

Electronic Supplementary Material (ESI)

## **$\gamma$ -Hydroxy- $\gamma$ -butyrolactams as 1,2-bis-electrophiles in a Brønsted/Lewis acid-free synthesis of condensed nitrogen heterocycles**

**Nicolai A. Aksenov,\* Igor A. Kurenkov, Nikolai A. Arutiunov, Vladimir V. Malyuga, Dmitrii A. Aksenov, Alexander V. Leontiev, Alexander V. Aksenov**

Department of Chemistry, North Caucasus Federal University, 1a Pushkin St., 355017 Stavropol, Russia

\*corresponding author: [naksenov@ncfu.ru](mailto:naksenov@ncfu.ru)

<b><math>^1\text{H}</math> and <math>^{13}\text{C}</math> NMR spectral charts.....</b>	<b>S2</b>
<b><math>^1\text{H}</math> and <math>^{13}\text{C}</math> NMR spectral charts for 5-hydroxy-5-(3-methoxyphenyl)-3-phenyl-1,5-dihydro-2H-pyrrol-2-one (1ca).....</b>	<b>S2</b>
<b><math>^1\text{H}</math> and <math>^{13}\text{C}</math> NMR spectral charts for quinoxalines 8.....</b>	<b>S4</b>
<b><math>^1\text{H}</math> and <math>^{13}\text{C}</math> NMR spectral charts for imidazopyridines 10.....</b>	<b>S18</b>
<b><math>^1\text{H}</math> and <math>^{13}\text{C}</math> NMR spectral charts for 3,5-diphenyl-3H-pyrrol-2-one 15aa.....</b>	<b>S52</b>
<b><math>^1\text{H}</math> and <math>^{13}\text{C}</math> NMR spectral charts for <i>N</i>-(2-aminophenyl)-2-phenylacetamide 16aa.....</b>	<b>S54</b>
<b><math>^1\text{H}</math> and <math>^{13}\text{C}</math> NMR spectral charts for 2-Benzyl-1<i>H</i>-benzo[<i>d</i>]imidazole 17aa.....</b>	<b>S56</b>
<b>HRMS spectral charts.....</b>	<b>S58</b>
<b>HRMS spectral chart for 5-hydroxy-5-(3-methoxyphenyl)-3-phenyl-1,5-dihydro-2H-pyrrol-2-one 1ca.....</b>	<b>S58</b>
<b>HRMS spectral charts for quinoxalines 8.....</b>	<b>S59</b>
<b>HRMS spectral charts for 2-aryl-3-benzylimidazo[1,2-<i>a</i>]pyridines 10.....</b>	<b>S63</b>
<b>HRMS spectral chart for 3,5-diphenyl-3H-pyrrol-2-one 15aa.....</b>	<b>S72</b>
<b>HRMS spectral chart for <i>N</i>-(2-aminophenyl)-2-phenylacetamide 16aa.....</b>	<b>S73</b>
<b>HRMS spectral chart for 2-Benzyl-1<i>H</i>-benzo[<i>d</i>]imidazole 17aa.....</b>	<b>S74</b>
<b>HRMS spectral chart of aqueous phase of the reaction between hydroxylactam 1aa and phenylenediamine 6a.....</b>	<b>S75</b>

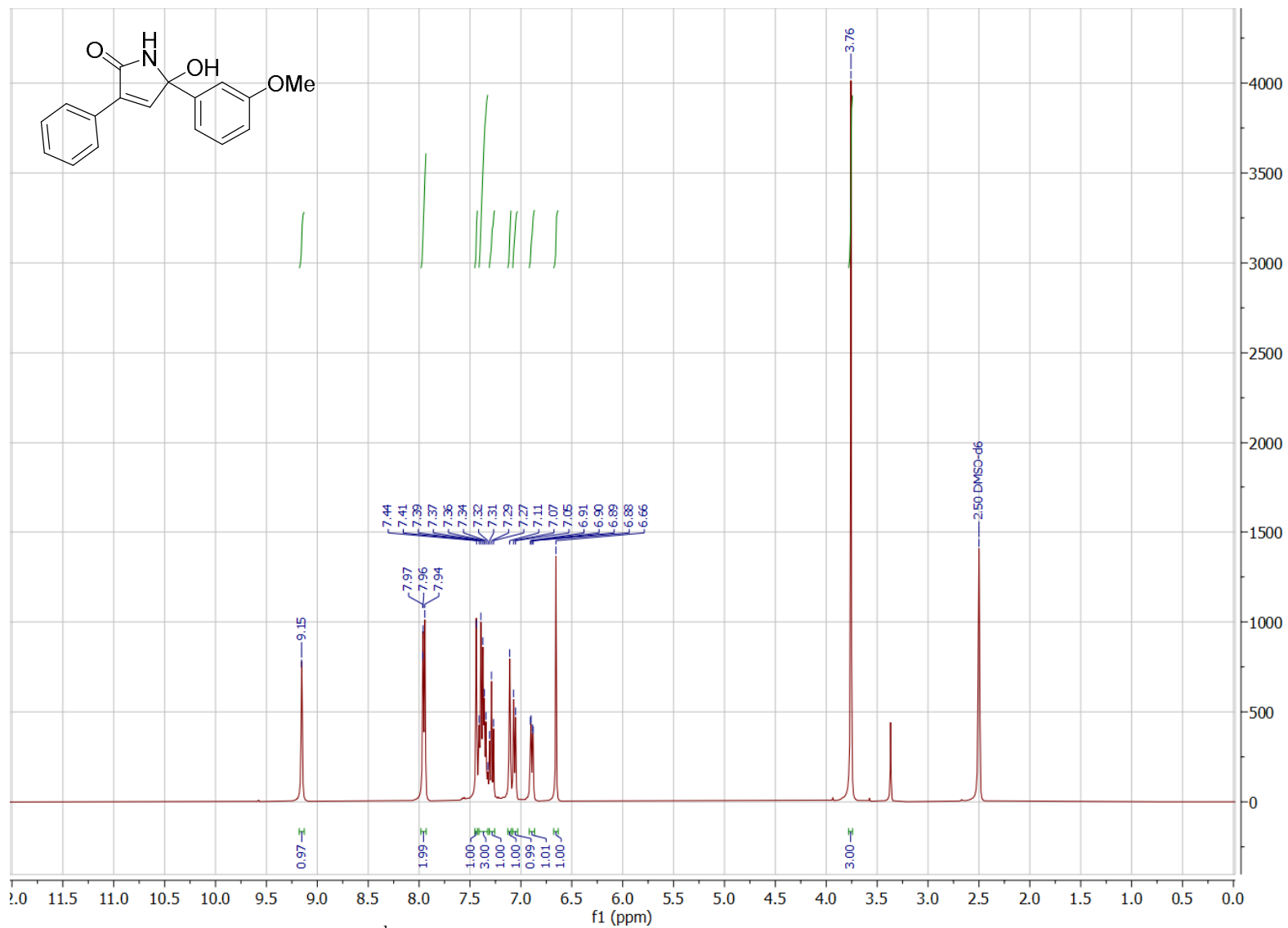


Figure S1. <sup>1</sup>H NMR spectrum of hydroxylactam **1ca** in DMSO-*d*<sub>6</sub> (400 MHz)

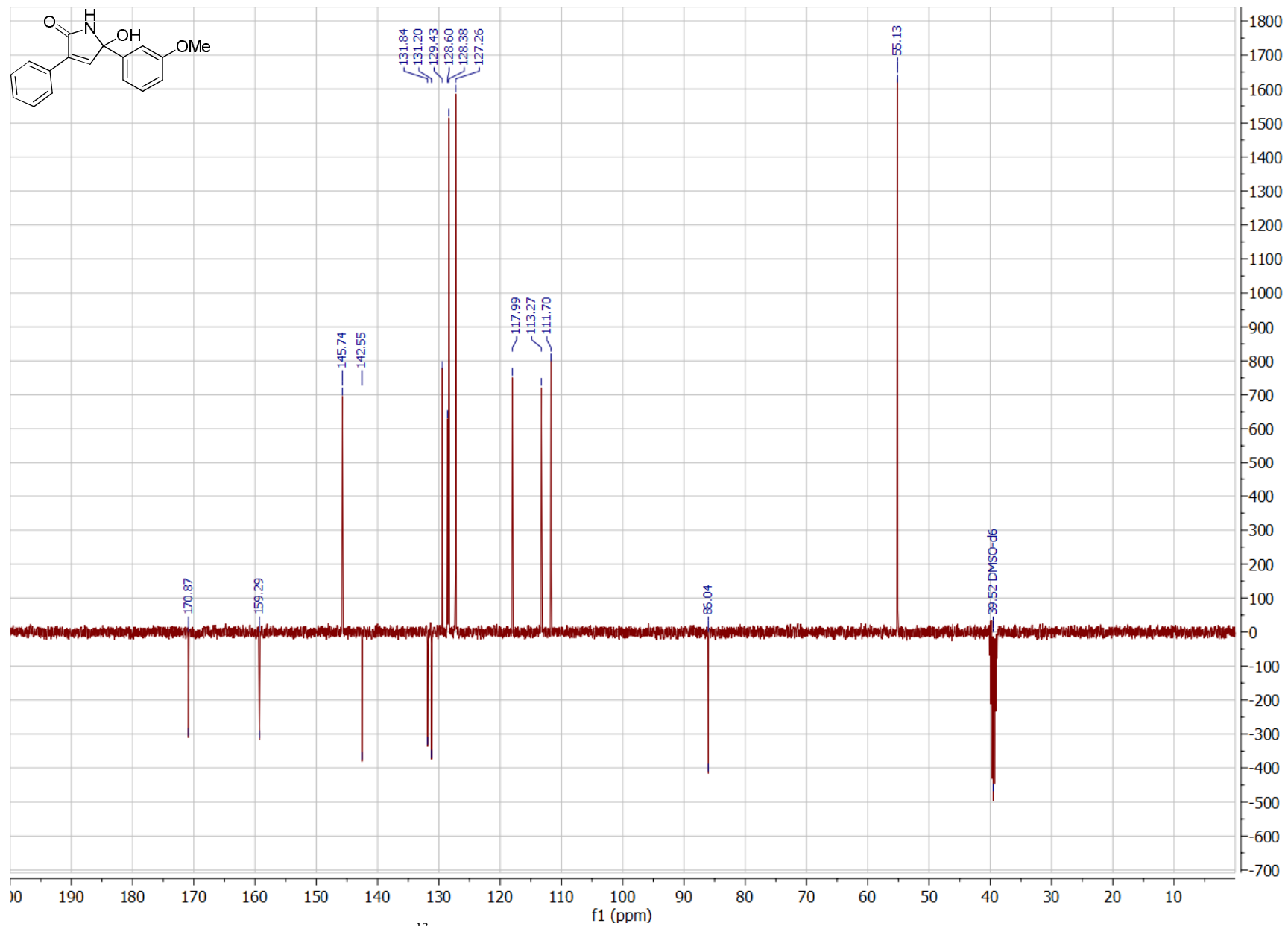


Figure S2.  $^{13}\text{C}$  NMR spectrum of hydroxylactam **1ca** in  $\text{DMSO-}d_6$  (101 MHz)

<sup>1</sup>H and <sup>13</sup>C NMR spectral charts for quinoxalines **8**

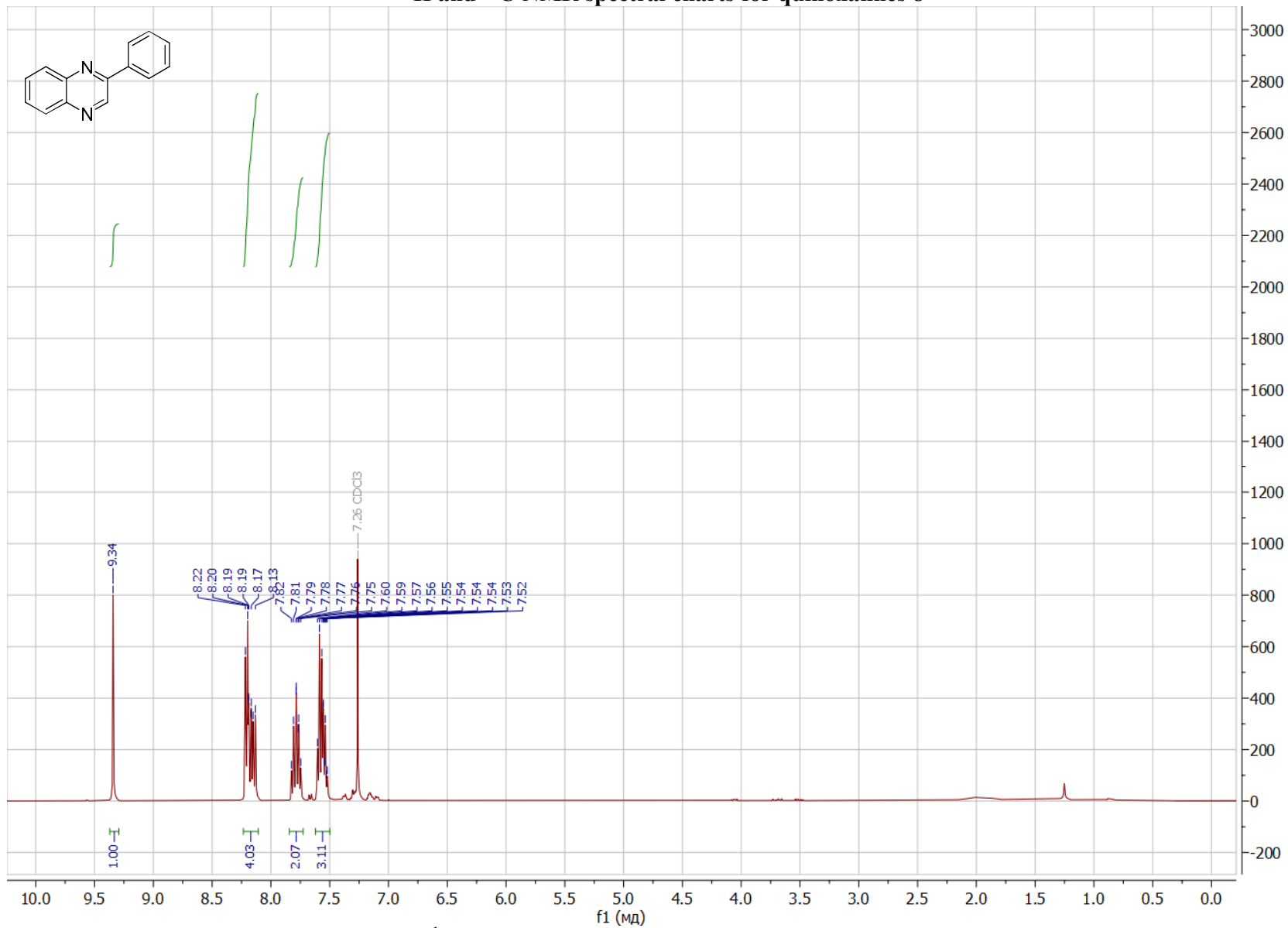


Figure S3. <sup>1</sup>H NMR spectrum of quinoxaline **8aa** in CDCl<sub>3</sub> (400 MHz)

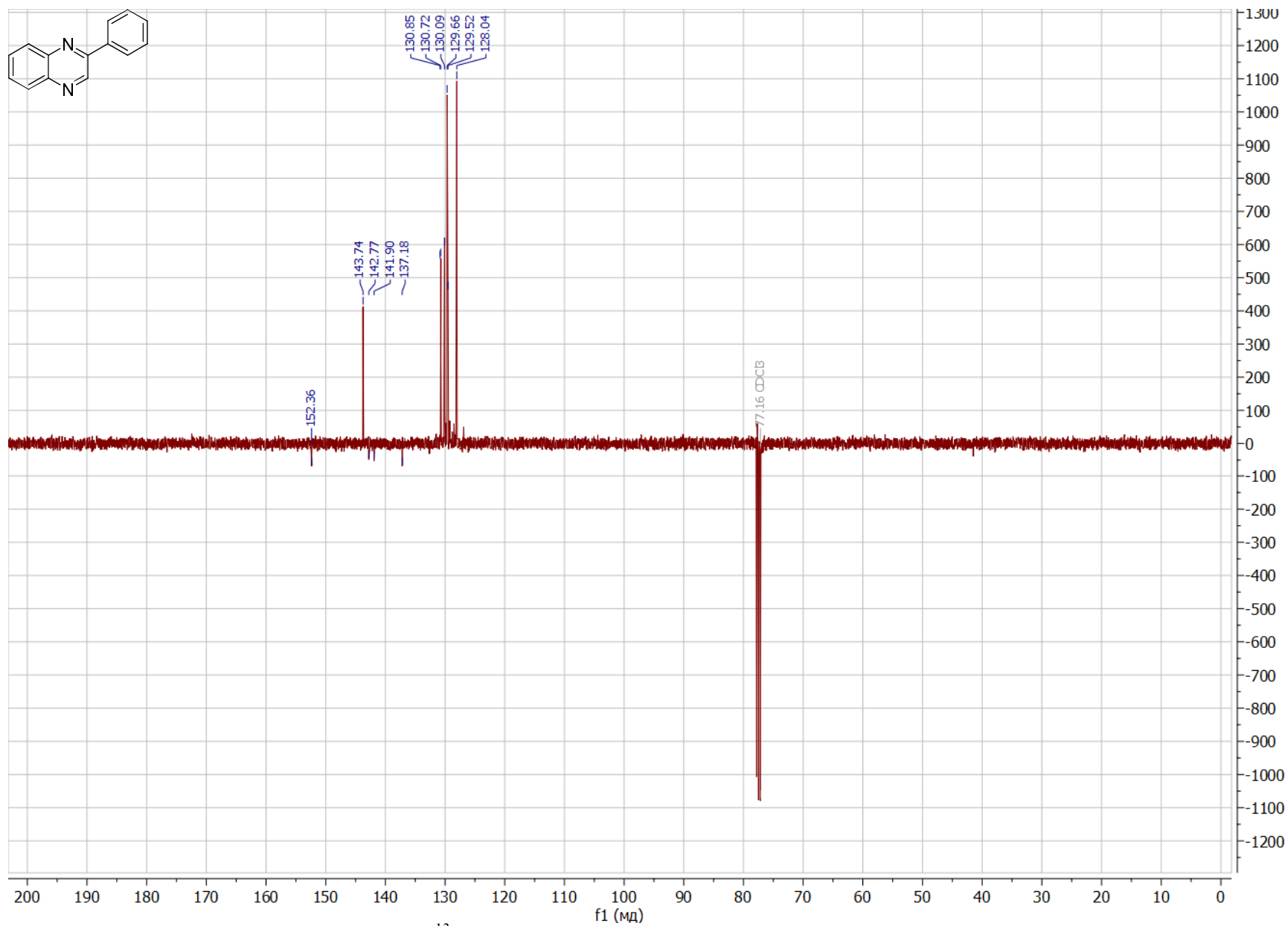


Figure S4.  $^{13}\text{C}$  NMR spectrum of quinoxaline **8aa** in  $\text{CDCl}_3$  (101 MHz)

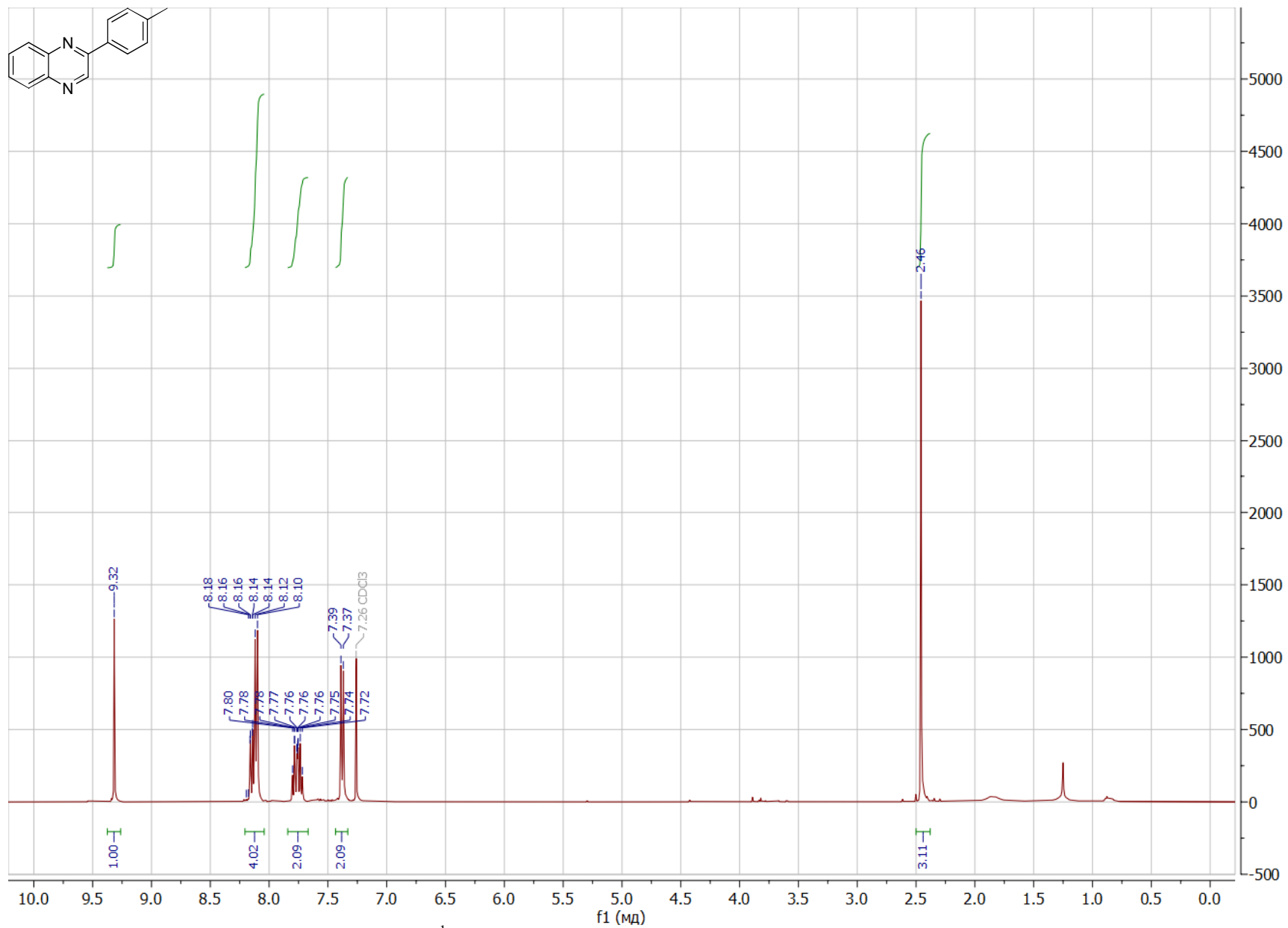


Figure S5. <sup>1</sup>H NMR spectrum of quinoxaline **8ba** in CDCl<sub>3</sub> (400 MHz)

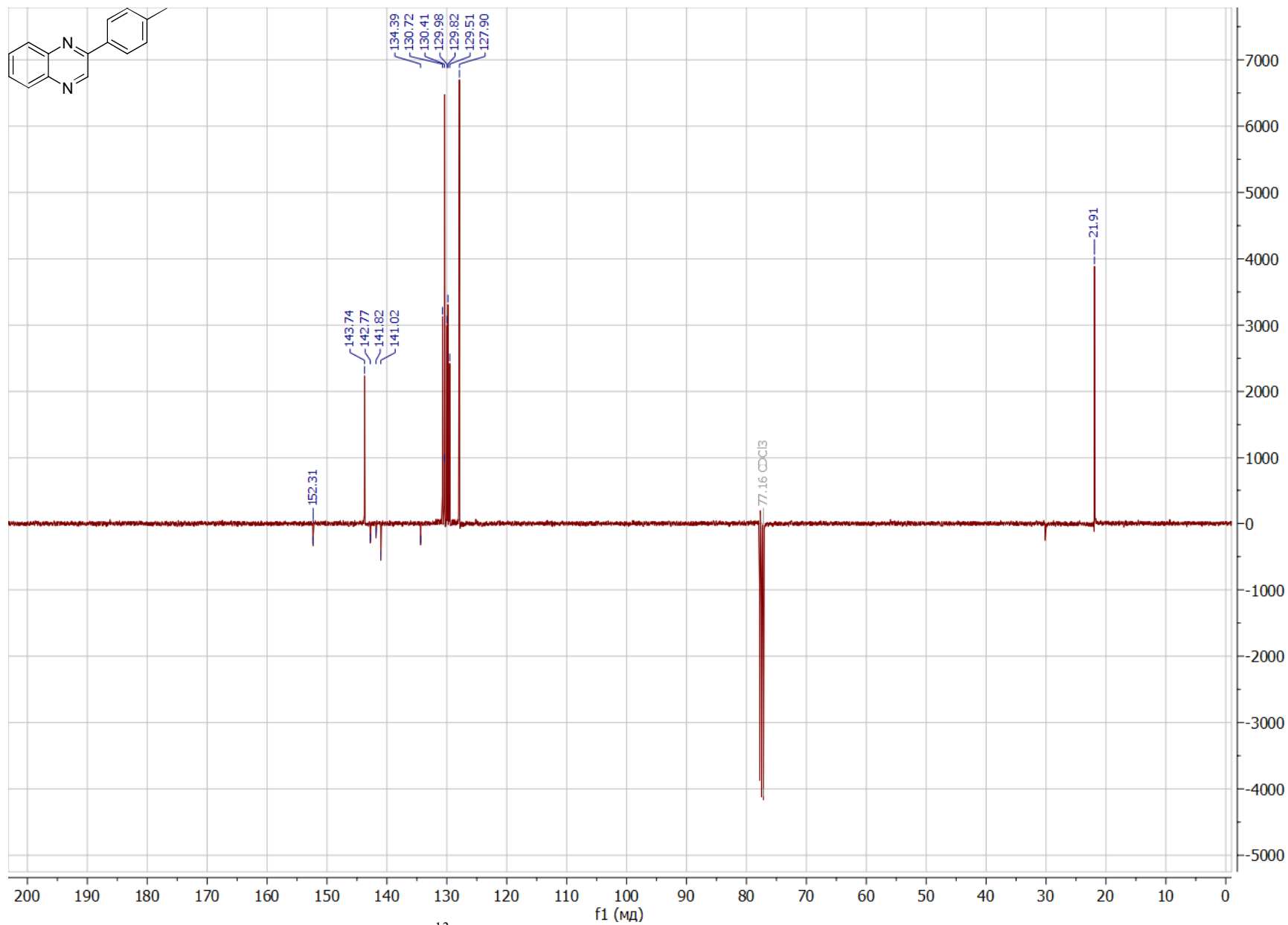


Figure S6.  $^{13}\text{C}$  NMR spectrum of quinoxaline **8ba** in  $\text{CDCl}_3$  (101 MHz)

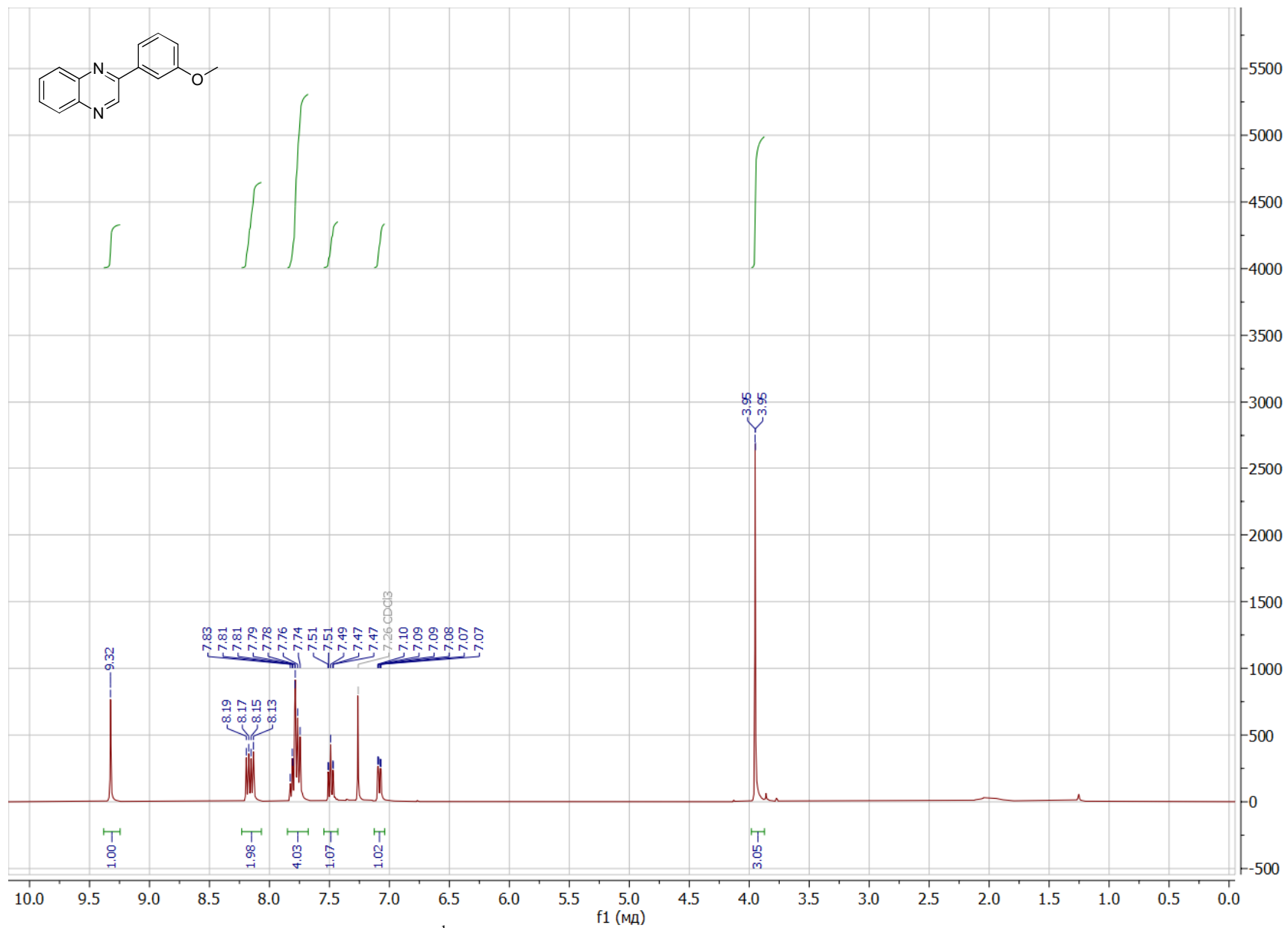


Figure S7. <sup>1</sup>H NMR spectrum of quinoxaline **8ca** in CDCl<sub>3</sub> (400 MHz)



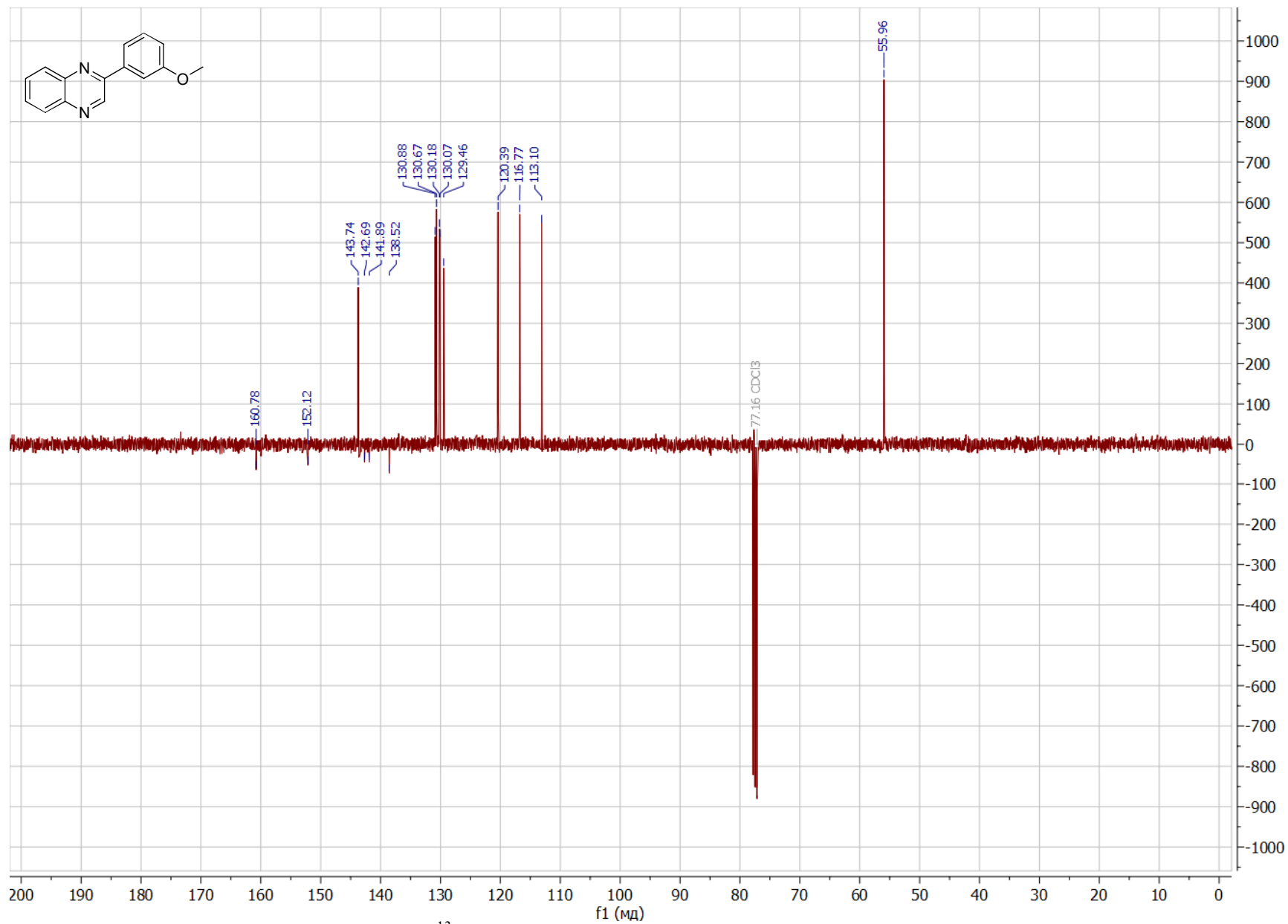


Figure S8.  $^{13}\text{C}$  NMR spectrum of quinoxaline **8ca** in  $\text{CDCl}_3$  (101 MHz)

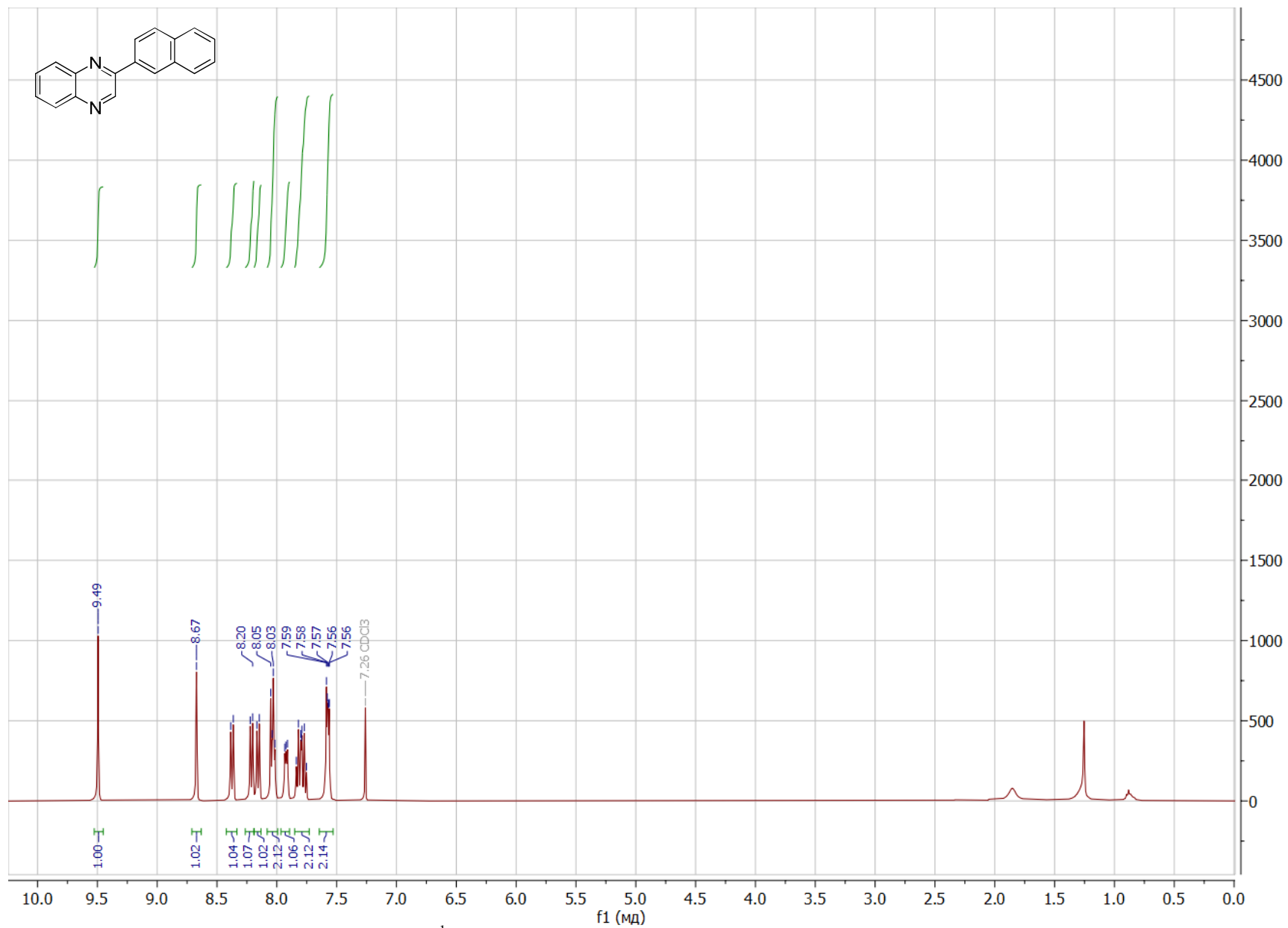


Figure S9. <sup>1</sup>H NMR spectrum of quinoxaline **8da** in CDCl<sub>3</sub> (400 MHz)

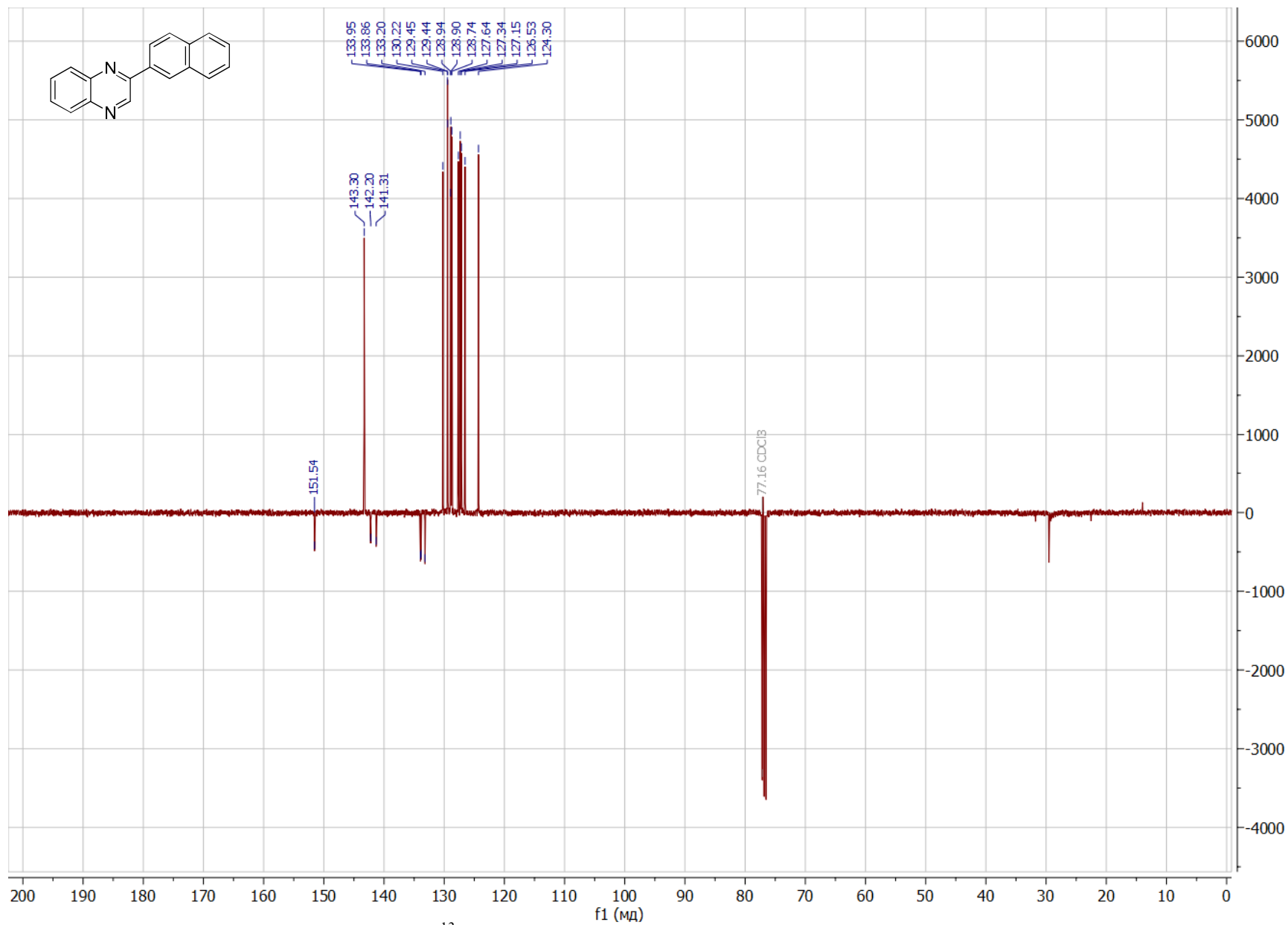


Figure S10.  $^{13}\text{C}$  NMR spectrum of quinoxaline **8da** in  $\text{CDCl}_3$  (101 MHz)

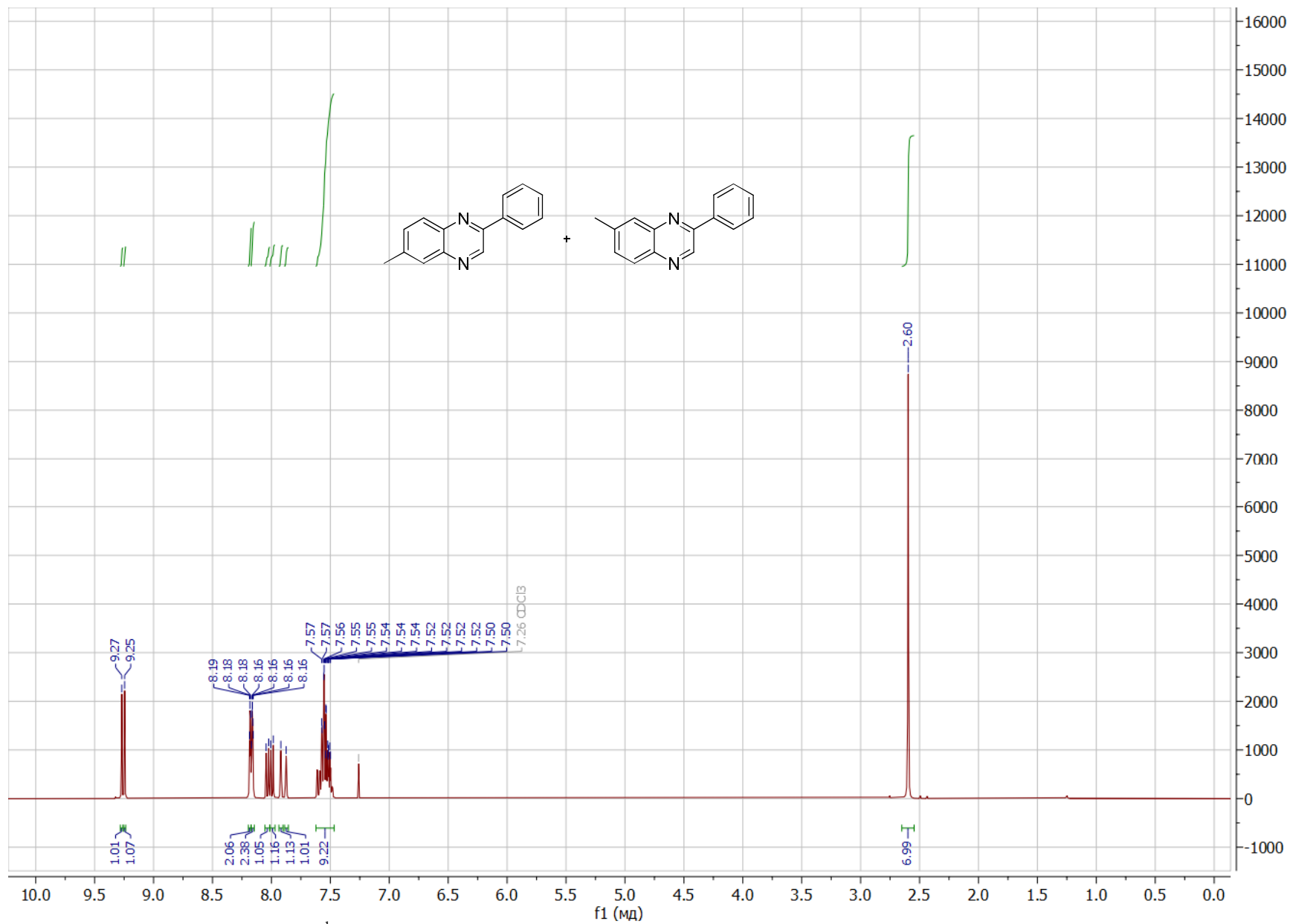


Figure S11. <sup>1</sup>H NMR spectrum of 1:1 mixture of quinoxalines **8ab'** and **8ab** in CDCl<sub>3</sub> (400 MHz)

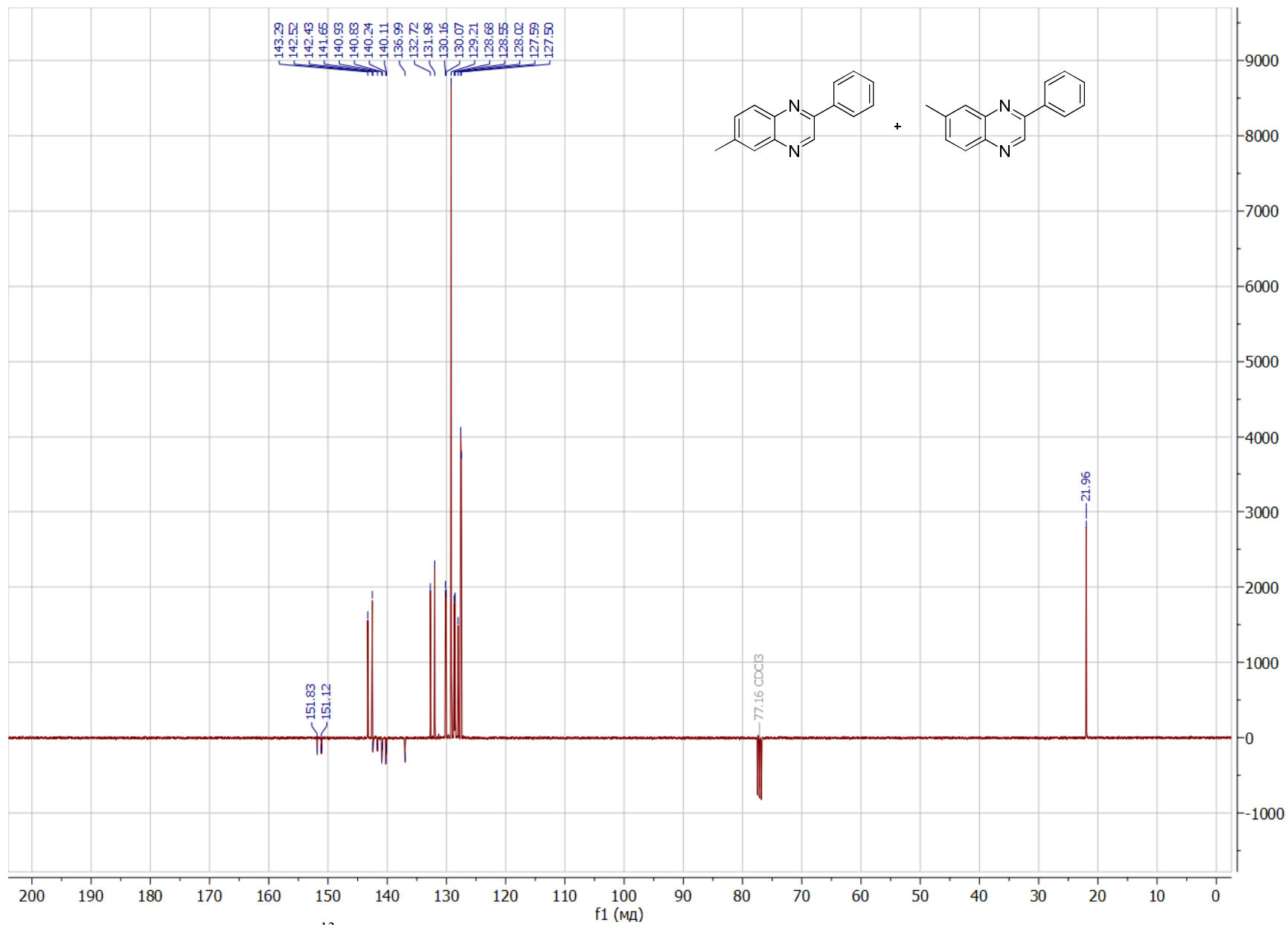


Figure S12.  $^{13}\text{C}$  NMR spectrum of 1:1 mixture of quinoxalines **8ab'** and **8ab** in  $\text{CDCl}_3$  (101 MHz)

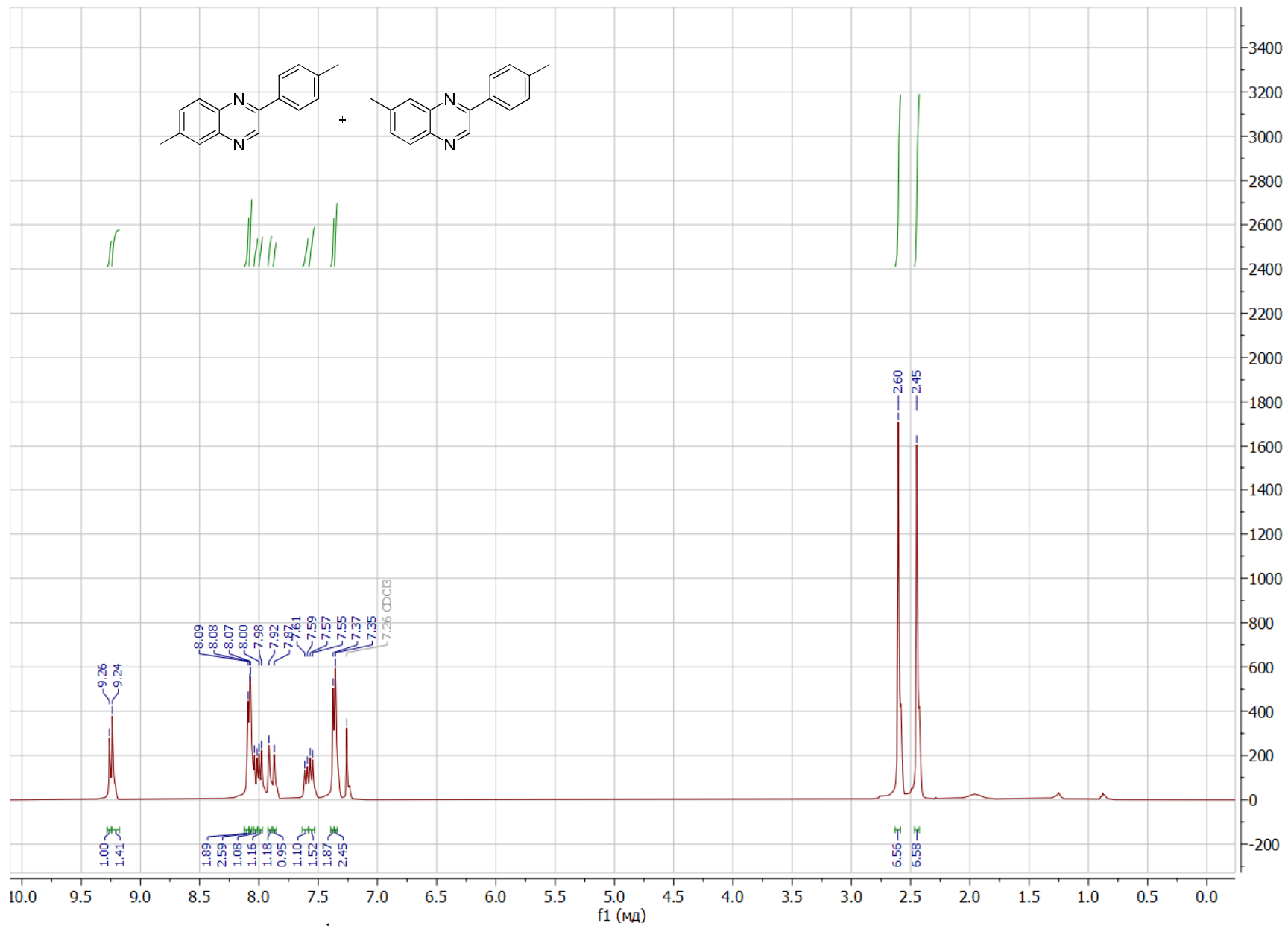


Figure S13.  $^1\text{H}$  NMR spectrum of 1:1 mixture of quinoxalines **8bb'** and **8bb** in  $\text{CDCl}_3$  (400 MHz)

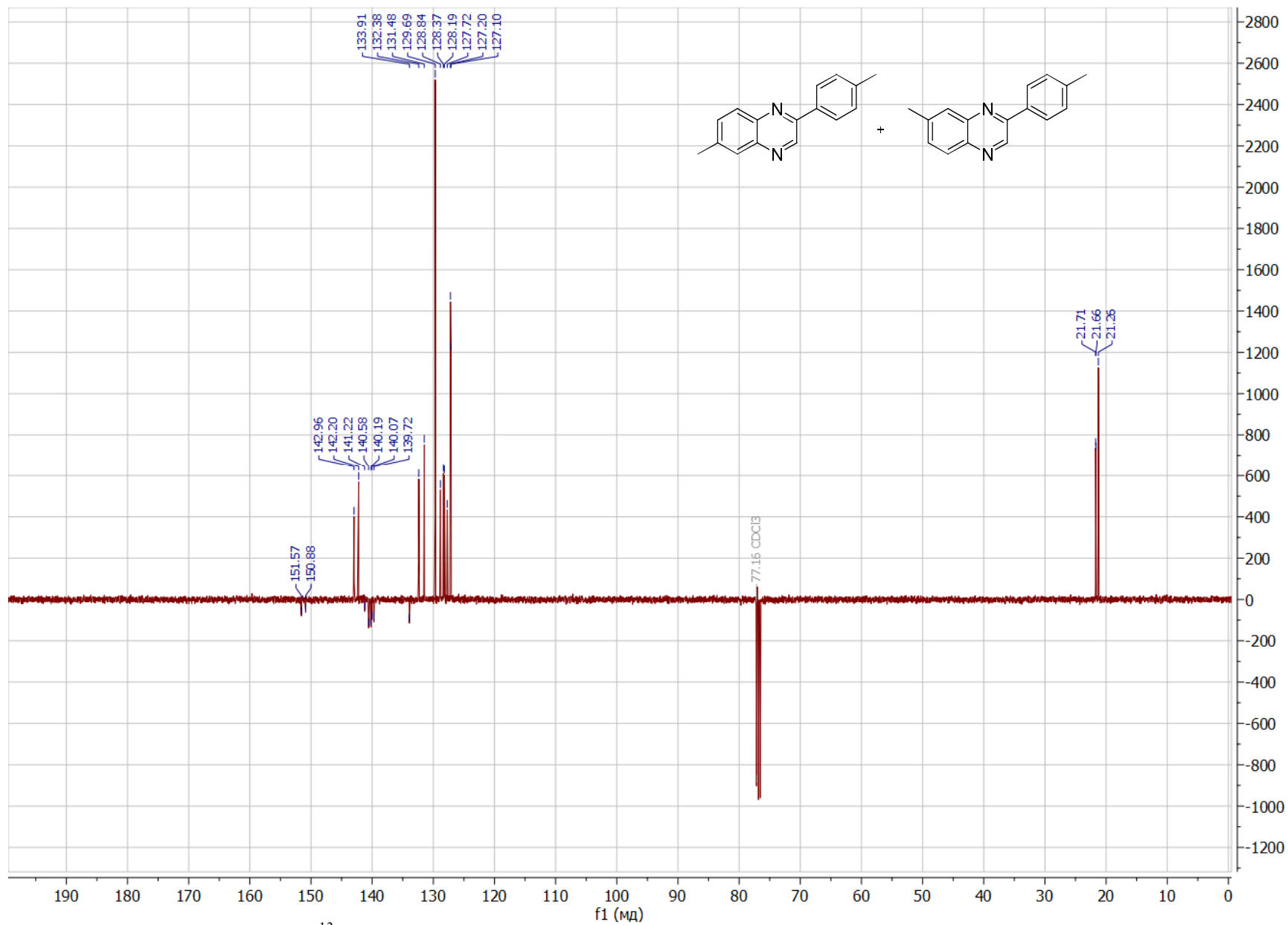


Figure S14.  $^{13}\text{C}$  NMR spectrum of 1:1 mixture of quinoxalines **8bb'** and **8bb** in  $\text{CDCl}_3$  (101 MHz)

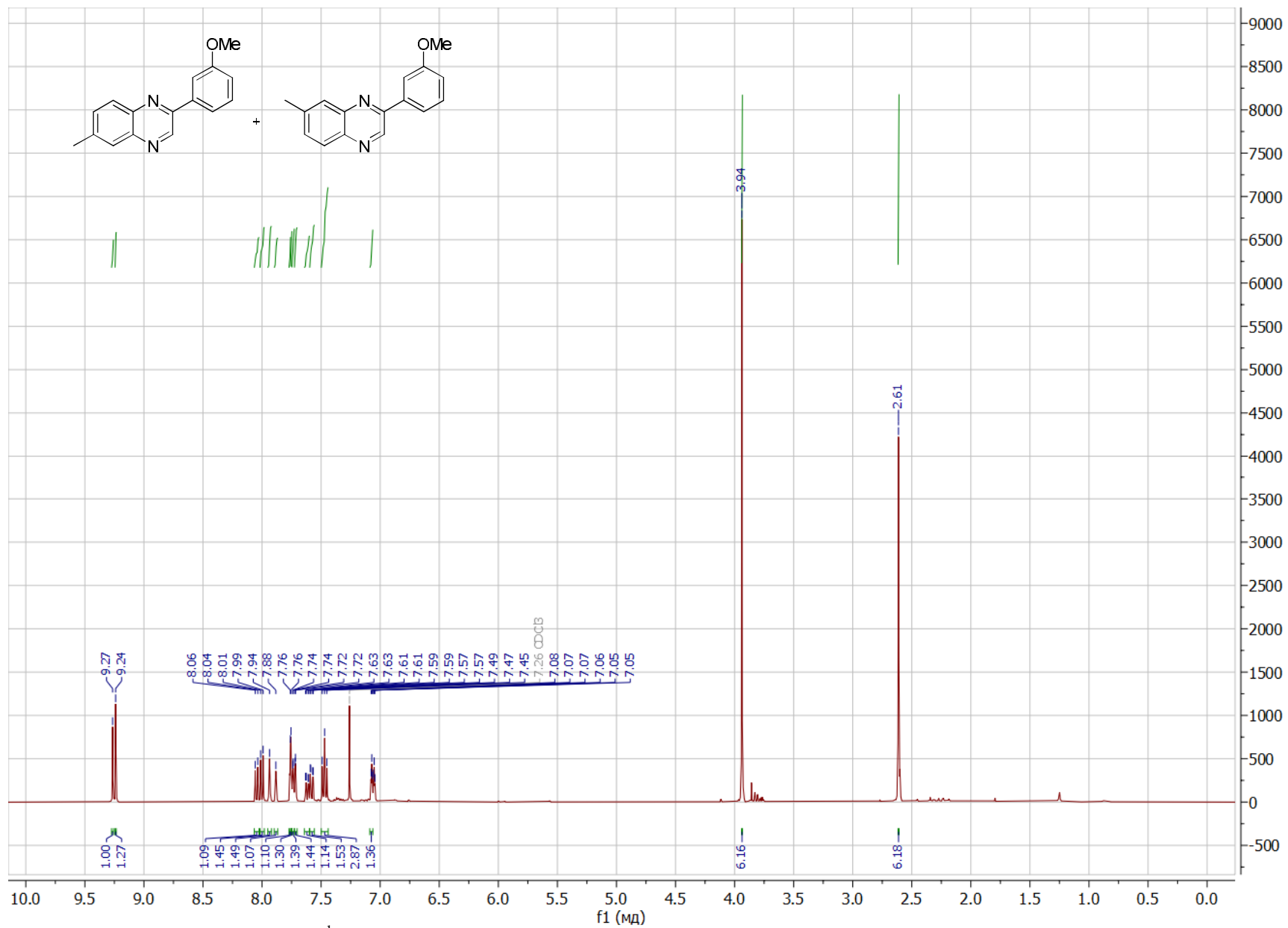


Figure S15.  $^1\text{H}$  NMR spectrum of 1:1 mixture of quinoxalines **8cb'** and **8cb** in  $\text{CDCl}_3$  (400 MHz)



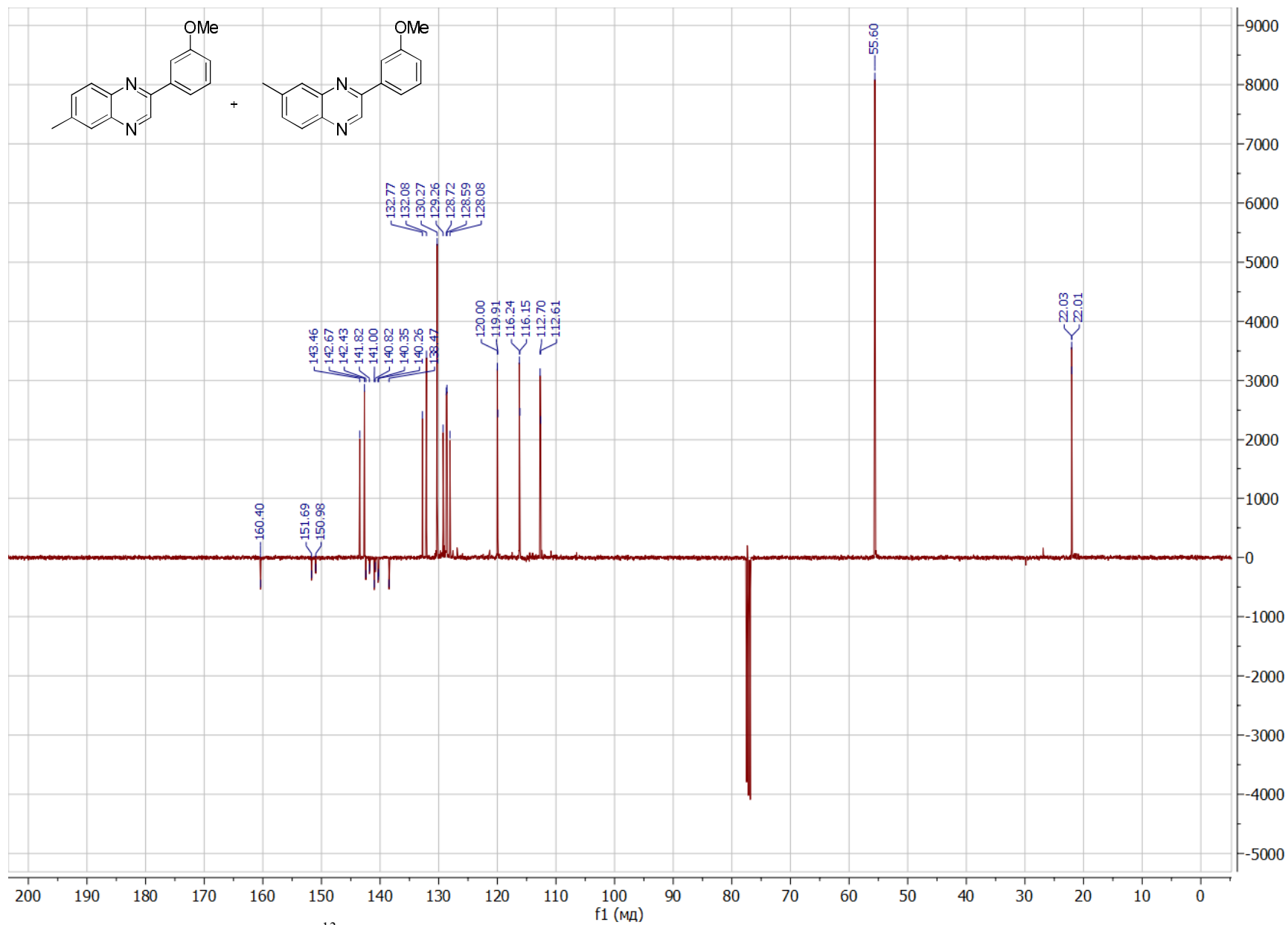


Figure S16.  $^{13}\text{C}$  NMR spectrum of 1:1 mixture of quinoxalines **8cb'** and **8cb** in  $\text{CDCl}_3$  (101 MHz)

**<sup>1</sup>H and <sup>13</sup>C NMR spectral charts for imidazopyridines 10**

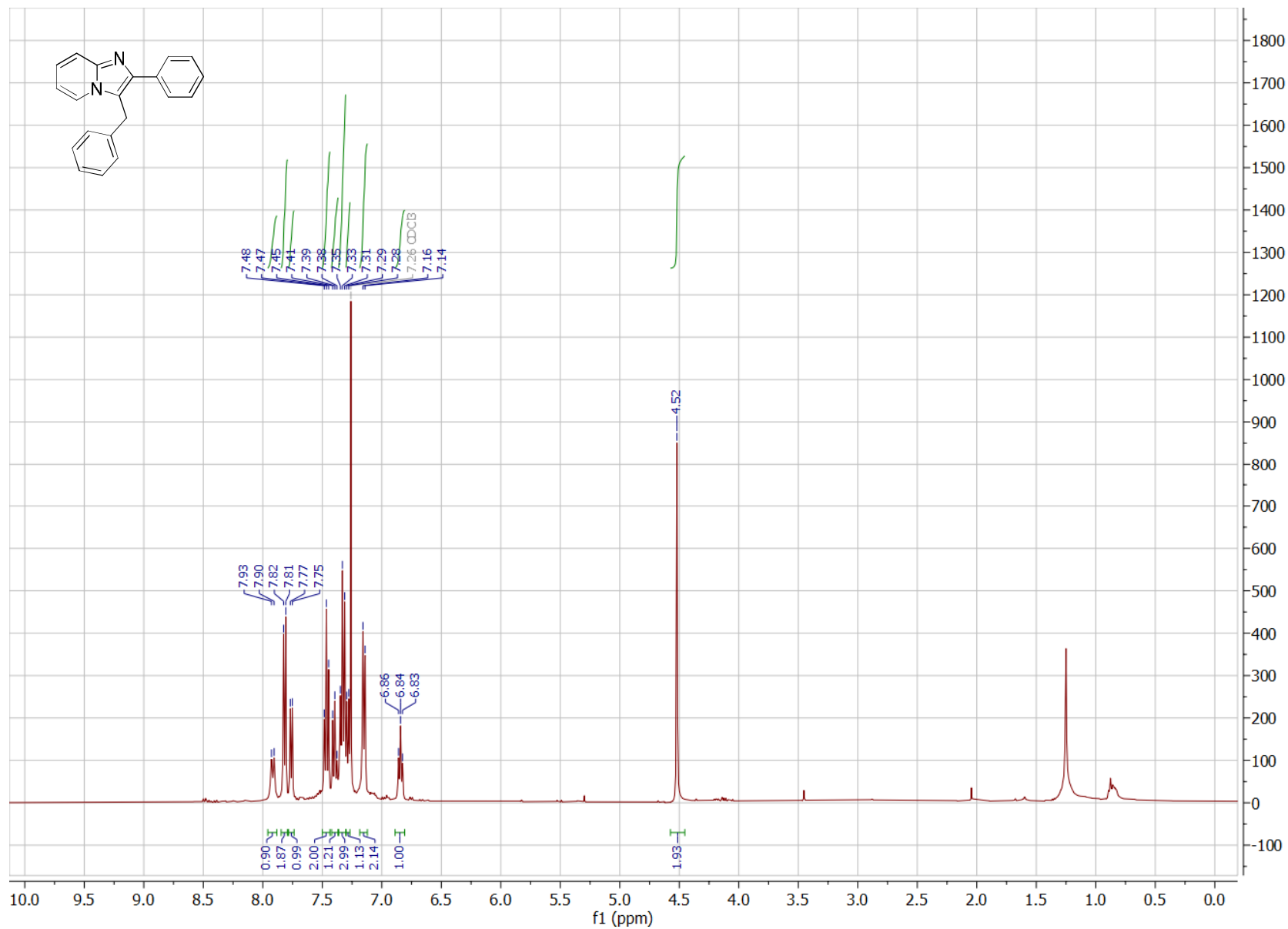


Figure S17. <sup>1</sup>H NMR spectrum of imidazo[1,2-a]pyridine **10aaa** in CDCl<sub>3</sub> (400 MHz)

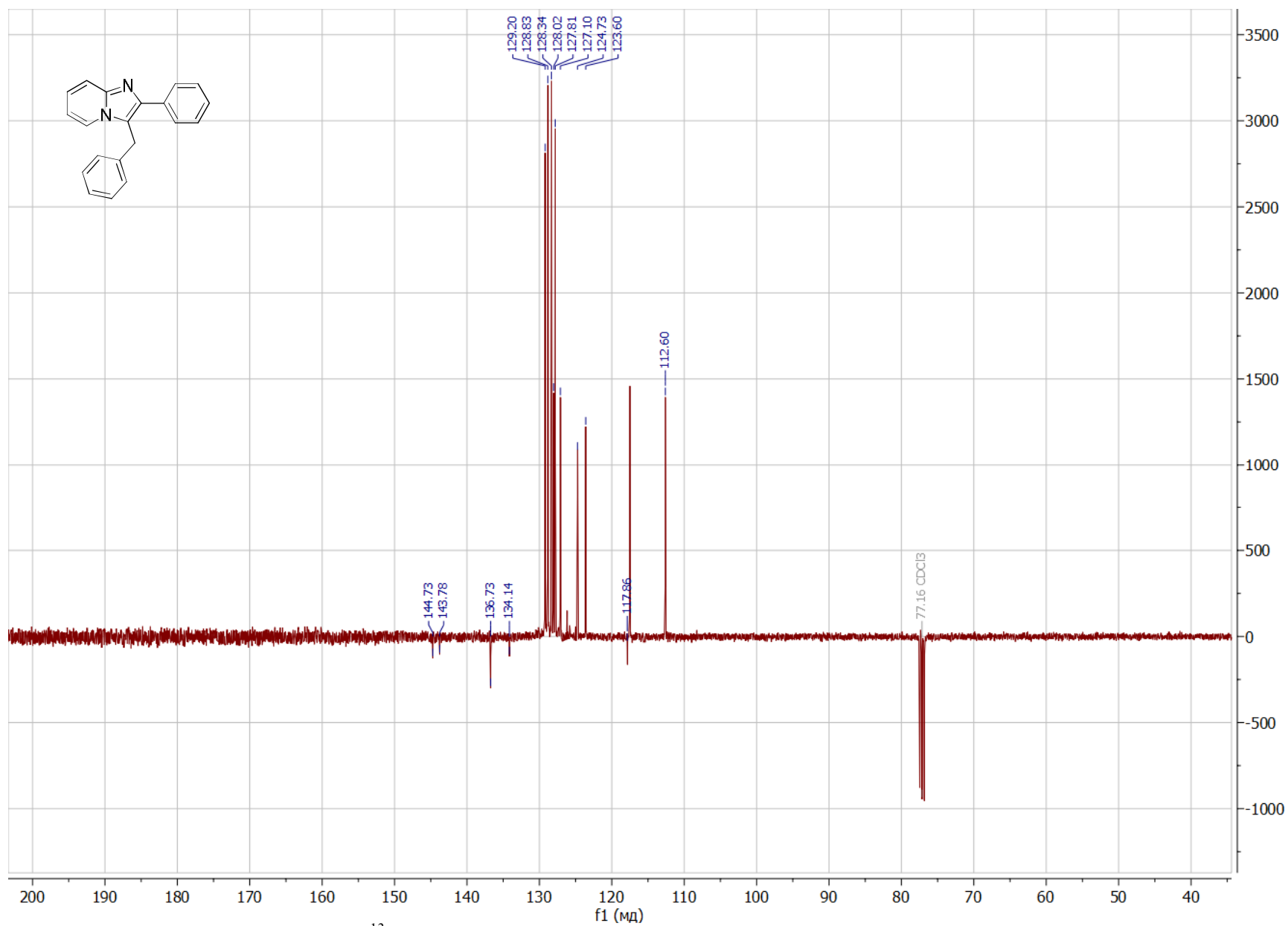


Figure S18.  $^{13}\text{C}$  NMR spectrum of imidazo[1,2-*a*]pyridine **10aaa** in  $\text{CDCl}_3$  (101 MHz)

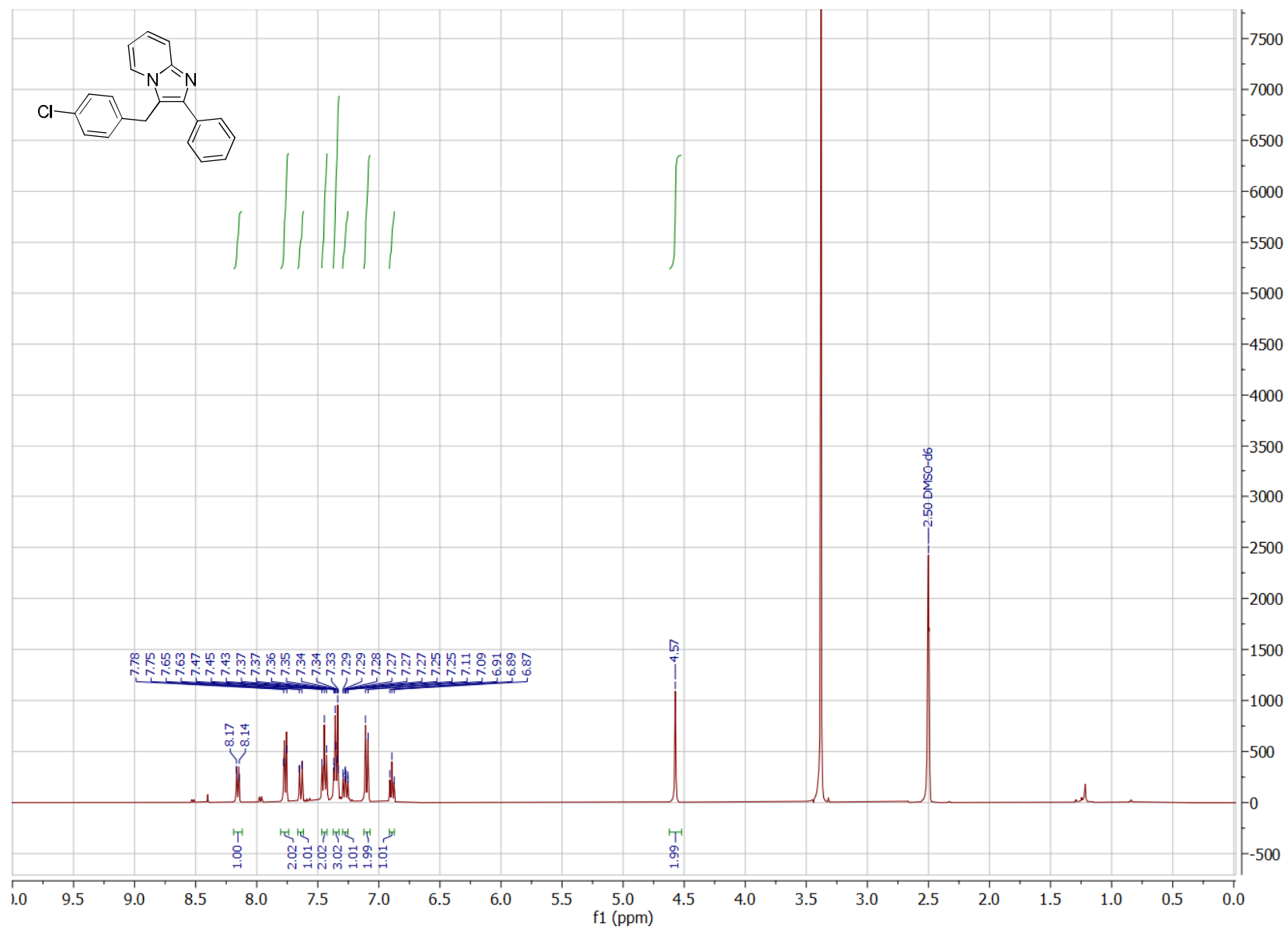


Figure S19. <sup>1</sup>H NMR spectrum of imidazo[1,2-*a*]pyridine **10aba** in DMSO-*d*<sub>6</sub> (400 MHz)

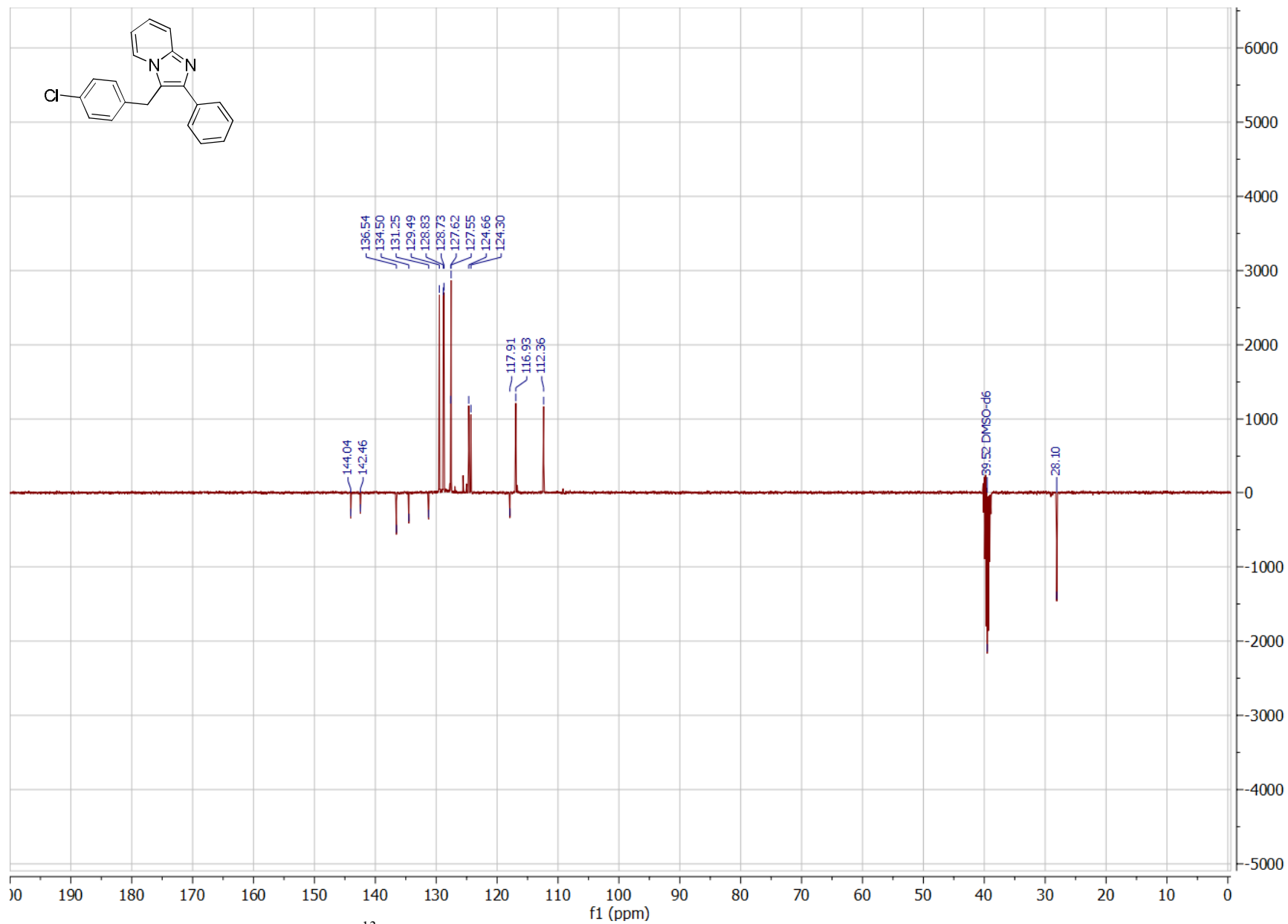


Figure S20.  $^{13}\text{C}$  NMR spectrum of imidazo[1,2-*a*]pyridine **10aba** in  $\text{DMSO-}d_6$  (101 MHz)

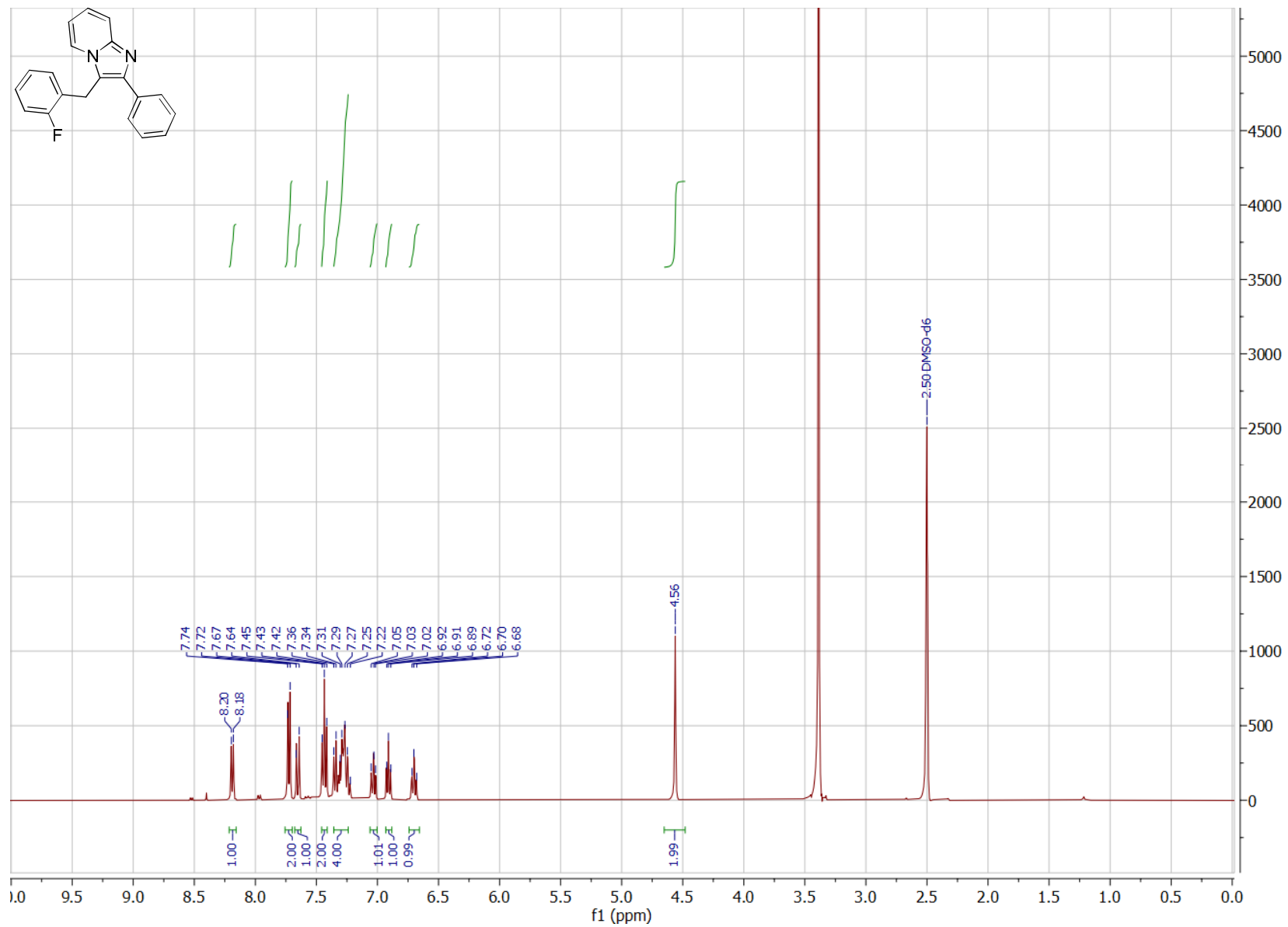


Figure S21. <sup>1</sup>H NMR spectrum of imidazo[1,2-*a*]pyridine **10aca** in DMSO-*d*<sub>6</sub> (400 MHz)

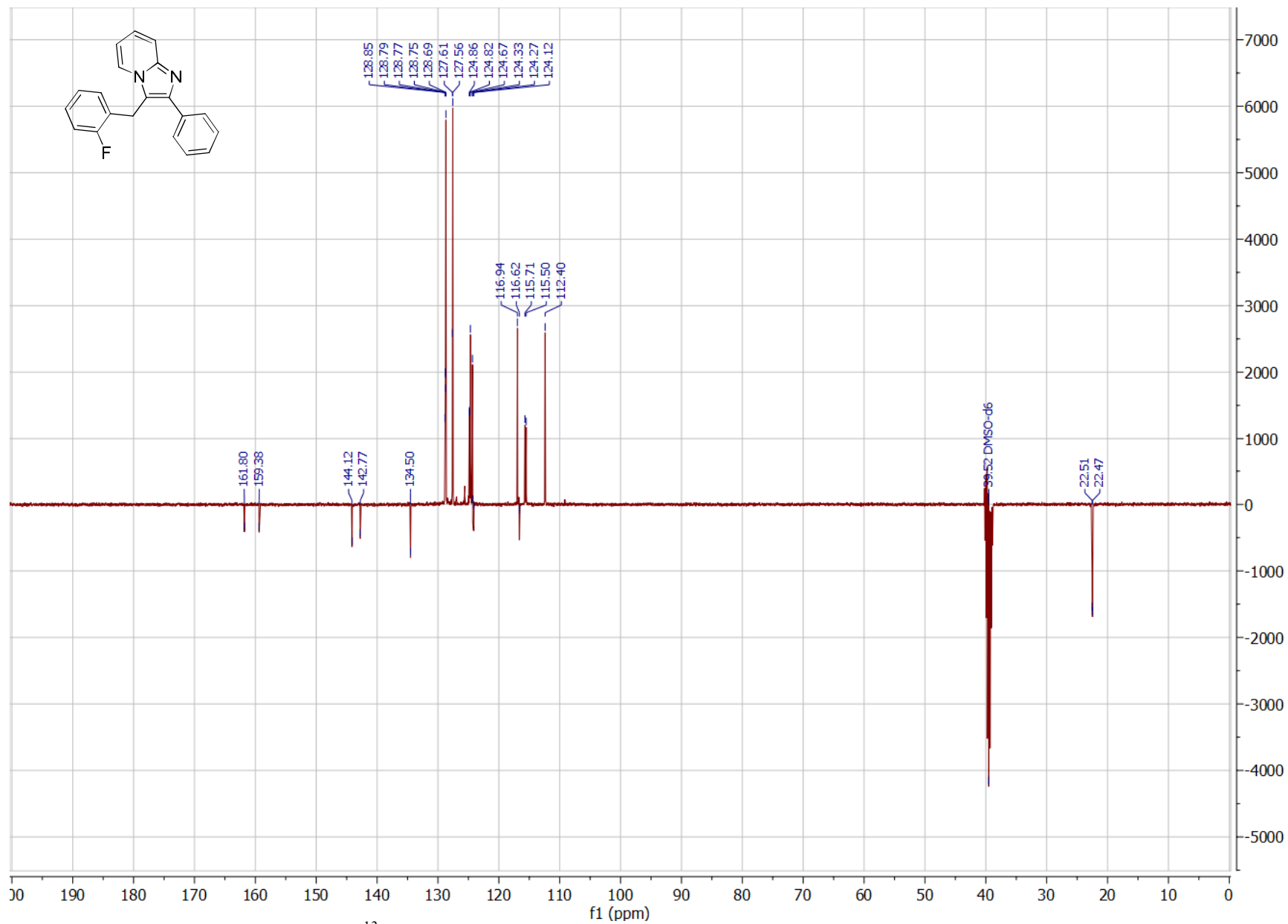


Figure S22.  $^{13}\text{C}$  NMR spectrum of imidazo[1,2-*a*]pyridine **10aca** in DMSO- $d_6$  (101 MHz)

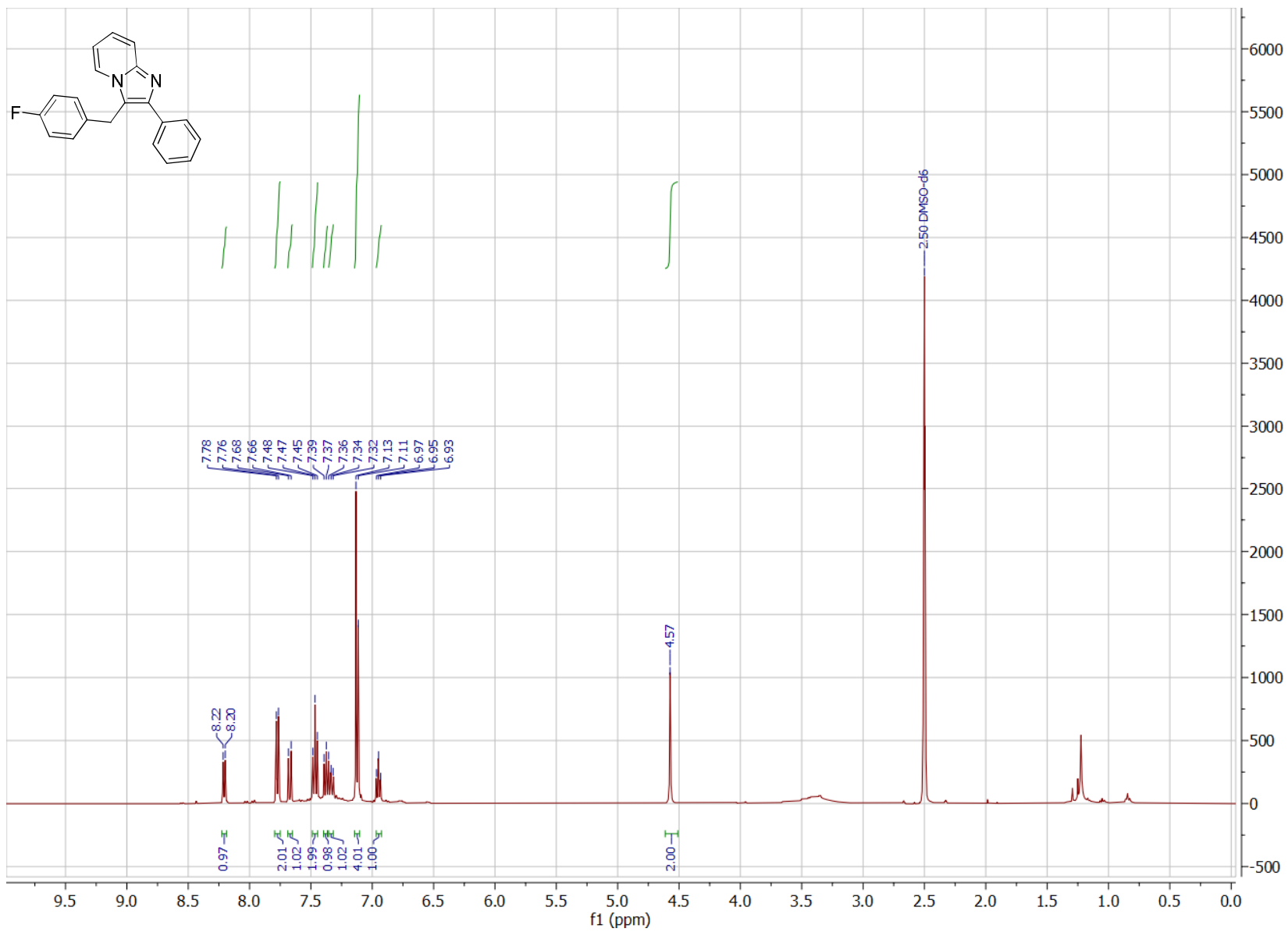


Figure S23. <sup>1</sup>H NMR spectrum of imidazo[1,2-*a*]pyridine **10ada** in DMSO-*d*<sub>6</sub> (400 MHz)



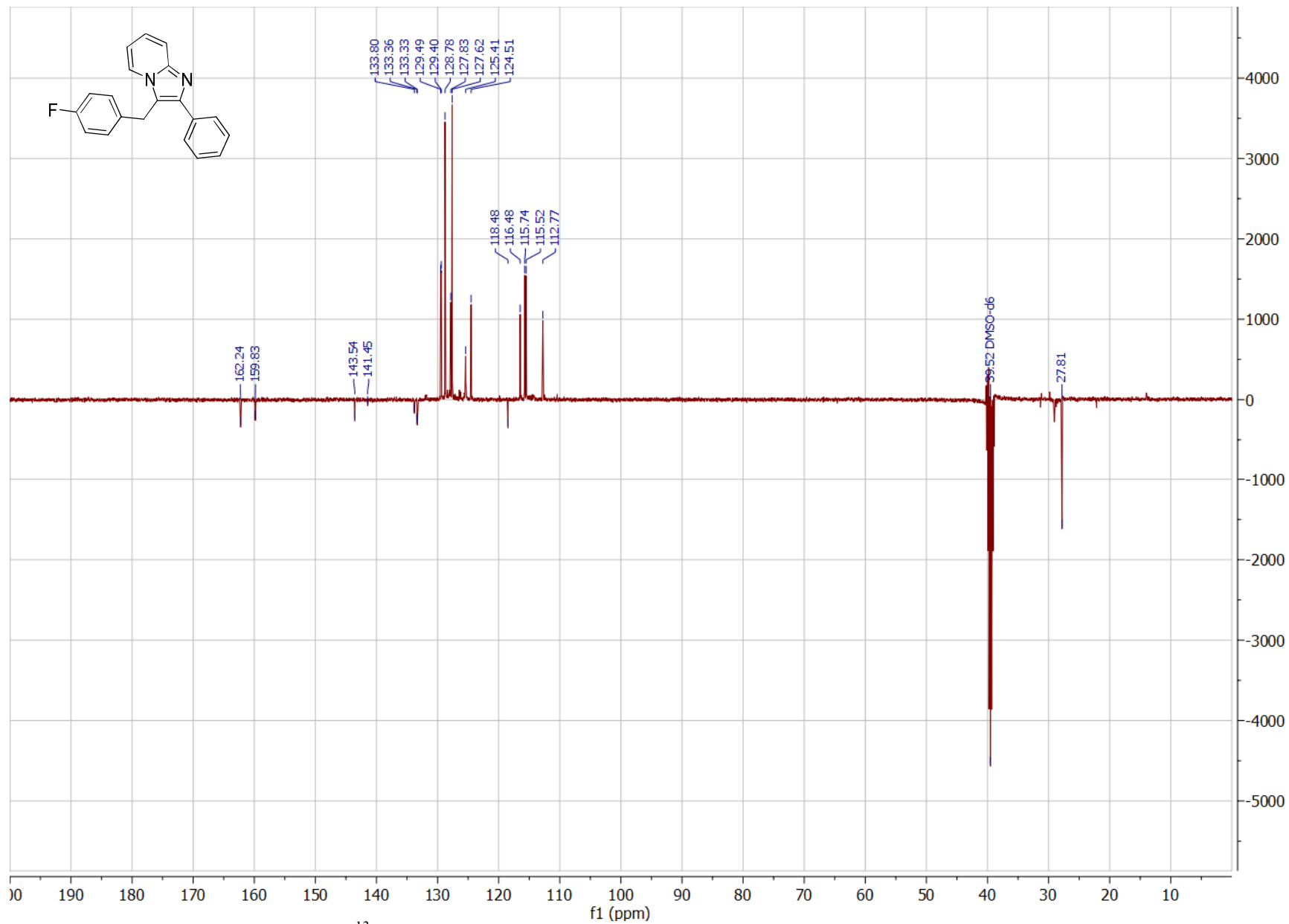


Figure S24. <sup>13</sup>C NMR spectrum of imidazo[1,2-a]pyridine **10ada** in DMSO-*d*<sub>6</sub> (101 MHz)

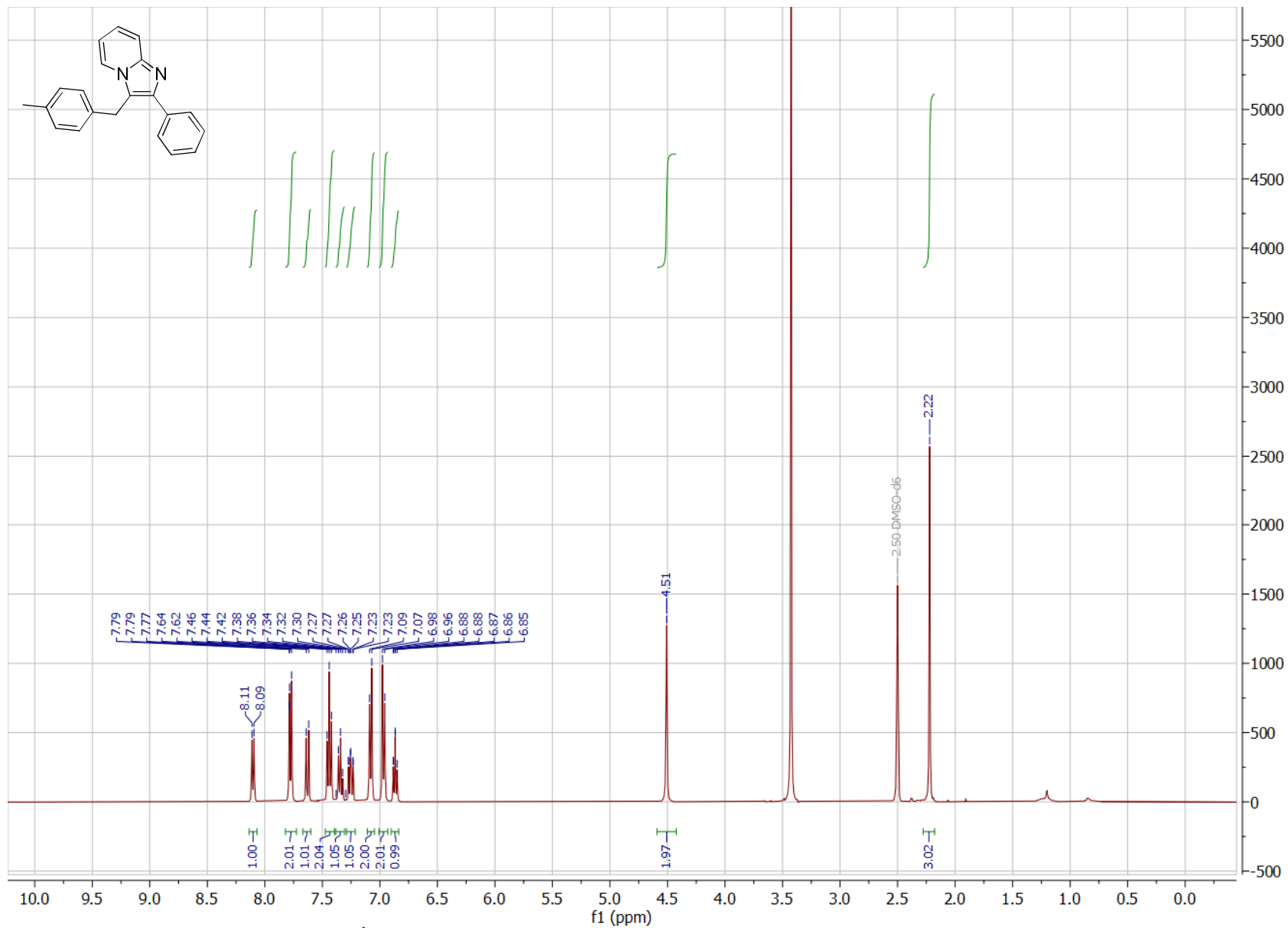


Figure S25. <sup>1</sup>H NMR spectrum of imidazo[1,2-*a*]pyridine **10aea** in DMSO-*d*<sub>6</sub> (400 MHz)

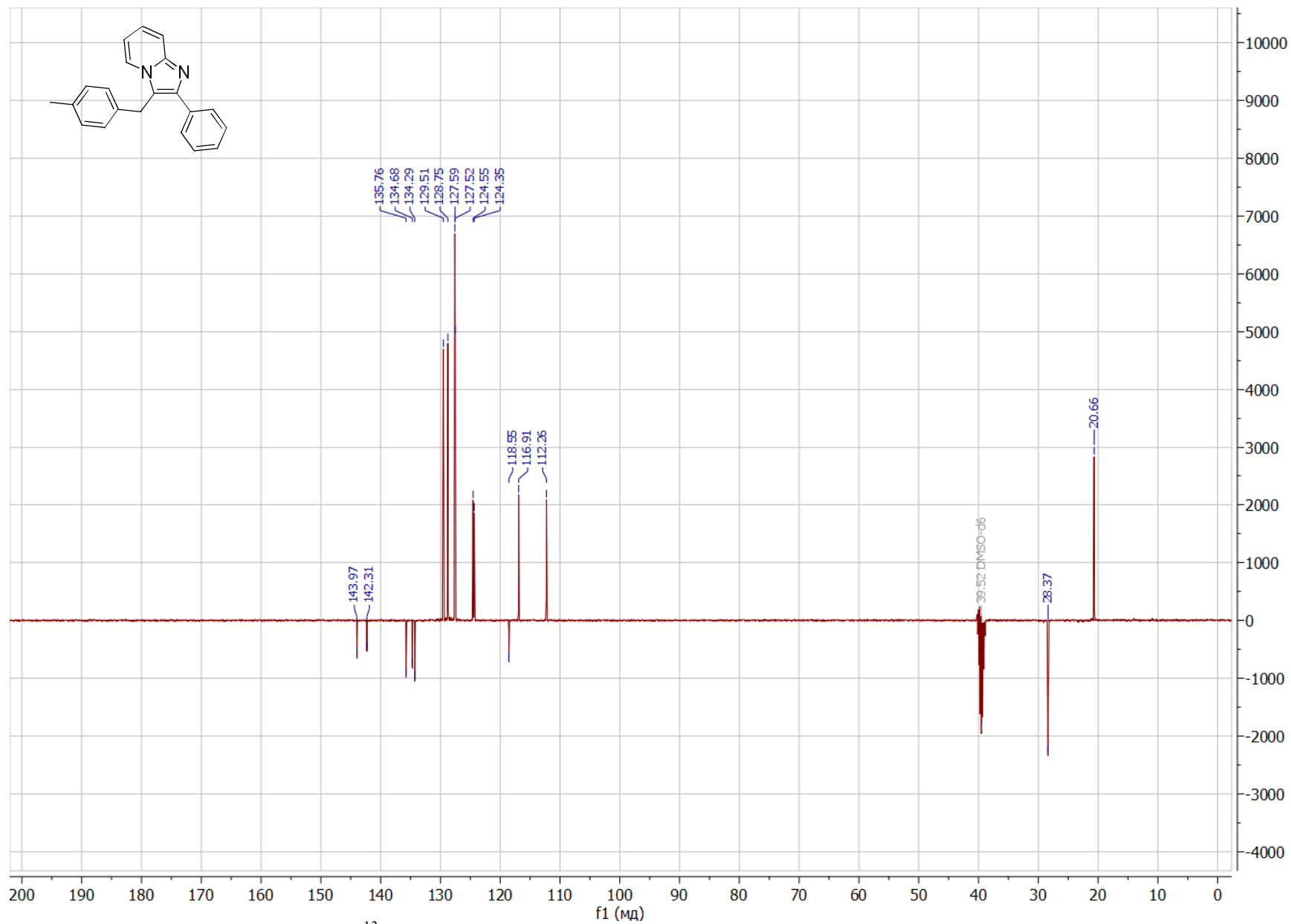


Figure S26. <sup>13</sup>C NMR spectrum of imidazo[1,2-*a*]pyridine **10aea** in DMSO-*d*<sub>6</sub> (101 MHz)

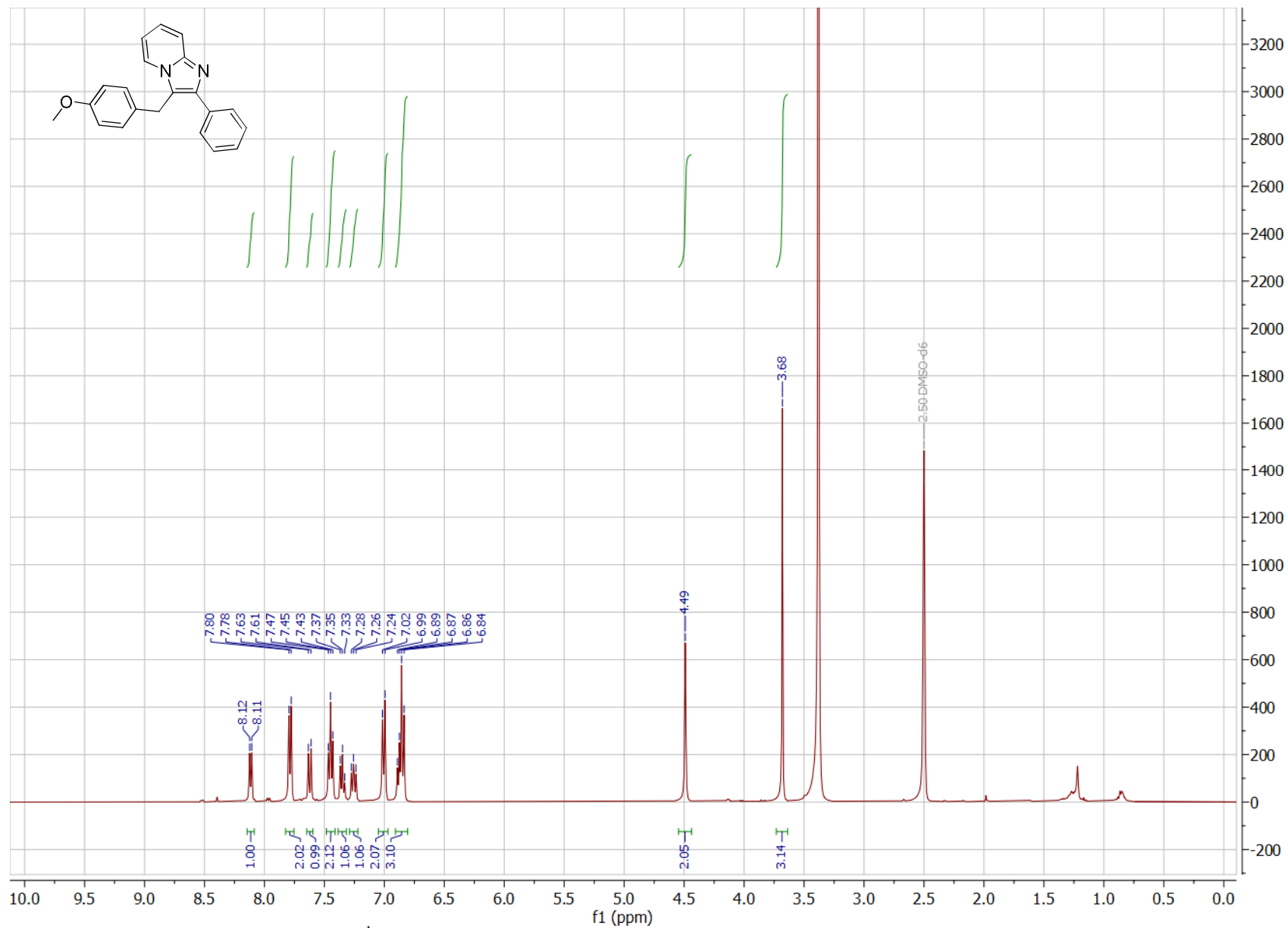


Figure S27. <sup>1</sup>H NMR spectrum of imidazo[1,2-a]pyridine **10afa** in DMSO-*d*<sub>6</sub> (400 MHz)

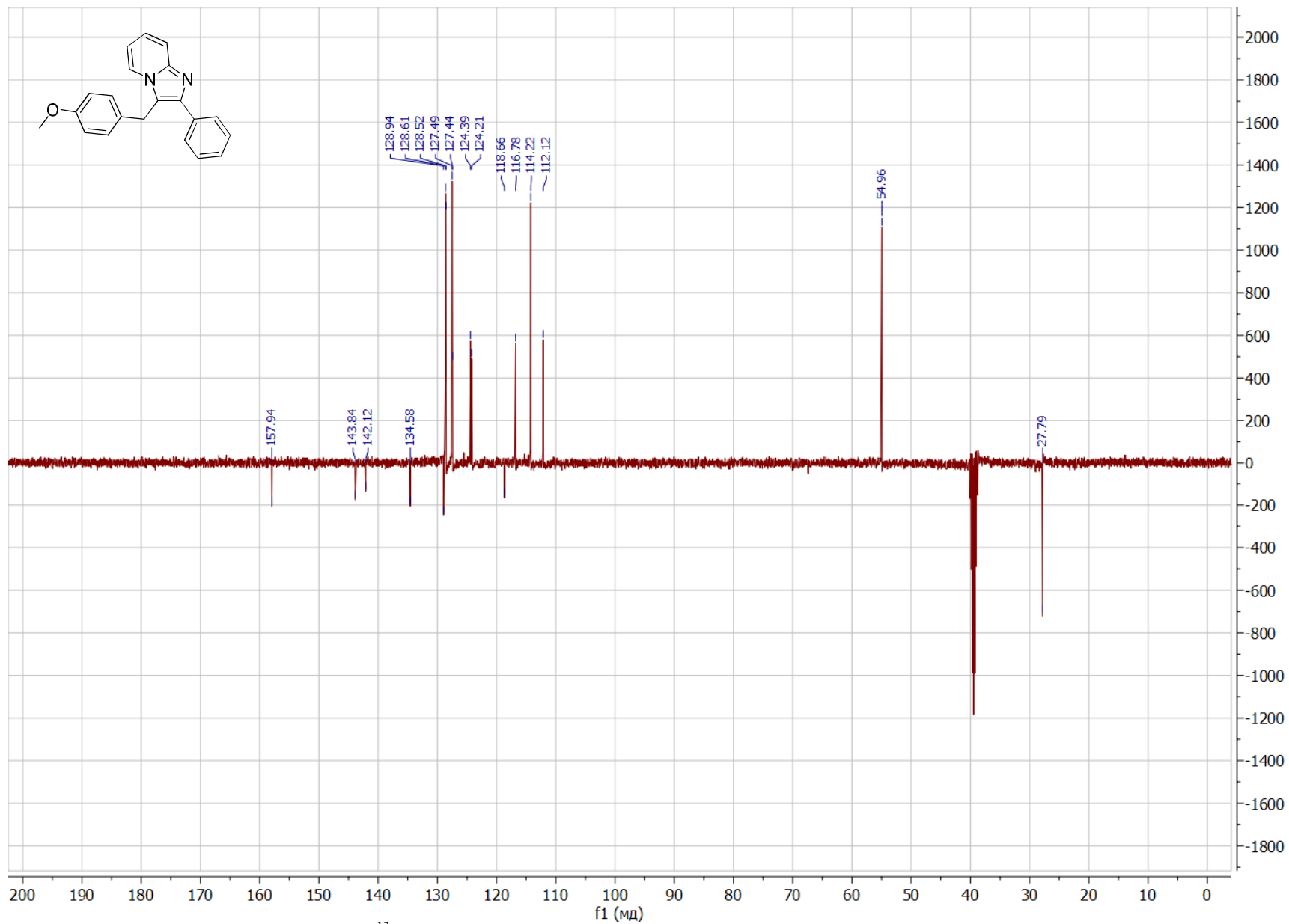


Figure S28.  $^{13}\text{C}$  NMR spectrum of imidazo[1,2-*a*]pyridine **10afa** in  $\text{DMSO-}d_6$  (101 MHz)

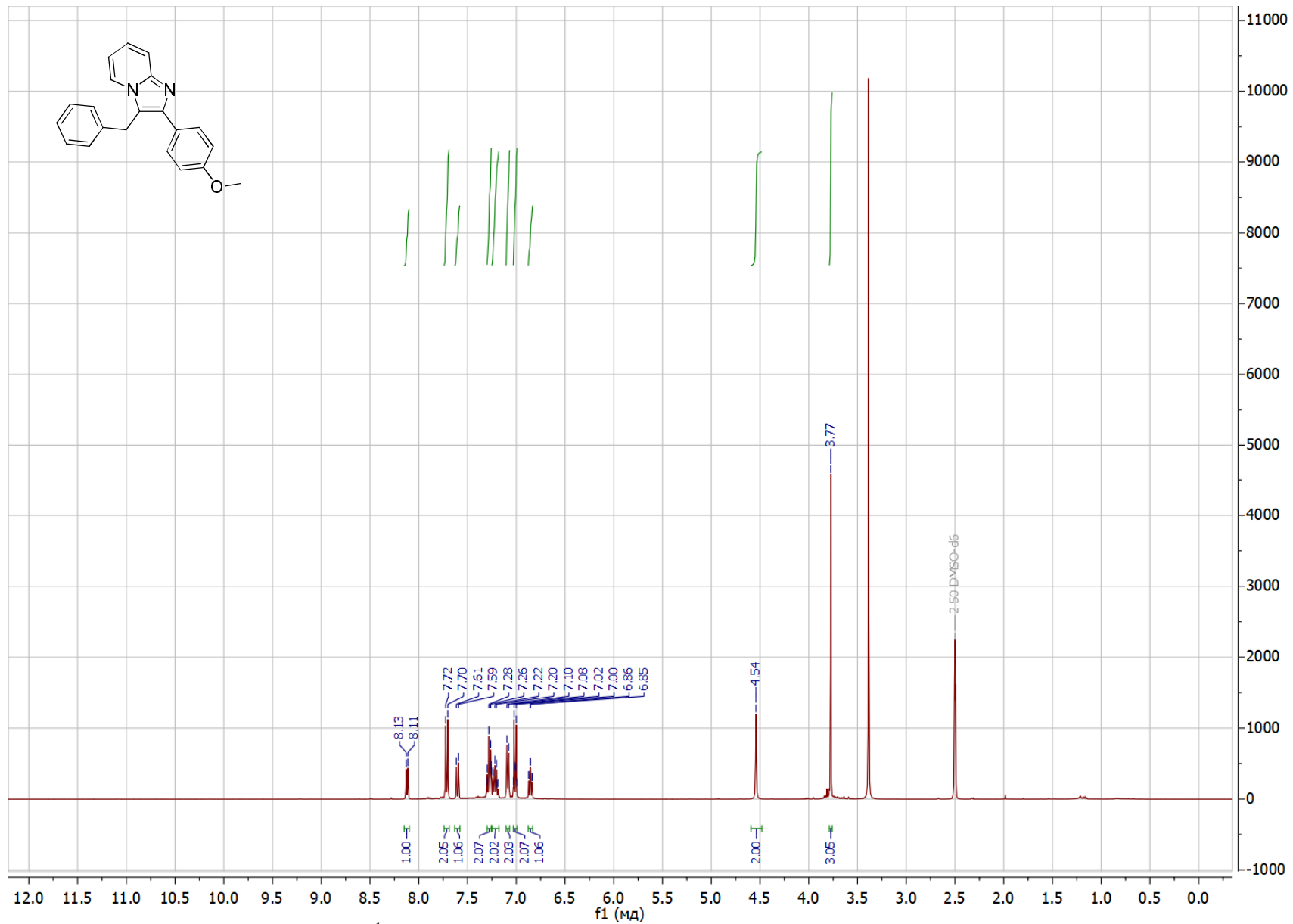


Figure S29. <sup>1</sup>H NMR spectrum of imidazo[1,2-*a*]pyridine **10caa** in DMSO-*d*<sub>6</sub> (400 MHz)

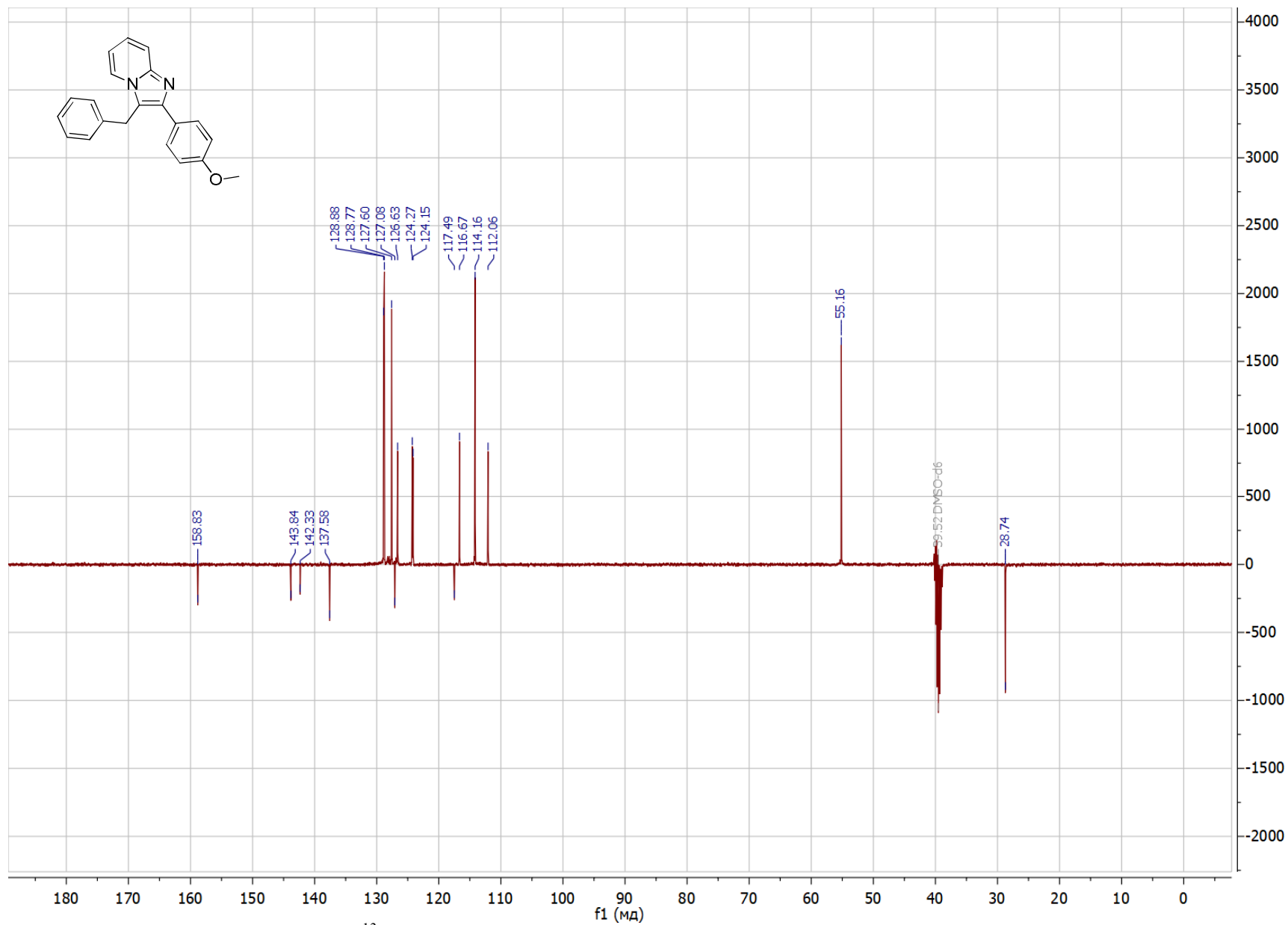


Figure S30.  $^{13}\text{C}$  NMR spectrum of imidazo[1,2-*a*]pyridine **10caa** in  $\text{DMSO-}d_6$  (101 MHz)

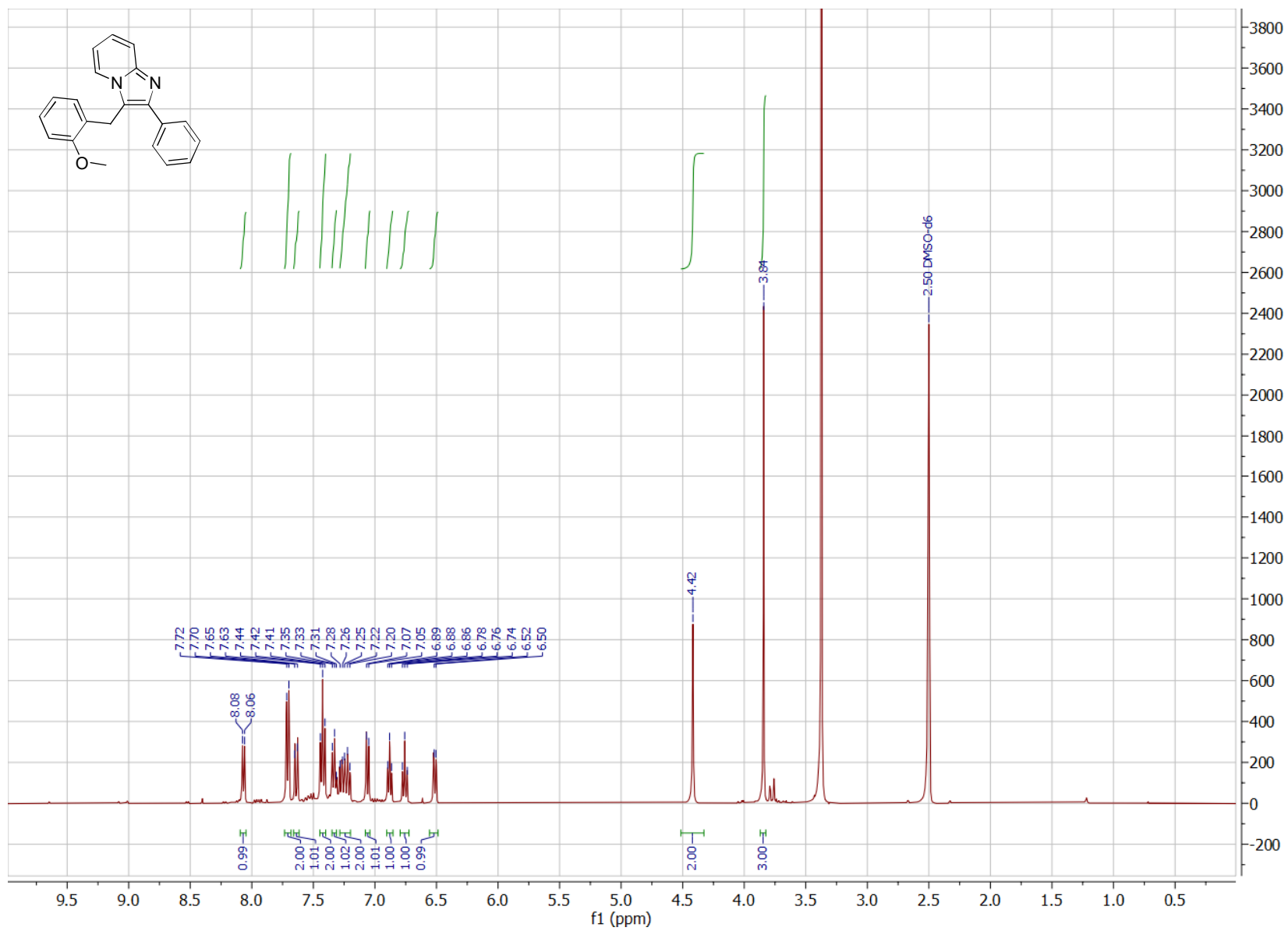


Figure S31. <sup>1</sup>H NMR spectrum of imidazo[1,2-*a*]pyridine **10ga** in DMSO-*d*<sub>6</sub> (400 MHz)



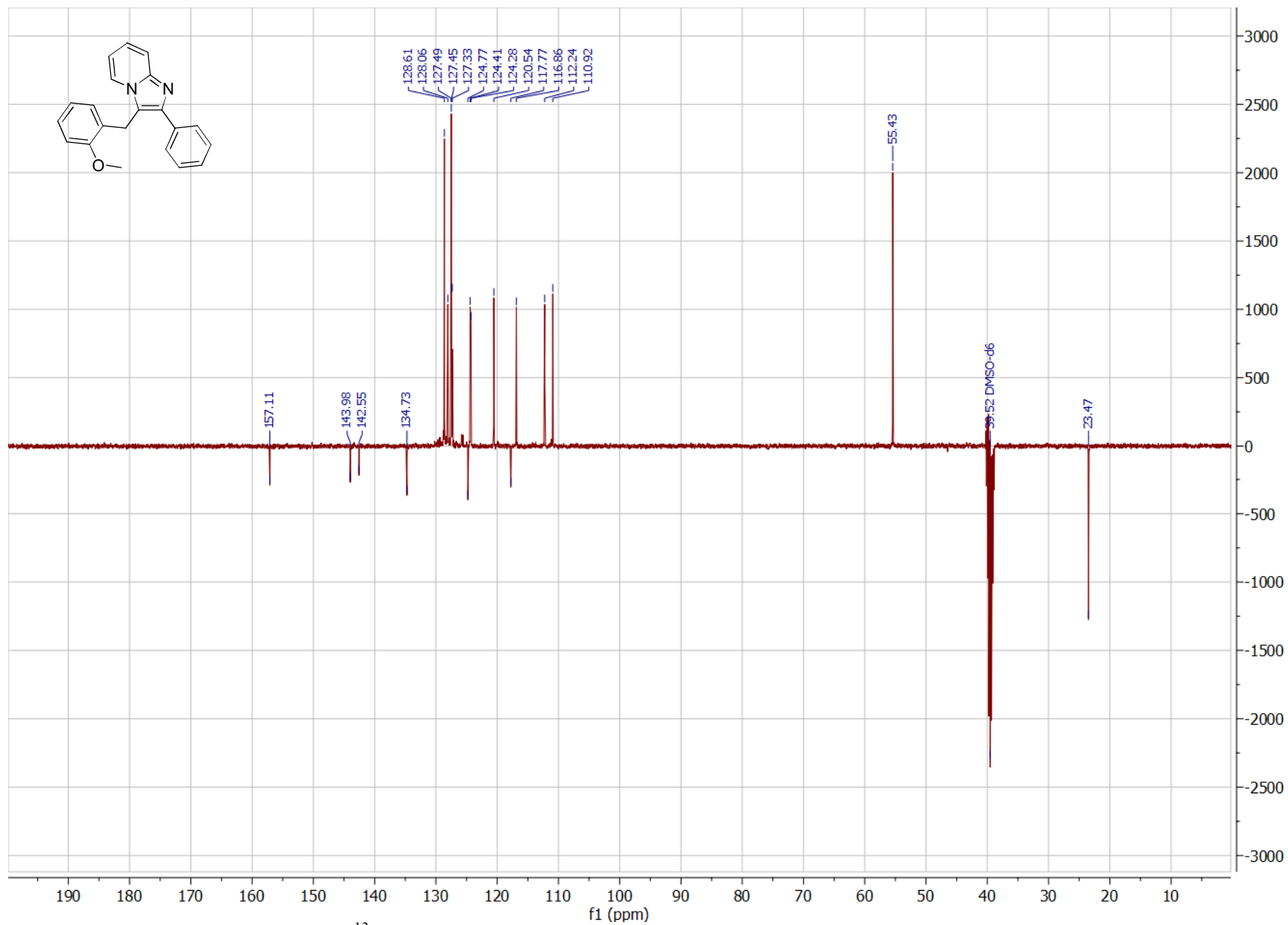


Figure S32.  $^{13}\text{C}$  NMR spectrum of imidazo[1,2-*a*]pyridine **10aga** in  $\text{DMSO-}d_6$  (101 MHz)

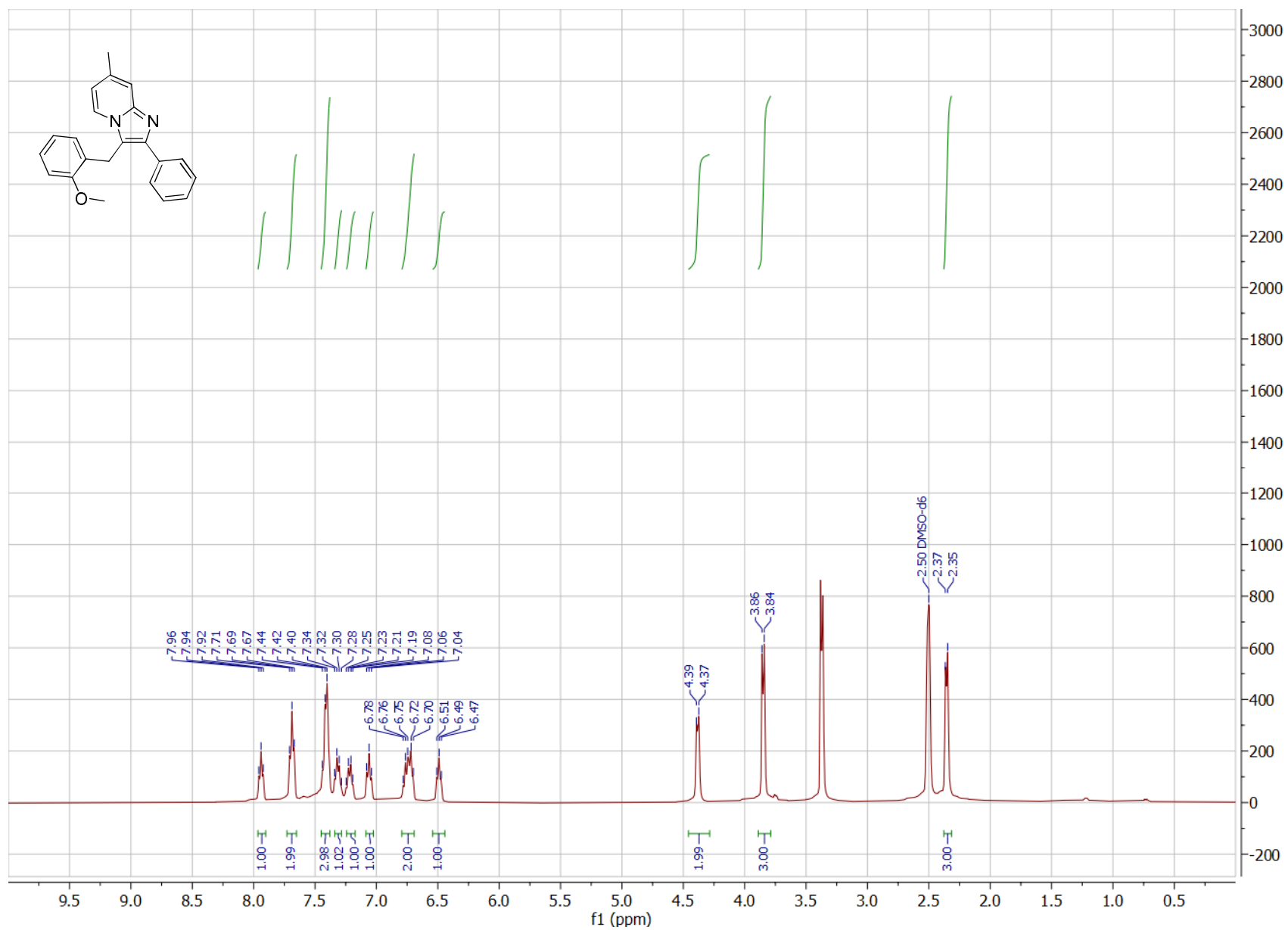


Figure S33. <sup>1</sup>H NMR spectrum of imidazo[1,2-*a*]pyridine **10agb** in DMSO-*d*<sub>6</sub> (400 MHz)

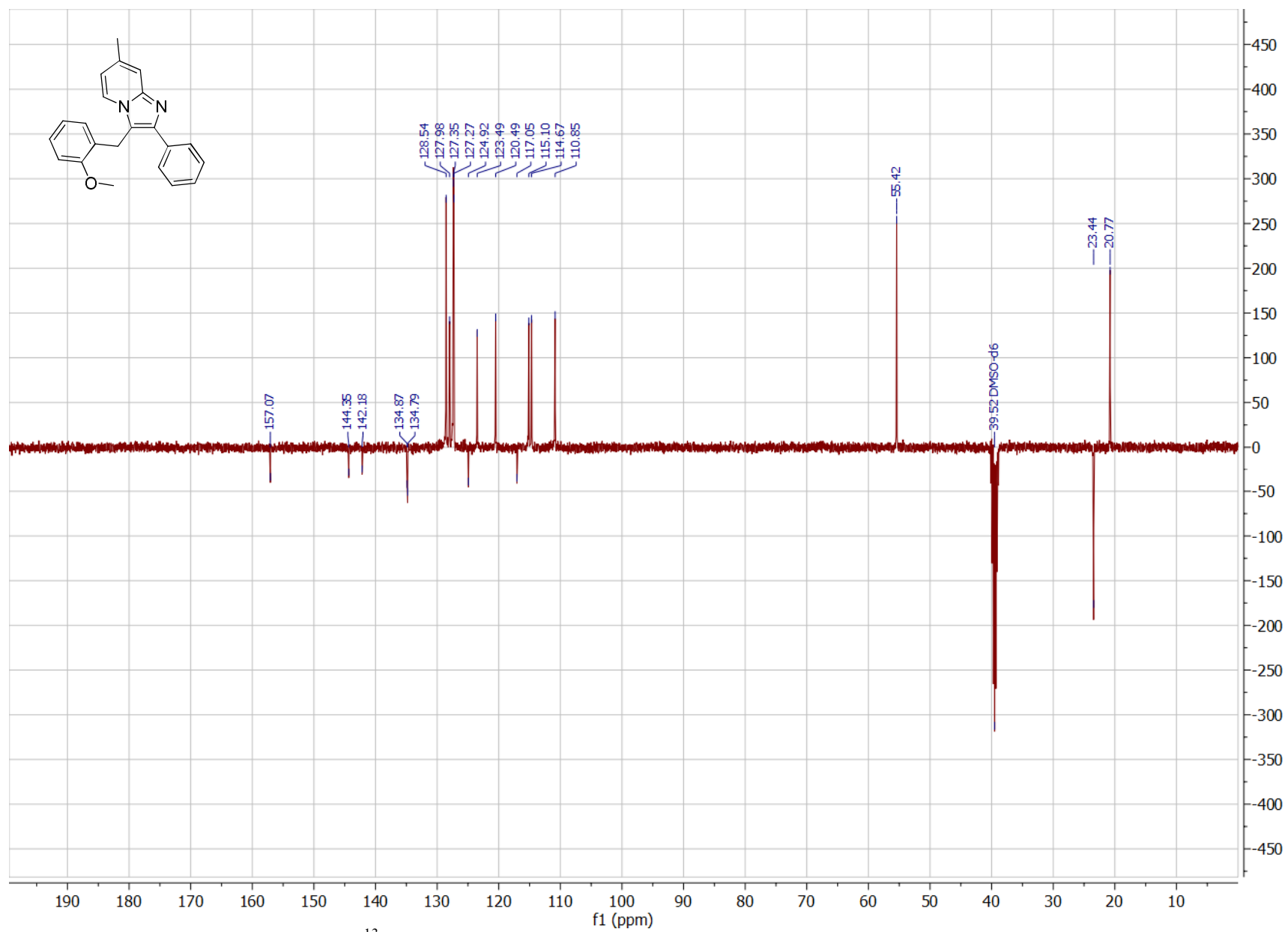


Figure S34.  $^{13}\text{C}$  NMR spectrum of imidazo[1,2-*a*]pyridine **10agb** in  $\text{DMSO-}d_6$  (101 MHz)

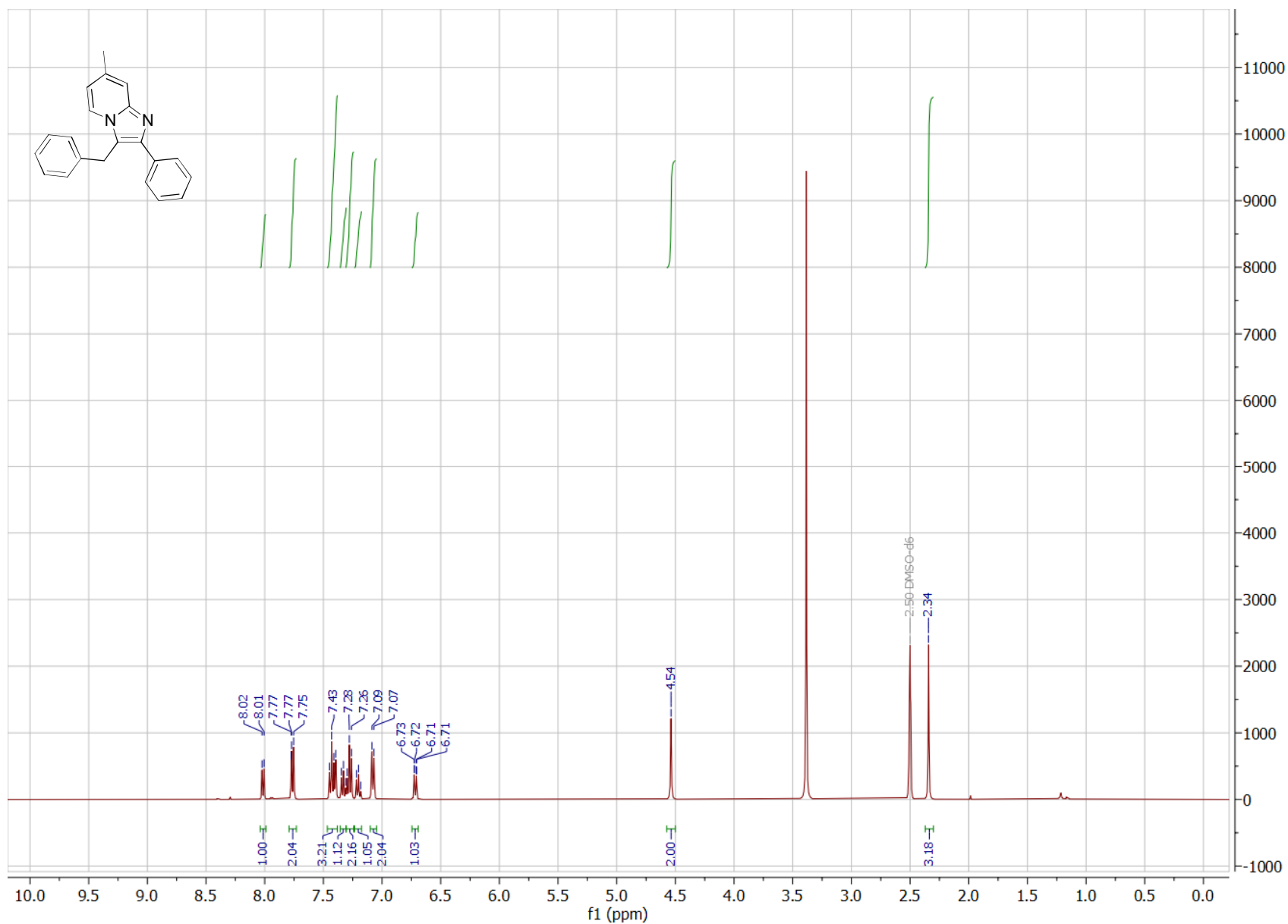


Figure S35. <sup>1</sup>H NMR spectrum of imidazo[1,2-*a*]pyridine **10aab** in DMSO-*d*<sub>6</sub> (400 MHz)

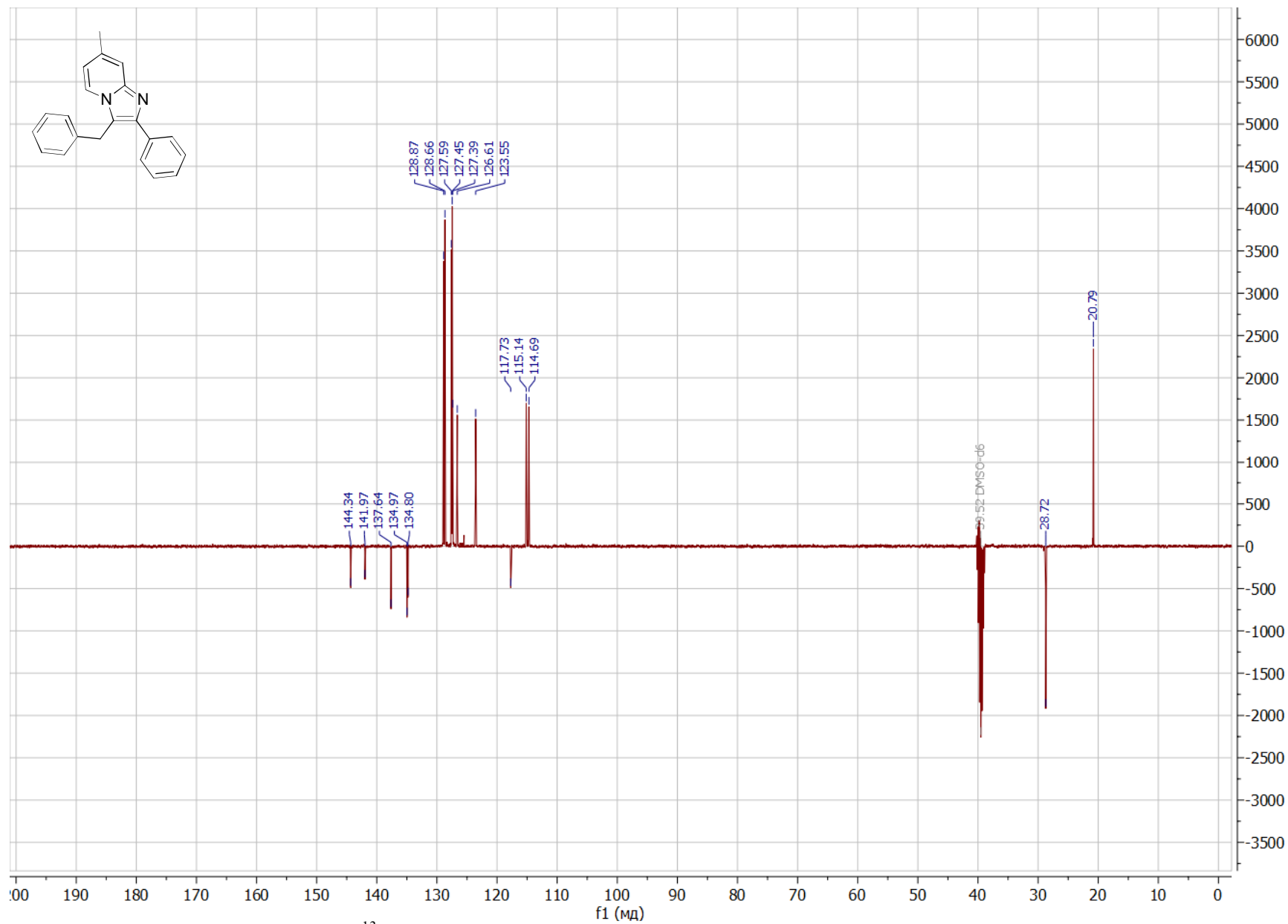


Figure S36.  $^{13}\text{C}$  NMR spectrum of imidazo[1,2-*a*]pyridine **10aab** in DMSO- $d_6$  (101 MHz)

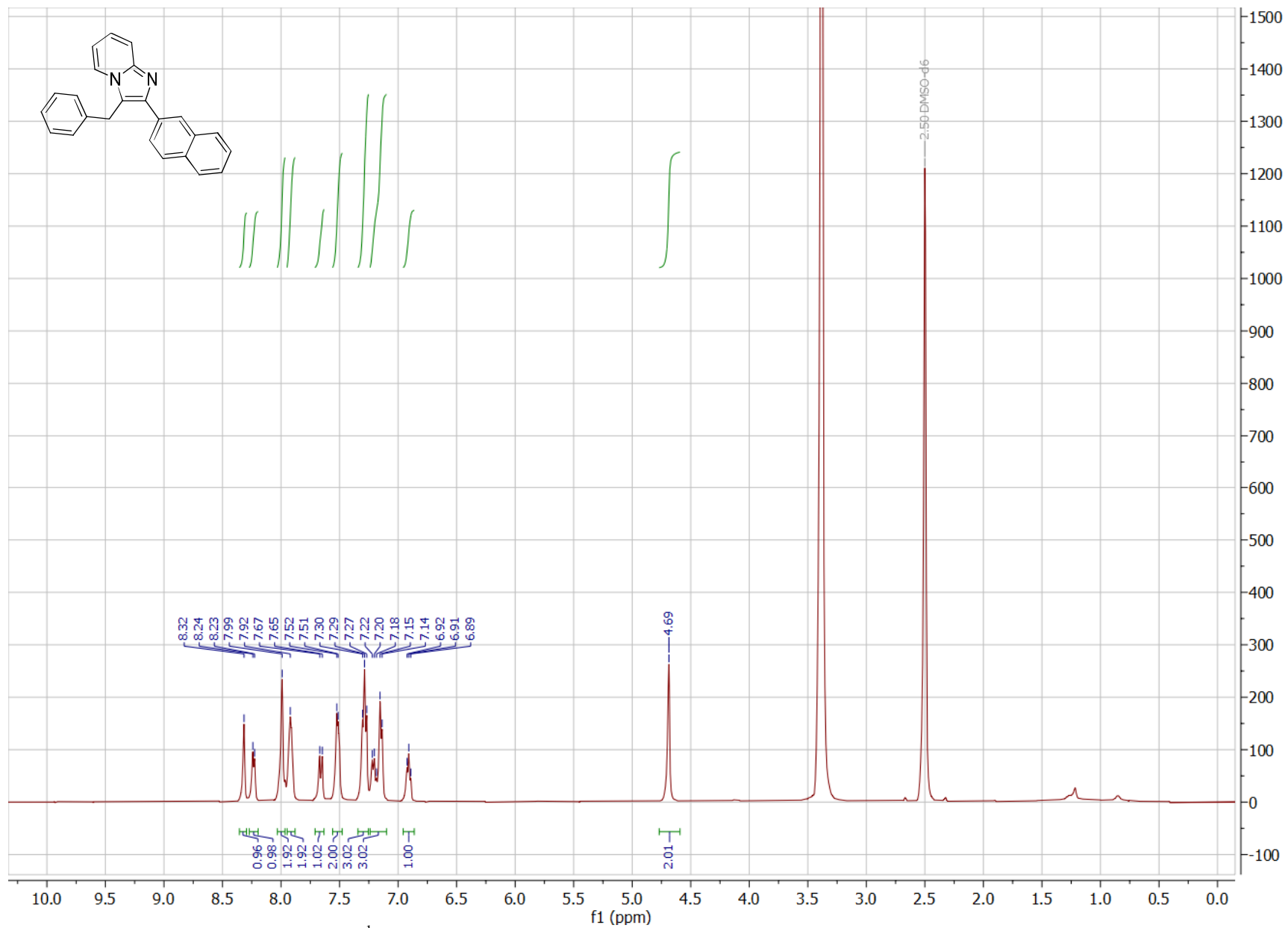


Figure S37. <sup>1</sup>H NMR spectrum of imidazo[1,2-*a*]pyridine **10daa** in DMSO-*d*<sub>6</sub> (400 MHz)

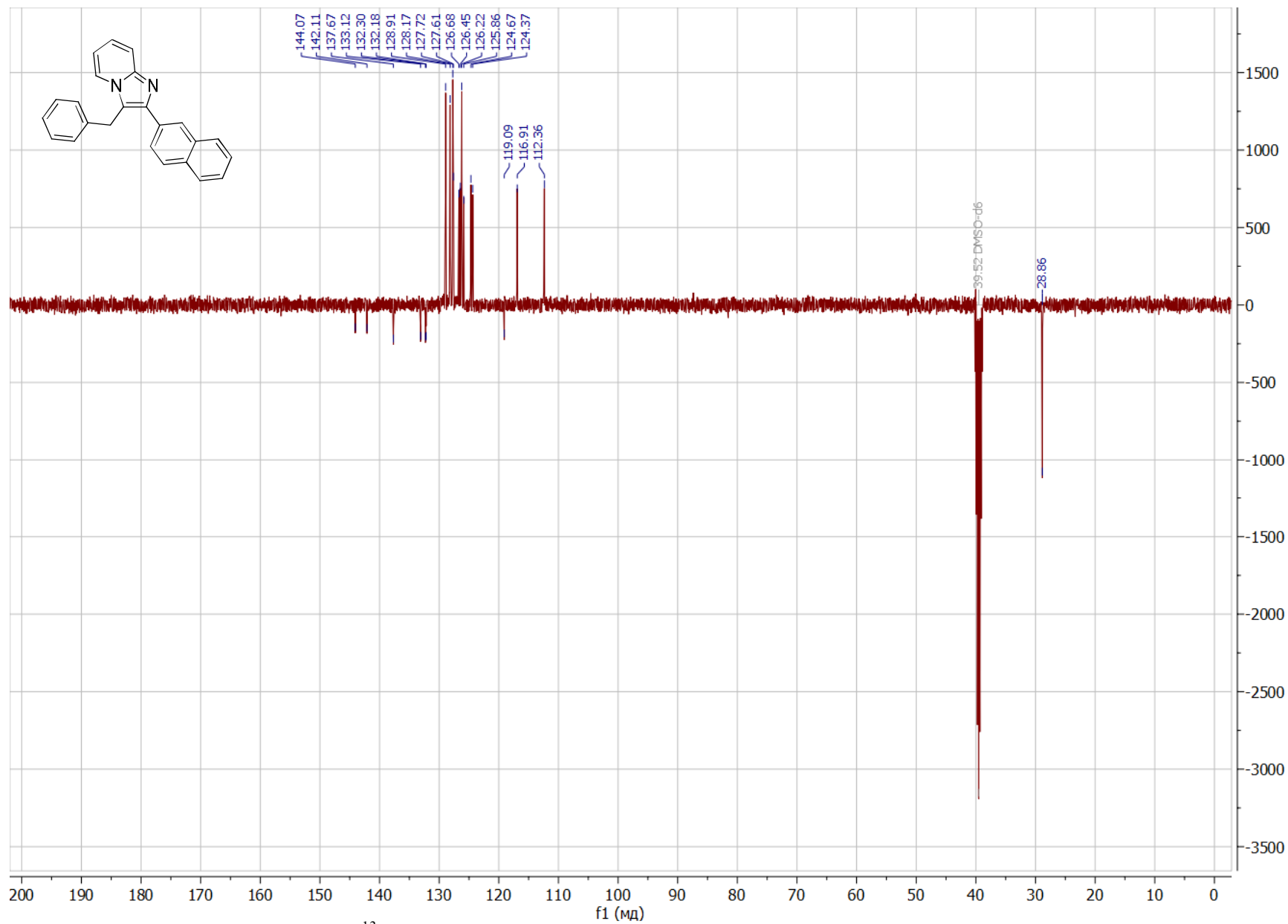


Figure S38.  $^{13}\text{C}$  NMR spectrum of imidazo[1,2-*a*]pyridine **10daa** in  $\text{DMSO-}d_6$  (101 MHz)

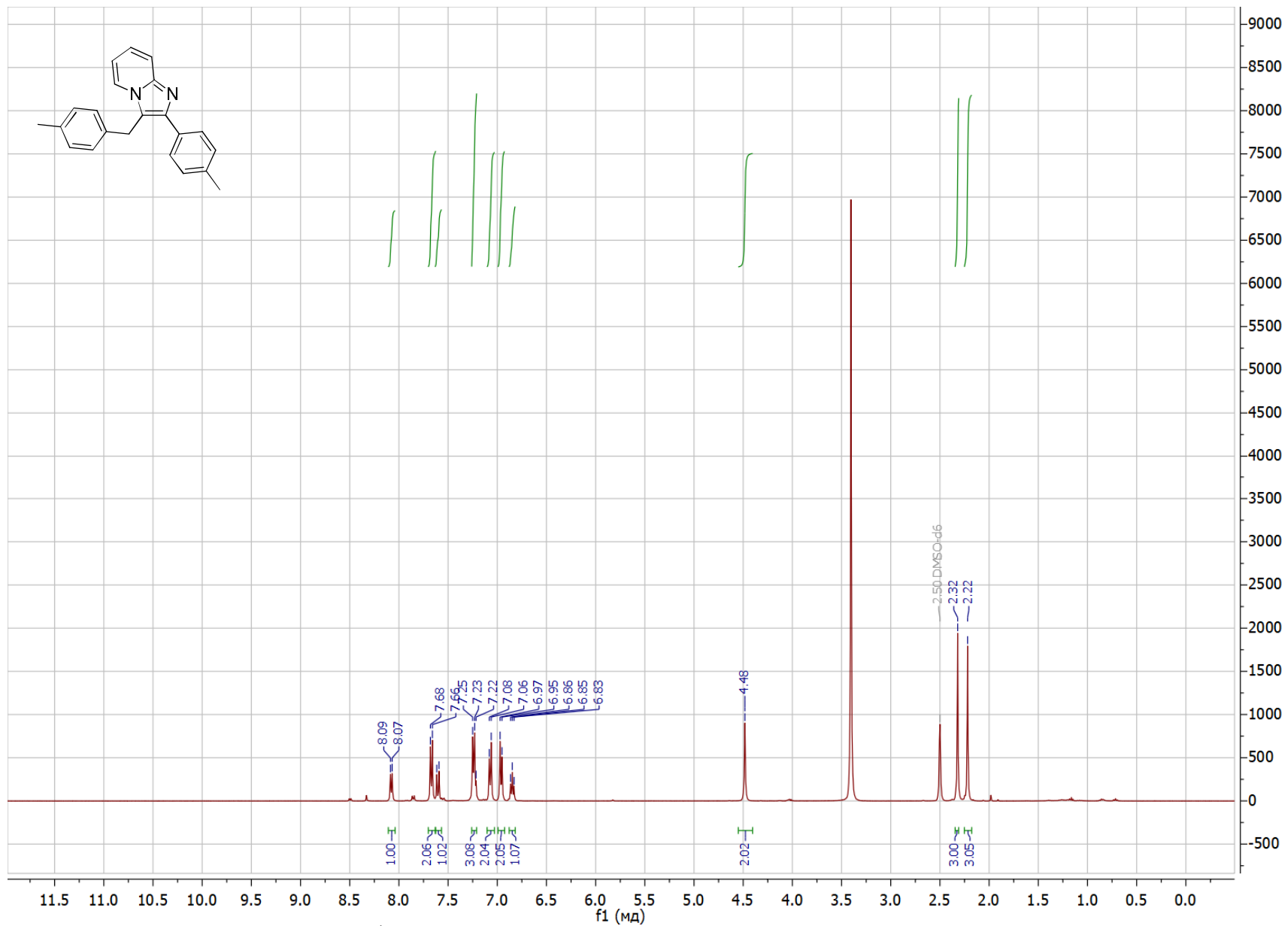


Figure S39. <sup>1</sup>H NMR spectrum of imidazo[1,2-a]pyridine **10bea** in DMSO-*d*<sub>6</sub> (400 MHz)



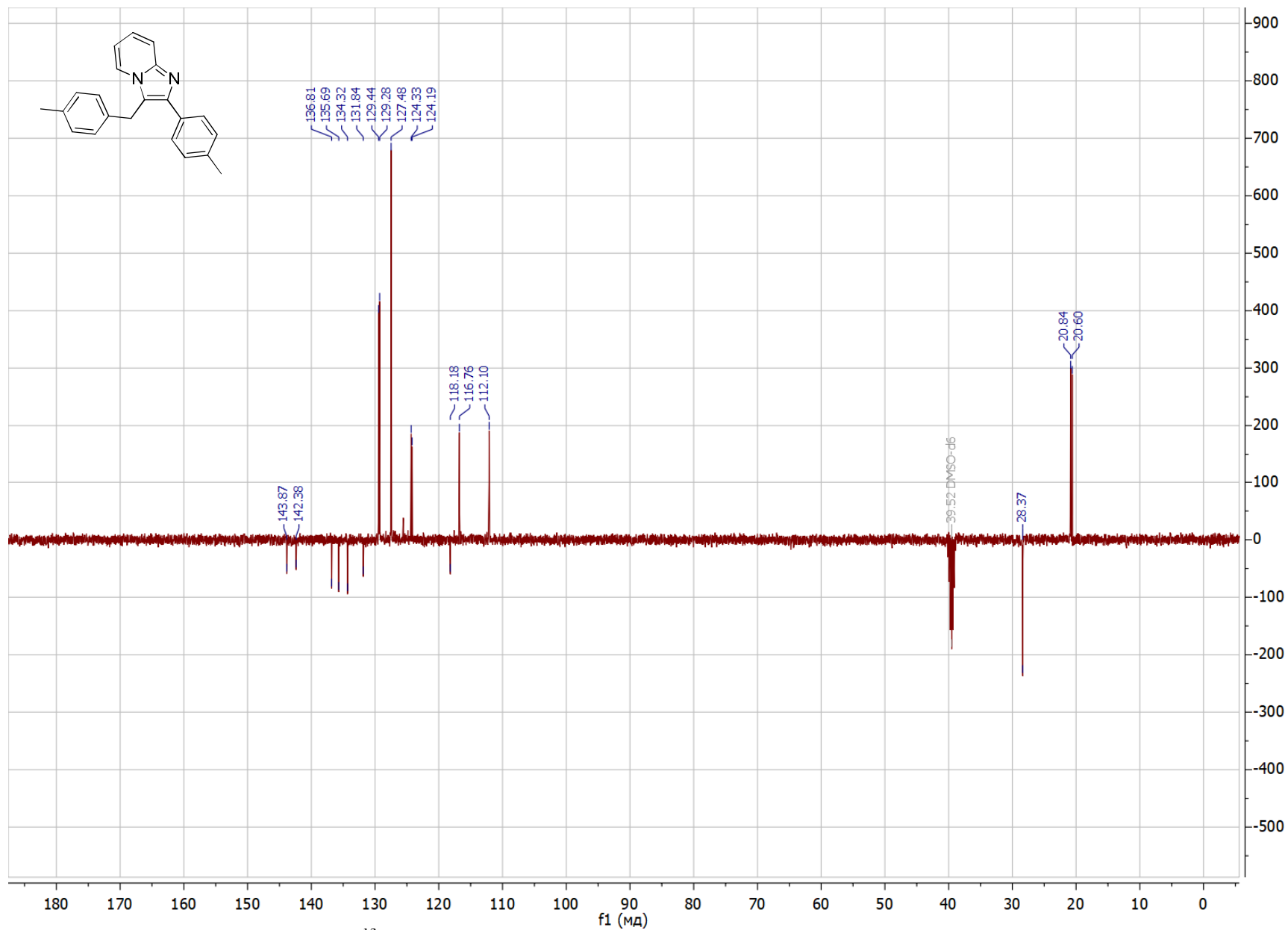


Figure S40.  $^{13}\text{C}$  NMR spectrum of imidazo[1,2-*a*]pyridine **10bea** in DMSO- $d_6$  (101 MHz)

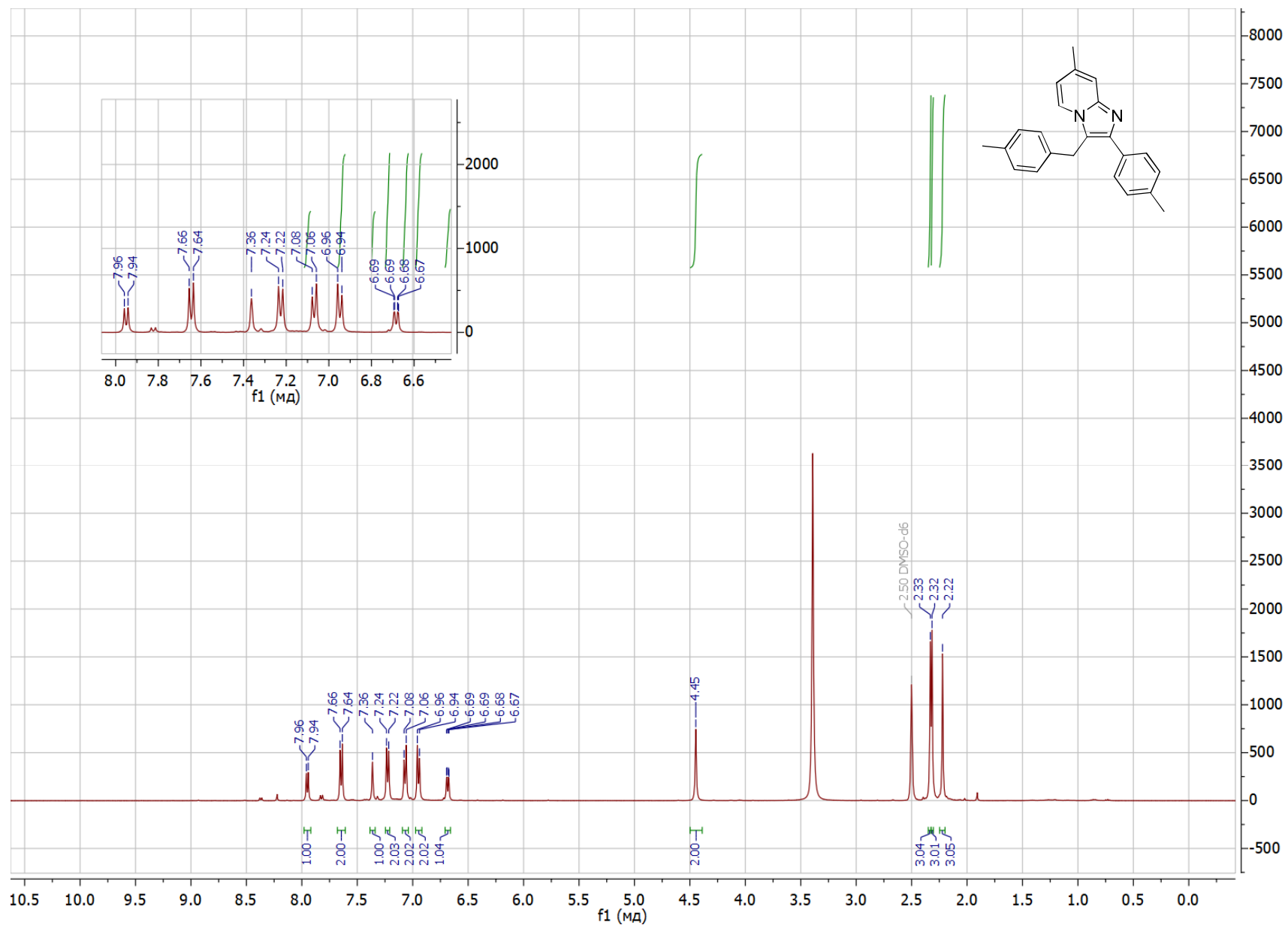


Figure S41. <sup>1</sup>H NMR spectrum of imidazo[1,2-*a*]pyridine **10beb** in DMSO-*d*<sub>6</sub> (400 MHz)

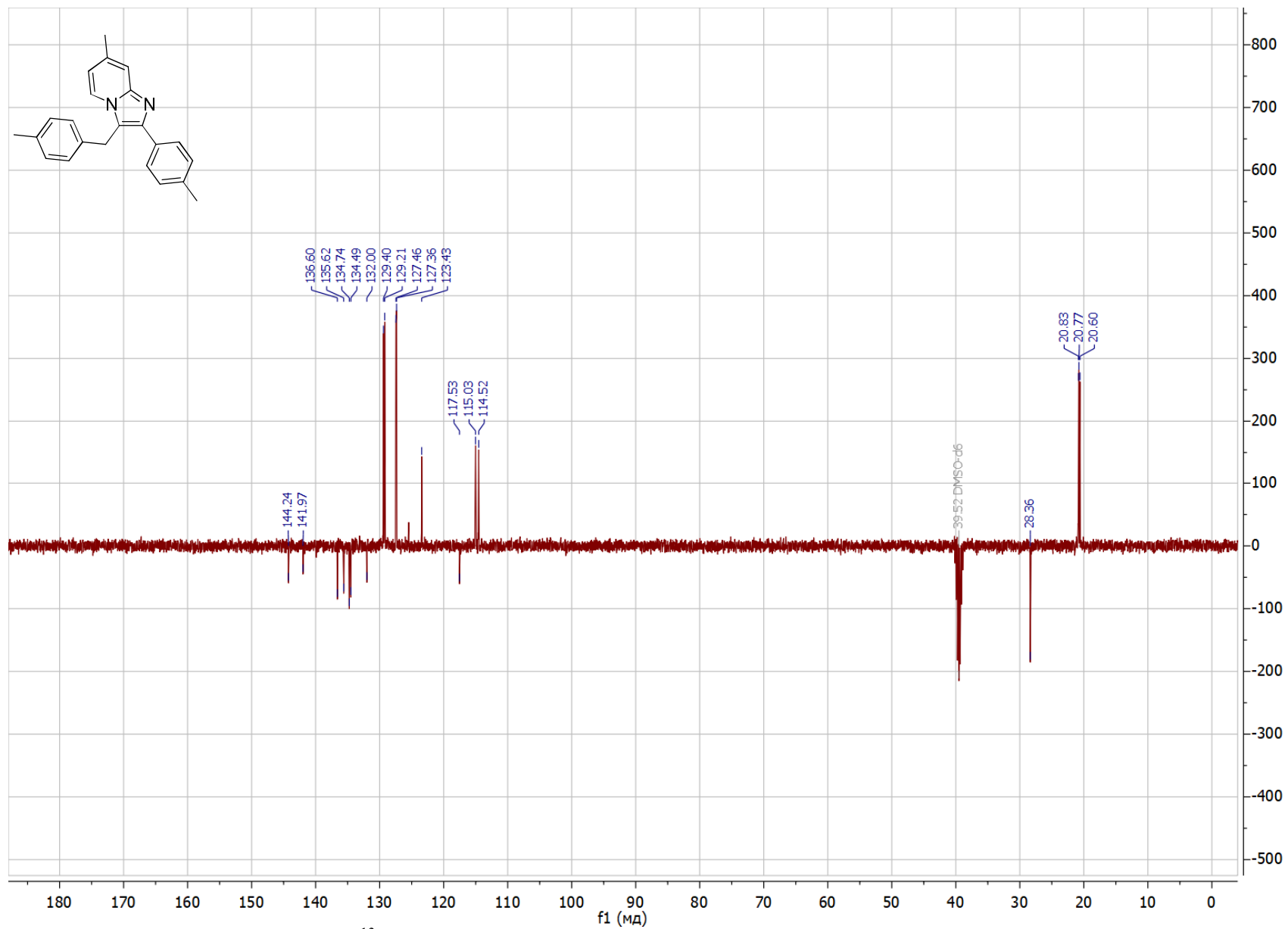


Figure S42.  $^{13}\text{C}$  NMR spectrum of imidazo[1,2-*a*]pyridine **10beb** in DMSO- $d_6$  (101 MHz)

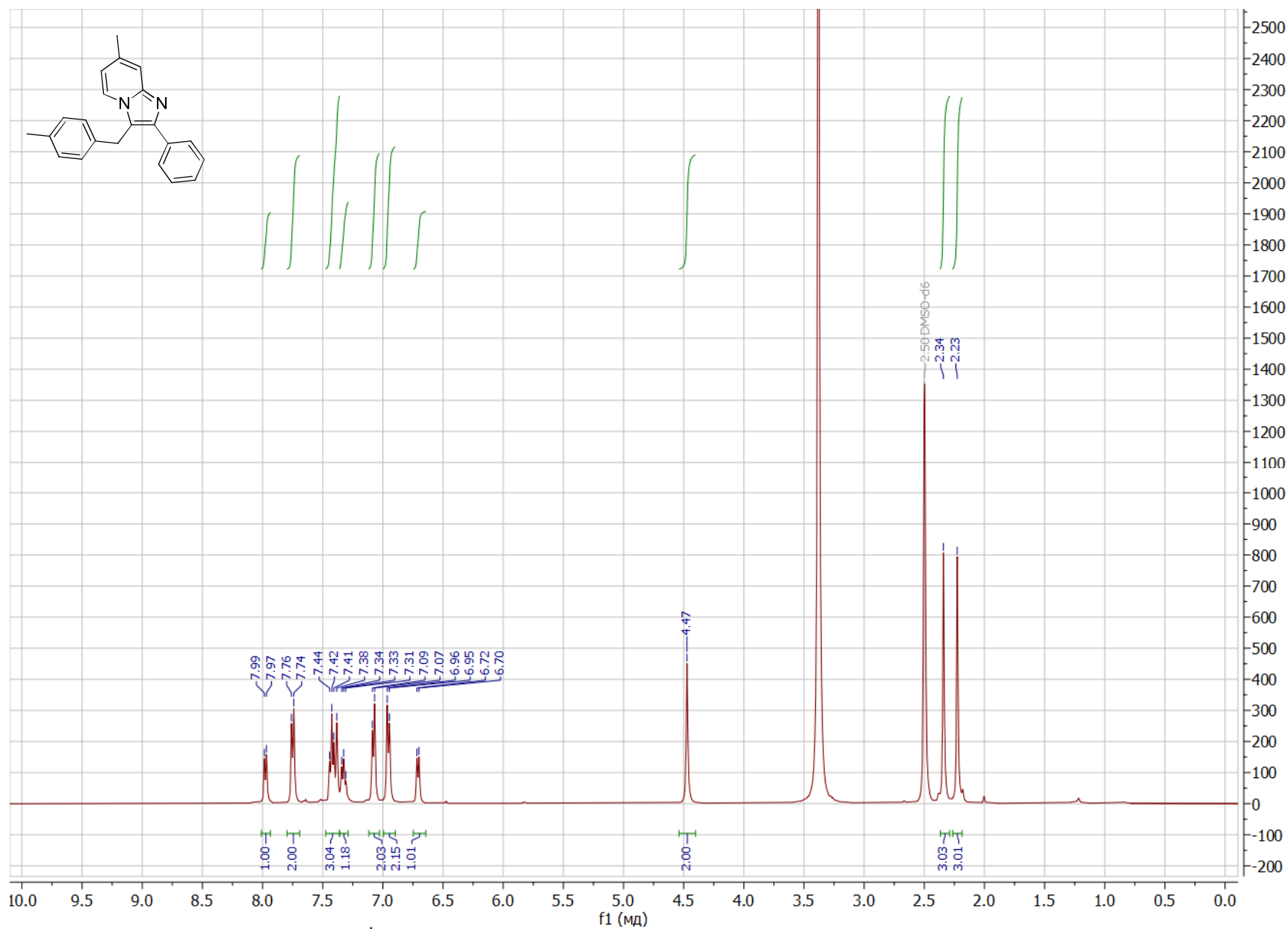


Figure S43. <sup>1</sup>H NMR spectrum of imidazo[1,2-*a*]pyridine **10aeb** in DMSO-*d*<sub>6</sub> (400 MHz)

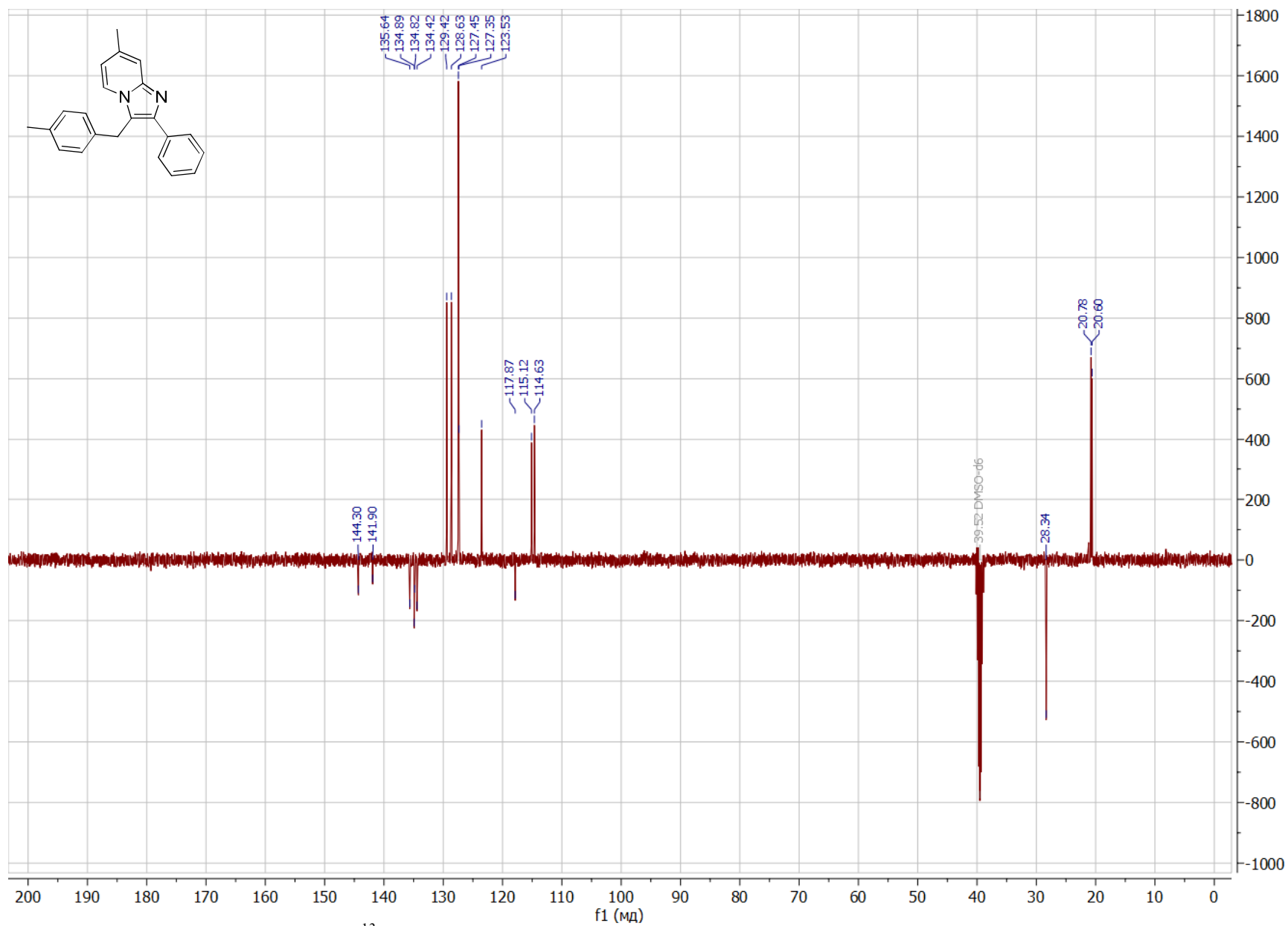


Figure S44.  $^{13}\text{C}$  NMR spectrum of imidazo[1,2-*a*]pyridine **10aeb** in DMSO- $d_6$  (101 MHz)

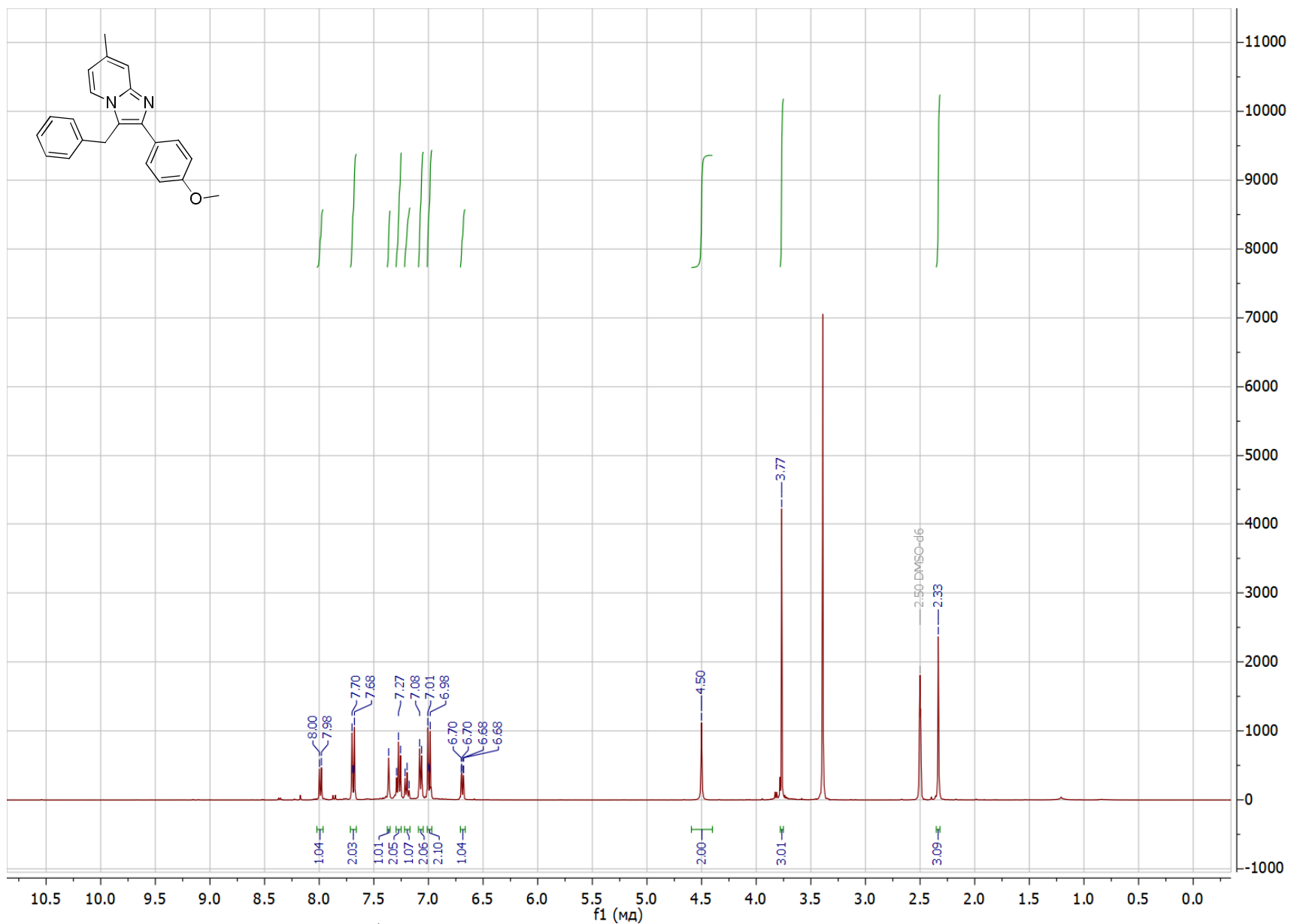


Figure S45. <sup>1</sup>H NMR spectrum of imidazo[1,2-*a*]pyridine **10cab** in DMSO-*d*<sub>6</sub> (400 MHz)

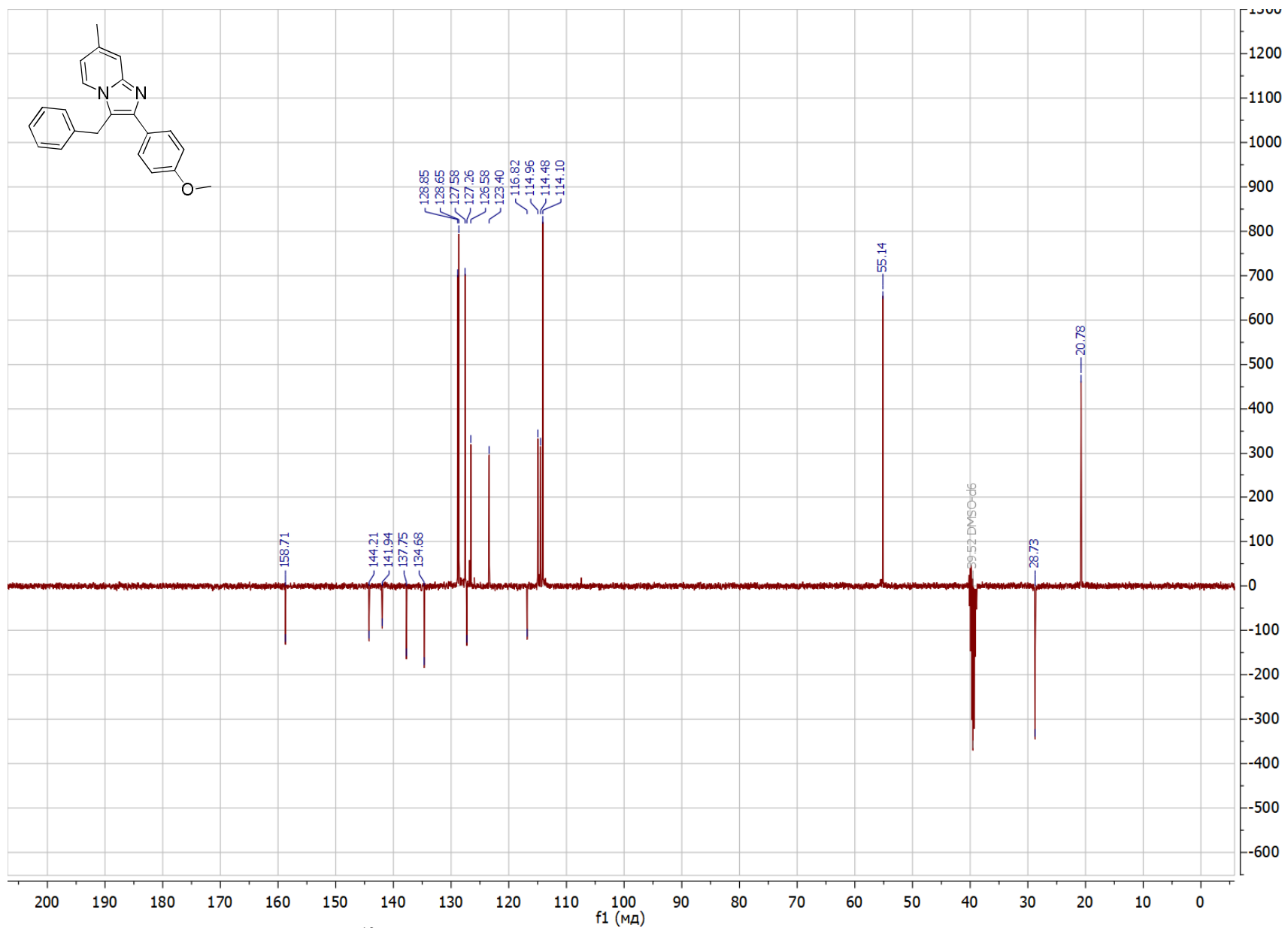


Figure S46. <sup>13</sup>C NMR spectrum of imidazo[1,2-*a*]pyridine **10cab** in DMSO-*d*<sub>6</sub> (101 MHz)

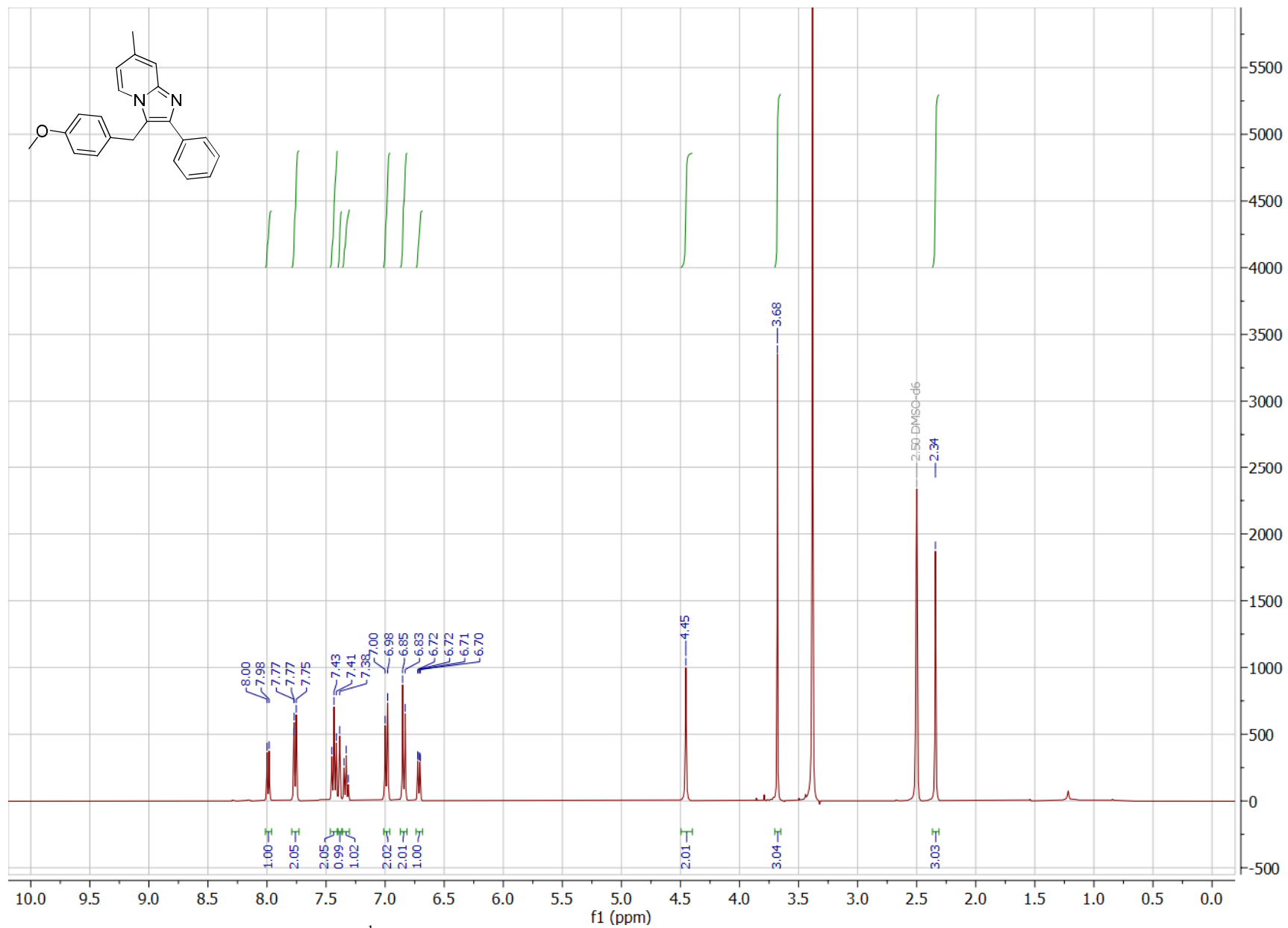


Figure S47. <sup>1</sup>H NMR spectrum of imidazo[1,2-*a*]pyridine **10afb** in DMSO-*d*<sub>6</sub> (400 MHz)



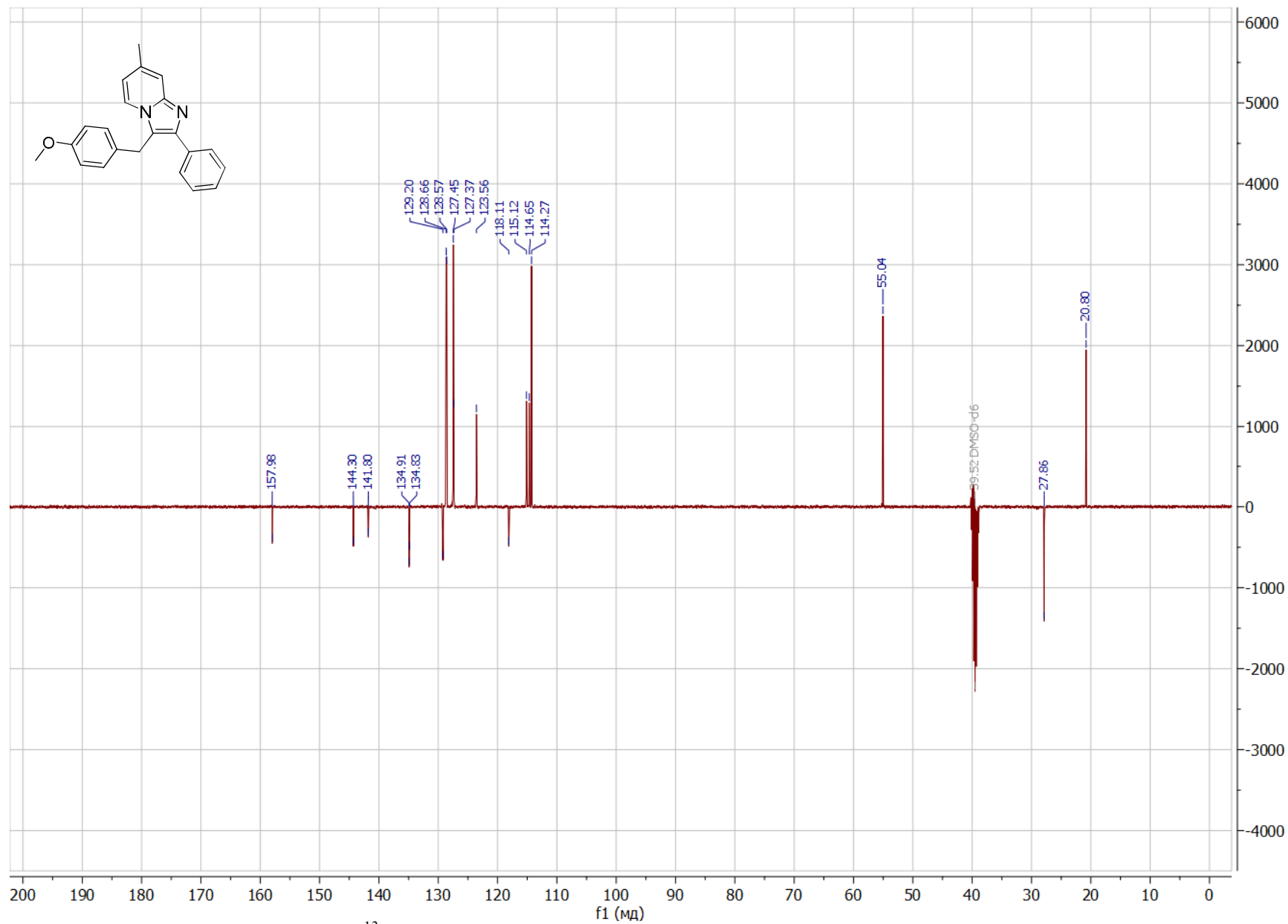


Figure S48. <sup>13</sup>C NMR spectrum of imidazo[1,2-*a*]pyridine **10afb** in DMSO-*d*<sub>6</sub> (101 MHz)

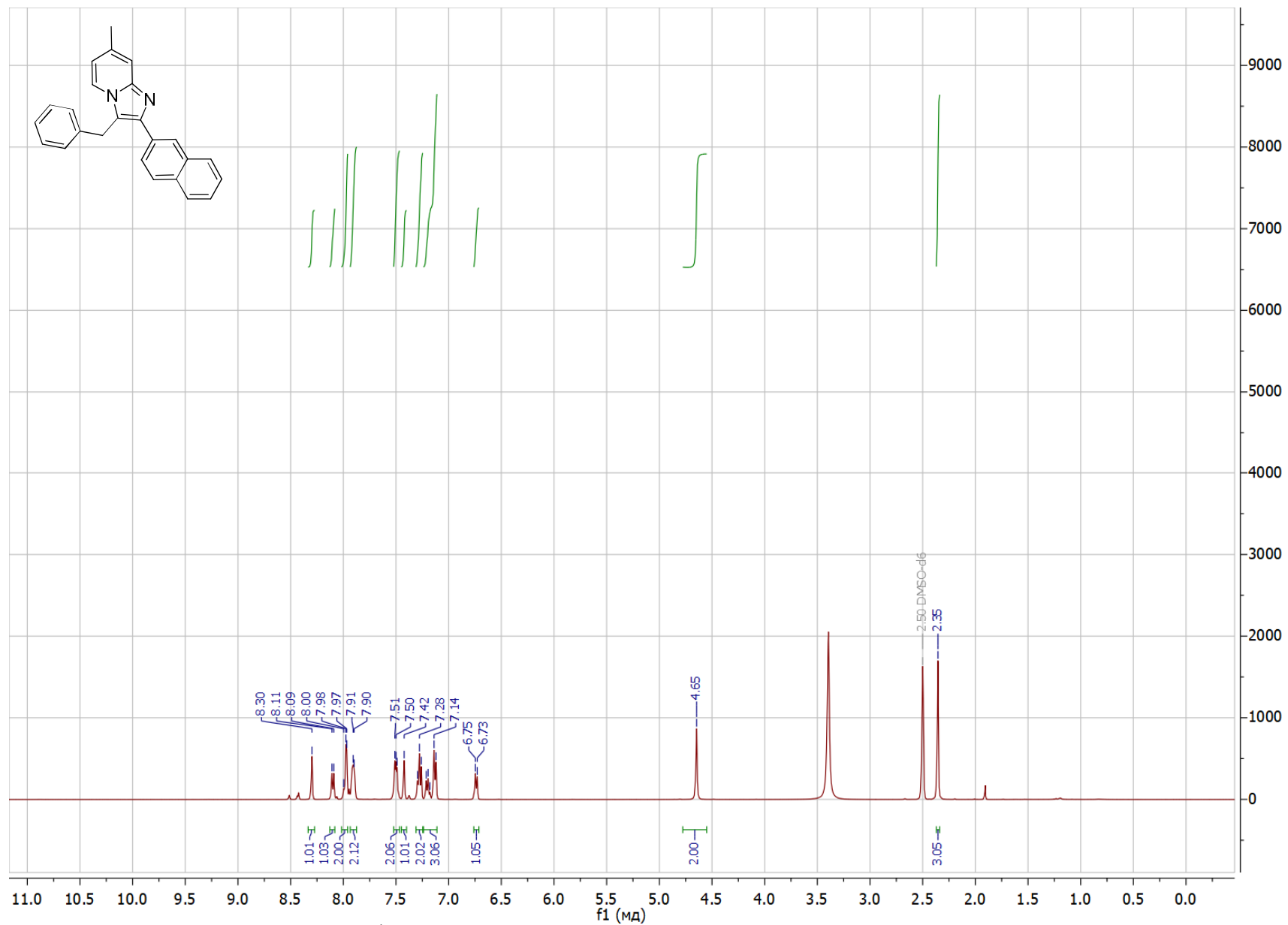


Figure S49.  $^1\text{H}$  NMR spectrum of imidazo[1,2-*a*]pyridine **10dab** in  $\text{DMSO}-d_6$  (400 MHz)

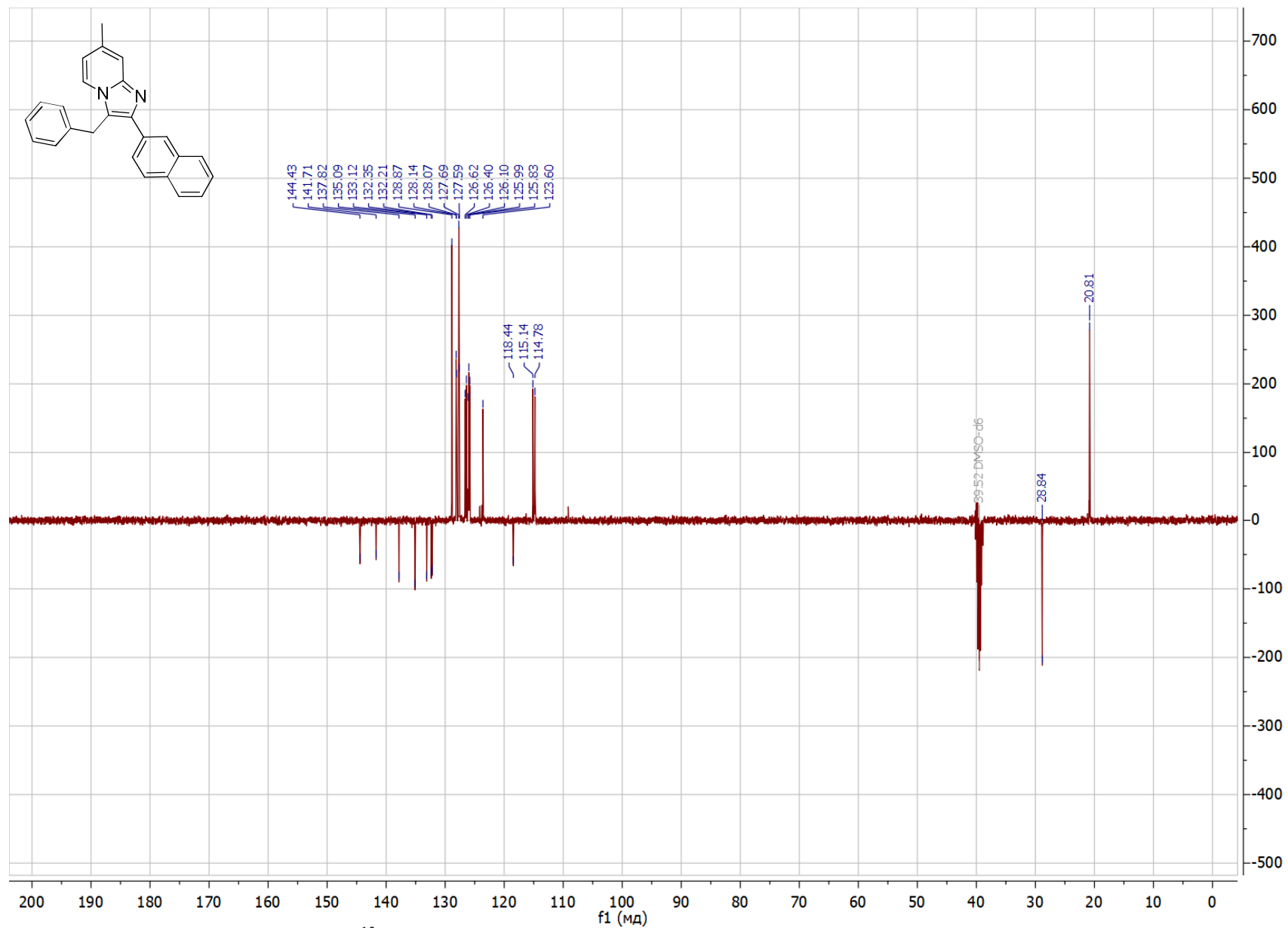


Figure S50.  $^{13}\text{C}$  NMR spectrum of imidazo[1,2-*a*]pyridine **10dab** in DMSO- $d_6$  (101 MHz)

**<sup>1</sup>H and <sup>13</sup>C NMR spectral charts for 3,5-diphenyl-3H-pyrrol-2-one 15aa**

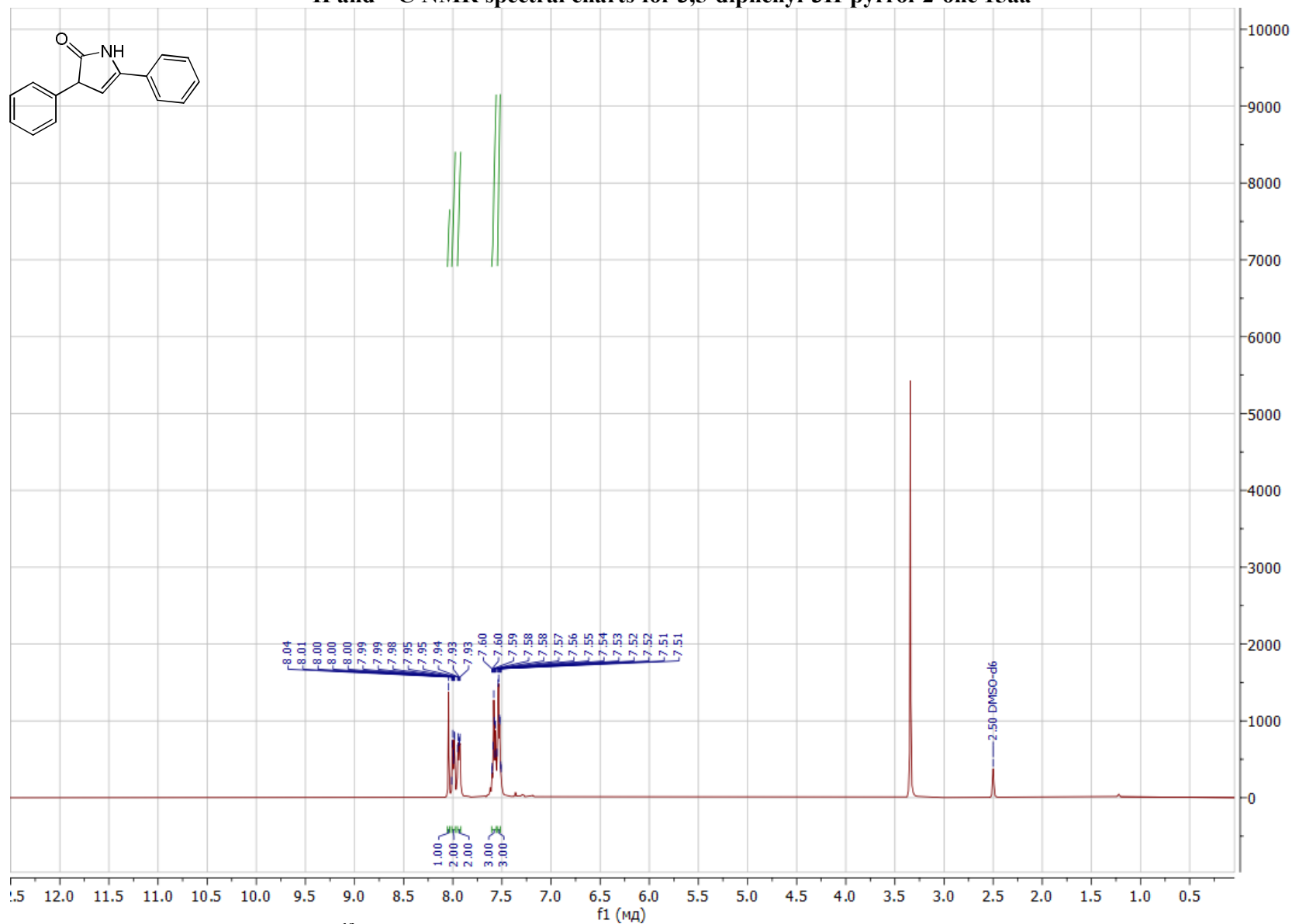


Figure S51. <sup>13</sup>C NMR spectrum of 3,5-diphenyl-3H-pyrrol-2-one **15aa** in DMSO-*d*<sub>6</sub> (101 MHz)

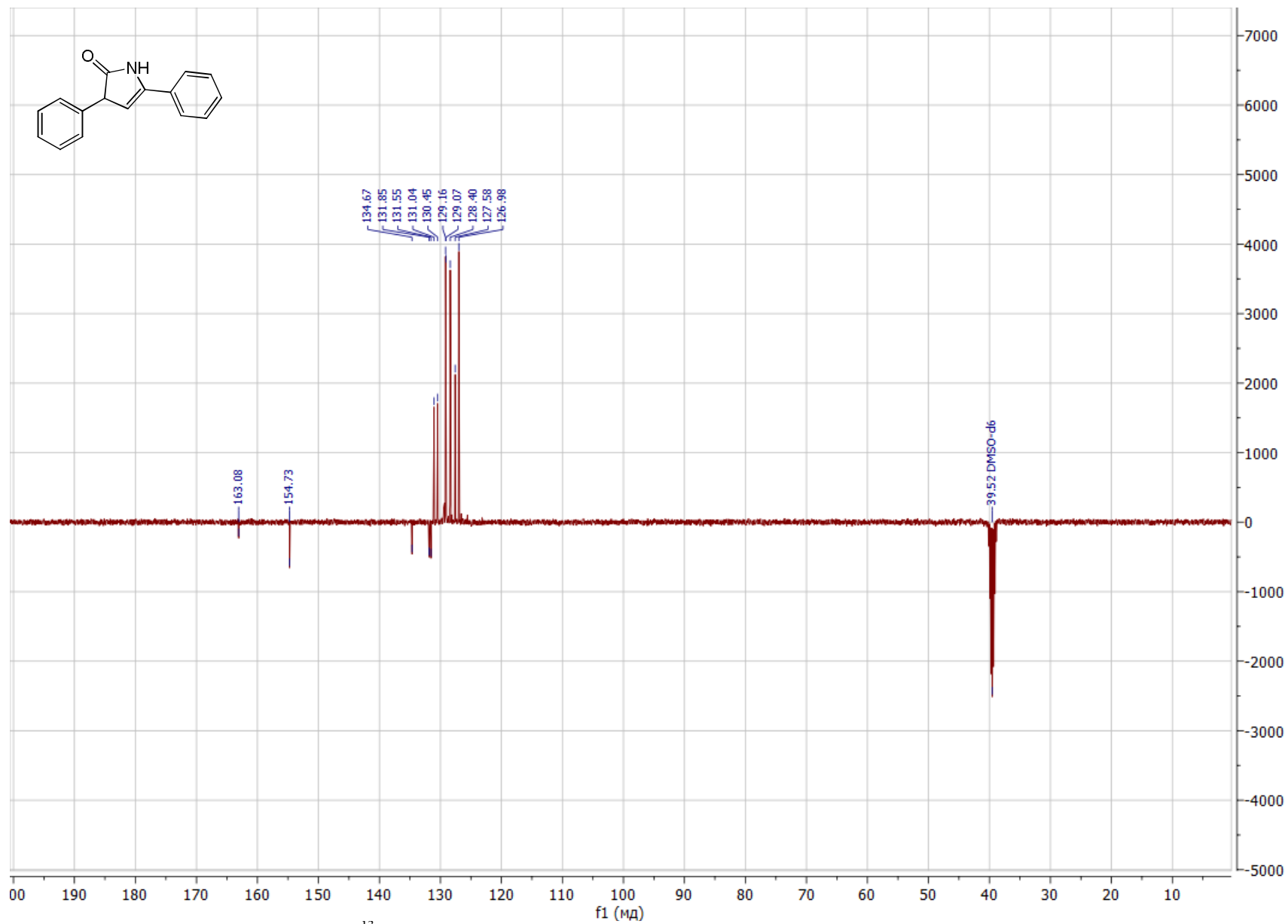


Figure S52.  $^{13}\text{C}$  NMR spectrum 3,5-diphenyl-3H-pyrrol-2-one **15aa** in  $\text{DMSO-}d_6$  (101 MHz)

<sup>1</sup>H and <sup>13</sup>C NMR spectral charts for *N*-(2-aminophenyl)-2-phenylacetamide **16aa**

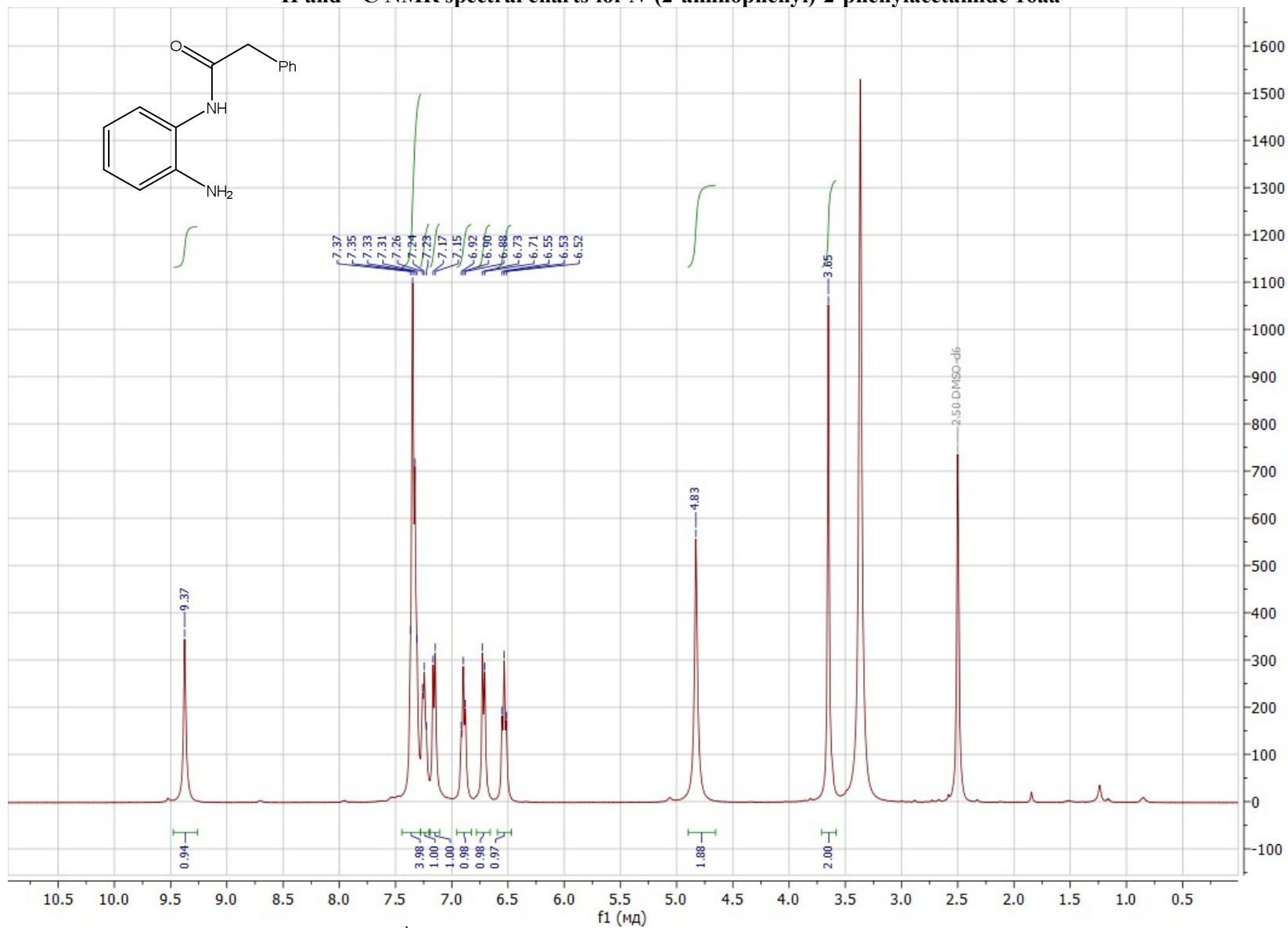


Figure S53. <sup>1</sup>H NMR spectrum of phenylacetamide **16aa** in DMSO-*d*<sub>6</sub> (400 MHz)

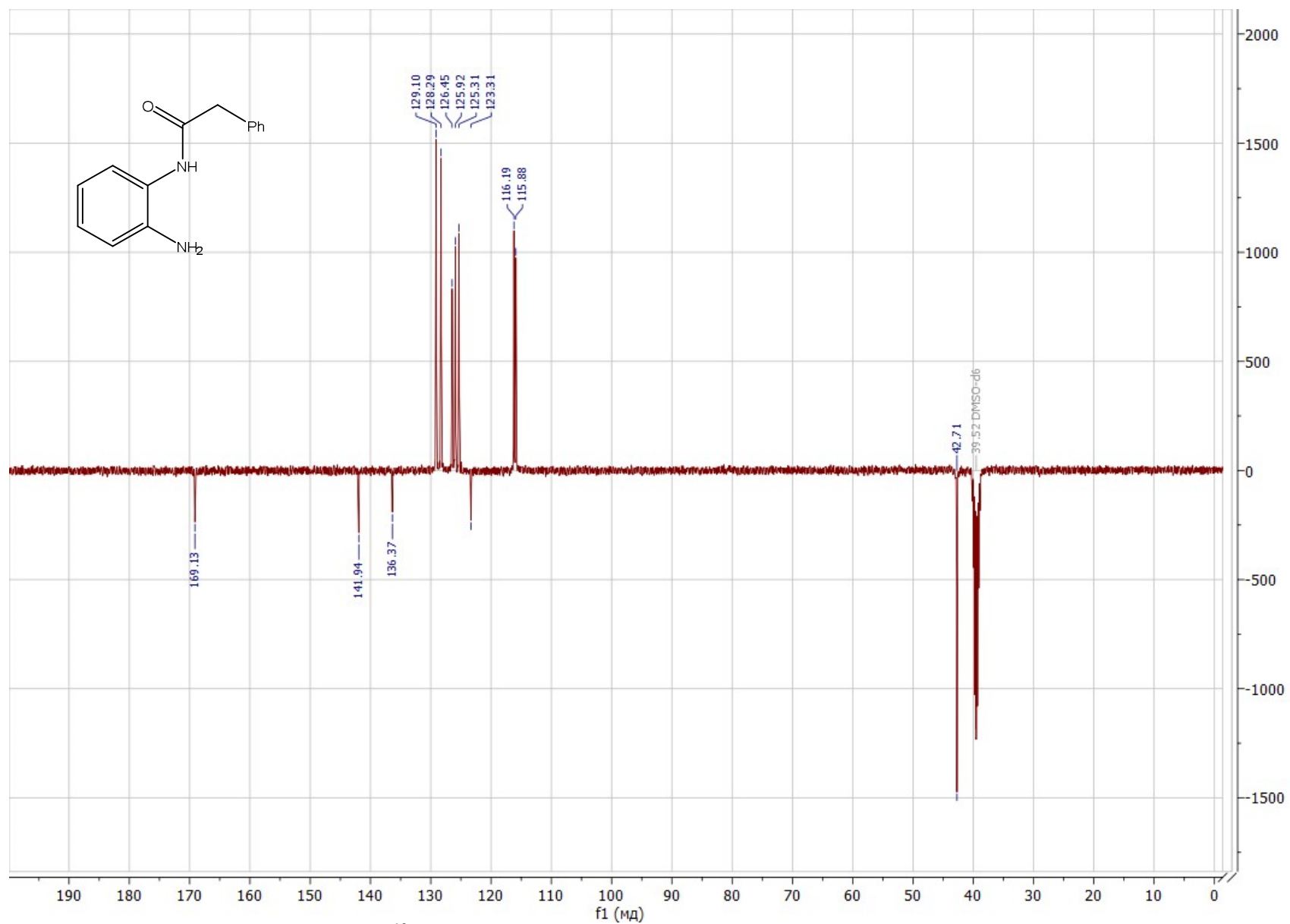


Figure S54.  $^{13}\text{C}$  NMR spectrum of phenylacetamide **16aa** in  $\text{DMSO-}d_6$  (101 MHz)

<sup>1</sup>H and <sup>13</sup>C NMR spectral charts for 2-Benzyl-1H-benzo[d]imidazole 17aa

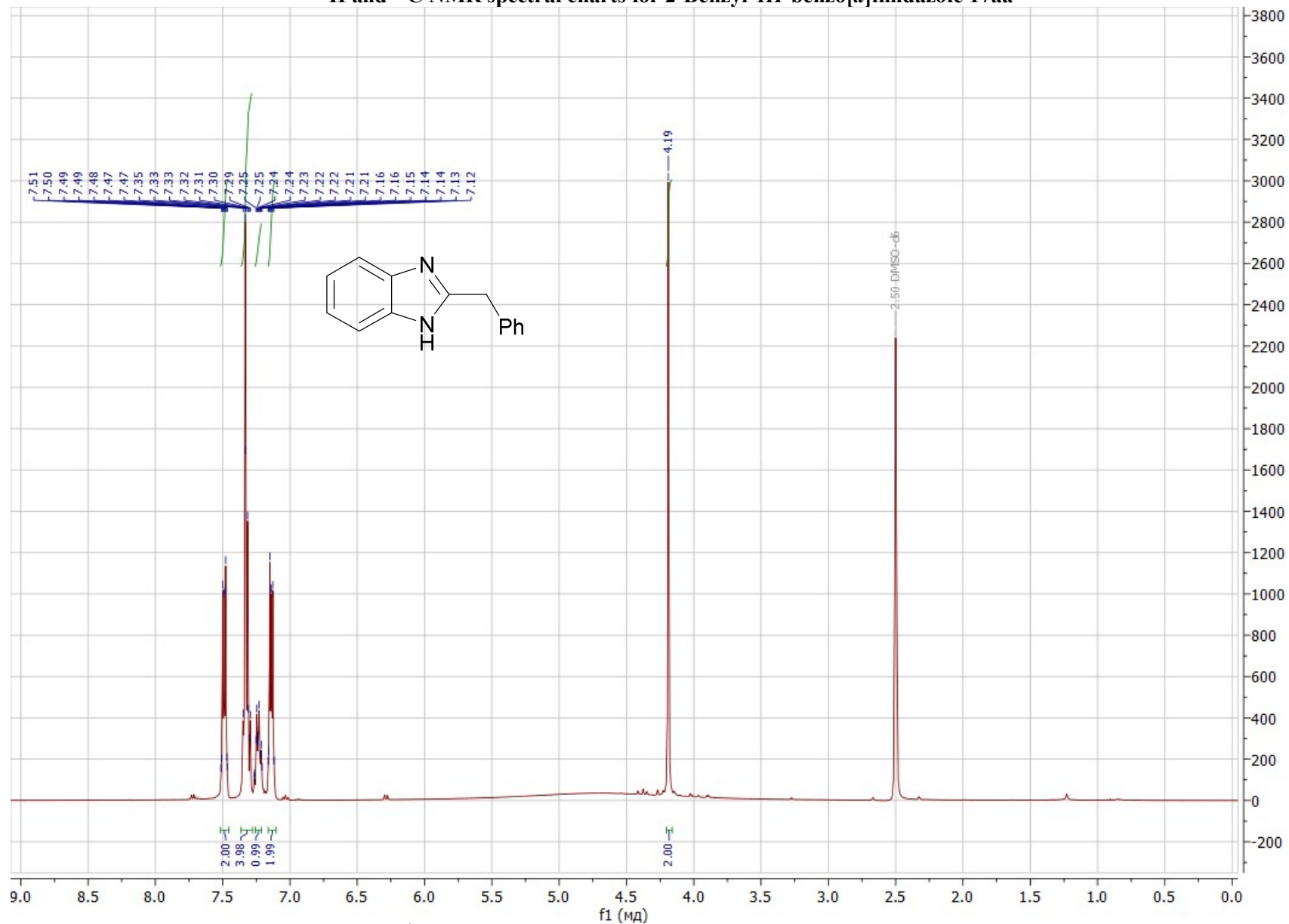


Figure S55. <sup>1</sup>H NMR spectrum of benzoimidazole 17aa in DMSO-*d*<sub>6</sub> (400 MHz)



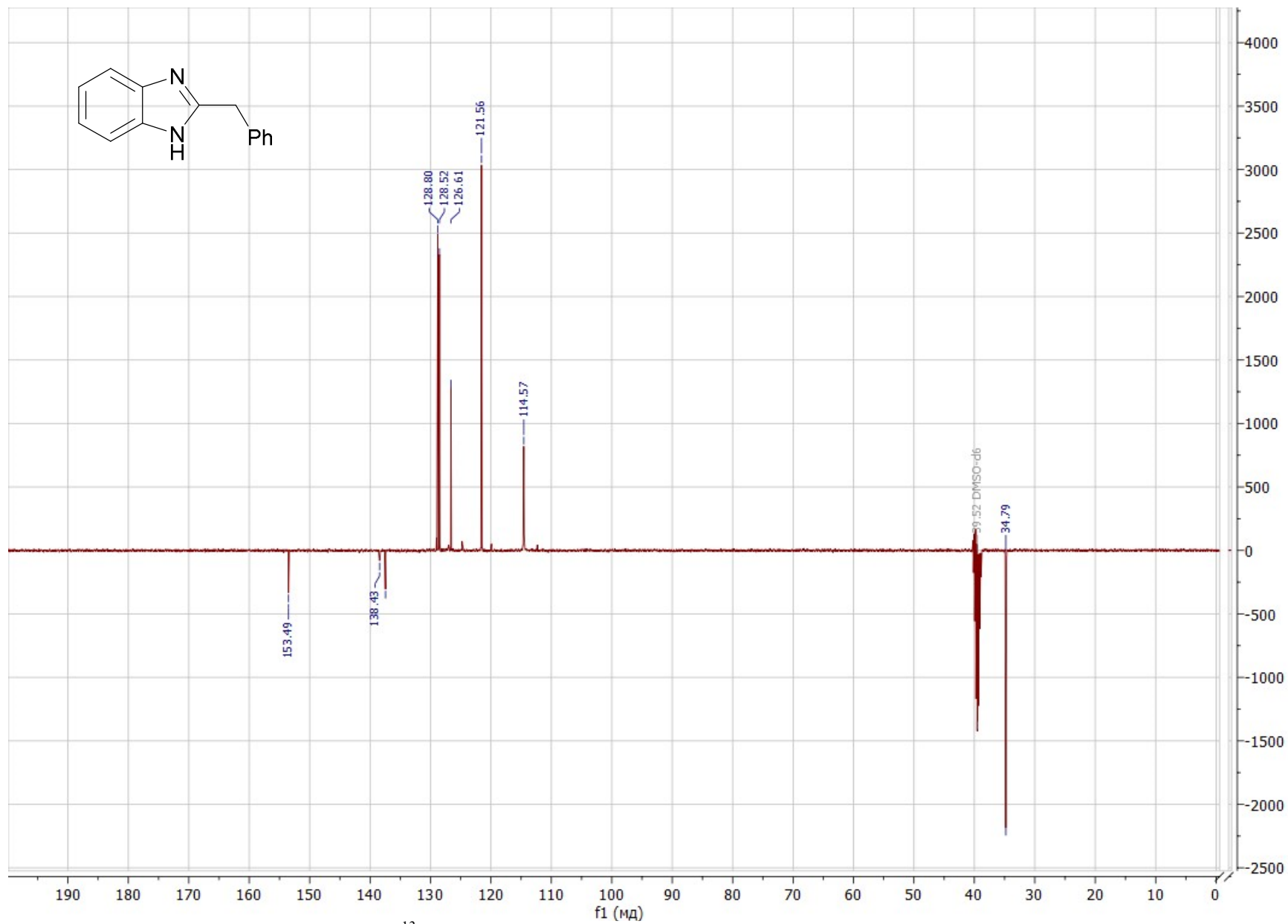


Figure S56.  $^{13}\text{C}$  NMR spectrum of benzoimidazole **17aa** in  $\text{DMSO-}d_6$  (400 MHz)

HRMS spectral chart for 5-hydroxy-5-(3-methoxyphenyl)-3-phenyl-1,5-dihydro-2H-pyrrol-2-one **1ca**

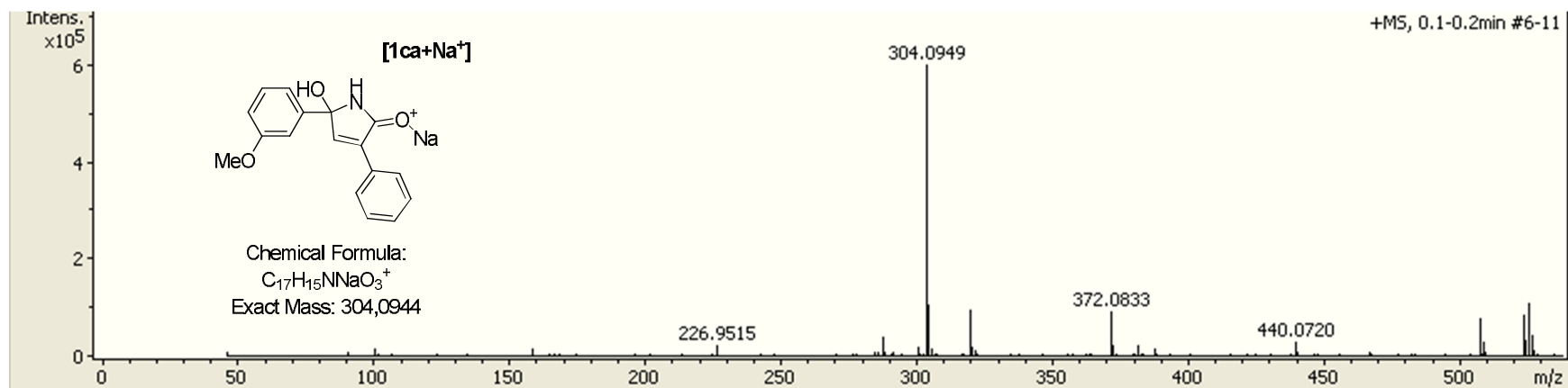


Figure S57. HRMS Chart for 5-hydroxy-5-(3-methoxyphenyl)-3-phenyl-1,5-dihydro-2H-pyrrol-2-one (**1ca**)

### HRMS spectral charts for quinoxalines 8

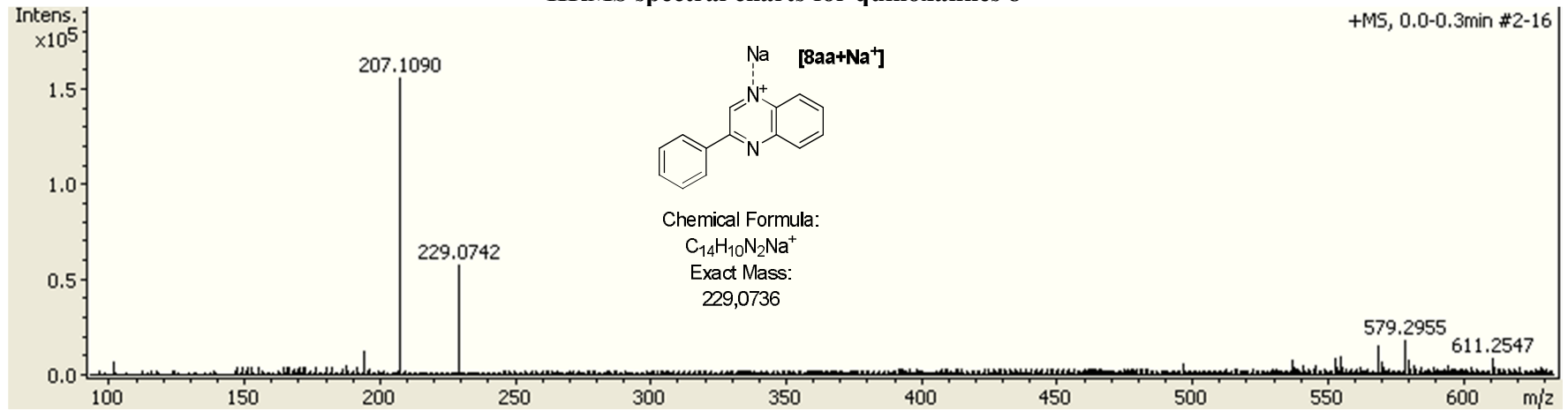


Figure S58. HRMS Chart for 2-Phenylquinoxaline (**8aa**)

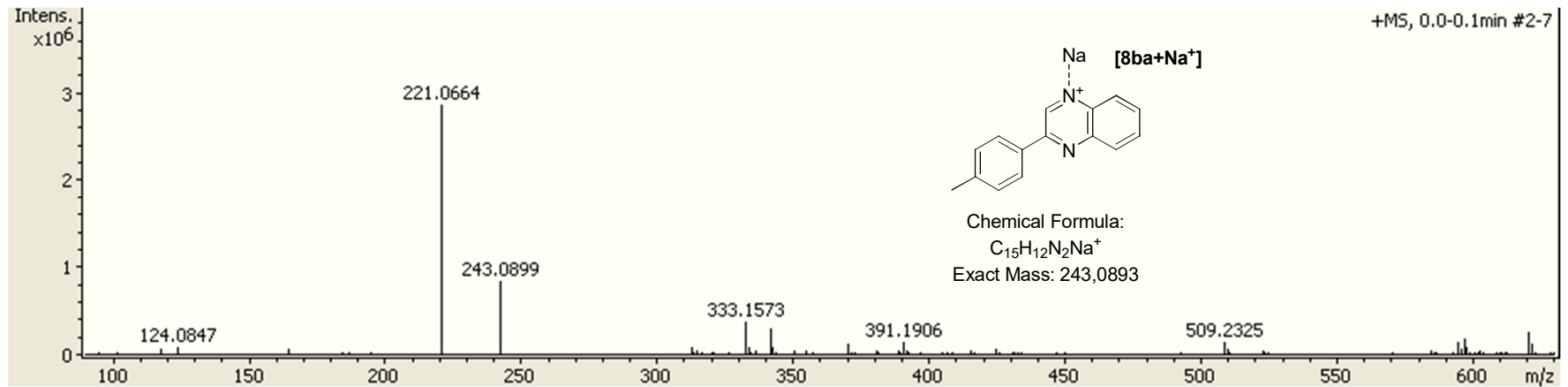


Figure S59. HRMS Chart for 2-(*p*-Tolyl)quinoxaline (**8ba**)

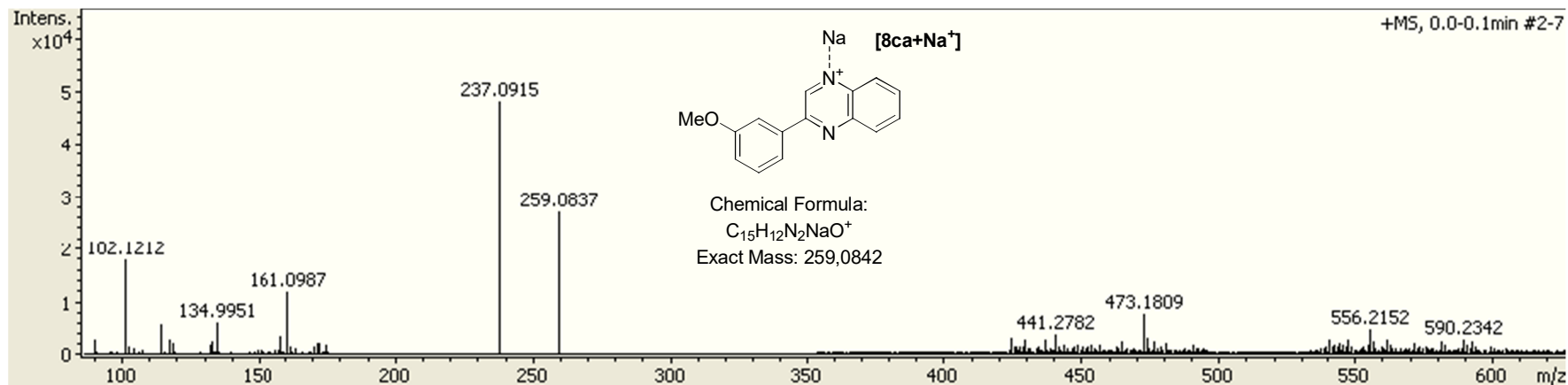


Figure S60. HRMS Chart for 2-(3-Methoxyphenyl)quinoxaline (**8ca**):

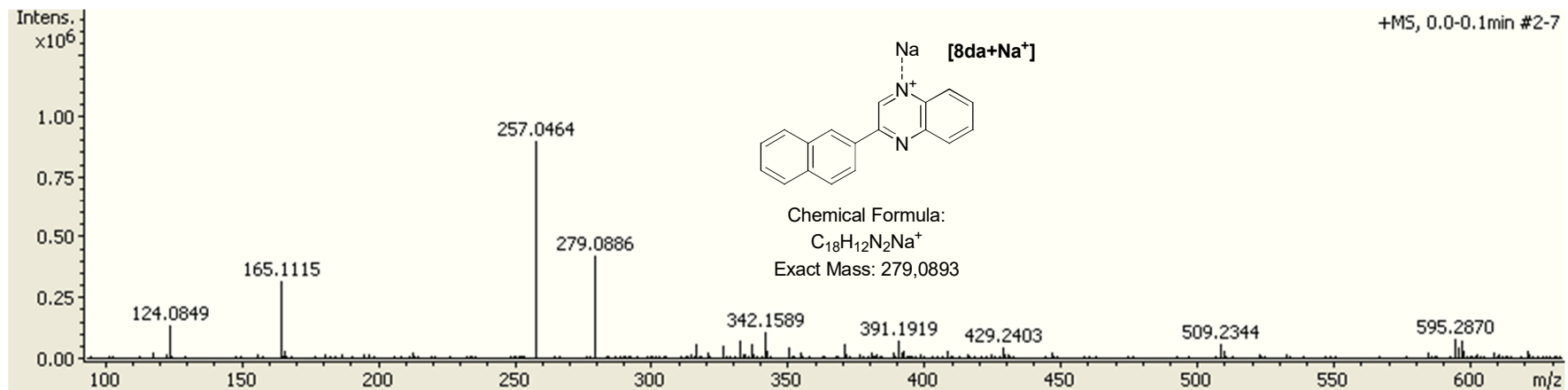


Figure S61. HRMS Chart for 2-(Naphthalen-2-yl)quinoxaline (**8da**):

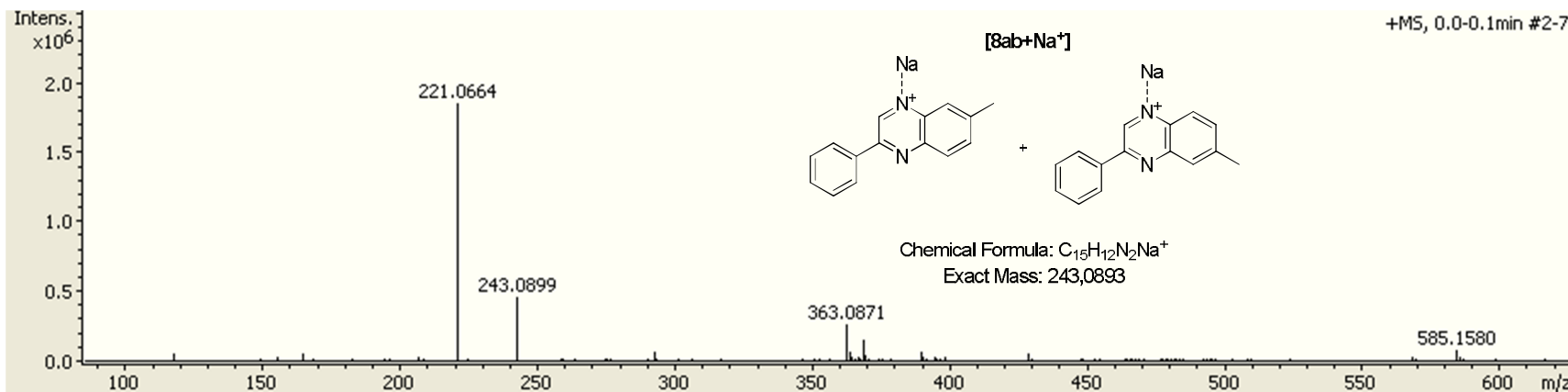


Figure S62. HRMS Chart for 7-Methyl-2-phenylquinoxaline (**8ab**) and 6-Methyl-2-phenylquinoxaline (**8ab'**)

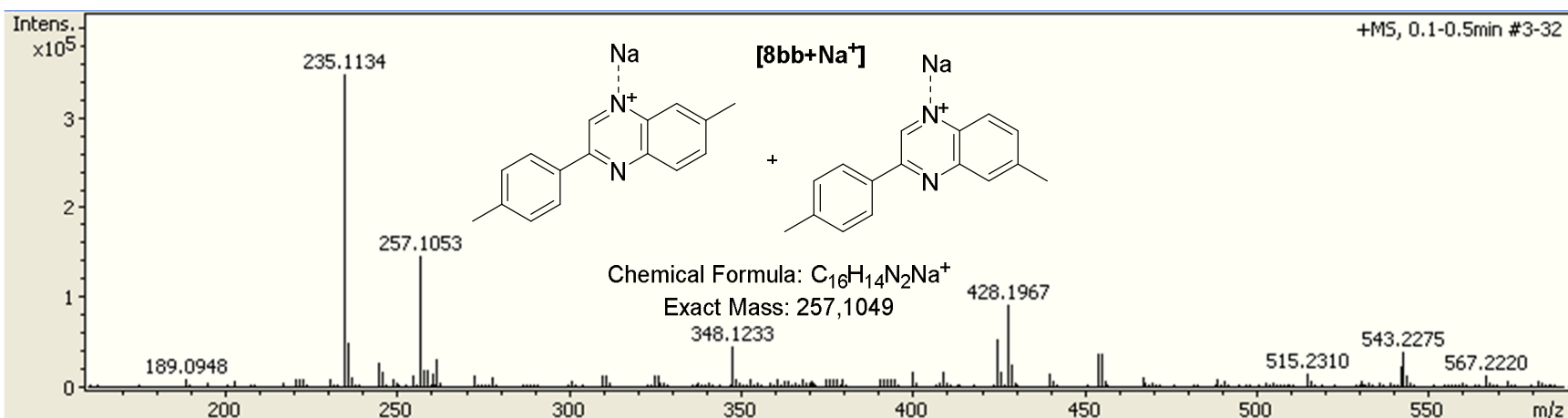


Figure S63. HRMS Chart for 7-Methyl-2-(*p*-tolyl)quinoxaline (**8bb**) and 6-Methyl-2-(*p*-tolyl)quinoxaline (**8bb'**)

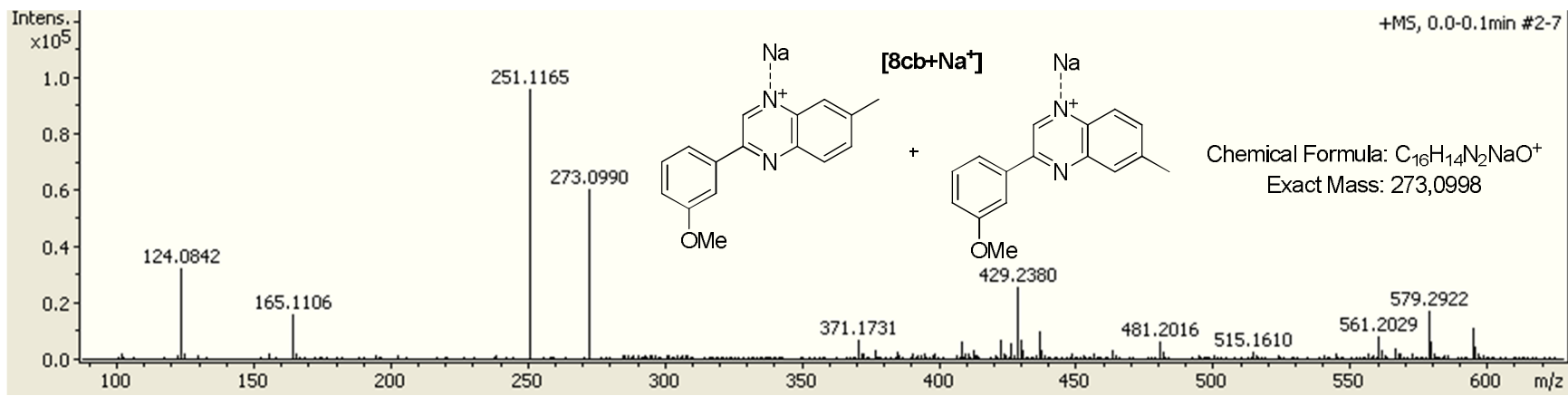


Figure S64. HRMS Chart for 2-(3-Methoxyphenyl)-7-methylquinoxaline (8cb) and 2-(3-Methoxyphenyl)-6-methylquinoxaline (8cb')

### HRMS spectral charts for 2-aryl-3-benzylimidazo[1,2-*a*]pyridines 10

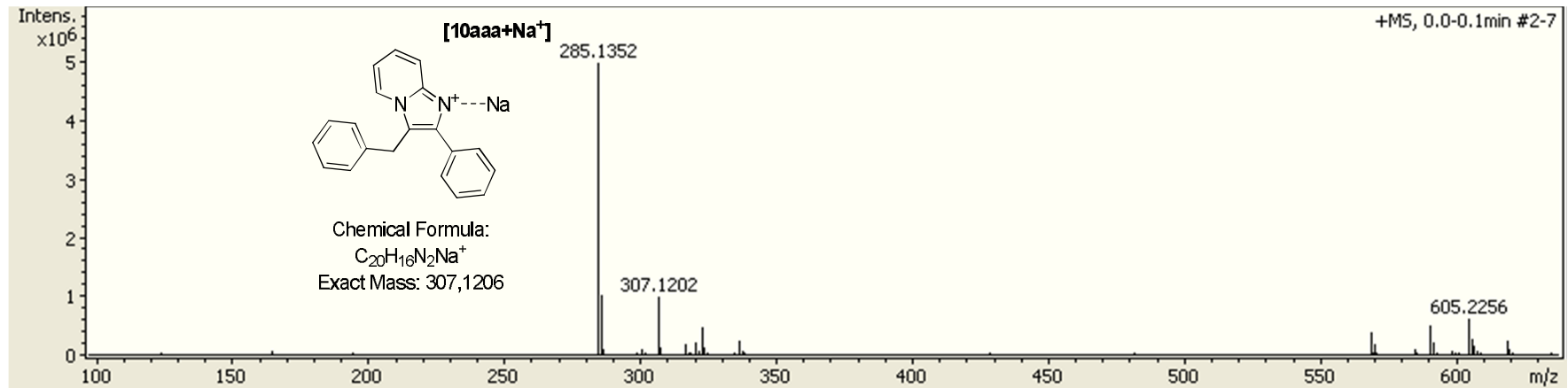


Figure S65. HRMS Chart for 3-Benzyl-2-phenylimidazo[1,2-*a*]pyridine (**10aaa**)

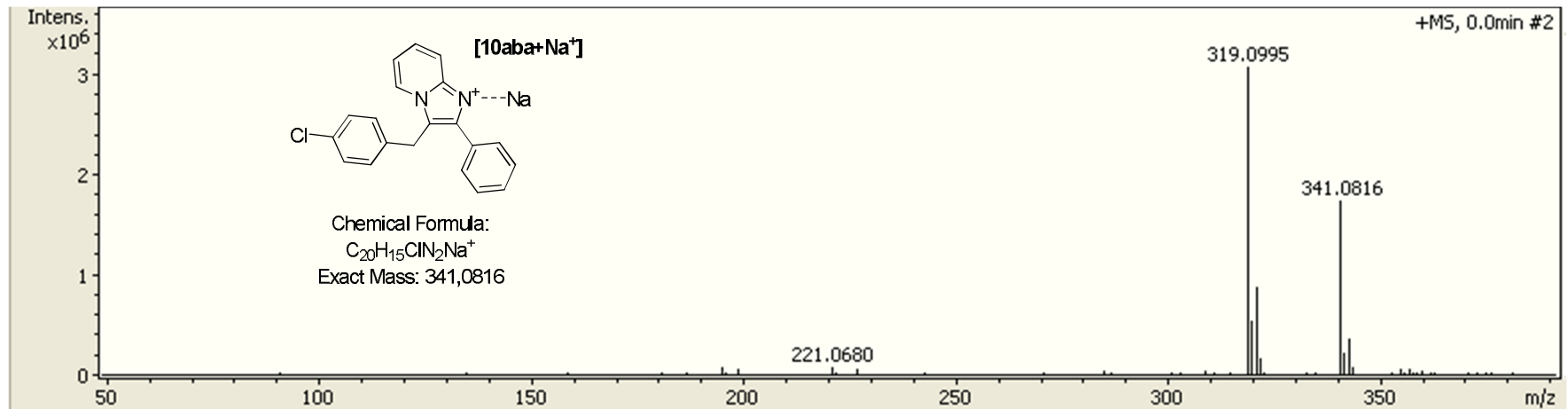


Figure S66. HRMS Chart for 3-(4-Chlorobenzyl)-2-phenylimidazo[1,2-*a*]pyridine (**10aba**)

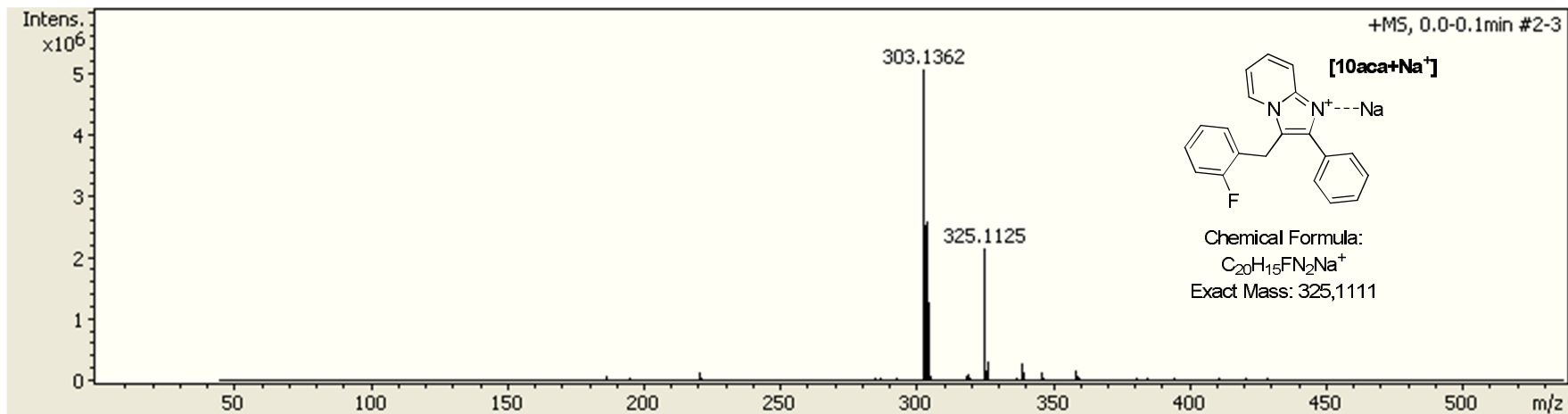


Figure S67. HRMS Chart for 3-(2-Fluorobenzyl)-2-phenylimidazo[1,2-*a*]pyridine (**10aca**)

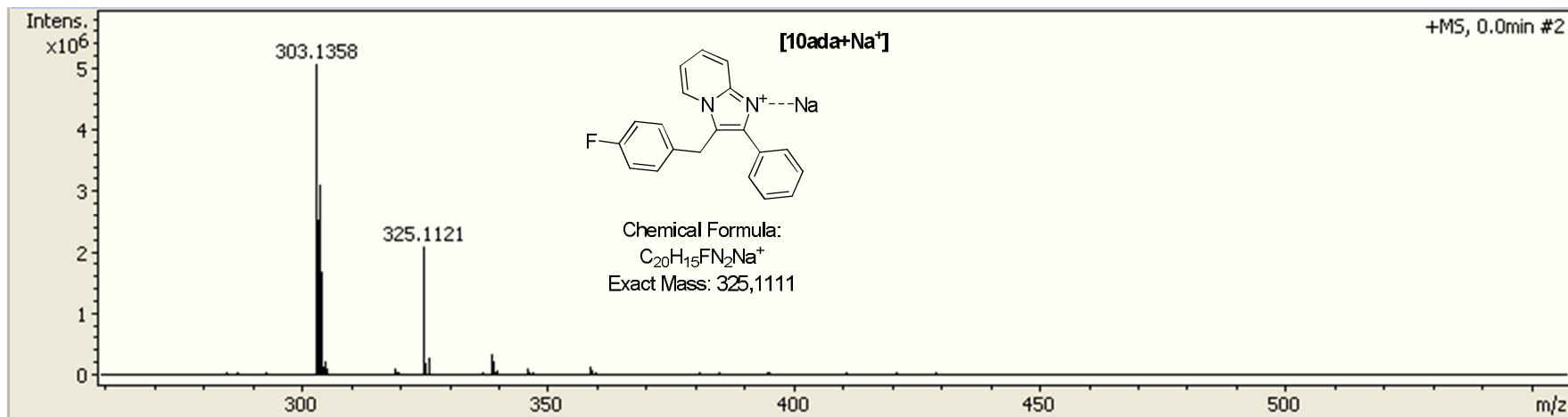


Figure S68. HRMS Chart for 3-(4-Fluorobenzyl)-2-phenylimidazo[1,2-*a*]pyridine (**10ada**)



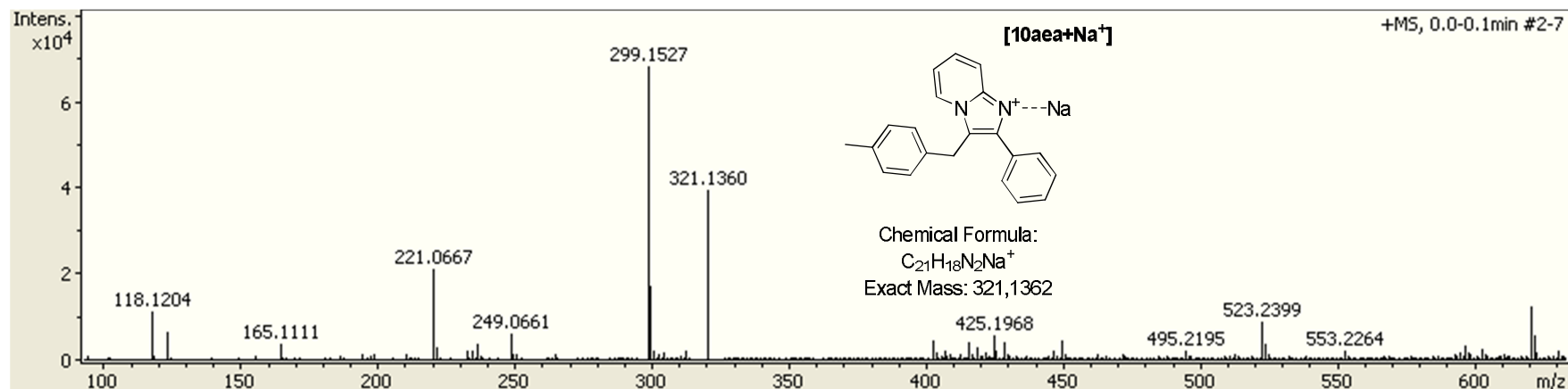


Figure S69. HRMS Chart for 3-(4-Methylbenzyl)-2-phenylimidazo[1,2-*a*]pyridine (**10aea**)

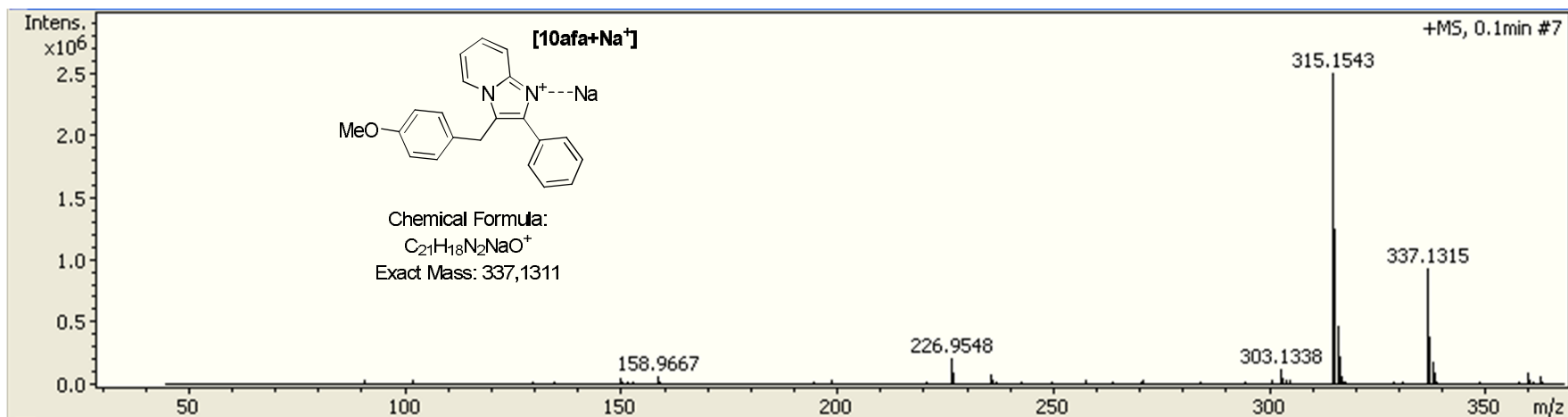


Figure S70. HRMS Chart 3-(4-Methoxybenzyl)-2-phenylimidazo[1,2-*a*]pyridine (**10afa**)

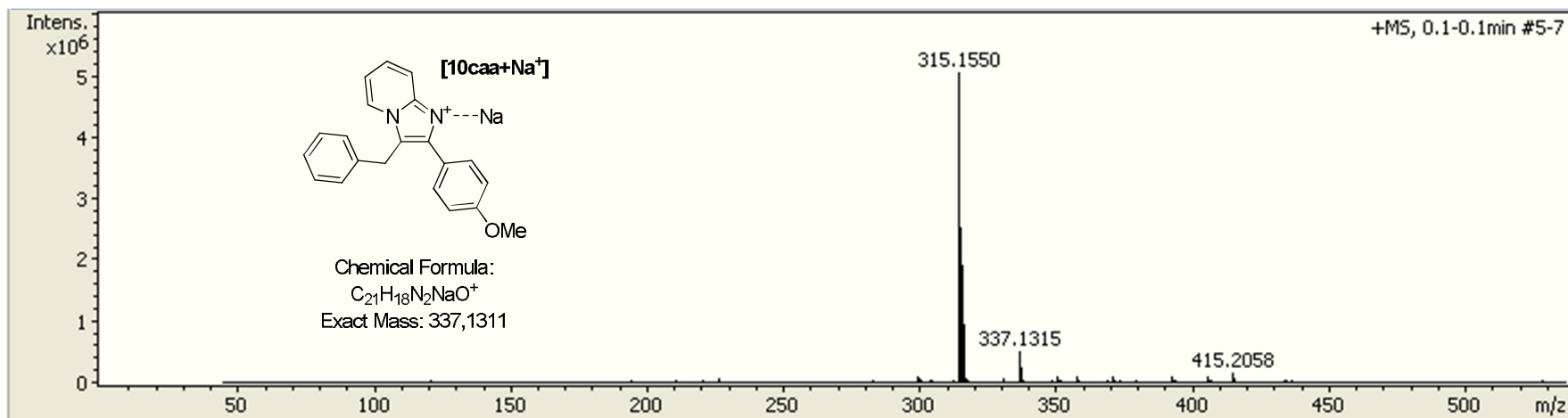


Figure S71. HRMS Chart for 3-Benzyl-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyridine (**10caa**)

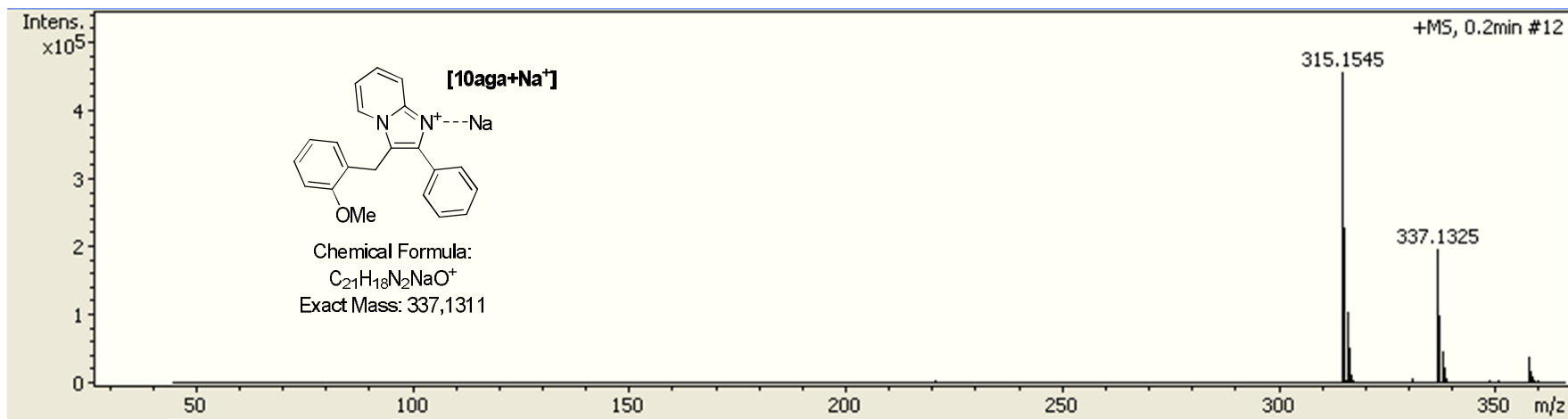


Figure S72. HRMS Chart for 3-(2-Methoxybenzyl)-2-phenylimidazo[1,2-*a*]pyridine (**10aga**)

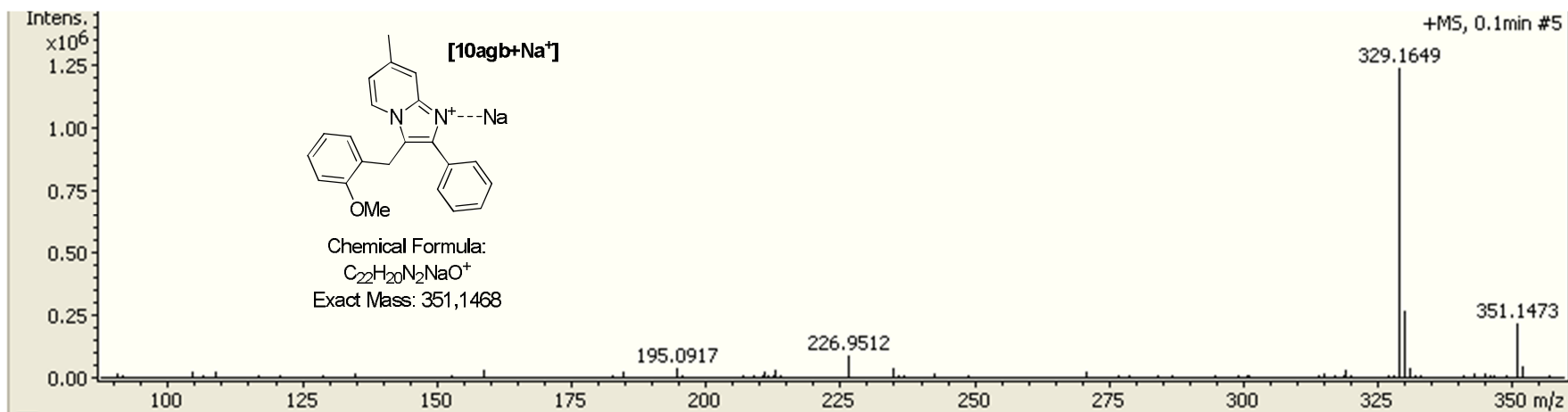


Figure S73. HRMS Chart for 3-(2-Methoxybenzyl)-7-methyl-2-phenylimidazo[1,2-a]pyridine (**10agb**)

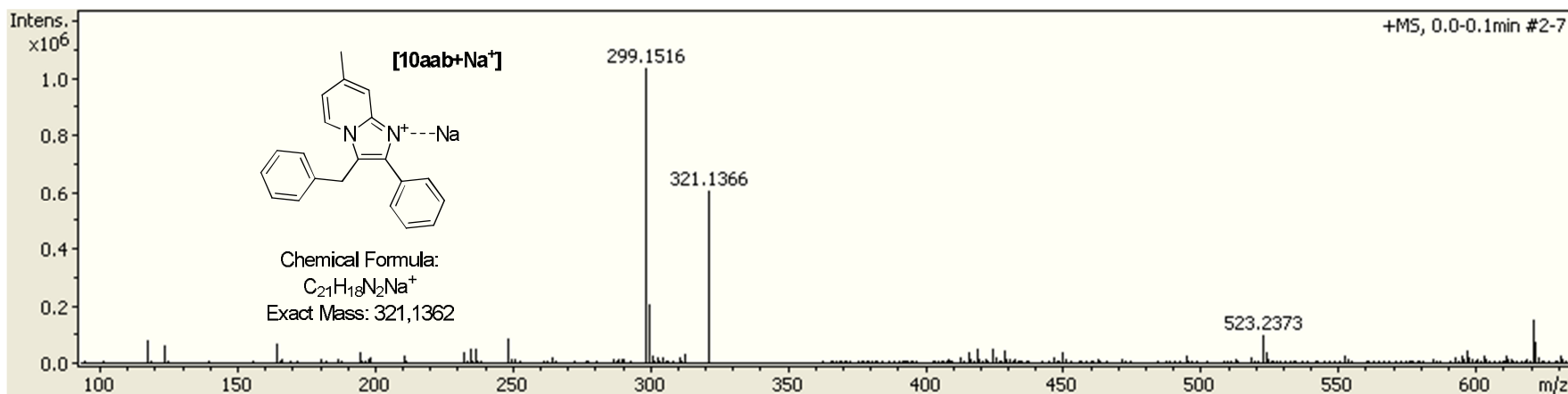


Figure S74. HRMS Chart for 3-Benzyl-7-methyl-2-phenylimidazo[1,2-a]pyridine (**10aab**)

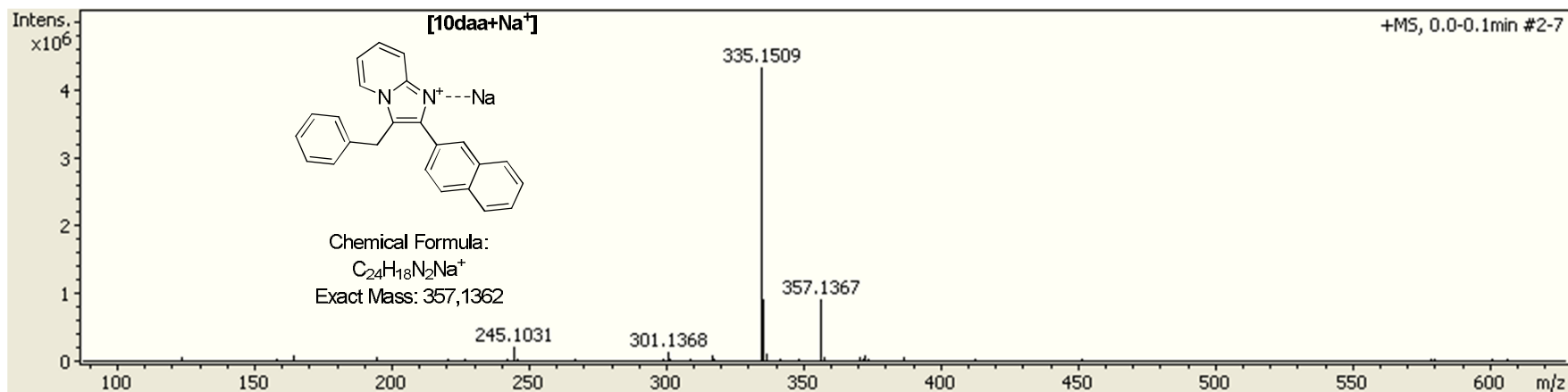


Figure S75. HRMS Chart for 3-Benzyl-2-(naphthalen-2-yl)imidazo[1,2-*a*]pyridine (**10daa**)

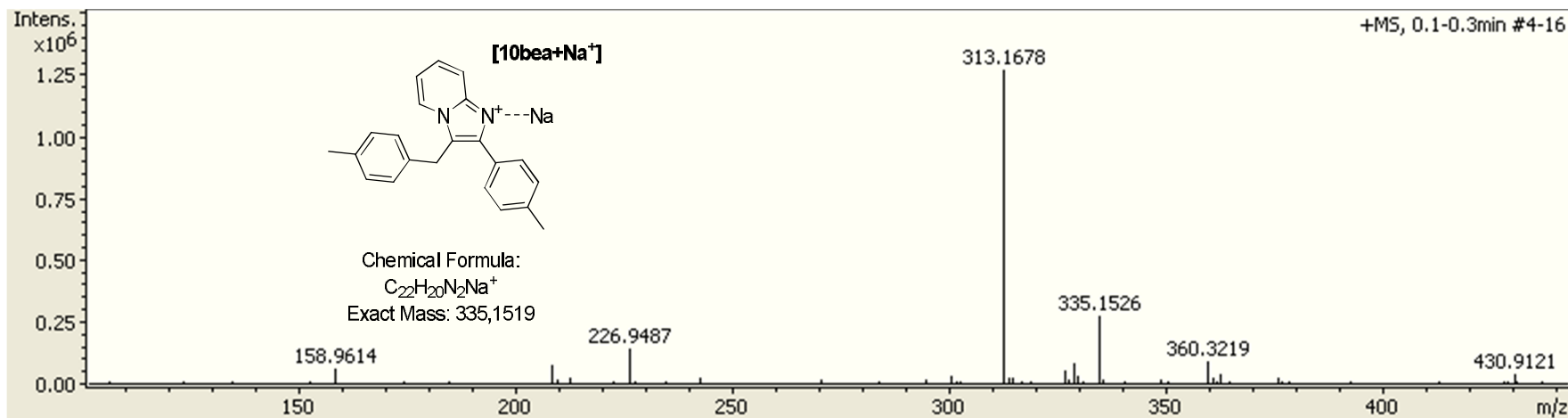


Figure S76. HRMS Chart for 3-(4-Methylbenzyl)-2-(*p*-tolyl)imidazo[1,2-*a*]pyridine (**10bea**)

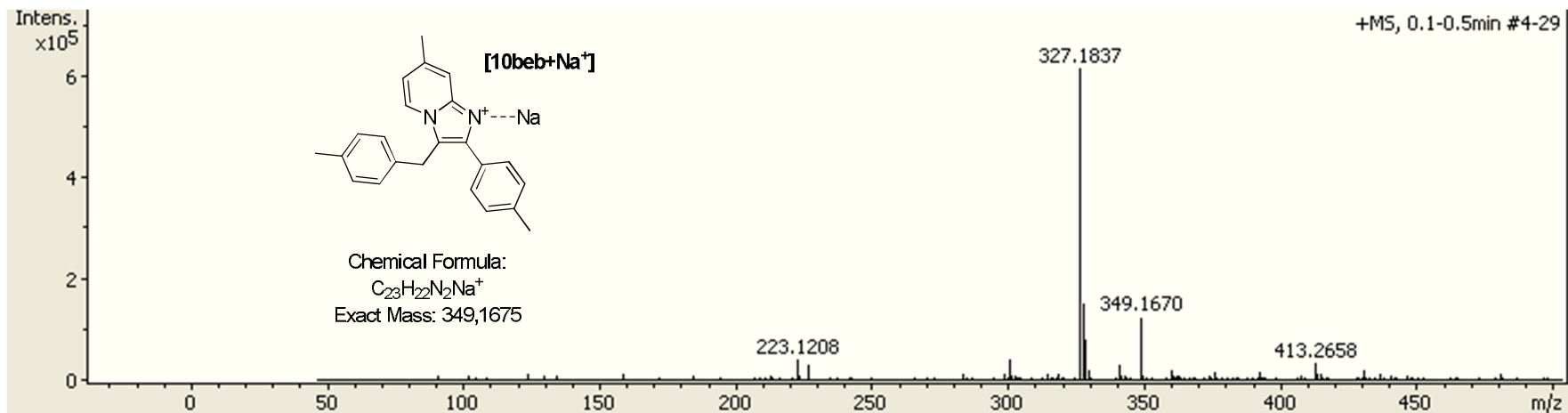


Figure S77. HRMS Chart for 7-Methyl-3-(4-methylbenzyl)-2-(*p*-tolyl)imidazo[1,2-*a*]pyridine (**10beb**)

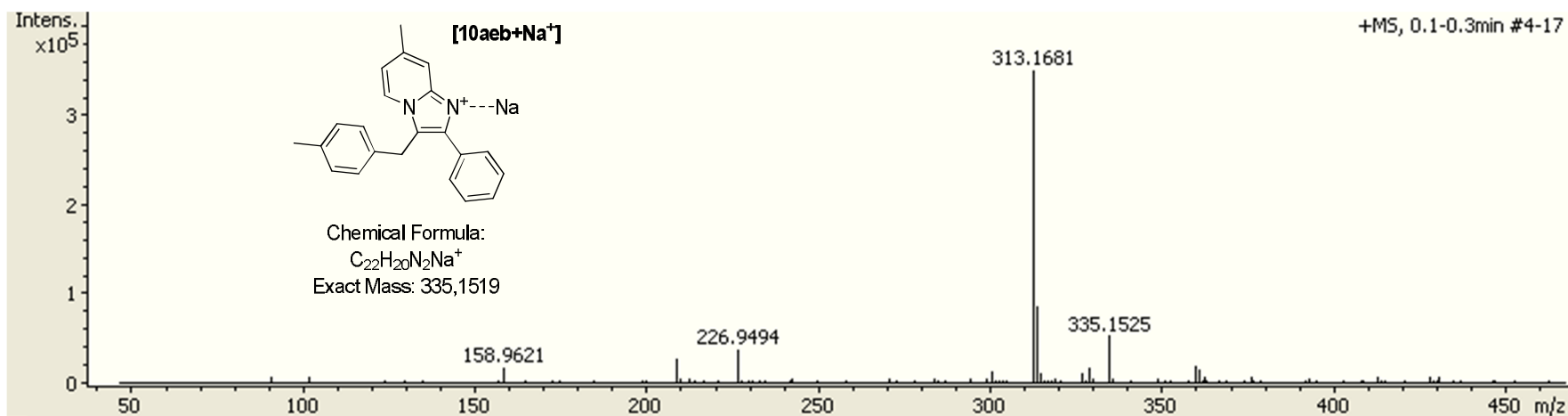


Figure S78. HRMS Chart for 7-Methyl-3-(4-methylbenzyl)-2-phenylimidazo[1,2-*a*]pyridine (**10aeb**)

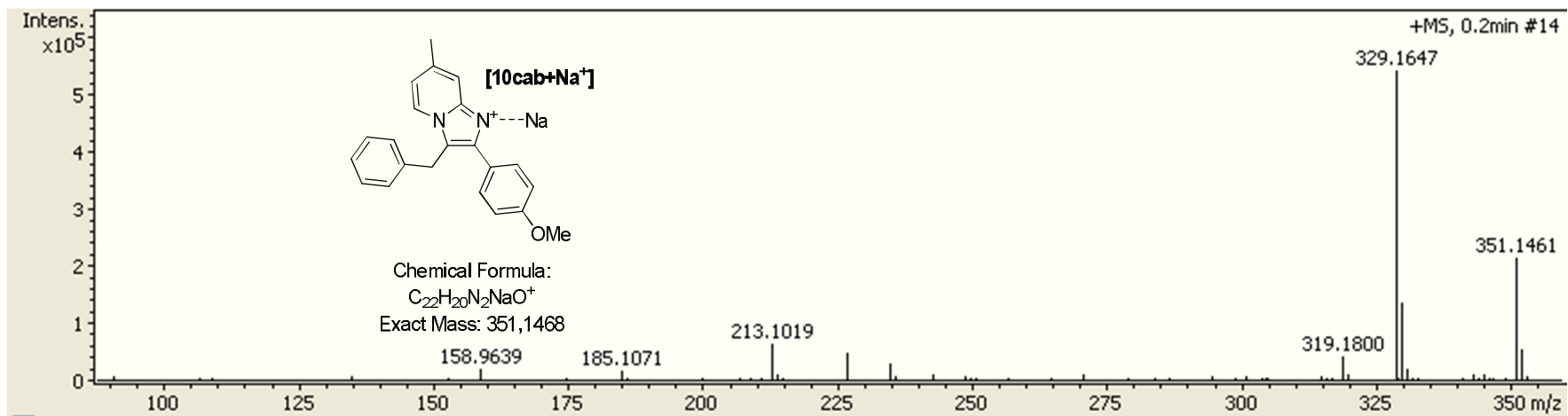


Figure S79. HRMS Chart for 3-Benzyl-2-(4-methoxyphenyl)-7-methylimidazo[1,2-*a*]pyridine (**10cab**)

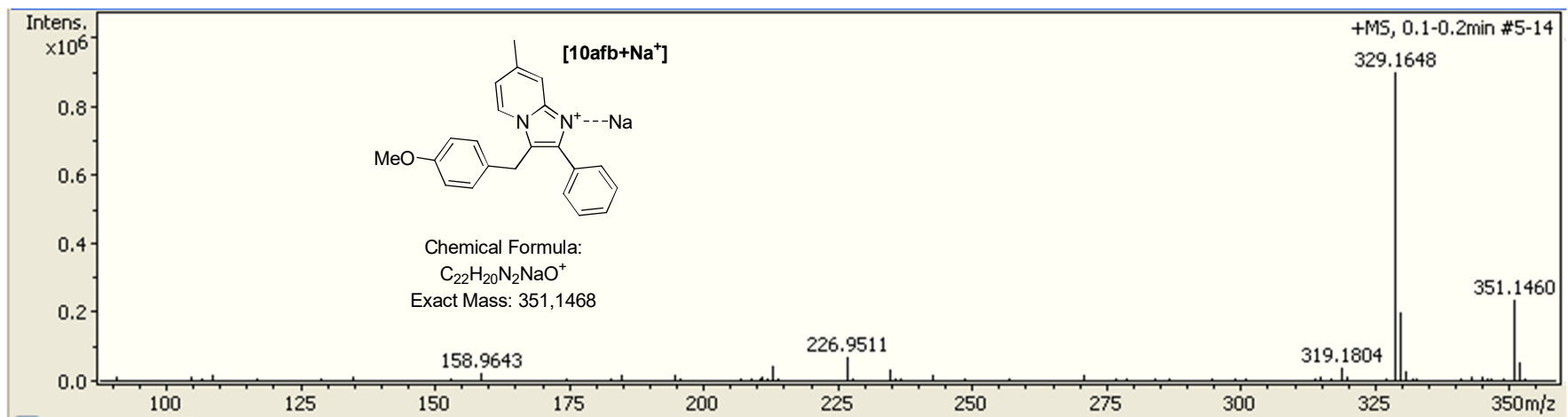


Figure S80. HRMS Chart for 3-(4-Methoxybenzyl)-7-methyl-2-phenylimidazo[1,2-*a*]pyridine (**10afb**)

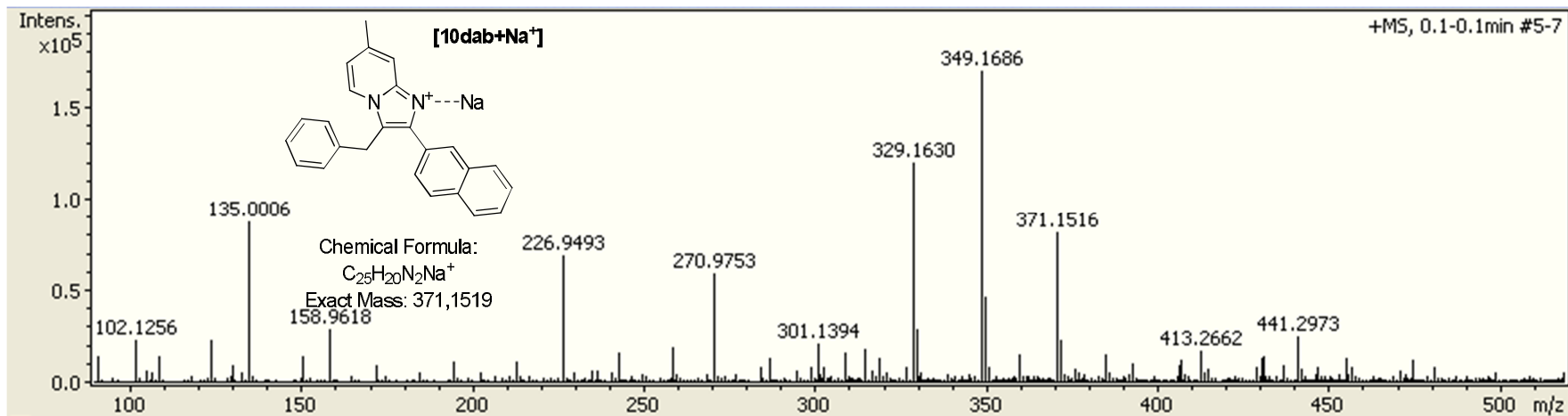


Figure S81. HRMS Chart for 3-Benzyl-2-(4-methoxyphenyl)-7-methylimidazo[1,2-*a*]pyridine (**10dab**)

### HRMS spectral chart for 3,5-diphenyl-3H-pyrrol-2-one 15aa

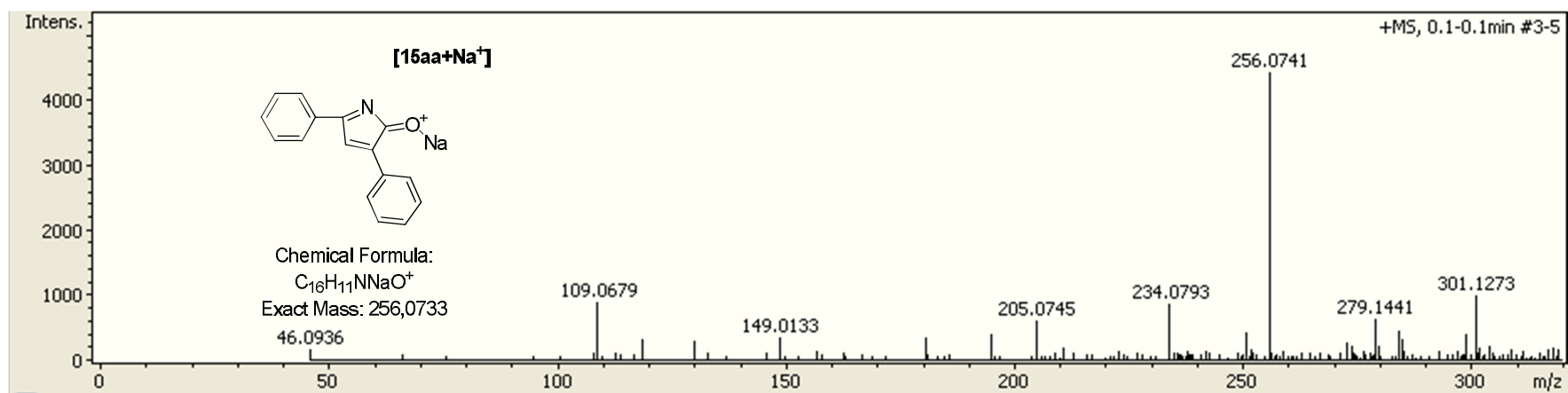


Figure S82. HRMS Chart for 3,5-diphenyl-3H-pyrrol-2-one (15aa)



HRMS spectral chart for *N*-(2-aminophenyl)-2-phenylacetamide **16aa**

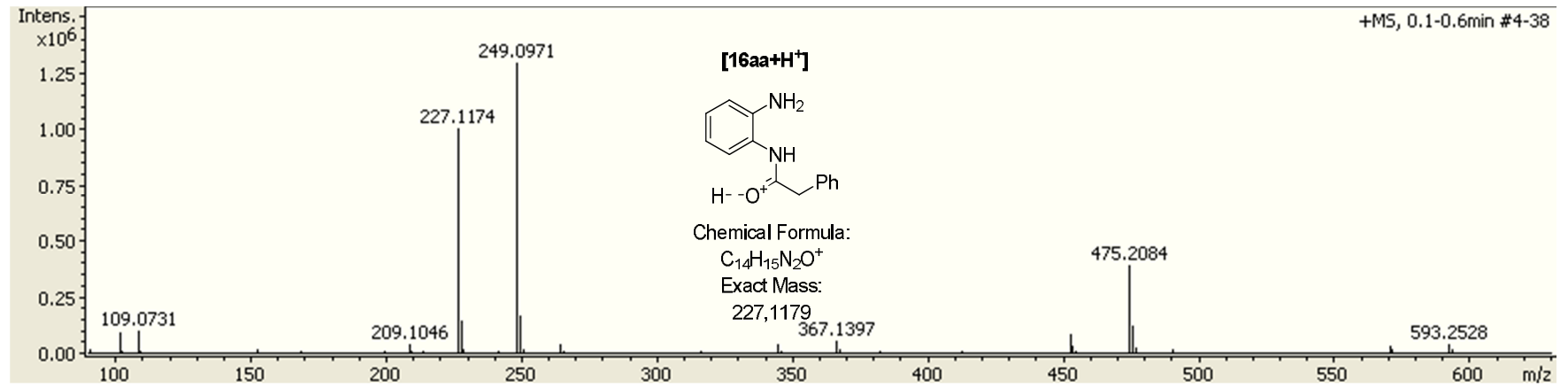


Figure S83. HRMS Chart for *N*-(2-aminophenyl)-2-phenylacetamide (**16aa**)

### HRMS spectral chart for 2-Benzyl-1*H*-benzo[*d*]imidazole 17aa

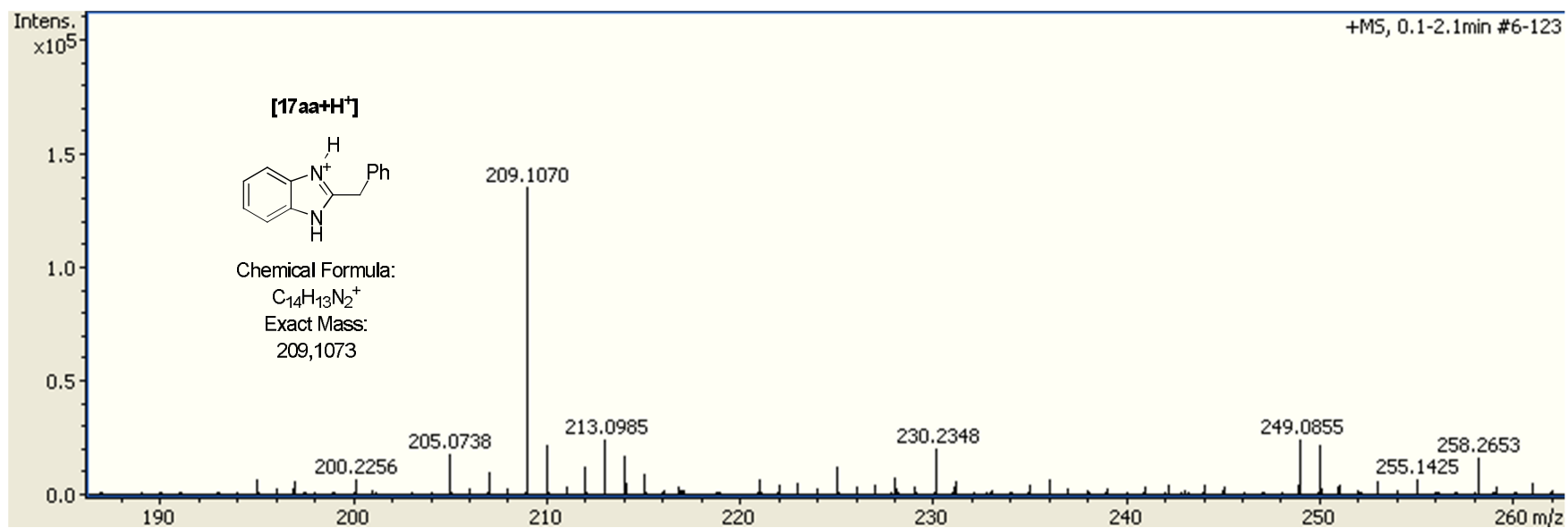


Figure S84. HRMS Chart for 2-Benzyl-1*H*-benzo[*d*]imidazole (**17aa**)

HRMS spectral chart of aqueous phase of the reaction between hydroxylactam **1aa** and phenylenediamine **6a**

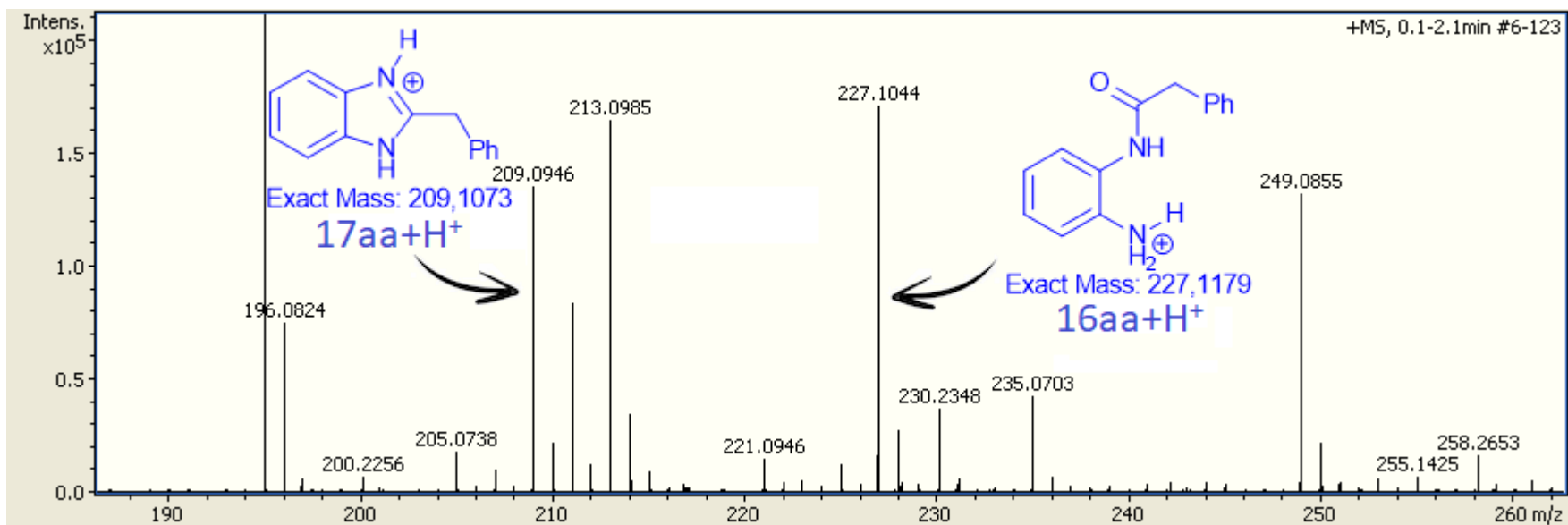


Figure S85. Mass spectrum of aqueous phase of the reaction between hydroxylactam **1aa** and phenylenediamine **6a**