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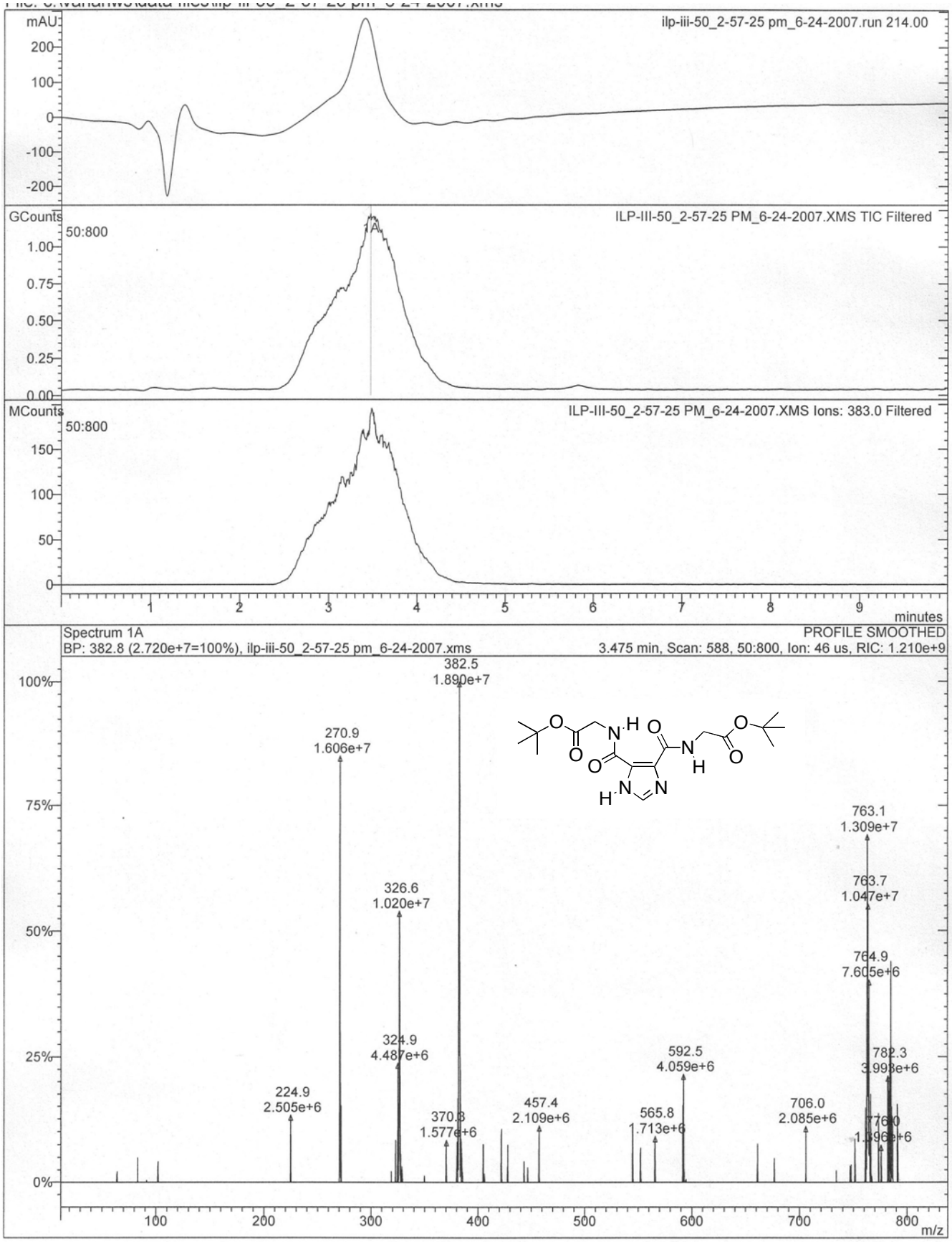
Table S1. Symmetrically-disubstituted Amino Acid Ester I45DCs, **4**{*1-9*}.

compound	formula	MW	C log*P*	form	R_f	R_t (min)
4{*1*}	$C_{17}H_{26}N_4O_6$	382.41	0.35	solid	0.79	3.40
4{*2*}	$C_{23}H_{22}N_4O_6$	450.44	1.30	solid	0.22	4.06
4{*3*}	$C_{19}H_{30}N_4O_6$	410.47	0.97	glass film	0.69	4.91
4{*4*}	$C_{25}H_{26}N_4O_6$	478.50	1.92	glass film	0.12	5.04
4{*5*}	$C_{25}H_{42}N_4O_6$	494.62	3.89	glass film	0.45	8.39
4{*6*}	$C_{31}H_{38}N_4O_6$	562.66	4.83	glass film	0.52	8.11
4{*7*}	$C_{31}H_{38}N_4O_6$	562.66	3.81	glass film	0.62	7.73
4{*8*}	$C_{37}H_{34}N_4O_6$	630.69	4.76	solid	0.23	7.37
4{*9*}	$C_{35}H_{60}N_6O_{10}$	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*P*	form	R_f	R_t (min)
4{*10*}	$C_{20}H_{24}N_4O_6$	416.43	1.17	glass film	0.83	3.67
4{*11*}	$C_{18}H_{28}N_4O_6$	396.44	0.66	glass film	0.86	4.00
4{*12*}	$C_{21}H_{26}N_4O_6$	430.45	1.14	glass film	0.85	4.31
4{*13*}	$C_{21}H_{34}N_4O_6$	438.52	2.12	glass film	0.91	5.86
4{*14*}	$C_{24}H_{32}N_4O_6$	472.53	2.59	glass film	0.83	6.04
4{*15*}	$C_{24}H_{32}N_4O_6$	472.53	2.42	glass film	0.78	6.00
4{*16*}	$C_{27}H_{30}N_4O_6$	506.55	2.90	glass film	0.84	6.18
4{*17*}	$C_{26}H_{43}N_5O_8$	553.31	2.11	glass film	0.61	5.45
4{*18*}	$C_{21}H_{26}N_4O_6$	430.56	1.48	glass film	0.56	4.36
4{*19*}	$C_{24}H_{24}N_4O_6$	464.47	1.61	solid	0.70	4.54
4{*20*}	$C_{24}H_{32}N_4O_6$	472.53	2.93	glass film	0.69	6.06
4{*21*}	$C_{27}H_{30}N_4O_6$	506.55	3.07	glass film	0.55	6.06
4{*22*}	$C_{27}H_{30}N_4O_6$	506.55	2.56	glass film	0.67	5.90
4{*23*}	$C_{30}H_{28}N_4O_6$	540.57	3.03	glass film	0.64	5.95
4{*24*}	$C_{29}H_{41}N_5O_8$	587.67	2.92	glass film	0.62	5.93
4{*25*}	$C_{22}H_{28}N_4O_6$	444.48	1.45	glass film	0.57	5.37
4{*26*}	$C_{22}H_{36}N_4O_6$	452.54	2.43	glass film	0.37	7.44
4{*27*}	$C_{25}H_{34}N_4O_6$	486.56	2.90	glass film	0.45	6.66
4{*28*}	$C_{25}H_{34}N_4O_6$	486.56	2.73	glass film	0.54	6.53
4{*29*}	$C_{28}H_{32}N_4O_6$	520.58	3.20	glass film	0.56	6.38
4{*30*}	$C_{27}H_{45}N_5O_8$	567.68	2.42	glass film	0.77	6.13
4{*31*}	$C_{25}H_{34}N_4O_6$	486.56	3.24	glass film	0.39	6.80
4{*32*}	$C_{28}H_{32}N_4O_6$	520.58	3.38	glass film	0.40	6.79
4{*33*}	$C_{28}H_{32}N_4O_6$	520.58	2.86	glass film	0.59	6.38
4{*34*}	$C_{31}H_{30}N_4O_6$	554.59	3.34	glass film	0.35	6.52
4{*35*}	$C_{39}H_{43}N_5O_8$	601.31	2.89	glass film	0.63	6.25
4{*36*}	$C_{28}H_{40}N_4O_6$	528.64	4.36	glass film	0.51	8.31
4{*37*}	$C_{28}H_{40}N_4O_6$	528.64	4.19	glass film	0.42	7.99
4{*38*}	$C_{31}H_{38}N_4O_6$	562.66	4.66	glass film	0.39	7.79
4{*39*}	$C_{30}H_{51}N_5O_8$	609.76	3.87	glass film	0.33	7.48
4{*40*}	$C_{31}H_{38}N_4O_6$	562.66	4.32	glass film	0.44	7.95
4{*41*}	$C_{34}H_{36}N_4O_6$	596.67	4.80	glass film	0.47	7.64
4{*42*}	$C_{33}H_{49}N_5O_8$	643.77	4.35	glass film	0.29	7.39
4{*43*}	$C_{34}H_{36}N_4O_6$	596.67	4.28	glass film	0.48	7.44
4{*44*}	$C_{33}H_{49}N_5O_8$	643.77	4.17	glass film	0.59	7.29
4{*45*}	$C_{36}H_{47}N_5O_8$	677.34	4.65	glass film	0.56	7.29



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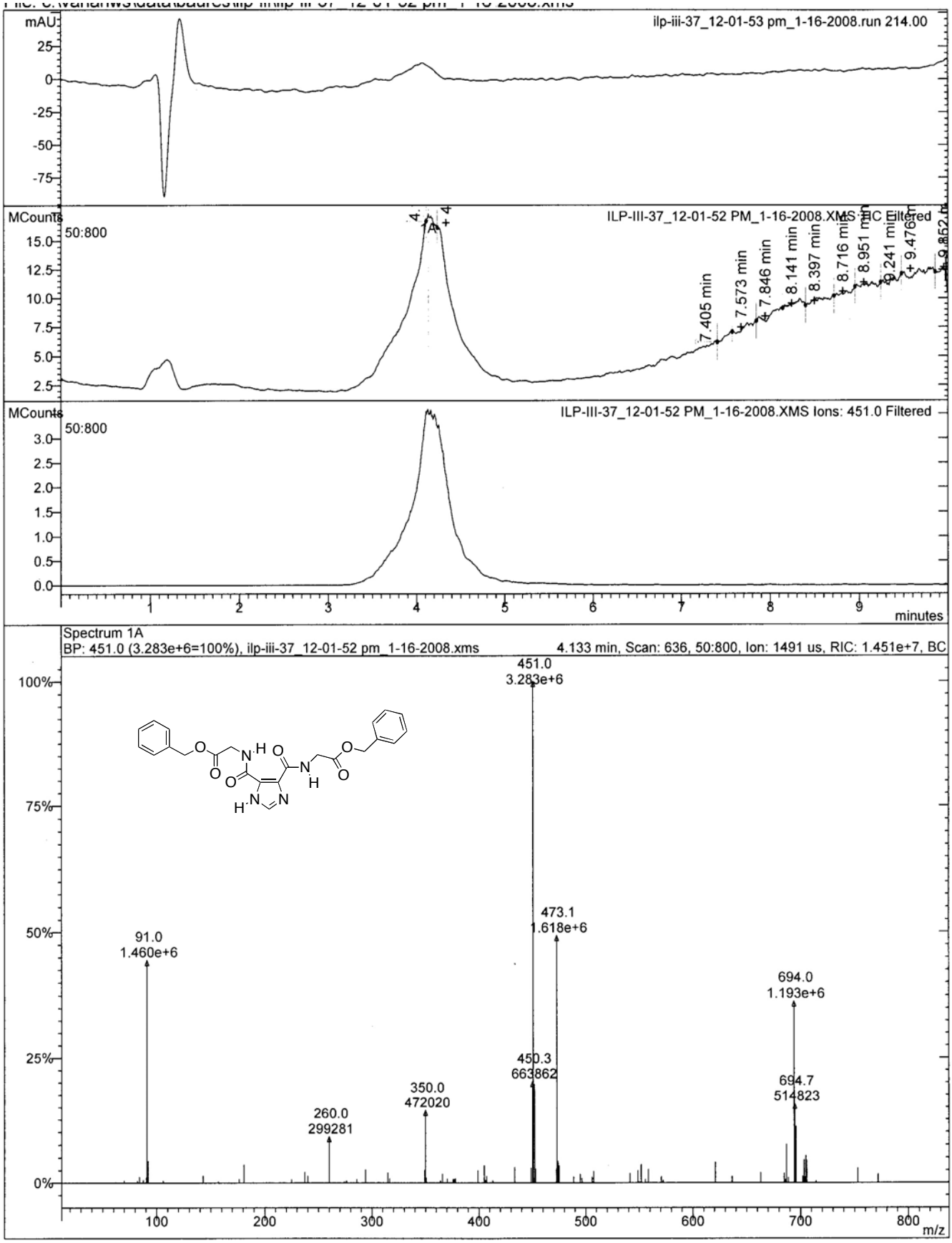

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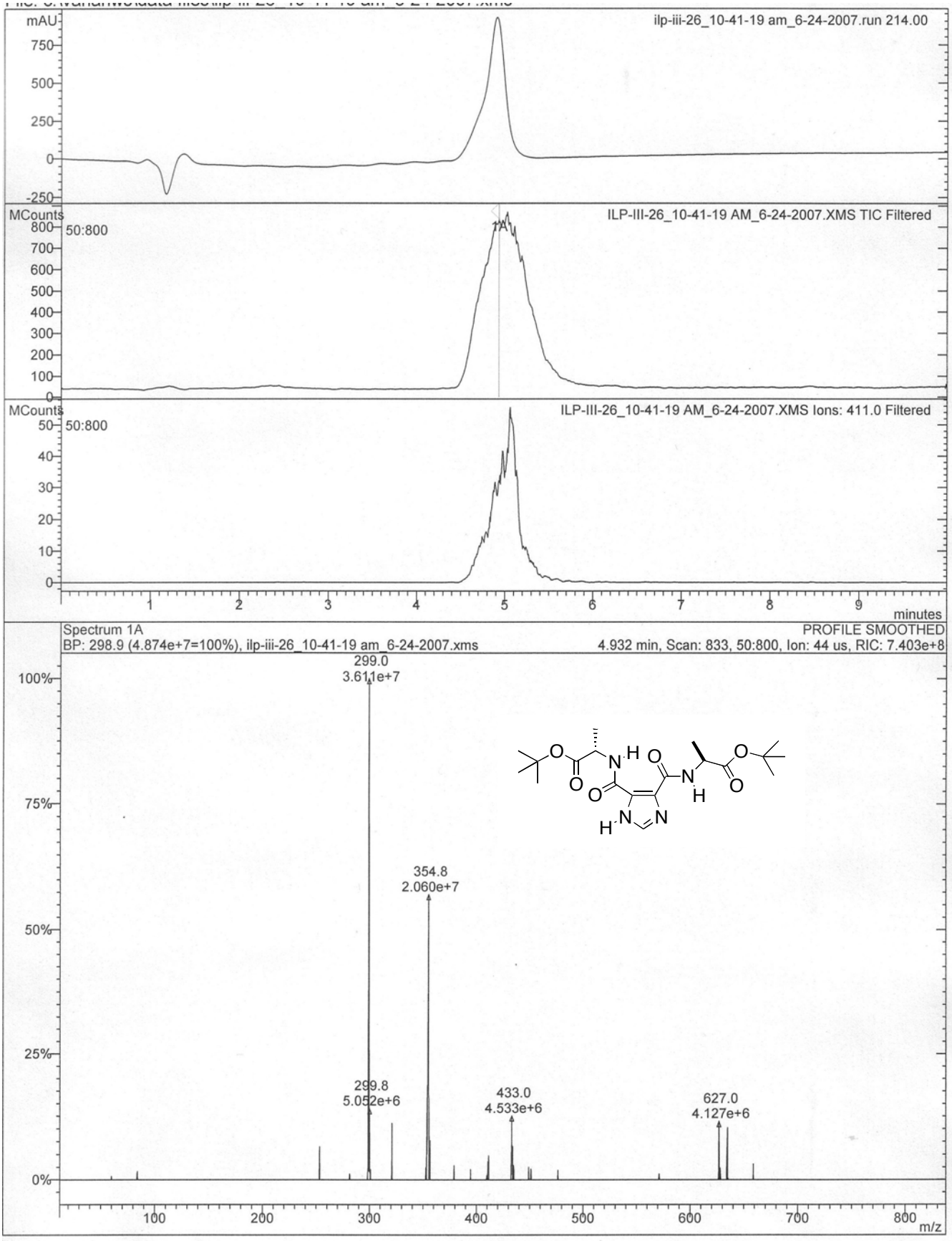

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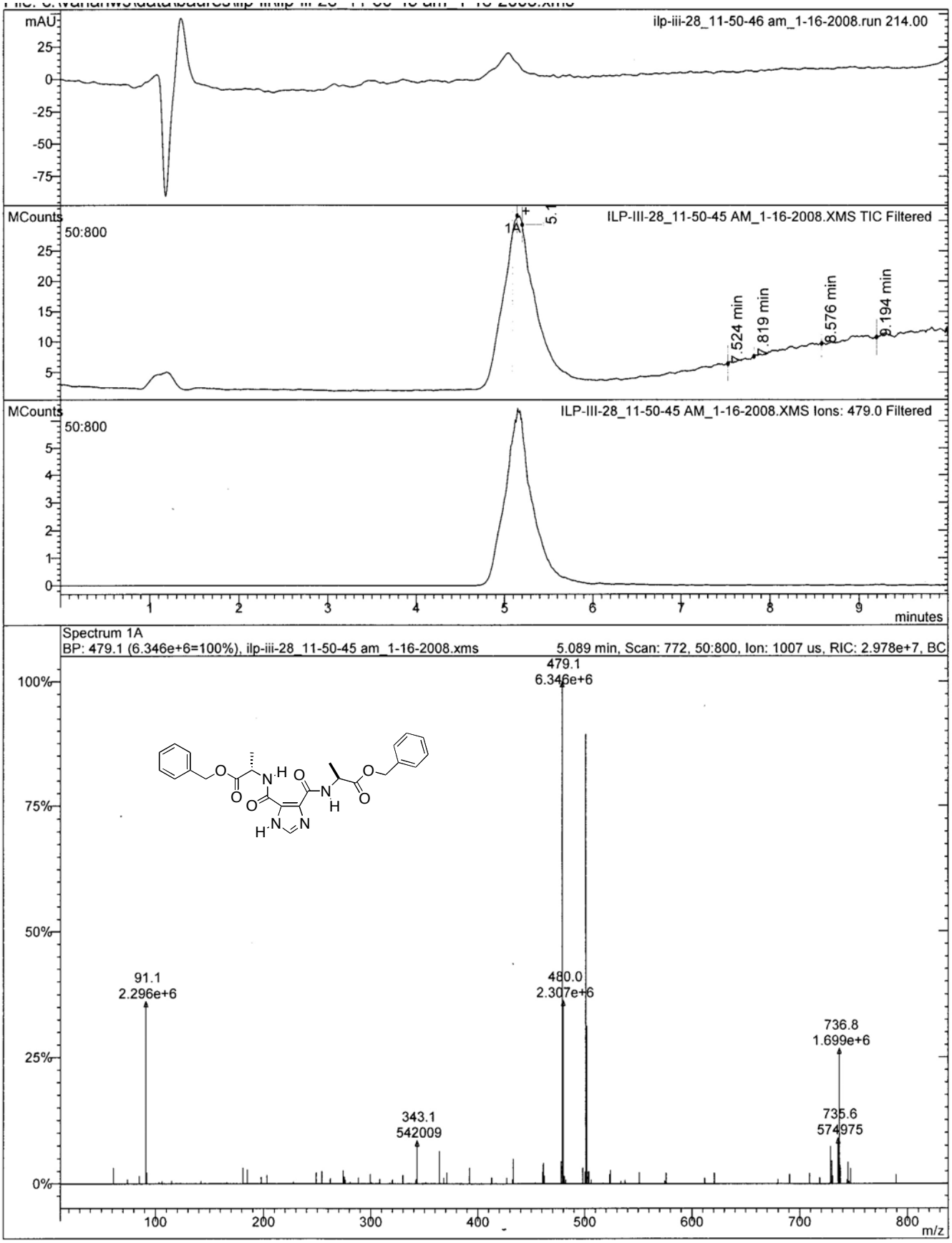

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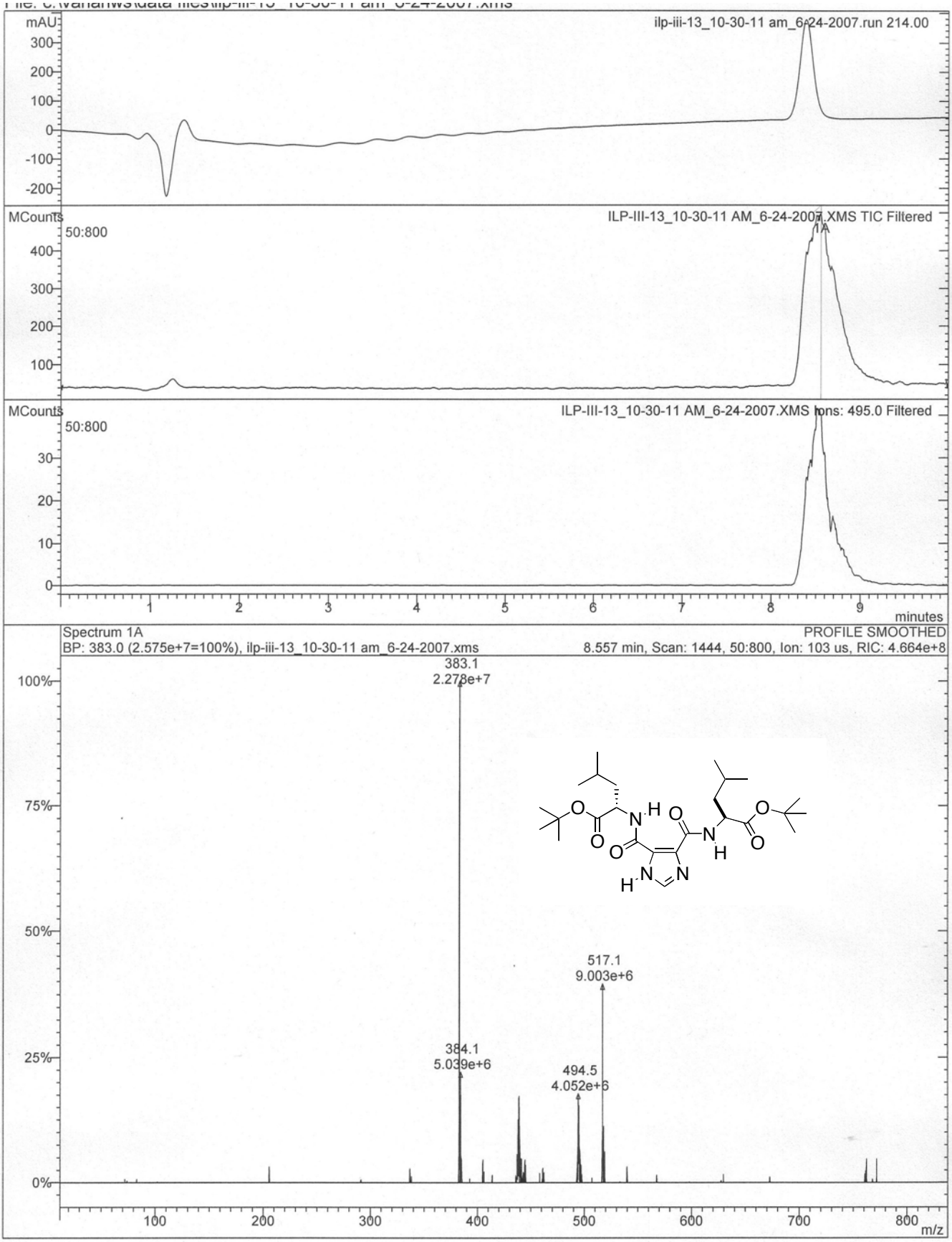

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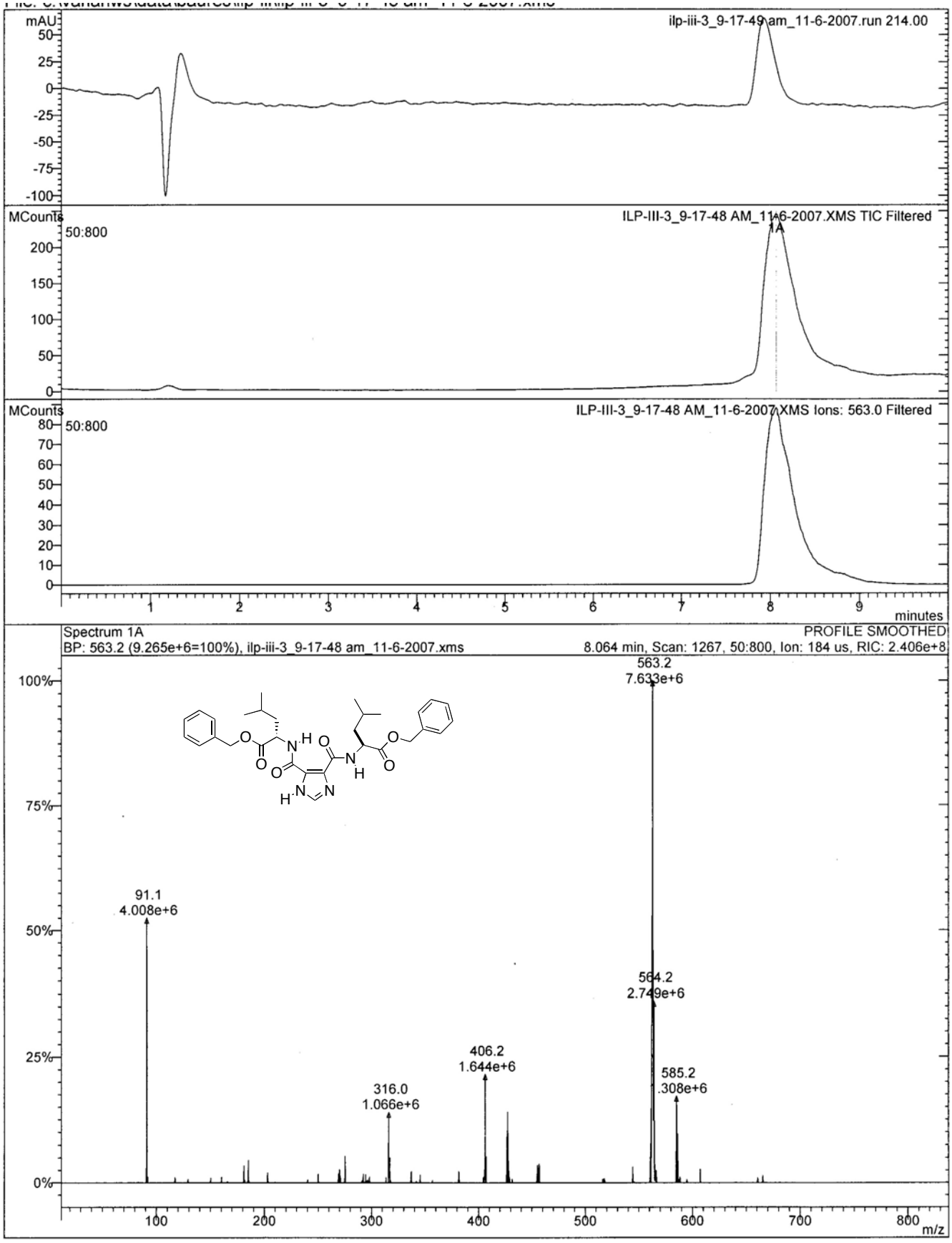

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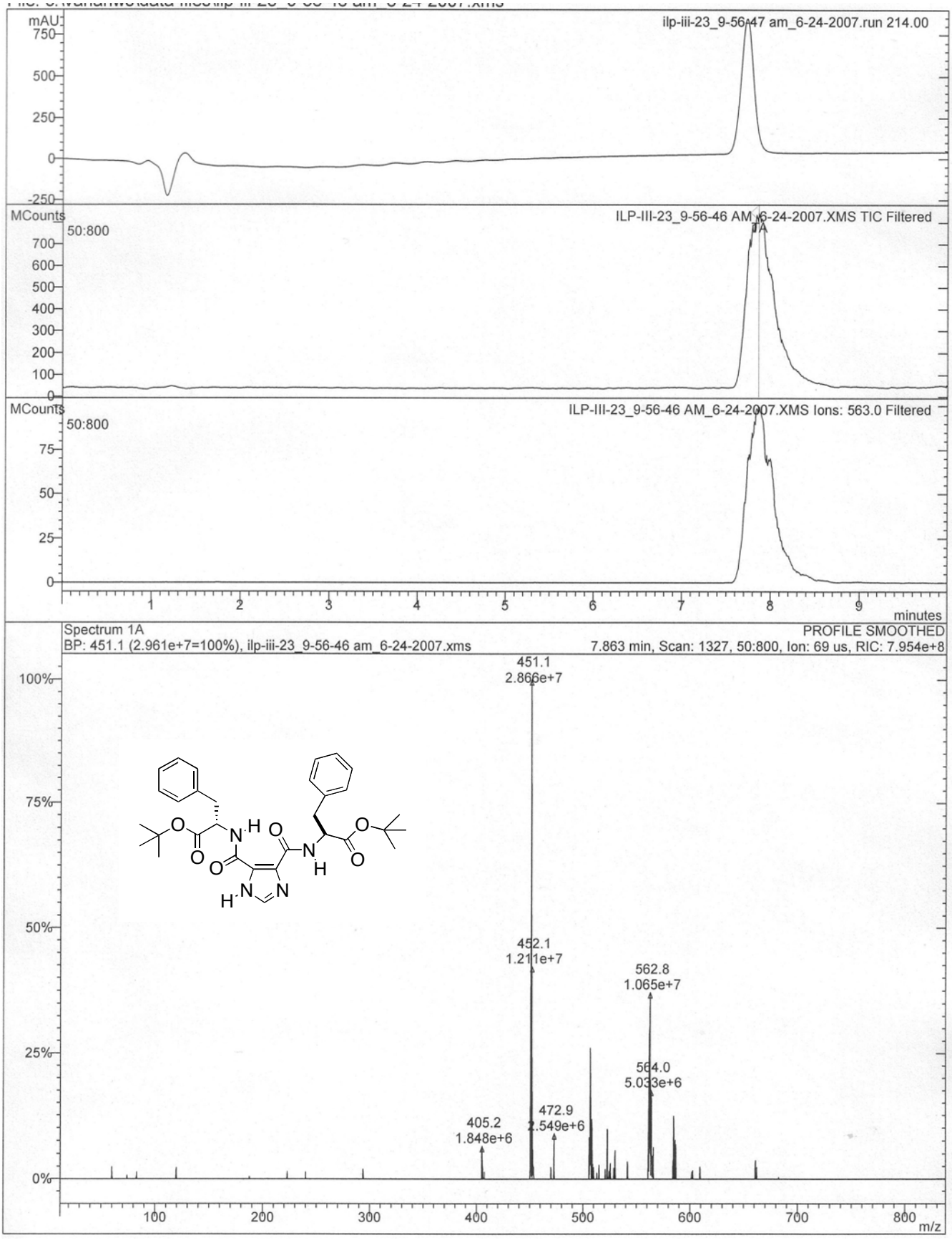

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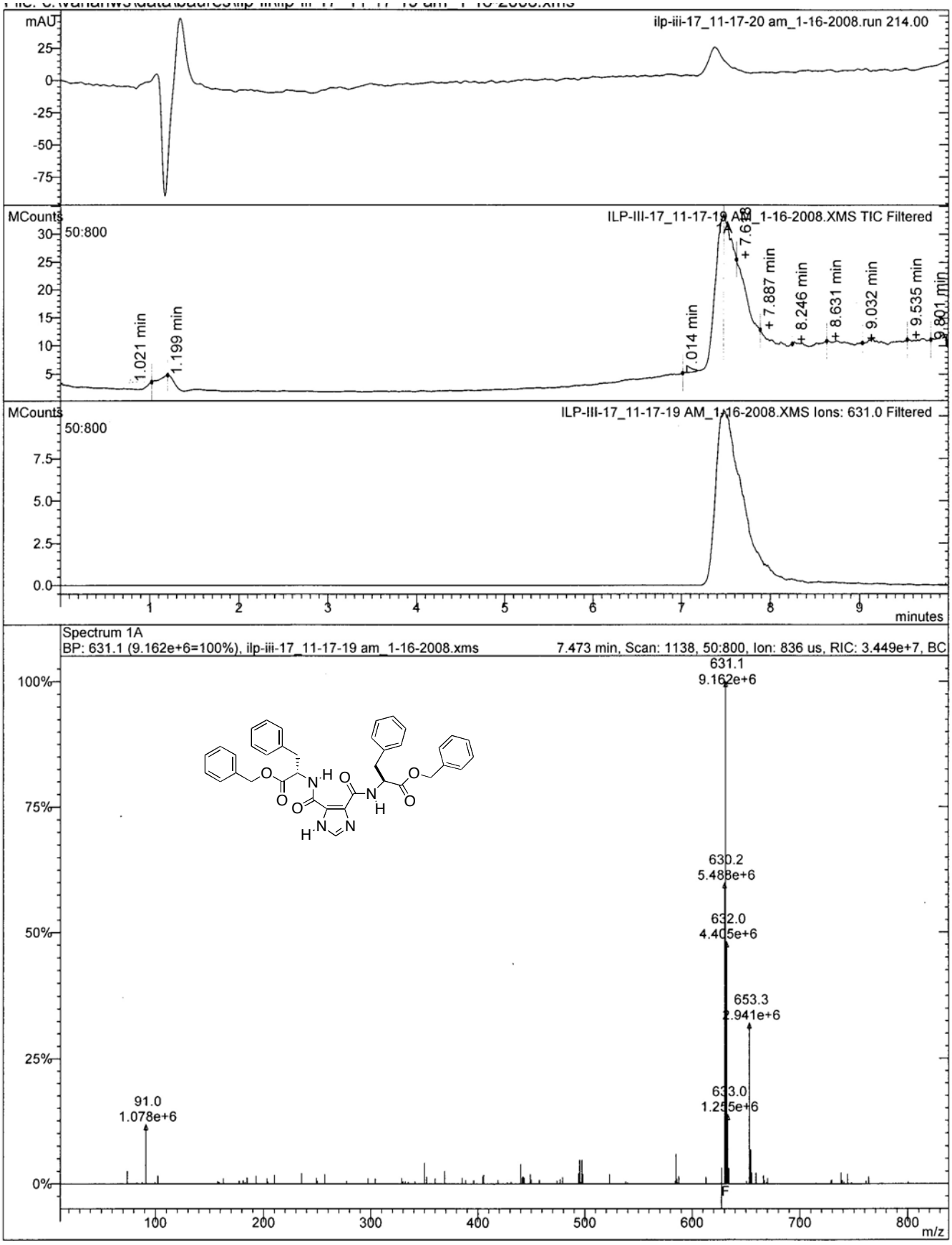

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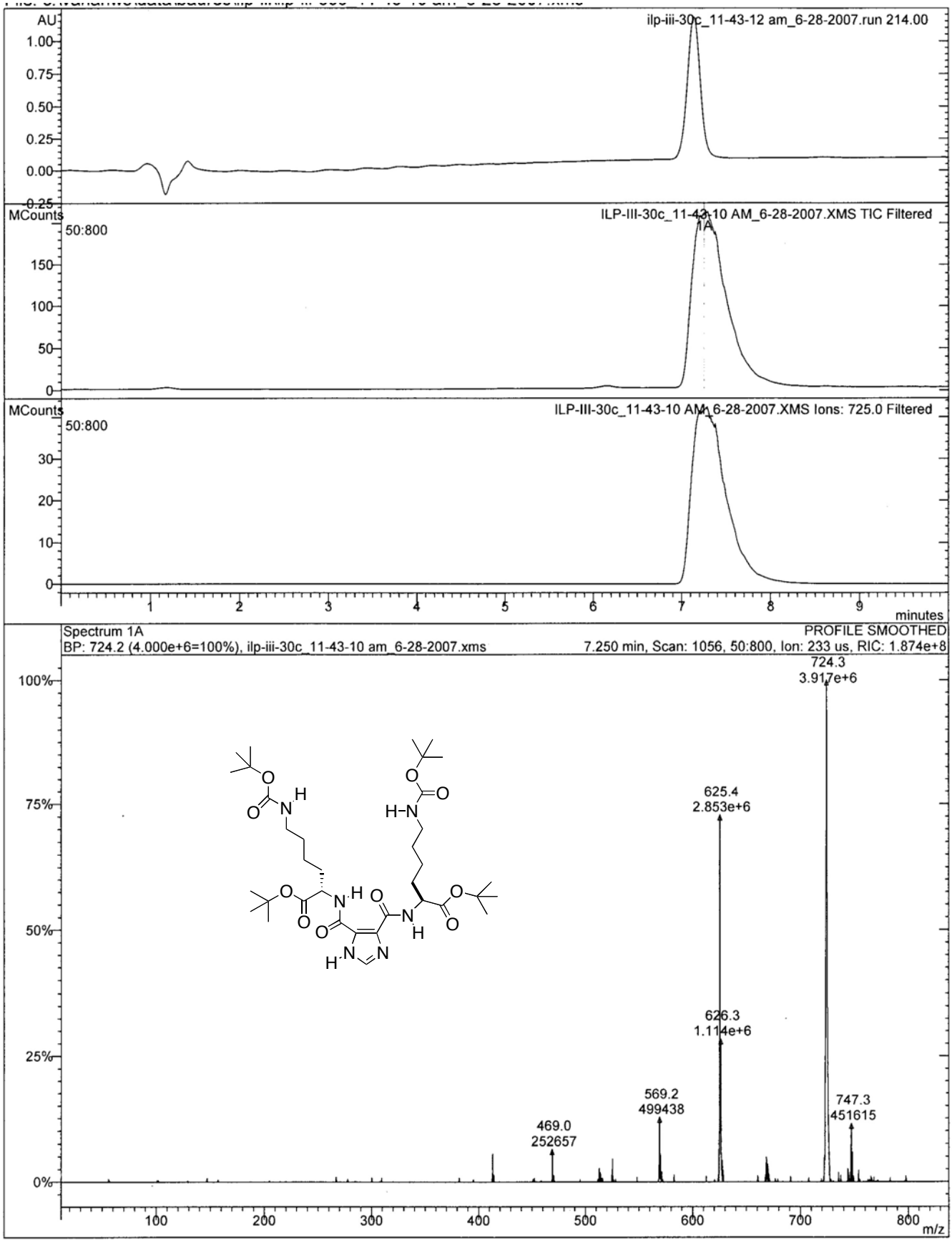

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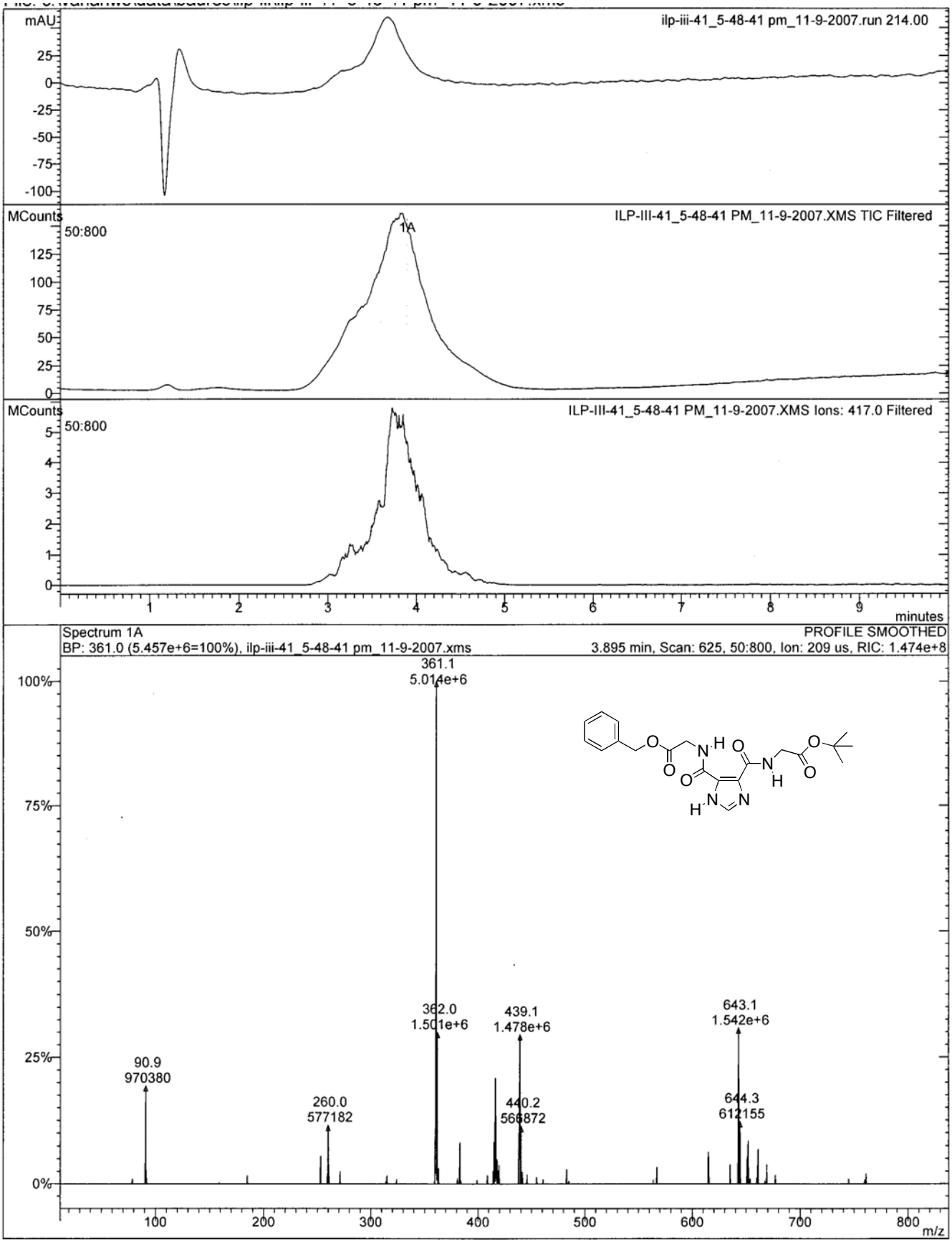

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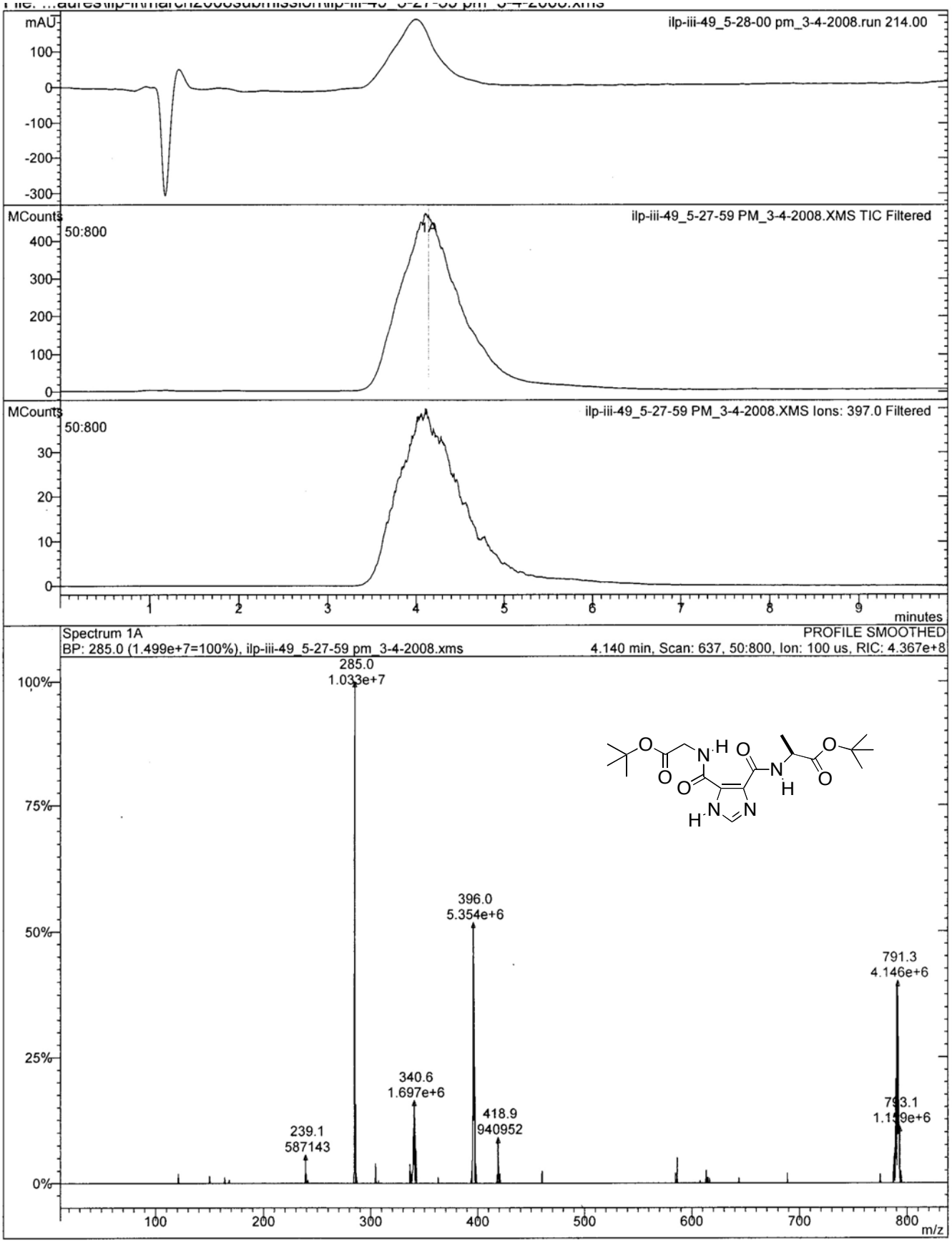

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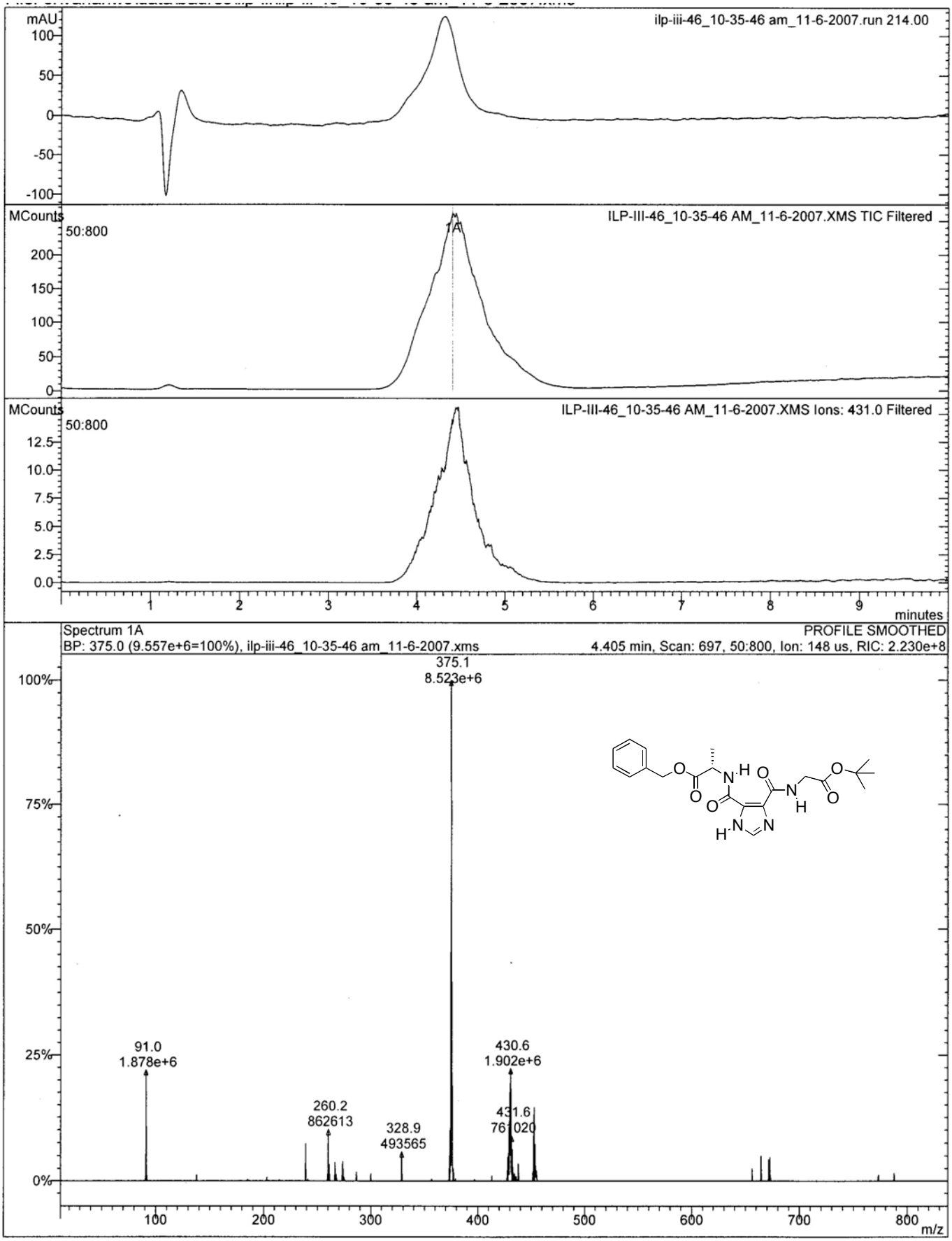

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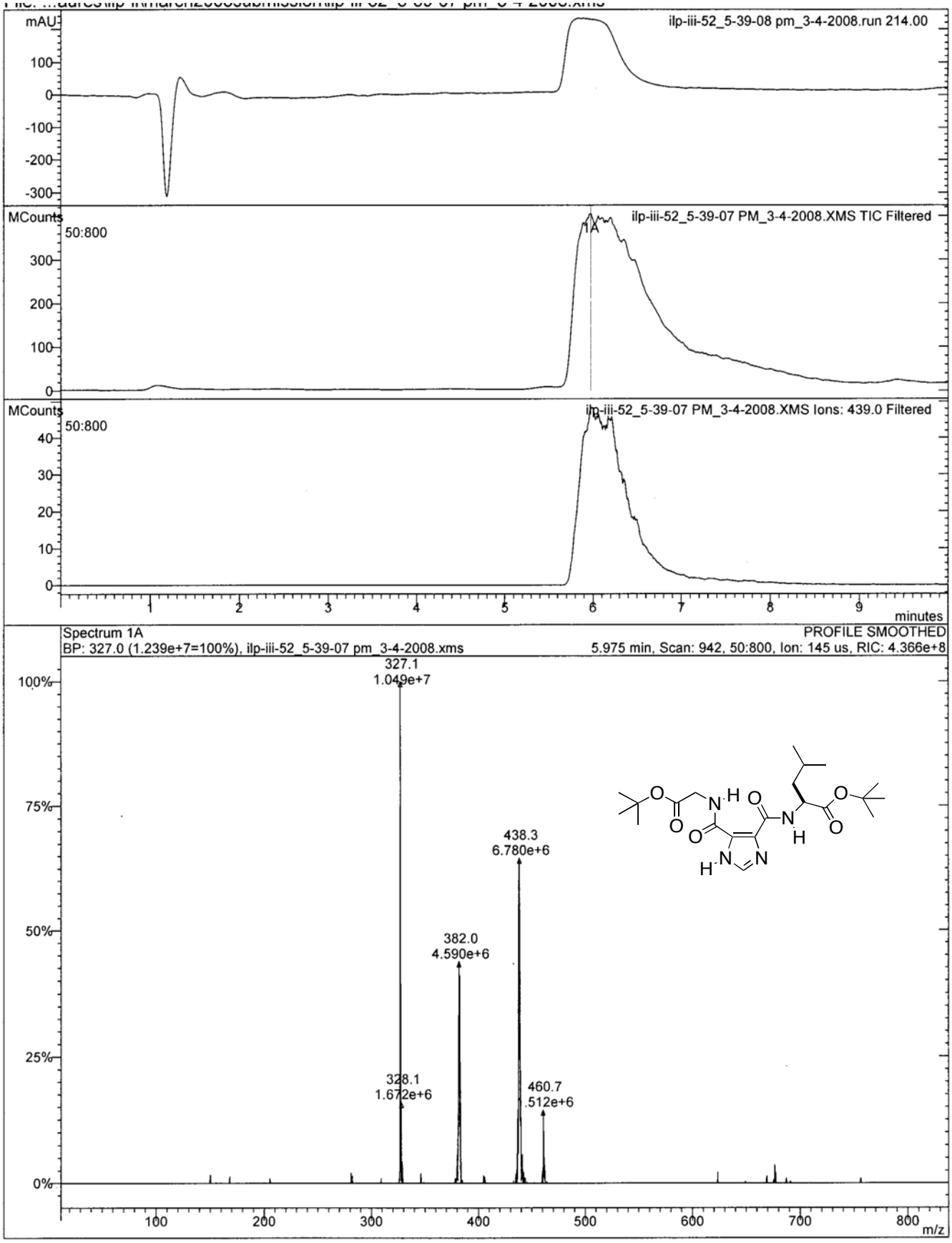

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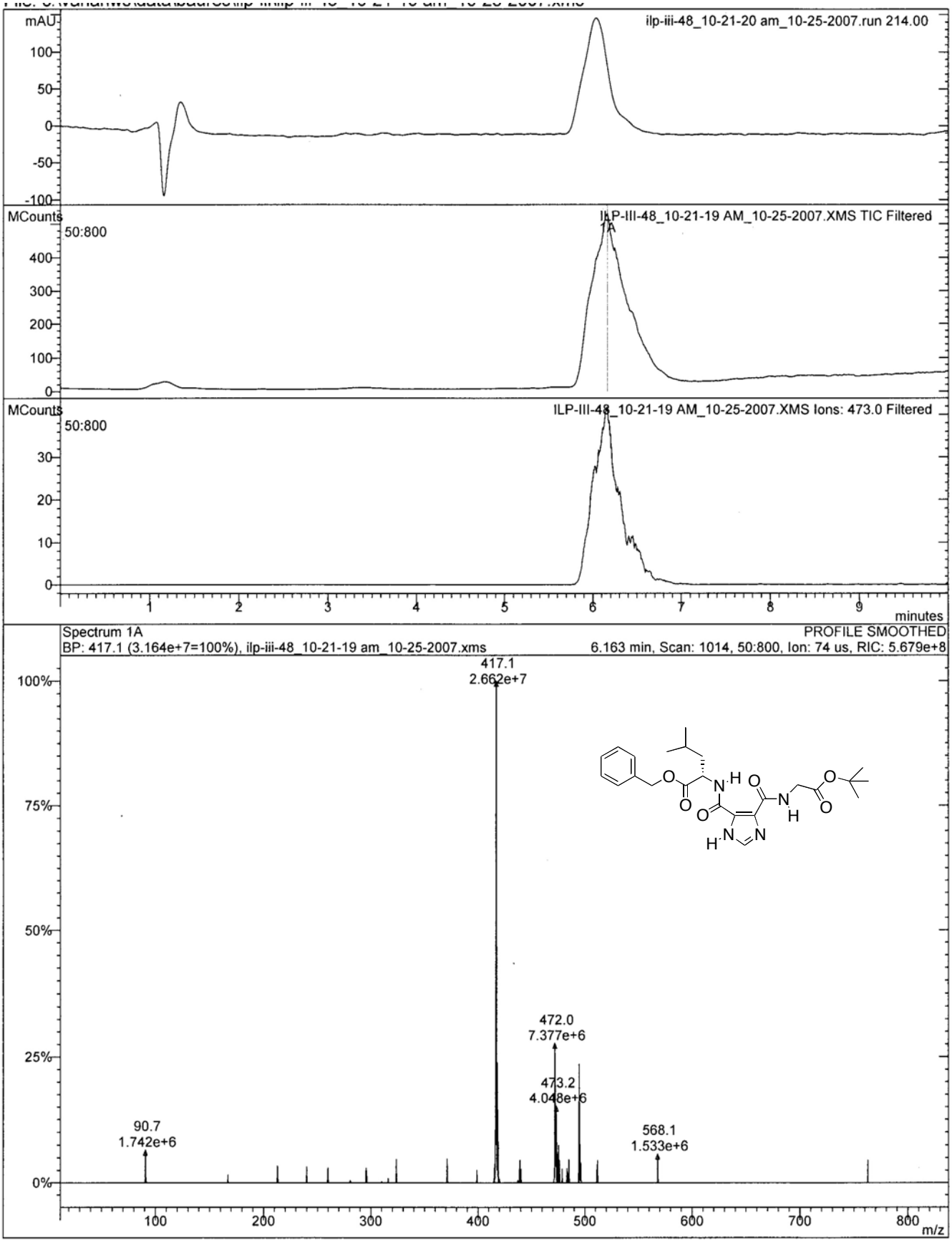

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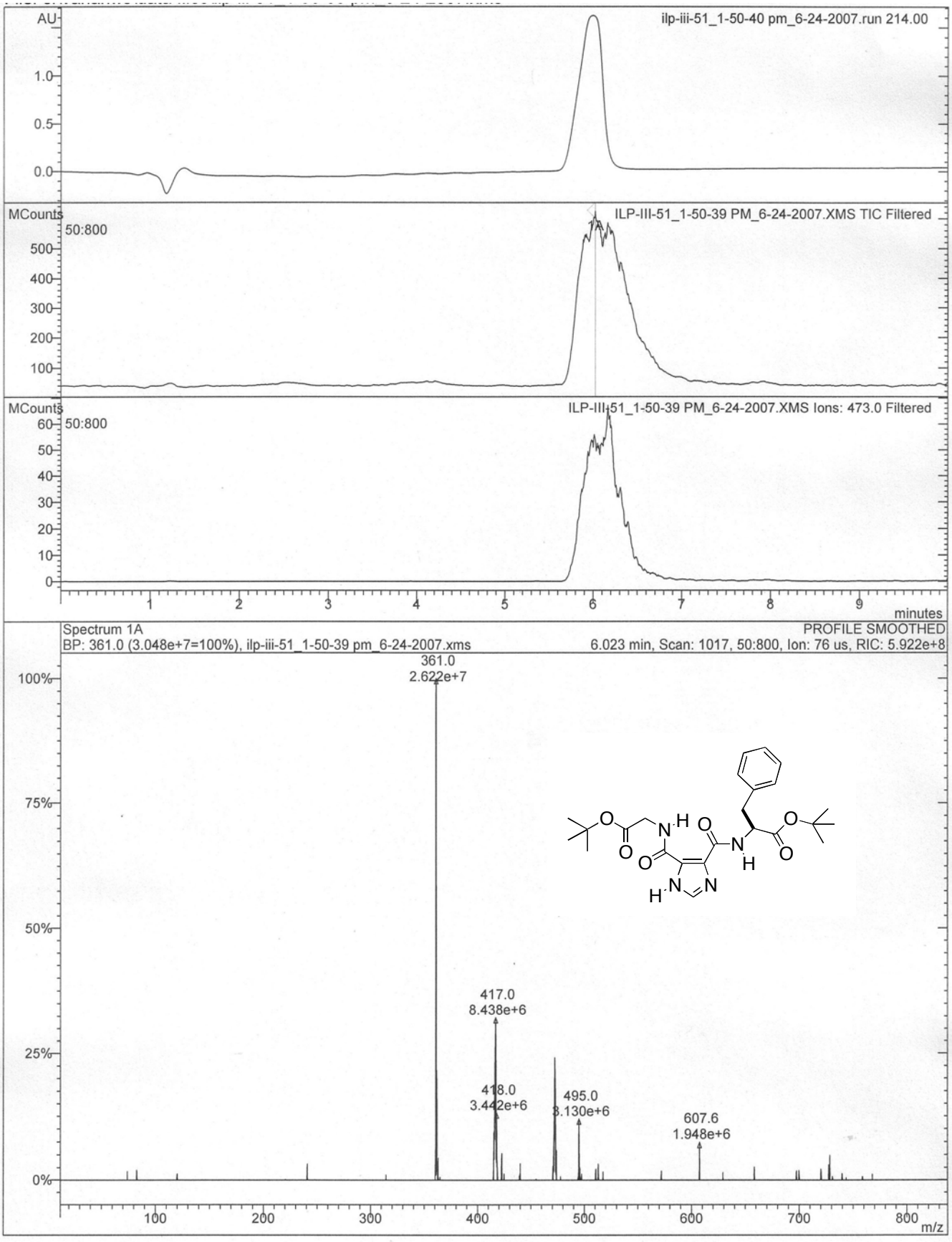

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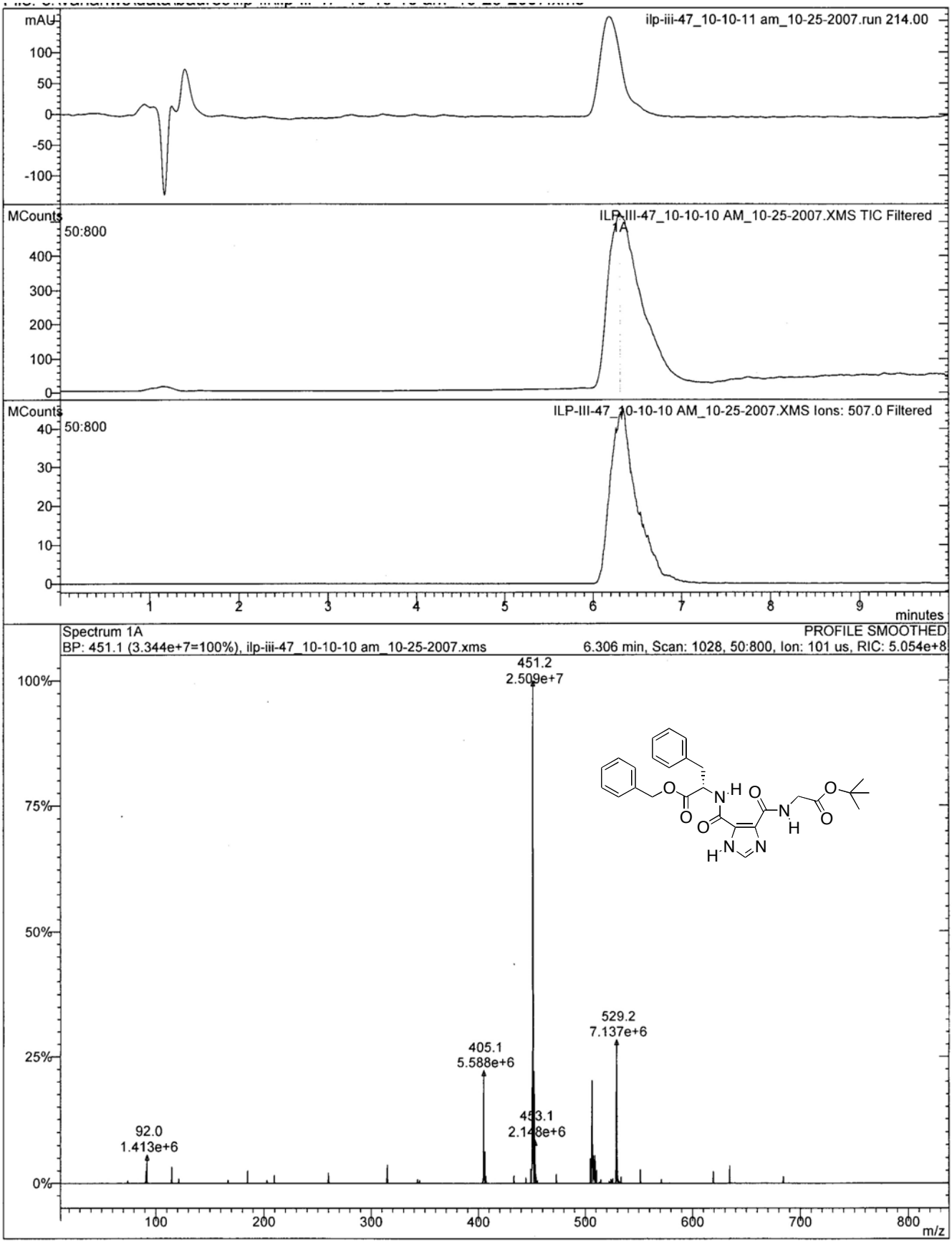

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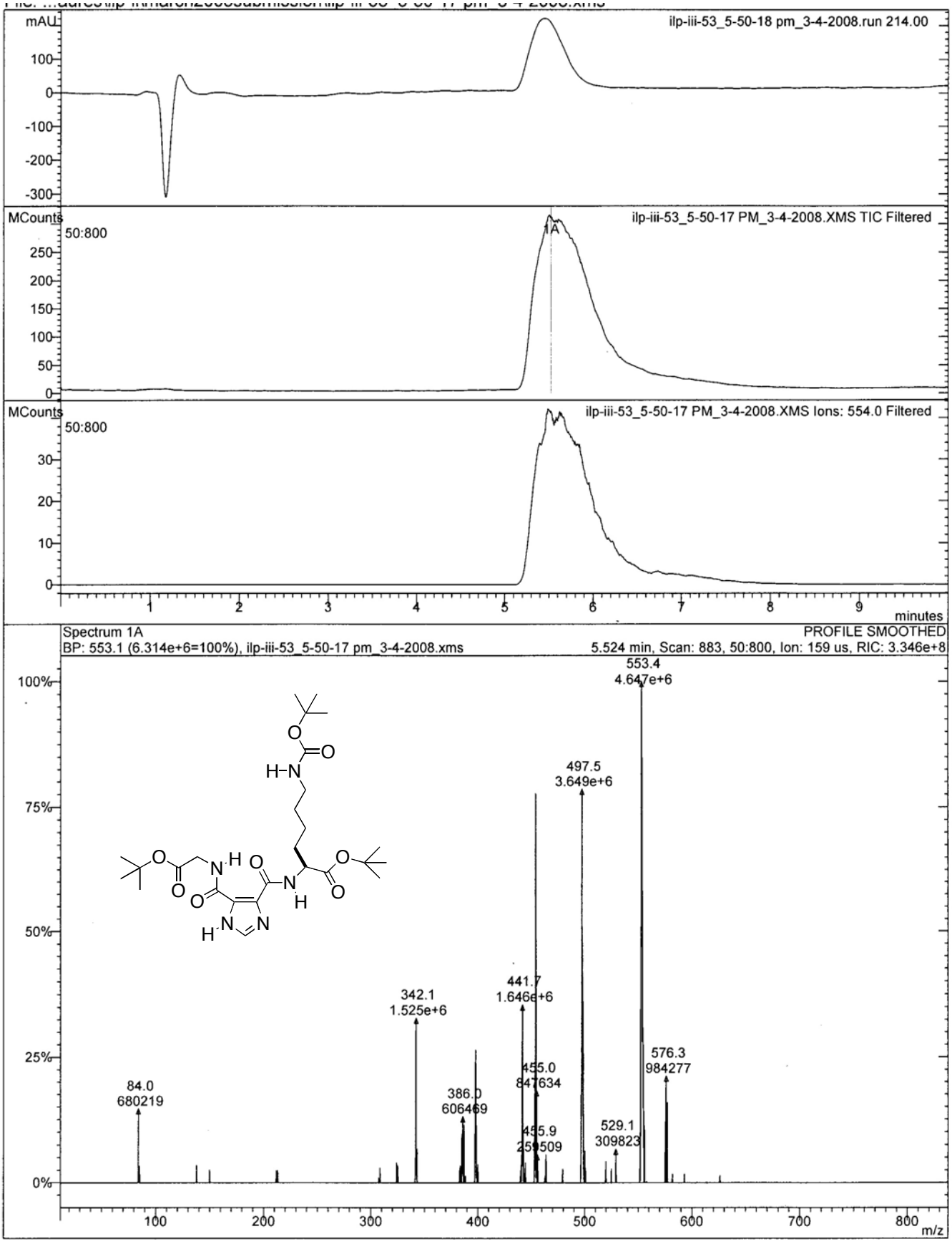

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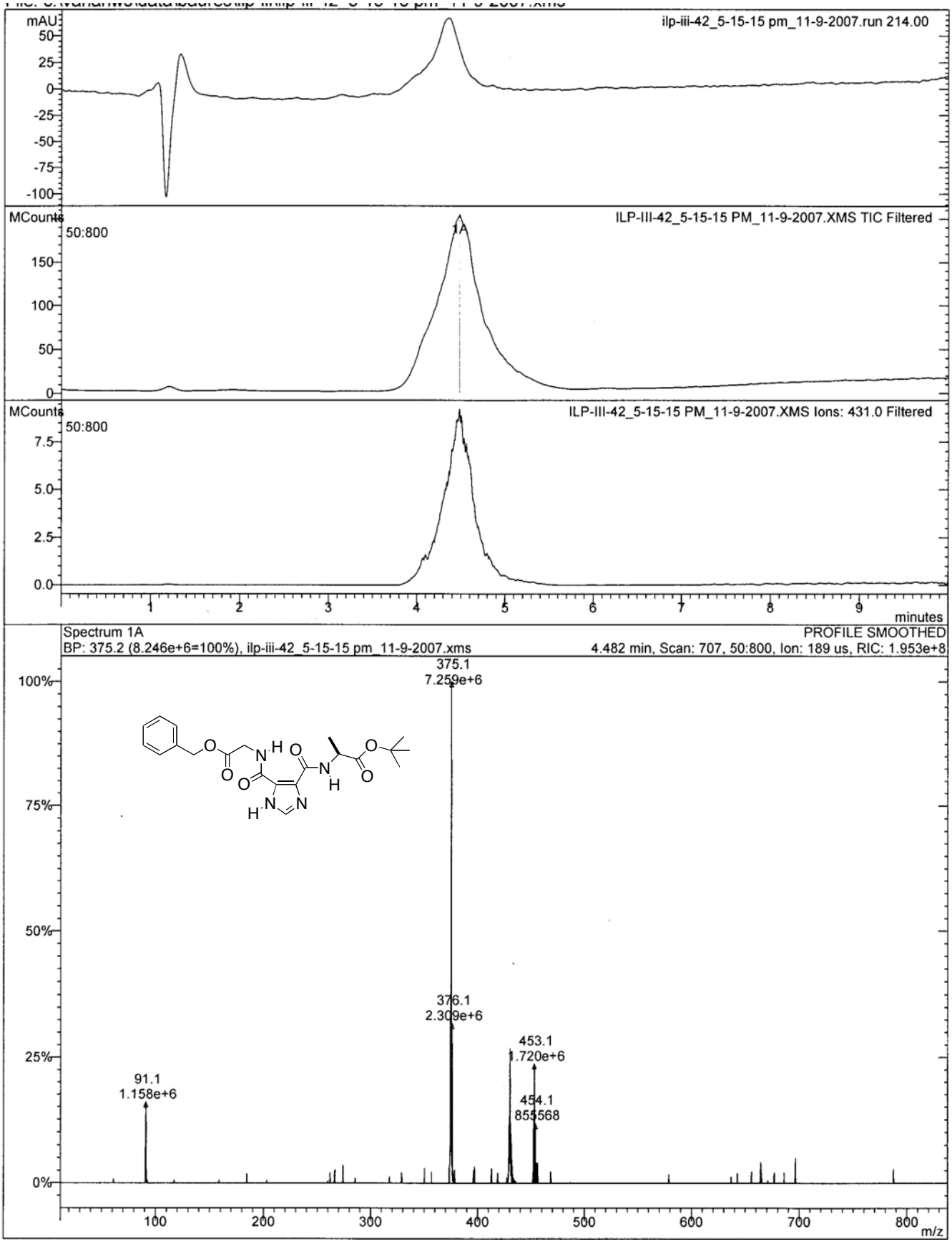

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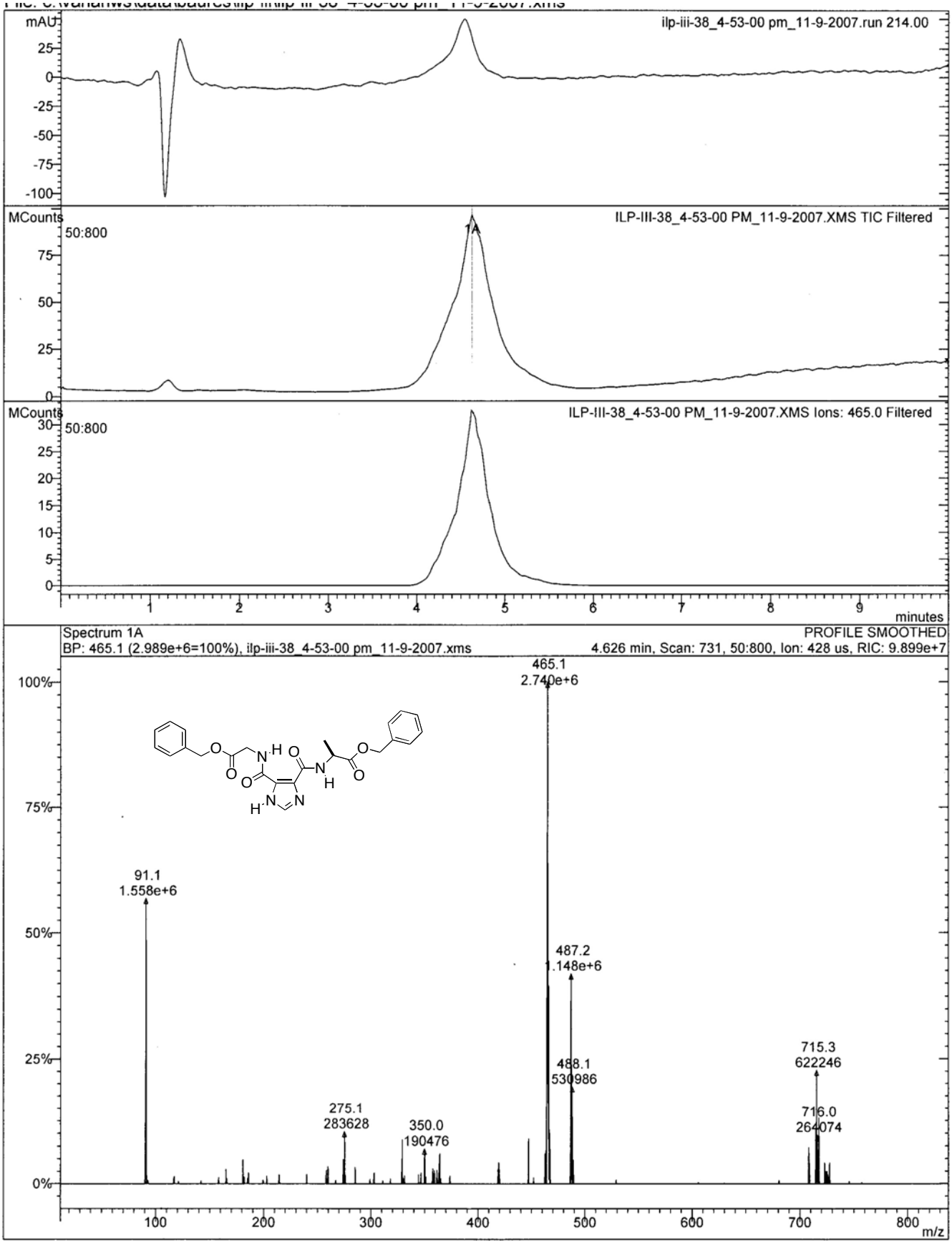

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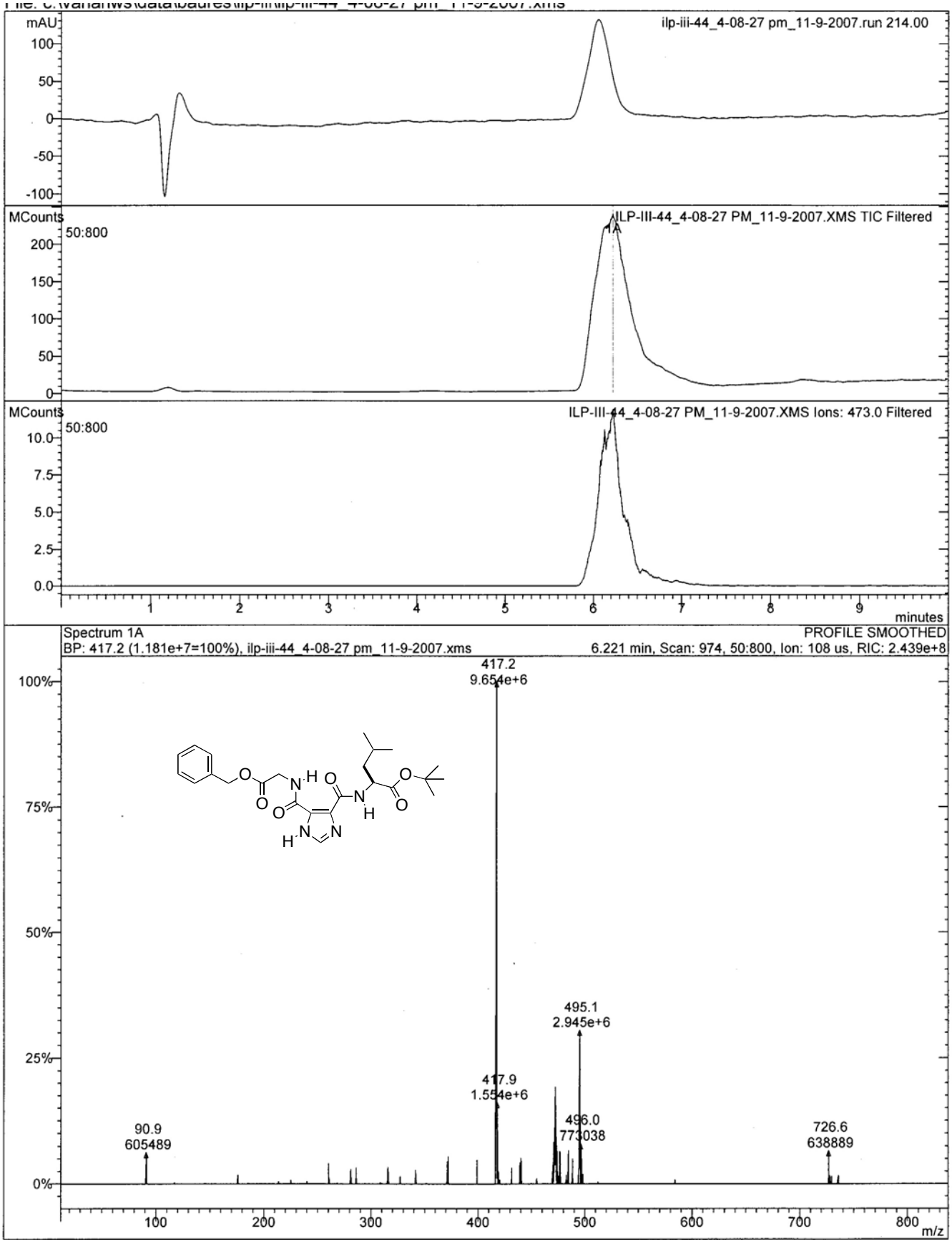

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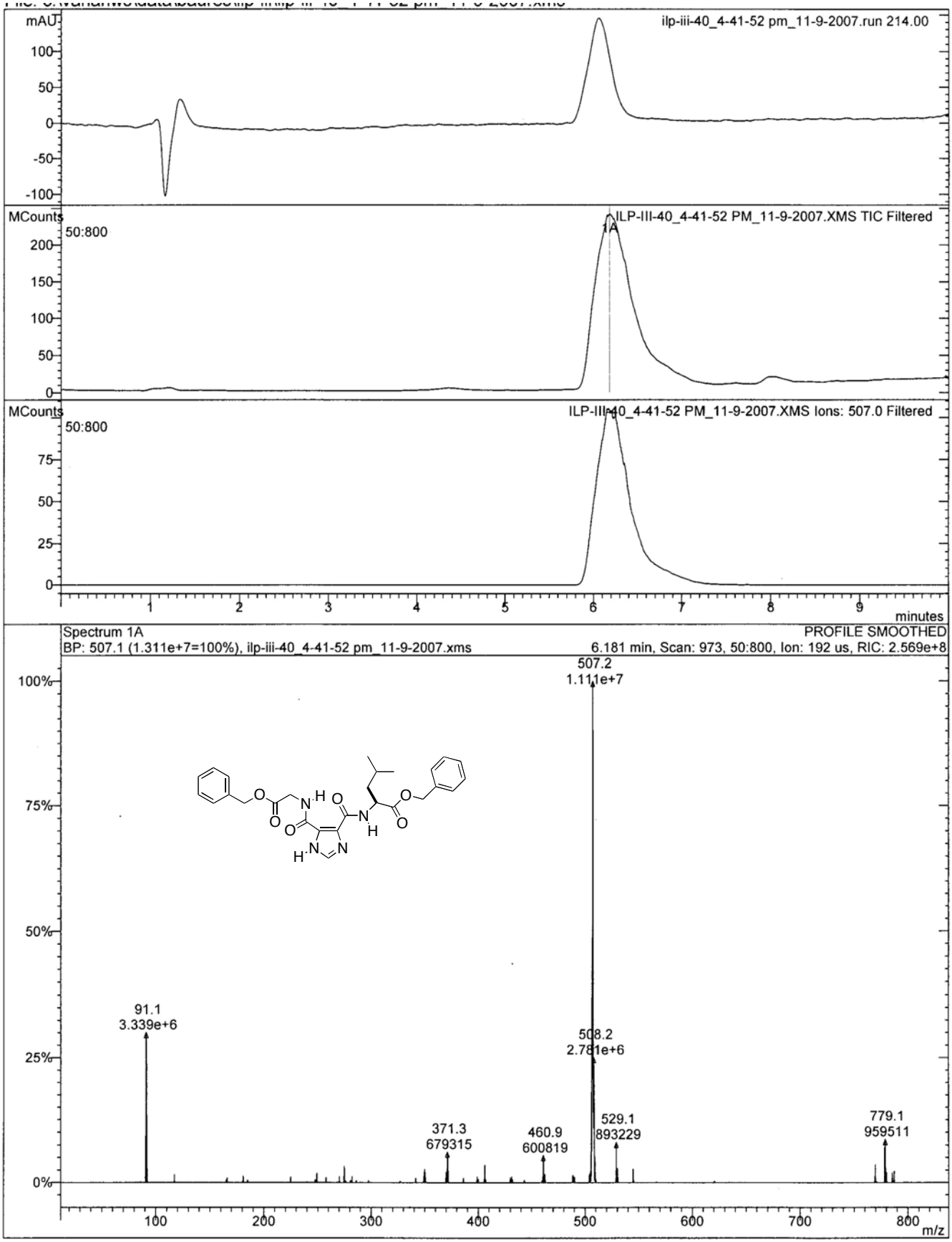

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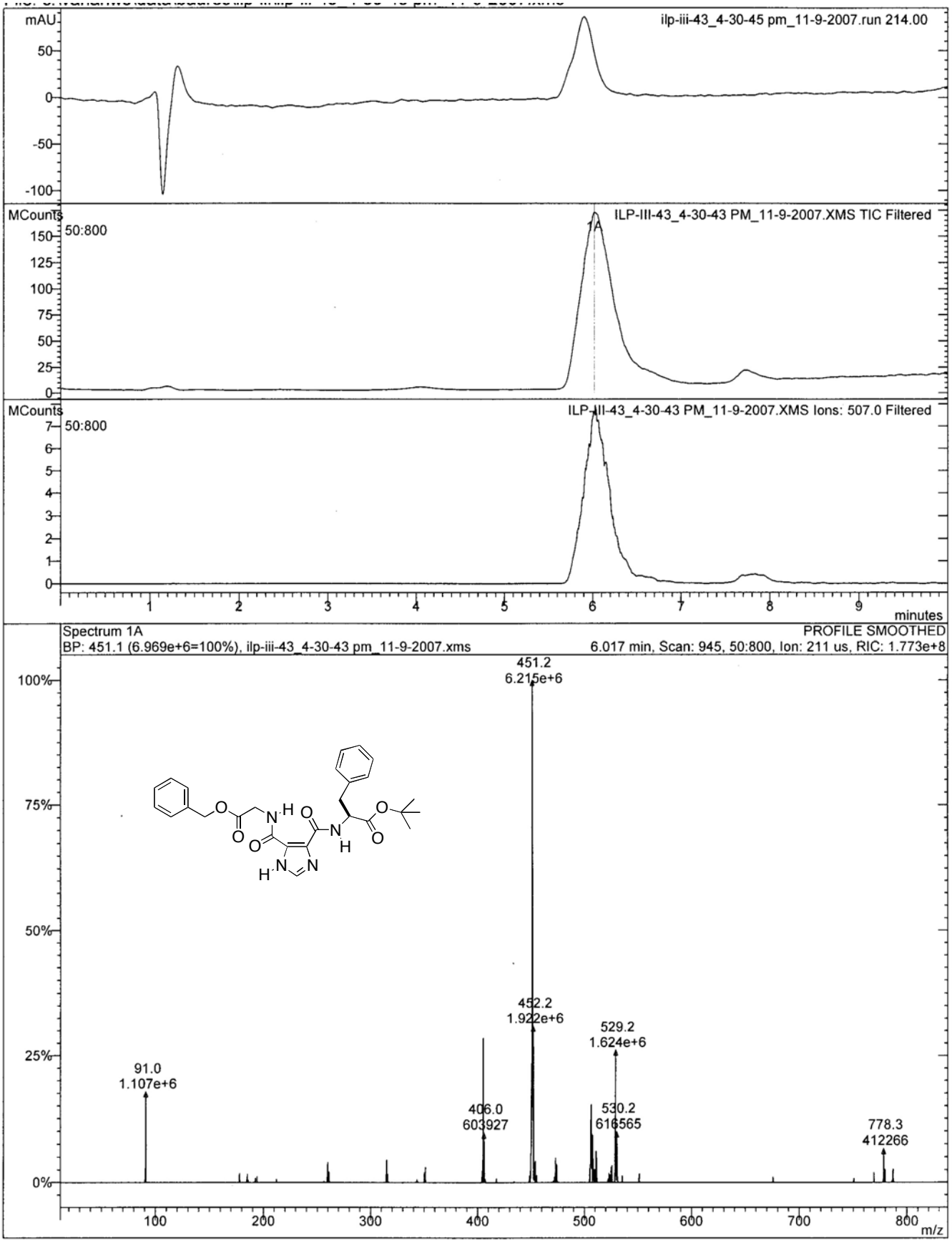

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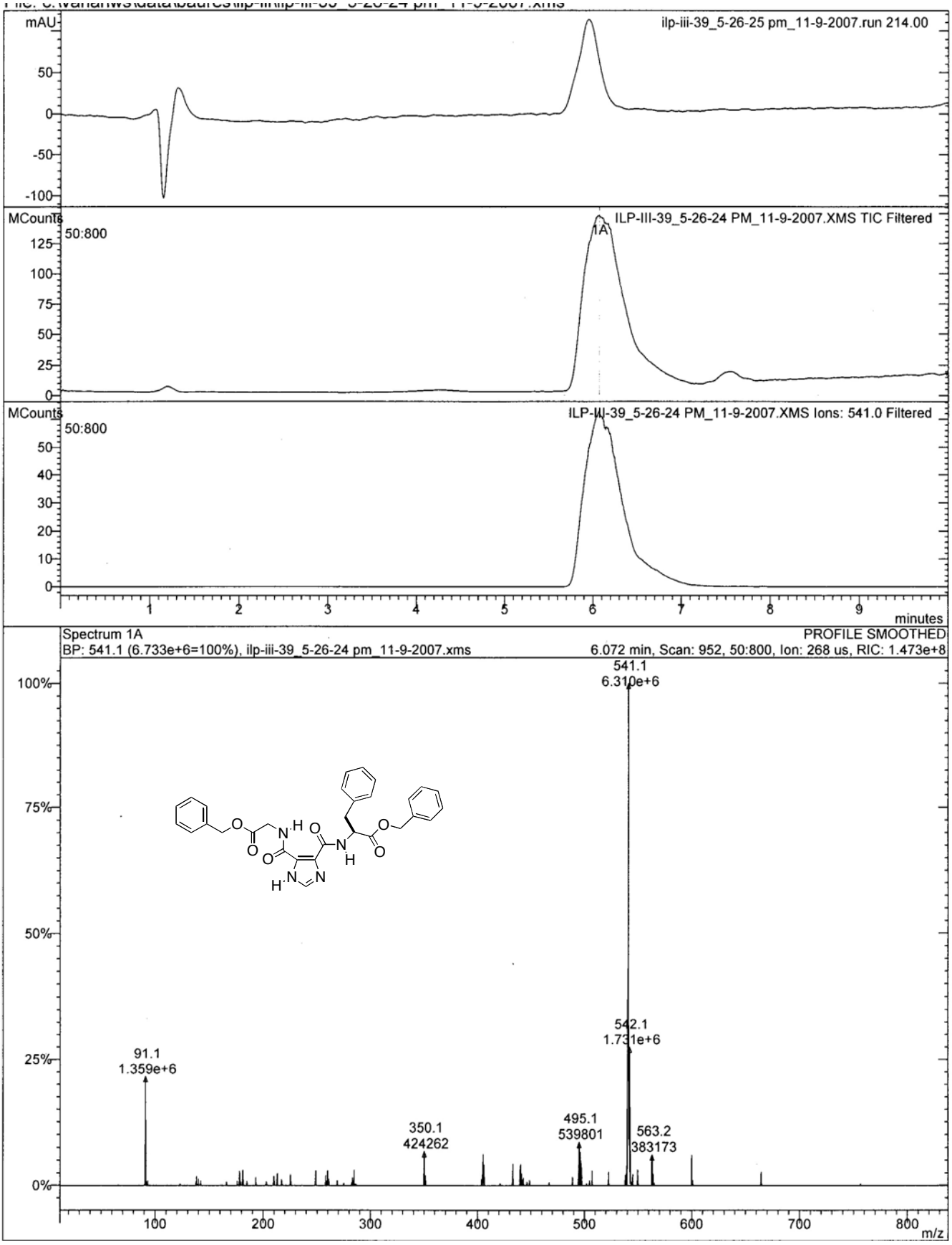

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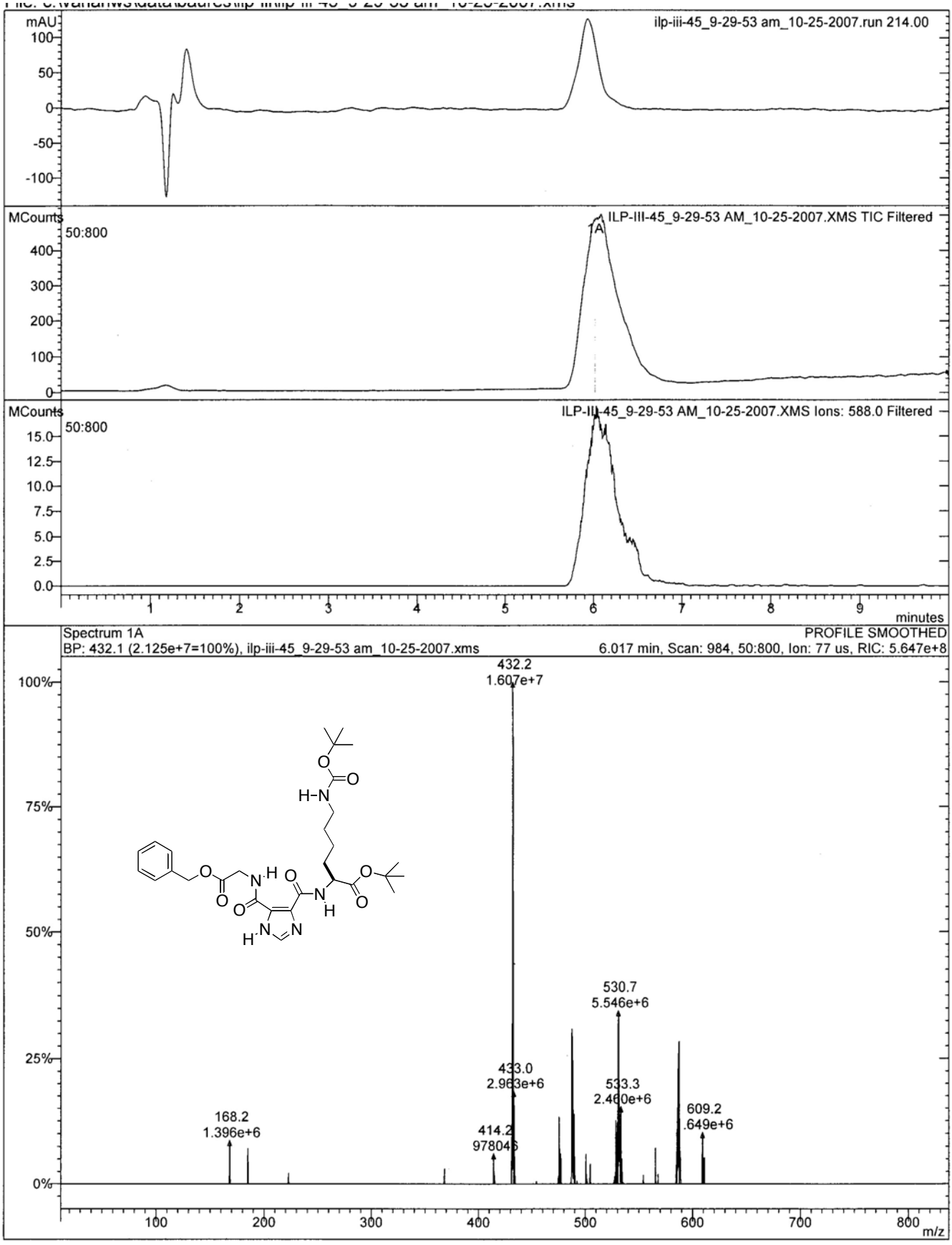

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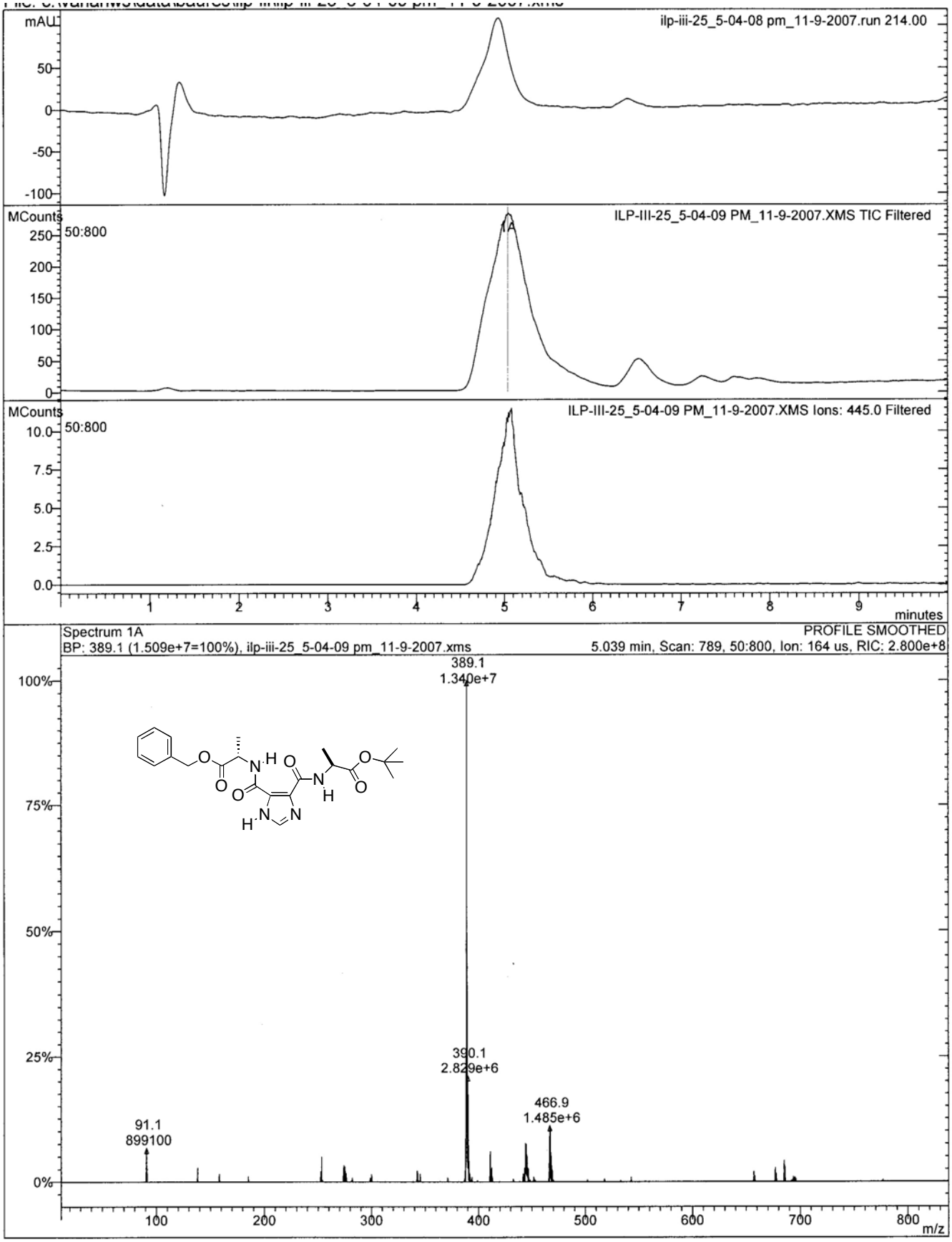

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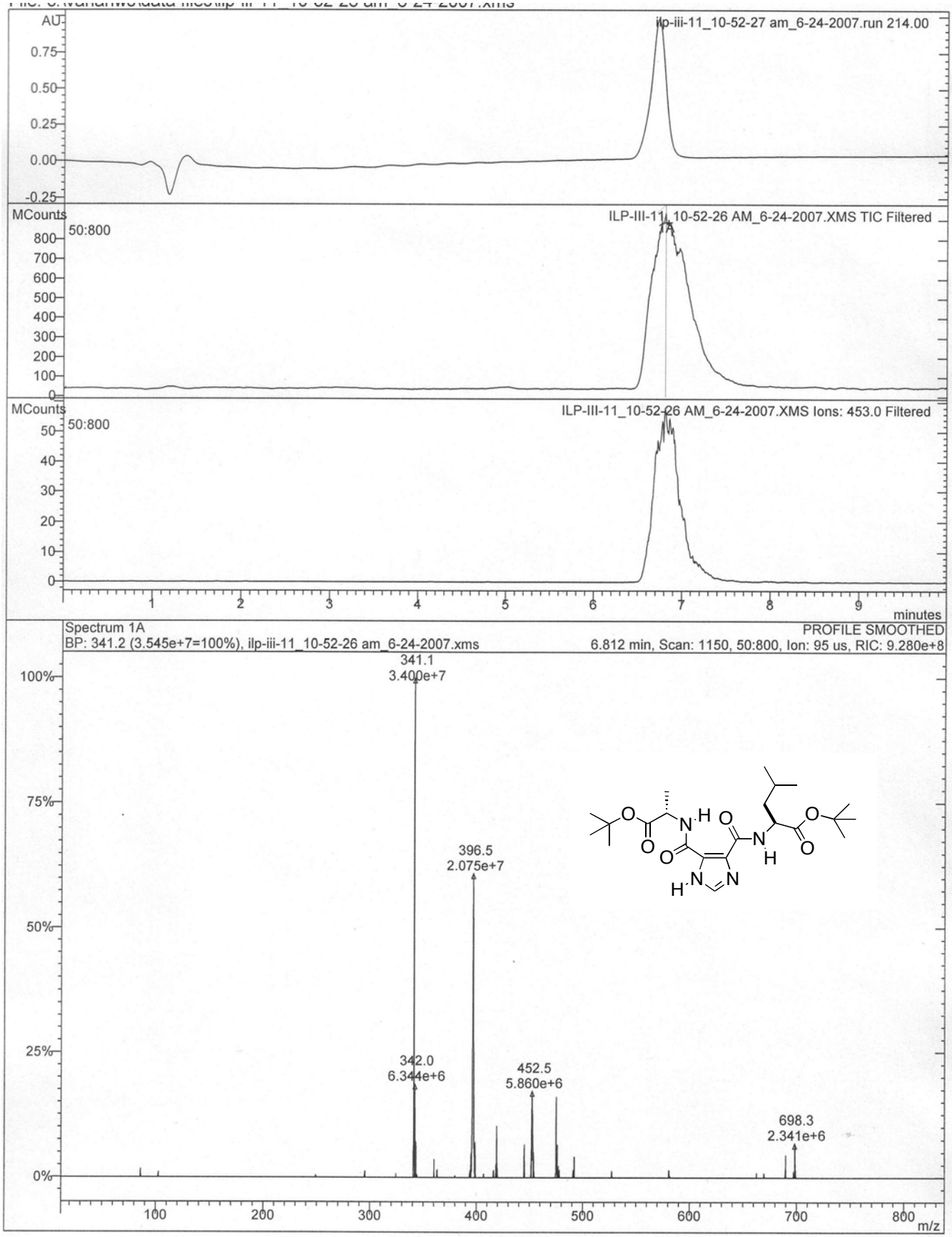

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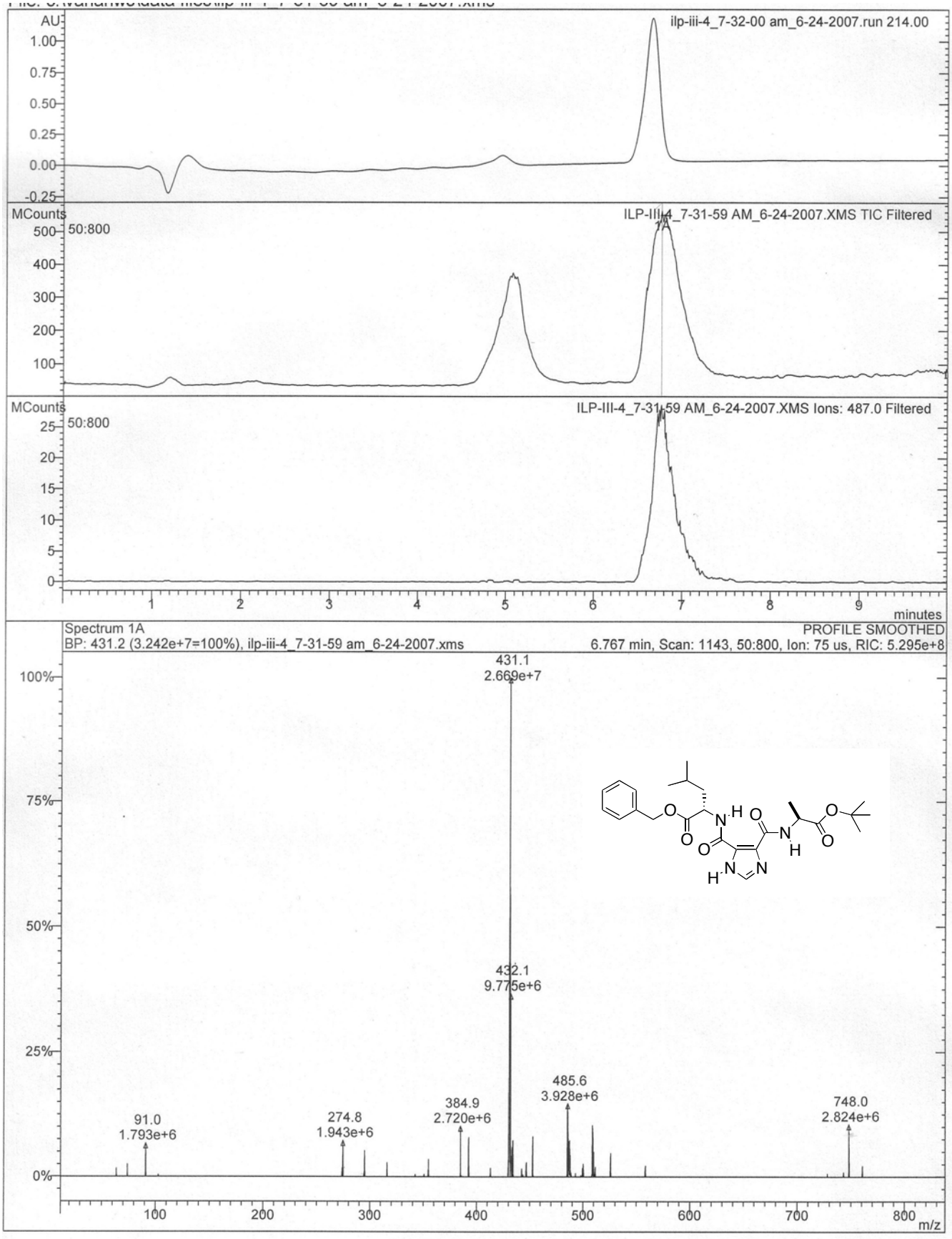

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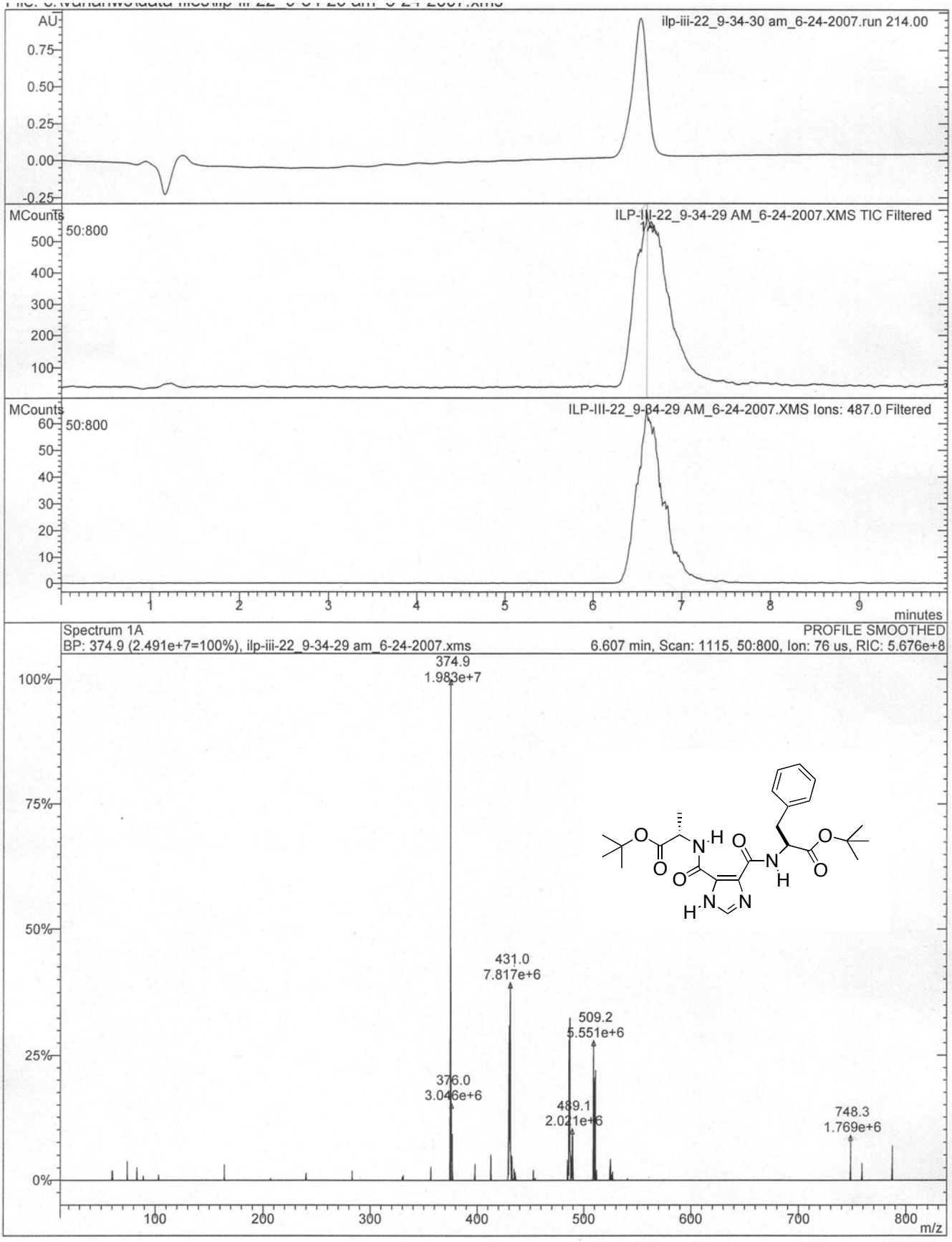

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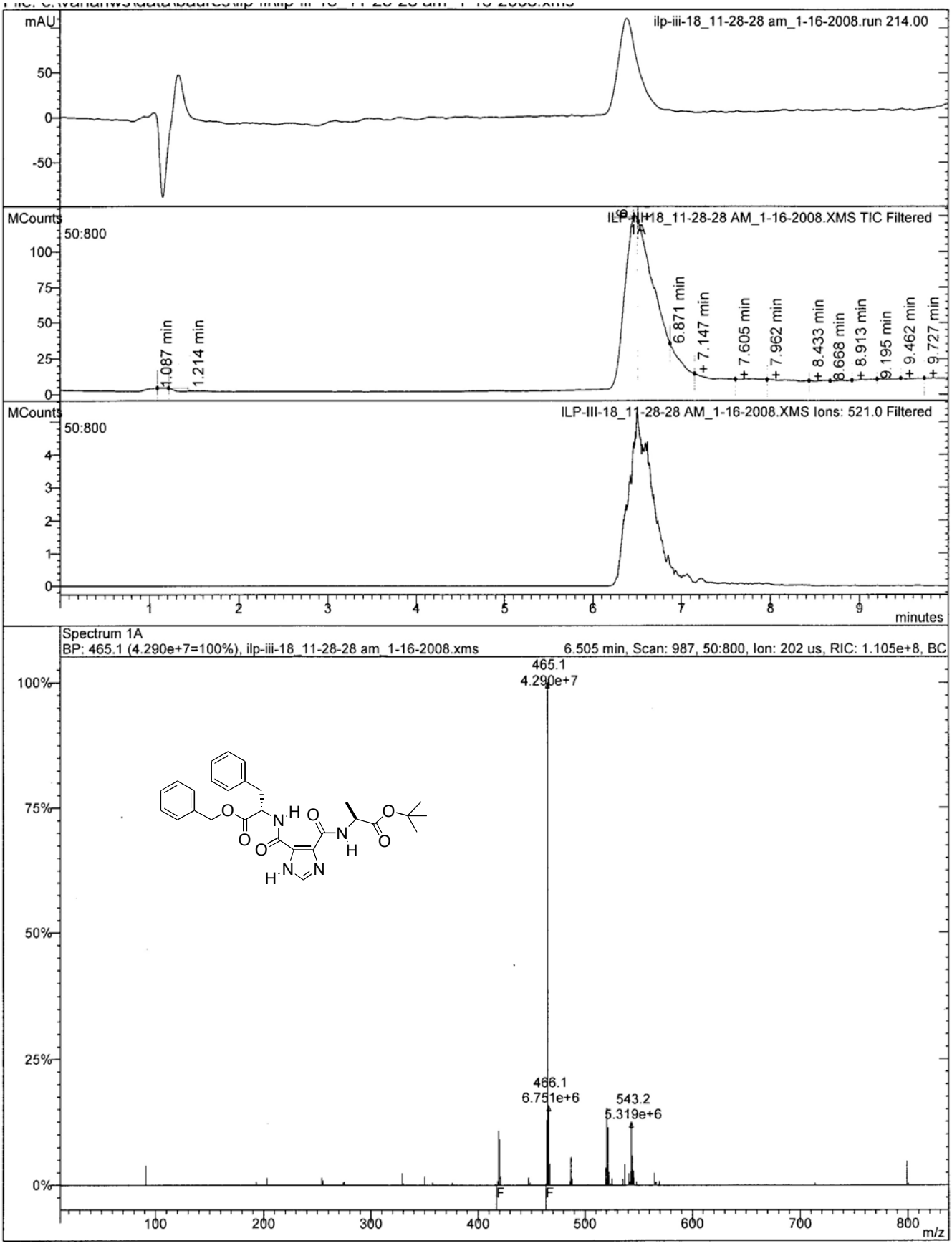

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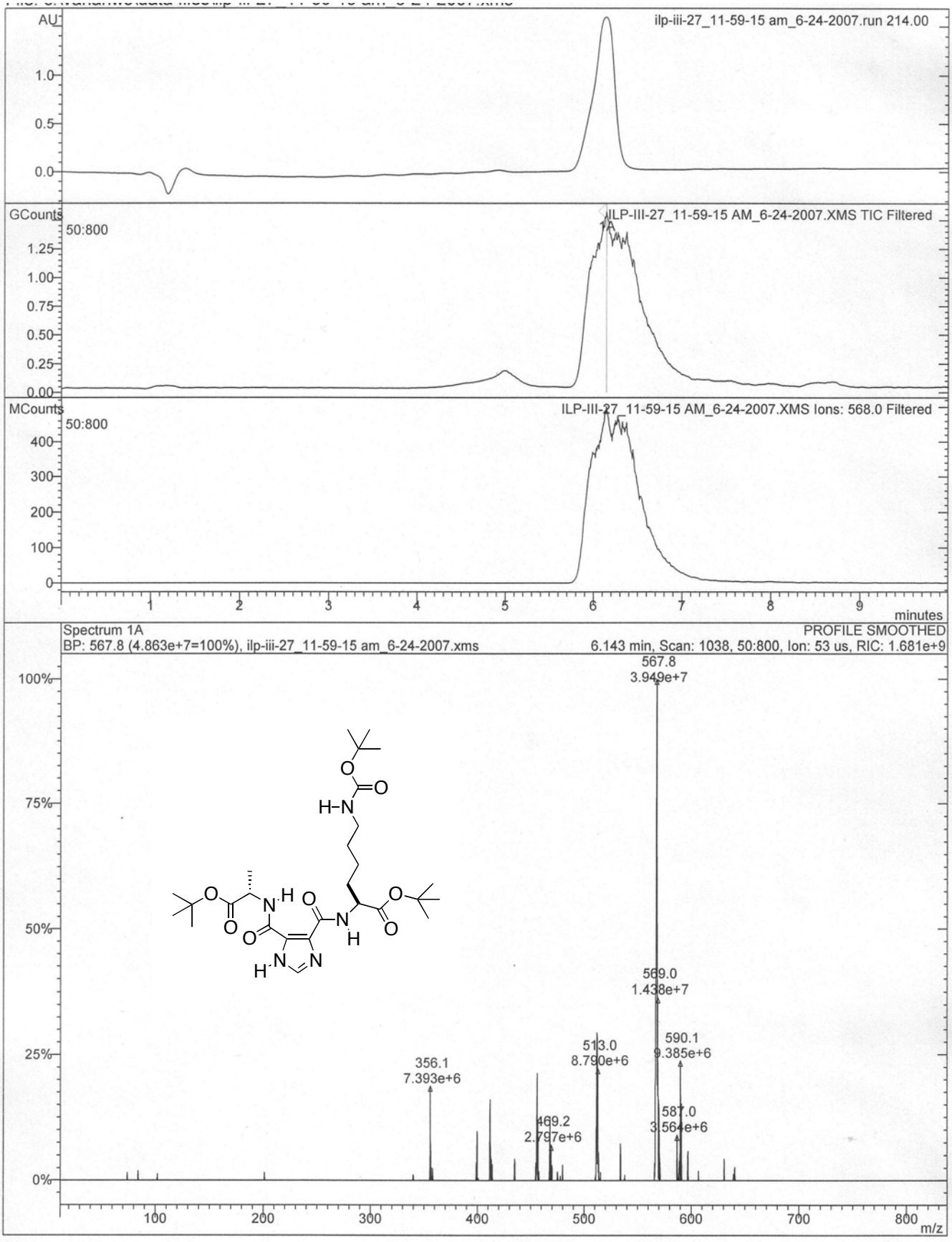

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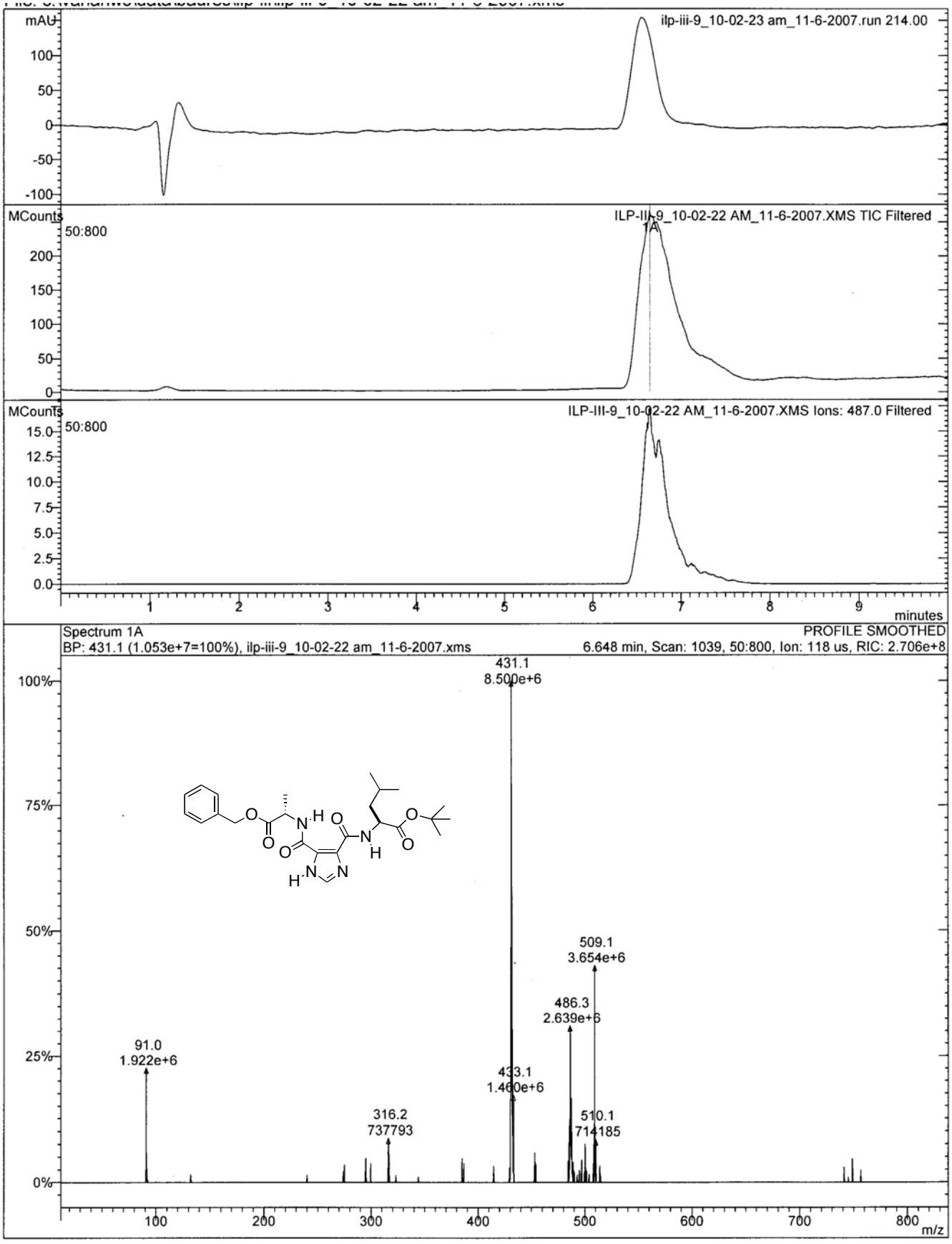

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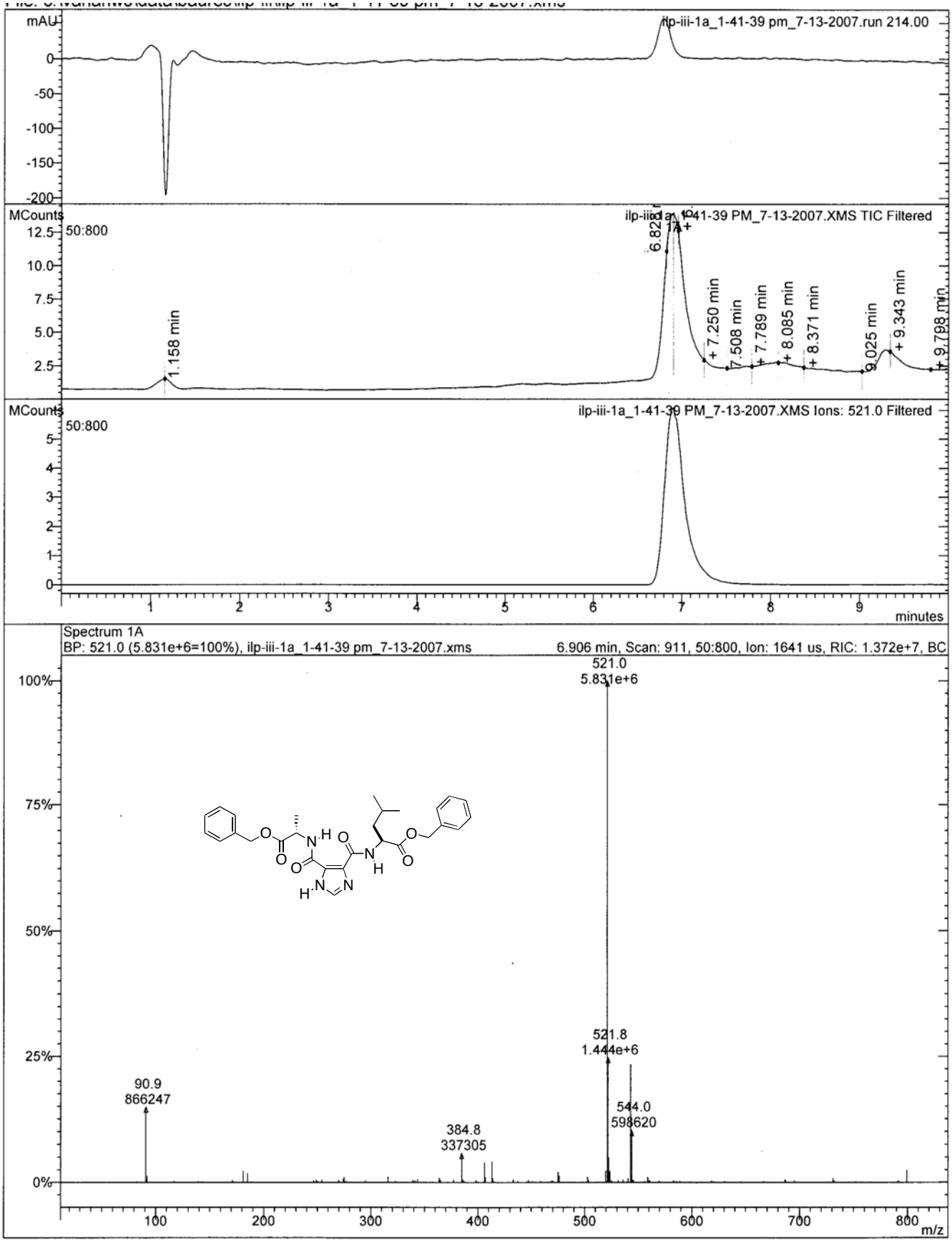

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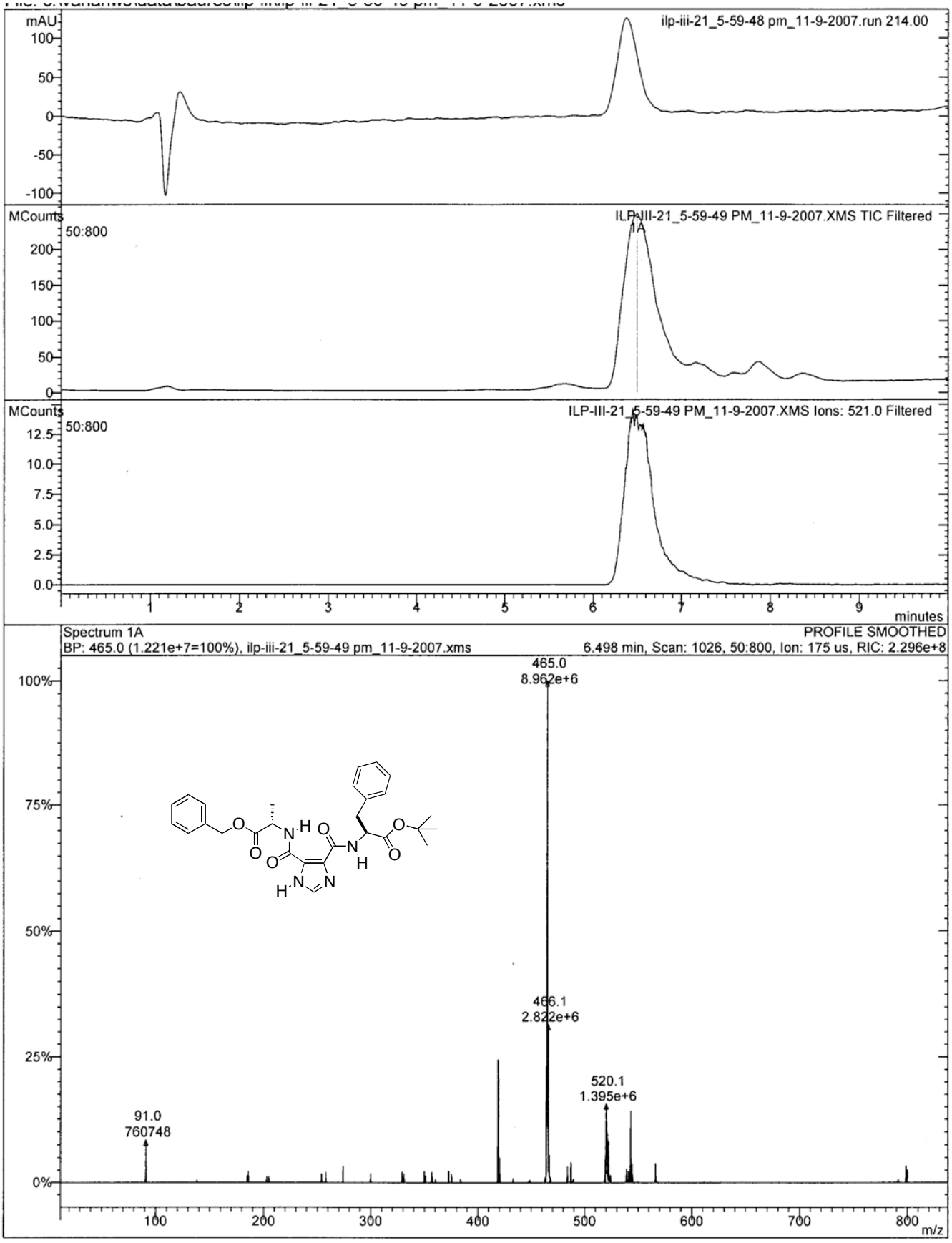

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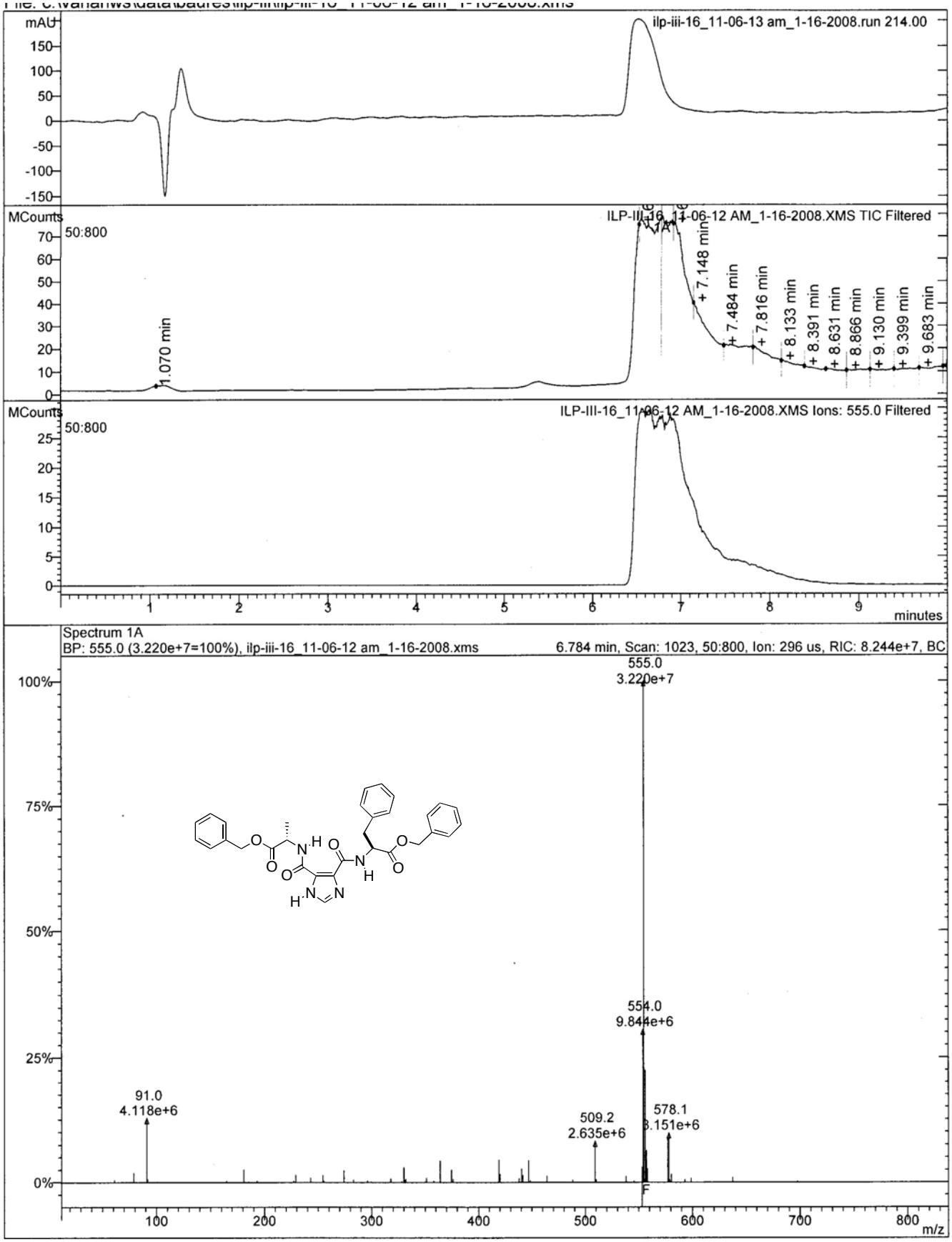

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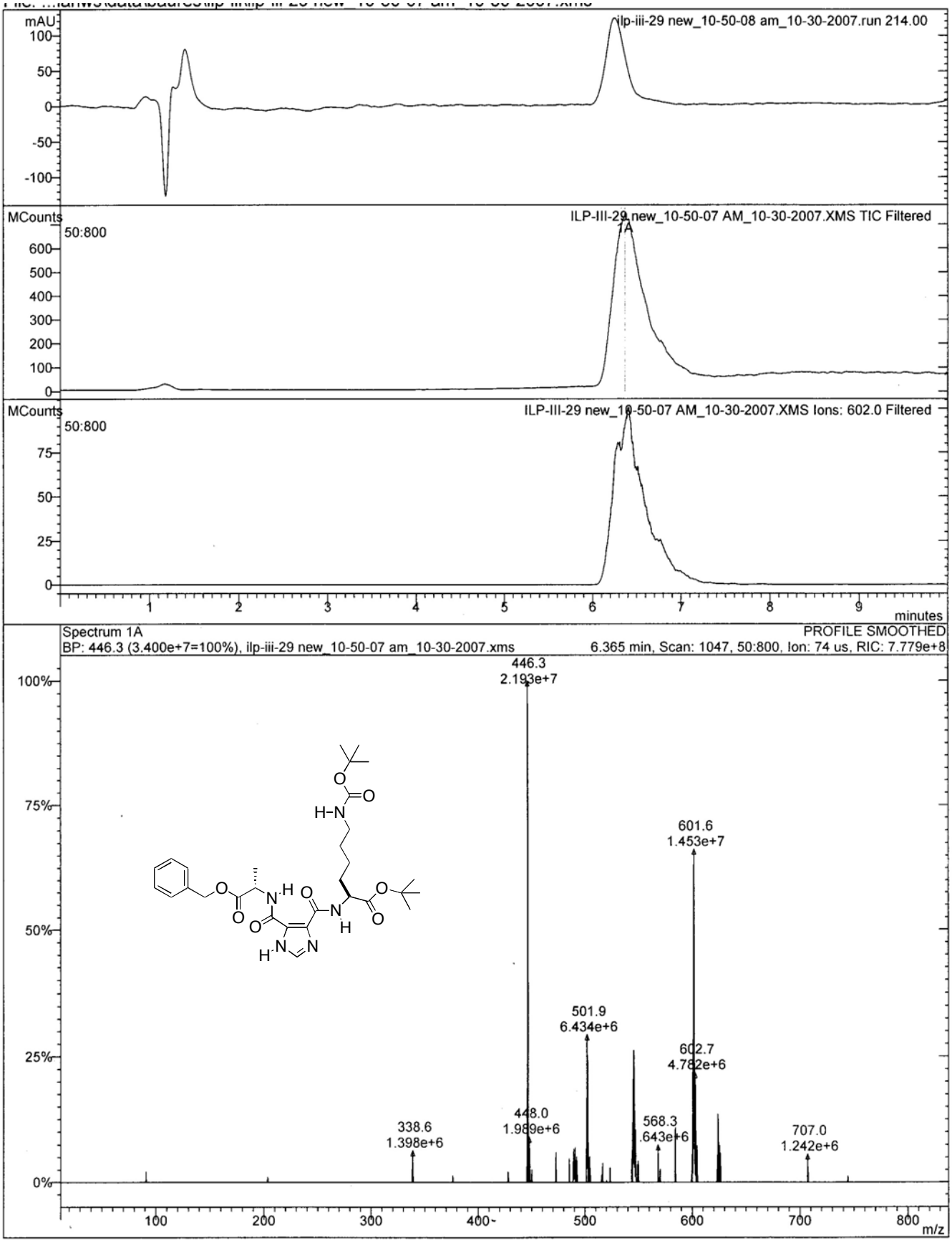

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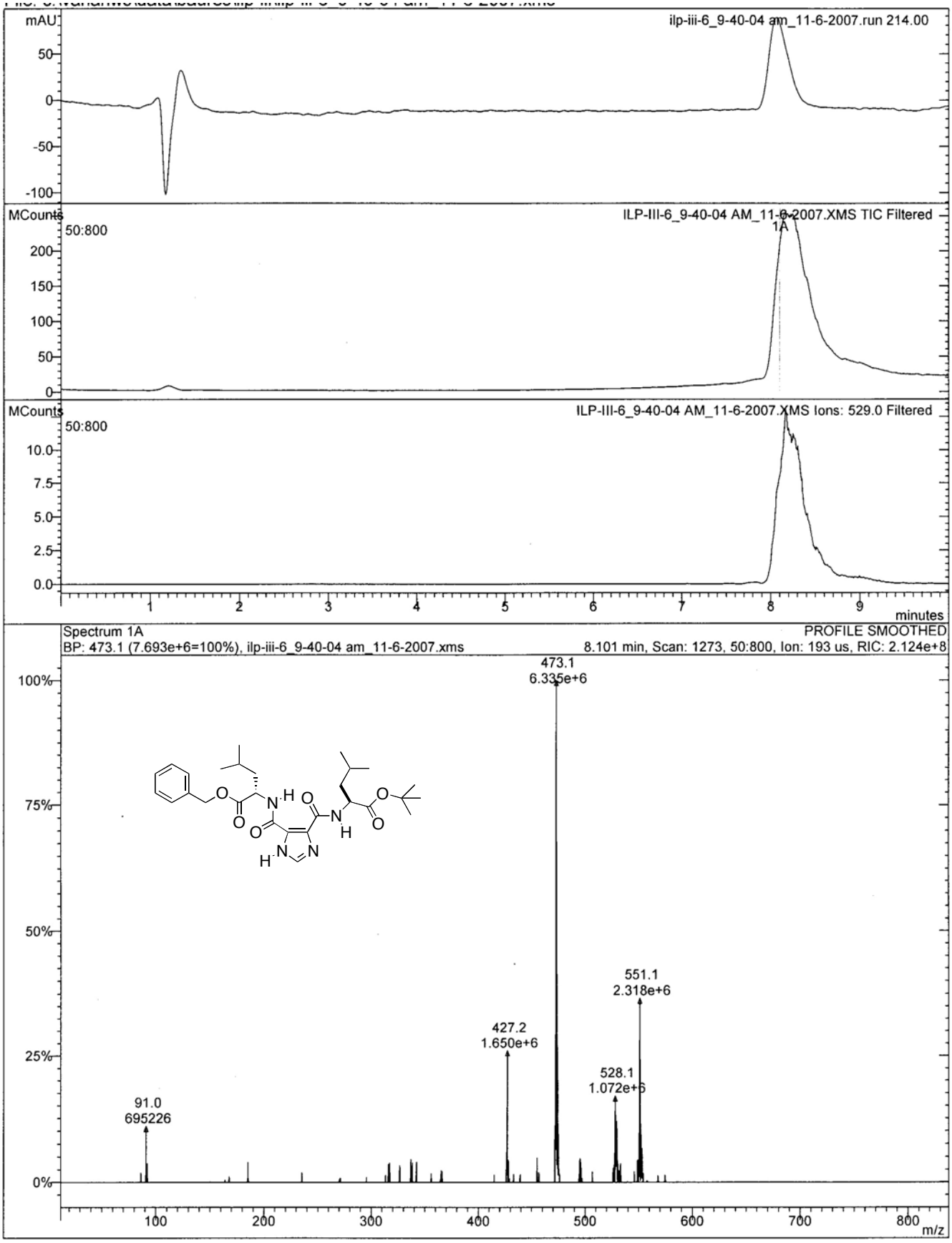

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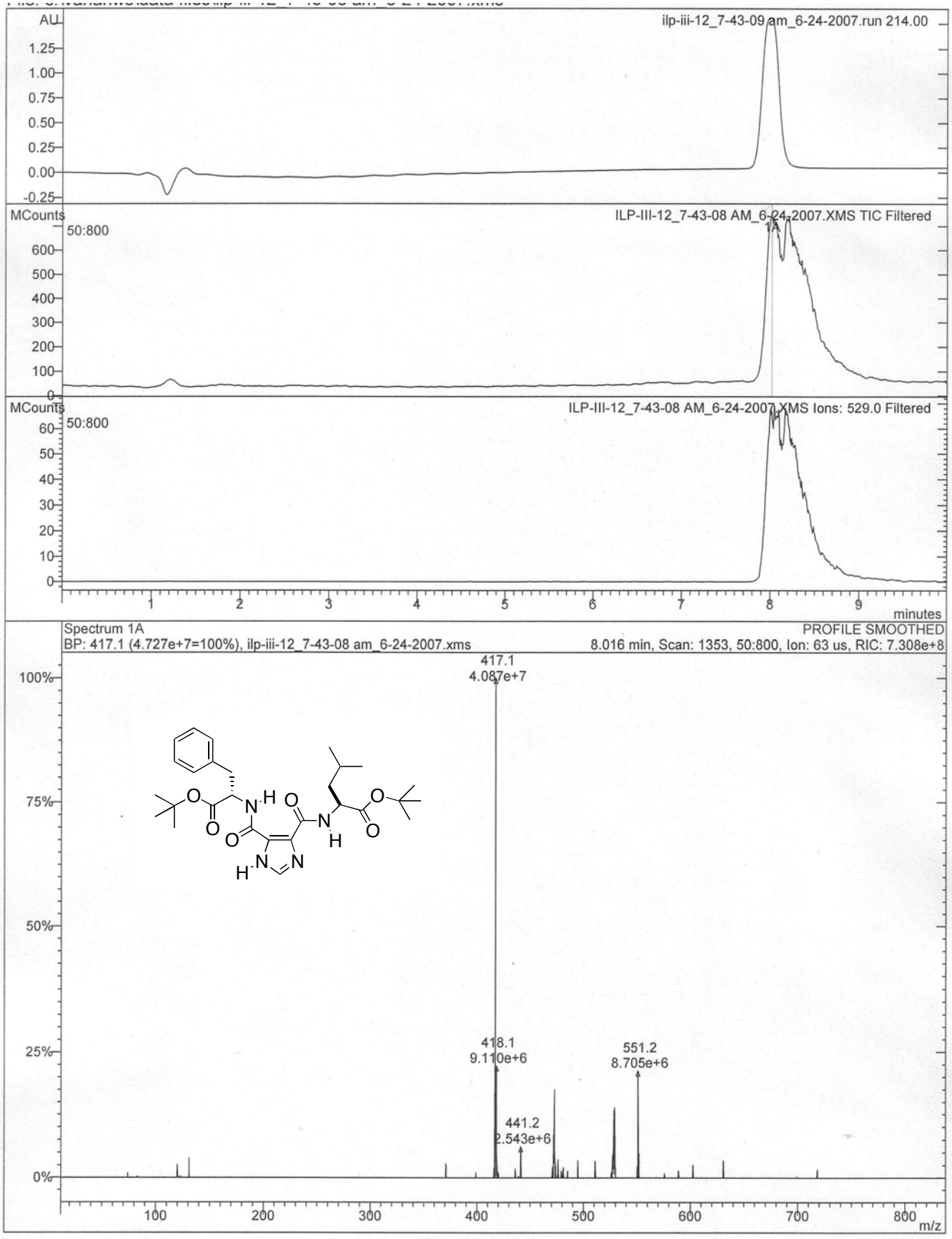

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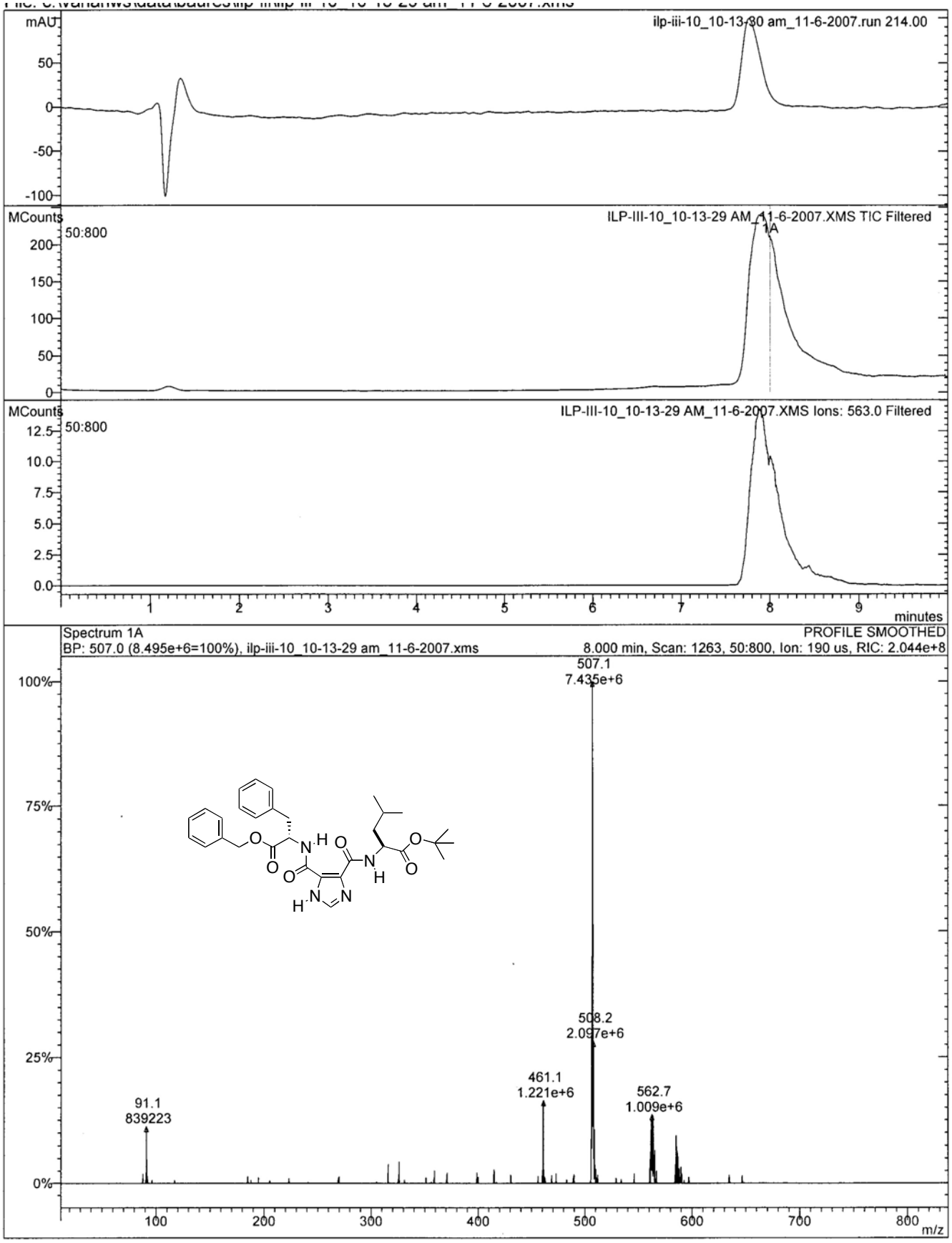

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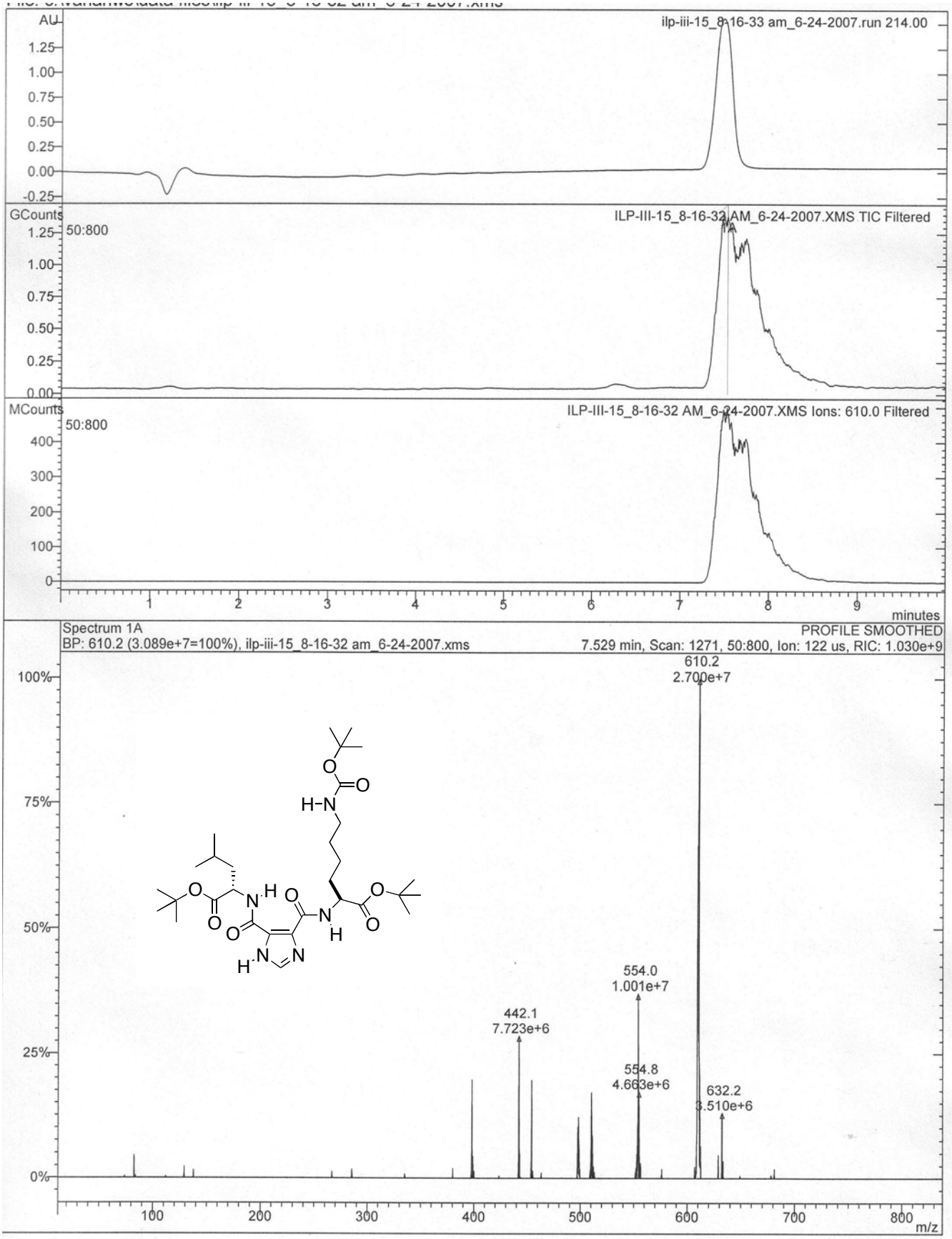

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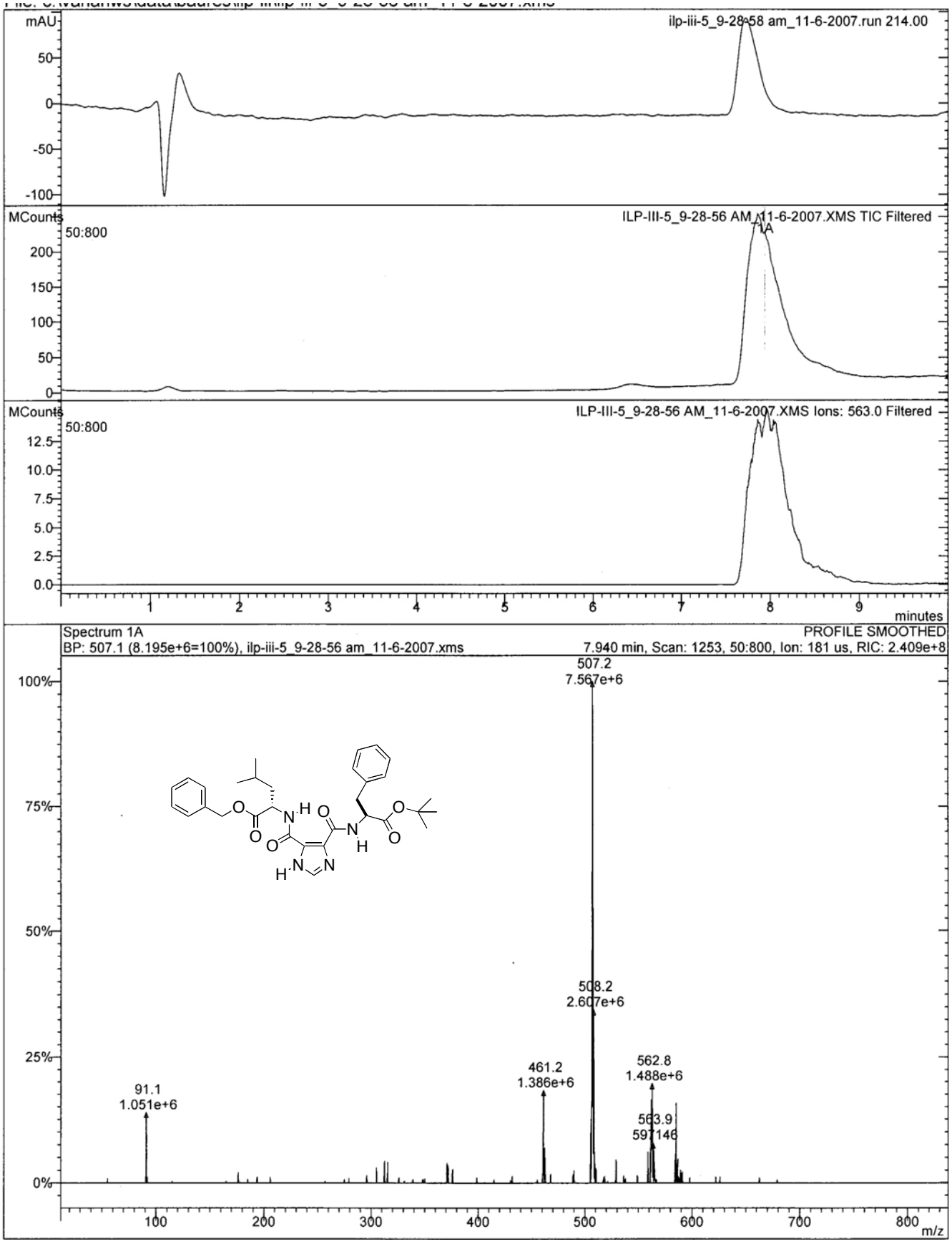

Figure S40. LC/MS data for **4{**40}.

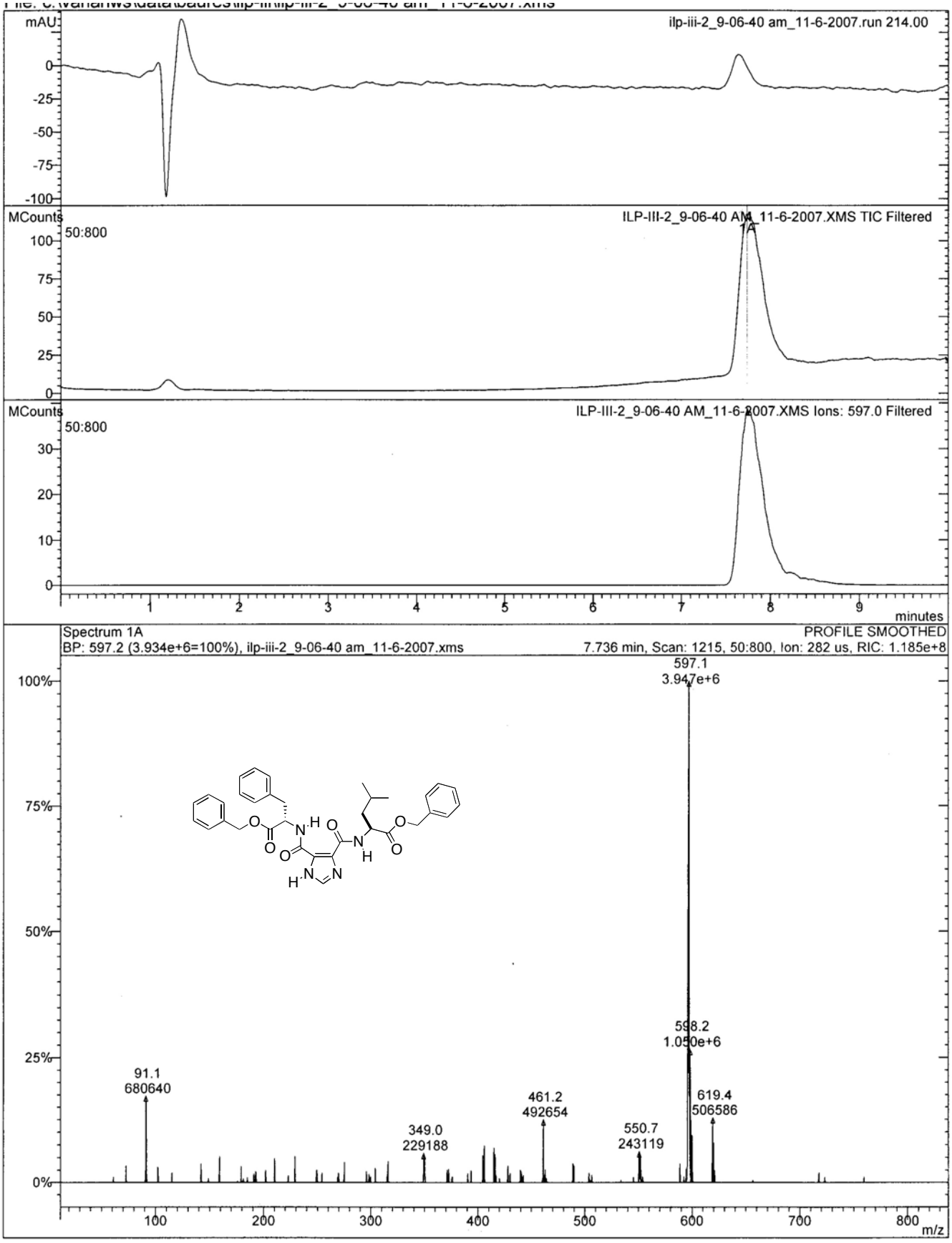

Figure S41. LC/MS data for **4{**41}.

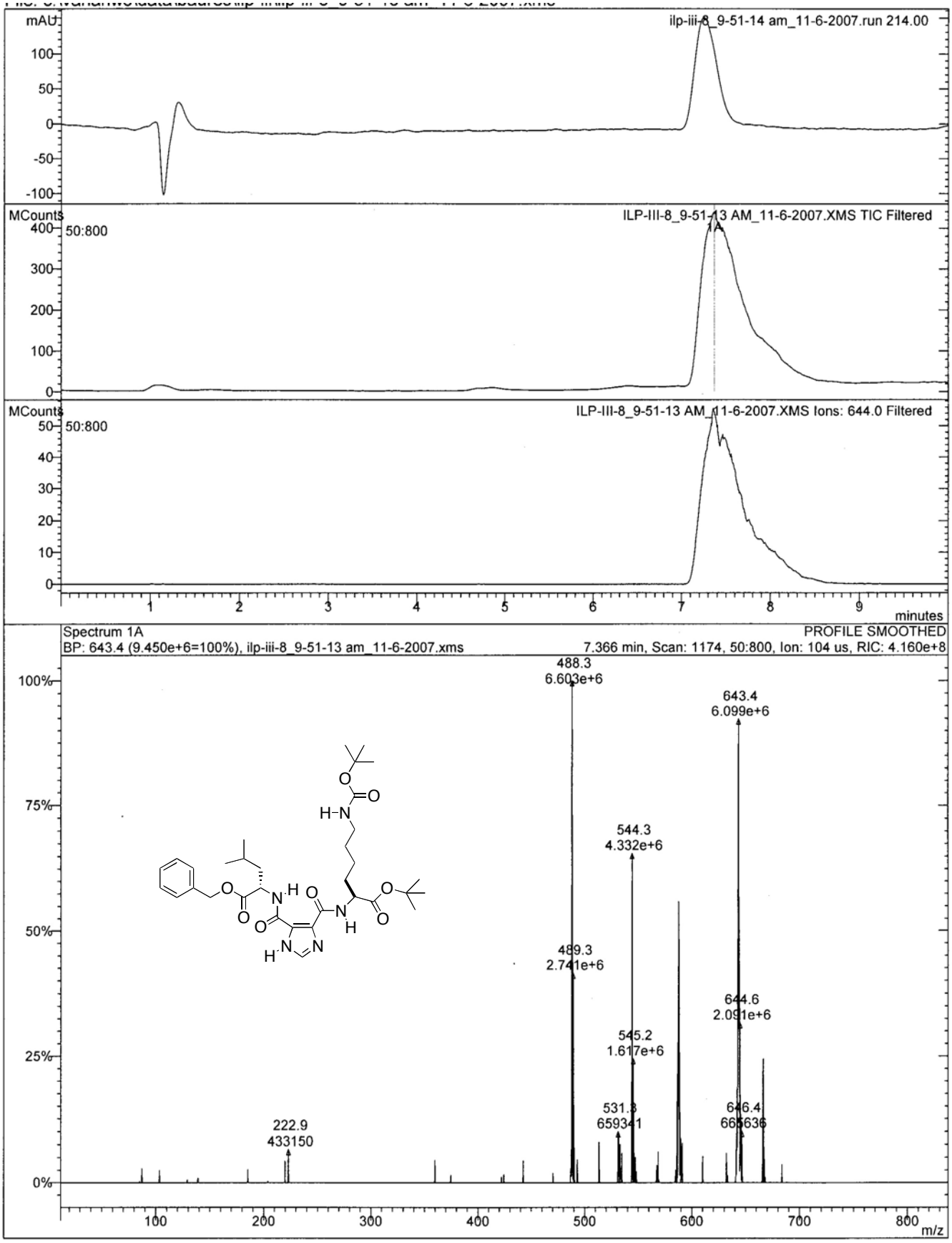

Figure S42. LC/MS data for **4{**42}.

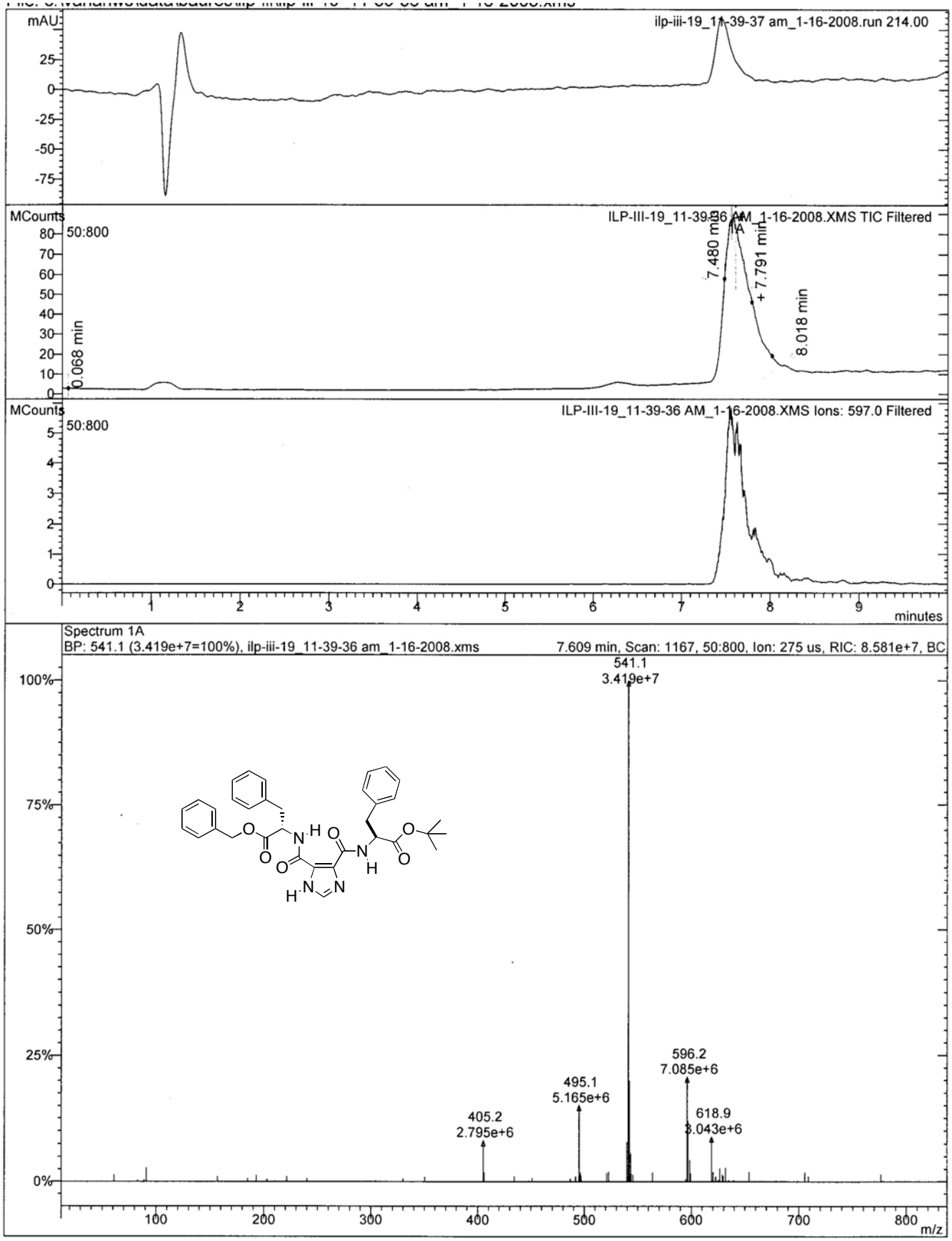

Figure S43. LC/MS data for **4{**43}.

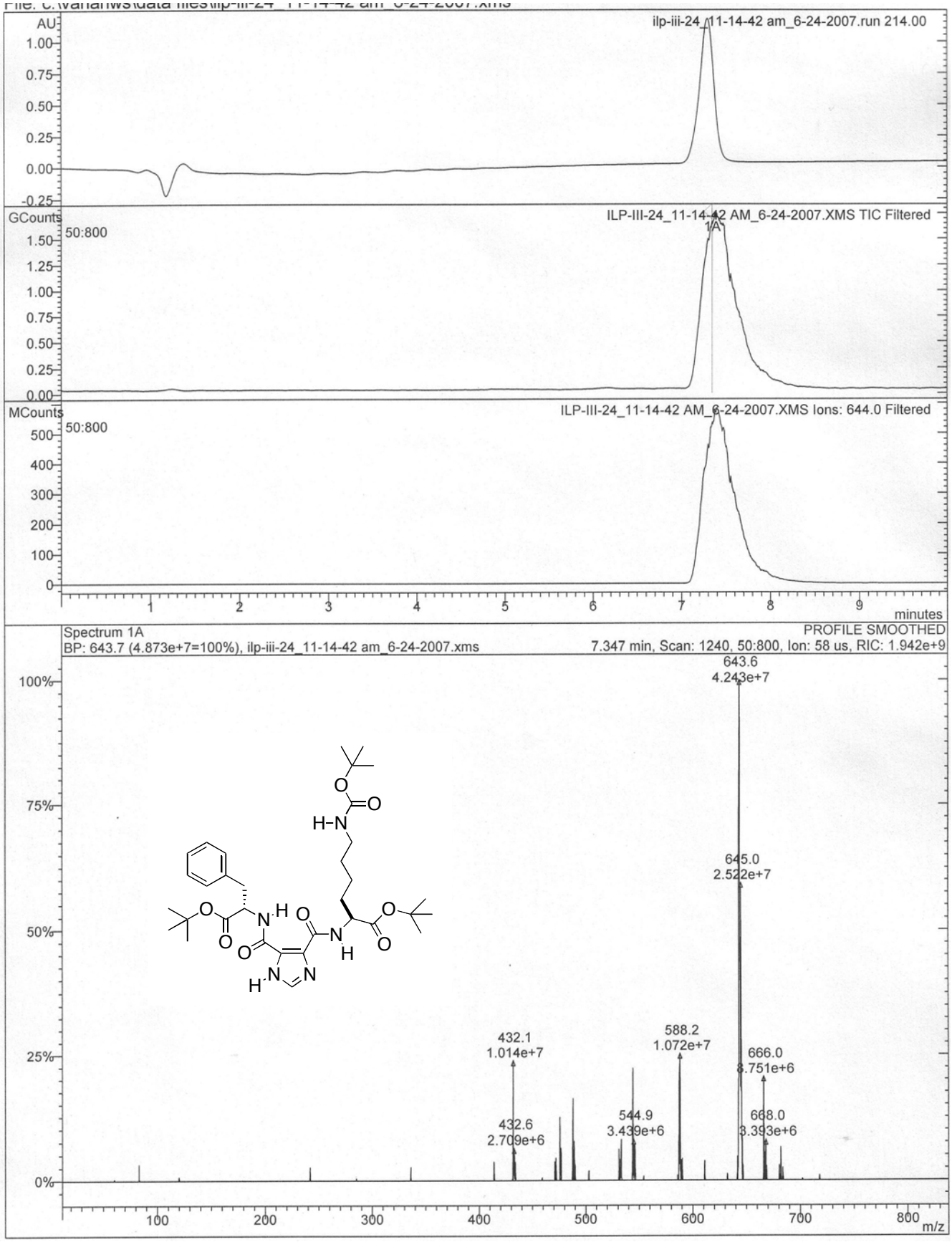

Figure S44. LC/MS data for **4{**44}.

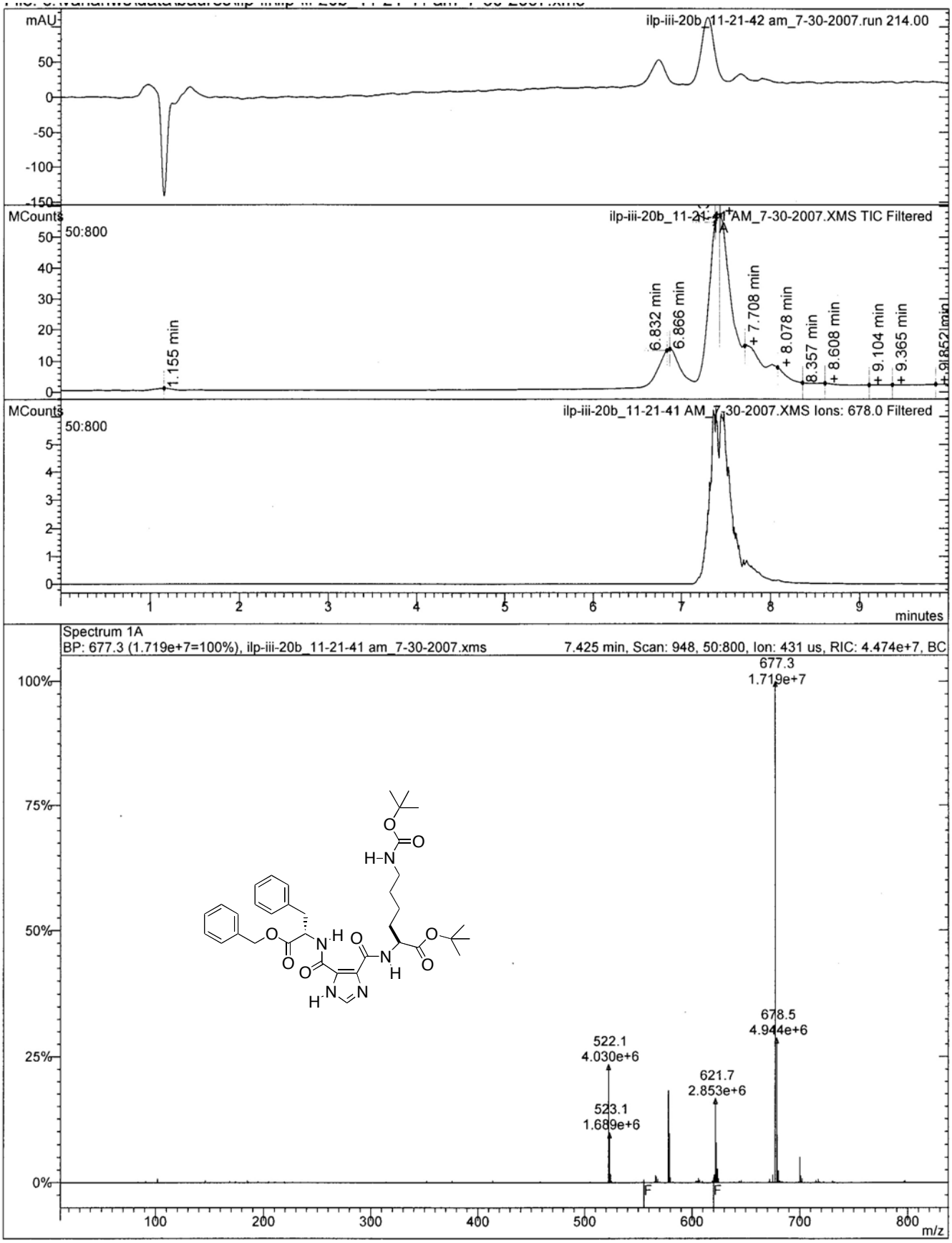

Figure S45. LC/MS data for **4{**45}.

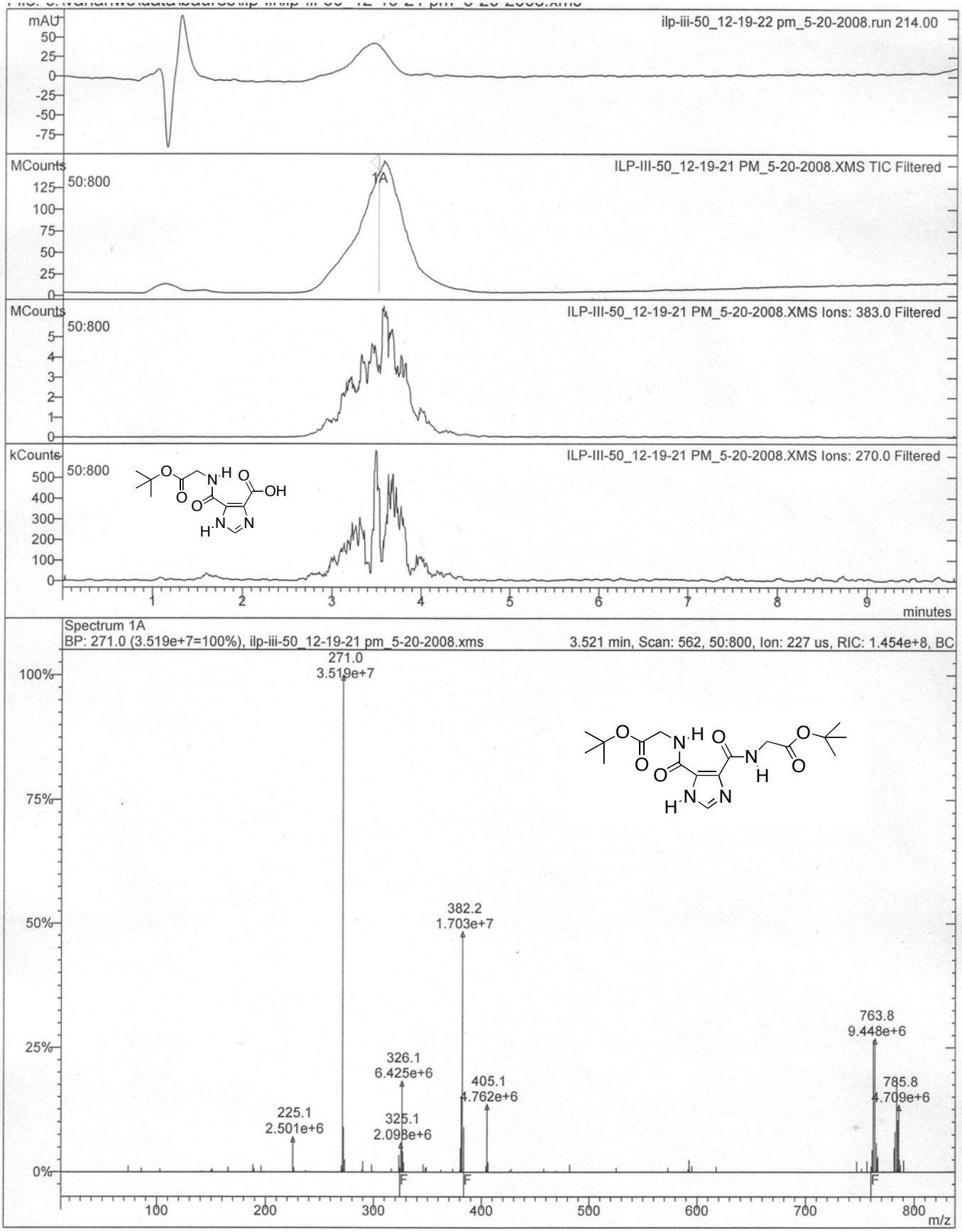

Figure S46. LC/MS data for the crude reaction to yield **4**{1}.

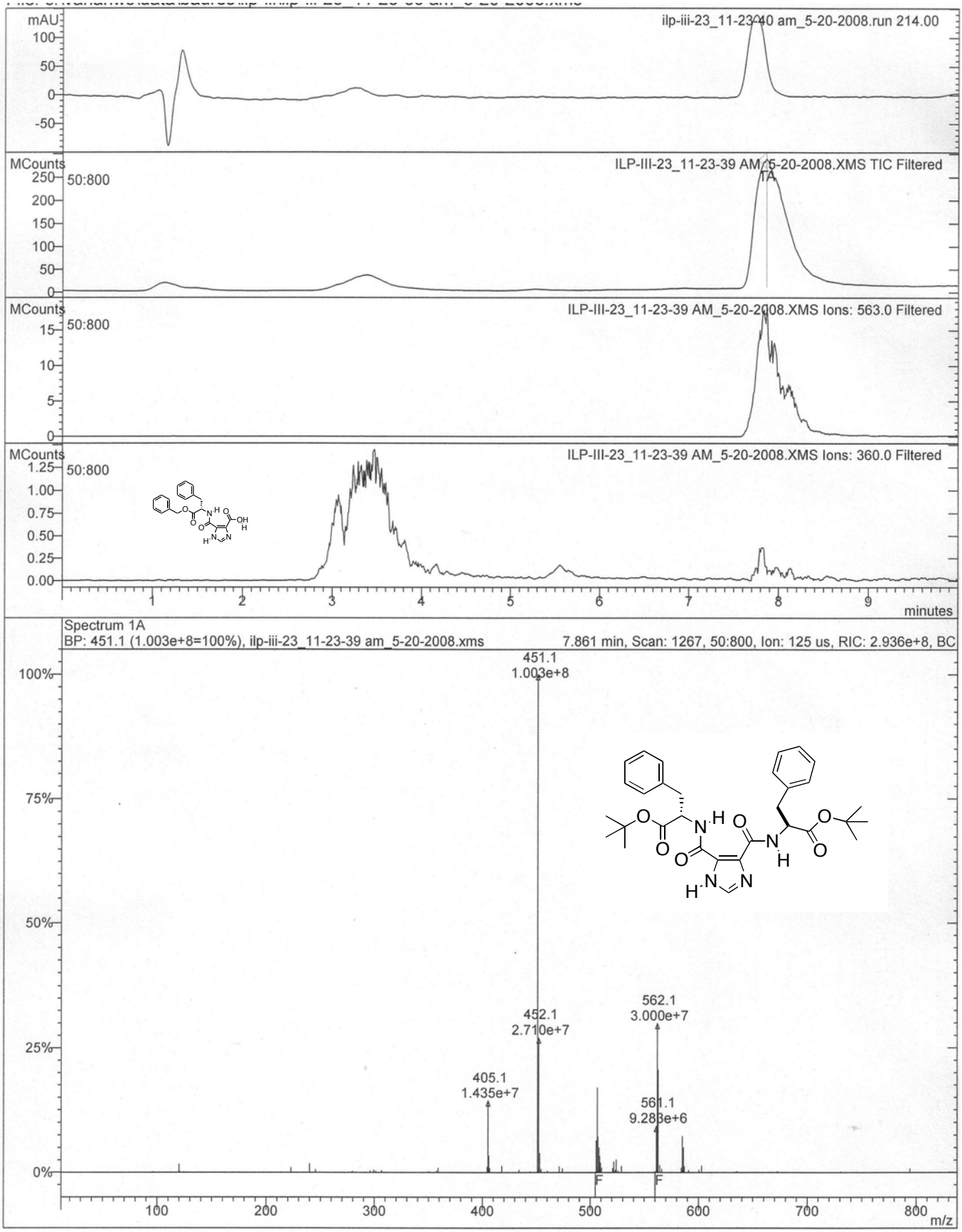

Figure S47. LC/MS data for the crude reaction to yield **4**{7}.

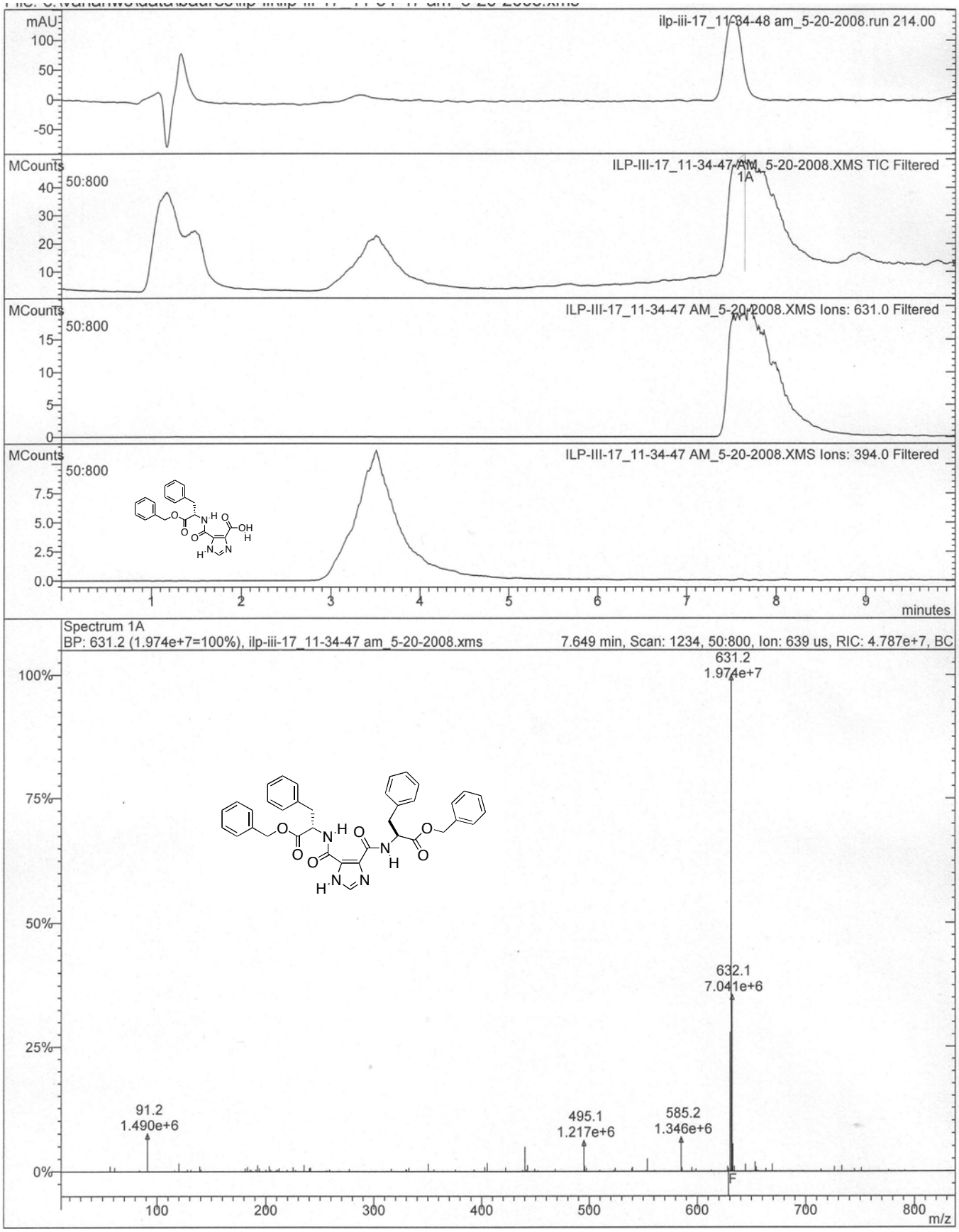

Figure S48. LC/MS data for the crude reaction to yield **4**{8}.

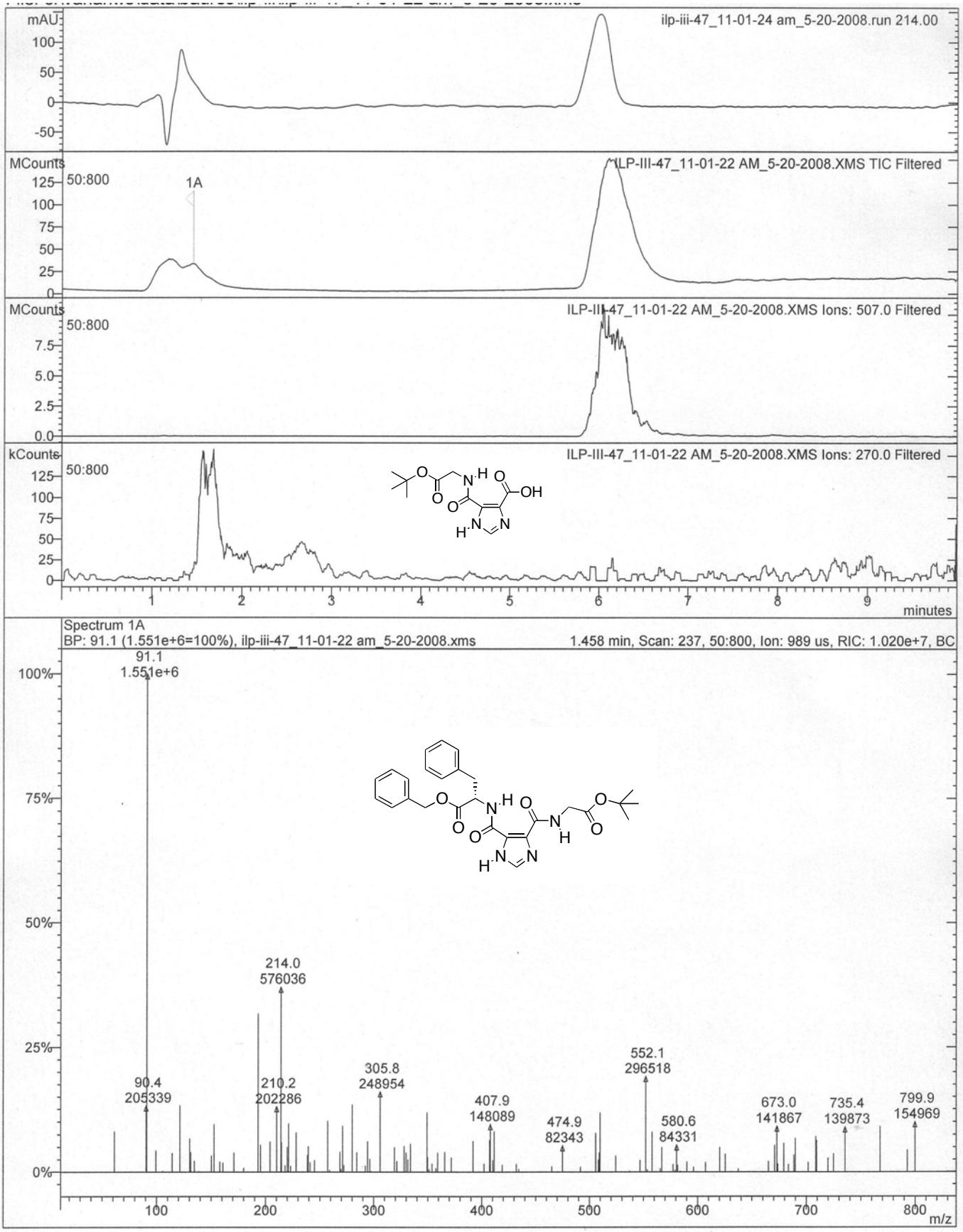

Figure S49. LC/MS data for the crude reaction to yield **4**{16}.

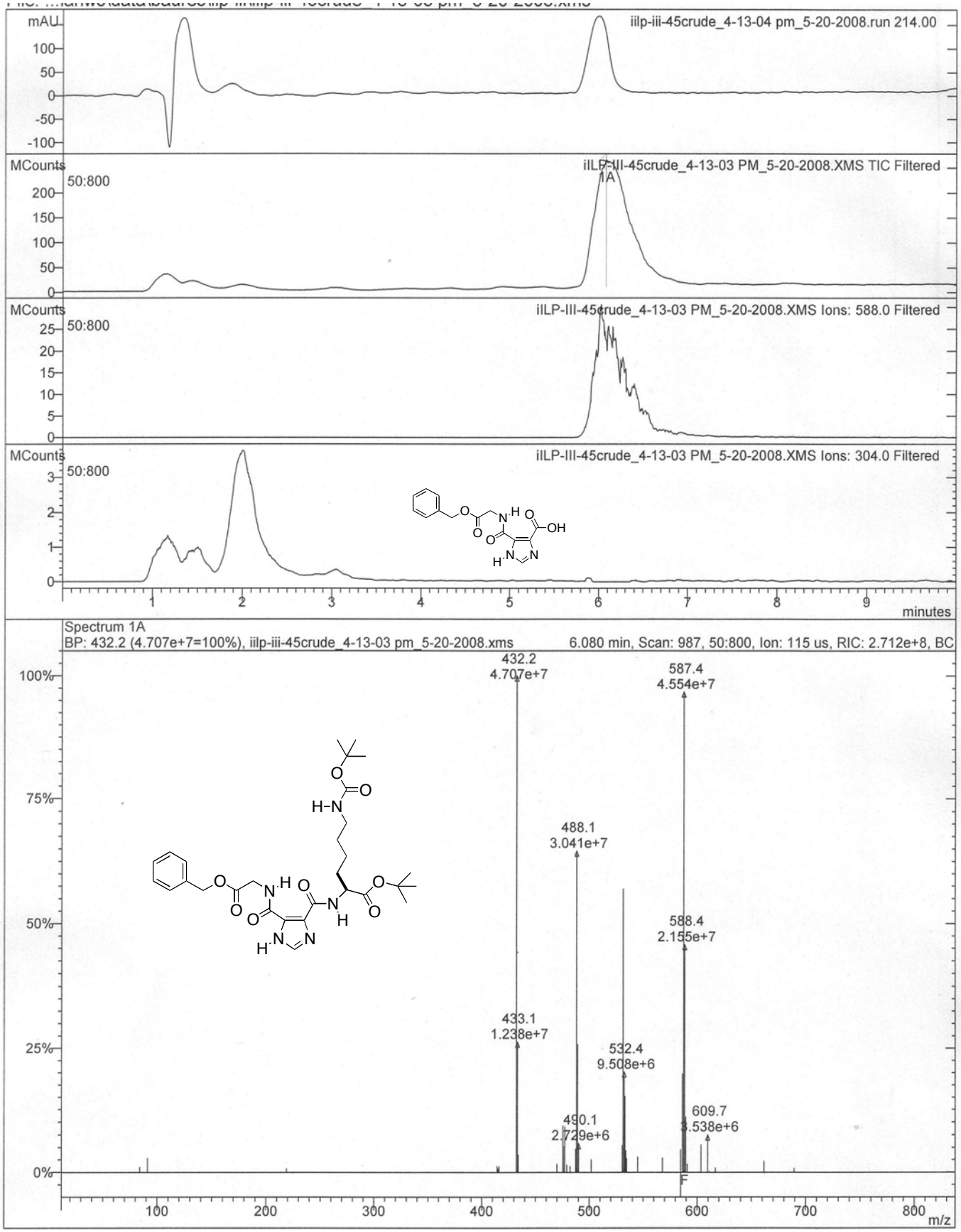

Figure S50. LC/MS data for the crude reaction to yield **4**{24}.

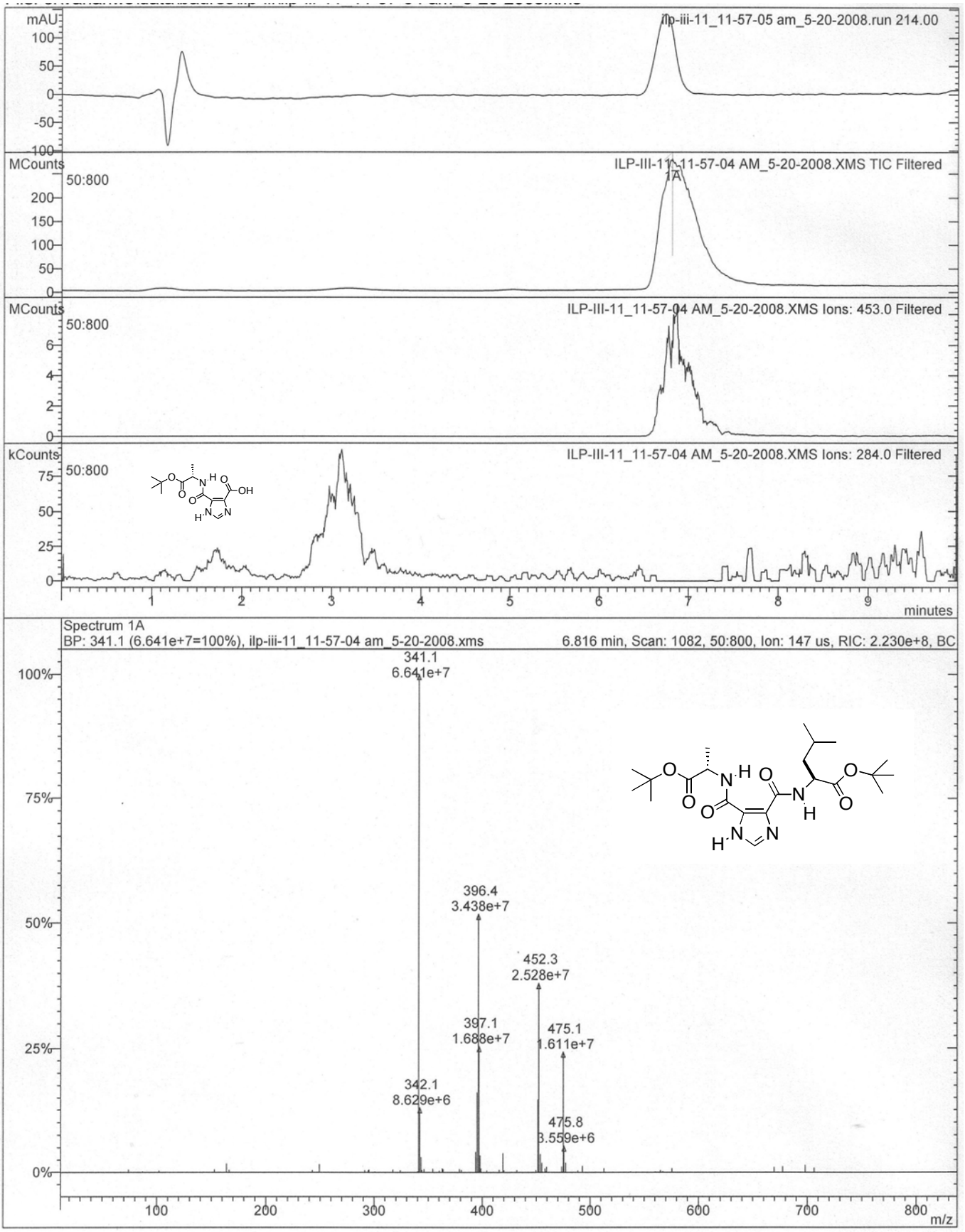

Figure S51. LC/MS data for the crude reaction to yield **4**{26}.

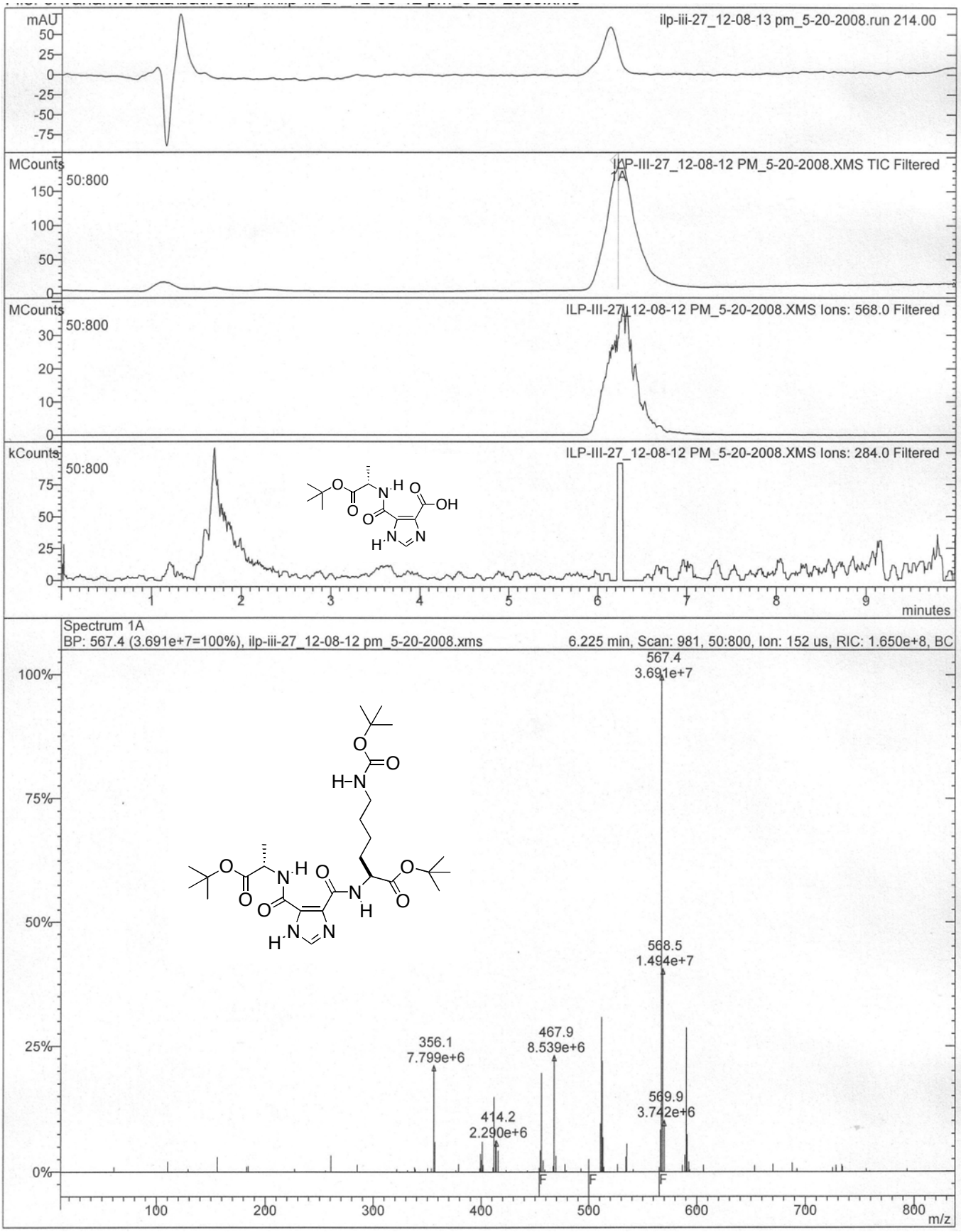

Figure S52. LC/MS data for the crude reaction to yield **4**{30}.

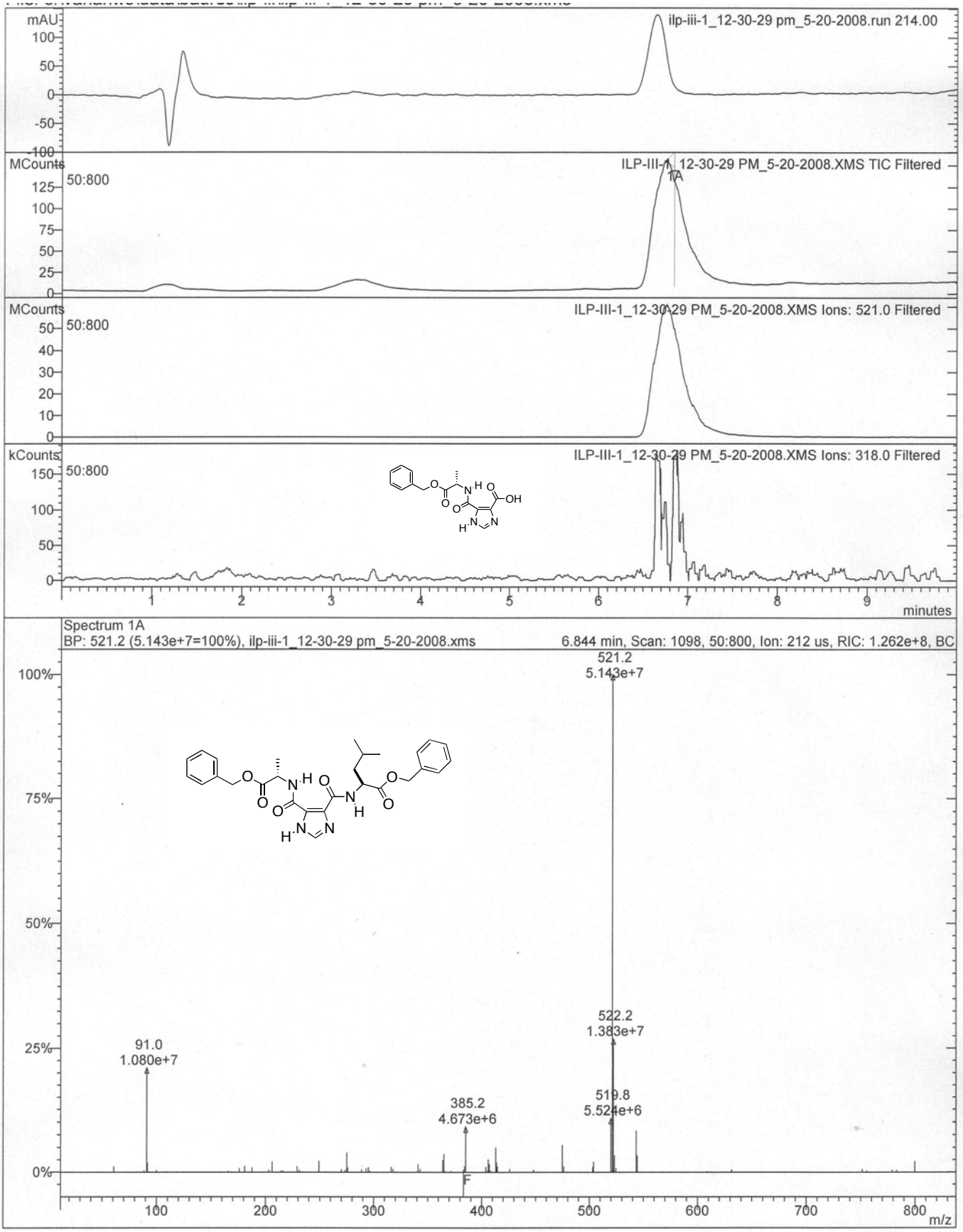

Figure S53. LC/MS data for the crude reaction to yield **4**{32}.

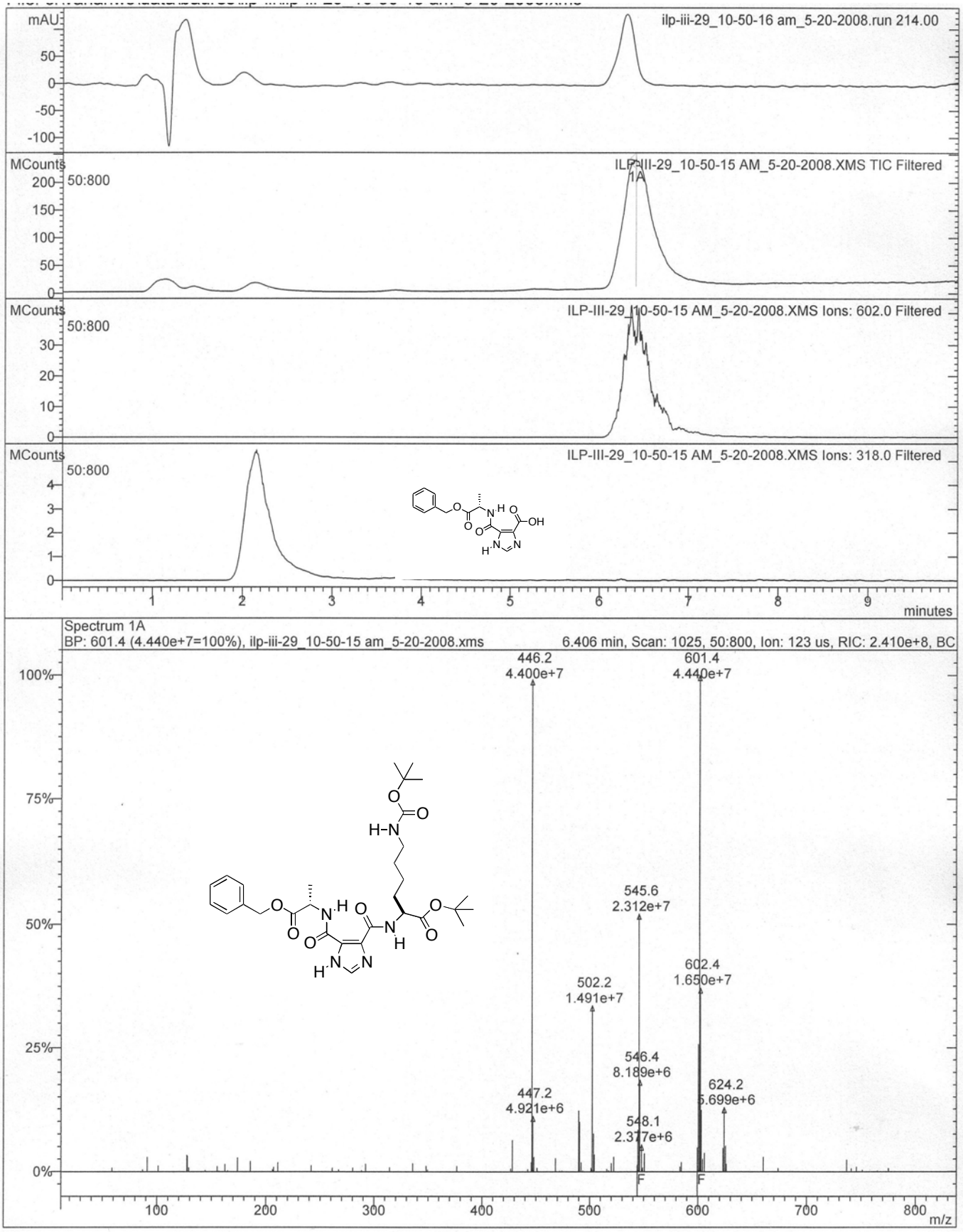

Figure S54. LC/MS data for the crude reaction to yield **4**{35}.

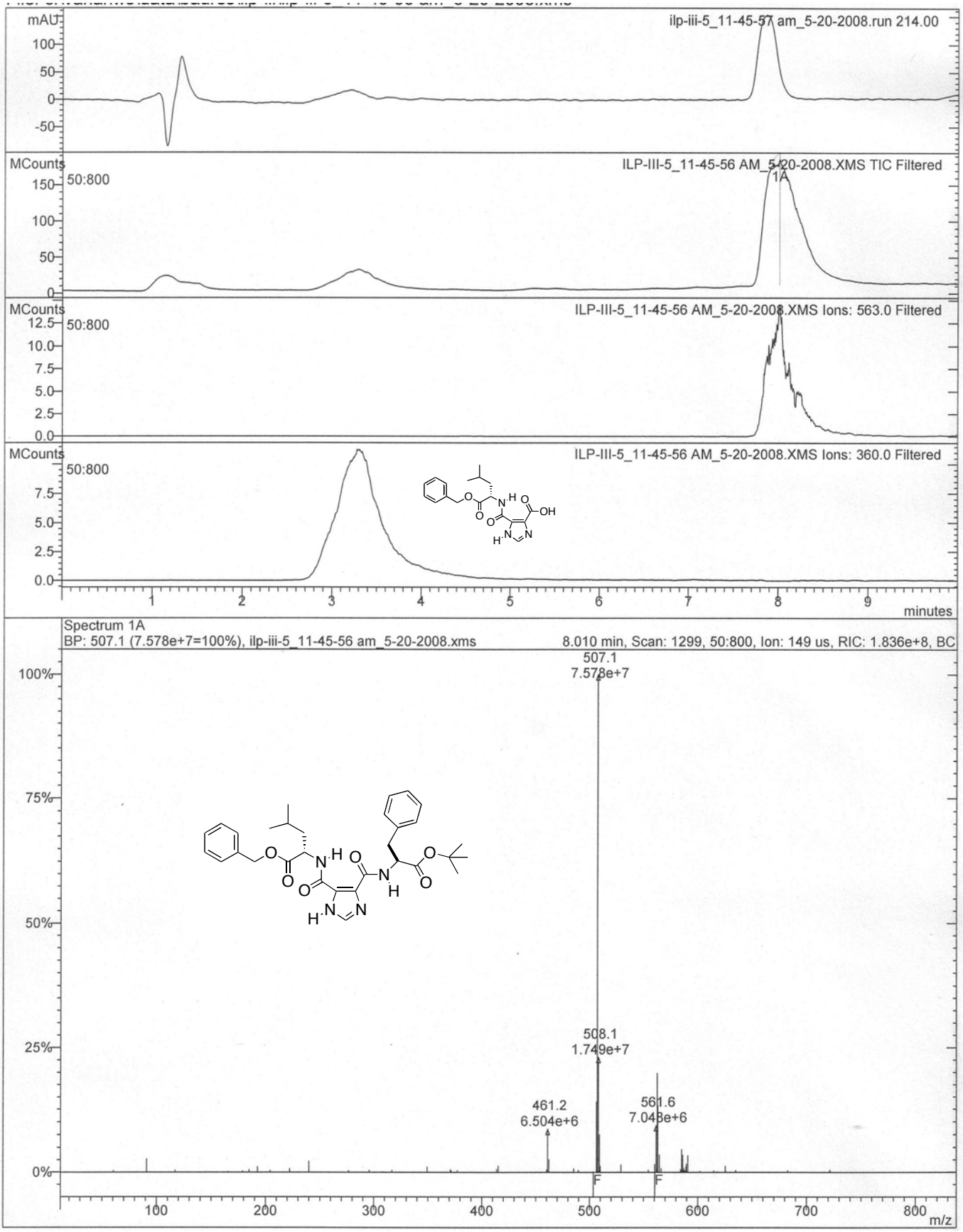

Figure S55. LC/MS data for the crude reaction to yield **4**{40}.

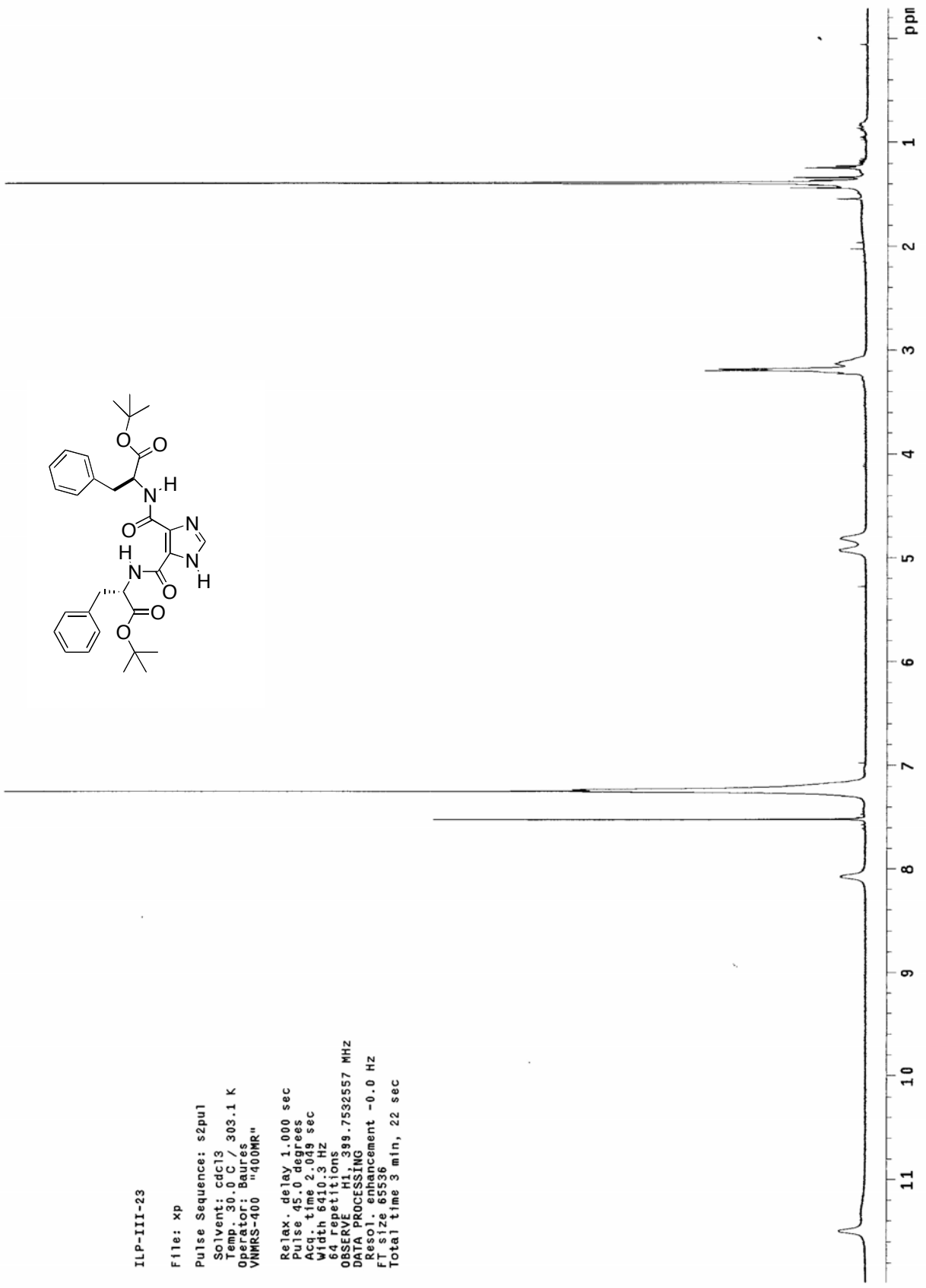

Figure S56. ^{1}H-NMR for **4{**7}.

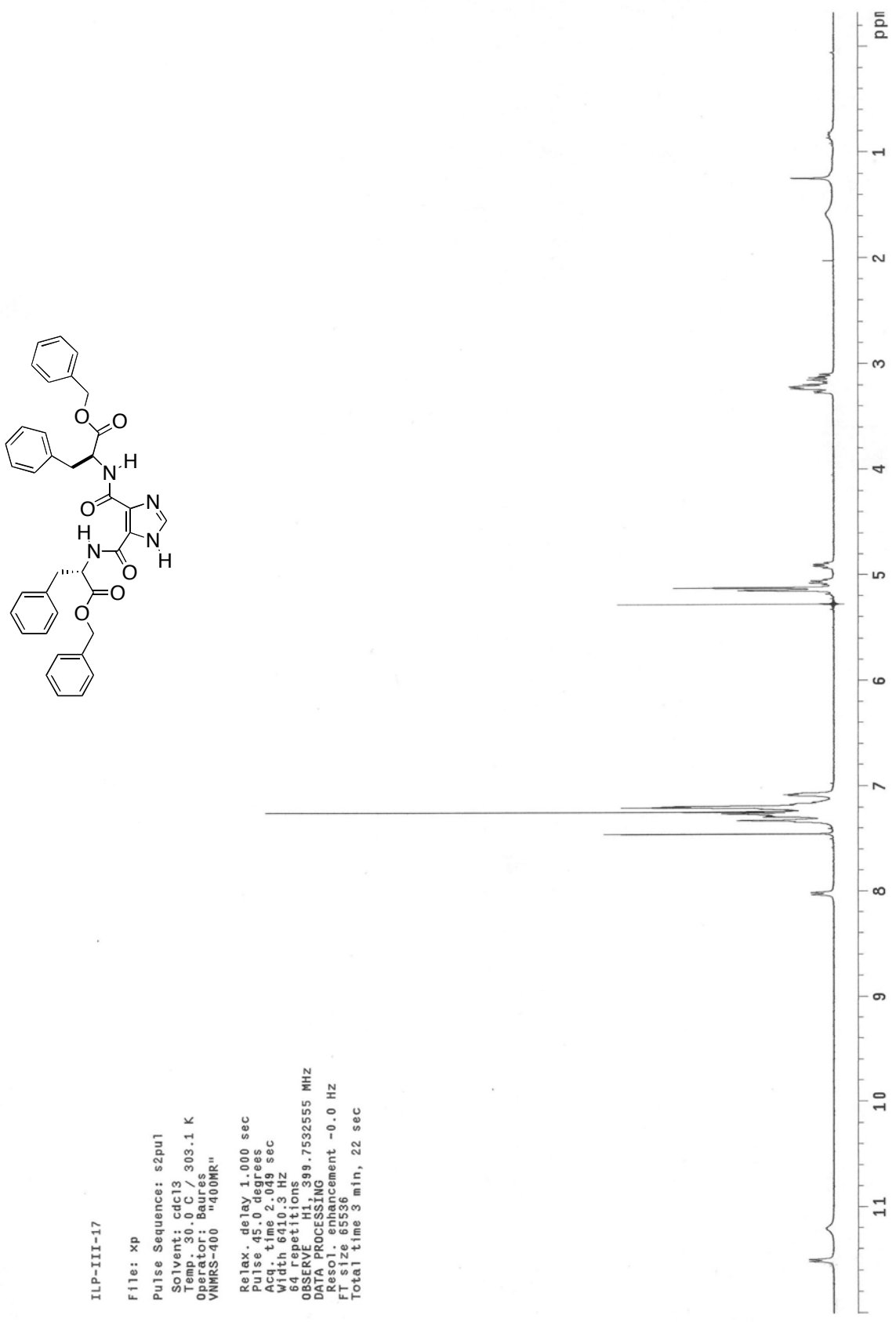

Figure S57. ^{1}H-NMR for **4{**8}.

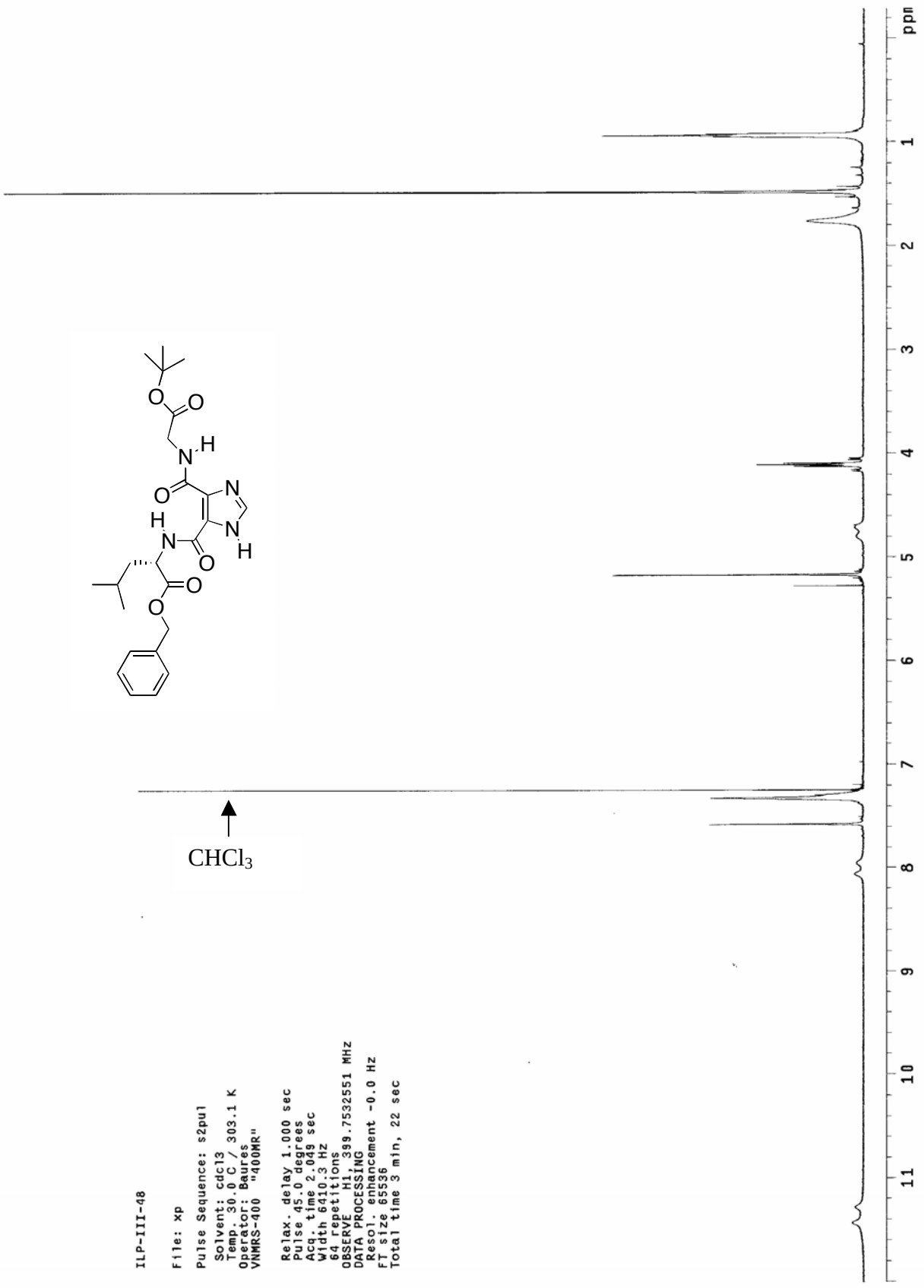

Figure S58. ^{1}H-NMR for **4{**14}.

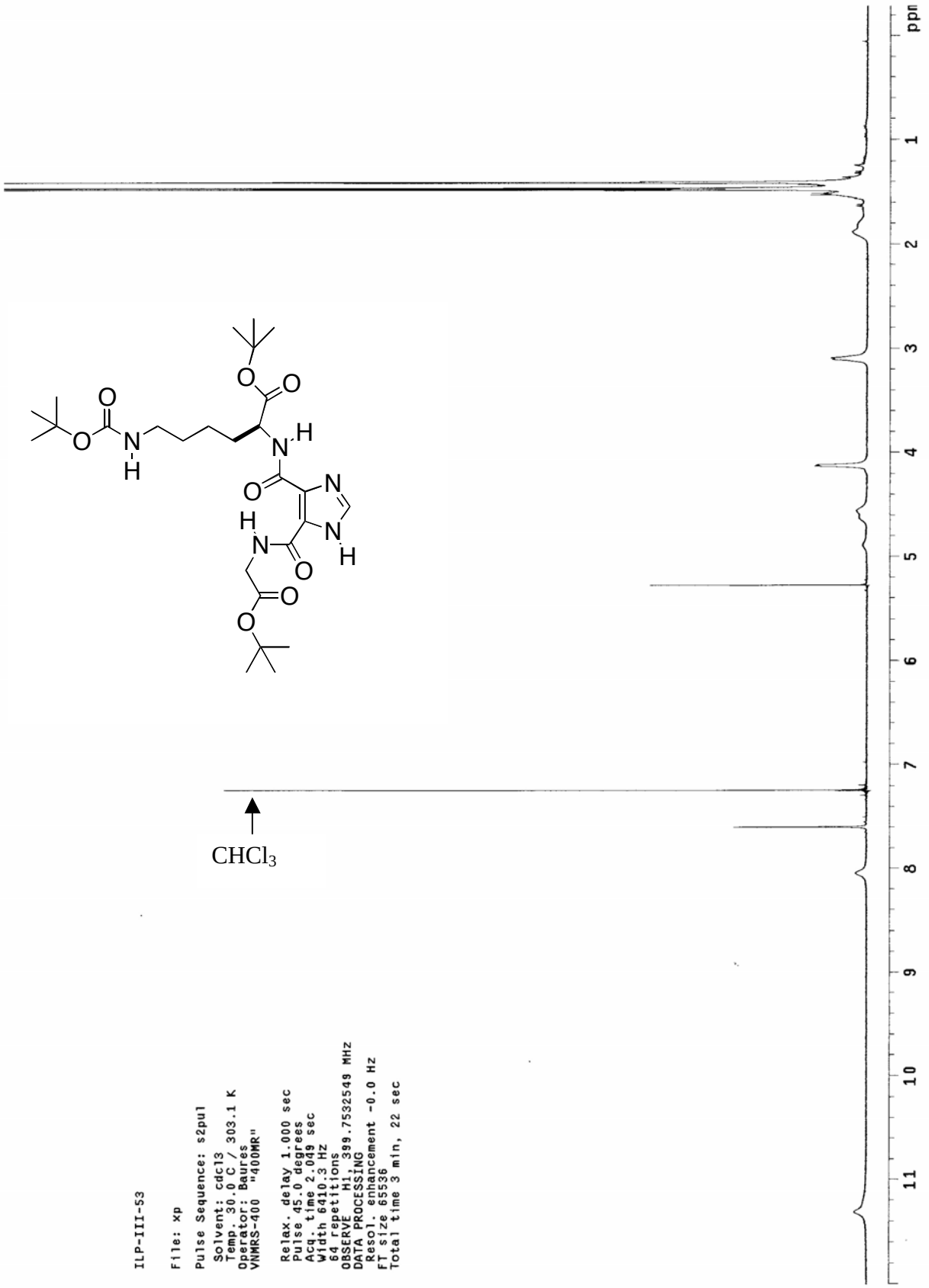

Figure 59. ^{1}H-NMR for **4{**17}.

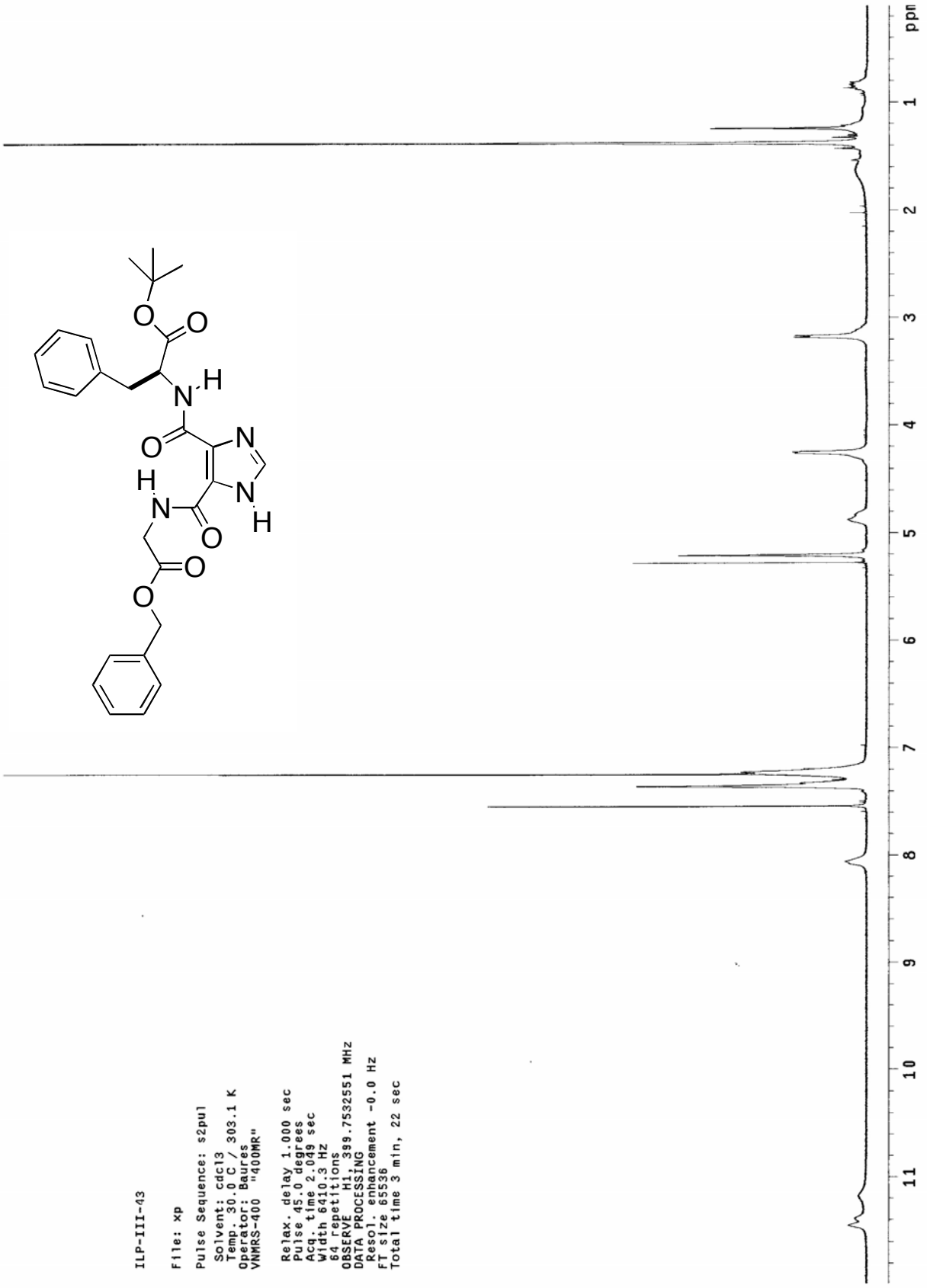

Figure S60. ^{1}H-NMR for **4{**22}.

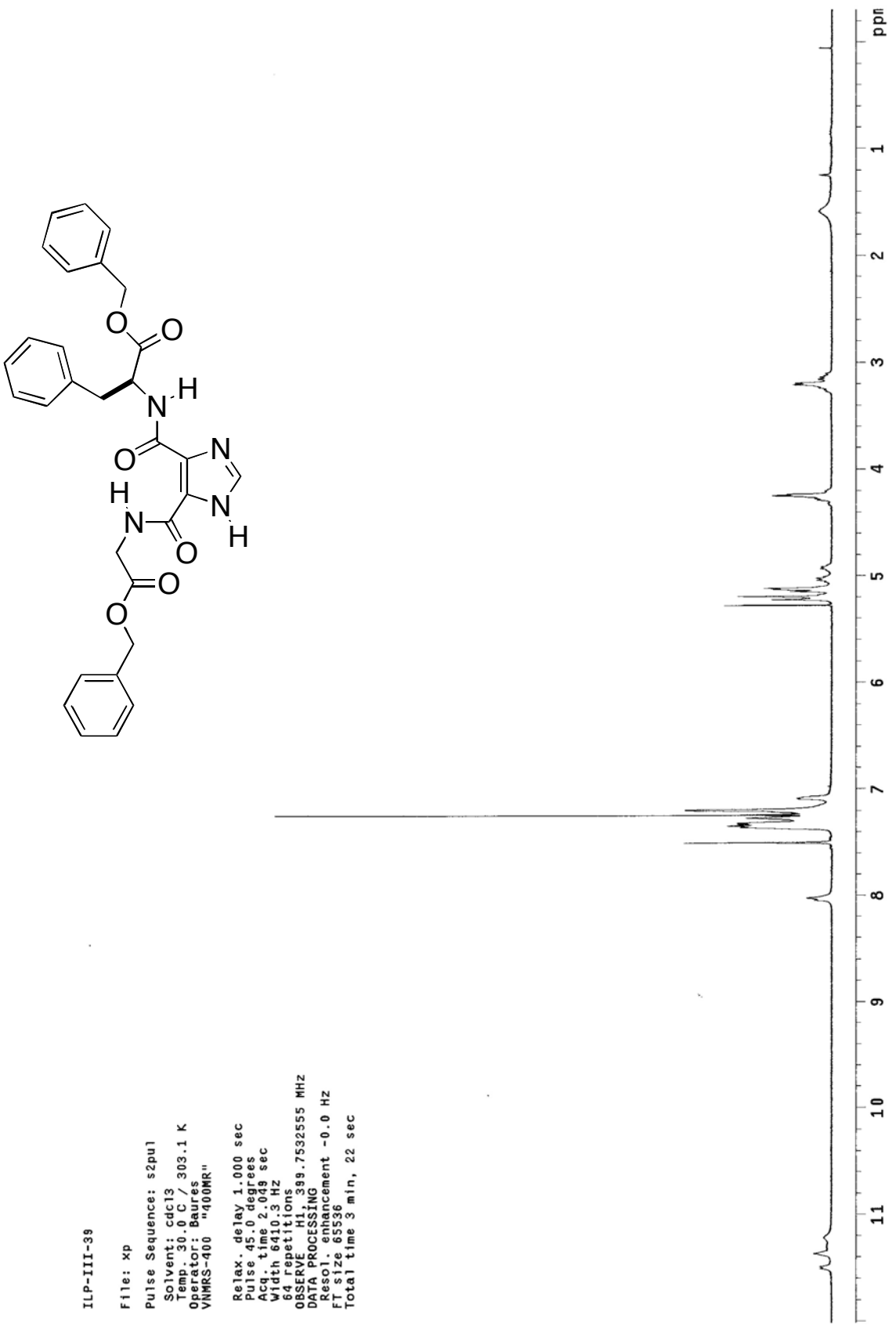

Figure S61. ^{1}H-NMR for **4{**23}.

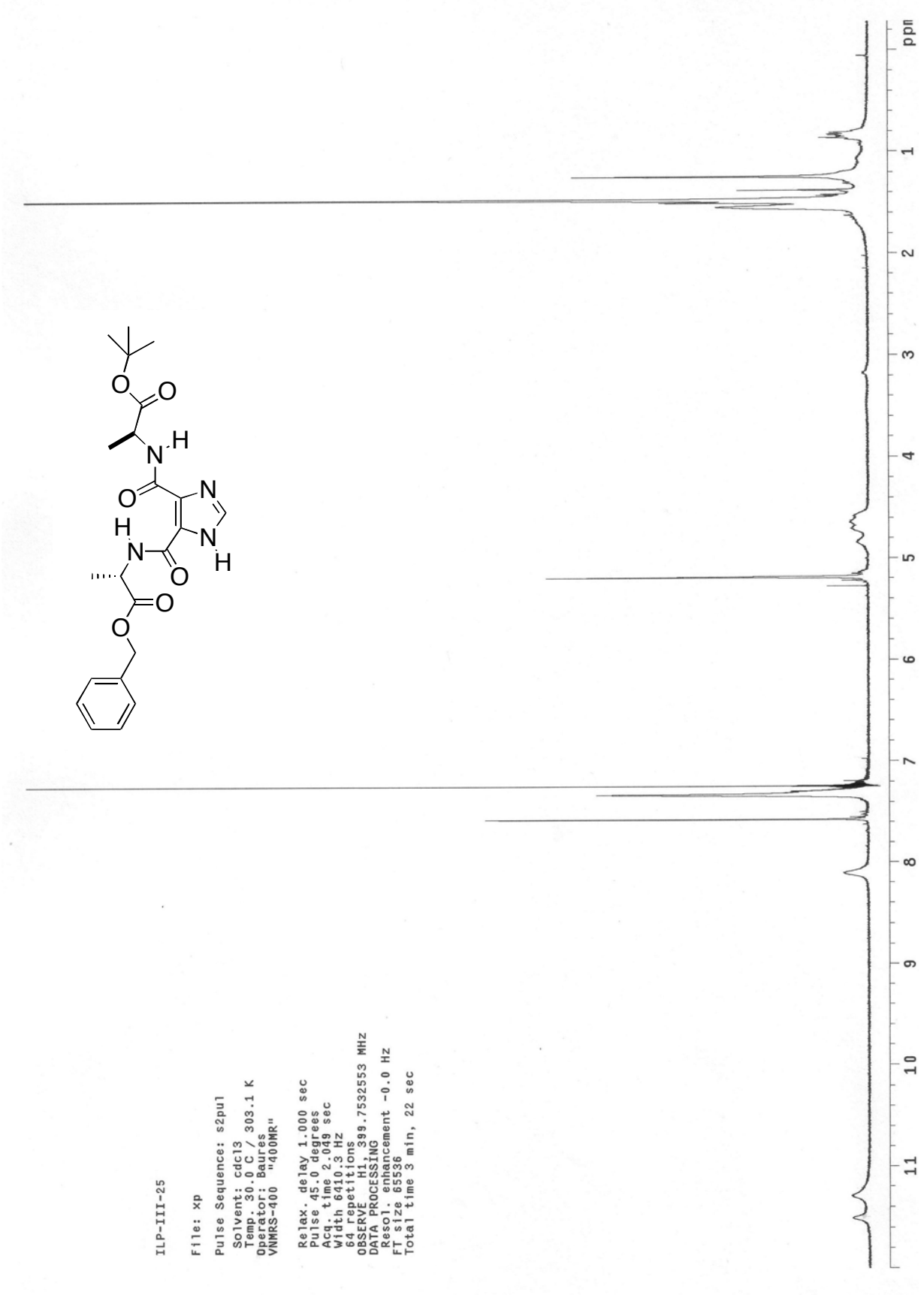

Figure S62. ^{1}H-NMR for **4{**25}.

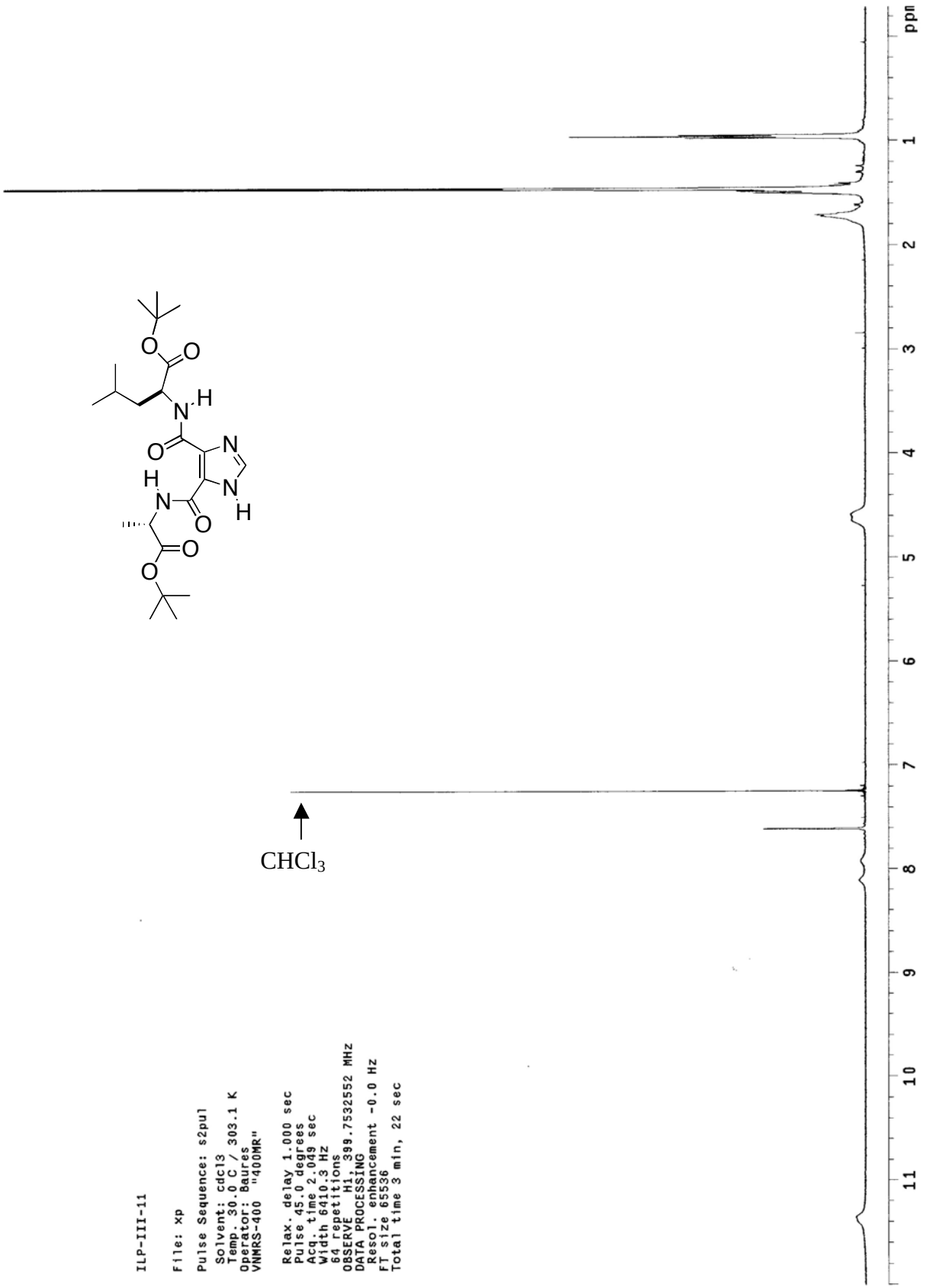

Figure S63. ^{1}H-NMR for **4{**26}.

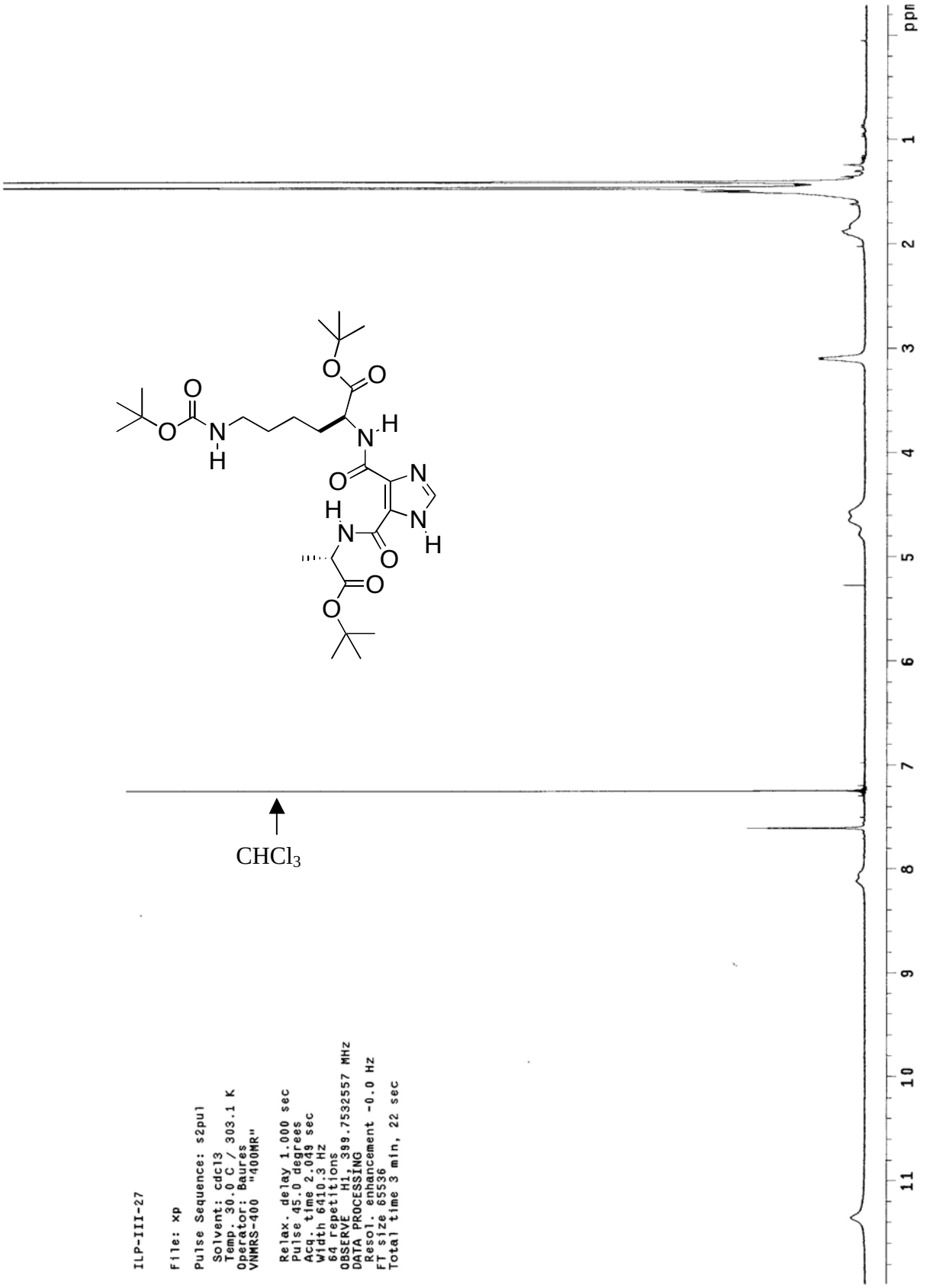

Figure S64. ^{1}H-NMR for **4{**30}.

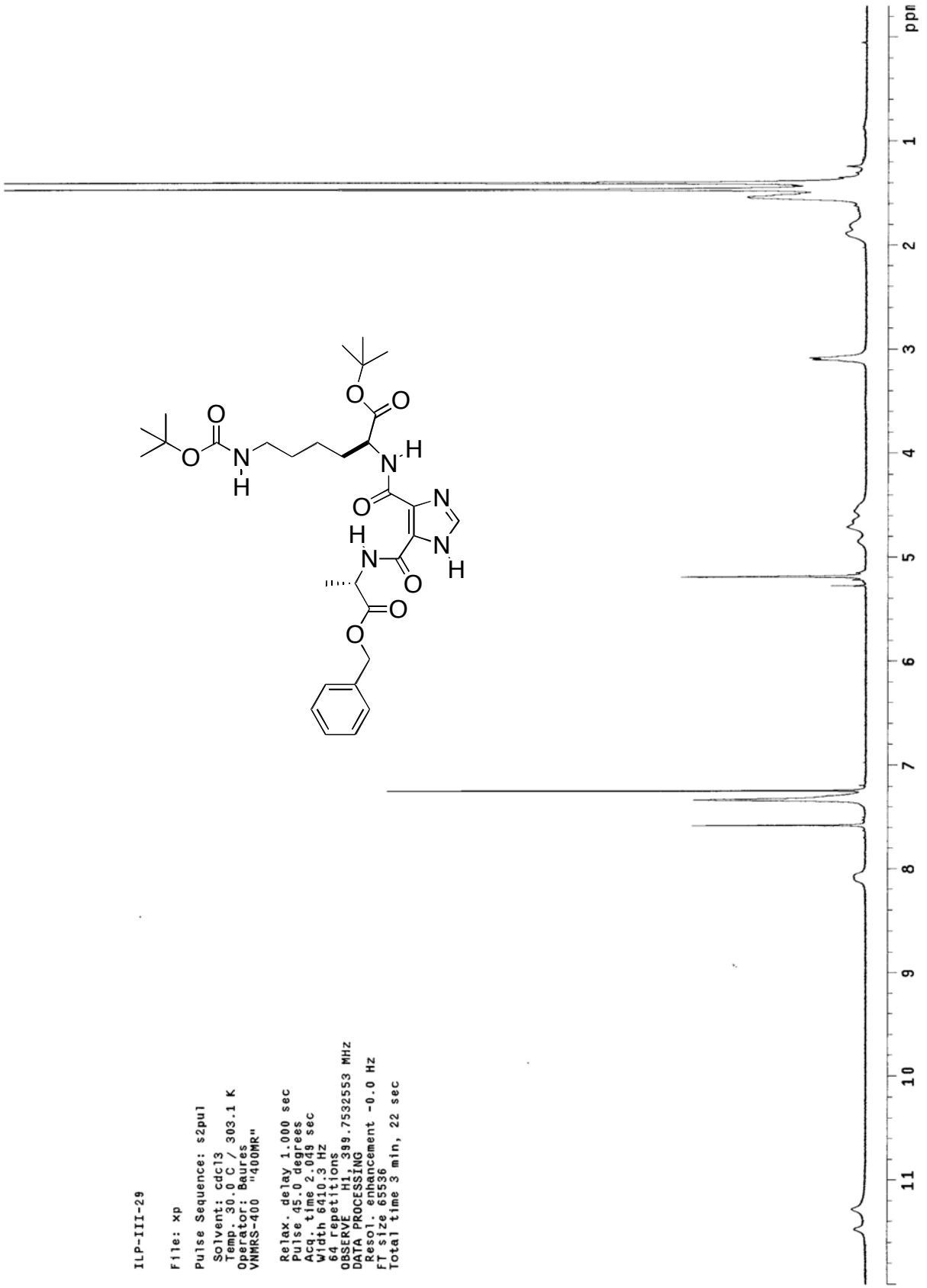

Figure S65. ^{1}H-NMR for **4{**35}.

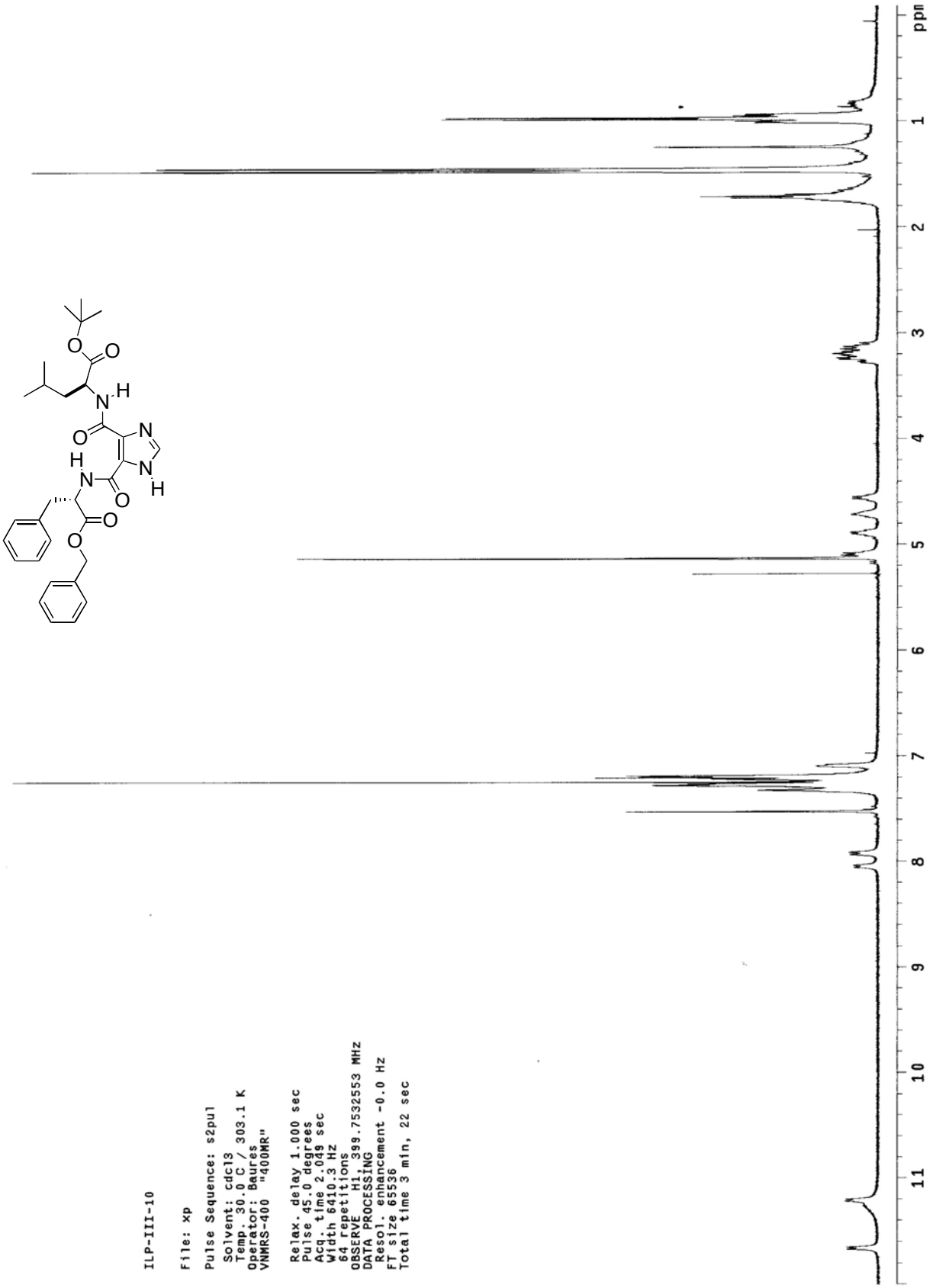

Figure S66. ^{1}H-NMR for **4{**38}.

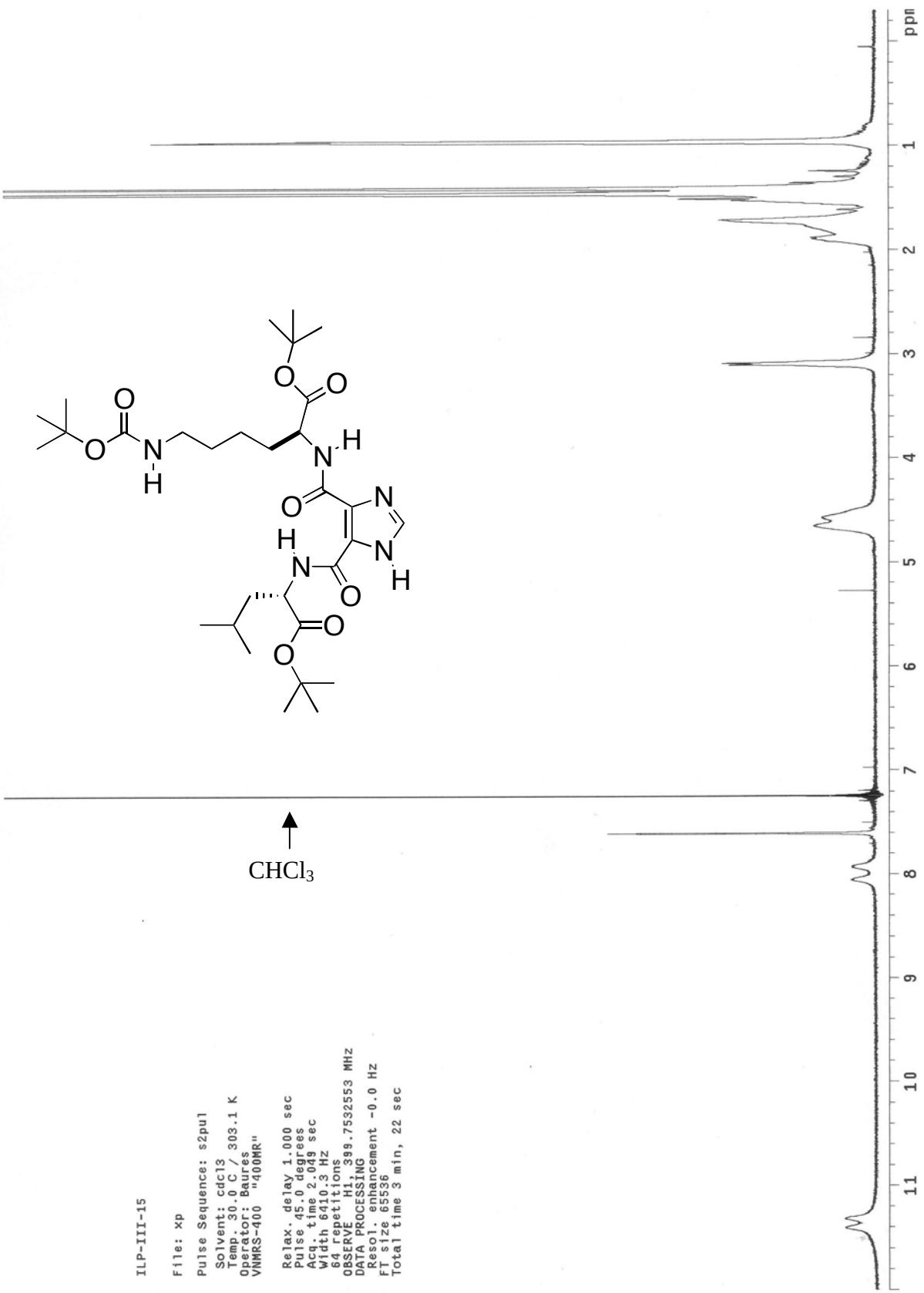

Figure S67. ^{1}H-NMR for **4{**39}.

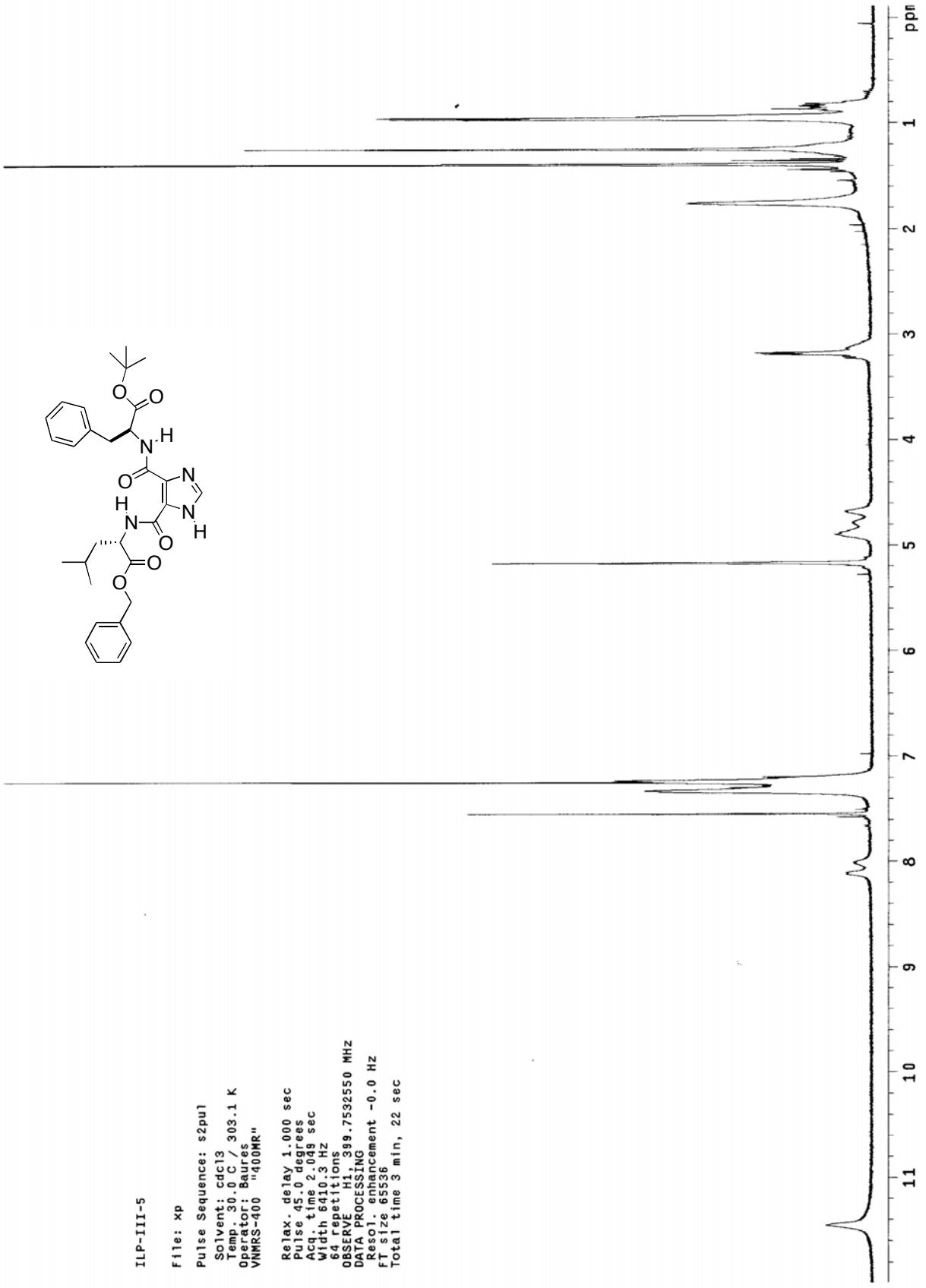

Figure S68. ^{1}H-NMR for **4{**40}.

Figure S69. ^{1}H-NMR for **4{**42}.

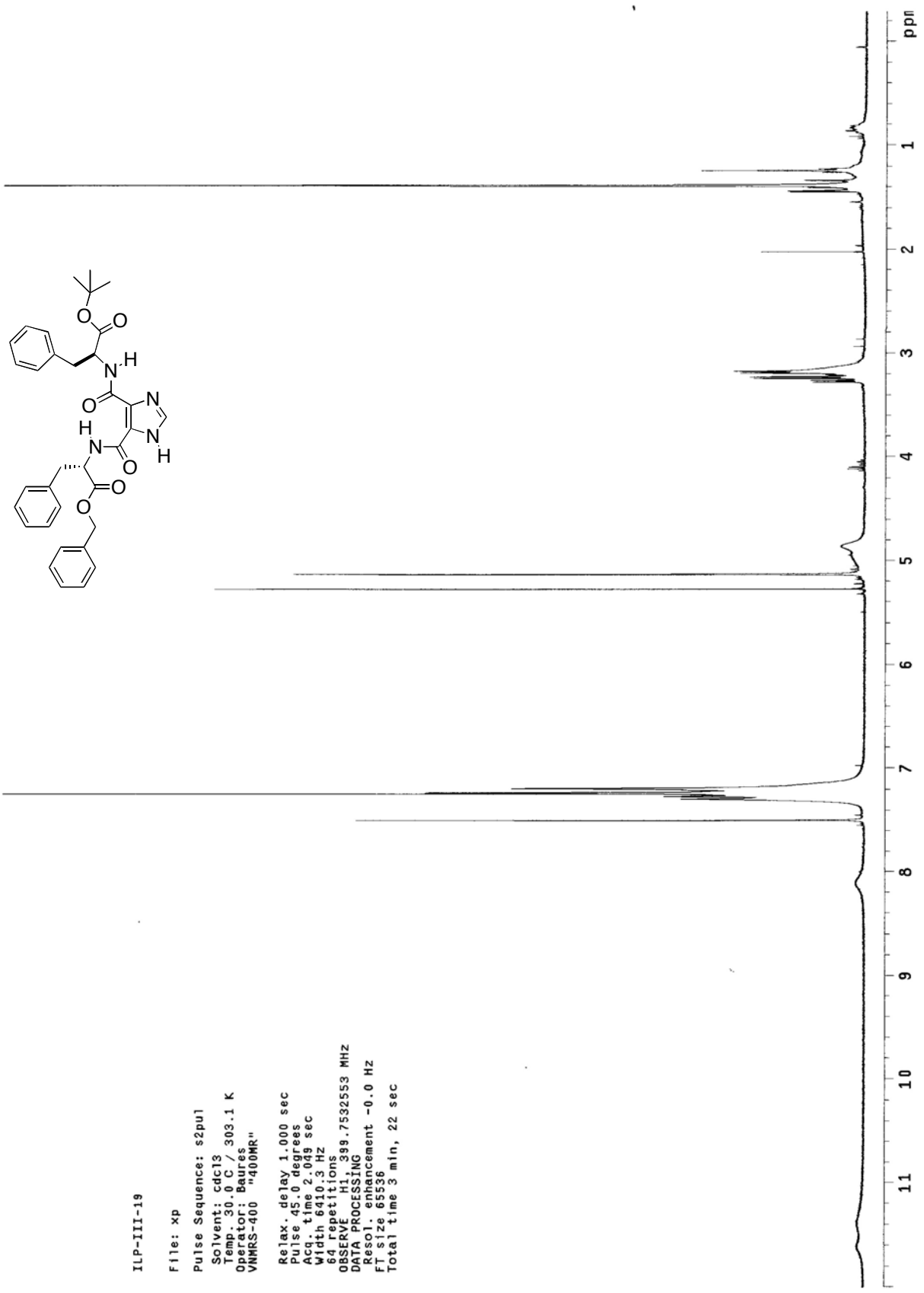

Figure S70. ^{1}H-NMR for **4{**43}.

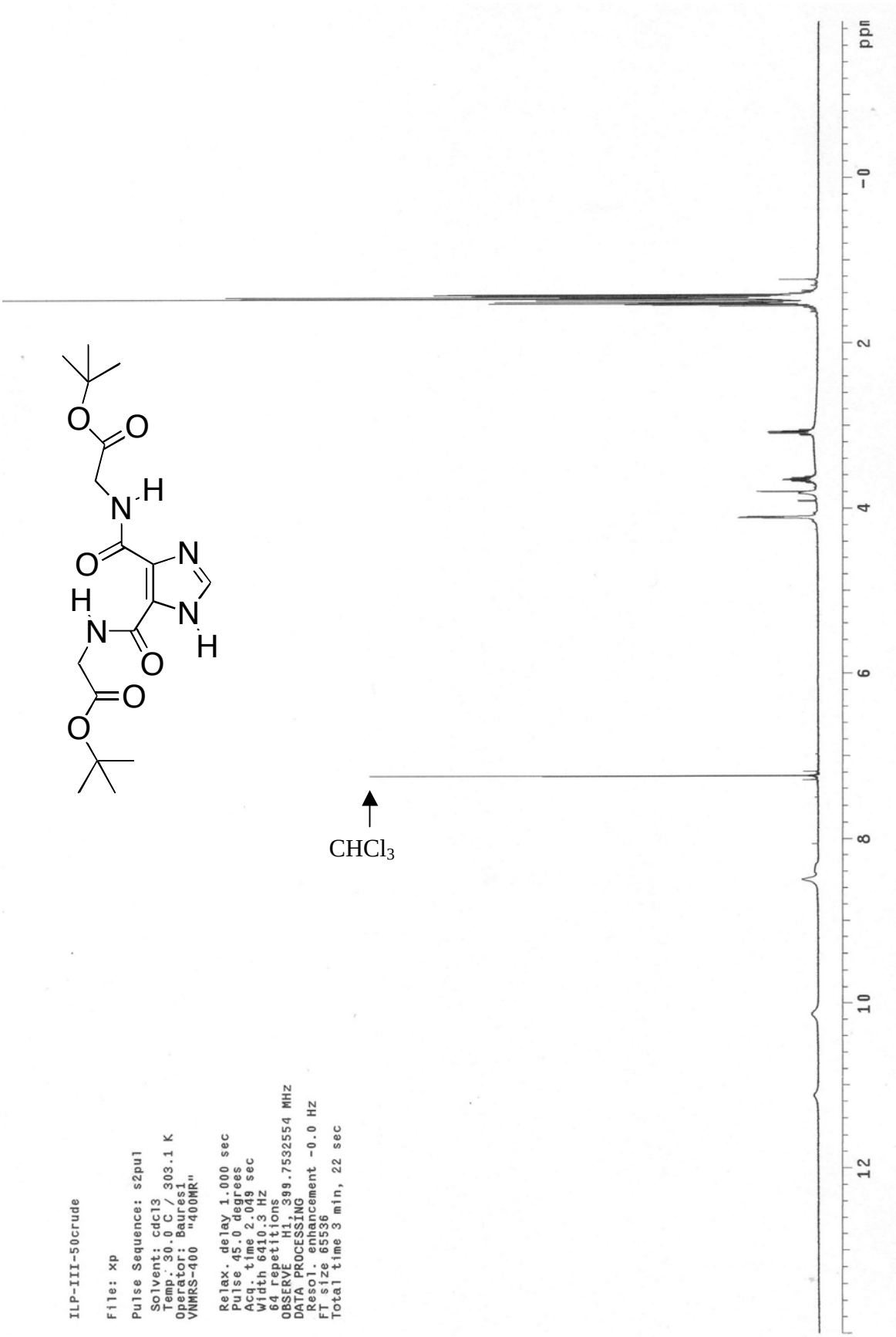

Figure S71. ^{1}H-NMR for the crude reaction to yield **4{**1}.

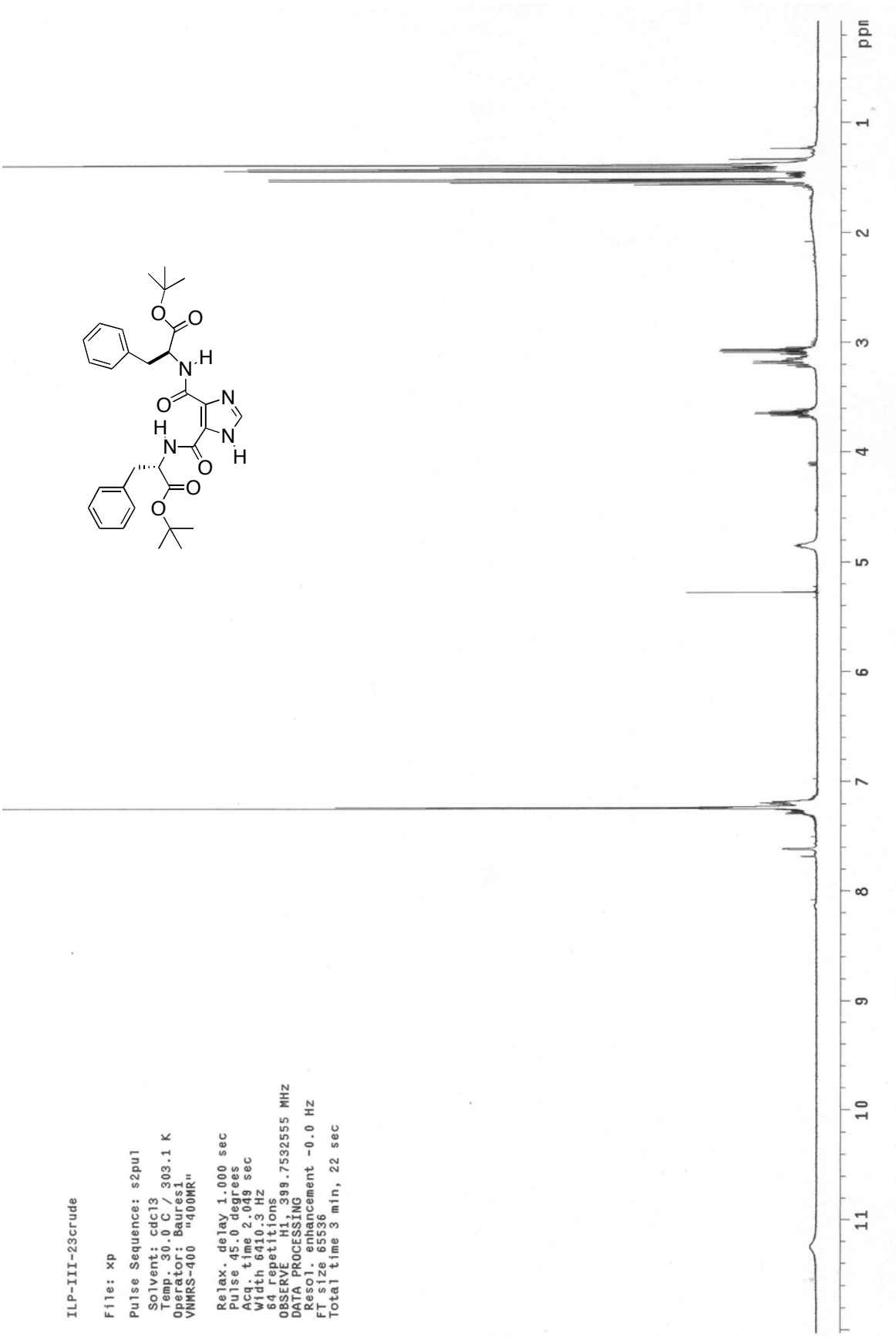

Figure S72. ^{1}H-NMR for the crude reaction to yield **4{**7}.

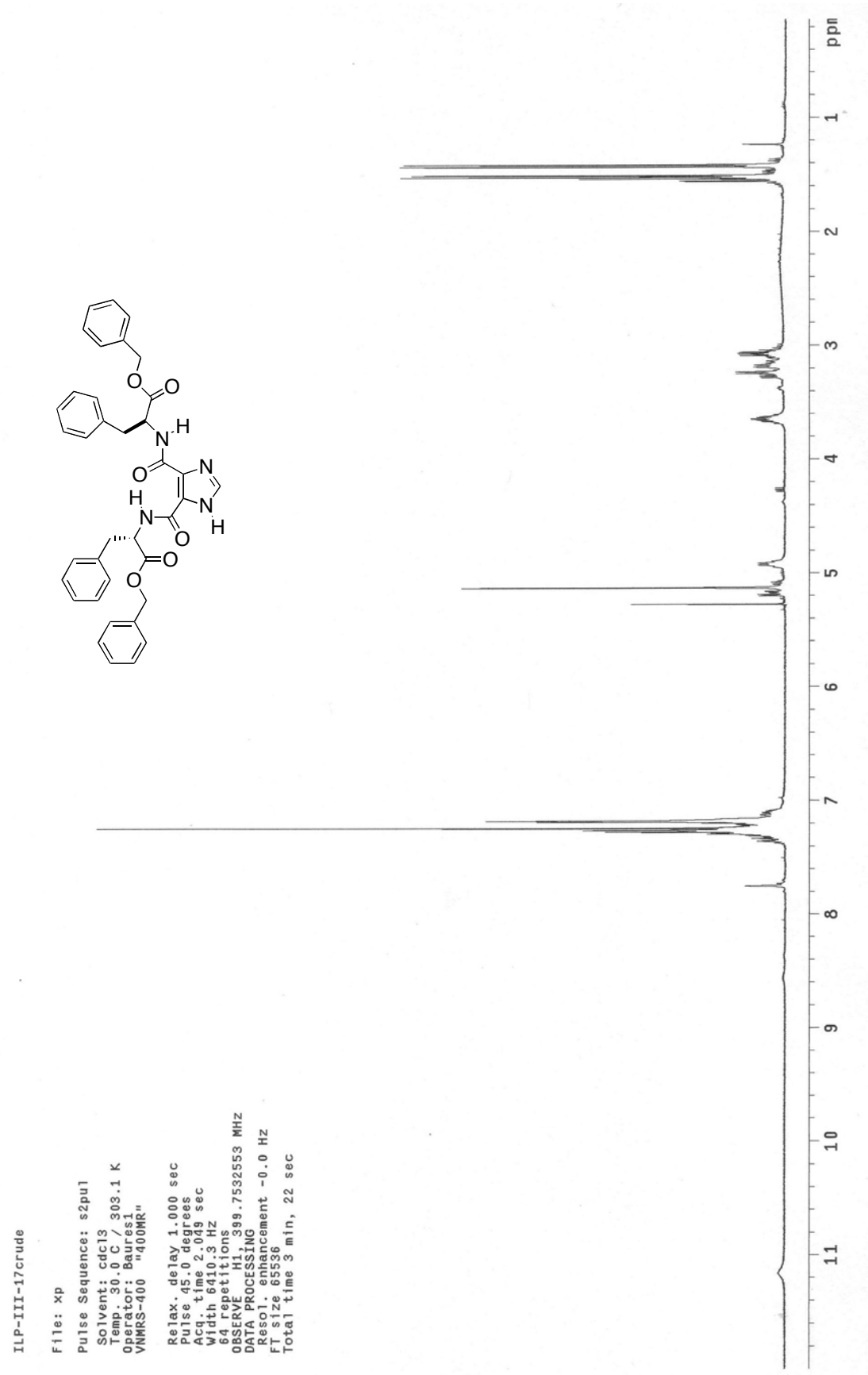

Figure S73. ^{1}H-NMR for the crude reaction to yield **4{**8}.

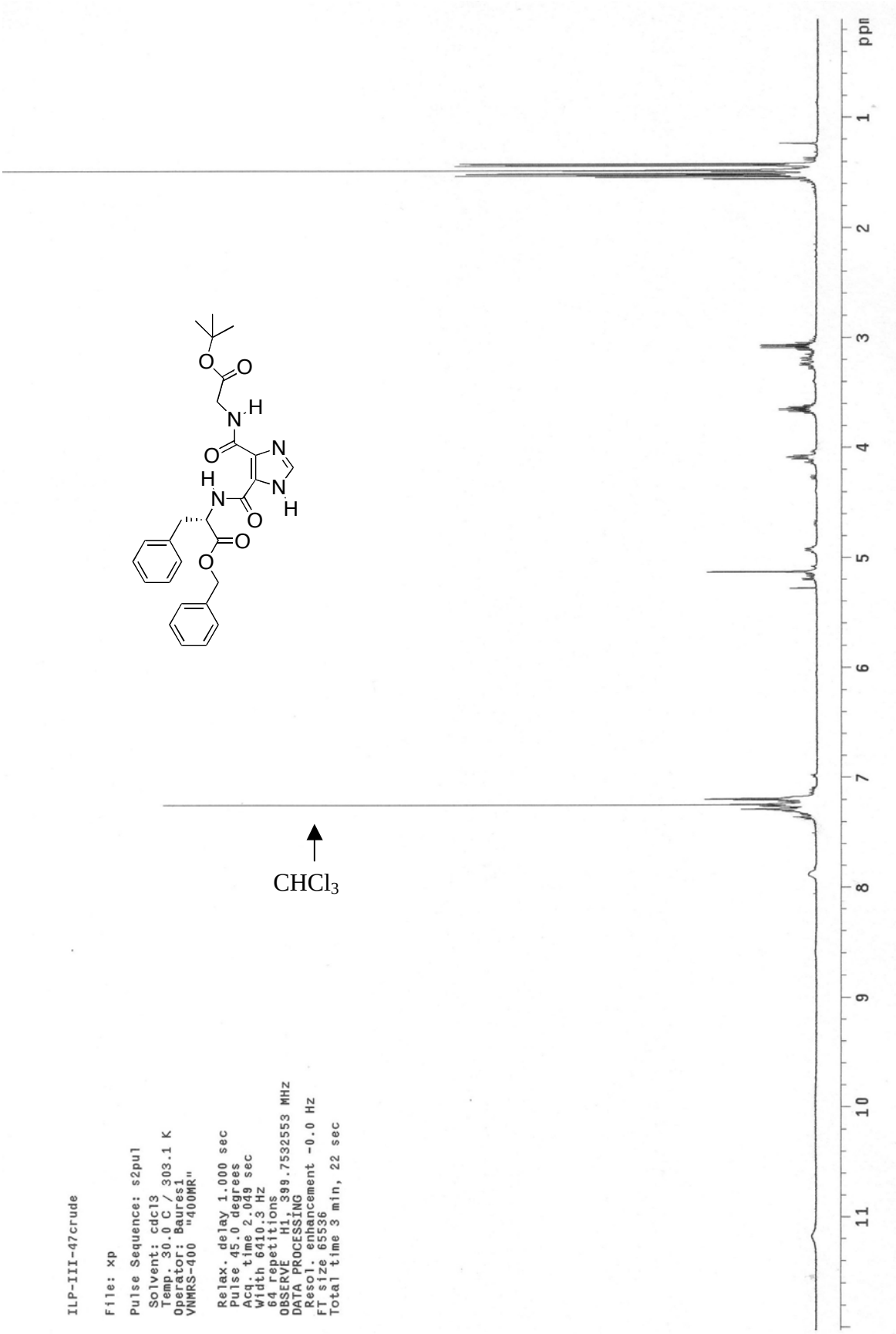

Figure S74. ^{1}H-NMR for the crude reaction to yield **4{**16}.

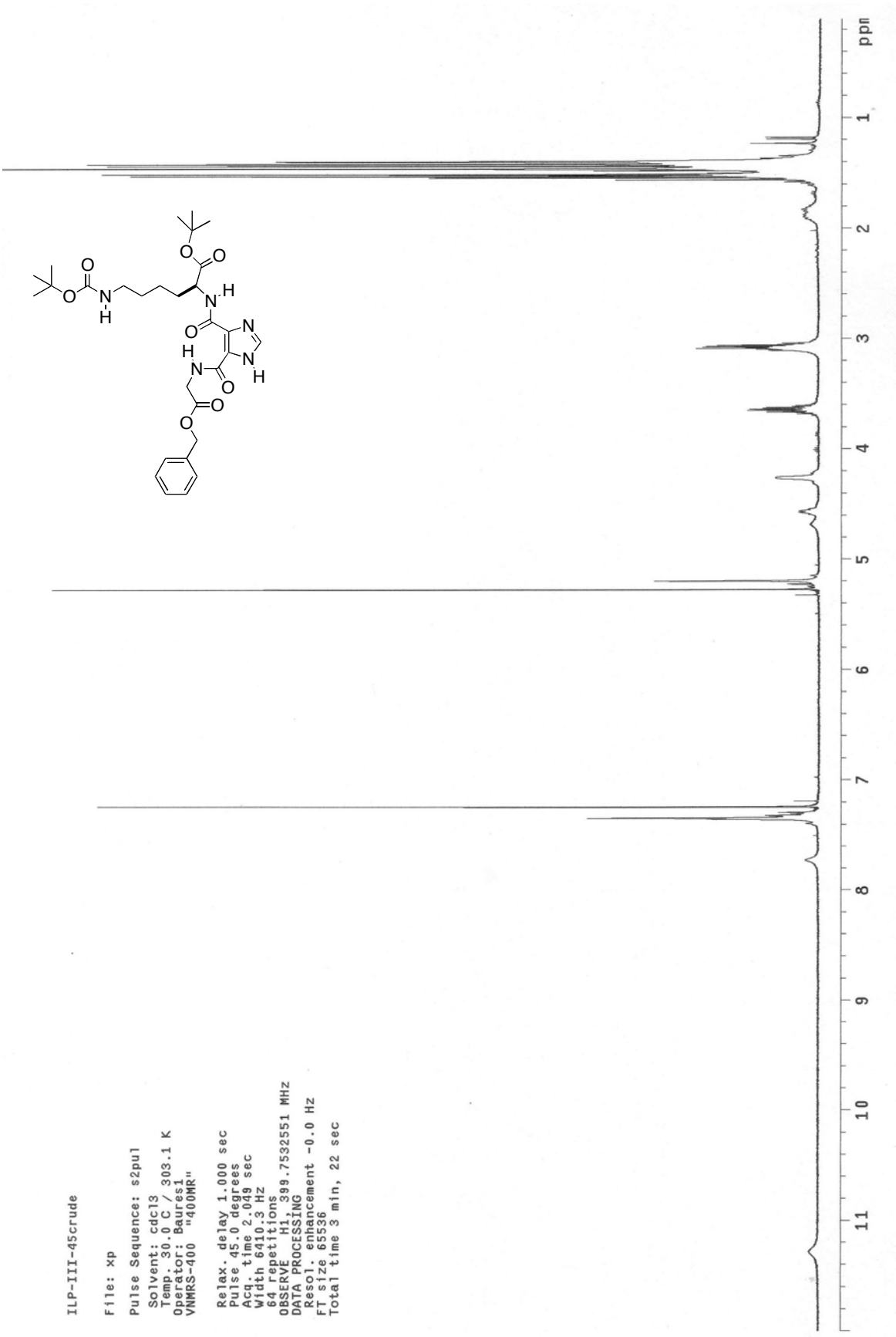

Figure S75. ^{1}H-NMR for the crude reaction to yield **4{**24}.

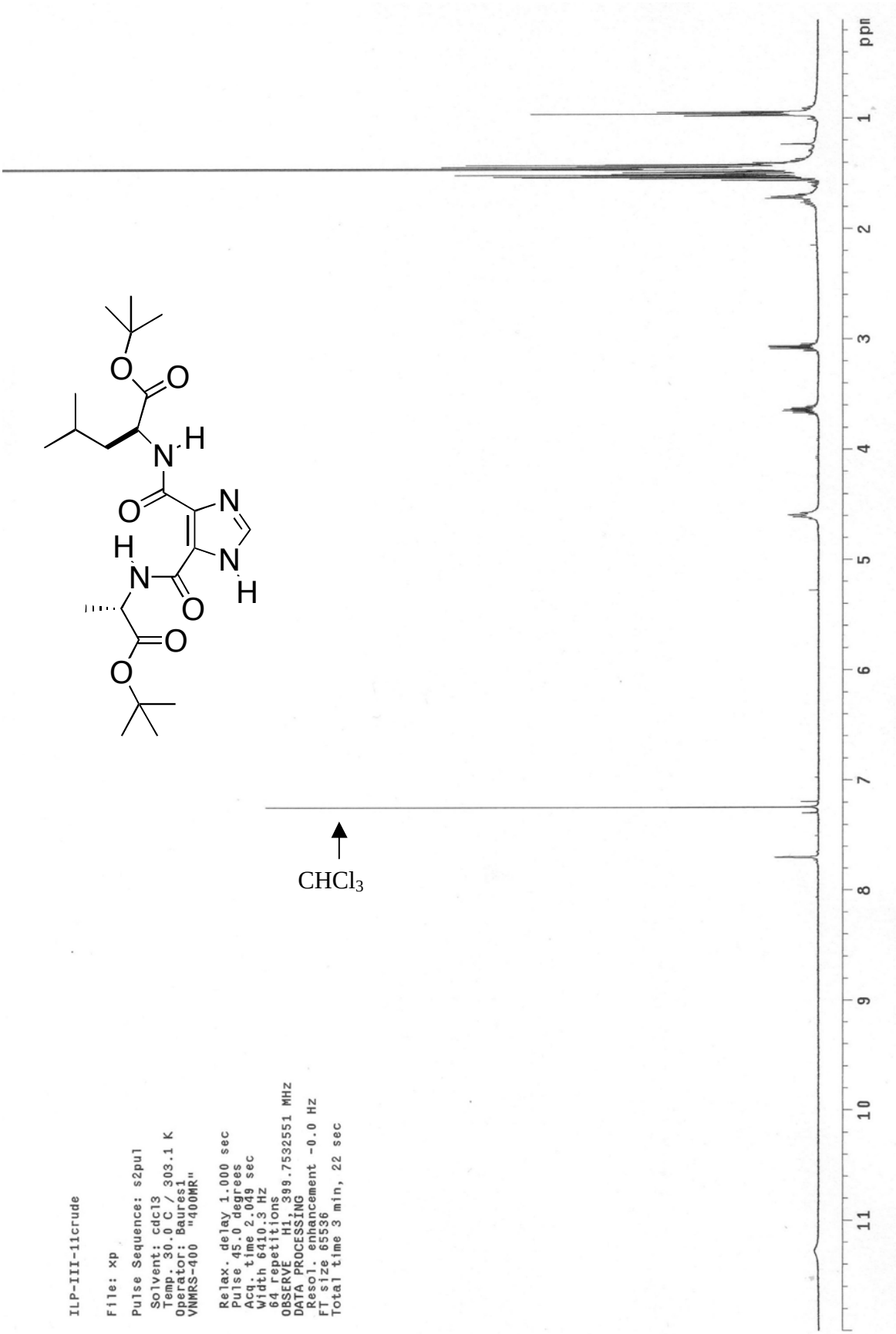

Figure S76. ^{1}H-NMR for the crude reaction to yield **4{**26}.

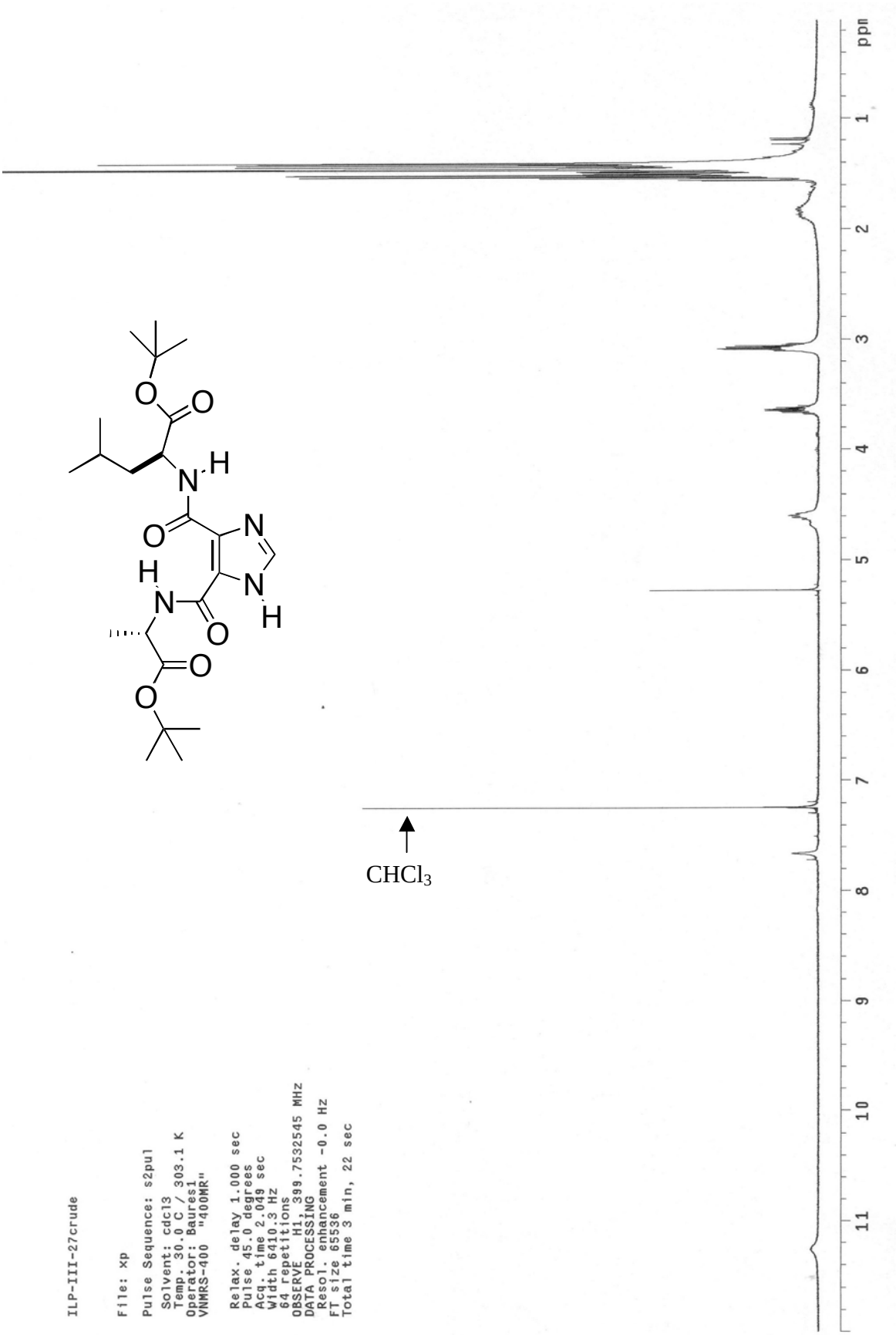

Figure S77. ^{1}H-NMR for the crude reaction to yield **4{**30}.

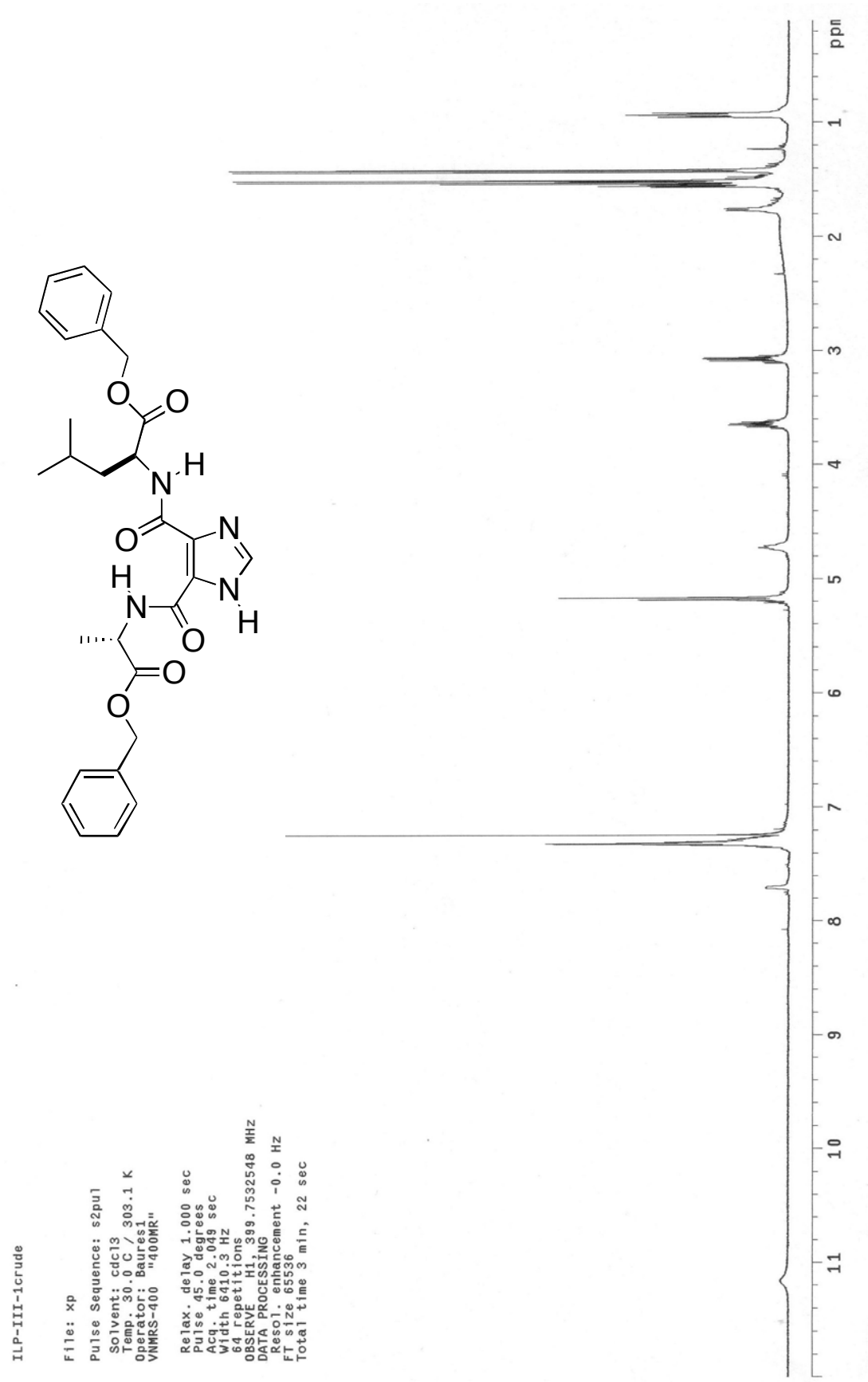

Figure S78. ^{1}H-NMR for the crude reaction to yield **4{**32}.

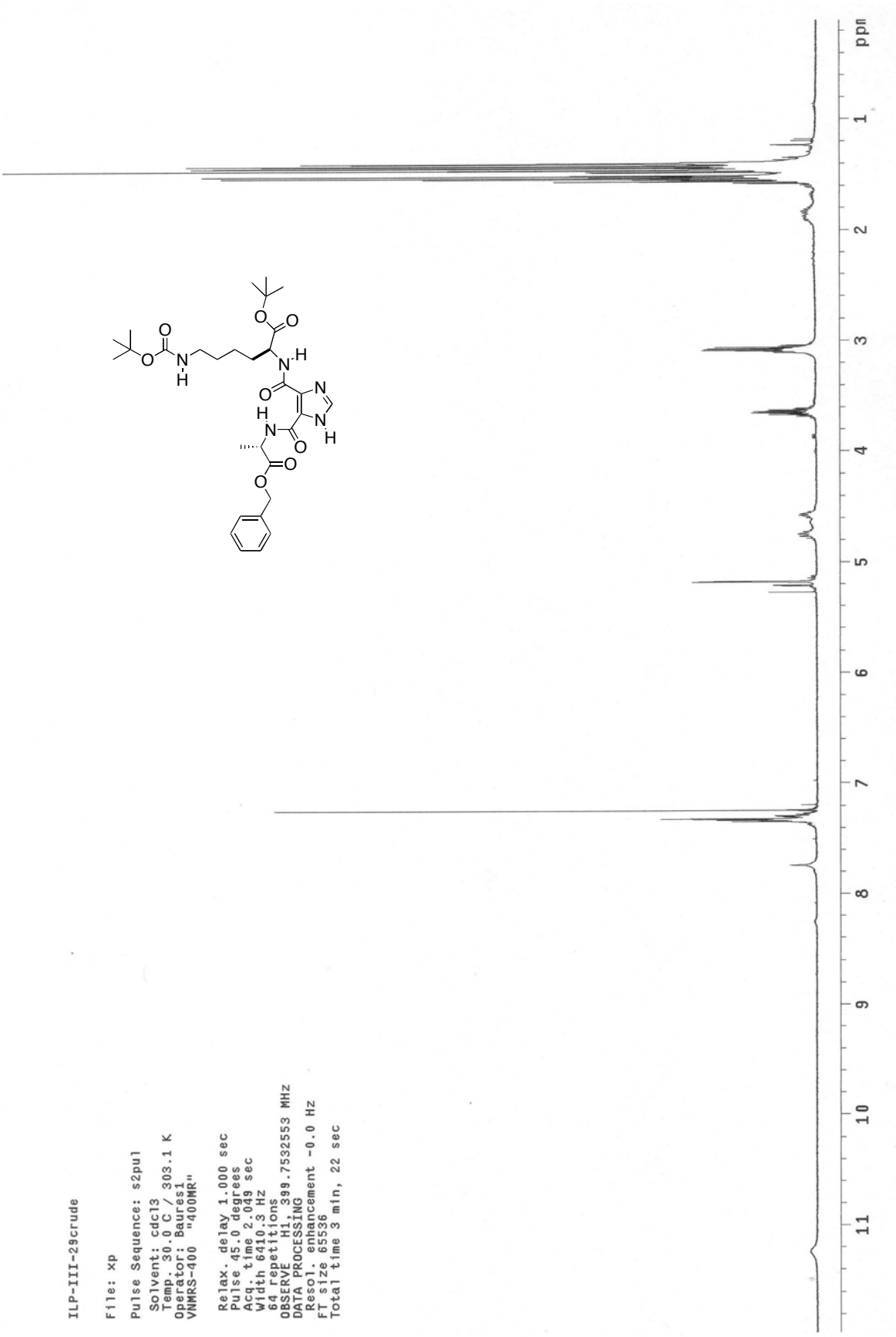

Figure S79. ^{1}H-NMR for the crude reaction to yield **4{**35}.

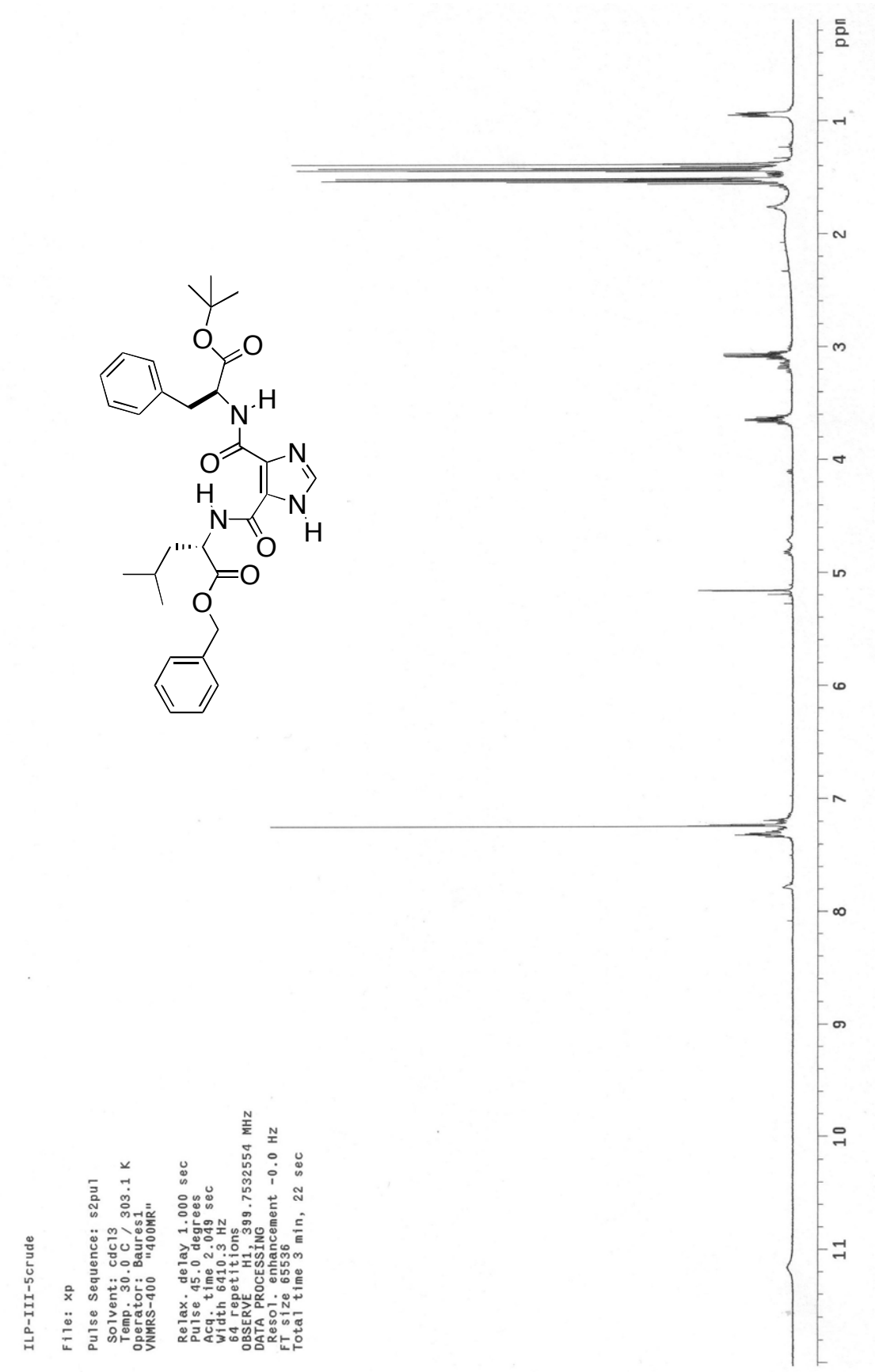

Figure S80. ^{1}H-NMR for the crude reaction to yield **4{**40}.