

Supporting Information

for

Parallel Synthesis of an Imidazole-4,5-dicarboxamide Library Bearing Amino Acid Esters and Alkanamines

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74104

Table of Contents

Page S1-3.	Title Page and Table of Contents	Page S20.	Figure S12. LC/MS data for 5{12} .
Page S4.	Table S1. Amino Acid Ester— Alkanamine Disubstituted I45DCs, 5{1-28} .	Page S21.	Figure S13. LC/MS data for 5{13} .
Page S5.	Table S2. Amino Acid Ester— Alkanamine Disubstituted I45DCs, 5{29-56} .	Page S22.	Figure S14. LC/MS data for 5{14} .
Page S6.	Table S3. Amino Acid Ester— Alkanamine Disubstituted I45DCs, 5{57-84} .	Page S23.	Figure S15. LC/MS data for 5{15} .
Page S7.	Table S4. Amino Acid Ester— Alkanamine Disubstituted I45DCs, 5{85-112} .	Page S24.	Figure S16. LC/MS data for 5{16} .
Page S8.	Table S5. Amino Acid Ester— Alkanamine Disubstituted I45DCs, 5{113-126} .	Page S25.	Figure S17. LC/MS data for 5{17} .
Page S9.	Figure S1. LC/MS data for 5{1} .	Page S26.	Figure S18. LC/MS data for 5{18} .
Page S10.	Figure S2. LC/MS data for 5{2} .	Page S27.	Figure S19. LC/MS data for 5{19} .
Page S11.	Figure S3. LC/MS data for 5{3} .	Page S28.	Figure S20. LC/MS data for 5{20} .
Page S12.	Figure S4. LC/MS data for 5{4} .	Page S29.	Figure S21. LC/MS data for 5{21} .
Page S13.	Figure S5. LC/MS data for 5{5} .	Page S30.	Figure S22. LC/MS data for 5{22} .
Page S14.	Figure S6. LC/MS data for 5{6} .	Page S31.	Figure S23. LC/MS data for 5{23} .
Page S15.	Figure S7. LC/MS data for 5{7} .	Page S32.	Figure S24. LC/MS data for 5{24} .
Page S16.	Figure S8. LC/MS data for 5{8} .	Page S33.	Figure S25. LC/MS data for 5{25} .
Page S17.	Figure S9. LC/MS data for 5{9} .	Page S34.	Figure S26. LC/MS data for 5{26} .
Page S18.	Figure S10. LC/MS data for 5{10} .	Page S35.	Figure S27. LC/MS data for 5{27} .
Page S19.	Figure S11. LC/MS data for 5{11} .	Page S36.	Figure S28. LC/MS data for 5{28} .
		Page S37.	Figure S29. LC/MS data for 5{29} .
		Page S38.	Figure S30. LC/MS data for 5{30} .
		Page S39.	Figure S31. LC/MS data for 5{31} .
		Page S40.	Figure S32. LC/MS data for 5{32} .
		Page S41.	Figure S33. LC/MS data for 5{33} .
		Page S42.	Figure S34. LC/MS data for 5{34} .
		Page S43.	Figure S35. LC/MS data for 5{35} .
		Page S44.	Figure S36. LC/MS data for 5{36} .
		Page S45.	Figure S37. LC/MS data for 5{37} .
		Page S46.	Figure S38. LC/MS data for 5{38} .

Page S47. **Figure S39.** LC/MS data for 5{39}.
 Page S48. **Figure S40.** LC/MS data for 5{40}.
 Page S49. **Figure S41.** LC/MS data for 5{41}.
 Page S50. **Figure S42.** LC/MS data for 5{42}.
 Page S51. **Figure S43.** LC/MS data for 5{43}.
 Page S52. **Figure S44.** LC/MS data for 5{44}.
 Page S53. **Figure S45.** LC/MS data for 5{45}.
 Page S54. **Figure S46.** LC/MS data for 5{46}.
 Page S55. **Figure S47.** LC/MS data for 5{47}.
 Page S56. **Figure S48.** LC/MS data for 5{48}.
 Page S57. **Figure S49.** LC/MS data for 5{49}.
 Page S58. **Figure S50.** LC/MS data for 5{50}.
 Page S59. **Figure S51.** LC/MS data for 5{51}.
 Page S60. **Figure S52.** LC/MS data for 5{52}.
 Page S61. **Figure S53.** LC/MS data for 5{53}.
 Page S62. **Figure S54.** LC/MS data for 5{54}.
 Page S63. **Figure S55.** LC/MS data for 5{55}.
 Page S64. **Figure S56.** LC/MS data for 5{56}.
 Page S65. **Figure S57.** LC/MS data for 5{57}.
 Page S66. **Figure S58.** LC/MS data for 5{58}.
 Page S67. **Figure S59.** LC/MS data for 5{59}.
 Page S68. **Figure S60.** LC/MS data for 5{60}.
 Page S69. **Figure S61.** LC/MS data for 5{61}.
 Page S70. **Figure S62.** LC/MS data for 5{62}.
 Page S71. **Figure S63.** LC/MS data for 5{63}.
 Page S72. **Figure S64.** LC/MS data for 5{64}.
 Page S73. **Figure S65.** LC/MS data for 5{65}.
 Page S74. **Figure S66.** LC/MS data for 5{66}.
 Page S75. **Figure S67.** LC/MS data for 5{67}.
 Page S76. **Figure S68.** LC/MS data for 5{68}.
 Page S77. **Figure S69.** LC/MS data for 5{69}.
 Page S78. **Figure S70.** LC/MS data for 5{70}.
 Page S79. **Figure S71.** LC/MS data for 5{71}.
 Page S80. **Figure S72.** LC/MS data for 5{72}.
 Page S81. **Figure S73.** LC/MS data for 5{73}.
 Page S82. **Figure S74.** LC/MS data for 5{74}.
 Page S83. **Figure S75.** LC/MS data for 5{75}.
 Page S84. **Figure S76.** LC/MS data for 5{76}.
 Page S85. **Figure S77.** LC/MS data for 5{77}.
 Page S86. **Figure S78.** LC/MS data for 5{78}.
 Page S87. **Figure S79.** LC/MS data for 5{79}.
 Page S88. **Figure S80.** LC/MS data for 5{80}.
 Page S89. **Figure S81.** LC/MS data for 5{81}.
 Page S90. **Figure S82.** LC/MS data for 5{82}.
 Page S91. **Figure S83.** LC/MS data for 5{83}.
 Page S92. **Figure S84.** LC/MS data for 5{84}.
 Page S93. **Figure S85.** LC/MS data for 5{85}.
 Page S94. **Figure S86.** LC/MS data for 5{86}.
 Page S95. **Figure S87.** LC/MS data for 5{87}.
 Page S96. **Figure S88.** LC/MS data for 5{88}.
 Page S97. **Figure S89.** LC/MS data for 5{89}.
 Page S98. **Figure S90.** LC/MS data for 5{90}.
 Page S99. **Figure S91.** LC/MS data for 5{91}.
 Page S100. **Figure S92.** LC/MS data for 5{92}.
 Page S101. **Figure S93.** LC/MS data for 5{93}.
 Page S102. **Figure S94.** LC/MS data for 5{94}.
 Page S103. **Figure S95.** LC/MS data for 5{95}.
 Page S104. **Figure S96.** LC/MS data for 5{96}.
 Page S105. **Figure S97.** LC/MS data for 5{97}.
 Page S106. **Figure S98.** LC/MS data for 5{98}.
 Page S107. **Figure S99.** LC/MS data for 5{99}.
 Page S108. **Figure S100.** LC/MS data for 5{100}.
 Page S109. **Figure S101.** LC/MS data for 5{101}.
 Page S110. **Figure S102.** LC/MS data for 5{102}.
 Page S111. **Figure S103.** LC/MS data for 5{103}.
 Page S112. **Figure S104.** LC/MS data for 5{104}.
 Page S113. **Figure S105.** LC/MS data for 5{105}.
 Page S114. **Figure S106.** LC/MS data for 5{106}.
 Page S115. **Figure S107.** LC/MS data for 5{107}.
 Page S116. **Figure S108.** LC/MS data for 5{108}.
 Page S117. **Figure S109.** LC/MS data for 5{109}.
 Page S118. **Figure S110.** LC/MS data for 5{110}.
 Page S119. **Figure S111.** LC/MS data for 5{111}.
 Page S120. **Figure S112.** LC/MS data for 5{112}.
 Page S121. **Figure S113.** LC/MS data for 5{113}.
 Page S122. **Figure S114.** LC/MS data for 5{114}.
 Page S123. **Figure S115.** LC/MS data for 5{115}.
 Page S124. **Figure S116.** LC/MS data for 5{116}.
 Page S125. **Figure S117.** LC/MS data for 5{117}.
 Page S126. **Figure S118.** LC/MS data for 5{118}.
 Page S127. **Figure S119.** LC/MS data for 5{119}.
 Page S128. **Figure S120.** LC/MS data for 5{120}.
 Page S129. **Figure S121.** LC/MS data for 5{121}.
 Page S130. **Figure S122.** LC/MS data for 5{122}.
 Page S131. **Figure S123.** LC/MS data for 5{123}.
 Page S132. **Figure S124.** LC/MS data for 5{124}.
 Page S133. **Figure S125.** LC/MS data for 5{125}.
 Page S134. **Figure S126.** LC/MS data for 5{126}.
 Page S135. **Figure S127.** LC/MS data for the crude reaction to yield 5{2}.
 Page S136. **Figure S128.** LC/MS data for the crude reaction to yield 5{6}.
 Page S137. **Figure S129.** LC/MS data for the crude reaction to yield 5{26}.
 Page S138. **Figure S130.** LC/MS data for the crude reaction to yield 5{28}.
 Page S139. **Figure S131.** LC/MS data for the crude reaction to yield 5{38}.

- Page S140. **Figure S132.** LC/MS data for the crude reaction to yield **5{39}**.
- Page S141. **Figure S133.** LC/MS data for the crude reaction to yield **5{44}**.
- Page S142. **Figure S134.** LC/MS data for the crude reaction to yield **5{48}**.
- Page S143. **Figure S135.** LC/MS data for the crude reaction to yield **5{59}**.
- Page S144. **Figure S136.** LC/MS data for the crude reaction to yield **5{63}**.
- Page S145. **Figure S137.** LC/MS data for the crude reaction to yield **5{72}**.
- Page S146. **Figure S138.** LC/MS data for the crude reaction to yield **5{74}**.
- Page S147. **Figure S139.** LC/MS data for the crude reaction to yield **5{93}**.
- Page S148. **Figure S140.** LC/MS data for the crude reaction to yield **5{97}**.
- Page S149. **Figure S141.** LC/MS data for the crude reaction to yield **5{100}**.
- Page S150. **Figure S142.** LC/MS data for the crude reaction to yield **5{104}**.
- Page S151. **Figure S143.** LC/MS data for the crude reaction to yield **5{119}**.
- Page S152. **Figure S144.** LC/MS data for the crude reaction to yield **5{126}**.
- Page S153. **Figure S145.** ¹H-NMR for **5{2}**.
- Page S154. **Figure S146.** ¹H-NMR for **5{6}**.
- Page S155. **Figure S147.** ¹H-NMR for **5{26}**.
- Page S156. **Figure S148.** ¹H-NMR for **5{28}**.
- Page S157. **Figure S149.** ¹H-NMR for **5{38}**.
- Page S158. **Figure S150.** ¹H-NMR for **5{39}**.
- Page S159. **Figure S151.** ¹H-NMR for **5{44}**.
- Page S160. **Figure S152.** ¹H-NMR for **5{48}**.
- Page S161. **Figure S153.** ¹H-NMR for **5{59}**.
- Page S162. **Figure S154.** ¹H-NMR for **5{63}**.
- Page S163. **Figure S155.** ¹H-NMR for **5{72}**.
- Page S164. **Figure S156.** ¹H-NMR for **5{74}**.
- Page S165. **Figure S157.** ¹H-NMR for **5{93}**.
- Page S166. **Figure S158.** ¹H-NMR for **5{97}**.
- Page S167. **Figure S159.** ¹H-NMR for **5{100}**.
- Page S168. **Figure S160.** ¹H-NMR for **5{104}**.
- Page S169. **Figure S161.** ¹H-NMR for **5{119}**.
- Page S170. **Figure S162.** ¹H-NMR for **5{126}**.
- Page S171. **Figure S163.** ¹H-NMR for the crude reaction to yield **5{26}**.
- Page S172. **Figure S164.** ¹H-NMR for the crude reaction to yield **5{2}**.
- Page S173. **Figure S165.** ¹H-NMR for the crude reaction to yield **5{6}**.
- Page S174. **Figure S166.** ¹H-NMR for the crude reaction to yield **5{26}**.
- Page S175. **Figure S167.** ¹H-NMR for the crude reaction to yield **5{28}**.
- Page S176. **Figure S168.** ¹H-NMR for the crude reaction to yield **5{39}**.
- Page S177. **Figure S169.** ¹H-NMR for the crude reaction to yield **5{44}**.
- Page S178. **Figure S170.** ¹H-NMR for the crude reaction to yield **5{48}**.
- Page S179. **Figure S171.** ¹H-NMR for the crude reaction to yield **5{59}**.
- Page S180. **Figure S172.** ¹H-NMR for the crude reaction to yield **5{63}**.
- Page S181. **Figure S173.** ¹H-NMR for the crude reaction to yield **5{72}**.
- Page S182. **Figure S174.** ¹H-NMR for the crude reaction to yield **5{74}**.
- Page S183. **Figure S175.** ¹H-NMR for the crude reaction to yield **5{93}**.
- Page S184. **Figure S176.** ¹H-NMR for the crude reaction to yield **5{97}**.
- Page S185. **Figure S177.** ¹H-NMR for the crude reaction to yield **5{100}**.
- Page S186. **Figure S178.** ¹H-NMR for the crude reaction to yield **5{104}**.
- Page S187. **Figure S179.** ¹H-NMR for the crude reaction to yield **5{119}**.
- Page S188. **Figure S180.** ¹H-NMR for the crude reaction to yield **5{126}**.

Table S1. Amino Acid Ester—Alkanamine Disubstituted I45DCs, **5**{1-28}.

compound	formula	MW	C log <i>P</i>	form	<i>R</i> _f	<i>R</i> _t (min)
5 {1}	C ₁₂ H ₁₈ N ₄ O ₄	282.30	-0.88	glass film	0.16	1.50
5 {2}	C ₂₁ H ₃₅ N ₅ O ₆	453.53	1.09	glass film	0.22	3.70
5 {3}	C ₁₈ H ₂₂ N ₄ O ₄	358.39	1.42	solid	0.27	3.45
5 {4}	C ₁₉ H ₂₄ N ₄ O ₄	372.42	1.39	glass film	0.26	4.10
5 {5}	C ₁₉ H ₂₄ N ₄ O ₄	372.42	1.39	glass film	0.26	4.10
5 {6}	C ₂₁ H ₃₃ N ₅ O ₆	451.52	1.00	solid	0.15	3.95
5 {7}	C ₂₄ H ₃₃ N ₅ O ₆	487.55	2.13	glass film	0.25	4.30
5 {8}	C ₂₄ H ₂₆ N ₄ O ₄	434.49	2.77	glass film	0.33	5.52
5 {9}	C ₁₉ H ₂₄ N ₄ O ₄	372.42	2.05	solid	0.19	2.40
5 {10}	C ₁₅ H ₂₄ N ₄ O ₄	324.38	0.92	glass film	0.26	1.65
5 {11}	C ₂₀ H ₃₁ N ₅ O ₆	437.49	2.00	solid	0.14	3.18
5 {12}	C ₂₀ H ₂₄ N ₄ O ₄	384.43	2.34	glass film	0.23	2.50
5 {13}	C ₁₇ H ₂₆ N ₄ O ₄	350.41	1.58	solid	0.18	2.05
5 {14}	C ₂₁ H ₂₇ N ₅ O ₄	413.47	1.20	solid	0.17	2.32
5 {15}	C ₁₅ H ₁₆ N ₄ O ₄	316.31	-0.07	solid	0.20	1.60
5 {16}	C ₂₄ H ₃₃ N ₅ O ₆	487.55	1.90	glass film	0.22	2.15
5 {17}	C ₂₁ H ₂₀ N ₄ O ₄	392.41	1.56	solid	0.46	3.80
5 {18}	C ₂₂ H ₂₂ N ₄ O ₄	406.43	1.87	glass film	0.20	4.85
5 {19}	C ₂₂ H ₂₂ N ₄ O ₄	406.43	1.87	glass film	0.20	4.85
5 {20}	C ₂₄ H ₃₁ N ₅ O ₆	485.53	1.13	glass film	0.31	4.25
5 {21}	C ₂₇ H ₃₁ N ₅ O ₆	521.56	2.26	solid	0.24	4.47
5 {22}	C ₂₇ H ₂₄ N ₄ O ₄	468.50	2.91	glass film	0.59	5.85
5 {23}	C ₂₂ H ₂₂ N ₄ O ₄	406.43	2.53	glass film	0.32	2.58
5 {24}	C ₁₉ H ₂₂ N ₄ O ₄	358.39	1.40	glass film	0.32	1.75
5 {25}	C ₂₃ H ₂₉ N ₅ O ₆	471.51	2.48	solid	0.20	2.35
5 {26}	C ₂₃ H ₂₂ N ₄ O ₄	418.45	2.81	solid	0.23	2.85
5 {27}	C ₂₀ H ₂₄ N ₄ O ₄	384.43	2.05	glass film	0.24	3.30
5 {28}	C ₂₄ H ₂₅ N ₅ O ₄	447.49	1.68	solid	0.22	3.95

Table S2. Amino Acid Ester—Alkanamine Disubstituted I45DCs, **5**{29-56}.

compound	formula	MW	C log <i>P</i>	form	<i>R</i> _f	<i>R</i> _t (min)
5 {29}	C ₁₃ H ₂₀ N ₄ O ₄	296.32	-0.58	glass film	0.14	1.70
5 {30}	C ₂₂ H ₃₇ N ₅ O ₆	467.56	1.40	glass film	0.14	4.40
5 {31}	C ₁₉ H ₂₄ N ₄ O ₄	372.42	1.73	glass film	0.22	4.30
5 {32}	C ₂₀ H ₂₆ N ₄ O ₄	386.44	2.04	glass film	0.30	4.90
5 {33}	C ₂₀ H ₂₆ N ₄ O ₄	386.44	2.04	glass film	0.30	4.90
5 {34}	C ₂₂ H ₃₅ N ₅ O ₆	465.54	1.31	glass film	0.13	4.72
5 {35}	C ₂₅ H ₃₅ N ₅ O ₆	501.58	2.44	glass film	0.19	4.87
5 {36}	C ₂₅ H ₂₈ N ₄ O ₄	448.51	3.08	glass film	0.32	6.10
5 {37}	C ₂₀ H ₂₆ N ₄ O ₄	386.44	2.36	glass film	0.15	3.10
5 {38}	C ₁₆ H ₂₆ N ₄ O ₄	338.40	1.23	glass film	0.24	1.95
5 {39}	C ₂₁ H ₃₃ N ₅ O ₆	451.52	2.31	glass film	0.10	2.75
5 {40}	C ₂₁ H ₂₆ N ₄ O ₄	398.46	2.65	glass film	0.15	3.50
5 {41}	C ₁₈ H ₂₈ N ₄ O ₄	364.44	1.89	solid	0.12	2.60
5 {42}	C ₂₂ H ₂₉ N ₅ O ₄	427.50	1.51	glass film	0.09	3.32
5 {43}	C ₁₆ H ₁₈ N ₄ O ₄	330.34	0.24	solid	0.11	1.80
5 {44}	C ₂₅ H ₃₅ N ₅ O ₆	501.58	1.87	glass film	0.14	4.60
5 {45}	C ₂₂ H ₂₂ N ₄ O ₄	406.43	1.87	glass film	0.26	4.42
5 {46}	C ₂₃ H ₂₄ N ₄ O ₄	420.46	2.18	glass film	0.25	4.95
5 {47}	C ₂₃ H ₂₄ N ₄ O ₄	420.46	2.18	glass film	0.25	4.95
5 {48}	C ₂₅ H ₃₃ N ₅ O ₆	499.56	1.44	glass film	0.14	4.82
5 {49}	C ₂₈ H ₃₃ N ₅ O ₆	535.59	2.57	glass film	0.14	4.97
5 {50}	C ₂₈ H ₂₆ N ₄ O ₄	482.53	3.21	glass film	0.30	6.05
5 {51}	C ₂₃ H ₂₄ N ₄ O ₄	420.46	2.84	glass film	0.14	3.57
5 {52}	C ₁₉ H ₂₄ N ₄ O ₄	372.42	1.71	solid	0.18	2.12
5 {53}	C ₂₄ H ₃₁ N ₅ O ₆	485.53	2.79	solid	0.11	4.18
5 {54}	C ₂₄ H ₂₄ N ₄ O ₄	432.47	3.12	glass film	0.18	3.92
5 {55}	C ₂₁ H ₂₆ N ₄ O ₄	398.46	2.36	solid	0.12	2.95
5 {56}	C ₂₅ H ₂₇ N ₅ O ₄	461.51	1.99	glass film	0.09	3.62

Table S3. Amino Acid Ester—Alkanamine Disubstituted I45DCs, **5**{57-84}.

compound	formula	MW	C log <i>P</i>	form	<i>R</i> _f	<i>R</i> _t (min)
5 {57}	C ₁₆ H ₂₆ N ₄ O ₄	338.40	0.88	glass film	0.26	3.75
5 {58}	C ₂₅ H ₄₃ N ₅ O ₆	509.64	2.85	glass film	0.23	6.22
5 {59}	C ₂₂ H ₃₀ N ₄ O ₄	414.50	3.19	glass film	0.41	6.23
5 {60}	C ₂₃ H ₃₂ N ₄ O ₄	428.52	3.50	glass film	0.42	6.73
5 {61}	C ₂₃ H ₃₂ N ₄ O ₄	428.52	3.50	glass film	0.42	6.73
5 {62}	C ₂₅ H ₄₁ N ₅ O ₆	507.62	2.77	glass film	0.29	6.55
5 {63}	C ₂₈ H ₄₁ N ₅ O ₆	543.66	3.89	glass film	0.26	6.52
5 {64}	C ₂₈ H ₃₄ N ₄ O ₄	490.59	4.54	glass film	0.52	7.67
5 {65}	C ₂₃ H ₃₂ N ₄ O ₄	428.52	3.82	solid	0.24	5.55
5 {66}	C ₁₉ H ₃₂ N ₄ O ₄	380.48	2.69	solid	0.33	4.45
5 {67}	C ₂₄ H ₃₉ N ₅ O ₆	493.60	3.77	solid	0.21	5.27
5 {68}	C ₂₄ H ₃₂ N ₄ O ₄	440.53	4.10	solid	0.28	5.73
5 {69}	C ₂₁ H ₃₄ N ₄ O ₄	406.52	3.34	solid	0.25	5.20
5 {70}	C ₂₅ H ₃₅ N ₅ O ₄	469.58	2.97	solid	0.19	5.60
5 {71}	C ₁₉ H ₂₄ N ₄ O ₄	372.42	1.70	glass film	0.16	4.80
5 {72}	C ₂₈ H ₄₁ N ₅ O ₆	543.66	3.33	glass film	0.16	6.20
5 {73}	C ₂₅ H ₂₈ N ₄ O ₄	448.51	3.32	glass film	0.30	6.90
5 {74}	C ₂₆ H ₃₀ N ₄ O ₄	462.54	3.63	glass film	0.47	6.75
5 {75}	C ₂₆ H ₃₀ N ₄ O ₄	462.54	3.63	glass film	0.47	6.75
5 {76}	C ₂₈ H ₃₉ N ₅ O ₆	541.64	2.90	glass film	0.27	6.47
5 {77}	C ₃₁ H ₃₉ N ₅ O ₆	577.67	4.02	solid	0.24	6.40
5 {78}	C ₃₁ H ₃₂ N ₄ O ₄	524.61	4.67	glass film	0.52	7.45
5 {79}	C ₂₆ H ₃₀ N ₄ O ₄	462.54	4.29	glass film	0.22	5.75
5 {80}	C ₂₂ H ₃₀ N ₄ O ₄	414.50	3.16	glass film	0.29	4.85
5 {81}	C ₂₇ H ₃₇ N ₅ O ₆	527.61	4.24	solid	0.13	5.45
5 {82}	C ₂₇ H ₃₀ N ₄ O ₄	474.55	4.58	glass film	0.23	5.85
5 {83}	C ₂₄ H ₃₂ N ₄ O ₄	440.54	3.82	solid	0.15	5.45
5 {84}	C ₂₈ H ₃₃ N ₅ O ₄	503.59	3.44	glass film	0.12	5.75

Table S4. Amino Acid Ester—Alkanamine Disubstituted I45DCs, **5{85-112}**.

compound	formula	MW	C log <i>P</i>	form	<i>R</i> _f	<i>R</i> _t (min)
5{85}	C ₁₉ H ₂₄ N ₄ O ₄	372.42	1.18	glass film	0.26	3.80
5{86}	C ₂₈ H ₄₁ N ₅ O ₆	543.66	3.15	glass film	0.29	6.10
5{87}	C ₂₅ H ₂₈ N ₄ O ₄	448.51	2.81	glass film	0.41	6.08
5{88}	C ₂₆ H ₃₀ N ₄ O ₄	462.54	3.12	glass film	0.36	6.65
5{89}	C ₂₆ H ₃₀ N ₄ O ₄	462.54	3.12	glass film	0.36	6.65
5{90}	C ₂₈ H ₃₉ N ₅ O ₆	541.64	2.39	glass film	0.26	6.40
5{91}	C ₃₁ H ₃₉ N ₅ O ₆	577.67	3.51	glass film	0.31	6.45
5{92}	C ₃₁ H ₃₂ N ₄ O ₄	524.61	4.16	glass film	0.48	7.50
5{93}	C ₂₆ H ₃₀ N ₄ O ₄	462.54	3.78	glass film	0.31	5.35
5{94}	C ₂₂ H ₃₀ N ₄ O ₄	414.50	2.65	glass film	0.36	4.30
5{95}	C ₂₇ H ₃₇ N ₅ O ₆	527.61	3.73	solid	0.21	5.12
5{96}	C ₂₇ H ₃₀ N ₄ O ₄	474.55	4.06	glass film	0.26	5.80
5{97}	C ₂₄ H ₃₀ N ₄ O ₄	462.54	3.12	glass film	0.36	5.09
5{98}	C ₂₈ H ₃₂ N ₅ O ₄	440.54	3.30	glass film	0.24	5.45
5{99}	C ₂₂ H ₂₂ N ₄ O ₄	406.43	1.66	solid	0.16	4.05
5{100}	C ₃₁ H ₃₉ N ₅ O ₆	577.67	3.63	glass film	0.19	6.12
5{101}	C ₂₈ H ₂₆ N ₄ O ₄	482.53	3.28	glass film	0.29	6.25
5{102}	C ₂₉ H ₂₈ N ₄ O ₄	496.56	3.59	glass film	0.29	6.75
5{103}	C ₂₉ H ₂₈ N ₄ O ₄	496.56	3.59	glass film	0.29	6.75
5{104}	C ₃₁ H ₃₇ N ₅ O ₆	575.66	2.86	glass film	0.18	6.35
5{105}	C ₃₄ H ₃₇ N ₅ O ₆	611.69	3.99	glass film	0.22	6.28
5{106}	C ₃₄ H ₃₀ N ₄ O ₄	558.63	4.63	glass film	0.35	7.25
5{107}	C ₂₉ H ₂₈ N ₄ O ₄	496.56	4.25	glass film	0.19	5.60
5{108}	C ₂₅ H ₂₈ N ₄ O ₄	448.51	3.12	glass film	0.19	5.30
5{109}	C ₃₀ H ₃₅ N ₅ O ₆	561.63	4.20	glass film	0.09	5.30
5{110}	C ₃₀ H ₂₈ N ₄ O ₄	508.57	4.54	glass film	0.22	5.73
5{111}	C ₂₇ H ₃₀ N ₄ O ₄	474.55	3.78	glass film	0.15	5.42
5{112}	C ₃₁ H ₃₁ N ₅ O ₄	537.61	3.40	glass film	0.12	5.75

Table S5. Amino Acid Ester—Alkanamine Disubstituted I45DCs, **5**{113-126}.

compound	formula	MW	C log <i>P</i>	form	<i>R</i> _f	<i>R</i> _t (min)
5 {113}	C ₂₁ H ₃₅ N ₅ O ₆	453.53	0.87	glass film	0.16	3.25
5 {114}	C ₃₀ H ₅₂ N ₆ O ₈	624.77	2.83	glass film	0.19	5.70
5 {115}	C ₂₇ H ₃₉ N ₅ O ₆	529.63	3.18	glass film	0.28	5.65
5 {116}	C ₂₈ H ₄₁ N ₅ O ₆	543.66	3.14	glass film	0.28	6.05
5 {117}	C ₂₈ H ₄₁ N ₅ O ₆	543.66	3.14	glass film	0.28	6.05
5 {118}	C ₃₀ H ₅₀ N ₆ O ₈	622.75	2.75	glass film	0.19	5.90
5 {119}	C ₃₃ H ₅₀ N ₆ O ₈	658.79	3.88	glass film	0.12	5.90
5 {120}	C ₃₃ H ₄₃ N ₅ O ₆	605.72	4.52	glass film	0.34	6.95
5 {121}	C ₂₈ H ₄₁ N ₅ O ₆	543.66	3.80	glass film	0.12	5.10
5 {122}	C ₂₄ H ₄₁ N ₅ O ₆	495.61	2.67	glass film	0.20	4.15
5 {123}	C ₂₉ H ₄₈ N ₆ O ₈	608.73	3.75	glass film	0.15	4.97
5 {124}	C ₂₉ H ₄₁ N ₅ O ₆	555.67	4.09	glass film	0.20	5.30
5 {125}	C ₂₆ H ₄₃ N ₅ O ₆	521.65	3.33	glass film	0.15	4.85
5 {126}	C ₃₀ H ₄₄ N ₆ O ₆	584.71	2.96	glass film	0.12	5.25

Note on Morphology of Samples. The purified products were transferred as CH₂Cl₂ solutions into vials for storage and allowed to evaporate at room temperature. It is noteworthy that a majority of the samples yield a transparent glass film (78%) from this process, with a smaller percentage of samples yielding largely amorphous white solids (22%). Primary amines yielded 8 solids from 72 samples (11%), while secondary amines yielded 20 solids from 54 samples (37%). This difference is likely due to a specific intramolecular hydrogen bonded conformation that forms in library members substituted with a secondary alkanamine as compared with the equilibrium of two intramolecular hydrogen bonded conformations for library members substituted with primary alkanamines. The library members are all readily soluble in CH₂Cl₂ and this volatile solvent is a good choice for the transfer of samples; however, we also know from our past research with I45DCs that this is a poor crystallization solvent and better results are obtained from either 2-propanone or methanol (Baures PW, Rush JR, Wiznycia AV, Desper J, Helfrich BA, Beatty AM: Intramolecular hydrogen bonding and intermolecular dimerization in the crystal structures of imidazole-4,5-dicarboxylic acid derivatives. *Cryst. Growth Des.* 2002, **2**:653-664). Thus, the observed percentages of solids versus transparent glass films, as well as percentages of amorphous solids versus crystalline solids, could very well change with a complete investigation of solvent choices.

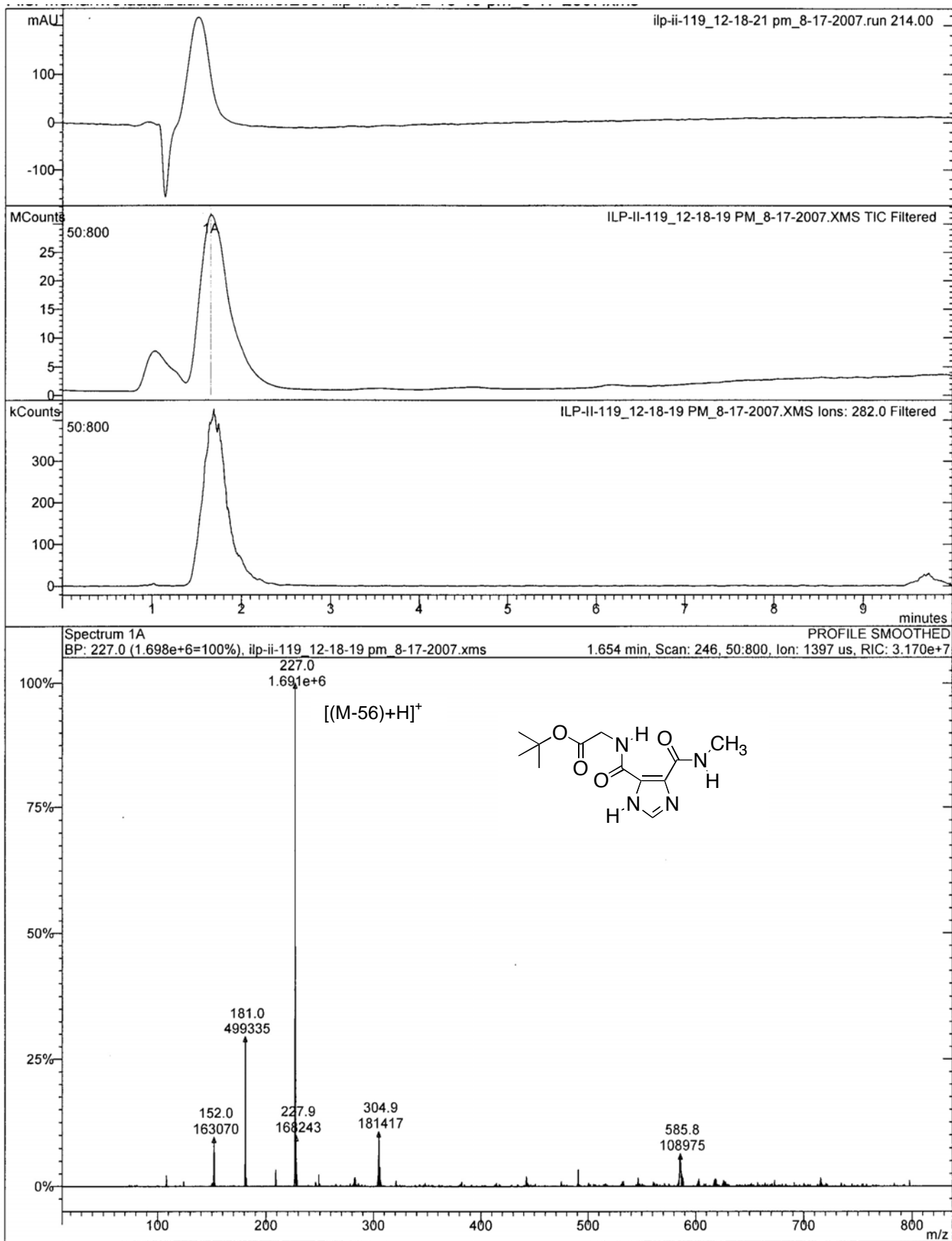


Figure S1. LC/MS data for 5{1}.

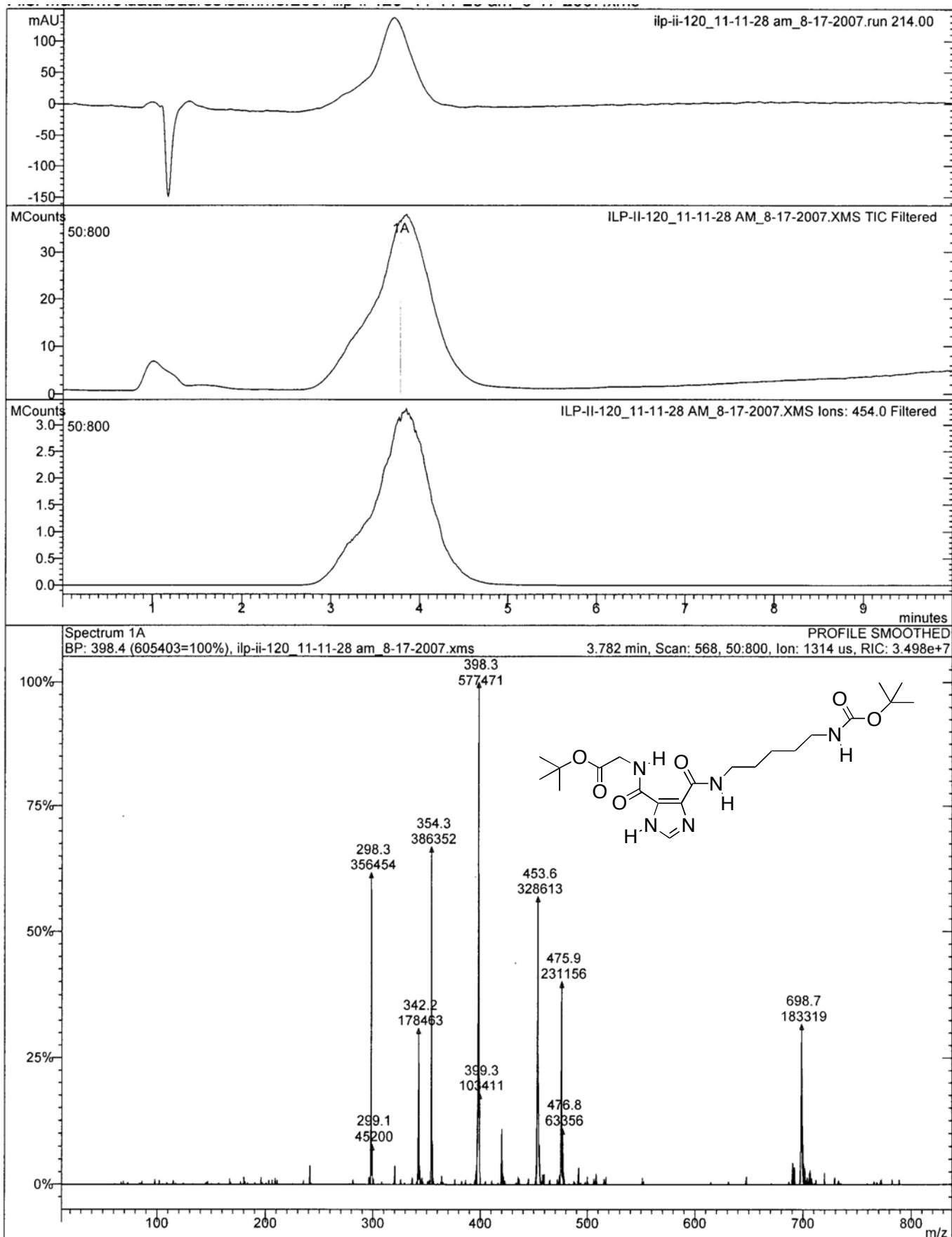


Figure S2. LC/MS data for 5{2}.

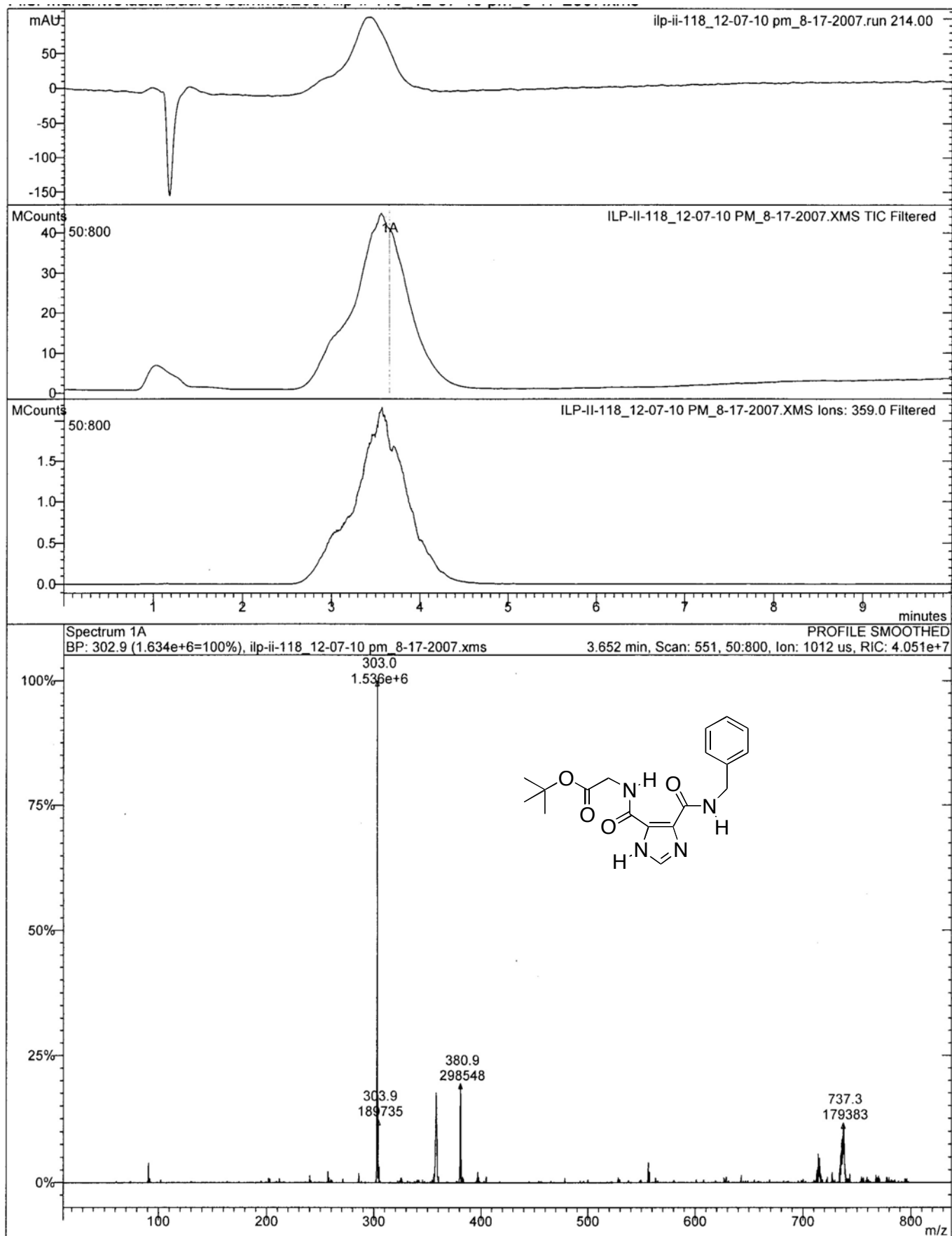


Figure S3. LC/MS data for 5{3}.

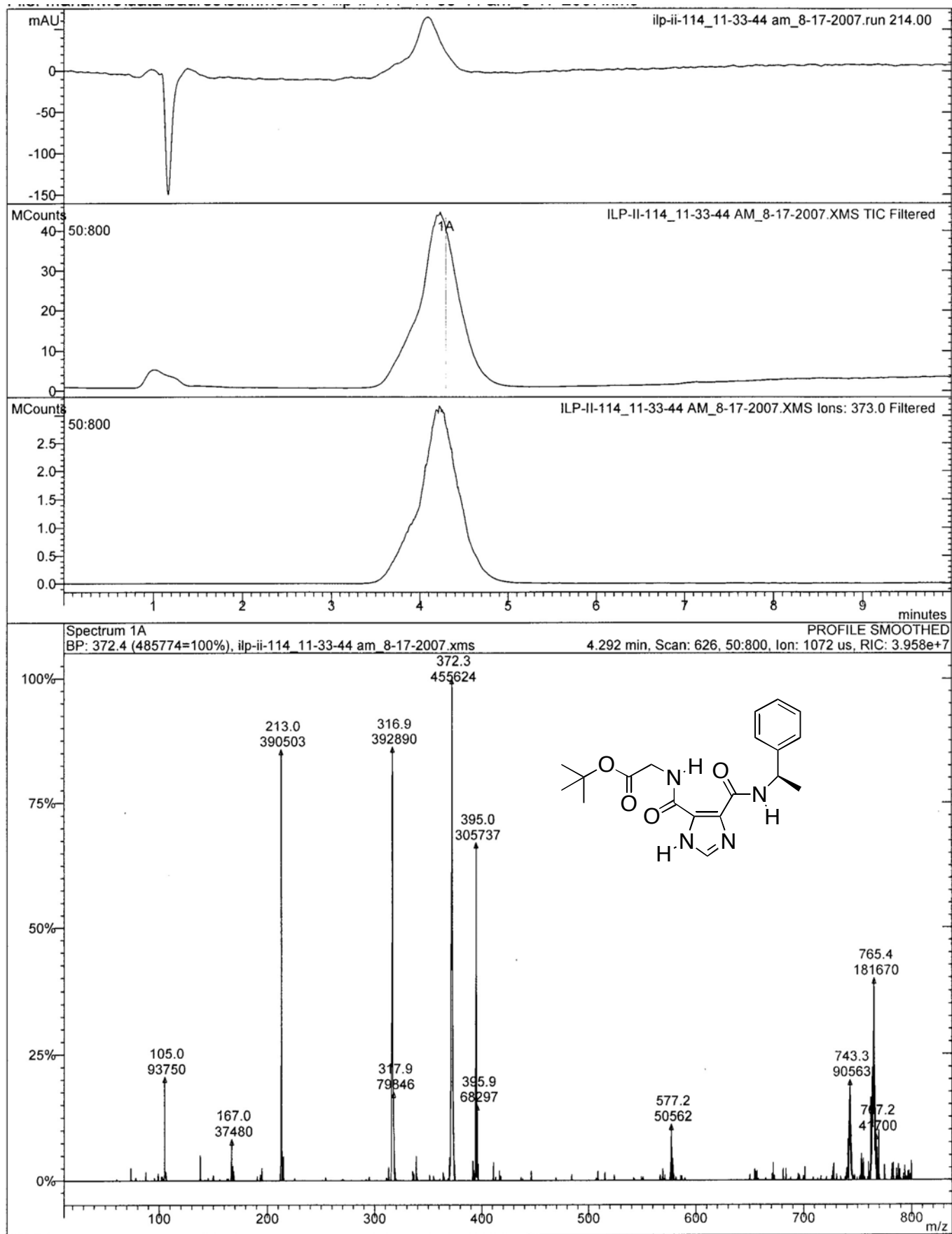


Figure S4. LC/MS data for 5{4}.

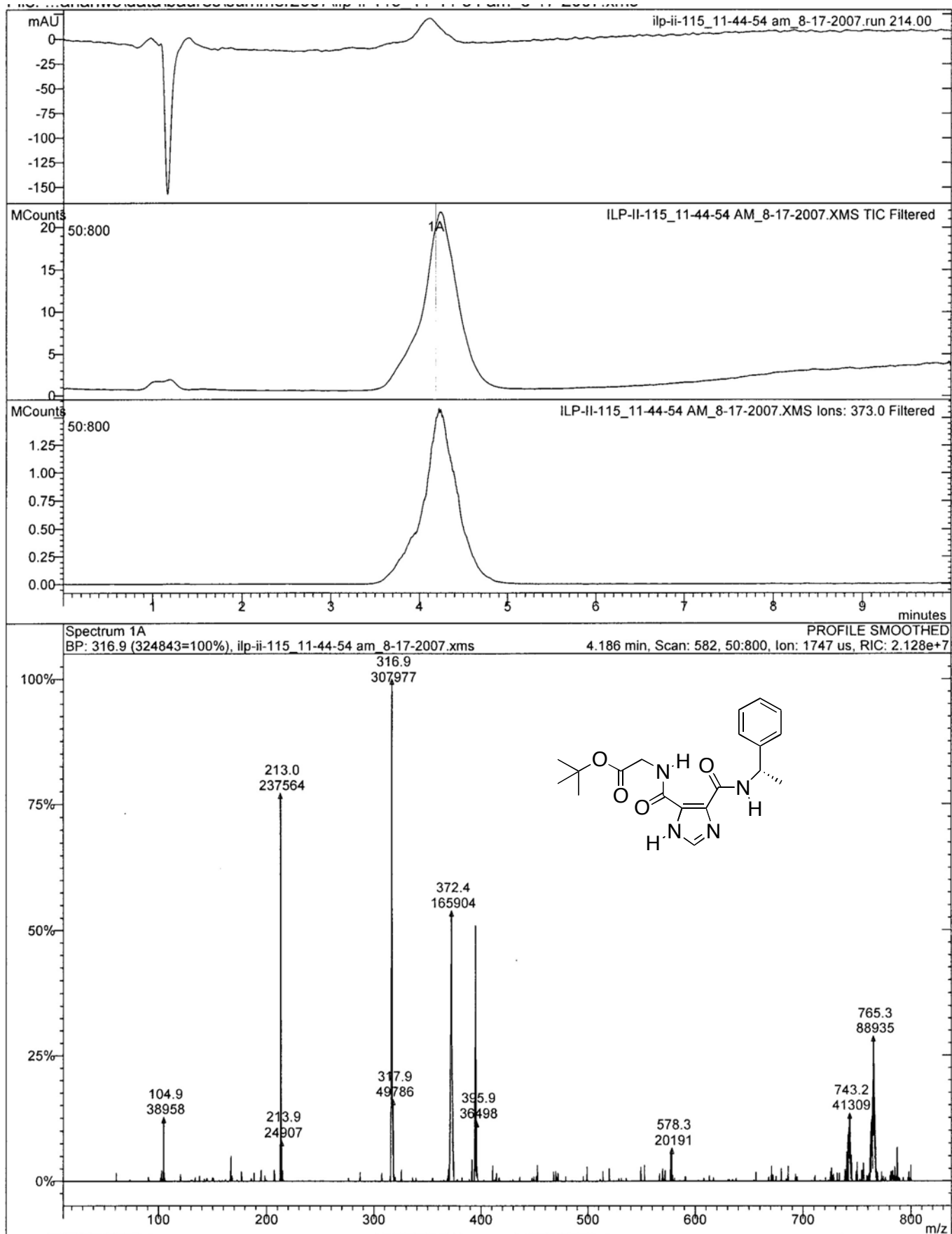


Figure S5. LC/MS data for 5{5}.

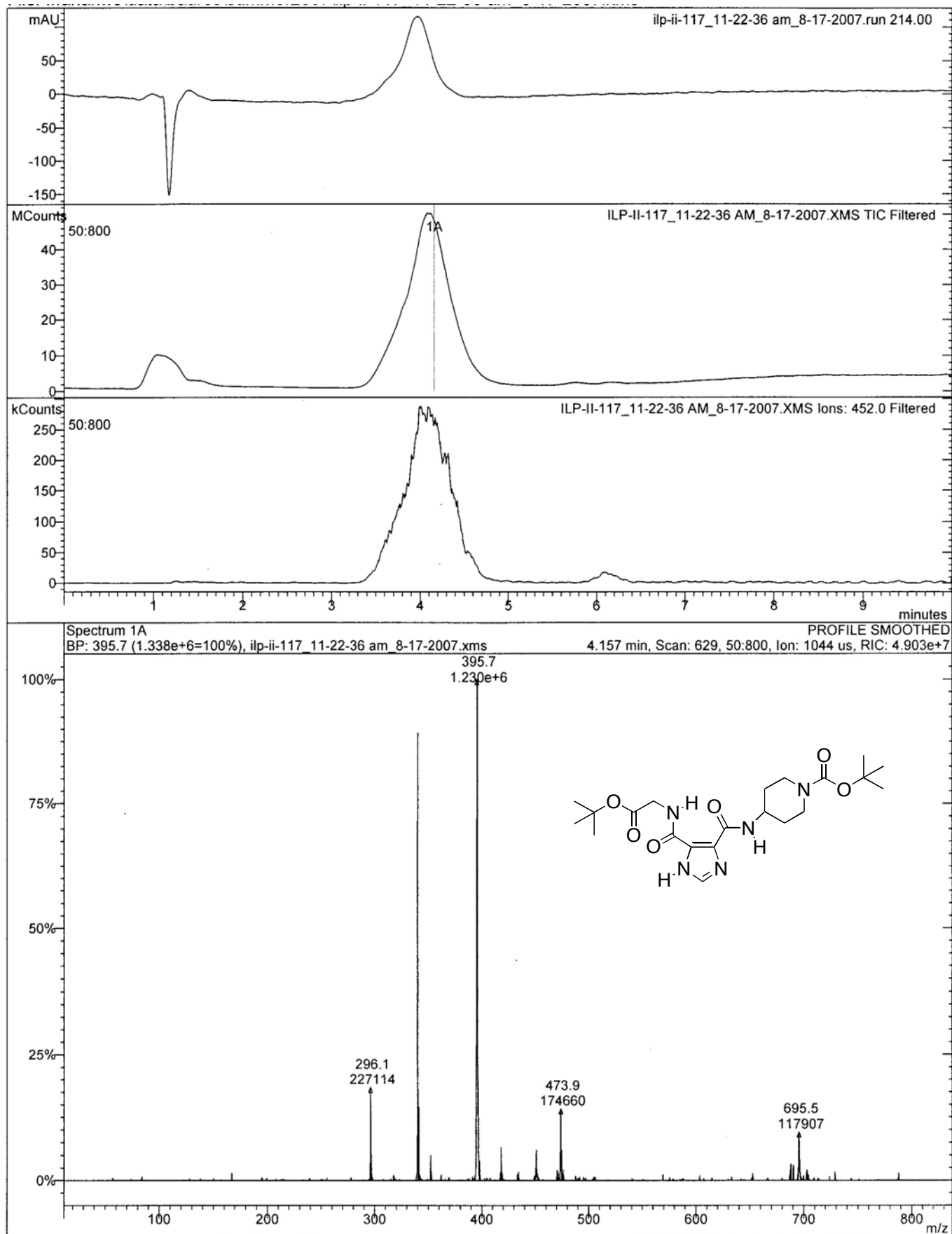


Figure S6. LC/MS data for 5{6}.

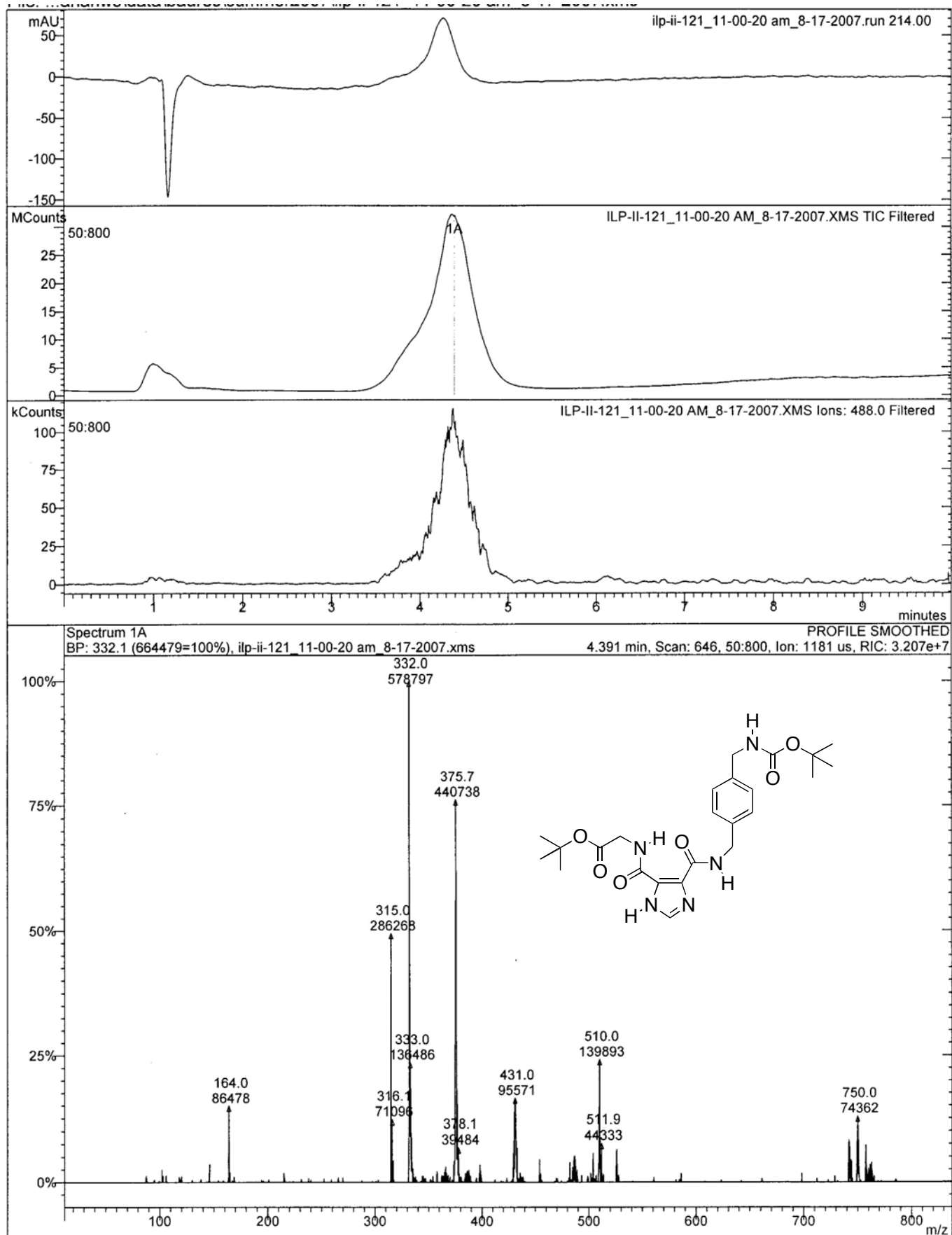


Figure S7. LC/MS data for 5{7}.

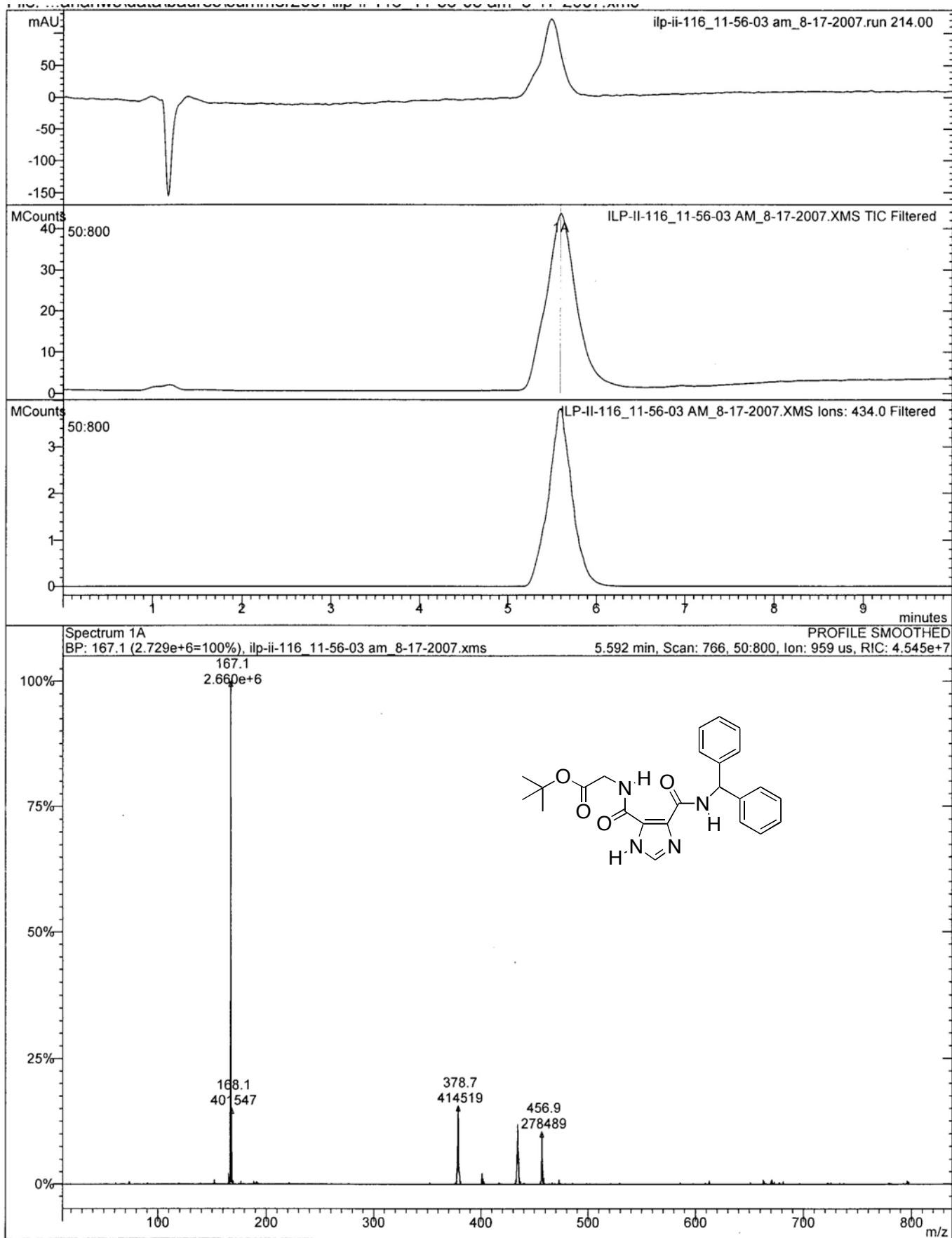


Figure S8. LC/MS data for 5{8}.

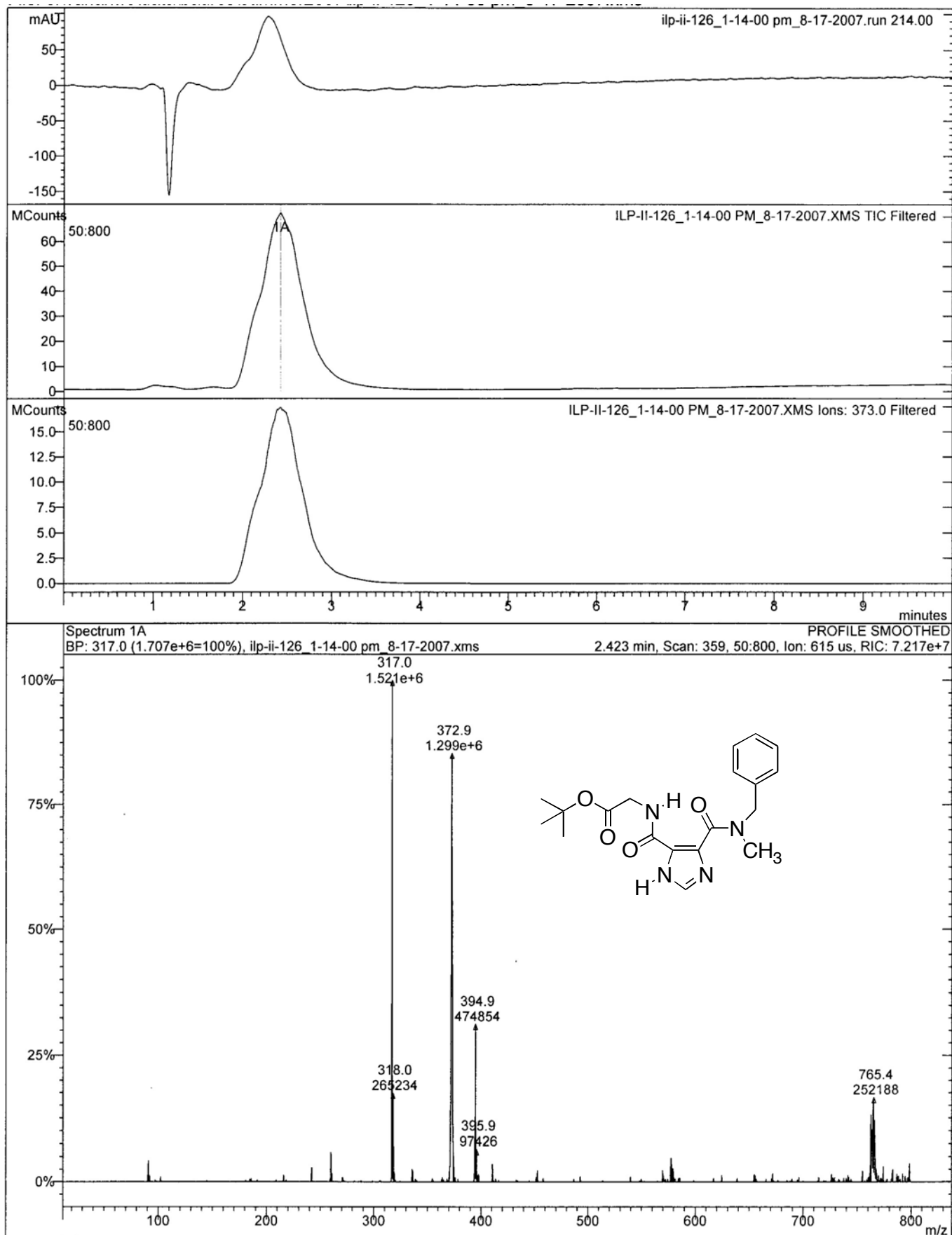


Figure S9. LC/MS data for 5{9}.

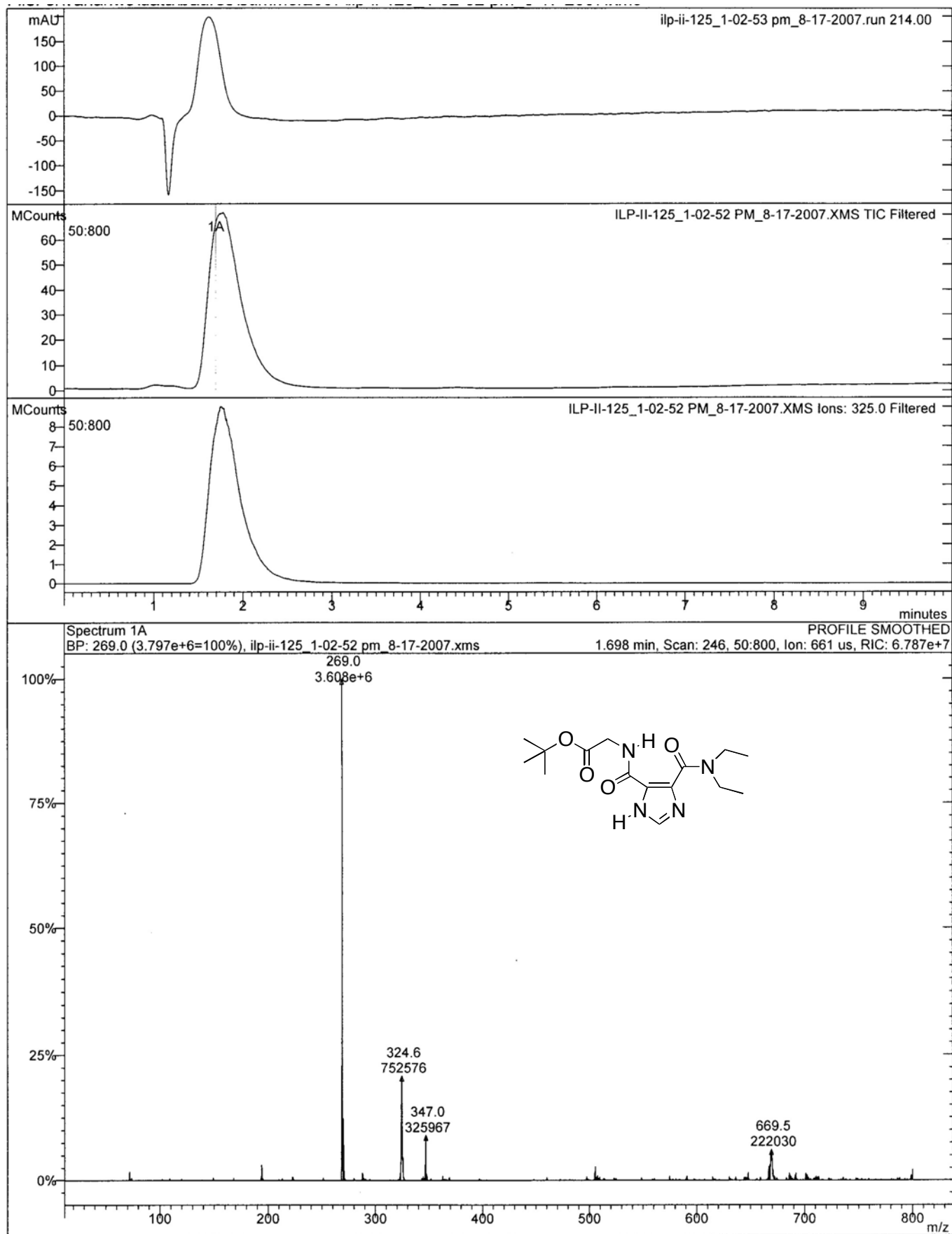


Figure S10. LC/MS data for 5{10}.

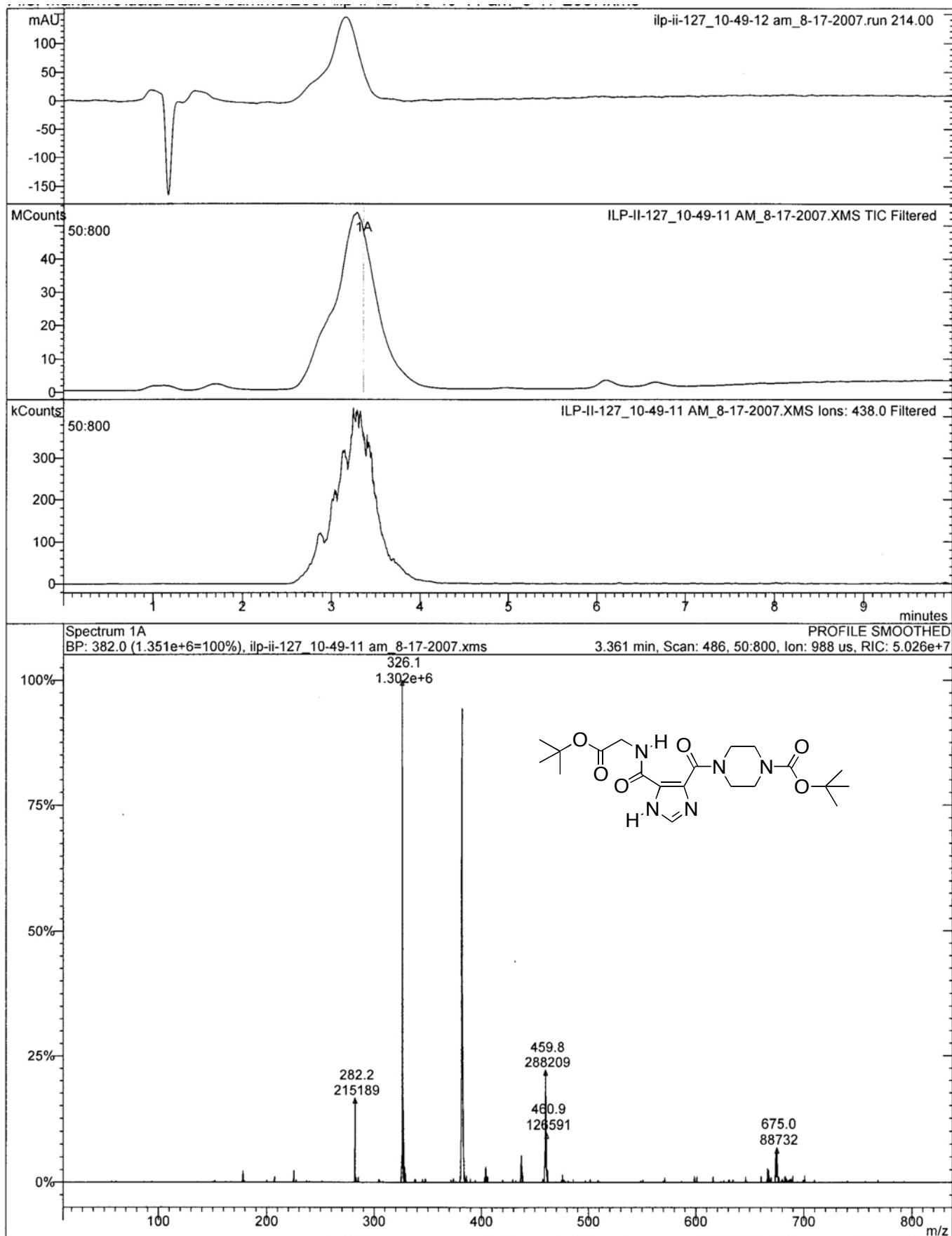


Figure S11. LC/MS data for 5{11}.

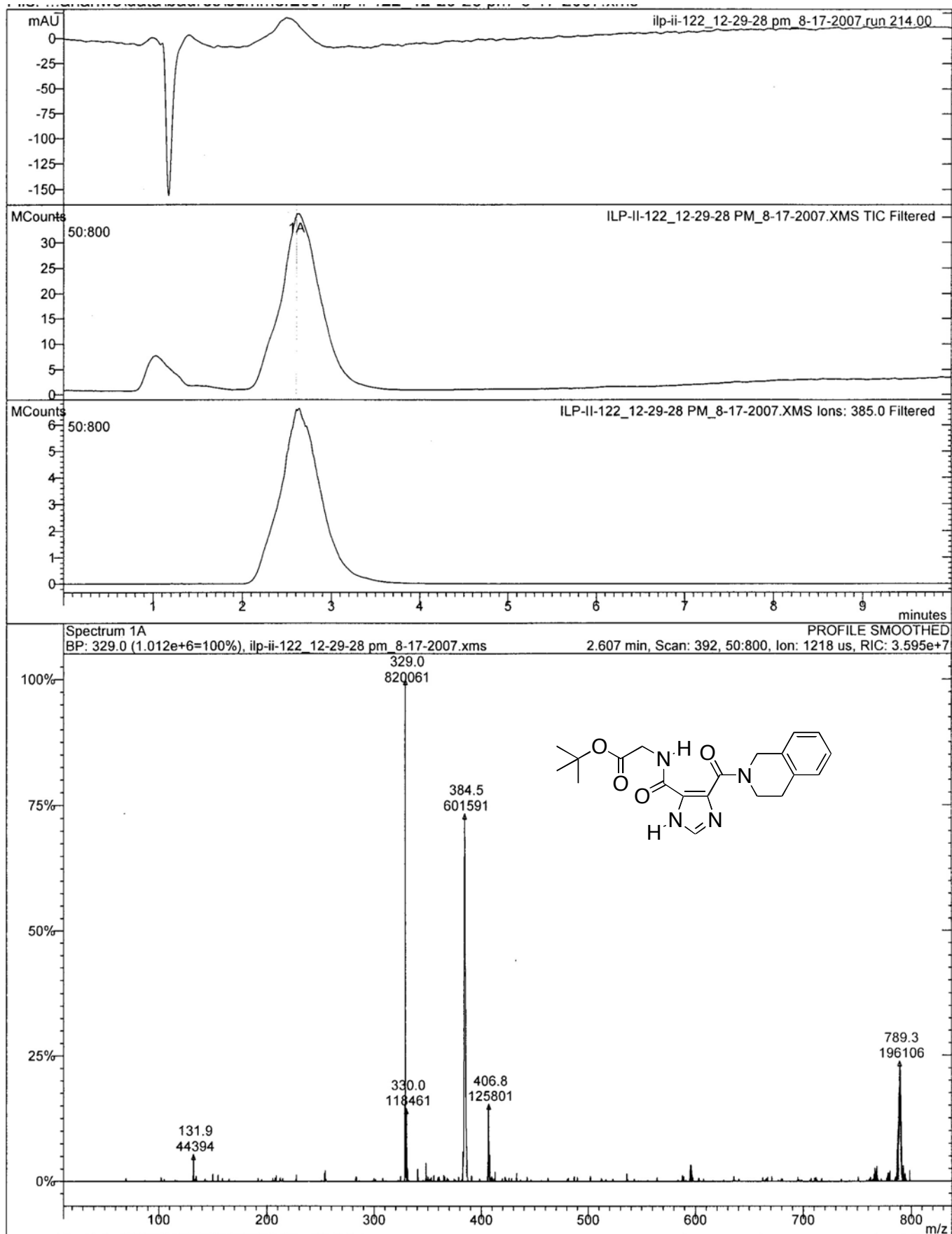


Figure S12. LC/MS data for 5{12}.

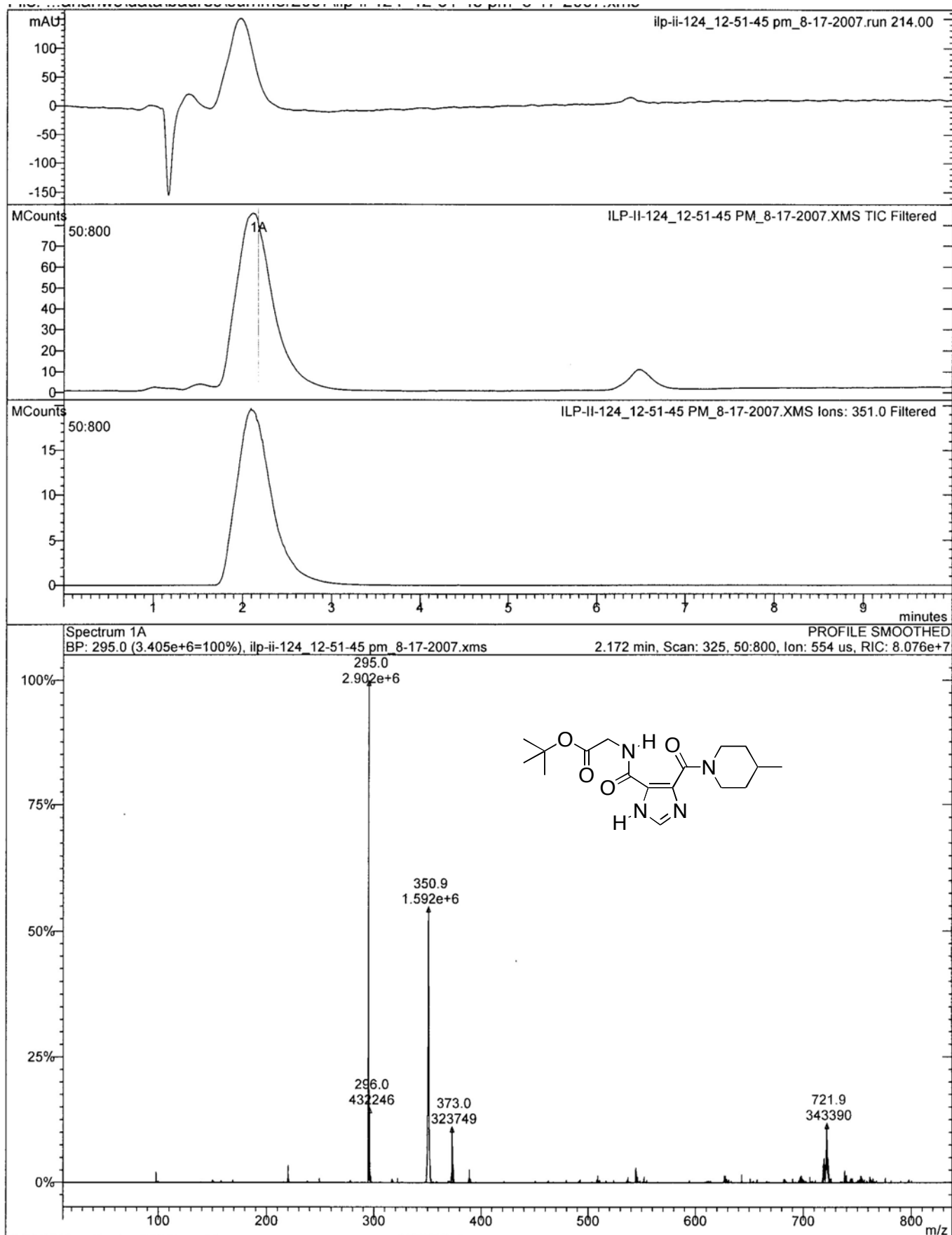


Figure S13. LC/MS data for 5{13}.

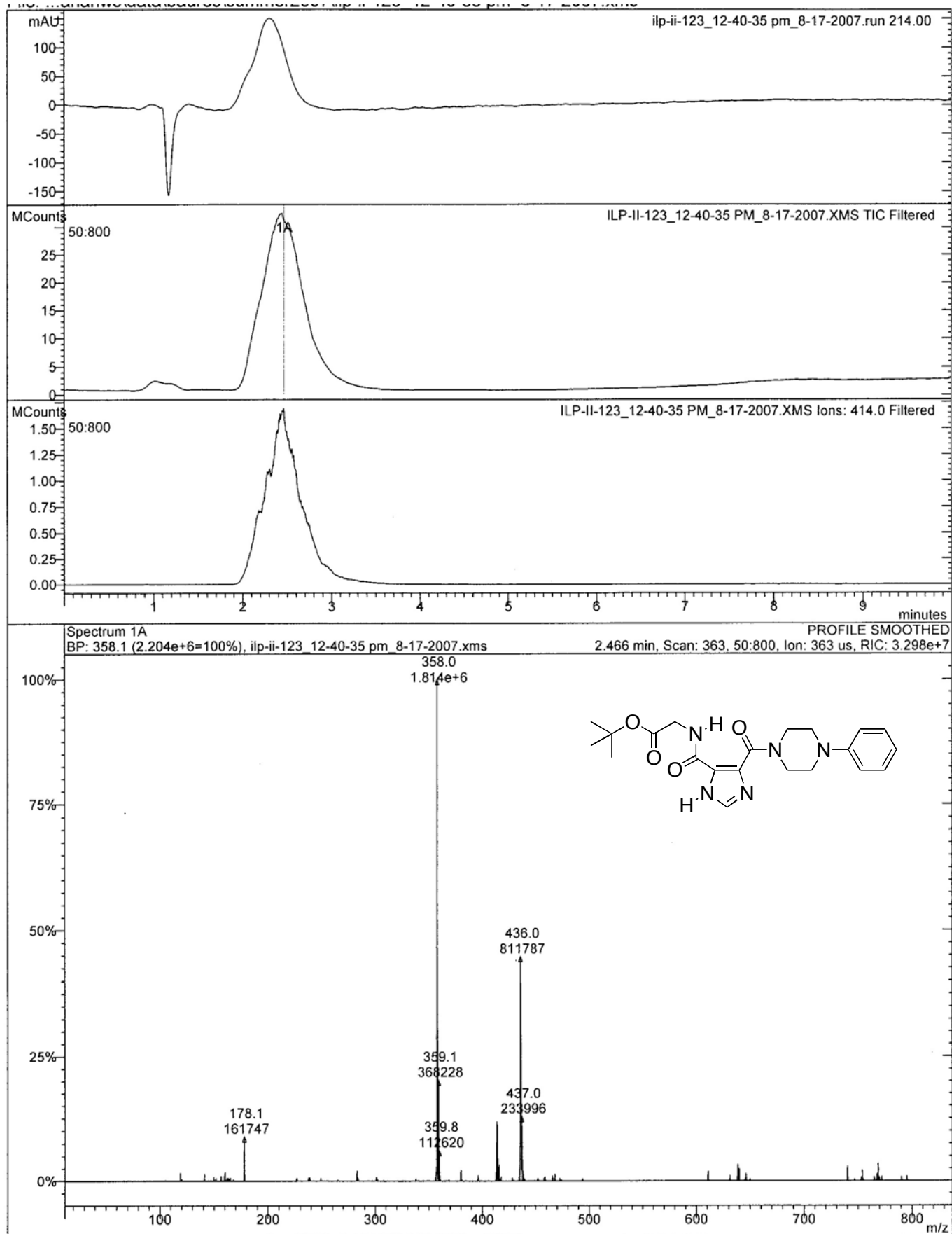


Figure S14. LC/MS data for 5{14}.

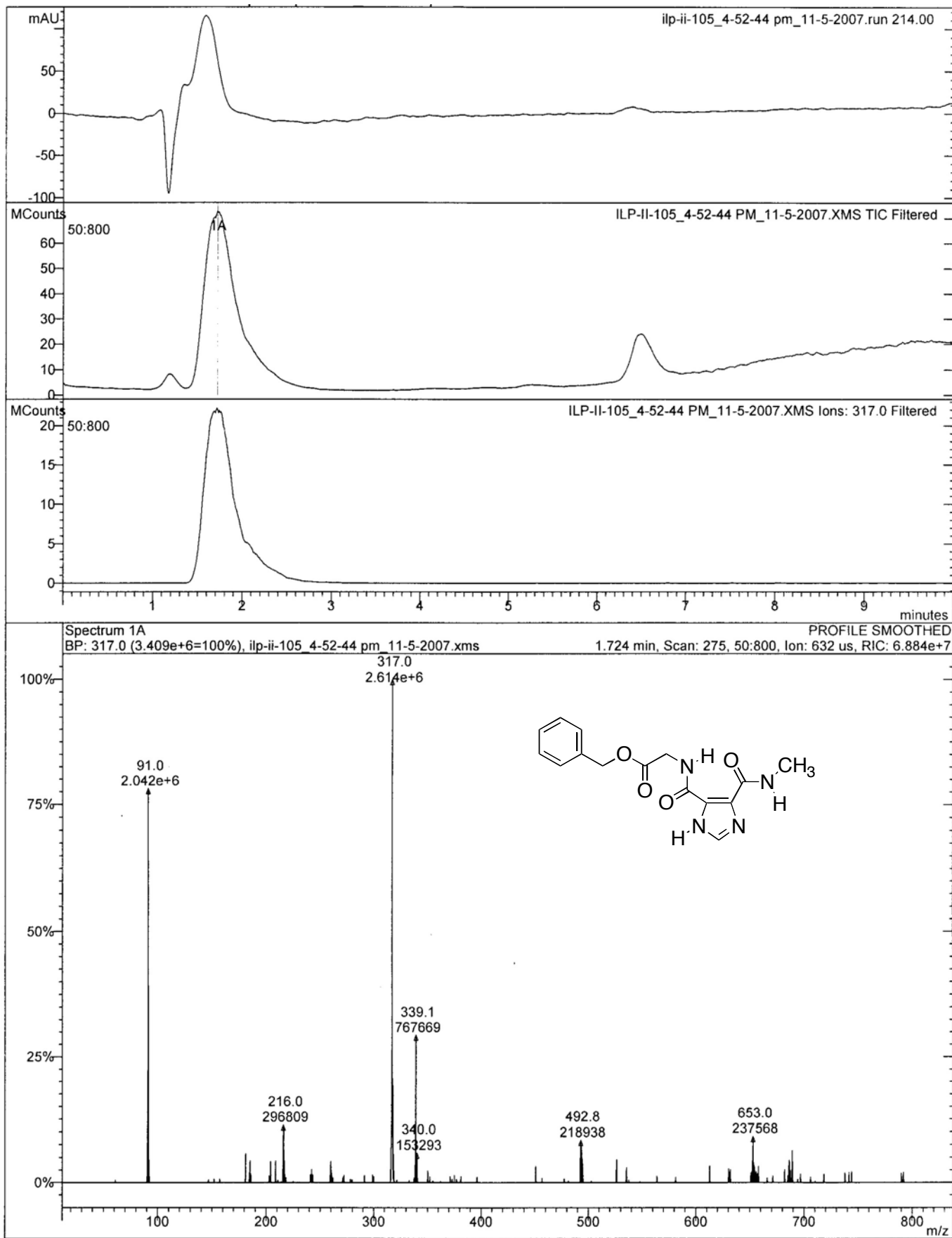


Figure S15. LC/MS data for 5{15}.

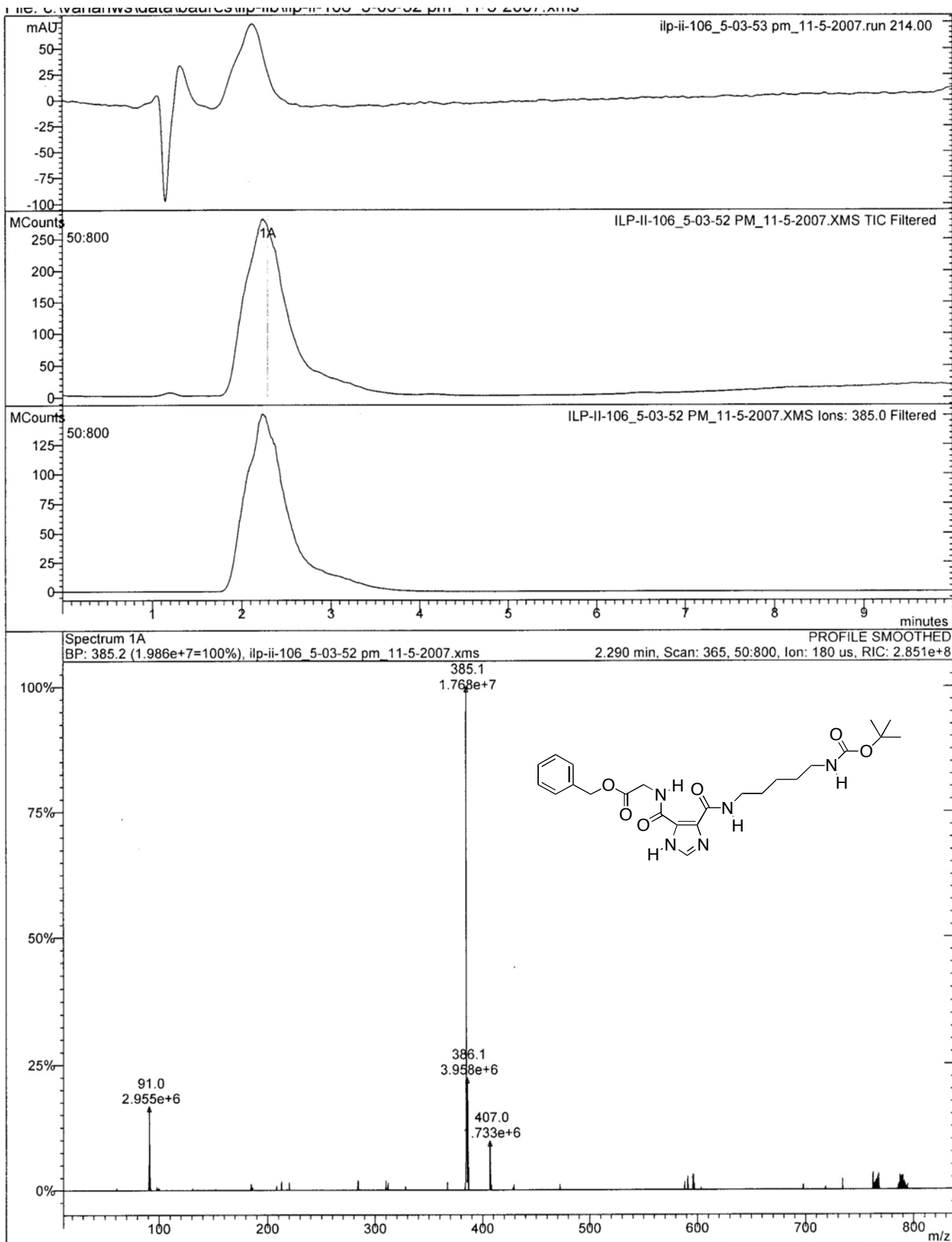


Figure S16. LC/MS data for 5{16}.

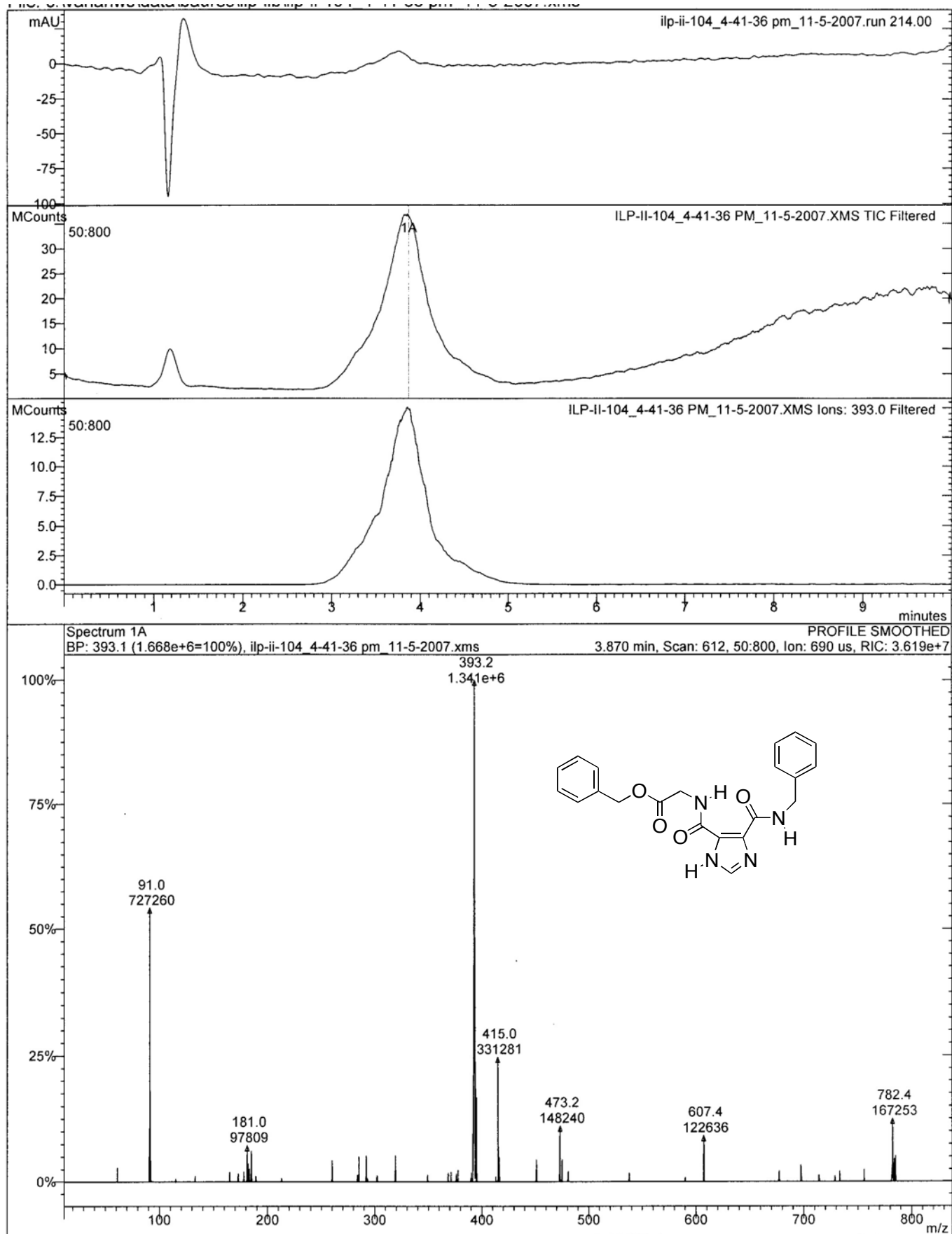


Figure S17. LC/MS data for 5{17}.

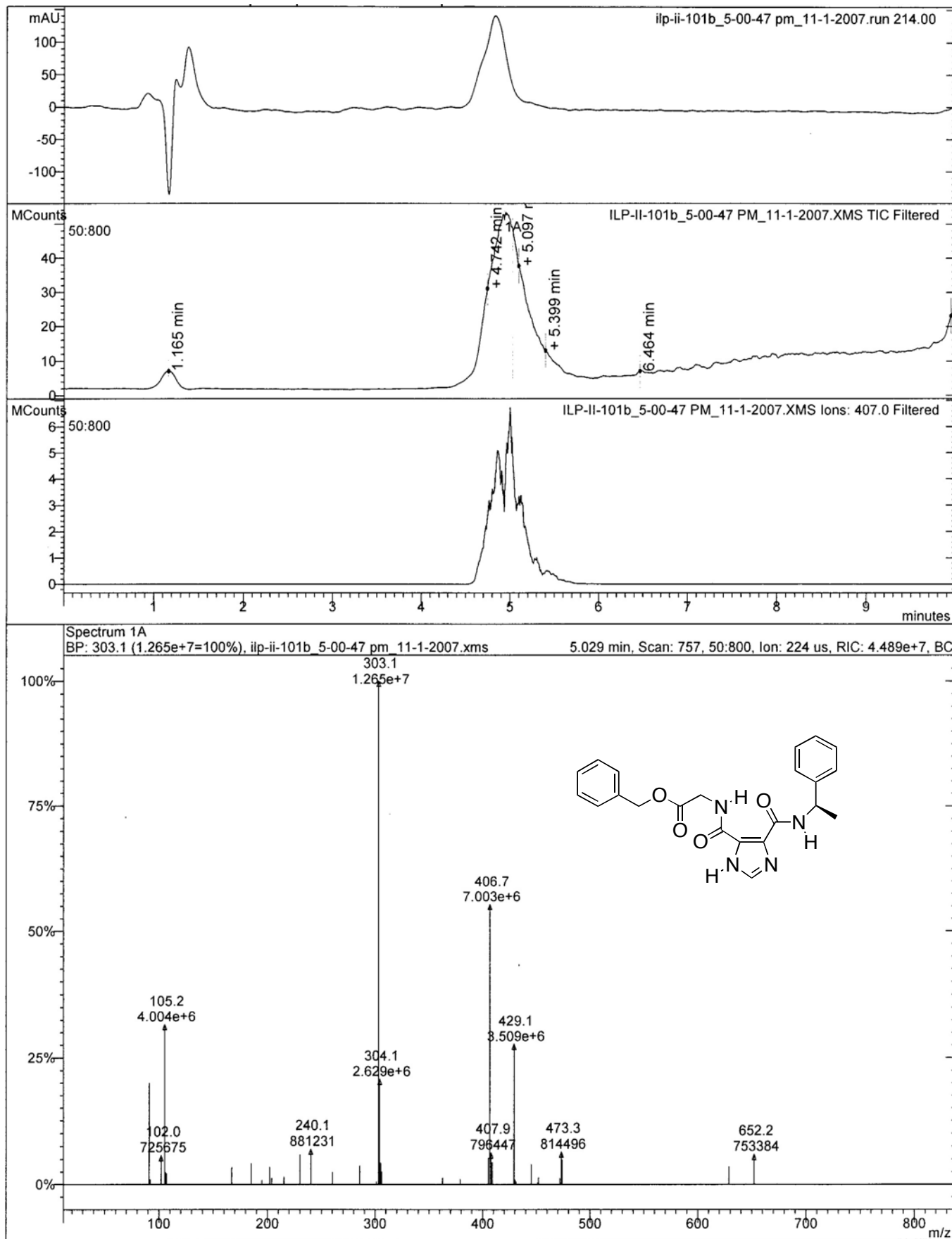


Figure S18. LC/MS data for 5{18}.

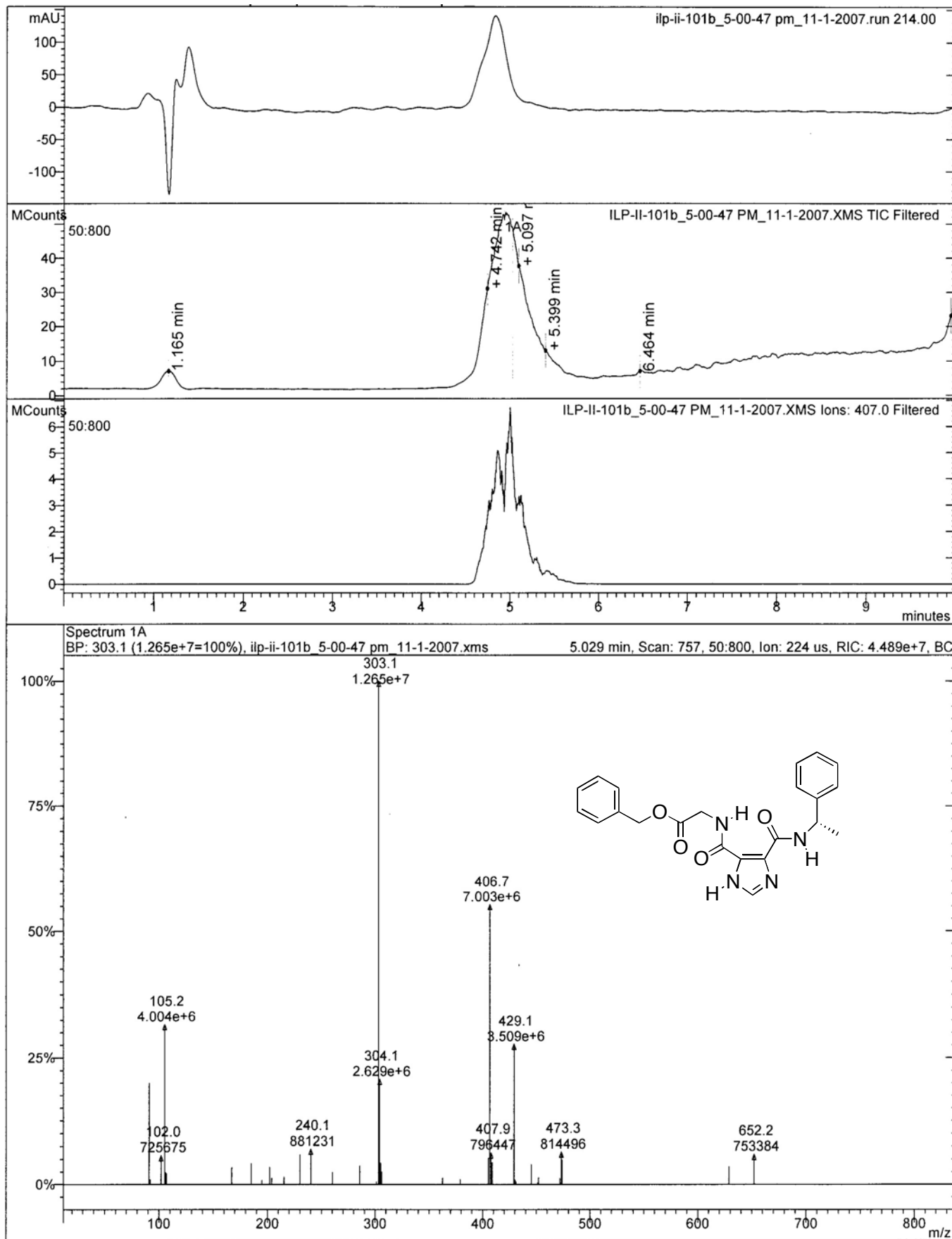


Figure S19. LC/MS data for 5{19}.

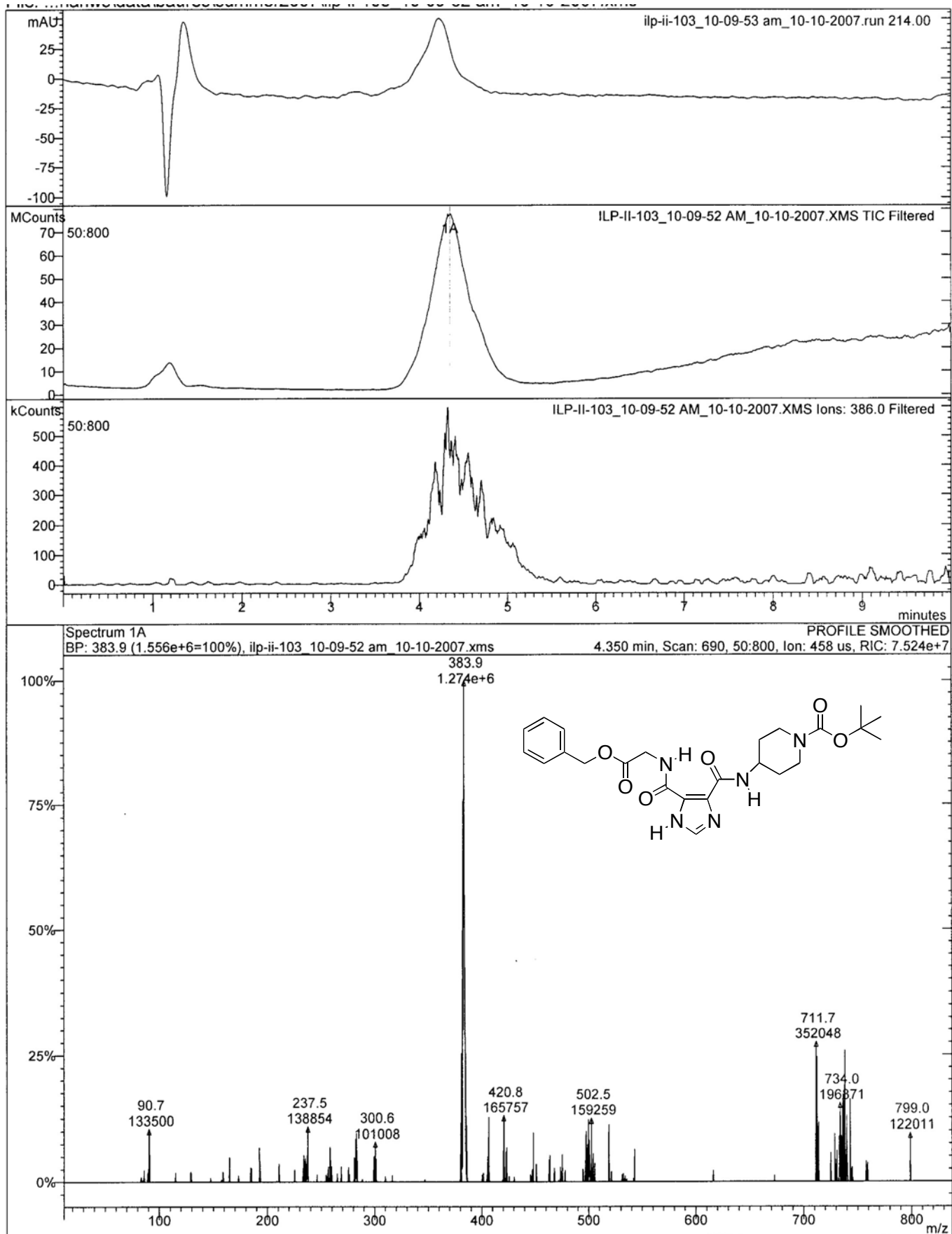


Figure S20. LC/MS data for 5{20}.

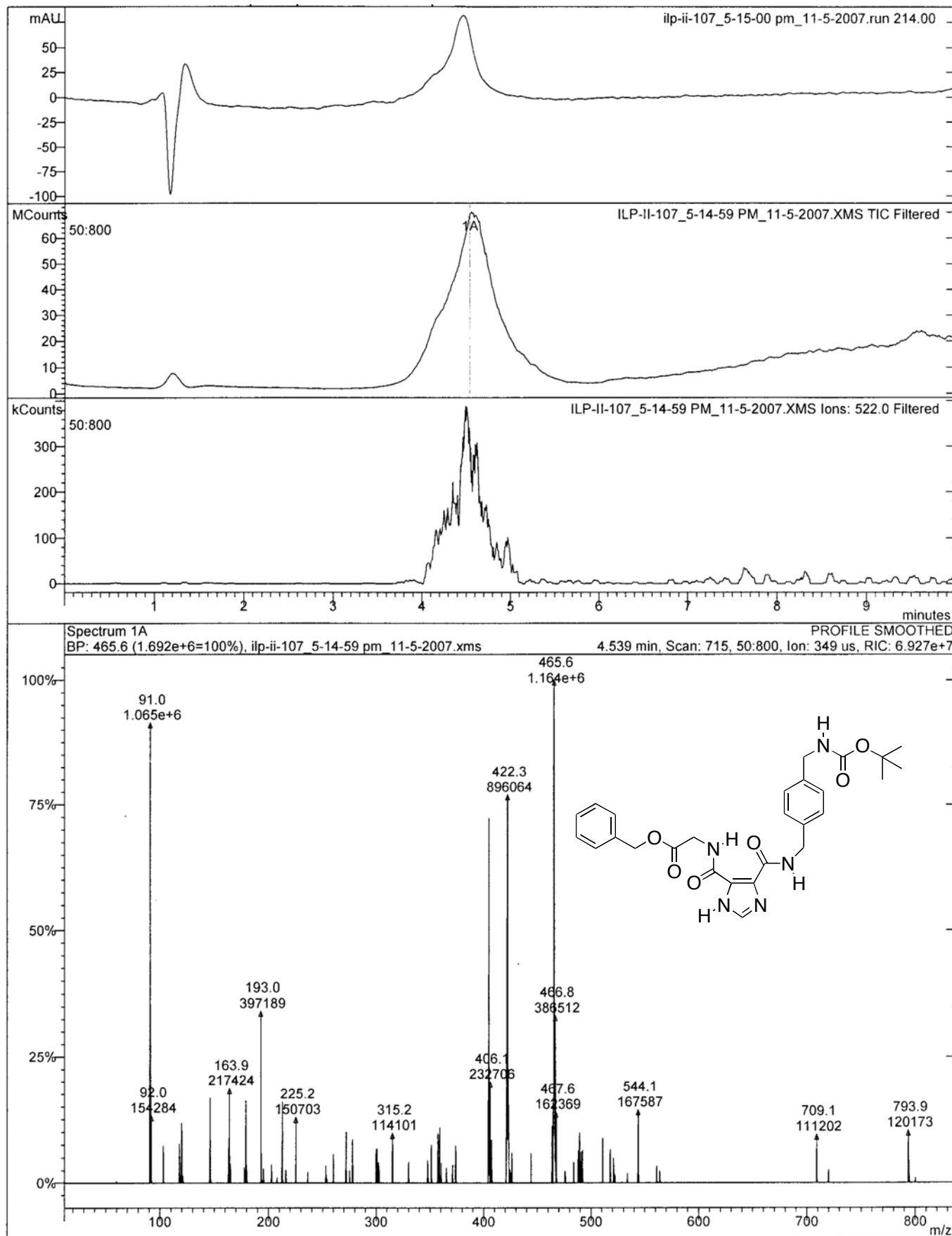


Figure S21. LC/MS data for 5{21}.

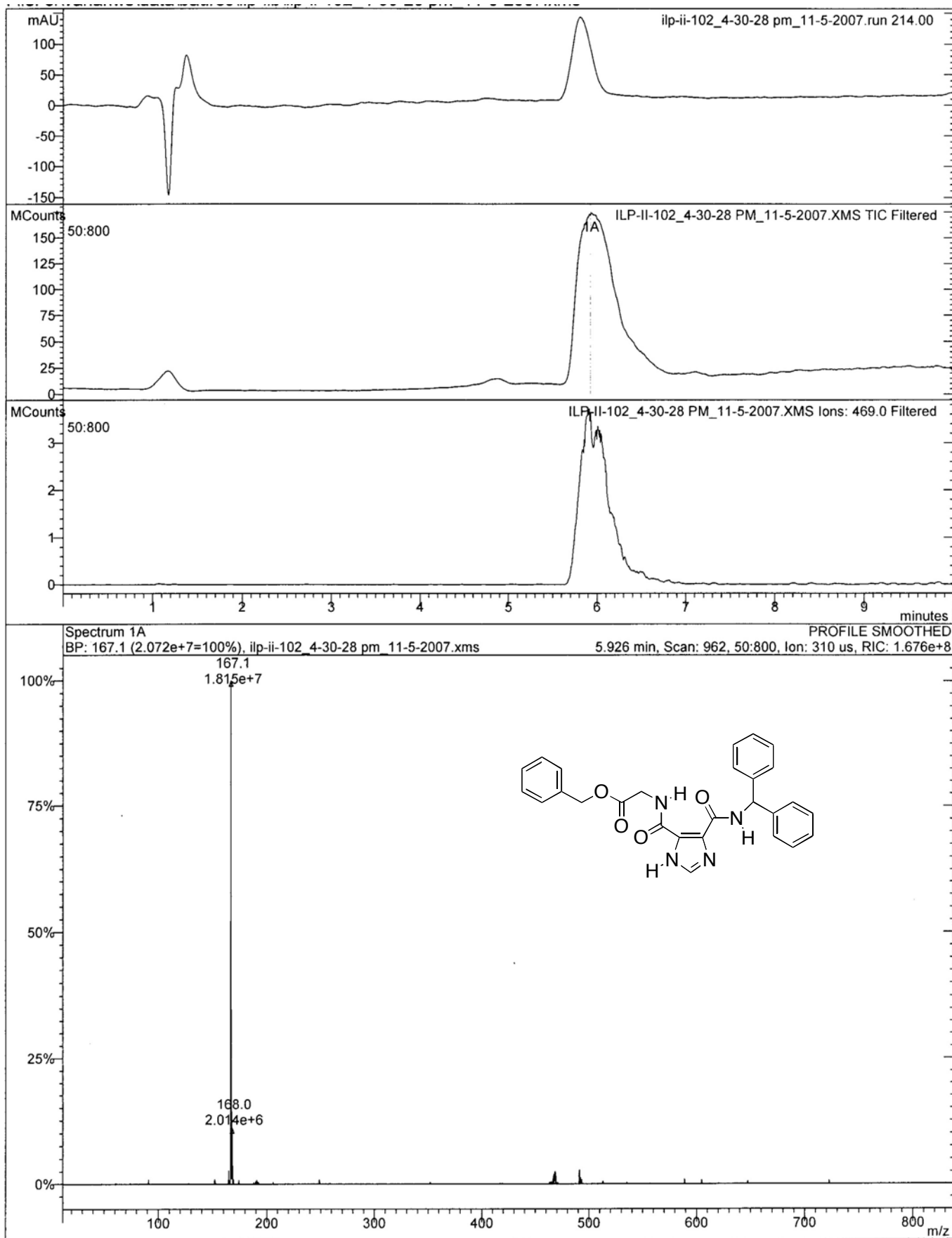


Figure S22. LC/MS data for 5{22}.

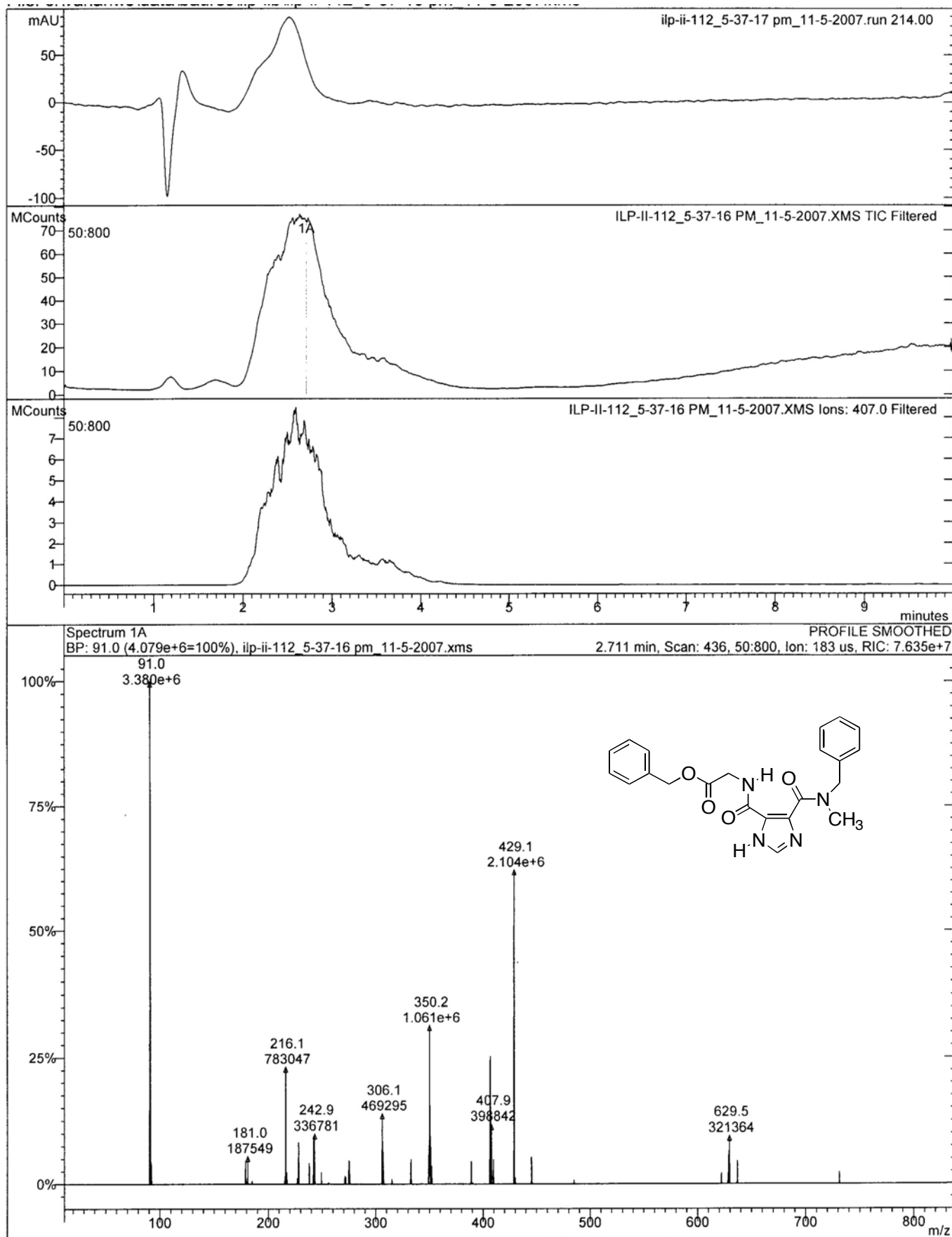


Figure S23. LC/MS data for 5{23}.

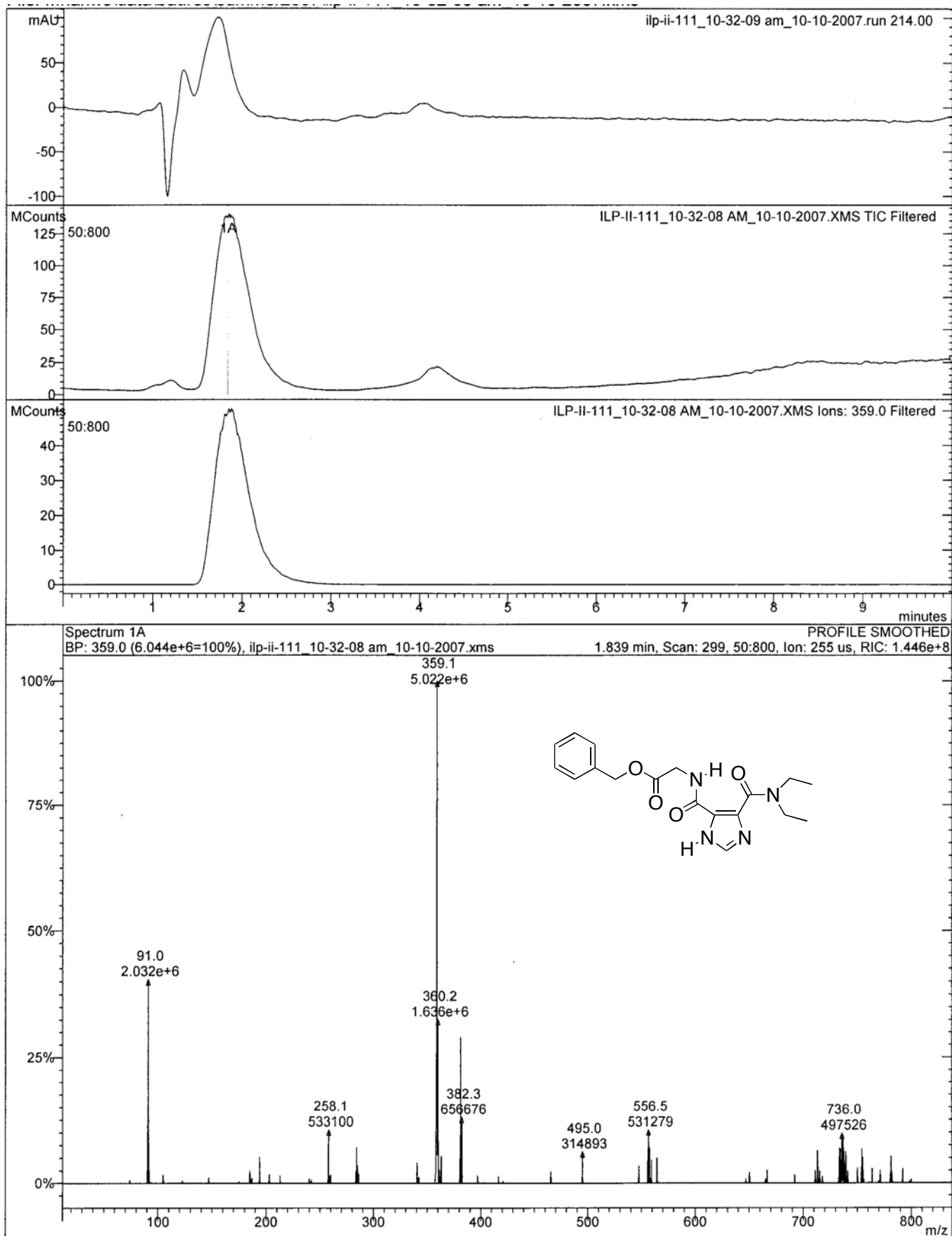


Figure S42. LC/MS data for 5{24}.

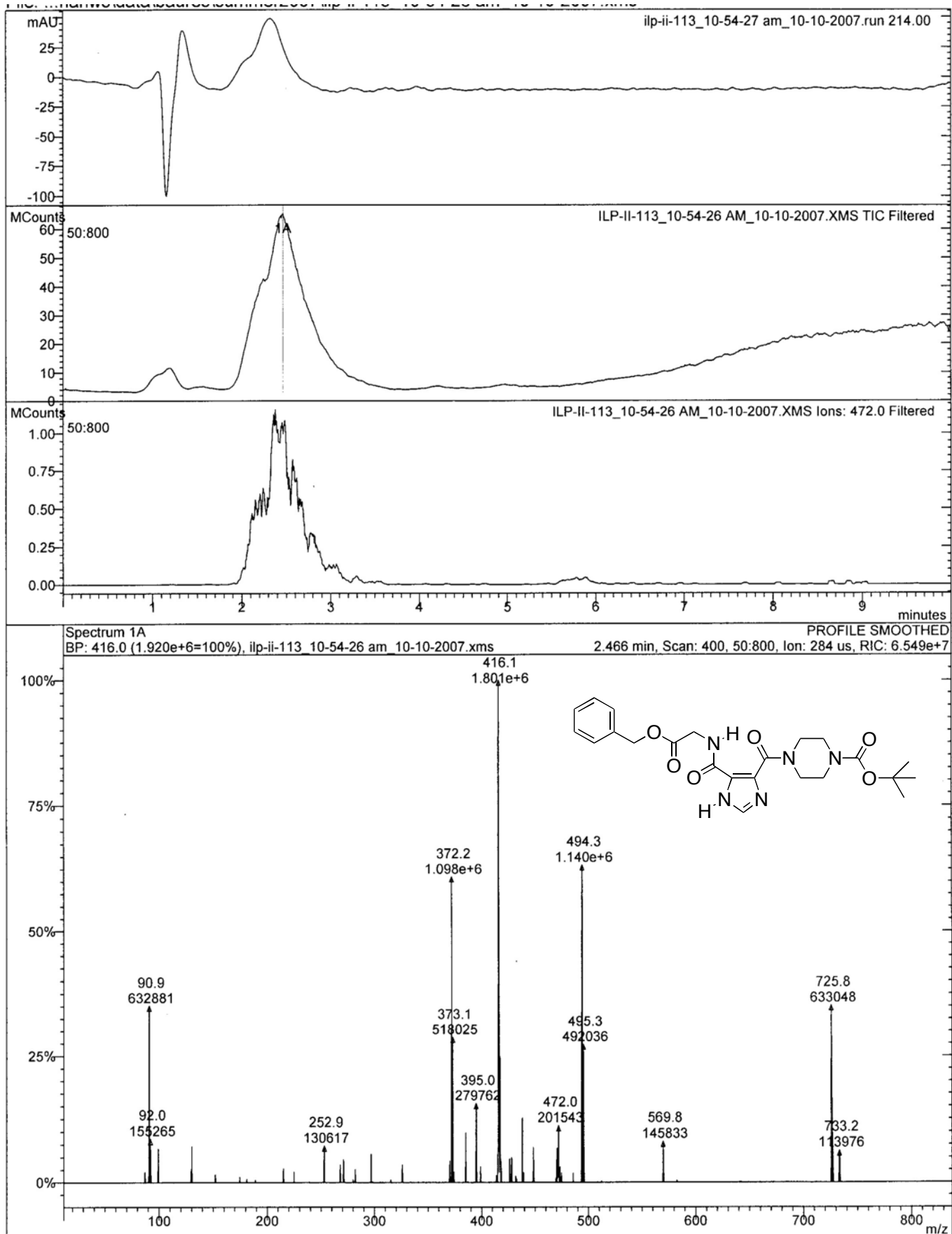


Figure S25. LC/MS data for 5{25}.

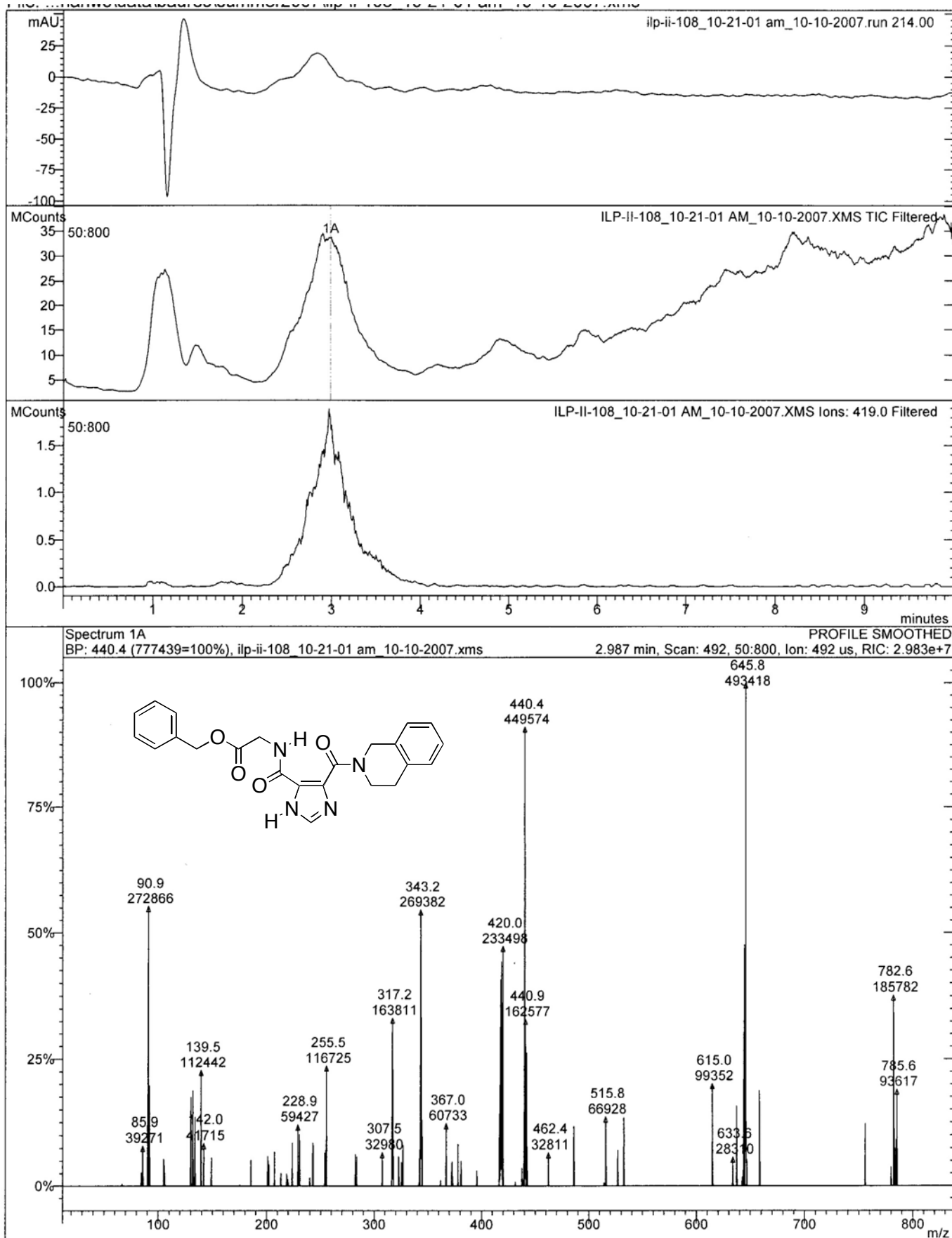
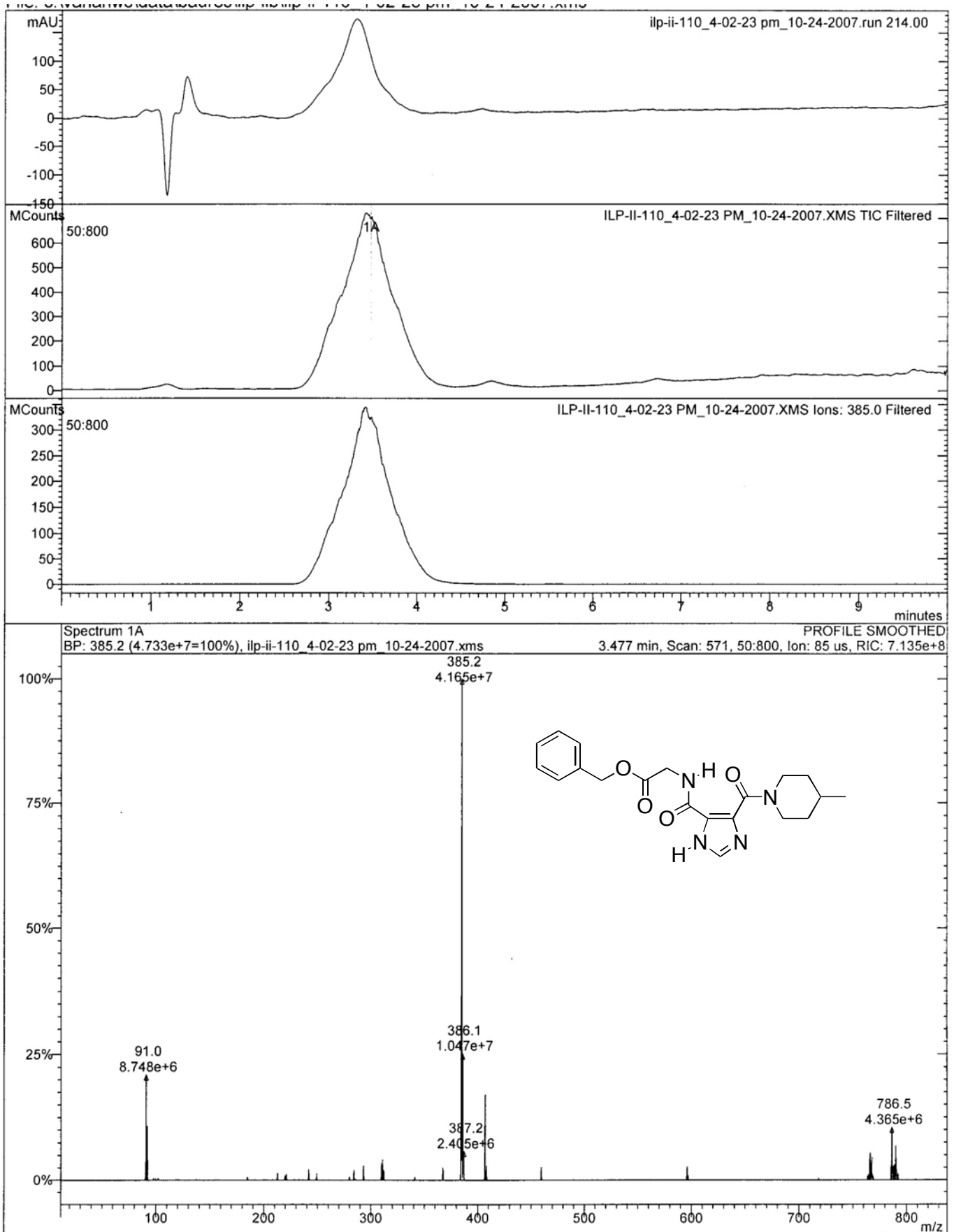


Figure S26. LC/MS data for 5{26}.



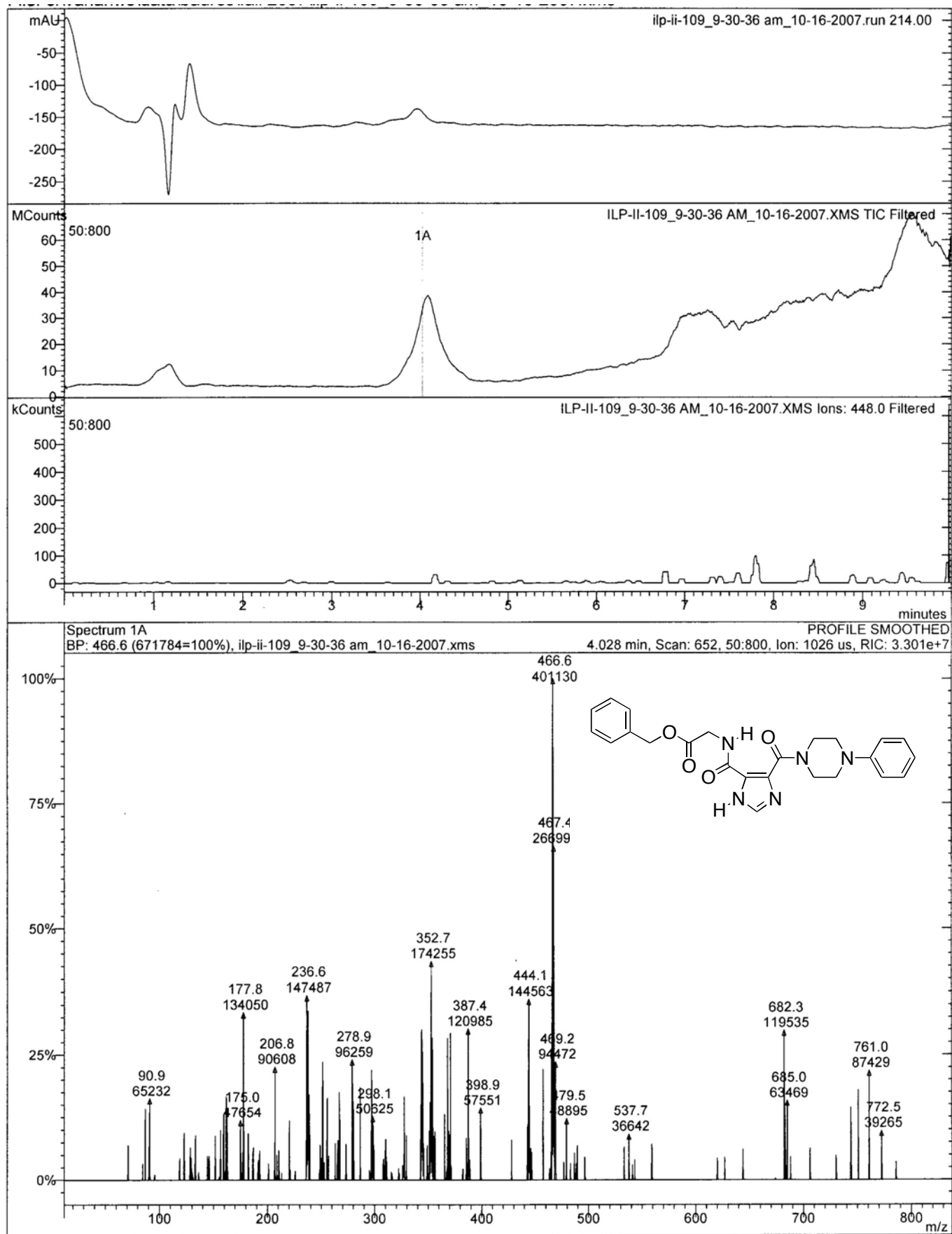


Figure S28. LC/MS data for 5{28}.

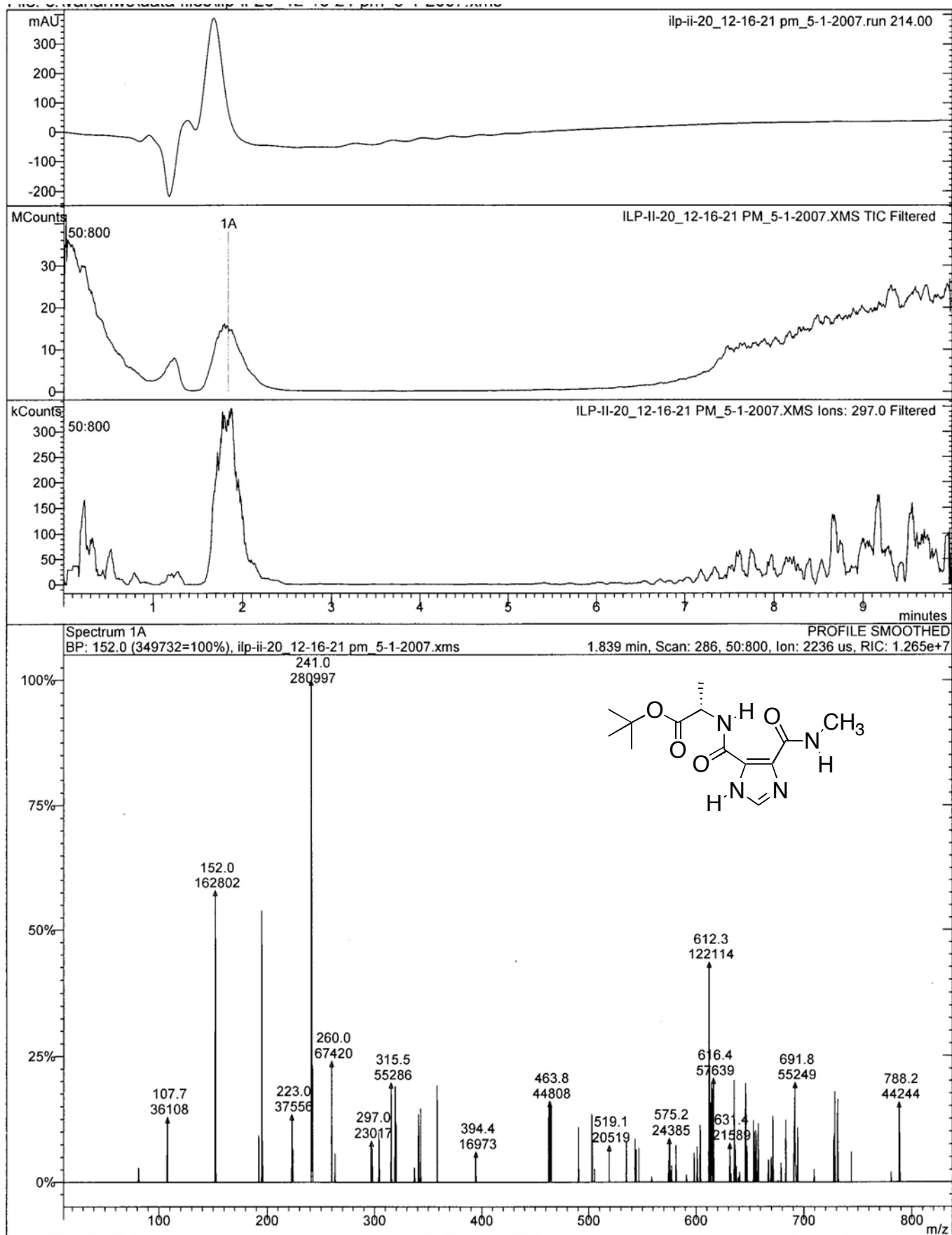


Figure S29. LC/MS data for 5{29}.

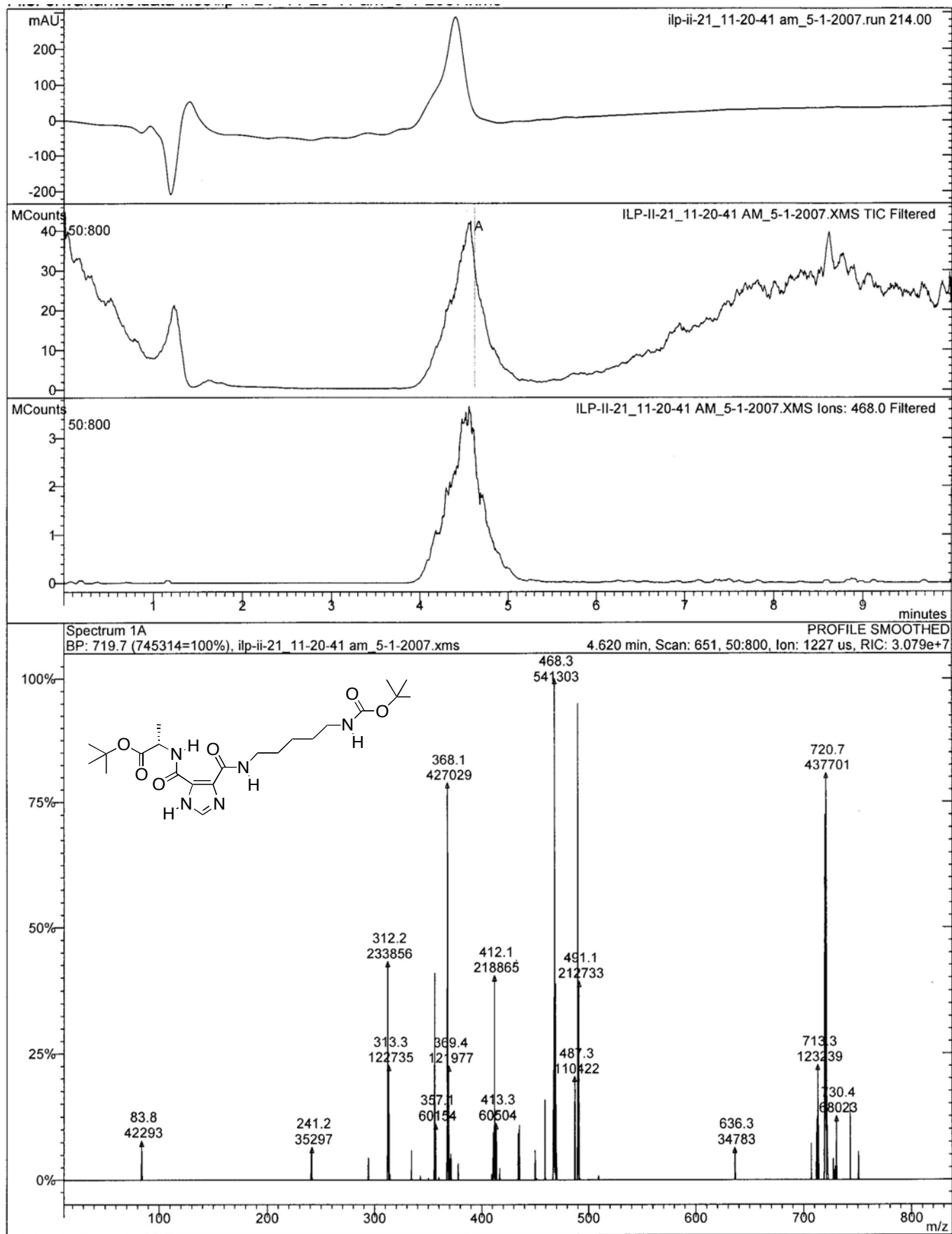


Figure S30. LC/MS data for 5{30}.

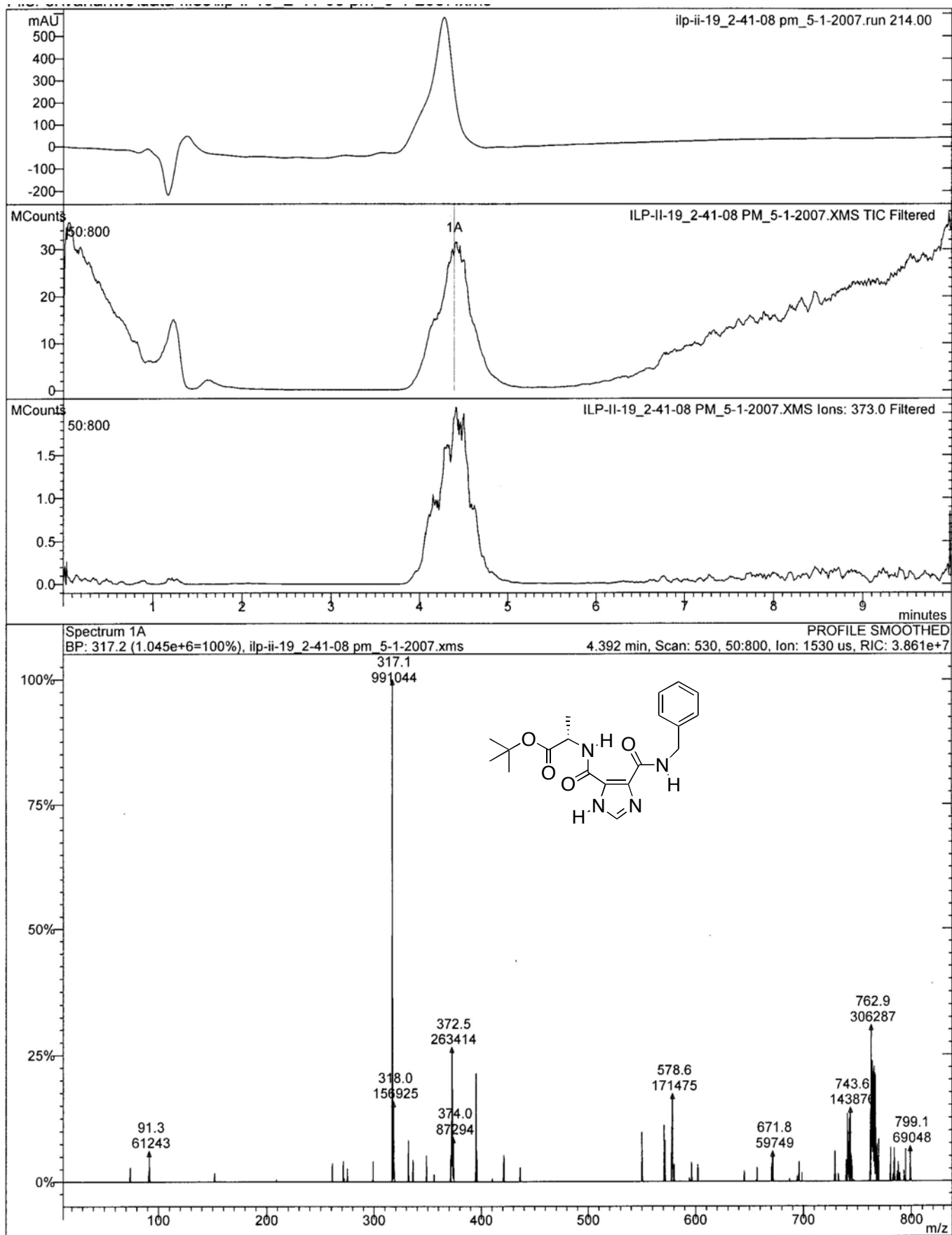


Figure S31. LC/MS data for 5{31}.

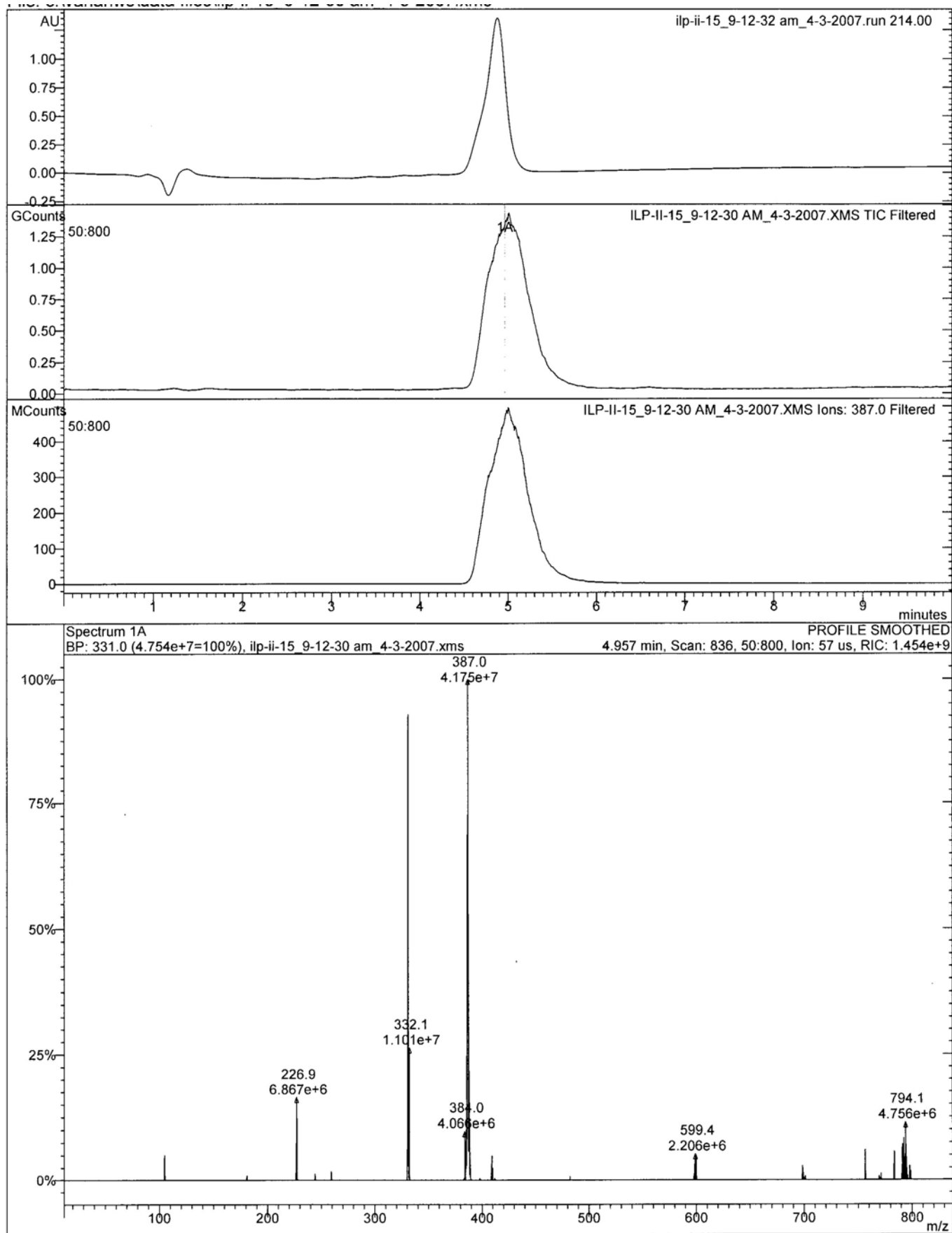


Figure S32. LC/MS data for 5{32}.

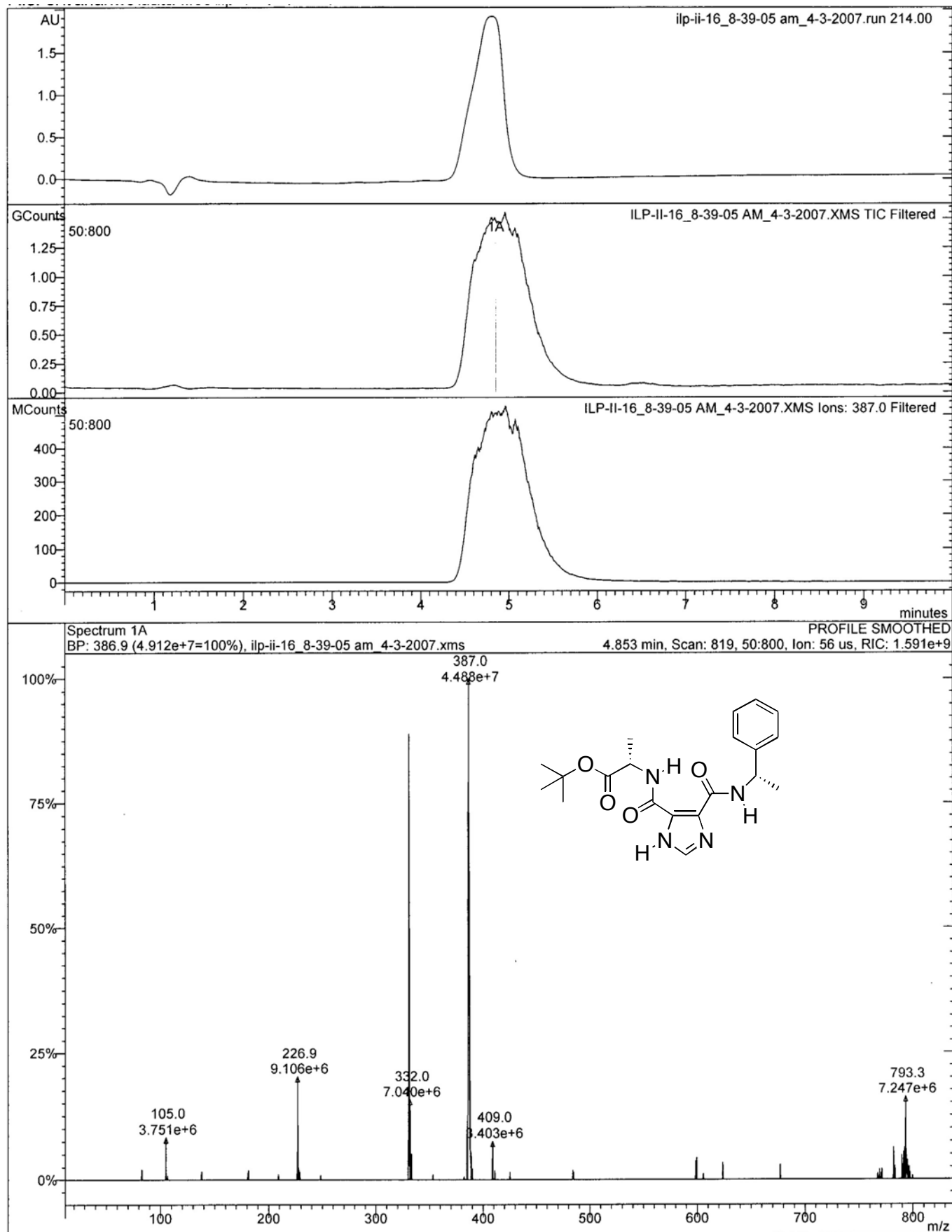


Figure S33. LC/MS data for 5{33}.

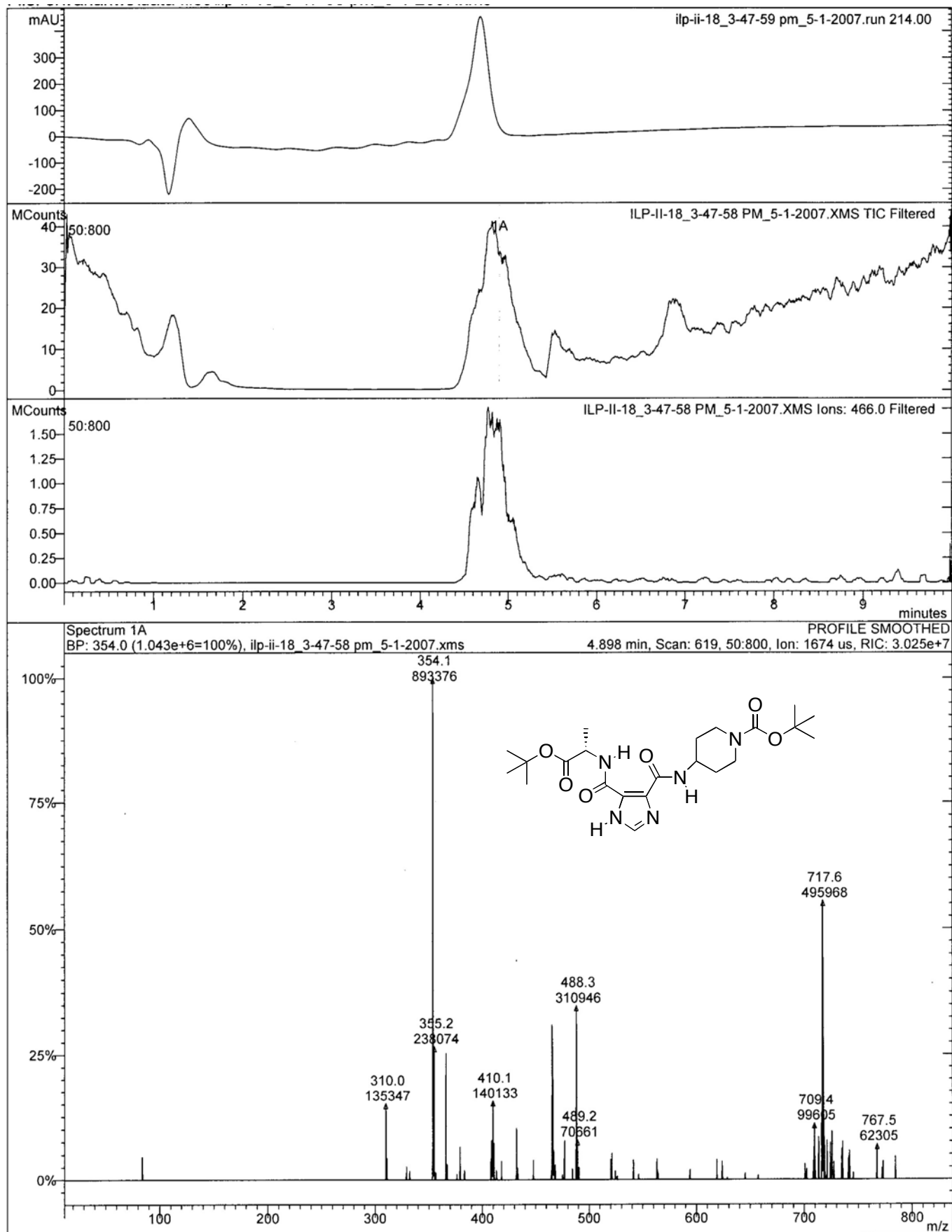


Figure S34. LC/MS data for 5{34}.

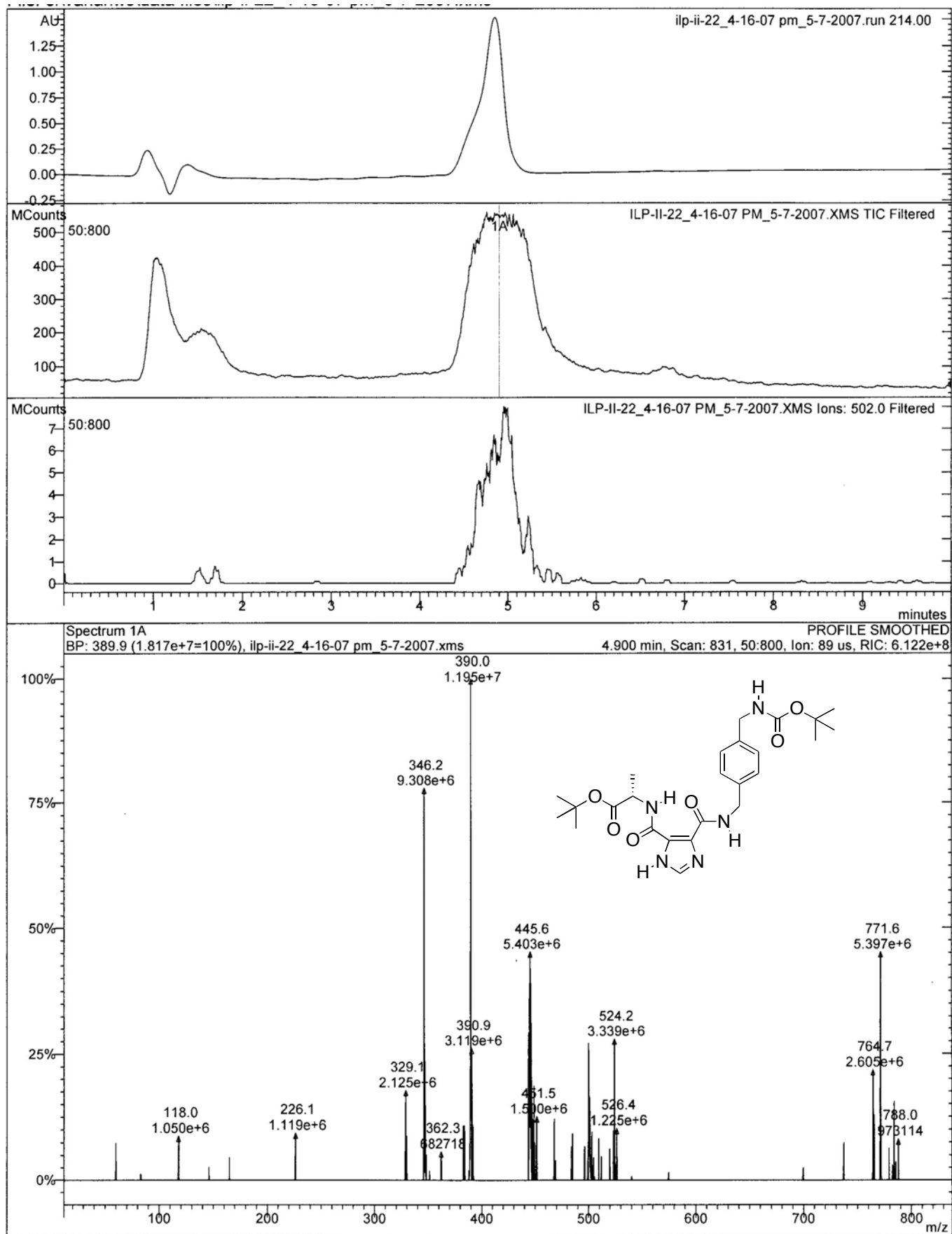


Figure S35. LC/MS data for 5{35}.

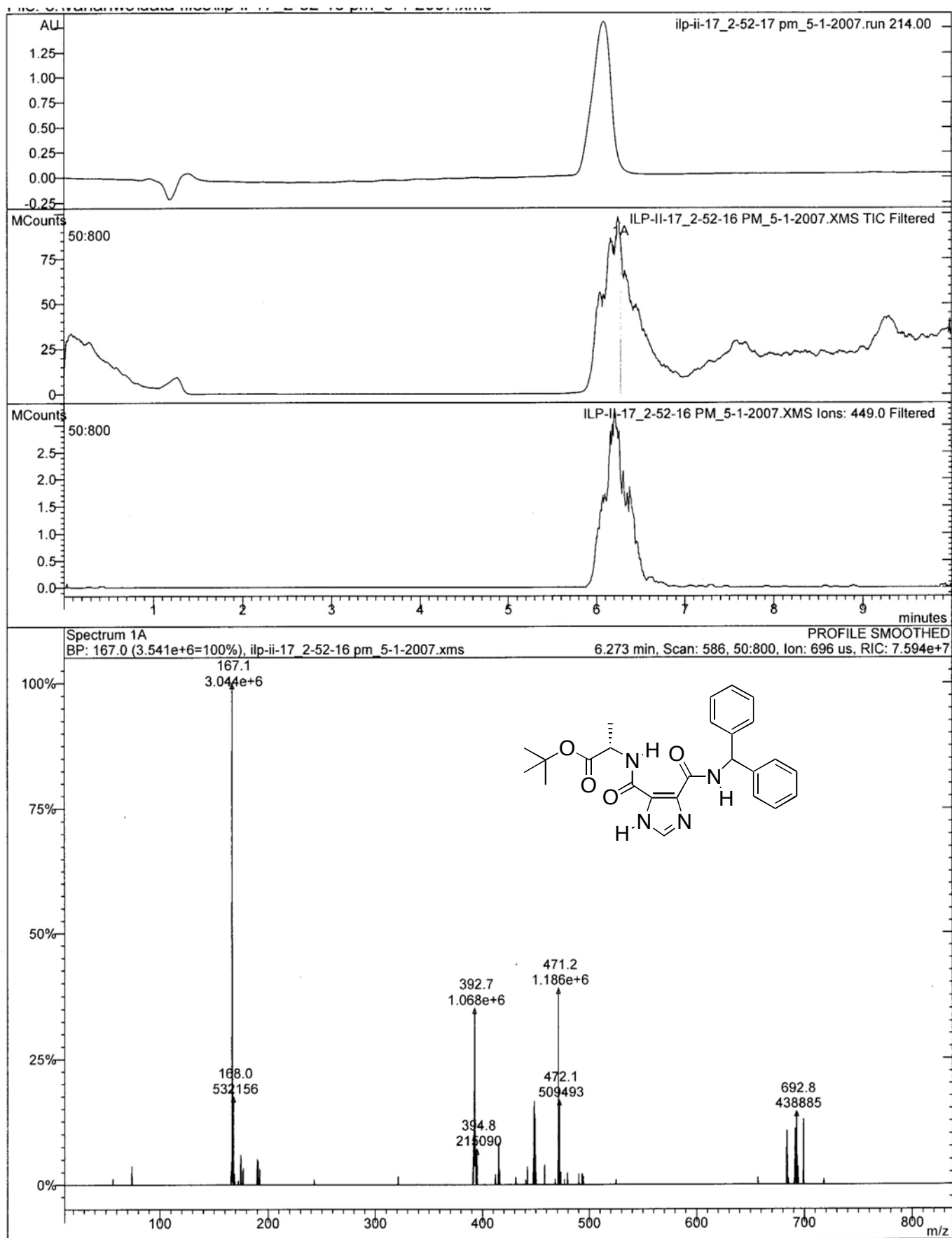


Figure S36. LC/MS data for 5{36}.

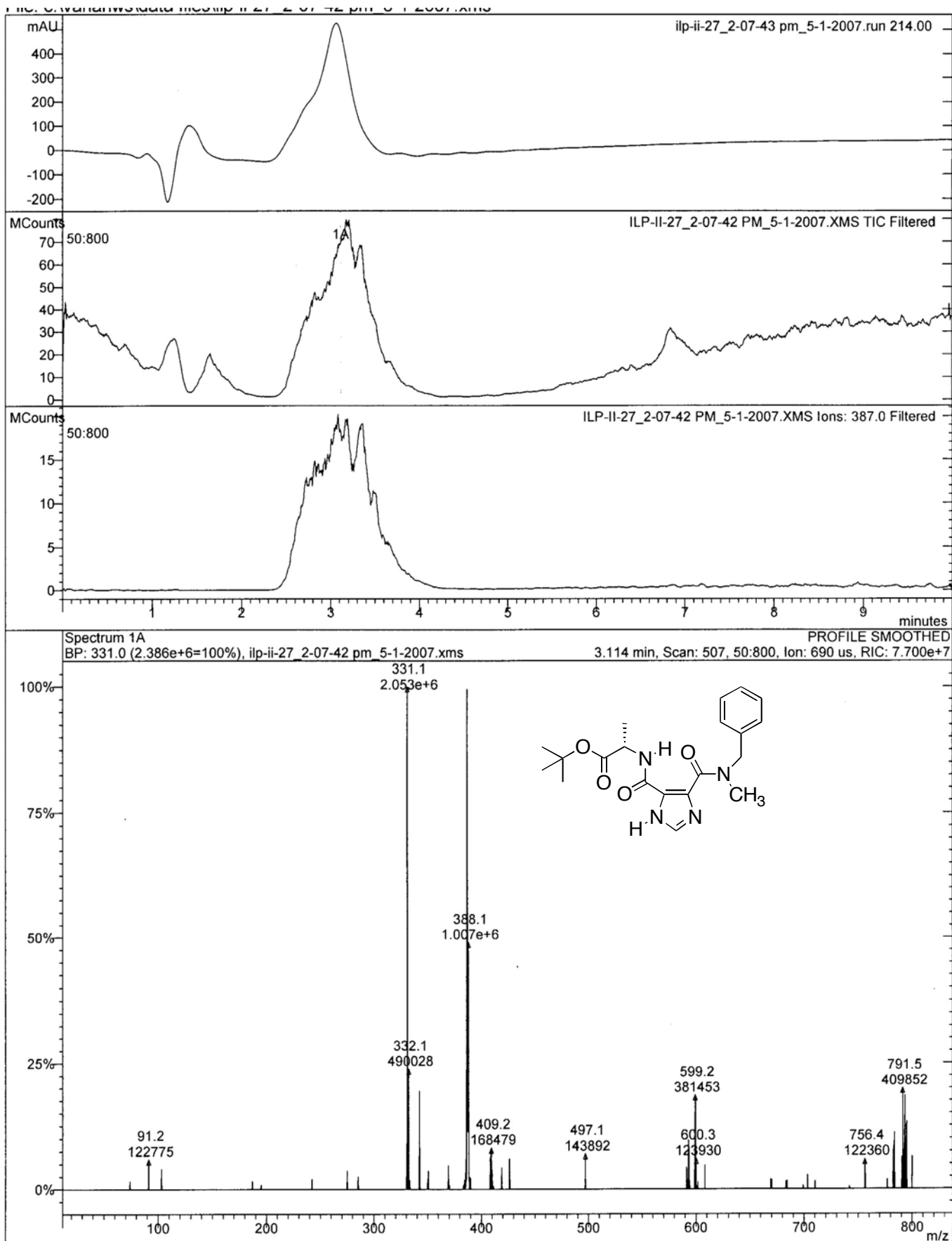


Figure S37. LC/MS data for 5{37}.

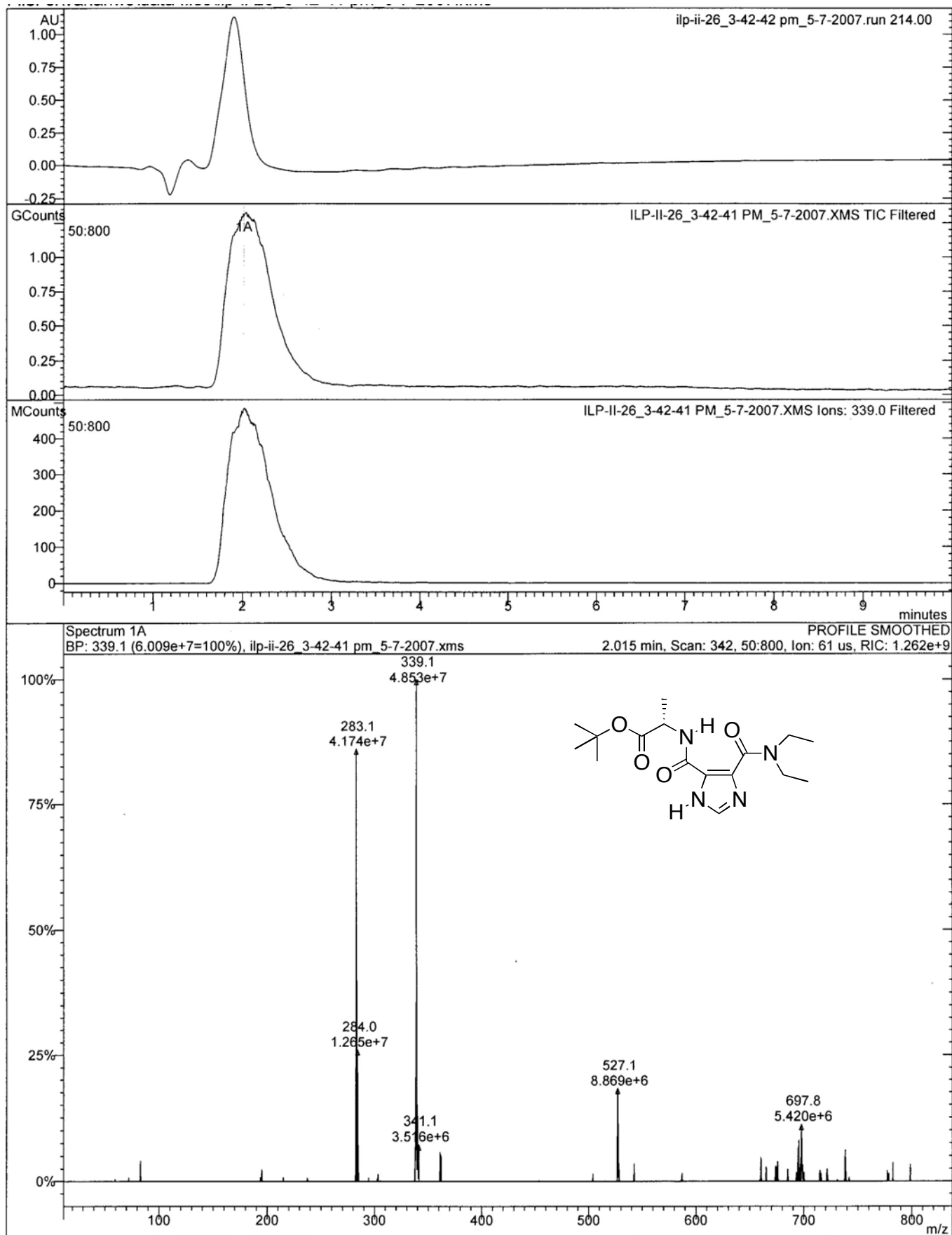


Figure S38. LC/MS data for 5{38}.

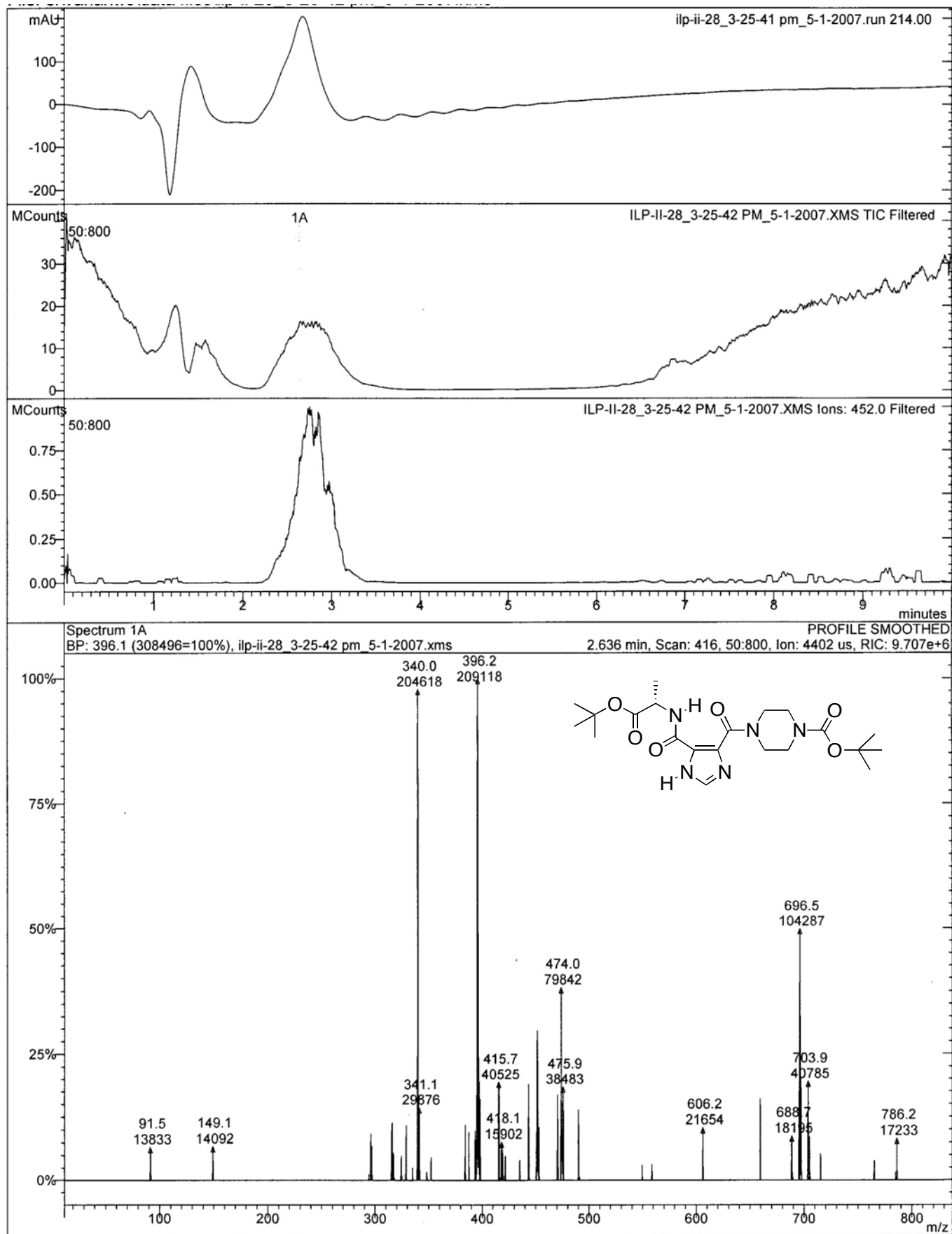


Figure S39. LC/MS data for 5{39}.

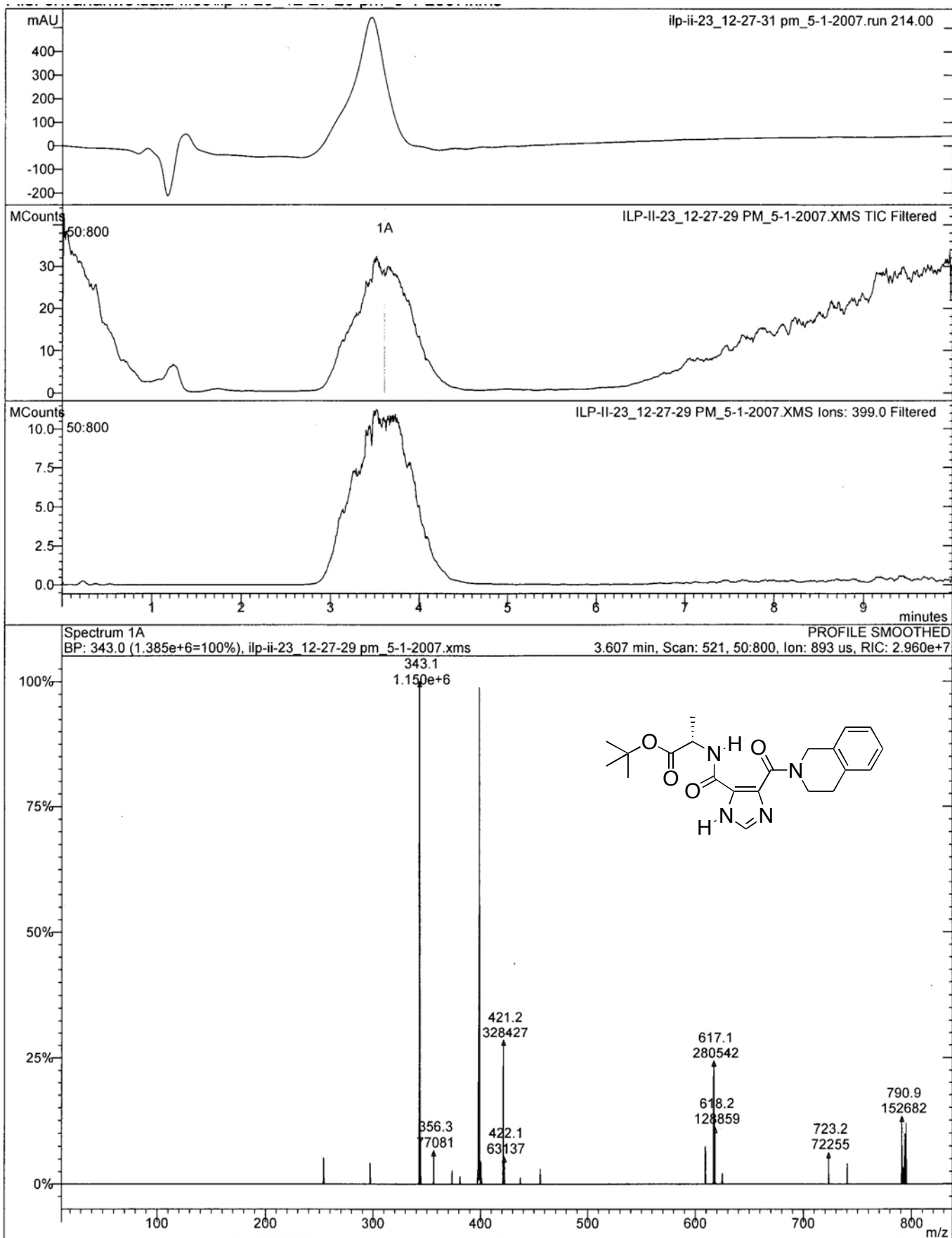


Figure S40. LC/MS data for 5{40}.

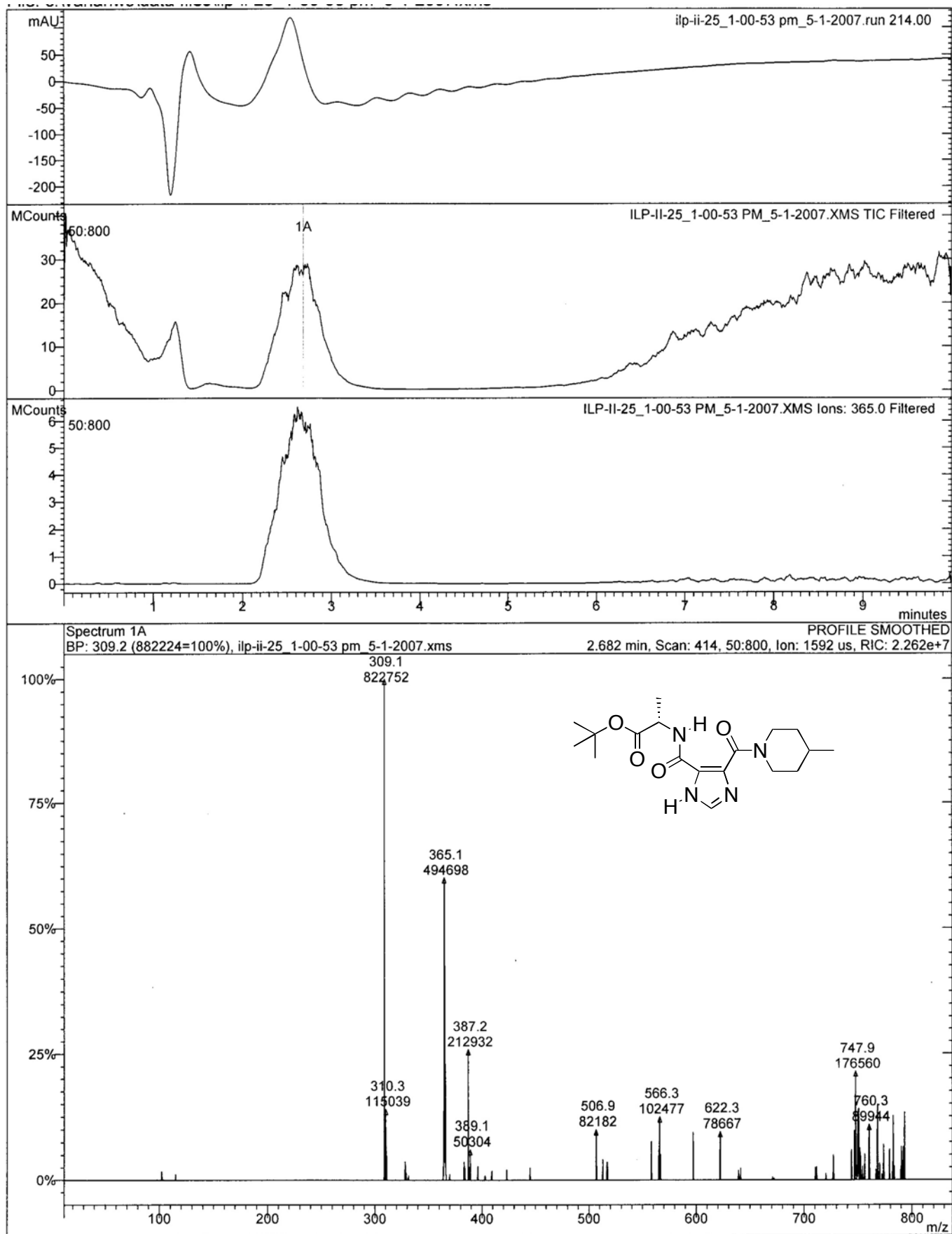


Figure S41. LC/MS data for 5{41}.

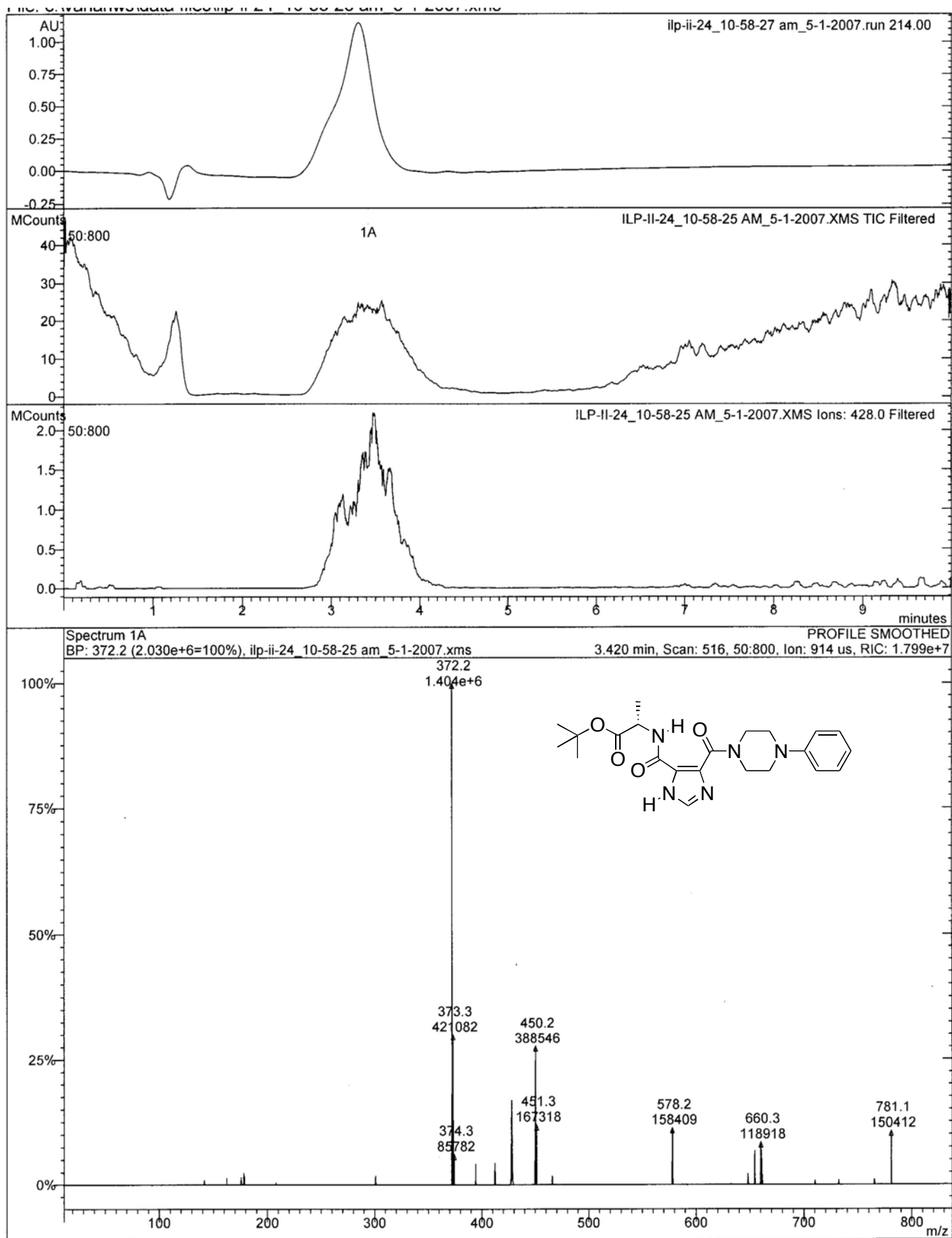


Figure S42. LC/MS data for 5{42}.

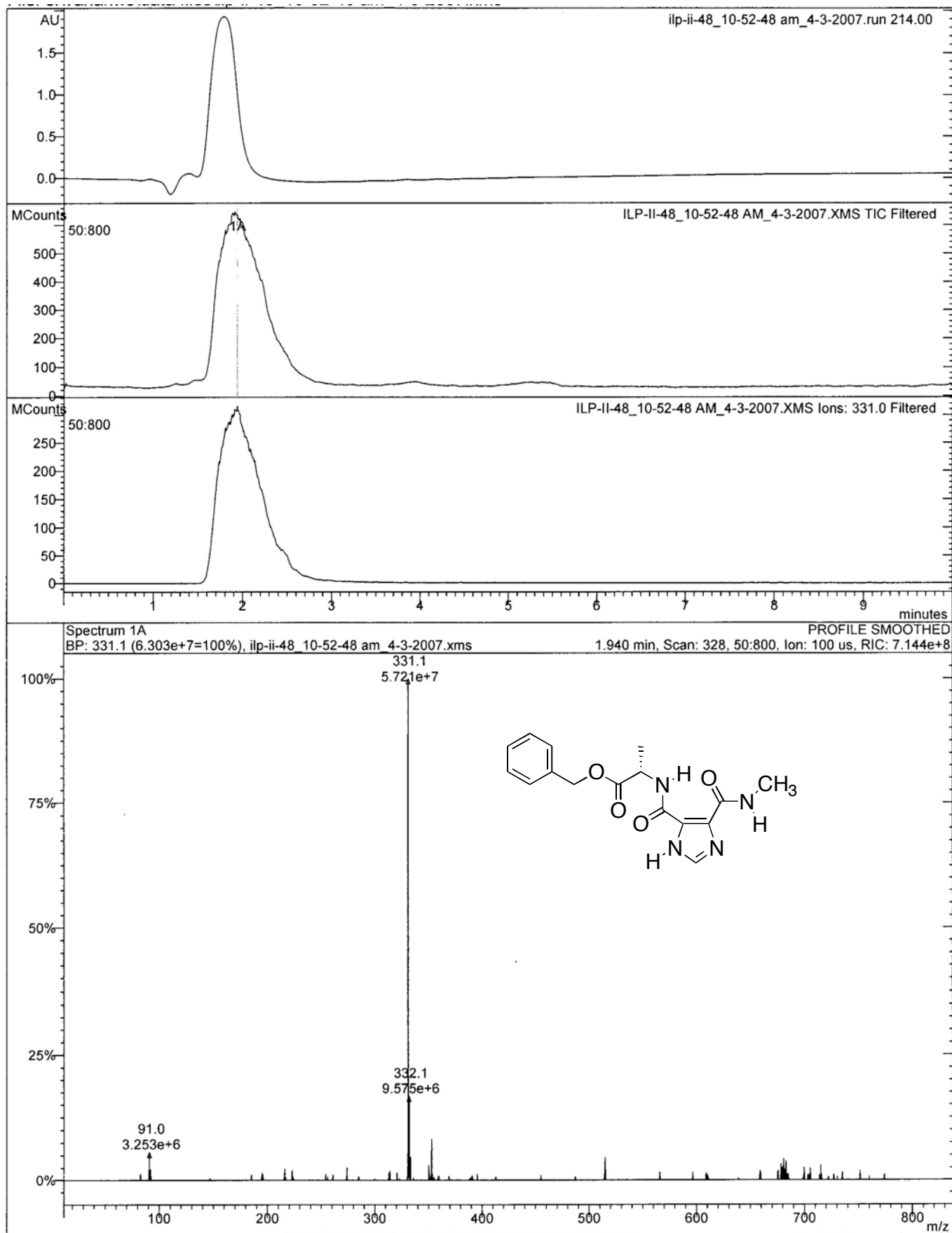


Figure S43. LC/MS data for 5{43}.

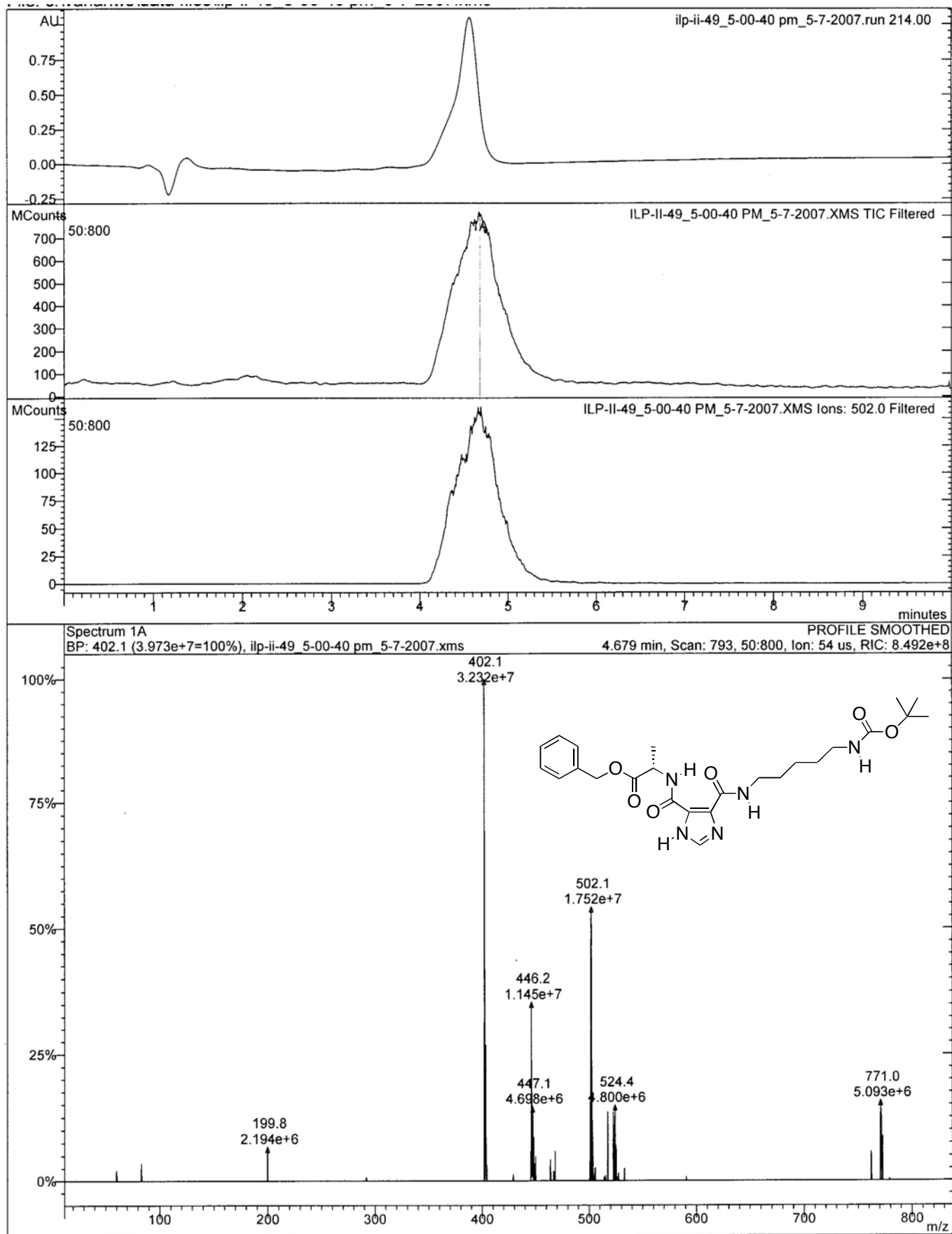


Figure S44. LC/MS data for 5{44}.

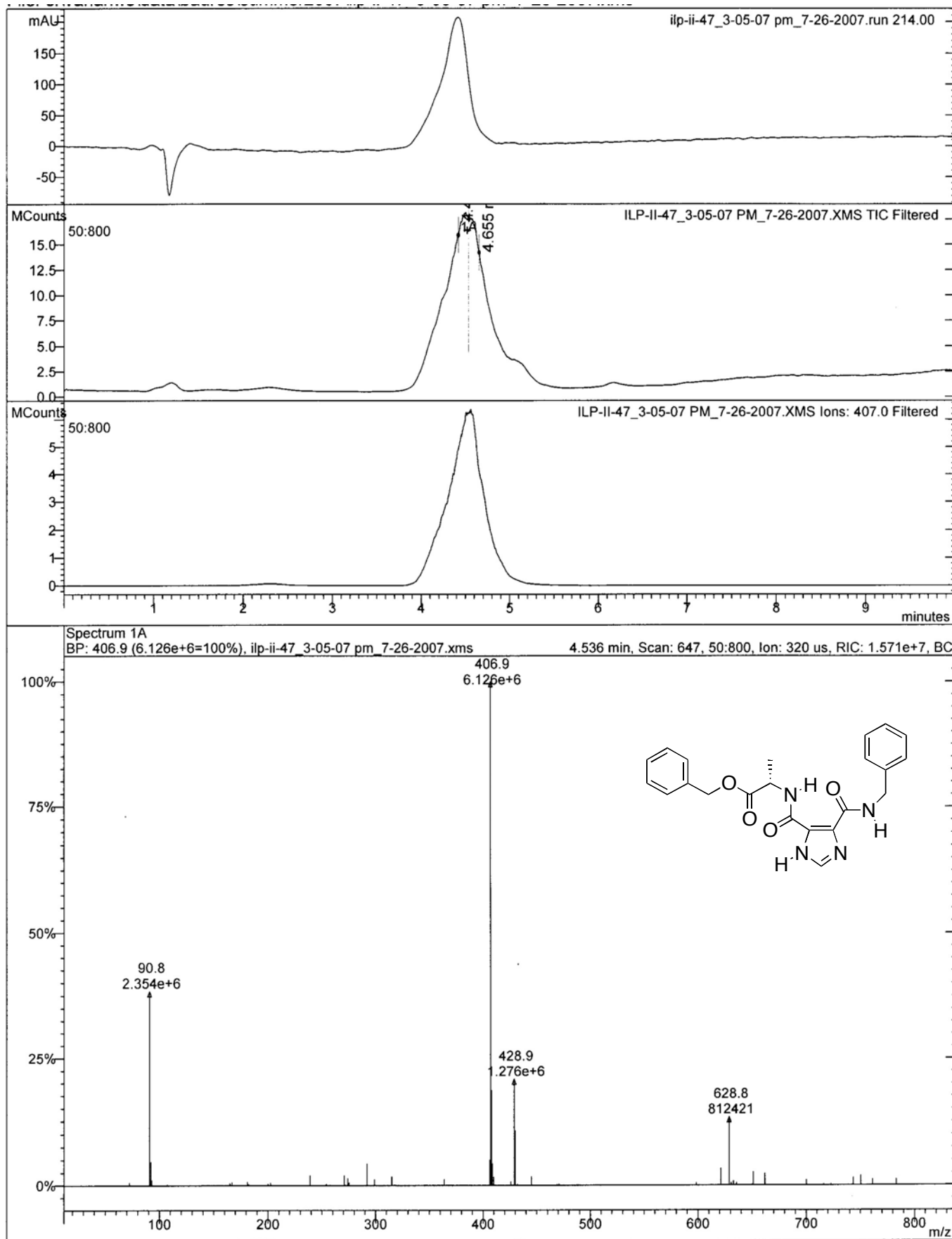


Figure S45. LC/MS data for 5{45}.

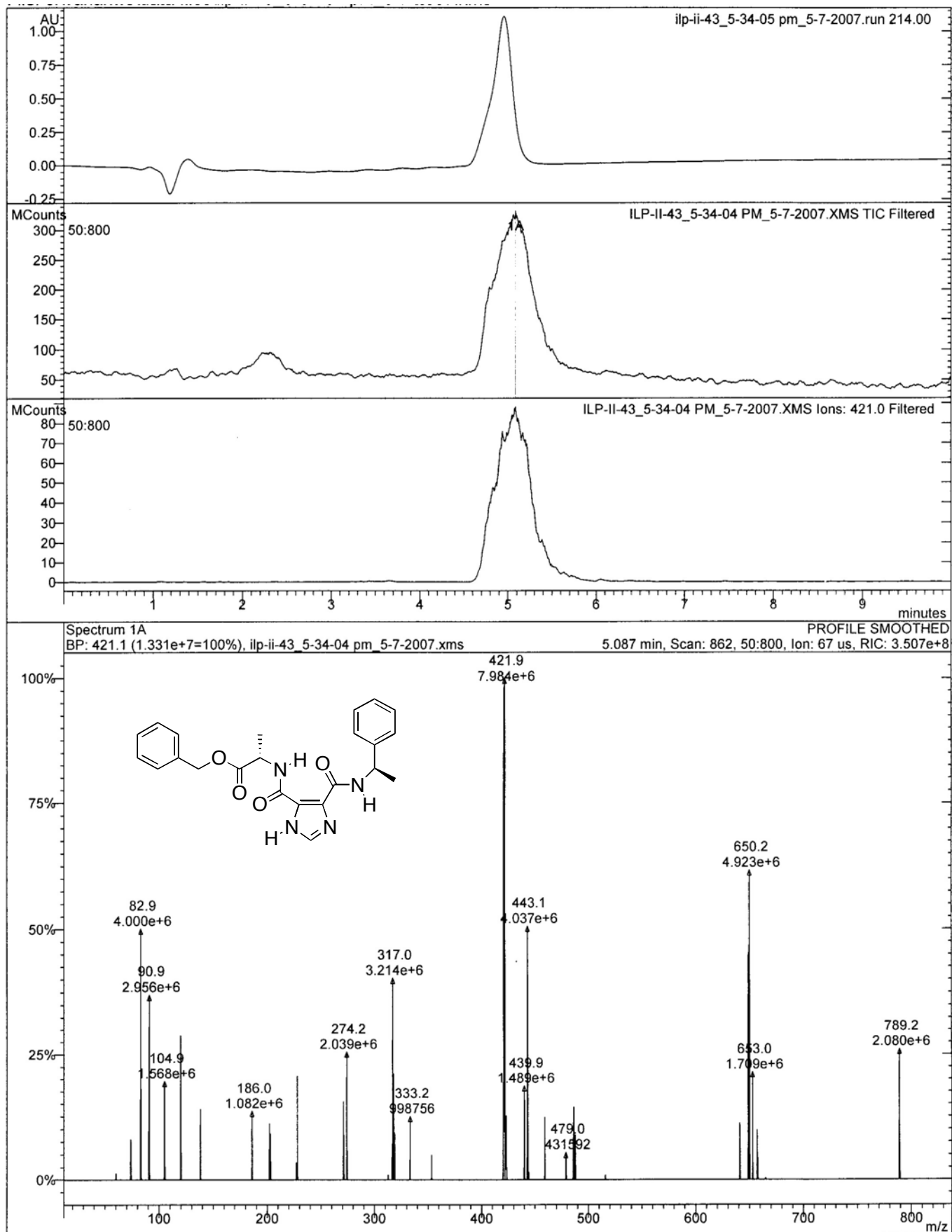


Figure S46. LC/MS data for 5{46}.

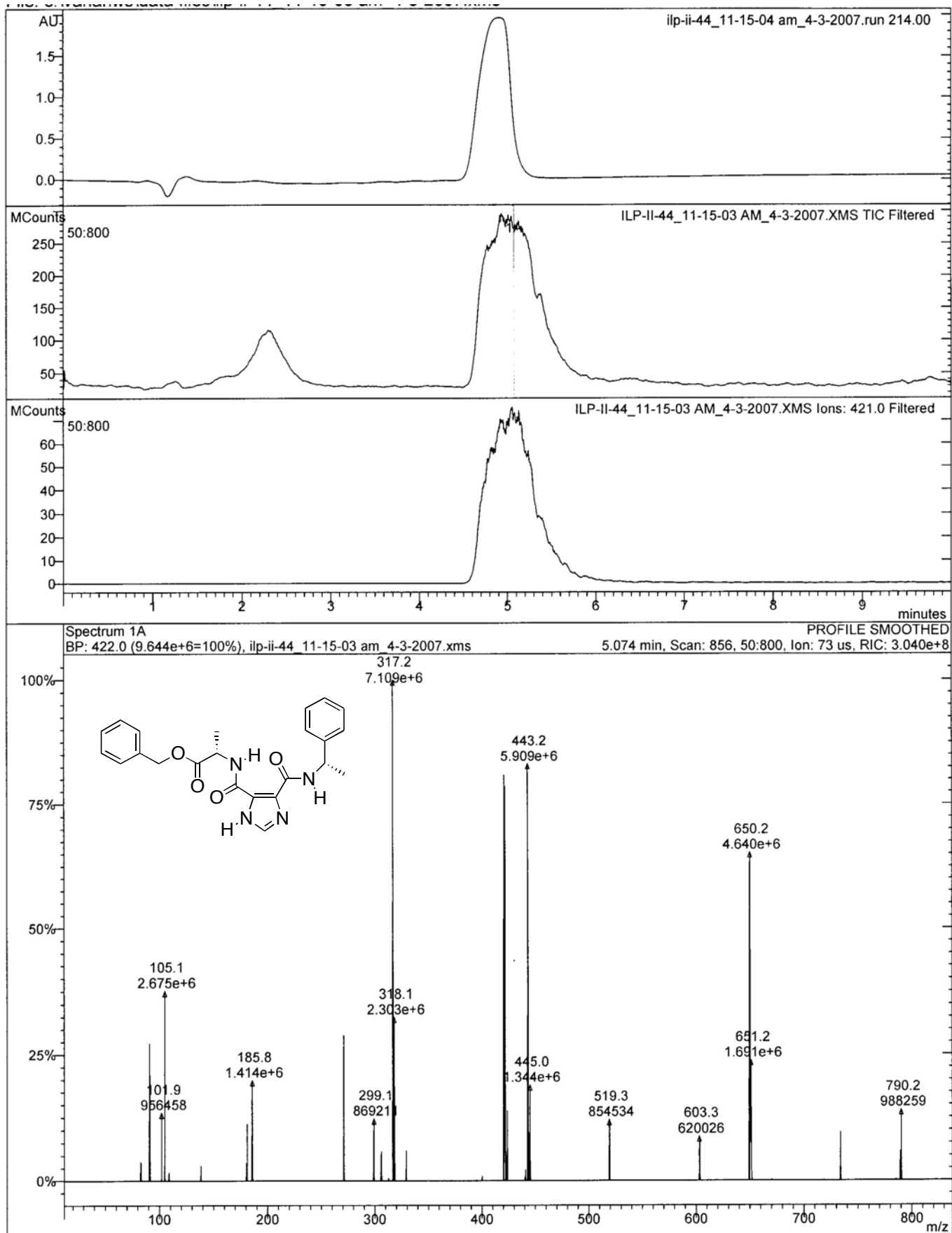


Figure S47. LC/MS data for 5{47}.

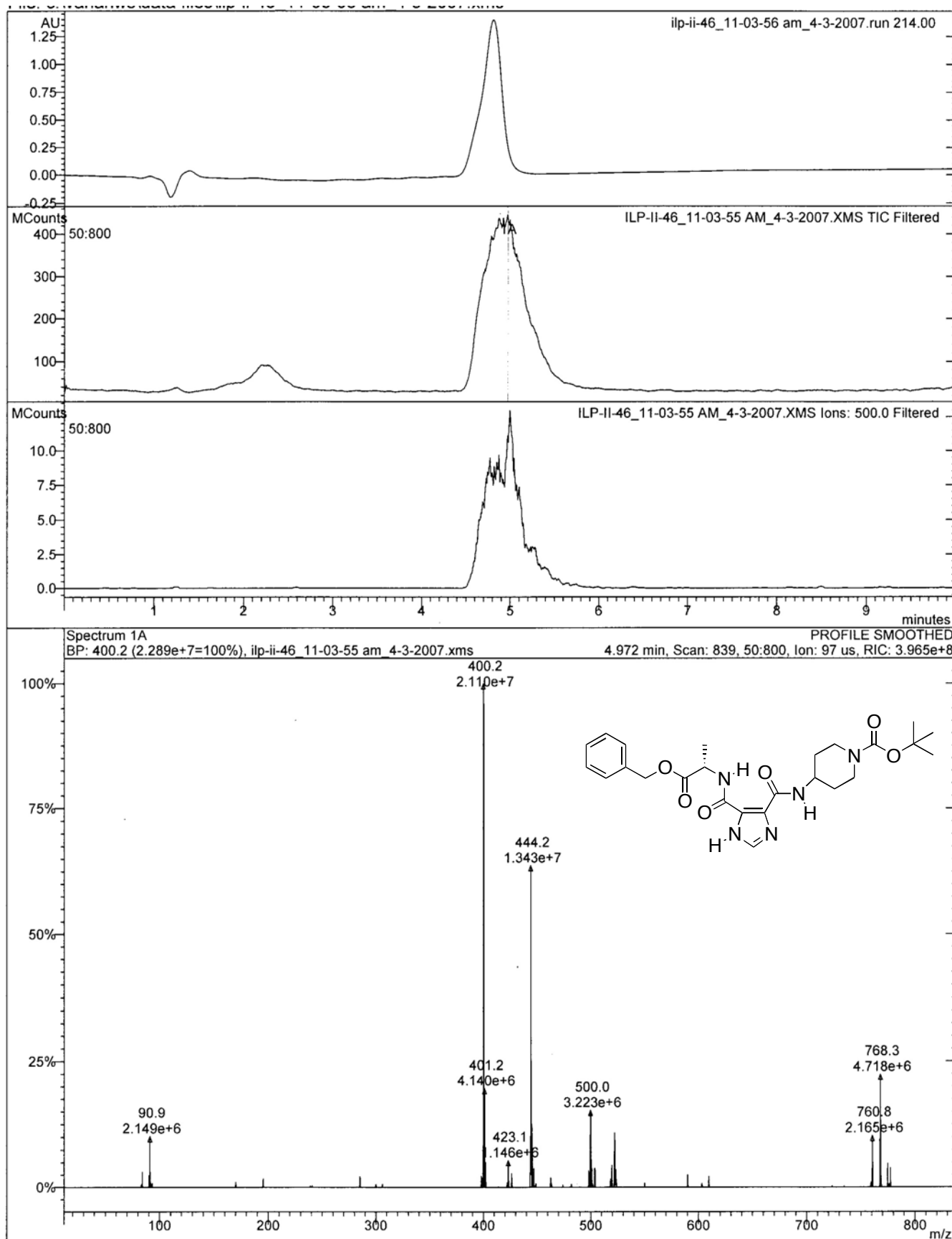


Figure S48. LC/MS data for 5{48}.

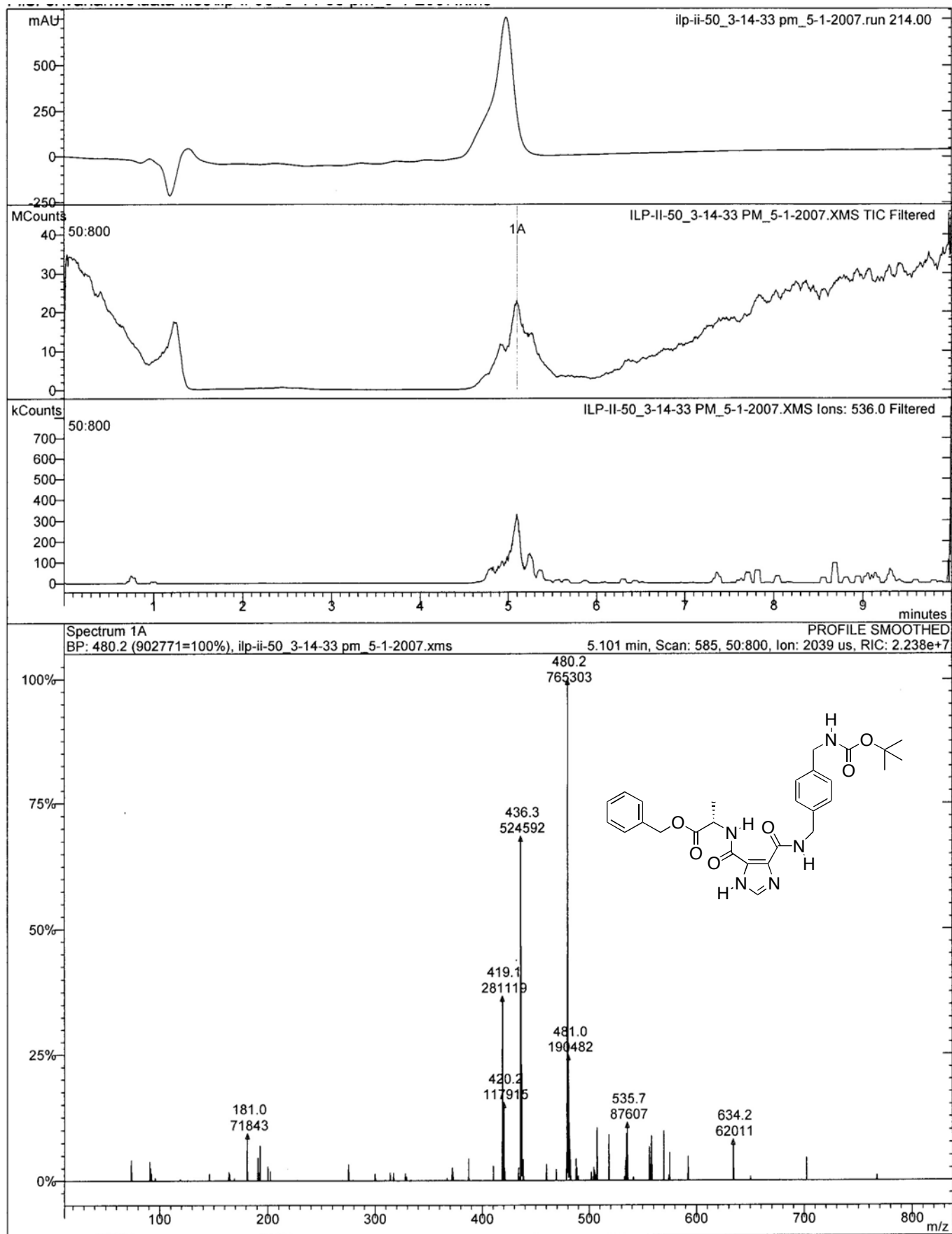


Figure S49. LC/MS data for 5{49}.

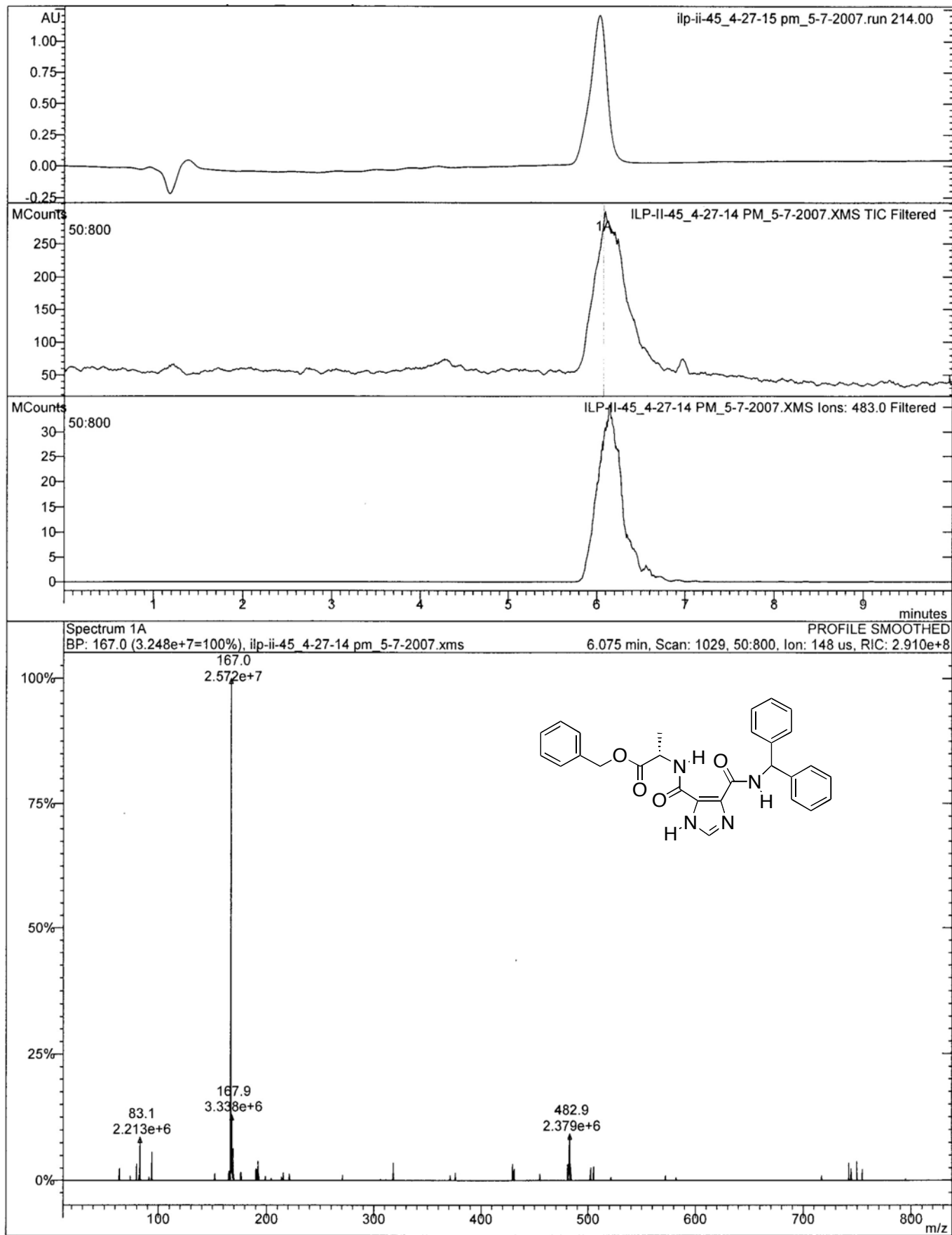


Figure S50. LC/MS data for 5{50}.

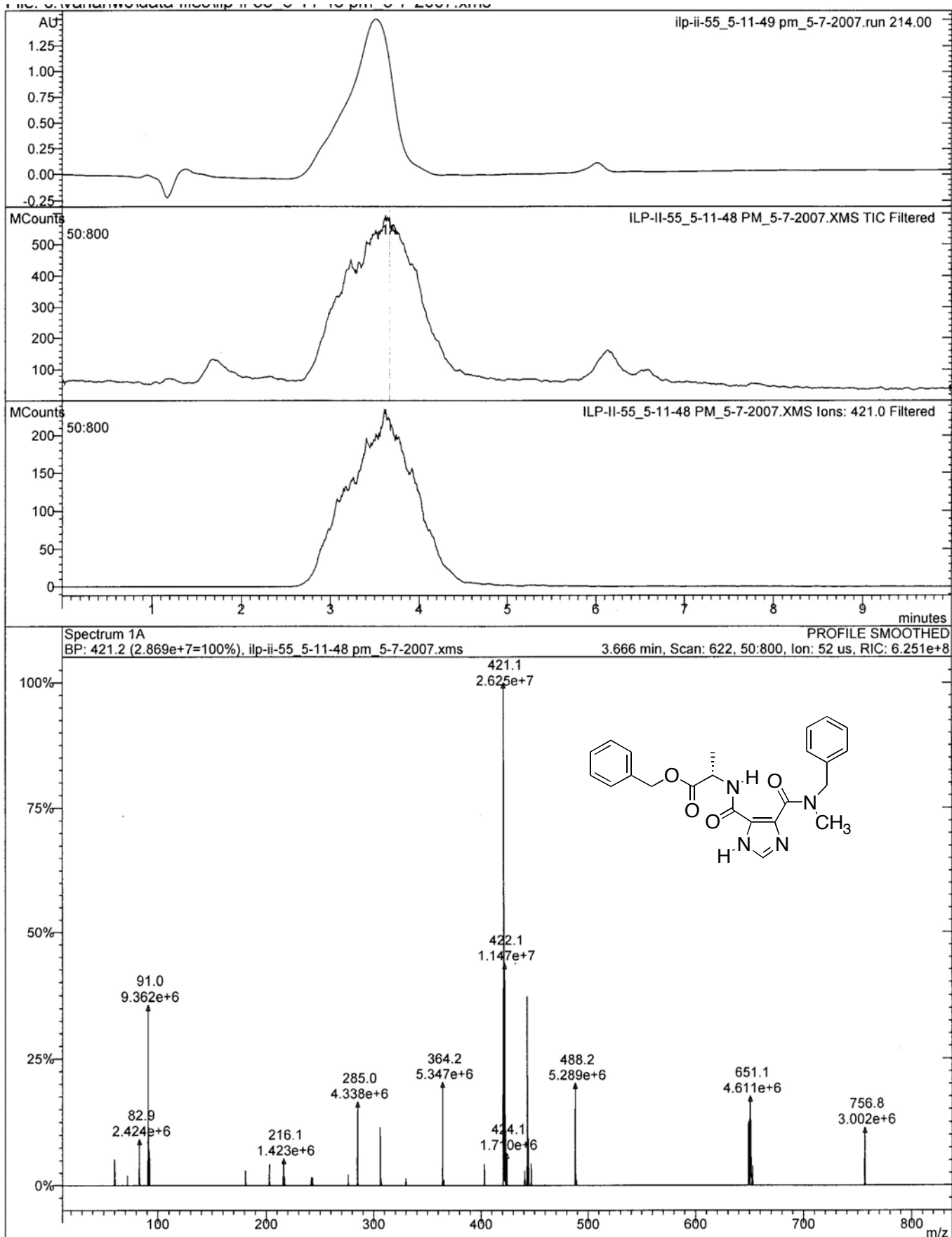


Figure S51. LC/MS data for 5{51}.

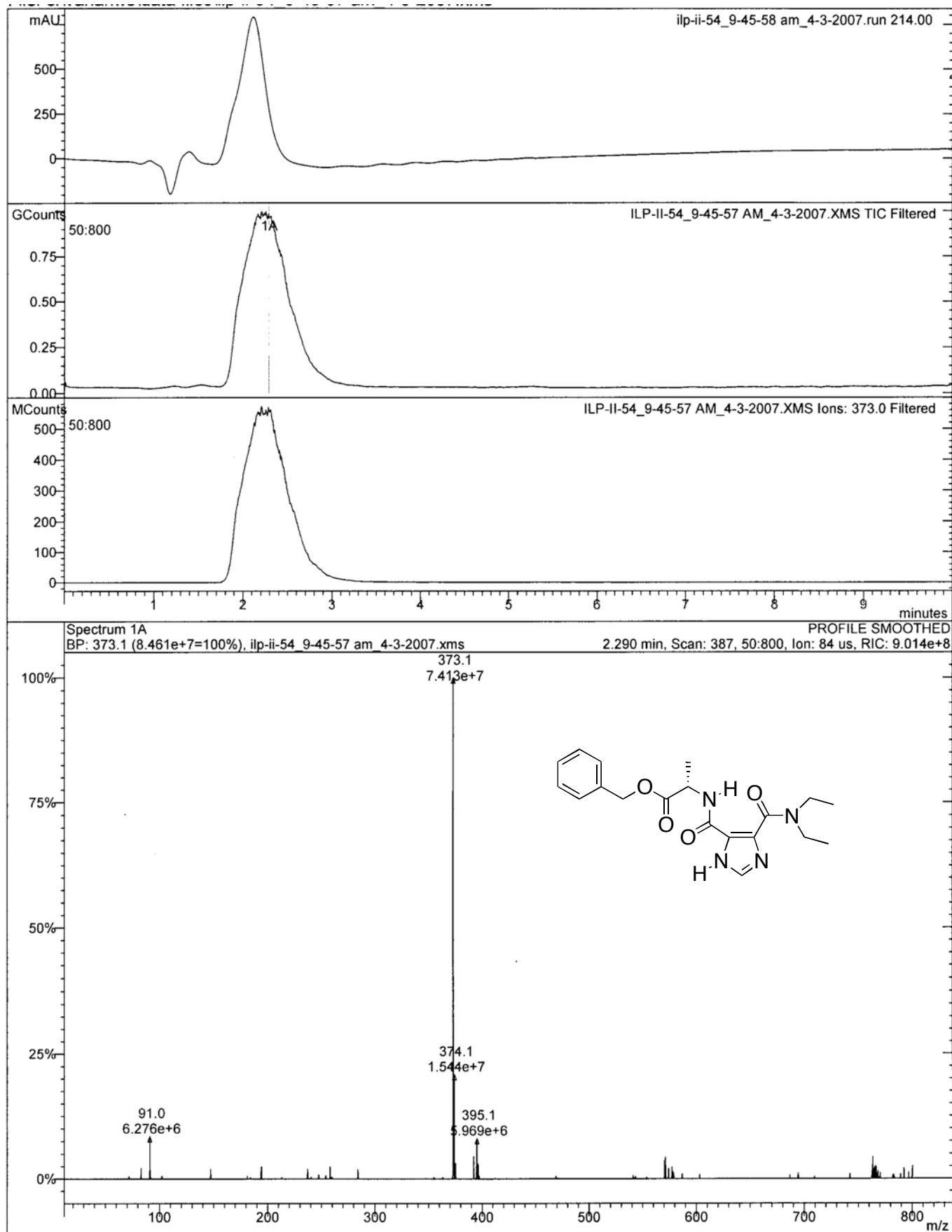


Figure S52. LC/MS data for 5{52}.

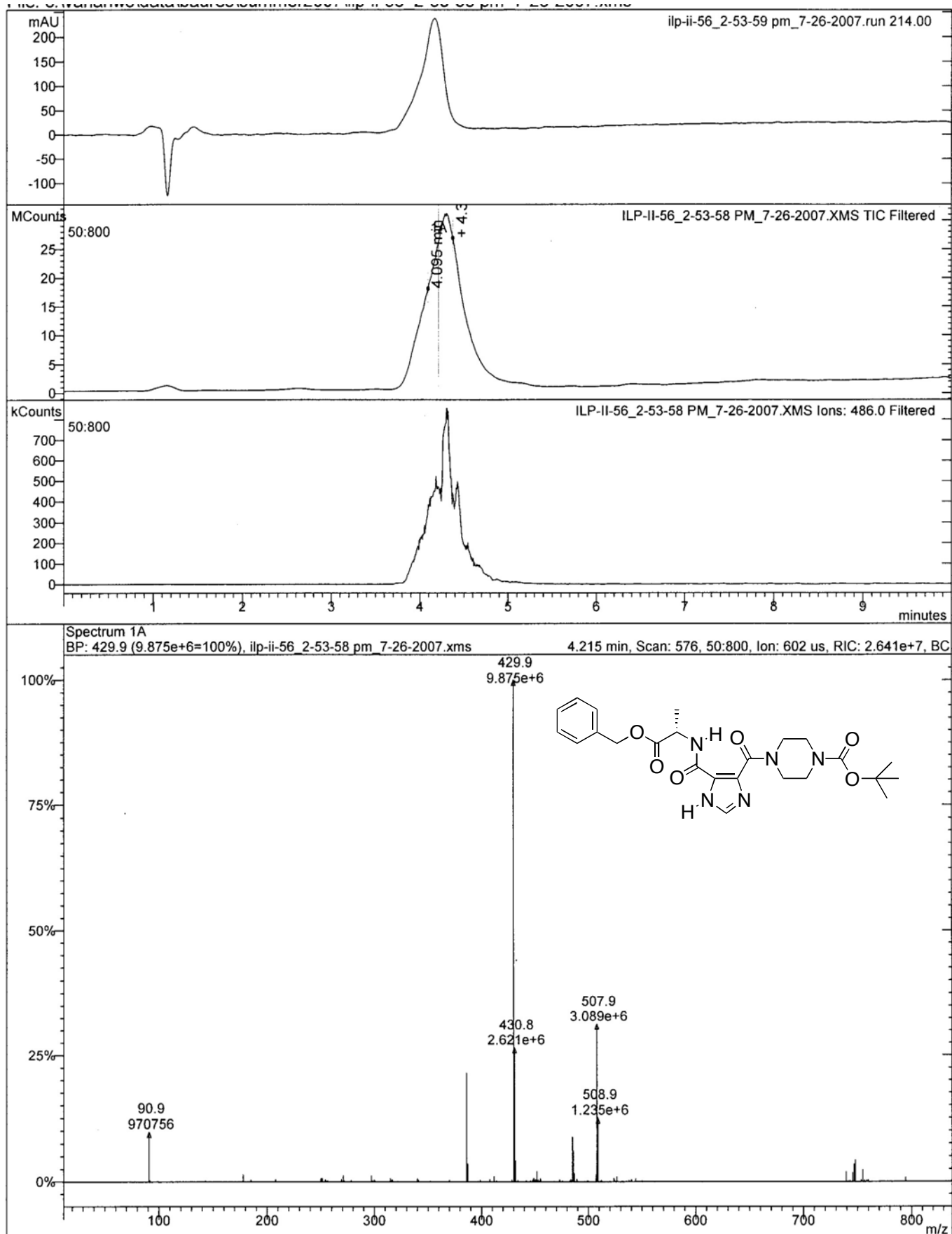


Figure S53. LC/MS data for 5{53}.

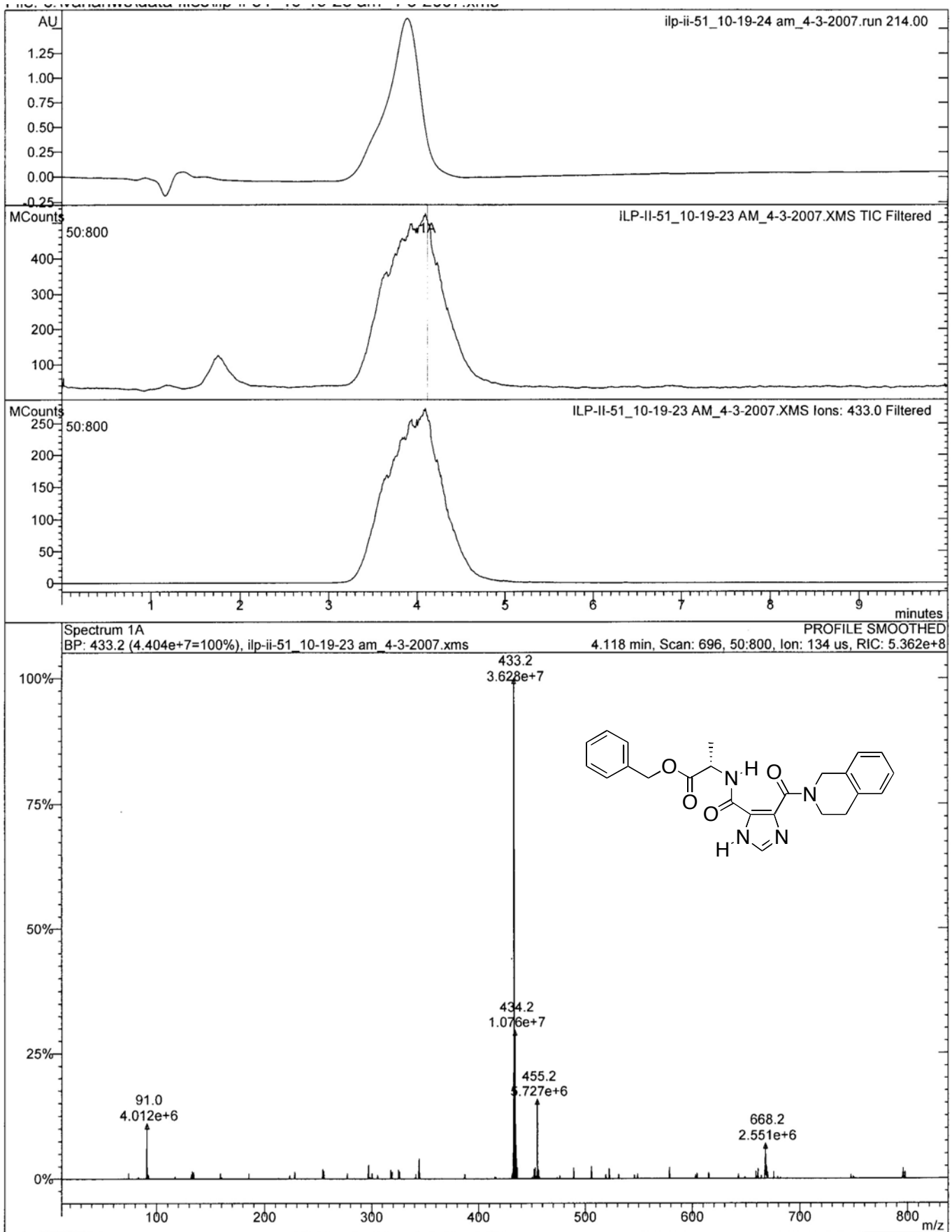


Figure S54. LC/MS data for 5{54}.

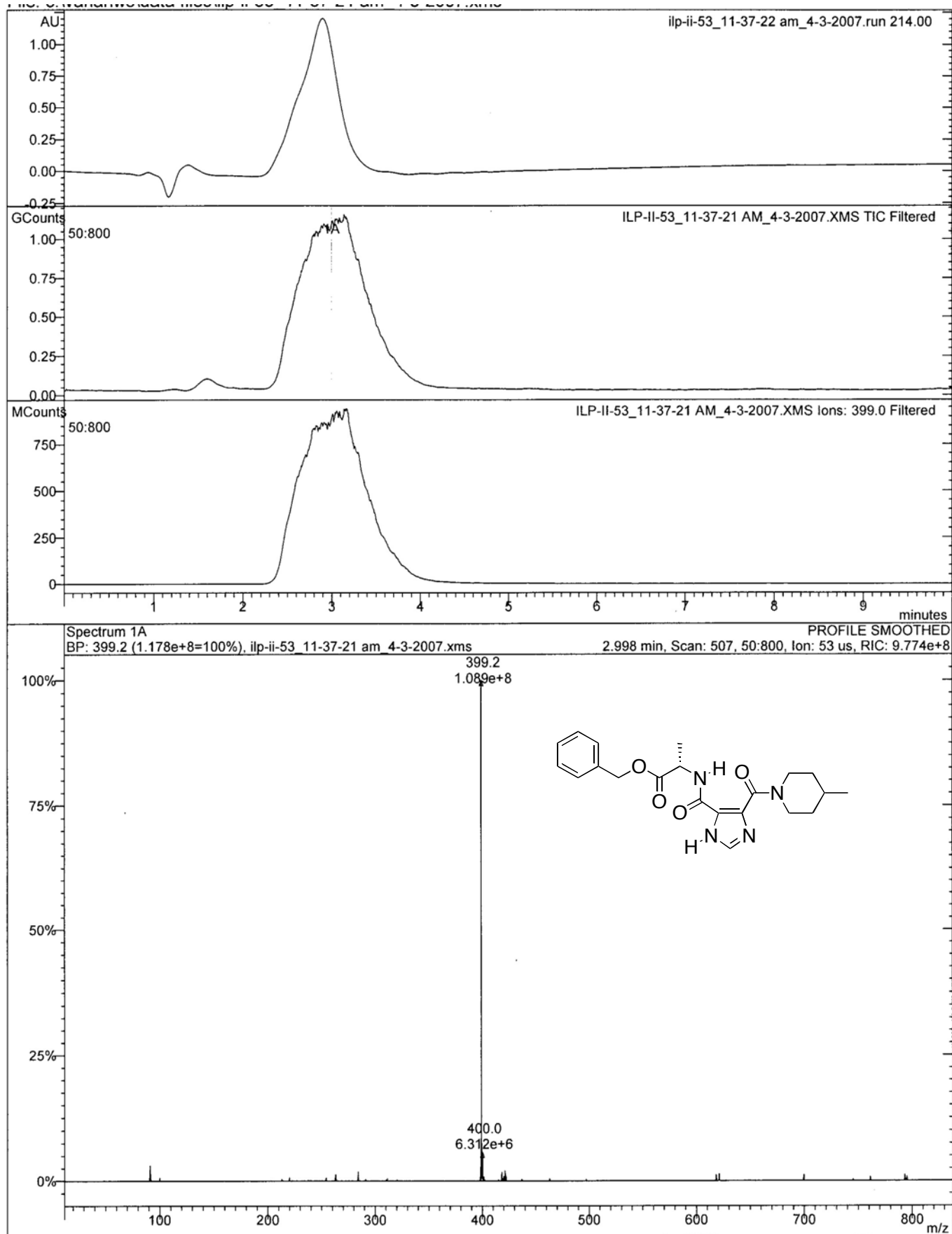
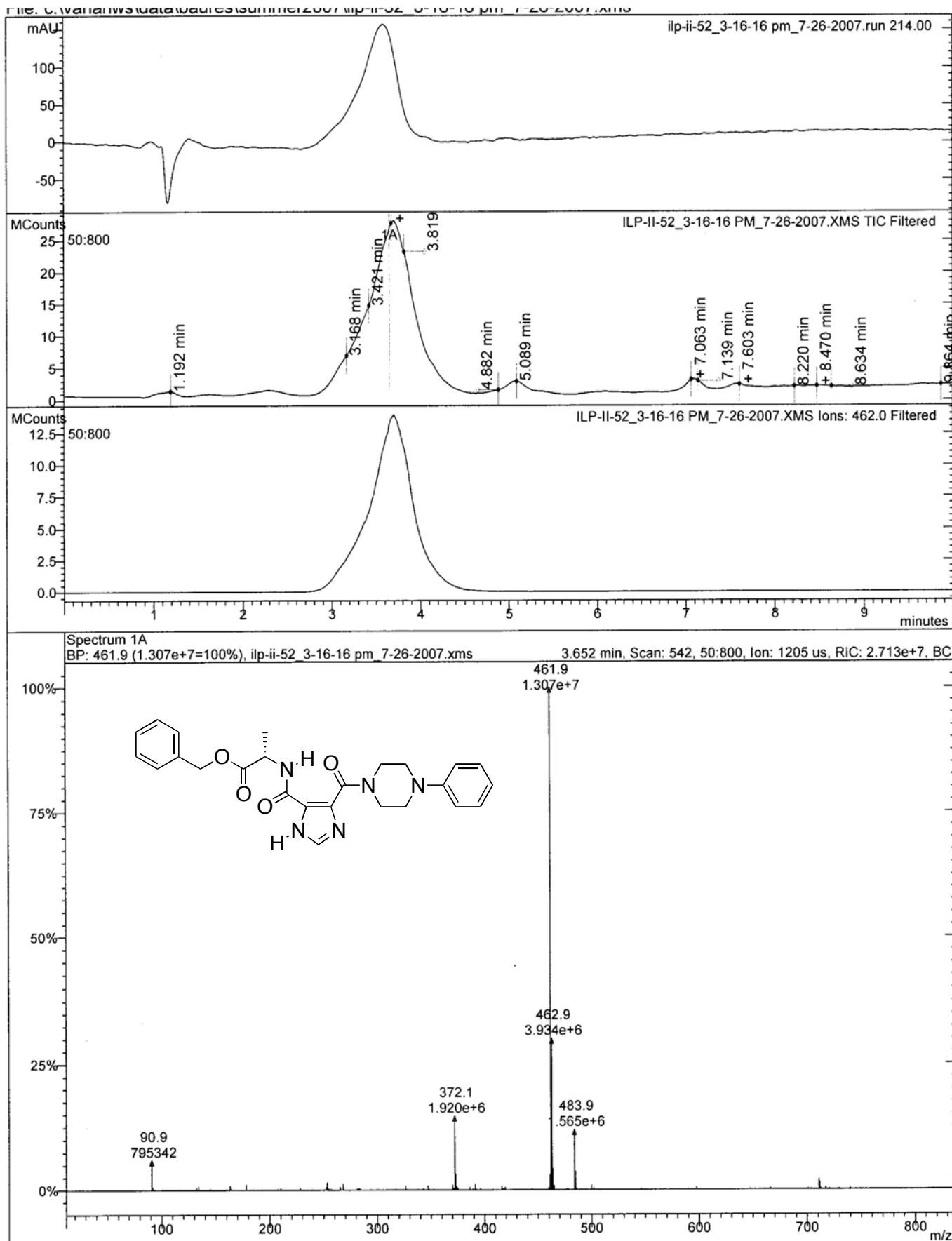


Figure S55. LC/MS data for 5{55}.



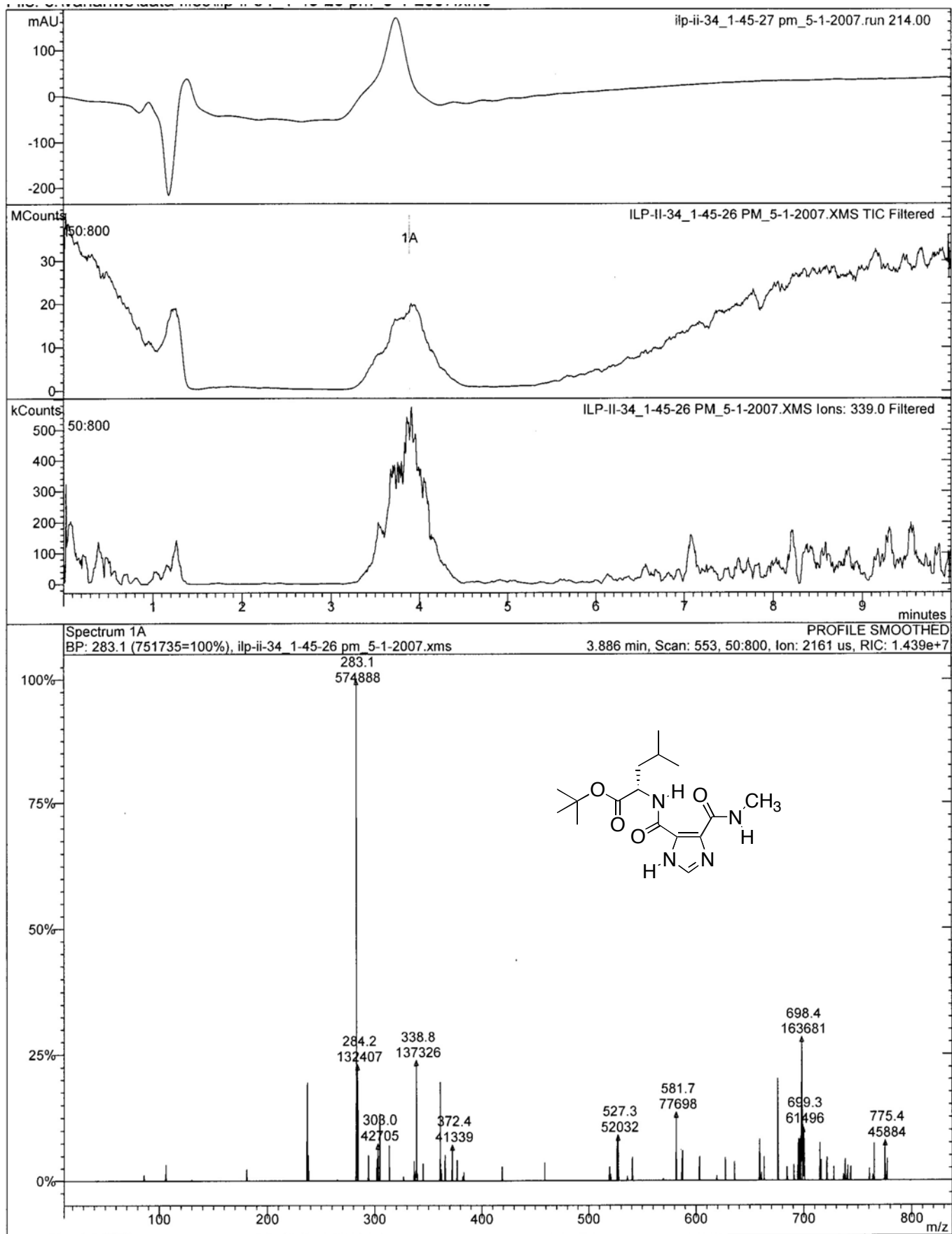


Figure S57. LC/MS data for 5{57}.

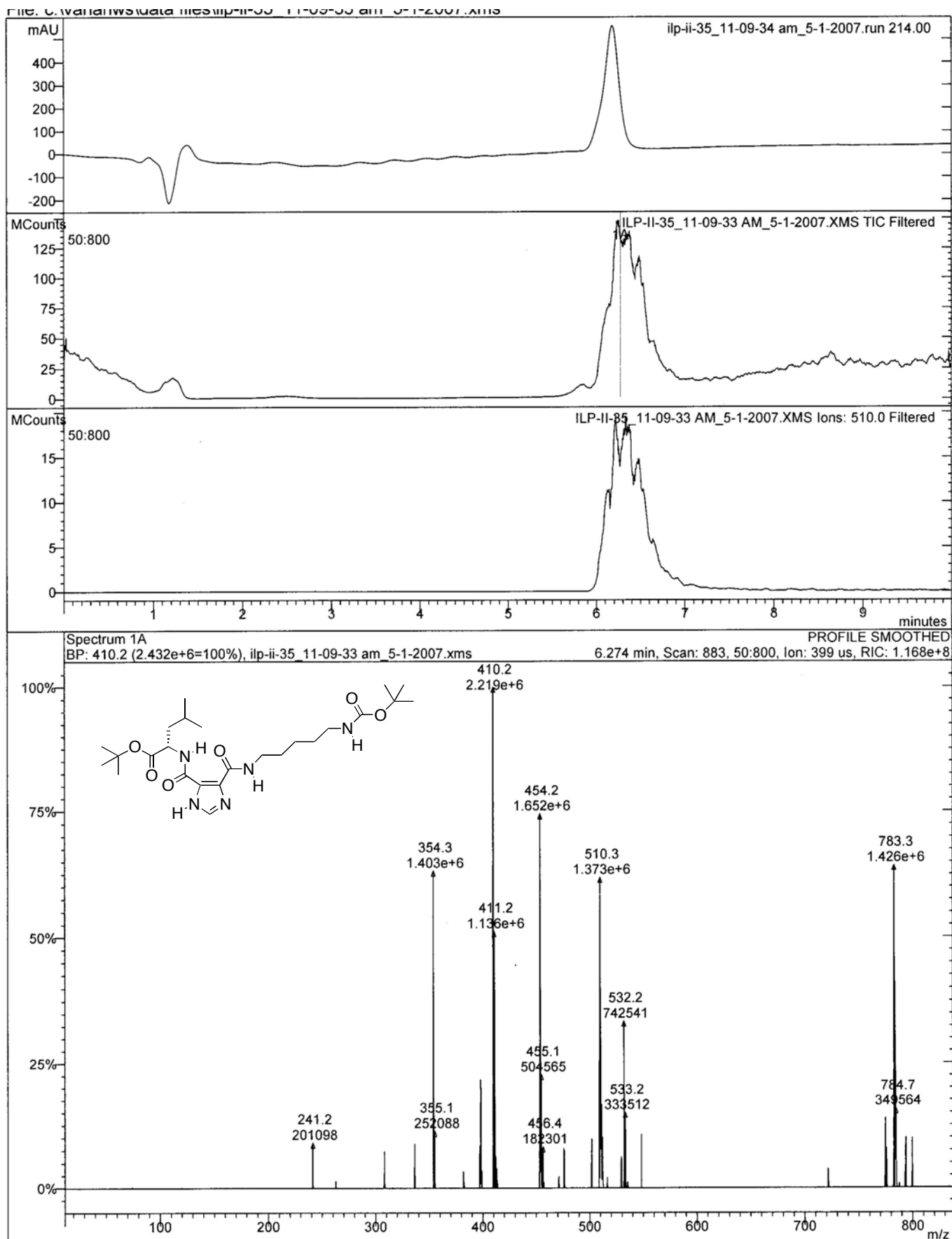


Figure S58. LC/MS data for 5{58}.

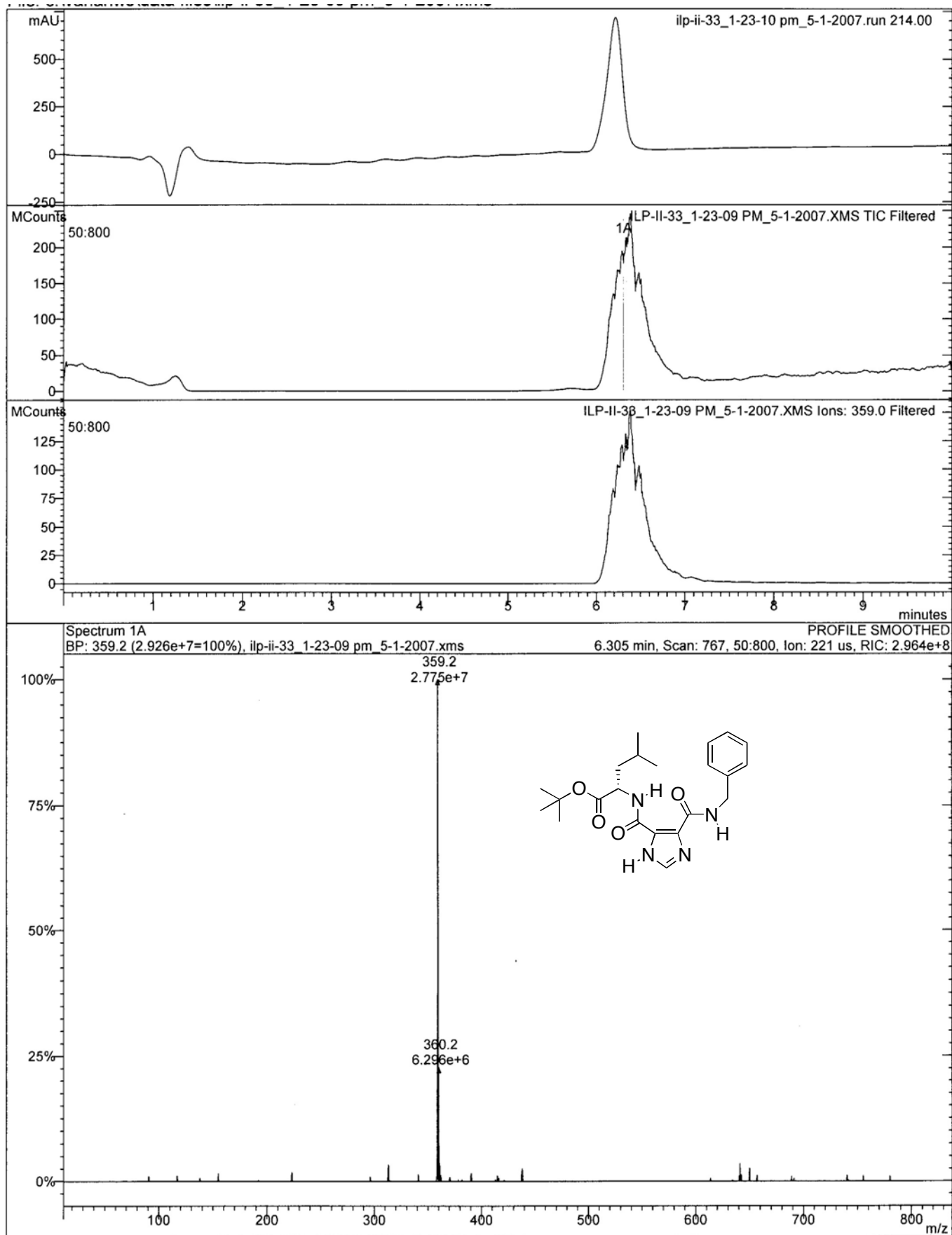


Figure S59. LC/MS data for 5{59}.

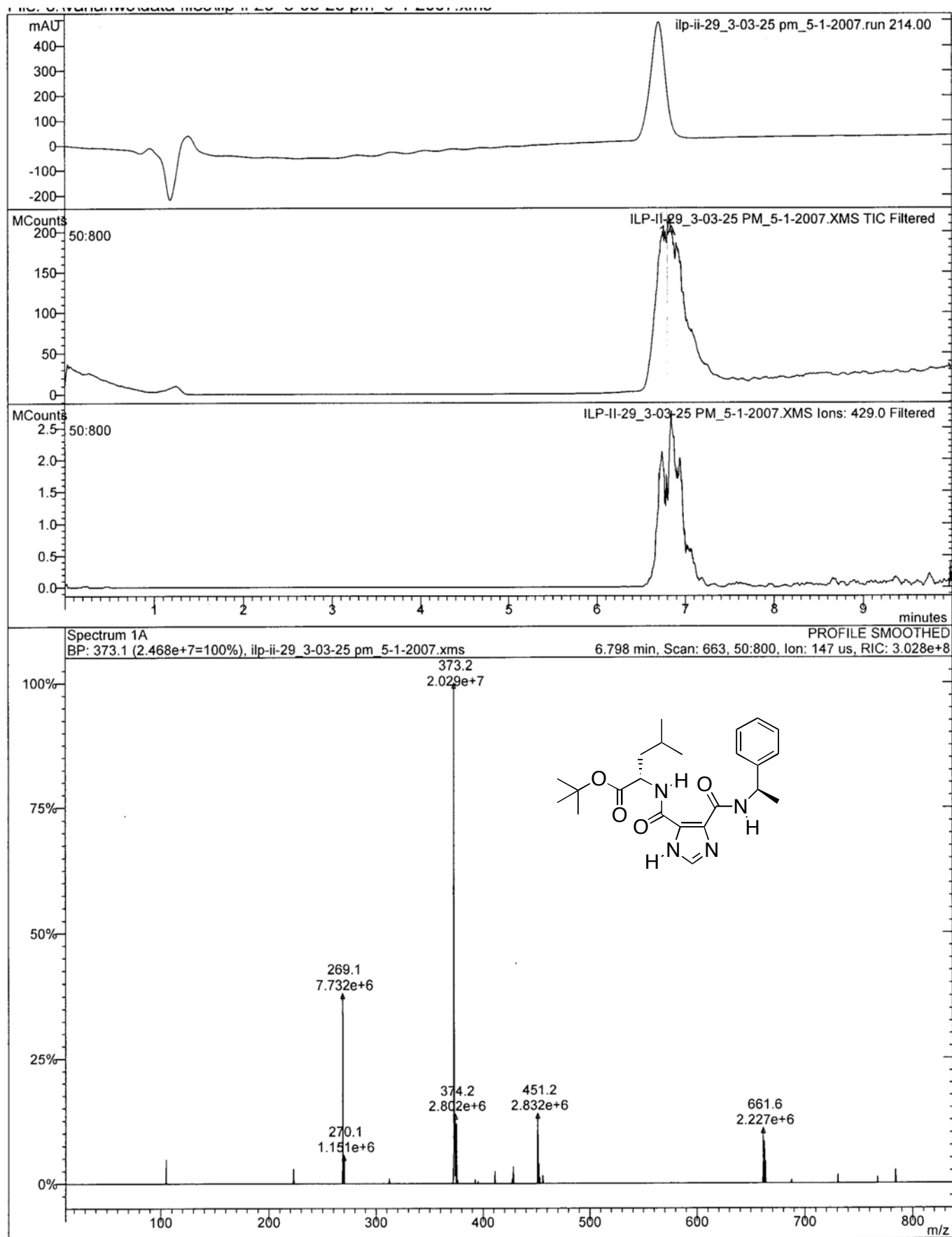


Figure S60. LC/MS data for **5{60}**.

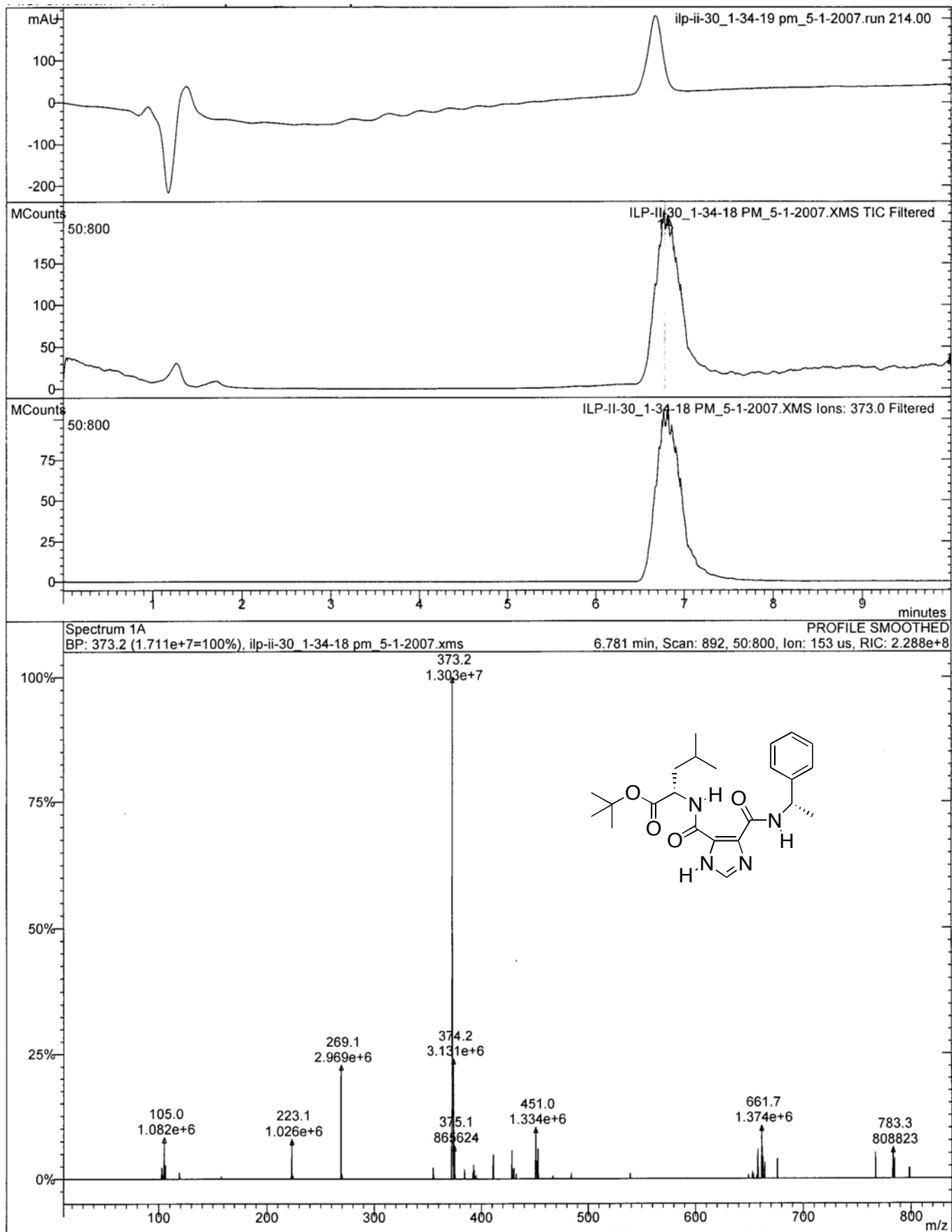


Figure S61. LC/MS data for 5{61}.

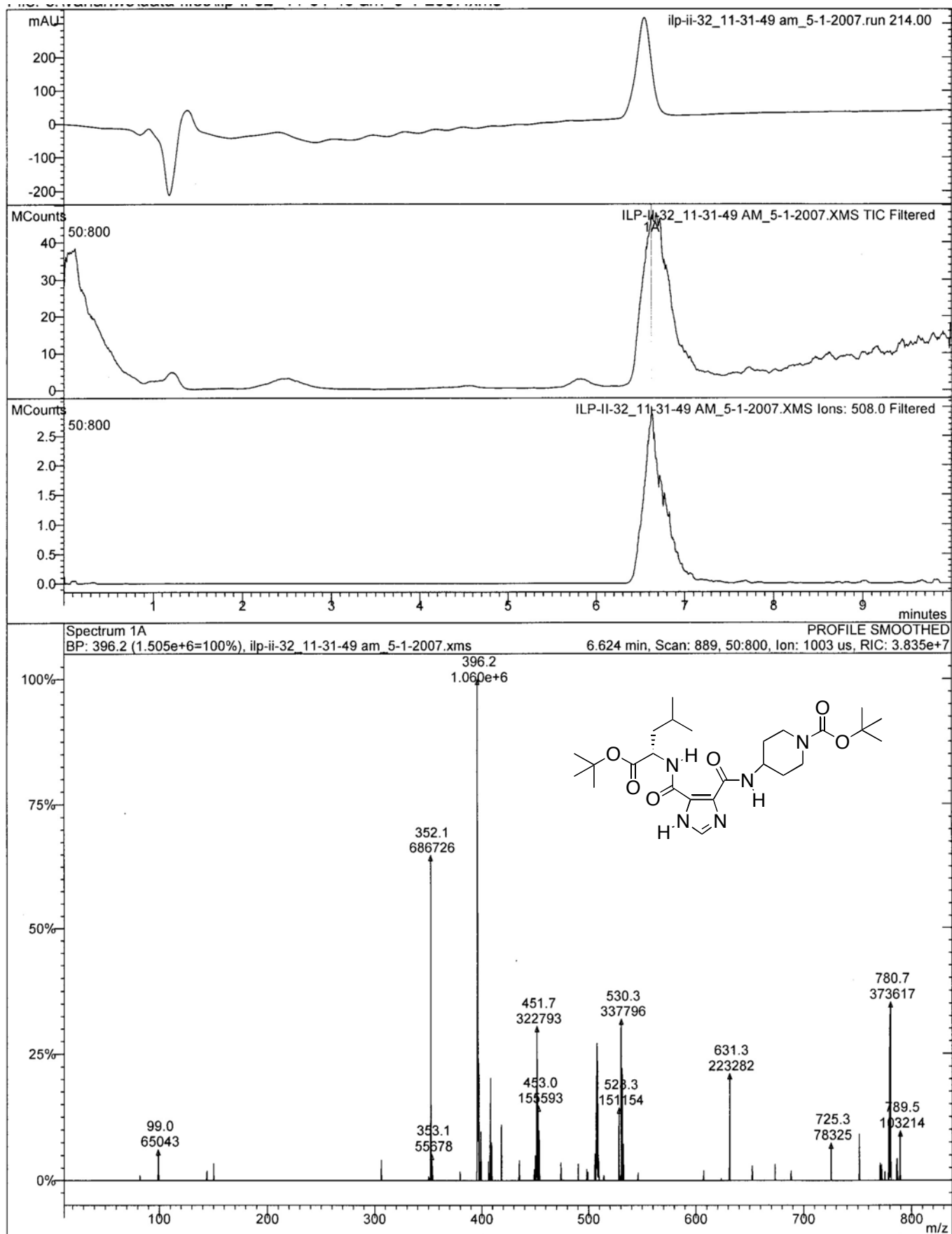


Figure S62. LC/MS data for 5{62}.

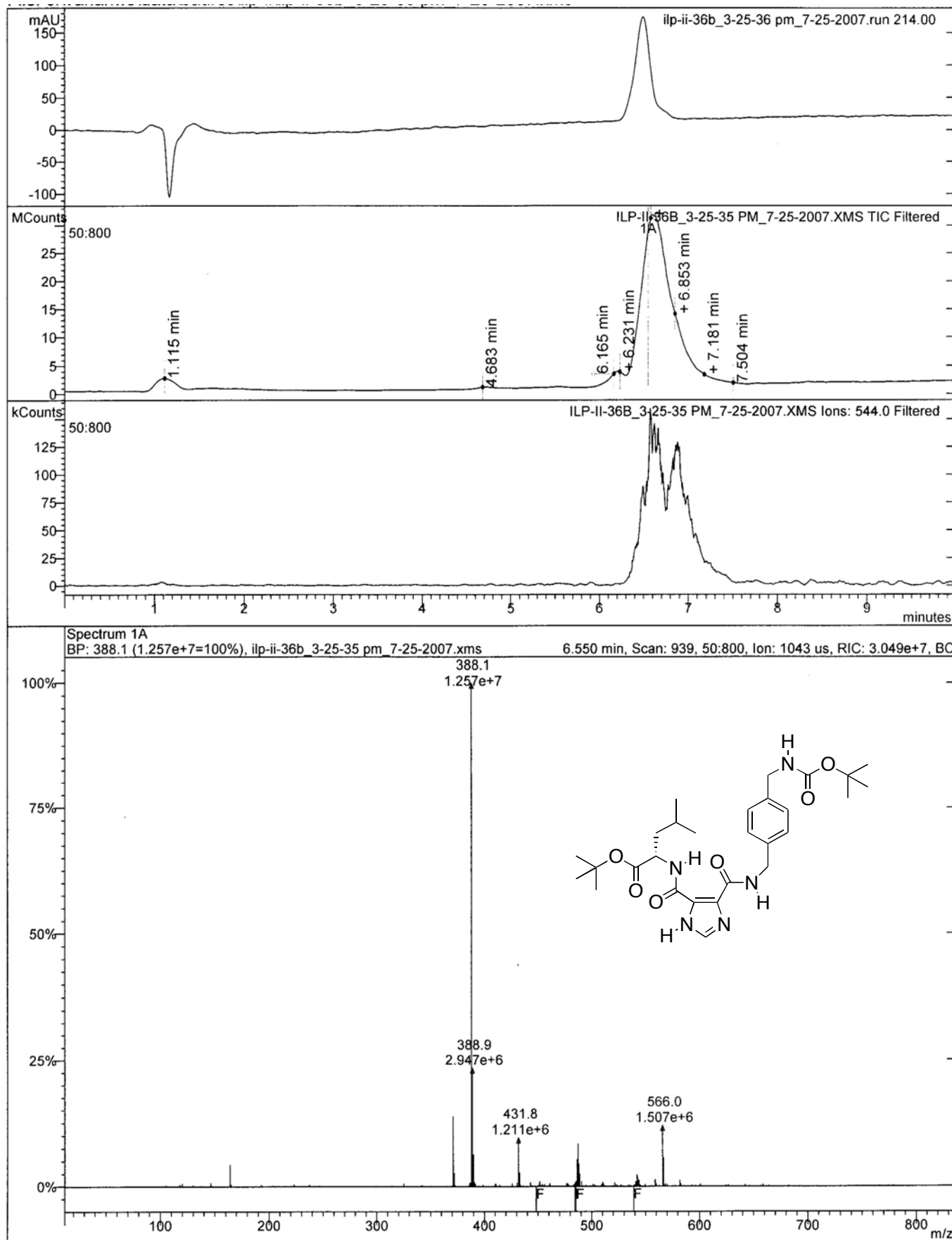


Figure S63. LC/MS data for 5{63}.

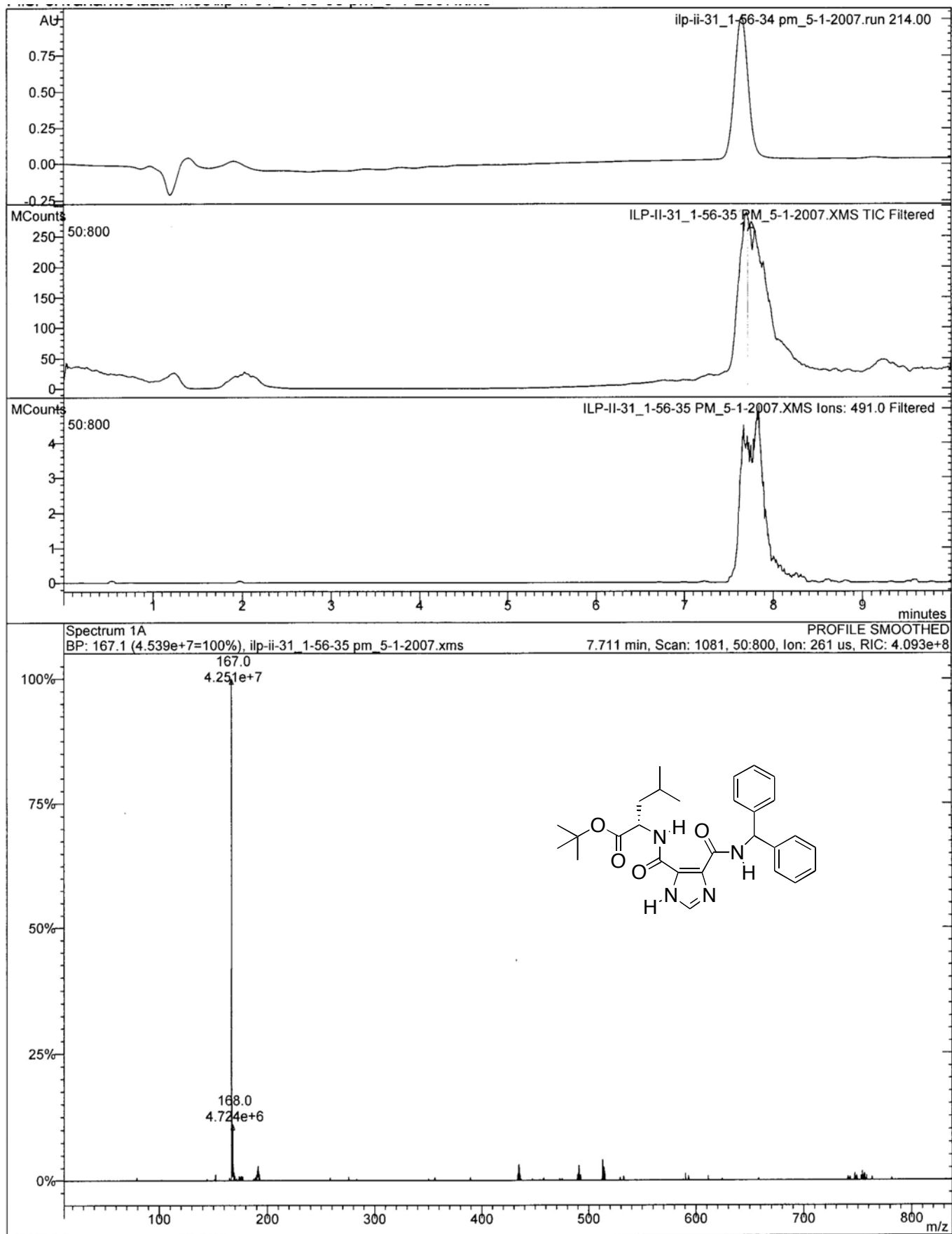


Figure S64. LC/MS data for 5{64}.

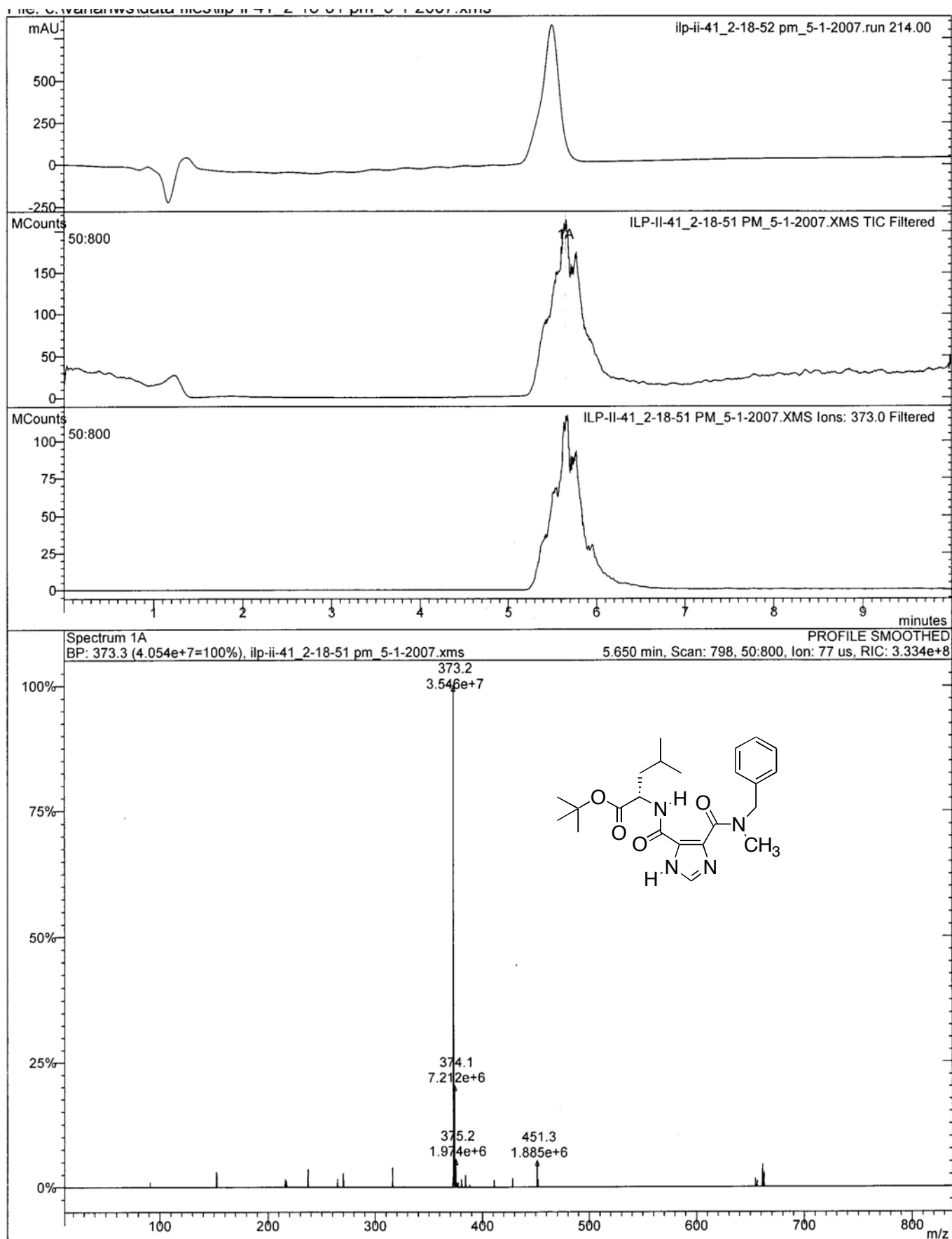


Figure S65. LC/MS data for 5{65}.

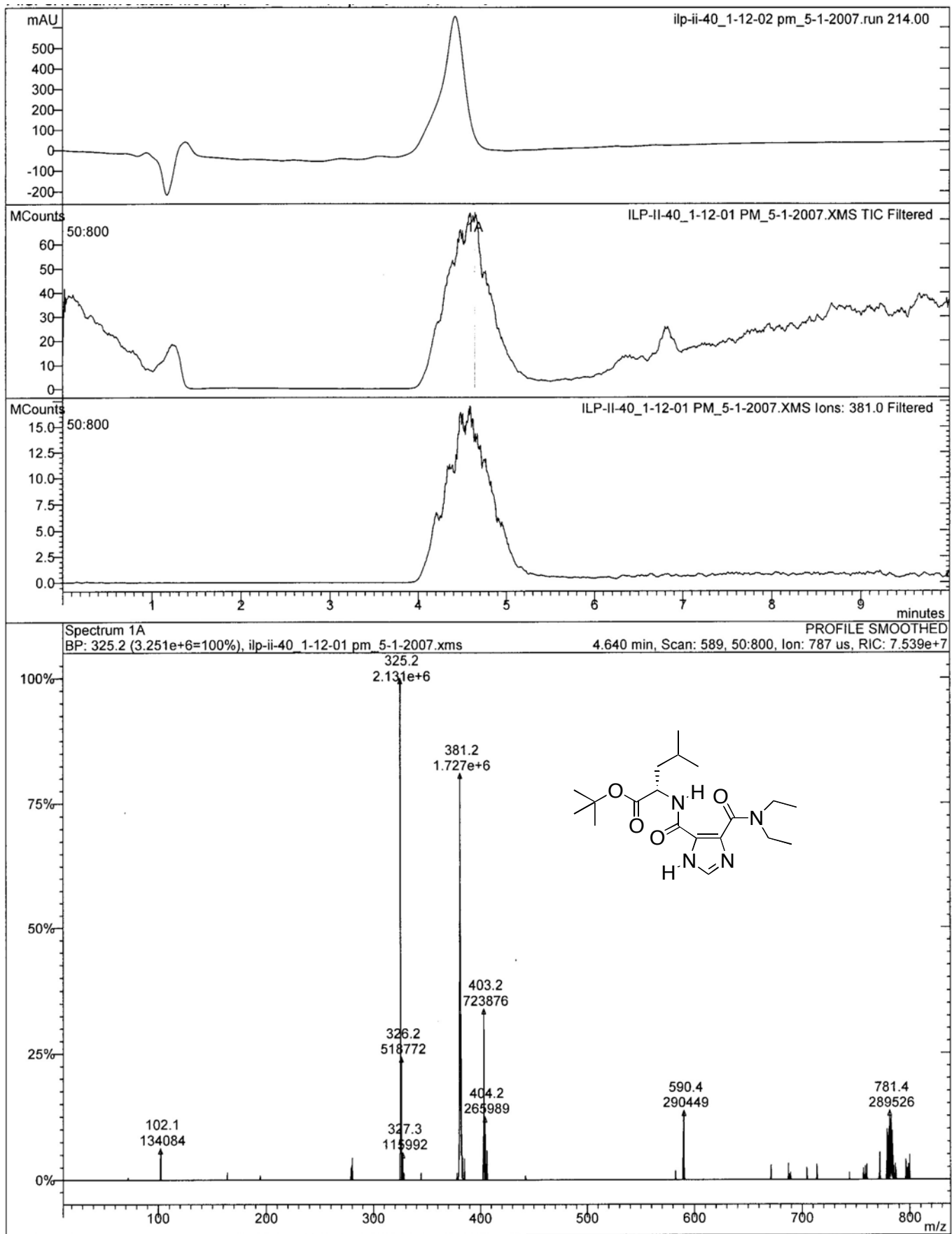


Figure S66. LC/MS data for 5{66}.

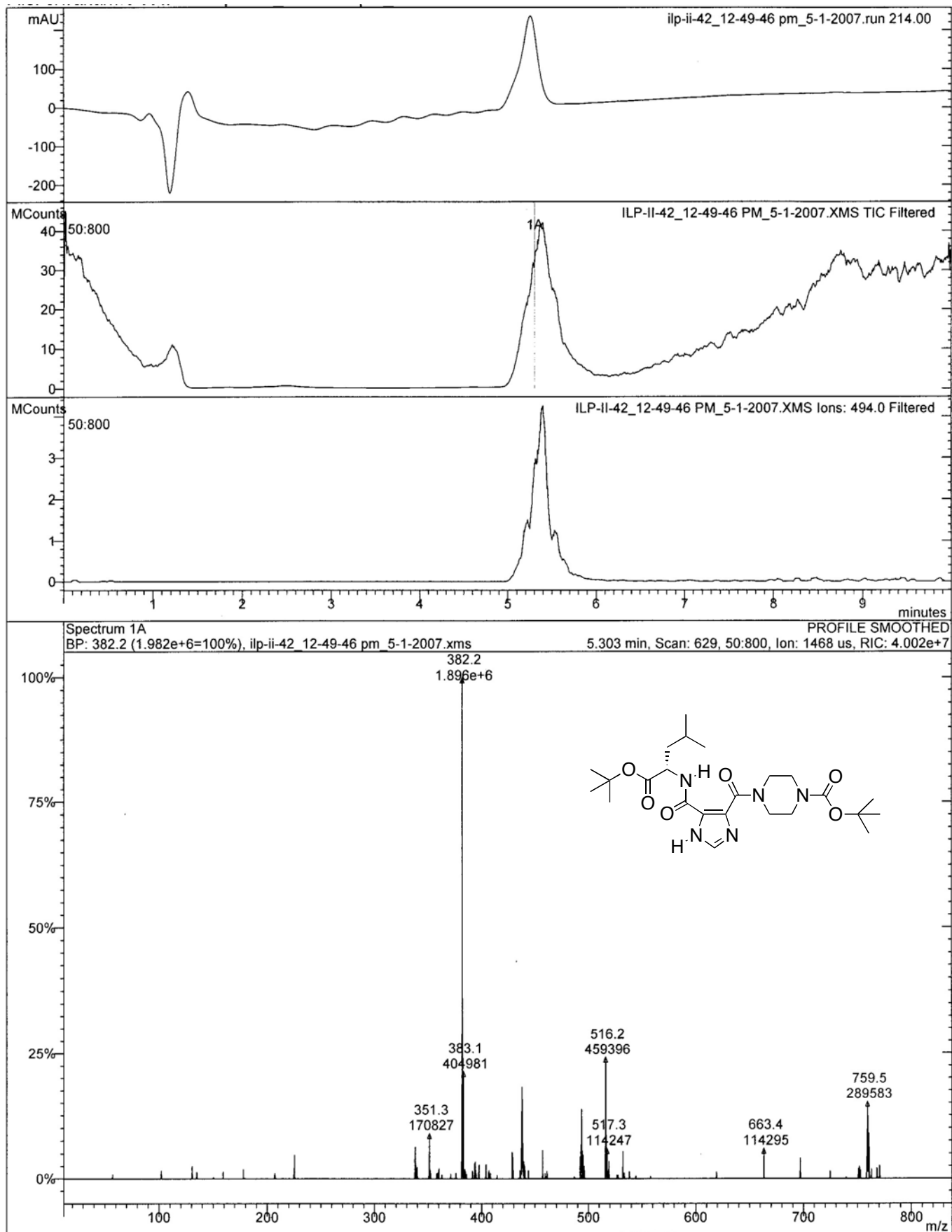


Figure S67. LC/MS data for 5{67}.

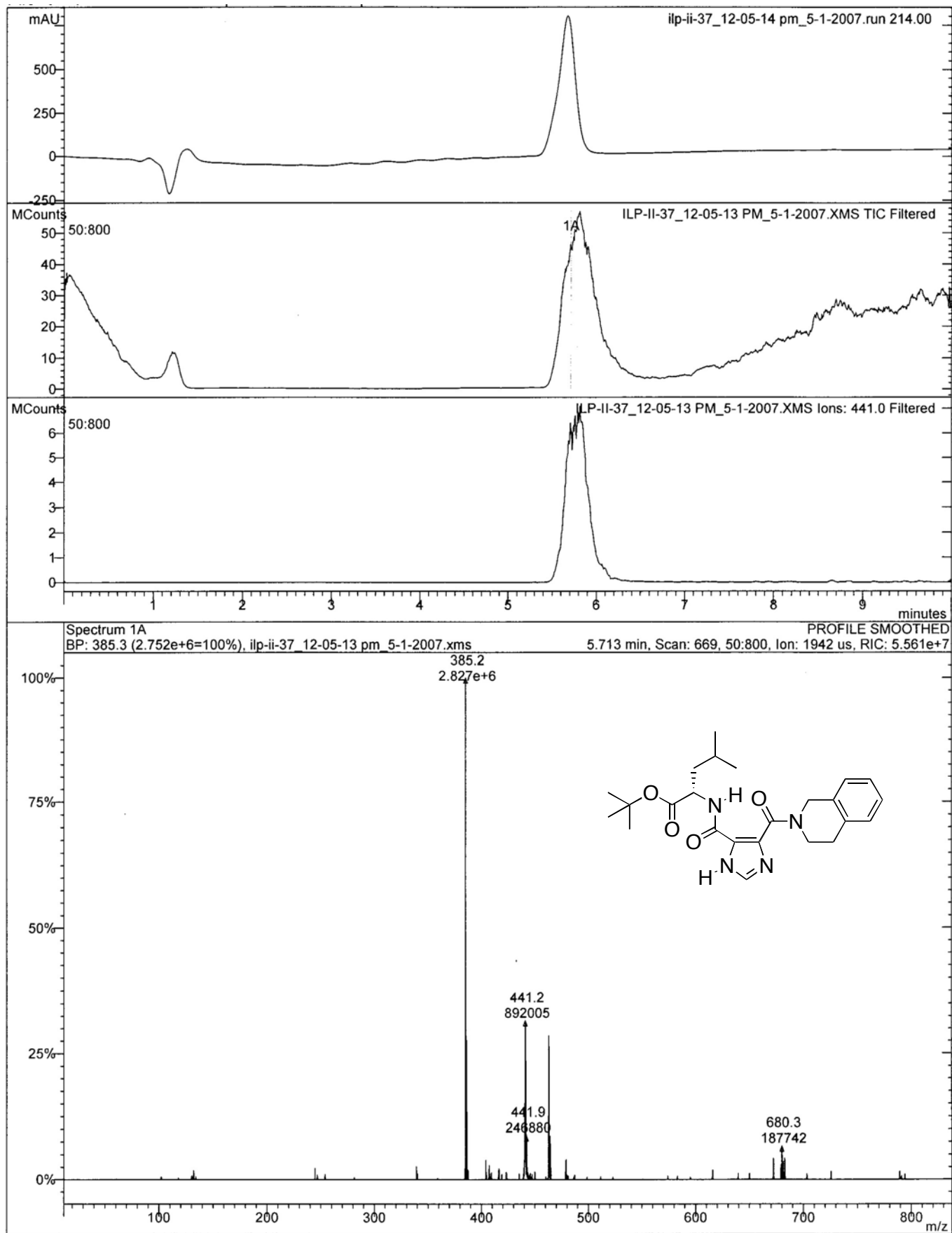


Figure S68. LC/MS data for 5{68}.

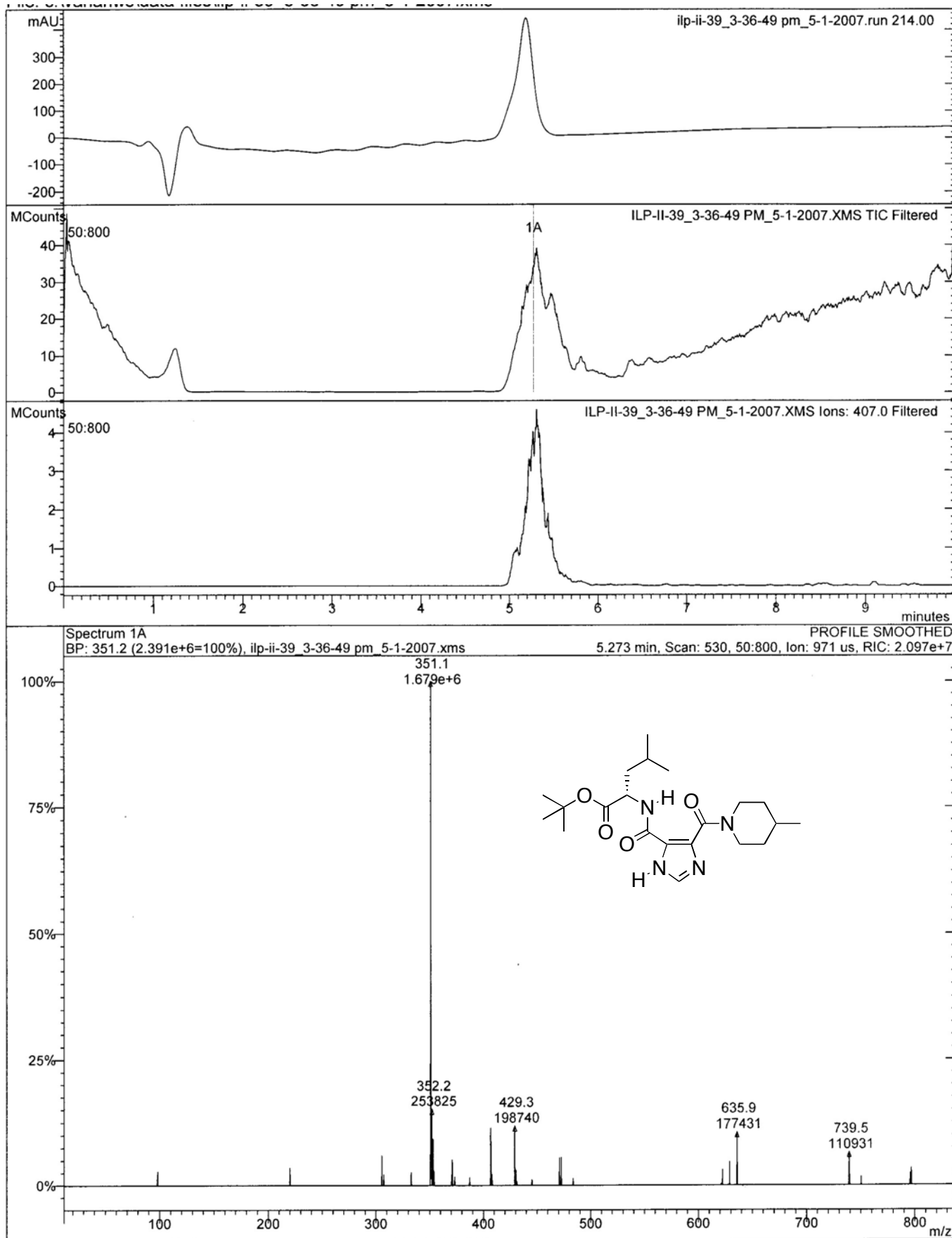


Figure S69. LC/MS data for 5{69}.

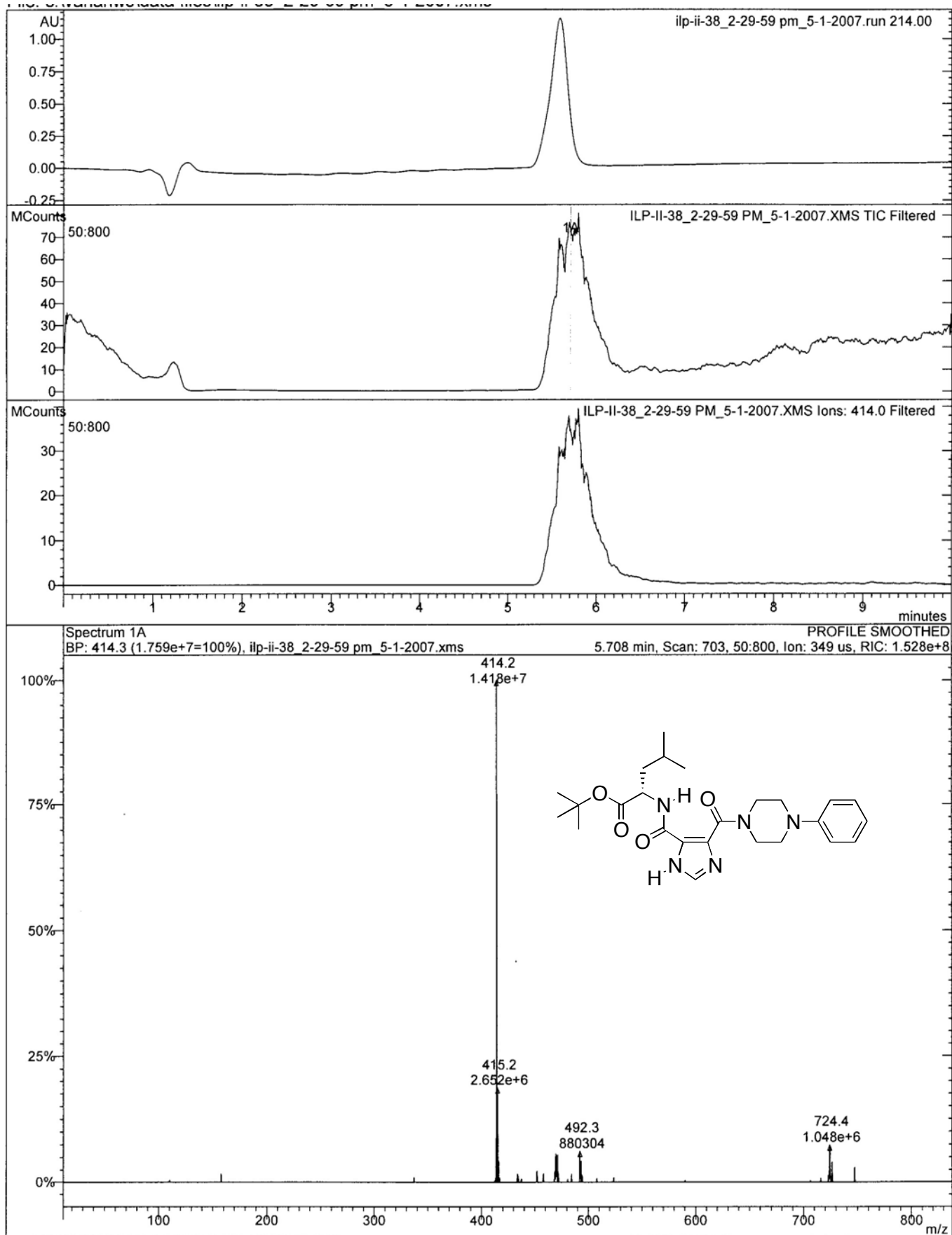


Figure S70. LC/MS data for 5{70}.

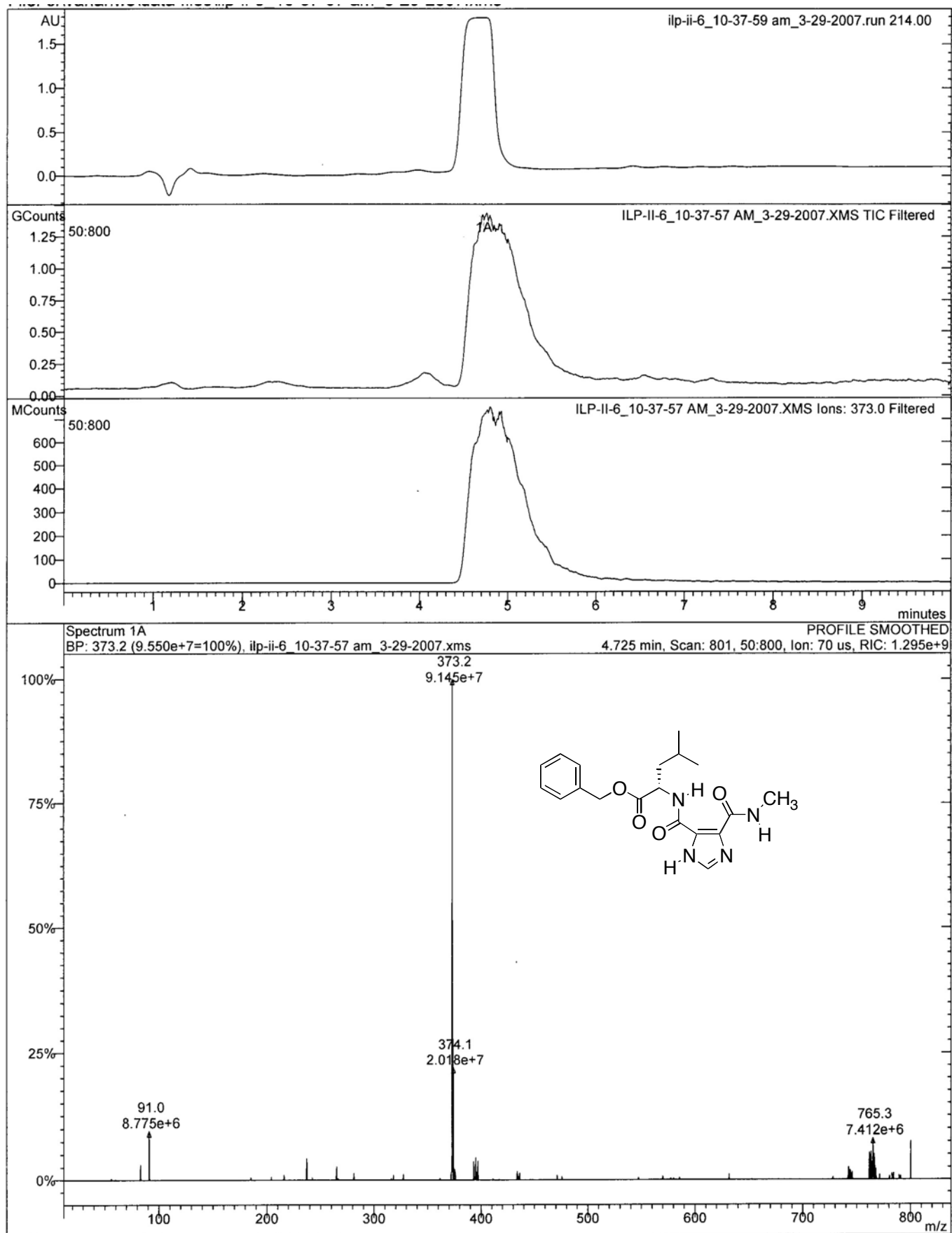


Figure S71. LC/MS data for 5{71}.

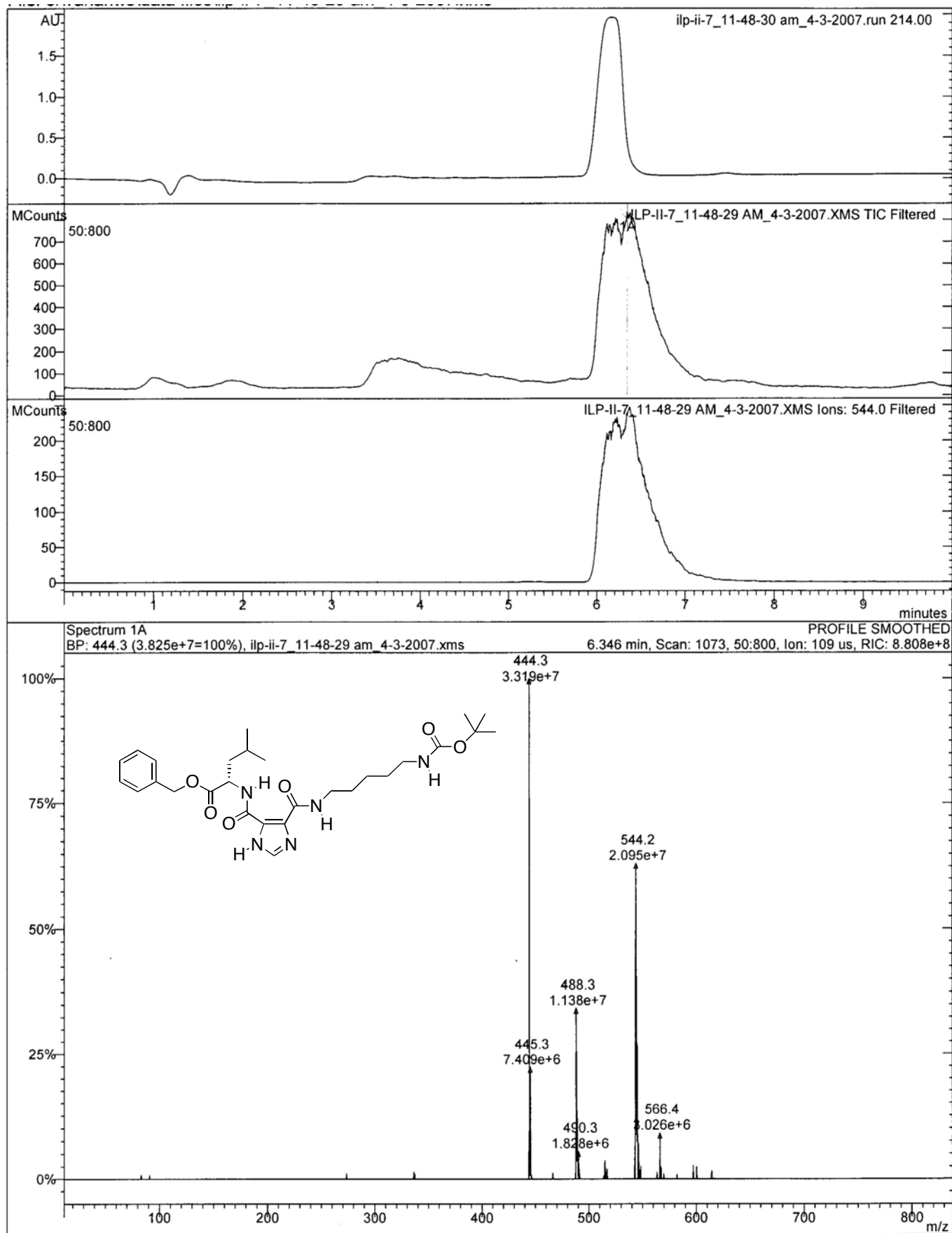


Figure S72. LC/MS data for 5{72}.

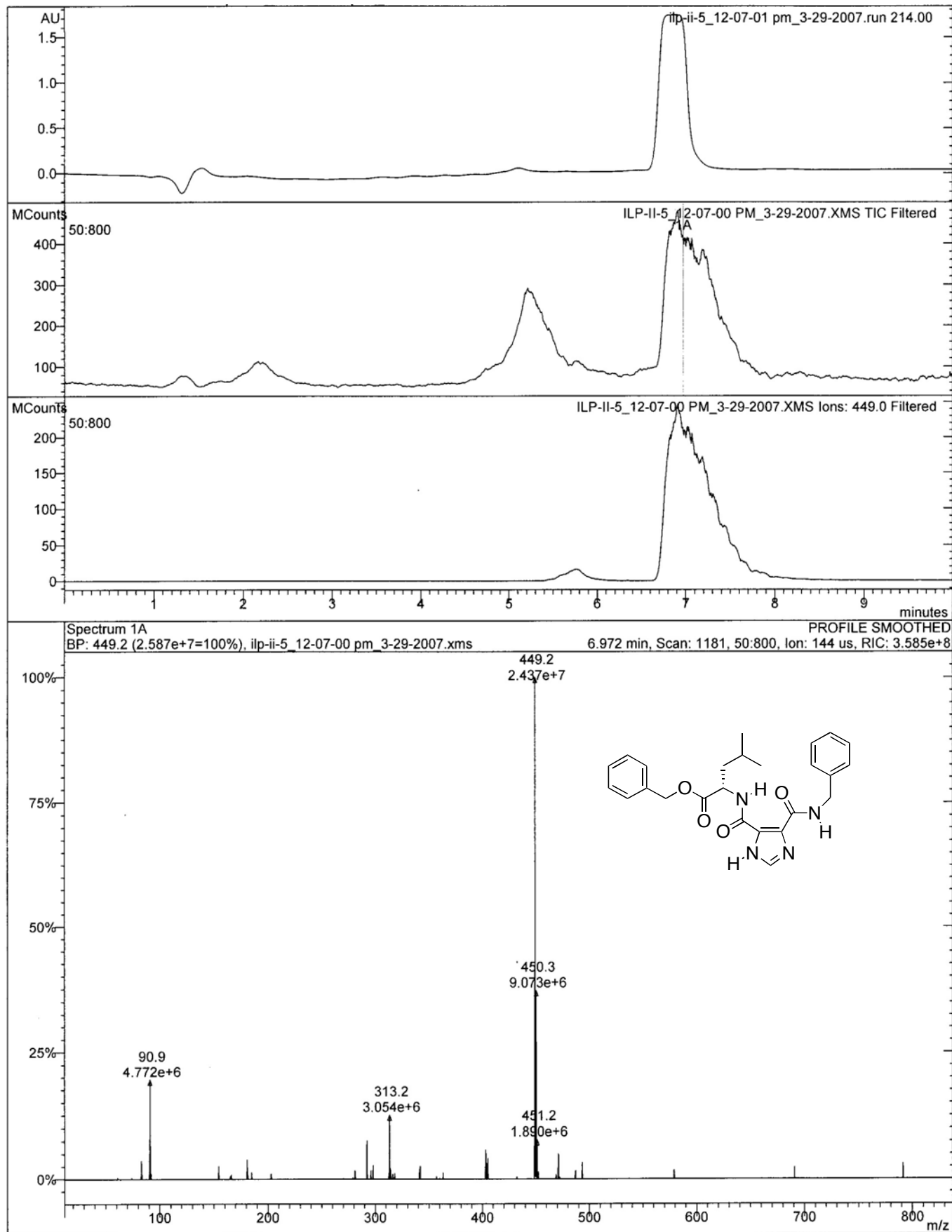


Figure S73. LC/MS data for 5{73}.

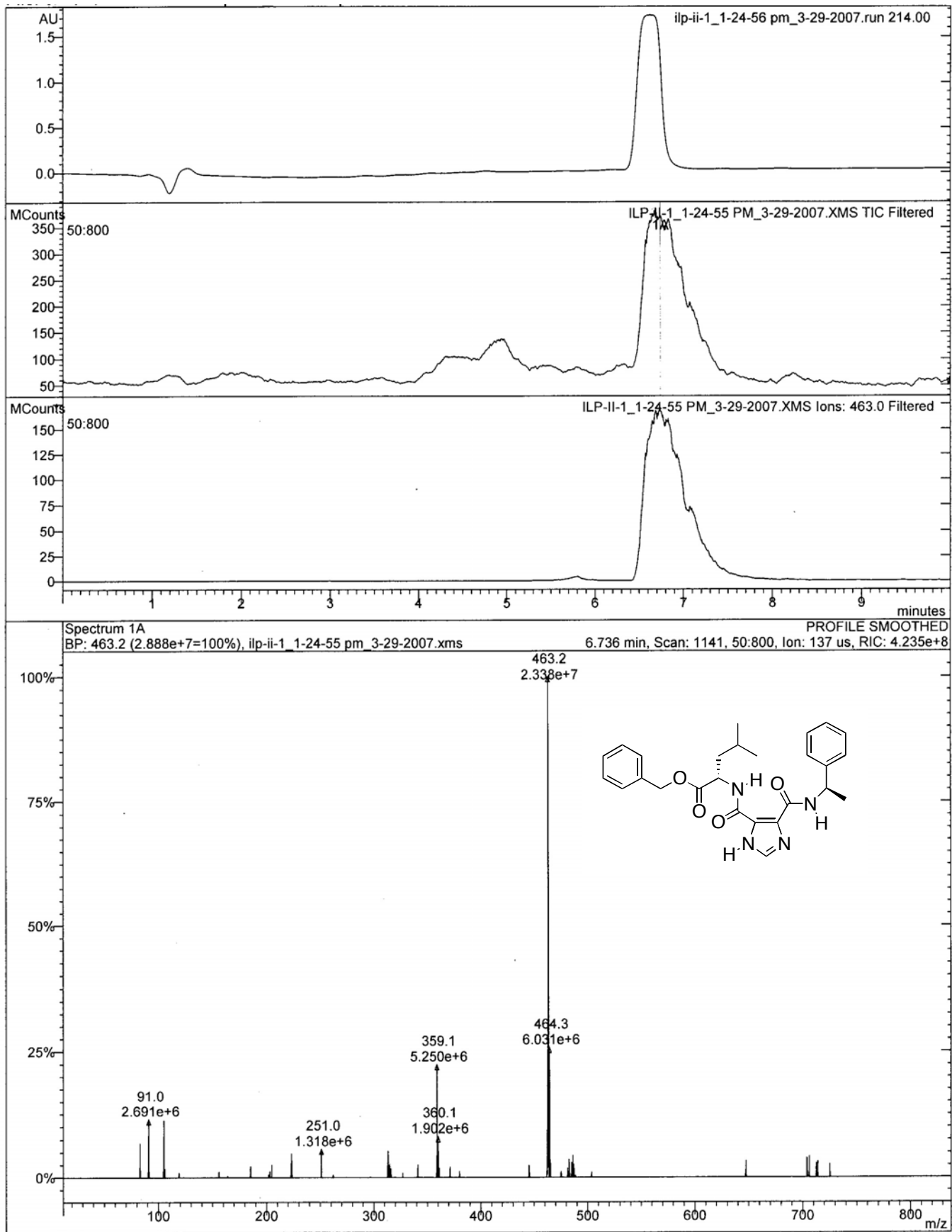


Figure S74. LC/MS data for 5{74}.

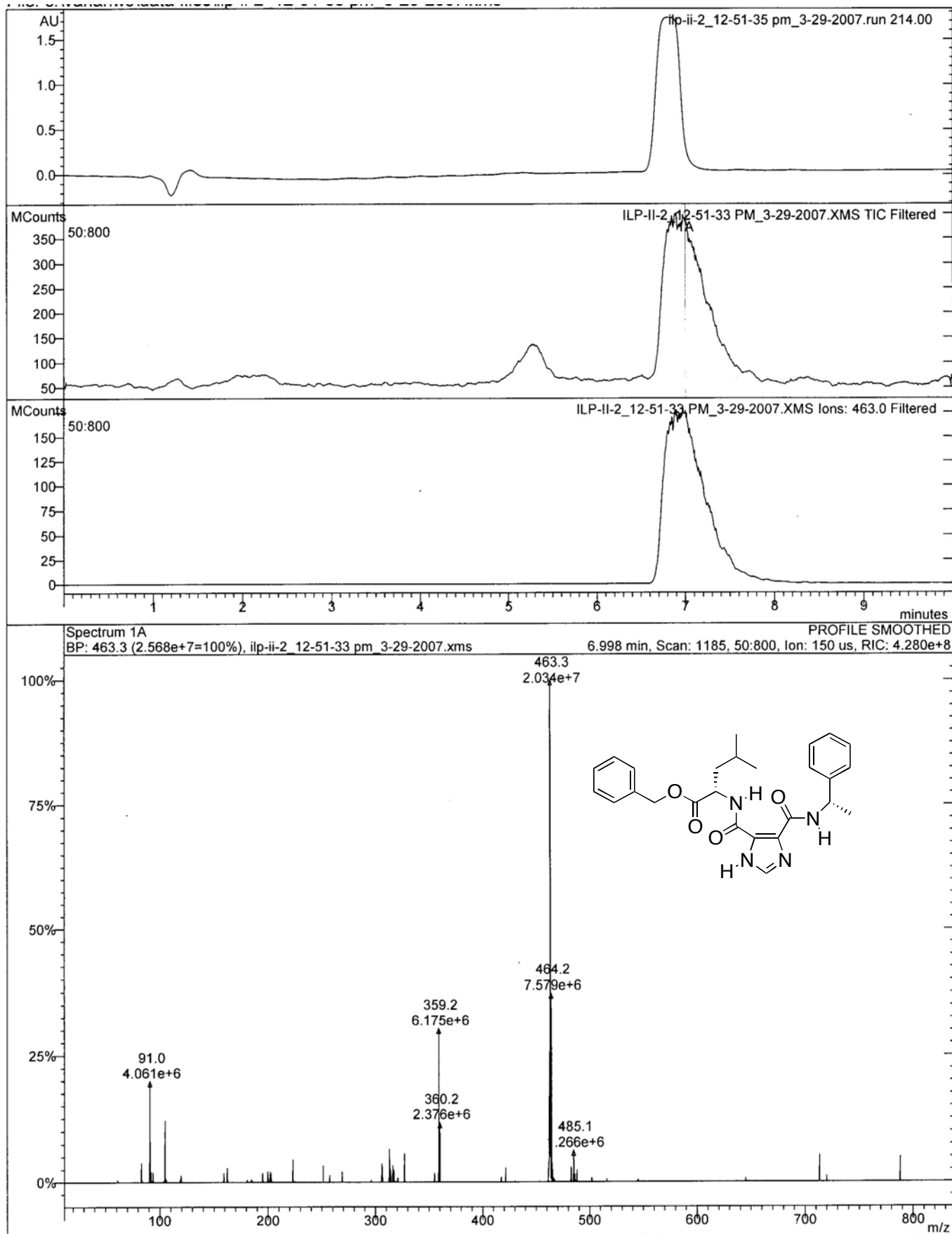


Figure S75. LC/MS data for 5{75}.

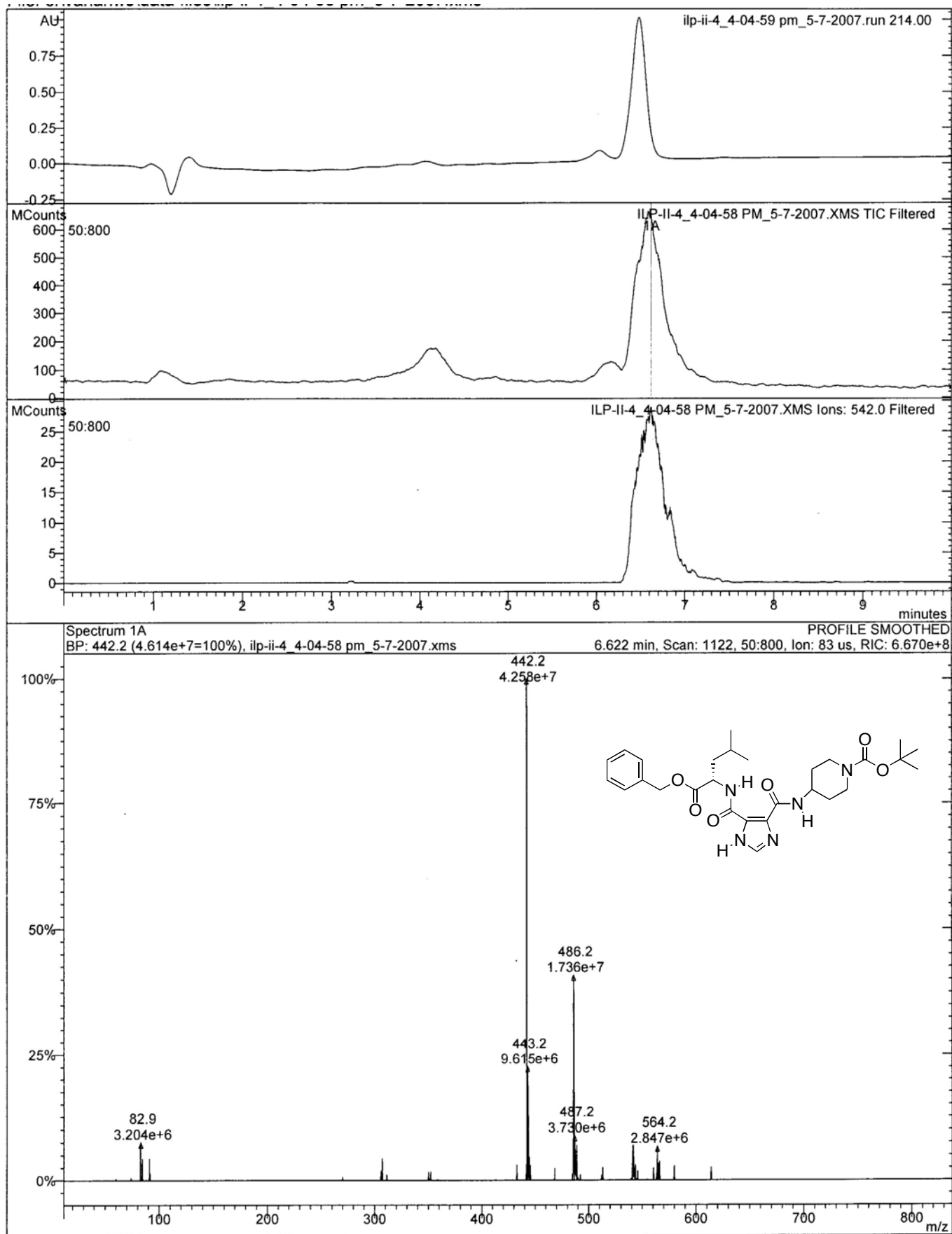


Figure S76. LC/MS data for 5{76}.

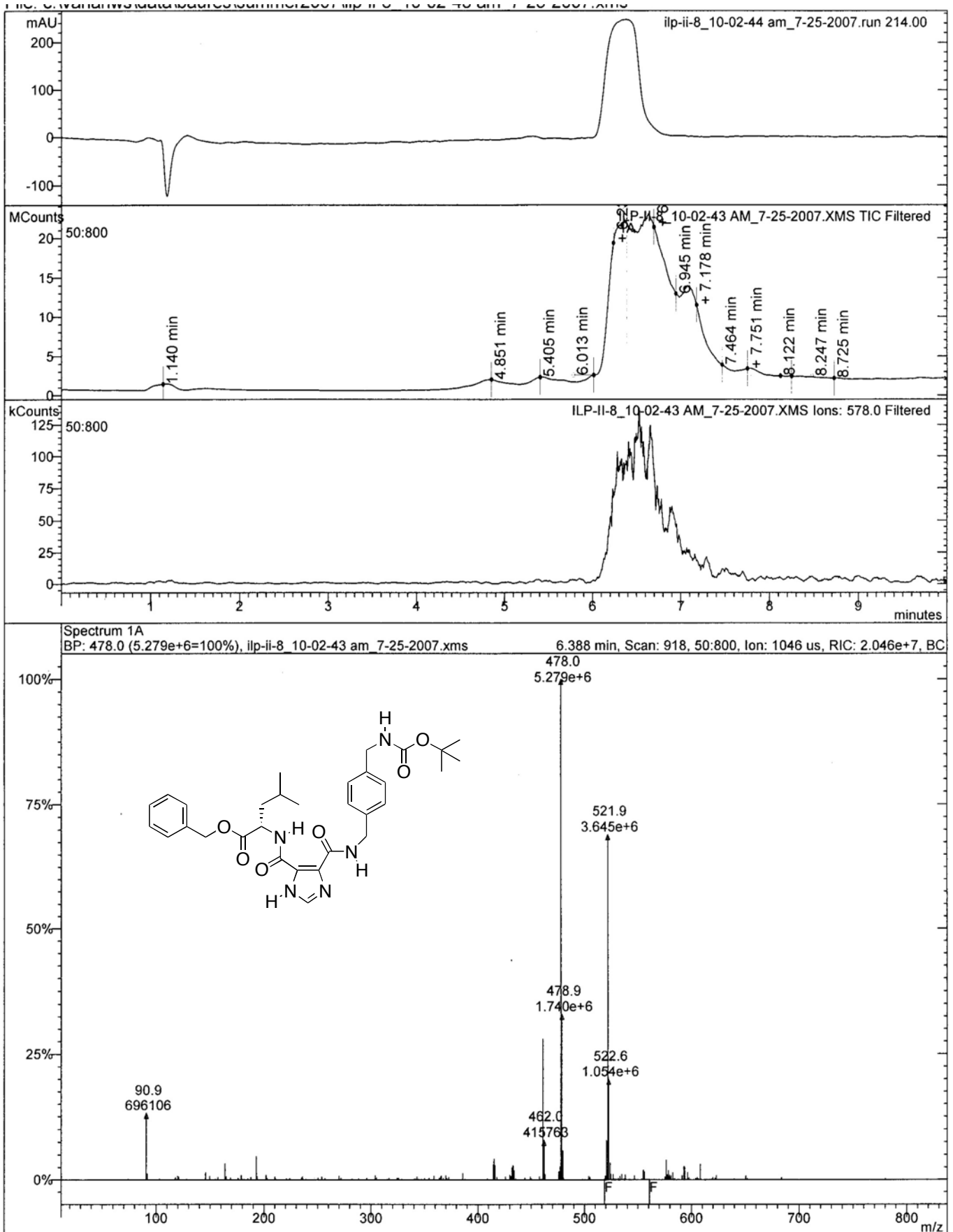


Figure S77. LC/MS data for 5{77}.

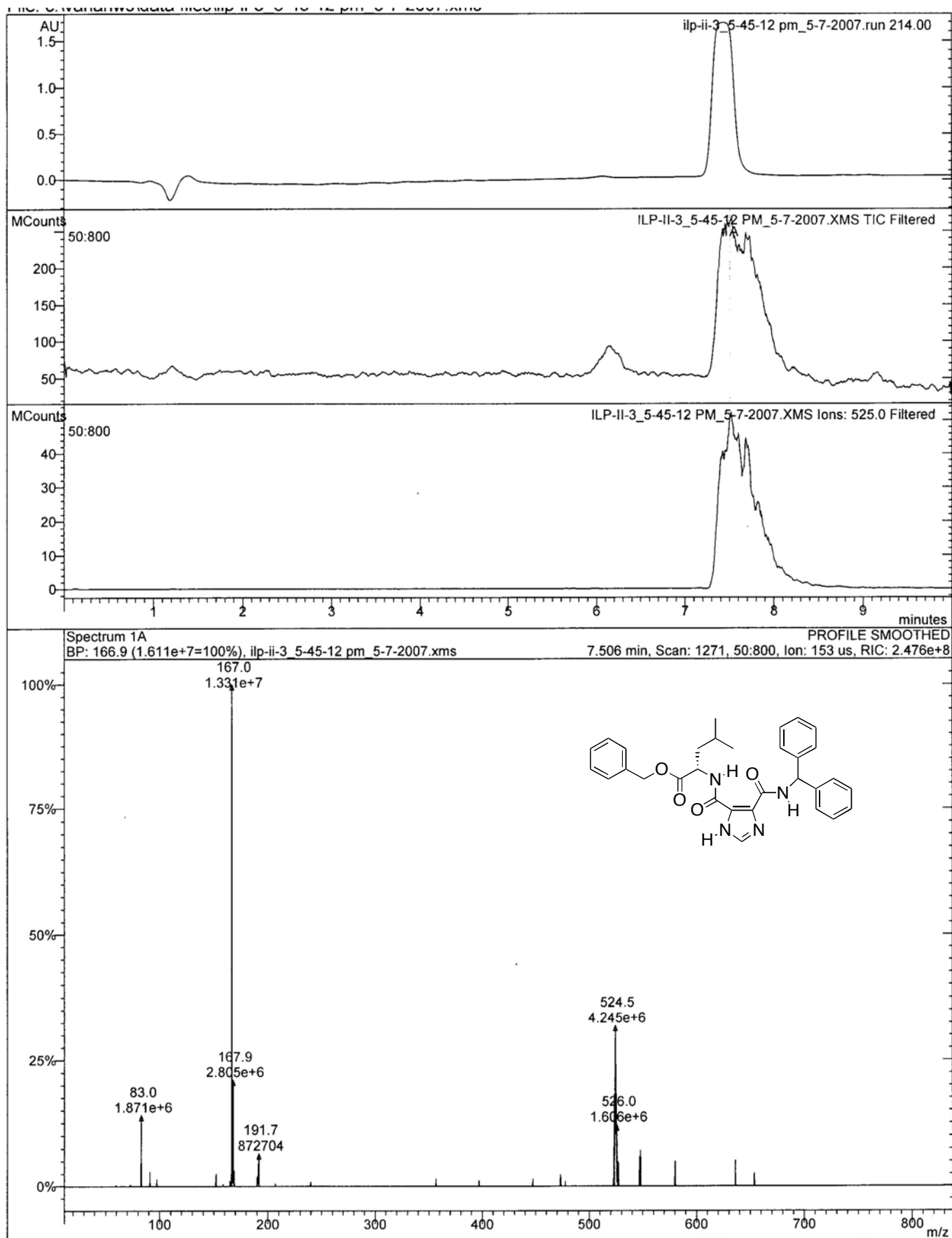


Figure S78. LC/MS data for 5{78}.

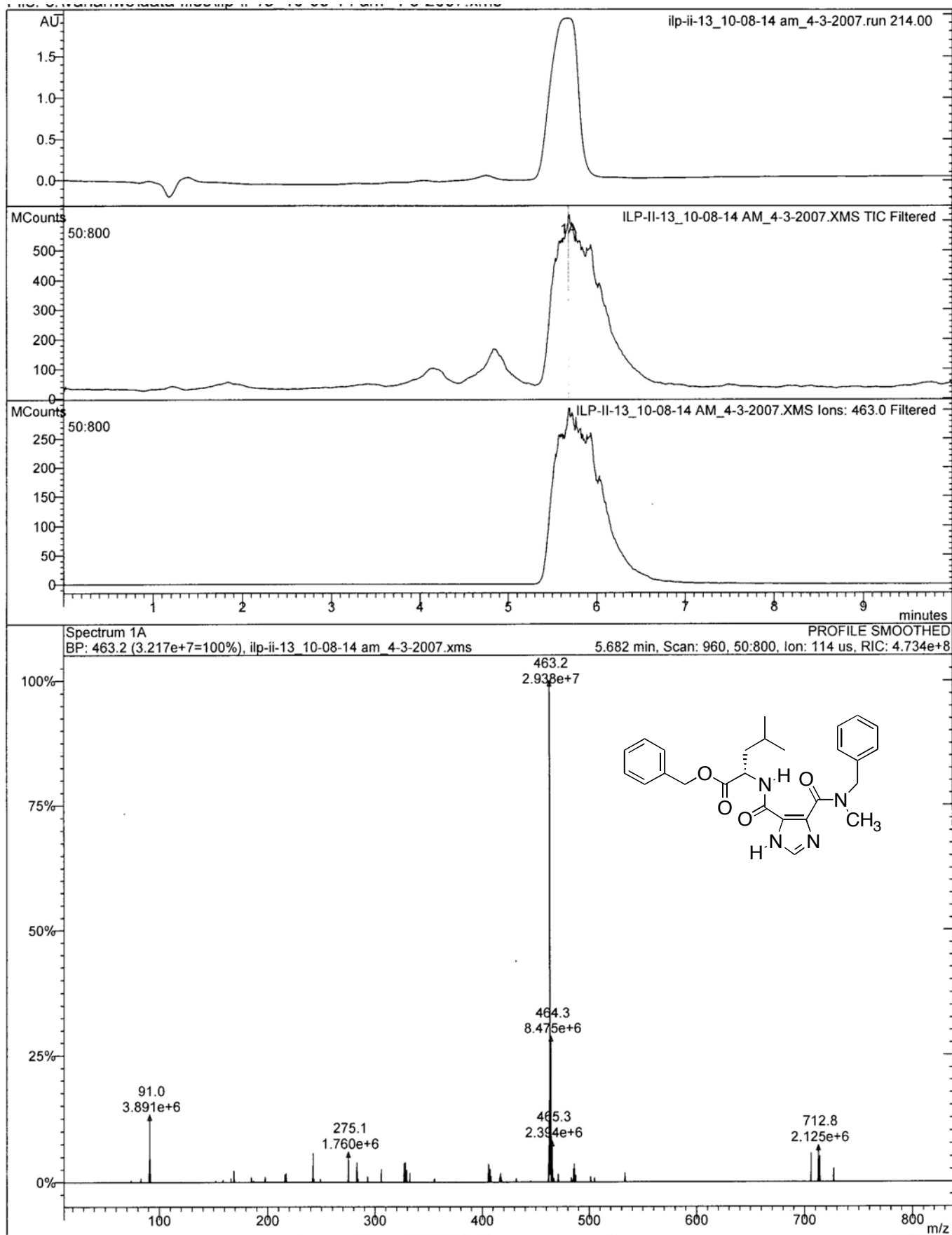


Figure S79. LC/MS data for 5{79}.

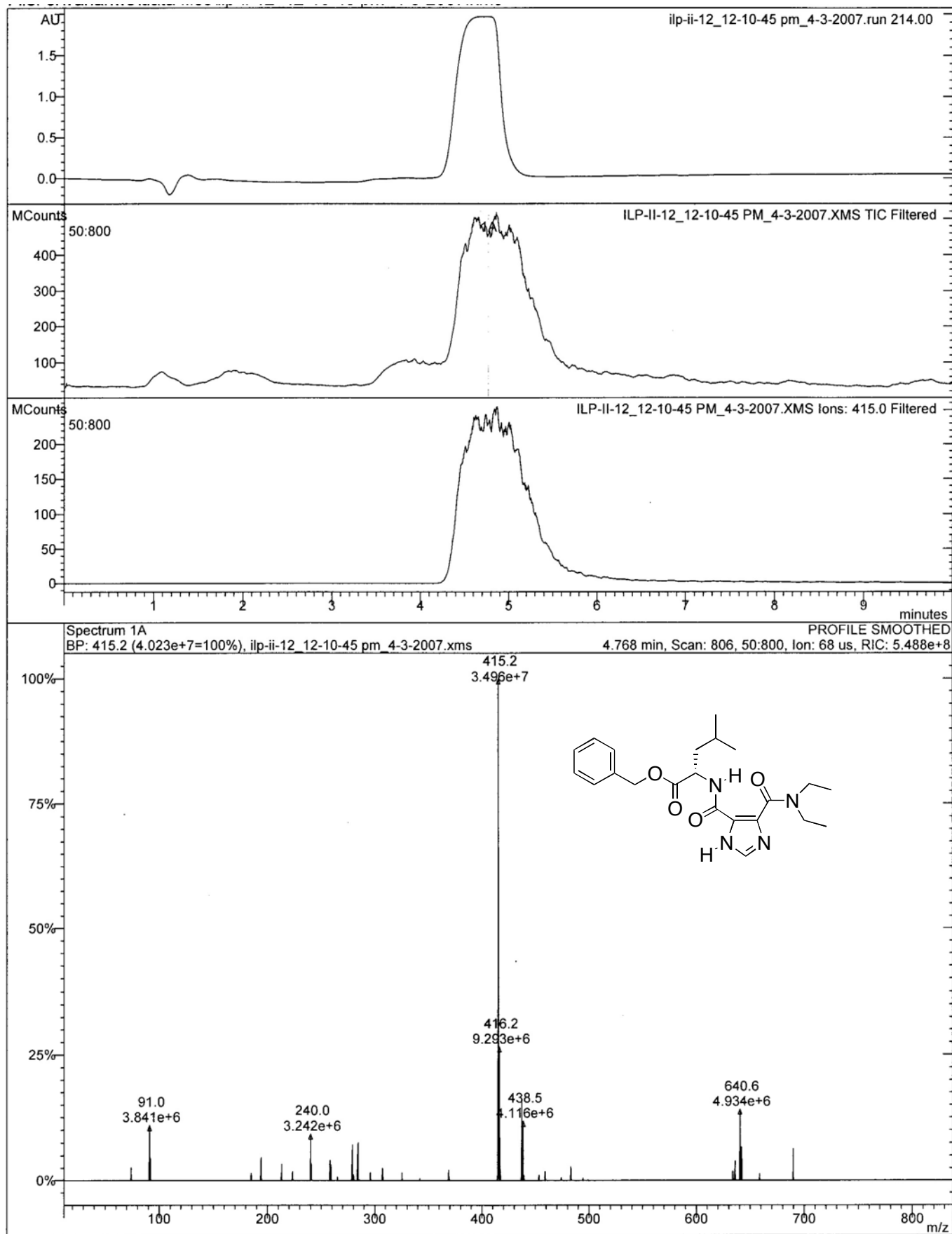


Figure S80. LC/MS data for 5{80}.

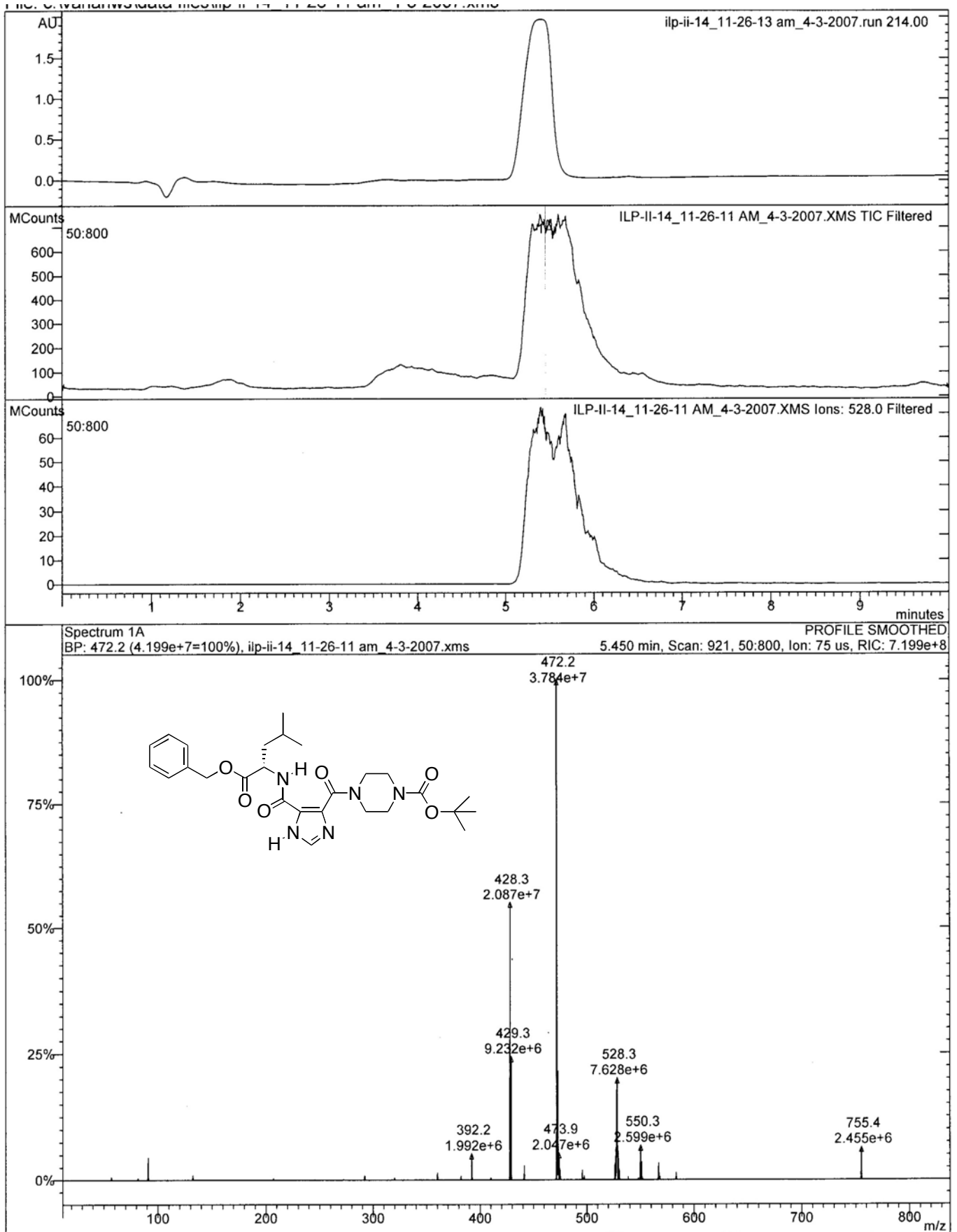


Figure S81. LC/MS data for 5{81}.

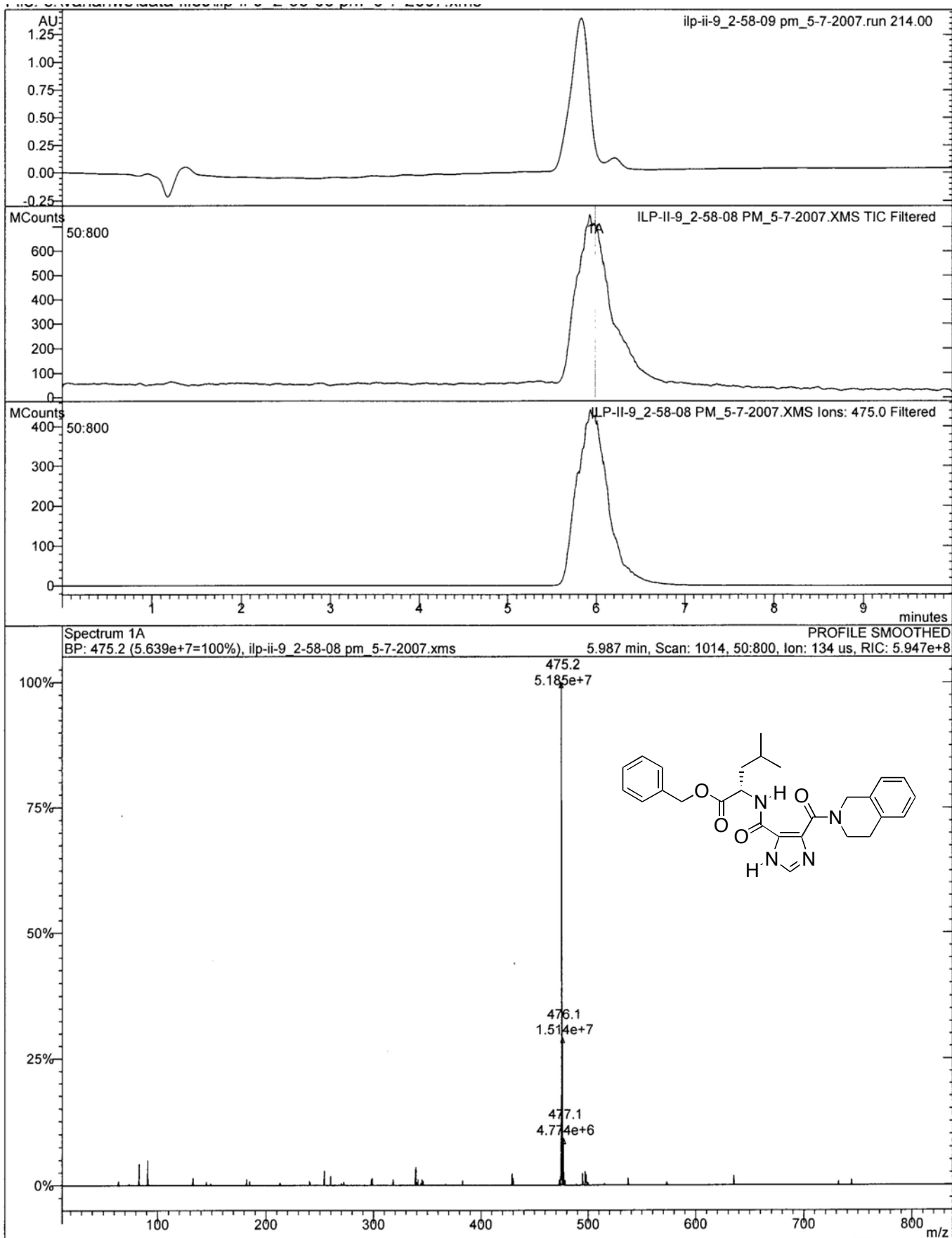


Figure S82. LC/MS data for 5{82}.

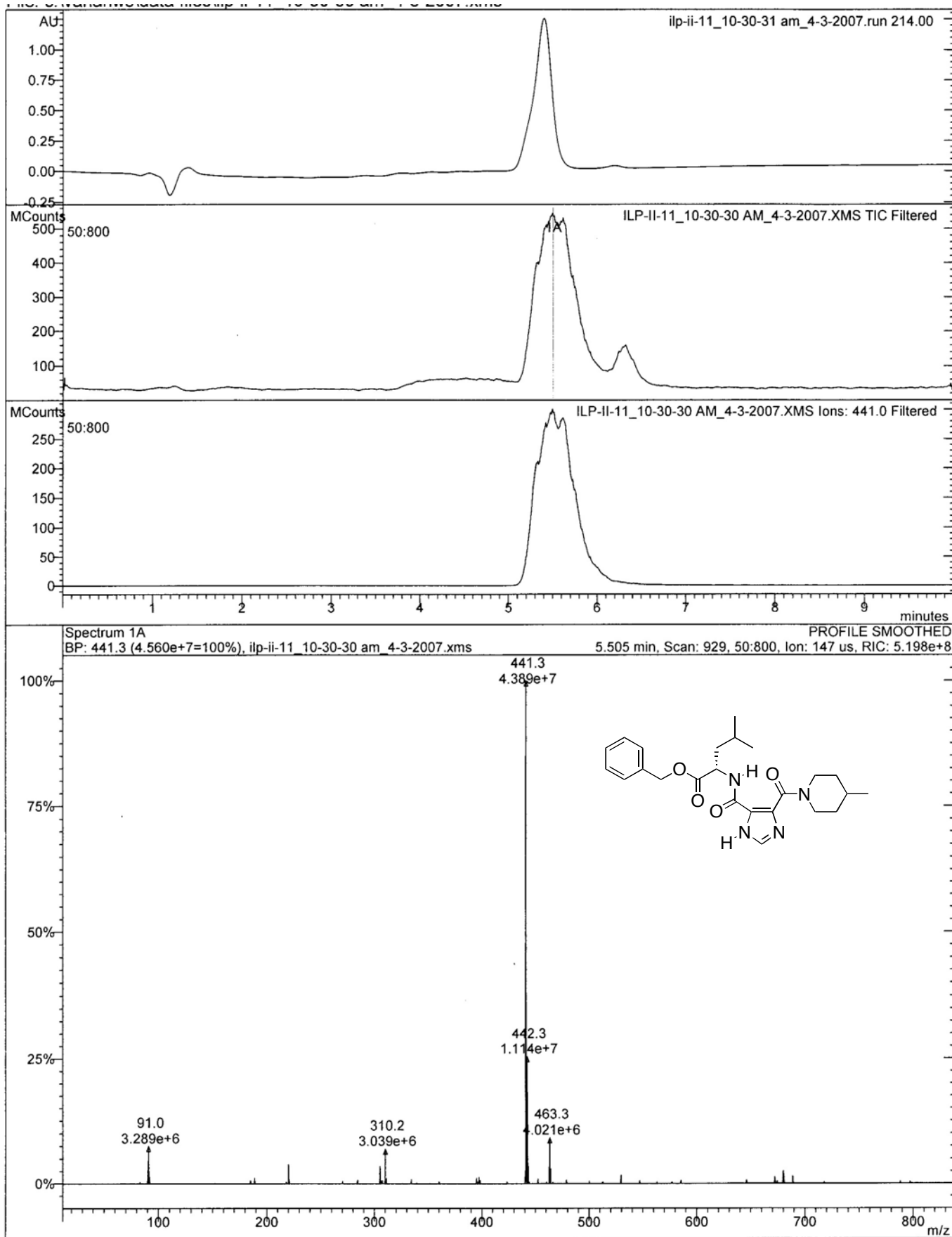


Figure S83. LC/MS data for 5{83}.

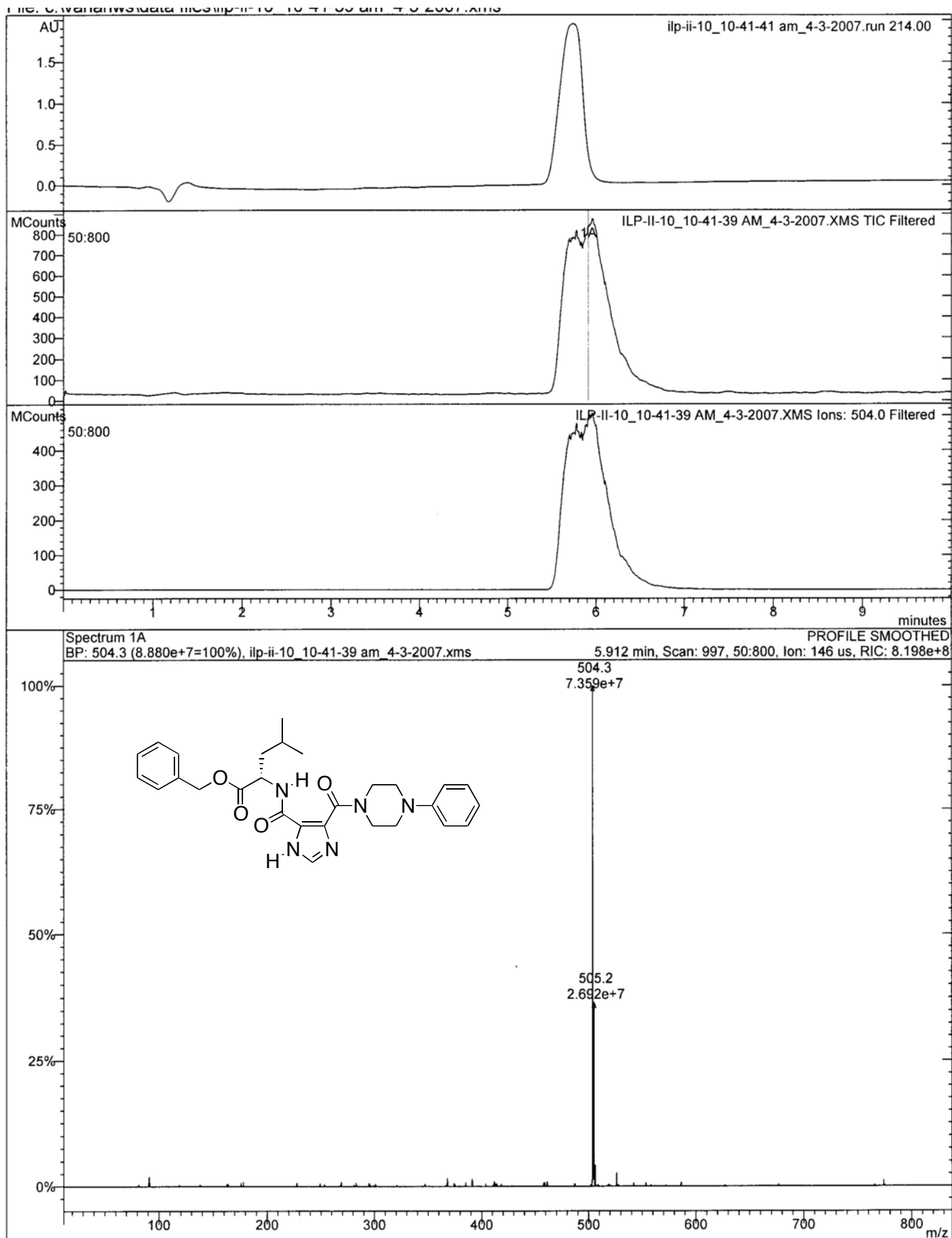


Figure S84. LC/MS data for 5{84}.

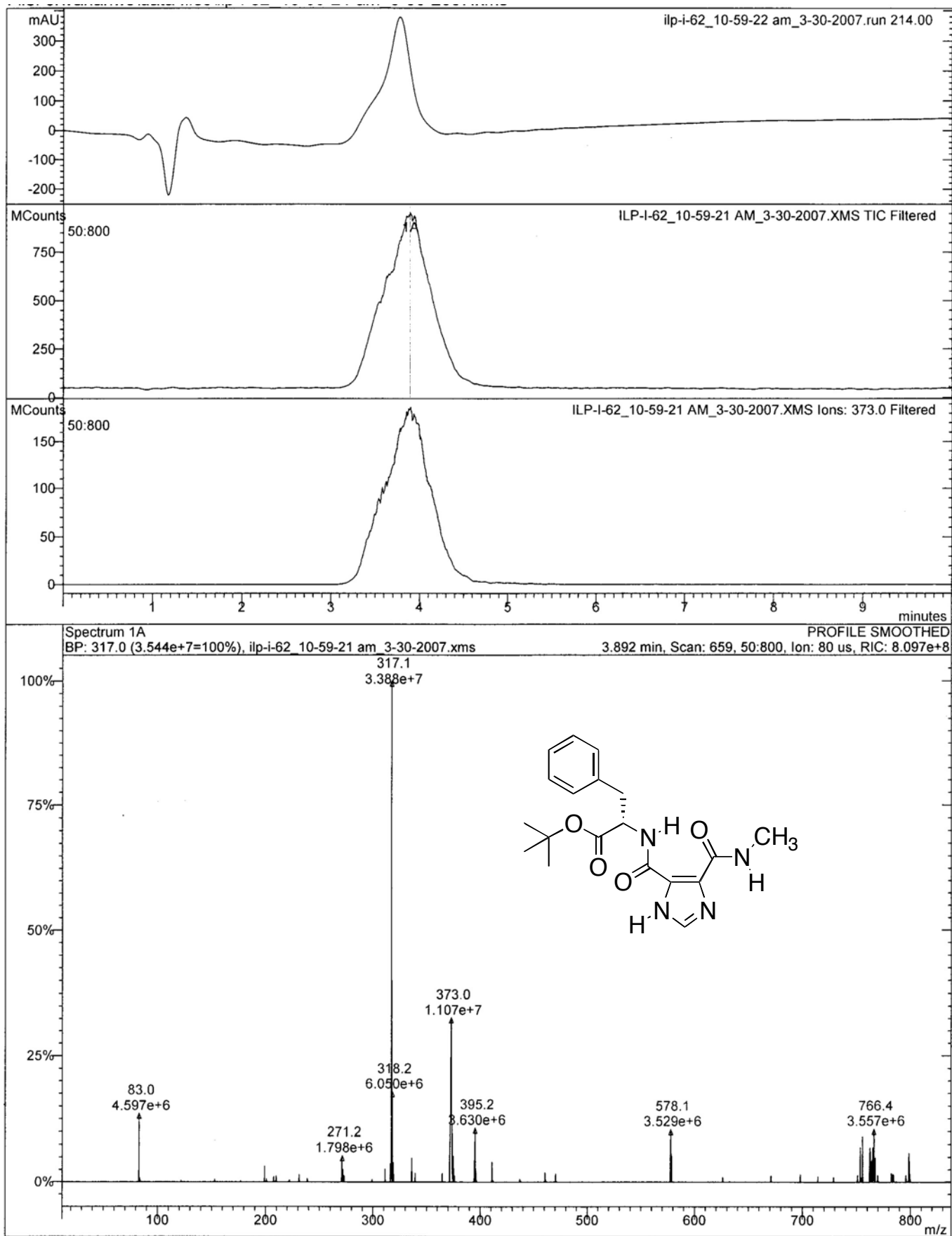


Figure S85. LC/MS data for 5{85}.

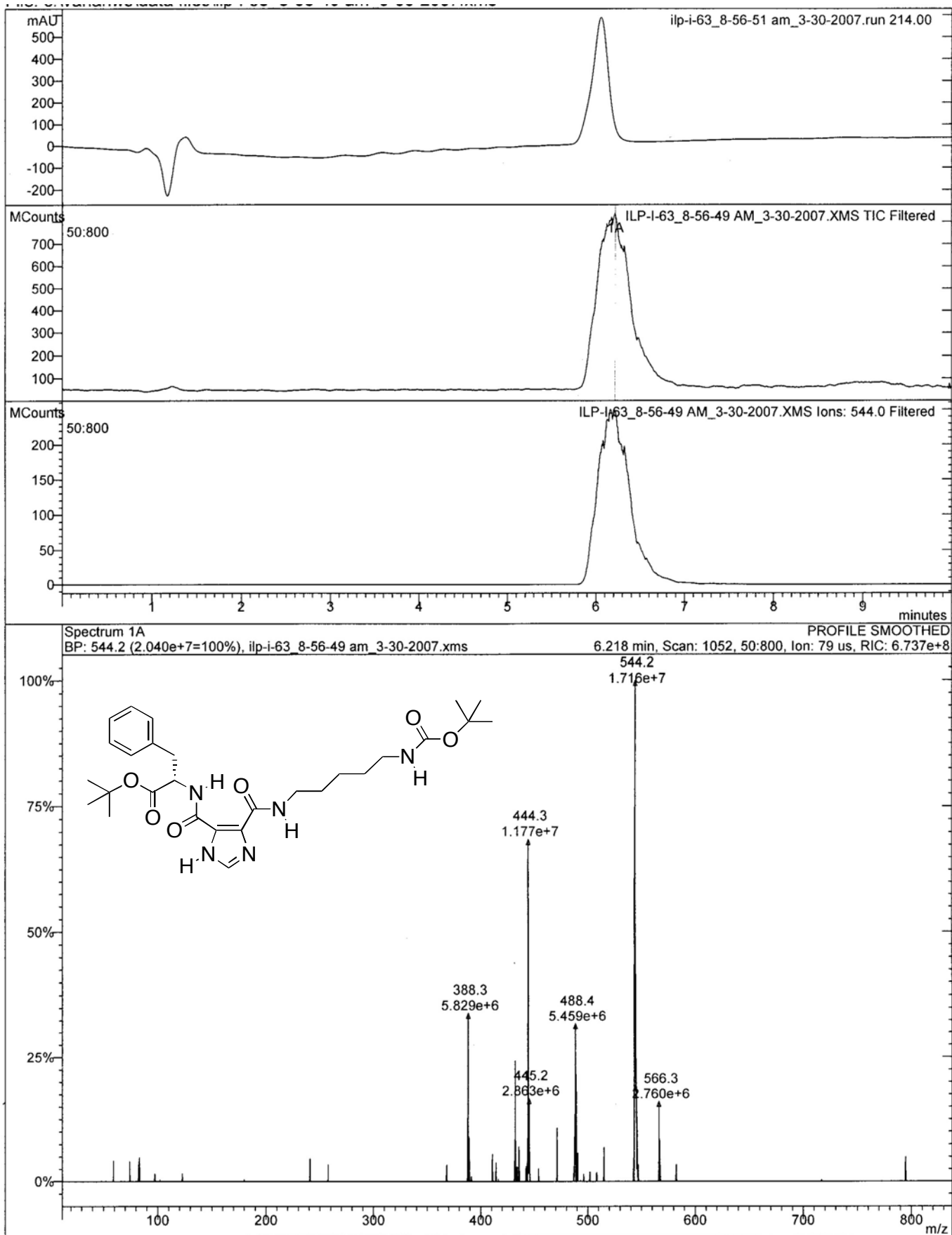


Figure S86. LC/MS data for 5{86}.

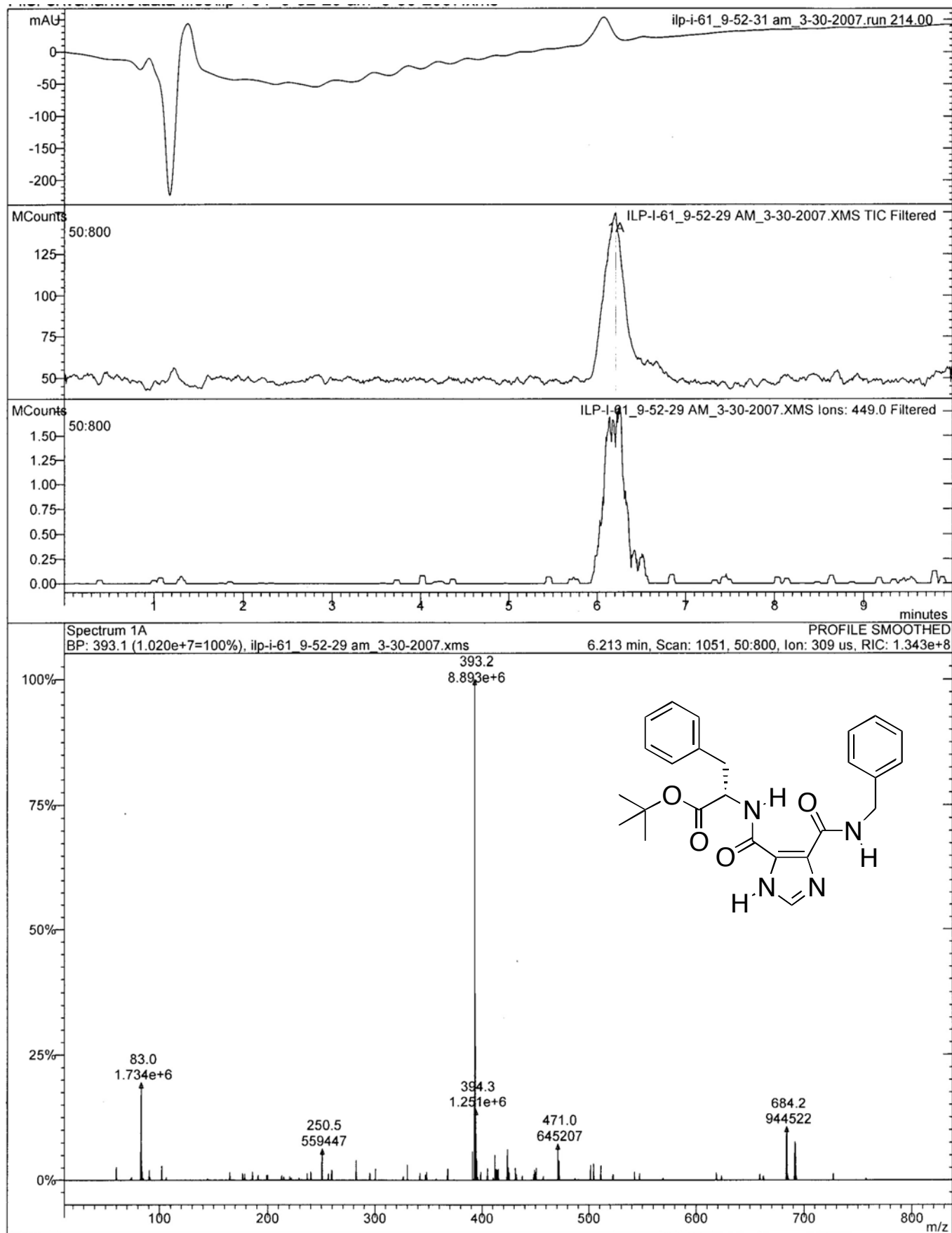


Figure S87. LC/MS data for 5{87}.

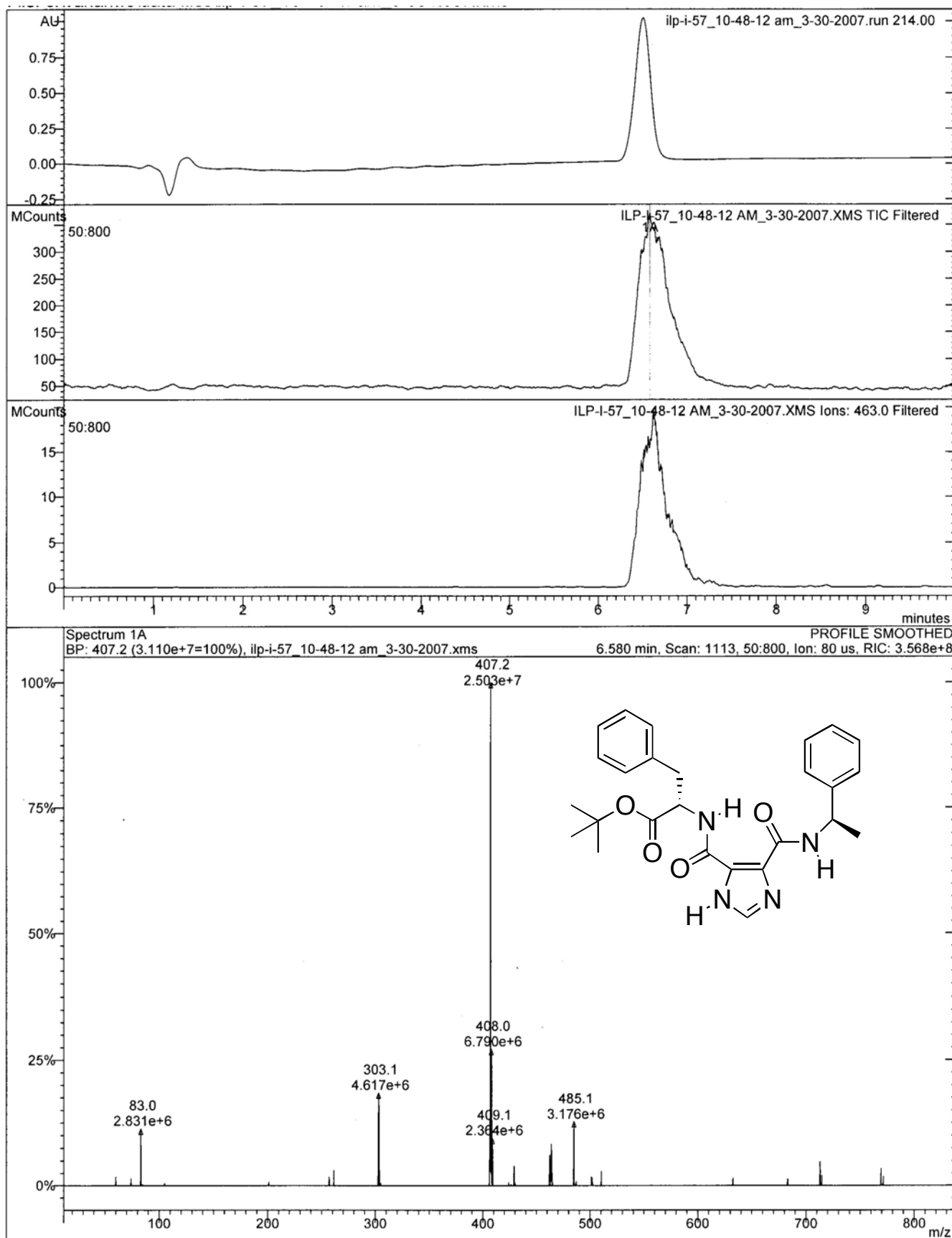


Figure S88. LC/MS data for 5{88}.

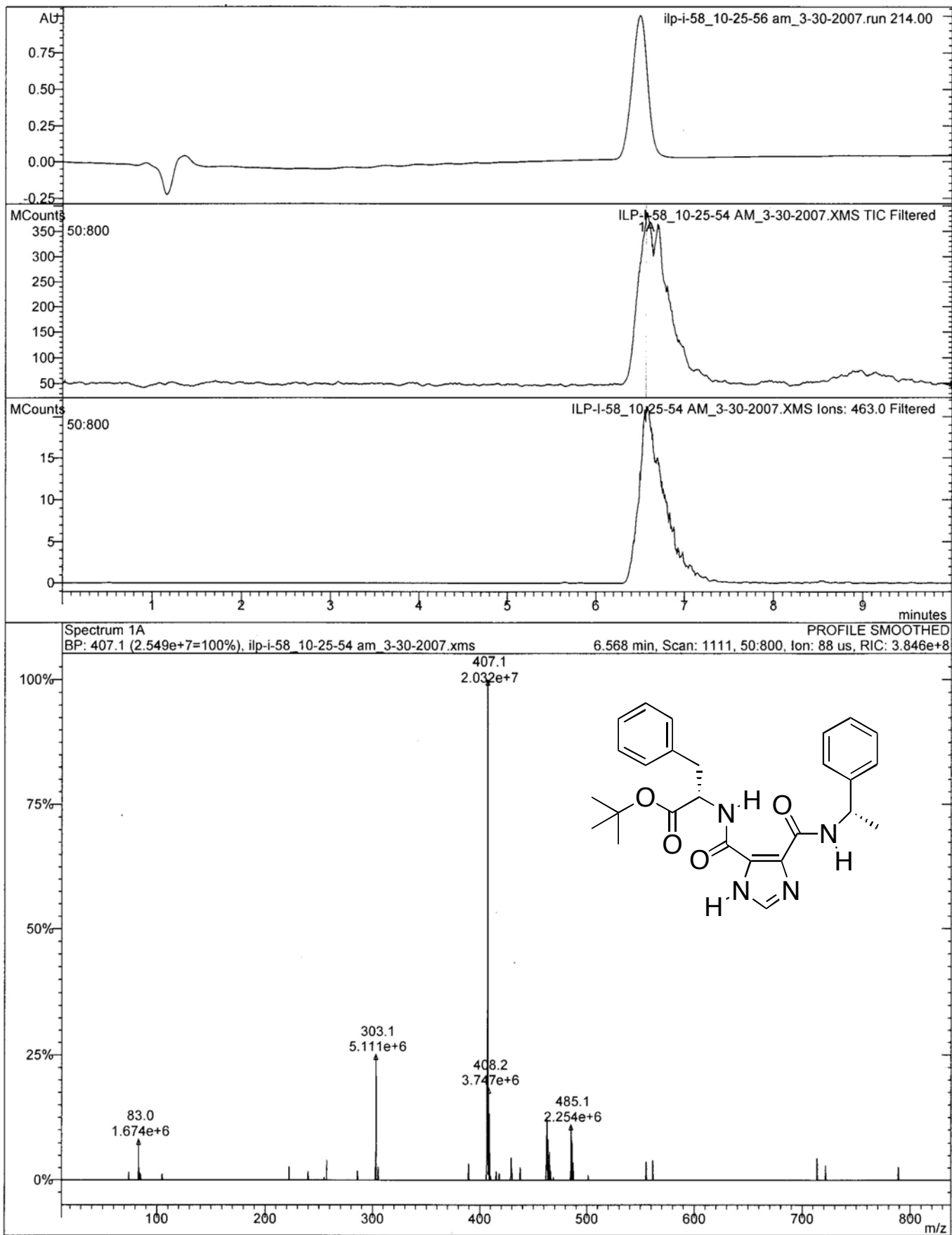


Figure S89. LC/MS data for 5{89}.

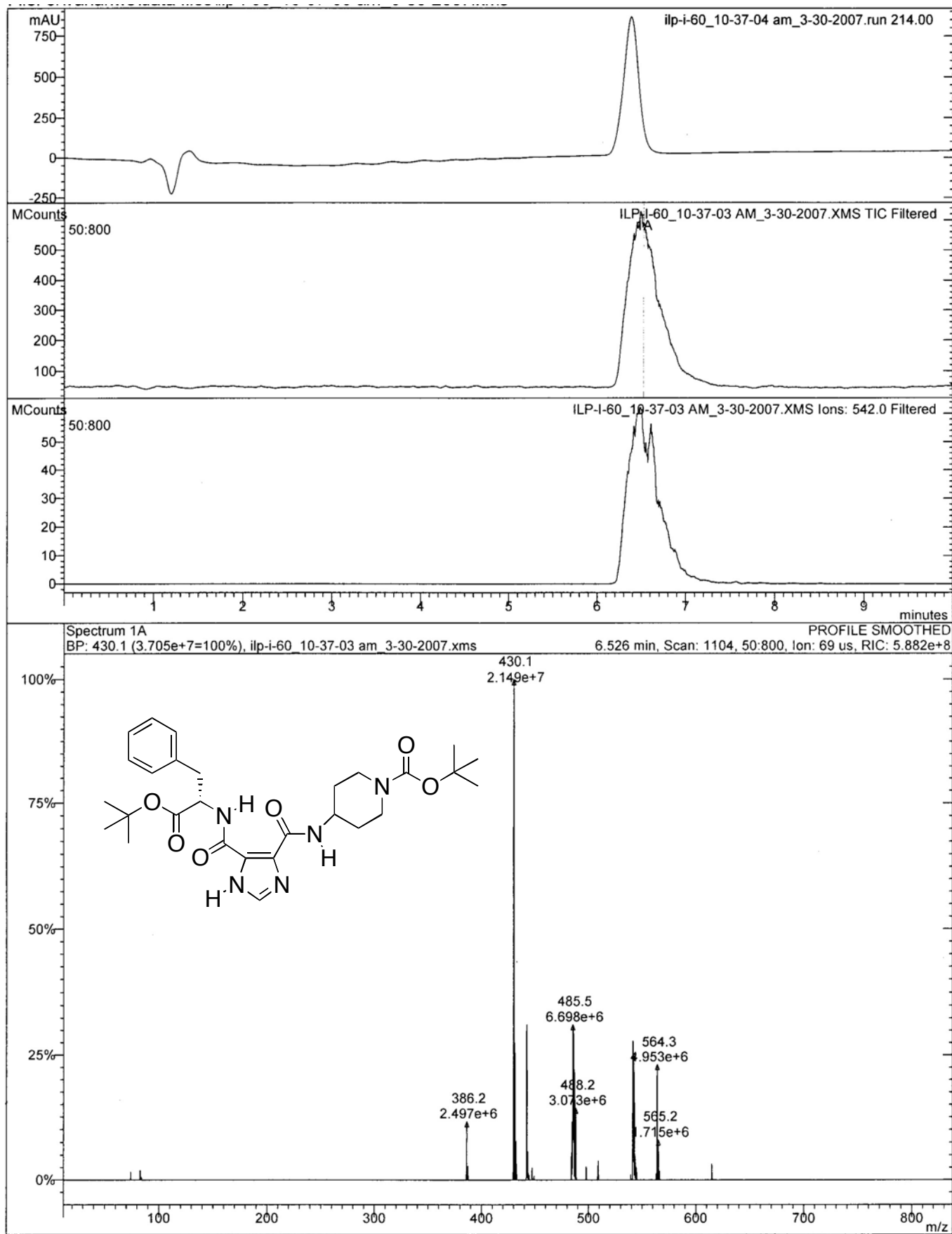


Figure S90. LC/MS data for 5{90}.

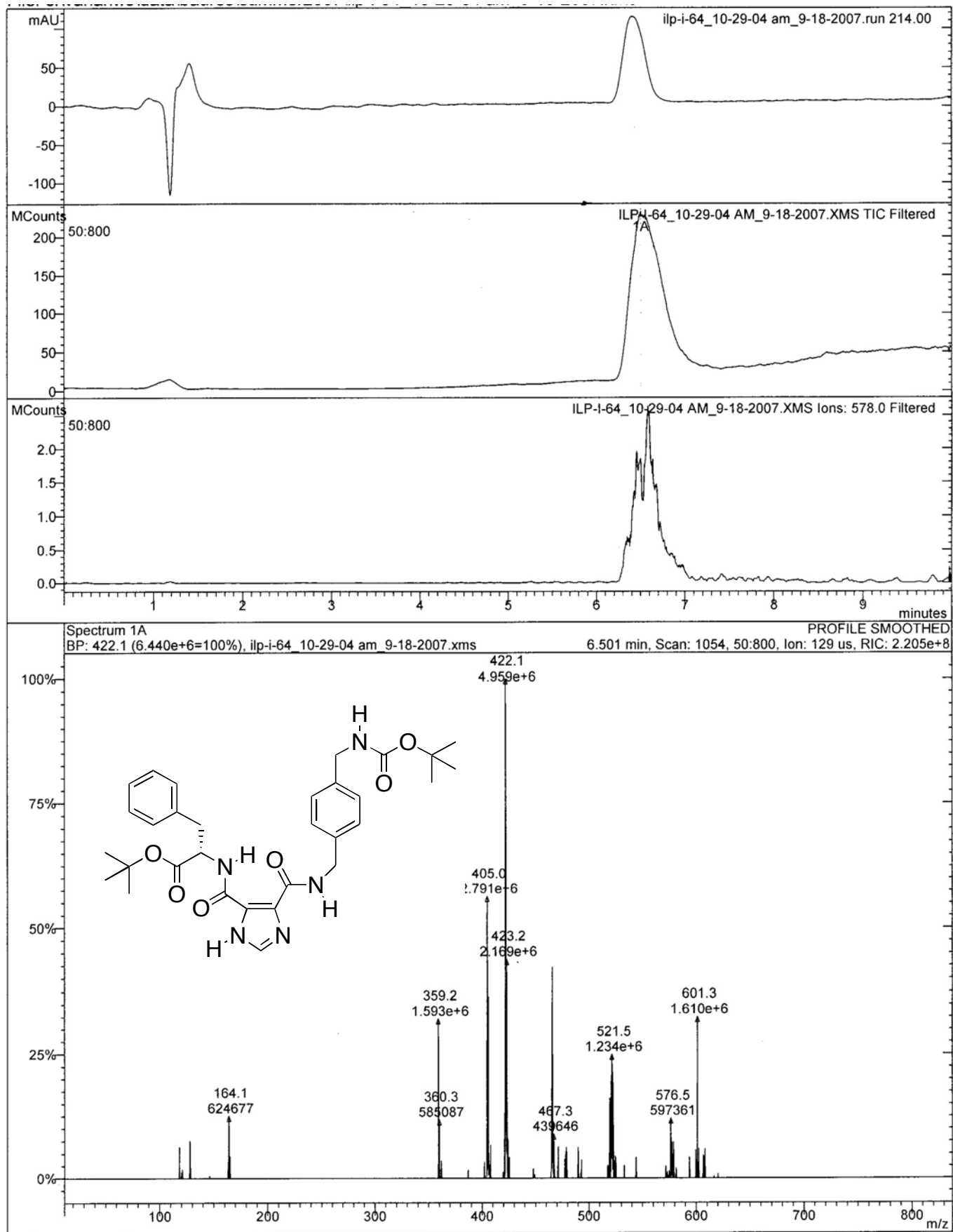


Figure S91. LC/MS data for 5{91}.

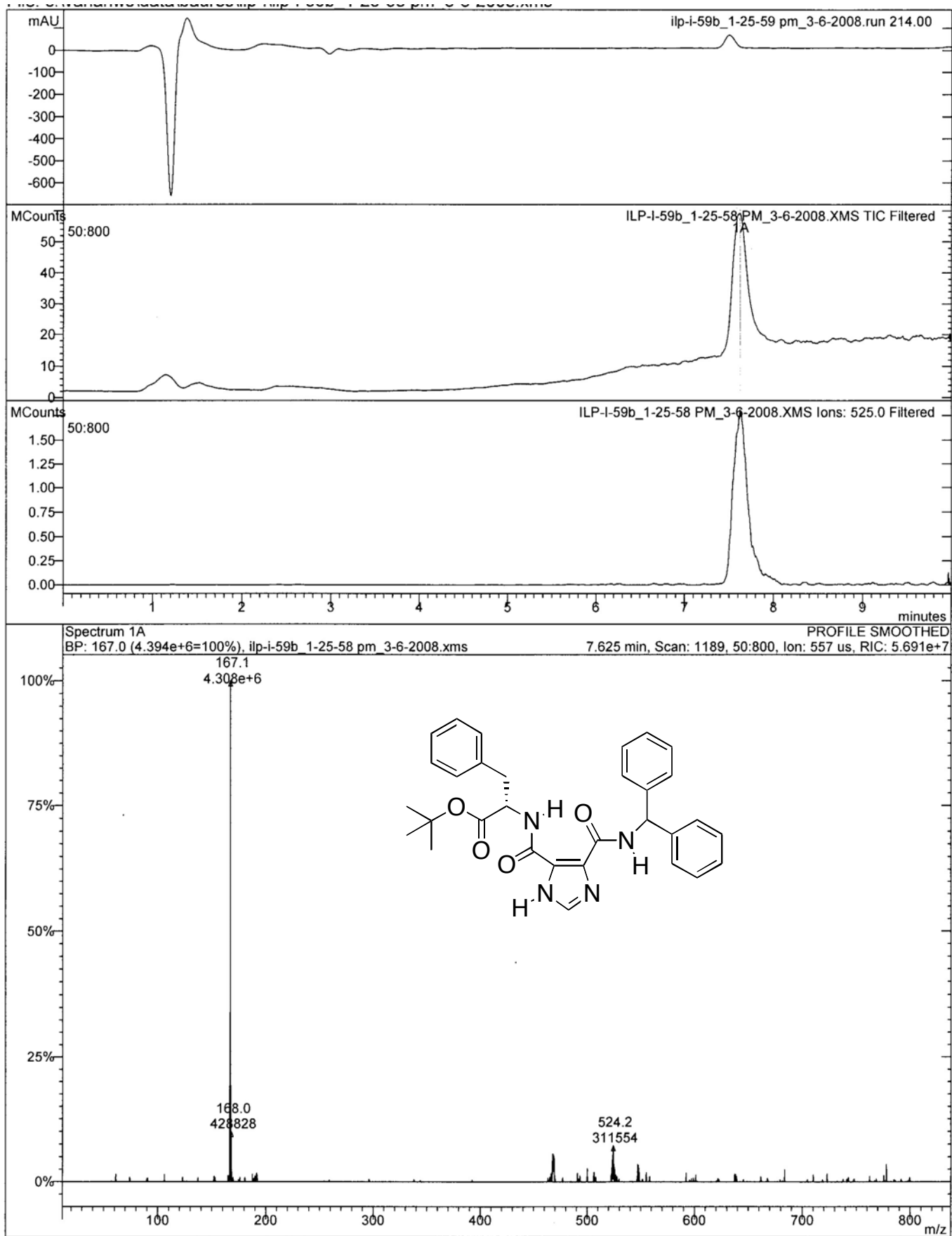


Figure S92. LC/MS data for 5{92}.

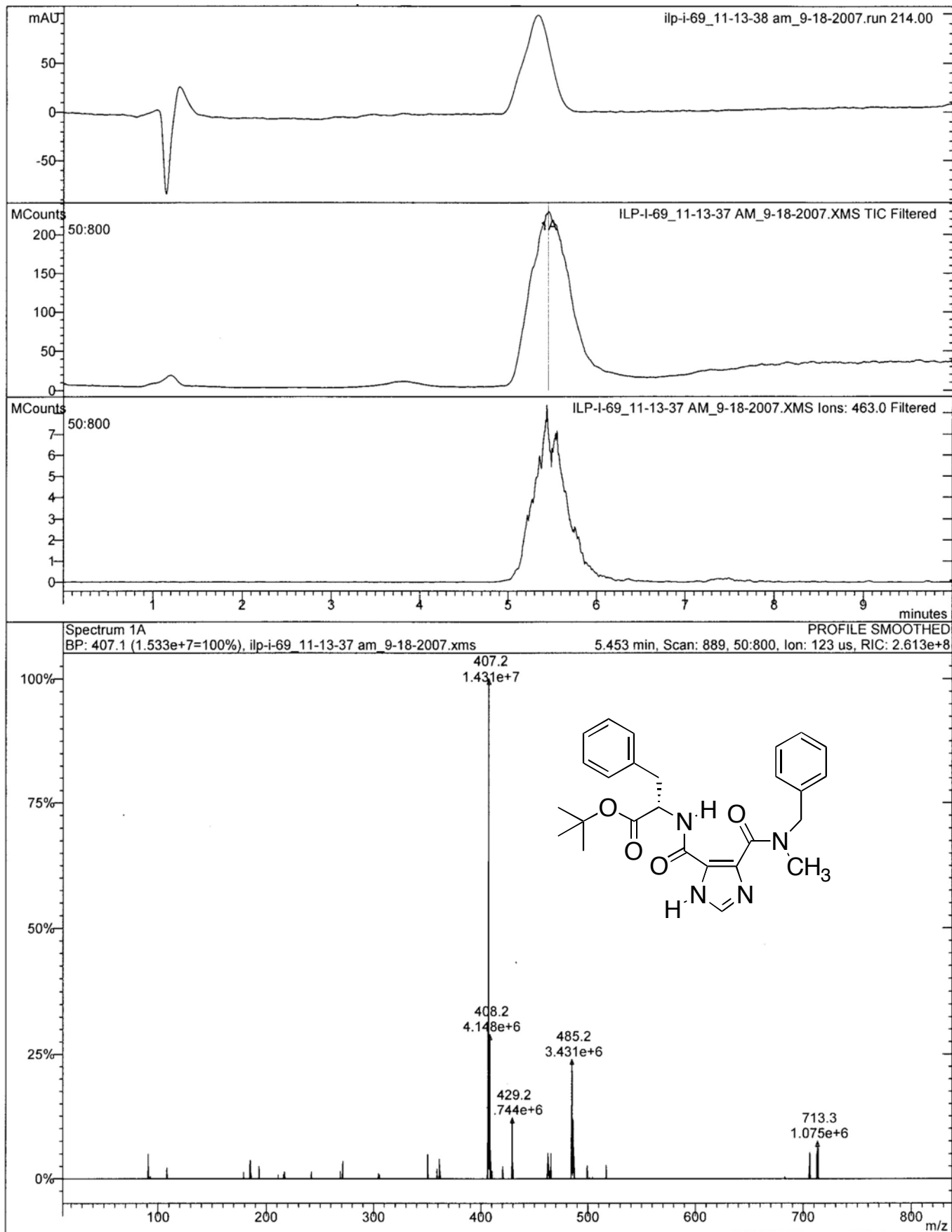


Figure S93. LC/MS data for 5{93}.

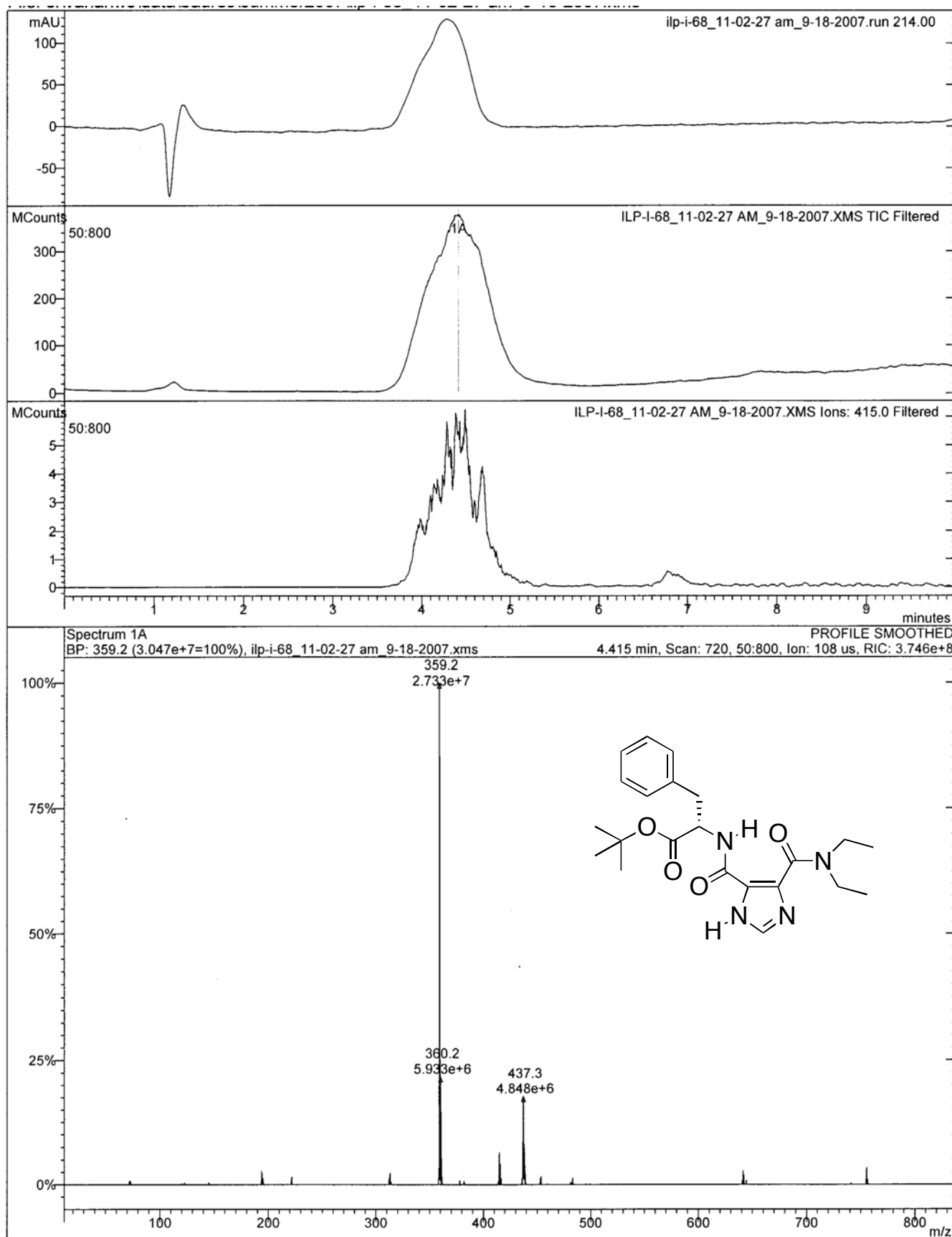


Figure S94. LC/MS data for 5{94}.

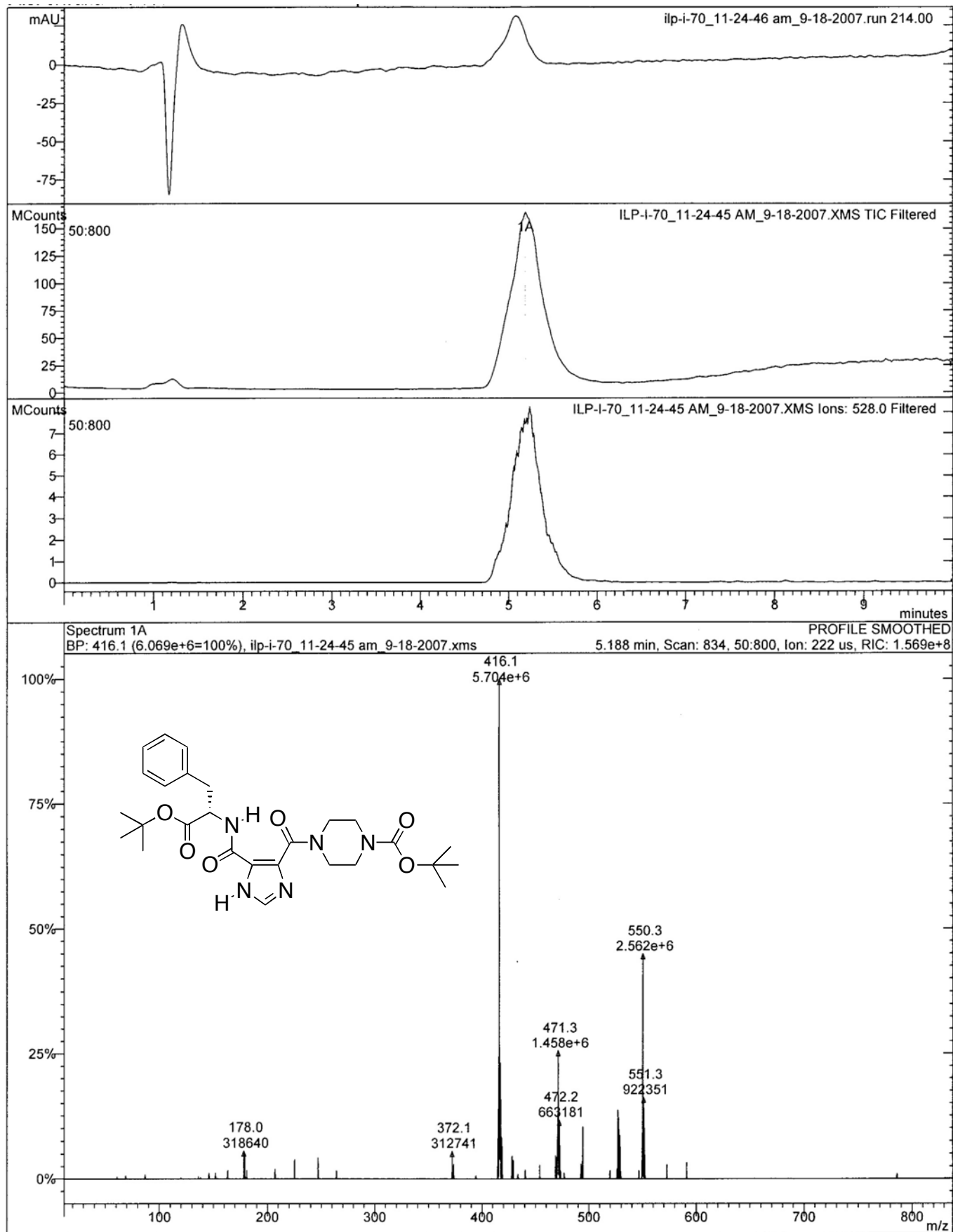


Figure S95. LC/MS data for 5{95}.

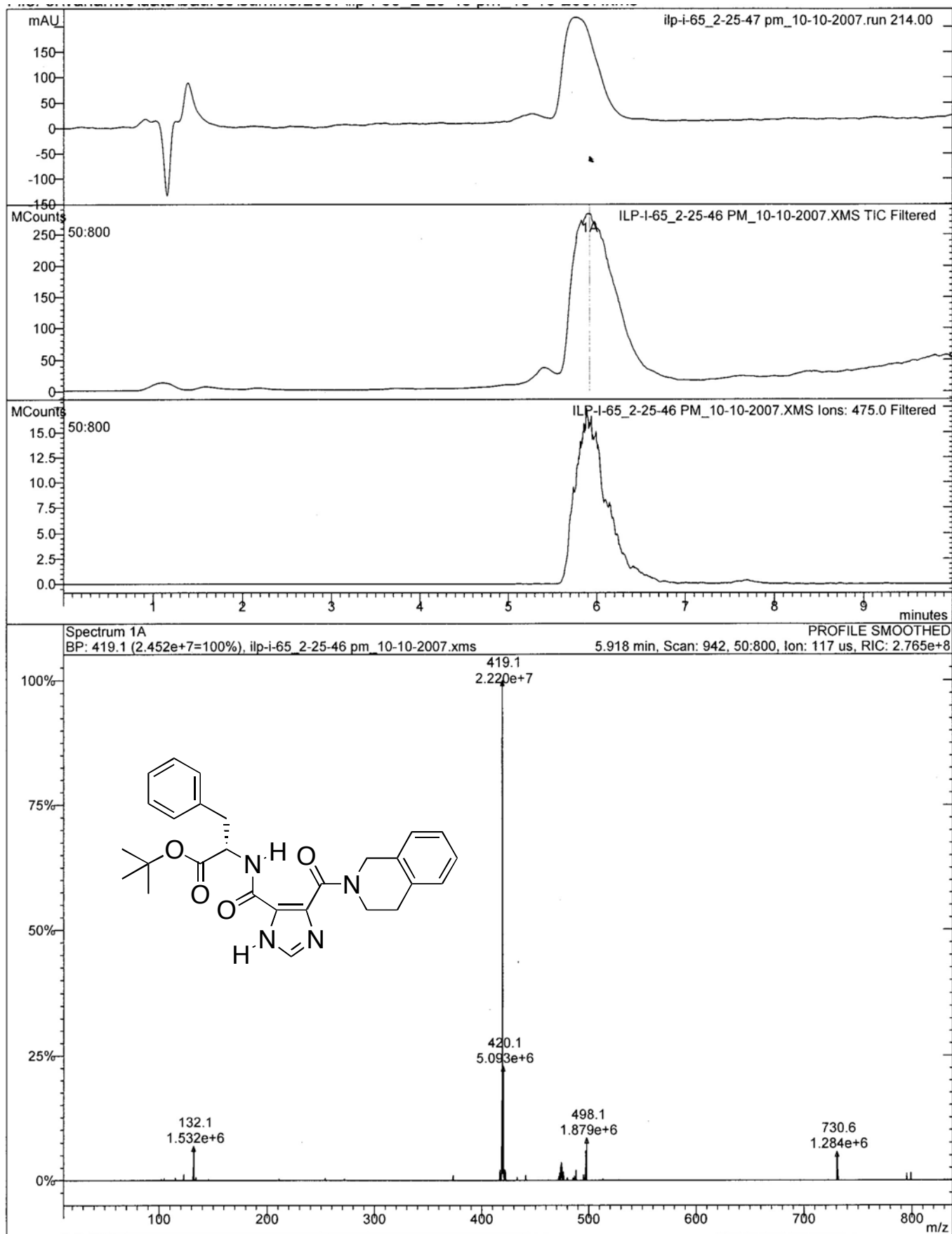


Figure S96. LC/MS data for 5{96}.

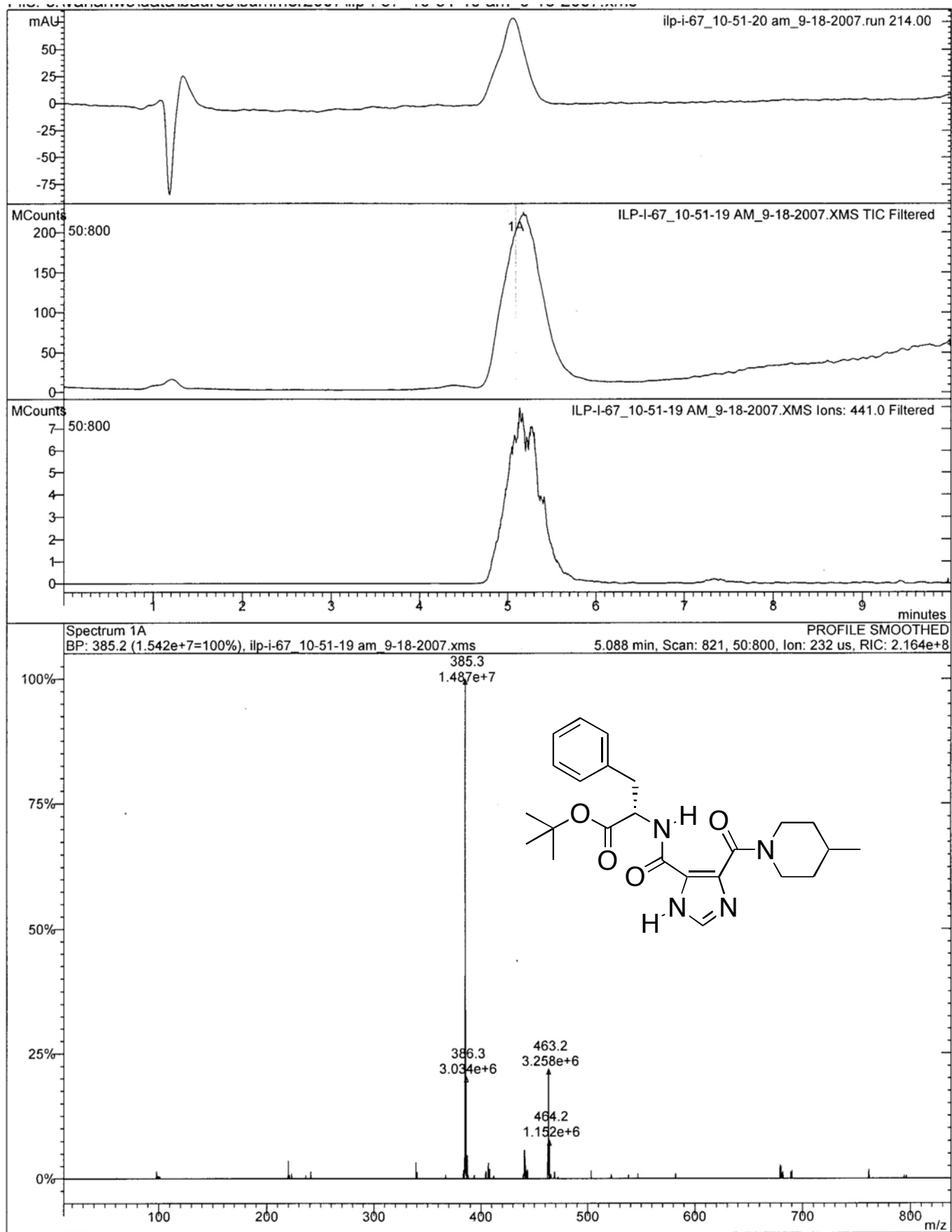


Figure S97. LC/MS data for 5{97}.

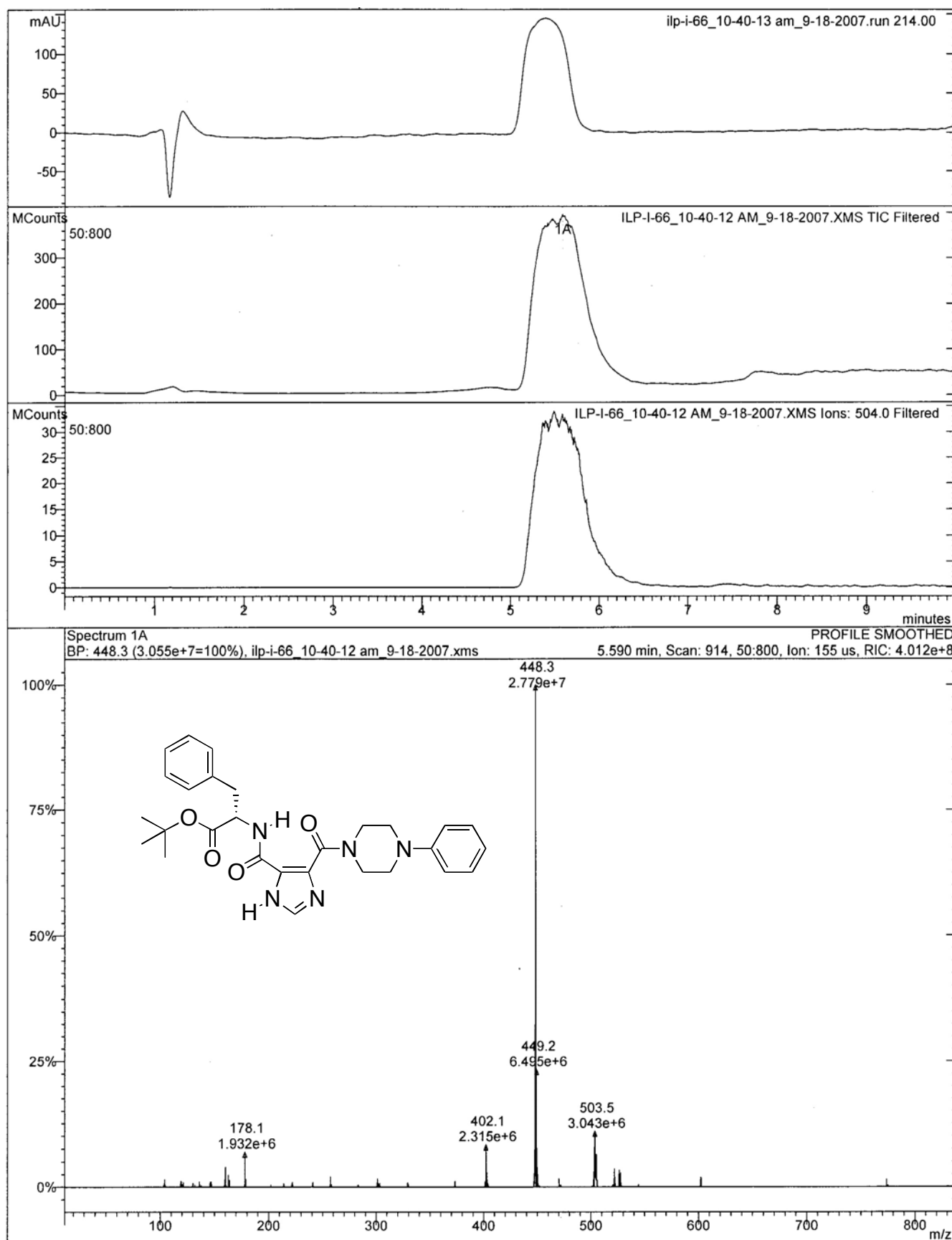


Figure S98. LC/MS data for 5{98}.

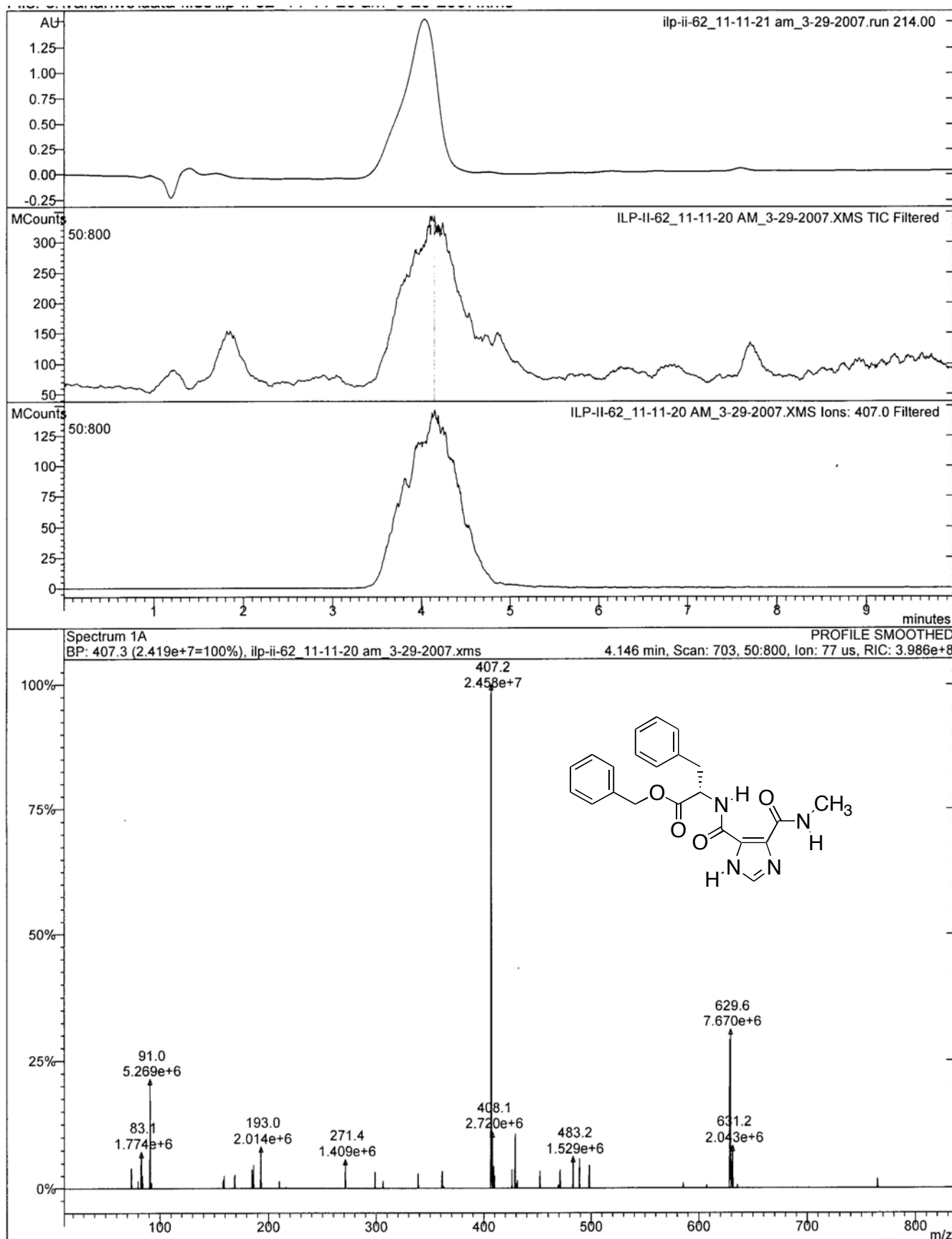


Figure S99. LC/MS data for 5{99}.

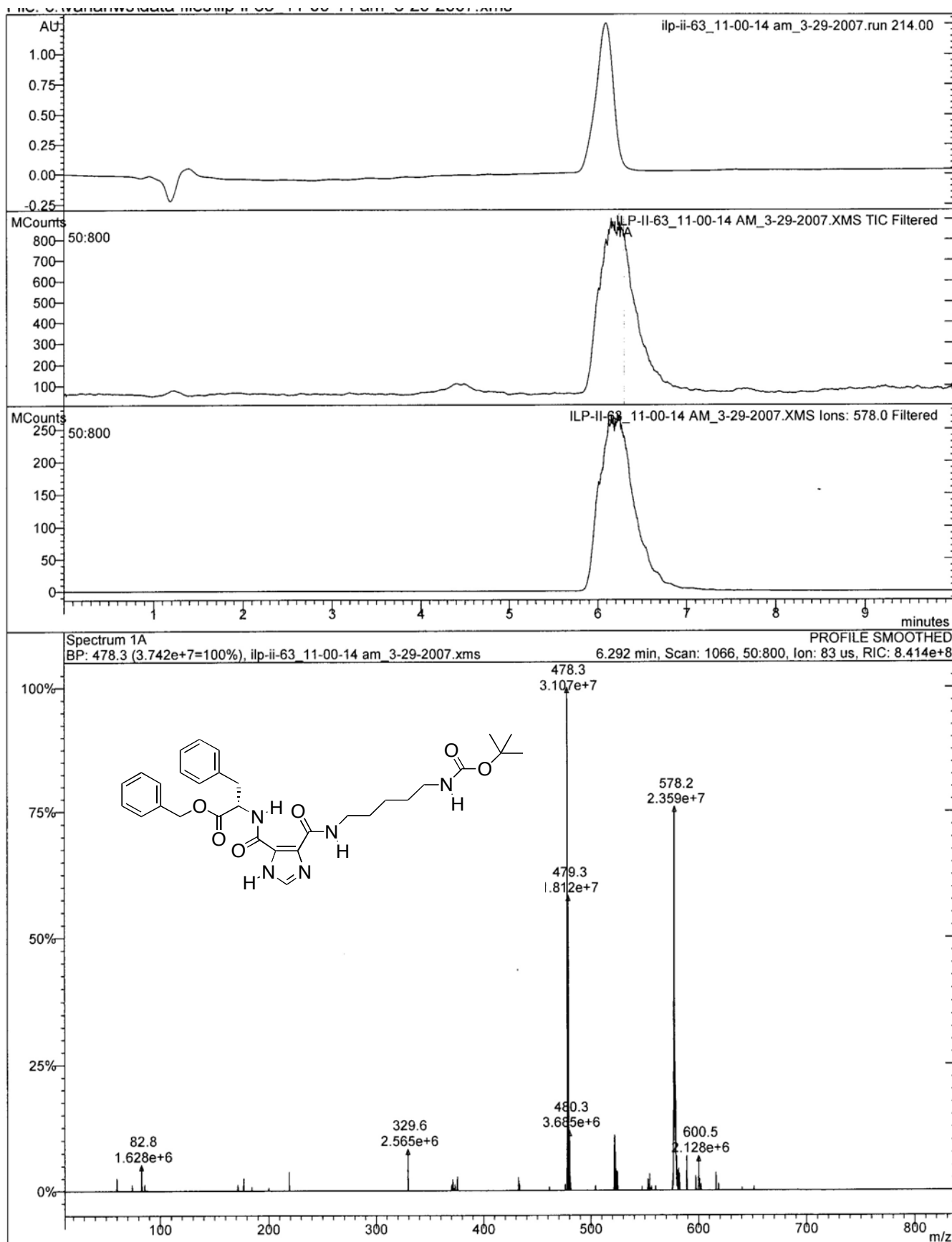


Figure S100. LC/MS data for 5{100}.

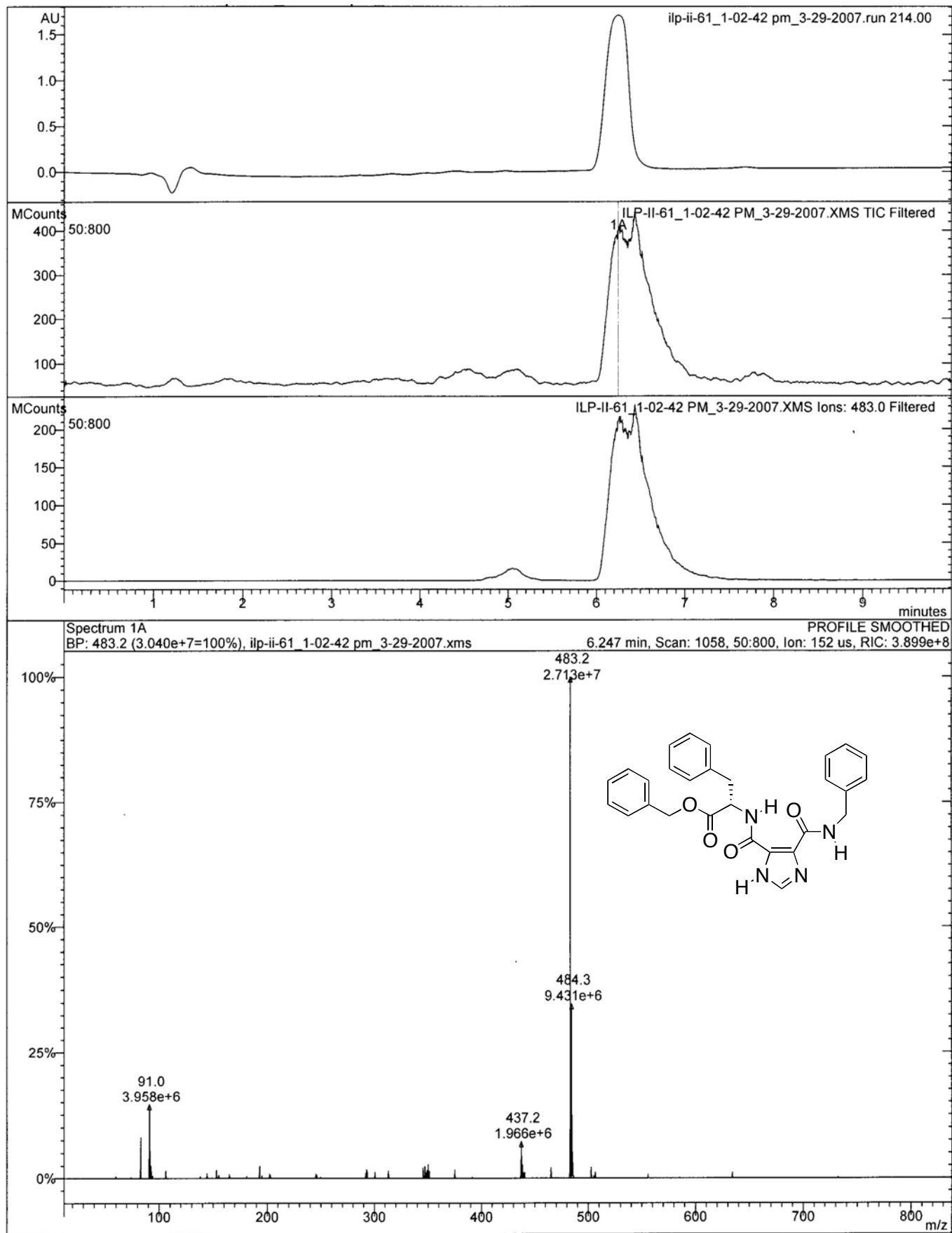


Figure S101. LC/MS data for 5{101}.

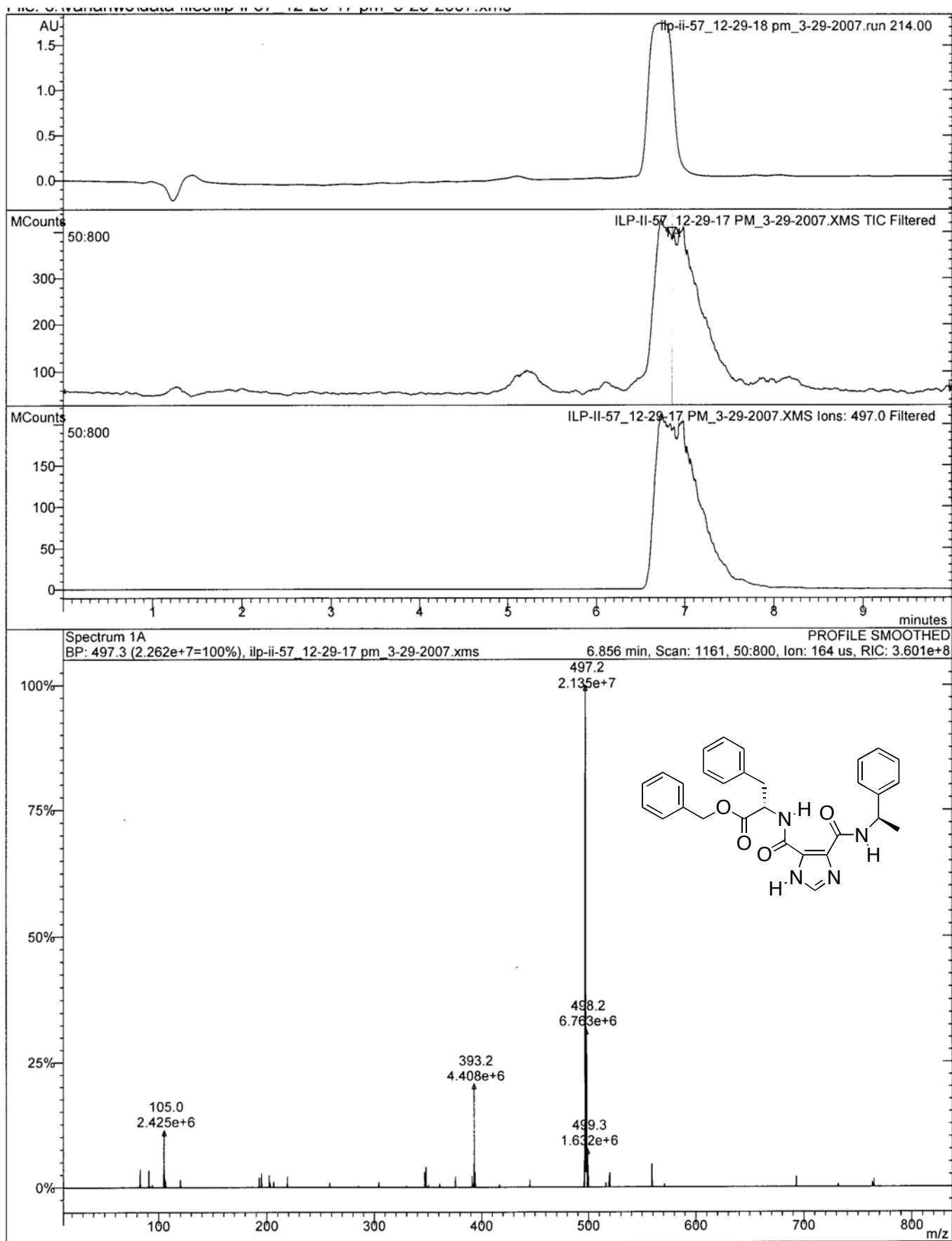


Figure S102. LC/MS data for **5{102}**.

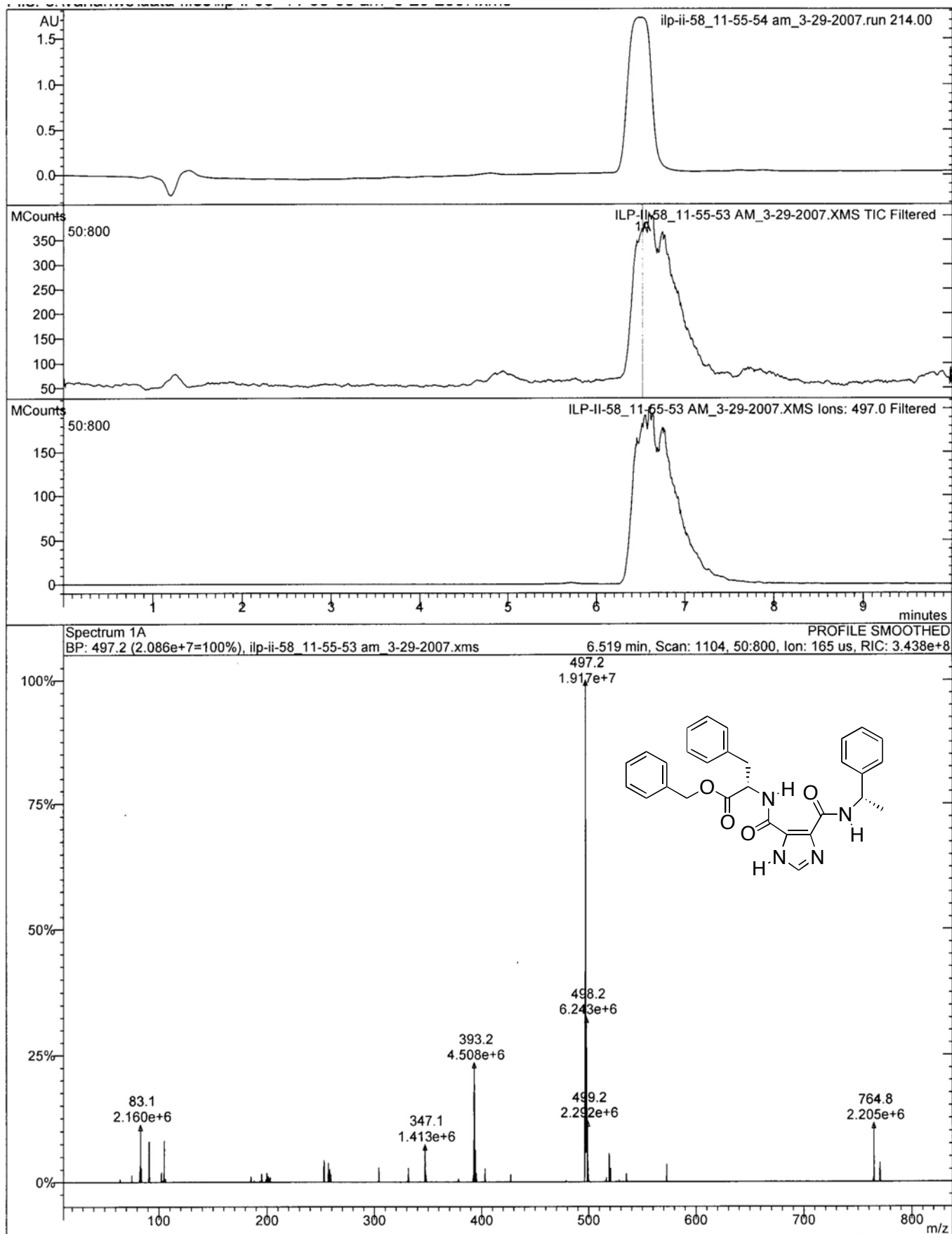


Figure S103. LC/MS data for **5{103}**.

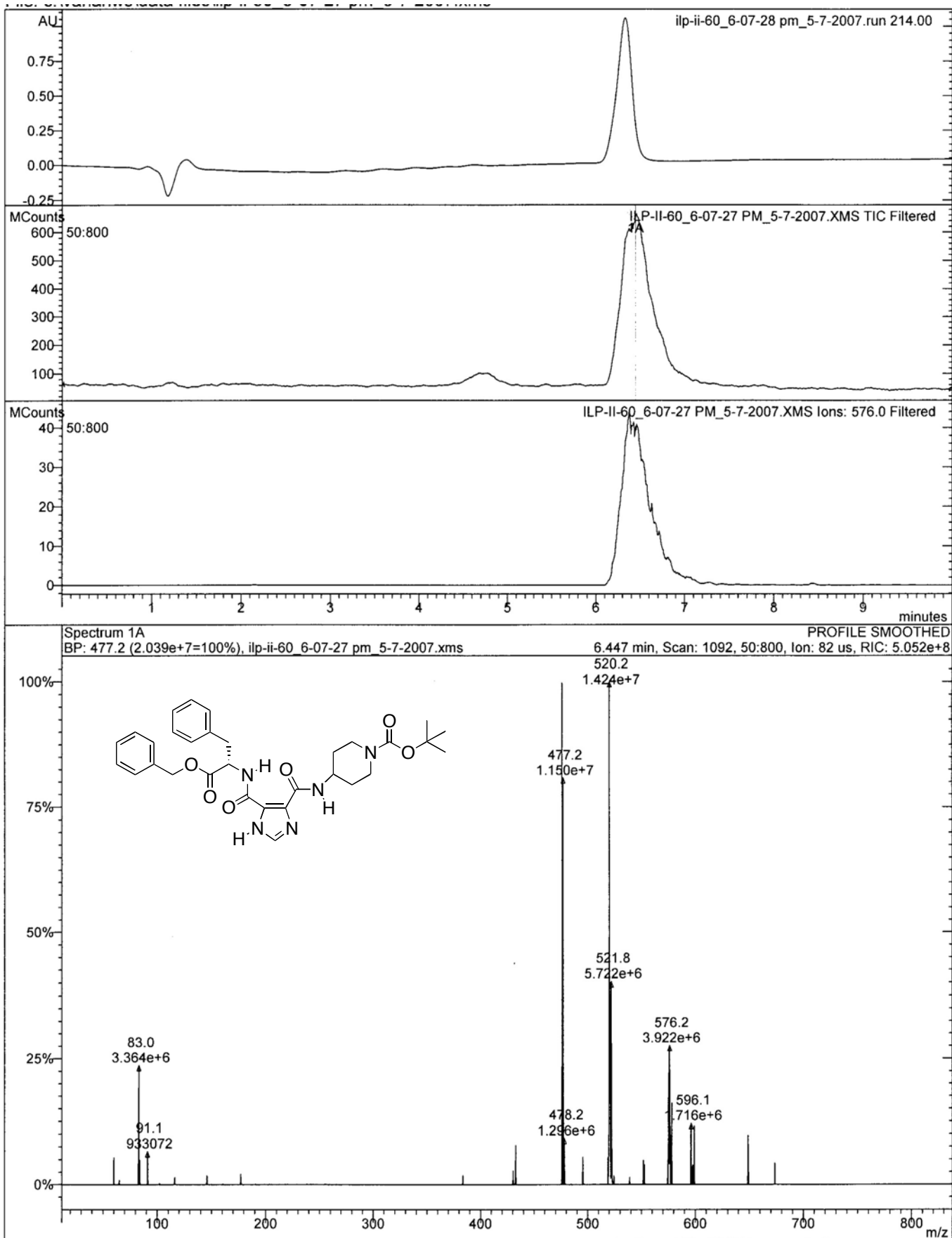


Figure S104. LC/MS data for 5{104}.

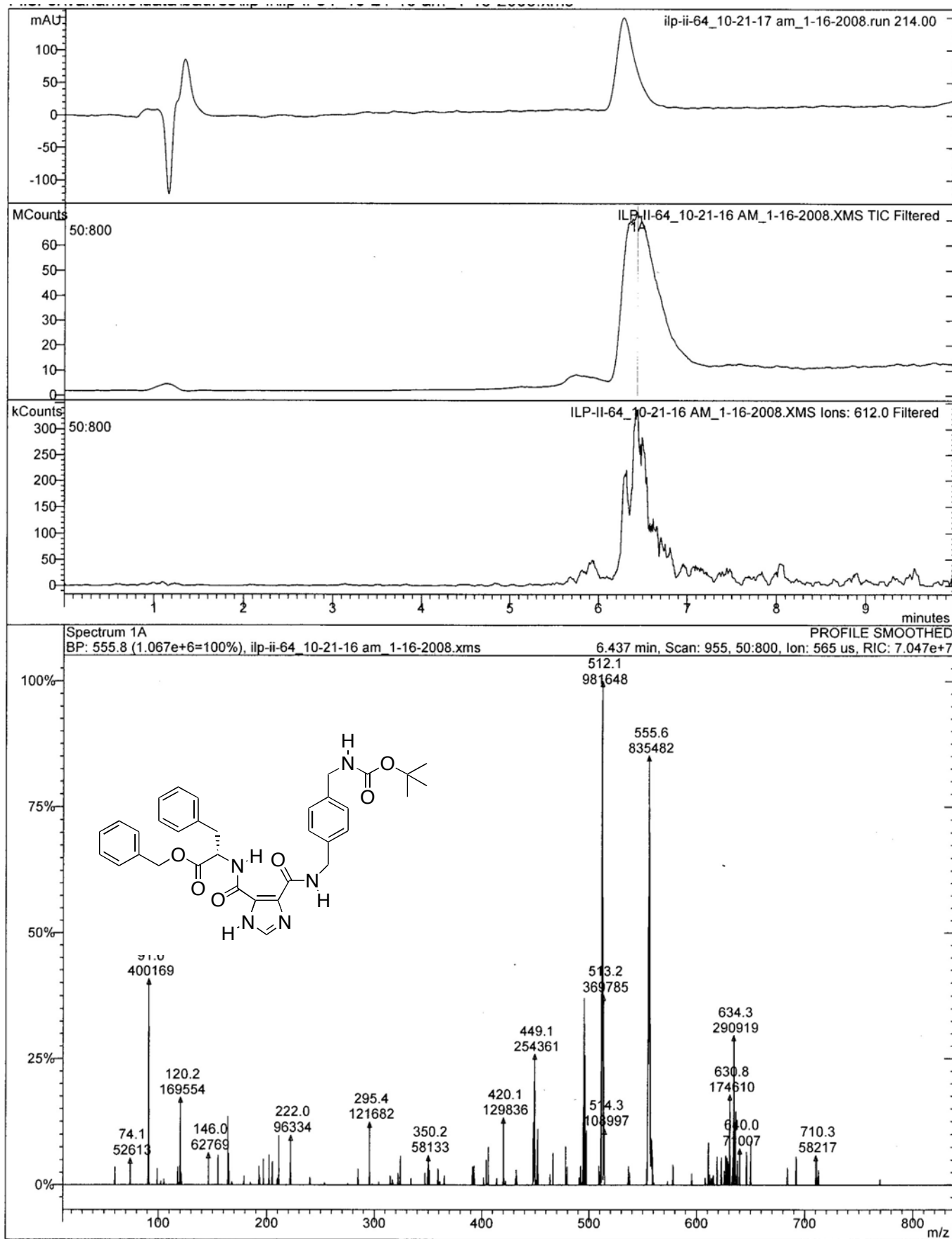


Figure S105. LC/MS data for 5{105}.

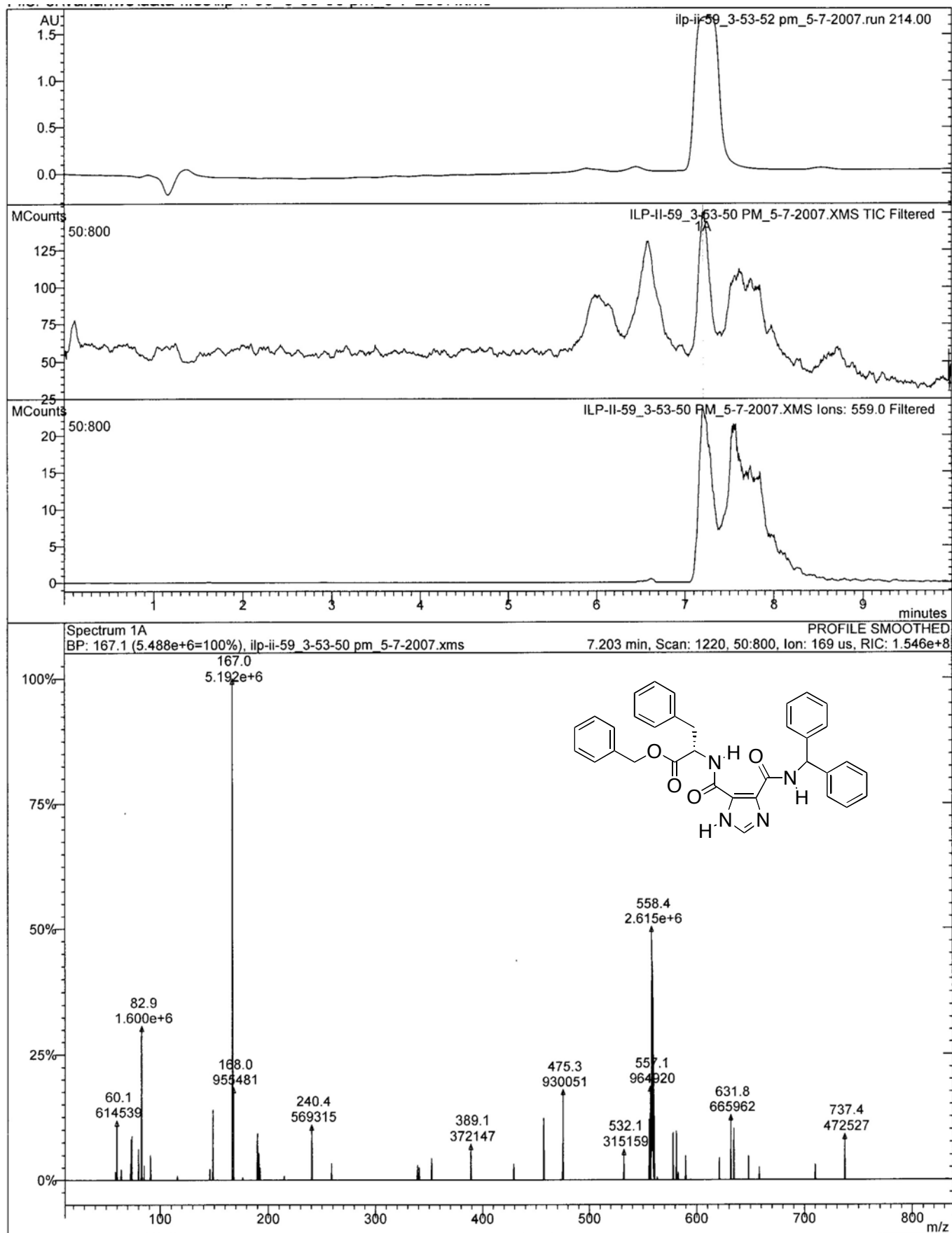


Figure S106. LC/MS data for 5{106}.

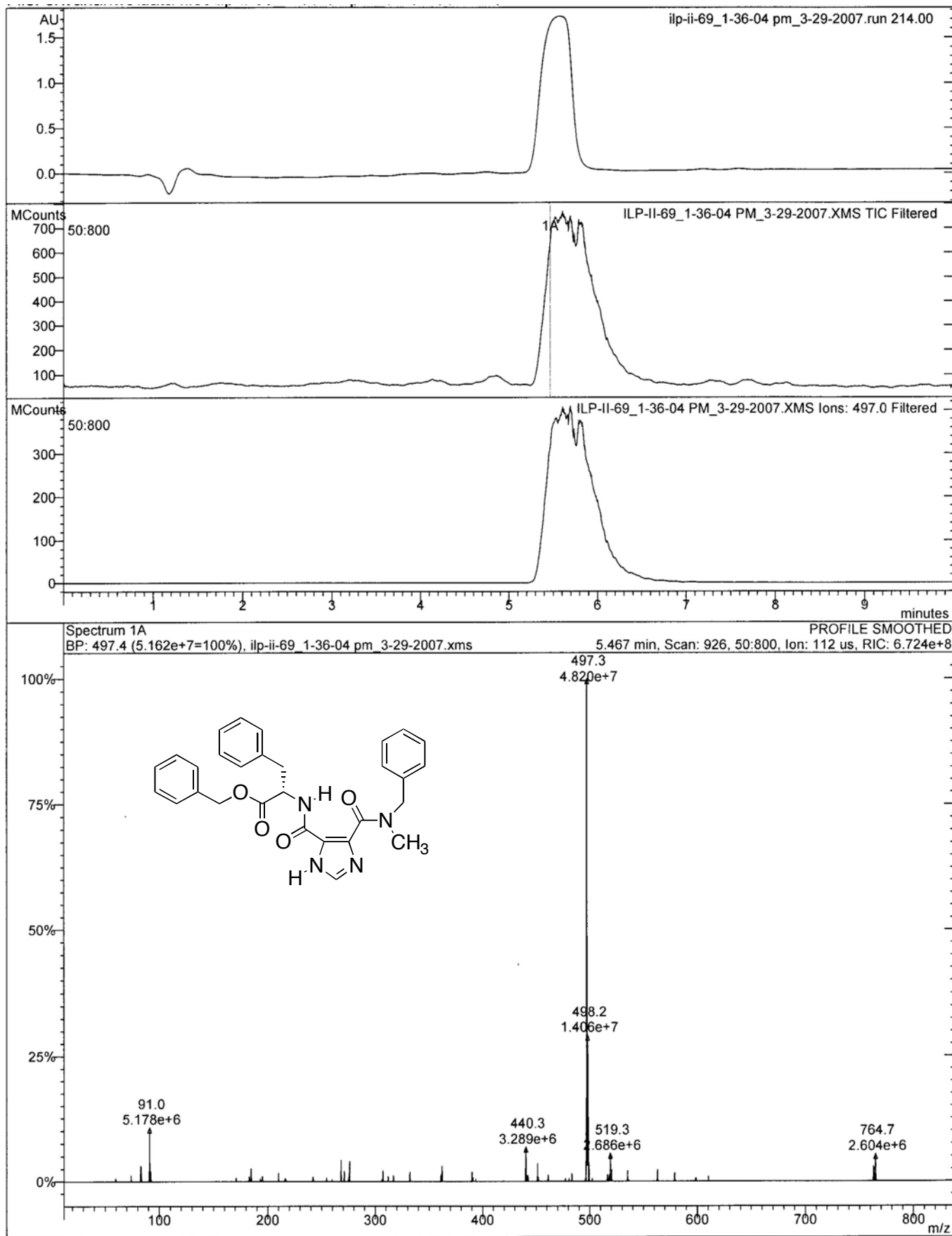


Figure S107. LC/MS data for 5{107}.

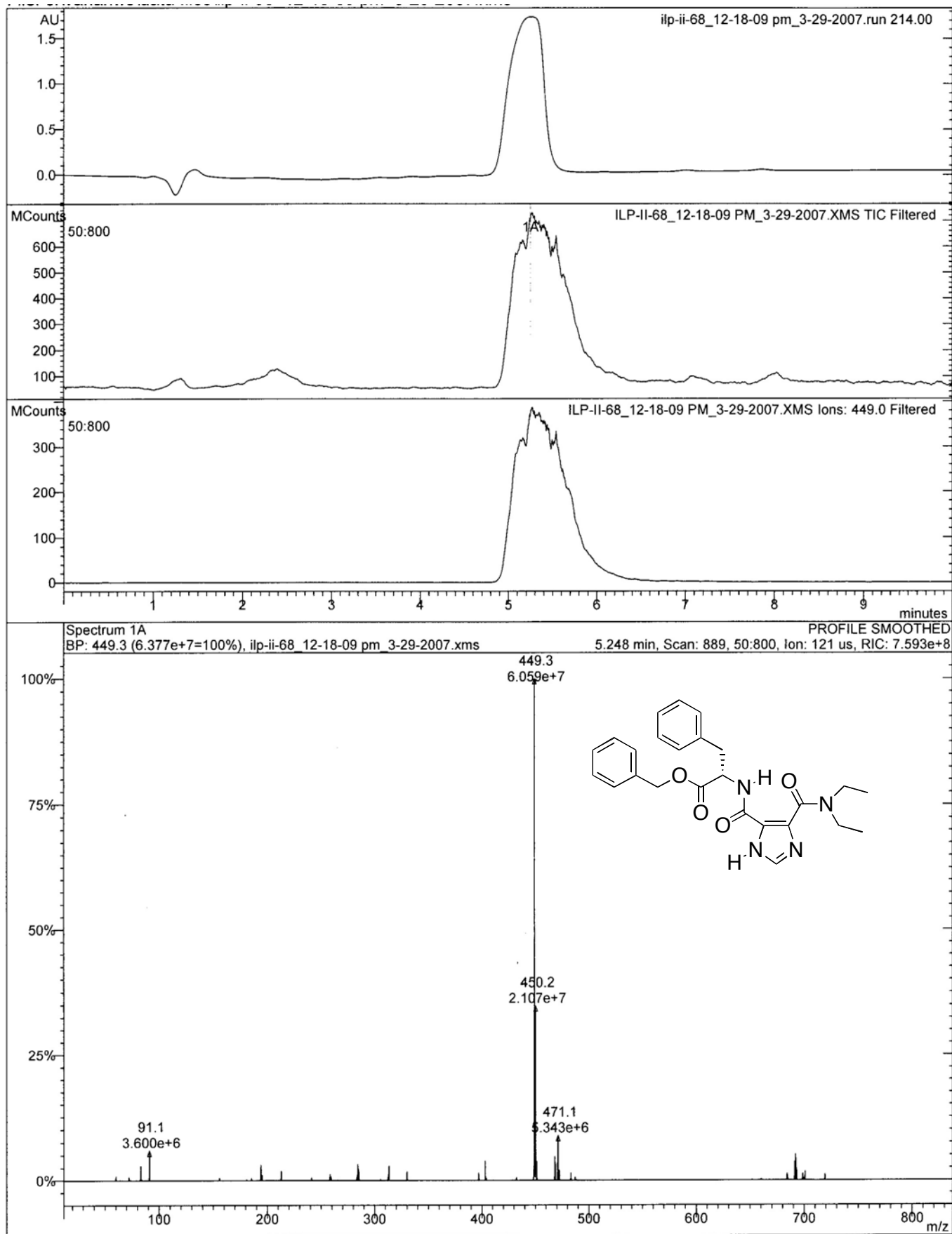


Figure S108. LC/MS data for 5{108}.

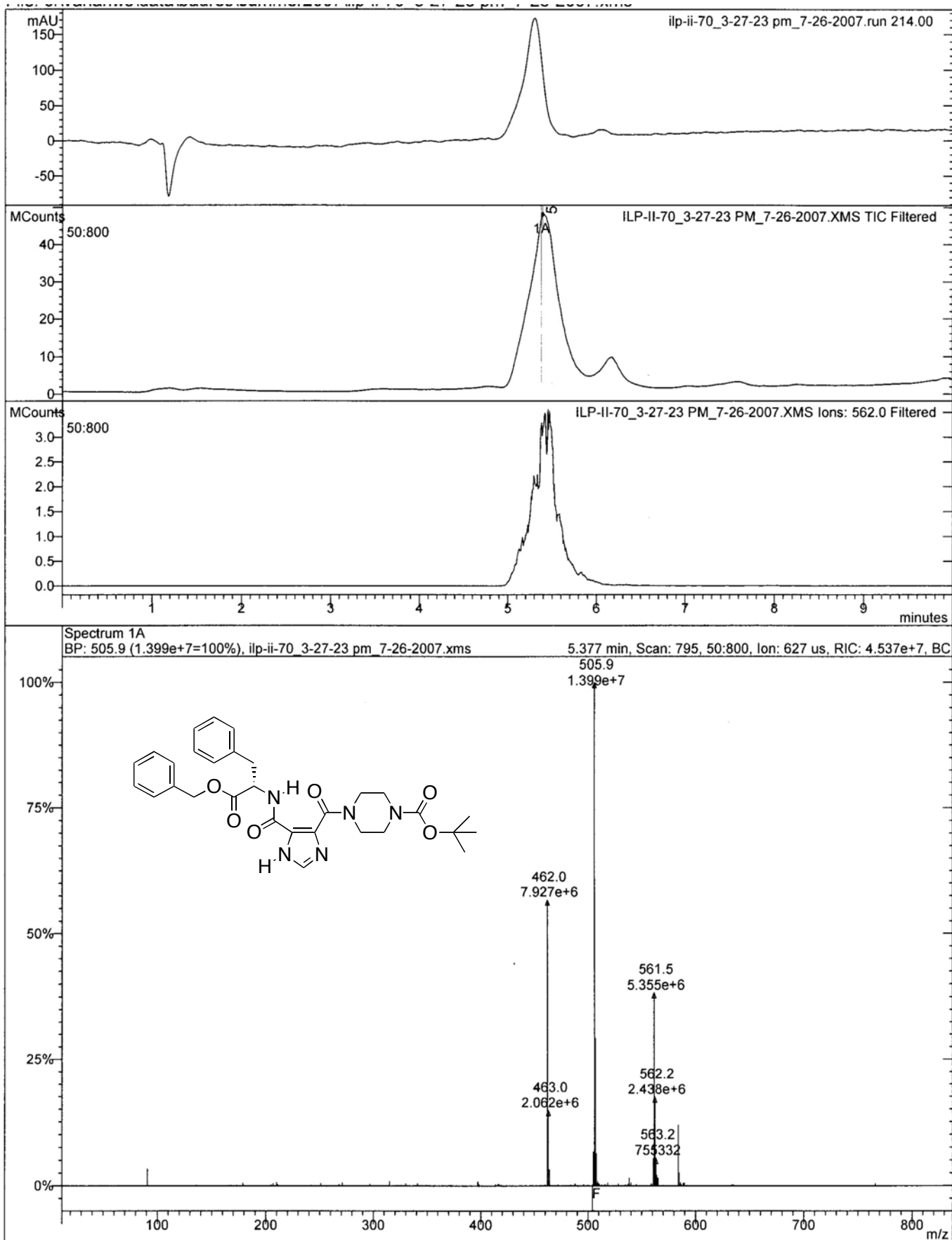


Figure S109. LC/MS data for 5{109}.

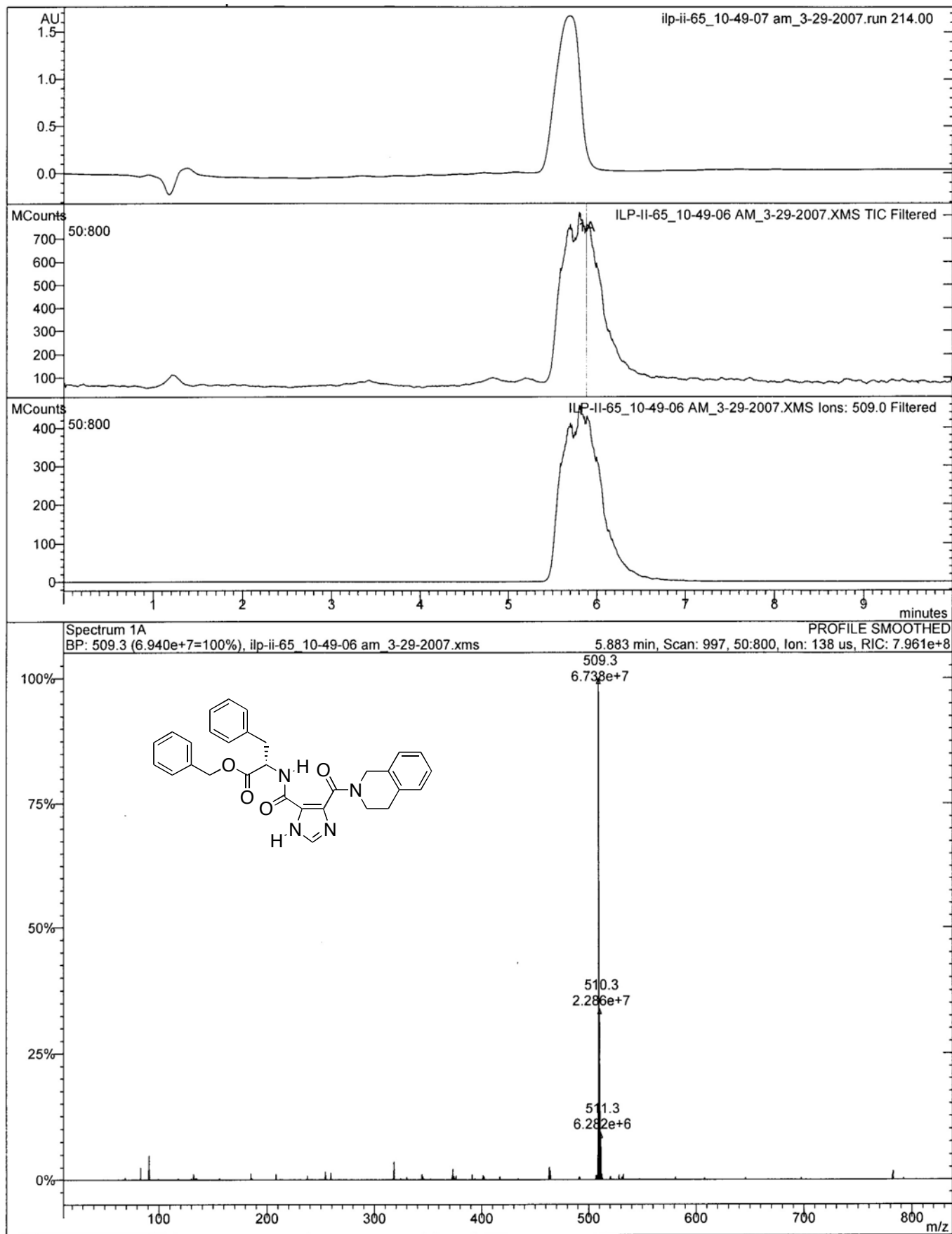


Figure S110. LC/MS data for 5{110}.

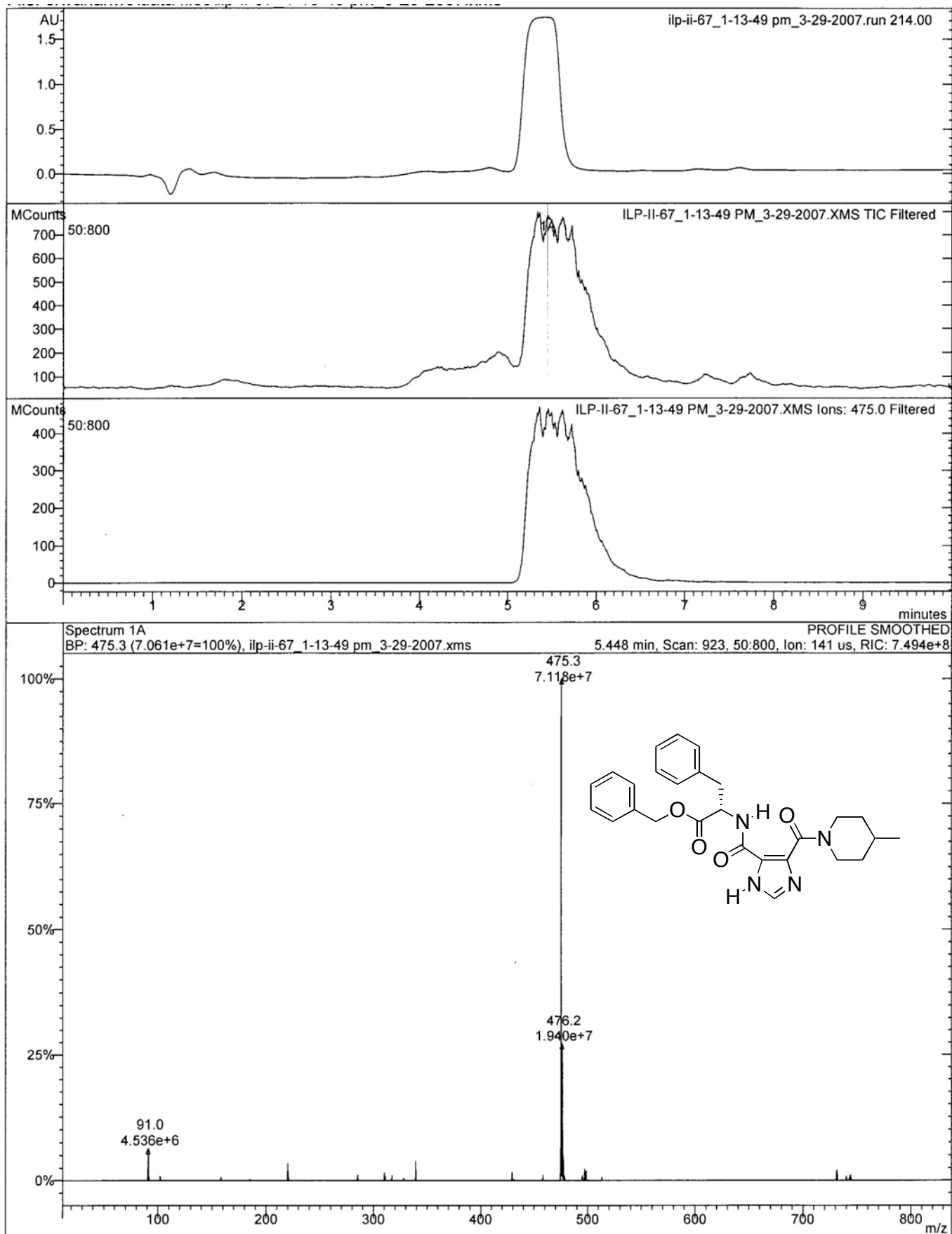


Figure S111. LC/MS data for 5{111}.

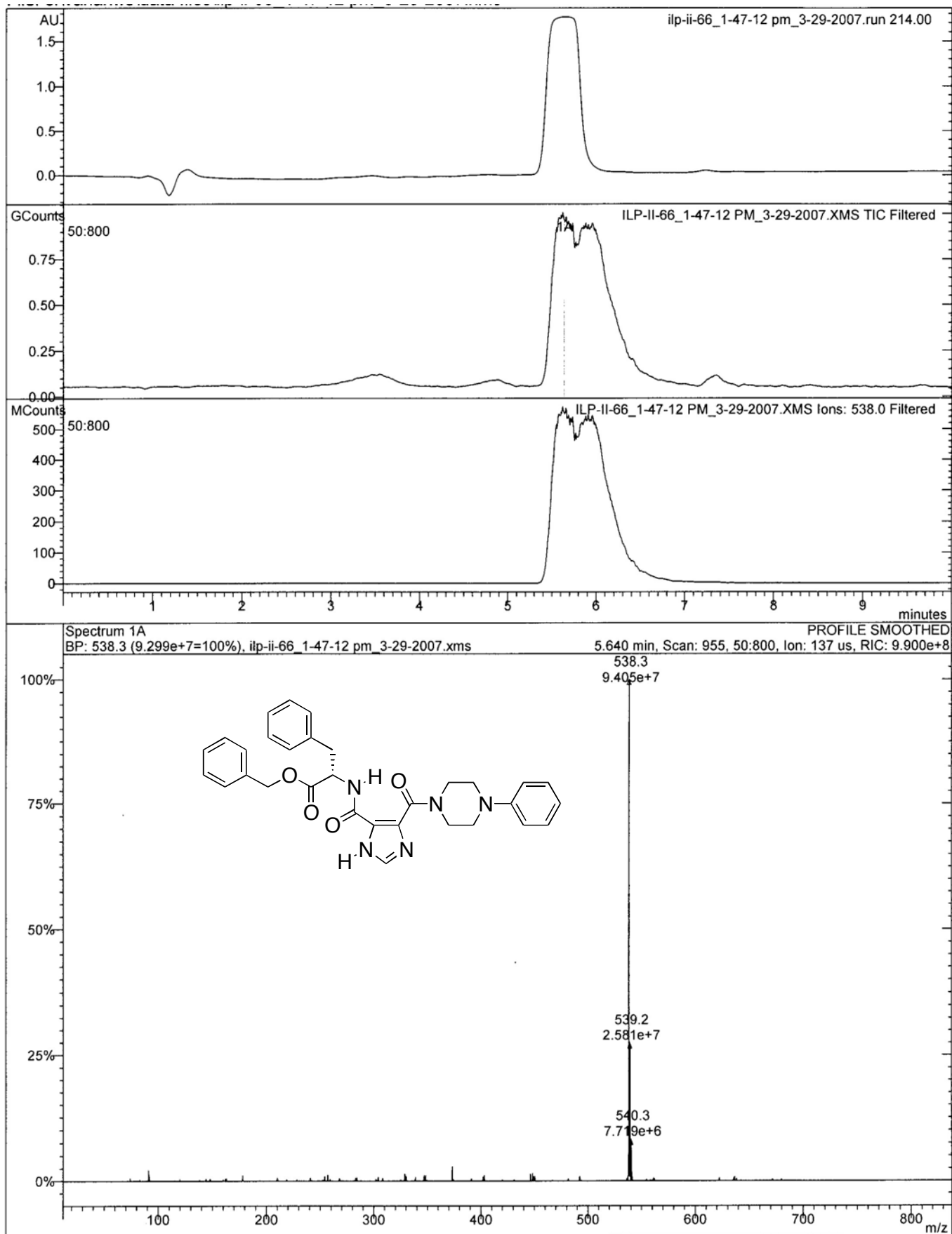


Figure S112. LC/MS data for **5{112}**.

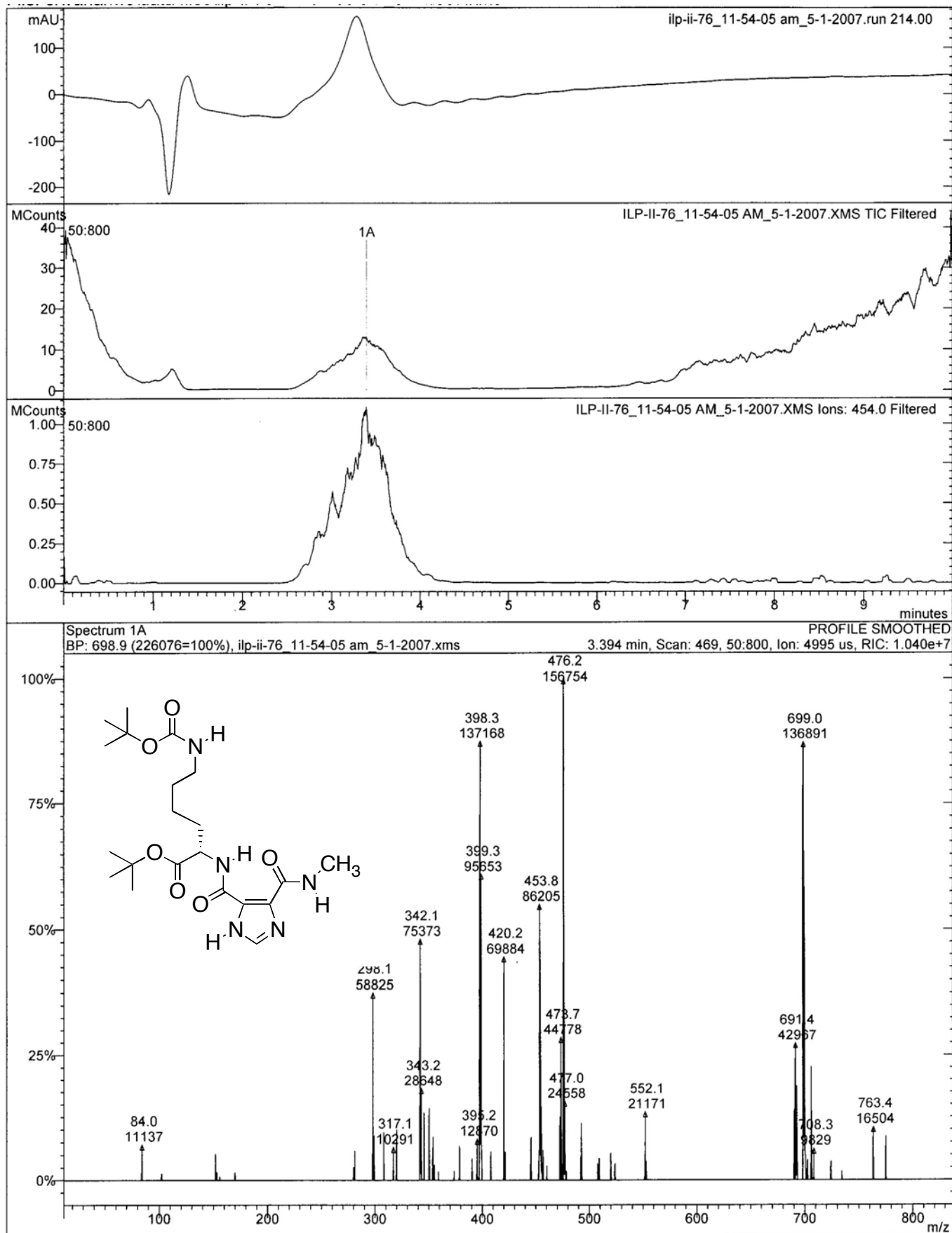


Figure S113. LC/MS data for 5{113}.

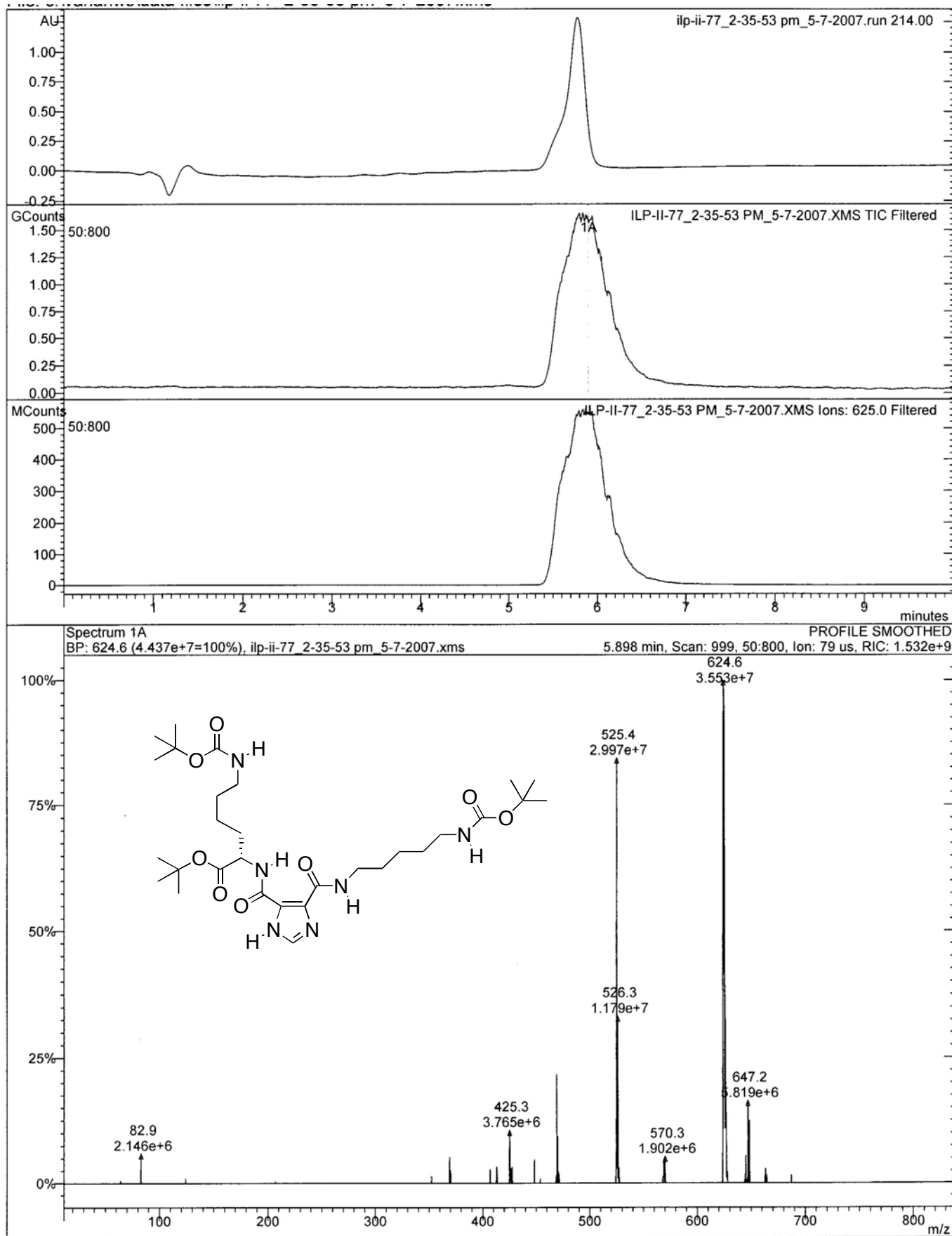


Figure S114. LC/MS data for **5{114}**.

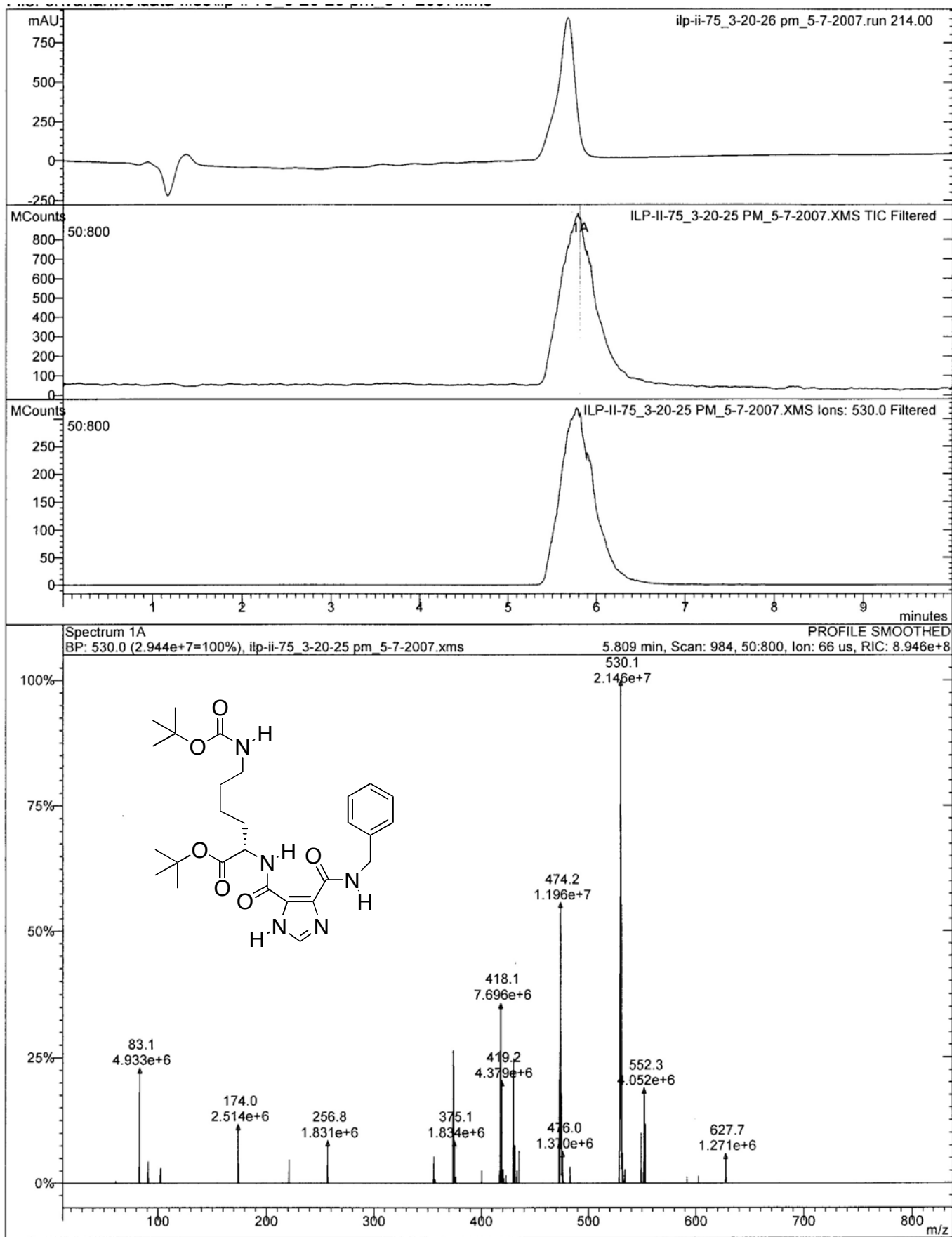


Figure S115. LC/MS data for 5{115}.

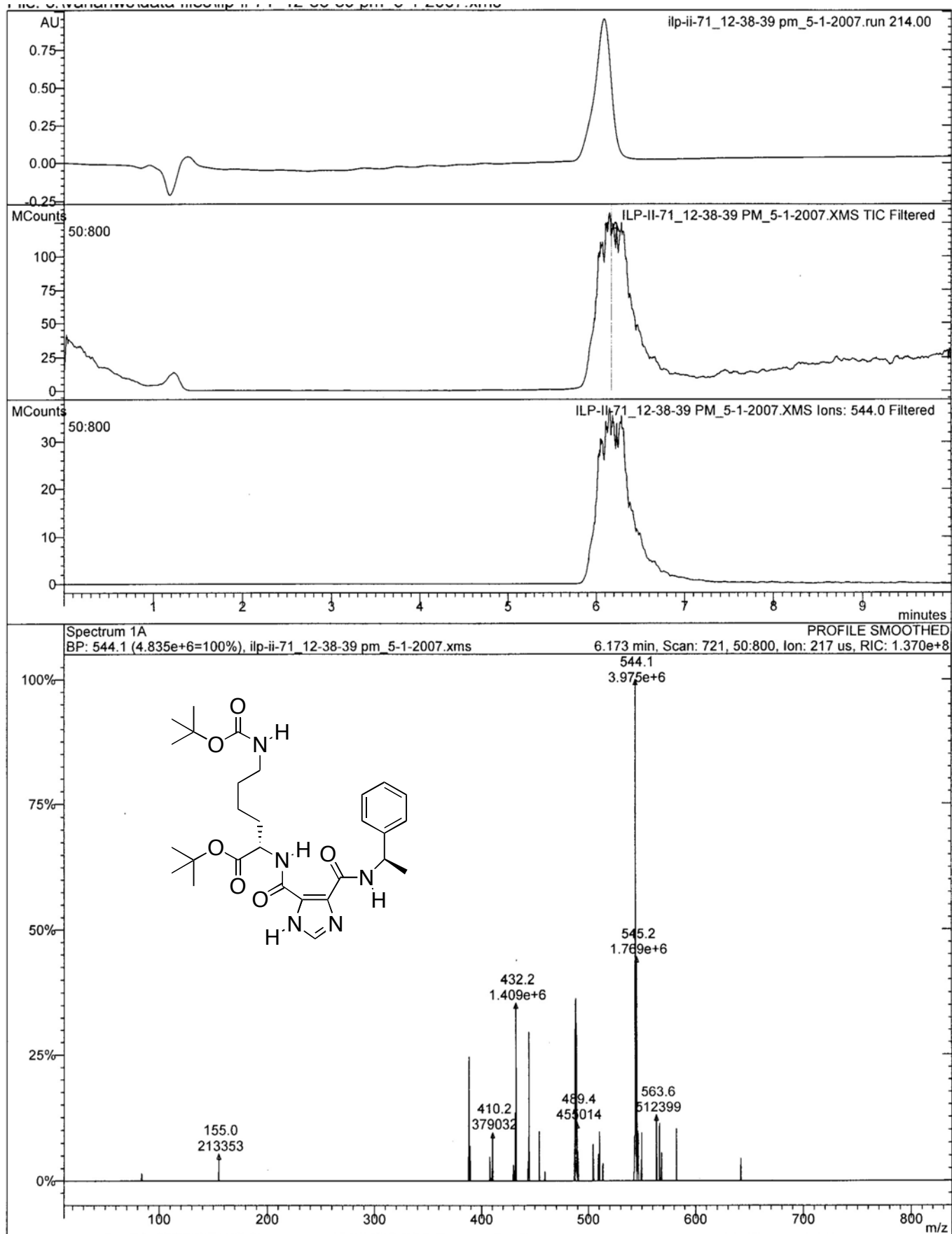


Figure S116. LC/MS data for 5{116}.

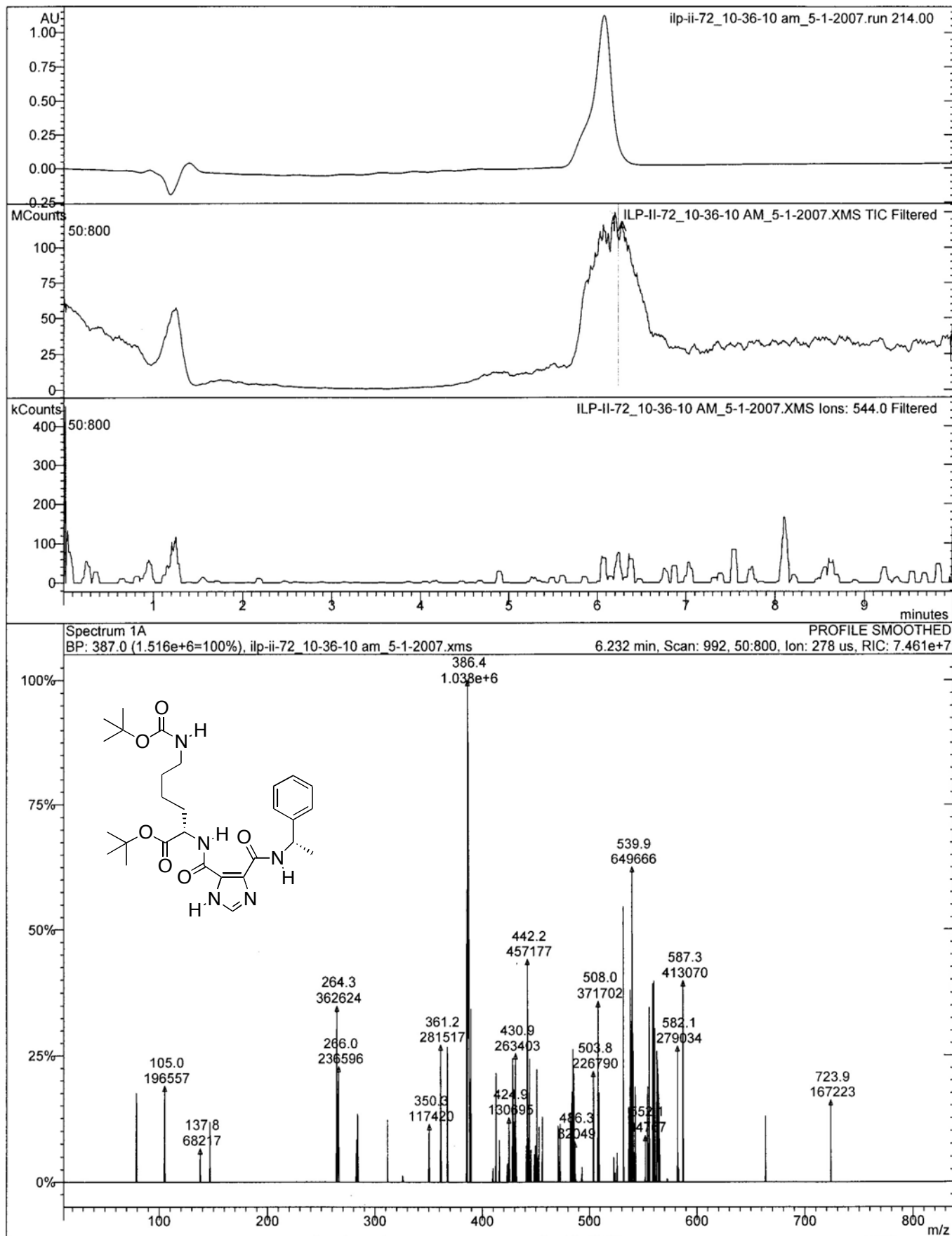


Figure S117. LC/MS data for 5{117}.

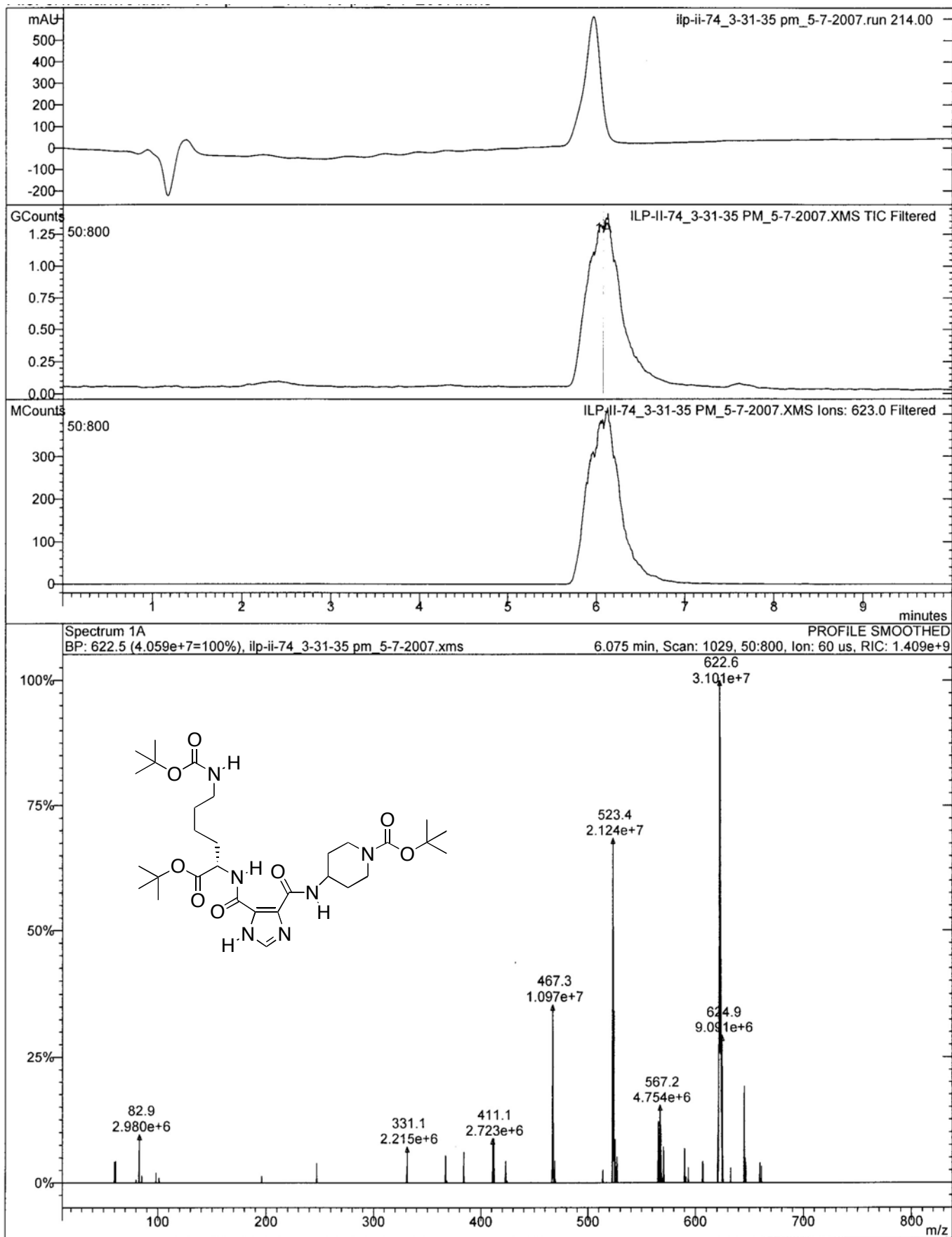


Figure S118. LC/MS data for 5{118}.

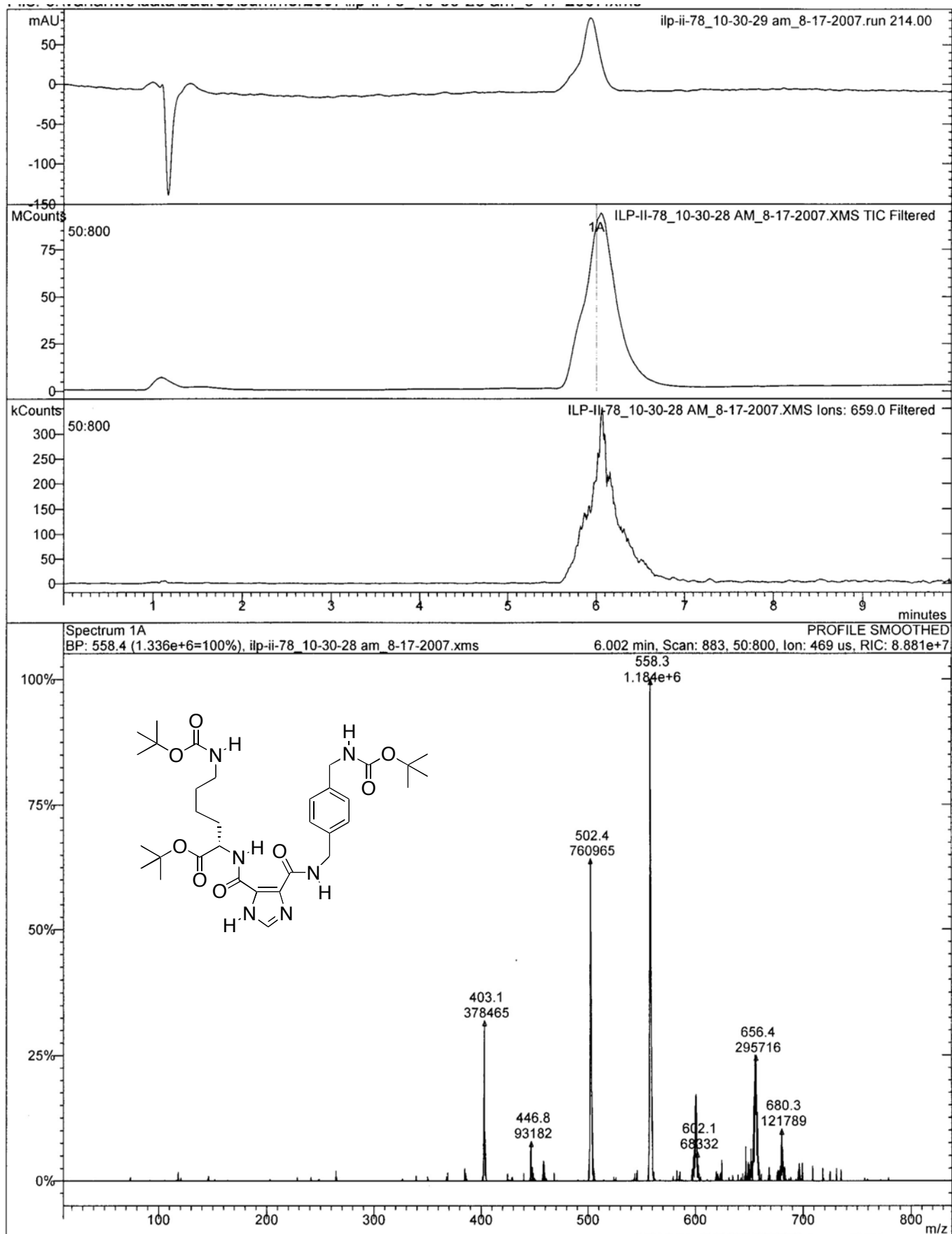


Figure S119. LC/MS data for 5{119}.

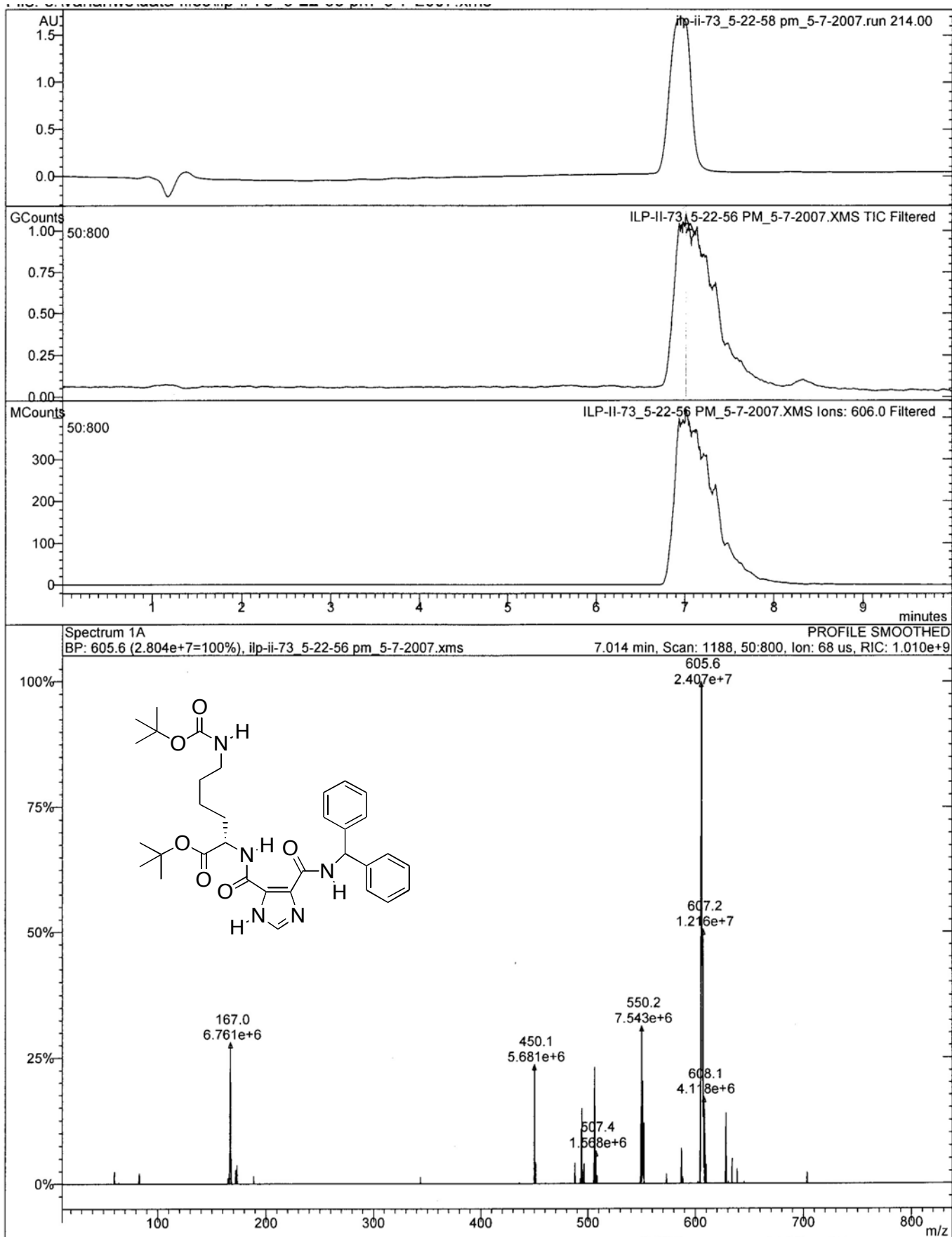


Figure S120. LC/MS data for 5{120}.

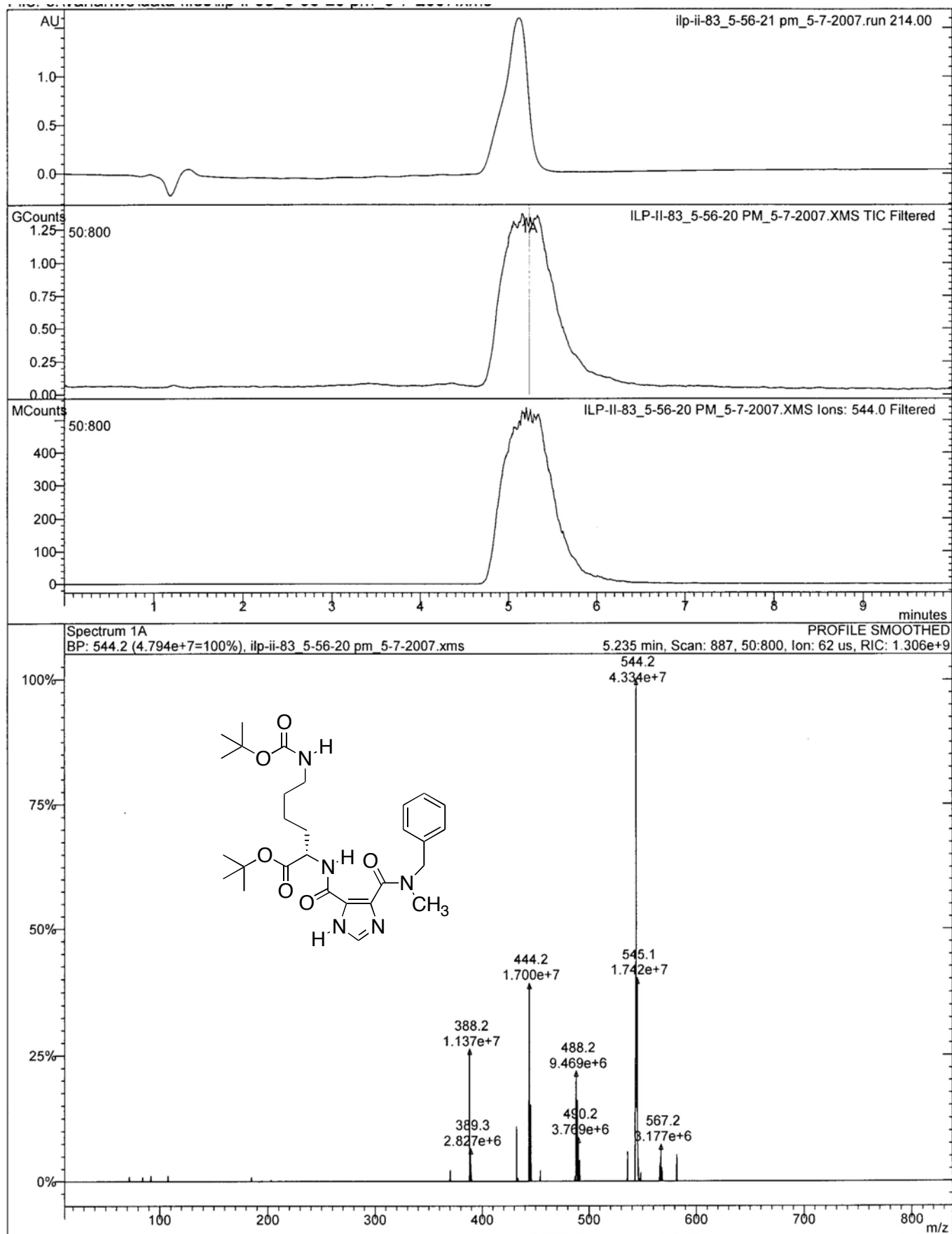


Figure S121. LC/MS data for 5{121}.

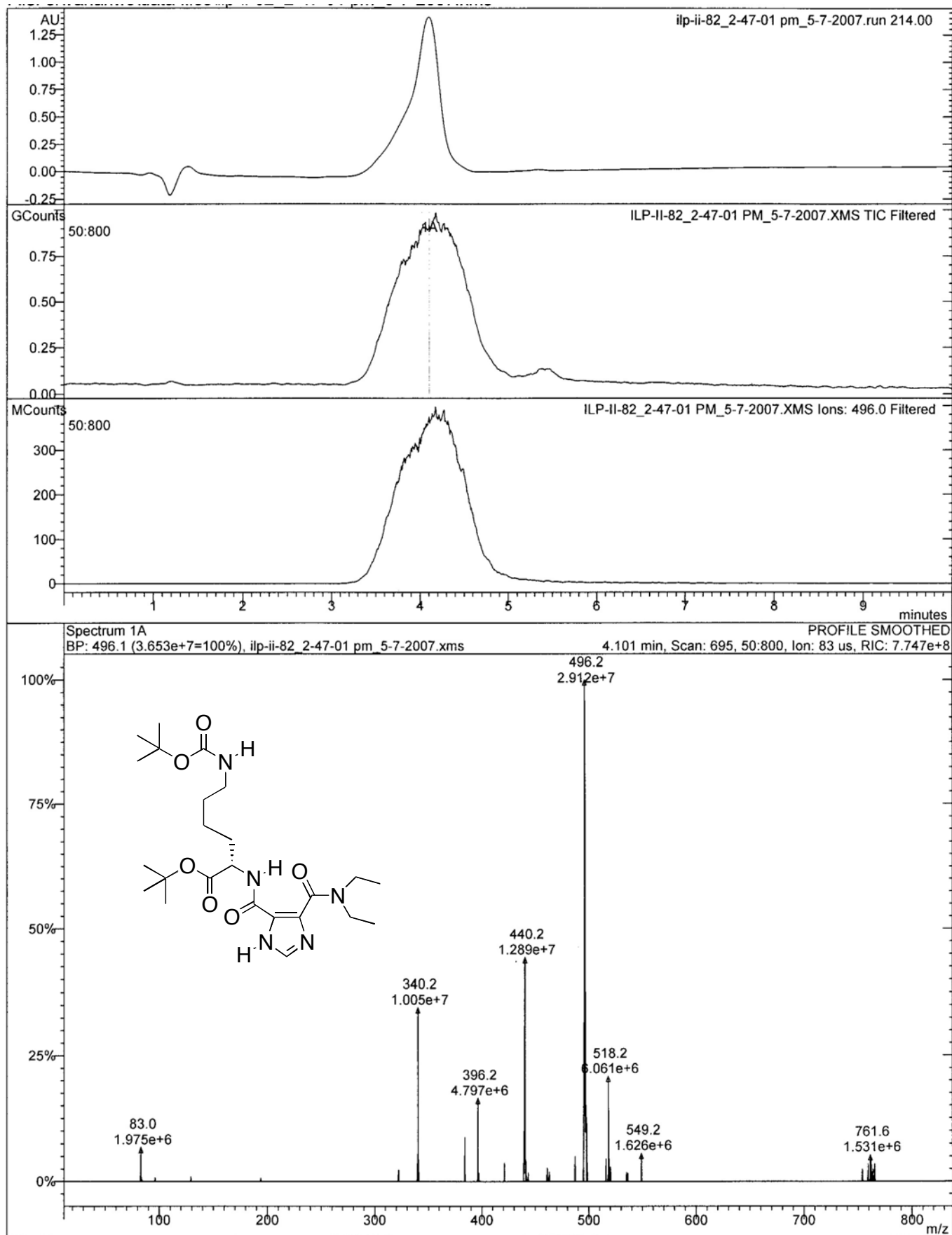


Figure S122. LC/MS data for 5{122}.

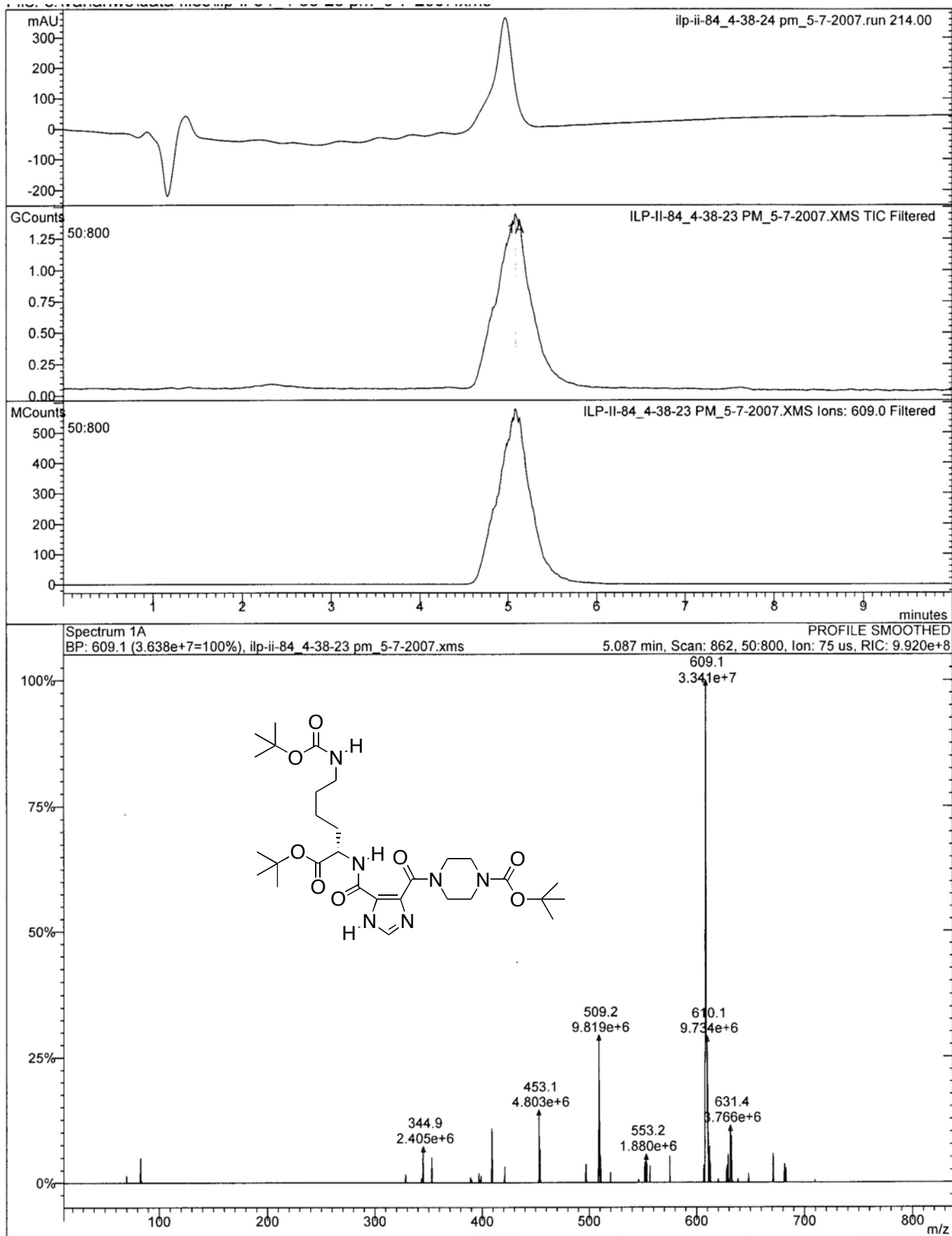


Figure S123. LC/MS data for 5{123}.

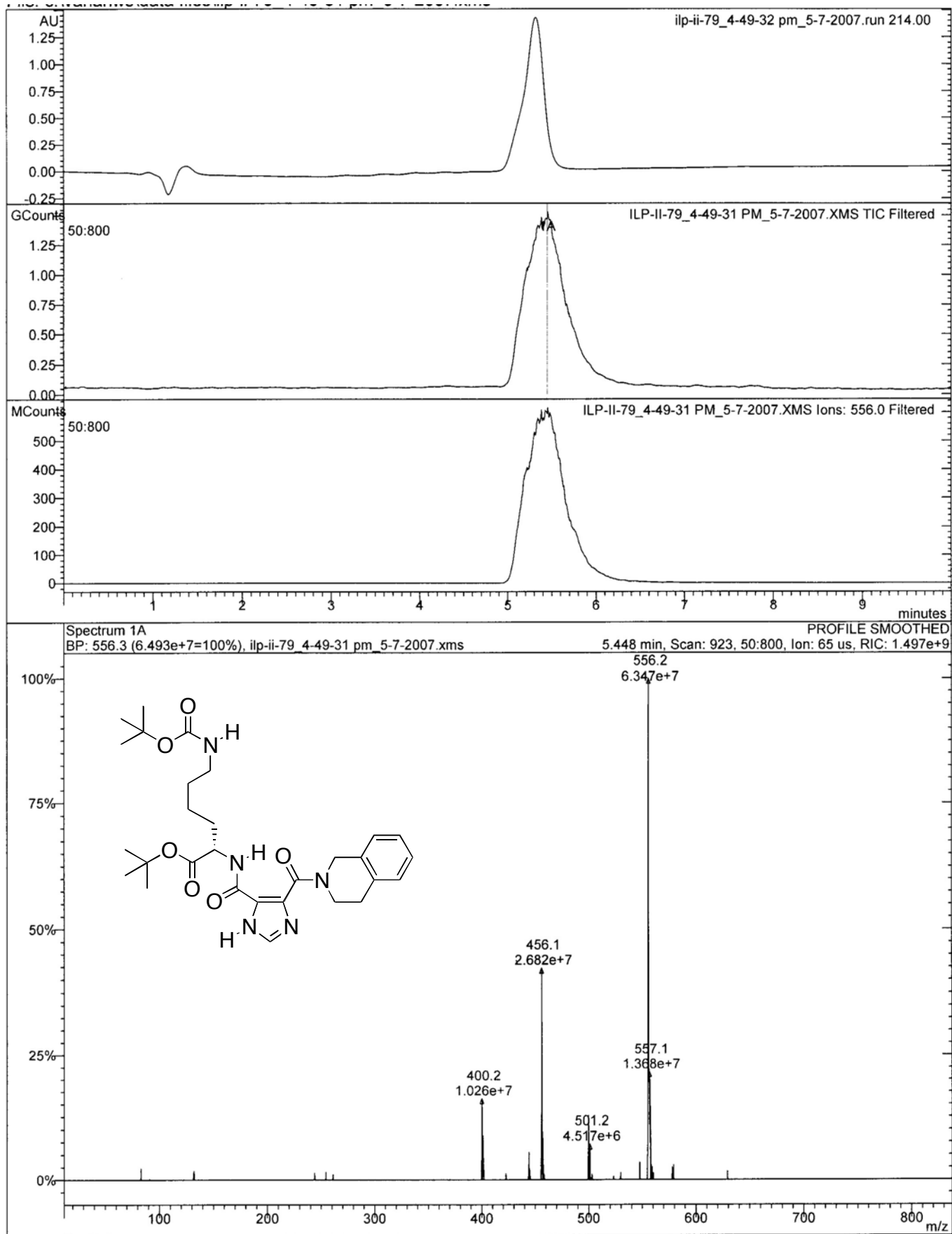


Figure S124. LC/MS data for 5{124}.

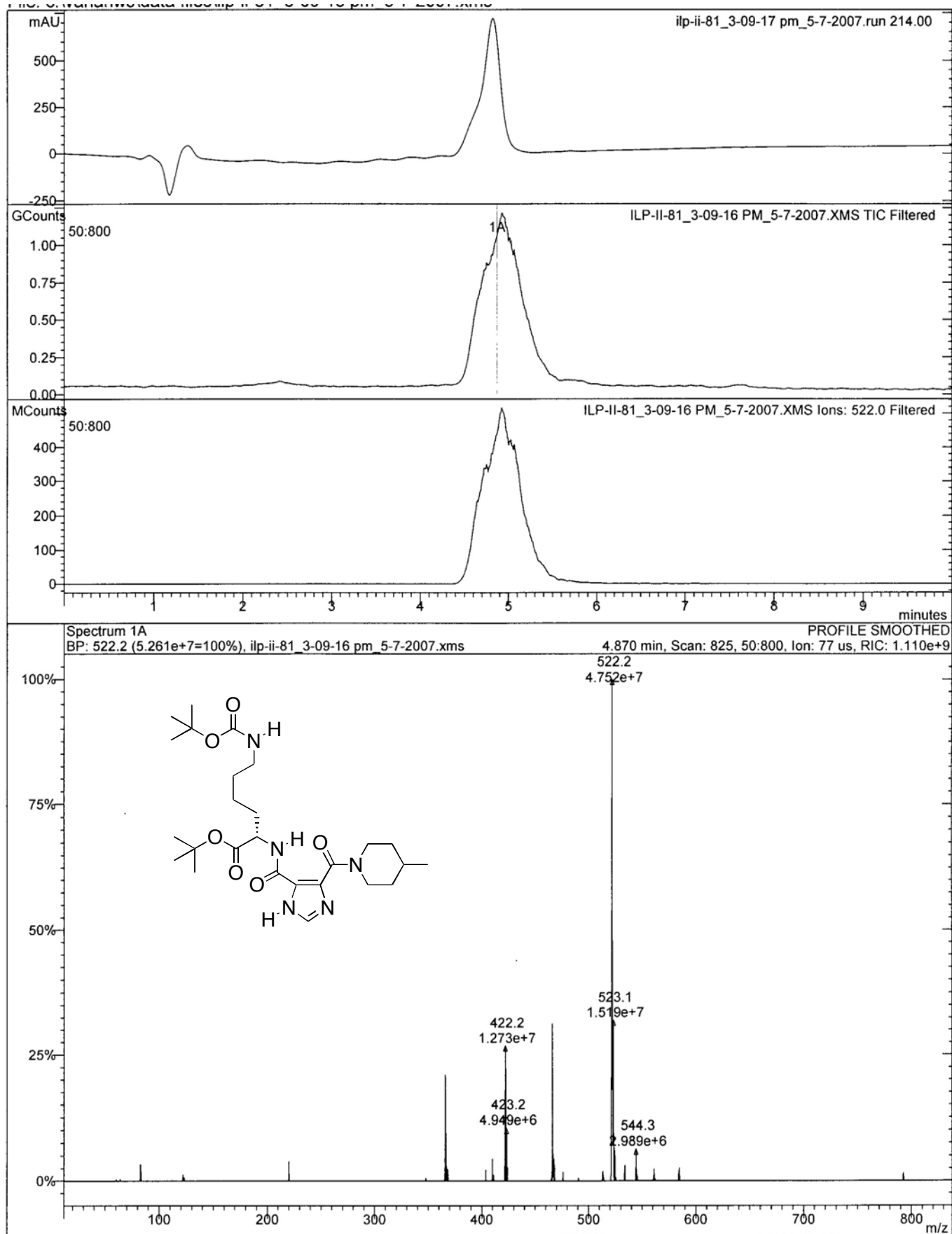


Figure S125. LC/MS data for 5{125}.

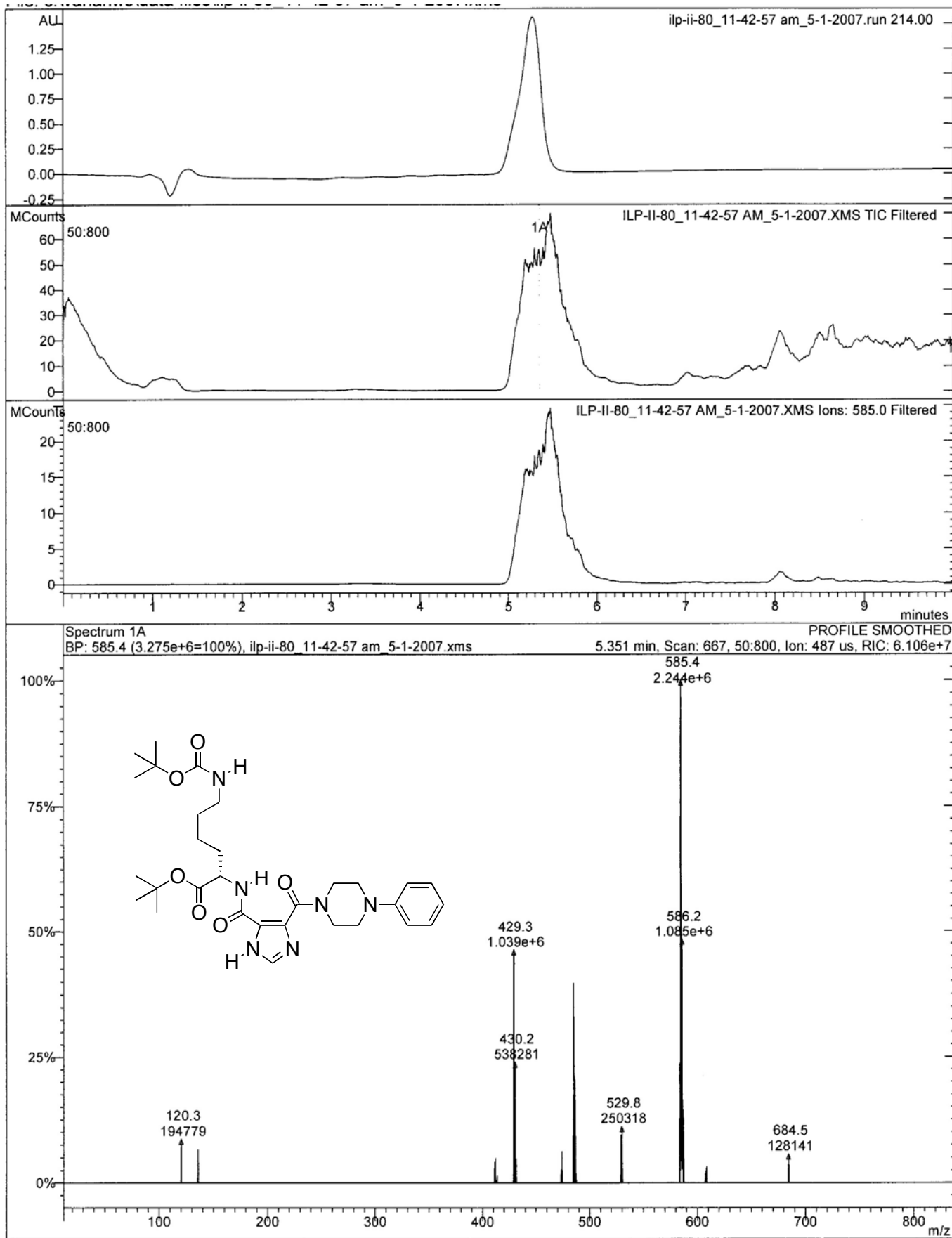


Figure S126. LC/MS data for 5{126}.

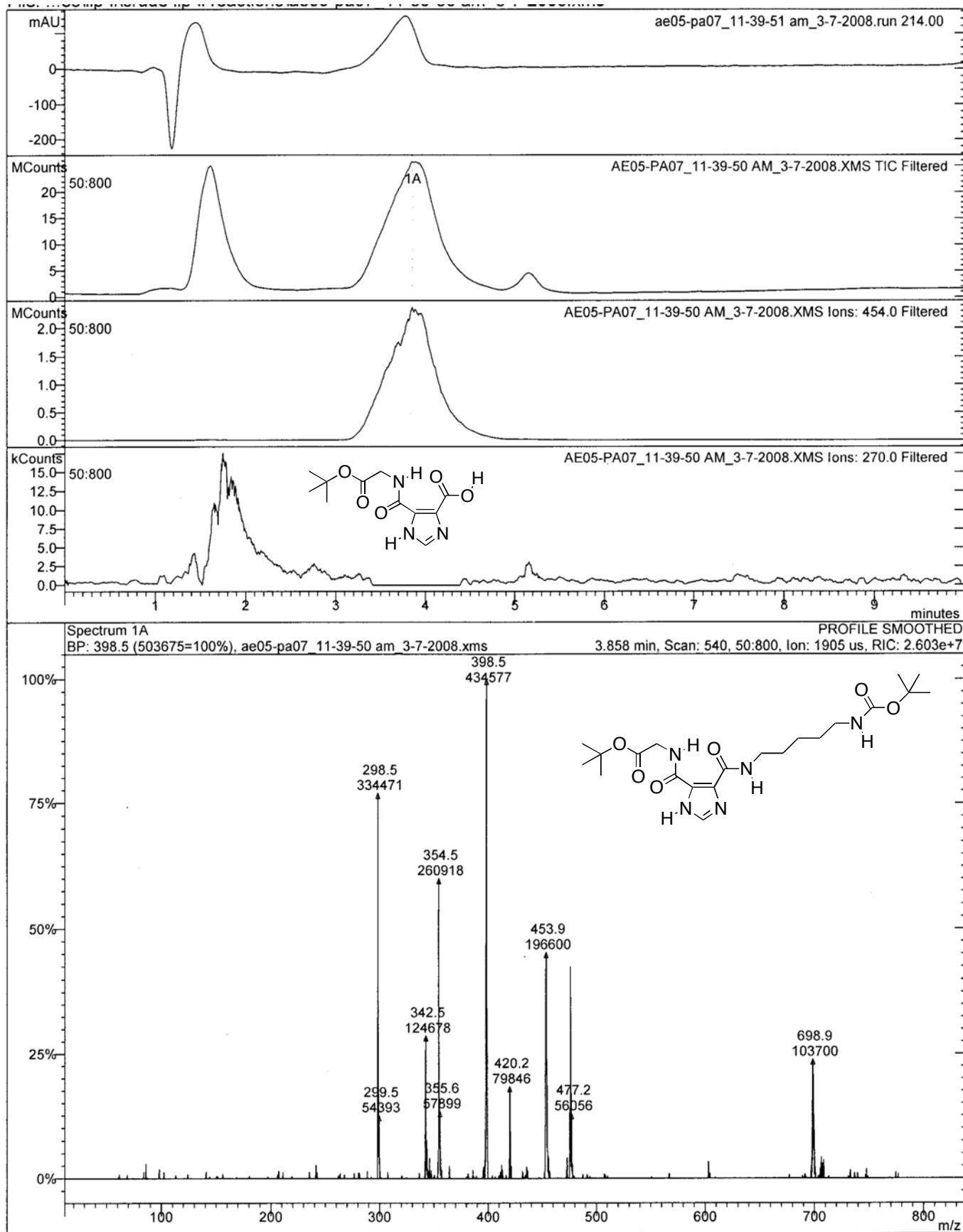


Figure S127. LC/MS data for the crude reaction to yield 5{2}.

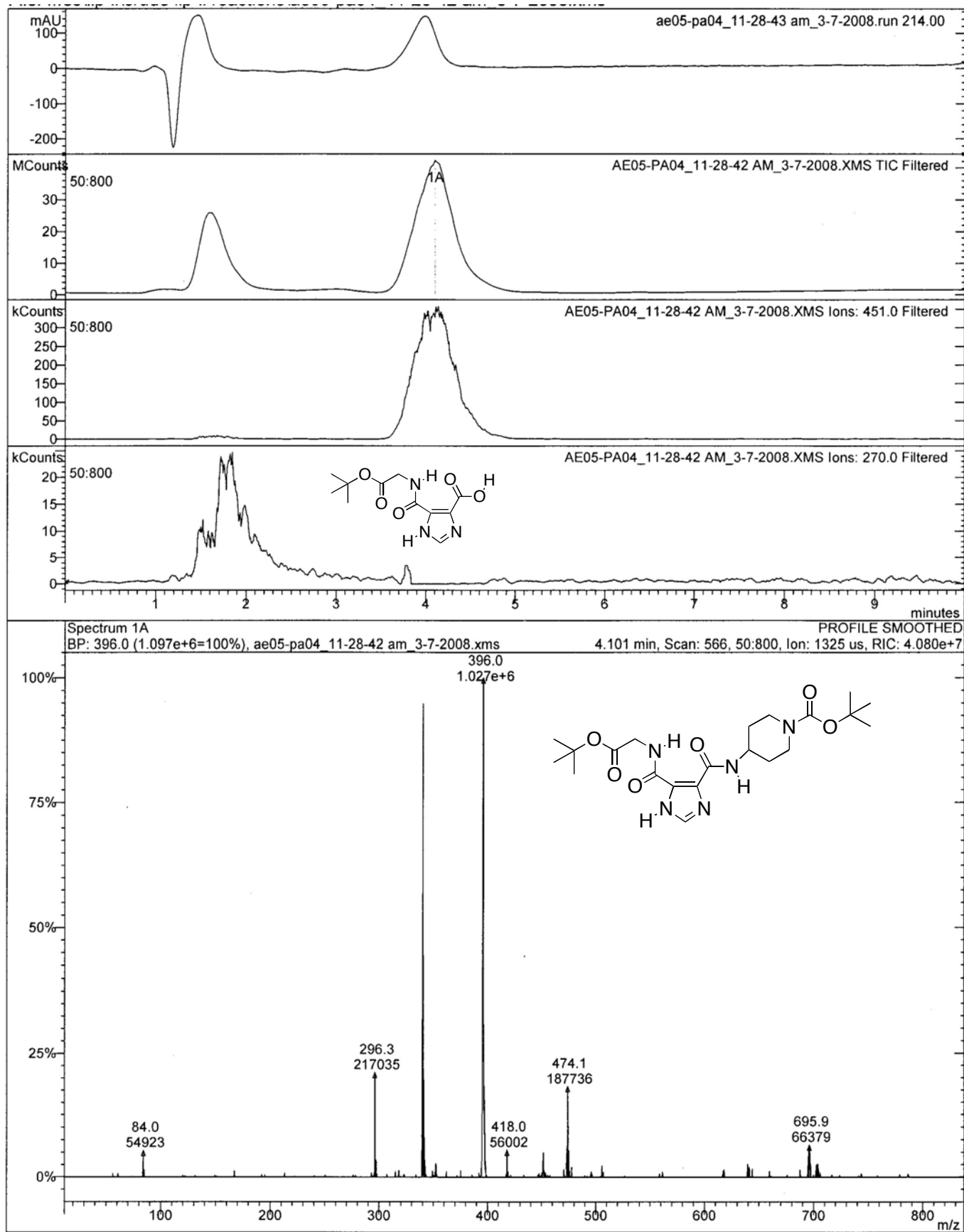


Figure S128. LC/MS data for the crude reaction to yield 5{6}.

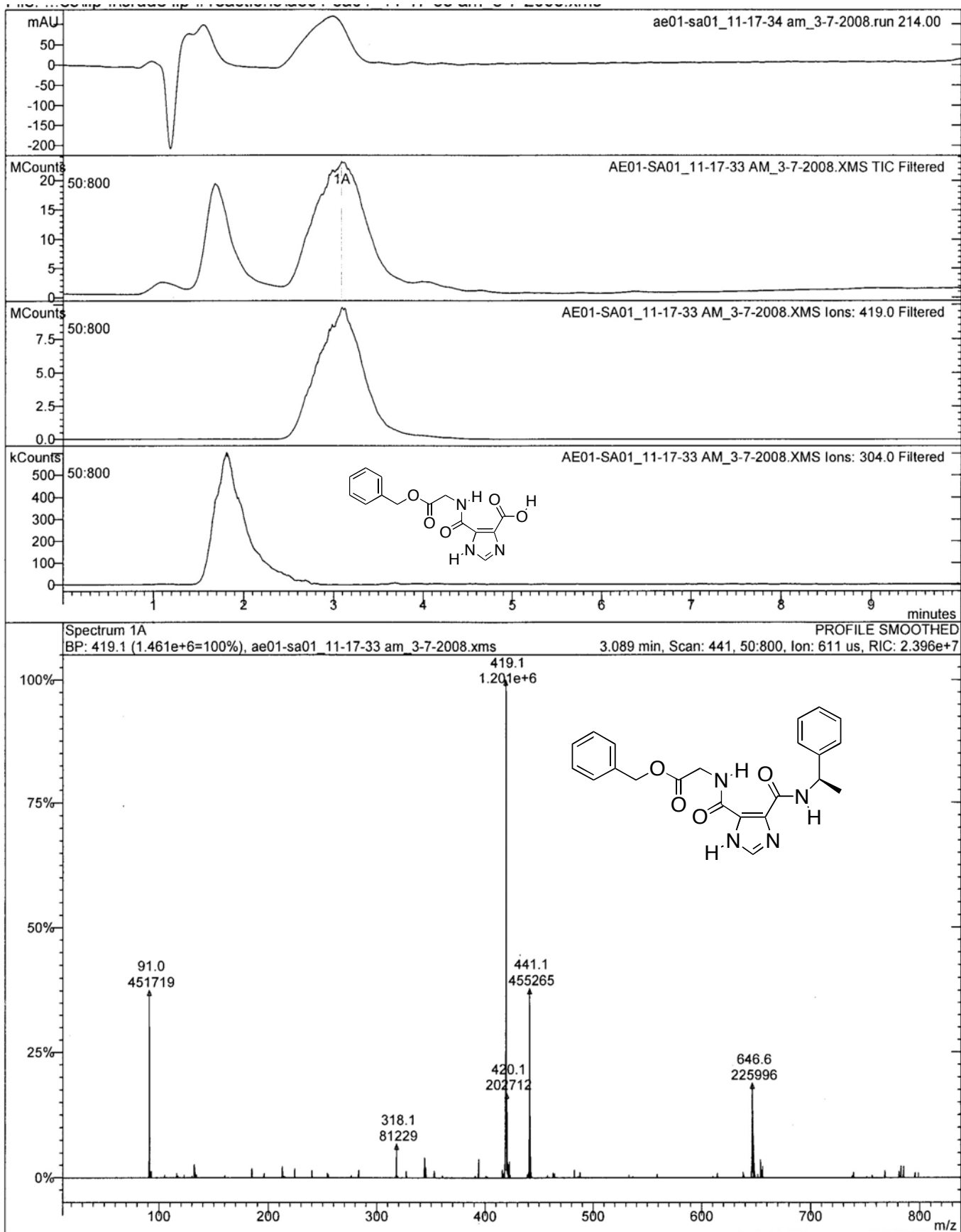


Figure S129. LC/MS data for the crude reaction to yield 5{26}.

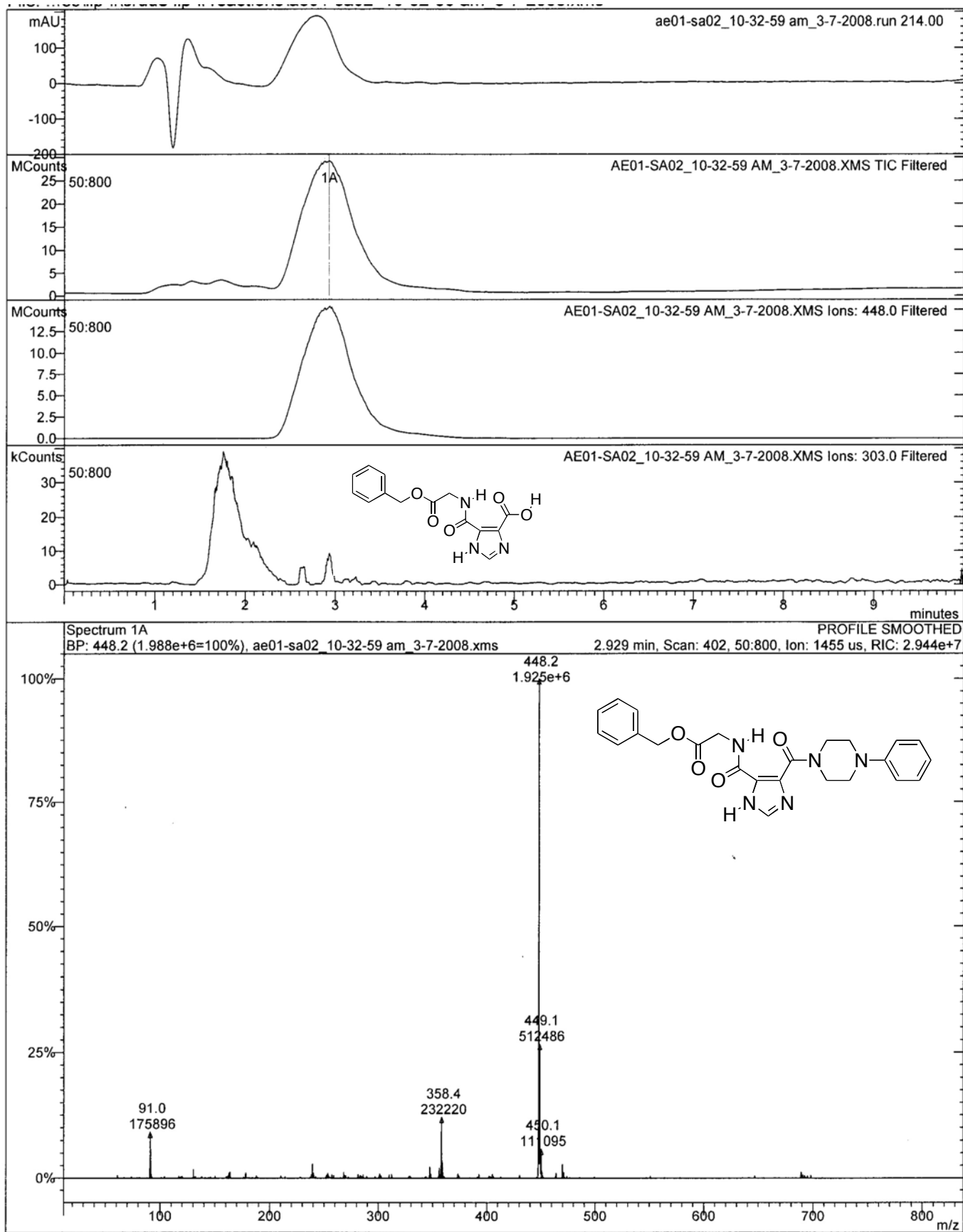


Figure S130. LC/MS data for the crude reaction to yield 5{28}.

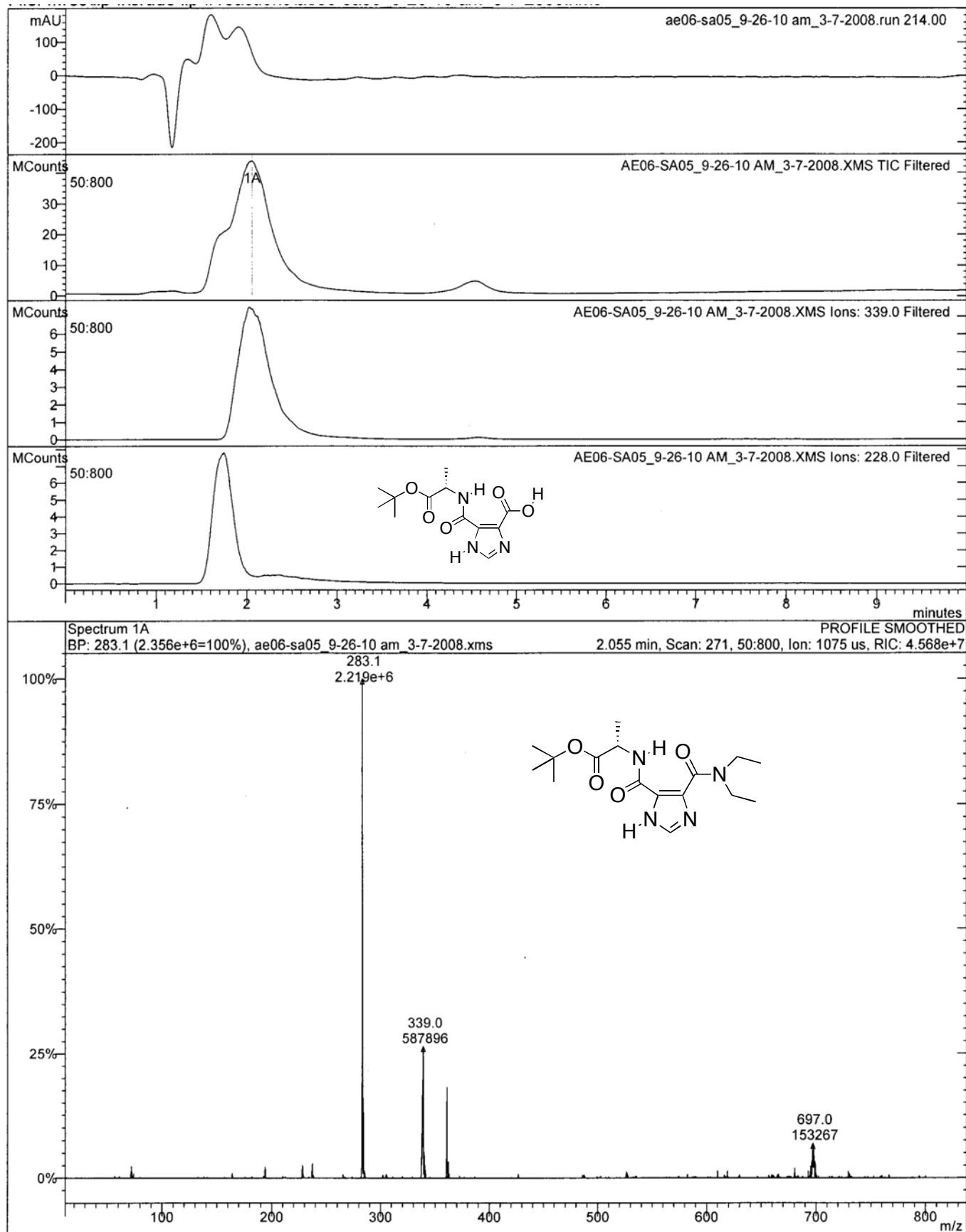


Figure S131. LC/MS data for the crude reaction to yield 5{38}.

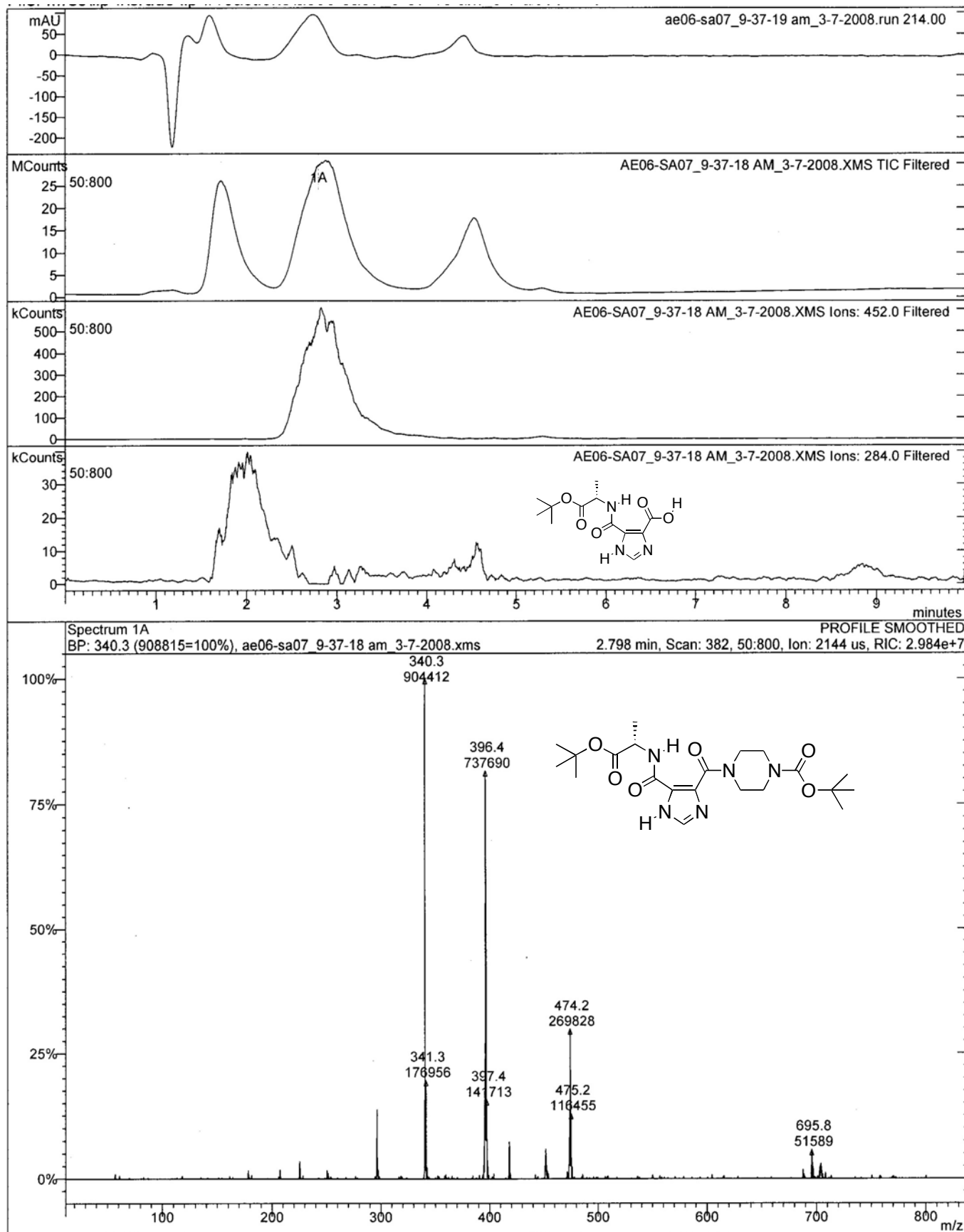


Figure S132. LC/MS data for the crude reaction to yield 5{39}.

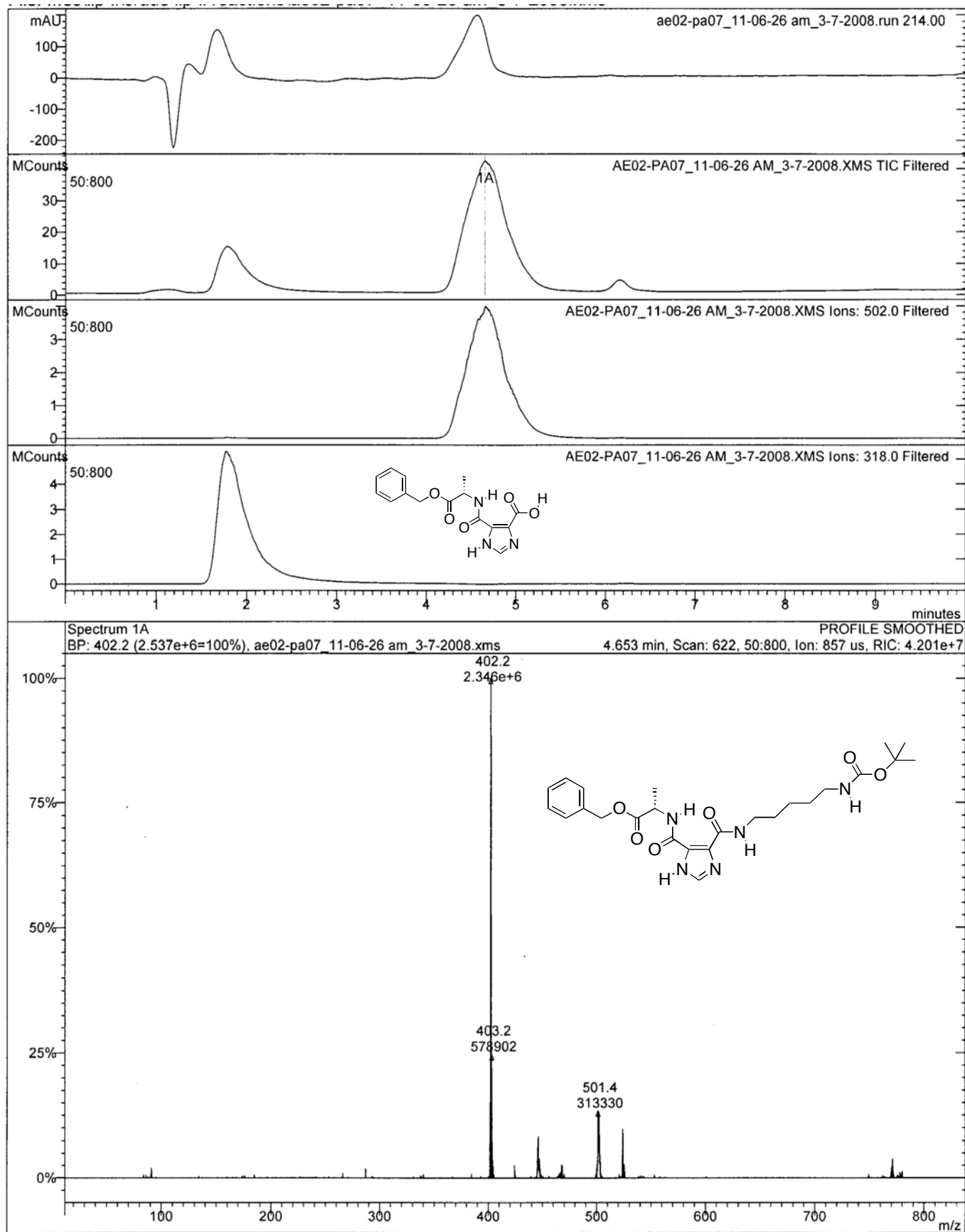


Figure S133. LC/MS data for the crude reaction to yield 5{44}.

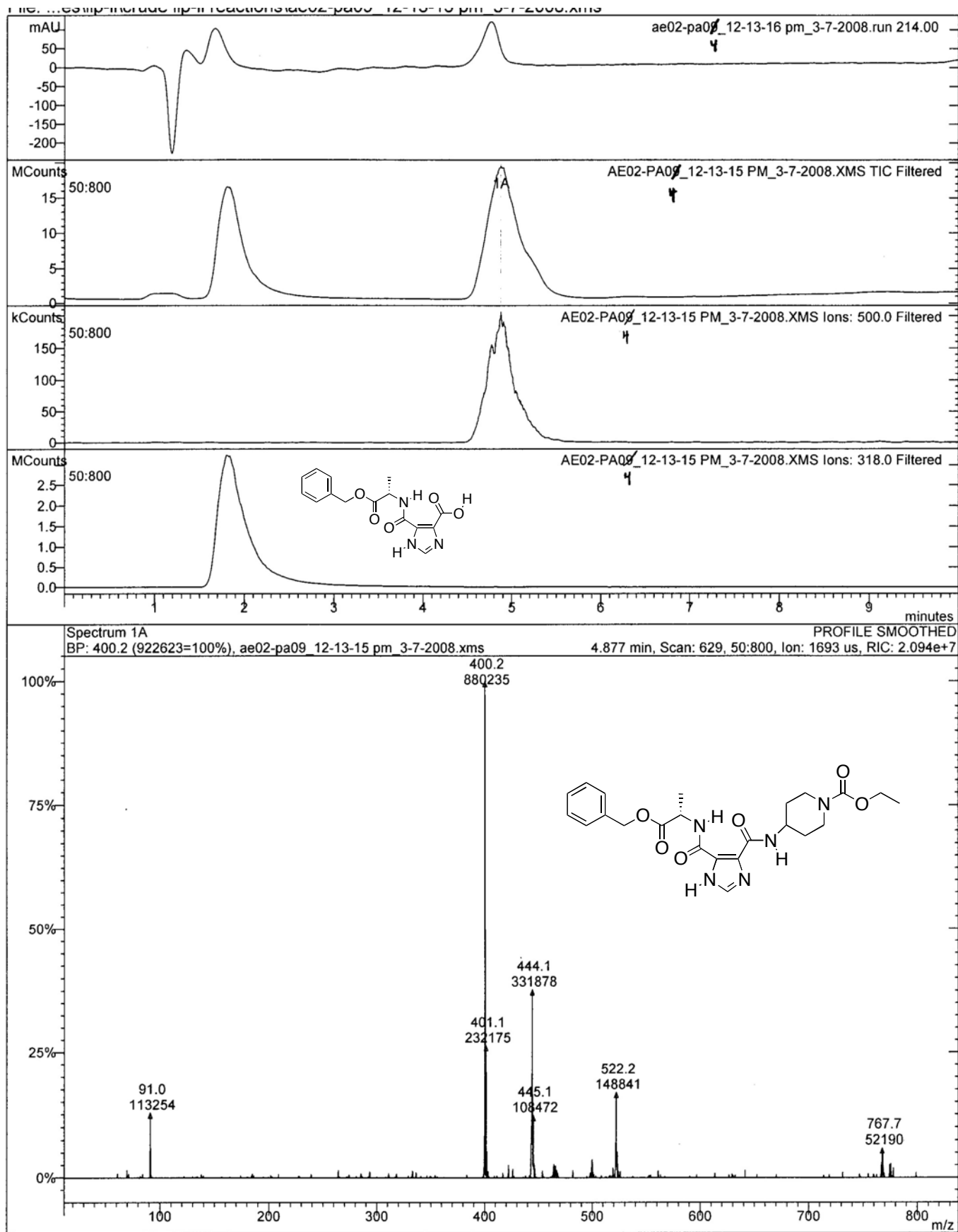


Figure S134. LC/MS data for the crude reaction to yield **5**{48}.

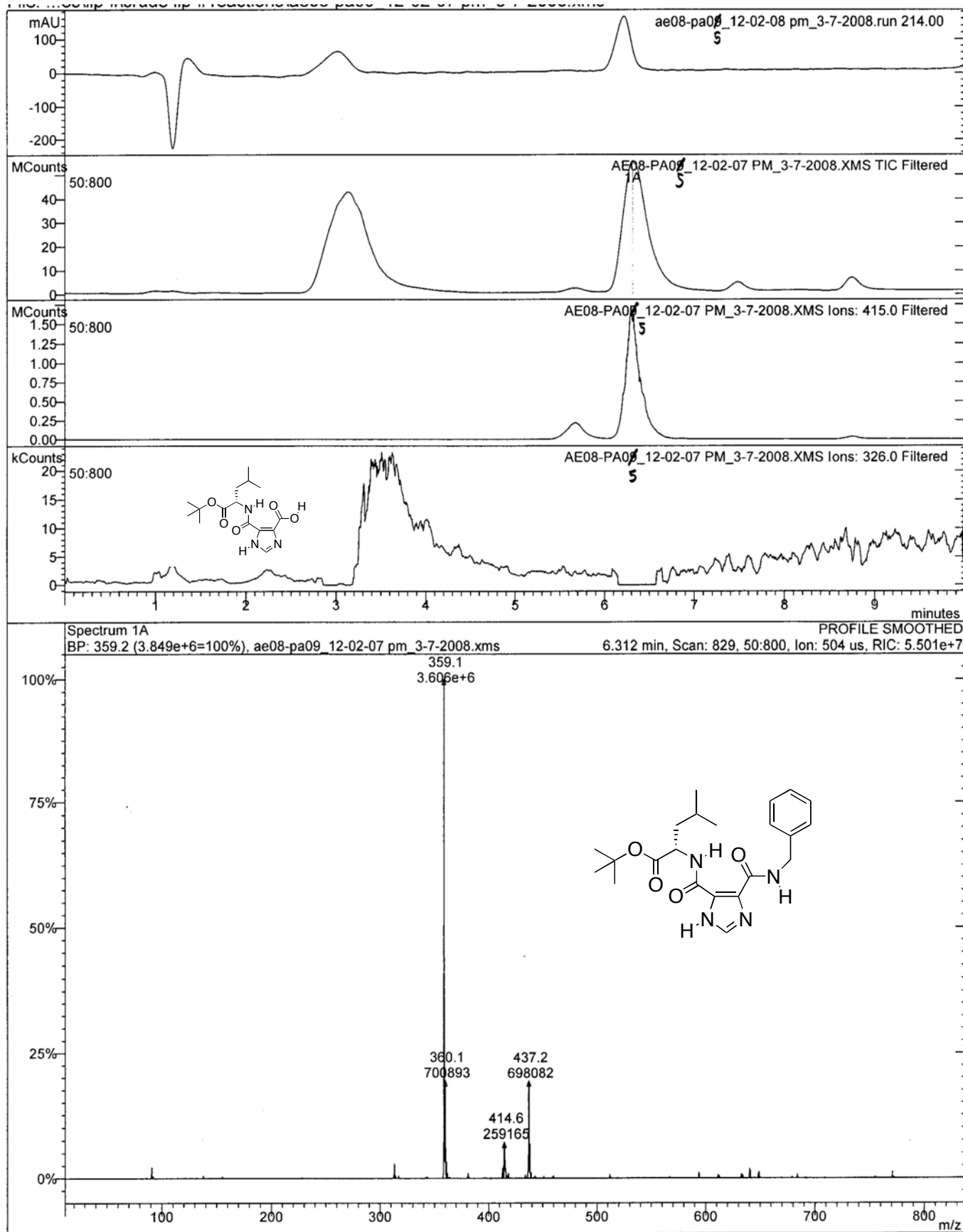


Figure S135. LC/MS data for the crude reaction to yield 5{59}.

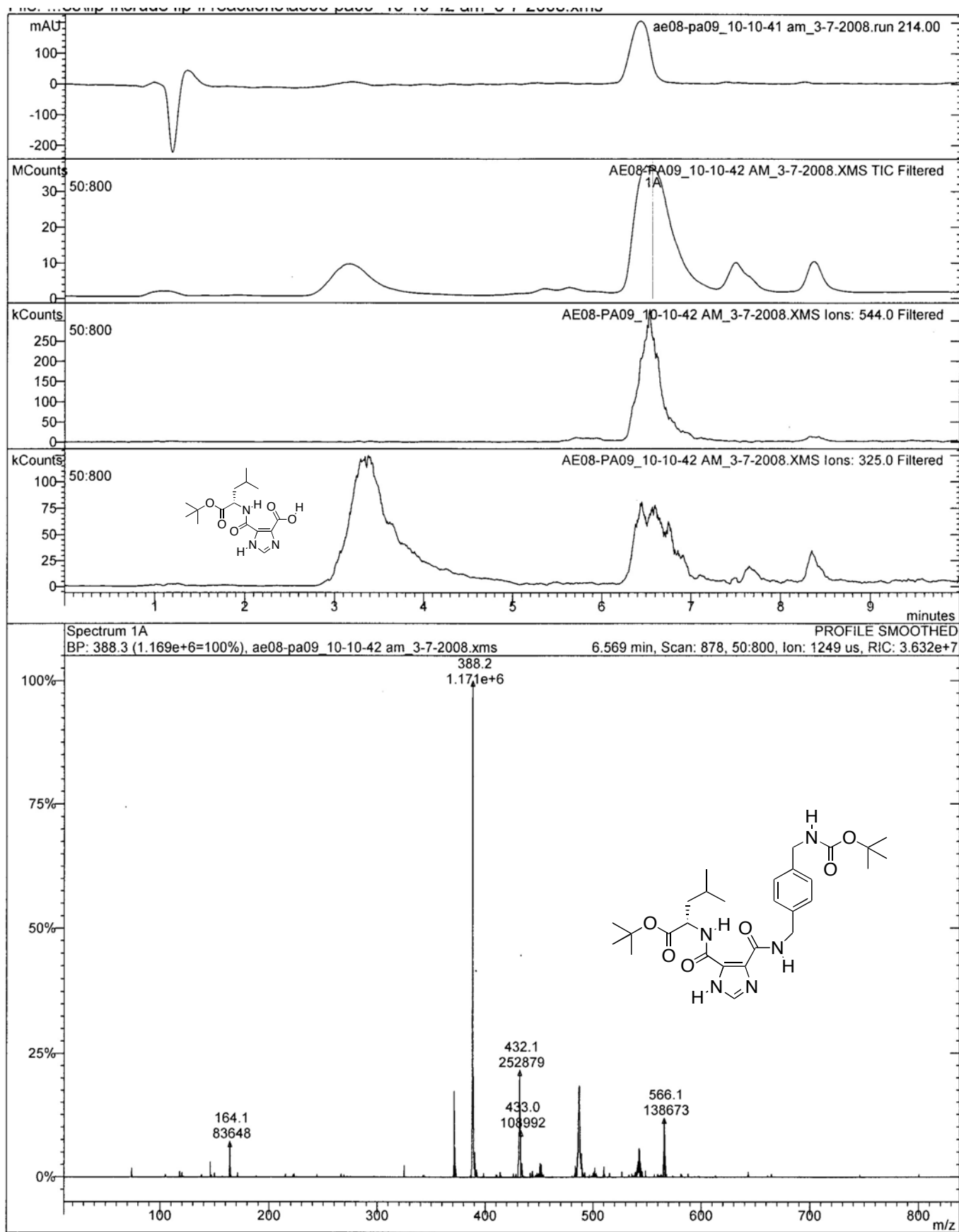


Figure S136. LC/MS data for the crude reaction to yield 5{63}.

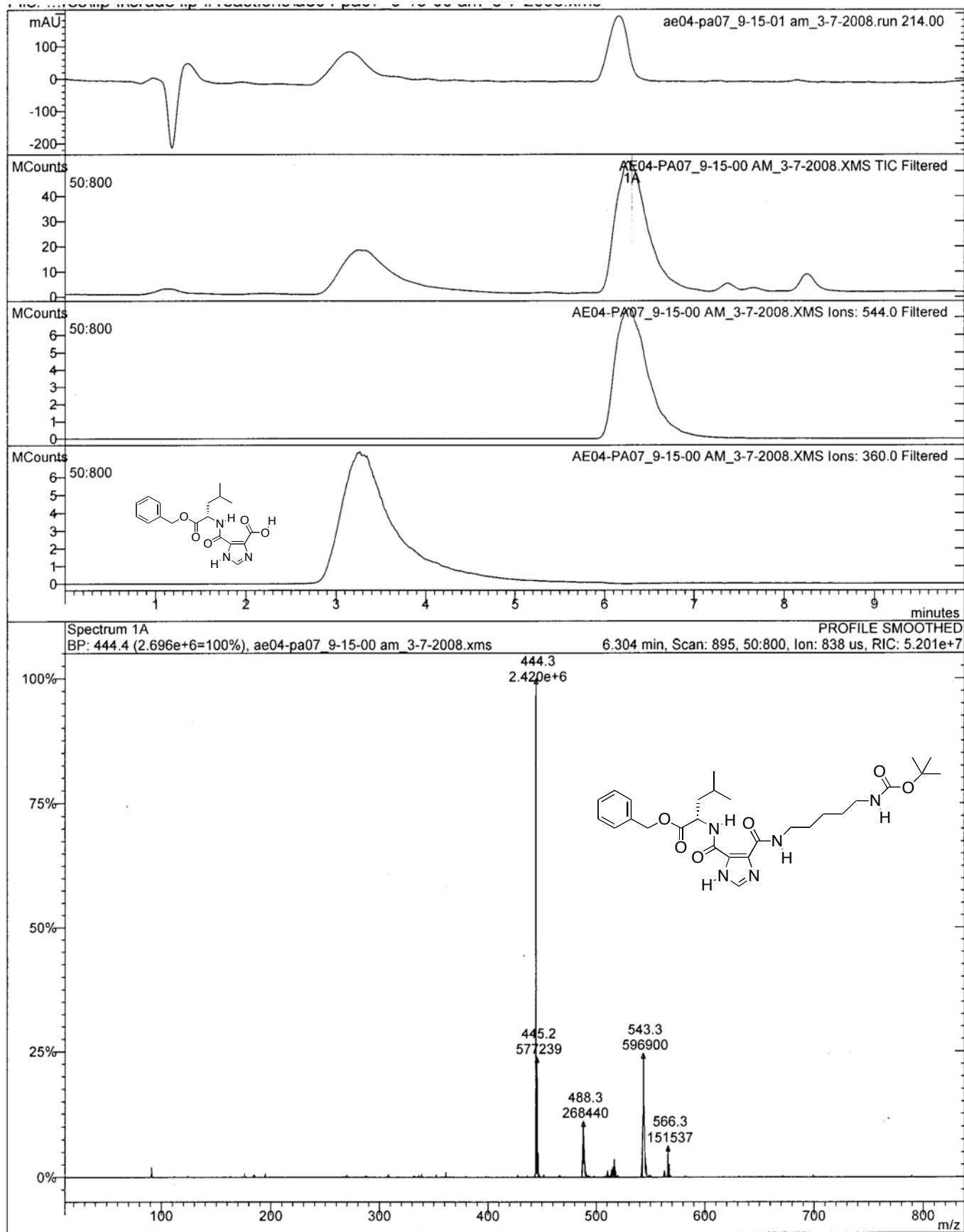


Figure S137. LC/MS data for the crude reaction to yield 5{72}.

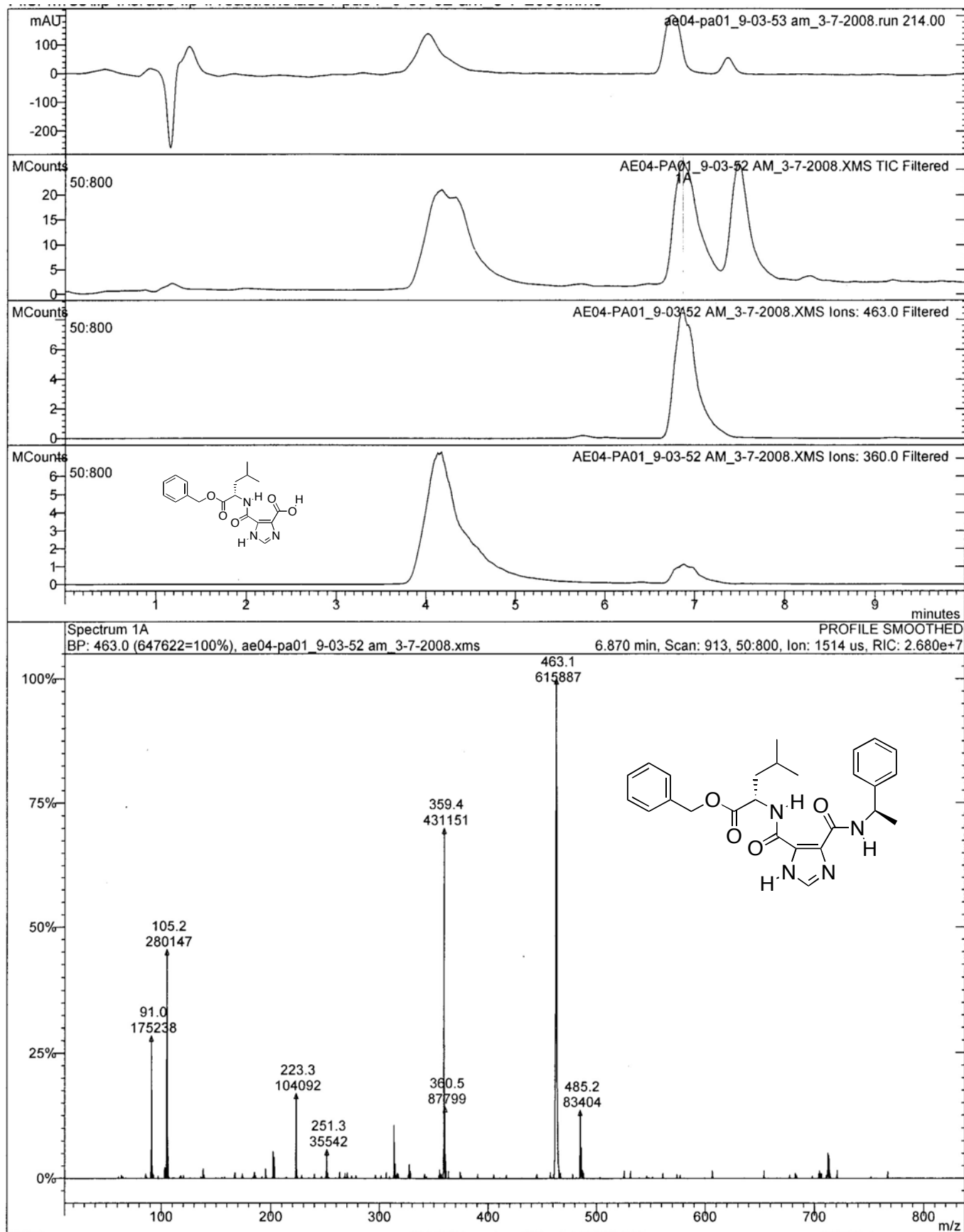


Figure S138. LC/MS data for the crude reaction to yield 5{74}.

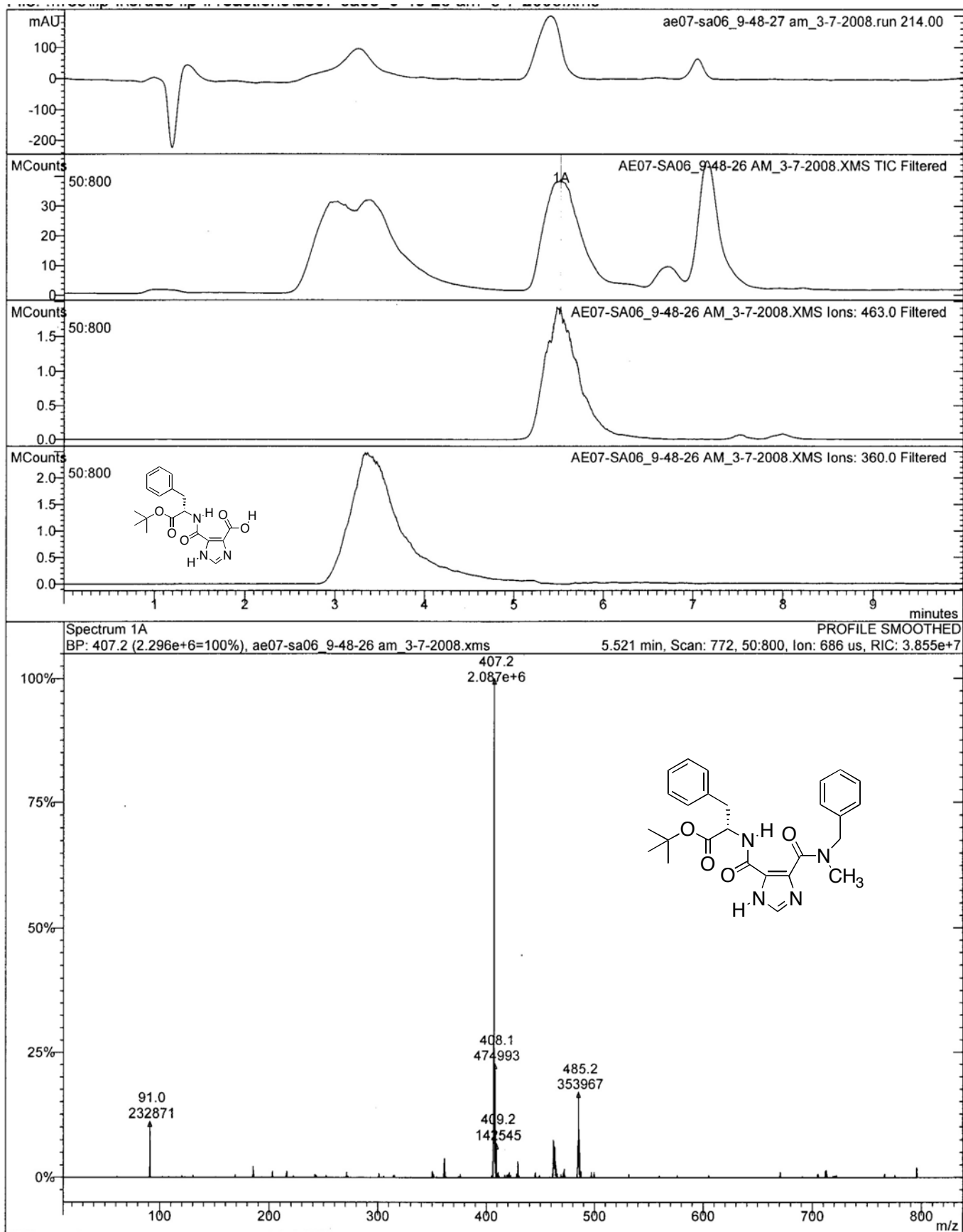


Figure S139. LC/MS data for the crude reaction to yield 5{93}.

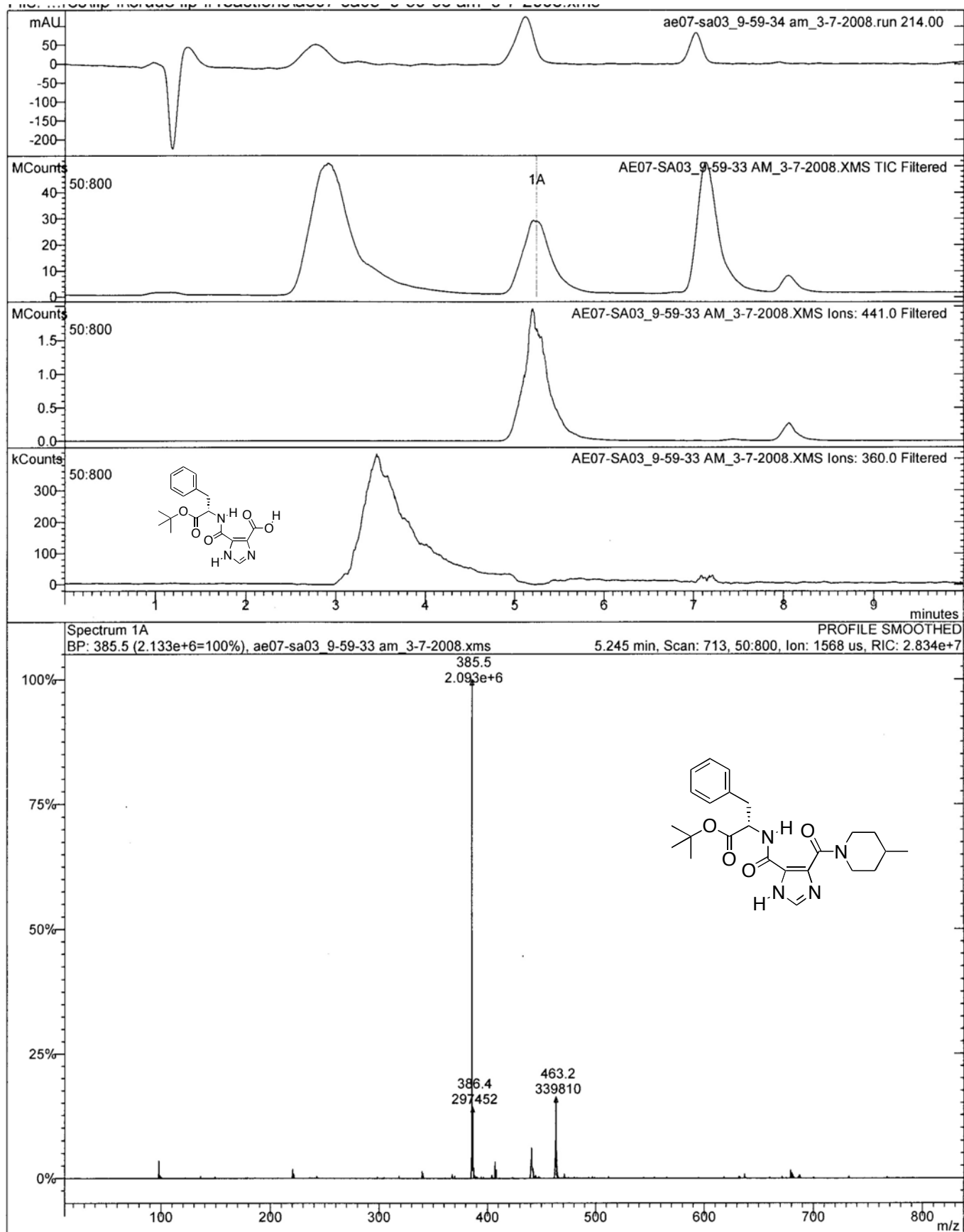


Figure S140. LC/MS data for the crude reaction to yield 5{97}.

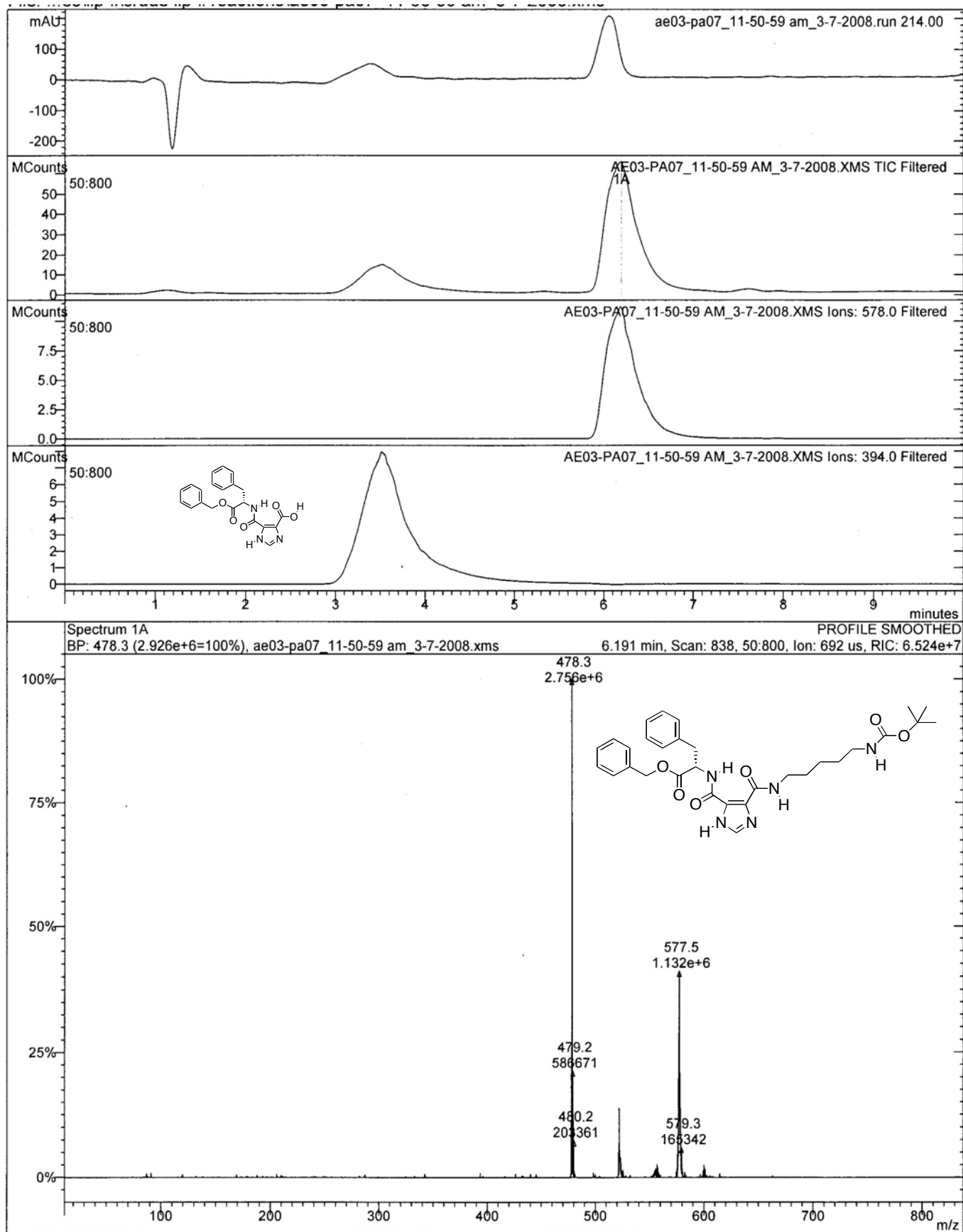


Figure S141. LC/MS data for the crude reaction to yield 5{100}.

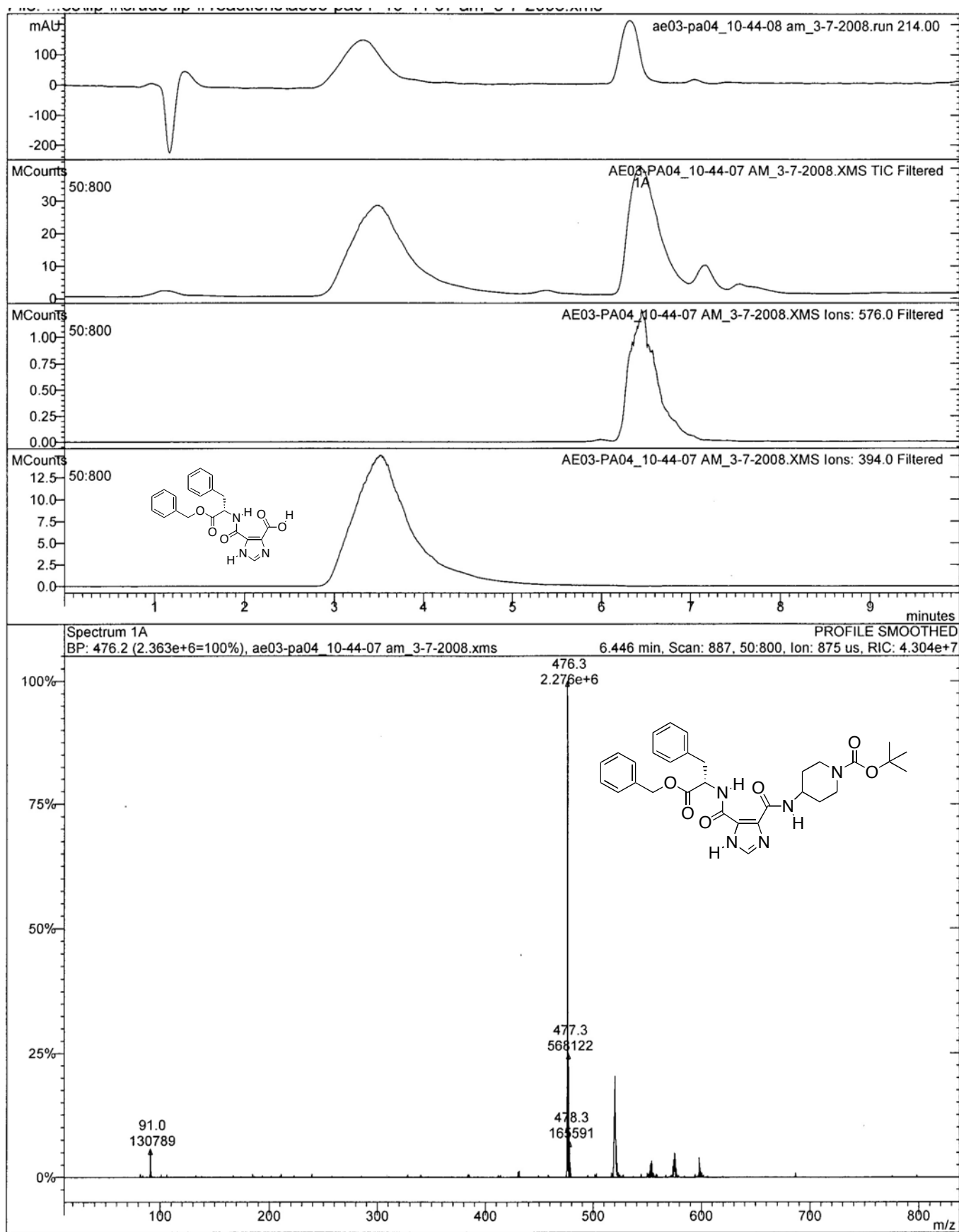


Figure S142. LC/MS data for the crude reaction to yield 6104}.

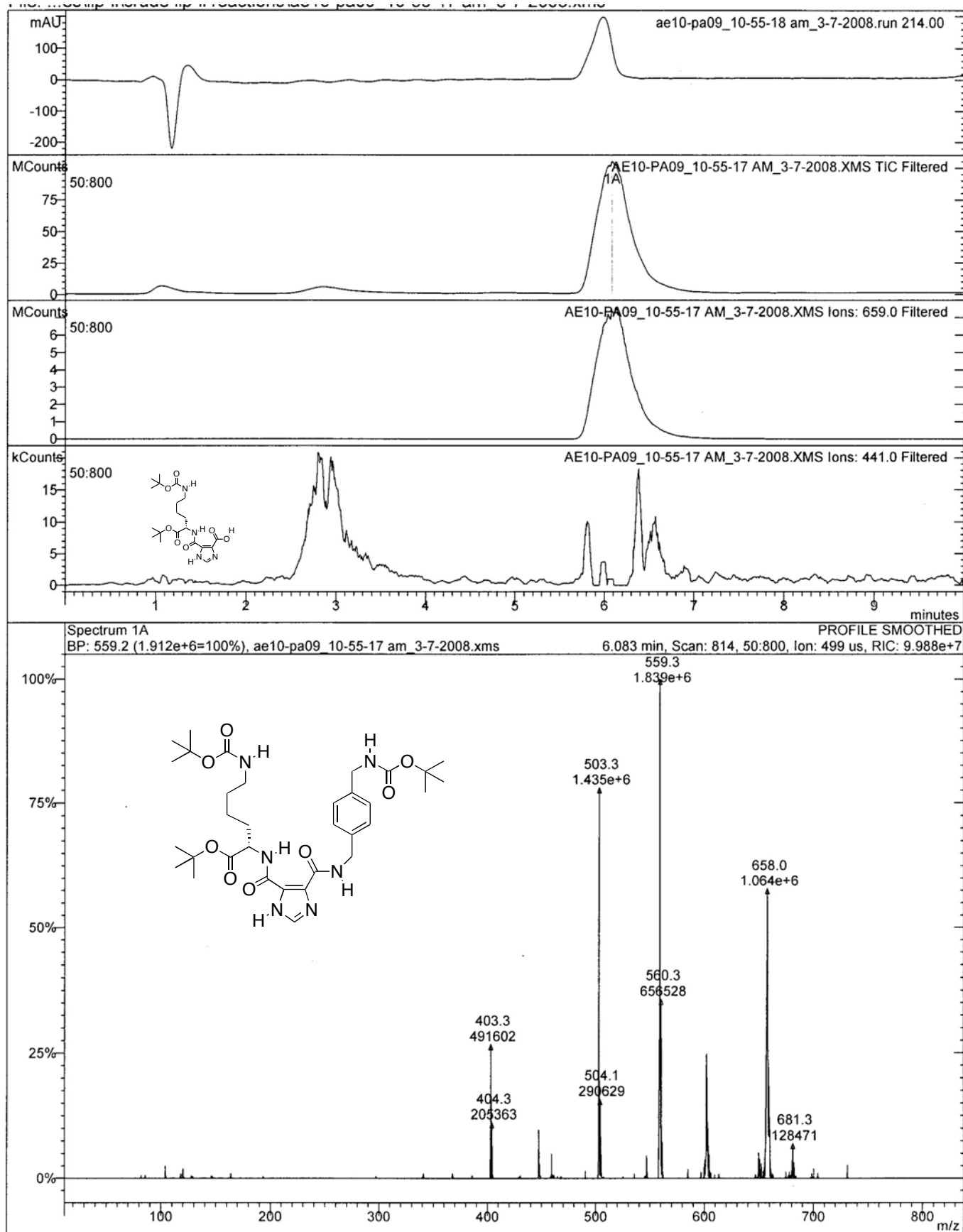


Figure S143. LC/MS data for the crude reaction to yield 5{119}.

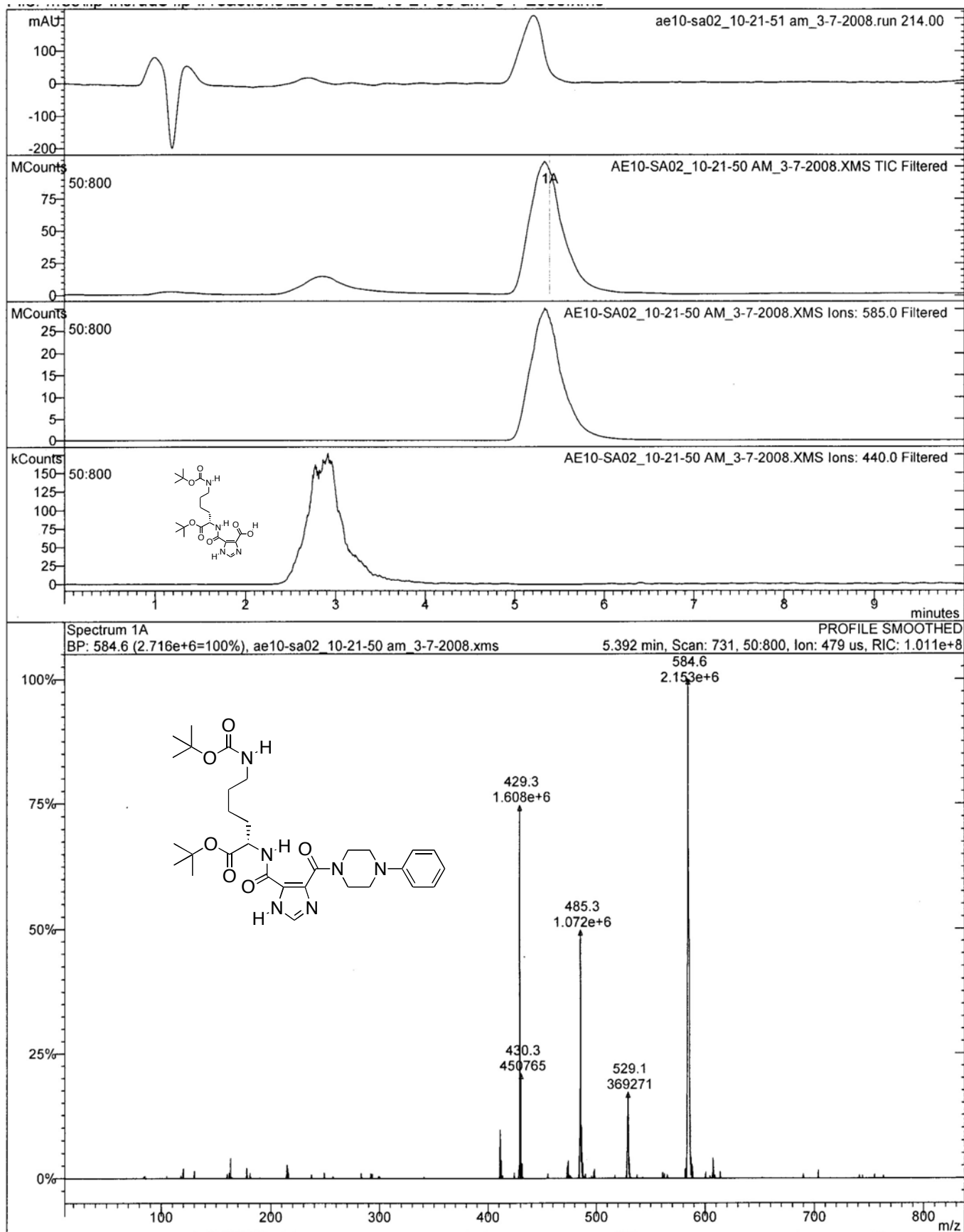


Figure S144. LC/MS data for the crude reaction to yield 5{126}.

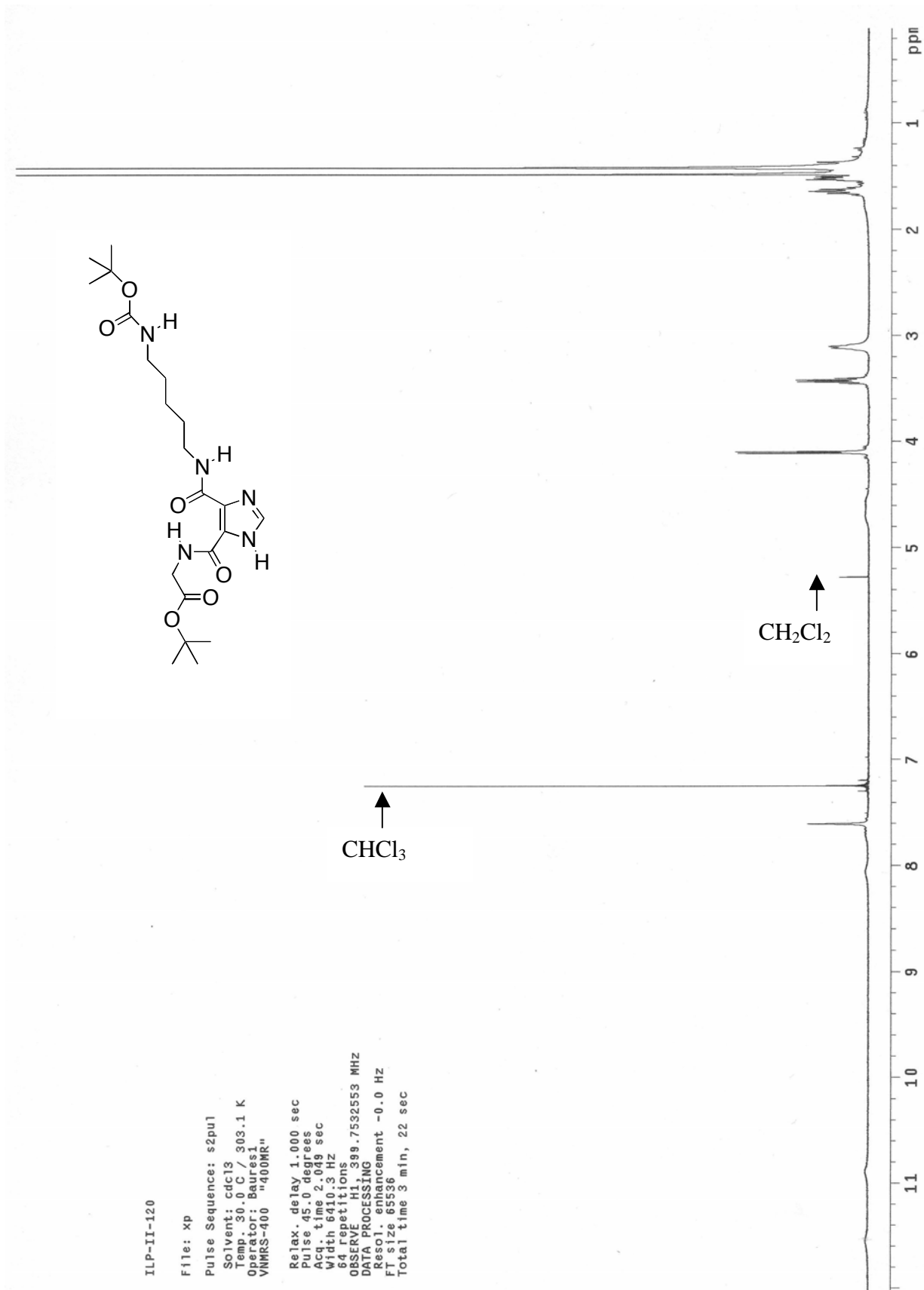


Figure S145. ¹H-NMR for 5{2}.

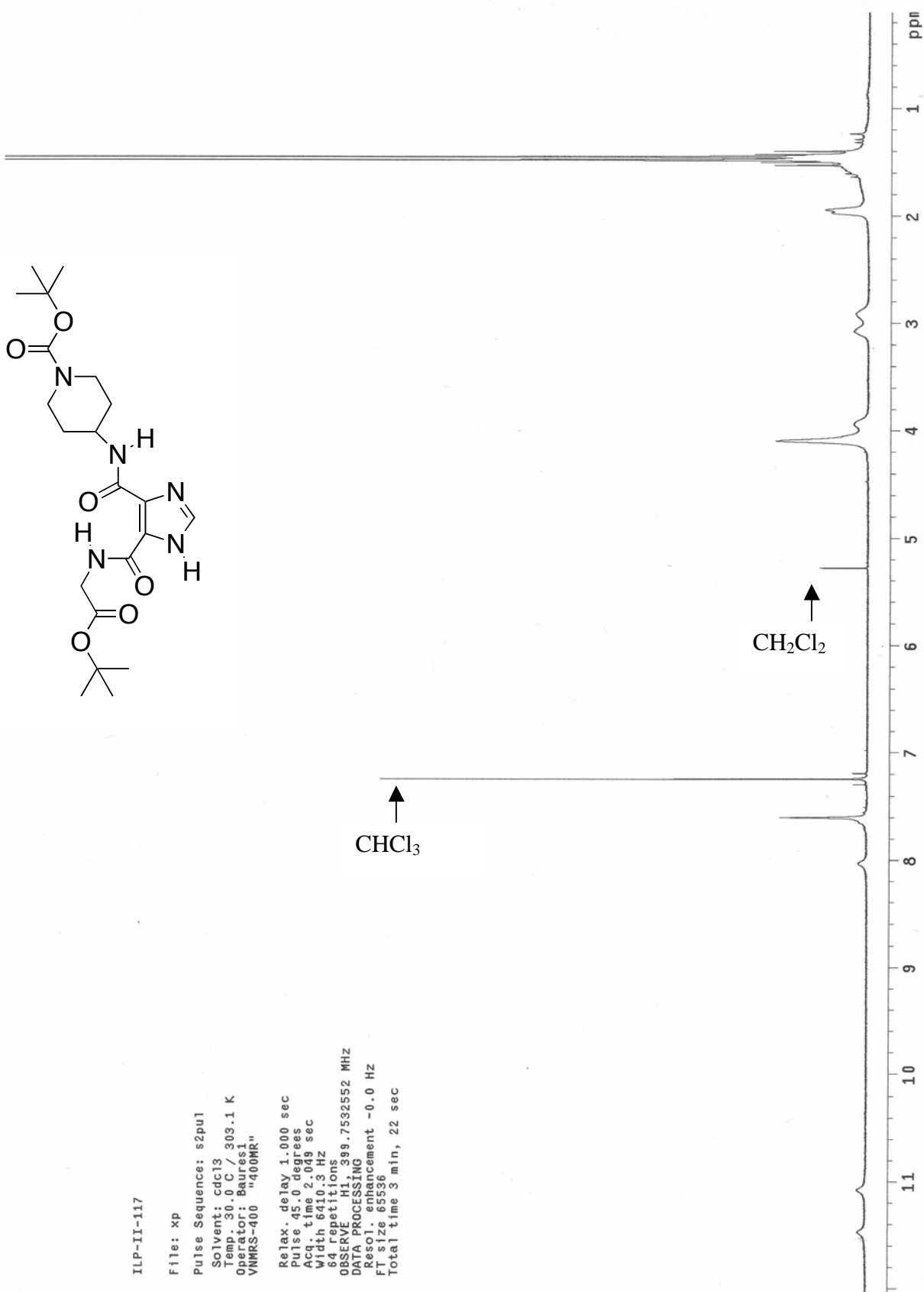
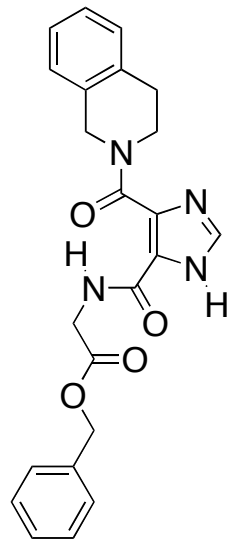


Figure S146. ¹H-NMR for 5{6}.



ILP-II-108

File: xp

Pulse Sequence: s2pul

Solvent: cdCl3

Temp: 30.0 C / 303.1 K

Operator: Baures1

VMRS-400 "400MR"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

64 repetitions

OBSERVE H1, 399.7532550 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 65536

Total time 3 min, 22 sec

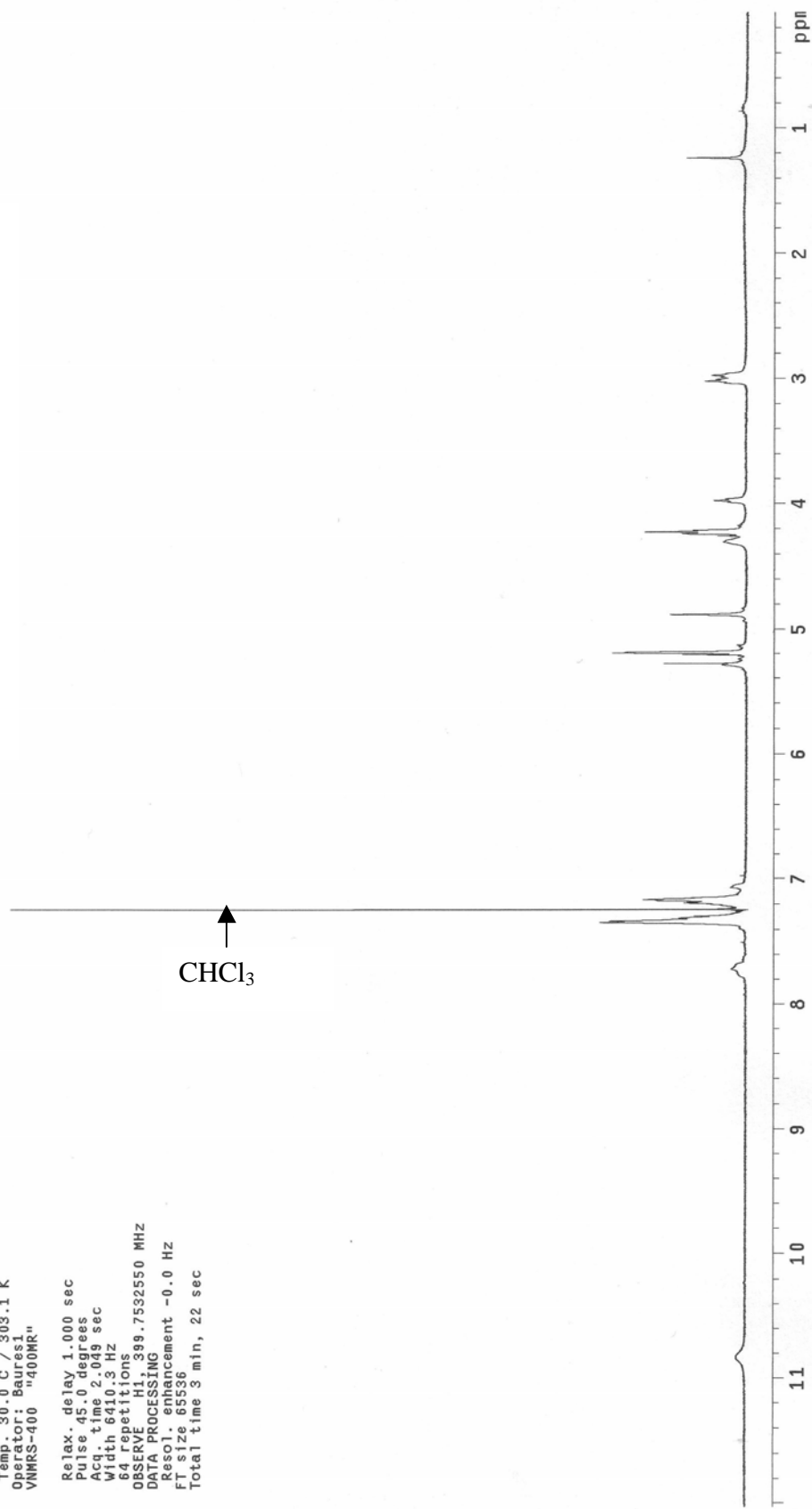
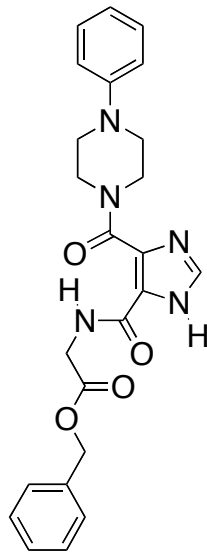


Figure S147. ¹H-NMR for 5{26}.



ILP-II-109

File: xp

Pulse Sequence: s2pu1

Solvent: cdcl3
Temp. 30.0 C / 303.1 K
Operator: BauresJ
VNMR5-400 "400MR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
64 repetitions
OBSERVE H1, 399.7532553 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 65536
Total time 3 min, 22 sec

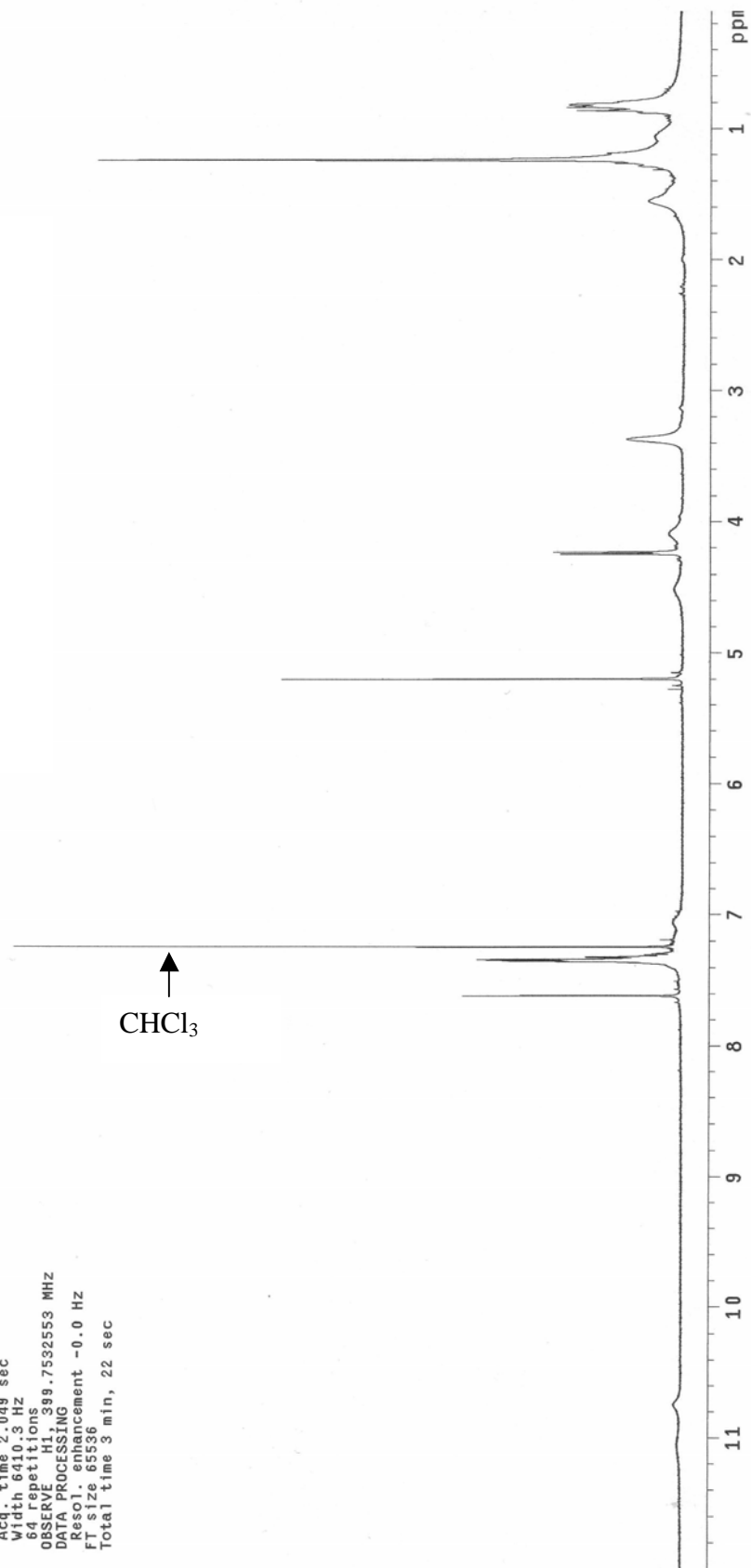


Figure S148. ¹H-NMR for 5{28}.

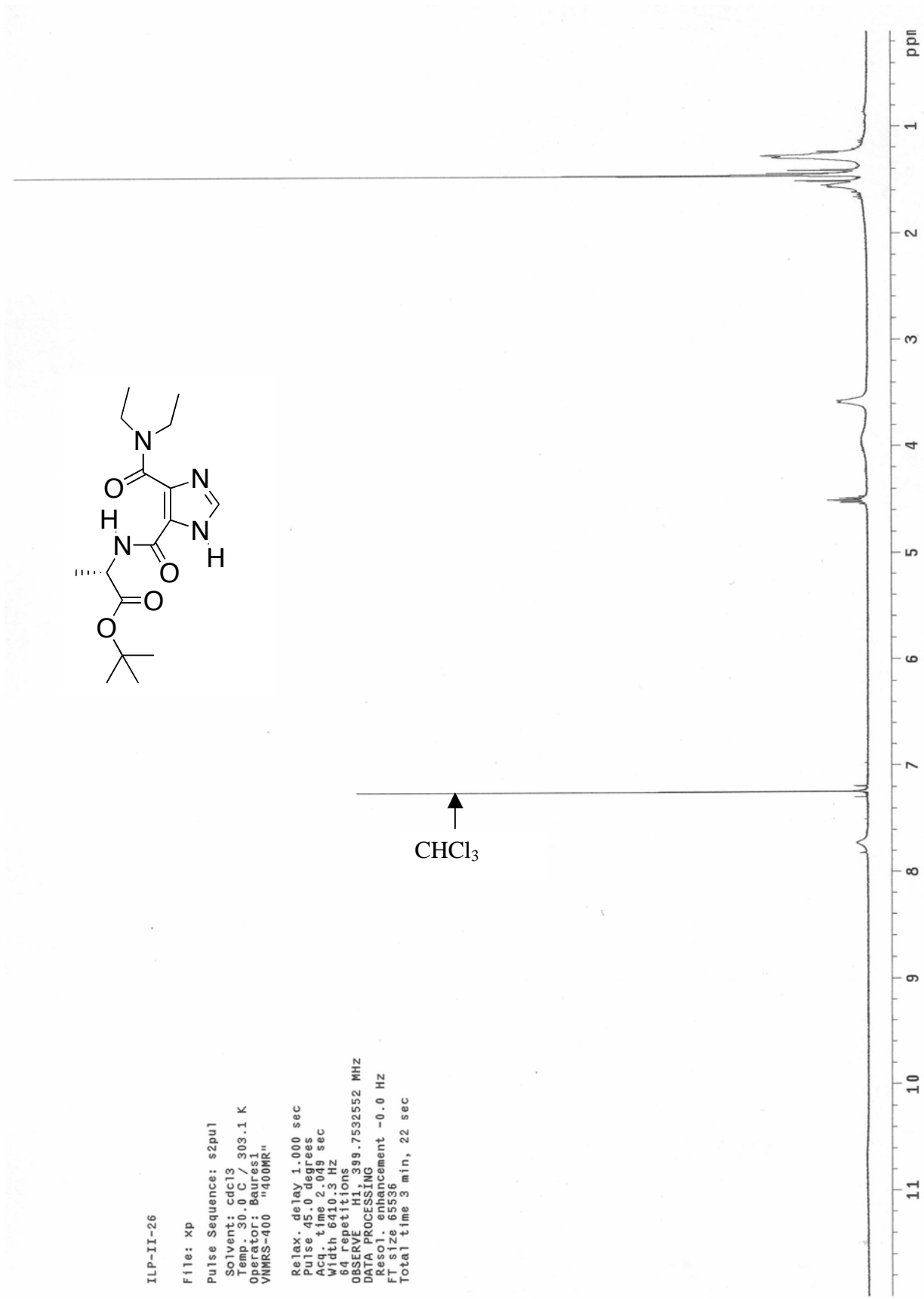


Figure S149. ¹H-NMR for 5{38}.

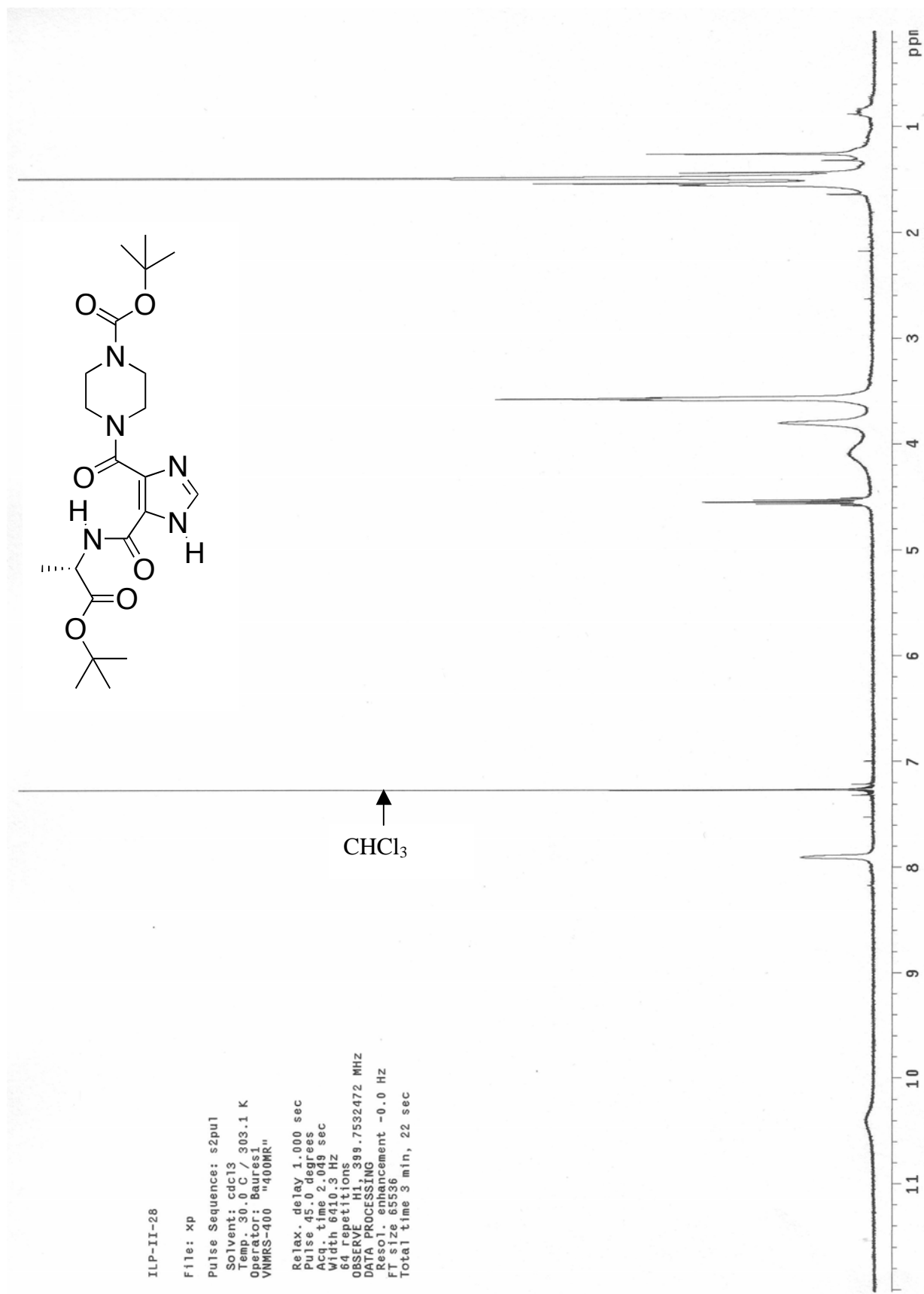


Figure S150. ¹H-NMR for 5{39}.

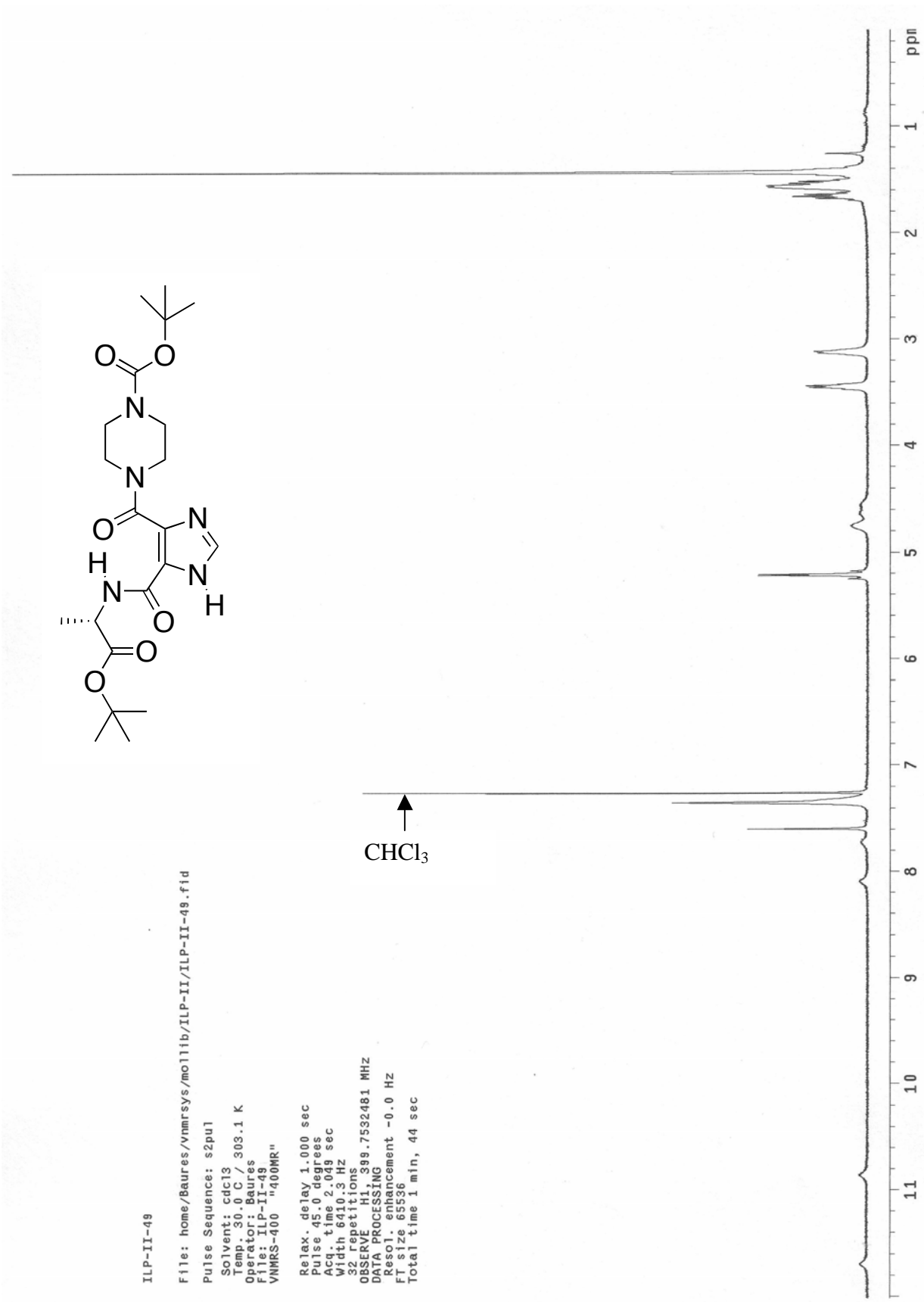


Figure S151. ¹H-NMR for 5{44}.

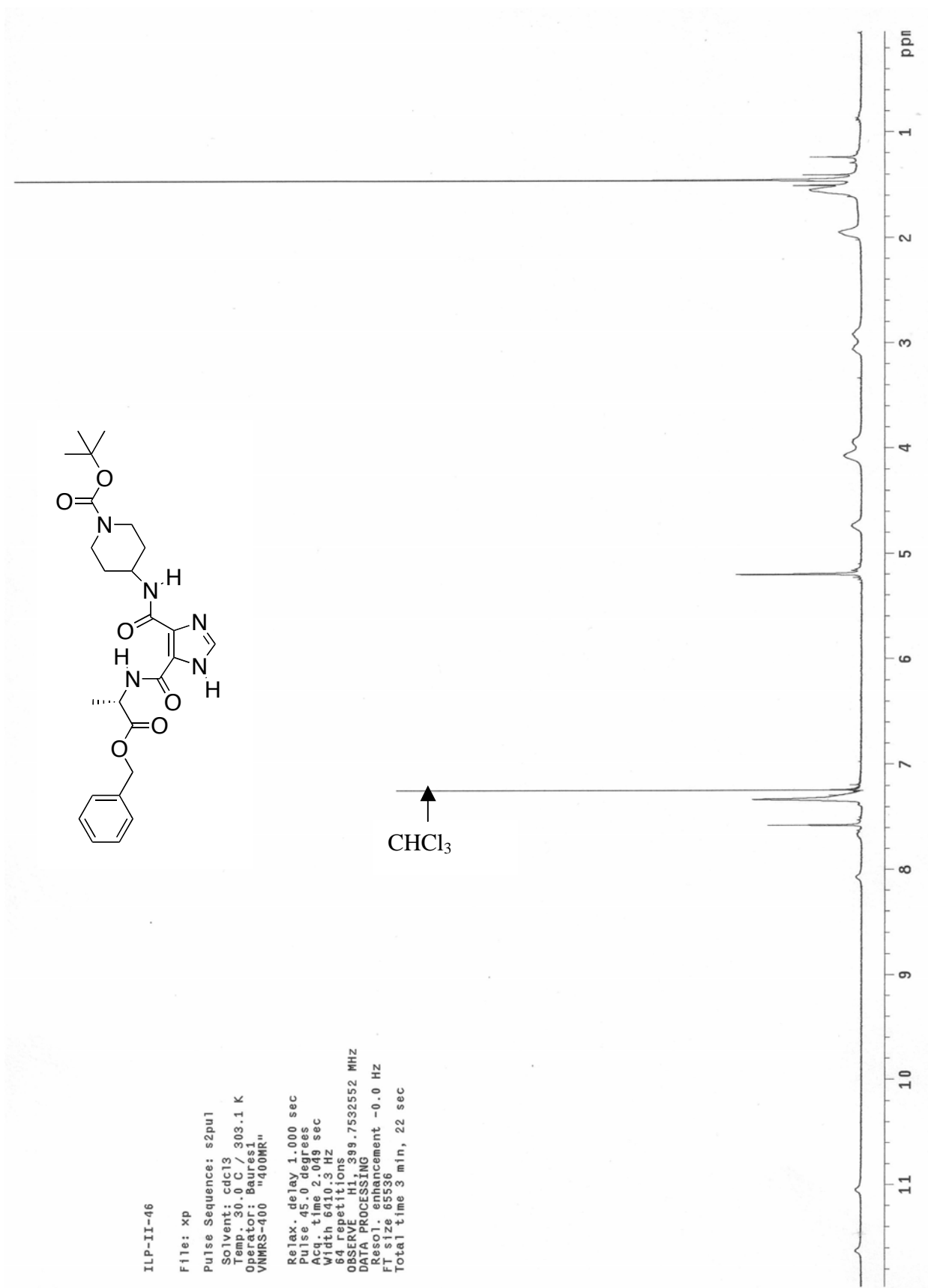


Figure S152. ¹H-NMR for 5{48}.

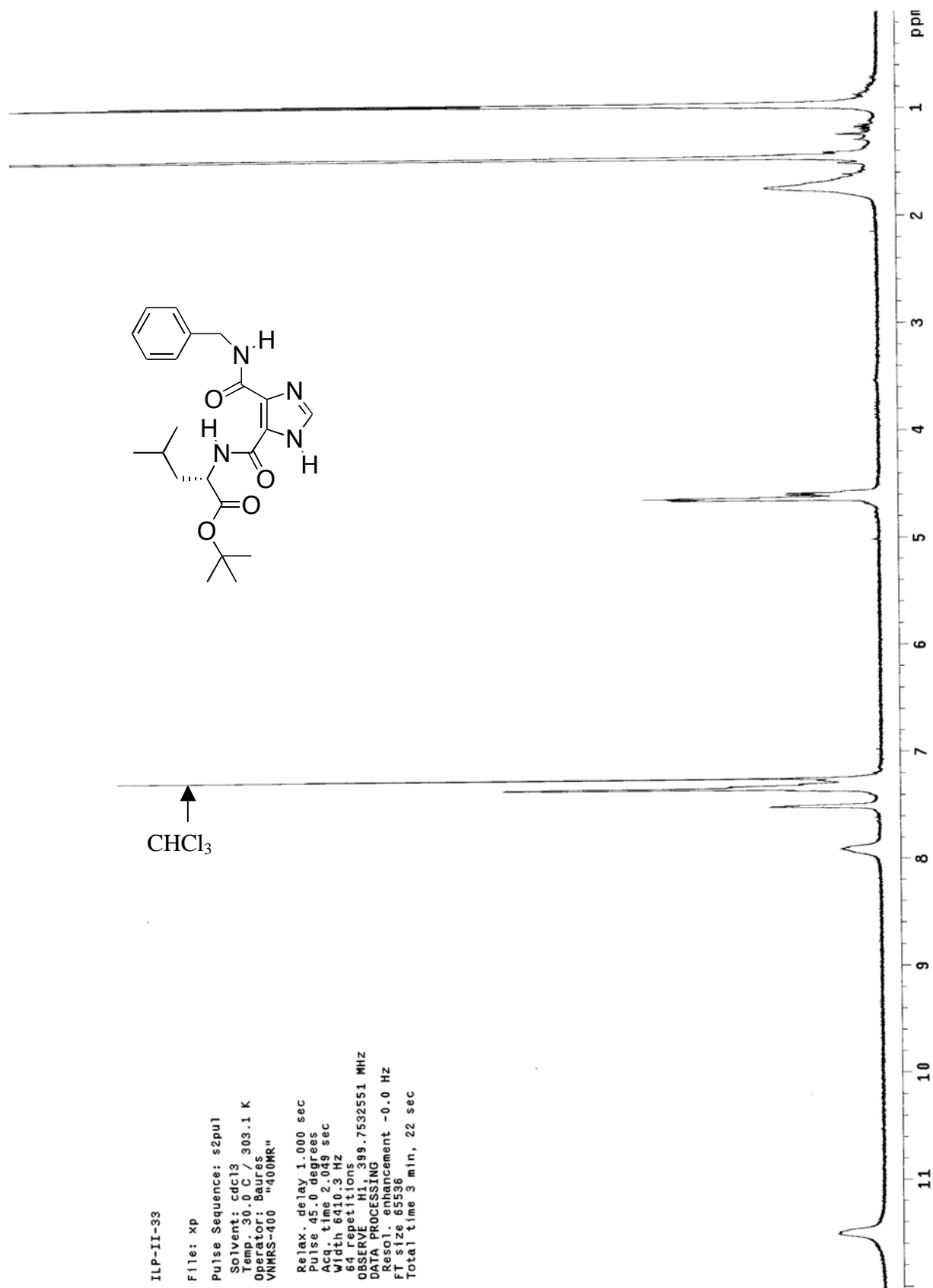


Figure S153. ¹H-NMR for 5{59}.

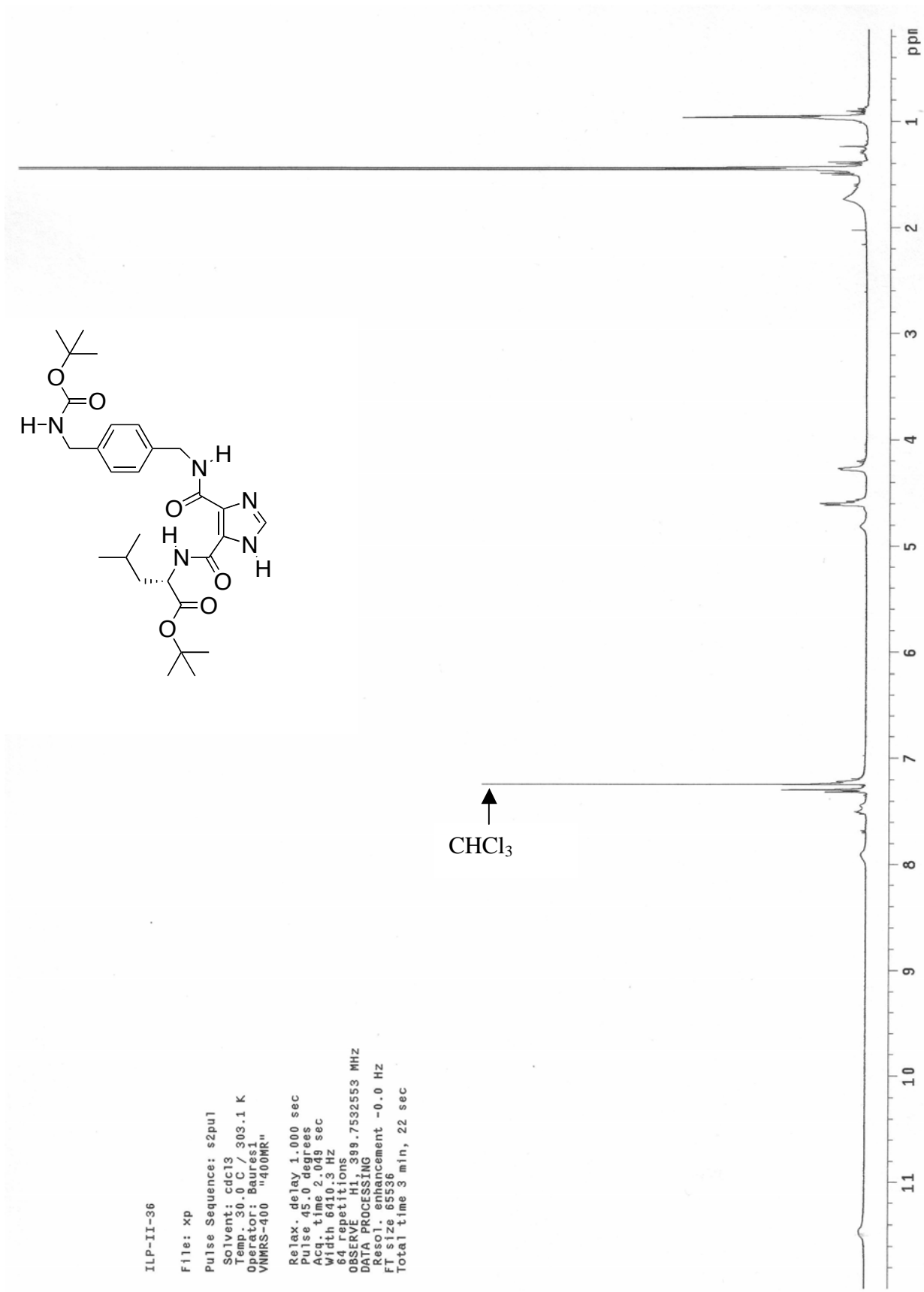


Figure S154. ¹H-NMR for 5{63}.

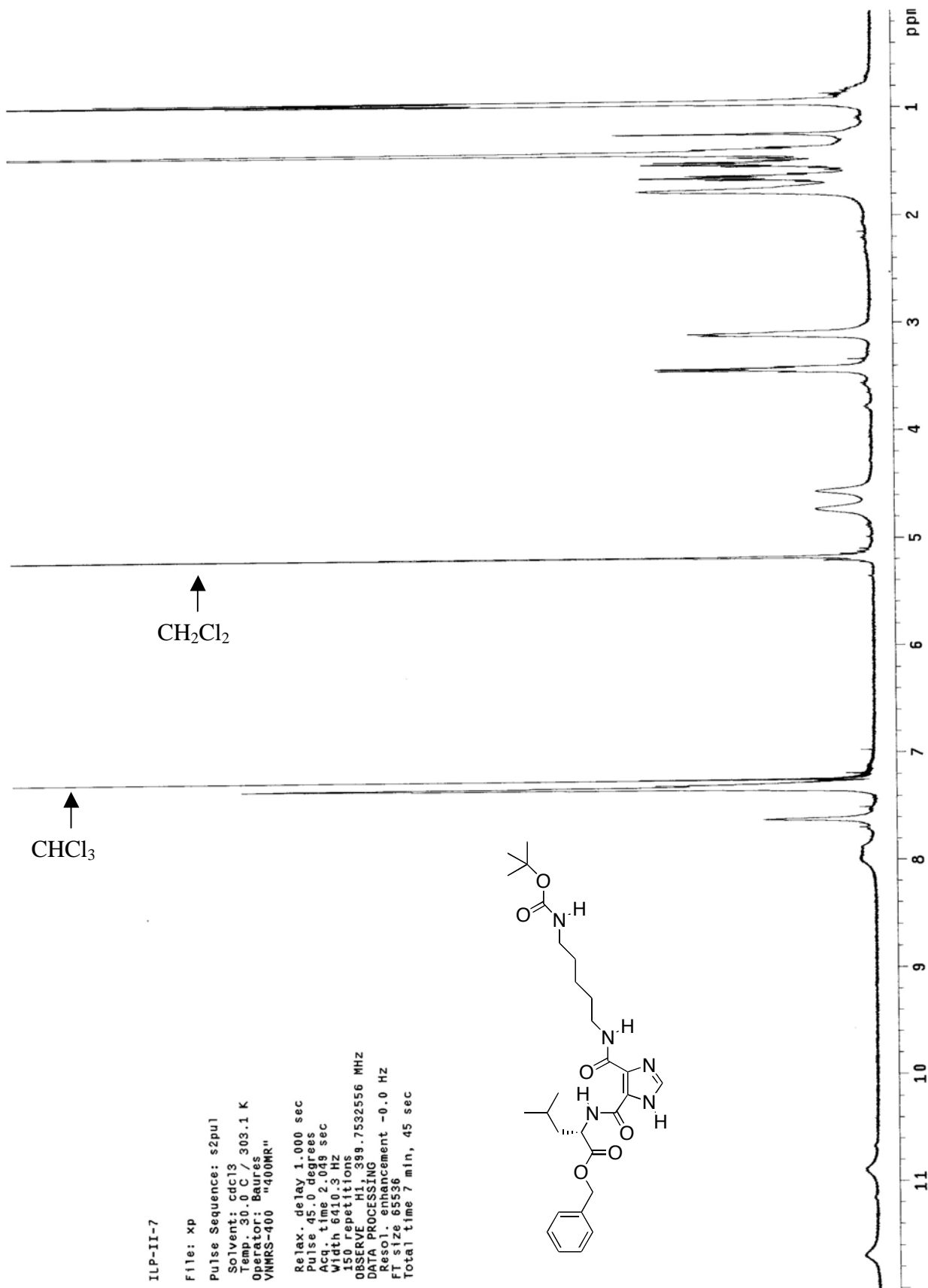
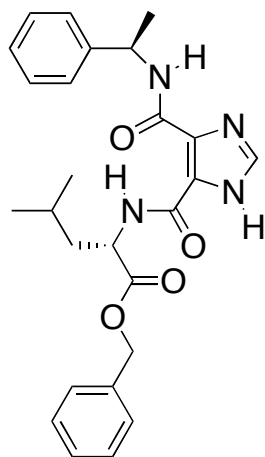


Figure S155. ¹H-NMR for 5{72}.



ILP-II-1

File: xp

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp: 30.0 C, 303.1 K

Origi: 01_Ba06a1

VNMR5-000 "400MR"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

64 repetitions

OBSERVE H1, 399.7532553 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 65536

Total time 3 min, 22 sec

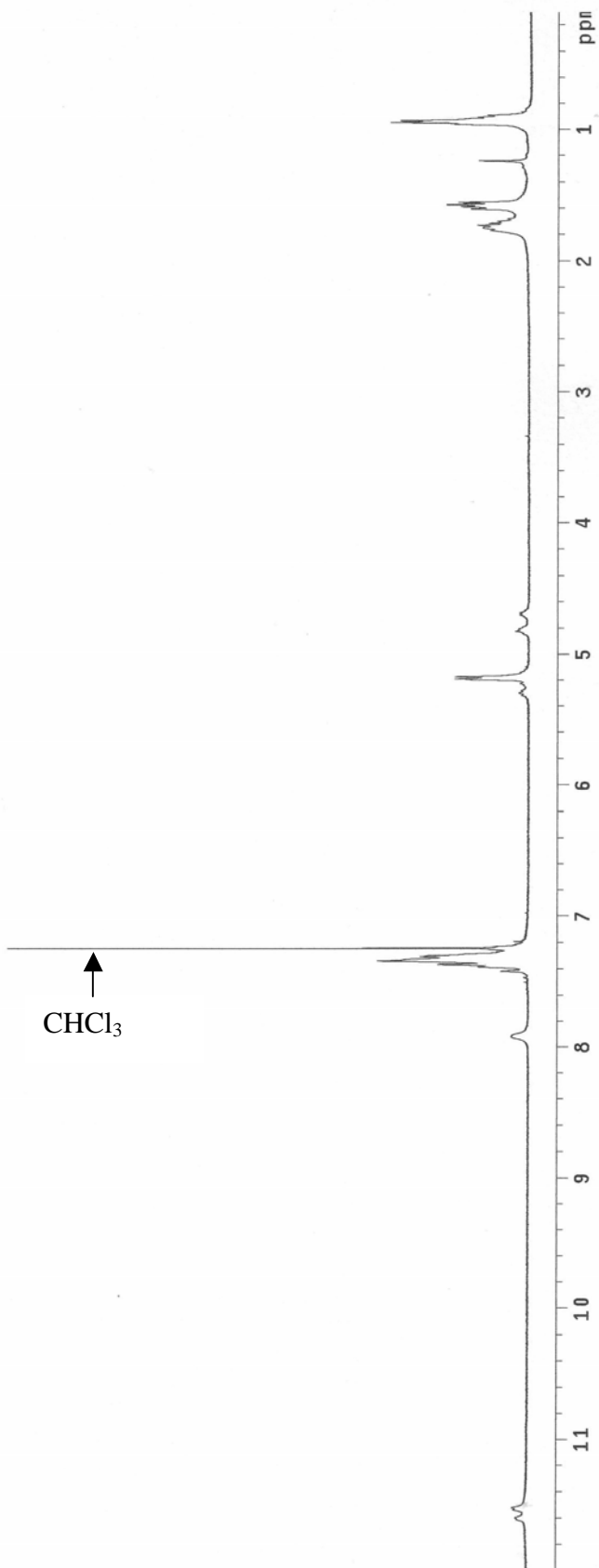


Figure S156. $^1\text{H-NMR}$ for 5{74}.

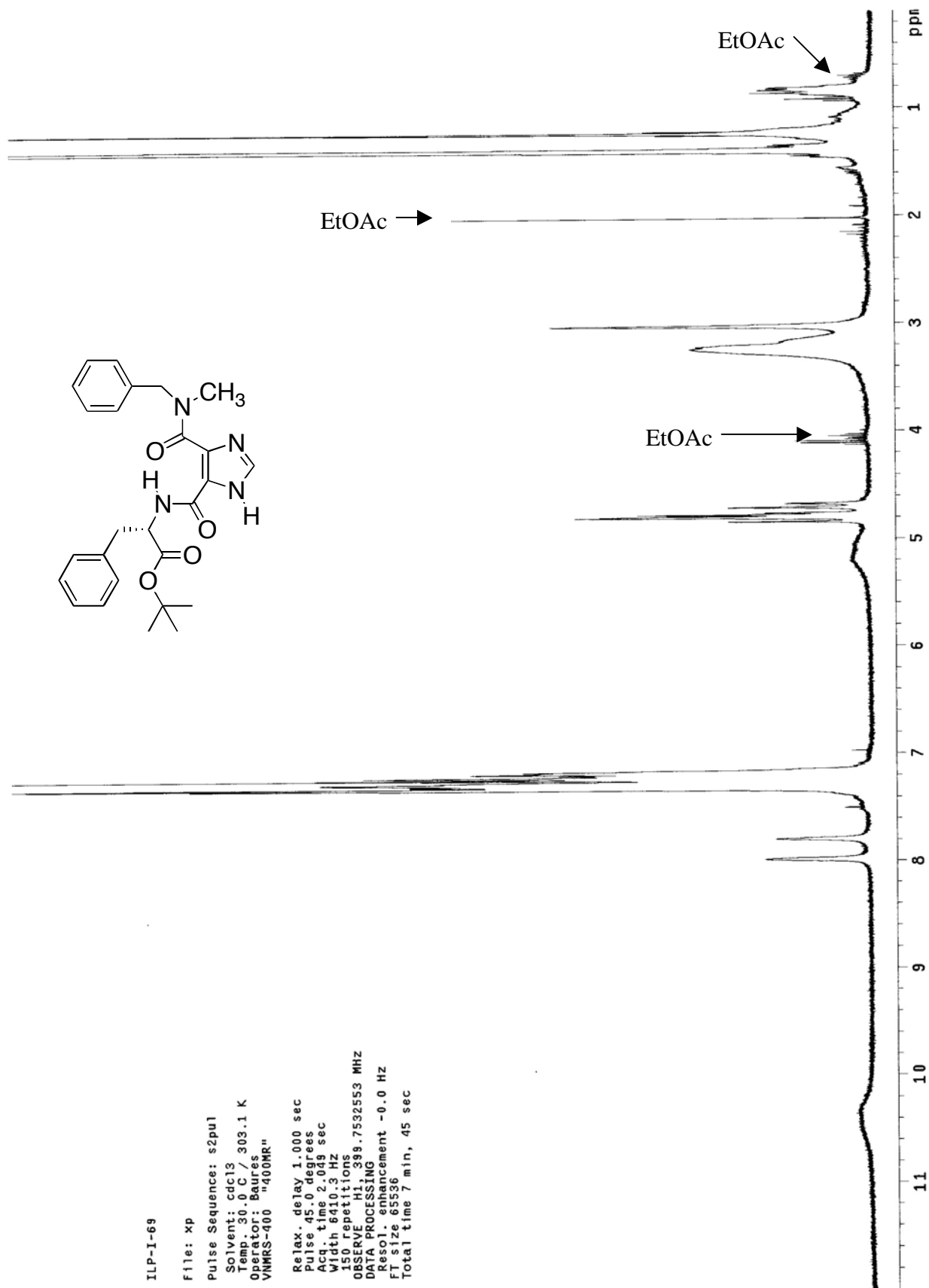


Figure S157. ¹H-NMR for 5{93}.

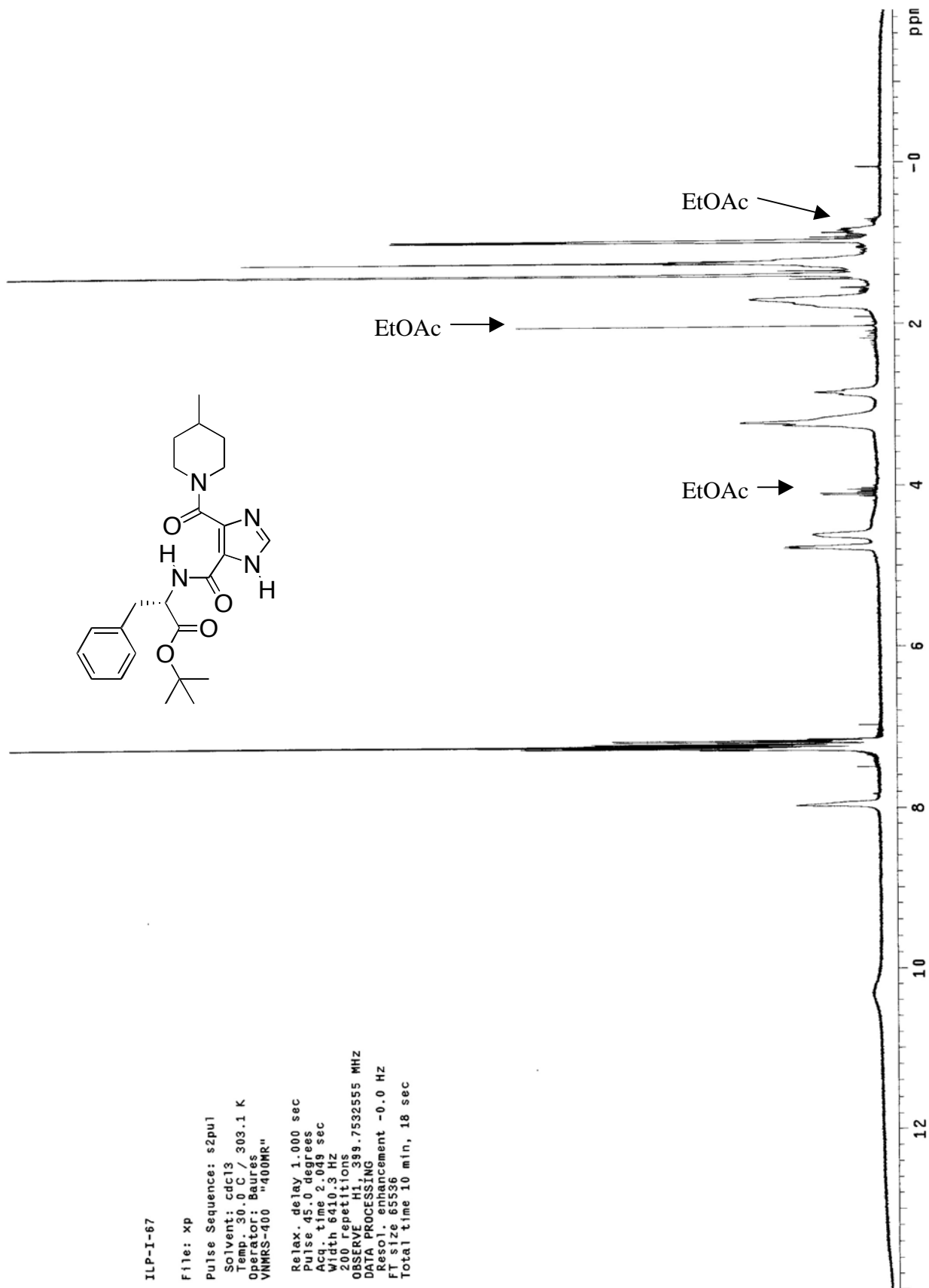


Figure S158. $^1\text{H-NMR}$ for 5{97}.

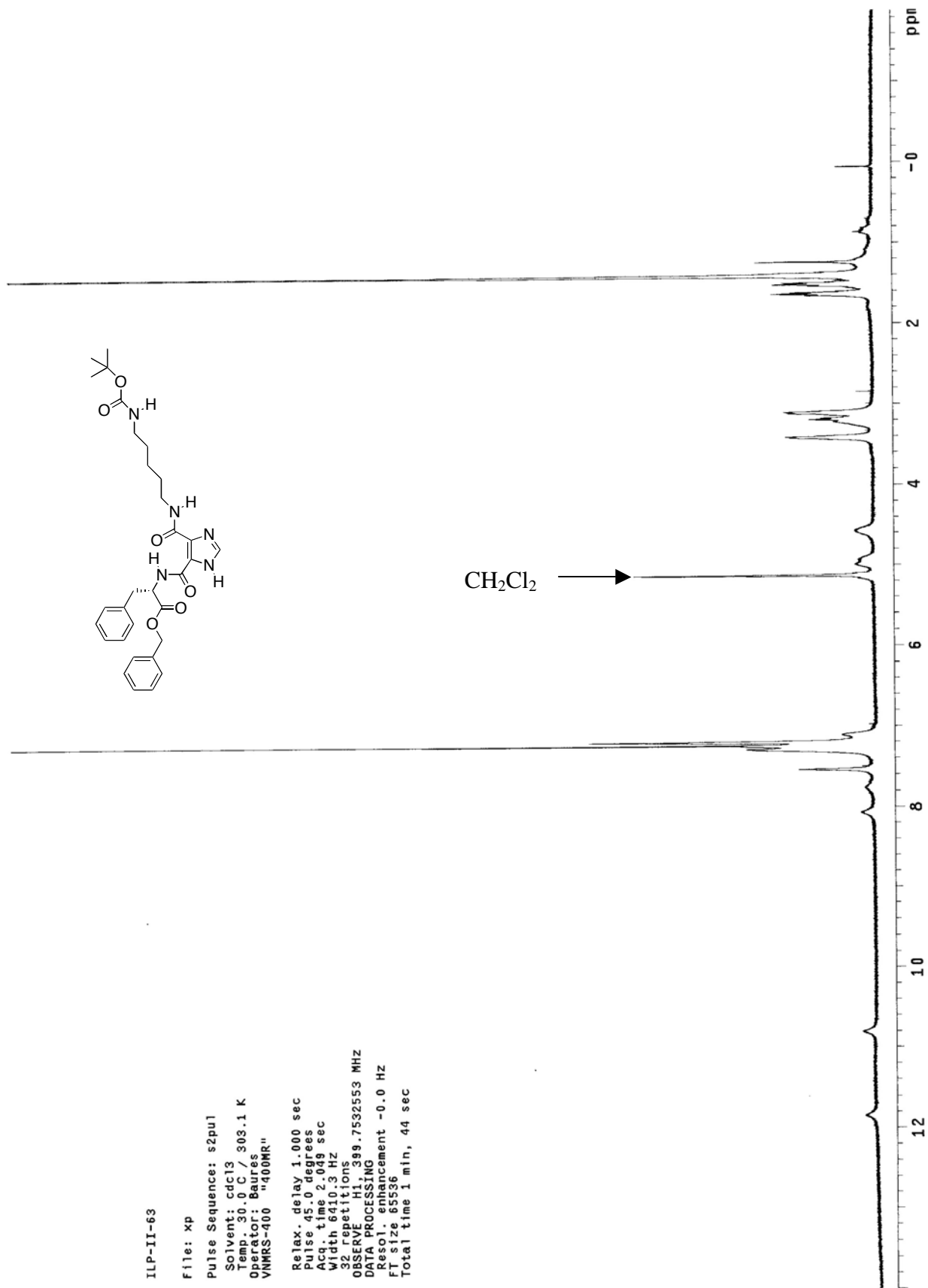


Figure S159. ¹H-NMR for 5{100}.

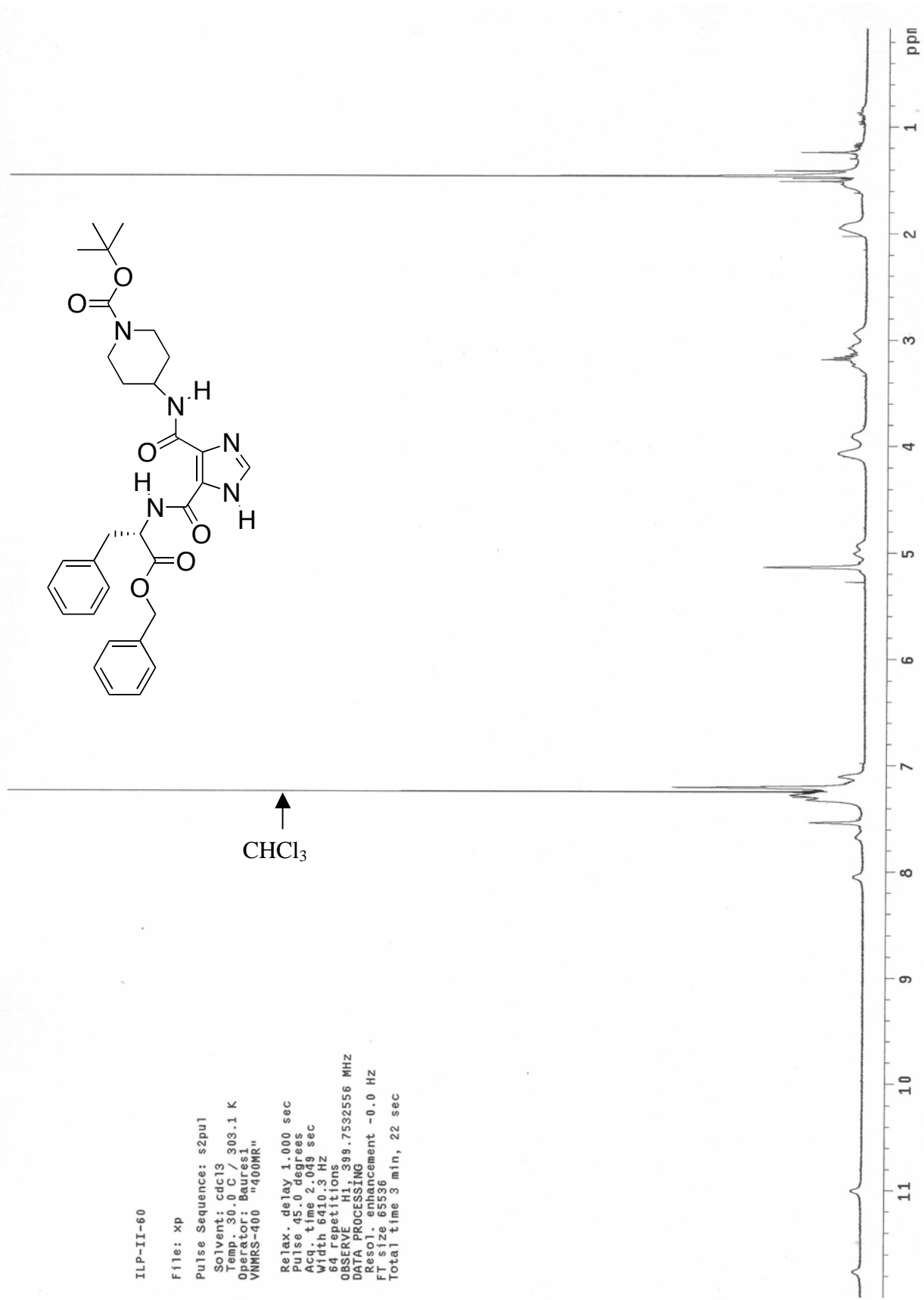


Figure S160. ¹H-NMR for 5{104}.

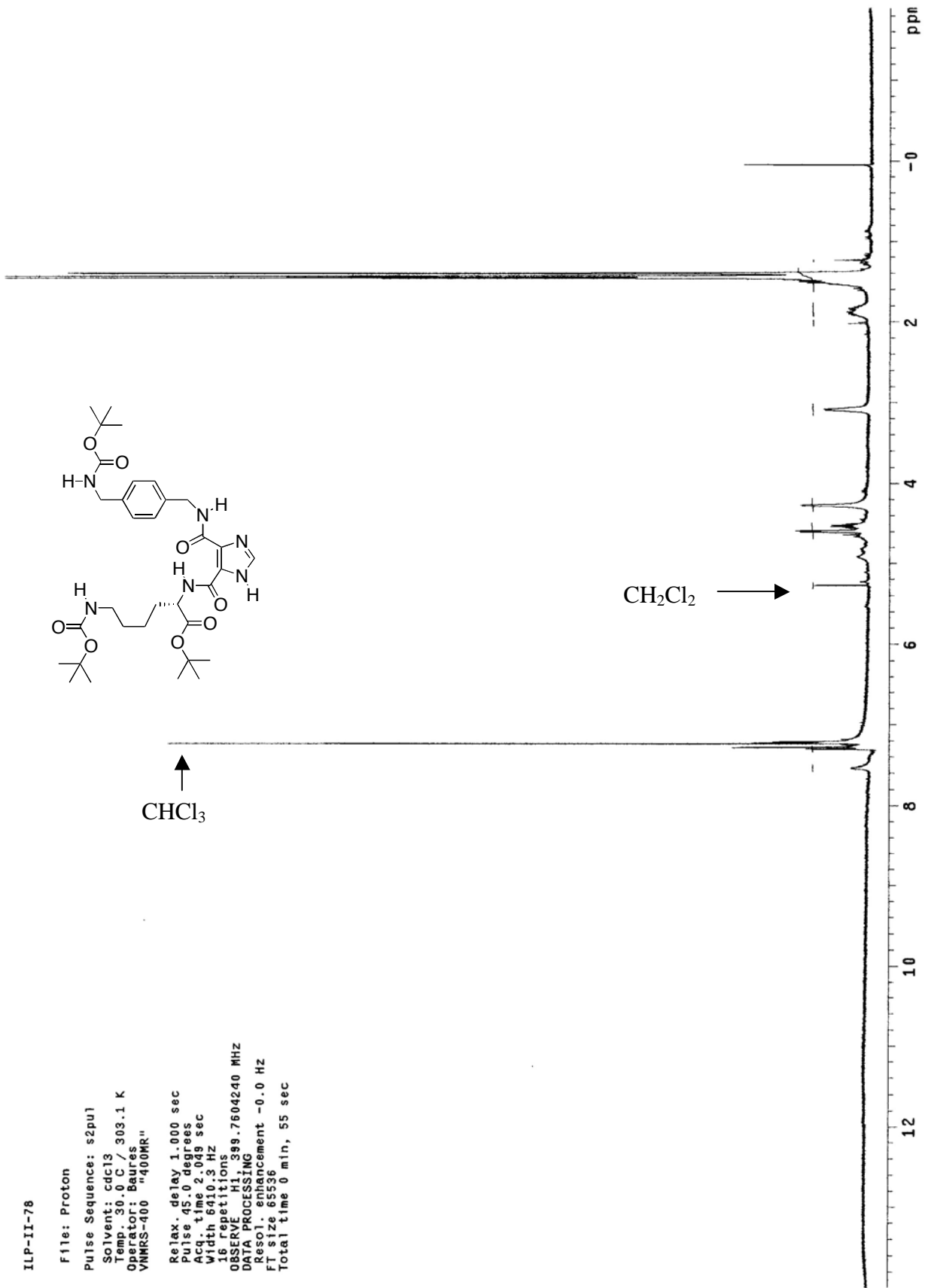


Figure S161. ¹H-NMR for 5{119}.

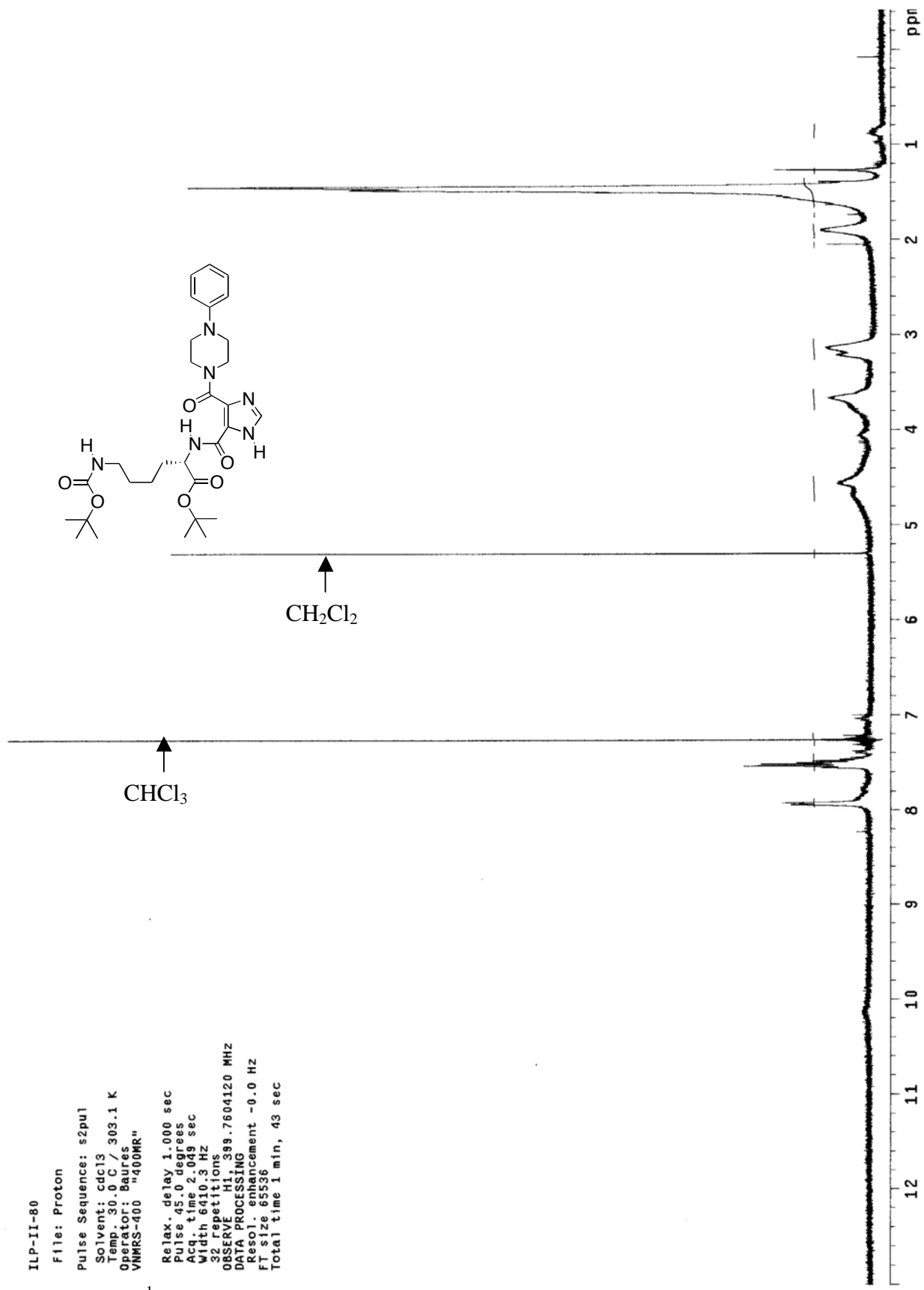


Figure S162. $^1\text{H-NMR}$ for 5{126}.

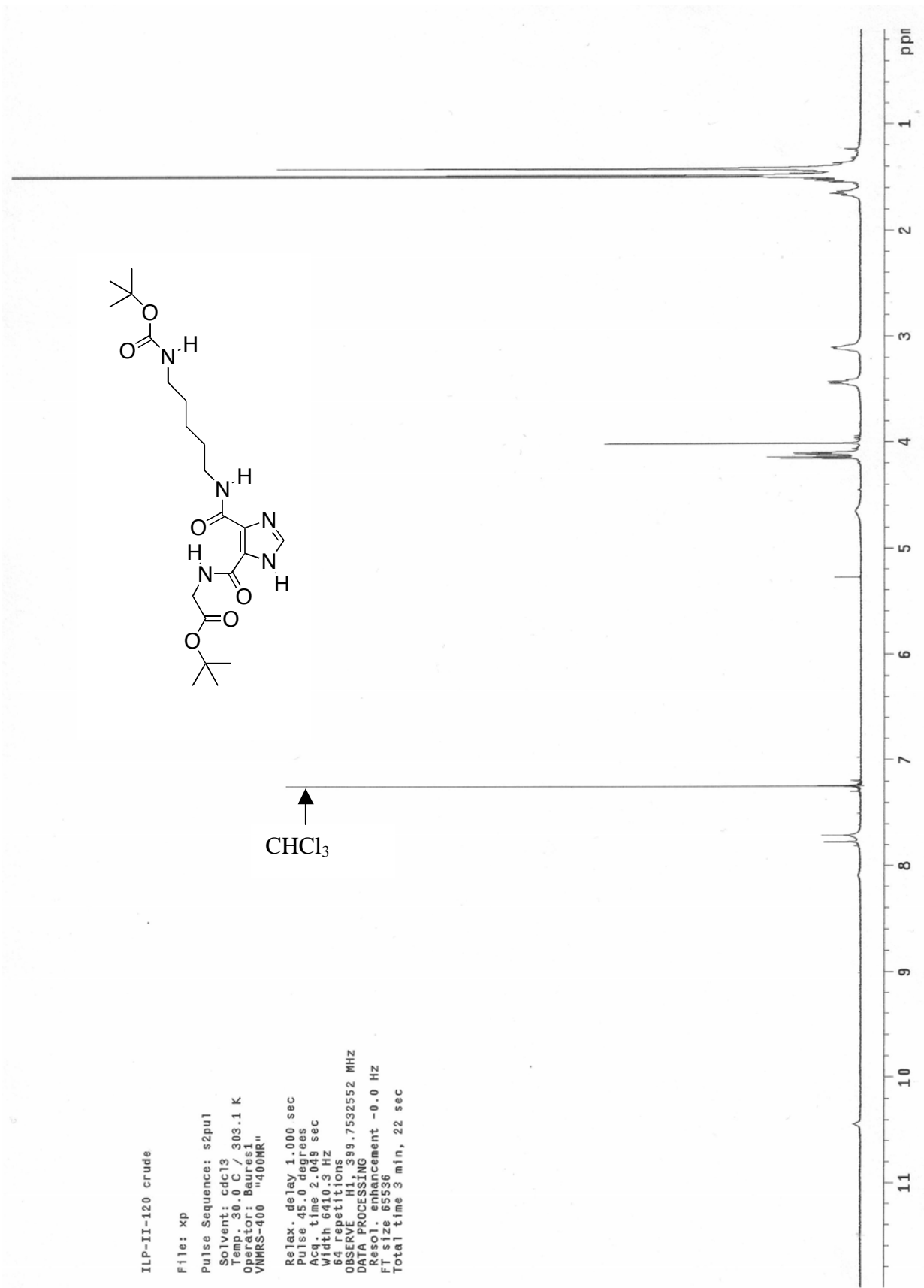


Figure S163. ¹H-NMR for the crude reaction to yield **5{2}**.

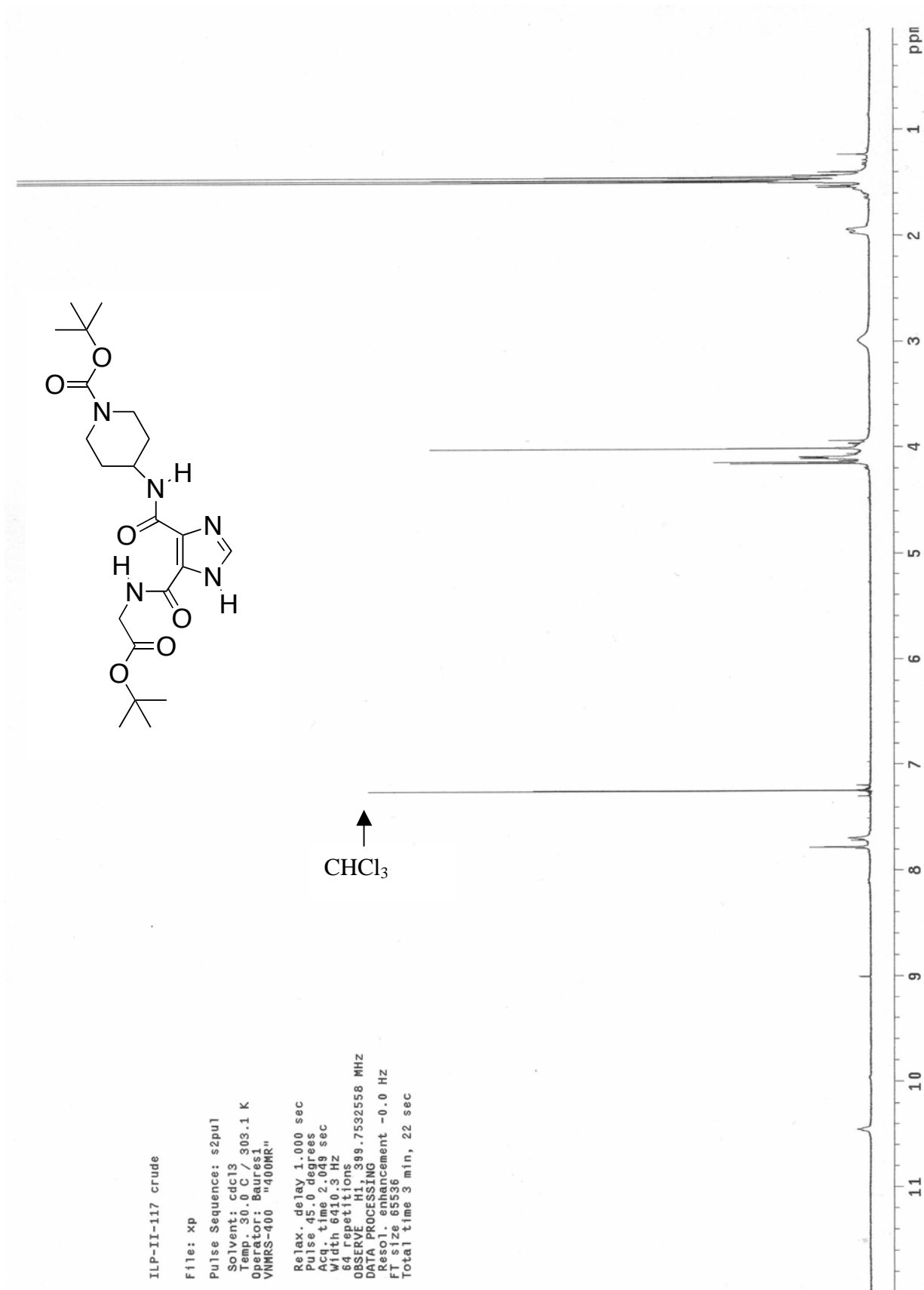


Figure S164. ¹H-NMR for the crude reaction to yield **5{6}**.

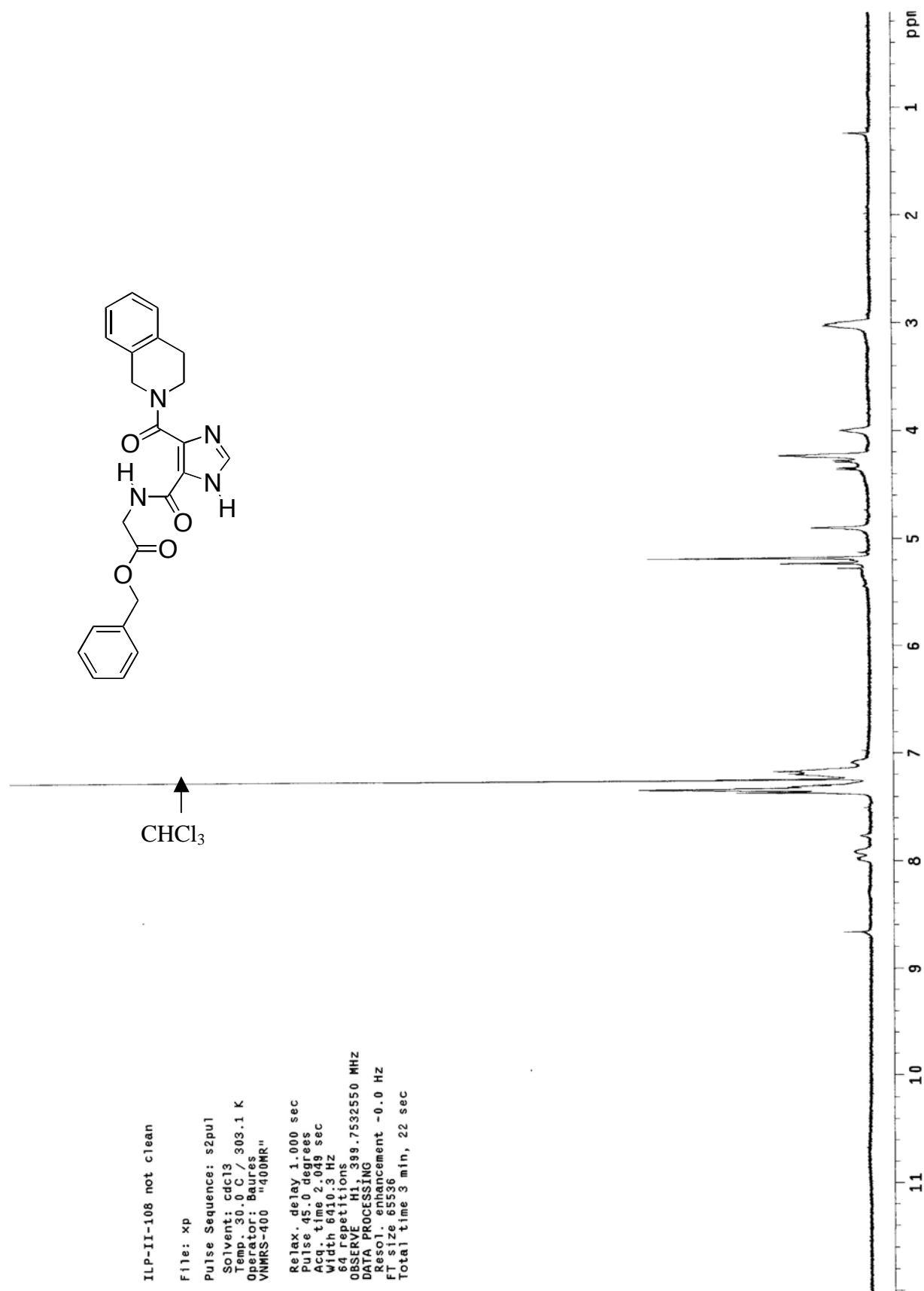


Figure S165. ¹H-NMR for the crude reaction to yield 5{26}.

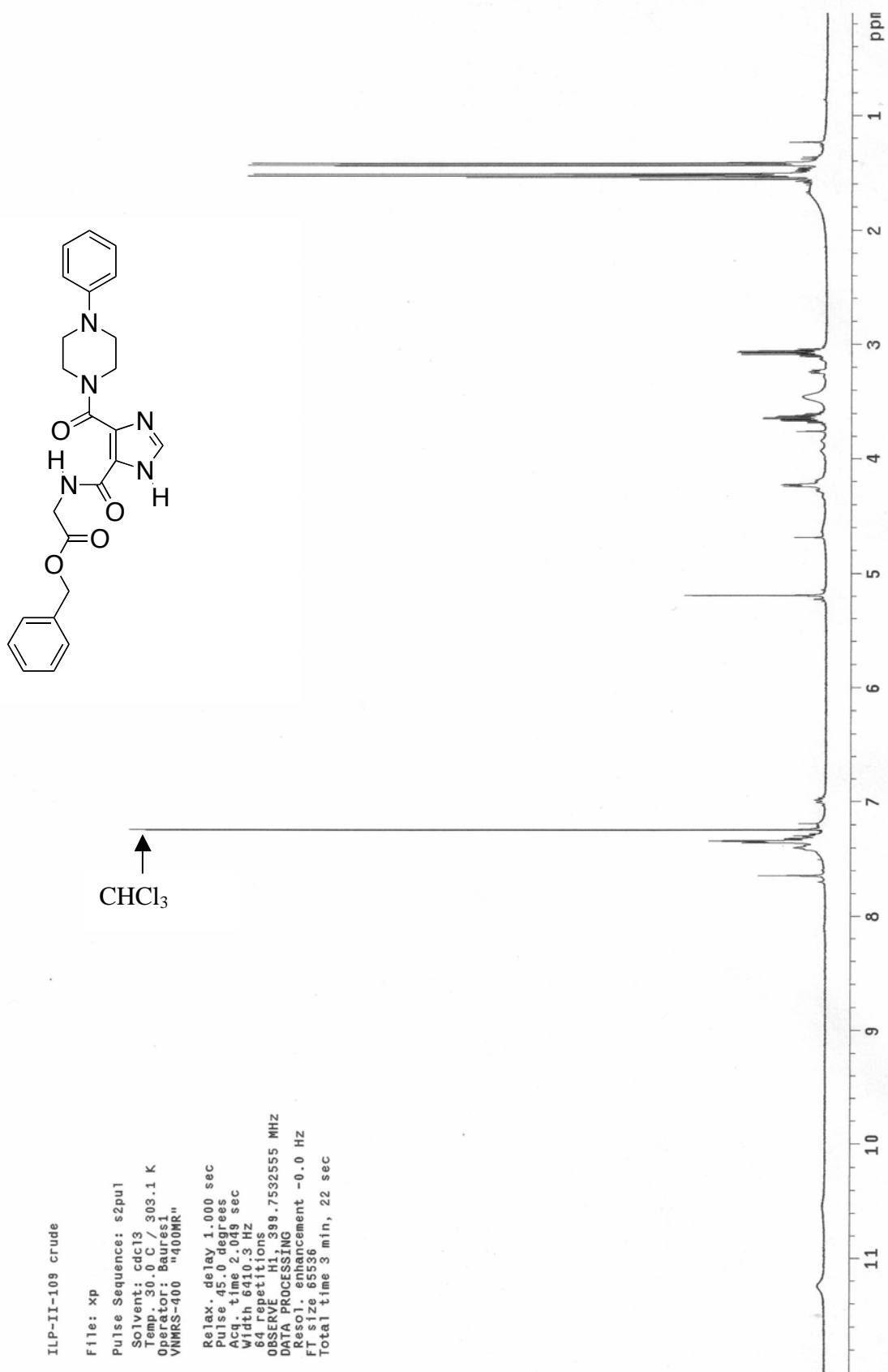


Figure S166. ¹H-NMR for the crude reaction to yield **5**{28}.

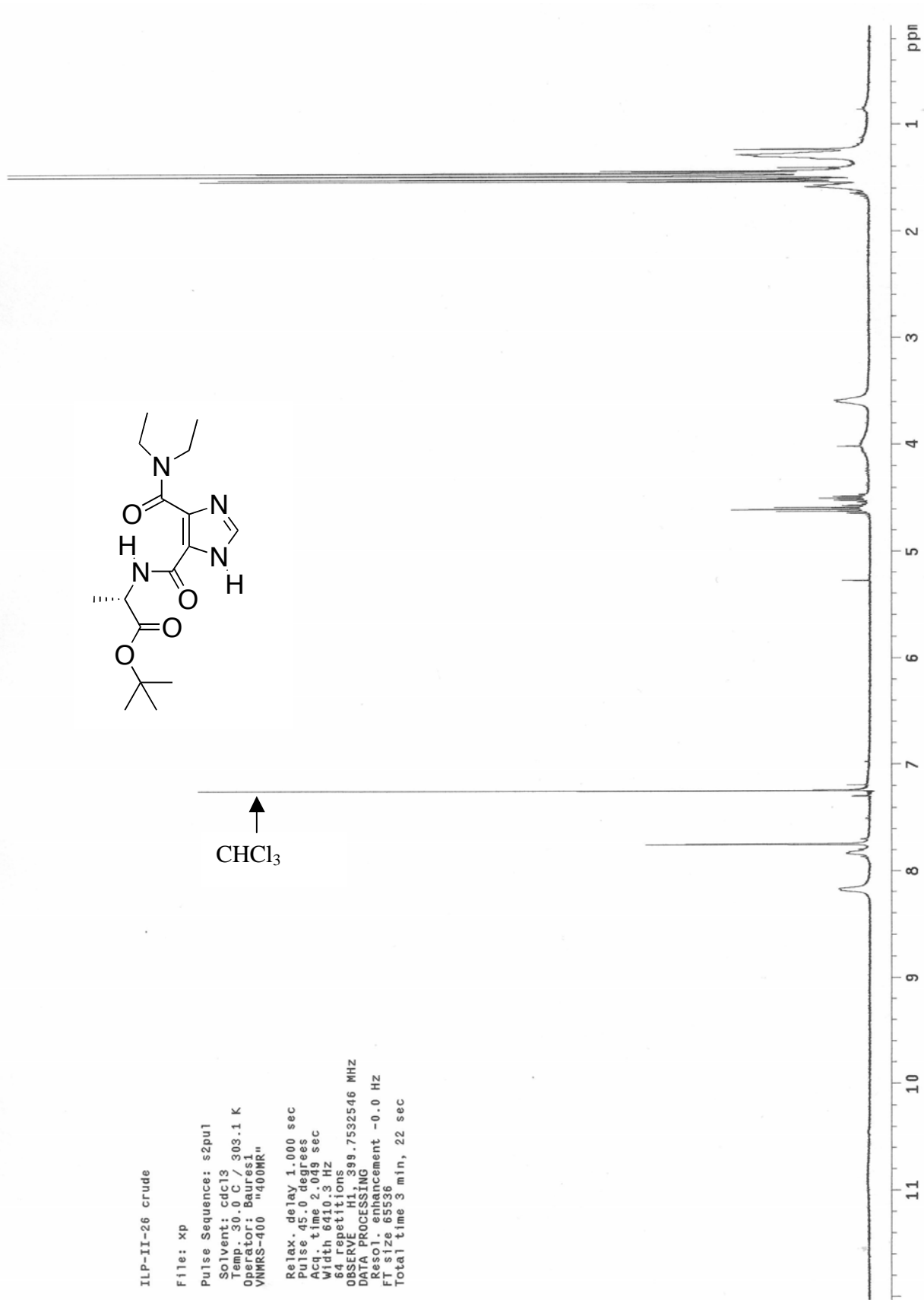


Figure S167. ¹H-NMR for the crude reaction to yield 5{38}.

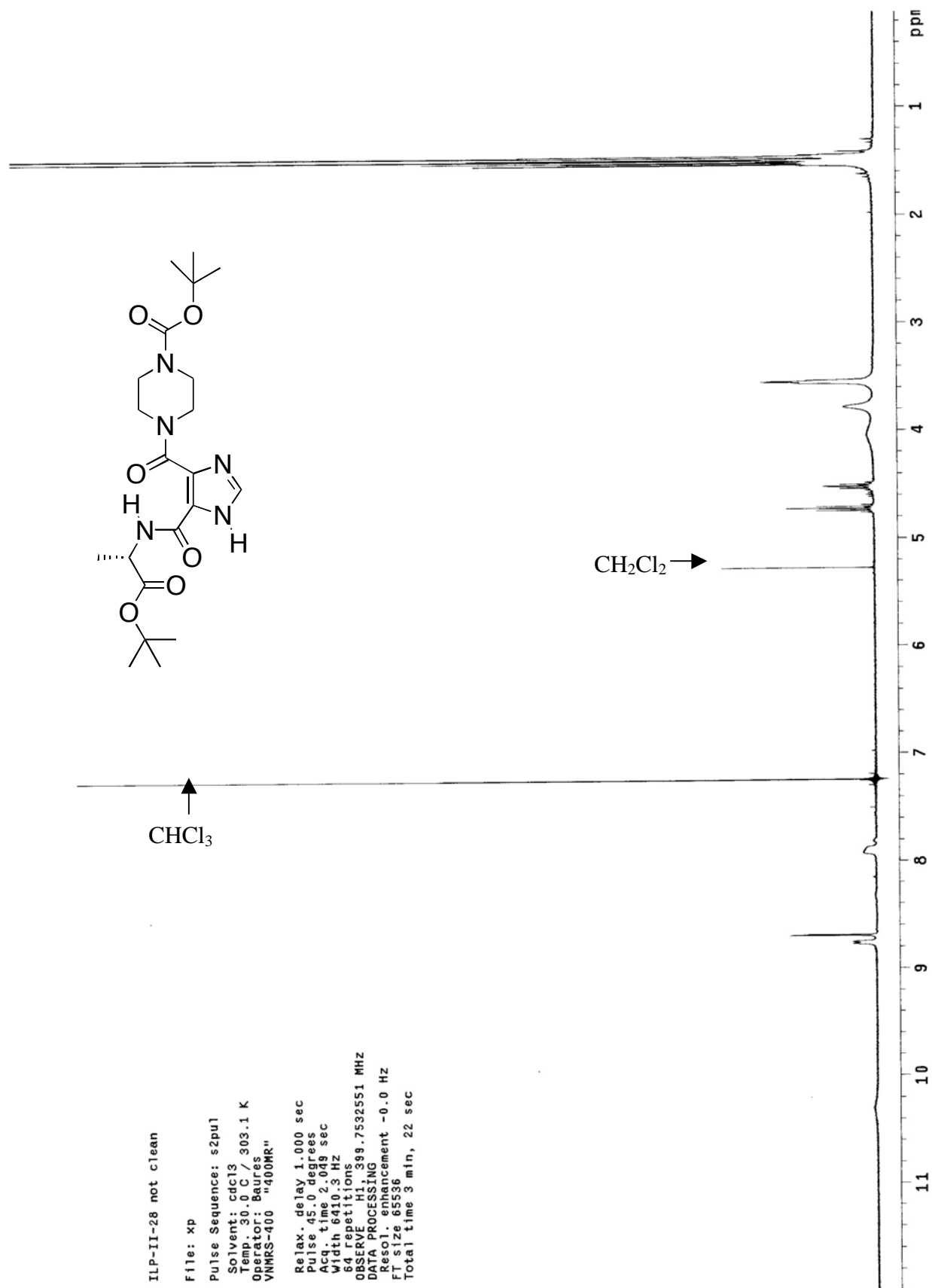


Figure S168. ¹H-NMR for the crude reaction to yield **5**{39}.

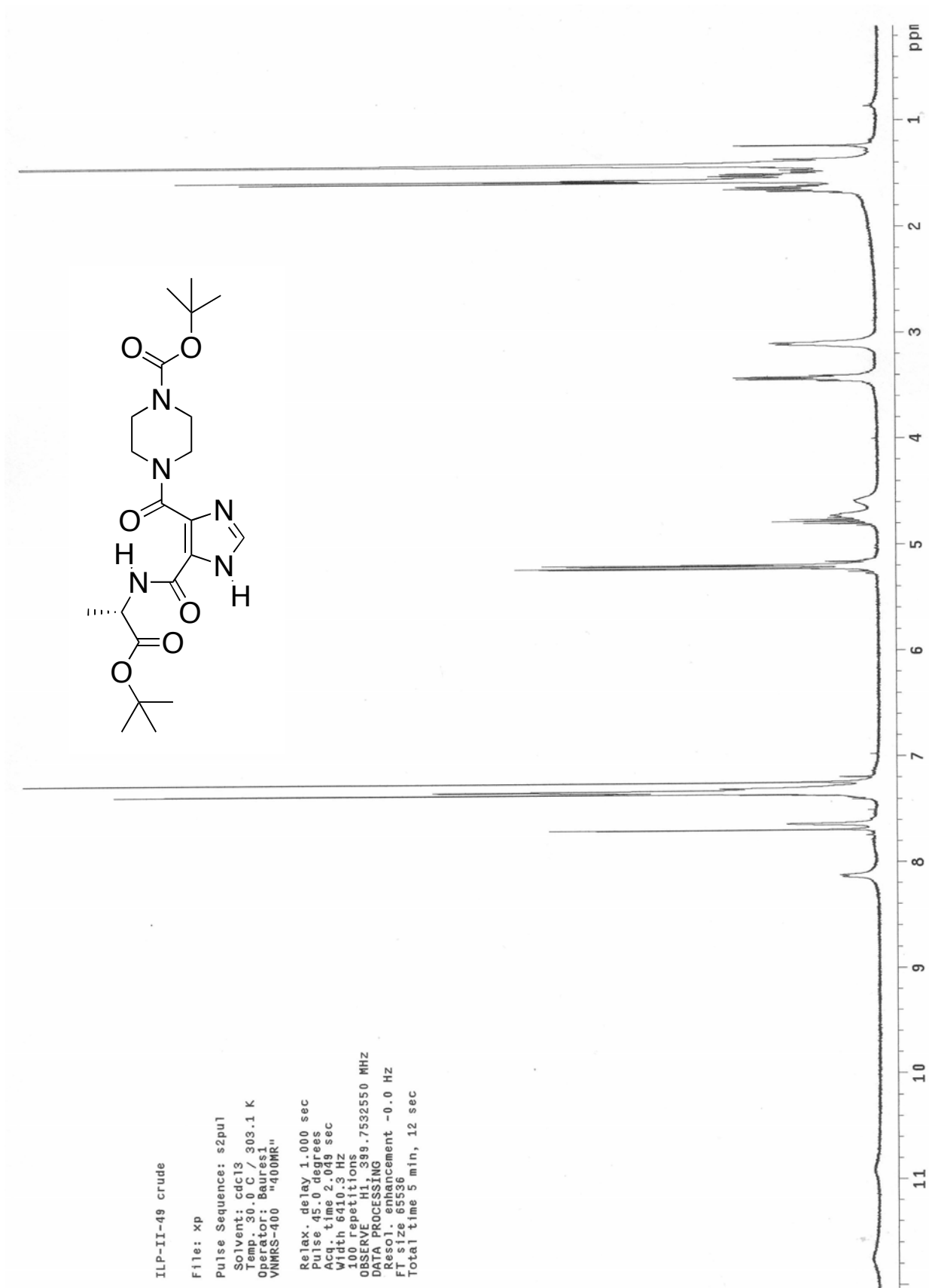


Figure S169. ¹H-NMR for the crude reaction to yield 5{44}.

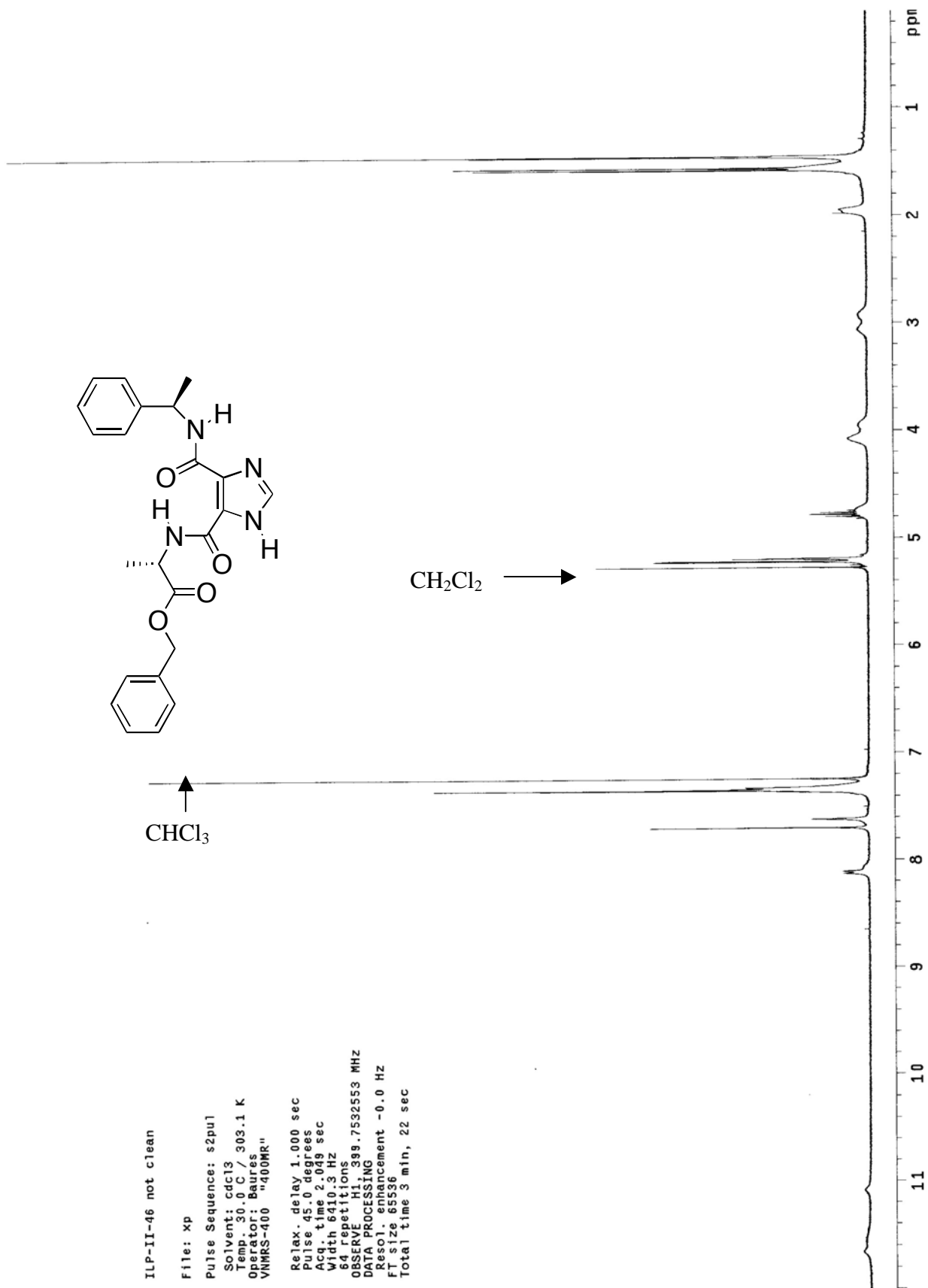


Figure S170. ¹H-NMR for the crude reaction to yield 5{48}.

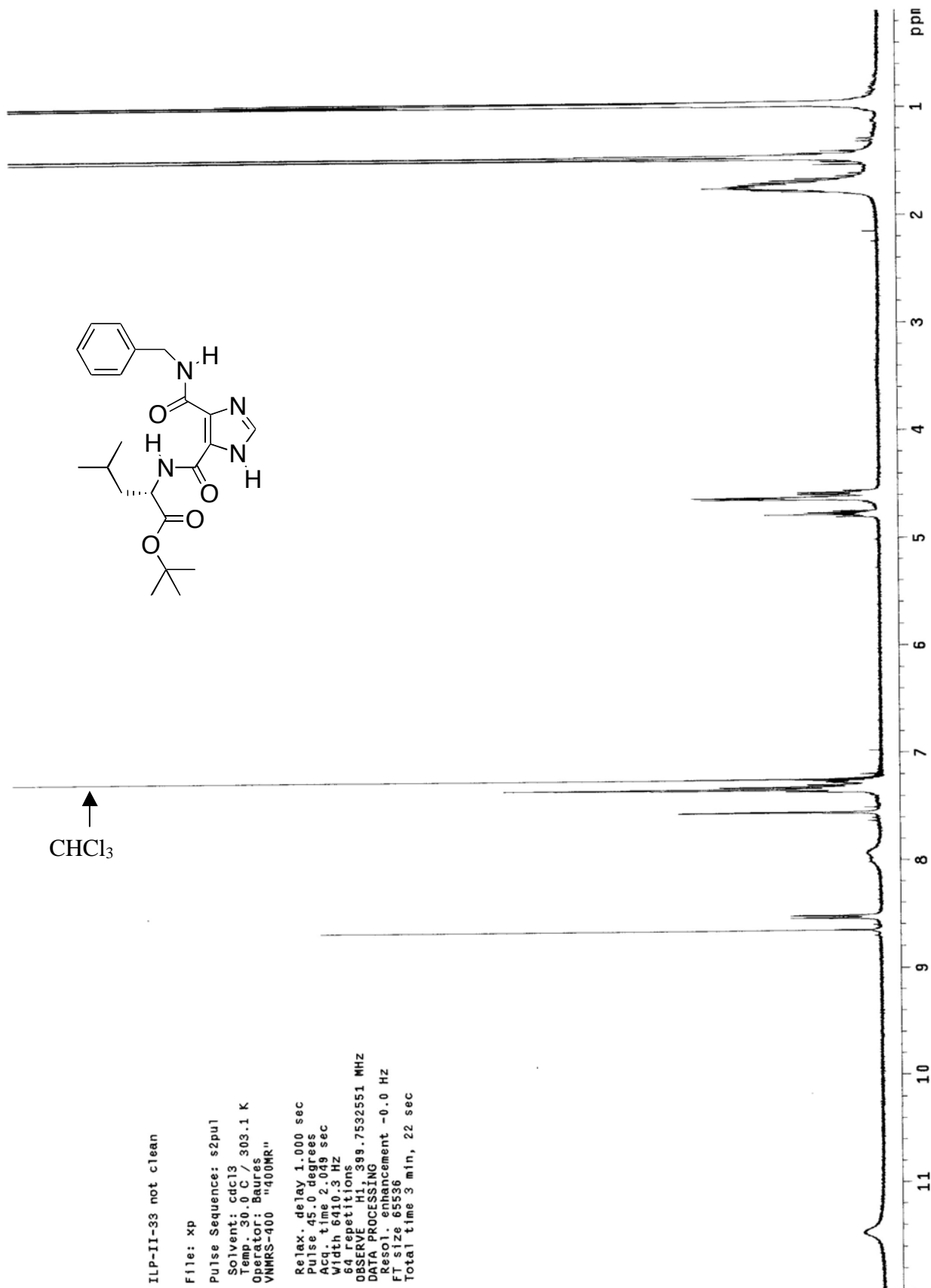


Figure S171. ¹H-NMR for the crude reaction to yield 5{59}.

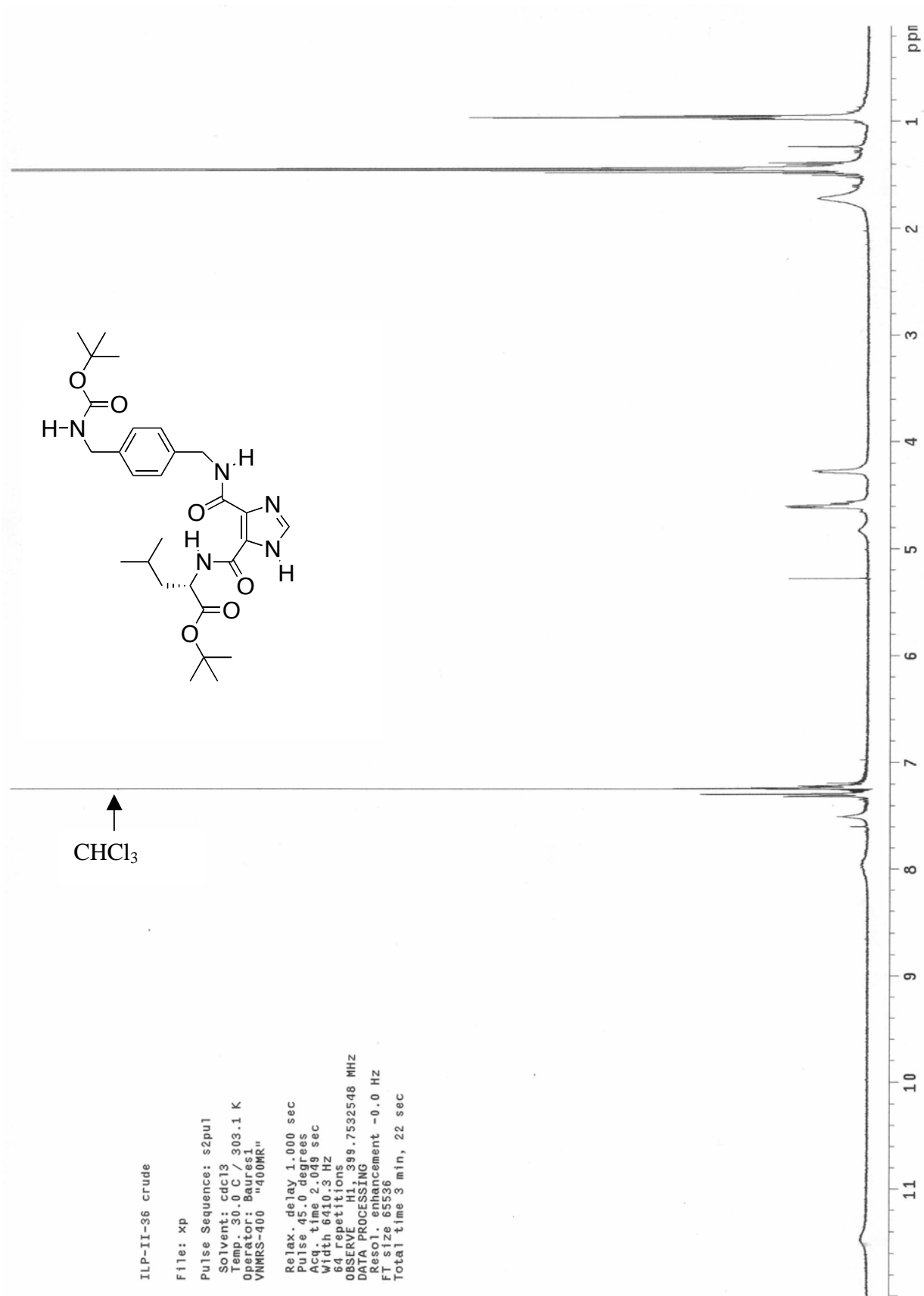


Figure S172. ¹H-NMR for the crude reaction to yield 5{63}.

ILP-II-7 not clean
File: xp
Pulse Sequence: s2pul
Solvent: cdcl3
Temp: 30.0 C / 303.1 K
Operator: Baures
VNMR-400 "400MR"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.099 sec
Width 6010.3 Hz
Sensitivity 1.3
OBSERVED F1 399.7532553 MHZ
DATA PROCESSING
Resol. enhancement -0.0 Hz
F1 size 65536
Total time 3 min, 22 sec

↑
CH₂Cl₂

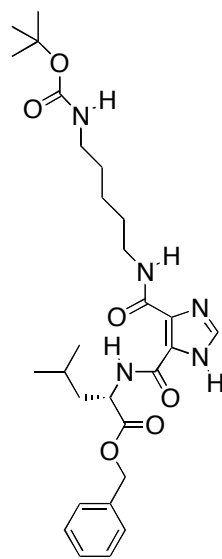


Figure S173. ¹H-NMR for the crude reaction to yield 5{72}.

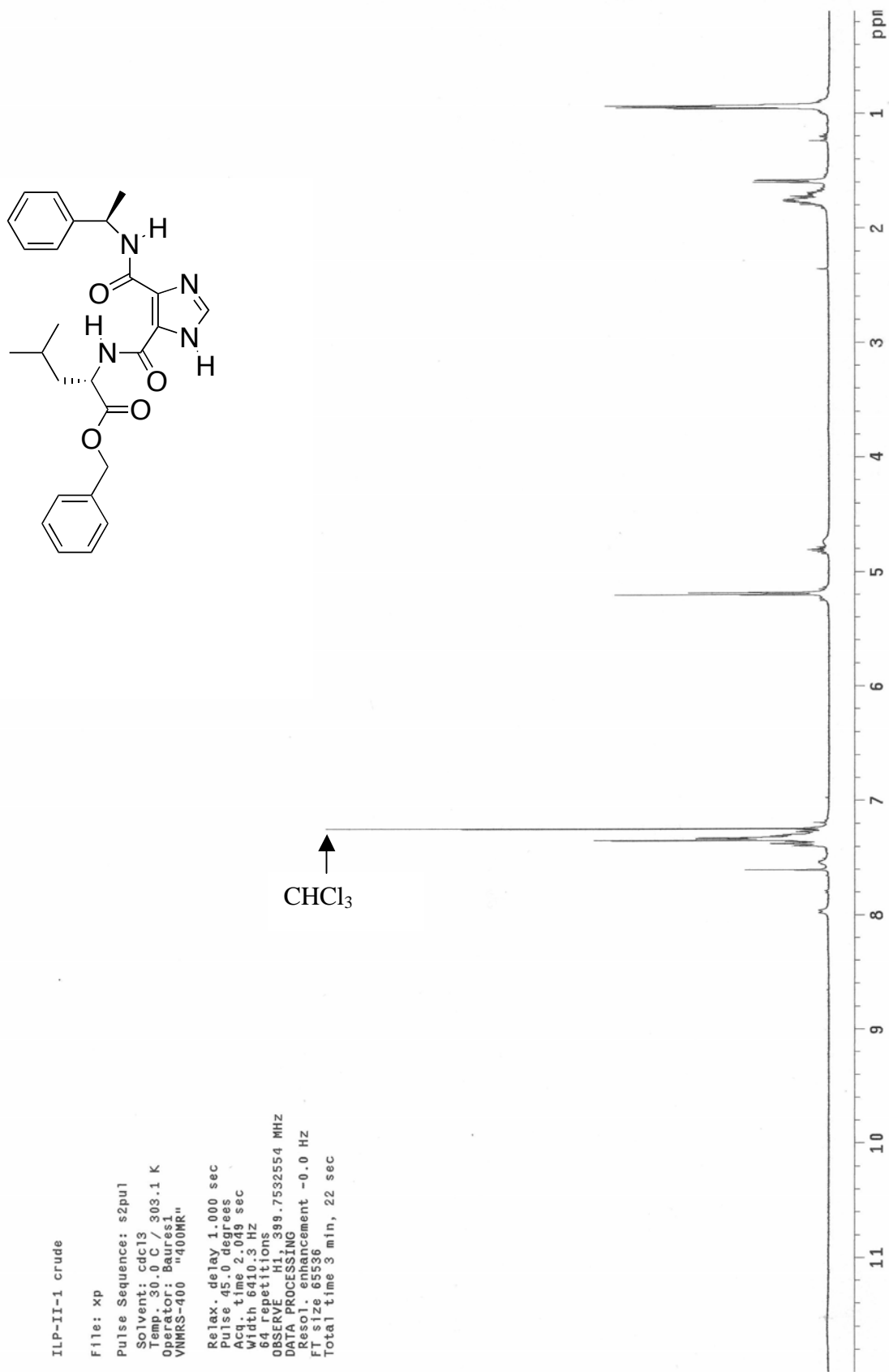


Figure S174. ¹H-NMR for the crude reaction to yield **5**{74}.

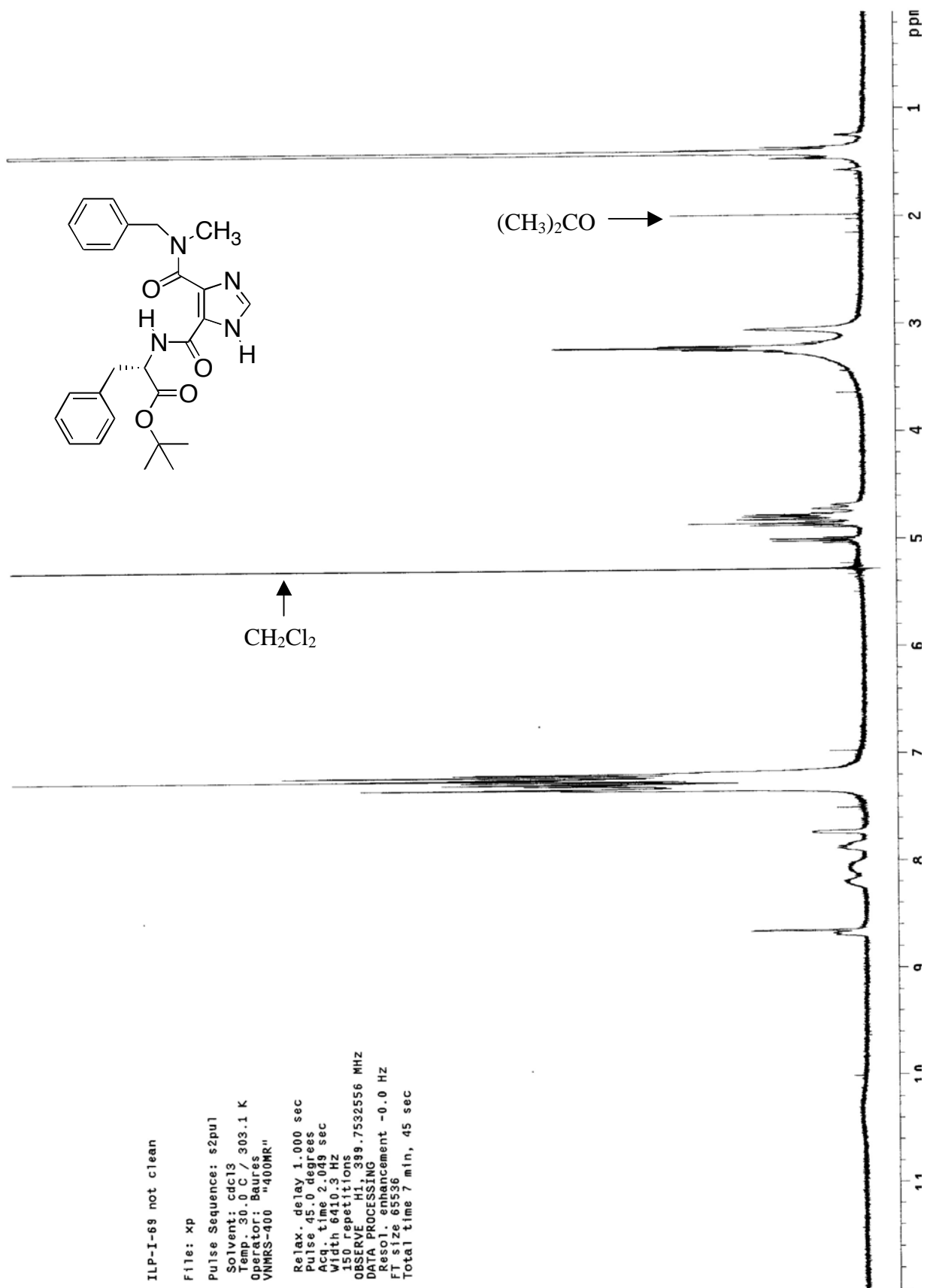


Figure S175. ¹H-NMR for the crude reaction to yield 5{93}.

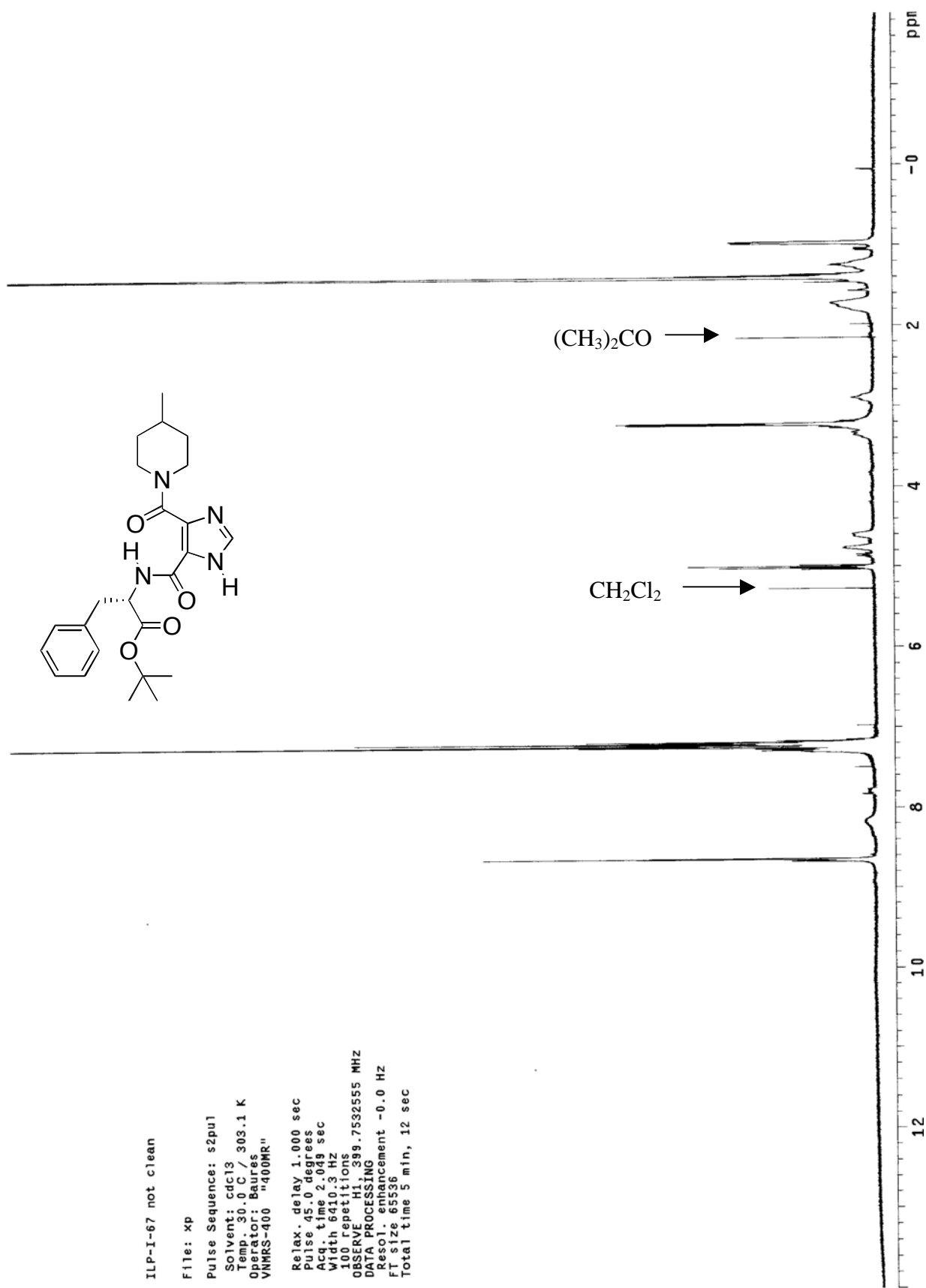


Figure S176. ¹H-NMR for the crude reaction to yield 5{97}.

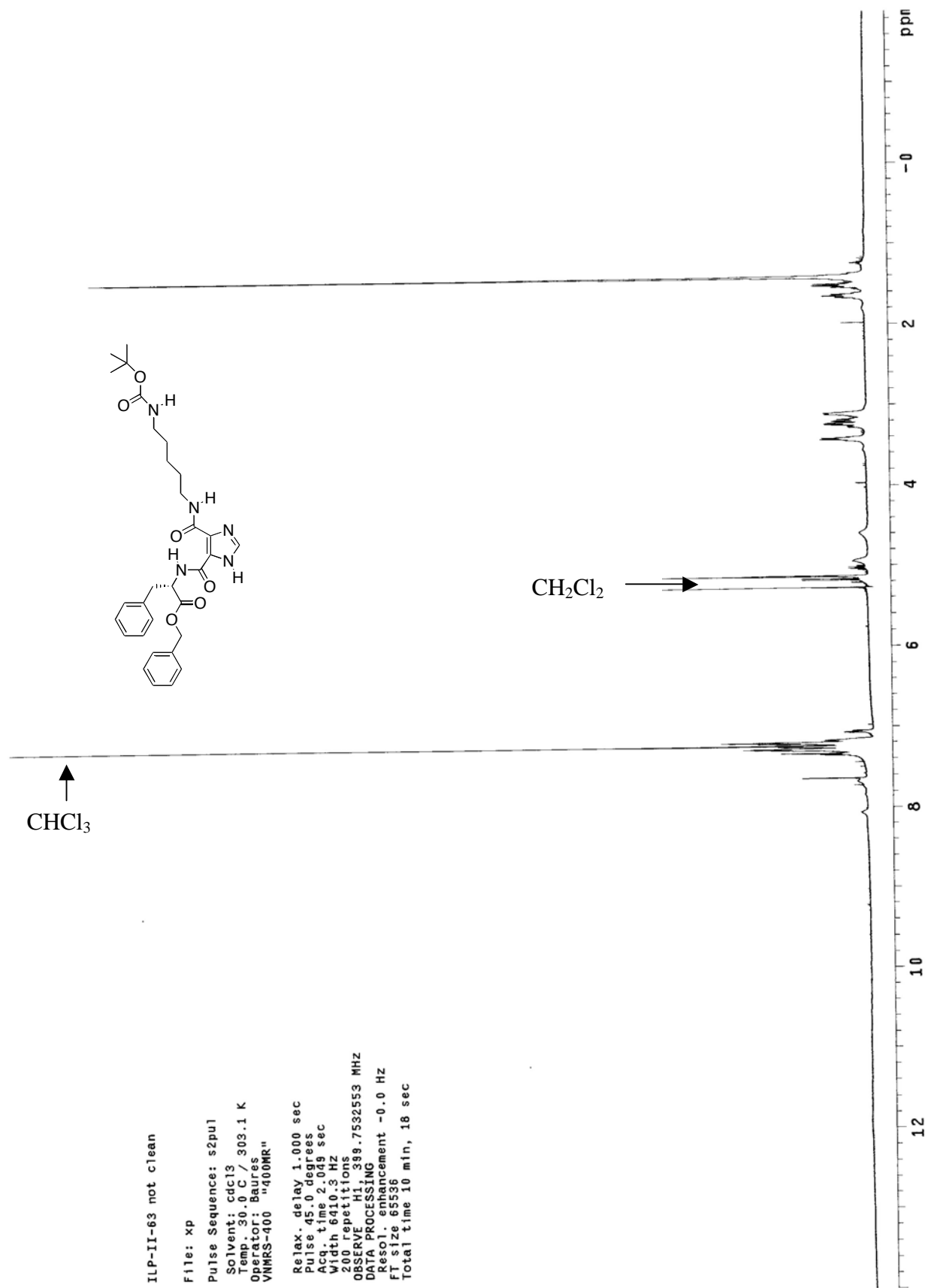


Figure S177. ¹H-NMR for the crude reaction to yield **5**{100}.

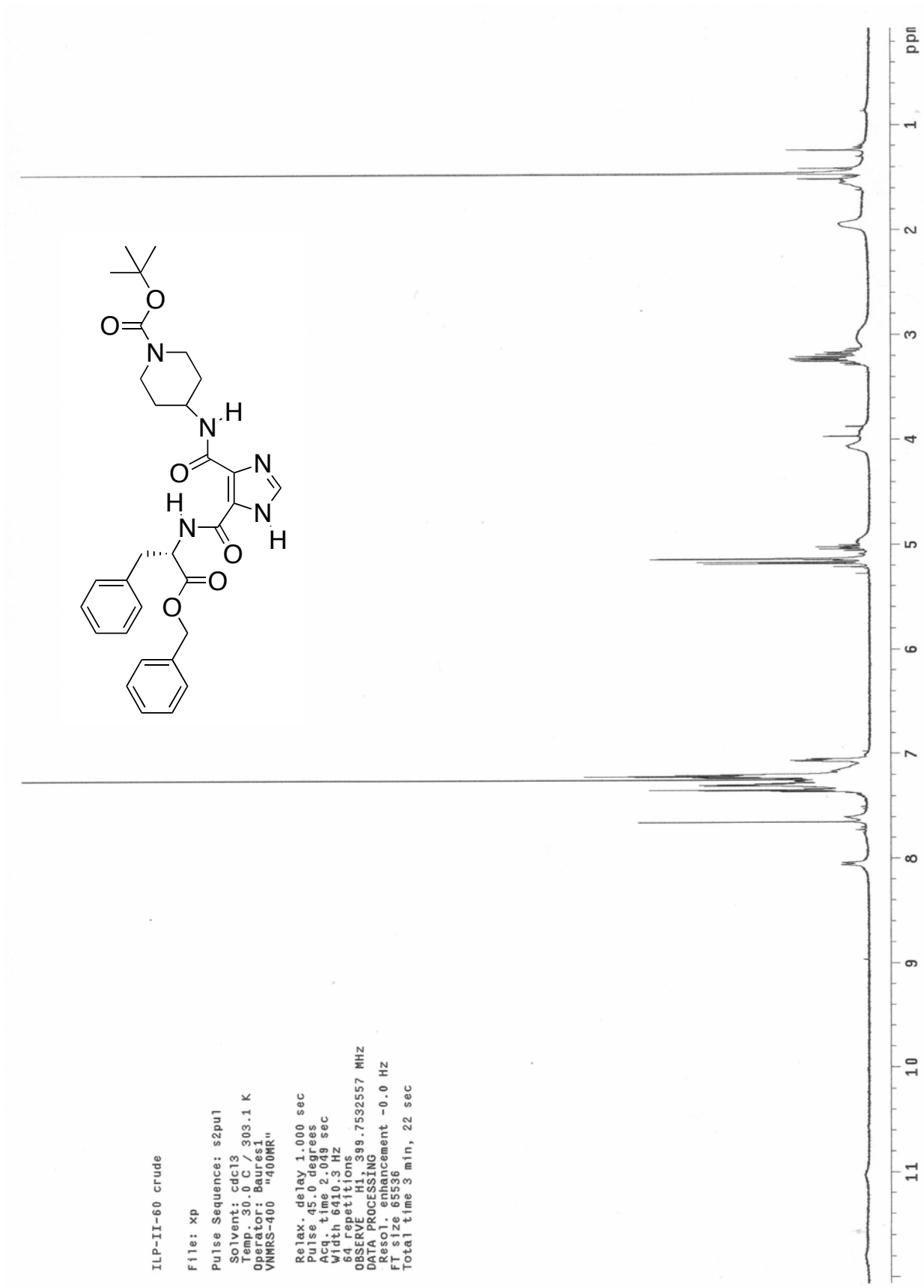


Figure S178. $^1\text{H-NMR}$ for the crude reaction to yield **5{104}**.

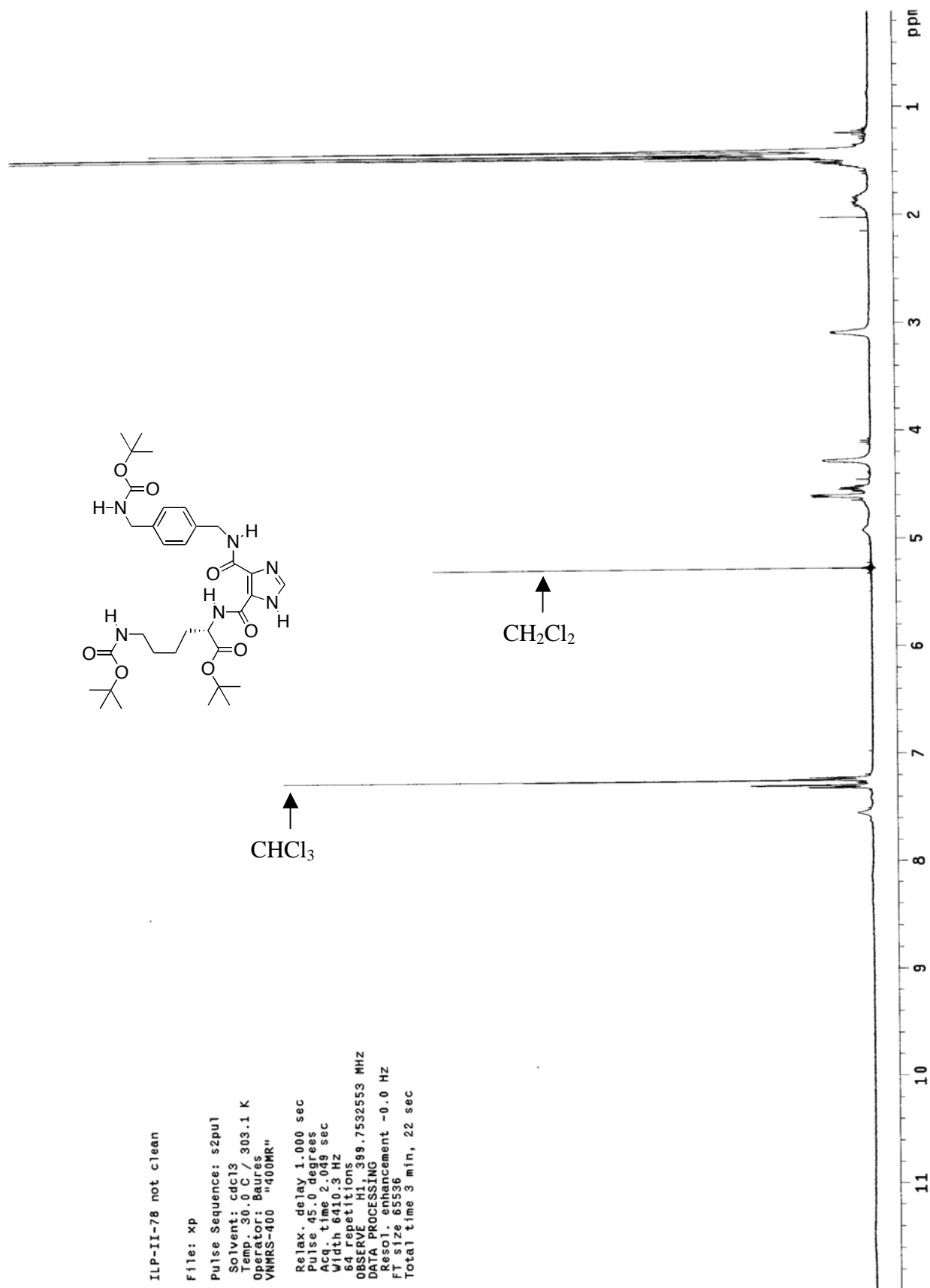


Figure S179. $^1\text{H-NMR}$ for the crude reaction to yield **5{119}**.

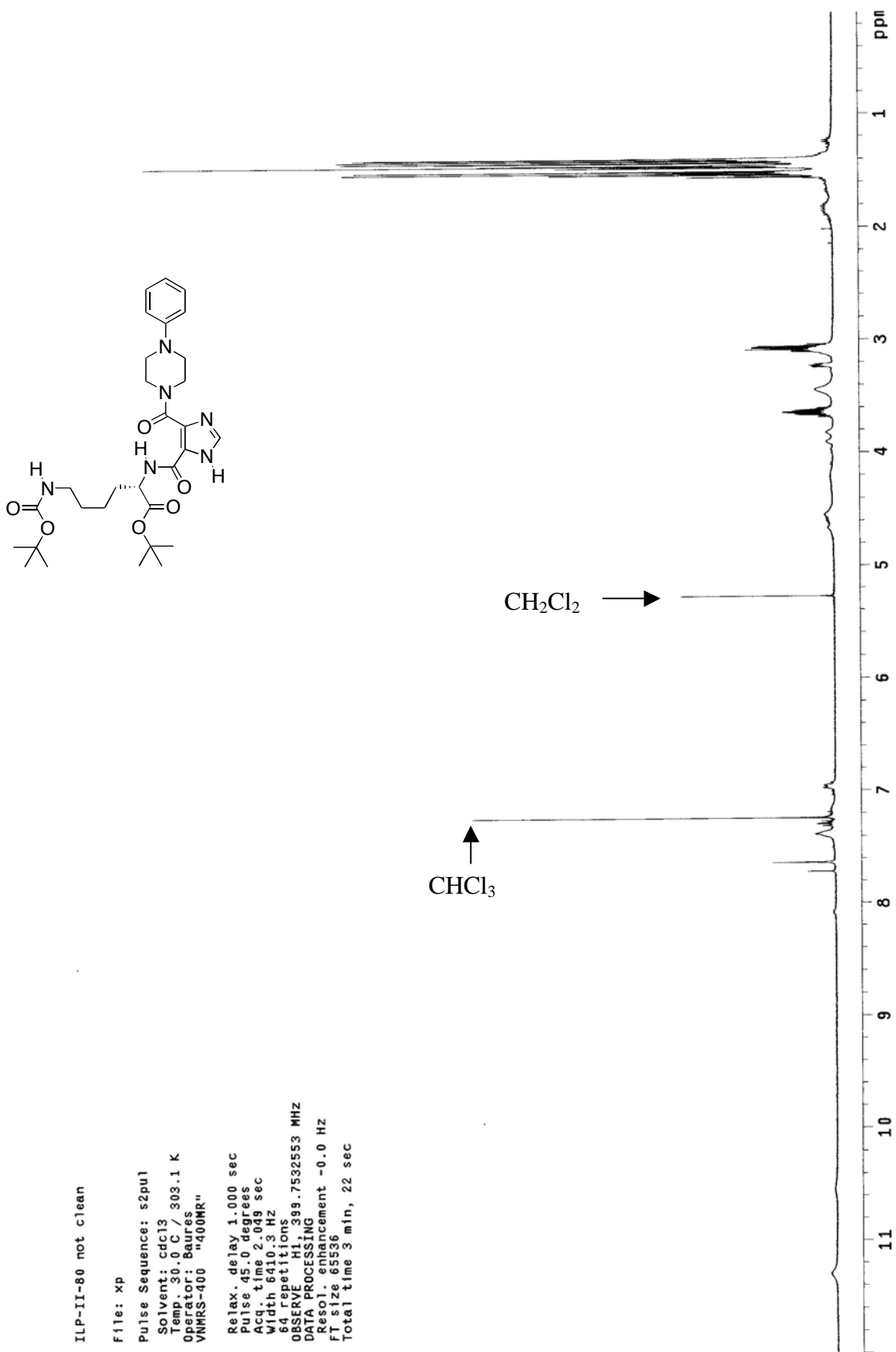


Figure S180. ¹H-NMR for the crude reaction to yield **5**{126}.