

## Supporting Information

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### Instrumentation and Chemicals

All the reagents were commercial grade and purified according to the established procedures. Organic extracts were dried over anhydrous sodium sulfate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60-120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F<sub>254</sub> (0.25mm). Melting points were recorded on melting point apparatus and are uncorrected. IR spectra were recorded on IR spectrophotometer. NMR spectra were recorded in CDCl<sub>3</sub> with tetramethylsilane as the internal standard for <sup>1</sup>H NMR (400 MHz) CDCl<sub>3</sub> solvent as the internal standard for <sup>13</sup>C NMR (100 MHz.) MS spectra were recorded using ESI mode. IR spectra were recorded in KBr or neat. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded on Varian 400 and Bruker 600 spectrometer by using TMS as internal reference; chemical shifts (δ scale) are reported in parts per million (ppm). Elemental analyses were carried out using analyzer. Column chromatographic separations were performed using Merck silica gel (60-120 mesh).

### Experimental procedure:

**General procedure for the preparation of symmetric anthranilate esters from alcohols 4a-u:** In a dried 25 mL round-bottomed flask a mixture of 2-nitrobenzaldehyde (1.0 mmol) and malononitrile (1.5 mmol) was taken in 3 mL of desired alcohol (**3a-d, f-g & q-u**) as reactant-cum-solvent. In rest of the cases required alcohol was used as reactant (2.0 mmol) with

acetonitrile as solvent. Then, 4-dimethylaminopyridine (DMAP) (1 equiv.) was added into it and the reaction mixture was kept for stirring at room temperature. The progress of the reaction was supervised through TLC time to time. After the reaction was complete, the solvent was removed in rotary evaporator. It was extracted with dichloromethane (2 x 10 mL), washed with water and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. It was concentrated *in vacuo*. The desired products **4** were obtained in 56-72 % yield after purification through column chromatography using ethylacetate/hexane (5:95) eluent.

**General procedure for the preparation of unsymmetrical anthranilate esters from amine & alcohols 6a-k:** In a dried 25 mL round-bottomed flask a mixture of 2-nitrobenzaldehyde (1.0 mmol), malononitrile (1.5 mmol) and requisite amine (1.0 mmol) was taken in 3 mL of desired alcohol as solvent. Then, 4-dimethylaminopyridine (DMAP) (20 mol%) was added into it and the reaction mixture was kept for stirring at room temperature. The progress of the reaction was monitored time to time through TLC. After completion of the reaction, the solvent was removed in rotary evaporator. It was then extracted with dichloromethane (2 x 10 mL), washed with water and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. It was concentrated *in vacuo*, purified through column chromatography with ethylacetate/hexane (15:85) and the desired product **6** were obtained in 64-74 % yields.

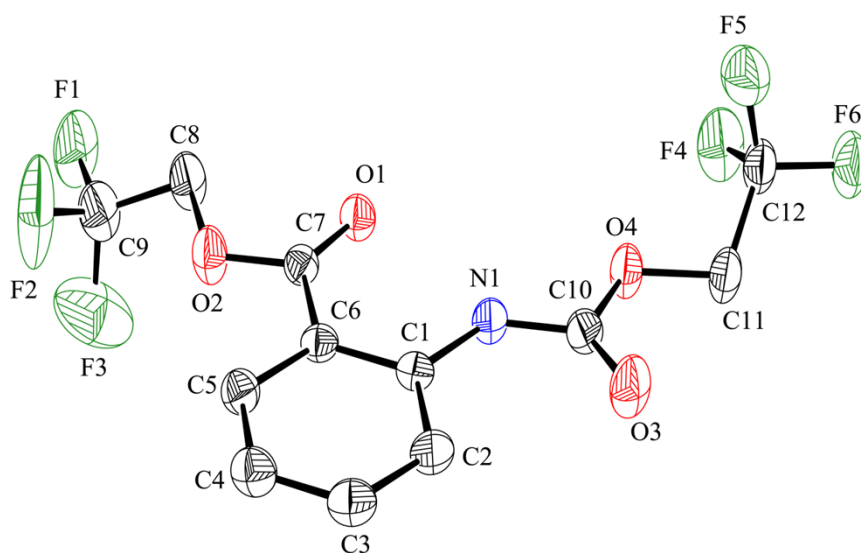
**General procedure for the preparation of *o*-amino benzoates 7a-c:** In a 25 mL round-bottomed flask a mixture of 2-nitrobenzaldehyde (1.0 mmol) and ethylcyanoacetate (1.5 mmol) was taken in 3 mL of desired alcohol as solvent. Then, 4-dimethylaminopyridine (DMAP) (1 equiv) was added into it and the reaction mixture was kept for stirring at room temperature. The progress of the reaction was monitored time to time through TLC. After completion of the reaction, the solvent was removed in rotary evaporator. It was then extracted with dichloromethane (2 x 10 mL), washed with water and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. It was concentrated *in vacuo*, purified through column chromatography with ethylacetate/hexane (15:85) and the desired products **7a-c** were obtained in 65-70 % yields.

**Procedure for the preparation of cross-coupling products 8a-b:** This reaction was conducted maintaining the procedure mentioned in the following paper, C. J. Taylor, M. Motevalli, and C. J. Richards, *Organometallics* 2006, **25**, 2899.

**Procedure for the O18 labelling reaction with H<sub>2</sub>O<sup>18</sup>:** In an oven dried 25 mL double necked round-bottomed flask a mixture of 2-nitrobenzaldehyde (1.0 mmol) and 4-dimethylaminopyridine (DMAP) (1 equiv.) was taken under argon atmosphere. 20 equiv of H<sub>2</sub>O<sup>18</sup> was added into in with 3 mL of anhydrous MeOH **3a**. At last 1.5 equiv of malononitrile was added and the reaction mixture was let to sitrr at room temperature for 2h. After the reaction was complete, the solvent was removed in rotary evaporator. It was extracted with dichloromethane (2 x 10 mL), washed with water and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. It was concentrated *in vacuo*. The desired product **4a** was obtained after purification through column chromatography using ethylacetate/hexane (5:95) eluent.

### Crystallographic Description:

Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite monochromated MoK $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) at 298 K. Cell parameters were retrieved using SMART<sup>[a]</sup> software and refined with SAINT<sup>[a]</sup> on all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS<sup>[b]</sup>. The structure was solved by direct methods implemented in SHELX-97<sup>[c]</sup> program and refined by full-matrix least-squares methods on F2. All non-hydrogen atomic positions were located in difference Fourier maps and refined anisotropically.



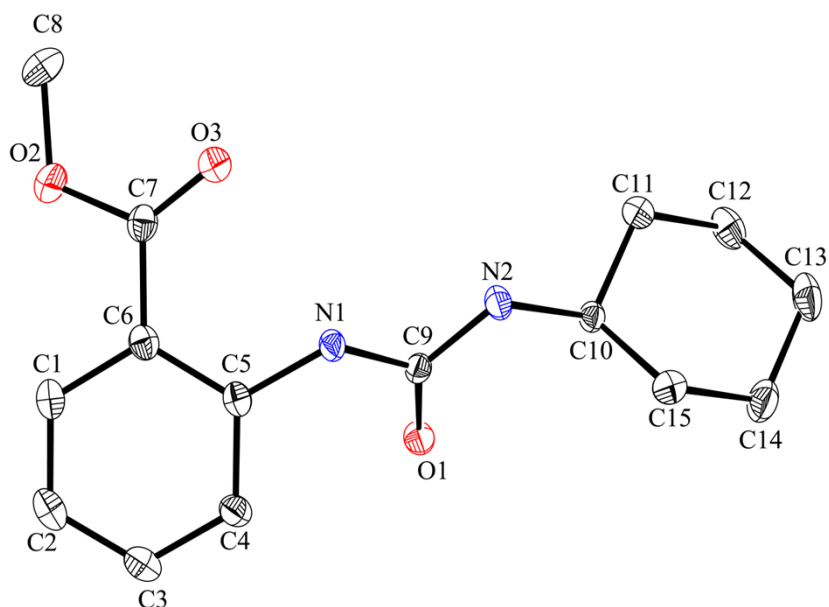
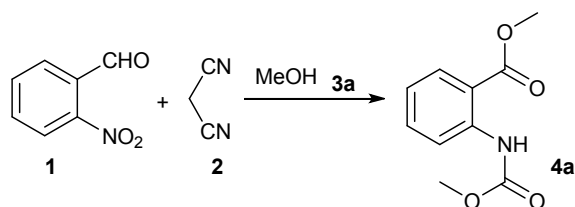


Fig. S1 X-ray crystal structure of **4n** (CCDC 1054296) and **6a** (CCDC 1060211)

	Compound <b>4n</b>	Compound <b>6a</b>
Formula	C <sub>12</sub> H <sub>9</sub> F <sub>6</sub> NO <sub>4</sub>	C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Mol. wt.	345.20	276.33
Crystal system	Monoclinic	Monoclinic
Space group	P1 21/c 1	P 21/c
Temperature /K	293 (2)	296
Wavelength /Å	0.71073	0.71073
<i>a</i> /Å	13.0242 (6)	4.8164 (4)
<i>b</i> /Å	13.3563 (6)	12.3382 (7)
<i>c</i> /Å	8.2205 (3)	24.06776(19)
<i>α</i> /°	90.00	90.00
<i>β</i> /°	100.660 (4)	94.39(7)
<i>γ</i> /°	90.00	90.00
<i>V</i> / Å <sup>3</sup>	1405.31 (10)	1426.02(17)
<i>Z</i>	4	4
Density/Mgm <sup>-3</sup>	1.632	1.287
Abs. co-eff. /mm <sup>-1</sup>	0.171	0.090
Abs. correction	multi-scan	multi-scan
F(000)	696	592
Total no. of reflections	2472	2652
Reflections, <i>I</i> > 2σ( <i>I</i> )	1634	1434
Max. 2θ/°	25.00	25.25
Ranges (h, k, l)	-15 ≤ h ≤ 15	-5 ≤ h ≤ 5

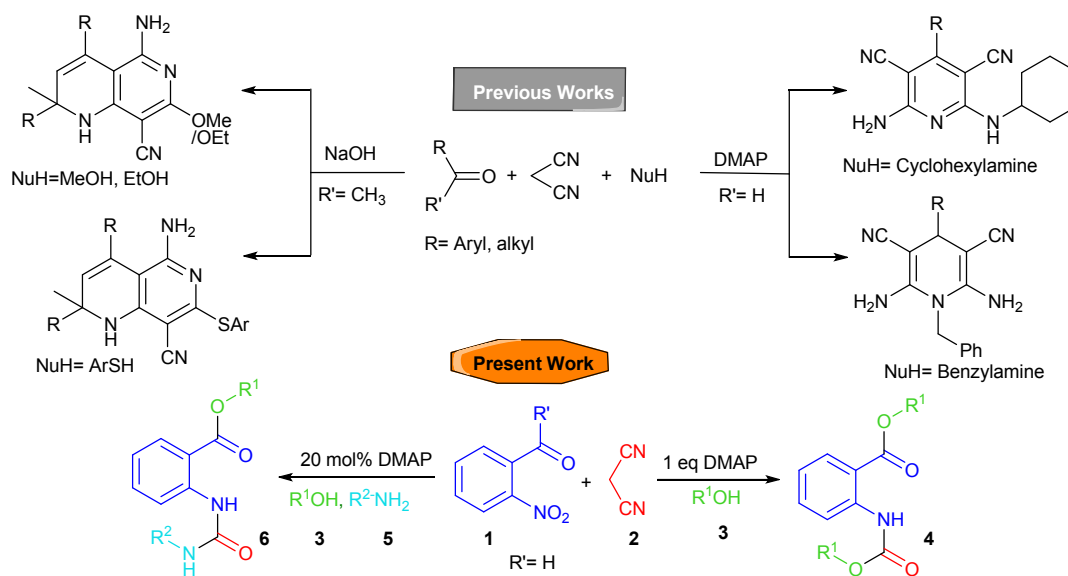
	-15 ≤ k ≤ 15 -9 ≤ l ≤ 6	-14 ≤ k ≤ 14 -29 ≤ l ≤ 29
Complete to 2θ (%)	99.9	99.9
Refinement method	Full-matrix least-squares on $F^2$	Full-matrix least-squares on $F^2$
Goof ( $F^2$ )	1.078	1.016
R <sub>1</sub> all	0.0986	0.1241
R <sub>1</sub> ( $\sigma > 2I$ )	0.0725	0.0669
wR <sub>2</sub> all	0.2215	0.1366
wR <sub>2</sub> ( $\sigma > 2I$ )	0.1985	0.1125

**Table S1:** Optimization of reaction conditions for the synthesis of anthranilate esters **4a**<sup>a</sup>.

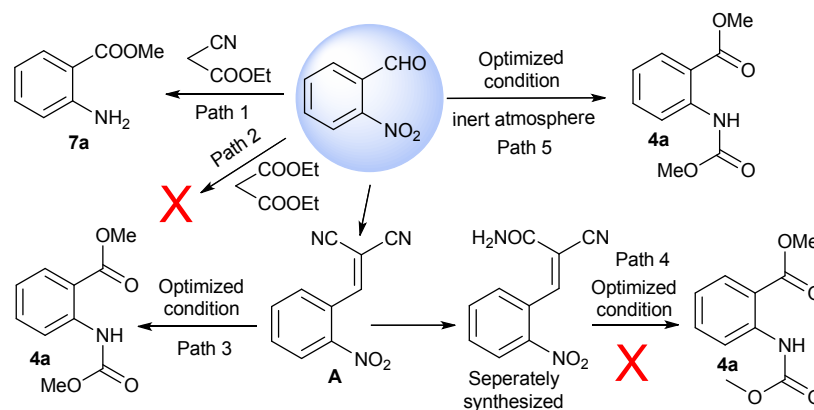


Sl.	Catalyst	Amount of catalyst	Solvent	Time (h)	Yield
1	DMAP	0.5	MeOH	3	54
2	<b>DMAP</b>	<b>1</b>	<b>MeOH</b>	<b>2</b>	<b>72</b>
3	DMAP	1.5	MeOH	2	73
4	DBU	1.5	MeOH	5	15
5	PPh <sub>3</sub>	1.5	MeOH	4	52
6	Et <sub>3</sub> N	1.5	MeOH	3	64
7	DMA	1.5	MeOH	12	---
8	NaOH	1.5	MeOH	3	61
9	DMAP	1.5	CH <sub>3</sub> CN <sup>c</sup>	2	71
10	DMAP	1.5	DMF <sup>c</sup>	10	7
11	DMAP	1.5	DCE <sup>c</sup>	5	17
12	DMAP	1.5	H <sub>2</sub> O <sup>c</sup>	12	---
13	-	-	MeOH	12	-

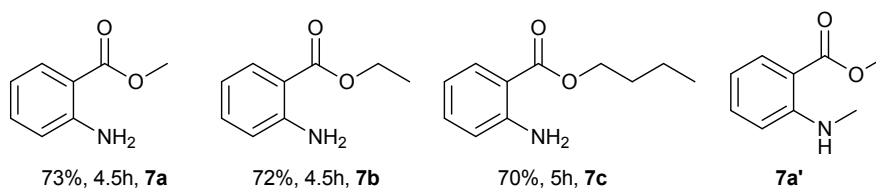
<sup>a</sup>Reaction conditions: 2-nitrobenzaldehyde and malononitrile taken in 1:1.5 ratio at rt. <sup>b</sup>Isolated yields. <sup>c</sup>MeOH (2 equiv) was used as reactant.



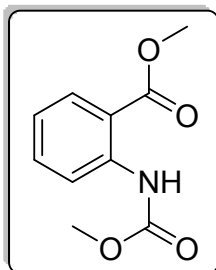
**Scheme S1.** Substrate Dependent Selectivity in Multicomponent Reaction



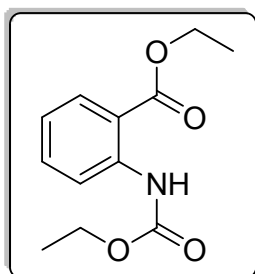
**Scheme S2.** Various control experiments during mechanistic study



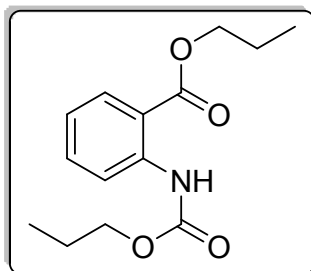
Structures of methyl anthranilate, ethyl anthranilate butyl anthranilate, n-methyl anthranilate (i.e 7a, 7b, 7c, 7a').

**Spectral Data:****Methyl 2-((methoxycarbonyl)amino)benzoate (4a):**

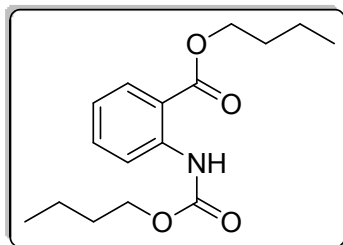
Gummy liquid;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  10.49 (s, 1H, NH), 8.42 (d,  $J=8.4$  Hz, 1H), 8.00 (d,  $J=7.8$  Hz, 1H), 7.52 (t,  $J=8.4$  Hz, 1H), 7.02 (t,  $J=7.8$  Hz, 1H), 3.91 (s, 3H, -OMe), 3.78 (s, 3H, -OMe);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.71, 154.31, 141.98, 134.79, 131.07, 121.75, 119.02, 114.78, 52.46; IR (KBr,  $\text{cm}^{-1}$ ): 3301, 2926, 1739, 1692, 1529, 1213, 1145; HRMS (ESI) calcd for  $\text{C}_{10}\text{H}_{11}\text{NO}_4$  ( $\text{M} + \text{H}^+$ ) 210.0766, found 210.0763.

**Ethyl 2-((ethoxycarbonyl)amino)benzoate (4b):**

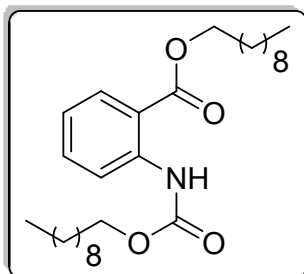
Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  10.49 (s, 1H, NH), 8.41 (d,  $J=8.8$  Hz, 1H), 7.99 (d,  $J=8.0$  Hz, 1H), 7.49 (t,  $J=8.0$  Hz, 1H), 6.99 (t,  $J=8.0$  Hz, 1H), 4.35 (q,  $J=7.6$  Hz, 2H), 4.20 (q,  $J=7.2$  Hz, 2H), 1.38 (t,  $J=7.2$  Hz, 3H), 1.29 (t,  $J=7.2$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.30, 153.92, 142.13, 134.65, 131.04, 121.56, 118.97, 114.95, 61.47, 61.33, 14.70, 14.39; IR (KBr,  $\text{cm}^{-1}$ ): 3300, 2982, 1737, 1690, 1591, 1529, 1242; HRMS (ESI) calcd for  $\text{C}_{12}\text{H}_{15}\text{NO}_4$  ( $\text{M} + \text{H}^+$ ) 238.1079, found 238.1079.

**Propyl 2-((propoxycarbonyl)amino)benzoate (4c):**

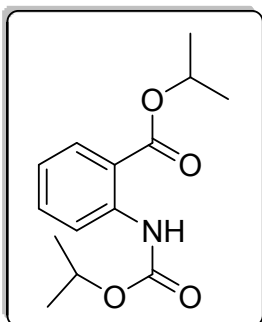
Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  10.51 (s, 1H, NH), 8.44 (d,  $J=8.0$  Hz, 1H), 8.02 (d,  $J=8.0$  Hz, 1H), 7.52 (t,  $J=7.2$  Hz, 1H), 7.02 (t,  $J=7.2$  Hz, 1H), 4.28 (t,  $J=6.4$  Hz, 2H), 4.13 (t,  $J=6.8$  Hz, 2H), 1.86-1.65 (m, 4H), 1.04 (t,  $J=7.6$  Hz, 3H), 0.98 (t,  $J=7.6$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.33, 154.04, 142.14, 134.64, 131.03, 121.56, 119.00, 115.00, 67.02, 66.99, 22.43, 22.18, 10.70, 10.55; IR (KBr,  $\text{cm}^{-1}$ ): 3300, 2969, 1738, 1690, 1591, 1528, 1240; HRMS (ESI) calcd for  $\text{C}_{14}\text{H}_{19}\text{NO}_4$  ( $\text{M} + \text{H}^+$ ) 266.1392, found 266.1394.

**Butyl 2-((butoxycarbonyl)amino)benzoate (4d):**

Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  10.50 (s, 1H, NH), 8.44 (d,  $J=8.0$  Hz, 1H), 8.01 (d,  $J=8.0$  Hz, 1H), 7.51 (t,  $J=7.2$  Hz, 1H), 7.01 (t,  $J=7.2$  Hz, 1H), 4.31 (t,  $J=6.8$  Hz, 2H), 4.16 (t,  $J=6.4$  Hz, 2H), 1.82-1.71 (m, 2H), 1.70-1.61 (m, 2H), 1.54-1.38 (m, 4H), 1.02-0.91 (m, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.33, 154.04, 142.13, 134.63, 131.03, 121.56, 118.99, 114.99, 65.32, 65.26, 31.14, 30.81, 19.47, 19.29, 13.92; IR (KBr,  $\text{cm}^{-1}$ ): 3299, 2960, 1737, 1690, 1561, 1528, 1242; HRMS (ESI) calcd for  $\text{C}_{16}\text{H}_{23}\text{NO}_4$  ( $\text{M} + \text{H}^+$ ) 294.1705, found 294.1707.

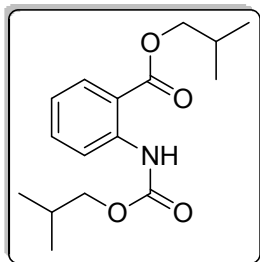
**Decyl 2-(((decyloxy)carbonyl)amino)benzoate (4e):**

Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  10.49 (s, 1H, NH), 8.44 (d,  $J=8.4$  Hz, 1H), 8.01 (d,  $J=7.8$  Hz, 1H), 7.51 (t,  $J=7.8$  Hz, 1H), 7.01 (t,  $J=7.8$  Hz, 1H), 4.30 (t,  $J=6.6$  Hz, 2H), 4.15 (t,  $J=6.6$  Hz, 2H), 1.72-1.63 (m, 2H), 1.62-1.52 (m, 2H), 1.49-1.20 (m, 28H), 0.93-0.81 (m, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.37, 154.08, 142.16, 134.66, 131.05, 121.58, 119.04, 115.05, 65.66, 65.62, 32.11, 29.74, 29.52, 29.47, 29.13, 28.80, 26.25, 26.10, 22.89, 14.31; IR (KBr,  $\text{cm}^{-1}$ ): 3310, 2925, 1739, 1691, 1591, 1528, 1241; HRMS (ESI) calcd for  $\text{C}_{28}\text{H}_{47}\text{NO}_4$  ( $\text{M} + \text{H}^+$ ) 462.3583, found 462.3573.

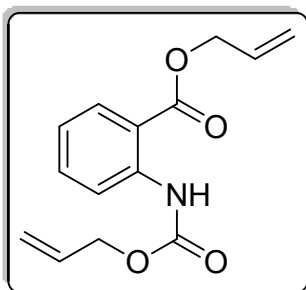
**Isopropyl 2-((isopropoxycarbonyl)amino)benzoate (4f):**

Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz): 10.49 (s, 1H, NH), 8.44 (d,  $J=8.4$  Hz, 1H), 8.00 (d,  $J=8.0$  Hz, 1H), 7.50 (t,  $J=7.6$  Hz, 1H), 7.00 (t,  $J=7.2$  Hz, 1H), 5.31-5.28 (m, 1H), 5.07-4.94 (m, 1H), 1.38 (d,  $J=6.0$  Hz, 6H), 1.30 (d,  $J=6.0$  Hz, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  167.83, 153.57, 142.27, 134.53, 131.06, 121.40, 118.92, 115.26, 69.11, 68.80, 22.27, 22.08; IR (KBr,  $\text{cm}^{-1}$ ): 3443, 2926, 1726, 1682, 1596, 1384, 1259; HRMS (ESI) calcd for  $\text{C}_{14}\text{H}_{19}\text{NO}_4$  ( $\text{M} + \text{H}^+$ ) 266.1392, found 266.1401.

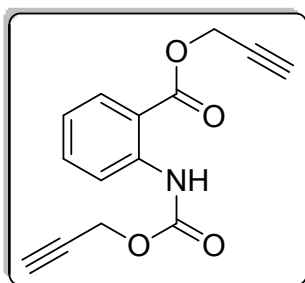


**Isobutyl 2-((isobutoxycarbonyl)amino)benzoate (4g):**

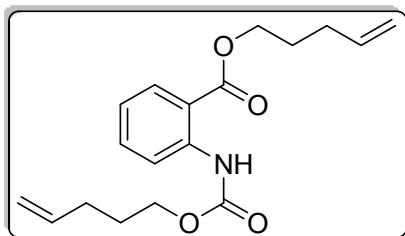
Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz): 10.49 (s, 1H, NH), 8.42 (d,  $J=8$  Hz, 1H), 8.0 (d,  $J=7.6$  Hz, 1H), 7.50 (t,  $J=7.6$  Hz, 1H), 7.00 (t,  $J=7.6$  Hz, 1H), 4.07 (d,  $J=6.0$  Hz, 2H), 3.93 (d,  $J=6.4$  Hz, 2H), 2.15-2.04 (m, 1H), 2.02-1.91 (m, 1H), 1.01 (d,  $J=6.8$  Hz, 6H), 0.95 (d,  $J=6.0$  Hz, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.27, 154.04, 142.14, 134.66, 130.99, 121.59, 119.03, 115.00, 71.51, 71.47, 28.12, 27.99, 19.37, 19.28; IR (KBr,  $\text{cm}^{-1}$ ): HRMS (ESI) calcd for  $\text{C}_{16}\text{H}_{23}\text{NO}_4$  ( $\text{M} + \text{H}^+$ ) 294.1705, found 294.1713.

**Allyl 2-(((allyloxy)carbonyl)amino)benzoate (4h):**

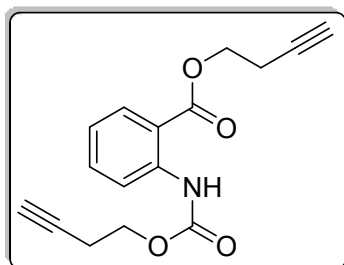
Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz): 10.51 (s, 1H, NH), 8.42 (d,  $J=8.8$  Hz, 1H), 8.03 (d,  $J=7.6$  Hz, 1H), 7.51 (t,  $J=7.2$  Hz, 1H), 7.01 (t,  $J=7.6$  Hz, 1H), 6.04-5.89 (m, 2H), 5.37 (t,  $J=17.2$  Hz, 2H), 5.29 (d,  $J=11.2$  Hz, 1H), 5.24 (d,  $J=10.8$  Hz, 1H), 4.80 (d,  $J=6.0$  Hz, 2H), 4.65 (d,  $J=6.0$  Hz, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  167.91, 153.55, 142.07, 134.88, 132.69, 131.98, 131.13, 121.81, 119.10, 118.94, 118.34, 114.81, 66.03, 65.99; IR (KBr,  $\text{cm}^{-1}$ ): 3406, 2931, 1739, 1692, 1591, 1529, 1239.

**Prop-2-yn-1-yl 2-(((prop-2-yn-1-yloxy)carbonyl)amino)benzoate (4i):**

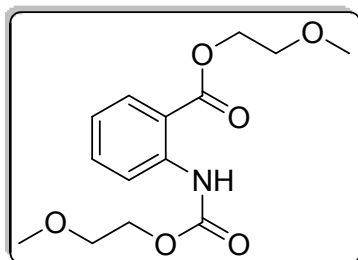
Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  10.50 (s, 1H, NH), 8.44 (d,  $J=8.4$  Hz, 1H), 8.07 (d,  $J=7.6$  Hz, 1H), 7.57 (t,  $J=8.0$  Hz, 1H), 7.07 (t,  $J=7.2$  Hz, 1H), 4.92 (s, 2H), 4.78 (s, 2H), 2.55 (s, 1H), 2.51 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  167.41, 152.77, 141.79, 135.31, 131.33, 122.22, 119.18, 114.28, 78.05, 75.64, 75.16, 52.92; IR (KBr,  $\text{cm}^{-1}$ ): 3283, 3245, 2951, 2128, 1721, 1689, 1596, 1384, 1256; HRMS (ESI) calcd for  $\text{C}_{14}\text{H}_{11}\text{NO}_4$  ( $\text{M} + \text{H}^+$ ) 258.0766, found 258.0758.

**Pent-4-en-1-yl 2-(((pent-4-en-1-yloxy)carbonyl)amino)benzoate (4j):**

Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz): 10.50 (s, 1H, NH), 8.44 (d,  $J=8.4$  Hz, 1H), 8.02 (d,  $J=7.8$  Hz, 1H), 7.52 (t,  $J=7.2$  Hz, 1H), 7.02 (t,  $J=7.2$  Hz, 1H), 5.89-5.12 (m, 2H), 5.12-4.98 (m, 4H), 4.33 (t,  $J=6.6$  Hz, 2H), 4.18 (t,  $J=6.6$  Hz, 2H), 2.28-2.21 (m, 2H), 2.20-2.01 (m, 2H), 1.94-1.86 (m, 2H), 1.82-1.74 (m, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.29, 153.93, 142.12, 137.76, 137.48, 137.45, 134.74, 131.03, 121.64, 119.03, 115.78, 115.46, 67.51, 64.85, 30.32, 30.19, 28.27, 27.95; IR (KBr,  $\text{cm}^{-1}$ ): 3486, 3451, 2943, 1737, 1690, 1591, 1528, 1384, 1241; HRMS (ESI) calcd for  $\text{C}_{18}\text{H}_{23}\text{NO}_4$  ( $\text{M} + \text{H}^+$ ) 318.1705, found 318.1719.

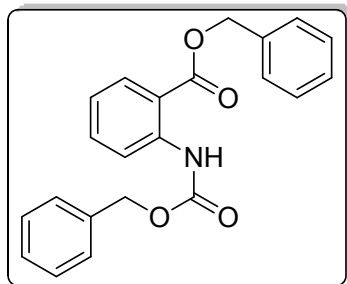
**But-3-yn-1-yl 2-(((but-3-yn-1-yloxy)carbonyl)amino)benzoate (4k):**

Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  10.45 (s, 1H, NH), 8.42 (d,  $J=8.4$  Hz, 1H), 8.05 (d,  $J=7.6$  Hz, 1H), 7.54 (t,  $J=7.8$  Hz, 1H), 7.04 (t,  $J=7.8$  Hz, 1H), 4.42 (t,  $J=7.2$  Hz, 2H), 4.28 (t,  $J=7.2$  Hz, 2H), 2.68 (td,  $J=6.6$  & 2.4 Hz, 2H), 2.60 (td,  $J=7.2$  & 2.4 Hz, 2H), 2.04 (t,  $J=2.4$  Hz, 1H), 2.02 (t,  $J=2.4$  Hz, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  167.92, 153.36, 141.89, 134.98, 131.21, 121.96, 119.10, 114.68, 80.18, 79.89, 70.48, 70.22, 63.08, 19.47, 19.21; IR (KBr,  $\text{cm}^{-1}$ ): 3447, 3280, 2923, 2126, 1718, 1688, 1596, 1384, 1266, 1146; HRMS (ESI) calcd for  $\text{C}_{16}\text{H}_{15}\text{NO}_4$  ( $\text{M} + \text{H}^+$ ) 286.1079, found 286.1086.

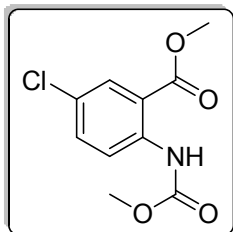
**2-Methoxyethyl 2-(((2-methoxyethoxy)carbonyl)amino)benzoate (4l):**

Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  10.44 (s, 1H, NH), 8.41 (d,  $J=8.4$  Hz, 1H), 8.04 (d,  $J=7.8$  Hz, 1H), 7.51 (t,  $J=8.4$  Hz, 1H), 7.01 (t,  $J=7.8$  Hz, 1H), 4.47-4.43 (m, 2H), 4.34-4.30 (m, 2H), 3.73-3.69 (m, 2H), 3.65-3.62 (m, 2H), 3.41 (s, 3H, -OMe), 3.39 (s, 3H, -OMe);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.04, 153.68, 141.86, 134.79, 131.25, 121.79, 119.05, 114.85, 70.81, 70.51, 64.38, 59.25, 59.15; IR (KBr,  $\text{cm}^{-1}$ ): 3299, 2889, 1737, 1686, 1592, 1262; HRMS (ESI) calcd for  $\text{C}_{14}\text{H}_{19}\text{NO}_6$  ( $\text{M} + \text{H}^+$ ) 298.1291, found 298.1294.

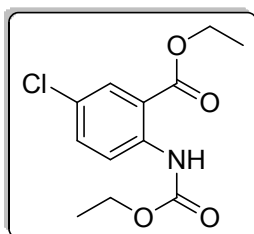


**Benzyl 2-(((benzyloxy)carbonyl)amino)benzoate (4p):**

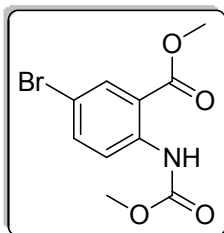
Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  10.56 (s, 1H, NH), 8.47 (d,  $J=8.4$  Hz, 1H), 8.06 (d,  $J=8.4$  Hz, 1H), 7.53 (t,  $J=7.8$  Hz, 1H), 7.47-7.42 (m, 4H), 7.41-7.32 (m, 6H), 7.02 (t,  $J=7.8$  Hz, 1H), 5.34 (s, 2H), 5.22 (s, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz): 167.99, 153.64, 142.05, 134.90, 131.20, 128.88, 128.79, 128.74, 128.66, 128.53, 128.47, 128.42, 128.40, 121.83, 119.09, 114.79, 67.13, 67.10; IR (KBr,  $\text{cm}^{-1}$ ): 3451, 3294, 2927, 1739, 1688, 1591, 1498, 1260, 1145; HRMS (ESI) calcd for  $\text{C}_{22}\text{H}_{19}\text{NO}_4$  ( $\text{M} + \text{H}^+$ ) 362.1392, found 362.1394.

**Methyl 5-chloro-2-((methoxycarbonyl)amino)benzoate (4q):**

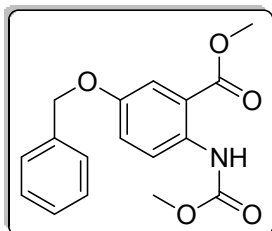
White solid; Mp 120–123 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  10.40 (s, 1H, NH), 8.40 (d,  $J=9$  Hz, 1H), 7.96 (d,  $J=3$  Hz, 1H), 7.47 (dd,  $J=9$  & 2.4 Hz, 1H), 3.91 (s, 3H, -OMe), 3.78 (s, 3H, -OMe);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  167.61, 154.14, 140.56, 134.61, 130.58, 126.82, 120.46, 115.89, 52.73, 52.61; IR (KBr,  $\text{cm}^{-1}$ ): 3439, 2925, 2854, 1743, 1464, 1263, 1059; HRMS (ESI) calcd for  $\text{C}_{10}\text{H}_9\text{ClNO}_4$  ( $\text{M} + \text{H}^+$ ) 244.0377, found 244.0378.

**Ethyl 5-chloro-2-((ethoxycarbonyl)amino)benzoate (4r):**

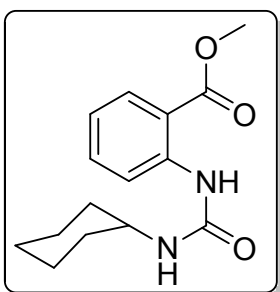
White solid; Mp 90–92 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  10.42 (s, 1H, NH), 8.41 (d,  $J=9$  Hz, 1H), 7.97 (d,  $J=2.4$  Hz, 1H), 7.46 (dd,  $J=9$  & 2.4 Hz, 1H), 4.38 (q,  $J=7.2$  Hz, 2H), 4.22 (q,  $J=7.2$  Hz, 2H), 1.41 (t,  $J=7.2$  Hz, 3H), 1.31 (t,  $J=7.2$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  167.24, 153.77, 140.74, 134.48, 130.54, 126.63, 120.46, 116.12, 61.94, 61.56, 14.67, 14.35; IR (KBr,  $\text{cm}^{-1}$ ): 3248, 2925, 2854, 1731, 1697, 1595, 1240, 1058; HRMS (ESI) calcd for  $\text{C}_{12}\text{H}_{14}\text{ClNO}_4$  ( $\text{M} + \text{H}^+$ ) 272.0690, found 272.0692.

**Methyl 5-bromo-2-((methoxycarbonyl)amino)benzoate (4s):**

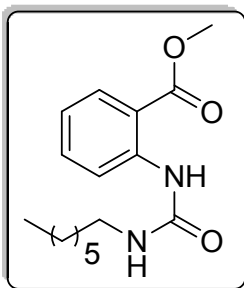
White solid; Mp 128–130 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  10.41 (s, 1H, NH), 8.35 (d,  $J=9$  Hz, 1H), 8.11 (d,  $J=2.4$  Hz, 1H), 7.61 (dd,  $J=9$  & 2.4 Hz, 1H), 3.91 (s, 3H, -OMe), 3.78 (s, 3H, -OMe);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  167.52, 154.09, 141.02, 137.47, 133.54, 120.74, 116.24, 114.03, 52.75, 52.62; IR (KBr,  $\text{cm}^{-1}$ ): 3259, 2953, 1743, 1690, 1588, 1430, 1252, 1067; HRMS (ESI) calcd for  $\text{C}_{10}\text{H}_{10}\text{BrNO}_4$  ( $\text{M} + \text{H}^+$ ) 287.9871, found 287.9870

**Methyl 5-(benzyloxy)-2-((methoxycarbonyl)amino)benzoate (4u):**

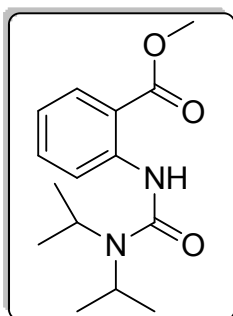
White solid; Mp 103–105 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  10.20 (s, 1H, NH), 8.33 (d,  $J=9.6$  Hz, 1H), 7.59 (d,  $J=3$  Hz, 1H), 7.42 (d,  $J=7.2$  Hz, 2H), 7.38 (t,  $J=7.8$  Hz, 2H), 7.33 (t,  $J=7.2$  Hz, 1H), 7.19 (dd,  $J=9$  & 3 Hz, 1H), 5.05 (s, 2H), 3.91 (s, 3H, -OMe), 3.76 (s, 3H, -OMe);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.32, 154.47, 153.24, 136.85, 135.83, 128.83, 128.32, 127.77, 122.32, 120.67, 116.05, 115.73, 70.74, 52.56, 52.43; IR (KBr,  $\text{cm}^{-1}$ ): 3309, 2924, 2854, 1729, 1690, 1527, 1263, 1019; HRMS (ESI) calcd for  $\text{C}_{17}\text{H}_{17}\text{NO}_5$  ( $\text{M} + \text{H}^+$ ) 316.1185, found 316.1185.

**Methyl 2-(3-cyclohexylureido)benzoate (6a):**

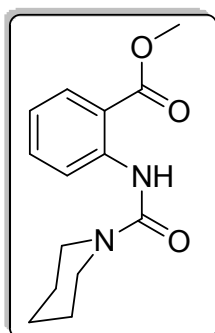
White solid; Mp 153–155 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz): 10.20 (s, 1H, NH), 8.45 (d,  $J=8.4$  Hz, 1H), 7.88 (d,  $J=7.6$  Hz, 1H), 7.39 (t,  $J=7.2$  Hz, 1H), 6.86 (t,  $J=6.4$  Hz, 1H), 4.63 (s, 1H), 3.81 (s, 3H), 3.57–3.53 (m, 1H), 2.02–1.86 (m, 2H), 1.73–1.62 (m, 2H), 1.61–1.52 (m, 1H), 1.4–1.21 (m, 2H), 1.18–1.00 (m, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  169.41, 154.42, 143.70, 134.76, 130.85, 120.61, 119.59, 113.72, 52.28, 49.56, 33.87, 25.75, 25.11; IR (KBr,  $\text{cm}^{-1}$ ): 3293, 2924, 1699, 1653, 1550, 1249; HRMS (ESI) calcd for  $\text{C}_{15}\text{H}_{20}\text{N}_2\text{O}_3$  ( $\text{M} + \text{H}^+$ ) 277.1552, found 277.1541.

**Methyl 2-(3-heptylureido)benzoate (6b):**

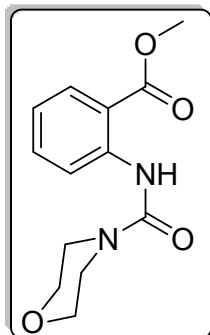
Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  10.30 (s, 1H, NH), 8.51 (d,  $J=8.4$  Hz, 1H), 7.95 (d,  $J=8.4$  Hz, 1H), 7.46 (t,  $J=8.0$  Hz, 1H), 6.92 (t,  $J=8.0$  Hz, 1H), 4.71 (s, 1H), 3.87 (s, 3H), 3.24 (q,  $J=6.8$  Hz, 2H), 1.6-1.49 (m, 2H), 1.38-1.31 (m, 4H), 1.30-1.29 (m, 4H), 0.85 (t,  $J=6.8$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  169.45, 155.24, 143.63, 134.84, 130.88, 120.74, 119.65, 113.78, 52.34, 40.86, 31.97, 30.22, 29.20, 27.05, 22.81, 14.26; IR (KBr,  $\text{cm}^{-1}$ ): 3454, 3319, 2929, 1654, 1607, 1547, 1261; MS (ESI) calcd for  $\text{C}_{16}\text{H}_{24}\text{N}_2\text{O}_3$  ( $\text{M} + \text{H}^+$ ) 293.1865, found 293.1900.

**Methyl 2-(3,3-diisopropylureido)benzoate (6c):**

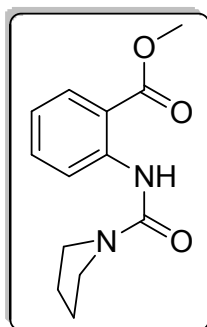
Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  10.29 (s, 1H, NH), 8.39 (dd,  $J=8.4$  & 0.8 Hz, 1H), 7.94 (dd,  $J=8.4$  & 2 Hz, 1H), 7.43 (td,  $J=7.2$  & 1.6 Hz, 1H), 6.89 (td,  $J=7.6$  & 1.2 Hz, 1H), 3.95-3.88 (m, 2H), 3.87 (s, 3H), 1.36 (s, 6H), 1.34 (s, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  169.36, 154.55, 144.06, 134.51, 130.87, 120.37, 114.23, 52.31, 46.59, 21.36; IR (KBr,  $\text{cm}^{-1}$ ): 3317, 2969, 1723, 1670, 1588, 1448, 1254; HRMS (ESI) calcd for  $\text{C}_{15}\text{H}_{23}\text{N}_2\text{O}_3$  ( $\text{M} + \text{H}^+$ ) 279.1709, found 279.1717.

**Methyl 2-(piperidine-1-carboxamido)benzoate (6d):**

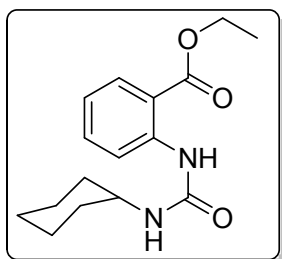
Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  10.64 (s, 1H, NH), 8.52 (d,  $J=8.8$  Hz, 1H), 7.96 (d,  $J=8.0$  Hz, 1H), 7.46 (t,  $J=8.8$  Hz, 1H), 6.92 (t,  $J=8.4$  Hz, 1H), 3.88 (s, 3H), 3.56-3.48 (m, 4H), 1.71-1.55 (m, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  169.60, 154.77, 144.02, 134.78, 130.87, 120.60, 119.81, 113.95, 52.39, 45.20, 25.98, 24.75; IR (KBr,  $\text{cm}^{-1}$ ): 3316, 2930, 1687, 1671, 1589, 1252; HRMS (ESI) calcd for  $\text{C}_{14}\text{H}_{18}\text{N}_2\text{O}_3$  ( $\text{M} + \text{H}^+$ ) 263.1396, found 263.1409.

**Methyl 2-(morpholine-4-carboxamido)benzoate (6e):**

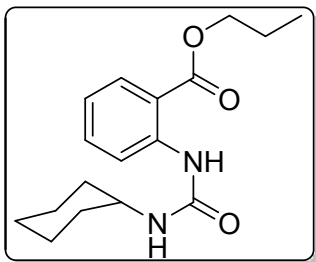
Gummy;  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  10.76 (s, 1H, NH), 8.55 (d,  $J=9.0$  Hz, 1H), 8.0 (dd,  $J=7.8$  & 1.2 Hz, 1H), 7.51 (t,  $J=9.0$ , 1.2 Hz, 1H), 6.98 (t,  $J=7.8$  Hz, 1H), 3.91 (s, 3H), 3.76 (t,  $J=4.8$  Hz, 4H), 3.58 (t,  $J=4.8$  Hz, 4H);  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.71, 154.95, 143.53, 134.95, 130.97, 121.11, 119.73, 114.11, 66.83, 52.51, 44.23; IR (KBr,  $\text{cm}^{-1}$ ): 3446, 2924, 1754, 1604, 1384, 1261; MS (ESI) calcd for  $\text{C}_{13}\text{H}_{16}\text{N}_2\text{O}_4$  ( $\text{M} + \text{H}^+$ ) 265.1188, found 265.1224.

**Methyl 2-(pyrrolidine-1-carboxamido)benzoate (6f):**

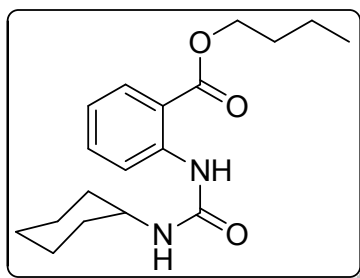
Gummy;  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  10.40 (s, 1H, NH), 8.57 (d,  $J=8.8$  Hz, 1H), 7.91 (d,  $J=7.6$  Hz, 1H), 7.42 (t,  $J=8.0$  Hz, 1H), 6.87 (t,  $J=7.6$  Hz, 1H), 3.83 (s, 3H), 3.51-3.39 (m, 4H), 2.01-1.34 (m, 4H);  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  169.54, 154.16, 143.89, 134.85, 130.87, 120.60, 119.52, 113.75, 52.35, 45.98, 25.76; IR (KBr,  $\text{cm}^{-1}$ ): 3315, 2925, 1671, 1606, 1532, 1252; HRMS (ESI) calcd for  $\text{C}_{13}\text{H}_{16}\text{N}_2\text{O}_3$  ( $\text{M} + \text{H}^+$ ) 249.1239, found 249.1237.

**Ethyl 2-(3-cyclohexylureido)benzoate (6g):**

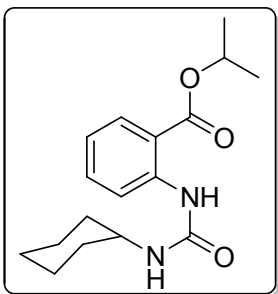
White solid; Mp 164–167 °C;  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  10.31 (s, 1H, NH), 8.50 (d,  $J=8.4$  Hz, 1H), 7.95 (d,  $J=8.0$  Hz, 1H), 7.45 (t,  $J=7.6$  Hz, 1H), 6.91 (t,  $J=7.2$  Hz, 1H), 4.60 (s, 1H), 4.32 (q,  $J=7.2$  Hz, 2H), 3.68-3.54 (m, 1H), 2.00-1.92 (m, 2H), 1.80-1.66 (m, 2H), 1.62-1.54 (m, 1H), 1.37 (t,  $J=6.4$  Hz, 3H), 1.36-1.29 (m, 2H), 1.21-1.09 (m, 3H);  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  169.05, 154.44, 143.73, 134.69, 130.85, 120.56, 119.52, 113.94, 61.33, 49.53, 33.88, 25.76, 25.11, 14.39; IR (KBr,  $\text{cm}^{-1}$ ): 3281, 2930, 1697, 1655, 1553, 1261; HRMS (ESI) calcd for  $\text{C}_{16}\text{H}_{22}\text{N}_2\text{O}_3$  ( $\text{M} + \text{H}^+$ ) 291.1709, found 291.1700.

**Propyl 2-(3-cyclohexylureido)benzoate (6h):**

White solid; Mp 152–153 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  10.31 (s, 1H, NH), 8.50 (d,  $J=8.4$  Hz, 1H), 7.96 (d,  $J=8.0$  Hz, 1H), 7.49 (t,  $J=8.0$  Hz, 1H), 6.91 (t,  $J=7.6$  Hz, 1H), 4.60 (d,  $J=7.6$  Hz, 1H), 4.22 (t,  $J=6.8$  Hz, 2H), 3.67–3.54 (m, 1H), 2.04–1.93 (m, 2H), 1.82–1.65 (m, 4H), 1.64–1.56 (m, 1H), 1.44–1.30 (m, 2H), 1.21–1.08 (m, 3H), 1.01 (t,  $J=7.6$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  169.07, 154.43, 143.71, 134.67, 130.80, 120.55, 119.52, 113.96, 66.88, 49.51, 33.86, 25.75, 25.10, 22.18, 10.70; IR (KBr,  $\text{cm}^{-1}$ ): 3292, 2936, 1697, 1657, 1549, 1245; HRMS (ESI) calcd for  $\text{C}_{17}\text{H}_{24}\text{N}_2\text{O}_3$  ( $\text{M} + \text{H}^+$ ) 305.1865, found 305.1863.

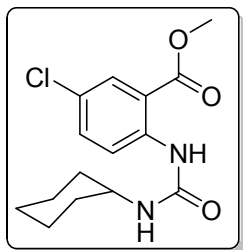
**Butyl 2-(3-cyclohexylureido)benzoate (6i):**

White solid;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  10.34 (s, 1H, NH), 8.52 (d,  $J=8.8$  Hz, 1H), 7.97 (d,  $J=8.0$  Hz, 1H), 7.47 (t,  $J=7.6$  Hz, 1H), 6.93 (t,  $J=7.6$  Hz, 1H), 4.66 (s, 1H), 4.28 (t,  $J=6.4$  Hz, 2H), 3.69–3.58 (m, 1H), 2.06–1.92 (m, 2H), 1.80–1.66 (m, 4H), 1.65–1.56 (m, 1H), 1.53–1.42 (m, 2H), 1.41–1.32 (m, 2H), 1.24–1.05 (m, 3H), 0.98 (t,  $J=7.2$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz): 169.08, 154.47, 143.69, 134.67, 130.80, 120.57, 119.54, 113.98, 65.18, 49.53, 33.85, 30.82, 25.75, 25.10, 19.46, 13.90; IR (KBr,  $\text{cm}^{-1}$ ): 3292, 2923, 1699, 1652, 1551, 1250; HRMS (ESI) calcd for  $\text{C}_{18}\text{H}_{26}\text{N}_2\text{O}_3$  ( $\text{M} + \text{H}^+$ ) 319.2022, found 319.2024.

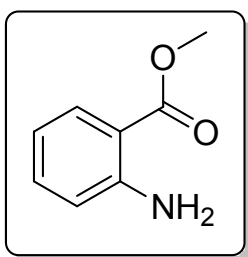
**Isopropyl 2-(3-cyclohexylureido)benzoate (6j):**

White solid; Mp 138–141 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  10.36 (s, 1H, NH), 8.49 (d,  $J=8.4$  Hz, 1H), 7.94 (d,  $J=8.4$  Hz, 1H), 7.43 (t,  $J=7.2$  Hz, 1H), 6.90 (t,  $J=7.6$  Hz, 1H), 5.24–5.12 (m, 1H), 4.60 (s, 1H), 3.68–3.54 (m, 1H), 2.14–1.93 (m, 2H), 1.77–1.65 (m, 2H), 1.64–1.56 (m, 1H), 1.34 (d,  $J=6.4$  Hz, 6H), 1.22–1.08 (m, 2H), 0.92–0.78 (m, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  168.57, 154.48, 143.72, 134.57, 130.84, 120.51, 119.48, 114.31, 68.97, 49.54, 33.88, 31.78, 25.77, 25.12, 22.84, 22.05, 14.30; IR (KBr,  $\text{cm}^{-1}$ ): 3292, 2969, 1697, 1657, 1549, 1245; HRMS (ESI) calcd for  $\text{C}_{17}\text{H}_{24}\text{N}_2\text{O}_3$  ( $\text{M} + \text{H}^+$ ) 305.1865, found 305.1864.

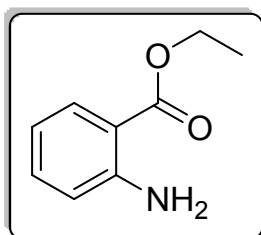


**Methyl 5-chloro-2-(3-cyclohexylureido)benzoate (6k):**

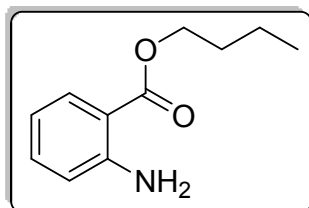
White solid; Mp 188–190 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz): 10.19 (s, 1H, NH), 8.52 (d,  $J=9$  Hz, 1H), 7.92 (d,  $J=2.4$  Hz, 1H), 7.41 (dd,  $J=9.6$  & 3 Hz, 1H), 4.66 (s, 1H), 3.90 (s, 3H), 3.58-5.65 (m, 1H), 2.05-1.93 (m, 2H), 1.81-1.68 (m, 2H), 1.65-1.58 (m, 1H), 1.45-1.32 (m, 2H), 1.22-1.10 (m, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.40, 154.14, 142.29, 134.62, 130.28, 125.57, 121.06, 114.75, 52.61, 49.63, 33.83, 25.71, 25.08; IR (KBr,  $\text{cm}^{-1}$ ): 3330, 3298, 2923, 2855, 1712, 1648, 1554, 1240, 1108; HRMS (ESI) calcd for  $\text{C}_{15}\text{H}_{19}\text{ClN}_2\text{O}_3$  ( $\text{M} + \text{H}^+$ ) 311.1162, found 311.1162.

**Methyl 2-aminobenzoate (7a):**

Gummy liquid;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.75 (d,  $J=8.0$  Hz, 1H), 7.15 (t,  $J=8.0$  Hz, 1H), 6.61-6.49 (m, 2H), 5.35 (s, 2H,  $\text{NH}_2$ ), 3.76 (s, 3H, -OMe);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  168.68, 150.54, 134.19, 131.31, 116.80, 116.36, 110.82, 51.60; IR (KBr,  $\text{cm}^{-1}$ ): 3482, 3373, 2951, 1694, 1617, 1248, 1162, 1106; HRMS (ESI) calcd for  $\text{C}_8\text{H}_9\text{NO}_2$  ( $\text{M} + \text{H}^+$ ) 152.0712, found 152.0711.

**Ethyl 2-aminobenzoate (7b):**

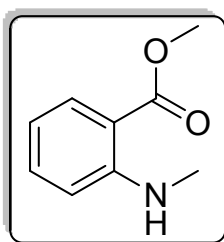
Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  7.87 (d,  $J=9.0$  Hz, 1H), 7.25 (t,  $J=7.2$  Hz, 1H), 6.67-6.61 (m, 2H), 5.72 (s, 2H,  $\text{NH}_2$ ), 4.31 (q,  $J=7.2$  Hz, 2H), 1.37 (t,  $J=6.6$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.31, 150.61, 134.10, 131.35, 116.80, 116.33, 111.18, 60.41, 14.49; IR (KBr,  $\text{cm}^{-1}$ ): 3483, 3373, 2981, 1689, 1616, 1589, 1246, 1161, 1103; HRMS (ESI) calcd for  $\text{C}_9\text{H}_{11}\text{NO}_2$  ( $\text{M} + \text{H}^+$ ) 166.0868, found 166.0867.

**Butyl 2-aminobenzoate (7c):**

Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  7.78 (dd,  $J=7.8$  & 1.2 Hz, 1H), 7.15 (td,  $J=9.0$  & 1.8 Hz, 1H), 6.61-6.53 (m, 2H), 5.65 (s, 2H,  $\text{NH}_2$ ), 4.18 (t,  $J=6.6$  Hz, 2H), 1.71-1.58 (m, 2H), 1.42-1.31 (m,

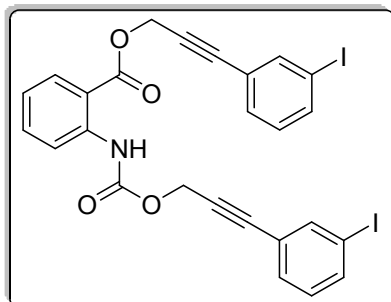
2H), 0.88 (t,  $J=7.8$ Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.32, 150.34, 134.08, 131.30, 116.93, 116.49, 111.34, 64.30, 30.92, 19.44, 13.89; IR (KBr,  $\text{cm}^{-1}$ ): 3485, 3373, 2960, 1692, 1616, 1589, 1246, 1161, 1104; HRMS (ESI) calcd for  $\text{C}_{11}\text{H}_{15}\text{NO}_2$  ( $\text{M} + \text{H}^+$ ) 194.1181, found 194.1184.

### Methyl 2-(methylamino)benzoate (7a')



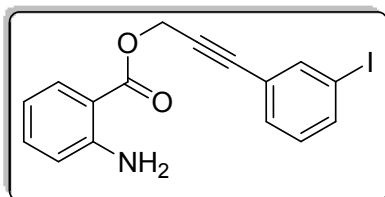
Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  7.93 (dd,  $J=7.8$  & 1.2 Hz, 1H), 7.44 (t,  $J=7.2$  Hz, 1H), 6.92 (d,  $J=8.4$  Hz, 1H), 6.76 (t,  $J=7.8$  Hz, 1H), 3.87 (s, 3H), 2.94 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.97, 150.36, 134.98, 131.80, 116.72, 112.98, 111.70, 51.95, 31.12; IR (KBr,  $\text{cm}^{-1}$ ): 3381, 2949, 1686, 1607, 1580, 1261, 1244, 1173, 1161; HRMS (ESI) calcd for  $\text{C}_9\text{H}_{11}\text{NO}_2$  ( $\text{M} + \text{H}^+$ ) 166.0868, found 166.0859.

### 3-(3-iodophenyl)prop-2-yn-1-yl 2-((((3-(3-iodophenyl)prop-2-yn-1-yl)oxy)carbonyl)amino)benzoate (8a):

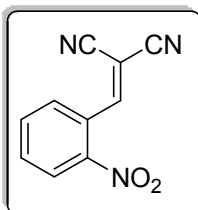


White solid; Mp 114–116 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  10.54 (s, 1H), 8.46 (d,  $J=8.4$  Hz, 1H), 8.10 (dd,  $J=7.8$  & 1.2 Hz, 1H), 7.87–7.8 (m, 2H), 7.71–7.64 (m, 2H), 7.61–7.56 (m, 1H), 7.45–7.39 (m, 2H), 7.07–7.02 (m, 3H), 5.13 (s, 2H), 4.99 (s, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  167.49, 152.85, 141.84, 140.68, 138.15, 137.96, 135.31, 131.40, 131.22, 131.20, 130.05, 130.00, 124.46, 124.21, 122.20, 119.18, 114.37, 93.73, 85.42, 85.00, 84.76, 84.06, 53.60, 53.57; IR (KBr,  $\text{cm}^{-1}$ ): 3444, 3281, 2923, 1739, 1685, 1604, 1419, 1384, 1208, 1051; HRMS (ESI) calcd for  $\text{C}_{26}\text{H}_{17}\text{I}_2\text{NO}_4$  ( $\text{M} + \text{K}^+$ ) 699.8884, found 699.8880.

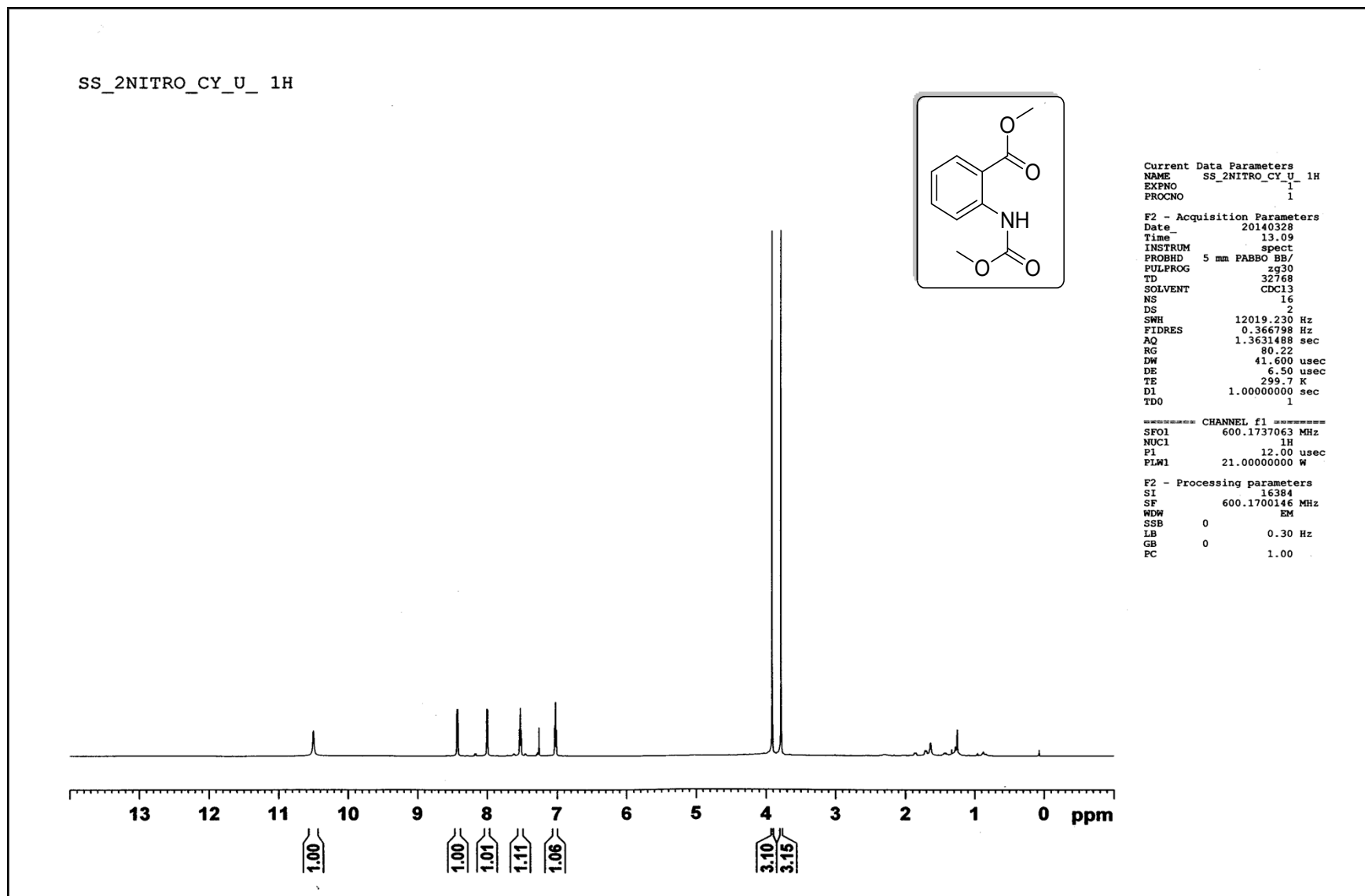
### 3-(3-iodophenyl)prop-2-yn-1-yl 2-aminobenzoate (8b):

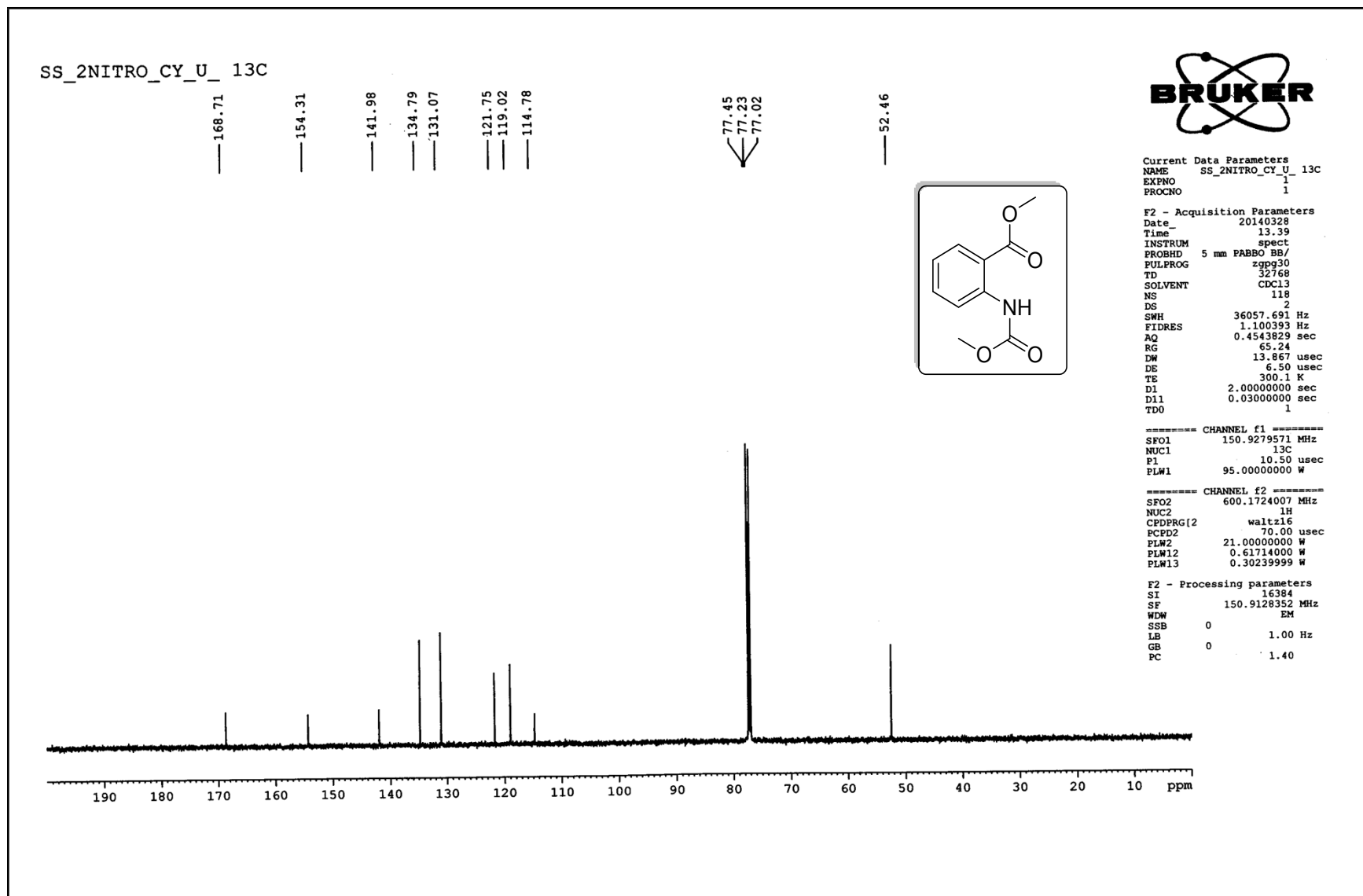


Gummy;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  7.93 (d,  $J=7.8$  Hz, 1H), 7.83 (s, 1H), 7.71–7.64 (m, 1H), 7.42 (d,  $J=7.8$  Hz, 1H), 7.31–7.25 (m, 1H), 7.08–7.00 (m, 1H), 6.71–6.62 (m, 2H), 5.72 (s, 2H), 5.08 (s, 2H); IR (KBr,  $\text{cm}^{-1}$ ): 3440, 3241, 2922, 1679, 1604, 1419, 1384, 1114; HRMS (ESI) calcd for  $\text{C}_{16}\text{H}_{12}\text{INO}_2$  ( $\text{M} + \text{H}^+$ ) 377.9991, found 378.0006.

**2-(2-nitrobenzylidene)malononitrile (A):**

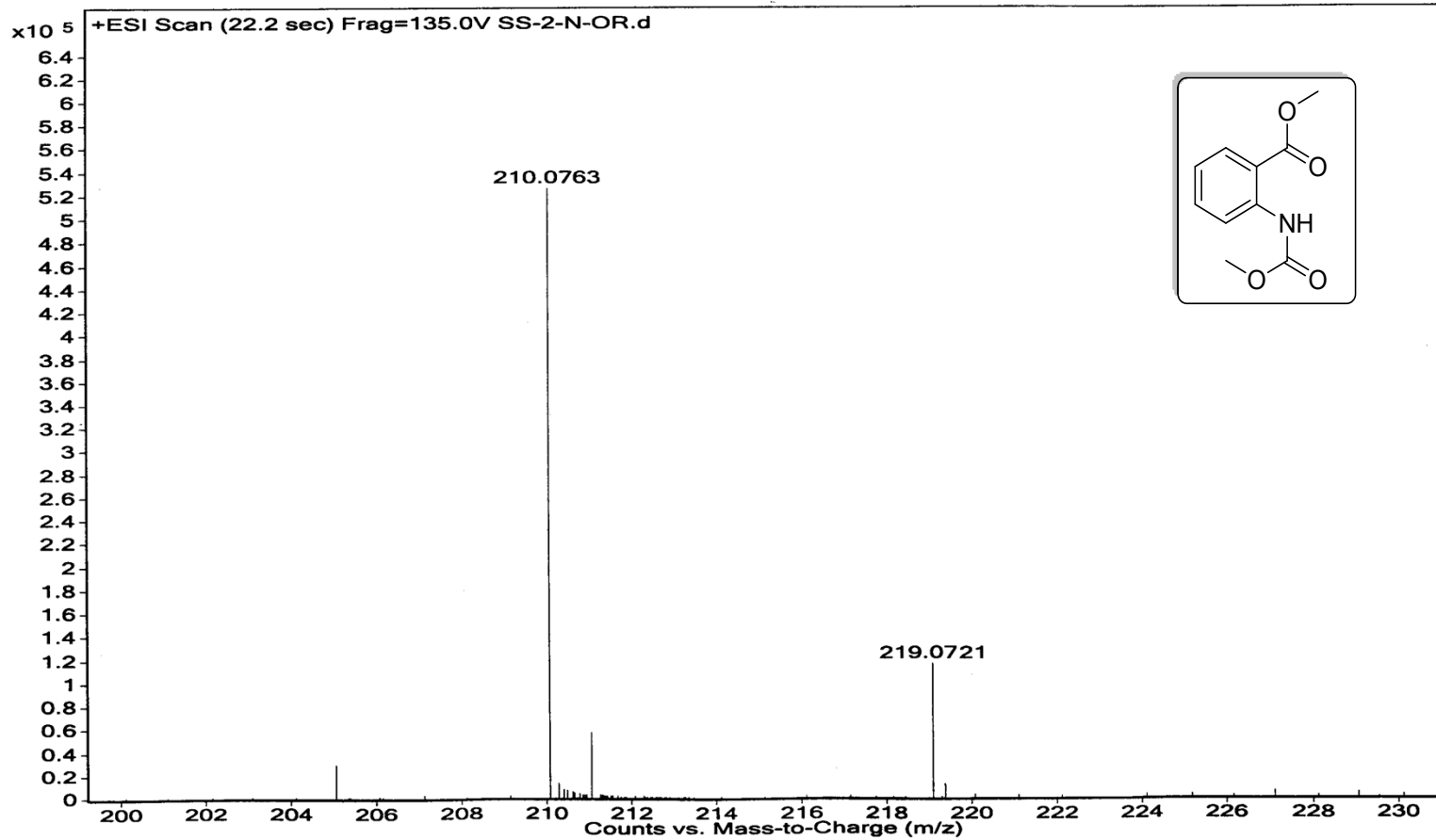
Yellow Solid;  $^1\text{H}$  NMR ( $\text{DMSO-}d_6$ , 400 MHz):  $\delta$  8.97 (s, 1H), 8.34 (d,  $J=8.4$  Hz, 1H), 8.01 (t,  $J=8.4$  Hz, 8H), 7.95 (d,  $J=6.8$  Hz, 1H), 7.89 (t,  $J=7.6$  Hz, 8H);  $^{13}\text{C}$  NMR ( $\text{DMSO-}d_6$ , 100 MHz):  $\delta$  161.32, 146.79, 135.03, 133.32, 130.43, 127.54, 125.40, 113.08, 111.77, 87.04; IR (KBr,  $\text{cm}^{-1}$ ): 3047, 2240, 1568, 1521, 1347, 870;

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): 4a

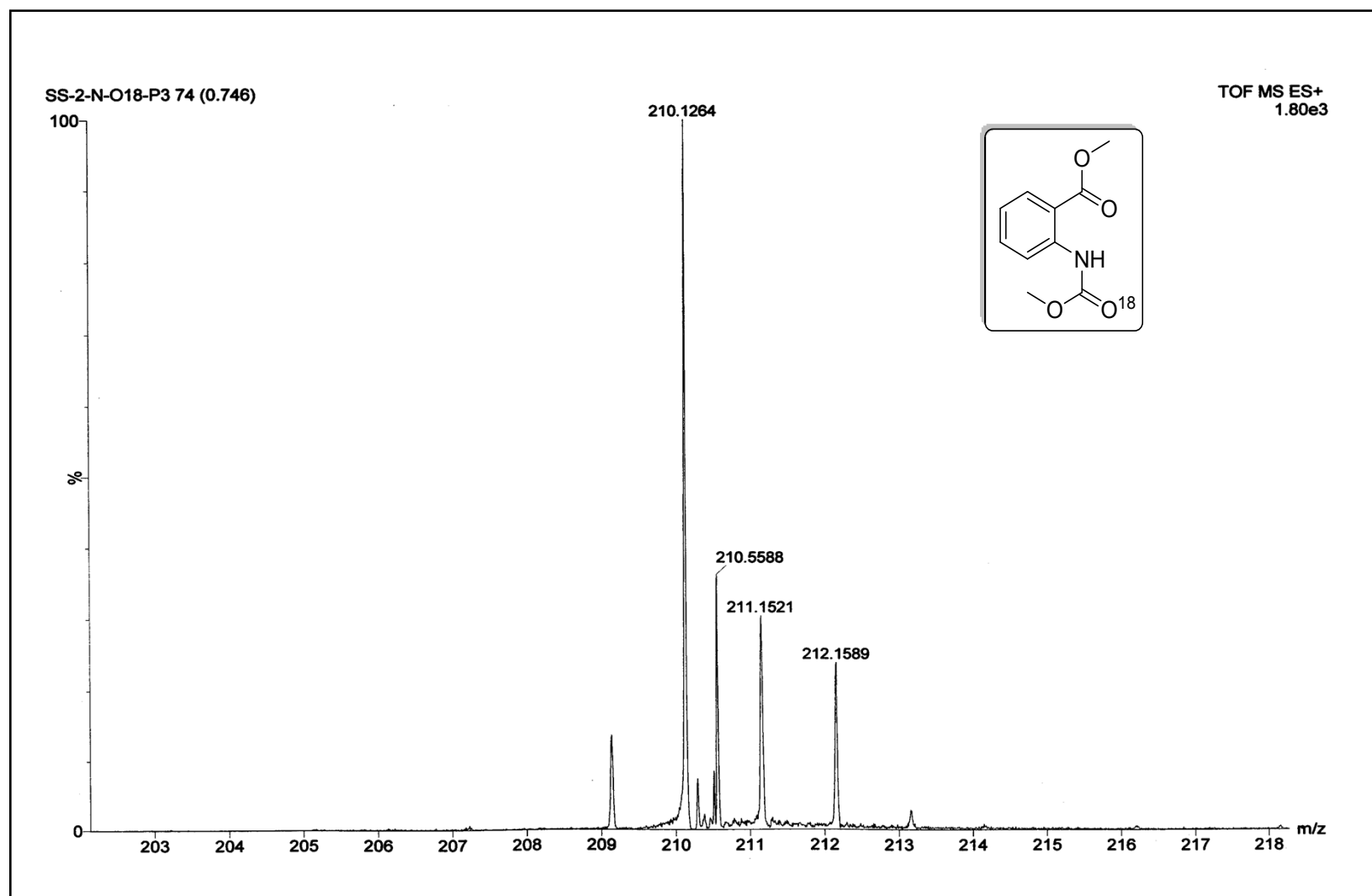
<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): 4a

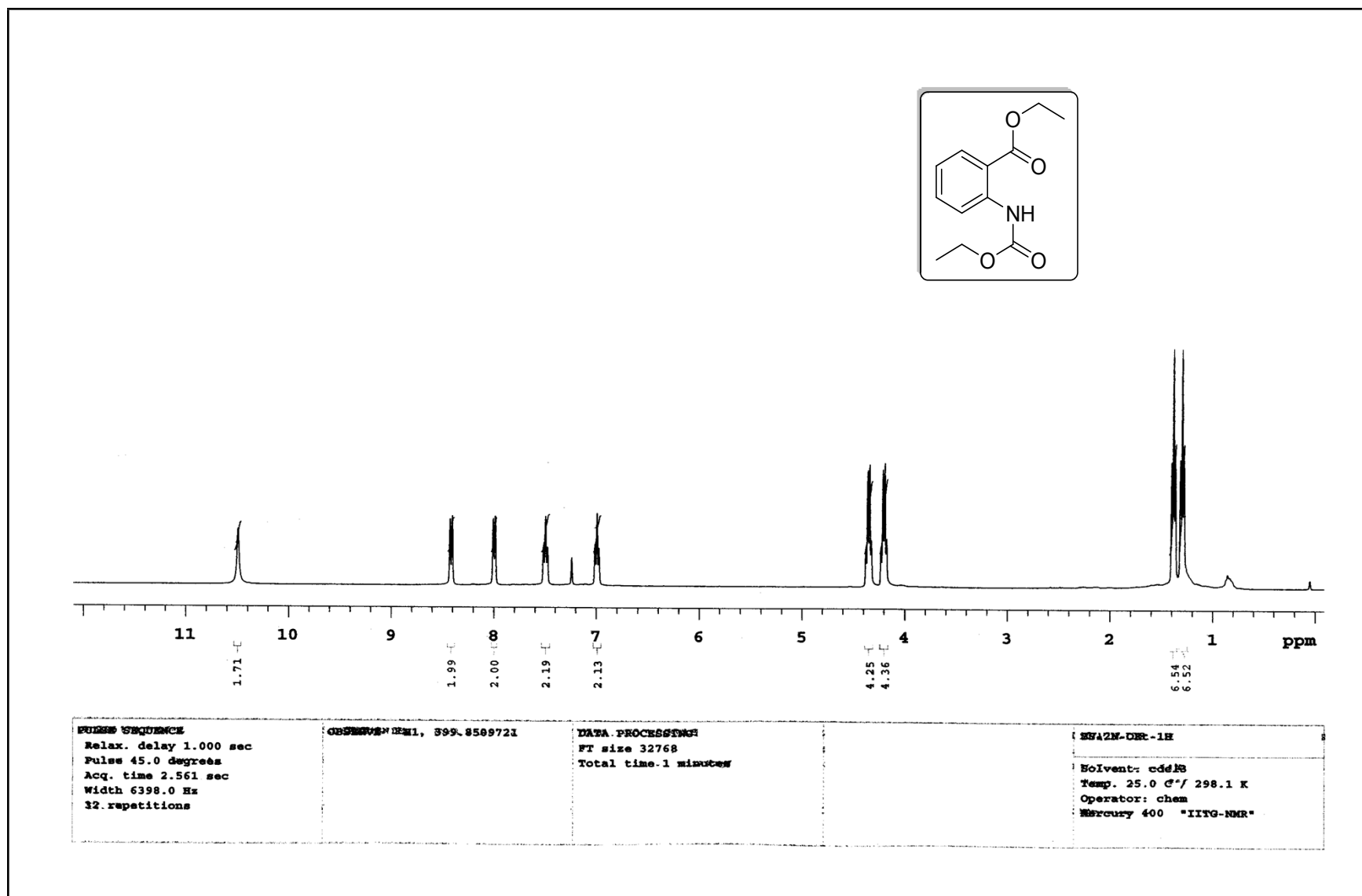
## Mass Spectra: 4a

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time

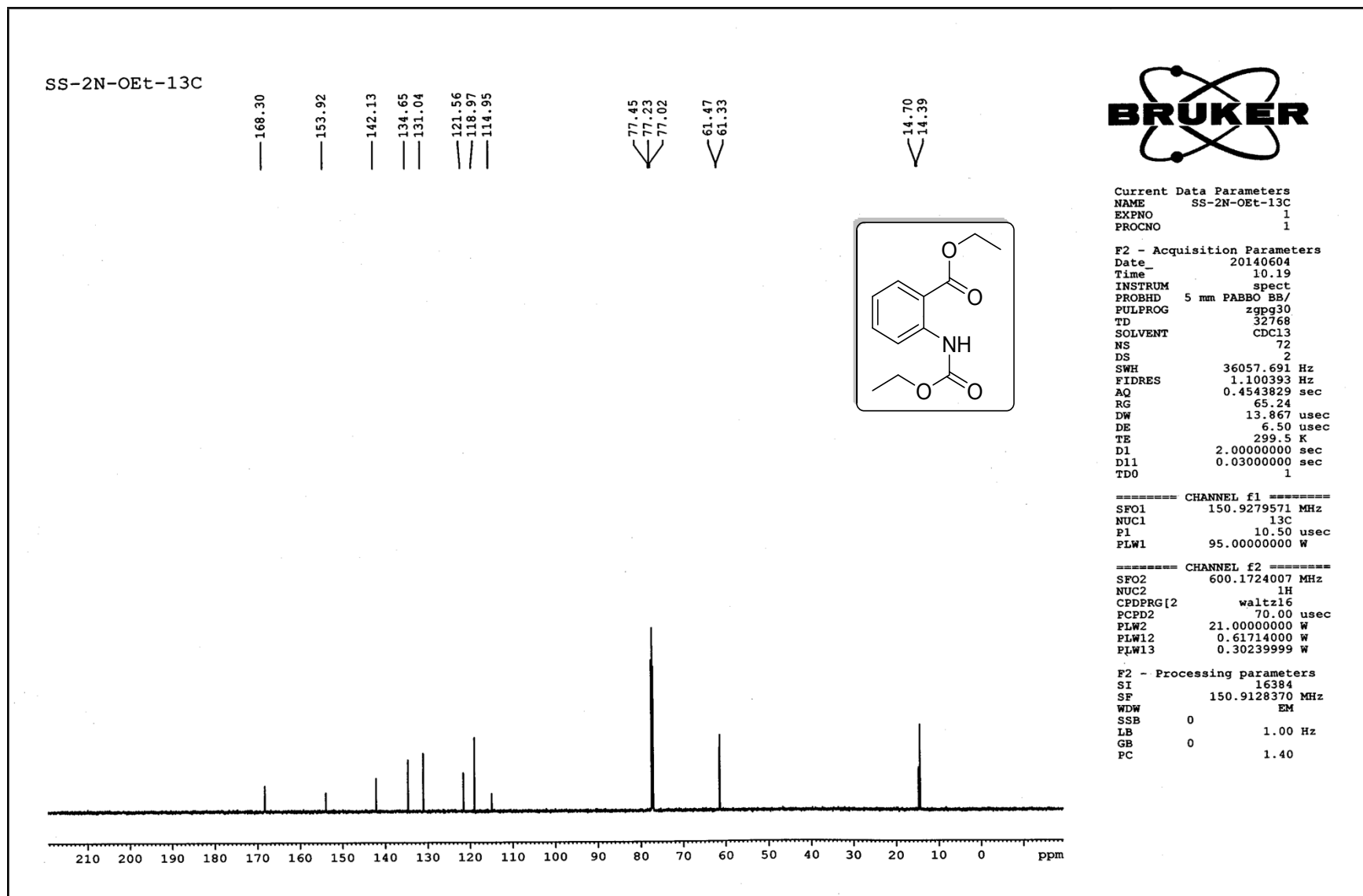


Mass Spectra: **4a** (After **O18** incorporation from  $\text{H}_2\text{O}^{18}$ )



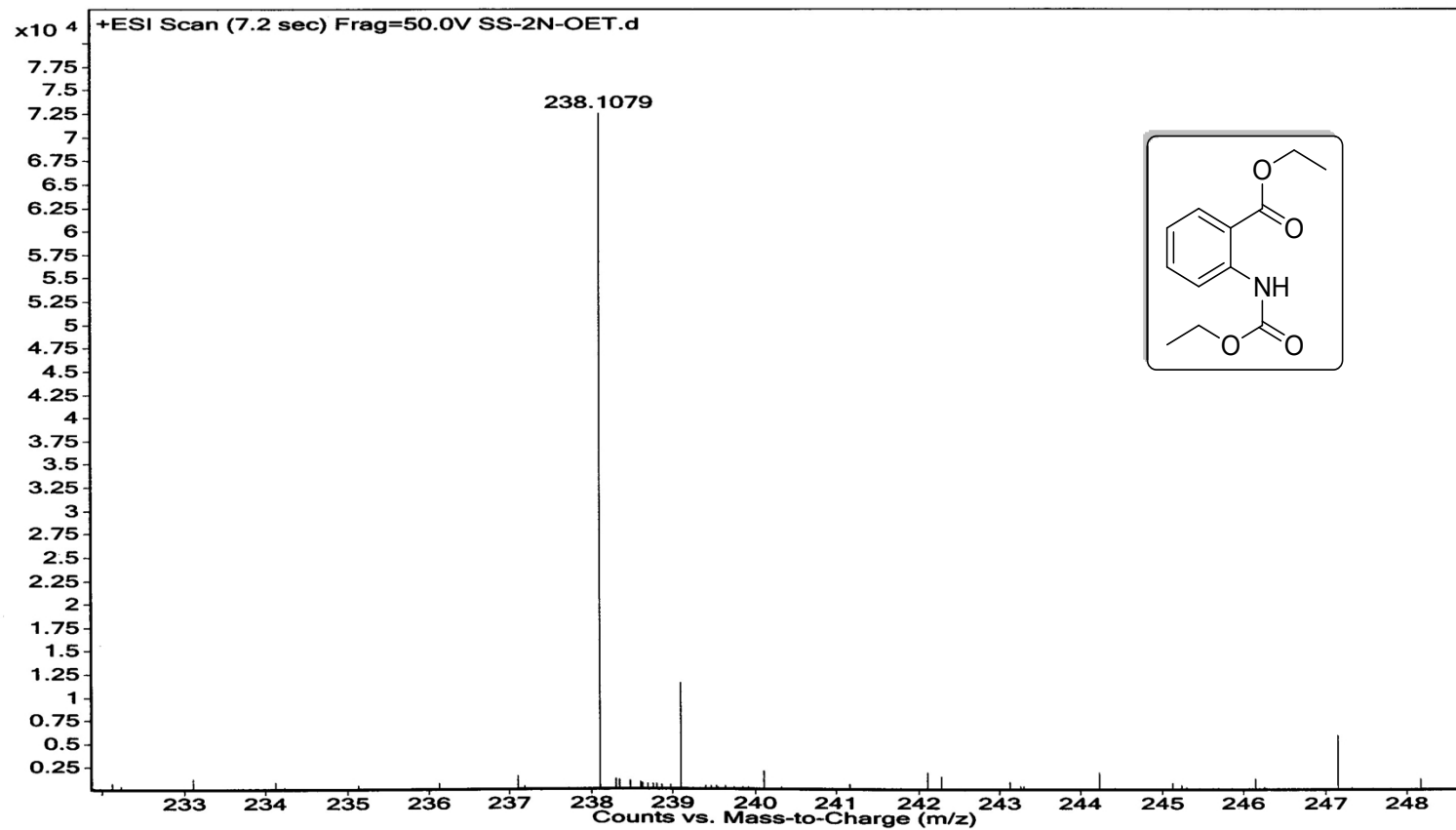
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): **4b**

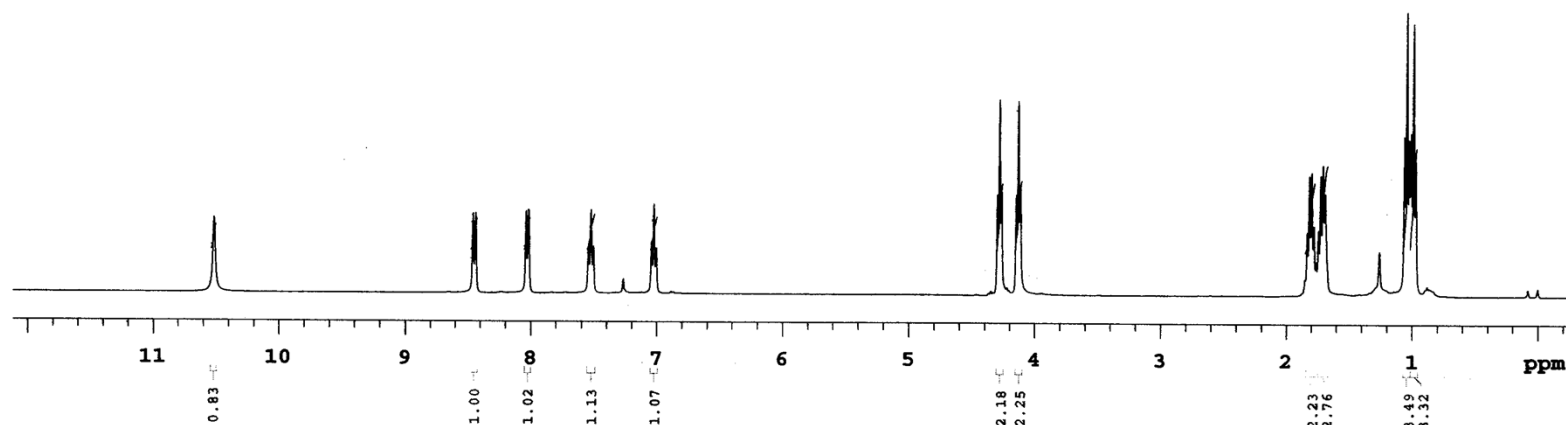
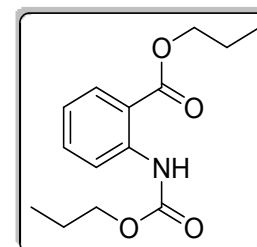


<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): **4b**

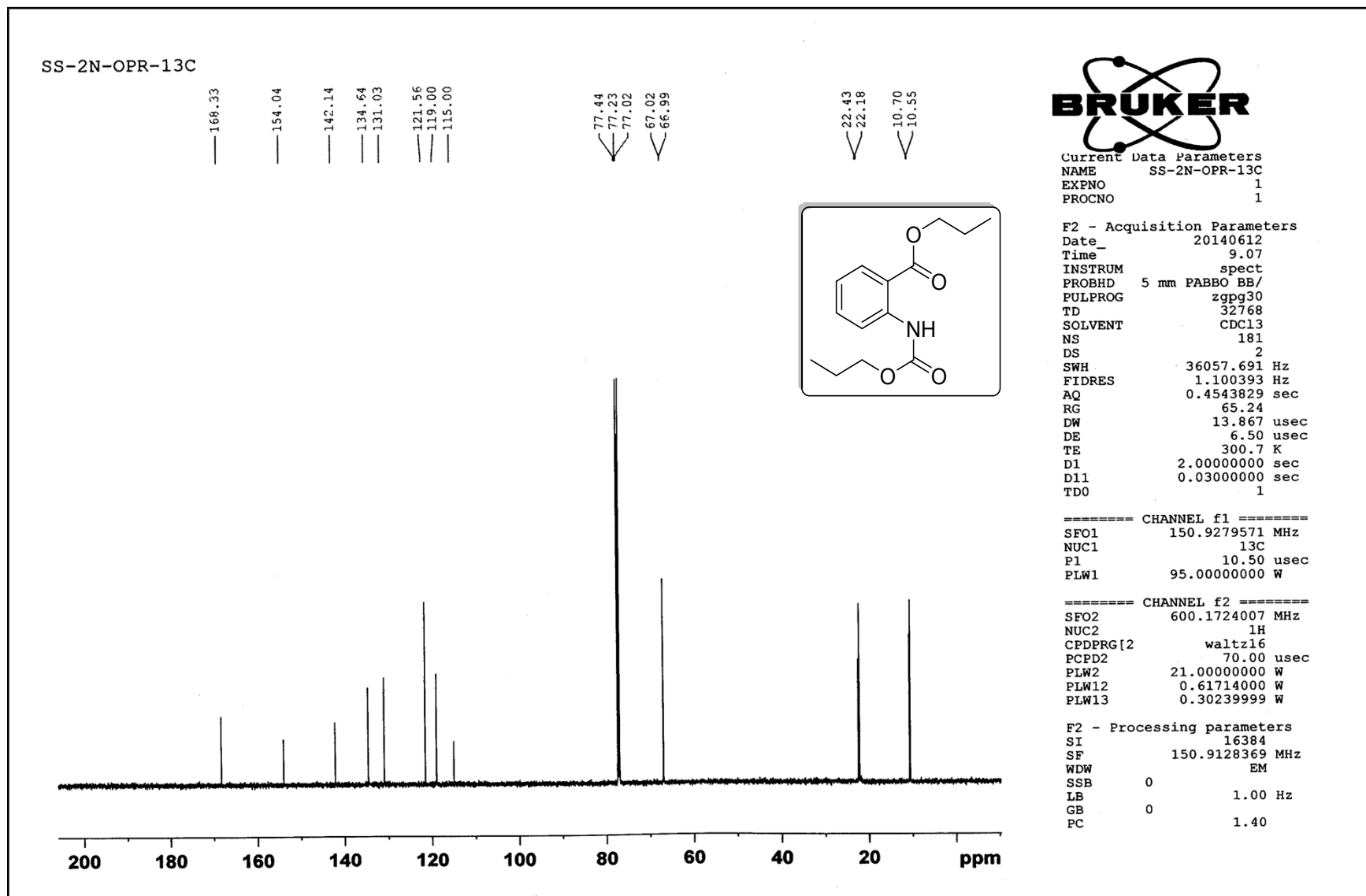
## Mass Spectra: 4b

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



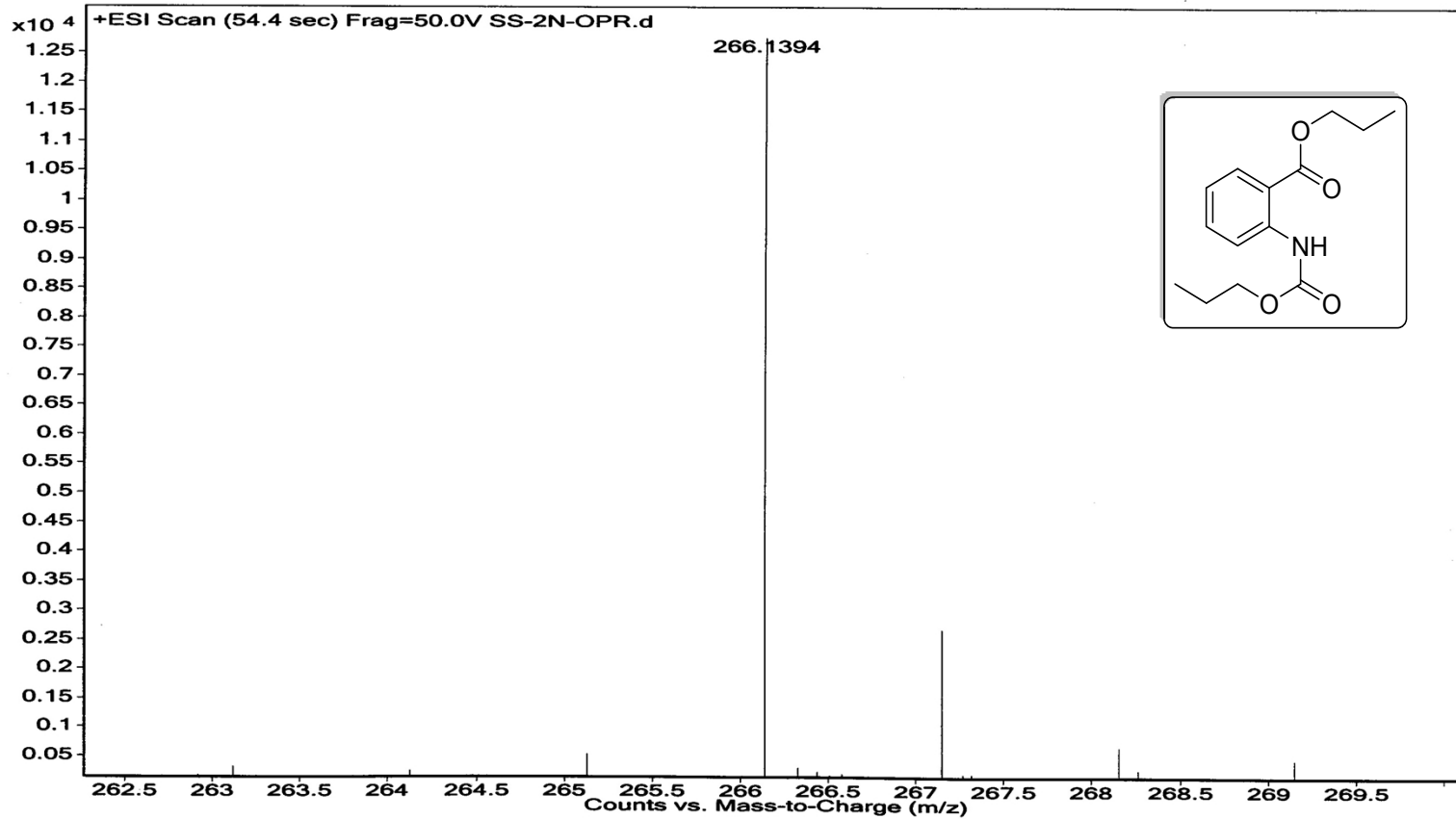
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): **4c**

<b>PULSE SEQUENCE</b> Relax. delay 1.000 secs Pulse 45:0 degree Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OPERATIVE FREQ</b> 399.8909613	<b>DATA PROCESSING</b> FT size 32768 Total time 1 minutes	<b>SR-2N-OPR</b> Solvent: cdc13 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *HITG-NMR*
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$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): **4c**

## Mass Spectra: 4c

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): **4d**

SS-2N-O-BU

Sample Name:  
SS-2N-O-BU

Data Collected on:  
IITG-NMR-mercury400

Archive directory:

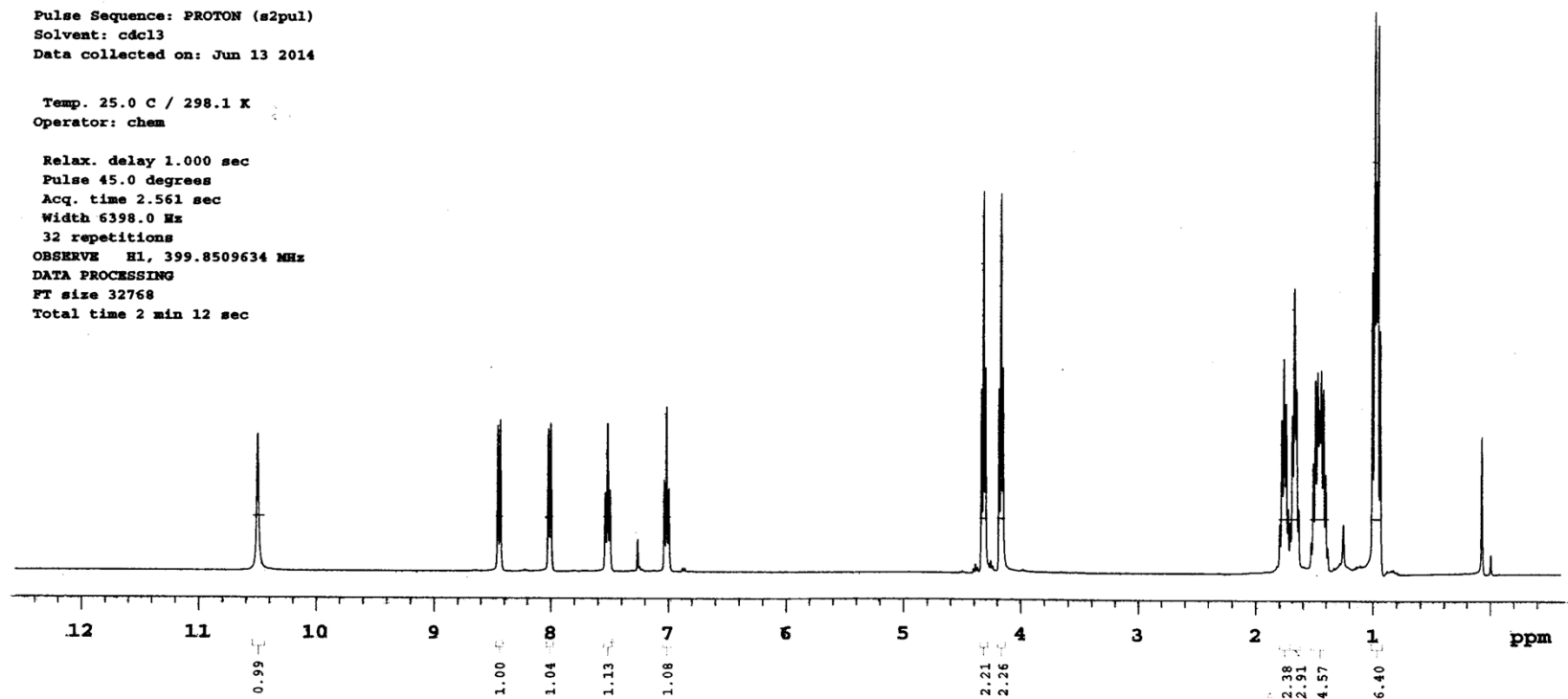
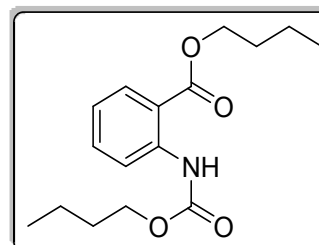
Sample directory:

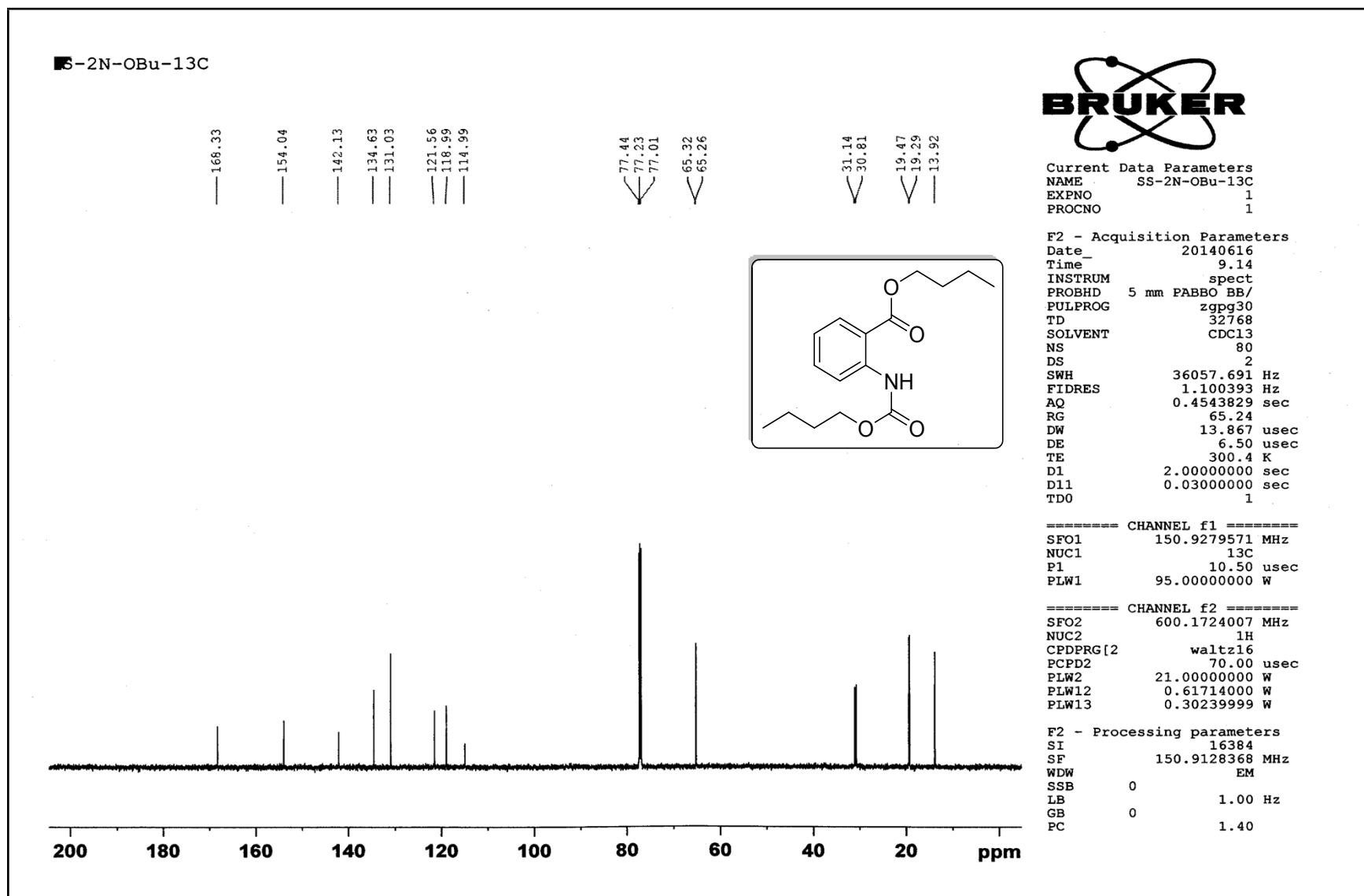
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Jun 13 2014

Temp. 25.0 C / 298.1 K  
Operator: chem

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions  
OBSERVE E1, 399.8509634 MHz  
DATA PROCESSING  
FT size 32768  
Total time 2 min 12 sec



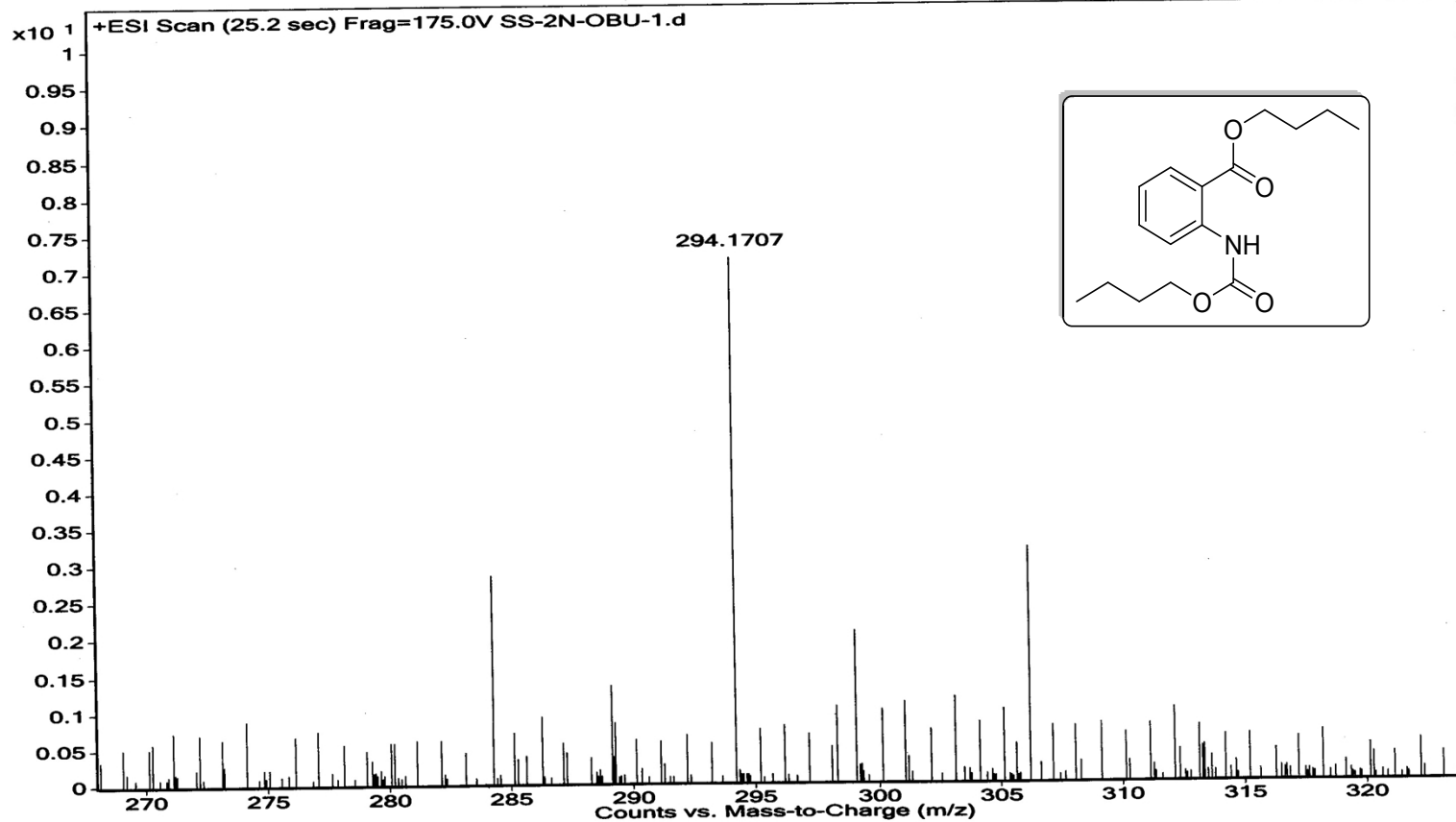
<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): 4d

Sample Name  
Inj Vol  
Data Filename

Position  
InjPosition  
ACQ Method

Instrument Name  
SampleType  
Comment

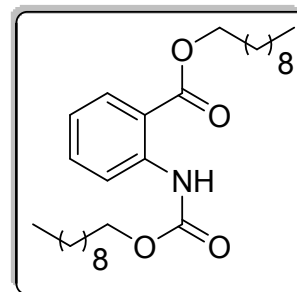
User Name  
IRM Calibration Status  
Acquired Time





<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): 4e

SS-2N-ODEC-1H

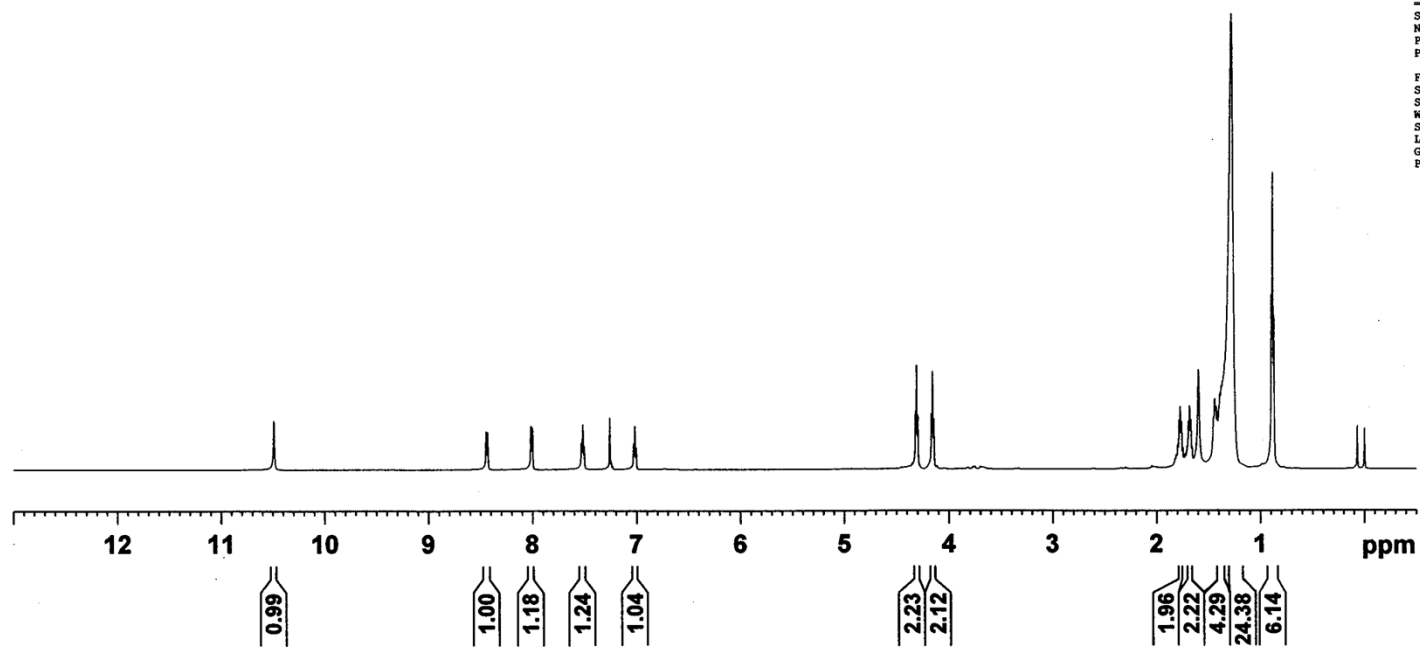


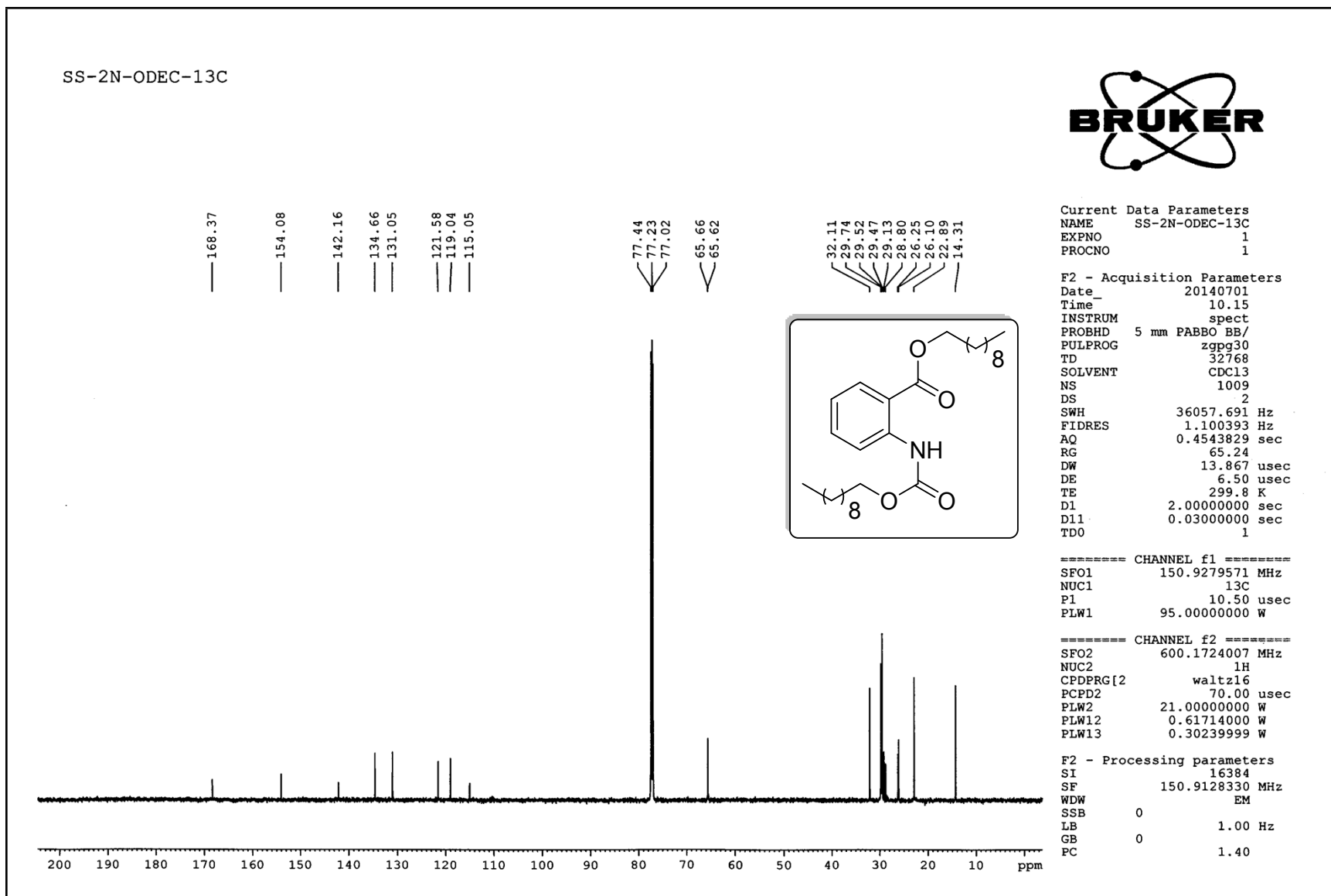
Current Data Parameters  
 NAME SS-2N-ODEC-1H  
 EXPNO 1  
 PROCNO 1

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 PULPROG zg30  
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 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 12019.230 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
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 DW 41.600 usec  
 DE 6.50 usec  
 TE 299.5 K  
 D1 1.0000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 SFO1 600.1737063 MHz  
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 P1 12.00 usec  
 PLW1 21.00000000 W

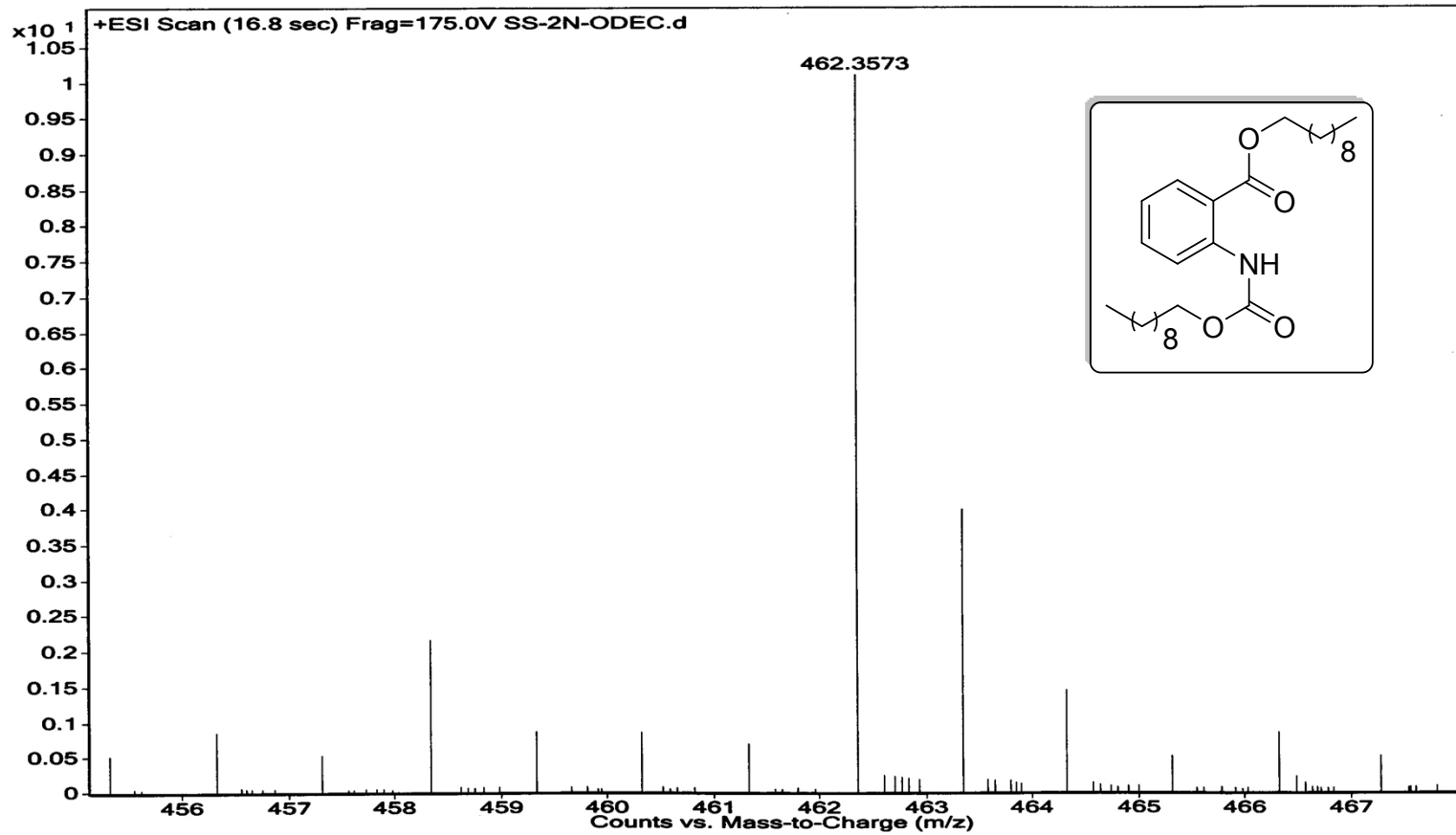
F2 - Processing parameters  
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 WDW EM  
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 LB 0.30 Hz  
 GB 0  
 PC 1.00



<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): 4e

## Mass Spectra:

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ): **4f**

SS-2N-IO-Pr-1H

Sample Name:  
SS-2N-IO-Pr-1H  
Data Collected on:  
IITG-NMR-mercury400  
Archive directory:

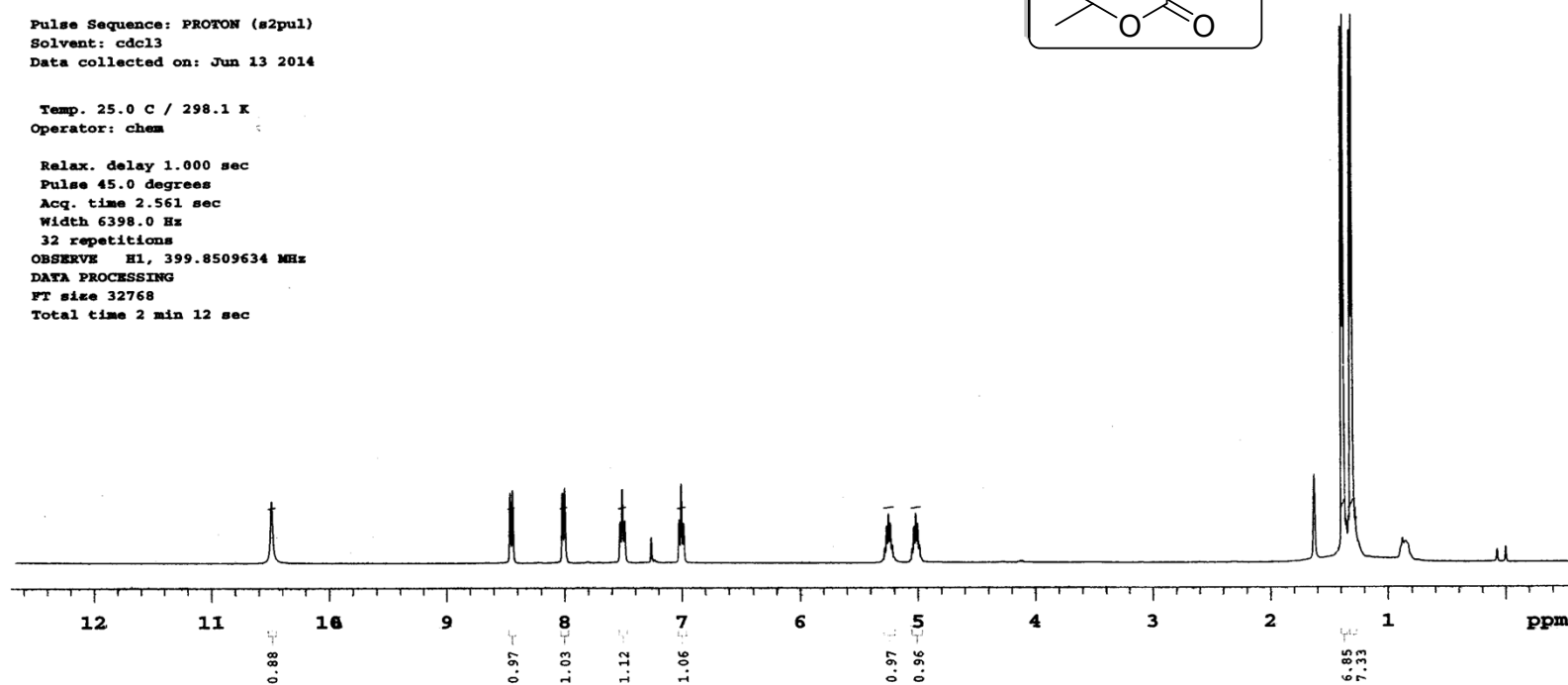
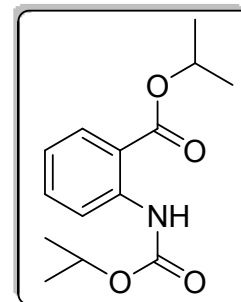
Sample directory:

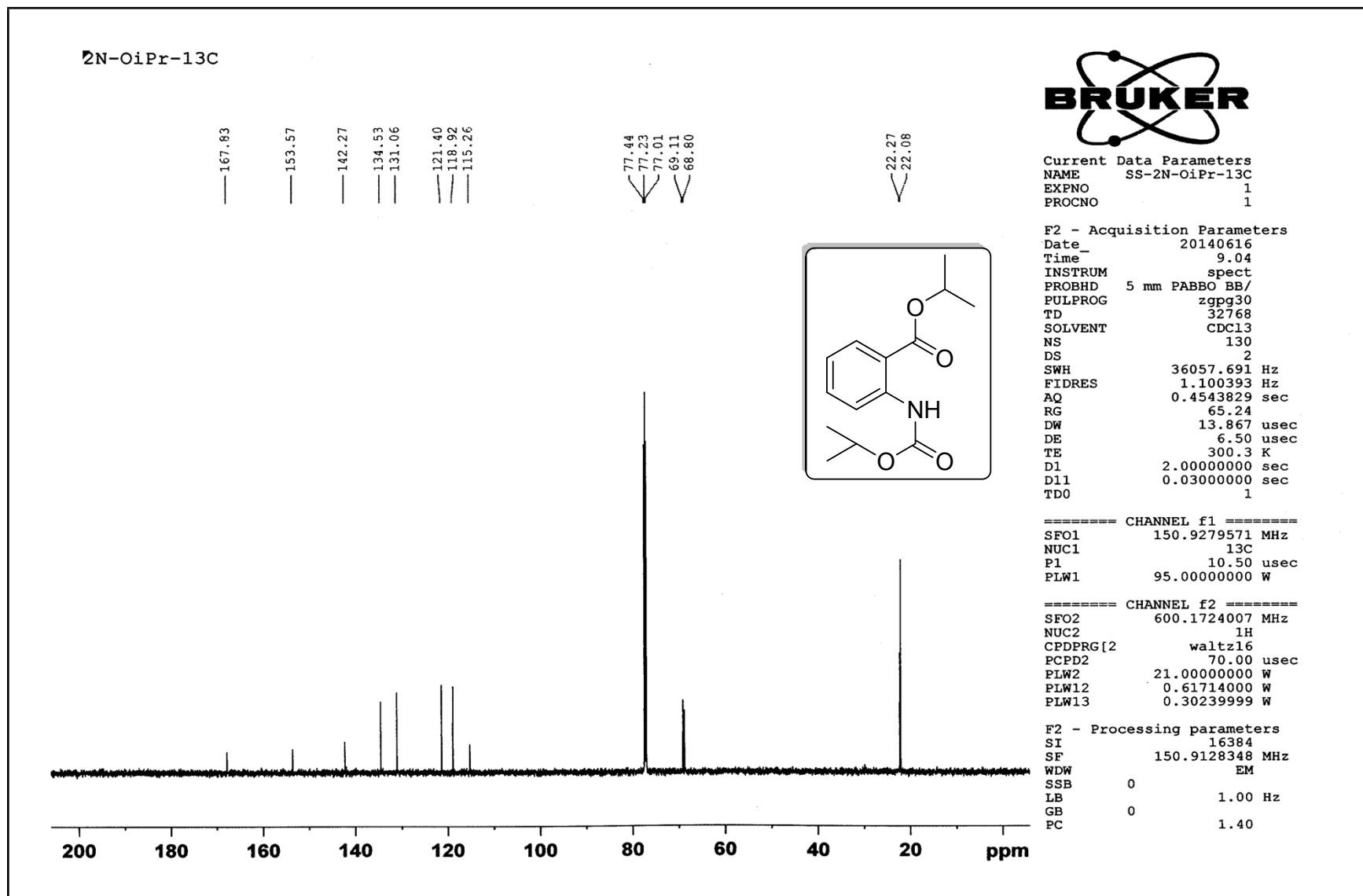
Fidfile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cdc13  
Data collected on: Jun 13 2014

Temp. 25.0 C / 298.1 K  
Operator: chem

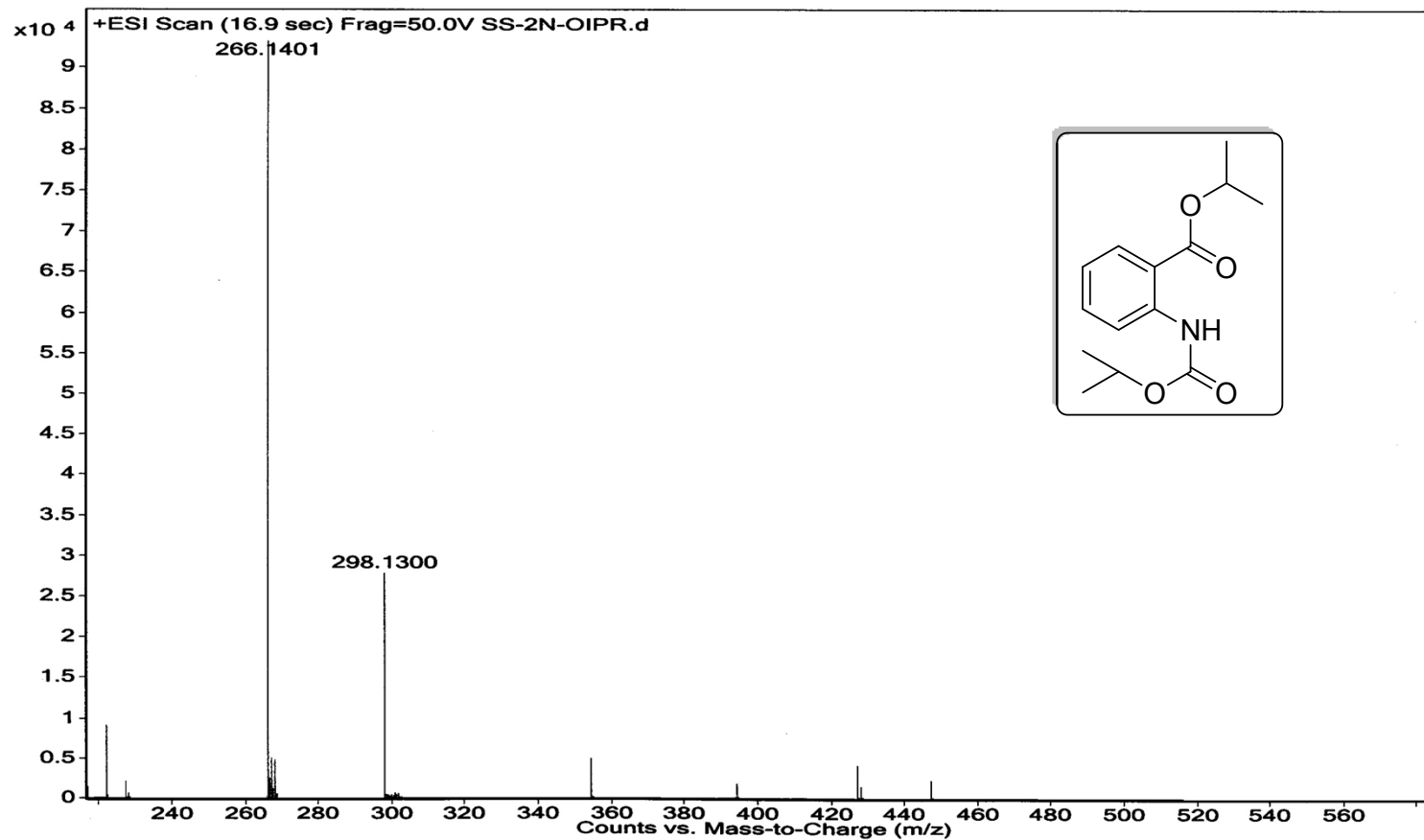
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions  
OBSERVE H1, 399.8509634 MHz  
DATA PROCESSING  
FT size 32768  
Total time 2 min 12 sec

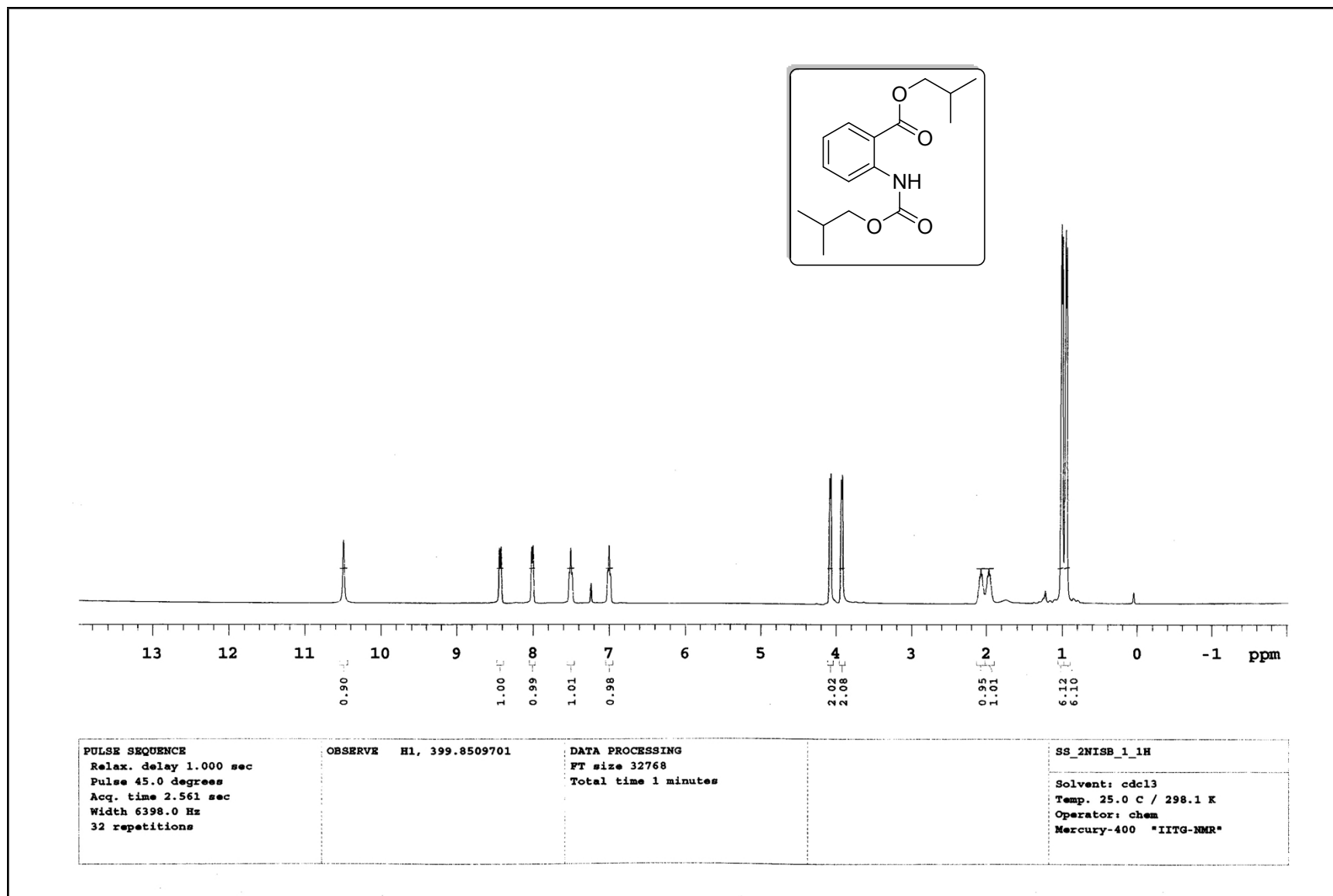


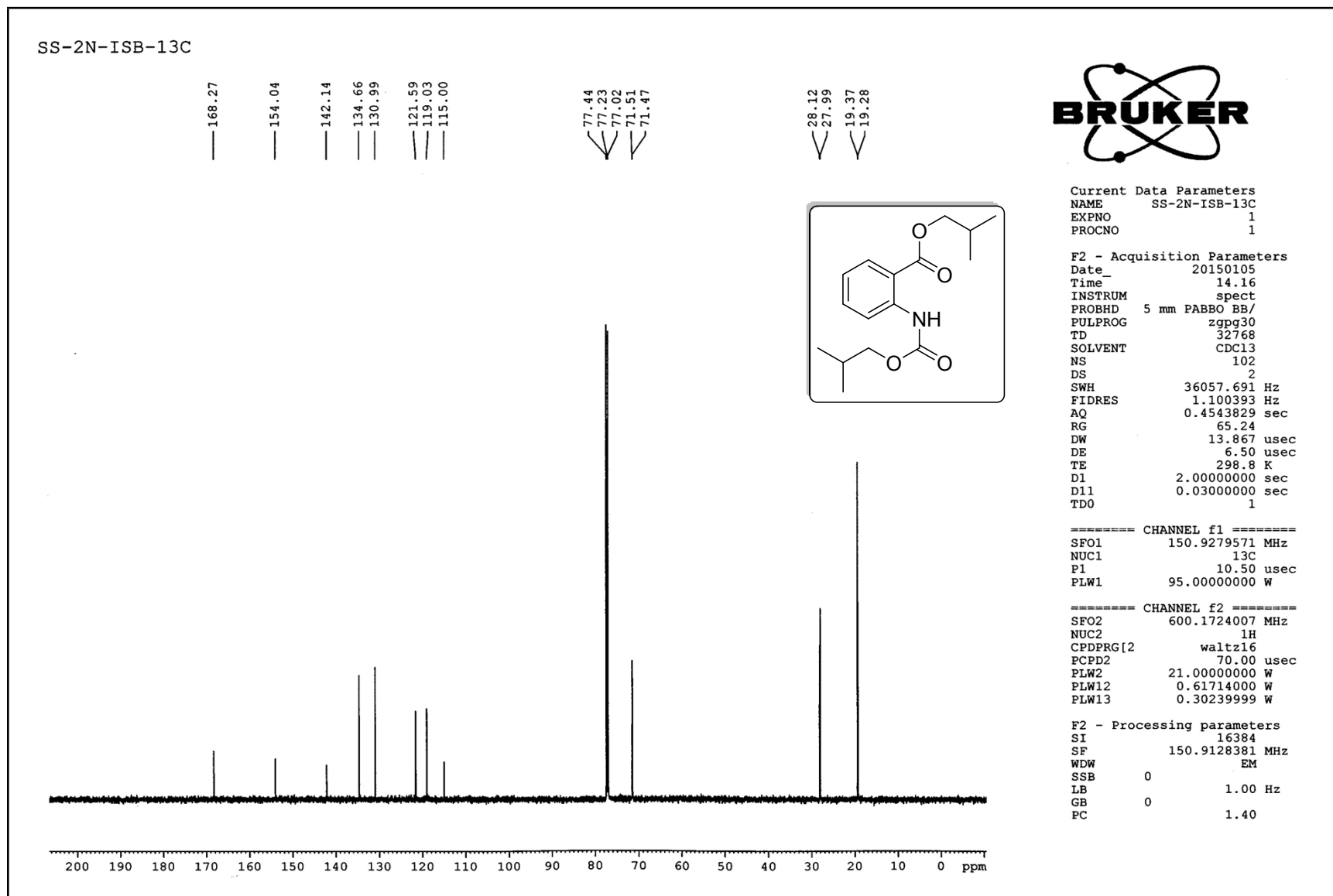
$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): **4f**

## Mass Spectra: 4f

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



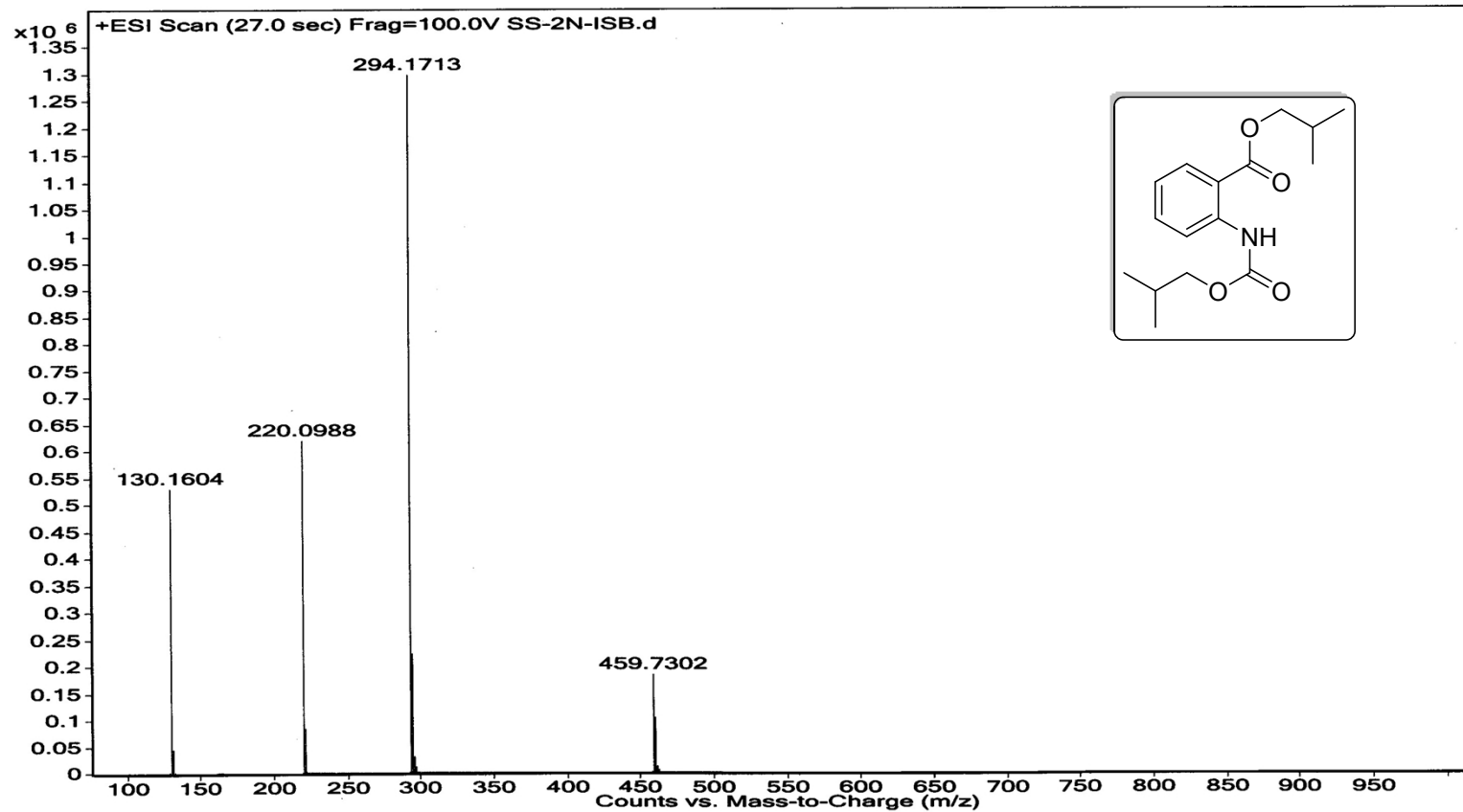
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): **4g**

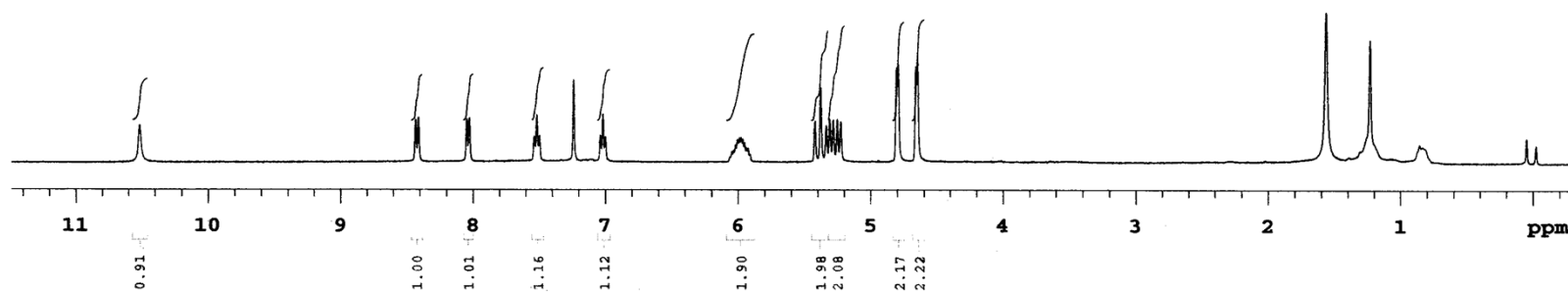
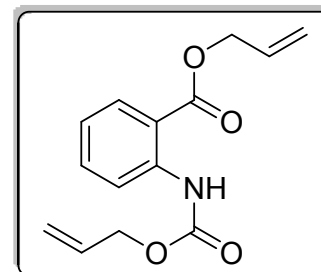
$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): 4g



Mass Spectra: 4g

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): **4h**

## PULSE SEQUENCE

Relax. delay 1.000 sec  
Pulse 45.0 degree  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions

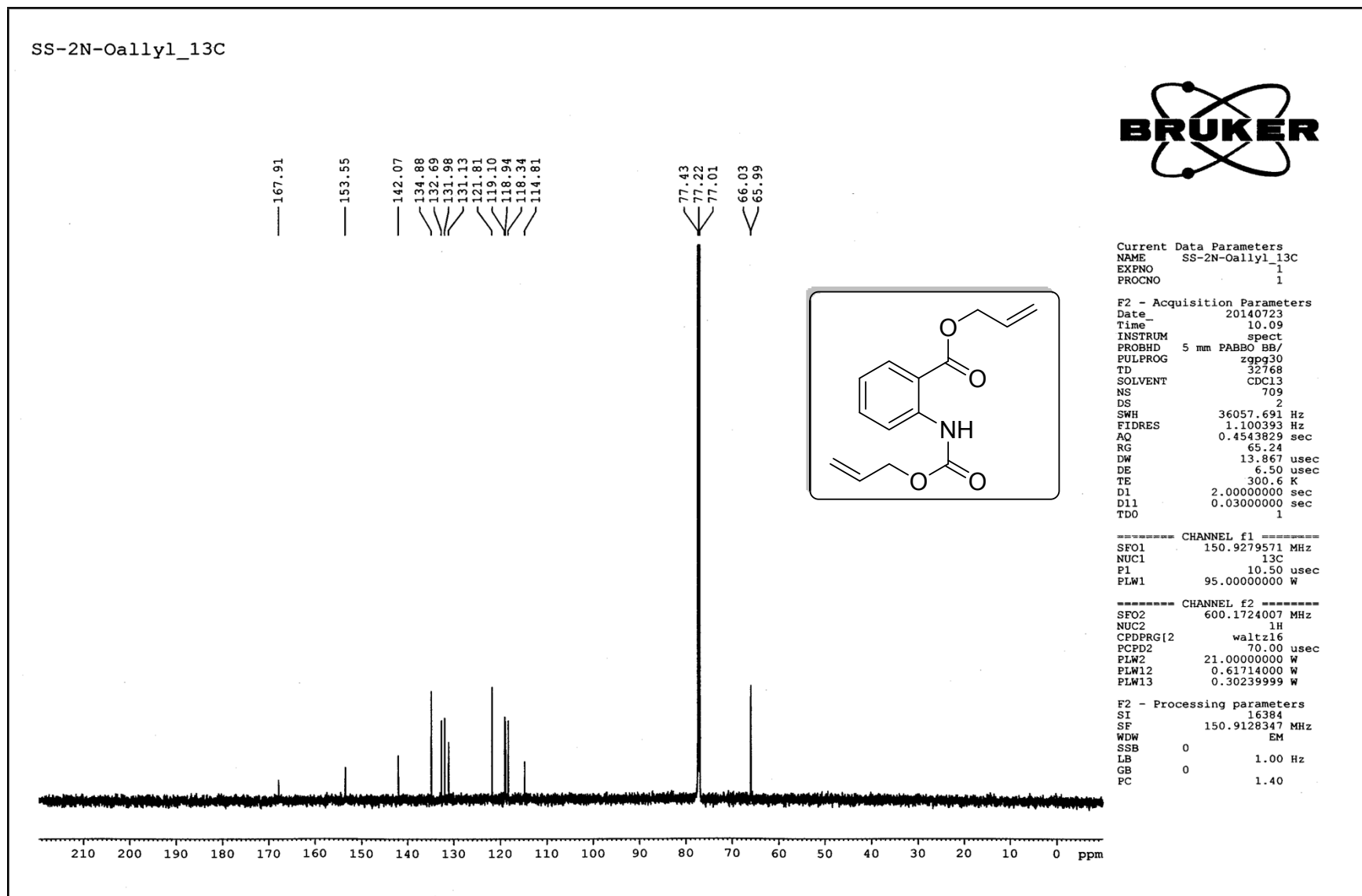
OBSERVE EL, 399:8509728

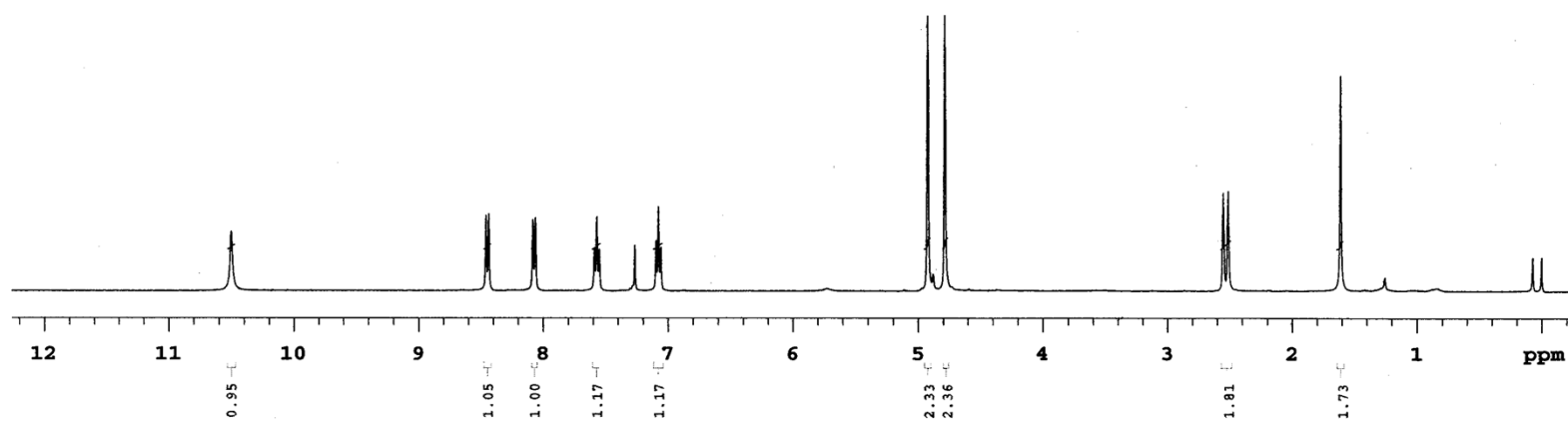
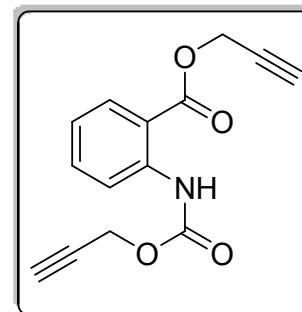
## DATA PROCESSING

FT size 32768  
Total time 1 minutes

SS-2NOAL-1-1H

Solvent: cdcl3  
Temp: 25.0 °C / 298.15 K  
Operator: chem  
Mercury-400 "IITG-NMR"

$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): 4h

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): **4i**

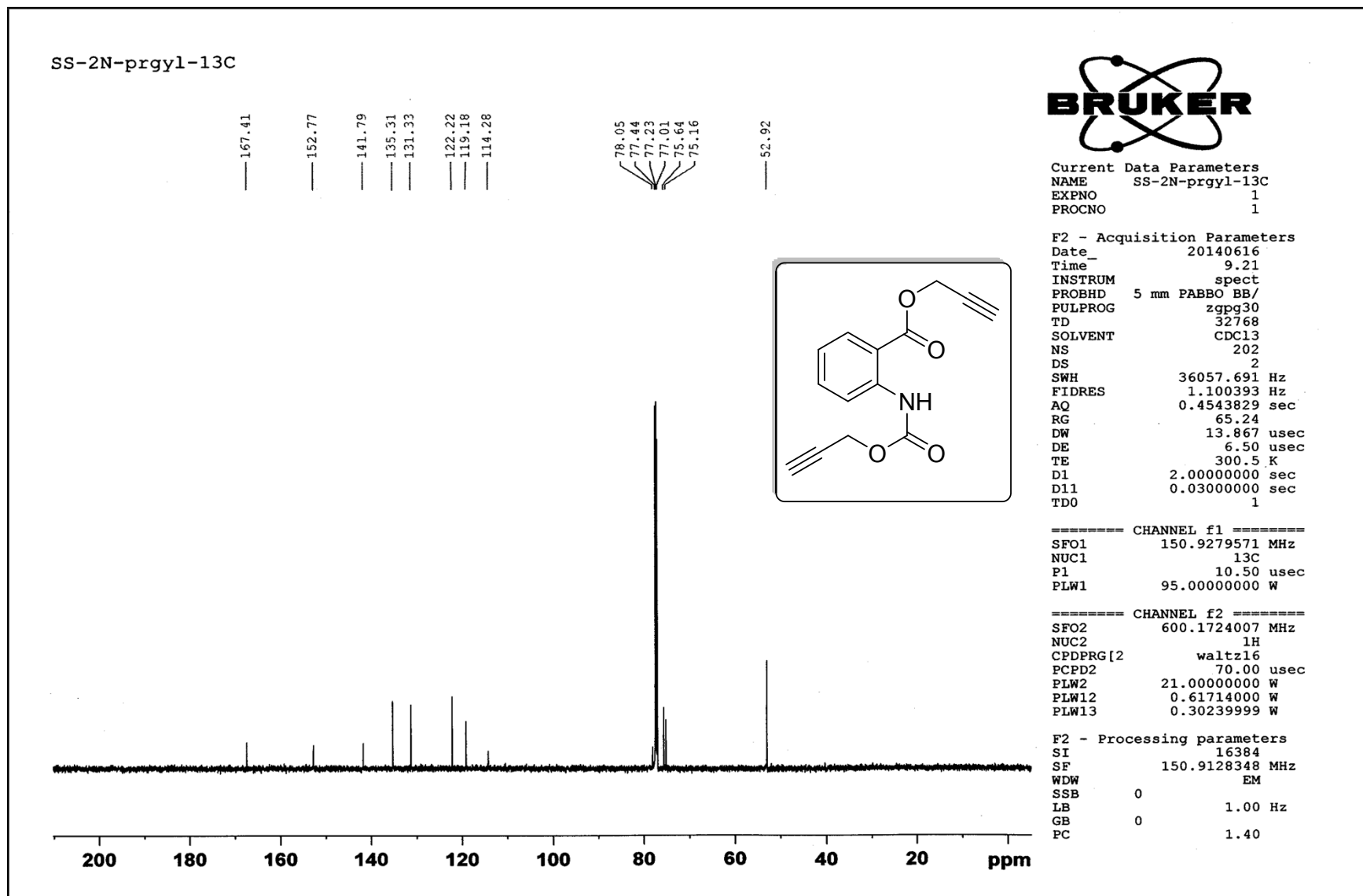
**PULSE SEQUENCE**  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions

**OBSERVE :** RL, 399.8509566

**DATA PROCESSING**  
FT size 32768  
Total time 1 minutes

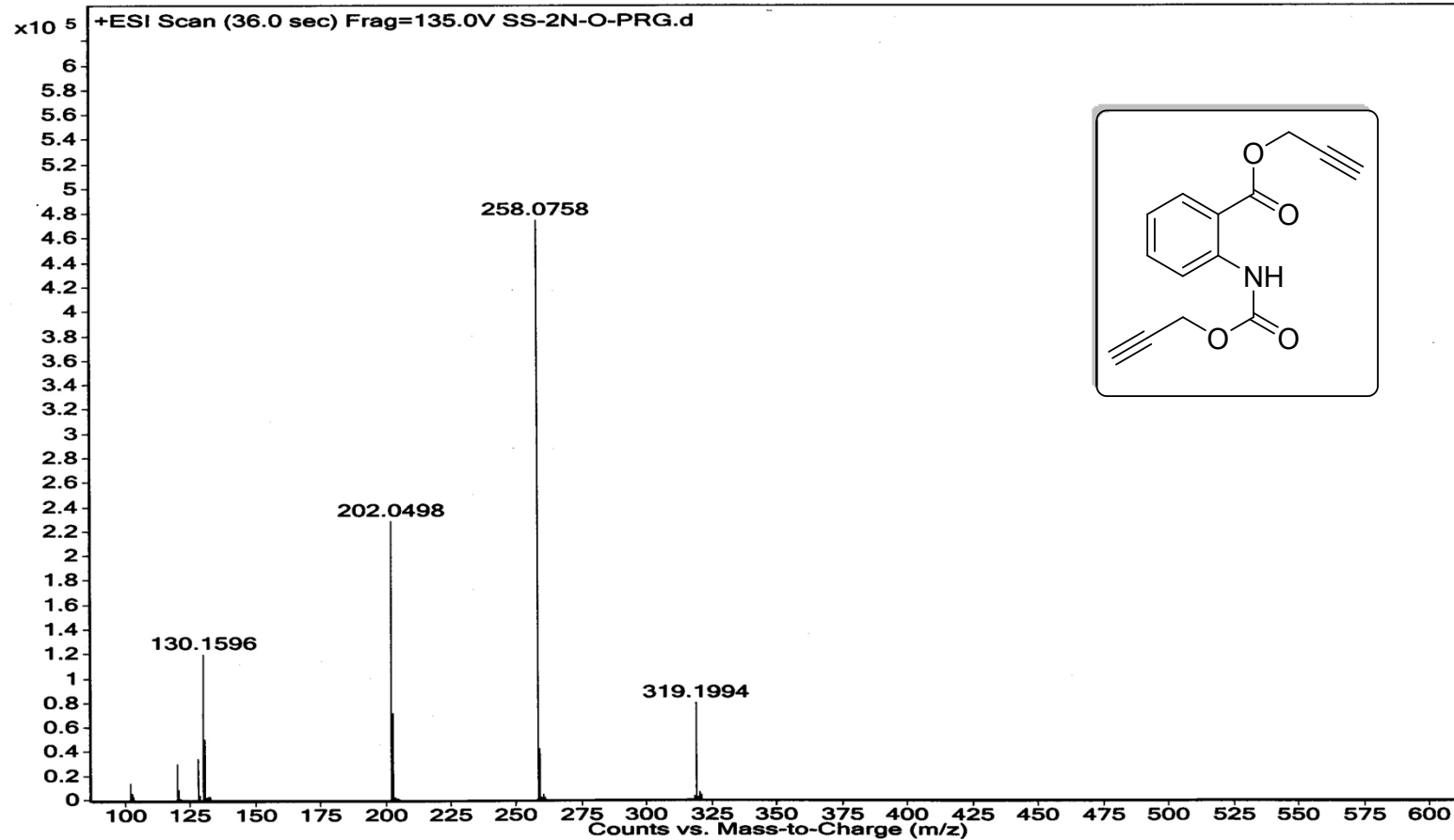
**SS-2N-PRgyl**

Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: chem  
File: SS-2N-PRgyl  
Mercury-400 "IITG-NMR"

<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): **4i**

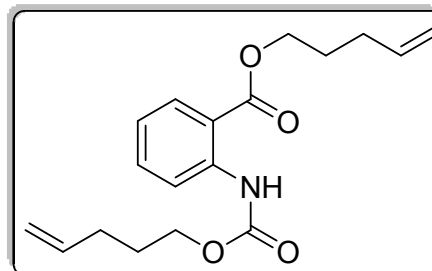
## Mass Spectra: 4i

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): 4j

SS-2N-Ptol\_1H

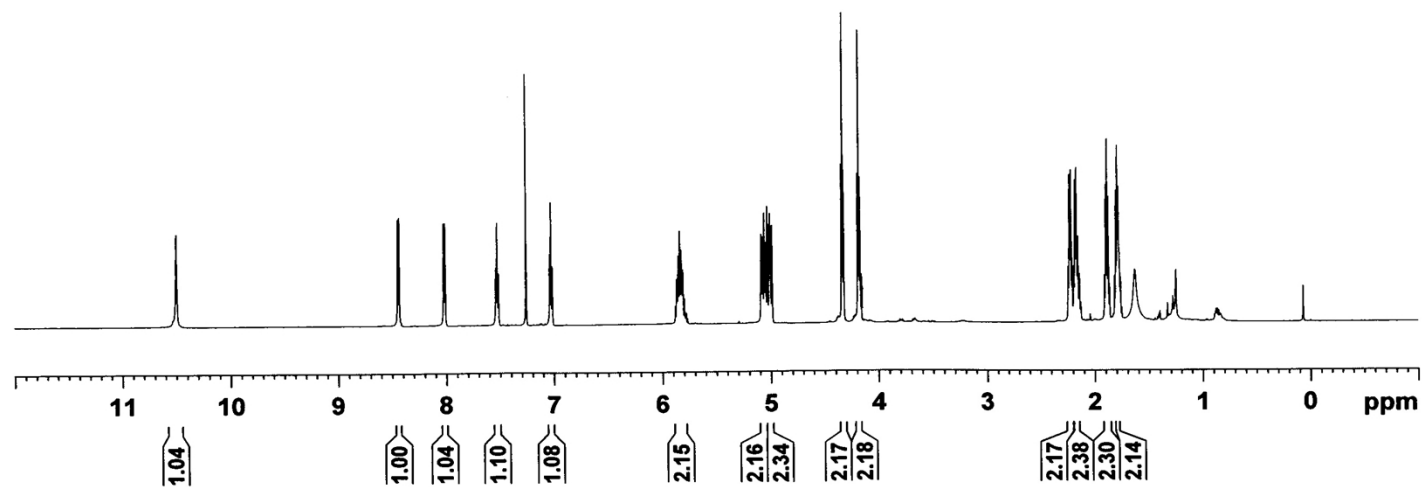


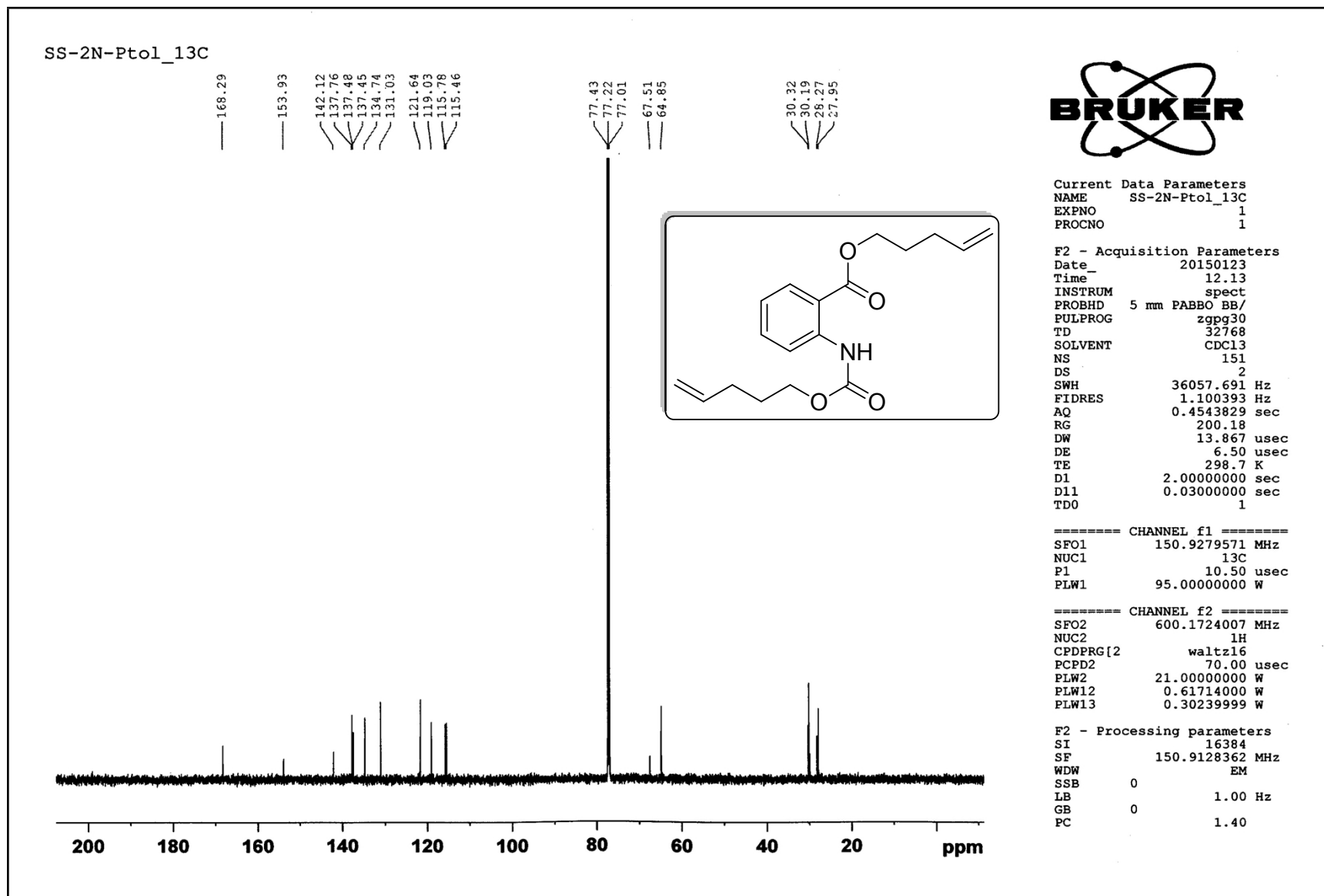
```
Current Data Parameters
NAME      SS-2N-Ptol_1H
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20150123
Time      12.10
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD        32768
SOLVENT   CDCl3
NS        16
DS        2
SWH       12019.230 Hz
FIDRES    0.366798 Hz
AQ        1.3631488 sec
RG        89.67
DW        41.600 usec
DE        6.50 usec
TE        298.2 K
D1        1.00000000 sec
TDO       1

----- CHANNEL f1 -----
SFO1      600.1720895 MHz
NUC1      1H
P1        12.00 usec
PLW1      21.00000000 W

F2 - Processing parameters
SI        16384
SF        600.1700141 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
```

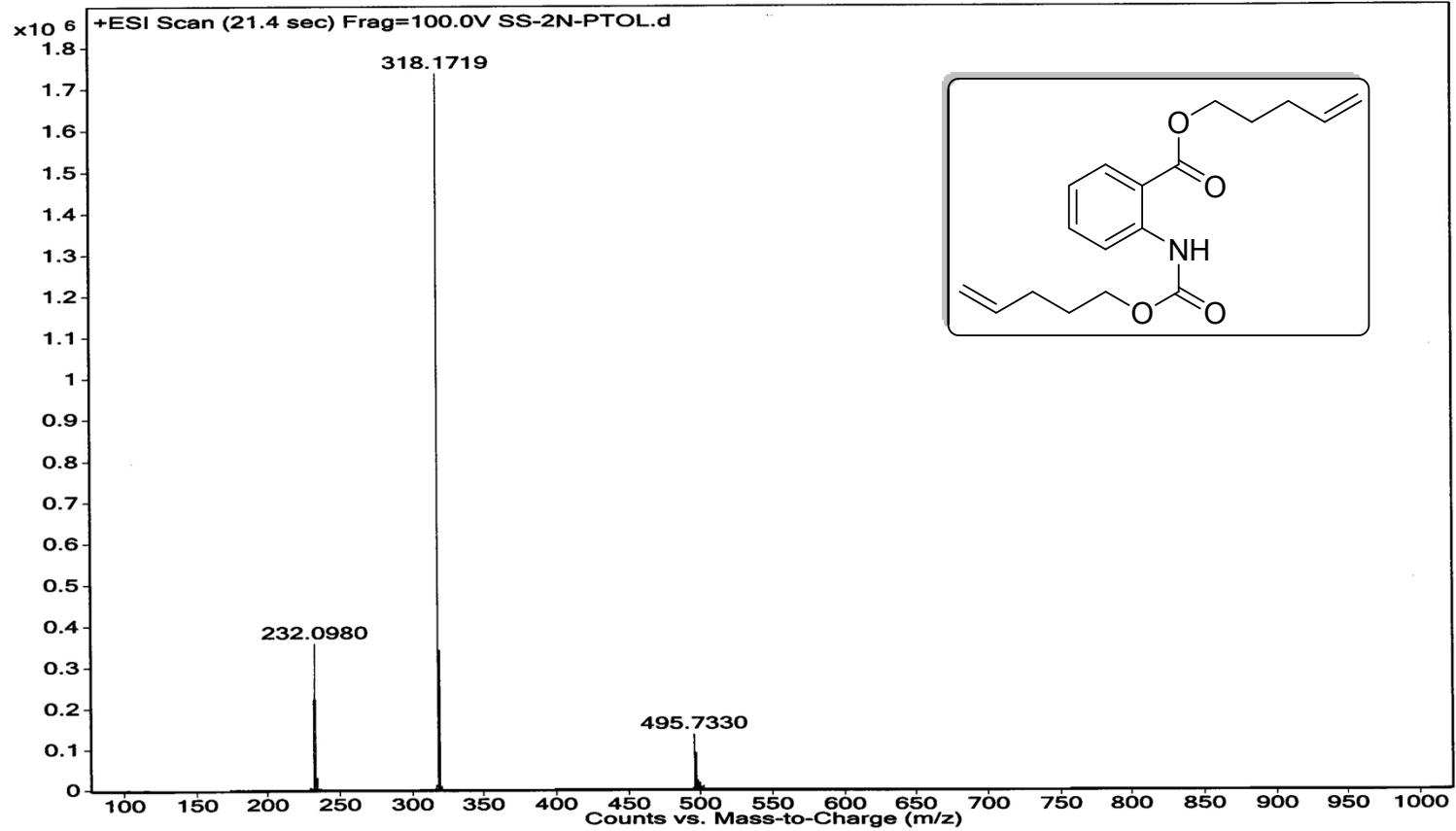


$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): 4j



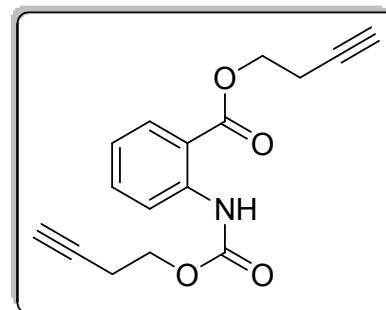
## Mass Spectra: 4j

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): **4k**

SS\_2N\_But\_YN\_1H



```

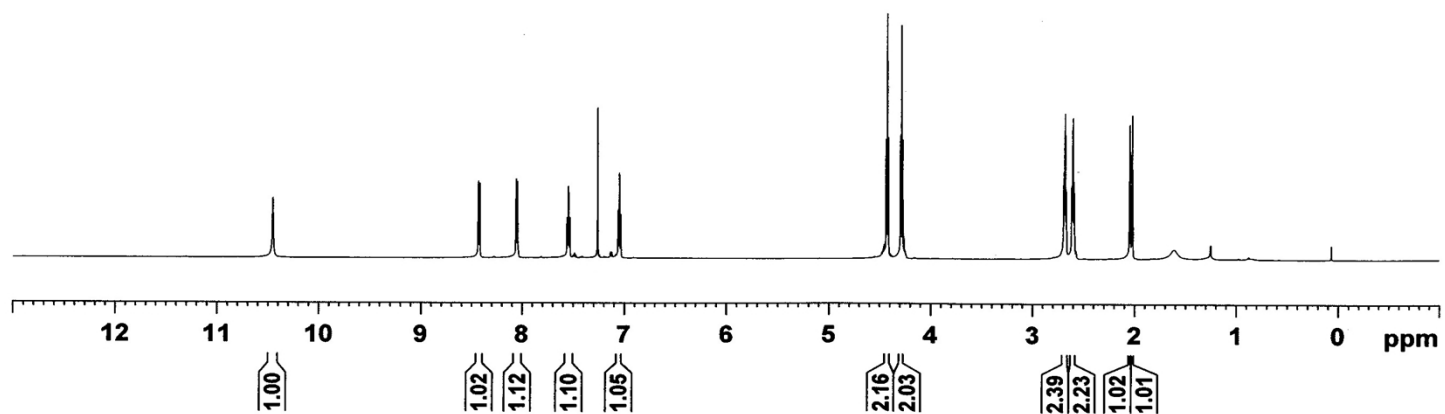
Current Data Parameters
NAME      SS_2N_But_YN_1H
EXPNO     1
PROCNO    1

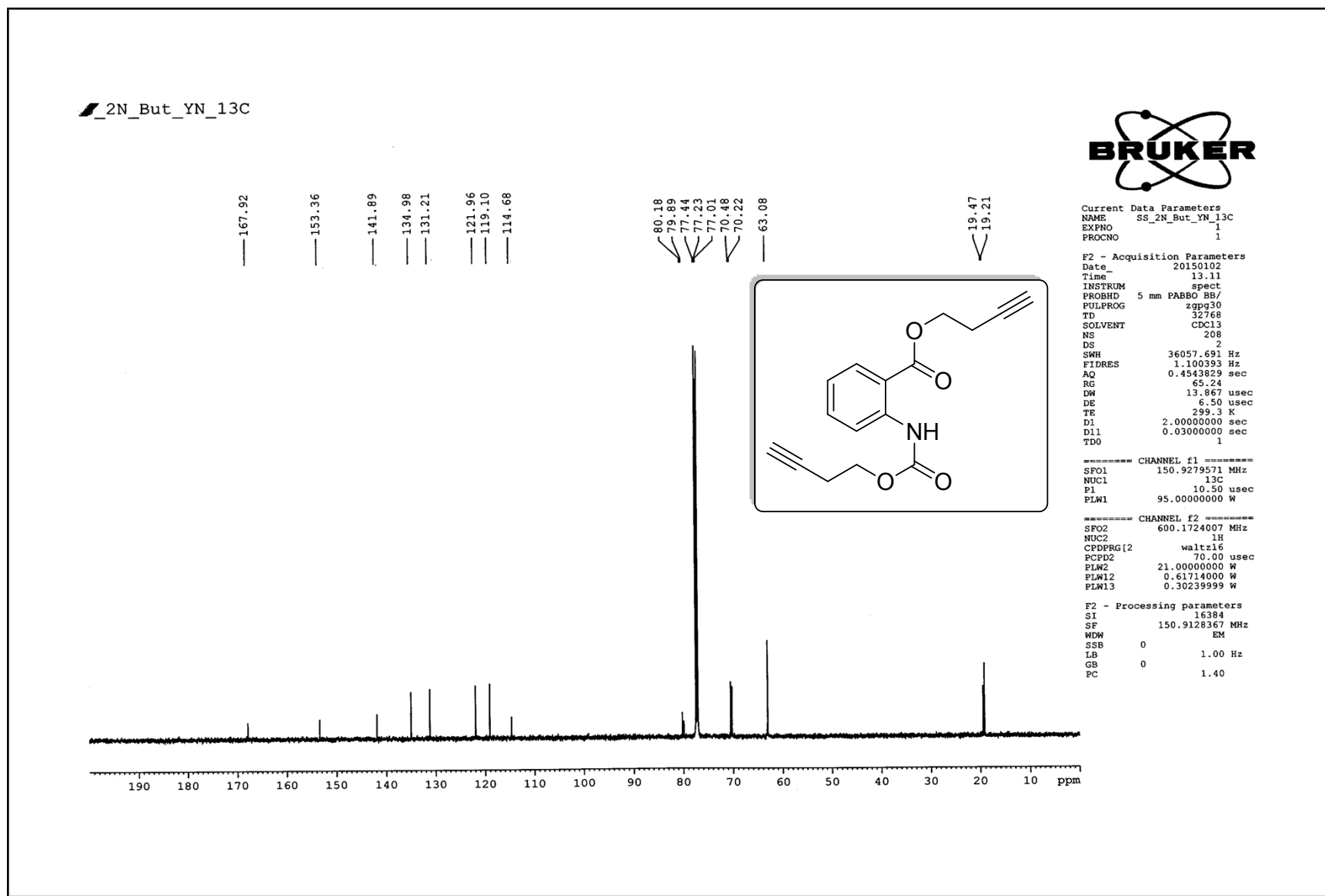
F2 - Acquisition Parameters
Date_     20150102
Time      13.06
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH       12019.230 Hz
FIDRES    0.366798 Hz
AQ         1.3631488 sec
RG         89.67
DW         41.600 usec
DE         6.50 usec
TE         298.2 K
D1         1.0000000 sec
TDO        1

===== CHANNEL f1 =====
SFO1      600.1737063 MHz
NUC1       1H
P1         12.00 usec
PLW1       21.0000000 W

F2 - Processing parameters
SI         16384
SF         600.1700148 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

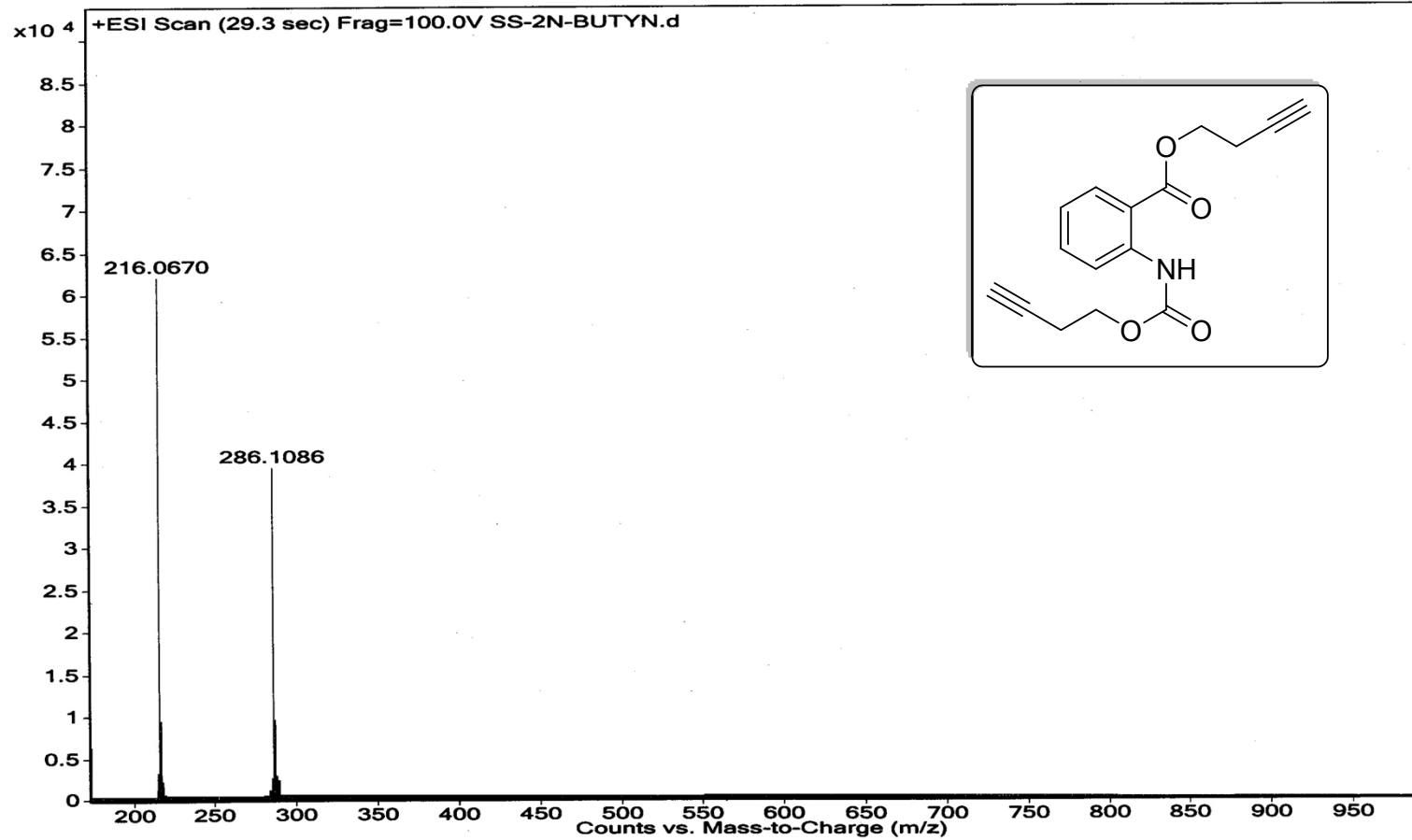
```



$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): 4k

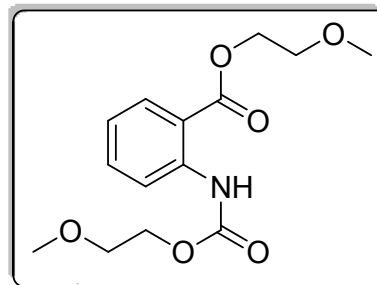
## Mass Spectra: 4k

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): 4I

SS-2N-OET-OMe\_1H

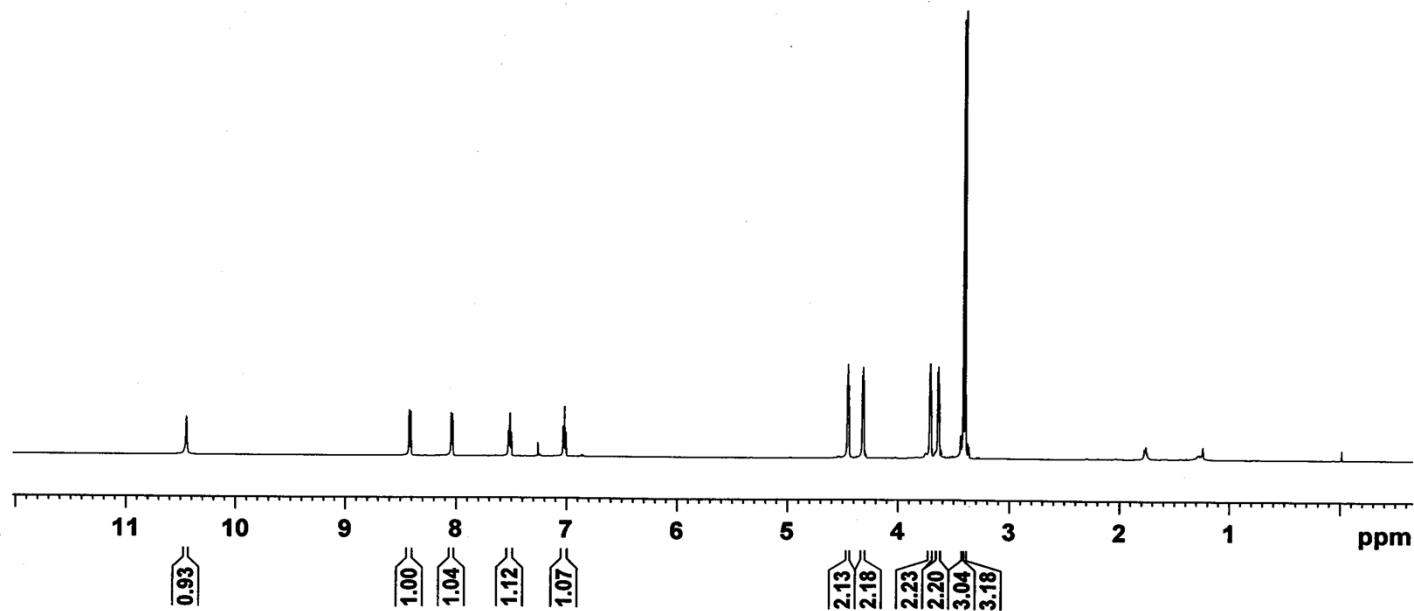


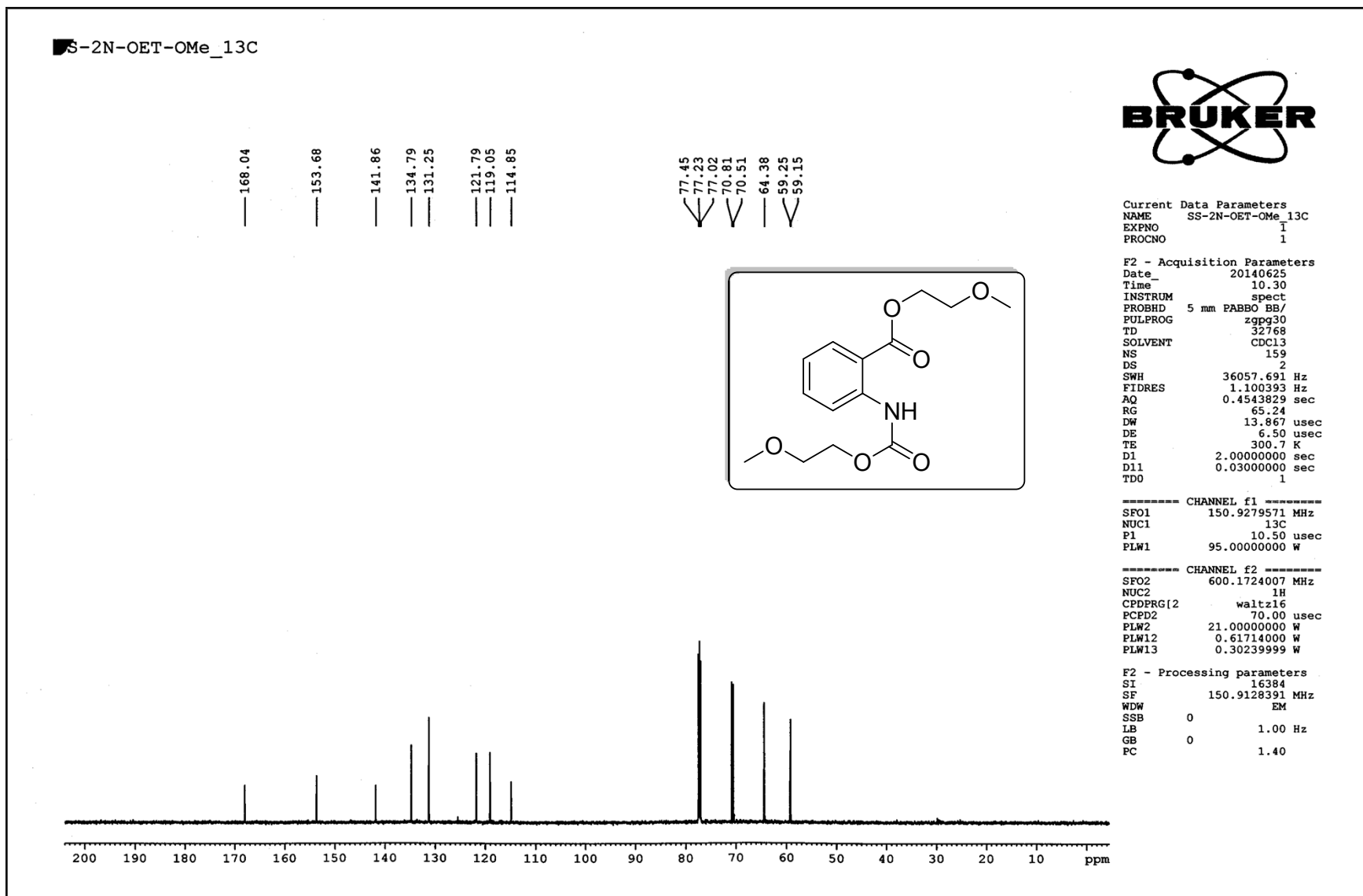
Current Data Parameters  
NAME SS-2N-OET-OMe\_1H  
EXNO 1  
PRCNO 1

F2 - Acquisition Parameters  
Date\_ 20140625  
Time 10.21  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 27.82  
DW 41.600 usec  
DE 6.50 usec  
TE 299.7 K  
D1 1.00000000 sec  
TDO 1

----- CHANNEL f1 -----  
SFO1 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

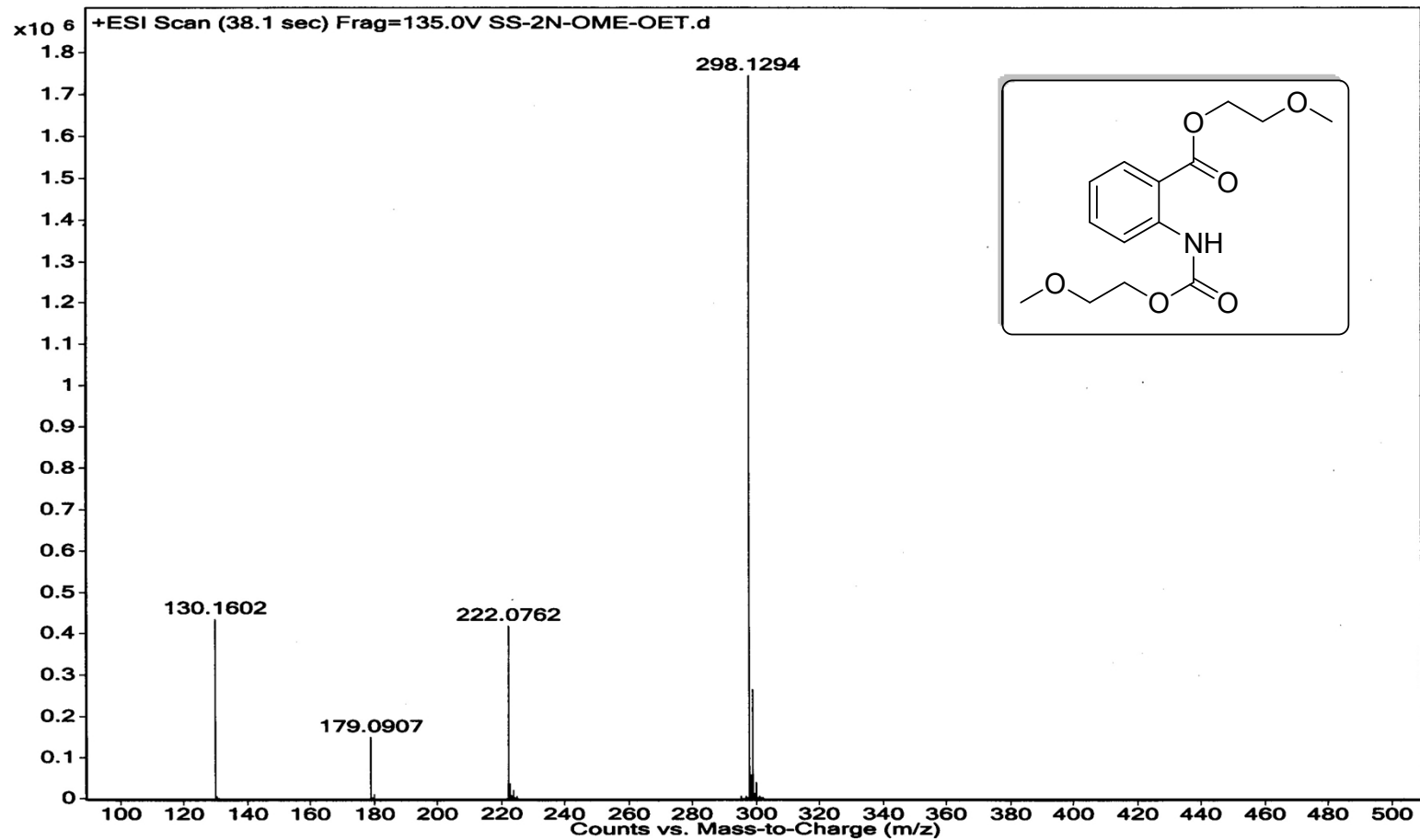
F2 - Processing parameters  
SI 16384  
SF 600.1700148 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
FC 1.00



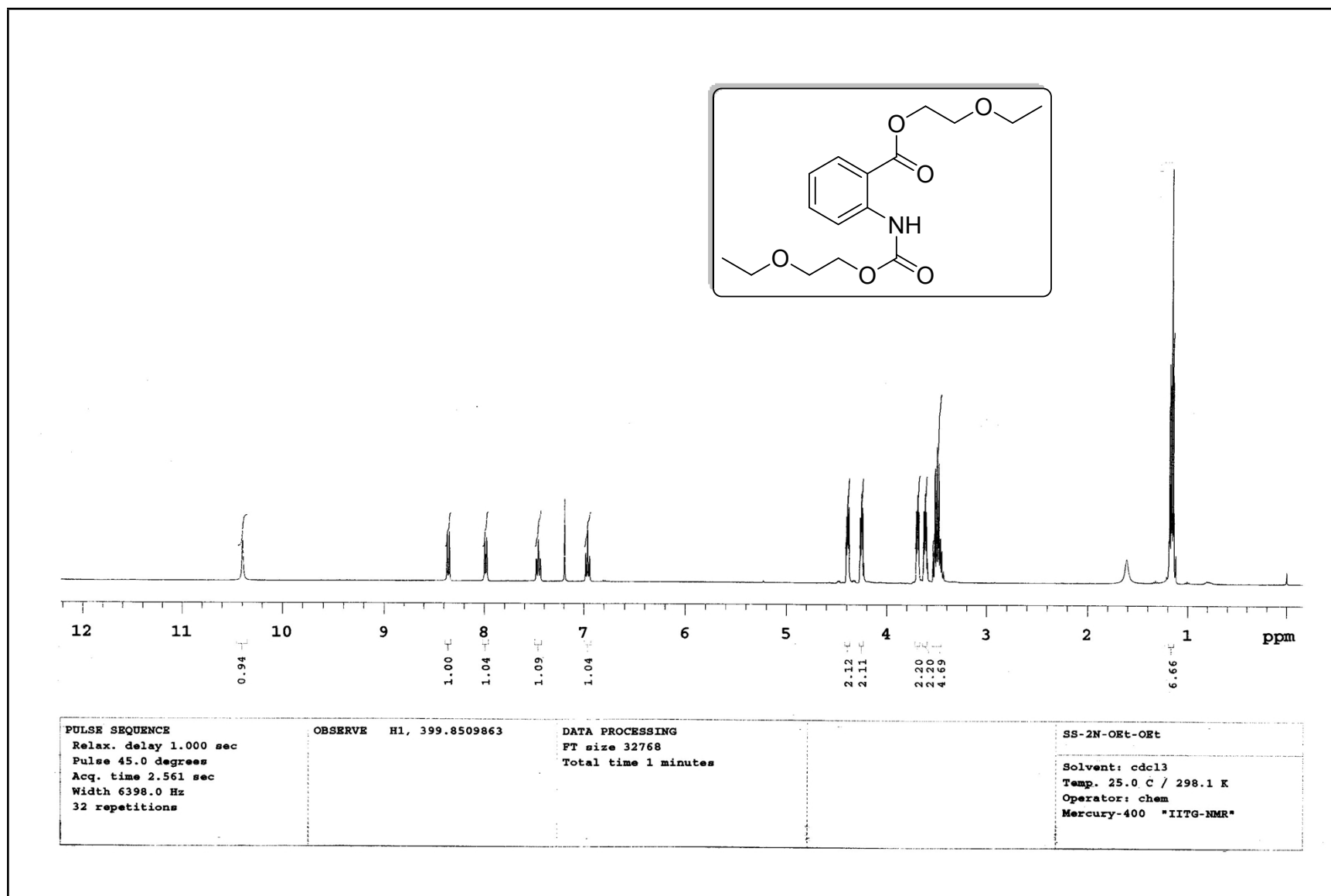
<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): 41

## Mass Spectra: 41

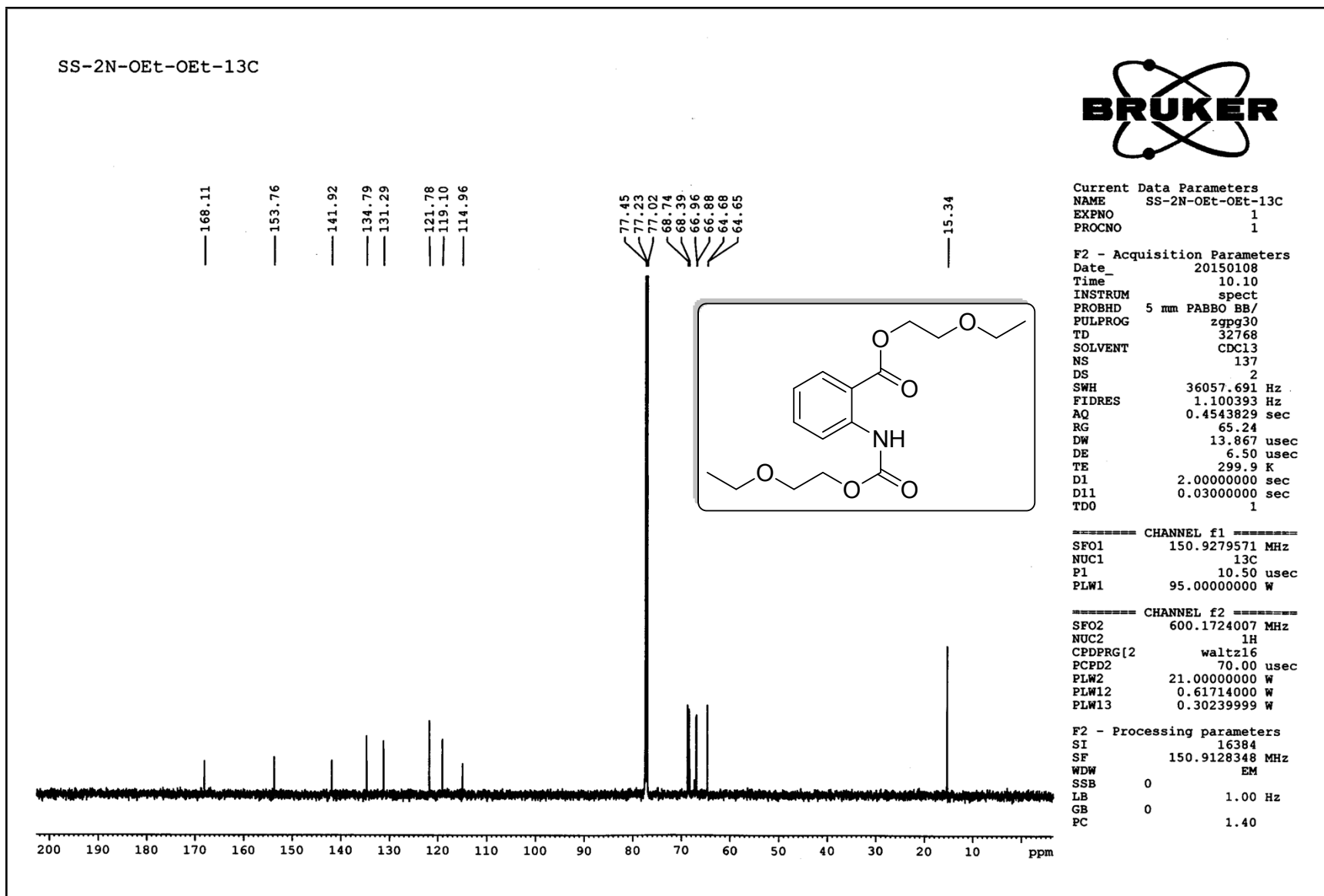
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): 4m

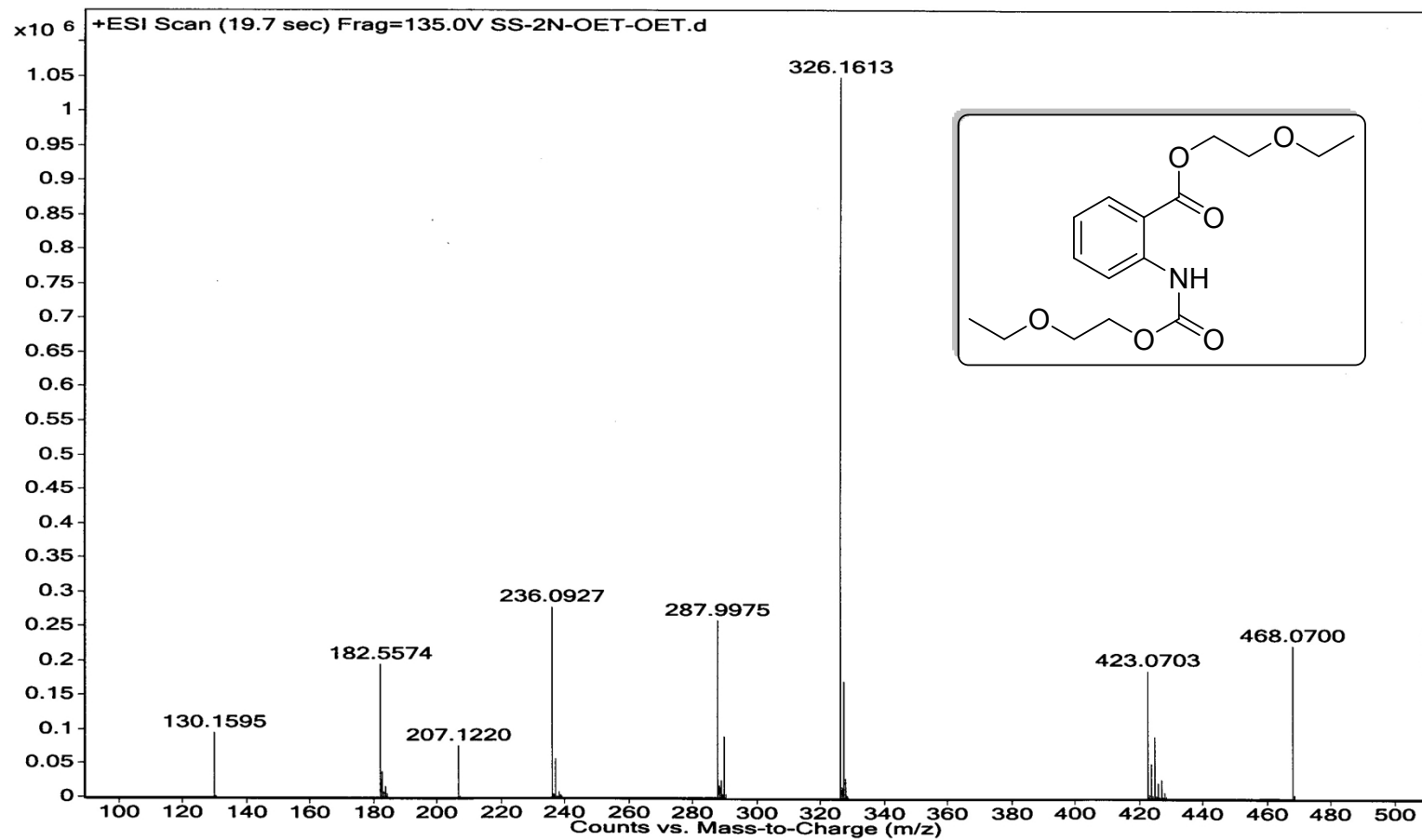




$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): 4m

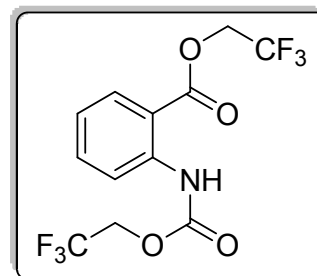
## Mass Spectra: 4m

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): **4n**

SS-2N-CF3-1H

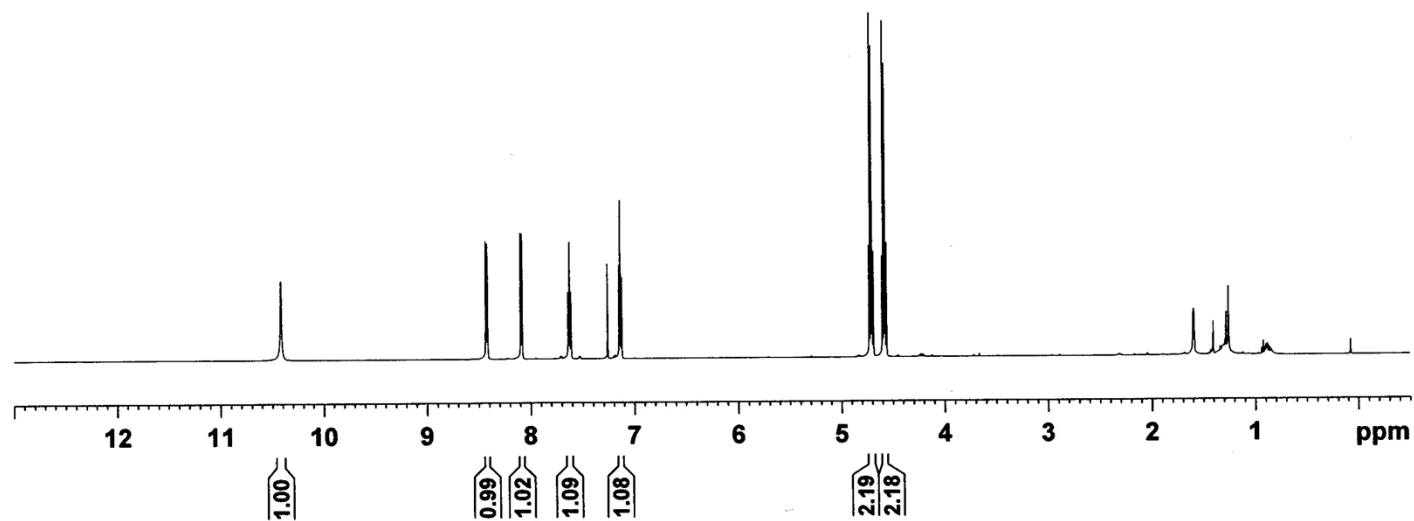


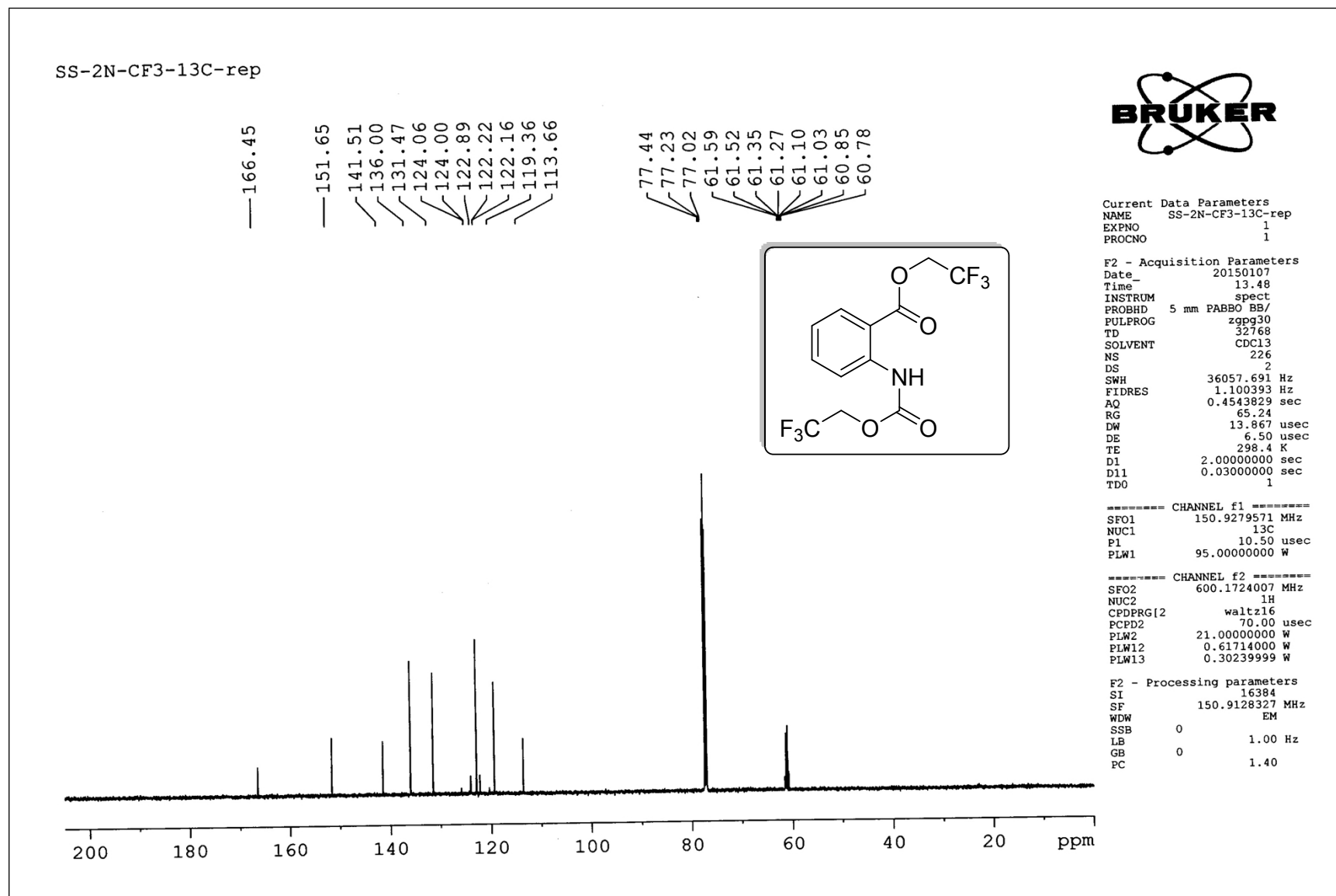
```
Current Data Parameters
NAME      SS-2N-CF3-1H
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20150107
Time      13.36
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        12019.230 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         43.16
DW         41.600 usec
DE         6.50 usec
TE         298.1 K
D1         1.0000000 sec
TDO        1

----- CHANNEL f1 -----
SFO1      600.1737063 MHz
NUC1       1H
P1         12.00 usec
PLW1       21.00000000 W

F2 - Processing parameters
SI         16384
SF         600.1700148 MHz
WDW        EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00
```



$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): **4n**

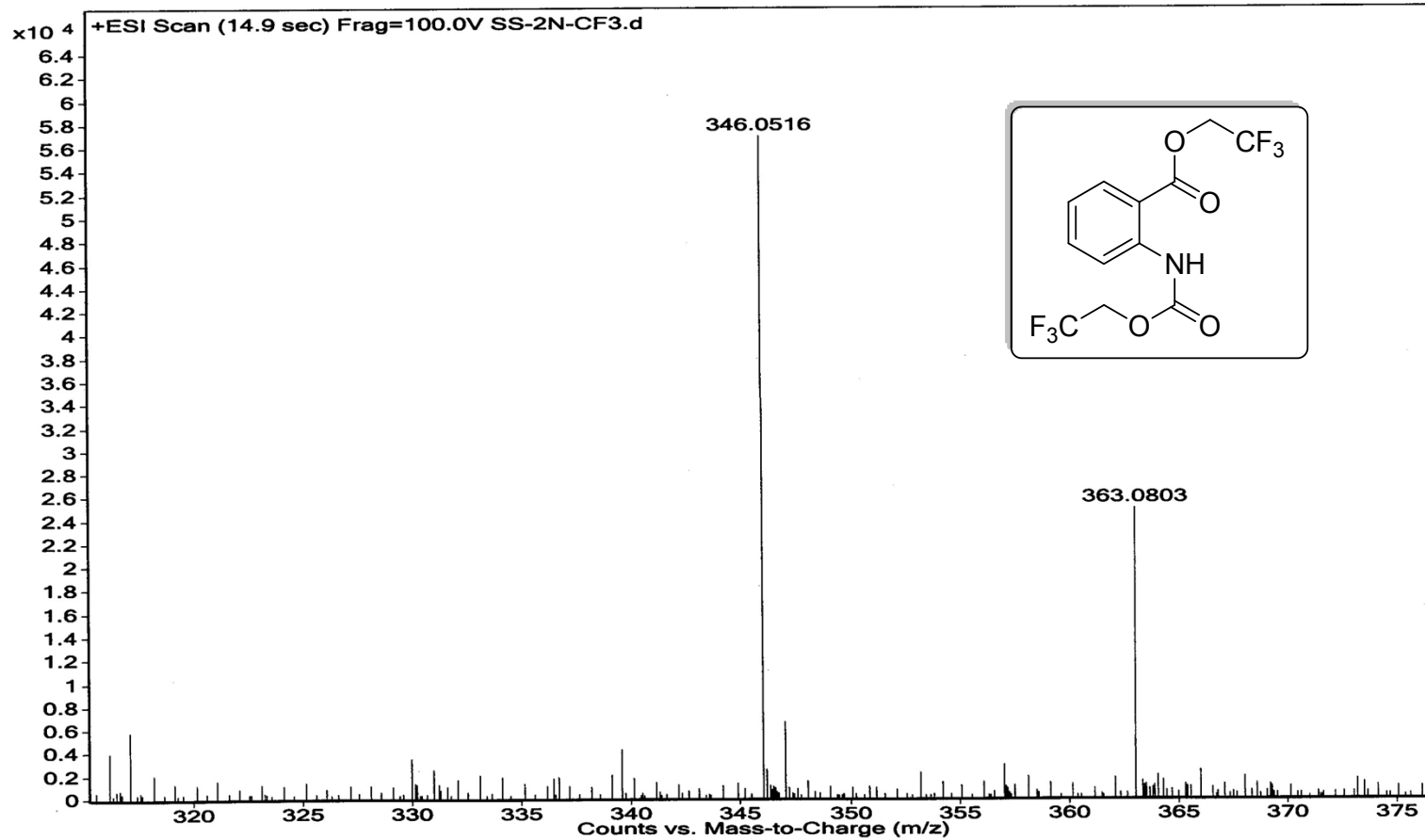
## Mass Spectra: 4n

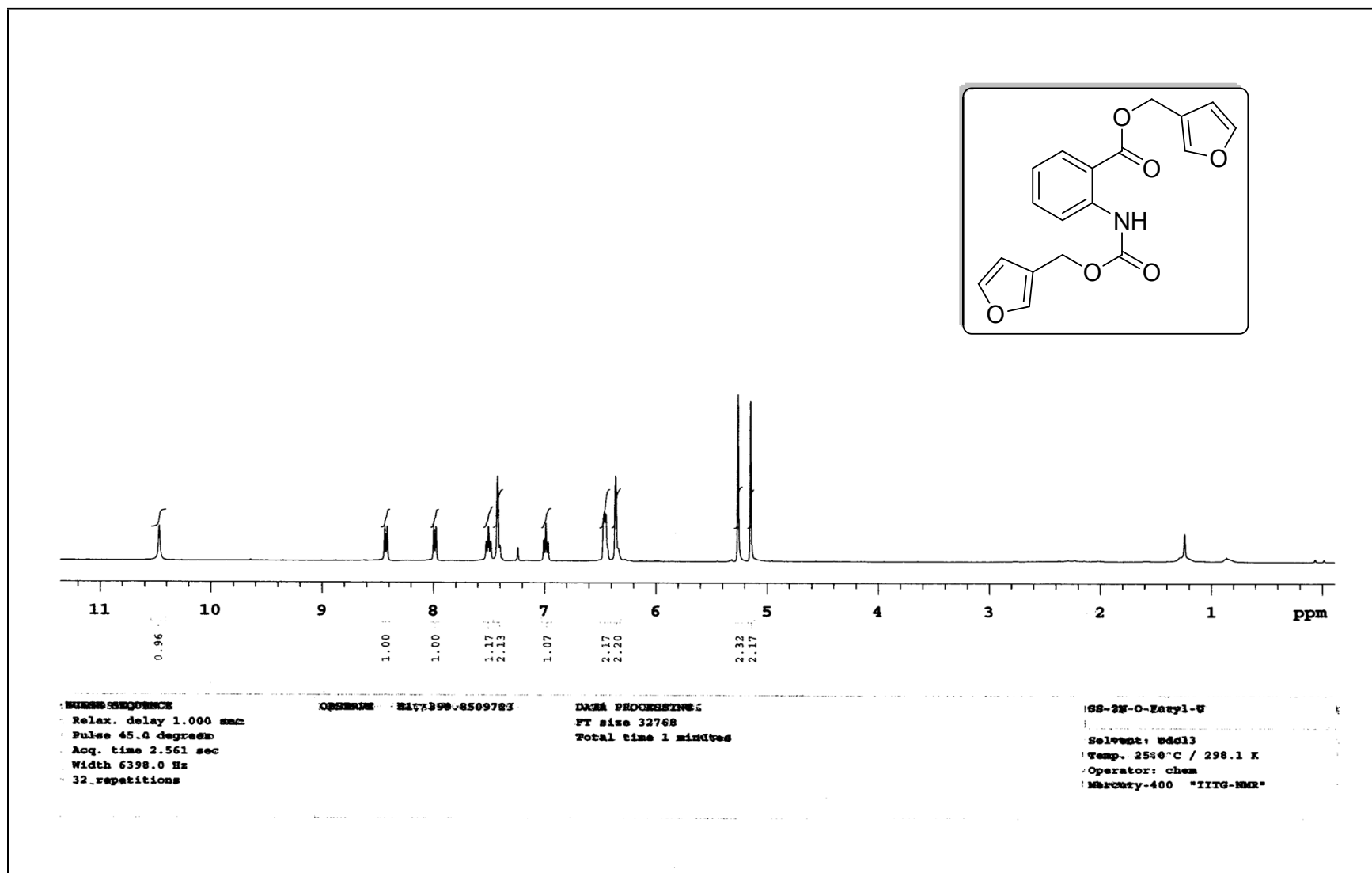
Sample Name  
Inj Vol  
Data Filename

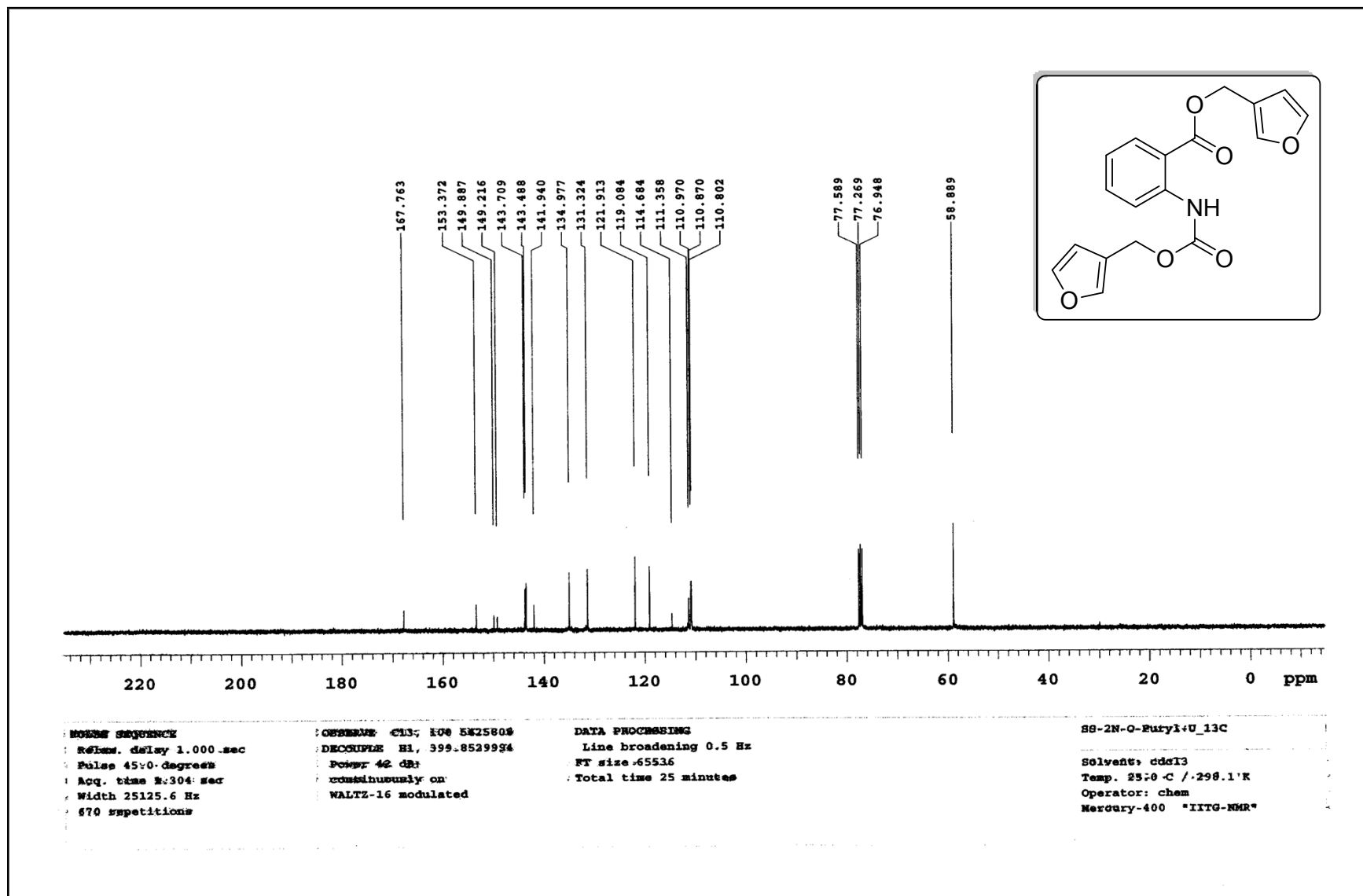
Position  
InjPosition  
ACQ Method

Instrument Name  
SampleType  
Comment

User Name  
IRM Calibration Status  
Acquired Time

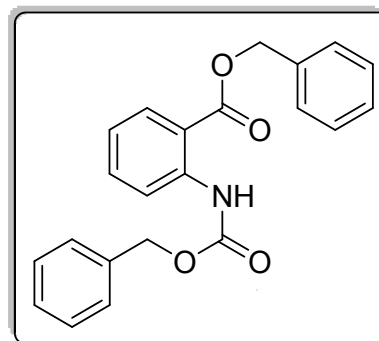


<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): **4o**

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 4o

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): **4p**

SS-2N-OC-Ph-1H

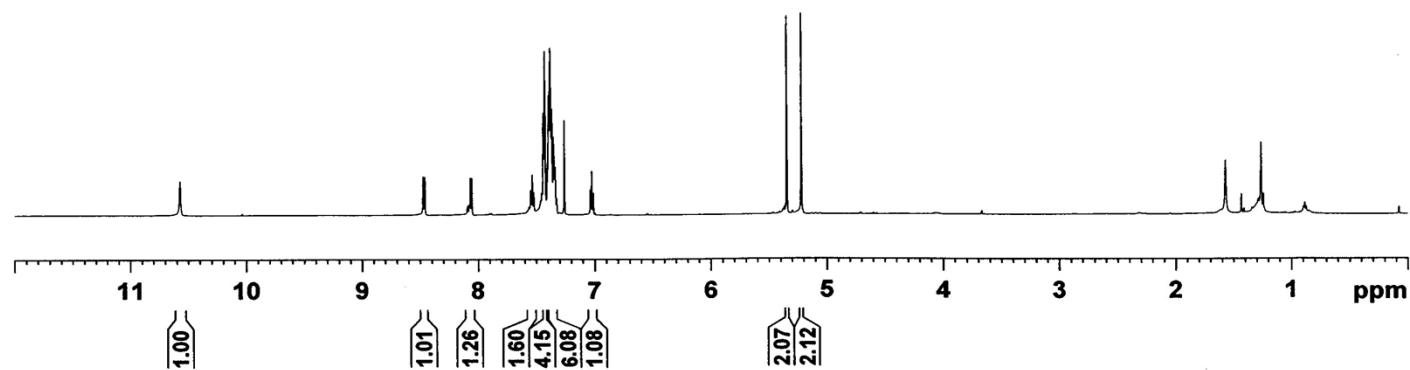


```
Current Data Parameters
NAME      SS-2N-OC-Ph-1H
EXPNO     1
PROCNO    1

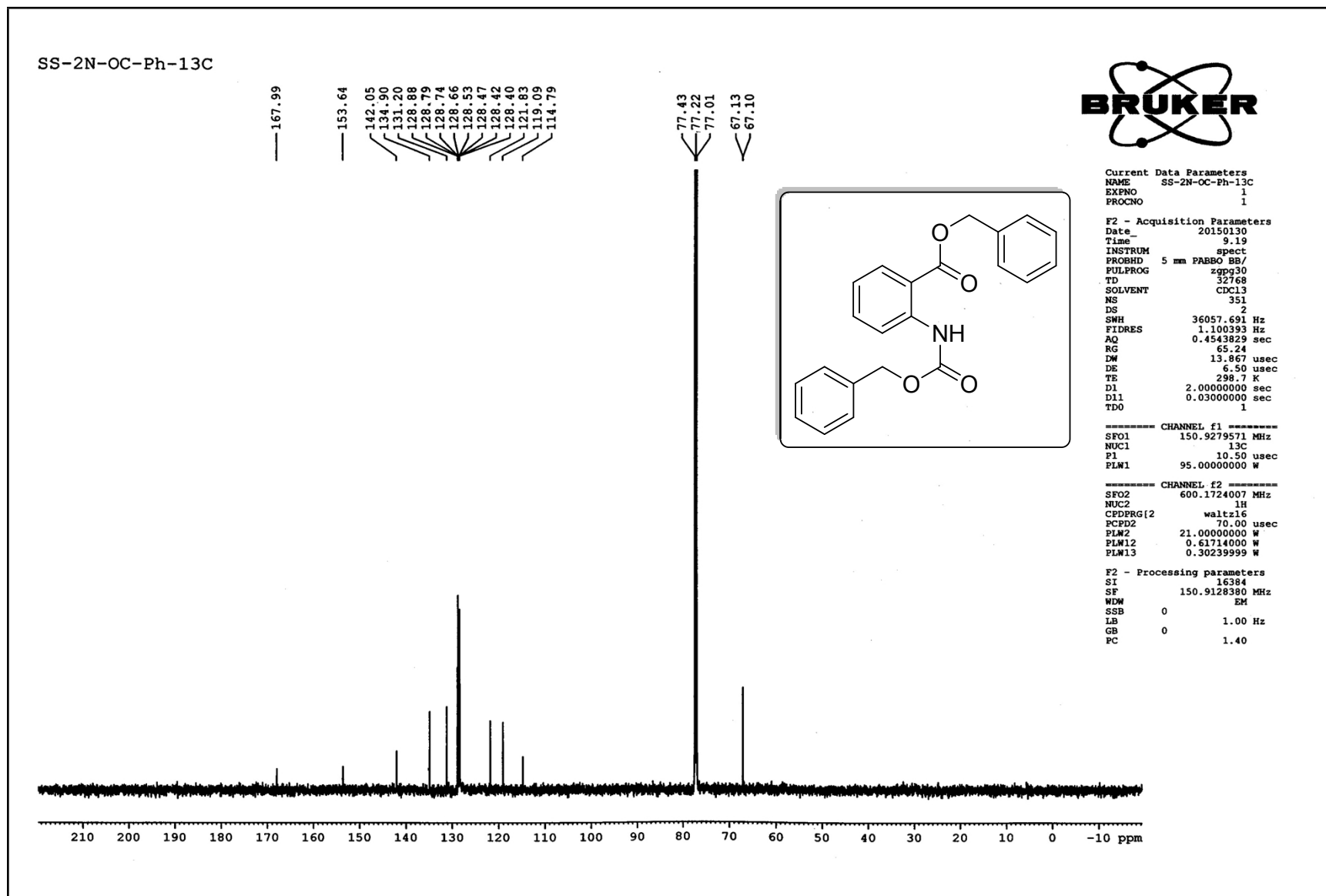
F2 - Acquisition Parameters
Date_     20150130
Time      9.16
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        12019.230 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         89.67
DW         41.600 usec
DE         6.50 usec
TE         298.1 K
D1         1.0000000 sec
TDO        1

===== CHANNEL f1 =====
SF01      600.1737063 MHz
NUC1       1H
P1         12.00 usec
PLW1      21.00000000 W

F2 - Processing parameters
SI         16384
SF         600.1700144 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

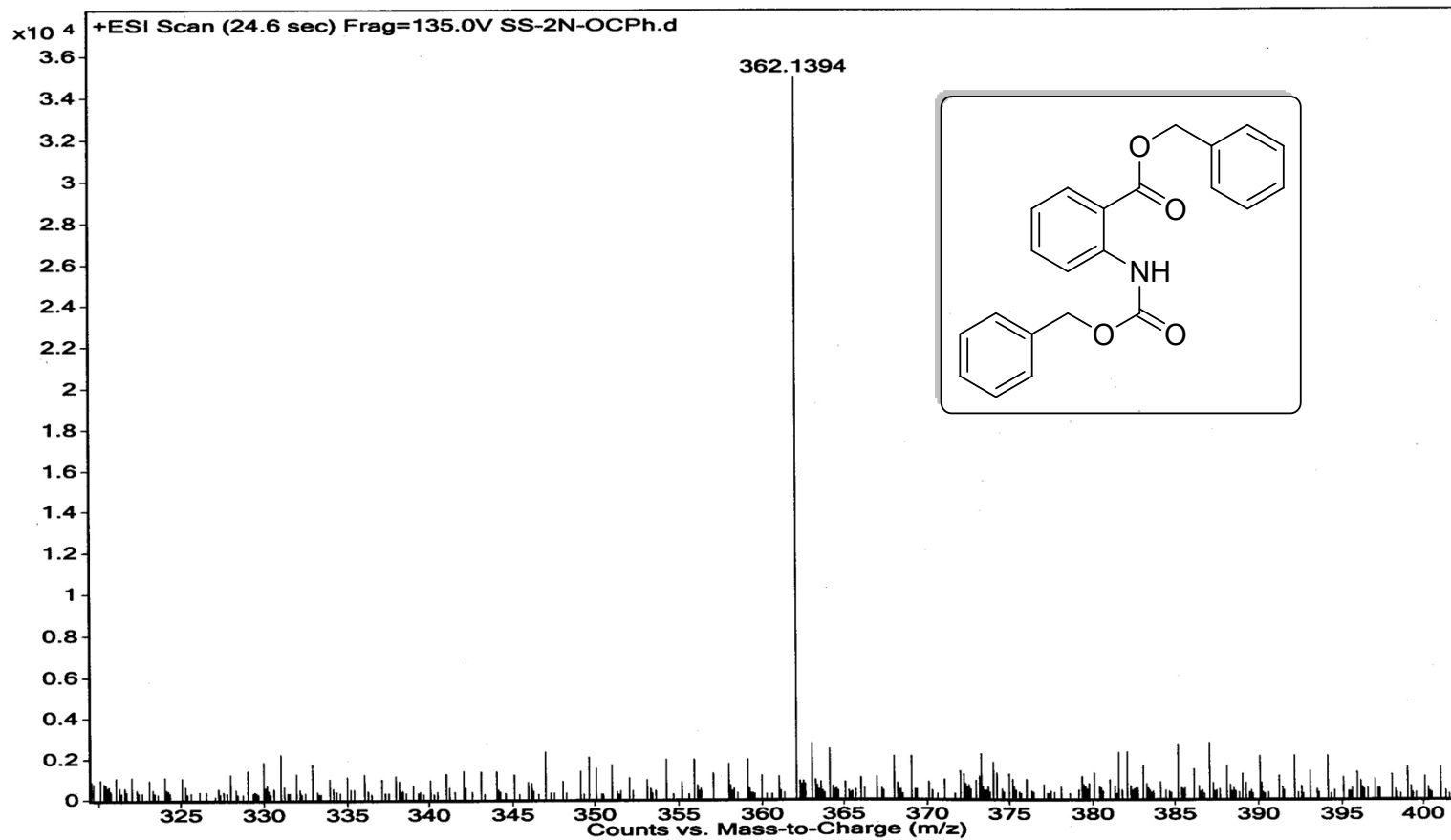


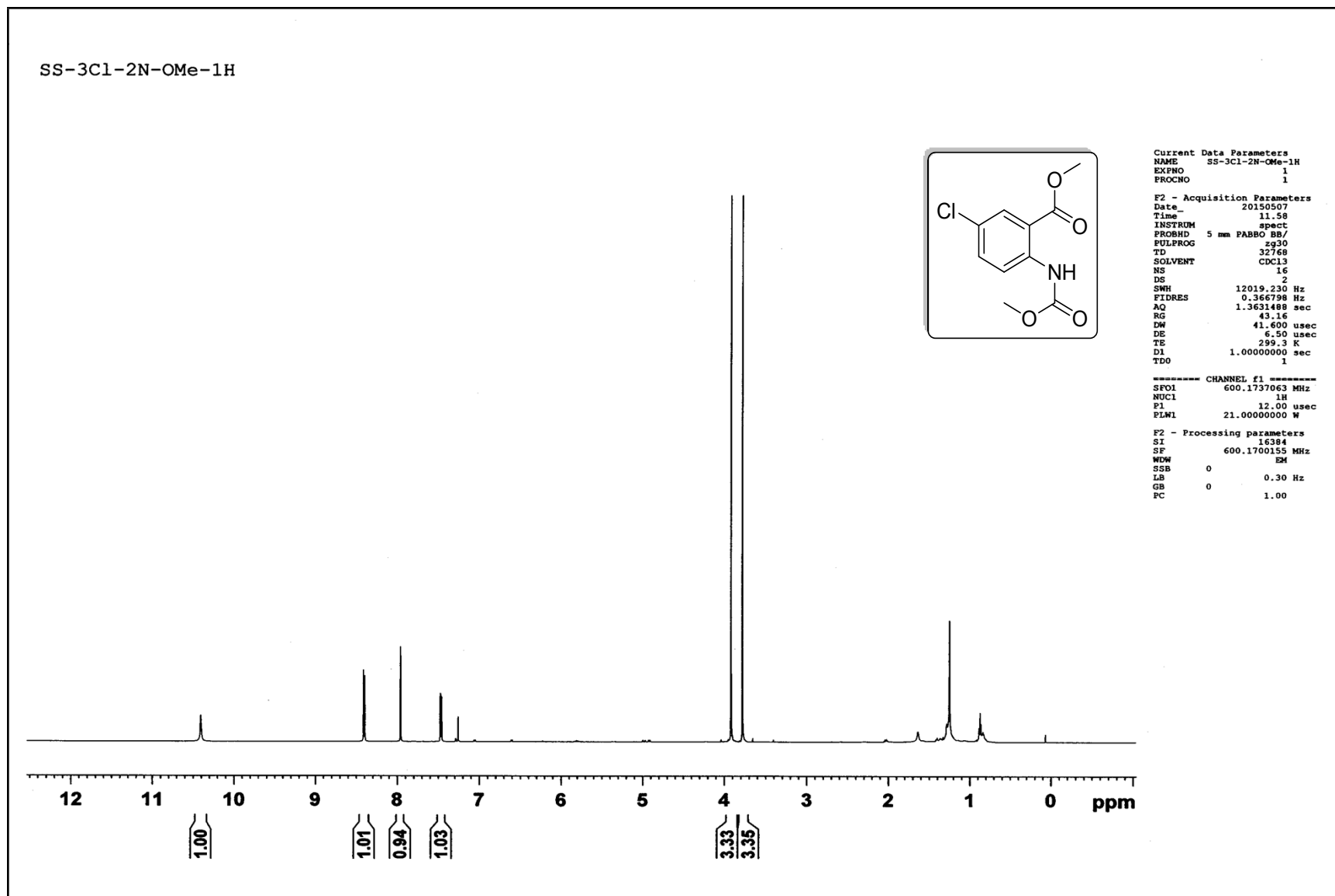


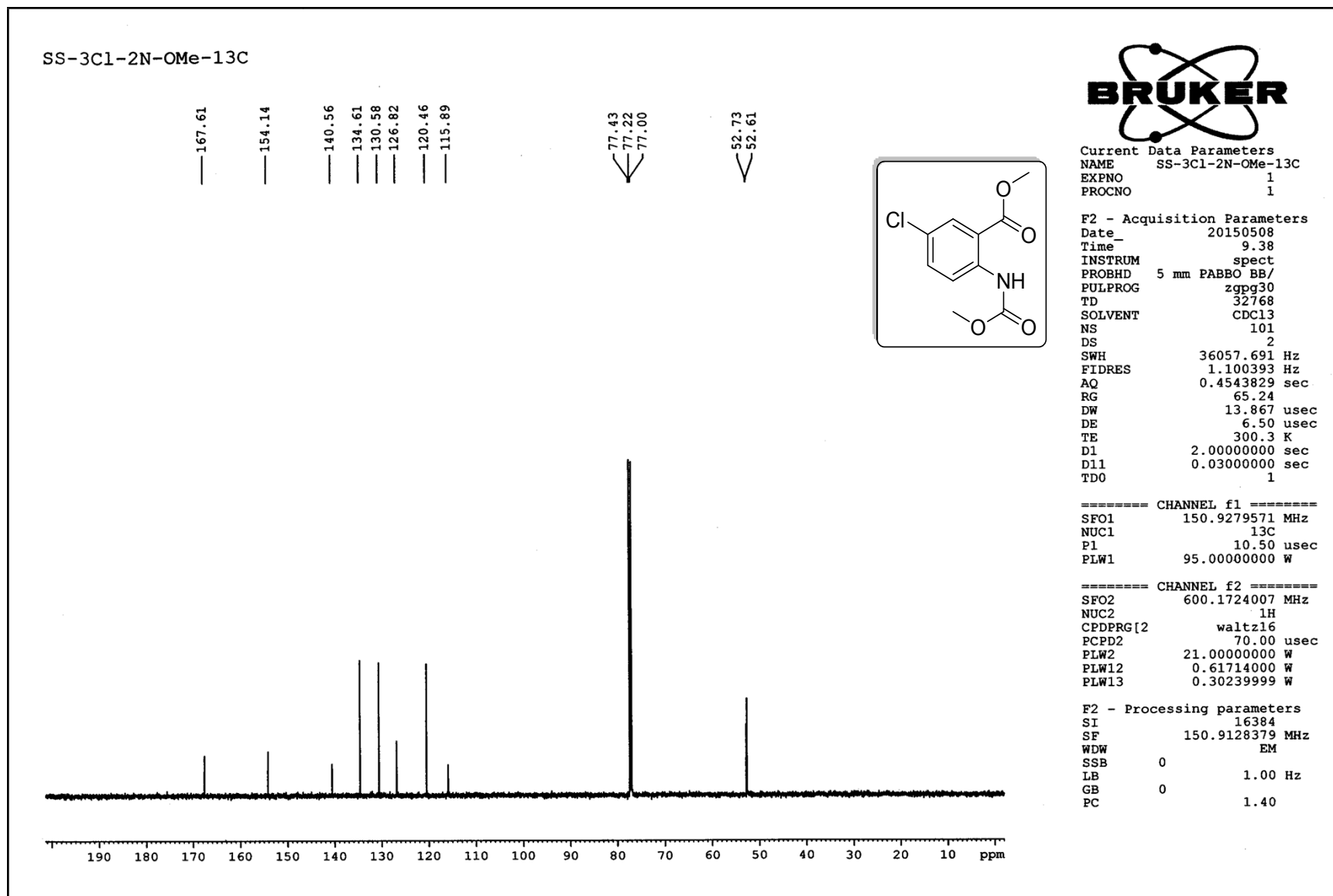
$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): 4p

## Mass Spectra: 4p

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time

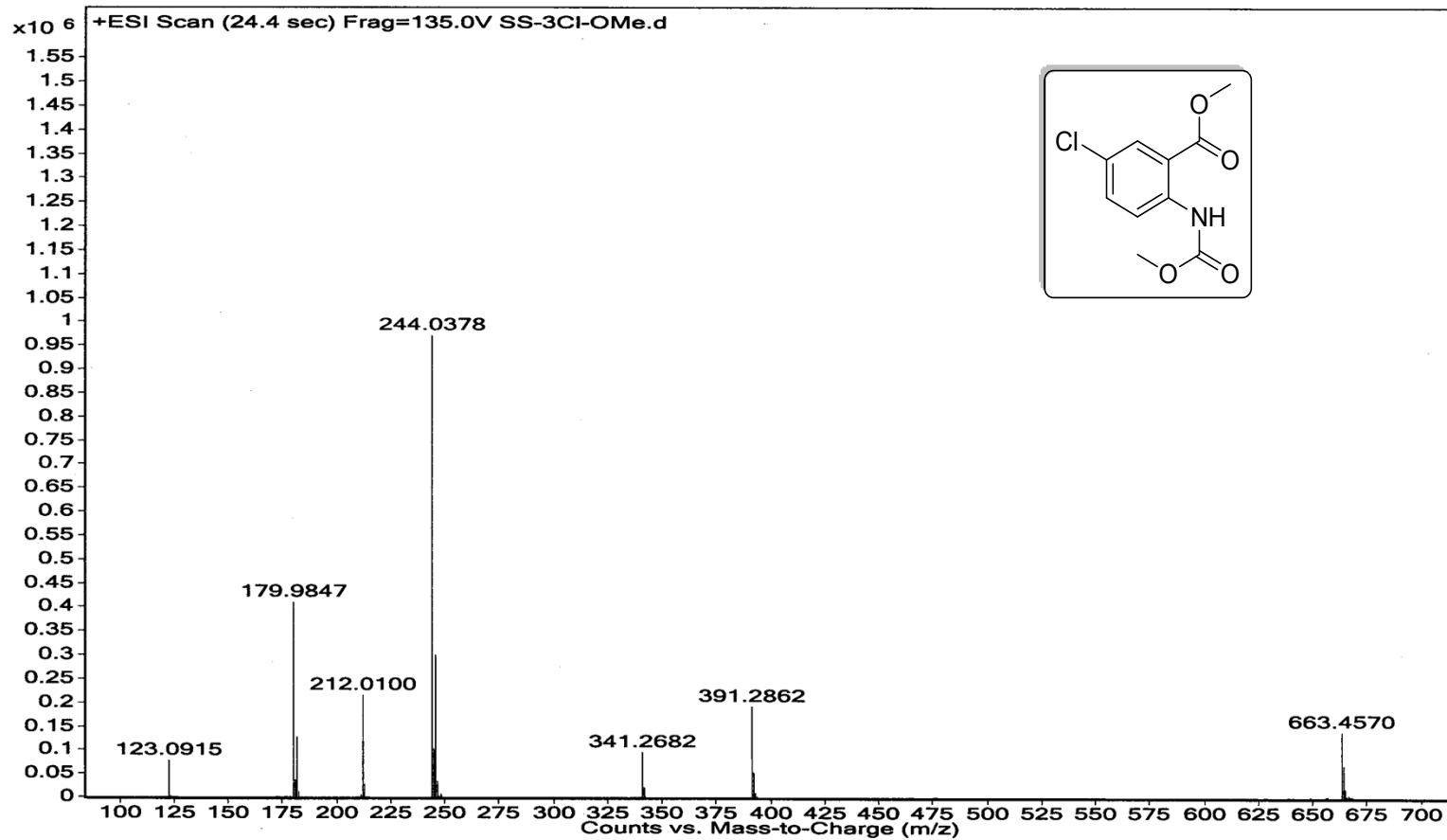


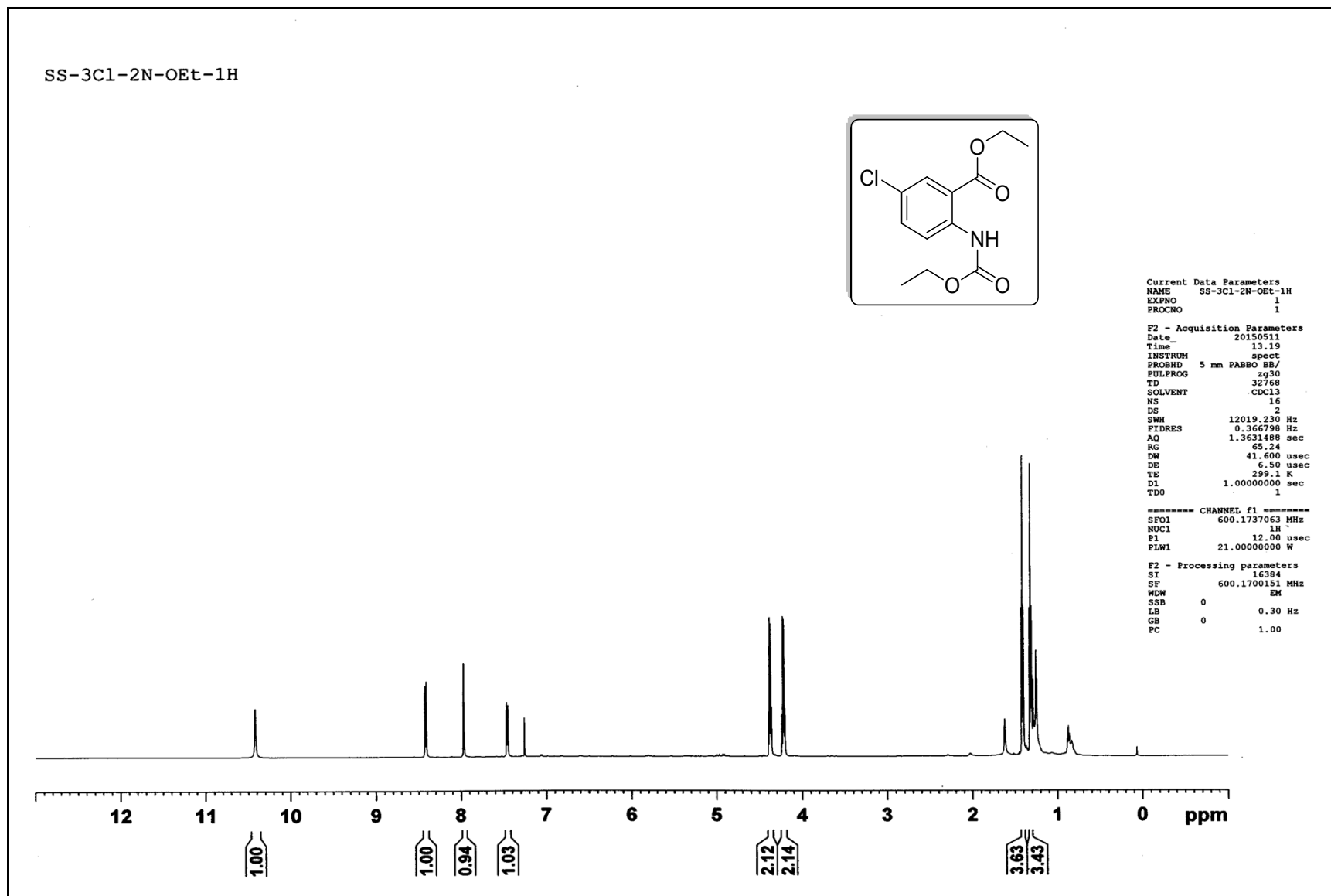
<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): **4q**

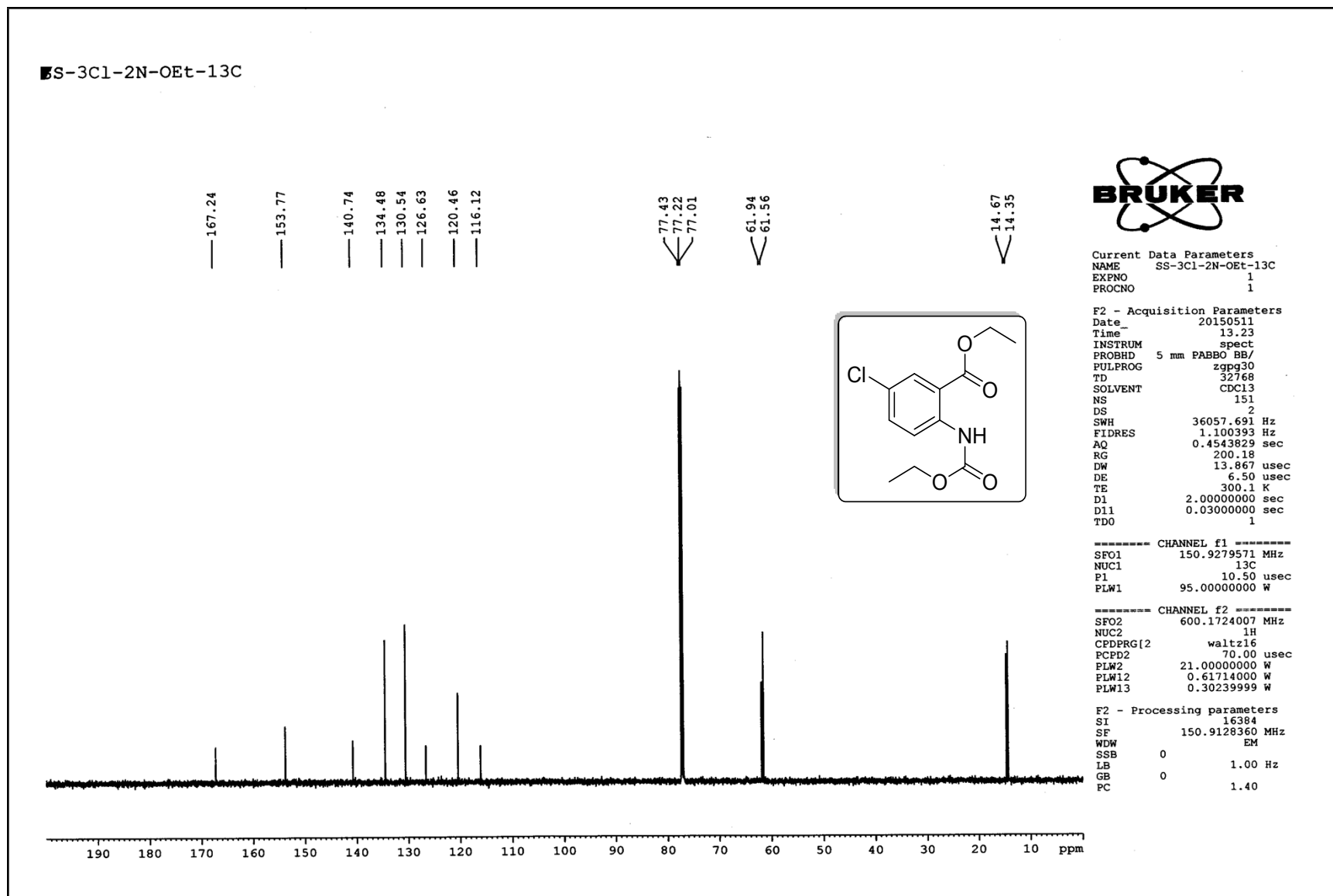
$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): 4q

## Mass Spectra: 4q

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time

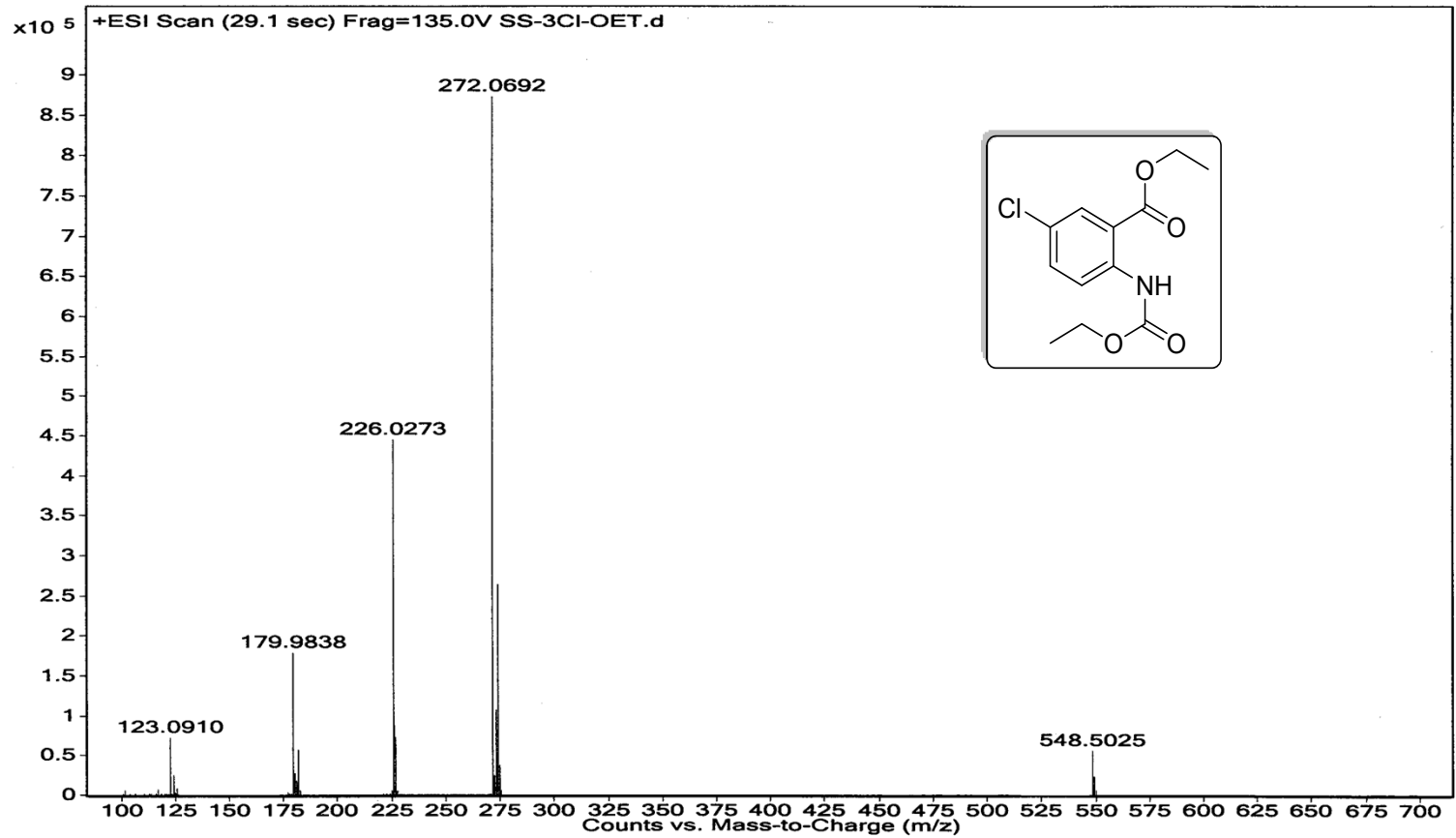


<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): **4r**

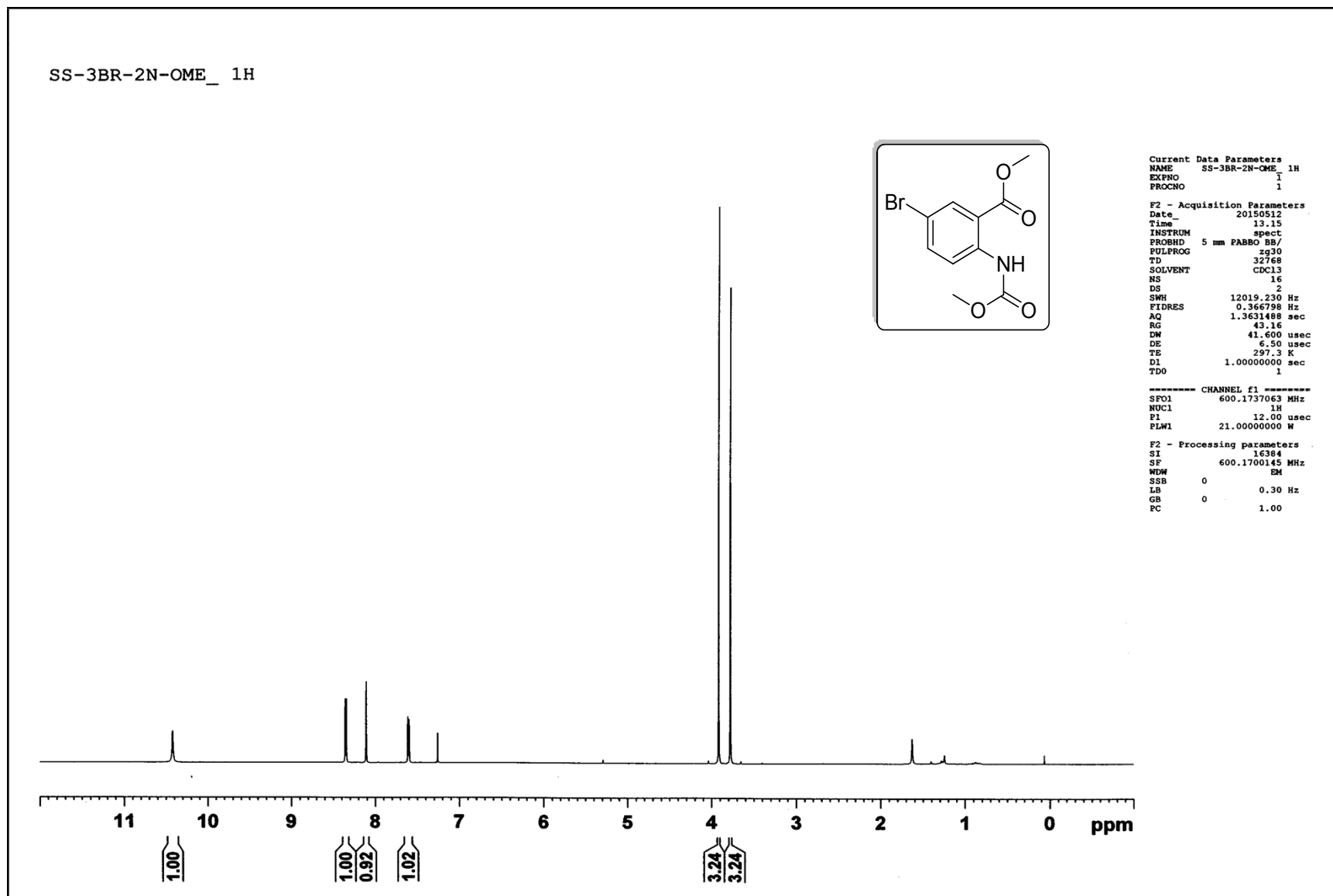
$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): 4r

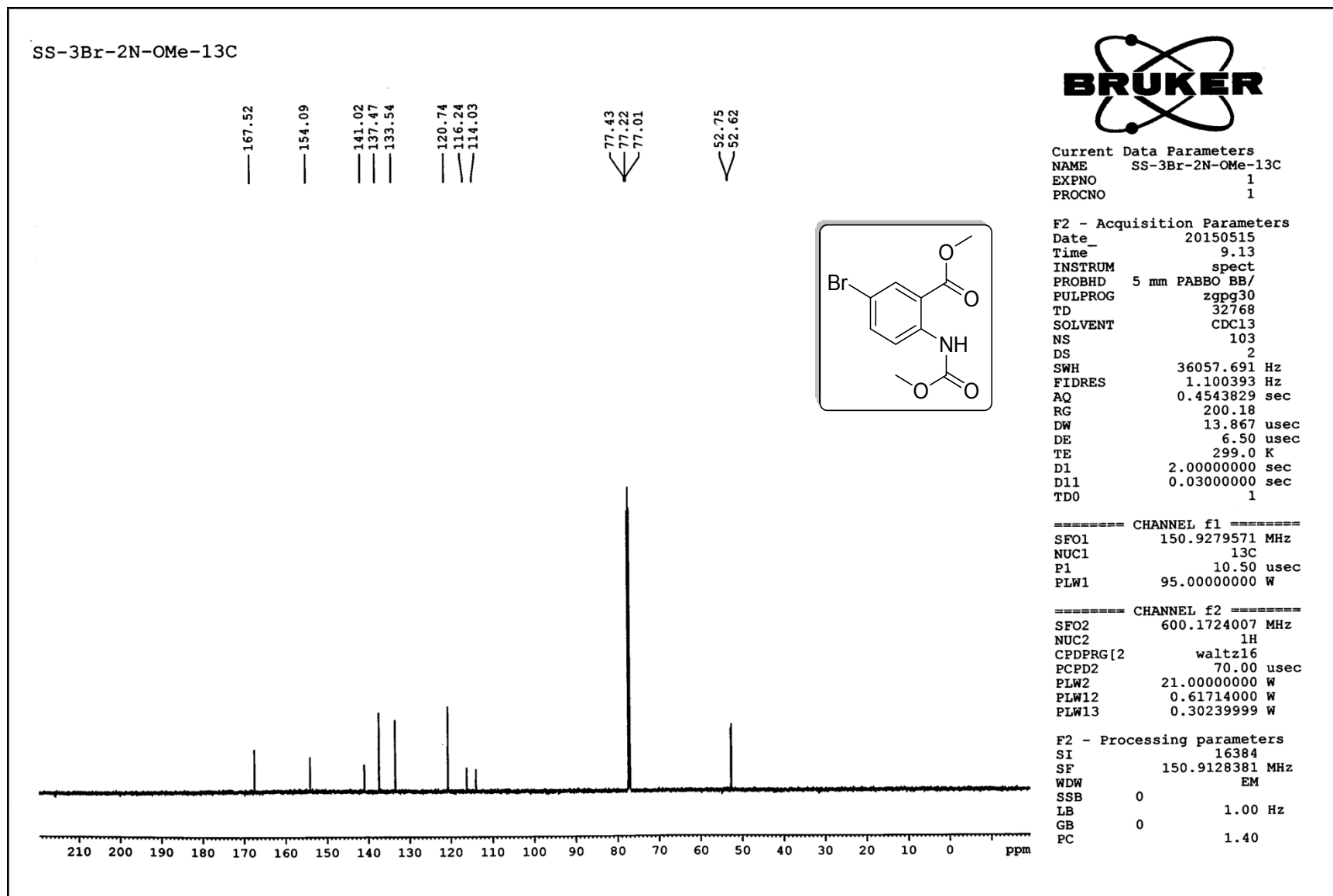
## Mass Spectra: 4r

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



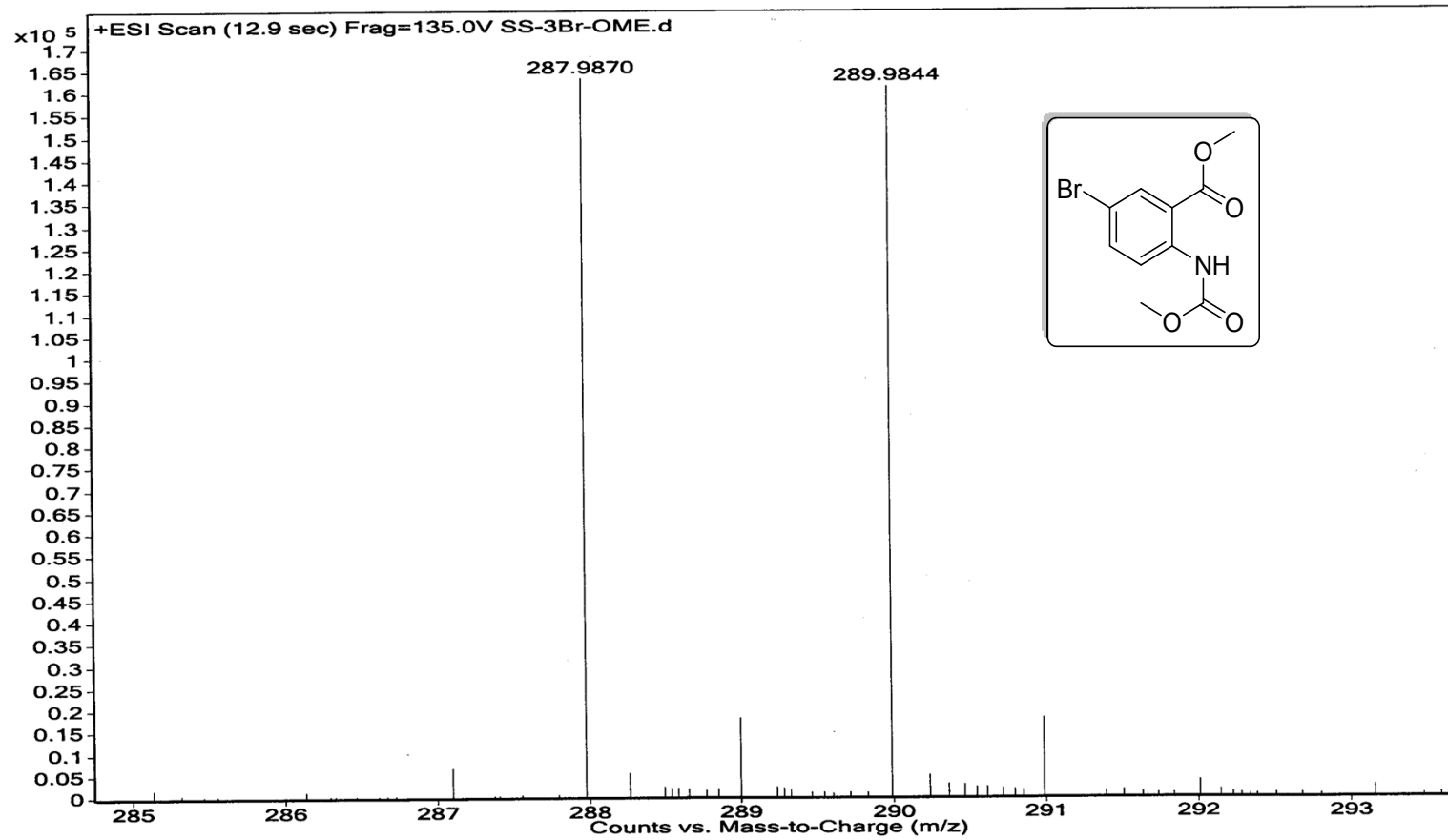


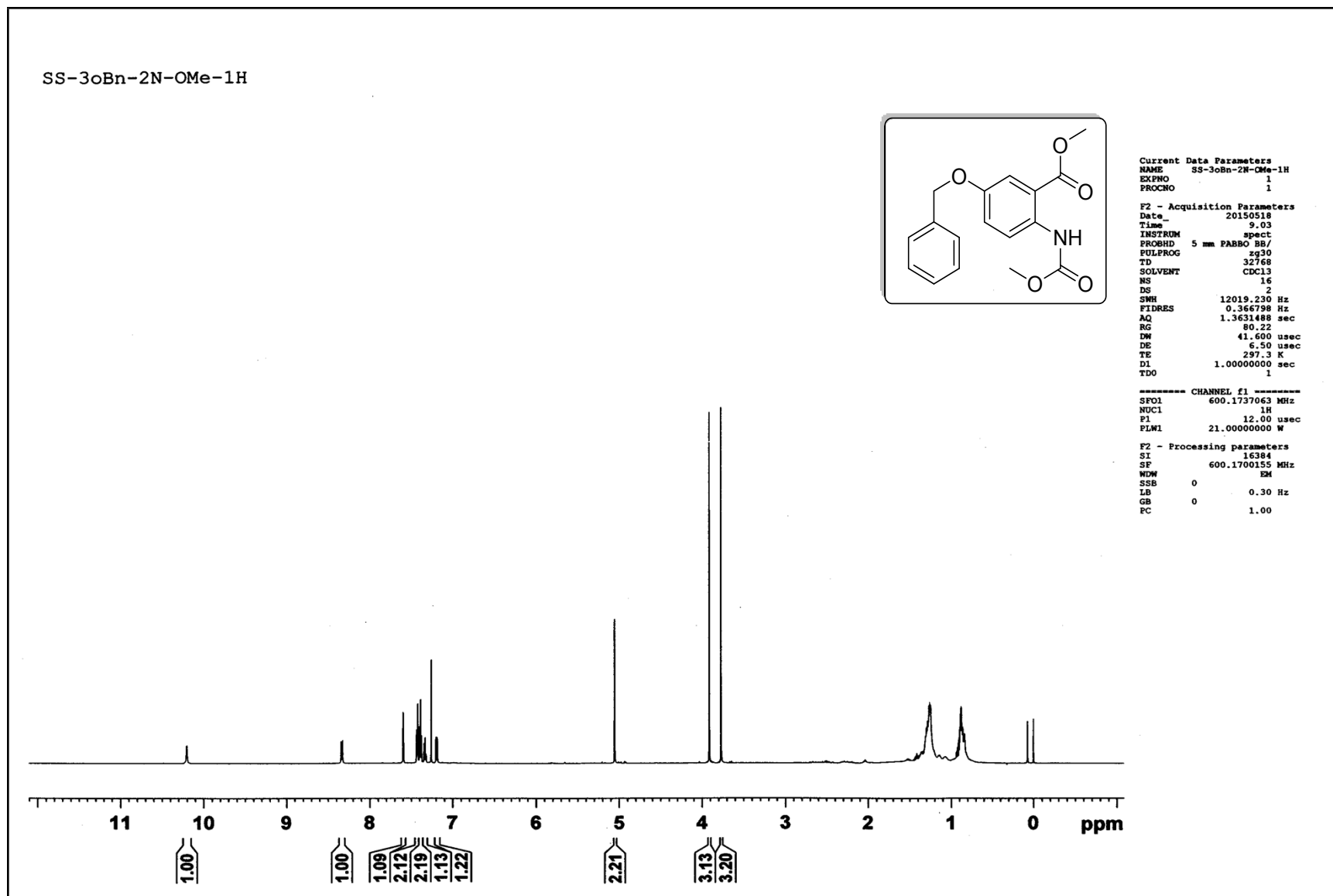
<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): 4s

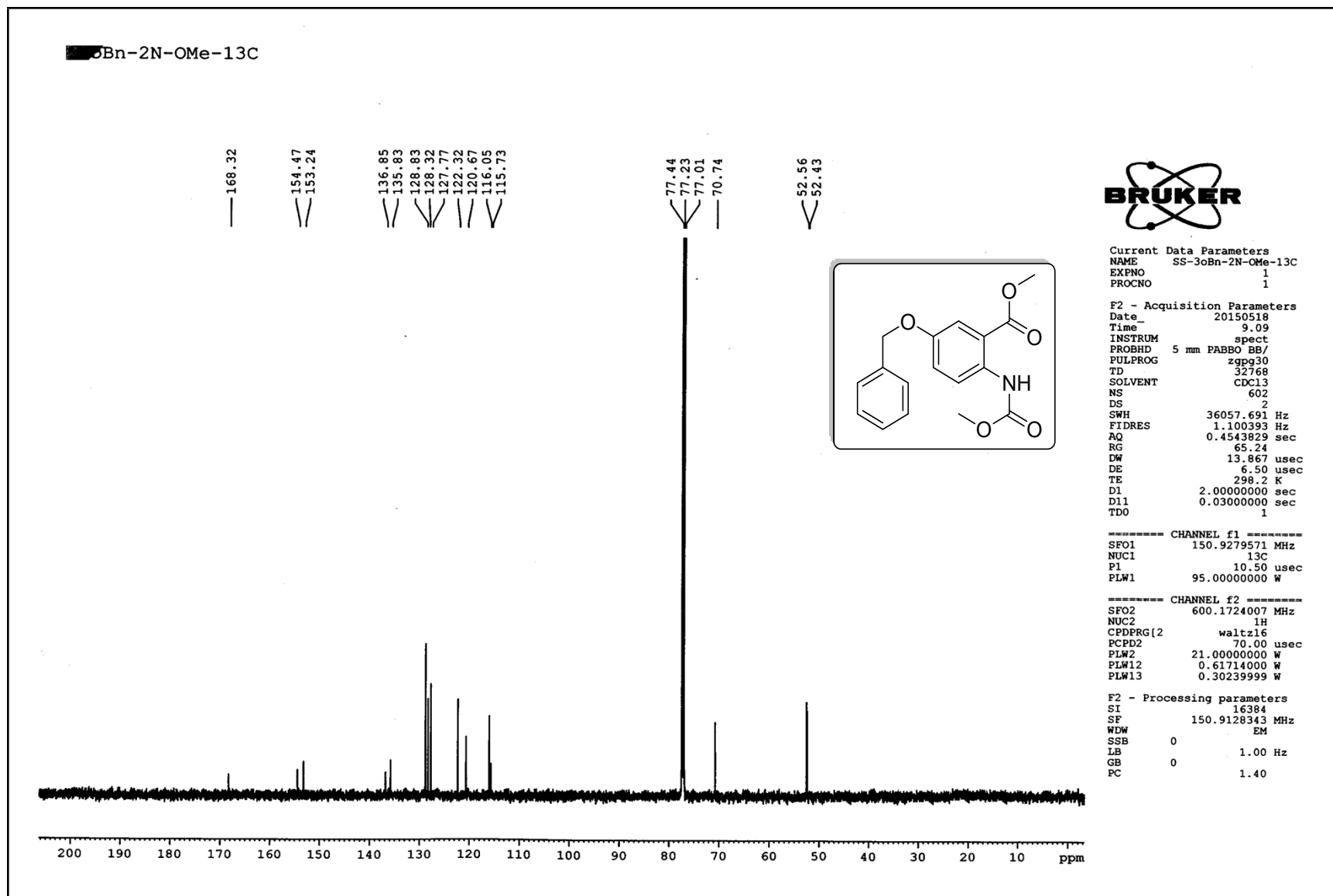
<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): 4s

## Mass Spectra: 4s

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time

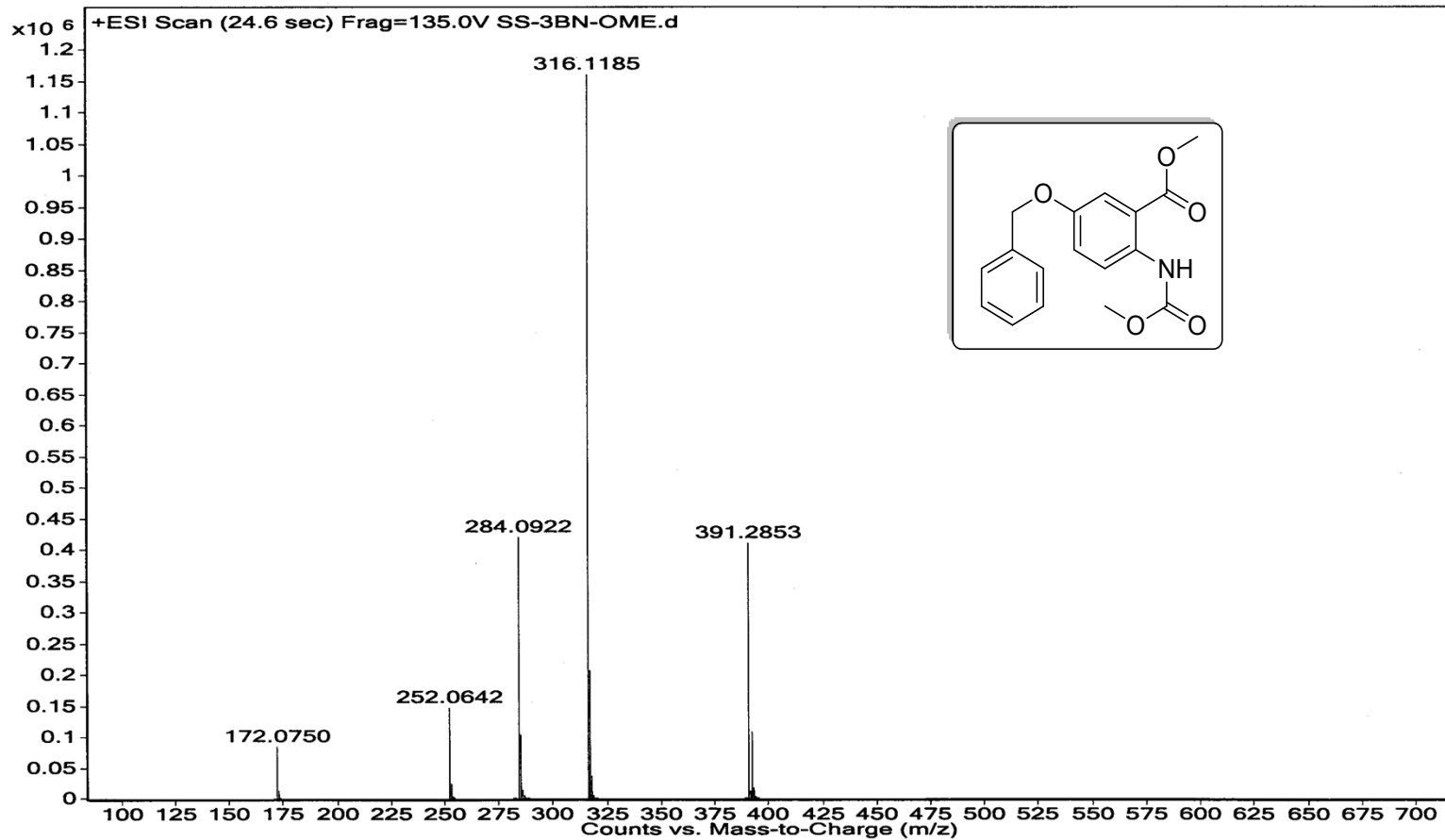


<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): **4u**

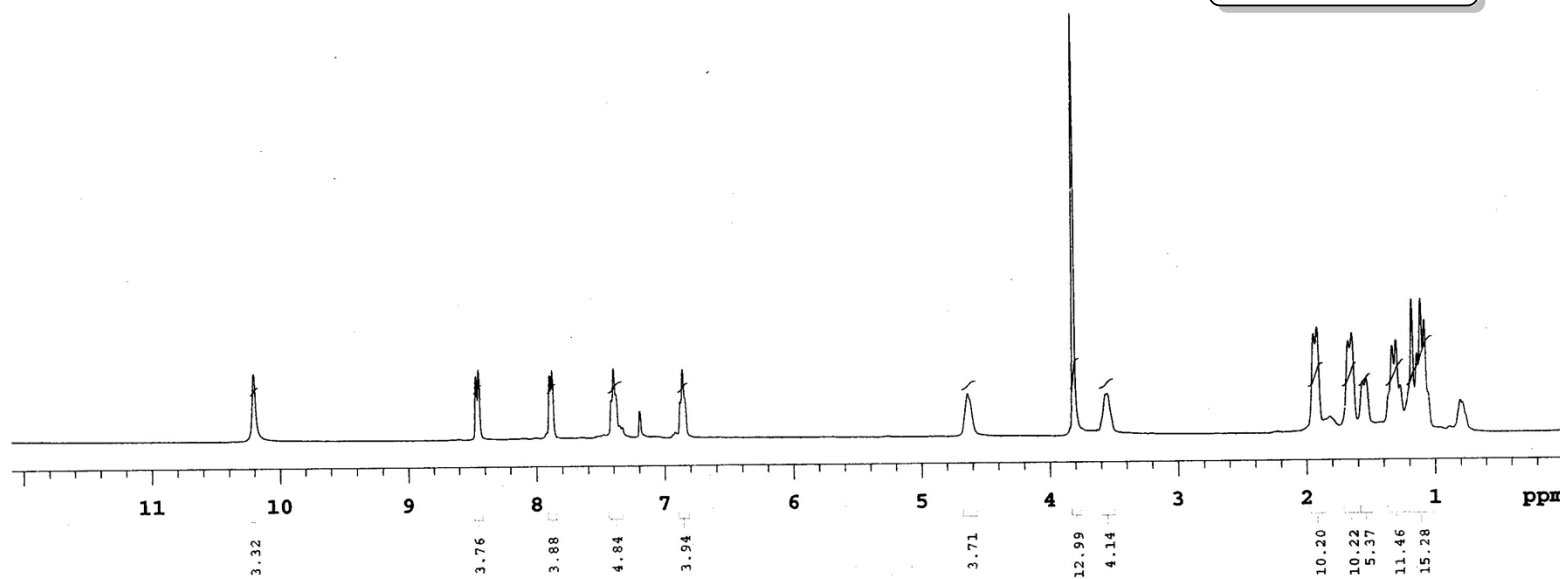
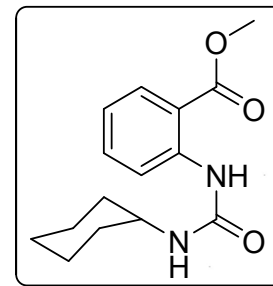
$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): **4u**

## Mass Spectra: 4u

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ): **6a**

**PULSE SEQUENCE**

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions

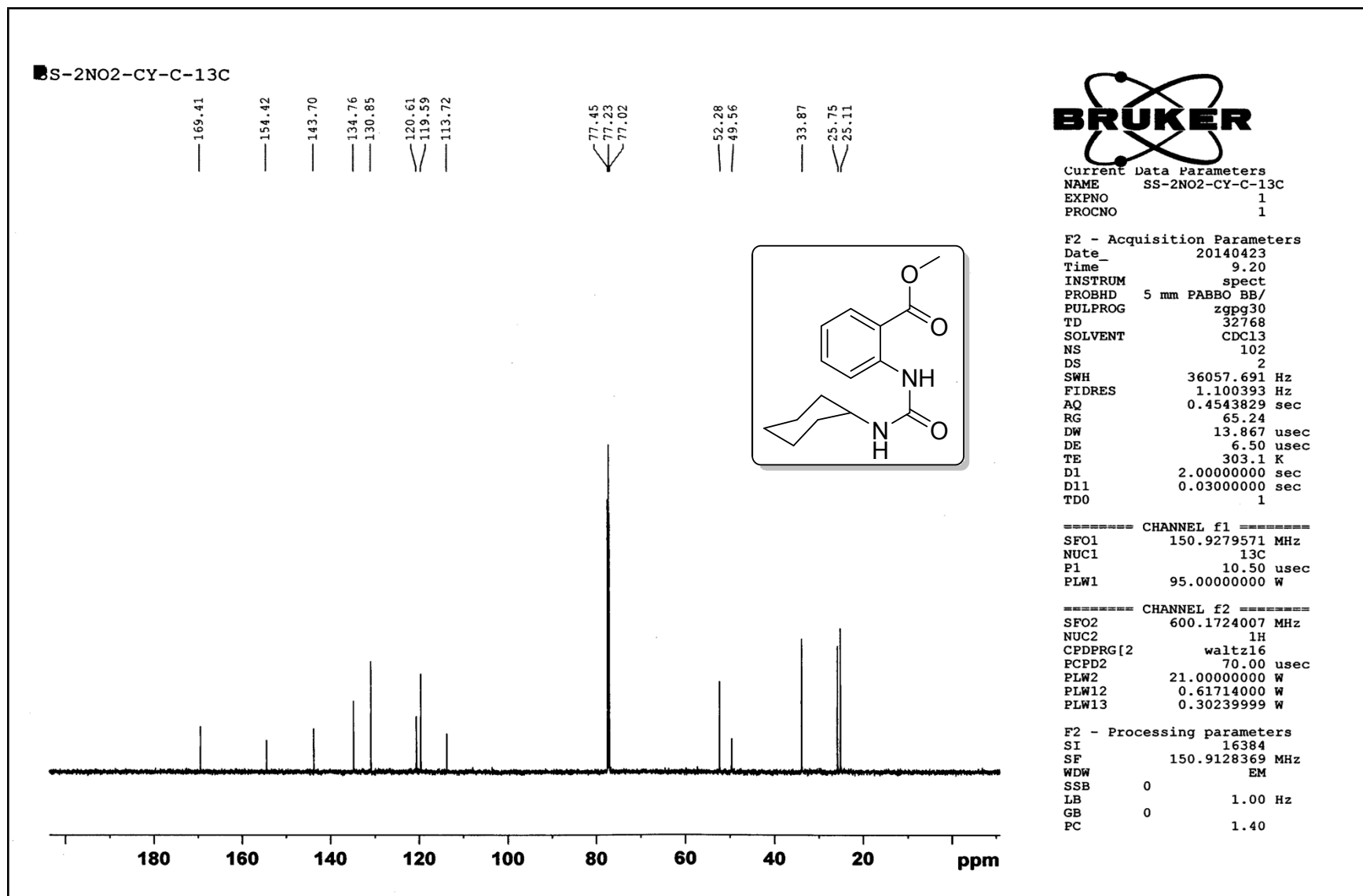
**DATA PROCESSING**

FT size 32768  
Total time 1 minutes

**SS\_2-NO2-CY-C-1H**

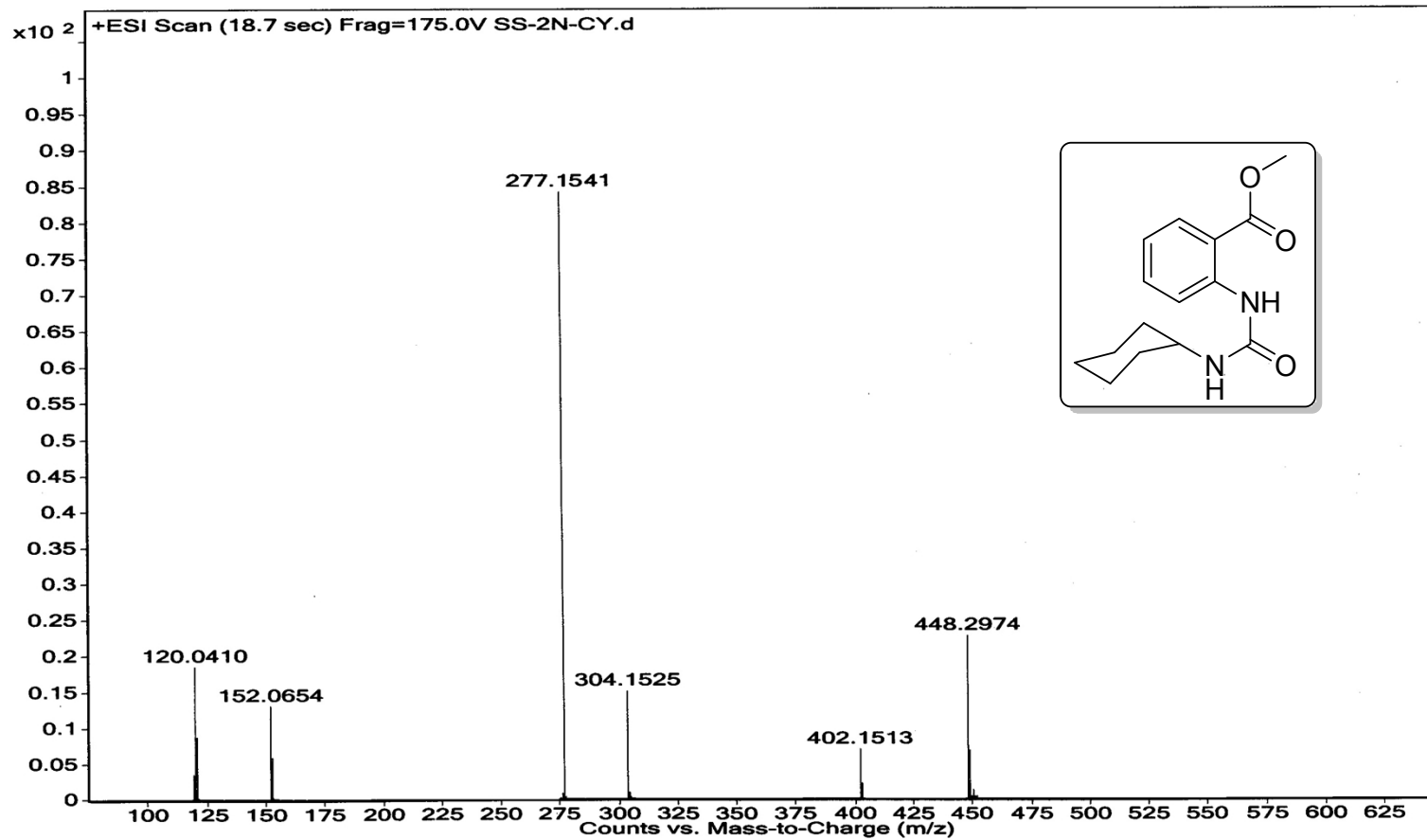
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: chem  
Mercury-400 "IITG-NMR"



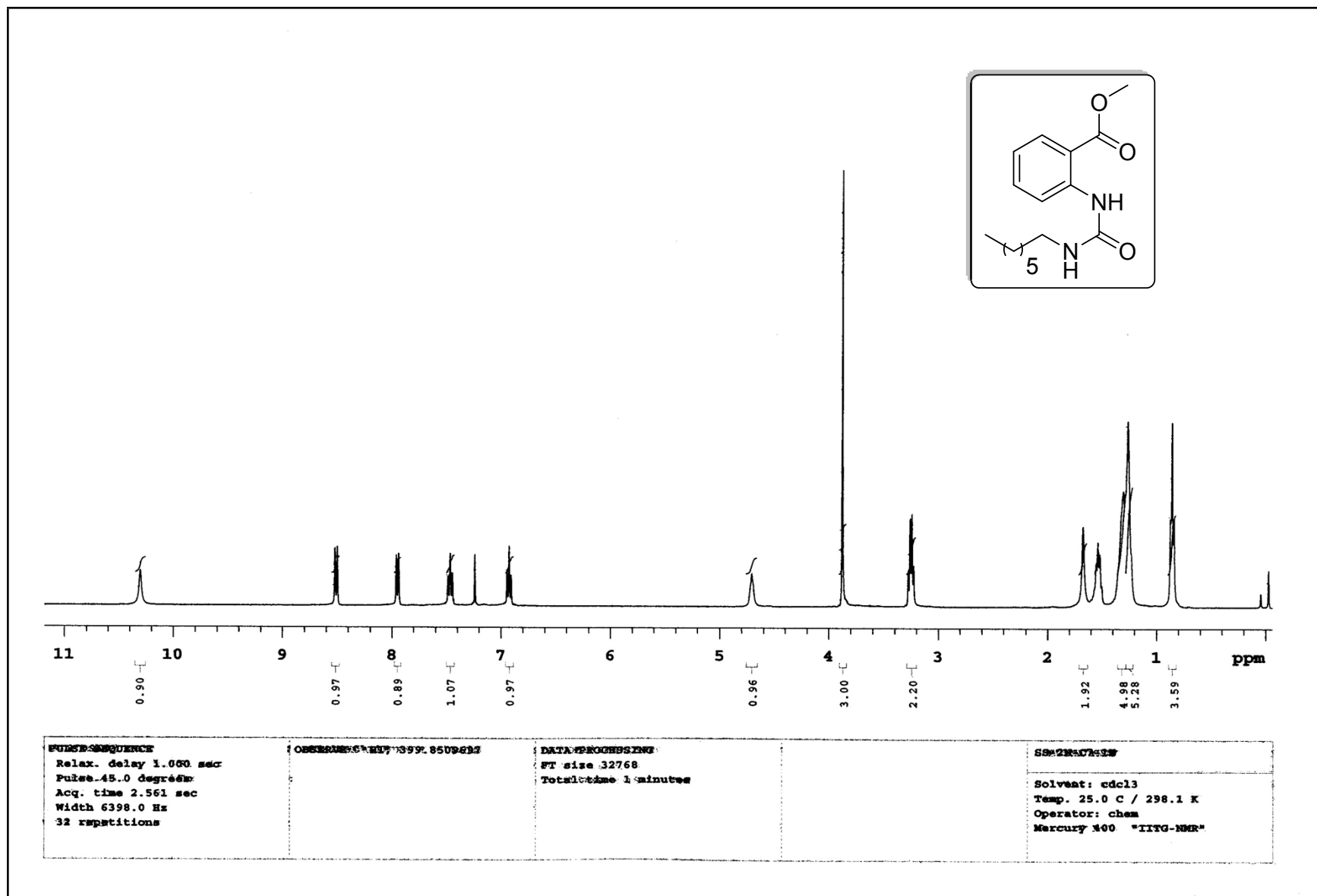
<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): 6a

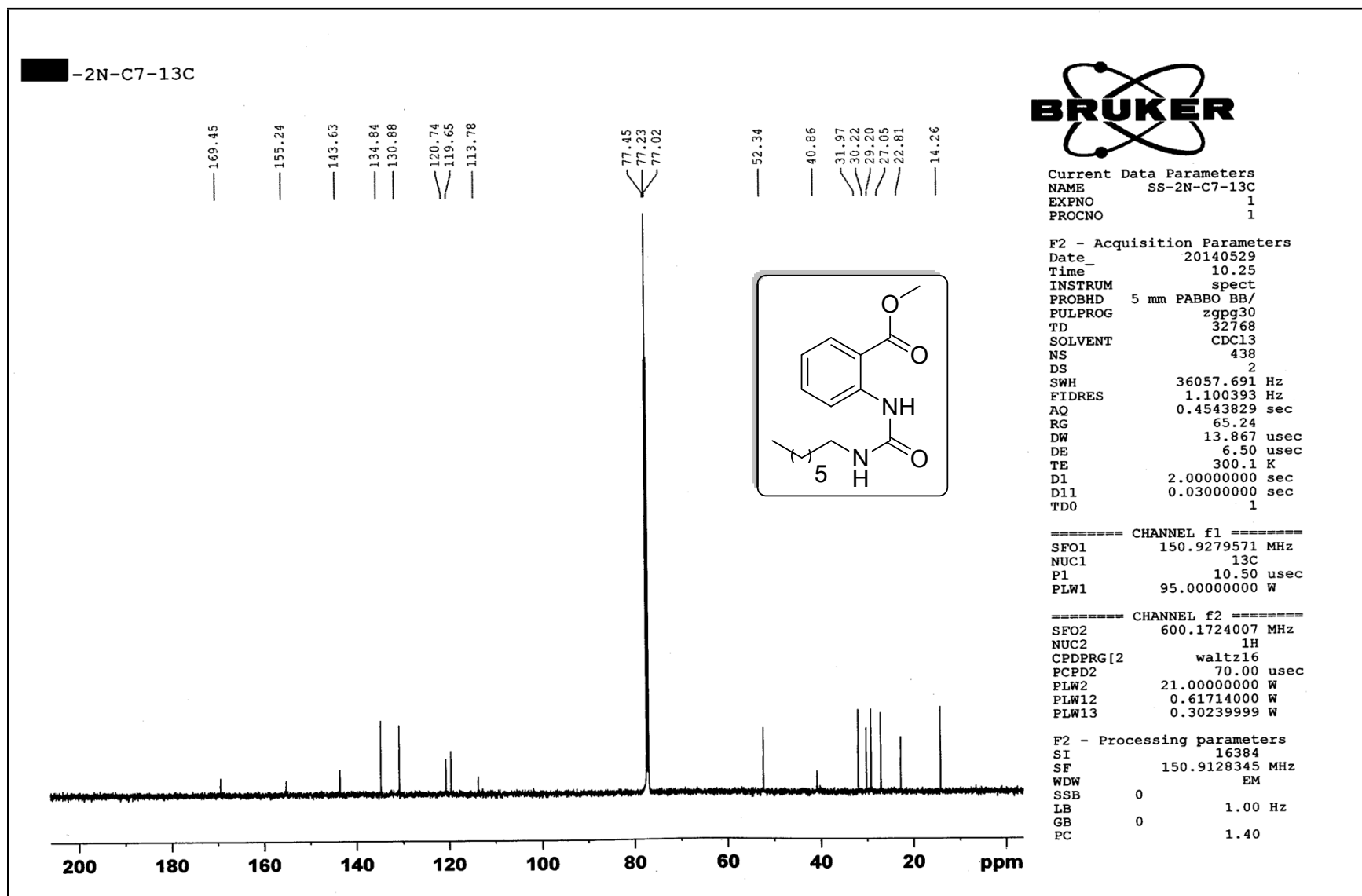
## Mass Spectra: 6a

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



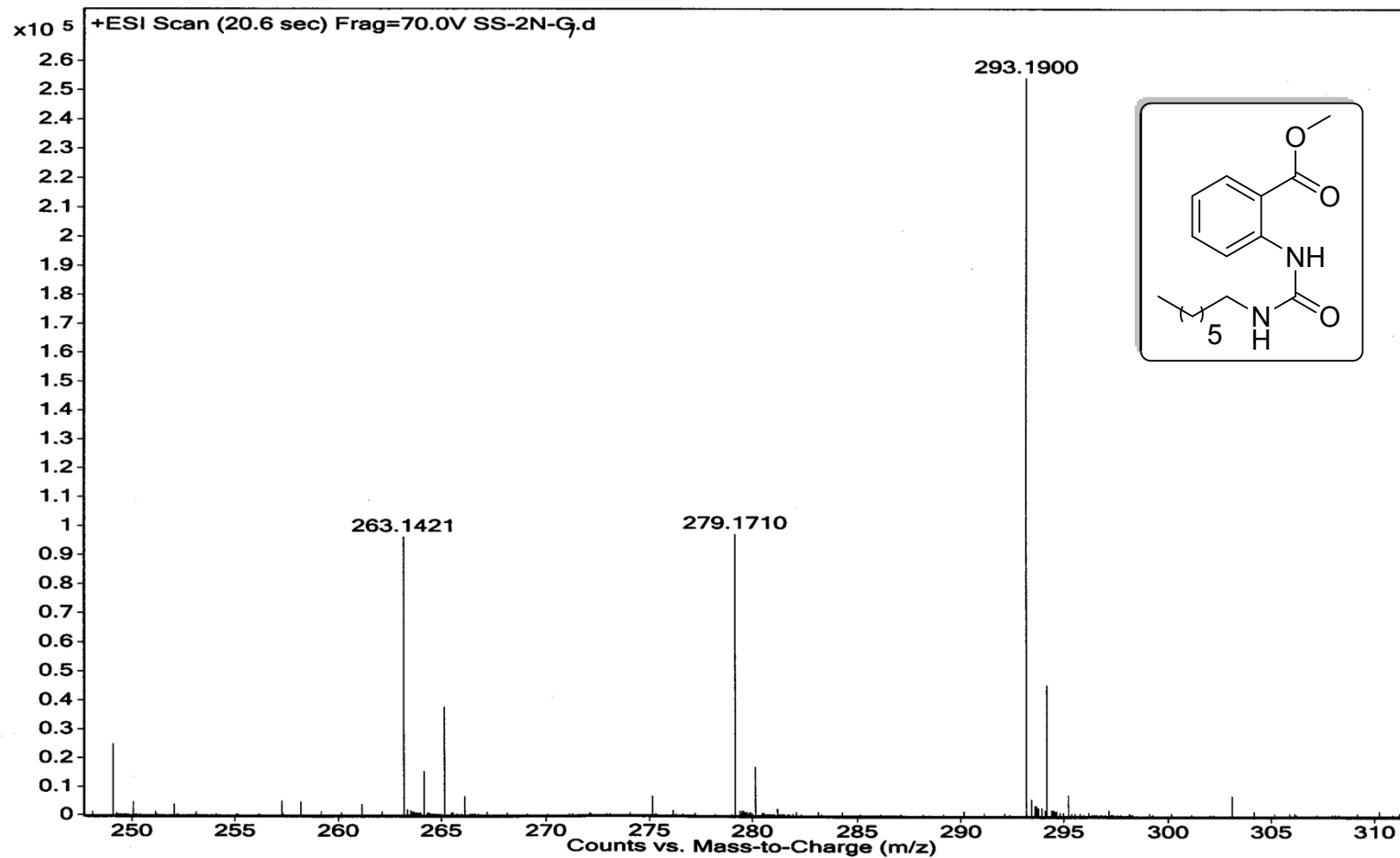
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): **6b**

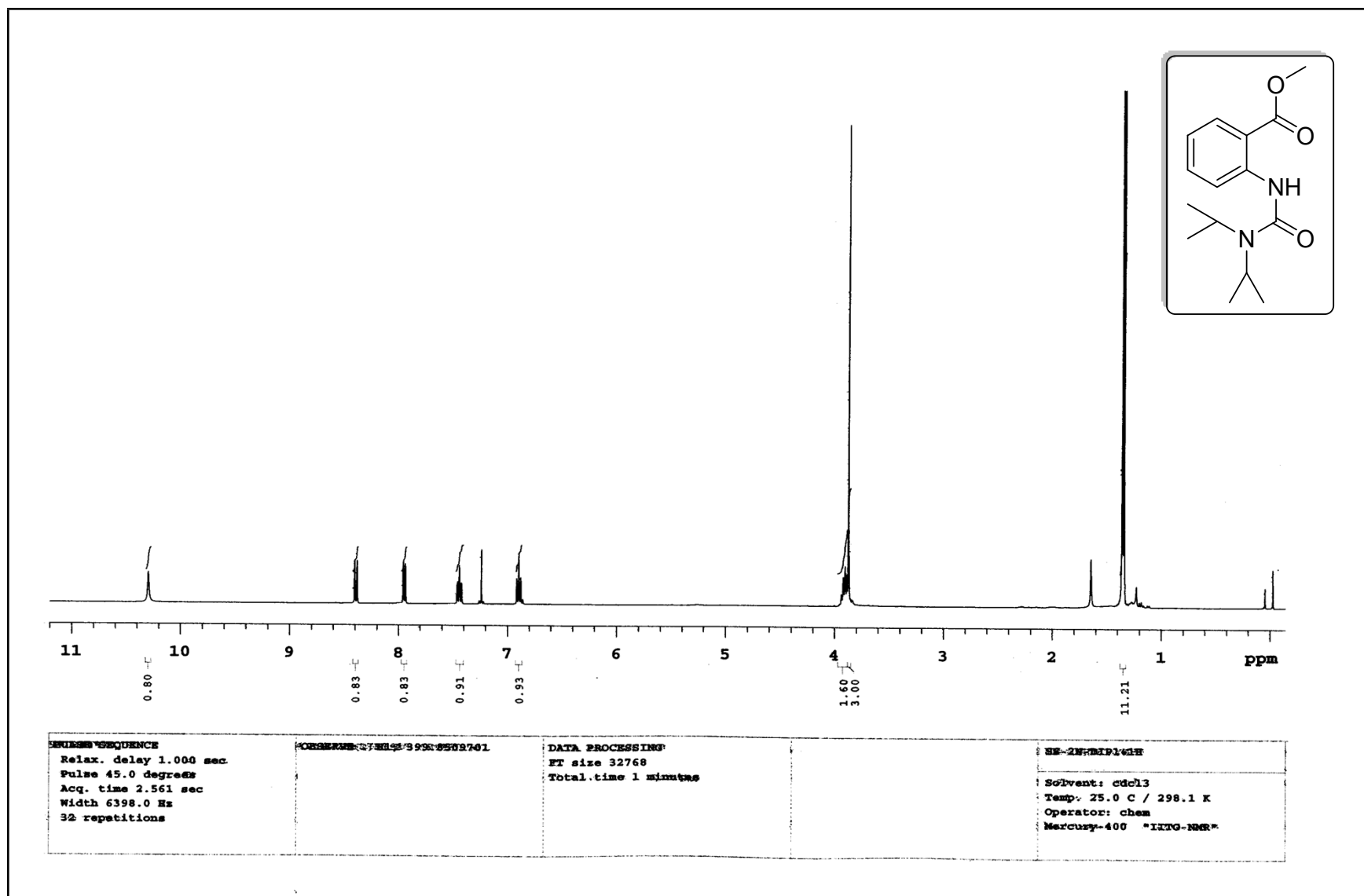


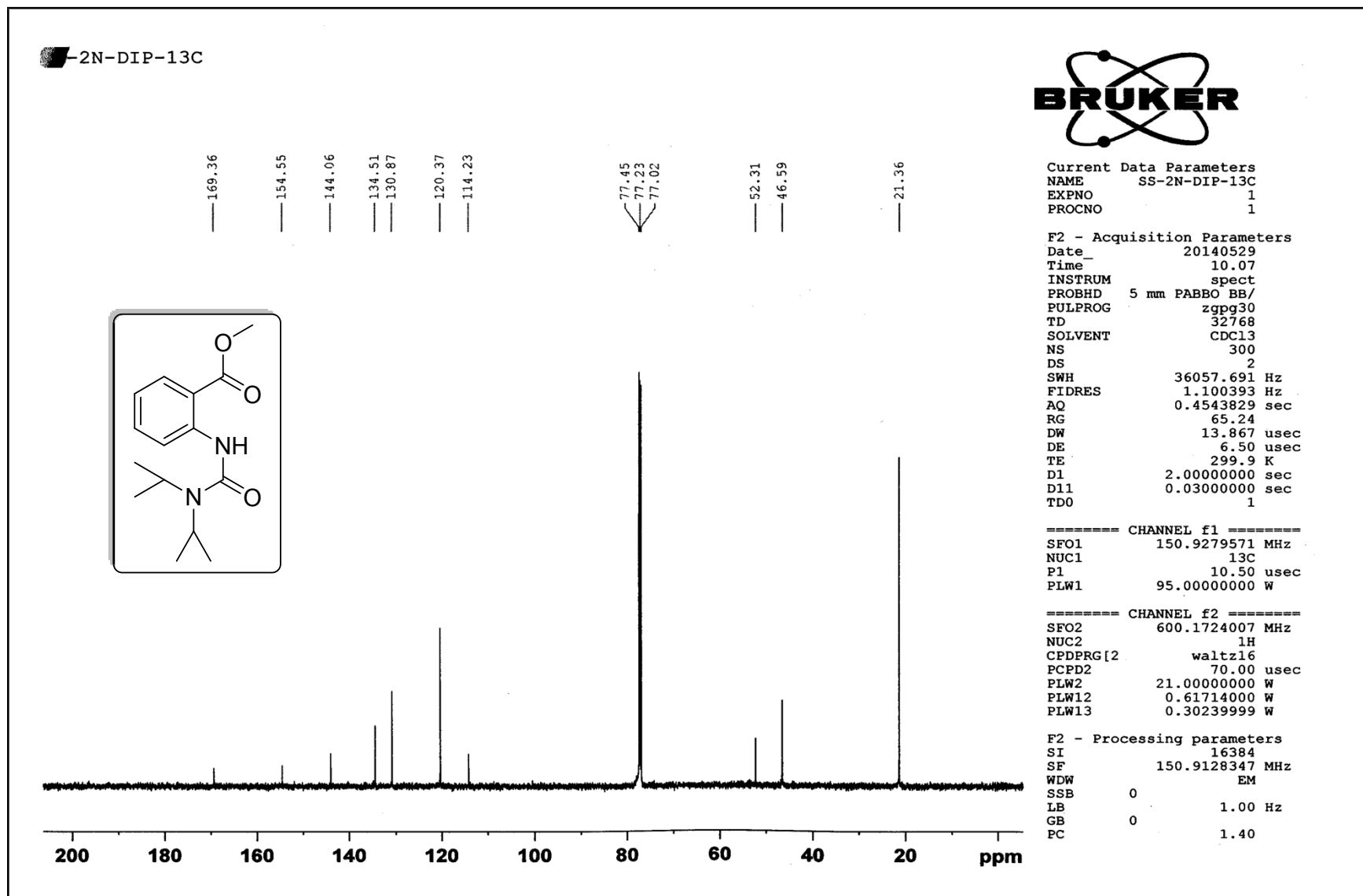
$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): **6b**

## Mass Spectra: 6b

<b>Sample Name</b>	SS-2N-G	<b>Position</b>	Vial 1	<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Inj Vol</b>	-10	<b>InjPosition</b>		<b>SampleType</b>	Sample	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	SS-2N-G.d	<b>ACQ Method</b>		<b>Comment</b>		<b>Acquired Time</b>	1/7/2015 3:28:32 PM

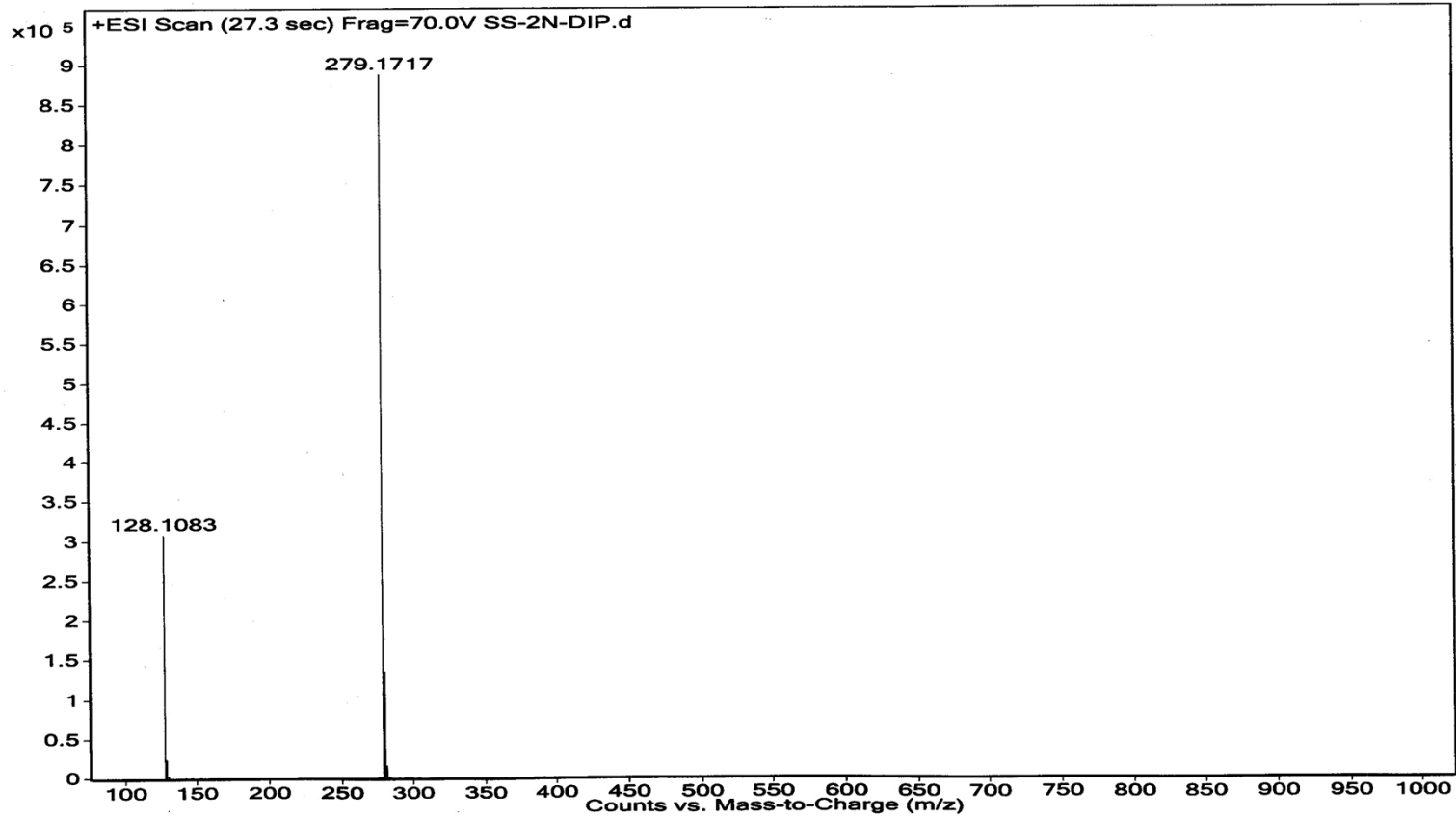


<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): **6c**

$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): **6c**

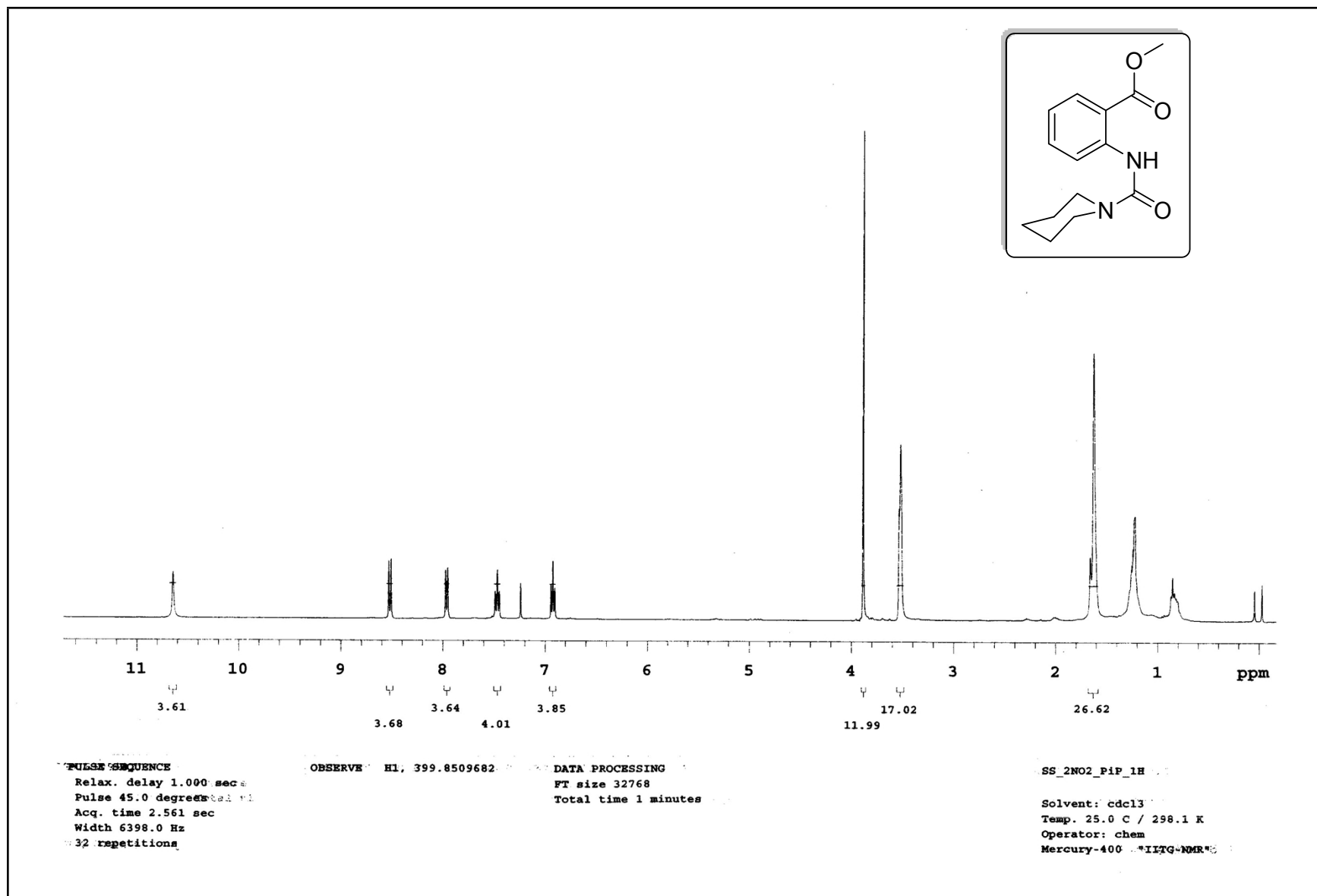
## Mass Spectra: 6c

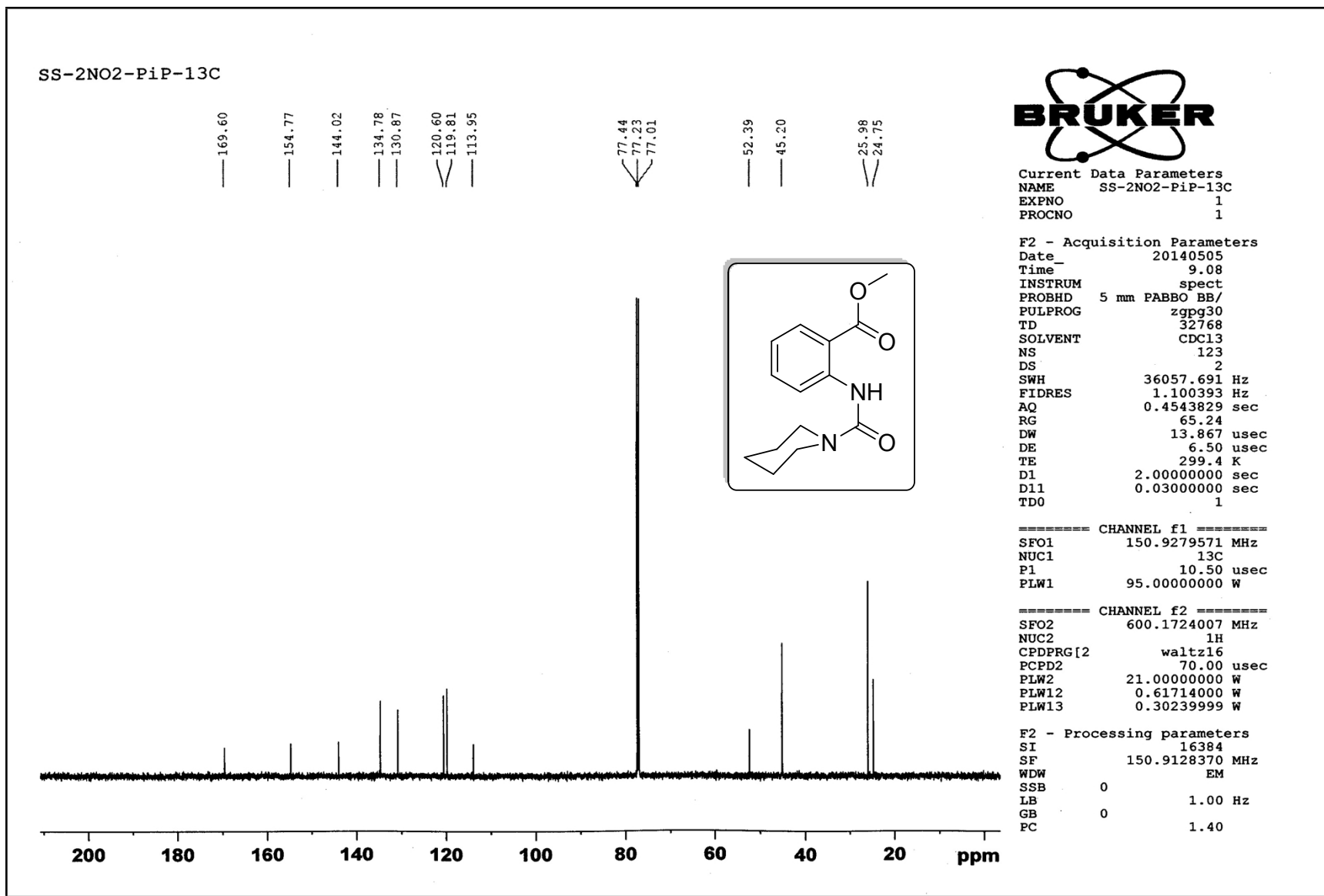
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time





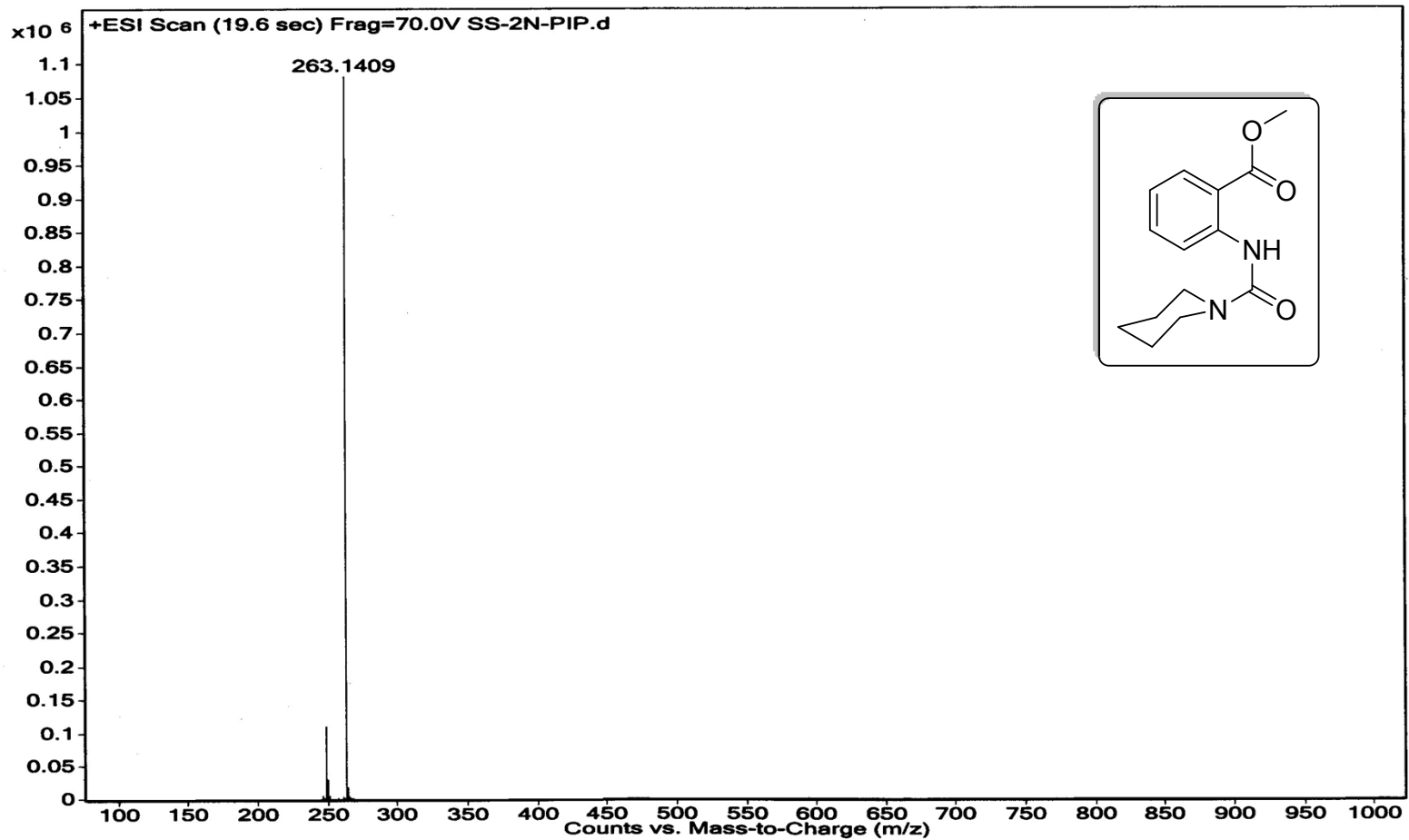
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ): **6d**



$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): **6d**

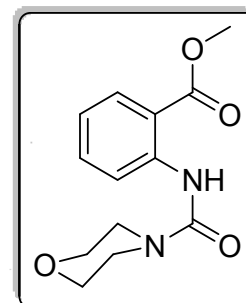
## Mass Spectra: 6d

<b>Sample Name</b>	SS-2N-PIP	<b>Position</b>	Vial 1	<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Inj Vol</b>	-10	<b>InjPosition</b>		<b>SampleType</b>	Sample	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	SS-2N-PIP.d	<b>ACQ Method</b>		<b>Comment</b>		<b>Acquired Time</b>	1/7/2015 3:23:11 PM



<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): 6e

SS-2N-M1-1H

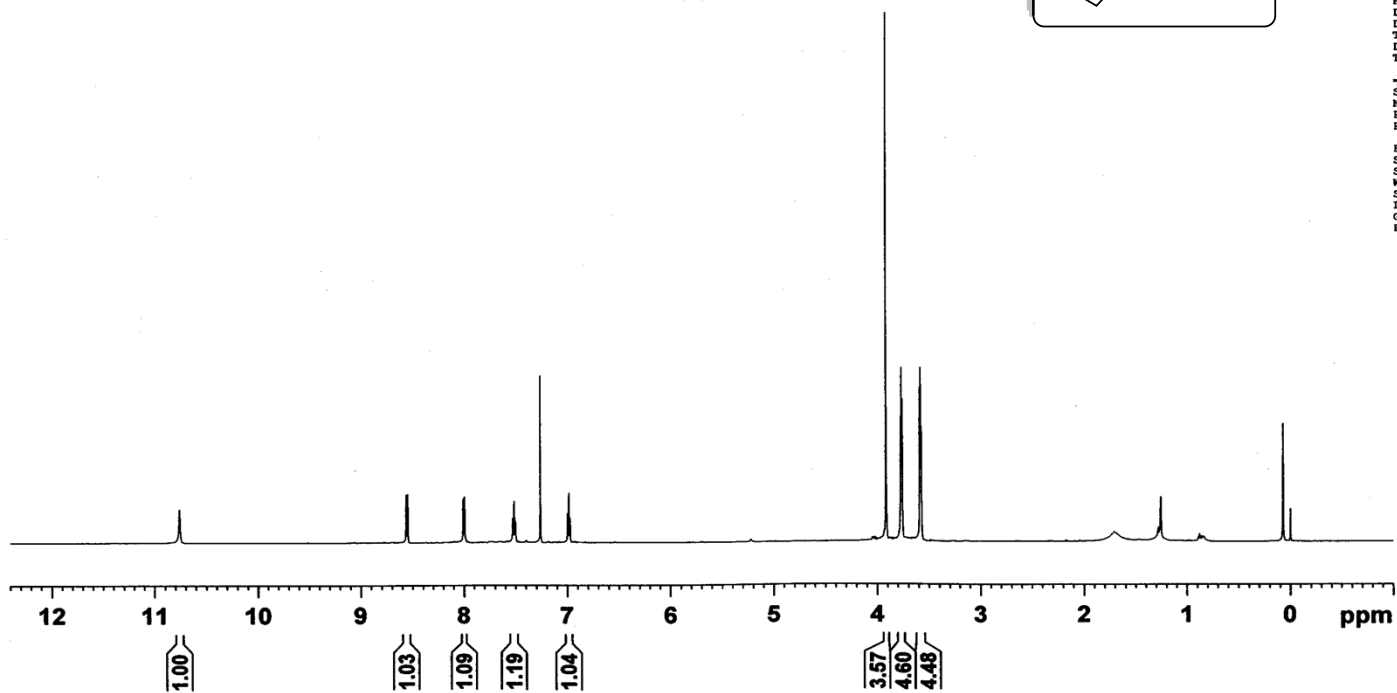


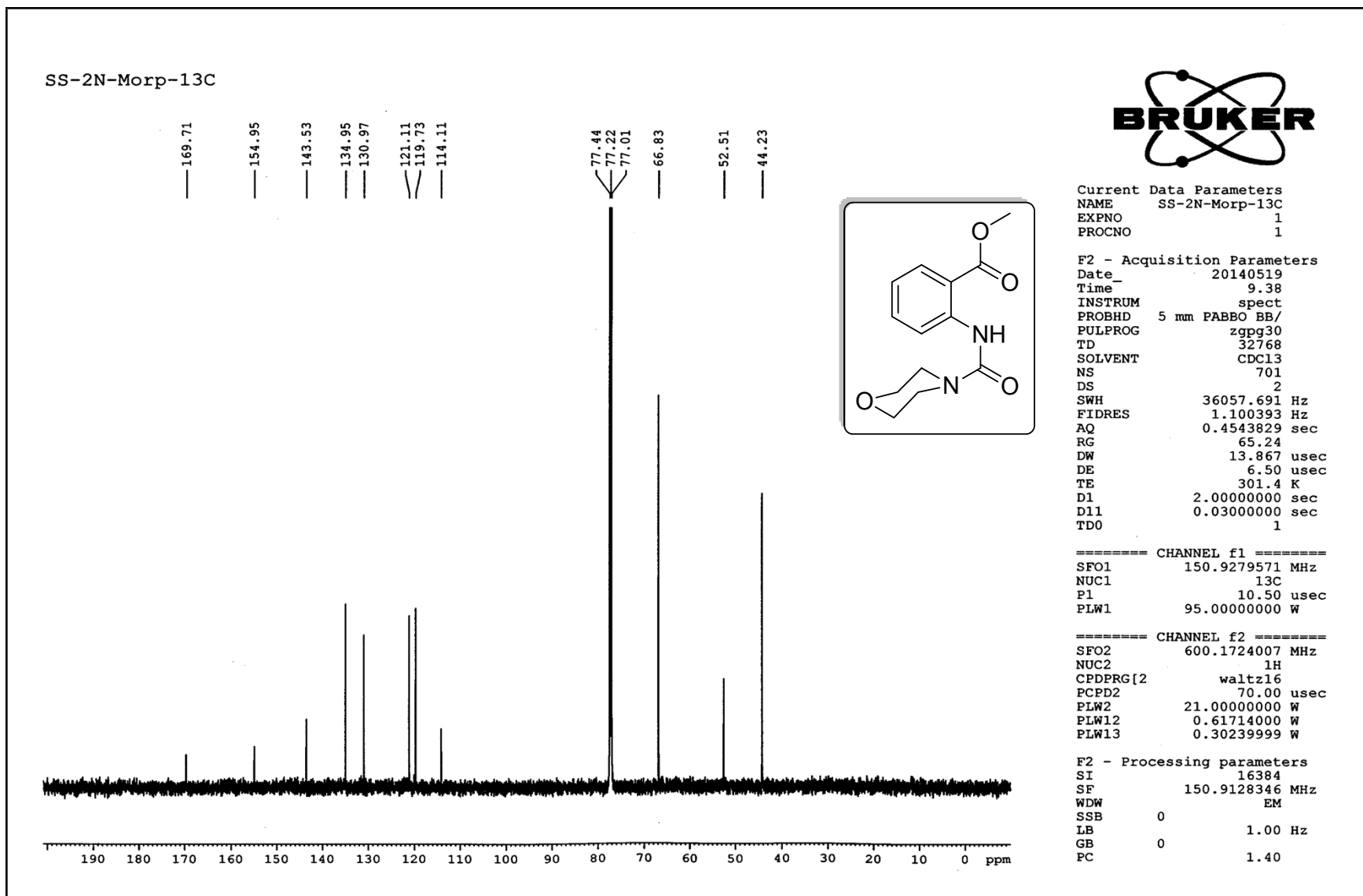
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Current Data Parameters
NAME      SS-2N-M1-1H
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20140604
Time      10.27
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        12019.230 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         99.36
DW         41.600 usec
DE         6.50 usec
TE         299.3 K
D1         1.0000000 sec
TD0        1

----- CHANNEL f1 -----
SF01      600.1737063 MHz
NUC1       1H
P1         12.00 usec
PLW1       21.00000000 W

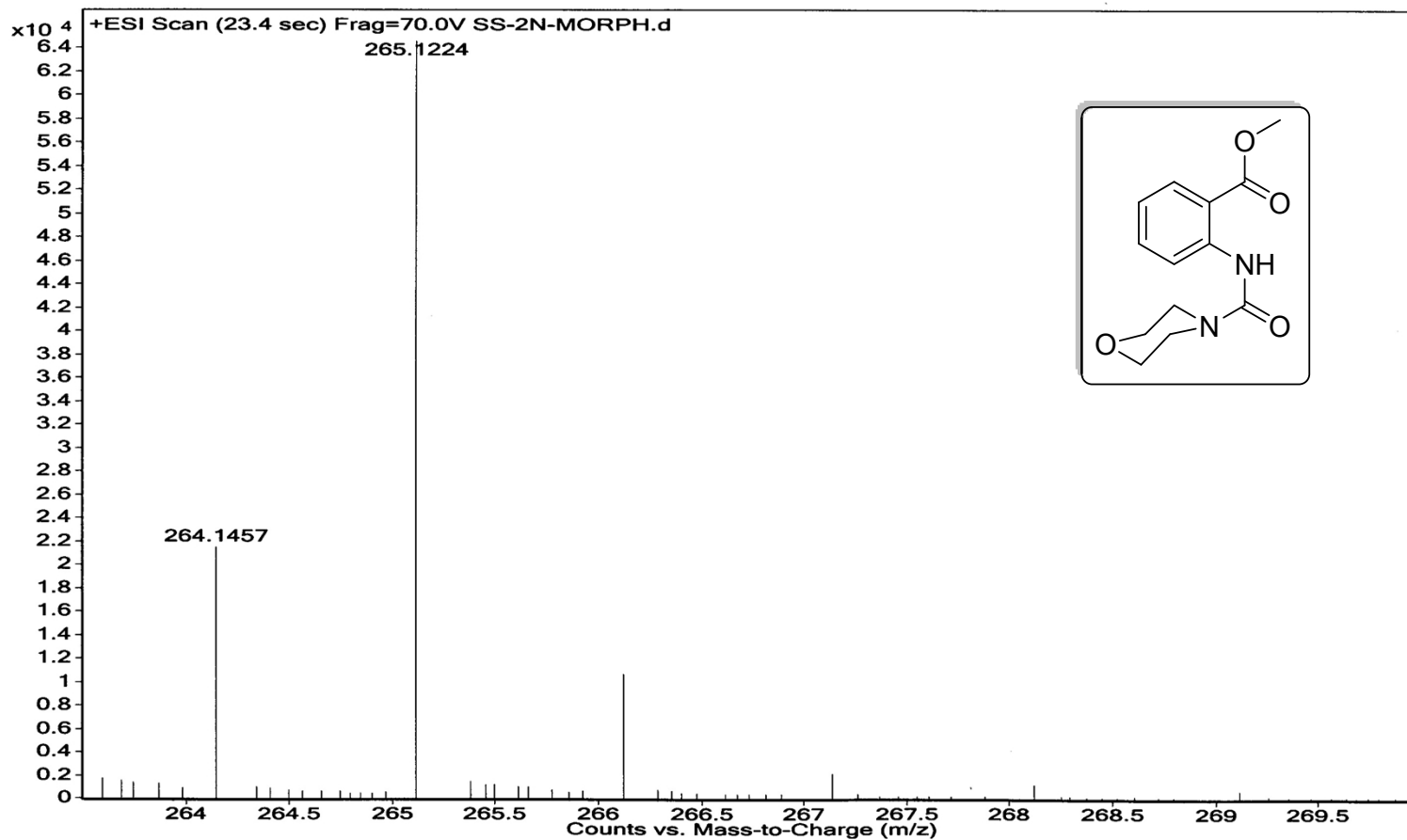
F2 - Processing parameters
SI         16384
SF         600.1700148 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
FC         1.00
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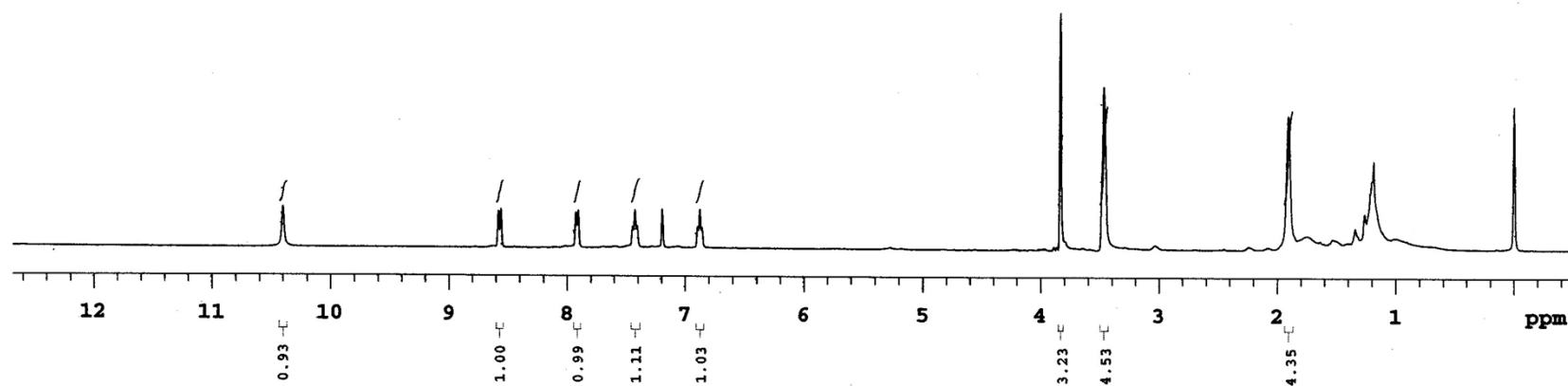
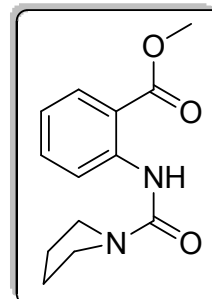


$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): **6e**

Mass spectra: 6e

<b>Sample Name</b>	SS-2N-MORPH	<b>Position</b>	Vial 1	<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Inj Vol</b>	-10	<b>InjPosition</b>		<b>SampleType</b>	Sample	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	SS-2N-MORPH.d	<b>ACQ Method</b>		<b>Comment</b>		<b>Acquired Time</b>	1/7/2015 3:26:53 PM



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): **6f****PULSE SEQUENCE**

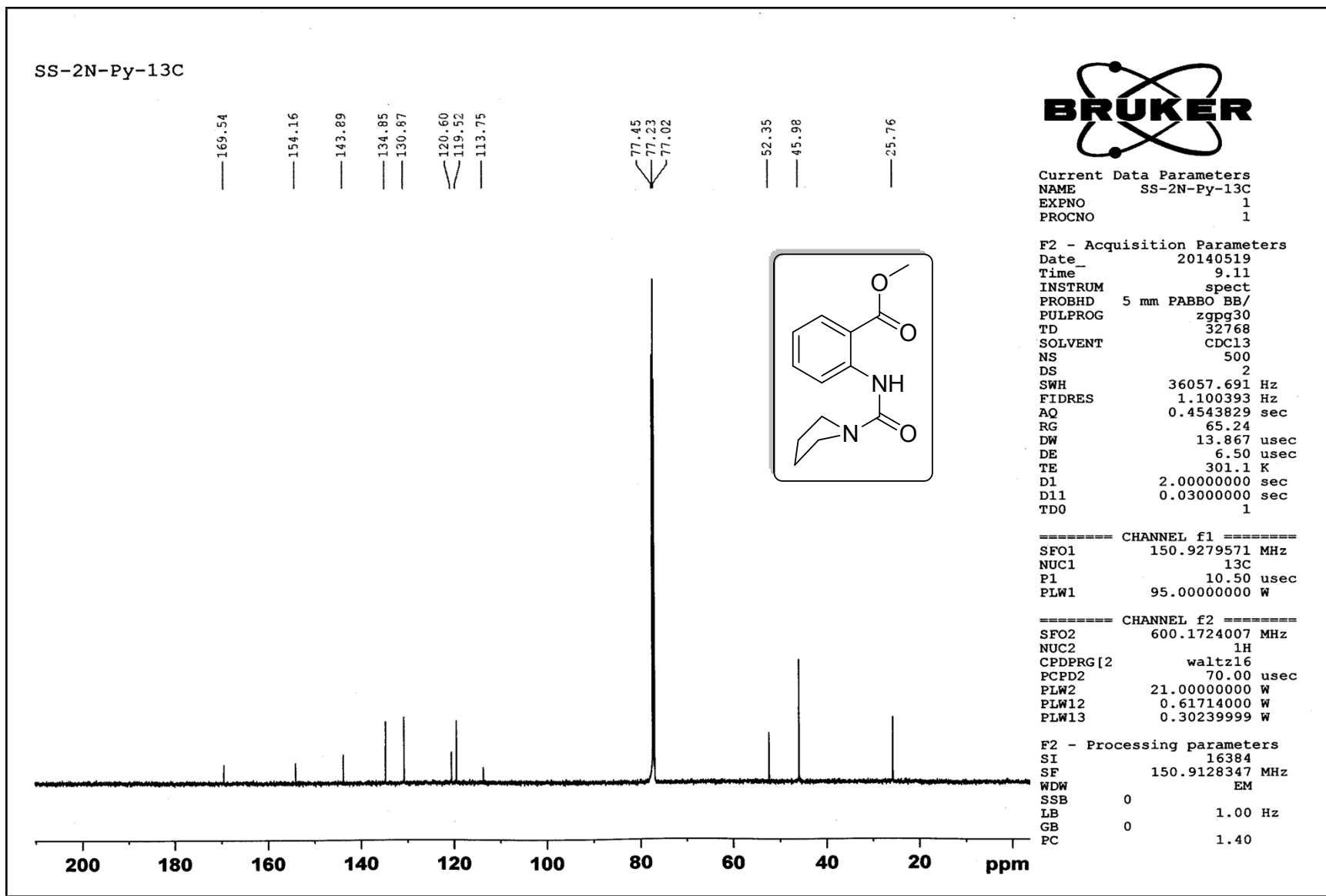
Relax. delay 1.000 sec  
Pulse 45.0 degree  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions

**OBSERVE** H1, 399.8509878**DATA PROCESSING**

FT size: 32768  
Total time 1 minutes

**SS-2N-Py**

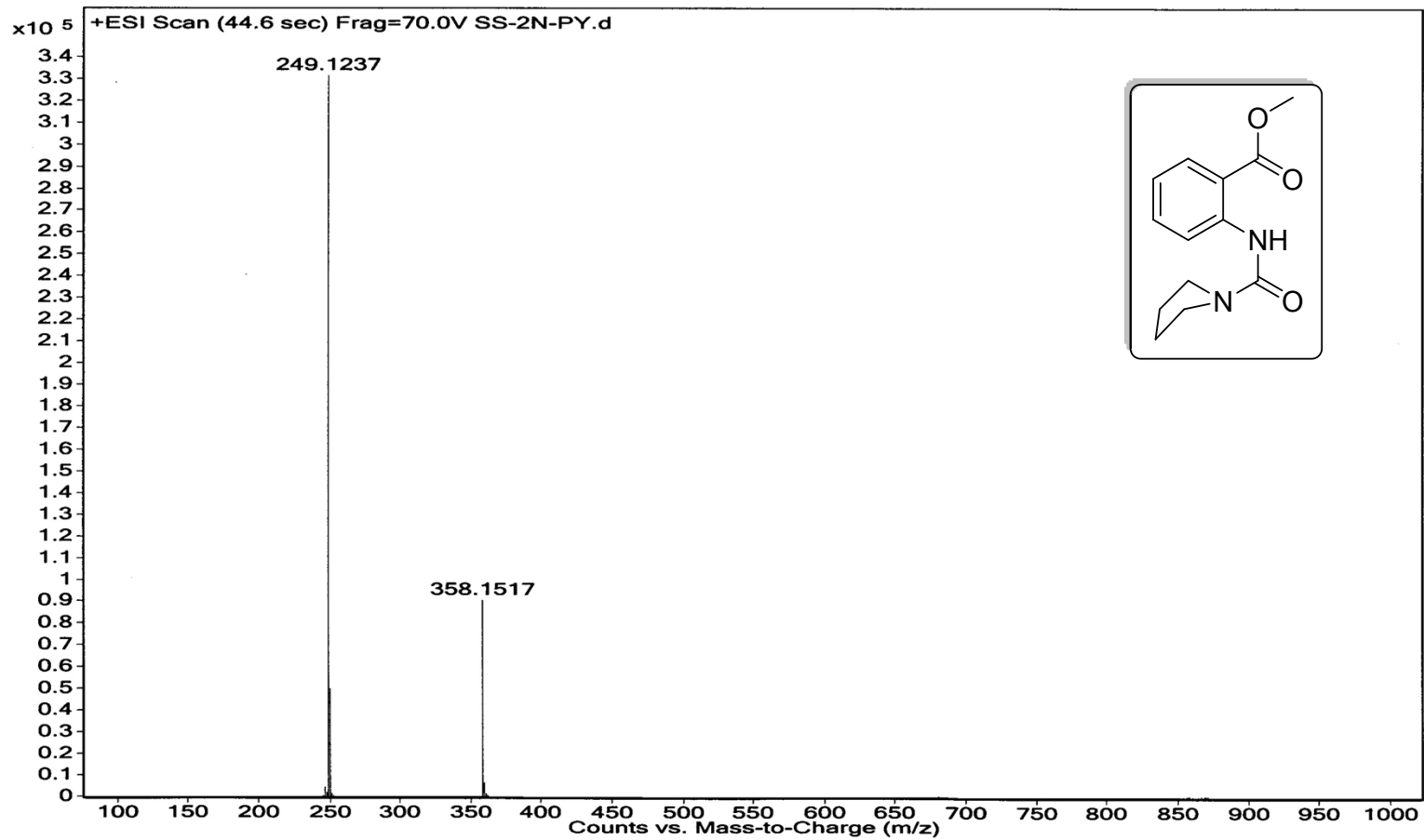
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: chem  
File: SS-2N-Py-1H  
Mercury-400 "1TG-NMR"

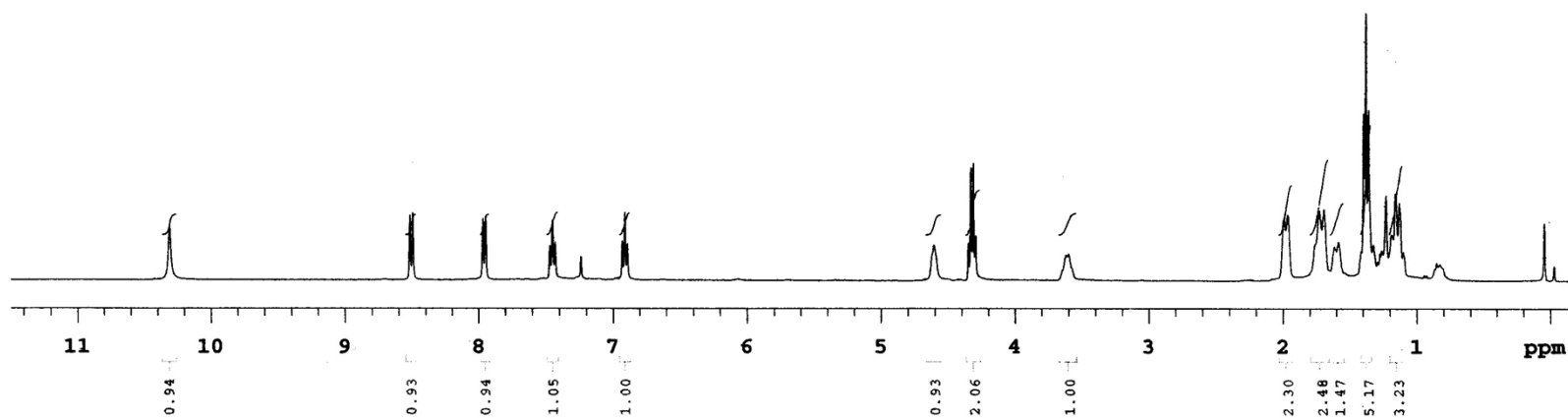
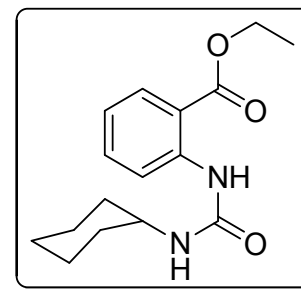
$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): **6f**



Mass spectra: 6f

<b>Sample Name</b>	SS-2N-PY	<b>Position</b>	Vial 1	<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Inj Vol</b>	-10	<b>InjPosition</b>		<b>SampleType</b>	Sample	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	SS-2N-PY.d	<b>ACQ Method</b>		<b>Comment</b>		<b>Acquired Time</b>	1/7/2015 3:21:26 PM



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): **6g**

## SUBSEQUENCE

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions

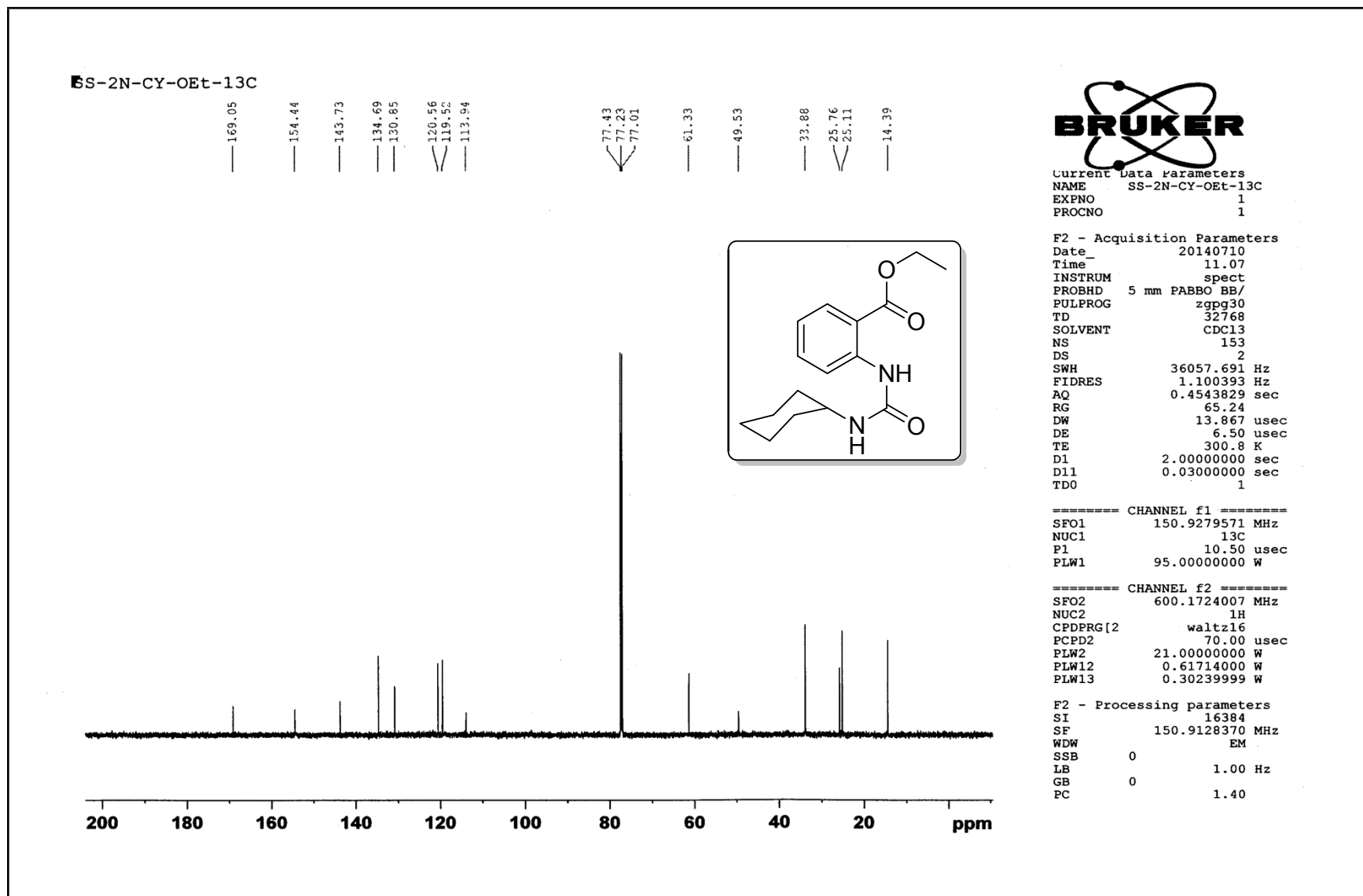
OBSERVE EL, 399.8509725

## DATA PROCESSING

FT size 32768  
Total time 1 minutes

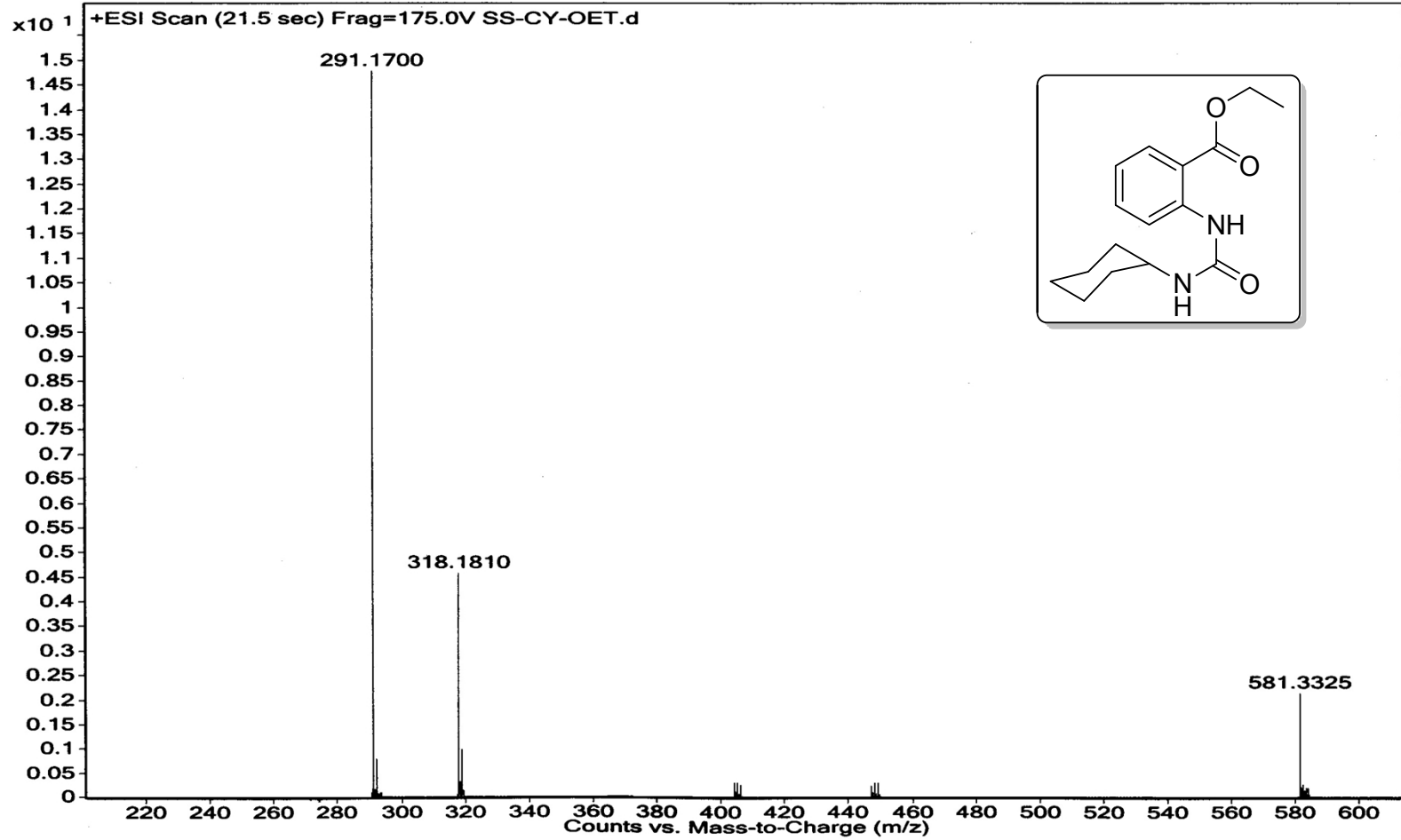
SS\_2N\_Cy\_OEt\_1H

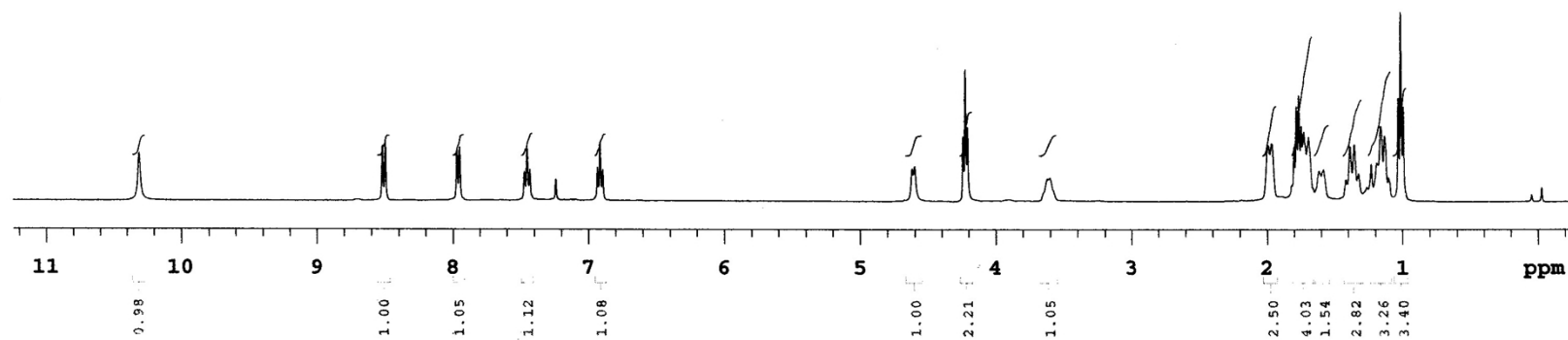
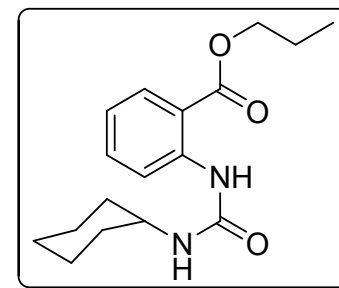
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: chem  
Mercury-400 "IITG-NMR"

<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): 6g

Mass spectra: 6g

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



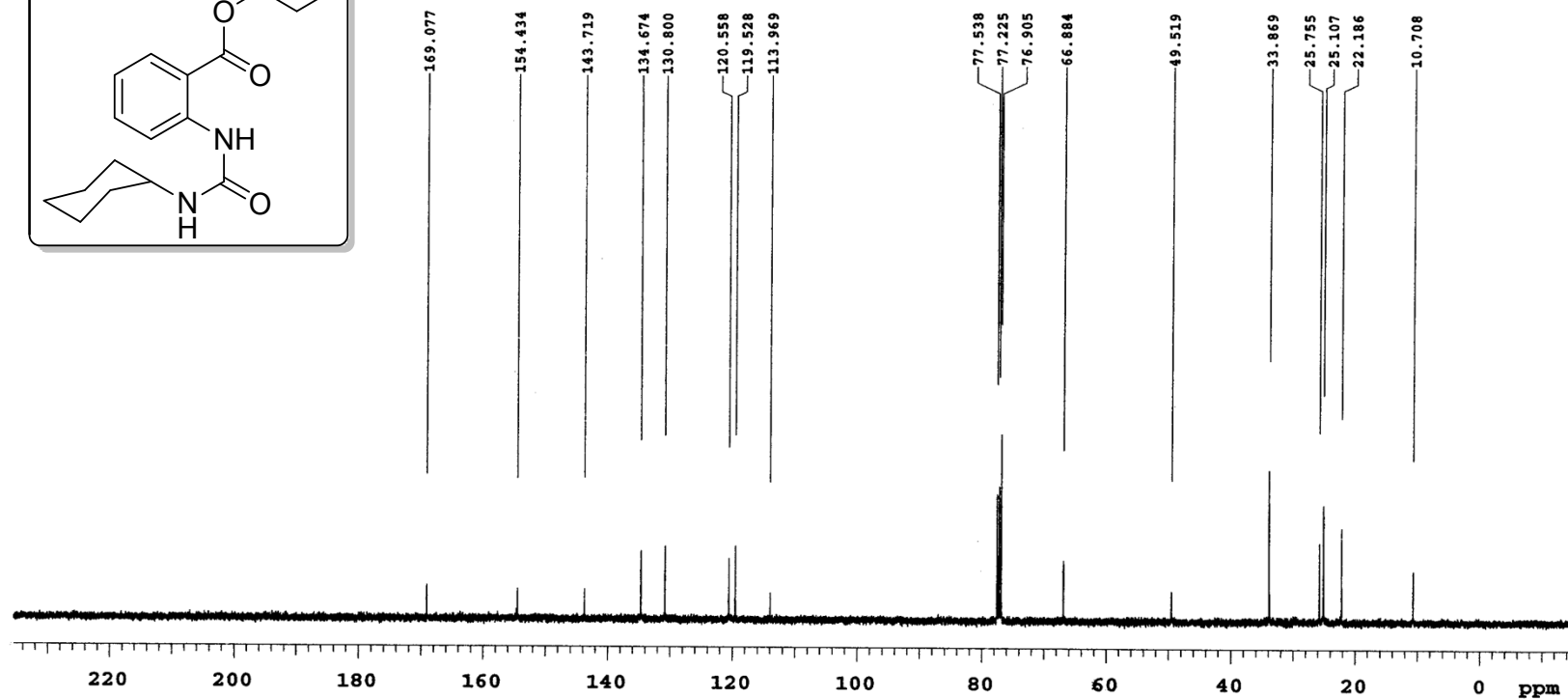
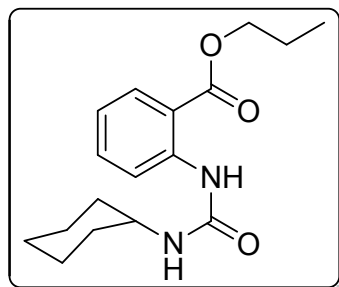
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): **6h**

SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degree  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions

OBSERVE: Cy-Pr- 399.8509721

DATA PROCESSING  
FT size 32768  
Total time 1 minutes

SE-2N-Cy-Pr-1H  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: chem  
Mercury-400 "1H-NMR"

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): **6h**

**PULSE SEQUENCE**  
 Relax delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq time 1.304 sec  
 Width 25125.6 Hz  
 528 repetitions

**OBSERVE** C13, 100.5425584  
**DECOUPLE** H1, 399.8529994  
 Power 42 dB  
 continuously on  
 WALTZ-16 modulated

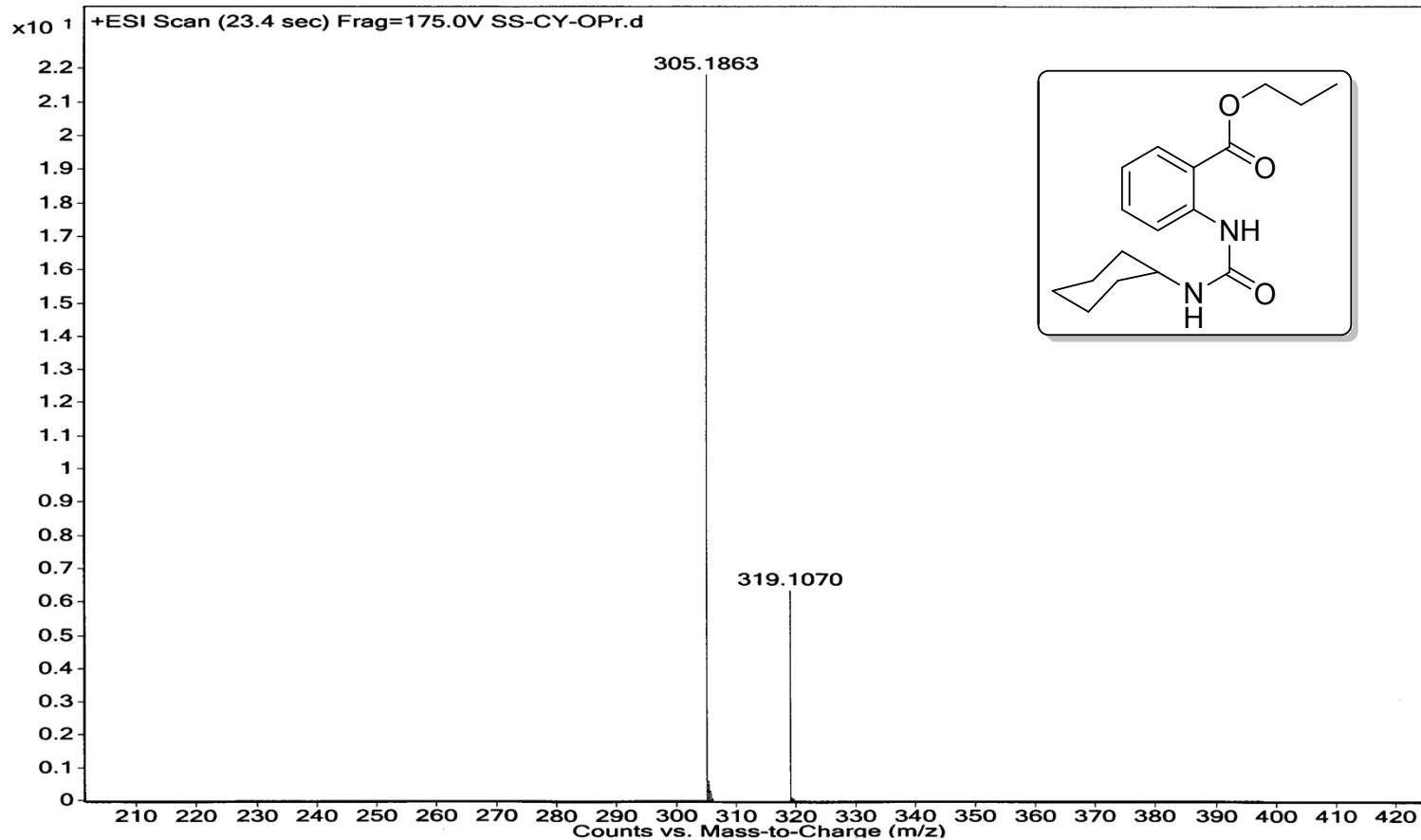
**DATA PROCESSING**  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 19 minutes

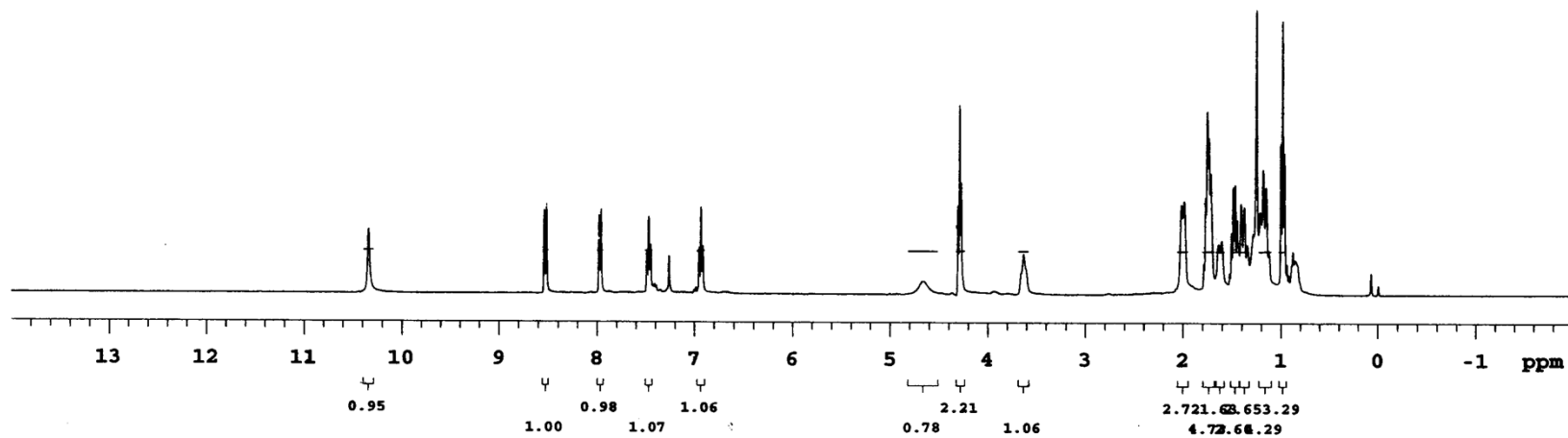
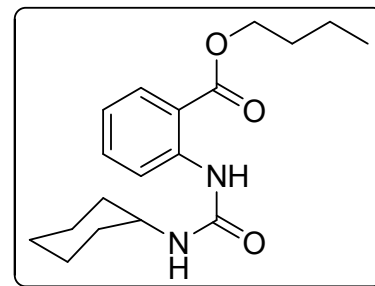
**SS-2N-Cy-Pr-13C**

Solvent: cdd13  
 Temp. 25.0 C / 298.1 K  
 Operator: chem  
 Mercury-400 "ITG-NMR"

Mass spectra: 6h

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



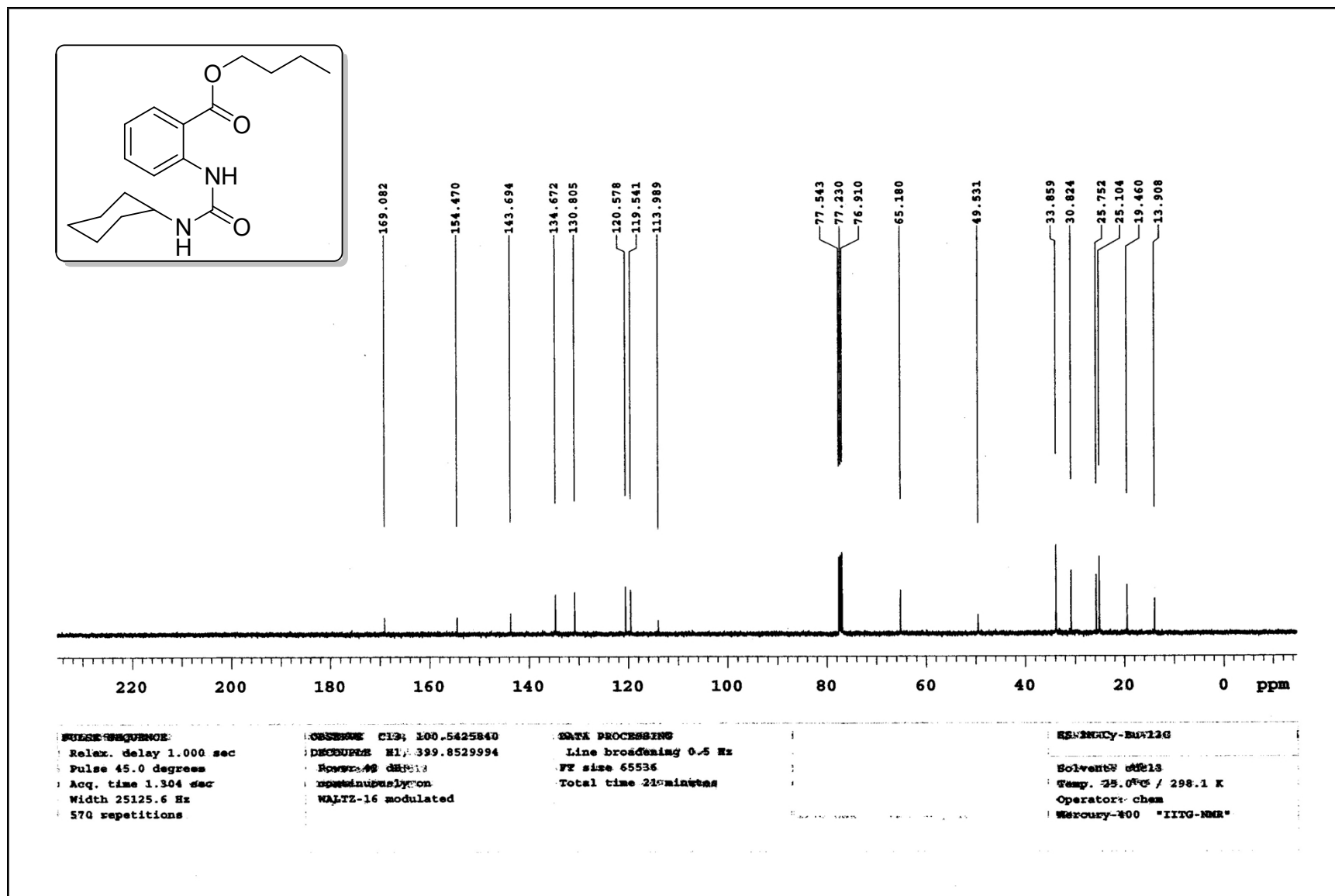
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): 6i

Relax. delay 1.000  
 Pulse 45.0 degree  
 Acq. time 2.561 sec  
 Width 6398.0 Hz  
 32 repetitions

Total time 1.141 sec  
 File size 32758

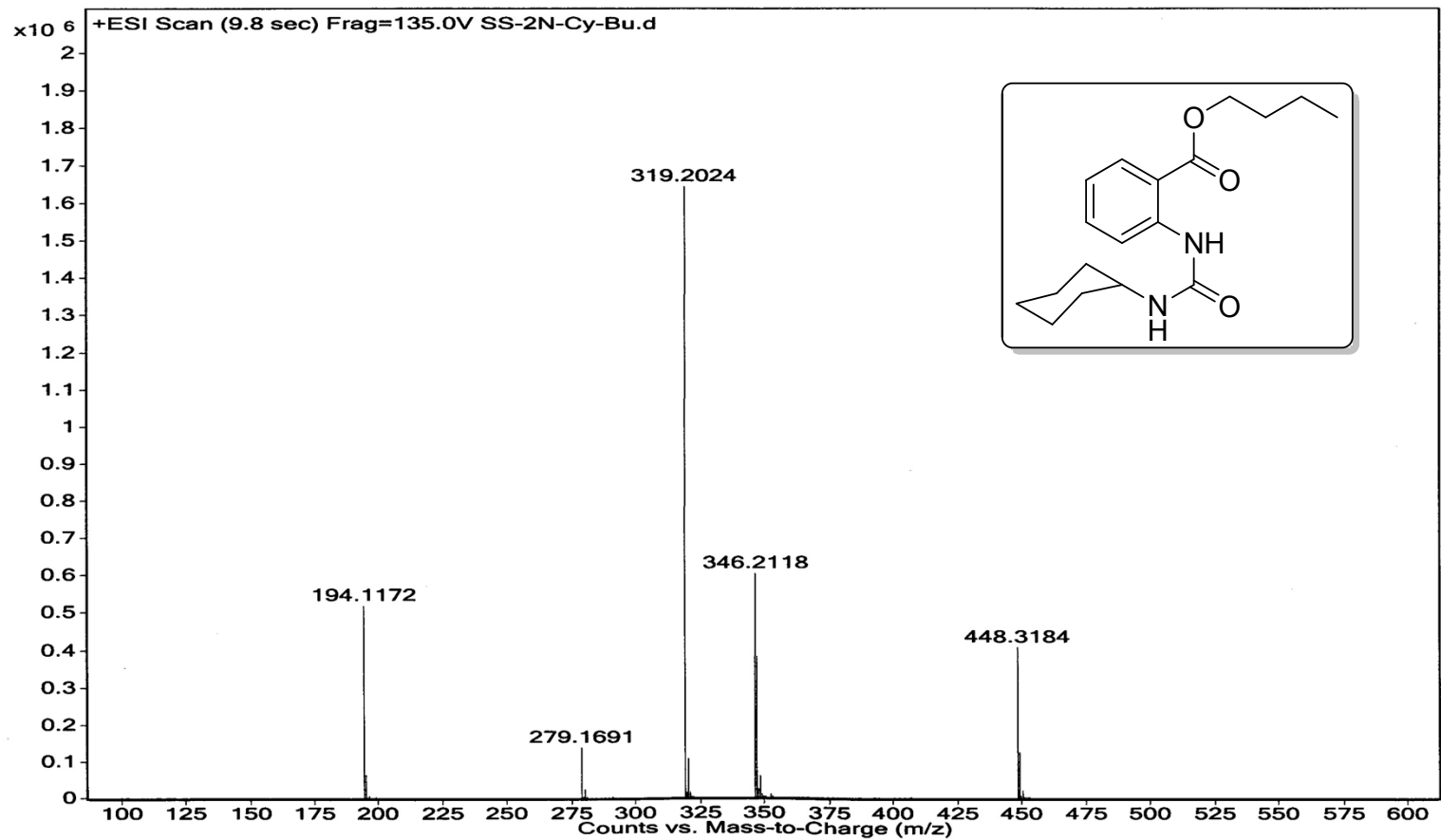
SS-2WgCy-Mn-1H  
 Solvent: cdcl3  
 Temp: 25.0 C / 298.1 K  
 Operator: chem  
 Mercury-400 #IITG-NMR

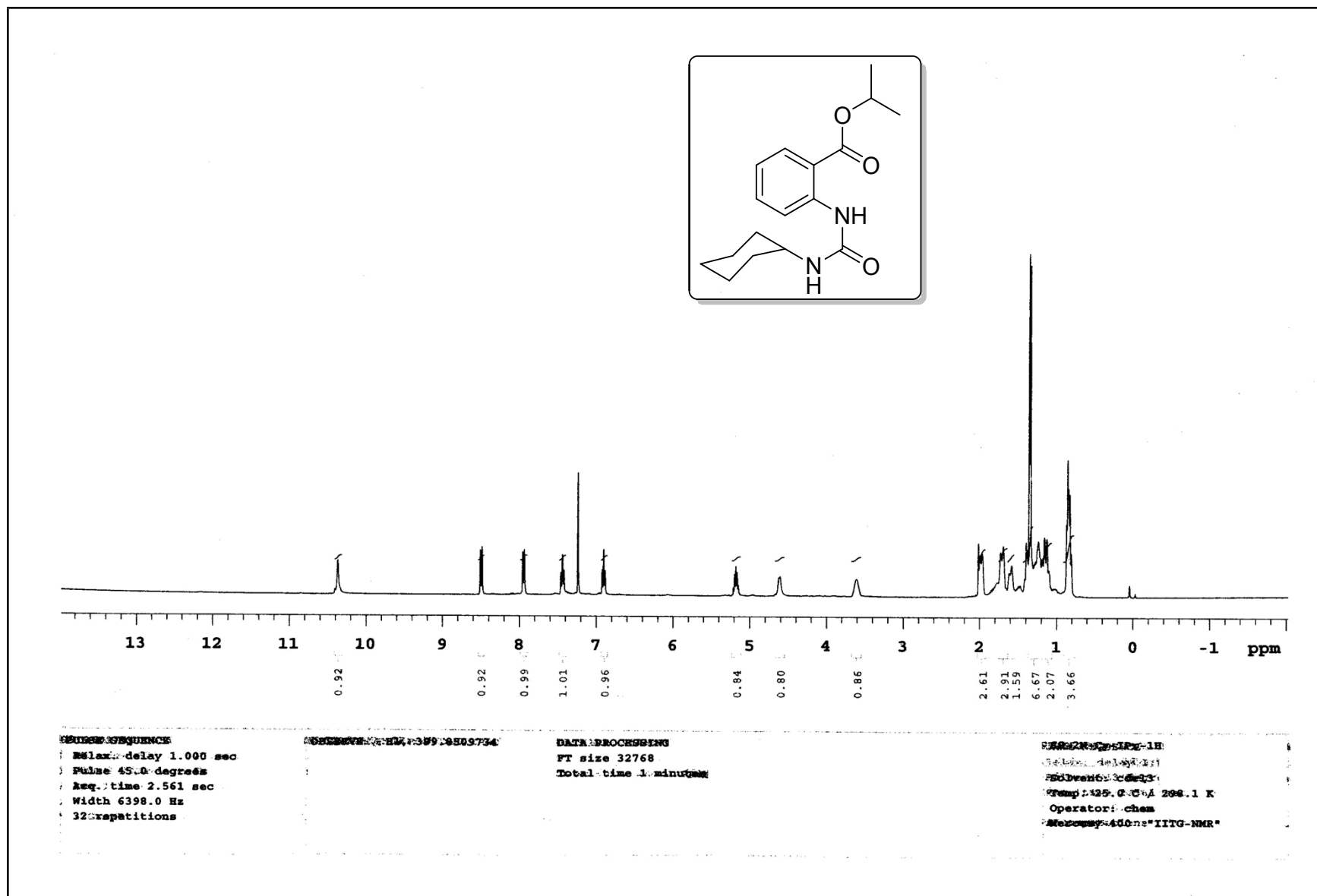


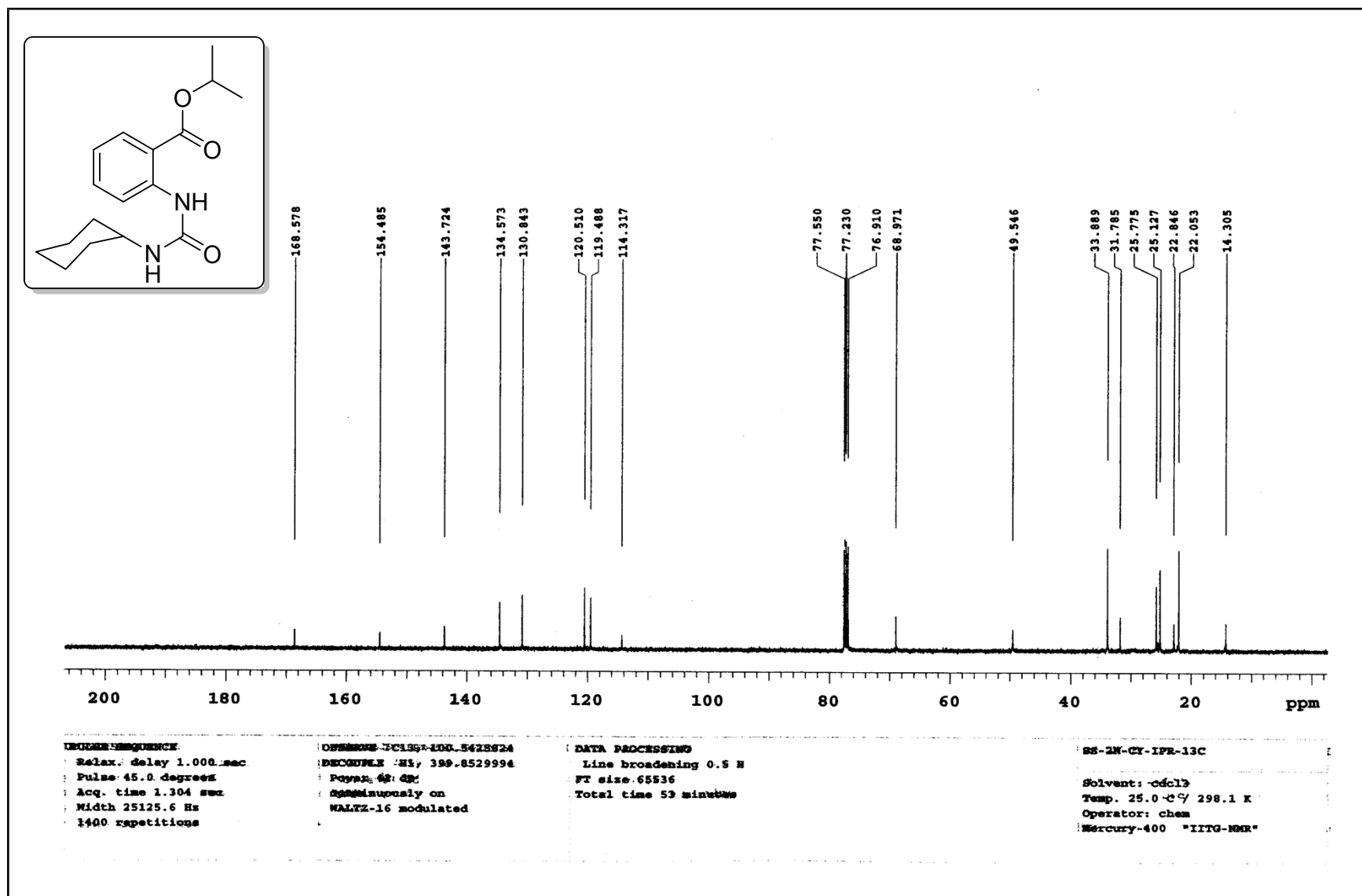
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): **6i**

Mass spectra: 6i

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time

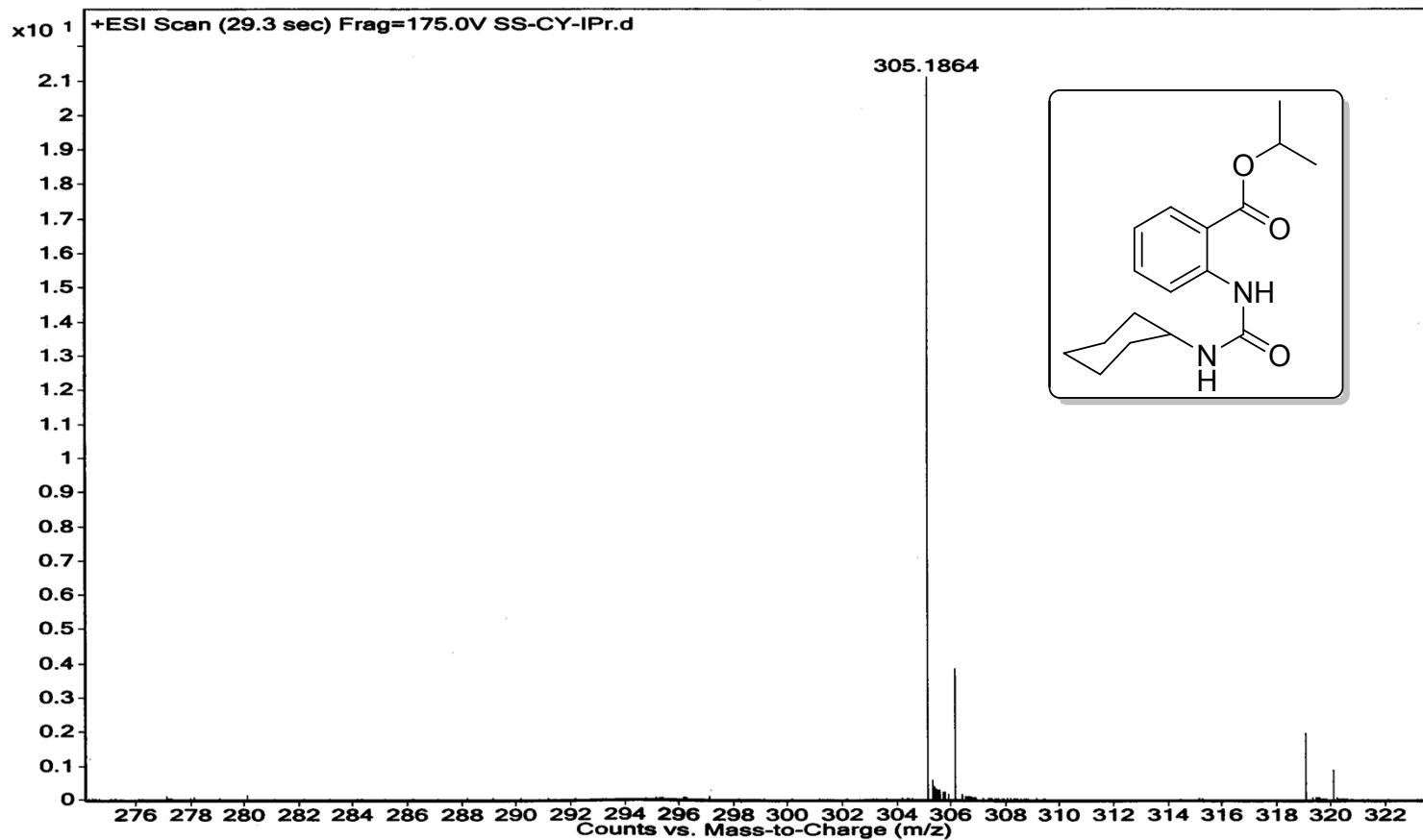


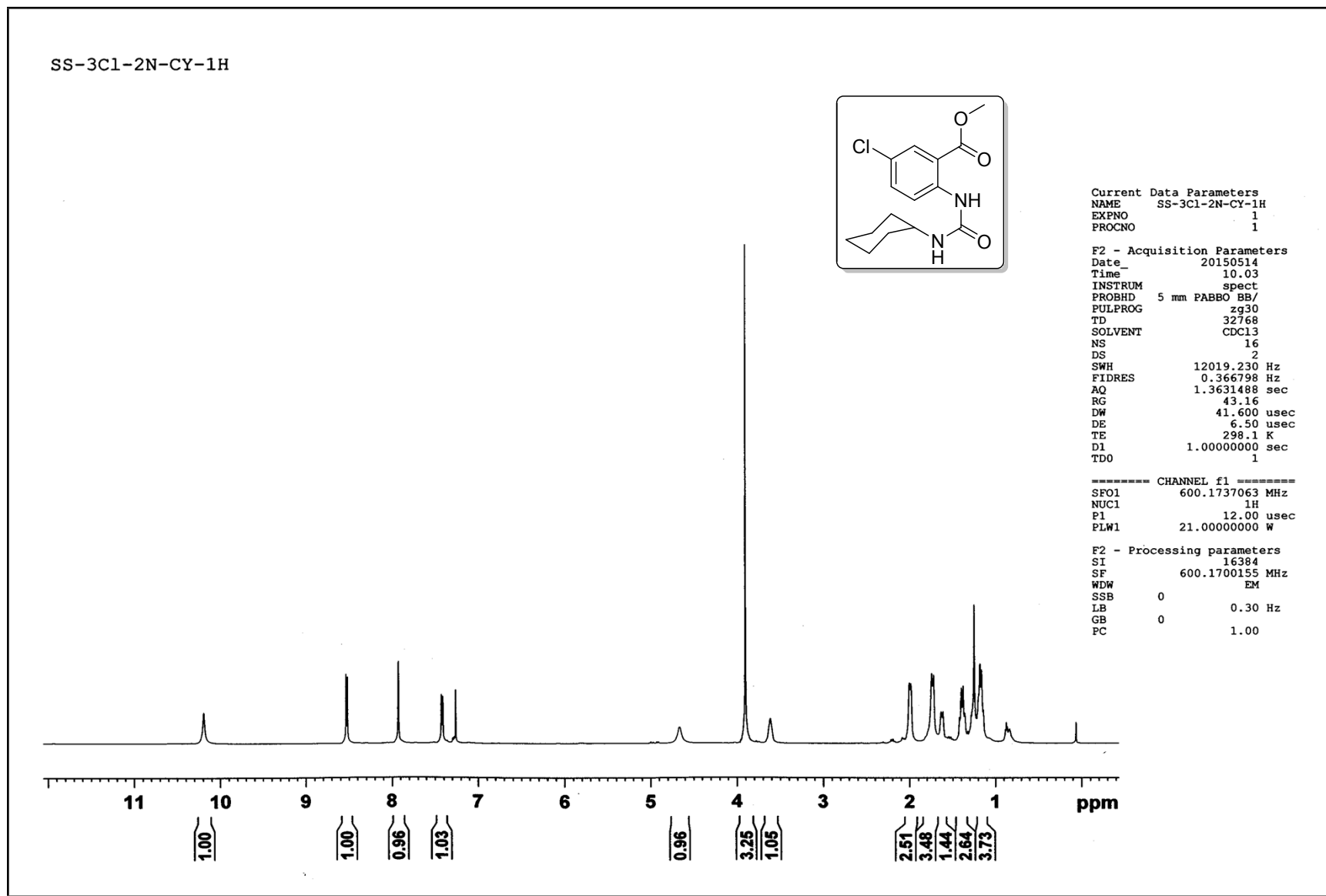
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): 6j

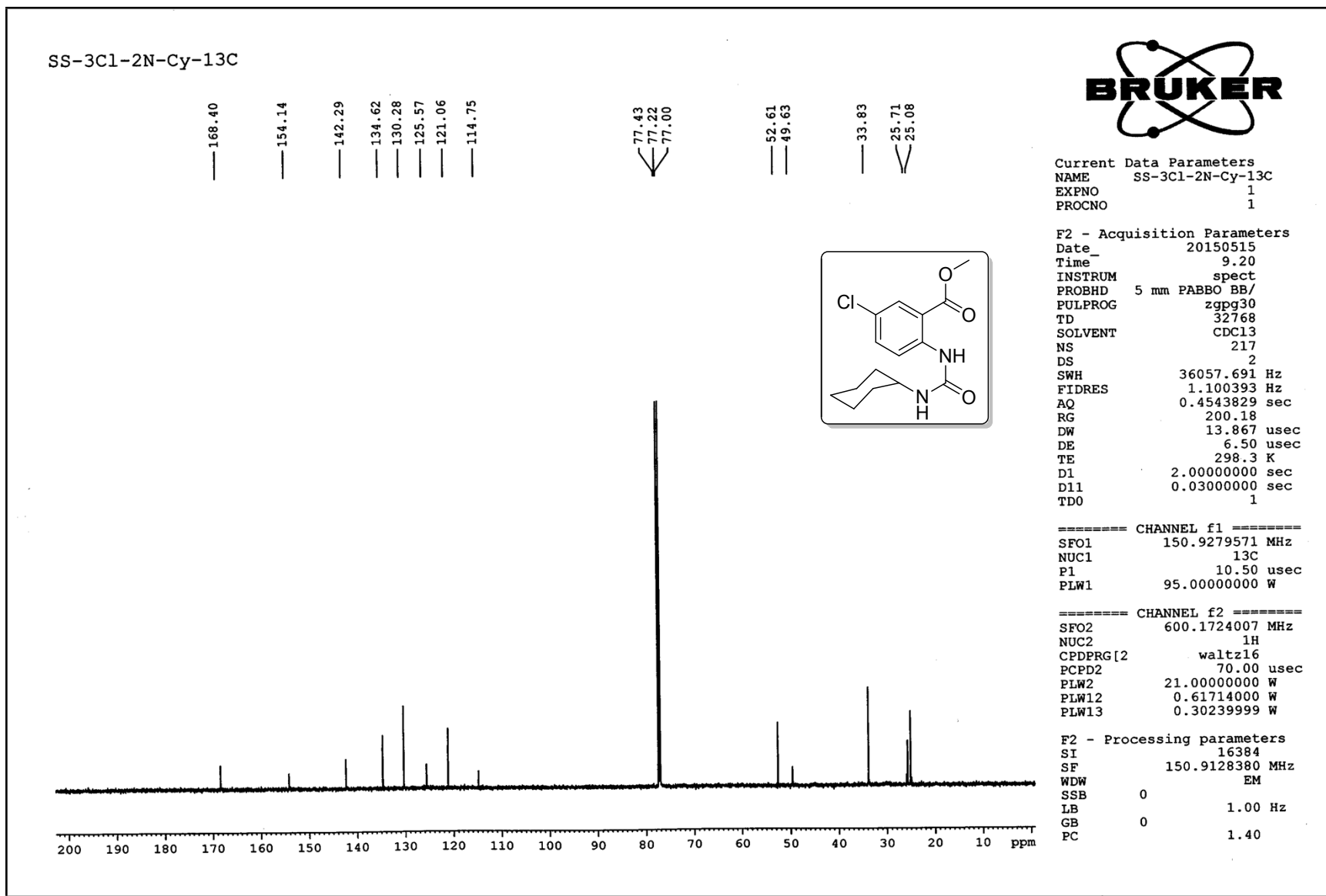
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): **6j**

Mass spectra: 6j

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time

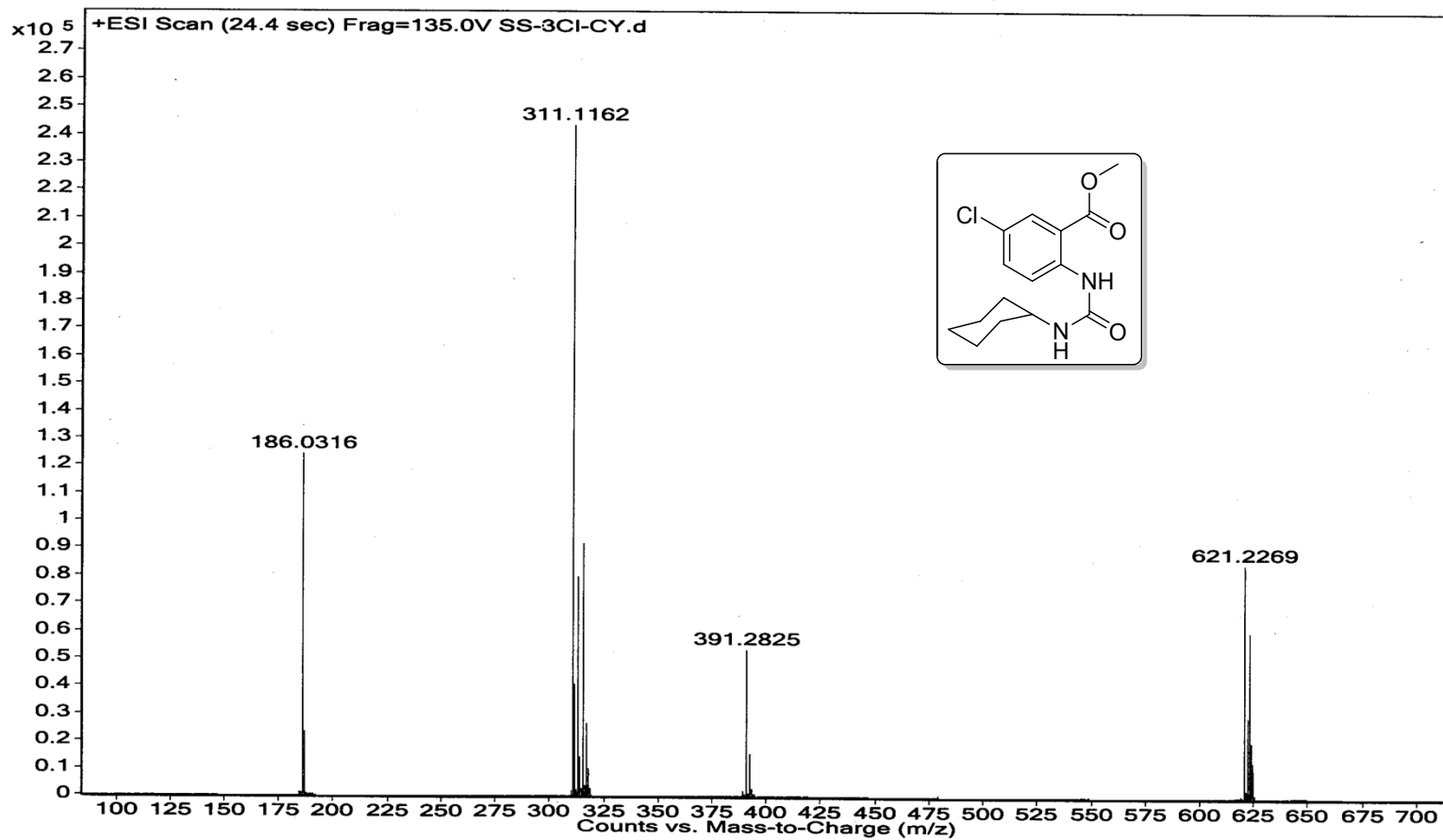


<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): **6k**

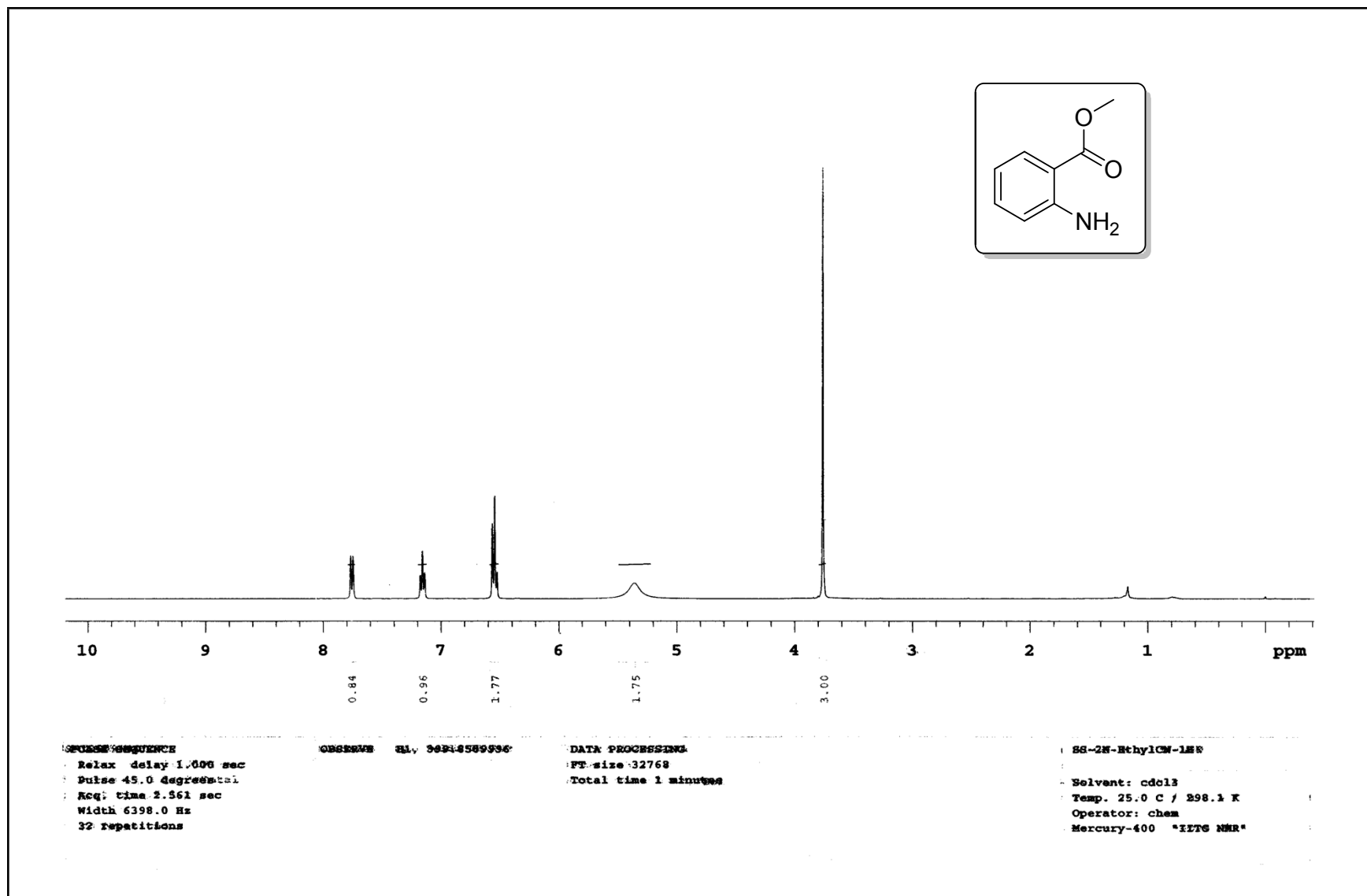
<sup>13</sup>CNMR (150 MHz, CDCl<sub>3</sub>): **6k**

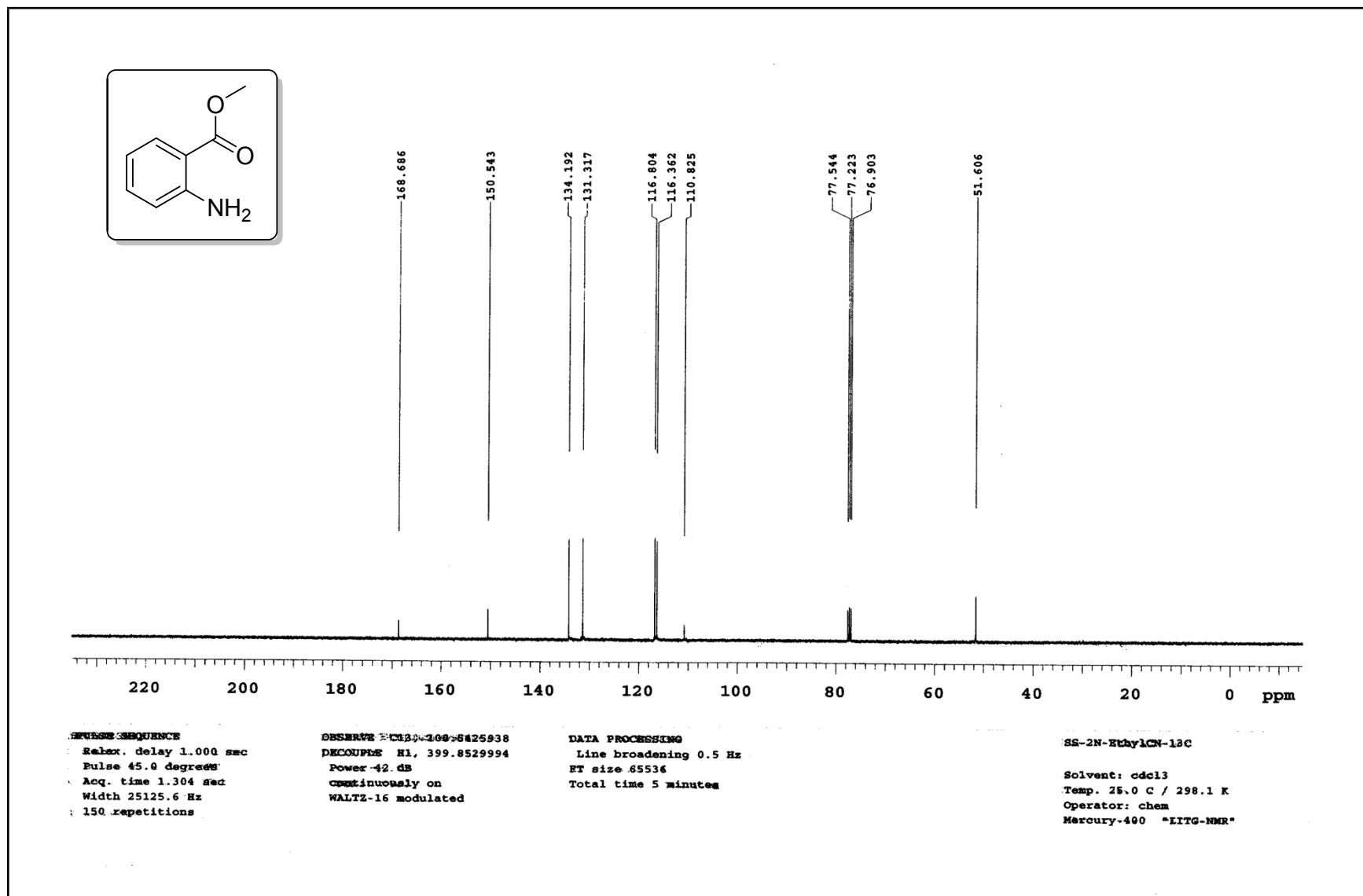
## Mass Spectra: 6k

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



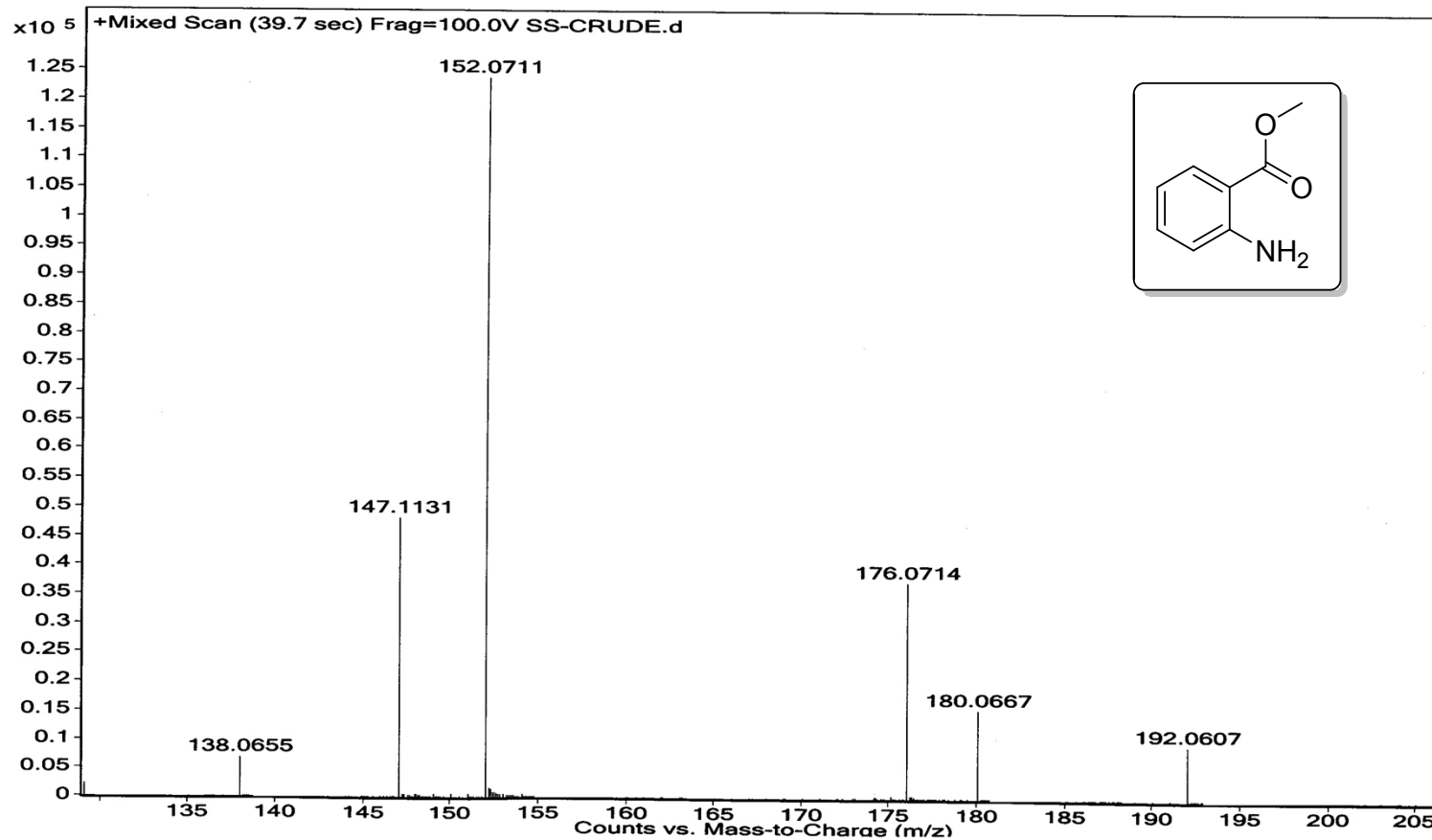


<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): 7a

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ): 7a

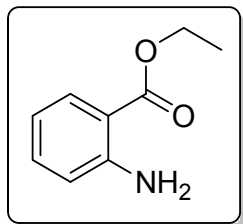
Mass spectra: 7a

<b>Sample Name</b>	SS-CRUDE	<b>Position</b>	Vial 1	<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Inj Vol</b>	-10	<b>InjPosition</b>		<b>SampleType</b>	Sample	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	SS-CRUDE.d	<b>ACQ Method</b>		<b>Comment</b>		<b>Acquired Time</b>	1/12/2015 3:18:32 PM



<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): **7b**

SS-2N-EtCN-EtOH-1H

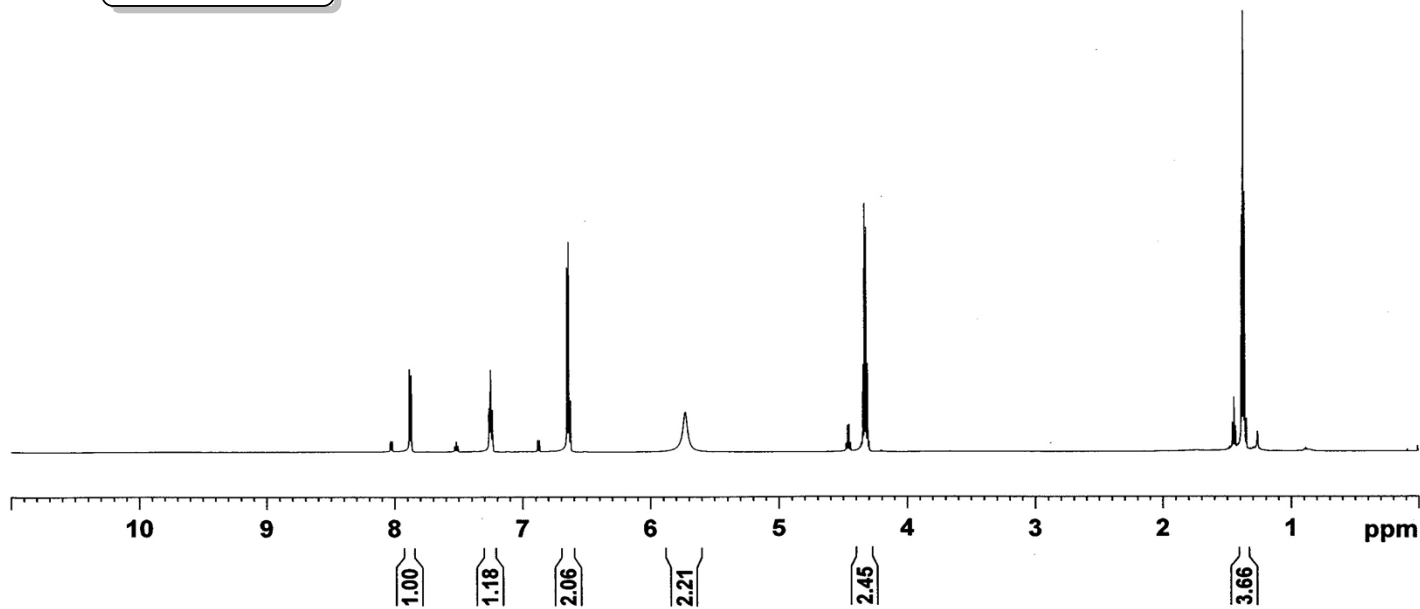


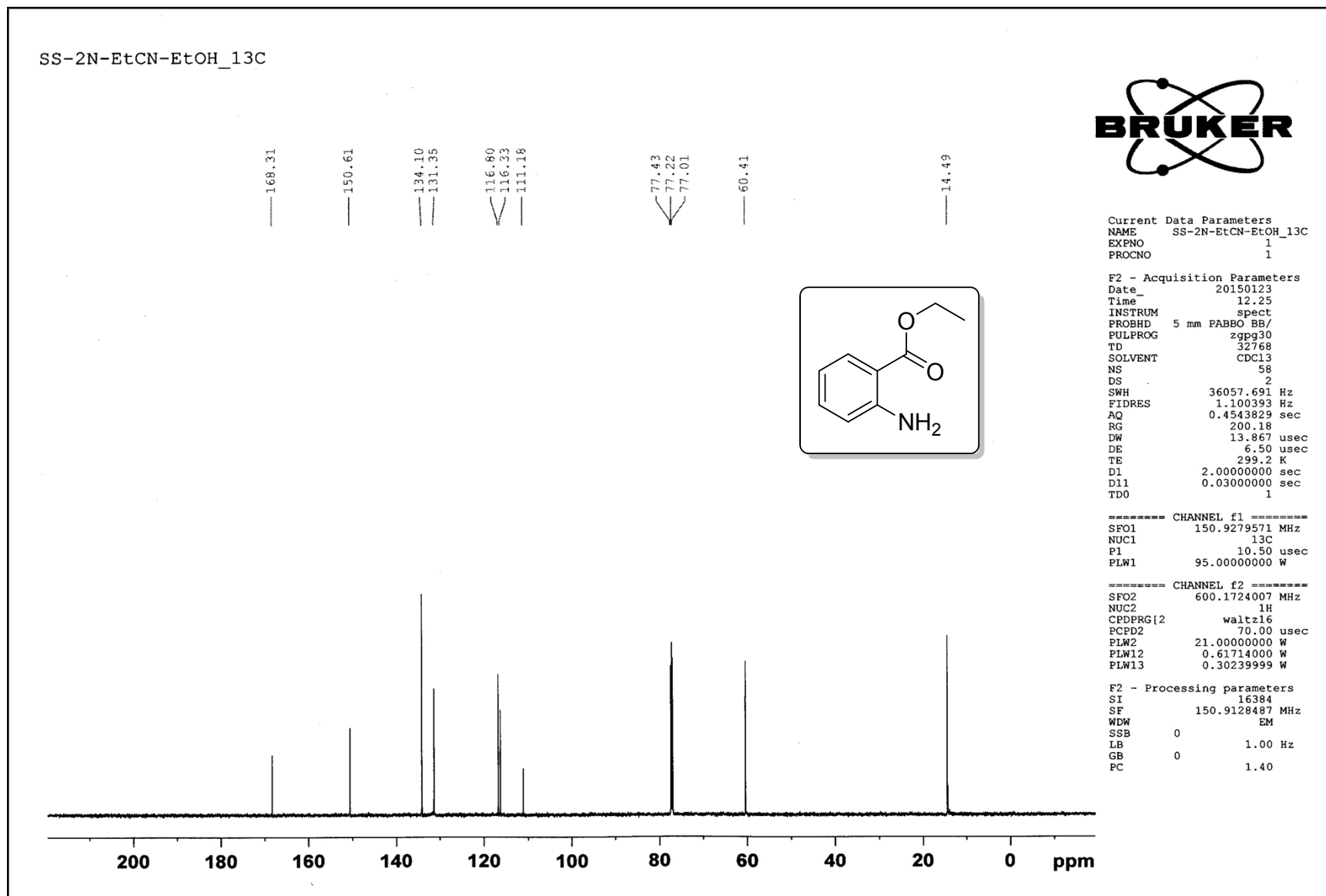
Current Data Parameters  
NAME SS-2N-EtCN-EtOH-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150205  
Time 9.58  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 18.03  
DM 41.600 usec  
DE 6.50 usec  
TE 297.7 K  
D1 1.0000000 sec  
TDO 1

----- CHANNEL f1 -----  
SF01 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLM1 21.0000000 W

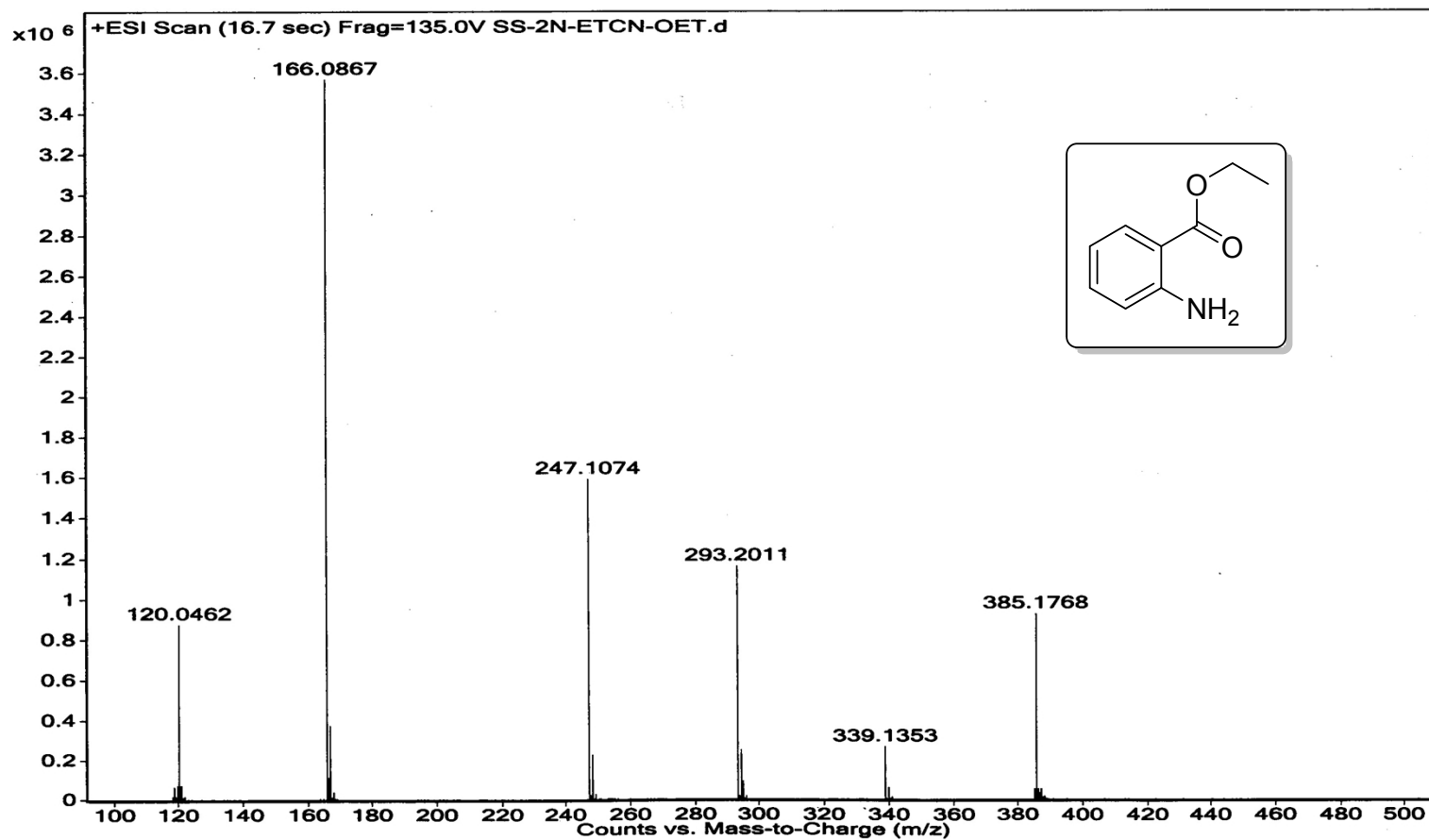
F2 - Processing parameters  
SI 16384  
SF 600.1700155 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

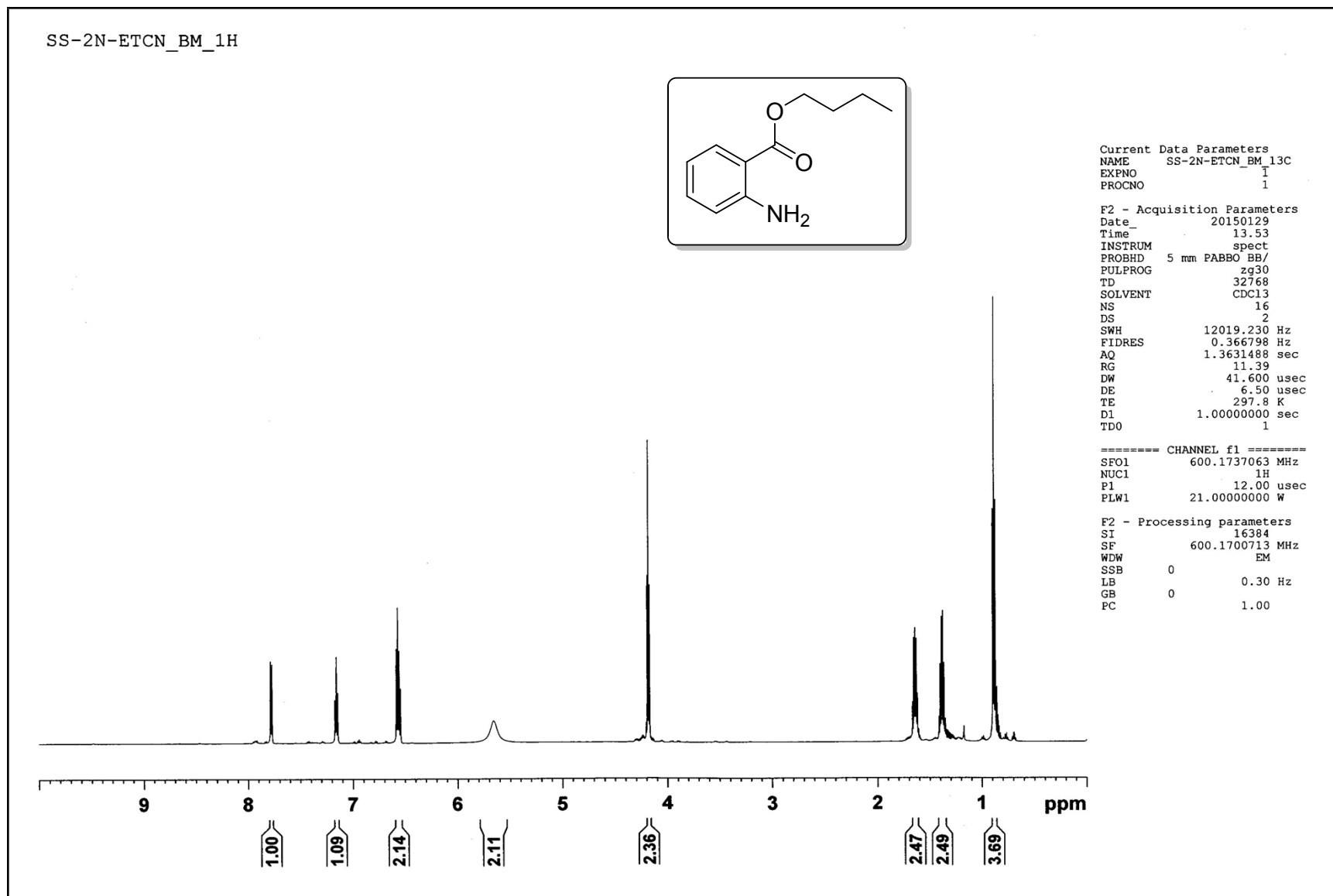


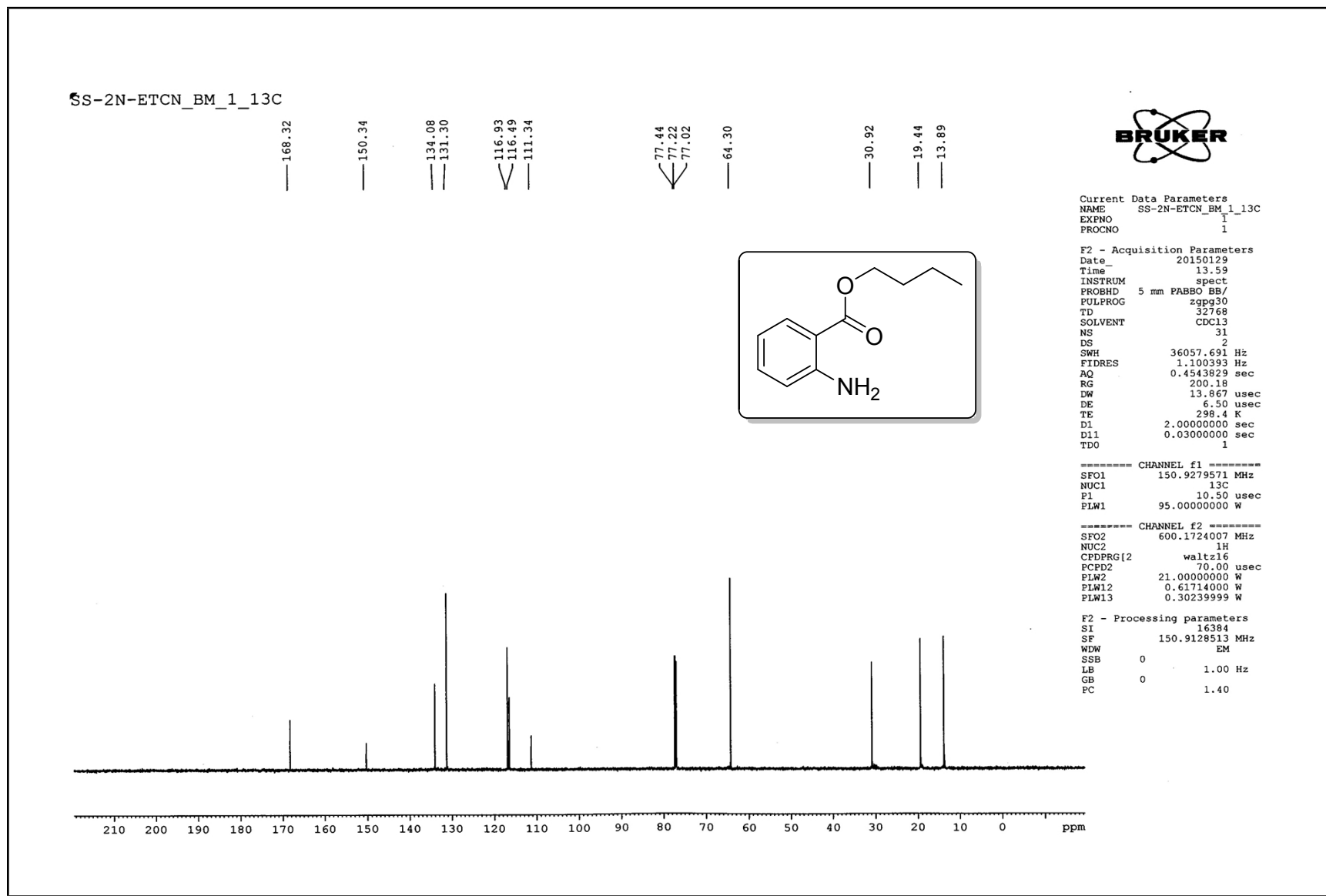
$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): **7b**

Mass spectra: 7b

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



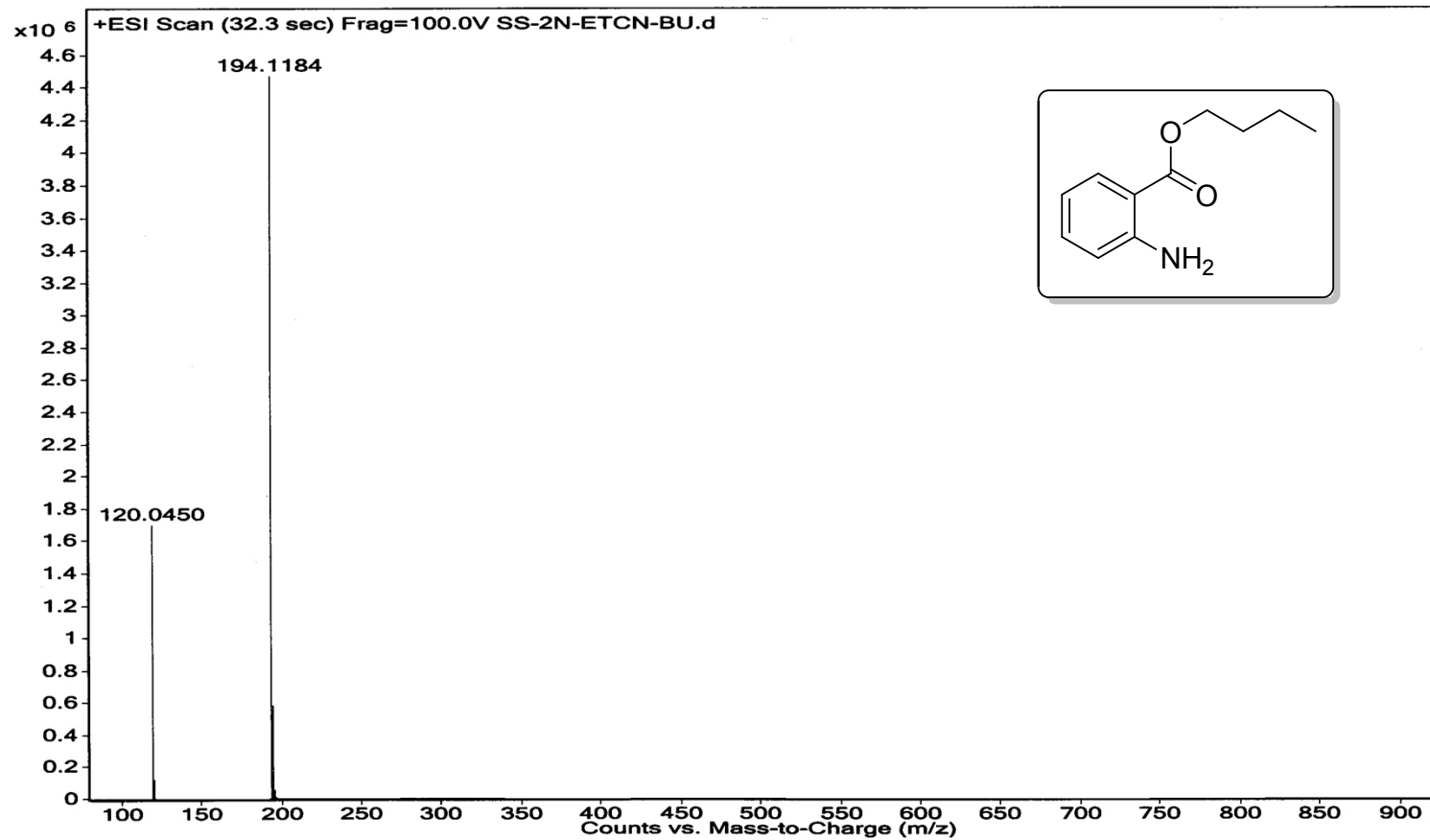
<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): 7c

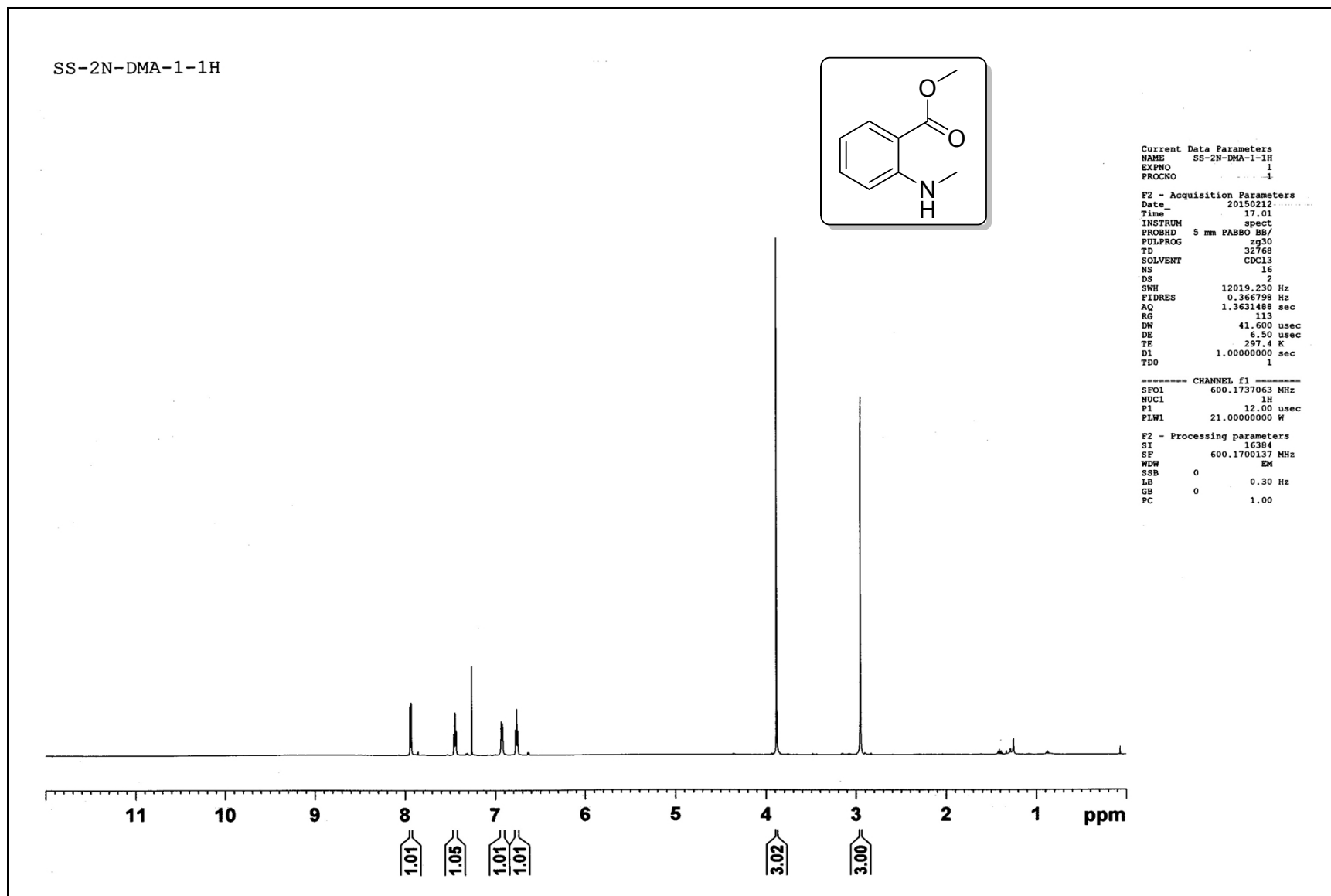
$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): **7c**

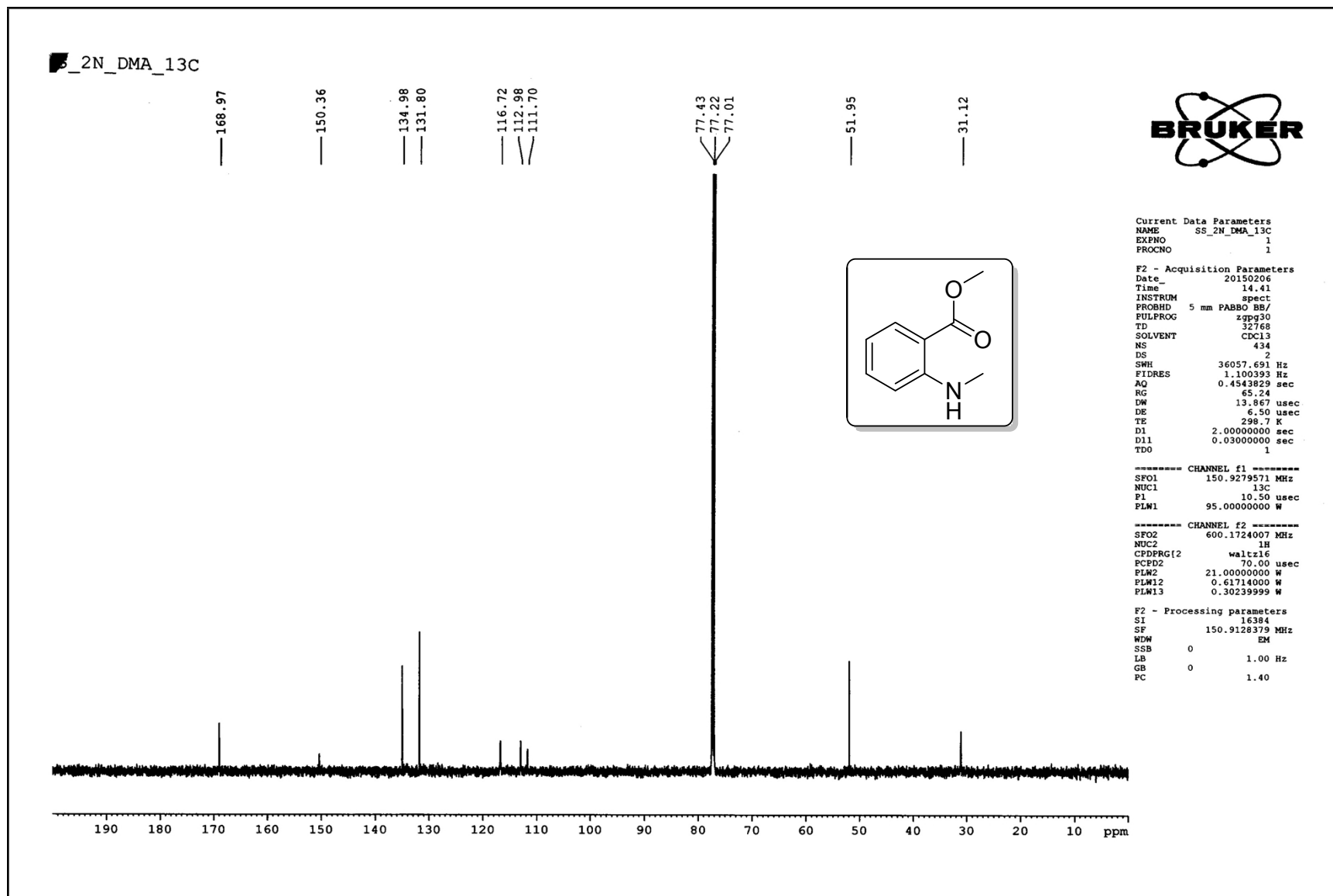


Mass spectra: 7c

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time

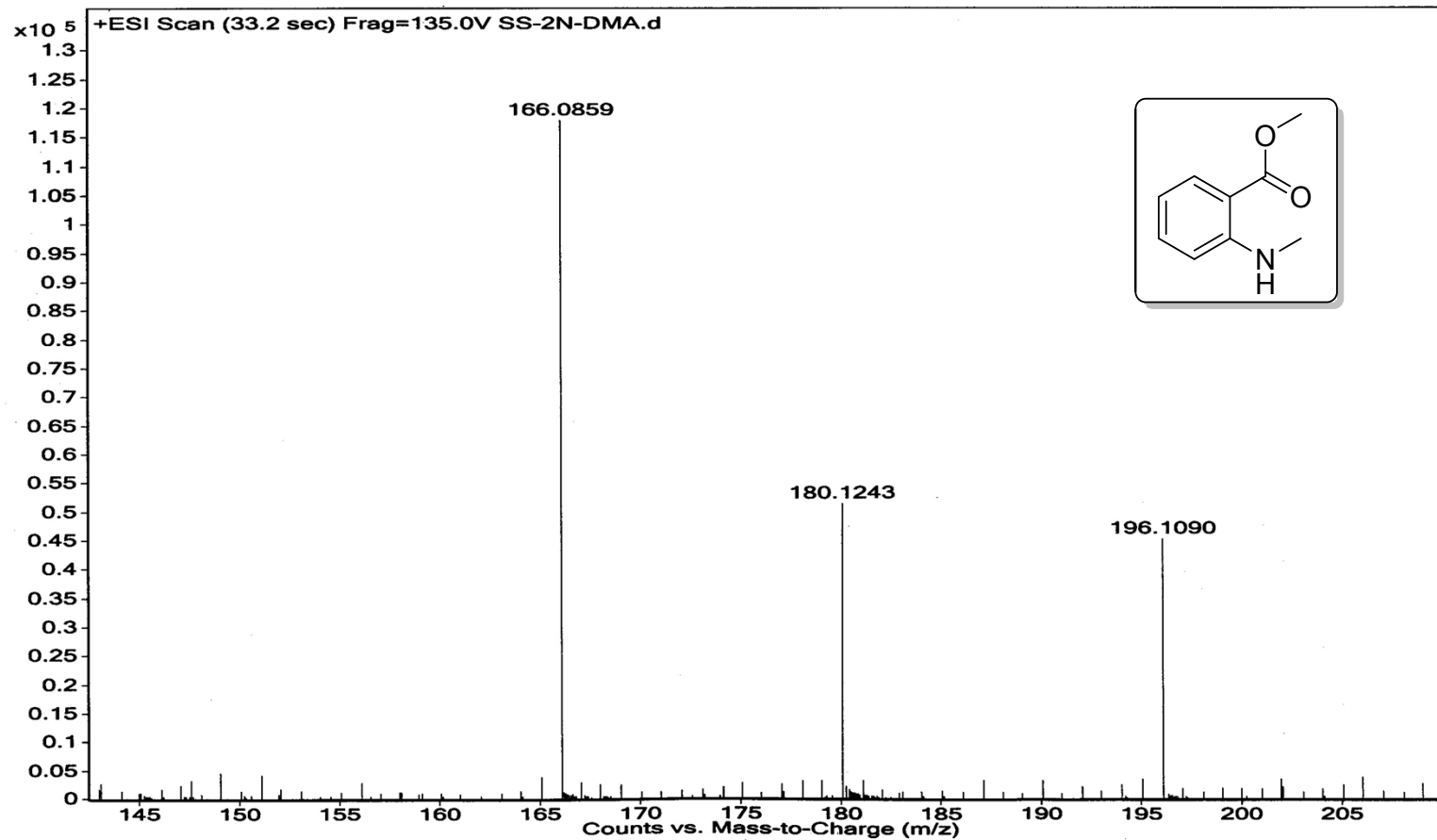


<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): **7a'**

$^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ): **7a'**

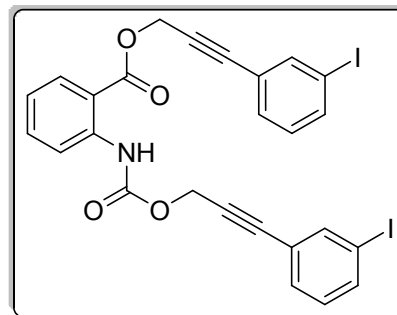
Mass spectra: 7a'

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): **8a**

SS-2N-SCDI-1H



```

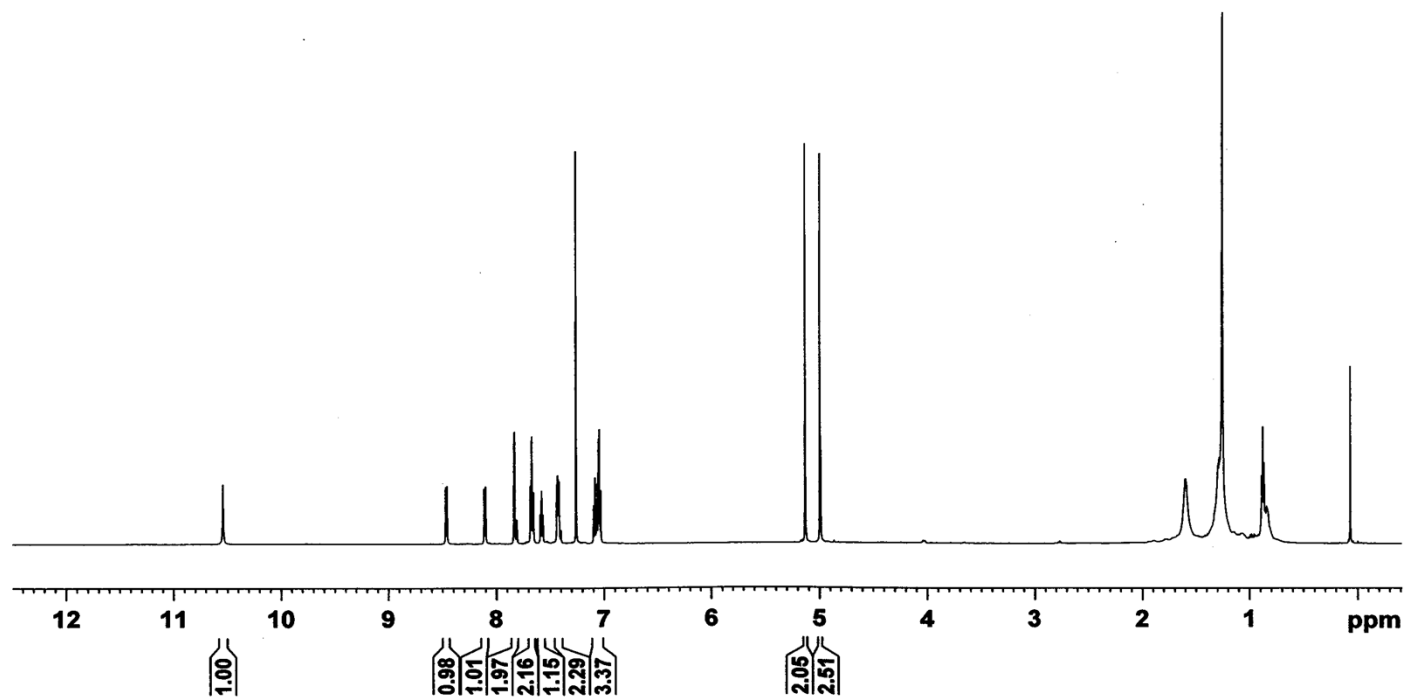
Current Data Parameters
NAME      SS-2N-SCDI-1H
EXPNO     1
PROCNO    1

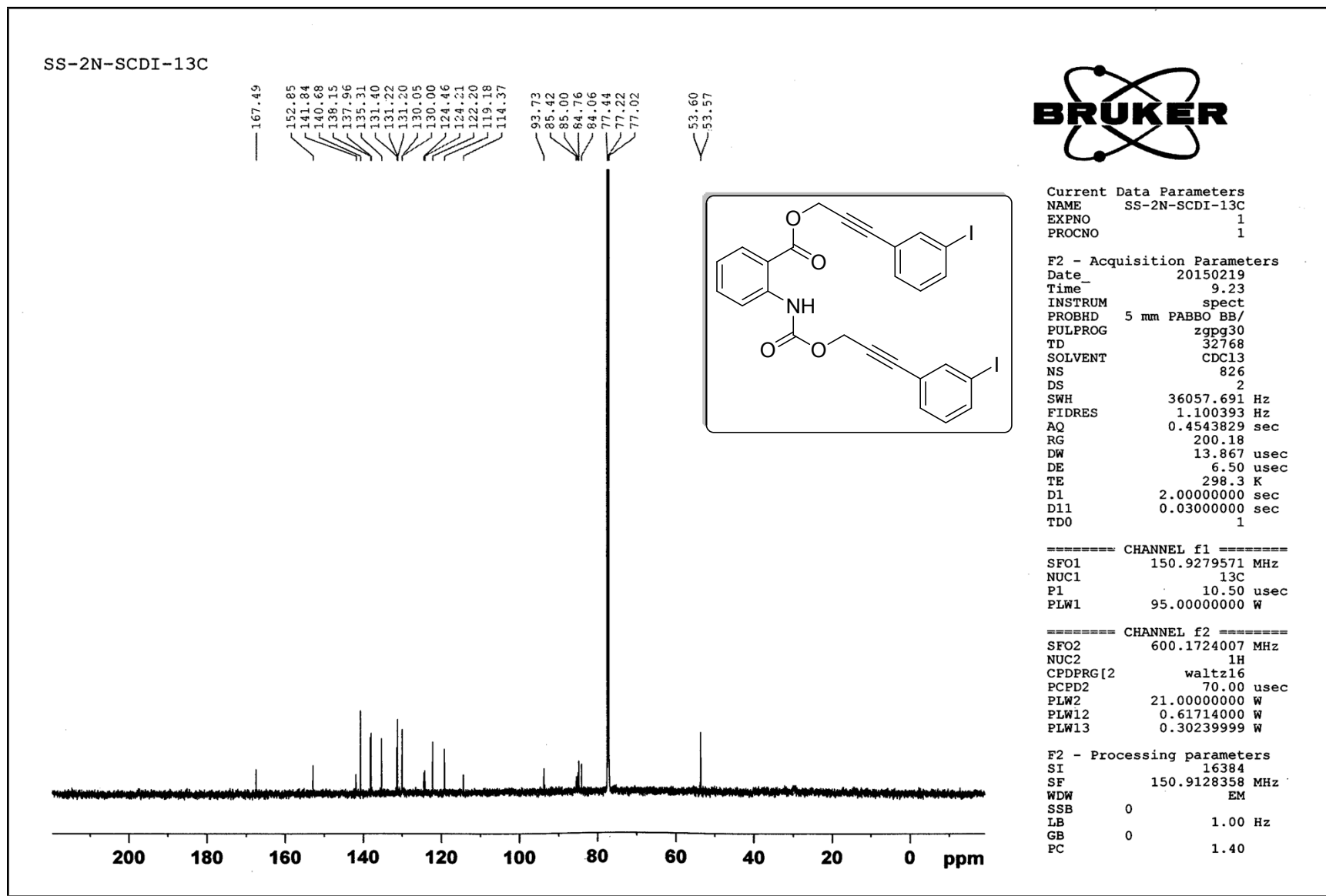
F2 - Acquisition Parameters
Date_     20150213
Time      9.49
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD        32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        12019.230 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         73.2
DW         41.600 usec
DE         6.50 usec
TE         297.9 K
D1         1.0000000 sec
TDO        1

----- CHANNEL f1 -----
SFO1      600.1737063 MHz
NUC1       1H
P1         12.00 usec
PLW1      21.00000000 W

F2 - Processing parameters
SI         16384
SF         600.1700144 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

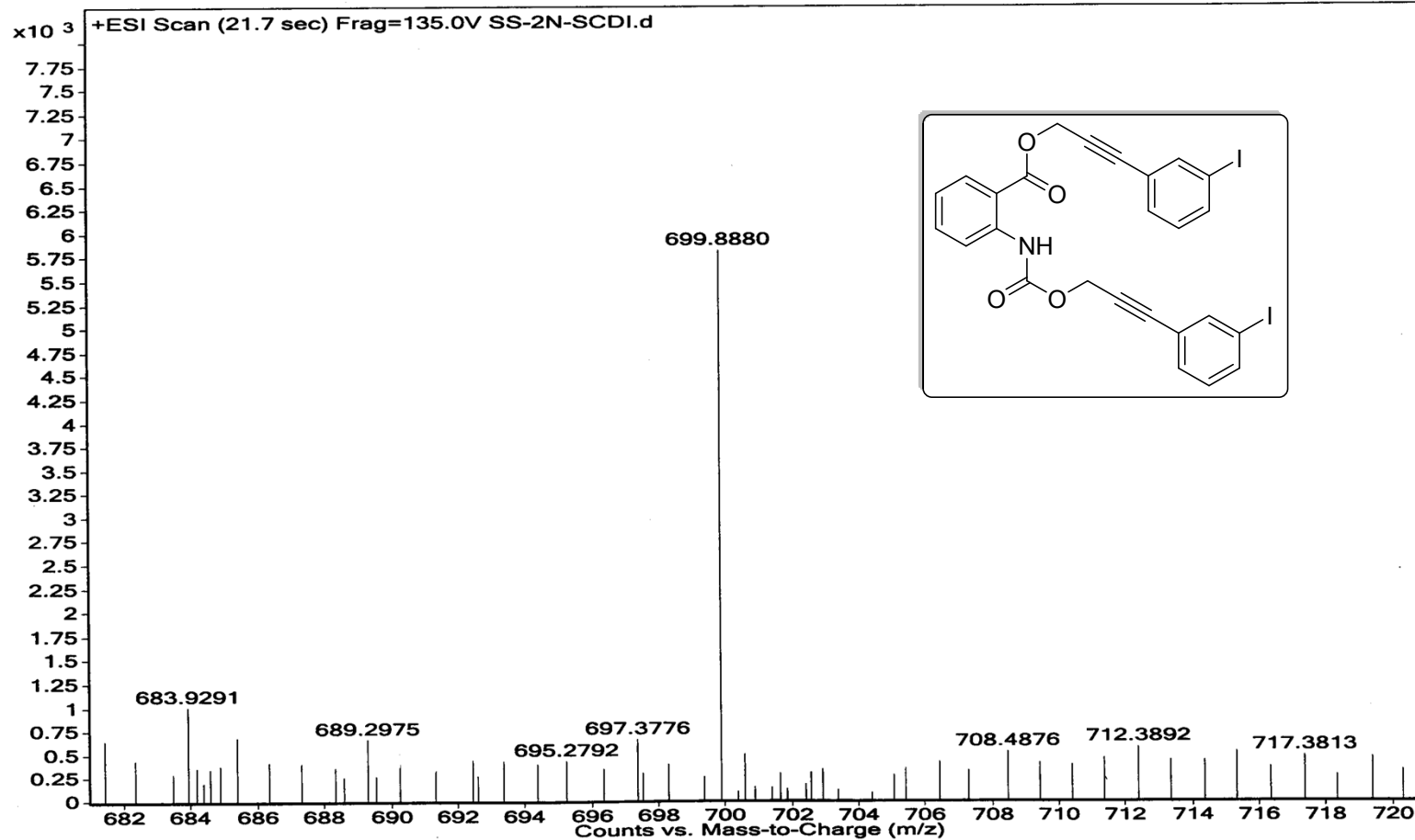
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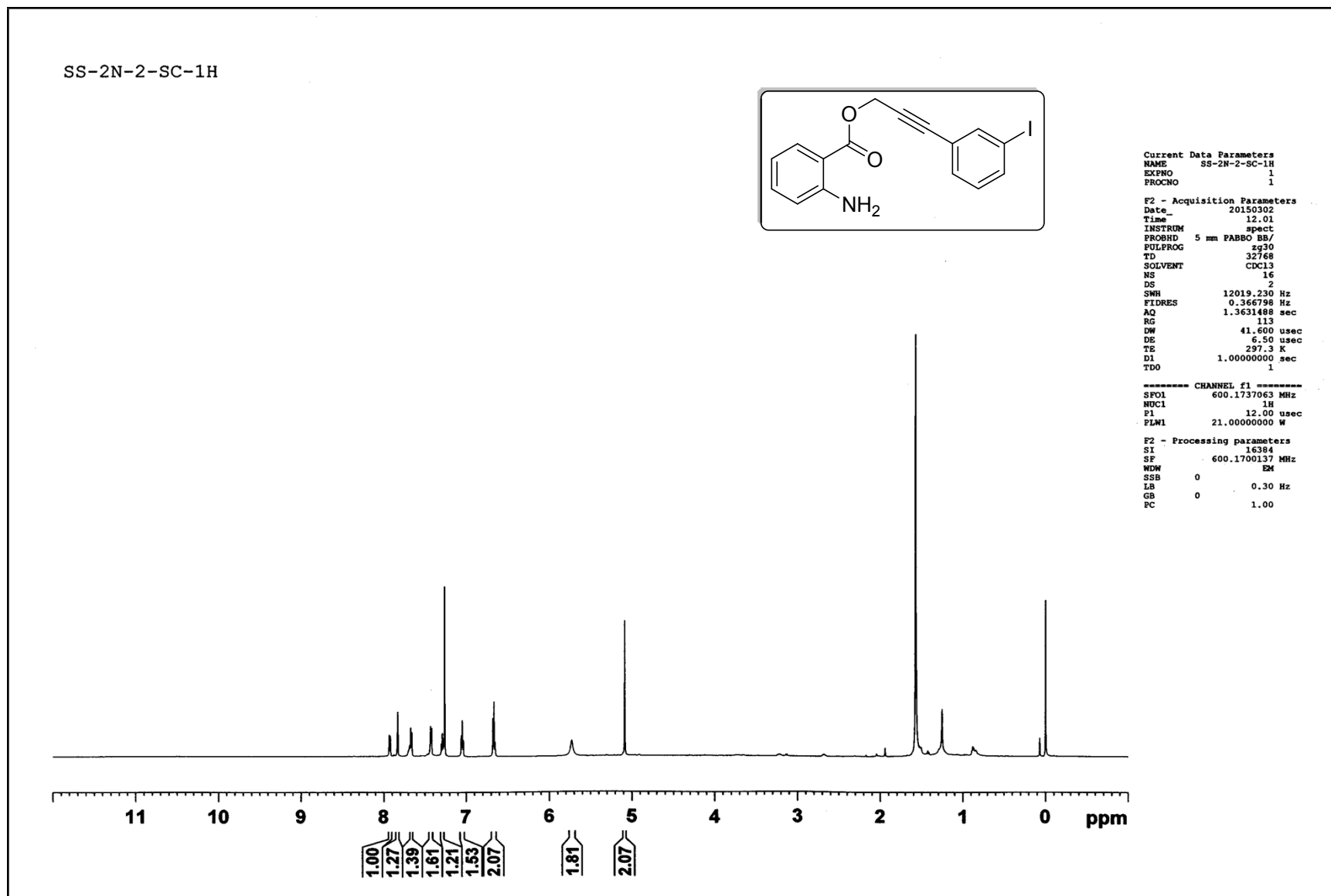


<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): **8a**

## Mass Spectra: 8a

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time

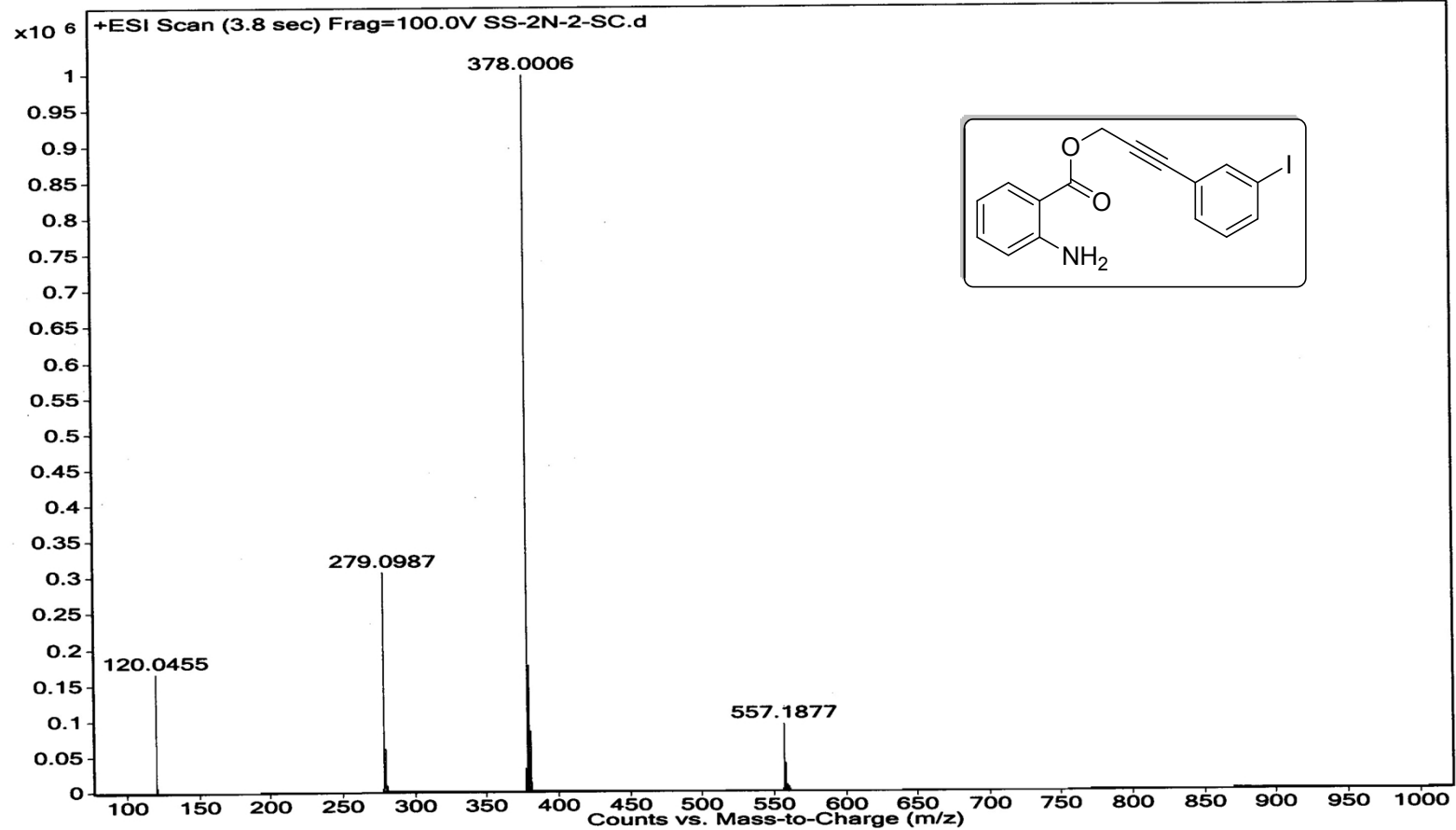


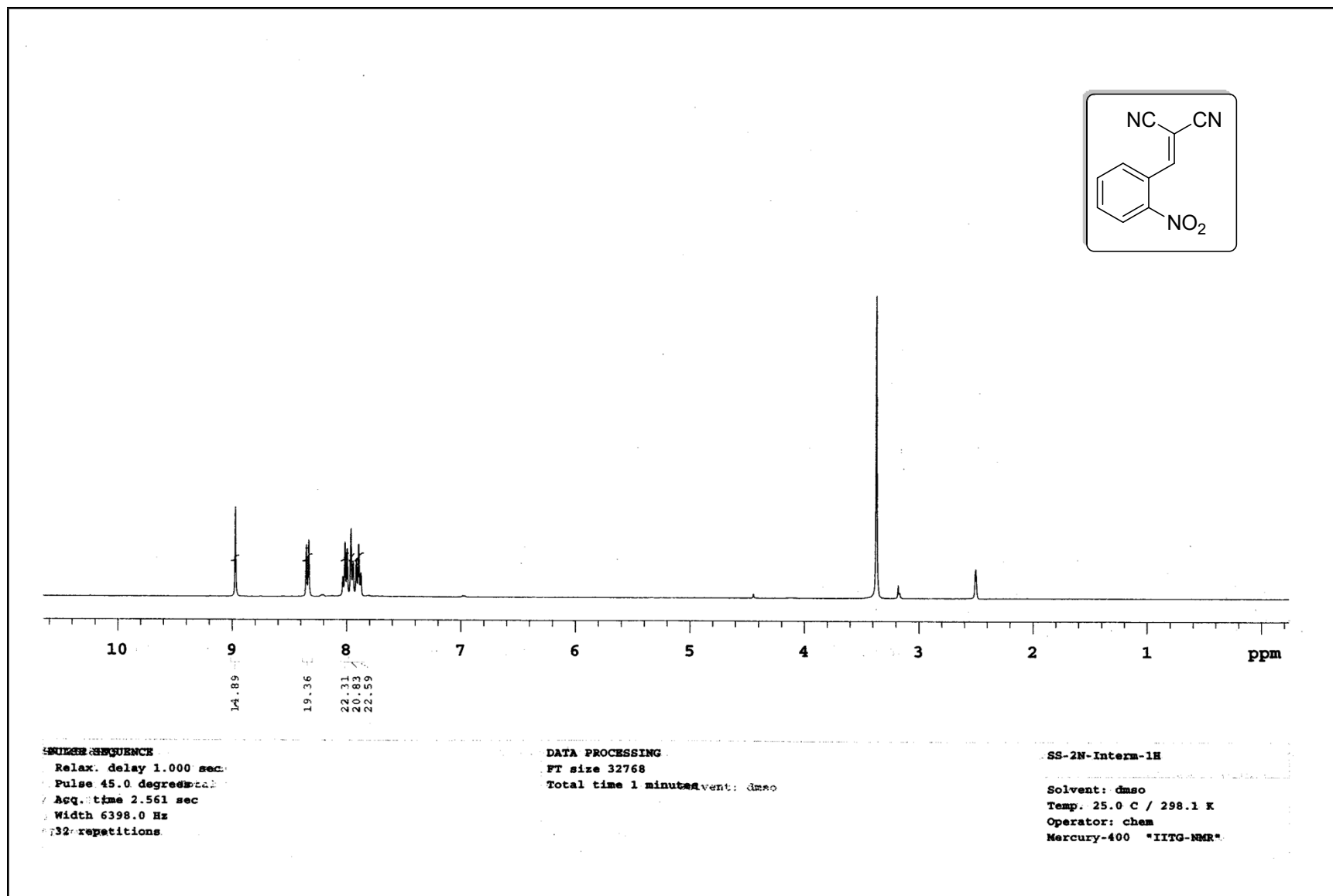
<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): **8b**



## Mass Spectra: 8b

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): A

<sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): A