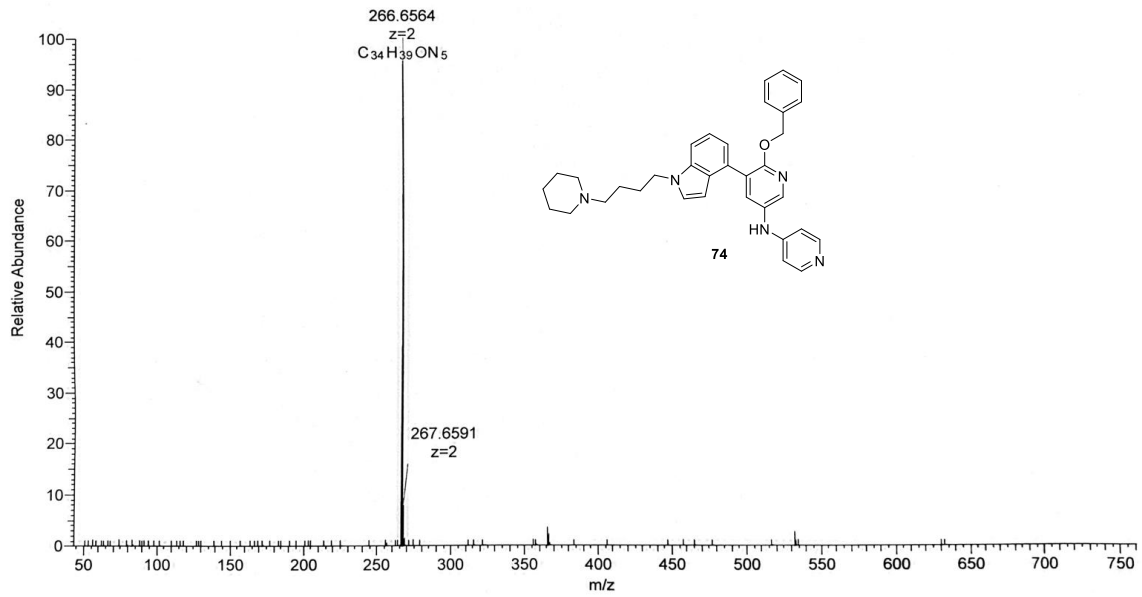
Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	259.6489	C <sub>33</sub> H <sub>37</sub> ON <sub>5</sub>	100	18	-1.9	C33H37ON5	259.64936

TF-1-173 #93 RT: 0.90 AV: 1 NL: 7.71E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

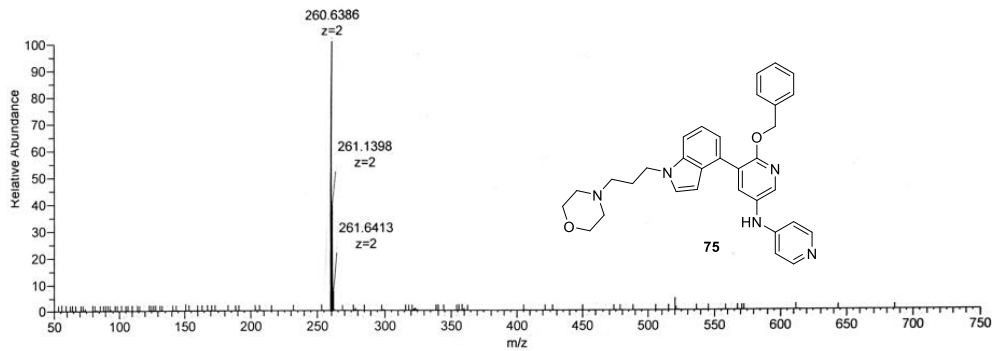


Rank	Peak Mass	Display Formula	RDB	Combined Score	Delta [ppm]	Theo. mass	MSMS Matched Fragm...
1	259.6489	C <sub>33</sub> H <sub>37</sub> ON <sub>5</sub>	18.00	97.19	-1.90	259.64936	(Collection)

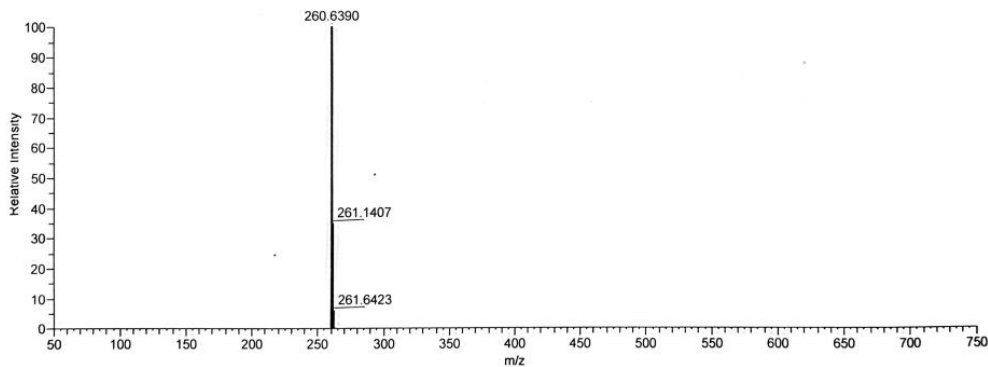
NC-006 #99 RT: 0.99 AV: 1 NL: 8.63E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]



Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments (Collection)
266.6564	C <sub>34</sub> H <sub>39</sub> ON <sub>5</sub>	-2.81	266.65718	91.66	95.22	



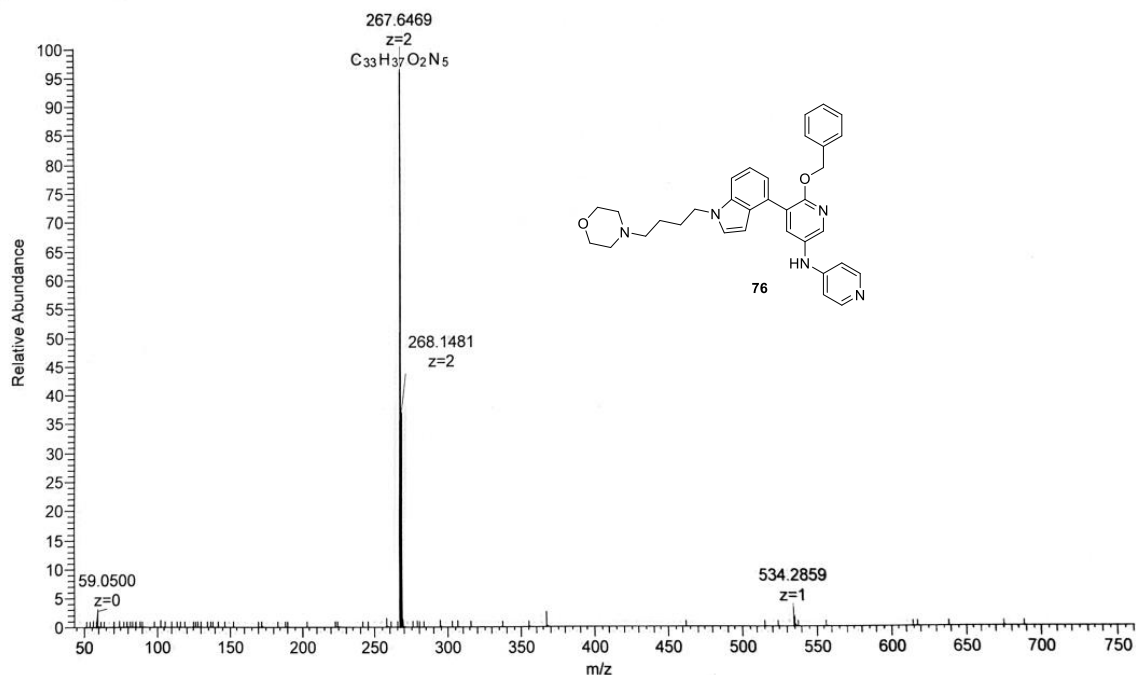
NL: 6.90E5  
 TF-1-149 #95 RT: 0.92 AV: 1 NL:  
 8.55E+009  
 T: FTMS + p ESI Full ms  
 [50.0000-750.0000]



NL: 6.90E5  
 C32H35O2N5 Chrg 2 R: 70707 Res. Pwr:  
 @FWHM

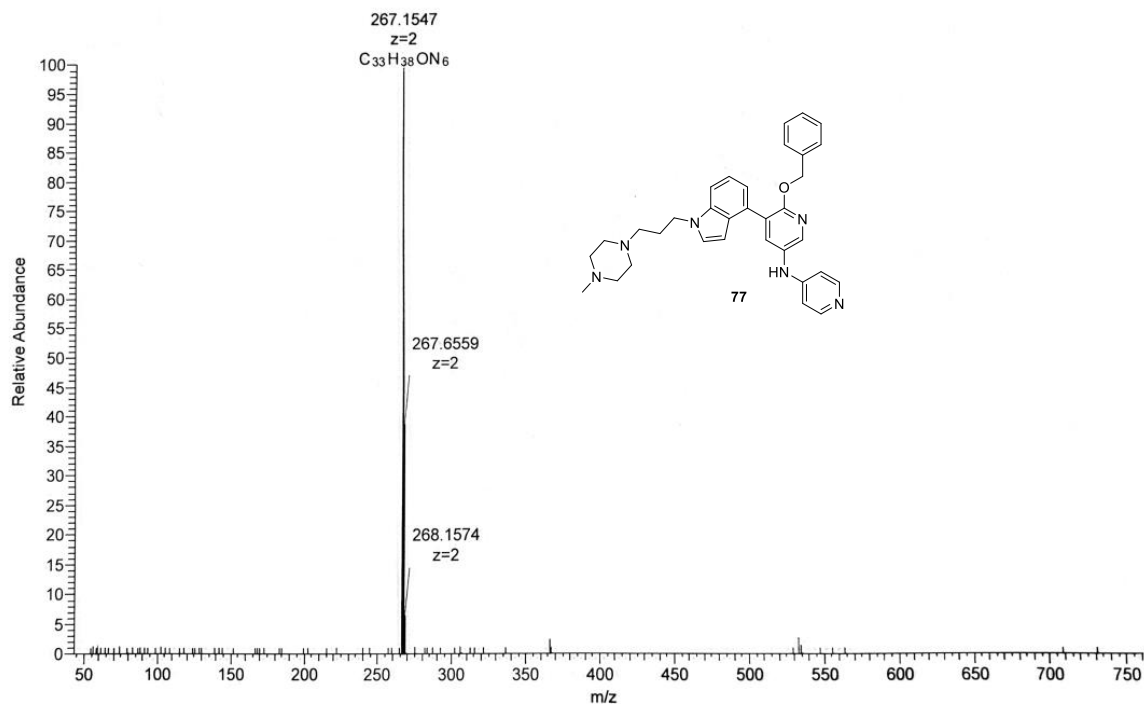
Index	m/z	Formula	Score	RDB	Delta ppm	Original Formula	Theo. Mass
1	260.6386	C <sub>32</sub> H <sub>35</sub> O <sub>2</sub> N <sub>5</sub>	100	18	-1.57	C32H35O2N5	260.63899

S-1-169 #93 RT: 0.92 AV: 1 NL: 7.56E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]



Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments (Collection)
267.6469	C <sub>33</sub> H <sub>37</sub> O <sub>2</sub> N <sub>5</sub>	0.25	267.64681	98.81	100	

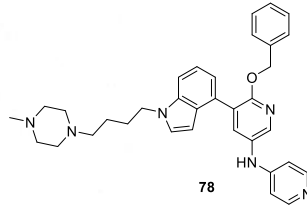
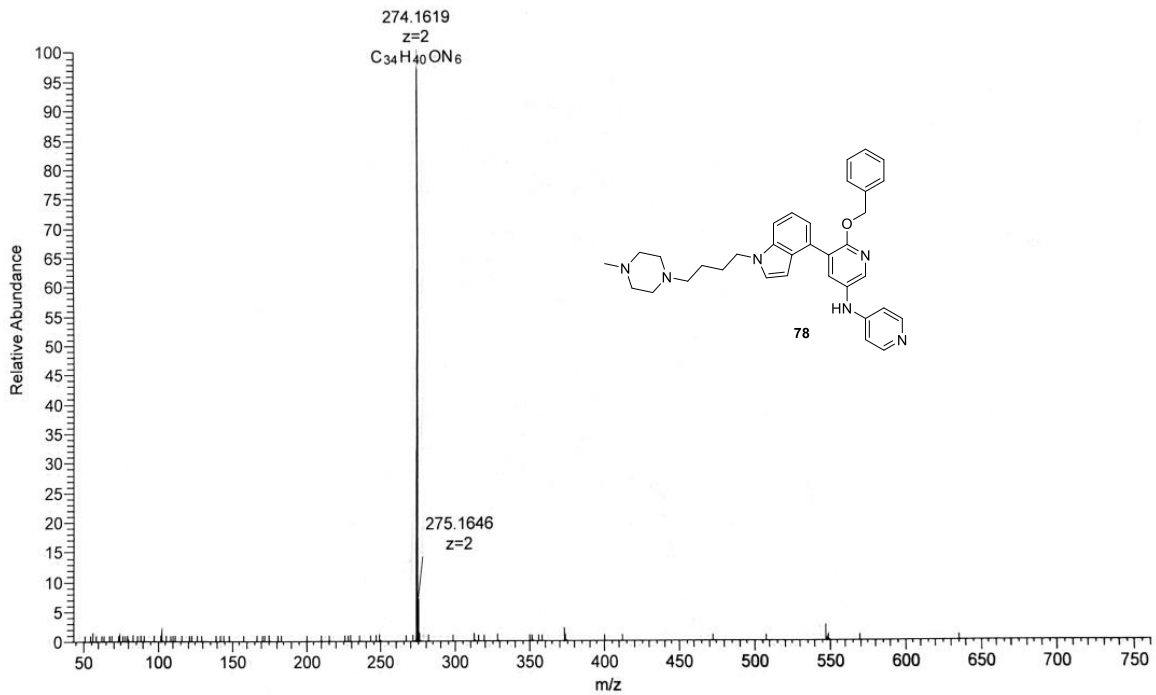
TF-1-174 #89 RT: 0.90 AV: 1 NL: 7.37E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]



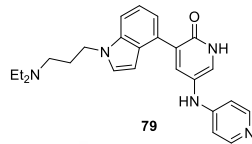
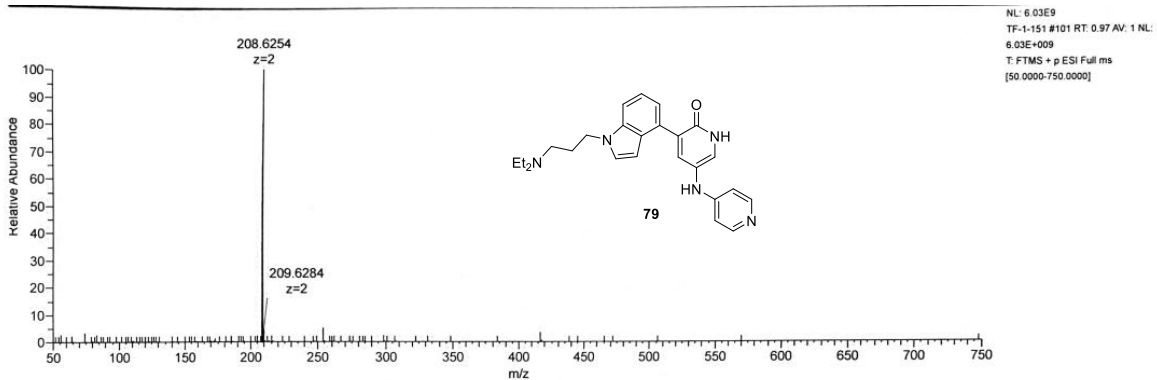
Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragment (Collection)
267.1547	C <sub>33</sub> H <sub>38</sub> ON <sub>6</sub>	-0.54	267.15481	98.49	100	



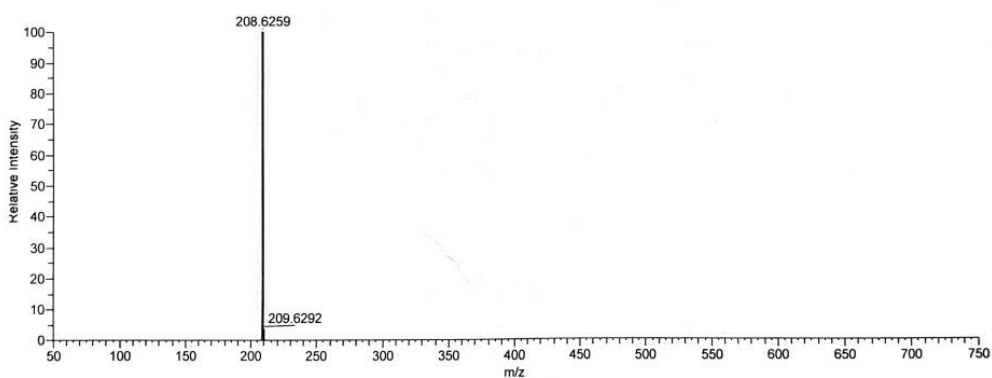
TF-1-192 #95 RT: 0.93 AV: 1 NL: 6.58E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]



Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragme
274.1619	C <sub>34</sub> H <sub>40</sub> ON <sub>6</sub>	-2.79	274.16263	96.92	100	(Collection)



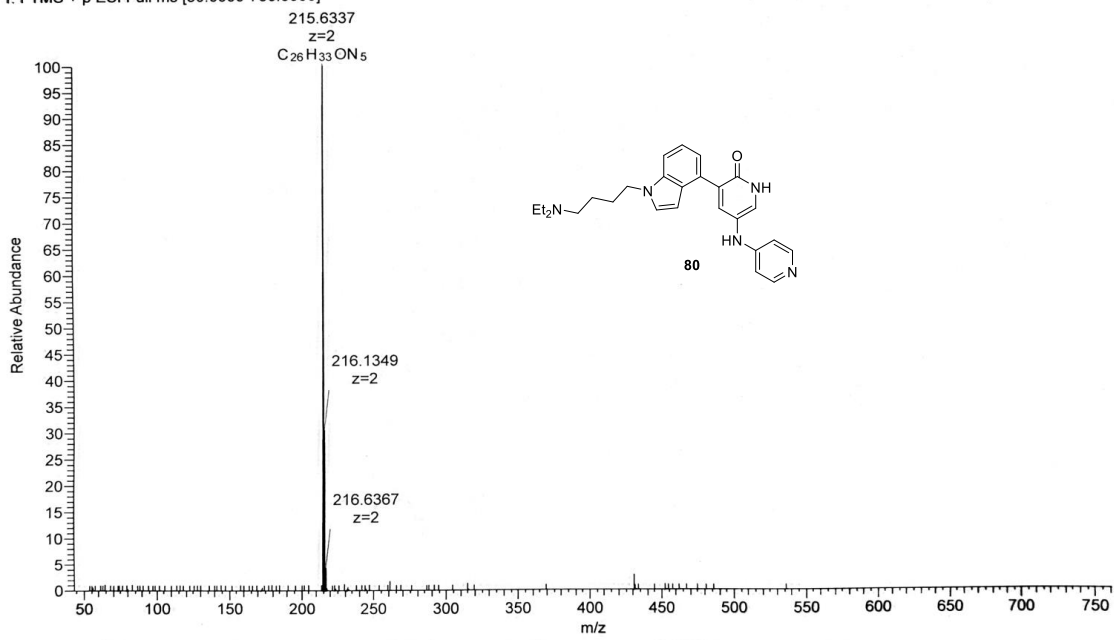
NL: 6.03E9  
 TF-1-151 #101 RT: 0.97 AV: 1 NL:  
 6.03E+009  
 T: FTMS + p ESI Full ms  
 [50.0000-750.0000]



NL: 7.46E5  
 C25H31ON5 Chrg 2 R: 79407 Res. Pwr.  
 @FWHM

index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	208.6254	C <sub>25</sub> H <sub>31</sub> ON <sub>5</sub>	93.9020117547757	13	-2.33	C25H31ON5	208.62588

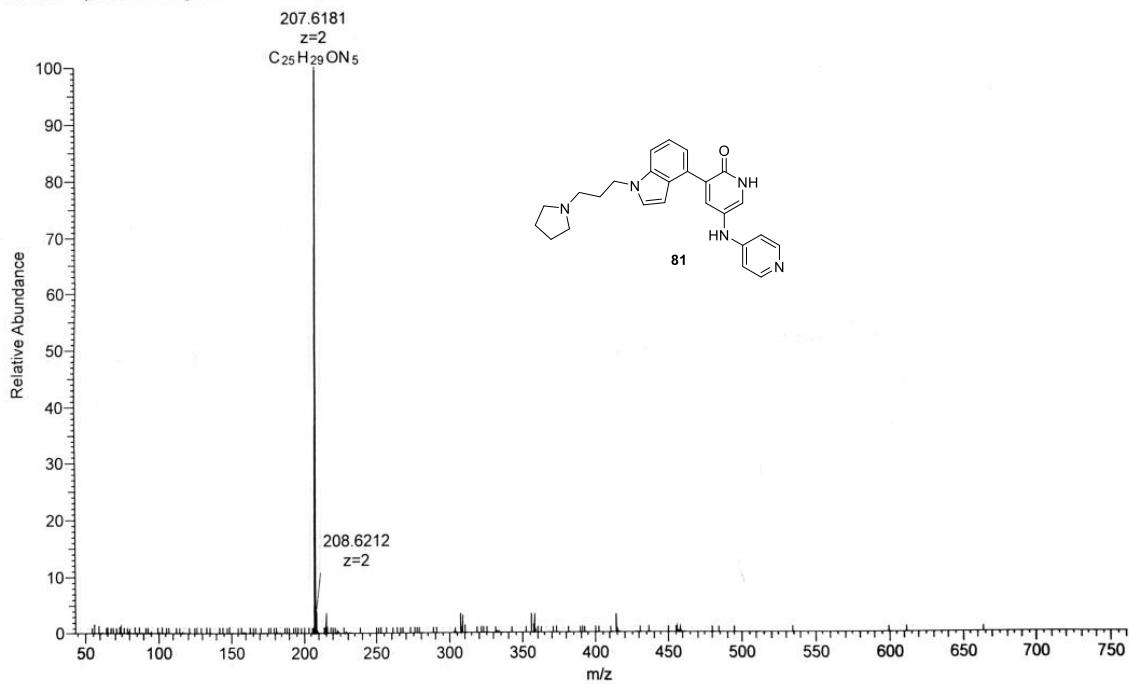
TF-1-198 #95 RT: 0.92 AV: 1 NL: 7.58E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]



Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments (Collection)
215.6337	C <sub>26</sub> H <sub>33</sub> ON <sub>5</sub>	-0.04	215.63371	96.88	99.72	

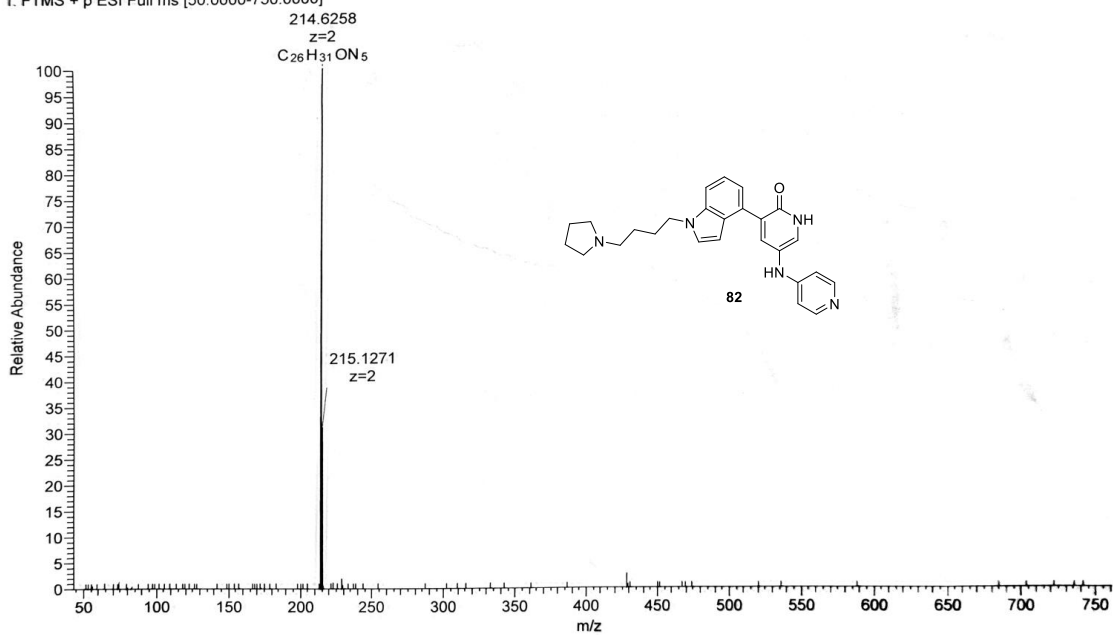
U:\ddid\ZZZZ\MMIDREURS DE KINASES\AB-1-U90.fidw

AB-1-098 #93 RT: 0.90 AV: 1 NL: 4.01E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]



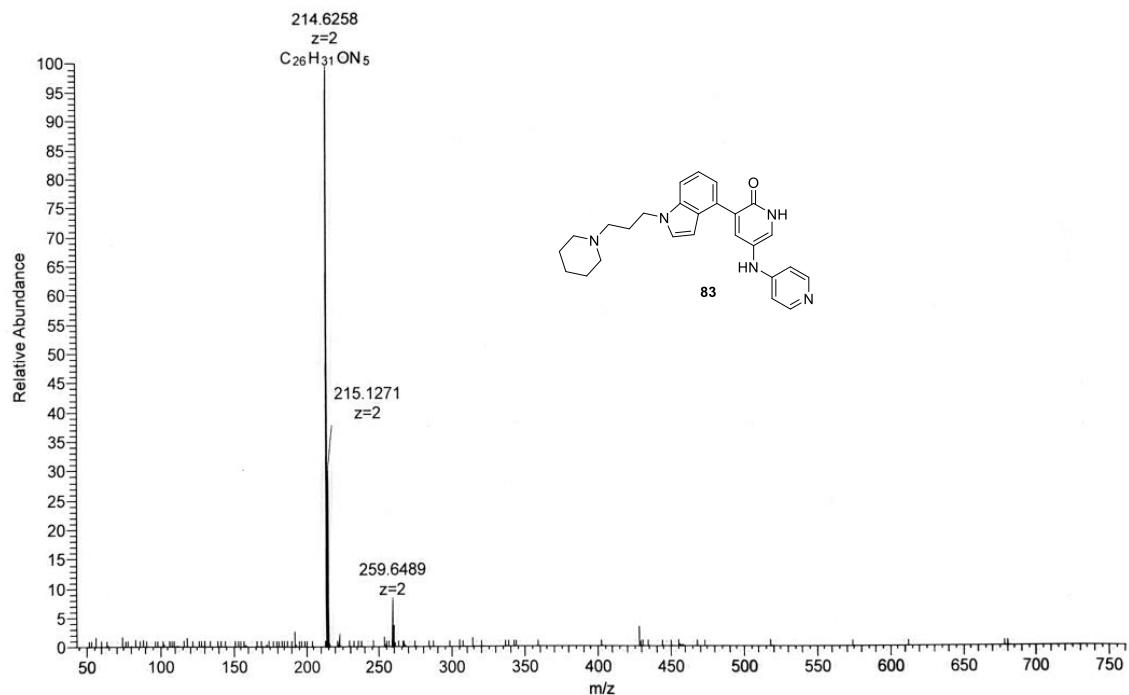
Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments (Collection)
207.6181	C <sub>25</sub> H <sub>29</sub> ON <sub>5</sub>	0.22	207.61806	98.04	100	

TF-1-200 #95 RT: 0.93 AV: 1 NL: 8.02E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]



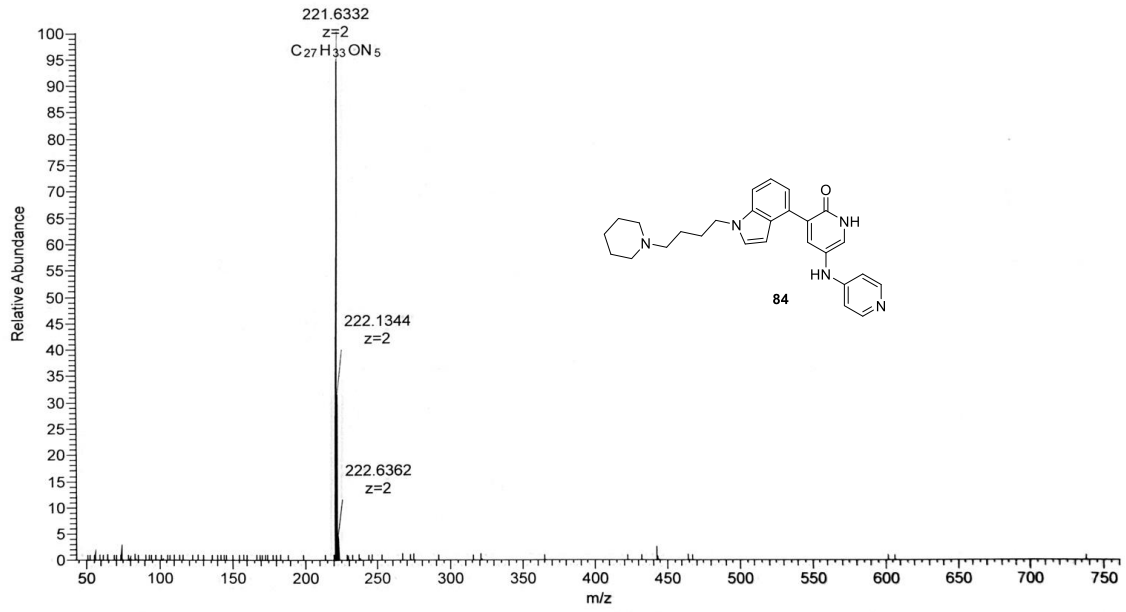
Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments
214.6258	C <sub>26</sub> H <sub>31</sub> ON <sub>5</sub>	-0.27	214.62588	98.54	100	(Collection)

TF-1-177 #91 RT: 0.92 AV: 1 NL: 6.68E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]

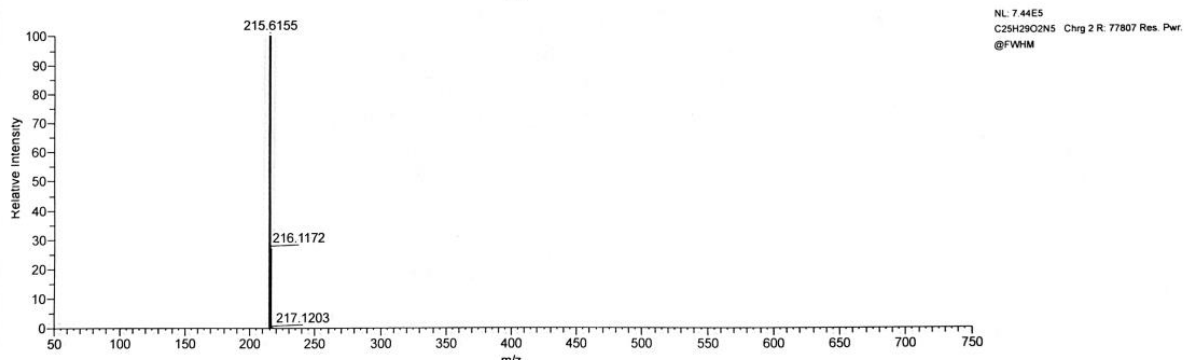
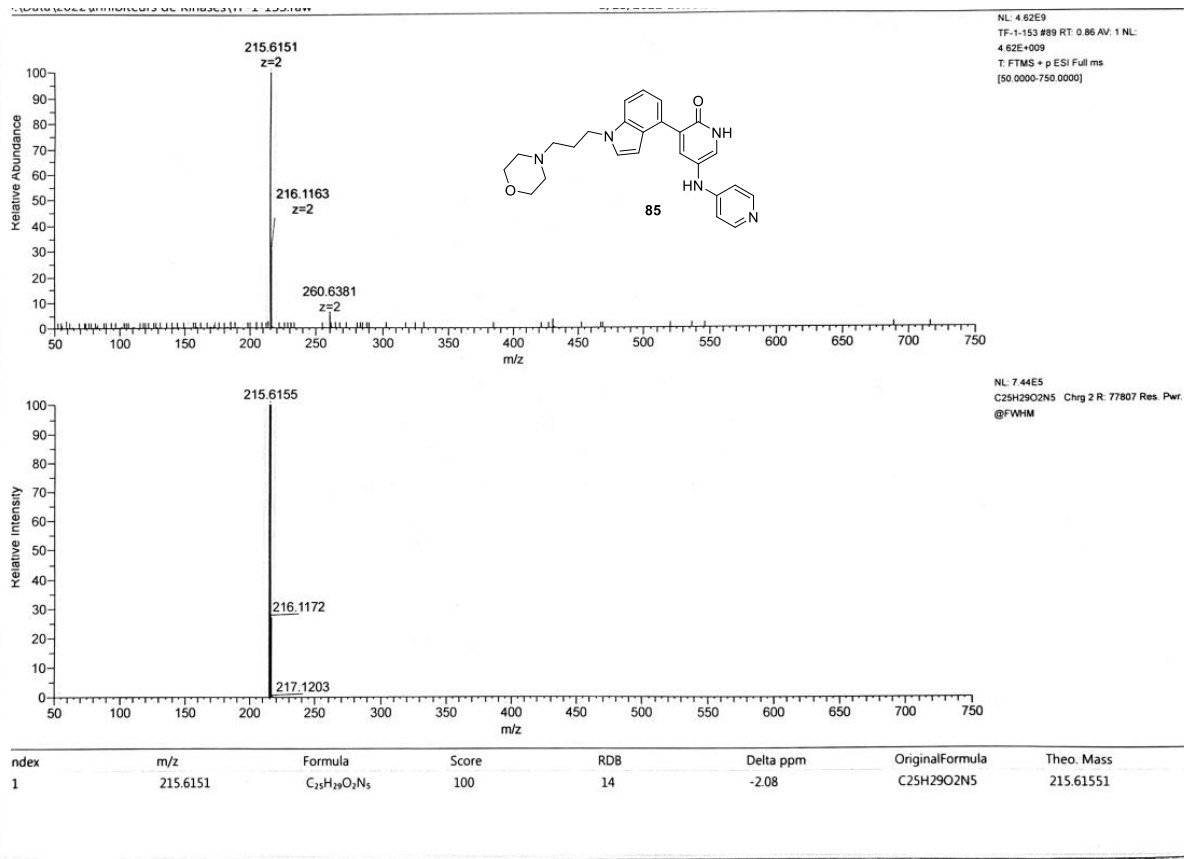


Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments
214.6258	C <sub>26</sub> H <sub>31</sub> ON <sub>5</sub>	-0.27	214.62588	98.63	100	(Collection)

TF-1-193 #101 RT: 1.00 AV: 1 NL: 4.31E9  
 T: FTMS + p ESI Full ms [50.0000-750.0000]

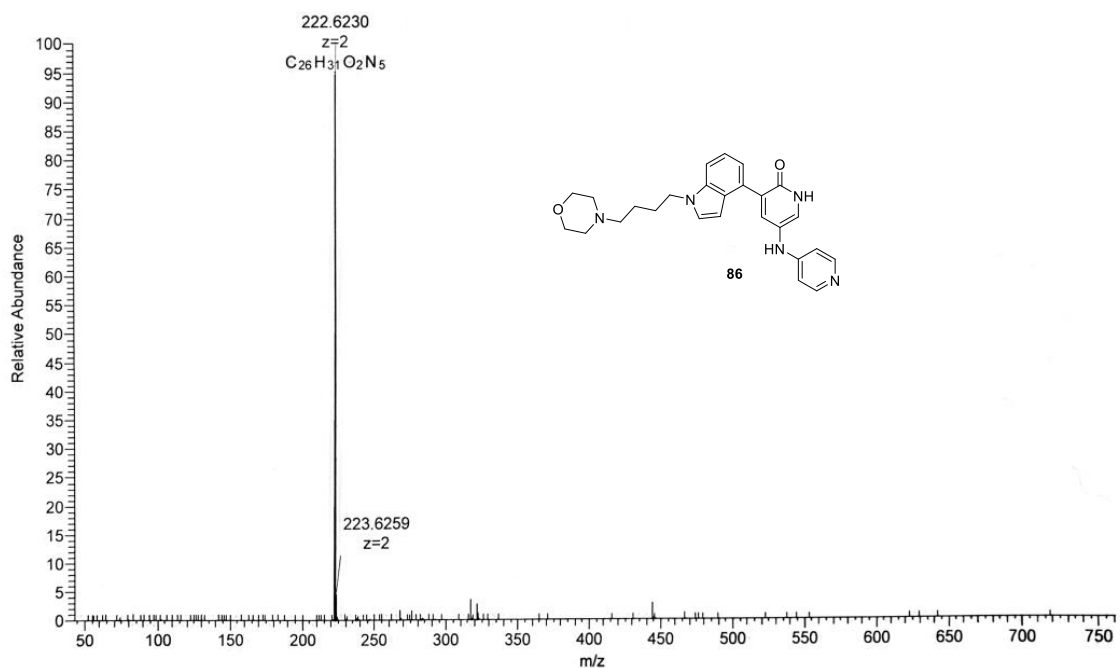


Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments
221.6332	C <sub>27</sub> H <sub>33</sub> ON <sub>5</sub>	-2.25	221.63371	97.16	100	(Collection)



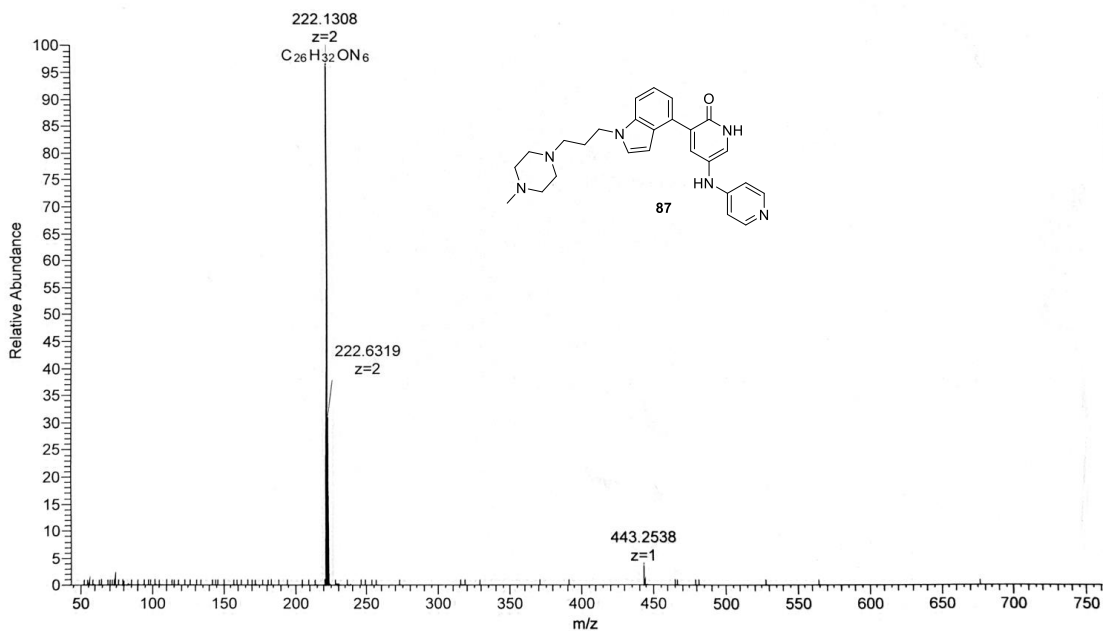
Index	m/z	Formula	Score	RDB	Delta ppm	Original Formula	Theo. Mass
1	215.6151	C <sub>25</sub> H <sub>29</sub> O <sub>2</sub> N <sub>5</sub>	100	14	-2.08	C <sub>25</sub> H <sub>29</sub> O <sub>2</sub> N <sub>5</sub>	215.61551

TF-1-187 #89 RT: 0.91 AV: 1 NL: 5.69E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]



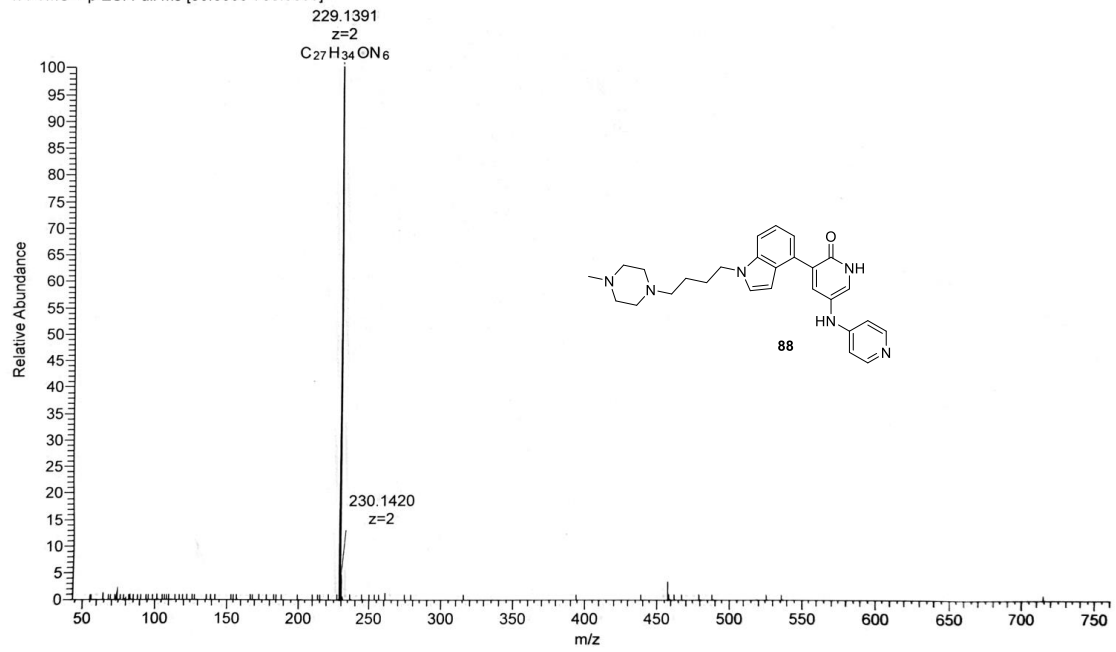
Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments (Collection)
222.6230	C <sub>26</sub> H <sub>31</sub> O <sub>2</sub> N <sub>5</sub>	-1.52	222.62334	97.64	100	

TF-1-188 #91 RT: 0.89 AV: 1 NL: 4.84E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]



Peak Mass	Display Formula	Delta [ppm]	Theo. mass	Combined Score	Pattern Cov. [%]	MSMS Matched Fragments (Collection)
222.1308	C <sub>26</sub> H <sub>32</sub> ON <sub>6</sub>	-2.47	222.13133	73.74	78.32	

TF-1-194 #95 RT: 0.92 AV: 1 NL: 6.53E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]



Peak Mass	Display Formula	Delta (ppm)	Theo. mass	Combined Score	Pattern Cov. (%)	MSMS Matched Fragments (Collection)
229.1391	C <sub>27</sub> H <sub>34</sub> ON <sub>6</sub>	-0.45	229.13916	98.63	100	