

## Supporting Information

Maxim D. Gotsko, Ivan V. Saliy, Igor A. Ushakov, Lyubov' N. Sobenina, Boris A. Trofimov

*A.E. Favorsky Irkutsk Institute of Chemistry, Siberian Branch of the Russian Academy of Sciences, 1  
Favorsky St., Irkutsk 664033, Russian Federation*

*\*Corresponding author: Tel.: 7 (3952) 51-14-31; fax 7 (3952) 41-93-46; e-mail:*

*boris\_trofimov@irioch.irk.ru*

### Table of contents

1. General information .....	2
2. Starting materials.....	2
3. The reaction of acylethynylpyrroles 1 with TosMIC.....	2
4. Characterization data of 2,3-bipyrroles 2a-o and pyrrolo[1,2-c]imidazoles 3a-j .....	3
5. The NMR spectra of 2,3-bipyrroles (2a-o) and pyrrolo[1,2-c]imidazoles (3a-j) and HRMS spectra.....	13

## 1. General information

IR spectra were obtained with a Bruker Vertex 70 spectrometer (400–4000  $\text{cm}^{-1}$ , films).  $^1\text{H}$  (400.13 MHz),  $^{13}\text{C}$  (100.6 MHz) spectra were recorded on a Bruker DPX-400 spectrometer at ambient temperature in  $\text{CDCl}_3$  and  $\text{DMSO-}d_6$  solutions and referenced to  $\text{CDCl}_3$  (residual protons of  $\text{CDCl}_3$  in  $^1\text{H}$  NMR  $\delta = 7.26$  ppm;  $^{13}\text{C}$  NMR  $\delta = 77.1$  ppm),  $\text{DMSO-}d_6$  (residual protons of  $\text{CDCl}_3$  in  $^1\text{H}$  NMR  $\delta = 2.50$  ppm;  $^{13}\text{C}$  NMR  $\delta = 39.52$  ppm).

The C, H, N microanalyses were performed on a Flash EA 1112 CHNS-O/MAS analyzer. Sulfur was determined by complexometric titration with Chlorasenazo III. Fluorine content was determined on a SPECOL 11 (Carl Zeiss Jena, Germany) spectrophotometer. Chlorine was determined by mercurimetric titration. Melting point (uncorrected) was determined on a Kofler micro hot-stage apparatus. High-resolution mass spectral analyses were performed from acetonitrile solution with 0.1% HFBA on HPLC Agilent 1200/Agilent 6210 TOF instrument equipped with an electrospray ionization (ESI) source (Agilent, USA).

All reactions were carried out in dried glassware in the presence of air.

## 2. Starting materials

Acylethynylpyrroles **1a-o** were prepared from corresponding pyrroles and acylbromoacetylenes in the presence of  $\text{Al}_2\text{O}_3$  according to the reported procedure<sup>1</sup>, tosylmethylisocyanide (TosMIC), *t*-BuONa, KOH, NaH and THF are commercial products.

## 3. The reaction of acylethynylpyrroles **1** with TosMIC

### 3.1. The reaction of acylethynylpyrroles **1a-o** with TosMIC in the presence of KOH. Synthesis of 2,3'-bipyrroles **2a-o** (General Procedure)

A solution of acylethynylpyrrole **1a-o** (1 mmol) and TosMIC (395 mg, 2 mmol) in THF (10 mL) was heated to reflux. Then, under reflux, suspension of  $\text{KOH}\cdot 0.5\text{H}_2\text{O}$  (130 mg, 2 mmol) in THF (10 mL) was added dropwise to reaction mixture for 1 hour. The residue, after removing solvent, was fractionated by column chromatography ( $\text{SiO}_2$ , *n*-hexane : diethyl ether, 5 : 1) to afford the 2,3'-bipyrrole **2a-o**.

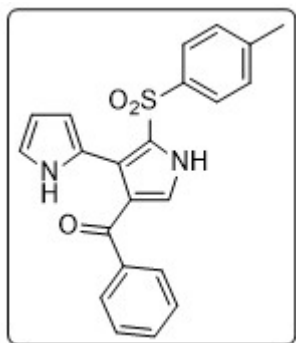
### 3.2. The reaction of acylethynylpyrroles **1a-d,i-n** with TosMIC in the presence of *t*-BuONa. Synthesis of 2,3'-bipyrroles **2a-b, d, h-n** and pyrrolo[1,2-*c*]imidazoles **3a-j** (General Procedure)

A solution of acylethynylpyrrole **1a-b, d, h-n** (1 mmol) and TosMIC (395 mg, 2 mmol) in THF (10 mL) was heated to reflux. Then, under reflux, solution of *t*-BuONa (224 mg, 2 mmol) in THF (10 mL) was added dropwise to reaction mixture for 1 hour. The residue, after removing solvent, was fractionated by column chromatography ( $\text{SiO}_2$ , *n*-hexane : diethyl ether, 5 : 1) to afford the 2,3'-bipyrrole **2a-b, d, h-n** then pyrrolo[1,2-*c*]imidazoles **3a-j**. Yields of 2,3'-bipyrrole **2a-b, d, h-n**, thus obtained, are: **2a** - 27%; **2b** - 32%; **2d** - 32%; **2h** - 24%; **2i** - 29%, **2j** - 24%; **2k** - 30%; **2l** - 22%; **2m** - 26%; **2n** - 24%.

#### 4. Characterization data of 2,3-bipyrroles 2a-o and pyrrolo[1,2-c]imidazoles 3a-j

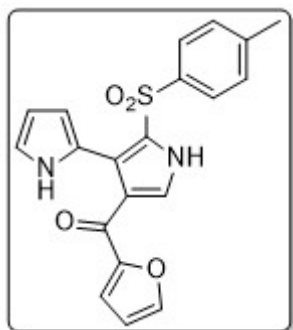
##### 4.1. Characterization data of 2,3-bipyrroles 2a-o

###### *Phenyl(2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)methanone (2a)*



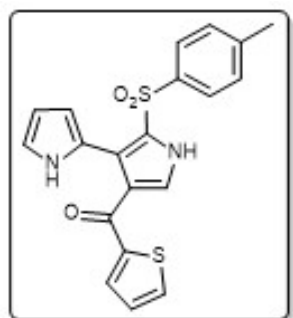
Yield 312 mg (80%). Yellow crystals, mp 163-165 °C. IR (KBr,  $\text{cm}^{-1}$ ): 3295 (NH), 3148, 3063 (=CH), 2920 (CH), 1636 (CO), 1597, 1517 (C=C), 1354, 1140 ( $\text{SO}_2$ ).  $^1\text{H}$  NMR (400.13 MHz,  $\text{CDCl}_3$ ):  $\delta$  10.89 (br.s, 1H, NH, CO-pyrrole), 9.92 (br.s, 1H, NH, pyrrole), 7.75-7.73 (m, 2H, Ph), 7.59-7.57 (m, 2H, Ph), 7.54-7.52 (m, 1H, Ph), 7.44-7.40 (m, 2H, Ph), 7.24 (d,  $J = 3.5$  Hz, 1H, H-5, CO-pyrrole), 7.16-7.14 (m, 2H, Ph), 6.84-6.83 (m, 2H, H-5, H-3, pyrrole), 6.20-6.18 (m, 1H, H-4, pyrrole), 2.34 (s, 3H,  $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100.6 MHz,  $\text{CDCl}_3$ ):  $\delta$  192.4, 144.7, 139.3, 137.5, 132.7, 129.8 (2C), 129.7 (2C), 129.3, 128.4 (2C), 127.2 (2C), 125.2, 124.3, 123.0, 121.4, 119.2, 113.1, 109.5, 21.7. Anal. Calcd for  $\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_3\text{S}$ : C, 67.68; H, 4.65; N, 7.17; S, 8.21%. Found: C, 67.84; H, 4.78; N, 7.32; S, 8.01%. HRMS (ESI-TOF): found 391,1116. Calcd. for  $[\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_4\text{S}+\text{H}]^+$  391,1121.

###### *Furan-2-yl(2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)methanone (2b)*



Yield 282 mg (74%). Yellow crystals, mp 95-97 °C. IR (KBr,  $\text{cm}^{-1}$ ): 3293 (NH), 3131 (=CH), 2923, 2859 (CH), 1620 (CO), 1563, 1520 (C=C), 1354, 1140 ( $\text{SO}_2$ ).  $^1\text{H}$  NMR (400.13 MHz,  $\text{CDCl}_3$ ):  $\delta$  10.71 (br.s, 1H, NH, CO-pyrrole), 9.94 (br.s, 1H, NH, pyrrole), 7.68 (d,  $J = 3.3$  Hz, 1H, H-5, CO-pyrrole), 7.62-7.61 (m, 1H, H-5, furan), 7.57-7.55 (m, 2H, Ph), 7.16-7.14 (m, 3H, H-3, furan, Ph), 6.86-6.84 (m, 2H, H-3, H-5, pyrrole), 6.54 (dd,  $J = 3.3, 1.4$  Hz, 1H, H-4, furan), 6.22-6.20 (m, 1H, H-4, pyrrole), 2.33 (s, 3H,  $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100.6 MHz,  $\text{CDCl}_3$ ):  $\delta$  177.8, 153.4, 146.9, 144.7, 137.9, 129.7 (2C), 127.5, 127.3 (2C), 125.7, 123.3, 123.0, 121.4, 119.8, 119.3, 113.2, 112.5, 109.5, 21.6. Anal. Calcd for  $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_4\text{S}$ : C, 63.15; H, 4.24; N, 7.36; S, 8.43%. Found: C, 63.27; H, 4.42; N, 7.53; S, 8.3%.

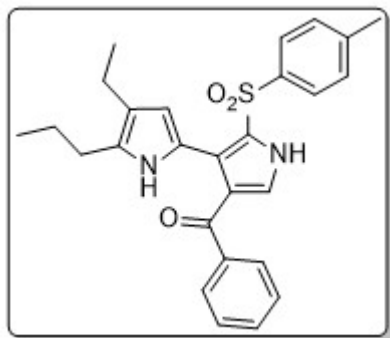
###### *Thiophen-2-yl(2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)methanone (2c)*



Yield 274 mg (69%). Yellow crystals, mp 175-177 °C. IR (KBr,  $\text{cm}^{-1}$ ): 3351 (NH), 3137, 3110 (=CH), 2922 (CH), 1614 (CO), 1569, 1520, 1484, 1458 (C=C), 1359, 1136 ( $\text{SO}_2$ ).  $^1\text{H}$  NMR (400.13 MHz,  $\text{CDCl}_3$ ):  $\delta$  10.64 (br.s, 1H, NH, CO-pyrrole), 10.16 (br.s, 1H, NH, pyrrole), 7.65 (d,  $J = 4.9$  Hz, 1H, H-5, thiophene), 7.57 (d,  $J = 8.1$  Hz, 2H, Ph), 7.54 (d,  $J = 3.5$  Hz, 1H, H-3, thiophene), 7.46 (d,  $J =$

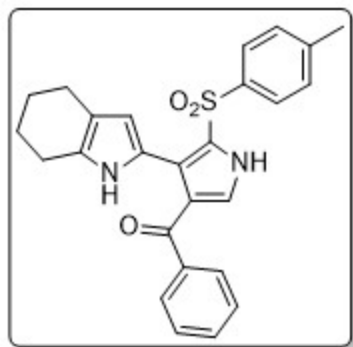
3.3 Hz, 1H, H-3, pyrrole), 7.14 (d,  $J = 8.1$  Hz, 2H, Ph), 7.09-7.07 (m, 1H, H-4, thiophene), 6.85-6.83 (m, 1H, H-4, pyrrole), 6.83-6.82 (m, 1H, H-3, pyrrole), 6.21-6.20 (m, 1H, H-5, pyrrole), 2.32 (s, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (100.6 MHz, CDCl<sub>3</sub>):  $\delta$  183.5, 145.0, 144.8, 137.5, 134.6, 134.4, 129.7 (2C), 128.2, 127.4, 127.2 (2C), 125.4, 124.1, 122.5, 121.4, 119.3, 113.0, 109.4, 21.7. Anal. Calcd for C<sub>20</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>S<sub>2</sub>: C, 60.59; H, 4.07; N, 7.07; S, 16.17%. Found: C, 60.73; H, 4.27; N, 7.18; S, 15.99%. HRMS (ESI-TOF): found 397,0681. Calcd. for [C<sub>20</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>S<sub>2</sub>+H]<sup>+</sup> 397,0685.

*(4-Ethyl-5-propyl-2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (2d)*



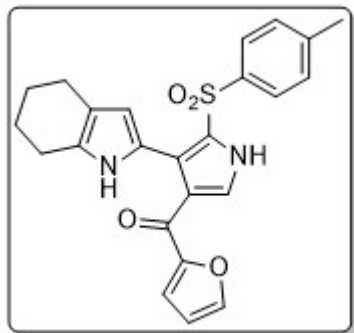
Yield 203 mg (44%). Yellow crystals, mp 170-172 °C. IR (KBr, cm<sup>-1</sup>): 3285 (NH), 3160 (=CH), 2958, 2927, 2869 (CH), 1630 (CO), 1596, 1575, 1519, 1495, 1461 (C=C), 1351, 1142, (SO<sub>2</sub>). <sup>1</sup>H NMR (400.13 MHz, CDCl<sub>3</sub>):  $\delta$  10.63 (br.s, 1H, NH, CO-pyrrole), 9.84 (br.s, 1H, NH, pyrrole), 7.72-7.70 (m, 2H, Ph), 7.63-7.61 (m, 2H, Ph), 7.54-7.51 (m, 1H, Ph), 7.43-7.39 (m, 2H, Ph), 7.22 (d,  $J = 3.5$  Hz, 1H, H-5, CO-pyrrole), 7.16-7.14 (m, 2H, Ph), 6.67-6.65 (m, 1H, pyrrole), 2.55-2.53 (m, 2H, CH<sub>2</sub>), 2.51-2.53 (m, 2H, CH<sub>2</sub>), 2.37 (s, 3H, CH<sub>3</sub>), 1.67-1.57 (m, 2H CH<sub>2</sub>), 1.12 (t,  $J = 7.6$  Hz, 3H, CH<sub>3</sub>), 0.90 (t,  $J = 7.3$  Hz, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (100.6 MHz, CDCl<sub>3</sub>):  $\delta$  192.5, 144.5, 139.8, 137.7, 132.4, 130.1, 129.7 (2C), 129.6 (2C), 129.5, 128.4 (2C), 127.3 (2C), 124.1, 124.0, 123.8, 123.2, 118.7, 113.5, 28.0, 23.1, 21.7, 19.0, 16.1, 13.9. Anal. Calcd for C<sub>27</sub>H<sub>28</sub>N<sub>2</sub>O<sub>3</sub>S: C, 70.41; H, 6.13; N, 6.08; S, 6.96%. Found: C, 70.6; H, 6.28; N, 6.25; S, 6.84%. HRMS (ESI-TOF): found 461,1899. Calcd. for [C<sub>27</sub>H<sub>28</sub>N<sub>2</sub>O<sub>3</sub>S +H]<sup>+</sup> 461,1902.

*Phenyl(4-(4,5,6,7-tetrahydro-1H-indol-2-yl)-5-tosyl-1H-pyrrol-3-yl)methanone (2e)*



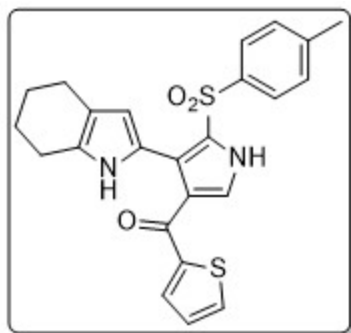
Yield 311 mg (70%). Yellow crystals, mp 235-237 °C. IR (KBr, cm<sup>-1</sup>): 3342 (NH), 3171 (=CH), 2922, 2851 (CH), 1633 (CO), 1594, 1574, 1521, 1495 (C=C), 1351, 1126 (SO<sub>2</sub>). <sup>1</sup>H NMR (400.13 MHz, CDCl<sub>3</sub>):  $\delta$  10.60 (br.s, 1H, NH, CO-pyrrole), 9.89 (br.s, 1H, NH, pyrrole), 7.73-7.71 (m, 2H, Ph), 7.65-7.63 (m, 2H, Ph), 7.56-7.52 (m, 1H, Ph), 7.44-7.40 (m, 2H, Ph), 7.20-7.19 (m, 2H, Ph), 7.17-7.15 (m, 1H, H-2, CO-pyrrole), 6.68-6.67 (m, 1H, H-3, pyrrole), 2.61-2.59 (m, 2H, CH<sub>2</sub>-7), 2.51-2.48 (m, 2H, CH<sub>2</sub>-4), 2.36 (s, 3H, CH<sub>3</sub>), 1.79-1.78 (m, 2H, CH<sub>2</sub>-5), 1.73-1.71 (m, 2H, CH<sub>2</sub>-6). <sup>13</sup>C NMR (100.61 MHz, CDCl<sub>3</sub>):  $\delta$  192.5, 144.5, 139.8, 137.7, 132.5, 129.7 (3C), 129.6 (2C), 129.2, 128.4 (2C), 127.2 (2C), 124.1, 123.9, 121.3, 119.5, 118.8, 112.4, 24.0, 23.6, 23.1, 23.1, 21.7. Anal. Calcd for C<sub>26</sub>H<sub>24</sub>N<sub>2</sub>O<sub>3</sub>S: C, 70.25; H, 5.44; N, 6.30; S, 7.21%. Found: C, 70.40; H, 5.25; N, 6.44; S, 7.04%. HRMS (ESI-TOF): found 445,1586. Calcd. for [C<sub>26</sub>H<sub>24</sub>N<sub>2</sub>O<sub>3</sub>S+H]<sup>+</sup> 445,1589.

*Furan-2-yl(4-(4,5,6,7-tetrahydro-1H-indol-2-yl)-5-tosyl-1H-pyrrol-3-yl)methanone (2f)*



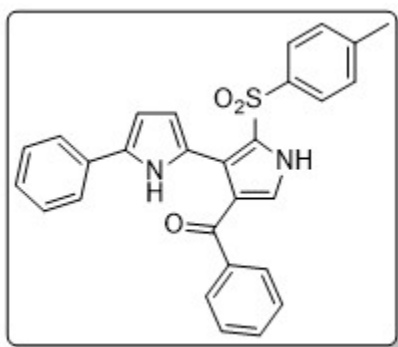
Yield 291 mg (67%). Yellow crystals, mp 173-175 °C. IR (KBr,  $\text{cm}^{-1}$ ): 3278 (NH), 3019 (=CH), 2924, 2850 (CH), 1618 (CO), 1609, 1524, 1464 (C=C), 1351, 1138 ( $\text{SO}_2$ ).  $^1\text{H}$  NMR (400.13 MHz,  $\text{CDCl}_3$ ):  $\delta$  10.39 (br.s, 1H, NH, CO-pyrrole), 10.27 (br.s, 1H, NH, pyrrole), 7.65-7.64 (m, 2H, Ph), 7.62-7.61 (m, 2H, H-5, H-3, furan), 7.16-7.14 (m, 2H, Ph), 7.12 (d,  $J = 3.5$  Hz, 1H, H-2, CO-pyrrole), 6.64 (d,  $J = 2.2$  Hz, 1H, H-3, pyrrole), 6.52 (dd,  $J = 3.5, 1.6$  Hz, 1H, H-4, furan), 2.60-2.57 (m, 2H,  $\text{CH}_2$ -7), 2.51-2.48 (m, 2H,  $\text{CH}_2$ -4), 2.33 (s, 3H,  $\text{CH}_3$ ), 1.81-1.75 (m, 2H,  $\text{CH}_2$ -5), 1.74-1.70 (m, 2H,  $\text{CH}_2$ -6).  $^{13}\text{C}$  NMR (100.6 MHz,  $\text{CDCl}_3$ ):  $\delta$  177.9, 153.2, 147.0, 144.5, 137.7, 129.6 (2C), 129.1, 128.5, 127.2 (2C), 124.0, 123.8, 122.4, 119.9, 119.3, 118.6, 112.4, 112.3, 24.0, 23.5, 23.1, 23.0, 21.7. Anal. Calcd for  $\text{C}_{24}\text{H}_{22}\text{N}_2\text{O}_4\text{S}$ : C, 66.34; H, 5.10; N, 6.45; S, 7.38%. Found: C, 66.41; H, 5.87; N, 6.18; S, 7.22%. HRMS (ESI-TOF): found 435,1379. Calcd. for  $[\text{C}_{24}\text{H}_{22}\text{N}_2\text{O}_4\text{S}+\text{H}]^+$  435,1383.

*(4-(4,5,6,7-Tetrahydro-1H-indol-2-yl)-5-tosyl-1H-pyrrol-3-yl)(thiophen-2-yl)methanone (2g)*



Yield 293 mg (65%). Yellow crystals, mp 198-200 °C. IR (KBr,  $\text{cm}^{-1}$ ): 3289 (NH), 3131 (=CH), 2924, 2851 (CH), 1613 (CO), 1595, 1514 (C=C), 1358, 1140 ( $\text{SO}_2$ ).  $^1\text{H}$  NMR (400.13 MHz,  $\text{CDCl}_3$ ):  $\delta$  10.23 (br.s, 1H, NH, CO-pyrrole), 10.02 (br.s, 1H, NH, pyrrole), 7.66-7.62 (m, 3H, Ph, H-5, thiophene), 7.56-7.55 (m, 1H, H-3, thiophene), 7.43 (d,  $J = 3.4$  Hz, 1H, H-2, CO-pyrrole), 7.17-7.15 (m, 2H, Ph), 7.10-7.08 (m, 1H, H-4 thiophene), 6.63-6.60 (m, 1H, H-3, pyrrole), 2.60-2.57 (m, 2H,  $\text{CH}_2$ -7), 2.51-2.48 (m, 2H,  $\text{CH}_2$ -4), 2.35 (s, 3H,  $\text{CH}_3$ ), 1.84-1.76 (m, 2H,  $\text{CH}_2$ -5), 1.74-1.69 (m, 2H,  $\text{CH}_2$ -6).  $^{13}\text{C}$  NMR (100.61 MHz,  $\text{CDCl}_3$ ):  $\delta$  183.5, 145.3, 144.5, 137.7, 134.3, 134.1, 129.6 (2C), 129.2, 128.1, 127.8, 127.3 (2C), 124.3, 123.7, 123.4, 119.4, 118.6, 112.3, 24.0, 23.6, 23.1, 23.0, 21.7. Anal. Calcd for  $\text{C}_{24}\text{H}_{22}\text{N}_2\text{O}_3\text{S}_2$ : C, 63.98; H, 4.92; N, 6.22; S, 14.23%. Found: C, 63.75; H, 5.07; N, 6.08; S, 14.12%. HRMS (ESI-TOF): found 451,1150. Calcd. for  $[\text{C}_{24}\text{H}_{22}\text{N}_2\text{O}_3\text{S}_2+\text{H}]^+$  451,1154.

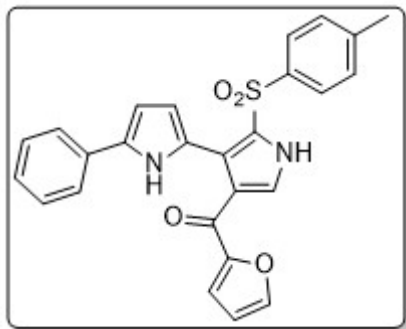
*Phenyl(5-phenyl-2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)methanone (2h)*



Yield 247 mg (53%). Yellow crystals, mp 205-207 °C. IR (KBr,  $\text{cm}^{-1}$ ): 3281 (NH), 3147 (=CH), 2923 (CH), 1629 (CO), 1597, 1677, 1508, 1477 (C=C), 1349, 1139 ( $\text{SO}_2$ ).  $^1\text{H}$  NMR (400.13 MHz,  $\text{CDCl}_3$ ):  $\delta$  11.77 (br.s, 1H, NH, CO-pyrrole), 9.89 (br.s, 1H, NH, pyrrole), 7.78-7.76 (m, 2H, Ph), 7.68-7.66 (m, 2H, Ph), 7.65-7.63 (m, 2H, Ph), 7.58-7.54 (m, 1H, Ph), 7.46-7.43 (m, 2H, Ph), 7.40-7.36 (m, 2H, Ph), 7.28 (d,  $J = 3.2$  Hz, 1H, H-5, CO-pyrrole), 7.21-7.19 (m, 1H, Ph), 7.18-7.16 (m, 2H, Ph), 7.04-7.02 (m, 1H, H-4, pyrrole), 6.56-6.55 (m, 1H, H-3, pyrrole), 2.32 (s, 3H,  $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100.6 MHz,  $\text{CDCl}_3$ ):  $\delta$  192.7, 144.9, 139.6, 137.4, 133.1, 132.7, 132.6, 129.9 (2C), 129.8 (2C), 129.0 (2C), 128.5 (2C), 127.2 (2C),

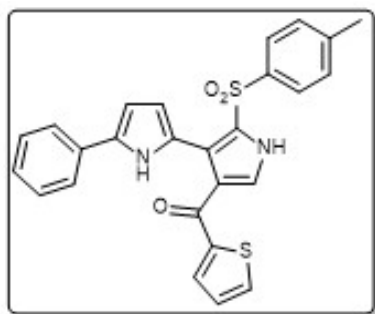
126.4, 125.1, 124.2, 123.9 (2C), 122.8, 122.8, 122.7, 120.2, 114.9, 107.4, 21.7. Anal. Calcd for  $C_{28}H_{22}N_2O_3S$ : C, 72.08; H, 4.75; N, 6.00; S, 6.87%. Found: C, 71.81; H, 4.85; N, 5.89; S, 6.75%. HRMS (ESI-TOF): found 467,1429. Calcd. for  $[C_{28}H_{22}N_2O_3S+H]^+$  467,1431.

*Furan-2-yl(5-phenyl-2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)methanone (2i)*



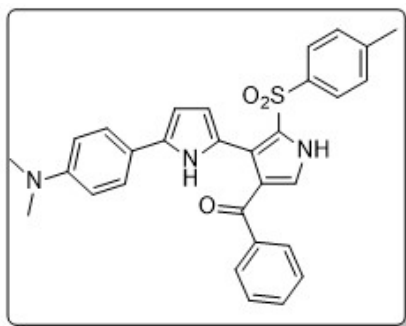
Yield 215 mg (47%). Yellow crystals, mp 90-92 °C. IR (KBr,  $cm^{-1}$ ): 3278 (NH), 3150 (=CH), 2923 (CH), 1619 (CO), 1519, 1561, 1531, 1509 (C=C), 1351, 1140 (SO<sub>2</sub>). <sup>1</sup>H NMR (400.13 MHz, CDCl<sub>3</sub>):  $\delta$  11.58 (br.s, 1H, NH of CO-pyrrole), 7.70-7.66 (m, 2H, H-5, furan, H-5, CO-pyrrole), 7.64-7.62 (m, 4H, Ph), 7.39-7.35 (m, 2H, Ph), 7.21-7.17 (m, 1H, Ph), 7.15-7.12 (m, 3H, H-3, furan, Ph), 7.05-7.03 (m, 1H, H-3, pyrrole), 6.57-5.55 (m, 1H, H-4, pyrrole), 6.52 (dd,  $J = 3.4, 1.5$  Hz, 1H, H-4, furan), 2.29 (s, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (100.6 MHz, CDCl<sub>3</sub>):  $\delta$  178.0, 153.0, 147.2, 144.8, 137.4, 132.9, 132.5, 129.8 (2C), 129.1, 129.0 (2C), 127.1 (2C), 126.3, 125.1, 123.8 (2C), 122.8 (2C), 122.6, 120.4, 114.7, 112.5, 107.3, 21.6. Anal. Calcd for  $C_{26}H_{20}N_2O_4S$ : C, 68.41; H, 4.42; N, 6.14; S, 7.02%. Found: C, 68.11; H, 4.29; N, 6.22; S, 6.91%. HRMS (ESI-TOF): found 457,1222. Calcd. for  $[C_{26}H_{20}N_2O_4S+H]^+$  457,1220.

*(5-Phenyl-2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)(thiophen-2-yl)methanone (2j)*



Yield 198 mg (42%). Yellow crystals, mp 105-107 °C. IR (KBr,  $cm^{-1}$ ): 3295 (NH), 3137 (=CH), 2922, 2853 (CH), 1613 (CO), 1582, 1562, 1511 (C=C), 1359, 1140 (SO<sub>2</sub>). <sup>1</sup>H NMR (400.13 MHz, CDCl<sub>3</sub>):  $\delta$  11.26 (br.s, 1H, NH, CO-pyrrole), 9.72 (br.s, 1H, NH, pyrrole), 7.68-7.67 (m, 1H, H-5 of thiophene), 7.65-7.60 (m, 5H, Ph, H-3, thiophene), 7.50-7.49 (m, 1H, H-5, CO-pyrrole), 7.40-7.36 (m, 2H, Ph), 7.22-7.18 (m, 1H, Ph), 7.16-7.14 (m, 2H, Ph), 7.12-7.10 (m, 1H, H-4, thiophene), 6.97 (dd,  $J = 3.6, 2.5$  Hz, 1H, H-3, pyrrole), 6.55-6.54 (m, 1H, H-4, pyrrole). <sup>13</sup>C NMR (100.6 MHz, CDCl<sub>3</sub>):  $\delta$  178.0, 153.0, 147.2, 144.8, 137.4, 132.9, 132.4, 129.7 (2C), 128.9 (2C), 128.0, 127.6, 127.0 (2C), 126.2, 125.1, 123.9, 123.7 (2C), 122.5, 122.1, 114.5, 107.1, 21.5. Anal. Calcd for  $C_{26}H_{20}N_2O_3S_2$ : C, 66.08; H, 4.27; N, 5.93; S, 13.57%. Found: C, 66.25; H, 4.46; N, 6.07; S, 13.38%. HRMS (ESI-TOF): found 473,0994. Calcd. for  $[C_{26}H_{20}N_2O_3S_2+H]^+$  473,0998.

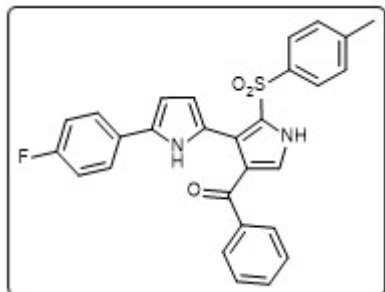
*(5-(4-(Dimethylamino)phenyl)-2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (2k)*



Yield 270 mg (53%). Yellow crystals, mp 213-215 °C. IR (KBr,  $cm^{-1}$ ): 3240 (NH), 2924, 2853 (CH), 1613 (CO), 1512, 1491 (C=C), 1350, 1141 (SO<sub>2</sub>). <sup>1</sup>H NMR (400.13 MHz, CDCl<sub>3</sub>):  $\delta$  11.58 (br.s, 1H, NH, CO-pyrrole), 10.03 (br.s, 1H, NH, pyrrole), 7.75-7.73 (m, 2H, Ph), 7.67-6.65 (m, 2H, Ph), 7.54-7.52 (m, 3H, Ph), 7.44-7.40 (m, 2H, Ph), 7.24-7.19 (m, 1H, H-5, CO-pyrrole), 7.16-7.14 (m, 2H, Ph), 6.98-6.96 (m, 1H, H-4, pyrrole), 6.78-6.76 (m, 2H, Ph), 6.40-6.38 (m, 1H, H-3 pyrrole), 2.96 (s,

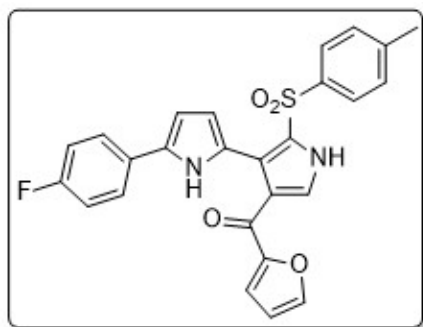
6H, N(CH<sub>3</sub>)<sub>2</sub>), 2.31 (s, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (100.6 MHz, CDCl<sub>3</sub>): δ 192.6, 149.4, 144.7, 139.7, 137.6, 133.9, 132.5, 130.0, 129.8 (2C), 129.7 (2C), 128.4 (2C), 127.1 (3C), 125.0 (2C), 124.3, 123.9, 123.2, 121.6, 121.3, 114.9, 113.2, 105.6, 40.8 (2C), 21.7. Anal. Calcd for C<sub>30</sub>H<sub>27</sub>N<sub>3</sub>O<sub>3</sub>S: C, 70.71; H, 5.34; N, 8.25; S, 6.29%. Found: C, 70.82; H, 5.48; N, 8.38; S, 6.18%. HRMS (ESI-TOF): found 510,1851. Calcd. for [C<sub>30</sub>H<sub>27</sub>N<sub>3</sub>O<sub>3</sub>S+H]<sup>+</sup> 510,1848.

*(5-(4-Fluorophenyl)-2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (2l)*



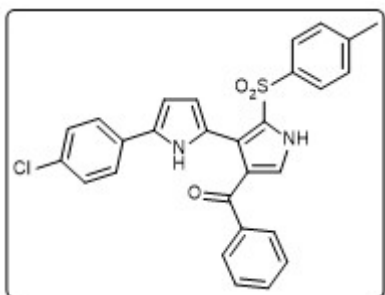
Yield 252 mg (52%). Yellow crystals, mp 130-132 °C. IR (KBr, cm<sup>-1</sup>): 3233 (NH), 3063 (=CH), 2969 (CH), 1613 (CO), 1597, 1486 (C=C), 1351, 1145 (SO<sub>2</sub>). <sup>1</sup>H NMR (400.13 MHz, DMSO-d<sub>6</sub>): δ 11.79 (br.s, 1H, NH, CO-pyrrole), 9.94 (br.s, 1H, NH, pyrrole), 7.77-7.75 (m, 2H, Ph), 7.68-7.66 (m, 2H, Ph), 7.60-7.55 (m, 3H, Ph), 7.47-7.43 (m, 2H, Ph), 7.28 (d, *J* = 3.5 Hz, 1H, H-5, CO-pyrrole), 7.19-7.17 (m, 2H, Ph), 7.09-7.03 (m, 3H, H-4, pyrrole, Ph), 6.49-6.47 (m, 1H, H-3, pyrrole), 2.33 (s, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (100.6 MHz DMSO-d<sub>6</sub>): δ 190.4, 160.5 (d, *J* = 242.4 Hz), 144.1, 138.8 (d, *J* = 29.4 Hz, 2C), 131.9, 130.9, 130.1, 129.8 (2C), 129.3 (d, *J* = 2.8 Hz), 129.0 (2C), 128.1 (2C), 126.7, 126.5 (2C), 125.3 (d, *J* = 7.8 Hz, 2C), 123.6, 122.5, 121.7, 115.6, 115.4, 112.7, 106.2, 21.0. Anal. Calcd for C<sub>28</sub>H<sub>21</sub>FN<sub>2</sub>O<sub>3</sub>S: C, 69.41; H, 4.37; F, 3.92; N, 5.78; S, 6.62%. Found: C, 69.56; H, 4.50; N, 5.95; S, 6.51; F, 4.04%.

*(5-(4-Fluorophenyl)-2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)(furan-2-yl)methanone (2m)*



Yield 228 mg (48%). Yellow crystals, mp 118-120 °C. IR (KBr, cm<sup>-1</sup>): 3281 (NH), 3152 (=CH), 2923, 2856 (CH), 1621 (CO), 1602, 1561, 1512, 1488 (C=C), 1351, 1141 (SO<sub>2</sub>). <sup>1</sup>H NMR (400.13 MHz, CDCl<sub>3</sub>): δ 11.58 (br.s, 1H, NH, CO-pyrrole), 7.72-7.70 (m, 1H, H-5, furan), 7.67-7.65 (m, 2H, Ph), 7.64-7.62 (m, 1H, H-3, furan), 7.59-7.55 (m, 2H, Ph), 7.17 (d, *J* = 3.6 Hz, 1H, H-5, CO-pyrrole), 7.16-7.14 (m, 2H, Ph), 7.08-7.03 (m, 3H, H-3 pyrrole, Ph), 6.54 (dd, *J* = 3.3, 1.5 Hz, 1H, H-4, furan), 6.49-6.48 (m, 1H, H-4 pyrrole), 2.31 (s, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (100.6 MHz, CDCl<sub>3</sub>): δ 178.0, 161.7 (d, *J* = 245.4 Hz), 153.1, 147.3, 144.9, 137.5, 132.2, 129.8 (2C), 129.0, 128.9 (d, *J* = 2.8 Hz), 127.2 (2C), 125.5 (d, *J* = 7.9 Hz, 2C), 125.1, 122.8, 122.7, 122.7, 120.5, 115.9 (d, *J* = 21.8 Hz, 2C), 114.8, 112.6, 107.1, 21.7. Anal. Calcd for C<sub>26</sub>H<sub>19</sub>FN<sub>2</sub>O<sub>4</sub>S: C, 65.81; H, 4.04; F, 4.00; N, 5.90; S, 6.76%. Found: C, 65.99; H, 4.21; F, 4.18; N, 6.09; S, 6.66%. HRMS (ESI-TOF): found 475,1128. Calcd. for [C<sub>26</sub>H<sub>19</sub>FN<sub>2</sub>O<sub>4</sub>S+H]<sup>+</sup> 475,1133.

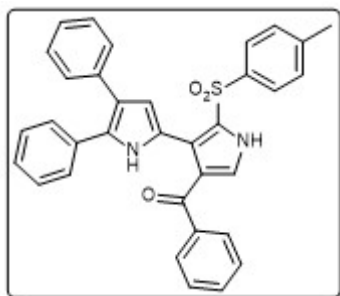
*(5-(4-Chlorophenyl)-2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (2n)*



Yield 225 mg (45%). Yellow crystals, mp 218-220 °C. IR (KBr, cm<sup>-1</sup>): 3275 (NH), 3118, 3092 (=CH), 1630 (CO), 1596, 1576, 1505, 1477 (C=C), 1351, 1145 (SO<sub>2</sub>). <sup>1</sup>H NMR (400.13 MHz, CDCl<sub>3</sub>): δ 11.83 (br.s, 1H, NH, CO-pyrrole), 9.89 (br.s, 1H, NH, pyrrole), 7.78-7.76 (m, 2H, Ph), 7.68-7.66

(m, 2H, Ph), 7.59-7.54 (m, 3H, Ph), 7.47-7.43 (m, 2H, Ph), 7.34-7.32 (m, 2H, Ph), 7.29 (d,  $J = 3.5$  Hz, 1H, H-5, CO-pyrrole), 7.19-7.17 (m, 2H, Ph), 7.05 (dd,  $J = 3.6, 2.4$  Hz, 1H, H-4, pyrrole), 6.54-6.52 (m, 1H, H-3, pyrrole), 2.33 (s, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (100.61 MHz, CDCl<sub>3</sub>):  $\delta$  192.8, 144.9, 139.6, 137.4, 132.7, 131.8, 131.7, 131.1, 130.3, 129.9 (2C), 129.8 (2C), 129.2 (2C), 128.5 (2C), 127.1 (2C), 125.1, 125.0 (2C), 124.0, 123.2, 122.6, 114.9, 107.8, 21.7. Anal. Calcd for C<sub>28</sub>H<sub>21</sub>ClN<sub>2</sub>O<sub>3</sub>S: C, 67.13; H, 4.23; Cl, 7.08; N, 5.59; S, 6.40%. Found: C, 67.33; H, 4.38; N, 5.70; S, 6.29%. HRMS (ESI-TOF): found 501,1040. Calcd. for [C<sub>28</sub>H<sub>21</sub>ClN<sub>2</sub>O<sub>3</sub>S+H]<sup>+</sup> 501,1044.

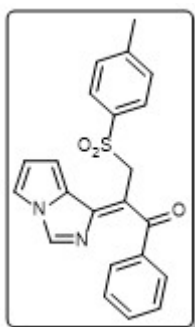
*(4,5-Diphenyl-2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (2o)*



Yield 250 mg (46%). Yellow crystals, mp 203-205 °C. IR (KBr, cm<sup>-1</sup>): 3296 (NH), 3059 (=CH), 2923 (CH), 1632 (CO), 1599, 1508, 1477 (C=C), 1351, 1132 (SO<sub>2</sub>). <sup>1</sup>H NMR (400.13 MHz, CDCl<sub>3</sub>):  $\delta$  11.36 (br.s, 1H, NH, CO-pyrrole), 9.82 (br.s, 1H, NH, pyrrole), 7.80-7.77 (m, 2H, Ph), 7.73-7.70 (m, 2H, Ph), 7.61-7.55 (m, 1H, H-5, CO-pyrrole), 7.48-7.45 (m, 4H, Ph), 7.36-7.27 (m, 7H, Ph), 7.24-7.20 (m, 4H, Ph), 7.05-7.03 (m, 1H, pyrrole), 2.36 (s, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (100.6 MHz, CDCl<sub>3</sub>):  $\delta$  192.6, 144.9, 139.6, 137.4, 137.0, 133.2, 132.7, 129.8 (3C), 129.6, 129.2, 128.8 (2C), 128.7 (2C), 128.5 (2C), 128.4 (2C), 127.4 (2C), 127.1 (2C), 126.8, 126.0, 125.5, 124.4, 123.6, 122.4, 121.8, 120.8, 115.7, 21.7. Anal. Calcd for C<sub>34</sub>H<sub>26</sub>N<sub>2</sub>O<sub>3</sub>S: C, 74.95; H, 4.68; N, 5.13; S, 5.91%. Found: C, 75.45; H, 4.98; N, 5.30; S, 5.79%. HRMS (ESI-TOF): found 543,1742. Calcd. for [C<sub>34</sub>H<sub>26</sub>N<sub>2</sub>O<sub>3</sub>S+H]<sup>+</sup> 543,1739.

## 4.2. Characterization data of pyrrolo[1,2-c]imidazoles 3a-j

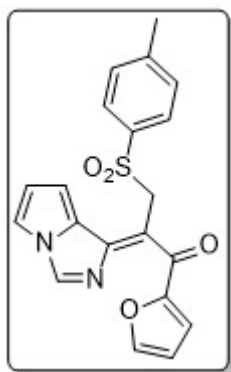
*(E)-1-Phenyl-2-(1H-pyrrolo[1,2-c]imidazol-1-ylidene)-3-tosylpropan-1-one (3a)*



Yield 144 mg (37%). Yellow crystals, mp 183-185°C. IR (KBr, cm<sup>-1</sup>): 3063(=CH), 2923, 1689 (CO), 1596, 1581, 1523, 1493 (C=C), 1320, 1153 (SO<sub>2</sub>). <sup>1</sup>H NMR (400.13 MHz, CDCl<sub>3</sub>):  $\delta$  8.64 (s, 1H, H-3, pyrroloimidazole), 8.14-8.12 (m, 2H, Ph), 7.90-7.88 (m, 2H, Ph), 7.66-7.62 (m, 1H, Ph), 7.56-7.53 (m, 2H, Ph), 7.44-7.43 (m, 1H, H-5, pyrroloimidazole), 7.29-7.27 (m, 2H, Ph), 6.94-6.93 (m, 1H, H-6, pyrroloimidazole), 6.67-6.65 (m, 1H, H-7, pyrroloimidazole), 5.17 (s, 2H, CH<sub>2</sub>), 2.39 (s, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (100.6 MHz, CDCl<sub>3</sub>):  $\delta$  195.2, 144.4, 138.3, 137.6, 136.9, 136.8, 133.7, 132.1, 129.6 (2C), 128.9 (2C), 128.8 (2C), 128.5 (2C), 124.2, 118.3, 114.2, 104.8, 38.1, 21.8. Anal. Calcd for C<sub>22</sub>H<sub>18</sub>N<sub>2</sub>O<sub>3</sub>S: C, 67.68; H, 4.65; N, 7.17; S, 8.21 %. Found: C, 67.80; H, 4.83; N, 7.30; S, 8.09%. HRMS (ESI-TOF): found 391,1116. Calcd. for [C<sub>22</sub>H<sub>18</sub>O<sub>3</sub>SN<sub>2</sub>+H]<sup>+</sup> 391,1120.

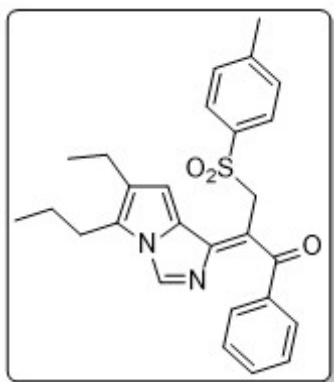


*(E)*-1-(Furan-2-yl)-2-(1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3b**)



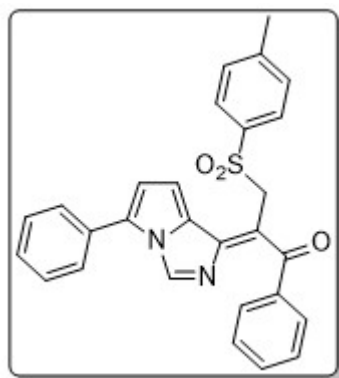
Yield 133 mg (35%). Yellow crystals, mp 90-92 °C. IR (KBr,  $\text{cm}^{-1}$ ): 3132 (=CH), 2923, 2853 (CH), 1679 (CO), 1621, 1595, 1521, 1467 (C=C), 1320, 1153 ( $\text{SO}_2$ ).  $^1\text{H}$  NMR (400.13 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.63 (s, 1H, H-3, pyrroloimidazole), 7.93-7.91 (m, 2H, Ph), 7.66-7.67 (m, 1H, H-5, furan), 7.43-7.41 (m, 1H, H-3, furan), 7.38-7.37 (m, 1H, H-5, pyrroloimidazole), 7.30-7.28 (m, 2H, Ph), 6.94-6.92 (m, 1H, H-6, pyrroloimidazole), 6.72-6.71 (m, 1H, H-7, pyrroloimidazole), 6.62 (dd,  $J = 3.4, 1.5$  Hz, 1H, H-4, furan), 5.05 (s, 2H,  $\text{CH}_2$ ), 2.40 (s, 3H,  $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100.6 MHz,  $\text{CDCl}_3$ ):  $\delta$  184.1, 152.4, 146.8, 144.4, 138.5, 137.6, 136.9, 132.0, 129.6 (2C), 128.9 (2C), 123.2, 118.4, 117.8, 114.2, 112.7, 104.9, 37.6, 21.8. Anal. Calcd for  $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_4\text{S}$ : C, 63.30; H, 4.24; N, 7.21; S, 8.43%. Found: C, 63.30; H, 4.39; N, 7.48; S, 8.31%. HRMS (ESI-TOF): found 381,0909. Calcd. for  $[\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_4\text{S}+\text{H}]^+$  381,0911.

*(E)*-2-(6-Ethyl-5-propyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (**3c**)



Yield 147 mg (32%). Yellow crystals, mp 153-155°C. IR (KBr,  $\text{cm}^{-1}$ ): 3129 (=CH), 2963, 2932, 2872 (CH), 1690 (CO), 1597, 1581, 1495 (C=C), 1318, 1129 ( $\text{SO}_2$ ).  $^1\text{H}$  NMR (400.13 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.51 (s, 1H, H-3, pyrroloimidazole), 8.15-8.13 (m, 2H, Ph), 7.90-7.88 (m, 2H, Ph), 7.65-7.61 (m, 1H, Ph), 7.56-7.52 (m, 2H, Ph), 7.28-7.26 (m, 2H, Ph), 6.55-6.53 (m, 1H, H-6, pyrroloimidazole), 5.13 (s, 2H,  $\text{CH}_2$ ), 2.85-2.81 (m, 2H,  $\text{CH}_2$ ), 2.62-2.57 (m, 2H,  $\text{CH}_2$ ), 2.38 (s, 3H,  $\text{CH}_3$ ), 1.63-1.57 (m, 2H,  $\text{CH}_2$ ), 1.19 (t,  $J = 7.5$  Hz, 3H,  $\text{CH}_3$ ), 0.94 (t,  $J = 7.3$  Hz, 3H,  $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100.6 MHz,  $\text{CDCl}_3$ ):  $\delta$  195.5, 144.1, 137.9, 136.9, 136.6, 133.9, 133.8, 133.5, 130.9, 129.5 (2C), 128.9 (2C), 128.7 (2C), 128.5 (2C), 124.3, 123.1, 103.9, 38.2, 25.6, 21.7, 21.6, 19.5, 15.2, 14.0. Anal. Calcd for  $\text{C}_{27}\text{H}_{28}\text{N}_2\text{O}_3\text{S}$ : C, 70.41; H, 6.13; N, 6.08; S, 6.96%. Found: C, 70.14; H, 6.15; N, 6.98; S, 6.77%. HRMS (ESI-TOF): found 461,1899. Calcd. for  $[\text{C}_{27}\text{H}_{28}\text{N}_2\text{O}_3\text{S}+\text{H}]^+$  461,1900.

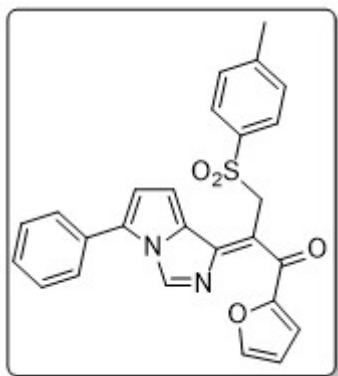
*(E)*-1-Phenyl-2-(5-phenyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3d**)



Yield 149 mg (32%). Yellow crystals, mp 165-167°C. IR (KBr,  $\text{cm}^{-1}$ ): 3134, 3061 (=CH), 2923, 2853 (CH), 1688 (CO), 1596, 1455 (C=C), 1318, 1145 ( $\text{SO}_2$ ).  $^1\text{H}$  NMR (400.13 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.91 (s, 1H, H-3, pyrroloimidazole), 8.17-8.15 (m, 2H, Ph), 7.90-7.88 (m, 2H, Ph), 7.68-7.64 (m, 1H, Ph), 7.58-7.55 (m, 2H, Ph), 7.49-7.48 (m, 4H, Ph), 7.43-7.39 (m, 1H, Ph), 7.29-7.27 (m, 2H, Ph), 6.98 (d,  $J = 3.7$  Hz, 1H, H-6, pyrroloimidazole), 6.76 (d,  $J = 3.7$  Hz, 1H, H-7, pyrroloimidazole), 5.20 (s, 2H,  $\text{CH}_2$ ), 2.39 (s, 3H,  $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100.61 MHz,  $\text{CDCl}_3$ ):  $\delta$  195.4, 144.4, 138.3, 137.6, 136.9, 135.1, 133.7, 132.8, 130.1, 129.5 (2C), 129.4 (2C), 129.0 (2C), 128.9 (2C), 128.8, 128.6 (3C), 128.5 (2C), 124.2, 118.2,

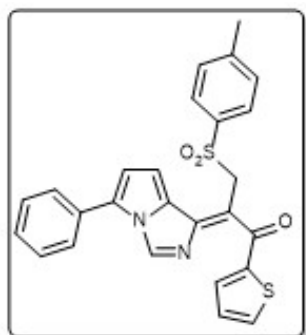
105.2, 38.1, 21.8. Anal. Calcd for  $C_{28}H_{22}N_2O_3S$ : C, 72.08; H, 4.75; N, 6.00; S, 6.87%. Found: C, 72.24; H, 4.94; N, 6.15; S, 6.74%. HRMS (ESI-TOF): found 467,1429. Calcd. for  $[C_{28}H_{22}N_2O_3S+H]^+$  467,1435.

*(E)*-1-(Furan-2-yl)-2-(5-phenyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3e**)



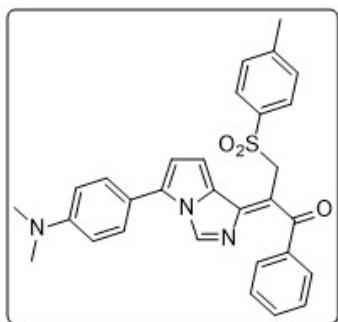
Yield 160 mg (35%). Yellow crystals, mp 183-185°C. IR (KBr,  $cm^{-1}$ ): 3133, 3063 (=CH), 2924 (CH), 1680 (CO), 1596, 1589, 1537 (C=C), 1317, 1145 ( $SO_2$ ).  $^1H$  NMR (400.13 MHz,  $CDCl_3$ ):  $\delta$  8.90 (s, 1H, H-3, pyrroloimidazole), 7.95-7.93 (m, 2H, Ph), 7.70-7.69 (m, 1H, H-5, furan), 7.52-7.48 (m, 4H, Ph), 7.42-7.41 (m, 2H, *p*-Ph, H-3, furan), 7.31-7.29 (m, 2H, Ph), 6.99 (d,  $J$  = 4.1 Hz, 1H, H-6, pyrroloimidazole), 6.82 (d,  $J$  = 4.1 Hz, 1H, H-7, pyrroloimidazole), 6.64 (dd,  $J$  = 3.6, 1.7 Hz, 1H, H-4, furan), 5.09 (s, 2H,  $CH_2$ ), 2.40 (s, 3H,  $CH_3$ ).  $^{13}C$  NMR (100.6 MHz,  $CDCl_3$ ):  $\delta$  184.0, 152.2, 146.6, 144.2, 138.3, 137.4, 134.9, 132.5, 129.8, 129.3 (2C), 129.2 (2C), 128.8 (2C), 128.7, 128.6, 128.4 (2C), 123.0, 118.0, 117.6, 112.5, 105.1, 37.5, 21.6. Anal. Calcd for  $C_{26}H_{20}N_2O_4S$ : C, 68.04; H, 4.42; N, 6.14; S, 7.02%. Found: C, 68.54; H, 4.56; N, 6.27; S, 6.88%. HRMS (ESI-TOF): found 457,1222. Calcd. for  $[C_{26}H_{20}N_2O_4S+H]^+$  457,1229.

*(E)*-2-(5-Phenyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-(thiophen-2-yl)-3-tosylpropan-1-one (**3f**)



Yield 175 mg (37%). Yellow crystals, mp 155-157°C. IR (KBr,  $cm^{-1}$ ): 3120, 3097 (=CH), 2861 (CH), 1663 (CO), 1595, 1518, 1494 (C=C), 1318, 1122 ( $SO_2$ ).  $^1H$  NMR (400.13 MHz,  $CDCl_3$ ):  $\delta$  8.87 (s, 1H, H-3, pyrroloimidazole), 7.99-7.98 (m, 1H, H-5, thiophene), 7.90-7.87 (m, 2H, Ph), 7.70-7.68 (m, 1H, H-3, thiophene), 7.45-7.40 (m, 4H, Ph), 7.39-7.34 (m, 1H, Ph), 7.27-7.25 (m, 2H, Ph), 7.21-7.18 (m, 1H, H-3, thiophene), 6.94-6.93 (m, 1H, H-6, pyrroloimidazole), 6.78-6.77 (m, 1H, H-7, pyrroloimidazole), 5.12 (s, 2H,  $CH_2$ ), 2.35 (s, 3H,  $CH_3$ ).  $^{13}C$  NMR (100.6 MHz,  $CDCl_3$ ):  $\delta$  187.9, 144.4, 143.5, 138.3, 137.5, 135.1, 134.2, 132.8, 132.6, 129.9, 129.5 (2C), 129.4 (2C), 128.9, 128.8 (2C), 128.6, 128.5 (2C), 128.4, 123.4, 118.2, 105.4, 38.4, 21.7. Anal. Calcd for  $C_{26}H_{20}N_2O_3S_2$ : C, 66.08; H, 4.27; N, 5.93; S, 13.57%. Found: C, 65.91; H, 4.05; N, 6.11; S, 13.39%. HRMS (ESI-TOF): found 473,0994. Calcd. for  $[C_{26}H_{20}N_2O_3S_2+H]^+$  473,0995.

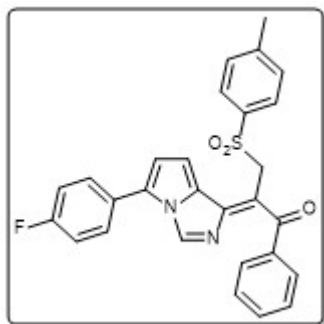
*(E)*-2-(5-(4-(Dimethylamino)phenyl)-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (**3g**)



Yield 143 mg (28%). Yellow crystals, mp 108-110°C. IR (KBr,  $cm^{-1}$ ): 3018 (=CH), 2924 (CH), 1688 (CO), 1612, 1597 (C=C), 1318, 1145 ( $SO_2$ ).  $^1H$  NMR (400.13 MHz,  $CDCl_3$ ):  $\delta$  8.89 (s, 1H, H-3, pyrroloimidazole), 8.17-8.15 (m, 2H, Ph), 7.90-7.88 (m, 2H, Ph), 7.67-7.62 (m, 1H, Ph), 7.57-7.54 (m, 2H, Ph), 7.35-7.33 (m, 2H, Ph), 7.28-7.26 (m, 2H, Ph), 6.87 (d,  $J$  = 3.9 Hz, 1H, H-6, pyrroloimidazole), 6.79-6.77 (m, 2H, Ph), 6.73 (d,  $J$  = 3.9 Hz, 1H, H-7, pyrroloimidazole).

pyrroloimidazole), 5.18 (s, 2H, CH<sub>2</sub>), 3.02 (s, 6H, N(CH<sub>3</sub>)<sub>2</sub>), 2.39 (s, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (100.6 MHz, CDCl<sub>3</sub>): δ 195.5, 150.6, 144.2, 137.8, 137.4, 136.9, 135.3, 133.6, 132.0, 130.5, 129.8, 129.6 (3C), 129.5 (2C), 128.9 (2C), 128.8 (2C), 128.5 (3C), 124.2, 117.3, 112.6, 105.1, 38.1 (2C), 21.8. Anal. Calcd for C<sub>30</sub>H<sub>27</sub>N<sub>3</sub>O<sub>3</sub>S: C, 70.71; H, 5.34; N, 8.25; S, 6.29%. Found: C, 70.85; H, 5.53; N, 8.39; S, 6.12%. HRMS (ESI-TOF): found 510,1851. Calcd. for [C<sub>30</sub>H<sub>27</sub>N<sub>3</sub>O<sub>3</sub>S+H]<sup>+</sup> 510,1856.

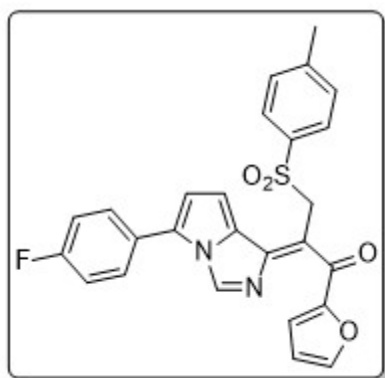
*(E)-2-(5-(4-Fluorophenyl)-1H-pyrrolo[1,2-c]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (3h)*



Yield 184 mg (38%). Yellow crystals, mp 95-97°C. IR (KBr, cm<sup>-1</sup>): 3131, 3063 (=CH), 2923 (CH), 1689 (CO), 1596, 1539, 1510, 1493 (C=C), 1316, 1146 (SO<sub>2</sub>). <sup>1</sup>H NMR (400.13 MHz, CDCl<sub>3</sub>): δ 8.81 (s, 1H, H-3, pyrroloimidazole), 8.16-8.14 (m, 2H, Ph), 7.90-7.88 (m, 2H, Ph), 7.67-7.63 (m, 1H, Ph), 7.58-7.54 (m, 2H, Ph), 7.47-7.44 (m, 2H, Ph), 7.29-7.27 (m, 2H, Ph), 7.20-7.16 (m, 2H, Ph), 6.93 (d, *J* = 4.0 Hz, 1H, H-6, pyrroloimidazole), 6.75 (d, *J* = 4.0 Hz, 1H, H-7, pyrroloimidazole), 5.20 (s, 2H, CH<sub>2</sub>), 2.39 (s, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (100.6

MHz, CDCl<sub>3</sub>): δ 195.3, 162.9 (d, <sup>1</sup>*J*<sub>CF</sub> = 250.5 Hz, C4, 4F-C<sub>6</sub>H<sub>4</sub>), 144.4, 138.3, 137.5, 136.8, 134.8, 133.7, 132.7, 130.6 (d, <sup>3</sup>*J*<sub>CF</sub> = 8.3 Hz, C-2,6 4F-C<sub>6</sub>H<sub>4</sub>, 2C), 129.5 (2C), 129.0 (2C), 128.9 (2C), 128.5 (2C), 127.4, 126.1 (d, <sup>4</sup>*J*<sub>CF</sub> = 3.3 Hz, C-1 4F-C<sub>6</sub>H<sub>4</sub>), 124.2, 118.2, 116.6 (d, <sup>2</sup>*J*<sub>CF</sub> = 21.8 Hz, C-3,5 4F-C<sub>6</sub>H<sub>4</sub>, 2C), 105.1, 38.1, 21.8. Anal. Calcd for C<sub>28</sub>H<sub>21</sub>FN<sub>2</sub>O<sub>3</sub>S: C, 69.41; H, 4.37; F, 3.92; N, 5.78; S, 6.62%. Found: C, 69.52; H, 4.51; N, 5.97; S, 6.47; F, 4.04%. HRMS (ESI-TOF): found 485,1335. Calcd. for [C<sub>28</sub>H<sub>21</sub>FN<sub>2</sub>O<sub>3</sub>S+H]<sup>+</sup> 485,1339.

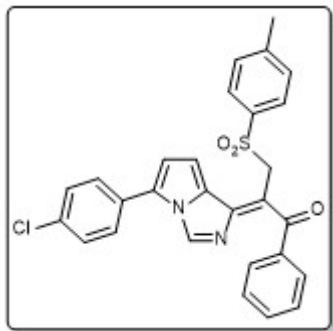
*(E)-2-(5-(4-Fluorophenyl)-1H-pyrrolo[1,2-c]imidazol-1-ylidene)-1-(furan-2-yl)-3-tosylpropan-1-one (3i)*



Yield 157 mg (33%). Yellow crystals, mp 188-190°C. IR (KBr, cm<sup>-1</sup>): 3131, 3056 (=CH), 2925 (CH), 1680 (CO), 1602, 1561, 1570, 1540, 1513 (C=C), 1317, 1161 (SO<sub>2</sub>). <sup>1</sup>H NMR (400.13 MHz, CDCl<sub>3</sub>): δ 8.80 (s, 1H, H-3, pyrroloimidazole), 7.93-7.91 (m, 2H, Ph), 7.68-7.67 (m, 1H, H-5, furan), 7.46-7.43 (m, 2H, H-3, furan), 7.41-7.40 (m, 1H, Ph), 7.30-7.28 (m, 2H, Ph), 7.19-7.15 (m, 2H, Ph), 6.93 (d, *J* = 4.0 Hz, 1H, H-6, pyrroloimidazole), 6.79 (d, *J* = 4.0 Hz, 1H, H-7, pyrroloimidazole), 6.63 (dd, *J* = 2.5, 1.4 Hz, 1H, H-4, furan), 5.08 (s, 2H, CH<sub>2</sub>), 2.39 (s, 3H, CH<sub>3</sub>).

<sup>13</sup>C NMR (100.6 MHz, CDCl<sub>3</sub>): δ 184.1, 162.9 (d, <sup>1</sup>*J*<sub>CF</sub> = 249.8 Hz, C4, 4F-C<sub>6</sub>H<sub>4</sub>), 152.3, 146.8, 144.4, 138.5, 137.5, 134.9, 132.6, 130.5 (d, <sup>3</sup>*J*<sub>CF</sub> = 8.3 Hz, C-2,6 4F-C<sub>6</sub>H<sub>4</sub>, 2C), 129.5 (2C), 128.9 (2C), 127.4, 126.1 (d, <sup>4</sup>*J*<sub>CF</sub> = 3.4 Hz, C-1 4F-C<sub>6</sub>H<sub>4</sub>), 123.2, 118.2, 117, 116.6 (d, <sup>2</sup>*J*<sub>CF</sub> = 21.8 Hz, C-3,5 4F-C<sub>6</sub>H<sub>4</sub>, 2C), 112.7, 105.3, 37.6, 21.7. Anal. Calcd for C<sub>26</sub>H<sub>19</sub>FN<sub>2</sub>O<sub>4</sub>S: C, 65.81; H, 4.04; F, 4.00; N, 5.90; S, 6.76%. Found: C, 65.99; H, 4.19; N, 6.10; S, 6.60; F, 4.12 %. HRMS (ESI-TOF): found 475,1128. Calcd. for [C<sub>26</sub>H<sub>19</sub>FN<sub>2</sub>O<sub>4</sub>S+H]<sup>+</sup> 475,1128.

*(E)*-2-(5-(4-chlorophenyl)-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (**3j**)

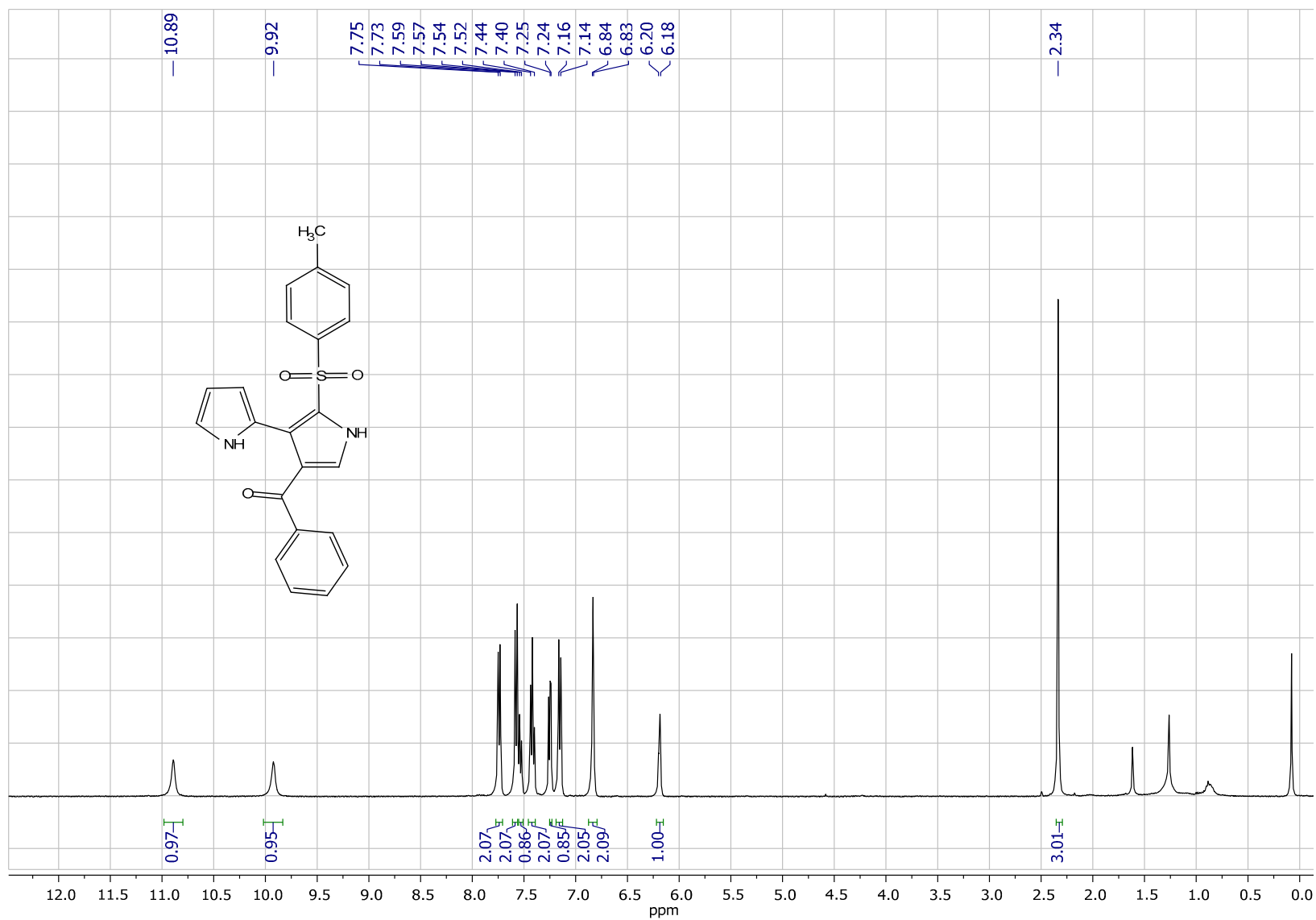


Yield 160 mg (32%). Yellow crystals, mp 135-137°C. IR (KBr,  $\text{cm}^{-1}$ ): 3056 ( $=\text{CH}$ ), 2924 (CH), 1688 (CO), 1596, 1581, 1532, 1494 ( $\text{C}=\text{C}$ ), 1315, 1145 ( $\text{SO}_2$ ).  $^1\text{H}$  NMR (400.13 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.84 (s, 1H, H-3, pyrroloimidazole), 8.16-8.14 (m, 2H, Ph), 7.90-7.88 (m, 2H, Ph), 7.67-7.64 (m, 1H, Ph), 7.58-7.54 (m, 2H, Ph), 7.47-7.41 (m, 4H, Ph), 7.29-7.27 (m, 2H, Ph), 6.96 (d,  $J = 4.1$  Hz, 1H, H-6, pyrroloimidazole), 6.76 (d,  $J = 4.1$  Hz, 1H, H-7, pyrroloimidazole), 5.20 (s, 2H,  $\text{CH}_2$ ), 2.39 (s, 3H,  $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100.6 MHz,  $\text{CDCl}_3$ ):  $\delta$  194.7, 143.8, 137.9, 136.8, 136.1, 134.3, 134.2, 133.1, 132.4, 129.1 (2C), 129.0 (2C), 128.9 (2C), 128.3 (2C), 128.2 (2C), 127.9 (2C), 127.8, 126.6, 123.6, 117.7, 104.6, 37.4, 21.1. Anal. Calcd for  $\text{C}_{28}\text{H}_{21}\text{ClN}_2\text{O}_3\text{S}$ : C, 67.13; H, 4.23; Cl, 7.08; N, 5.59; S, 6.40%. Found: C, 67.25; H, 4.39; N, 5.78; S, 6.25%.

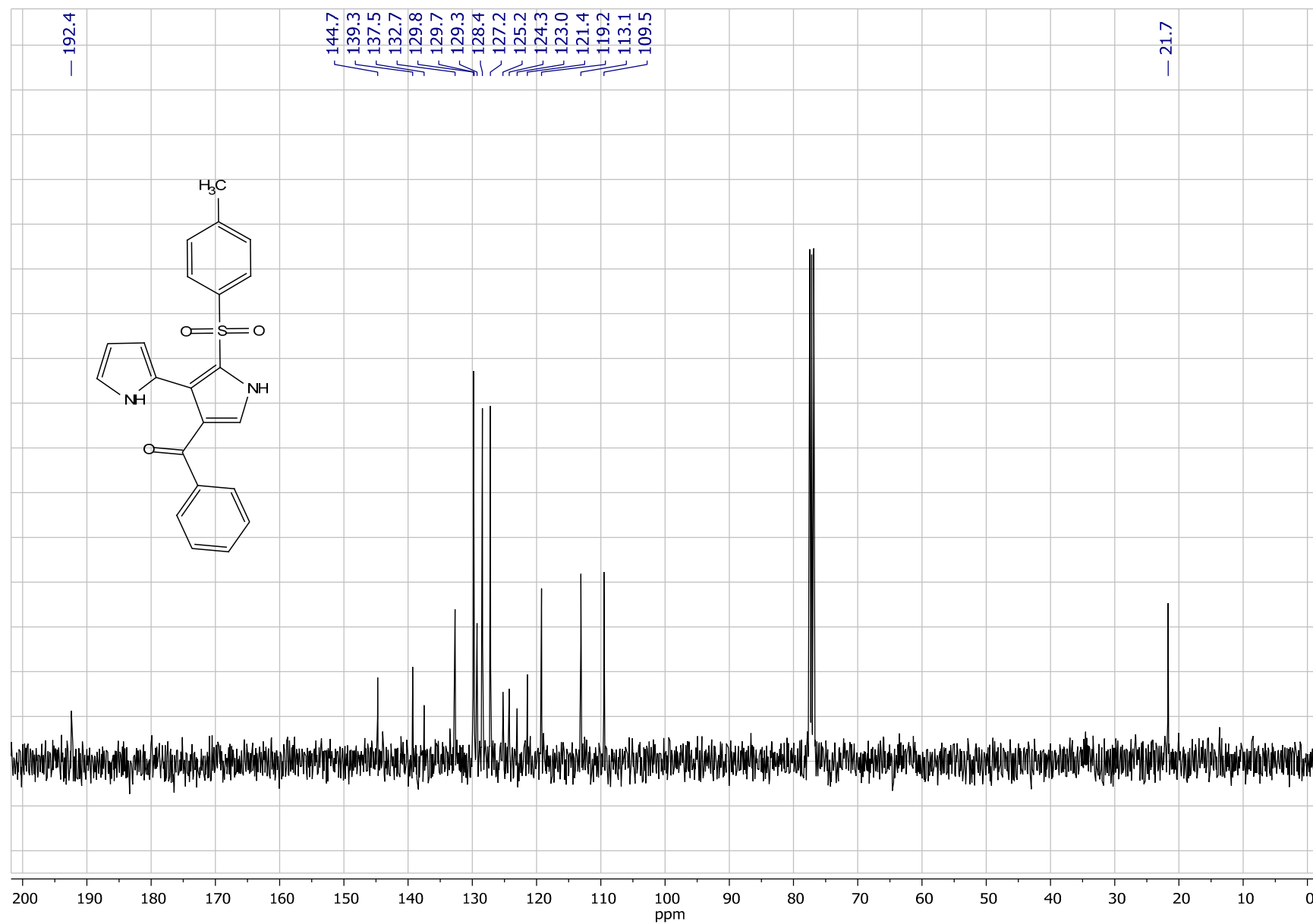
(1) Trofimov, B. A.; Stepanova, Z. V.; Sobenina, L. N.; Mikhaleva, A. b. I.; Ushakov, I. A., Ethynylation of pyrroles with 1-acyl-2-bromoacetylenes on alumina: a formal ‘inverse Sonogashira coupling’. *Tetrahedron Lett.* 2004, 45, 6513-6516.

## 5. The NMR spectra of 2,3-bipyrroles (2a-o) and pyrrolo[1,2-c]imidazoles (3a-j) and HRMS spectra

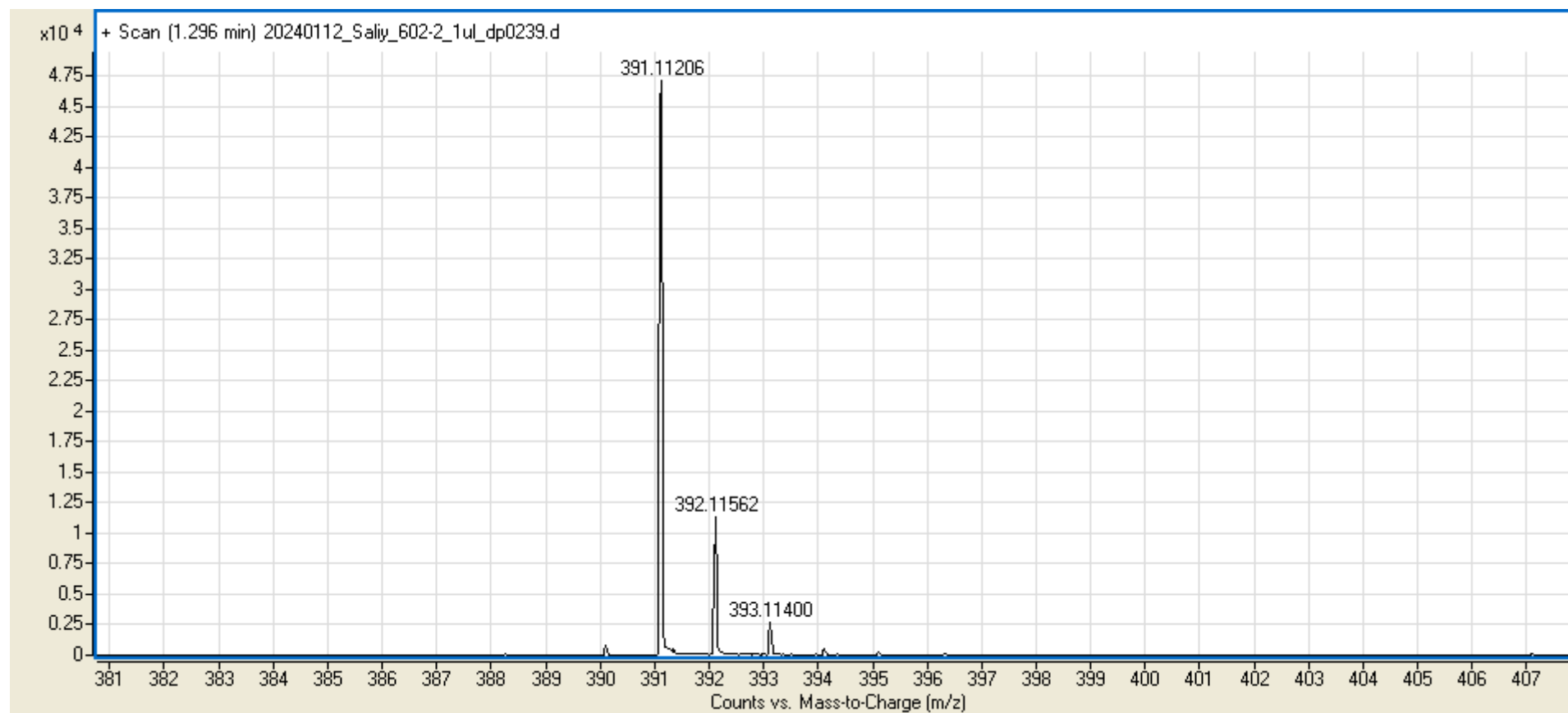
<sup>1</sup>H NMR spectrum of phenyl(2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)methanone (2a) in CDCl<sub>3</sub>.



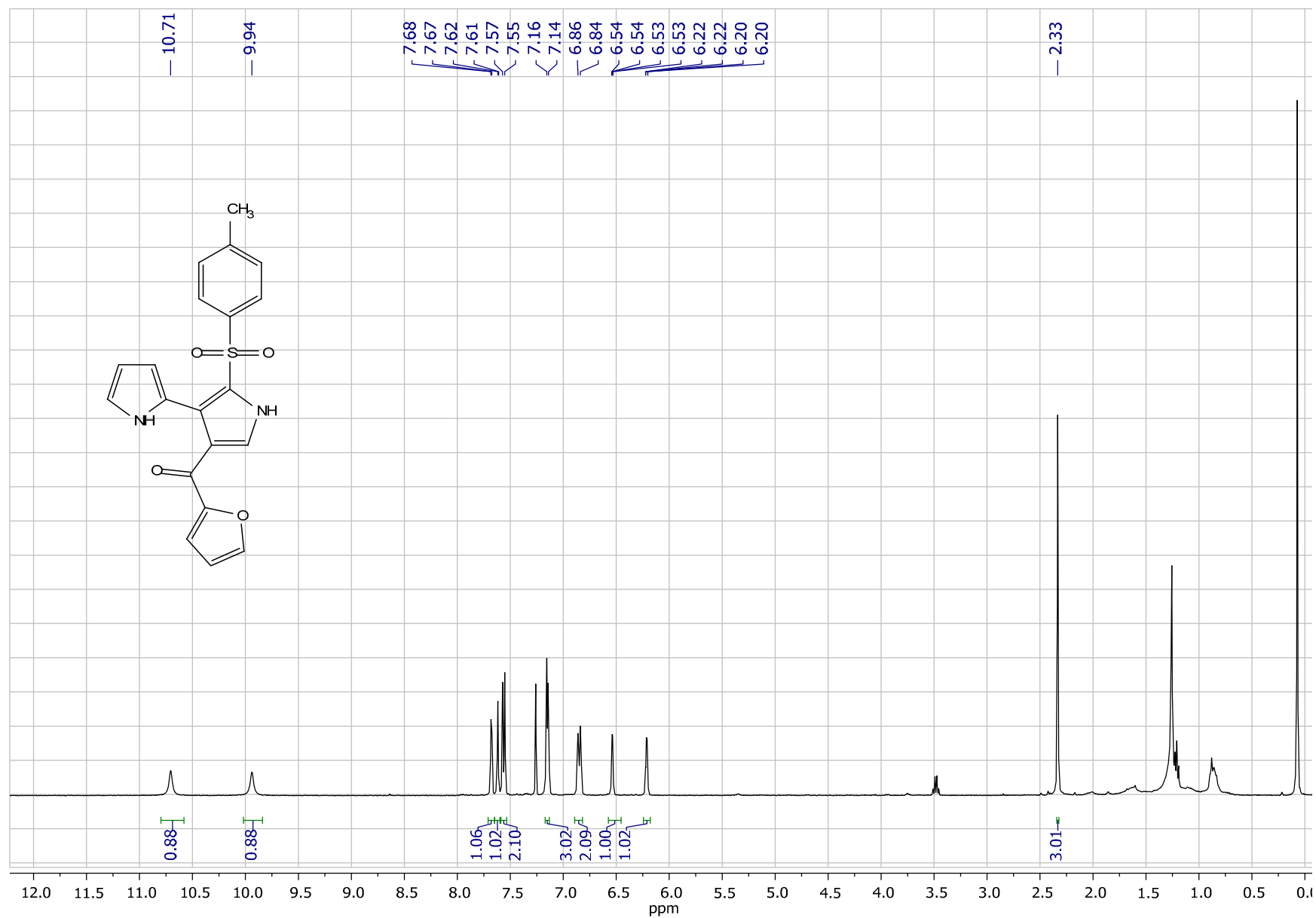
$^{13}\text{C}$  NMR spectrum of phenyl(2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)methanone (**2a**) in  $\text{CDCl}_3$ .



HRMS spectrum of phenyl(2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)methanone (**2a**)

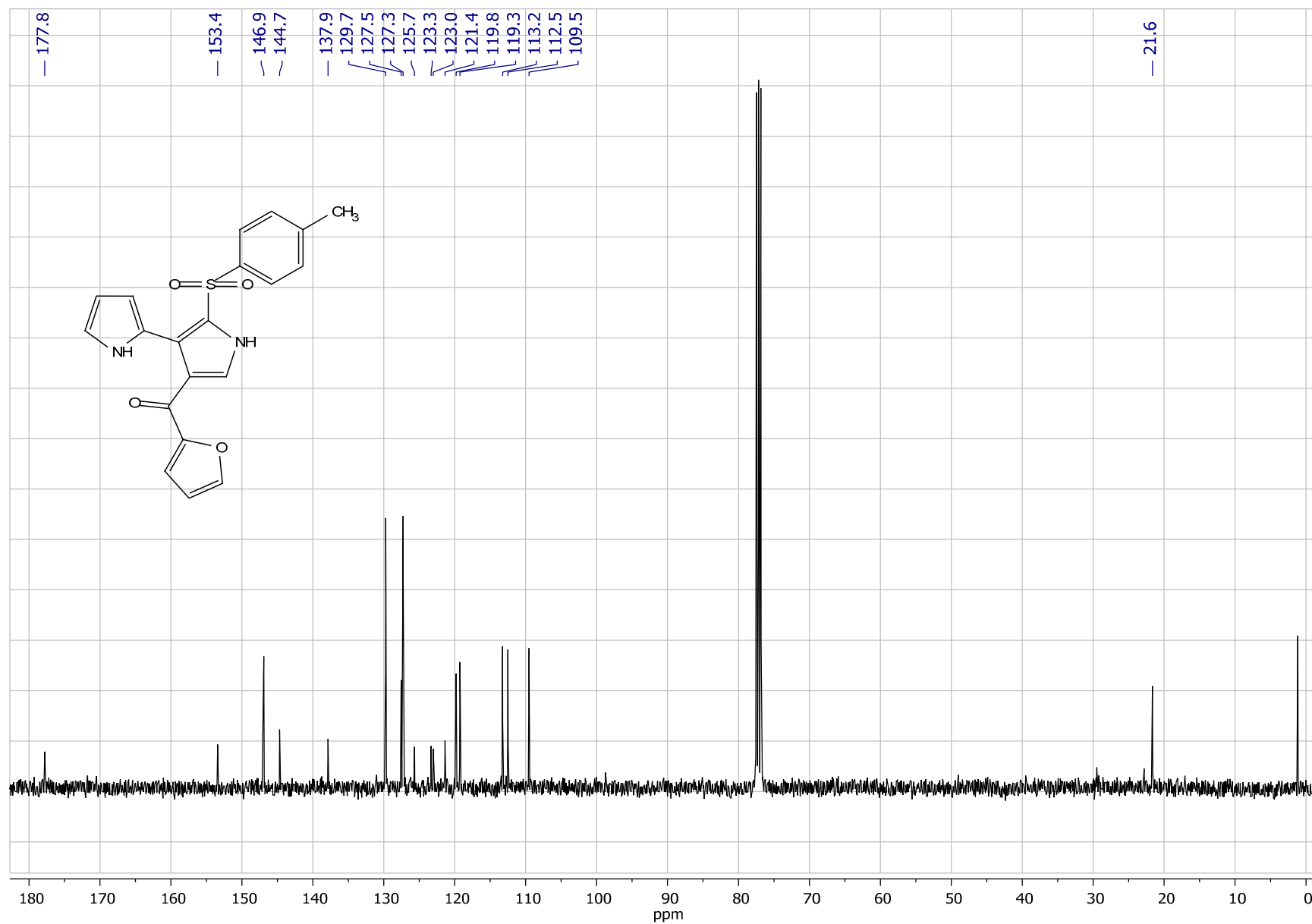


$^1\text{H}$  NMR spectrum of furan-2-yl(2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)methanone (**2b**) in  $\text{CDCl}_3$ .

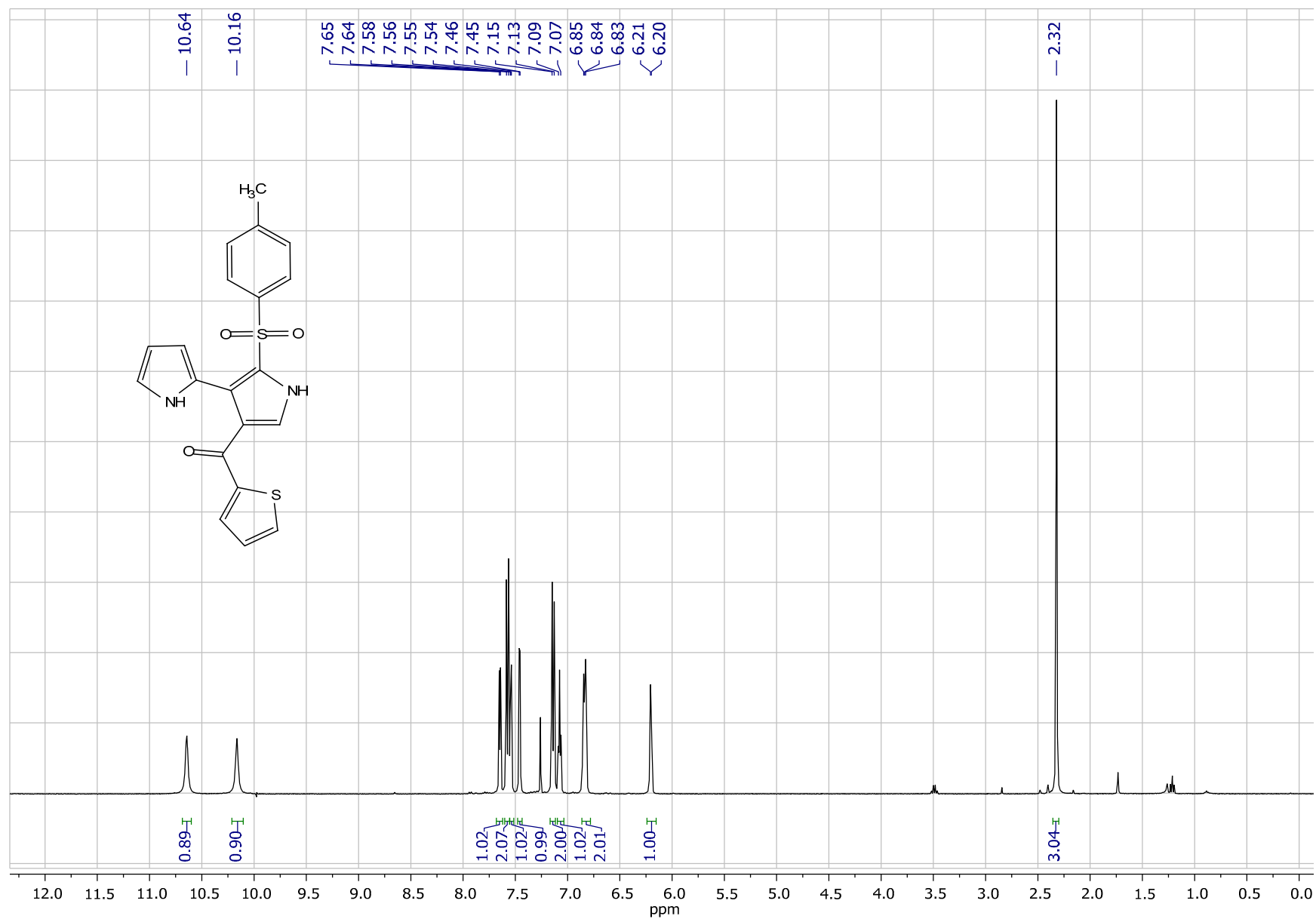




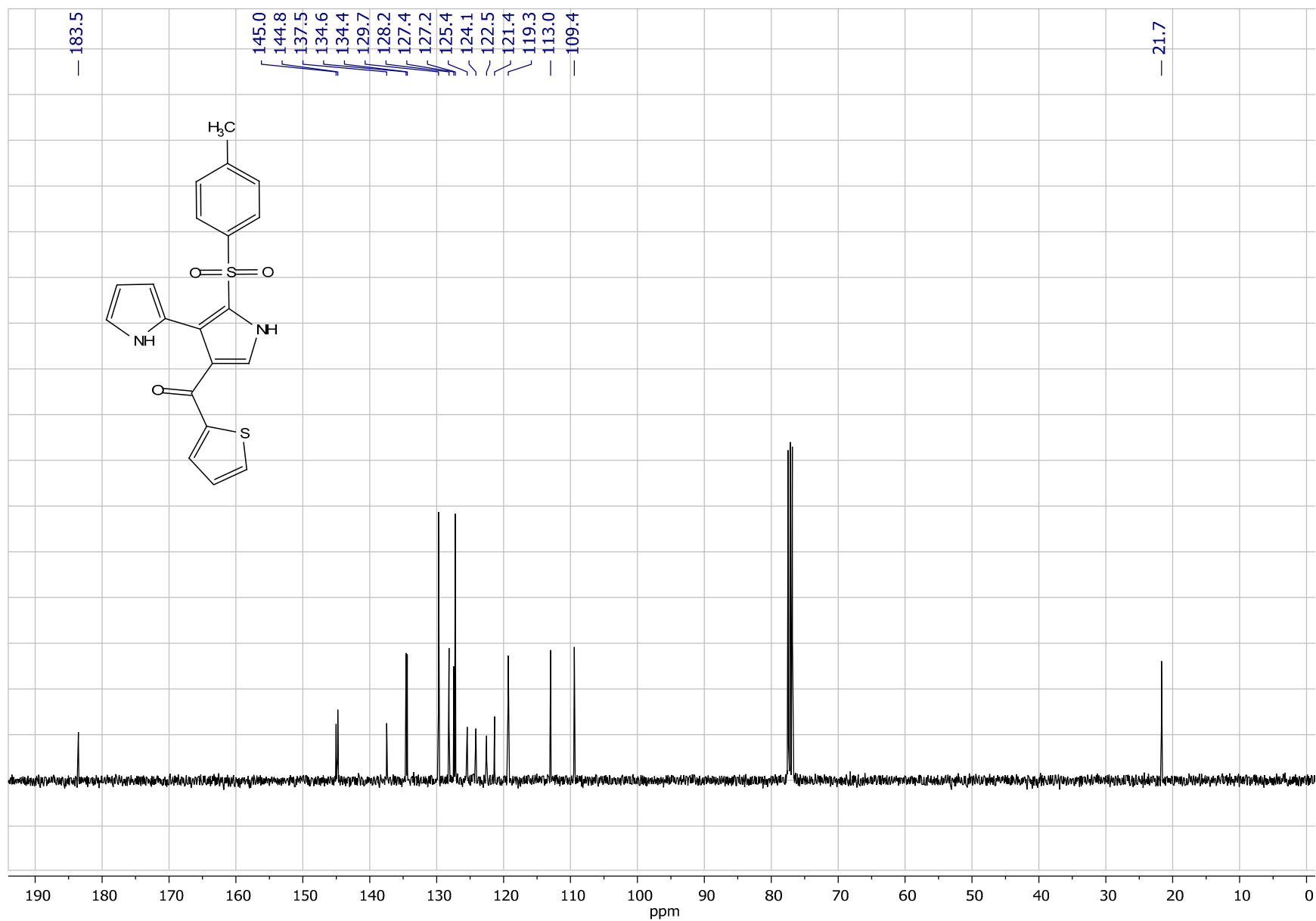
$^{13}\text{C}$  NMR spectrum of furan-2-yl(2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)methanone (**2b**) in  $\text{CDCl}_3$ .



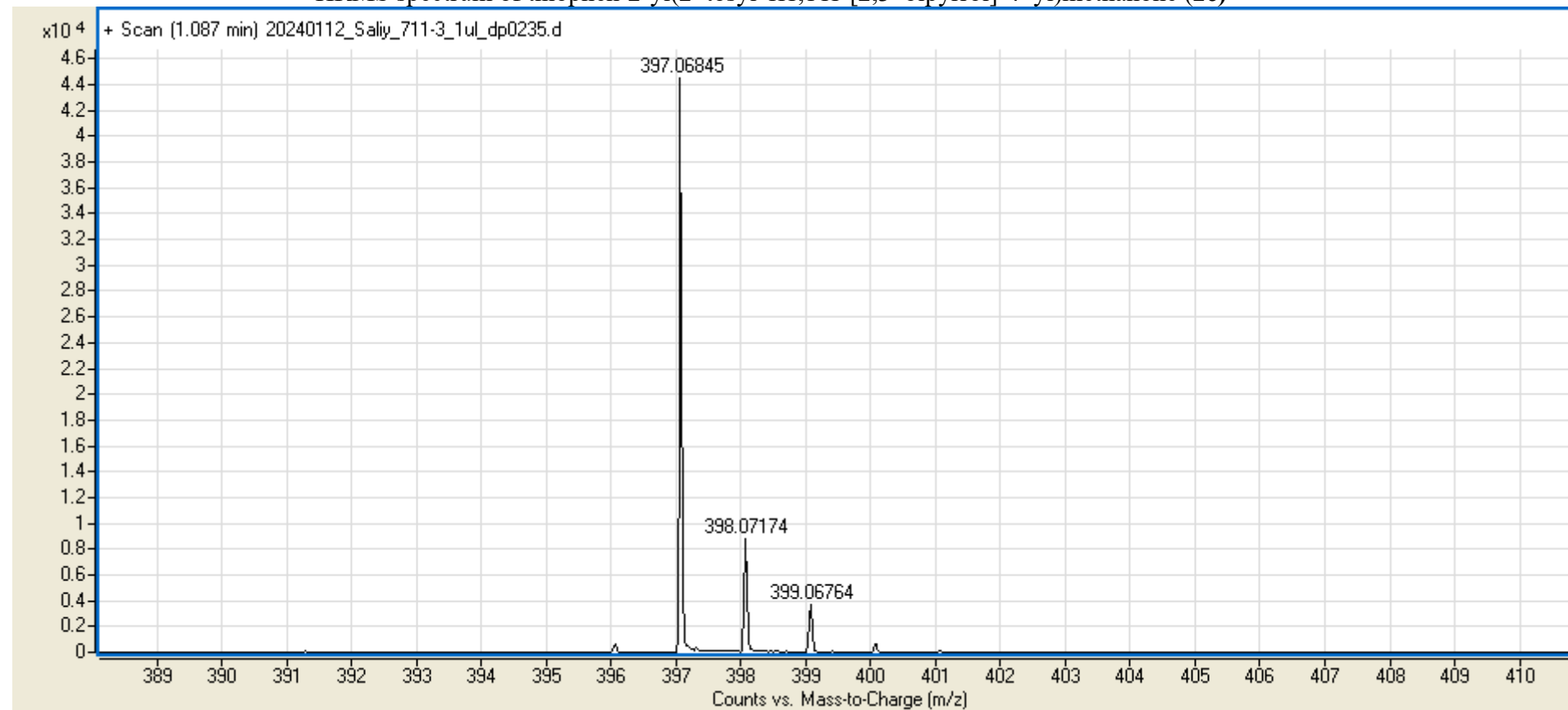
$^1\text{H}$  NMR spectrum of thiophen-2-yl(2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)methanone (**2c**) in  $\text{CDCl}_3$ .



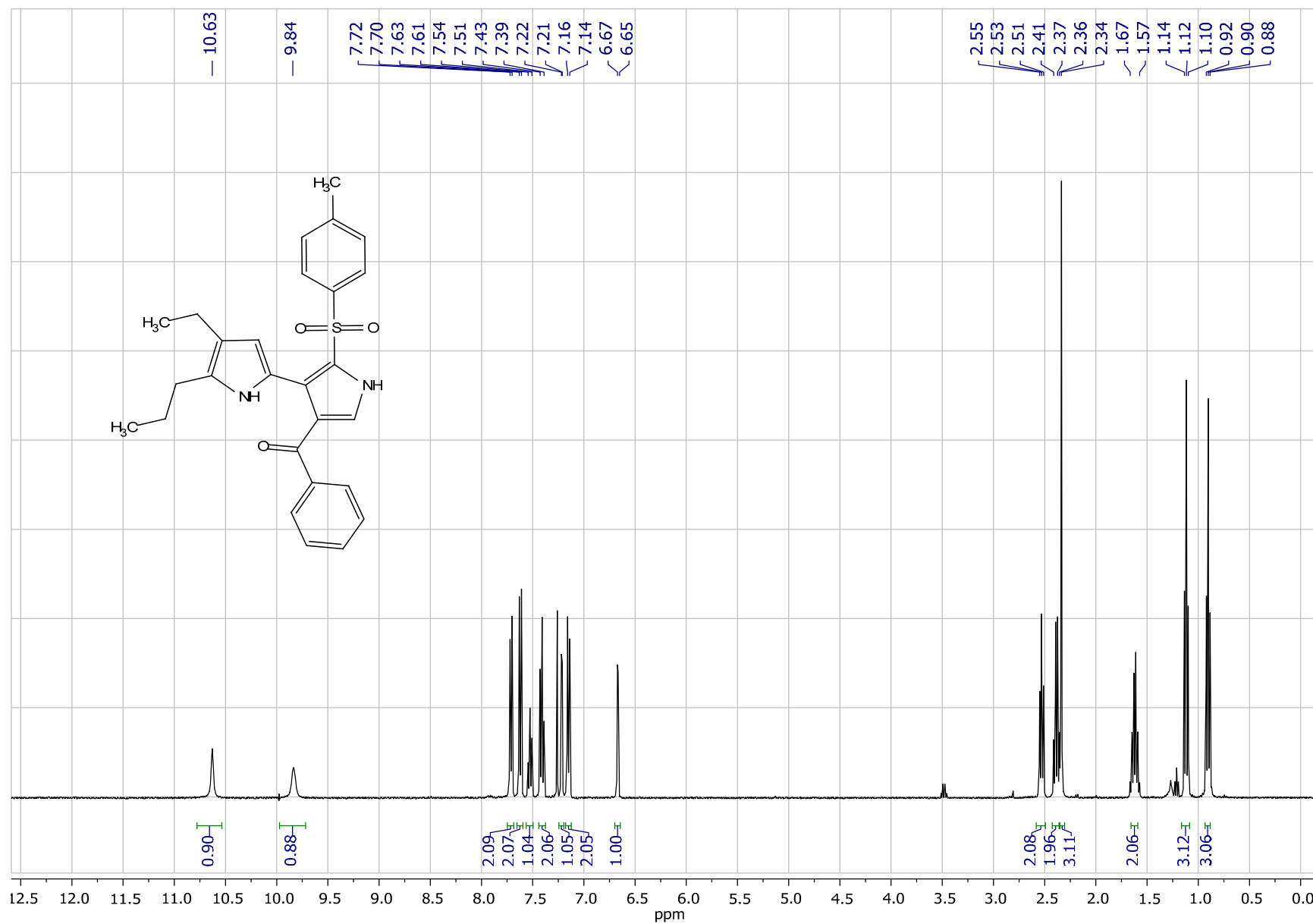
$^{13}\text{C}$  NMR spectrum of thiophen-2-yl(2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)methanone (**2c**) in  $\text{CDCl}_3$ .



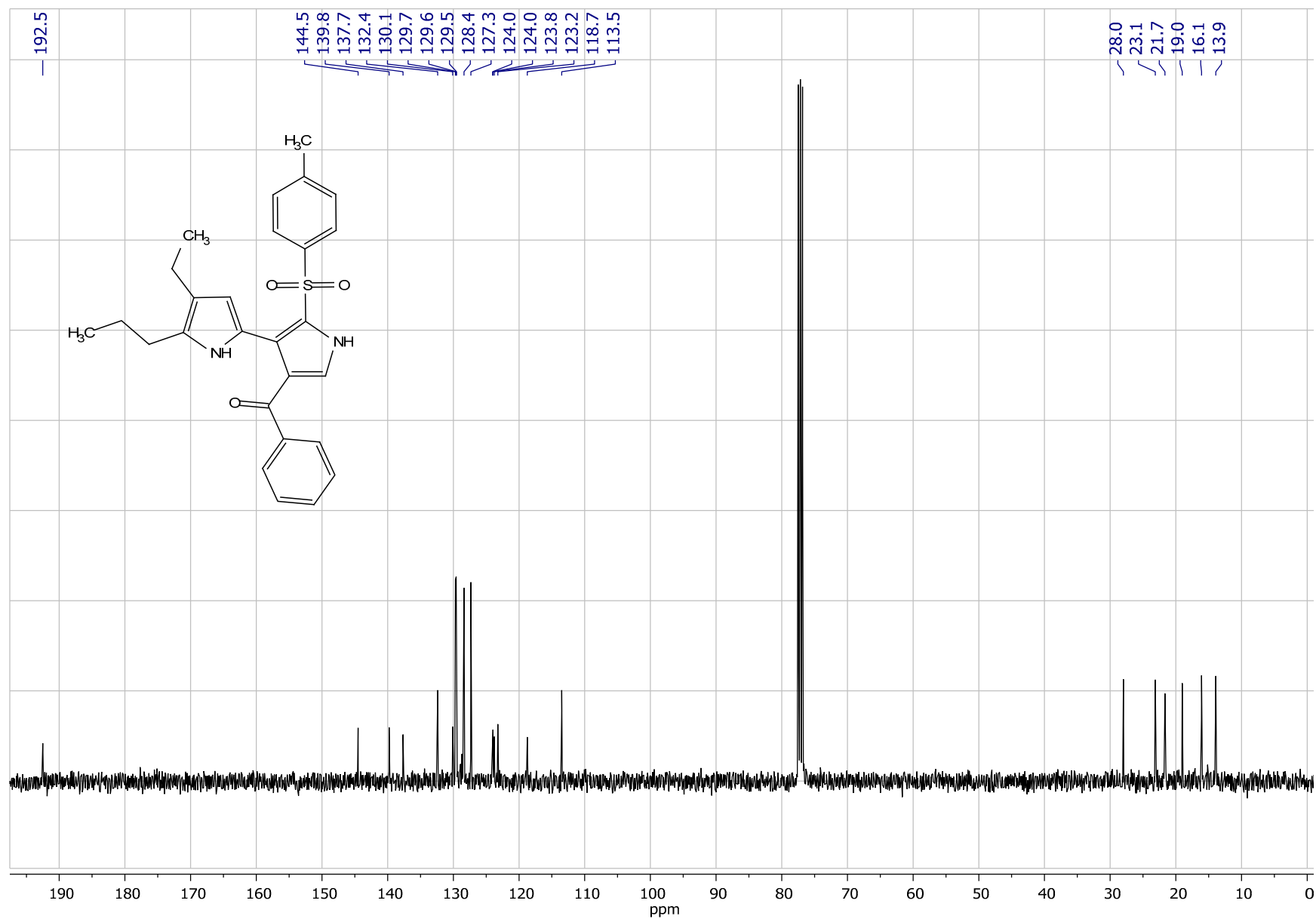
HRMS spectrum of thiophen-2-yl(2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)methanone (**2c**)



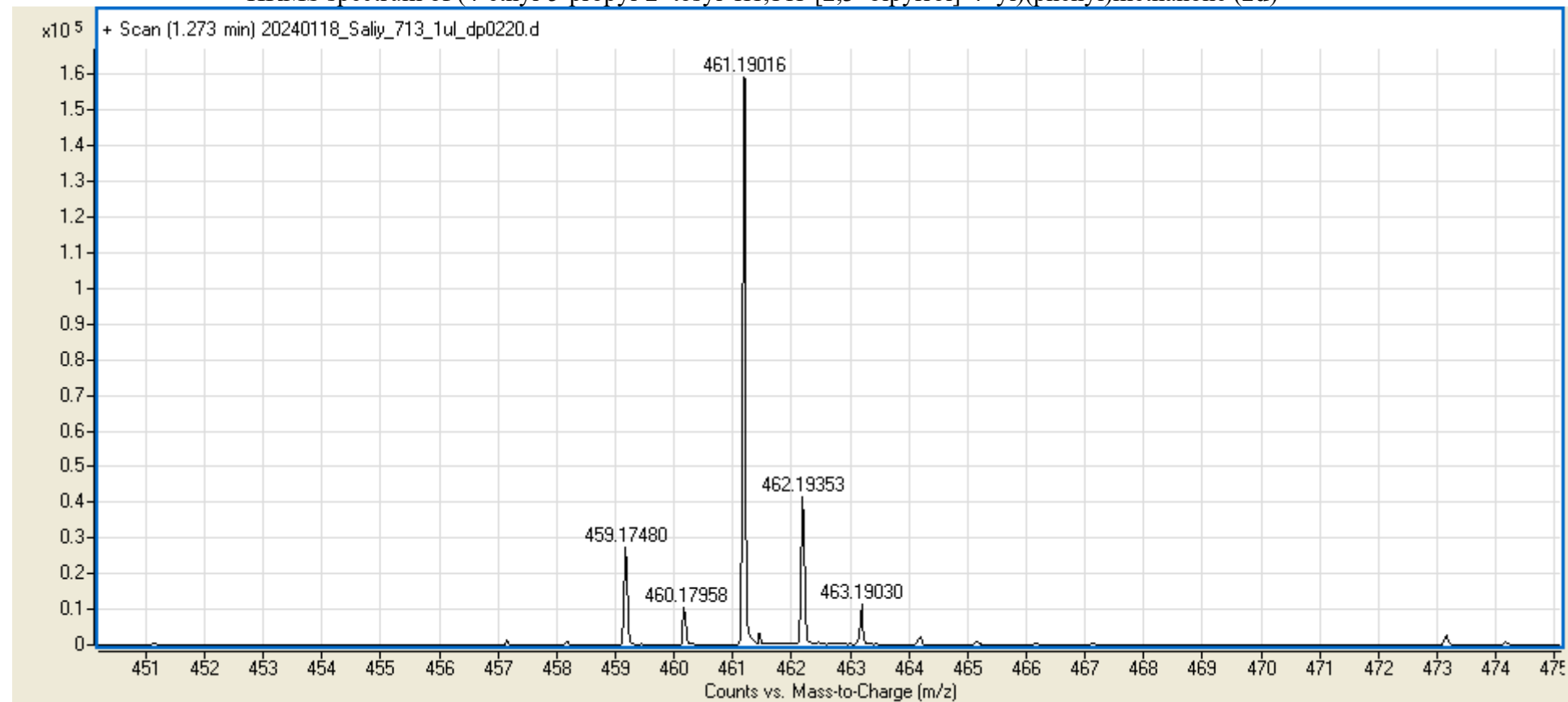
$^1\text{H}$  NMR spectrum of (4-ethyl-5-propyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (**2d**) in  $\text{CDCl}_3$ .



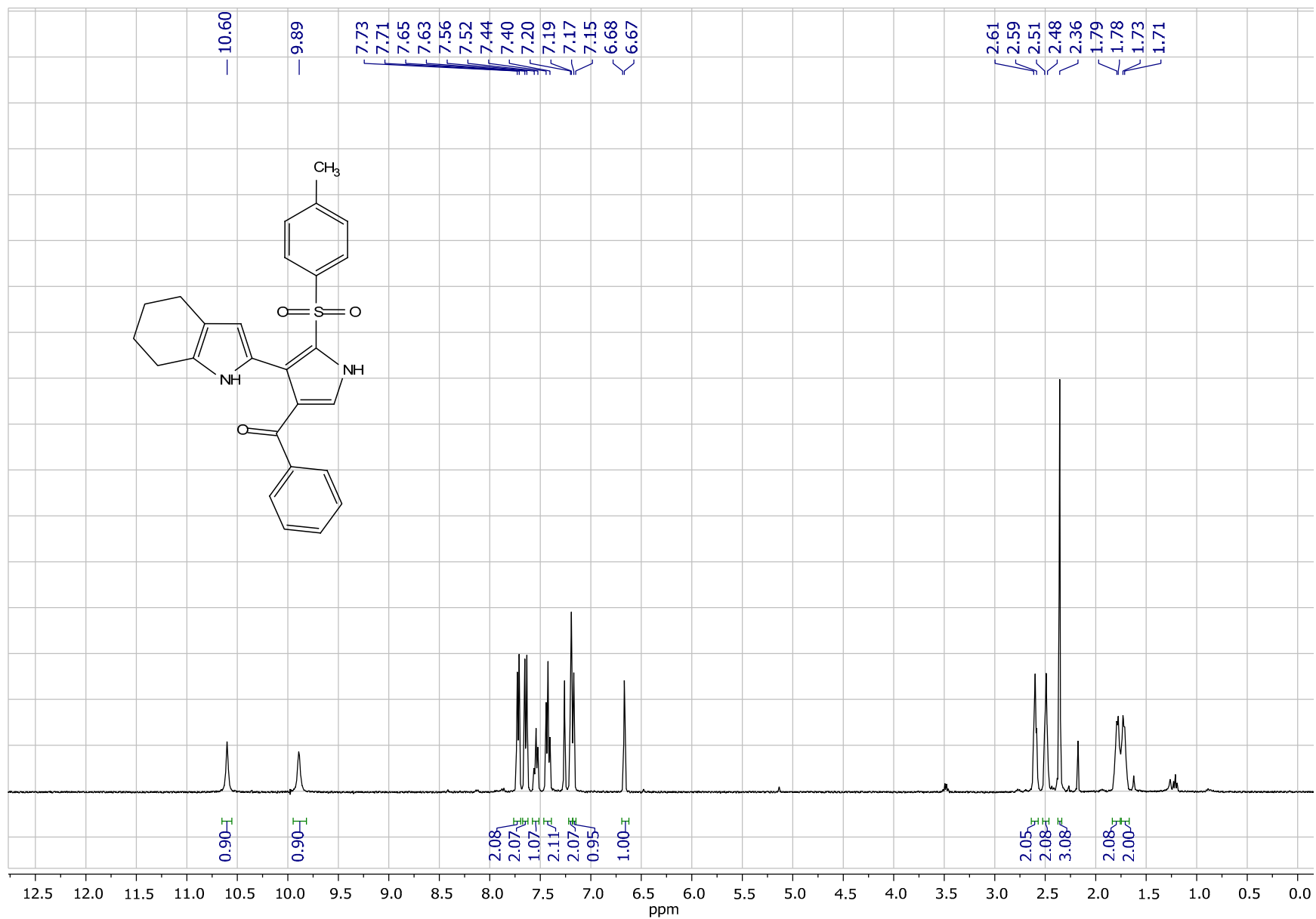
$^{13}\text{C}$  NMR spectrum of (4-ethyl-5-propyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (**2d**) in  $\text{CDCl}_3$ .



HRMS spectrum of (4-ethyl-5-propyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (**2d**)

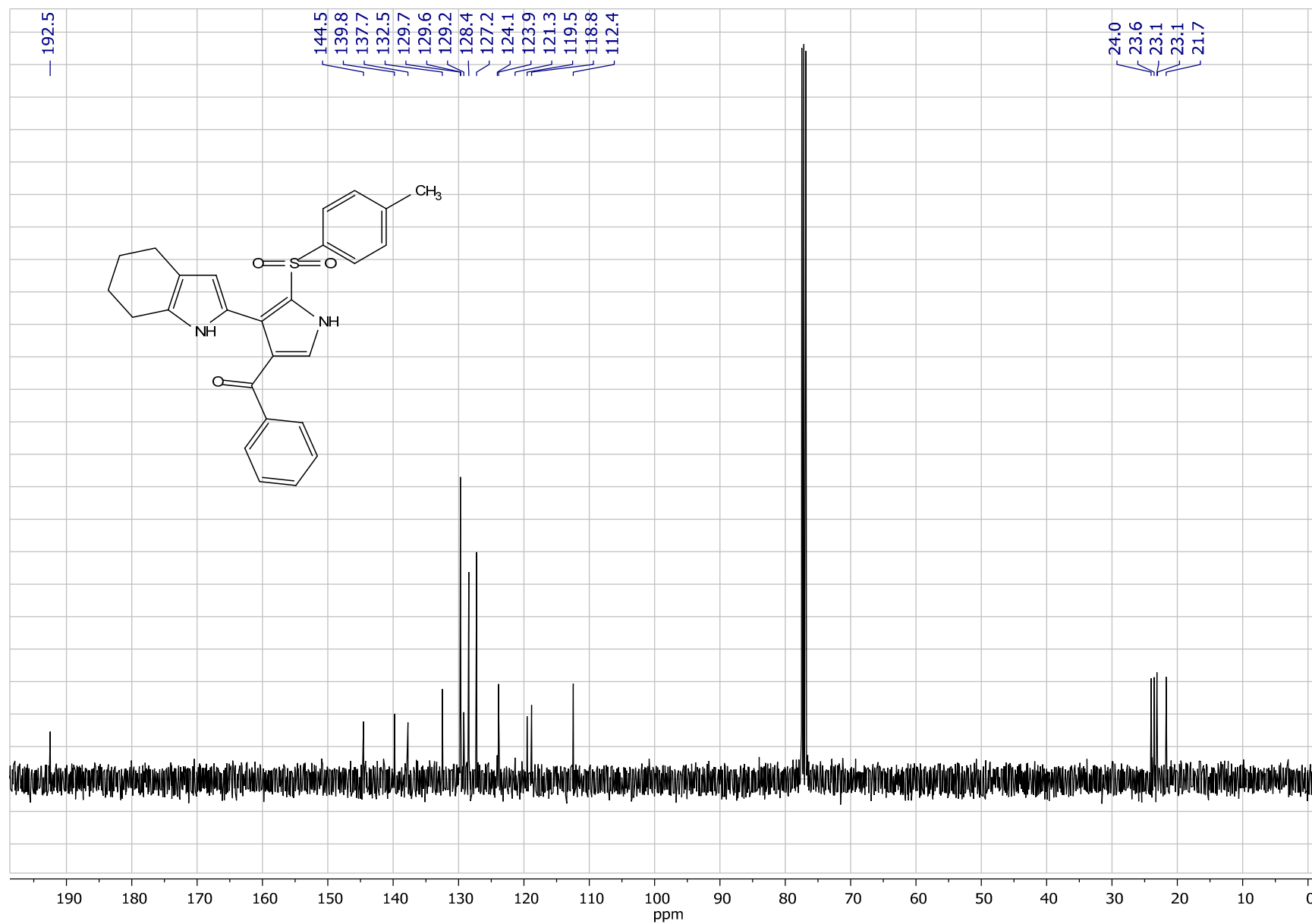


$^1\text{H}$  NMR spectrum of phenyl(4-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-5-tosyl-1*H*-pyrrol-3-yl)methanone (**2e**) in  $\text{CDCl}_3$ .

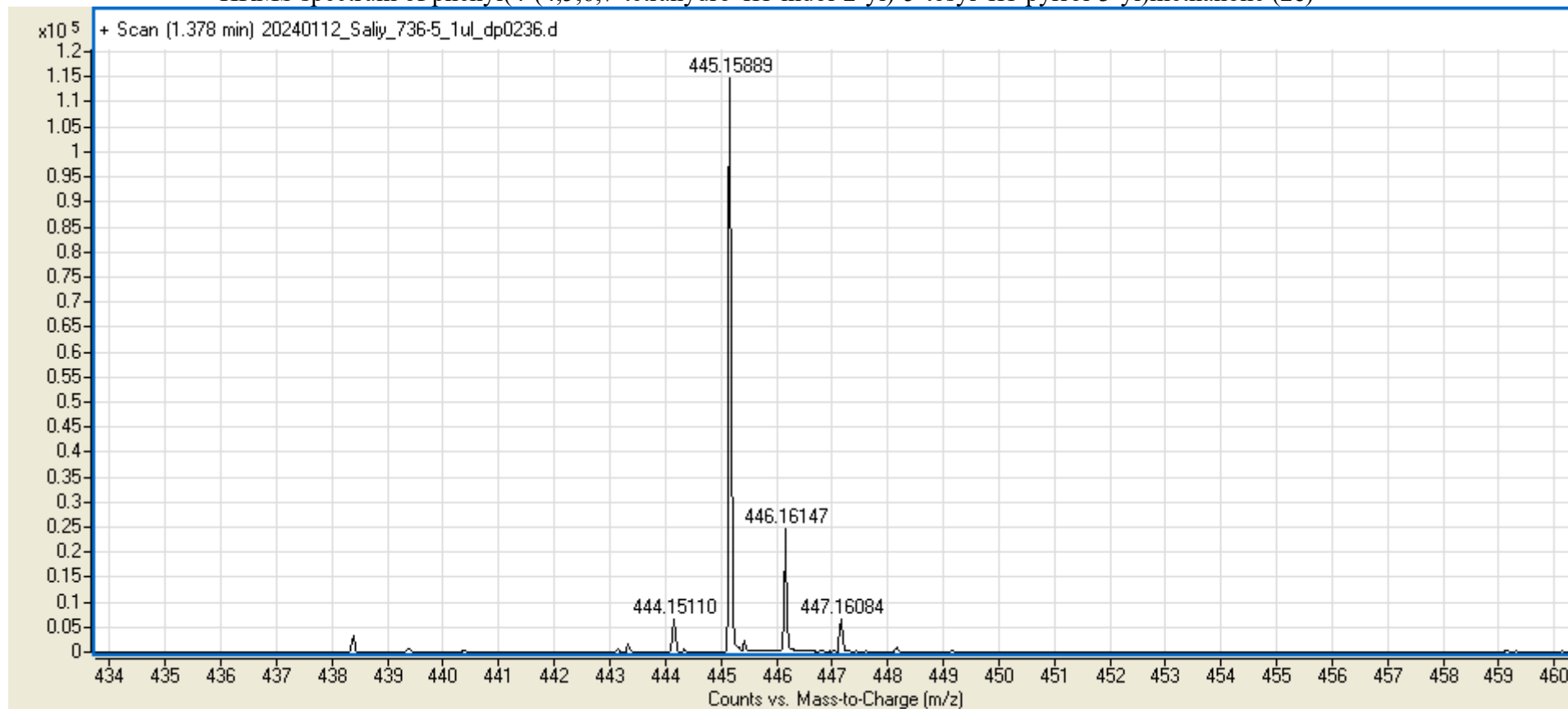




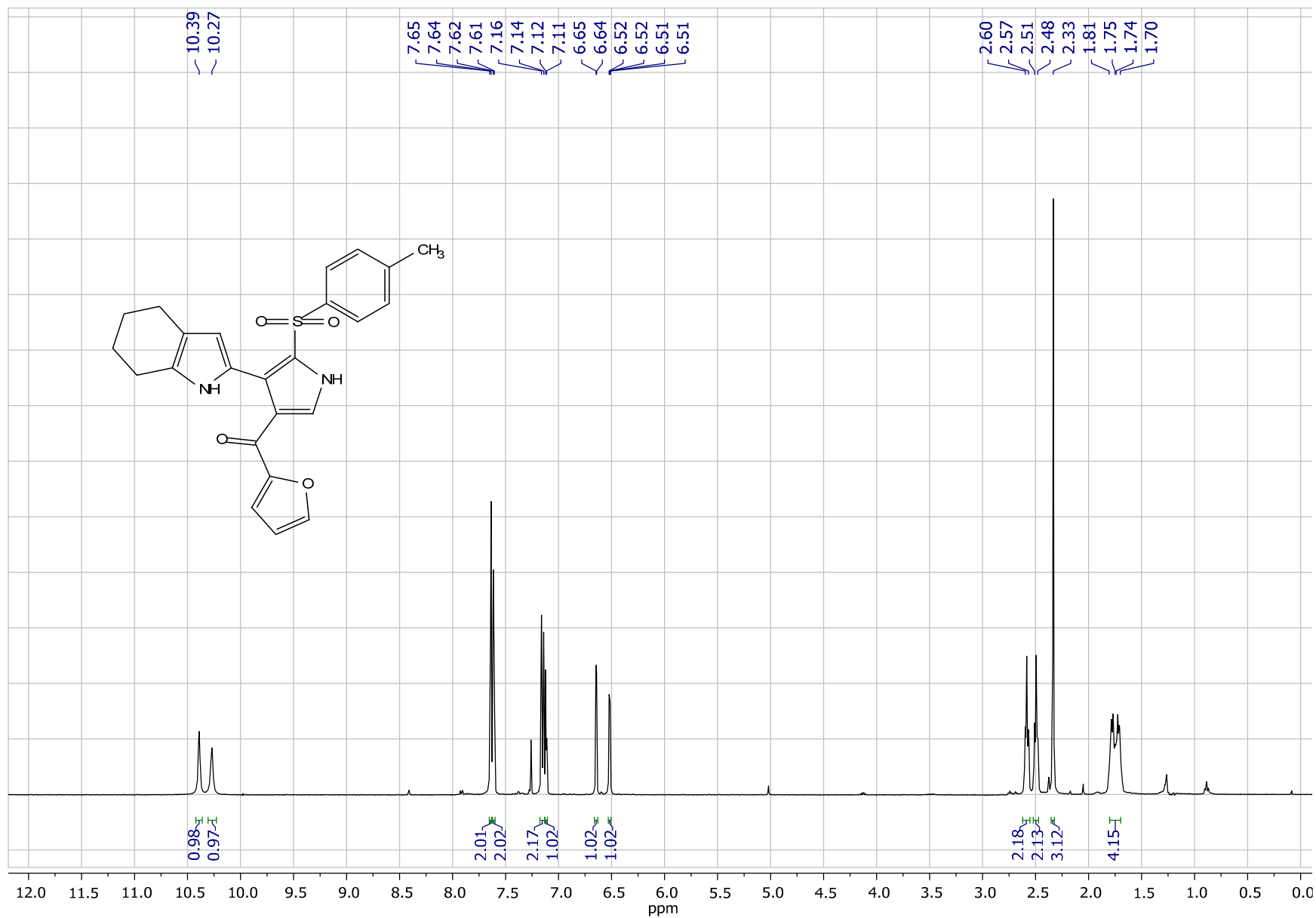
$^{13}\text{C}$  NMR spectrum of phenyl(4-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-5-tosyl-1*H*-pyrrol-3-yl)methanone (**2e**) in  $\text{CDCl}_3$ .



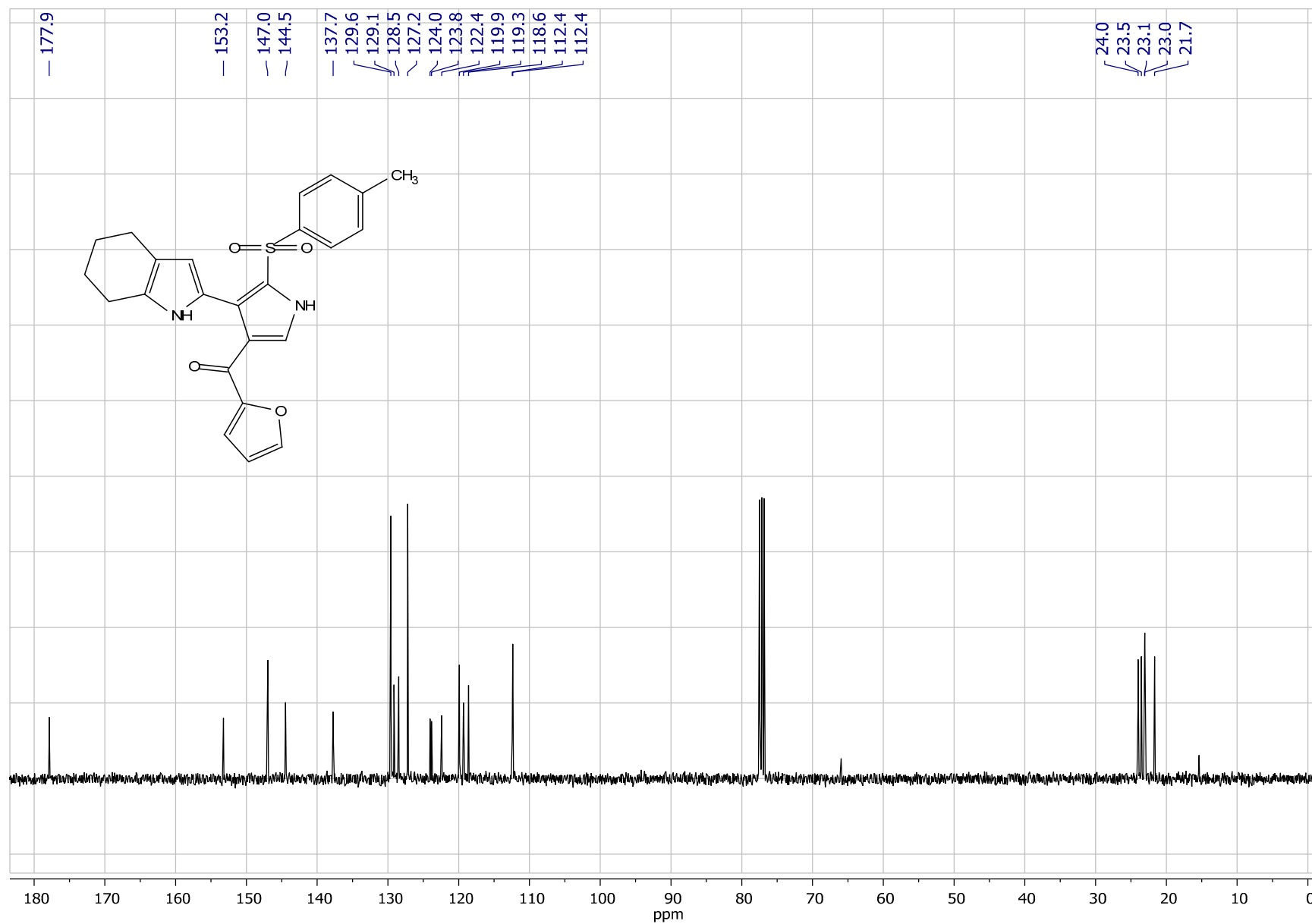
HRMS spectrum of phenyl(4-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-5-tosyl-1*H*-pyrrol-3-yl)methanone (**2e**)



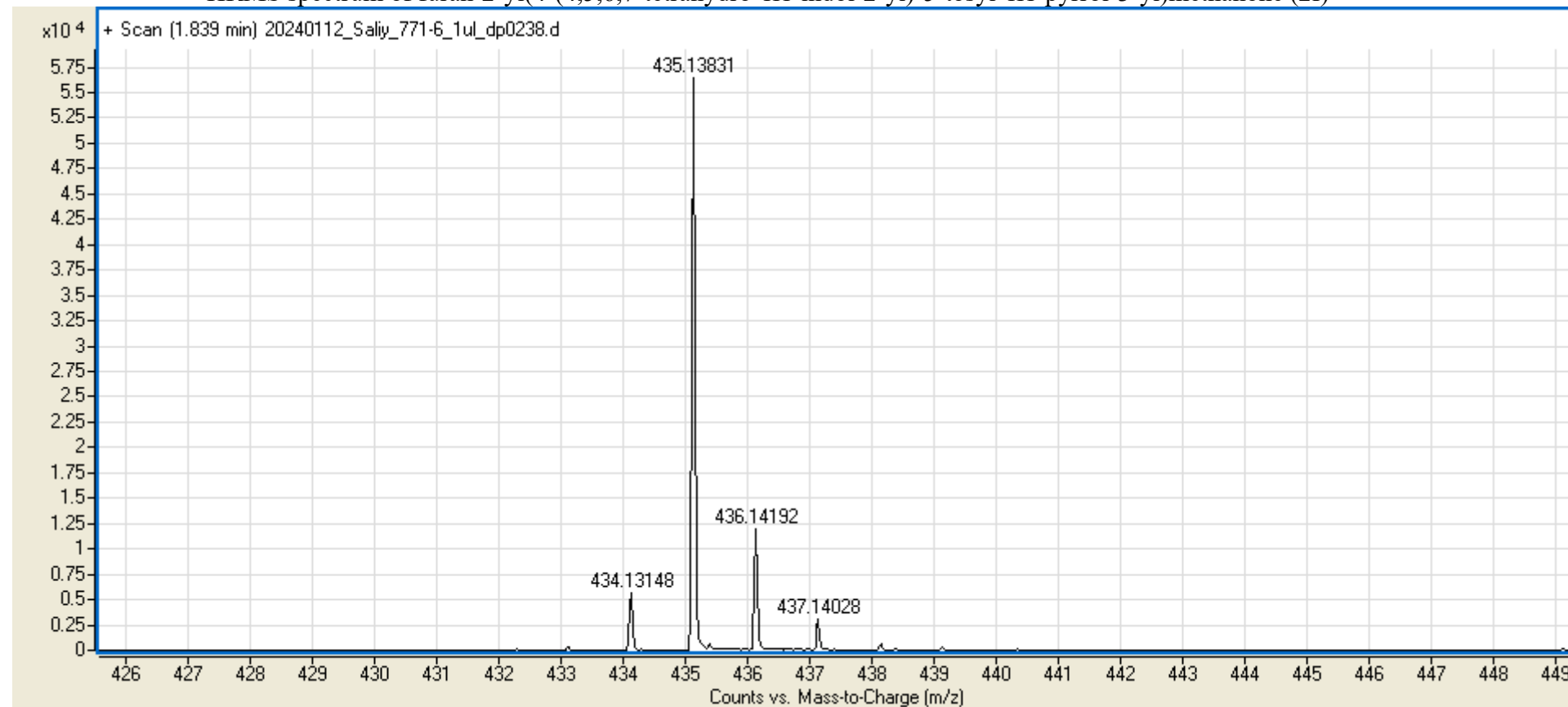
$^1\text{H}$  NMR spectrum of furan-2-yl(4-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-5-tosyl-1*H*-pyrrol-3-yl)methanone (**2f**) in  $\text{CDCl}_3$ .



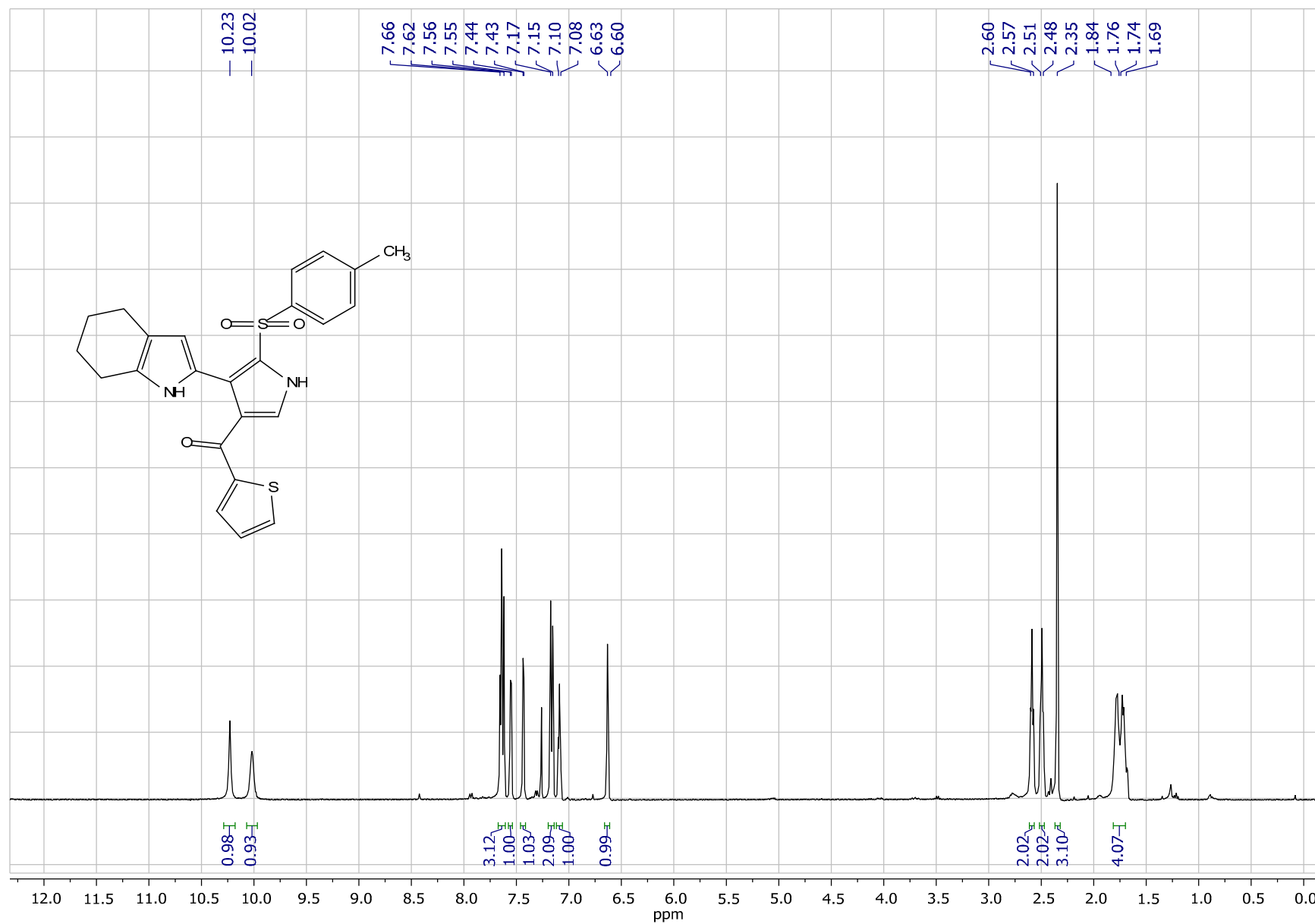
$^{13}\text{C}$  NMR spectrum of furan-2-yl(4-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-5-tosyl-1*H*-pyrrol-3-yl)methanone (**2f**) in  $\text{CDCl}_3$ .



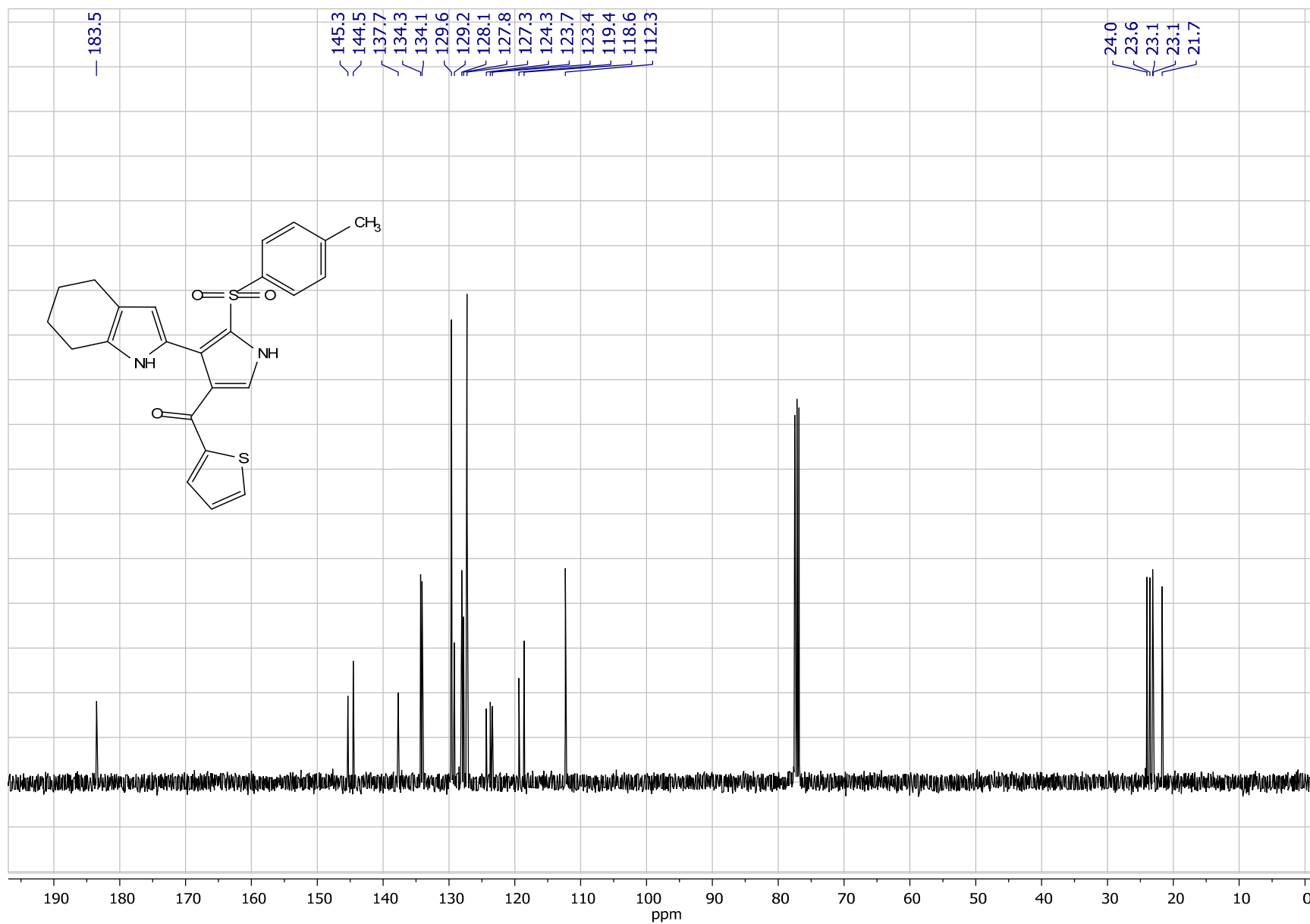
HRMS spectrum of furan-2-yl(4-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-5-tosyl-1*H*-pyrrol-3-yl)methanone (**2f**)



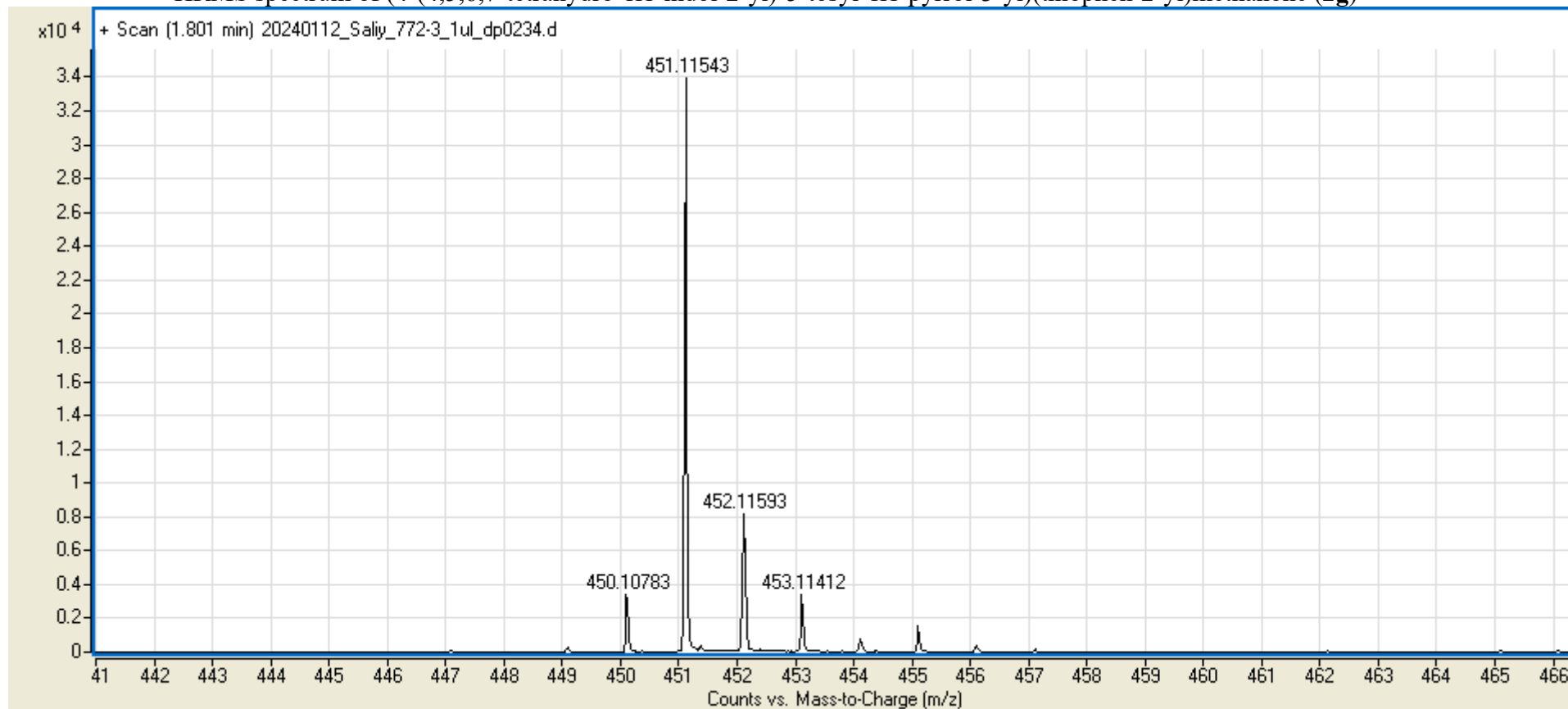
$^1\text{H}$  NMR spectrum of (4-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-5-tosyl-1*H*-pyrrol-3-yl)(thiophen-2-yl)methanone (**2g**) in  $\text{CDCl}_3$ .



$^{13}\text{C}$  NMR spectrum of (4-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-5-tosyl-1*H*-pyrrol-3-yl)(thiophen-2-yl)methanone (**2g**) in  $\text{CDCl}_3$ .

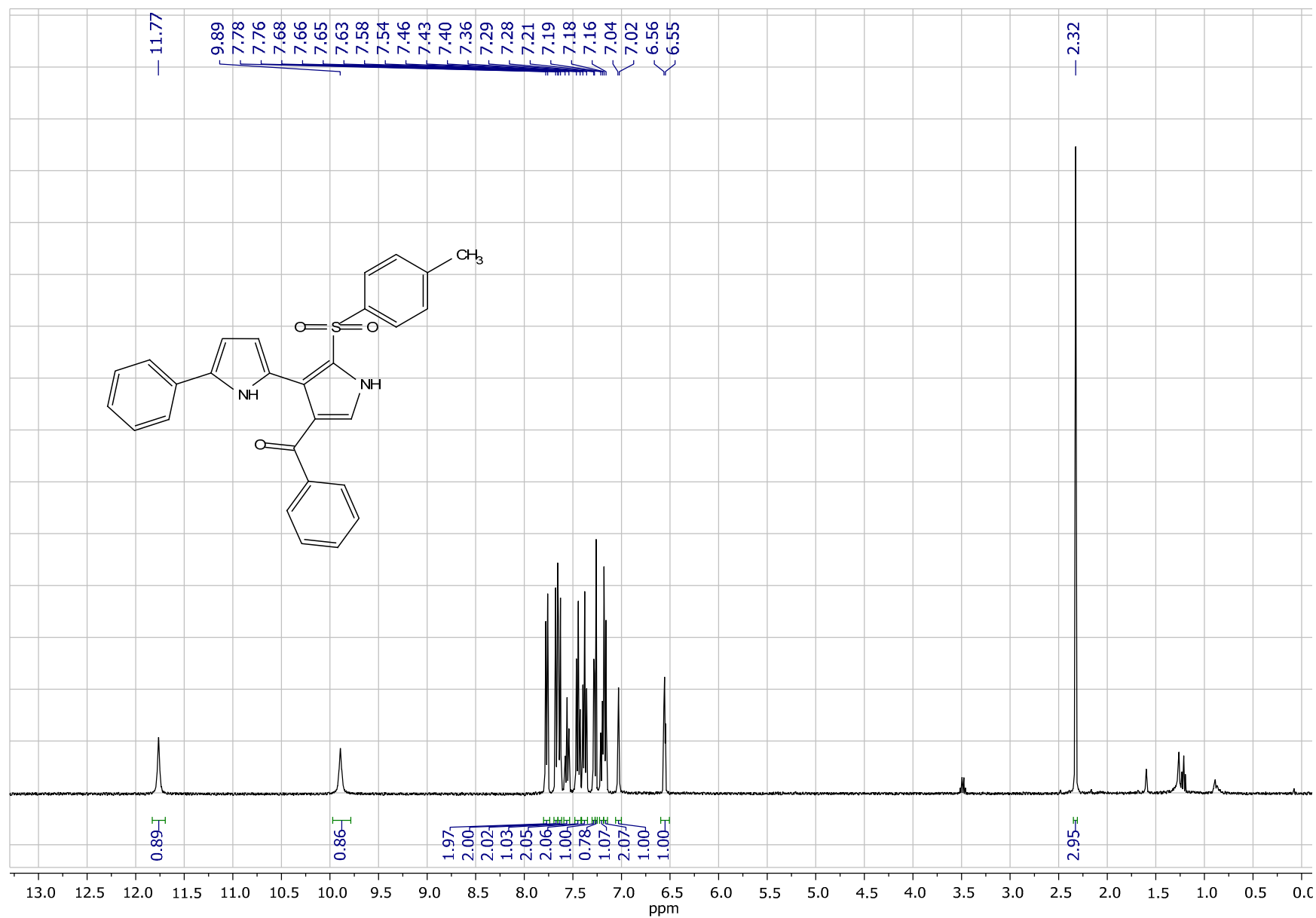


HRMS spectrum of (4-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)-5-tosyl-1*H*-pyrrol-3-yl)(thiophen-2-yl)methanone (**2g**)

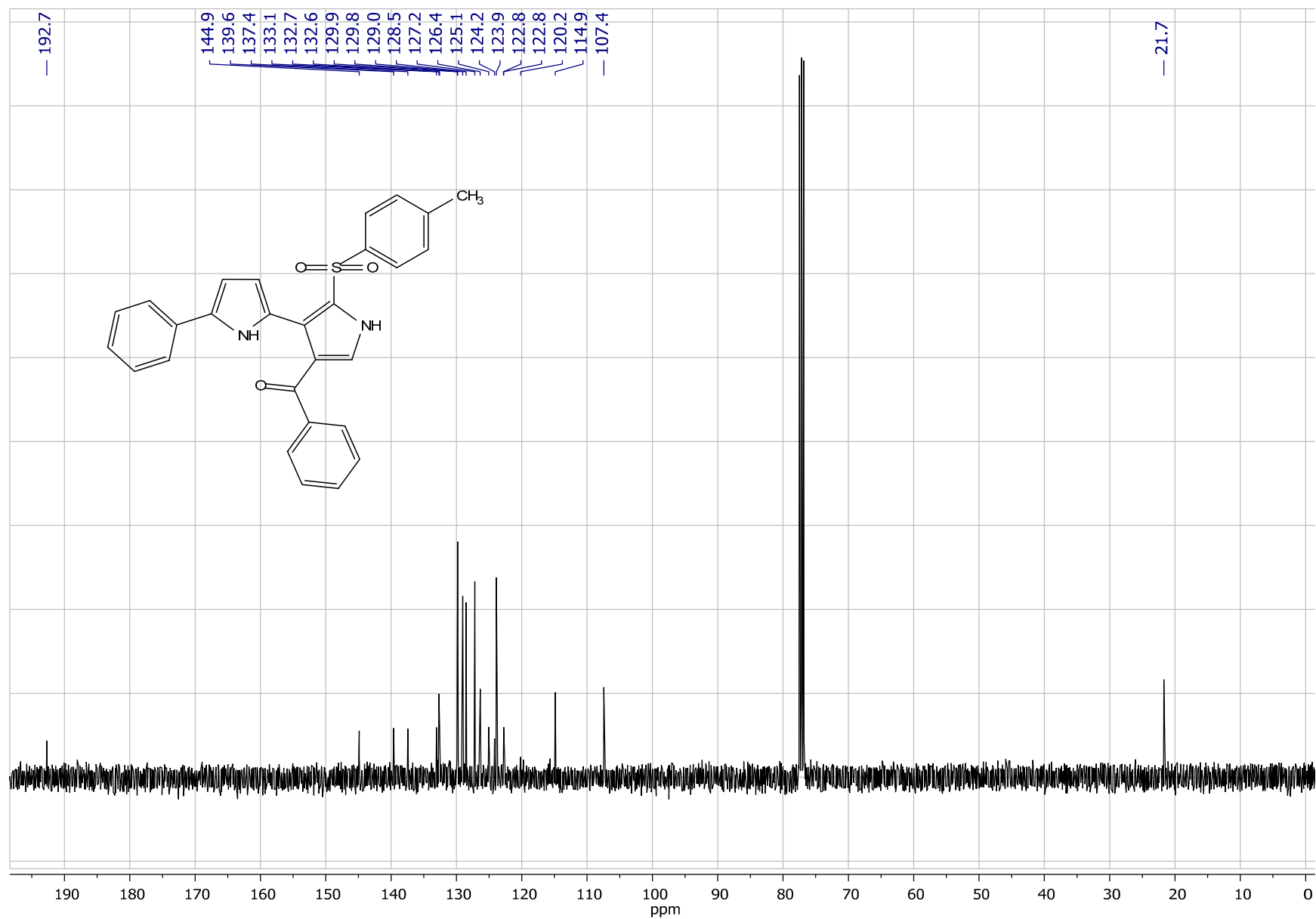




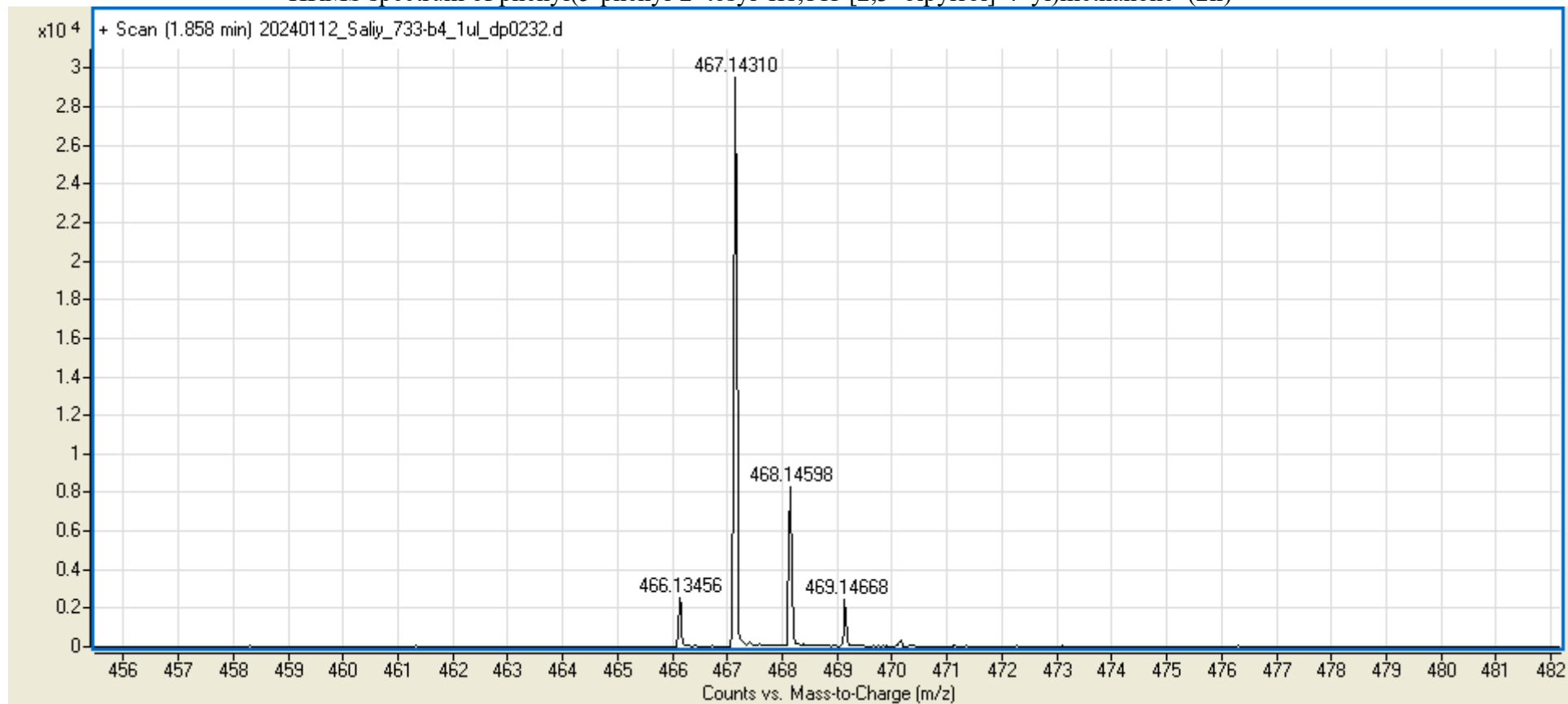
$^1\text{H}$  NMR spectrum of phenyl(5-phenyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)methanone (**2h**) in  $\text{CDCl}_3$ .



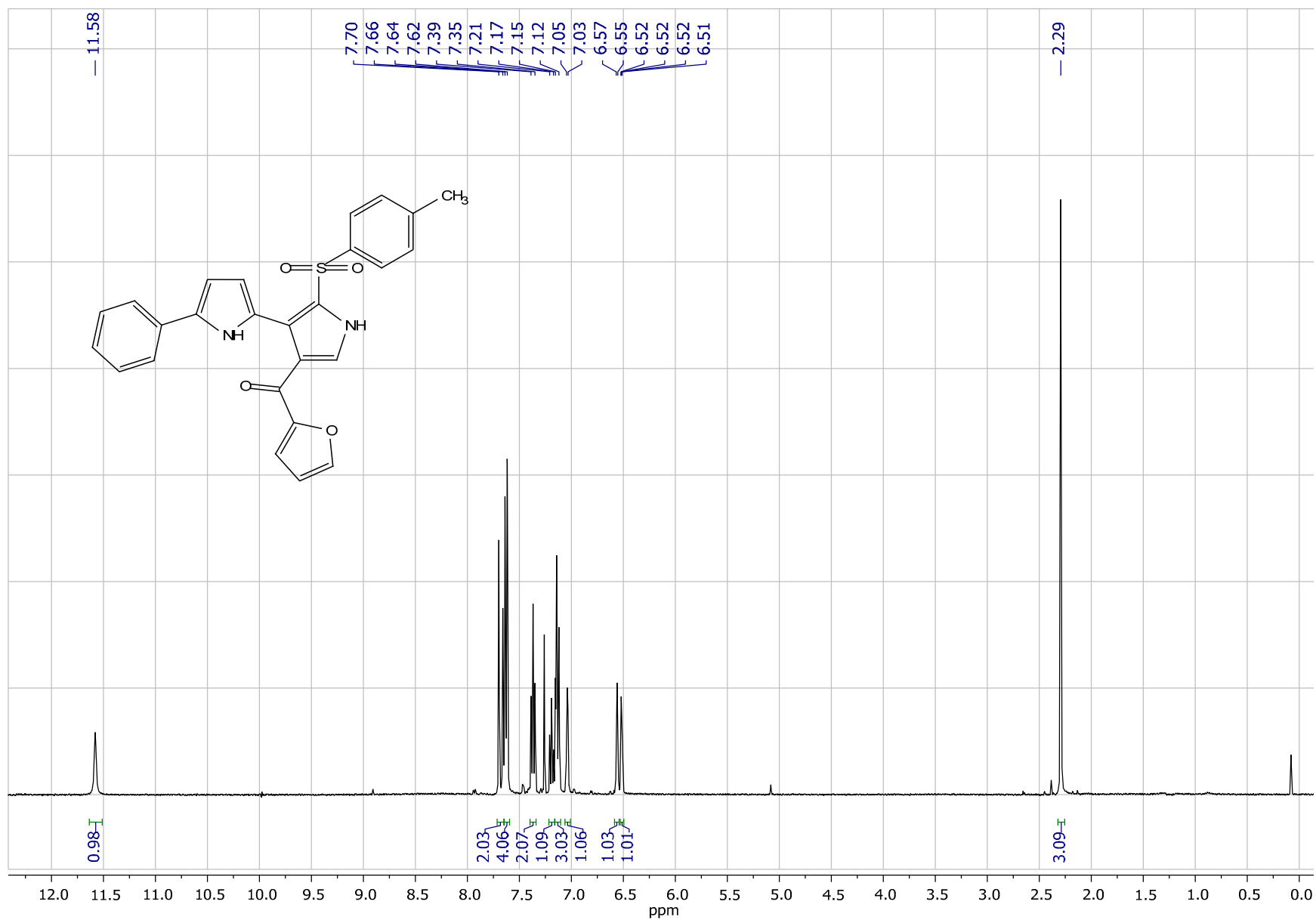
$^{13}\text{C}$  NMR spectrum of phenyl(5-phenyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)methanone (**2h**) in  $\text{CDCl}_3$ .



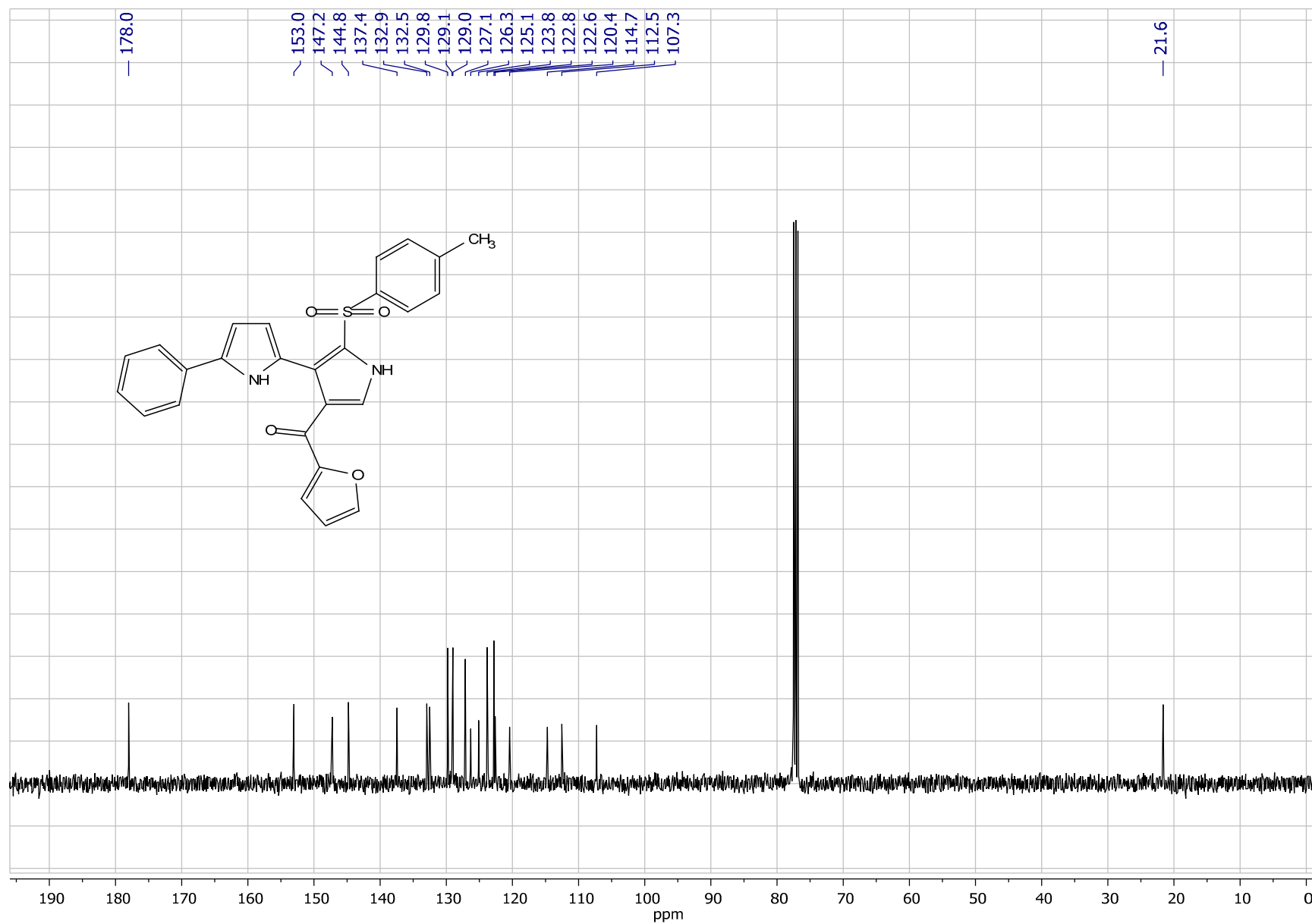
HRMS spectrum of phenyl(5-phenyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)methanone (**2h**)



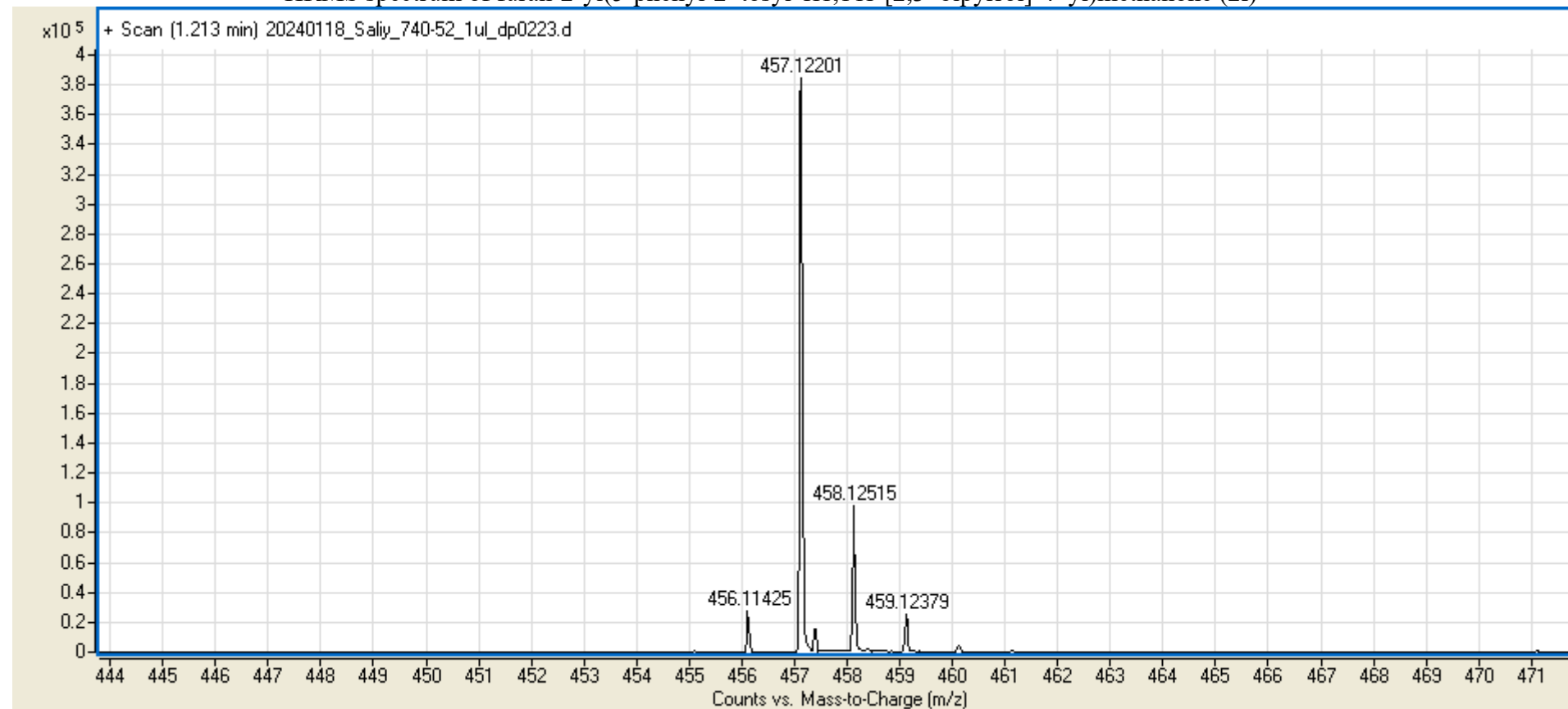
$^1\text{H}$  NMR spectrum of furan-2-yl(5-phenyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)methanone (**2i**) in  $\text{CDCl}_3$ .



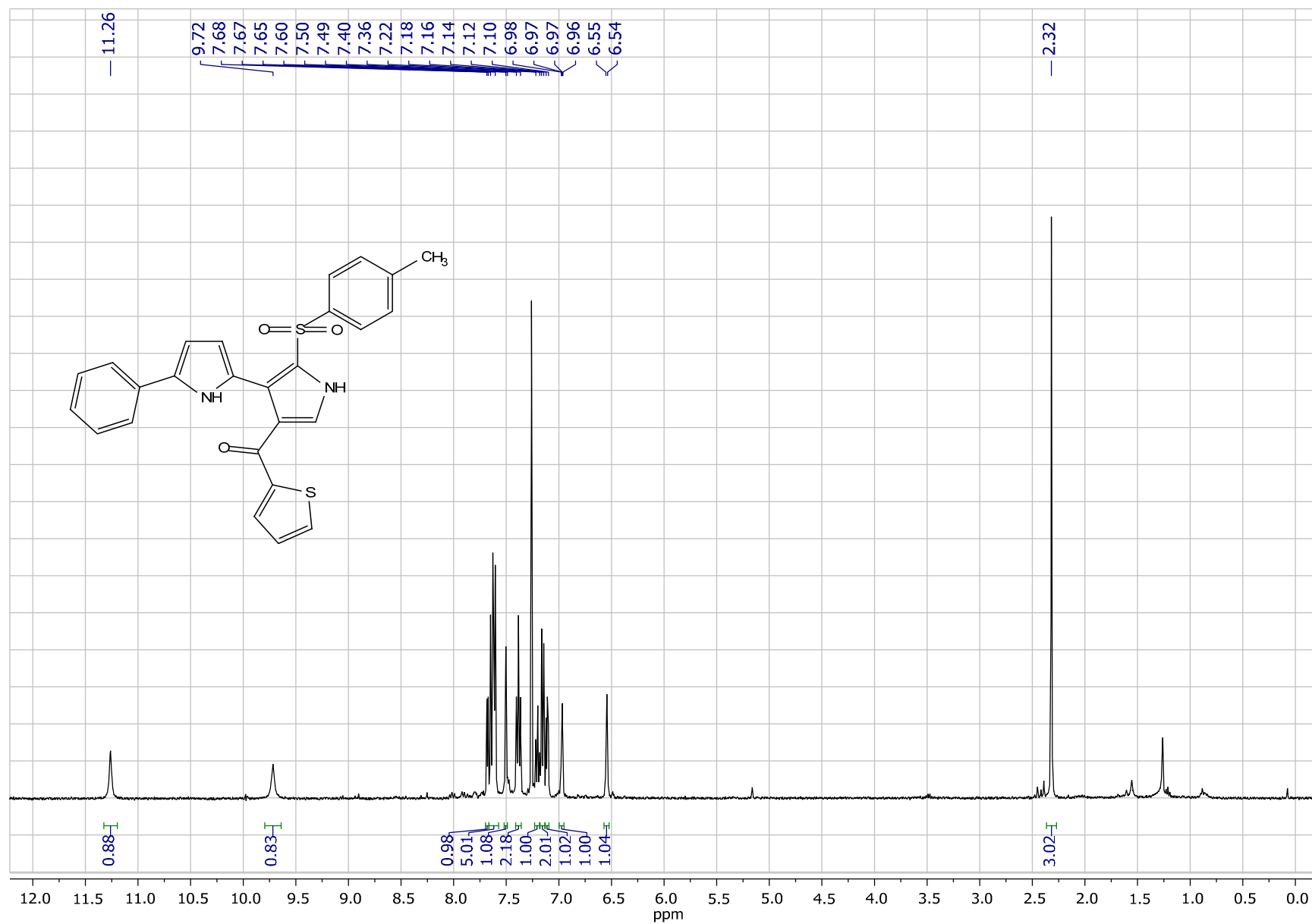
$^{13}\text{C}$  NMR spectrum of furan-2-yl(5-phenyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)methanone (**2i**) in  $\text{CDCl}_3$ .



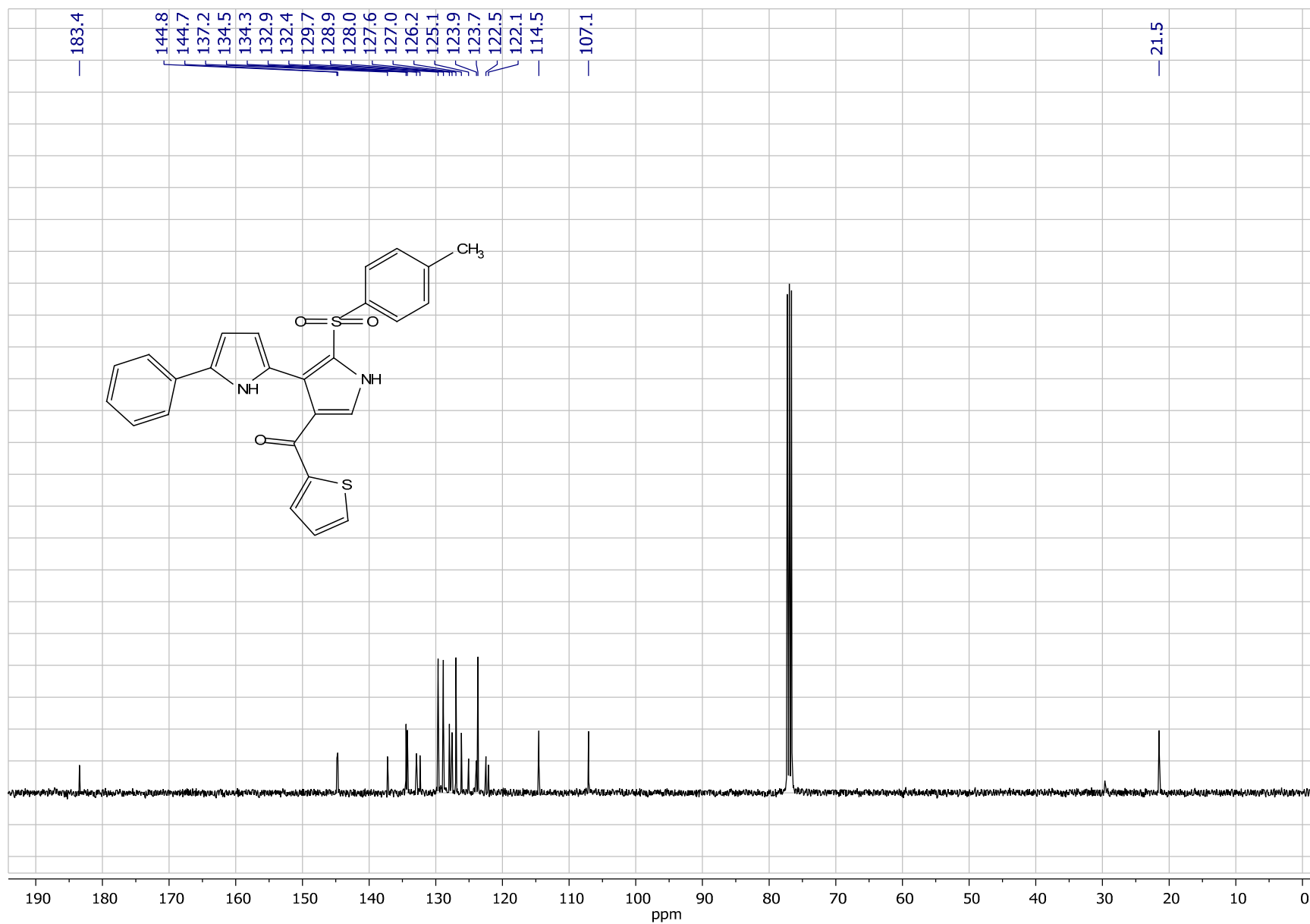
HRMS spectrum of furan-2-yl(5-phenyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)methanone (**2i**)



$^1\text{H}$  NMR spectrum of (5-phenyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(thiophen-2-yl)methanone (**2j**) in  $\text{CDCl}_3$ .

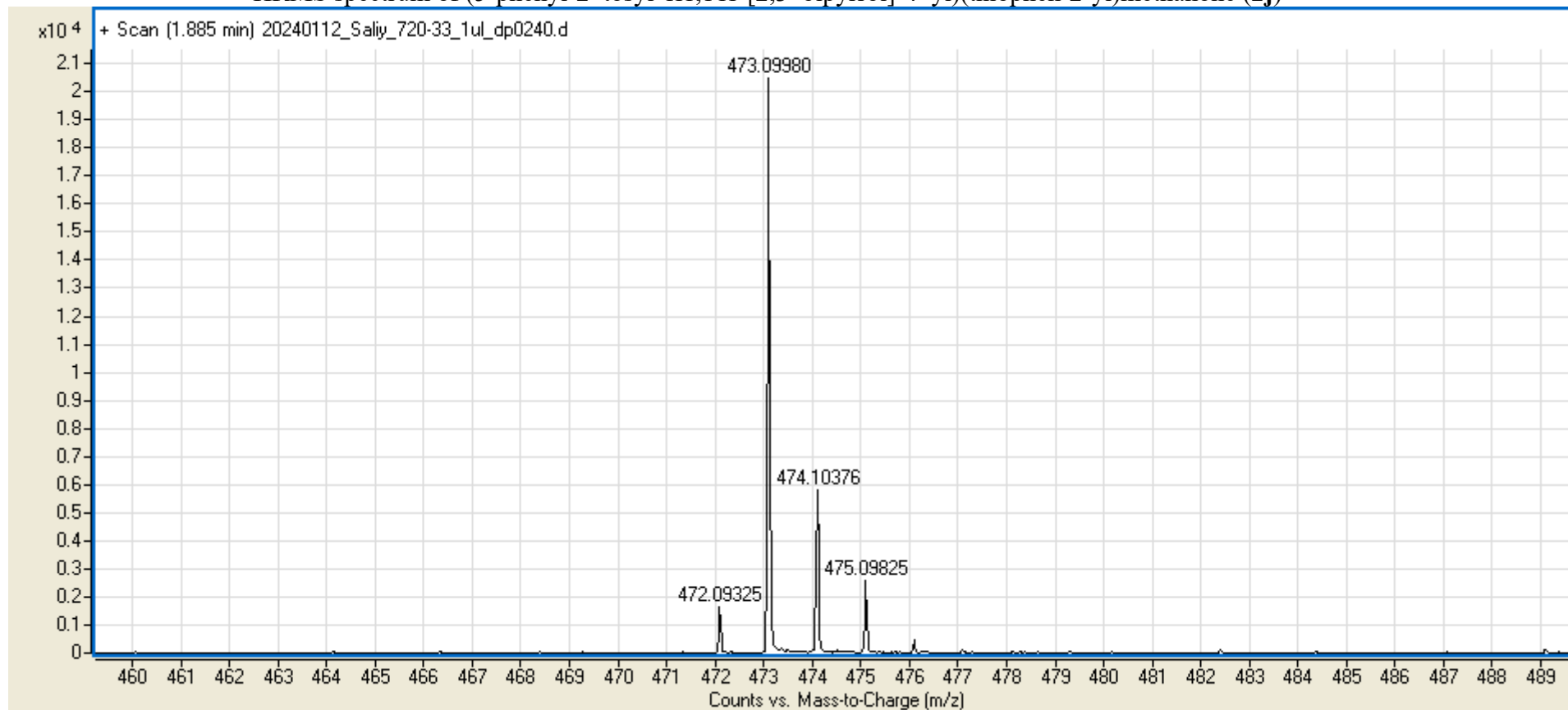


$^{13}\text{C}$  NMR spectrum of (5-phenyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(thiophen-2-yl)methanone (**2j**) in  $\text{CDCl}_3$ .

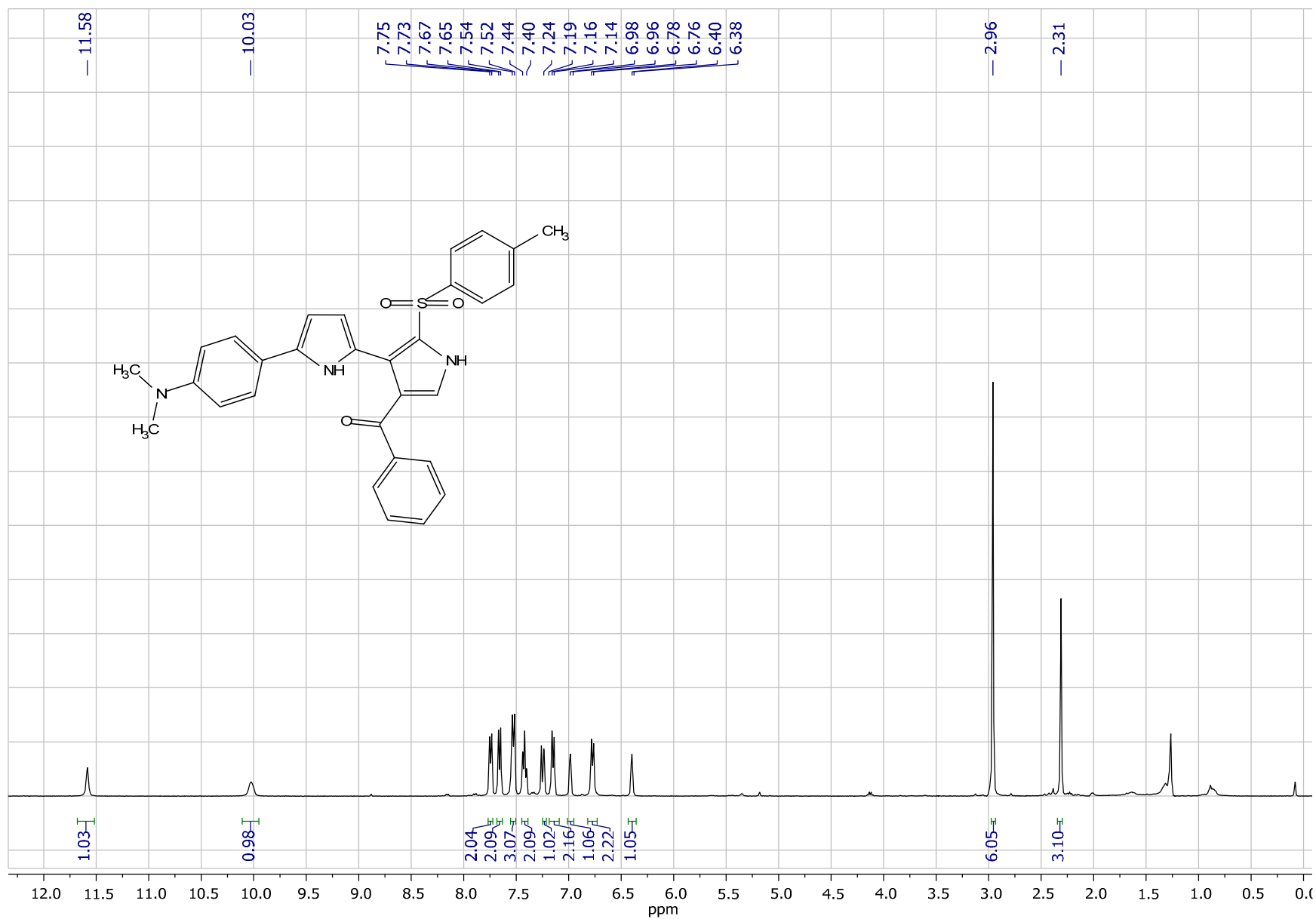




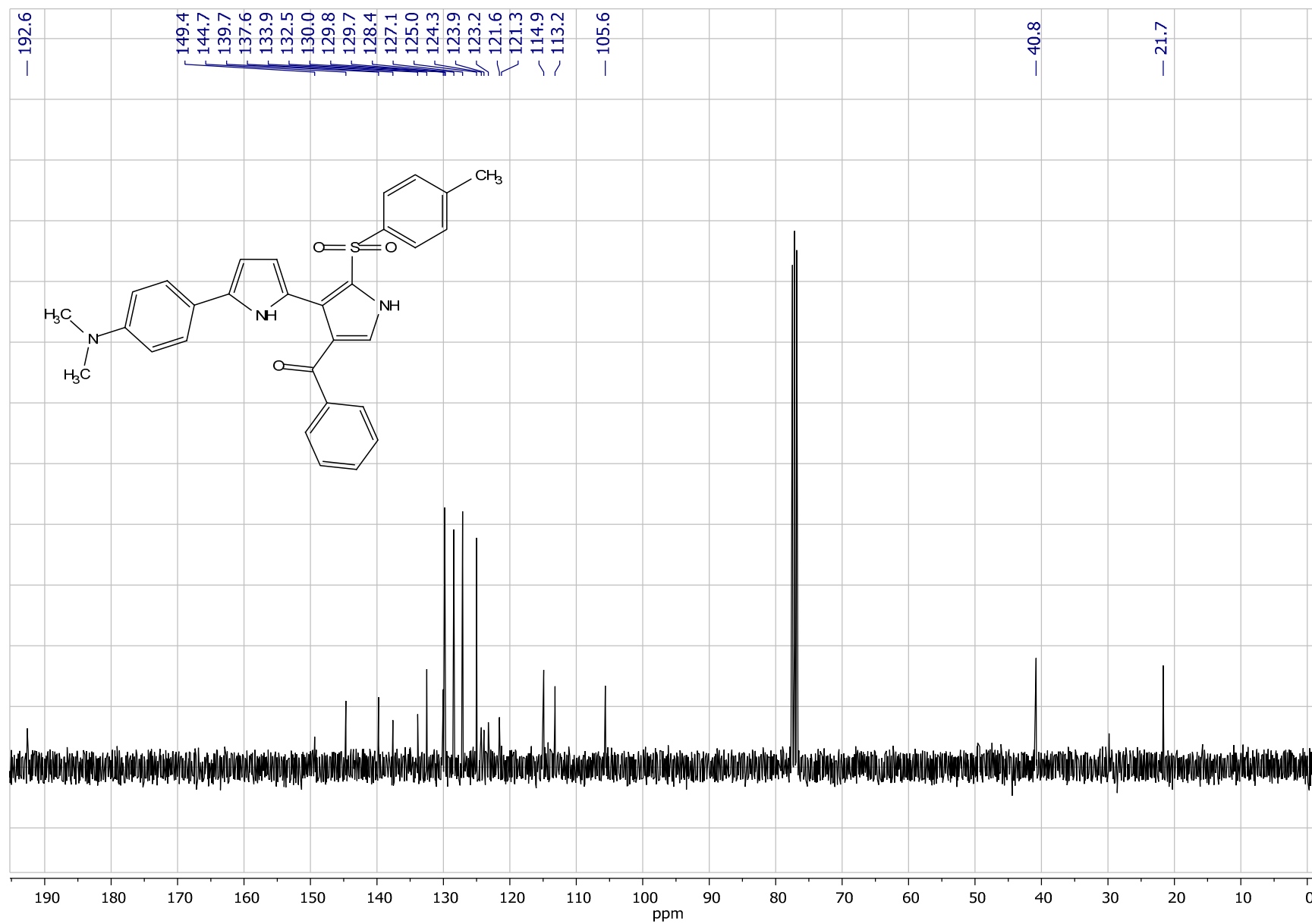
HRMS spectrum of (5-phenyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(thiophen-2-yl)methanone (**2j**)



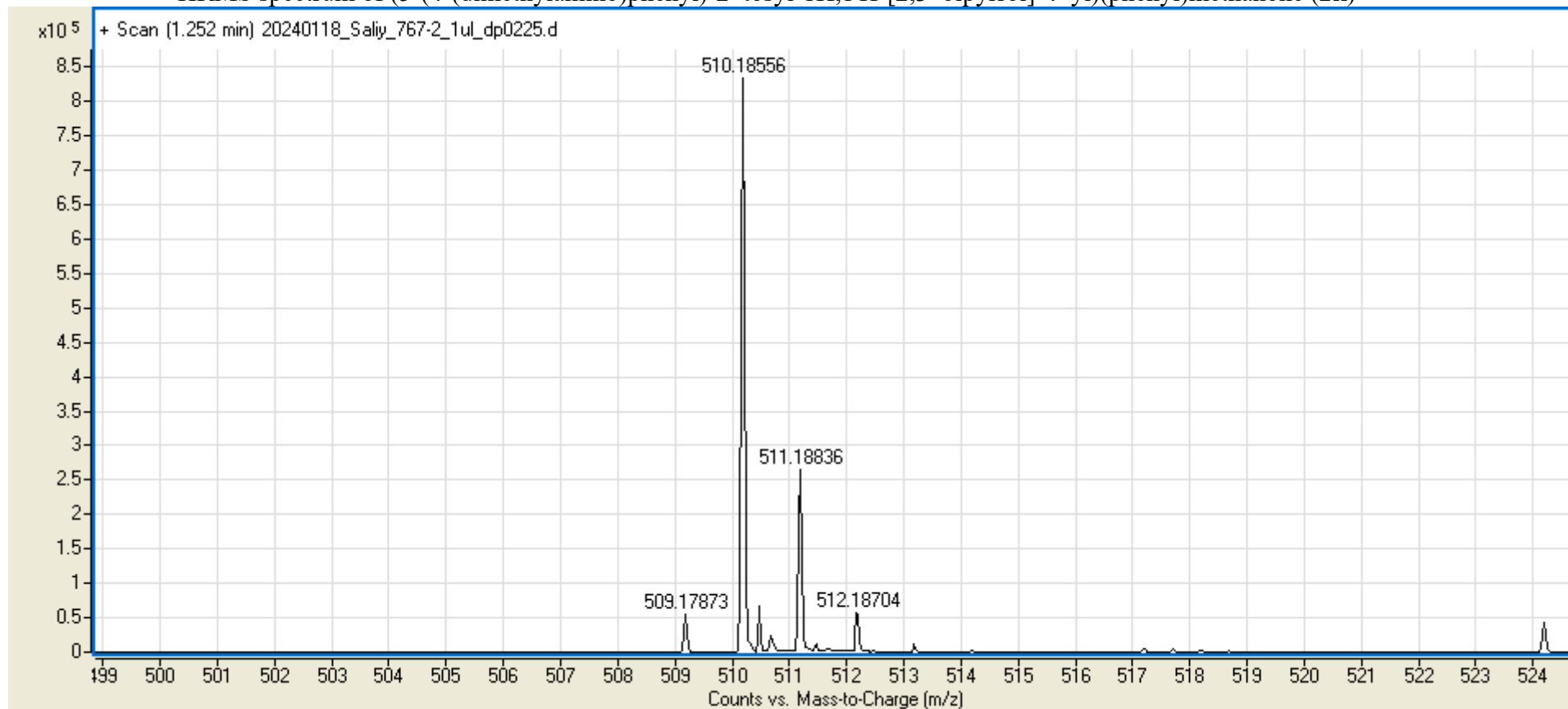
$^1\text{H}$  NMR spectrum of (5-(4-(dimethylamino)phenyl)-2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (**2k**) in  $\text{CDCl}_3$ .



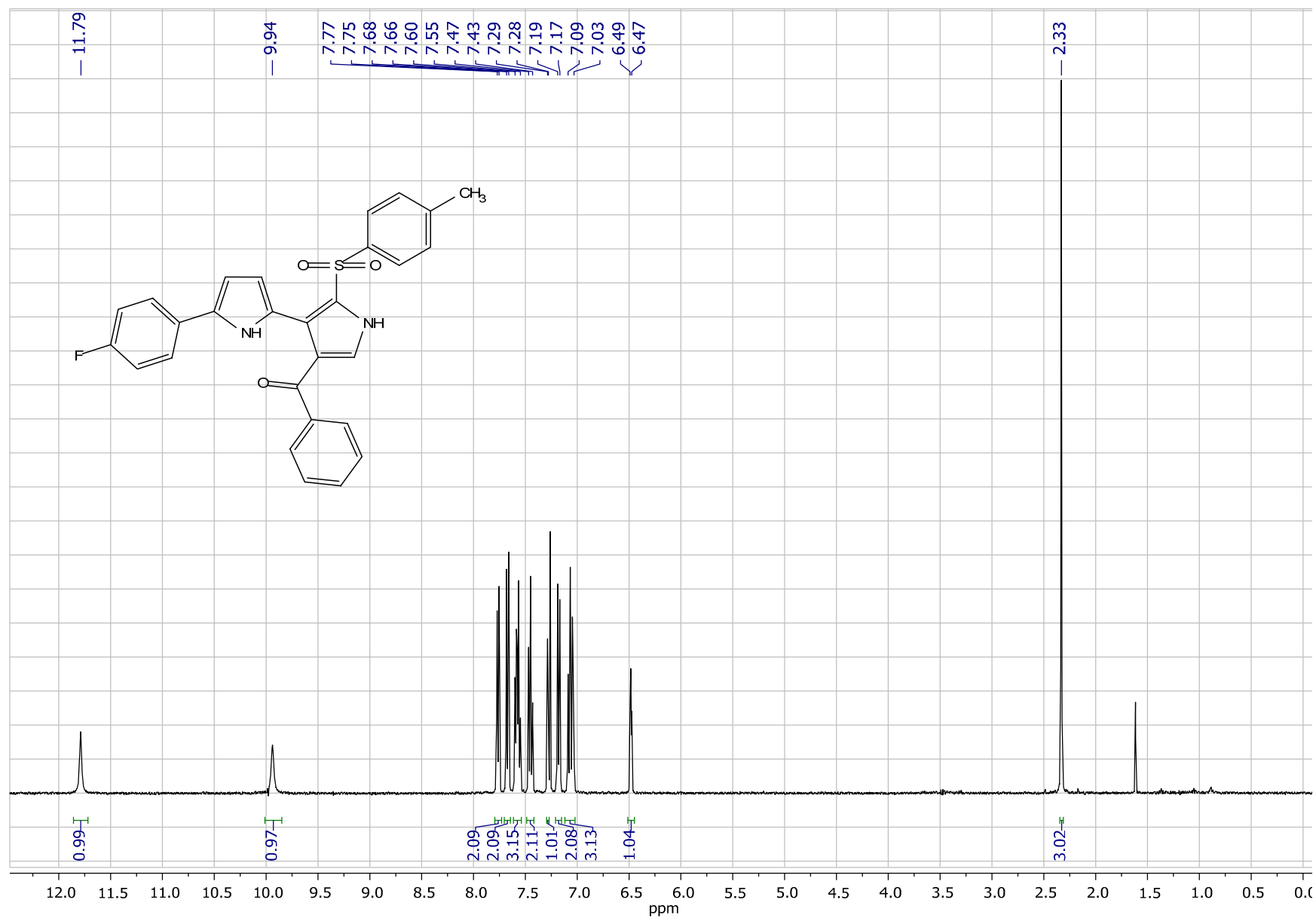
$^{13}\text{C}$  NMR spectrum of (5-(4-(dimethylamino)phenyl)-2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (**2k**) in  $\text{CDCl}_3$ .



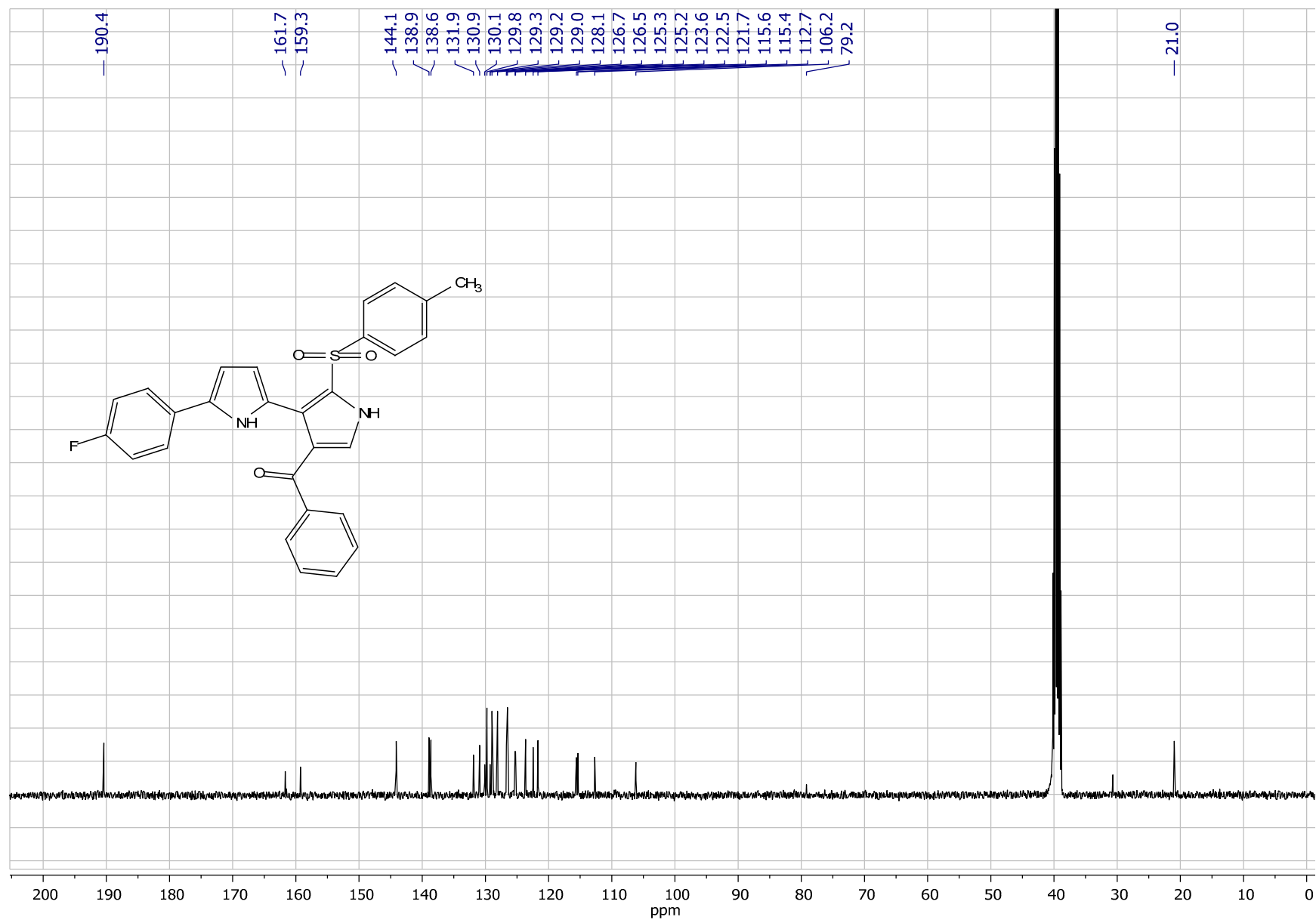
HRMS spectrum of (5-(4-(dimethylamino)phenyl)-2'-tosyl-1H,1'H-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (**2k**)



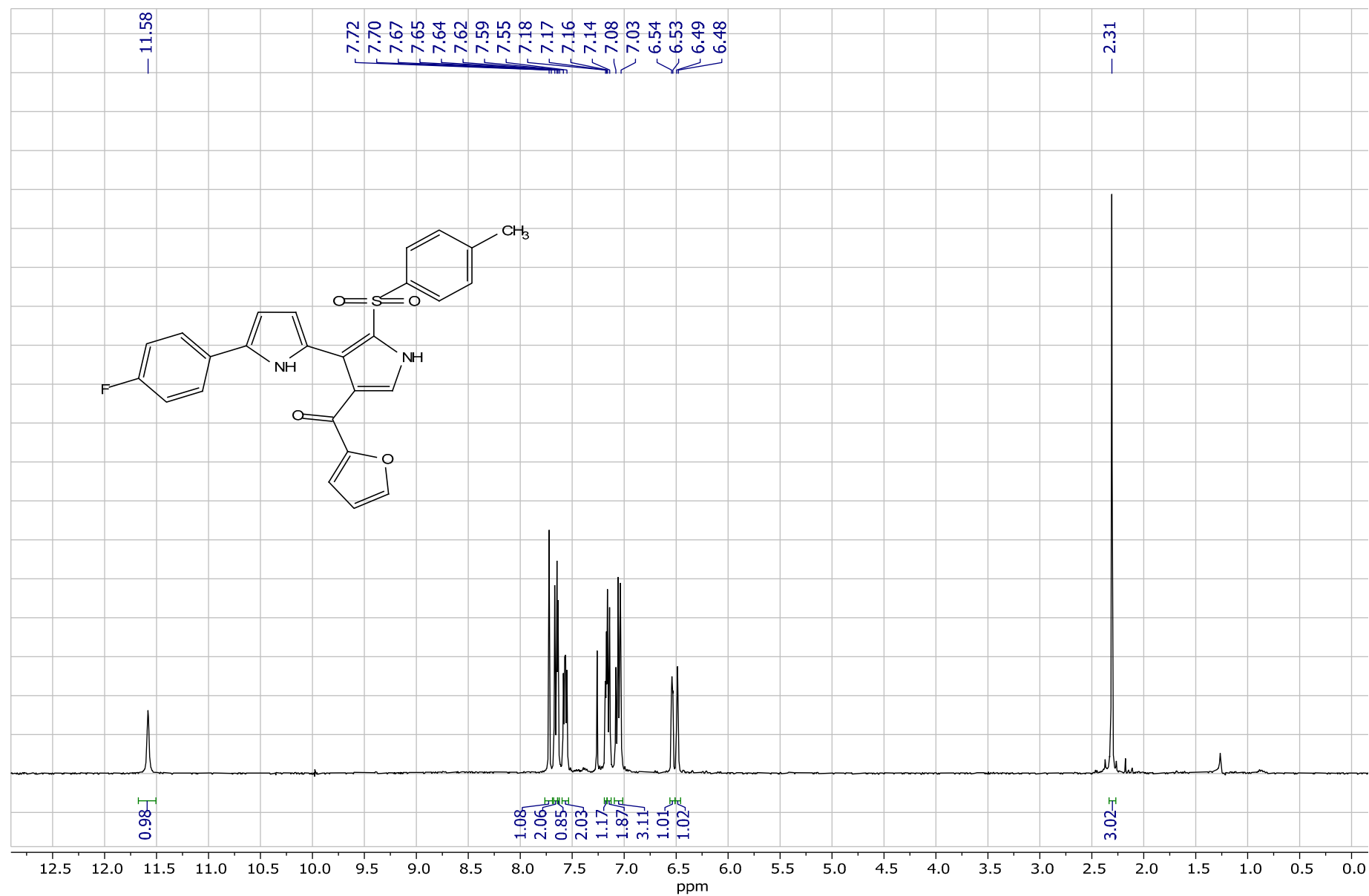
<sup>1</sup>H NMR spectrum of (5-(4-fluorophenyl)-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (**21**) in CDCl<sub>3</sub>.



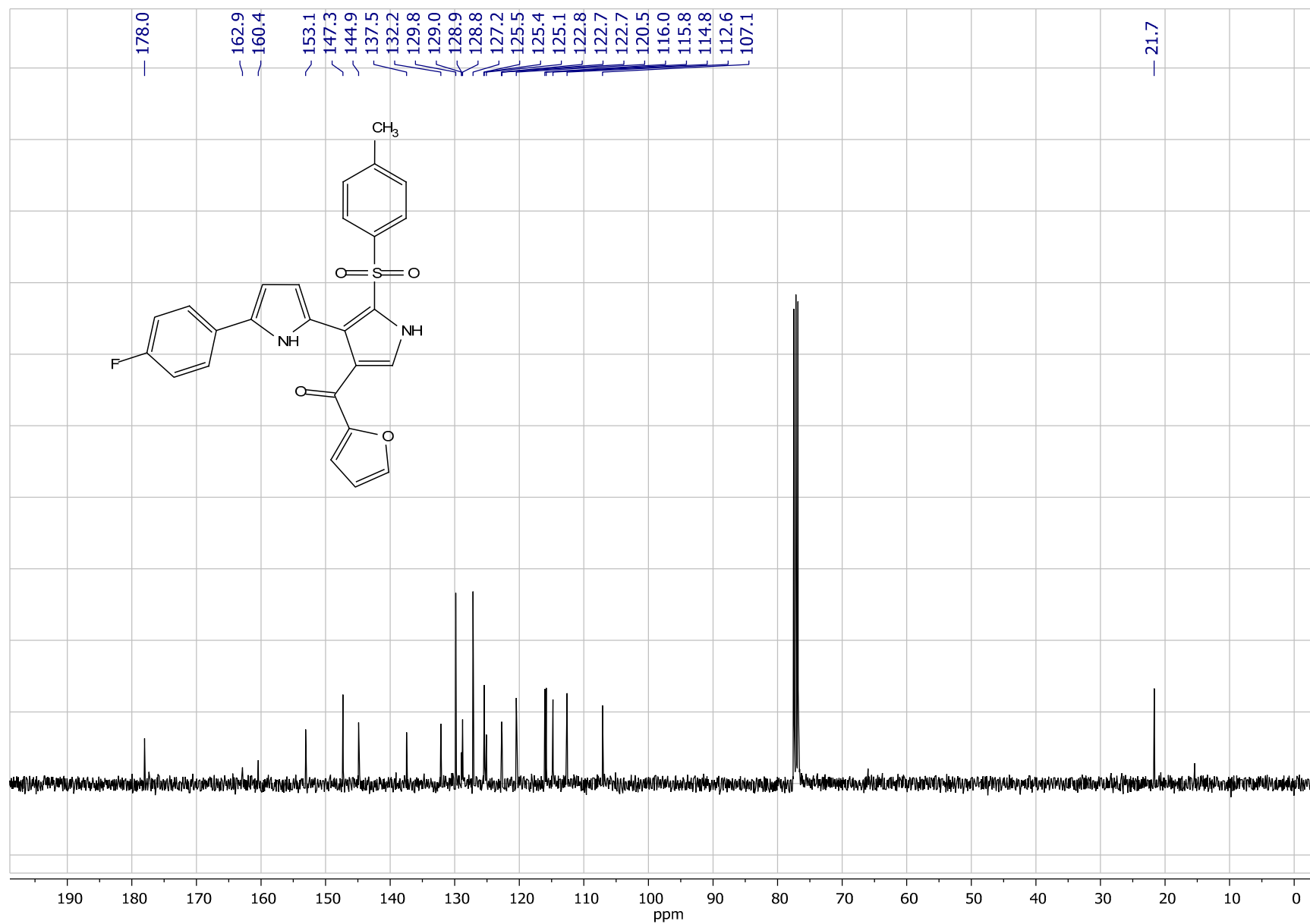
$^{13}\text{C}$  NMR spectrum of (5-(4-fluorophenyl)-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (**21**) in DMSO- $\text{d}_6$ .



$^1\text{H}$  NMR spectrum of (5-(4-fluorophenyl)-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(furan-2-yl)methanone (**2m**) in  $\text{CDCl}_3$ .

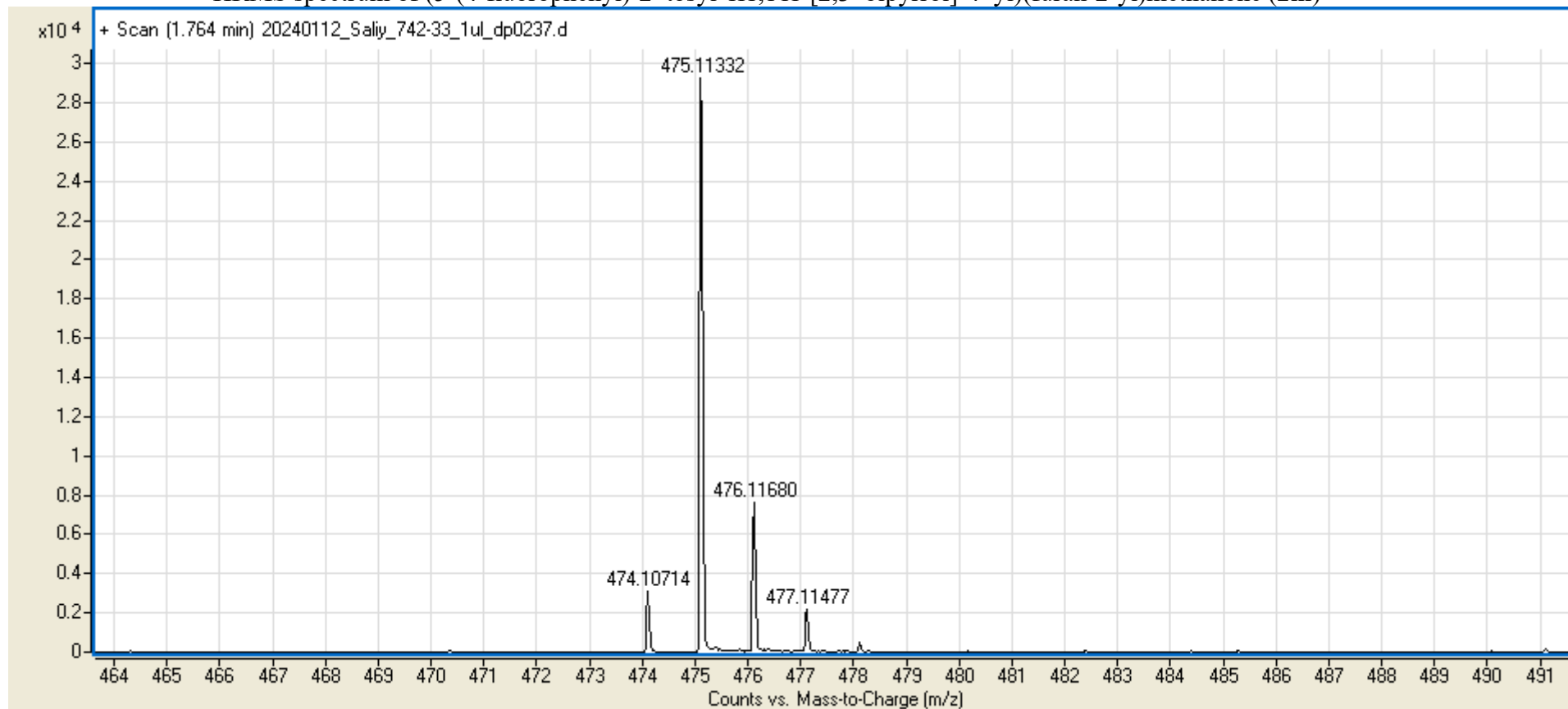


$^{13}\text{C}$  NMR spectrum of (5-(4-fluorophenyl)-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(furan-2-yl)methanone (**2m**) in  $\text{CDCl}_3$ .

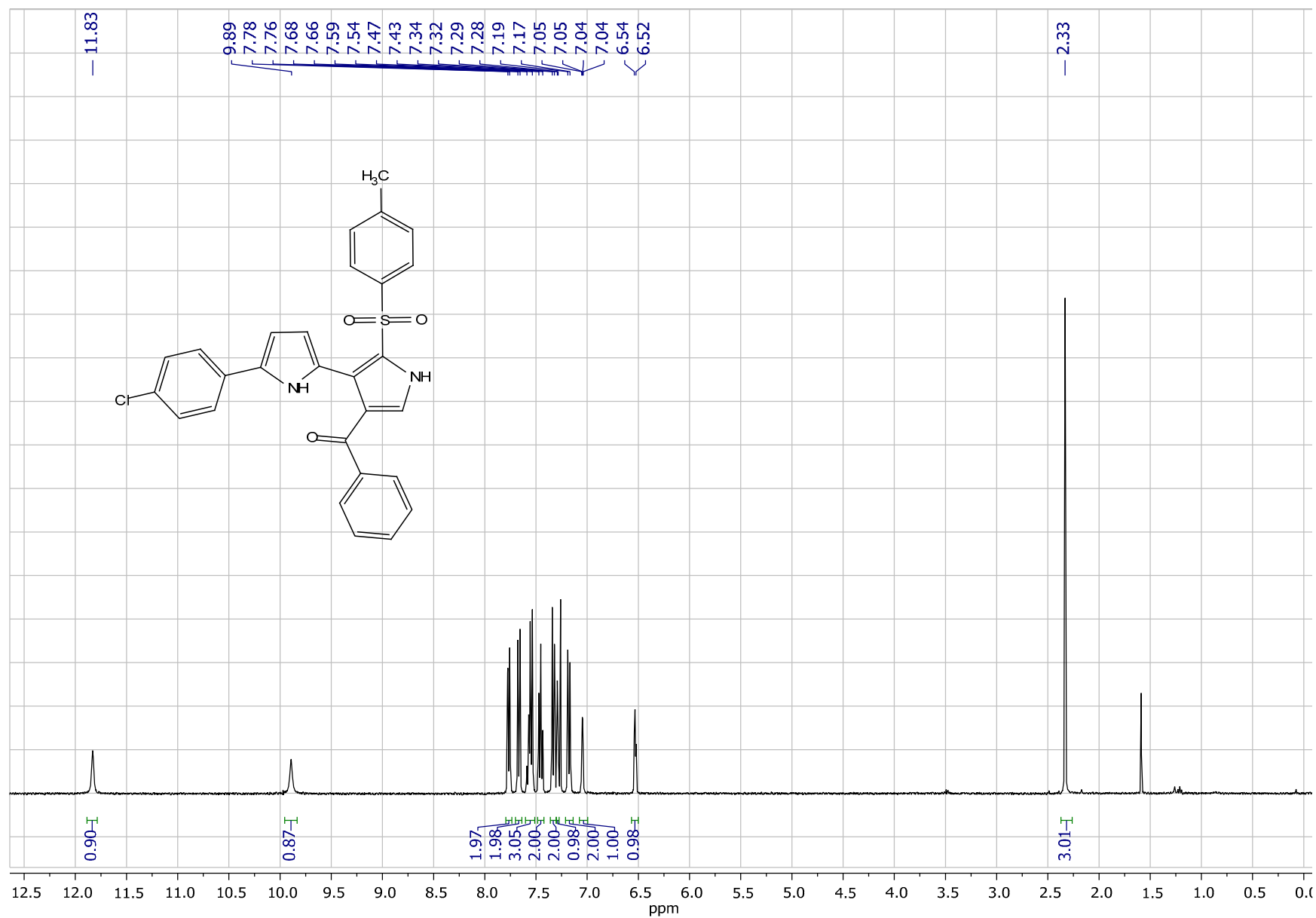




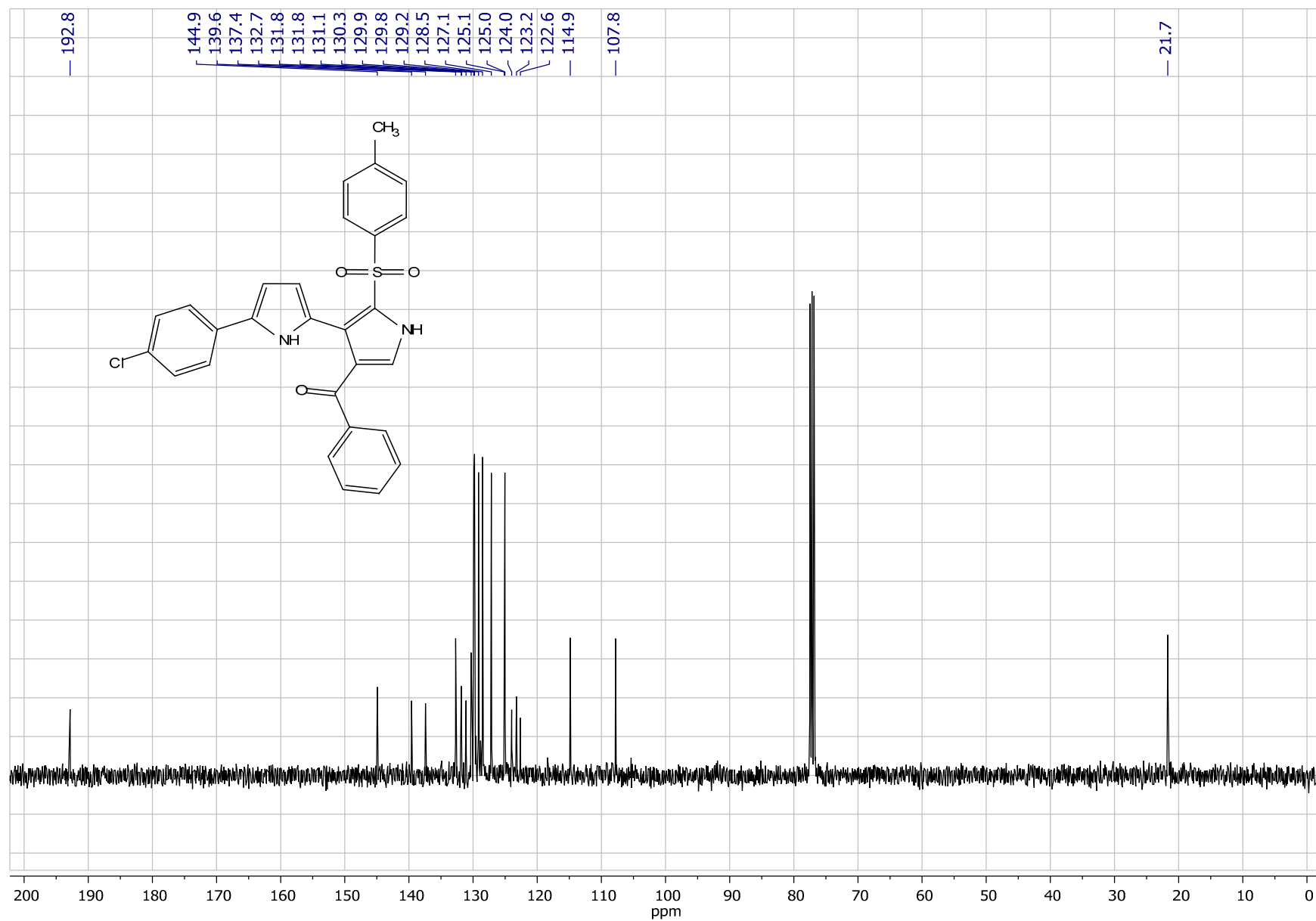
HRMS spectrum of (5-(4-fluorophenyl)-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(furan-2-yl)methanone (**2m**)



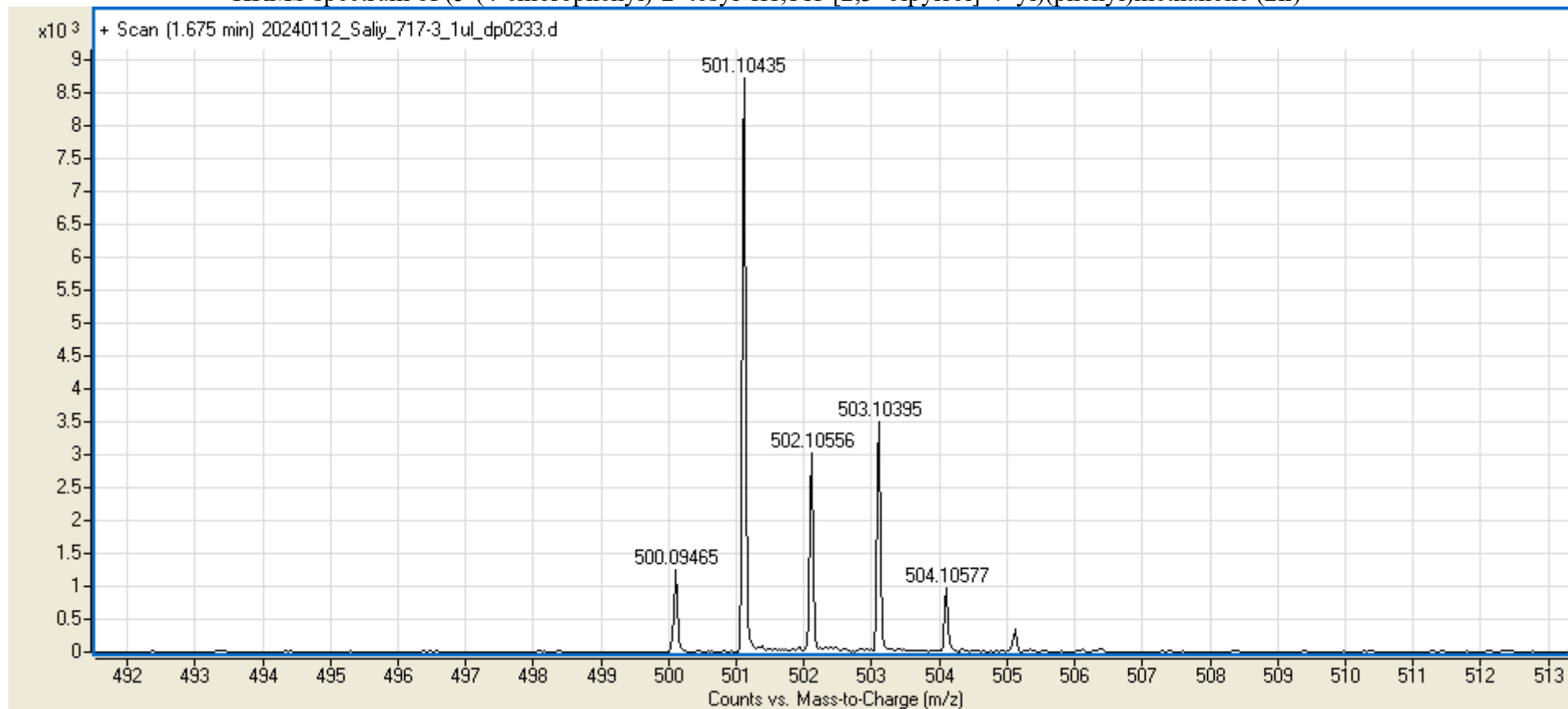
$^1\text{H}$  NMR spectrum of (5-(4-chlorophenyl)-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (**2n**) in  $\text{CDCl}_3$ .



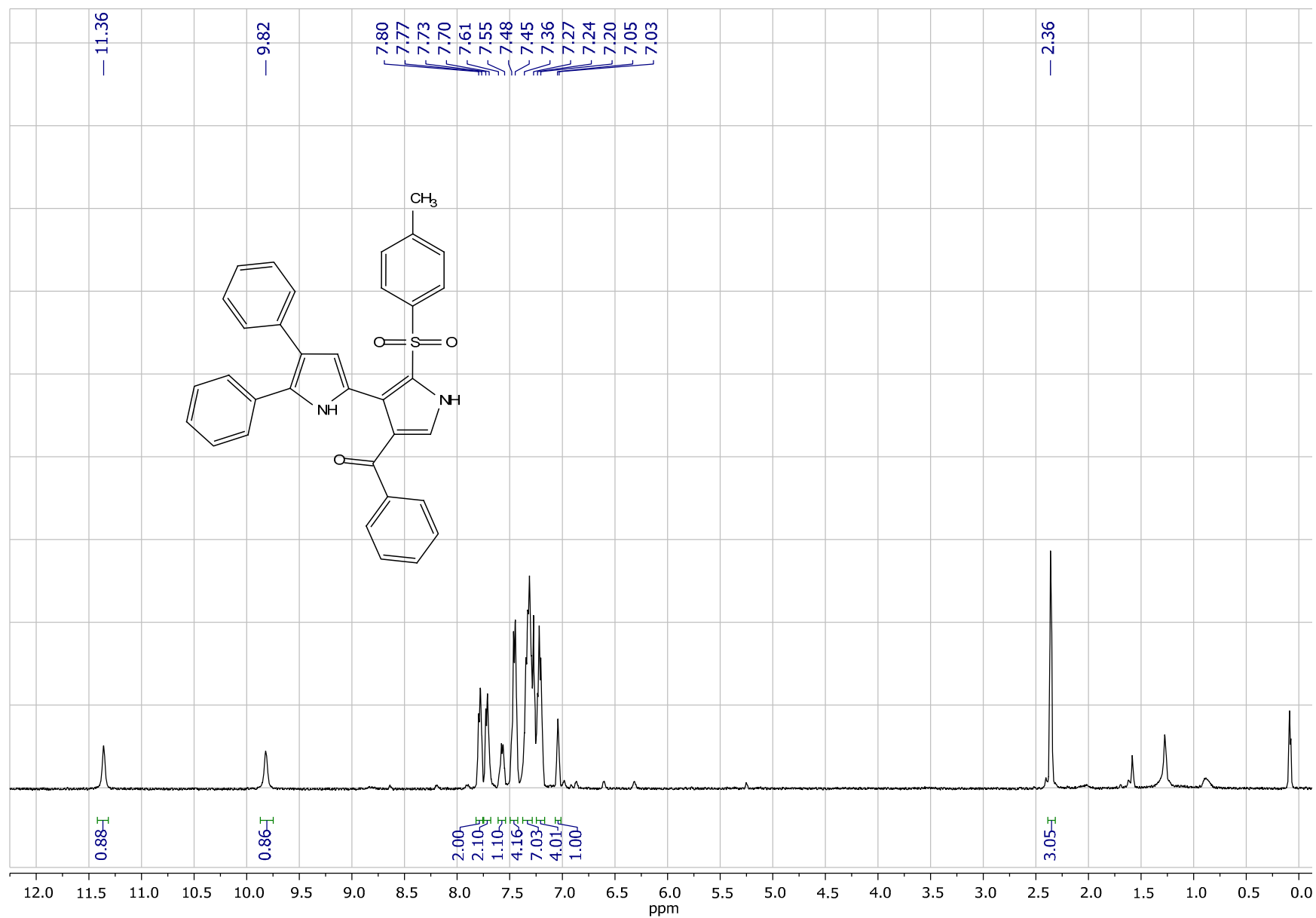
$^{13}\text{C}$  NMR spectrum of (5-(4-chlorophenyl)-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (**2n**) in  $\text{CDCl}_3$ .



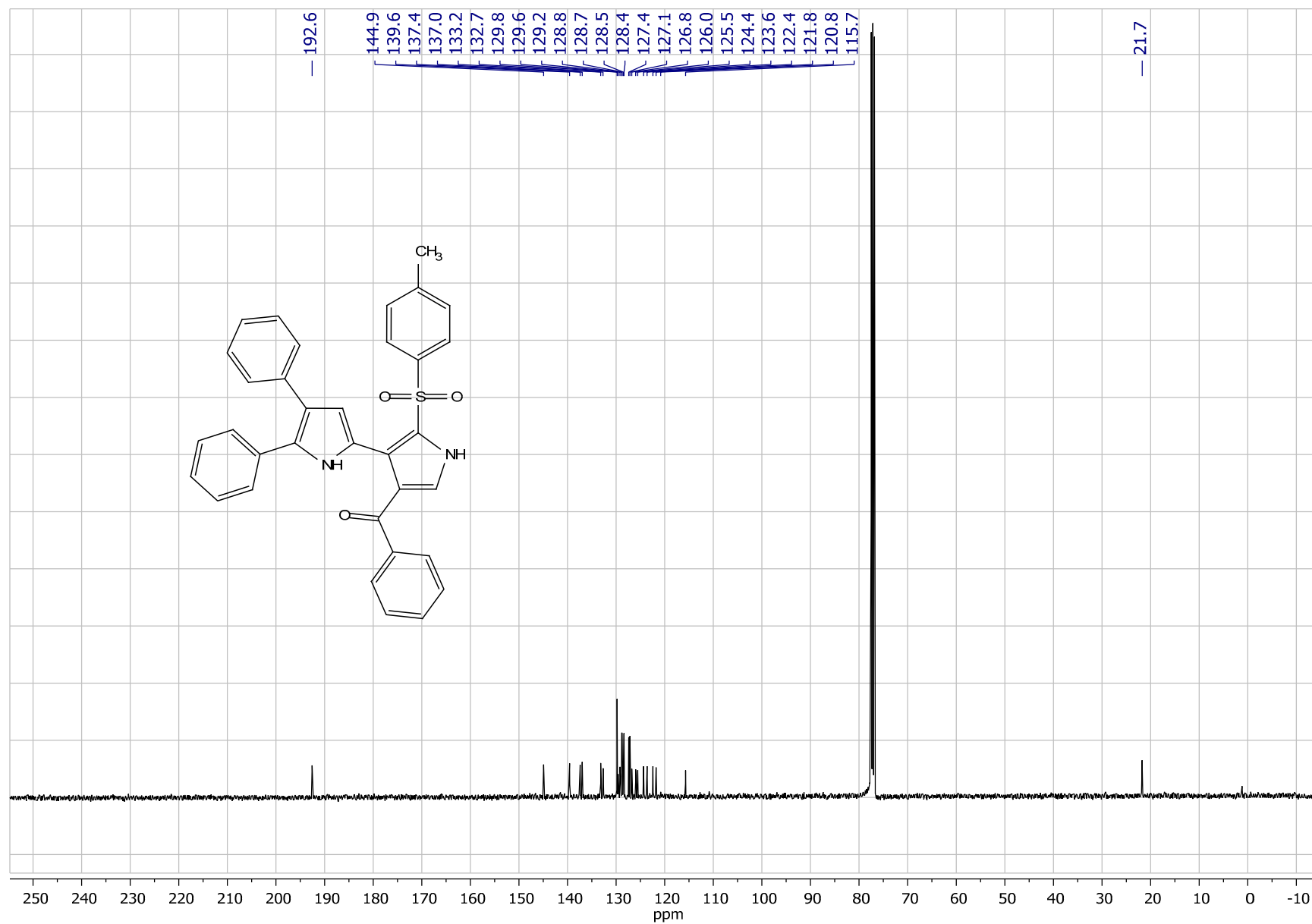
HRMS spectrum of (5-(4-chlorophenyl)-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (**2n**)



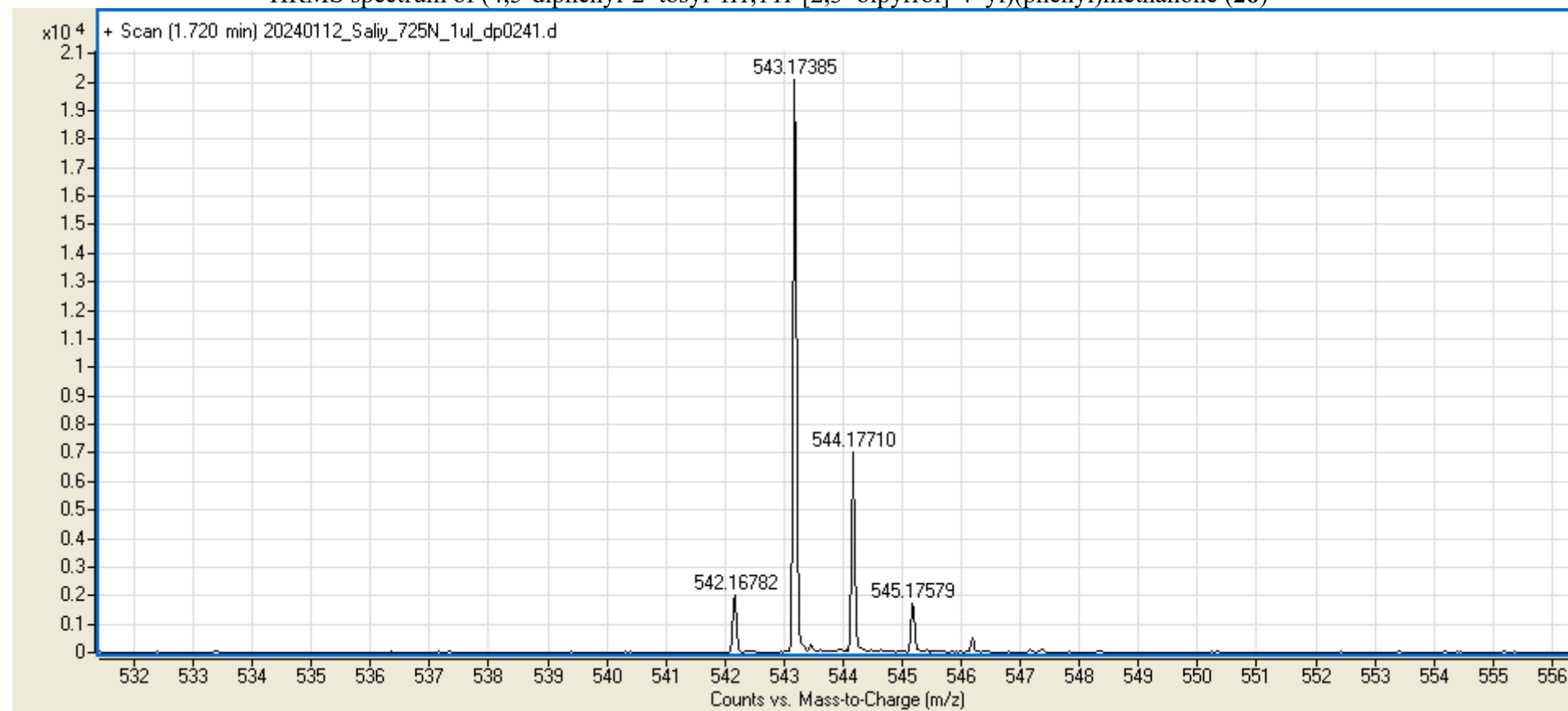
$^1\text{H}$  NMR spectrum of (4,5-diphenyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (**2o**) in  $\text{CDCl}_3$ .



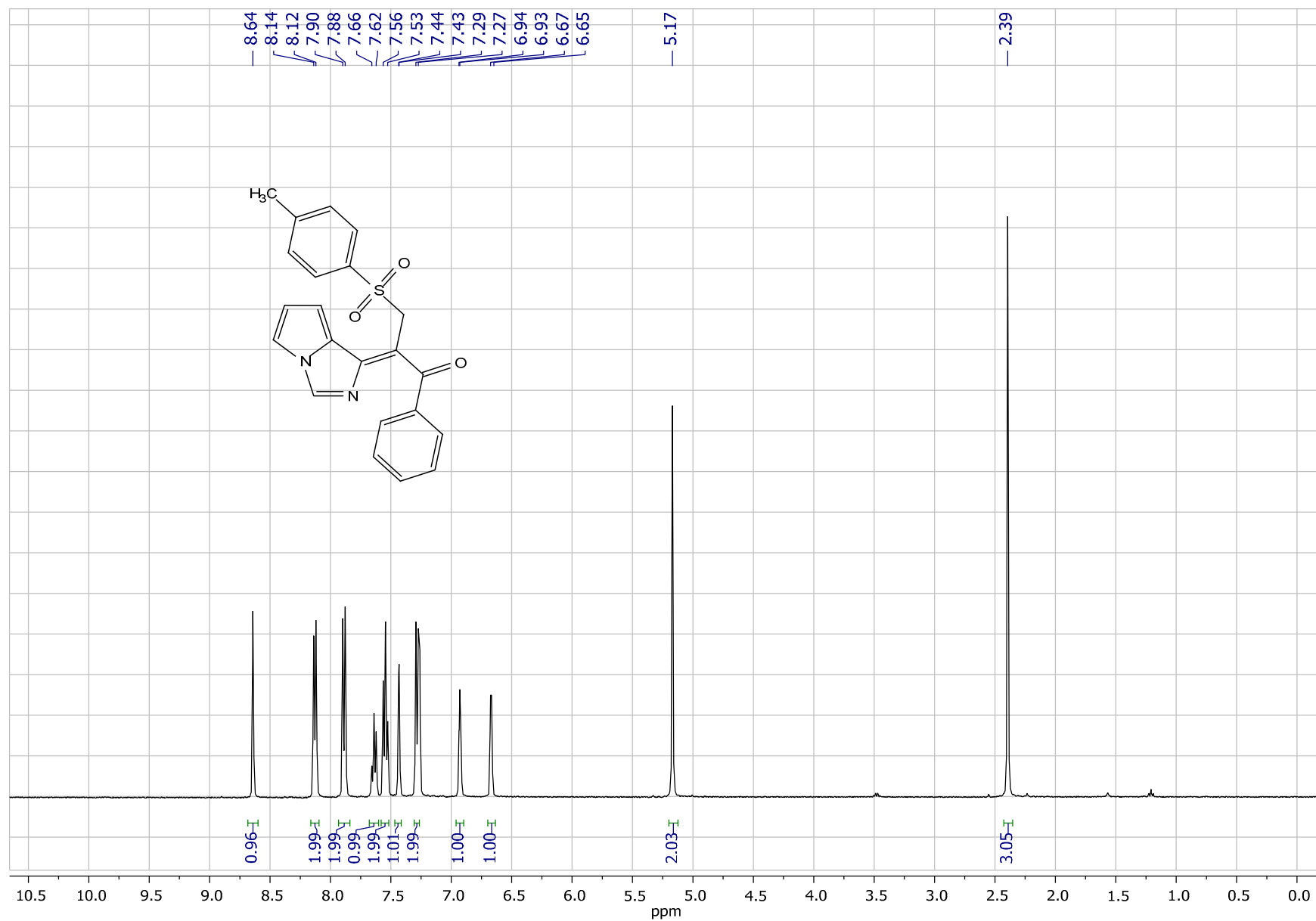
$^{13}\text{C}$  NMR spectrum of (4,5-diphenyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (**2o**) in  $\text{CDCl}_3$ .



HRMS spectrum of (4,5-diphenyl-2'-tosyl-1*H*,1'*H*-[2,3'-bipyrrol]-4'-yl)(phenyl)methanone (**2o**)

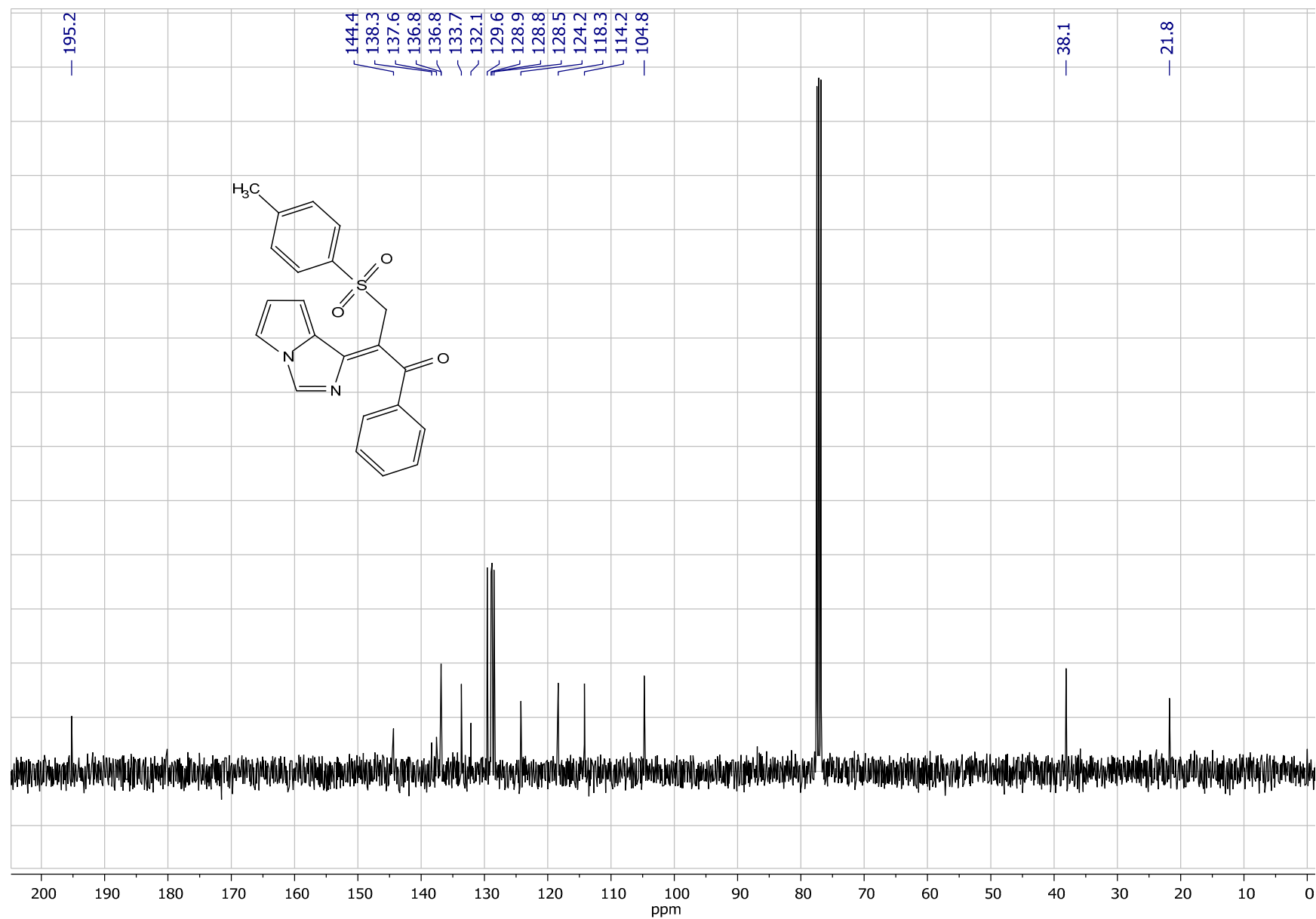


$^1\text{H}$  NMR spectrum of (*E*)-1-phenyl-2-(1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3a**) in  $\text{CDCl}_3$ .

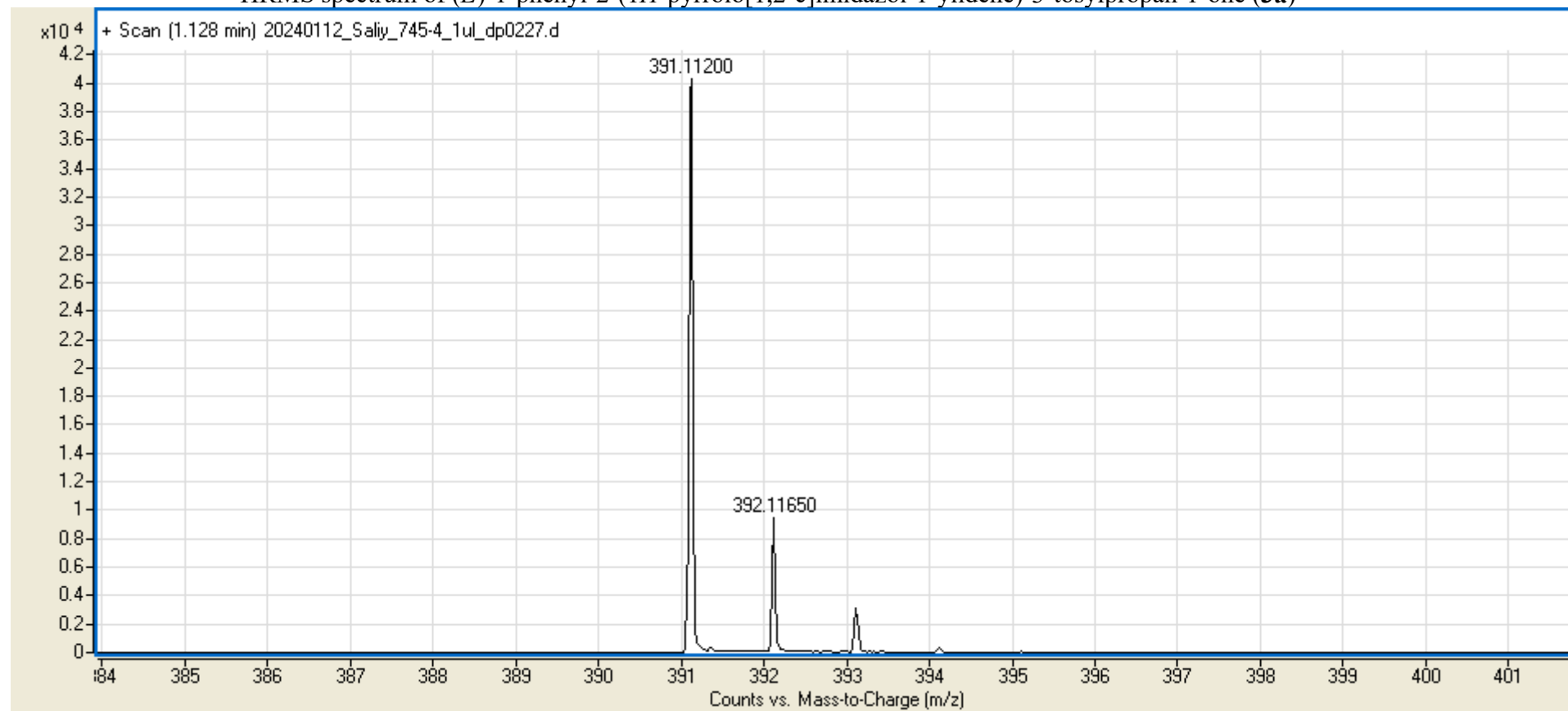




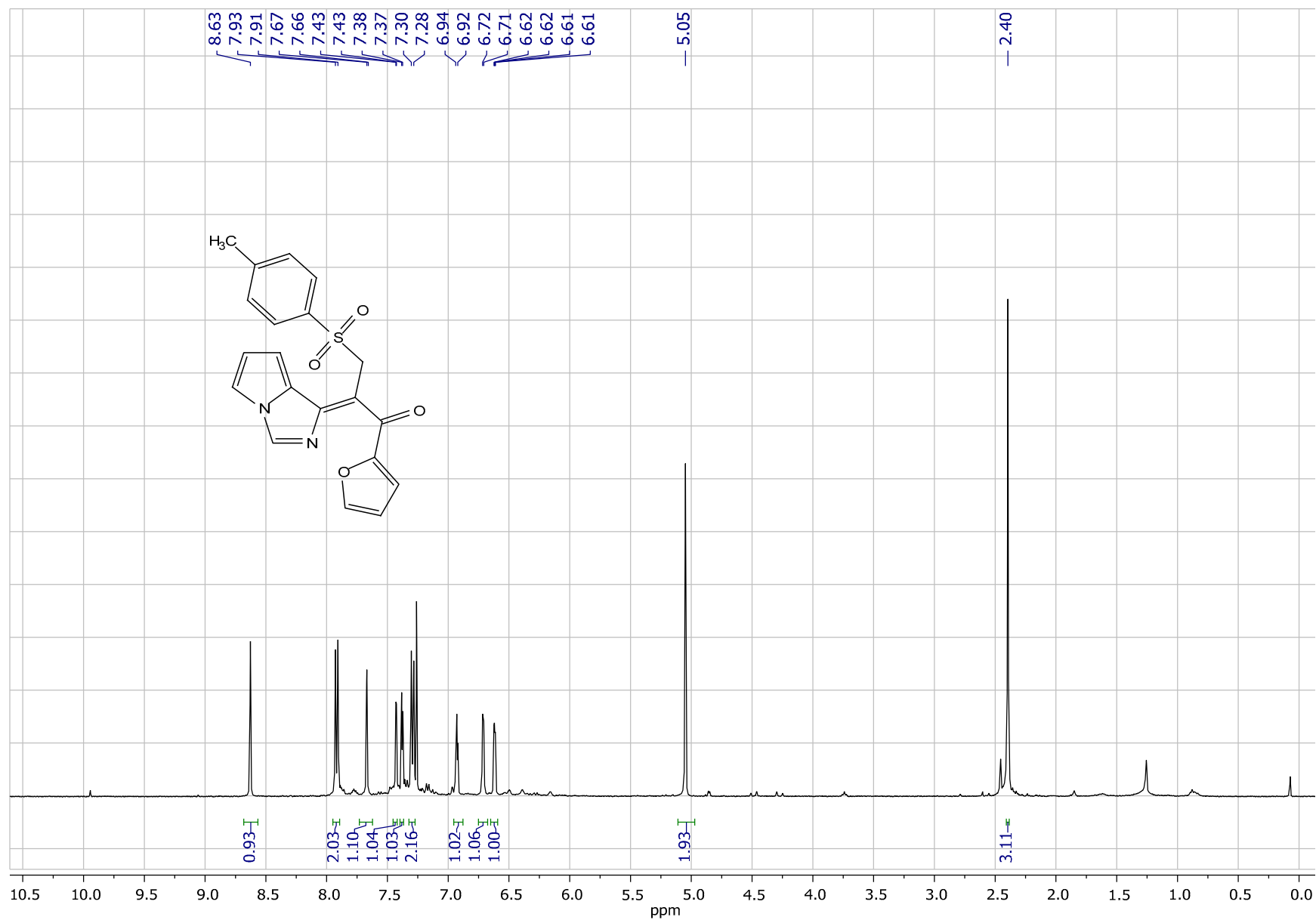
$^{13}\text{C}$  NMR spectrum of (*E*)-1-phenyl-2-(1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3a**) in  $\text{CDCl}_3$ .



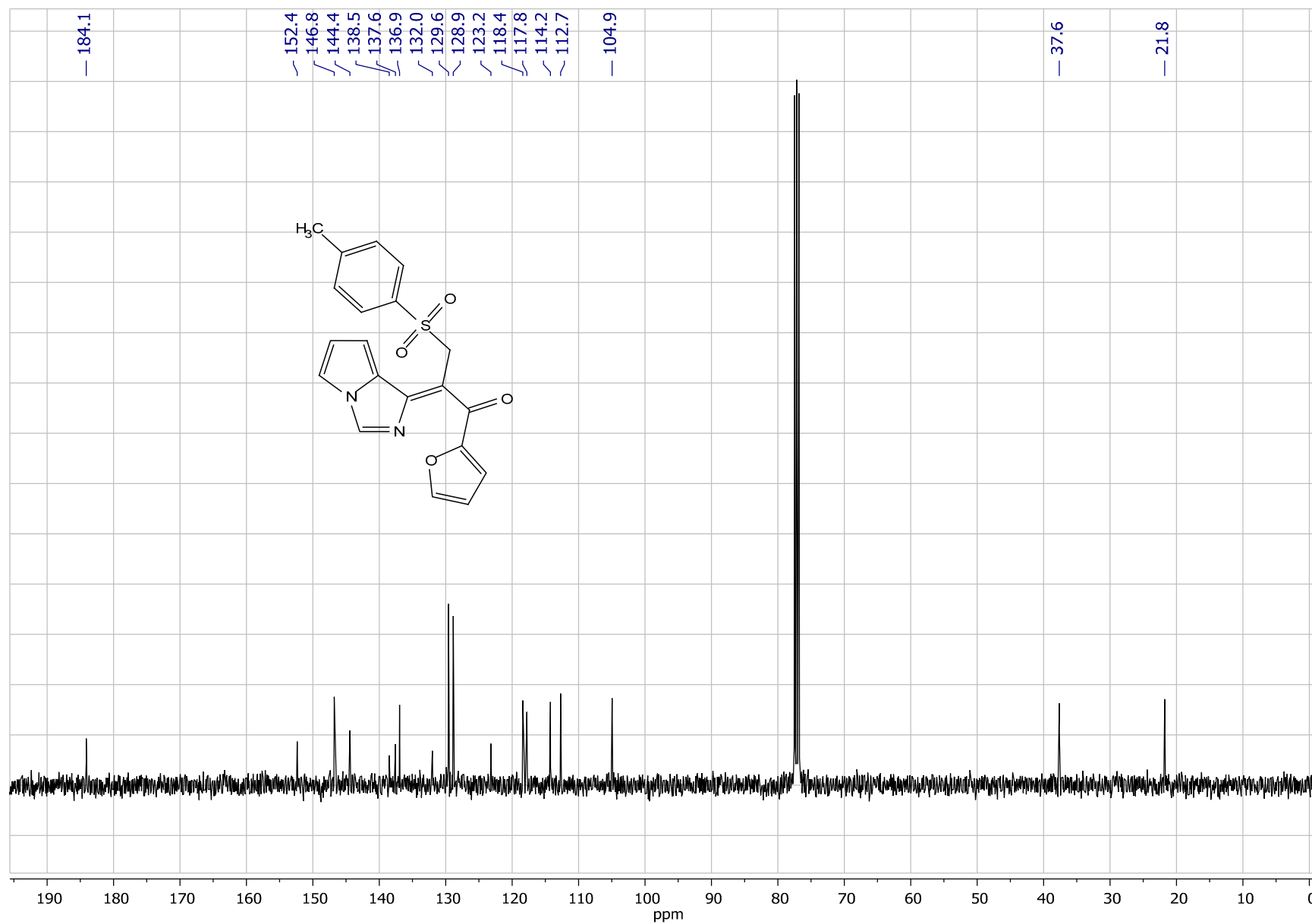
HRMS spectrum of (*E*)-1-phenyl-2-(1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3a**)



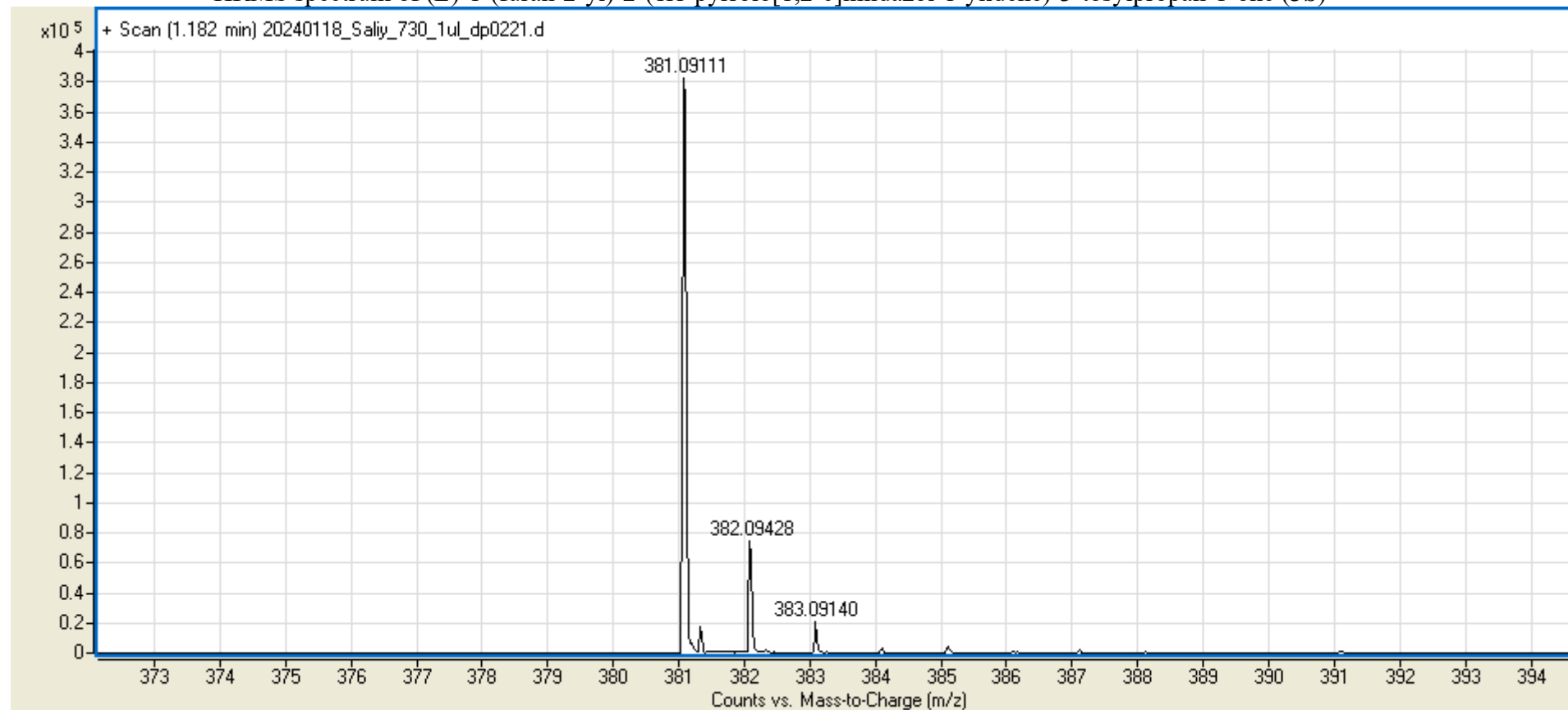
$^1\text{H}$  NMR spectrum of (*E*)-1-(furan-2-yl)-2-(1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3b**) in  $\text{CDCl}_3$ .



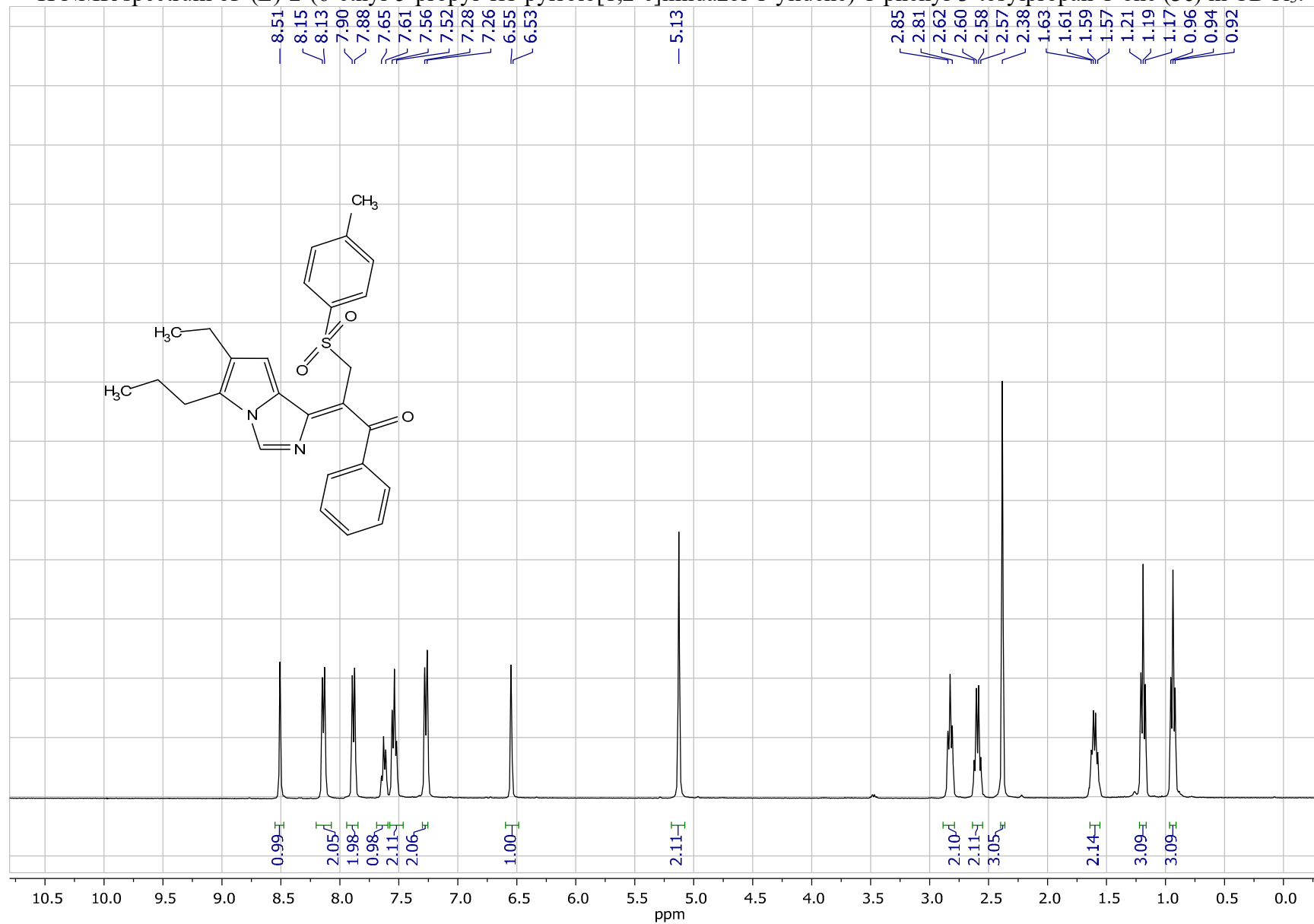
$^{13}\text{C}$  NMR spectrum of (*E*)-1-(furan-2-yl)-2-(1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3b**) in  $\text{CDCl}_3$ .



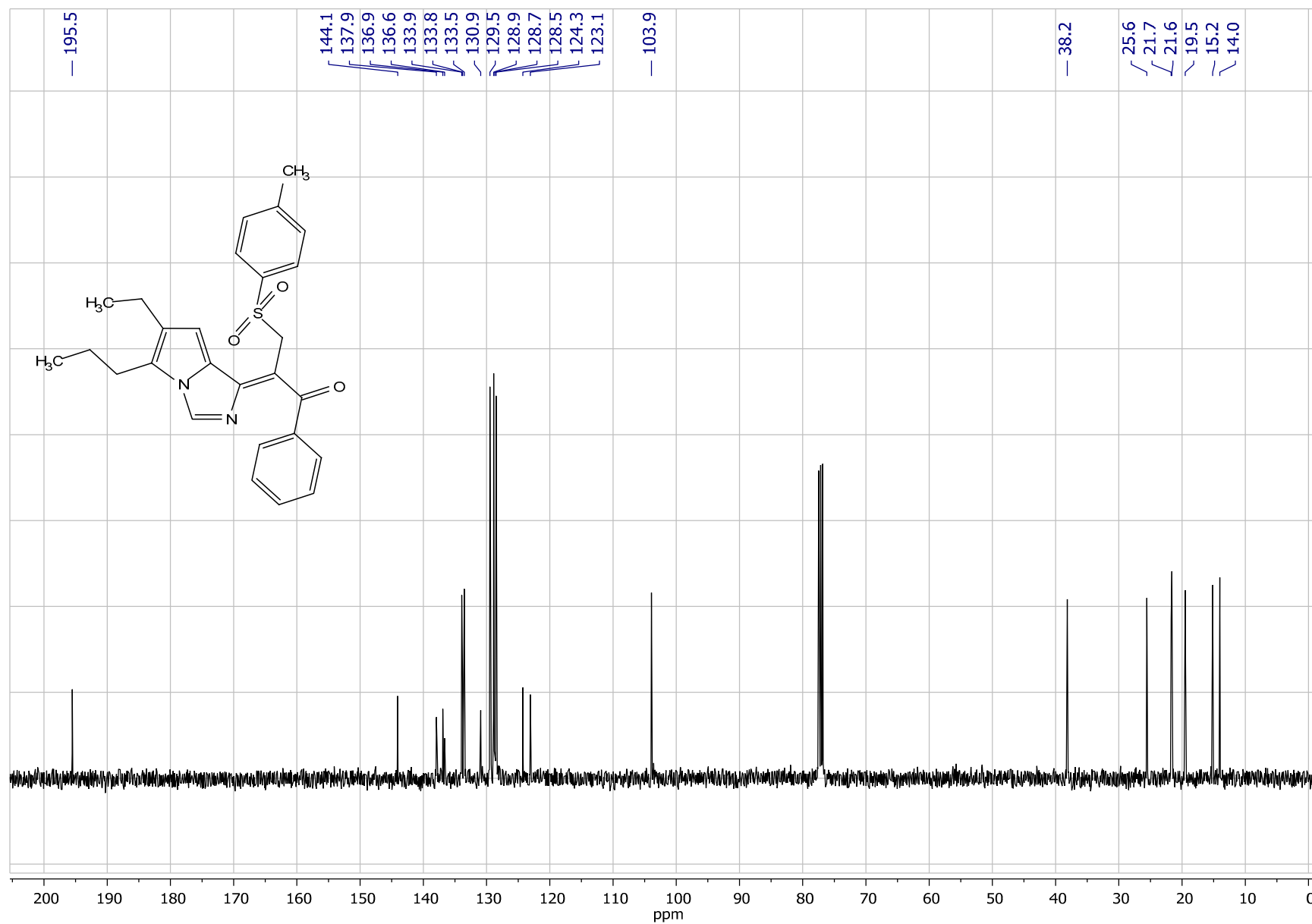
HRMS spectrum of (*E*)-1-(furan-2-yl)-2-(1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3b**)



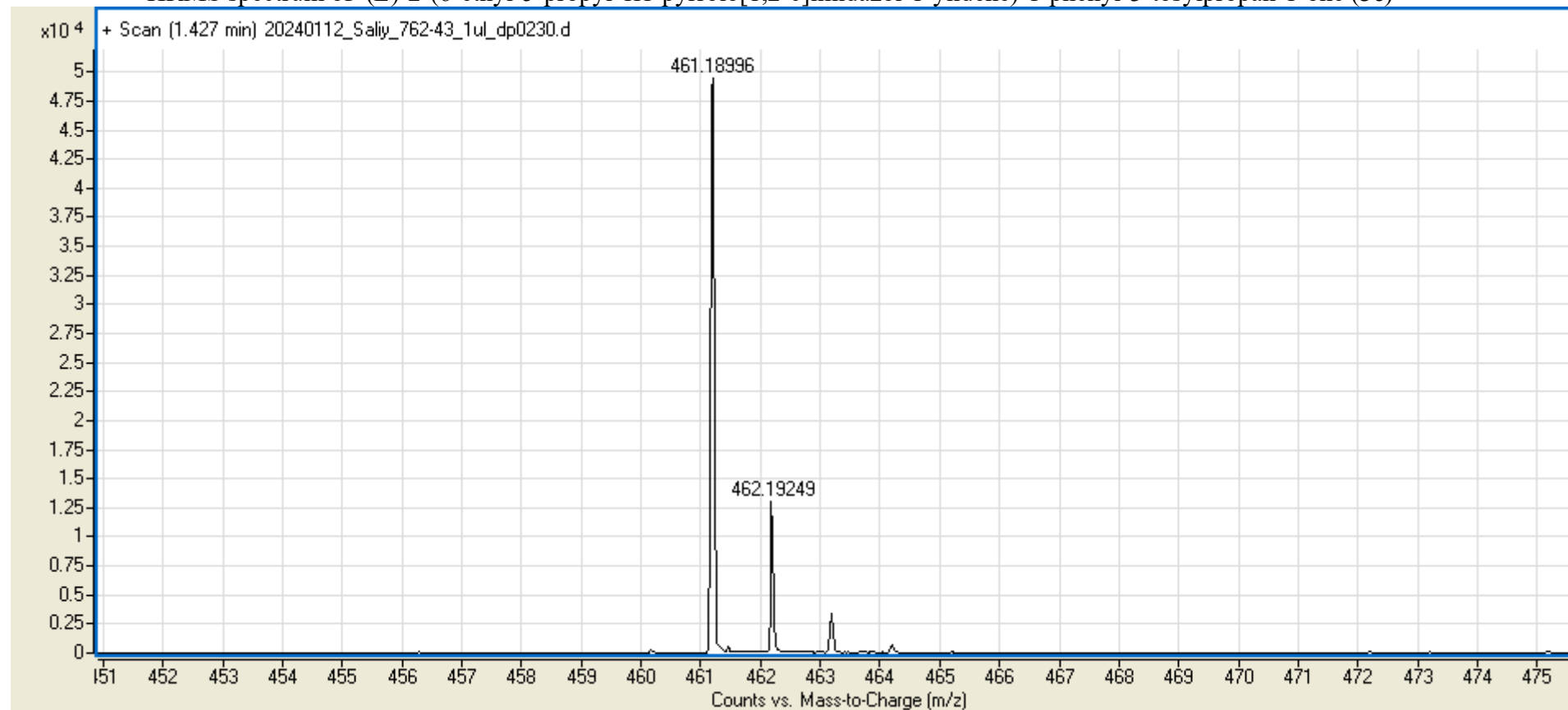
$^1\text{H}$  NMR spectrum of (*E*)-2-(6-ethyl-5-propyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (**3c**) in  $\text{CDCl}_3$ .



$^{13}\text{C}$  NMR spectrum of (*E*)-2-(6-ethyl-5-propyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (**3c**) in  $\text{CDCl}_3$ .

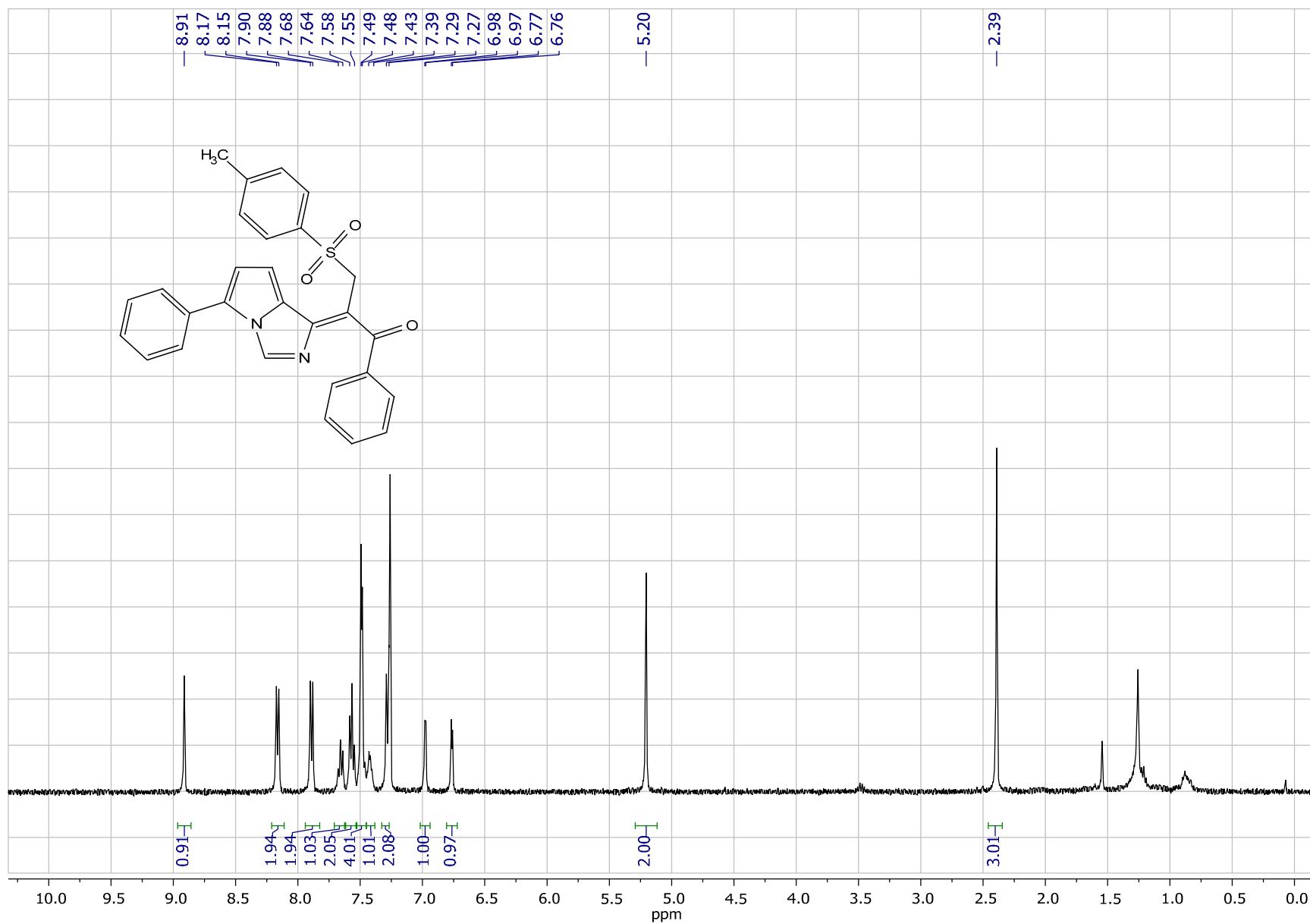


HRMS spectrum of (*E*)-2-(6-ethyl-5-propyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (**3c**)

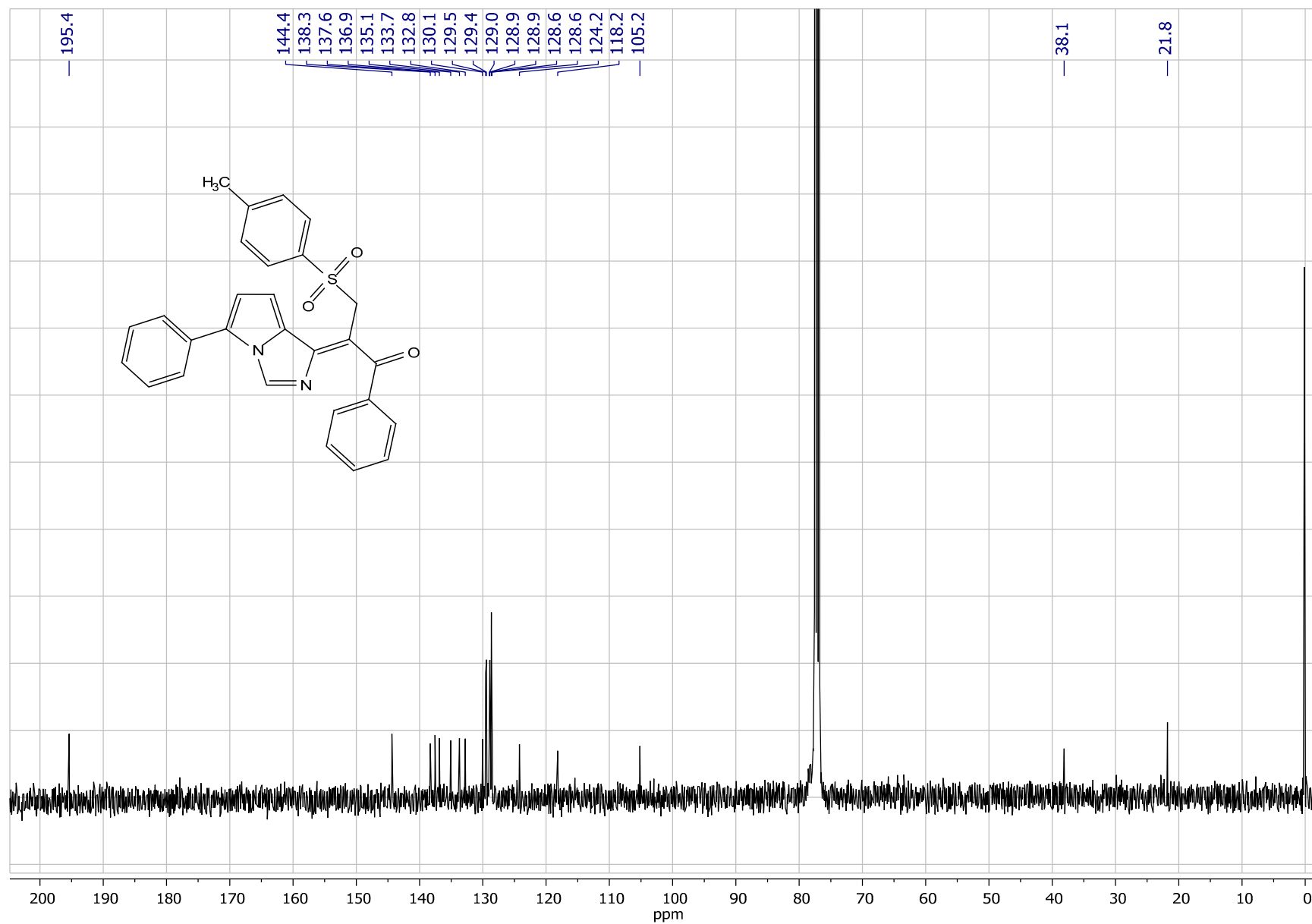




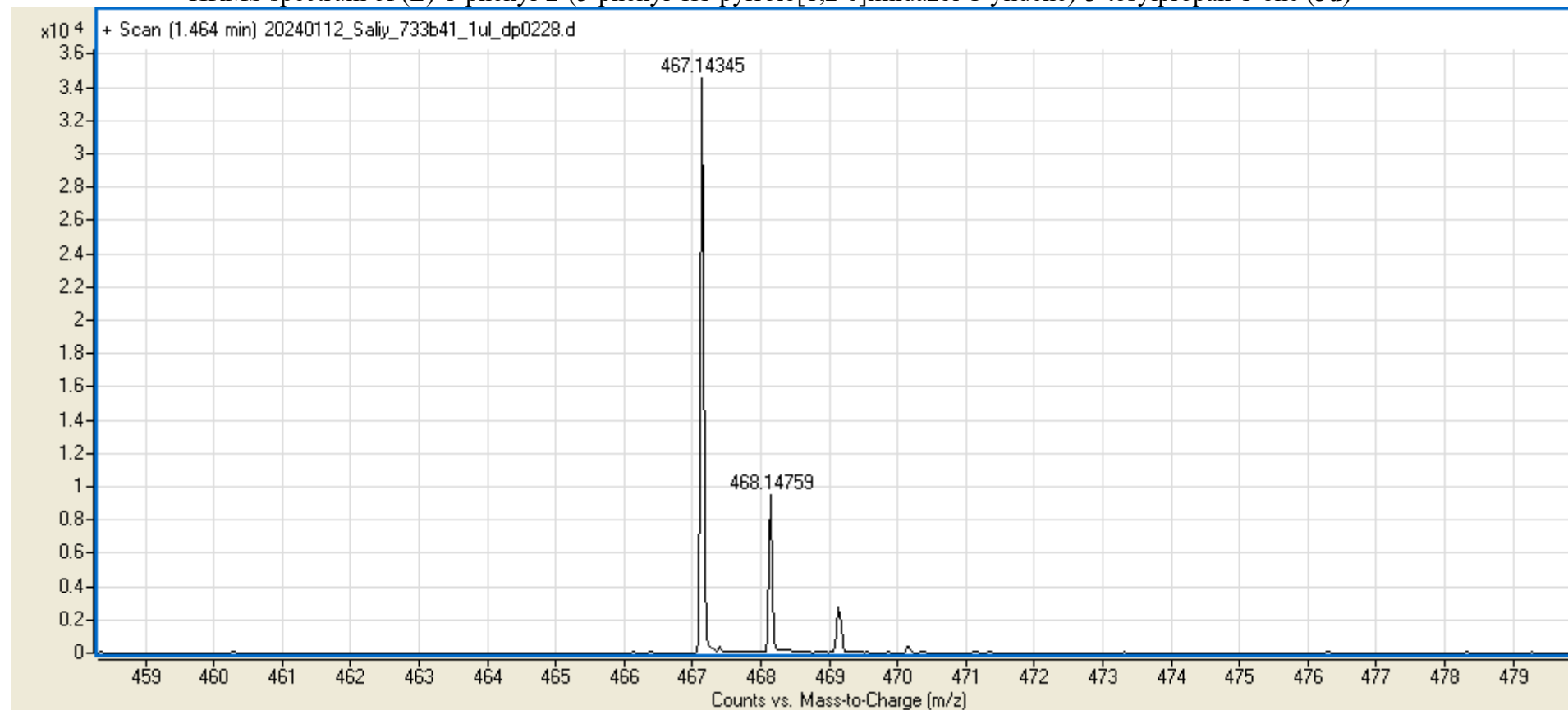
$^1\text{H}$  NMR spectrum of (*E*)-1-phenyl-2-(5-phenyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3d**) in  $\text{CDCl}_3$ .



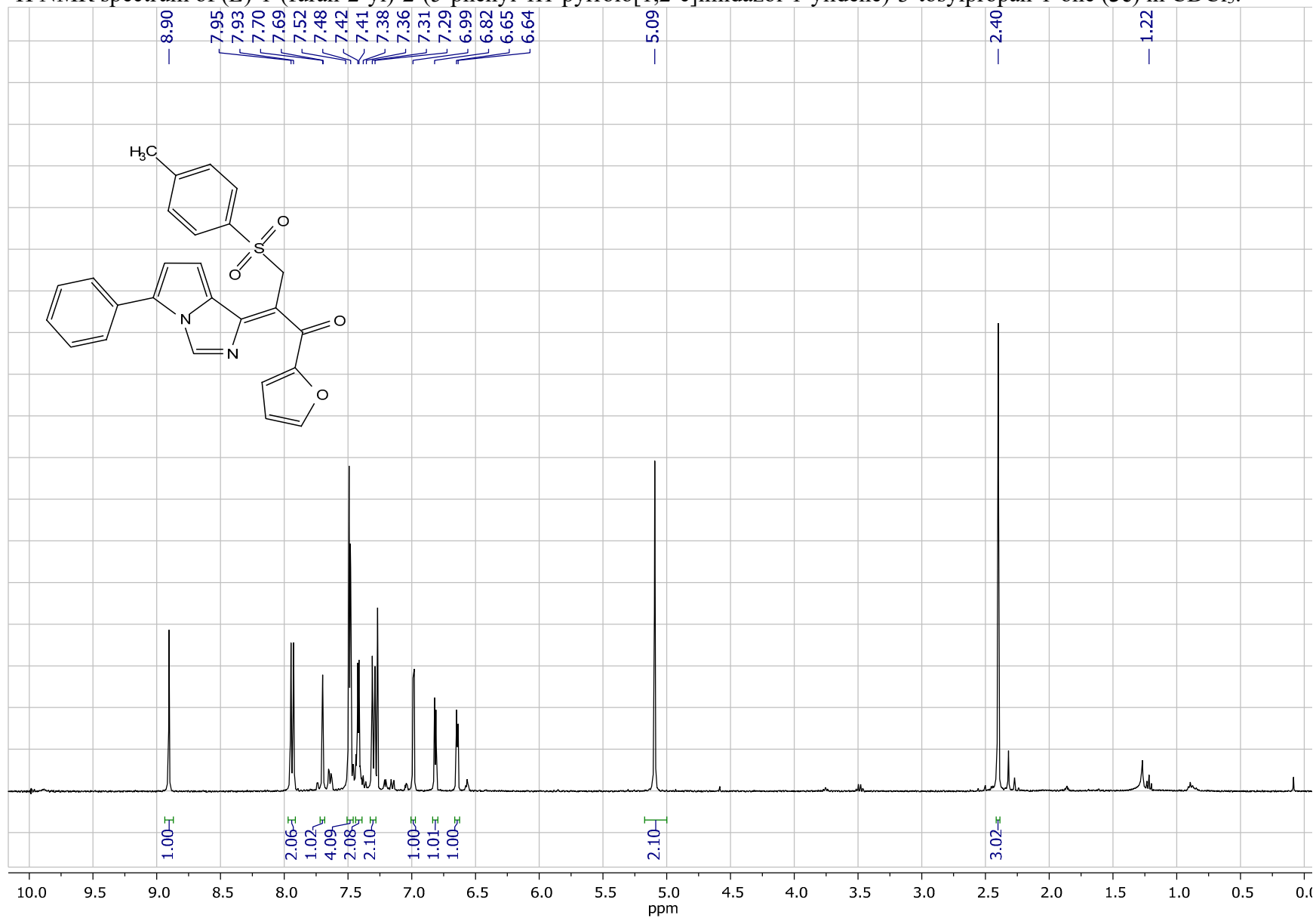
$^{13}\text{C}$  NMR spectrum of (*E*)-1-phenyl-2-(5-phenyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3d**) in  $\text{CDCl}_3$ .



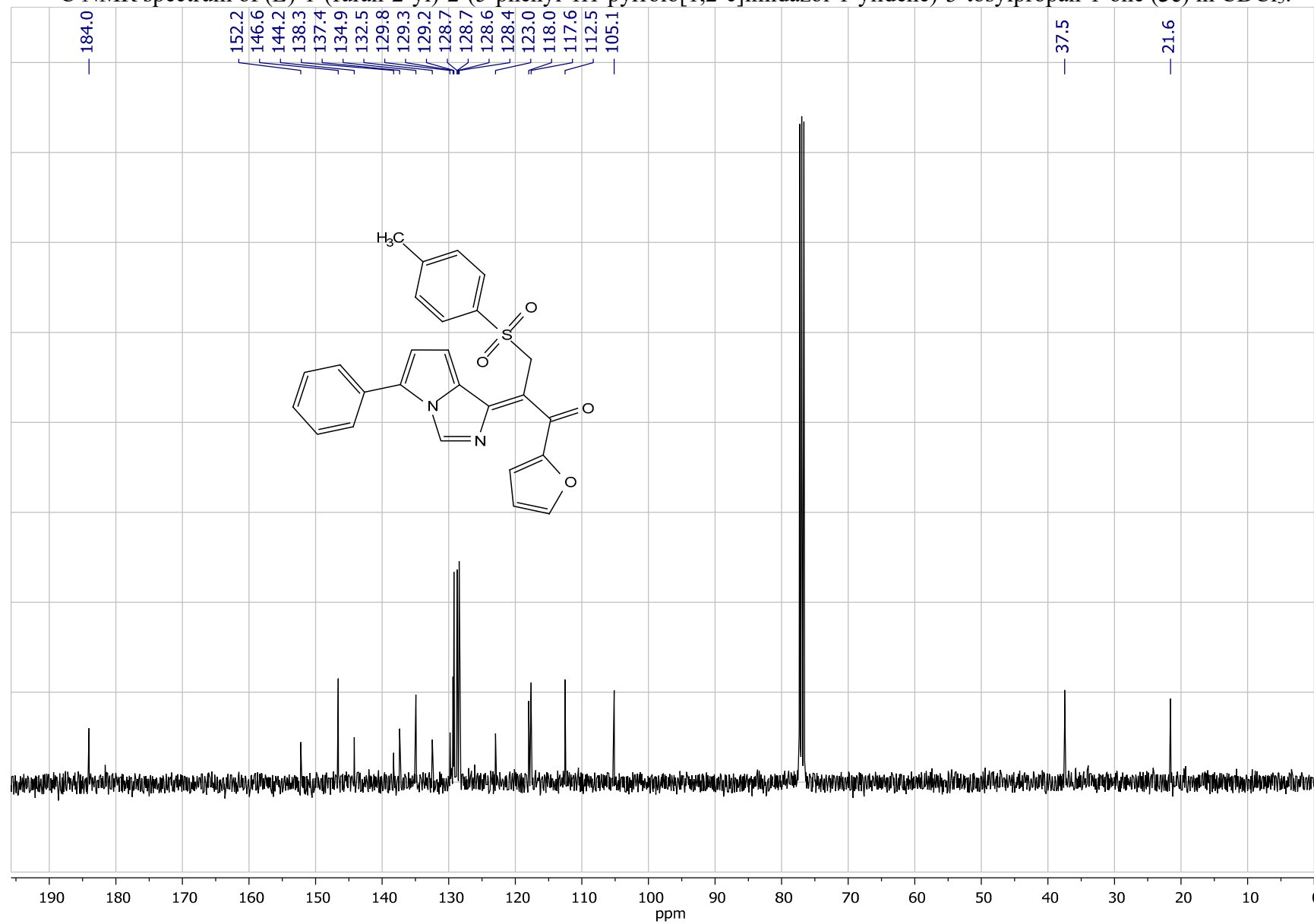
HRMS spectrum of (*E*)-1-phenyl-2-(5-phenyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3d**)



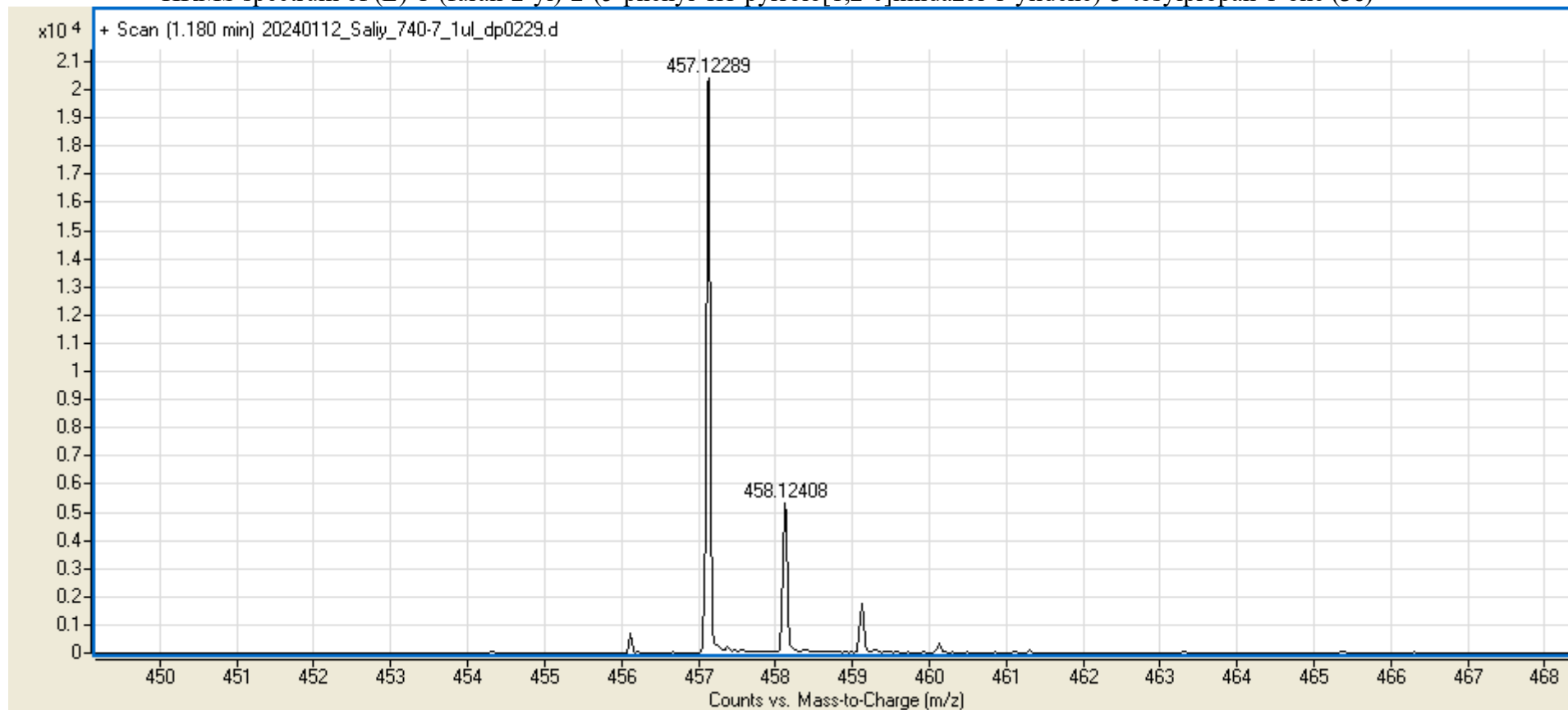
$^1\text{H}$  NMR spectrum of (*E*)-1-(furan-2-yl)-2-(5-phenyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3e**) in  $\text{CDCl}_3$ .



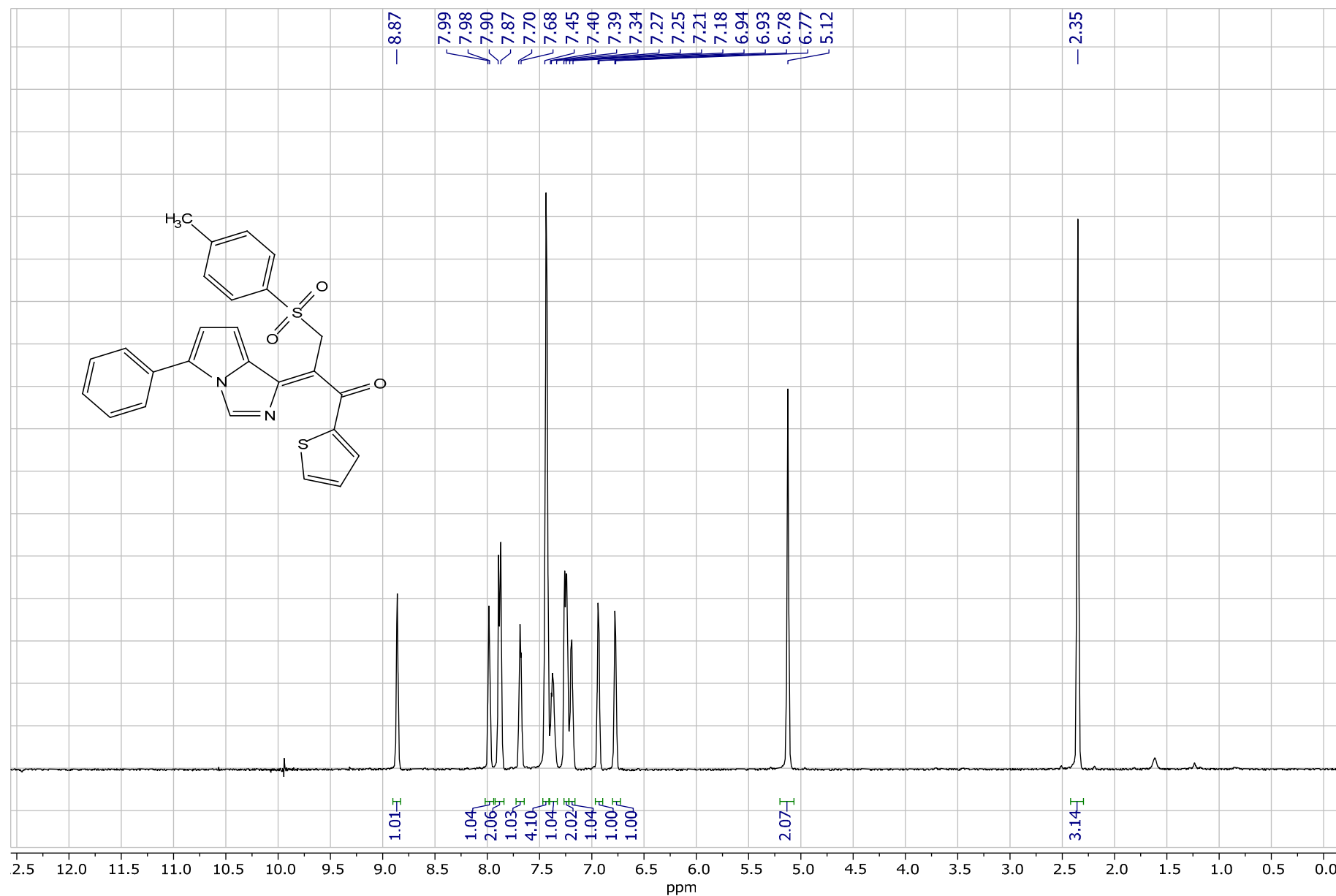
$^{13}\text{C}$  NMR spectrum of (*E*)-1-(furan-2-yl)-2-(5-phenyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3e**) in  $\text{CDCl}_3$ .



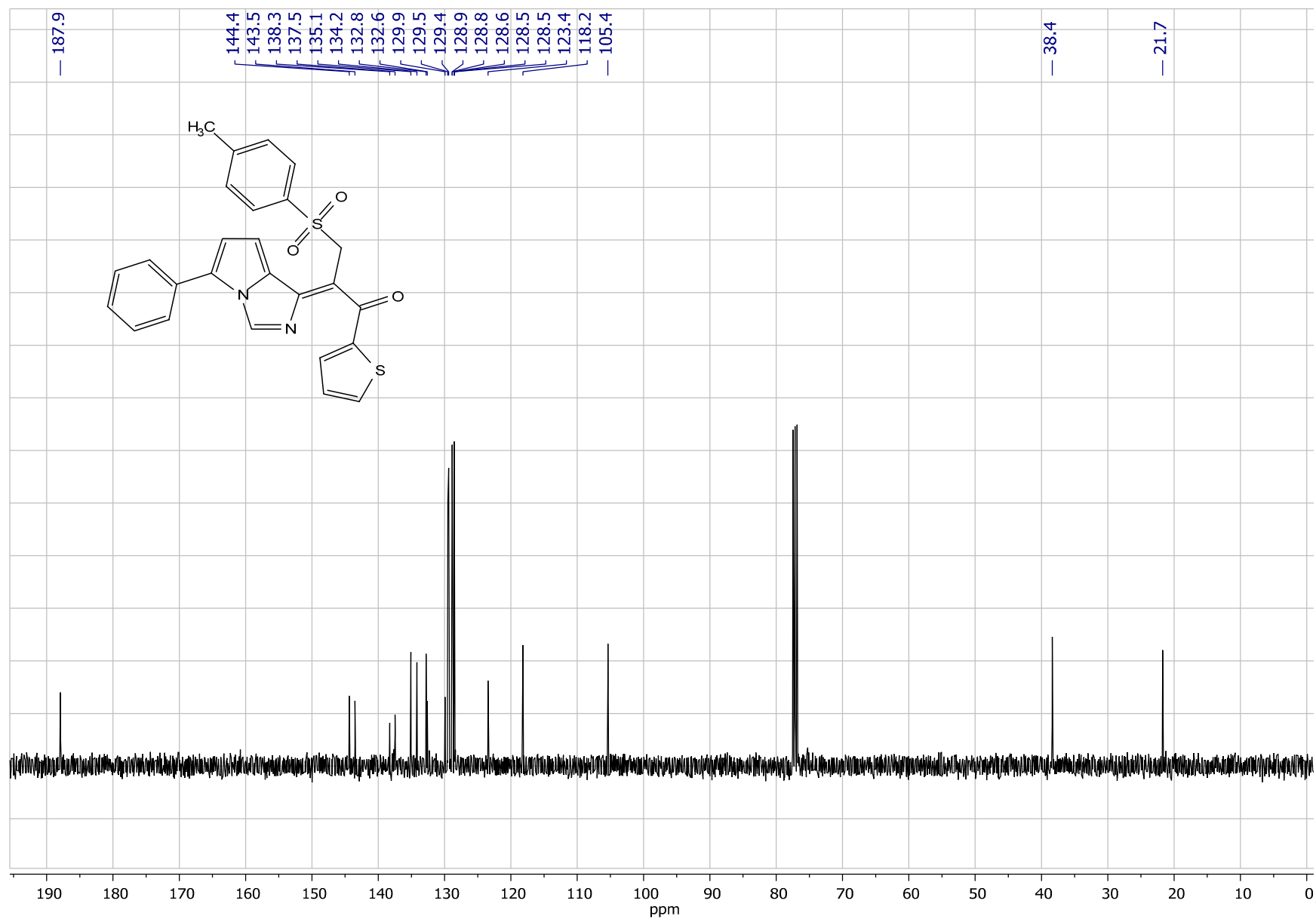
HRMS spectrum of (*E*)-1-(furan-2-yl)-2-(5-phenyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-3-tosylpropan-1-one (**3e**)



$^1\text{H}$  NMR spectrum of (*E*)-2-(5-phenyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-(thiophen-2-yl)-3-tosylpropan-1-one (**3f**) in  $\text{CDCl}_3$ .

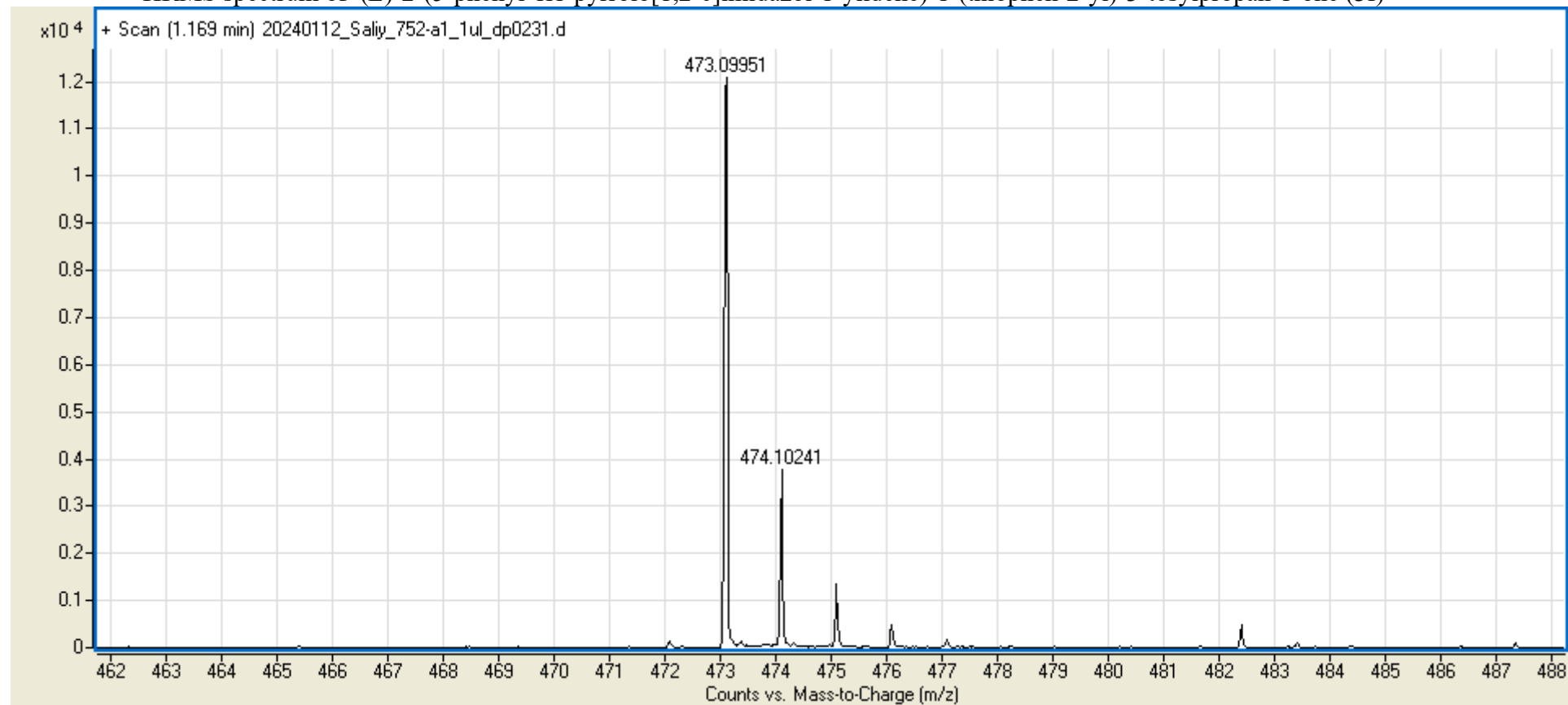


$^{13}\text{C}$  NMR spectrum of (*E*)-2-(5-phenyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-(thiophen-2-yl)-3-tosylpropan-1-one (**3f**) in  $\text{CDCl}_3$ .

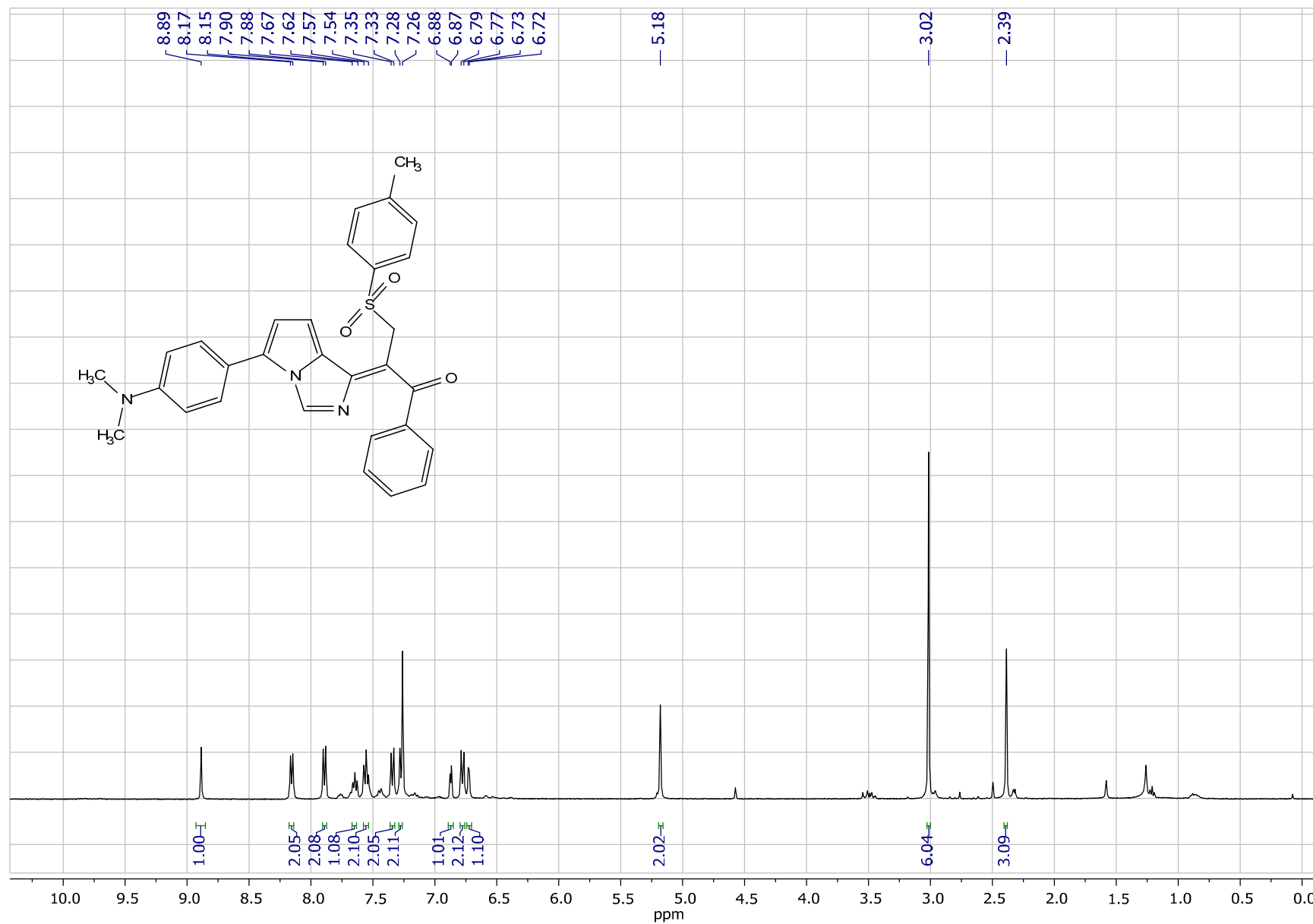




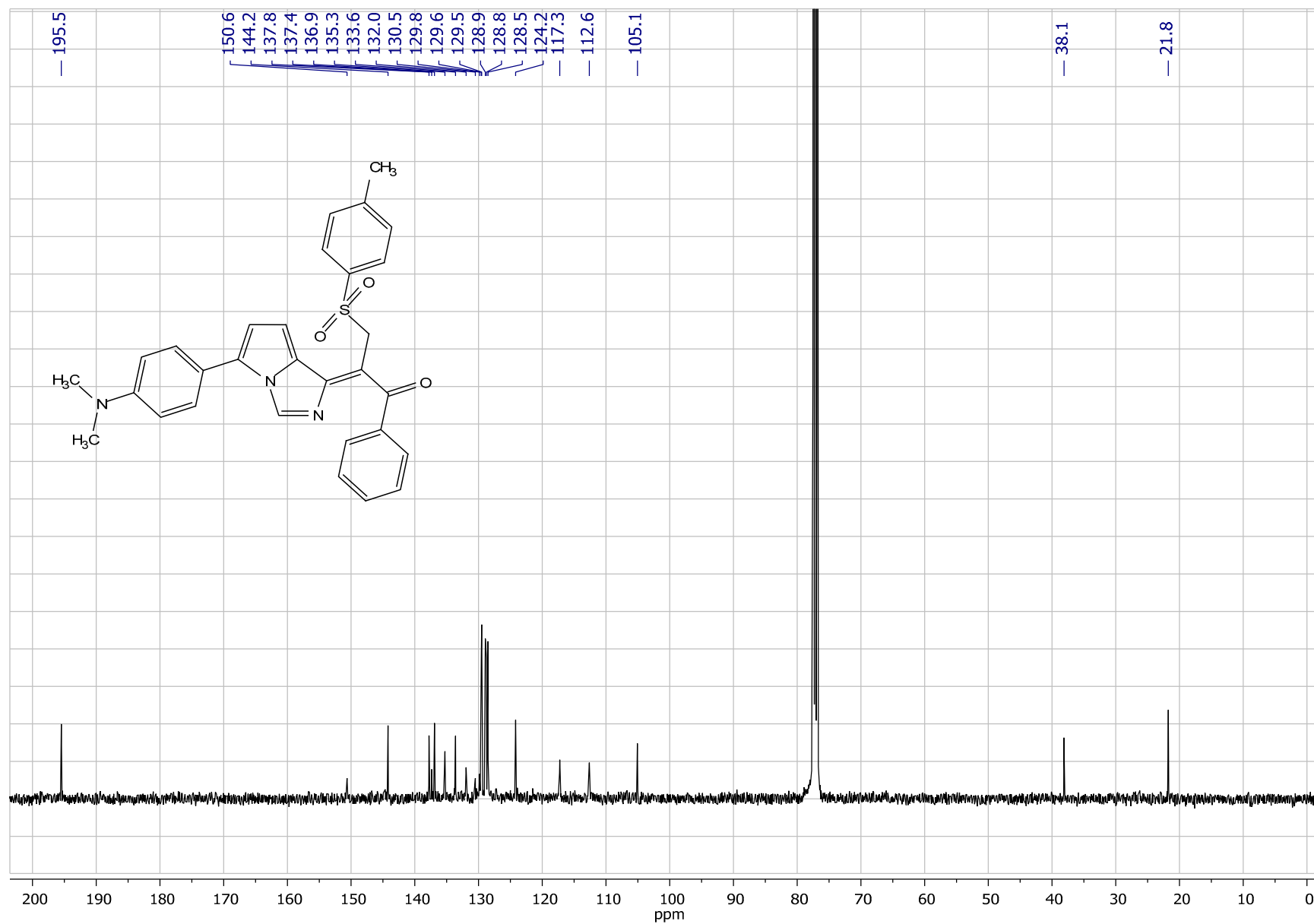
HRMS spectrum of (*E*)-2-(5-phenyl-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-(thiophen-2-yl)-3-tosylpropan-1-one (**3f**)



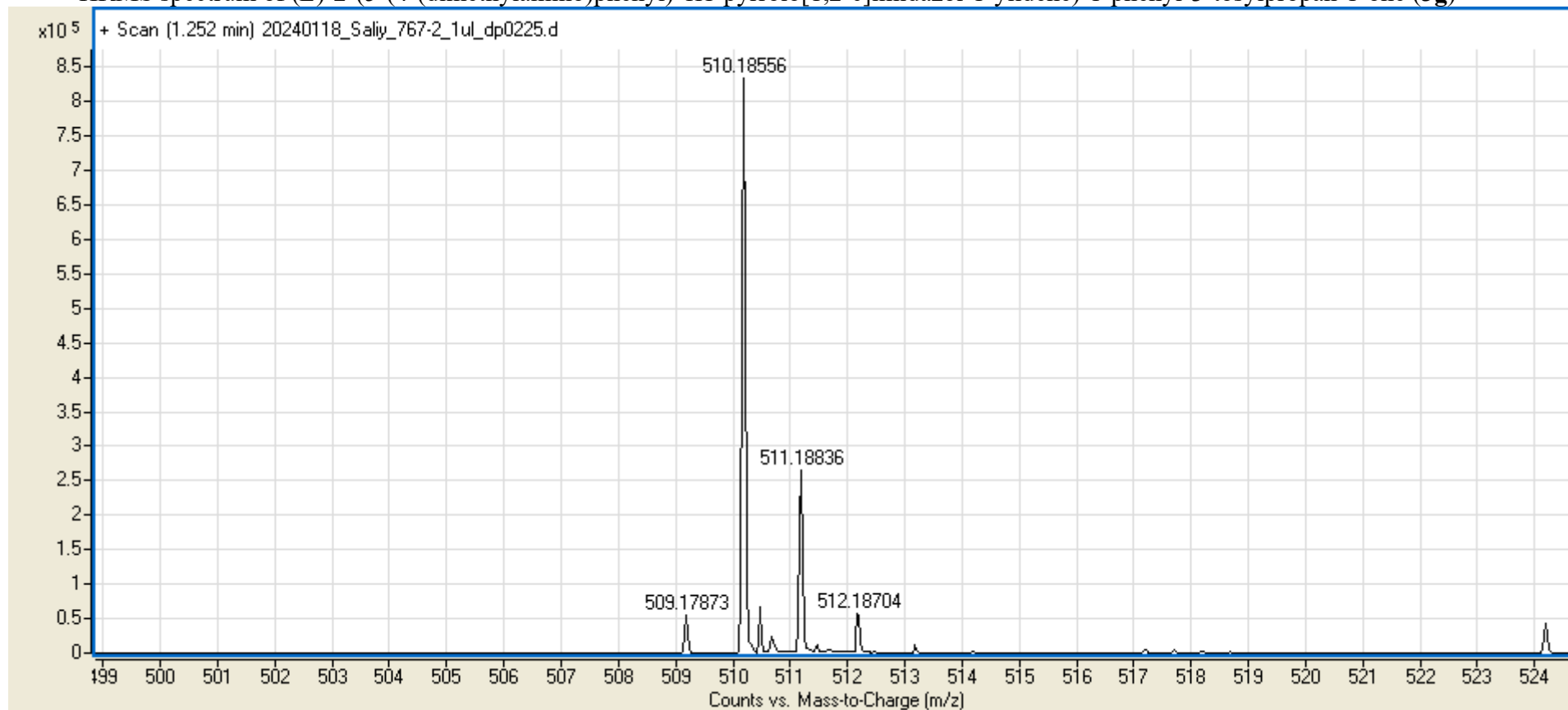
$^1\text{H}$  NMR spectrum of (*E*)-2-(5-(4-(dimethylamino)phenyl)-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (**3g**) in  $\text{CDCl}_3$ .



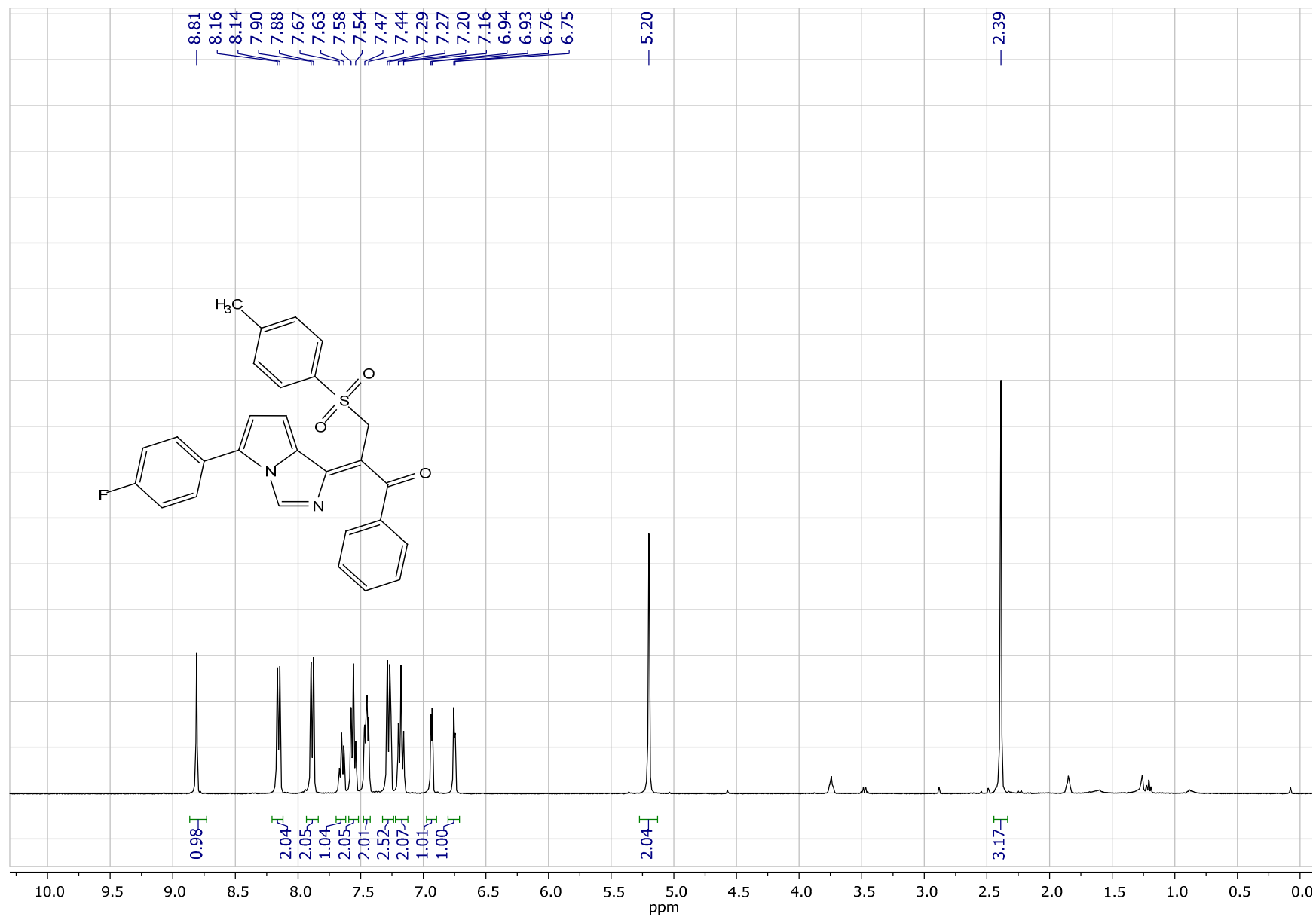
$^{13}\text{C}$  NMR spectrum of (*E*)-2-(5-(4-(dimethylamino)phenyl)-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (**3g**) in  $\text{CDCl}_3$ .



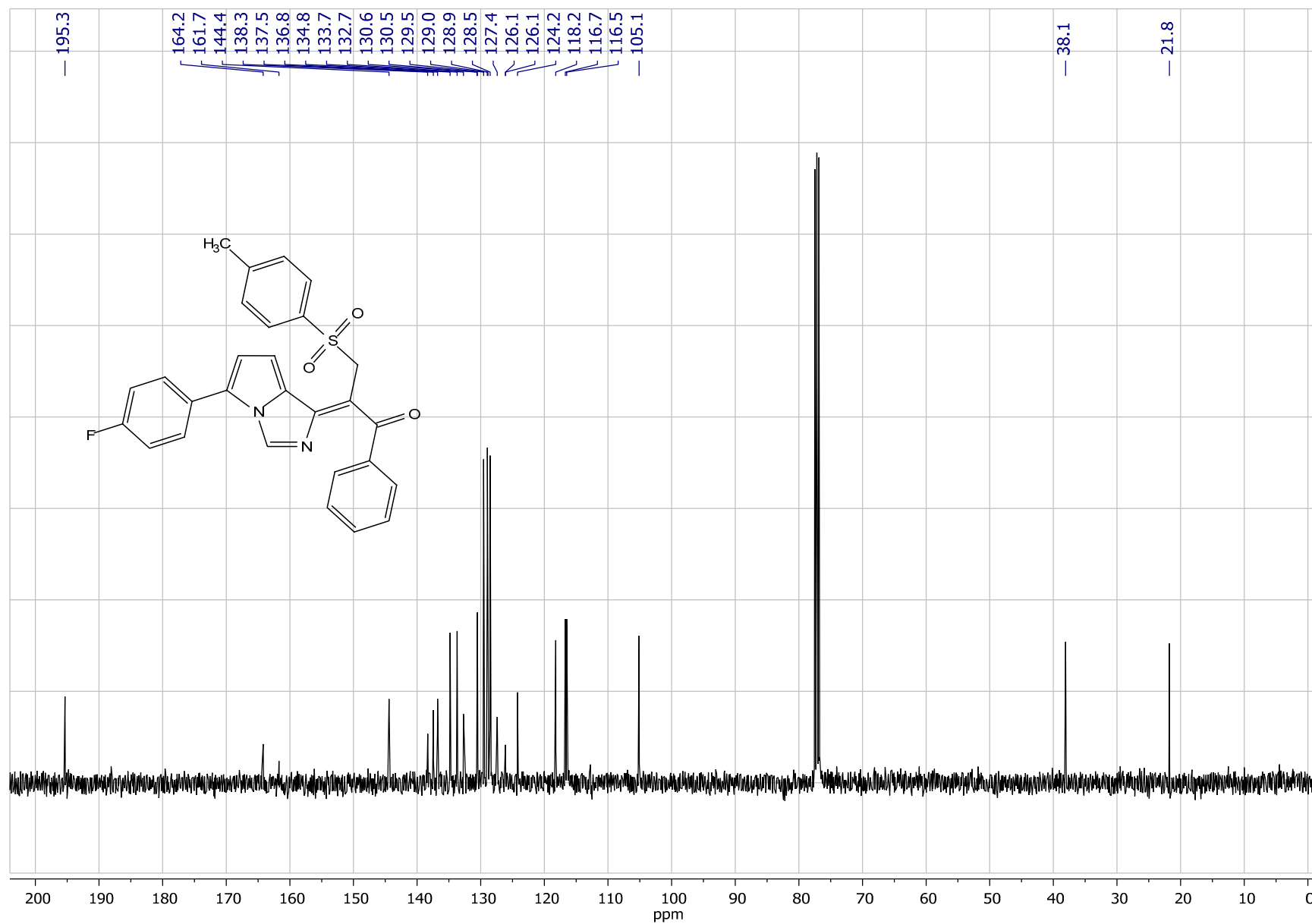
HRMS spectrum of (*E*)-2-(5-(4-(dimethylamino)phenyl)-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (**3g**)



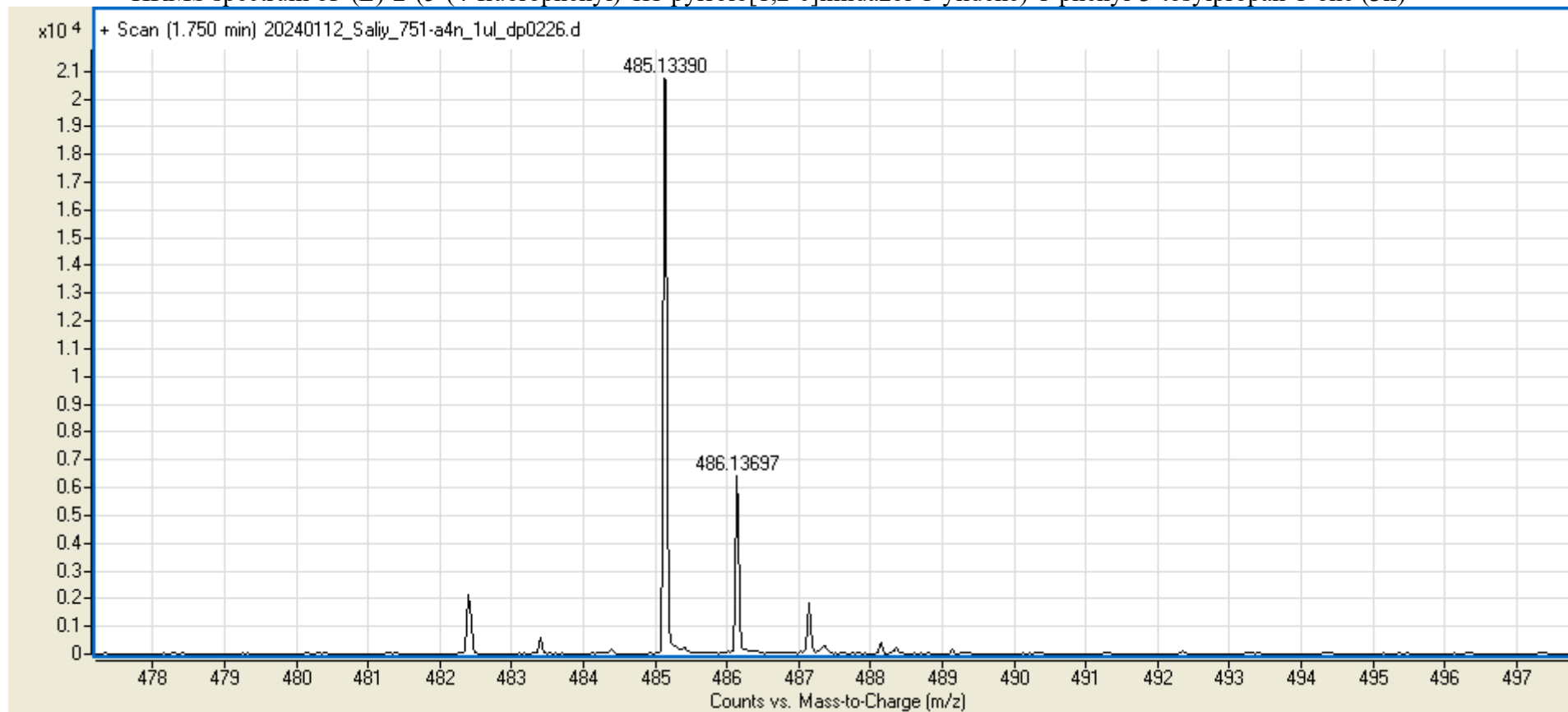
$^1\text{H}$  NMR spectrum of (*E*)-2-(5-(4-fluorophenyl)-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (**3h**) in  $\text{CDCl}_3$ .



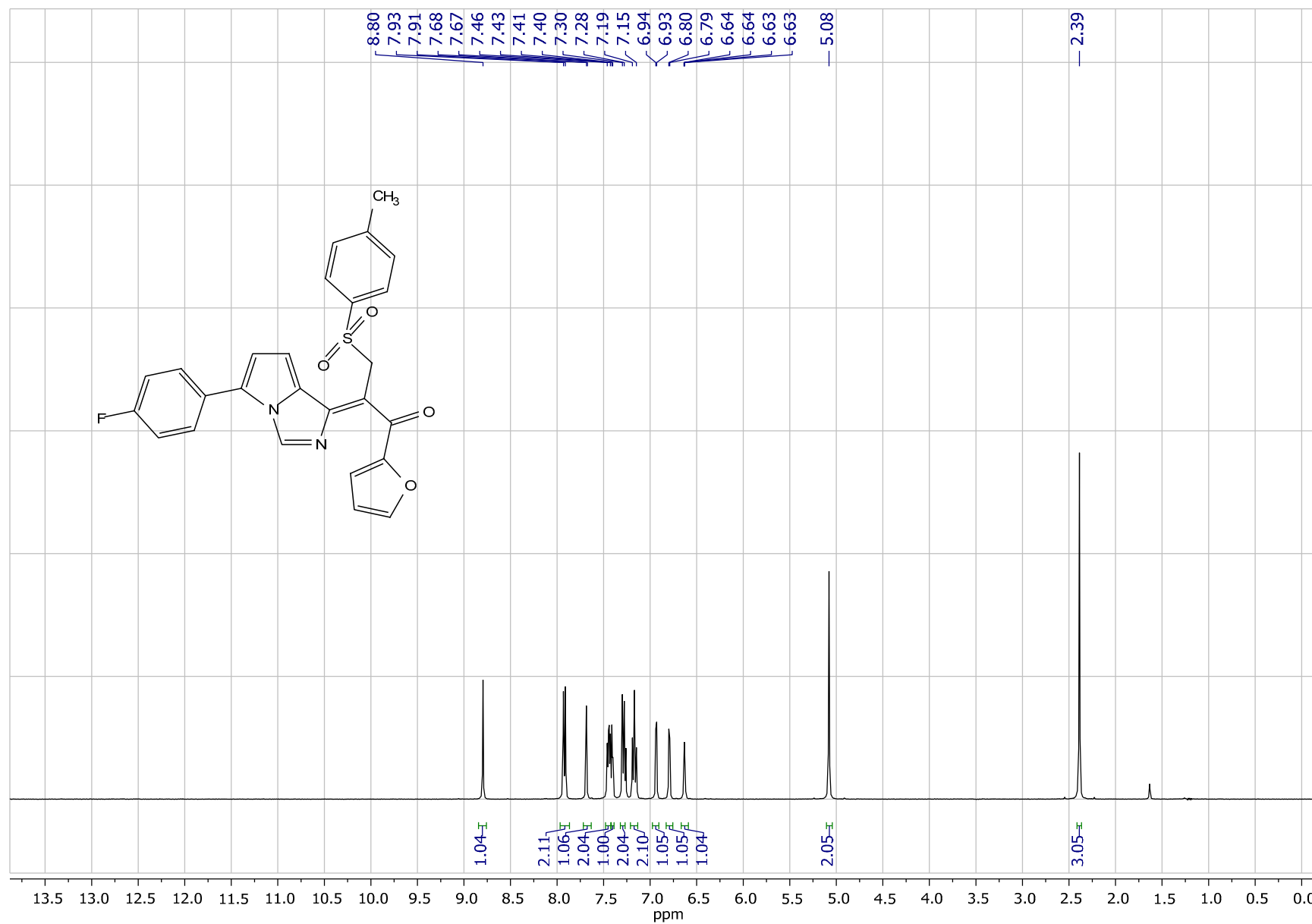
$^{13}\text{C}$  NMR spectrum of (*E*)-2-(5-(4-fluorophenyl)-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (**3h**) in  $\text{CDCl}_3$ .



HRMS spectrum of (*E*)-2-(5-(4-fluorophenyl)-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (**3h**)

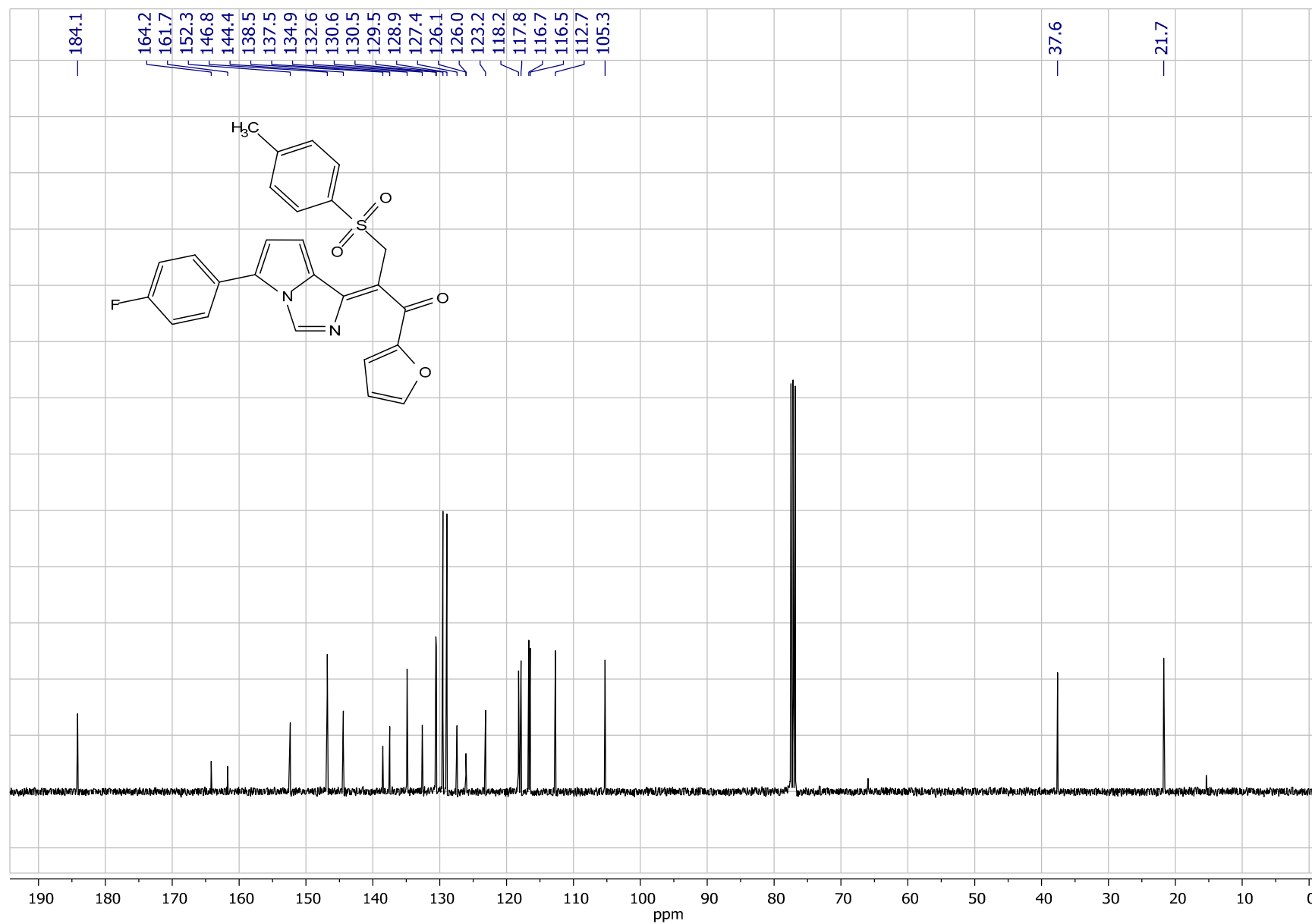


$^1\text{H}$  NMR spectrum of (*E*)-2-(5-(4-fluorophenyl)-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-(furan-2-yl)-3-tosylpropan-1-one (**3i**) in  $\text{CDCl}_3$ .

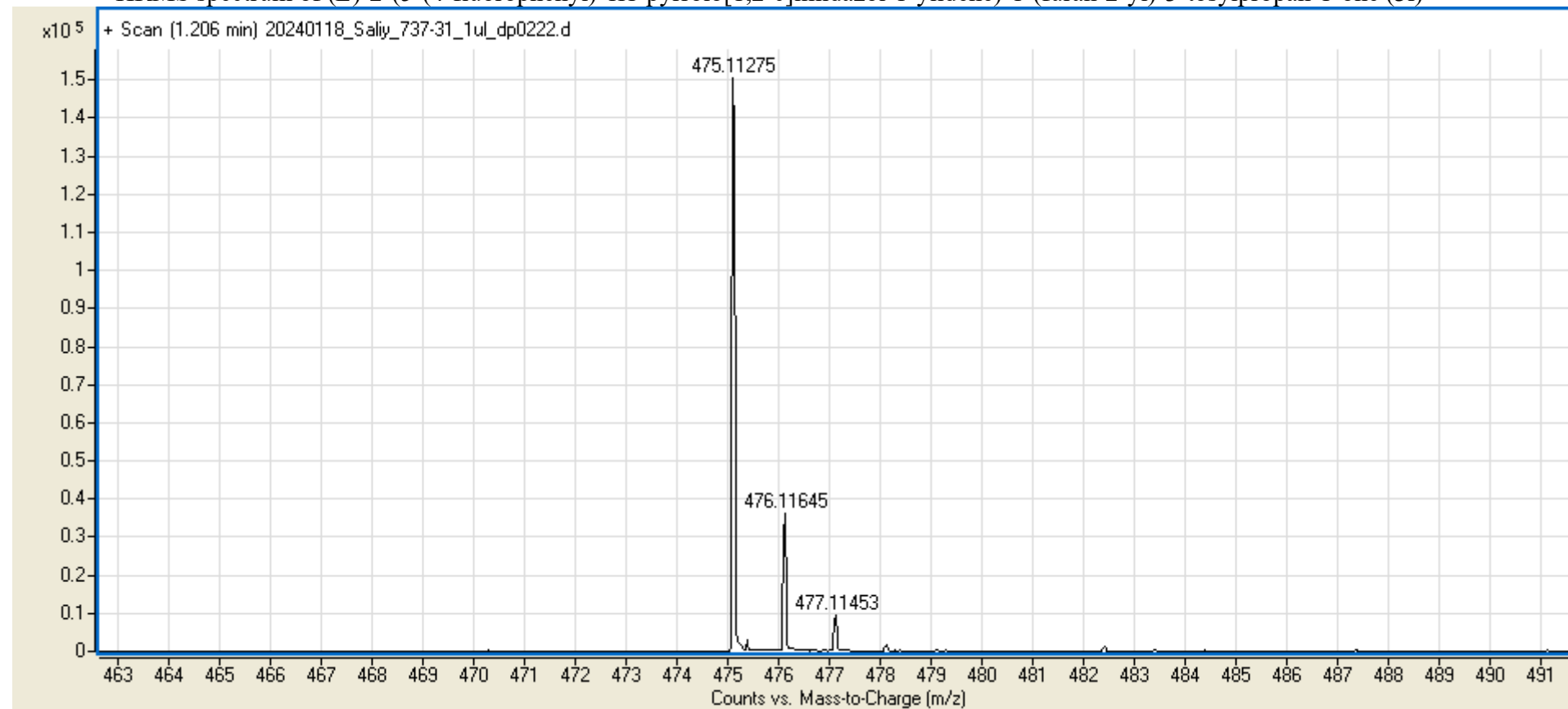




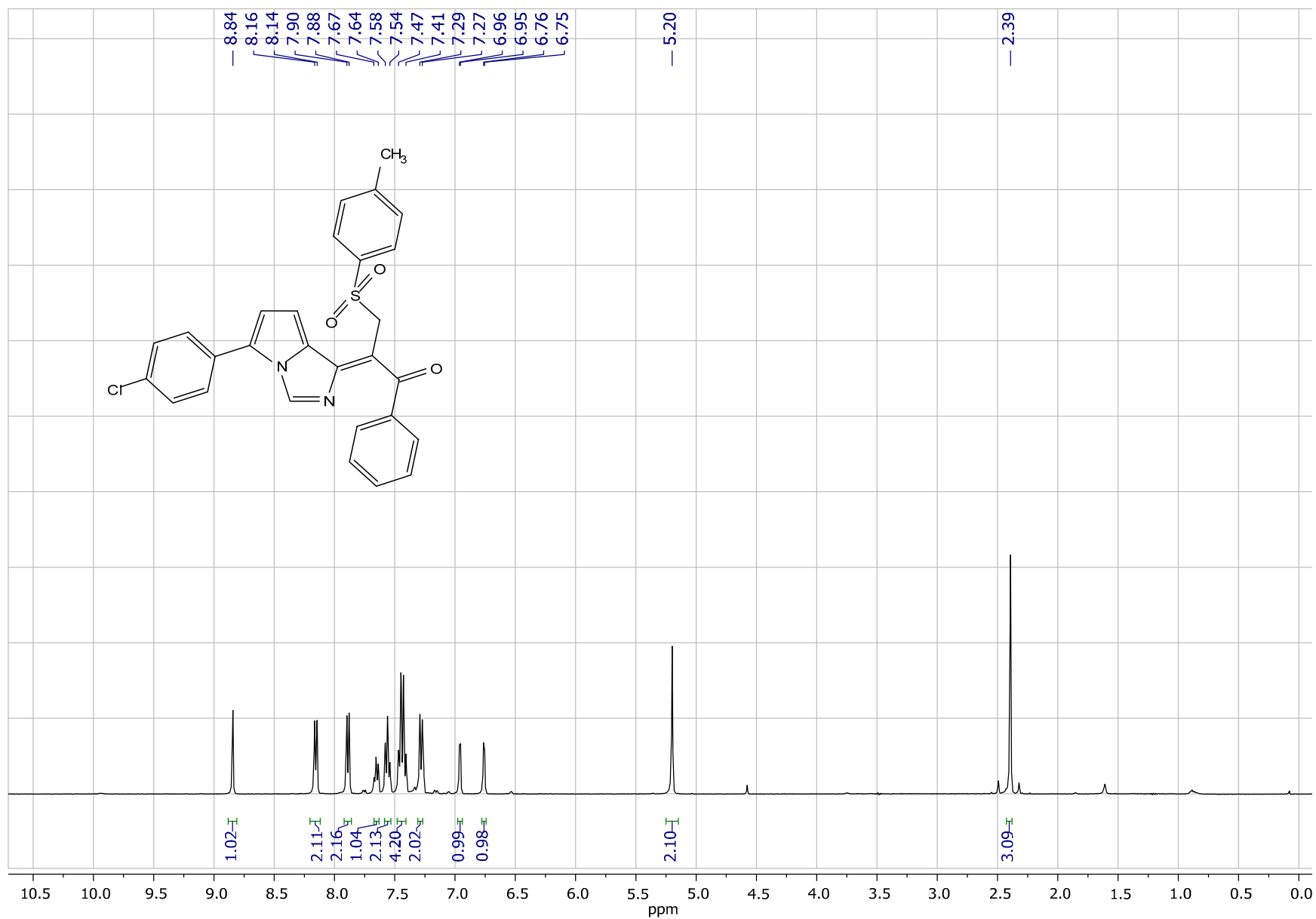
$^{13}\text{C}$  NMR spectrum of (*E*)-2-(5-(4-fluorophenyl)-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-(furan-2-yl)-3-tosylpropan-1-one (**3i**) in  $\text{CDCl}_3$ .



HRMS spectrum of (*E*)-2-(5-(4-fluorophenyl)-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-(furan-2-yl)-3-tosylpropan-1-one (**3i**)



$^1\text{H}$  NMR spectrum of (*E*)-2-(5-(4-chlorophenyl)-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (**3j**) in  $\text{CDCl}_3$ .



$^{13}\text{C}$  NMR spectrum of (*E*)-2-(5-(4-chlorophenyl)-1*H*-pyrrolo[1,2-*c*]imidazol-1-ylidene)-1-phenyl-3-tosylpropan-1-one (**3j**) in  $\text{CDCl}_3$ .

