

## Supporting Information

### Decarboxylative/Oxidative Amidation of Aryl $\alpha$ -Ketocarboxylic Acids with Nitroarenes and Nitroso Compounds in Aqueous Medium

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## 1. General Experimental Details

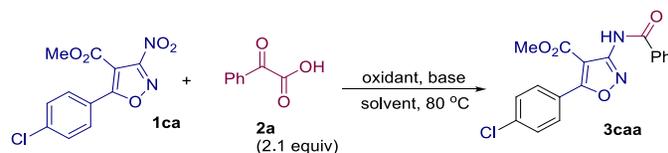
Unless otherwise stated all reactions were performed in non-dry glassware under an air atmosphere and were monitored by analytical thin layer chromatography (TLC). For all reactions requiring heating, it was carried out by placing the reaction vessel in an oil bath and the temperature indicated is the temperature of the oil bath. TLC was performed on pre-coated silica gel plates. After elution, plate was visualized under UV illumination at 254 nm for UV active materials. The melting points were recorded on a hot stage apparatus and are uncorrected.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded on 300 or 400 or 500 MHz NMR spectrometers with  $\text{CDCl}_3$  or  $\text{DMSO-}d^6$  as solvent, using TMS as an internal standard (chemical shifts in  $\delta$ ). Peak multiplicities of  $^1\text{H}$ -NMR signals were designated as s (singlet), brs (broad singlet), d (doublet), dd (doublet of doublet), t (triplet), q (quartet), m (multiplet) etc. Coupling constants ( $J$ ) are in Hz. The ESI-MS were recorded on triple quadrupole Mass spectrometer. Column chromatography was performed using silica gel (100-200 mesh). Analytical grade solvents for the column chromatography were used as received. GC-MS & GC (Agilent Technology) were obtained from Centre of Biomedical Research Institute and for the analysis, RAM temperature was used 50 °C for each sample

## 2 Starting Material Synthesis

All the 3-nitroisoxazole-4-carboxylates and some nitroso compounds were prepared by using previously reported methods.<sup>1</sup>

## 3. Reaction Optimization

### General Procedure for the Reaction Optimization



A tube equipped with a stirring bar was charged with **1ca** (0.2 g, 0.71 mmol), **2a** (1.48 mmol), oxidant (2.0–3.0 equiv.) and base (1.5–2.0 equiv.) in solvent (6 mL) at room temperature. The reaction mixture was heated at 80 °C for 12→23 h. After completion of the reaction (as monitored by TLC) the solvent was removed under vacuum and the residue was diluted with H<sub>2</sub>O (20 mL) and extracted with EtOAc (3 X 20 mL). The combined organic layers were washed with brine, dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered and evaporated to furnish crude product. Purification by column chromatography on silica gel, eluting with hexanes/ EtOAc (7:3, v/v), gave desired product methyl 3-benzamido-5-phenylisoxazole-4-carboxylate (**3caa**)

**Table 1.** . Results of optimization study with methyl 5-(4-chlorophenyl)-3-nitroisoxazole-4-carboxylate (**1ca**)<sup>a</sup>

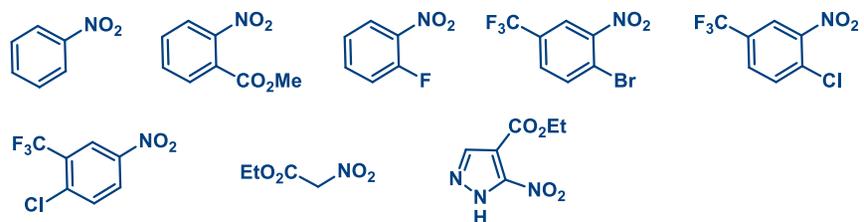
Entry	oxidant (equiv)	solvent	base (equiv)	time	yield (%) <sup>b</sup> <b>3caa</b>	<b>1ca</b> recovered (%)
1	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (3.0)	MeCN:H <sub>2</sub> O	-	20 h	45 <sup>c</sup>	46
2	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (3.0)	MeCN:H <sub>2</sub> O	K <sub>2</sub> CO <sub>3</sub> (1.0)	20 h	66	17
3	<b>K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> (3.0)</b>	<b>MeCN:H<sub>2</sub>O</b>	<b>K<sub>2</sub>CO<sub>3</sub> (1.5)</b>	<b>12 h</b>	<b>80</b>	-

4	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (3.0)	MeCN:H <sub>2</sub> O	K <sub>2</sub> CO <sub>3</sub> (2.0)	12 h	69 <sup>d</sup>	-
5	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (4.0)	MeCN:H <sub>2</sub> O	K <sub>2</sub> CO <sub>3</sub> (1.5)	20 h	64	
6	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (2.5)	MeCN:H <sub>2</sub> O	K <sub>2</sub> CO <sub>3</sub> (1.5)	20 h	73	trace
7	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (2.0)	MeCN:H <sub>2</sub> O	K <sub>2</sub> CO <sub>3</sub> (1.5)	20 h	61	25
8	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (1.5)	MeCN:H <sub>2</sub> O	K <sub>2</sub> CO <sub>3</sub> (1.5)	20 h	44	43
9	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (1.0)	MeCN:H <sub>2</sub> O	K <sub>2</sub> CO <sub>3</sub> (1.5)	20 h	31	61
10	Na <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (3.0)	MeCN:H <sub>2</sub> O	K <sub>2</sub> CO <sub>3</sub> (1.5)	23 h	70	11
11	(NH <sub>4</sub> ) <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (3.0)	MeCN:H <sub>2</sub> O	K <sub>2</sub> CO <sub>3</sub> (1.5)	14 h	76	trace
12	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (3.0)	MeCN:H <sub>2</sub> O	Na <sub>2</sub> CO <sub>3</sub> (1.5)	20 h	68	15
13	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (3.0)	MeCN:H <sub>2</sub> O	Cs <sub>2</sub> CO <sub>3</sub> (1.5)	20 h	57	29
14	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (3.0)	MeCN	K <sub>2</sub> CO <sub>3</sub> (1.5)	20 h	-	98 <sup>c</sup>
15	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (3.0)	DMSO: H <sub>2</sub> O	K <sub>2</sub> CO <sub>3</sub> (1.5)	20 h	61	23
16	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (3.0)	DMF:H <sub>2</sub> O	K <sub>2</sub> CO <sub>3</sub> (1.5)	20 h	47 <sup>c</sup>	43
17	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (3.0)	Toluene: H <sub>2</sub> O	K <sub>2</sub> CO <sub>3</sub> (1.5)	20 h	27 <sup>c</sup>	66
18	K <sub>2</sub> S <sub>2</sub> O <sub>8</sub> (3.0)	THF: H <sub>2</sub> O	K <sub>2</sub> CO <sub>3</sub> (1.5)	20 h	- <sup>c</sup>	98

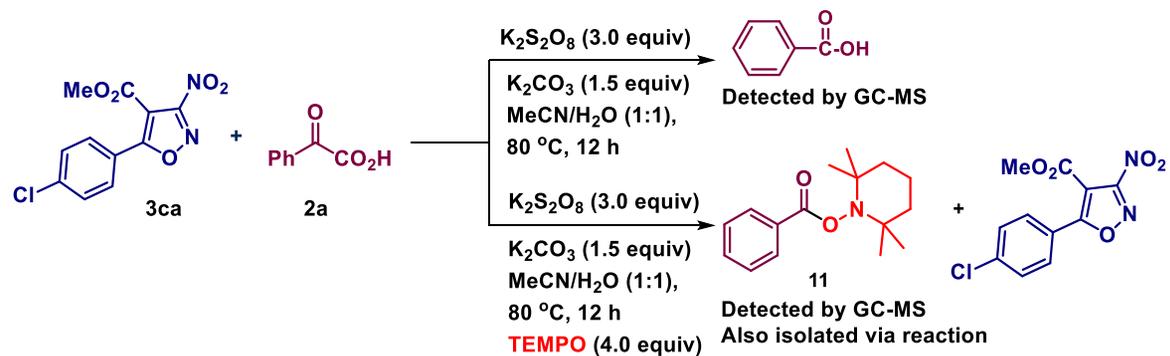
<sup>a</sup> The reactions were performed using **1ca** (0.2 g, 0.71 mmol), **2a** (1.48 mmol) and base (1.06 mmol) in solvent and H<sub>2</sub>O (3.0 and 3.0 mL) under heating for indicated time. <sup>b</sup> Isolated yields after purification. <sup>c</sup> Starting material was recovered as such. <sup>d</sup> Polar inseparable impurities were formed.

#### 4. Investigations of scope with nitroarene

Reaction of following nitro derivatives with aryl  $\alpha$ -ketocarboxylic acid under the standardized conditions were unsuccessful.



#### 5. Control Experiments



The GCMS plots are given below.

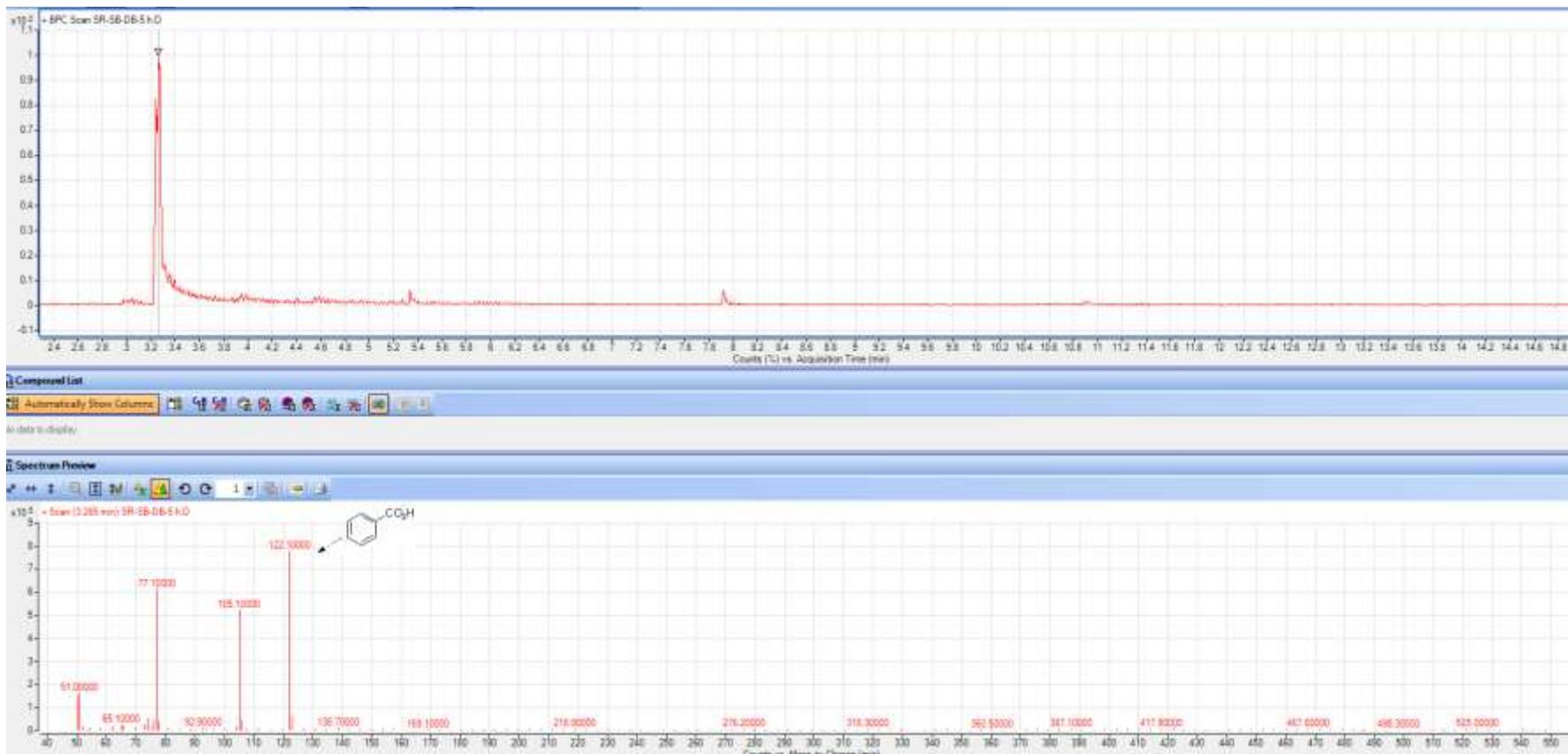


Figure S-1. GCMS spectrum showing the presence of benzoic acid

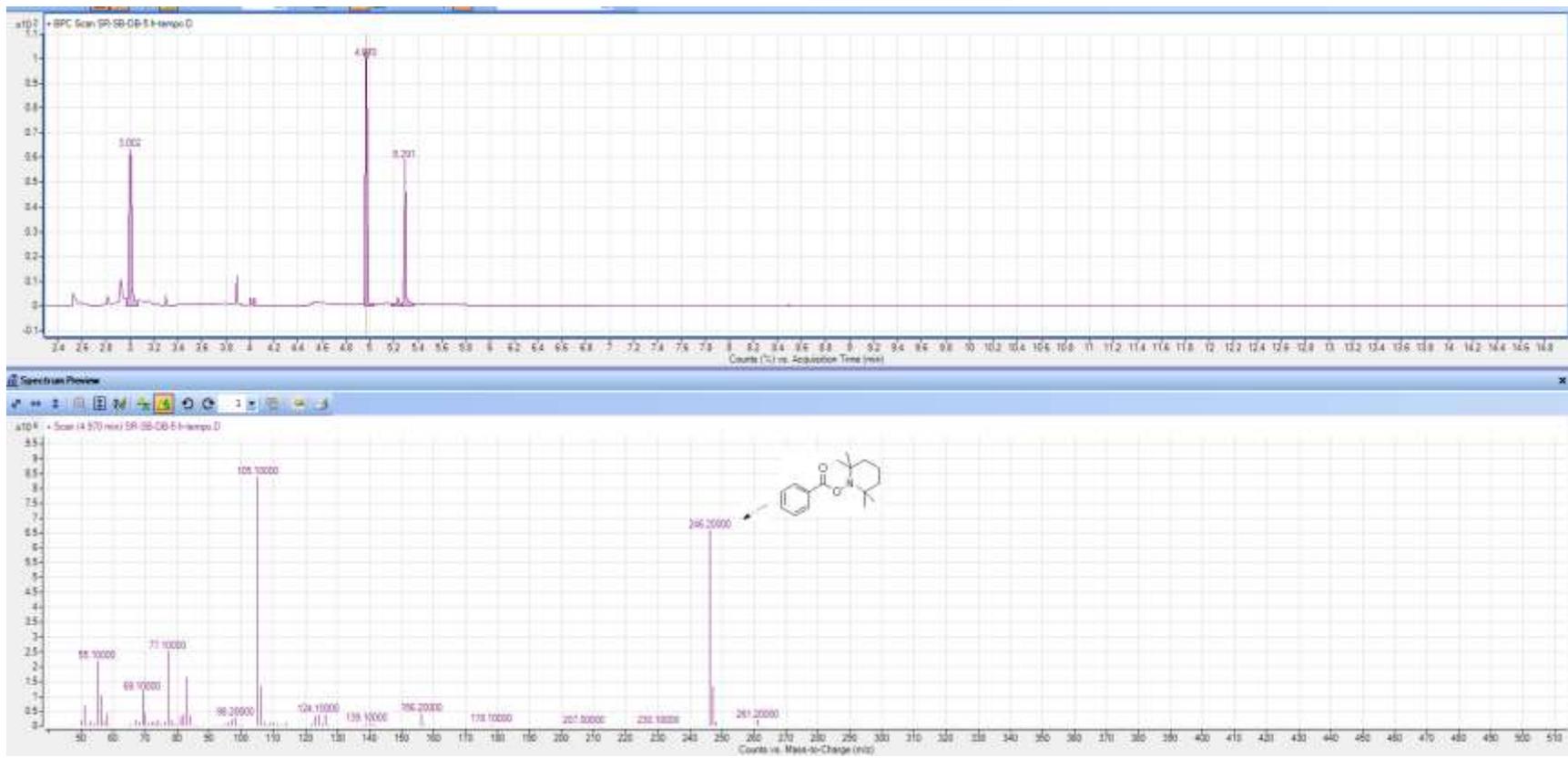


Figure S-2. The GCMS spectrum displaying the trapping of the benzoyloxy radical with TEMPO

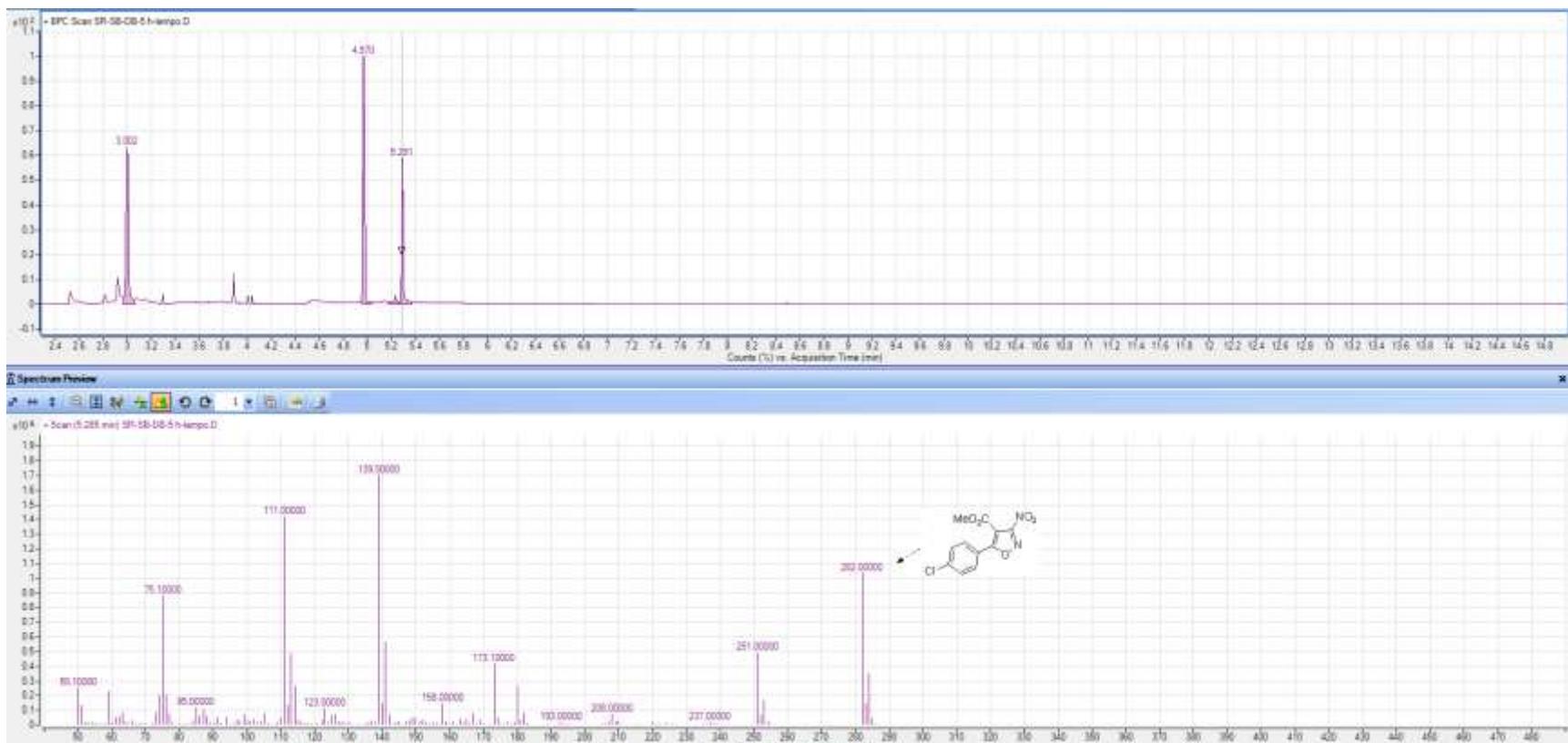
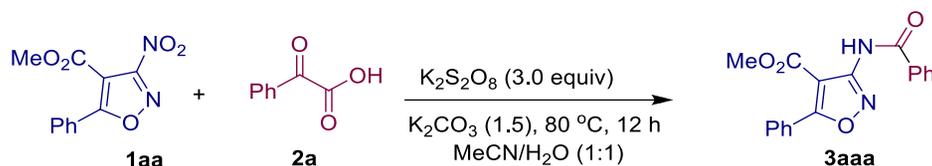


Figure S-3. GCMS spectrum displaying the presence of the starting substrate

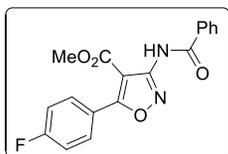
## 6. Substrate Scope

**General Procedure for the Synthesis of Alkyl 3-benzamido-5-aryllisoxazole-4-carboxylate (3aaa-7ca) as exemplified for the synthesis of 3aaa.**



To a stirred solution **1aa** (0.2 g, 0.81mmol) in MeCN/H<sub>2</sub>O (1:1) (6 mL) was added **2a** (0.254 g, 1.69 mmol), K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> (0.667 g, 2.41mmol) and K<sub>2</sub>CO<sub>3</sub> (0.166 g, 1.21mmol) at room temperature and the reaction was heated at 80 °C for 12 h. After completion of the reaction (as monitored by TLC) the solvent was removed under vacuum and the residue was diluted with H<sub>2</sub>O (20 mL) and extracted with EtOAc (3 X 20 mL). The combined organic layer was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and evaporated to furnish crude product that was purified by column chromatography over silica gel using hexanes/ EtOAc (7:3, v/v) as eluent to afford 0.199 g (77%) of **3aaa** as a white solid. Methyl 3-benzamido-5-phenylisoxazole-4-carboxylate (**3aaa**). Mp 122-124 °C; R<sub>f</sub> = 0.48 (hexanes: EtOAc, 7:3, v/v); IR (KBr) ν<sub>max</sub>: 1649, 1718 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 3.92 (s, 3H), 7.47 (t, *J* = 7.7 Hz, 1H), 7.54 (t, *J* = 7.7 Hz, 1H), 7.59-7.63 (m, 1H), 7.66 (d, *J* = 8.5 Hz, 2H), 7.73 (d, *J* = 8.5 Hz, 2H), 8.00-8.52 (m, 2H), 10.40 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 52.4, 99.2, 126.6, 127.6, 128.4, 129.0, 129.4, 131.8, 132.7, 133.0, 157.5, 163.5, 163.9, 172.7 ppm. MS (ESI<sup>+</sup>): *m/z* = 323.1. ESI-HR-MS calculated for C<sub>18</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub>(M+H<sup>+</sup>): 323.1026, found: 323.1028.

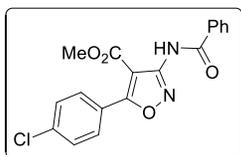
**Methyl 3-benzamido-5-(4-fluorophenyl)isoxazole-4-carboxylate (3baa)**. Yield: 78% (0.199 g from 0.2 g); a white solid, mp 123-



125 °C; R<sub>f</sub> = 0.48 (hexanes: EtOAc, 7:3, v/v); IR (KBr) ν<sub>max</sub>: 1642, 1729 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 3.84 (s, 3H), 7.31 (t, *J* = 8.5 Hz, 2H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.78-7.82 (m, 2H), 7.93 (d, *J* = 7.3 Hz, 2H), 10.29 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 52.5, 99.2, 115.8 (d, *J* = 22.0 Hz), 122.7,

122.8, 129.0, 131.8 (d,  $J = 8.9$  Hz), 132.7, 132.9, 157.5, 163.7, 164.8(d,  $J = 256.5$  Hz), 171.6 ppm. MS (ESI+):  $m/z = 341.1$ . ESI-HR-MS calculated for  $C_{18}H_{13}FN_2O_4(M+H^+)$ : 341.0932, found: 341.0935.

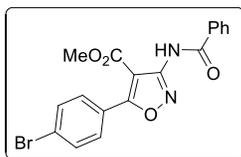
**Methyl 3-benzamido-5-(4-chlorophenyl)isoxazole-4-carboxylate (3caa).** Yield: 80% (0.201 g from 0.2 g); white solid, mp 123-124



$^{\circ}C$ ;  $R_f = 0.45$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{max}$ : 1645, 1726  $cm^{-1}$ .  $^1H$  NMR (300 MHz,  $CDCl_3$ ):  $\delta = 3.94$  (s, 3H), 7.51-7.64 (m, 5H), 7.83 (d,  $J = 8.4$  Hz, 2H), 8.04 (d,  $J = 7.2$  Hz, 2H), 10.39 (s, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ): 52.5, 99.5, 125.0, 127.6, 128.9, 129.0, 130.7, 132.7, 132.9, 138.2, 157.6, 163.4, 163.7, 171.4 ppm. MS (ESI+):  $m/z = 357.1$ . ESI-HR-MS calculated for  $C_{18}H_{13}ClN_2O_4(M+H^+)$ : 357.0637, found:

357.0639.

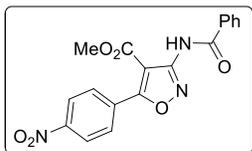
**Methyl 3-benzamido-5-(4-bromophenyl)isoxazole-4-carboxylate (3daa).** Yield: 81% (0.197 g from 0.2 g); a white solid, mp 130-



132  $^{\circ}C$ ;  $R_f = 0.45$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{max}$ : 1638, 1723  $cm^{-1}$ .  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta = 3.94$  (s, 3H), 7.54-7.64 (m, 3H), 7.69 (d,  $J = 8.7$  Hz, 2H), 7.75 (d,  $J = 8.7$  Hz, 2H), 8.03 (d,  $J = 7.0$  Hz, 2H), 10.39 (s, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ): 52.5, 99.5, 125.4, 127.6, 129.0, 130.9, 131.8, 132.7, 132.9, 157.6, 163.4, 163.6, 171.ppm. MS (ESI+):  $m/z = 401.0$ . ESI-HR-MS calculated for  $C_{18}H_{13}BrN_2O_4(M+H^+)$ : 401.0131,

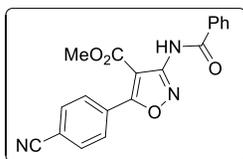
found: 401.0134.

**Methyl 3-benzamido-5-(4-nitrophenyl)isoxazole-4-carboxylate (3eaa).** Yield: 77% (0.192 g from 0.2 g); a white solid, mp 138-140



$^{\circ}C$ ;  $R_f = 0.47$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{max}$ : 1649, 1716  $cm^{-1}$ .  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta = 3.94$  (s, 3H), 7.55 (t,  $J = 7.8$  Hz, 2H), 7.61-7.65 (m, 1H), 8.01 (d,  $J = 7.1$  Hz, 2H), 8.06 (d,  $J = 8.9$  Hz, 2H), 8.38 (d,  $J = 8.9$  Hz, 2H), 10.32 (s, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ): 52.8, 100.9, 123.6, 127.6, 129.1, 130.6, 132.2, 132.7, 132.9, 149.5, 157.6, 163.2, 163.4, 169.9 ppm. MS (ESI+):  $m/z = 368.1$ . ESI-HR-MS calculated for  $C_{18}H_{13}N_3O_6(M+H^+)$ : 368.0877, found: 368.0881.

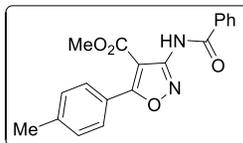
**Methyl 3-benzamido-5-(4-cyanophenyl)isoxazole-4-carboxylate (3faa).** Yield: 70% (0.177 g from 0.2 g); a white solid, mp 124-



126 °C;  $R_f = 0.48$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1646, 1721  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 3.86$  (s, 3H), 7.48 (t,  $J = 7.7$  Hz, 2H), 7.56-7.57 (m, 1H), 7.75 (d,  $J = 8.6$  Hz, 2H), 7.90-7.95 (m, 4H), 10.24 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 52.8, 115.3, 117.8, 127.6, 129.1, 130.0, 132.2, 132.7, 132.9, 157.6, 163.2, 163.4, 170.2 ppm. MS (ESI+):  $m/z = 348.1$ . ESI-HR-MS calculated for  $\text{C}_{19}\text{H}_{13}\text{N}_3\text{O}_4(\text{M}+\text{H}^+)$ : 348.0979, found:

348.0981.

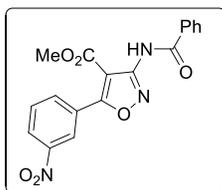
**Methyl 3-benzamido-5-p-tolylisoxazole-4-carboxylate (3gaa).** Yield: 73% (0.235 g from 0.2 g); a white solid, mp 106-108 °C;  $R_f =$



0.48 (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1649, 1723  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 2.45$  (s, 3H), 3.93 (s, 3H), 7.32 (d,  $J = 8.0$  Hz, 2H), 7.52-7.56 (m, 2H), 7.58-7.61 (m, 1H), 7.72 (d,  $J = 8.2$  Hz, 2H), 8.01-8.03 (m, 2H), 10.40 (s, 1H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO}-d_6$ ): 21.7, 52.3, 98.7, 123.8, 127.6, 129.0, 129.1, 129.3, 132.6, 142.4, 157.5, 163.5, 164.1, 172.8 ppm. MS (ESI+):  $m/z = 337.1$ . ESI-HR-MS calculated for  $\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}_4(\text{M}+\text{H}^+)$ : 337.1183, found: 337.1182.

for  $\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}_4(\text{M}+\text{H}^+)$ : 337.1183, found: 337.1182.

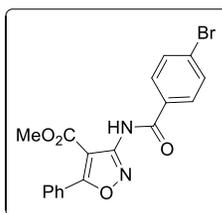
**Methyl 3-benzamido-5-(3-nitrophenyl)isoxazole-4-carboxylate (3haa).** Yield: 61% (0.152 g from 0.2 g); a white solid, mp 131-133



°C;  $R_f = 0.47$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1643, 1726  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 3.97$  (s, 3H), 7.57 (t,  $J = 7.1$  Hz, 2H), 7.61-7.65 (m, 1H), 7.75 (t,  $J = 7.0$  Hz, 1H), 8.02 (d,  $J = 7.3$  Hz, 2H), 8.21 (d,  $J = 7.8$  Hz, 1H), 8.43 (dd,  $J_1 = 8.2$  Hz,  $J_2 = 1.2$  Hz, 1H), 8.85 (s, 1H), 10.36 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 52.8, 100.6, 124.7, 126.2, 127.6, 128.0, 129.0, 129.8, 132.7, 132.8, 134.9, 148.1, 157.7, 163.2, 163.4, 169.5 ppm.

MS (ESI+):  $m/z = 368.1$ . ESI-HR-MS calculated for  $\text{C}_{18}\text{H}_{13}\text{N}_3\text{O}_6(\text{M}+\text{H}^+)$ : 368.0877, found: 368.0879.

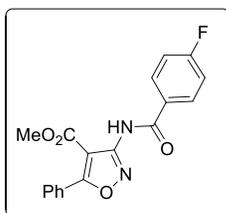
**Methyl 3-(4-bromobenzamido)-5-phenylisoxazole-4-carboxylate (3aab).** Yield: 76% (0.245 g from 0.2 g); a white solid, mp 137-



139°C;  $R_f = 0.47$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1642, 1728  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta =$

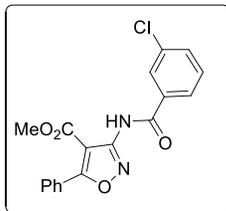
3.90 (s, 3H), 7.50-7.59 (m, 3H) 7.68 (d,  $J = 8.5$  Hz, 2H), 7.84 (d,  $J = 7.1$  Hz, 2H), 7.88 (d,  $J = 8.5$  Hz, 2H), 10.41 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 52.9, 99.1, 126.5, 127.7, 128.4, 129.2, 129.4, 131.7, 131.8, 132.3, 127.4, 162.5, 164.0, 172.7. MS (ESI+):  $m/z = 401.0$  ppm. ESI-HR-MS calculated for  $\text{C}_{18}\text{H}_{13}\text{BrN}_2\text{O}_4(\text{M}+\text{H}^+)$ : 401.0131, found: 401.0132.

**Methyl 3-(4-fluorobenzamido)-5-phenylisoxazole-4-carboxylate (3aad).** Yield: 74% (0.202 g from 0.2 g); a white solid, mp 125-



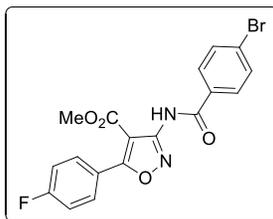
127°C;  $R_f = 0.46$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\text{max}}$ : 1639, 1721  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta = 3.90$  (s, 3H), 7.21 (d,  $J = 8.6$  Hz, 2H), 7.50-7.58 (m, 3H), 7.82-7.84 (m, 2H), 8.02-8.05 (m, 2H), 10.39 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 52.4, 99.1, 116.1 (d,  $J = 22.1$  Hz), 126.5, 128.4, 129.0, 129.4, 130.2, 131.8, 157.5, 162.3, 164.1, 165.3 (d,  $J = 253.9$  Hz), 172.7 ppm. MS (ESI+):  $m/z = 341.1$ . ESI-HR-MS calculated for  $\text{C}_{18}\text{H}_{13}\text{FN}_2\text{O}_4(\text{M}+\text{H}^+)$ : 341.0932, found: 341.0930.

**Methyl 3-(3-chlorobenzamido)-5-phenylisoxazole-4-carboxylate (3aaf).** Yield: 71% (0.203 g from 0.2 g); a yellow oil;  $R_f = 0.48$



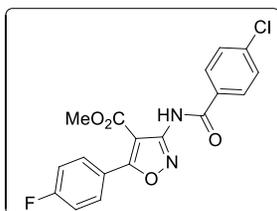
(hexanes: EtOAc, 7:3, v/v); IR ( $\text{CHCl}_3$ )  $\nu_{\text{max}}$ : 1634, 1721  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta = 3.93$  (s, 3H), 7.50-7.61 (m, 5H), 7.85-7.89 (m, 3H), 8.03 (s, 1H), 10.44 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 52.5, 99.2, 125.3, 126.5, 128.1, 128.4, 129.4, 130.2, 131.8, 132.7, 134.7, 135.3, 157.3, 162.1, 163.9, 172.7 ppm. MS (ESI+):  $m/z = 357.0$ . ESI-HR-MS calculated for  $\text{C}_{18}\text{H}_{13}\text{ClN}_2\text{O}_4(\text{M}+\text{H}^+)$ : 357.0637, found: 357.0639.

**Methyl 3-(4-bromobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (3bab).** Yield: 79% (0.248 g from 0.2 g); a white solid,



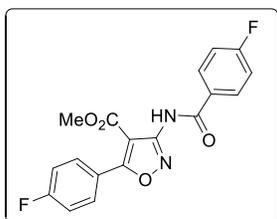
mp 131-133 °C;  $R_f = 0.45$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\text{max}}$ : 1641, 1731  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta = 3.94$  (s, 3H), 7.14 (t,  $J = 8.5$  Hz, 2H), 7.70 (d,  $J = 8.2$  Hz, 2H), 7.89-7.92 (m, 4H), 10.41 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 52.5, 99.1, 115.8 (d,  $J = 22.1$  Hz), 127.8, 129.2, 131.7 (d,  $J = 8.9$  Hz), 131.8, 132.3, 157.4, 162.5, 163.8, 171.6 ppm. MS (ESI+):  $m/z = 419.0$ . ESI-HR-MS calculated for  $\text{C}_{18}\text{H}_{12}\text{FBrN}_2\text{O}_4(\text{M}+\text{H}^+)$ : 419.0037, found: 419.0035.

**Methyl 3-(4-chlorobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (3bac).** Yield: 77% (0.202 g from 0.2 g); a white solid,



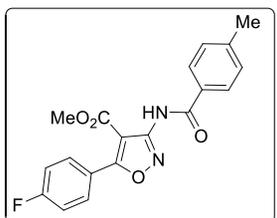
mp 118-120 °C;  $R_f = 0.45$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1647, 1731  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 3.92$  (s, 3H), 7.22 (t,  $J = 8.5$  Hz, 2H), 7.68 (d,  $J = 8.1$  Hz, 2H), 7.86 (d,  $J = 8.3$  Hz, 4H), 10.37 (s, 1H)  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 52.5, 99.1, 115.7 (d,  $J = 22.1$  Hz), 122.7, 127.8, 129.2, 131.8 (d,  $J = 9.0$  Hz), 132.3, 163.5, 163.8 ppm. MS (ESI+):  $m/z = 375.0$ . ESI-HR-MS calculated for  $\text{C}_{18}\text{H}_{12}\text{FCIN}_2\text{O}_4(\text{M}+\text{H}^+)$ : 375.0542, found: 375.0545.

**Methyl 3-(4-fluorobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (3bad).** Yield: 75% (0.202 g from 0.2 g); a white solid,



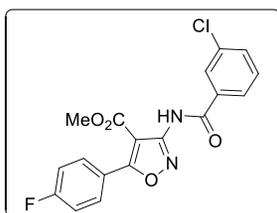
mp 131-133 °C;  $R_f = 0.46$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1632, 1731  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 3.91$  (s, 3H), 7.19-7.29 (m, 4H), 7.86-7.89 (m, 2H), 8.02-8.05 (m, 2H), 10.36 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 52.5, 99.1, 115.8 (d,  $J = 22.0$  Hz), 116.1 (d,  $J = 22.1$  Hz), 129.1, 130.0, 130.1, 131.7, 131.8, 157.5, 162.3, 163.9, 171.6 ppm. MS (ESI+):  $m/z = 359.1$ . ESI-HR-MS calculated for  $\text{C}_{18}\text{H}_{12}\text{F}_2\text{N}_2\text{O}_4(\text{M}+\text{H}^+)$ : 359.0838, found: 359.0838.

**Methyl 5-(4-fluorophenyl)-3-(4-methylbenzamido)isoxazole-4-carboxylate (3bae).** Yield: 75% (0.199 g from 0.2 g); a white solid,



mp 107-109 °C;  $R_f = 0.46$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1636, 1726  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 2.44$  (s, 3H), 3.91 (s, 3H), 7.55 (t,  $J = 8.5$  Hz, 2H), 7.33 (d,  $J = 7.9$  Hz, 2H), 7.86-7.92 (m, 4H), 10.31 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 21.6, 52.4, 99.2, 115.7 (d,  $J = 22.2$  Hz), 122.8, 127.6, 129.7, 130.1, 131.8 (d,  $J = 8.9$  Hz), 143.4, 157.6, 163.4, 163.7, 166.0, 171.5 ppm. MS (ESI+):  $m/z = 355.1$ . ESI-HR-MS calculated for  $\text{C}_{19}\text{H}_{15}\text{FN}_2\text{O}_4(\text{M}+\text{H}^+)$ : 355.1089, found: 355.1085.

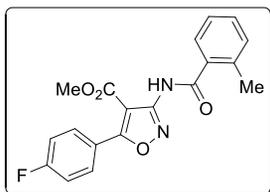
**Methyl 3-(3-chlorobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (3baf).** Yield: 72% (0.202 g from 0.2 g); a white solid,



mp 118-120 °C;  $R_f = 0.48$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1642, 1731  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,

CDCl<sub>3</sub>):  $\delta$  = 3.85 (s, 3H), 7.12-7.17 (m, 2H), 7.41 (t,  $J$  = 8.0 Hz, 1H), 7.51 (t,  $J$  = 8.0 Hz, 1H), 7.78-7.82 (m, 3H), 7.93 (s, 1H), 10.37 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 52.6, 99.1, 115.8 (d,  $J$  = 22.2 Hz), 122.6, 125.4, 128.1, 130.3, 131.7 (d,  $J$  = 8.1 Hz), 132.8, 134.7, 135.3, 157.4, 162.1, 163.7, 171.7 ppm. MS (ESI<sup>+</sup>):  $m/z$  = 375.0. ESI-HR-MS calculated for C<sub>18</sub>H<sub>12</sub>ClFN<sub>2</sub>O<sub>4</sub>(M+H<sup>+</sup>): 375.0542, found: 375.0544.

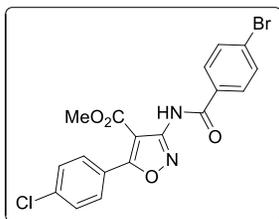
**Methyl 5-(4-fluorophenyl)-3-(2-methylbenzamido)isoxazole-4-carboxylate (3bag).** Yield: 65% (0.173 g from 0.2 g); a white solid,



mp 95-97 °C;  $R_f$  = 0.47 (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1637, 1725 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.61 (s, 3H), 3.87 (s, 3H), 7.21 (t,  $J$  = 8.3 Hz, 2H), 7.32 (d,  $J$  = 3.6 Hz, 2H), 7.41 (d,  $J$  = 7.2 Hz, 1H), 7.63 (d,  $J$  = 7.8 Hz, 1H), 7.88 (d,  $J$  = 7.0 Hz, 2H), 9.85 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 20.4, 52.4, 99.3, 115.8 (d,  $J$  = 22.2 Hz), 126.1, 127.1, 131.2, 131.7, 131.8, 134.0, 138.0, 157.4, 163.3, 165.8, 166.0

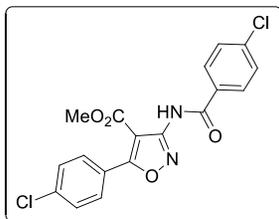
171.6 ppm. MS (ESI<sup>+</sup>):  $m/z$  = 355.1. ESI-HR-MS calculated for C<sub>19</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>4</sub>(M+H<sup>+</sup>): 355.1089, found: 355.1085.

**Methyl 3-(4-bromobenzamido)-5-(4-chlorophenyl)isoxazole-4-carboxylate (3cab).** Yield: 76% (0.233 g from 0.2 g); a white solid,



mp 127-129 °C;  $R_f$  = 0.45 (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1634, 1719 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 3.92 (s, 3H), 7.52 (d,  $J$  = 8.6 Hz, 2H), 7.68 (d,  $J$  = 8.5 Hz, 2H), 7.80 (d,  $J$  = 8.6 Hz, 2H), 7.88 (d,  $J$  = 8.5 Hz, 2H), 10.37 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 52.6, 99.4, 124.9, 127.8, 128.9, 129.2, 130.7, 132.3, 138.3, 157.5, 162.5, 163.8, 171.5 ppm. MS (ESI<sup>+</sup>):  $m/z$  = 434.9. ESI-HR-MS calculated for C<sub>18</sub>H<sub>12</sub>BrClN<sub>2</sub>O<sub>4</sub>(M+H<sup>+</sup>): 434.9742, found: 434.9740.

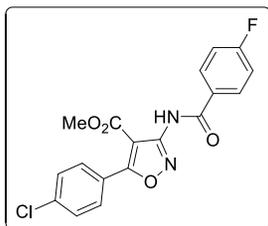
**Methyl 3-(4-chlorobenzamido)-5-(4-chlorophenyl)isoxazole-4-carboxylate (3cac).** Yield: 78% (0.215 g from 0.2 g); a white solid,



mp 136-138 °C;  $R_f$  = 0.48 (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1639, 1719 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 3.95 (s, 3H), 7.52-7.56 (m, 4H), 7.83 (d,  $J$  = 8.5 Hz, 2H), 7.98 (d,  $J$  = 8.4 Hz, 2H), 10.41 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 52.6, 99.4, 128.9, 129.0, 129.3, 130.7, 131.2, 138.3, 139.2, 157.5,

162.4, 163.7, 171.4 ppm. MS (ESI+):  $m/z = 391.0$ . ESI-HR-MS calculated for  $C_{18}H_{12}Cl_2N_2O_4(M+H^+)$ : 391.0247, found: 391.0248.

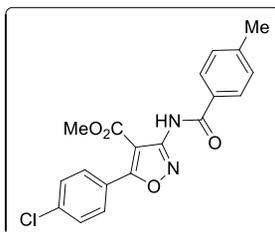
**Methyl 5-(4-chlorophenyl)-3-(4-fluorobenzamido)isoxazole-4-carboxylate (3cad)**. Yield: 78% (0.206 g from 0.2 g); a white solid,



mp 116-118 °C ;  $R_f = 0.48$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{max}$ : 1648, 1721  $cm^{-1}$ .  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta = 3.92$  (s, 3H), 7.22 (t,  $J = 8.5$  Hz, 2H), 7.50 (d,  $J = 8.5$  Hz, 2H), 7.80 (d,  $J = 8.5$  Hz, 2H), 8.01-8.05 (dd,  $J_1 = 8.7$  Hz,  $J_2 = 3.7$  Hz, 2H), 10.35 (s, 1H);  $^{13}C$  NMR (75 MHz,  $CDCl_3$ ): 52.6, 99.4, 116.2 (d,  $J = 22.2$  Hz), 124.9, 128.9, 130.1 (d,  $J = 9.3$  Hz), 130.7, 138.3, 157.5, 162.3, 163.8, 165.4 (d,  $J = 255.1$  Hz), 171.4 ppm. MS (ESI+):  $m/z = 375.0$ . ESI-HR-MS calculated for  $C_{18}H_{12}FCIN_2O_4(M+H^+)$ : 375.0542, found:

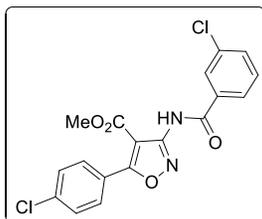
375.0539.

**Methyl 5-(4-chlorophenyl)-3-(4-methylbenzamido)isoxazole-4-carboxylate (3cae)**. Yield: 77% (0.202 g from 0.2 g); a white solid,



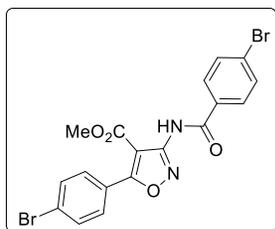
mp 110-112 °C;  $R_f = 0.47$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{max}$ : 1639, 1733  $cm^{-1}$ .  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta = 2.44$  (s, 3H), 3.92 (s, 3H), 7.32 (d,  $J = 8.0$  Hz, 2H), 7.50 (d,  $J = 8.5$  Hz, 2H), 7.80 (d,  $J = 8.5$  Hz, 2H), 7.90 (d,  $J = 8.0$  Hz, 2H), 10.30 (s, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ): 21.6, 52.5, 99.5, 125.0, 127.6, 128.8, 129.7, 130.1, 130.7, 138.2, 143.4, 157.6, 163.4, 163.6, 171.4 ppm. MS (ESI+):  $m/z = 371.1$ . ESI-HR-MS calculated for  $C_{19}H_{15}ClN_2O_4(M+H^+)$ : 371.0793, found: 371.0795.

**Methyl 3-(3-chlorobenzamido)-5-(4-chlorophenyl)isoxazole-4-carboxylate (3caf)**. Yield: 70% (0.193 g from 0.2 g); a white solid,



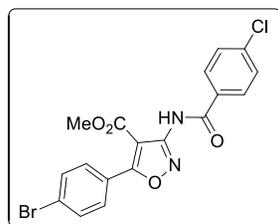
mp 103-105 °C;  $R_f = 0.46$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{max}$ : 1633, 1724  $cm^{-1}$ .  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta = 3.92$  (s, 3H), 7.46-7.52 (m, 3H), 7.57-7.60 (m, 1H), 7.79-7.86 (m, 3H), 8.00 (s, 1H), 10.35 (s, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ): 52.6, 99.5, 124.8, 125.4, 128.1, 128.9, 130.3, 130.7, 132.8, 134.6, 135.4, 138.3, 157.4, 162.1, 163.6, 171.5 ppm. MS (ESI+):  $m/z = 391.0$ . ESI-HR-MS calculated for  $C_{18}H_{12}Cl_2N_2O_4(M+H^+)$ : 391.0247, found: 391.0248.

**Methyl 3-(4-bromobenzamido)-5-(4-bromophenyl)isoxazole-4-carboxylate (3dab).** Yield: 80% (0.232 g from 0.2 g); a white solid,



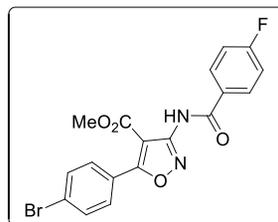
mp 143-145 °C;  $R_f = 0.48$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1647, 1732  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 3.93$  (s, 3H), 7.67-7.76 (m, 4H), 7.65-7.73 (m, 2H), 7.89 (dd,  $J_1 = 6.73$  Hz,  $J_2 = 1.8$  Hz, 2H), 10.39 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 52.6, 99.4, 125.3, 126.8, 127.8, 129.1, 130.8, 131.7, 131.8, 132.3, 157.5, 162.5, 163.7, 171.5 ppm. MS (ESI+):  $m/z = 478.9$ . ESI-HR-MS calculated for  $\text{C}_{18}\text{H}_{12}\text{Br}_2\text{N}_2\text{O}_4(\text{M}+\text{H}^+)$ : 480.9217, found: 480.9214.

**Methyl 5-(4-bromophenyl)-3-(4-chlorobenzamido)isoxazole-4-carboxylate (3dac).** Yield: 78% (0.205 g from 0.2 g); a white solid,



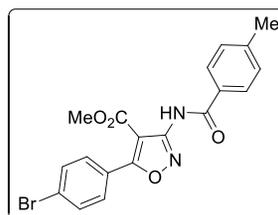
mp 128-130 °C;  $R_f = 0.47$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1640, 1730  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 3.92$  (s, 3H), 7.66-7.669 (m, 4H), 7.72 (d,  $J = 8.5$  Hz, 2H), 7.87 (d,  $J = 8.3$  Hz, 2H), 10.36 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 52.6, 99.4, 125.3, 126.8, 127.8, 129.1, 130.8, 131.7, 131.9, 132.3, 163.7, 171.5 ppm. MS (ESI+):  $m/z = 434.9$ . ESI-HR-MS calculated  $\text{C}_{18}\text{H}_{12}\text{BrClN}_2\text{O}_4$  ( $\text{M}+\text{H}^+$ ): 436.9722, found: 436.9724.

**Methyl 5-(4-bromophenyl)-3-(4-fluorobenzamido)isoxazole-4-carboxylate (3dad).** Yield: 79% (0.201 g from 0.2 g); a white solid,



mp 125-127 °C;  $R_f = 0.47$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1635, 1728  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 3.92$  (s, 3H), 7.22 (t,  $J = 8.6$  Hz, 2H), 7.66 (d,  $J = 8.7$  Hz, 2H), 7.72 (d,  $J = 8.7$  Hz, 2H), 8.01-8.05 (m, 2H), 10.35 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 52.6, 99.4, 116.1 (d,  $J = 22.0$  Hz), 125.4, 126.8, 128.9, 130.1 (d,  $J = 9.2$  Hz), 130.8, 131.8, 157.5, 162.3, 163.8, 165.6 (d,  $J = 255.8$  Hz), 171.5 ppm. MS (ESI+):  $m/z = 419.0$ . ESI-HR-MS calculated for  $\text{C}_{18}\text{H}_{12}\text{BrFN}_2\text{O}_4(\text{M}+\text{H}^+)$ : 419.0037, found: 419.0039.

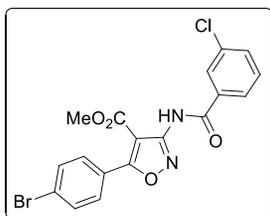
**Methyl 5-(4-bromophenyl)-3-(4-methylbenzamido)isoxazole-4-carboxylate (3dae).** Yield: 77% (0.194 g from 0.2 g); a white solid,



mp 115-117 °C;  $R_f = 0.46$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1641, 1730  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,

CDCl<sub>3</sub>):  $\delta$  = 2.44 (s, 3H), 3.91 (s, 3H), 7.33 (d,  $J$  = 8.0 Hz, 2H), 7.66 (d,  $J$  = 8.5 Hz, 2H), 7.73 (d,  $J$  = 8.6 Hz, 2H), 7.90 (d,  $J$  = 8.0 Hz, 2H), 10.30 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 21.6, 52.5, 99.6, 125.5, 126.6, 127.6, 129.7, 130.1, 130.8, 131.8, 143.5, 157.6, 163.4, 163.6, 171.4 ppm. MS (ESI+):  $m/z$  = 415.0. ESI-HR-MS calculated for C<sub>19</sub>H<sub>15</sub>BrN<sub>2</sub>O<sub>4</sub>(M+H<sup>+</sup>): 415.0288, found: 415.0290.

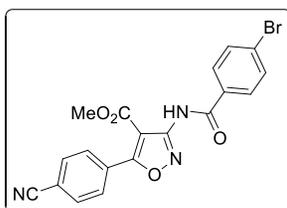
**Methyl 3-(3-chlorobenzamido)-5-(4-bromophenyl)isoxazole-4-carboxylate (3daf).** Yield: 78% (0.205 g from 0.2 g); a white solid,



mp 108-110 °C;  $R_f$  = 0.48 (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1637, 1725 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 3.93 (s, 3H), 7.48 (t,  $J$  = 7.8 Hz, 1H), 7.58 (d,  $J$  = 8.0 Hz, 1H), 7.67 (d,  $J$  = 8.6 Hz, 2H), 7.73 (d,  $J$  = 8.6 Hz, 2H), 7.86 (d,  $J$  = 7.7 Hz, 1H), 8.00 (s, 1H), 10.35 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 52.6, 99.4, 125.3, 125.4, 126.8, 128.1, 130.3, 130.8, 131.8, 132.8, 134.6, 135.4, 157.4, 162.1, 163.6, 171.5 ppm. MS (ESI+):  $m/z$  = 434.9. ESI-HR-MS calculated C<sub>18</sub>H<sub>12</sub>BrClN<sub>2</sub>O<sub>4</sub> (M+H<sup>+</sup>): 436.9722, found:

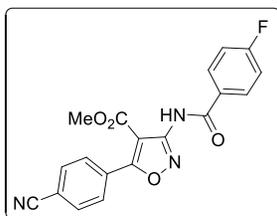
436.9725.

**Methyl 3-(4-bromobenzamido)-5-(4-cyanophenyl)isoxazole-4-carboxylate (3fab).** Yield: 72% (0.224 g from 0.2 g); a white solid,



mp 135-137 °C;  $R_f$  = 0.46 (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1631, 1718 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 3.86 (s, 3H), 7.61 (d,  $J$  = 8.5 Hz, 2H), 7.74-7.81 (m, 4H), 7.90 (d,  $J$  = 8.4 Hz, 2H), 10.23 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 52.8, 100.5, 115.4, 117.8, 127.9, 129.1, 130.0, 130.5, 131.5, 132.2, 132.4, 157.5, 162.5, 163.3, 170.2 ppm. MS (ESI+):  $m/z$  = 426.0. ESI-HR-MS calculated for C<sub>19</sub>H<sub>12</sub>BrN<sub>3</sub>O<sub>4</sub>(M+H<sup>+</sup>): 426.0084, found: 426.0079.

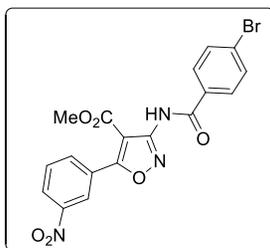
**Methyl 5-(4-cyanophenyl)-3-(4-fluorobenzamido)isoxazole-4-carboxylate (3fad).** Yield: 73% (0.195 g from 0.2 g); a white solid,



mp 128-130 °C;  $R_f$  = 0.44 (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1636, 1719 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 3.93 (s, 3H), 7.23 (t,  $J$  = 8.5 Hz, 2H), 7.82 (d,  $J$  = 8.4 Hz, 2H), 7.98 (d,  $J$  = 8.5 Hz, 2H), 8.02-8.05 (m, 2H), 10.31 (s, 1H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sup>6</sup>): 52.8, 100.6, 115.4, 116.2 (d,  $J$  = 21.9

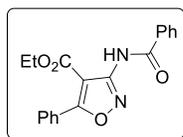
Hz), 117.8, 128.9, 130.0, 130.1, 130.5, 132.2, 157.6, 162.3, 163.3, 170.2 ppm. MS (ESI+):  $m/z = 366.1$ . ESI-HR-MS calculated for  $C_{19}H_{12}FN_3O_4(M+H^+)$ : 366.0885, found: 366.0887.

**Methyl 3-(4-bromobenzamido)-5-(3-nitrophenyl)isoxazole-4-carboxylate (3hab).** Yield: 67% (0.203 g from 0.2 g); a white solid,



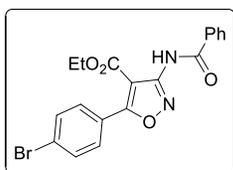
mp 142-144 °C;  $R_f = 0.42$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{max}$ : 1643, 1723  $cm^{-1}$ .  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta = 3.97$  (s, 3H), 7.69 (d,  $J = 8.6$  Hz, 2H), 7.75-7.77 (m, 1H), 7.89 (d,  $J = 8.6$  Hz, 2H), 8.19-8.21 (m, 1H), 8.42-8.45 (m, 1H), 8.84 (t,  $J = 1.9$  Hz, 1H), 10.37 (s, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ): 52.9, 100.5, 124.4, 124.7, 126.3, 127.9, 129.2, 131.5, 132.4, 134.9, 148.1, 157.6, 162.5, 163.3, 169.6 ppm. MS (ESI+):  $m/z = 445.9$ . ESI-HR-MS calculated for  $C_{18}H_{12}BrN_3O_6(M+H^+)$ : 445.9982, found: 445.9982.

**Ethyl 3-benzamido-5-phenylisoxazole-4-carboxylate (3aba).** Yield: 75% (0.203 g from 0.2 g); a yellow oil, mp 112-114 °C;  $R_f =$



0.48 (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{max}$ : 1639, 1718  $cm^{-1}$ .  $^1H$  NMR (300 MHz,  $CDCl_3$ ):  $\delta = 1.32$  (t,  $J = 7.2$  Hz, 3H), 4.38 (q,  $J = 7.2$  Hz, 2H), 7.49-7.60 (m, 6H), 7.86 (dd,  $J_1 = 8.6$  Hz,  $J_2 = 1.6$  Hz, 2H), 8.01-8.03 (m, 2H), 10.40 (s, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ): 13.9, 61.9, 99.5, 126.7, 127.6, 128.2, 129.0, 129.6, 131.7, 132.6, 133.0, 157.5, 163.5, 172.6 ppm. MS (ESI+):  $m/z = 337.1$ . ESI-HR-MS calculated for  $C_{19}H_{16}N_2O_4(M+H^+)$ : 337.1183, found: 337.1180.

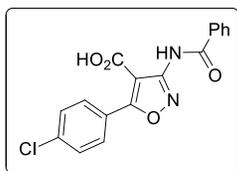
**Ethyl 3-benzamido-5-(4-bromophenyl)isoxazole-4-carboxylate (3dba).** Yield: 76% (0.192 g from 0.2 g); a white solid, mp 121-123



°C;  $R_f = 0.46$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{max}$ : 1649, 1727  $cm^{-1}$ .  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta = 1.34$  (t,  $J = 7.2$  Hz, 3H), 4.40 (q,  $J = 7.2$  Hz, 2H), 7.53 (t,  $J = 7.1$  Hz, 2H), 7.59-7.62 (m, 1H), 7.65 (d,  $J = 8.6$  Hz, 2H), 7.76 (d,  $J = 8.6$  Hz, 2H), 8.00-8.02 (m, 2H), 10.38 (s, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ): 14.0, 62.1, 99.7, 125.5, 126.6, 127.6, 129.0, 131.0, 131.6, 132.7, 132.9, 157.6, 163.2, 163.4, 171.4 ppm. MS (ESI+):  $m/z = 415.0$ .

ESI-HR-MS calculated for  $C_{19}H_{16}BrN_2O_4(M+H^+)$ : 417.0268, found: 417.0267.

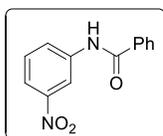
**3-Benzamido-5-(4-chlorophenyl)isoxazole-4-carboxylic acid (3cca).** Yield: 52% (0.132 g from 0.2 g); a pale yellow solid, mp 220-



222 °C;  $R_f = 0.37$  ( $\text{CHCl}_3$ : MeOH, 9:1, v/v); IR (KBr)  $\nu_{\text{max}}$ : 1631, 1708  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 7.50$ -7.52 (m, 3H), 7.59 (t,  $J = 7.2$  Hz, 2H), 7.64-7.66 (m, 1H), 7.99 (d,  $J = 7.2$  Hz, 2H), 8.36-8.37 (m, 2H), 13.5 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 106.5, 127.8, 128.2, 128.5, 129.3, 129.4, 130.8, 132.8, 133.9, 158.8, 162.9, 164.8, 167.1 ppm. MS (ESI+):  $m/z = 343.0$ . ESI-HR-MS calculated for  $\text{C}_{17}\text{H}_{11}\text{ClN}_2\text{O}_4(\text{M}+\text{H}^+)$ :

343.0480, found: 343.0478.

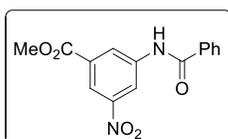
**N-(3-Nitrophenyl)benzamide (5a).** Yield: 17% (0.048 g from 0.2 g); a pale yellow solid, mp 153-155 °C;  $R_f = 0.44$  (Hexanes: EtOAc,



8:2, v/v); IR (KBr)  $\nu_{\text{max}}$ : 1641  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta = 7.49$ -7.59 (m, 4H), 7.89 (d,  $J = 7.3$  Hz, 2H), 8.01-8.05 (dd,  $J_1 = 8.1$  Hz,  $J_2 = 1.2$  Hz, 1H), 8.10 (d,  $J = 8.3$  Hz, 2H), 8.49 (s, 1H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ): 114.9, 119.1, 125.9, 127.1, 129.0, 130.0, 132.5, 134.0, 139.1, 148.6, 165.9 ppm. MS (ESI+):  $m/z = 243.1$ . ESI-HR-

MS calculated for  $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_3(\text{M}+\text{H}^+)$ : 243.0764, found: 243.0762. Data in accordance with the literature<sup>4</sup>

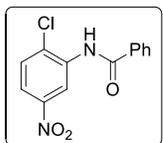
**Methyl 3-benzamido-5-nitrobenzoate (5b).** Yield: 52% (0.138 g from 0.2 g); a pale yellow solid, mp 163-165 °C;  $R_f = 0.41$



(Hexanes: EtOAc, 8:2, v/v); IR (KBr)  $\nu_{\text{max}}$ : 1647  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 3.98$  (s, 3H), 7.52 (t,  $J = 7.1$  Hz, 2H), 7.61 (t,  $J = 7.2$  Hz, 1H), 7.89-7.92 (m, 2H), 8.25 (s, 1H), 8.55 (d,  $J = 1.6$  Hz, 1H), 8.62 (d,  $J = 1.5$  Hz, 1H), 8.92 (d,  $J = 2.0$  Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 52.9, 118.7, 119.9, 126.1, 127.1, 129.0, 132.4,

132.7, 133.6, 139.5, 148.8, 164.8, 165.9 ppm. MS (ESI+):  $m/z = 301.1$ . ESI-HR-MS calculated for  $\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}_5(\text{M}+\text{H}^+)$ : 301.0819, found: 301.0818.

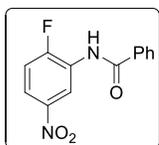
**N-(2-Chloro-5-nitrophenyl)benzamide (5c).** Yield: 47% (0.129 g from 0.2 g); a pale yellow solid, mp 165-167 °C;  $R_f = 0.44$



(Hexanes: EtOAc, 8:2, v/v); IR (KBr)  $\nu_{\text{max}}$ : 1645  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 7.57$  (t,  $J = 7.2$  Hz, 2H), 7.66 (t,  $J = 7.2$  Hz, 1H), 7.89 (d,  $J = 8.8$  Hz, 1H), 8.02 (d,  $J = 7.3$  Hz, 2H), 8.13 (dd,  $J_1 = 8.8$  Hz,  $J_2 = 2.6$  Hz, 1H), 8.57 (d,  $J$

= 2.6 Hz, 1H), 10.35 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 122.1, 122.5, 128.3, 129.1, 131.3, 132.7, 133.9, 136.2, 136.7, 146.8, 166.1 ppm. MS (ESI+):  $m/z = 277.0$ . ESI-HR-MS calculated for  $\text{C}_{13}\text{H}_9\text{ClN}_2\text{O}_3$  ( $\text{M}+\text{H}^+$ ): 277.0374, found: 277.0373. Data in accordance with the literature<sup>5</sup>

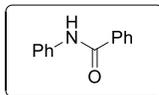
***N*-(2-Fluoro-5-nitrophenyl)benzamide (5d)**. Yield: 42% (0.117 g from 0.2 g); a white solid, mp157-159 °C;  $R_f = 0.44$  (Hexanes:



EtOAc, 8:2, v/v); IR (KBr)  $\nu_{\text{max}}$ :  $1653\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 7.29$  (t,  $J = 9.4$  Hz, 1H), 7.54 (t,  $J = 7.1$  Hz, 2H), 7.62 (t,  $J = 7.3$  Hz, 1H), 7.91 (d,  $J = 7.2$  Hz, 2H), 8.01-8.05 (m, 2H), 8.16 (s, 1H), 9.48 (dd,  $J_1 = 8.1$  Hz,  $J_2 = 1.2$  Hz, 1H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ): 115.4 (d,  $J = 22.4$  Hz), 117.4, 117.4, 119.9, 120.0, 127.2, 129.1, 132.8,

133.6, 144.7, 165.4 ppm. MS (ESI+):  $m/z = 261.1$ . ESI-HR-MS calculated for  $\text{C}_{13}\text{H}_9\text{FN}_2\text{O}_3$  ( $\text{M}+\text{H}^+$ ): 261.0670, found: 261.0671. Data in accordance with the literature<sup>6</sup>

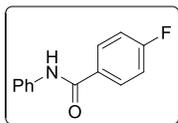
***N*-Phenylbenzamide (7aa)**. Yield: 78% (0.287 g from 0.2 g); a white solid, mp162-164°C;  $R_f = 0.42$  (Hexanes: EtOAc, 8:2, v/v); IR



(KBr)  $\nu_{\text{max}}$ :  $1642\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 7.13$ -7.17 (m, 1H), 7.35-7.39 (m, 2H), 7.46-7.50 (m, 2H), 7.53-7.56 (m, 1H), 7.63-7.65 (m, 2H), 7.83-7.87 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 120.2, 124.6, 127.0, 128.8, 129.1, 131.8, 135.0, 137.9, 165.7 ppm. MS (ESI+):  $m/z = 198.1$ . ESI-HR-MS calculated for  $\text{C}_{13}\text{H}_{11}\text{NO}$  ( $\text{M}+\text{H}^+$ ):

198.0913, found: 198.0911. Data in accordance with the literature.<sup>2</sup>

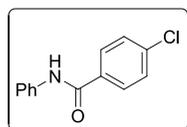
**4-Fluoro-*N*-phenylbenzamide (7ab)**. Yield: 76% (0.307 g from 0.2 g); a white solid, mp181-183°C;  $R_f = 0.45$  (Hexanes: EtOAc, 8:2,



v/v); IR (KBr)  $\nu_{\text{max}}$ :  $1649$ ,  $1708\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 7.16$  (t,  $J = 8.7$  Hz, 3H), 7.37 (d,  $J = 8.3$  Hz, 2H), 7.62 (d,  $J = 7.7$  Hz, 2H), 7.76 (s, 1H), 7.86-7.90 (m, 2H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ): 115.9 (d,  $J = 21.9$  Hz), 120.3, 1240.7, 129.1, 129.4, 129.4, 131.2, 137.8, 164.4, 165.0 (d,  $J = 252.4$  Hz) ppm. MS (ESI+):  $m/z = 216.1$ . ESI-

HR-MS calculated for  $\text{C}_{13}\text{H}_{10}\text{FNO}$  ( $\text{M}+\text{H}^+$ ): 216.0819, found: 216.0820. Data in accordance with the literature.<sup>3</sup>

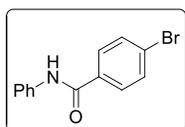
**4-Chloro-*N*-phenylbenzamide (7ac).** Yield: 79% (0.341 g from 0.2 g); a white solid, mp 196-198°C;  $R_f = 0.48$  (Hexanes: EtOAc, 8:2,



v/v); IR (KBr)  $\nu_{\max}$ : 1625  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 7.16$  (t,  $J = 7.4$  Hz, 1H), 7.38 (d,  $J = 8.1$  Hz, 2H), 7.47 (d,  $J = 8.6$  Hz, 2H), 7.62 (d,  $J = 7.7$  Hz, 2H), 7.76 (s, 1H), 7.81 (d,  $J = 8.5$  Hz, 2H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ): 120.3, 124.8, 128.5, 129.1, 129.2, 133.4, 137.7, 138.2, 164.6 ppm. MS (ESI+):  $m/z = 232.0$ . ESI-HR-MS

calculated for  $\text{C}_{13}\text{H}_{10}\text{ClNO}(\text{M}+\text{H}^+)$ : 232.0524, found: 232.0521. Data in accordance with the literature.<sup>2</sup>

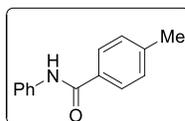
**4-Bromo-*N*-phenylbenzamide (7ad).** Yield: 82% (0.419 g from 0.2 g); a white solid, mp 203-205°C;  $R_f = 0.44$  (Hexanes: EtOAc, 8:2,



v/v); IR (KBr)  $\nu_{\max}$ : 1634  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 7.17$  (t,  $J = 7.5$  Hz, 1H), 7.38 (t,  $J = 8.3$  Hz, 2H), 7.61-7.64 (m, 4H), 7.74 (d,  $J = 8.5$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 120.3, 124.8, 126.6, 128.6, 129.2, 132.1, 133.8, 137.6, 164.1 ppm. MS (ESI+):  $m/z = 276.0$ . ESI-HR-MS calculated for  $\text{C}_{13}\text{H}_{10}\text{BrNO}(\text{M}+\text{H}^+)$ : 276.0019,

found: 276.0015. Data in accordance with the literature.<sup>2</sup>

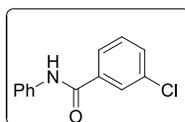
**4-Methyl-*N*-phenylbenzamide (7ae).** Yield: 77% (0.303 g from 0.2 g); a white solid, mp 183-185°C;  $R_f = 0.42$  (Hexanes: EtOAc, 8:2,



v/v); IR (KBr)  $\nu_{\max}$ : 1628  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 2.42$  (s, 3H), 7.12-7.16 (m, 1H), 7.28 (d,  $J = 8.0$  Hz, 2H), 7.36 (t,  $J = 8.4$  Hz, 2H), 7.62-7.64 (m, 2H), 7.77 (d,  $J = 8.2$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ): 21.5, 120.1, 124.4, 127.0, 129.1, 129.4, 132.2, 138.0, 142.4, 165.6 ppm. MS (ESI+):  $m/z = 212.1$ . ESI-HR-MS calculated

for  $\text{C}_{14}\text{H}_{13}\text{N}_2\text{O}_4(\text{M}+\text{H}^+)$ : 212.1070, found: 212.1071. Data in accordance with the literature.<sup>2</sup>

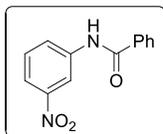
**3-Chloro-*N*-phenylbenzamide (7af).** Yield: 79% (0.341 g from 0.2 g); a white solid, mp 136-138°C;  $R_f = 0.46$  (Hexanes: EtOAc, 8:2,



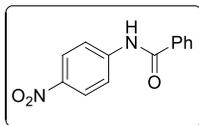
v/v); IR (KBr)  $\nu_{\max}$ : 1639, 1708  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 7.10$  (t,  $J = 7.4$  Hz, 1H), 7.29-7.37 (m, 3H), 7.44-7.47 (m, 1H), 7.55 (d,  $J = 7.7$  Hz, 2H), 7.66 (d,  $J = 7.6$  Hz, 1H), 7.71 (s, 1H), 7.78 (t,  $J = 1.8$  Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 120.3, 124.9, 125.1, 127.4, 129.2, 130.1, 131.9, 135.0, 136.8, 137.6, 163.4 ppm. MS

(ESI+):  $m/z = 232.0$ . ESI-HR-MS calculated for  $\text{C}_{13}\text{H}_{10}\text{ClNO}(\text{M}+\text{H}^+)$ : 232.0524, found: 232.0524. Data in accordance with the literature.<sup>2</sup>

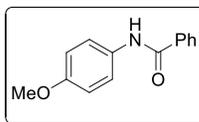
***N*-(3-Nitrophenyl)benzamide (7ba)**. Yield: 71% (0.226 g from 0.2 g); a white solid, mp153-155°C;  $R_f = 0.44$  (Hexanes: EtOAc, 8:2, v/v); IR (KBr)  $\nu_{\max}$ : 1641cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta = 7.49$ -7.59 (m, 4H), 7.89 (d,  $J = 7.3$  Hz, 2H), 8.01-8.05 (dd,  $J_1 = 8.1$  Hz,  $J_2 = 1.2$  Hz, 1H), 8.10 (d,  $J = 8.3$  Hz, 2H), 8.49 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 114.9, 119.1, 125.9, 127.1, 129.0, 130.0, 132.5, 134.0, 139.1, 148.6, 165.9 ppm. MS (ESI+):  $m/z = 243.1$ . ESI-HR-MS calculated for C<sub>13</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>(M+H<sup>+</sup>): 243.0764, found: 243.0763. Data in accordance with the literature.<sup>4</sup>



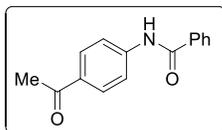
***N*-(4-nitrophenyl)benzamide (7ca)**. Yield: 69% (0.219 g from 0.2 g); a pale yellow solid, mp195-197 °C;  $R_f = 0.42$  (Hexanes: EtOAc, 8:2, v/v); IR (KBr)  $\nu_{\max}$ : 1642cm<sup>-1</sup>. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta = 7.55$ -7.67 (m, 3H), 7.99 (d,  $J = 7.0$  Hz, 2H), 8.07 (d,  $J = 9.1$  Hz, 2H), 8.27 (d,  $J = 9.3$  Hz, 2H), 10.80 (s, 1H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): 120.3, 125.2, 128.4, 129.0, 132.6, 134.7, 142.9, 146.0, 166.8 ppm. MS (ESI+):  $m/z = 243.1$ . ESI-HR-MS calculated for C<sub>13</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>(M+H<sup>+</sup>): 243.0764, found: 243.0764. Data in accordance with the literature.<sup>7</sup>



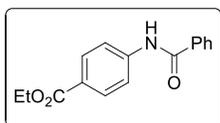
***N*-(4-methoxyphenyl)benzamide (7da)**. Yield: 63% (0.208 g from 0.2 g); a white solid, mp153-155°C;  $R_f = 0.43$  (Hexanes: EtOAc, 8:2, v/v); IR (KBr)  $\nu_{\max}$ : 1651cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta = 3.81$  (s, 3H), 6.89 (d,  $J = 9.1$  Hz, 2H), 7.46 (t,  $J = 7.1$  Hz, 2H), 7.51-7.54 (m, 3H), 7.82-7.86 (m, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 55.5, 114.2, 122.2, 127.0, 128.7, 131.0, 131.7, 135.0, 156.7, 165.7 ppm. MS (ESI+):  $m/z = 228.1$ . ESI-HR-MS calculated for C<sub>14</sub>H<sub>13</sub>NO<sub>2</sub>(M+H<sup>+</sup>): 228.1019, found: 228.1018. Data in accordance with the literature.<sup>8</sup>



***N*-(4-acetylphenyl)benzamide (7ea)**. Yield: 72% (0.230 g from 0.2 g); a white solid, mp 64-65°C;  $R_f = 0.44$  (Hexanes: EtOAc, 8:2, v/v); IR (KBr)  $\nu_{\max}$ : 1649, 1740 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta = 2.60$  (s, 3H), 7.50-7.53 (m, 2H), 7.57-7.61 (m, 1H), 7.77 (d,  $J = 8.7$  Hz, 2H), 7.87-7.90 (m, 2H), 7.99 (d,  $J = 8.7$  Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 26.5, 119.2, 127.1, 128.9, 129.8, 132.3, 134.5, 142.3, 165.8, 196.9 ppm. MS (ESI+):  $m/z = 240.1$ . ESI-HR-MS calculated for C<sub>15</sub>H<sub>13</sub>NO<sub>2</sub>(M+H<sup>+</sup>): 240.1019, found: 240.1019. Data in accordance with the literature.<sup>8</sup>



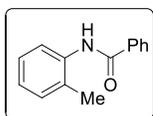
**Ethyl 4-benzamidobenzoate (7fa)**. Yield: 79% (0.237 g from 0.2 g); a white solid, mp148-150 °C;  $R_f = 0.41$  (Hexanes: EtOAc, 8:2,



v/v); IR (KBr)  $\nu_{\max}$ : 1645, 1735  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 1.40$  (t,  $J = 7.2$  Hz, 3H), 4.37 (q,  $J = 7.1$  Hz, 2H), 7.47-7.51 (m, 2H), 7.55-7.59 (m, 1H), 7.74 (d,  $J = 8.8$  Hz, 2H), 7.86-7.89 (m, 2H), 8.05 (d,  $J = 8.8$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ): 14.3, 60.9, 119.2, 126.2, 127.1, 128.9, 130.8, 132.2, 134.6, 142.1, 165.8,

166.1 ppm. MS (ESI+):  $m/z = 270.1$ . ESI-HR-MS calculated for  $\text{C}_{16}\text{H}_{15}\text{NO}_3$  ( $\text{M}+\text{H}^+$ ): 270.1125, found: 270.1126. Data in accordance with the literature.<sup>8</sup>

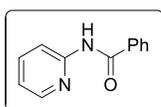
***N*-o-Tolylbenzamide (7ga)**. Yield: 71% (0.247 g from 0.2 g); a white solid, mp144-146 °C;  $R_f = 0.44$  (Hexanes: EtOAc, 8:2, v/v); IR



(KBr)  $\nu_{\max}$ : 1644 $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 2.32$  (s, 3H), 7.09-7.14 (m, 1H), 7.23-7.27 (m, 2H), 7.47-7.51 (m, 2H), 7.53-7.58 (m, 1H), 7.71 (s, 1H), 7.86-7.93 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 17.8, 123.2, 125.2, 126.9,

127.0, 128.8, 129.4, 130.6, 131.8, 135.0, 135.8, 165.7 ppm. MS (ESI+):  $m/z = 212.1$ . ESI-HR-MS calculated for  $\text{C}_{14}\text{H}_{13}\text{NO}$  ( $\text{M}+\text{H}^+$ ): 212.1070, found: 212.1071. Data in accordance with the literature.<sup>8</sup>

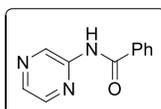
***N*-(Pyridin-2-yl)benzamide (7ha)**. Yield: 64% (0.234 g from 0.2 g); a white solid, mp 86-88 °C;  $R_f = 0.44$  (Hexanes: EtOAc, 8:2,



v/v); IR (KBr)  $\nu_{\max}$ : 1641 $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta = 7.07$ -7.12 (m, 1H), 7.56-7.59 (m, 1H), 7.48-7.54 (m, 2H), 7.77-7.83 (m, 1H), 8.01-8.04 (m, 2H), 8.25-8.27 (m, 1H), 8.48 (d,  $J = 8.5$  Hz, 1H), 9.59 (s, 1H);  $^{13}\text{C}$  NMR (75

MHz,  $\text{CDCl}_3$ ): 114.8, 119.9, 127.6, 128.7, 129.9, 132.2, 139.0, 147.1, 151.8, 166.2 ppm. MS (ESI+):  $m/z = 199.1$ . ESI-HR-MS calculated for  $\text{C}_{12}\text{H}_{10}\text{N}_2\text{O}$  ( $\text{M}+\text{H}^+$ ): 199.0866, found: 199.0865. Data in accordance with the literature.<sup>9</sup>

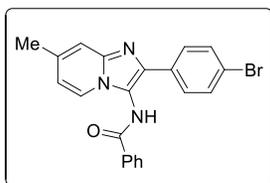
***N*-(Pyrazin-2-yl)benzamide (7ia)**. Yield: 41% (0.149 g from 0.2 g); a white solid, mp165-167 °C;  $R_f = 0.42$  (Hexanes: EtOAc, 8:2,



v/v); IR (KBr)  $\nu_{\max}$ : 1640 $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 7.48$ -7.54 (m, 2H), 7.60 (t,  $J = 7.4$  Hz, 1H), 7.94 (d,  $J = 7.5$  Hz, 2H), 8.24 (s, 1H), 8.37 (d,  $J = 2.4$  Hz, 1H), 8.70 (s, 1H), 9.72 (s, 1H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):

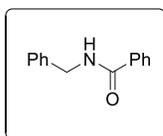
109.0, 127.4, 129.0, 132.7, 137.3, 140.4, 142.1, 148.4, 165.6 ppm. MS (ESI+):  $m/z = 200.1$ . ESI-HR-MS calculated for  $\text{C}_{11}\text{H}_9\text{N}_3\text{O}$  ( $\text{M}+\text{H}^+$ ): 200.0818, found: 200.0819. Data in accordance with the literature.<sup>10</sup>

**N-(2-(4-Bromophenyl)-7-methylimidazo[1,2-a]pyridin-3-yl)benzamide (7ja)**. Yield: 68% (0.174 g from 0.2 g); a white solid, mp



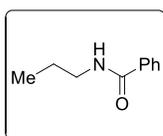
220-222 °C;  $R_f = 0.38$  (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1636  $\text{cm}^{-1}$ .  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 2.47$  (s, 3H), 7.03 (d,  $J = 4.9$  Hz, 1H), 7.48 (t,  $J = 7.6$  Hz, 2H), 7.60 (d,  $J = 7.4$  Hz, 1H), 8.10 (d,  $J = 7.3$  Hz, 2H), 8.17 (d,  $J = 4.0$  Hz, 1H), 8.28 (d,  $J = 8.7$  Hz, 2H), 8.37 (d,  $J = 8.9$  Hz, 3H), 10.82 (s, 1H);  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ ): 116.1, 121.6, 123.8, 128.4, 129.2, 130.0, 133.3, 139.6, 145.6, 150.0, 131.3, 152.0, 164.5, 171.2 ppm. MS (ESI+):  $m/z = 406.0$ . ESI-HR-MS calculated for  $\text{C}_{21}\text{H}_{16}\text{BrN}_3\text{O}(\text{M}+\text{H}^+)$ : 406.0550, found: 406.0552.

**N-Benzylbenzamide (7ka)**. Yield: 81% (0.282 g from 0.2 g); a white solid, mp 102-104 °C;  $R_f = 0.42$  (Hexanes: EtOAc, 8:2, v/v); IR



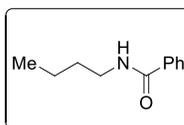
(KBr)  $\nu_{\max}$ : 1647  $\text{cm}^{-1}$ .  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 4.65$  (d,  $J = 5.6$  Hz, 2H), 6.43 (m, 1H), 7.27-7.31 (m, 1H), 7.32-7.36 (m, 4H), 7.40-7.44 (m, 2H), 7.47-7.51 (m, 1H), 7.77-7.79 (m, 2H);  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ ): 44.1, 127.6, 127.9, 128.6, 128.8, 131.6, 134.4, 138.2, 167.4 ppm. MS (ESI+):  $m/z = 212.1$ . ESI-HR-MS calculated for  $\text{C}_{14}\text{H}_{13}\text{NO}(\text{M}+\text{H}^+)$ : 212.1070, found: 212.1069. Data in accordance with the literature.<sup>11</sup>

**N-Isopropylbenzamide (7la)**. Yield: 74% (0.330 g from 0.2 g); a white solid, mp 82-84 °C;  $R_f = 0.44$  (Hexanes: EtOAc, 8:2, v/v); IR



(KBr)  $\nu_{\max}$ : 1639  $\text{cm}^{-1}$ .  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ ):  $\delta = 0.97$  (s, 3H), 1.59-1.67 (m, 2H), 3.39-3.43 (m, 2H), 6.30 (s, 1H), 7.39-7.48 (m, 3H), 7.75 (d,  $J = 7.3$  Hz, 2H);  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ ): 11.4, 22.9, 41.8, 126.9, 128.5, 131.3, 134.9, 167.7 ppm. MS (ESI+):  $m/z = 164.1$ . ESI-HR-MS calculated for  $\text{C}_{10}\text{H}_{13}\text{NO}(\text{M}+\text{H}^+)$ : 164.1070, found: 164.1067. Data in accordance with the literature.<sup>12</sup>

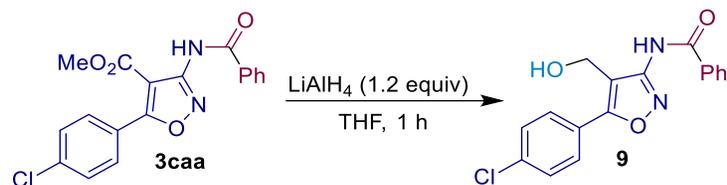
**N-Butylbenzamide (7ma)**. Yield: 62% (0.252 g from 0.2 g); a yellow oil;  $R_f = 0.45$  (Hexanes: EtOAc, 8:2, v/v); IR (KBr)  $\nu_{\max}$ :



1635  $\text{cm}^{-1}$ .  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 0.91$ -0.95 (m, 3H), 1.36-1.42 (m, 2H), 1.56-1.61 (m, 2H), 3.42-3.45 (m, 2H), 6.54 (s, 1H), 7.36-7.45 (m, 3H), 7.76-7.78 (m, 2H);  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ ): 13.7, 20.1, 31.5, 39.8, 126.8, 128.3, 131.1, 134.7, 167.7 ppm. MS (ESI+):  $m/z = 178.1$ . ESI-HR-MS calculated for  $\text{C}_{11}\text{H}_{15}\text{NO}(\text{M}+\text{H}^+)$ :

178.1226, found: 178.1224. Data in accordance with the literature.<sup>13</sup>

**Procedure for the Synthesis of *N*-(5-(4-chlorophenyl)-4-(hydroxymethyl)isoxazol-3-yl)benzamide (9).**



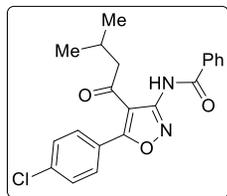
To a stirred solution **3caa** (0.1 g, 0.28 mmol) in THF (4 mL) was added  $\text{LiAlH}_4$  (0.012 g, 0.34 mmol), at 0 °C and the reaction was allowed to stirred at room temperature for 1 h. After completion of the reaction (as monitored by TLC) the solvent was removed under vacuum and the residue was diluted with  $\text{H}_2\text{O}$  (20 mL) and extracted with EtOAc (3 X 20 mL). The combined organic layer was dried over anhydrous  $\text{Na}_2\text{SO}_4$  and evaporated to furnish crude product that was purified by column chromatography over silica gel using hexanes/ EtOAc (7:3, v/v) as eluent to afford the desired product *N*-(5-(4-chlorophenyl)-4-(hydroxymethyl)isoxazol-3-yl)benzamide (**9**) (0.066 g from 0.1 g, 72%) as a white solid, mp 151-153 °C;  $R_f$  = 0.48 (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\text{max}}$ : 3335, 1735  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 4.45 (d,  $J$  = 5.2 Hz, 2H), 5.13 (t,  $J$  = 5.4 Hz, 1H), 7.57 (t,  $J$  = 7.3 Hz, 2H), 7.64-7.69 (m, 3H), 7.91 (d,  $J$  = 8.7 Hz, 2H), 8.00-8.04 (m, 2H), 10.85 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 52.6, 113.1, 126.5, 128.5, 129.0, 129.3, 129.8, 132.9, 133.3, 135.7, 159.0, 166.4, 166.7 ppm. MS (ESI<sup>+</sup>):  $m/z$  = 329.1. ESI-HR-MS calculated for  $\text{C}_{17}\text{H}_{13}\text{ClN}_2\text{O}_3(\text{M}+\text{H}^+)$ : 329.0687, found: 329.0683.

**General Procedure for the Grignard reaction of 3caa as exemplified for the synthesis of 10a.**

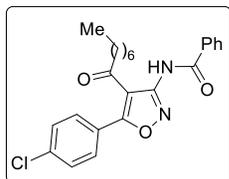


To a stirred solution **3caa** (0.1 g, 0.28 mmol) in THF (4 mL) was added  $i$ PrMgBr (0.16 mL, 0.34 mmol), at room temperature and the reaction was allowed to stirred at room temperature for 4 h. After completion of the reaction (as monitored by TLC) the solvent was removed under vacuum and the residue was diluted with H<sub>2</sub>O (20 mL) and extracted with EtOAc (3 X 20 mL). The combined organic layer was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and evaporated to furnish crude product that was purified by column chromatography over silica gel using hexanes/ EtOAc (7:3, v/v) as eluent to afford the product *N*-(5-(4-chlorophenyl)-4-isobutyrylisoxazol-3-yl)benzamide (**10a**) (0.074 g from 0.1 g, 72%) as a white solid, mp 109-111 °C;  $R_f$  = 0.45 (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1695, 1721 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 0.94 (s, 3H), 0.97 (s, 3H), 2.09 (s, 1H), 7.58 (t,  $J$  = 7.5 Hz, 2H), 7.67-7.69 (m, 3H), 7.85 (d,  $J$  = 8.6 Hz, 2H), 8.03 (d,  $J$  = 7.3 Hz, 2H), 11.50 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 18.2, 67.5, 112.5, 125.7, 128.5, 129.2, 130.1, 132.7, 133.3, 136.9, 156.8, 166.7, 168.8, 199.6 ppm. MS (ESI+):  $m/z$  = 369.1. ESI-HR-MS calculated for C<sub>20</sub>H<sub>17</sub>ClN<sub>2</sub>O<sub>3</sub>(M+H<sup>+</sup>): 369.1000, found: 369.1003.

*N*-(5-(4-chlorophenyl)-4-(3-methylbutanoyl)isoxazol-3-yl)benzamide (**10b**). Yield: 74% (0.078 g from 0.1 g); a white solid, mp 117-119 °C;  $R_f$  = 0.45 (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1689, 1727 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 0.74 (s, 3H), 0.76 (s, 3H), 1.96-2.03 (m, 1H), 2.47-2.49 (m, 2H), 7.59 (t,  $J$  = 7.6 Hz, 2H), 7.66-7.70 (m, 3H), 7.86 (d,  $J$  = 8.6 Hz, 2H), 8.01-8.03 (m, 2H), 11.39 (s, 1H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): 22.7, 24.5, 50.7, 113.9, 125.7, 128.4, 129.2, 129.7, 130.6, 132.8, 133.3, 137.0, 156.9, 166.5, 168.9, 195.7 ppm. MS (ESI+):  $m/z$  = 383.1. ESI-HR-MS calculated for C<sub>21</sub>H<sub>19</sub>ClN<sub>2</sub>O<sub>3</sub>(M+H<sup>+</sup>): 383.1157, found: 383.1160.

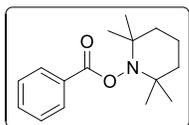


*N*-(5-(4-chlorophenyl)-4-octanoylisoxazol-3-yl)benzamide (**10c**). Yield: 70% (0.083 g from 0.1 g); a white solid, mp 93-95 °C;  $R_f$  = 0.45 (hexanes: EtOAc, 7:3, v/v); IR (KBr)  $\nu_{\max}$ : 1683, 1731 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 0.85-0.88 (m, 3H), 1.17-1.12 (m, 8H), 1.56-1.59 (m, 2H), 2.52 (t,  $J$  = 6.6 Hz, 2H), 7.54-7.63 (m, 7H), 8.05 (d,  $J$  = 7.9 Hz, 2H), 10.82 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 14.0, 22.5, 24.1, 28.8, 28.9, 31.5, 41.5, 108.7, 125.7, 127.7, 129.0, 129.5, 130.7, 132.7, 132.8, 138.4, 157.1, 163.7, 172.0, 198.5 ppm. MS (ESI+):  $m/z$  = 425.2. ESI-HR-MS



calculated for C<sub>24</sub>H<sub>26</sub>ClN<sub>2</sub>O<sub>3</sub>(M+H<sup>+</sup>): 425.1626, found: 425.1627.

**2,2,6,6-Tetramethylpiperidin-1-yl benzoate (11).** Yield: 21% (0.081 g from 0.223 g); a yellow oil; R<sub>f</sub> = 0.45 (Hexanes: EtOAc, 9:1,



v/v); IR (KBr)  $\nu_{\max}$ : 1735cm<sup>-1</sup>. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  = 1.15 (s, 6H), 1.31 (s, 6H), 1.46-1.51 (m, 1H), 1.60-1.64 (m, 2H), 1.74-1.82 (m, 3H), 7.49 (t, *J* = 7.3 Hz, 2H), 7.61 (t, *J* = 7.3 Hz, 2H), 8.09-8.12 (m, 2H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): 17.1, 20.9, 32.0, 39.1, 60.4, 128.5, 129.6, 129.8, 132.9, 166.4 ppm. MS (ESI<sup>+</sup>): *m/z* = 262.2.

ESI-HR-MS calculated for C<sub>16</sub>H<sub>23</sub>NO<sub>2</sub> (M+H<sup>+</sup>): 262.1802, found: 262.1803. Data in accordance with the literature.<sup>14</sup>

## 7. References

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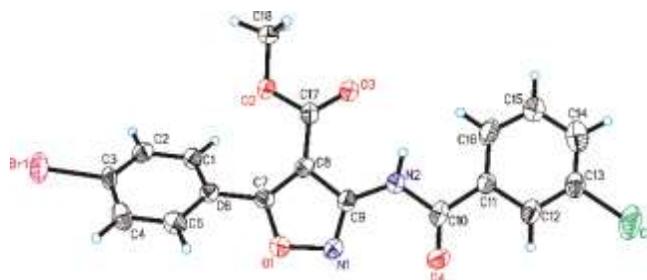
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## 8. X-ray Crystallography Data for compound **3daf**:

Crystals of compound **3daf** were grown from the solvent chloroform by slow evaporation method. A good quality colorless single crystal of size 0.58 x 0.23 x 0.21 mm, was selected under a polarizing microscope and was mounted on a glass fiber for data collection. Single crystal X-ray data for compound **3daf** were collected on the Rigaku Kappa 3 circle diffractometer equipped with the AFC12 goniometer and enhanced sensitivity (HG) Saturn724+ CCD detector in the 4x4 bin mode using the monochromated Mo-K $\alpha$  radiation generated from the microfocus sealed tube MicroMax-003 X-ray generator equipped with specially designed confocal multilayer optics. Data collection was performed using  $\omega$ -scans of 0.5 $^\circ$  steps at 293(2) K. Cell determination, data collection and data reduction was performed using the Rigaku CrystalClear-SM Expert 2.1 b24<sup>1</sup> software. Asymmetric unit contains four molecules of compound **3daf** along with two water molecules. Structure solution and refinement were performed by using SHELXTL-NT.<sup>2</sup> Refinement of coordinates and anisotropic thermal parameters of non-hydrogen atoms were carried out by the full-matrix least-squares method. The hydrogen atoms attached to carbon atoms were generated with idealized geometries and isotropically refined using a riding model.

1. CrystalClear 2.1, Rigaku Corporation, Tokyo, Japan
2. Sheldrick, G. M. Acta Crystallogr., Sect. A 2008, 64, 112–122.



**Figure S-4** ORTEP diagram drawn with 30% ellipsoid probability for non-H atoms of the crystal structure of compound **3daf** determined at 293 K.

<b>Compound</b>	<b>3daf</b>
Empirical formula	C <sub>18</sub> H <sub>12</sub> Br Cl N <sub>2</sub> O <sub>4</sub>
Formula weight	435.66
Crystal System	Monoclinic
Space group	<i>P</i> 2 1
<i>a</i> (Å)	7.339(3)
<i>b</i> (Å)	15.226(5)
<i>c</i> (Å)	8.541(3)
$\alpha$ (°)	90.00
$\beta$ (°)	109.747(4)
$\gamma$ (°)	90.00
<i>V</i> (Å <sup>3</sup> )	898.3(6)
<i>Z</i>	2
D <sub>c</sub> (g/cm <sup>3</sup> )	1.611
<i>F</i> <sub>000</sub>	436
$\mu$ (mm <sup>-1</sup> )	2.463
$\theta_{\max}$ (°)	25.37
Total reflections	6250
Unique reflections	2390
Reflections [ <i>I</i> > 2σ( <i>I</i> )]	1474
Parameters	240
<i>R</i> <sub>int</sub>	0.1295
Goodness-of-fit	0.892
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )]	0.0751
<i>wR</i> ( <i>F</i> <sup>2</sup> , all data)	0.1794
CCDC No.	1940609





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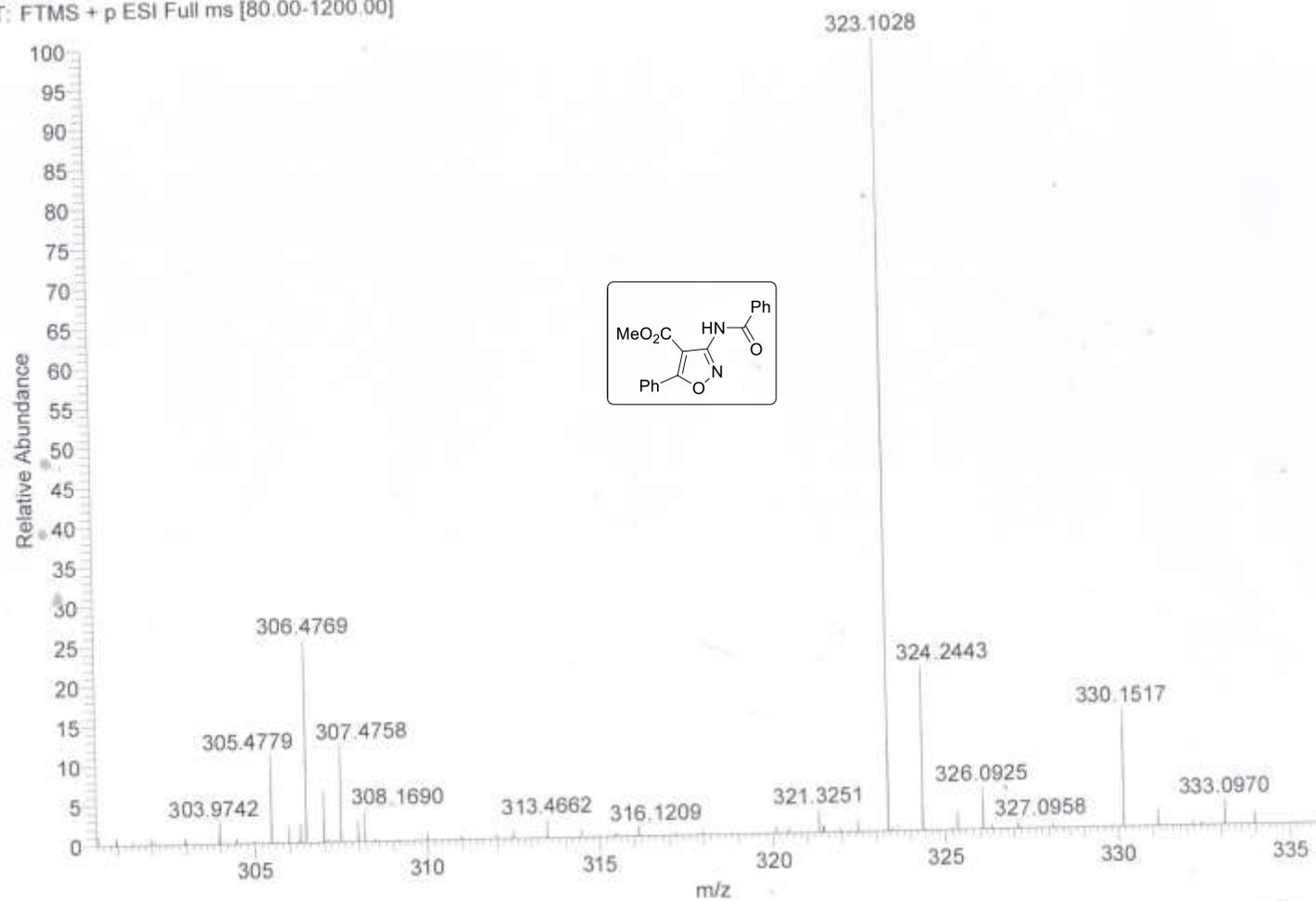


Figure S-7. HRMS spectrum of methyl 3-benzamido-5-phenylisoxazole-4-carboxylate (**3aaa**).

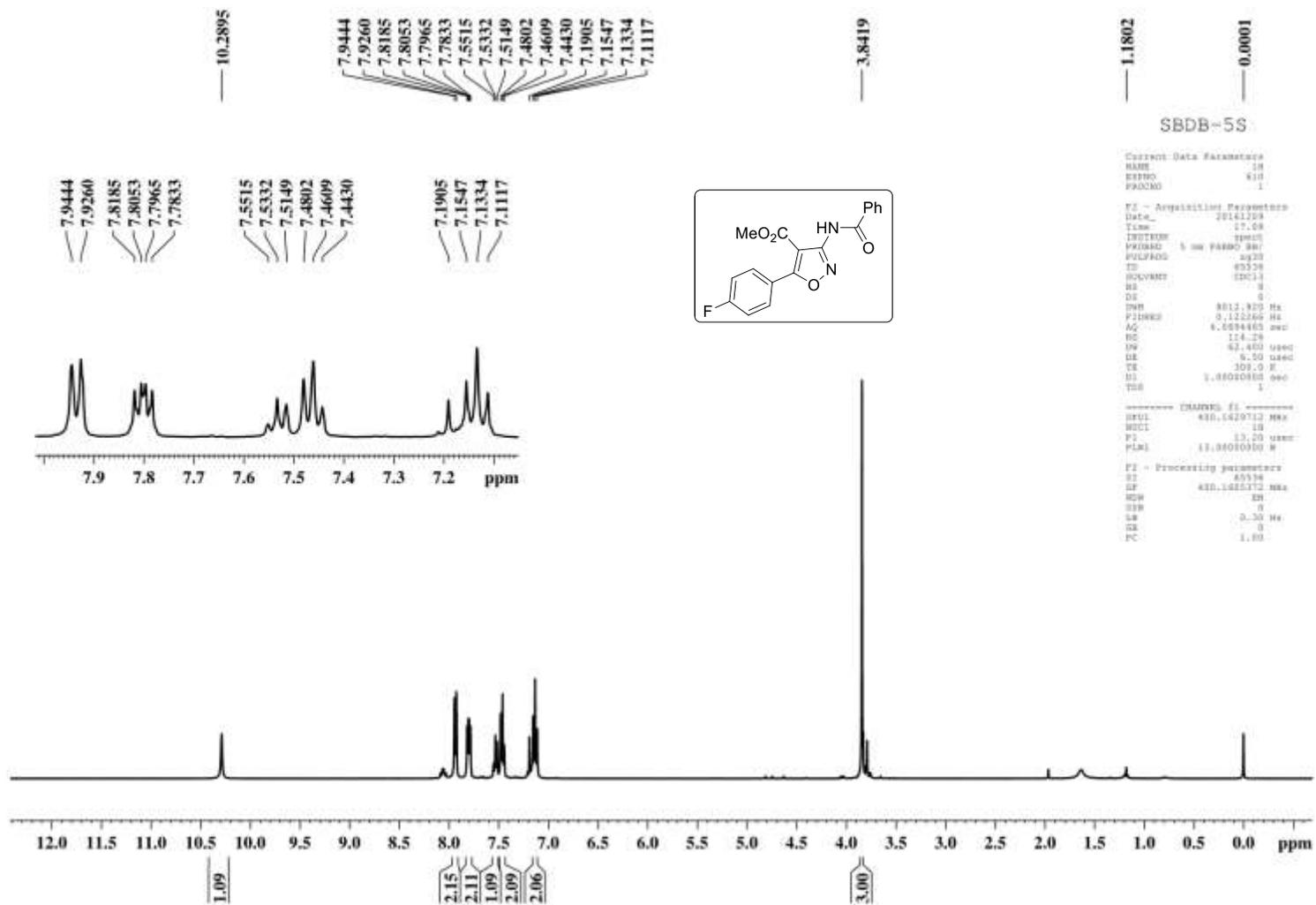


Figure S-8. <sup>1</sup>H-NMR spectrum of methyl 3-benzamido-5-(4-fluorophenyl)isoxazole-4-carboxylate (**3baa**).

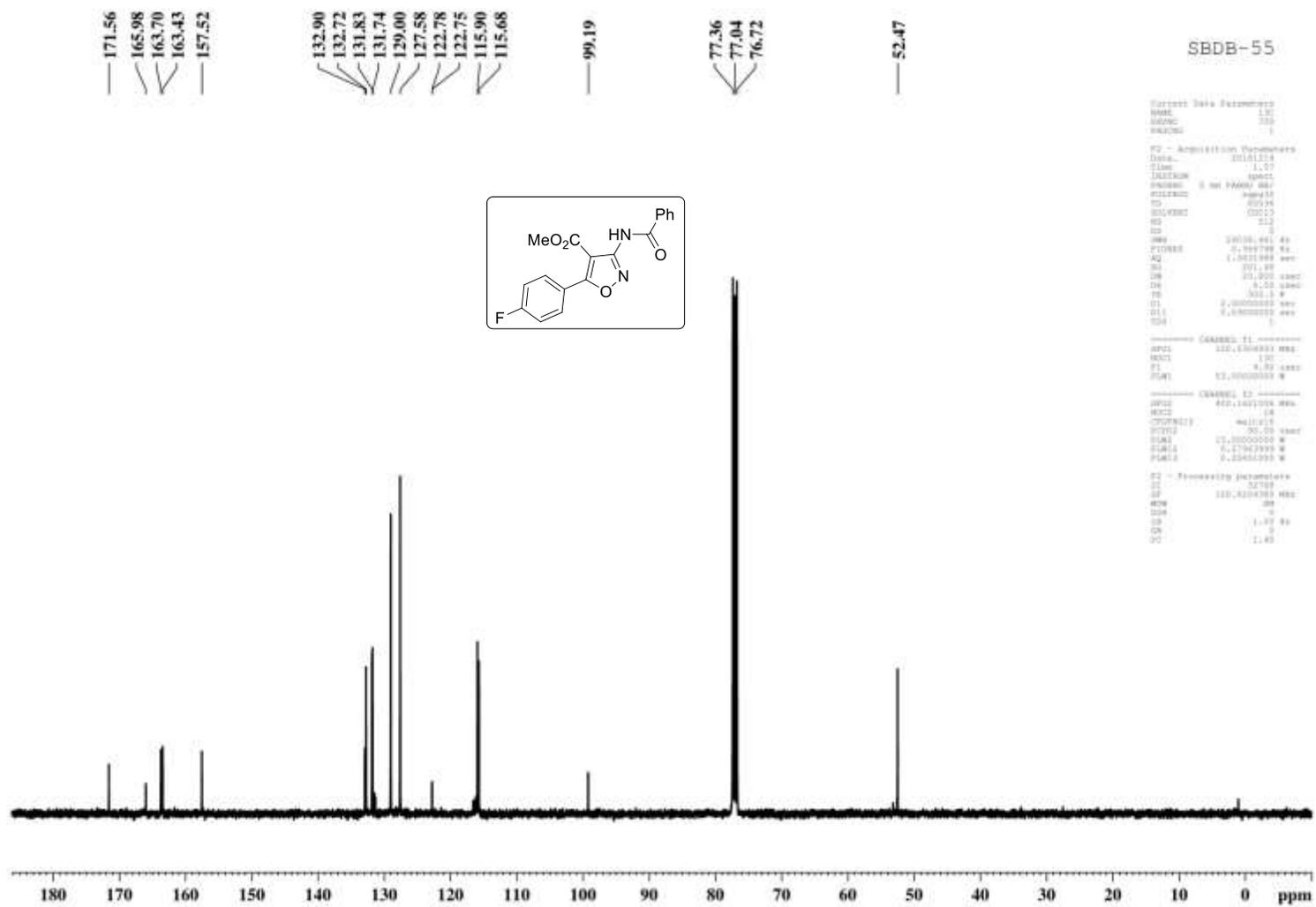


Figure S-9. <sup>13</sup>C-NMR spectrum of methyl 3-benzamido-5-(4-fluorophenyl)isoxazole-4-carboxylate (3baa).

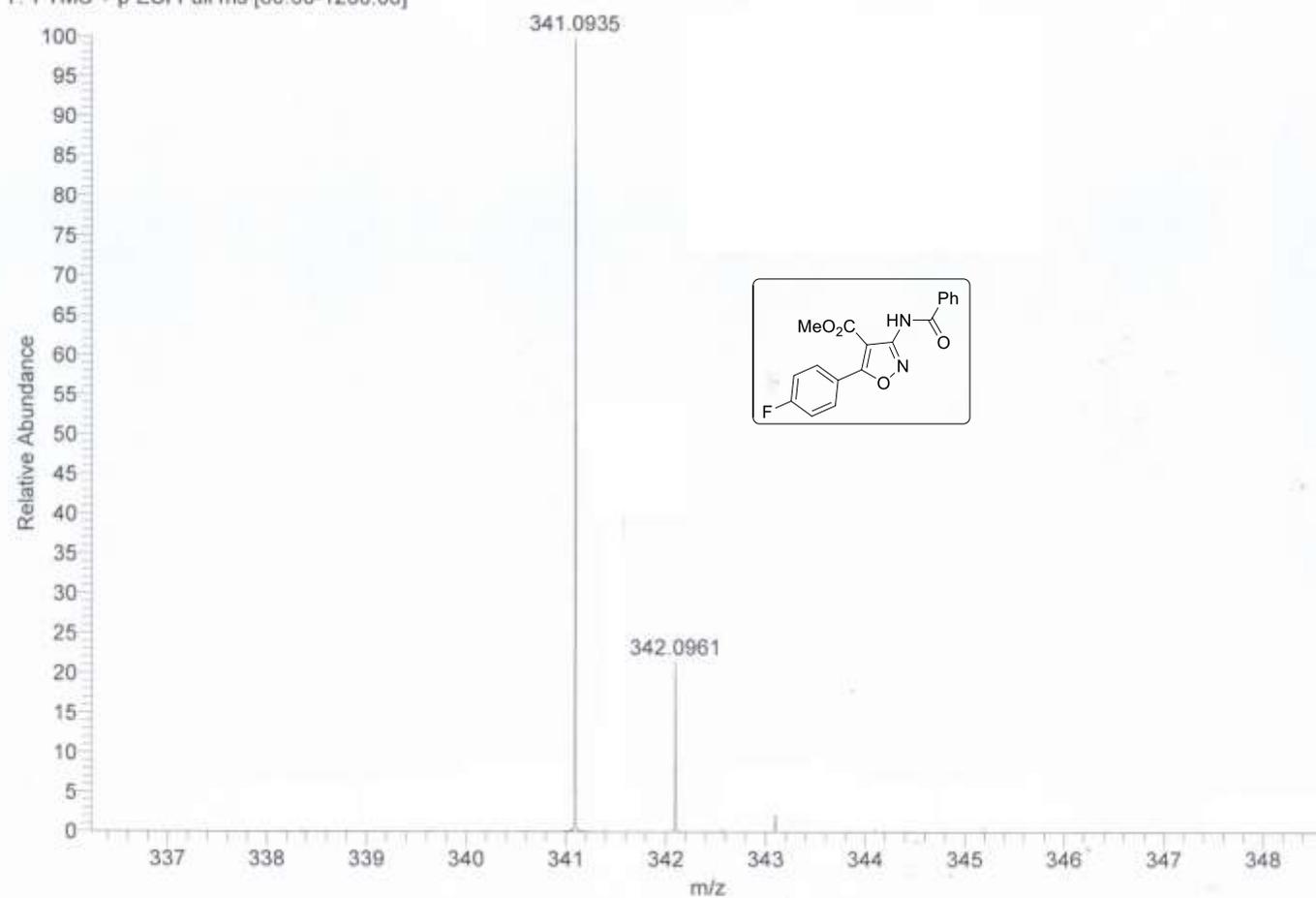
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**Figure S-10.** HRMS spectrum of methyl 3-benzamido-5-(4-fluorophenyl)isoxazole-4-carboxylate (**3baa**).

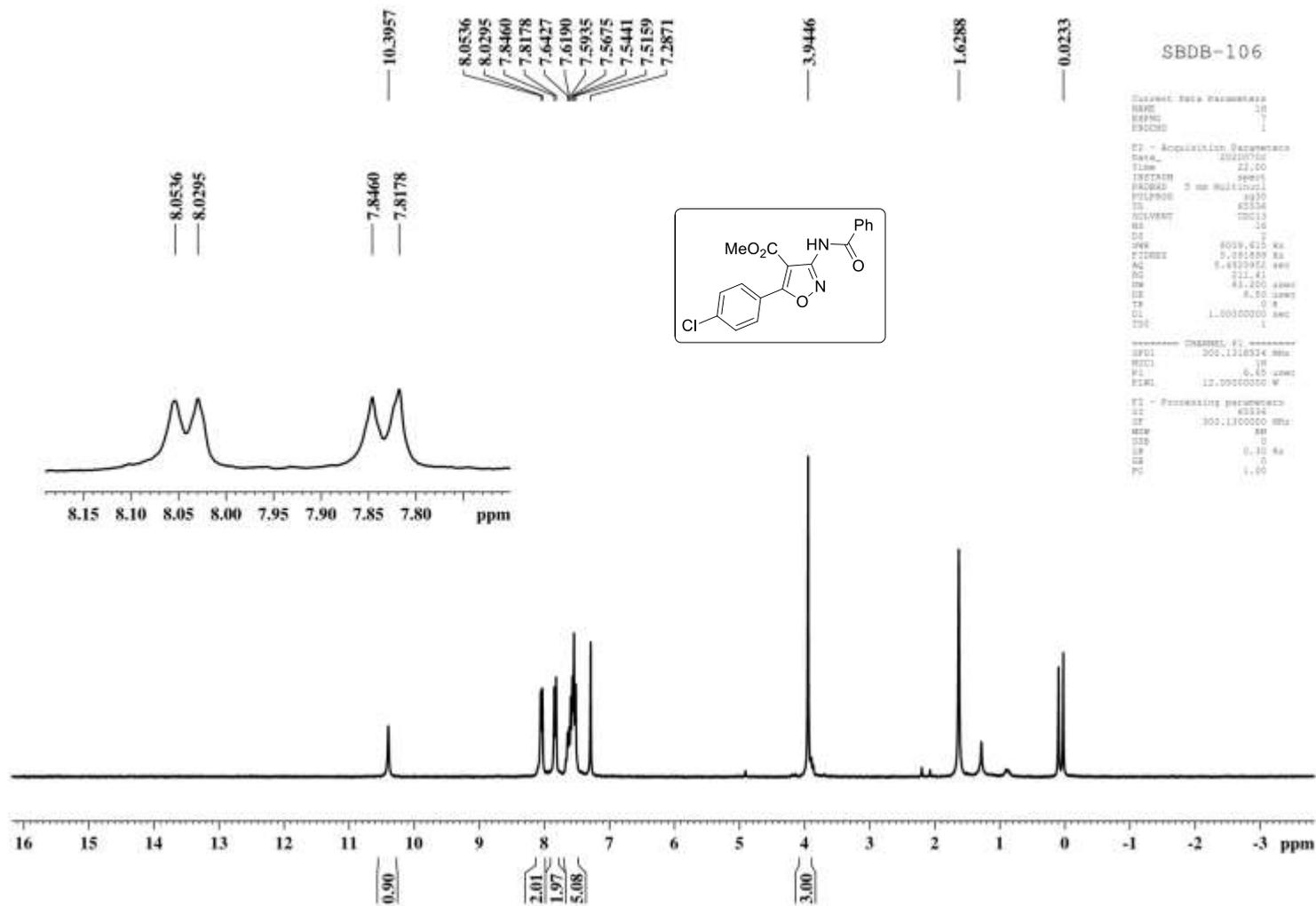


Figure S-11. <sup>1</sup>H-NMR spectrum of methyl 3-benzamido-5-(4-chlorophenyl)isoxazole-4-carboxylate (**3caa**).

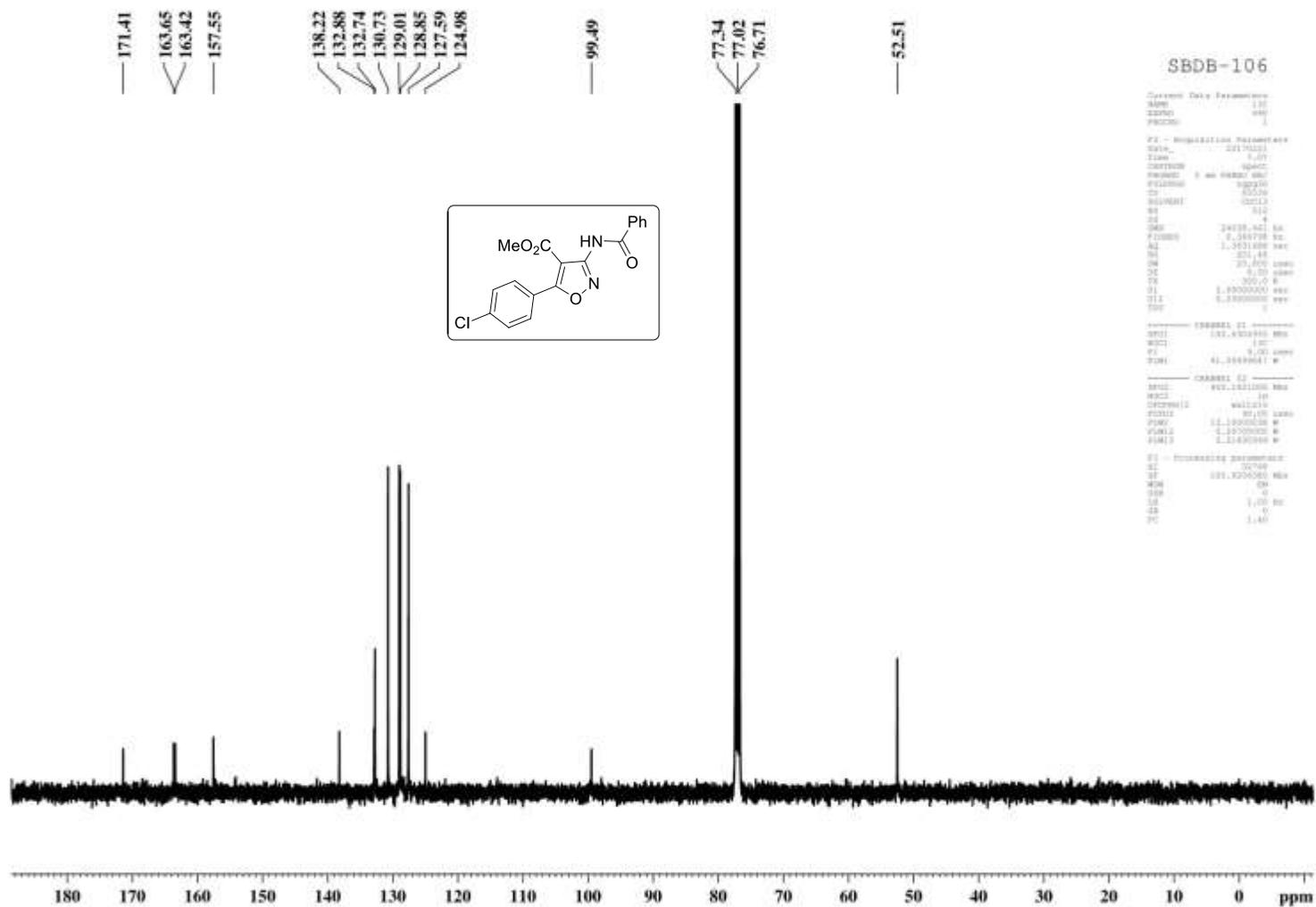
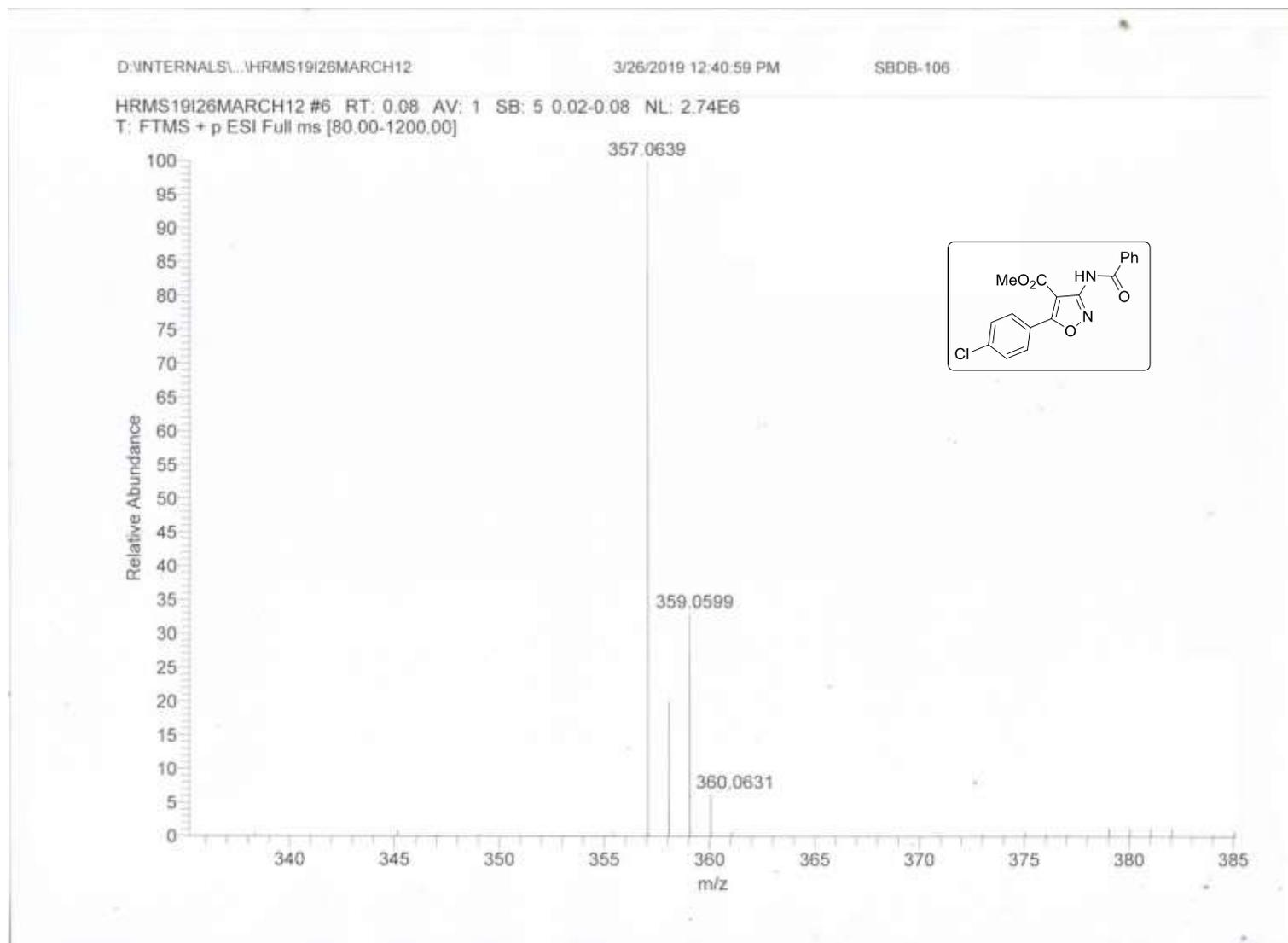


Figure S-12.  $^{13}\text{C}$ -NMR spectrum of methyl 3-benzamido-5-(4-chlorophenyl)isoxazole-4-carboxylate (**3caa**).



**Figure S-13.** HRMS spectrum of methyl 3-benzamido-5-(4-chlorophenyl)isoxazole-4-carboxylate (**3caa**).

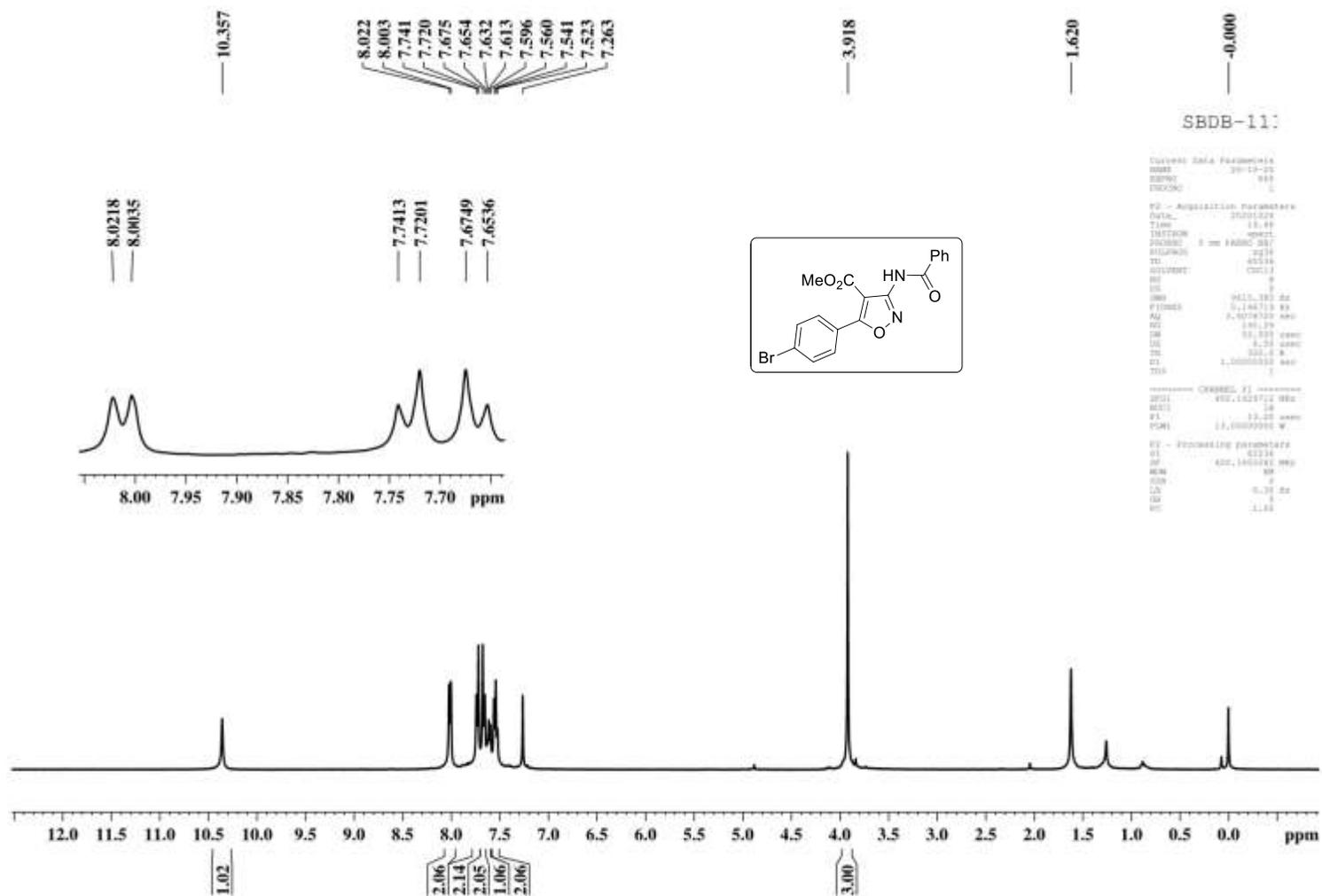


Figure S-14. <sup>1</sup>H-NMR spectrum of methyl 3-benzamido-5-(4-bromophenyl)isoxazole-4-carboxylate (**3daa**).



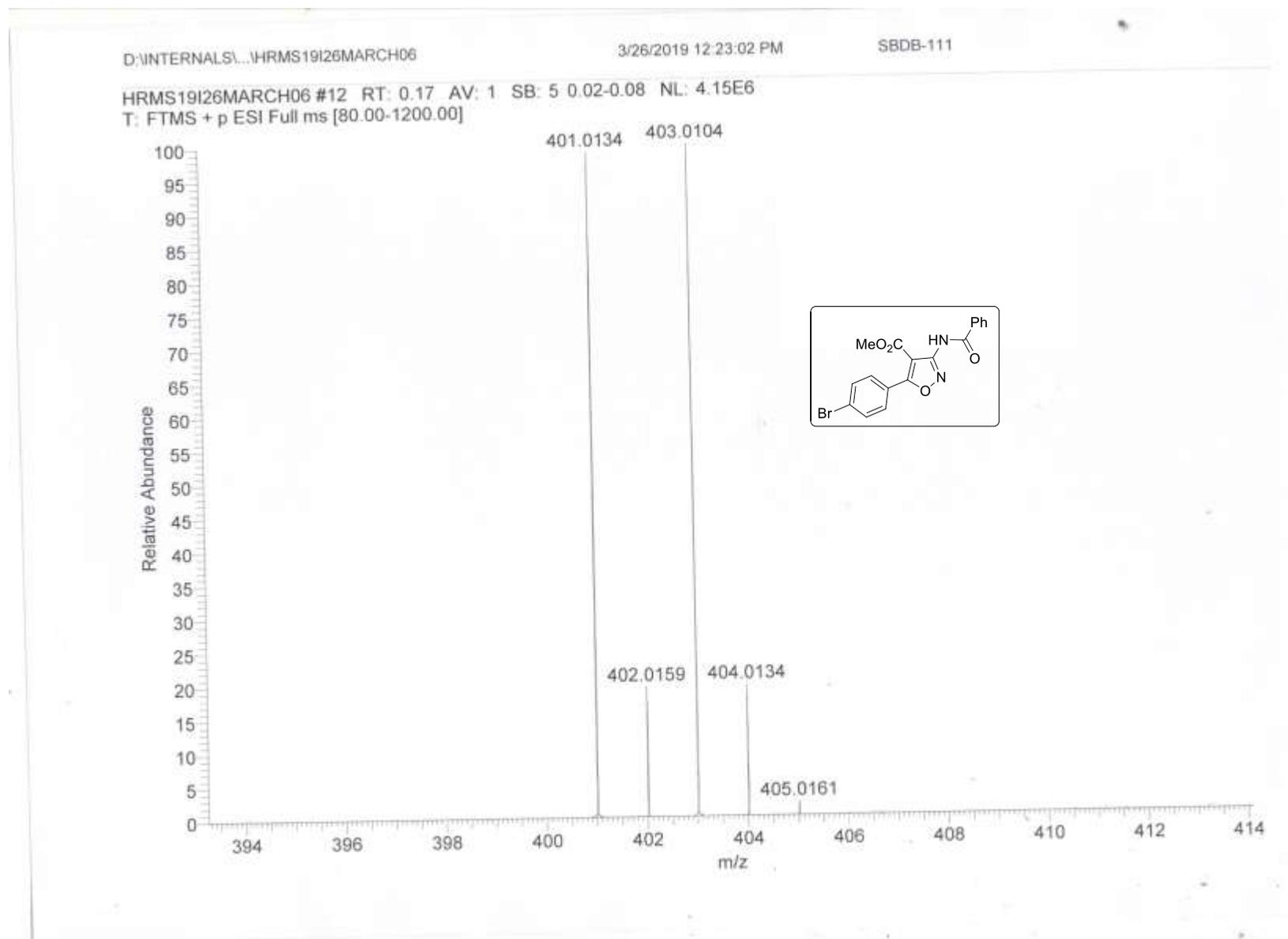


Figure S-16. HRMS spectrum of methyl 3-benzamido-5-(4-bromophenyl)isoxazole-4-carboxylate (**3daa**).

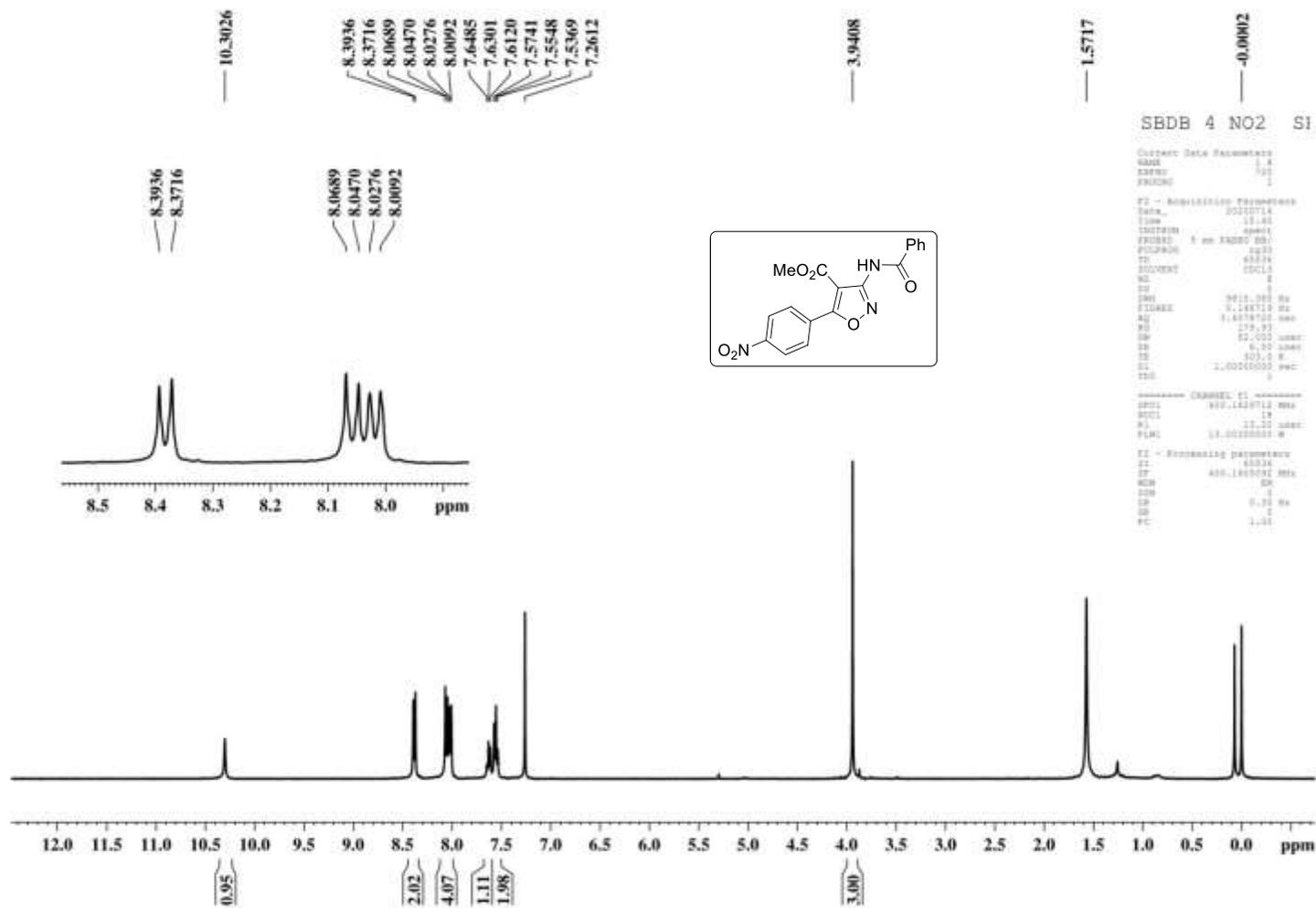


Figure S-17. <sup>1</sup>H-NMR spectrum of methyl 3-benzamido-5-(4-nitrophenyl)isoxazole-4-carboxylate (**3eaa**).

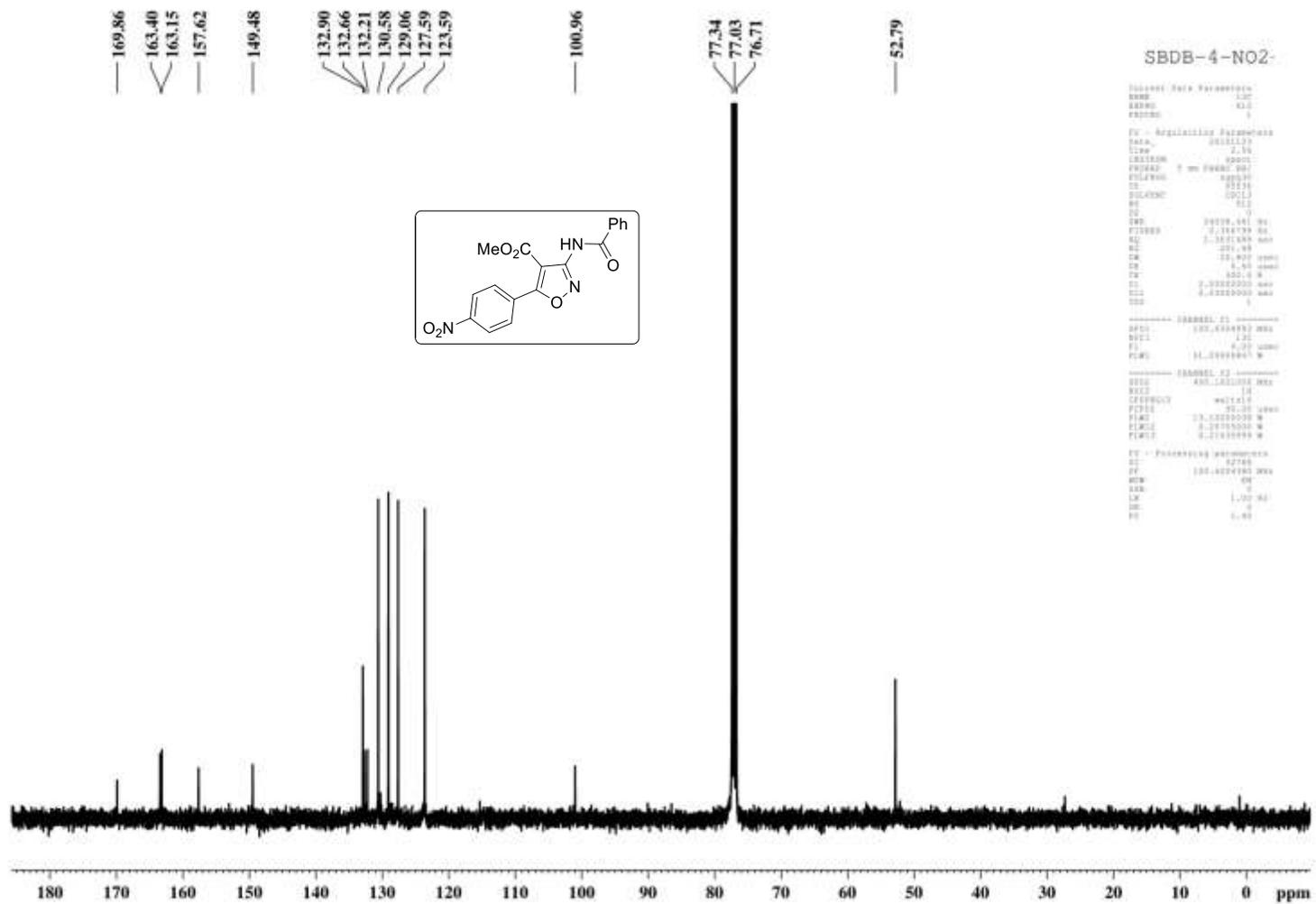


Figure S-18.  $^{13}\text{C}$ -NMR spectrum of methyl 3-benzamido-5-(4-nitrophenyl)isoxazole-4-carboxylate (**3eaa**).

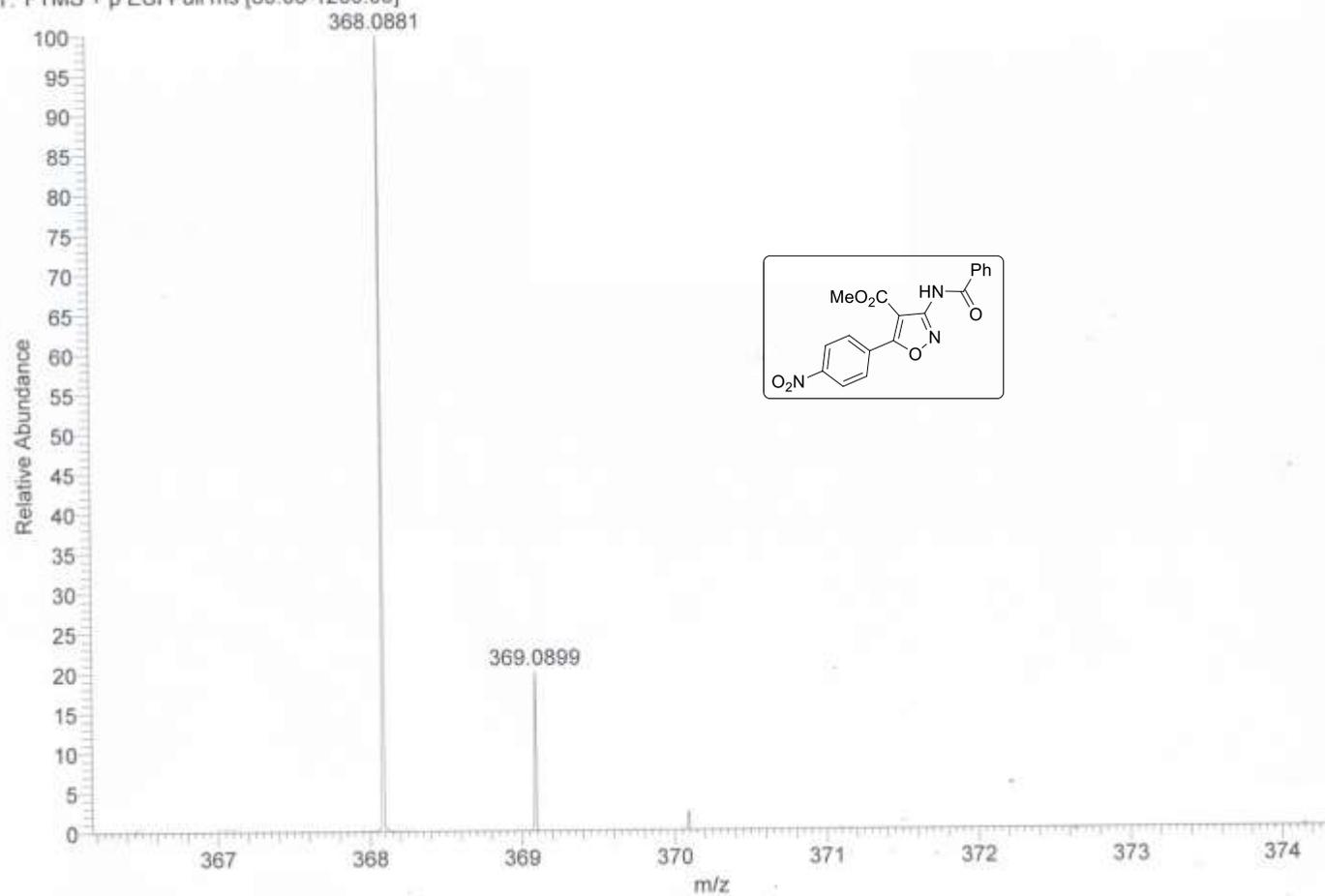
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**Figure S-19.** HRMS spectrum of methyl 3-benzamido-5-(4-nitrophenyl)isoxazole-4-carboxylate (**3eaa**).



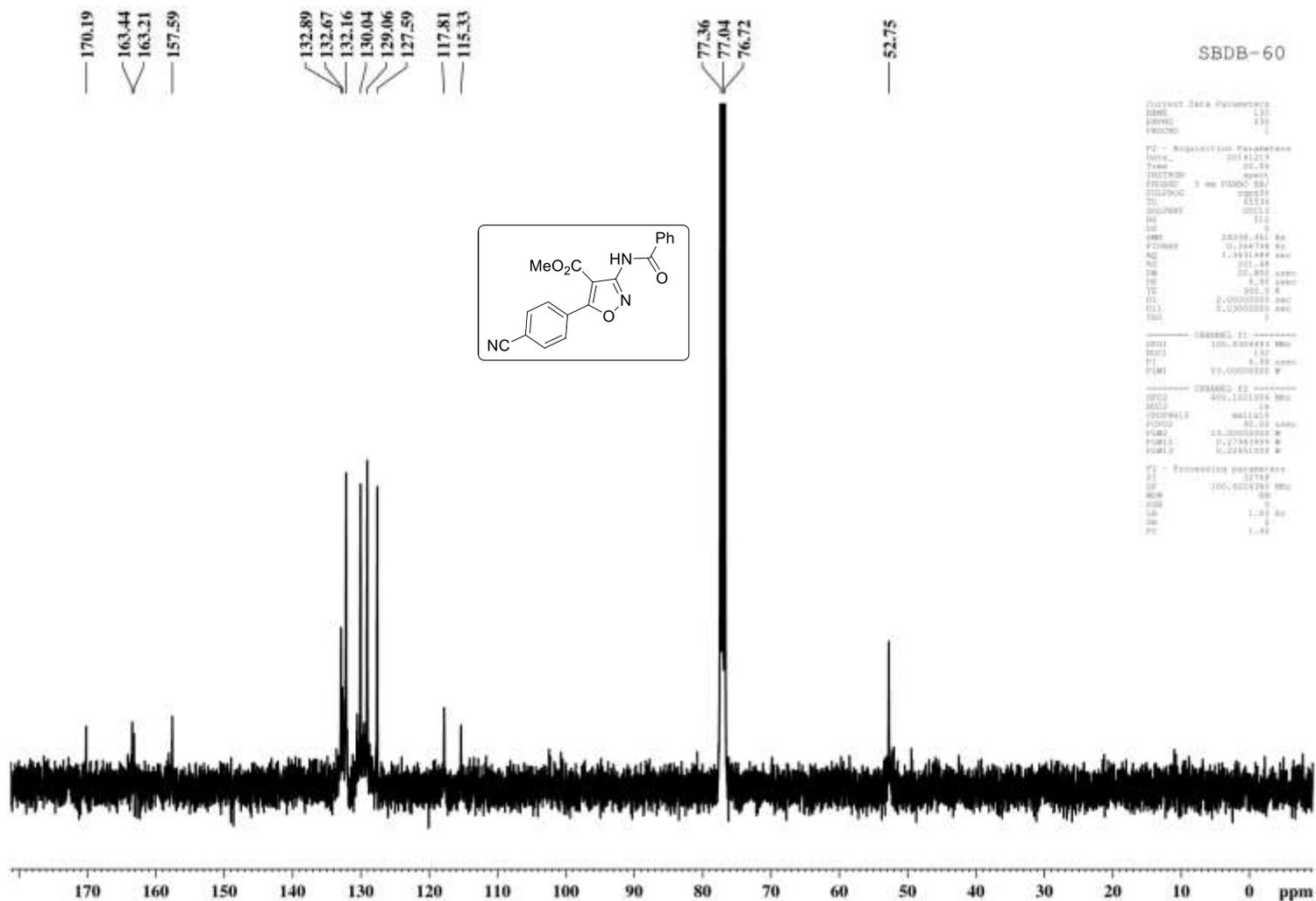


Figure S-21. <sup>13</sup>C-NMR spectrum of methyl 3-benzamido-5-(4-cyanophenyl)isoxazole-4-carboxylate (**3faa**).

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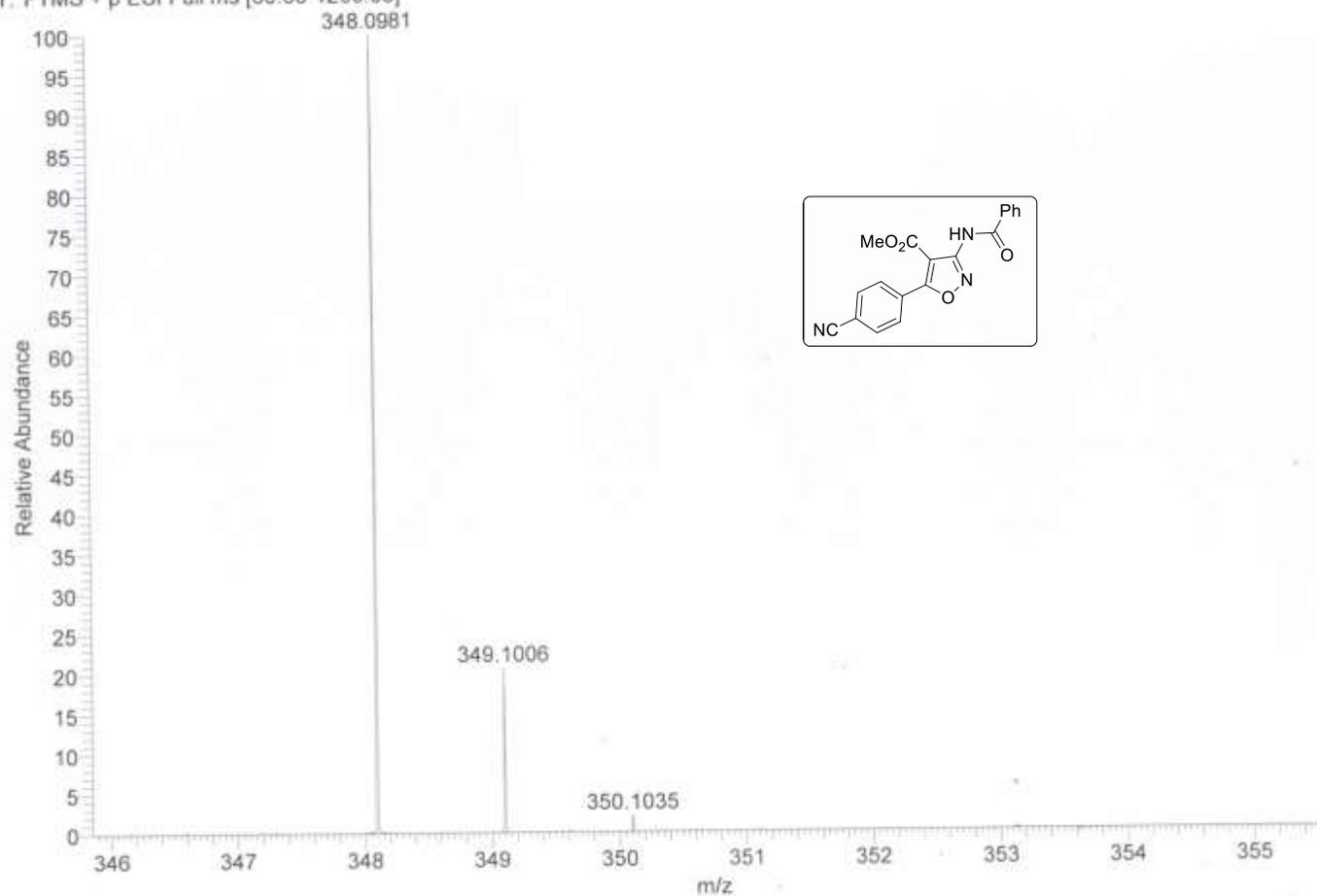


Figure S-22. HRMS spectrum of methyl 3-benzamido-5-(4-cyanophenyl)isoxazole-4-carboxylate (**3faa**).

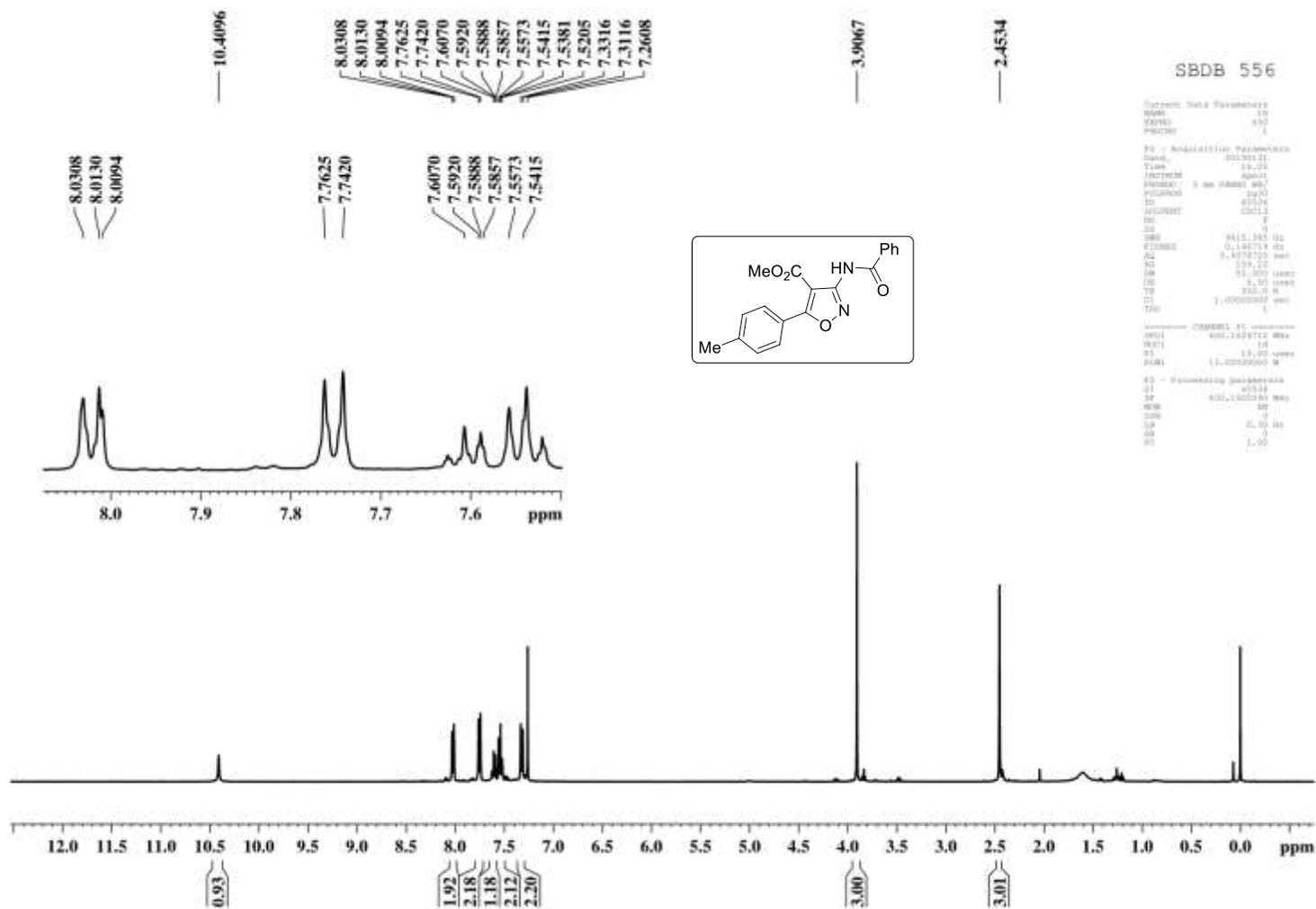


Figure S-23. <sup>1</sup>H-NMR spectrum of methyl 3-benzamido-5-p-tolylisoxazole-4-carboxylate (**3gaa**).

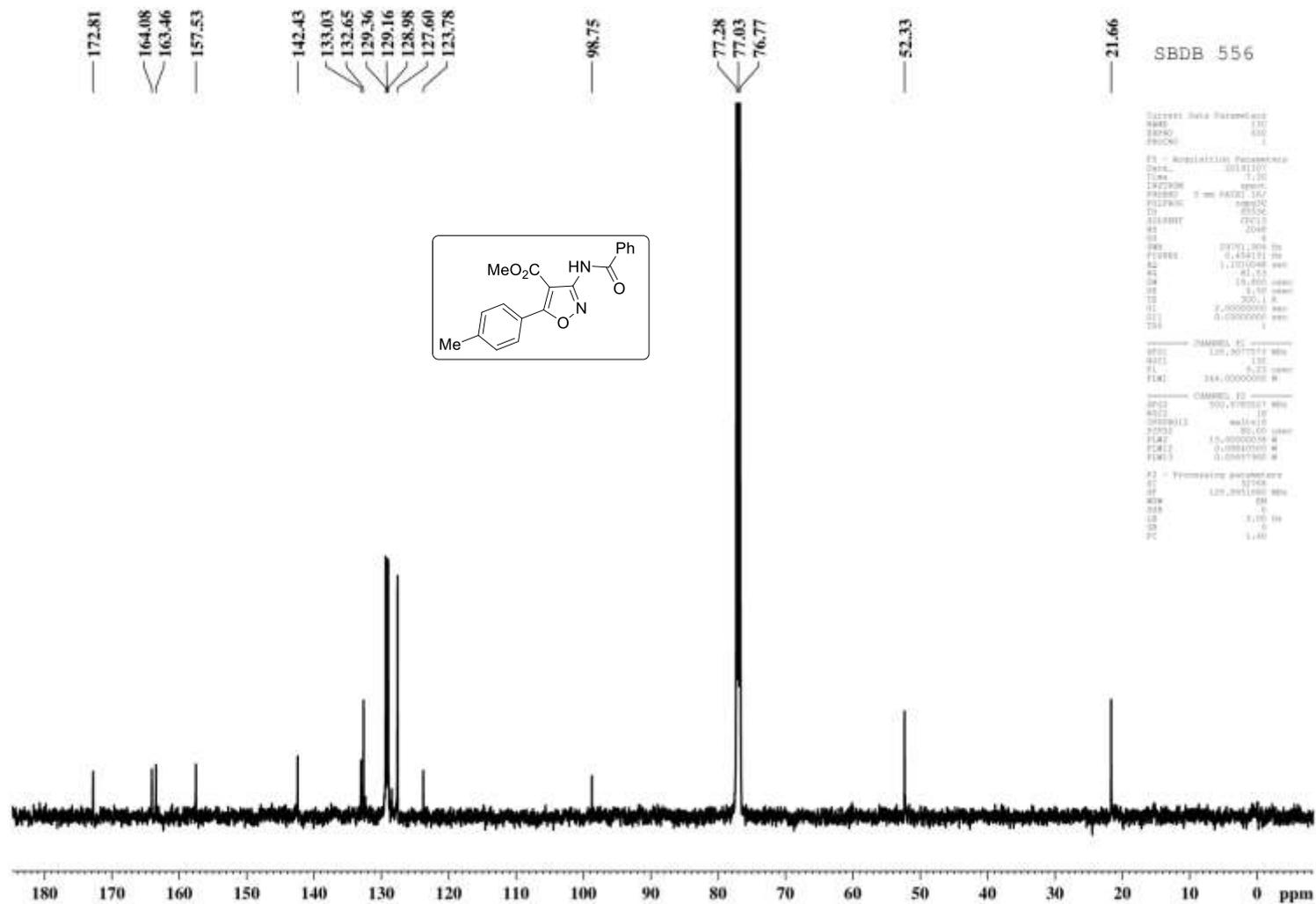


Figure S-24. <sup>13</sup>C-NMR spectrum of methyl 3-benzamido-5-p-tolylisoxazole-4-carboxylate (**3gaa**).

### SAIF [HRMS Report]

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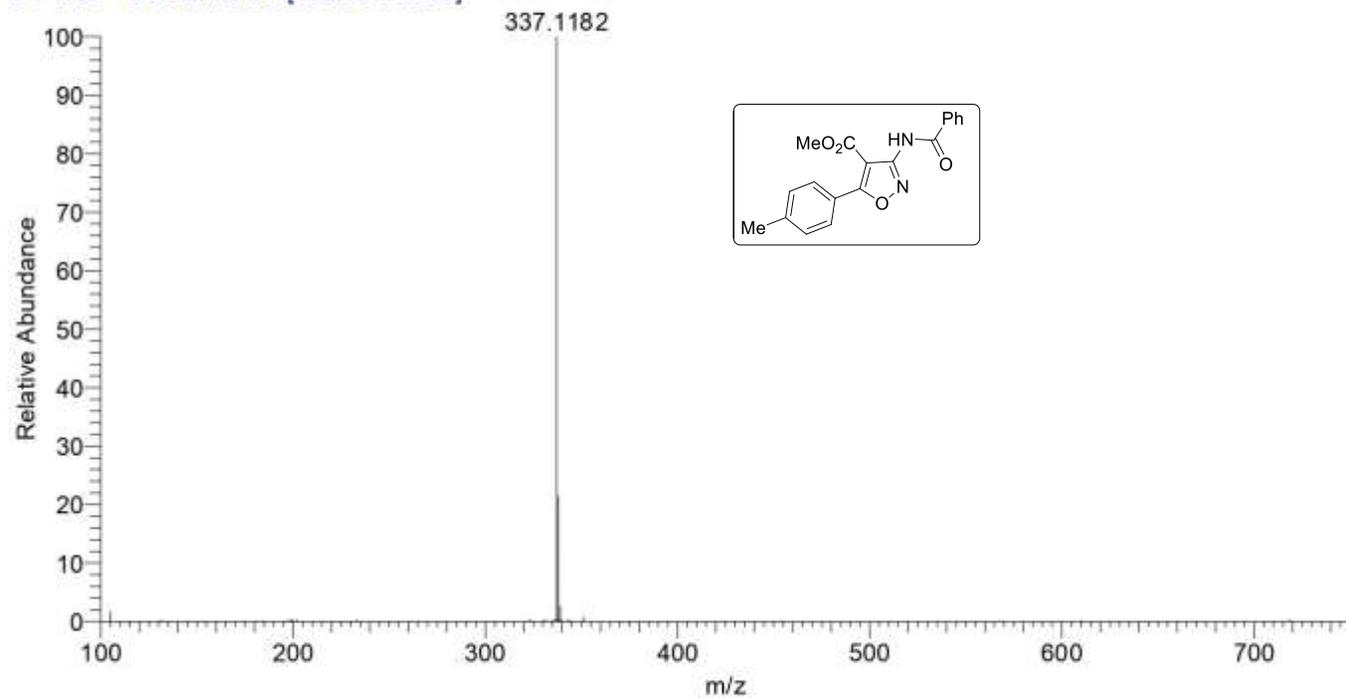


Figure S-25. HRMS spectrum of methyl 3-benzamido-5-p-tolylisoxazole-4-carboxylate (**3gaa**).

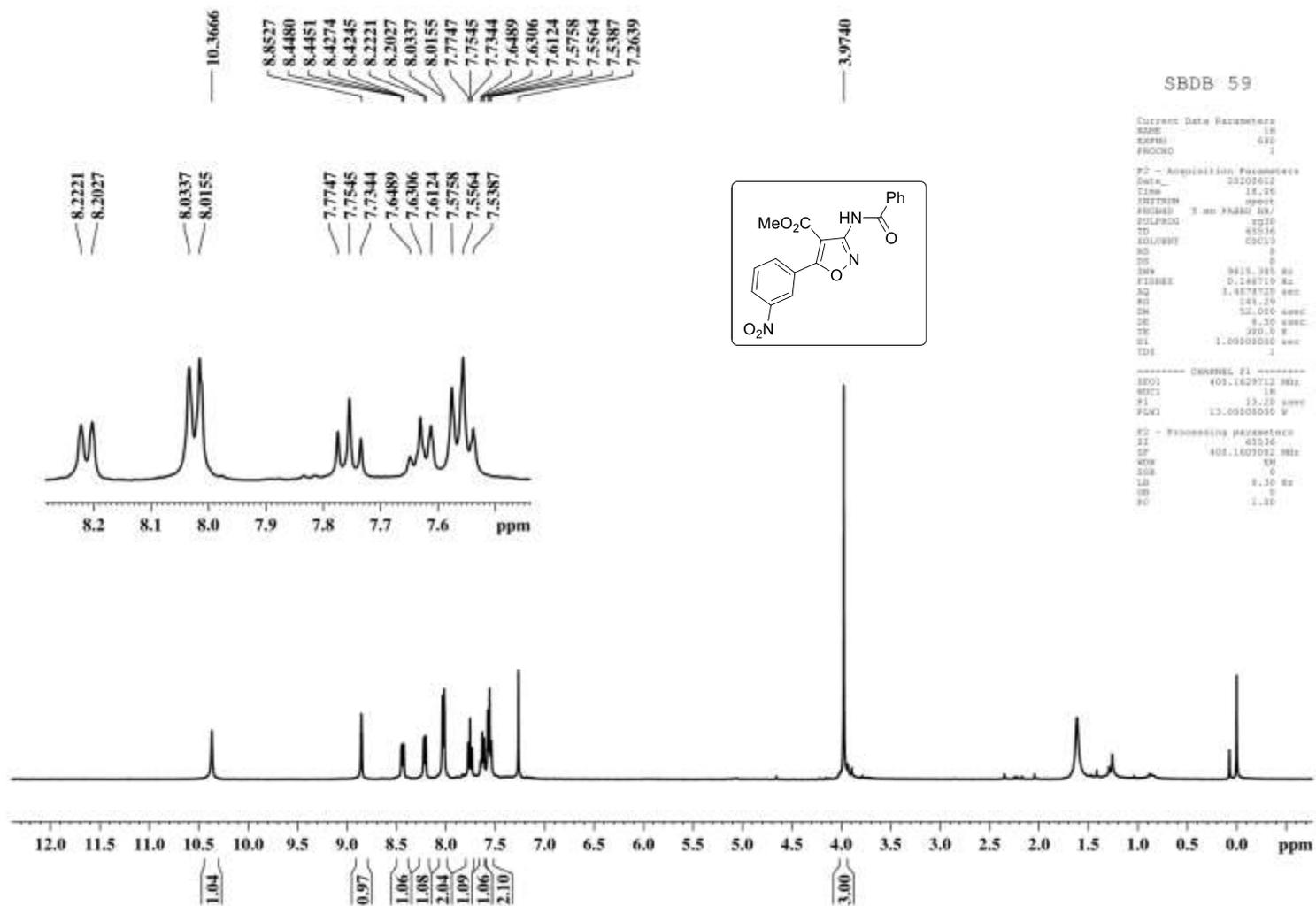


Figure S-26. <sup>1</sup>H-NMR spectrum of methyl 3-benzamido-5-(3-nitrophenyl)isoxazole-4-carboxylate (**3haa**).

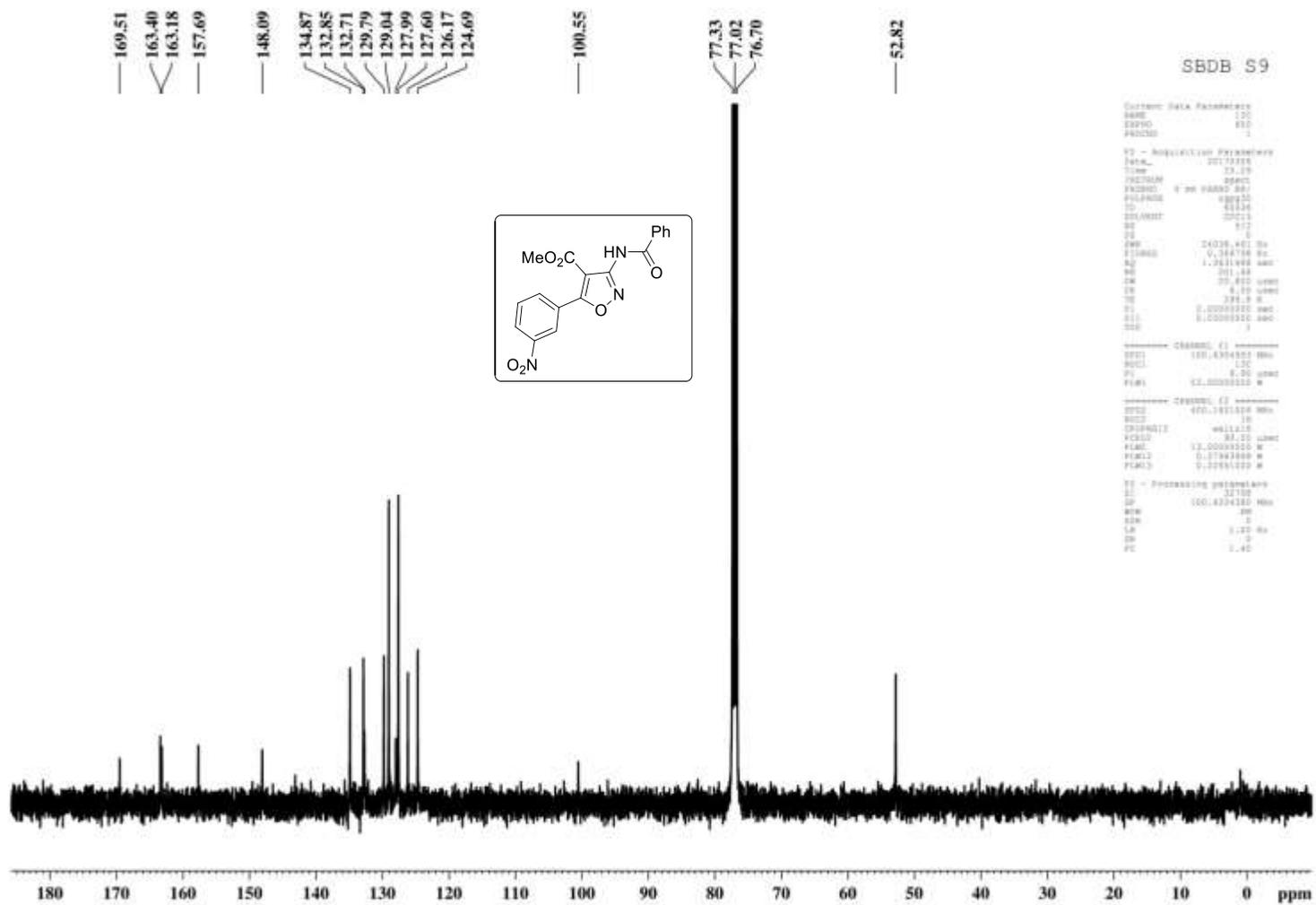


Figure S-27.  $^{13}\text{C}$ -NMR spectrum of methyl 3-benzamido-5-(3-nitrophenyl)isoxazole-4-carboxylate (**3haa**).

### SAIF [HRMS Report]

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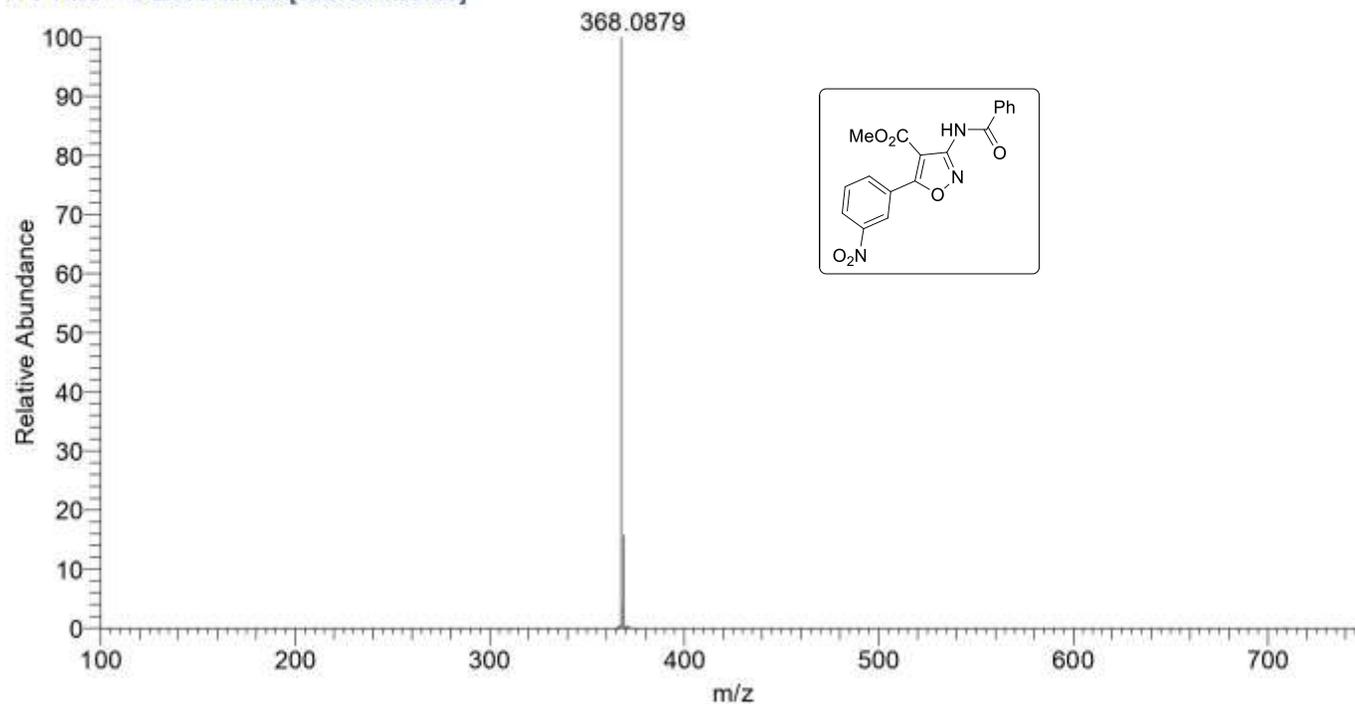


Figure S-28. HRMS spectrum of methyl 3-benzamido-5-(3-nitrophenyl)isoxazole-4-carboxylate (**3haa**).



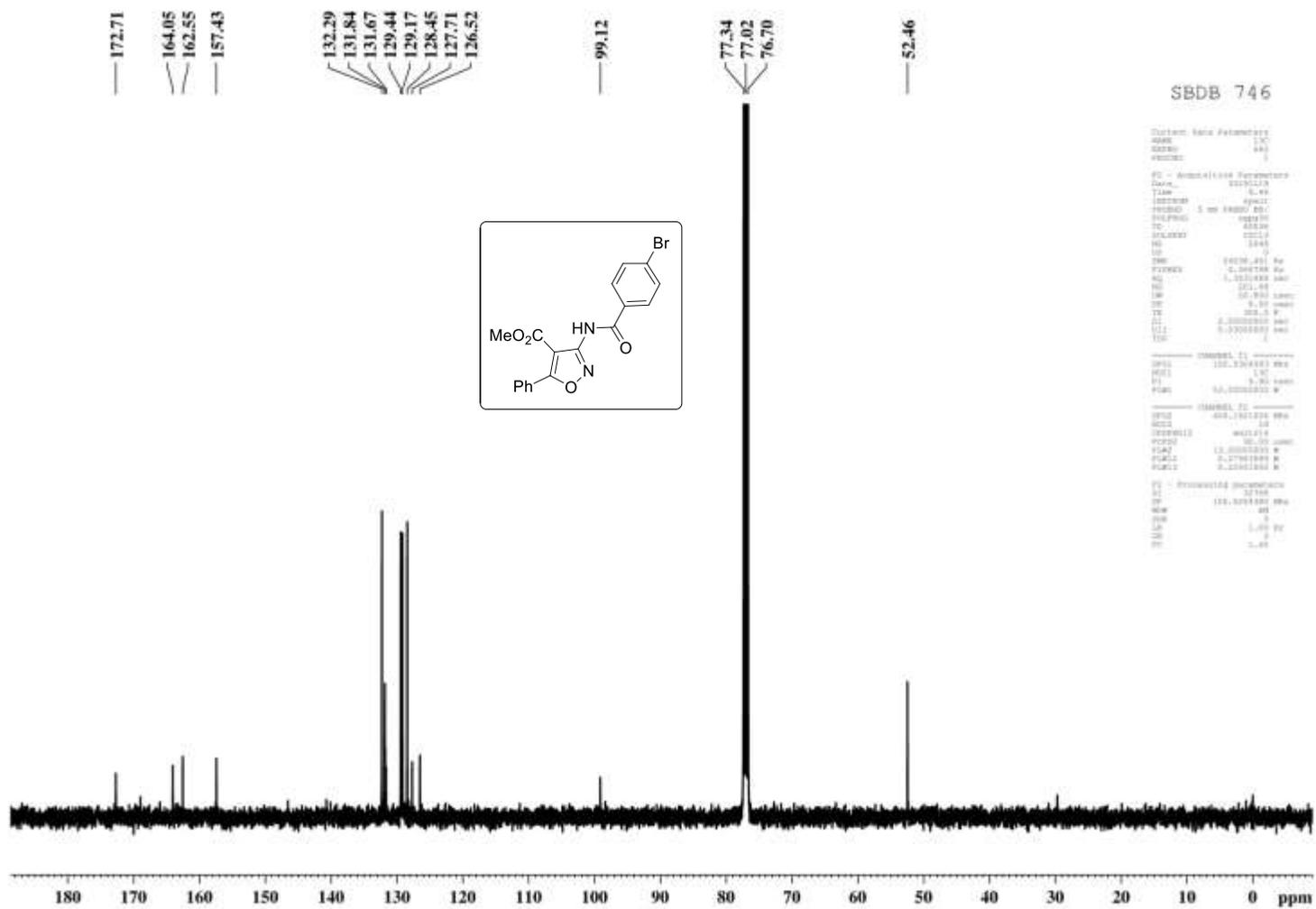


Figure S-30.  $^{13}\text{C}$ -NMR spectrum of methyl 3-(4-bromobenzamido)-5-phenylisoxazole-4-carboxylate (**3aab**).

HRMS19119NOV13 #14-29 RT: 0.12-0.24 AV: 16 SB: 6 0.03-0.07 NL: 9.87E4  
T: FTMS + p ESI Full ms [100.00-1000.00]

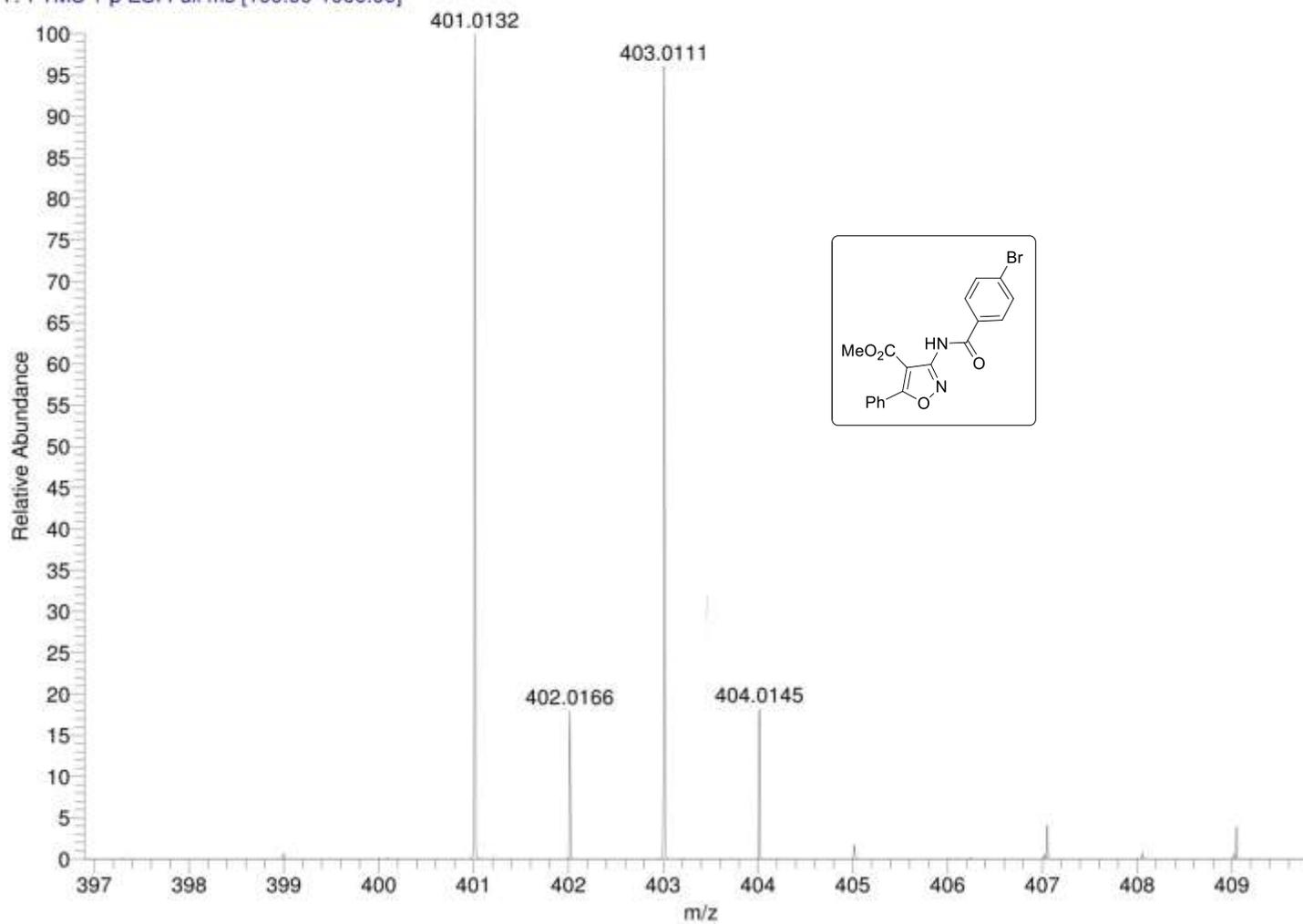


Figure S-31. HRMS spectrum of methyl 3-(4-bromobenzamido)-5-phenylisoxazole-4-carboxylate (**3aab**).

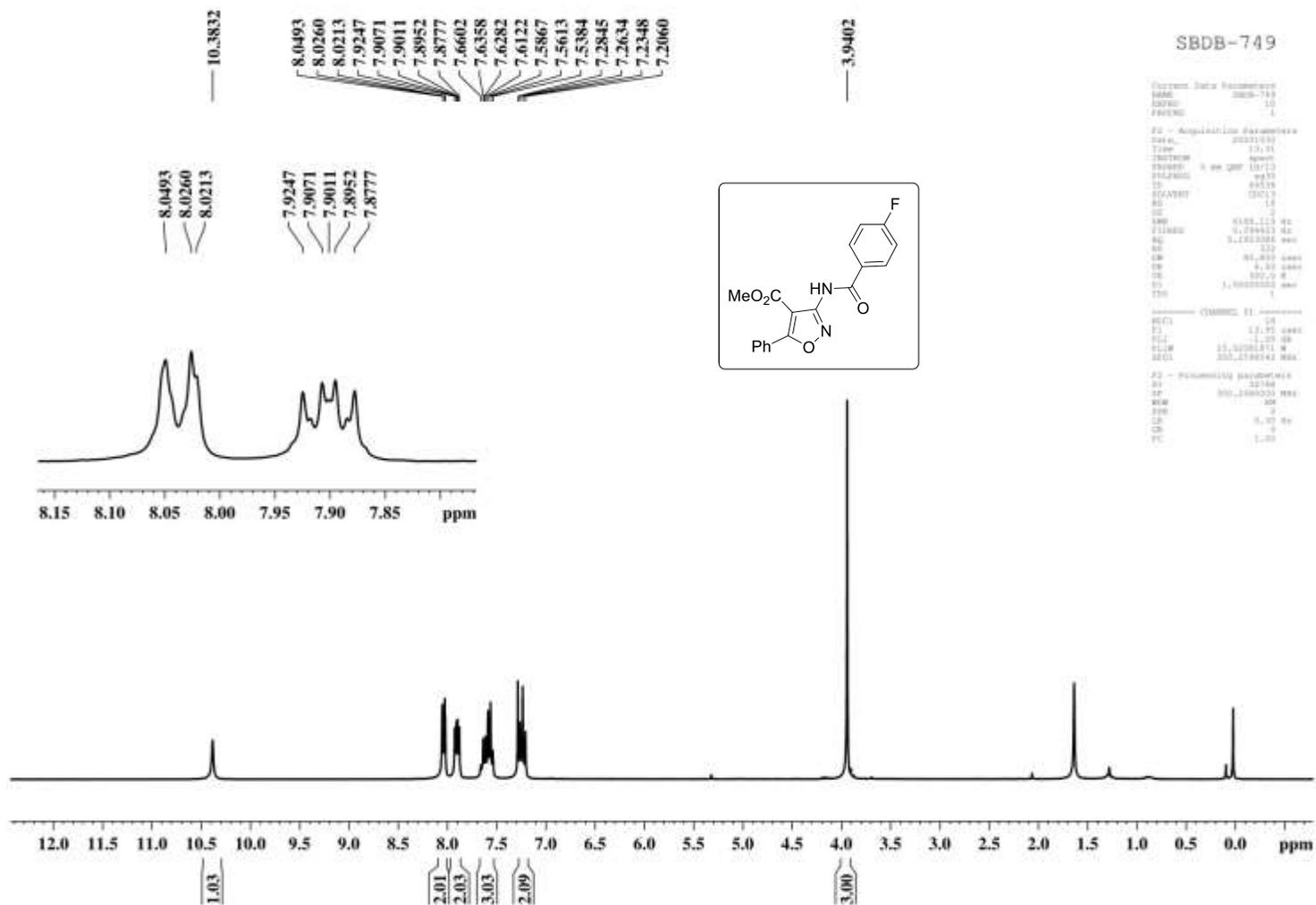
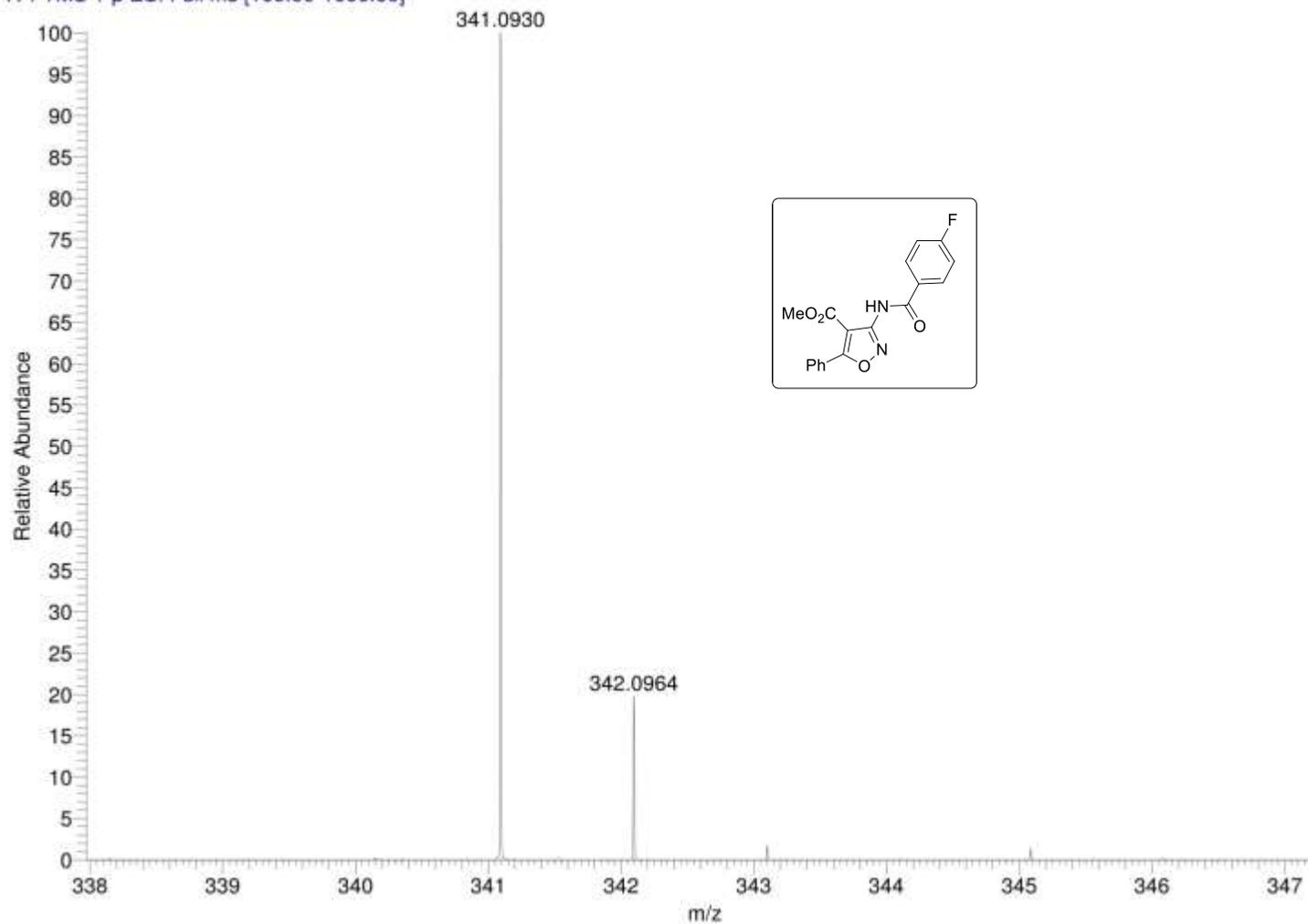


Figure S-32. <sup>1</sup>H-NMR spectrum of methyl 3-(4-fluorobenzamido)-5-phenylisoxazole-4-carboxylate (**3aad**).



HRMS19\19NOV14 #14-28 RT: 0.12-0.24 AV: 15 SB: 6 0.03-0.07 NL: 1.07E5

T: FTMS + p ESI Full ms [100.00-1000.00]



**Figure S-34.** HRMS spectrum of methyl 3-(4-fluorobenzamido)-5-phenylisoxazole-4-carboxylate (**3aad**).



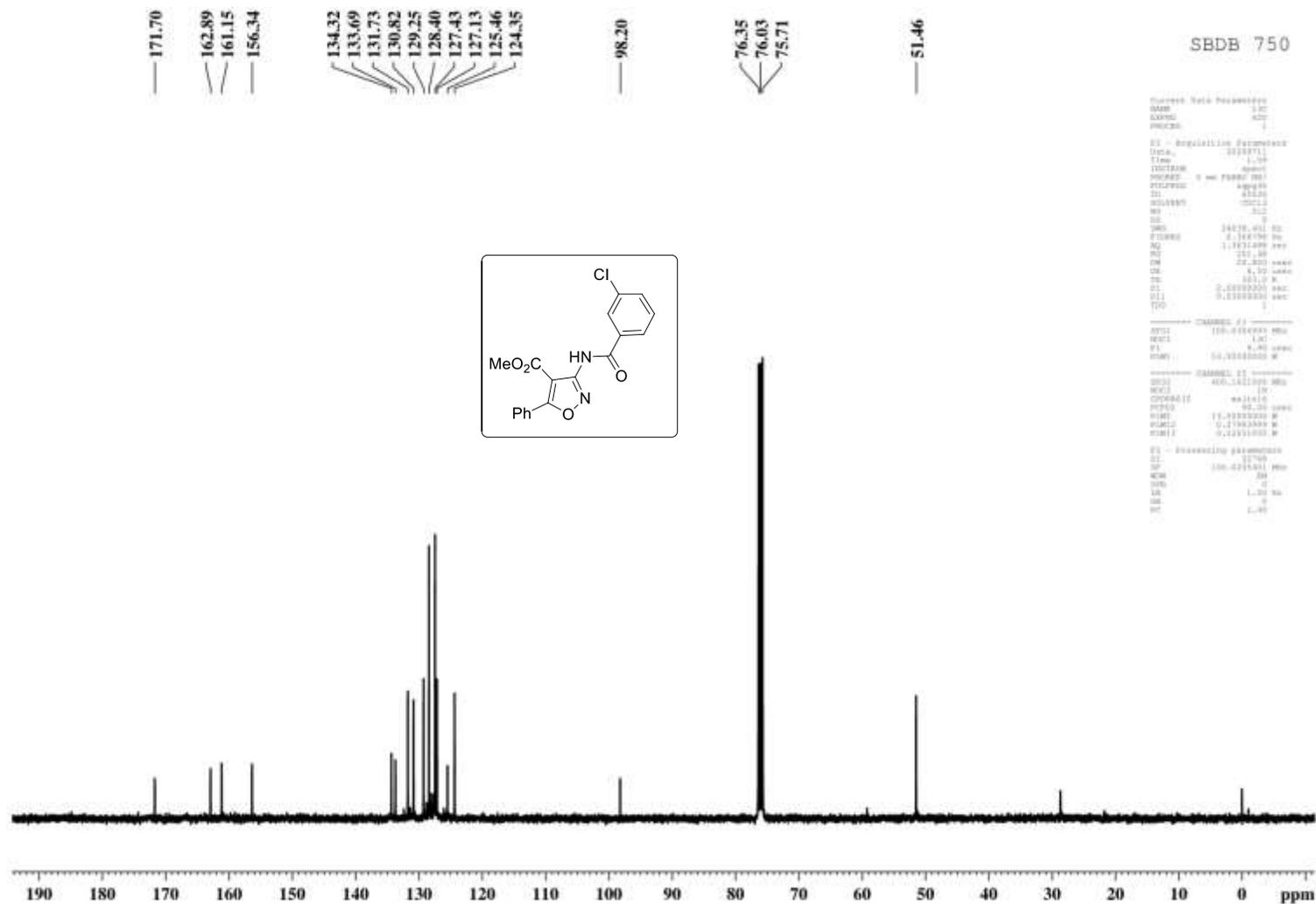
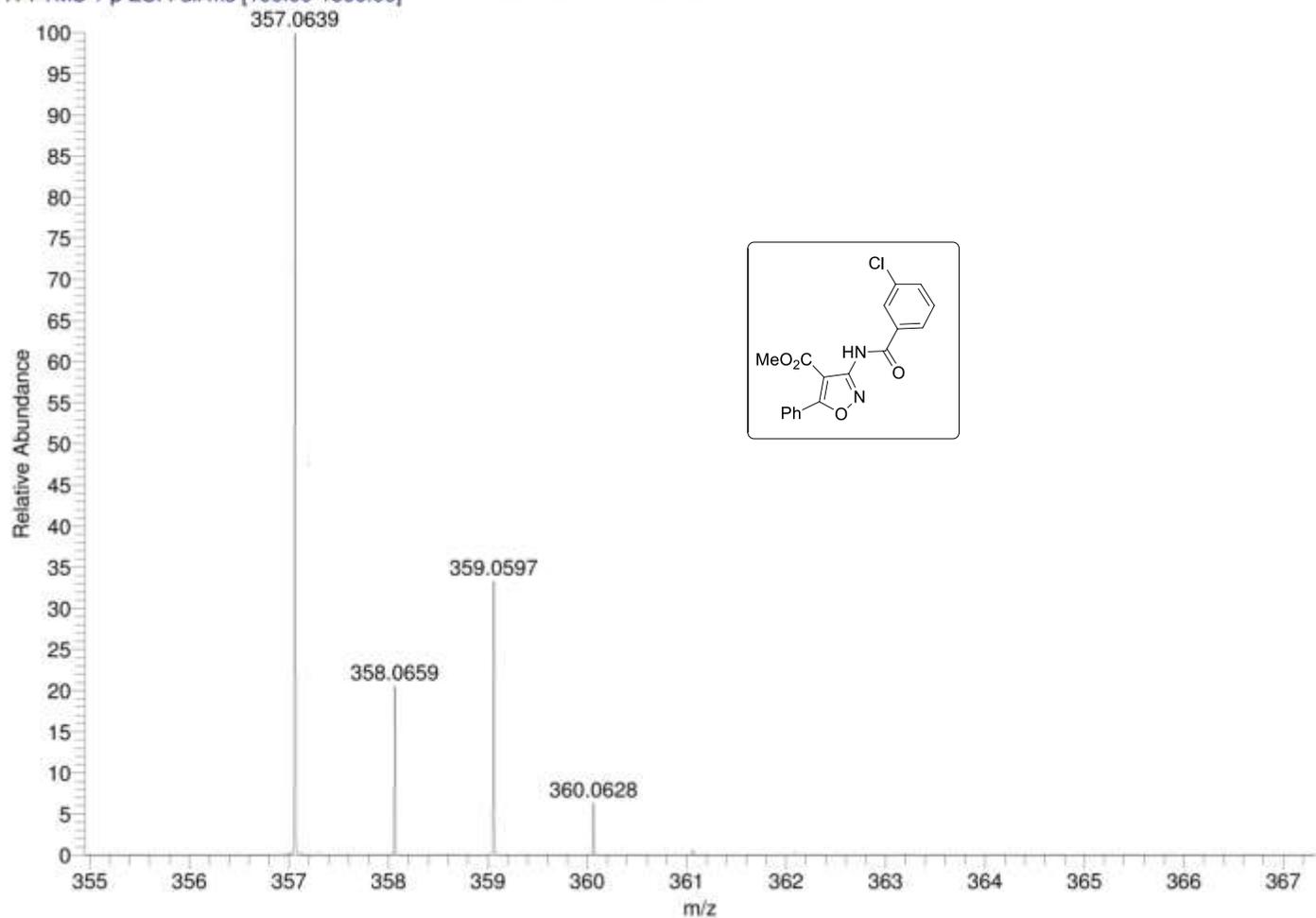


Figure S-36. <sup>13</sup>C-NMR spectrum of methyl 3-(3-chlorobenzamido)-5-phenylisoxazole-4-carboxylate (**3aaf**).

HRMS19I17MAY12 #18 RT: 0.25 AV: 1 SB: 4 0.03-0.08 NL: 7.95E6

T: FTMS + p ESI Full ms [100.00-1500.00]



**Figure S-37.** HRMS spectrum of methyl 3-(3-chlorobenzamido)-5-phenylisoxazole-4-carboxylate (**3aaf**).

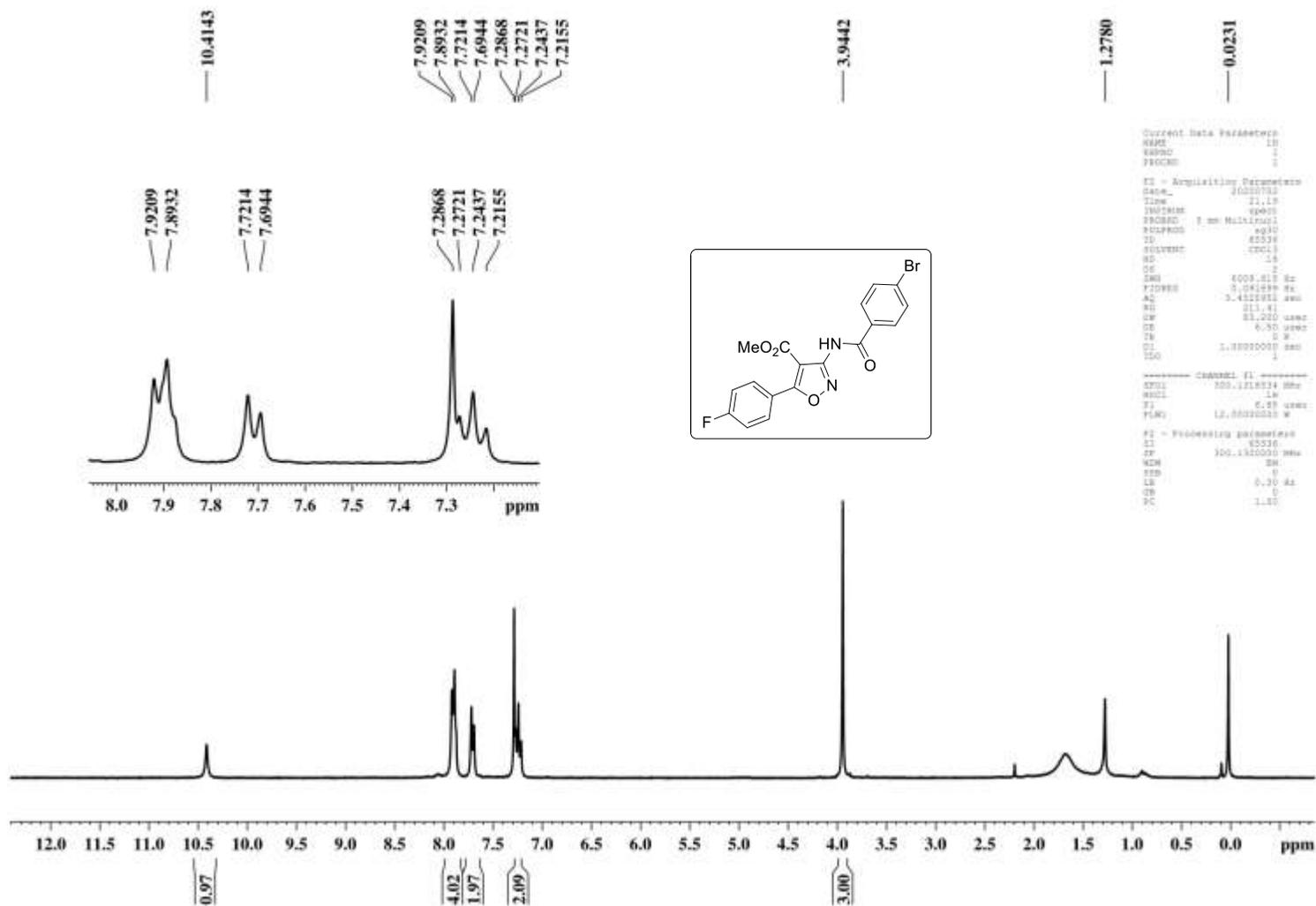


Figure S-38. <sup>1</sup>H-NMR spectrum of Methyl 3-(4-bromobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (**3bab**).

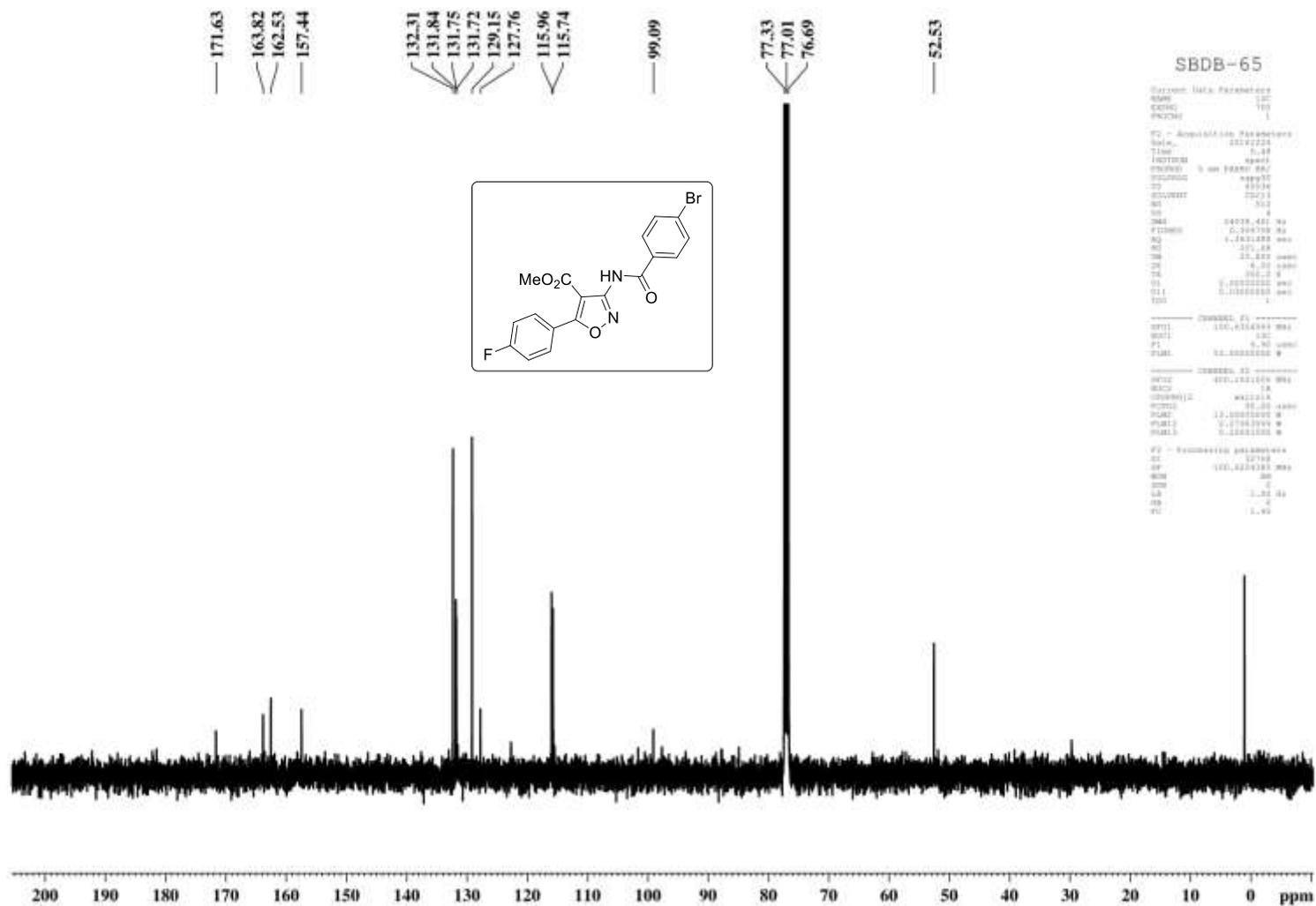
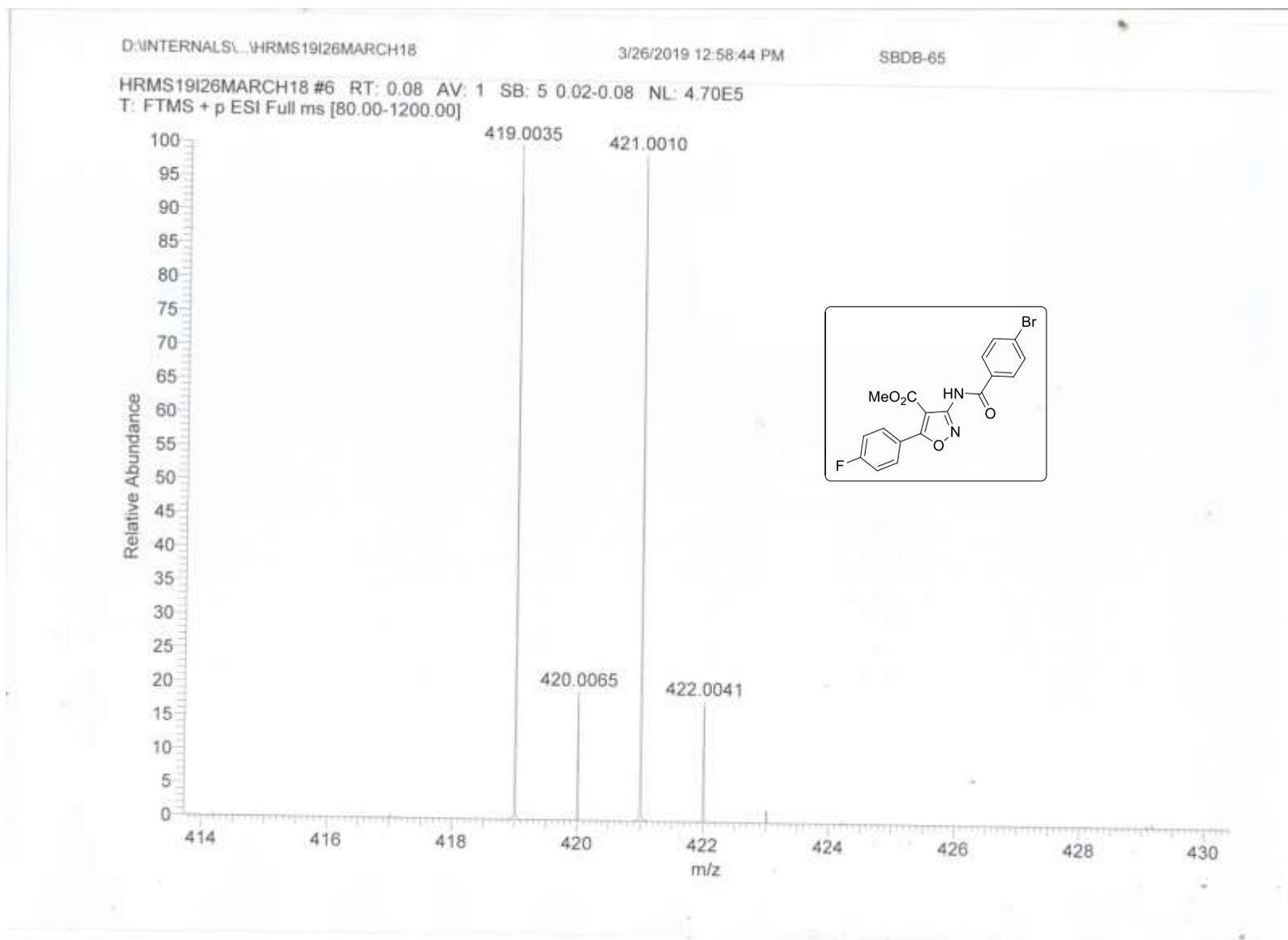
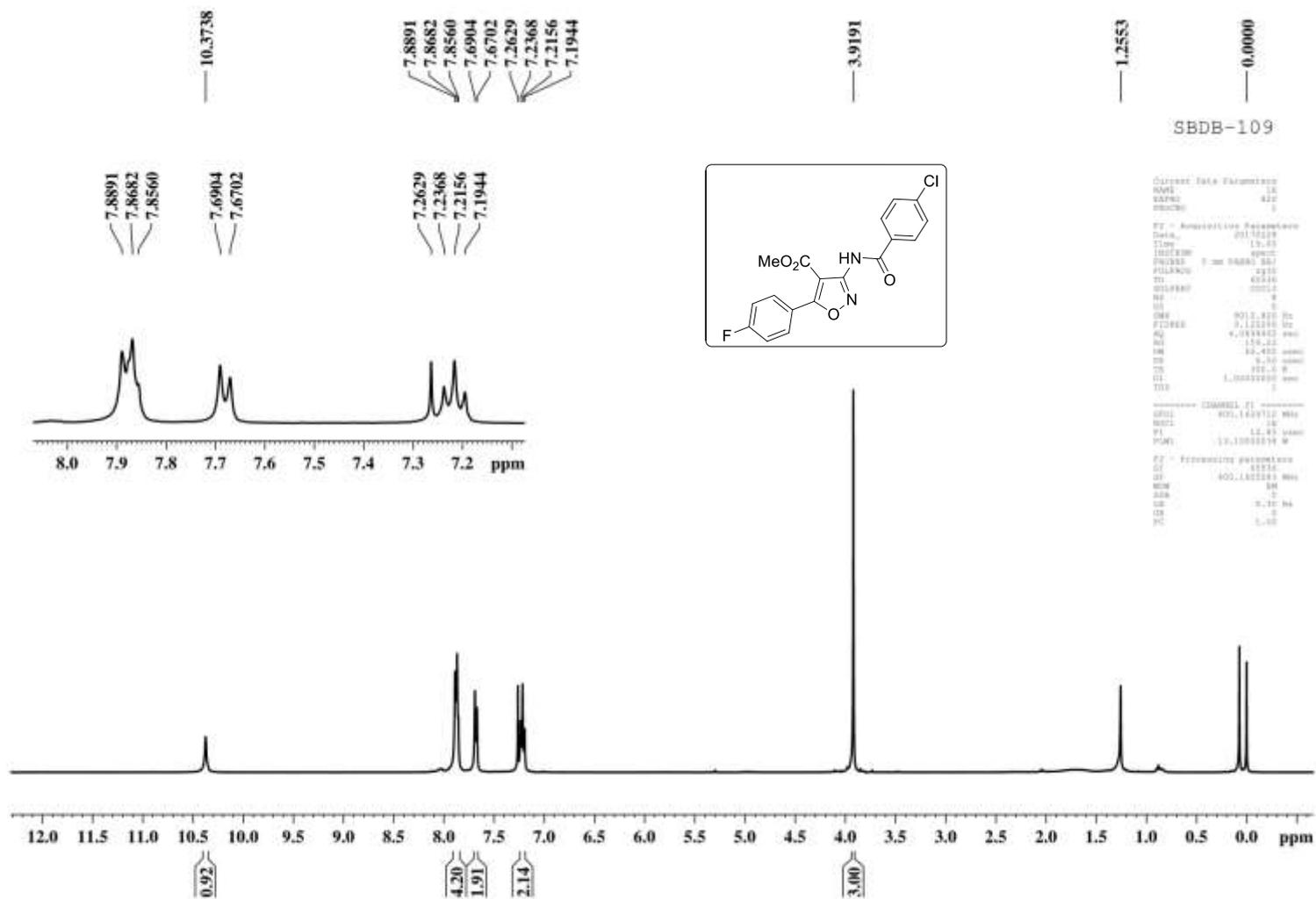


Figure S-39.  $^{13}\text{C}$ -NMR spectrum of methyl 3-(4-bromobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (**3bab**).



**Figure S-40.** HRMS spectrum of methyl 3-(4-bromobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (**3bab**).



**Figure S-41.**  $^1\text{H-NMR}$  spectrum of methyl 3-(4-chlorobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (**3bac**).

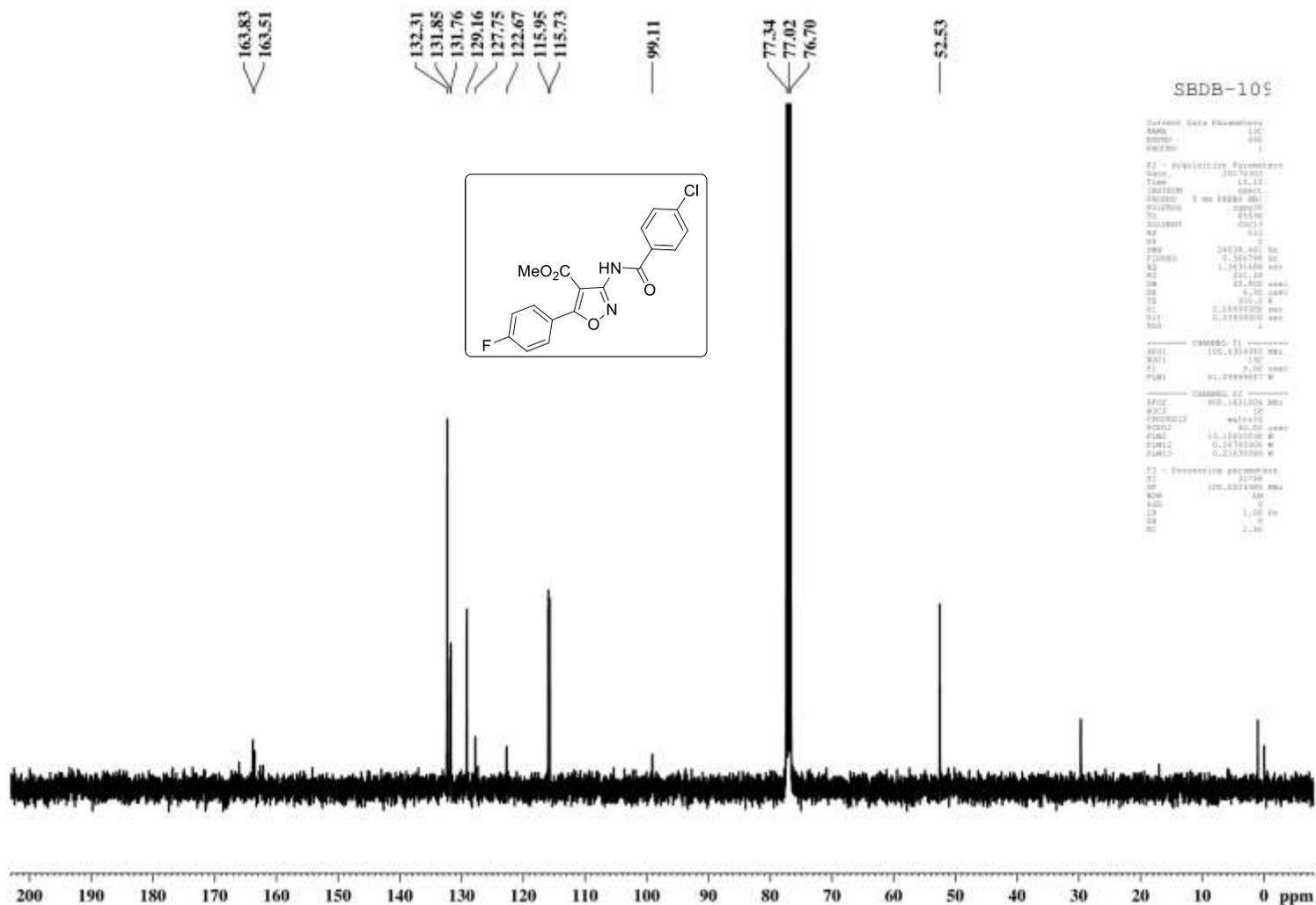


Figure S-42. <sup>13</sup>C-NMR spectrum of methyl 3-(4-chlorobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (**3bac**).

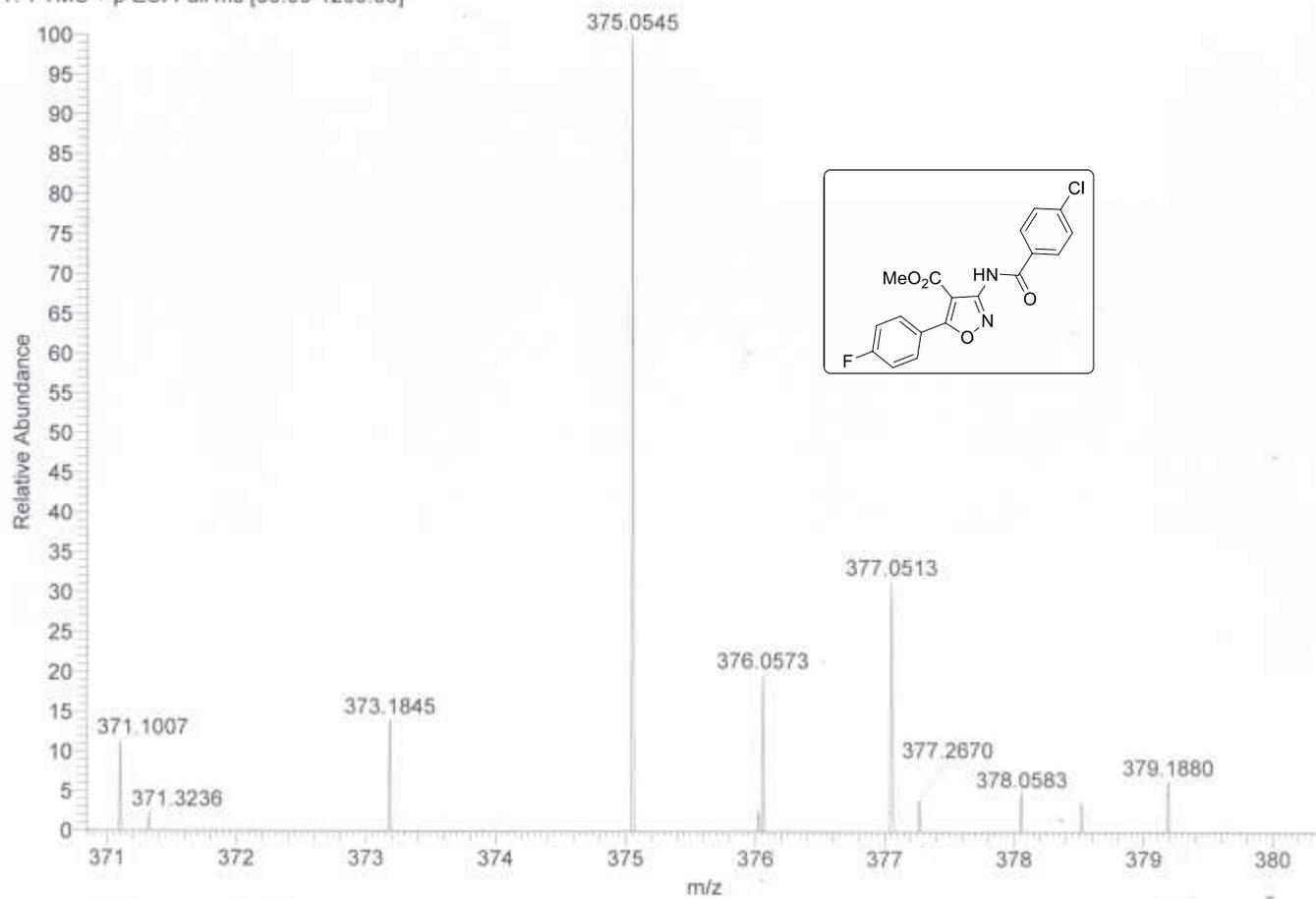
D:\INTERNALS\HRMS19I26MARCH19

3/26/2019 1:01:39 PM

SBDB-109

HRMS19I26MARCH19 #7 RT: 0.10 AV: 1 SB: 5 0.02-0.08 NL: 2.57E4

T: FTMS + p ESI Full ms [80.00-1200.00]



**Figure S-43.** HRMS spectrum of methyl 3-(4-chlorobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (**3bac**).

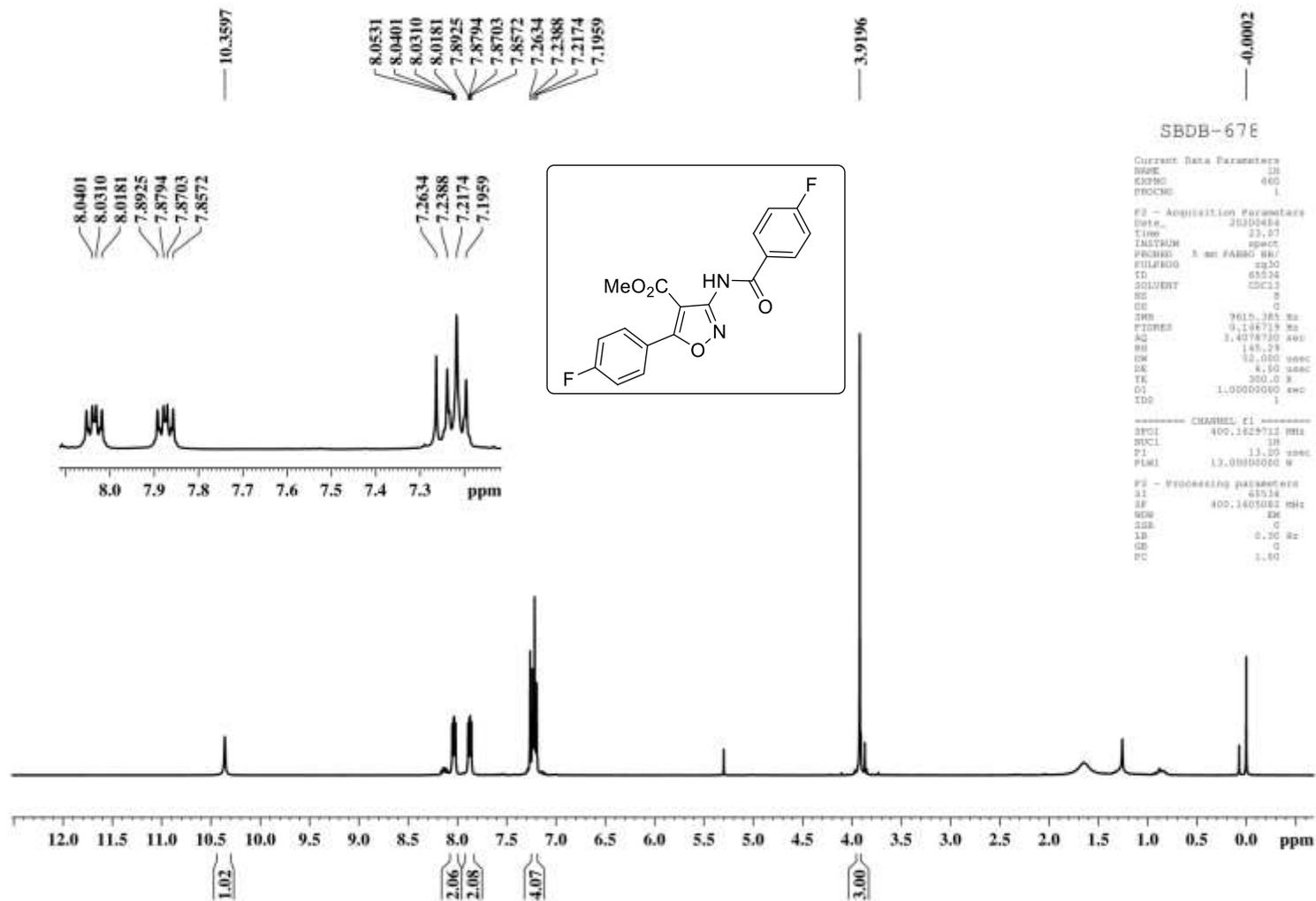
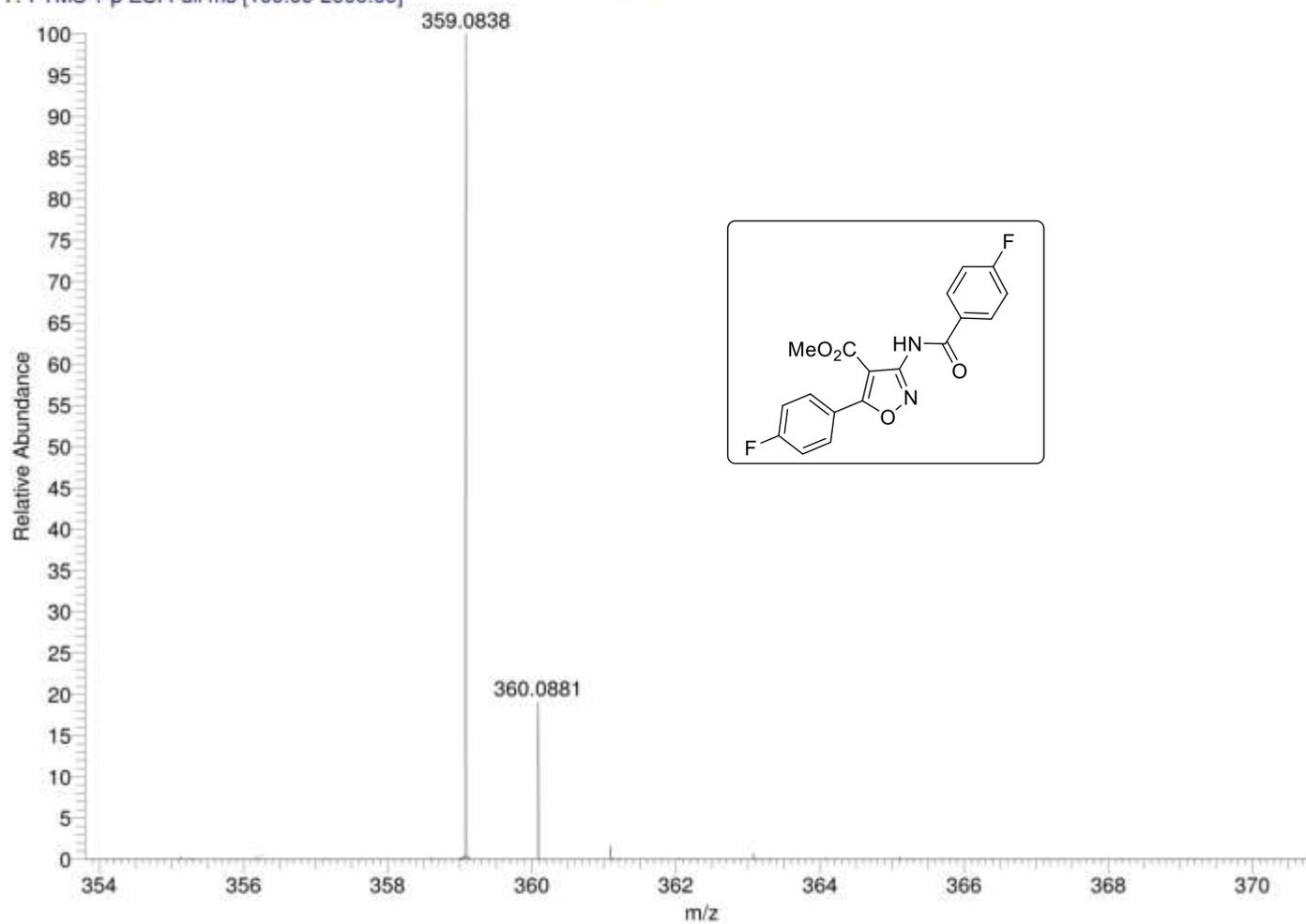


Figure S-44. <sup>1</sup>H-NMR spectrum of methyl 3-(4-fluorobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (**3bad**).



HRMS19I22AUG07 #10 RT: 0.15 AV: 1 SB: 5 0.02-0.08 NL: 9.27E5

T: FTMS + p ESI Full ms [100.00-2000.00]



**Figure S-46.** HRMS spectrum of methyl 3-(4-fluorobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (**3bad**).

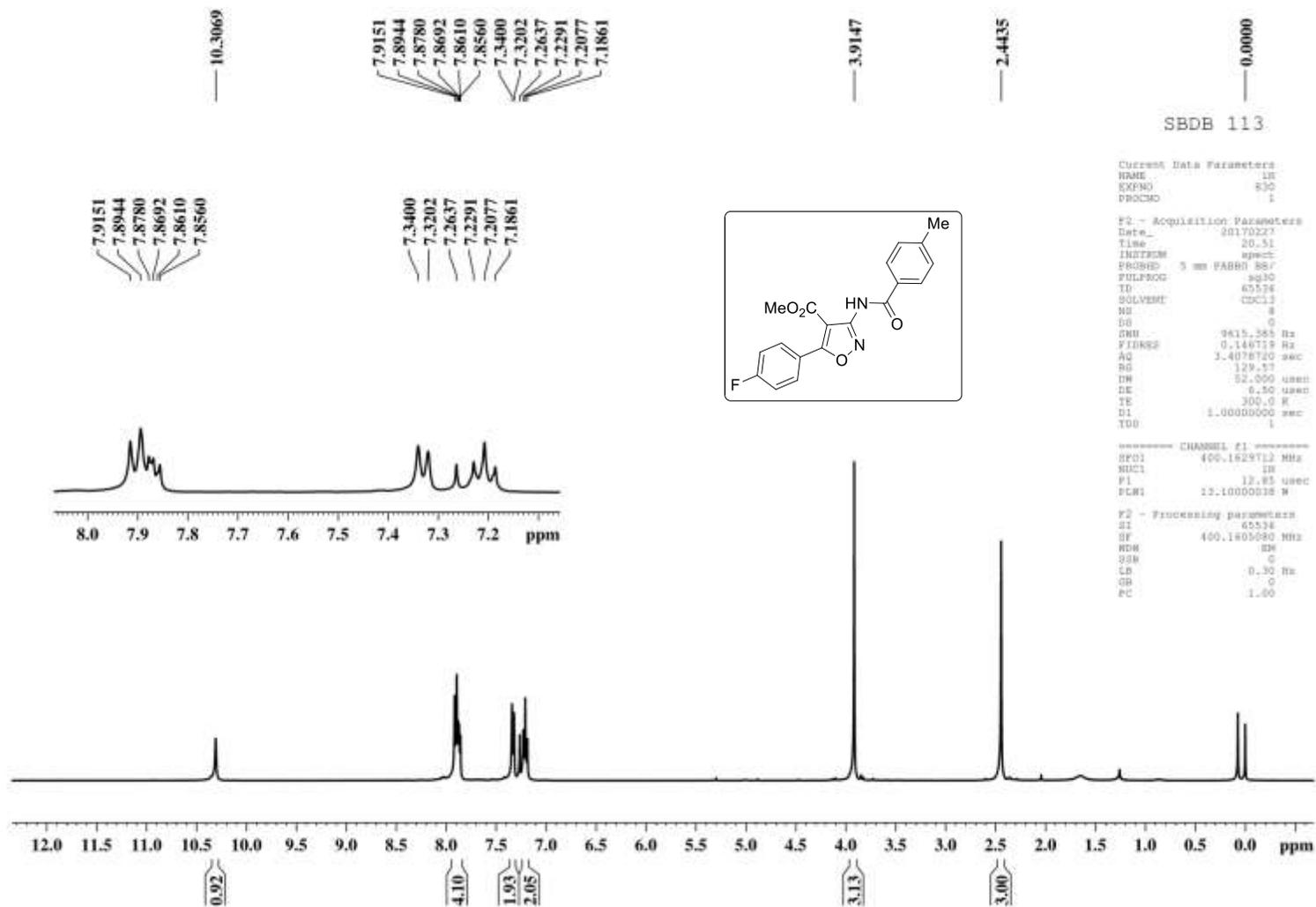


Figure S-47. <sup>1</sup>H-NMR spectrum of methyl 5-(4-fluorophenyl)-3-(4-methylbenzamido)isoxazole-4-carboxylate (**3bae**).

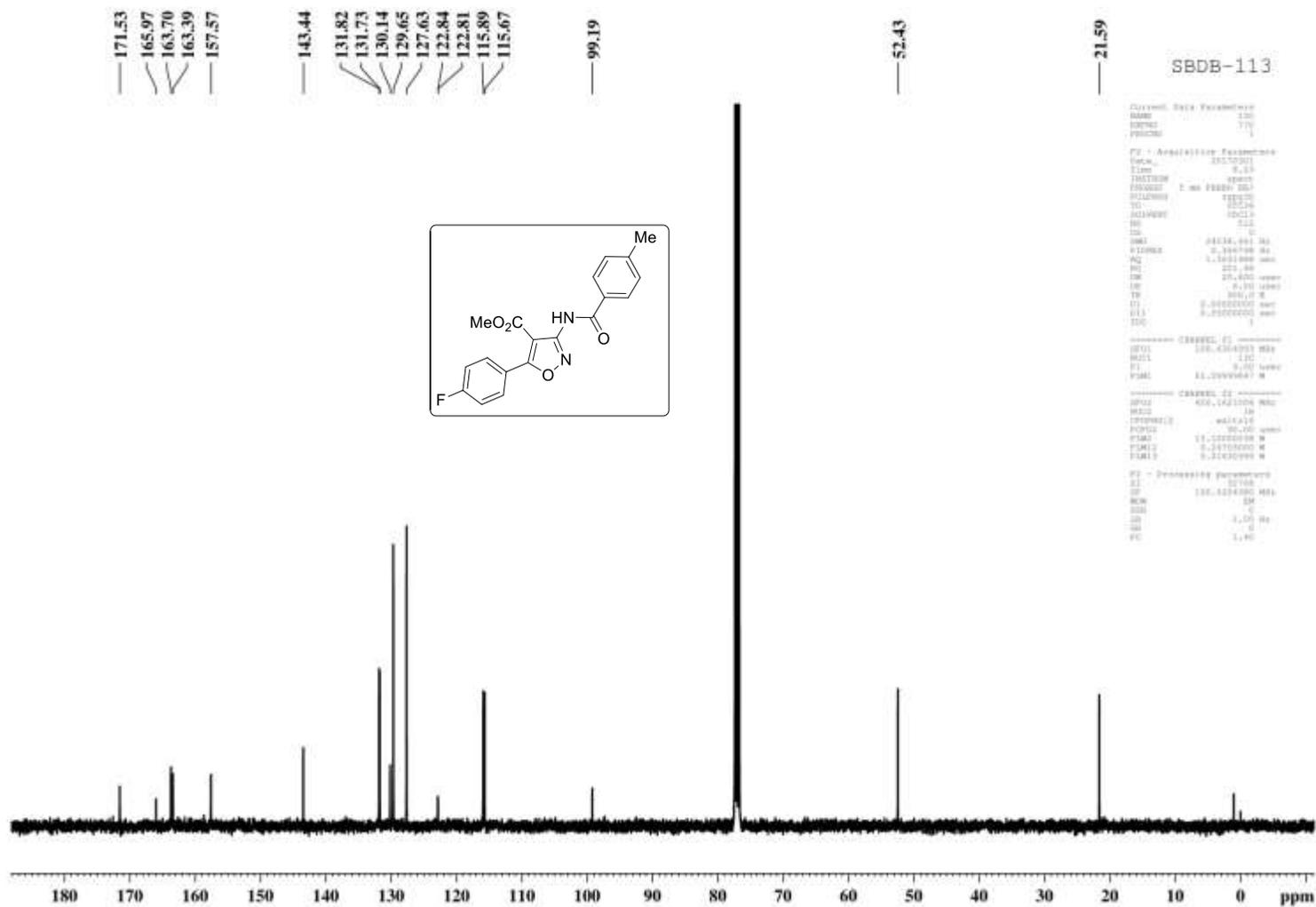
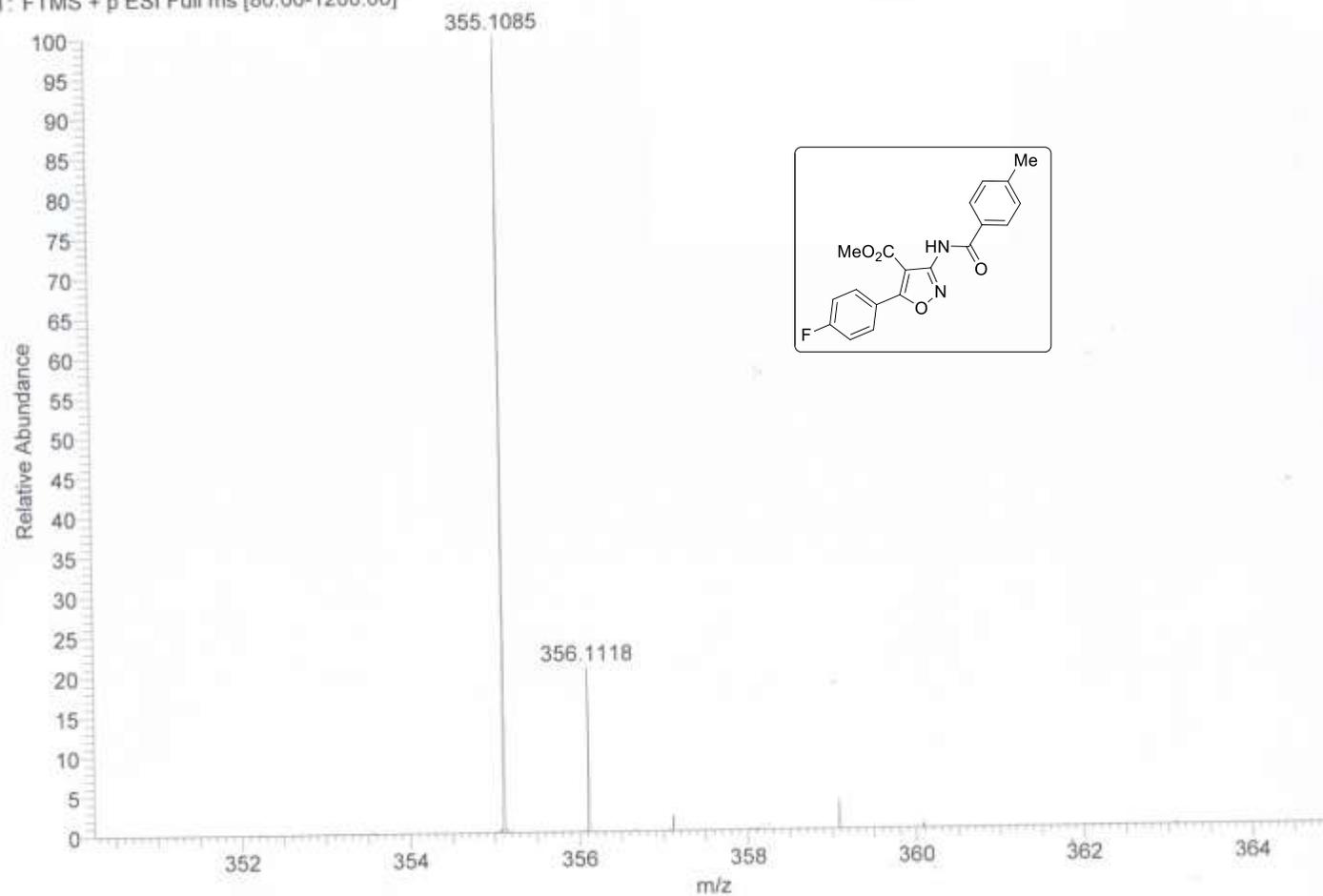


Figure S-48. <sup>13</sup>C-NMR spectrum of methyl 5-(4-fluorophenyl)-3-(4-methylbenzamido)isoxazole-4-carboxylate (**3bae**).

HRMS19I26MARCH20 #6 RT: 0.08 AV: 1 SB: 5 0.02-0.08 NL: 9.75E5  
T: FTMS + p ESI Full ms [80.00-1200.00]



**Figure S-49.** HRMS spectrum of methyl 5-(4-fluorophenyl)-3-(4-methylbenzamido)isoxazole-4-carboxylate (**3bae**).

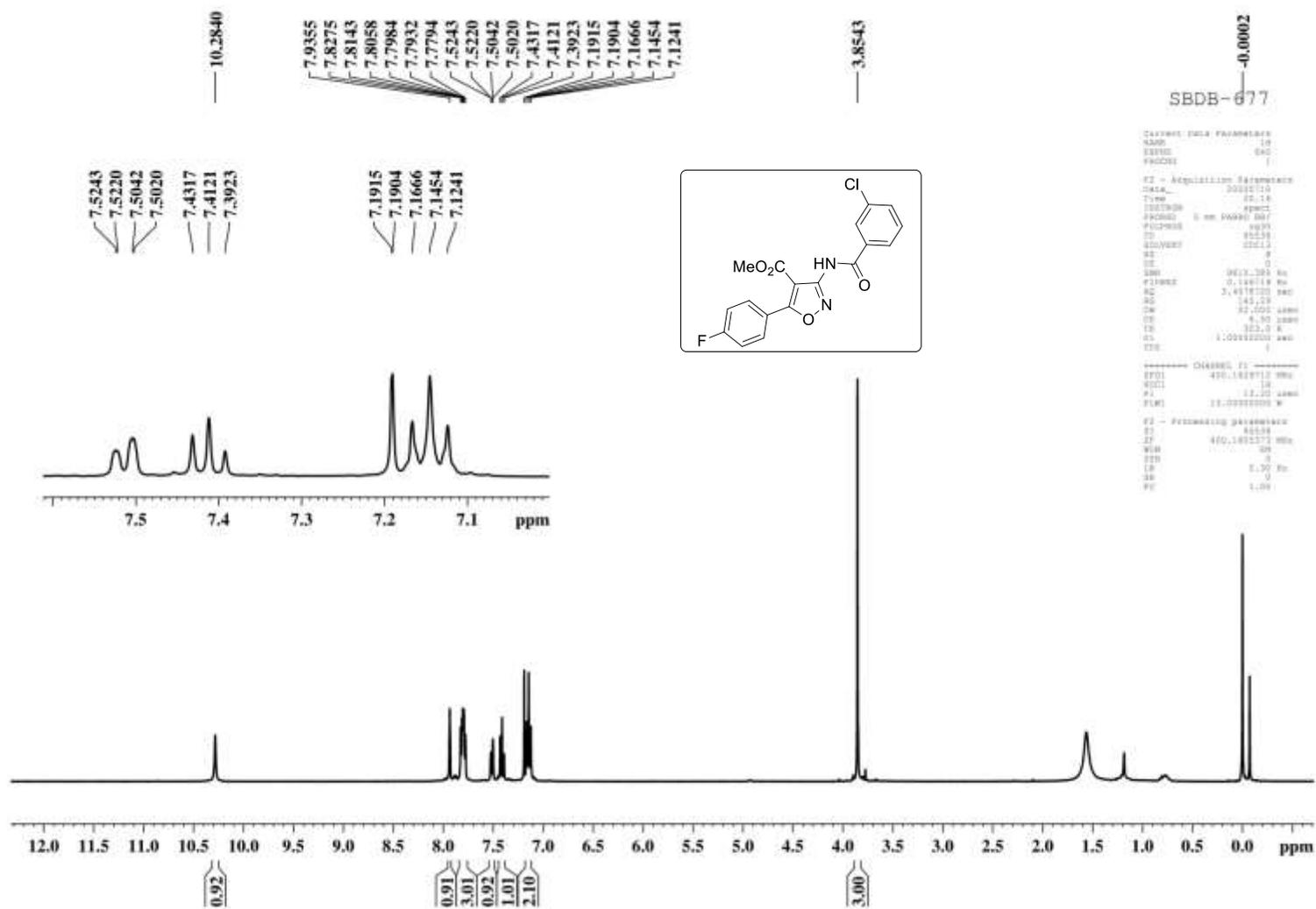


Figure S-50. <sup>1</sup>H-NMR spectrum of methyl 3-(3-chlorobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (**3baf**).

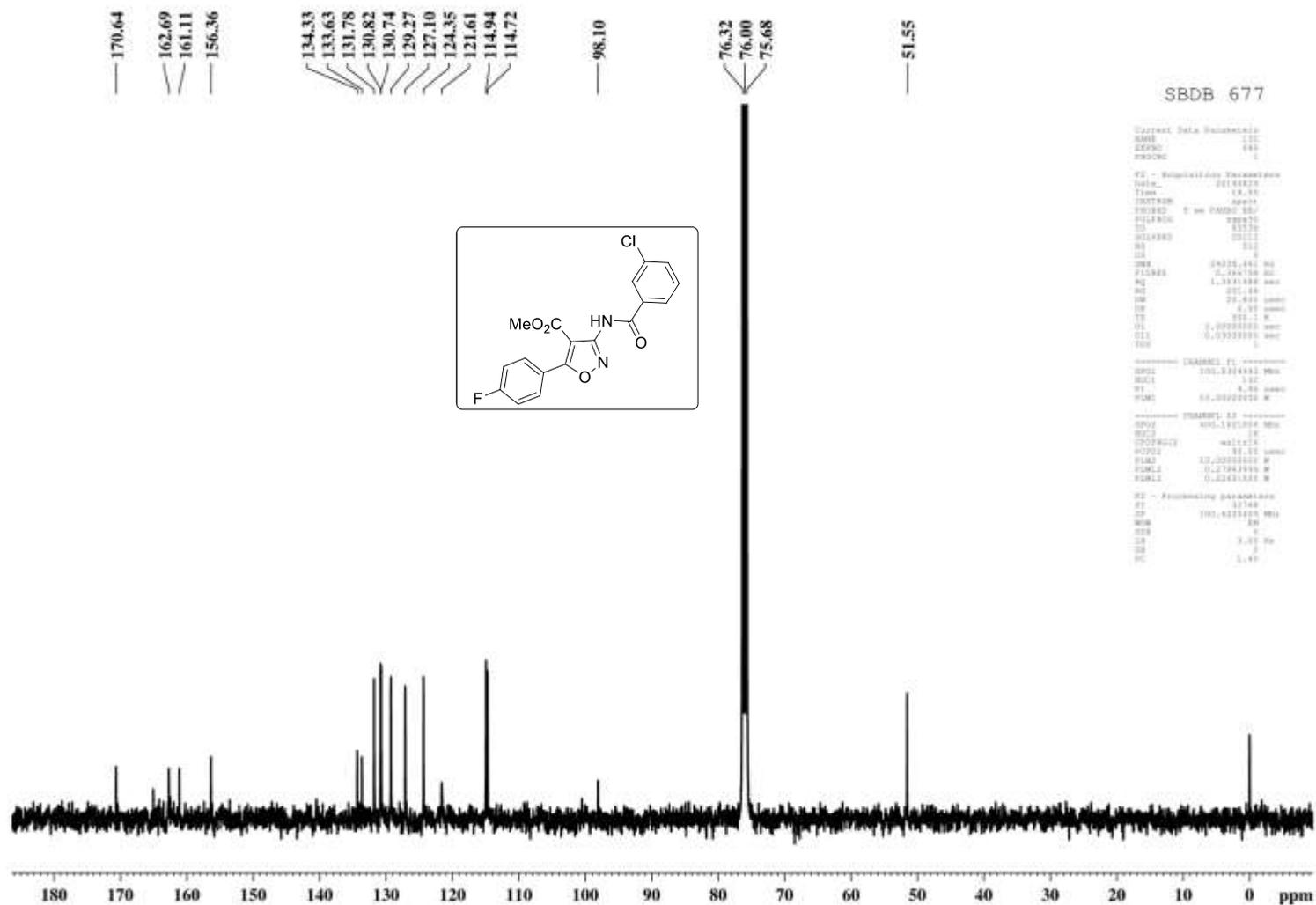
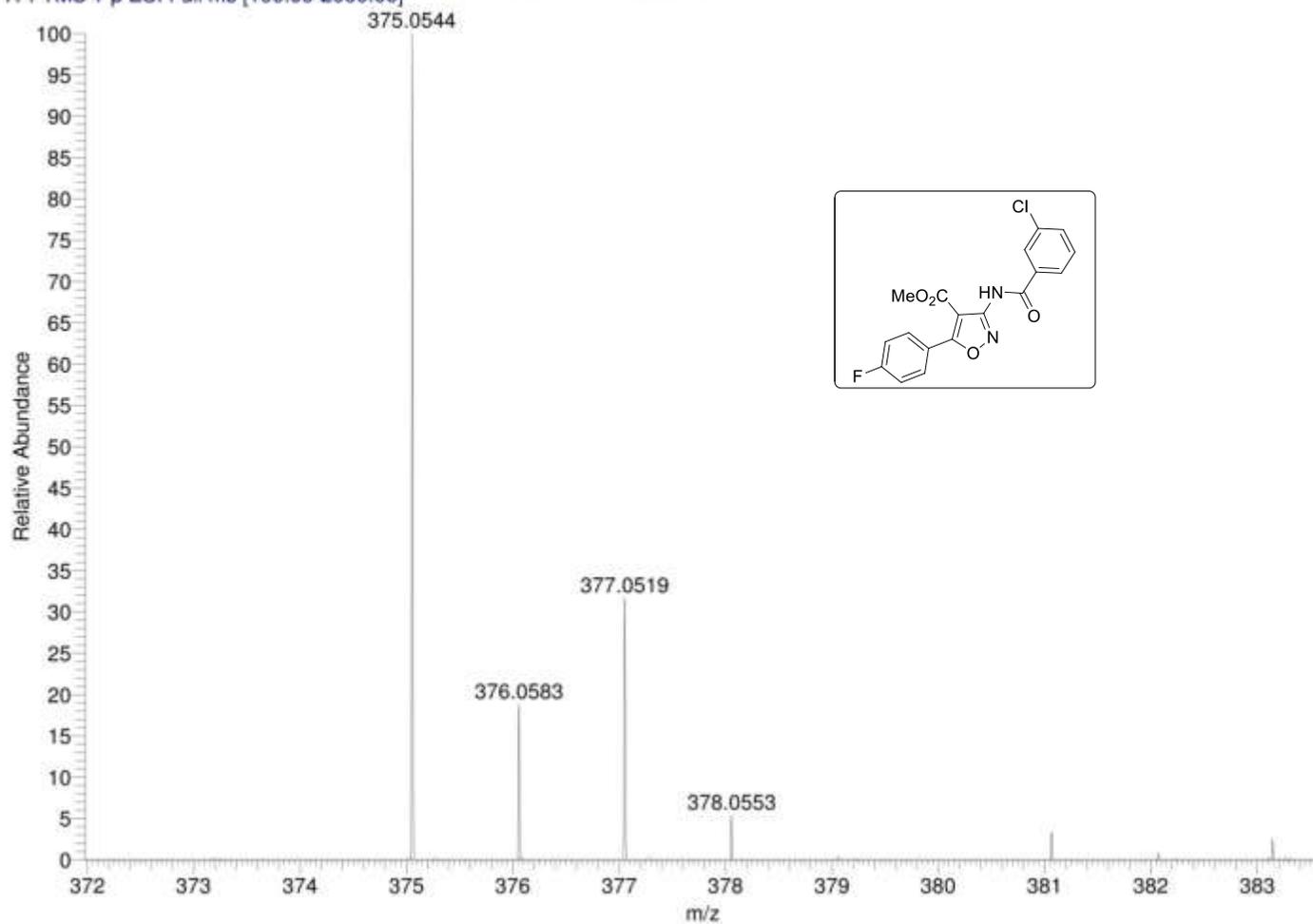


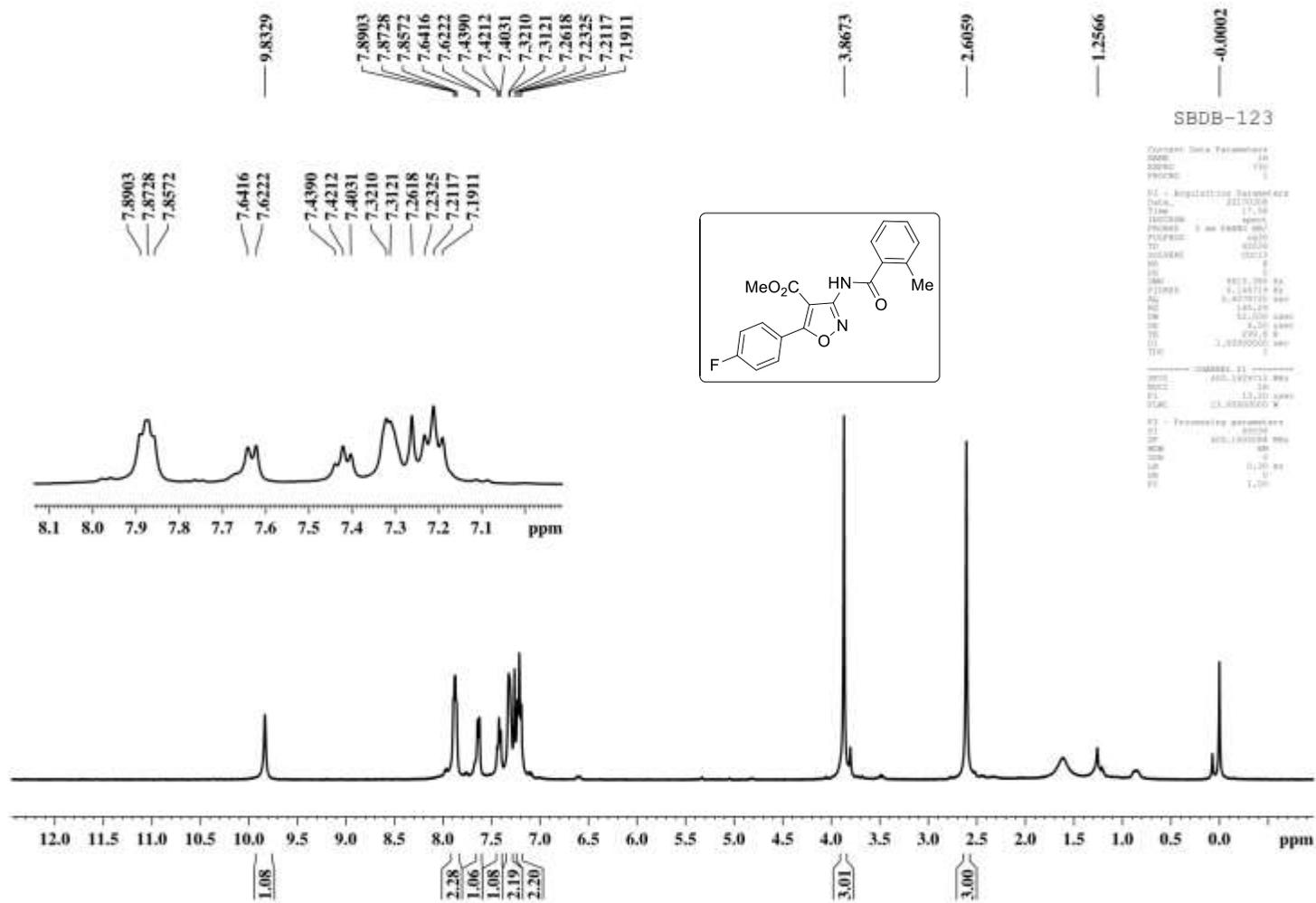
Figure S-51.  $^{13}\text{C}$ -NMR spectrum of methyl 3-(3-chlorobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (**3baf**).

HRMS19I22AUG06 #9 RT: 0.13 AV: 1 SB: 5 0.02-0.08 NL: 5.79E5

T: FTMS + p ESI Full ms [100.00-2000.00]



**Figure S-52.** HRMS spectrum of methyl 3-(3-chlorobenzamido)-5-(4-fluorophenyl)isoxazole-4-carboxylate (**3baf**).



**Figure S-53.** <sup>1</sup>H-NMR spectrum of methyl 5-(4-fluorophenyl)-3-(2-methylbenzamido)isoxazole-4-carboxylate (**3bag**).

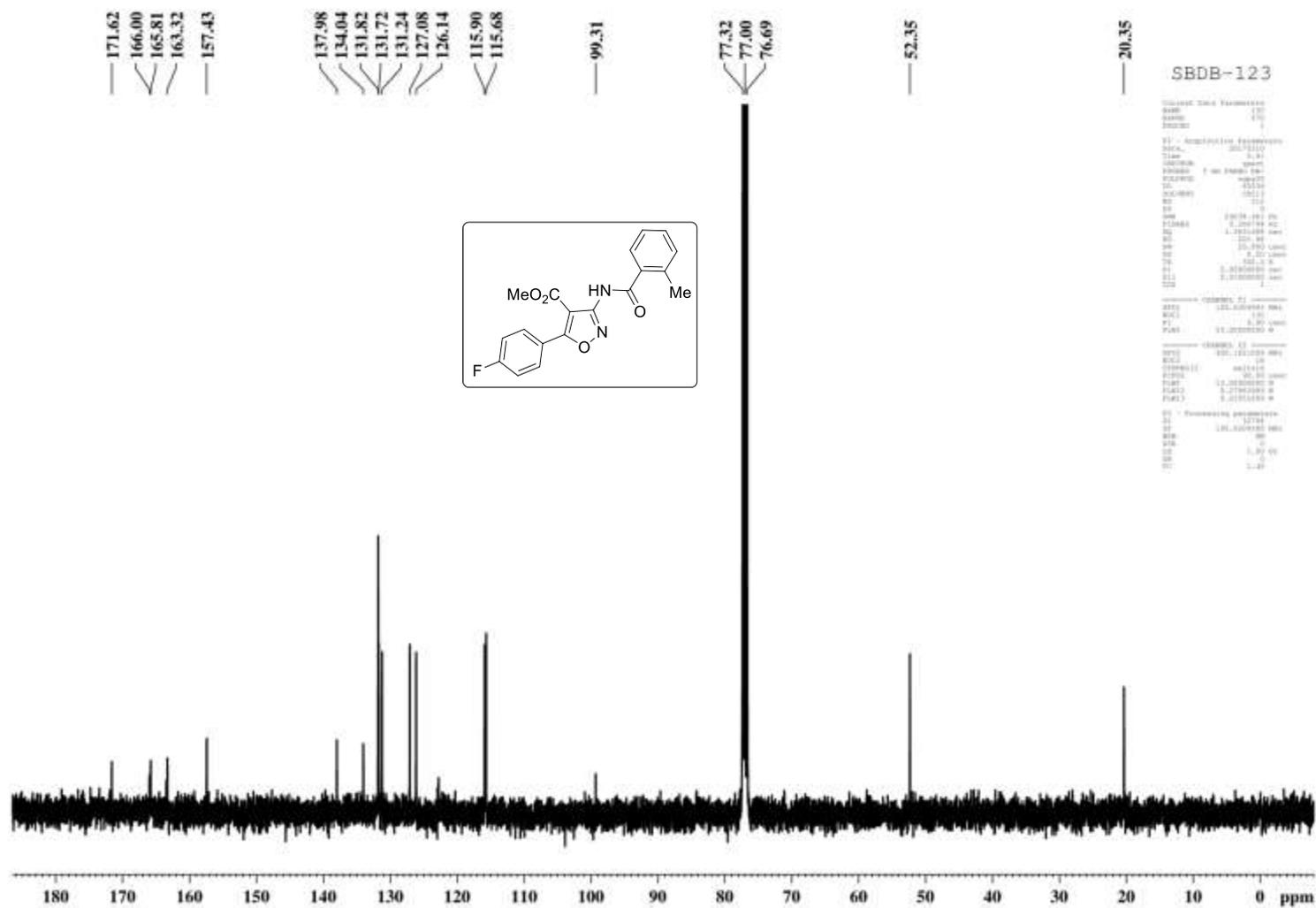


Figure S-54. <sup>13</sup>C-NMR spectrum of methyl 5-(4-fluorophenyl)-3-(2-methylbenzamido)isoxazole-4-carboxylate (**3bag**).

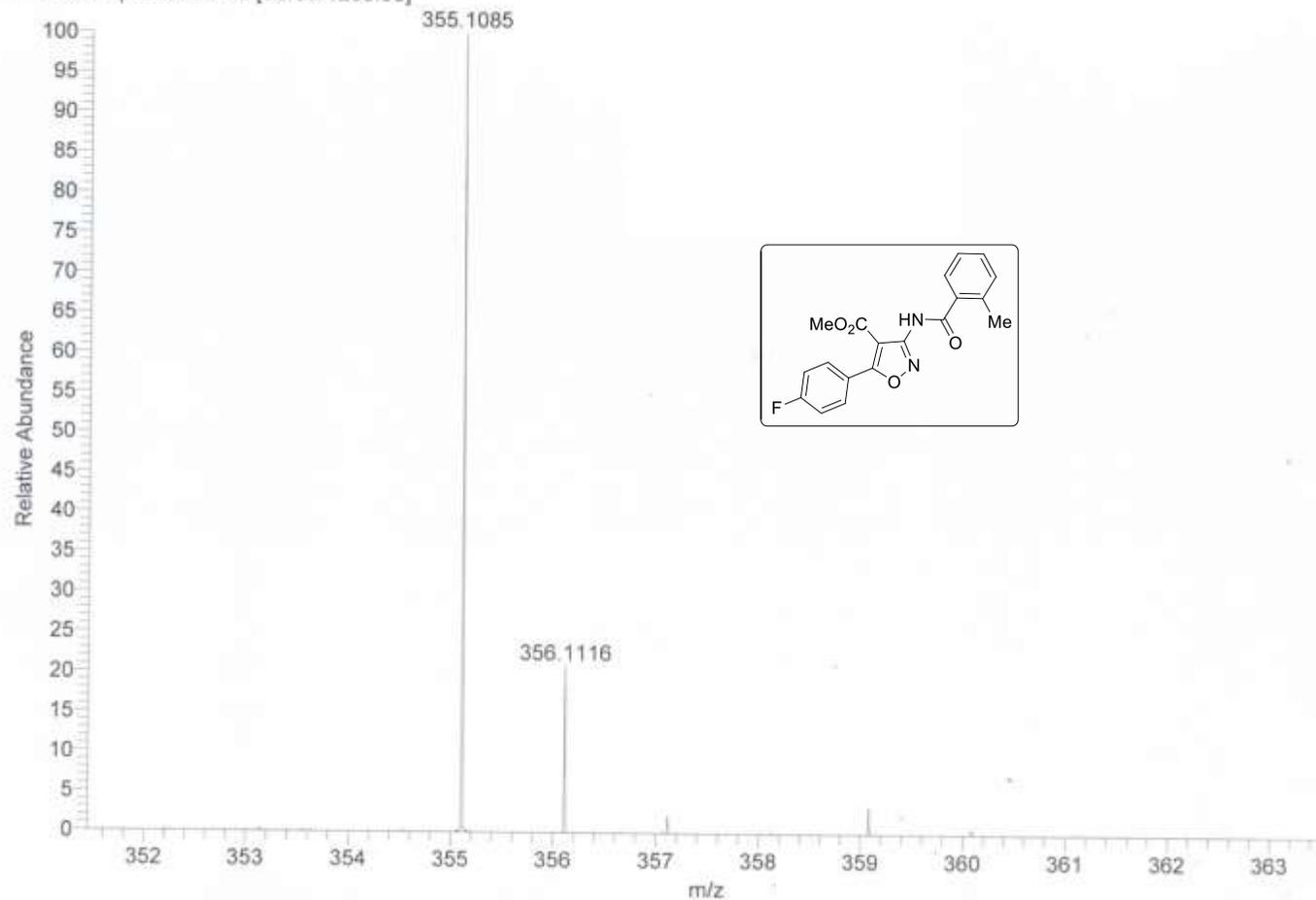
D:\INTERNALS\...HRMS19I26MARCH17

3/26/2019 12:55:43 PM

SBDB-123

HRMS19I26MARCH17 #6 RT: 0.08 AV: 1 SB: 5 0.02-0.08 NL: 2.09E6

T: FTMS + p ESI Full ms [80.00-1200.00]



**Figure S-55.** HRMS spectrum of methyl 5-(4-fluorophenyl)-3-(2-methylbenzamido)isoxazole-4-carboxylate (**3bag**).

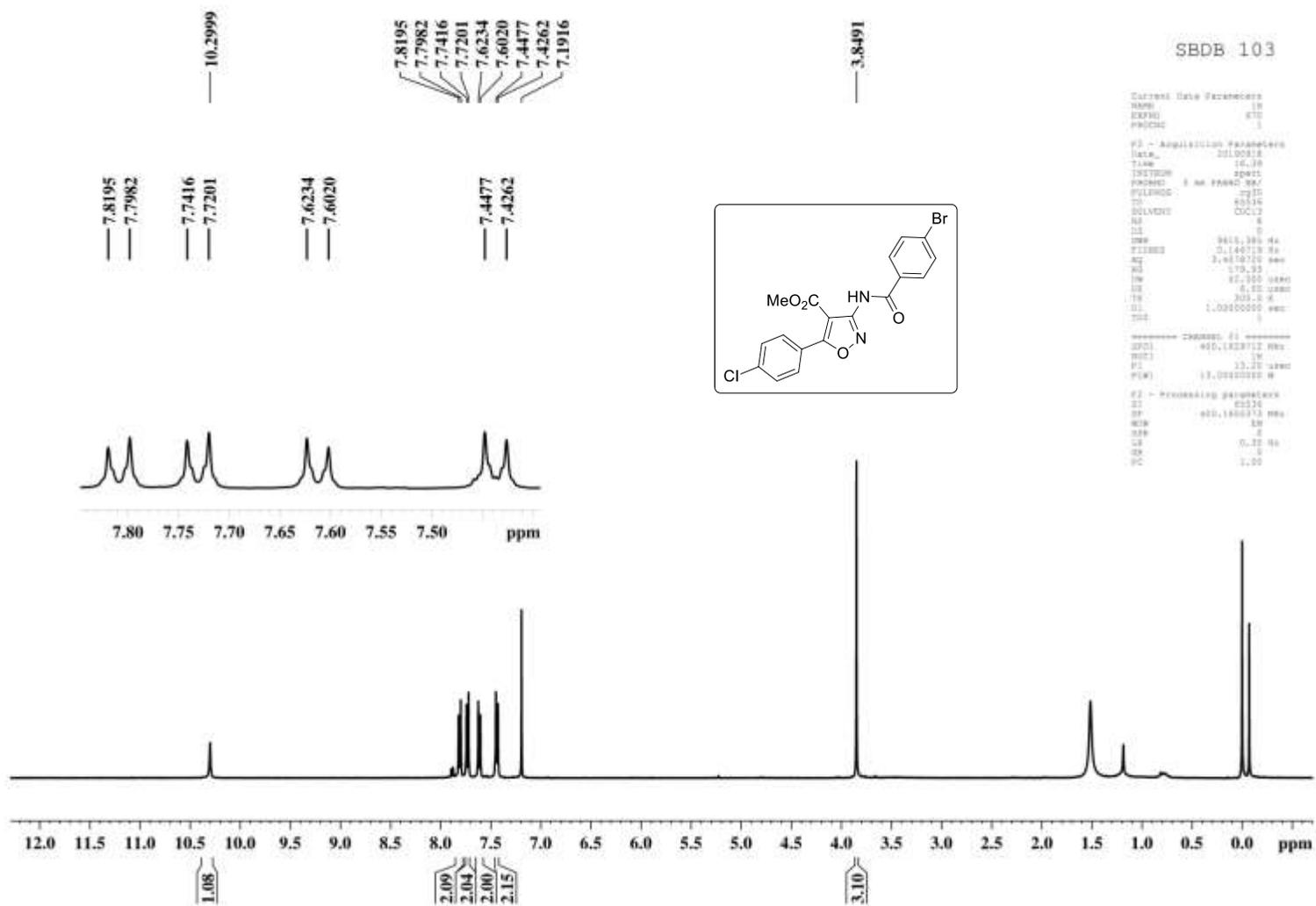


Figure S-56. <sup>1</sup>H-NMR spectrum of methyl 3-(4-bromobenzamido)-5-(4-chlorophenyl)isoxazole-4-carboxylate (**3cab**).

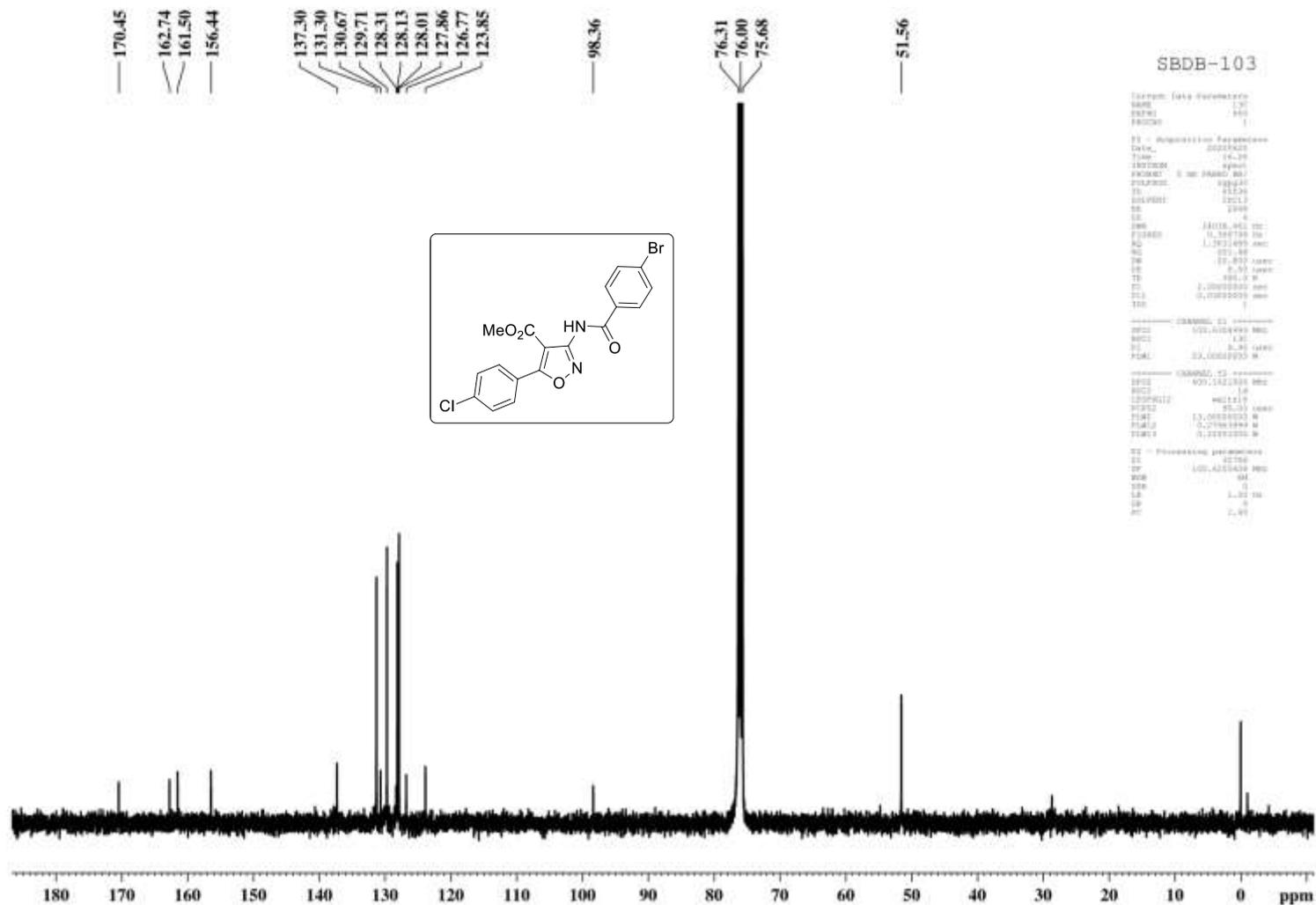
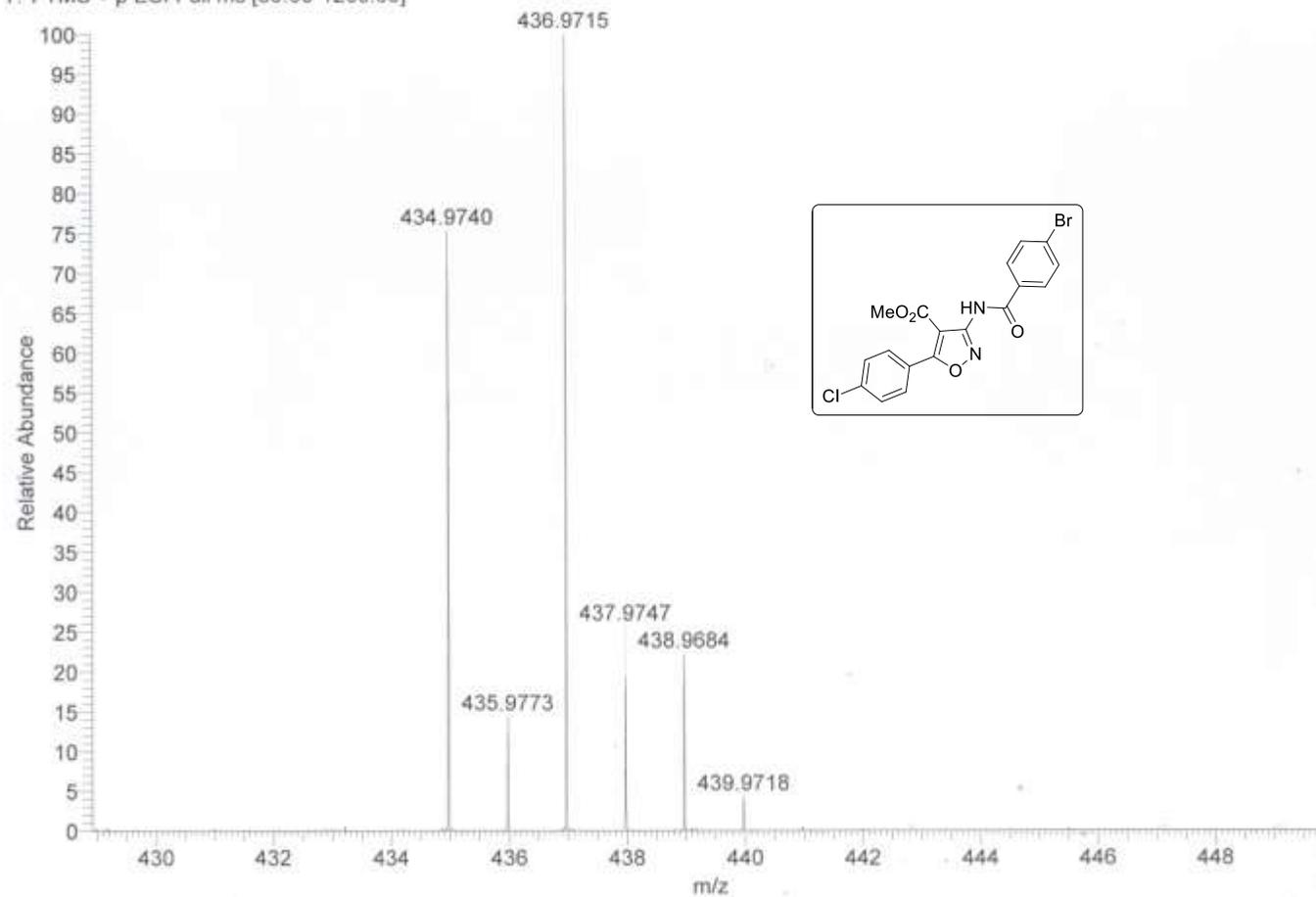


Figure S-57. <sup>13</sup>C-NMR spectrum of methyl 3-(4-bromobenzamido)-5-(4-chlorophenyl)isoxazole-4-carboxylate (**3cab**).

HRMS19I26MARCH09 #11 RT: 0.15 AV: 1 SB: 5 0.02-0.08 NL: 2.56E6

T: FTMS + p ESI Full ms [80.00-1200.00]



**Figure S-58.** HRMS spectrum of methyl 3-(4-bromobenzamido)-5-(4-chlorophenyl)isoxazole-4-carboxylate (**3cab**).

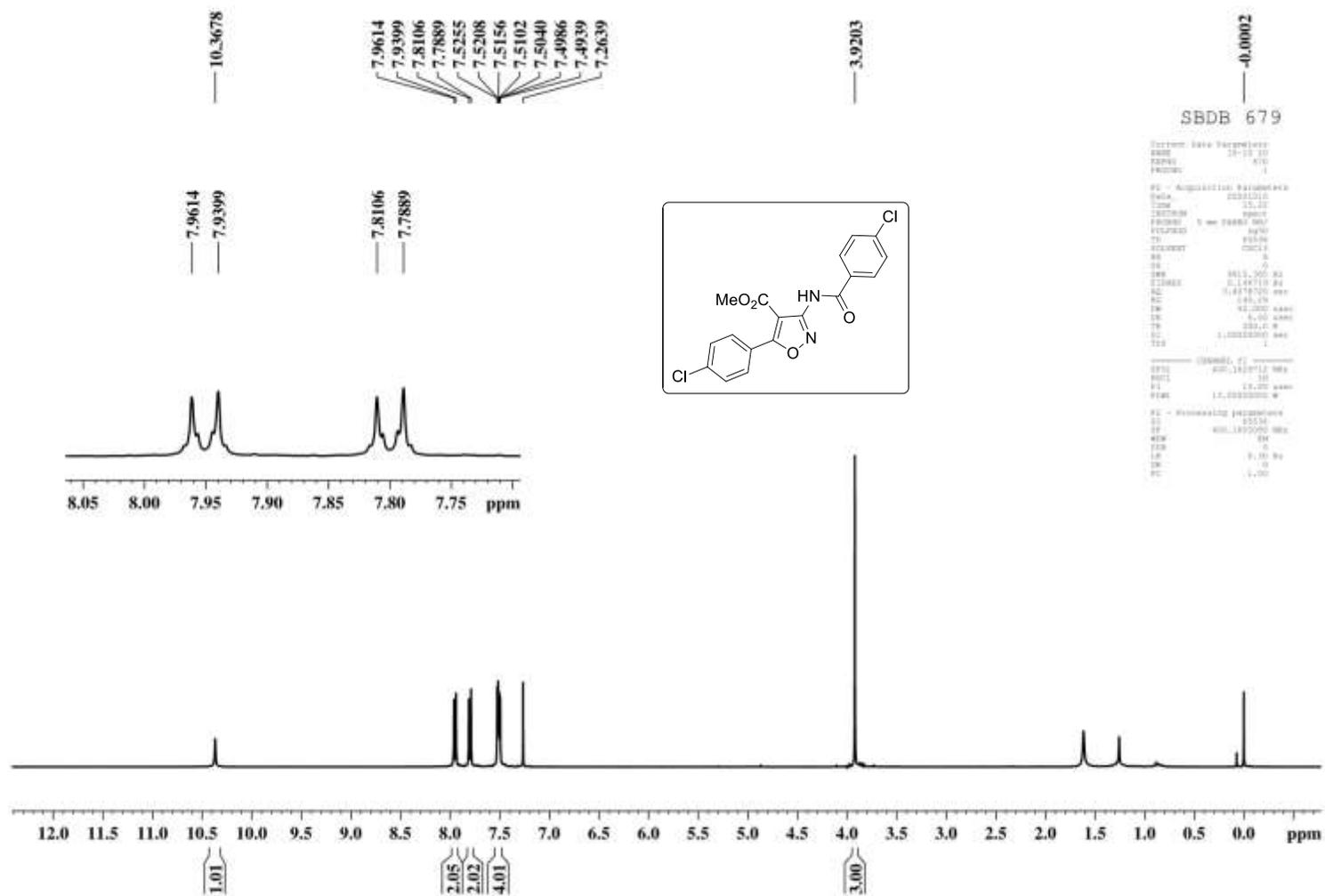


Figure S-59. <sup>1</sup>H-NMR spectrum of methyl 3-(4-chlorobenzamido)-5-(4-chlorophenyl)isoxazole-4-carboxylate (**3cac**).

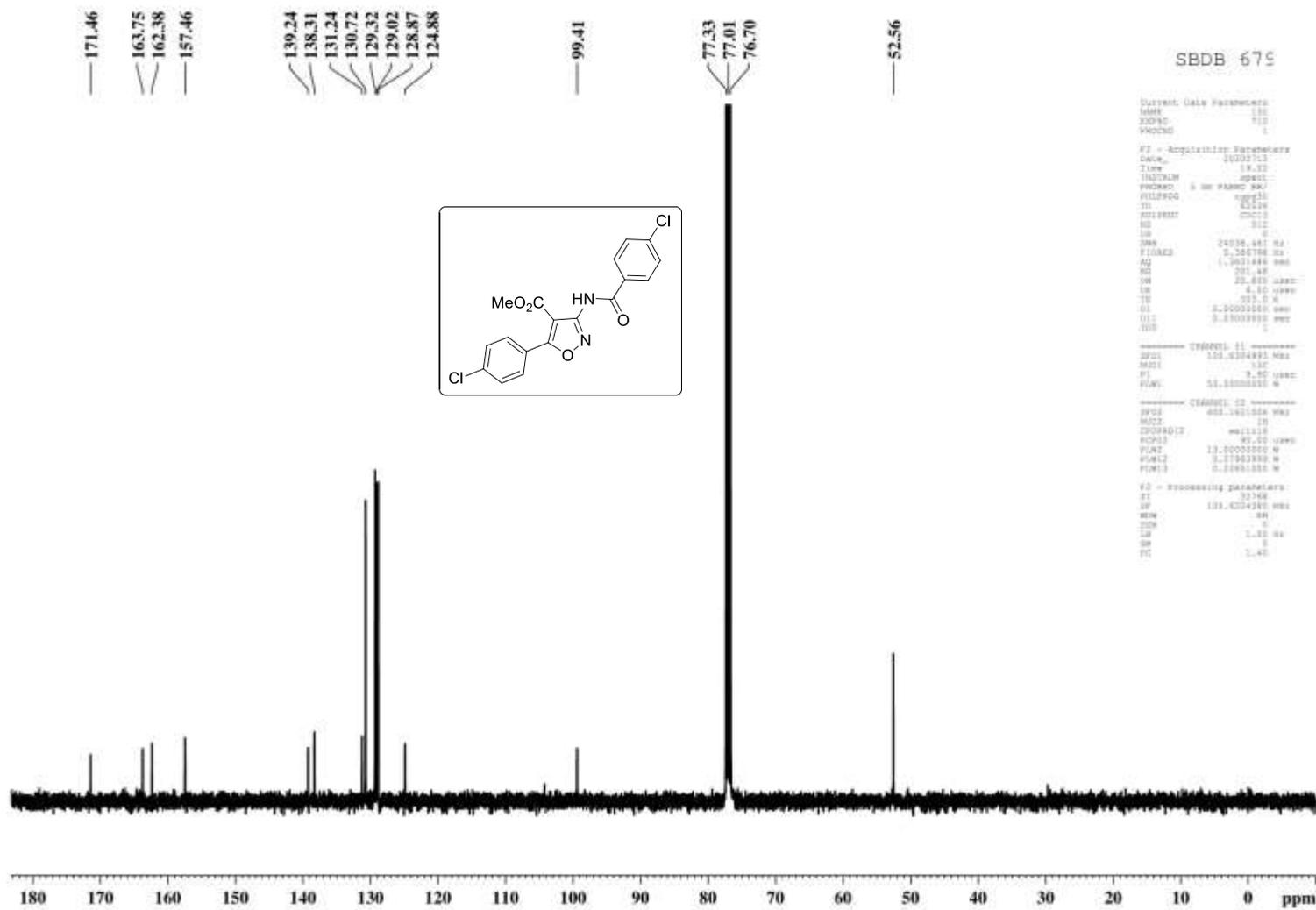
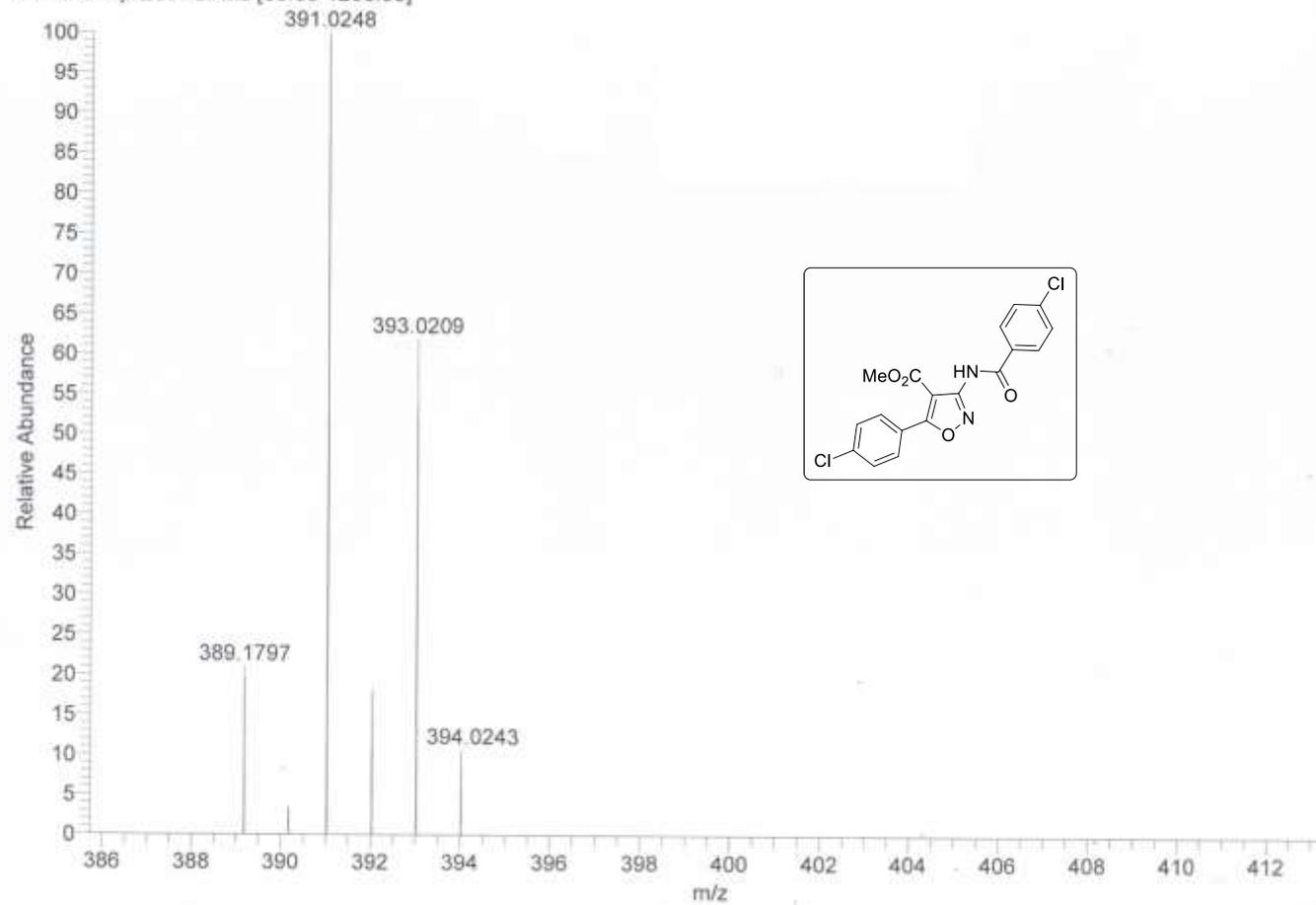


Figure S-60. <sup>13</sup>C-NMR spectrum of methyl 3-(4-chlorobenzamido)-5-(4-chlorophenyl)isoxazole-4-carboxylate (**3cac**).

HRMS19I20MARCH09 #19 RT: 0.18 AV: 1 SB: 5 0.02-0.08 NL: 1.55E5

T: FTMS + p ESI Full ms [80.00-1200.00]



**Figure S-61.** HRMS spectrum of methyl 3-(4-chlorobenzamido)-5-(4-chlorophenyl)isoxazole-4-carboxylate (**3cac**).

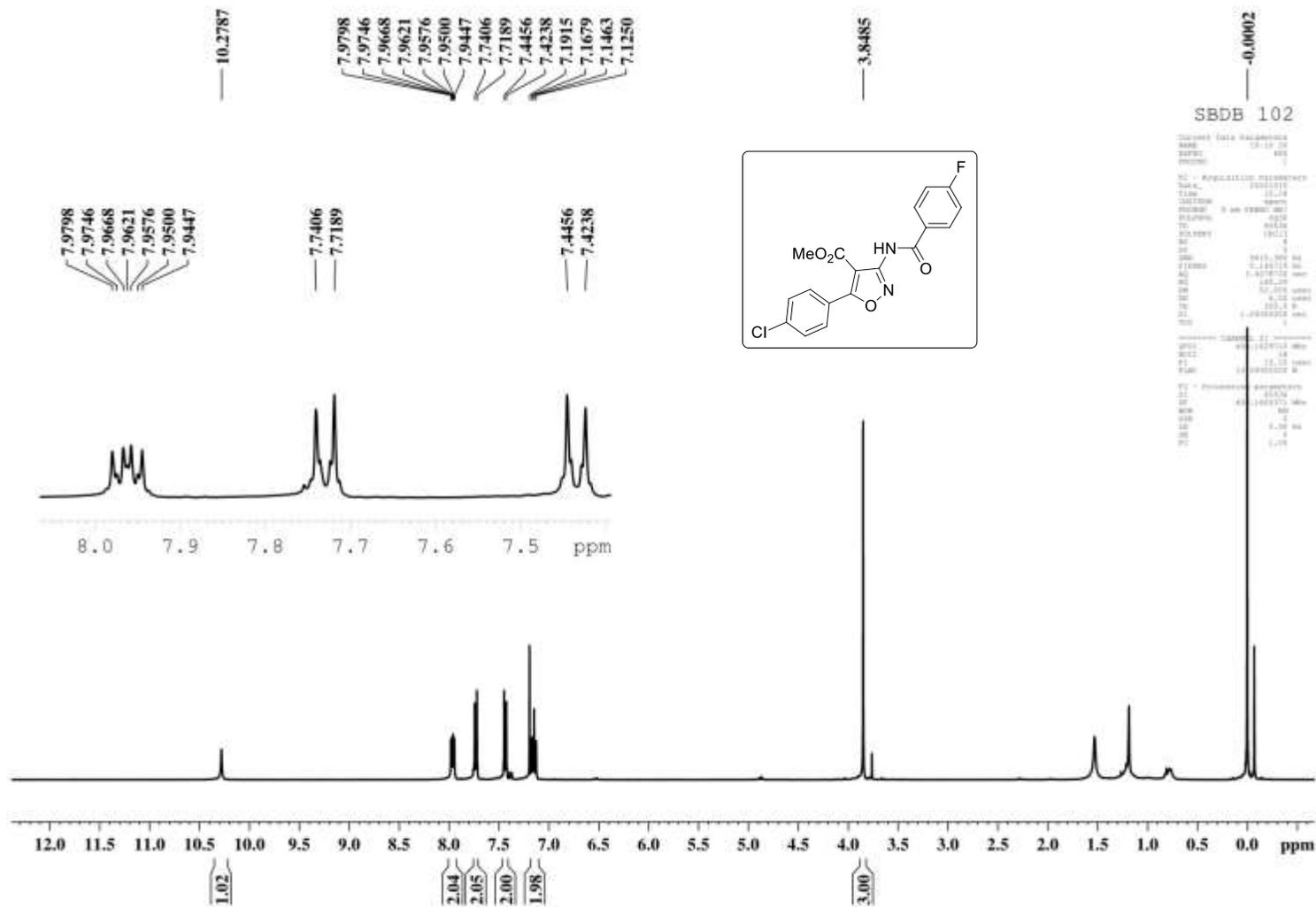


Figure S-62. <sup>1</sup>H-NMR spectrum of methyl 5-(4-chlorophenyl)-3-(4-fluorobenzamido)isoxazole-4-carboxylate (**3cad**).

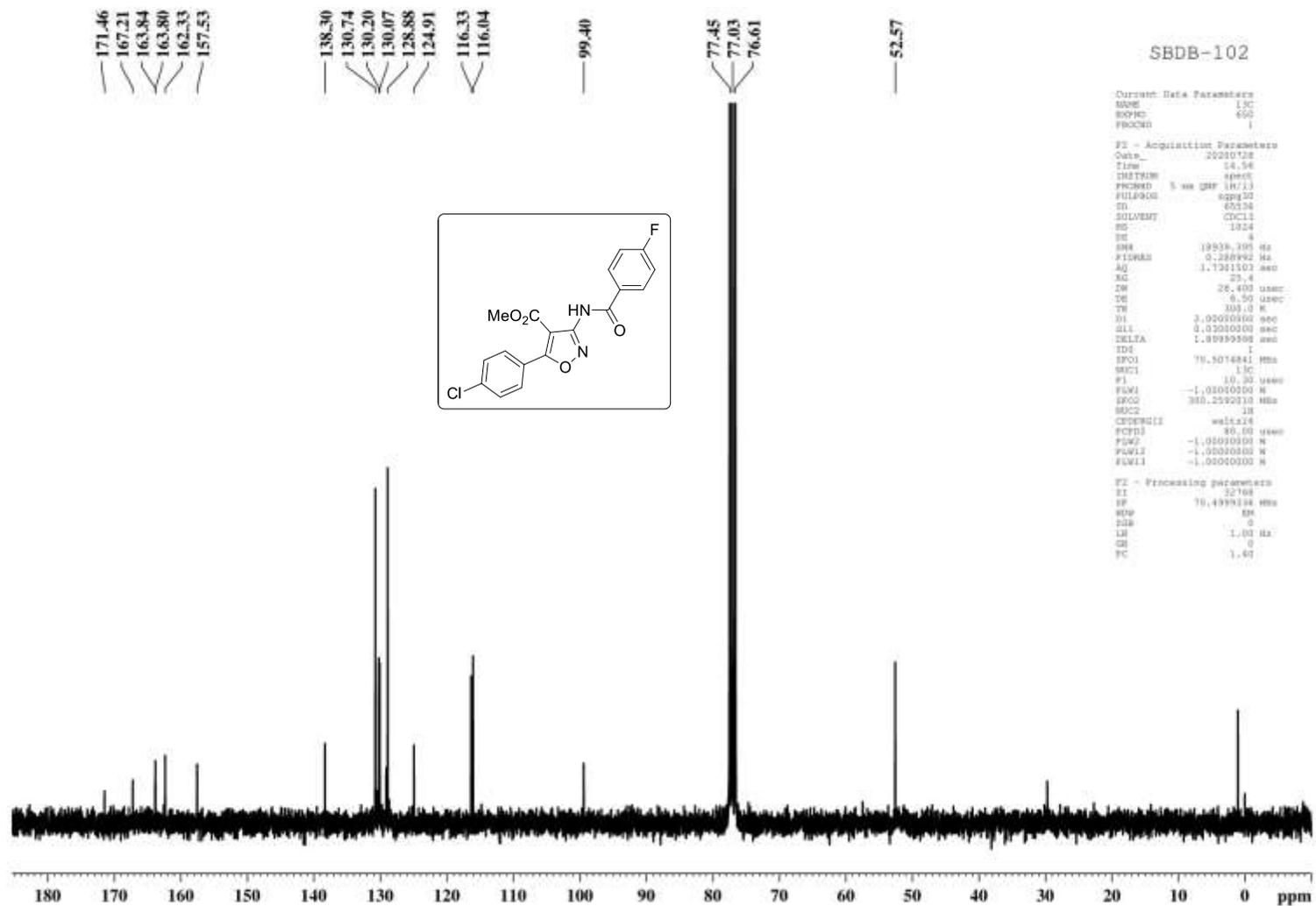
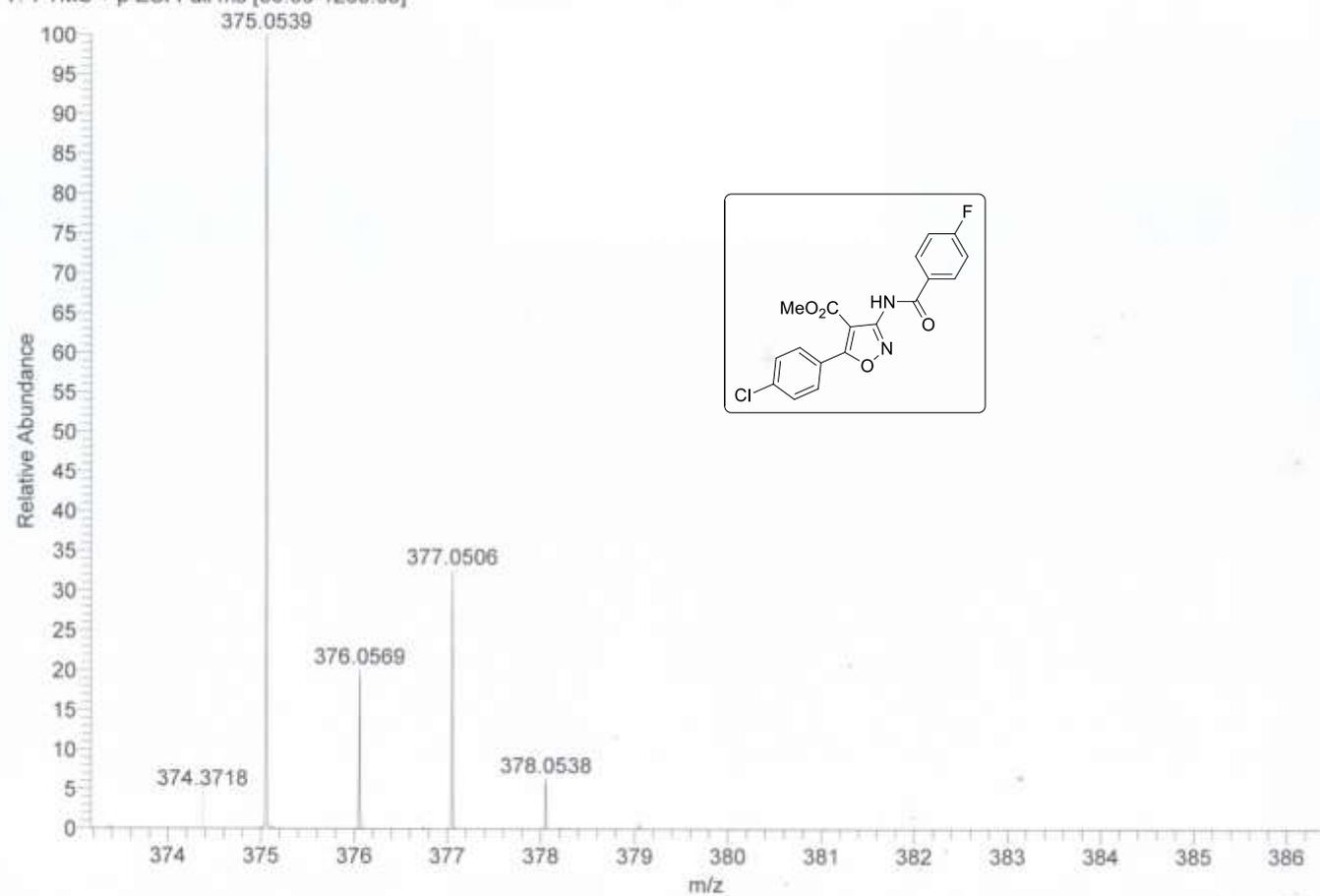


Figure S-63.  $^{13}\text{C}$ -NMR spectrum of methyl 5-(4-chlorophenyl)-3-(4-fluorobenzamido)isoxazole-4-carboxylate (**3cad**).

HRMS19I26MARCH10 #7 RT: 0.09 AV: 1 SB: 5 0.02-0.08 NL: 2.89E6

T: FTMS + p ESI Full ms [80.00-1200.00]



**Figure S-64.** HRMS spectrum of methyl 5-(4-chlorophenyl)-3-(4-fluorobenzamido)isoxazole-4-carboxylate (**3cad**).

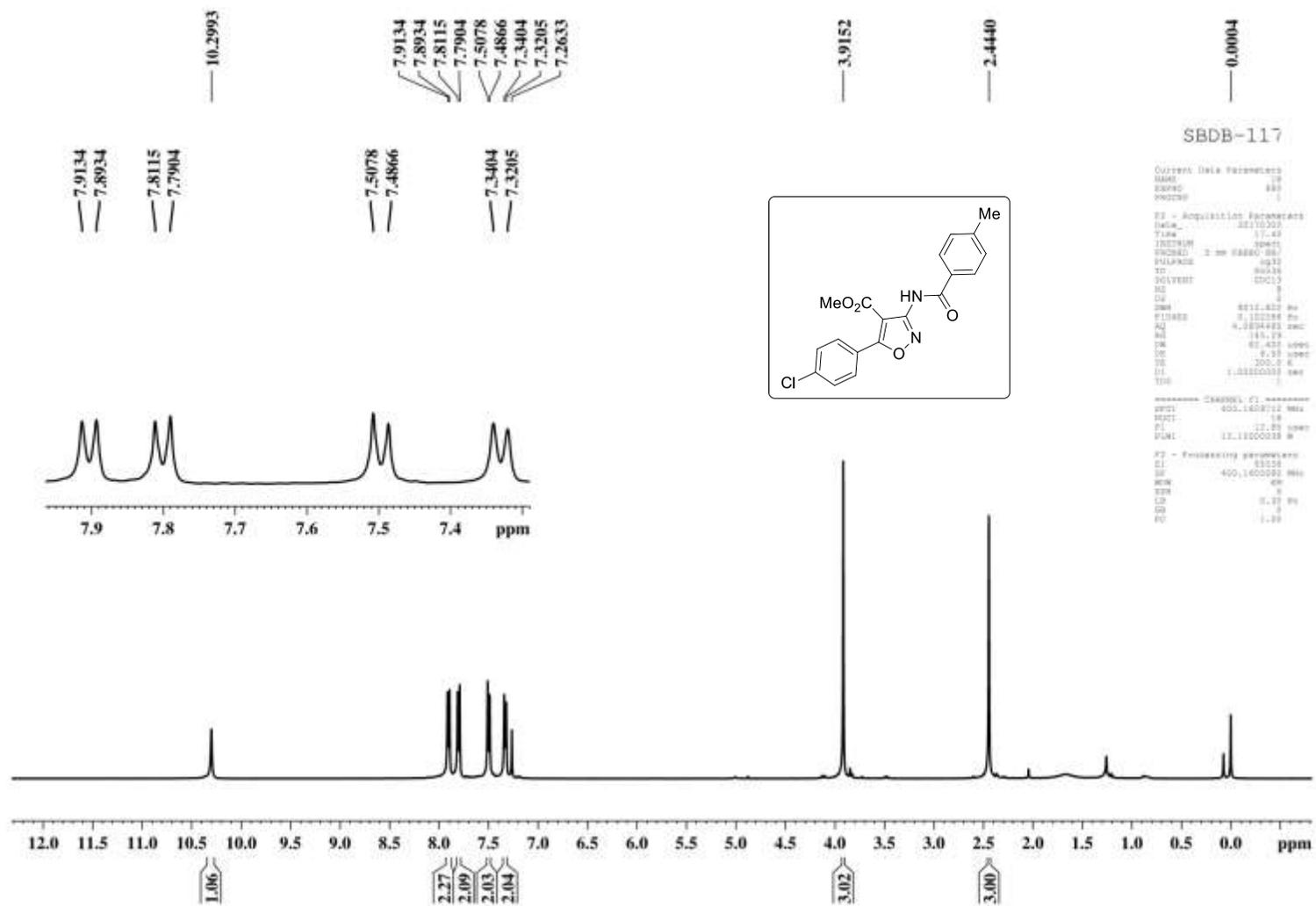


Figure S-65. <sup>1</sup>H-NMR spectrum of methyl 5-(4-chlorophenyl)-3-(4-methylbenzamido)isoxazole-4-carboxylate (**3cae**).

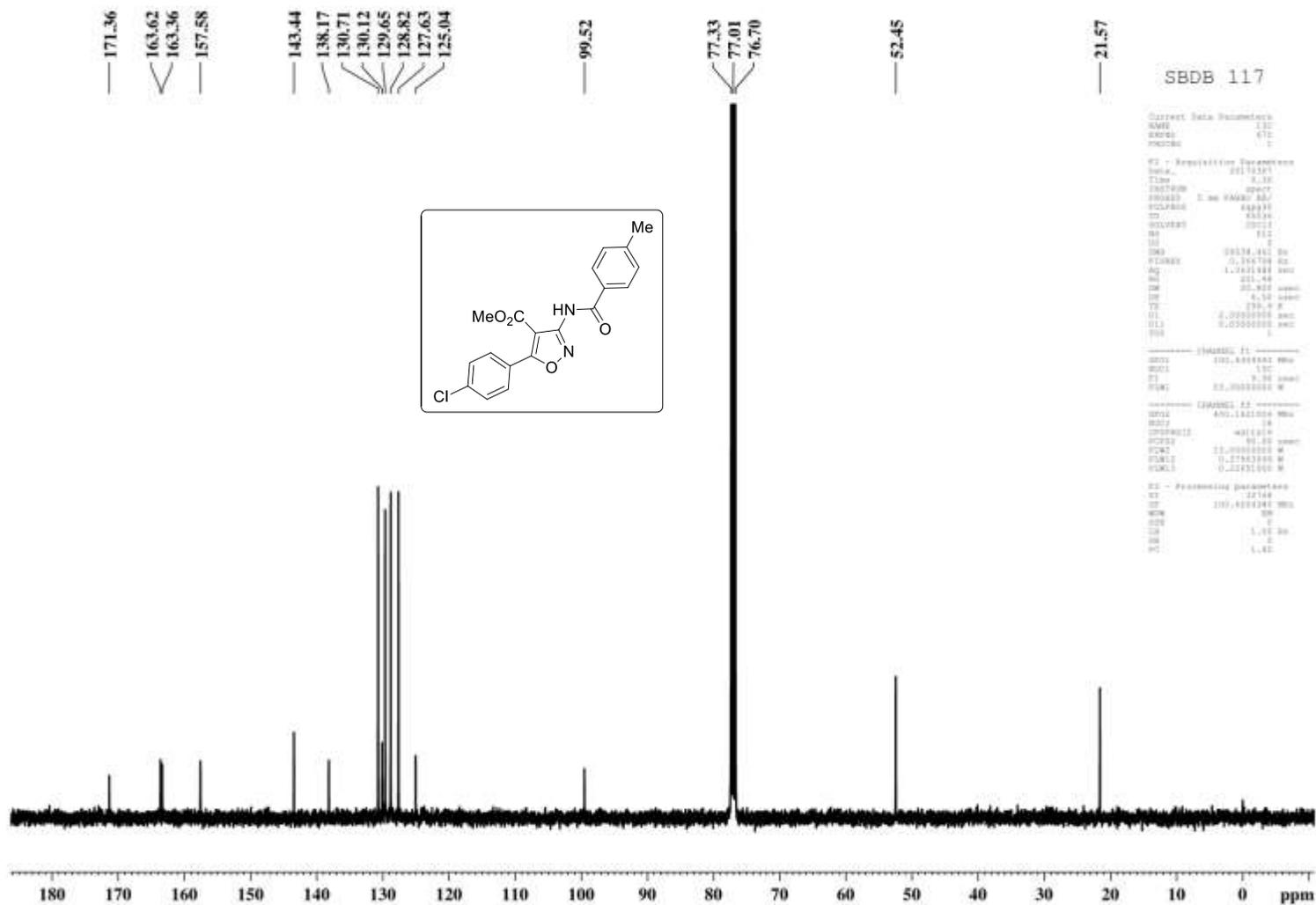
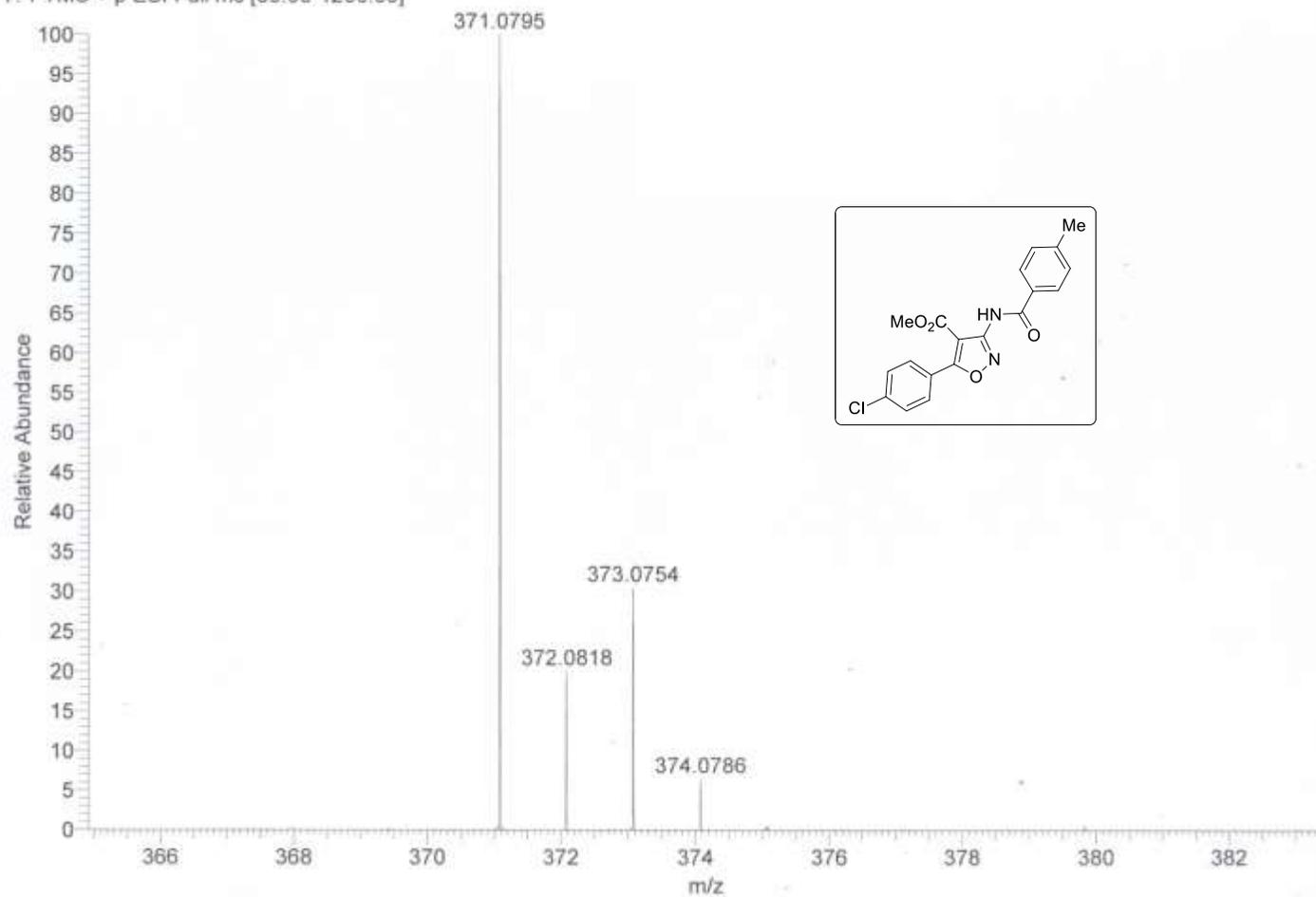
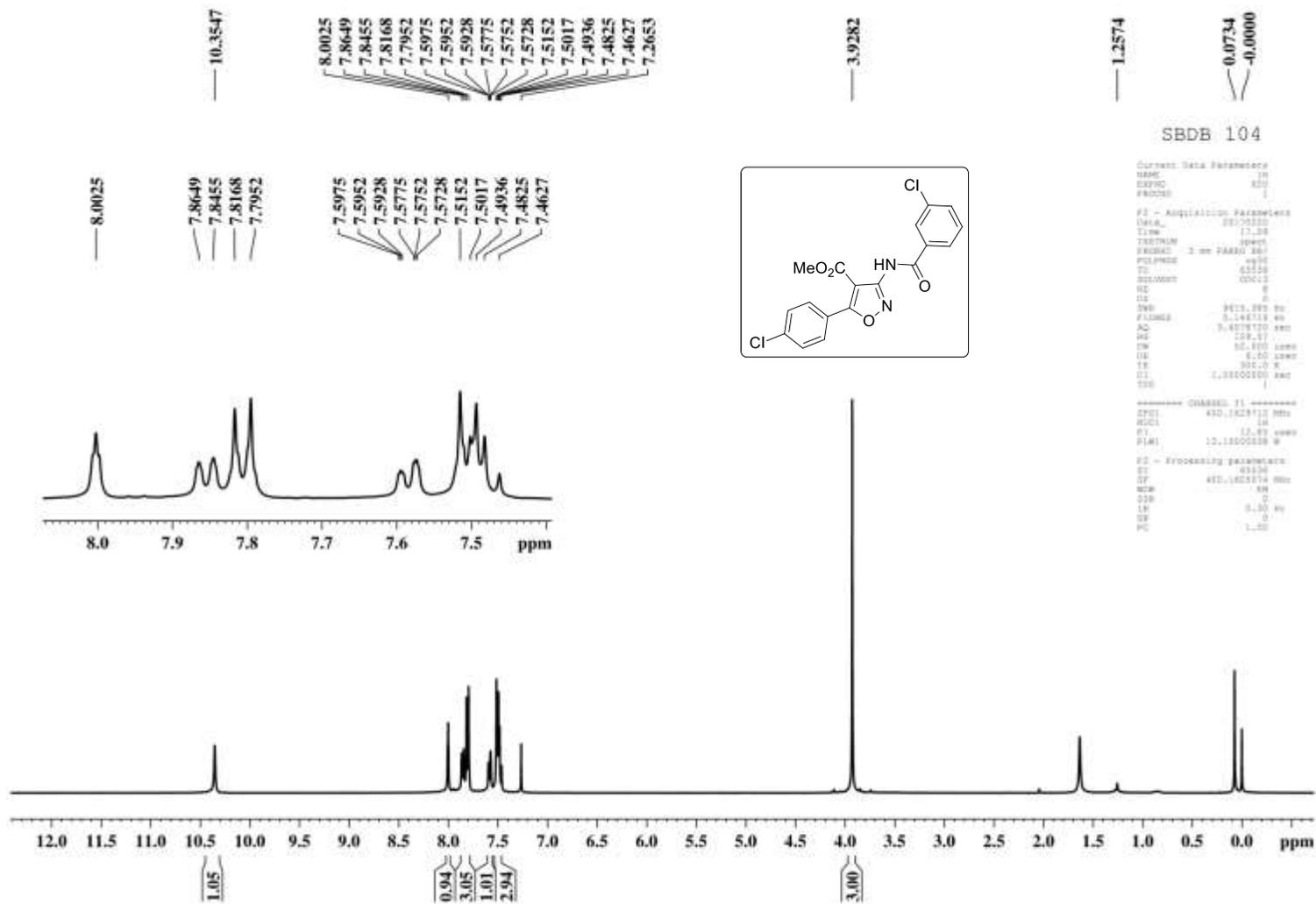


Figure S-66. <sup>13</sup>C-NMR spectrum of methyl 5-(4-chlorophenyl)-3-(4-methylbenzamido)isoxazole-4-carboxylate (**3cae**).

HRMS19I26MARCH11 #11 RT: 0.15 AV: 1 SB: 5 0.02-0.08 NL: 3.43E6  
T: FTMS + p ESI Full ms [80.00-1200.00]



**Figure S-67.** HRMS spectrum of methyl 5-(4-chlorophenyl)-3-(4-methylbenzamido)isoxazole-4-carboxylate (**3cae**).



**Figure S-68.** <sup>1</sup>H-NMR spectrum of methyl 3-(3-chlorobenzamido)-5-(4-chlorophenyl)isoxazole-4-carboxylate (**3caf**).

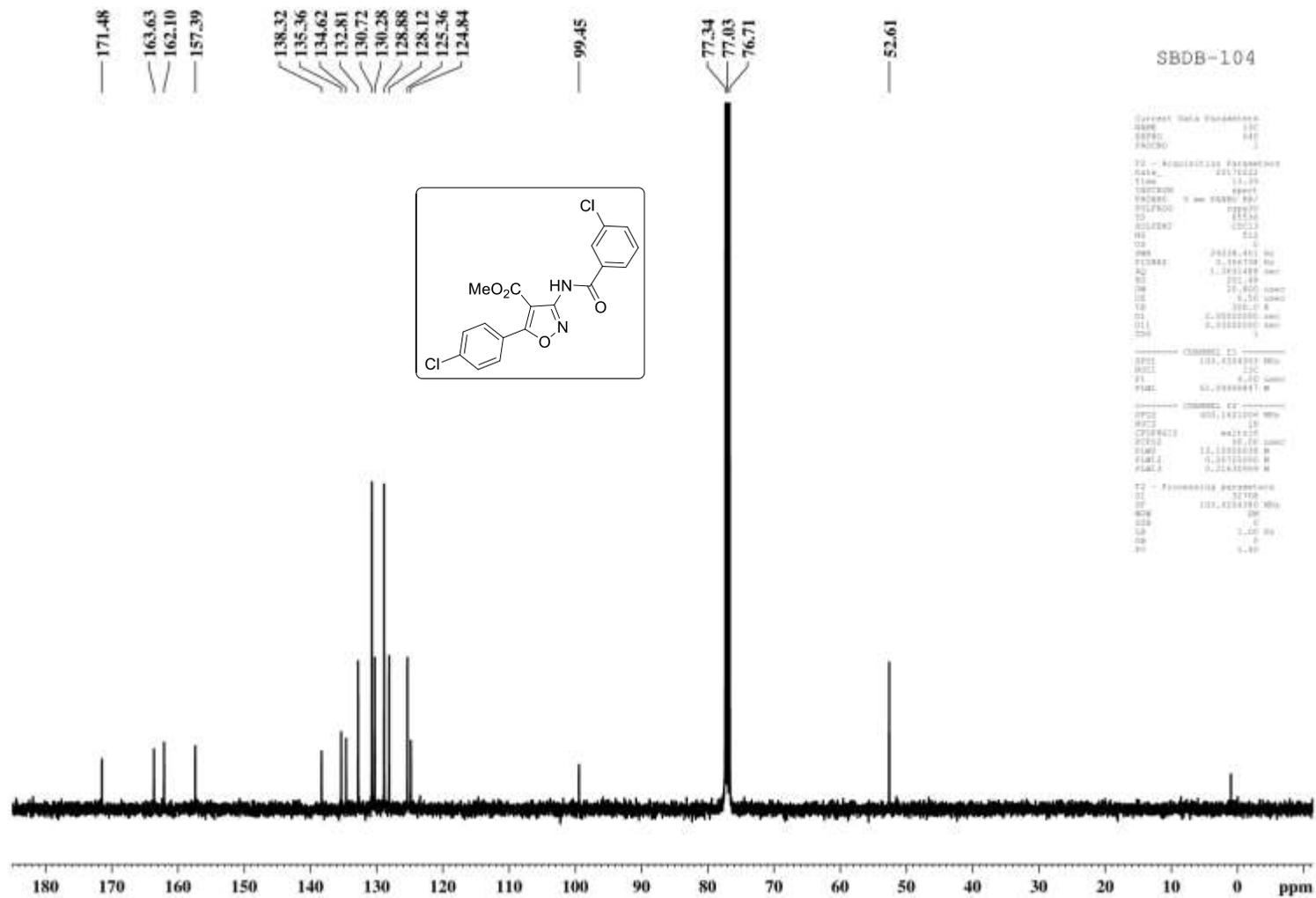
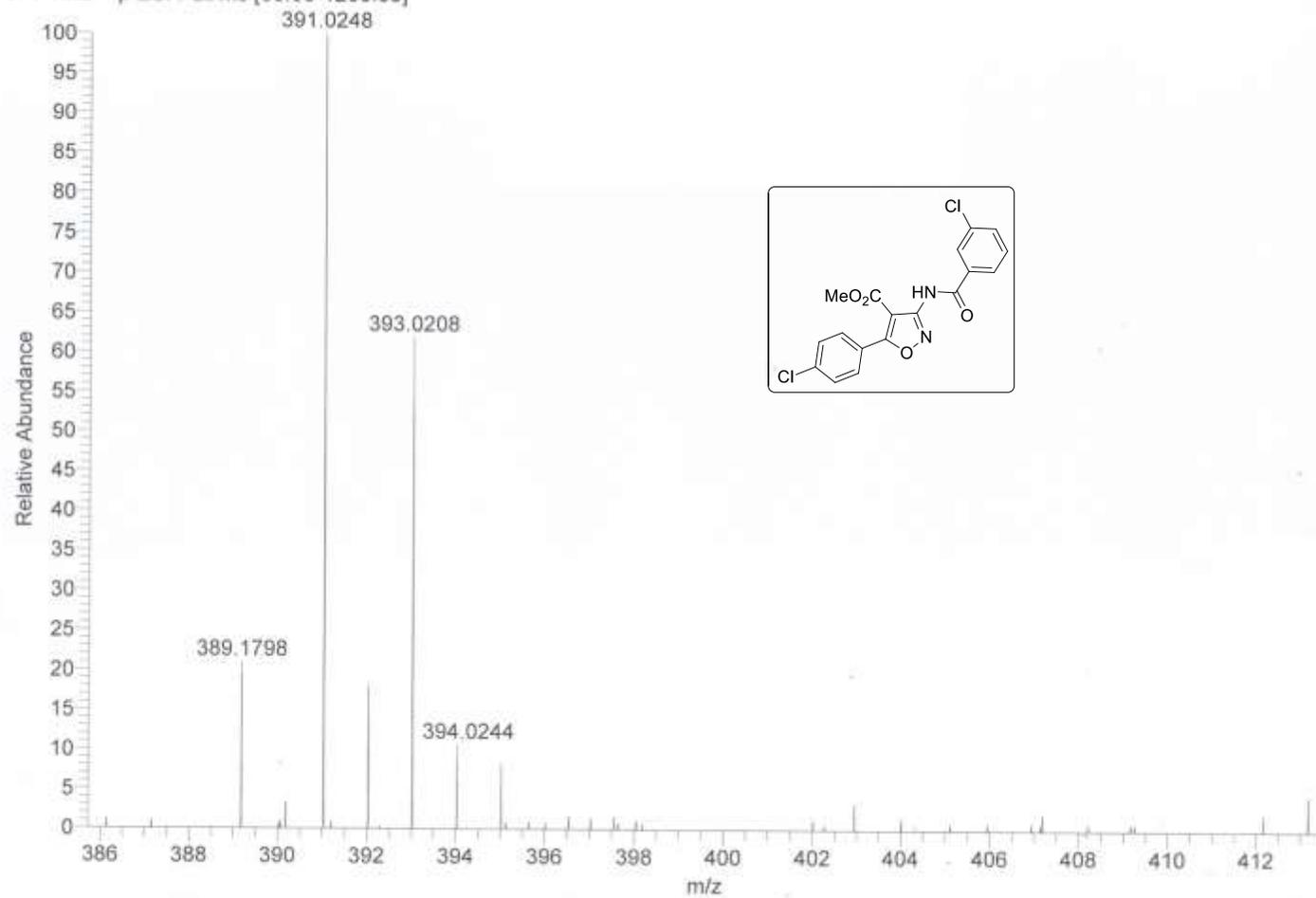


Figure S-69.  $^{13}\text{C}$ -NMR spectrum of methyl 3-(3-chlorobenzamido)-5-(4-chlorophenyl)isoxazole-4-carboxylate (**3caf**).

HRMS19I26MARCH08 #13 RT: 0.18 AV: 1 SB: 5 0.02-0.08 NL: 1.59E5

T: FTMS + p ESI Full ms [80.00-1200.00]



**Figure S-70.** HRMS spectrum of methyl 3-(3-chlorobenzamido)-5-(4-chlorophenyl)isoxazole-4-carboxylate (**3caf**).

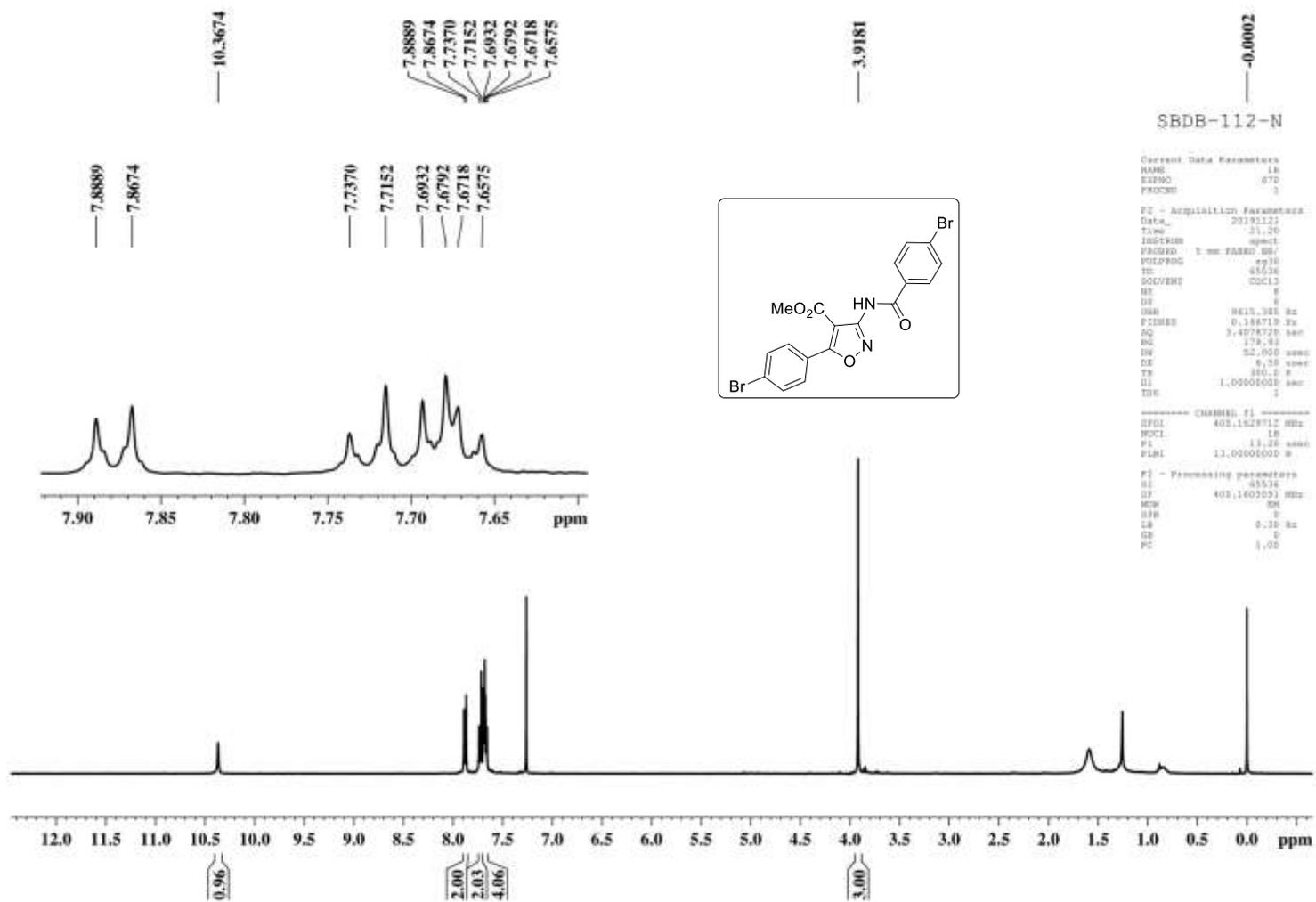


Figure S-71. <sup>1</sup>H-NMR spectrum of methyl 3-(4-bromobenzamido)-5-(4-bromophenyl)isoxazole-4-carboxylate (**3dab**).

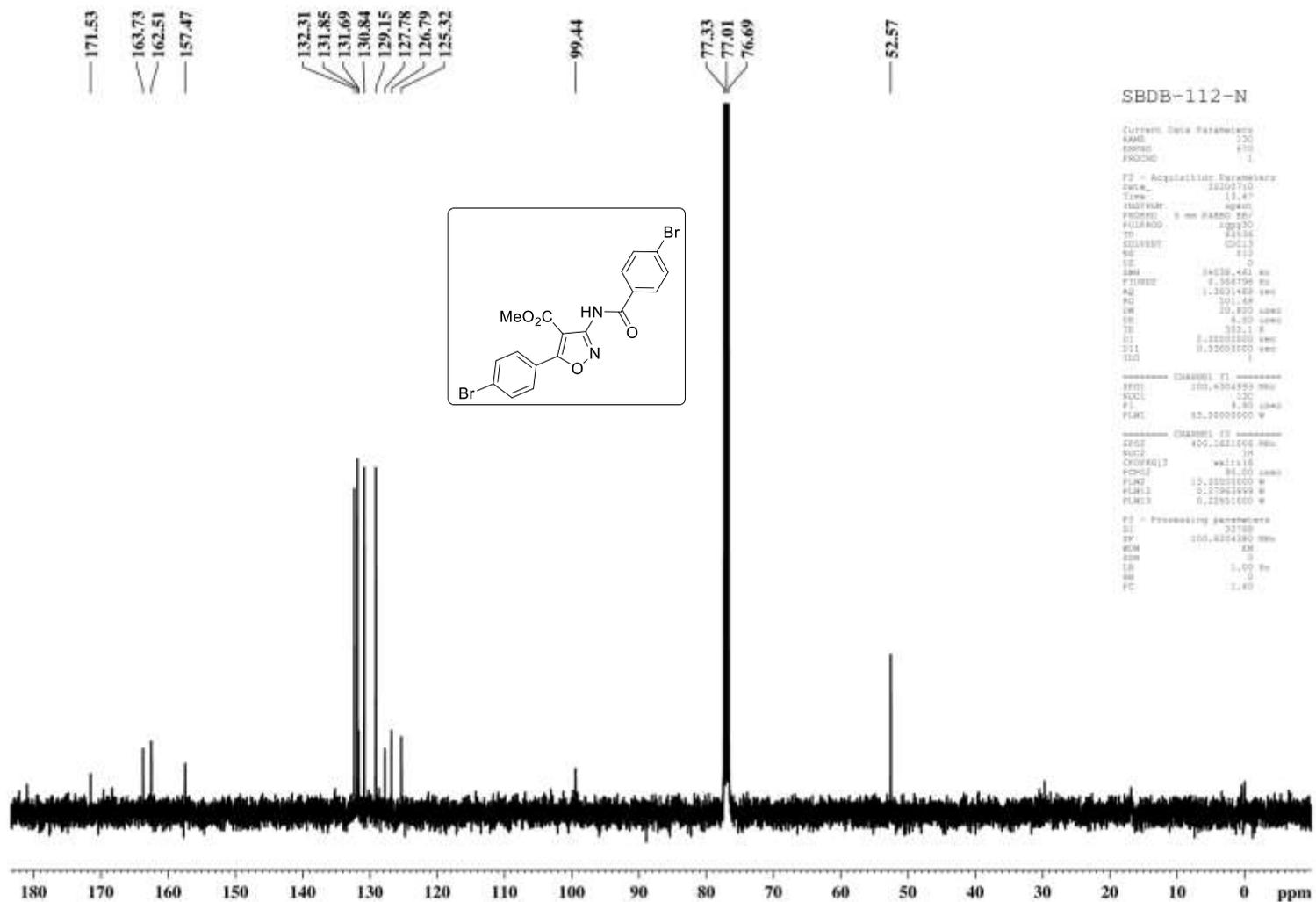


Figure S-72.  $^{13}\text{C}$ -NMR spectrum of methyl 3-(4-bromobenzamido)-5-(4-bromophenyl)isoxazole-4-carboxylate (**3dab**).

### SAIF [HRMS Report]

Data File:	HRMS20I15SEP02	Original Data Path:	D:\INTERNAL NEW\2020\Sep 2020
Sample ID:	sbdb-112 N	Sample Name:	
Acquisition Date:	09/15/20 10:25:32 AM	Run Time(min):	0.00
Vial:	CS1k1-01:2	Injection Volume(μl):	1.00

HRMS20I15SEP02 #12-23 RT: 0.11-0.21 AV: 12 SB: 1 0.01 NL: 4.06E5  
T: FTMS + c ESI Full ms [100.00-750.00]

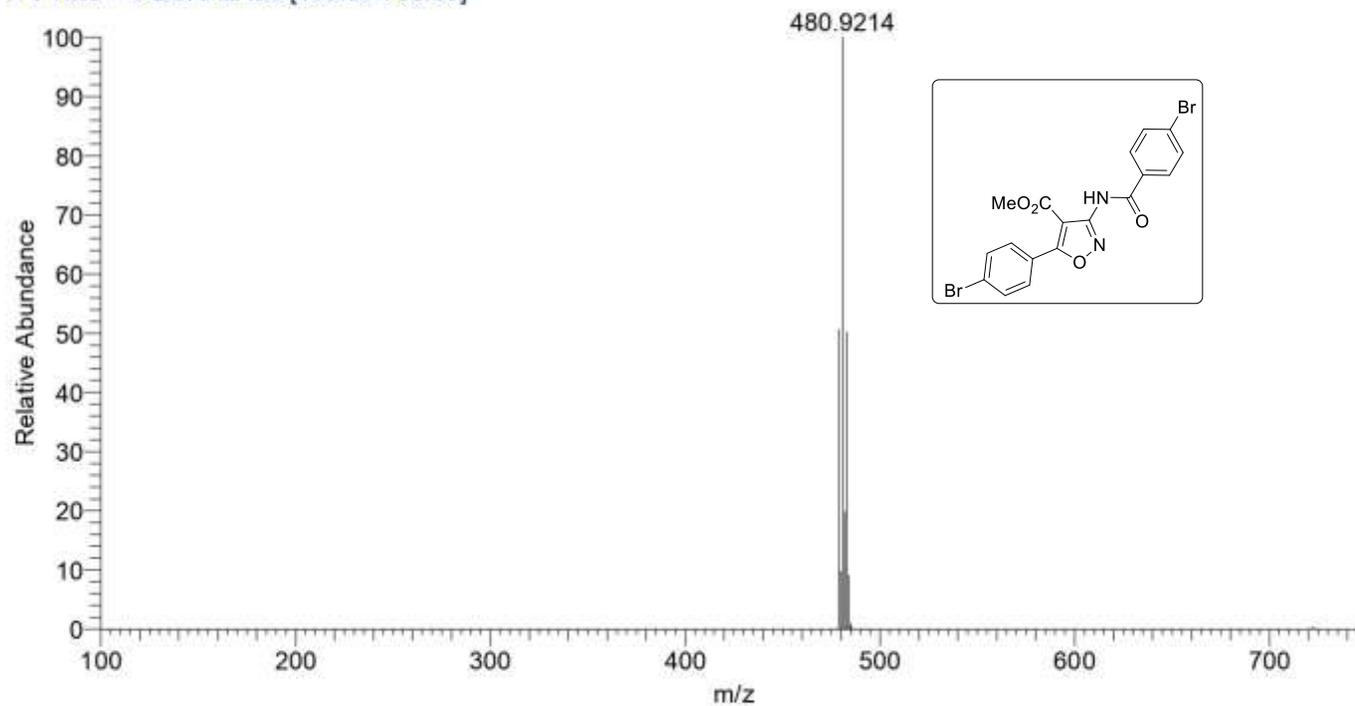


Figure S-73. HRMS spectrum of methyl 3-(4-bromobenzamido)-5-(4-bromophenyl)isoxazole-4-carboxylate (**3dab**).

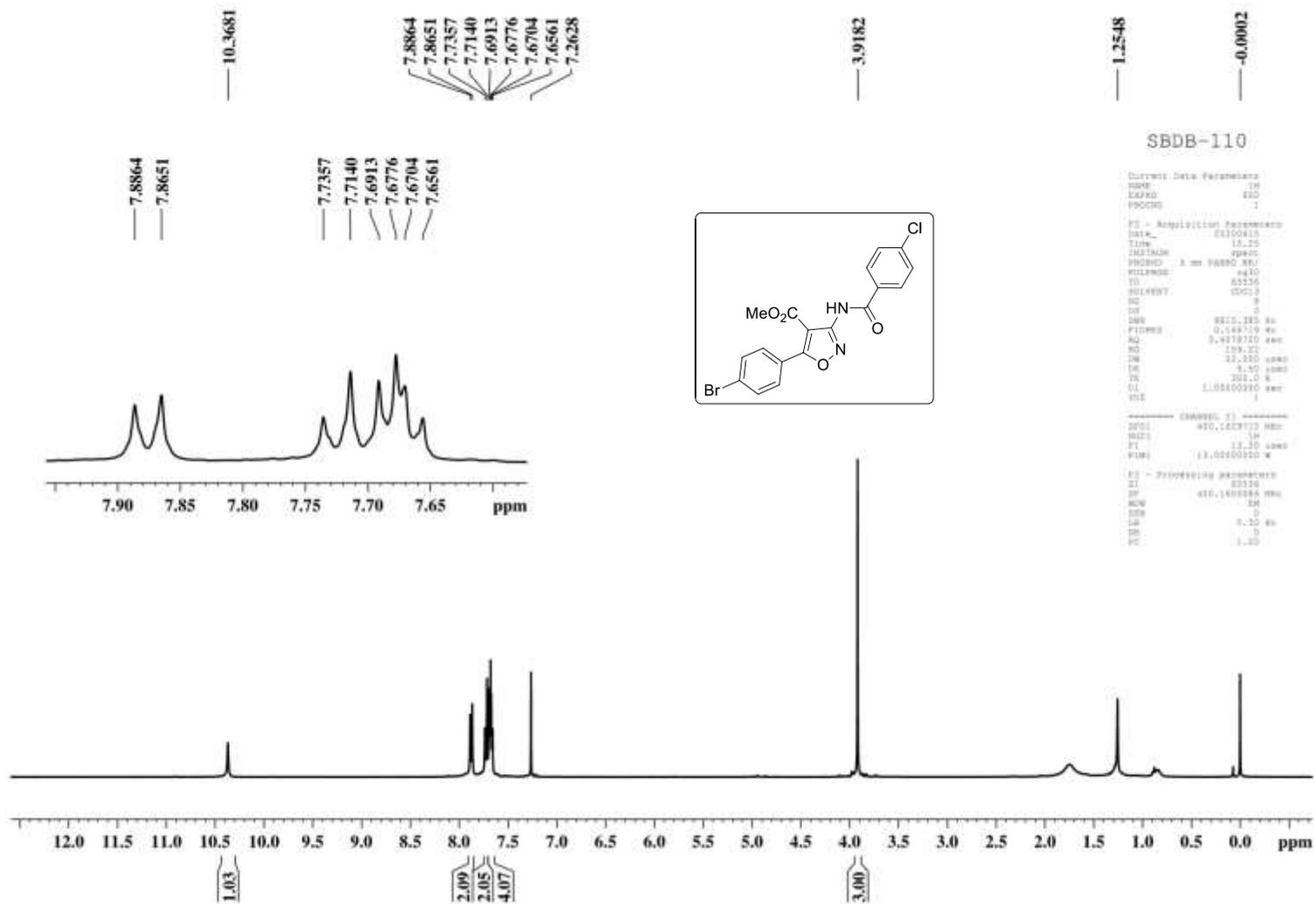


Figure S-74. <sup>1</sup>H-NMR spectrum of methyl 5-(4-bromophenyl)-3-(4-chlorobenzamido)isoxazole-4-carboxylate (**3dac**).

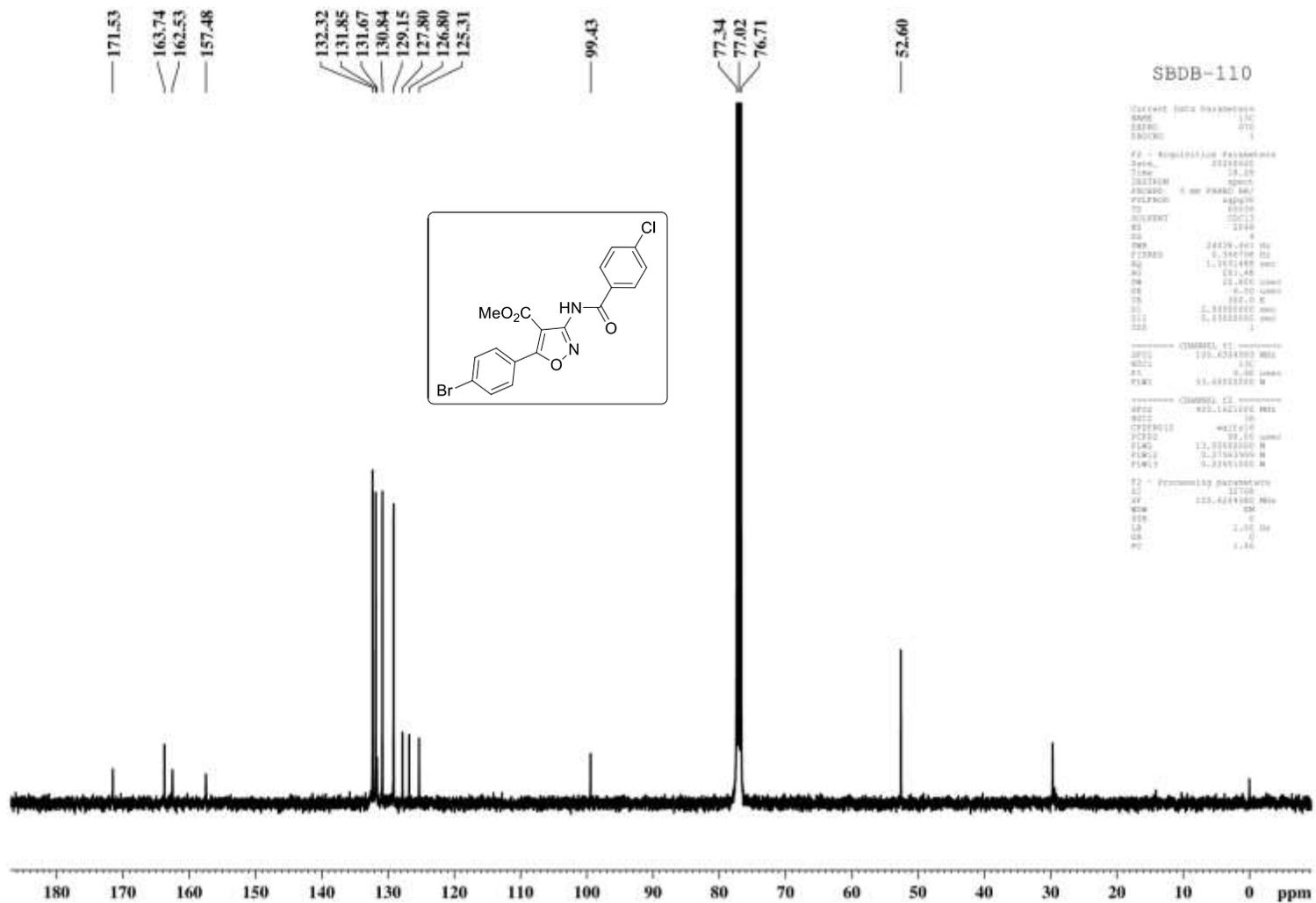


Figure S-75.  $^{13}\text{C}$ -NMR spectrum of methyl 5-(4-bromophenyl)-3-(4-chlorobenzamido)isoxazole-4-carboxylate (**3dac**).

### SAIF [HRMS Report]

Data File:	HRMS20I21SEP16	Original Data Path:	D:\INTERNAL NEW\2020\Sep 2020
Sample ID:	SBDB-112	Sample Name:	
Acquisition Date:	09/21/20 11:22:02 AM	Run Time(min):	0.00
Vial:	CSik1-01:16	Injection Volume( $\mu$ l):	1.00

HRMS20I21SEP16 #12-24 RT: 0.11-0.21 AV: 13 SB: 1 0.01 NL: 4.77E5  
T: FTMS + c ESI Full ms [100.00-750.00]

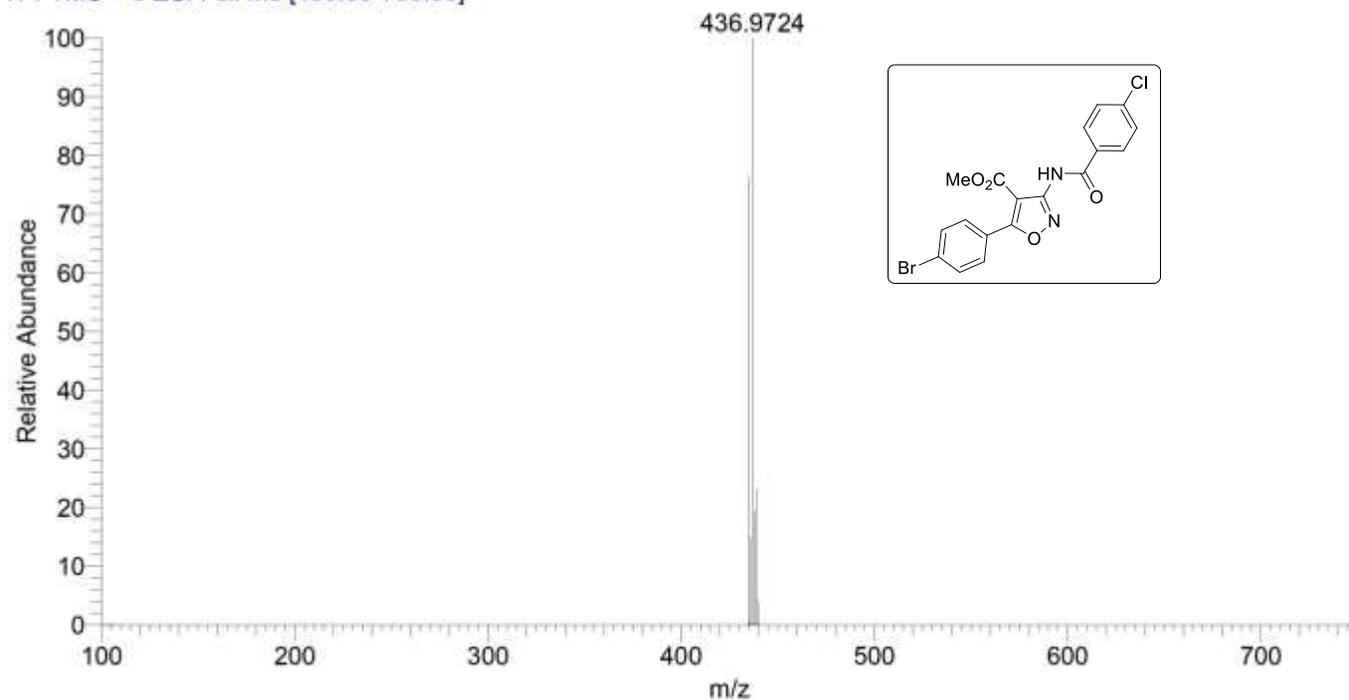


Figure S-76. HRMS spectrum of methyl 5-(4-bromophenyl)-3-(4-chlorobenzamido)isoxazole-4-carboxylate (**3dac**).



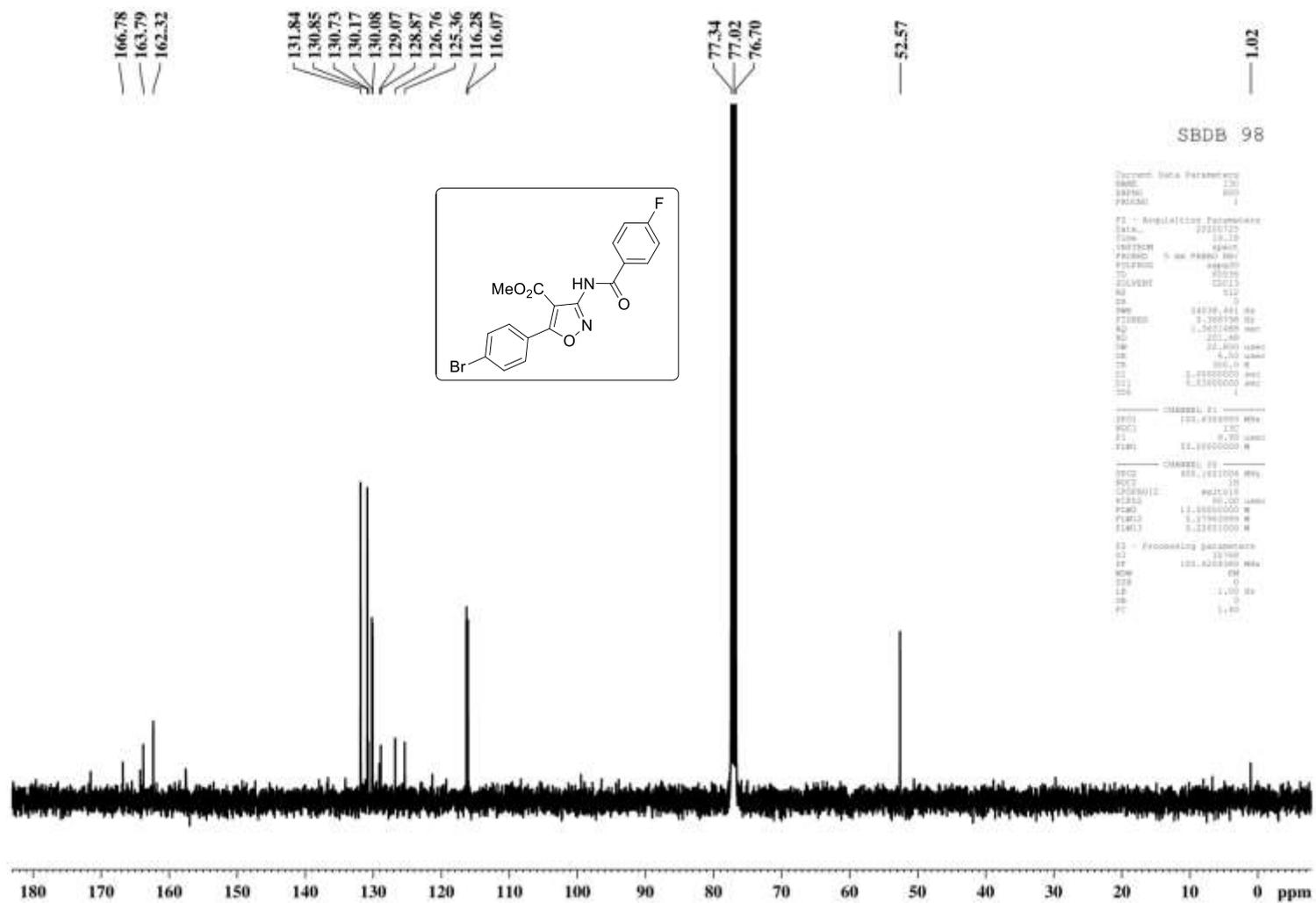
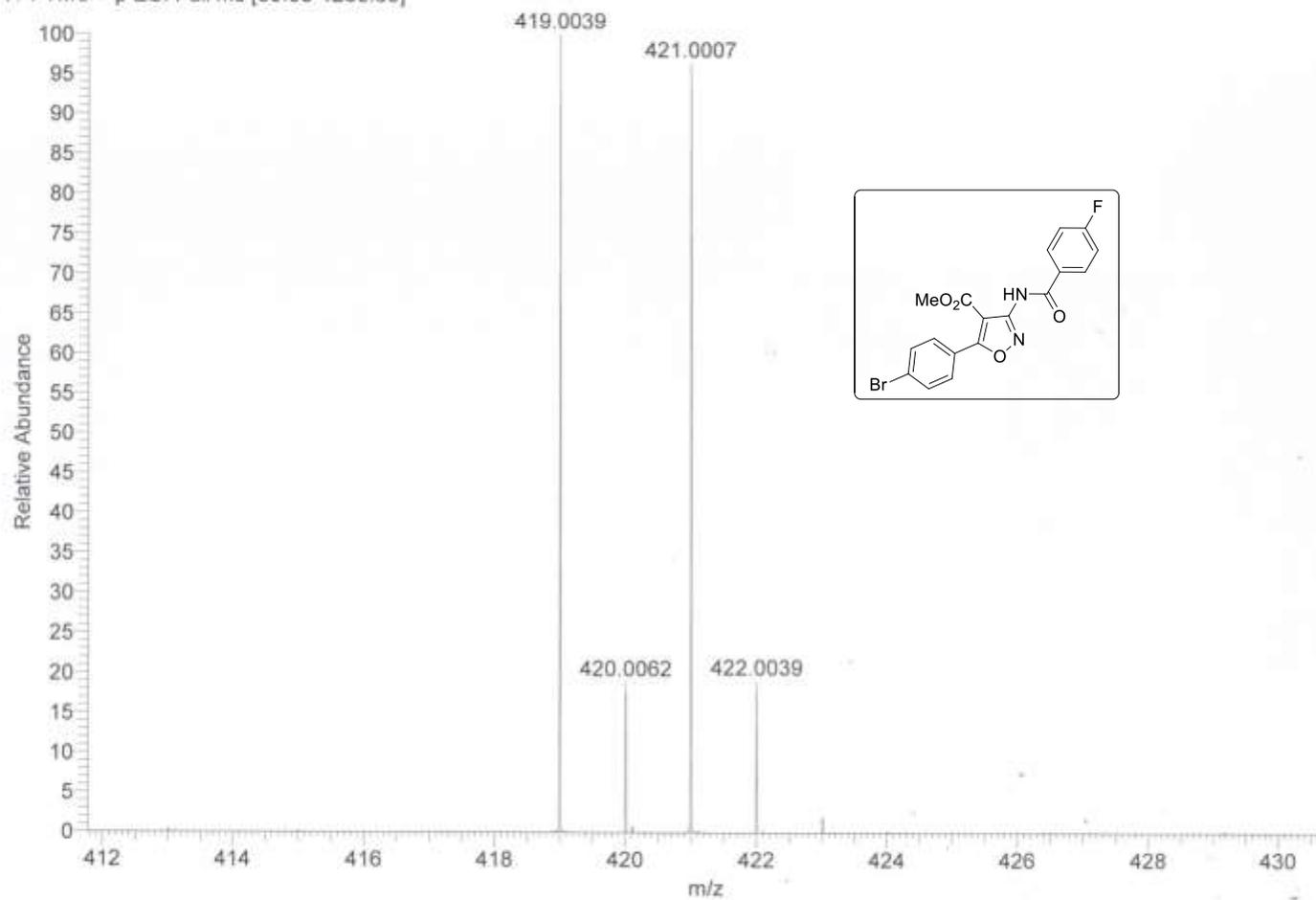
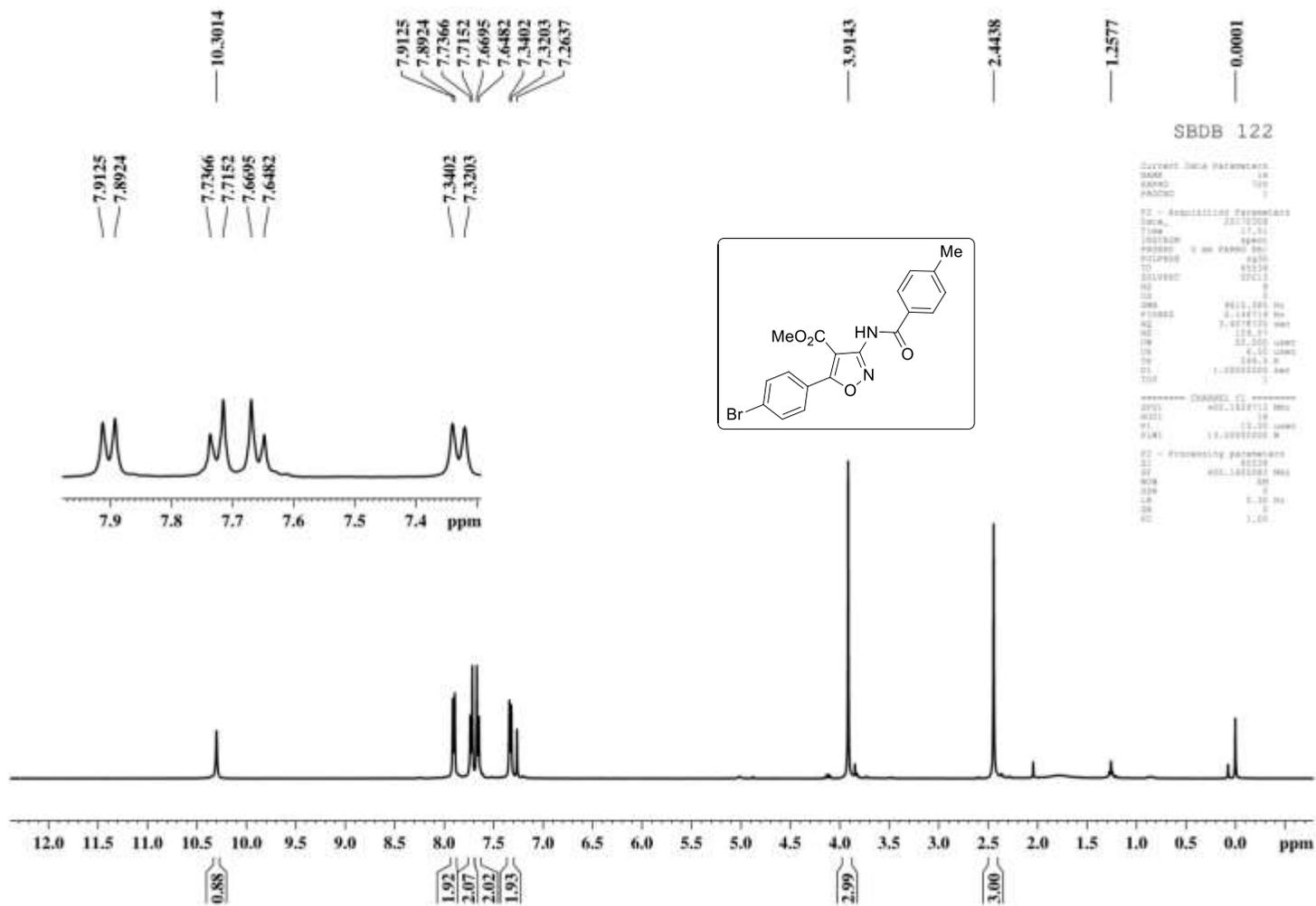


Figure S-78.  $^{13}\text{C}$ -NMR spectrum of methyl 5-(4-bromophenyl)-3-(4-fluorobenzamido)isoxazole-4-carboxylate (**3dad**).

HRMS19I26MARCH07 #18 RT: 0.26 AV: 1 SB: 5 0.02-0.08 NL: 1.59E6  
T: FTMS + p ESI Full ms [80.00-1200.00]



**Figure S-79.** HRMS spectrum of methyl 5-(4-bromophenyl)-3-(4-fluorobenzamido)isoxazole-4-carboxylate (**3dad**).



**Figure S-80.**  $^1\text{H-NMR}$  spectrum of methyl 5-(4-bromophenyl)-3-(4-methylbenzamido)isoxazole-4-carboxylate (**3dae**).

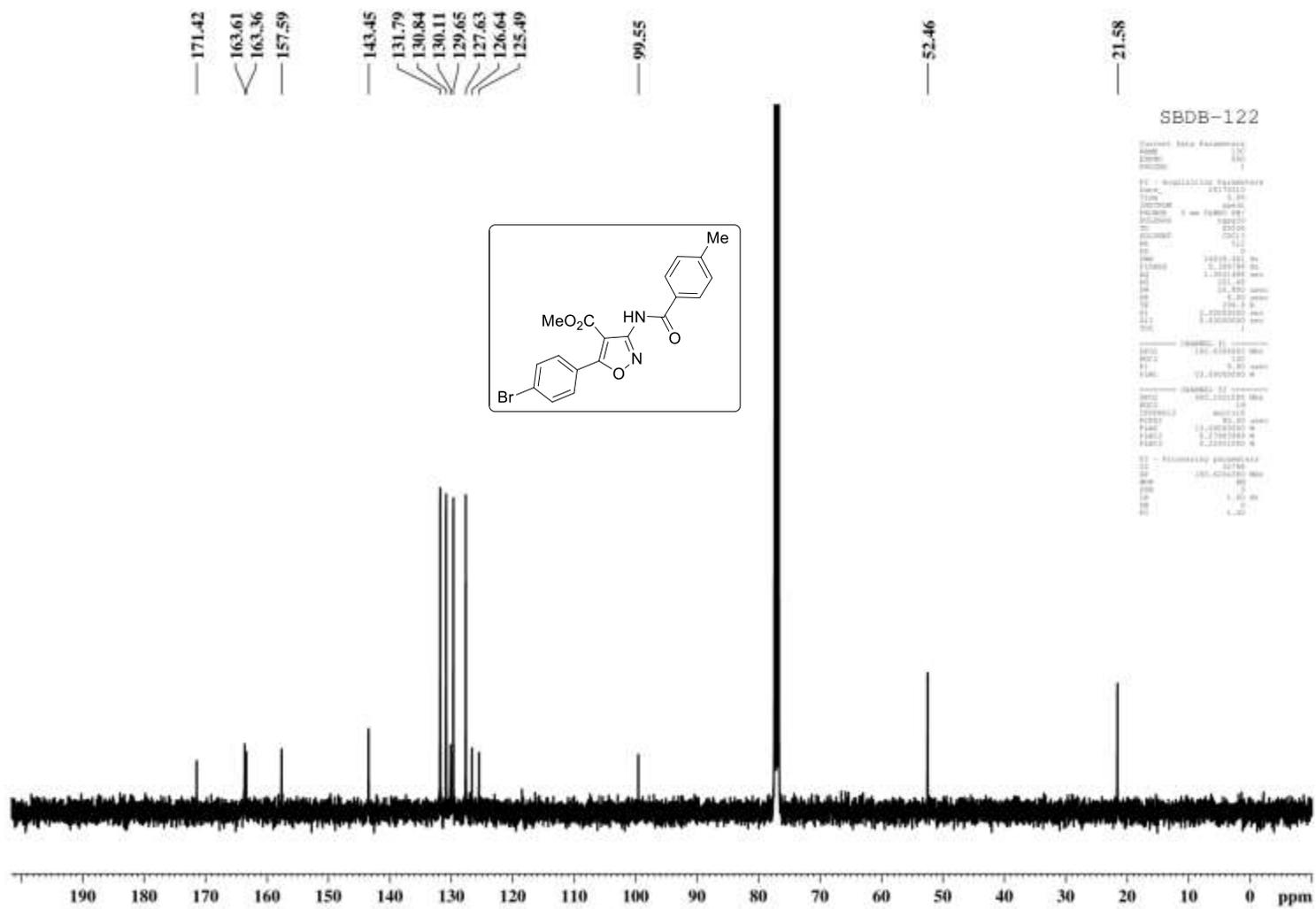


Figure S-81.  $^{13}\text{C}$ -NMR spectrum of methyl 5-(4-bromophenyl)-3-(4-methylbenzamido)isoxazole-4-carboxylate (**3dae**).

HRMS19126MARCH03 #13-14 RT: 0.19-0.20 AV: 2 SB: 5 0.02-0.08 NL: 1.00E6  
T: FTMS + p ESI Full ms [80.00-1200.00]

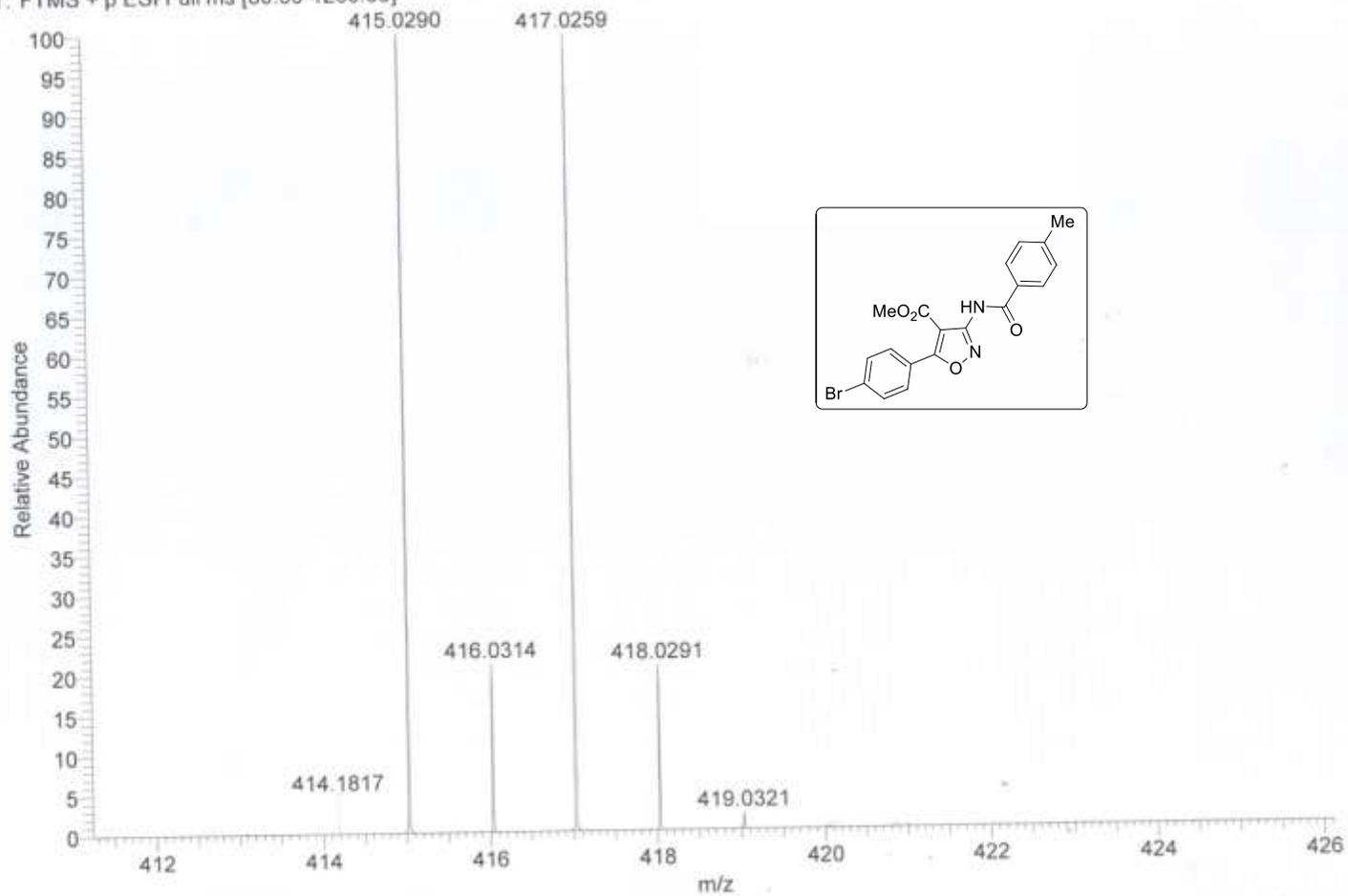


Figure S-82. HRMS spectrum of methyl 5-(4-bromophenyl)-3-(4-methylbenzamido)isoxazole-4-carboxylate (**3dae**).



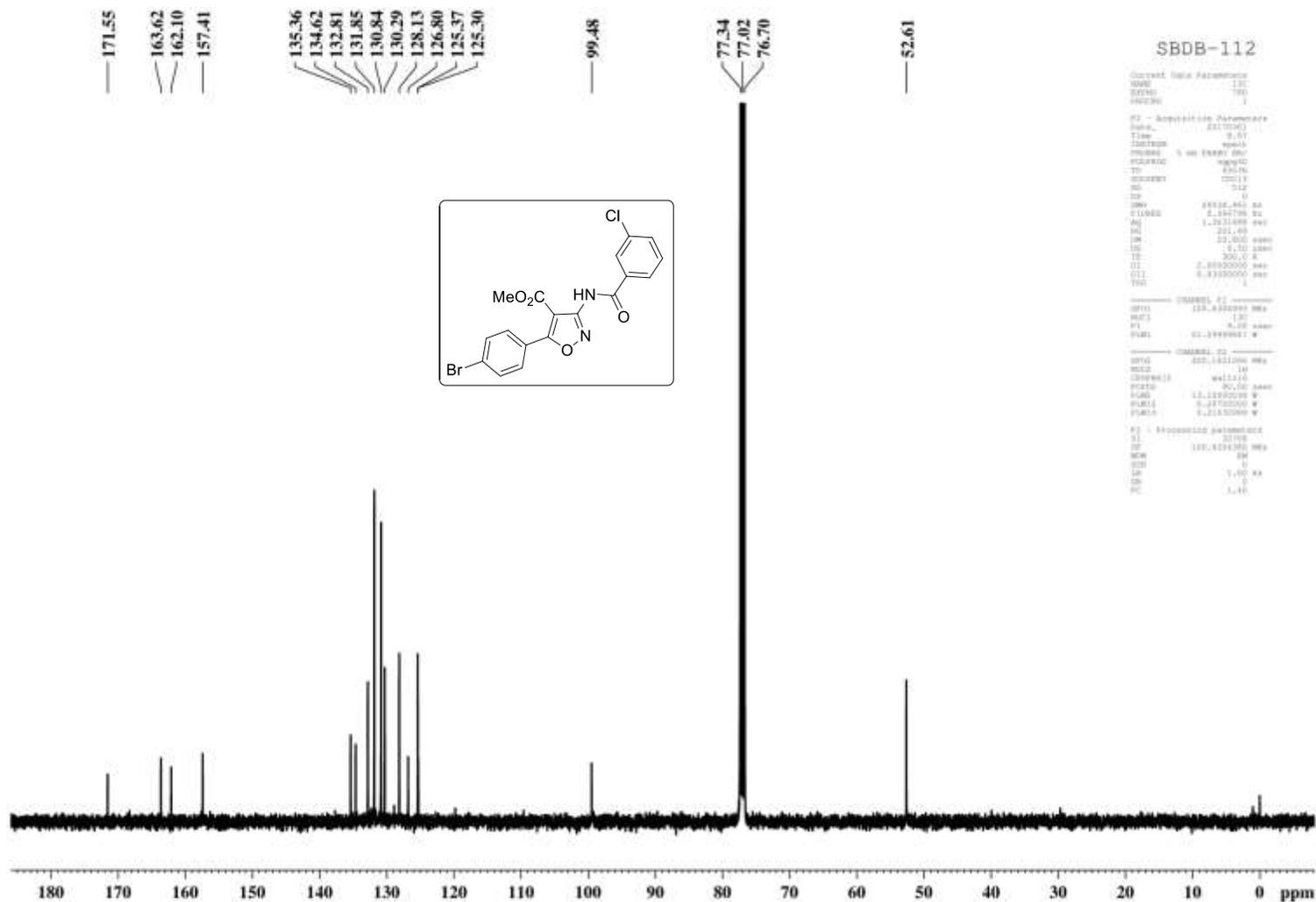


Figure S-84. <sup>13</sup>C-NMR spectrum of methyl 3-(3-chlorobenzamido)-5-(4-bromophenyl)isoxazole-4-carboxylate (**3daf**).

### SAIF [HRMS Report]

Data File:	HRMS20I21SEP15	Original Data Path:	D:\INTERNAL NEW\2020\Sep 2020
Sample ID:	SBDB-110	Sample Name:	
Acquisition Date:	09/21/20 11:20:03 AM	Run Time(min):	0.00
Vial:	CSik1-01:15	Injection Volume(μl):	1.00

HRMS20I21SEP15 #12-24 RT: 0.11-0.21 AV: 13 SB: 1 0.01 NL: 4.70E5  
T: FTMS + c ESI Full ms [100.00-750.00]

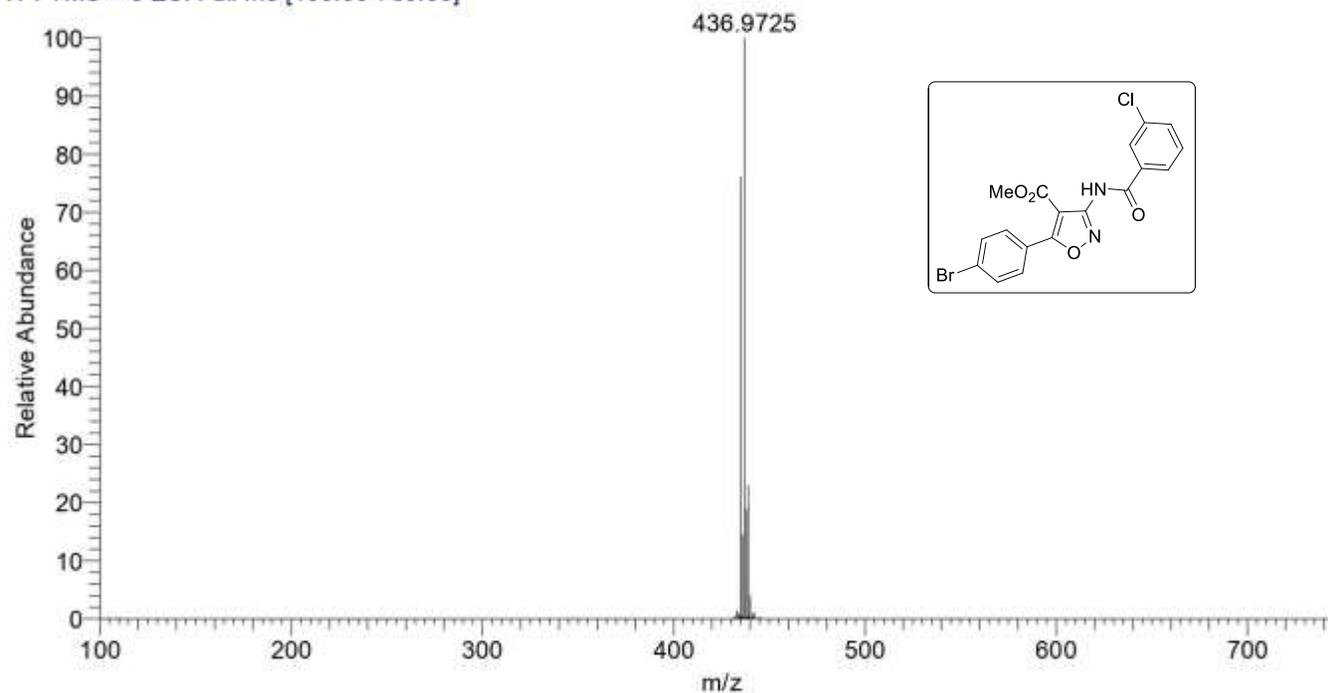


Figure S-85. HRMS spectrum of methyl 3-(3-chlorobenzamido)-5-(4-bromophenyl)isoxazole-4-carboxylate (**3daf**).

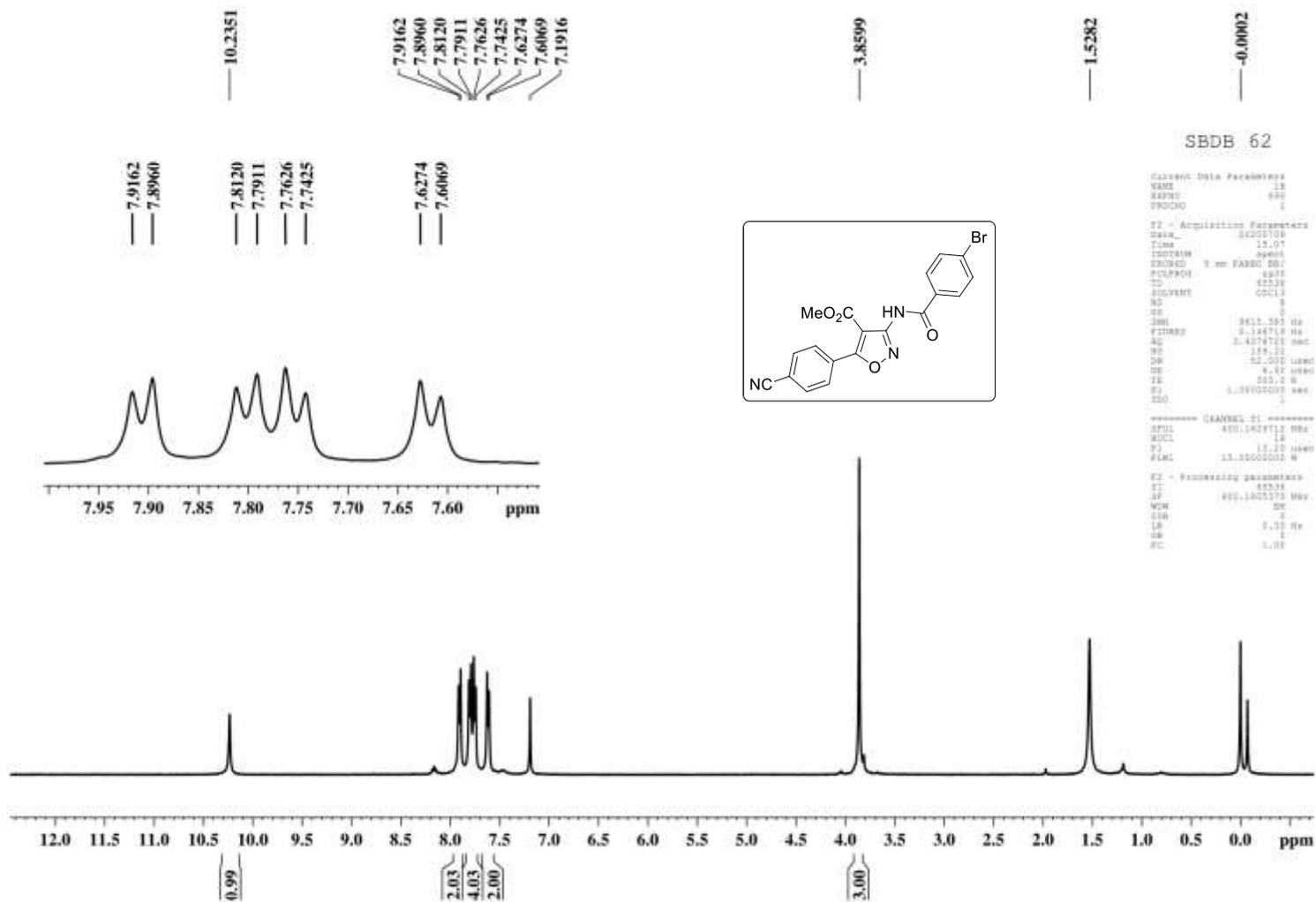
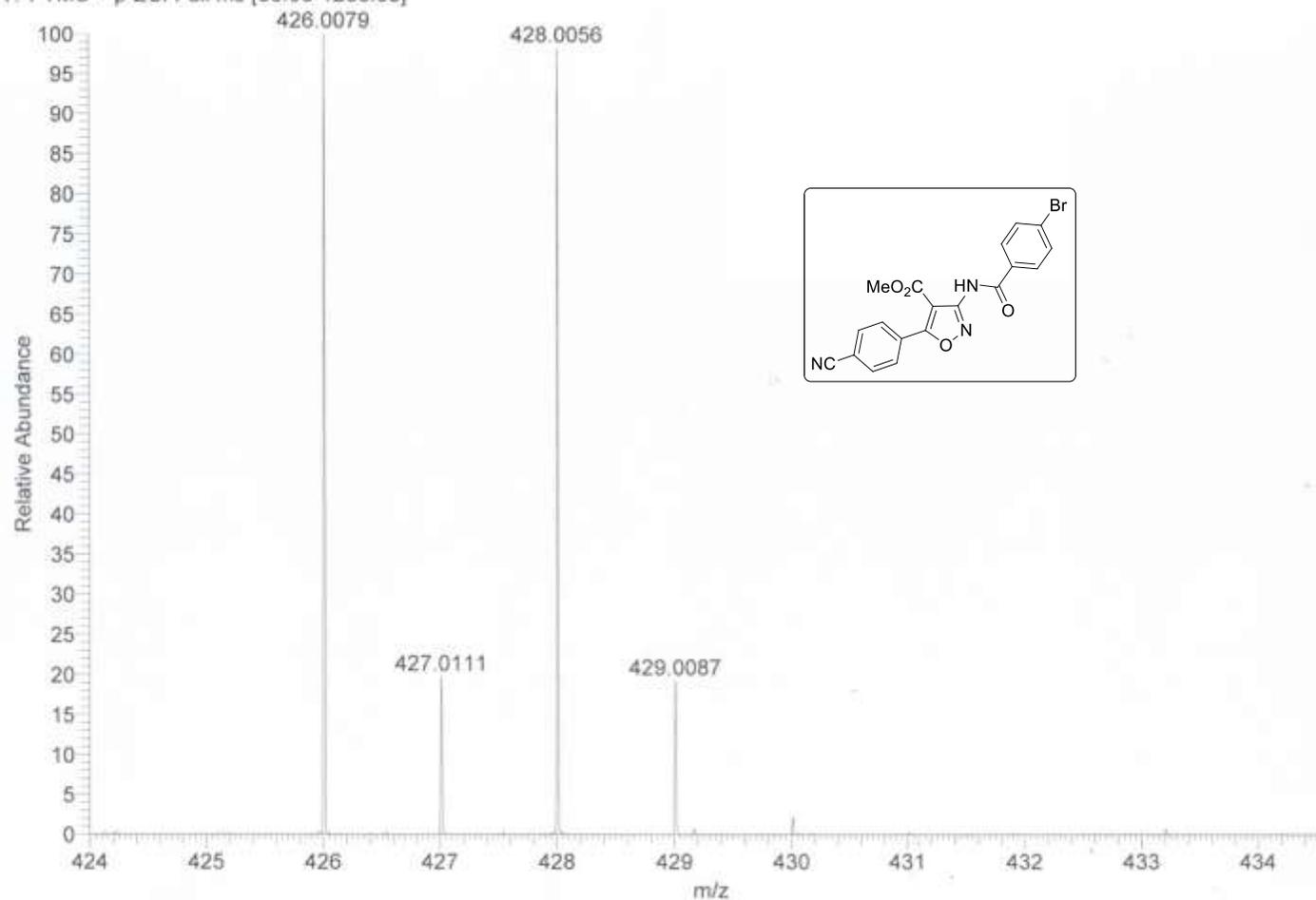


Figure S-86. <sup>1</sup>H-NMR spectrum of methyl 3-(4-bromobenzamido)-5-(4-cyanophenyl)isoxazole-4-carboxylate (**3fab**).



HRMS19I26MARCH14 #10 RT: 0.14 AV: 1 SB: 5 0.02-0.08 NL: 2.27E6  
T: FTMS + p ESI Full ms [80.00-1200.00]



**Figure S-88.** HRMS spectrum of methyl 3-(4-bromobenzamido)-5-(4-cyanophenyl)isoxazole-4-carboxylate (**3fab**).

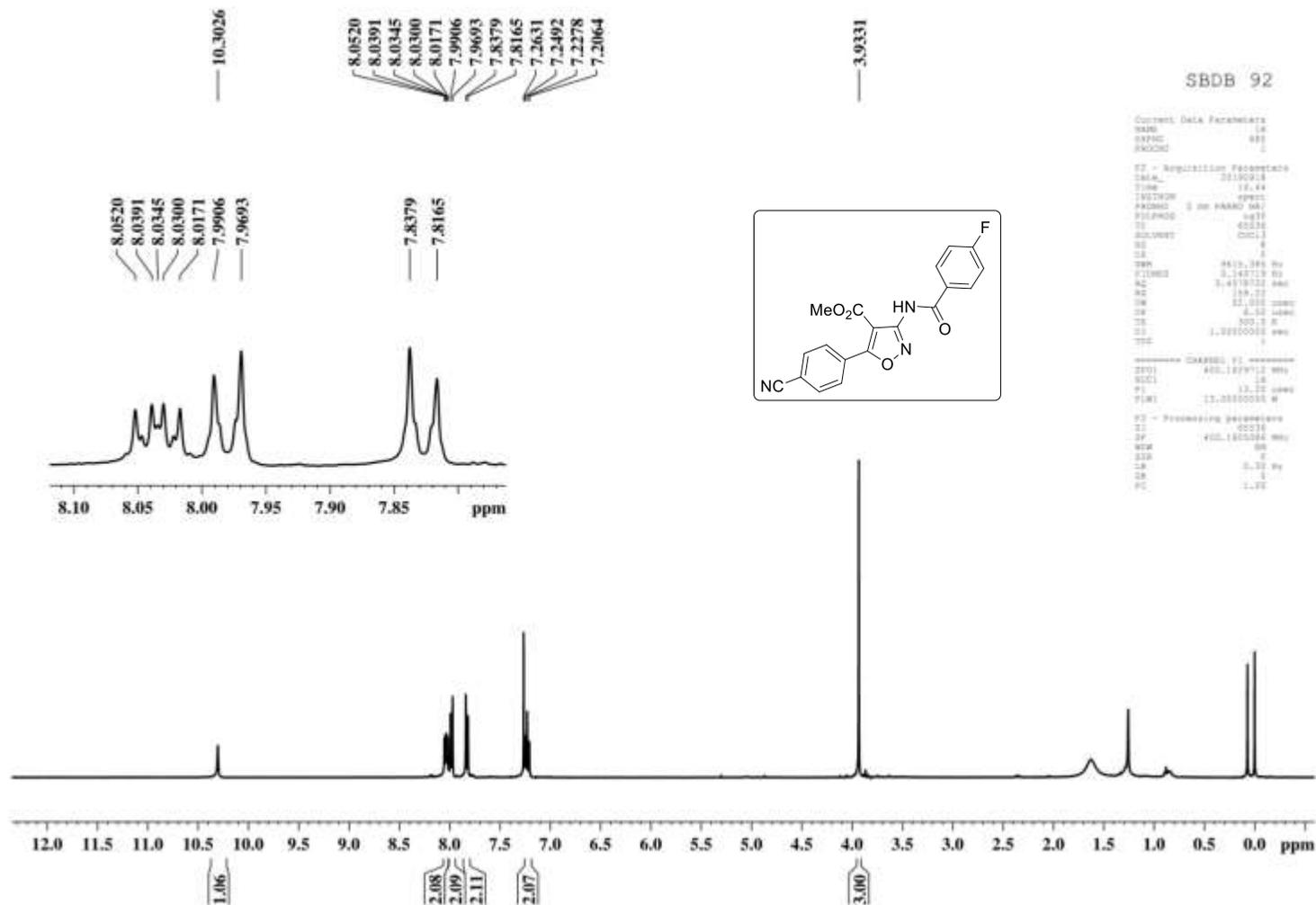


Figure S-89. <sup>1</sup>H-NMR spectrum of methyl 5-(4-cyanophenyl)-3-(4-fluorobenzamido)isoxazole-4-carboxylate (**3fad**).

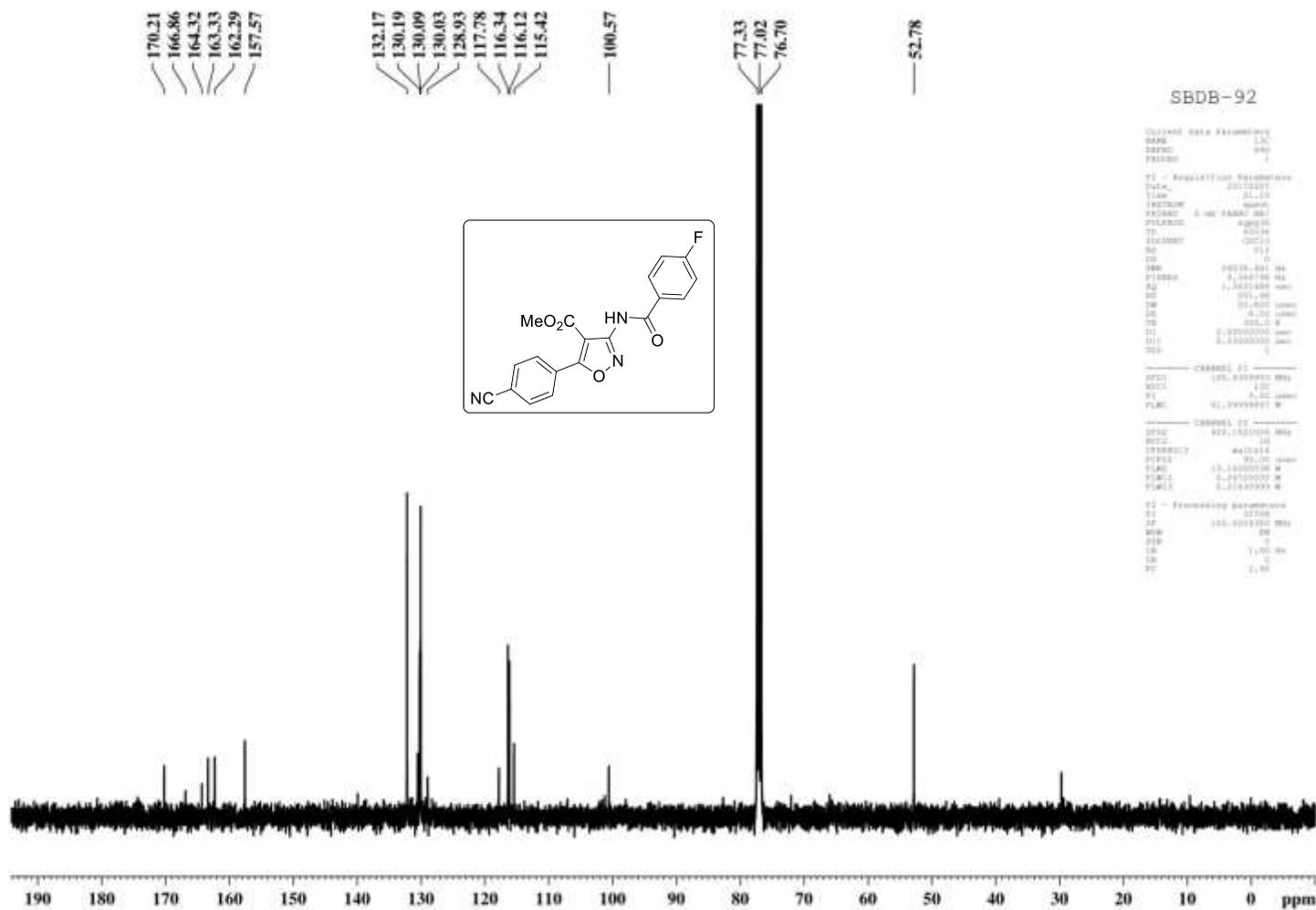


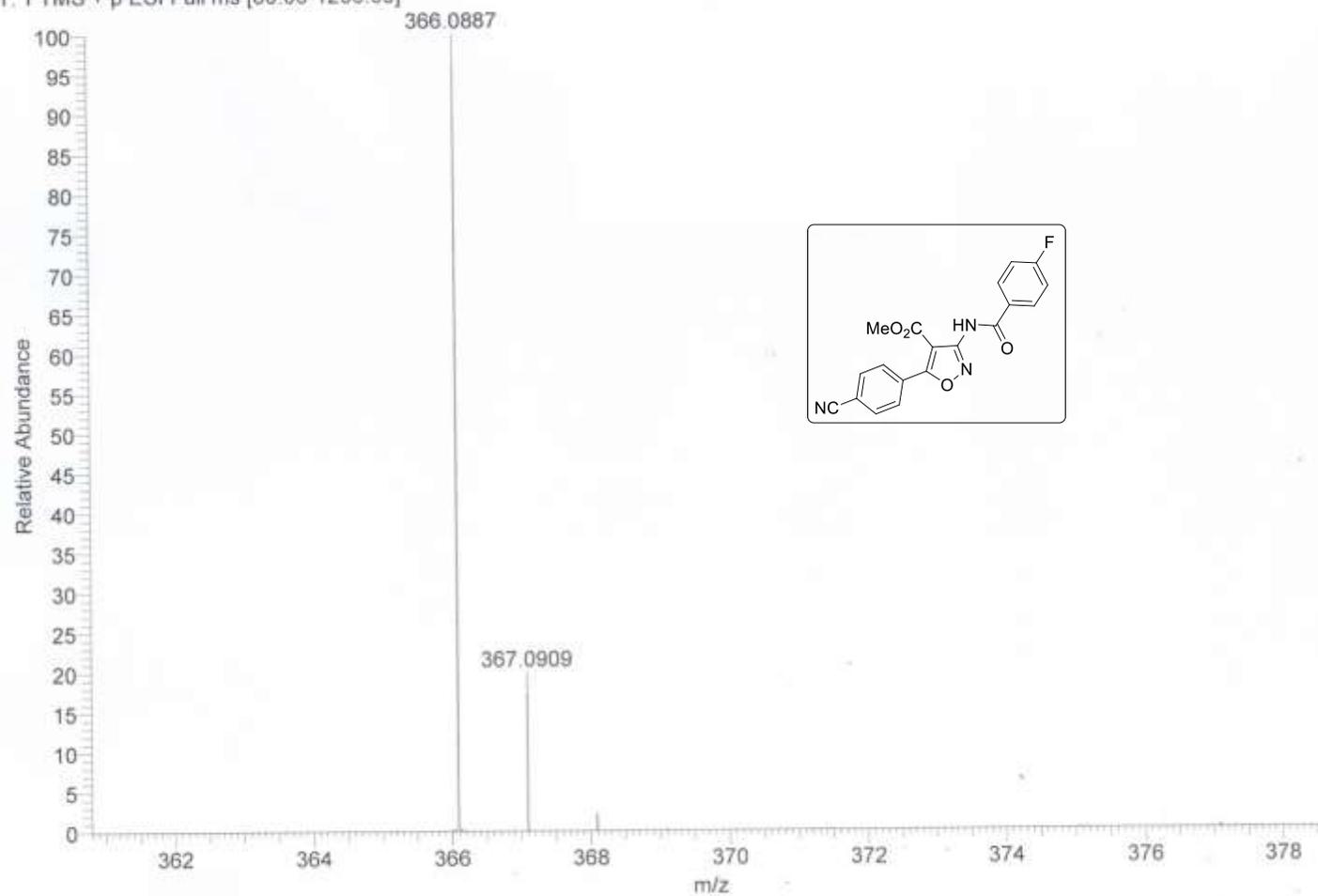
Figure S-90.  $^{13}\text{C}$ -NMR spectrum of methyl 5-(4-cyanophenyl)-3-(4-fluorobenzamido)isoxazole-4-carboxylate (**3fad**).

D:\INTERNALSL\HRMS19I26MARCH15

3/26/2019 12:49:54 PM

SBDB-92

HRMS19I26MARCH15 #8 RT: 0.11 AV: 1 SB: 5 0.02-0.08 NL: 4.32E6  
T: FTMS + p ESI Full ms [80.00-1200.00]



**Figure S-91.** HRMS spectrum of methyl 5-(4-cyanophenyl)-3-(4-fluorobenzamido)isoxazole-4-carboxylate (**3fad**).

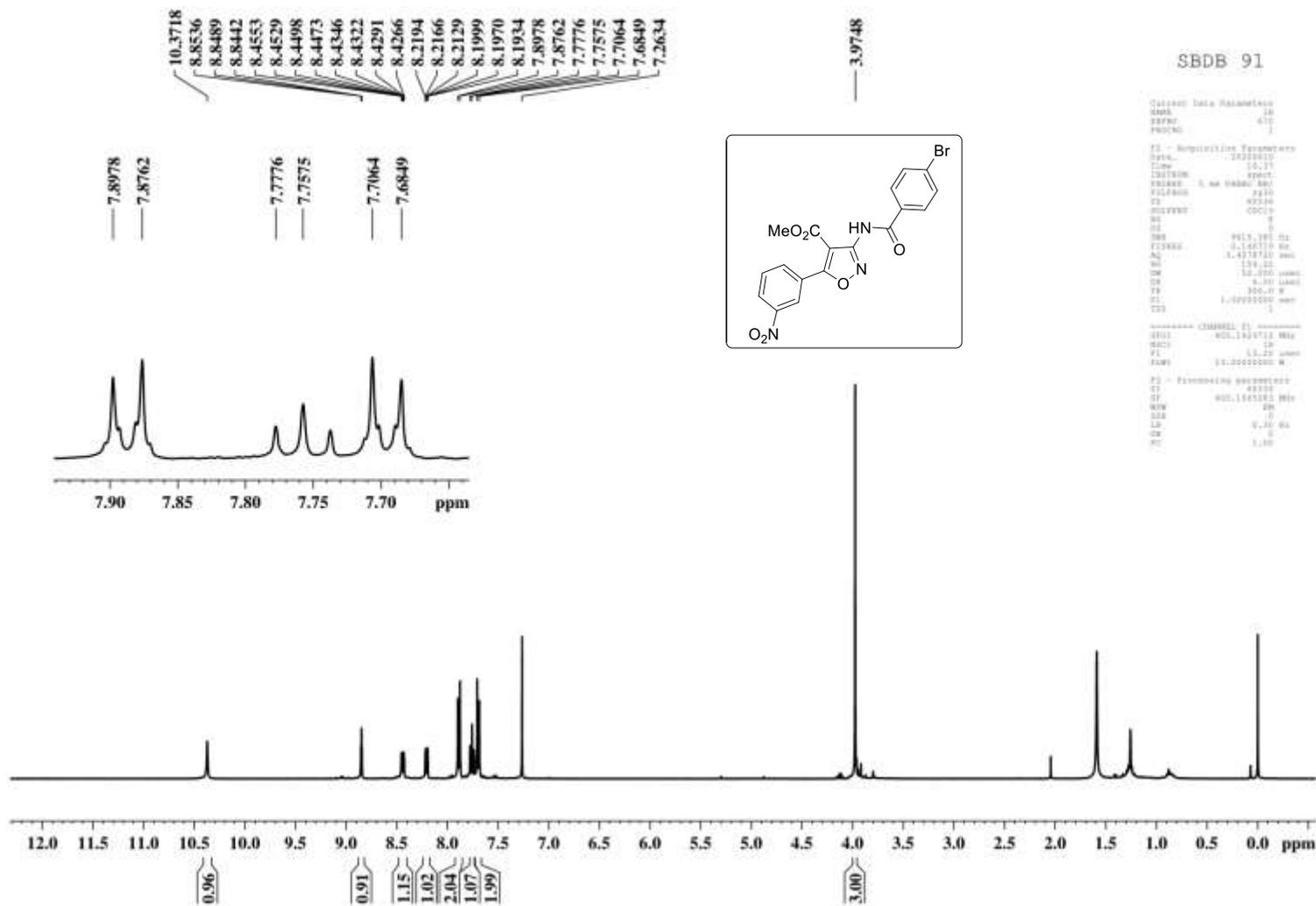
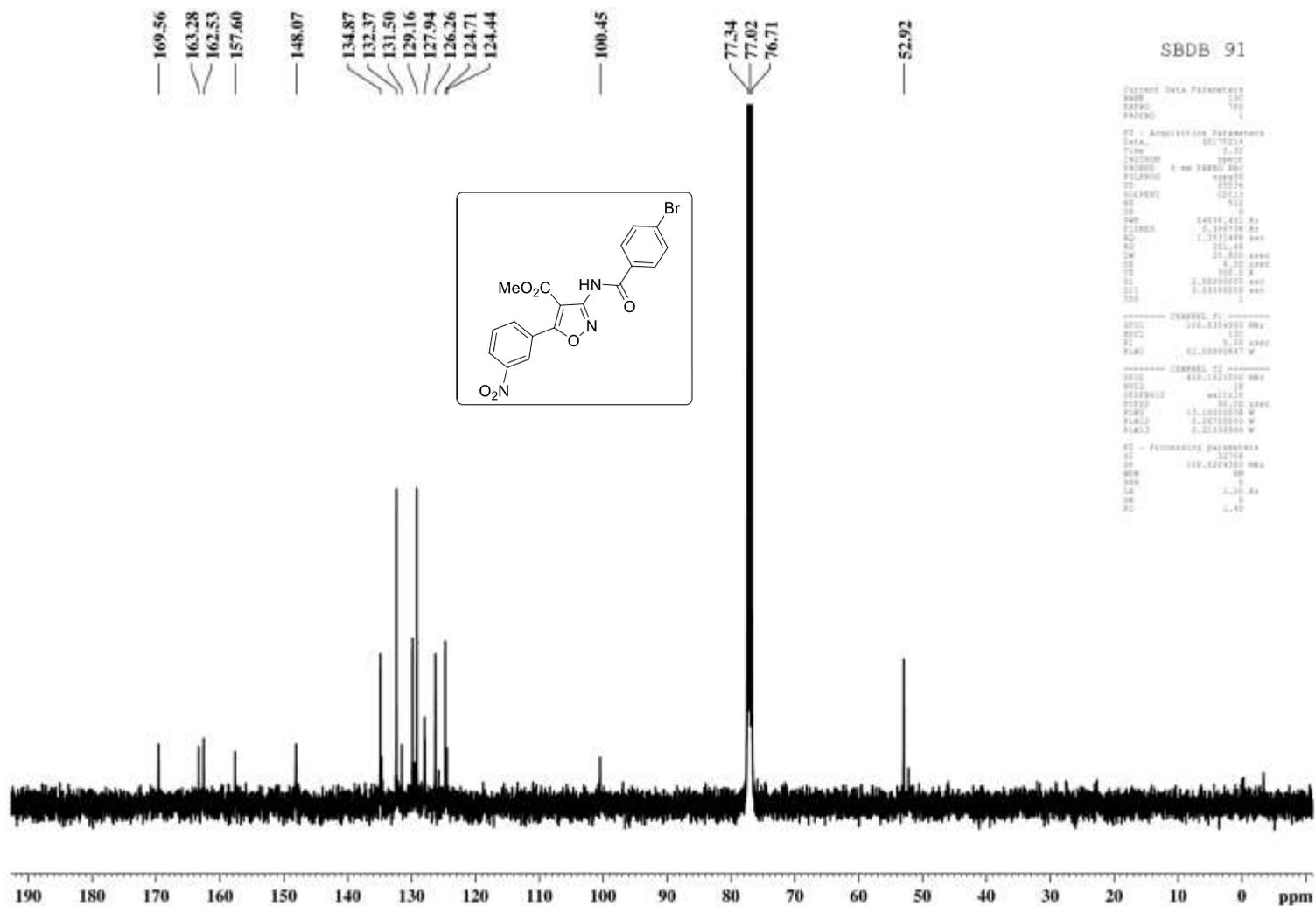
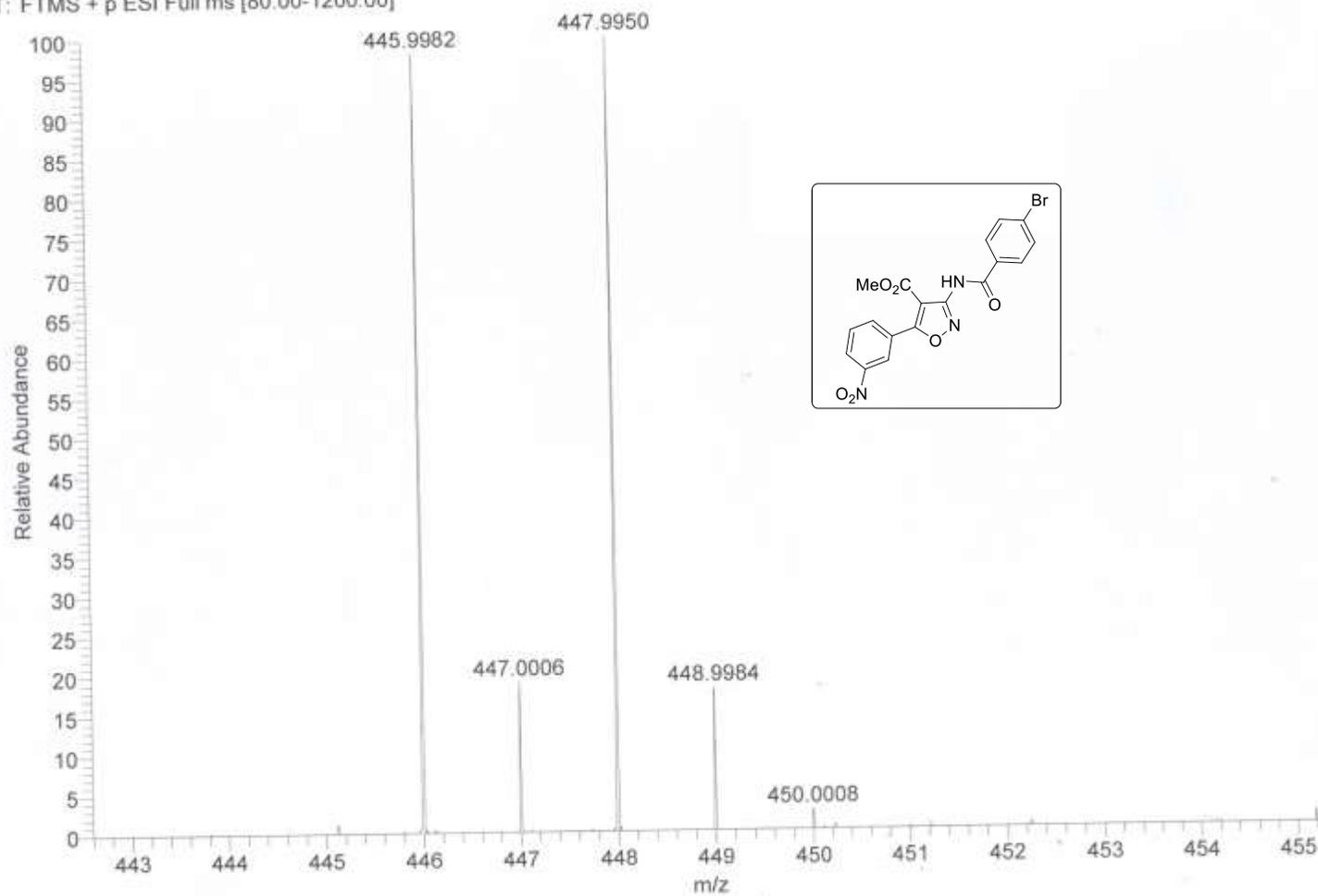


Figure S-92. <sup>1</sup>H-NMR spectrum of methyl 3-(4-bromobenzamido)-5-(3-nitrophenyl)isoxazole-4-carboxylate (**3hab**).



**Figure S-93.**  $^{13}\text{C}$ -NMR spectrum of methyl 3-(4-bromobenzamido)-5-(3-nitrophenyl)isoxazole-4-carboxylate (**3hab**).

HRMS19I26MARCH02 #16 RT: 0.23 AV: 1 SB: 5 0.02-0.08 NL: 7.74E5  
T: FTMS + p ESI Full ms [80.00-1200.00]



**Figure S-94.** HRMS spectrum of methyl 3-(4-bromobenzamido)-5-(3-nitrophenyl)isoxazole-4-carboxylate (**3hab**).



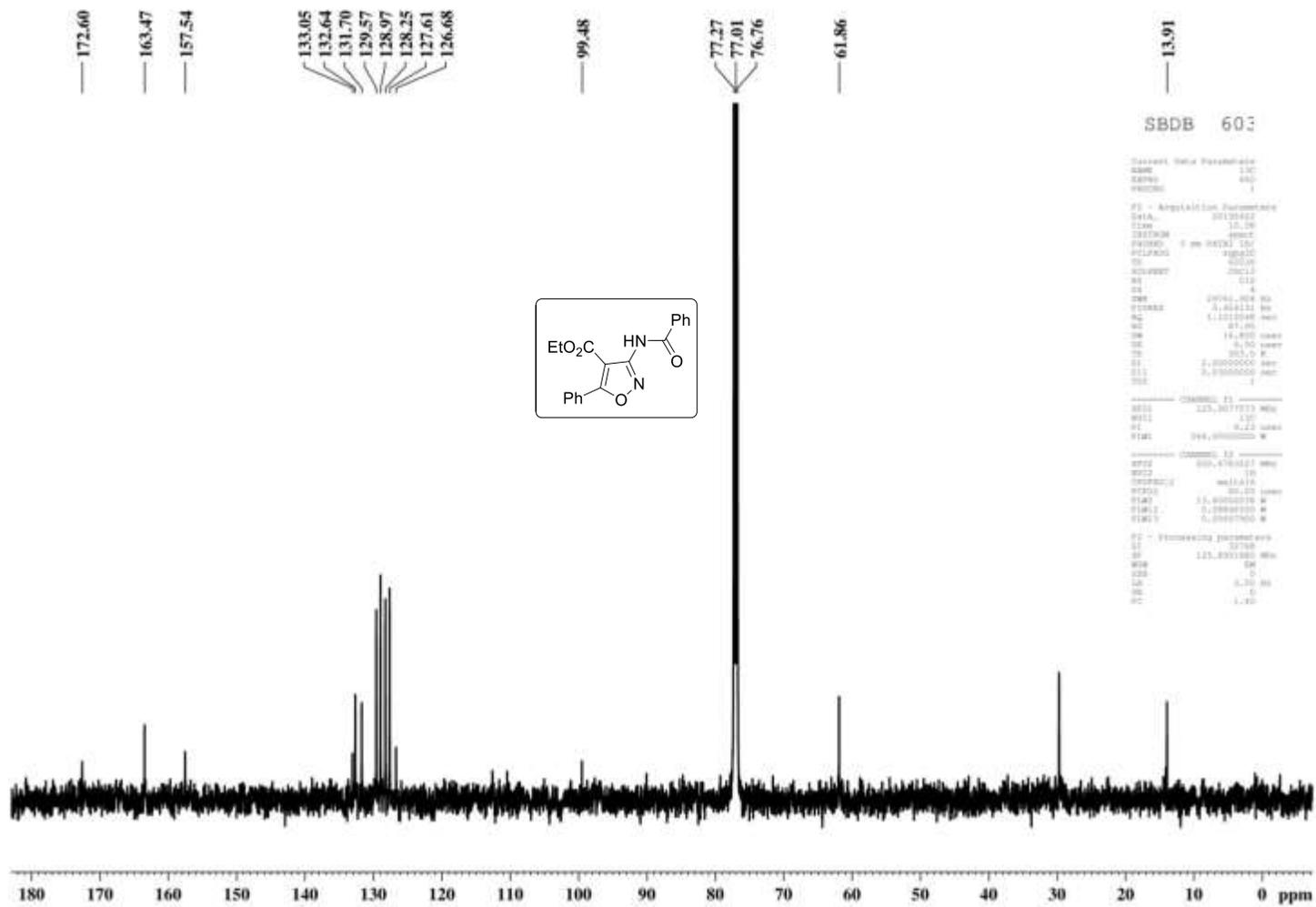
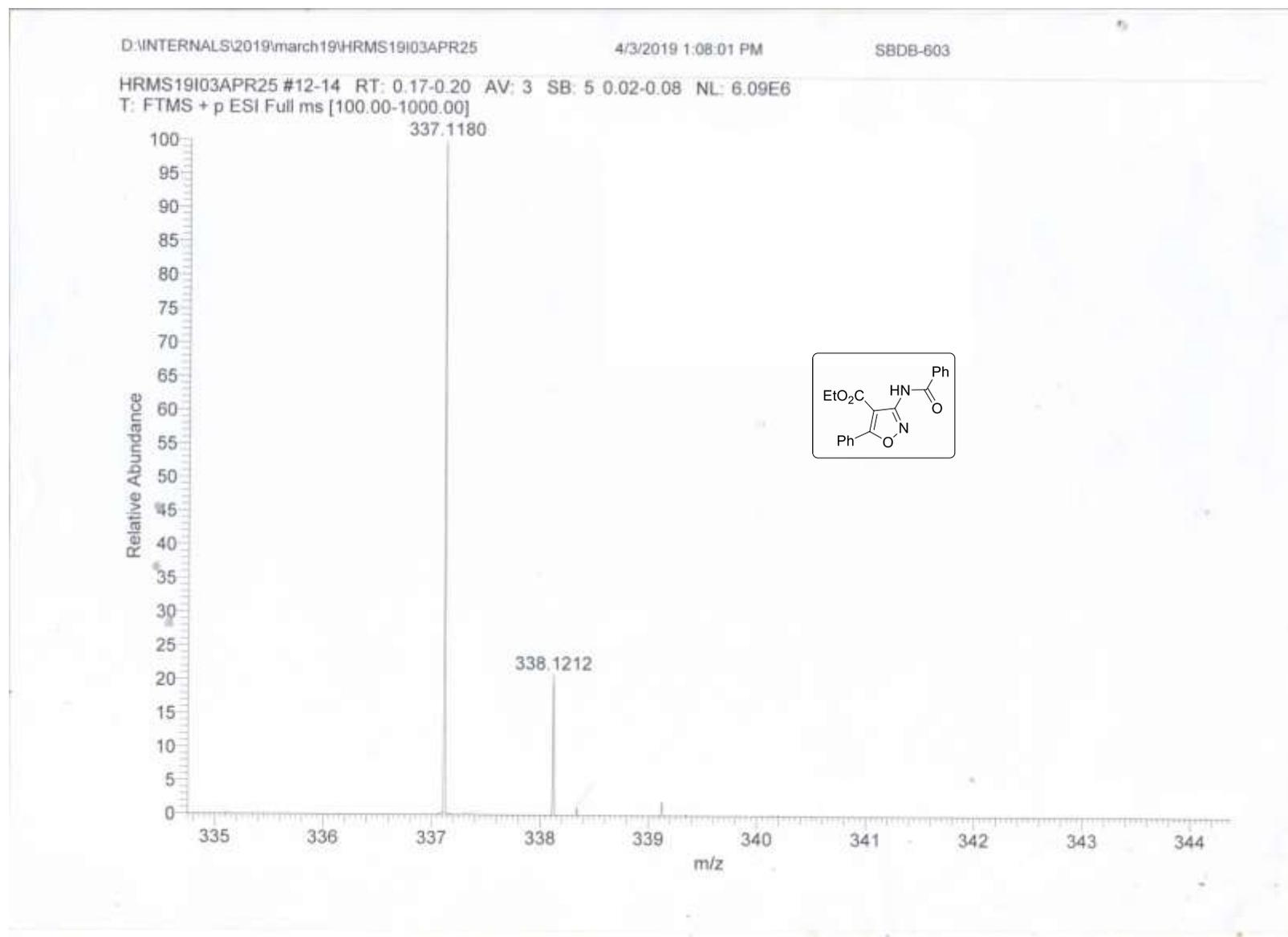


Figure S-96.  $^{13}\text{C}$ -NMR spectrum of ethyl 3-benzamido-5-phenylisoxazole-4-carboxylate (**3aba**).



**Figure S-97.** HRMS spectrum of ethyl 3-benzamido-5-phenylisoxazole-4-carboxylate (**3aba**).

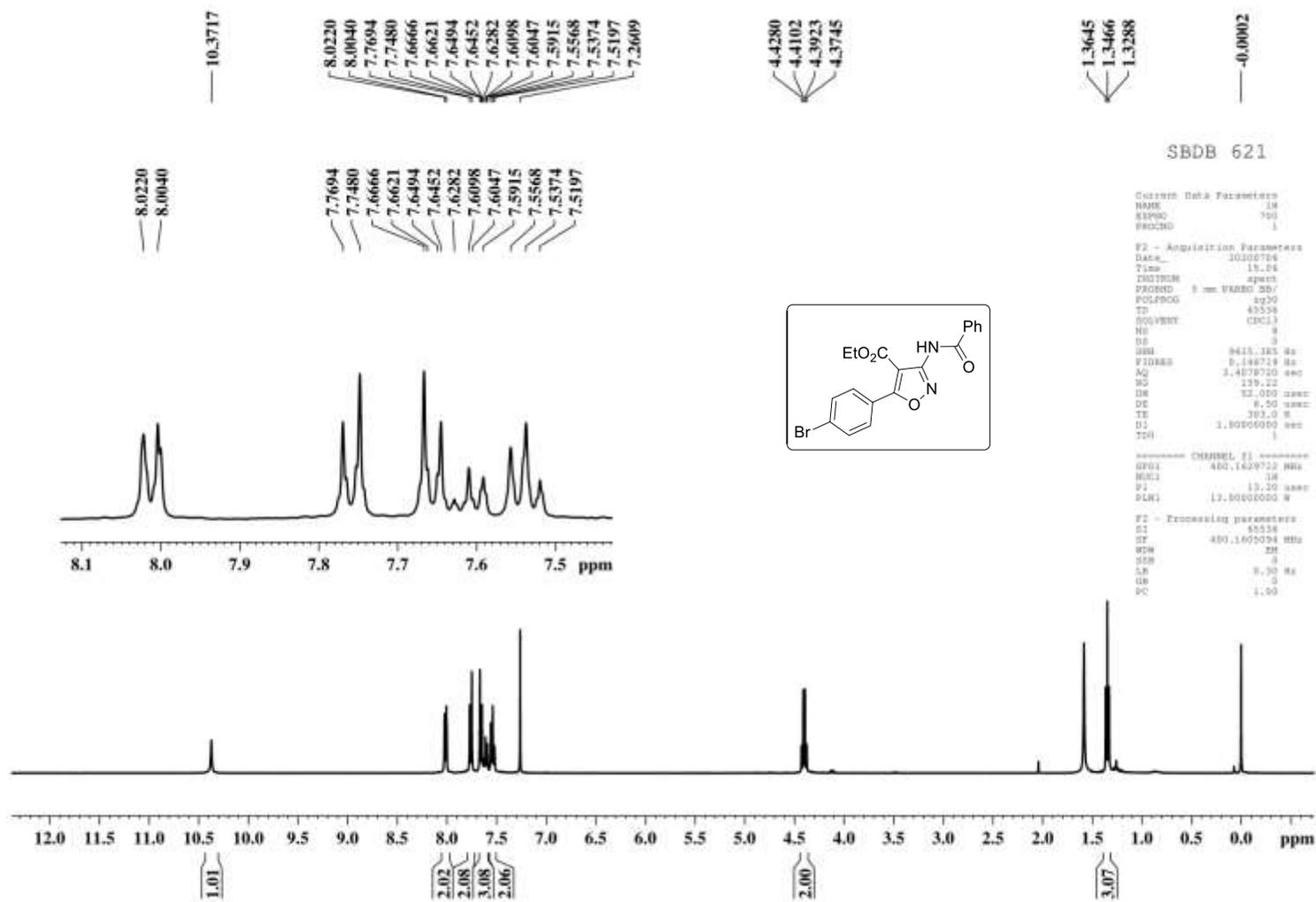


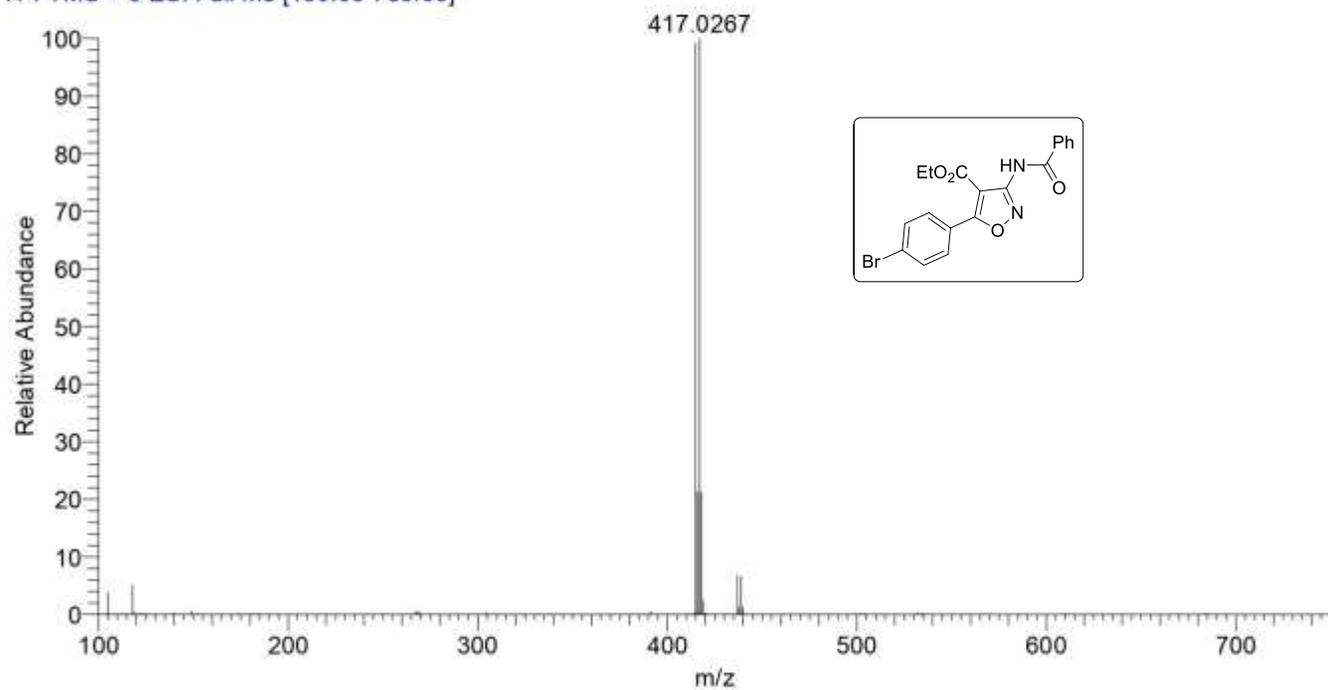
Figure S-98. <sup>1</sup>H-NMR spectrum of ethyl 3-benzamido-5-(4-bromophenyl)isoxazole-4-carboxylate (**3dba**).



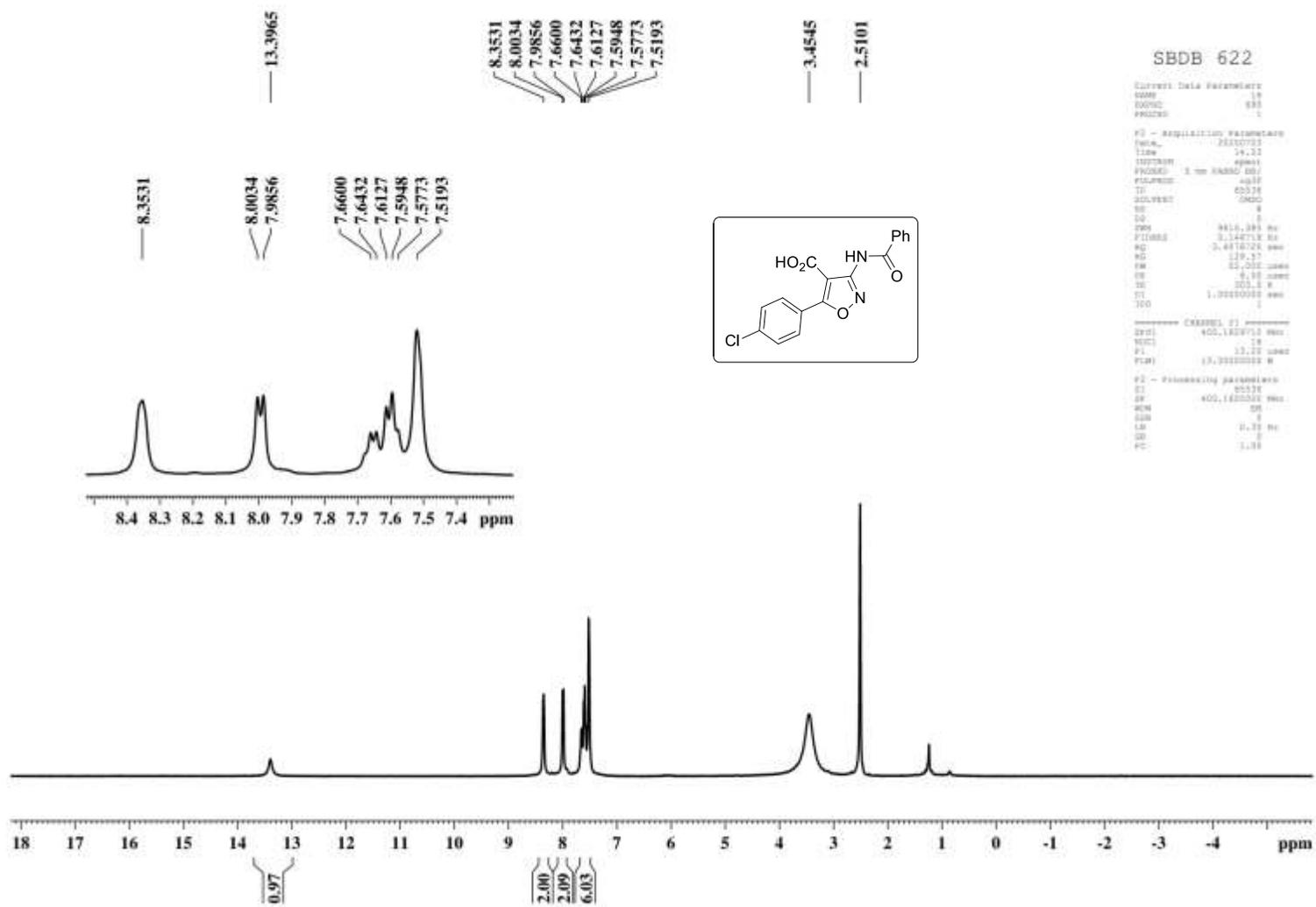
### SAIF [HRMS Report]

Data File:	HRMS20115SEP04	Original Data Path:	D:\INTERNAL NEW\2020\Sep 2020
Sample ID:	SBDB-621	Sample Name:	
Acquisition Date:	09/15/20 10:29:30 AM	Run Time(min):	0.00
Vial:	CStk1-01:4	Injection Volume( $\mu$ l):	1.00

HRMS20115SEP04 #12-24 RT: 0.11-0.21 AV: 13 SB: 1 0.01 NL: 4.34E6  
T: FTMS + c ESI Full ms [100.00-750.00]



**Figure S-100.** HRMS spectrum of ethyl 3-benzamido-5-(4-bromophenyl)isoxazole-4-carboxylate (**3dba**).



**Figure S-101.** <sup>1</sup>H-NMR spectrum of 3-benzamido-5-(4-chlorophenyl)isoxazole-4-carboxylic acid (**3cca**).

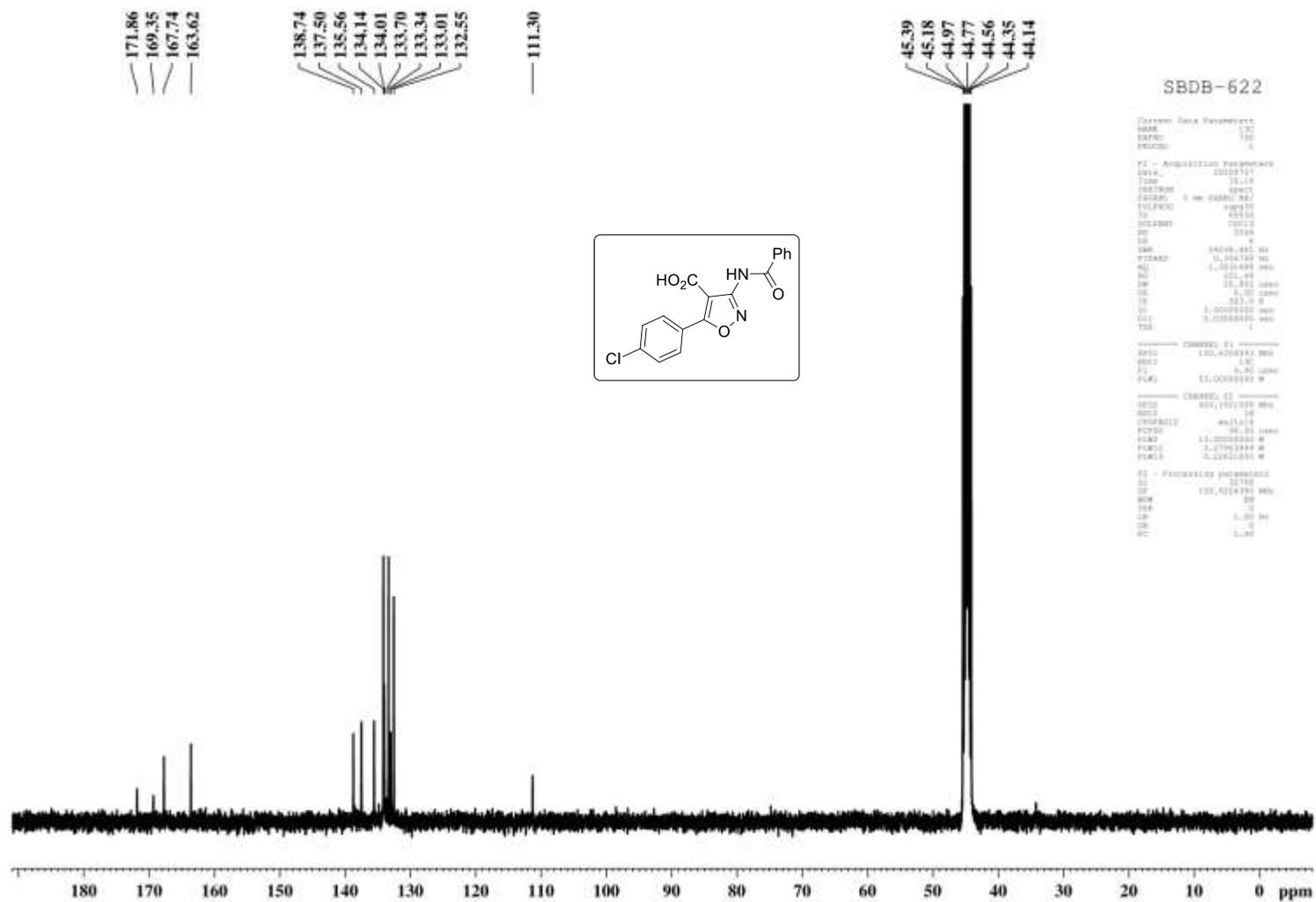


Figure S-102. <sup>13</sup>C-NMR spectrum of 3-benzamido-5-(4-chlorophenyl)isoxazole-4-carboxylic acid (**3cca**).

HRMS19I30APR5 #11 RT: 0.15 AV: 1 SB: 4 0.03-0.08 NL: 3.02E5

T: FTMS + p ESI Full ms [100.00-1000.00]

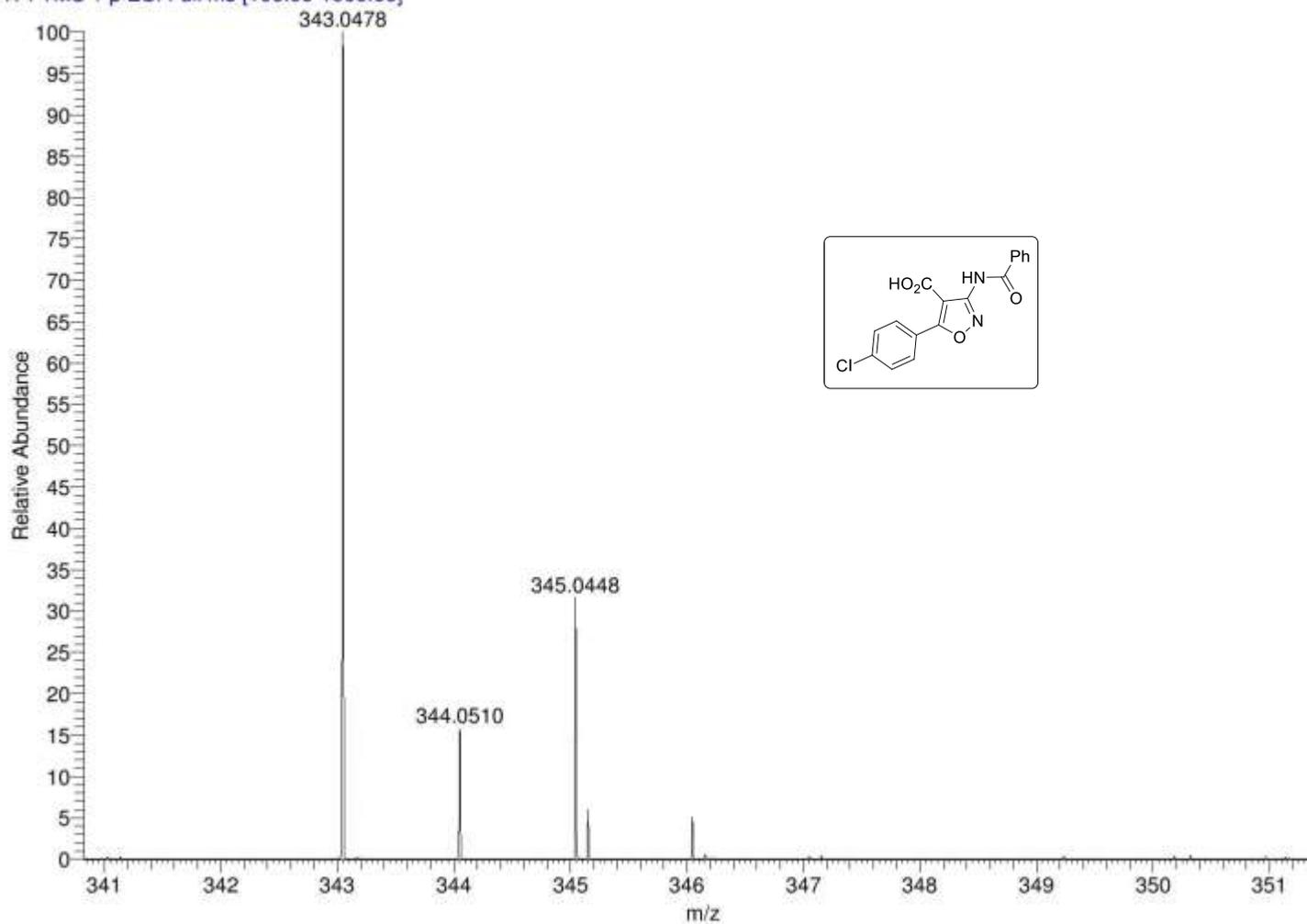
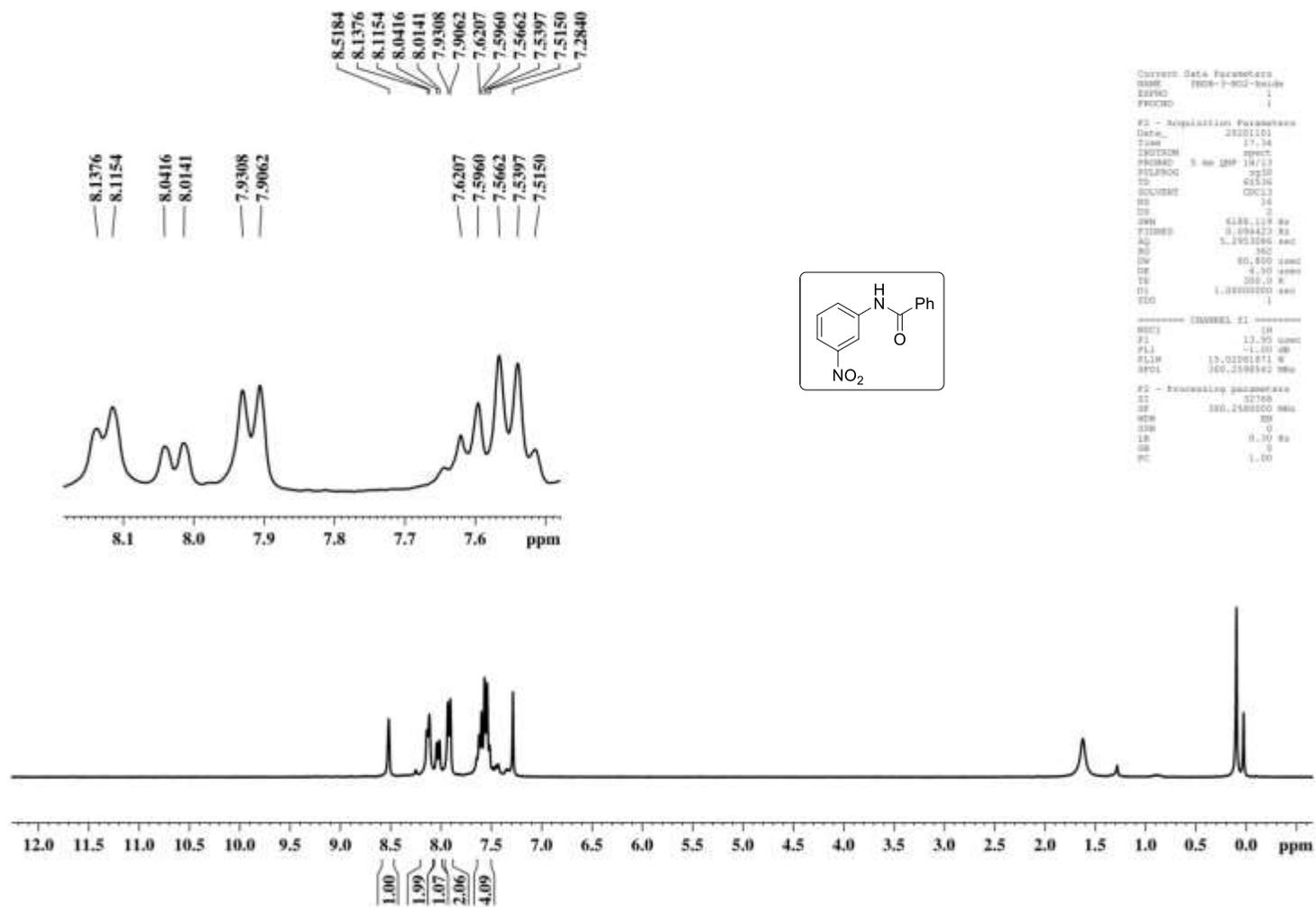


Figure S-103. HRMS spectrum of 3-benzamido-5-(4-chlorophenyl)isoxazole-4-carboxylic acid (**3cca**).



**Figure S-104.**  $^1\text{H-NMR}$  spectrum of *N*-(3-nitrophenyl)benzamide (5a).

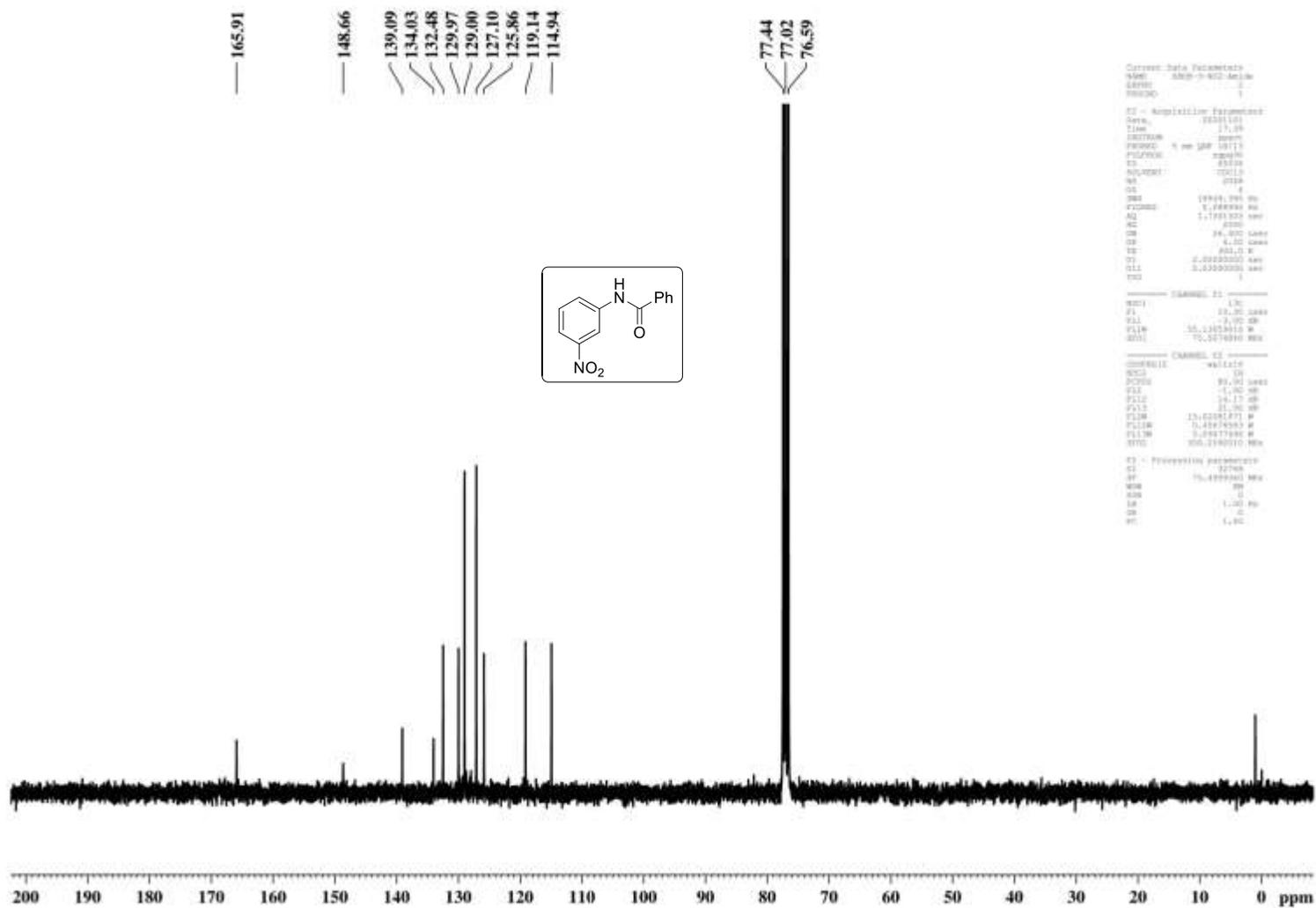
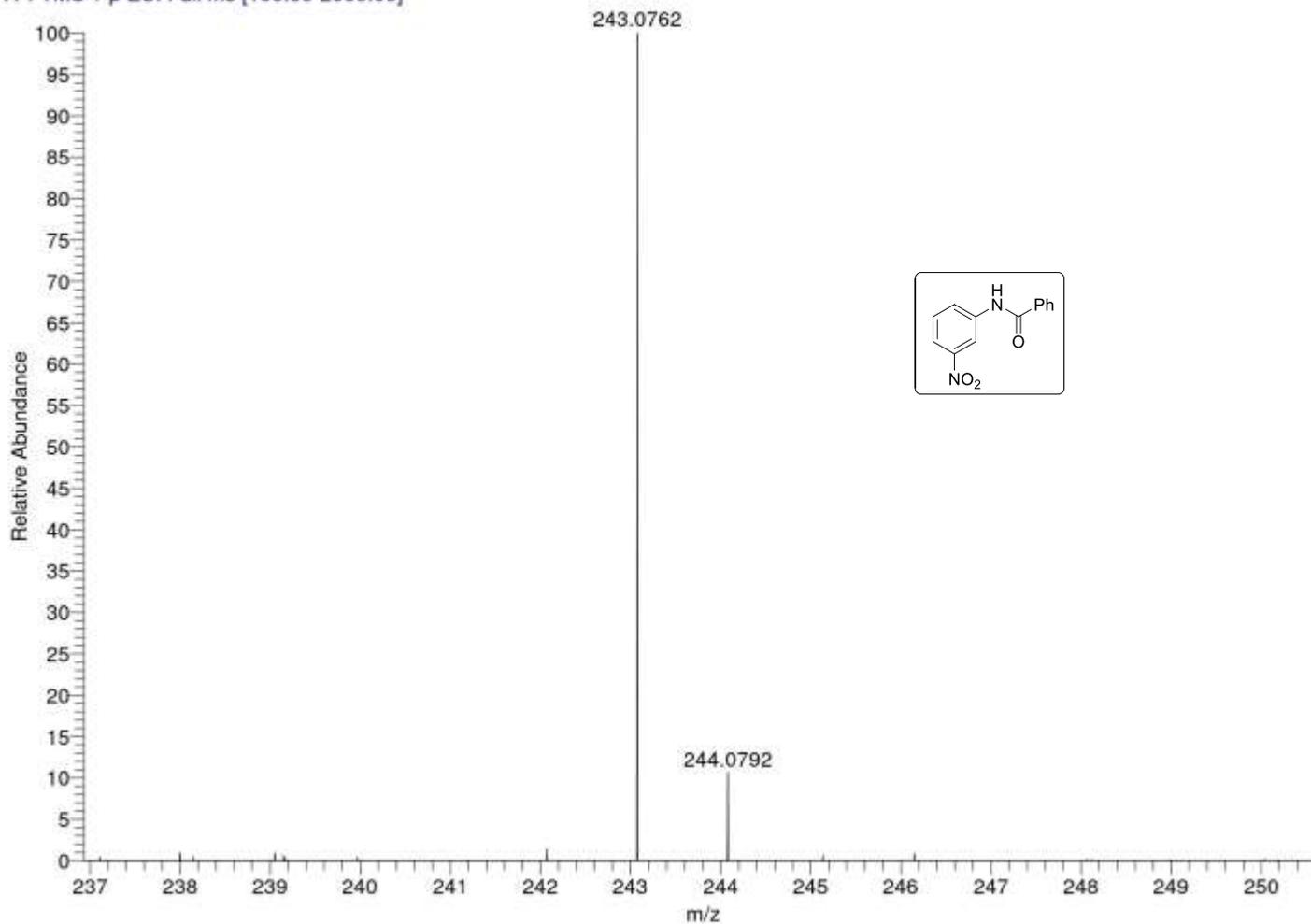


Figure S-105.  $^{13}\text{C}$ -NMR spectrum of *N*-(3-nitrophenyl)benzamide (**5a**).

HRMS19I22SEP10 #10 RT: 0.15 AV: 1 SB: 5 0.02-0.08 NL: 8.62E4

T: FTMS +p ESI Full ms [100.00-2000.00]



**Figure S-106.** HRMS spectrum of *N*-(3-nitrophenyl)benzamide (**5a**).

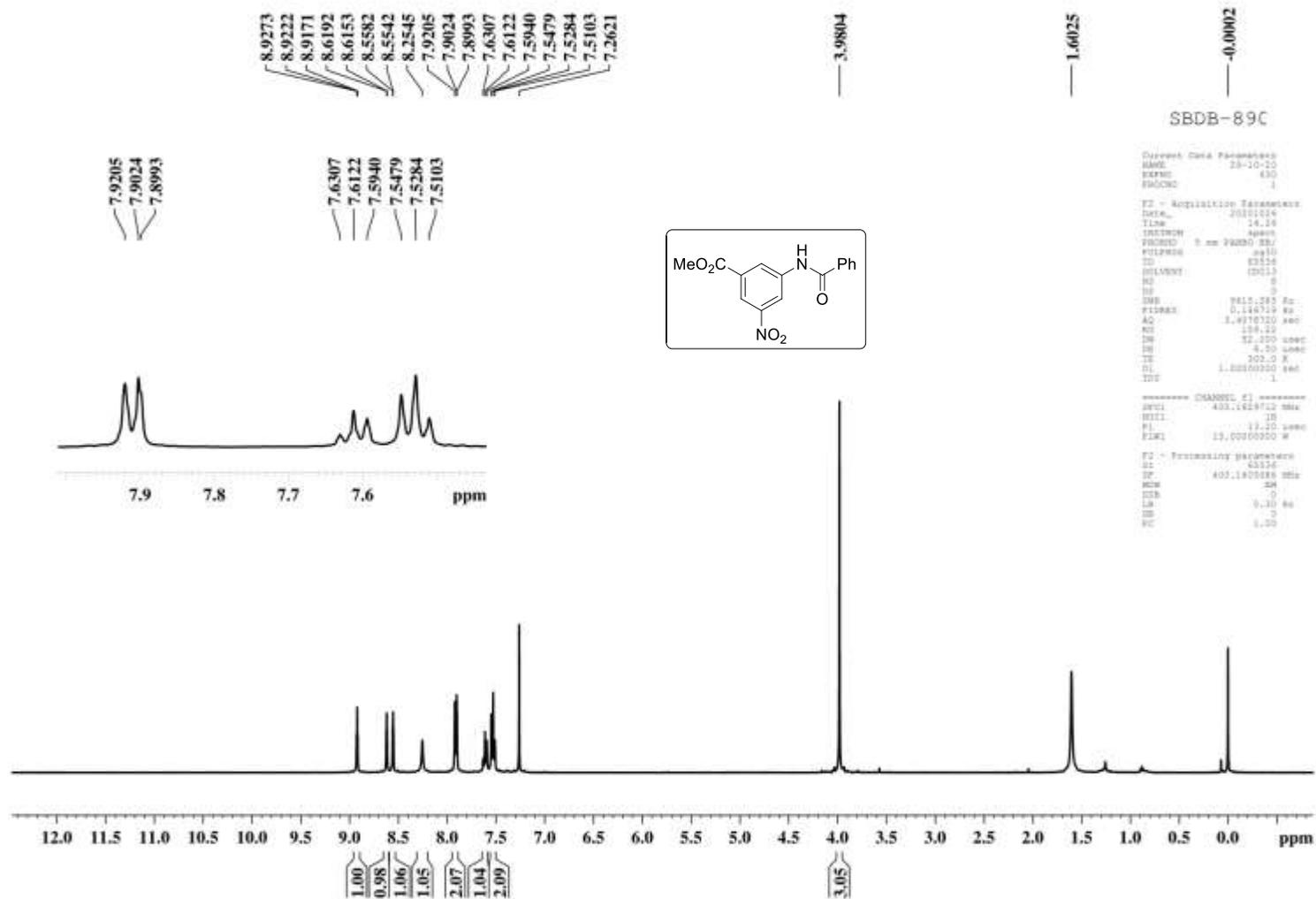


Figure S-107. <sup>1</sup>H-NMR spectrum of methyl 3-benzamido-5-nitrobenzoate (**5b**).

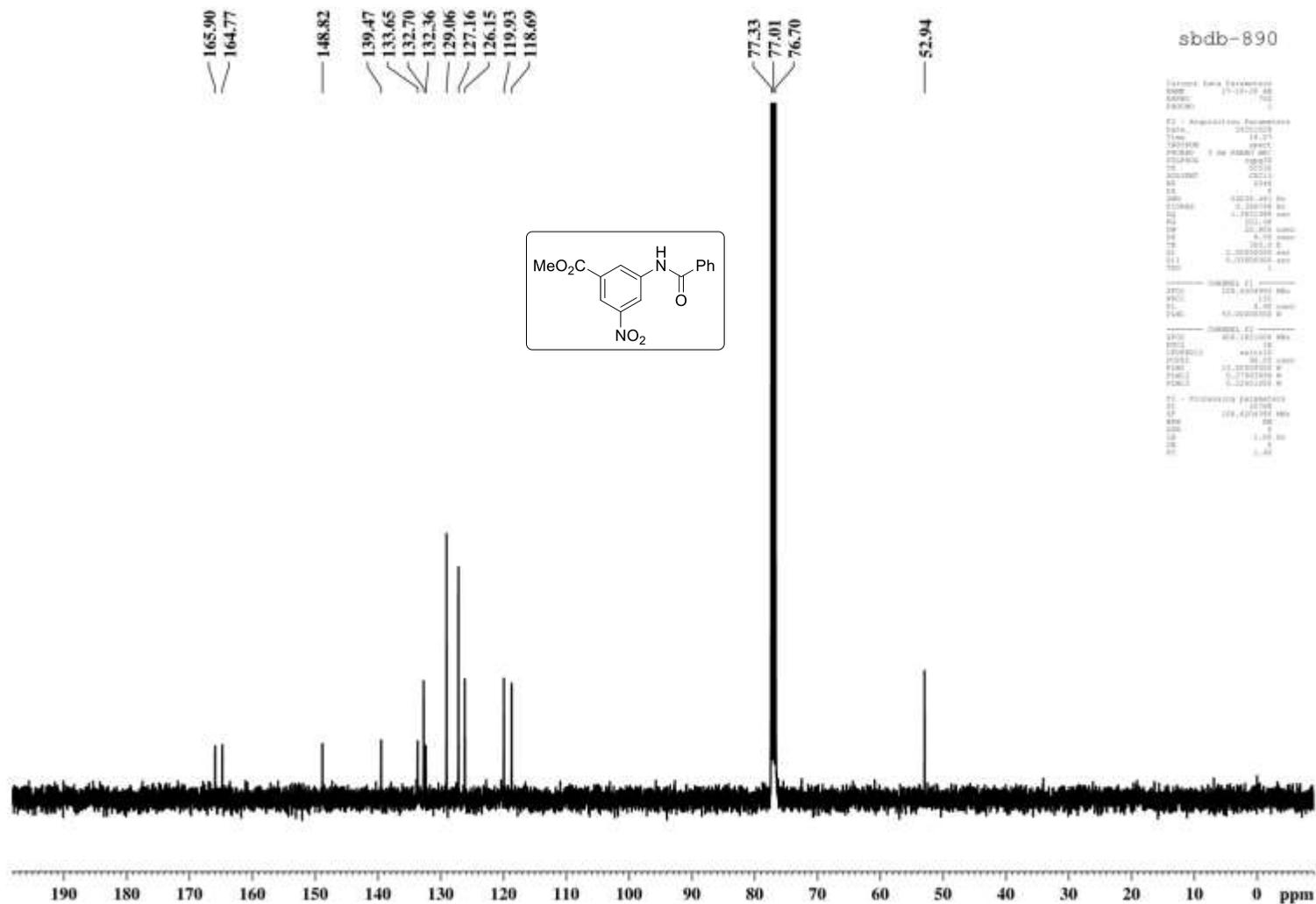
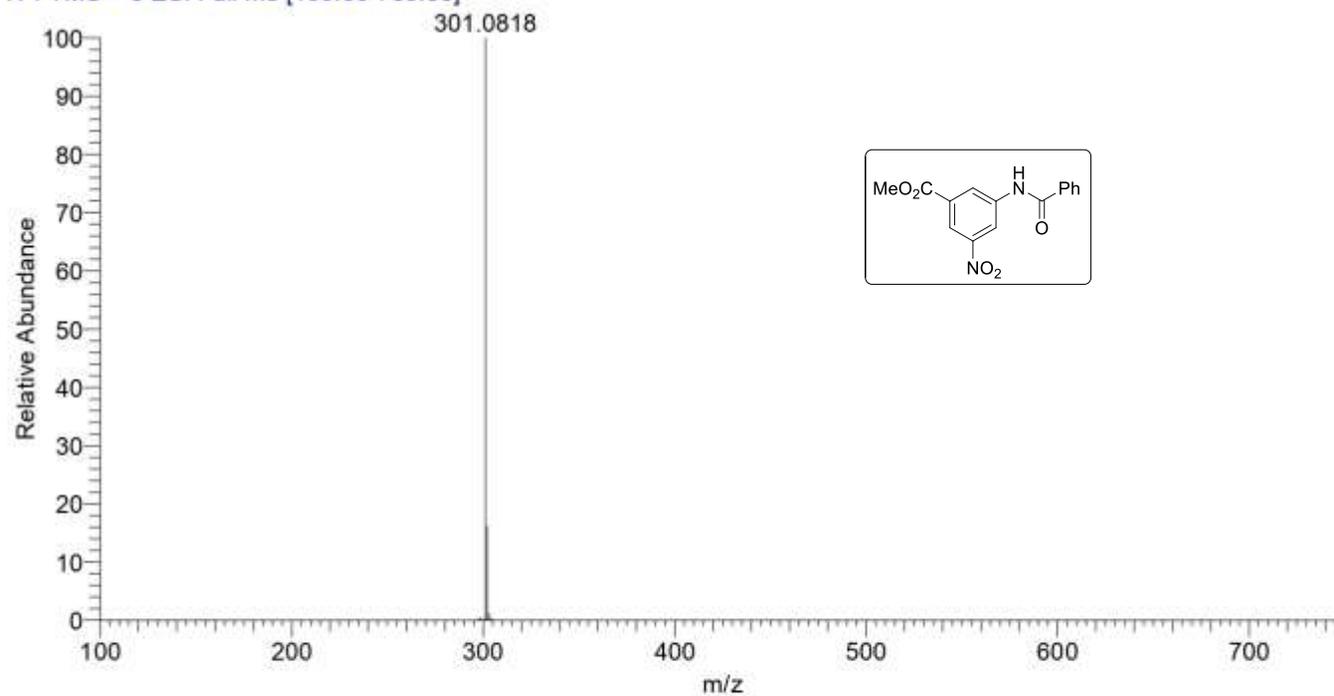


Figure S-108.  $^{13}\text{C}$ -NMR spectrum of methyl 3-benzamido-5-nitrobenzoate (**5b**).

**SAIF [HRMS Report]**

Data File:	HRMS20I21OCT27	Original Data Path:	D:\INTERNAL NEW\2020\OCT 2020
Sample ID:	SBDB-890	Sample Name:	
Acquisition Date:	10/21/20 12:11:31 PM	Run Time(min):	0.00
Vial:	CStk1-01:27	Injection Volume(μl):	1.00

HRMS20I21OCT27 #11-23 RT: 0.11-0.21 AV: 13 SB: 1 0.01 NL: 6.41E5  
T: FTMS + c ESI Full ms [100.00-750.00]



**Figure S-109.** HRMS spectrum of methyl 3-benzamido-5-nitrobenzoate (**5b**).

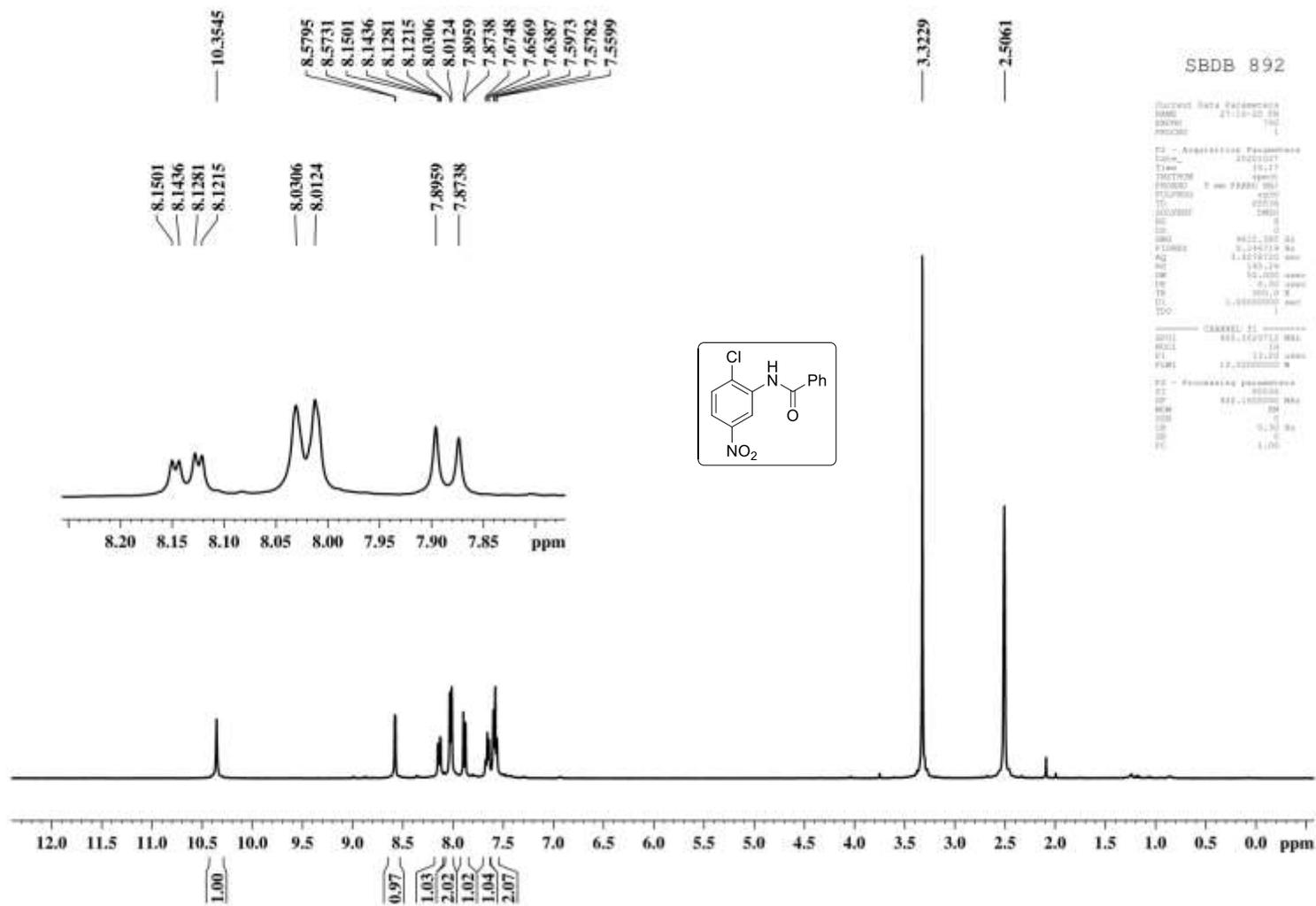


Figure S-110. <sup>1</sup>H-NMR spectrum of *N*-(2-chloro-5-nitrophenyl)benzamide (5c).

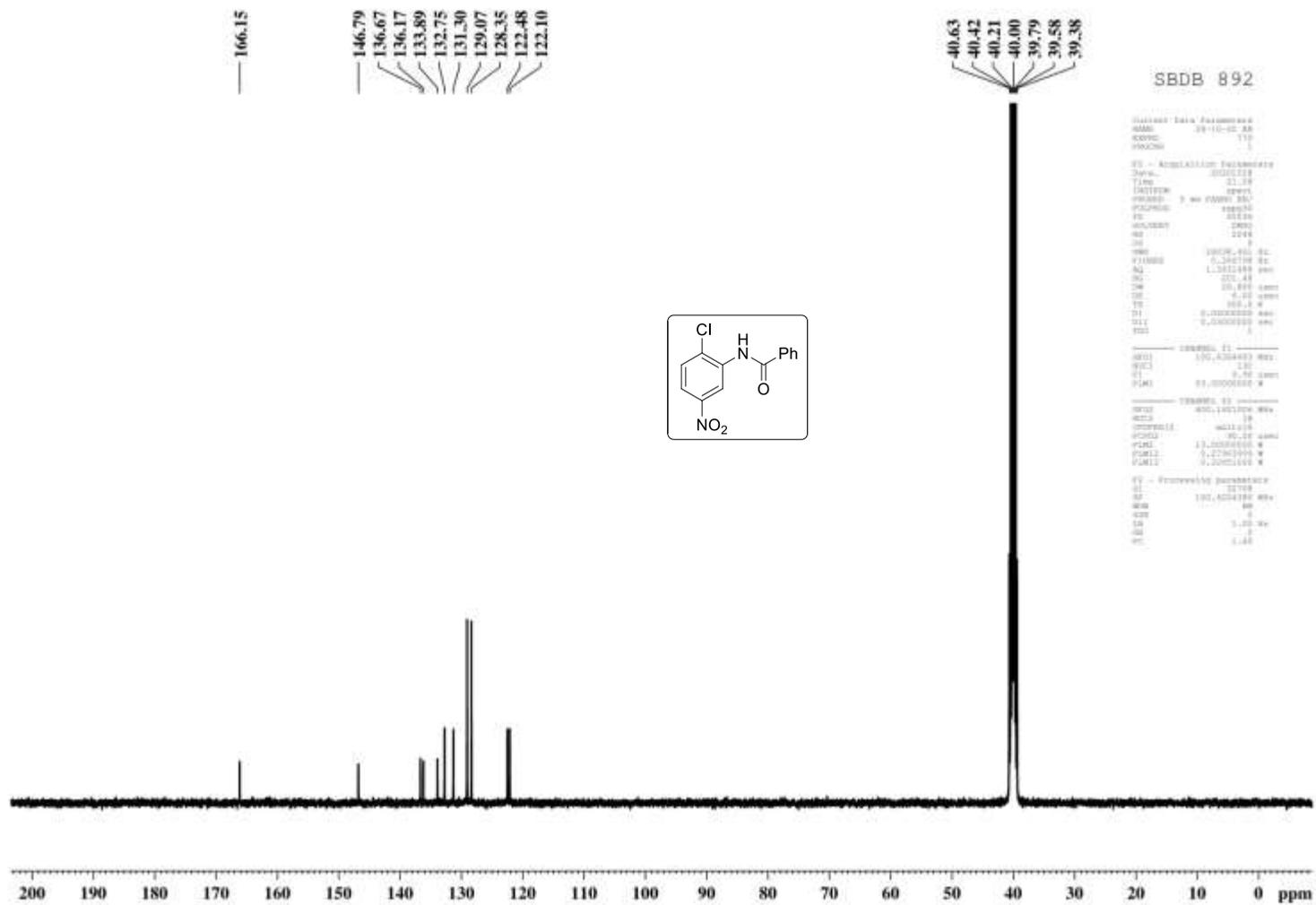
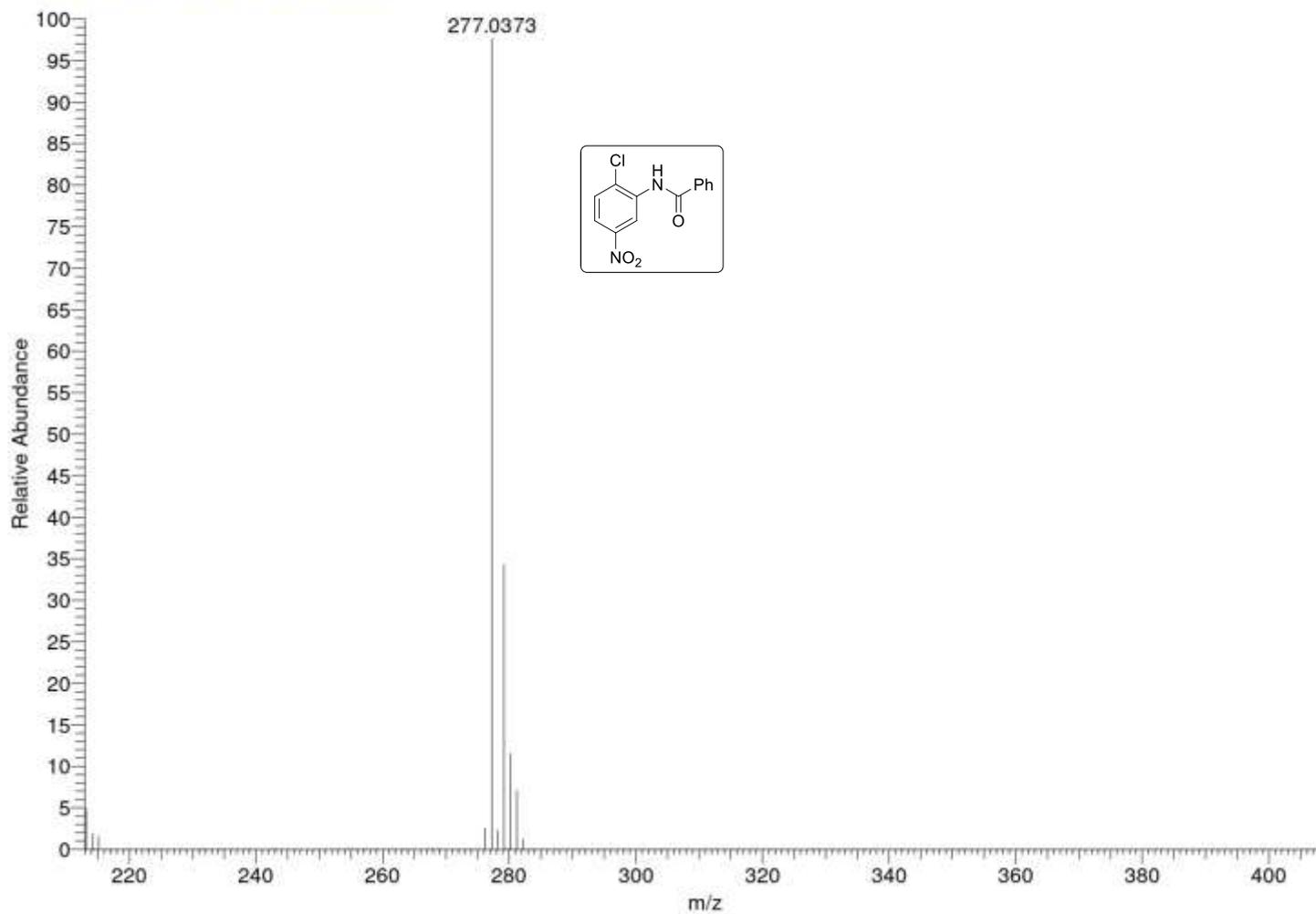


Figure S-111.  $^{13}\text{C}$ -NMR spectrum of *N*-(2-chloro-5-nitrophenyl)benzamide (5c).

HRMS20121OCT28\_201021125313 #18-29 RT: 0.17-0.27 AV: 12 SB: 6 0.02-0.07 NL: 4.14E4  
T: FTMS + c ESI Full ms [100.00-750.00]



**Figure S-112.** HRMS spectrum of *N*-(2-chloro-5-nitrophenyl)benzamide (**5c**).

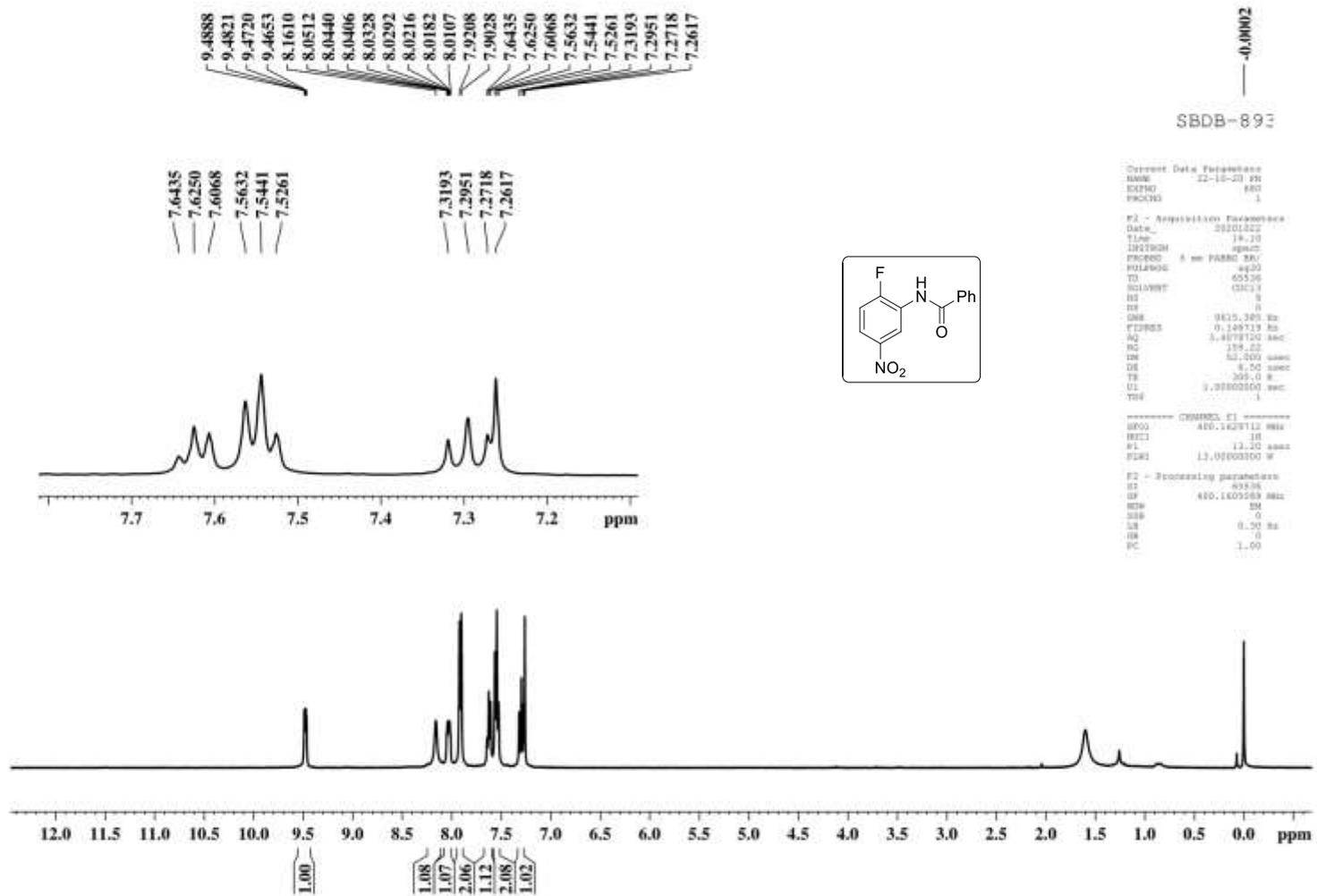


Figure S-113. <sup>1</sup>H-NMR spectrum of *N*-(2-fluoro-5-nitrophenyl)benzamide (5d).



### SAIF [HRMS Report]

Data File:	HRMS20I23OCT23	Original Data Path:	D:\INTERNAL NEW\2020\OCT 2020
Sample ID:	SBDB-893	Sample Name:	
Acquisition Date:	10/23/20 12:06:00 PM	Run Time(min):	0.00
Vial:	CStk1-01:23	Injection Volume(μl):	1.00

HRMS20I23OCT23 #11-22 RT: 0.11-0.21 AV: 12 SB: 1 0.01 NL: 1.65E5  
T: FTMS + c ESI Full ms [100.00-750.00]

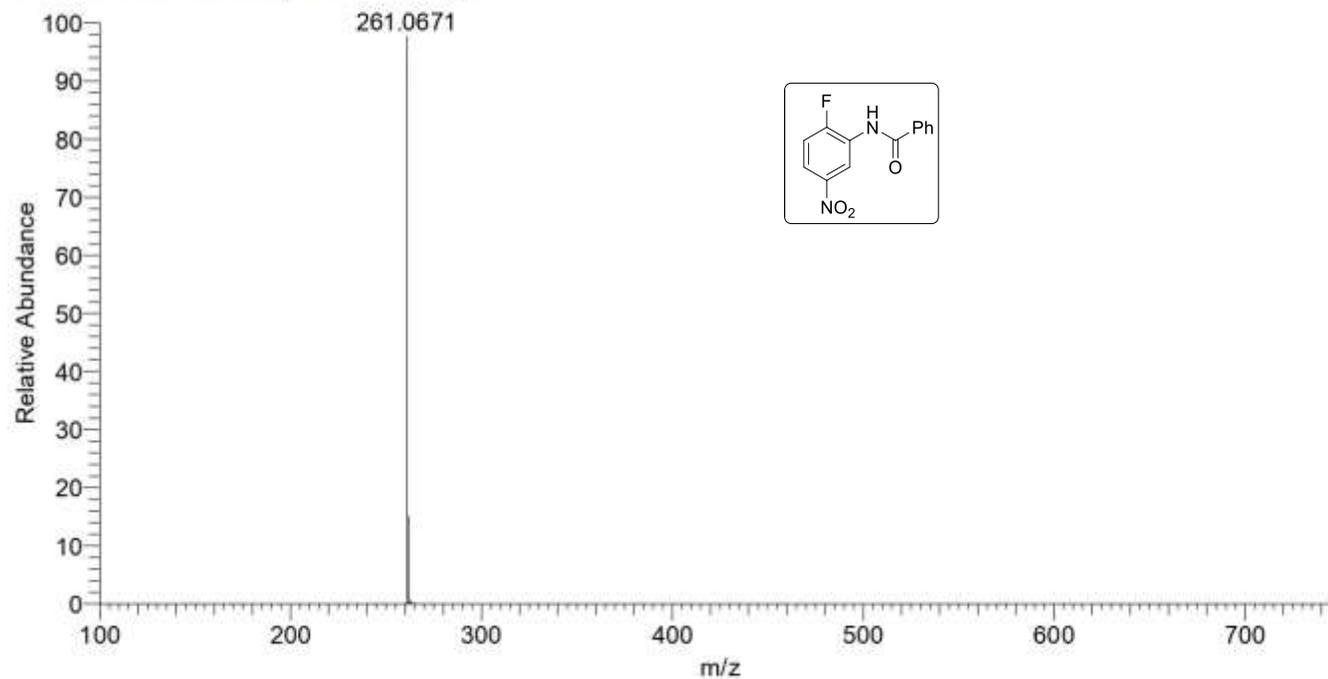


Figure S-115. HRMS spectrum of *N*-(2-fluoro-5-nitrophenyl)benzamide (**5d**).

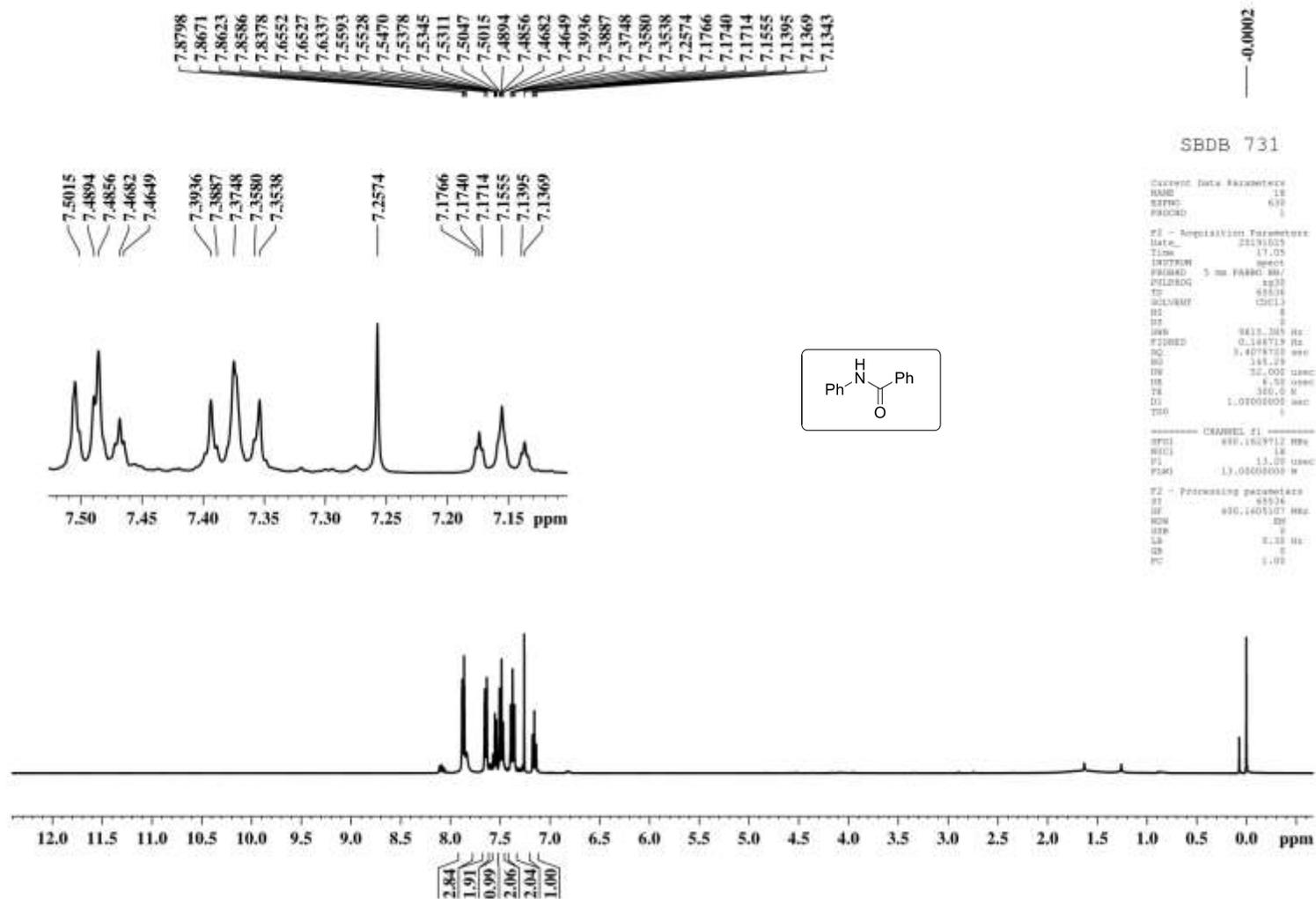


Figure S-116. <sup>1</sup>H-NMR spectrum of *N*-phenylbenzamide (7aa).

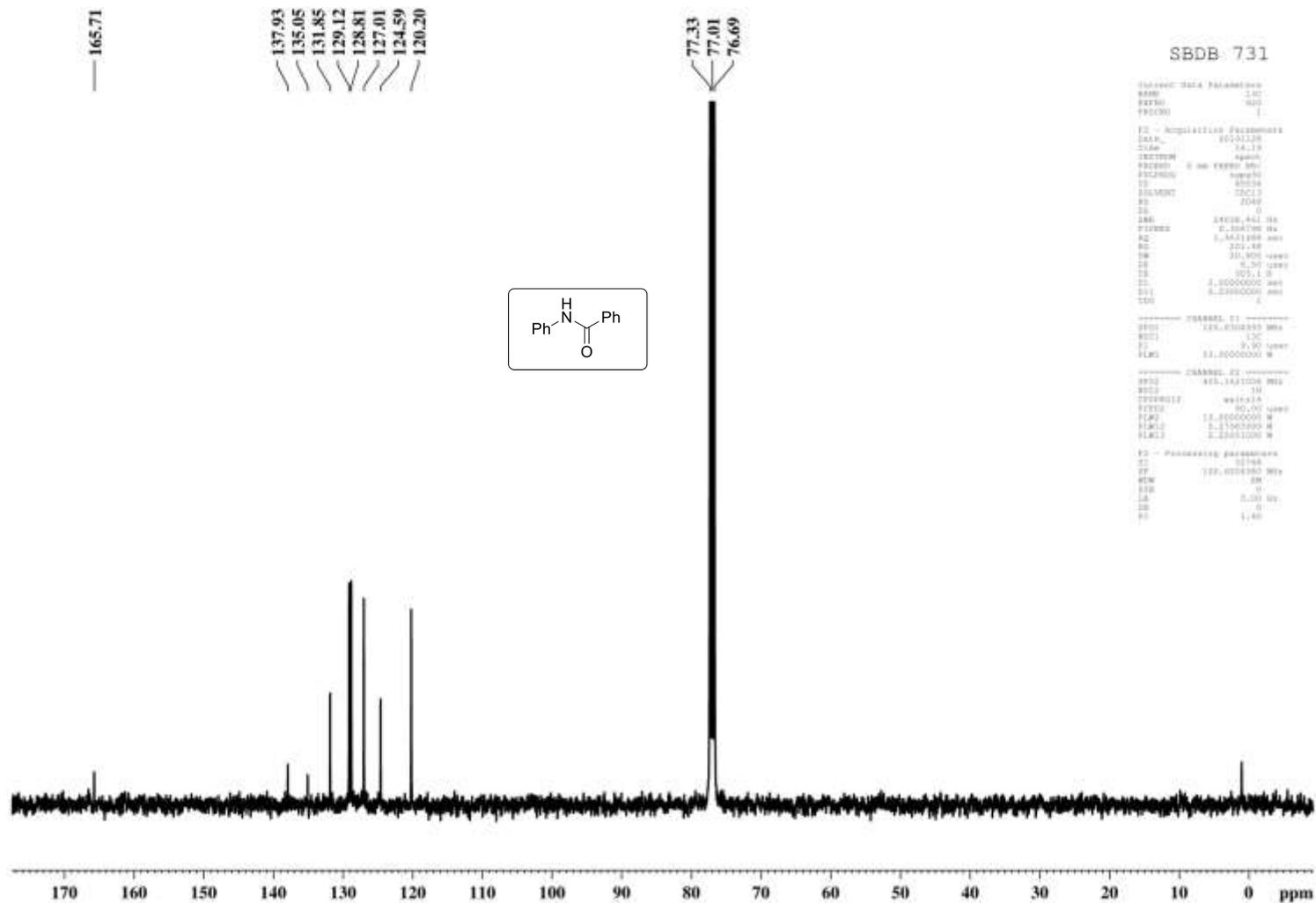


Figure S-117. <sup>13</sup>C-NMR spectrum *N*-phenylbenzamide (7aa).

HRMS19I24SEP09 #12 RT: 0.18 AV: 1 SB: 5 0.02-0.08 NL: 2.17E6  
T: FTMS + p ESI Full ms [100.00-2000.00]

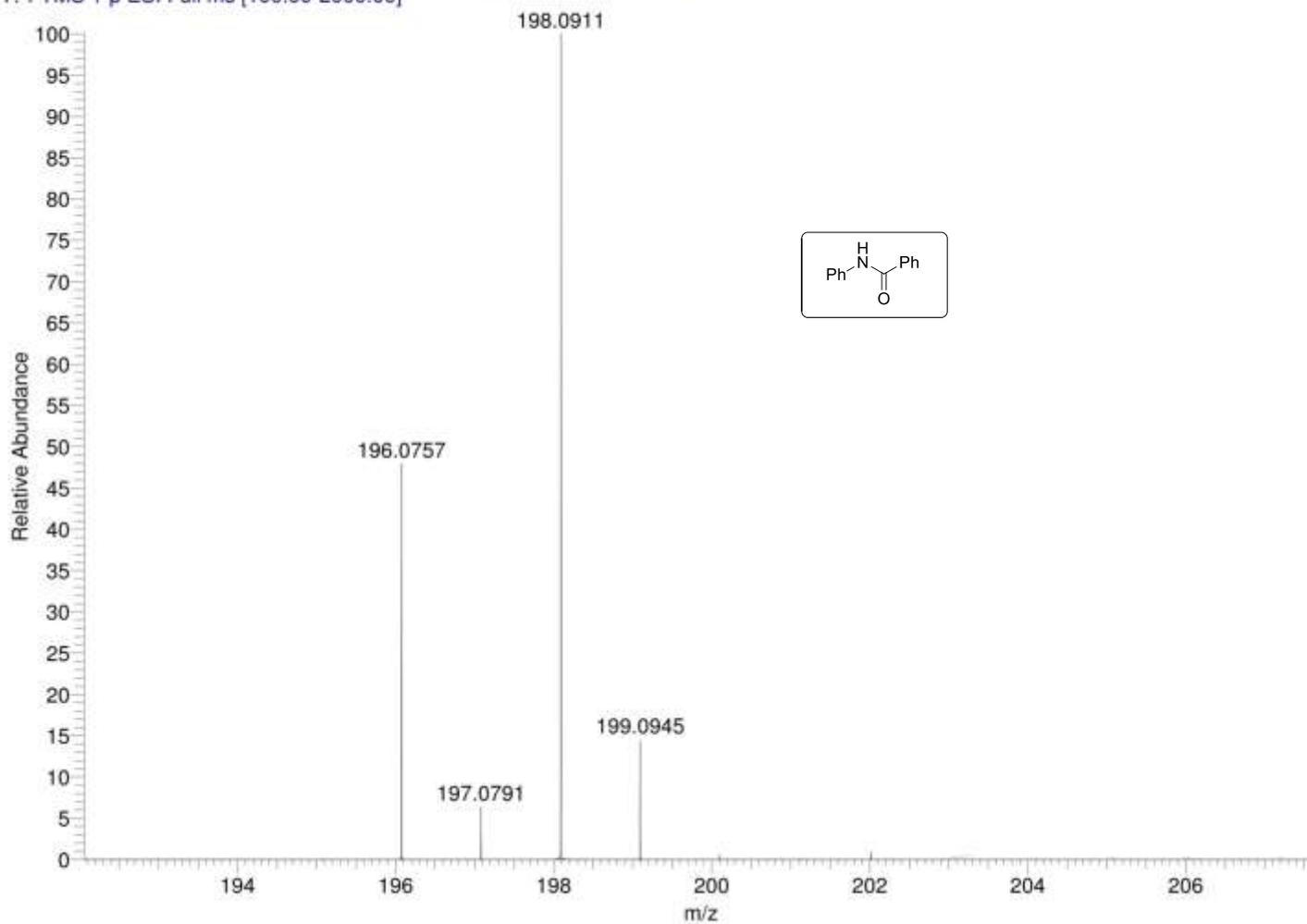


Figure S-118. HRMS spectrum of *N*-phenylbenzamide (**7aa**).

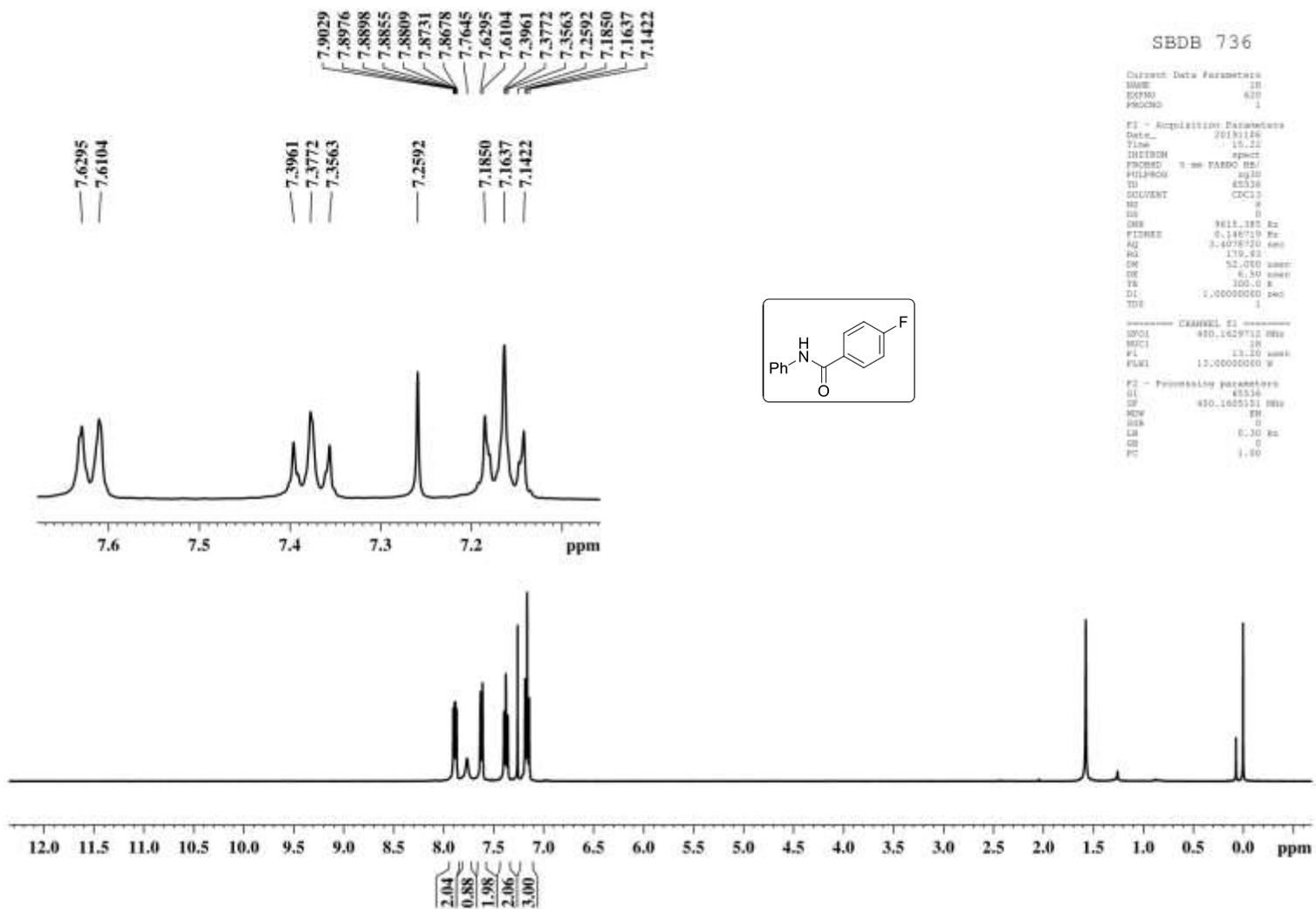


Figure S-119. <sup>1</sup>H-NMR spectrum of 4-fluoro-N-phenylbenzamide (7ab).

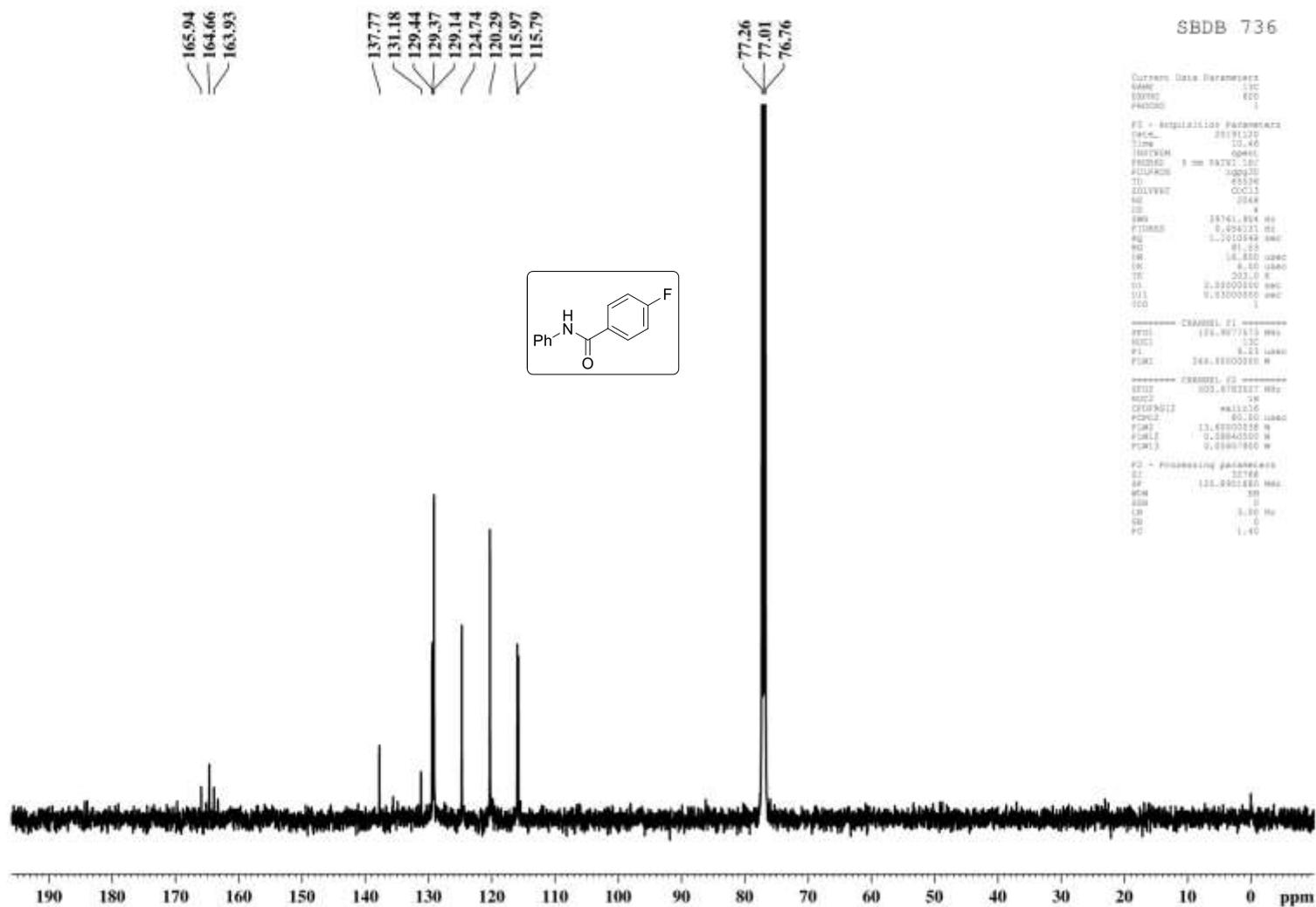
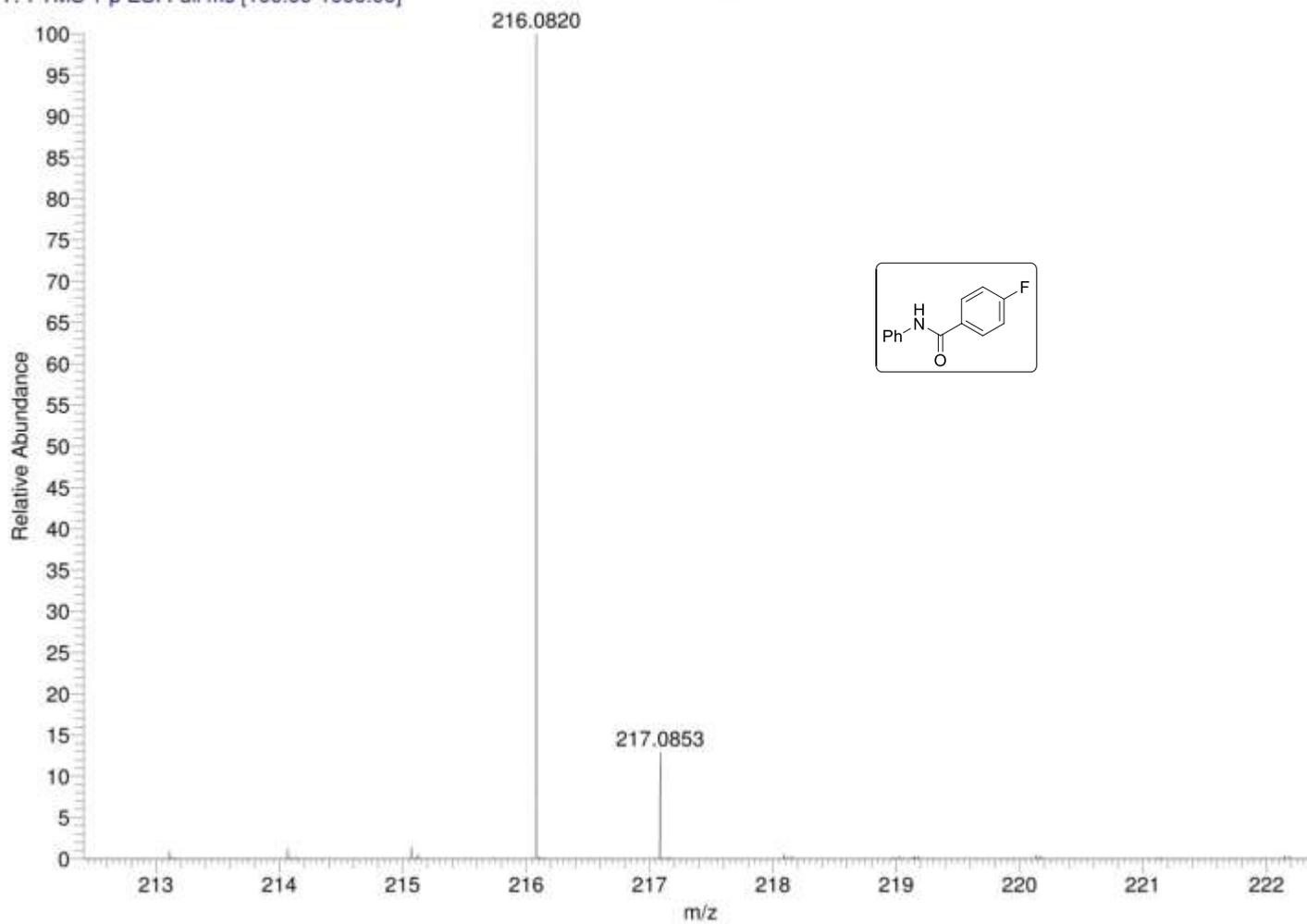


Figure S-120.  $^{13}\text{C}$ -NMR spectrum of 4-fluoro-*N*-phenylbenzamide (7ab).

HRMS19114NOV12 #12-20 RT: 0.10-0.17 AV: 9 SB: 6 0.03-0.07 NL: 5.85E4  
T: FTMS + p ESI Full ms [100.00-1000.00]



**Figure S-121.** HRMS spectrum of 4-fluoro-*N*-phenylbenzamide (**7ab**).





HRMS19126SEP24 #8 RT: 0.12 AV: 1 SB: 5 0.02-0.08 NL: 3.11E5  
T: FTMS + p ESI Full ms [100.00-2000.00]

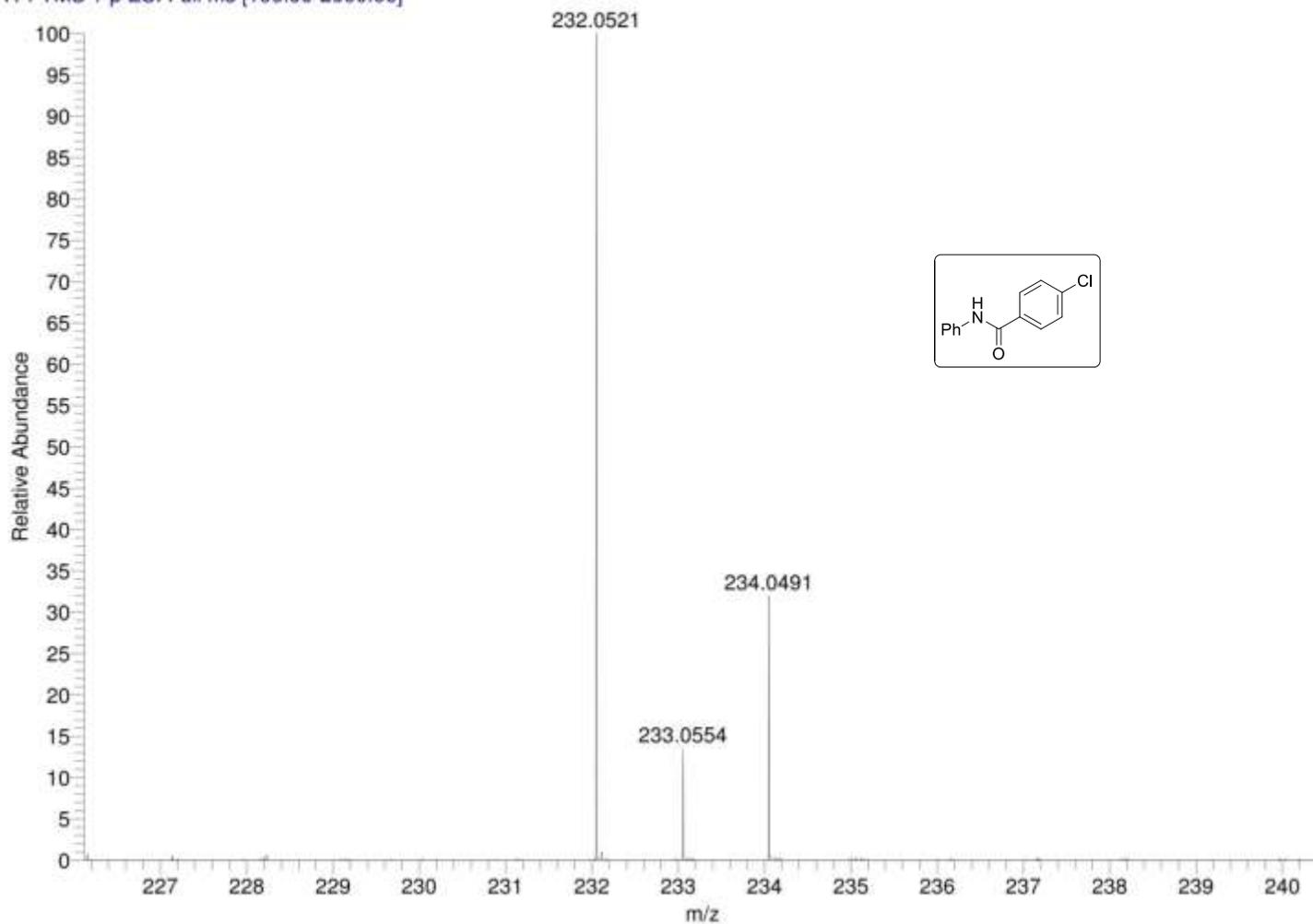


Figure S-124. HRMS spectrum of 4-chloro-N-phenylbenzamide (7ac).

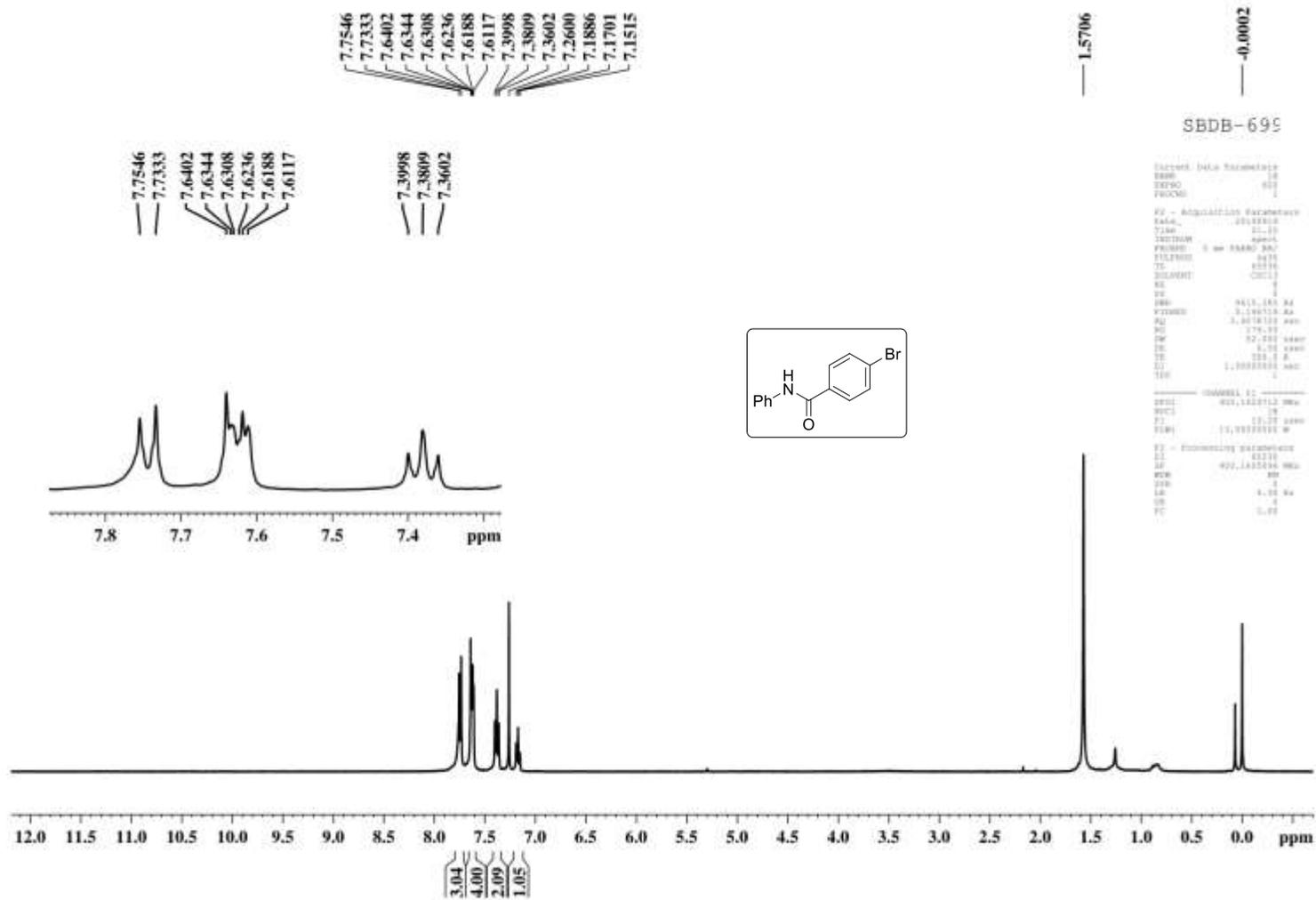


Figure S-125. <sup>1</sup>H-NMR spectrum of 4-bromo-N-phenylbenzamide (7ad).

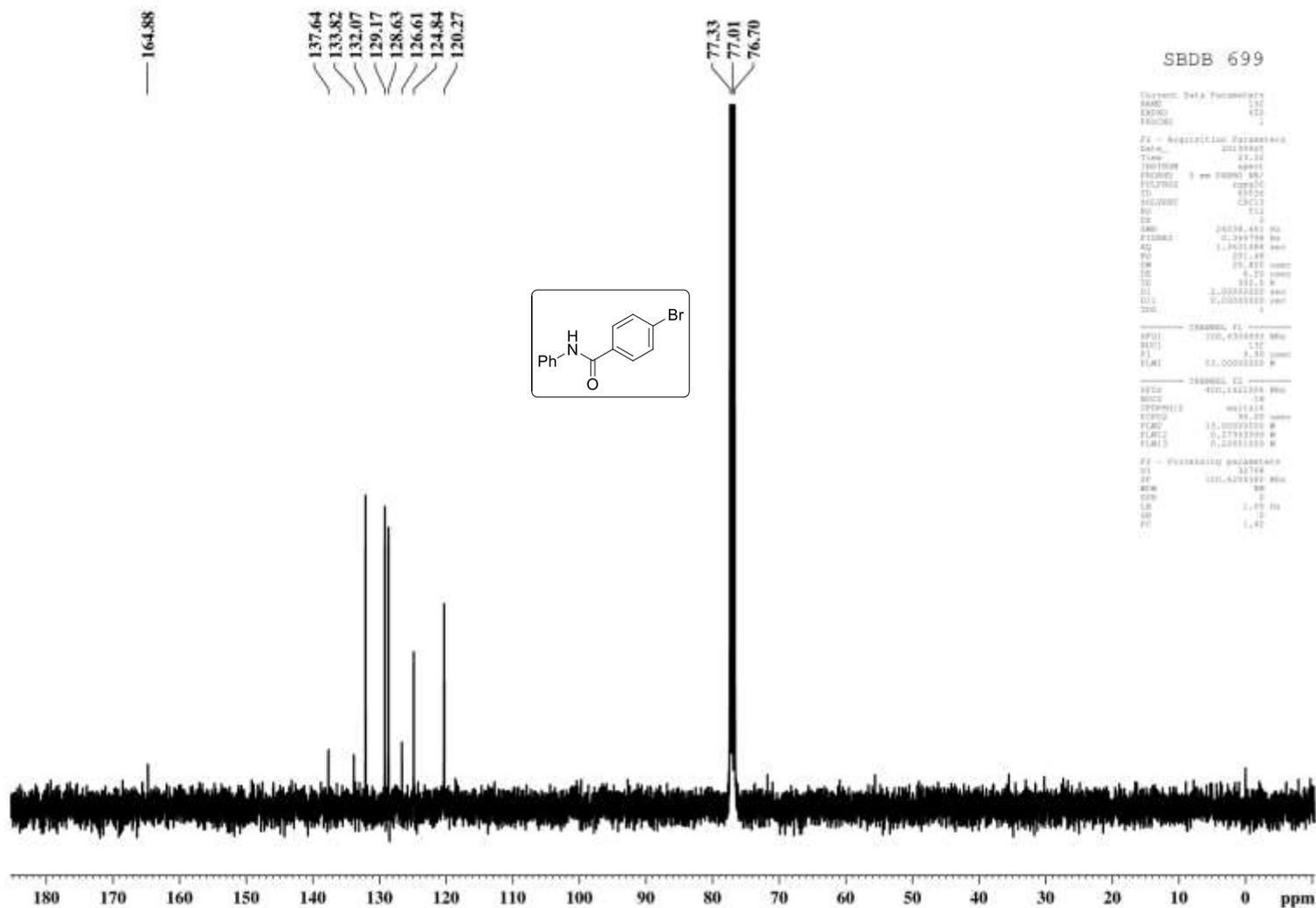


Figure S-126.  $^{13}\text{C}$ -NMR spectrum of 4-bromo-*N*-phenylbenzamide (**7ad**).

HRMS19I24SEP11 #10 RT: 0.15 AV: 1 SB: 5 0.02-0.08 NL: 2.30E5

T: FTMS + p ESI Full ms [100.00-2000.00]

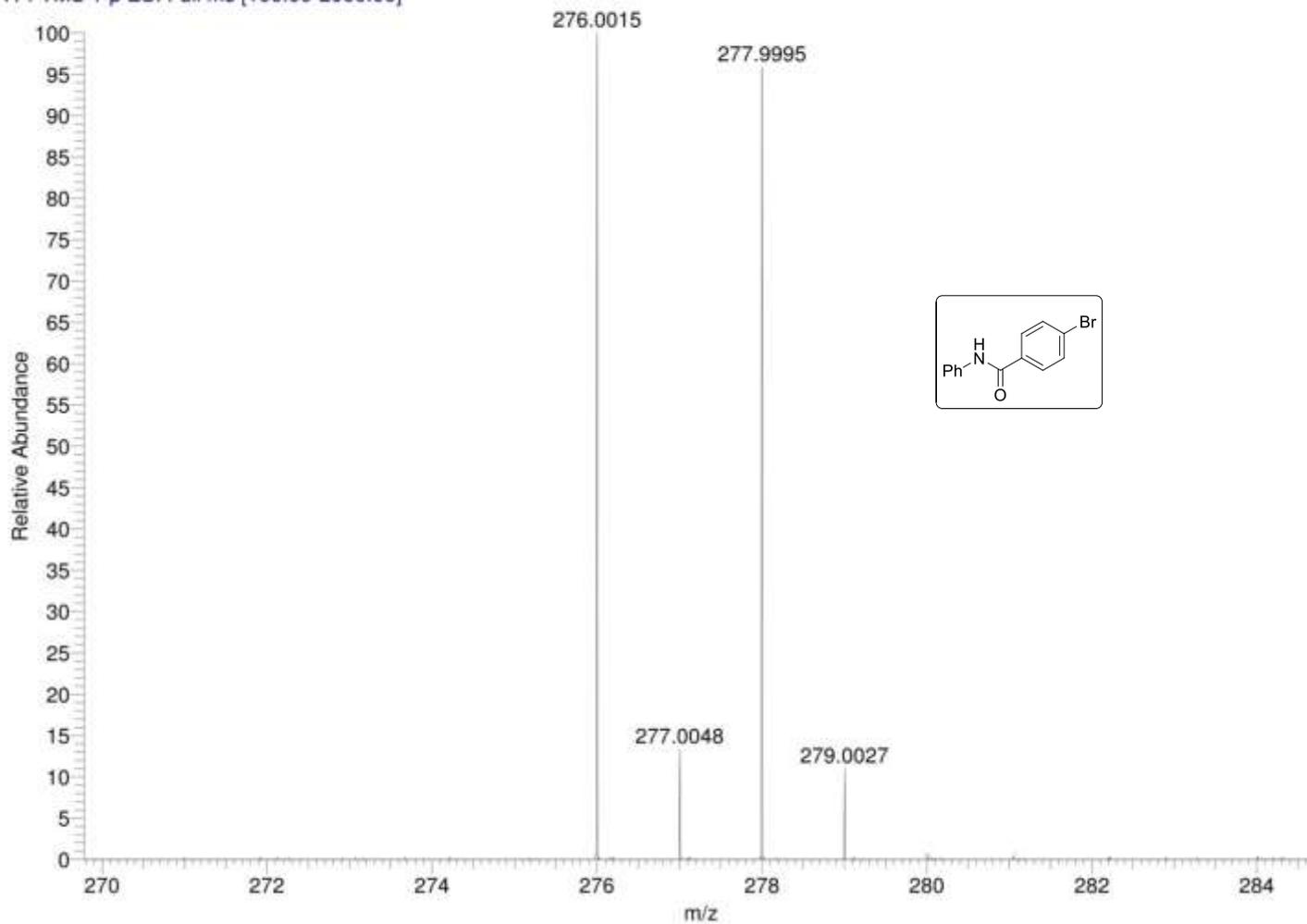


Figure S-127. HRMS spectrum of 4-bromo-N-phenylbenzamide (7ad).

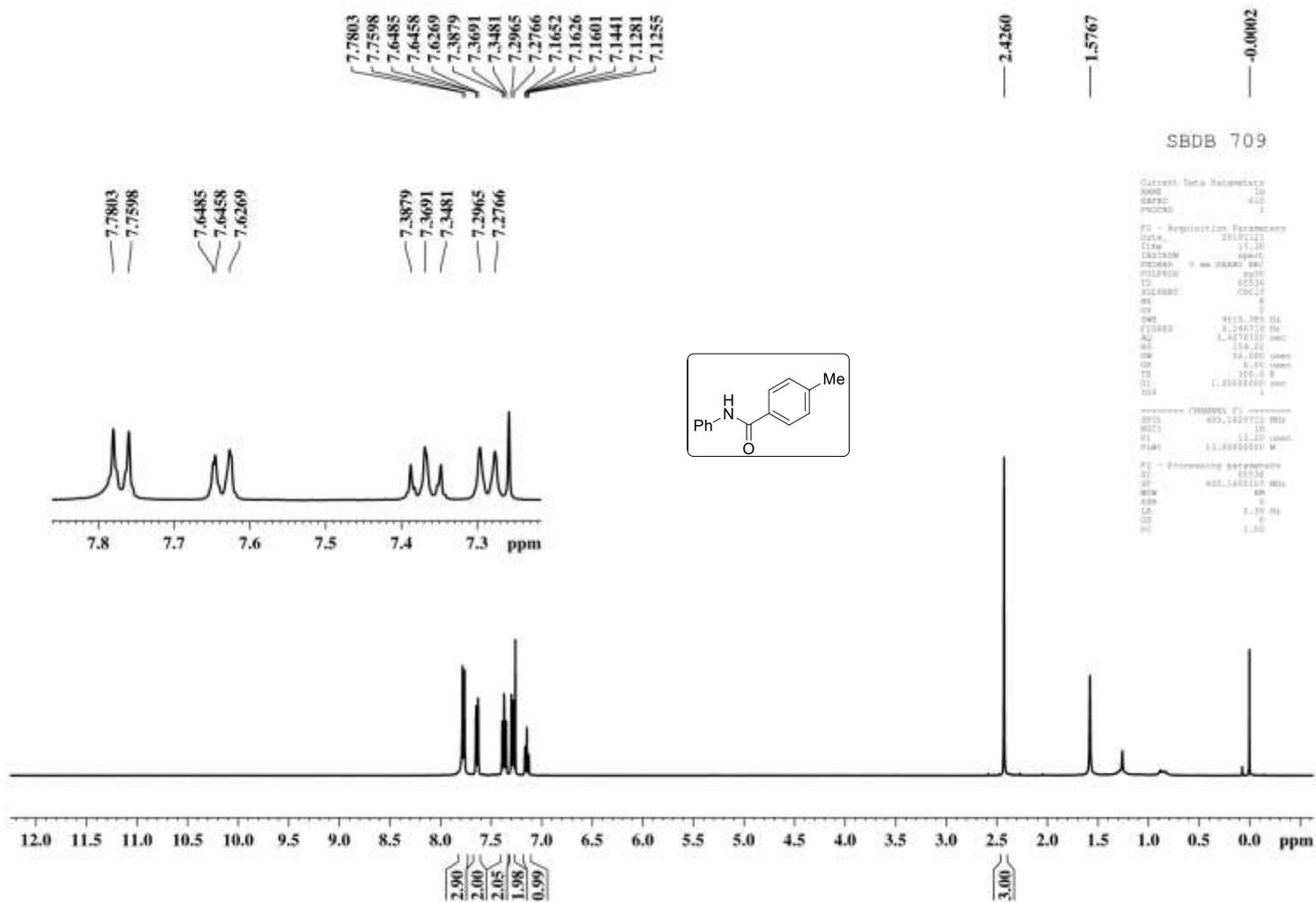


Figure S-128. <sup>1</sup>H-NMR spectrum of 4-methyl-N-phenylbenzamide (7ae).



HRMS19114NOV10 #14-24 RT: 0.12-0.20 AV: 11 SB: 7 0.02-0.07 NL: 6.93E5  
T: FTMS + p ESI Full ms [100.00-1000.00]

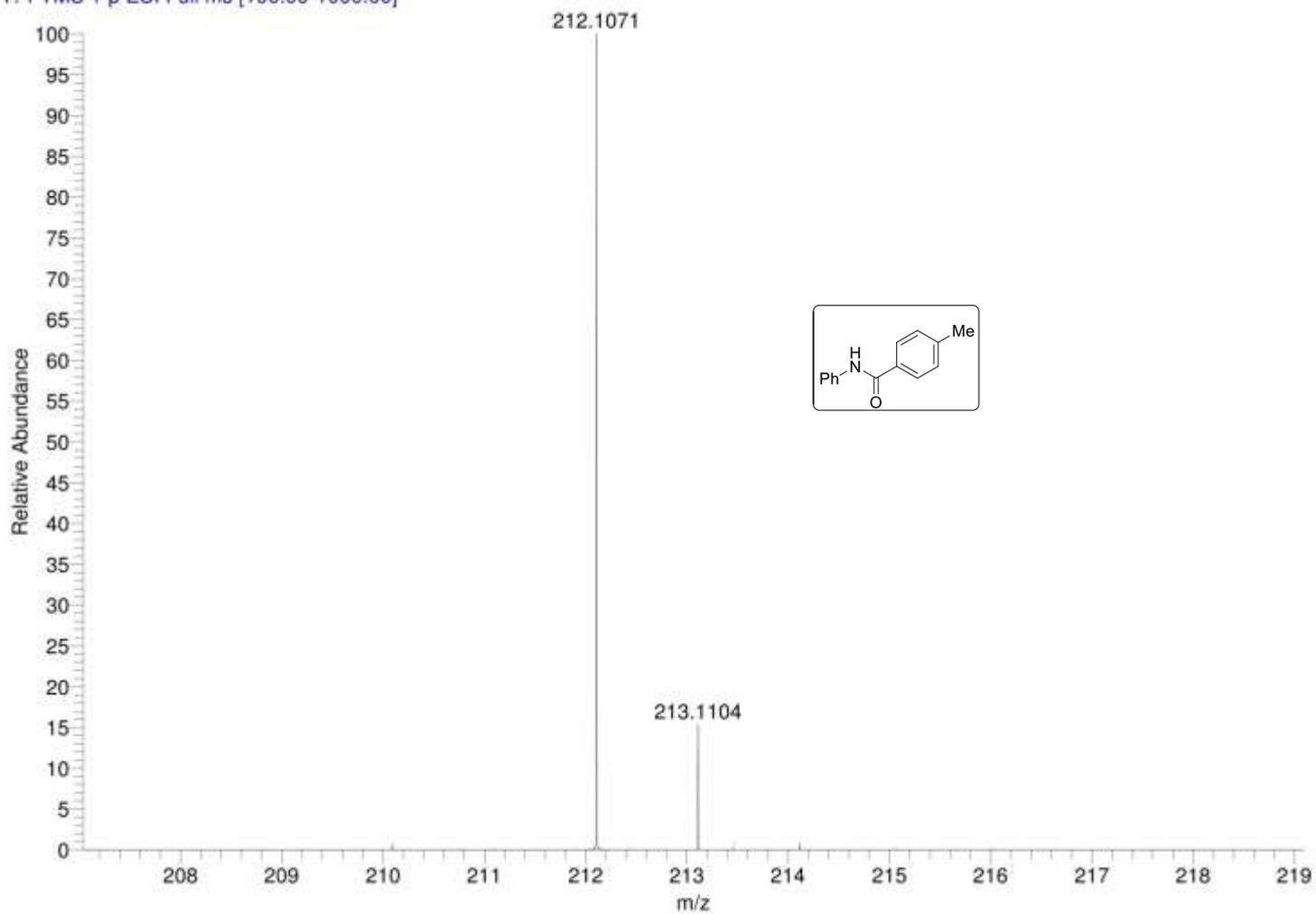


Figure S-130. HRMS spectrum of 4-methyl-N-phenylbenzamide (7ae).



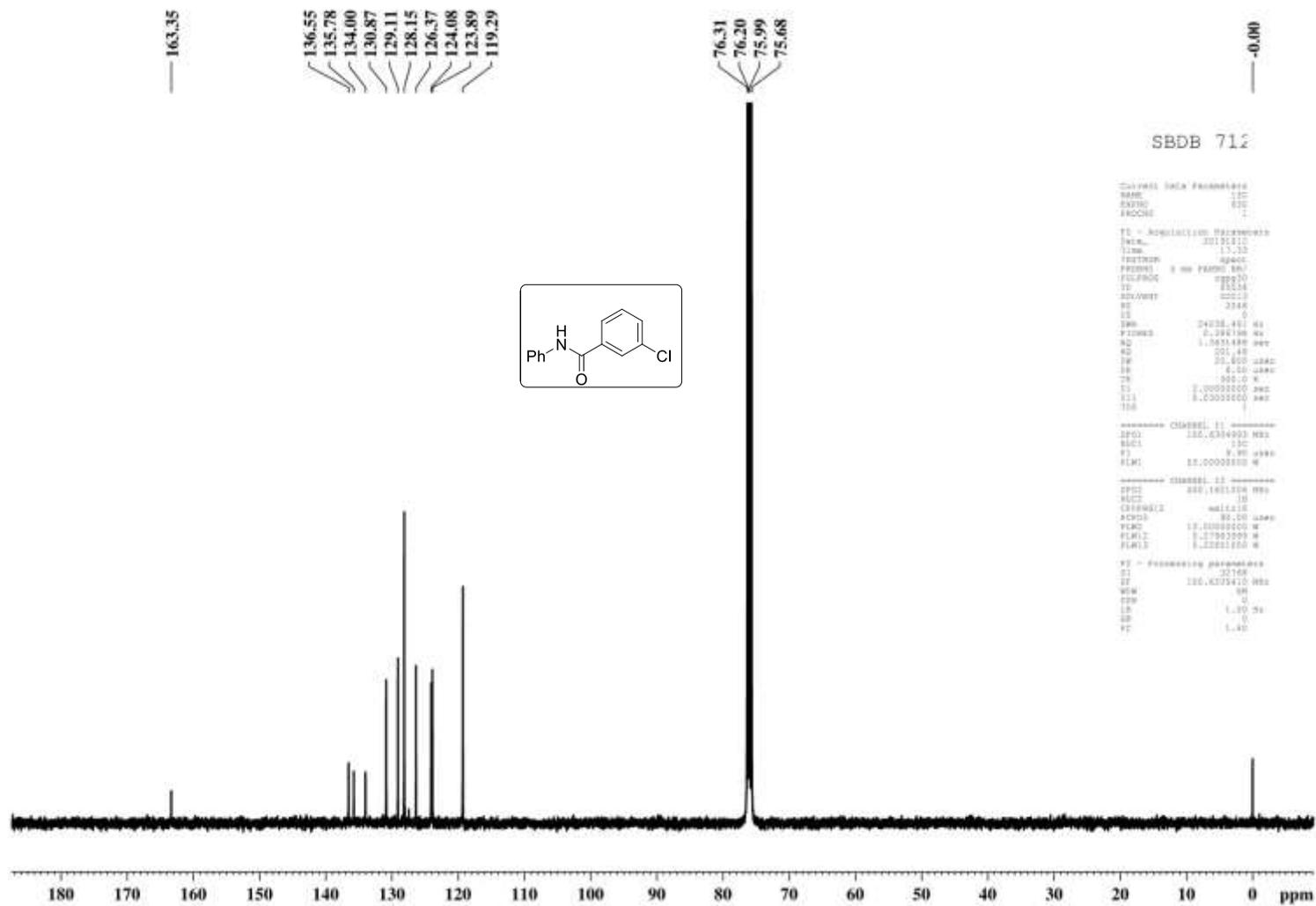


Figure S-132. <sup>13</sup>C-NMR spectrum 3-chloro-N-phenylbenzamide (7af).

HRMS19114NOV11 #12-26 RT: 0.10-0.22 AV: 15 SB: 7 0.02-0.07 NL: 2.23E5  
T: FTMS + p ESI Full ms [100.00-1000.00]

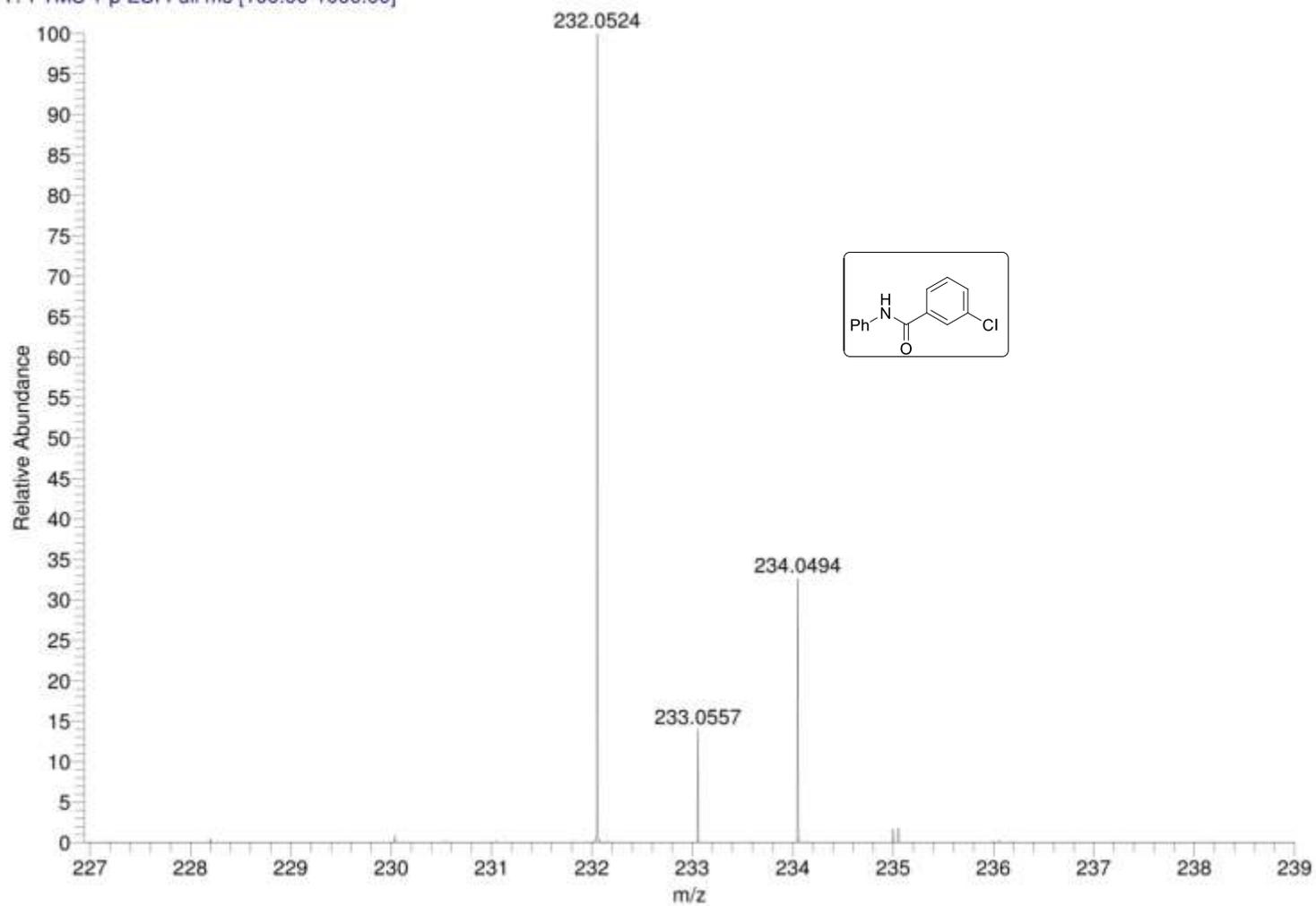


Figure S-133. HRMS spectrum of 3-chloro-*N*-phenylbenzamide (**7af**).

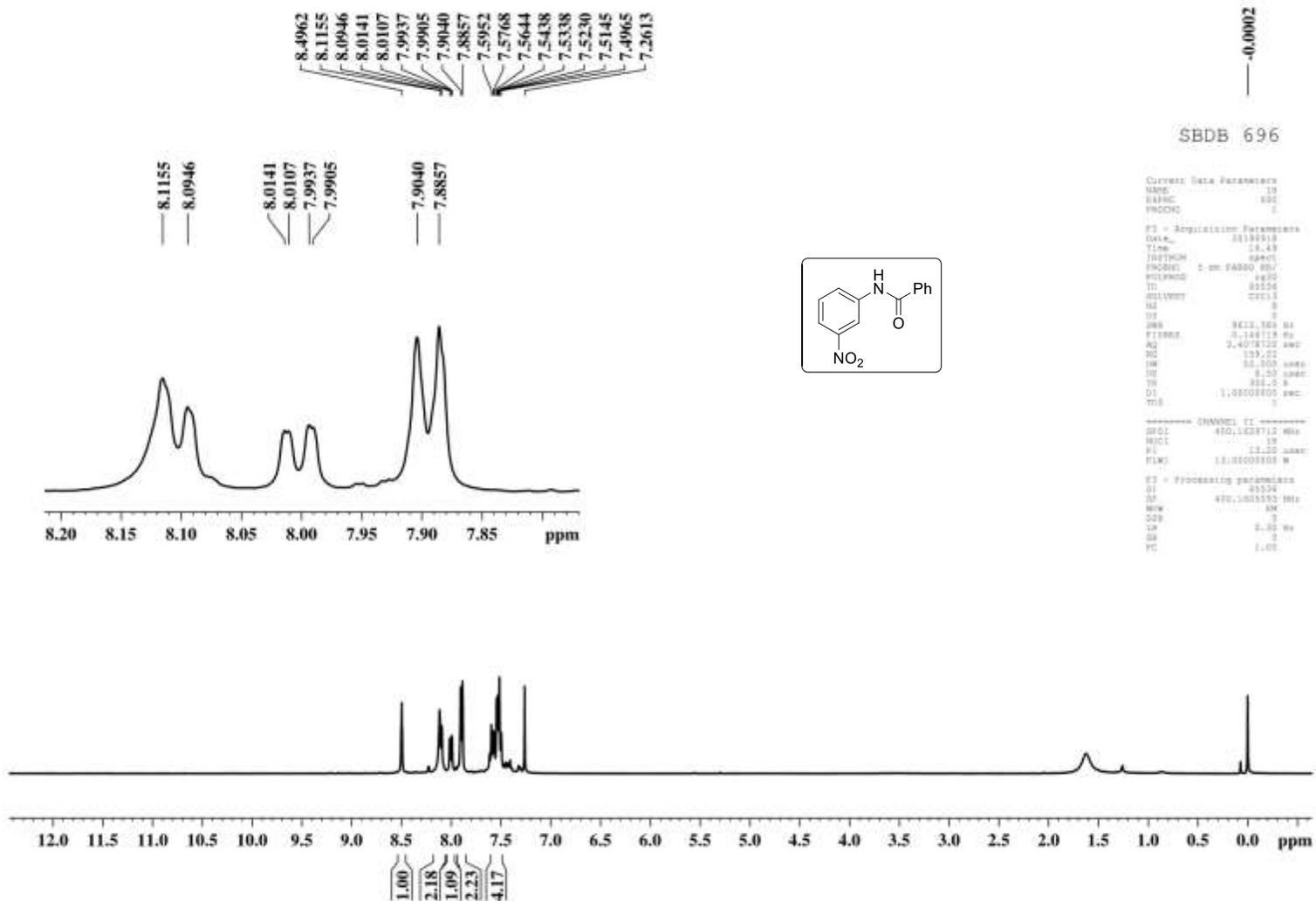


Figure S-134. <sup>1</sup>H-NMR spectrum of *N*-(3-nitrophenyl)benzamide (7ba).

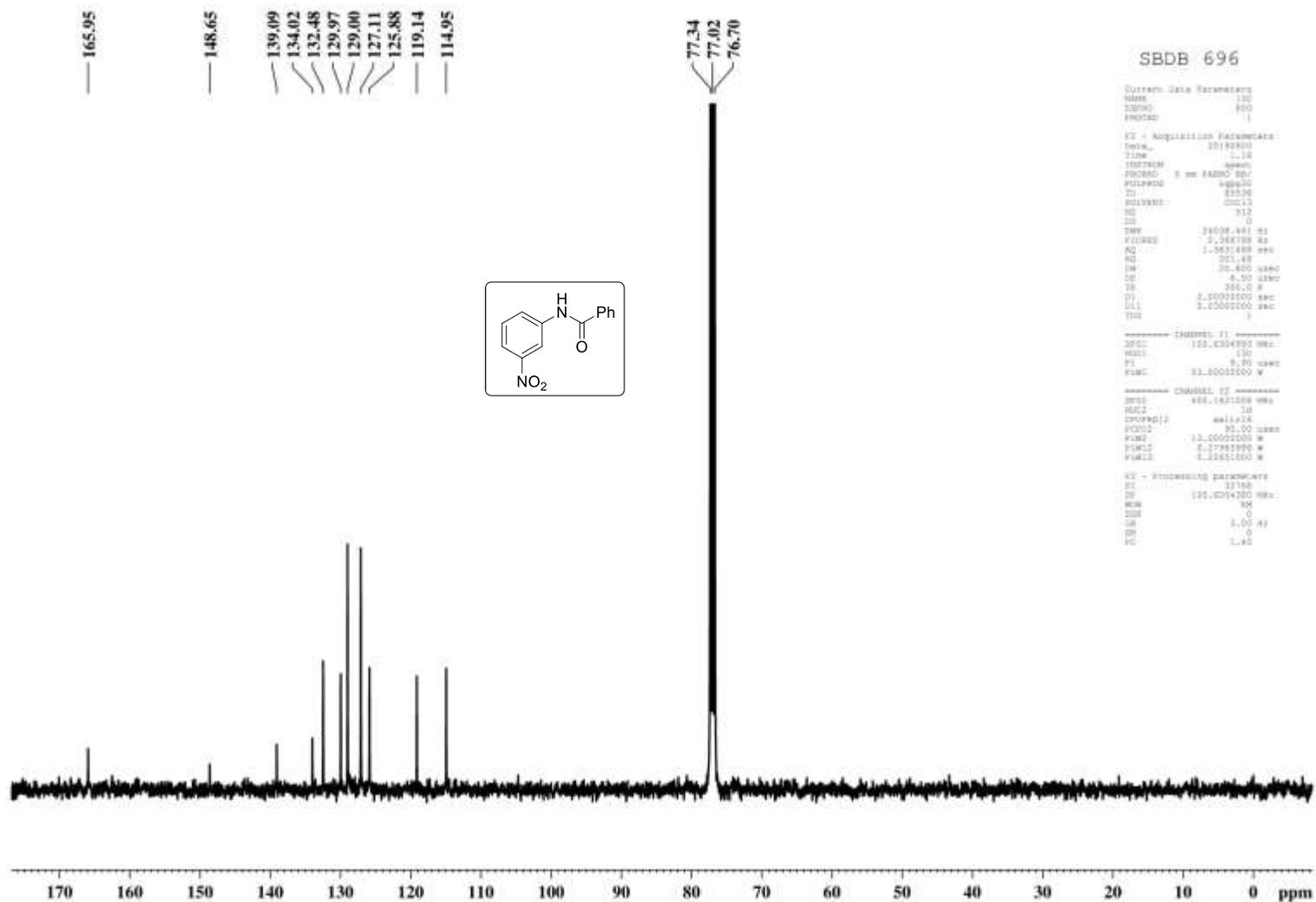


Figure S-135.  $^{13}\text{C}$ -NMR spectrum of *N*-(3-nitrophenyl)benzamide (**7ba**).

HRMS19I24SEP10 #10 RT: 0.15 AV: 1 SB: 5 0.02-0.08 NL: 8.61E4  
T: FTMS + p ESI Full ms [100.00-2000.00]

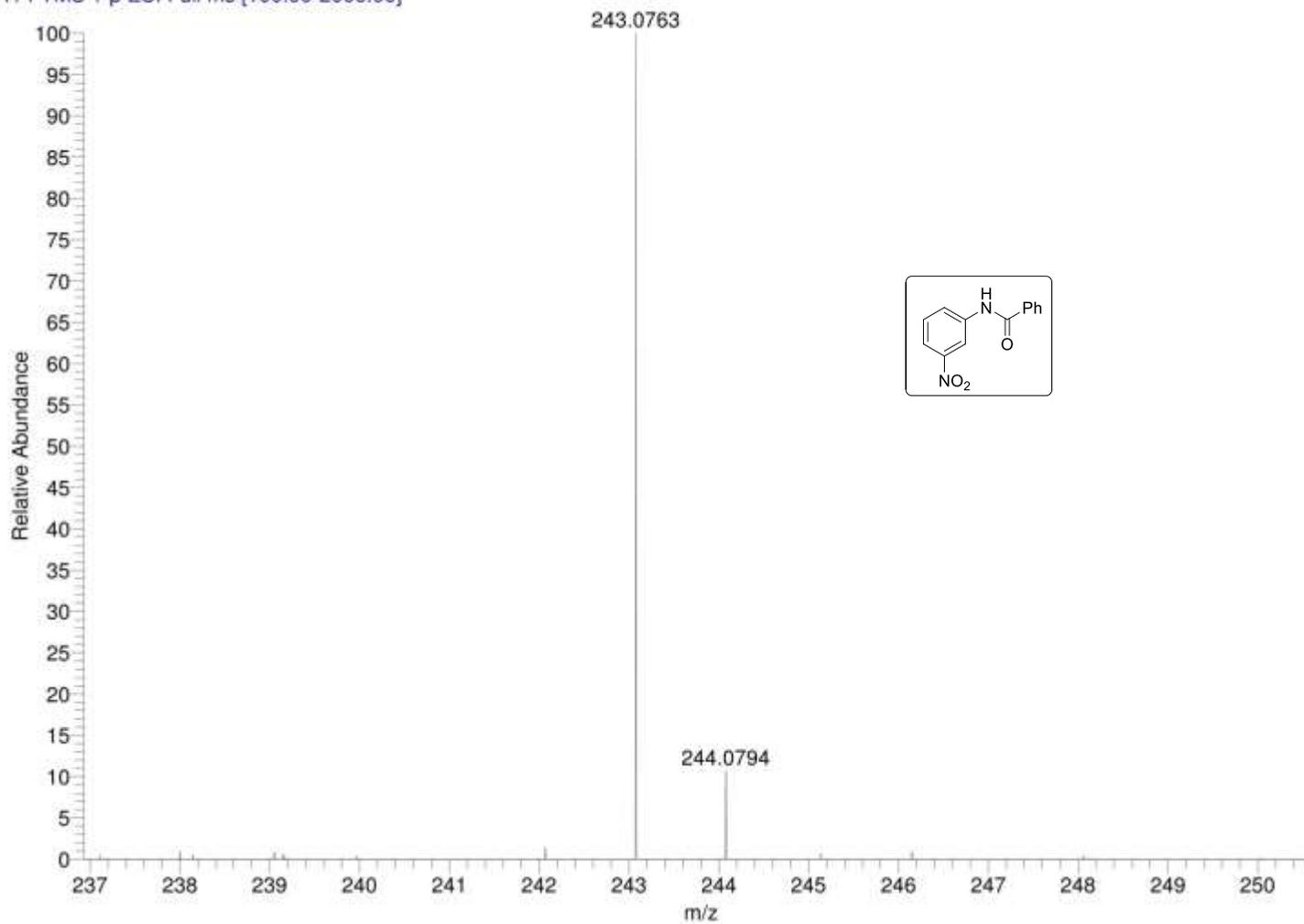
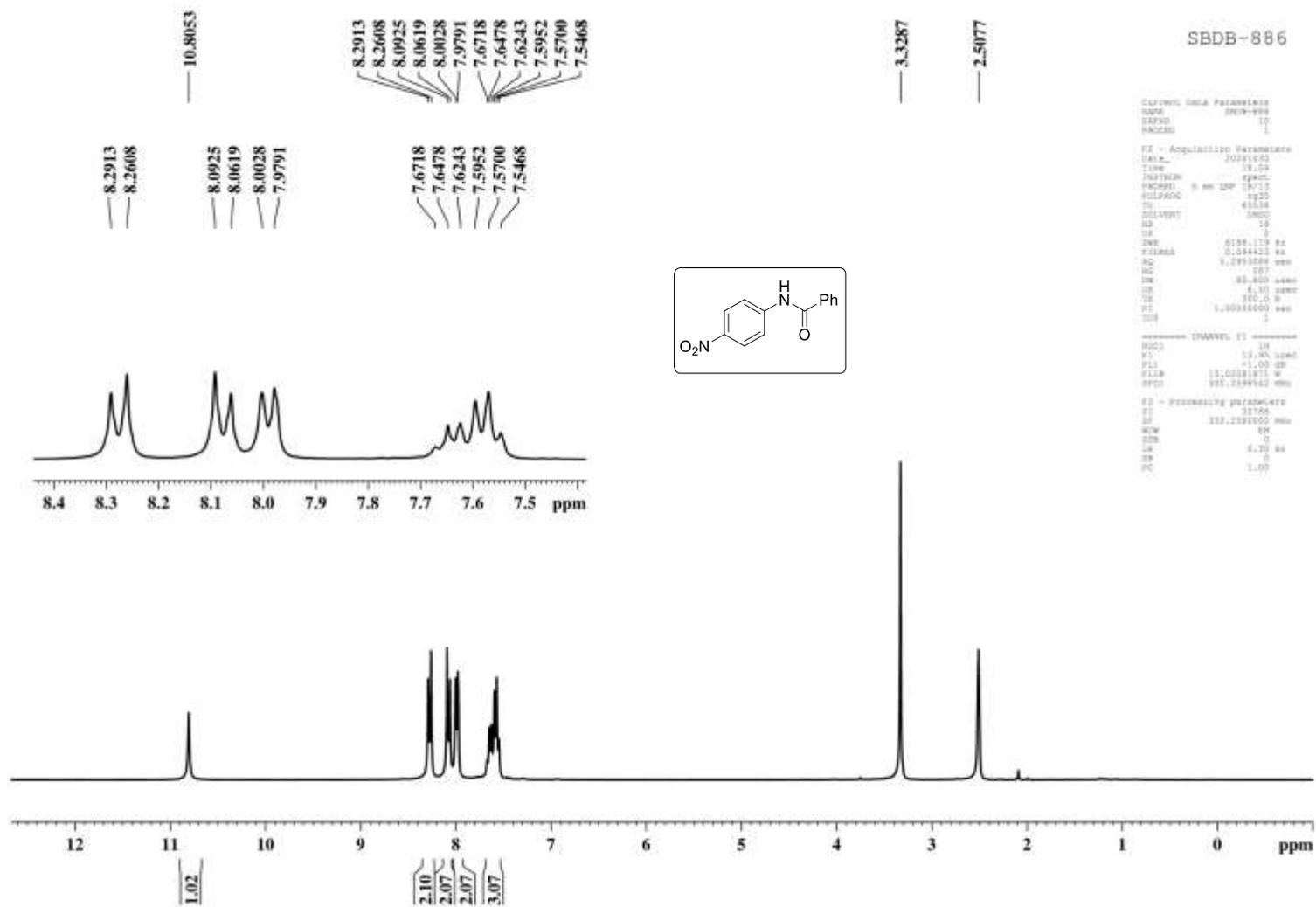


Figure S-136. HRMS spectrum of *N*-(3-nitrophenyl)benzamide (**7ba**).



**Figure S-137.**  $^1\text{H-NMR}$  spectrum of *N*-(4-nitrophenyl)benzamide (7ca).

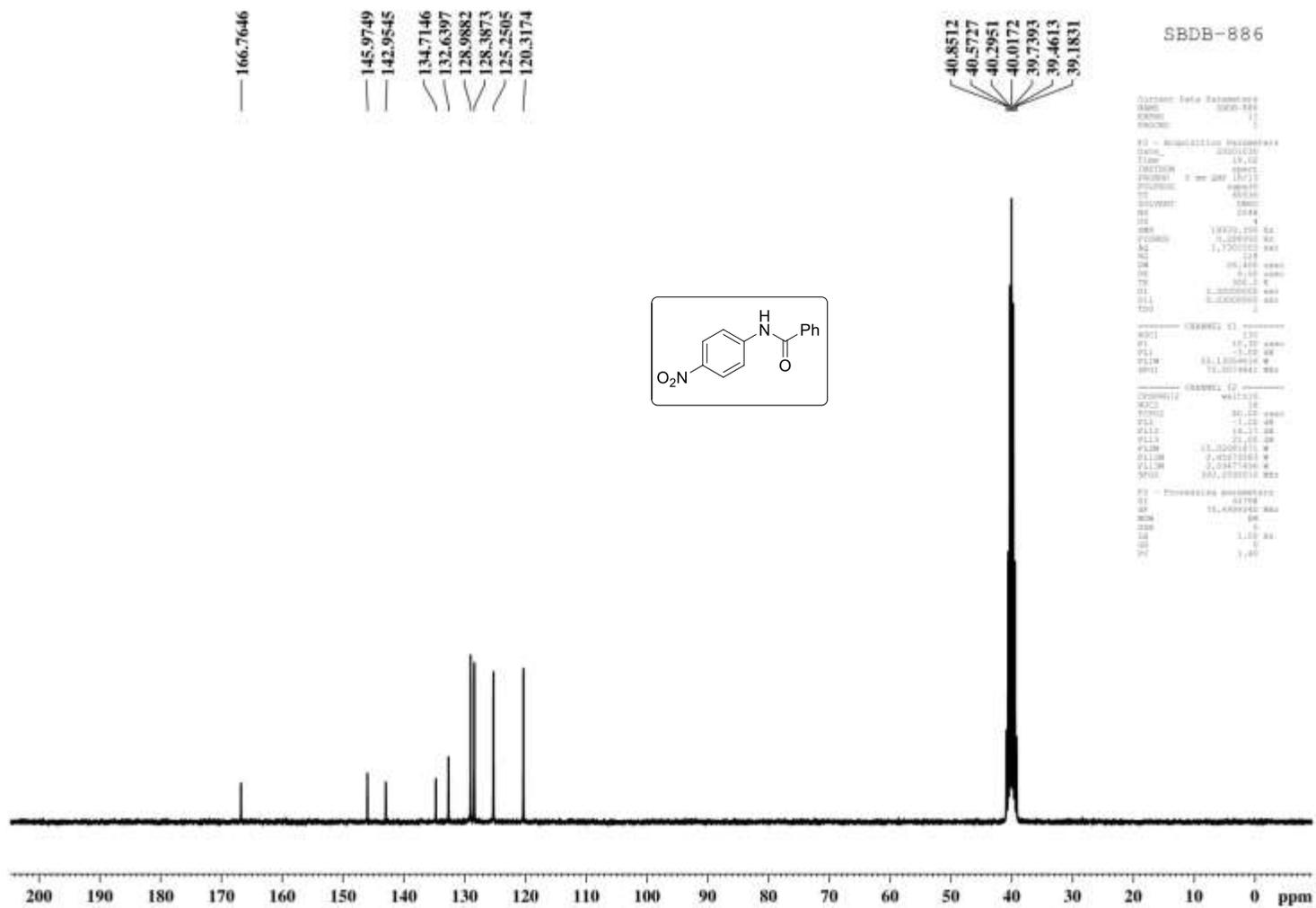


Figure S-138. <sup>13</sup>C-NMR spectrum of *N*-(4-nitrophenyl)benzamide (**7ca**).

### SAIF [HRMS Report]

Data File:	HRMS20I20OCT03	Original Data Path:	D:\INTERNAL NEW\2020\OCT 2020
Sample ID:	SBDB-886	Sample Name:	
Acquisition Date:	10/20/20 10:58:10 AM	Run Time(min):	0.00
Vial:	CStk1-01:3	Injection Volume(μl):	1.00

HRMS20I20OCT03 #11-22 RT: 0.11-0.21 AV: 12 SB: 1 0.01 NL: 1.39E5  
T: FTMS + c ESI Full ms [100.00-750.00]

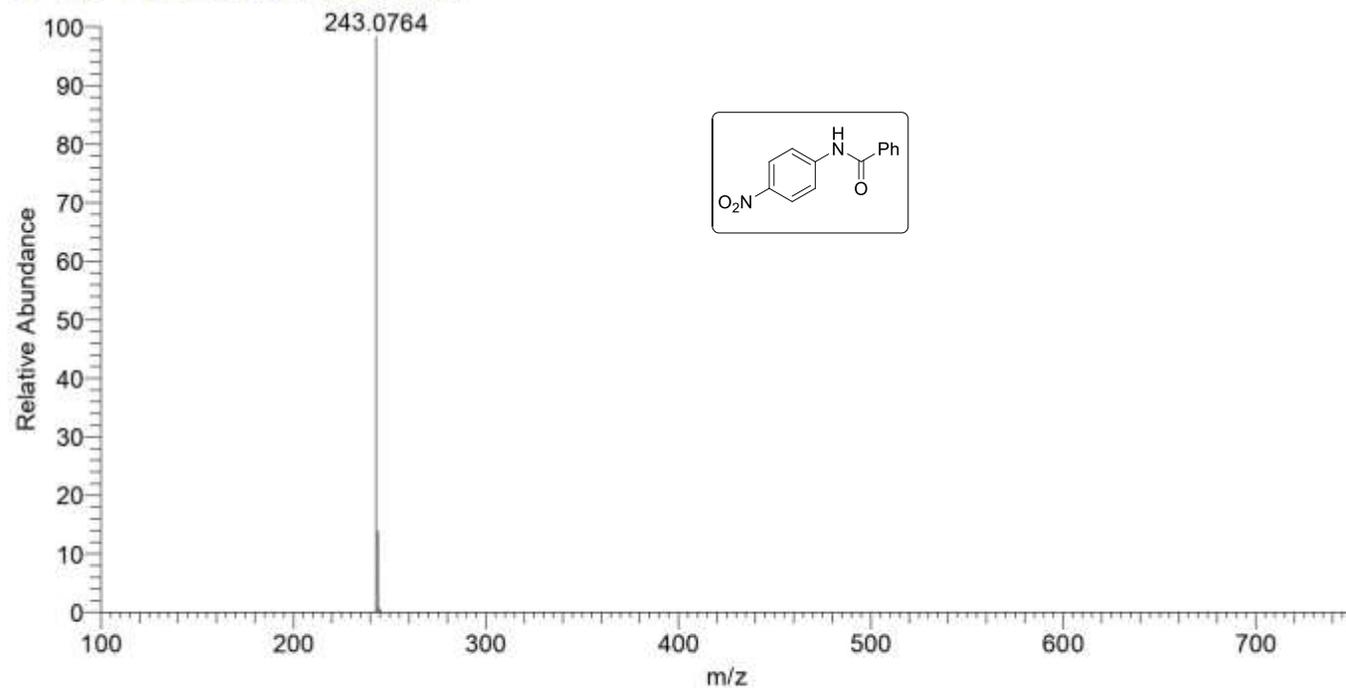


Figure S-139. HRMS spectrum of *N*-(4-nitrophenyl)benzamide (**7ca**).

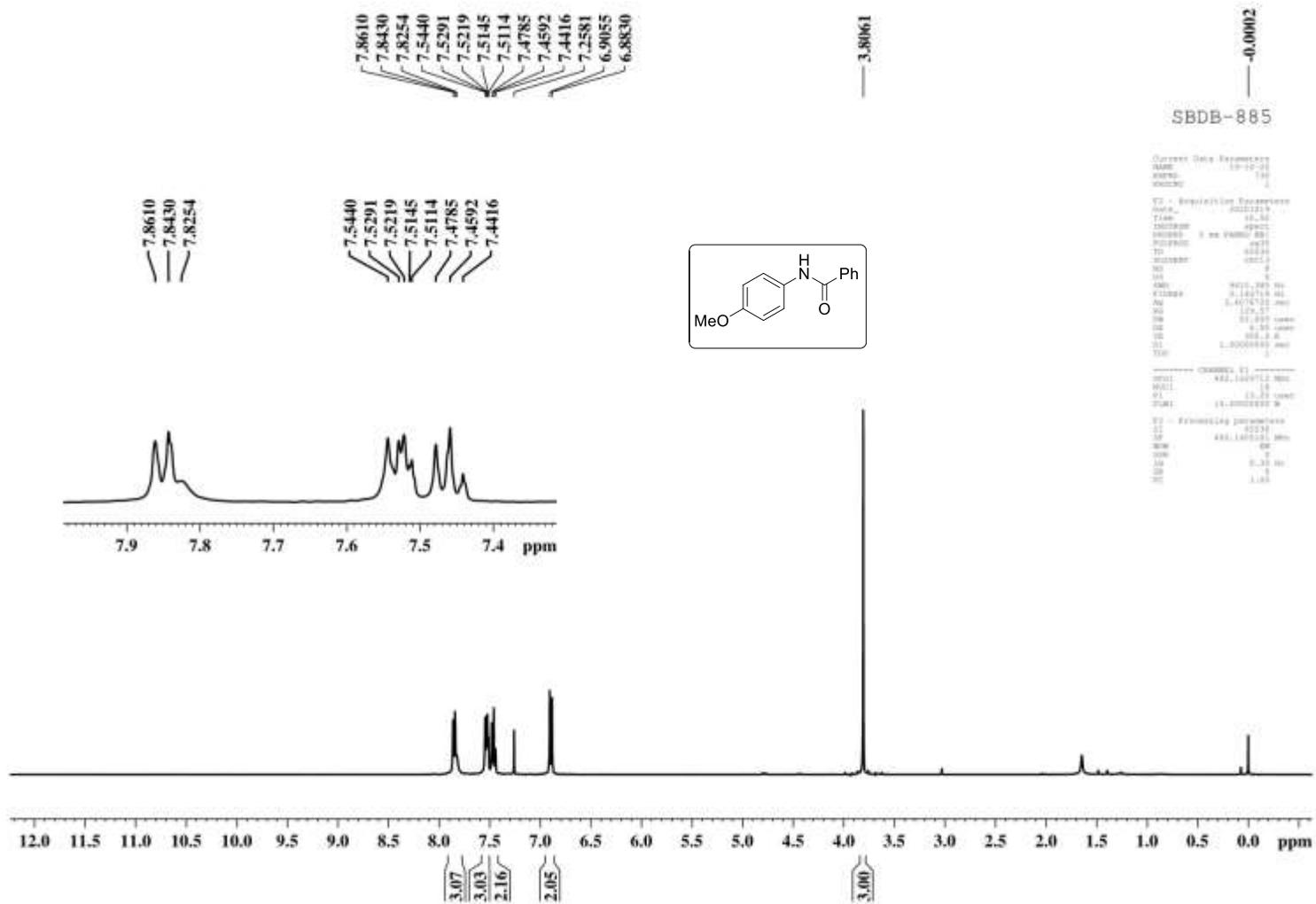


Figure S-140. <sup>1</sup>H-NMR spectrum of *N*-(4-methoxyphenyl)benzamide (7da).



### SAIF [HRMS Report]

Data File:	HRMS20I20OCT02	Original Data Path:	D:\INTERNAL NEW\2020\OCT 2020
Sample ID:	SBDB-885	Sample Name:	
Acquisition Date:	10/20/20 10:56:12 AM	Run Time(min):	0.00
Vial:	CS4k1-01:2	Injection Volume( $\mu$ l):	1.00

HRMS20I20OCT02 #12-23 RT: 0.12-0.21 AV: 12 SB: 1 0.01 NL: 1.09E6  
T: FTMS + c ESI Full ms [100.00-750.00]

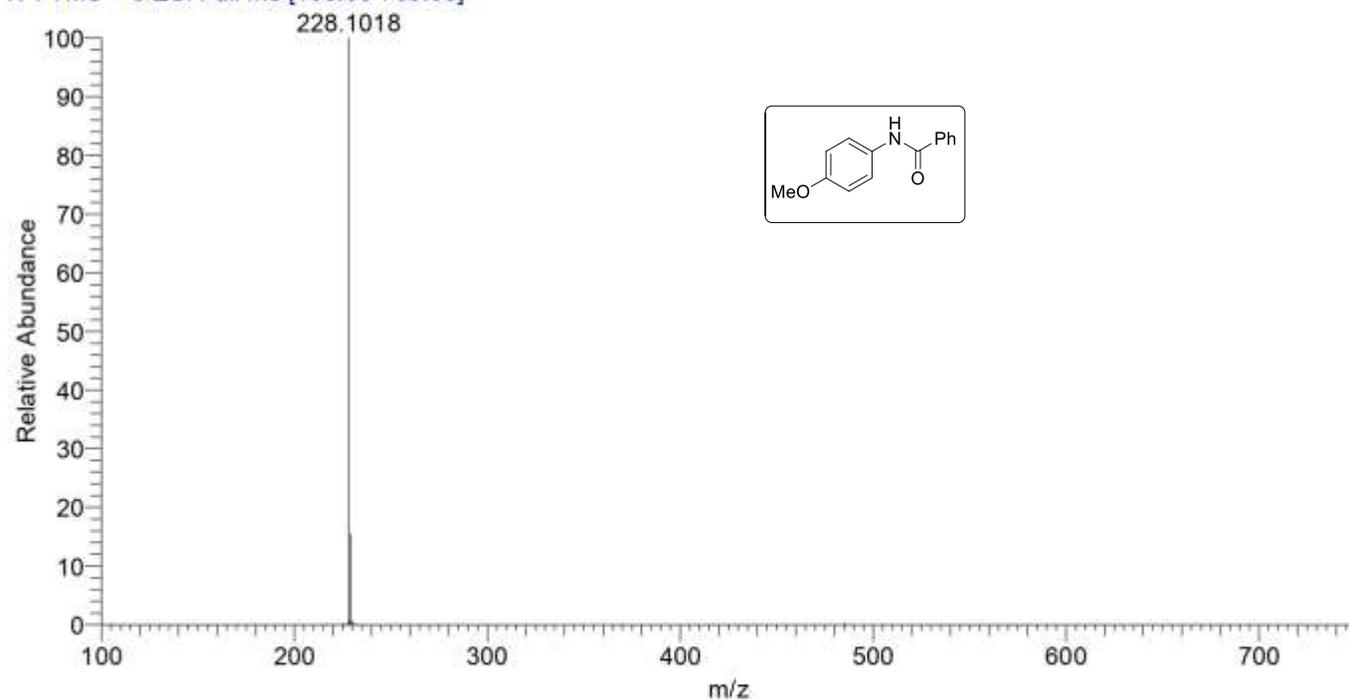


Figure S-142. HRMS spectrum of *N*-(4-methoxyphenyl)benzamide (**7da**).



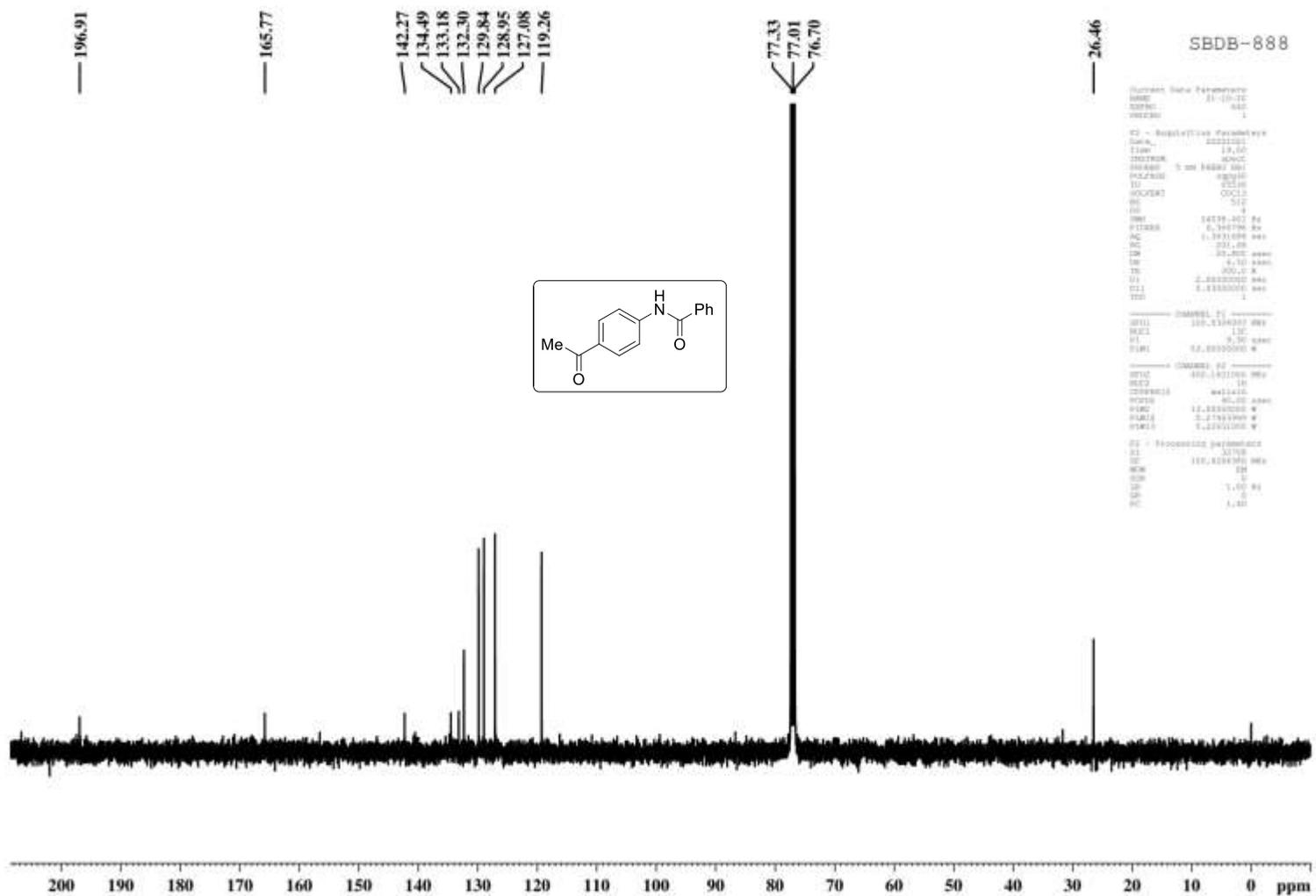


Figure S-144.  $^{13}\text{C}$ -NMR spectrum of *N*-(4-acetylphenyl)benzamide (7ea).

### SAIF [HRMS Report]

Data File:	HRMS20I20OCT04	Original Data Path:	D:\INTERNAL NEW\2020\OCT 2020
Sample ID:	SBDB-888	Sample Name:	
Acquisition Date:	10/20/20 11:00:07 AM	Run Time(min):	0.00
Vial:	CSfk1-01:4	Injection Volume(μl):	1.00

HRMS20I20OCT04 #11-22 RT: 0.11-0.21 AV: 12 SB: 1 0.01 NL: 6.55E5  
T: FTMS + c ESI Full ms [100.00-750.00]

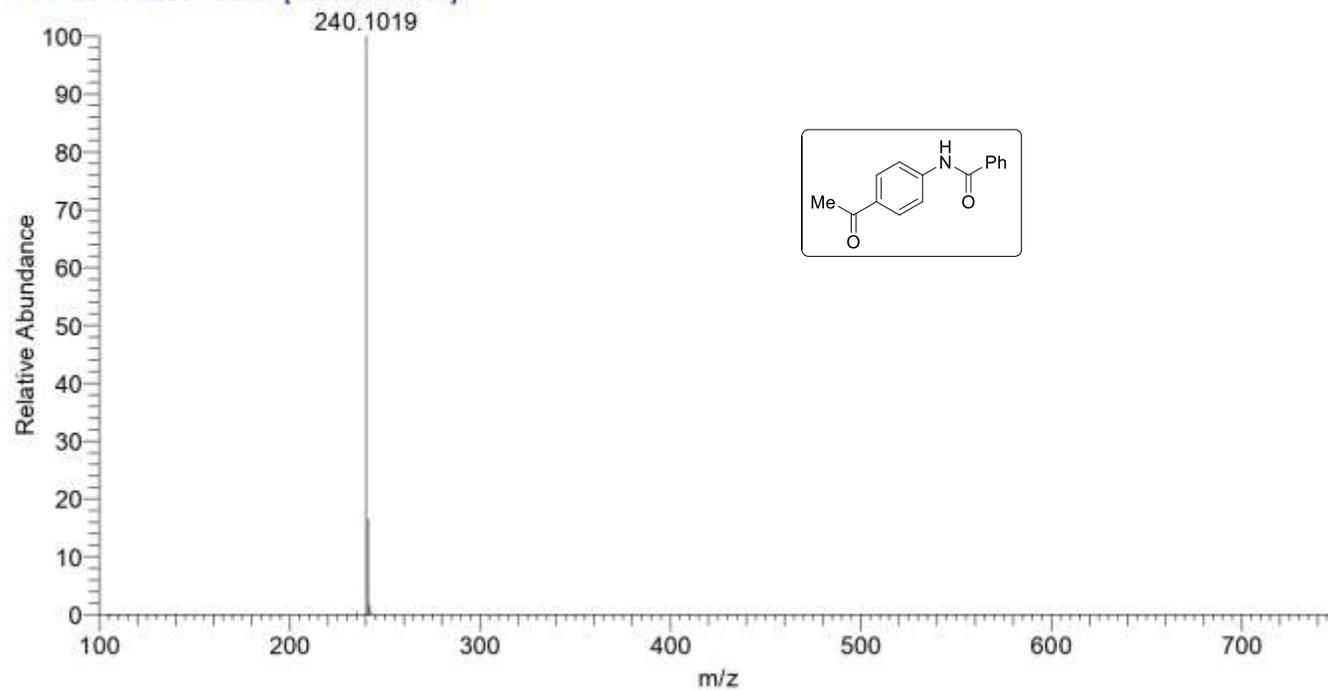


Figure S-145. HRMS spectrum of *N*-(4-acetylphenyl)benzamide (**7ea**).

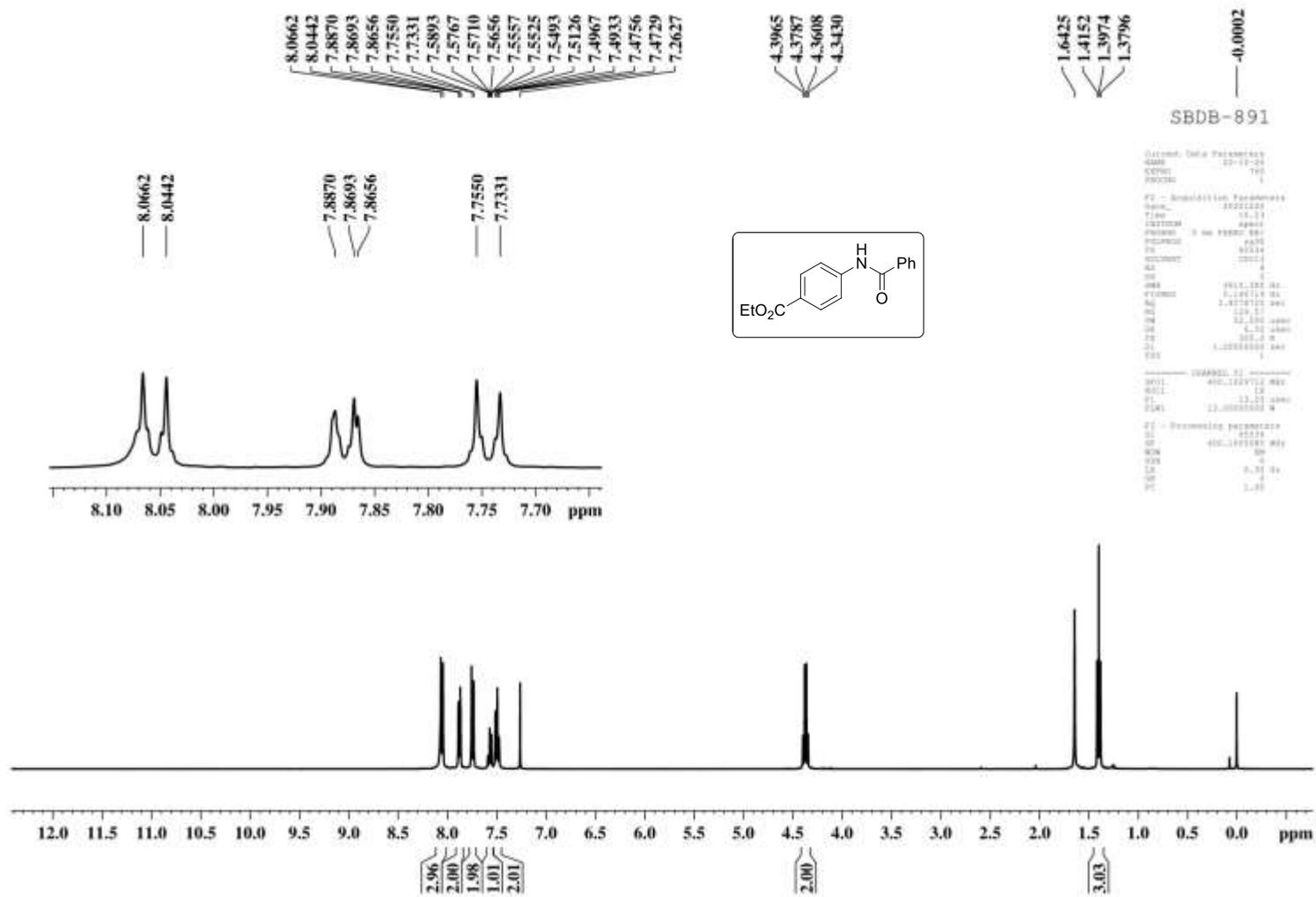


Figure S-146. <sup>1</sup>H-NMR spectrum of ethyl 4-benzamidobenzoate (7fa).

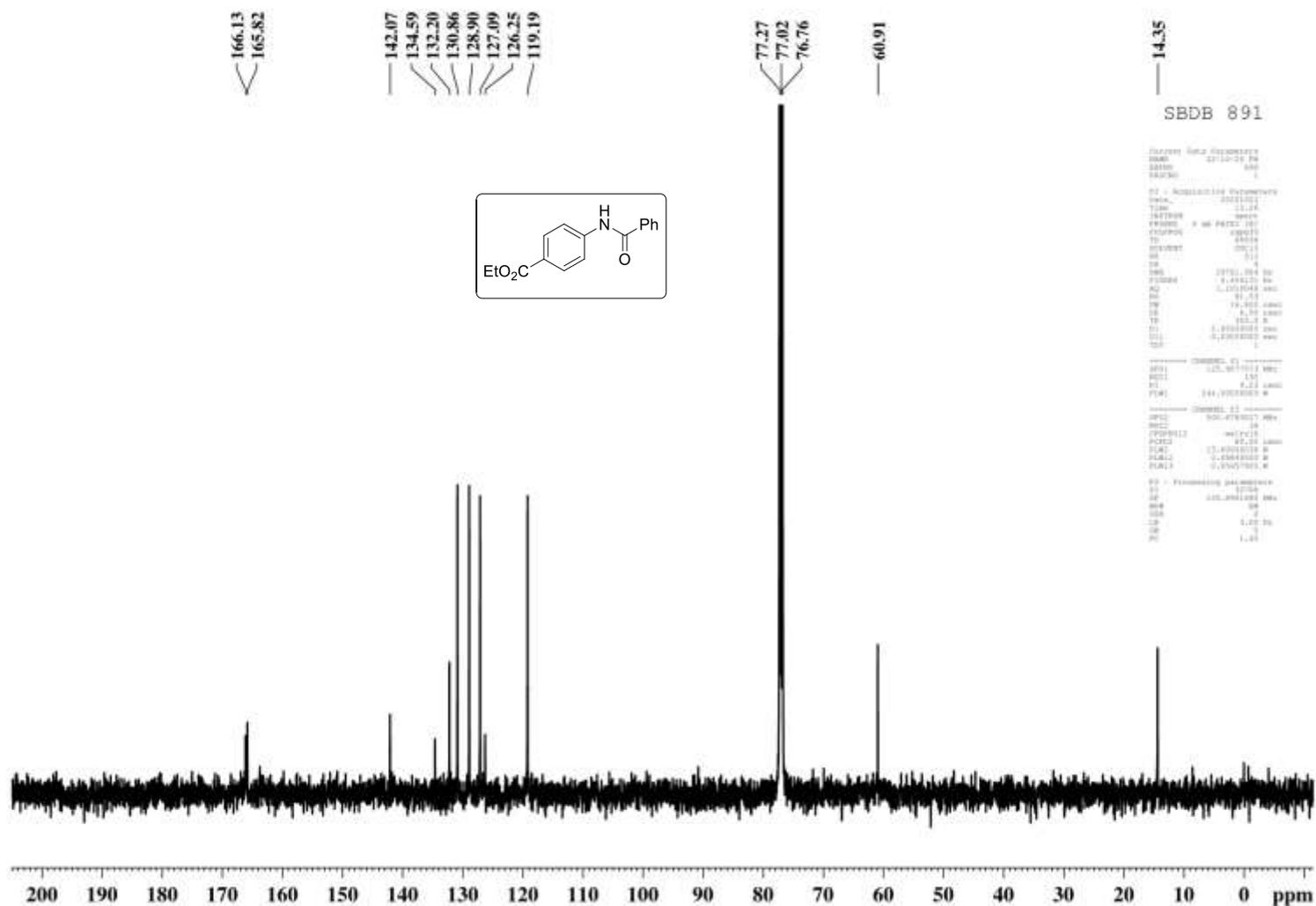


Figure S-147. <sup>13</sup>C-NMR spectrum of ethyl 4-benzamidobenzoate (7fa).

### SAIF [HRMS Report]

Data File:	HRMS20I20OCT26	Original Data Path:	D:\INTERNAL NEW\2020\OCT 2020
Sample ID:	sdbf-891	Sample Name:	
Acquisition Date:	10/20/20 11:43:05 AM	Run Time(min):	0.00
Vial:	CStk1-01:26	Injection Volume( $\mu$ l):	1.00

HRMS20I20OCT26 #11-22 RT: 0.11-0.21 AV: 12 SB: 1 0.01 NL: 8.27E4  
T: FTMS + c ESI Full ms [100.00-750.00]

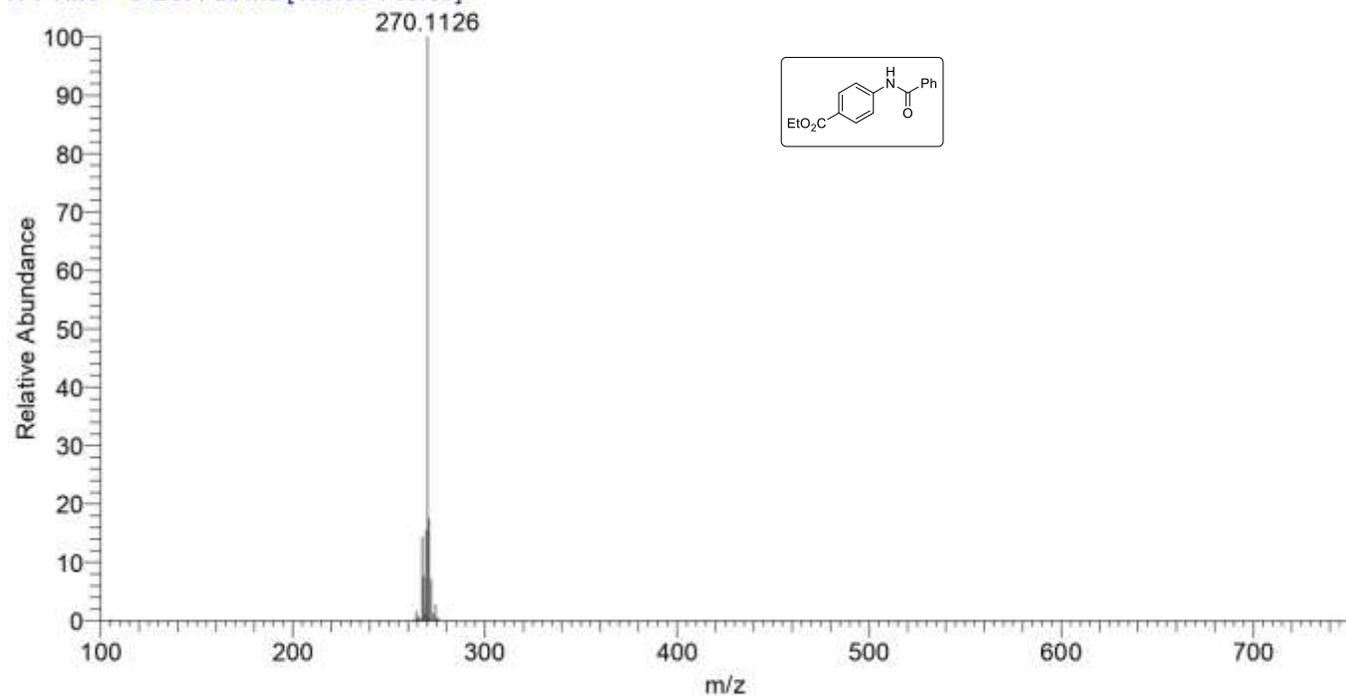
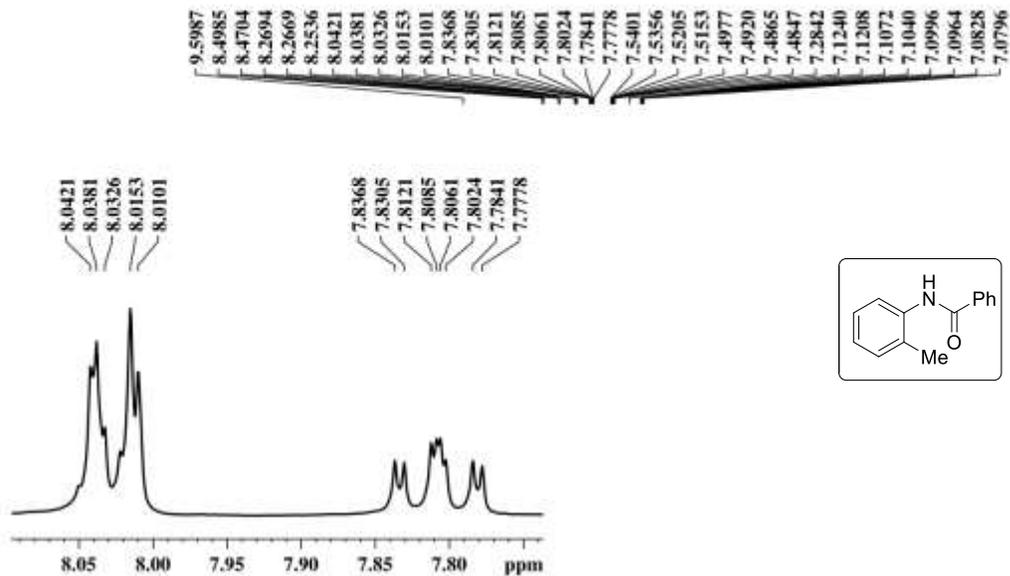


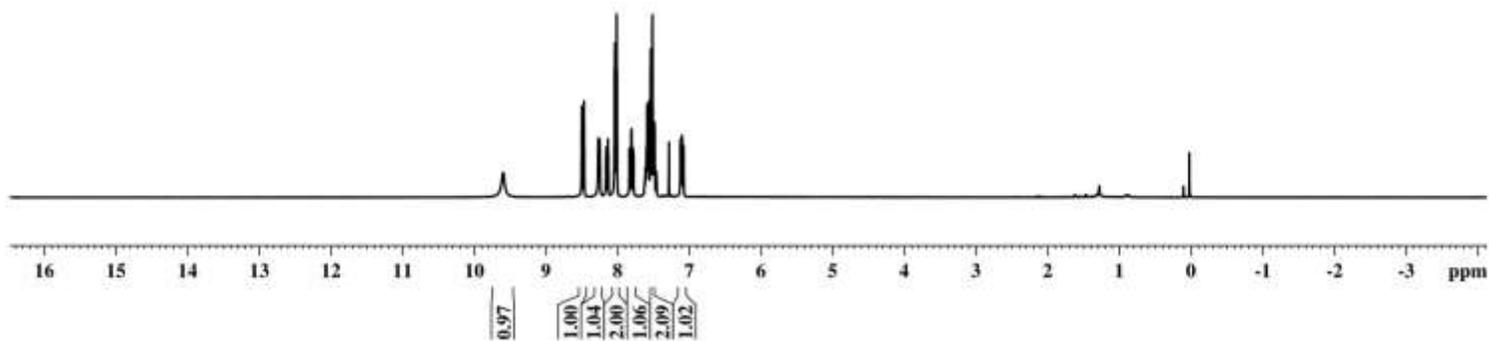
Figure S-148. HRMS spectrum of ethyl 4-benzamidobenzoate (**7fa**).



SBDB-894

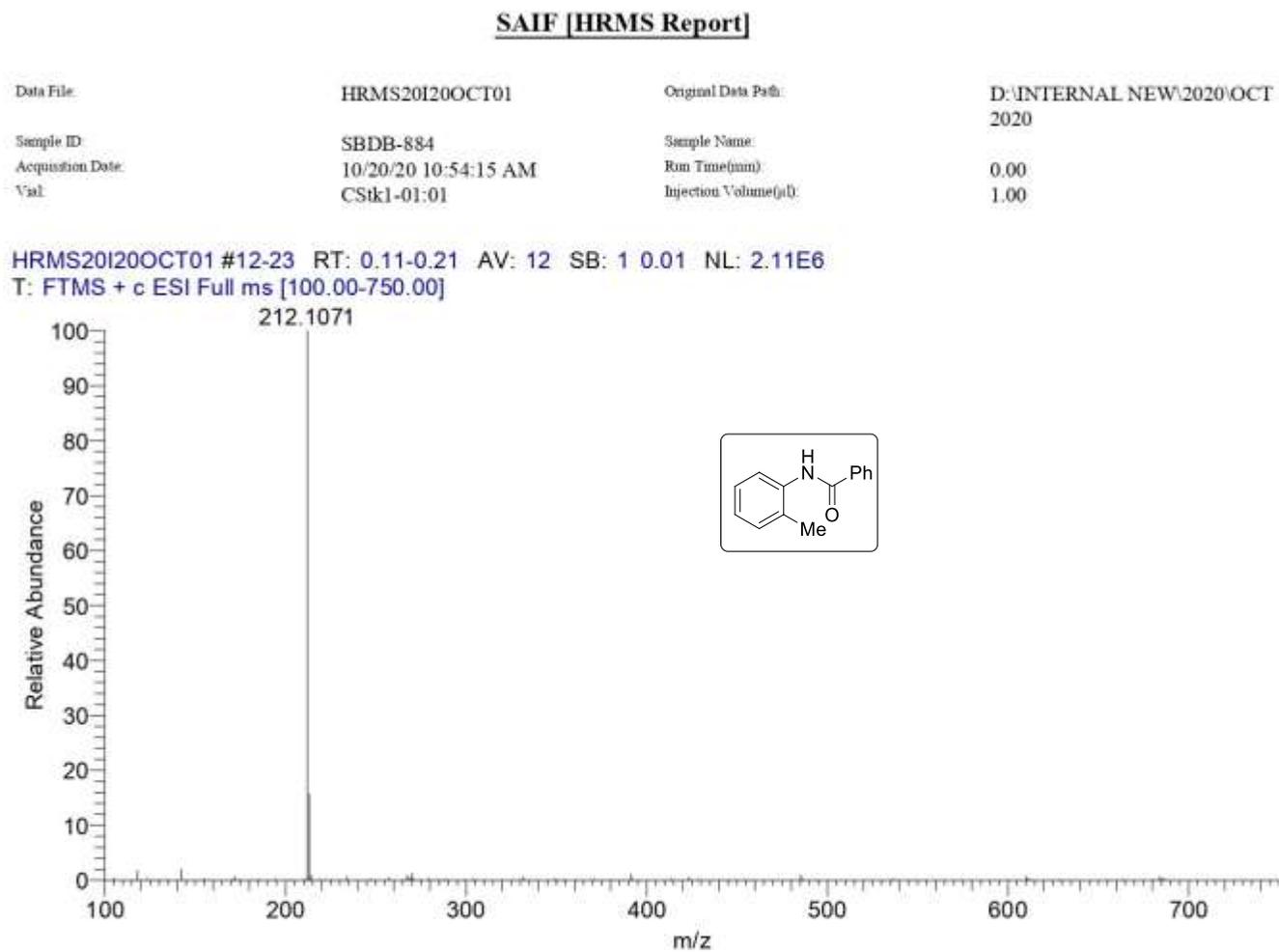
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PROCNO    1
F2 - Acquisition Parameters
Date_     20070324
Time      13:34
INSTRUM   spect
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PULPROG   zgpg30
PR      4024
SOLVENT   CDCl3
NUC1       13
NUC2       1
FWD       634.115 Hz
AQ        6.034223 Hz
RG         2.233333 sec
AQ        121
SF         400.600 MHz
DS         4.00 umm
TE         300.0 K
NUC1       13C(101320) MHz
TDS       1
===== CHANNEL f1 =====
NUC1       13
P1         12.00 umm
PL1        -1.00 dB
PL12       12.0000000 MHz
PC1        100.2300000 MHz
F2 - Processing parameters
SI         32768
SF         100.2300000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.04
  
```





**Figure S-150.**  $^{13}\text{C}$ -NMR spectrum of *N*-*o*-tolylbenzamide (**7ga**).



**Figure S-151.** HRMS spectrum of *N*-*o*-tolylbenzamide (**7ga**).

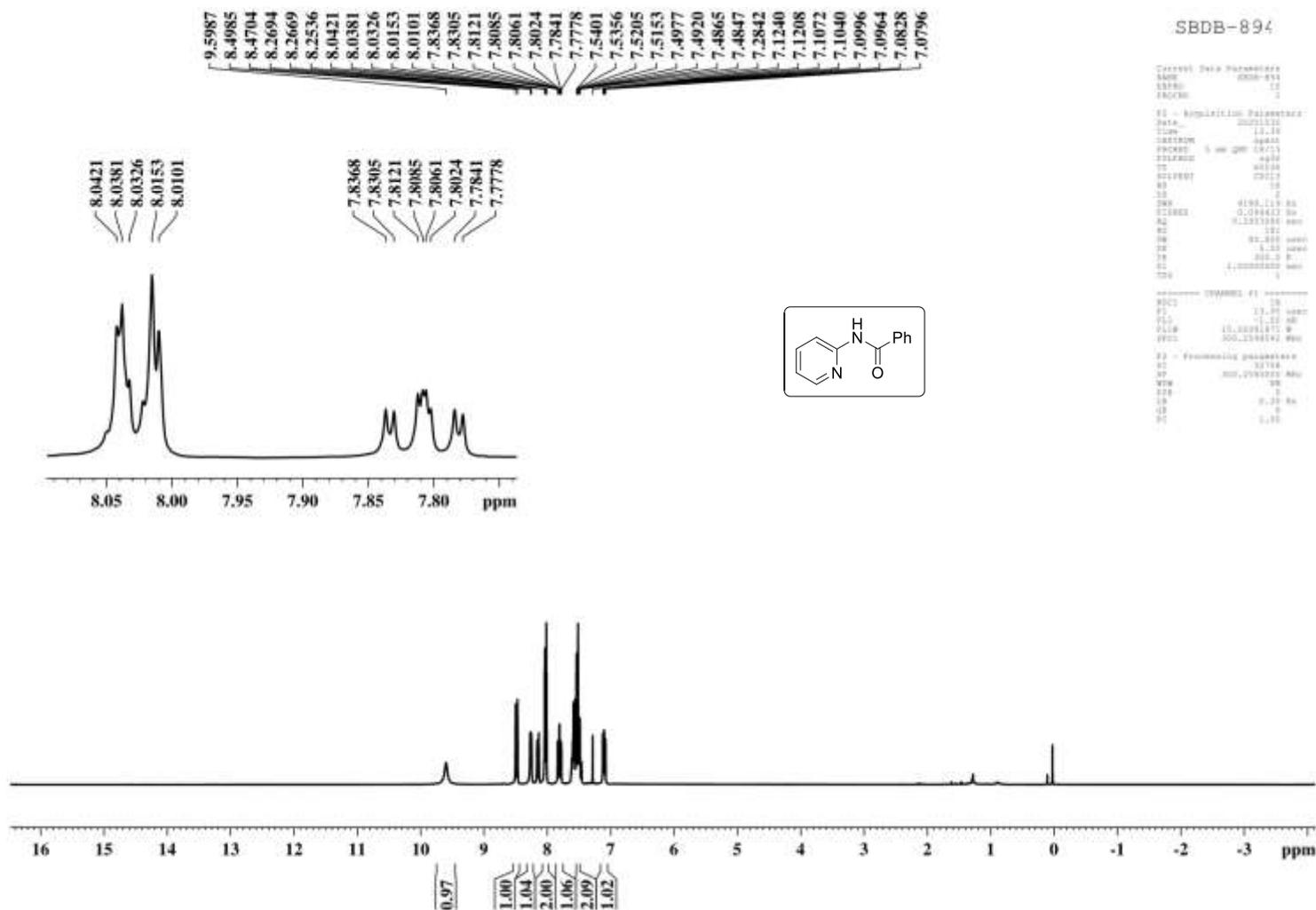


Figure S-152. <sup>1</sup>H-NMR spectrum of *N*-(pyridin-2-yl)benzamide (7ha).

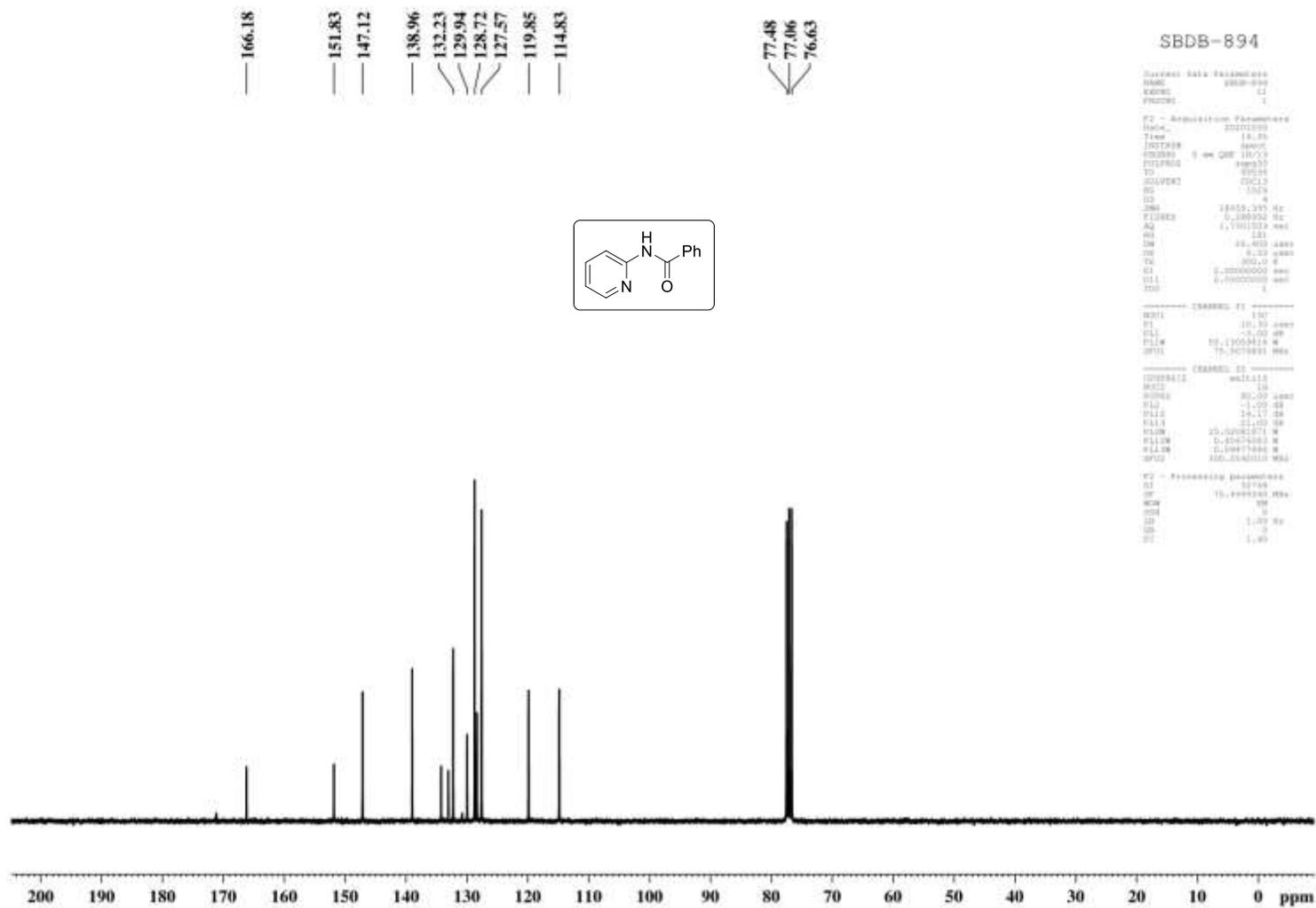


Figure S-153. <sup>13</sup>C-NMR spectrum of *N*-(pyridin-2-yl)benzamide (7ha).

### SAIF [HRMS Report]

Data File:	HRMS20I28OCT28	Original Data Path:	D:\INTERNAL NEW\2020\OCT 2020
Sample ID:	SBDB-894	Sample Name:	
Acquisition Date:	10/28/20 11:36:47 AM	Run Time(min):	0.00
Vial:	CStk1-01:28	Injection Volume( $\mu$ l):	1.00

HRMS20I28OCT28 #13-26 RT: 0.11-0.21 AV: 14 SB: 1 0.01 NL: 1.74E7  
T: FTMS + p ESI Full ms [100.00-500.00]

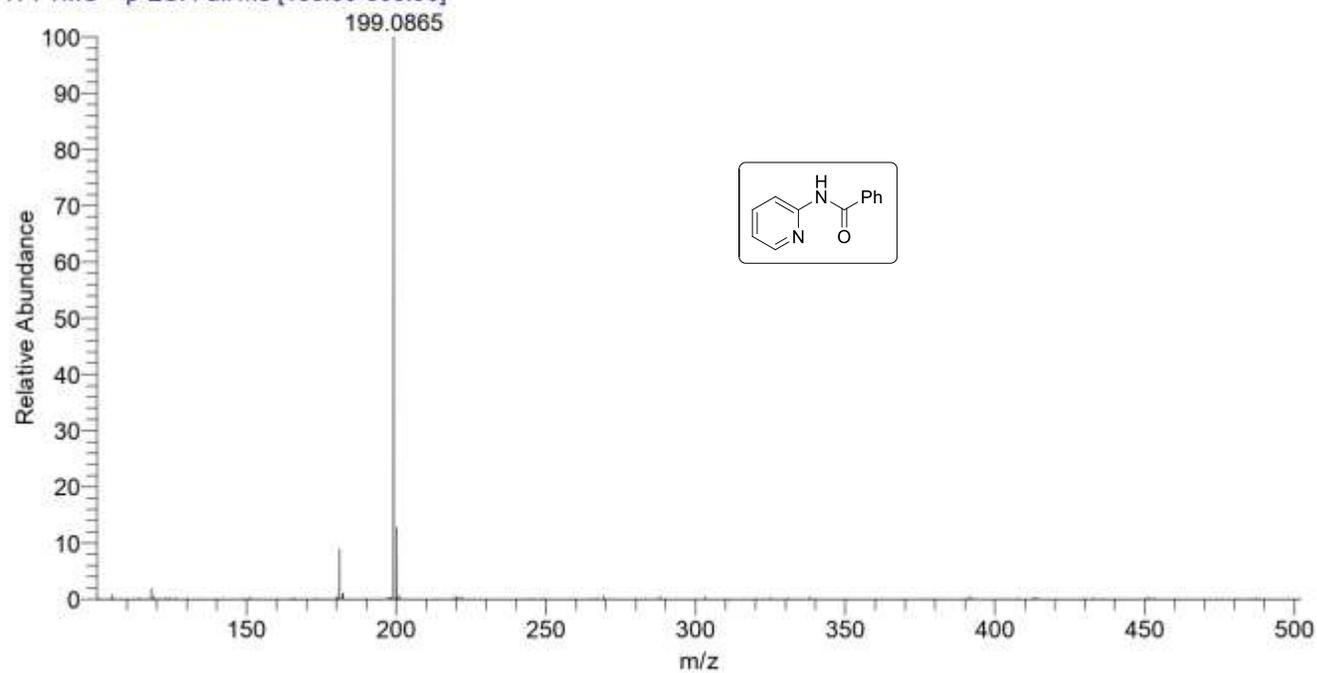


Figure S-154. HRMS spectrum of *N*-(pyridin-2-yl)benzamide (**7ha**).

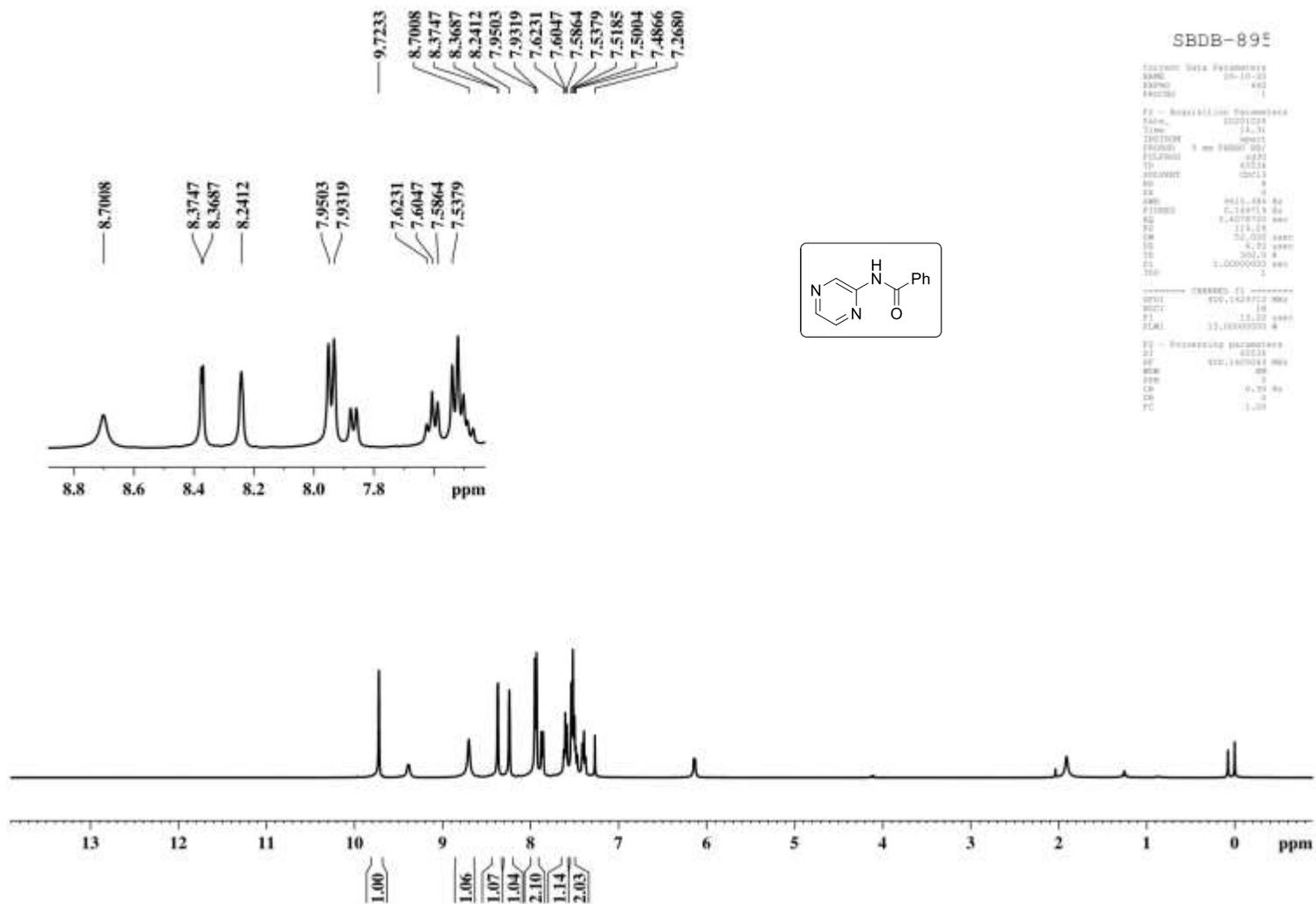


Figure S-155. <sup>1</sup>H-NMR spectrum of *N*-(pyrazin-2-yl)benzamide (7ia).

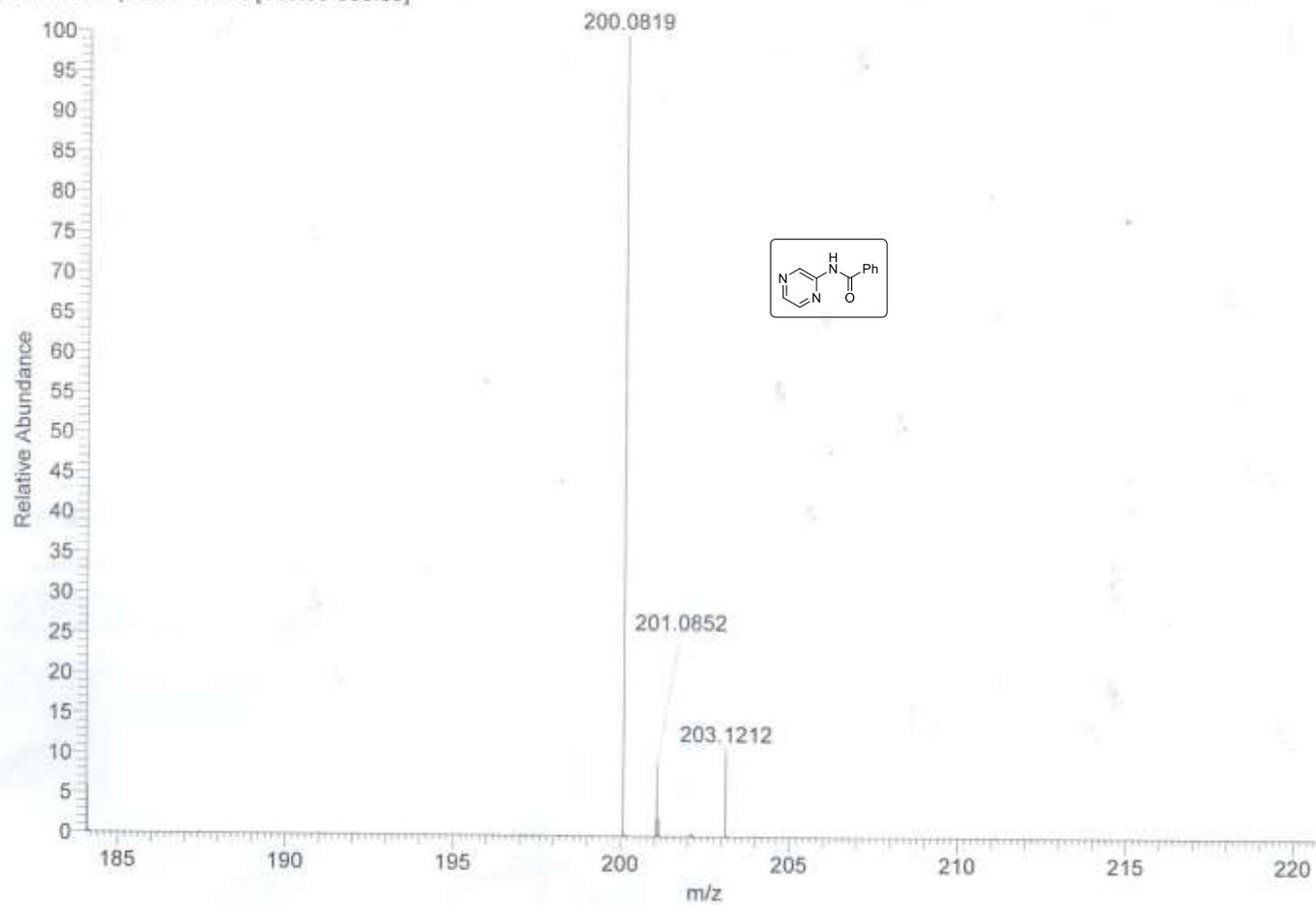


D:\INTERNAL NEW...HRMS20I27OCT25

10/27/2020 11:27:44 AM

SBDB-895-I

HRMS20I27OCT25 #23-34 RT: 0.19-0.28 AV: 12 SB: 7 0.03-0.08 NL: 1.65E5  
T: FTMS + p ESI Full ms [100.00-500.00]



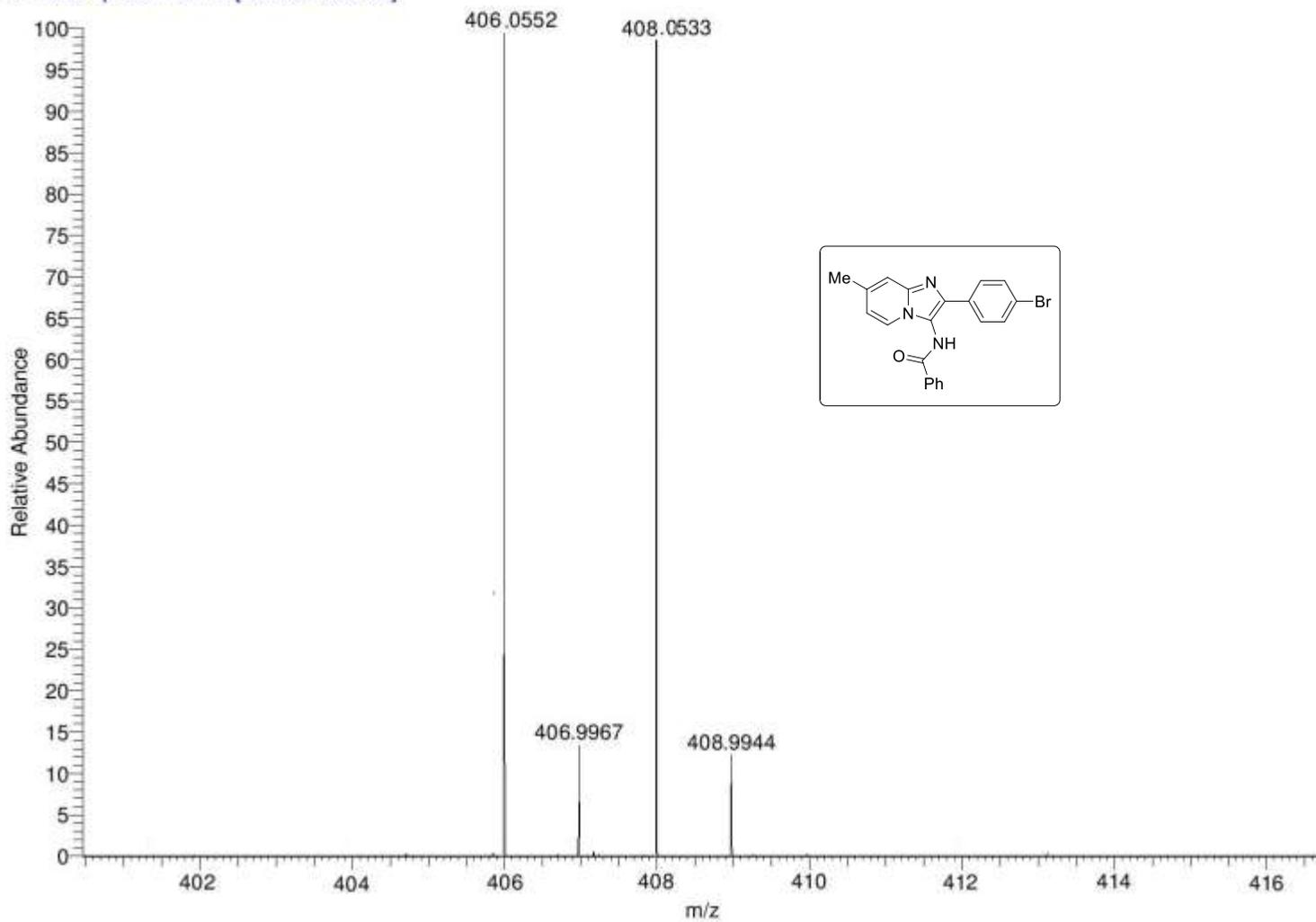
**Figure S-157.** HRMS spectrum of *N*-(pyrazin-2-yl)benzamide (**7ia**).





HRMS19I11APR10 #5-8 RT: 0.15-0.18 AV: 4 SB: 25 0.46-0.71 , 0.12 NL: 4.80E5

T: FTMS - p ESI Full ms [100.00-1000.00]



**Figure S-160.** HRMS spectrum of *N*-(2-(4-bromophenyl)-7-methylimidazo[1,2-*a*]pyridin-3-yl)benzamide (**7ja**).

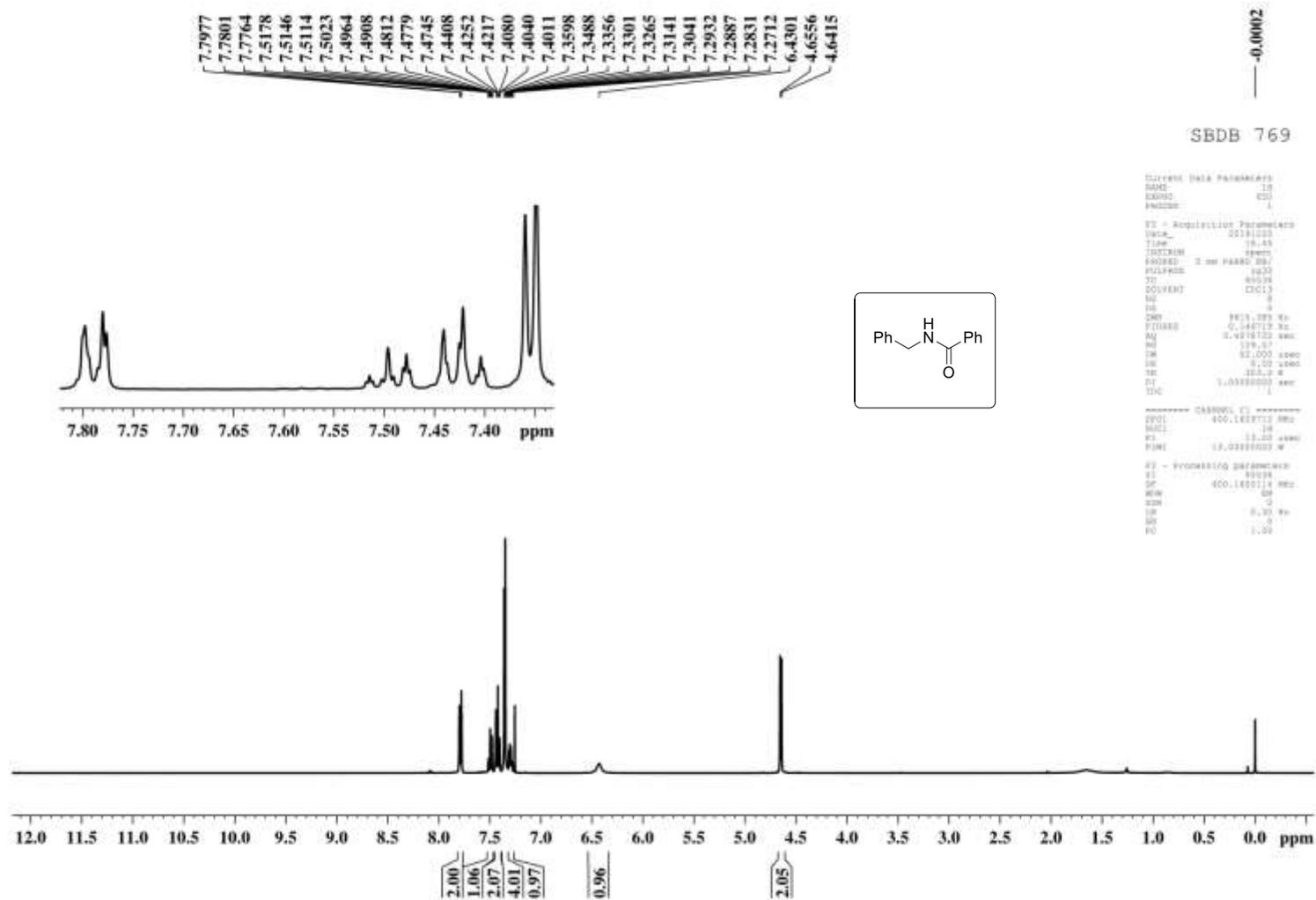


Figure S-161. <sup>1</sup>H-NMR spectrum of *N*-benzylbenzamide (7ka).

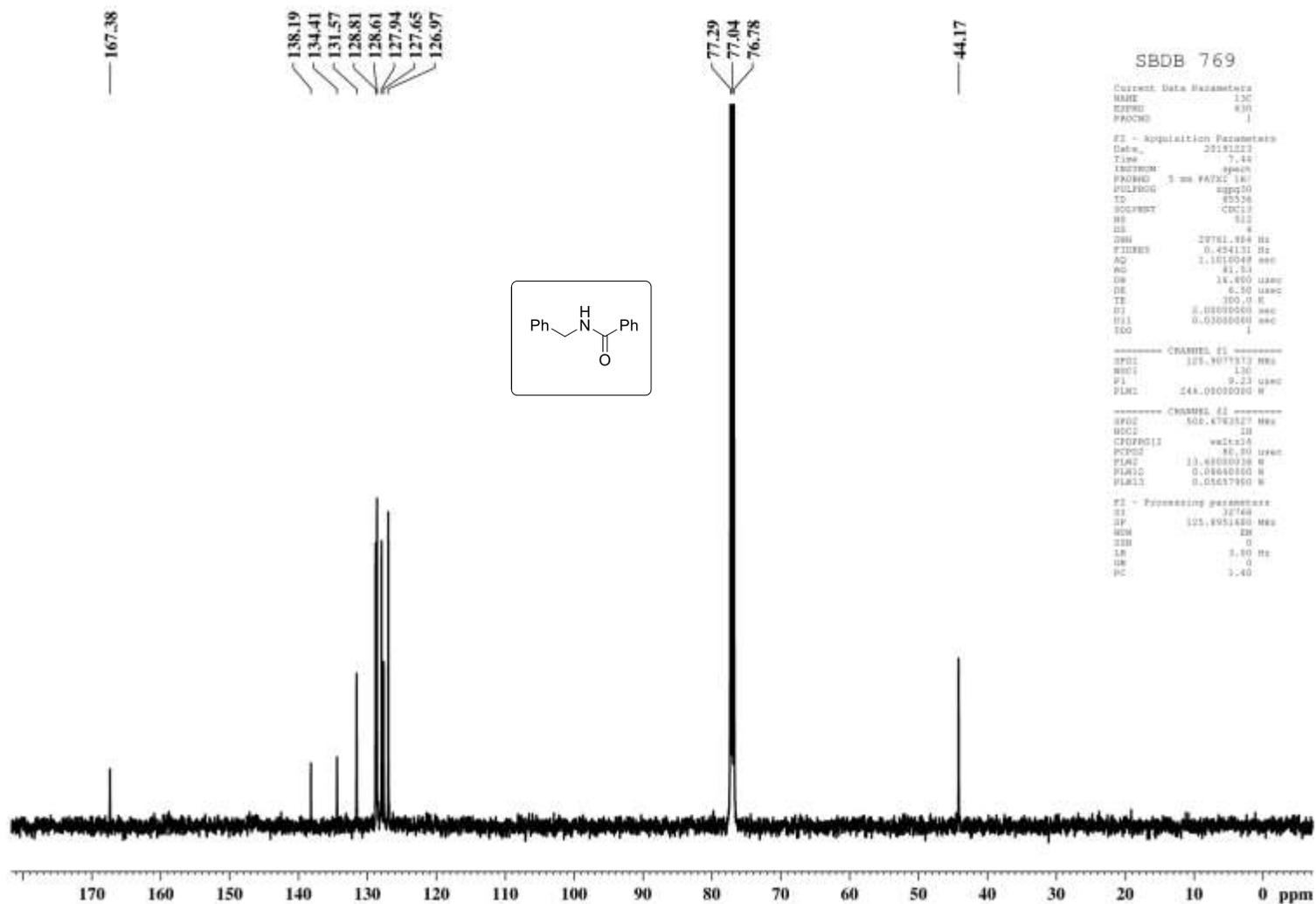
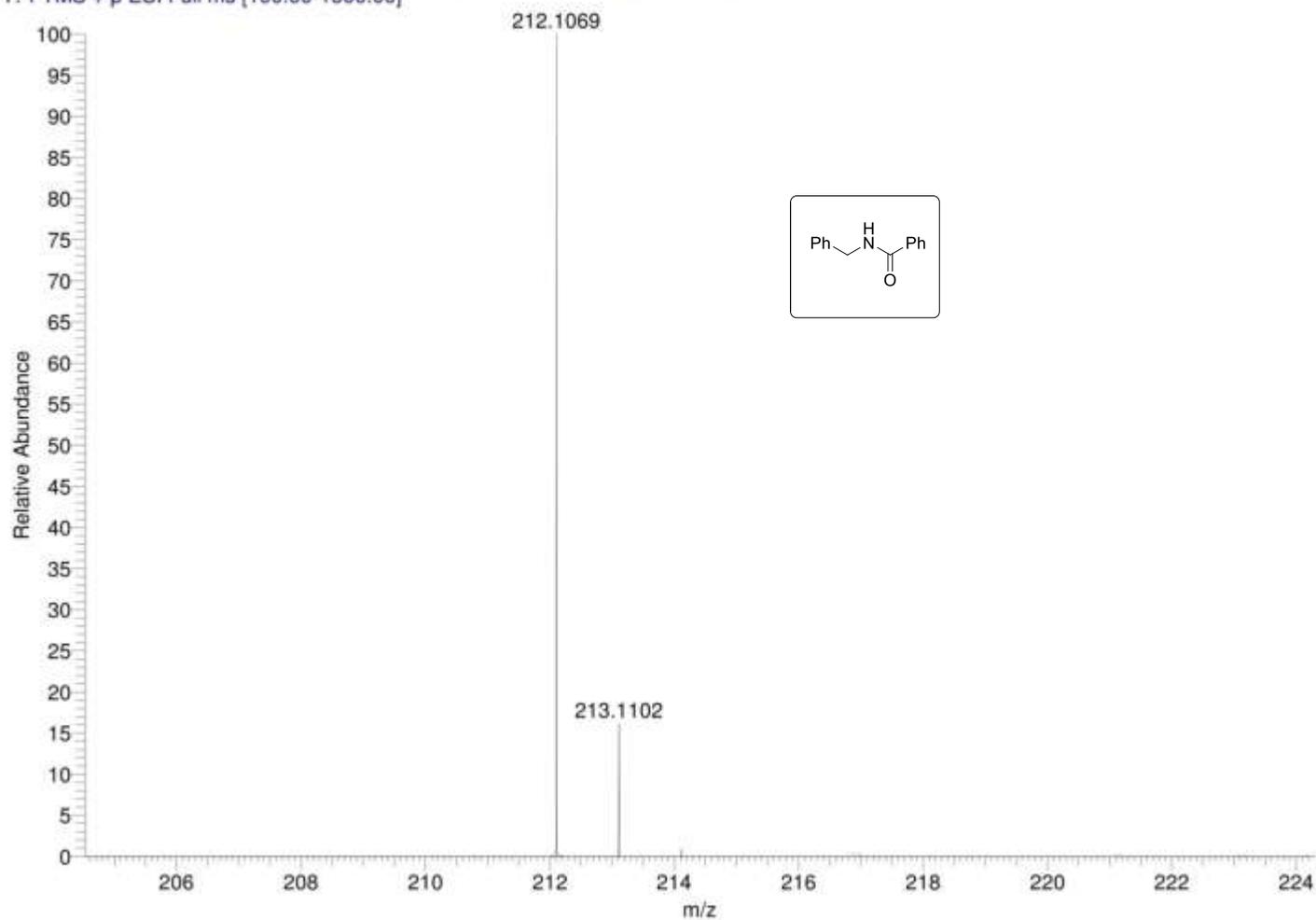


Figure S-162. <sup>13</sup>C-NMR spectrum of N-benzylbenzamide (7ka).

HRMS19I23DEC41 #13-40 RT: 0.10-0.30 AV: 28 SB: 8 0.02-0.08 NL: 7.13E6

T: FTMS +p ESI Full ms [100.00-1500.00]



**Figure S-163.** HRMS spectrum of *N*-benzylbenzamide (**7ka**).

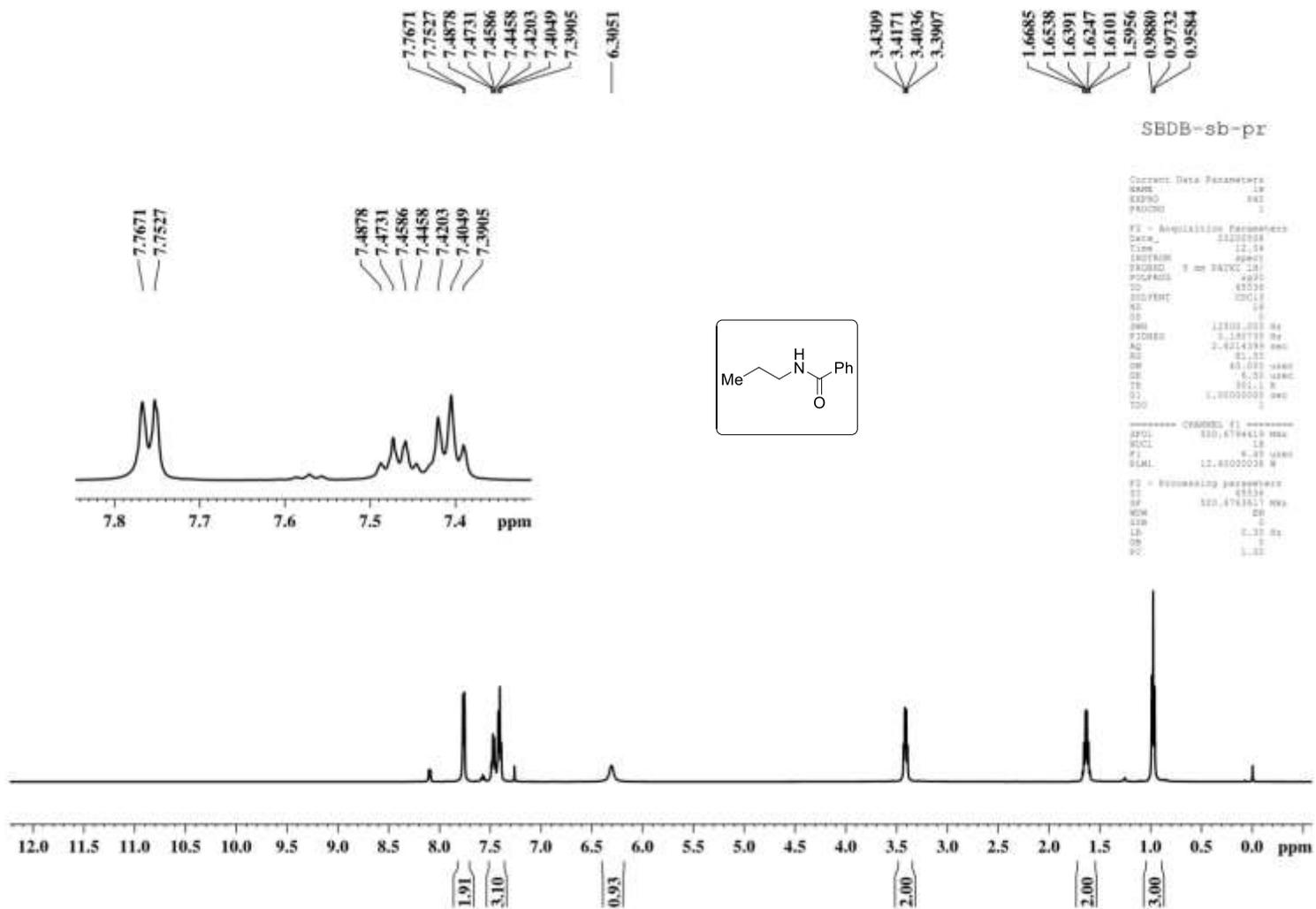


Figure S-164. <sup>1</sup>H-NMR spectrum of *N*-isopropylbenzamide (71a).

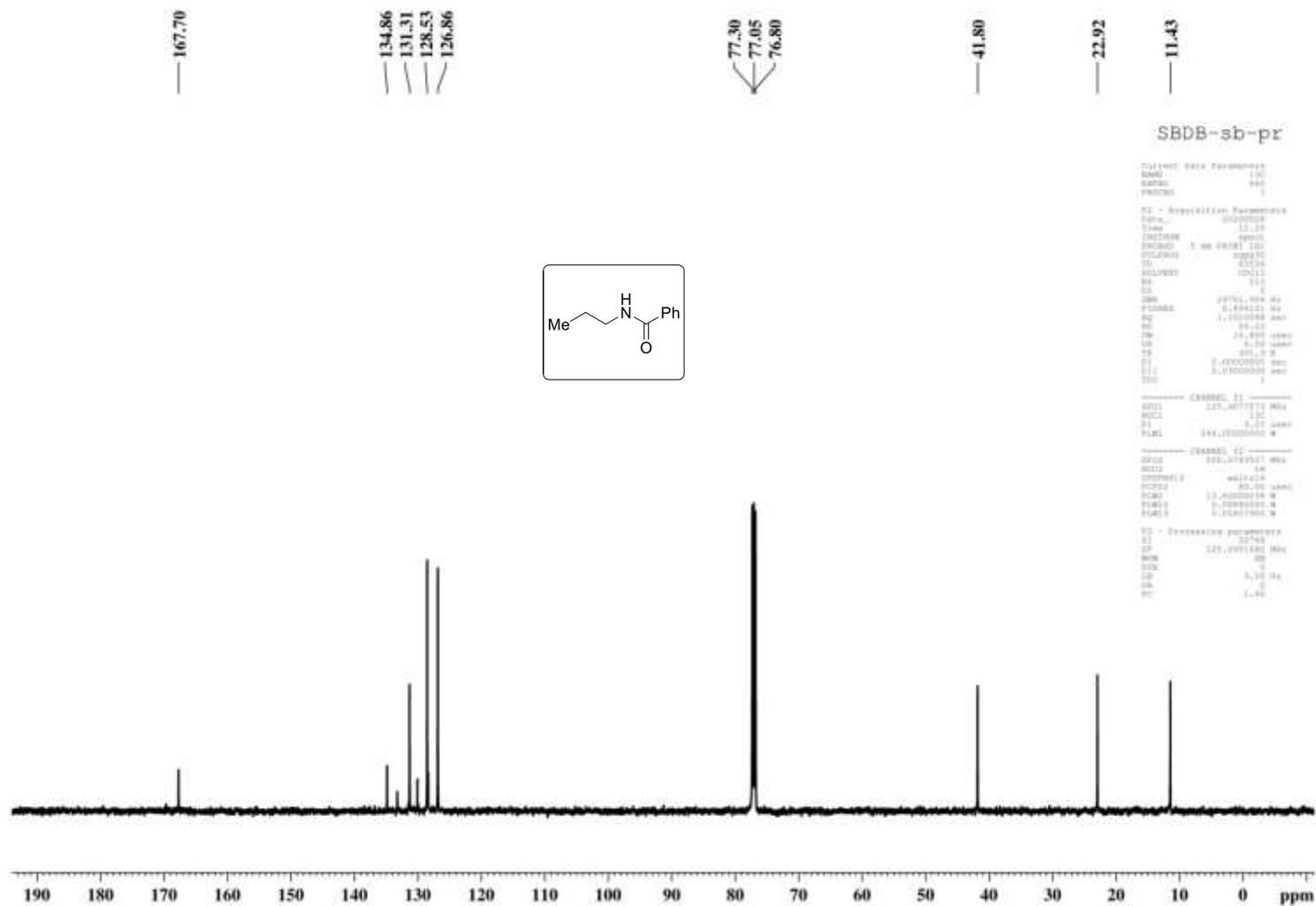
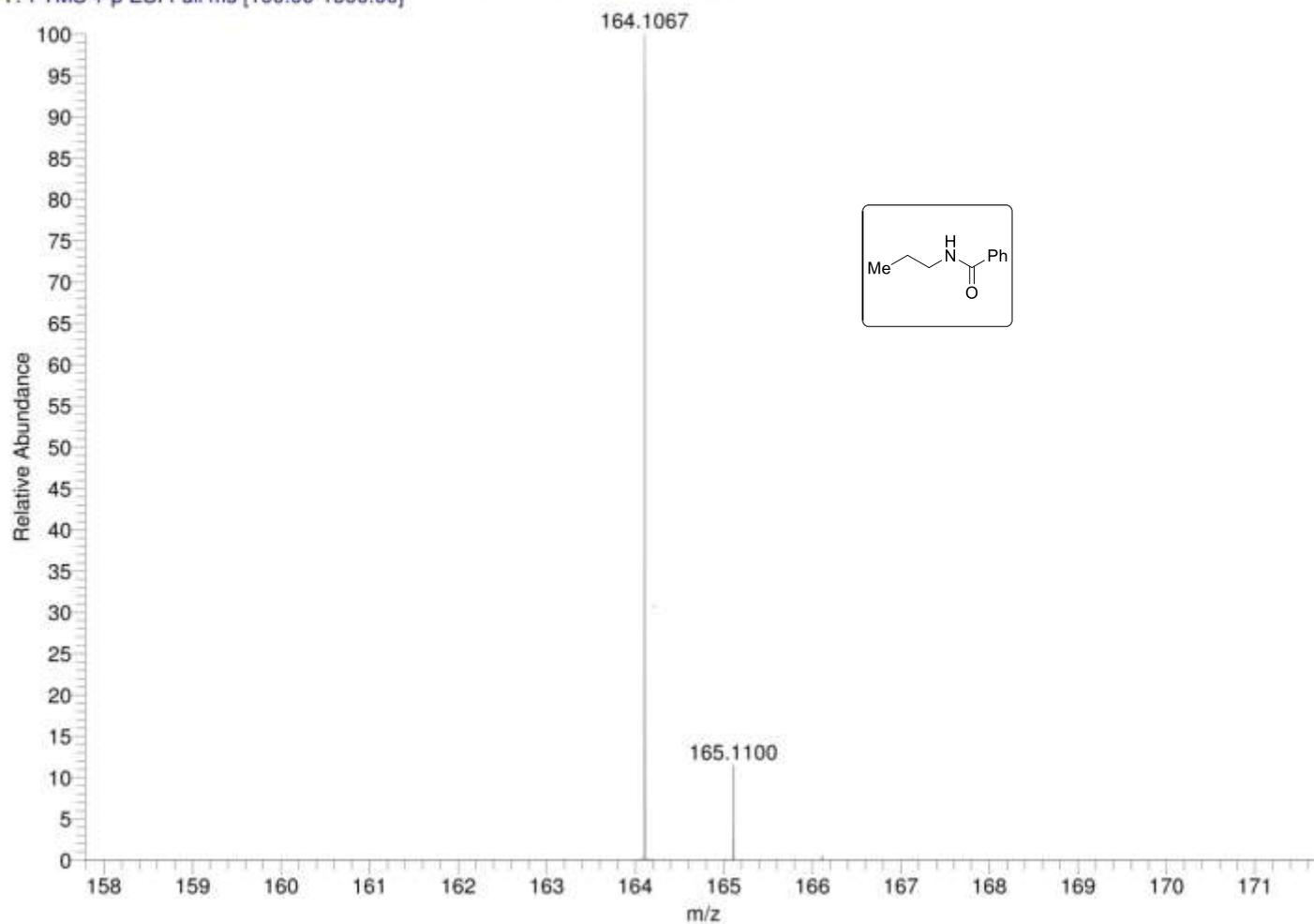


Figure S-165. <sup>13</sup>C-NMR spectrum of *N*-isopropylbenzamide (71a).

HRMS19I23DEC42 #17-32 RT: 0.13-0.24 AV: 16 SB: 8 0.02-0.08 NL: 2.03E7  
T: FTMS + p ESI Full ms [100.00-1500.00]



**Figure S-166.** HRMS spectrum of *N*-isopropylbenzamide (**71a**).

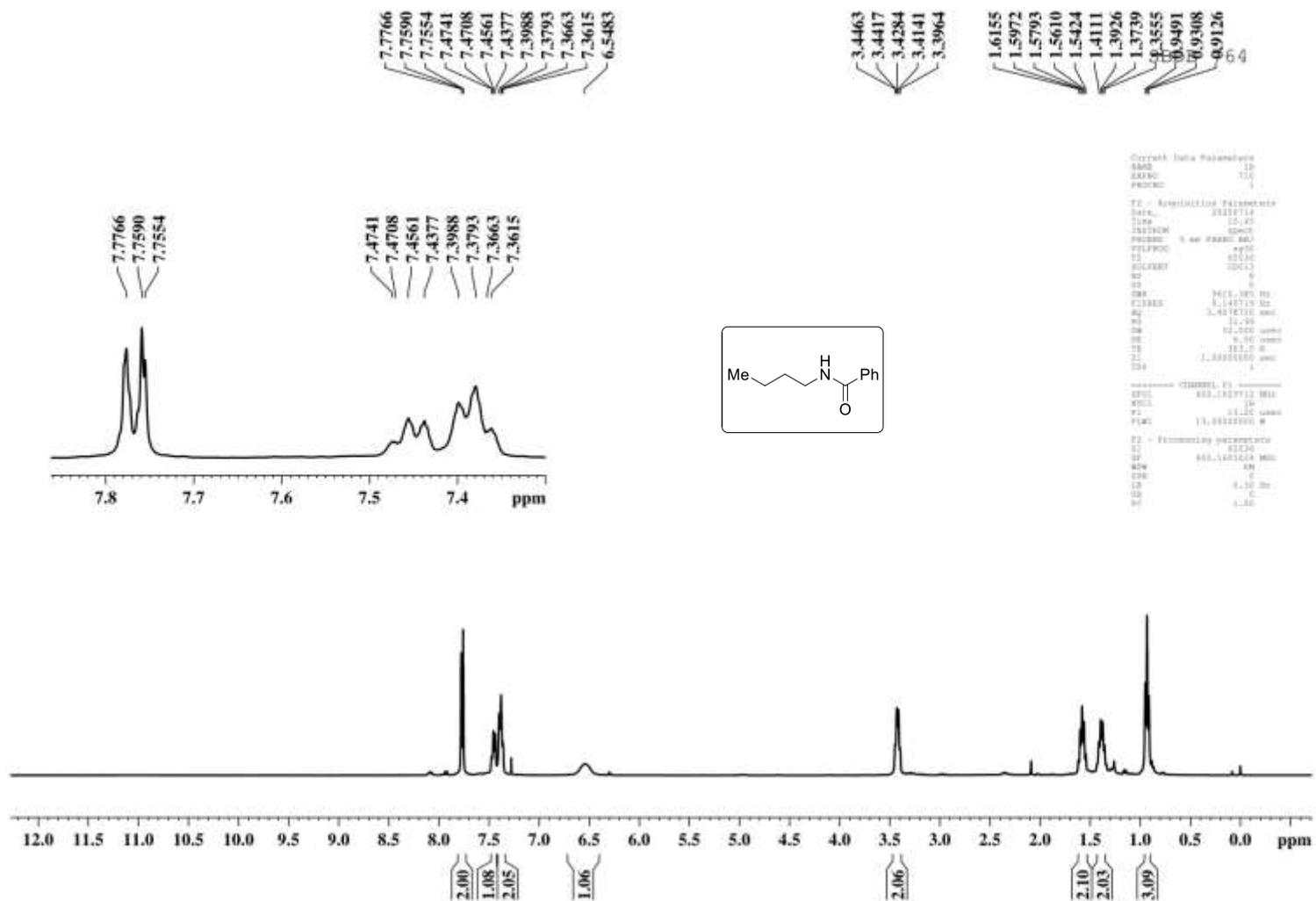
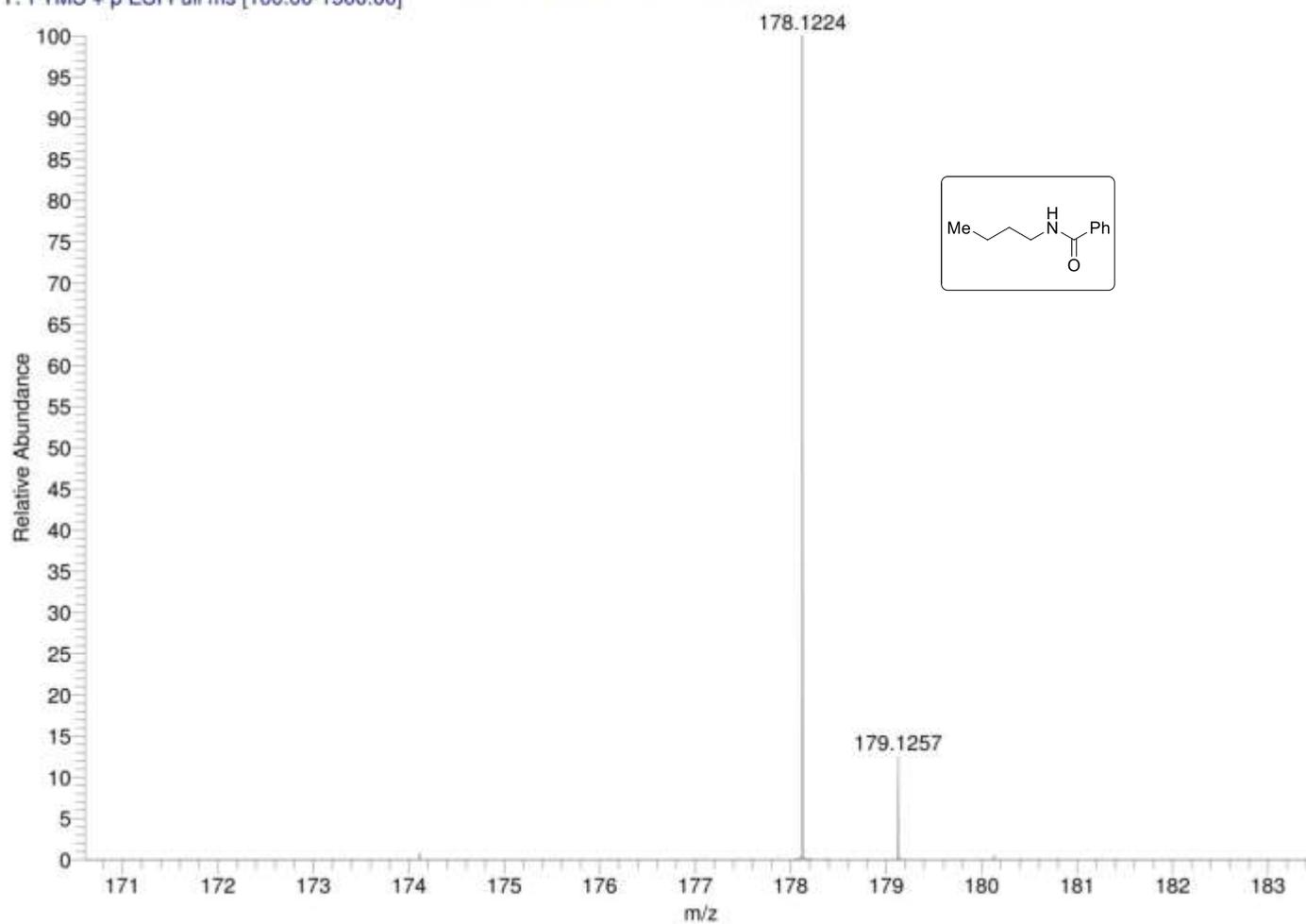


Figure S-167. <sup>1</sup>H-NMR spectrum of *N*-butylbenzamide (7ma).

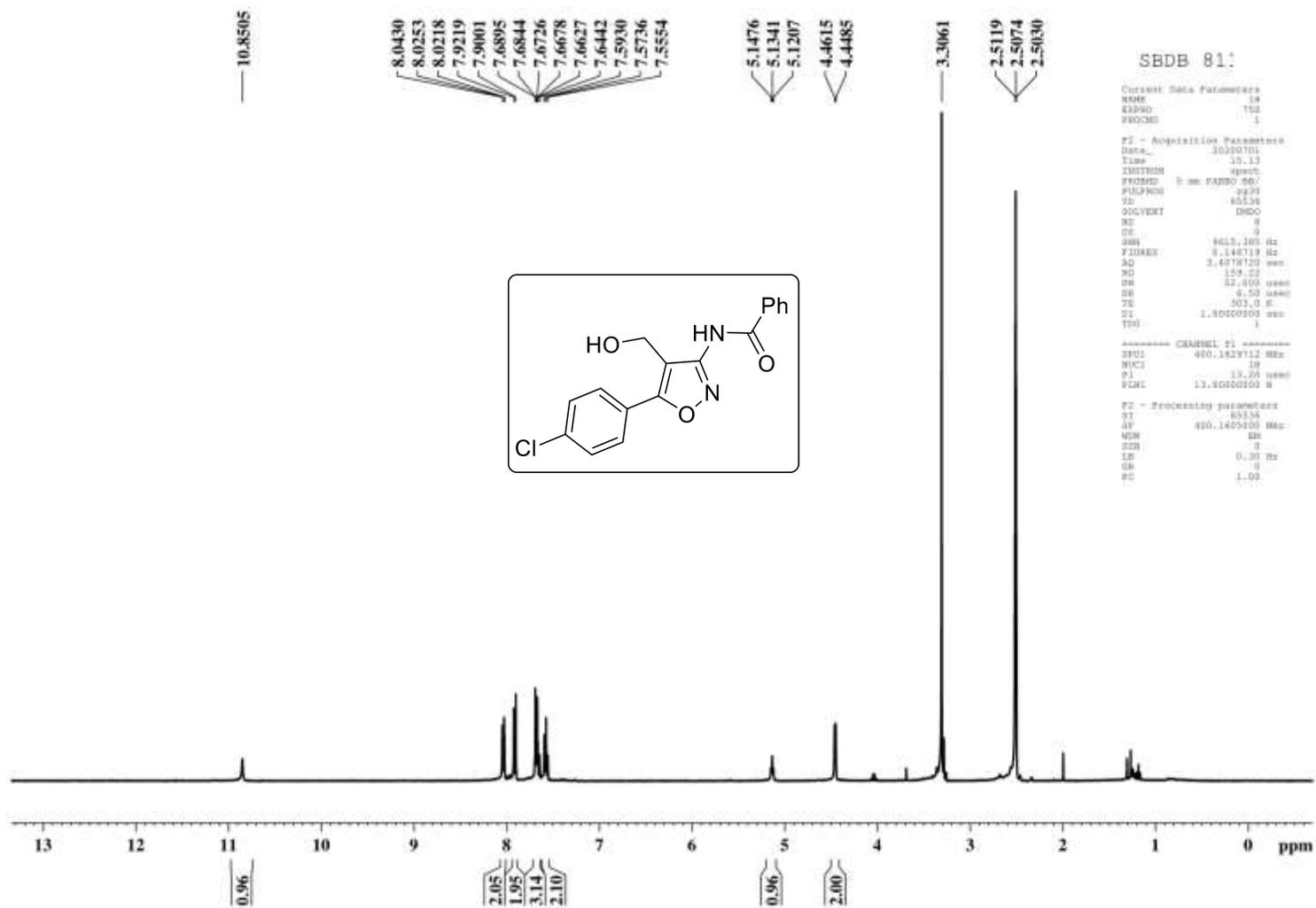


HRMS19119DEC22 #18-33 RT: 0.13-0.24 AV: 16 SB: 8 0.02-0.08 NL: 5.89E7

T: FTMS + p ESI Full ms [100.00-1500.00]



**Figure S-169.** HRMS spectrum of *N*-butylbenzamide (**7ma**).



**Figure S-170.**  $^1\text{H-NMR}$  spectrum of *N*-(5-(4-chlorophenyl)-4-(hydroxymethyl)isoxazol-3-yl)benzamide (**9**).

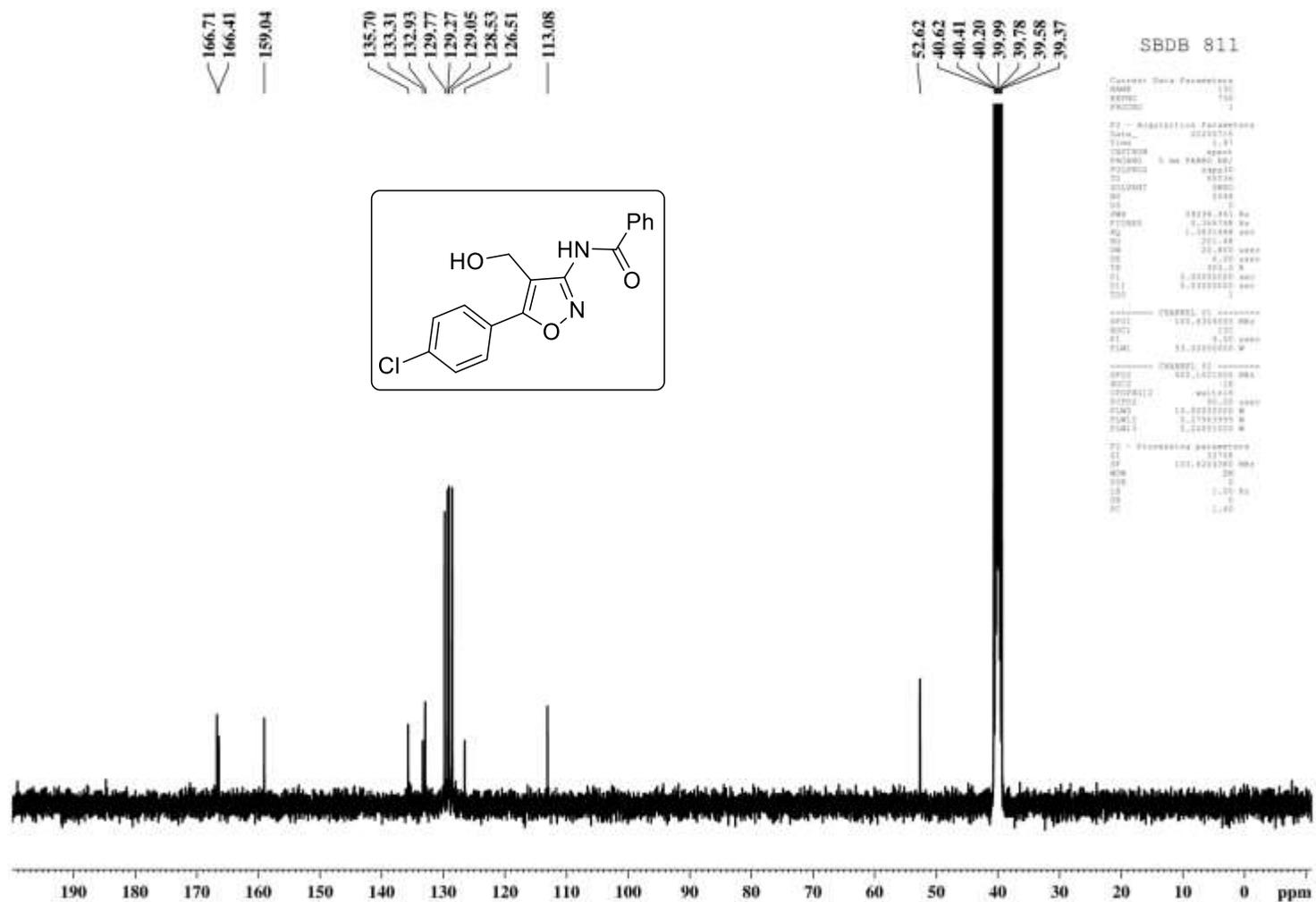
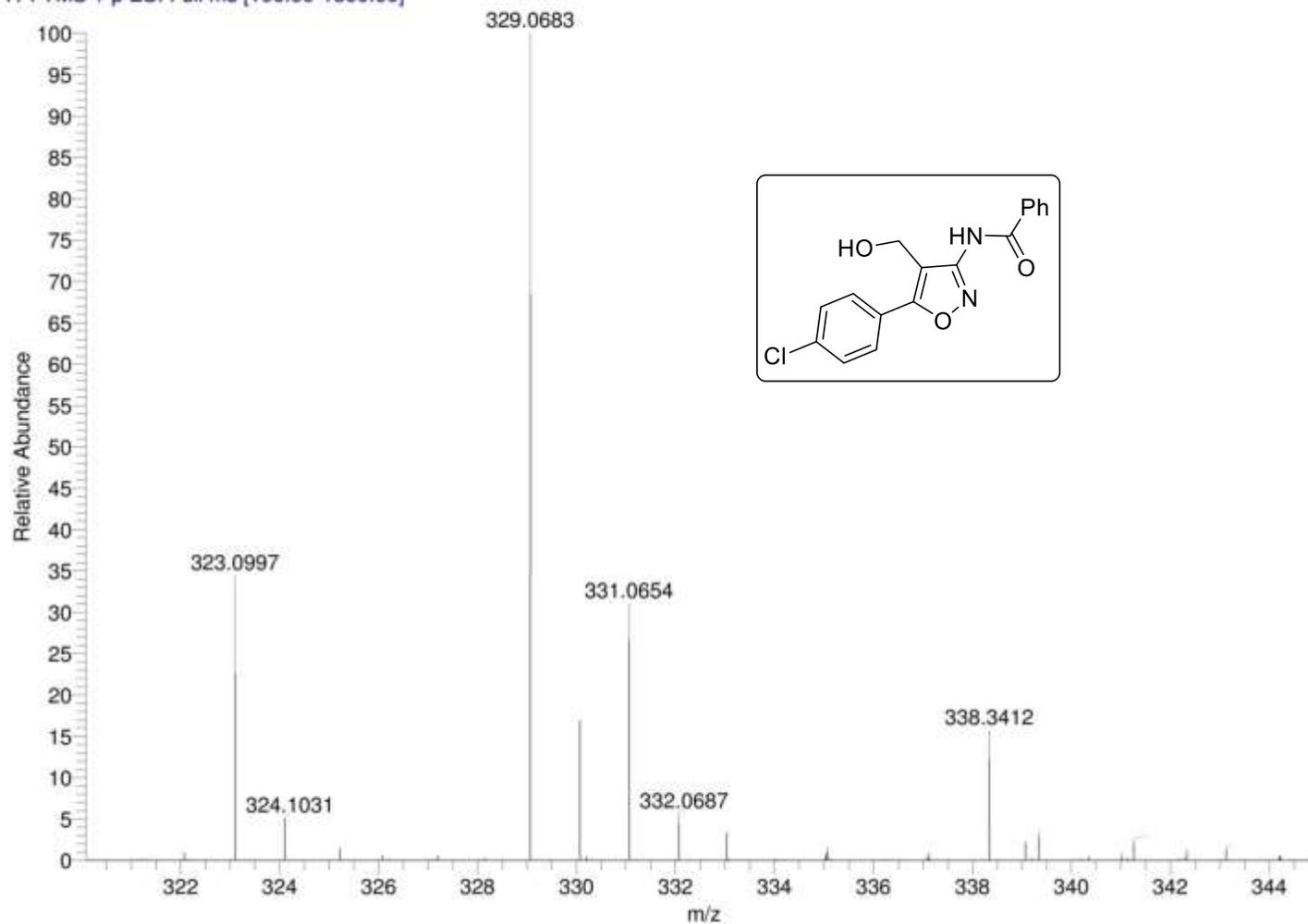


Figure S-171.  $^{13}\text{C}$ -NMR spectrum of *N*-(5-(4-chlorophenyl)-4-(hydroxymethyl)isoxazol-3-yl)benzamide (9).

HRMS20106MAR19 #27-37 RT: 0.20-0.28 AV: 11 SB: 7 0.02-0.07 NL: 1.21E5

T: FTMS + p ESI Full ms [100.00-1500.00]

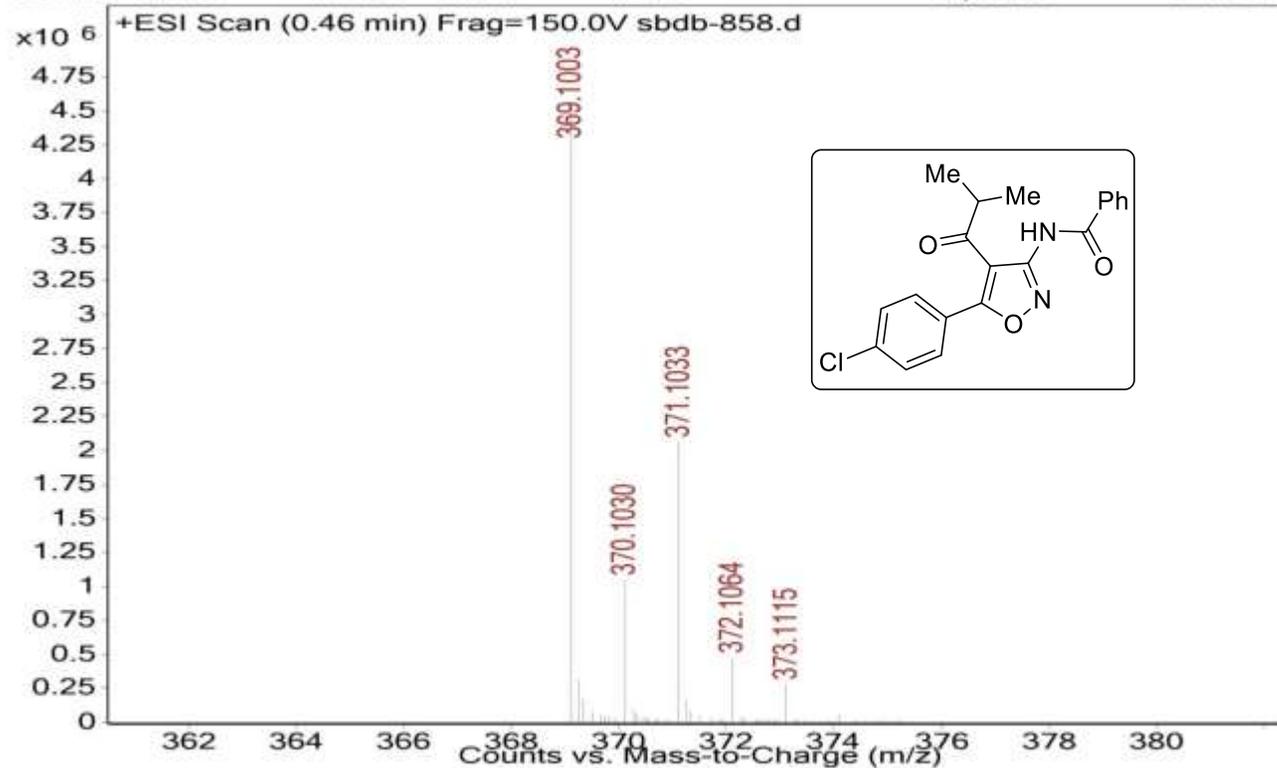


**Figure S-172.** HRMS spectrum of *N*-(5-(4-chlorophenyl)-4-(hydroxymethyl)isoxazol-3-yl)benzamide (9).





Sample Name	HRMS20107AUG22	Position	Vial 22	Instrument Name	Instrument 1	User Name	
Inj Vol	3	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	sbdb-858.d	ACQ Method	ISOCRATIC.m	Comment		Acquired Time	8/7/2020 1:42:06 PM



**Figure S-175.** HRMS spectrum of *N*-(5-(4-chlorophenyl)-4-isobutyrylisoxazol-3-yl)benzamide (**10a**).

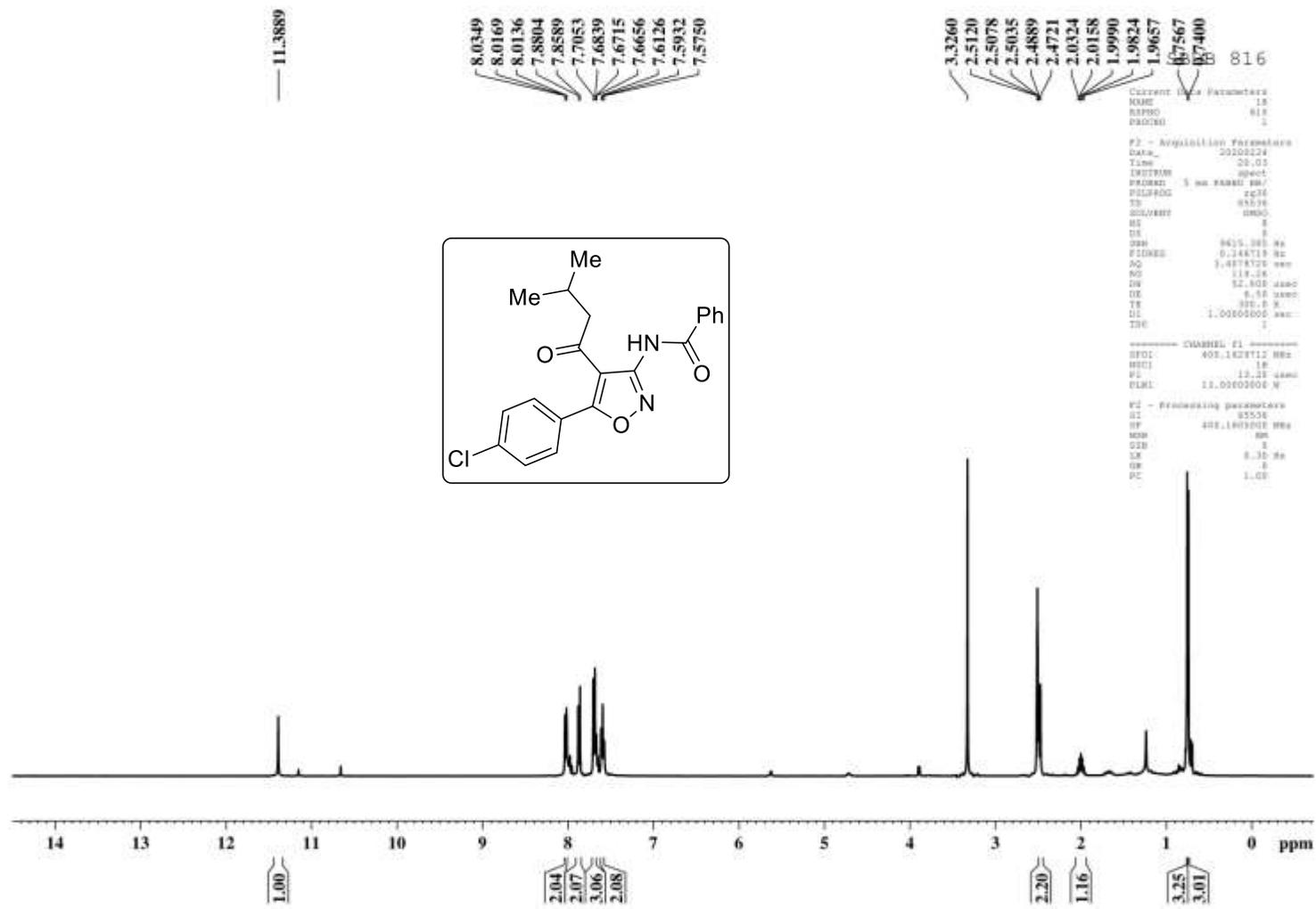


Figure S-176. <sup>1</sup>H-NMR spectrum of *N*-(5-(4-chlorophenyl)-4-(3-methylbutanoyl)isoxazol-3-yl)benzamide (10b).



### SAIF [HRMS Report]

Data File:	HRMS20I20MAR16	Original Data Path:	D:\INTERNALS\2020\Mar2020
Sample ID:	SBDB-816	Sample Name:	
Acquisition Date:	03/20/20 12:53:08 PM	Run Time(min):	0.00
Vial:	CStk1-01:16	Injection Volume(μl):	1.00

HRMS20I20MAR16 #15-28 RT: 0.11-0.21 AV: 14 SB: 1 0.01 NL: 1.52E6  
T: FTMS + p ESI Full ms [100.00-750.00]

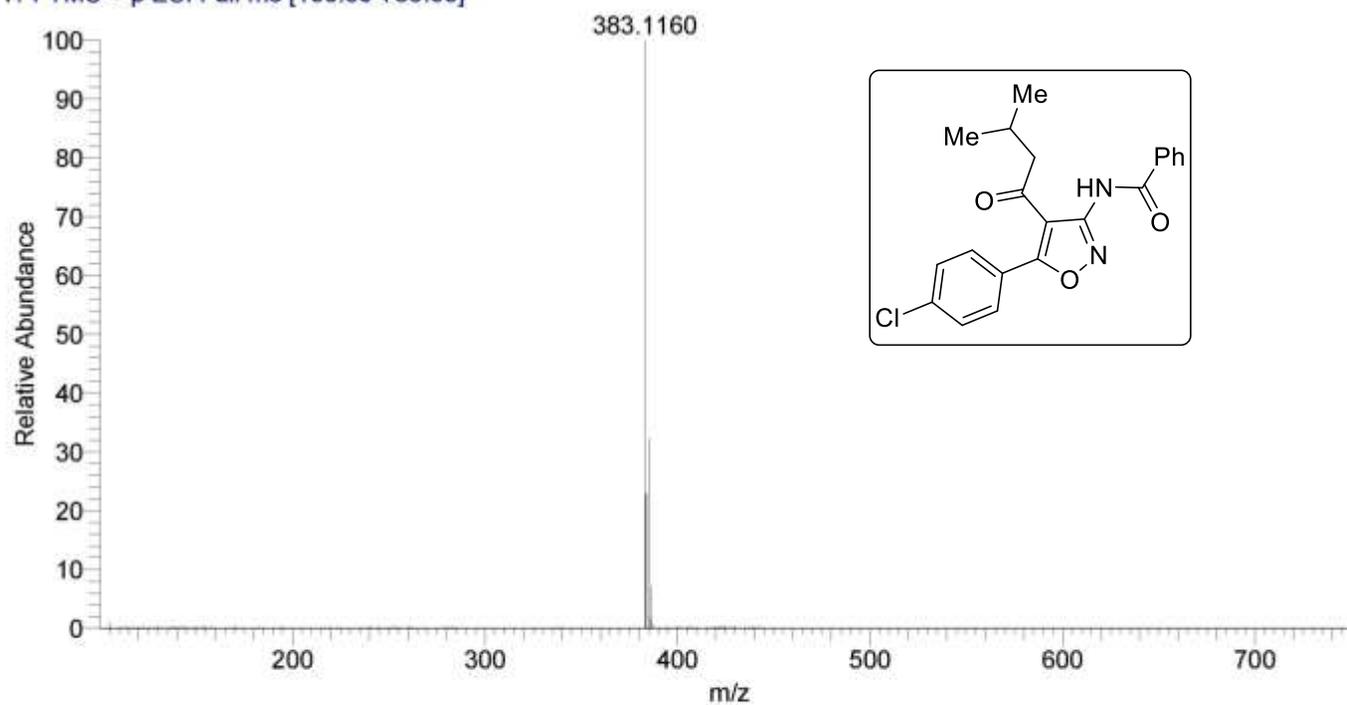
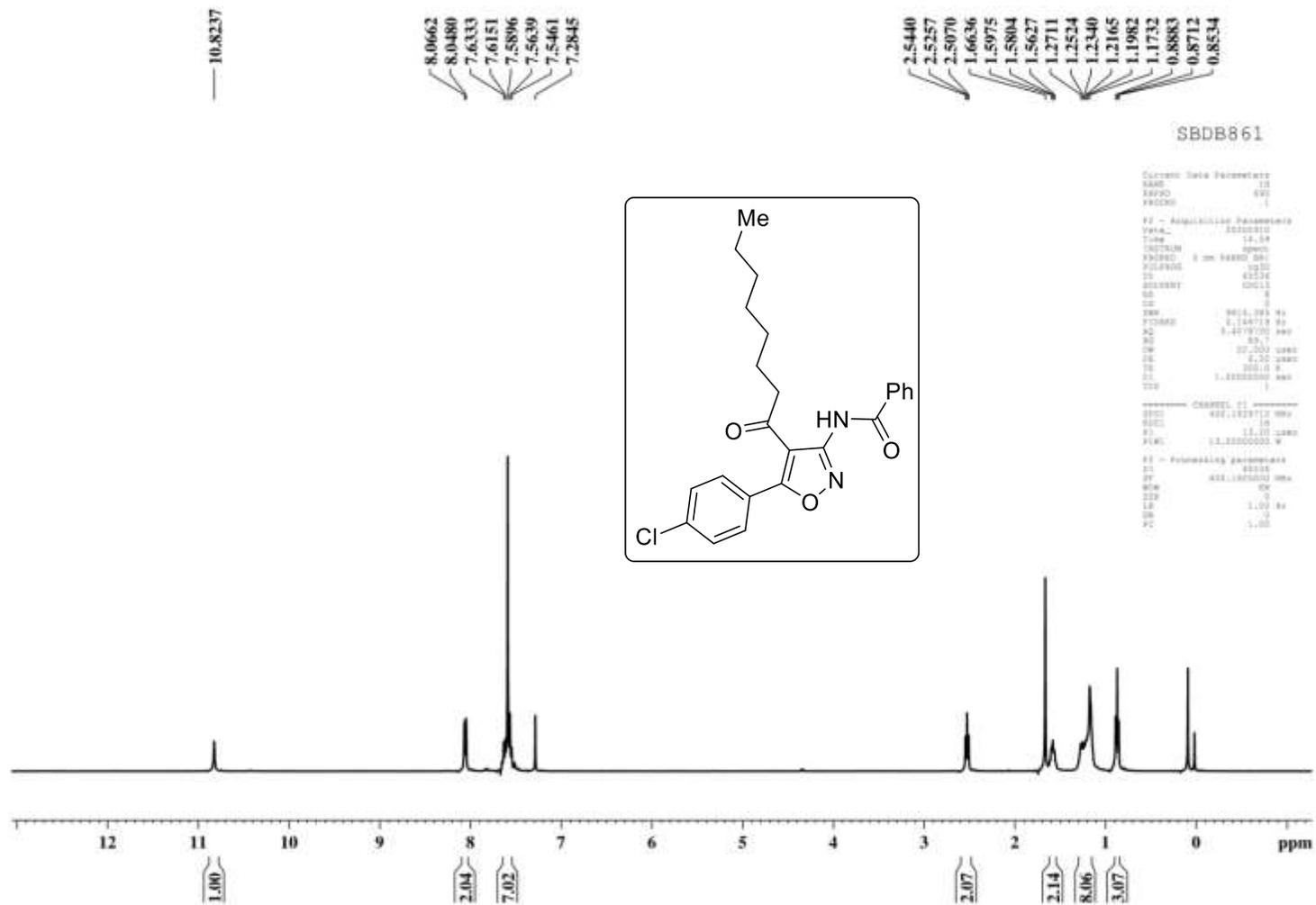


Figure S-178. HRMS spectrum of *N*-(5-(4-chlorophenyl)-4-(3-methylbutanoyl)isoxazol-3-yl)benzamide (**10b**).



**Figure S-179.** <sup>1</sup>H-NMR spectrum of *N*-(5-(4-chlorophenyl)-4-octanoylisoxazol-3-yl)benzamide (**10c**).

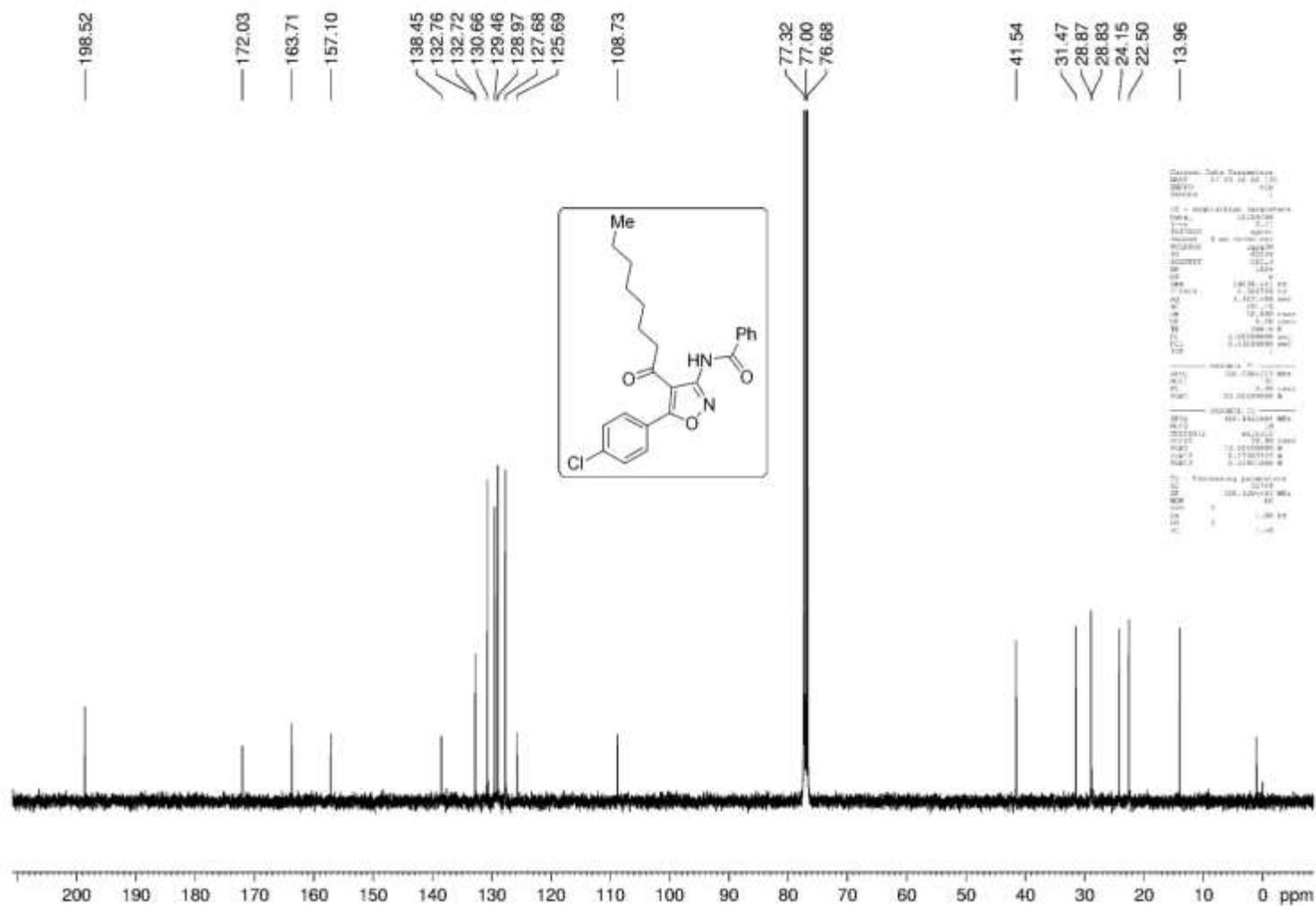


Figure S-180.  $^{13}\text{C}$ -NMR spectrum of *N*-(5-(4-chlorophenyl)-4-octanoylisoxazol-3-yl)benzamide (**10c**).

Sample Name	HRMS20107AUG23	Position	Vial 23	Instrument Name	Instrument 1	User Name	
Inj Vol	3	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SBDB-861.d	ACQ Method	ISOCRATIC.m	Comment		Acquired Time	8/7/2020 1:45:44 PM

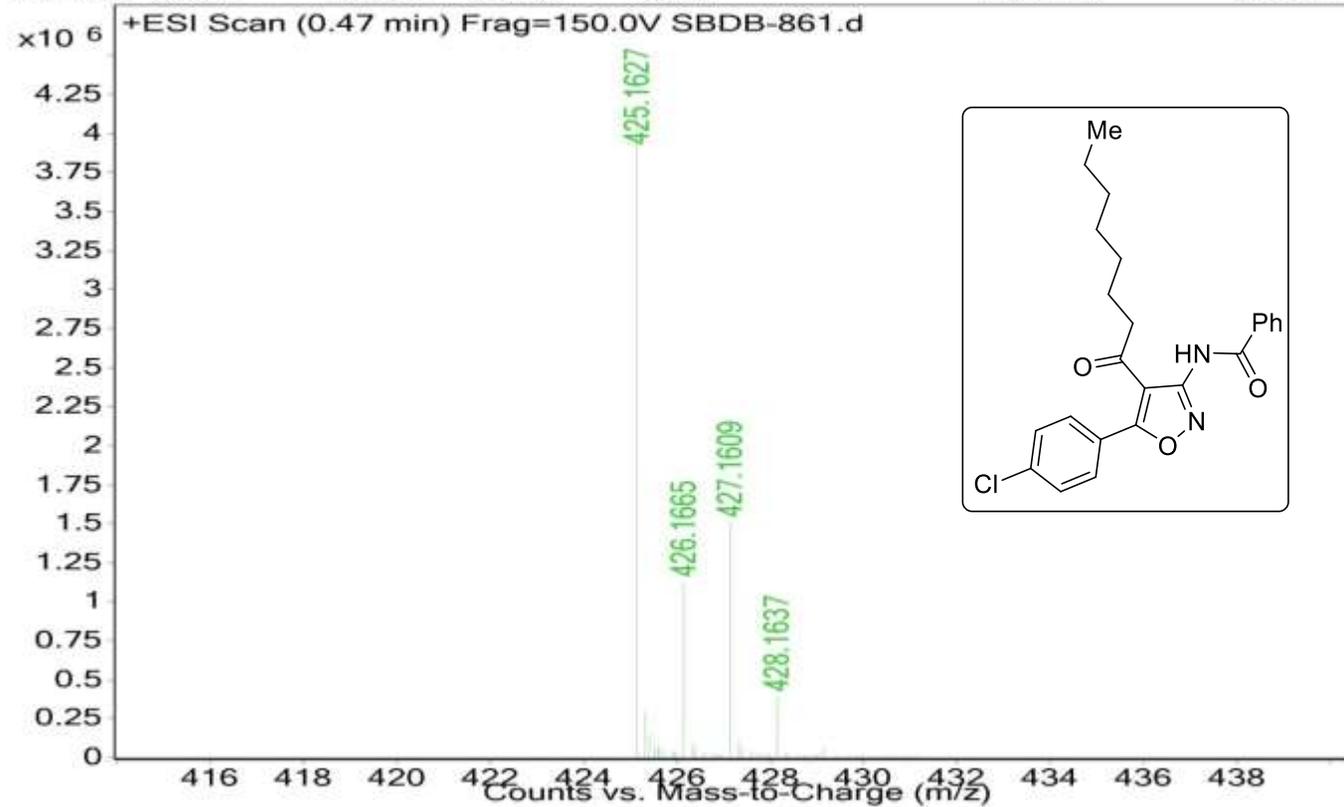


Figure S-181. HRMS spectrum of *N*-(5-(4-chlorophenyl)-4-octanoylisoxazol-3-yl)benzamide (**10c**).





### SAIF [HRMS Report]

Data File:	HRMS20I22OCT01	Original Data Path:	D:\INTERNAL NEW\2020\OCT 2020
Sample ID:	SBDB-882	Sample Name:	
Acquisition Date:	10/22/20 10:54:15 AM	Run Time(min):	0.00
Vial:	CSik1-01:01	Injection Volume(μl):	1.00

HRMS20I22OCT01 #12-23 RT: 0.11-0.21 AV: 12 SB: 1 0.01 NL: 2.21E6  
T: FTMS + c ESI Full ms [100.00-750.00]

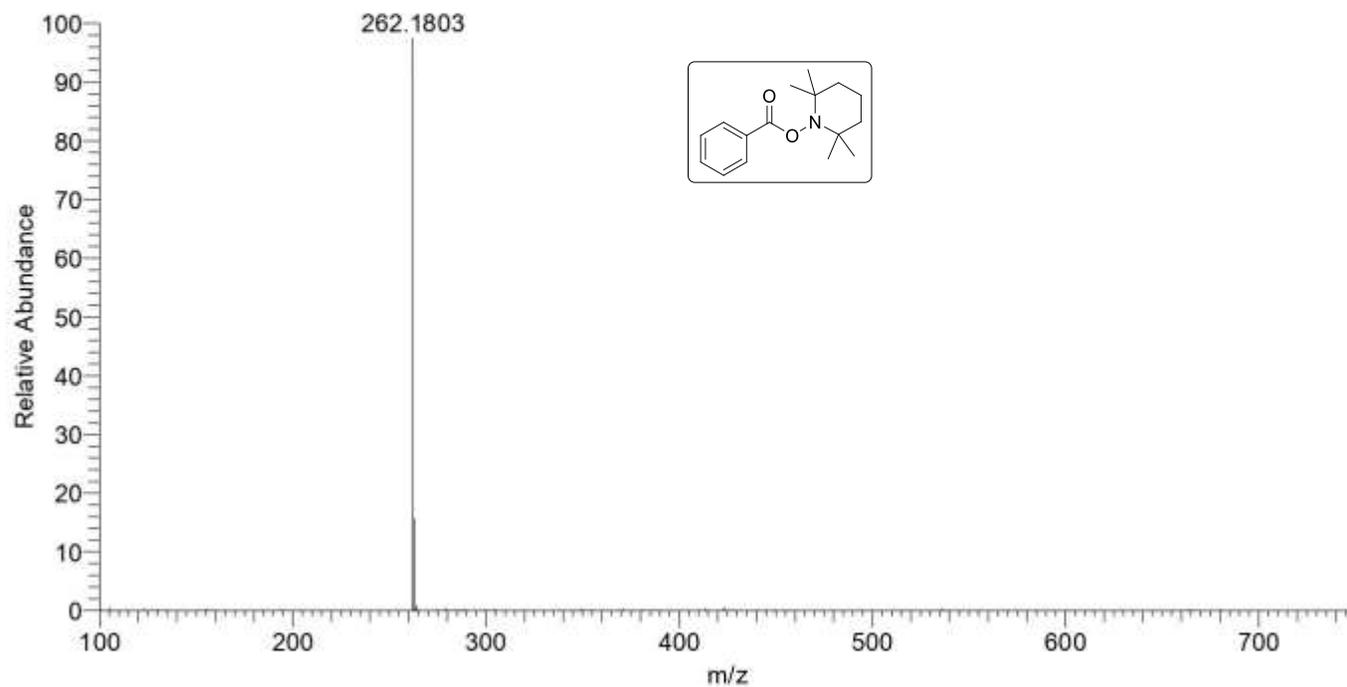


Figure S-184. HRMS spectrum of 2,2,6,6-tetramethylpiperidin-1-yl benzoate (**11**).