

Parallel Synthesis of a Library of Symmetrically- and Dissymmetrically-disubstituted
Imidazole-4,5-dicarboxamides Bearing Amino Acid Esters

*Rosanna Solinas, John C. DiCesare, and Paul W. Baures**

Department of Chemistry and Biochemistry, The University of Tulsa, 800 South Tucker Drive, Tulsa, OK

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Supporting Information

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Table S1. Symmetrically-disubstituted Amino Acid Ester I45DCs, **4**{1-9}.

compound	formula	MW	C log <i>P</i>	form	<i>R_f</i>	<i>R_t</i> (min)
4 {1}	C ₁₇ H ₂₆ N ₄ O ₆	382.41	0.35	solid	0.79	3.40
4 {2}	C ₂₃ H ₂₂ N ₄ O ₆	450.44	1.30	solid	0.22	4.06
4 {3}	C ₁₉ H ₃₀ N ₄ O ₆	410.47	0.97	glass film	0.69	4.91
4 {4}	C ₂₅ H ₂₆ N ₄ O ₆	478.50	1.92	glass film	0.12	5.04
4 {5}	C ₂₅ H ₄₂ N ₄ O ₆	494.62	3.89	glass film	0.45	8.39
4 {6}	C ₃₁ H ₃₈ N ₄ O ₆	562.66	4.83	glass film	0.52	8.11
4 {7}	C ₃₁ H ₃₈ N ₄ O ₆	562.66	3.81	glass film	0.62	7.73
4 {8}	C ₃₇ H ₃₄ N ₄ O ₆	630.69	4.76	solid	0.23	7.37
4 {9}	C ₃₅ H ₆₀ N ₆ O ₁₀	724.44	3.86	glass film	0.86	7.14

Table S2. Dissymmetrically-disubstituted Amino Acid Ester I45DCs, 4{10-45}.

compound	formula	MW	C log <i>P</i>	form	<i>R</i> _f	<i>R</i> _t (min)
4{10}	C ₂₀ H ₂₄ N ₄ O ₆	416.43	1.17	glass film	0.83	3.67
4{11}	C ₁₈ H ₂₈ N ₄ O ₆	396.44	0.66	glass film	0.86	4.00
4{12}	C ₂₁ H ₂₆ N ₄ O ₆	430.45	1.14	glass film	0.85	4.31
4{13}	C ₂₁ H ₃₄ N ₄ O ₆	438.52	2.12	glass film	0.91	5.86
4{14}	C ₂₄ H ₃₂ N ₄ O ₆	472.53	2.59	glass film	0.83	6.04
4{15}	C ₂₄ H ₃₂ N ₄ O ₆	472.53	2.42	glass film	0.78	6.00
4{16}	C ₂₇ H ₃₀ N ₄ O ₆	506.55	2.90	glass film	0.84	6.18
4{17}	C ₂₆ H ₄₃ N ₅ O ₈	553.31	2.11	glass film	0.61	5.45
4{18}	C ₂₁ H ₂₆ N ₄ O ₆	430.56	1.48	glass film	0.56	4.36
4{19}	C ₂₄ H ₂₄ N ₄ O ₆	464.47	1.61	solid	0.70	4.54
4{20}	C ₂₄ H ₃₂ N ₄ O ₆	472.53	2.93	glass film	0.69	6.06
4{21}	C ₂₇ H ₃₀ N ₄ O ₆	506.55	3.07	glass film	0.55	6.06
4{22}	C ₂₇ H ₃₀ N ₄ O ₆	506.55	2.56	glass film	0.67	5.90
4{23}	C ₃₀ H ₂₈ N ₄ O ₆	540.57	3.03	glass film	0.64	5.95
4{24}	C ₂₉ H ₄₁ N ₅ O ₈	587.67	2.92	glass film	0.62	5.93
4{25}	C ₂₂ H ₂₈ N ₄ O ₆	444.48	1.45	glass film	0.57	5.37
4{26}	C ₂₂ H ₃₆ N ₄ O ₆	452.54	2.43	glass film	0.37	7.44
4{27}	C ₂₅ H ₃₄ N ₄ O ₆	486.56	2.90	glass film	0.45	6.66
4{28}	C ₂₅ H ₃₄ N ₄ O ₆	486.56	2.73	glass film	0.54	6.53
4{29}	C ₂₈ H ₃₂ N ₄ O ₆	520.58	3.20	glass film	0.56	6.38
4{30}	C ₂₇ H ₄₅ N ₅ O ₈	567.68	2.42	glass film	0.77	6.13
4{31}	C ₂₅ H ₃₄ N ₄ O ₆	486.56	3.24	glass film	0.39	6.80
4{32}	C ₂₈ H ₃₂ N ₄ O ₆	520.58	3.38	glass film	0.40	6.79
4{33}	C ₂₈ H ₃₂ N ₄ O ₆	520.58	2.86	glass film	0.59	6.38
4{34}	C ₃₁ H ₃₀ N ₄ O ₆	554.59	3.34	glass film	0.35	6.52
4{35}	C ₃₉ H ₄₃ N ₅ O ₈	601.31	2.89	glass film	0.63	6.25
4{36}	C ₂₈ H ₄₀ N ₄ O ₆	528.64	4.36	glass film	0.51	8.31
4{37}	C ₂₈ H ₄₀ N ₄ O ₆	528.64	4.19	glass film	0.42	7.99
4{38}	C ₃₁ H ₃₈ N ₄ O ₆	562.66	4.66	glass film	0.39	7.79
4{39}	C ₃₀ H ₅₁ N ₅ O ₈	609.76	3.87	glass film	0.33	7.48
4{40}	C ₃₁ H ₃₈ N ₄ O ₆	562.66	4.32	glass film	0.44	7.95
4{41}	C ₃₄ H ₃₆ N ₄ O ₆	596.67	4.80	glass film	0.47	7.64
4{42}	C ₃₃ H ₄₉ N ₅ O ₈	643.77	4.35	glass film	0.29	7.39
4{43}	C ₃₄ H ₃₆ N ₄ O ₆	596.67	4.28	glass film	0.48	7.44
4{44}	C ₃₃ H ₄₉ N ₅ O ₈	643.77	4.17	glass film	0.59	7.29
4{45}	C ₃₆ H ₄₇ N ₅ O ₈	677.34	4.65	glass film	0.56	7.29

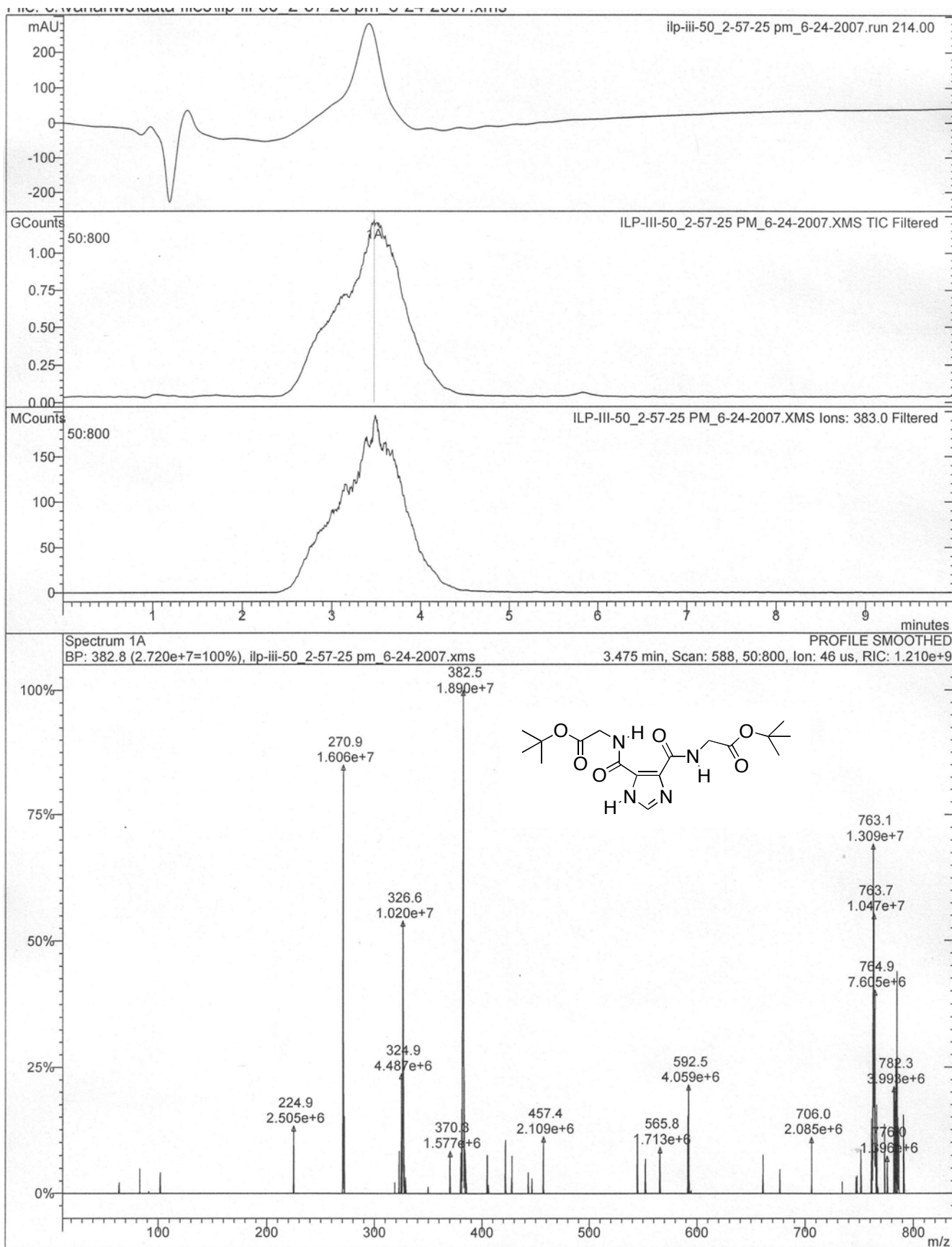


Figure S1. LC/MS data for 4{1}.

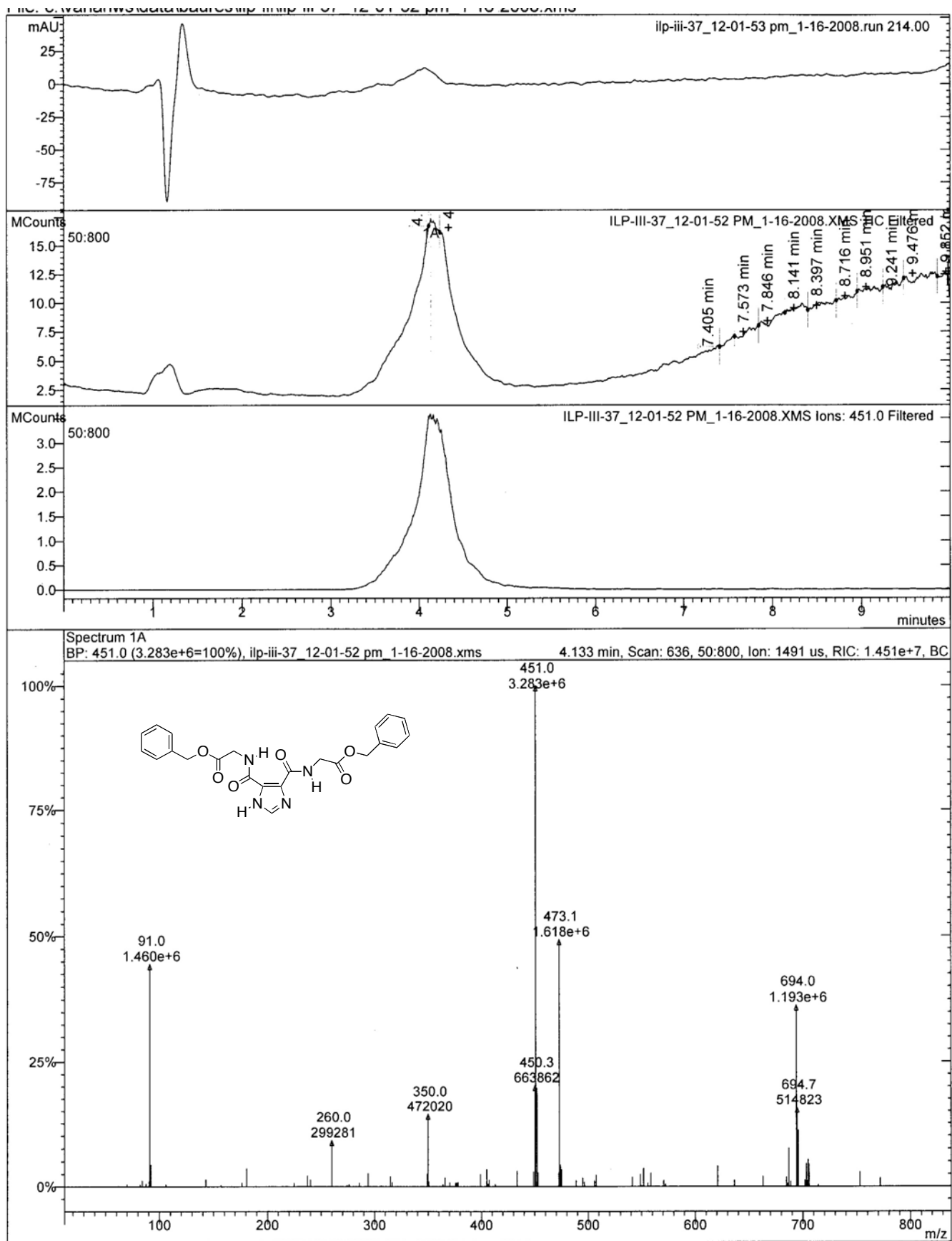


Figure S2. LC/MS data for 4{2}.

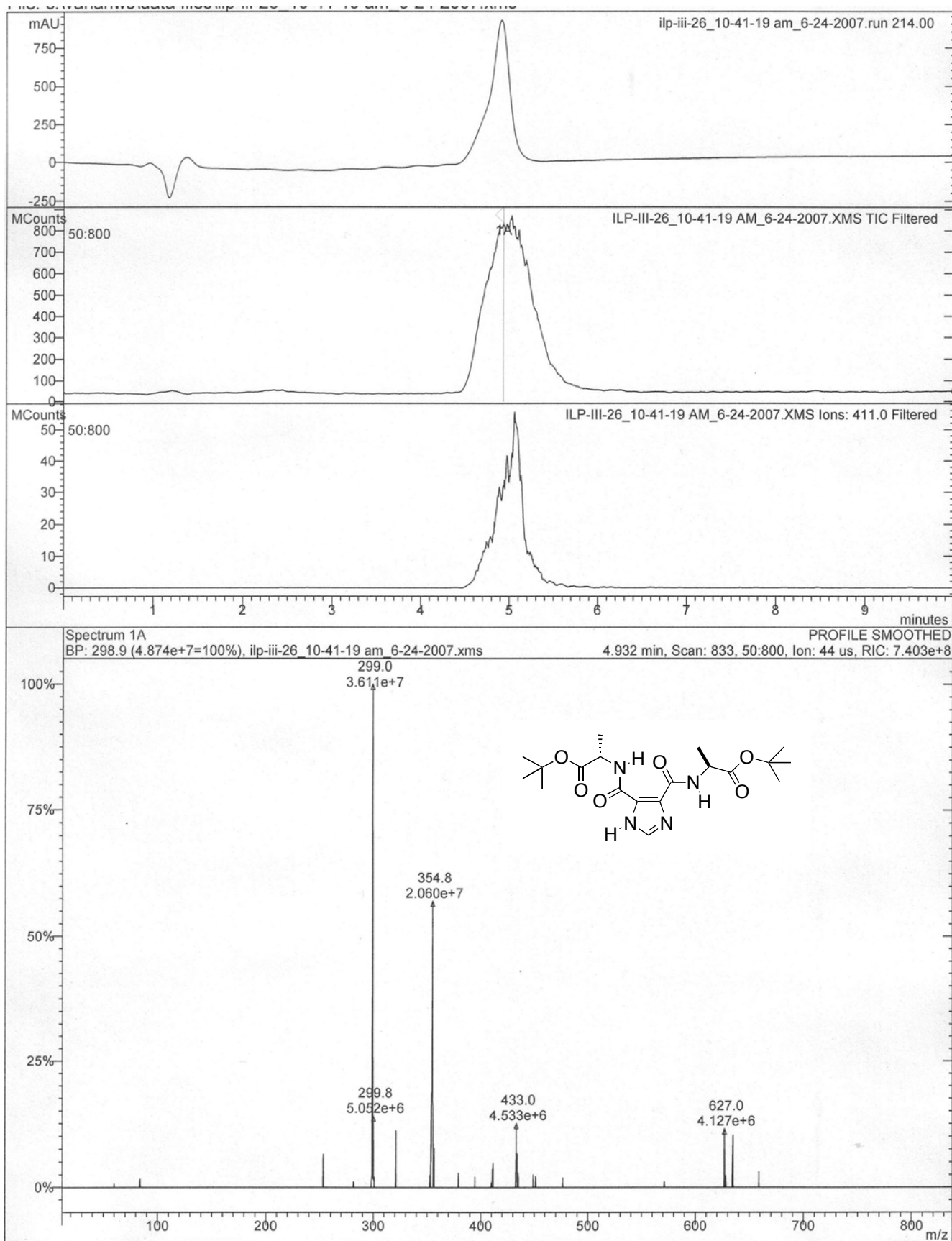


Figure S3. LC/MS data for 4{3}.

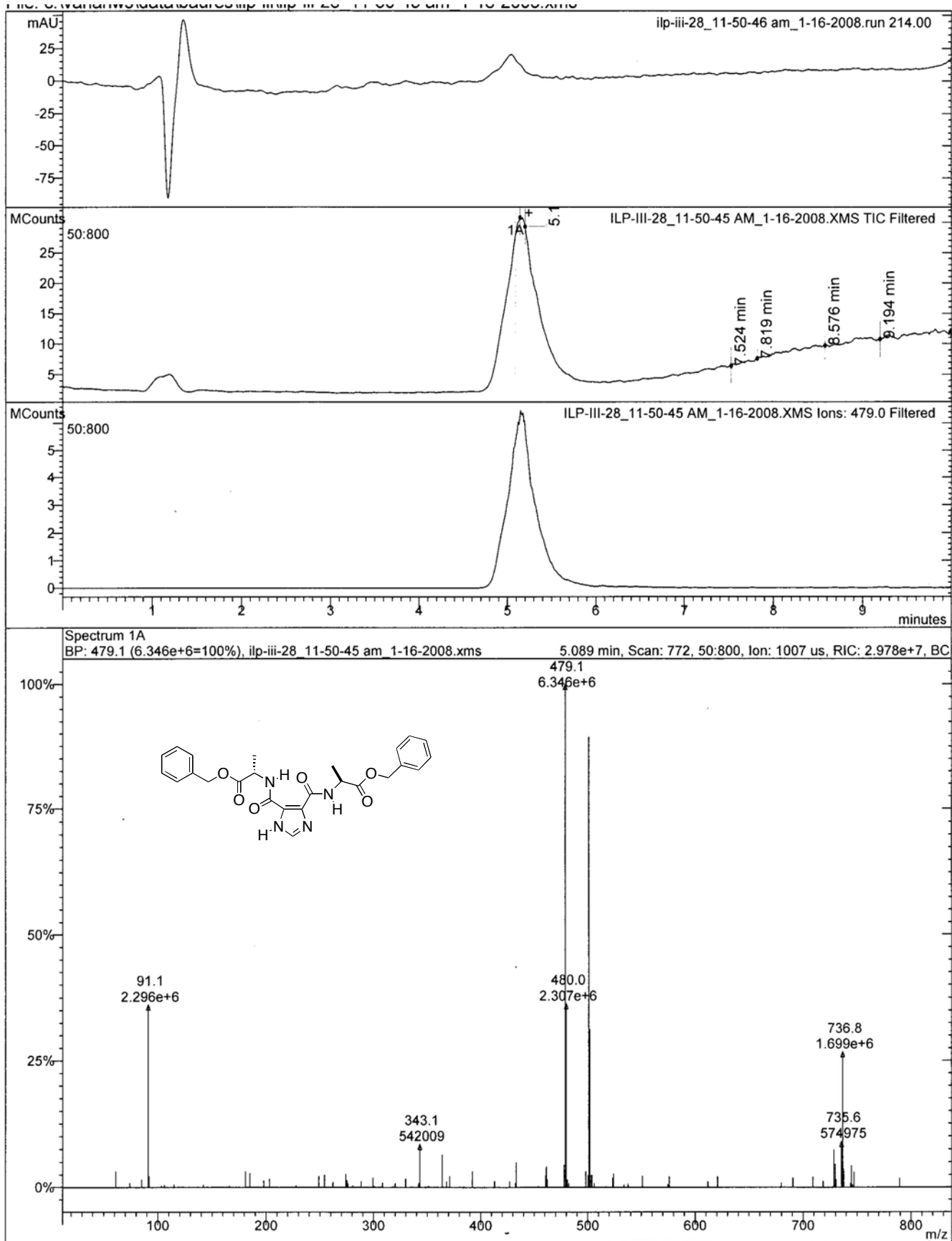


Figure S4. LC/MS data for 4{4}.

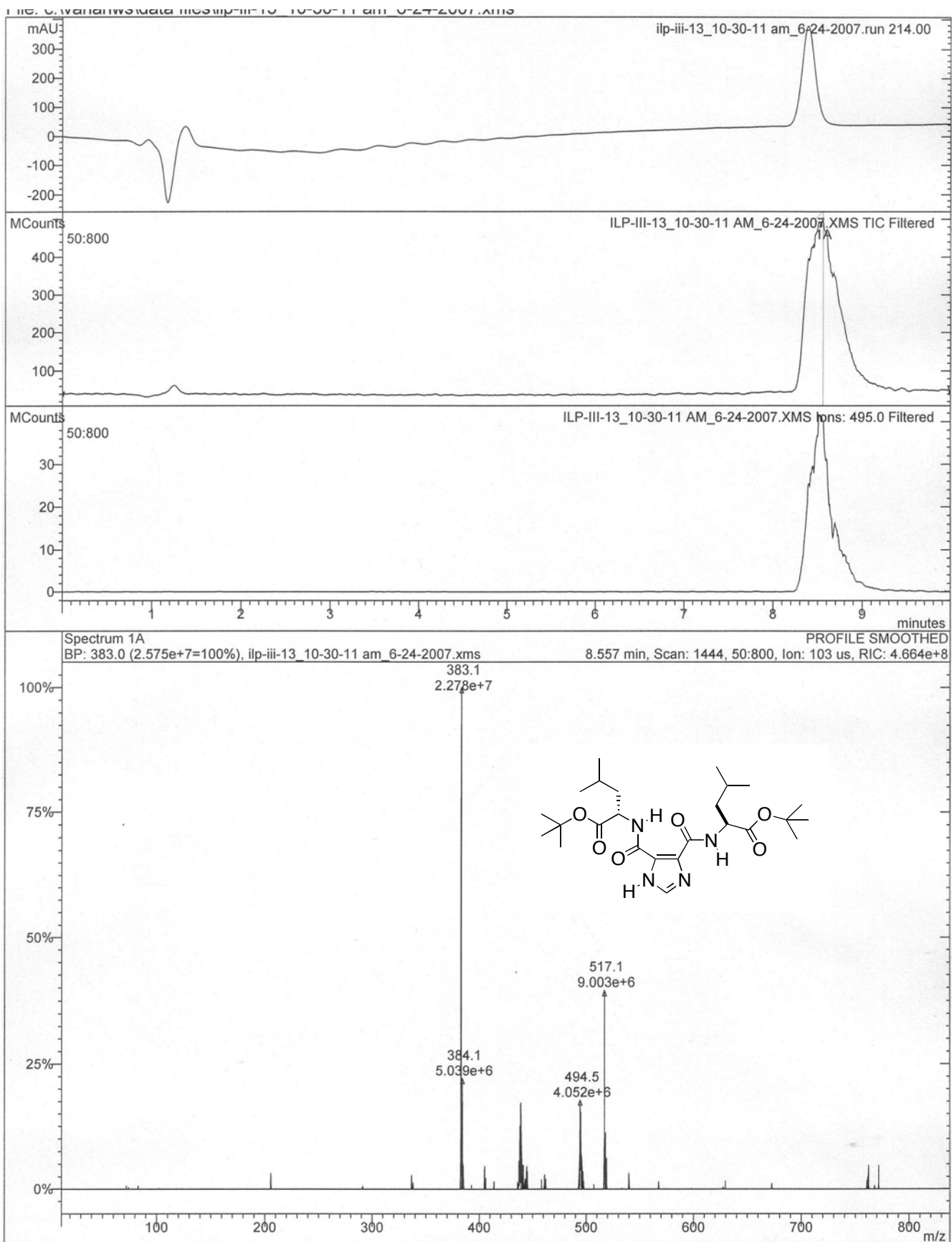


Figure S5. LC/MS data for 4{5}.

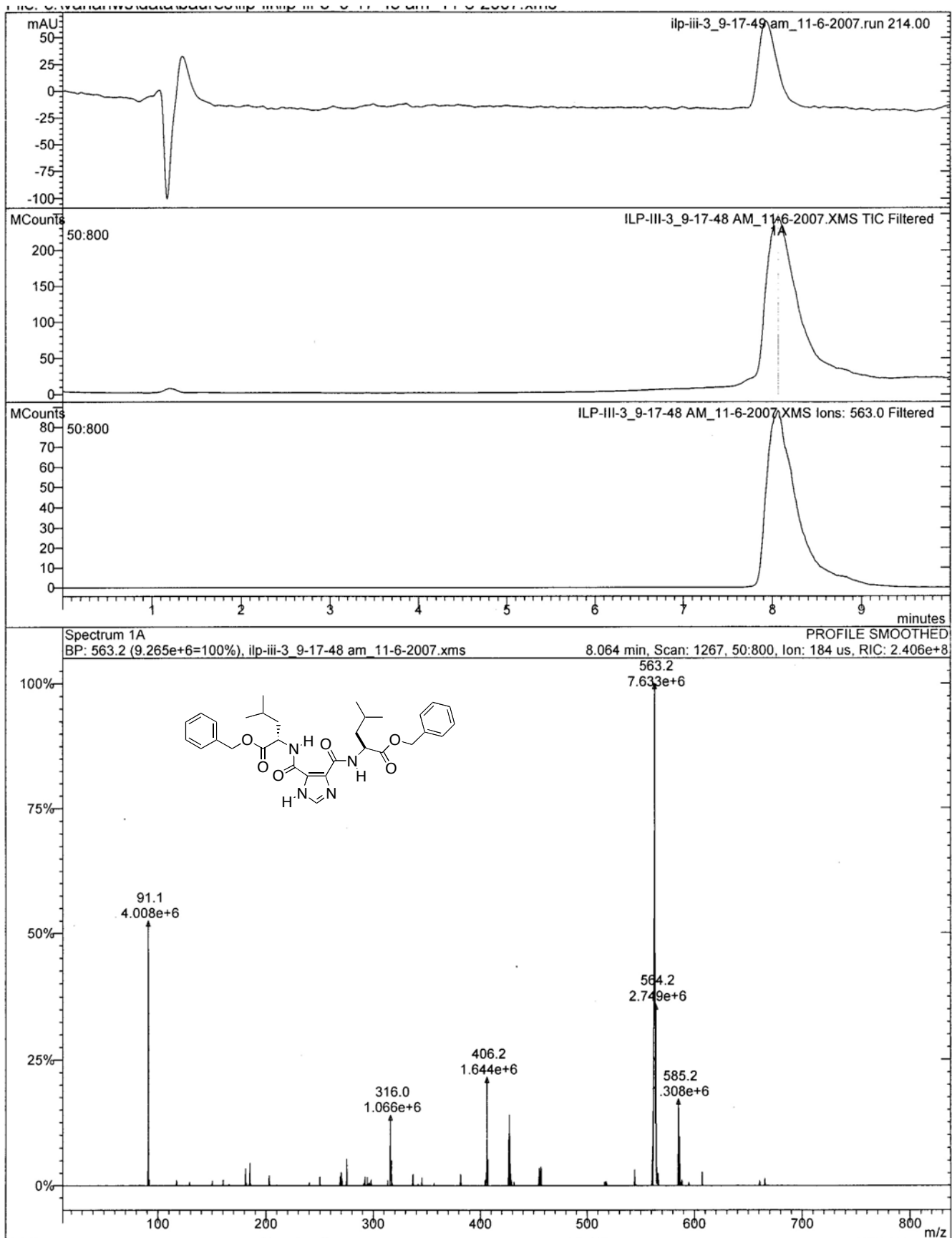


Figure S6. LC/MS data for 4{6}.

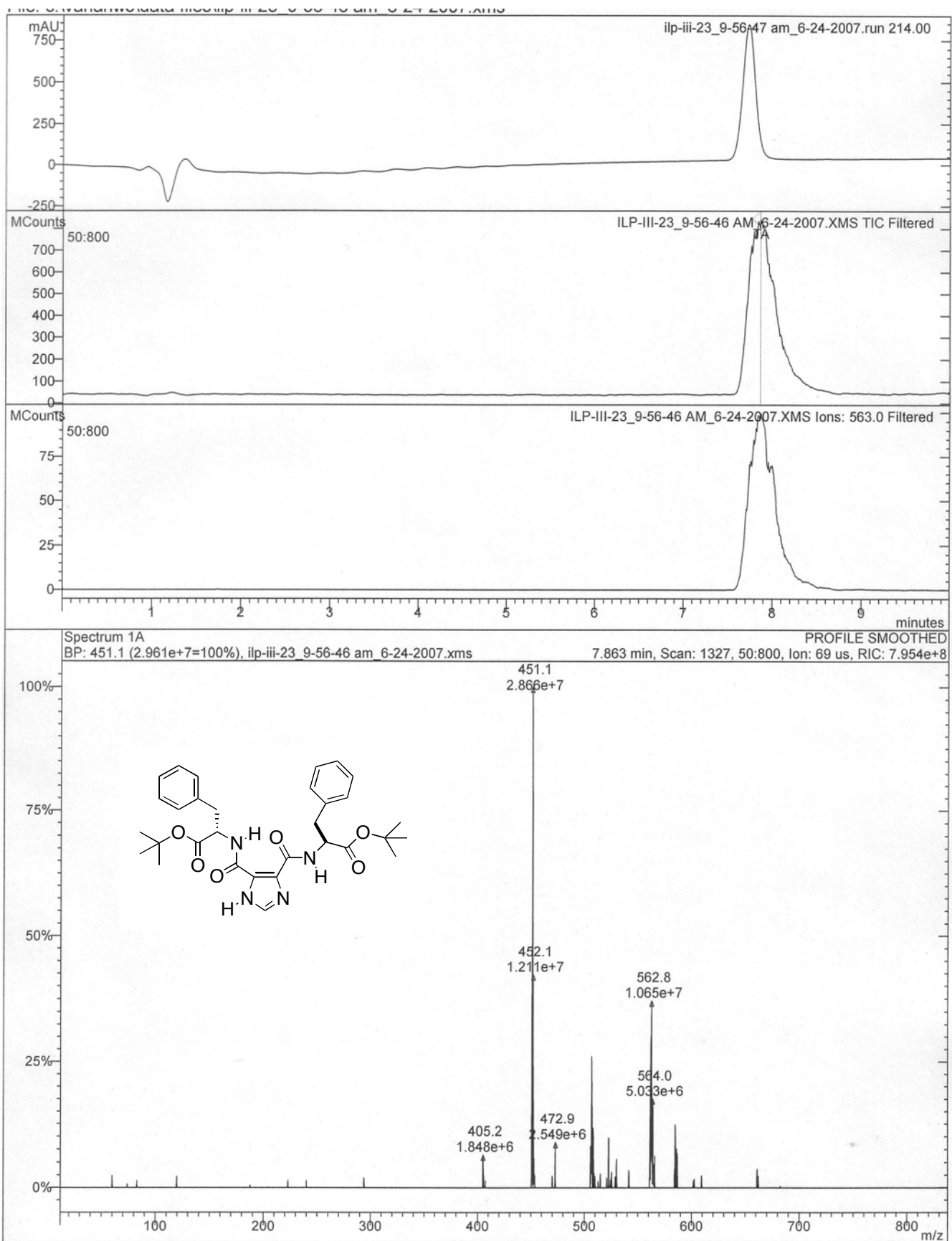


Figure S7. LC/MS data for 4{7}.

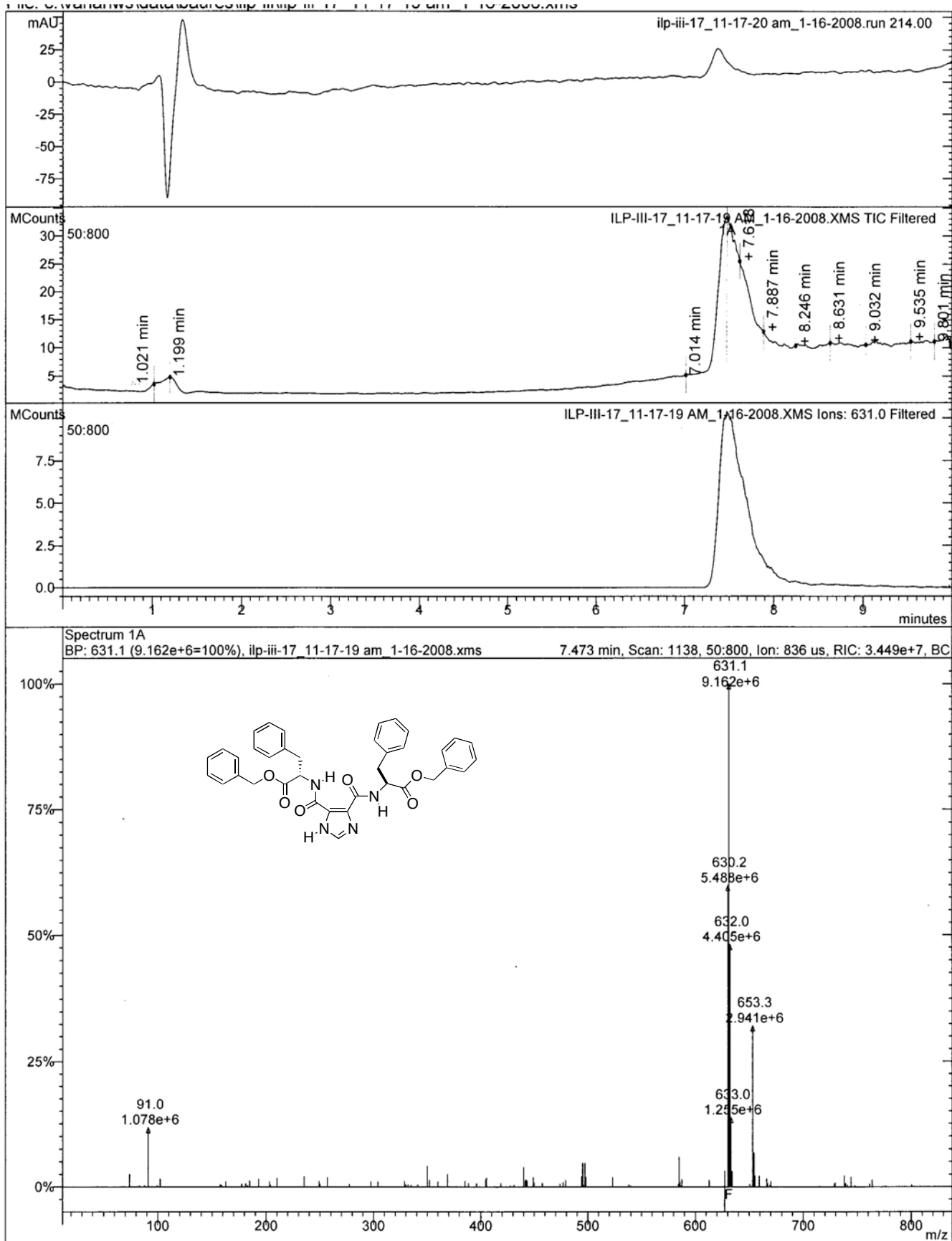


Figure S8. LC/MS data for 4{8}.

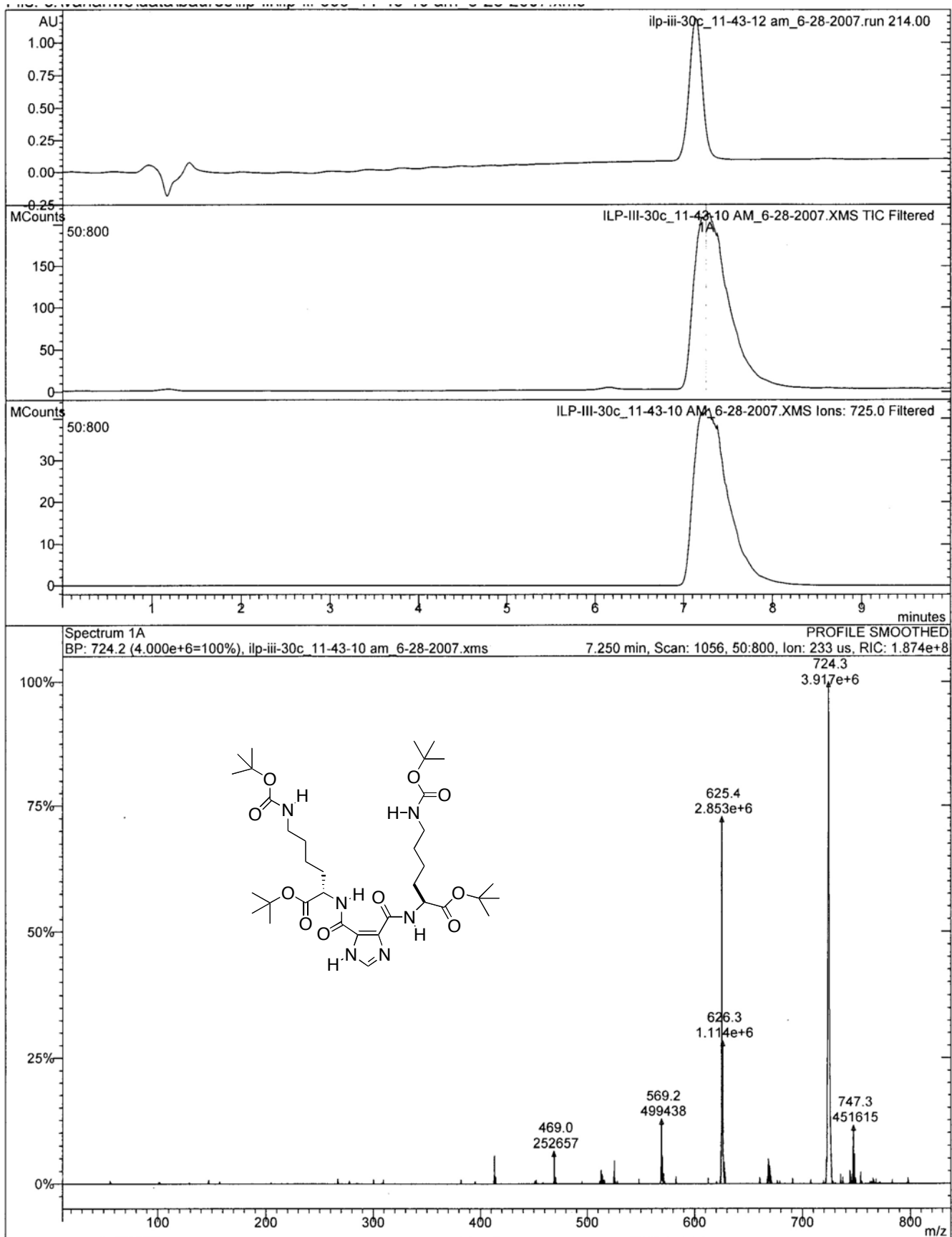


Figure S9. LC/MS data for 4{9}.

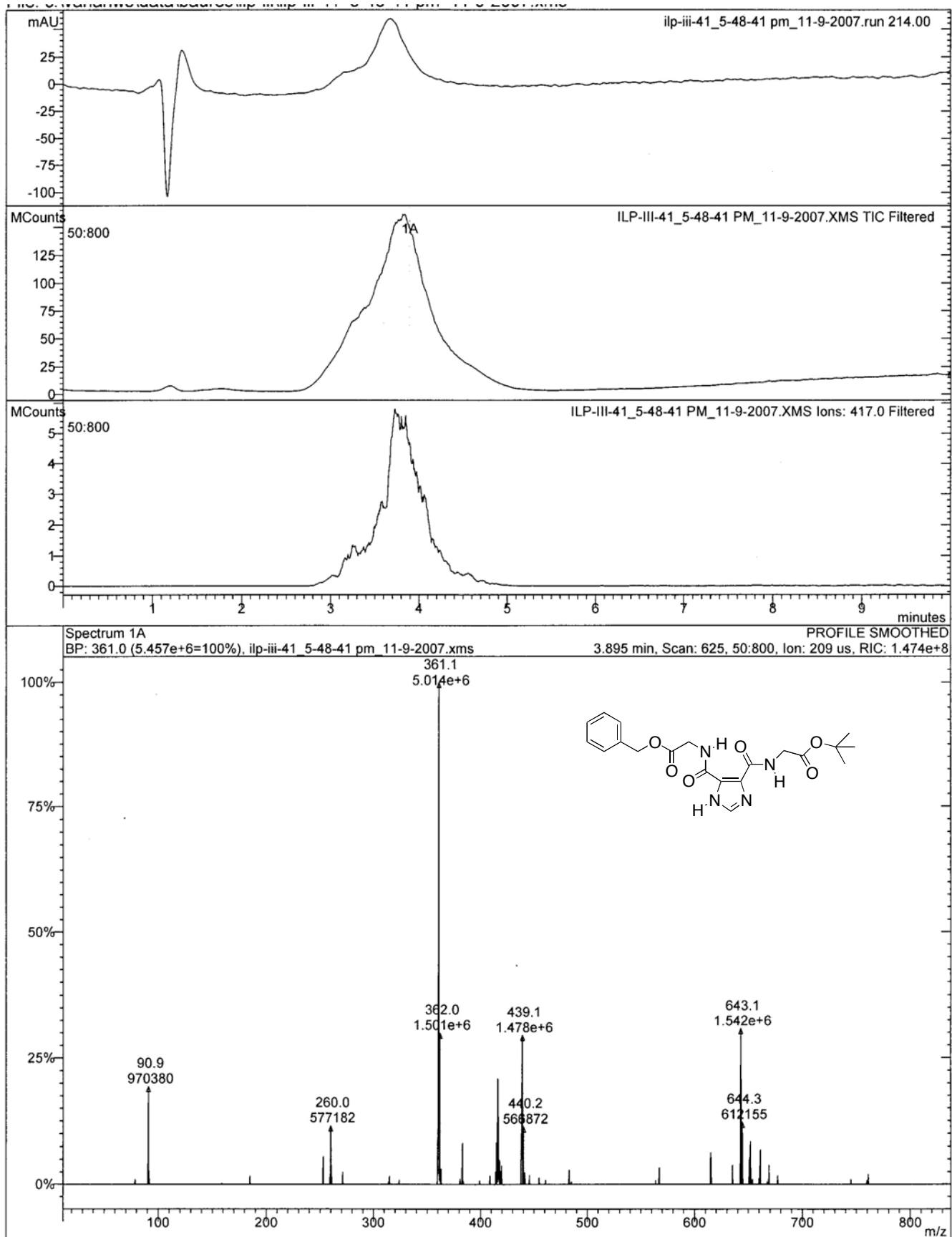


Figure S10. LC/MS data for 4{10}.

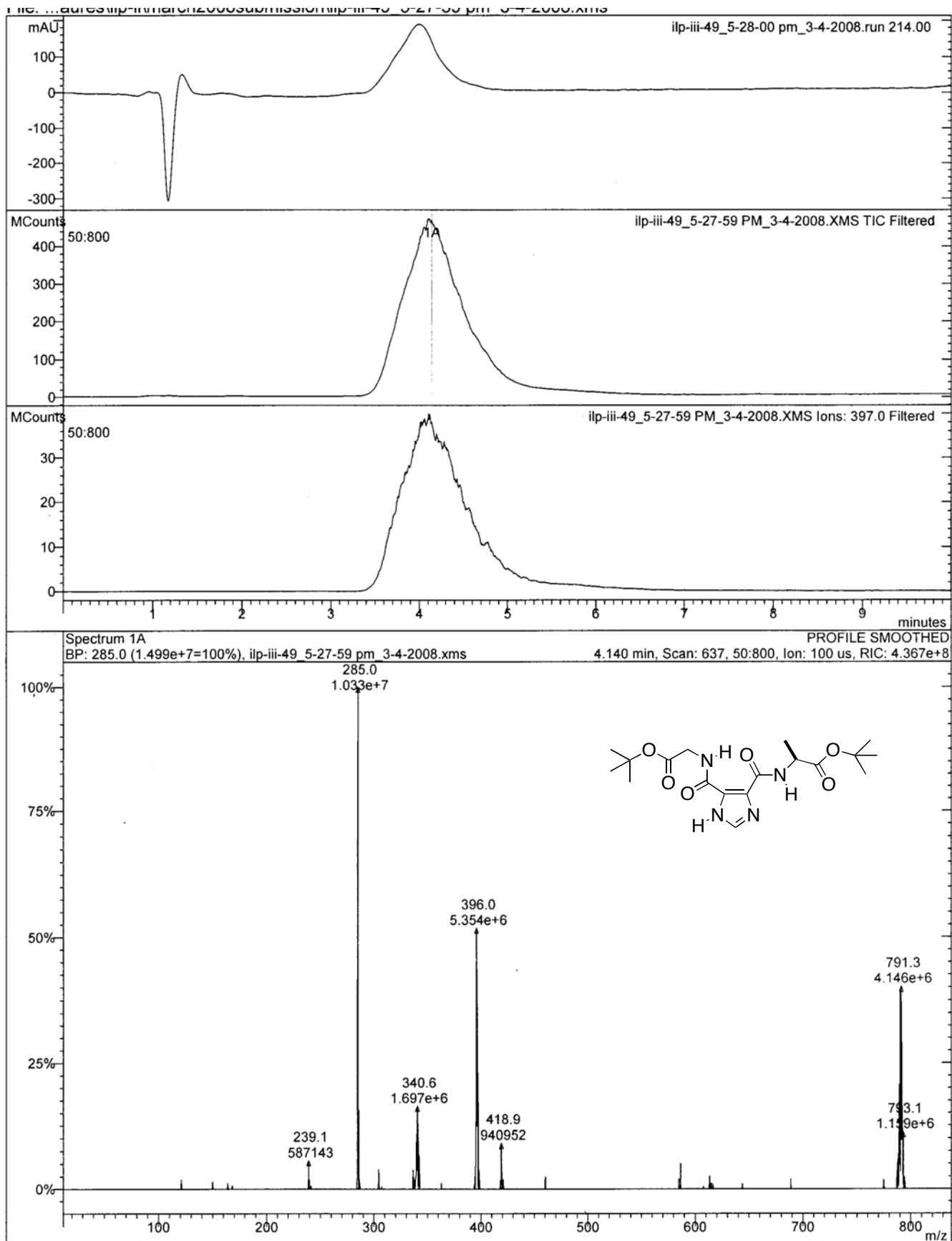


Figure S11. LC/MS data for 4{11}.

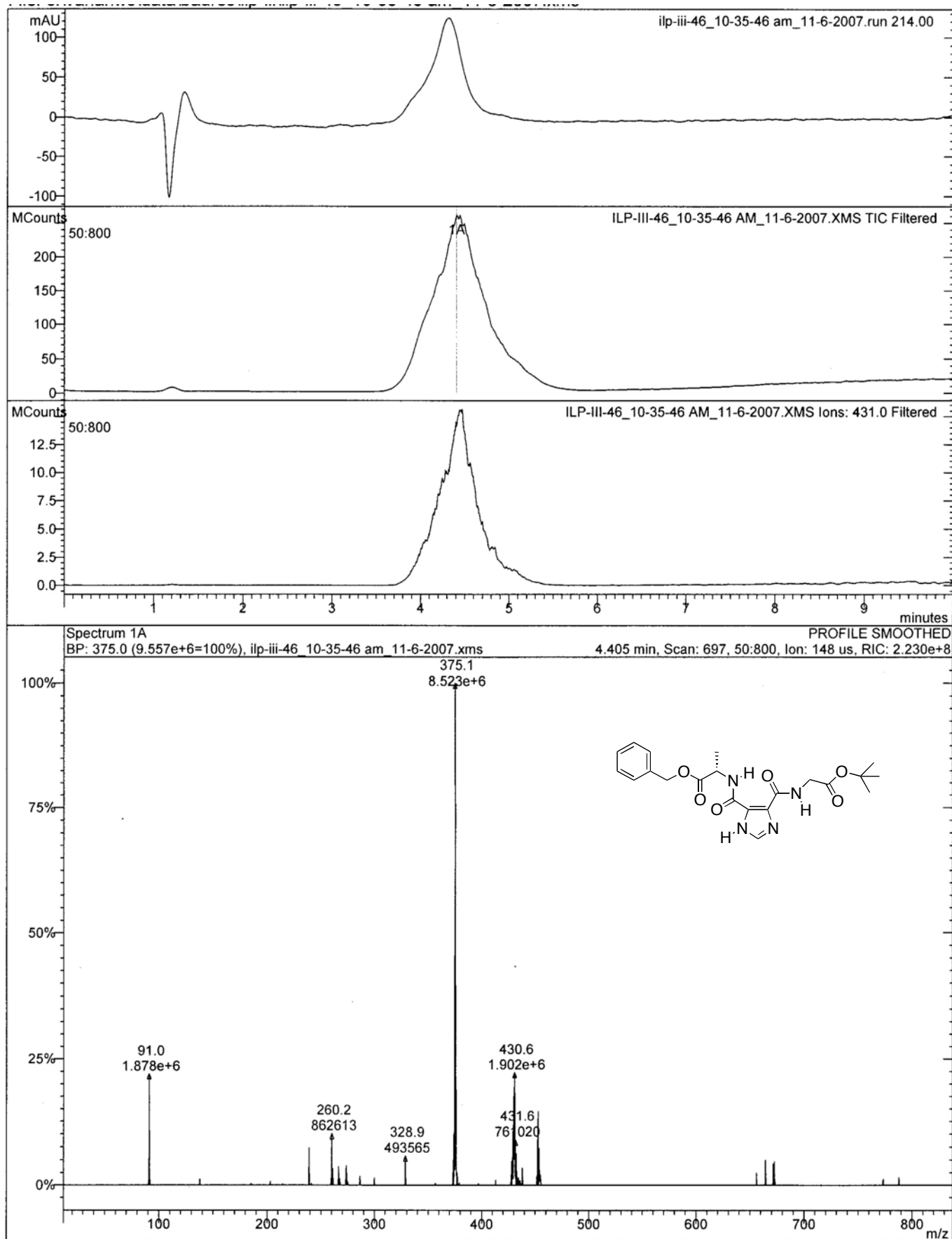


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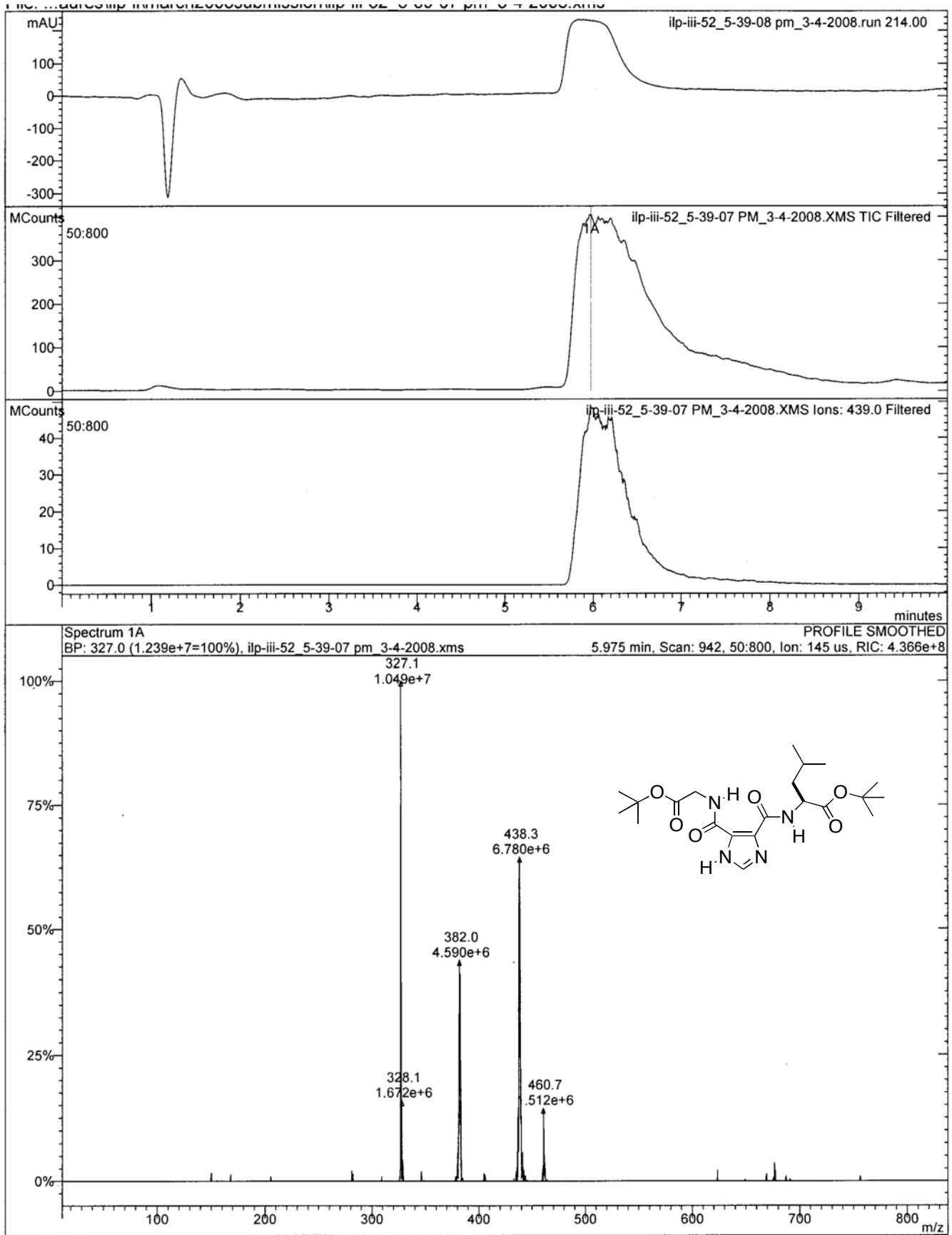


Figure S13. LC/MS data for 4{13}.

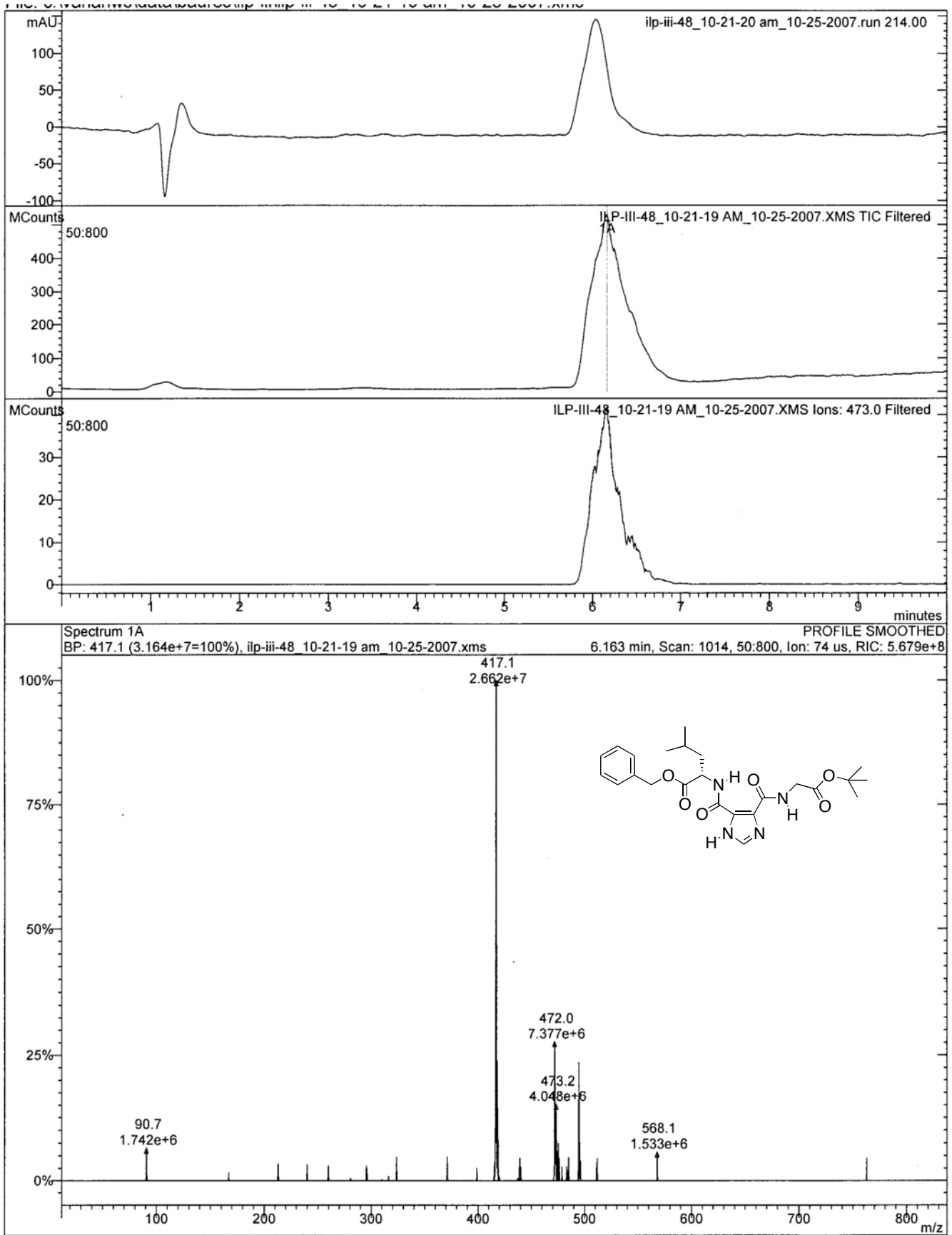


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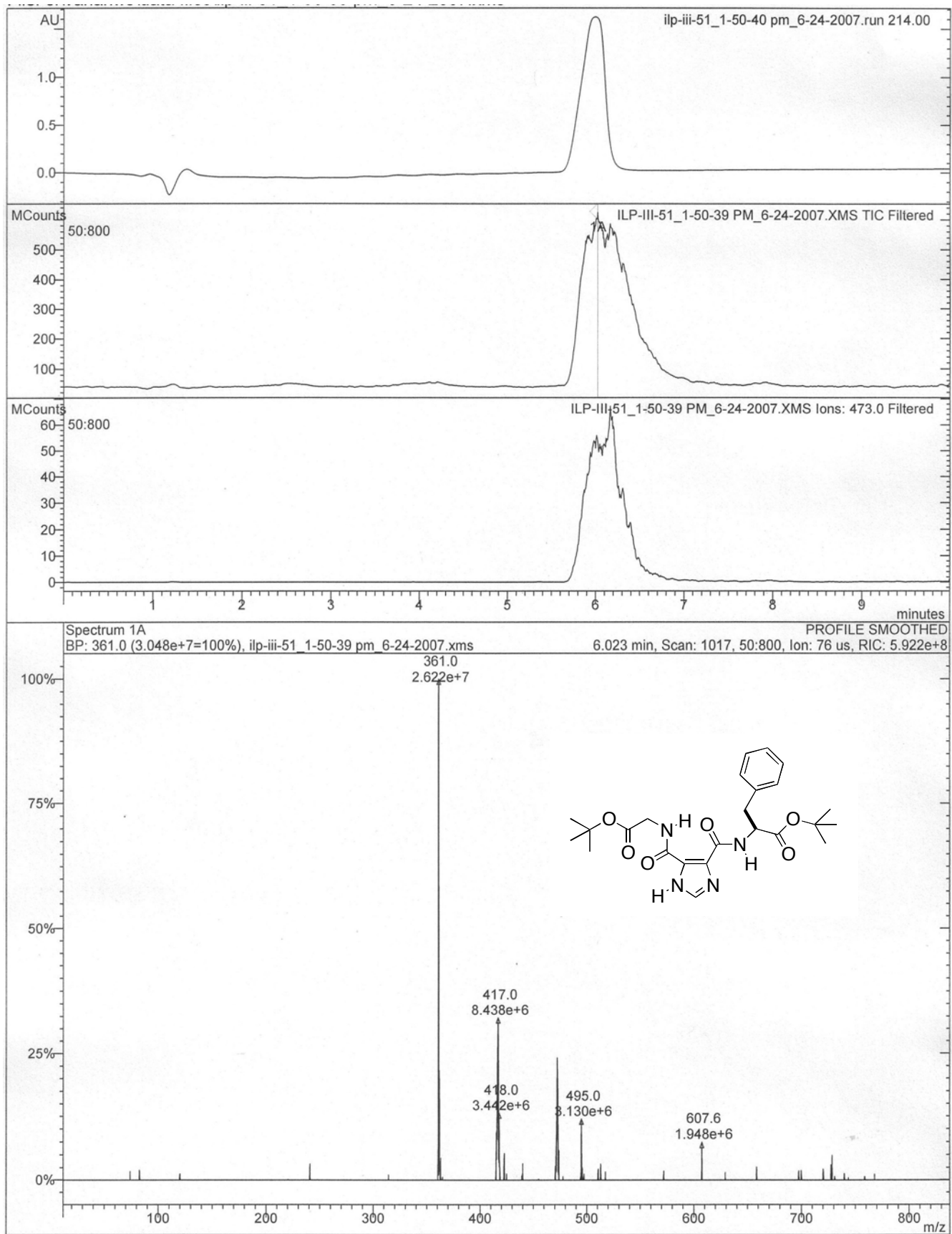


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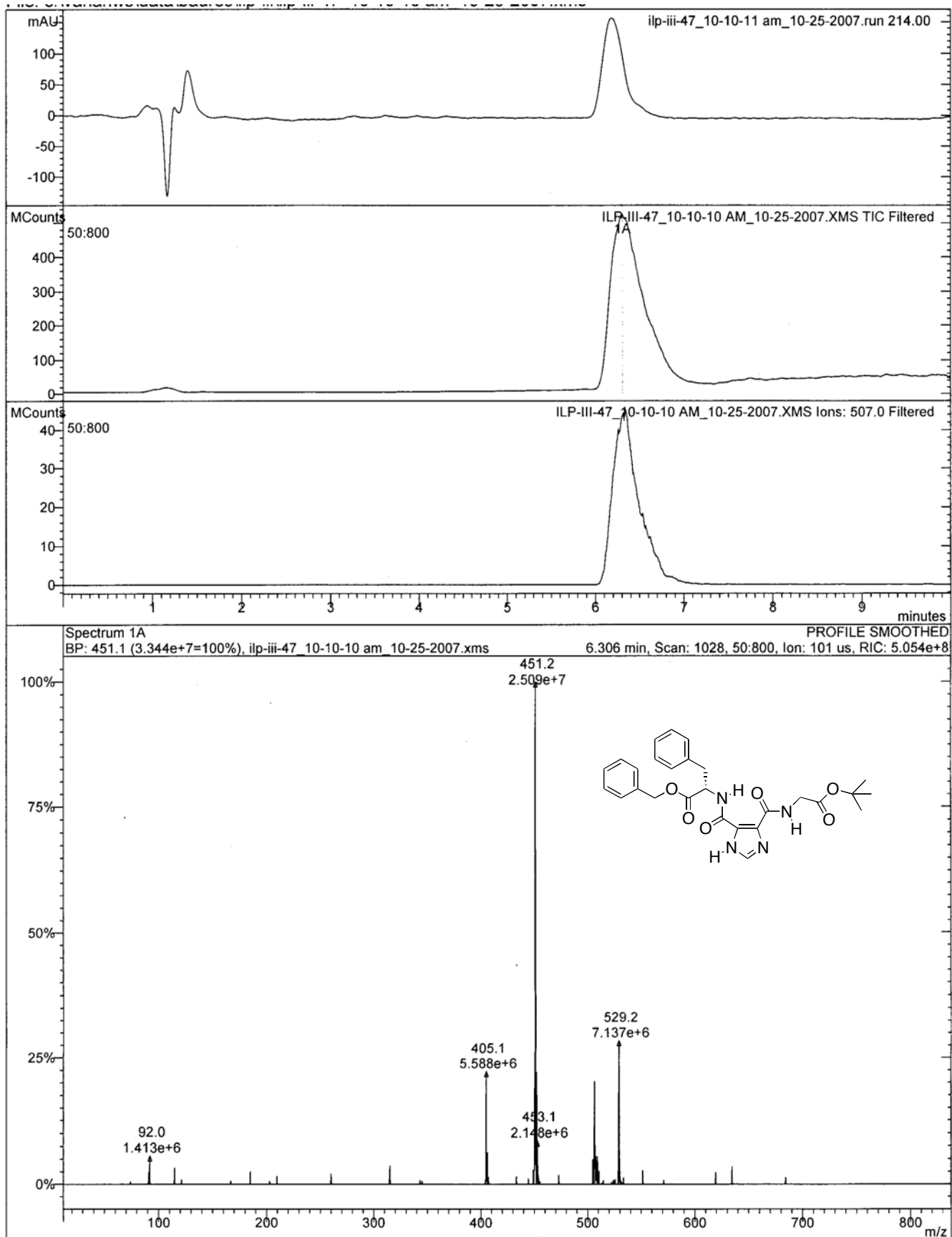


Figure S16. LC/MS data for 4{16}.

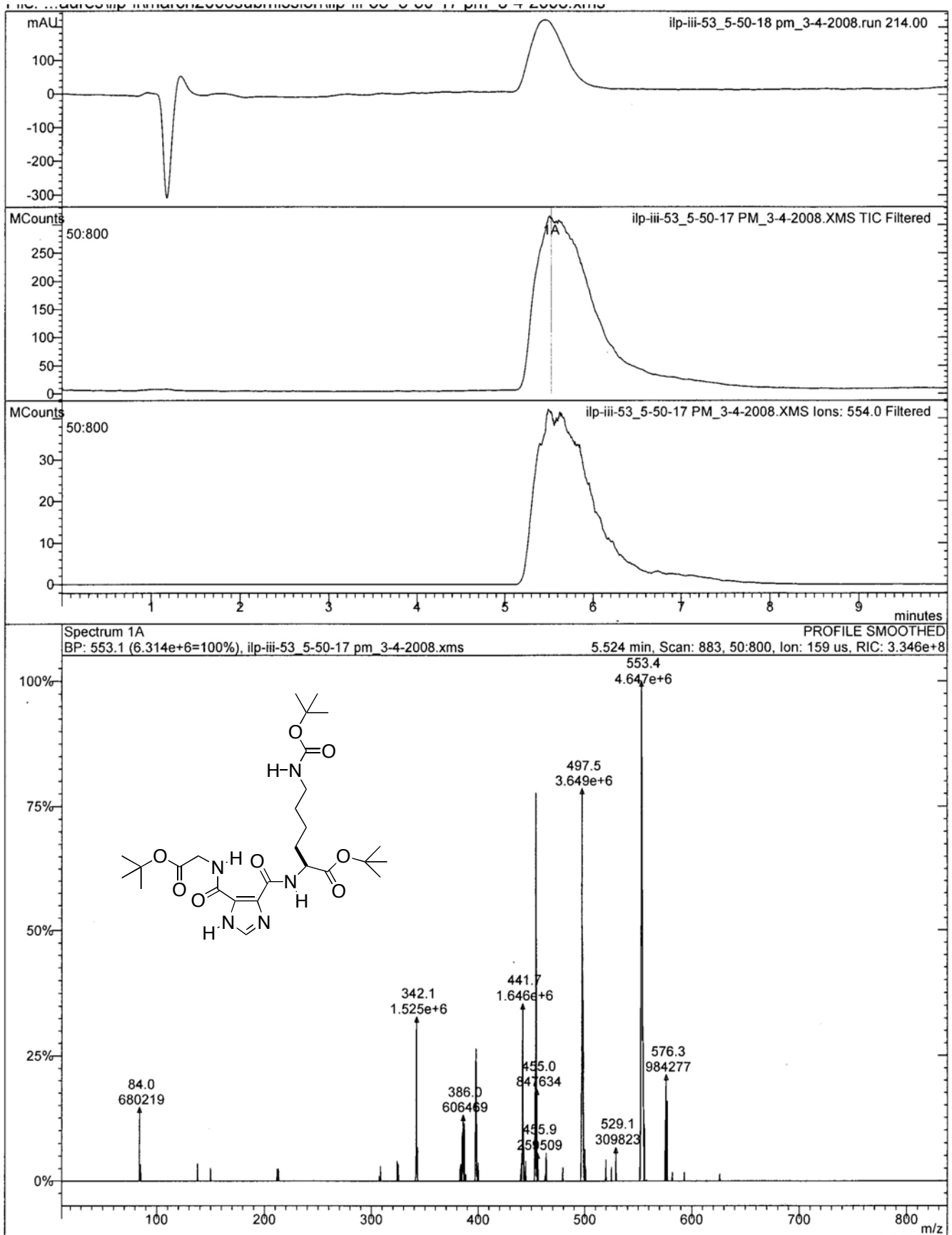


Figure S17. LC/MS data for 4{17}.

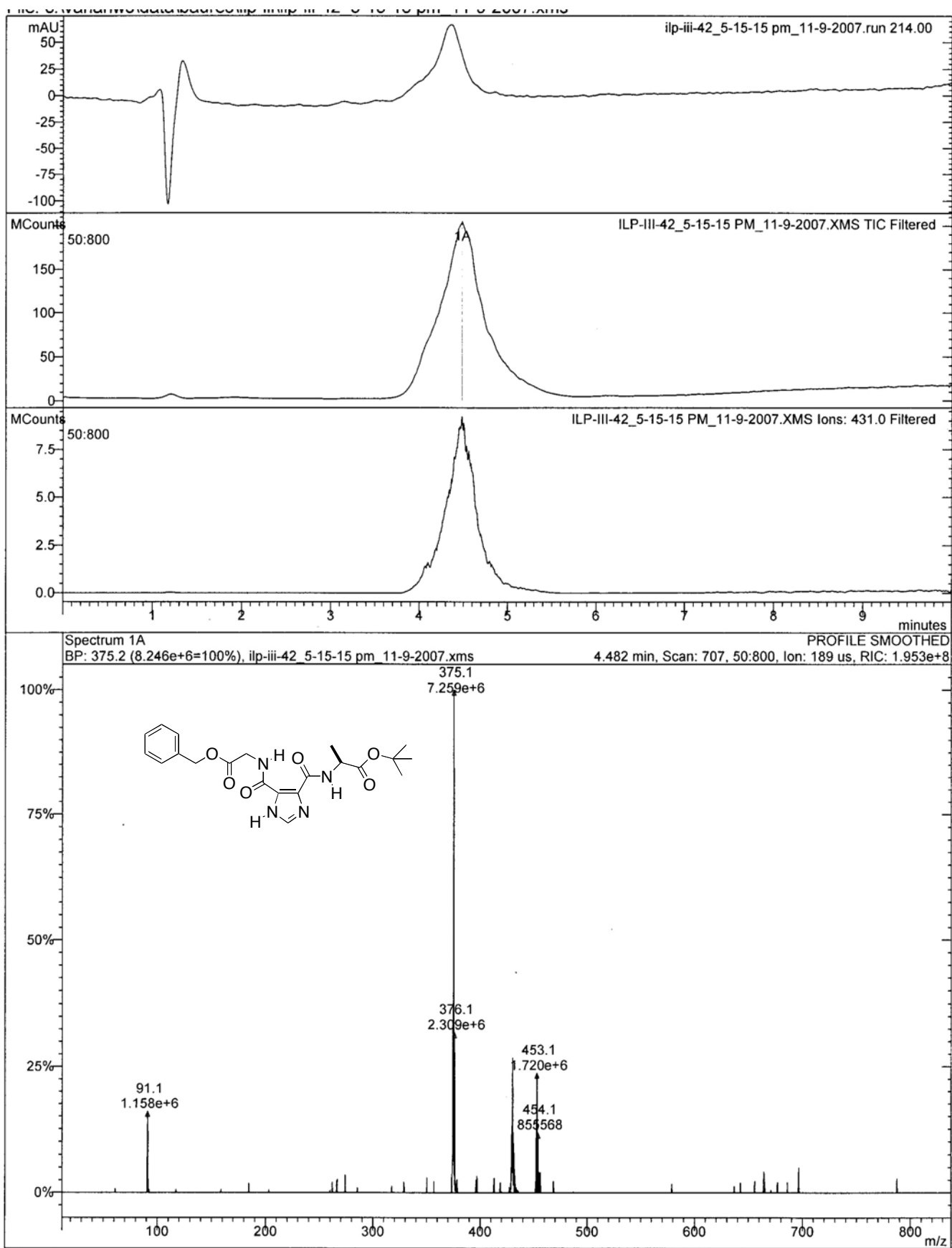


Figure S18. LC/MS data for 4{18}.

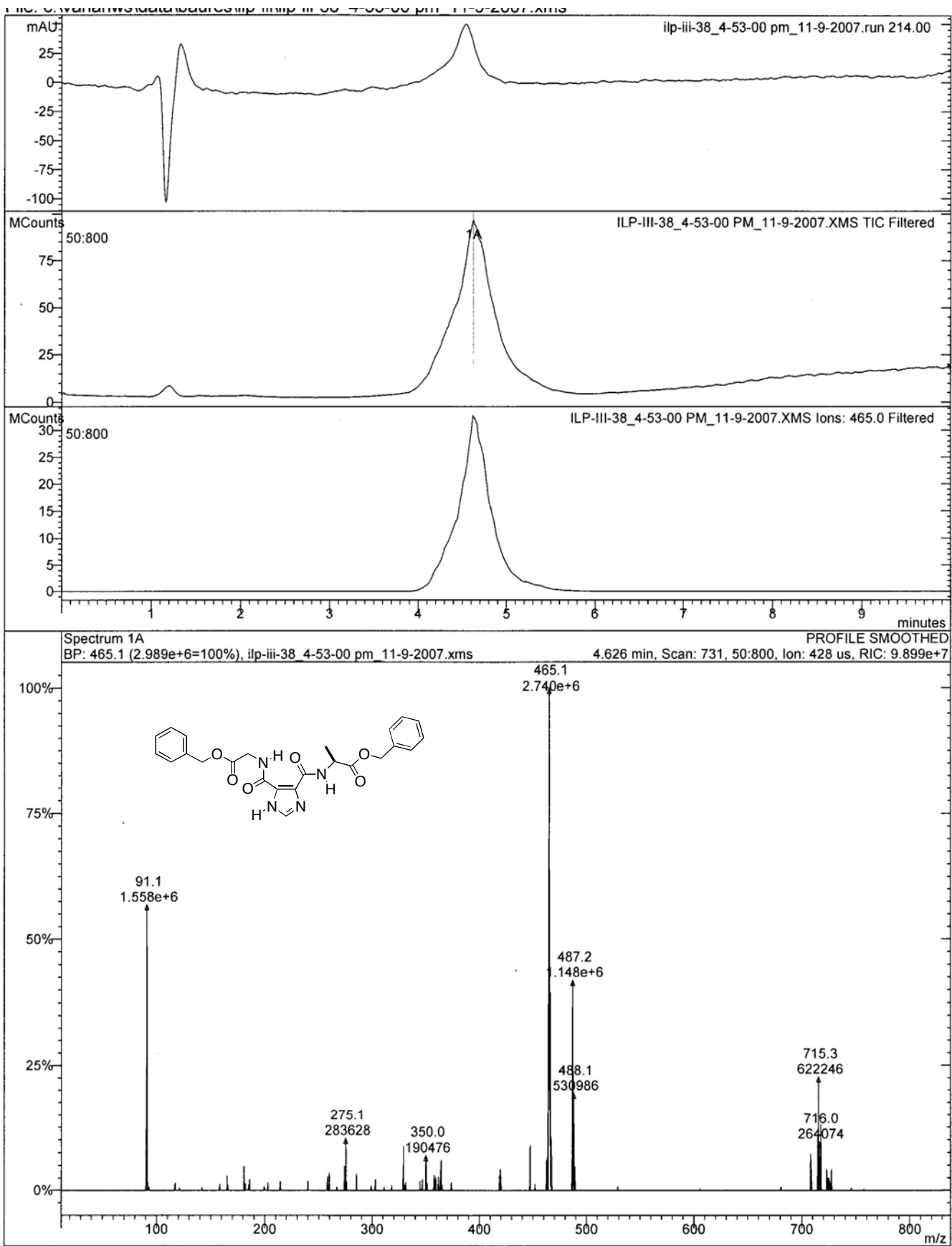


Figure S19. LC/MS data for 4{19}.

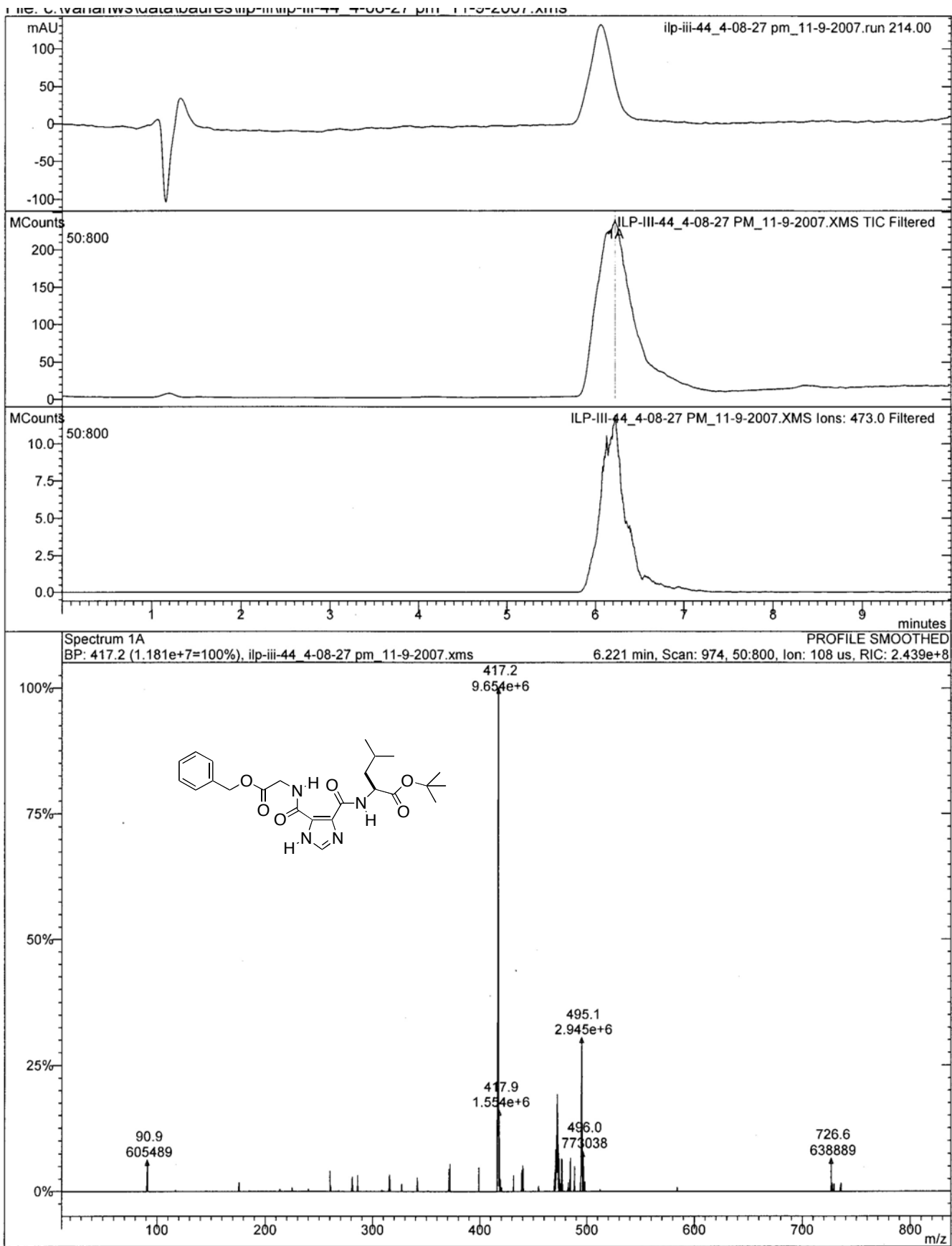


Figure S20. LC/MS data for 4{20}.

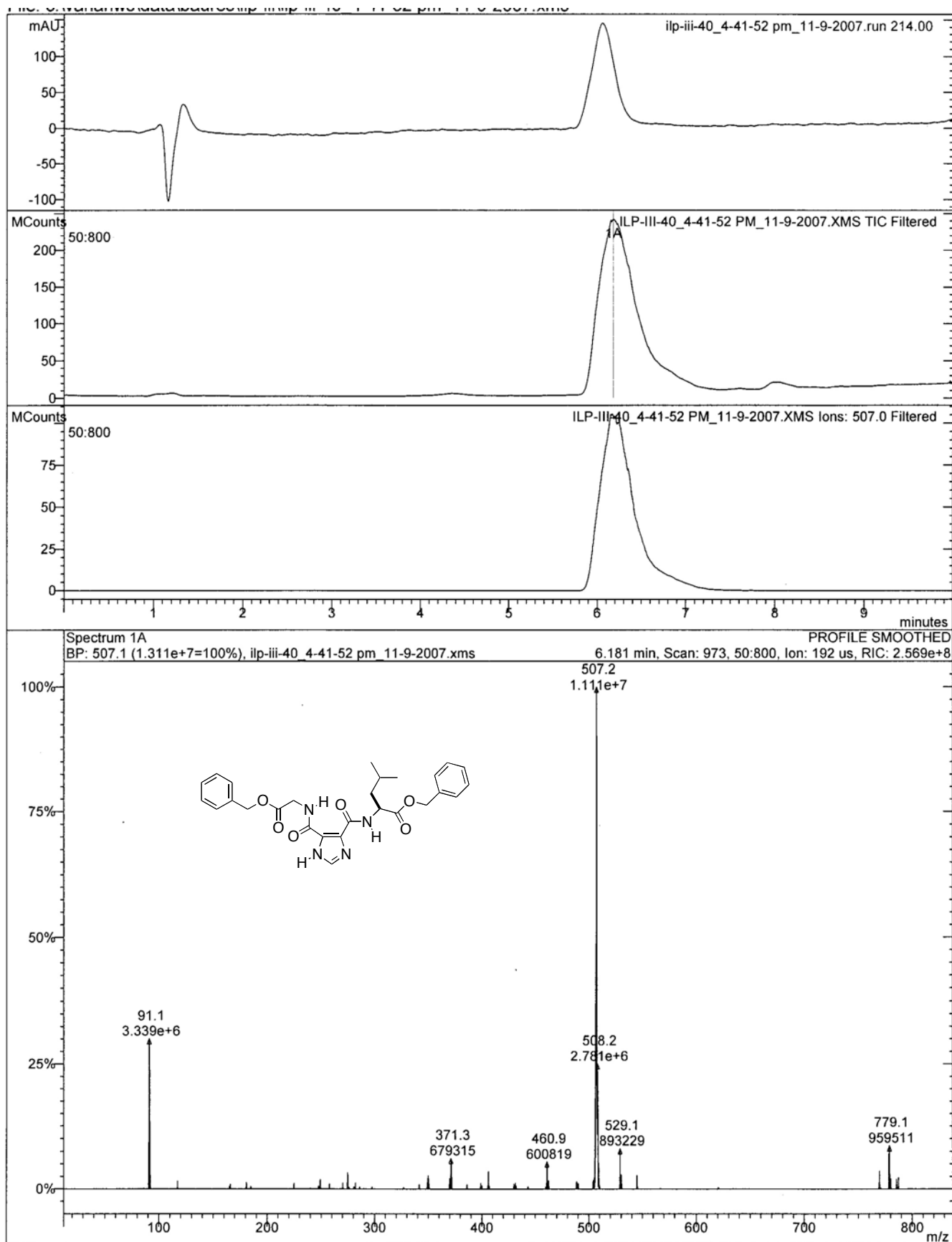


Figure S21. LC/MS data for 4{21}.

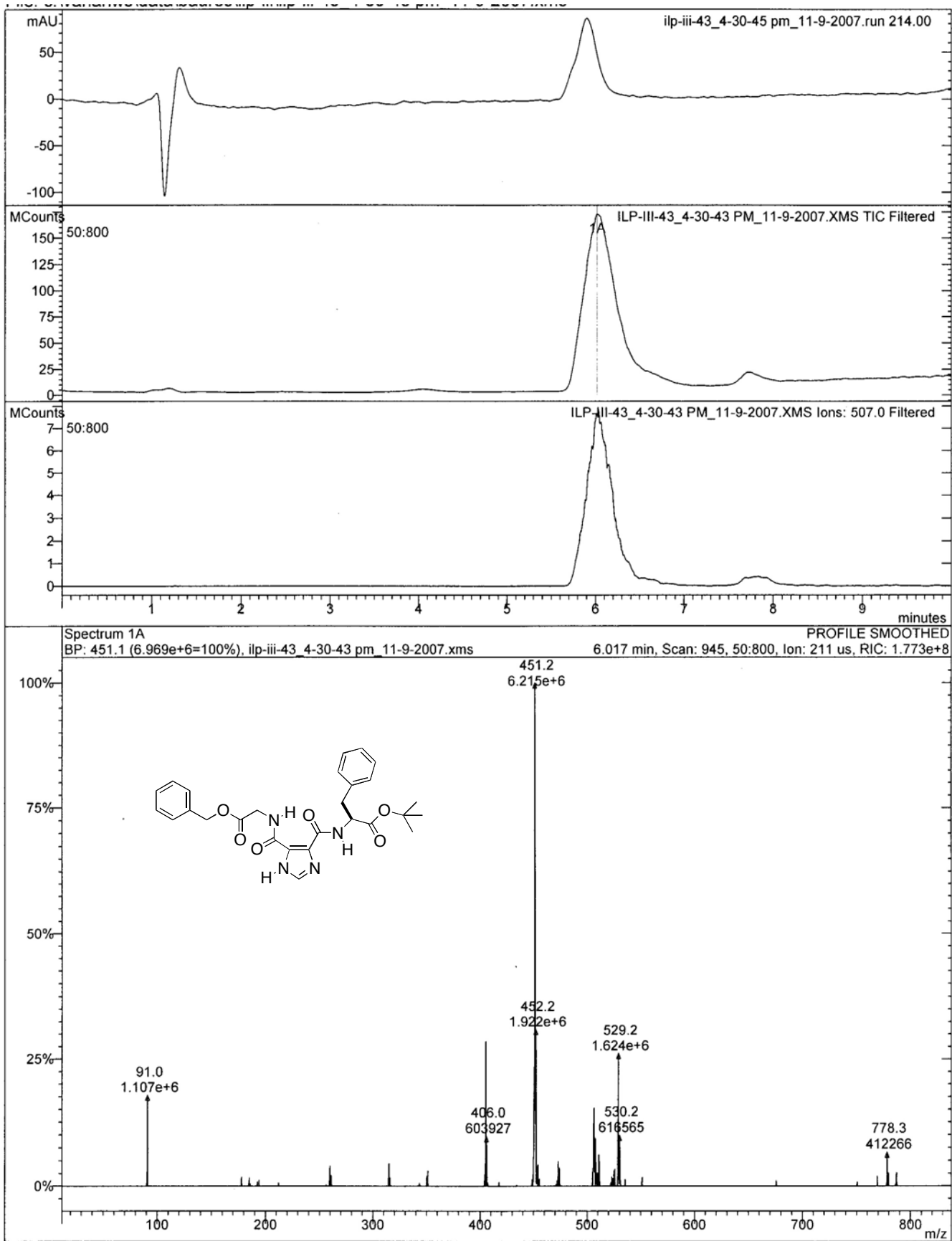


Figure S22. LC/MS data for 4{22}.

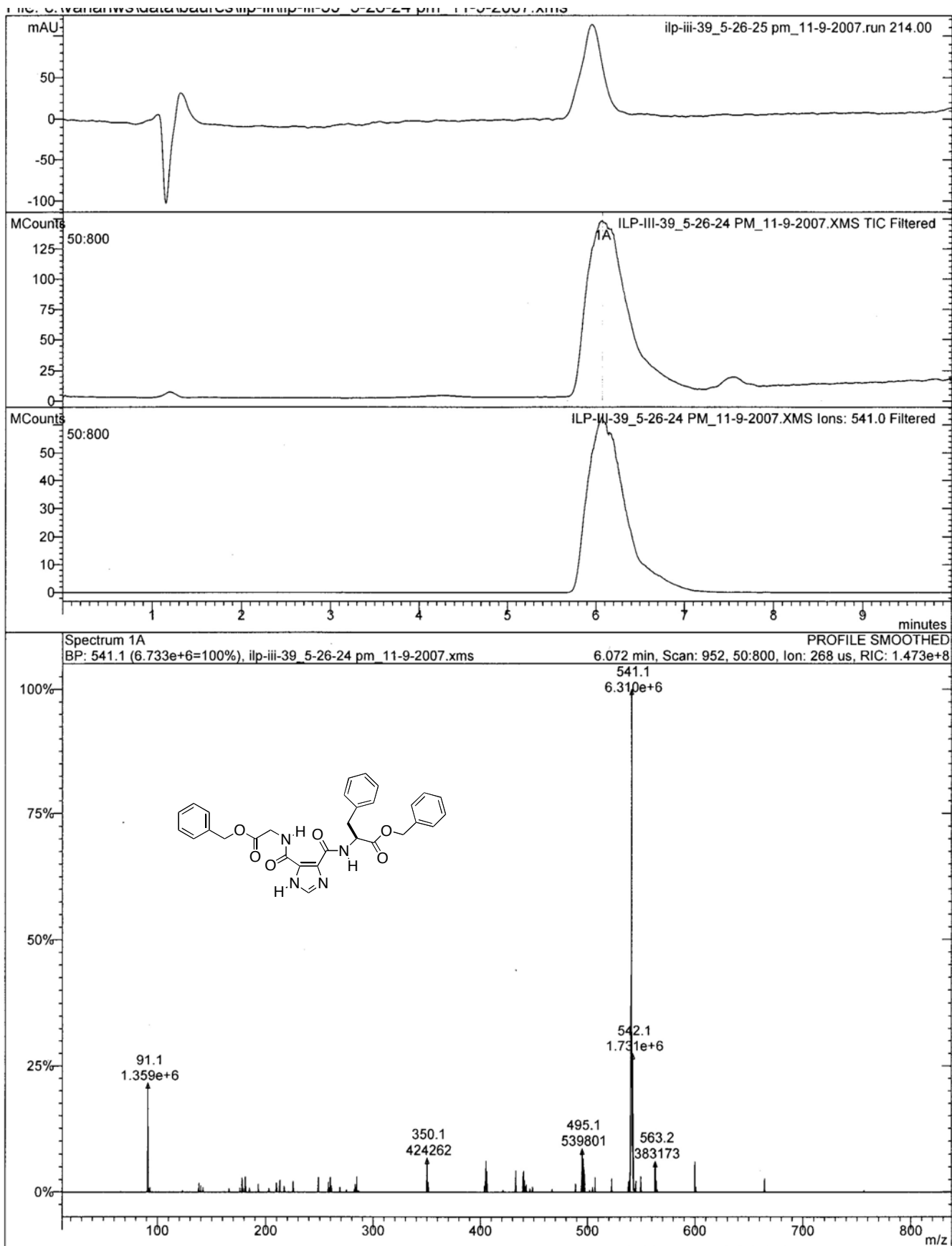


Figure S23. LC/MS data for 4{23}.

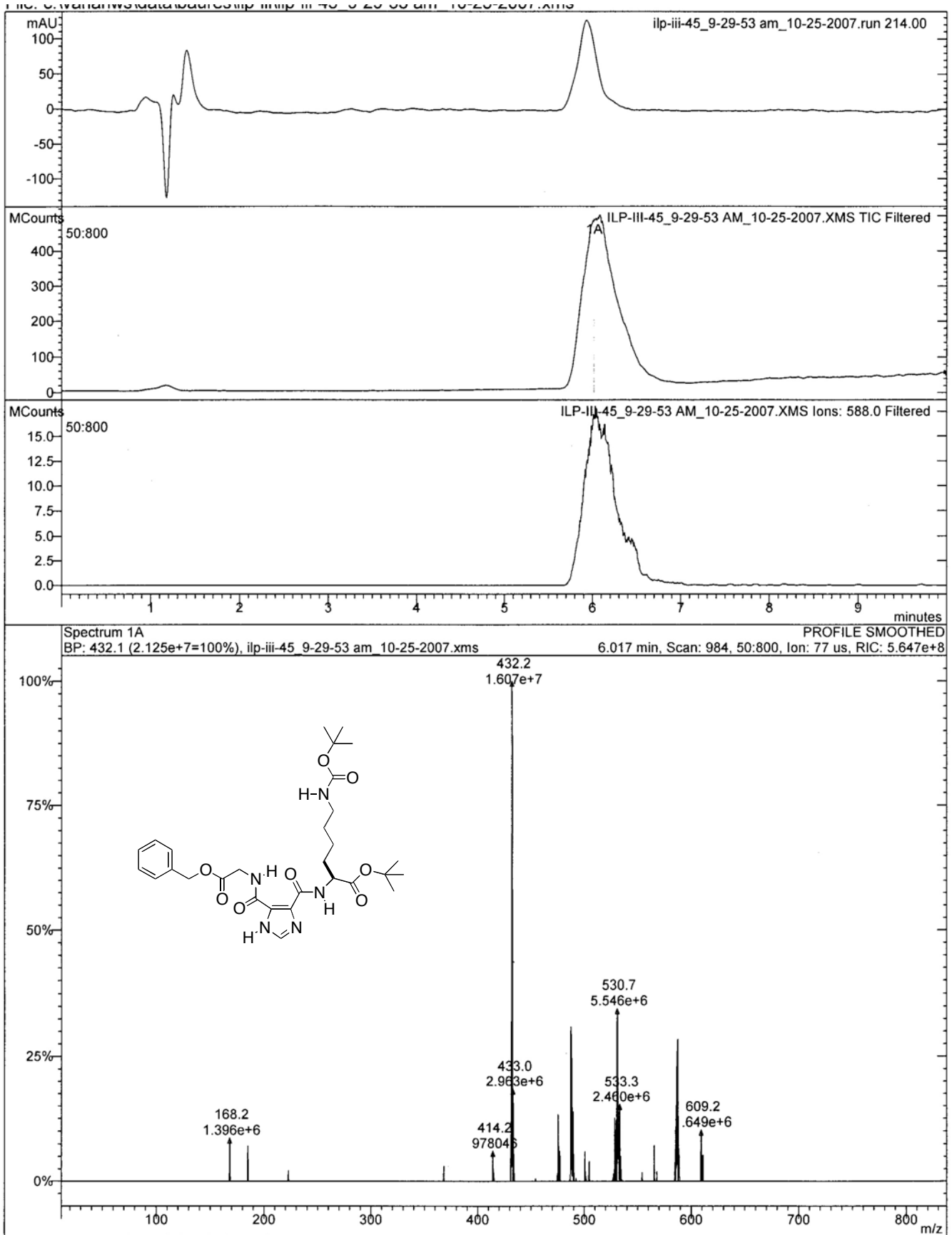


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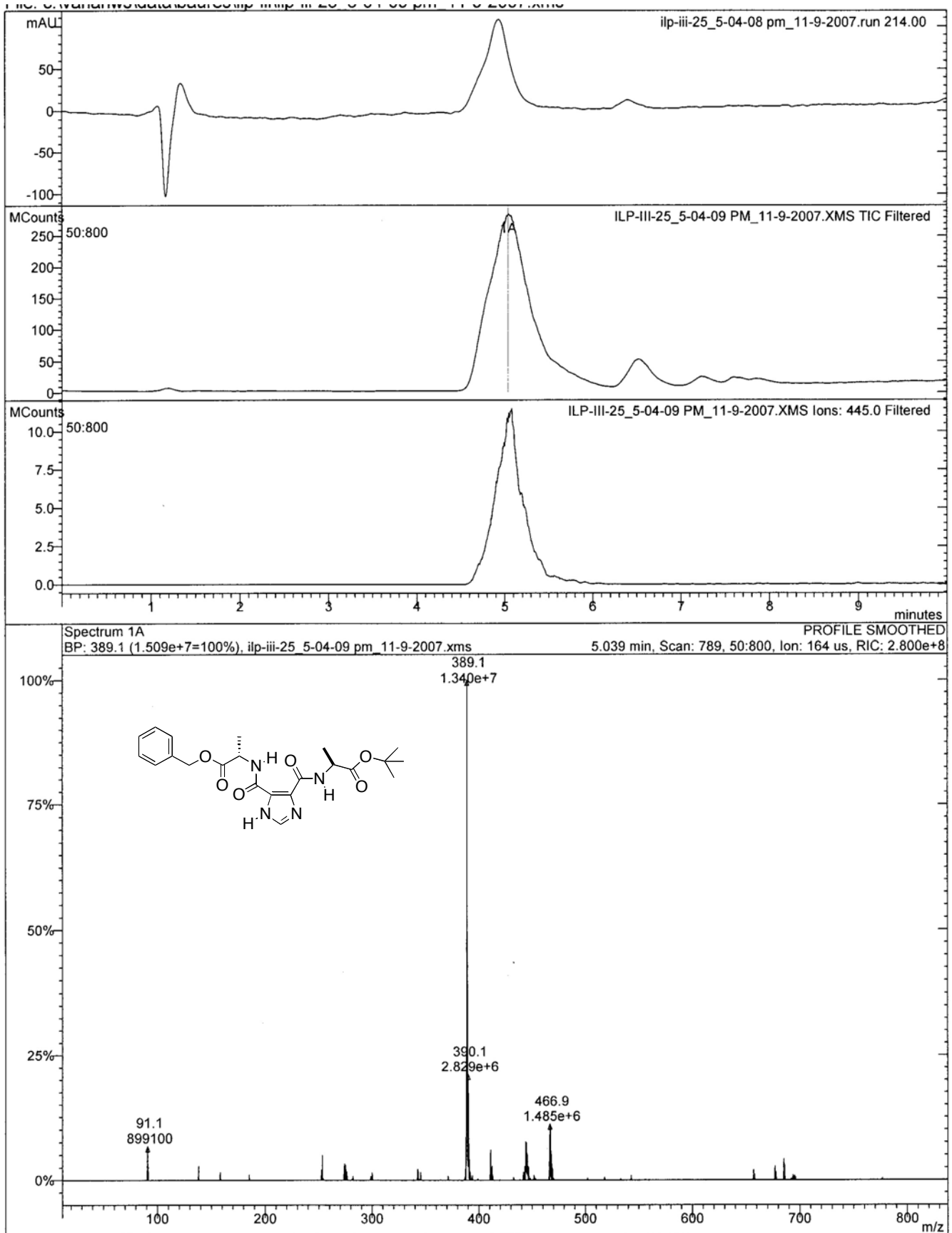


Figure S25. LC/MS data for 4{25}.

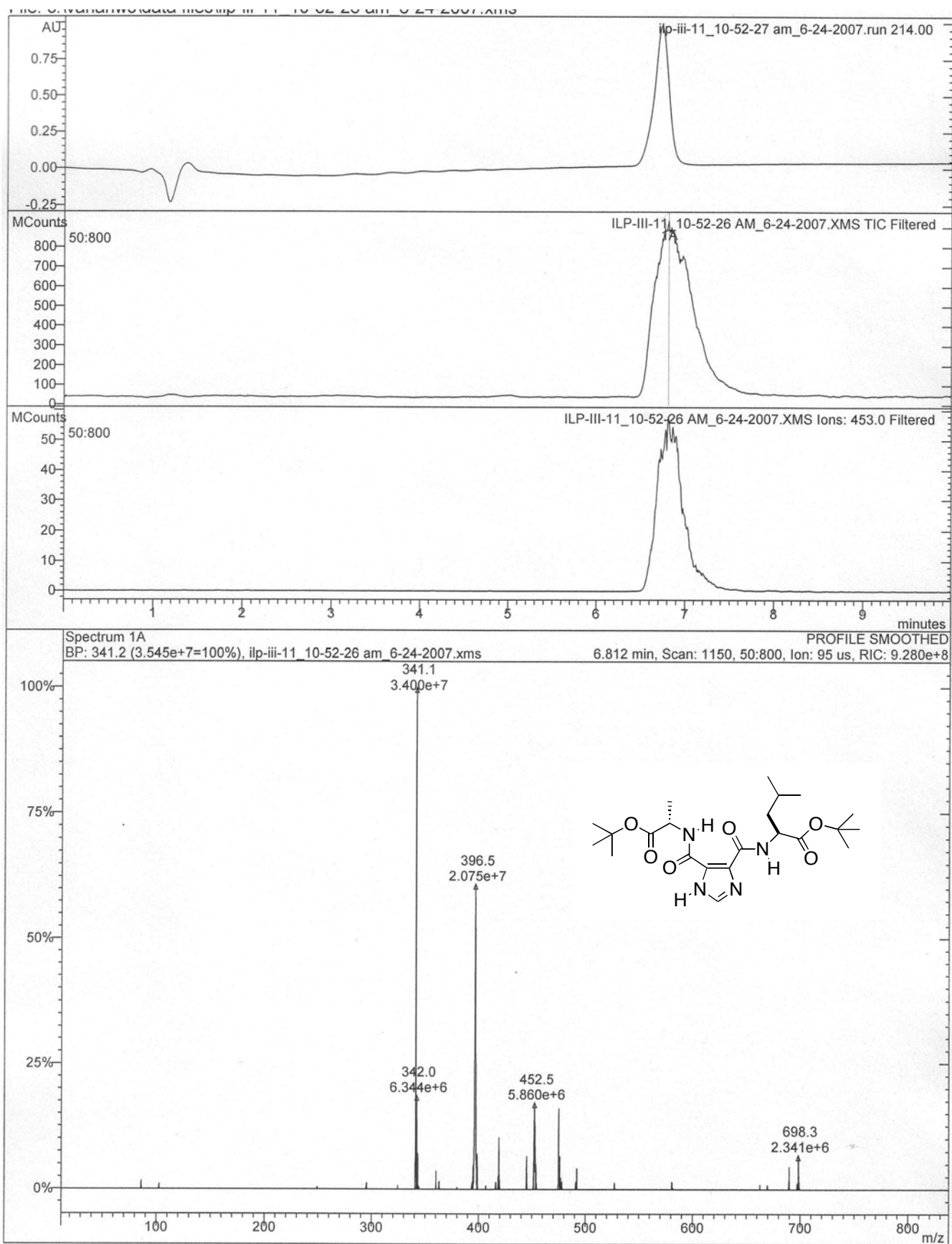


Figure S26. LC/MS data for 4{26}.

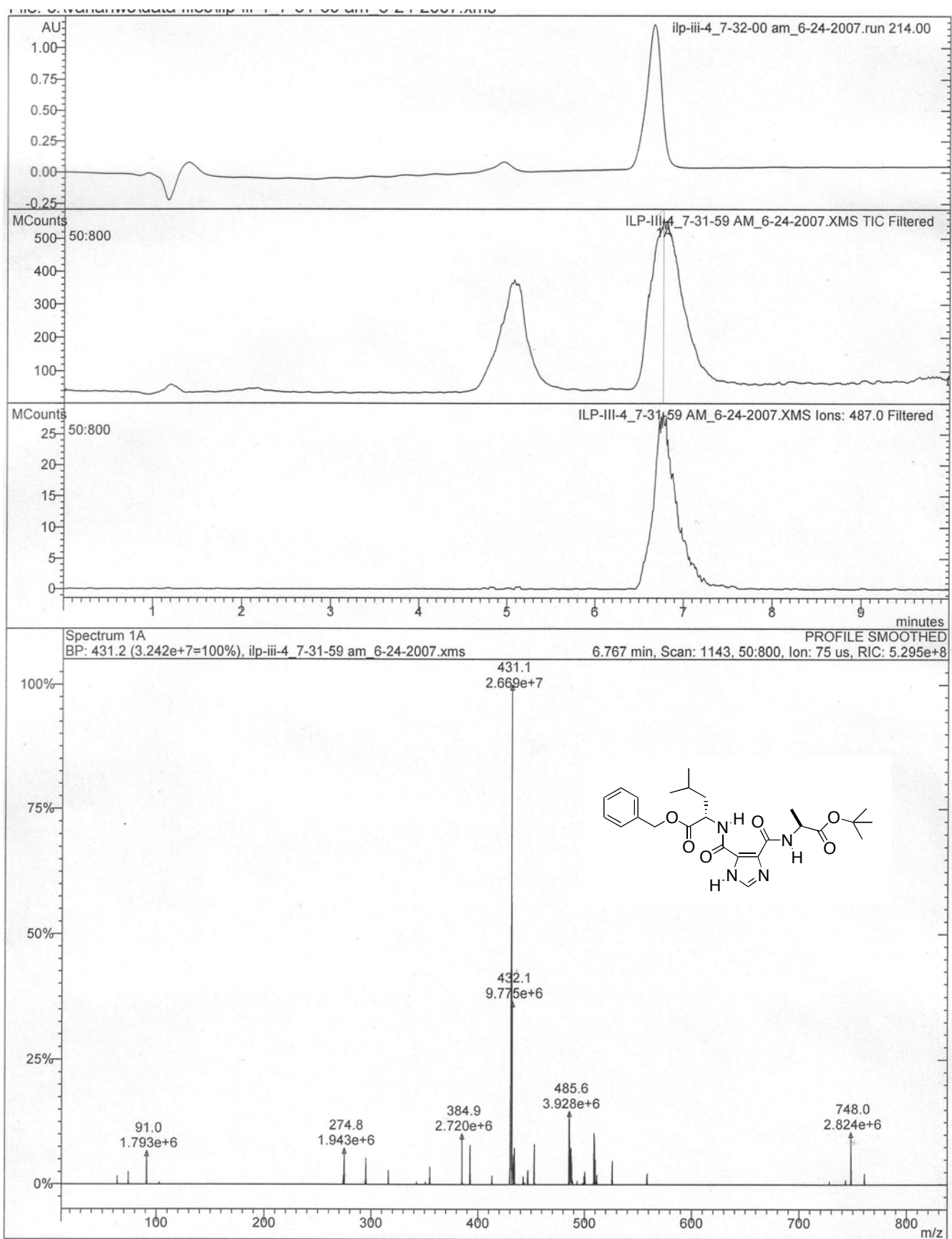


Figure S27. LC/MS data for 4{27}.

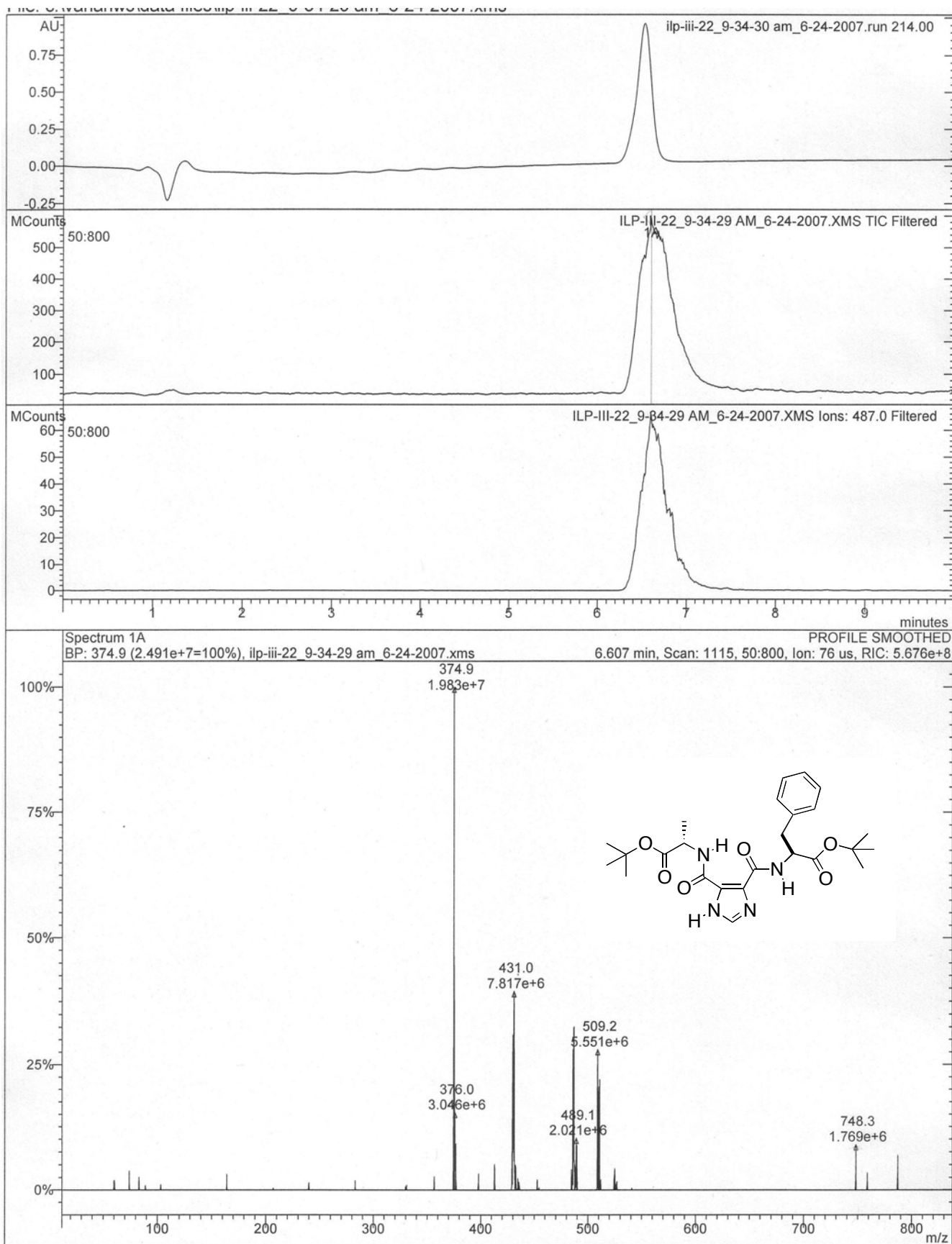


Figure S28. LC/MS data for 4{28}.

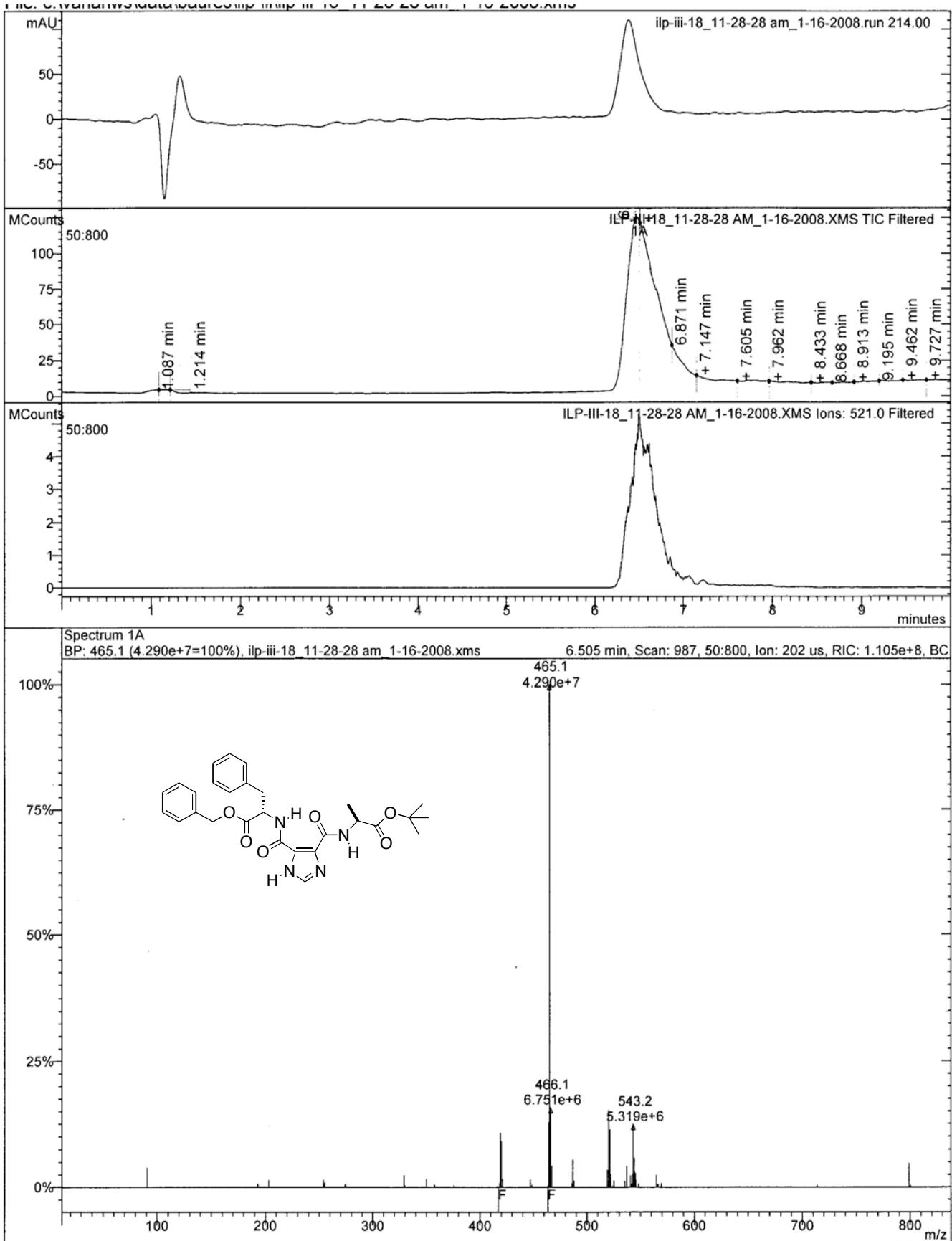


Figure S29. LC/MS data for 4{29}.

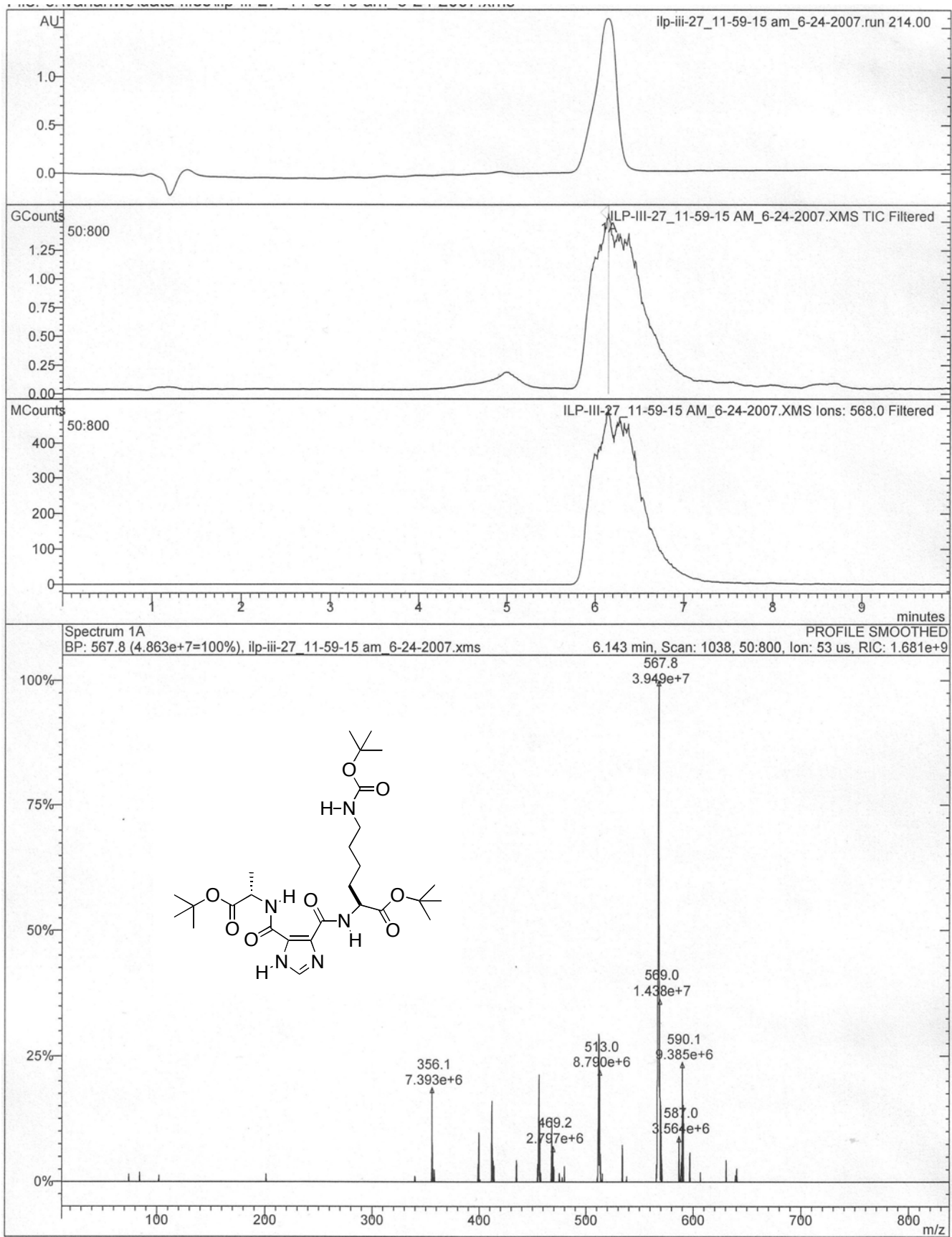


Figure S30. LC/MS data for 4{30}.

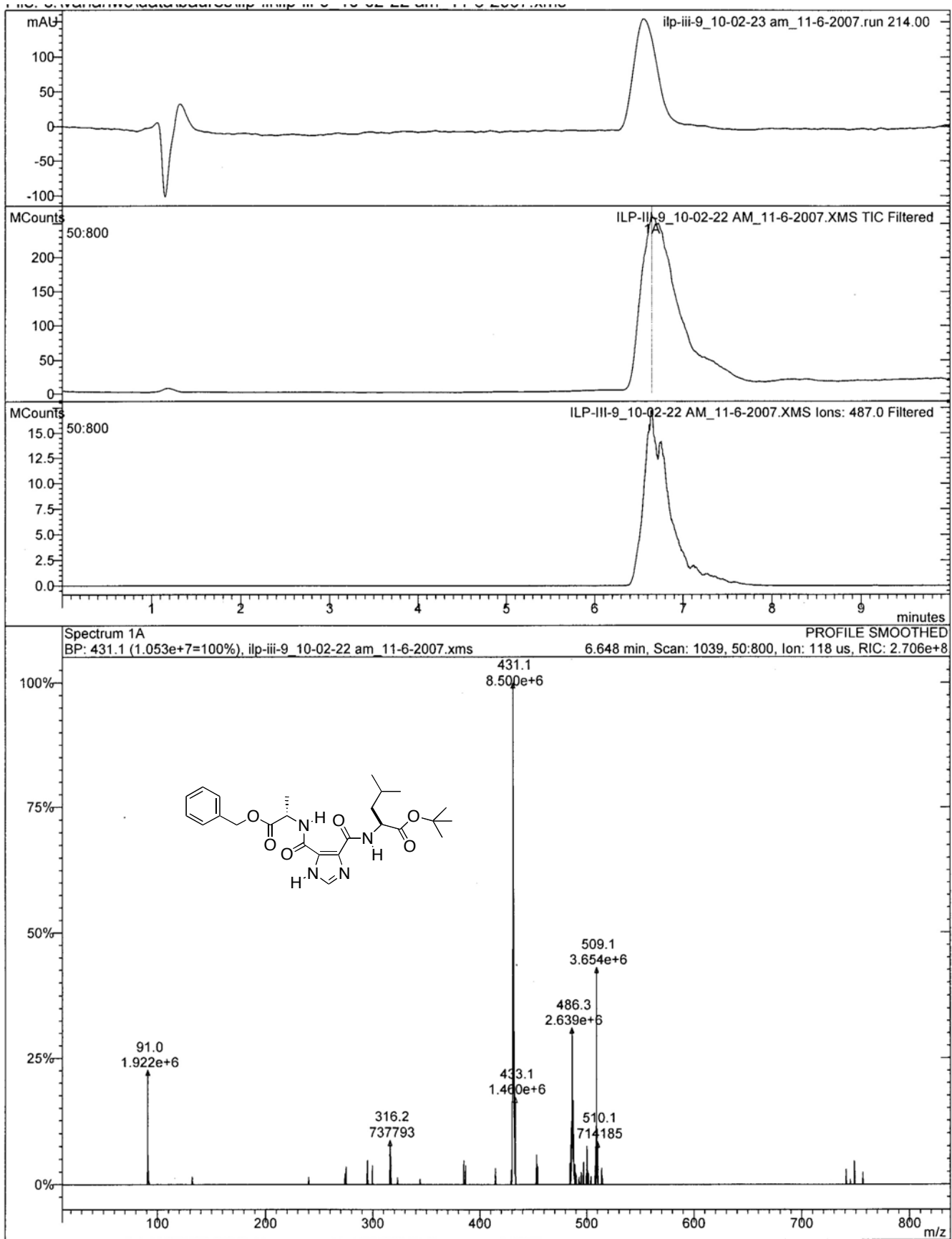


Figure S31. LC/MS data for 4{31}.

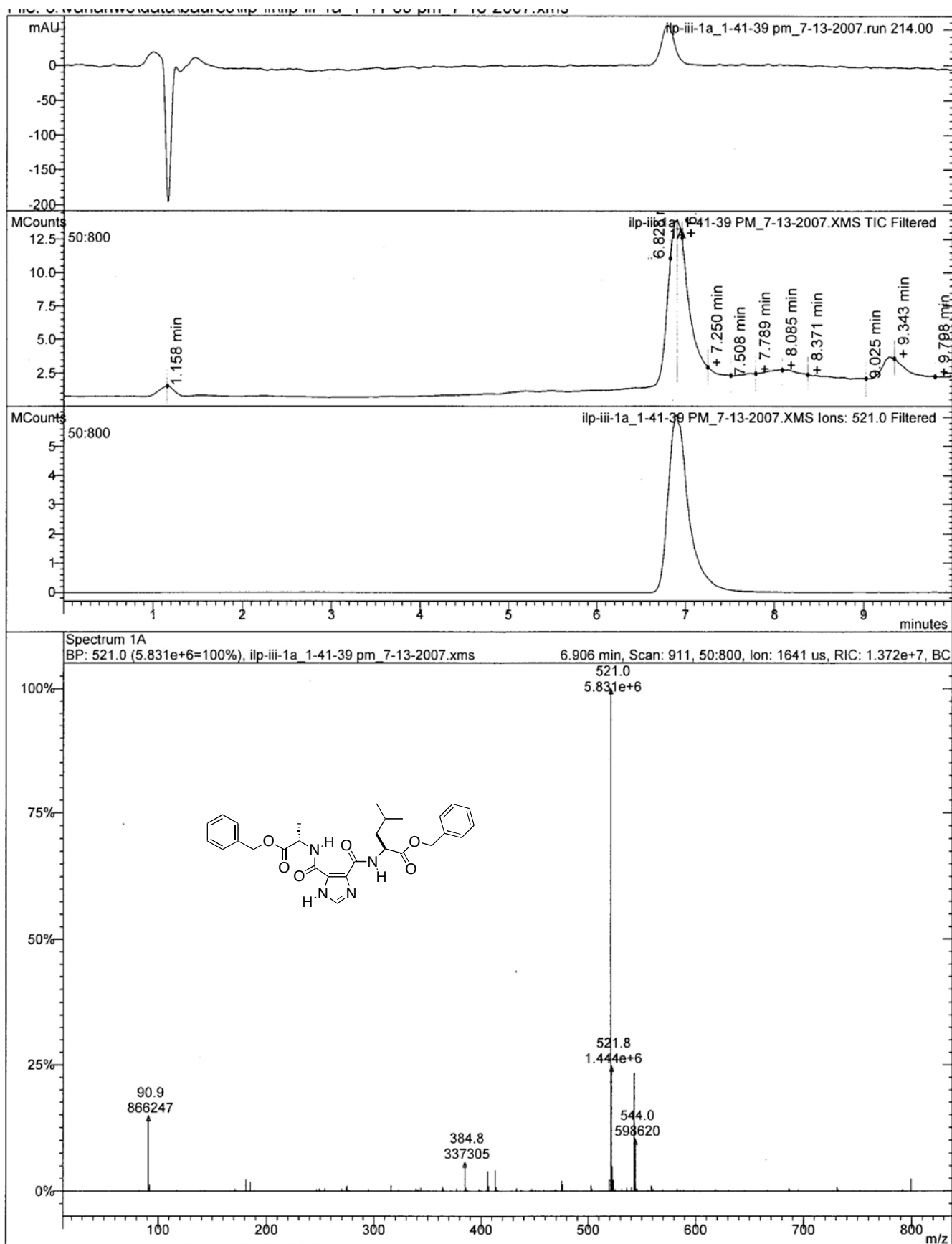


Figure S32. LC/MS data for 4{32}.

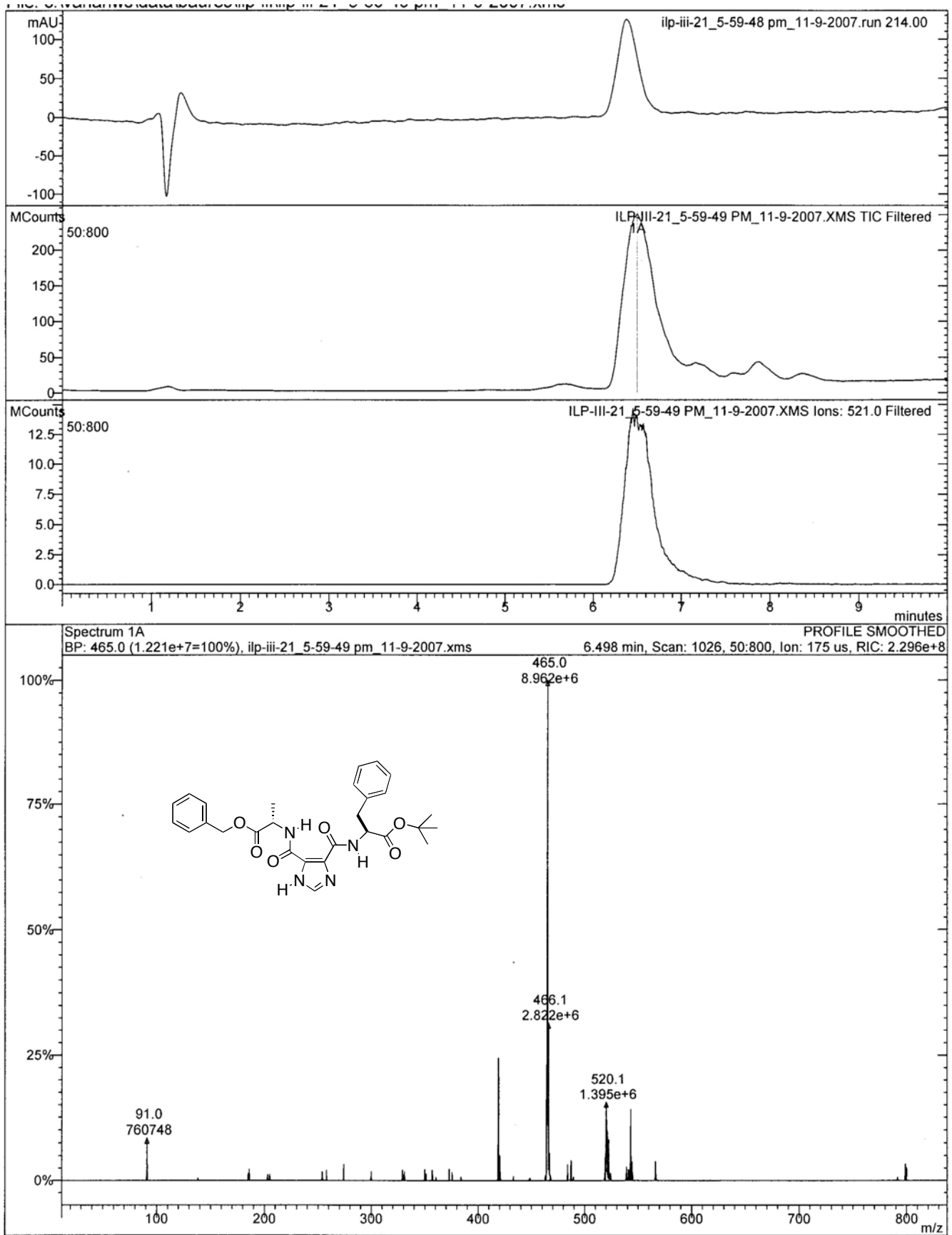


Figure S33. LC/MS data for 4{33}.

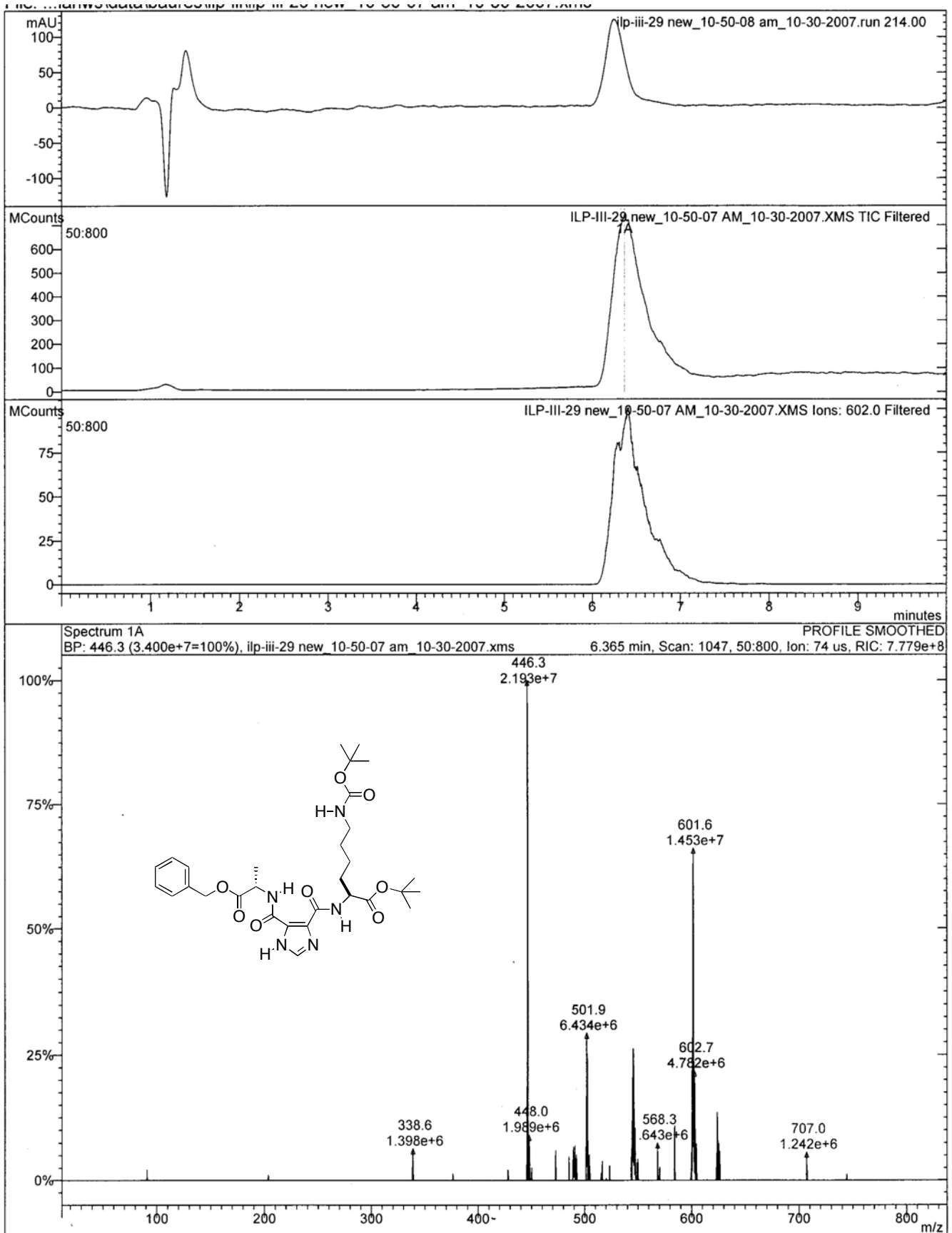


Figure S35. LC/MS data for 4{35}.

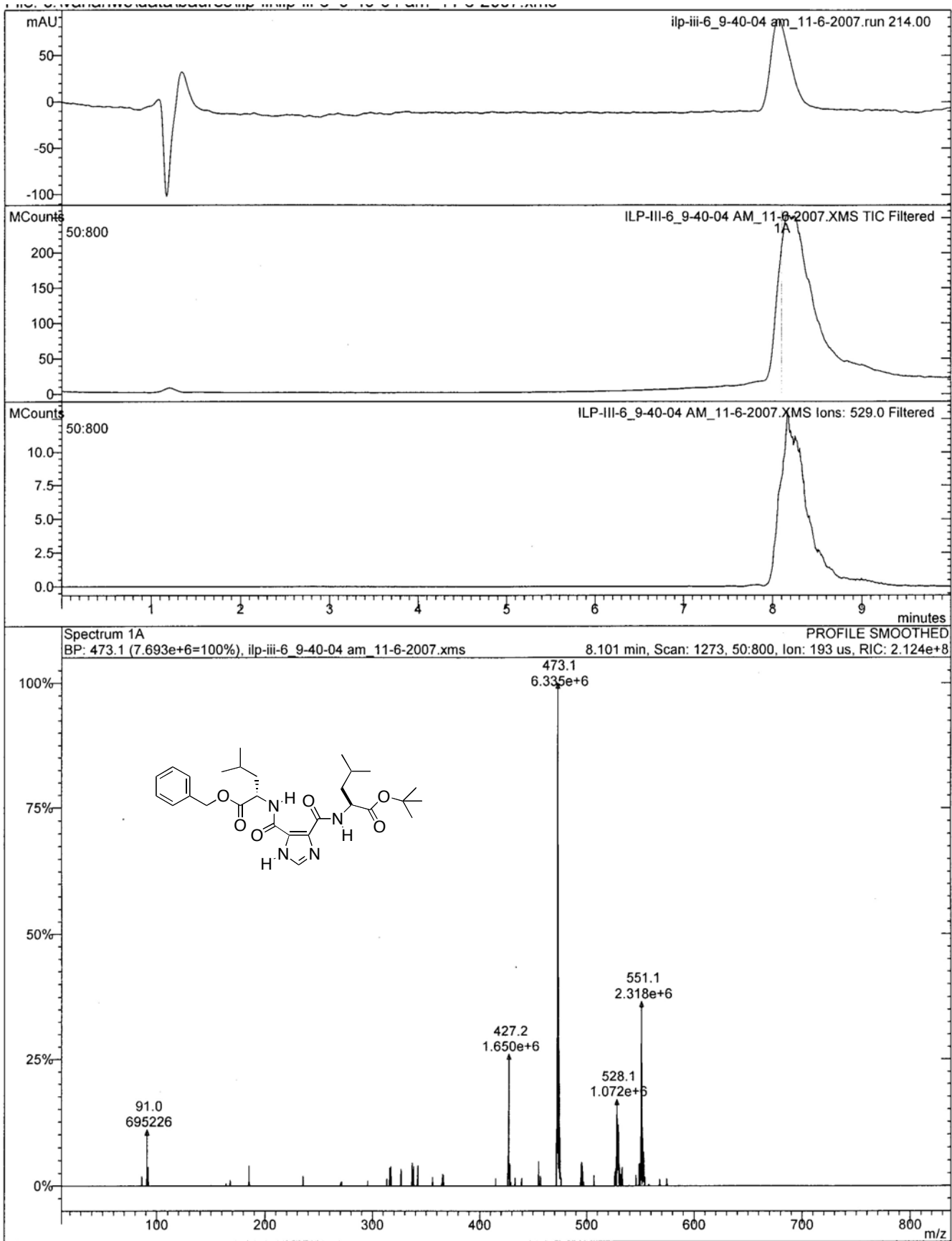


Figure S36. LC/MS data for 4{36}.

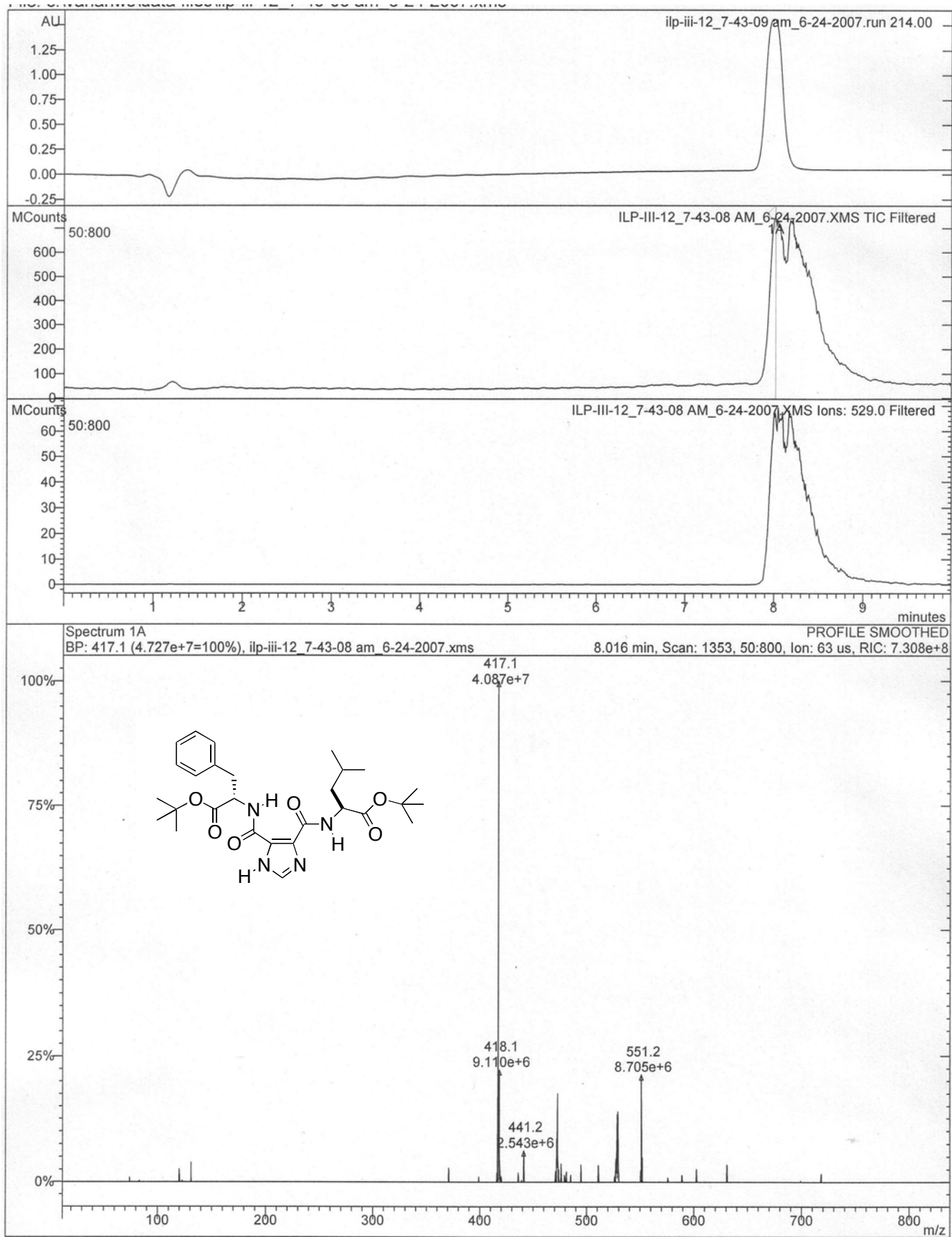


Figure S37. LC/MS data for 4{37}.

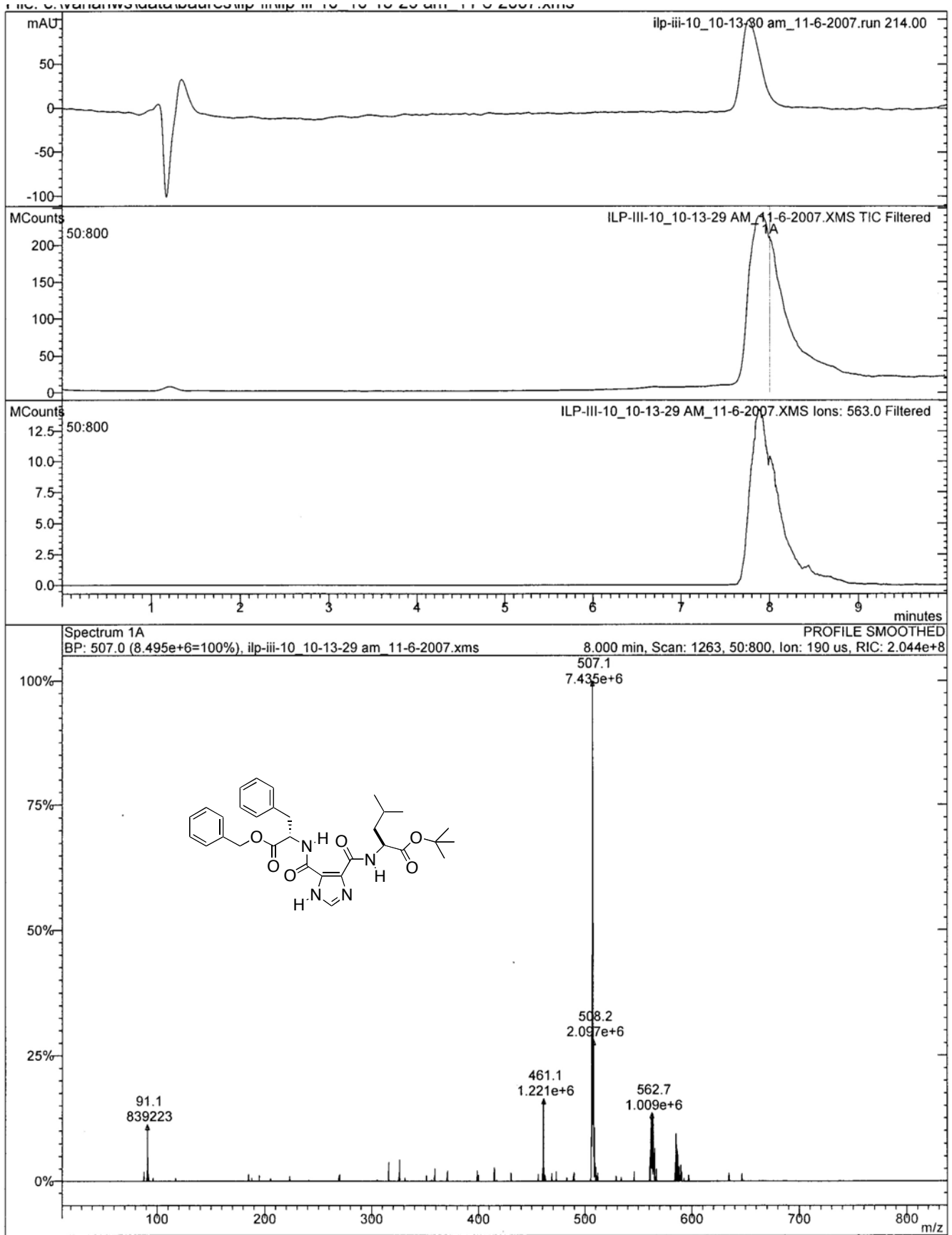


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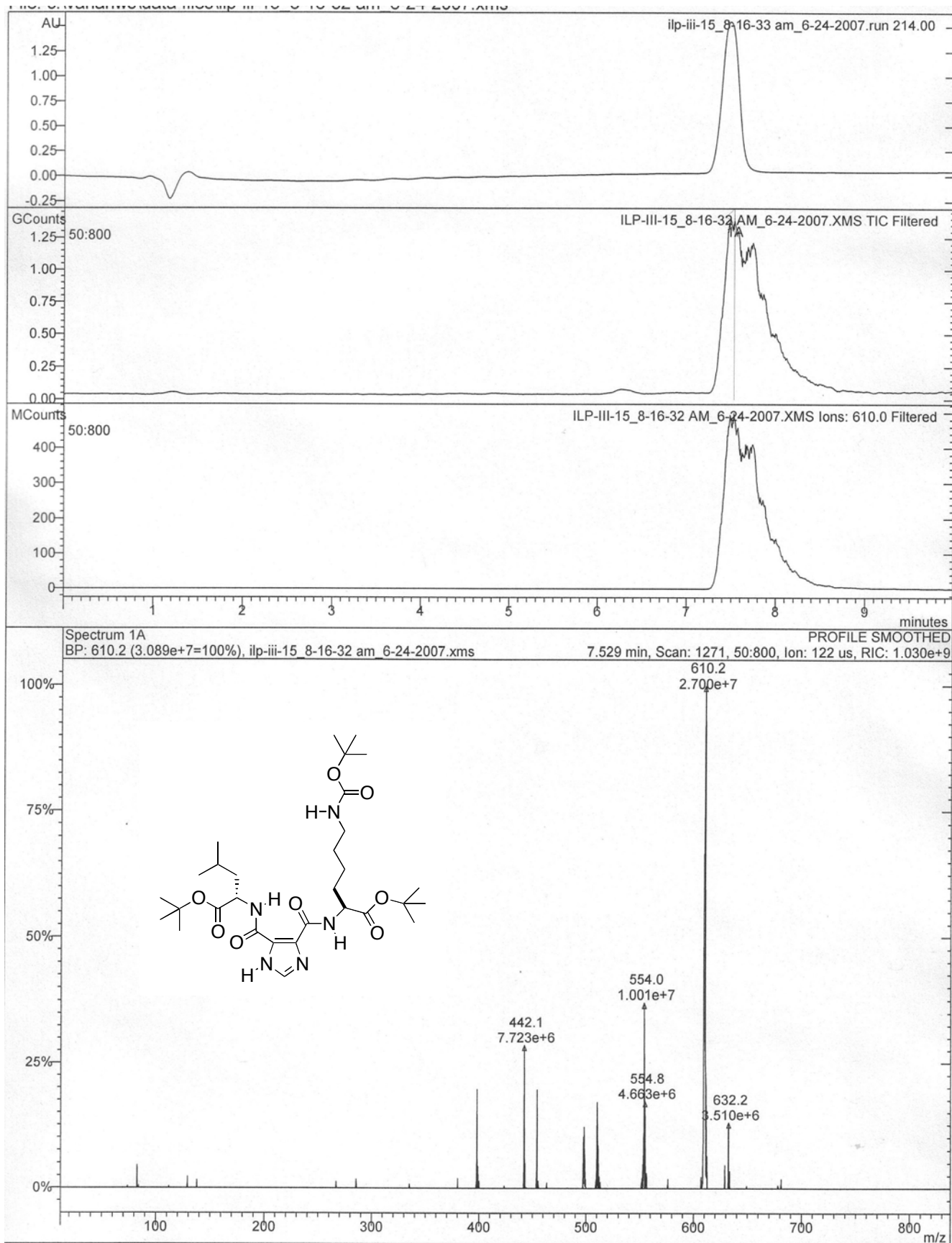


Figure S39. LC/MS data for 4{39}.

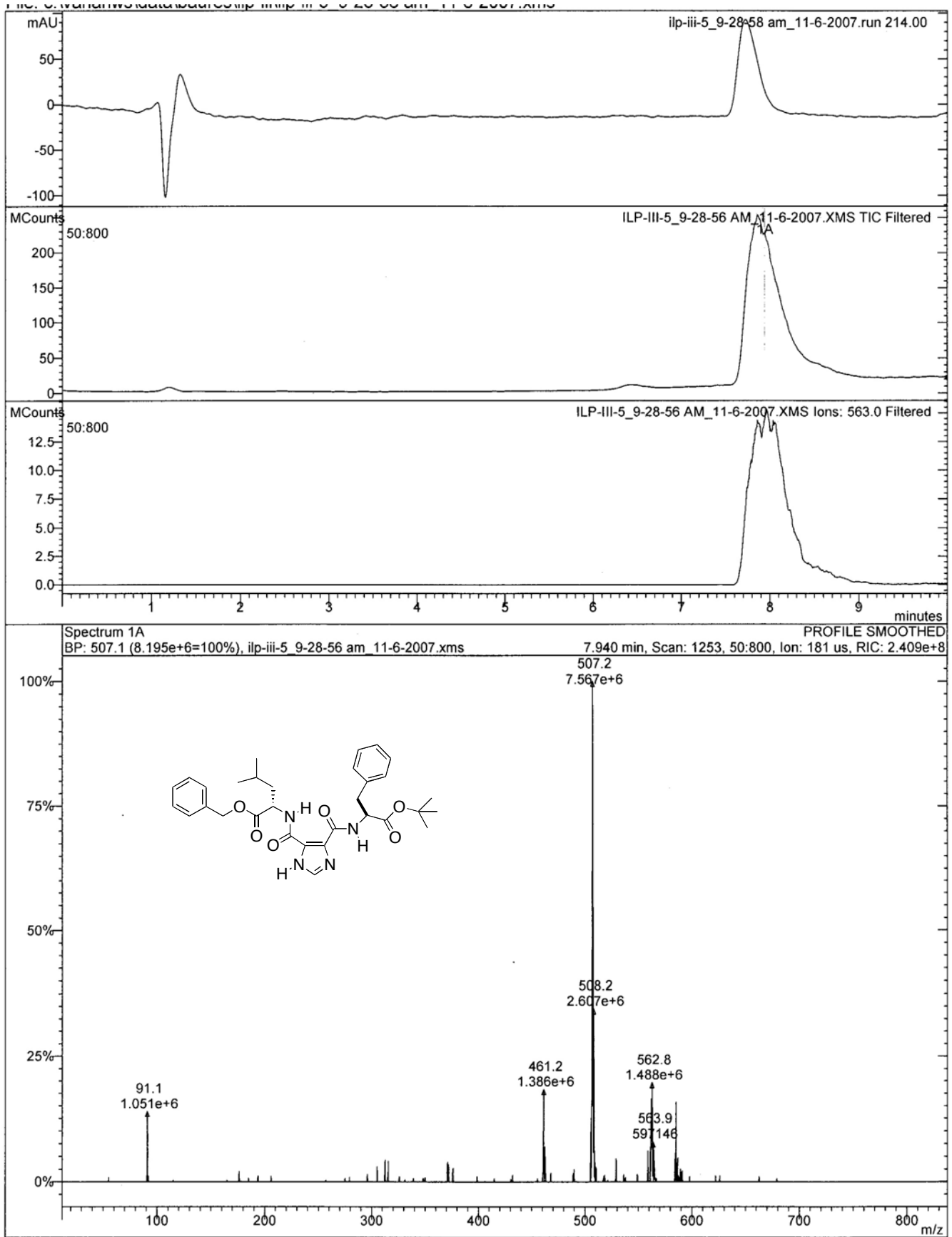


Figure S40. LC/MS data for 4{40}.

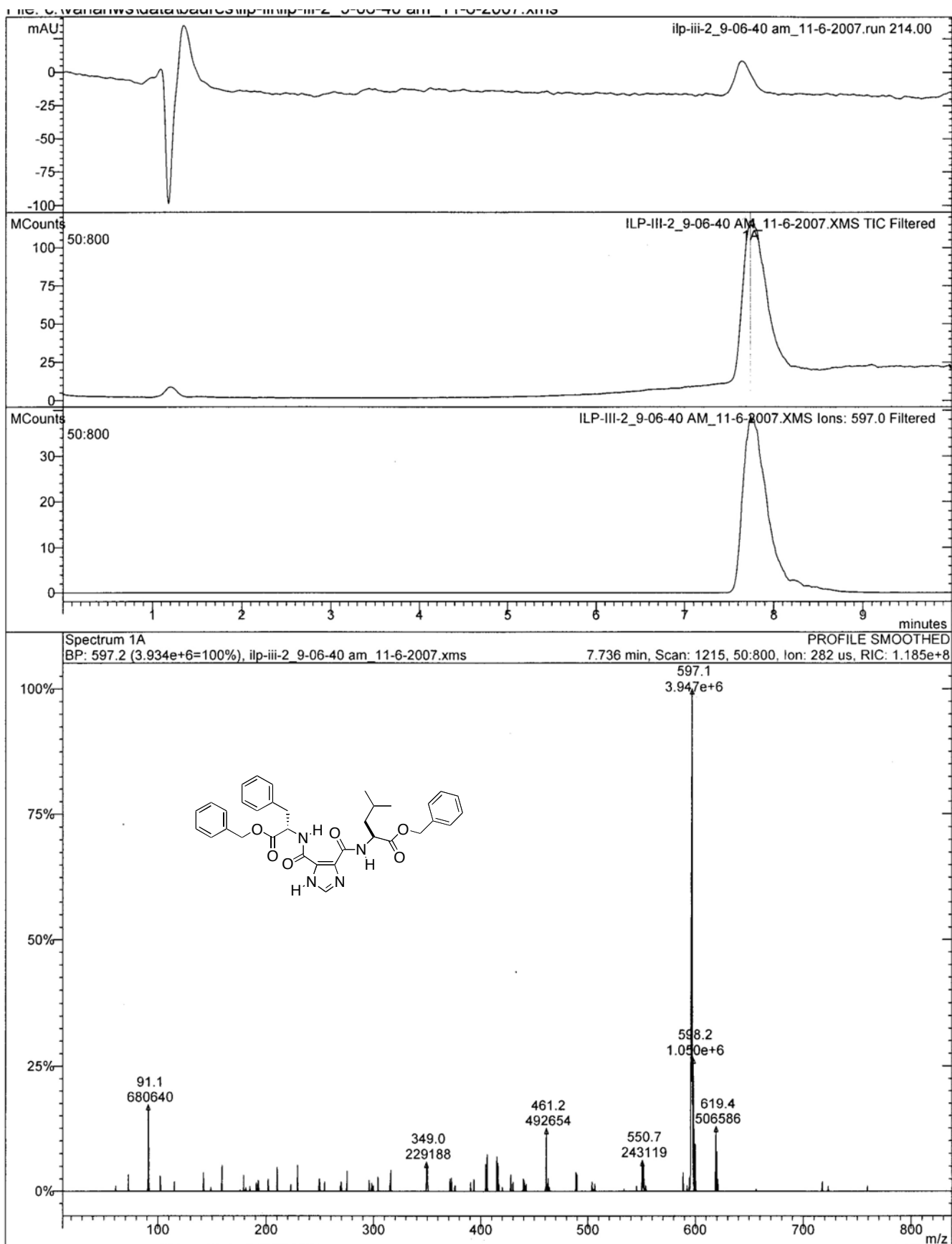


Figure S41. LC/MS data for 4{41}.

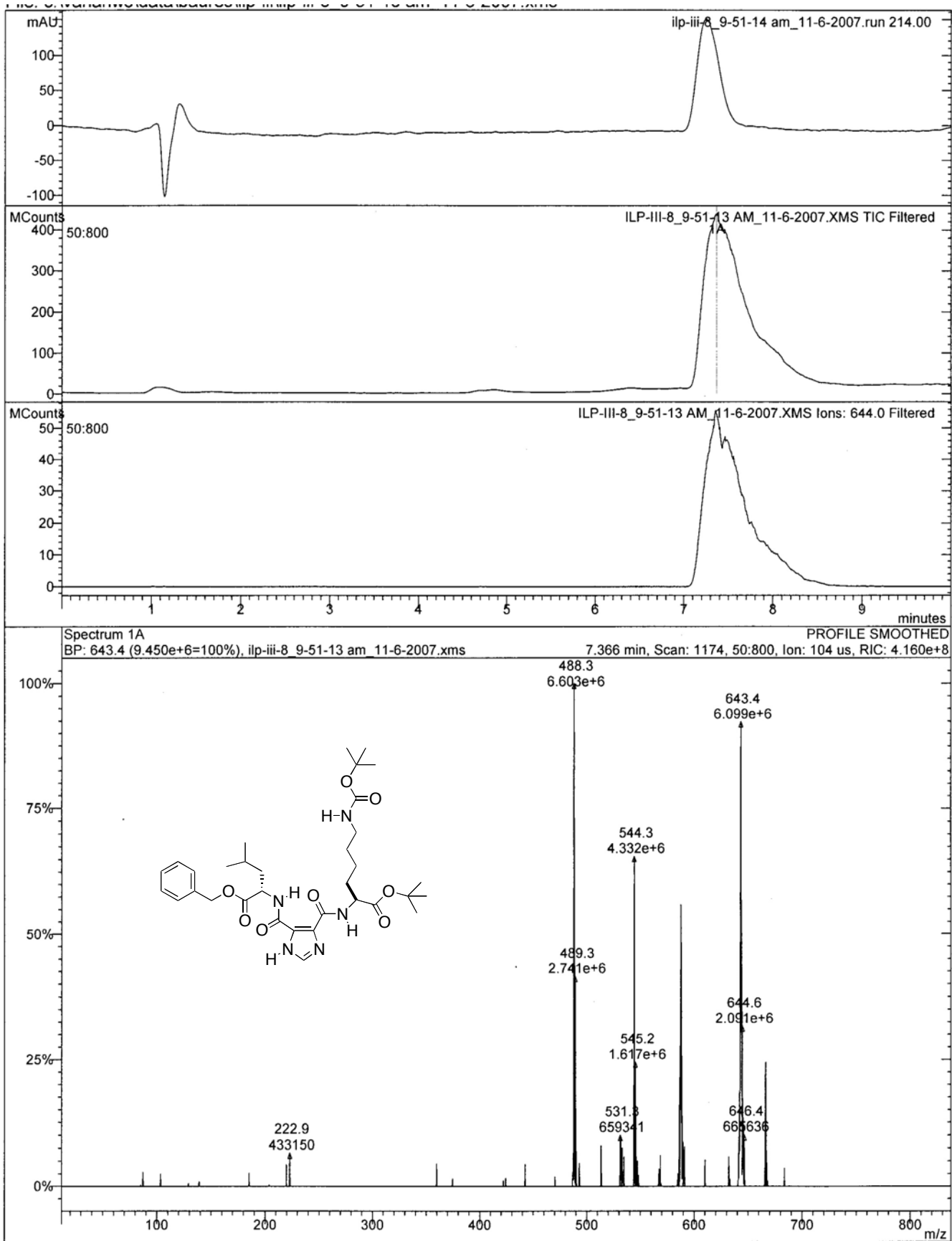


Figure S42. LC/MS data for 4{42}.

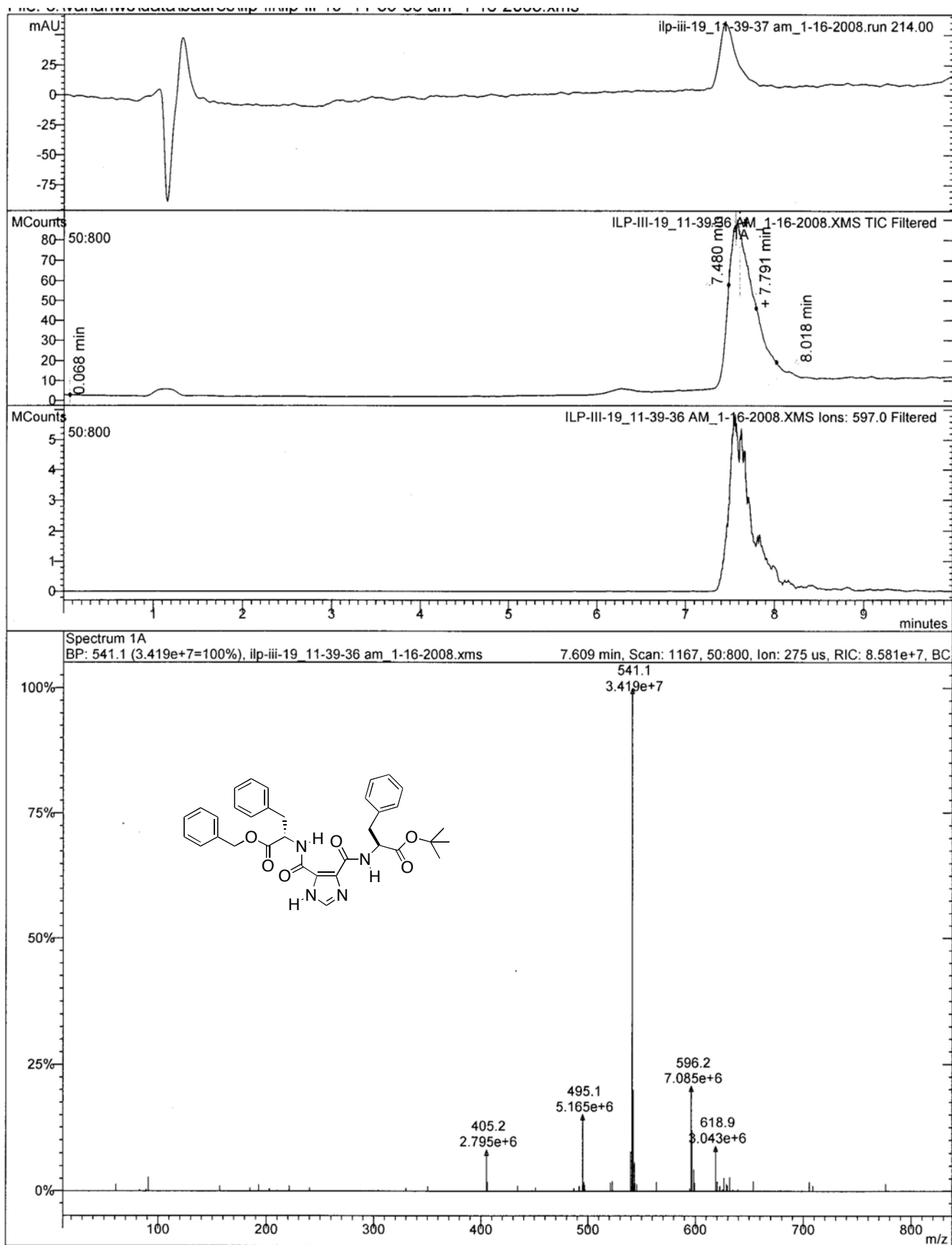


Figure S43. LC/MS data for 4{43}.

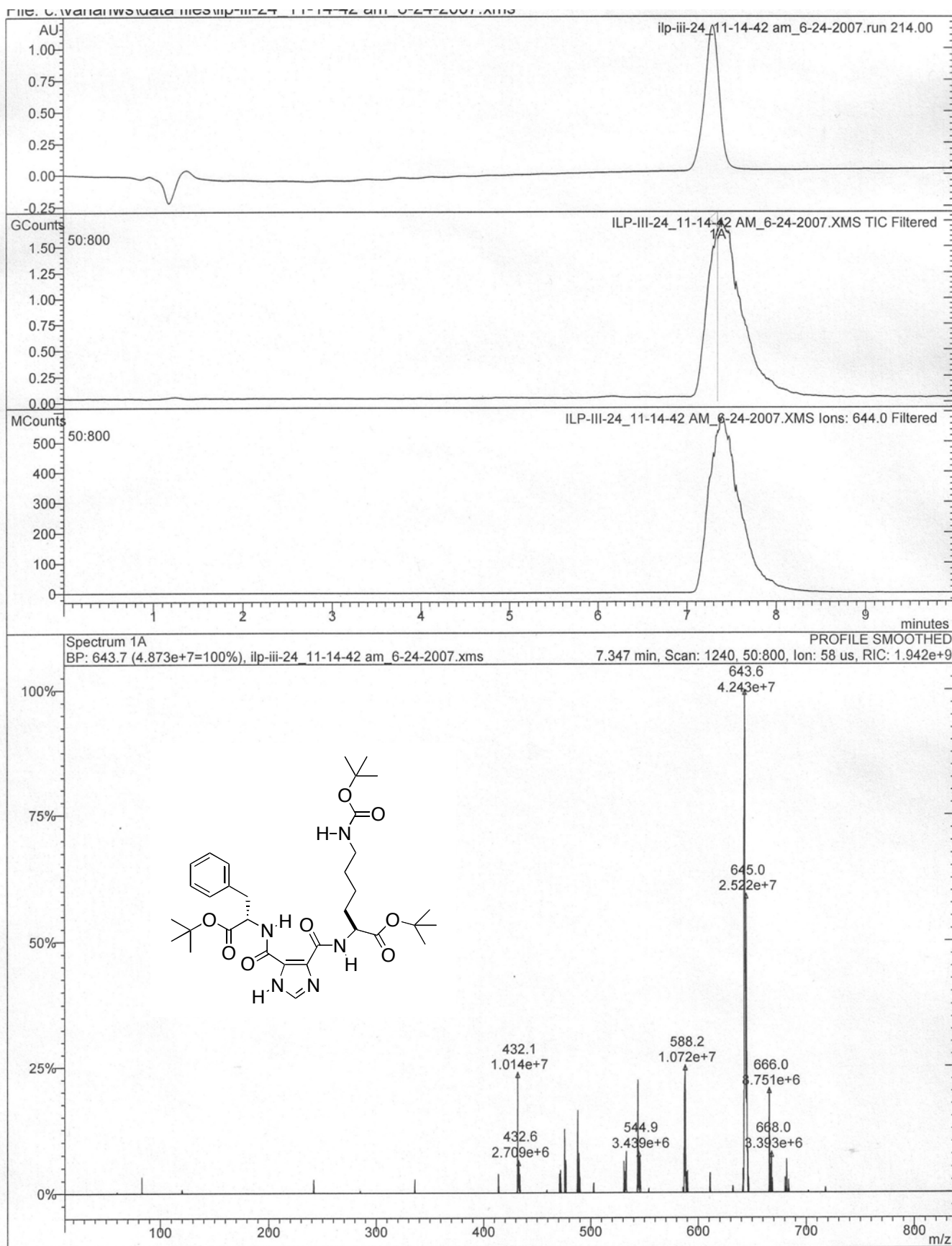


Figure S44. LC/MS data for 4{44}.

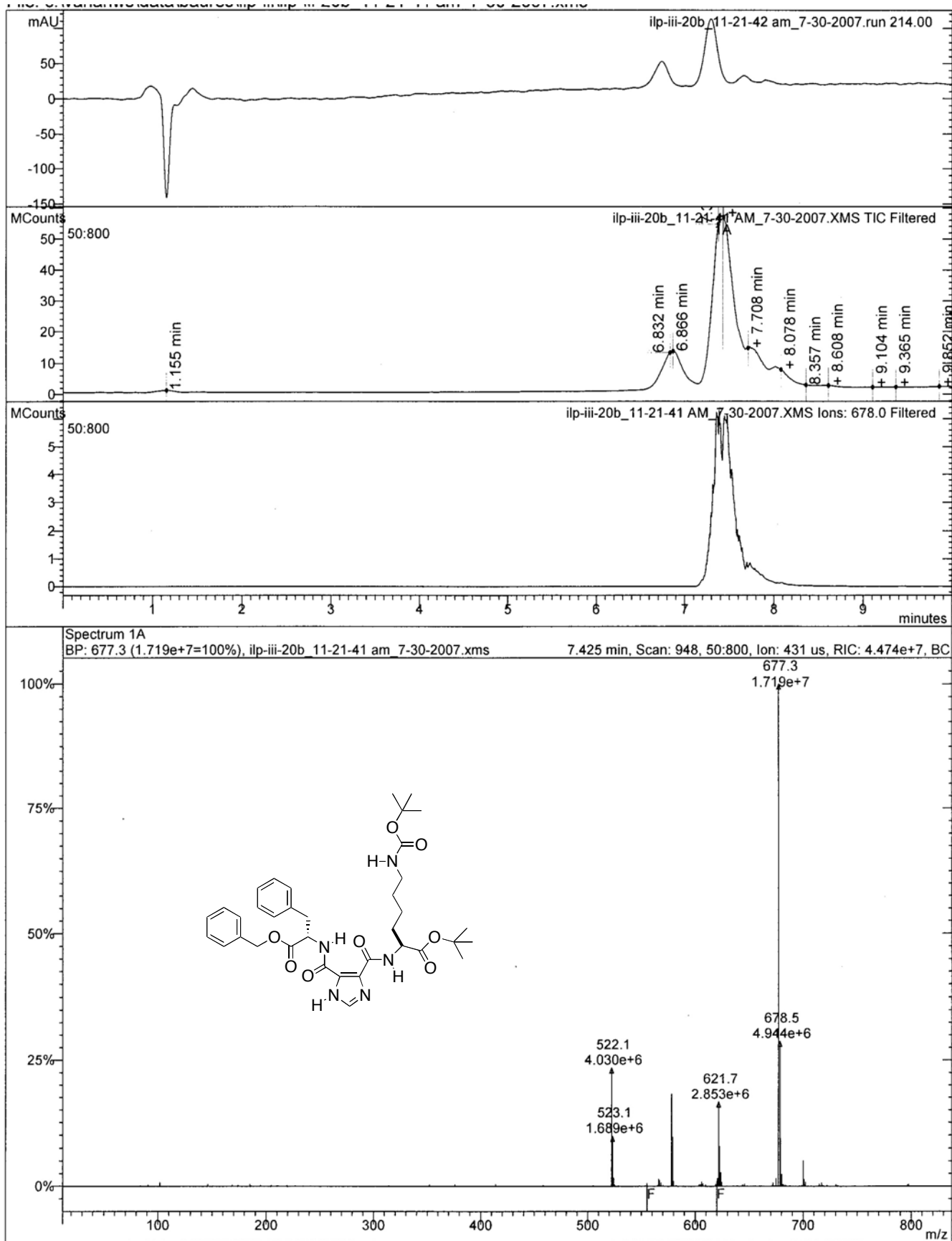


Figure S45. LC/MS data for 4{45}.

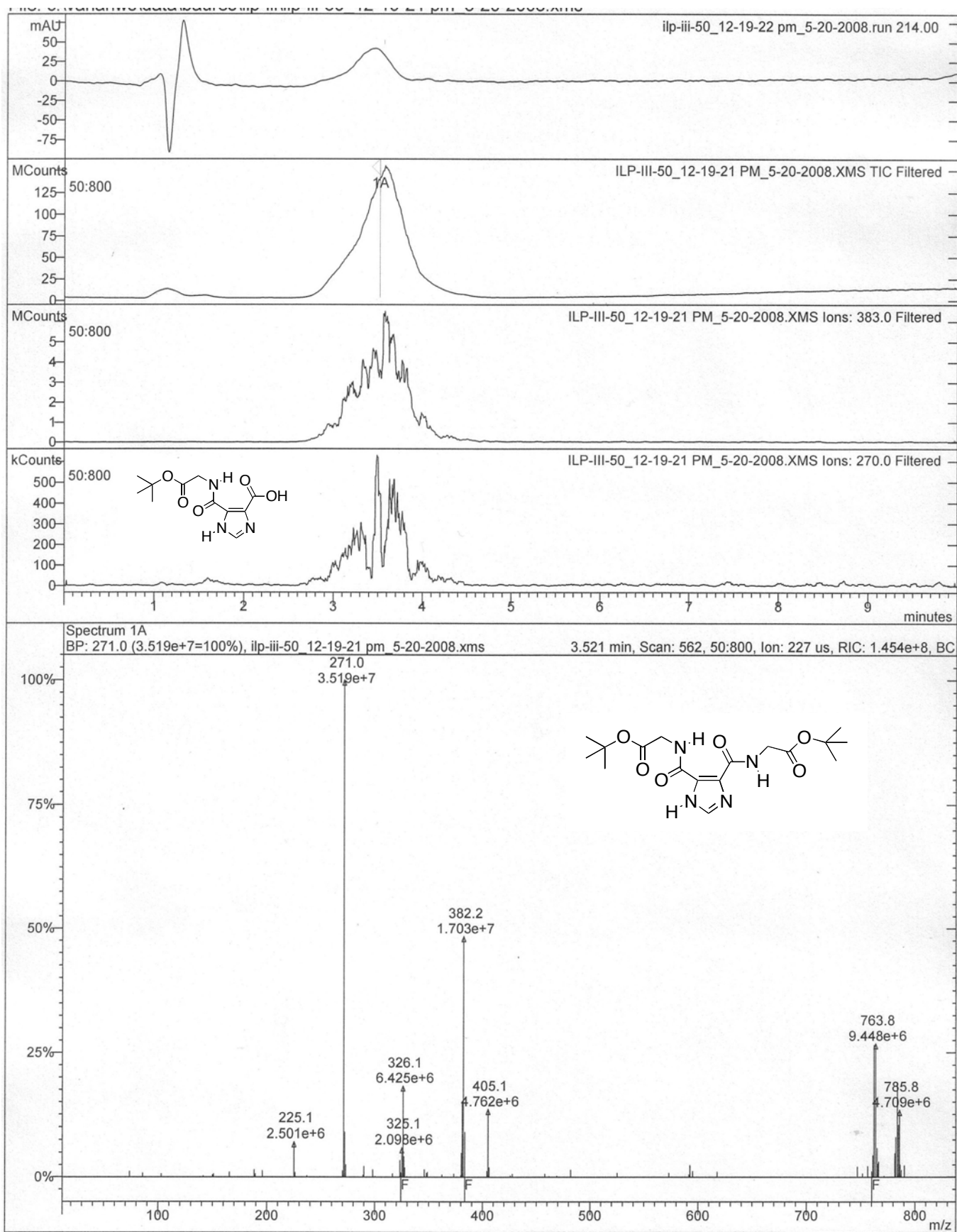


Figure S46. LC/MS data for the crude reaction to yield 4{1}.

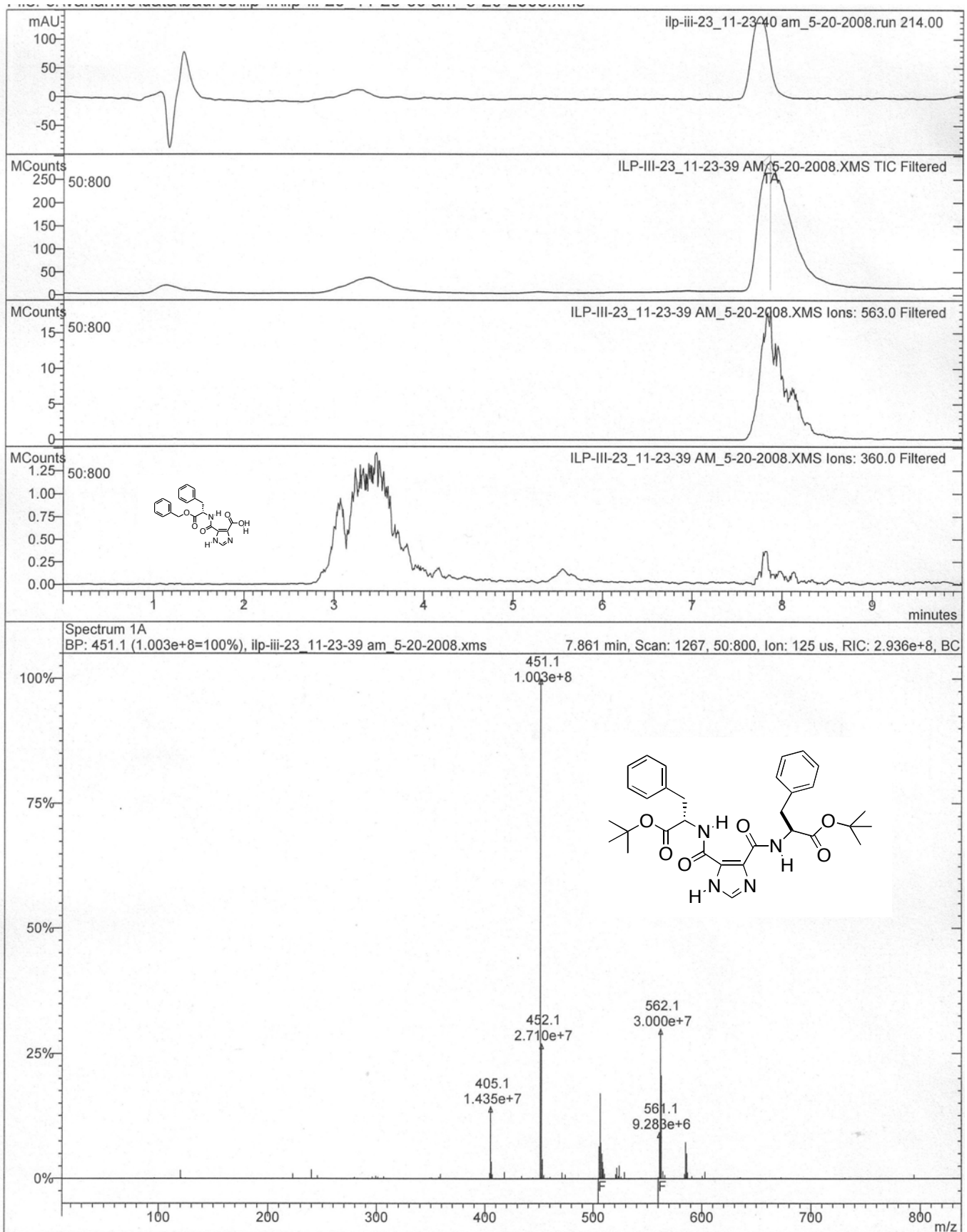


Figure S47. LC/MS data for the crude reaction to yield 4{7}.

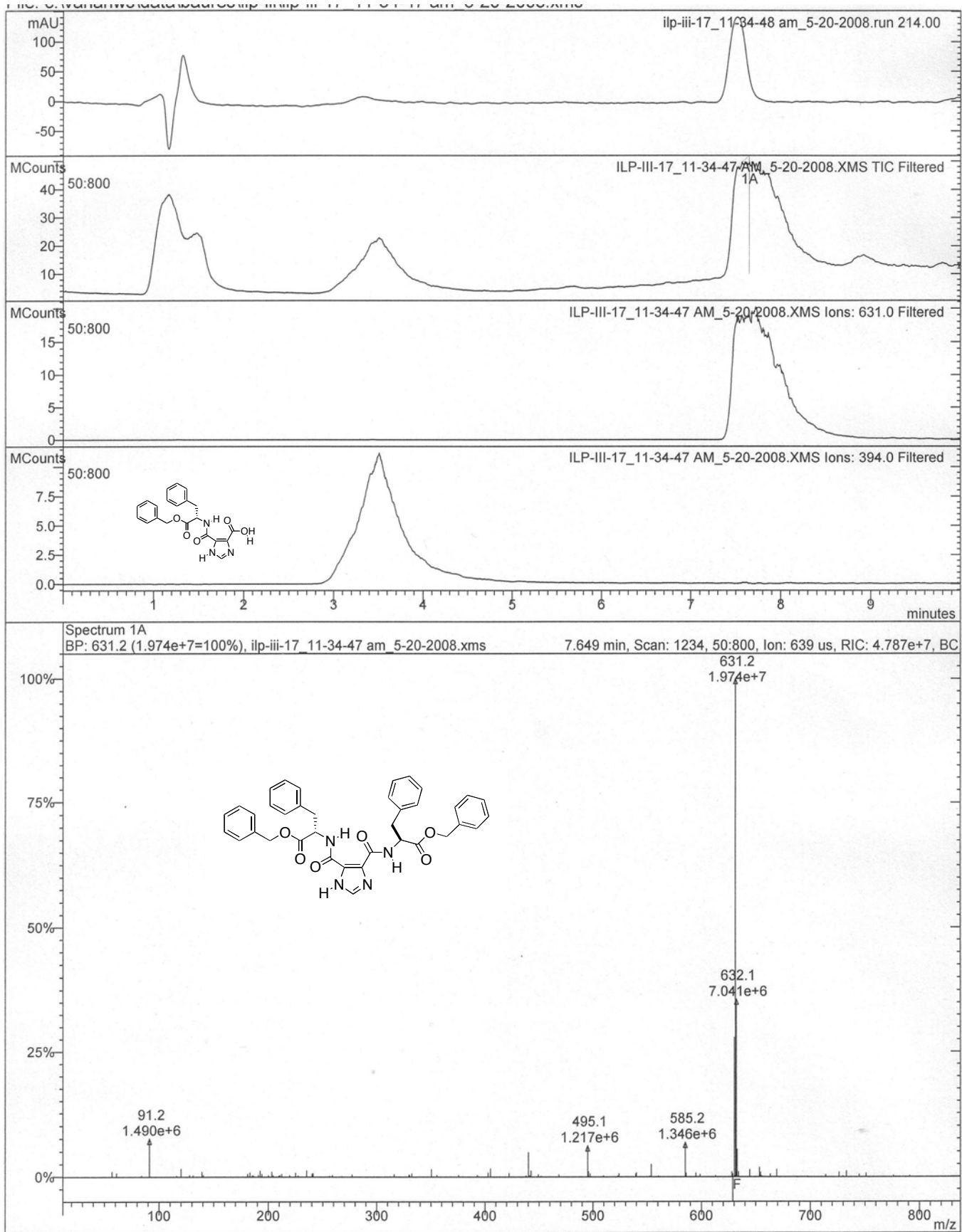


Figure S48. LC/MS data for the crude reaction to yield 4{8}.

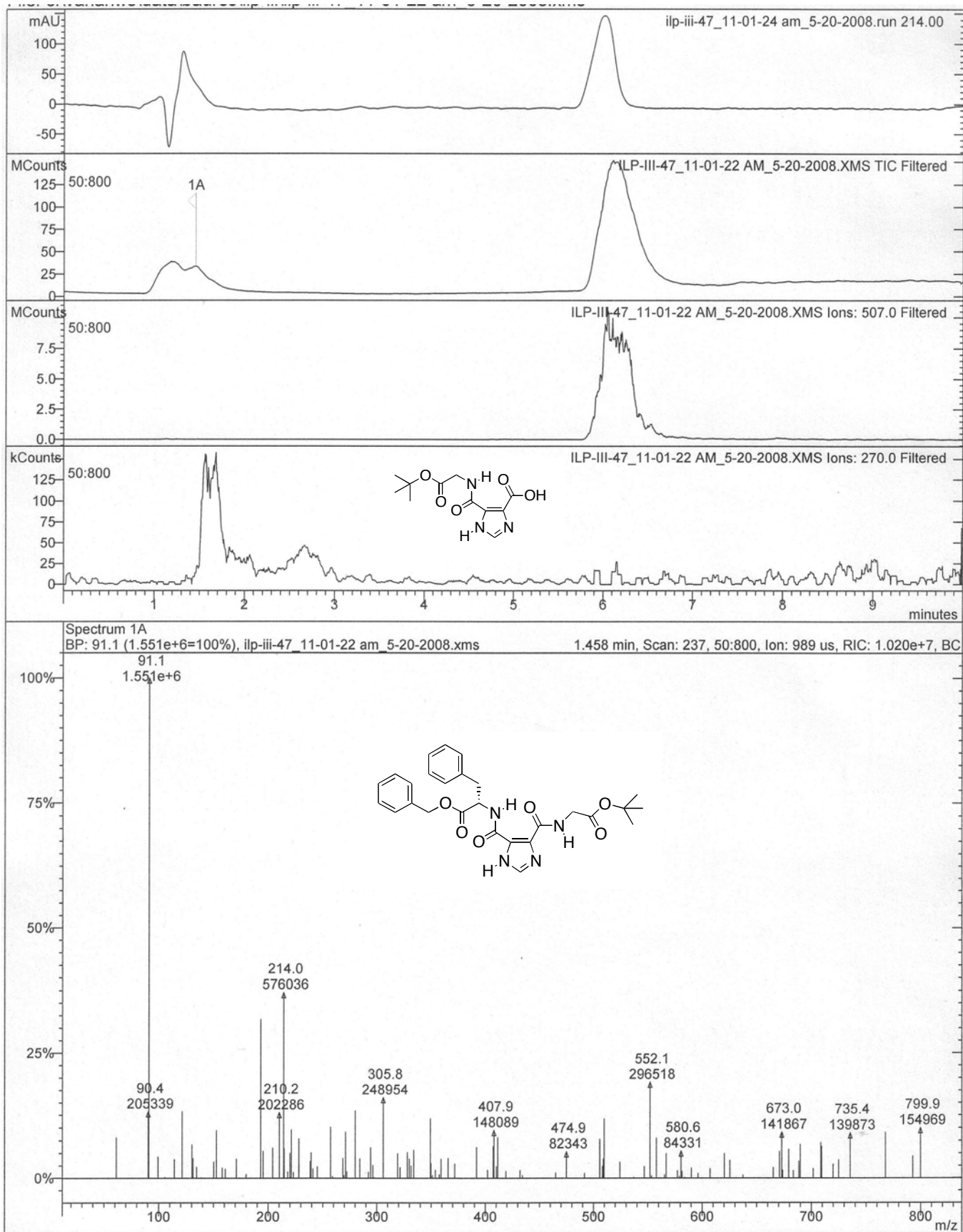


Figure S49. LC/MS data for the crude reaction to yield 4{16}.

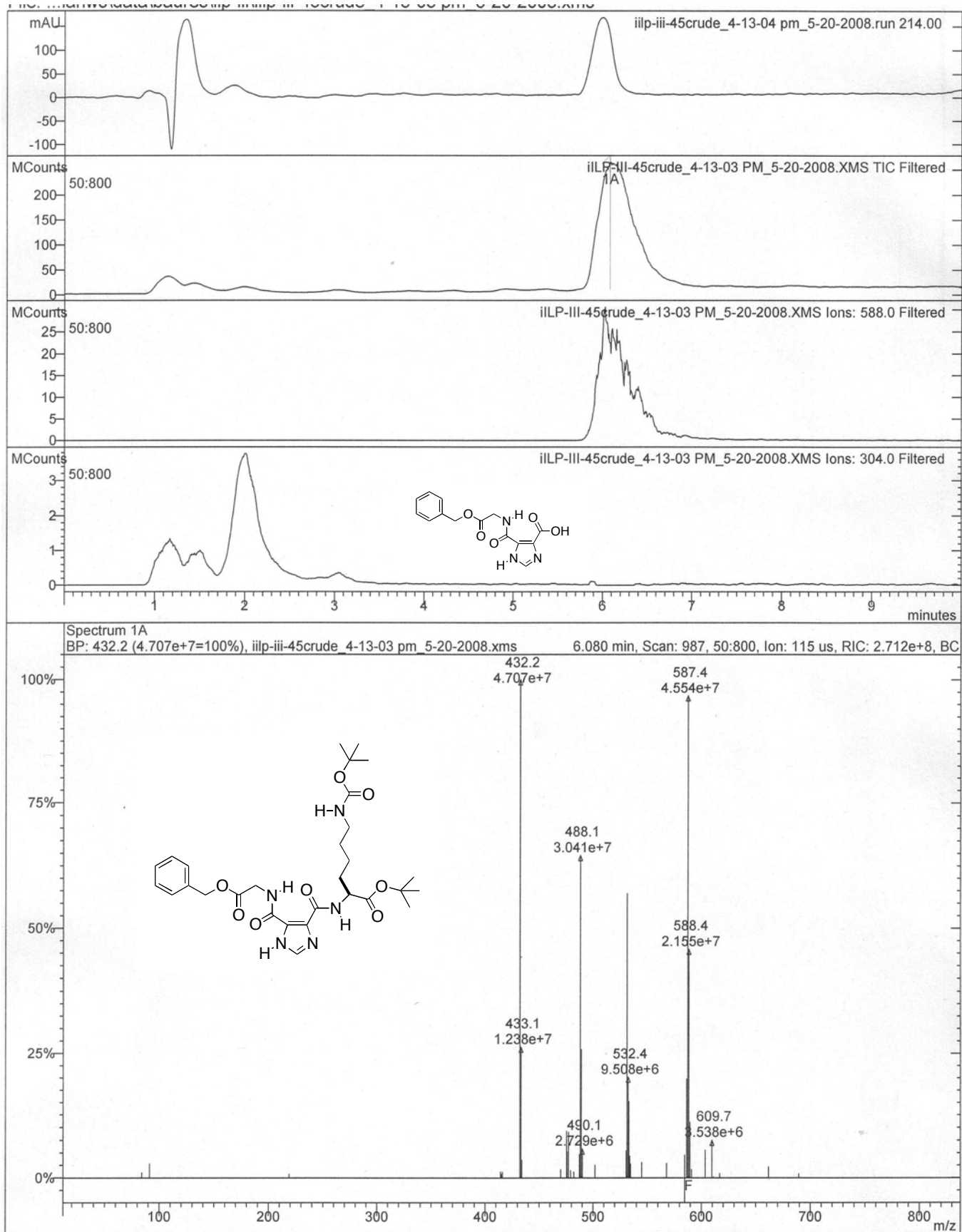


Figure S50. LC/MS data for the crude reaction to yield 4{24}.

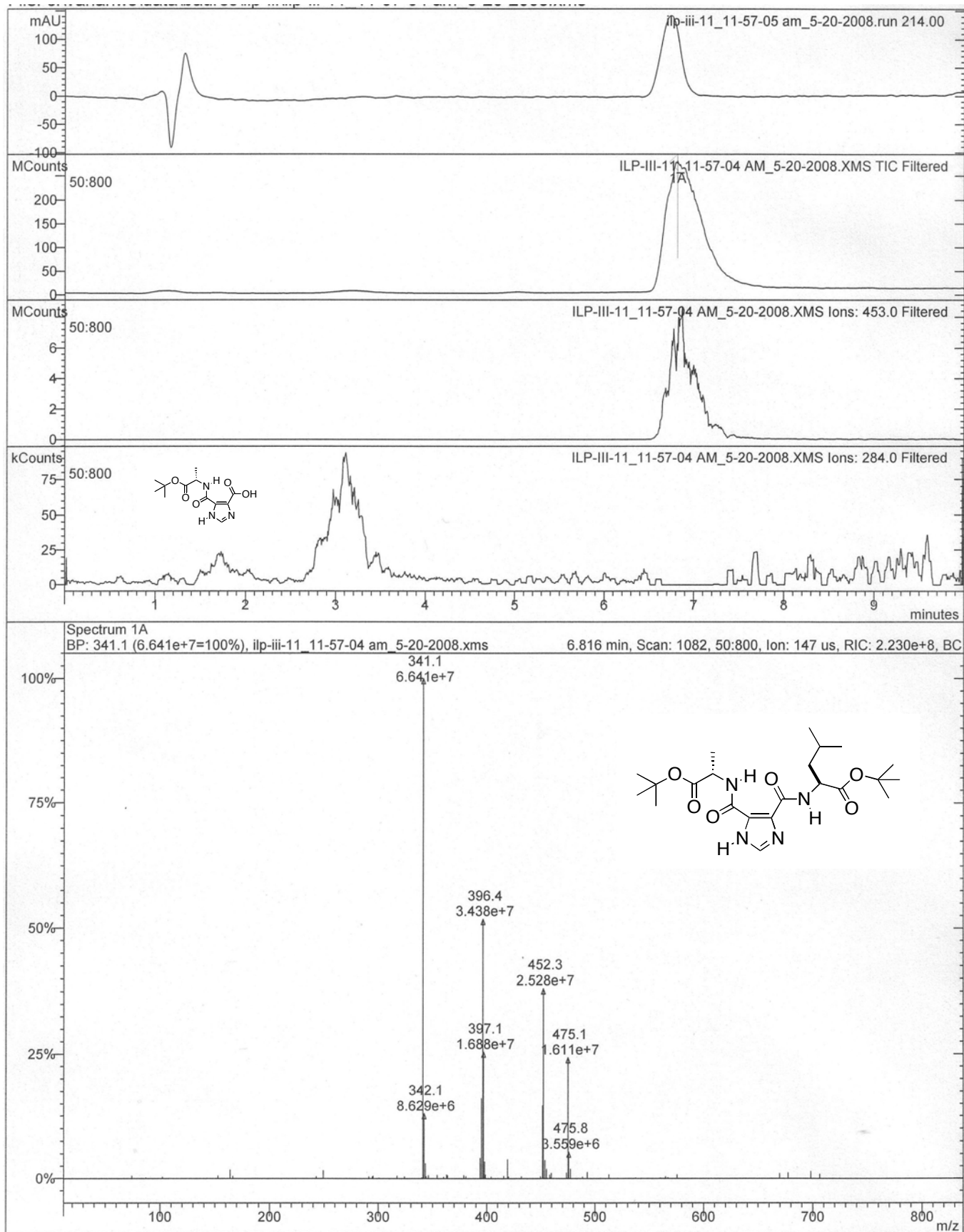


Figure S51. LC/MS data for the crude reaction to yield 4{26}.

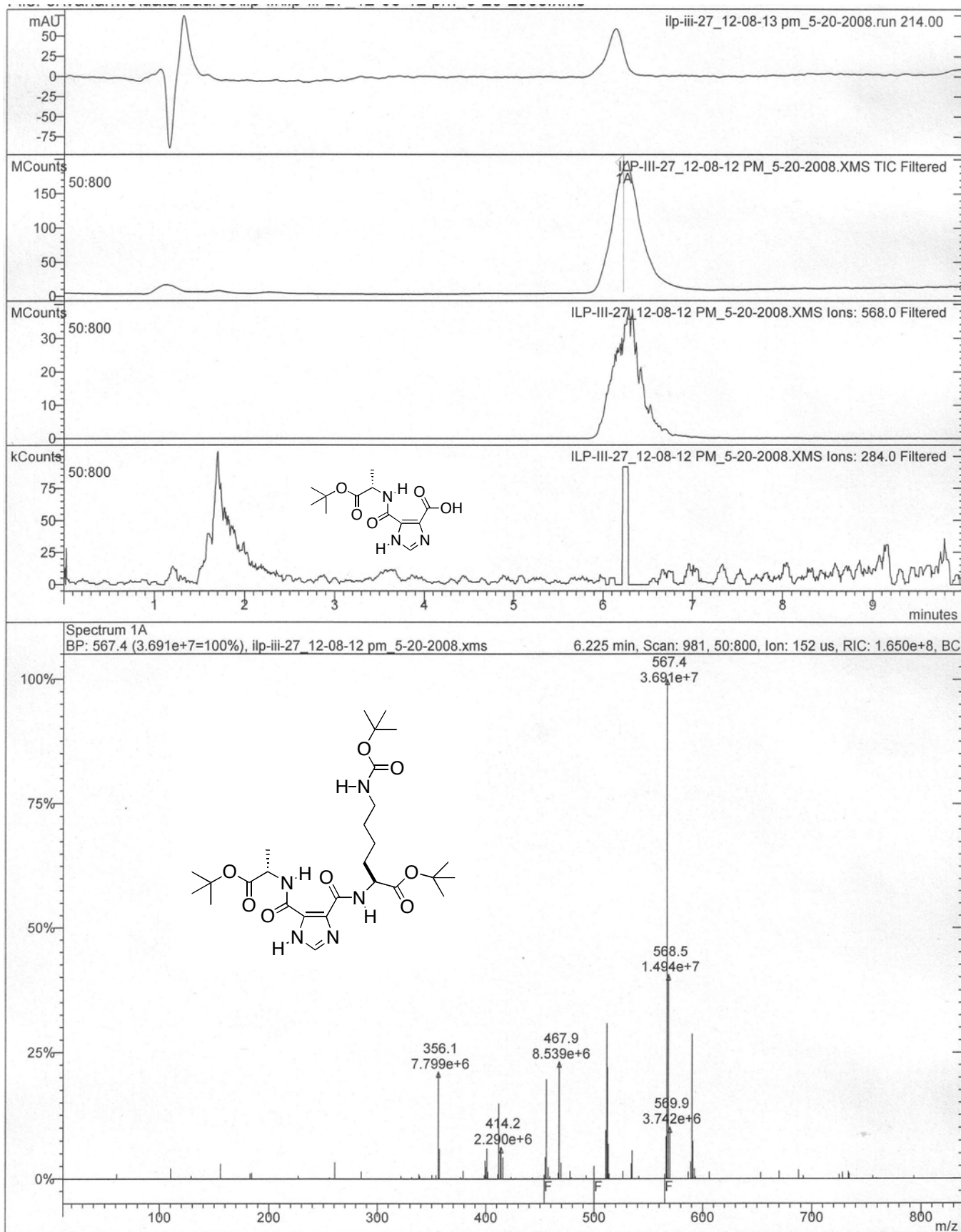


Figure S52. LC/MS data for the crude reaction to yield 4{30}.

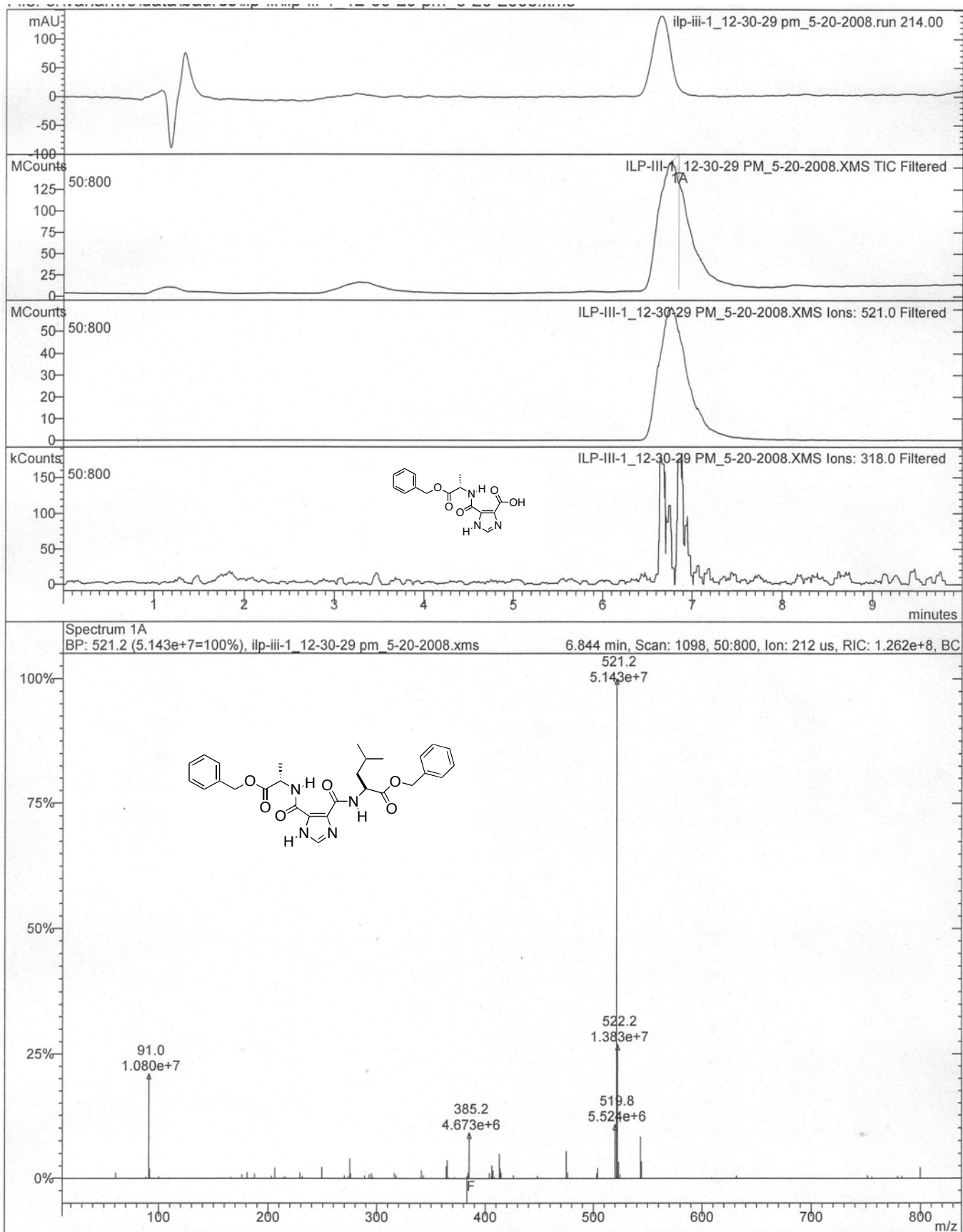


Figure S53. LC/MS data for the crude reaction to yield 4{32}.

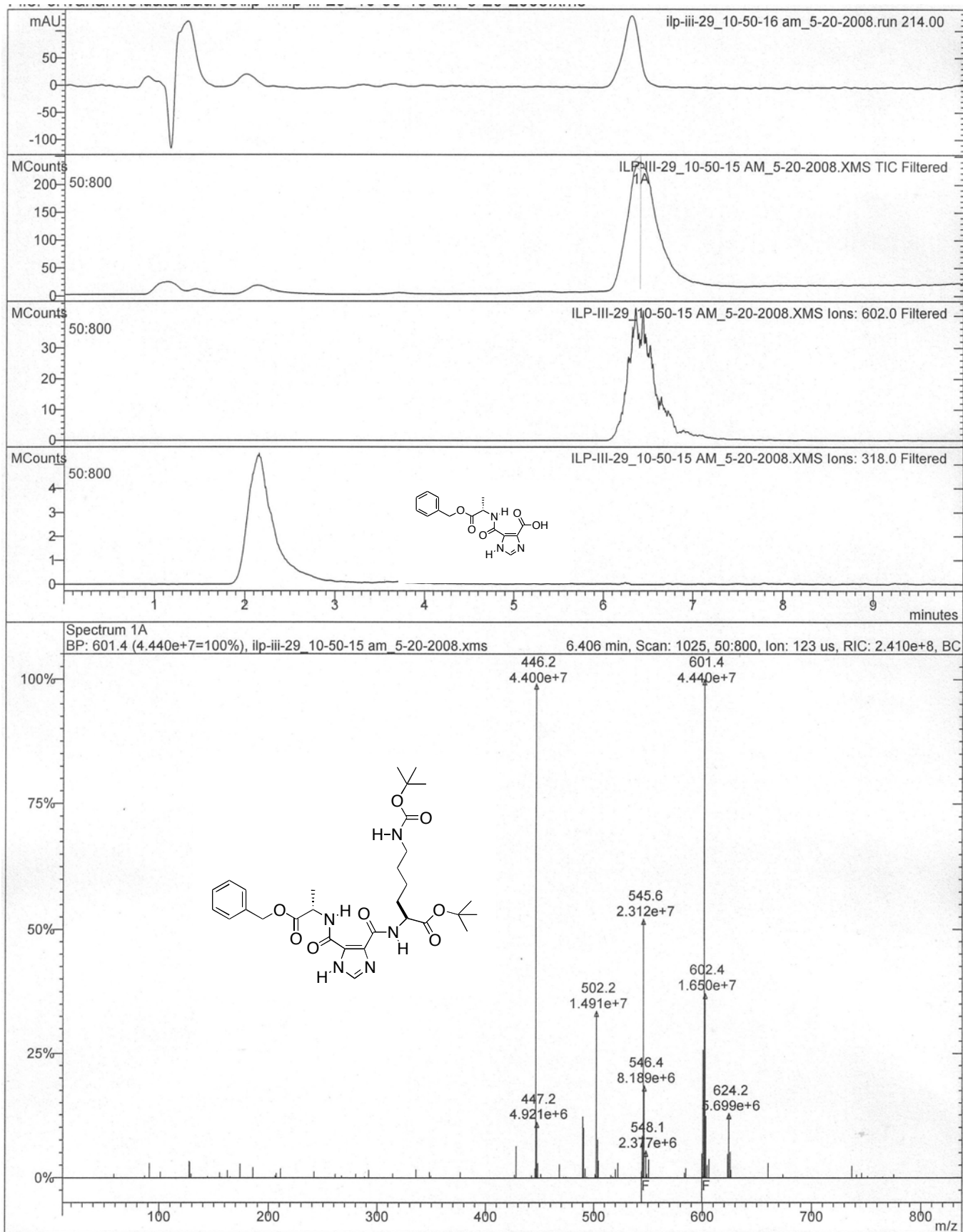


Figure S54. LC/MS data for the crude reaction to yield 4{35}.

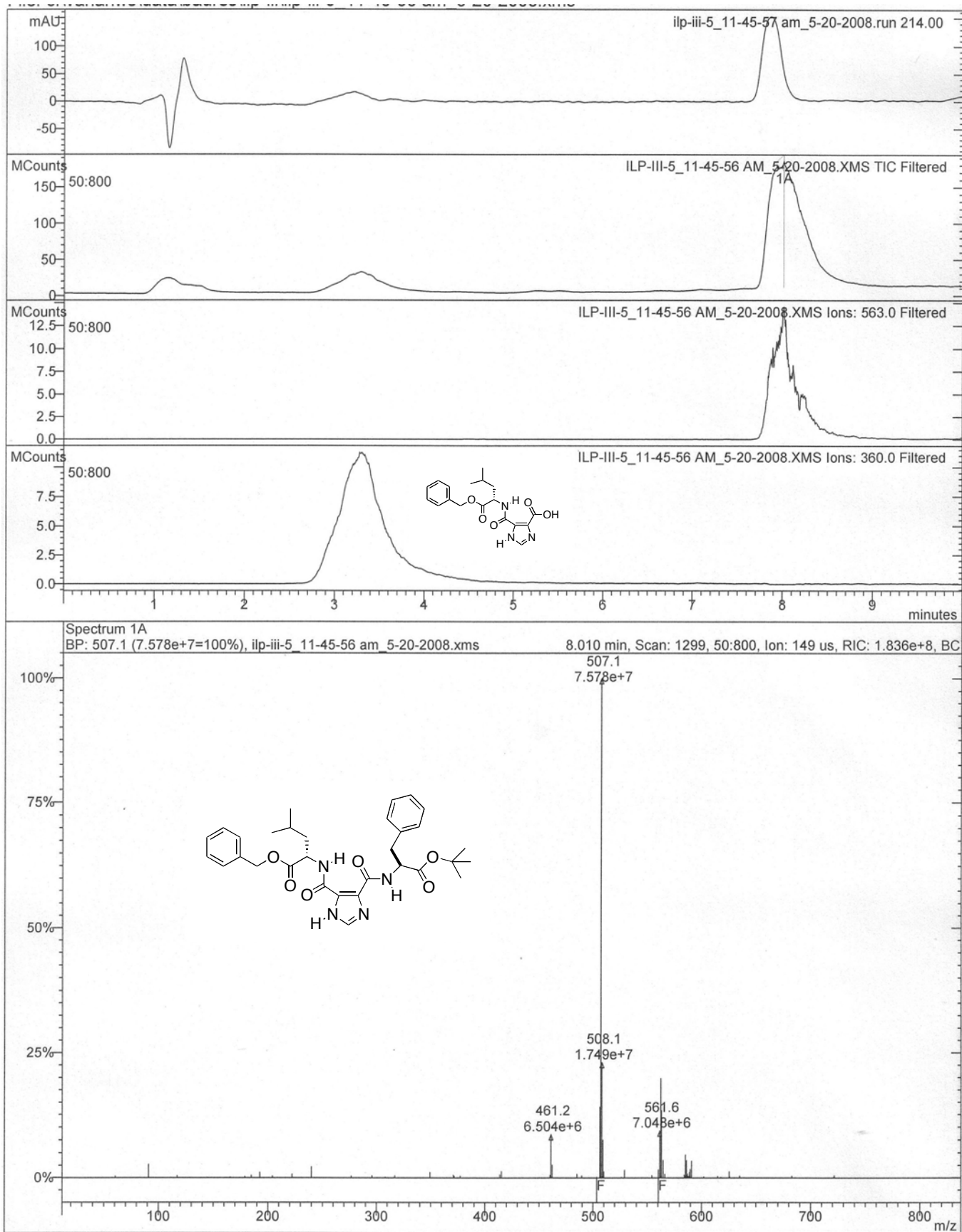


Figure S55. LC/MS data for the crude reaction to yield 4{40}.

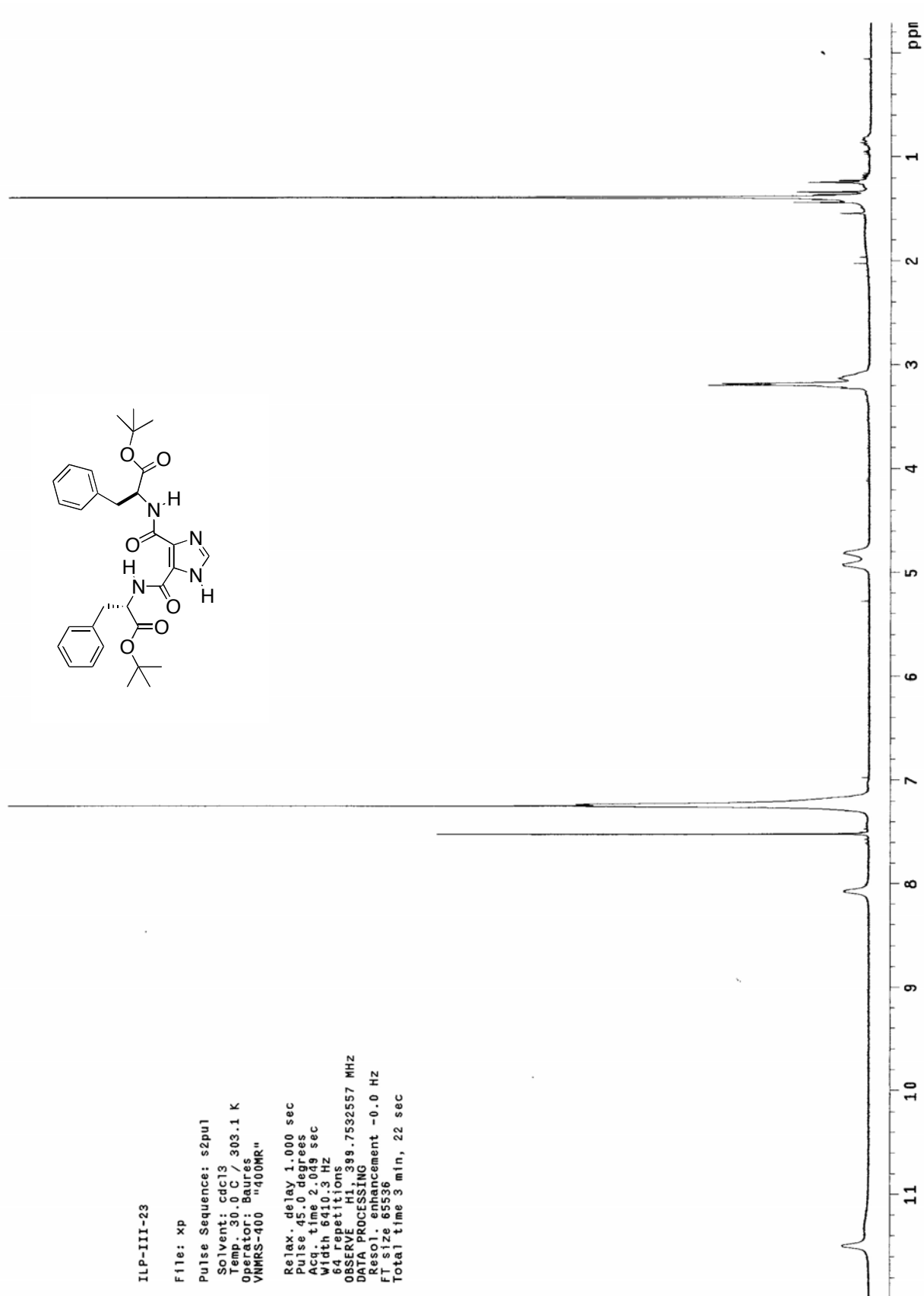
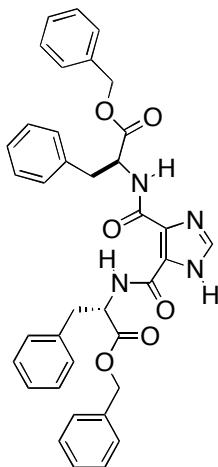


Figure S56. ¹H-NMR for 4{7}.



ILP-III-17

File: xp

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 30.0 C / 303.1 K

Operator: Baures

VNMRK-400 "400MR"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

64 repetitions

OBSERVE H1, 399.7532555 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 65536

Total time 3 min, 22 sec

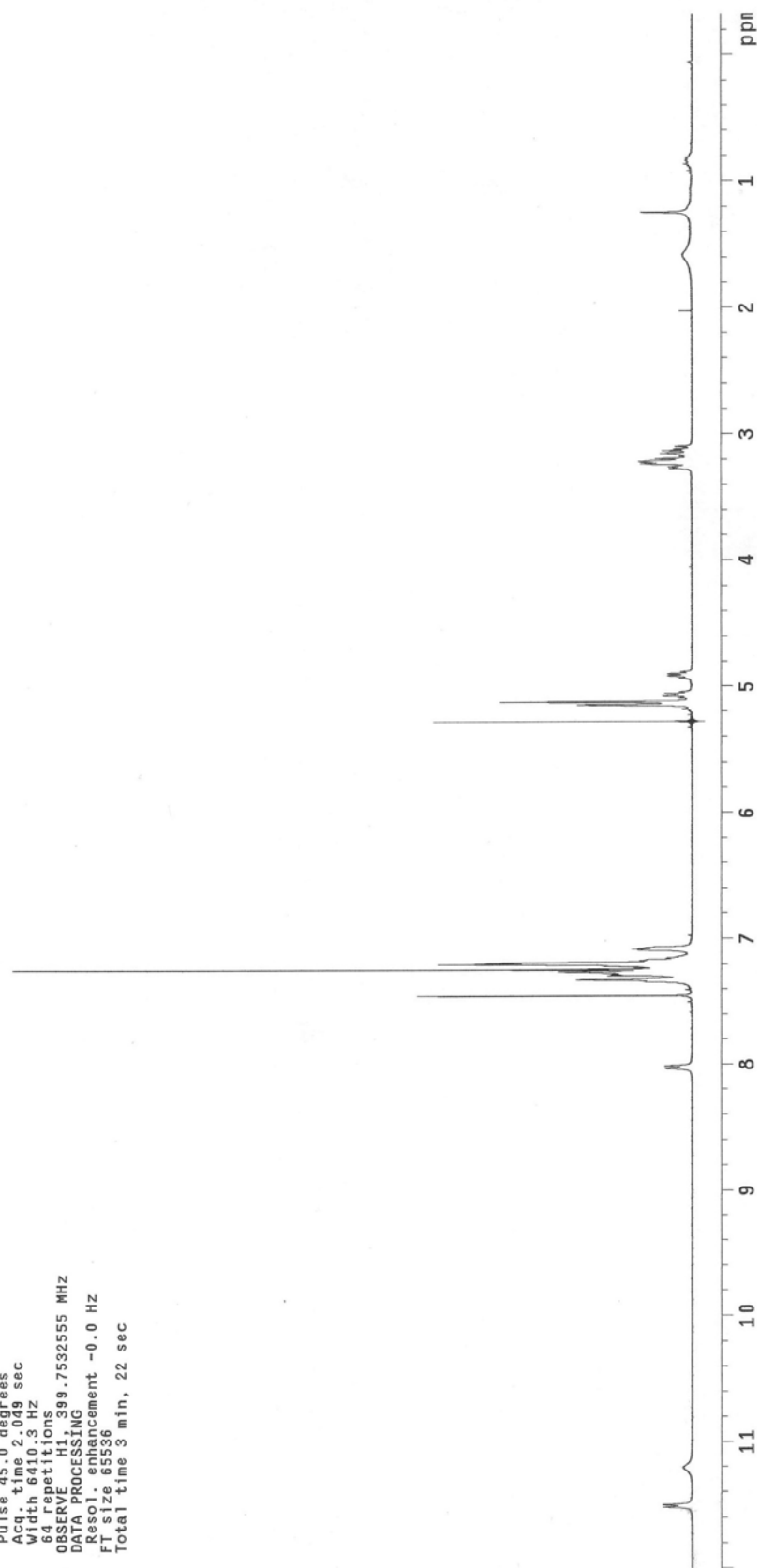


Figure S57. ¹H-NMR for 4{8}.

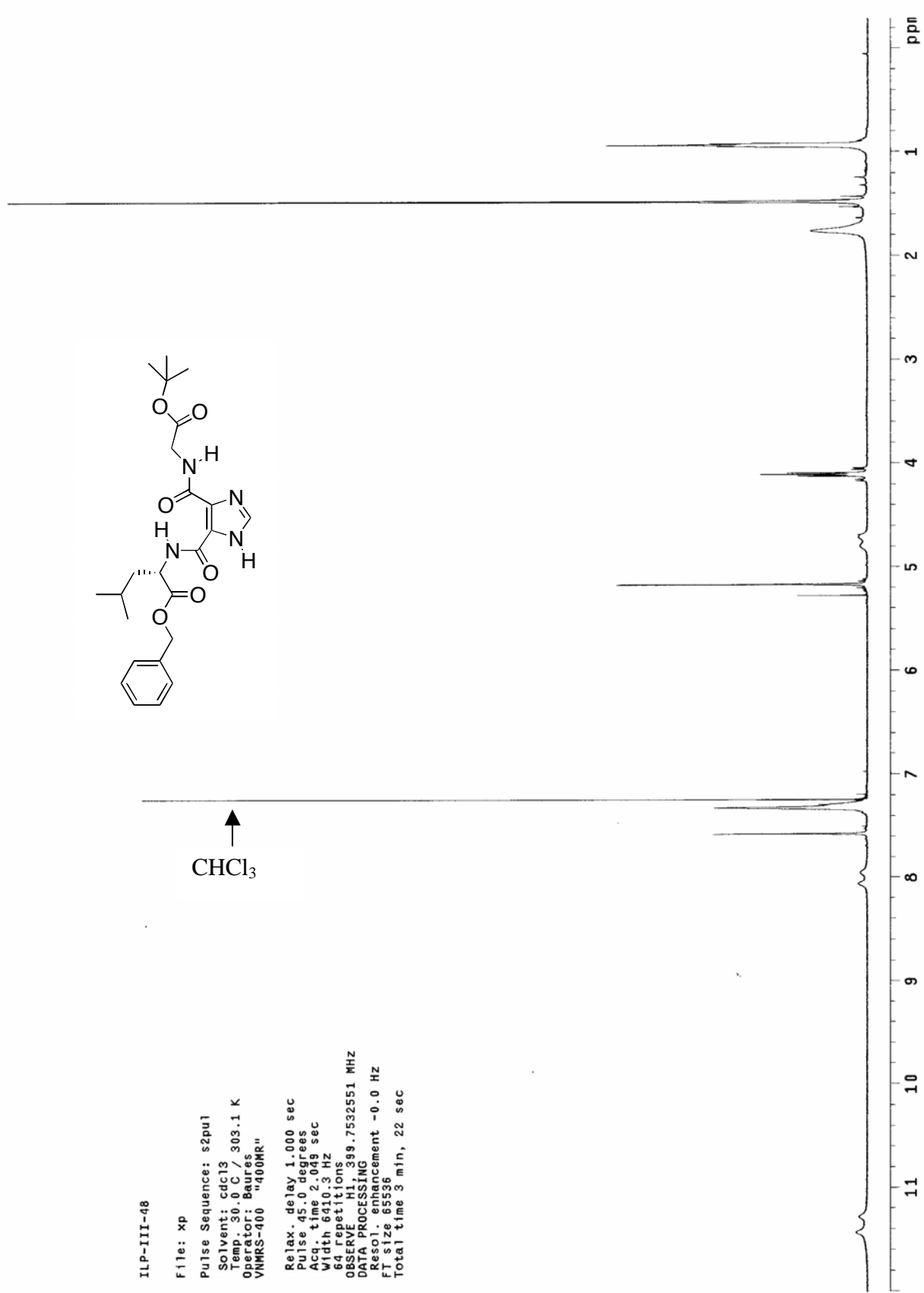


Figure S58. ¹H-NMR for 4{14}.

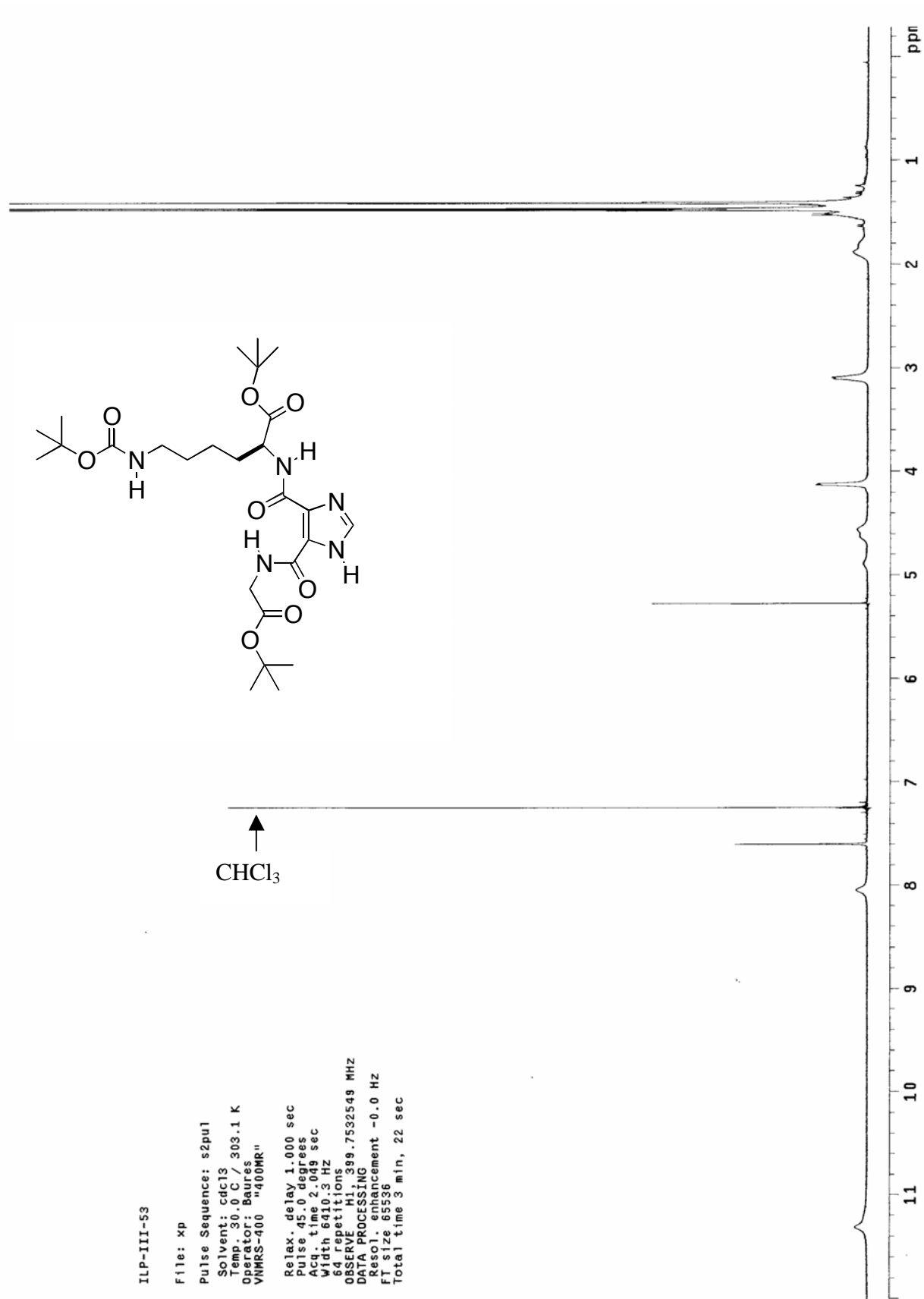


Figure 59. ¹H-NMR for 4{17}.

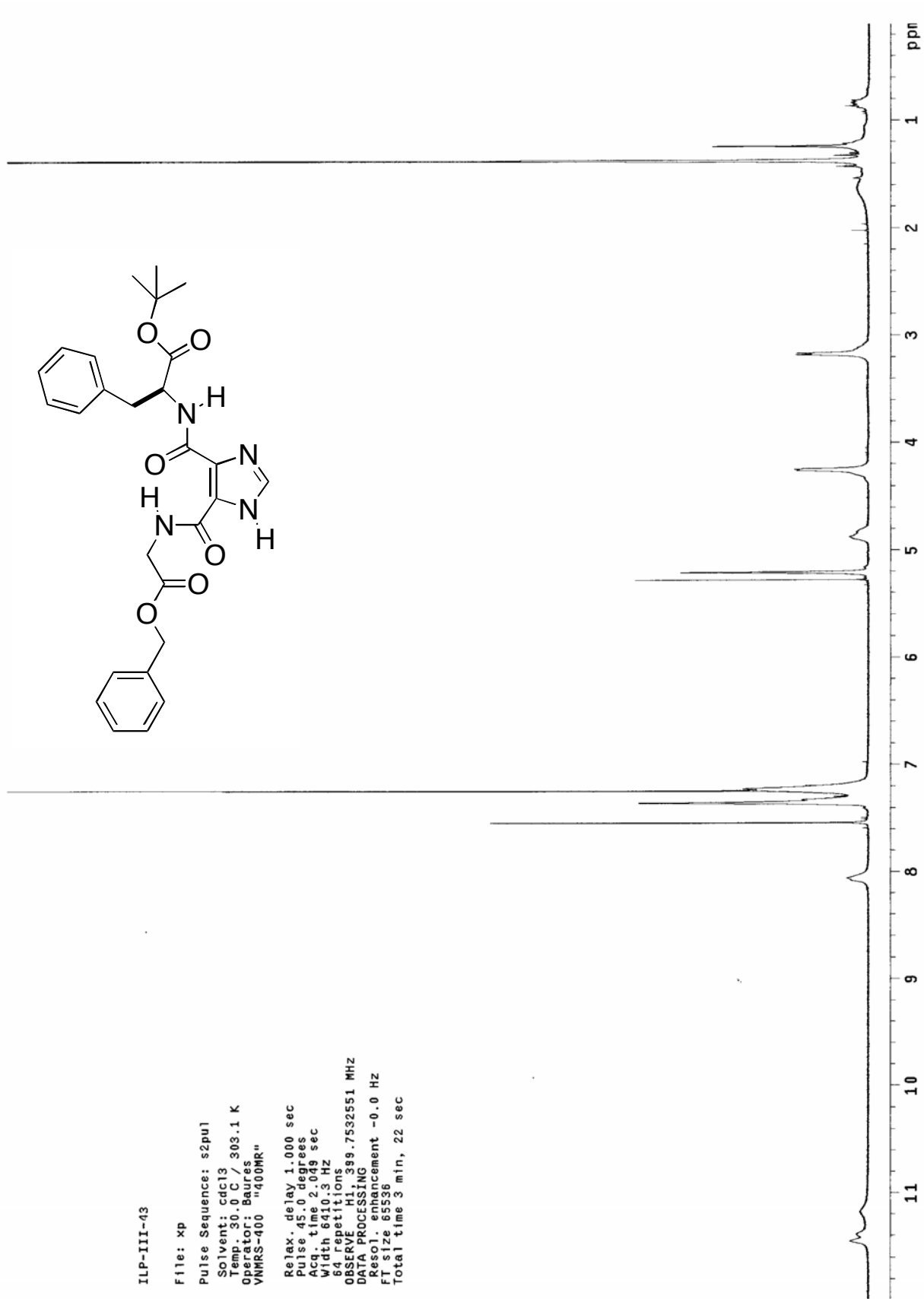


Figure S60. $^1\text{H-NMR}$ for 4{22}.

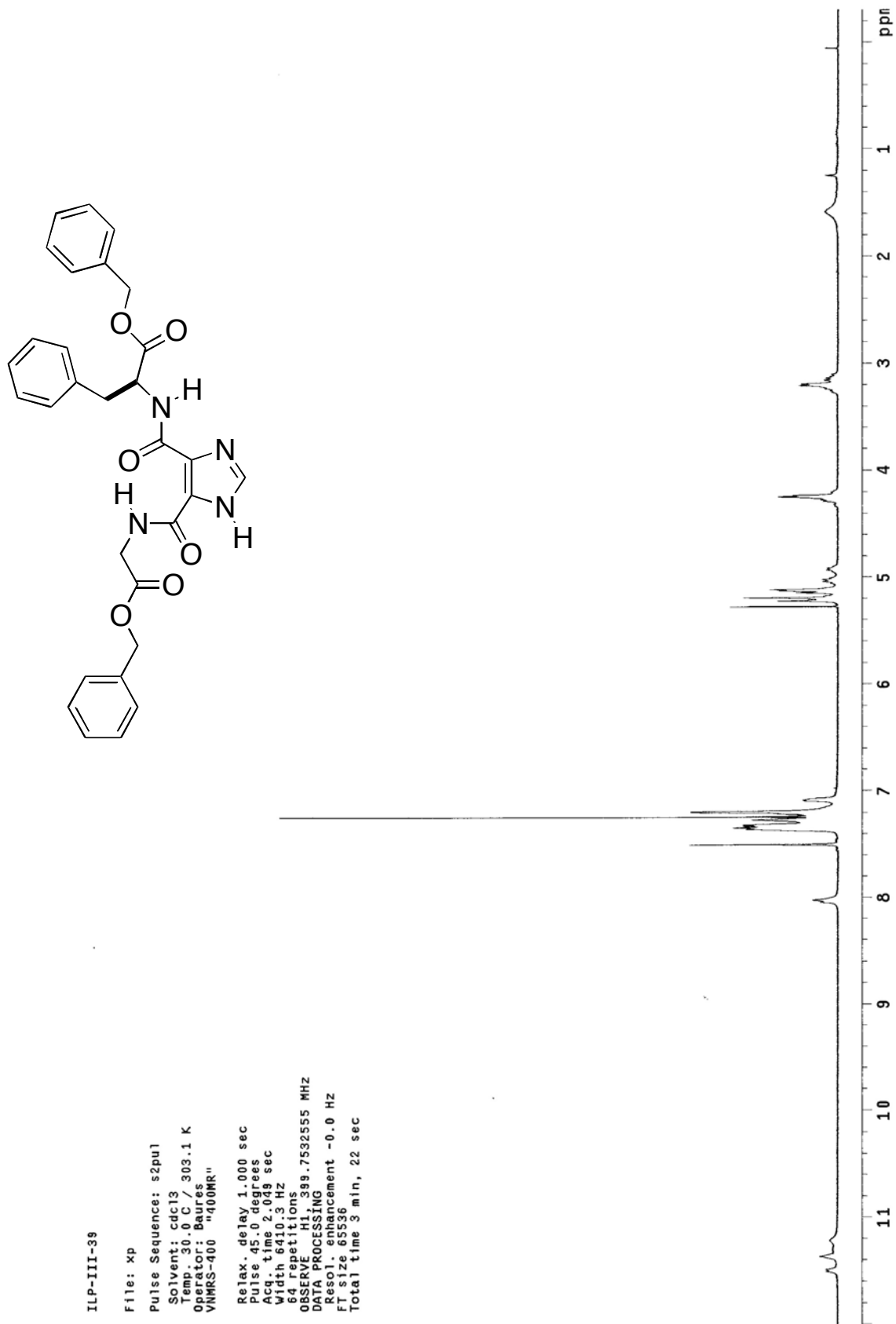


Figure S61. $^1\text{H-NMR}$ for 4{23}.

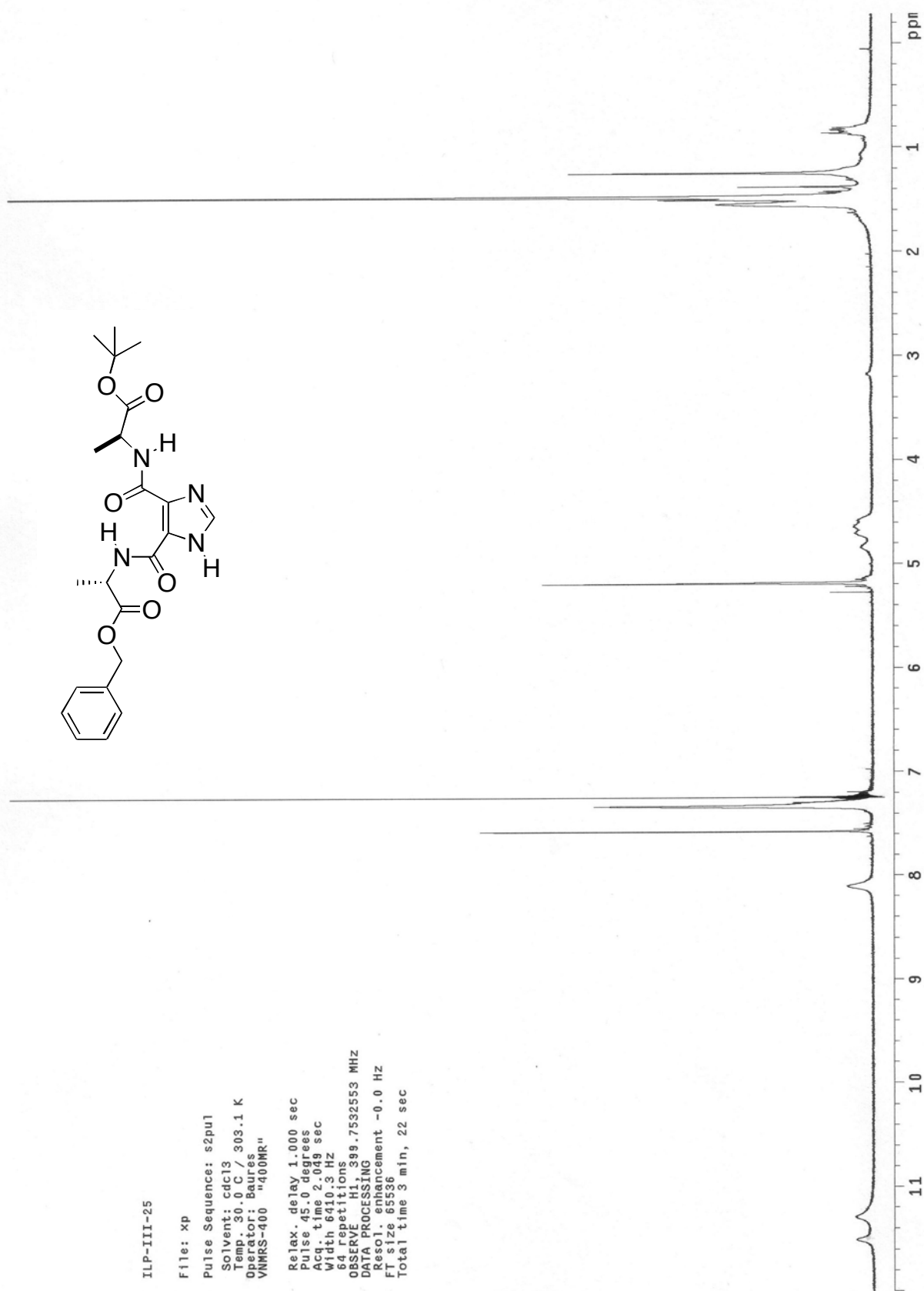


Figure S62. ¹H-NMR for 4{25}.

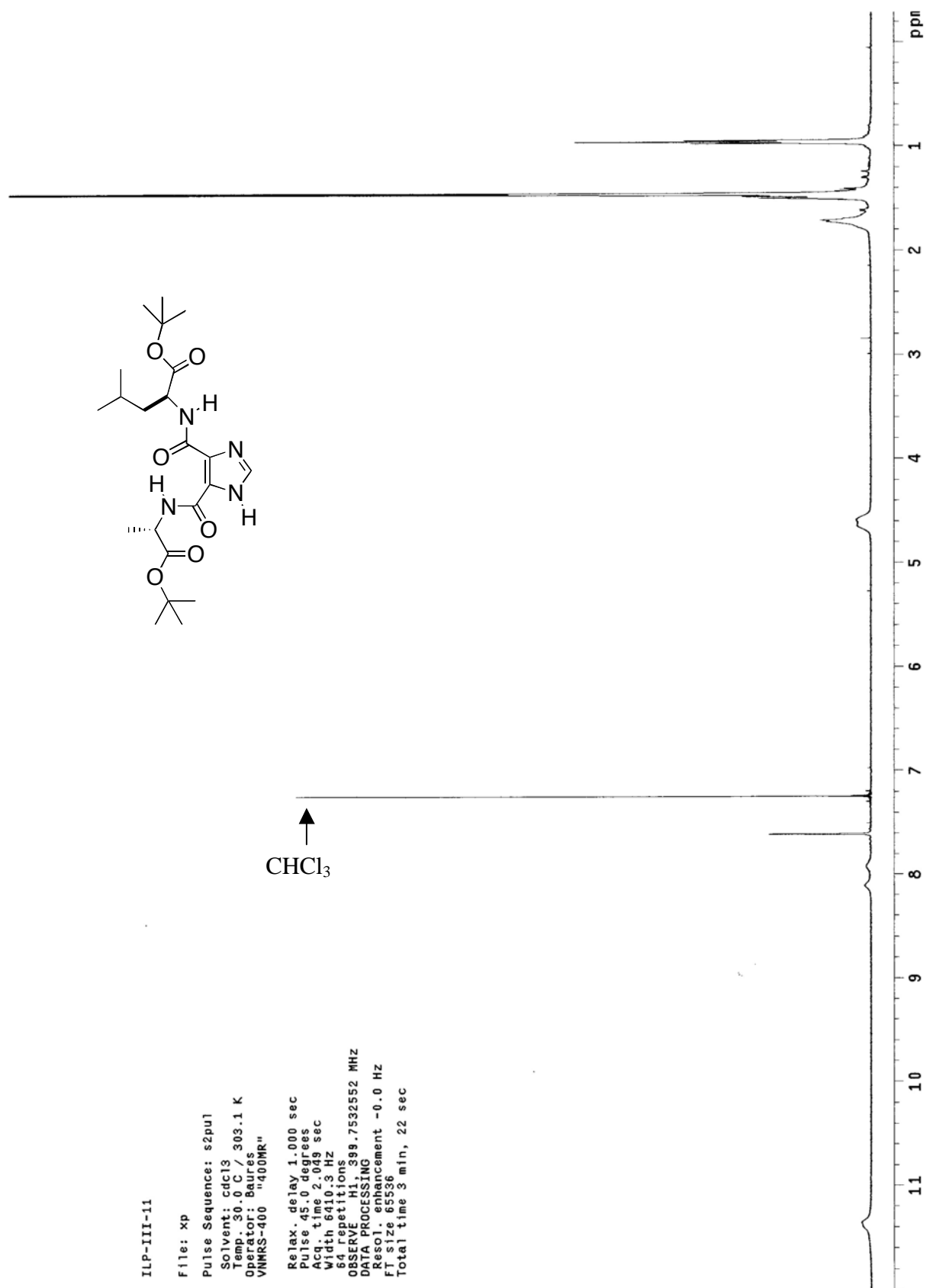


Figure S63. ¹H-NMR for 4{26}.

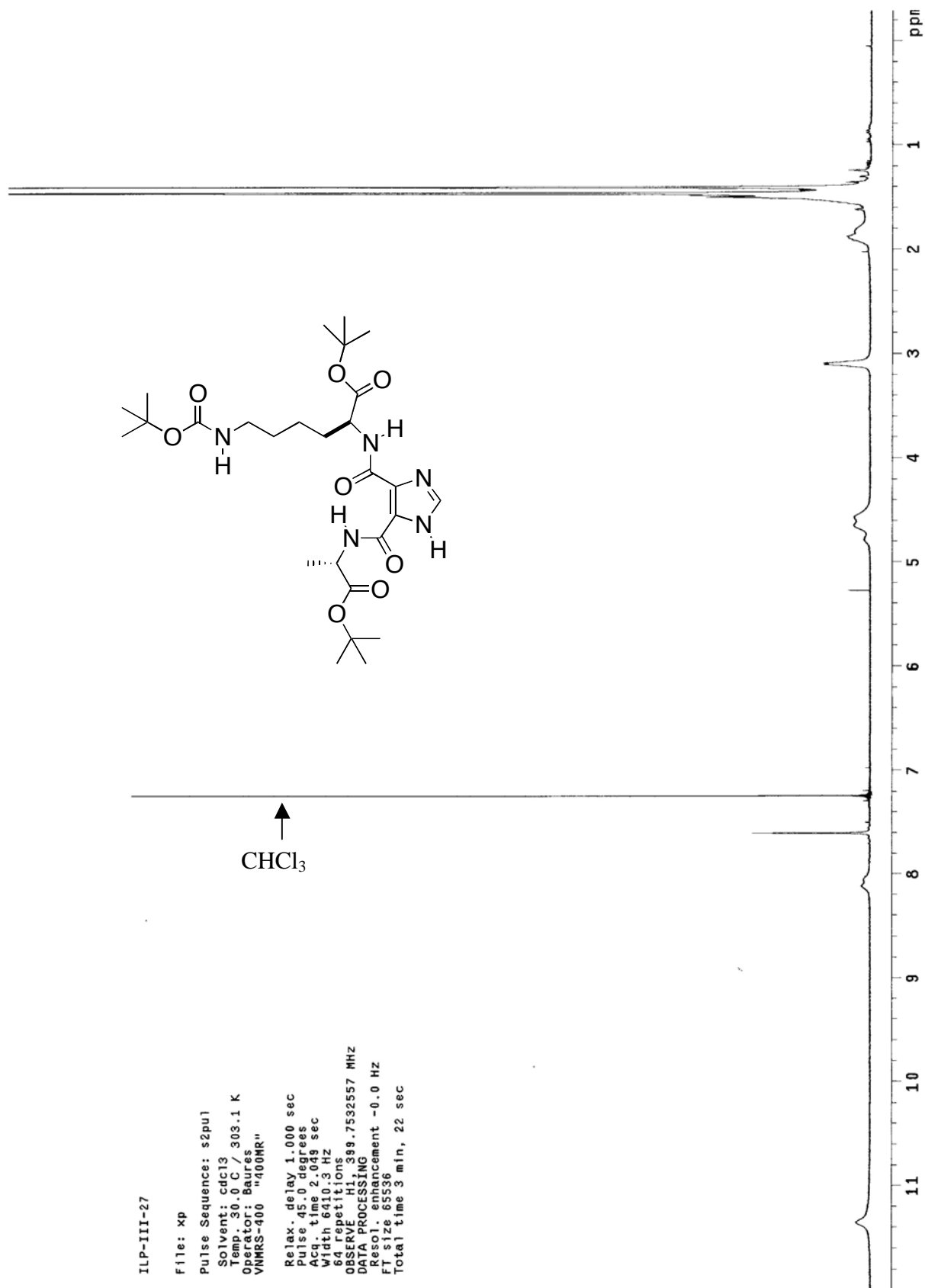


Figure S64. ¹H-NMR for 4{30}.

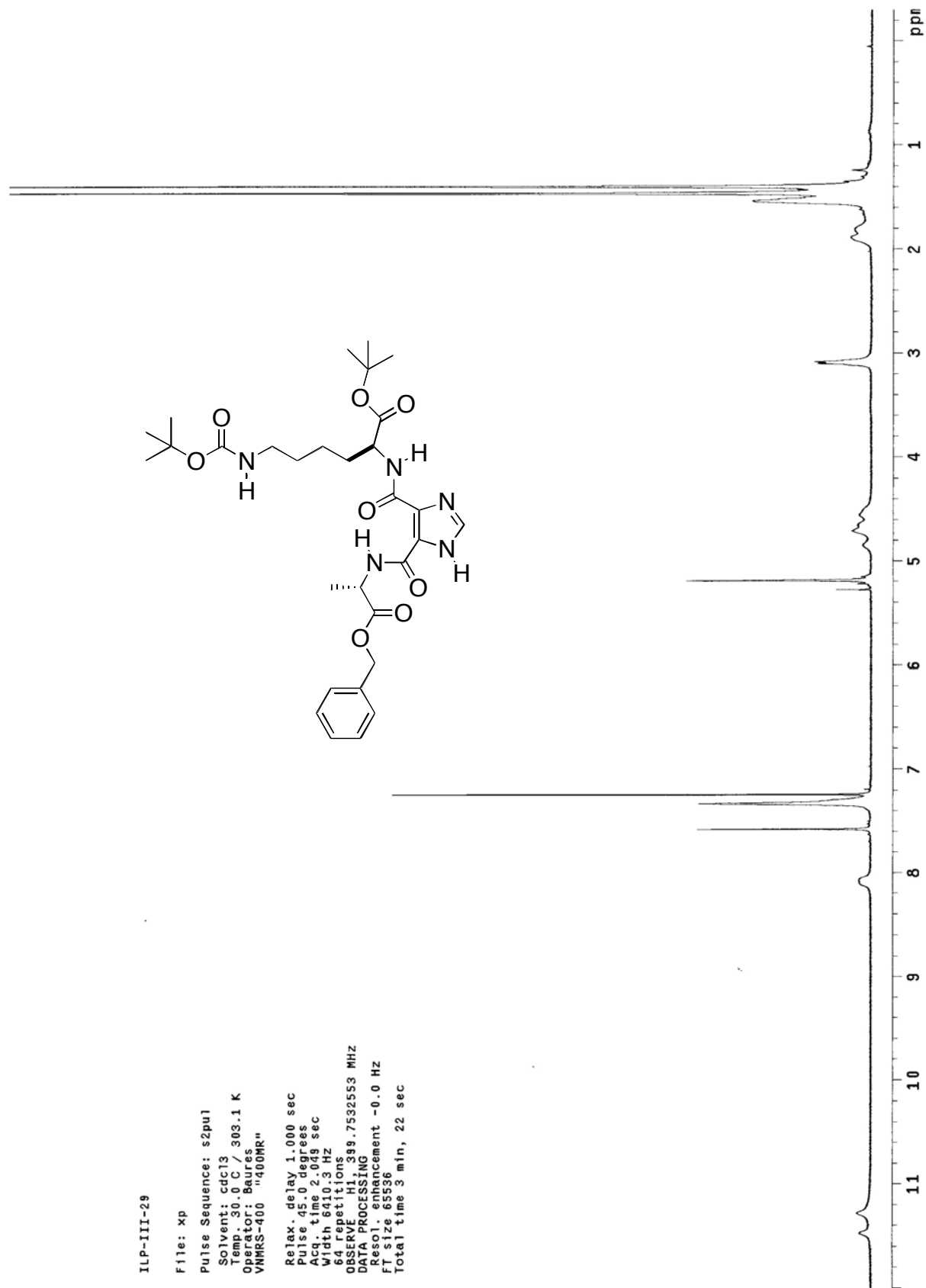


Figure S65. $^1\text{H-NMR}$ for 4{35}.

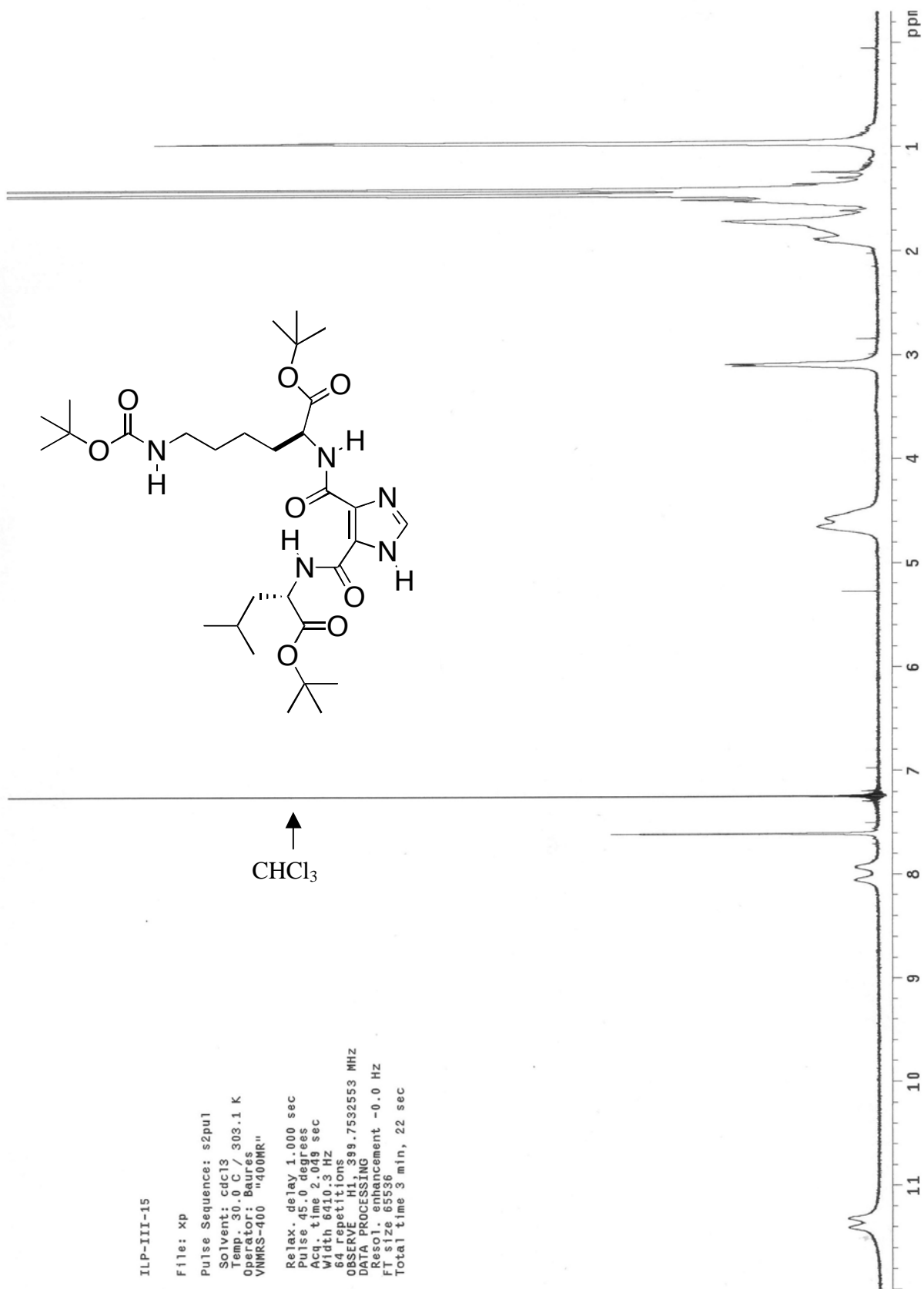


Figure S67. ¹H-NMR for 4{39}.

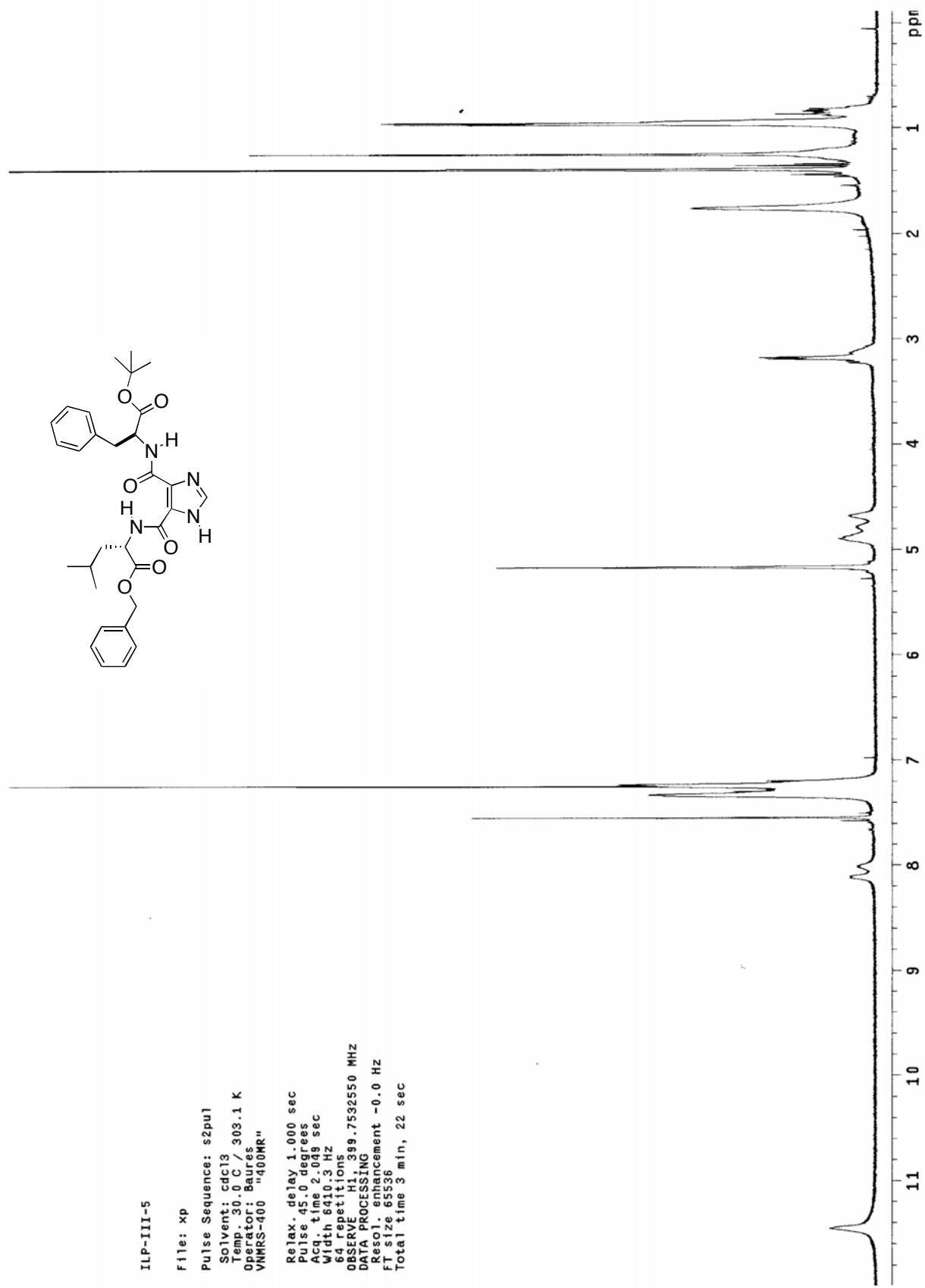


Figure S68. $^1\text{H-NMR}$ for 4{40}.

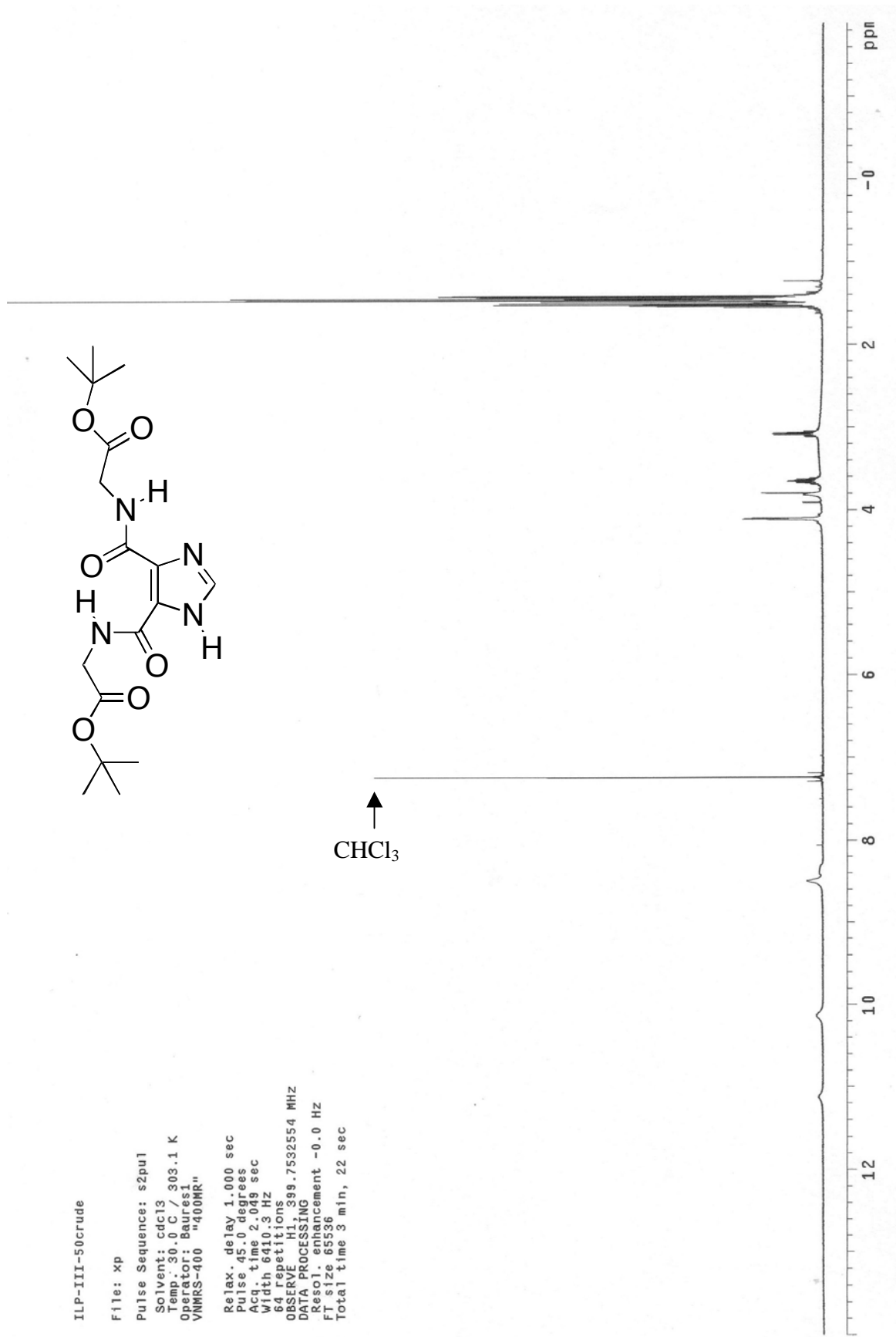


Figure S71. ¹H-NMR for the crude reaction to yield 4{1}.

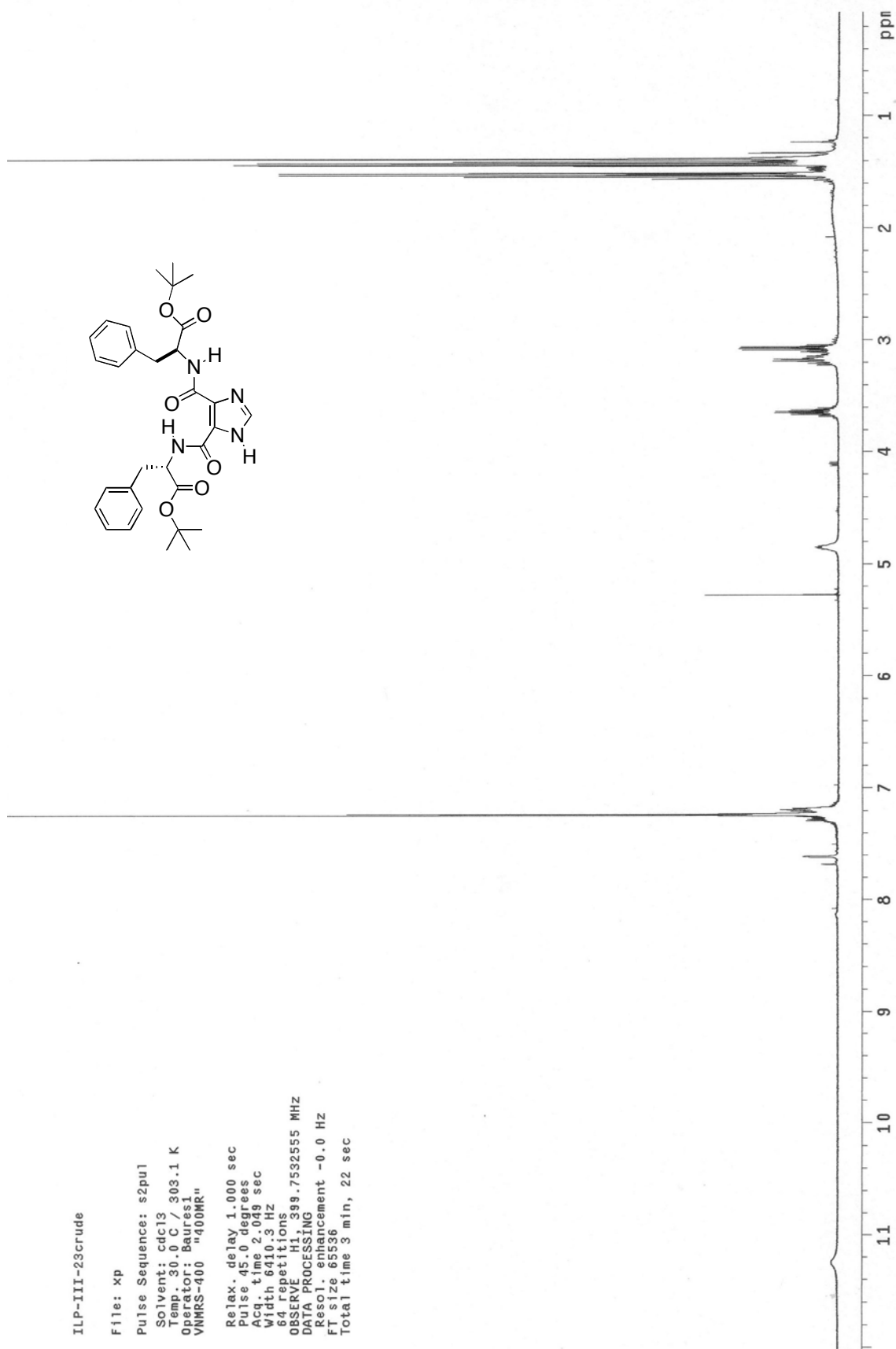


Figure S72. ¹H-NMR for the crude reaction to yield **4{7}**.

ILP-III-17crude

File: xp

Pulse Sequence: s2pu1

Solvent: cdcl3
Temp. 30.0 C / 303.1 K
Operator: Baures1
VNMR-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
F1 size 65536
Total time 3 min, 22 sec

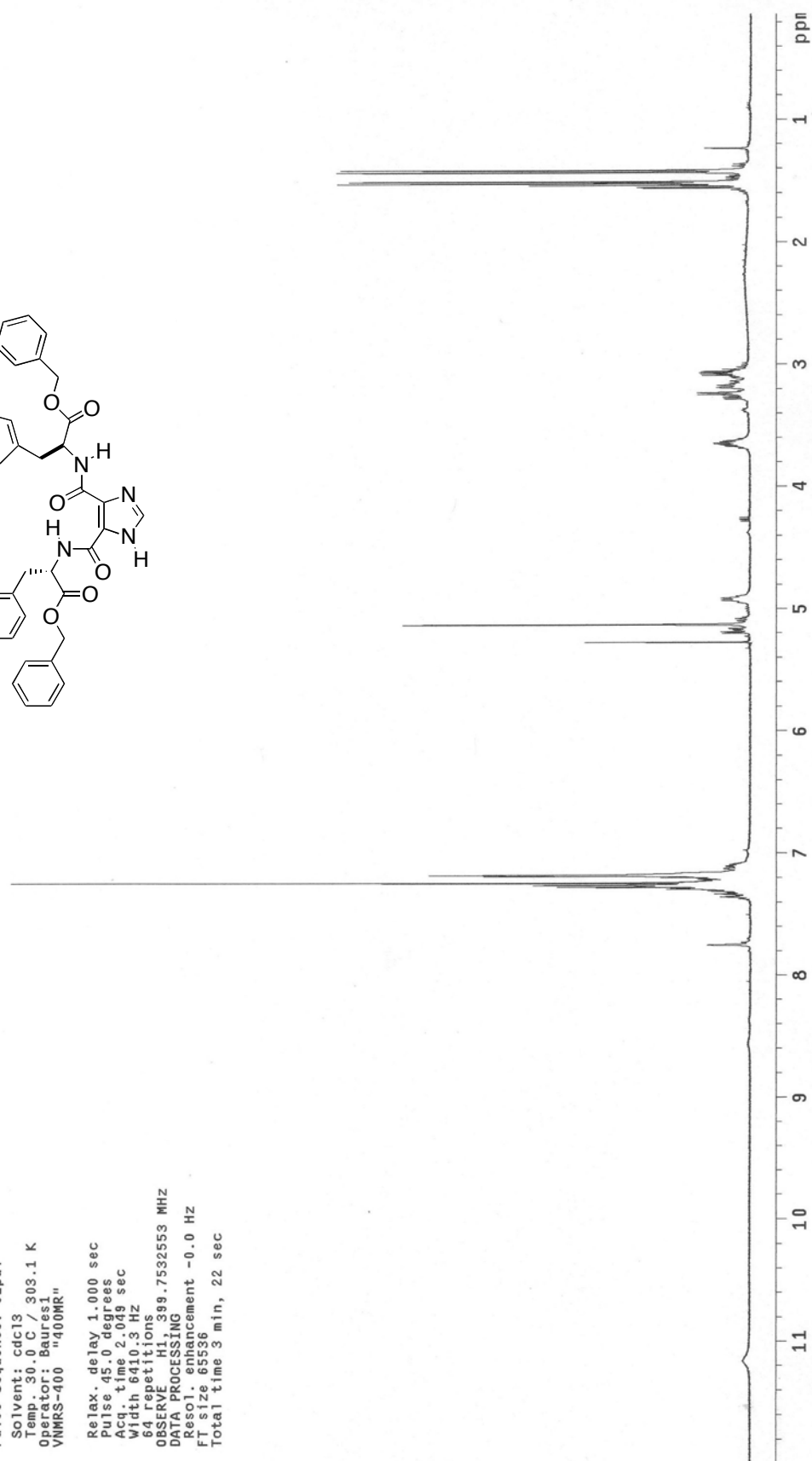
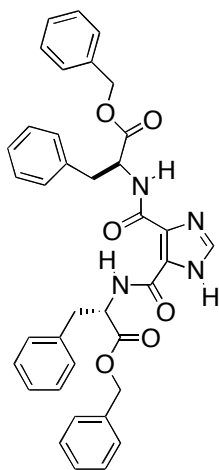


Figure S73. ¹H-NMR for the crude reaction to yield 4{8}.

ILP-III-47crude

File: xp

Pulse Sequence: s2pu1

Solvent: cdCl3

Temp. 30.0 C / 303.1 K

Operator: Baures1

VNMR5-400

"400MR"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

64 repetitions

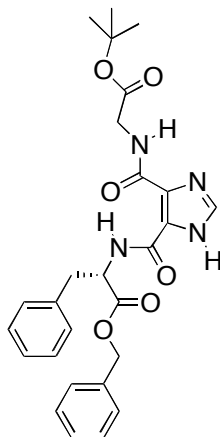
OBSERVE H1, 399.7532553 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 65536

Total time 3 min, 22 sec



CHCl₃

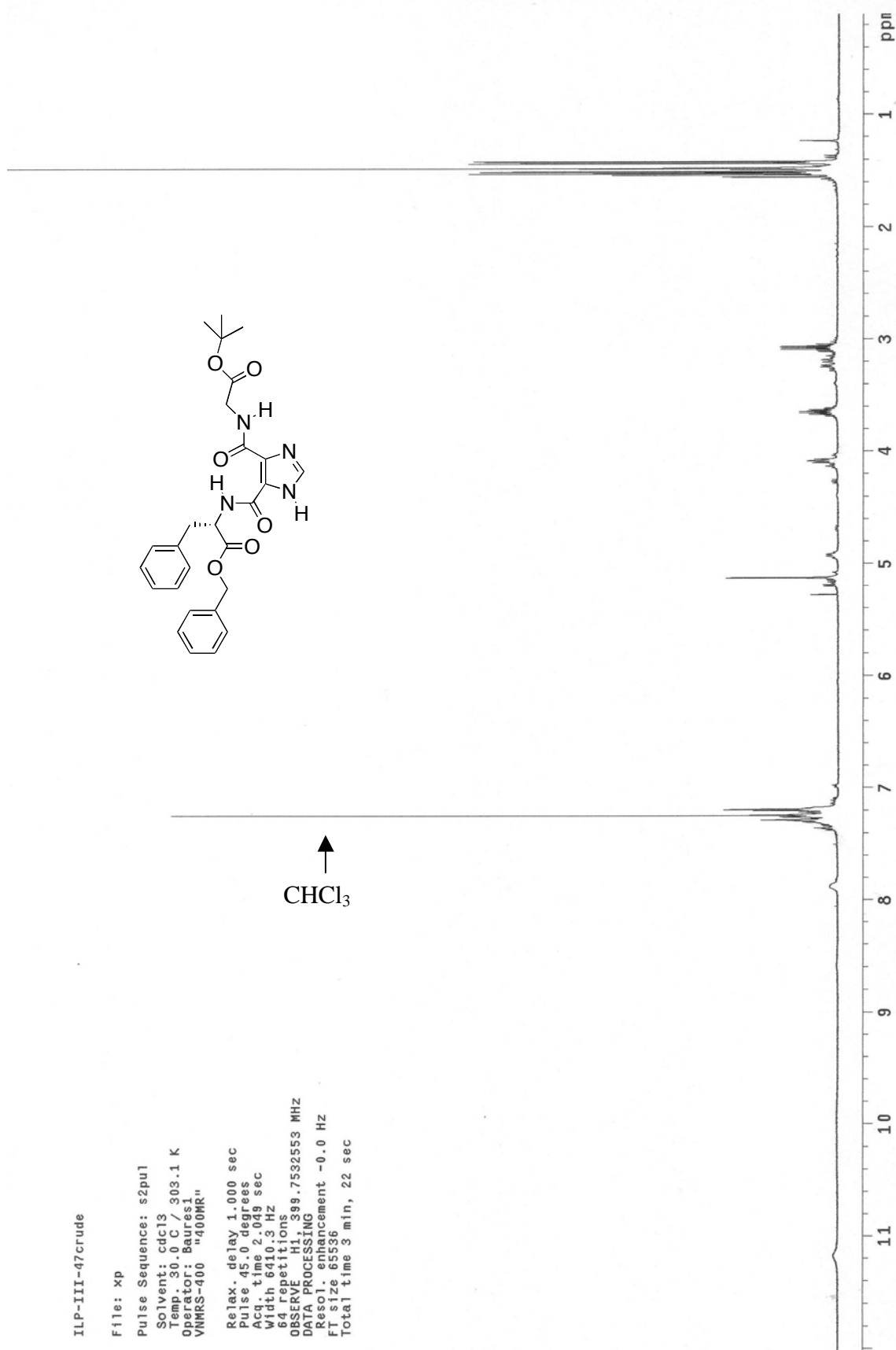


Figure S74. ¹H-NMR for the crude reaction to yield 4{16}.

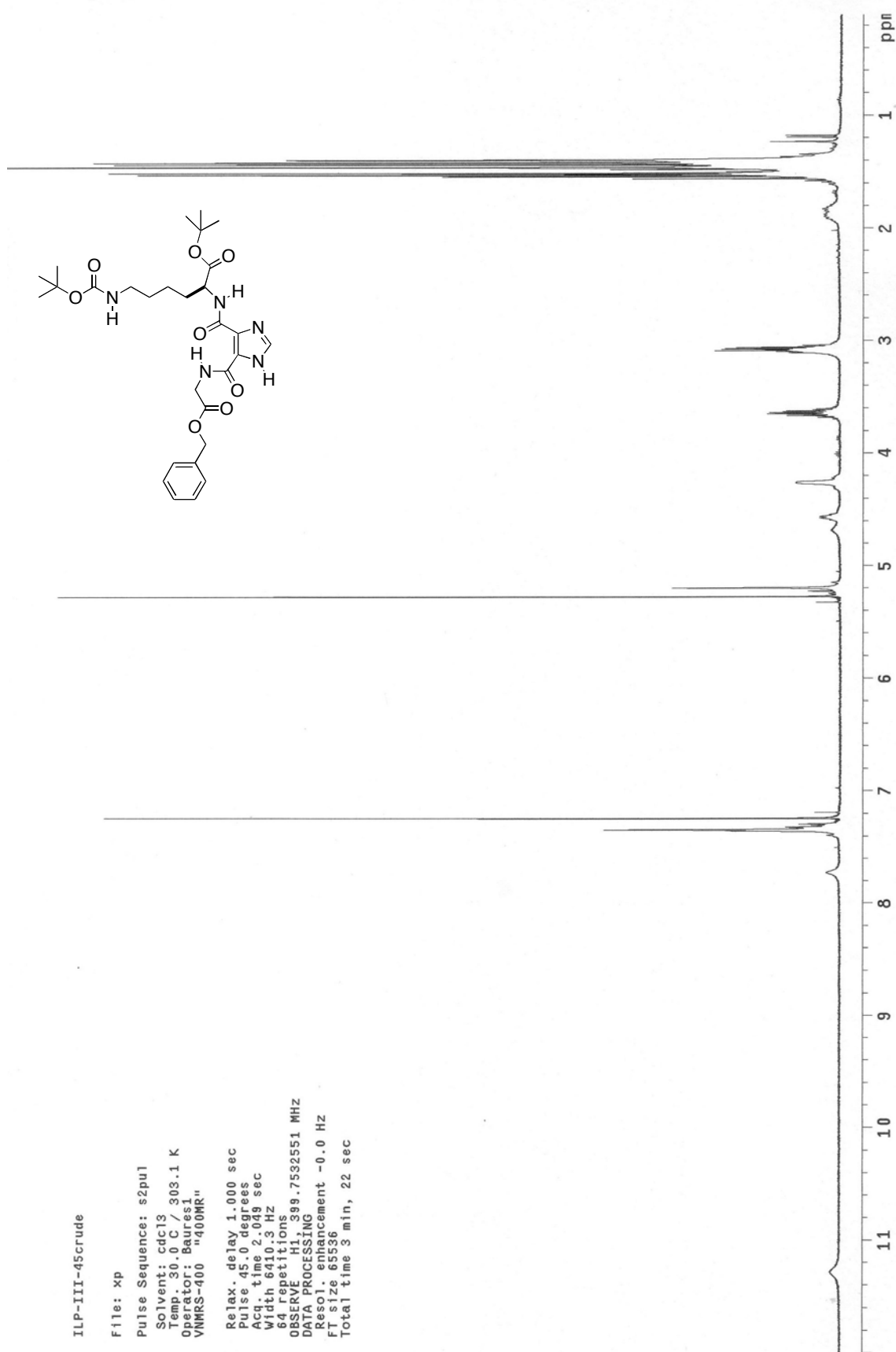


Figure S75. $^1\text{H-NMR}$ for the crude reaction to yield **4{24}**.

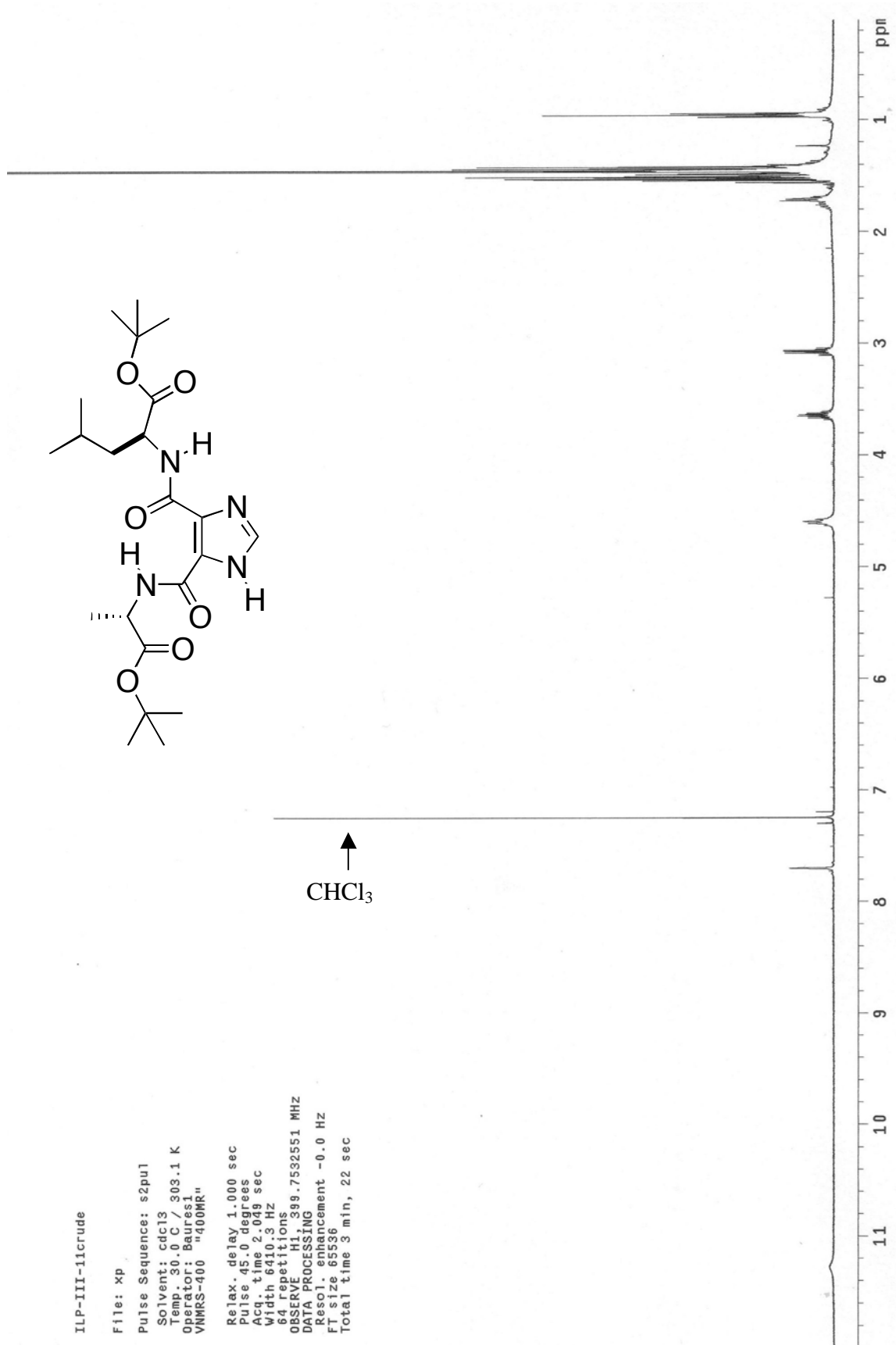


Figure S76. $^1\text{H-NMR}$ for the crude reaction to yield **4{26}**.

ILP-III-27crude

File: xp

Pulse Sequence: s2pul

Solvent: cdc13

Temp. 30.0 C / 303.1 K

Operator: Baures1

VNMR5-400 "400MR"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

64 repetitions

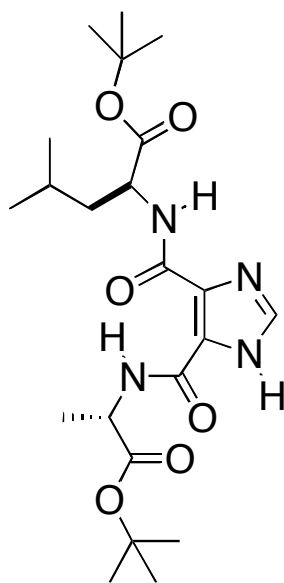
OBSERVE H1, 399.7532545 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 65536

Total time 3 min, 22 sec



↑
CHCl₃

Figure S77. ¹H-NMR for the crude reaction to yield 4{30}.

ILP-III-1crude

File: xp

Pulse Sequence: s2pul

Solvent: cdc13

Temp. 30.0 C / 303.1 K

Operator: Baures1

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, 399.7532548 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 65536

Total time 3 min, 22 sec

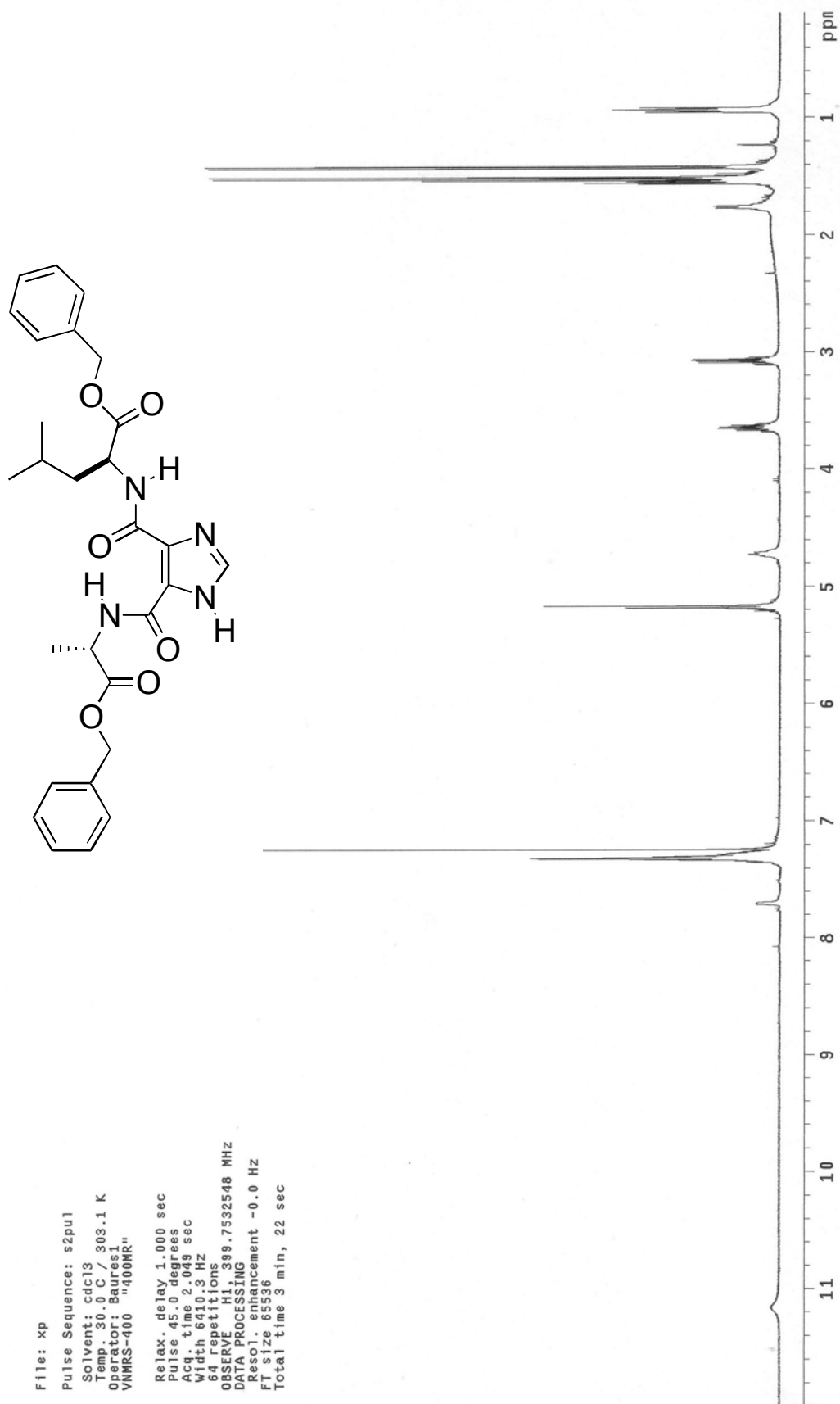


Figure S78. ¹H-NMR for the crude reaction to yield 4{32}.

IILP-III-5crude

File: xp

Pulse Sequence: s2pul

Solvent: cdc13

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, 398.7532554 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 65536

Total time 3 min, 22 sec

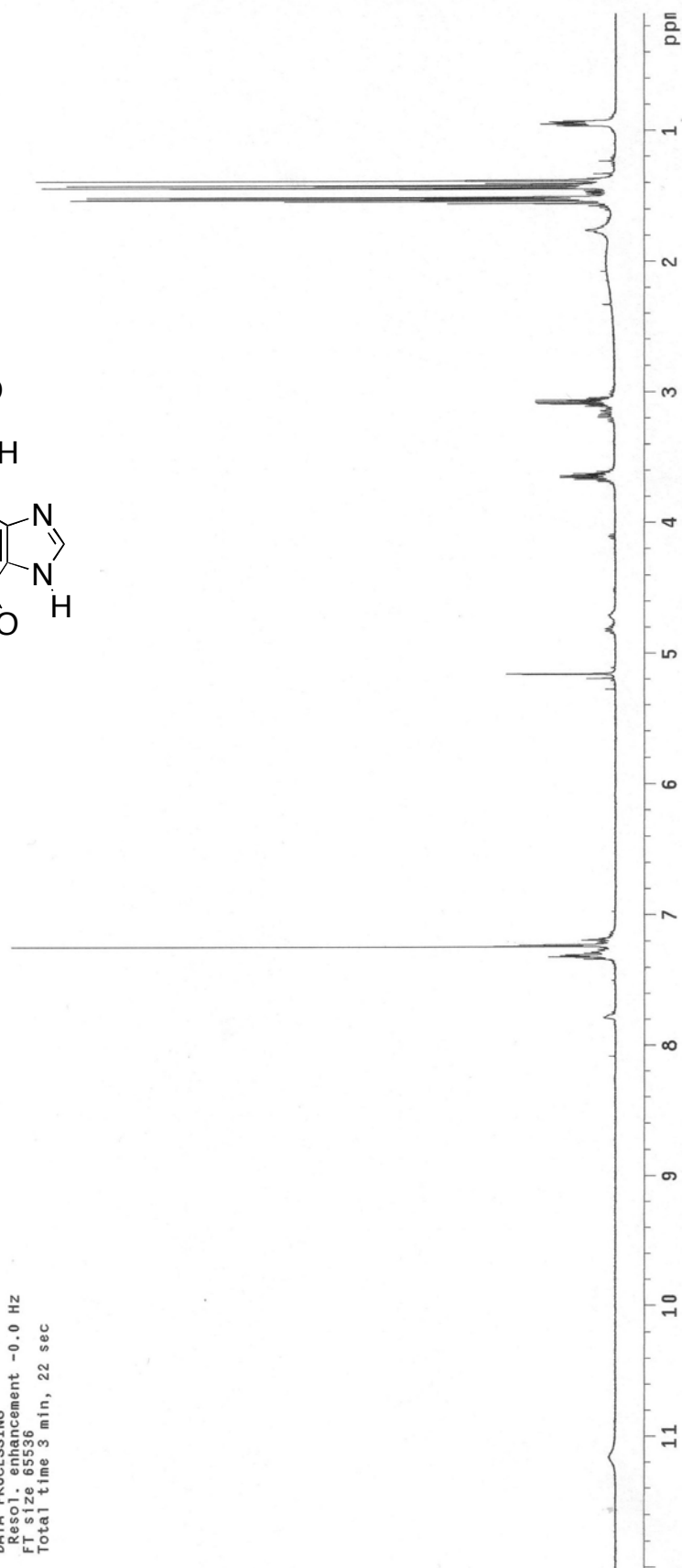
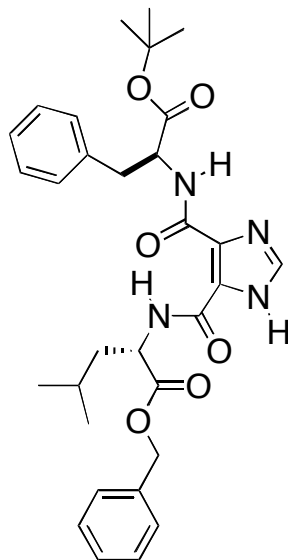


Figure S80. ¹H-NMR for the crude reaction to yield 4{40}.