

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

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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

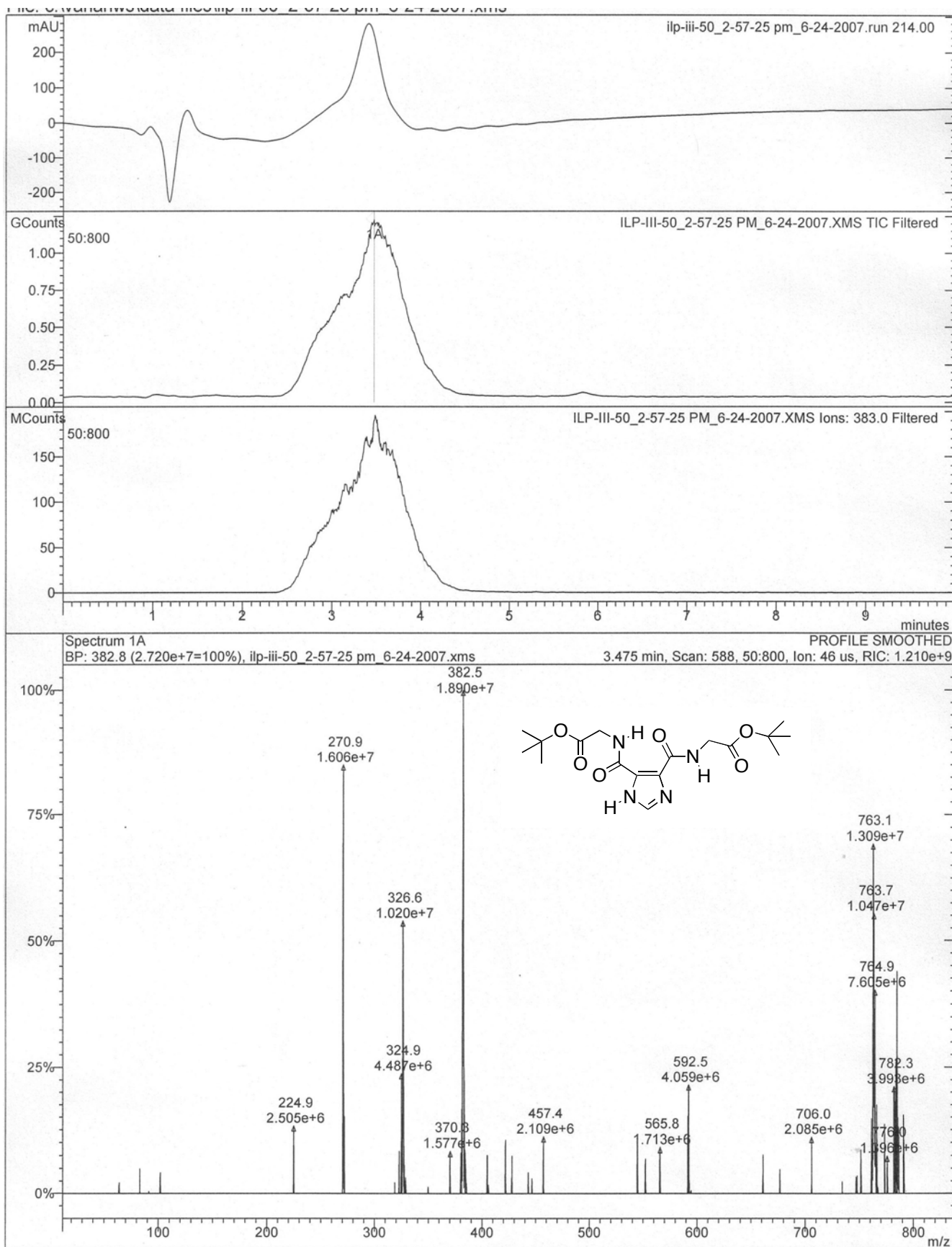


Figure S1. LC/MS data for 4{1}.

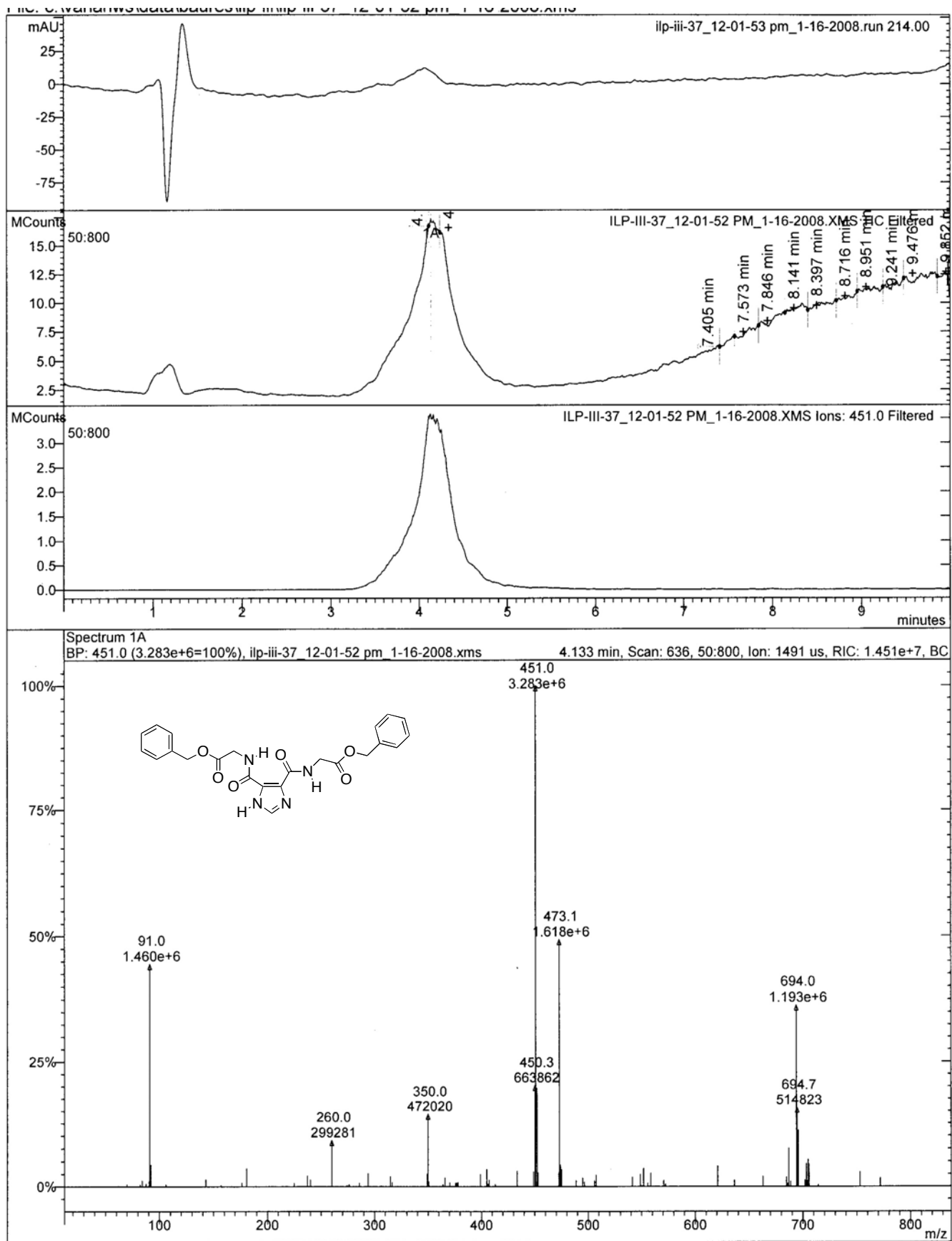


Figure S2. LC/MS data for 4{2}.

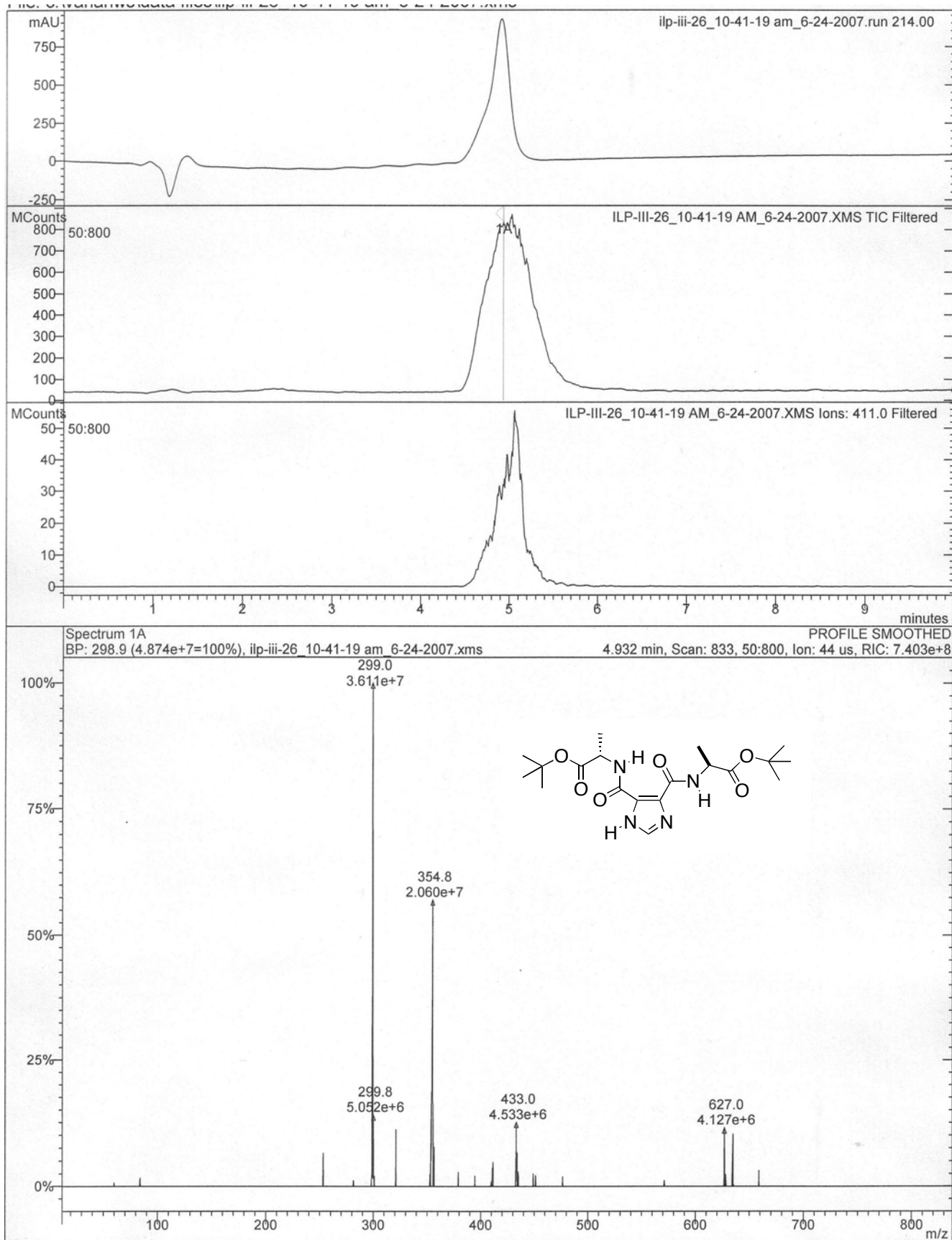


Figure S3. LC/MS data for 4{3}.

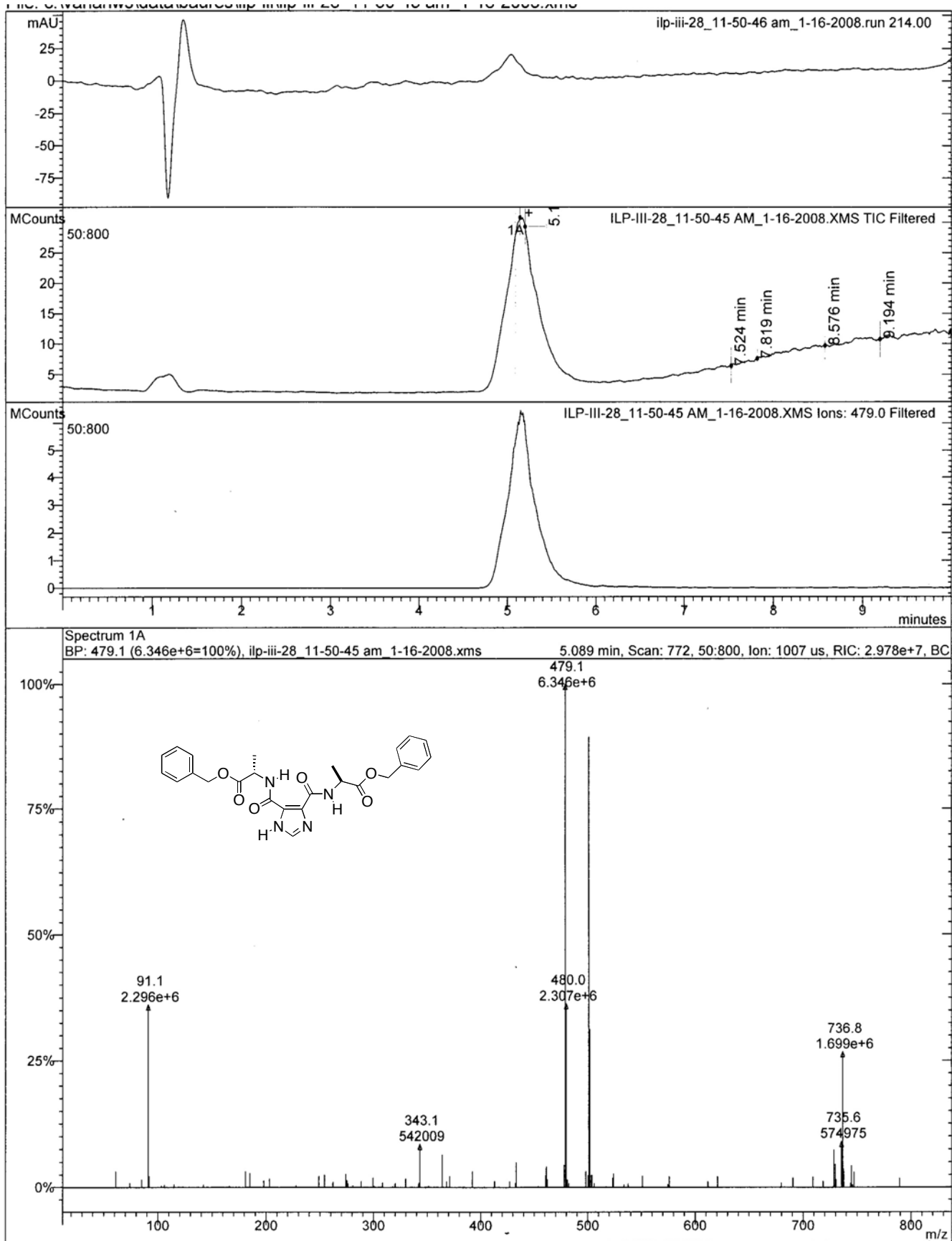


Figure S4. LC/MS data for 4{4}.

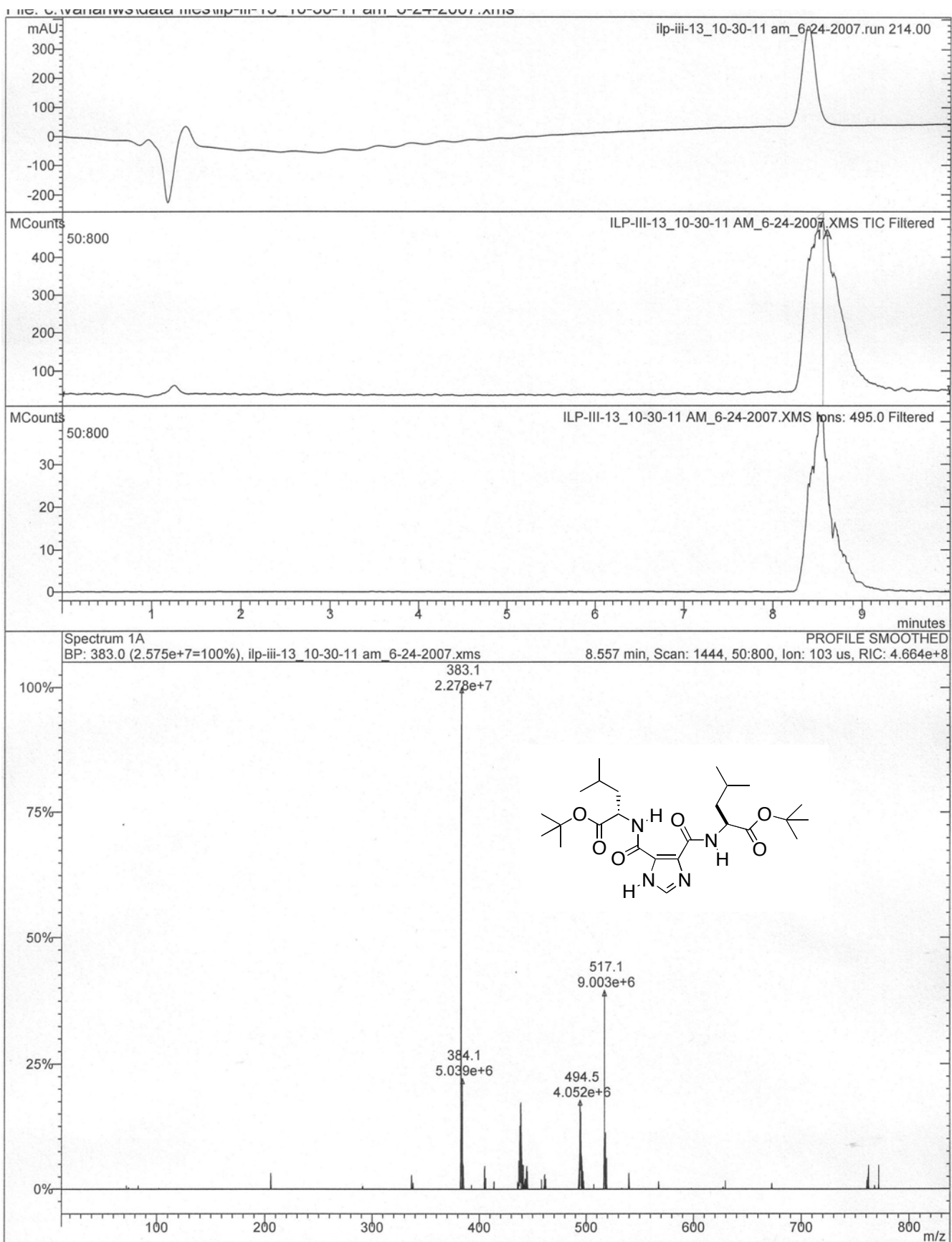


Figure S5. LC/MS data for 4{5}.

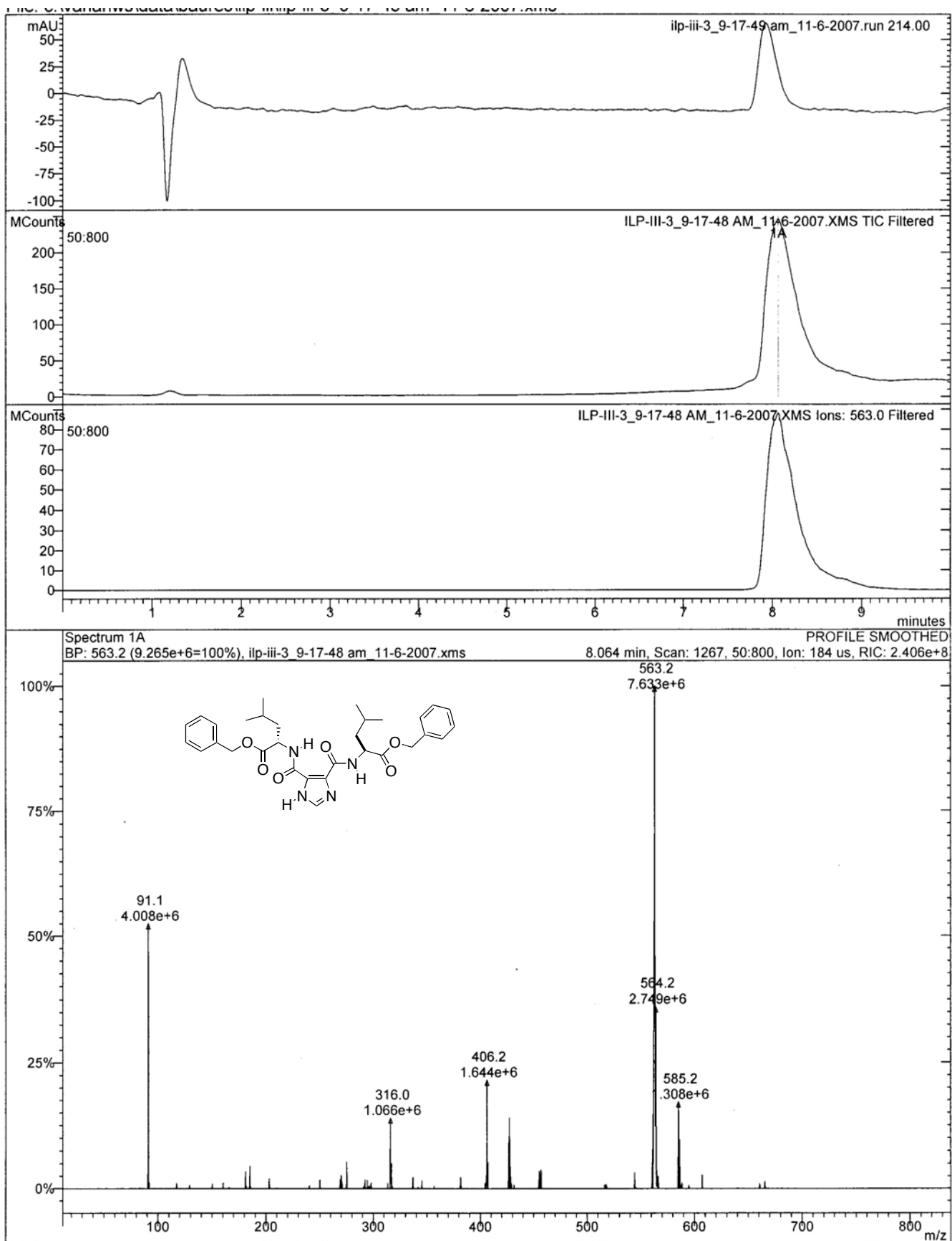


Figure S6. LC/MS data for 4{6}.

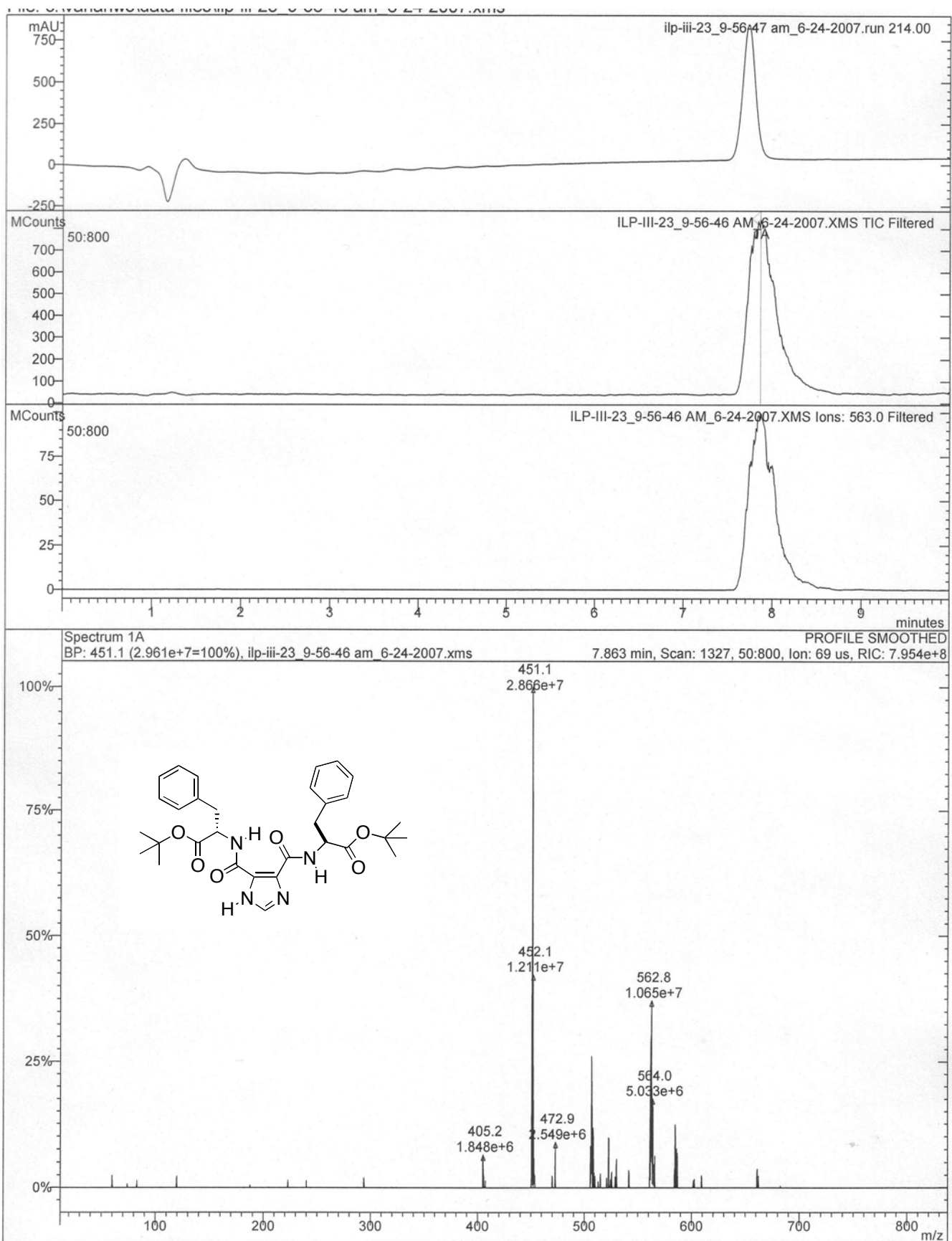


Figure S7. LC/MS data for 4{7}.

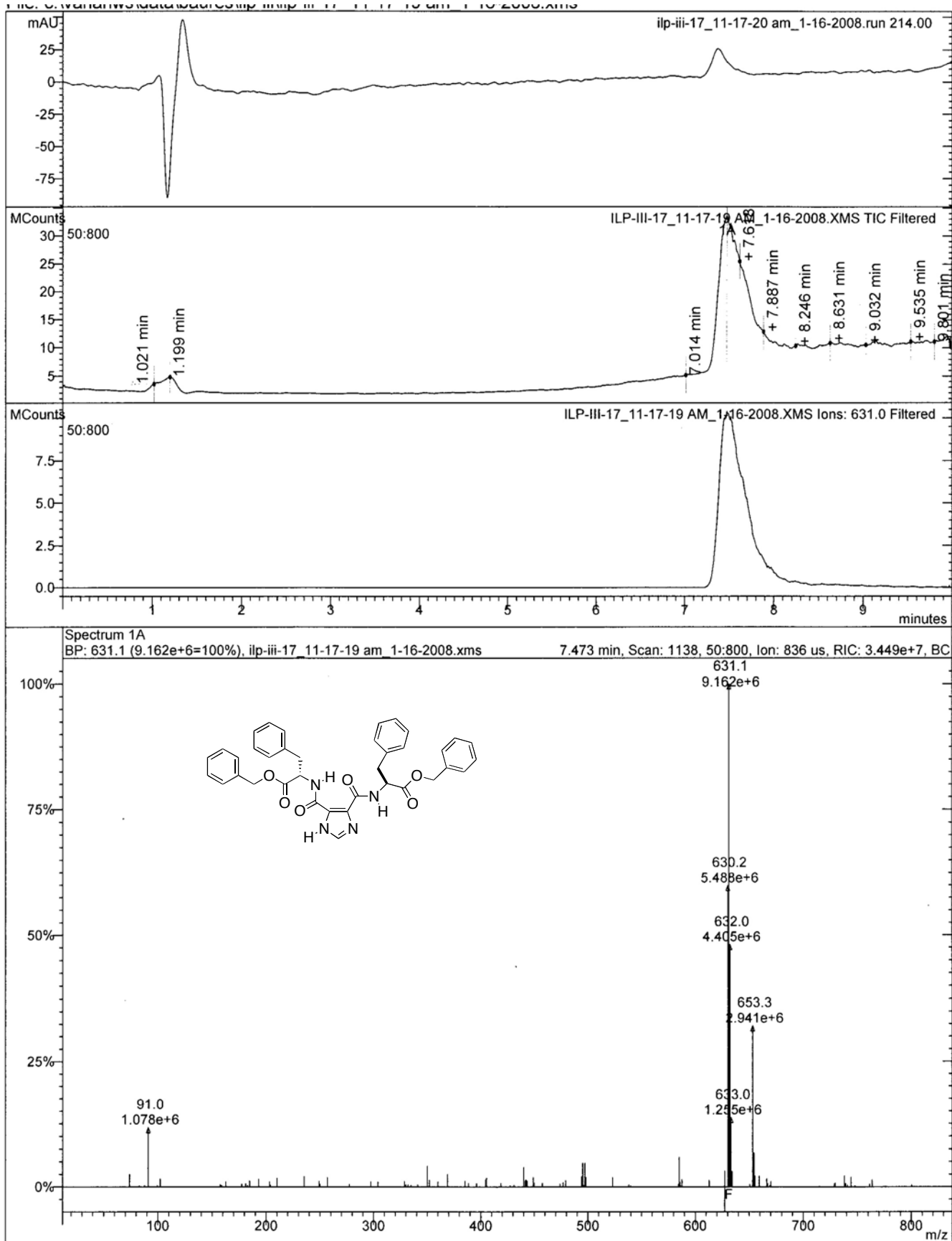


Figure S8. LC/MS data for 4{8}.

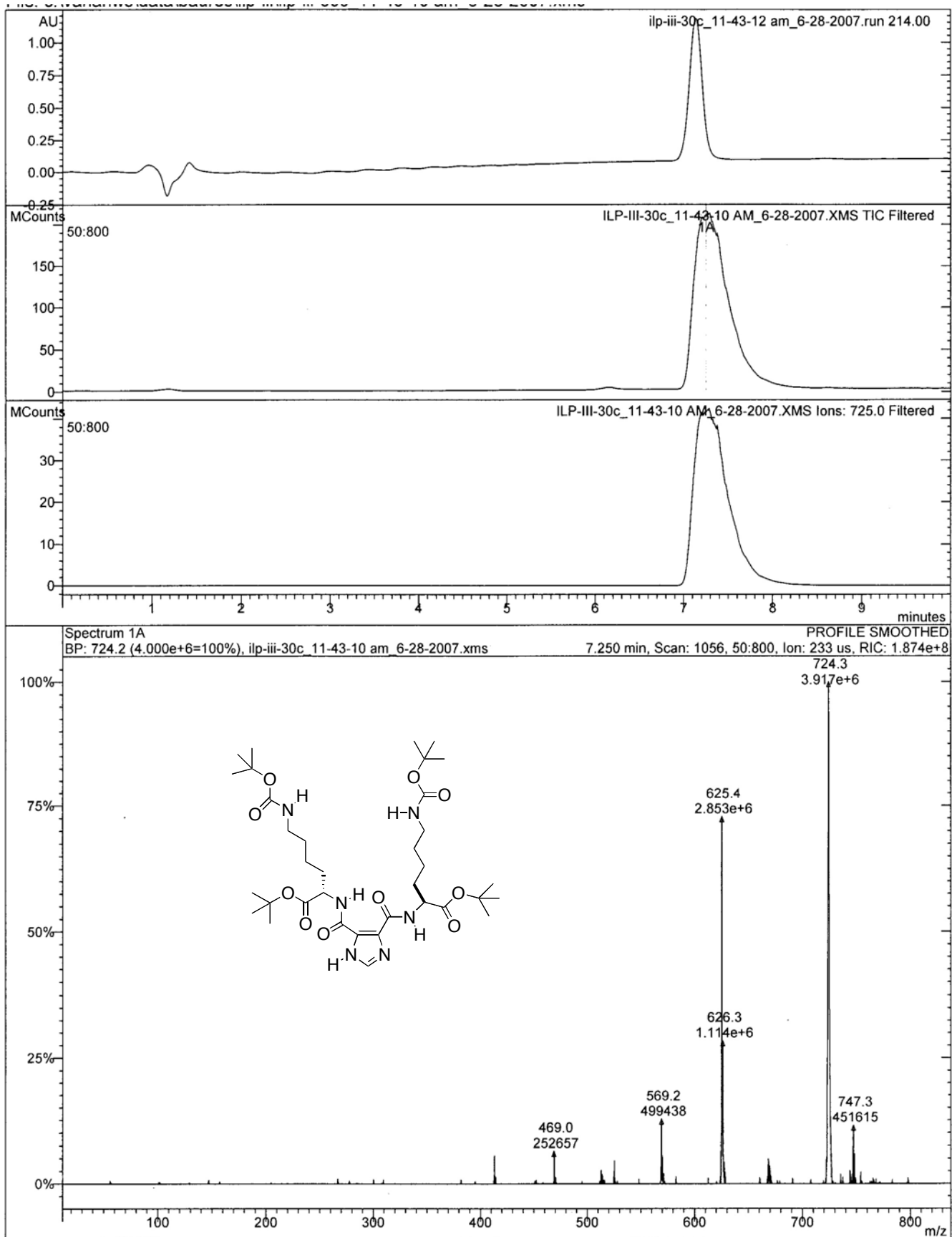


Figure S9. LC/MS data for 4{9}.

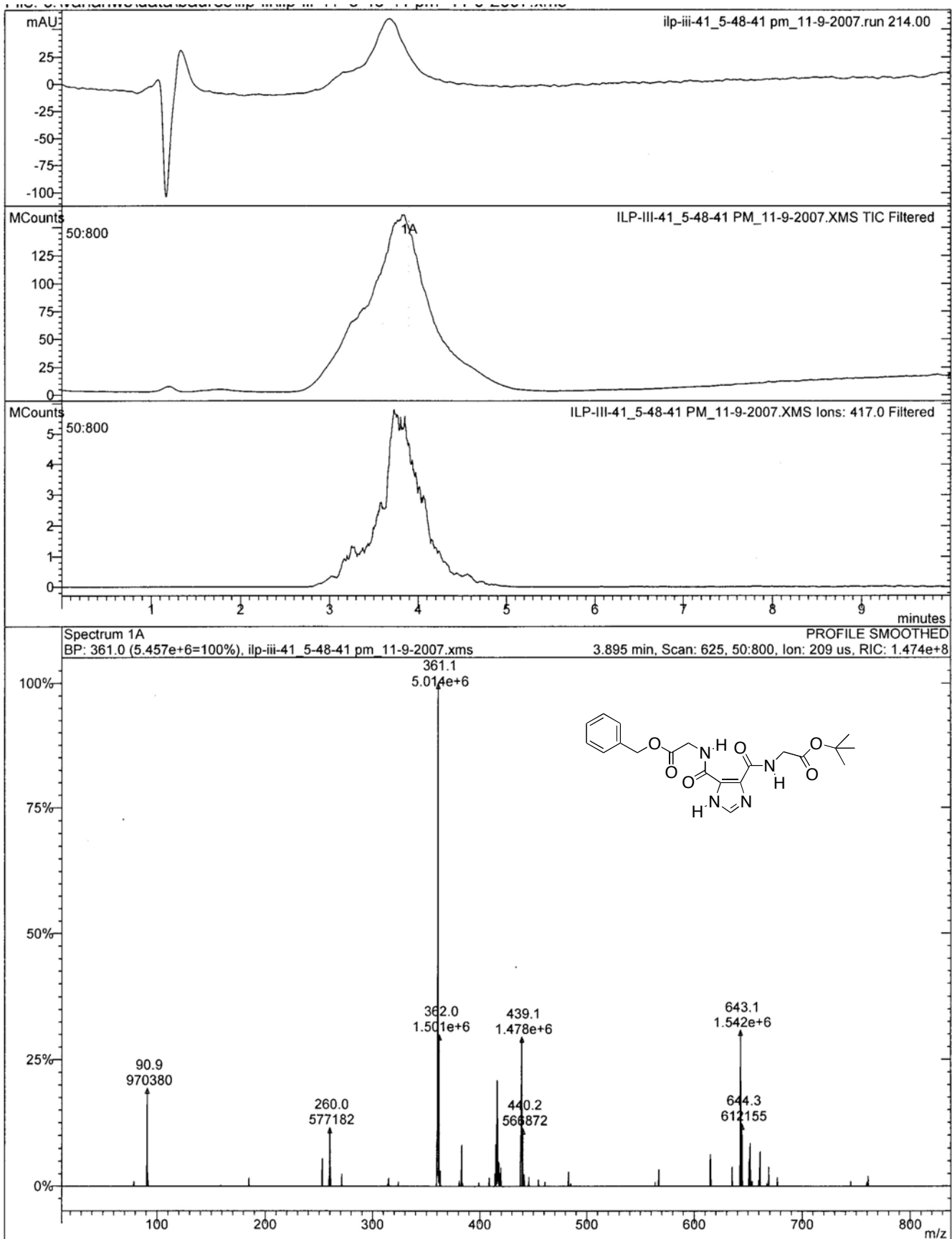


Figure S10. LC/MS data for 4{10}.

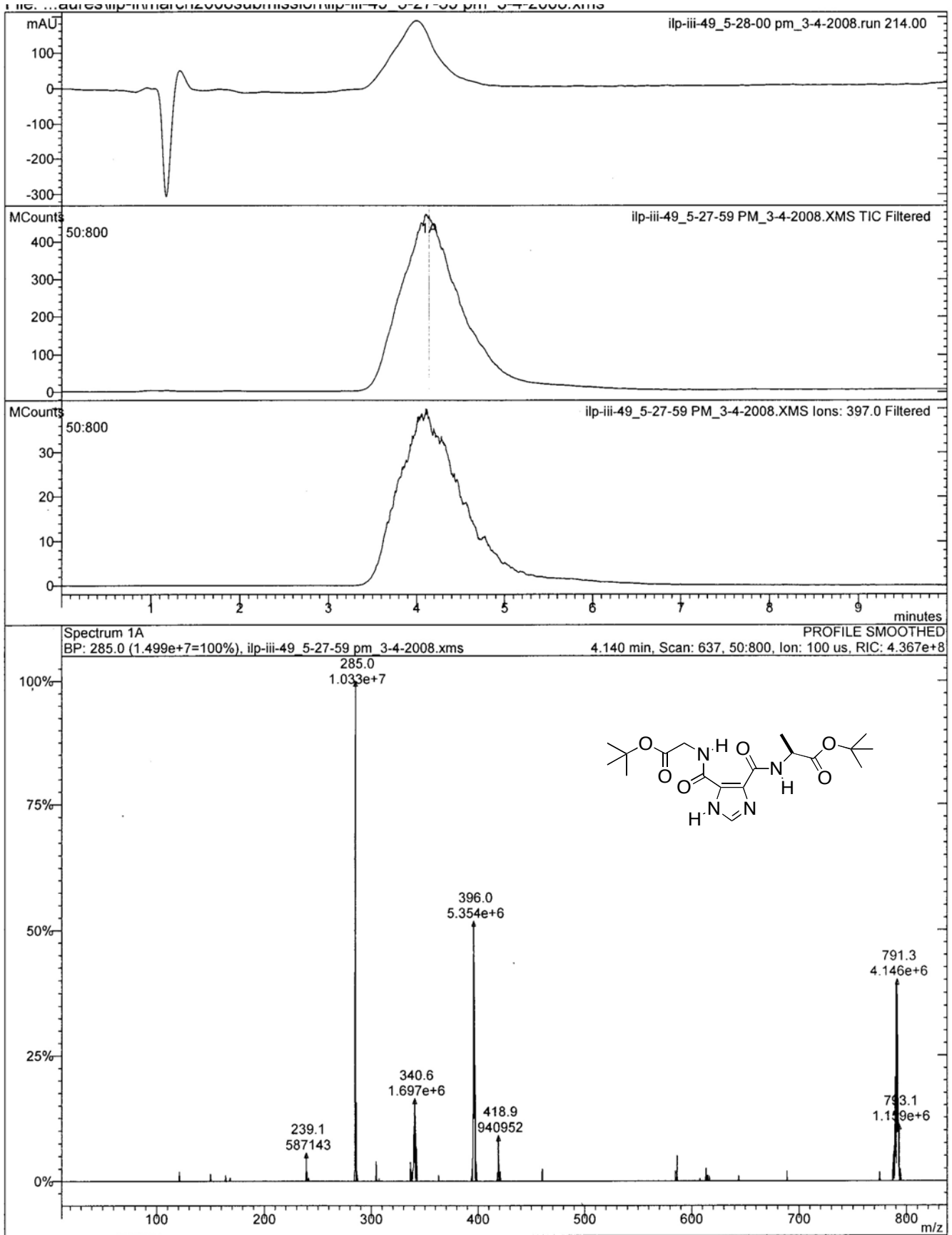


Figure S11. LC/MS data for 4{11}.

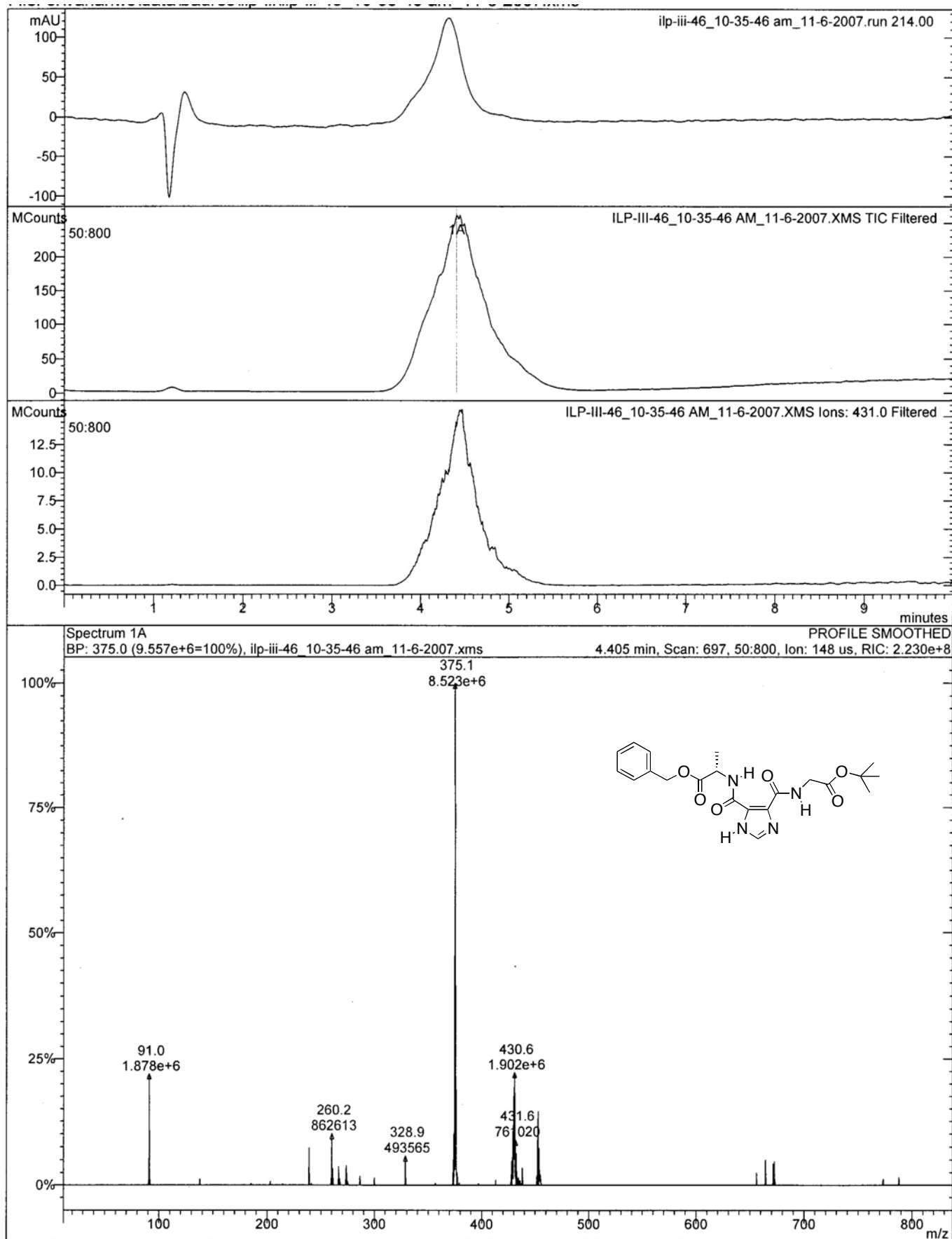


Figure S12. LC/MS data for 4{12}.

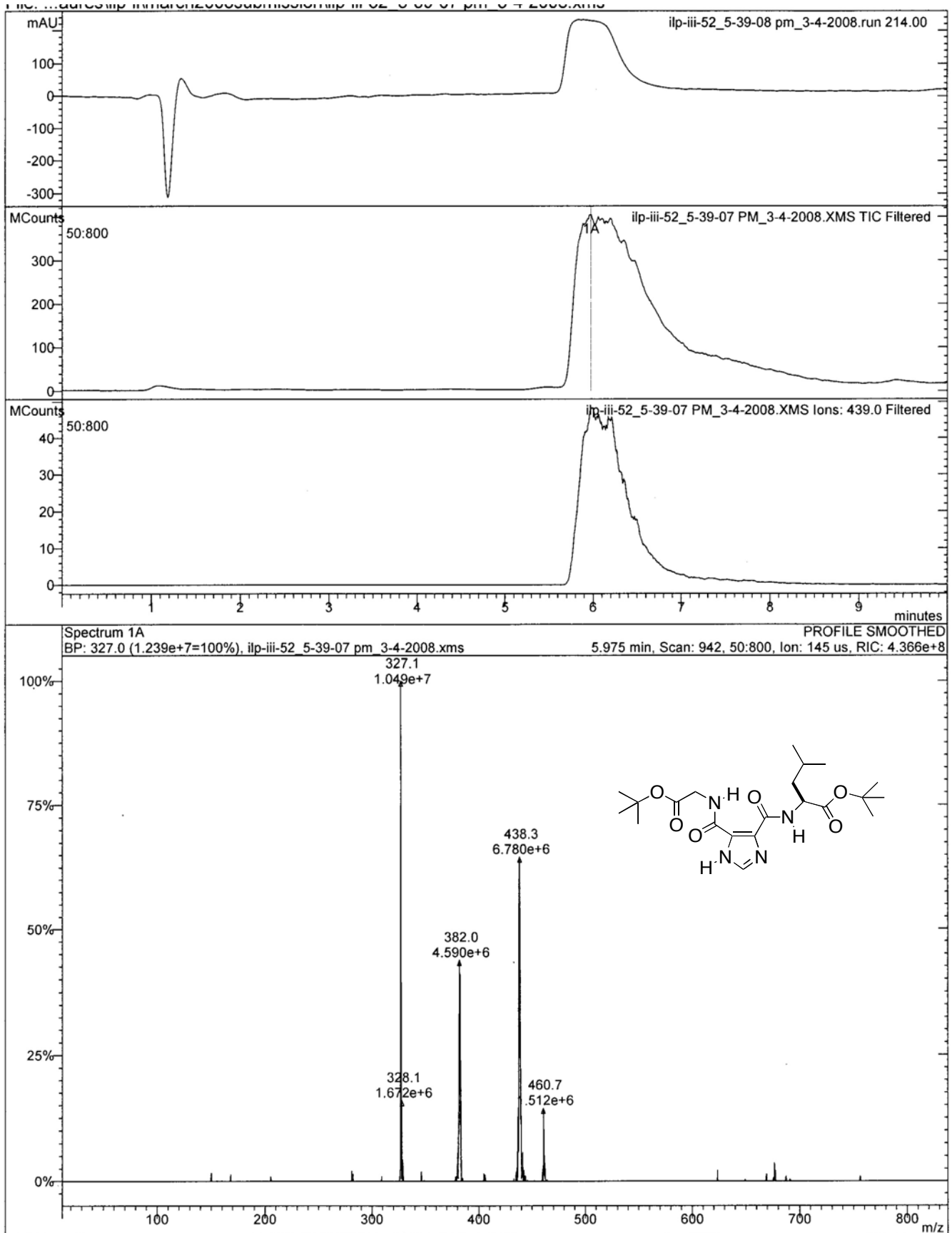


Figure S13. LC/MS data for 4{13}.

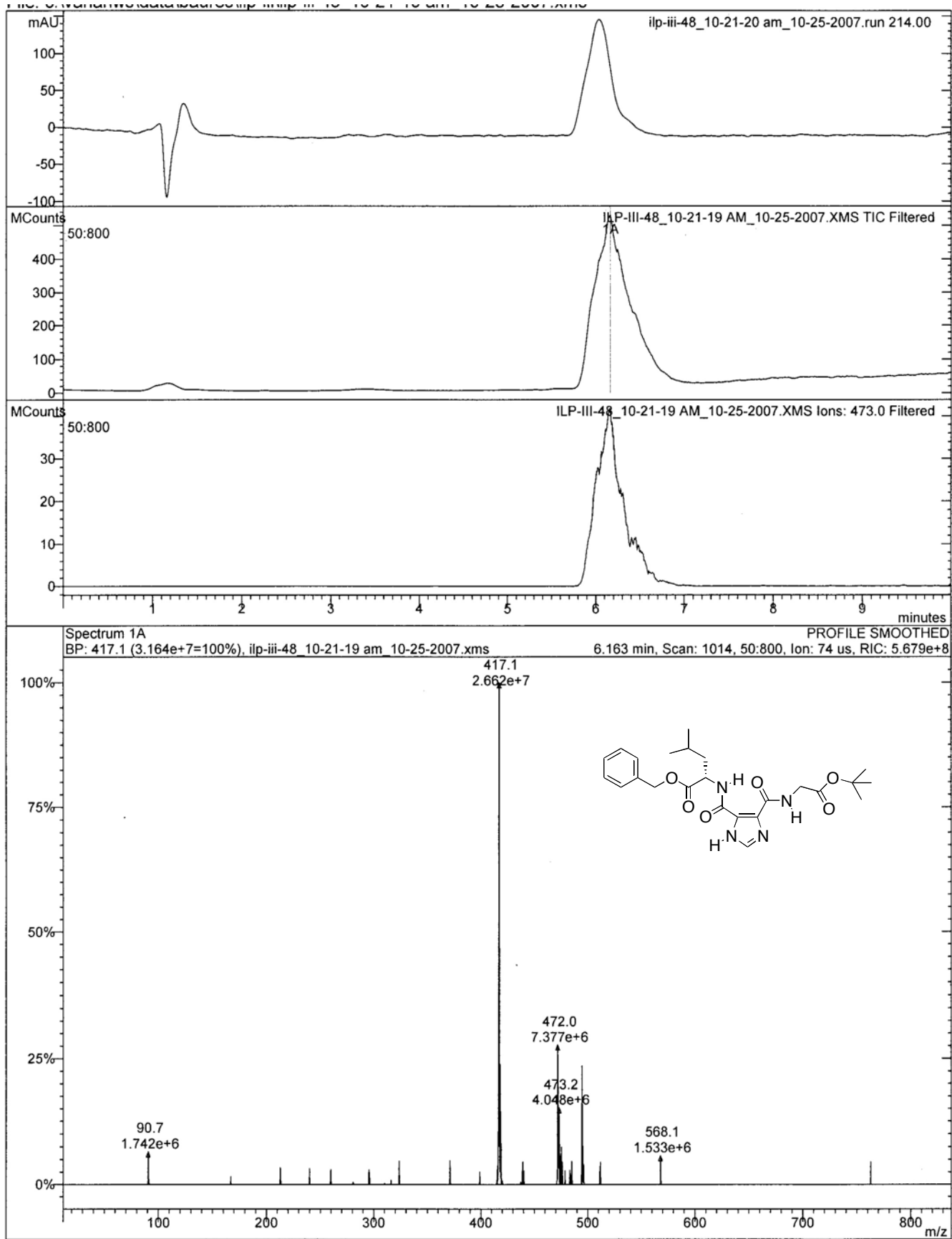


Figure S14. LC/MS data for 4{14}.

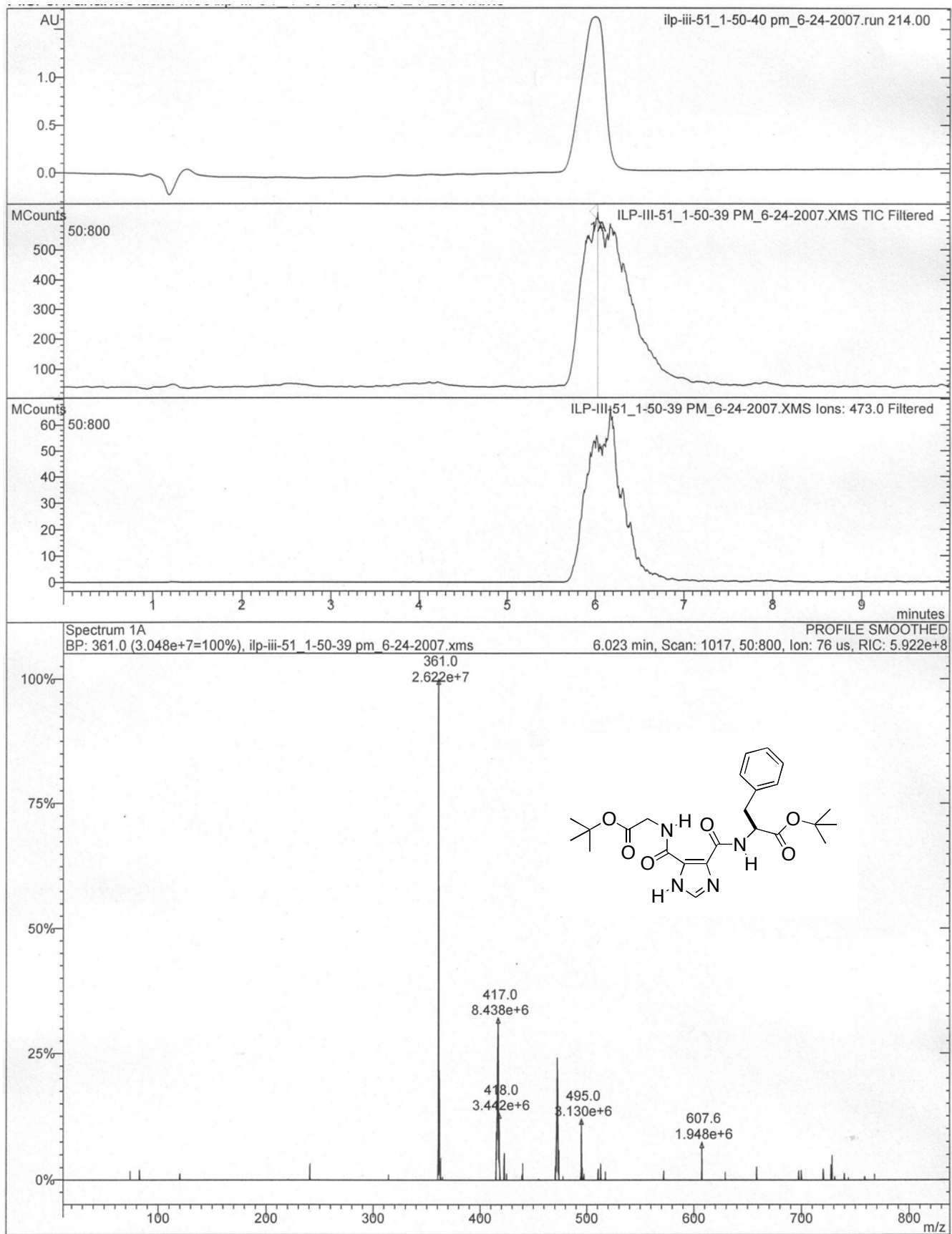


Figure S15. LC/MS data for 4{15}.

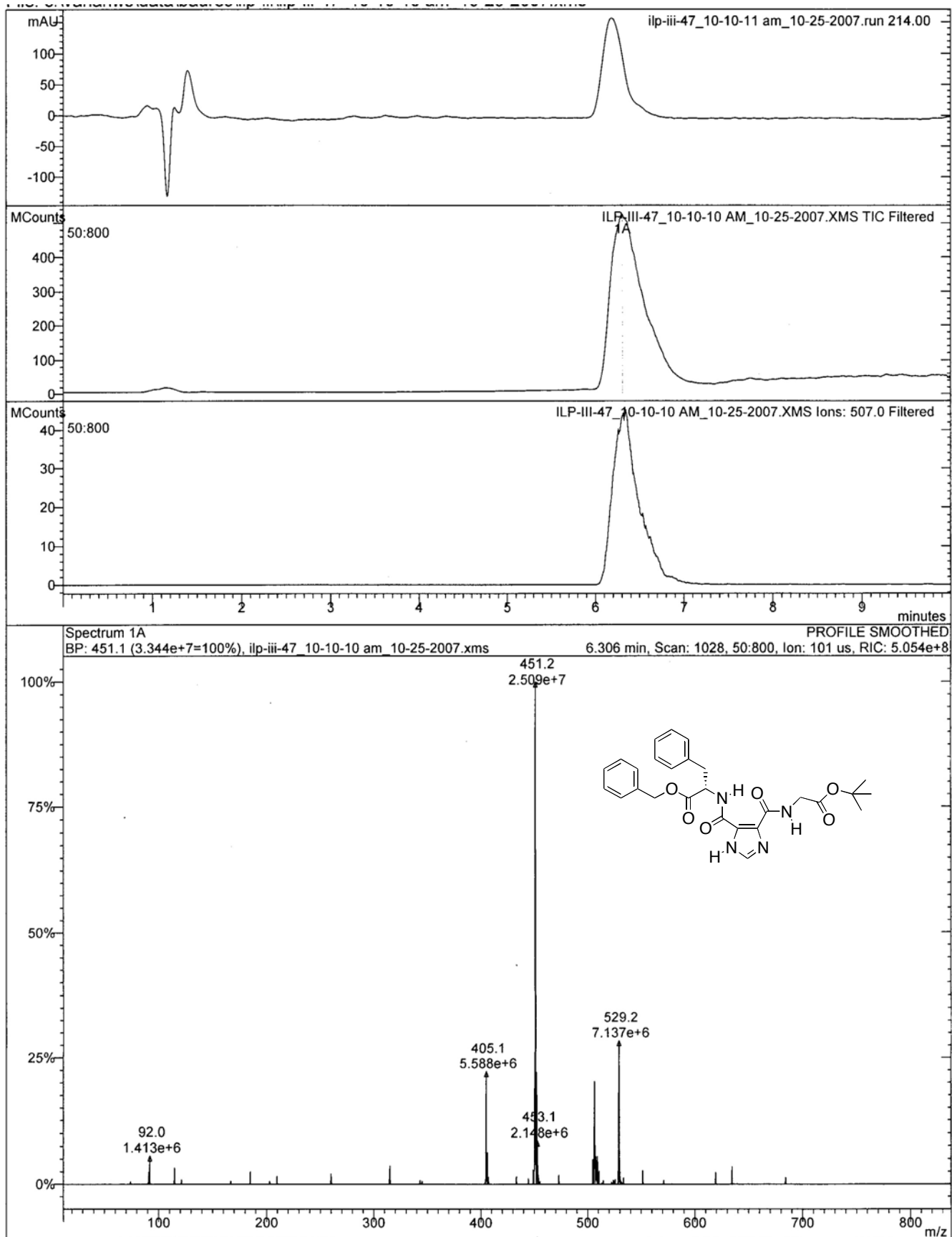


Figure S16. LC/MS data for 4{16}.

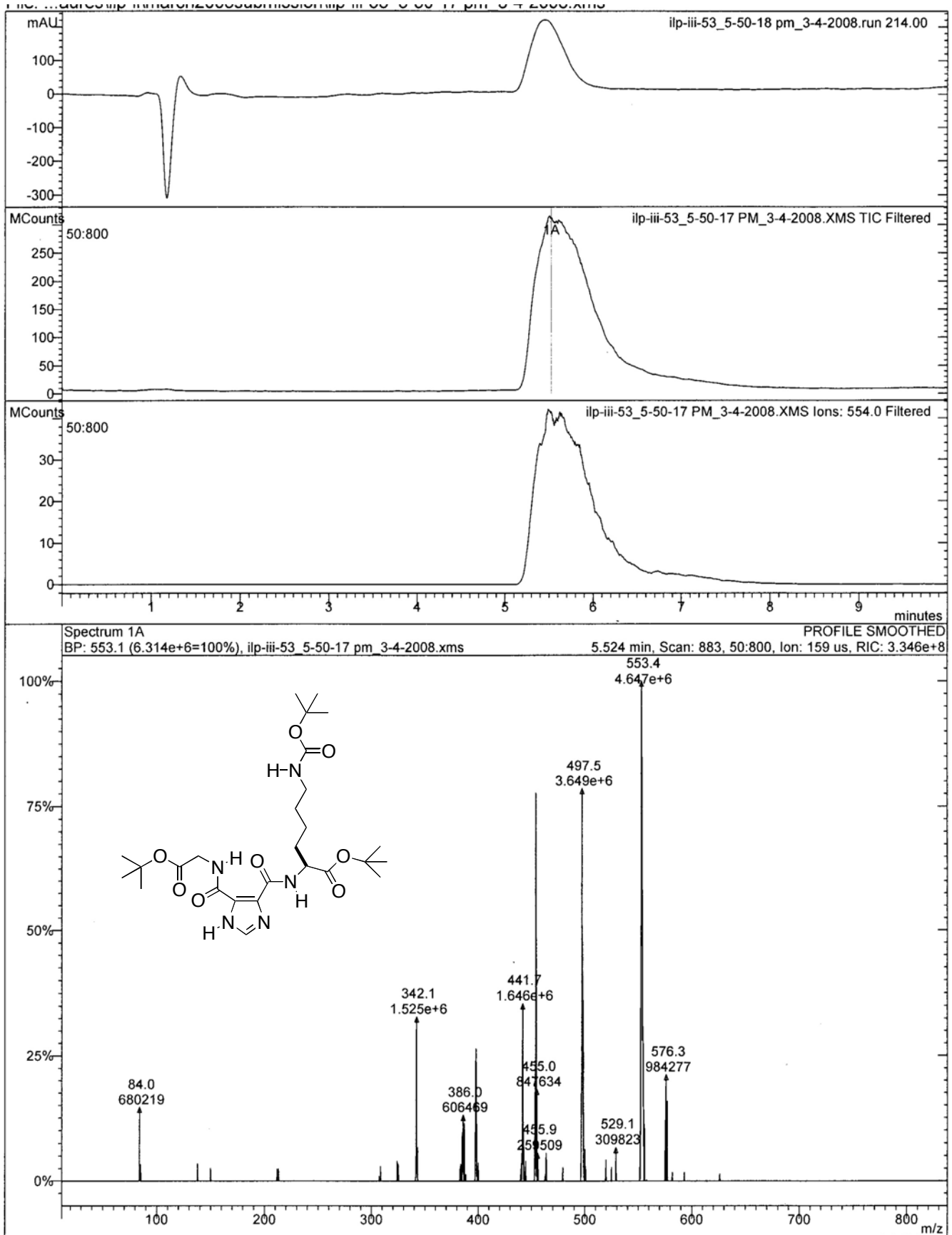


Figure S17. LC/MS data for 4{17}.

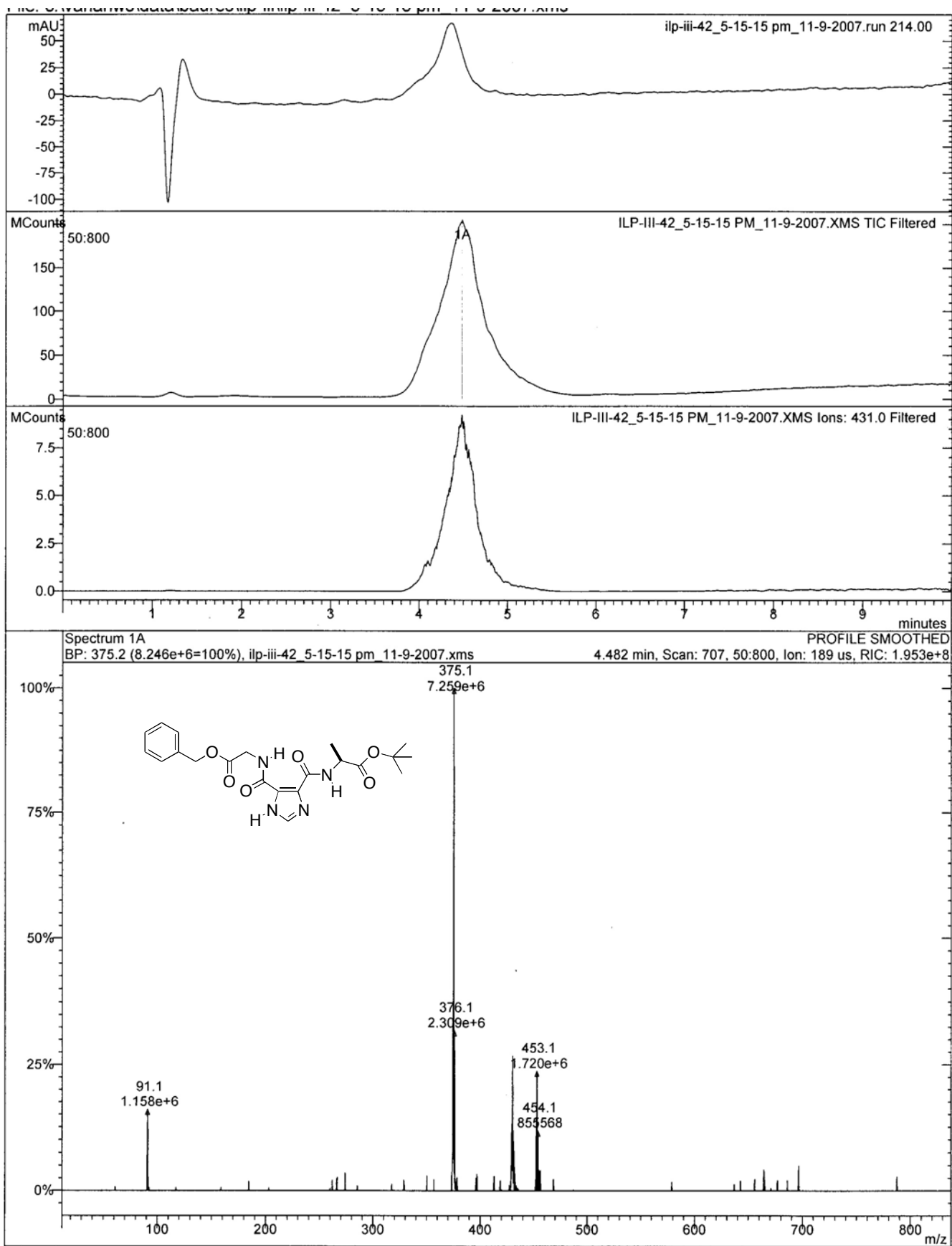


Figure S18. LC/MS data for 4{18}.

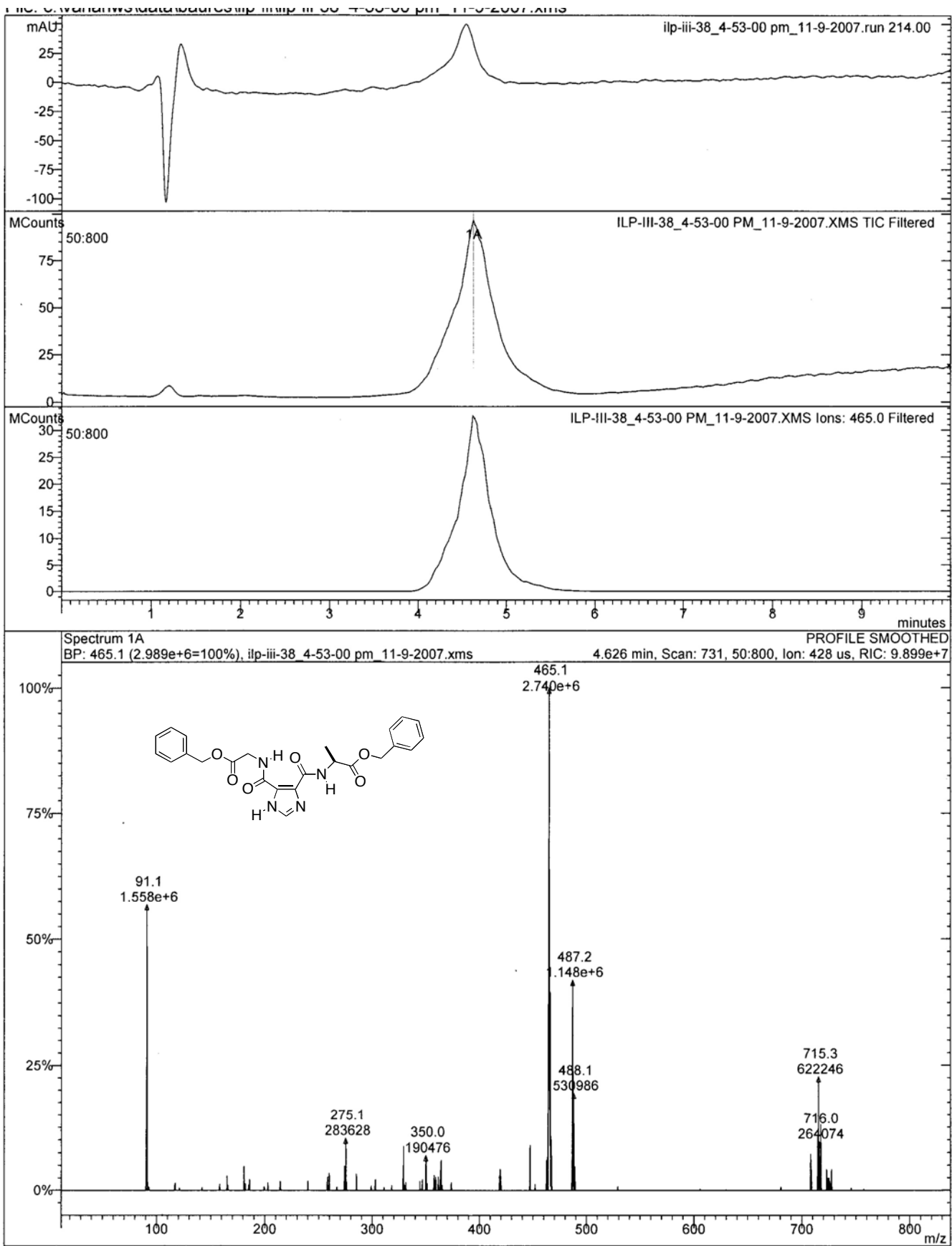


Figure S19. LC/MS data for 4{19}.

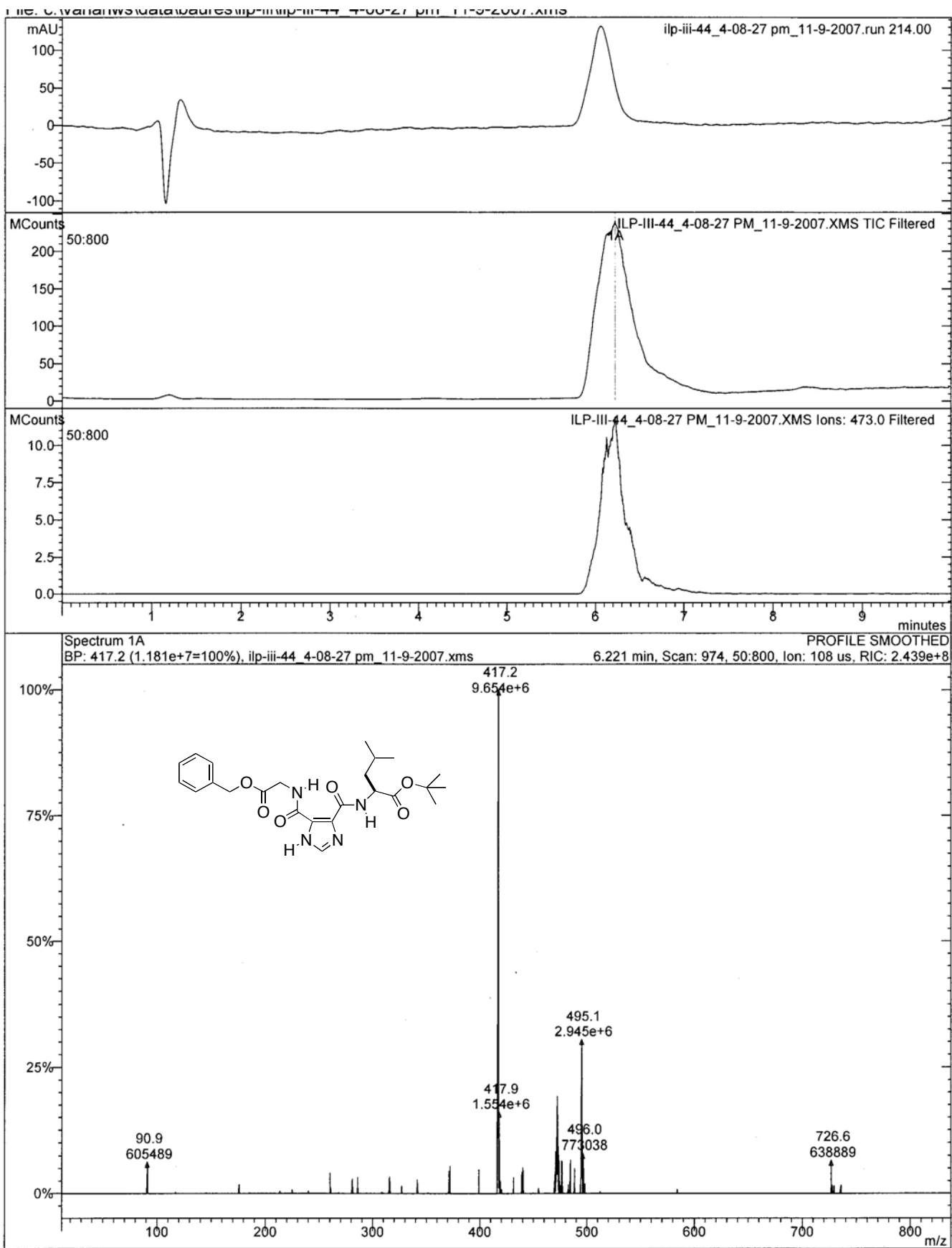


Figure S20. LC/MS data for 4{20}.

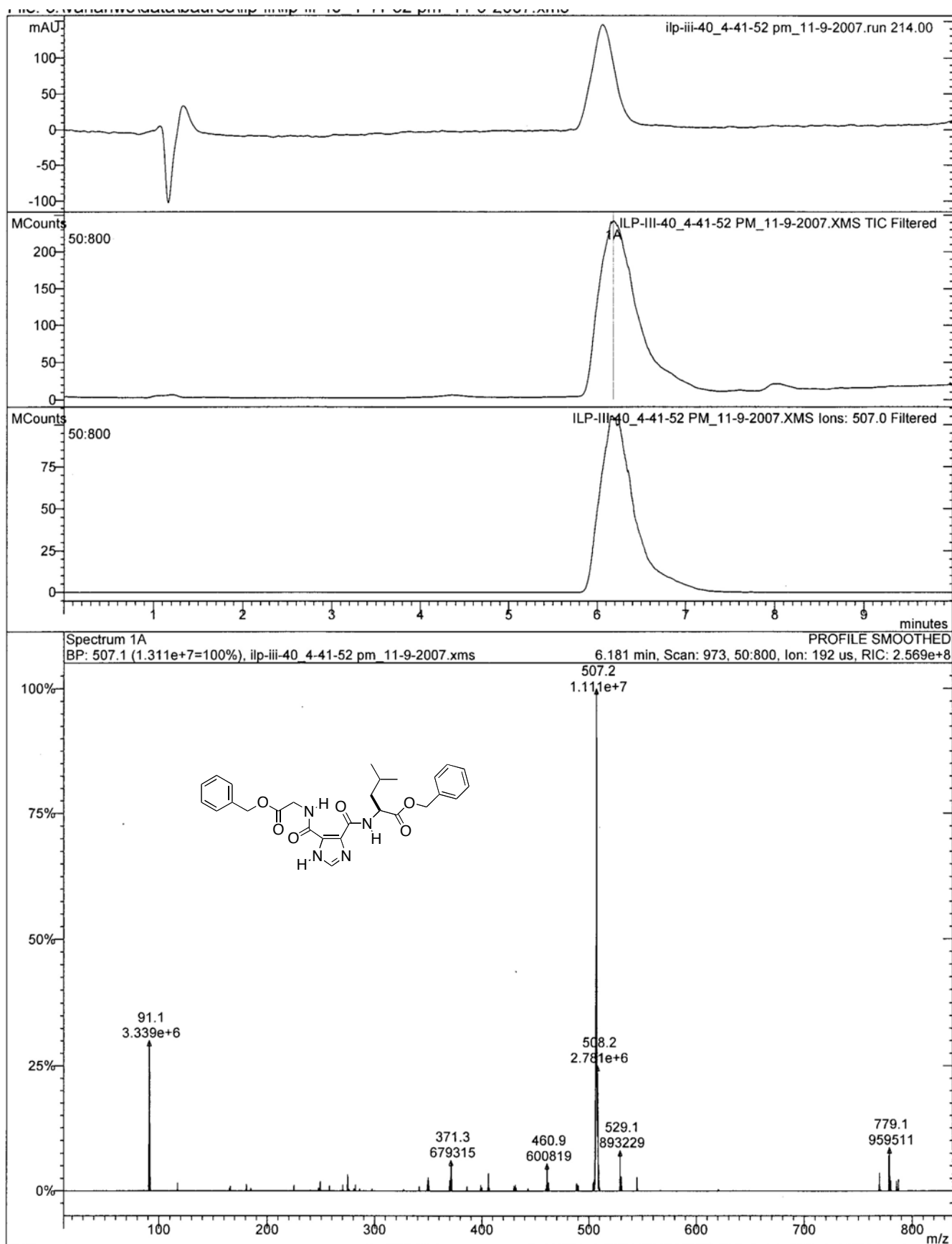


Figure S21. LC/MS data for 4{21}.

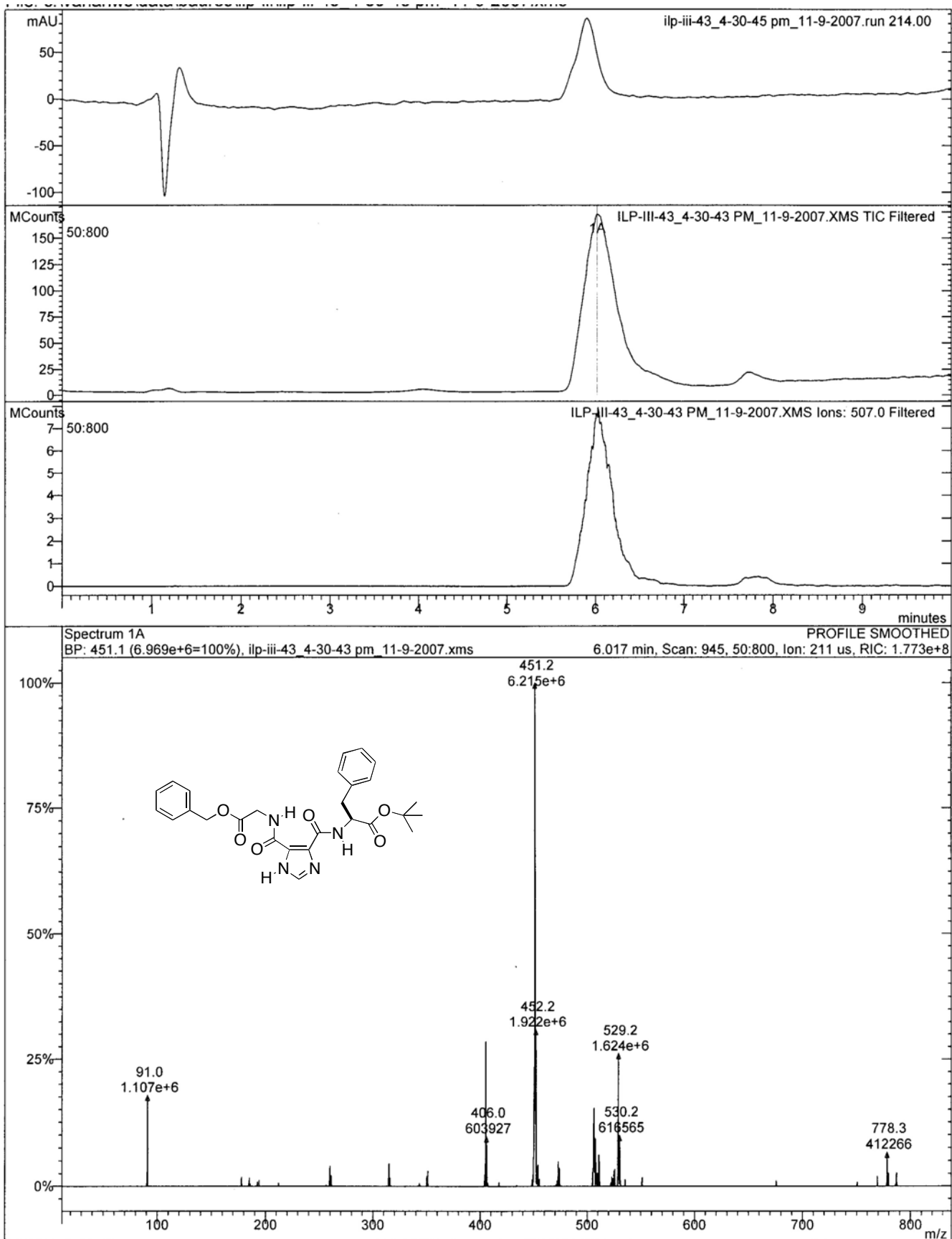


Figure S22. LC/MS data for 4{22}.

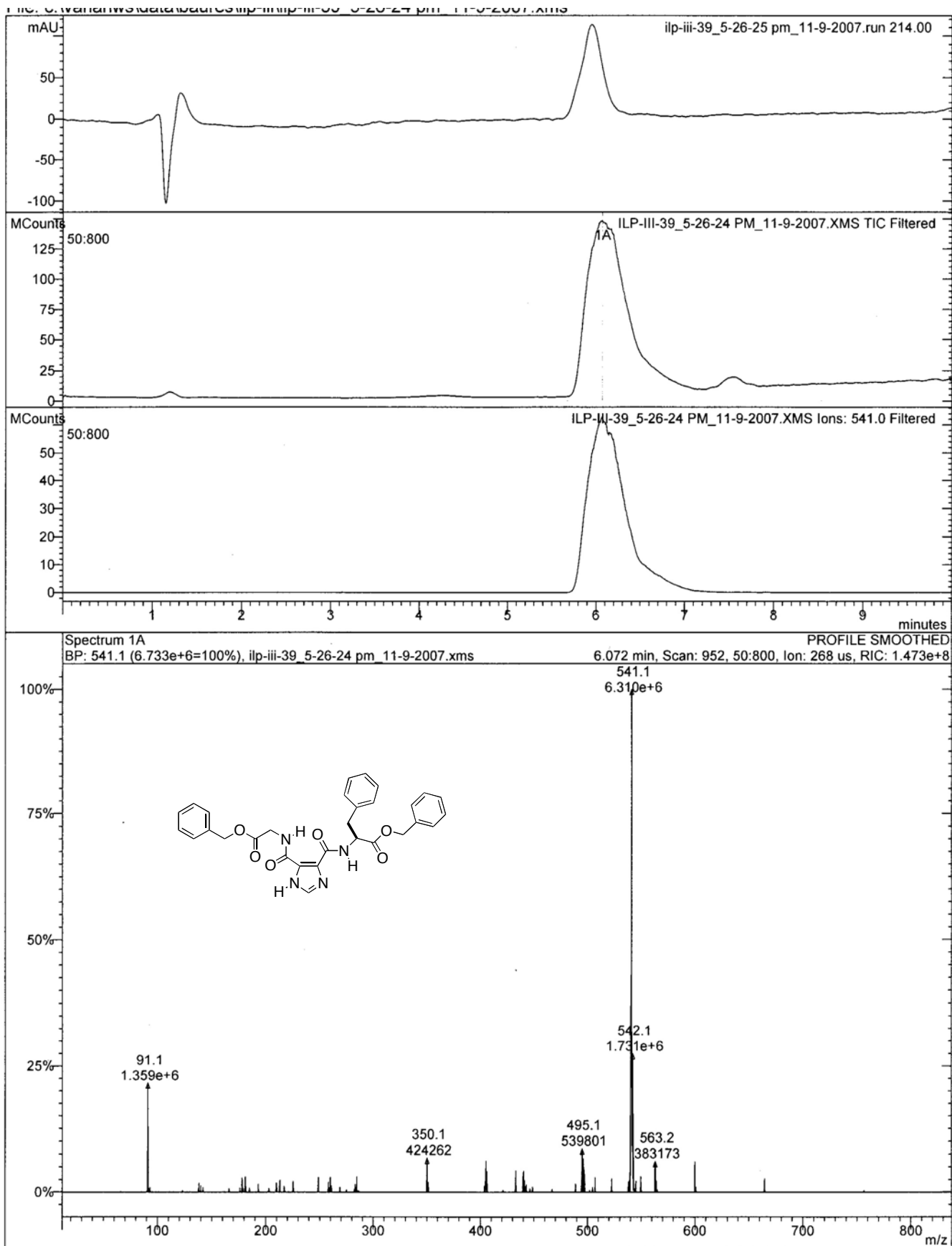


Figure S23. LC/MS data for 4{23}.

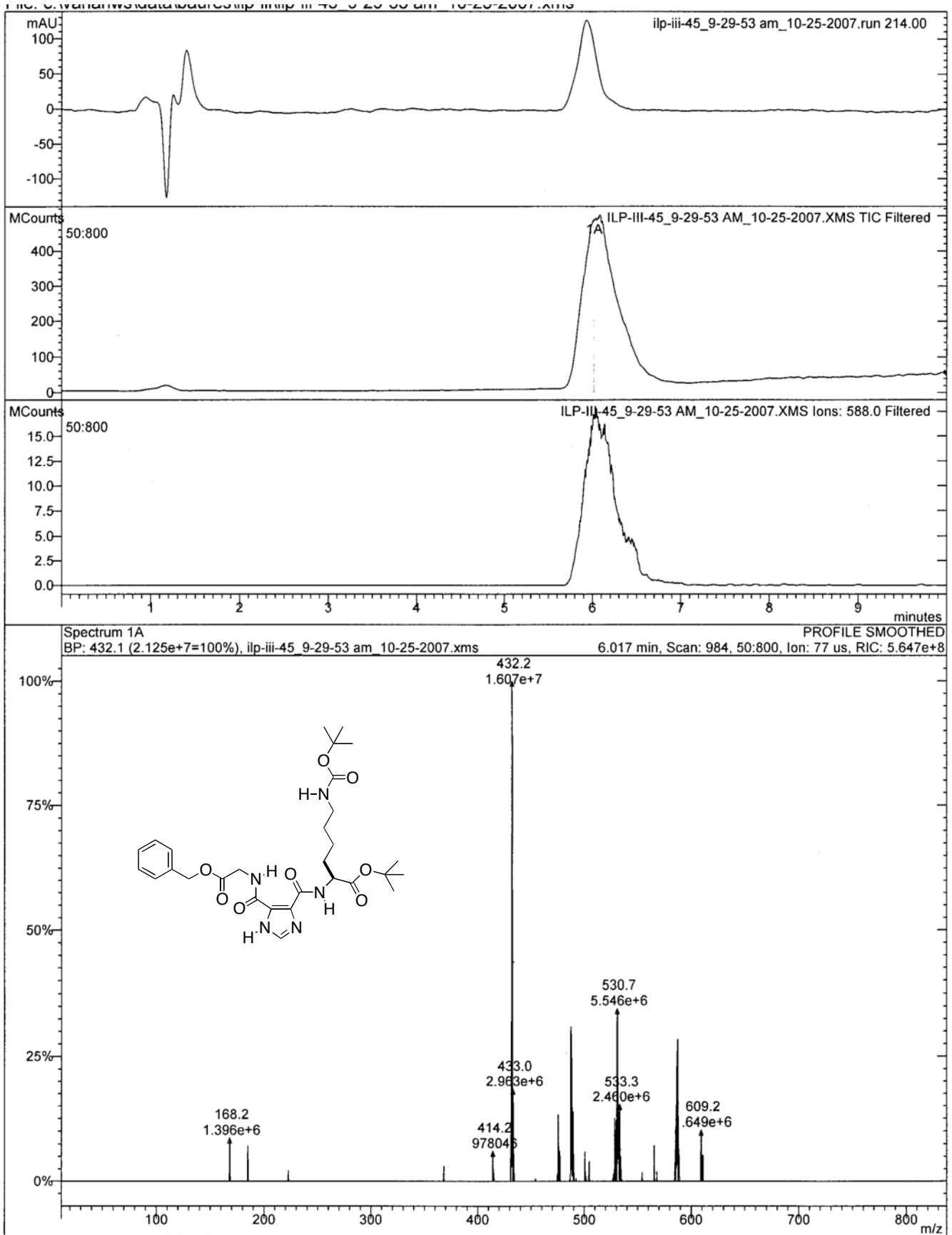


Figure S24. LC/MS data for 4{24}.

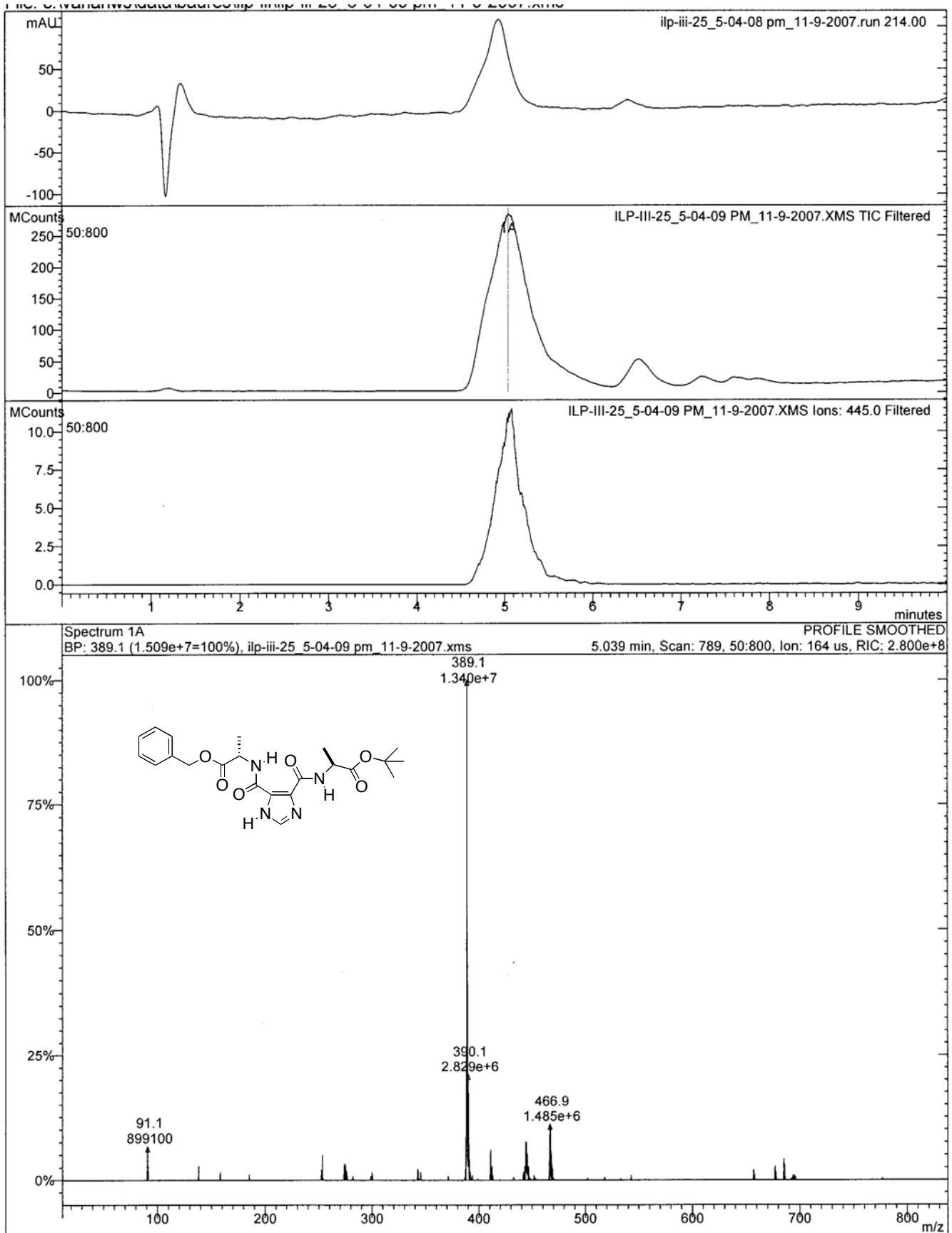


Figure S25. LC/MS data for 4{25}.

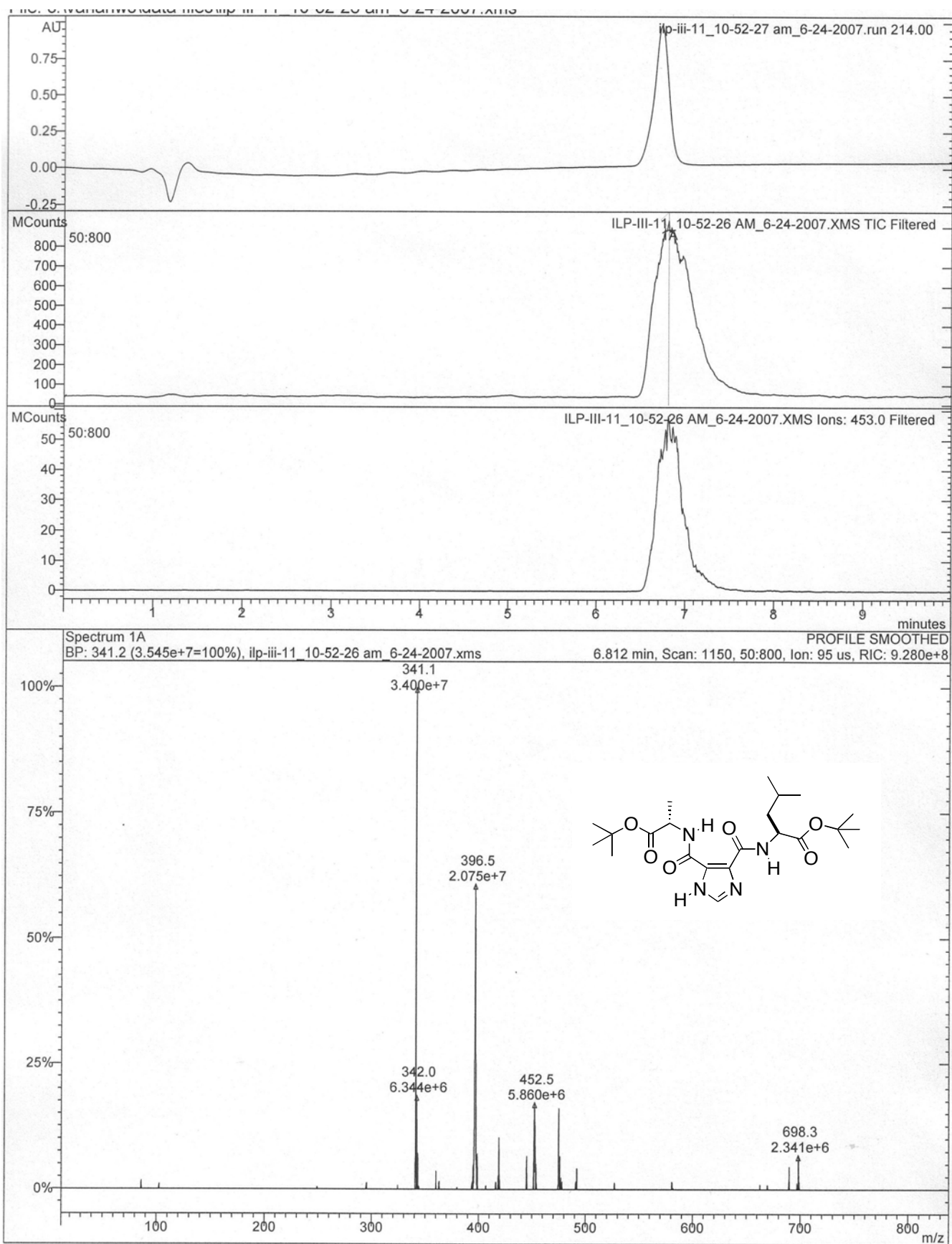


Figure S26. LC/MS data for 4{26}.