Supporting Information

Synthesis of Sansalvamide A Peptidomimetics: Triazole, Oxazole, Thiazole, and Pseudoproline containing compounds

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Contents

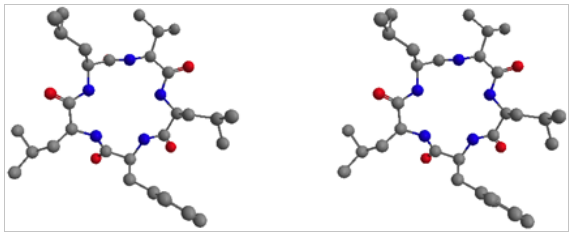
Table of compounds with text describing structural variations

Comp #		aa_1	aa_2	aa_3	aa_4	aa_5
1	A-Tri-III	Phe	Leu	Val-Triazole	Leu	Leu
2	B-Tri-III	Phe	Leu	Val-Triazole	Leu	NMe-Leu
3	A-Ox-III	Phe	Leu	Oxazole	Leu	Leu
4	B-Ox-III	Phe	Leu	Oxazole	Leu	NMe-Leu
5	C-Ox-III	Phe	NMe-D-Phe	Oxazole	Leu	Lys(Cbz)
6	D-Ox-III	(2R,3R)-β-Benzoxy-Phe	Leu	Oxazole	D-Leu	D-Phe
7	D-Ox-II	(2R,3R)-β-Benzoxy-Phe	Oxazole	NMe-Val	D-Leu	D-Phe
8	D-Ox-I	Phenyl-Oxazole	Leu	NMe-Val	D-Leu	D-Phe
9	A-Th-III	Phe	Leu	Thiazole	Leu	Leu
10	B-Th-III	Phe	Leu	Thiazole	Leu	NMe-Leu
11	C-Th-III	Phe	NMe-D-Phe	Thiazole	Leu	Lys(Cbz)
12	A-PP-II	Phe	Thr(ΨMe,Me-Pro)	Val	Leu	Leu
13	A-PP-III	Phe	Leu	Thr(ΨMe,Me-Pro)	Leu	Leu

Table of cytotoxicity of additional compounds

Compound		PGI at 25μM	Error
B		86%	±0.3%
C		78.8%	±1.4%
D		47.5%	±5.1%
2	B-Tri-III	60.9%	±3.7%
4	B-Ox-III	23.4%	±6.0%
5	C-Ox-III	42.2%	±0.8%
6	D-Ox-III	2.3%	±1.3%
7	D-Ox-II	4.6%	±2.5%
8	D-Ox-I	2.9%	±1.6%
10	B-Th-III	14.0%	±5.0%
11	C-Th-III	6.1%	±1.9%
12	A-PP-II	7.7%	±3.3%

Molecular models of all compounds in stereo



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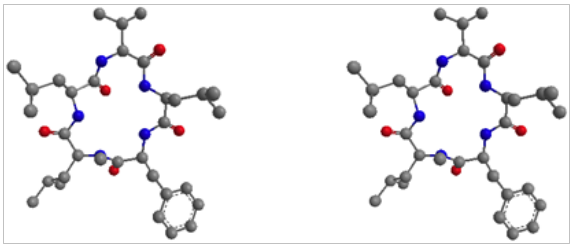

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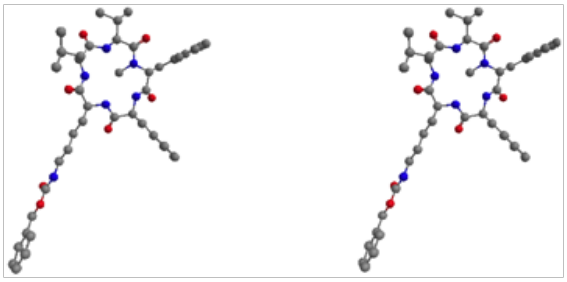
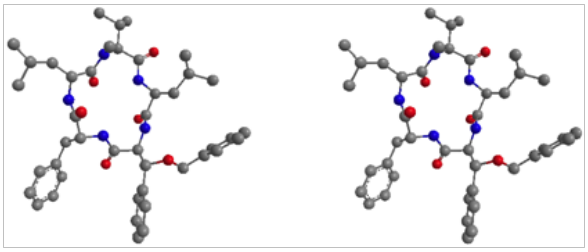
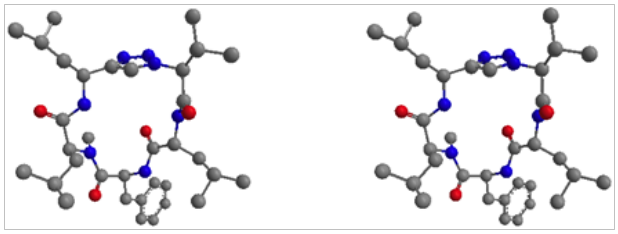


Compound C



Compound D

Compound 1



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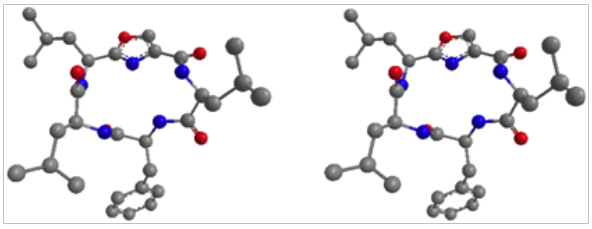

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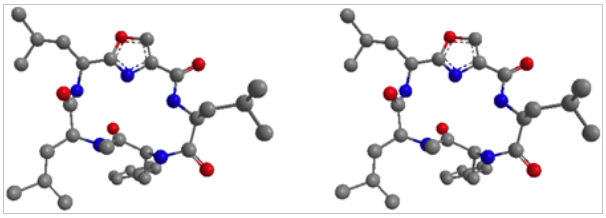

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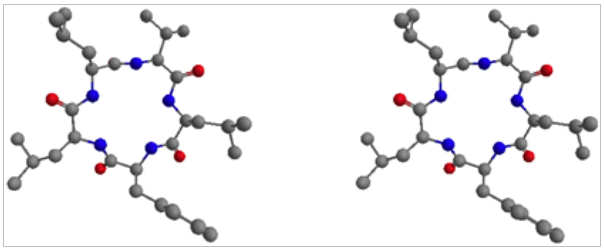

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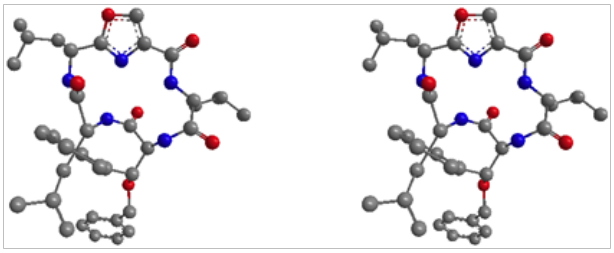

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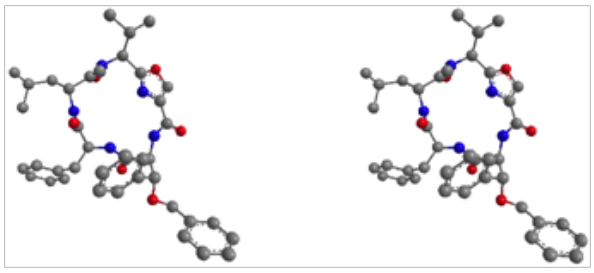

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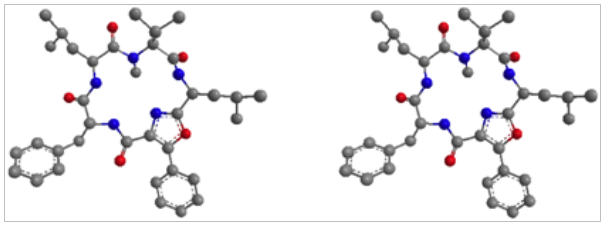
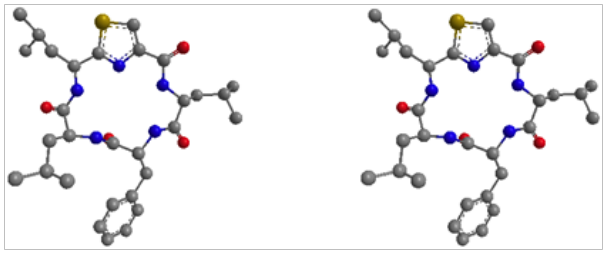


Compound 8



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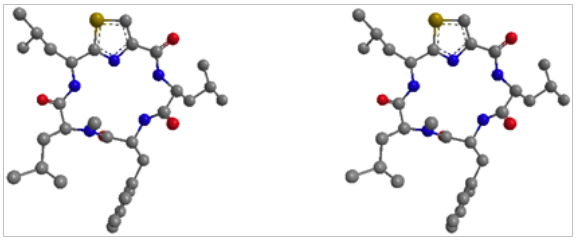

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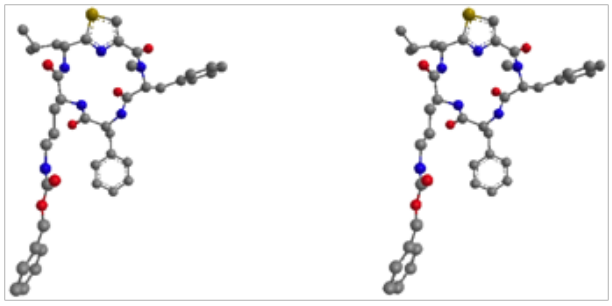

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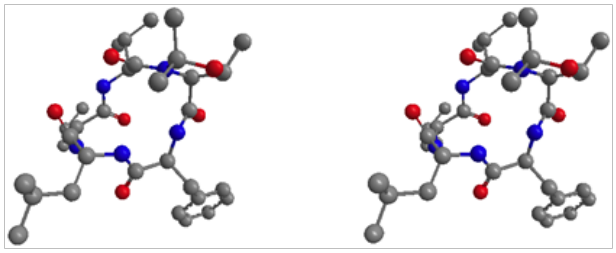

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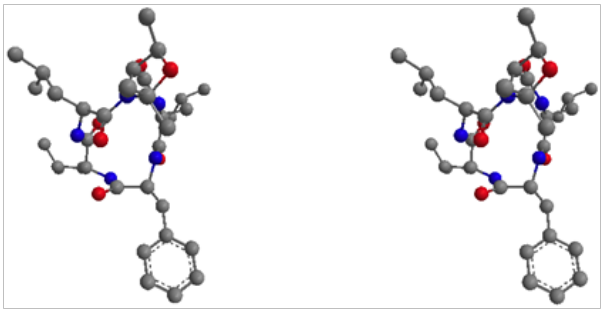

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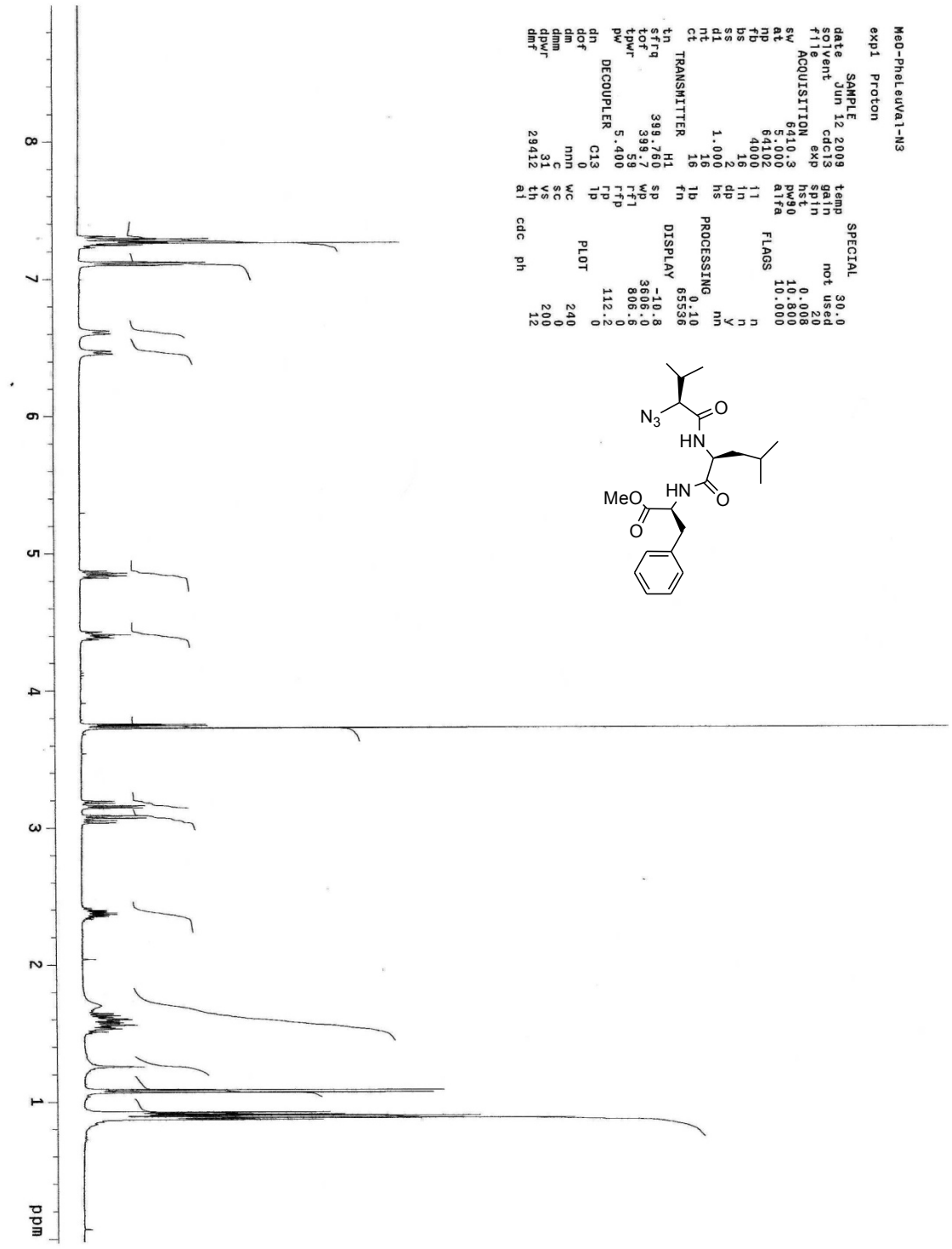
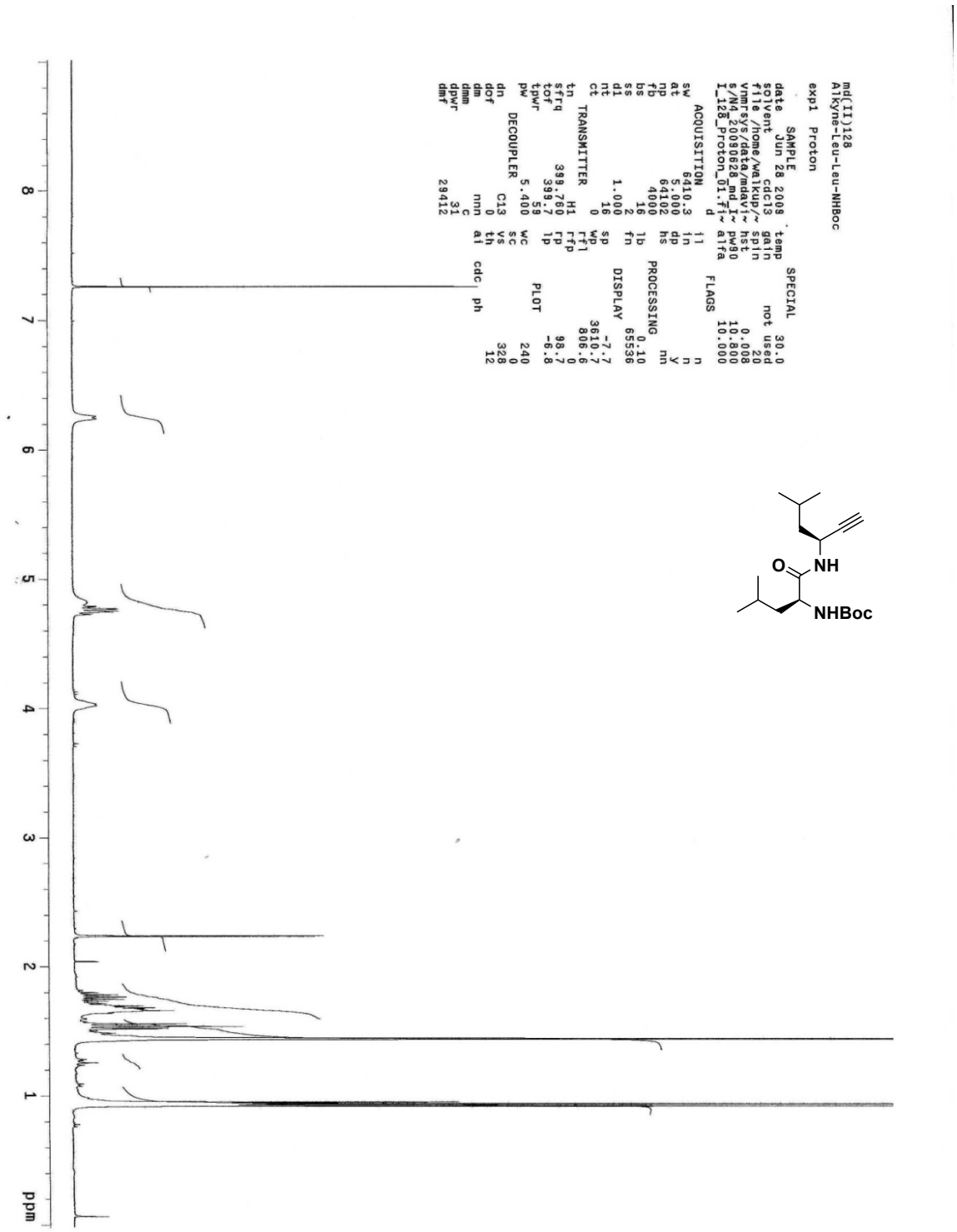


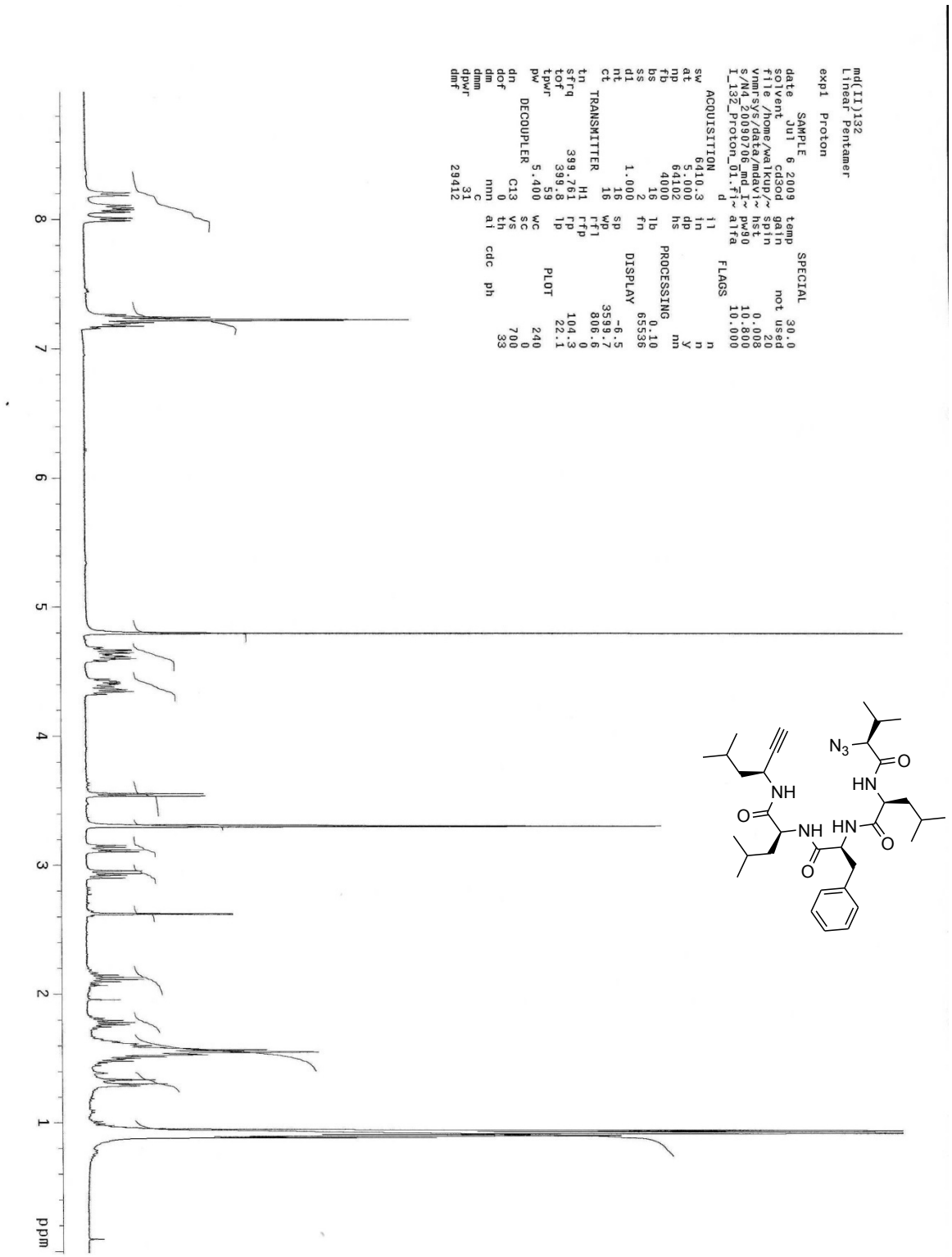
Compound 1: A-Tri-III

NMR Tripeptide MeO-Phe-Leu-Val-N_3 (22)



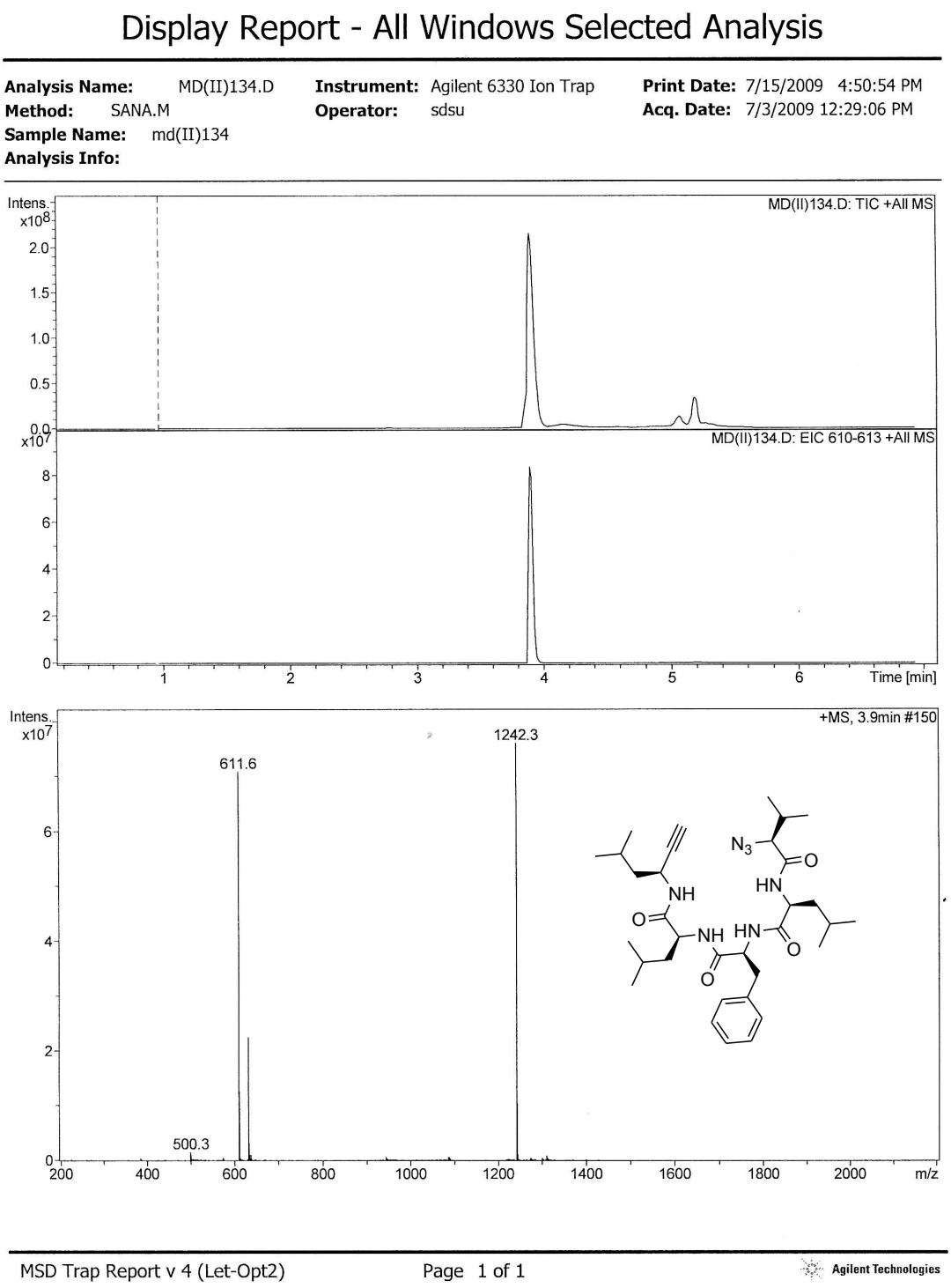
Compound 1: A-Tri-III

NMR Dipeptide Alkyne-Leu-Leu-NHBoc



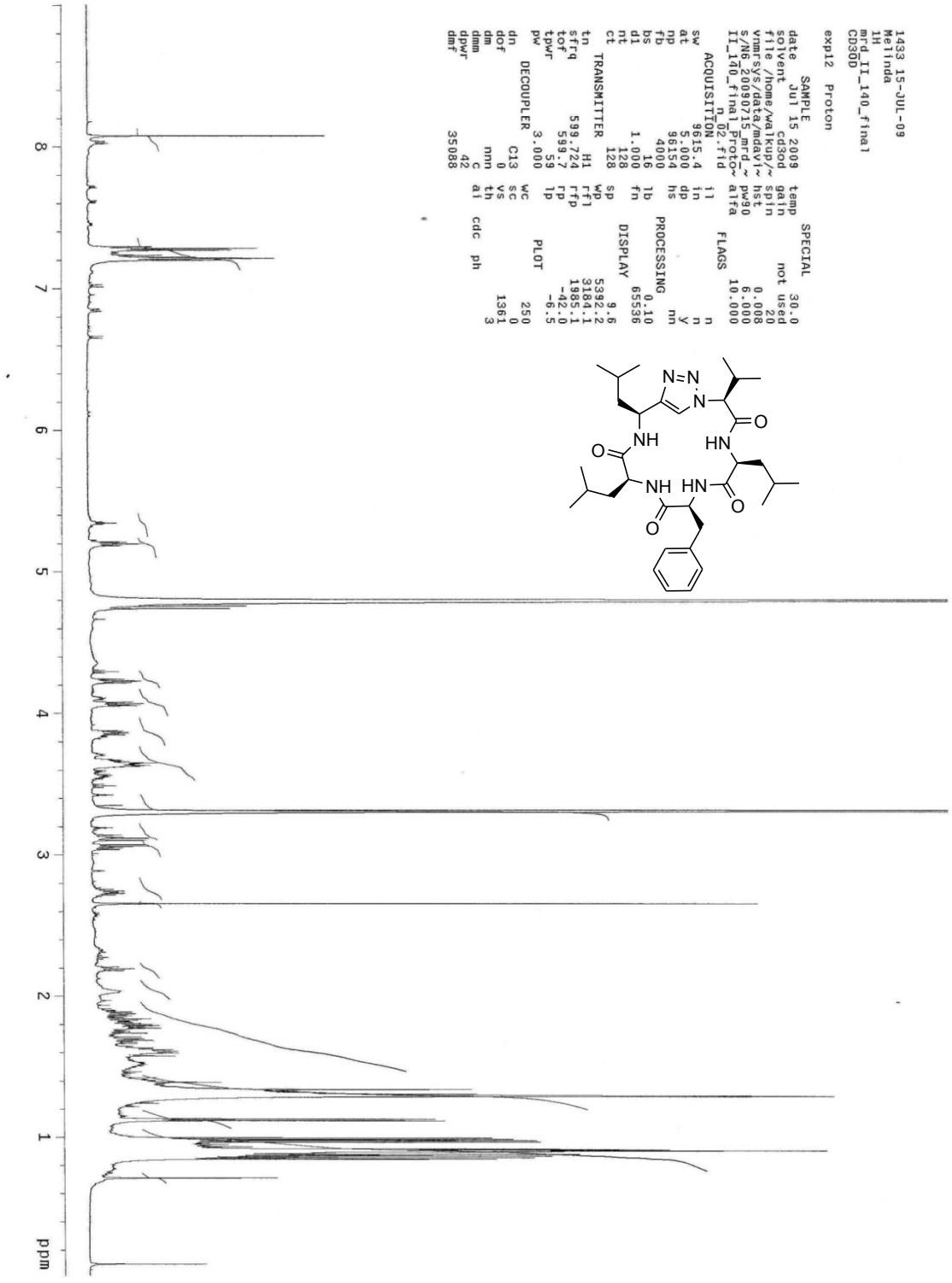
Compound 1: A-Tri-III

NMR Pentapeptide Alkyne-Leu-Leu-Phe-Leu-Val-N_3 (23)



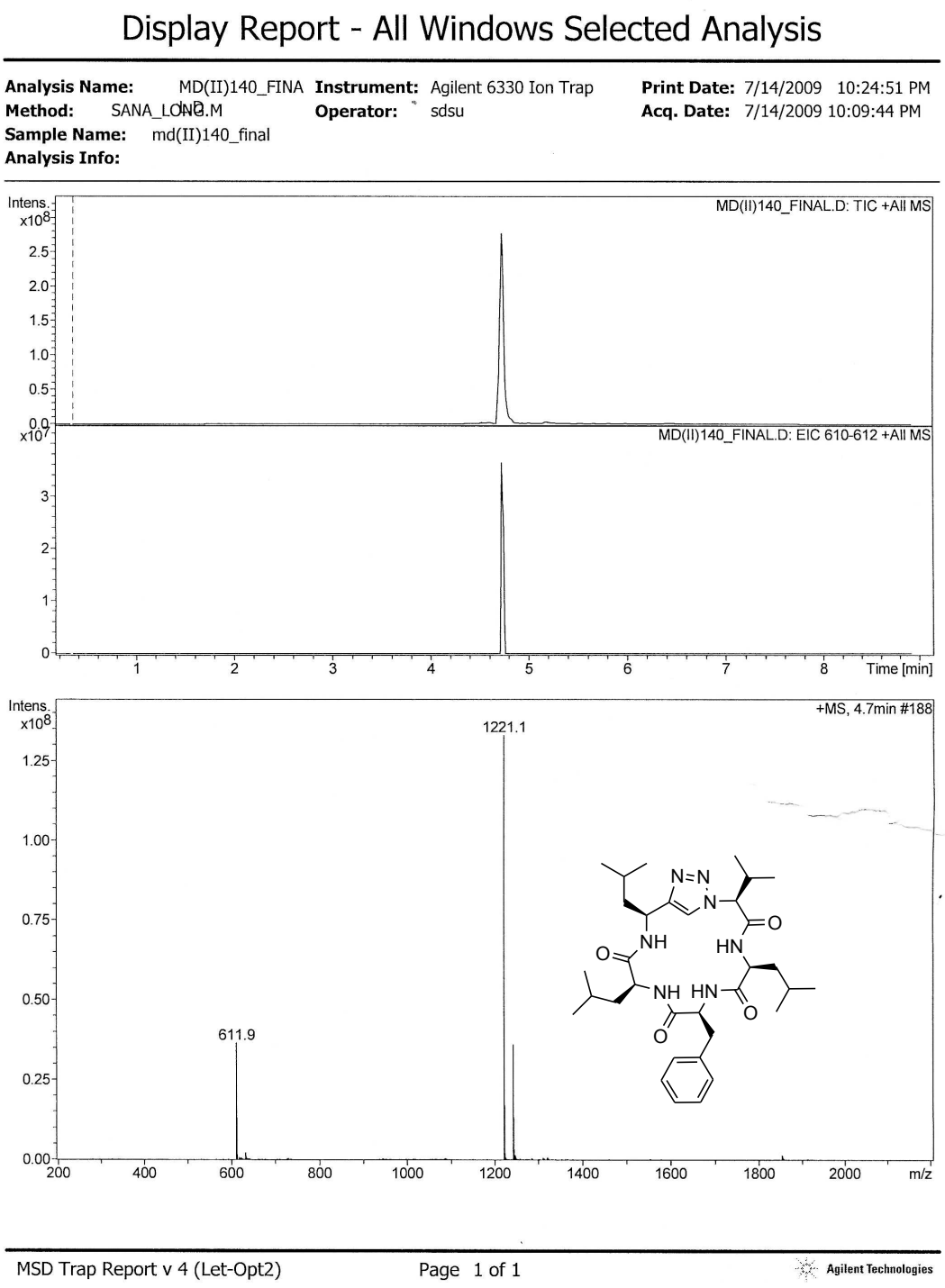
Compound 1: A-Tri-III

LCMS Pentapeptide Alkyne-Leu-Leu-Phe-Leu-Val-N_3 (23) (MW = 611)



Compound 1: A-Tri-III

NMR Macrocycle Phe-Leu-Val-Triazole-Leu-Leu (1)



Compound 1: A-Tri-III

LCMS Macrocycle Phe-Leu-Val-Triazole-Leu-Leu (1) (MW = 610)

SDSU

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Reported by User: System

Breeze

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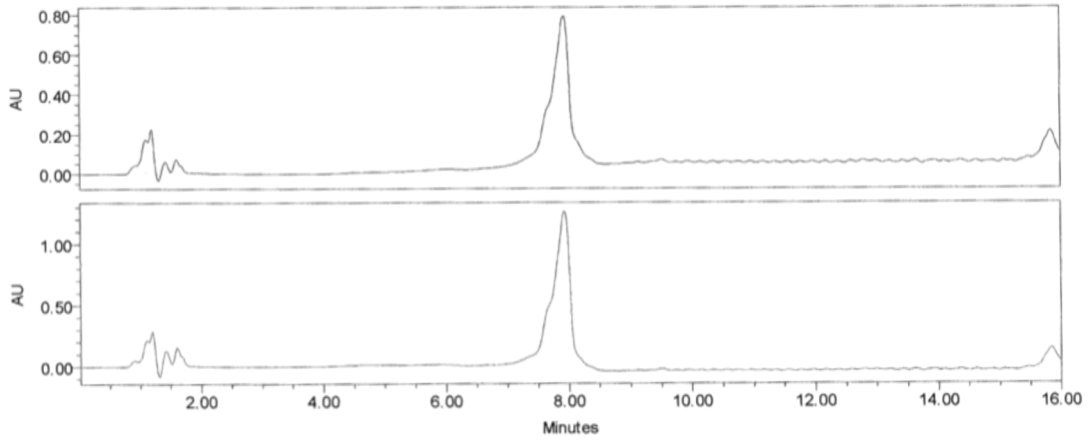

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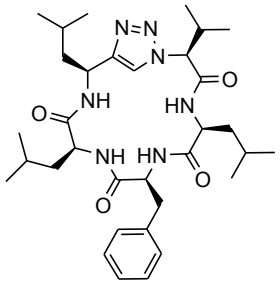

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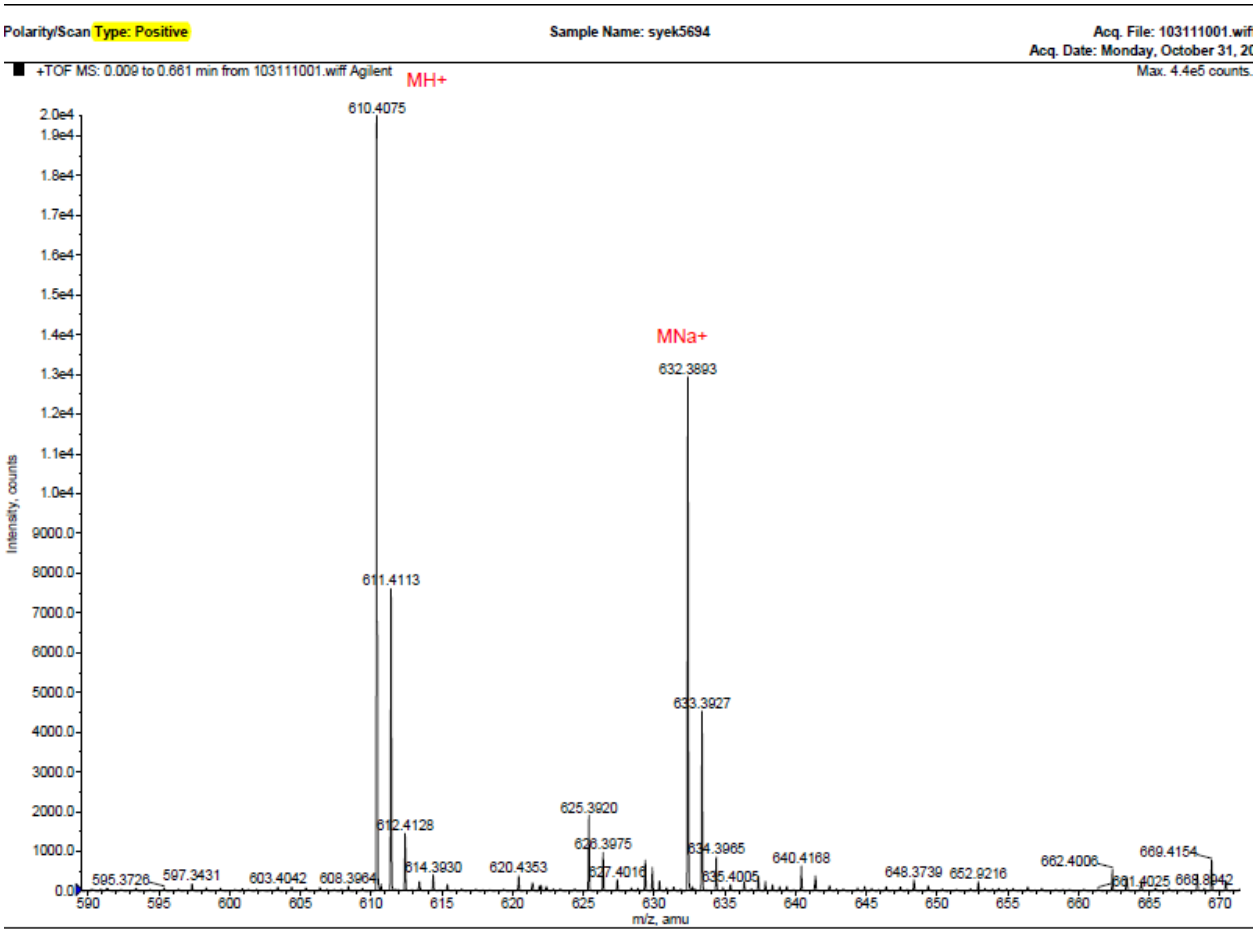
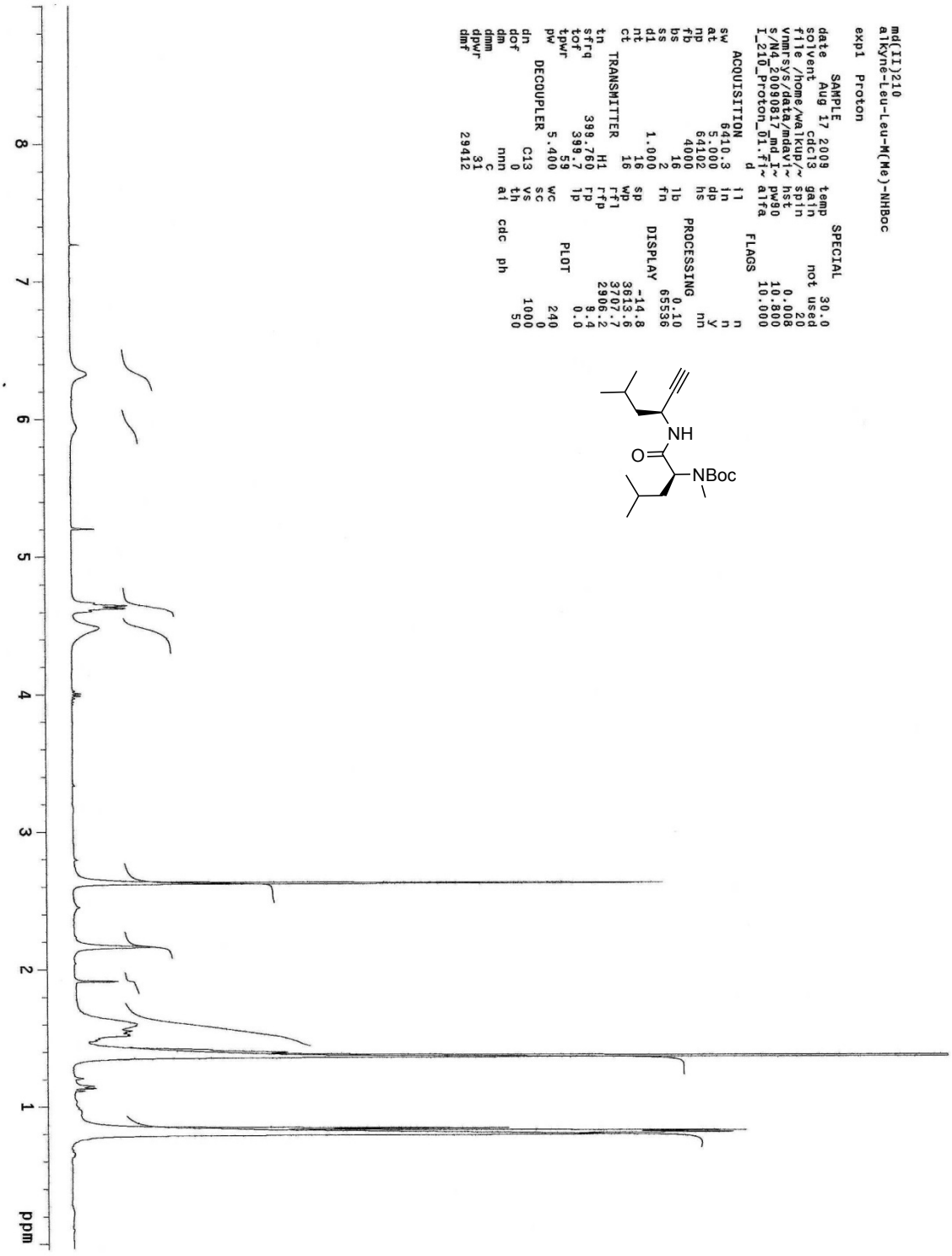
Compound 1: A-Tri-III

HPLC Macrocycle Phe-Leu-Val-Triazole-Leu-Leu (1)



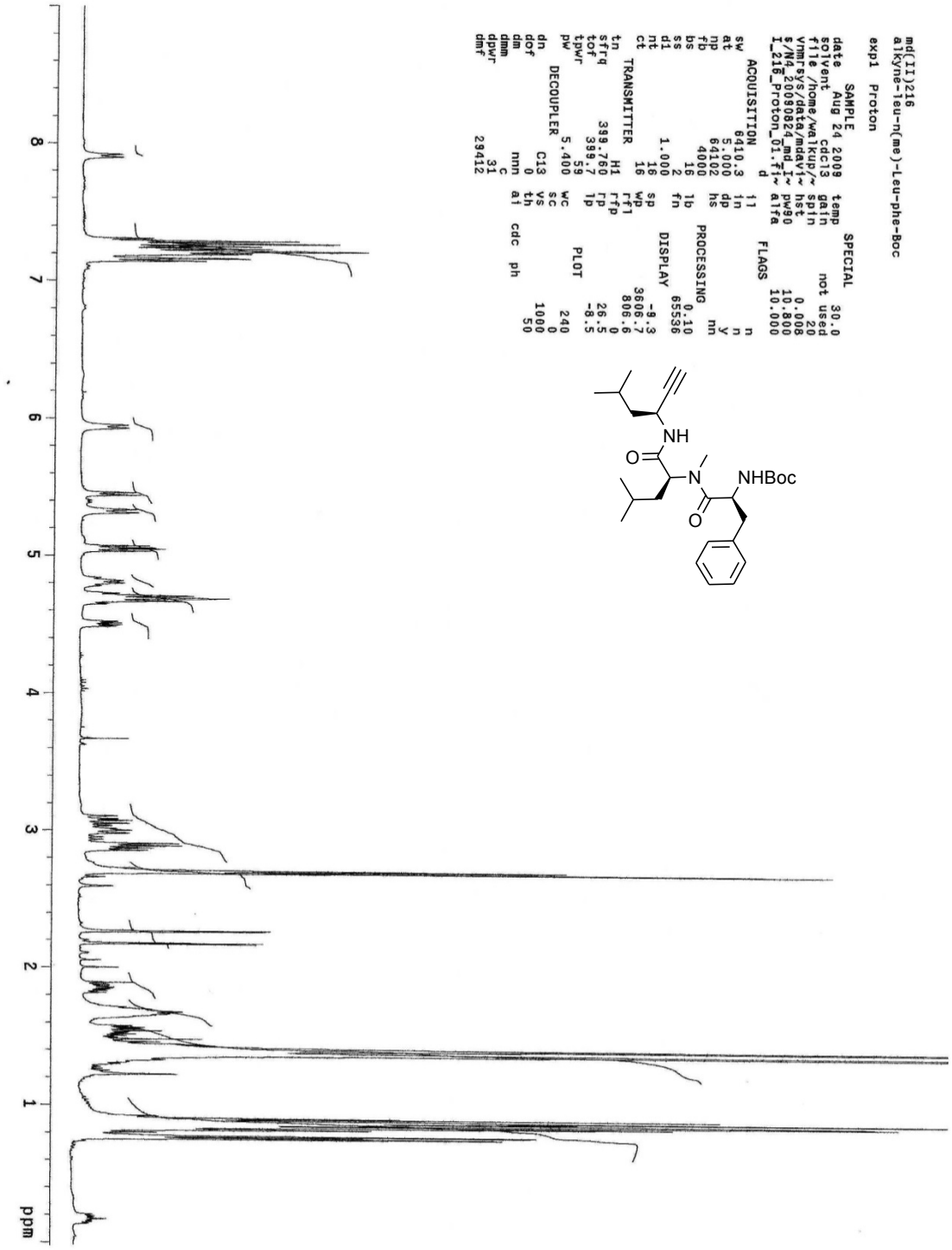
Compound 1: A-Tri-III

HRMS Macrocycle Phe-Leu-Val-Triazole-Leu-Leu (1) (MW = 610.4075)



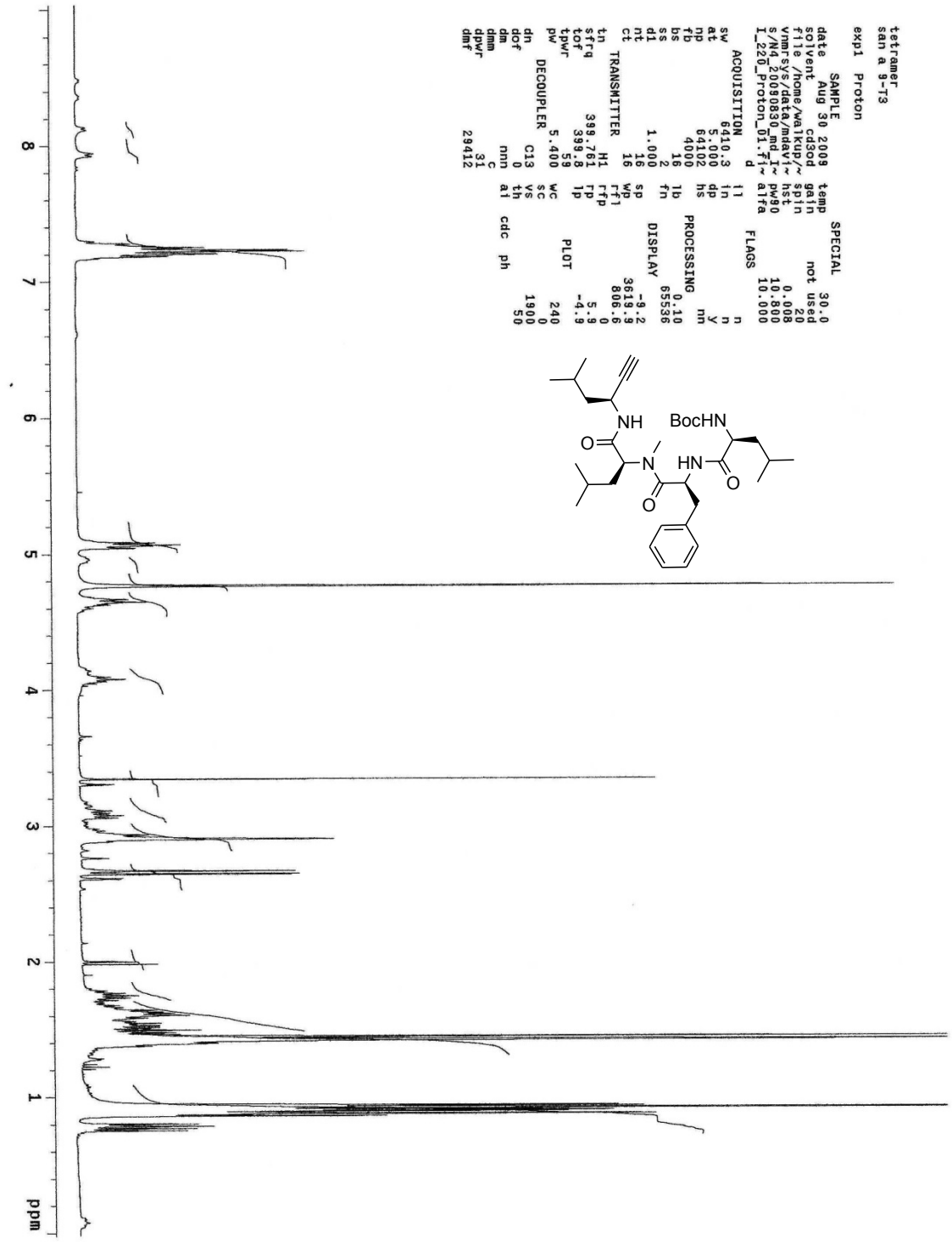
Compound 2: B-Tri-III

NMR Dipeptide Alkyne-Leu-Leu-N(Me)Boc



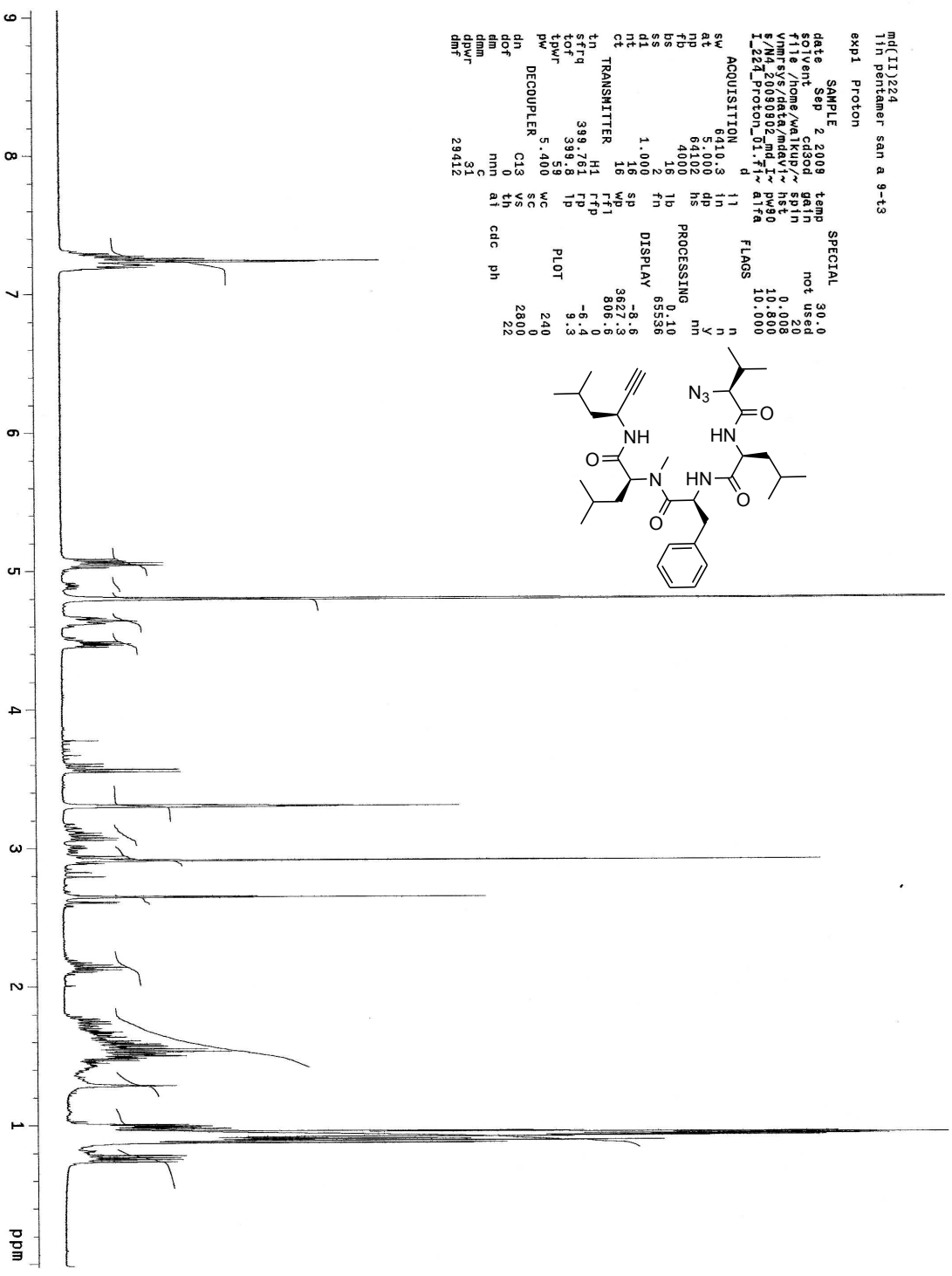
Compound 2: B-Tri-III

NMR Tripeptide Alkyne-Leu-Leu-N(Me)-Phe-NHBoc



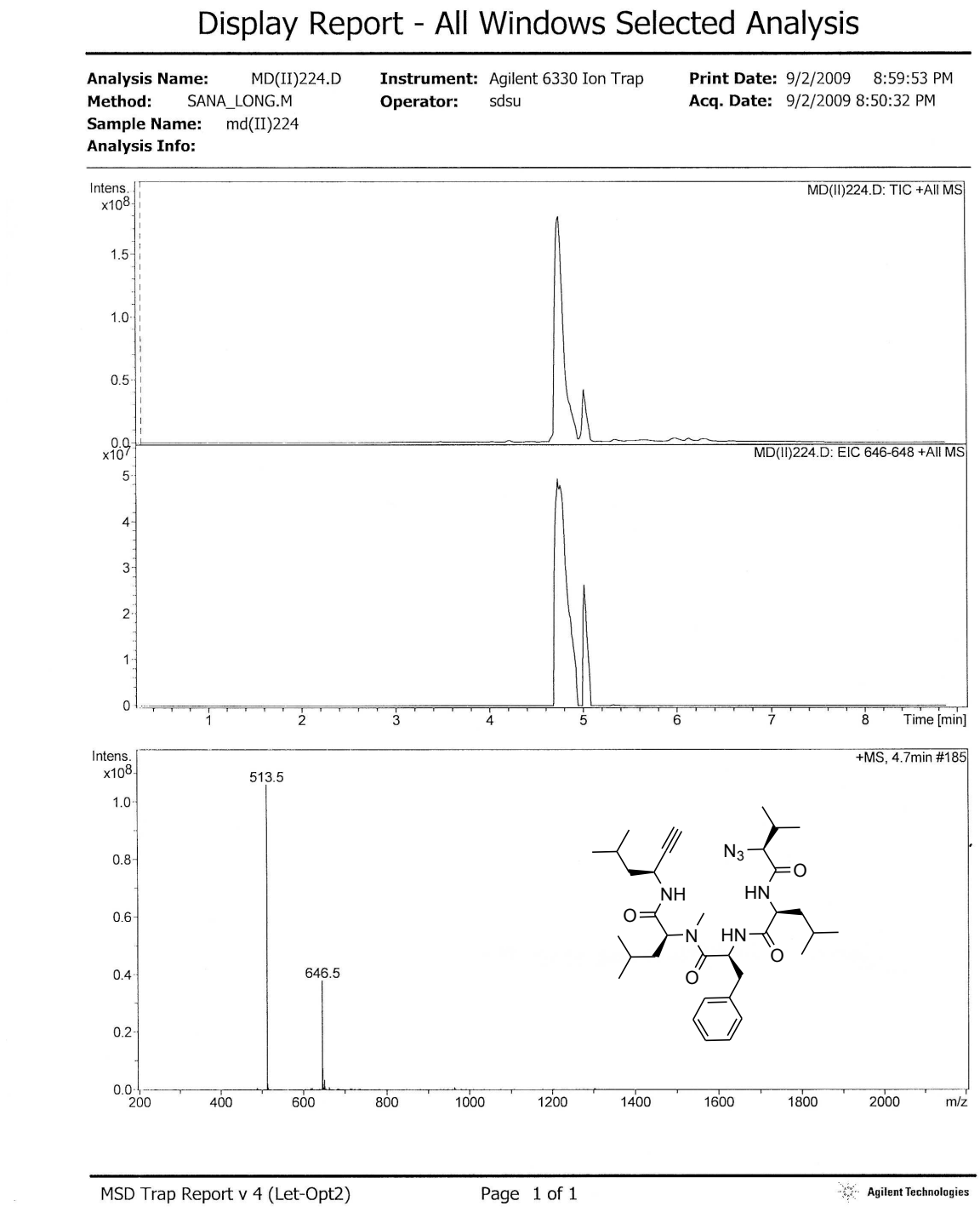
Compound 2: B-Tri-III

NMR Tetrapeptide Alkyne-Leu-Leu-N(Me)-Phe-Leu-NHBoc



Compound 2: B-Tri-III

NMR Pentapeptide Alkyne-Leu-Leu-N(Me)-Phe-Leu-Val-N_3 (33)



Compound 2: B-Tri-III

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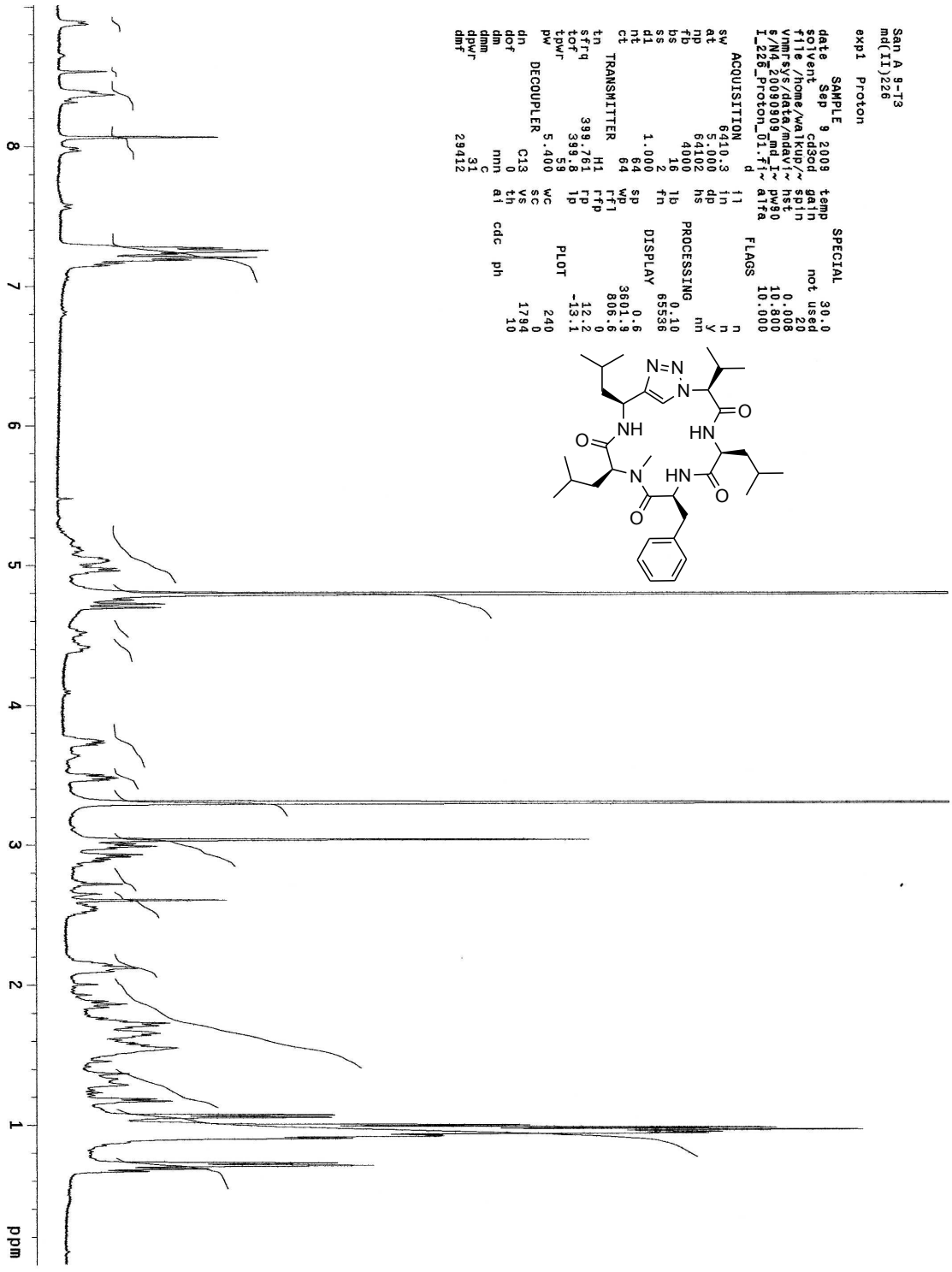

Compound 2: B-Tri-III

NMR Macrocycle Phe-Leu-Val-Triazole-Leu-Leu-N(Me) (2)

Display Report - All Windows Selected Analysis

Analysis Name: MD(II)226_FINA **Instrument:** Agilent 6330 Ion Trap **Print Date:** 9/9/2009 9:04:20 PM
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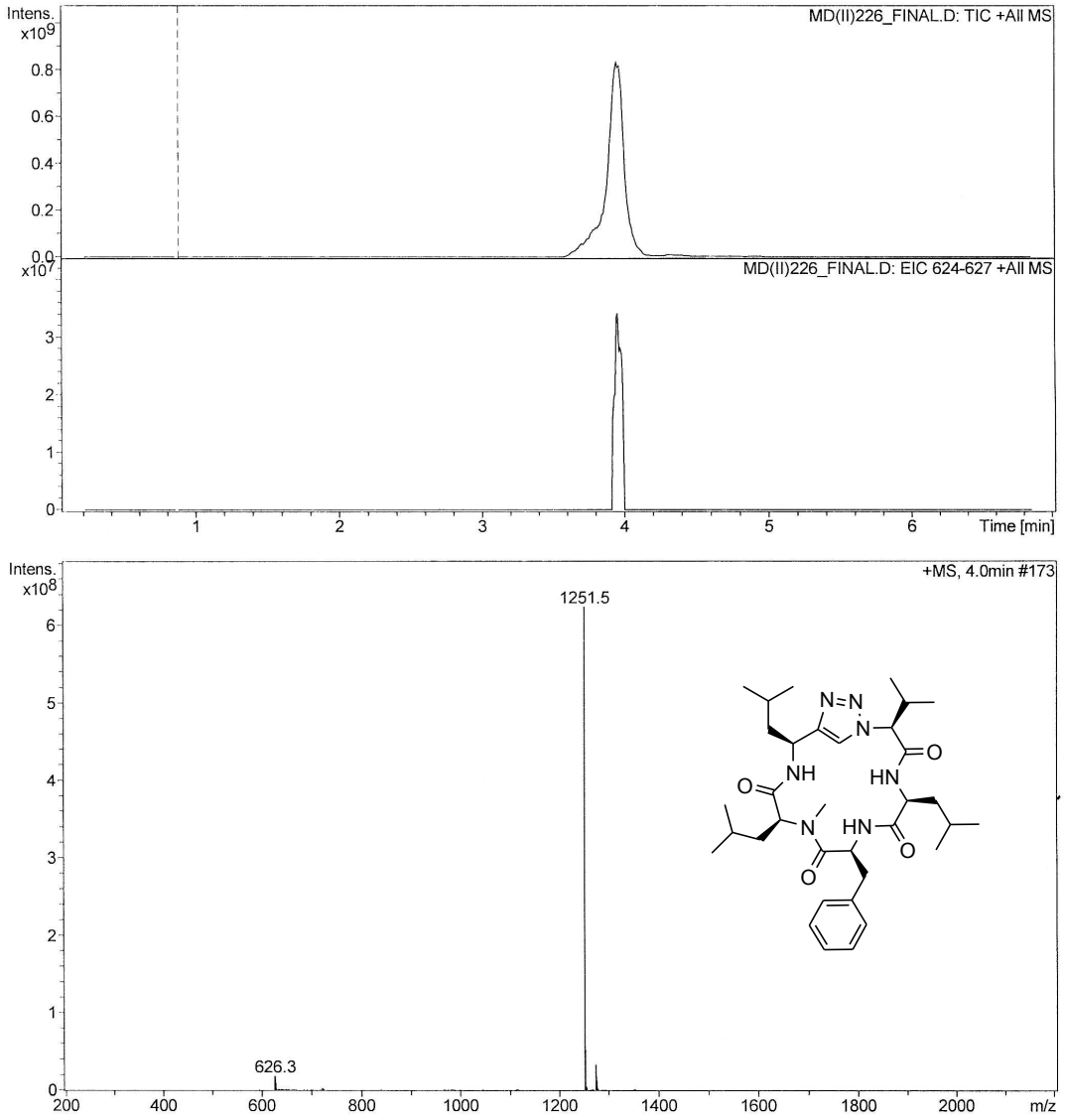
Analysis Info:



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Compound 2: B-Tri-III

LCMS Macrocycle Phe-Leu-Val-Triazole-Leu-Leu-N(Me) (2) (MW = 624)

SDSU

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

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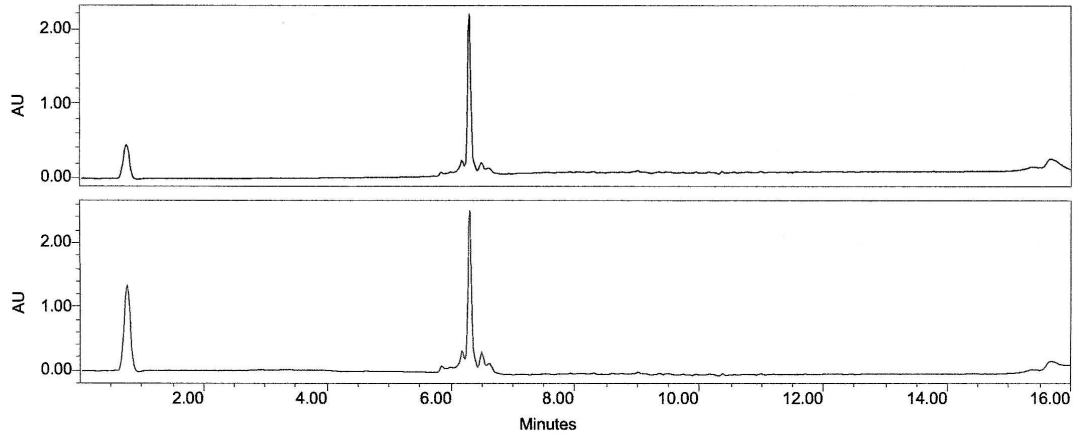
Run Time:	16.00 Minutes	Injection Volume:	50.00 ul



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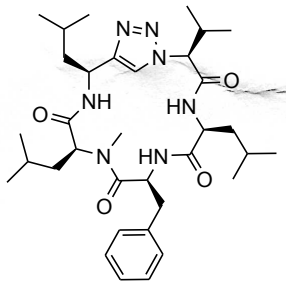
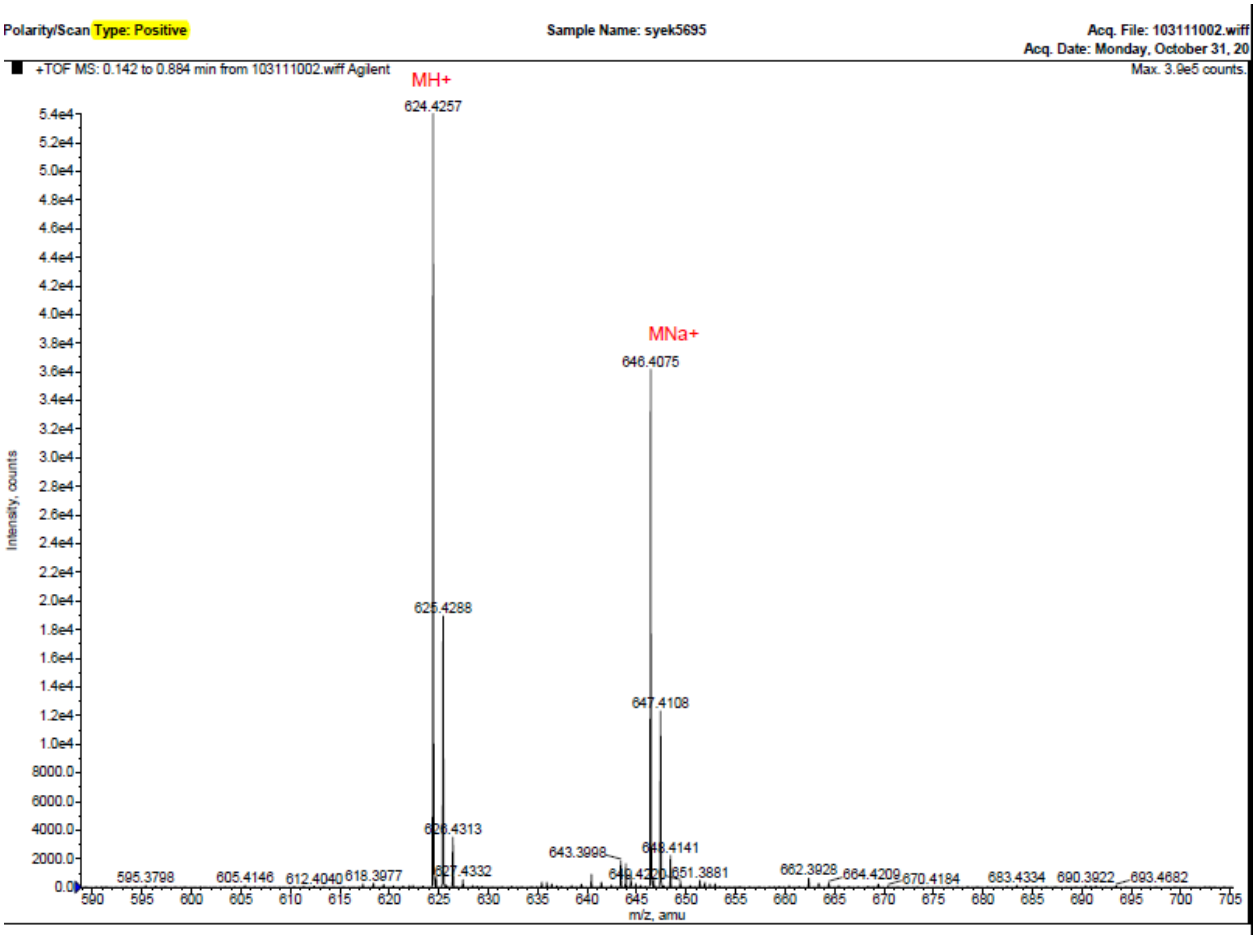


Report Method: Injection Summary Report Printed 10:59:54 PM 9/7/2009 Page: 1 of 1

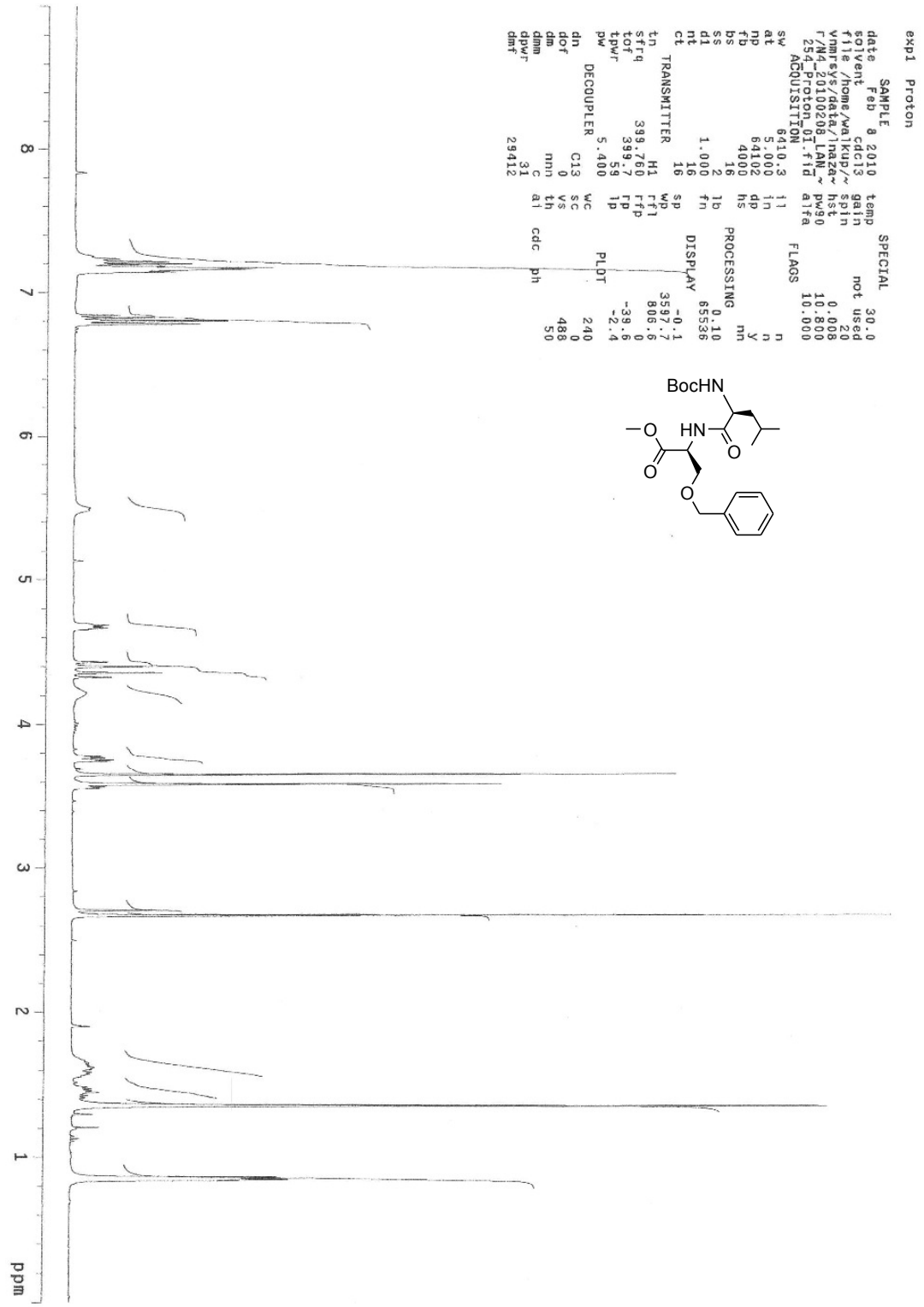
Compound 2: B-Tri-III

HPLC Macrocycle Phe-Leu-Val-Triazole-Leu-Leu-N(Me) (2)



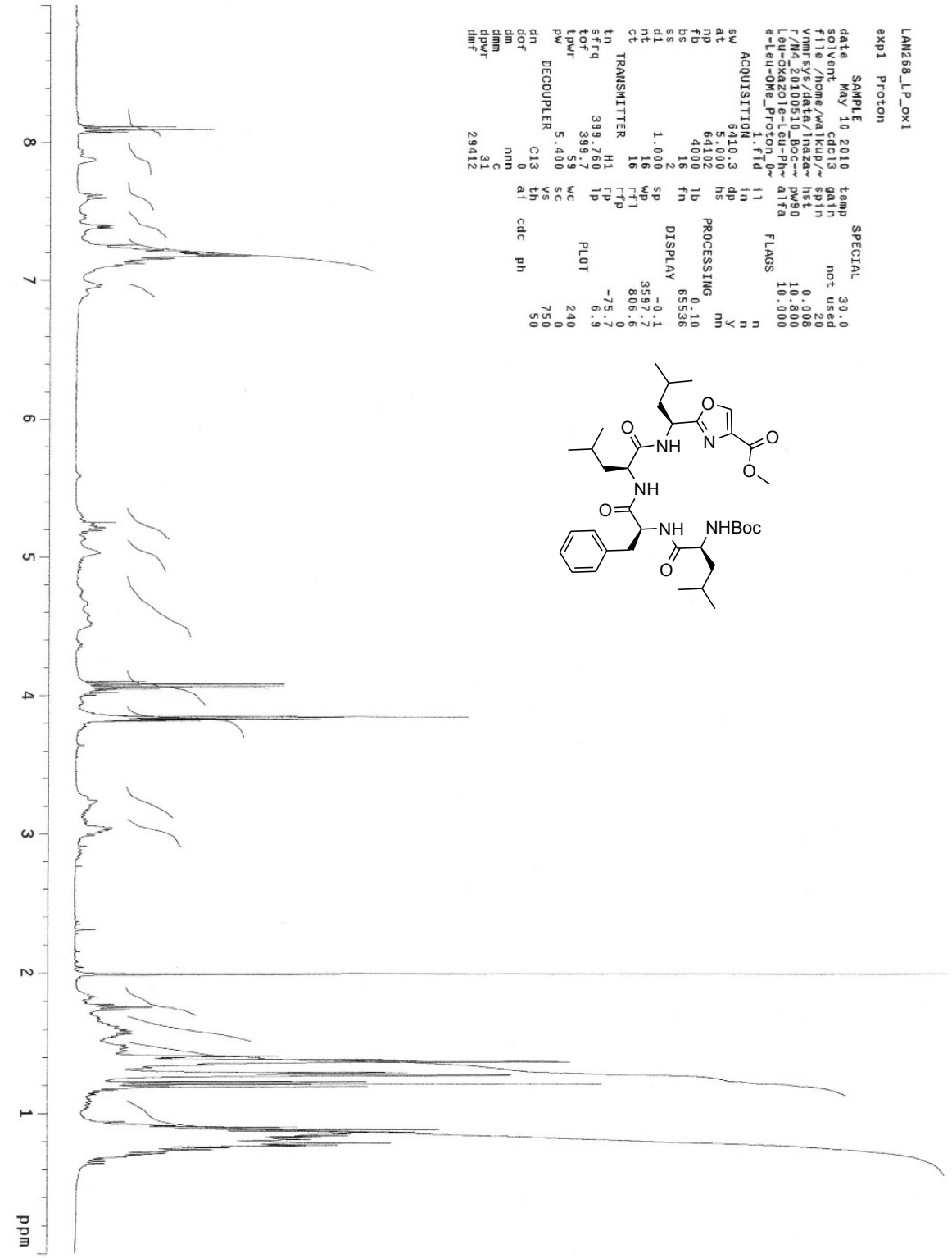
Compound 2: B-Tri-III

HRMS Macrocycle Phe-Leu-Val-Triazole-Leu-Leu-N(Me) (2) (MW = 624.4257)



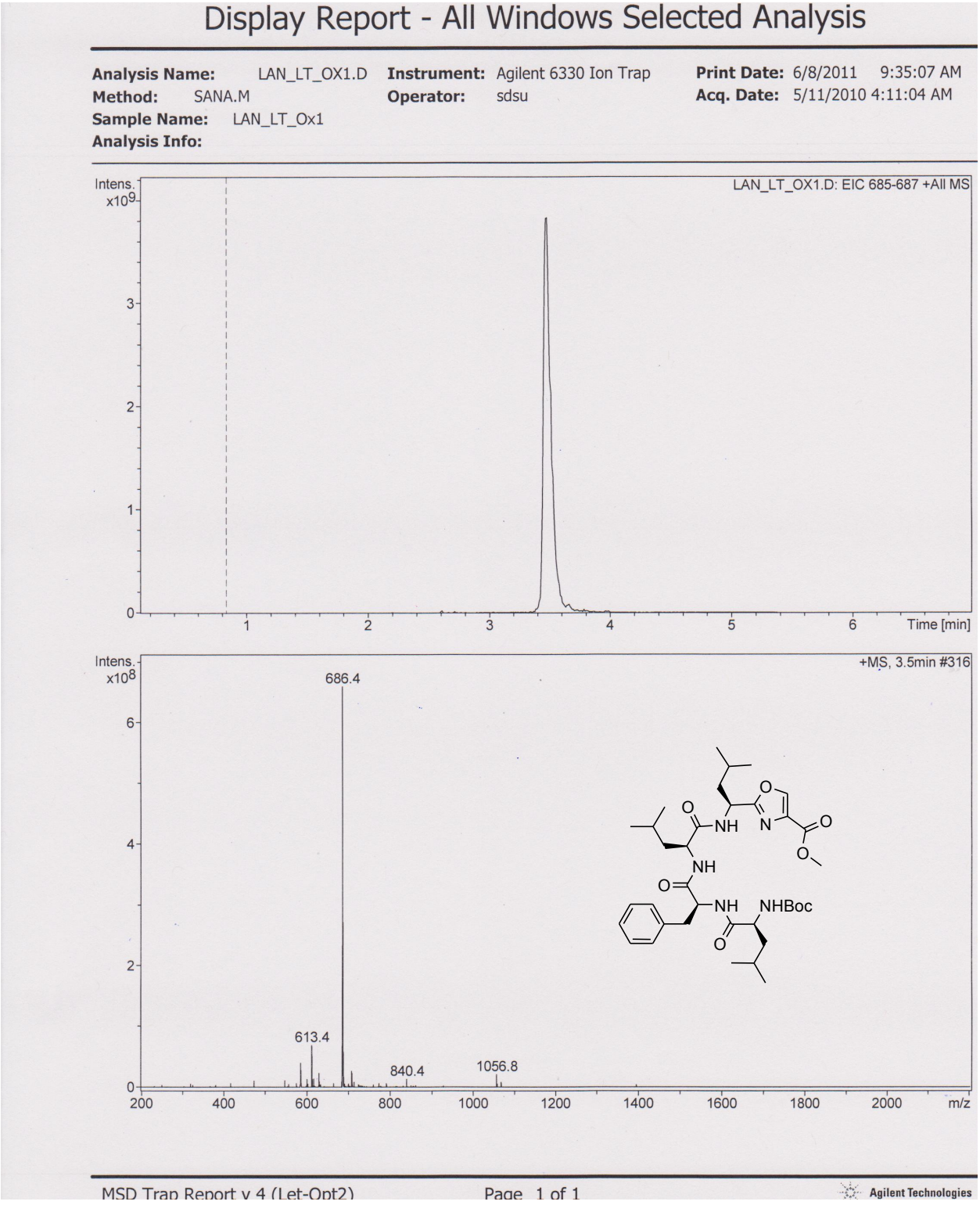
Compound 3: A-Ox-III

NMR Dipeptide MeO-Ser(Bzl)-Leu-NHBoc



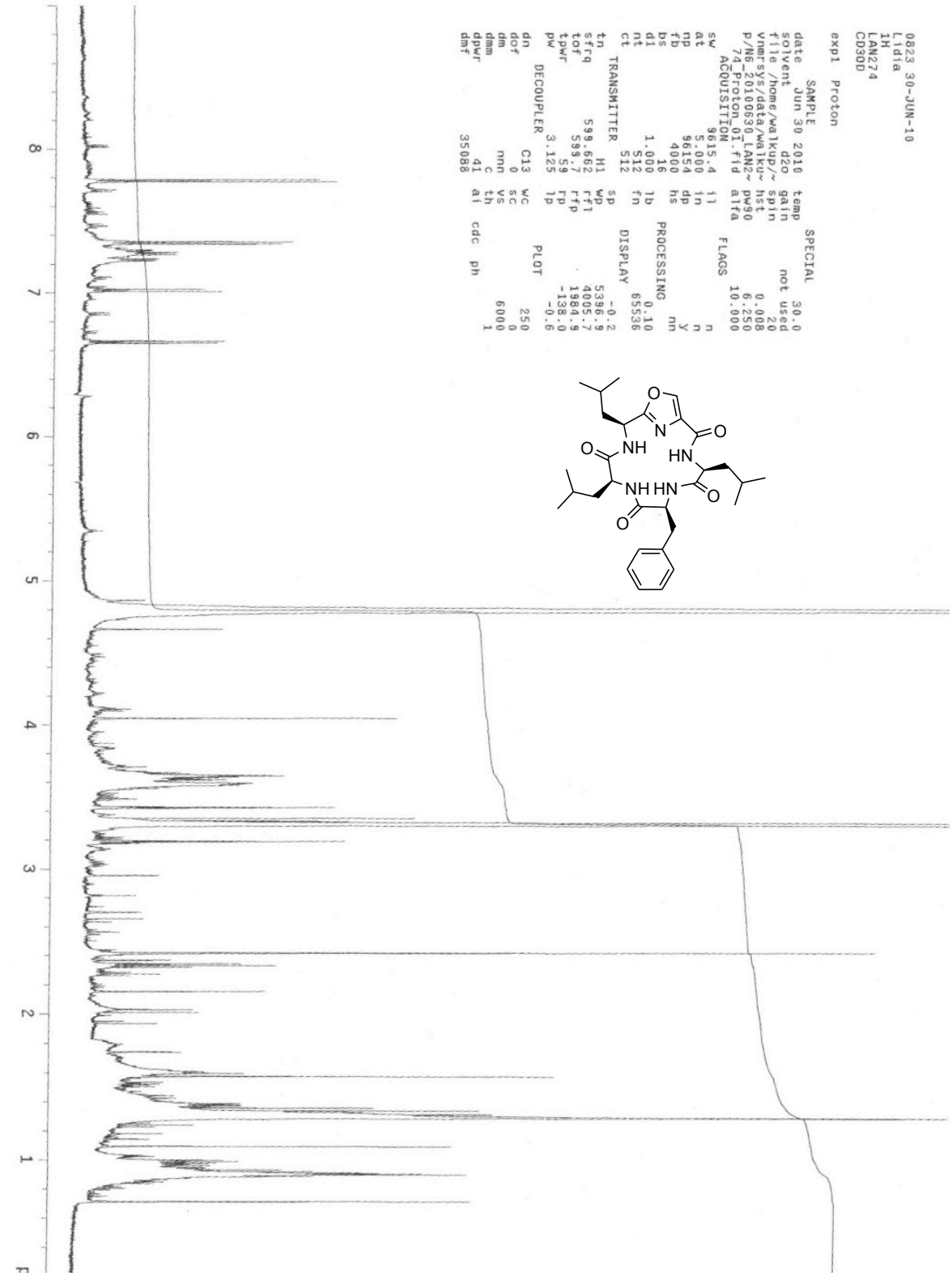
Compound 3: A-Ox-III

NMR Pentapeptide MeO-Oxazole-Leu-Leu-Phe-Leu-NHBoc (43)



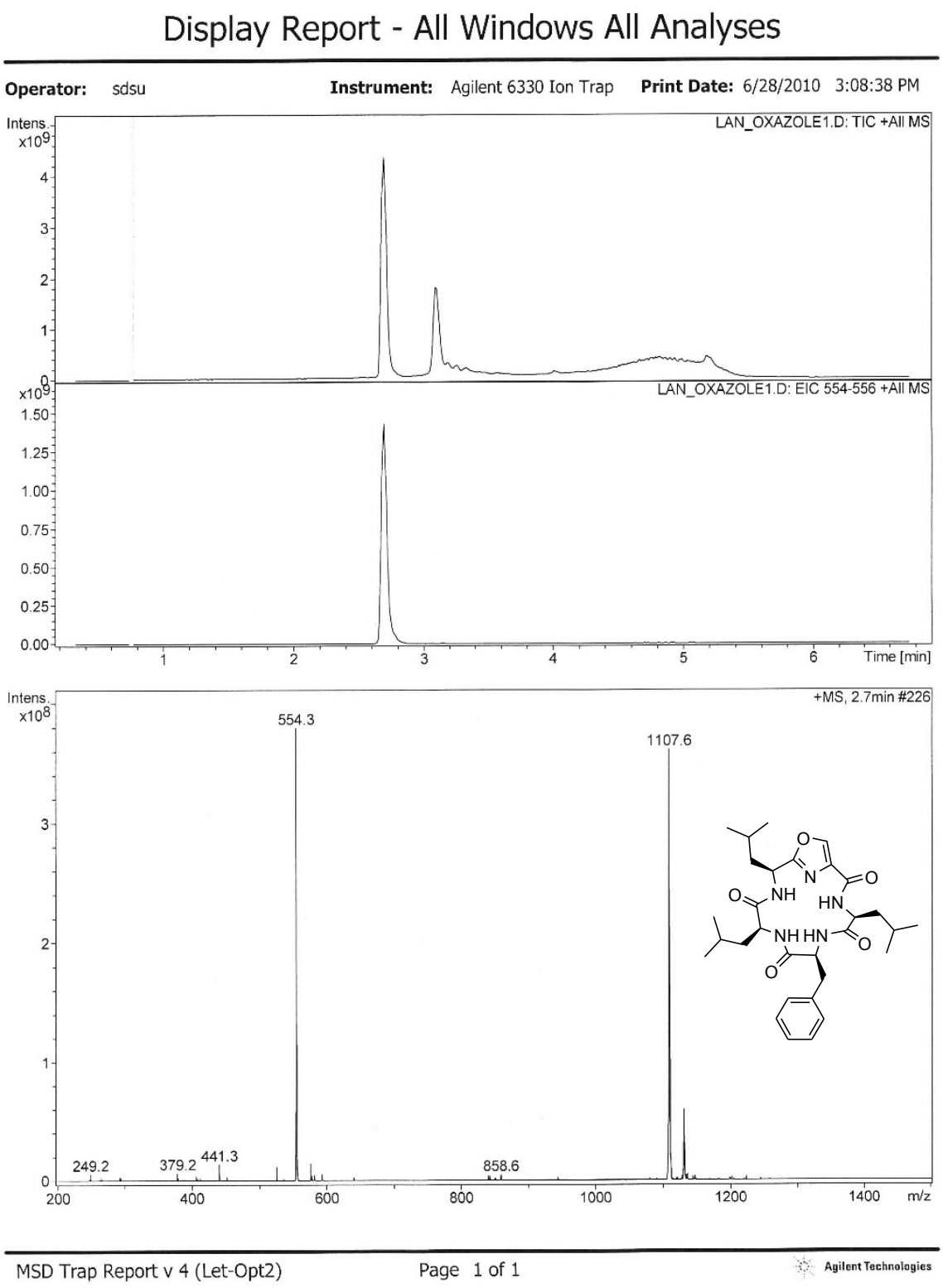
Compound 3: A-Ox-III

LCMS Linear pentapeptide MeO-Oxazole-Leu-Leu-Phe-Leu-NHBoc (43) (MW = 685.85)



Compound 3: A-Ox-III

NMR Macrocycle Phe-Leu-Oxazole-Leu-Leu (3)



Compound 3: A-Ox-III

LCMS Macrocycle Phe-Leu-Oxazole-Leu-Leu (3) (MW = 553.69)

SDSU

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

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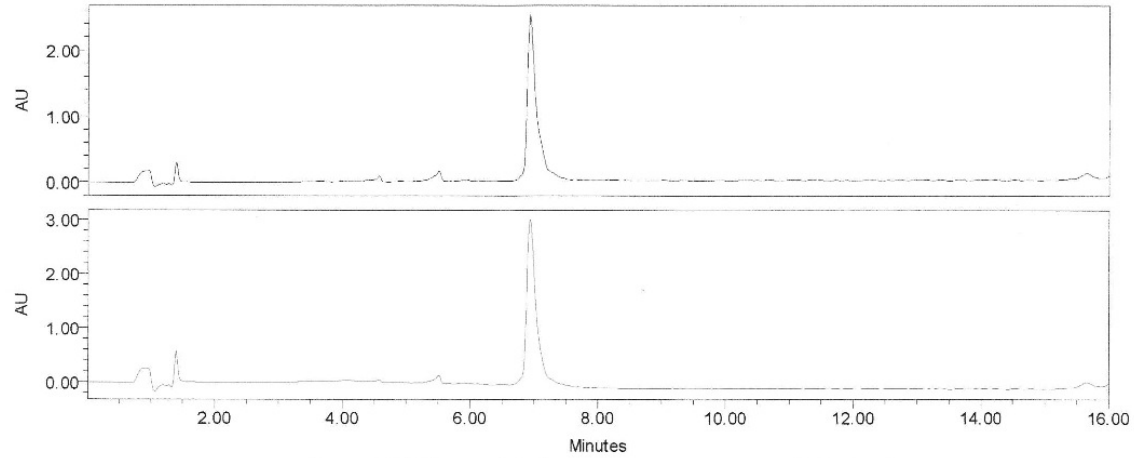

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Channel: 2487Channel 2 Channel Desc.: Processing Method: ****

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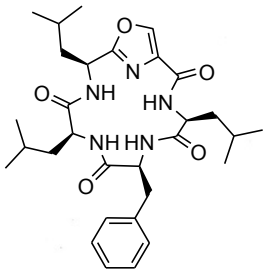

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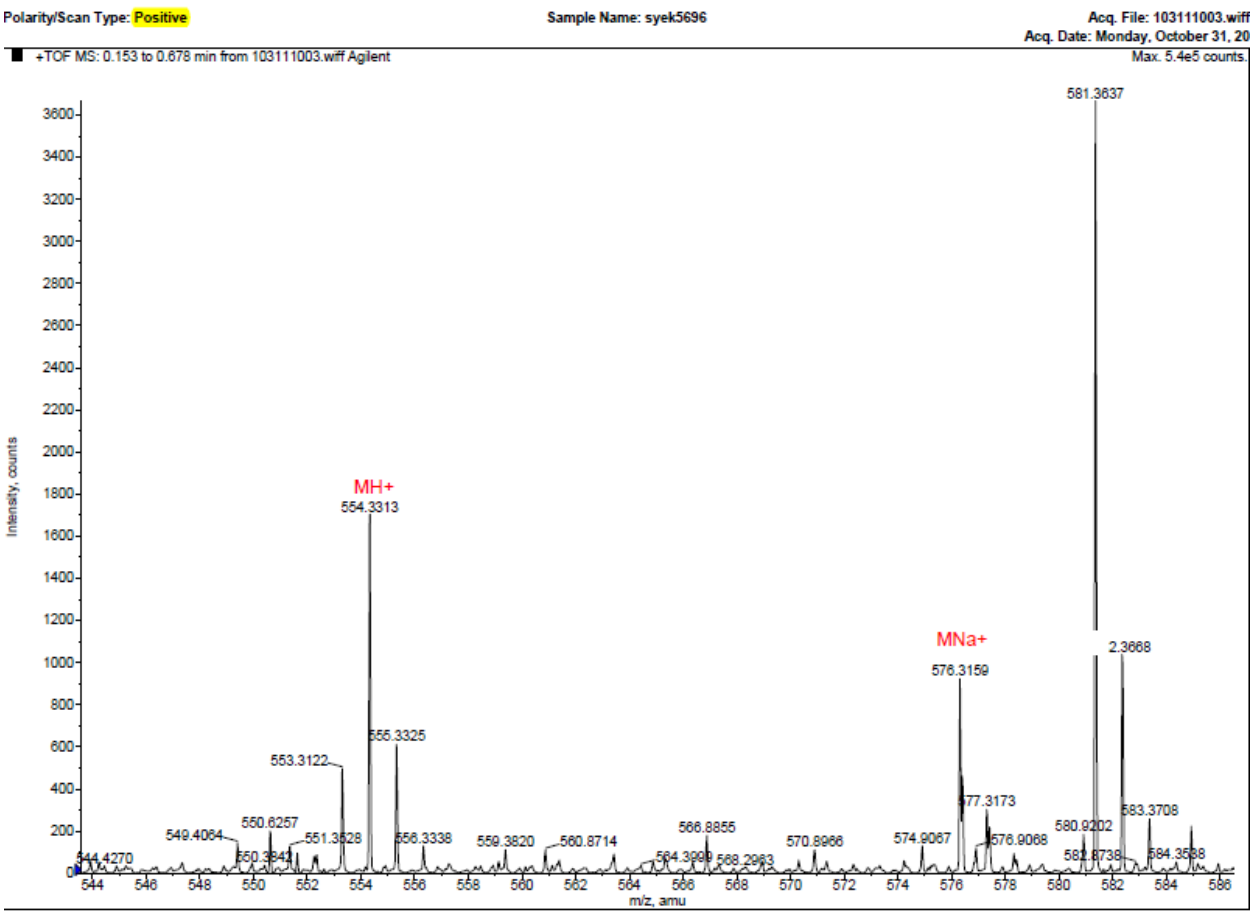
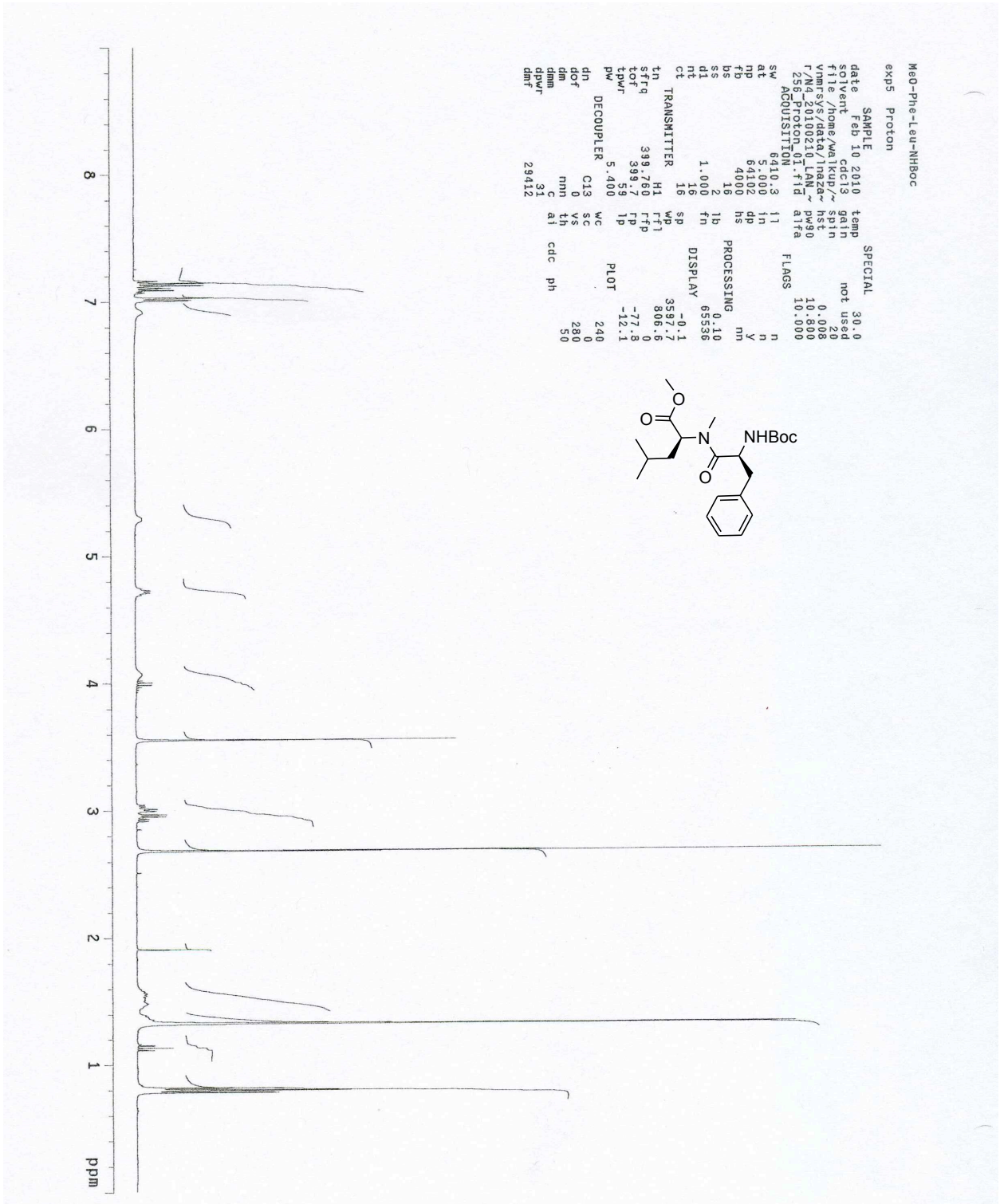
Compound 3: A-Ox-III

HPLC Macrocycle Phe-Leu-Oxazole-Leu-Leu (3)



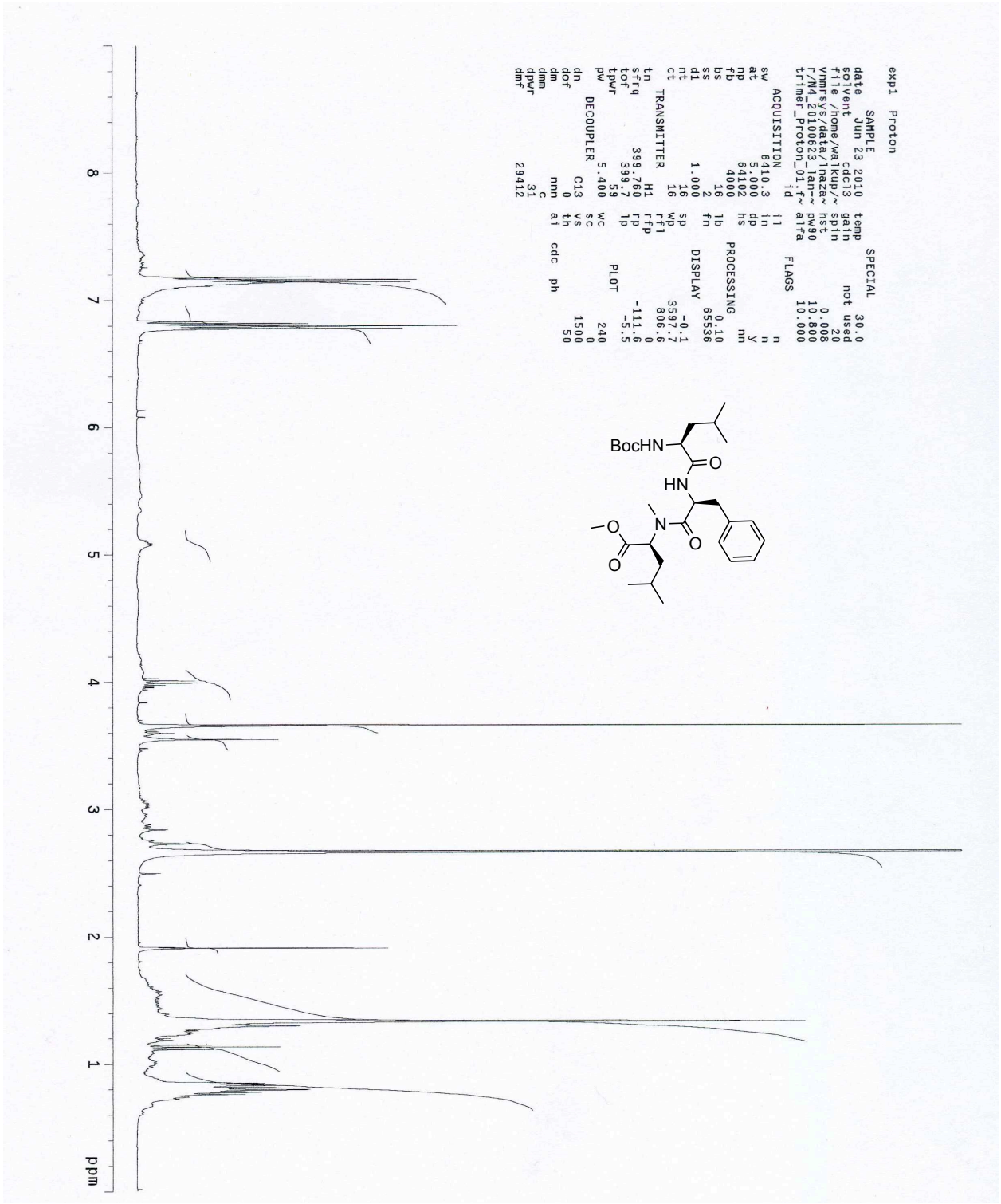
Compound 3: A-Ox-III

HRMS Macrocycle Phe-Leu-Oxazole-Leu-Leu (3) (MW = 554.3313)



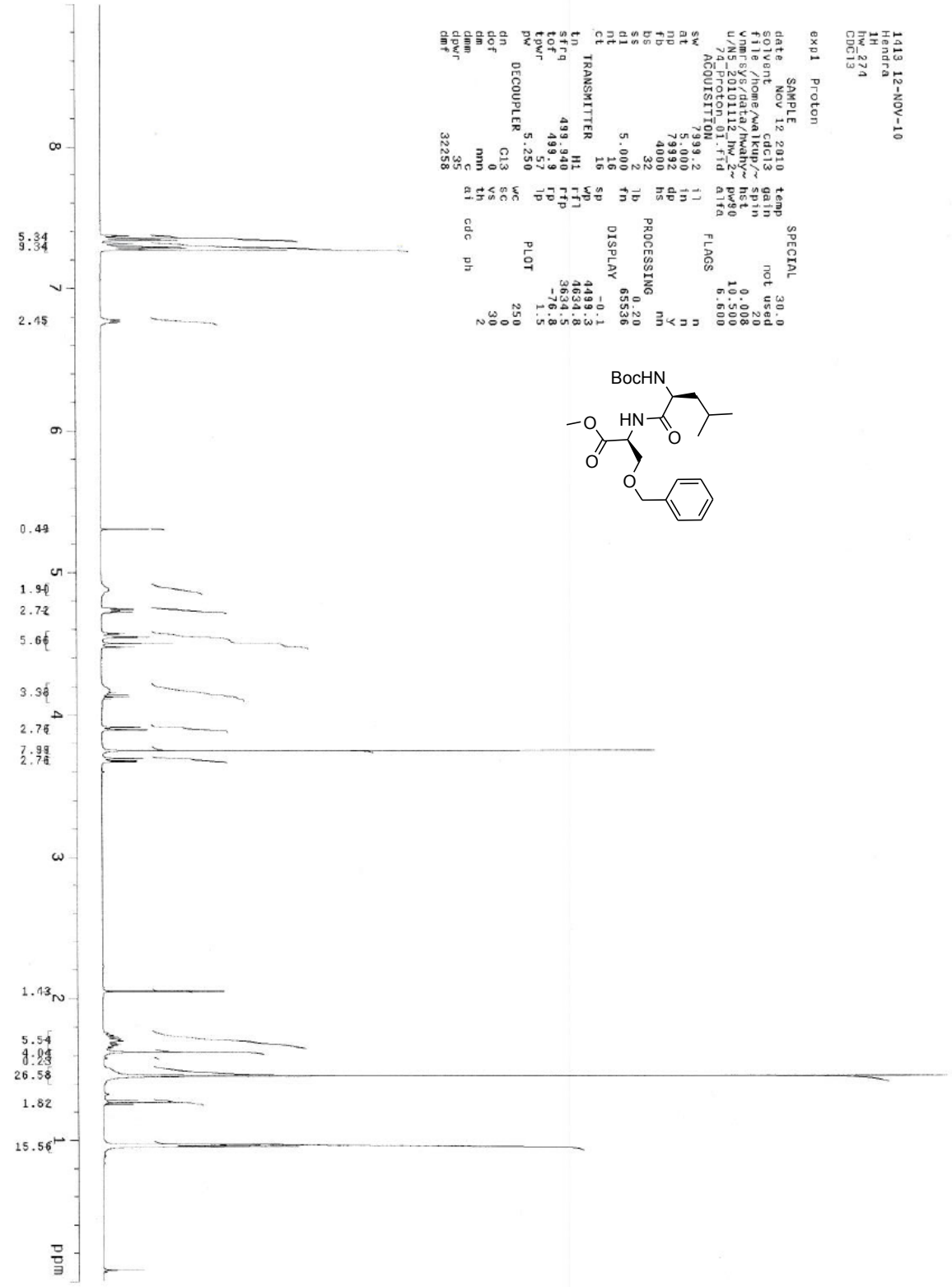
Compound 4: B-Ox-III

NMR Dipeptide MeO-Leu-N(Me)-Phe-NHBoc



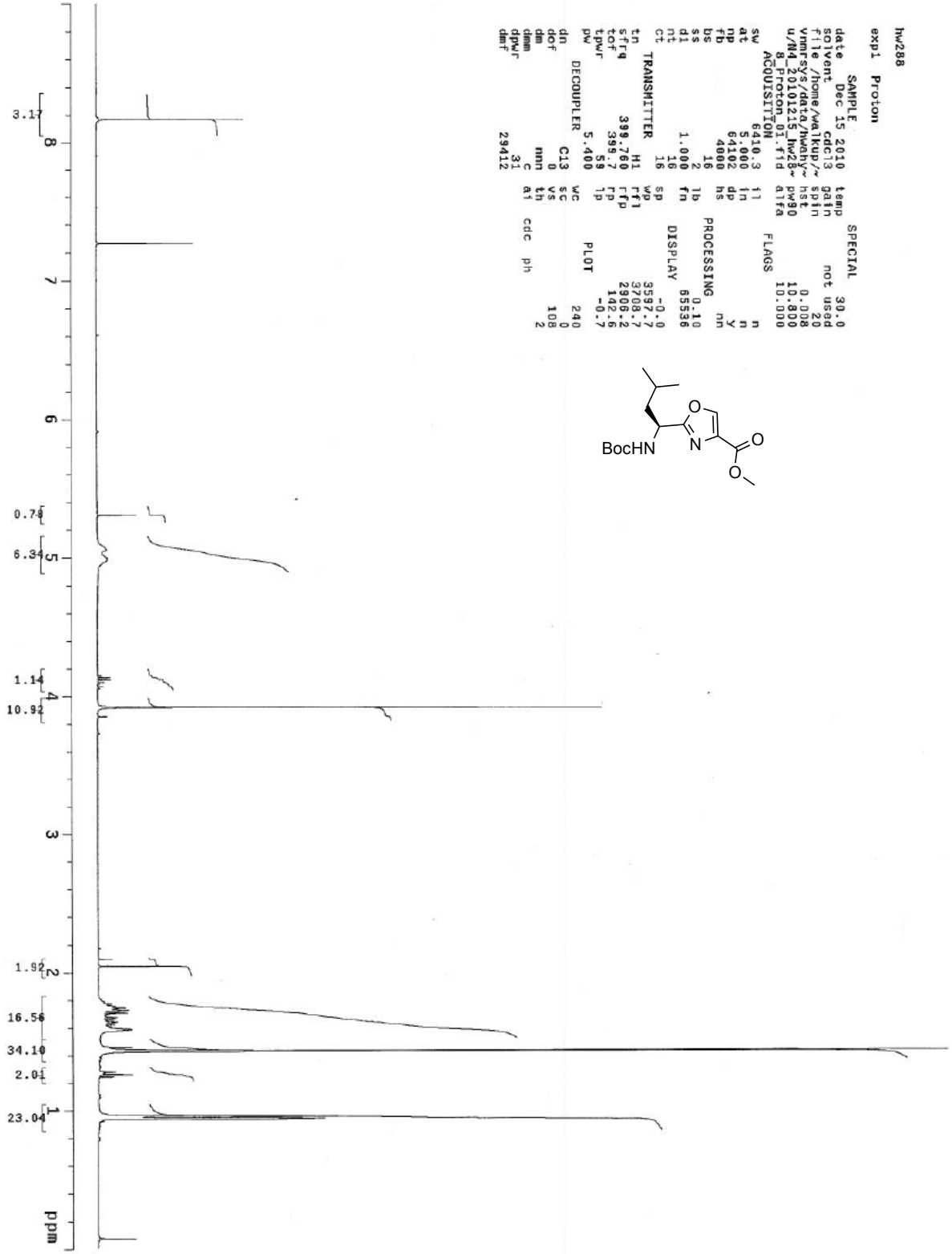
Compound 4: B-Ox-III

NMR Tripeptide MeO-Leu-N(Me)-Phe-Leu-NHBoc



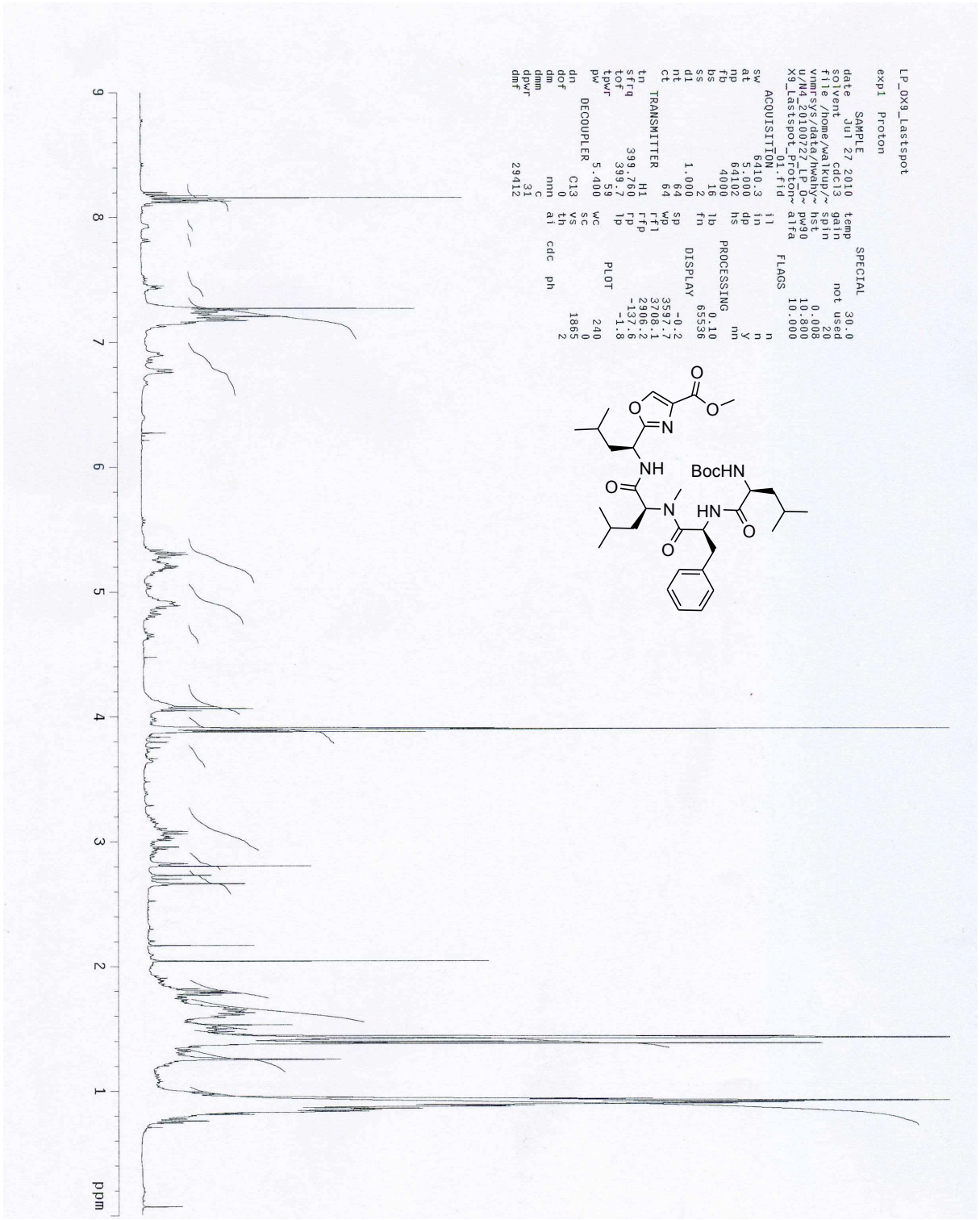
Compound 4: B-Ox-III

NMR Dipeptide MeO-Ser(Bzl)-Leu-NHBoc



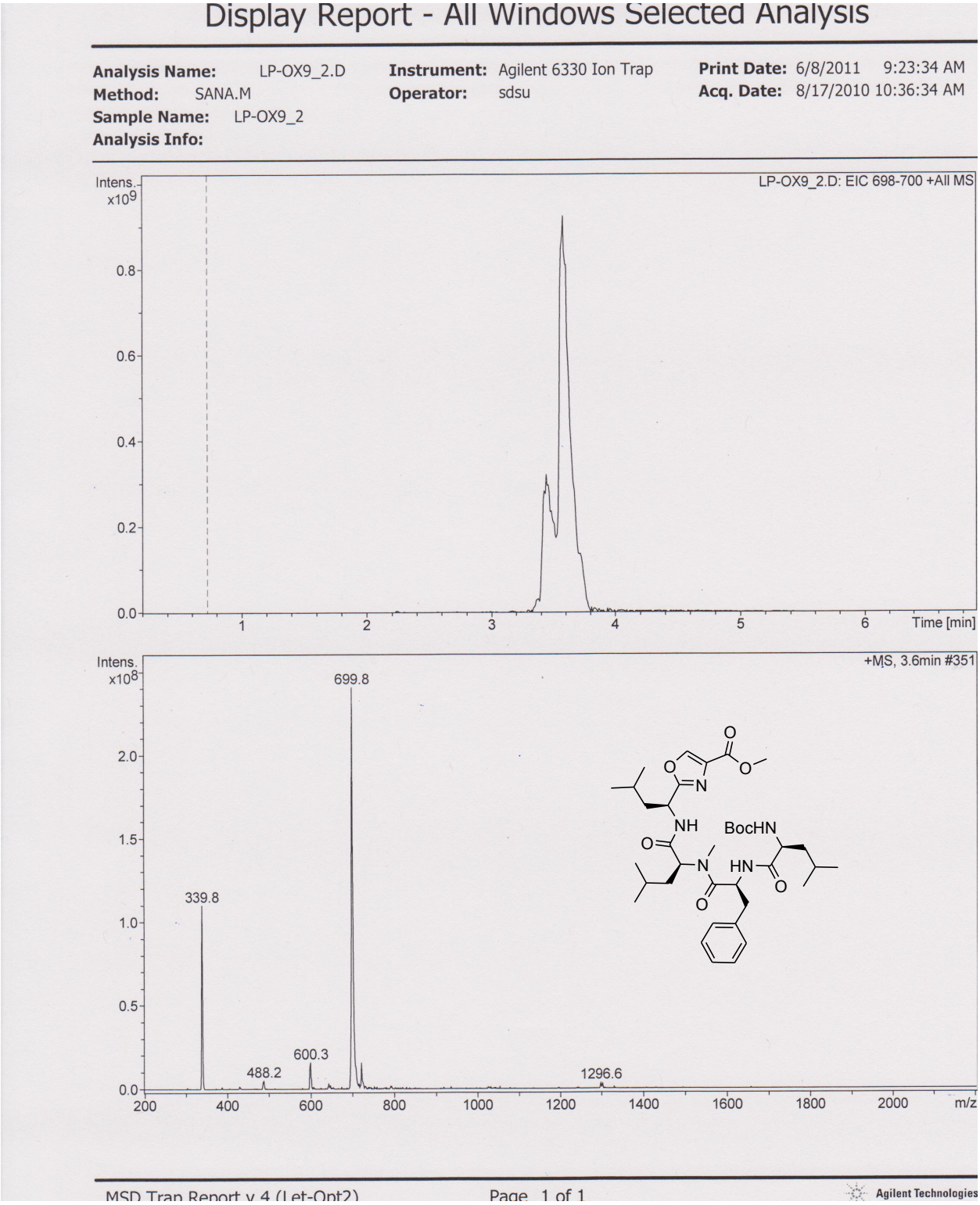
Compound 4: B-Ox-III

NMR Dipeptide MeO-Oxazole-Leu-NHBoc



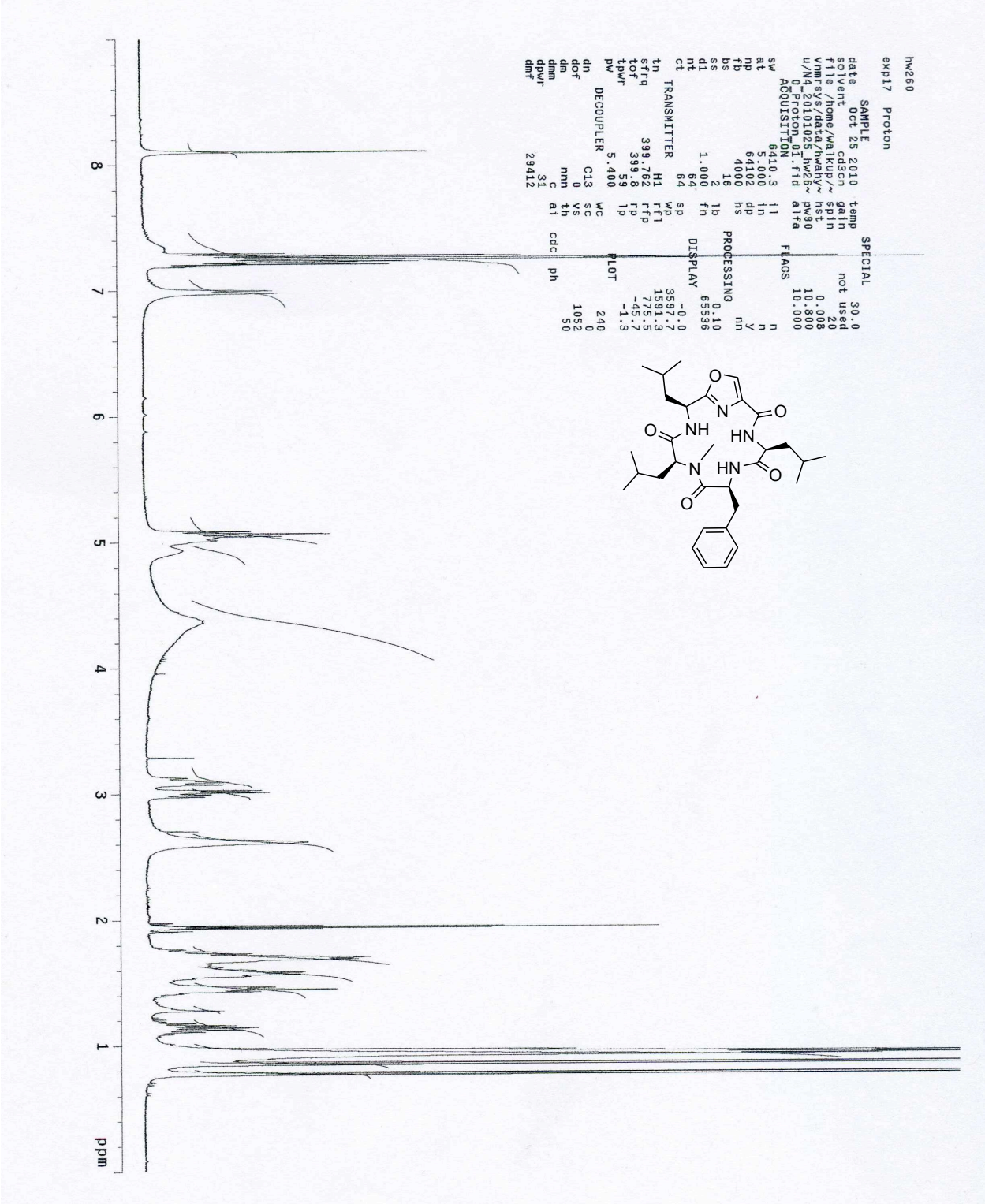
Compound 4: B-Ox-III

NMR Pentapeptide MeO-Oxazole-Leu-Leu-N(Me)-Phe-Leu-NHBoc



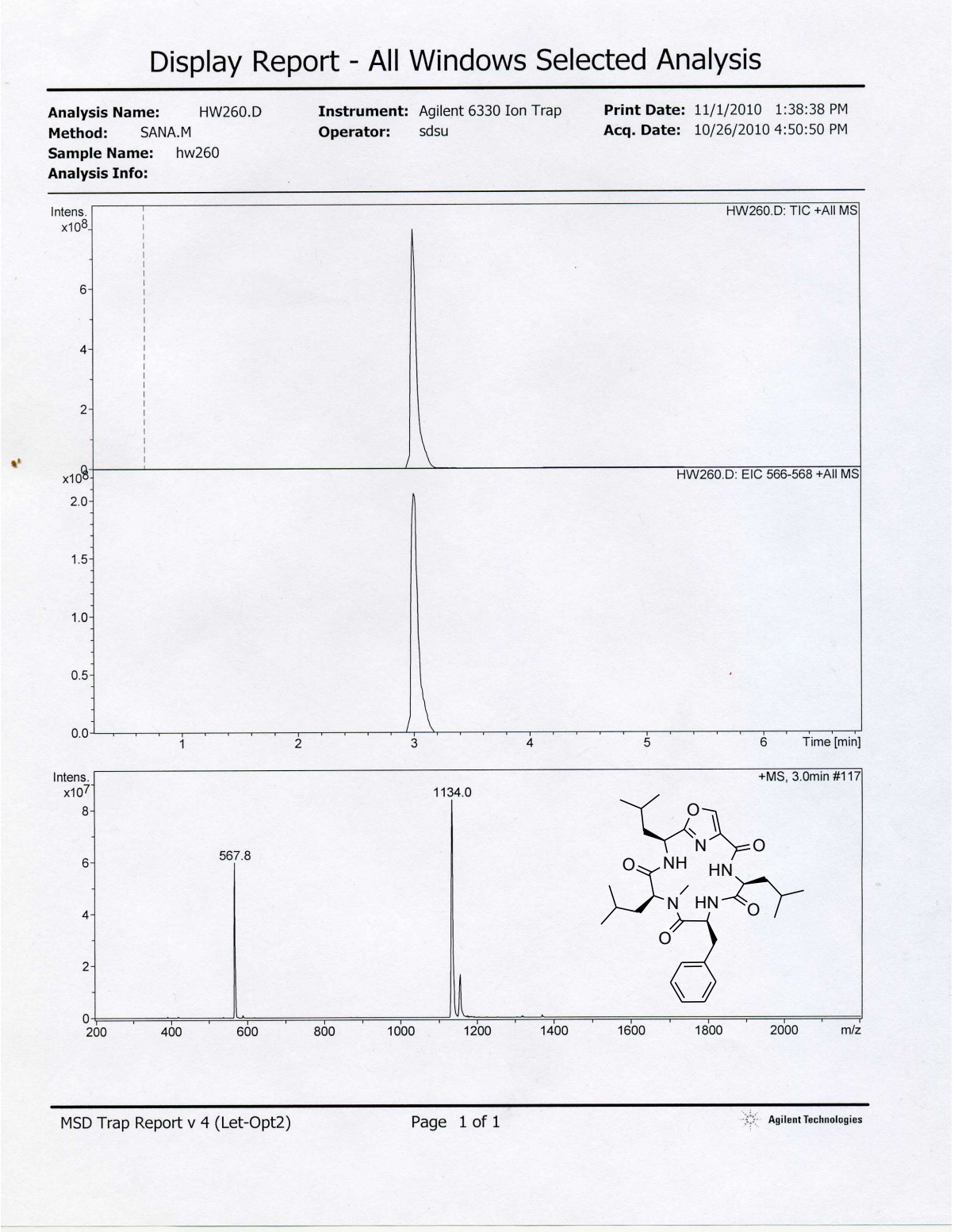
Compound 4: B-Ox-III

LCMS Pentapeptide MeO-Oxazole-Leu-Leu-N(Me)-Phe-Leu-NHBoc (MW = 699)



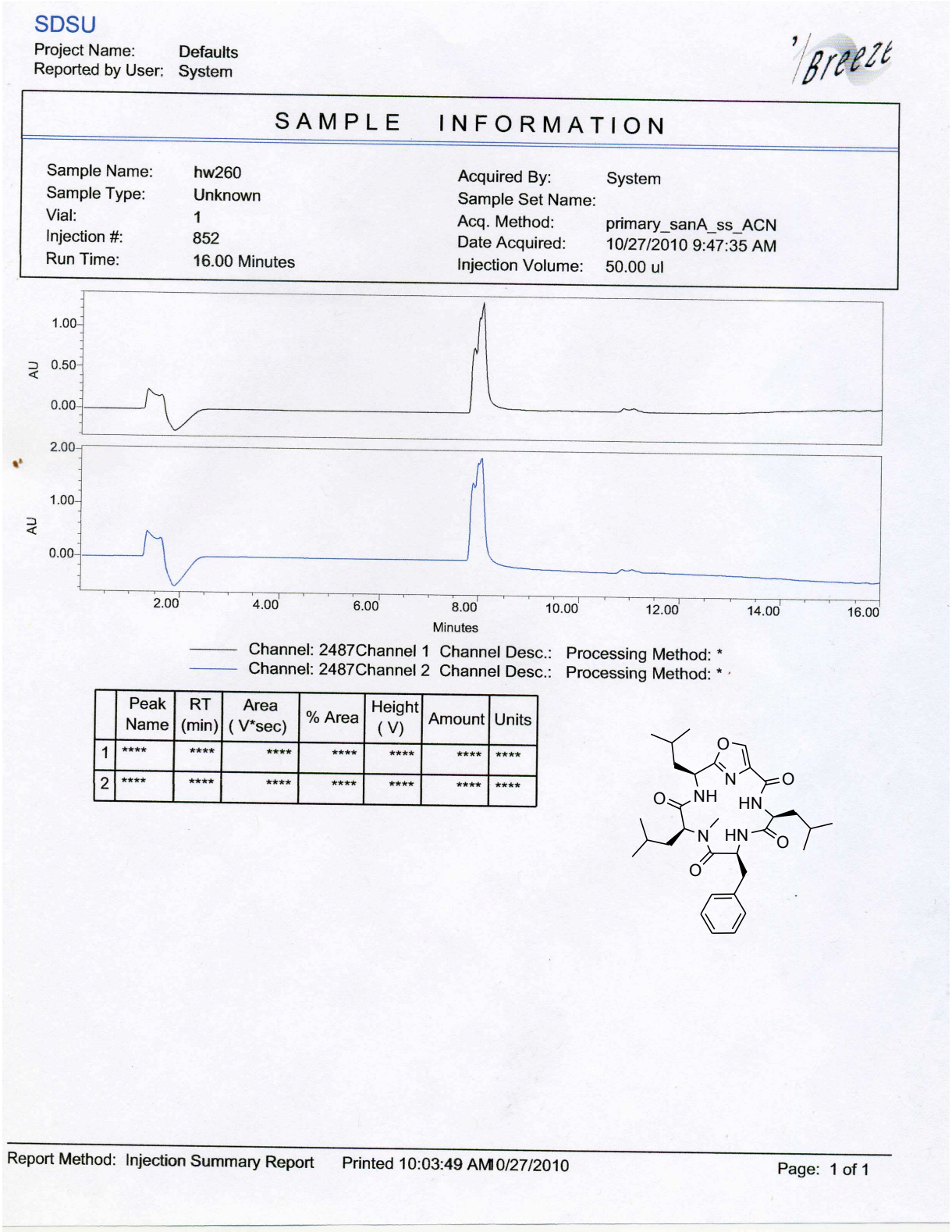
Compound 4: B-Ox-III

NMR Macrocycle Phe-Leu-Oxazole-Leu-Leu-N(Me) (4)



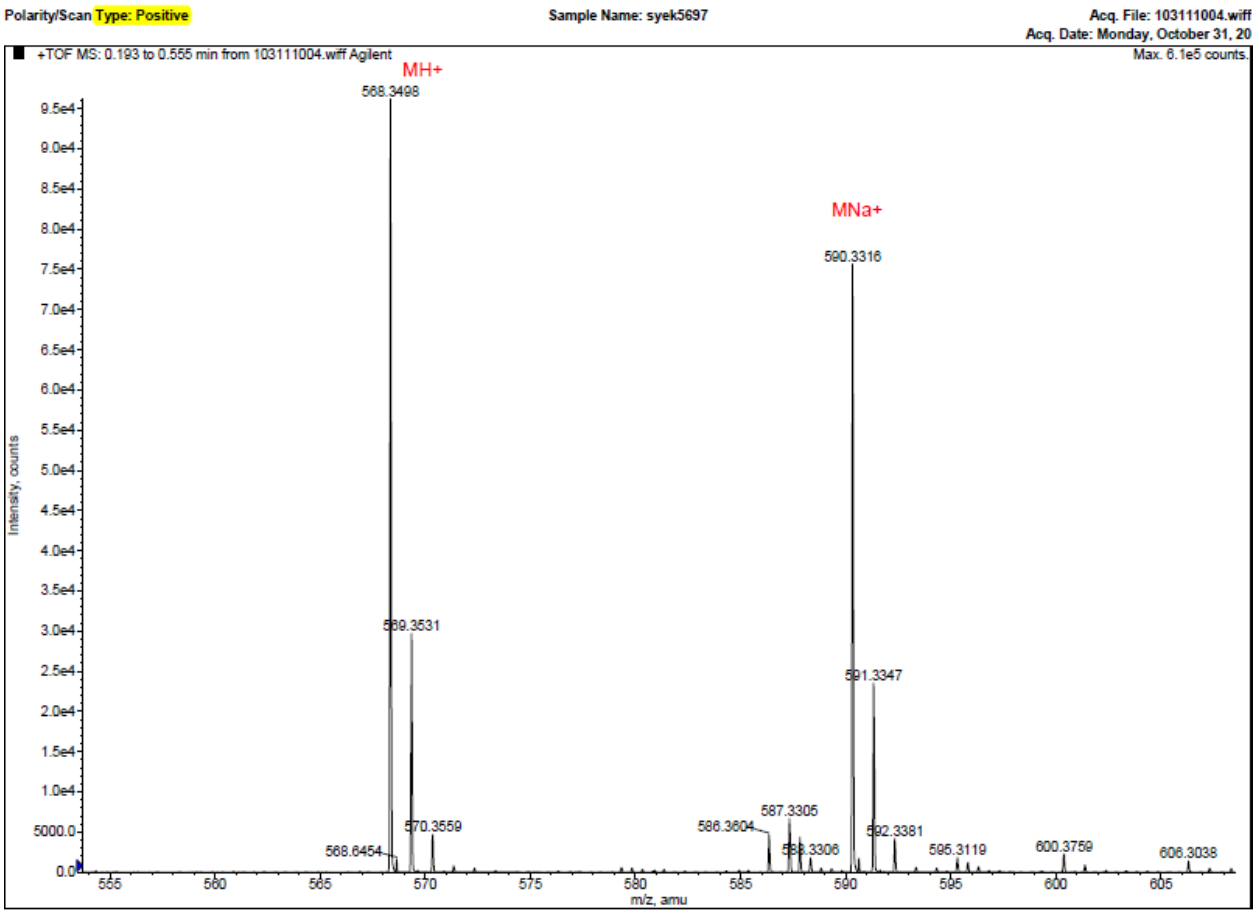
Compound 4: B-Ox-III

LCMS Macrocycle Phe-Leu-Oxazole-Leu-Leu-N(Me) (4) (MW = 567)



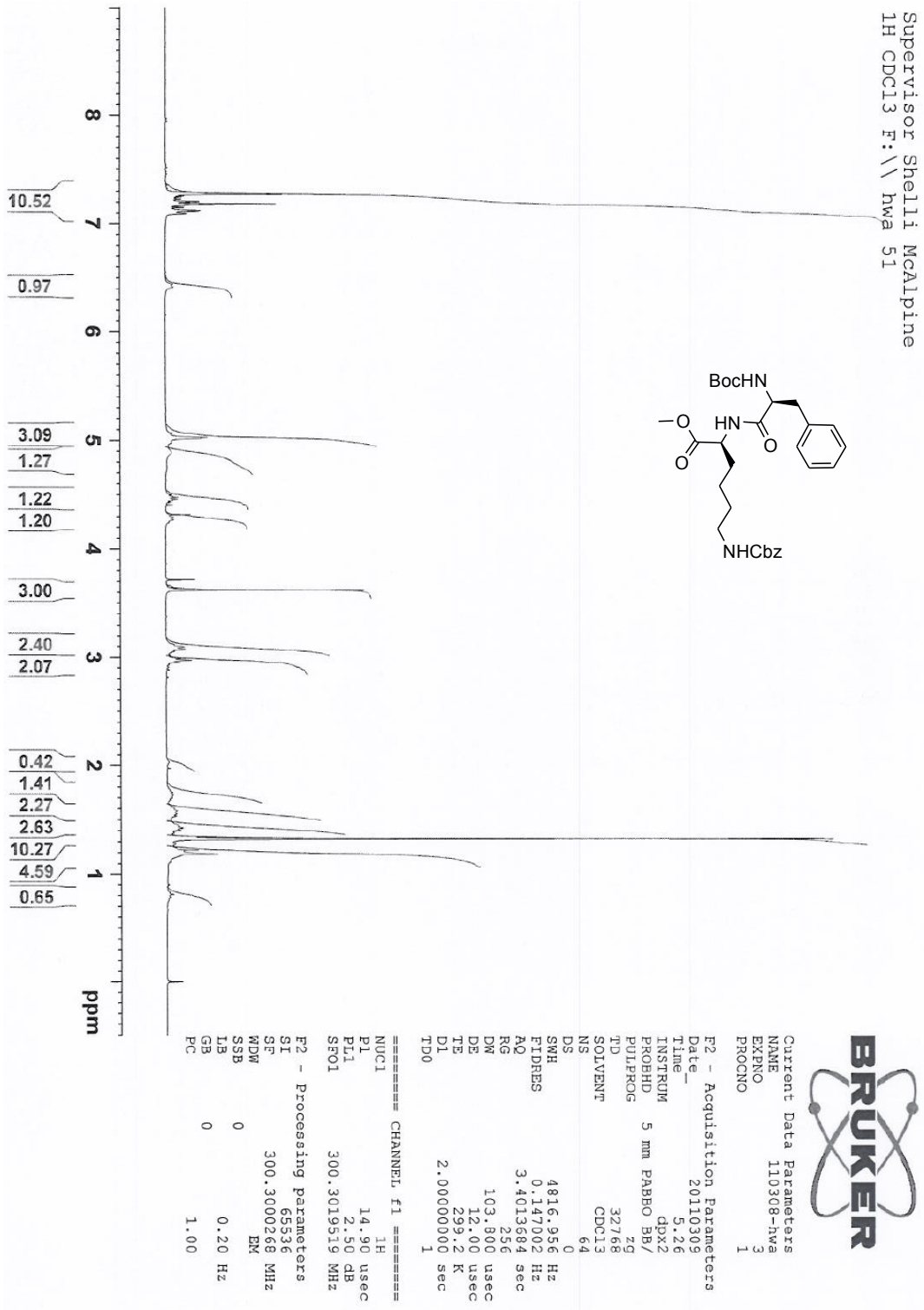
Compound 4: B-Ox-III

HPLC Macrocycle Phe-Leu-Oxazole-Leu-Leu-N(Me) (4)



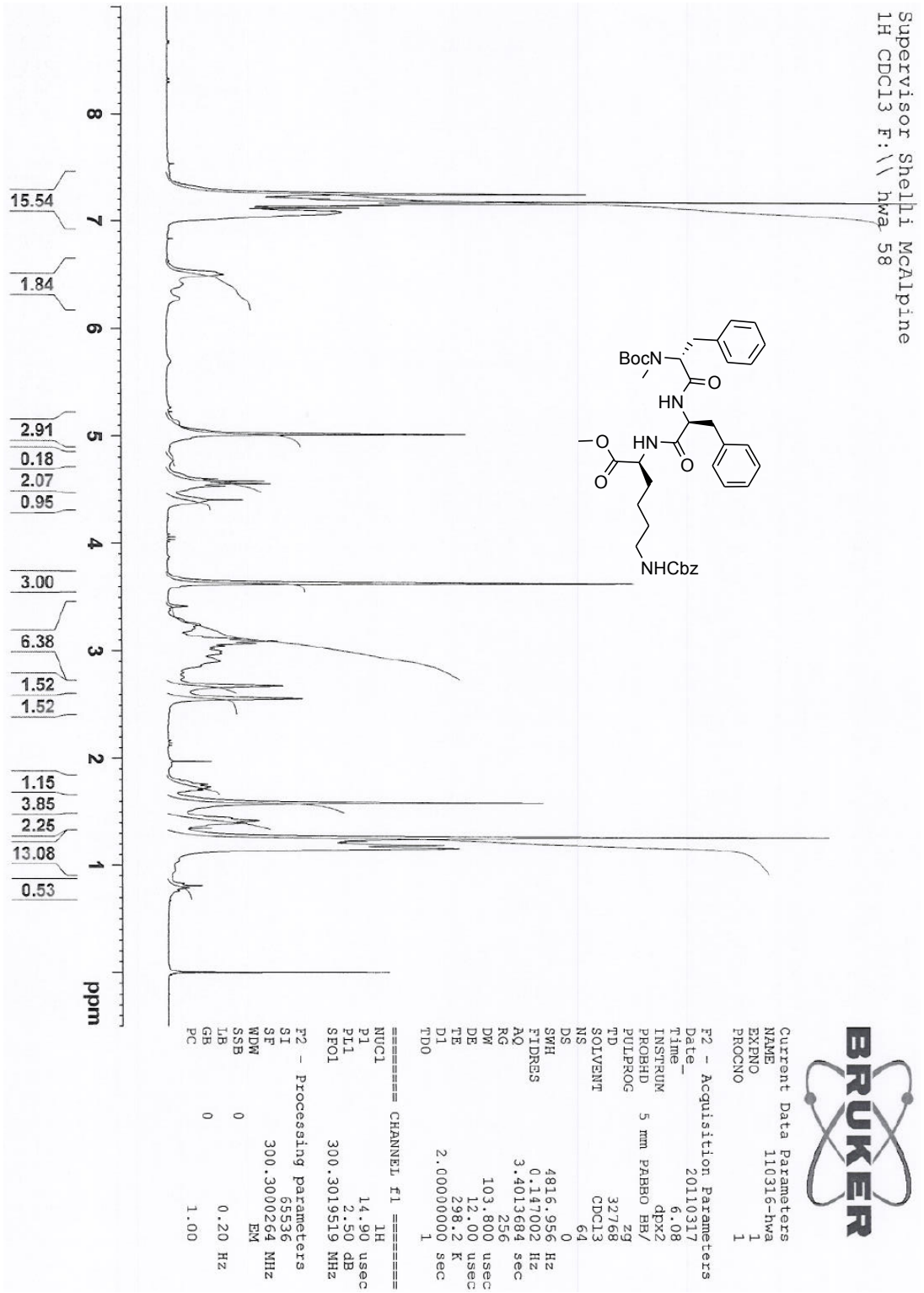
Compound 4: B-Ox-III

HRMS Macrocycle Phe-Leu-Oxazole-Leu-Leu-N(Me) (4) (MW = 568.3520)



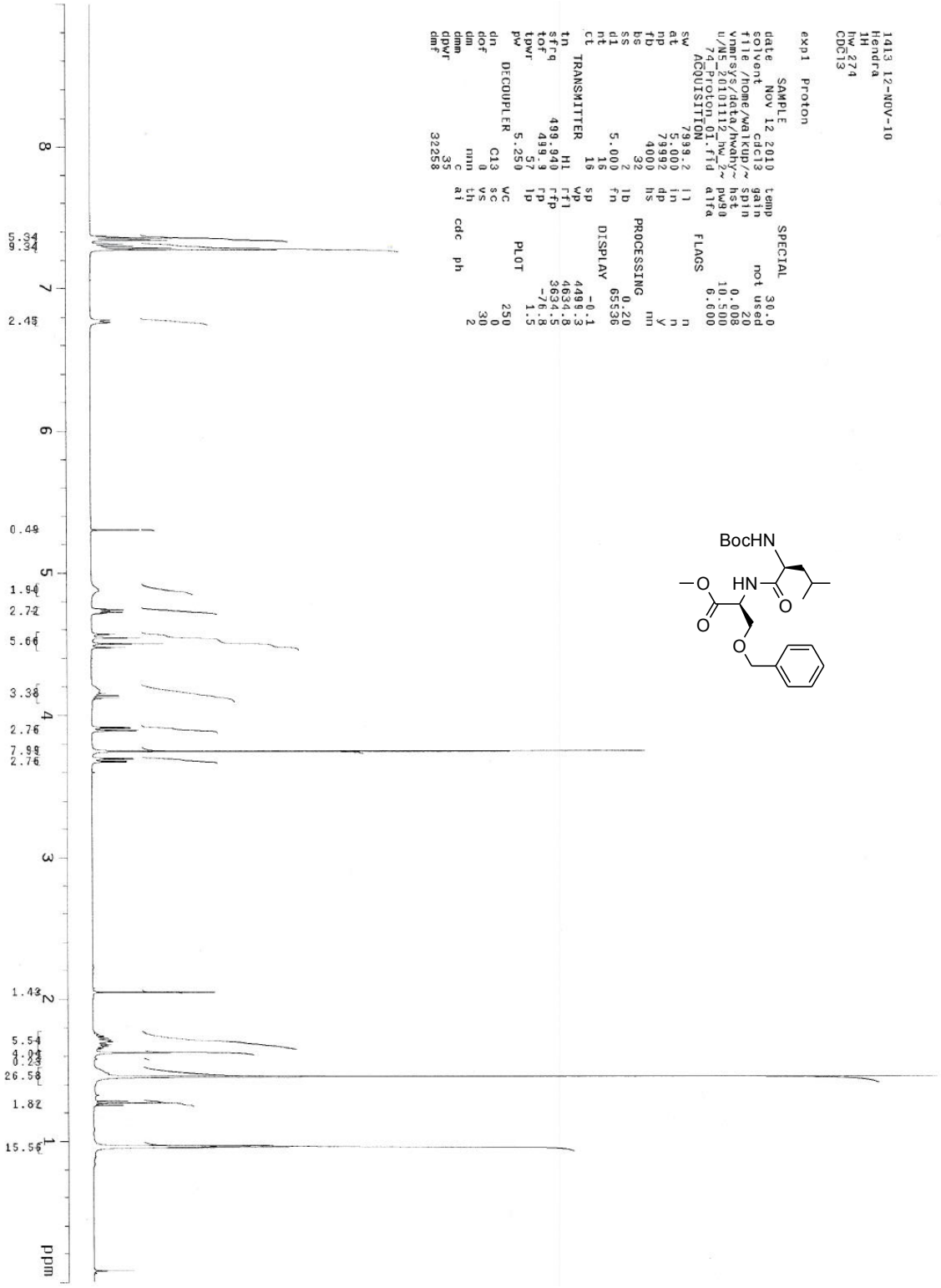
Compound 5: C-Ox-III

NMR Dipeptide MeO-Lys(Cbz)-Phe-NHBoc



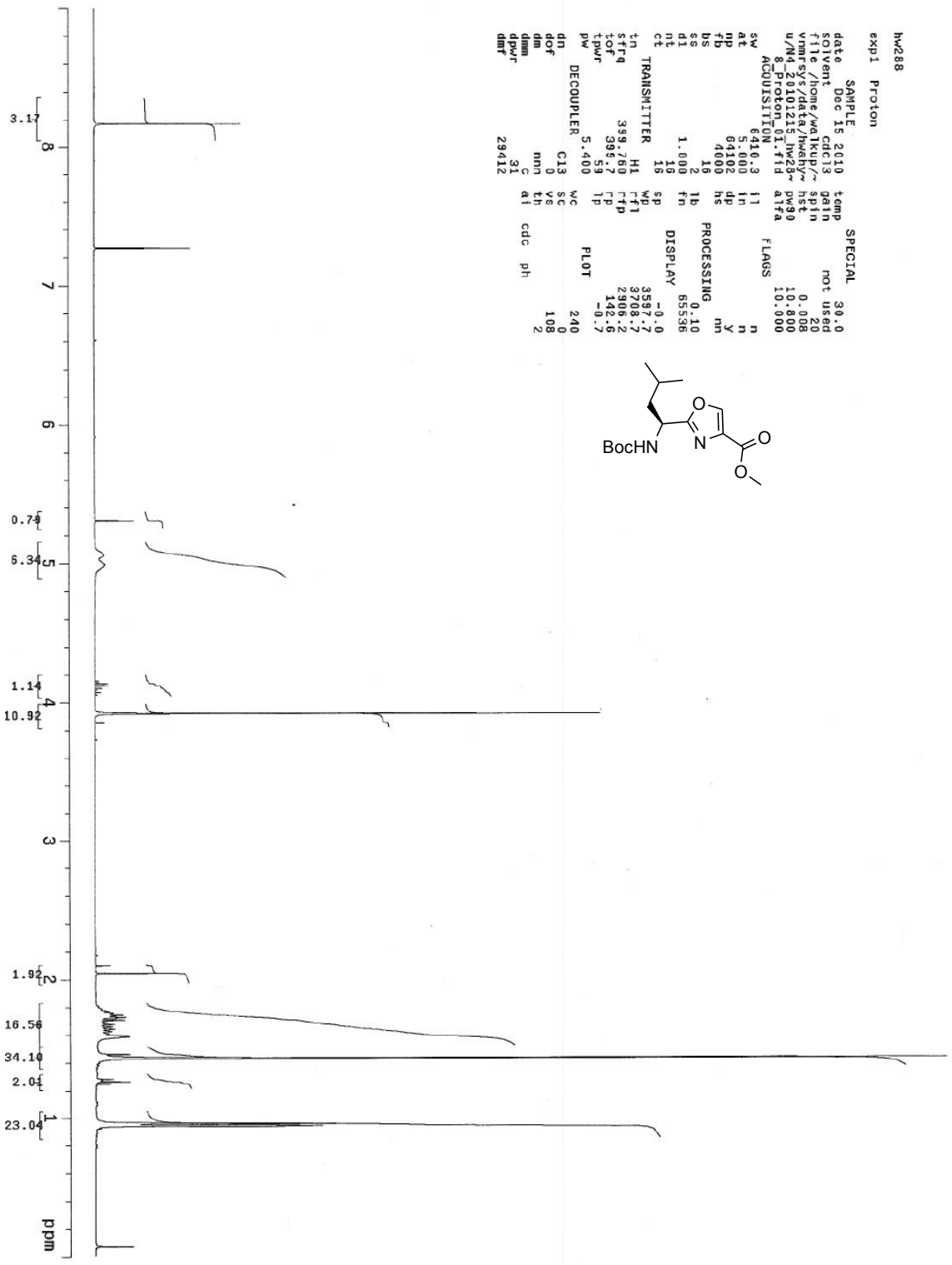
Compound 5: C-Ox-III

NMR Tripeptide MeO-Lys(Cbz)-Phe-D-Phe-N(Me)Boc



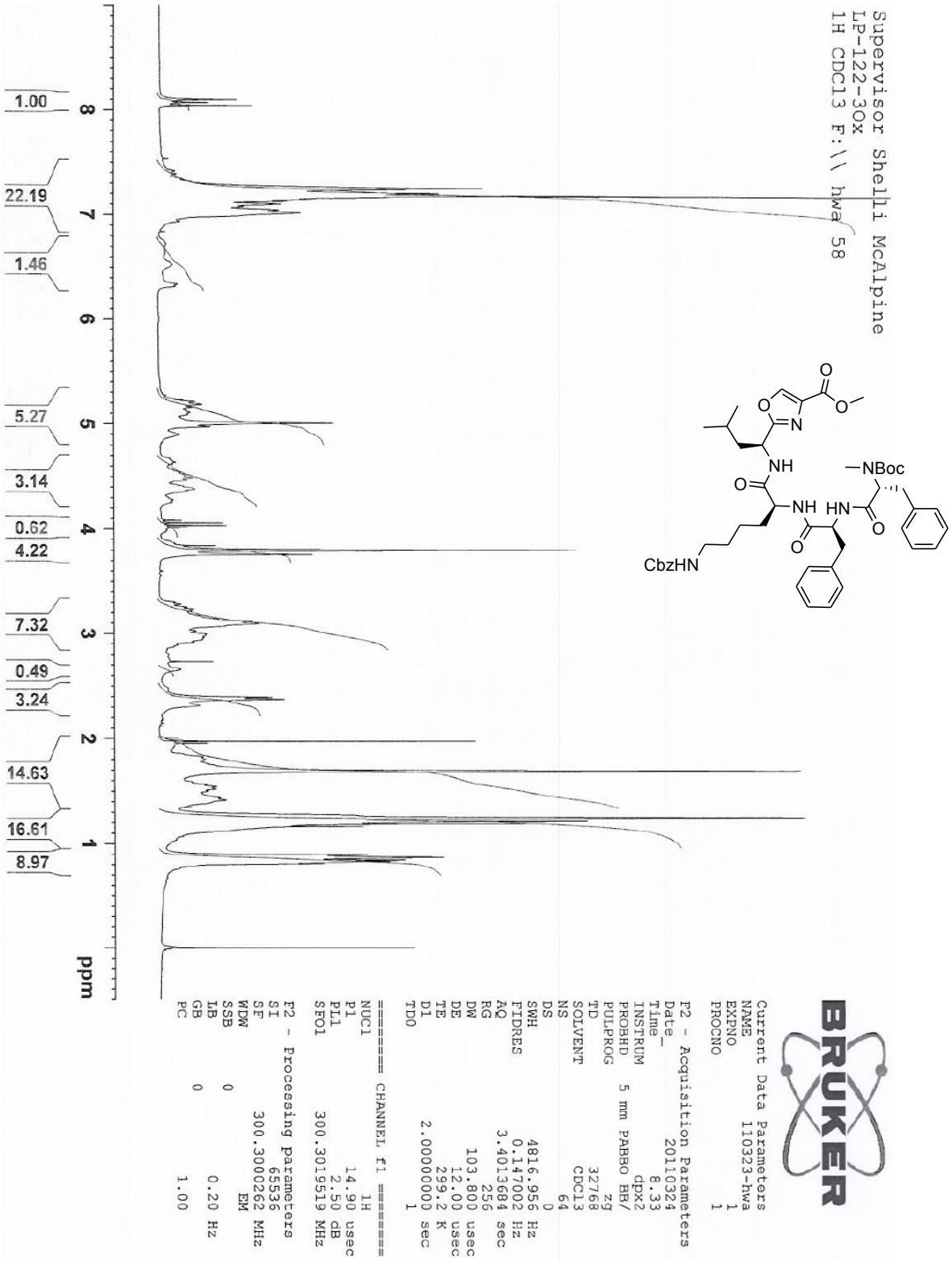
Compound 5: C-Ox-III

NMR Dipeptide MeO-Ser(Bzl)-Leu-NHBoc



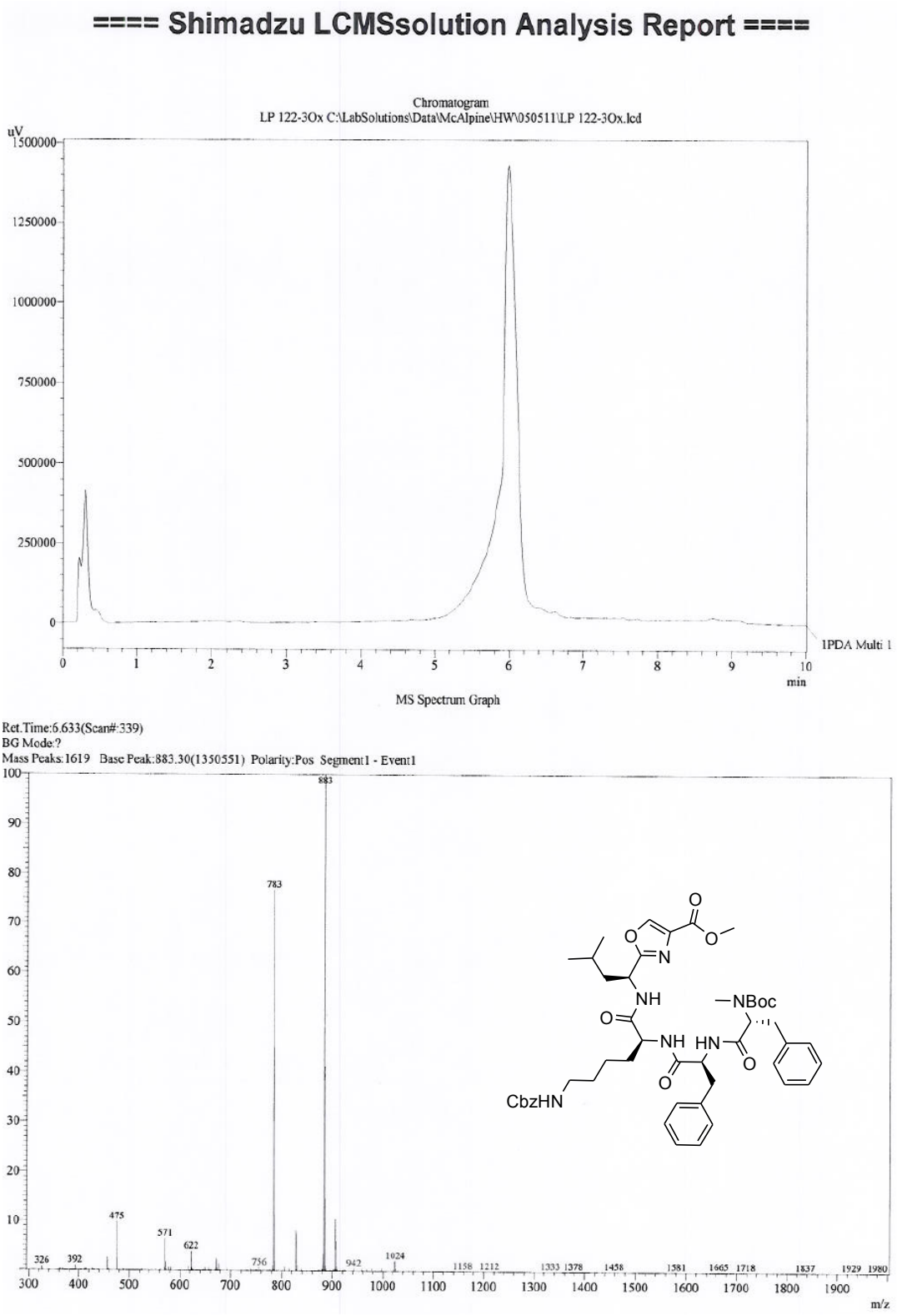
Compound 5: C-Ox-III

NMR Dipeptide MeO-Oxazole-Leu-NHBoc



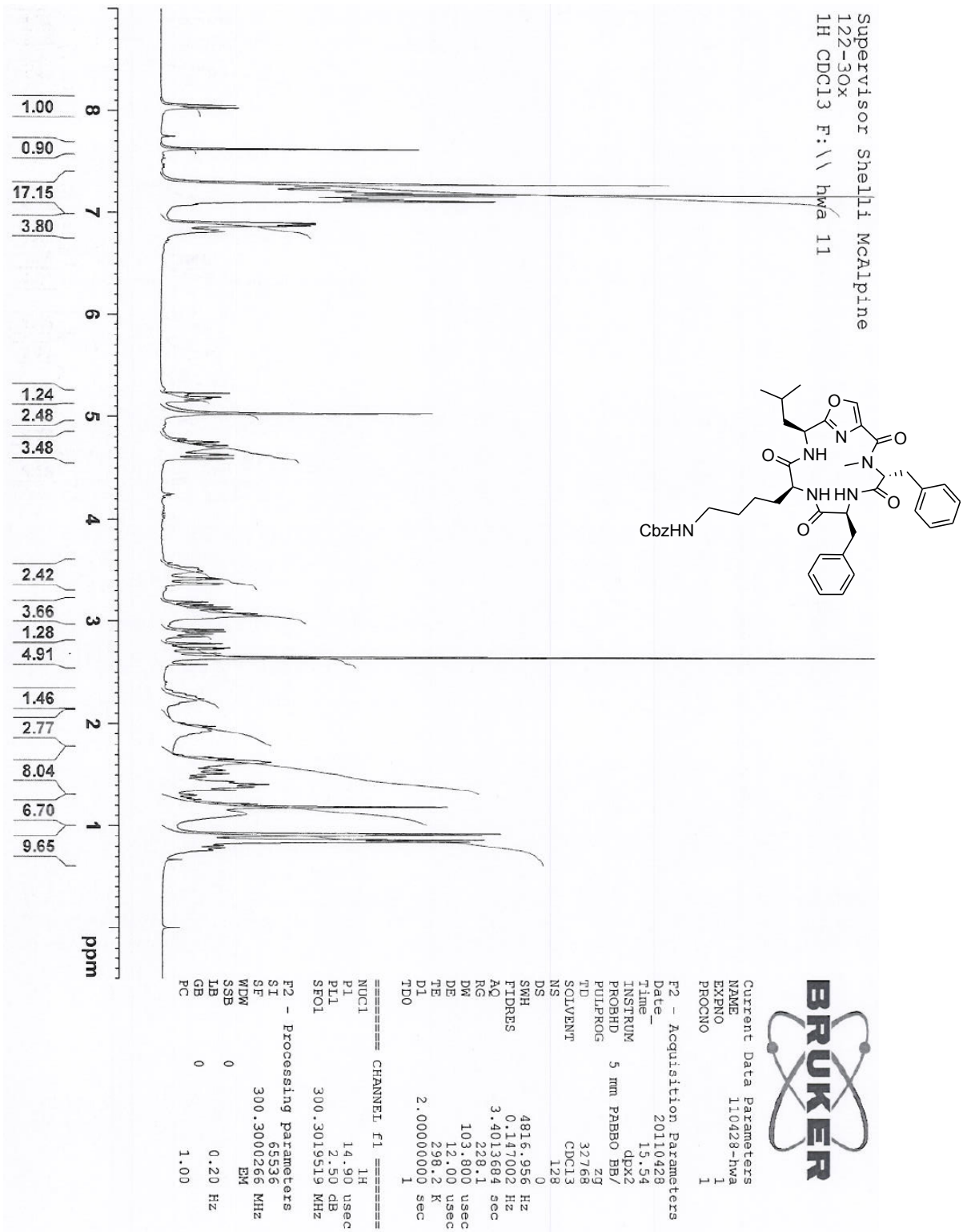
Compound 5: C-Ox-III

NMR Pentapeptide MeO-Oxazole-Leu-Lys(Cbz)-Phe-D-Phe-N(Me)Boc



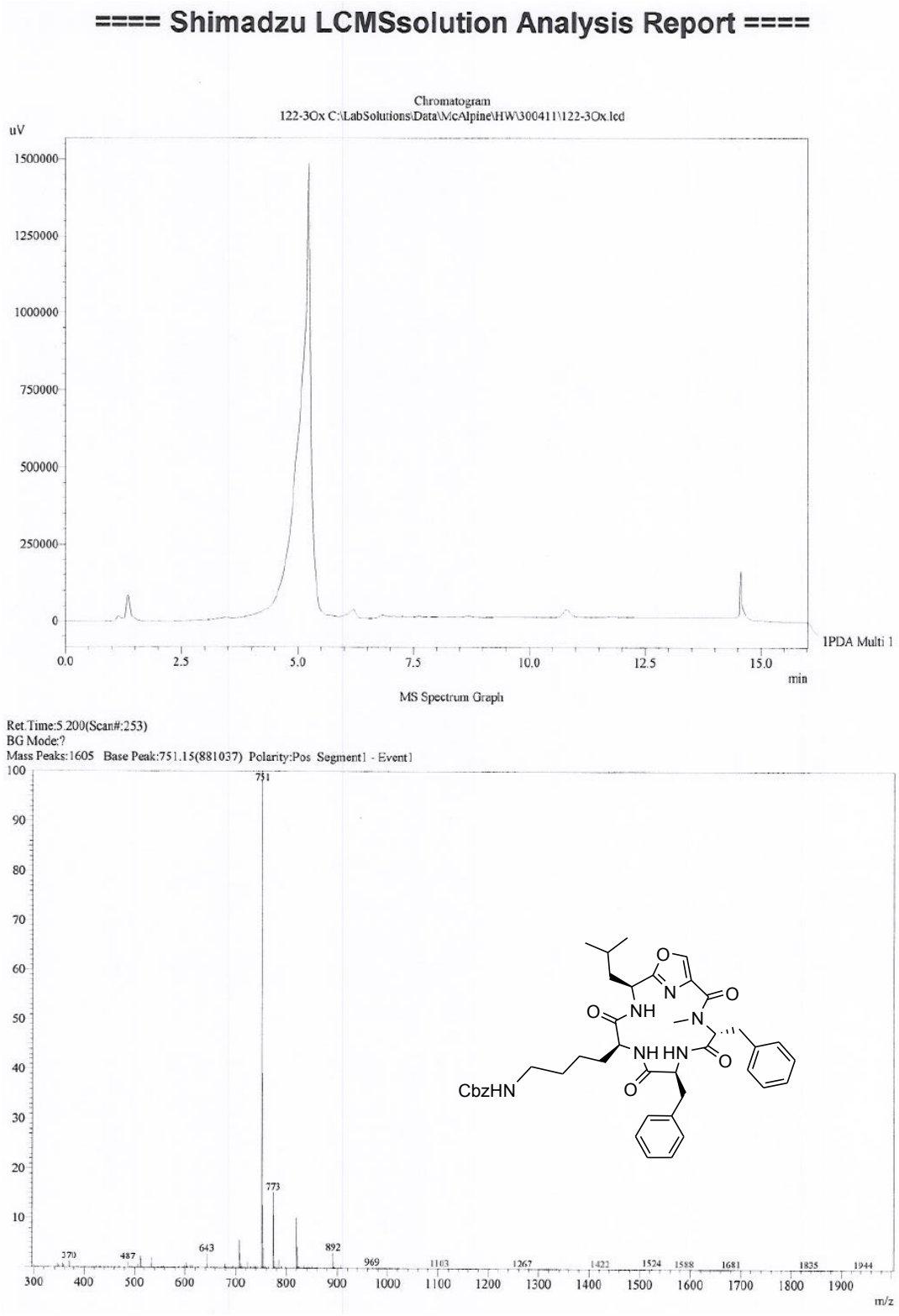
Compound 5: C-Ox-III

HPLC/LCMS Pentapeptide MeO-Oxazole-Leu-Lys(Cbz)-Phe-D-Phe-N(Me)Boc (MW = 882)



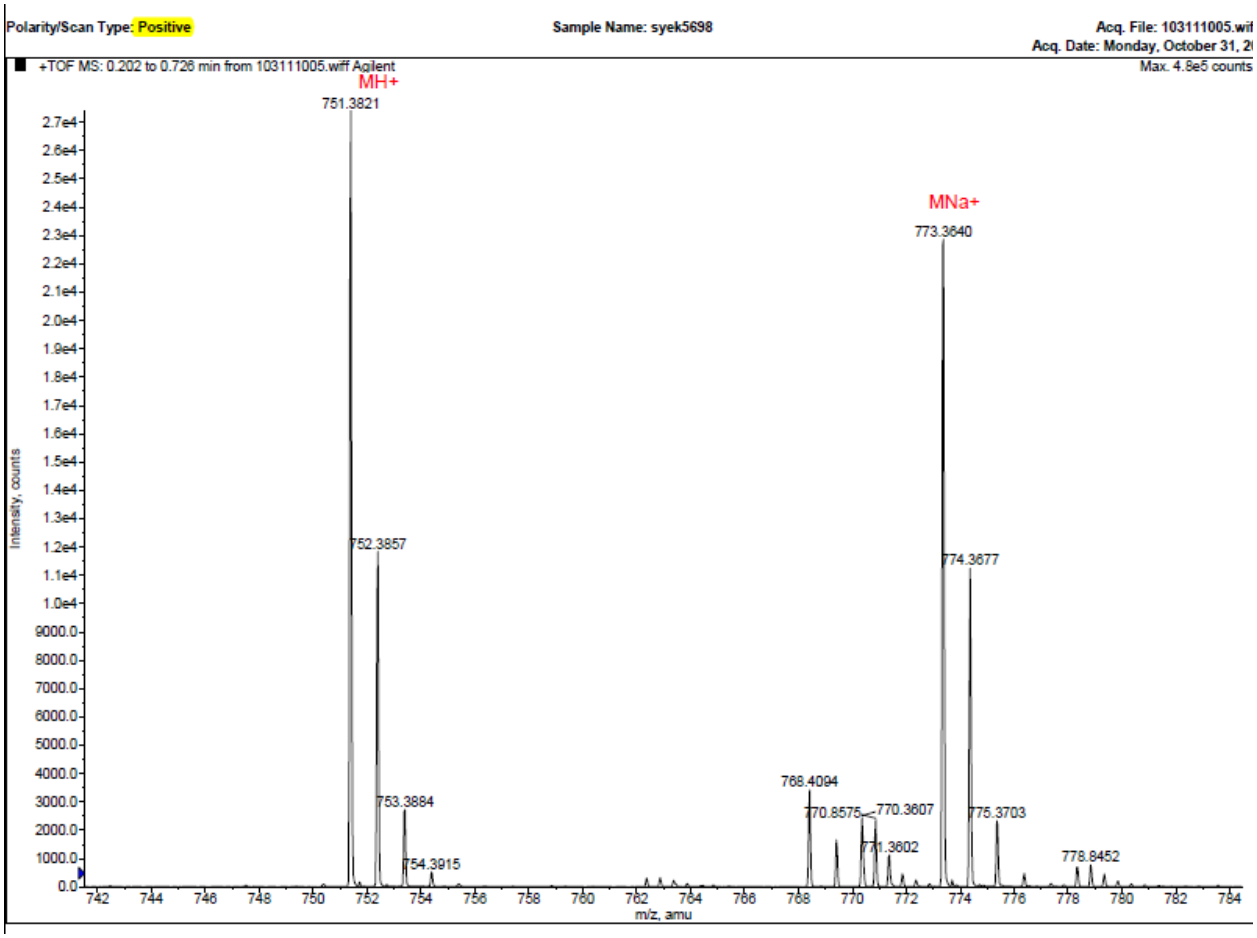
Compound 5: C-Ox-III

NMR Macrocycle Phe-D-Phe-N(Me)-Oxazole-Leu-Lys(Cbz) (5)



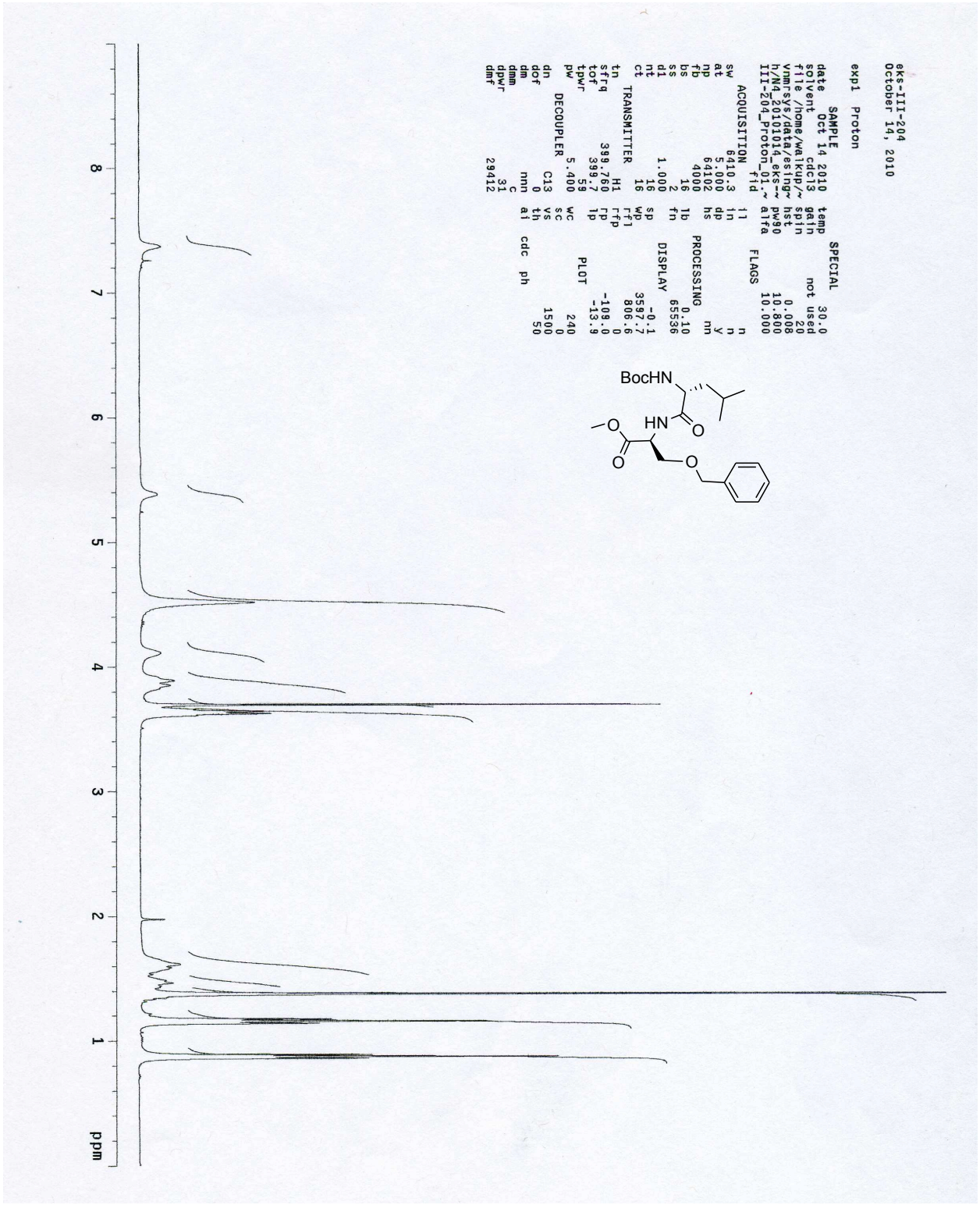
Compound 5: C-Ox-III

HPLC+LCMS Macrocycle Phe-D-Phe-N(Me)-Oxazole-Leu-Lys(Cbz) (5) (MW=750)



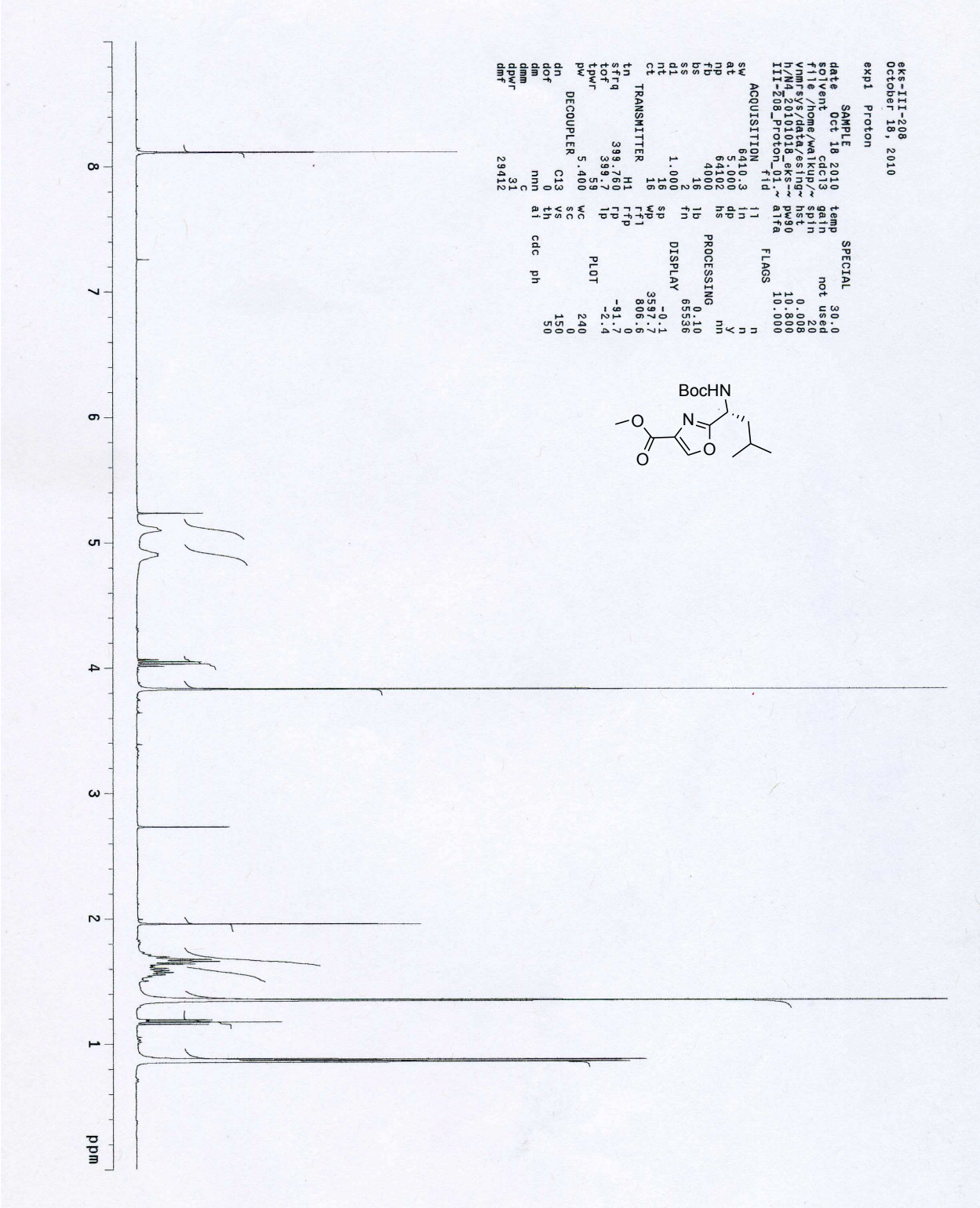
Compound 5: C-Ox-III

HRMS Macrocycle Phe-D-Phe-N(Me)-Oxazole-Leu-Lys(Cbz) (5) (MW= 751.3821)



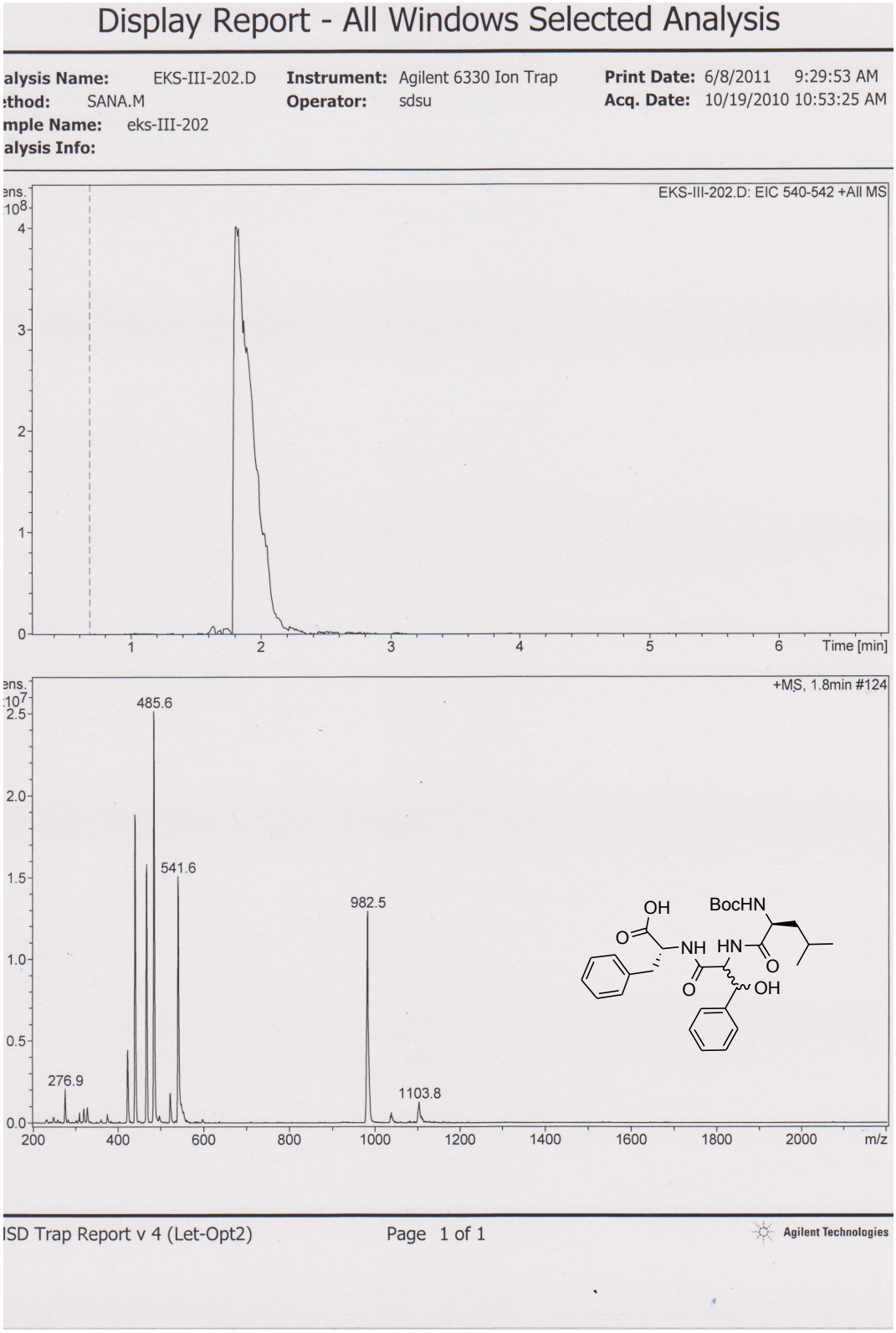
Compound 6: D-Ox-III

NMR Dipeptide MeO-Ser(Bzl)-D-Leu-NHBoc



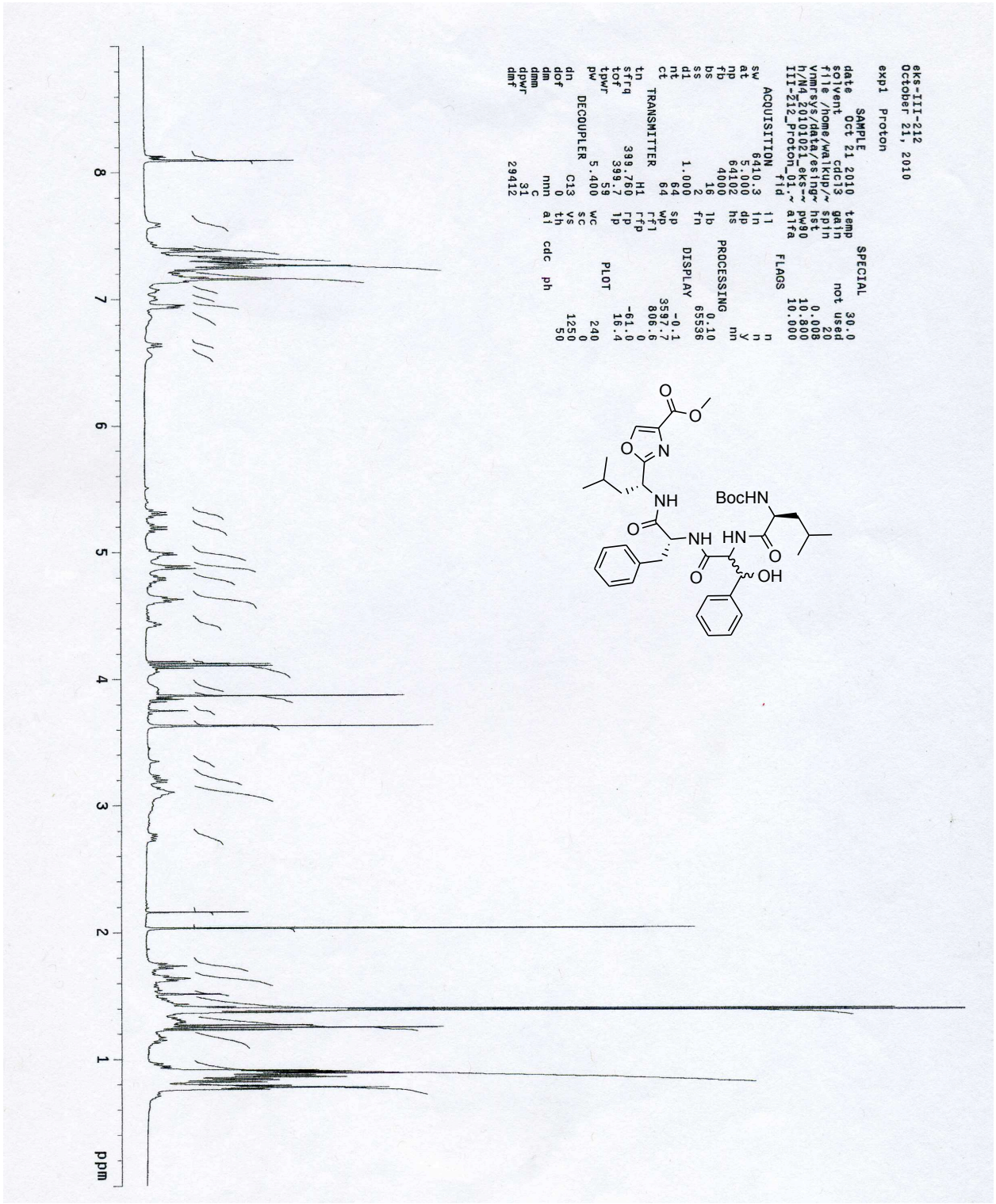
Compound 6: D-Ox-III

NMR Dipeptide MeO-Oxazole-D-Leu-NHBoc



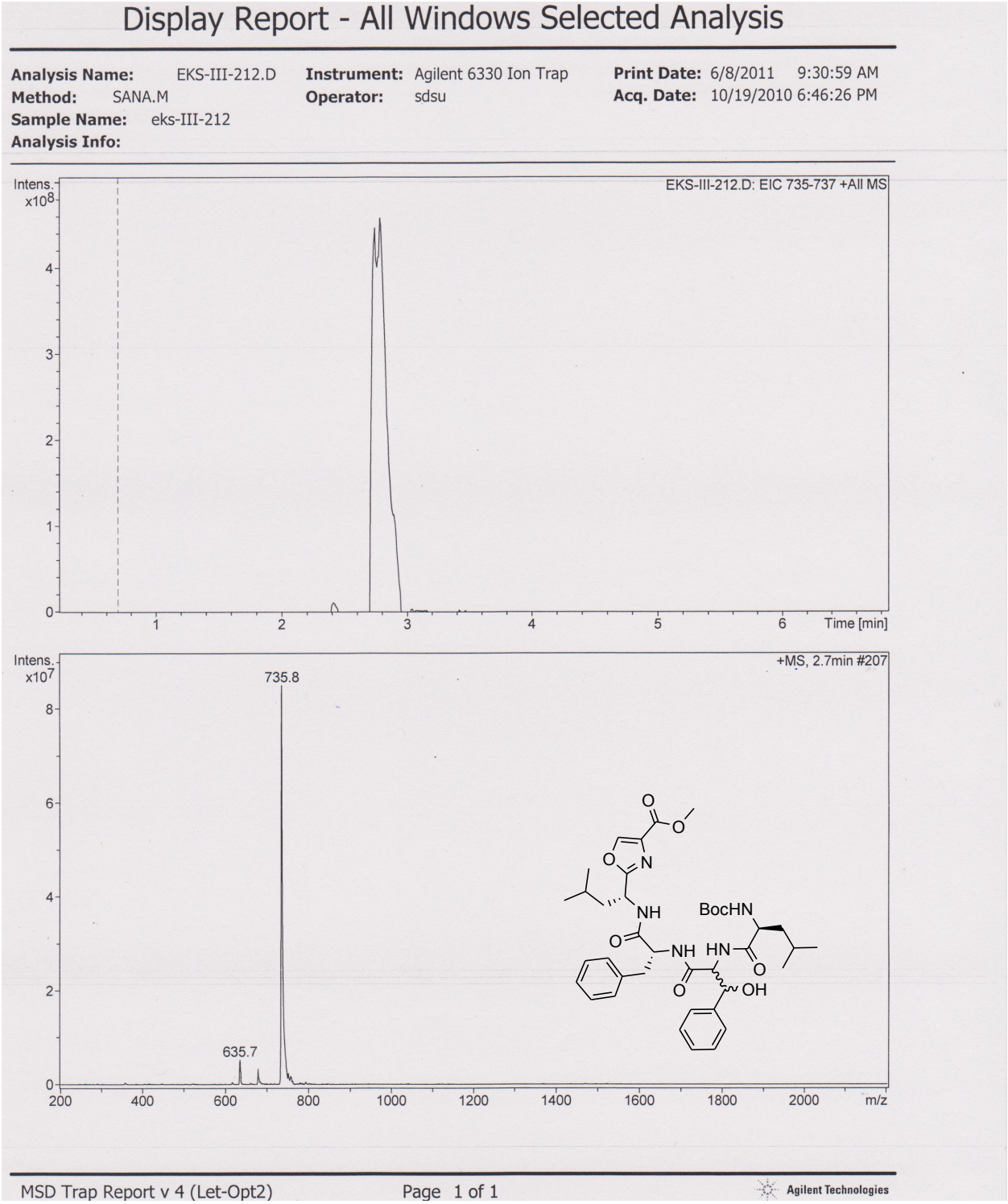
Compound 6: D-Ox-III

LCMS Tripeptide HO-D-Phe-Phe-(2R,3R)/(2S,3S)-β-OH-Leu-NHBoc (MW = 541)



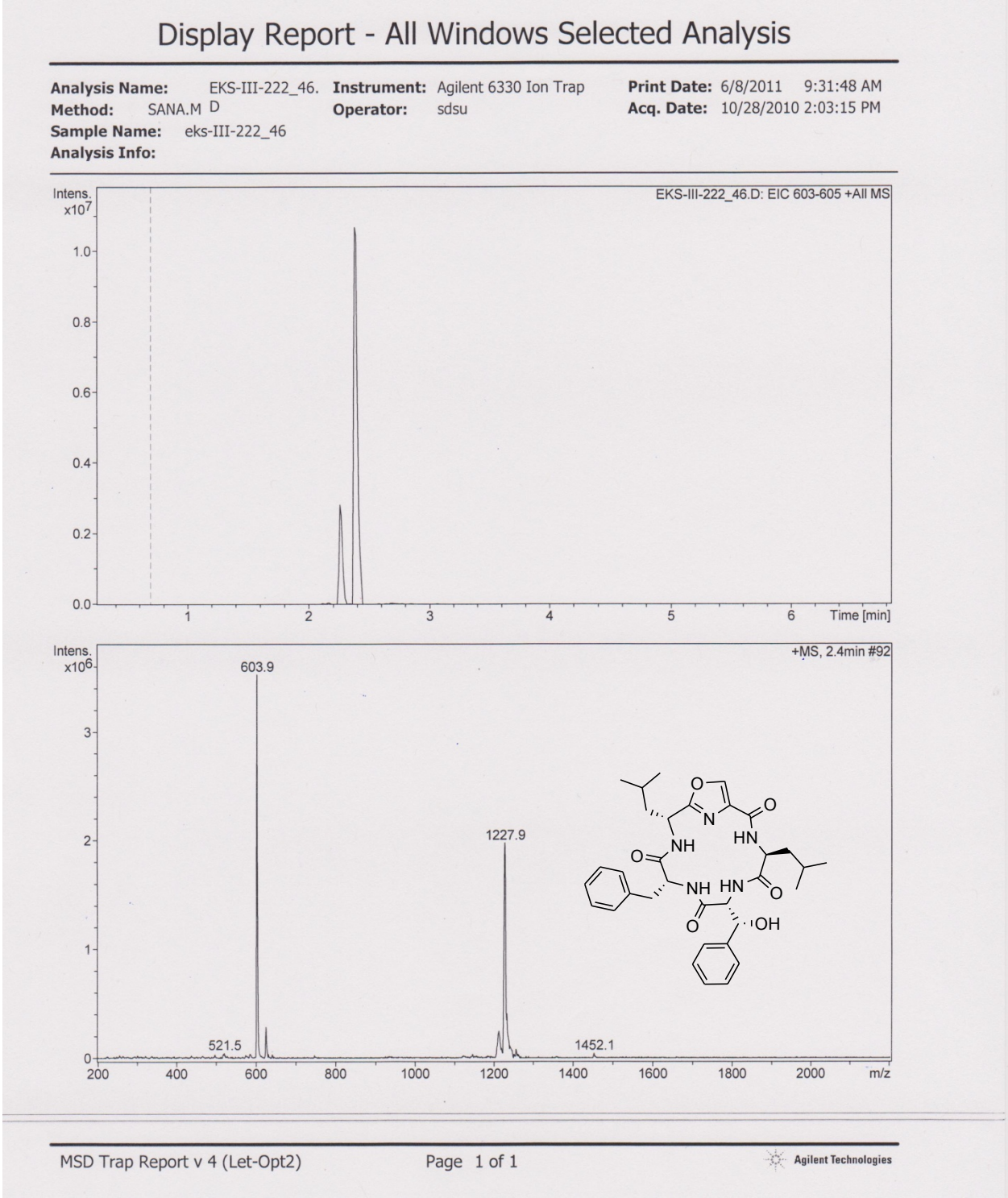
Compound 6: D-Ox-III

NMR Pentapeptide MeO-Oxazole-D-Leu-D-Phe-(2R,3R)/(2S,3S)-β-OH-Phe-Leu-NHBoc



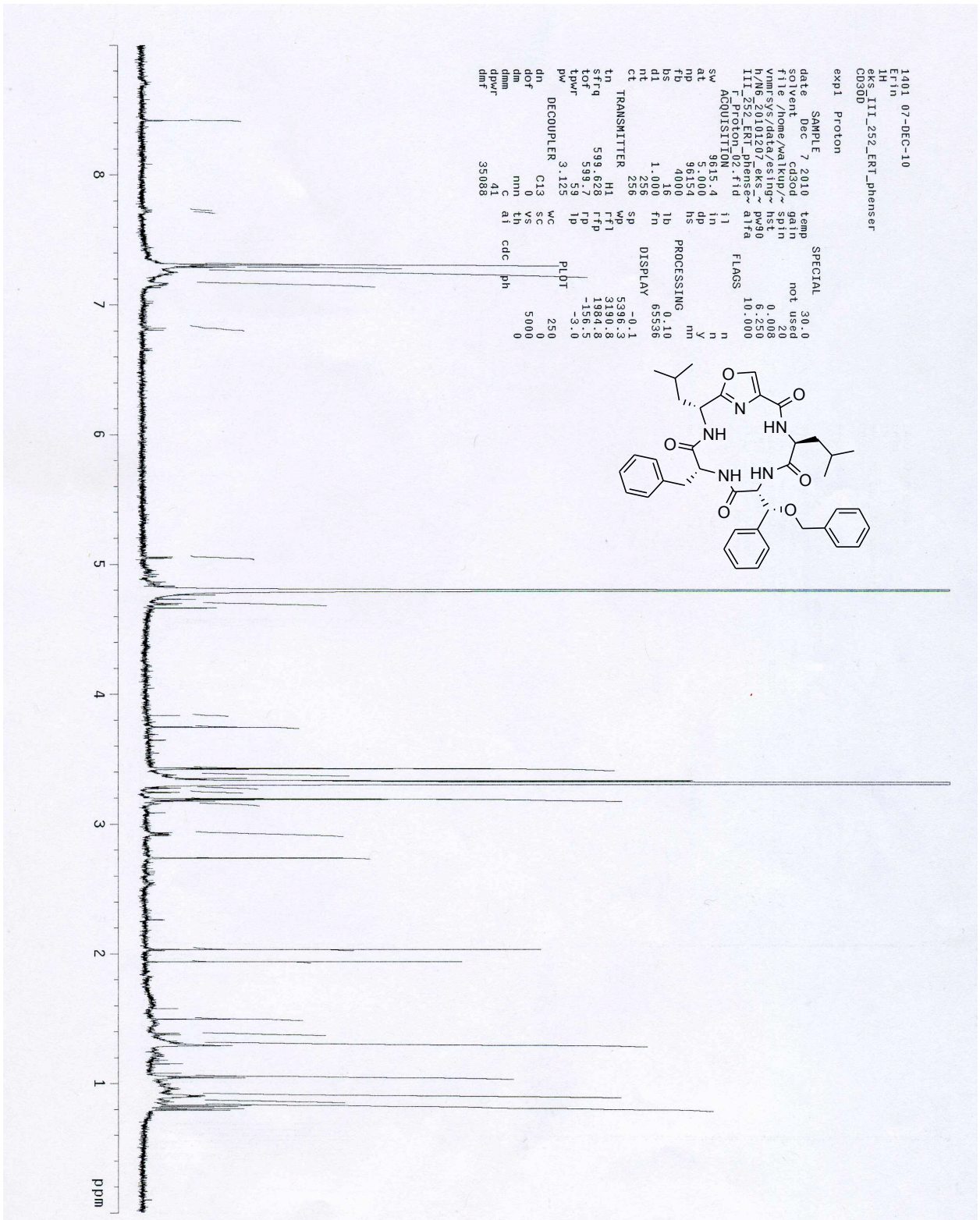
Compound 6: D-Ox-III

LCMS Pentapeptide MeO-Oxazole-D-Leu-D-Phe-(2R,3R)/(2S,3S)-β-OH-Phe-Leu-NHBoc (MW = 736)



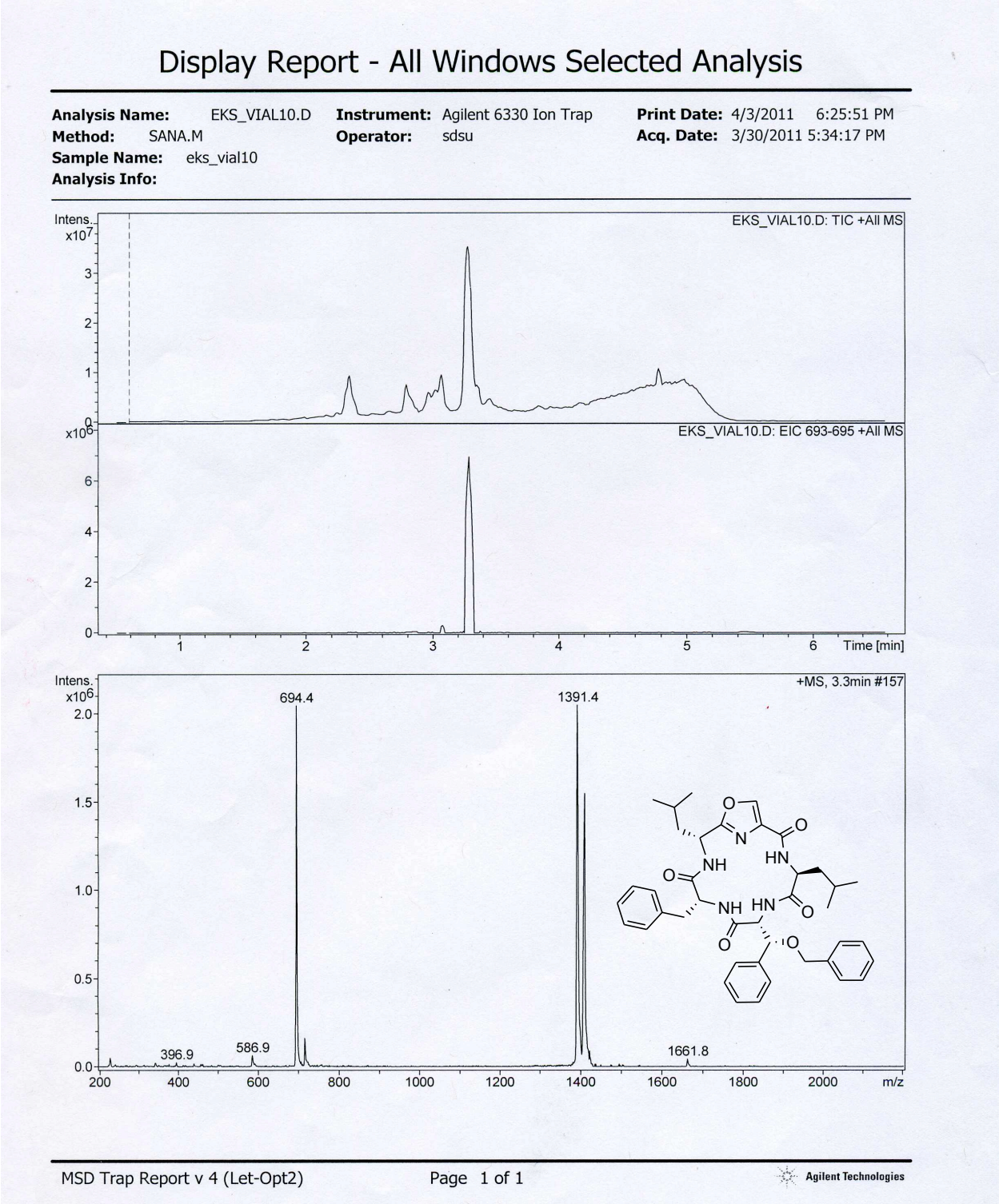
Compound 6: D-Ox-III

LCMS Macrocycle (2R,3R)-β-hydroxy-Phe-Leu-Oxazole-D-Leu-D-Phe (MW = 604)



Compound 6: D-Ox-III

NMR Macrocycle (2R,3R)-β-benzoxy-Phe-Leu-Oxazole-D-Leu-D-Phe (6)



Compound 6: D-Ox-III

LCMS Macrocycle (2R,3R)-β-benzoxy-Phe-Leu-Oxazole-D-Leu-D-Phe (6) (MW = 694)

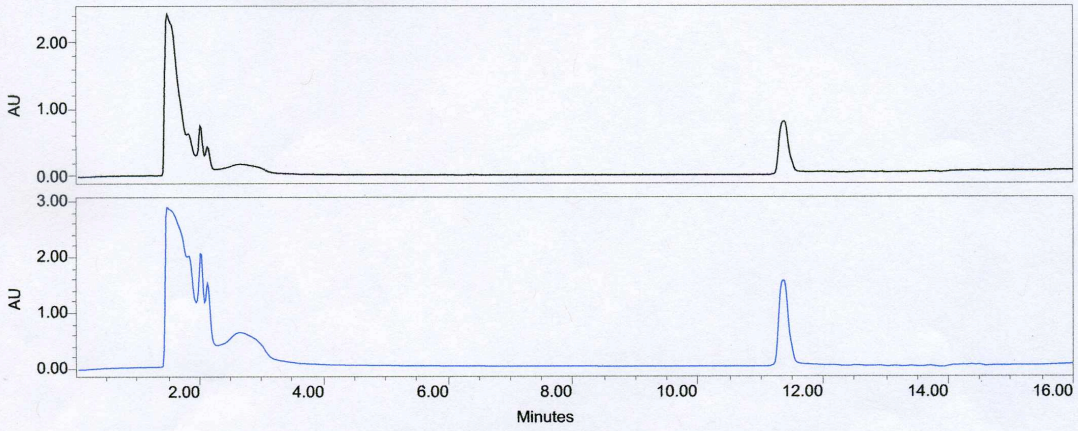
SDSU

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	eks_comp145_3ox	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	240	Date Acquired:	3/16/2011 1:22:10 PM
Run Time:	16.00 Minutes	Injection Volume:	50.00 ul



Channel: 2487Channel 1 Channel Desc.: Processing Method: *
Channel: 2487Channel 2 Channel Desc.: Processing Method: *

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	Amount	Units
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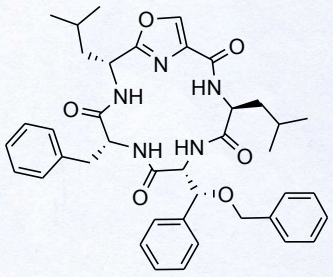
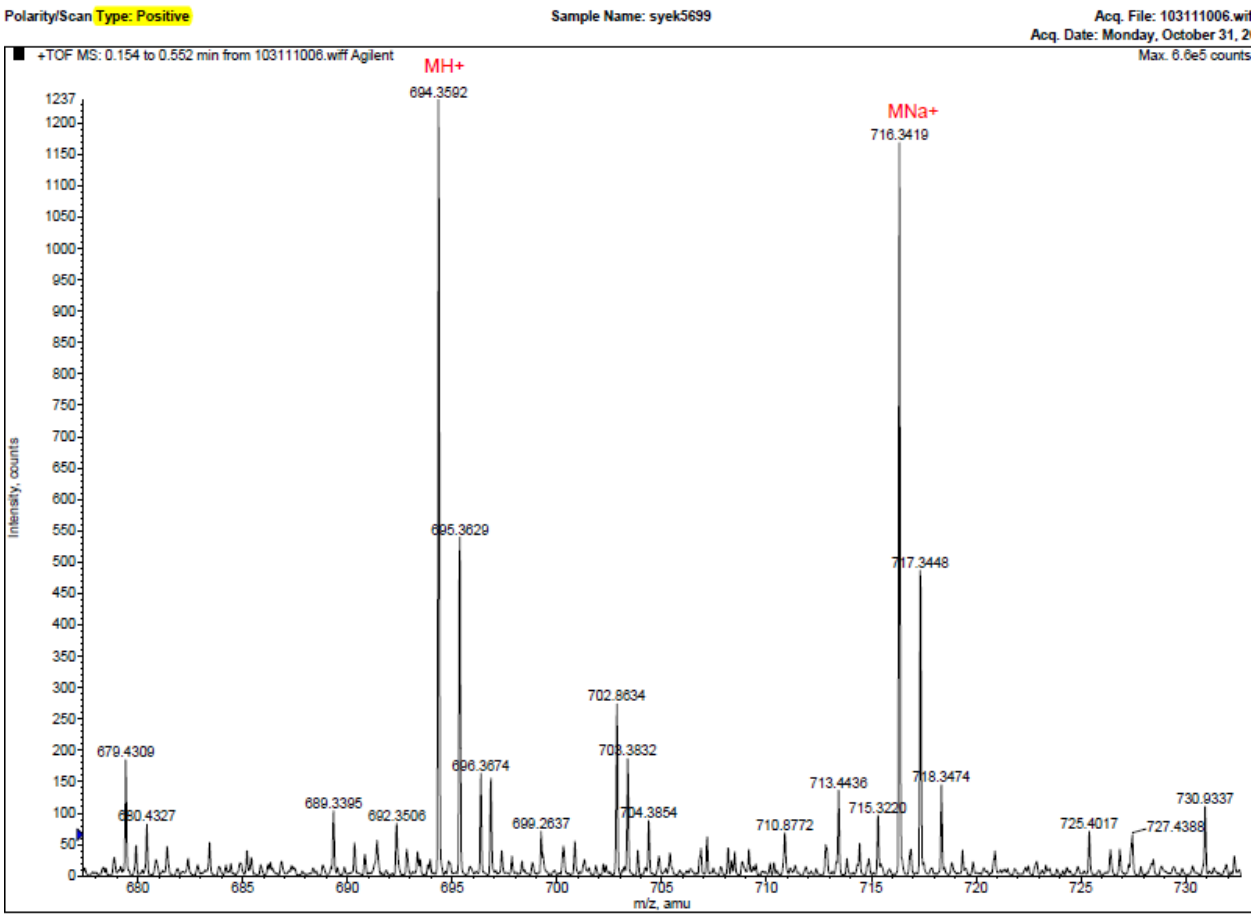
2	****	****	****	****	****	****	****



Report Method: Injection Summary Report Printed 1:38:23 PM 3/16/2011 Page: 1 of 1

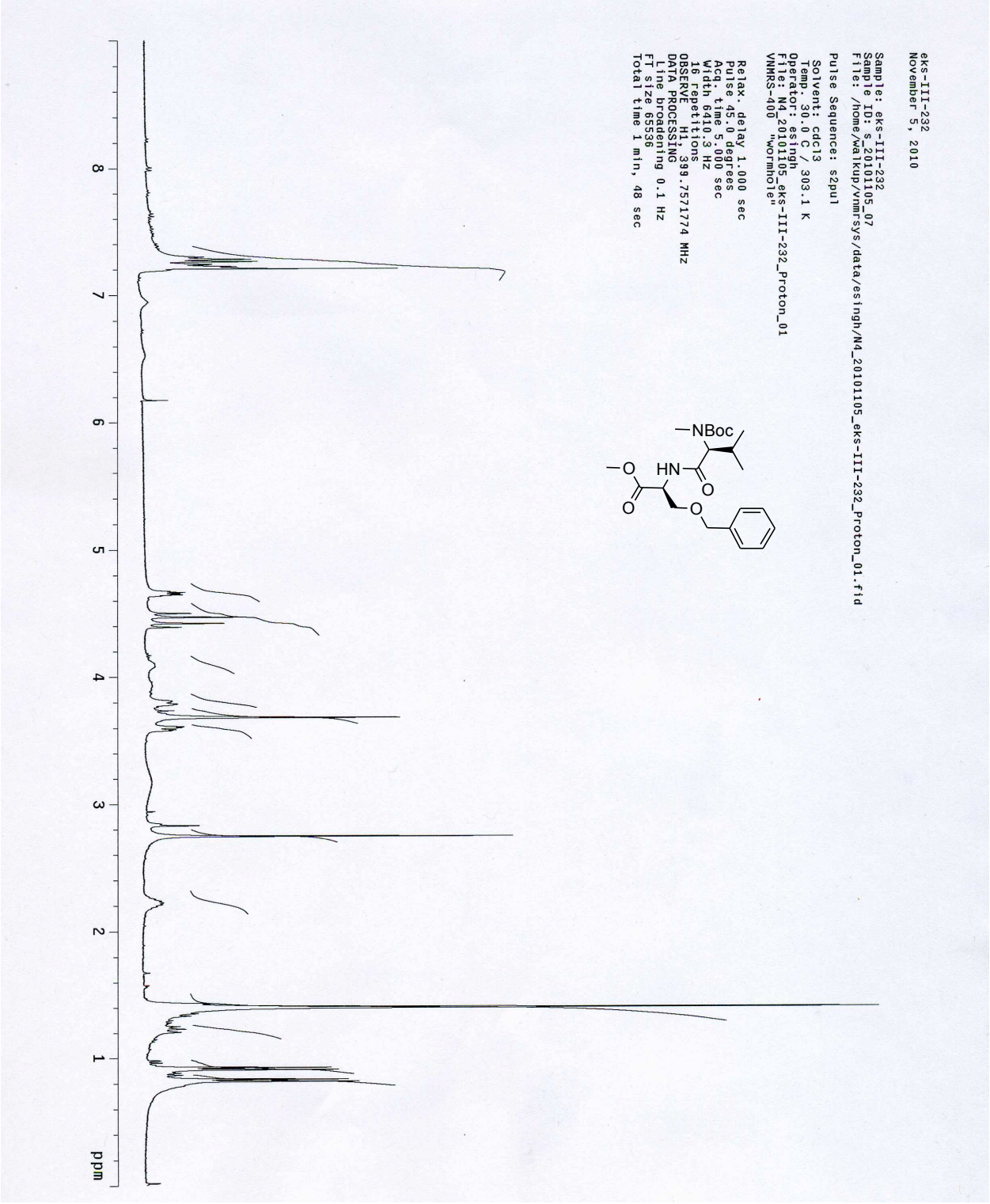
Compound 6: D-Ox-III

HPLC Macrocycle (2R,3R)-β-benzoxy-Phe-Leu-Oxazole-D-Leu-D-Phe (6)



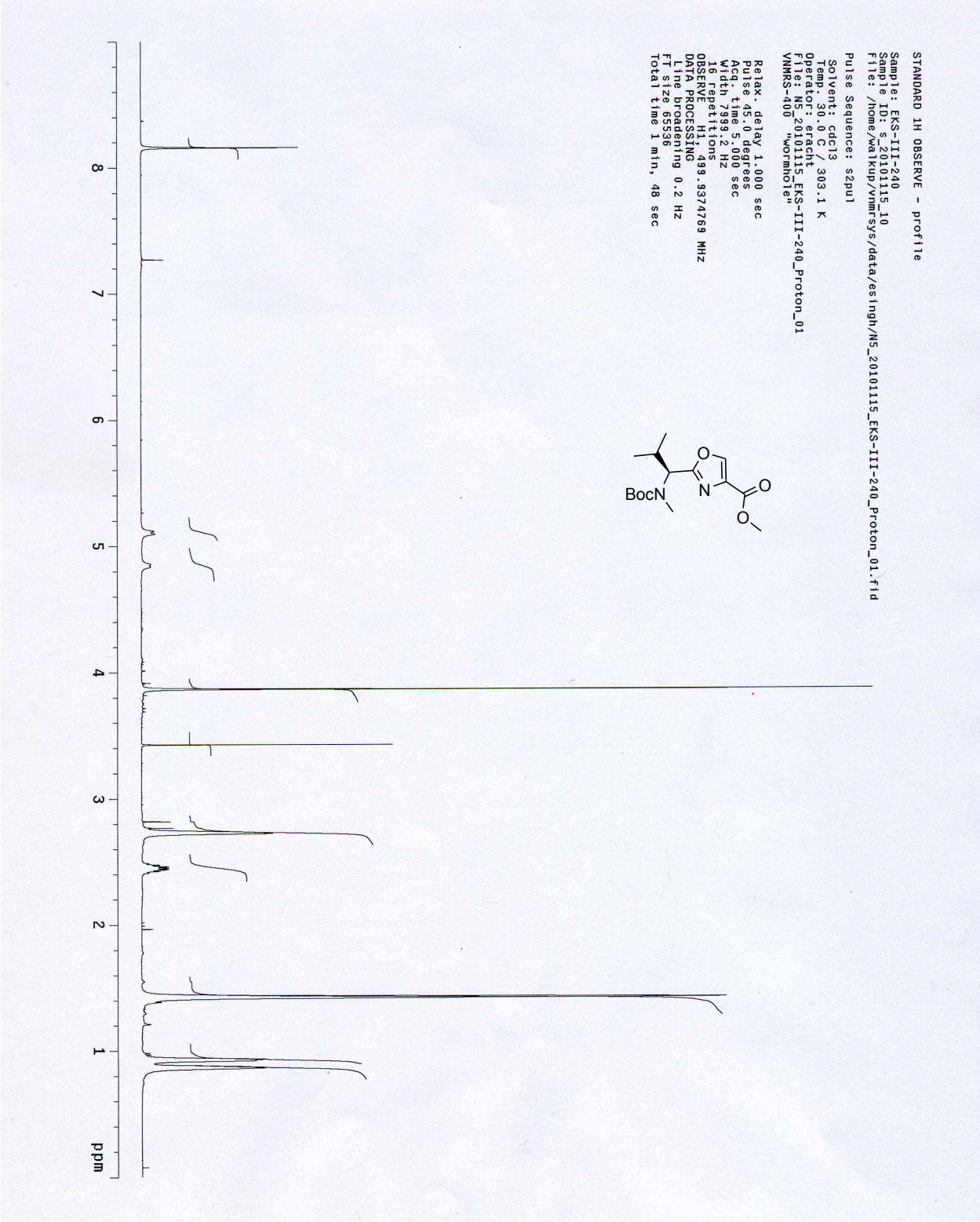
Compound 6: D-Ox-III

HRMS Macrocycle (2R,3R)-β-benzoxy-Phe-Leu-Oxazole-D-Leu-D-Phe (6) (MW = 694.3592)



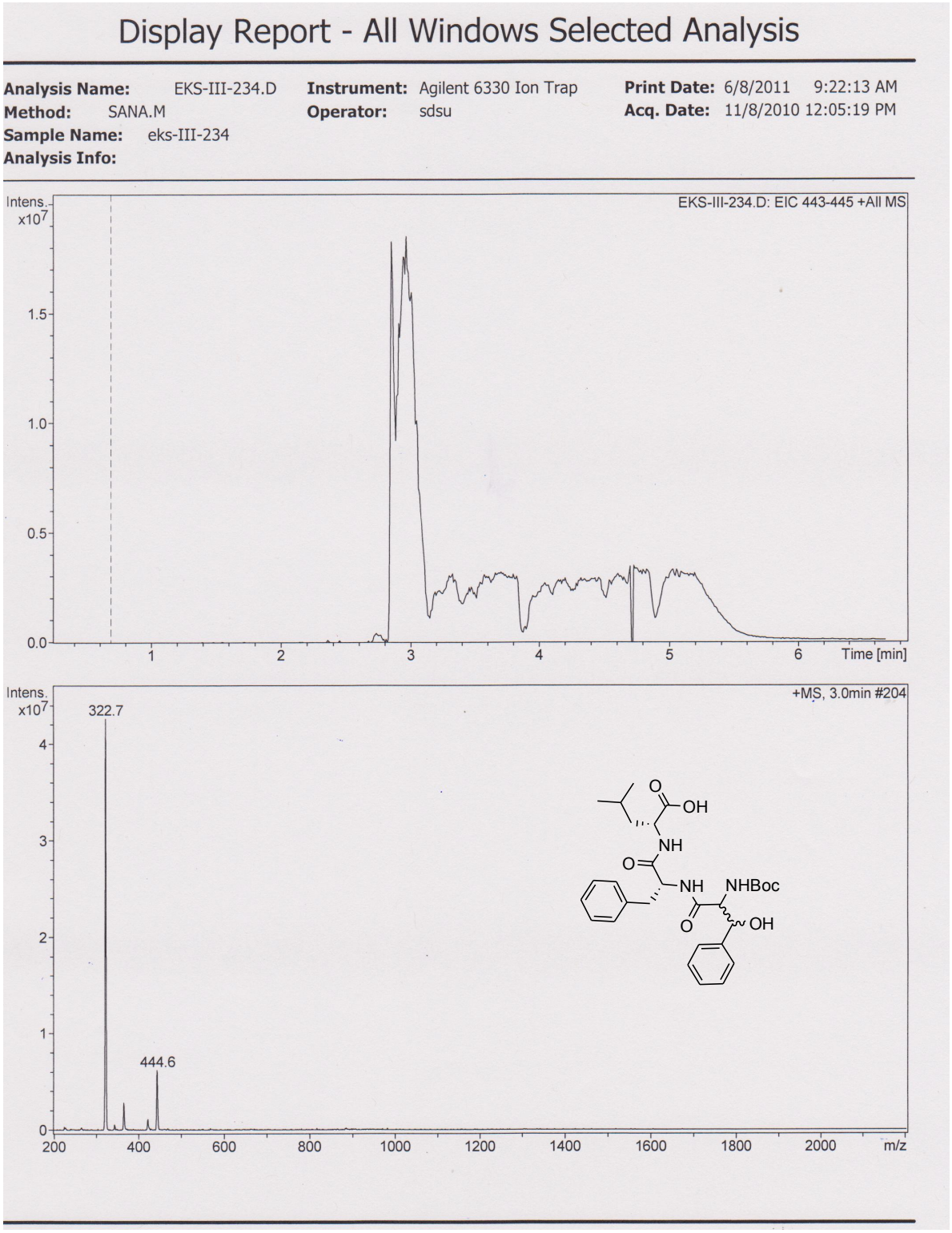
Compound 7: D-Ox-II

NMR Dipeptide MeO-Ser(Bzl)-Val-N(Me)Boc



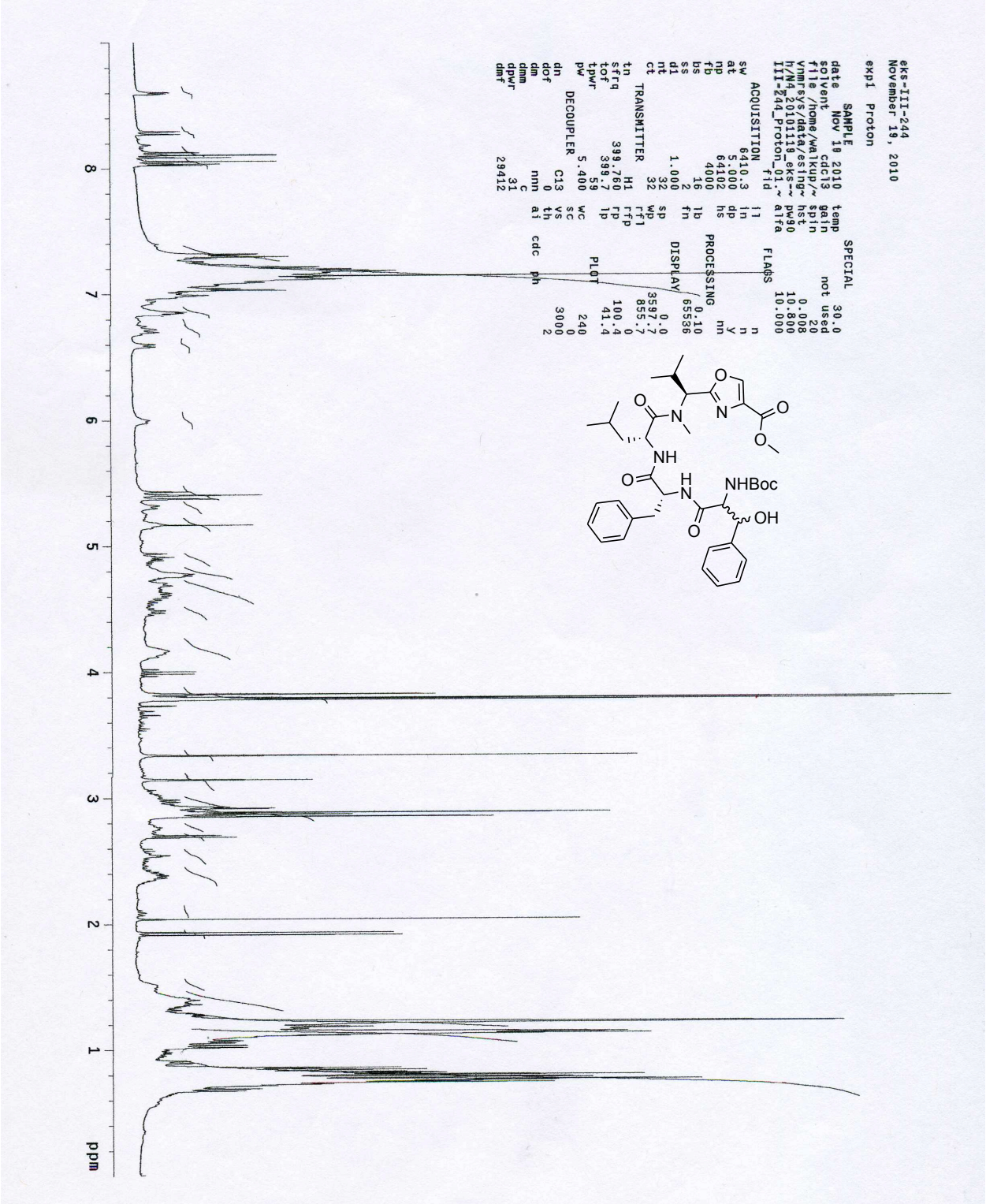
Compound 7: D-Ox-II

NMR Dipeptide MeO-Oxazole-Val-N(Me)Boc



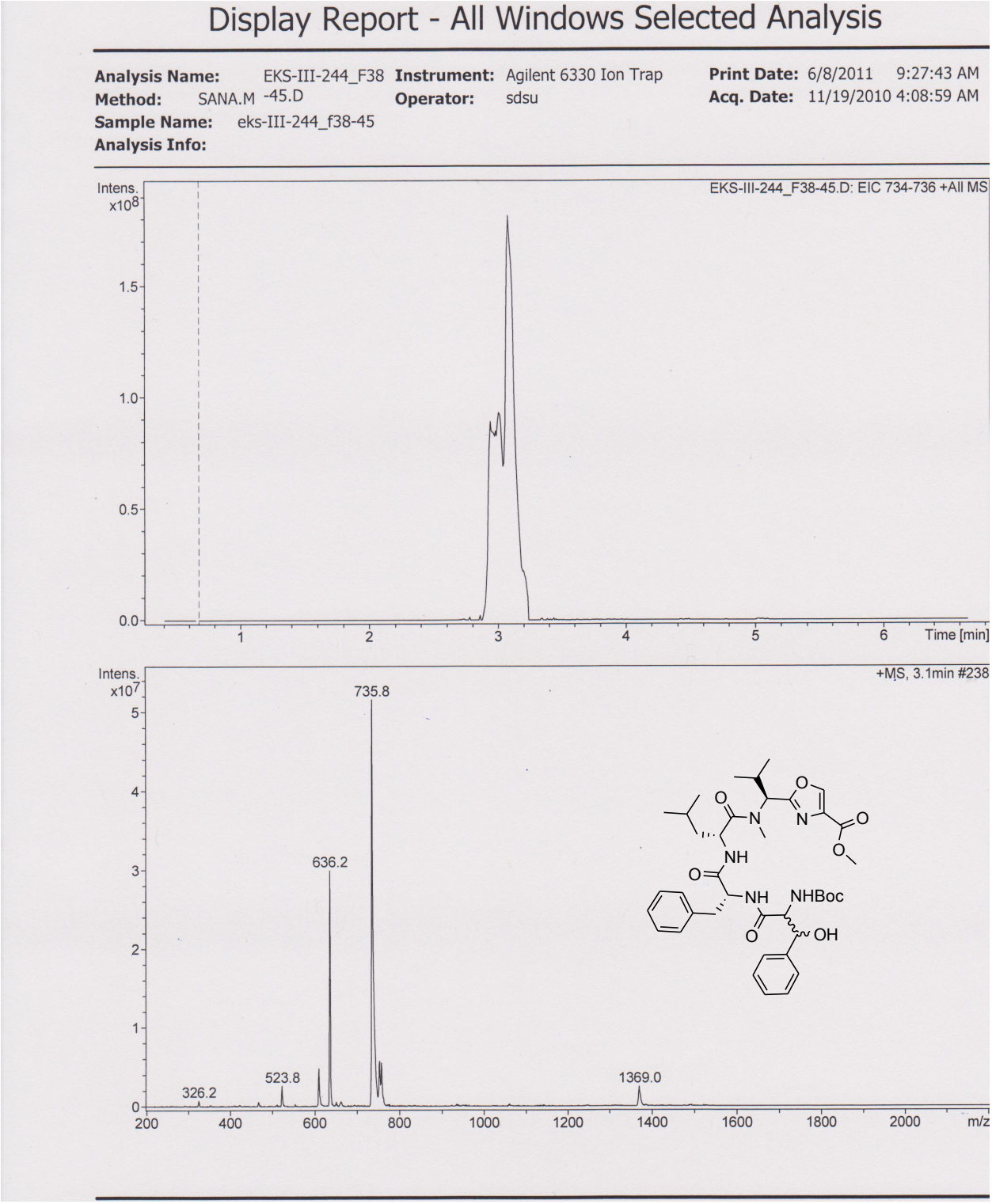
Compound 7: D-Ox-II

LCMS Tripeptide HO-D-Leu-D-Phe- β-OH-(2R,3R)/(2S,3S)-NHBoc (MW = 444)



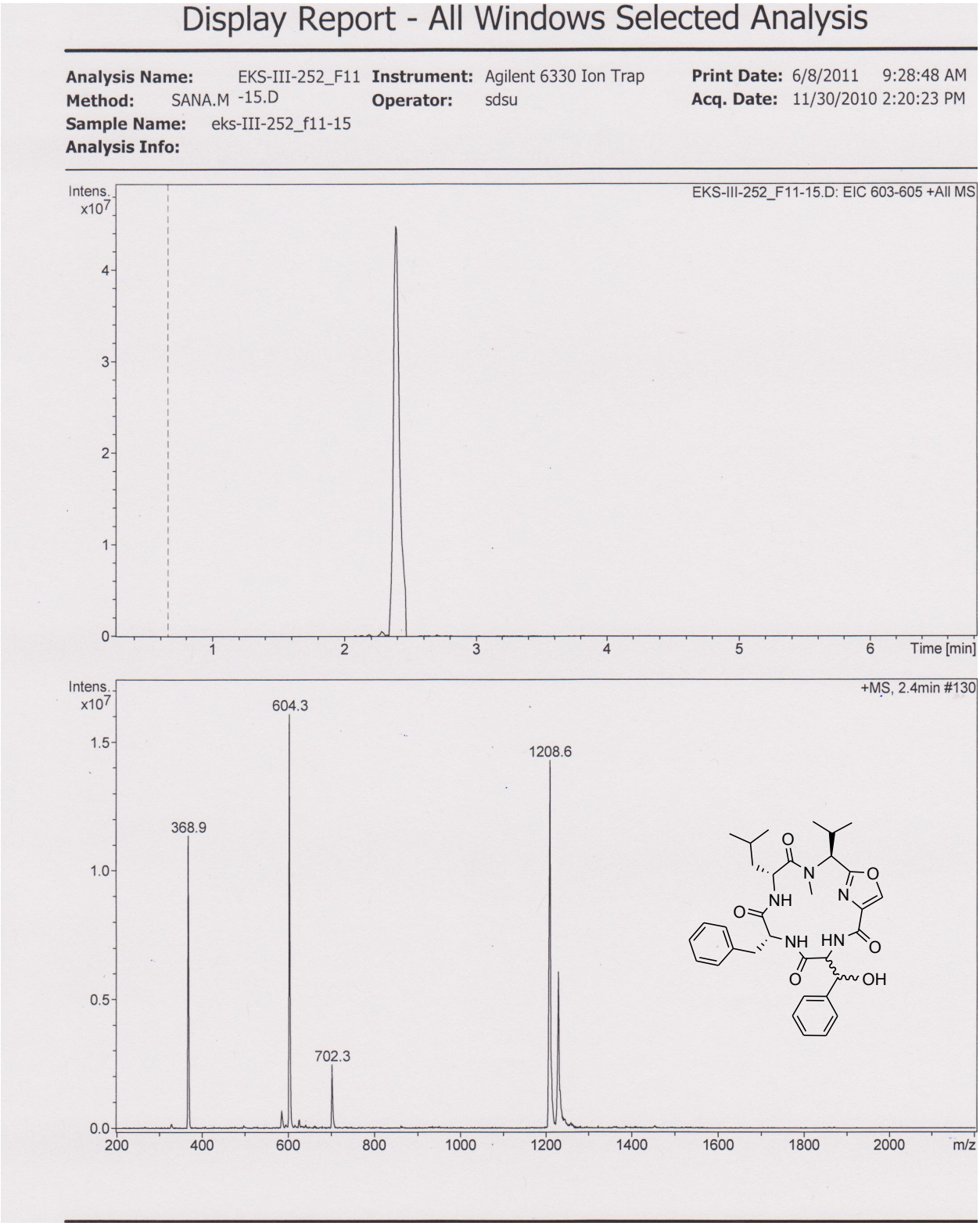
Compound 7: D-Ox-II

NMR Pentapeptide MeO-Oxazole-Val-N(Me)-D-Leu-D-Phe-(2R,3R)/(2S,3S)-β-OH-Phe-NHBoc



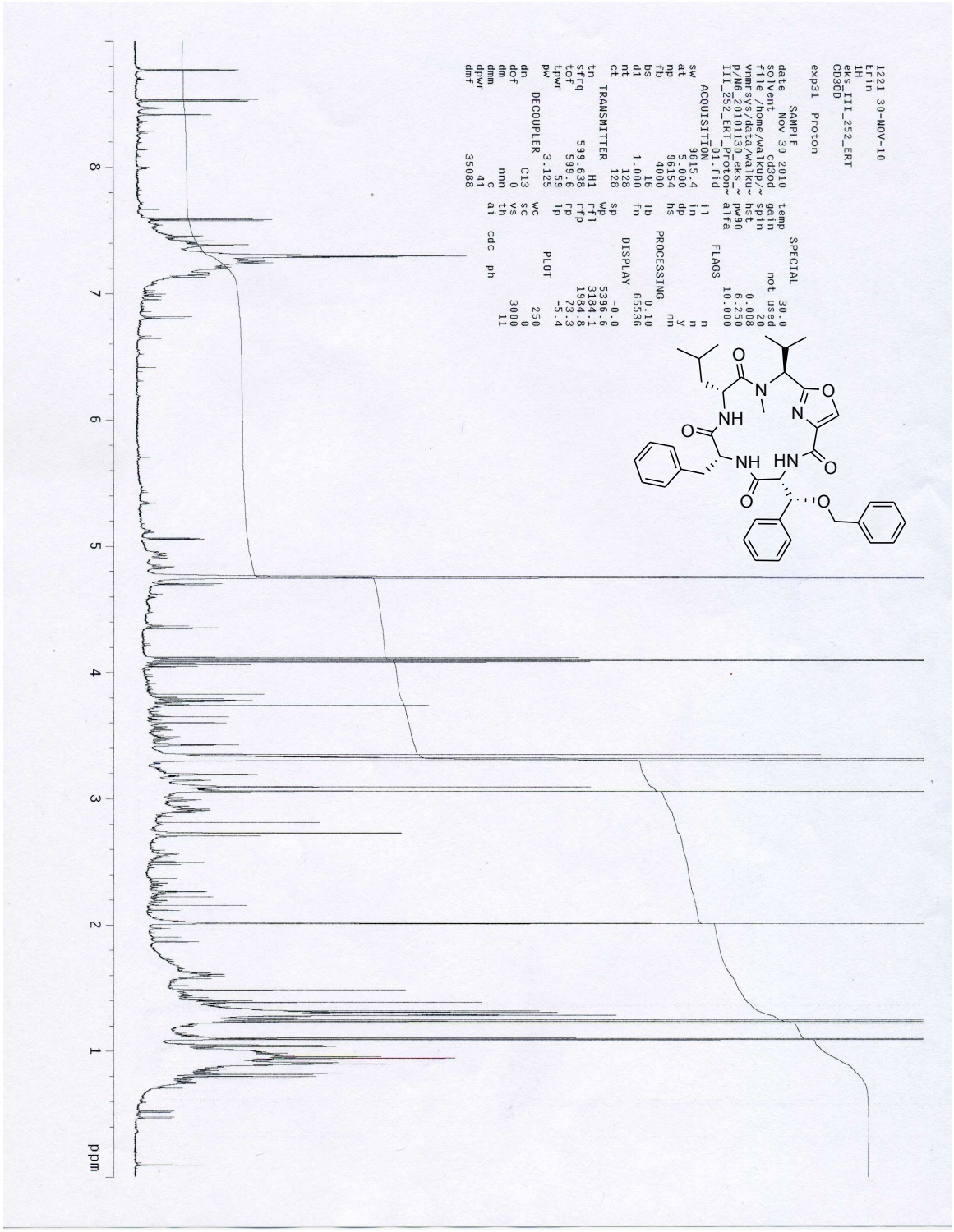
Compound 7: D-Ox-II

LCMS Pentapeptide MeO-oxazole-Val-N(Me)-D-Leu-D-Phe-(2R,3R)/(2S,3S)-β-OH-Phe-NHBoc (MW = 736)



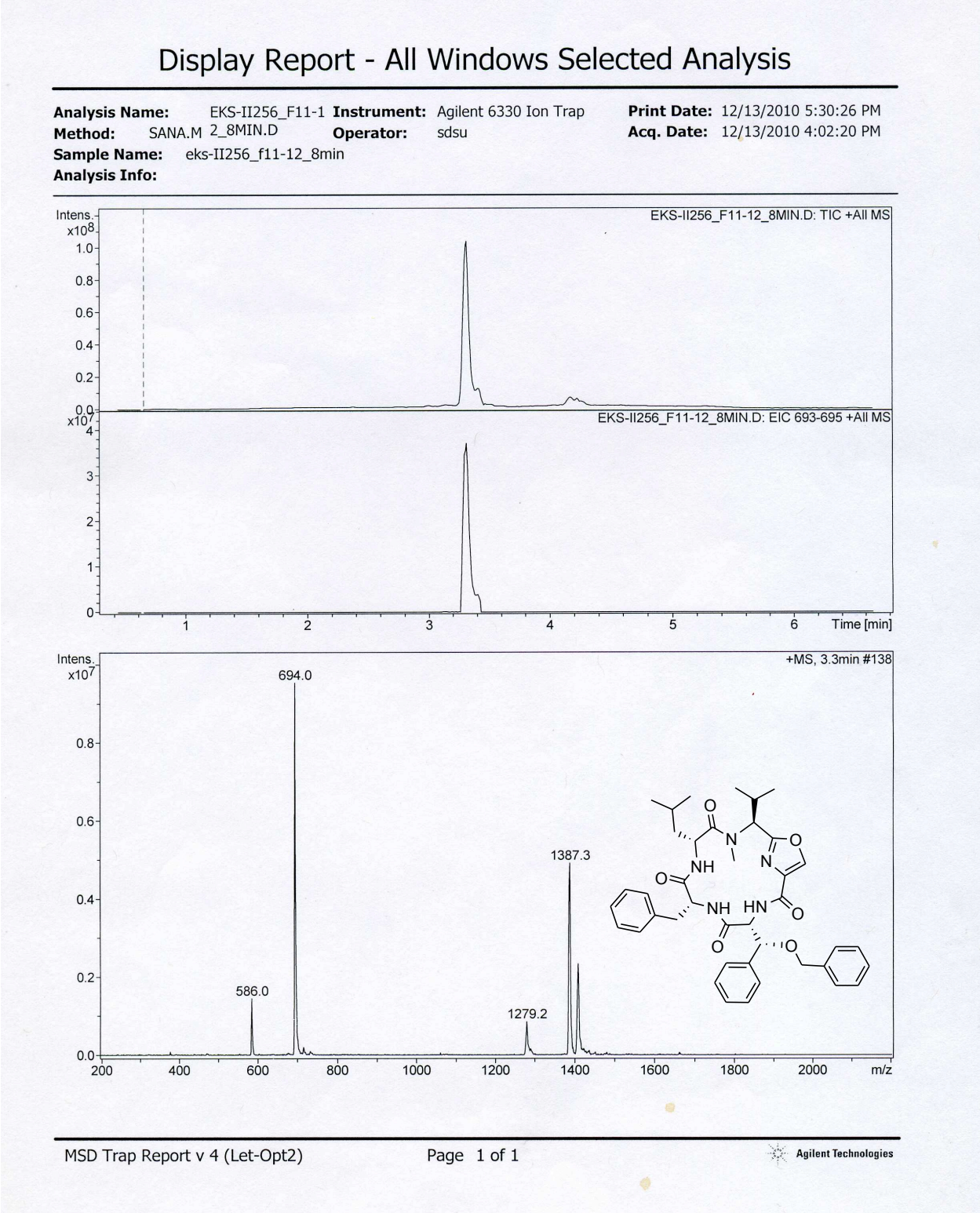
Compound 7: D-Ox-II

LCMS Macrocycle (2R,3R)-β-OH-Phe-Oxazole-Val-N(Me)-D-Leu-D-Phe (MW = 604)



Compound 7: D-Ox-II

NMR Macrocycle (2R,3R)-β-benzoxy-Phe-oxazole-Val-N(Me)-D-Leu-D-Phe (7)



Compound 7: D-Ox-II

LCMS Macrocycle (2R,3R)-β-benzoxy-Phe-oxazole-Val-N(Me)-D-Leu-D-Phe (7) (MW = 694)

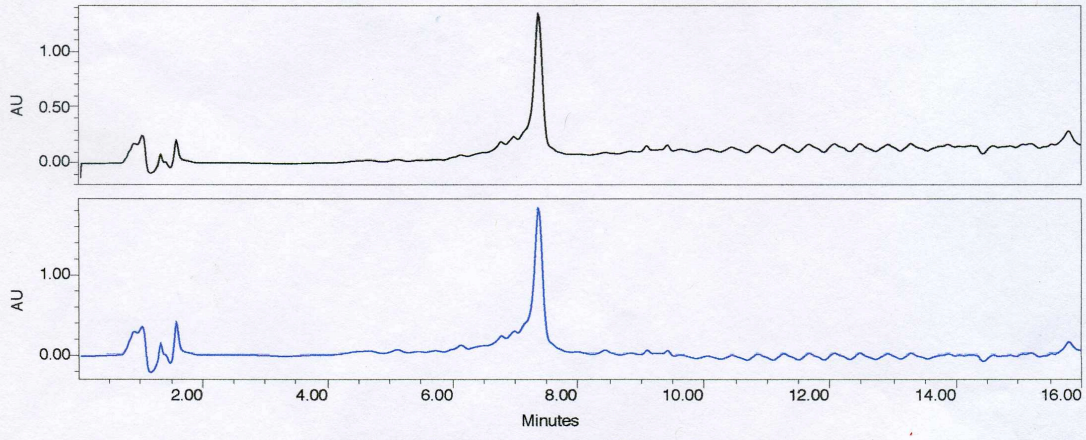
SDSU

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	eks-III-252_ERT-208	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	42	Date Acquired:	12/7/2010 4:31:57 PM
Run Time:	16.00 Minutes	Injection Volume:	75.00 ul



	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	Amount	Units
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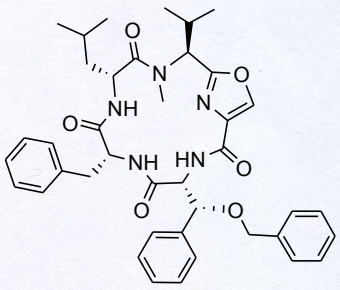
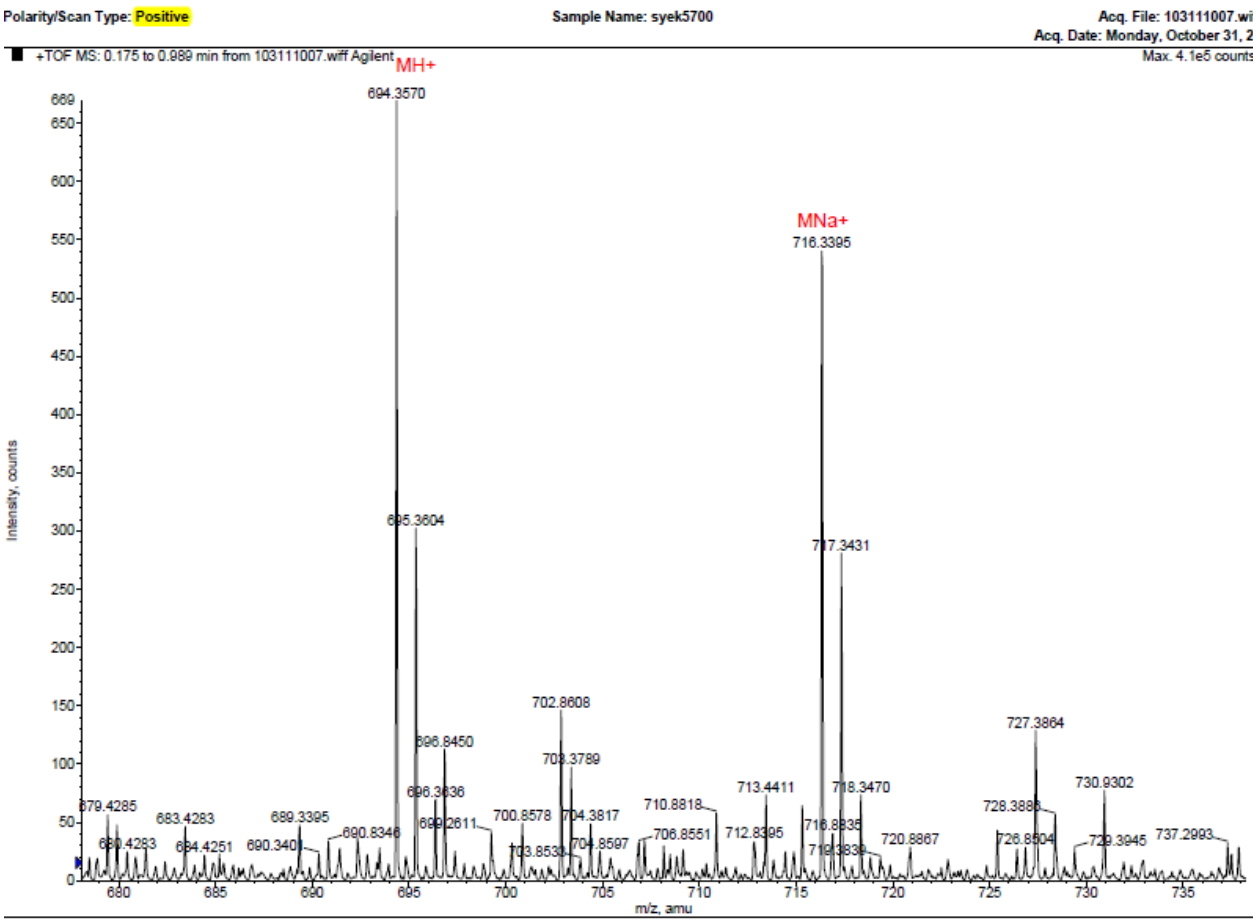
2	****	****	****	****	****	****	****



Report Method: Injection Summary Report Printed 4:48:11 PM 12/7/2010 Page: 1 of 1

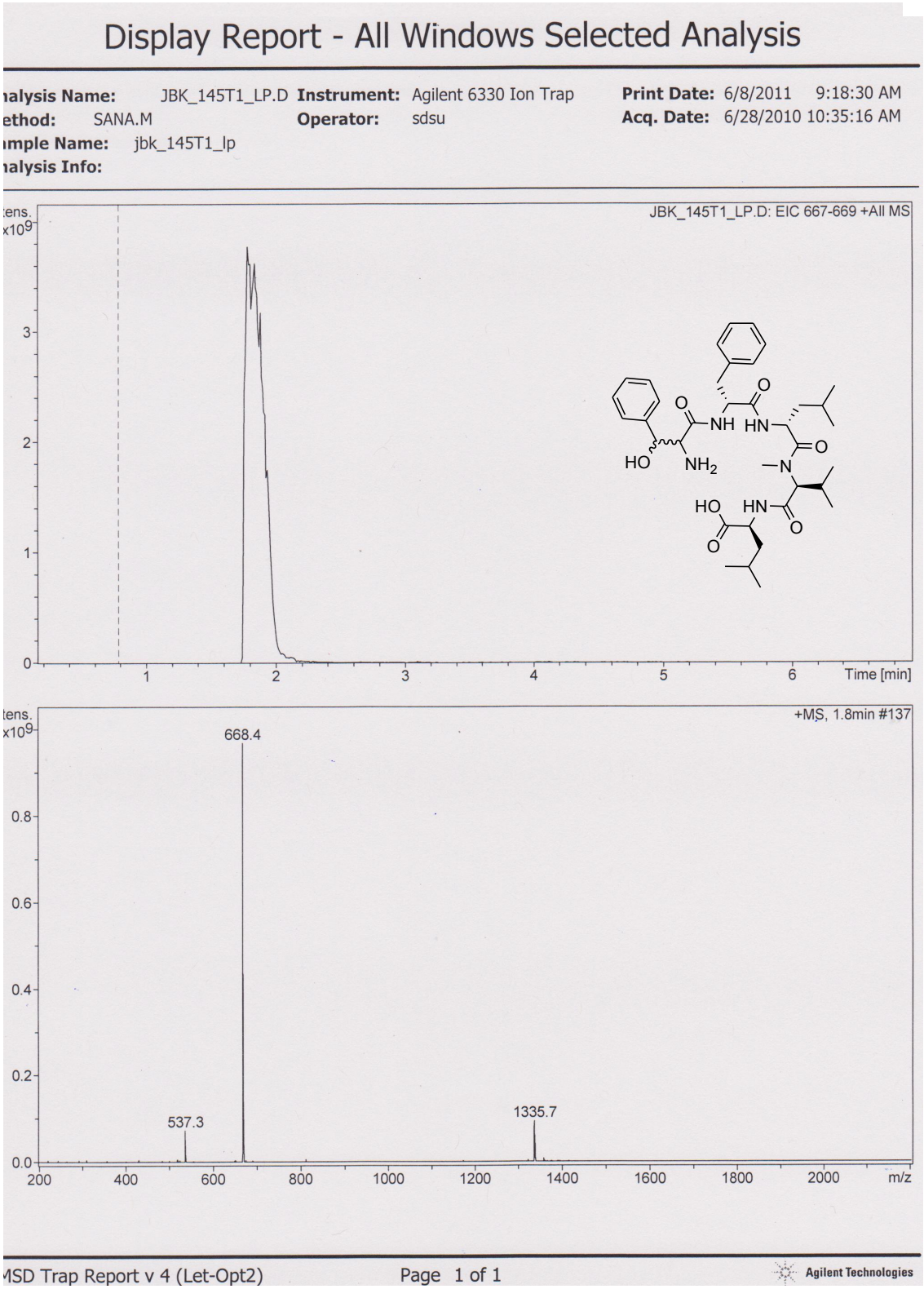
Compound 7: D-Ox-II

HPLC Macrocycle (2R,3R)-β-benzoxy-Phe-oxazole-Val-N(Me)-D-Leu-D-Phe (7)



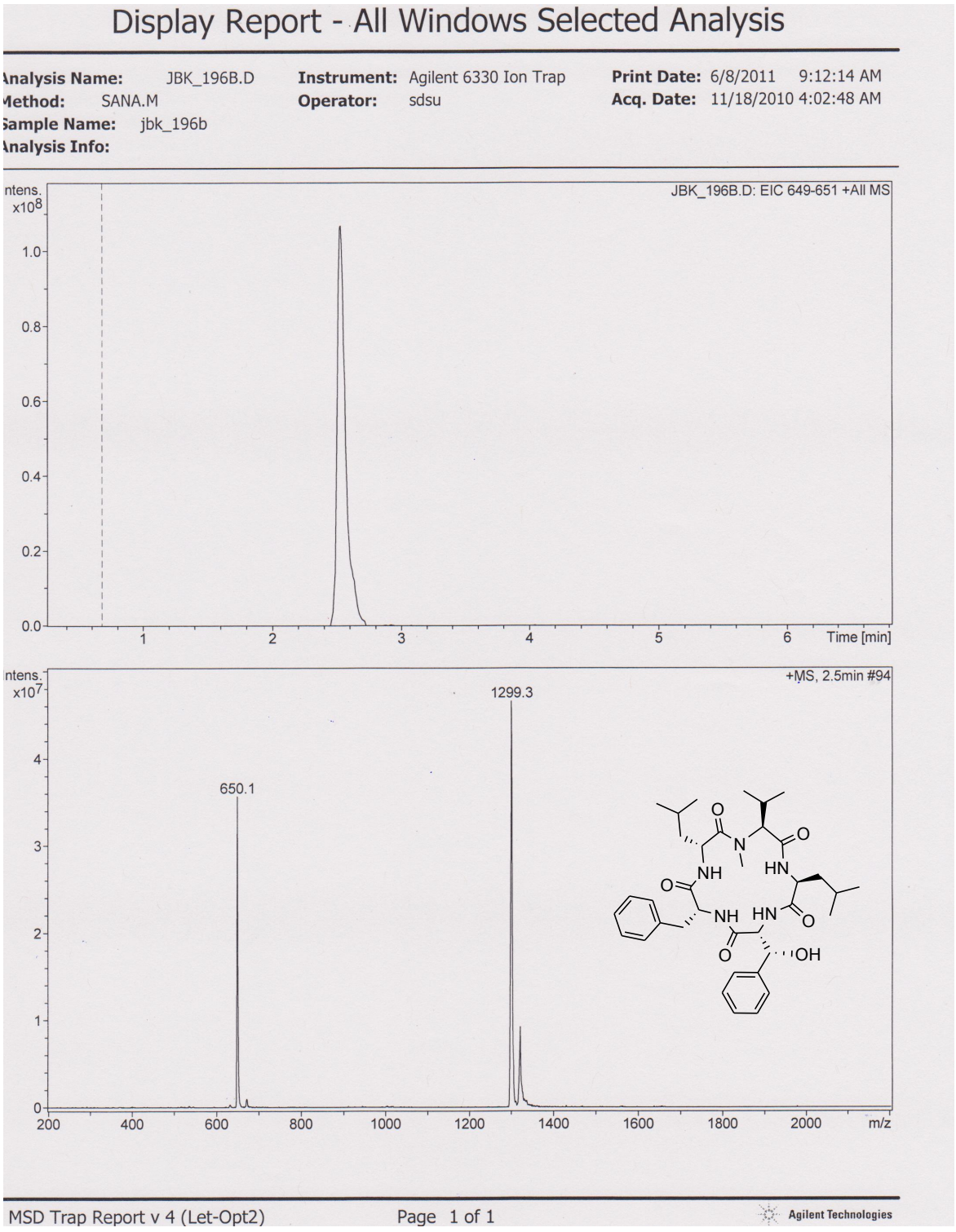
Compound 7: D-Ox-II

HRMS Macrocycle (2R,3R)-β-benzoxy-Phe-oxazole-Val-N(Me)-D-Leu-D-Phe (7) (MW = 694.3570)



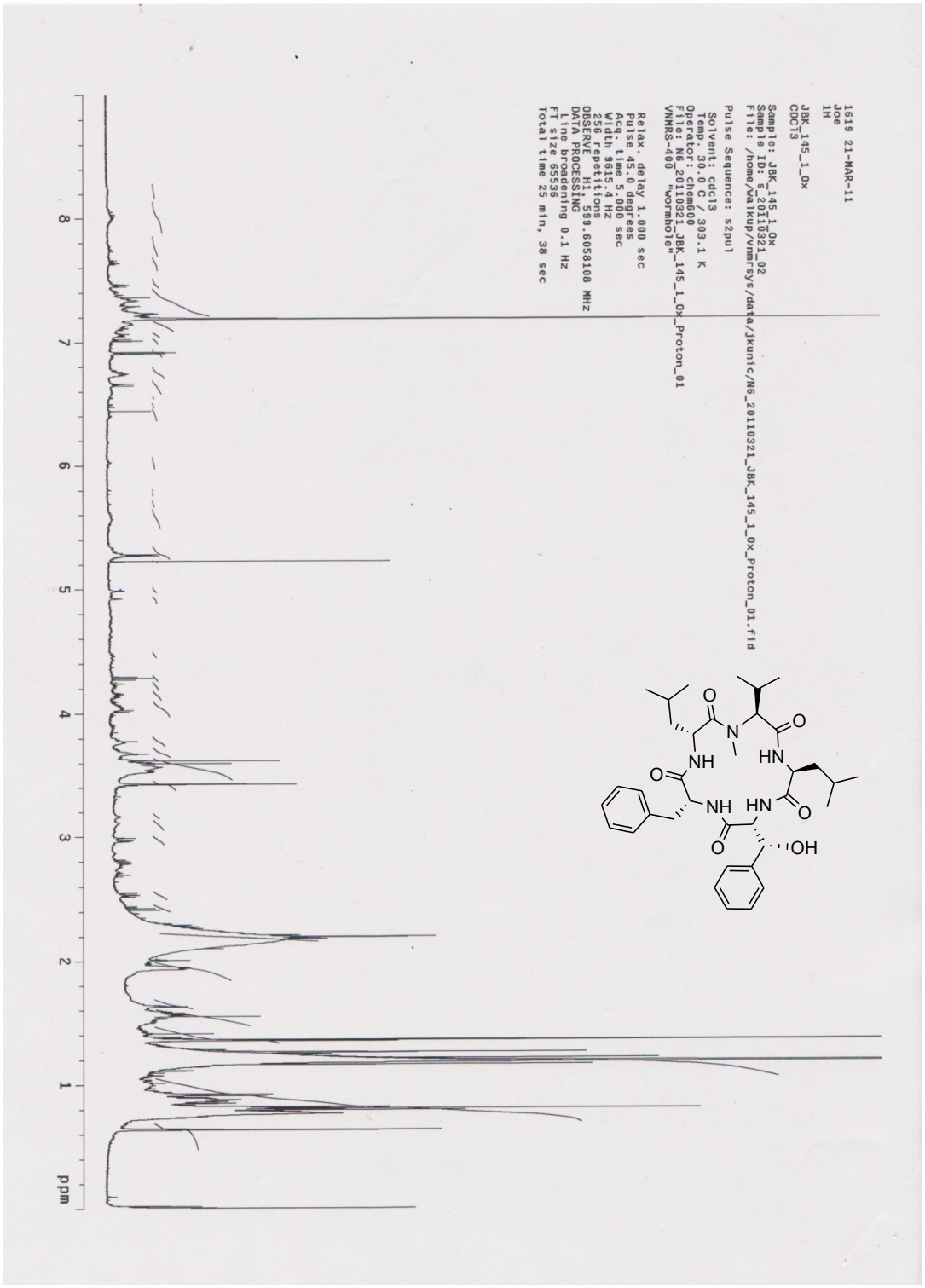
Compound 8: D-Ox-I

LCMS Pentapeptide HO- Leu-Val-N(Me)-D-Leu-D-Phe-β-OH(2R,3R)(2S,3S)-Phe-NH_2
(MW = 668)



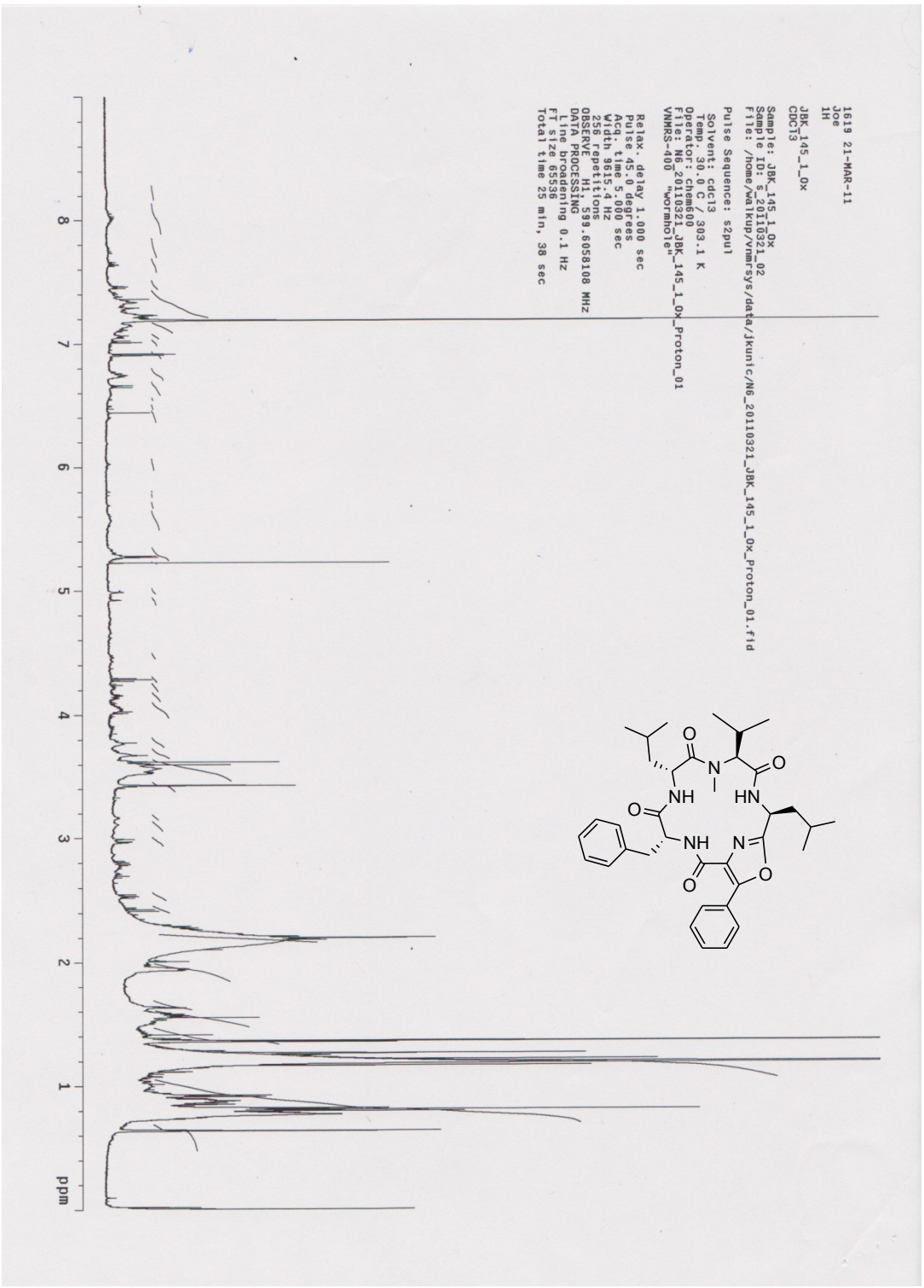
Compound 8: D-Ox-I

LCMS Macrocycle β-OH(2R,3R)-Phe-Leu-Val-N(Me)-D-Leu-D-Phe (MW = 649.82)



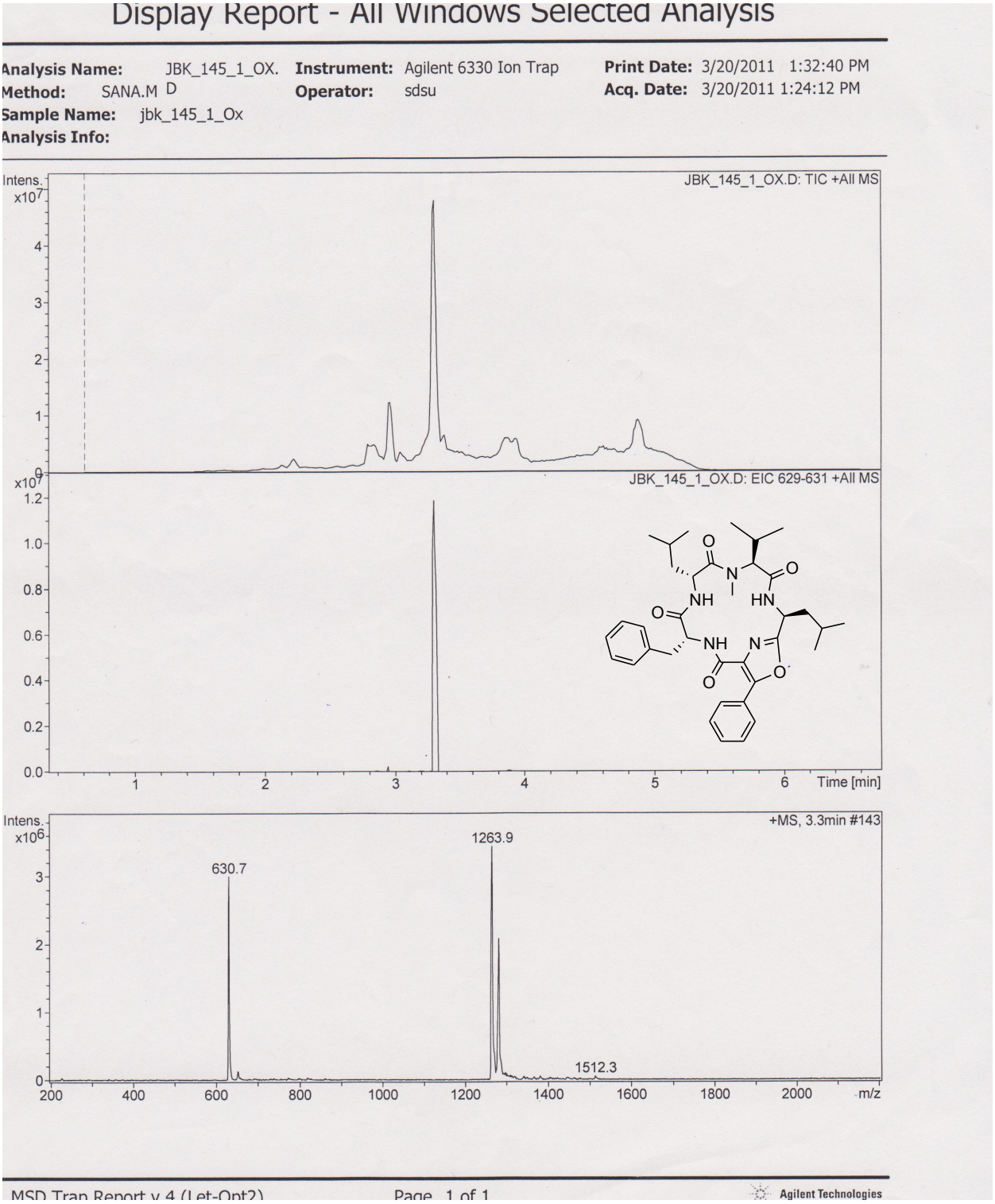
Compound 8: D-Ox-I

NMR Macrocycle β-OH(2*R*,3*R*)-Phe-Leu-Val-N(Me)-D-Leu-D-Phe (8)



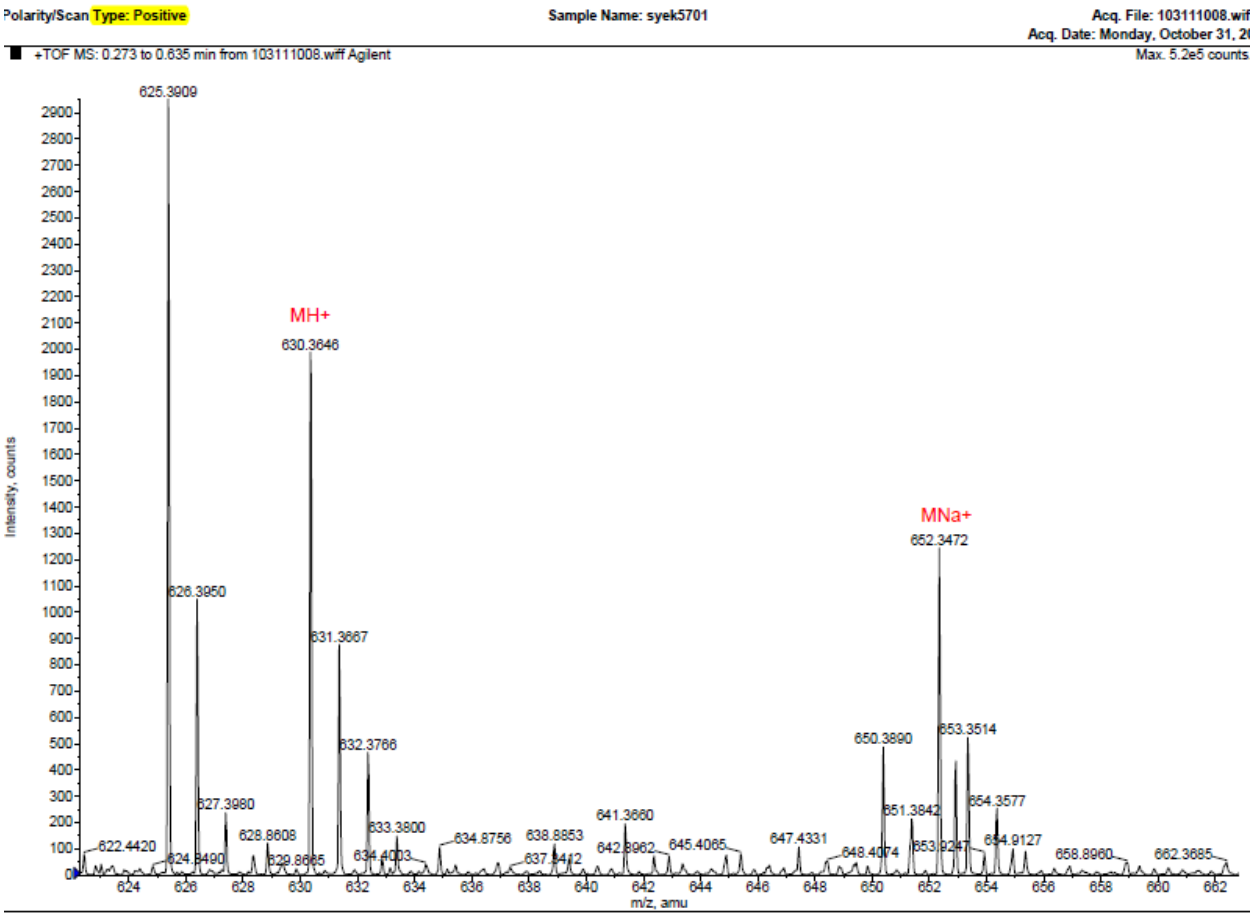
Compound 8: D-Ox-I

NMR Macrocycle Phe-Oxazole-Leu-Val-N(Me)-D-Leu-D-Phe (8)



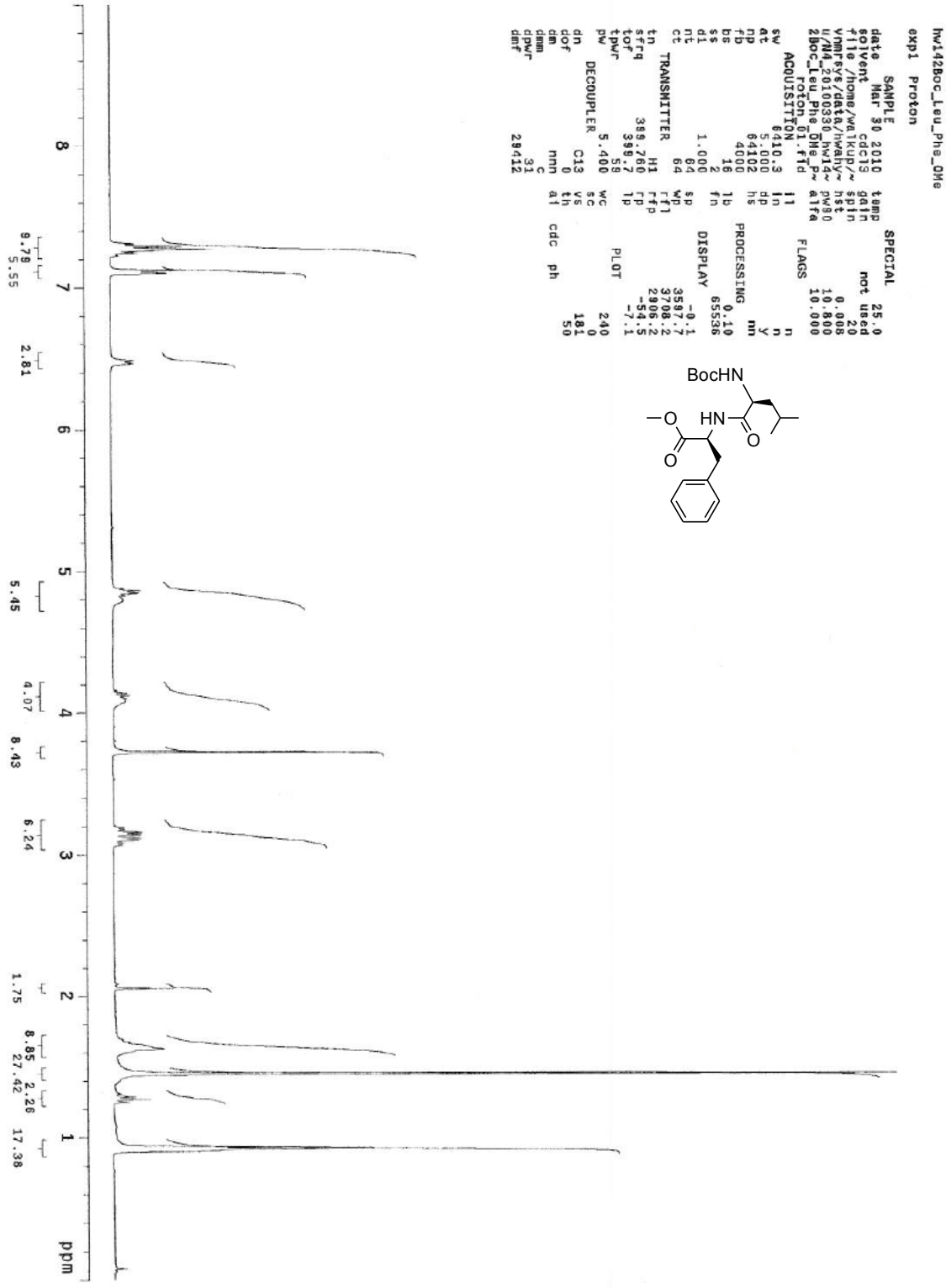
Compound 8: D-Ox-I

LCMS Macrocycle Phe-Oxazole-Leu-Val-N(Me)-D-Leu-D-Phe (8) (MW = 629.79)



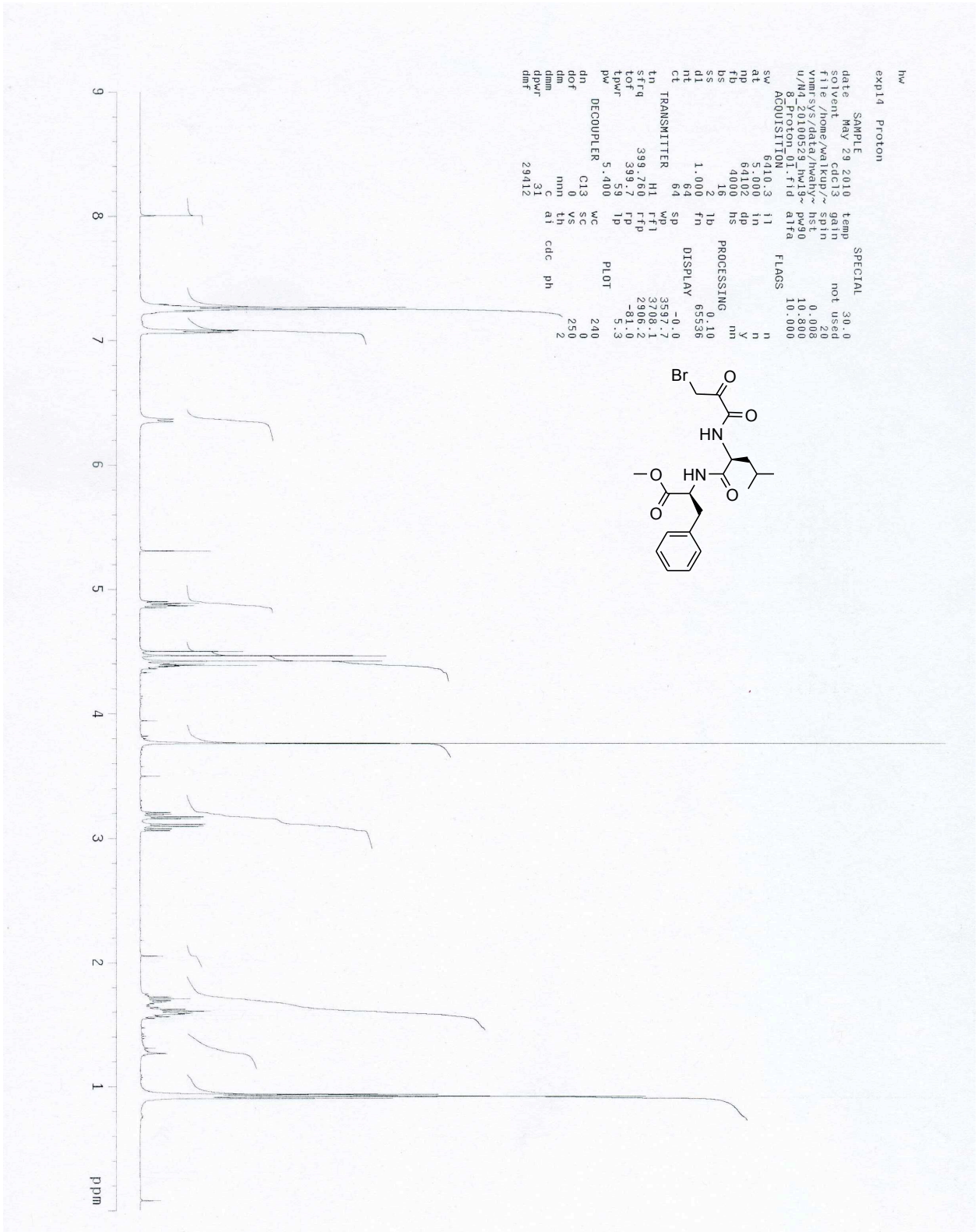
Compound 8: D-Ox-I

HRMS Macrocycle Phe-Oxazole-Leu-Val-N(Me)-D-Leu-D-Phe (8) (MW = 630.3646)



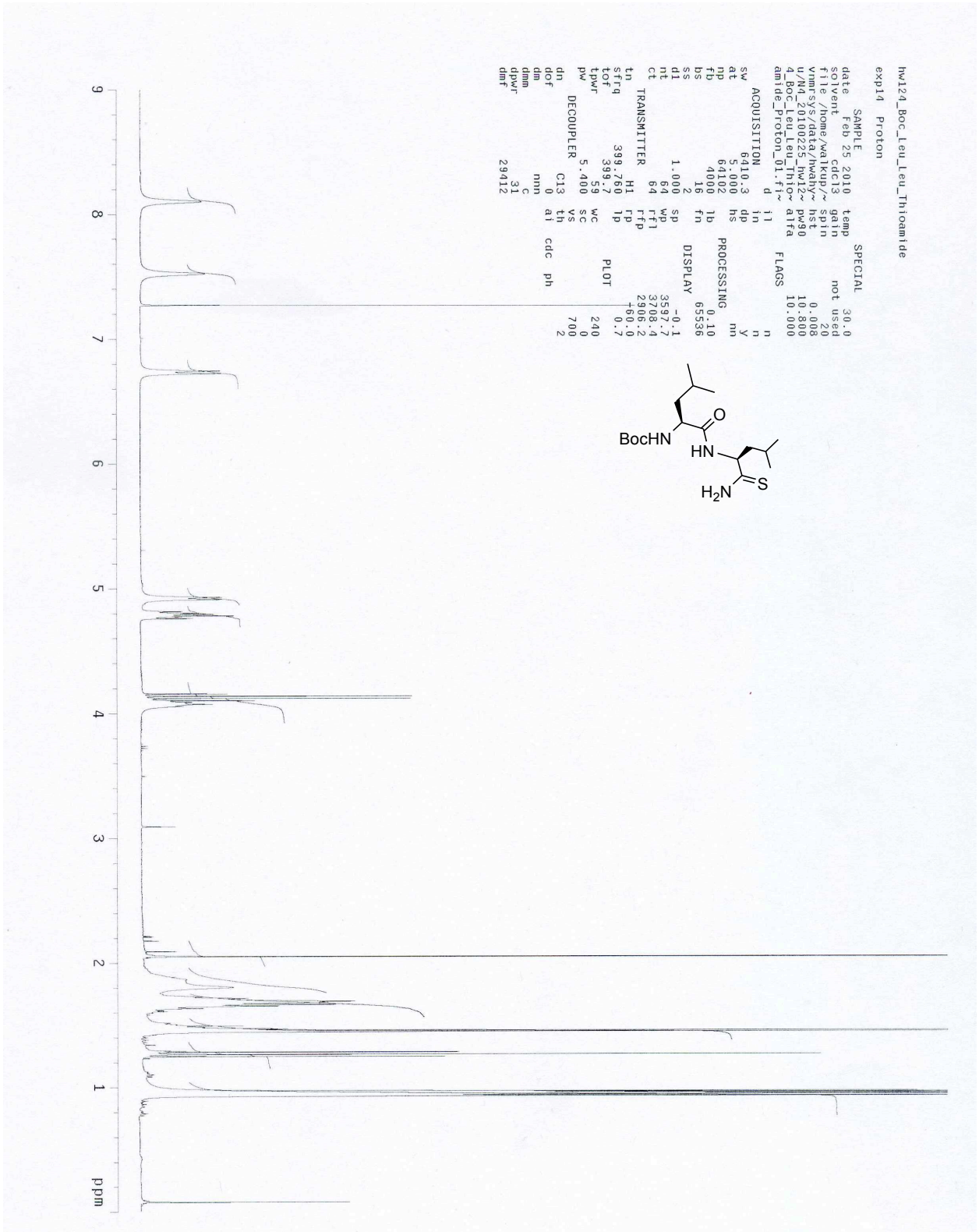
Compound 9: A-Th-III

NMR Dipeptide MeO-Phe-Leu-NHBoc



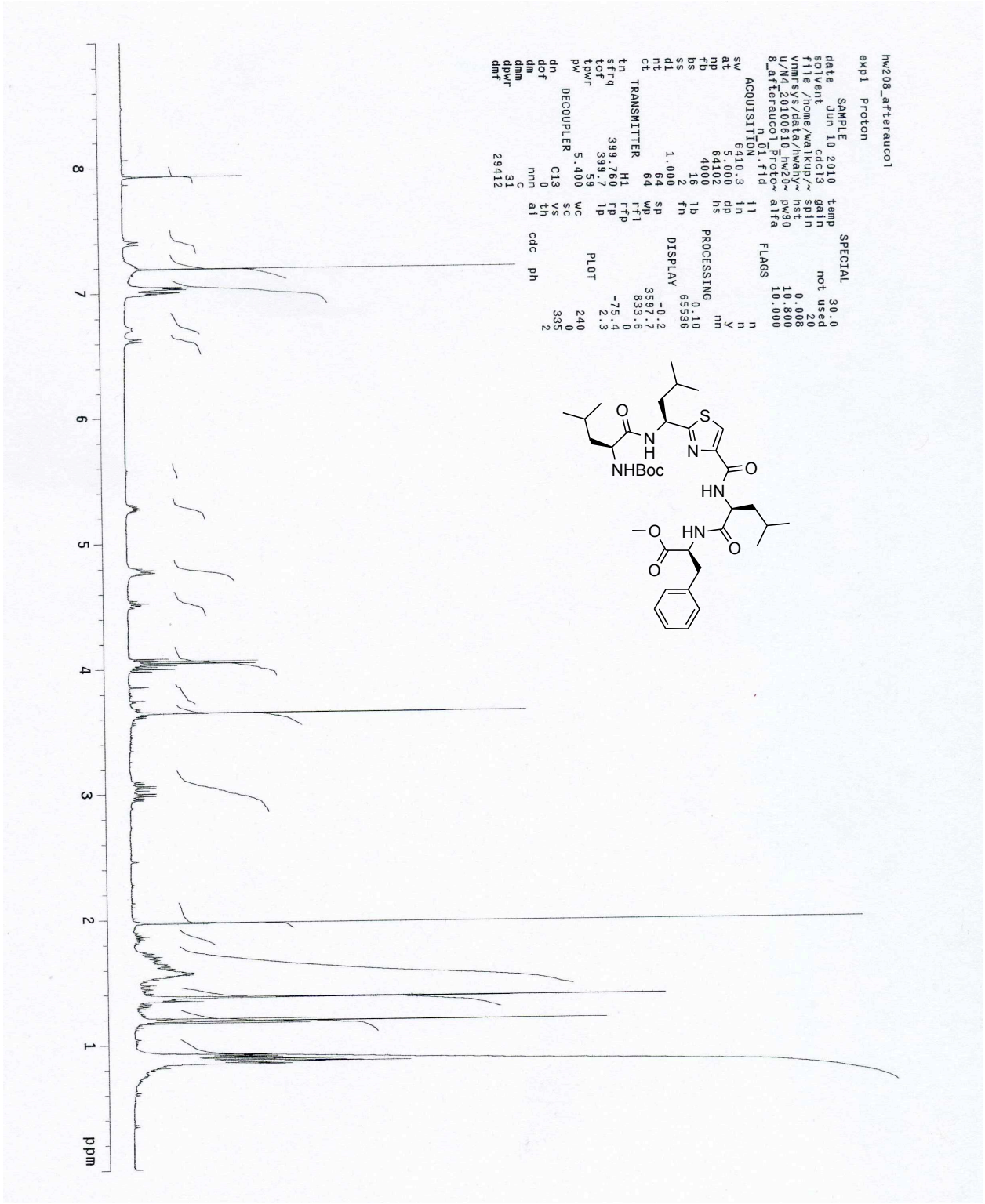
Compound 9: A-Th-III

NMR Tripeptide MeO-Phe-Leu-Ketone-Br (48)



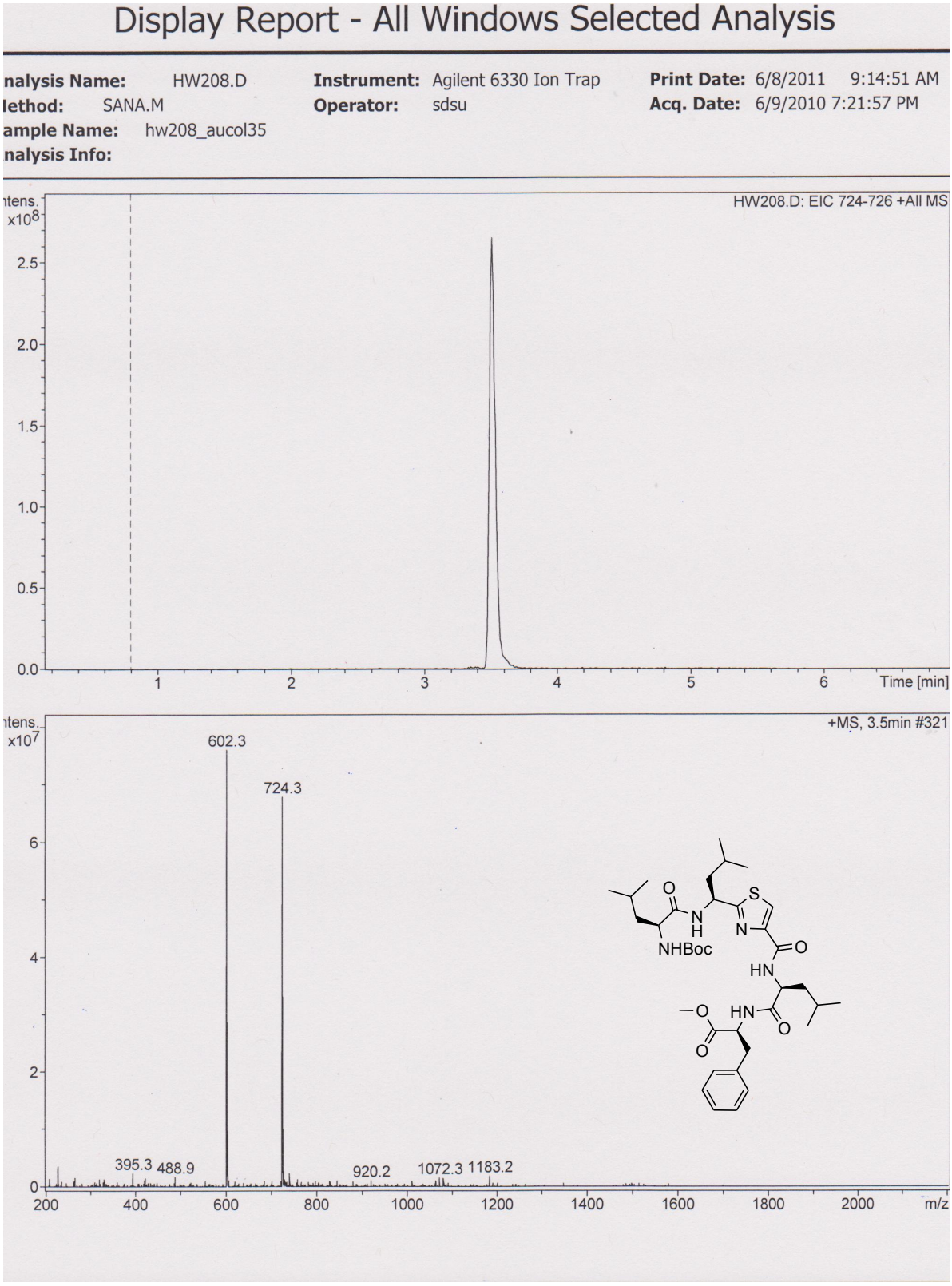
Compound 9: A-Th-III

NMR Dipeptide Thioamide-Leu-Leu-NHBoc (52)



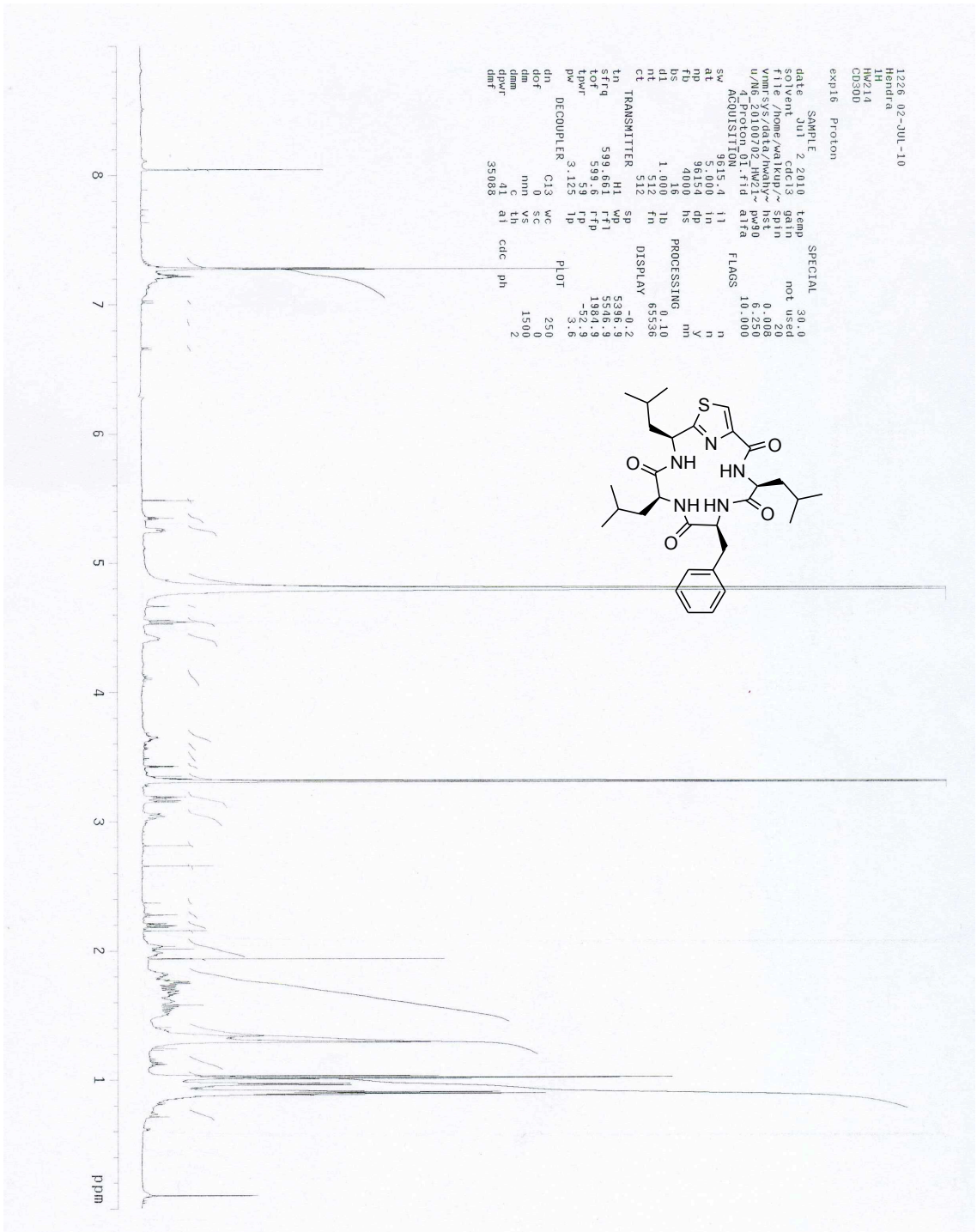
Compound 9: A-Th-III

NMR Pentapeptide MeO-Phe-Leu-Thiazole-Leu-Leu-NHBoc (53)



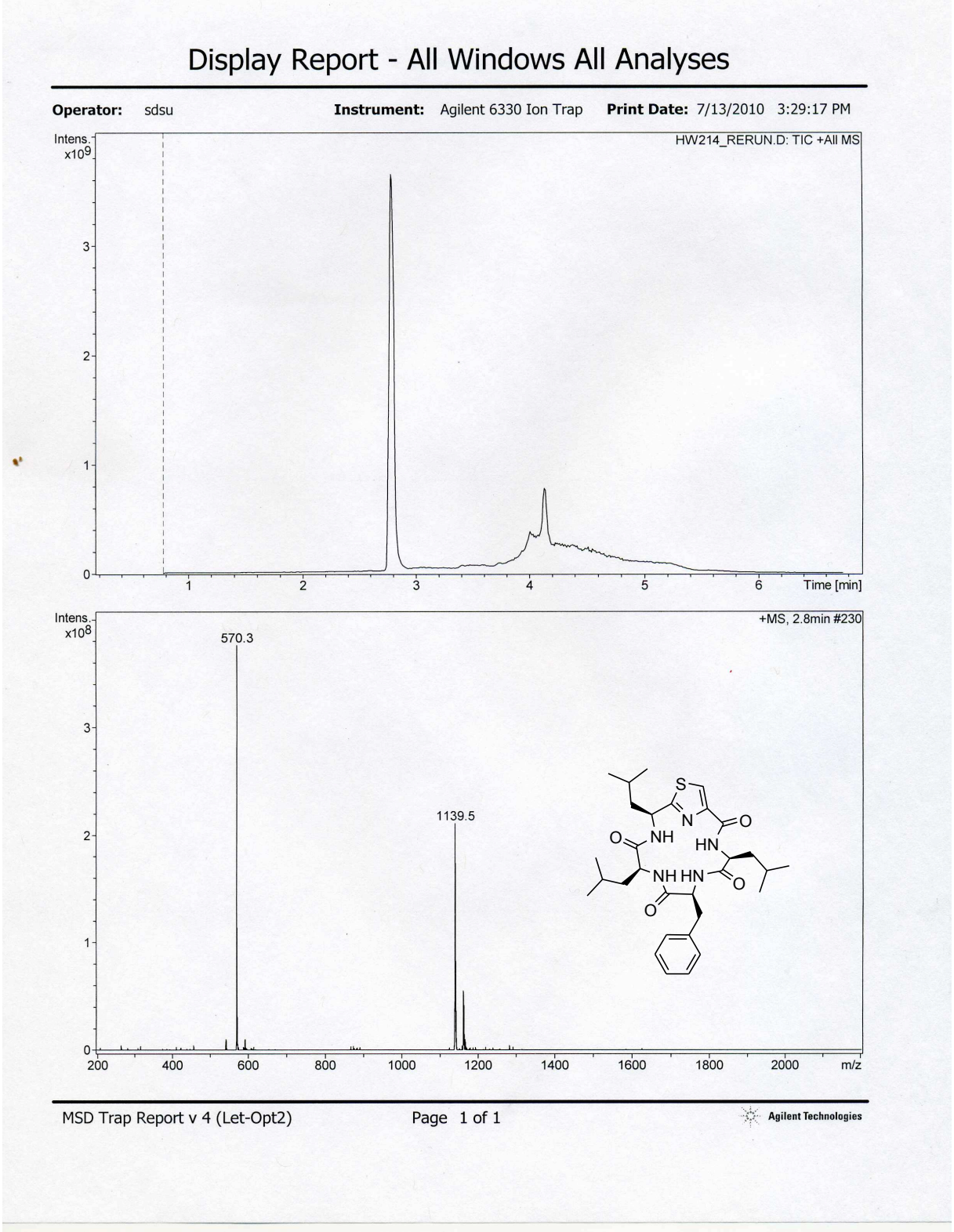
Compound 9: A-Th-III

LCMS Pentapeptide MeO-Phe-Leu-Thiazole-Leu-Leu-NHBoc (53) (MW=701)



Compound 9: A-Th-III

NMR Macrocycle Phe-Leu-Thiazole-Leu-Leu (9)



Compound 9: A-Th-III

LCMS Macrocycle Phe-Leu-Thiazole-Leu-Leu (9) (MW=569)

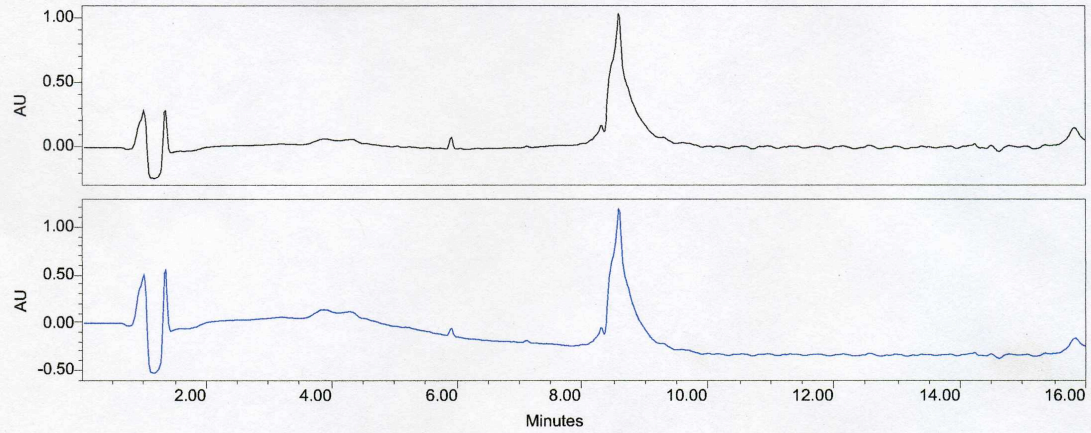
SDSU

Project Name: Defaults
Reported by User: System

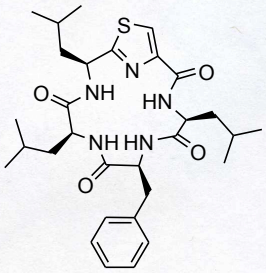
Breeze

SAMPLE INFORMATION

Sample Name:	hw214	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	377	Date Acquired:	6/30/2010 6:29:30 PM
Run Time:	16.00 Minutes	Injection Volume:	40.00 ul



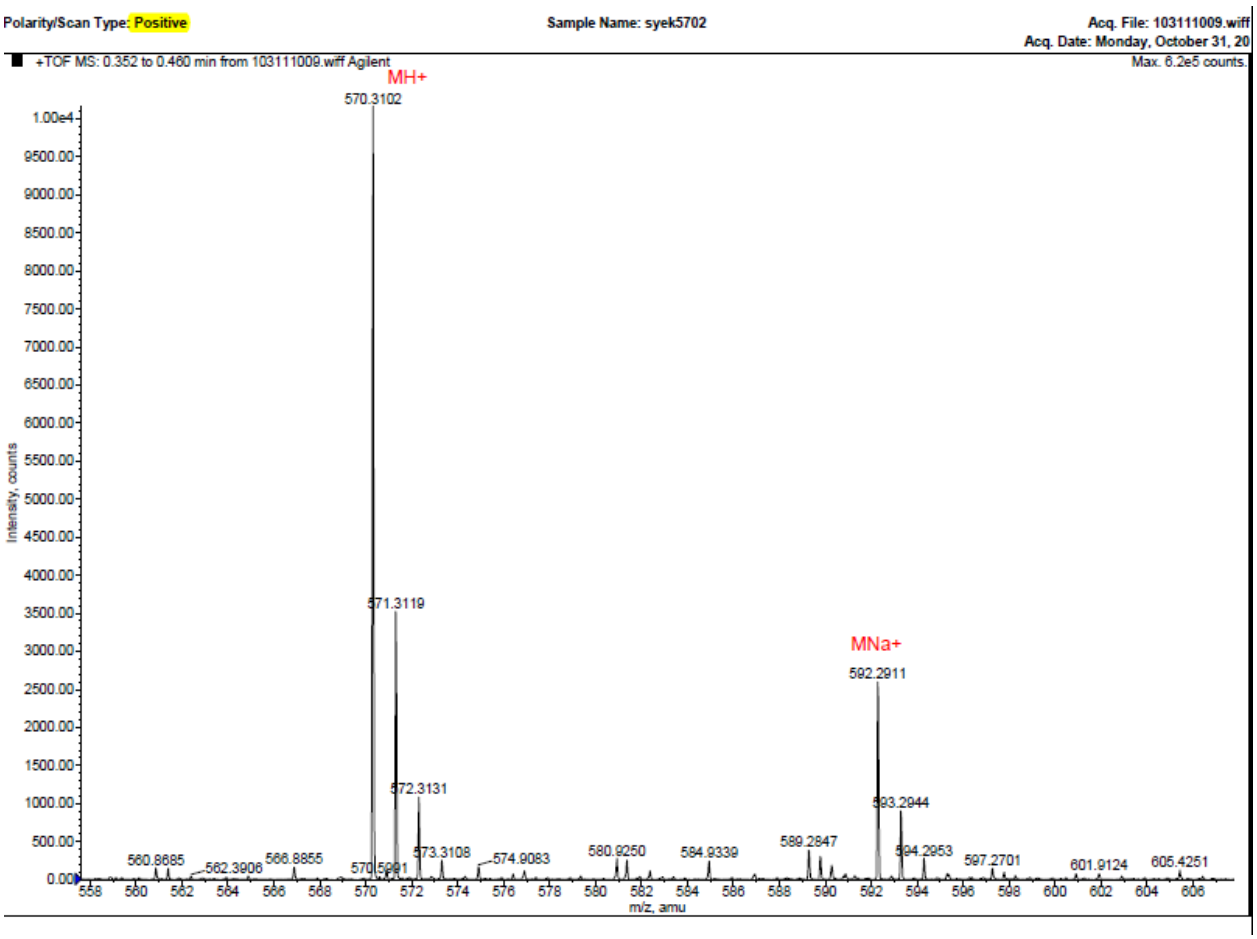
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	Amount	Units
1	****	****	****	****	****	****	****
2	****	****	****	****	****	****	****



Report Method: Injection Summary Report Printed 6:45:44 PM 6/30/2010 Page: 1 of 1

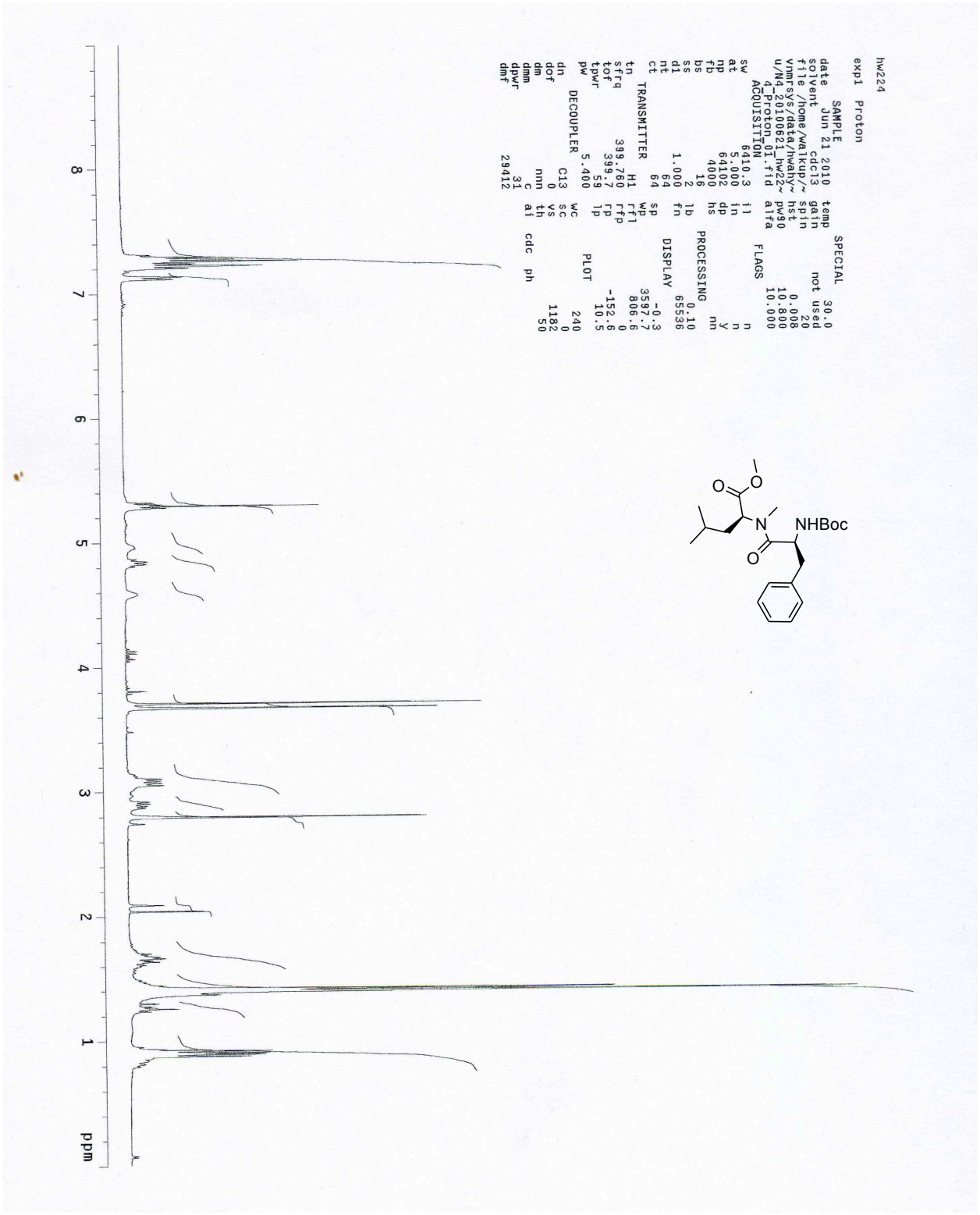
Compound 9: A-Th-III

HPLC Macrocycle Phe-Leu-Thiazole-Leu-Leu (9)



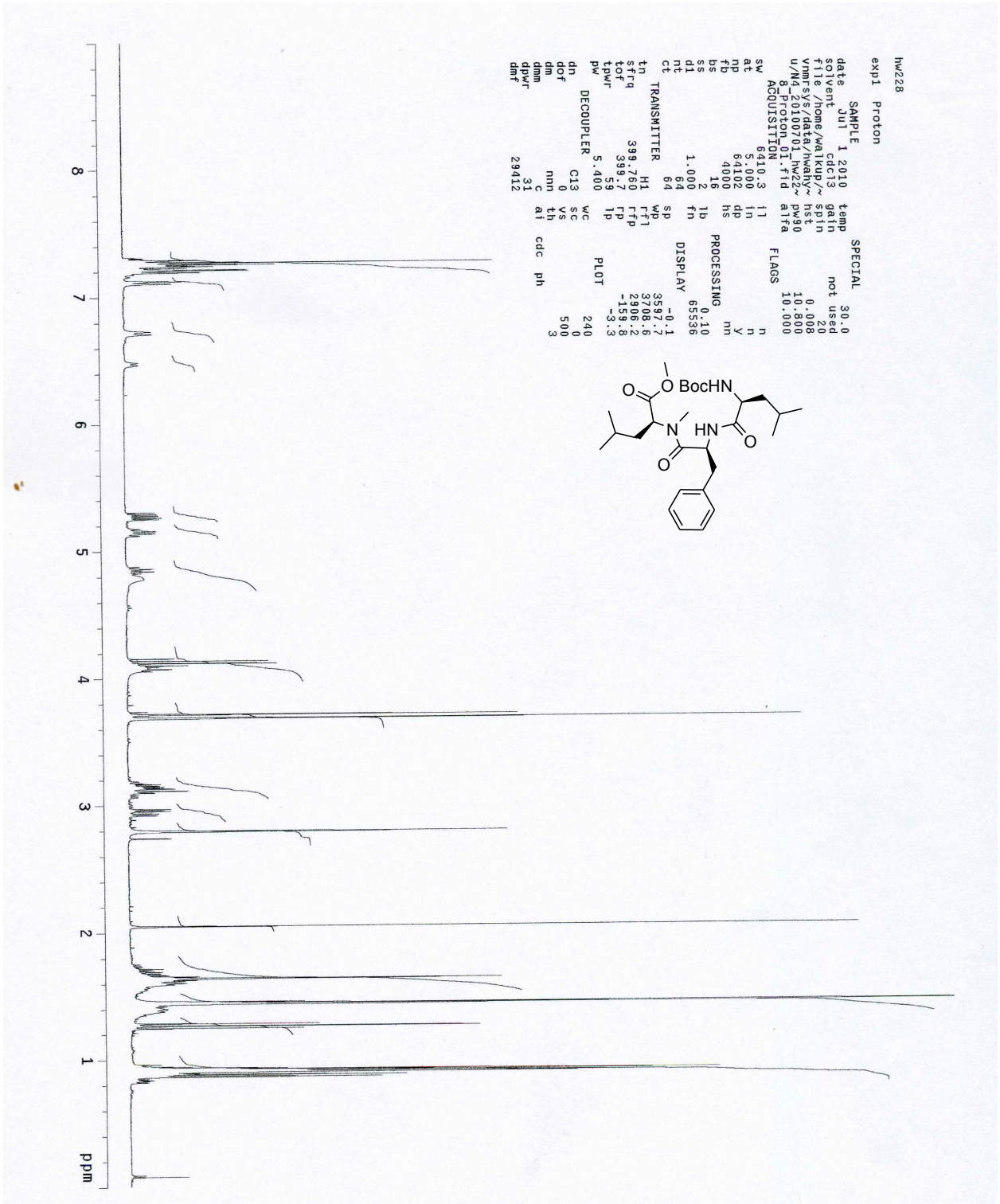
Compound 9: A-Th-III

HRMS Macrocycle Phe-Leu-Thiazole-Leu-Leu (9) (MW= 570.3102)



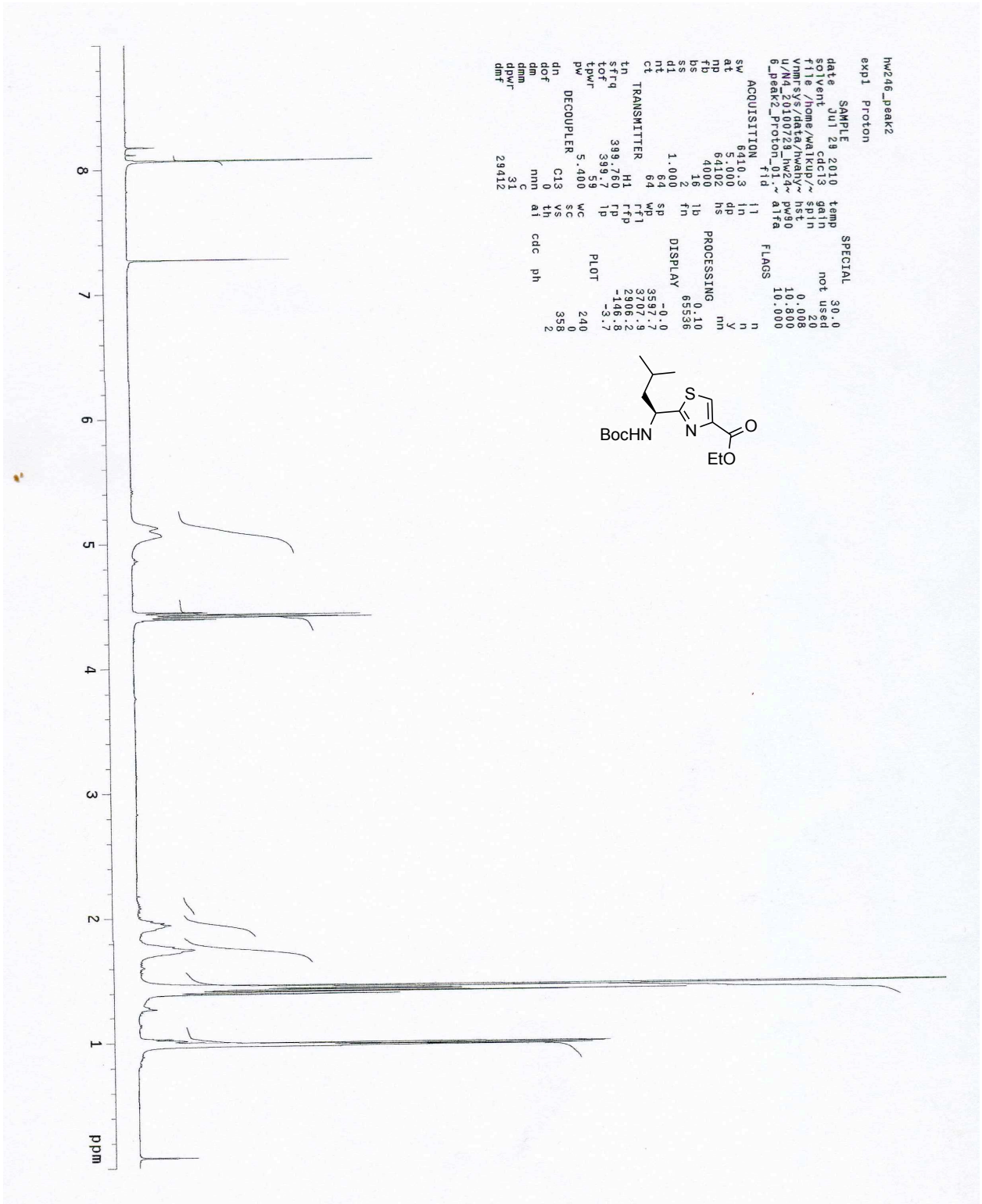
Compound 10: B-Th-III

NMR Dipeptide MeO-Leu-N(Me)-Phe-NHBoc



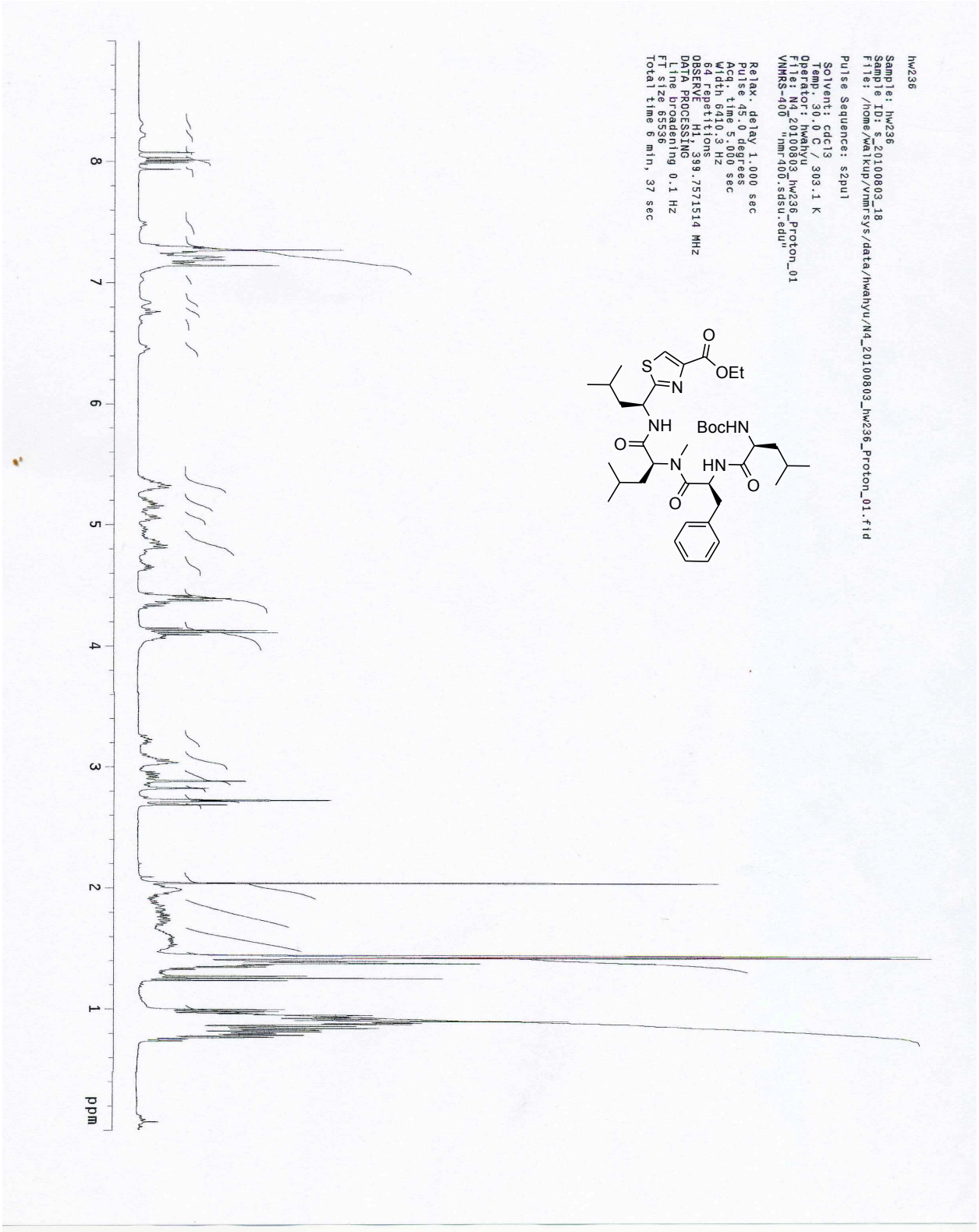
Compound 10: B-Th-III

NMR Tripeptide MeO-Leu-N(Me)-Phe-Leu-NHBoc



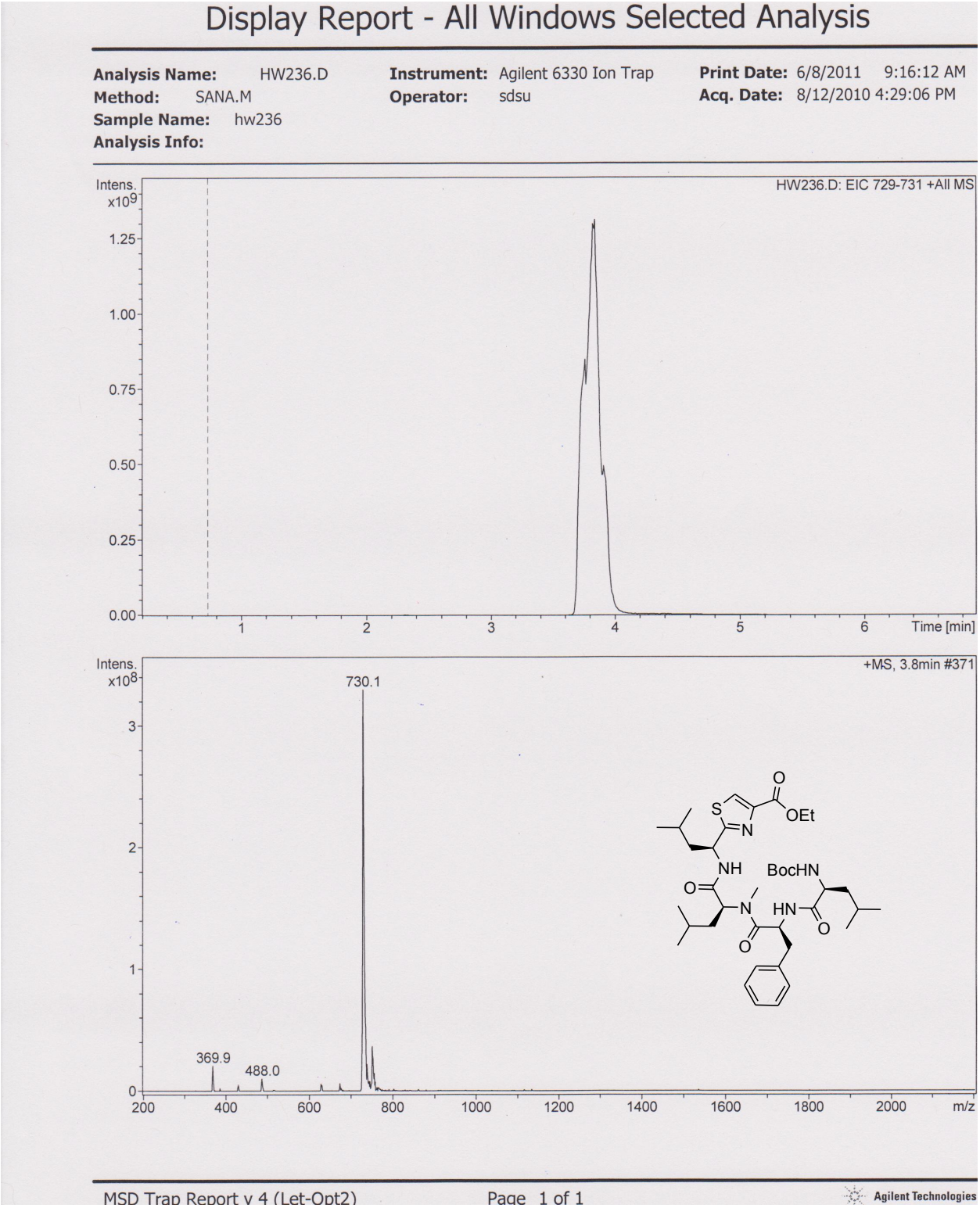
Compound 10: B-Th-III

NMR Dipeptide EtO-Thiazole-Leu-NHBoc (57)



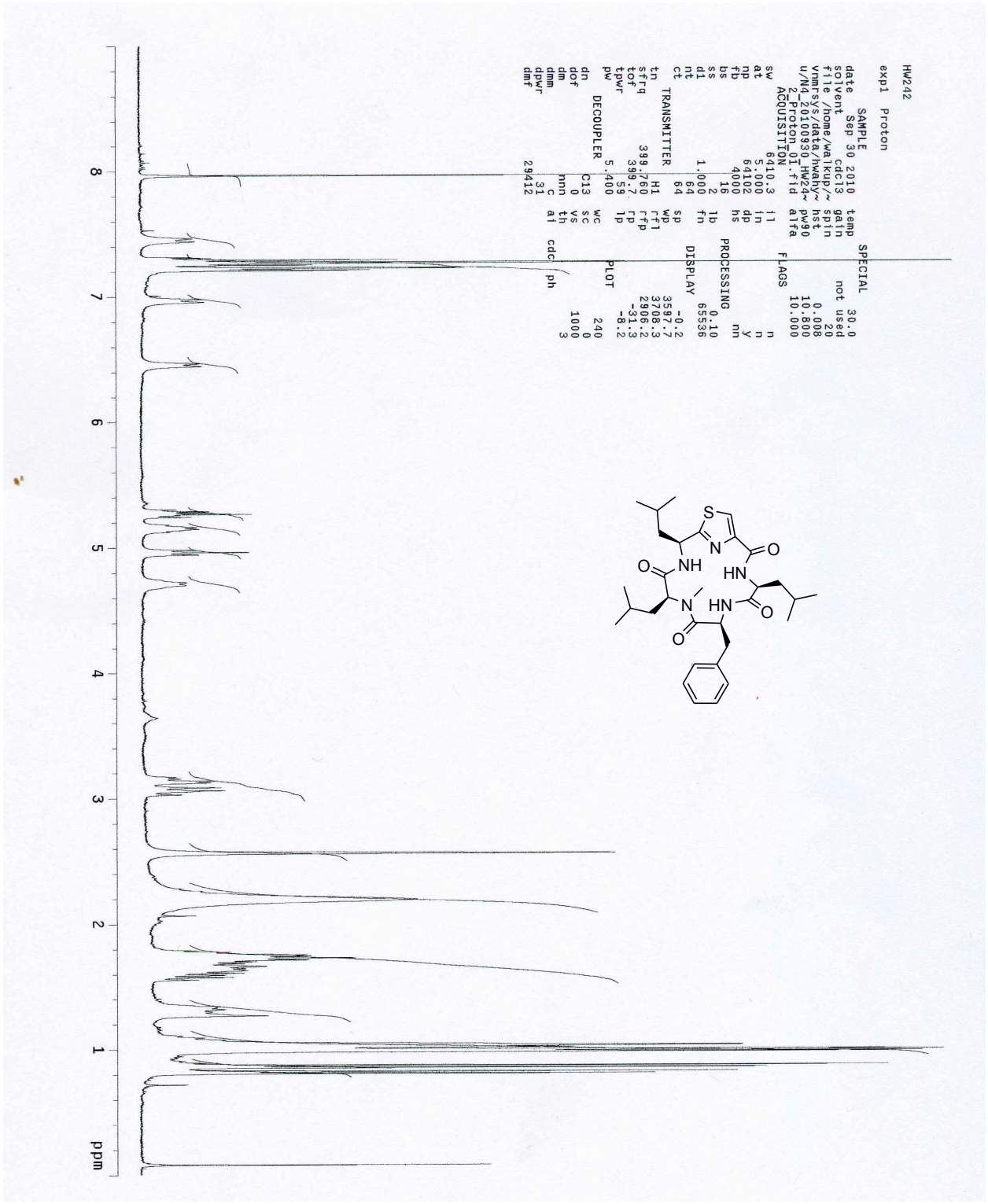
Compound 10: B-Th-III

NMR Pentapeptide EtO-Thiazole-Leu-Leu-N(Me)-Phe-Leu-NHBoc (63)



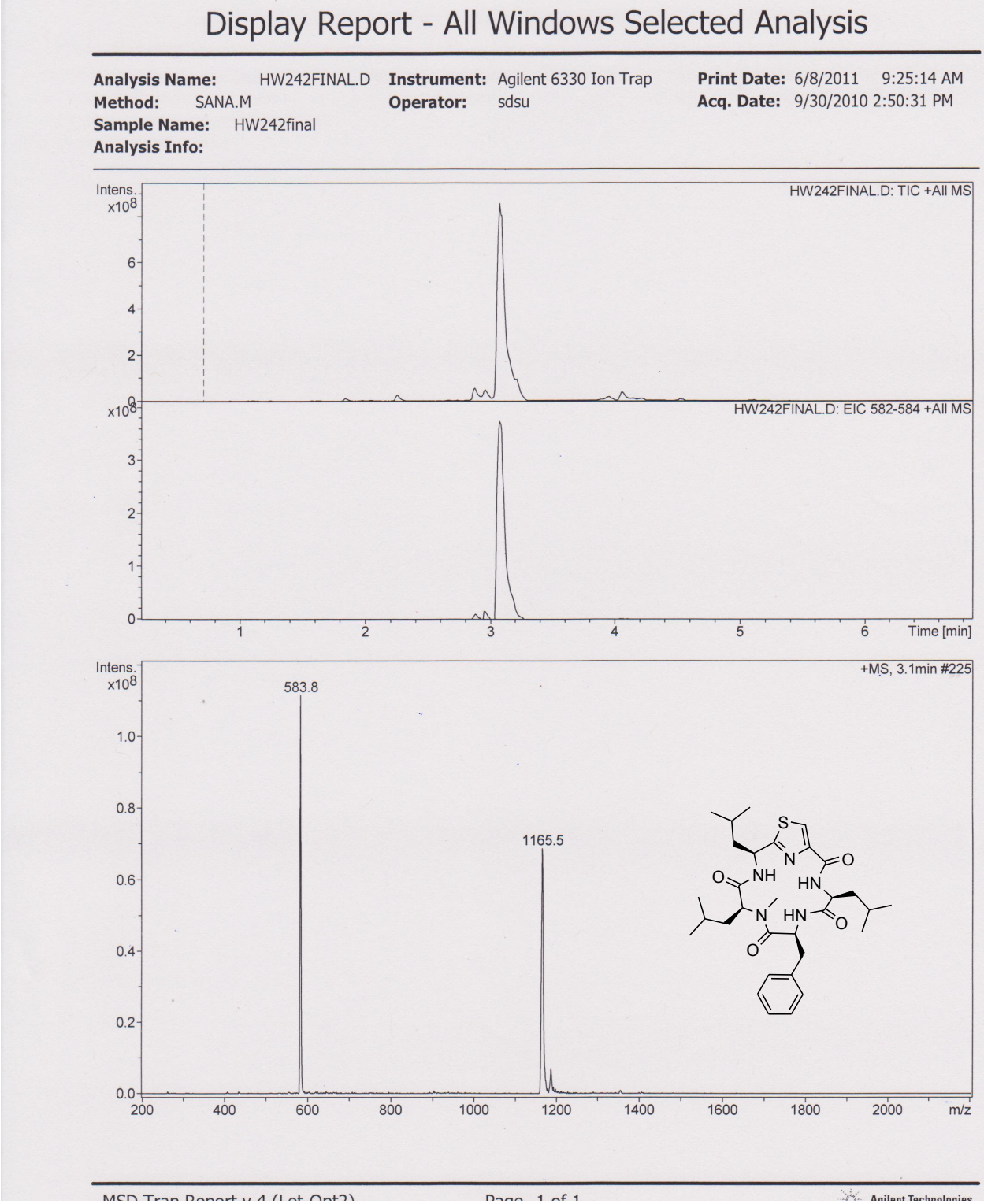
Compound 10: B-Th-III

LCMS Pentapeptide EtO-Thiazole-Leu-Leu-N(Me)-Phe-Leu-NHBoc (63) (MW = 729)



Compound 10: B-Th-III

NMR Macrocycle Phe-Leu-Thiazole-Leu-Leu-N(Me) (10)



Compound 10: B-Th-III

LCMS Macrocycle Phe-Leu-Thiazole-Leu-Leu-N(Me) (10) (MW = 583)

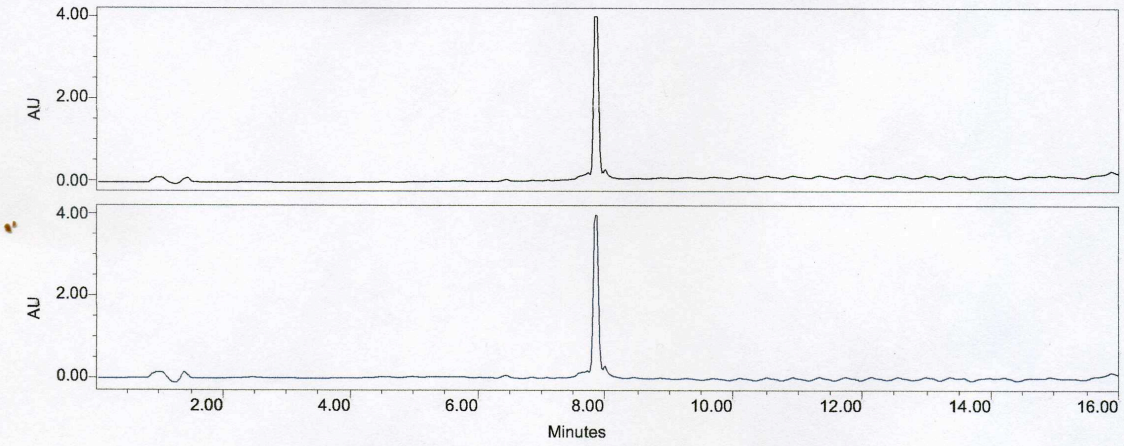
SDSU

Project Name: Defaults
Reported by User: System

Breeze

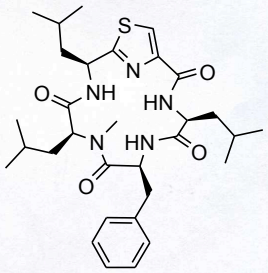
SAMPLE INFORMATION

Sample Name:	hw242	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss
Injection #:	749	Date Acquired:	9/29/2010 11:33:03 AM
Run Time:	16.00 Minutes	Injection Volume:	100.00 ul



Channel: 2487Channel 1 Channel Desc.: Processing Method: *
Channel: 2487Channel 2 Channel Desc.: Processing Method: *

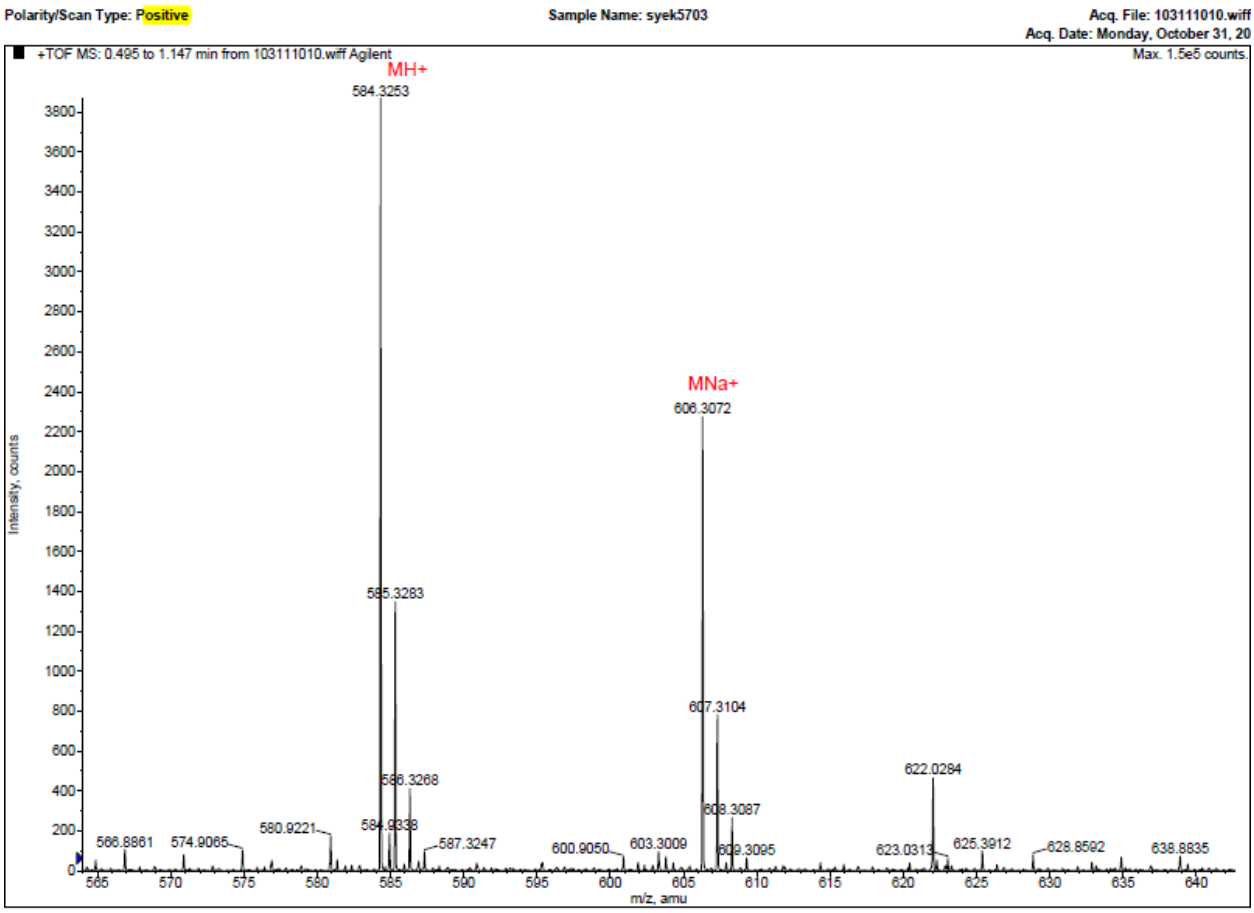
	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	Amount	Units
1	****	****	****	****	****	****	****
2	****	****	****	****	****	****	****



Report Method: Injection Summary Report Printed 11:49:17 AM 9/29/2010 Page: 1 of 1

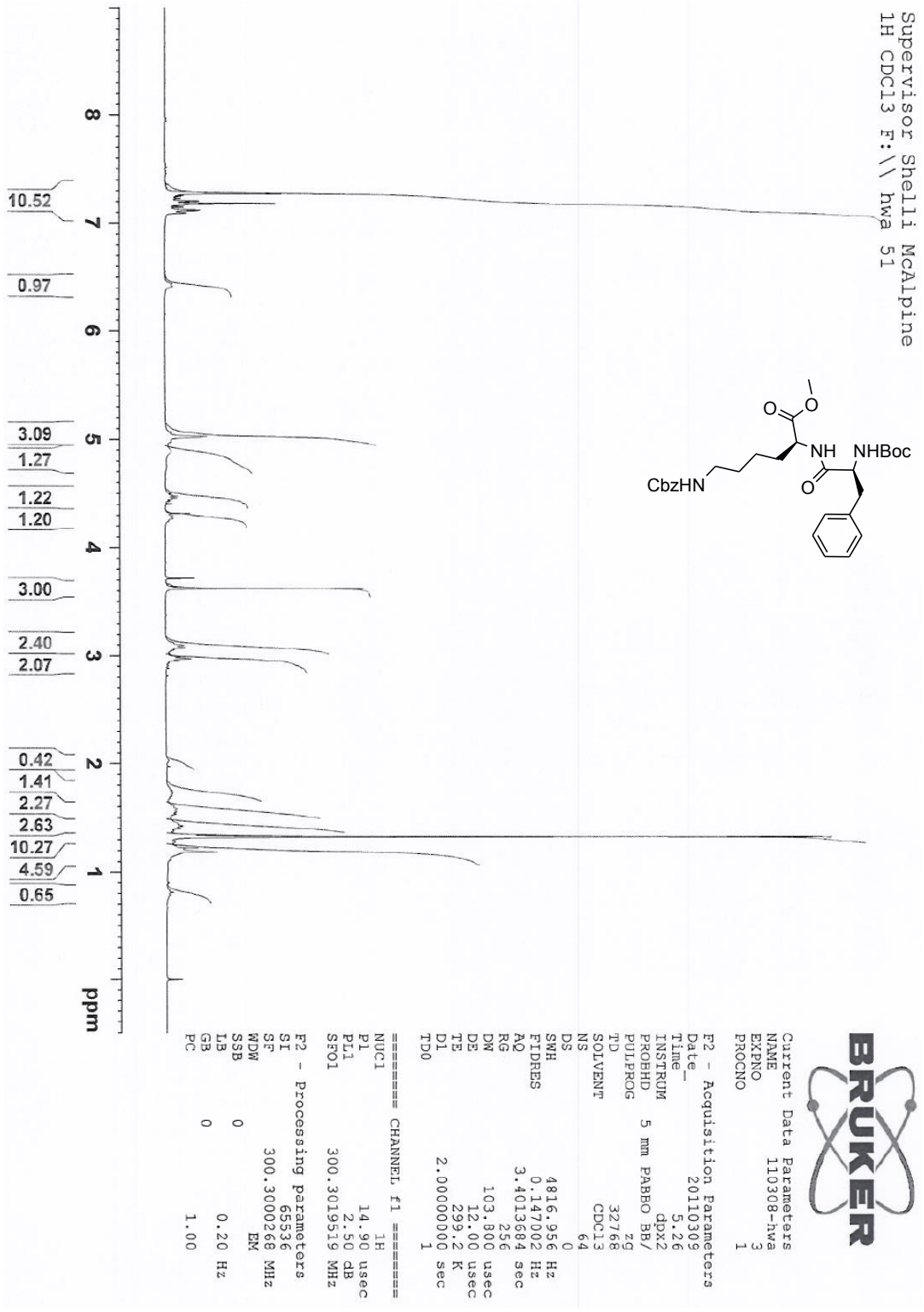
Compound 10: B-Th-III

HPLC Macrocycle Phe-Leu-Thiazole-Leu-Leu-N(Me) (10)



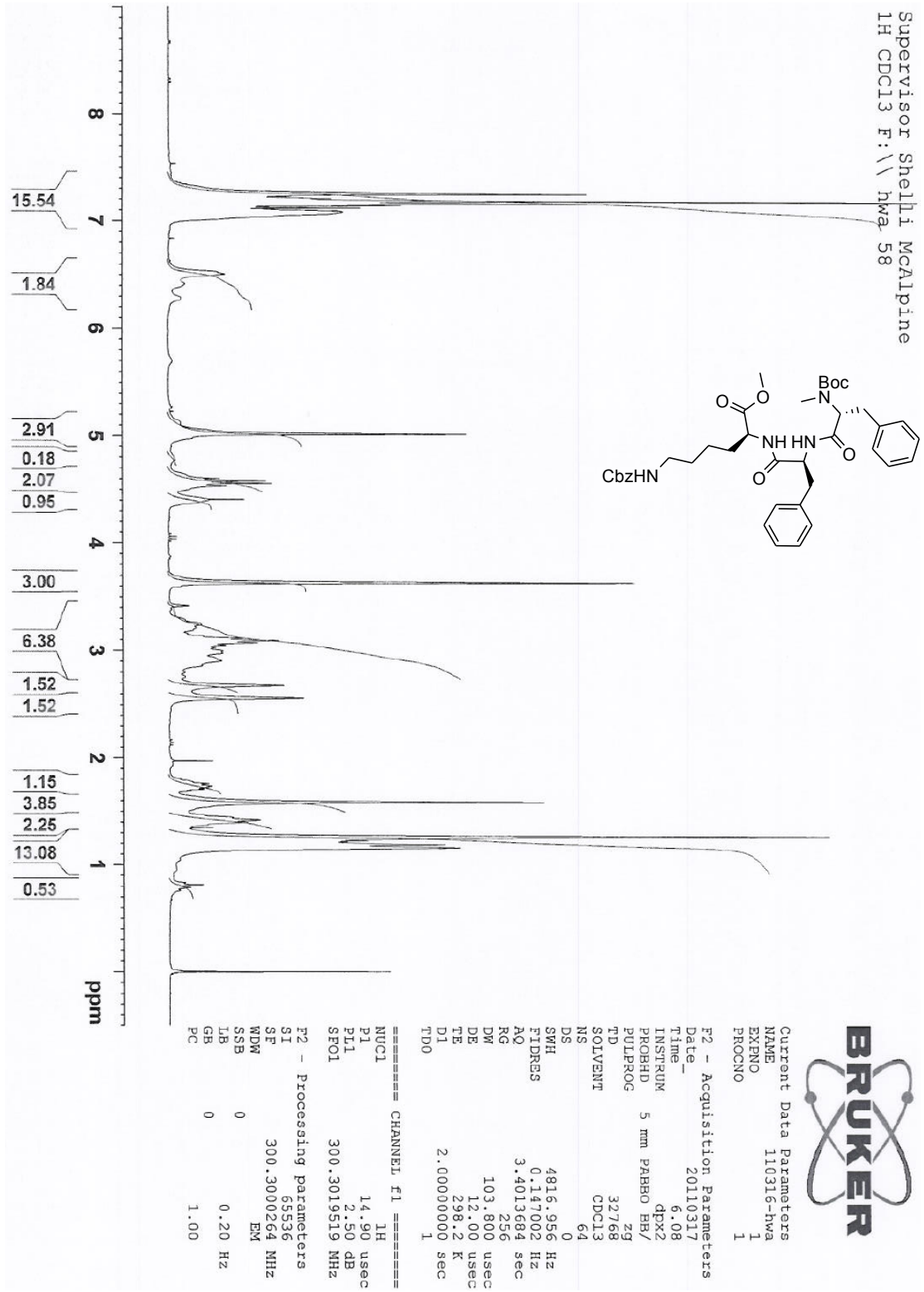
Compound 10: B-Th-III

HRMS Macrocycle Phe-Leu-Thiazole-Leu-Leu-N(Me) (10) (MW = 584.3253)



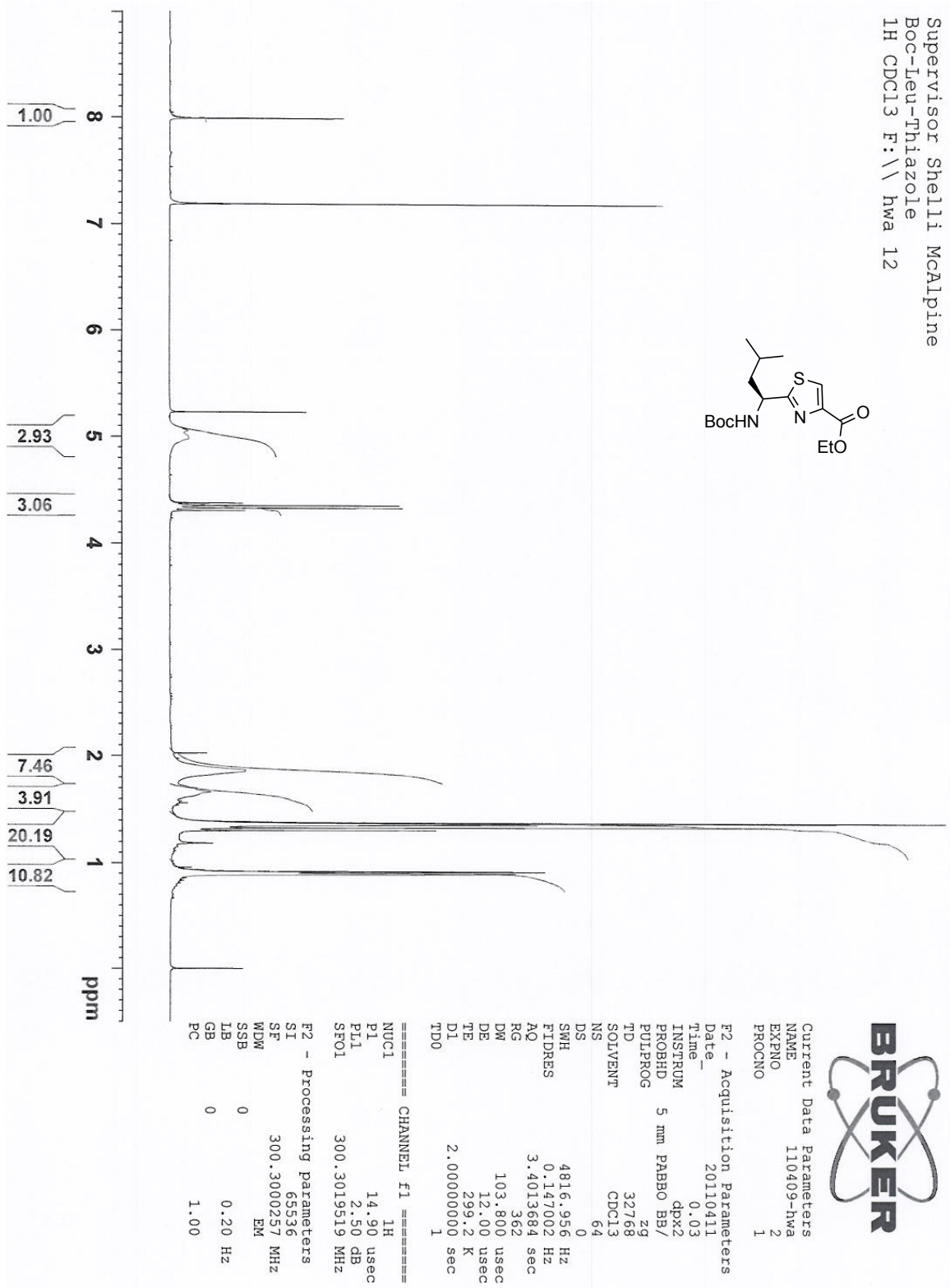
Compound 11: C-Th-III

NMR Dipeptide MeO-Lys(Cbz)-Phe-NHBoc



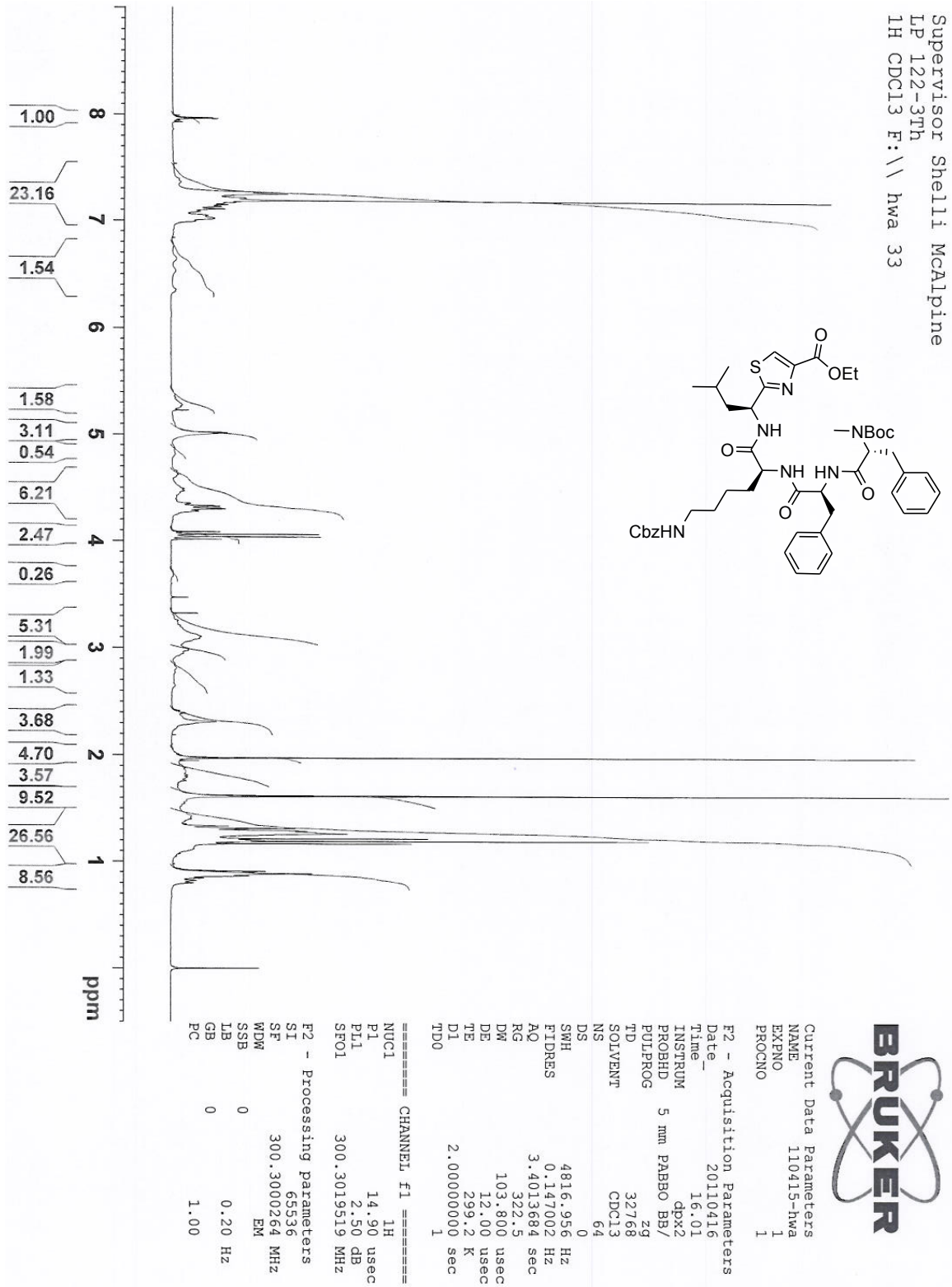
Compound 11: C-Th-III

NMR Tripeptide MeO-Lys(Cbz)-Phe-D-Phe-N(Me)Boc



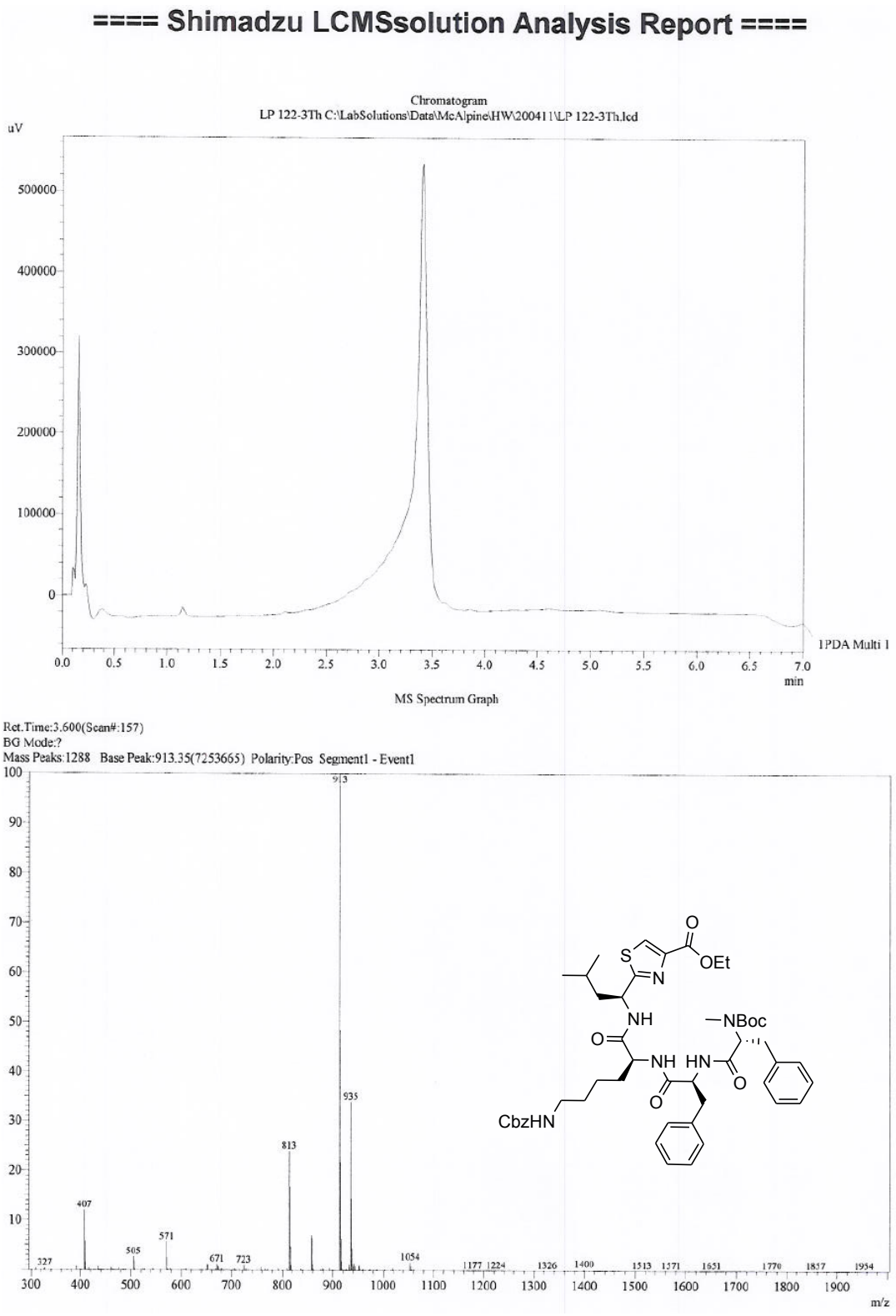
Compound 11: C-Th-III

NMR Dipeptide EtO-Thiazole-Leu-NHBoc



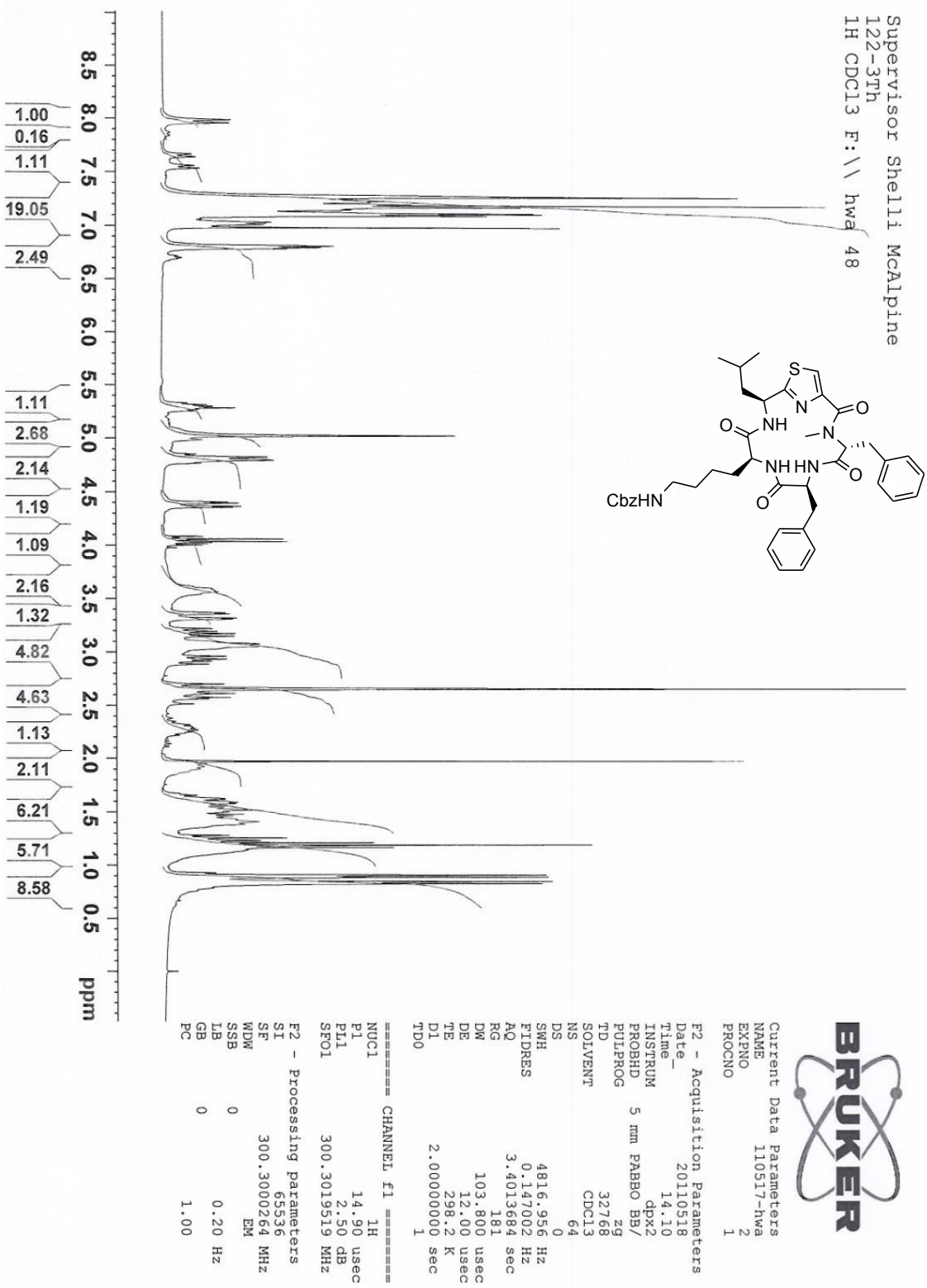
Compound 11: C-Th-III

NMR Pentapeptide EtO-Thiazole-Leu-Lys(Cbz)-Phe-D-Phe-N(Me)Boc



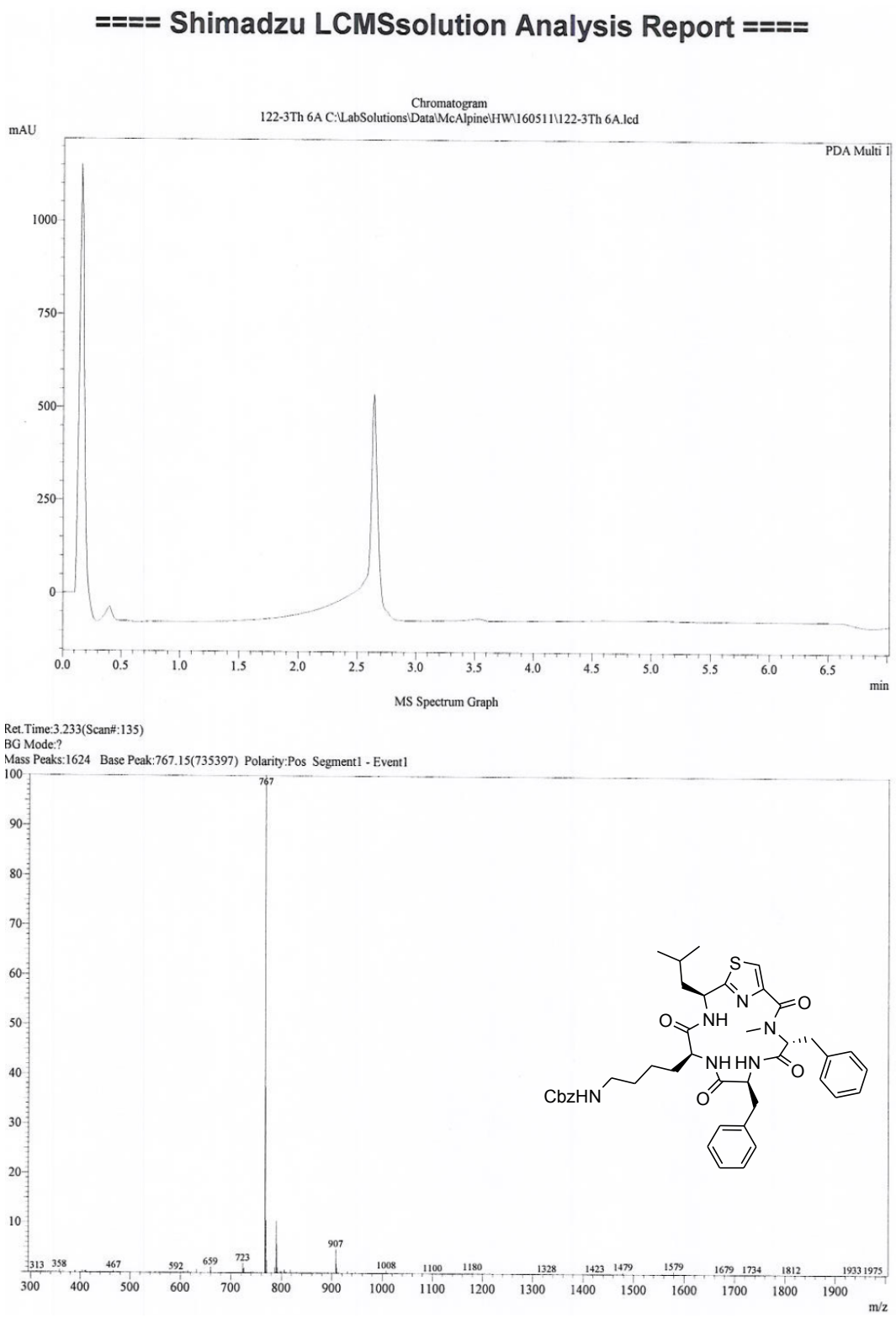
Compound 11: C-Th-III

HPLC+LCMS Pentapeptide EtO-Thiazole-Leu-Lys(Cbz)-Phe-D-Phe-N(Me)Boc (MW = 912)



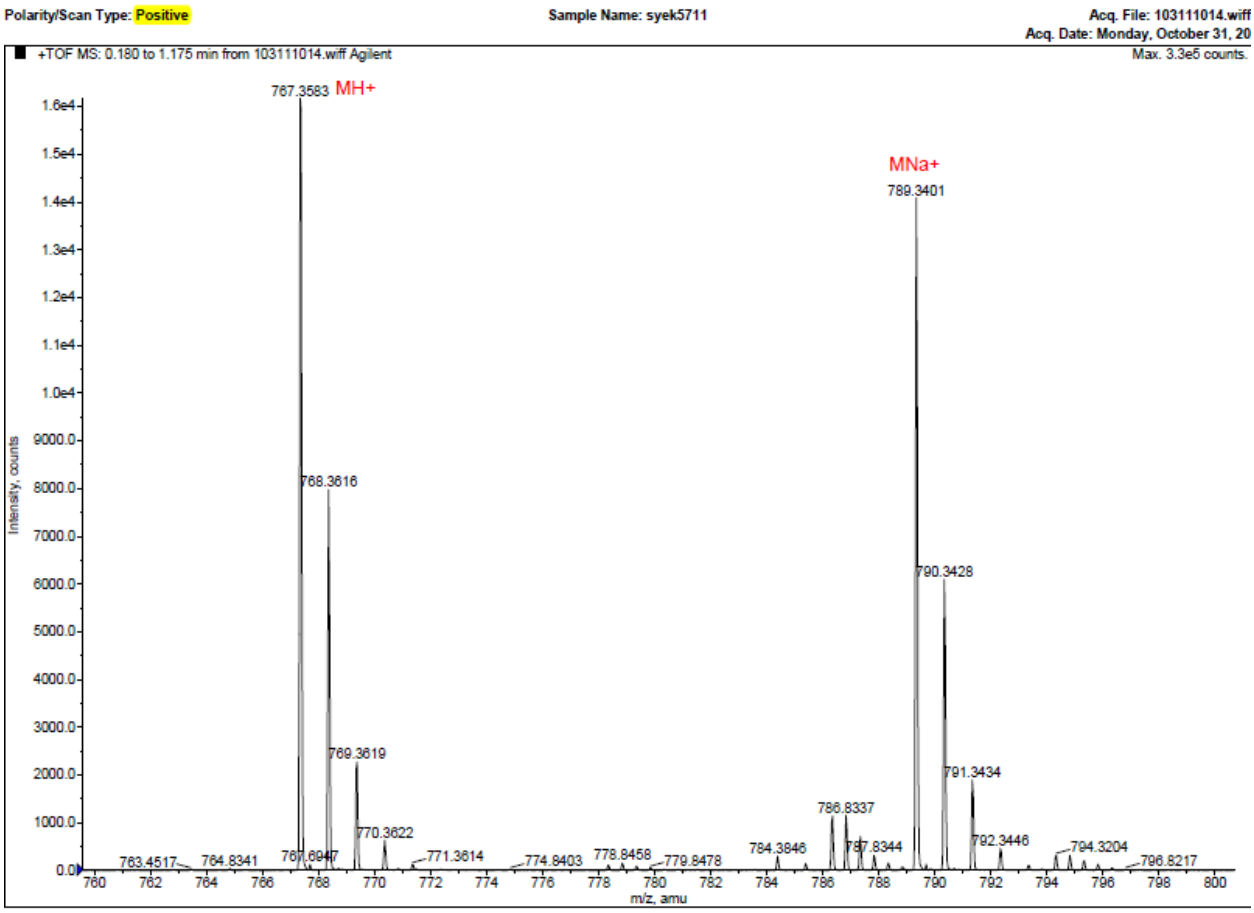
Compound 11: C-Th-III

NMR Macrocycle Phe-D-Phe-N(Me)-Thiazole-Leu-Lys(Cbz) (11)



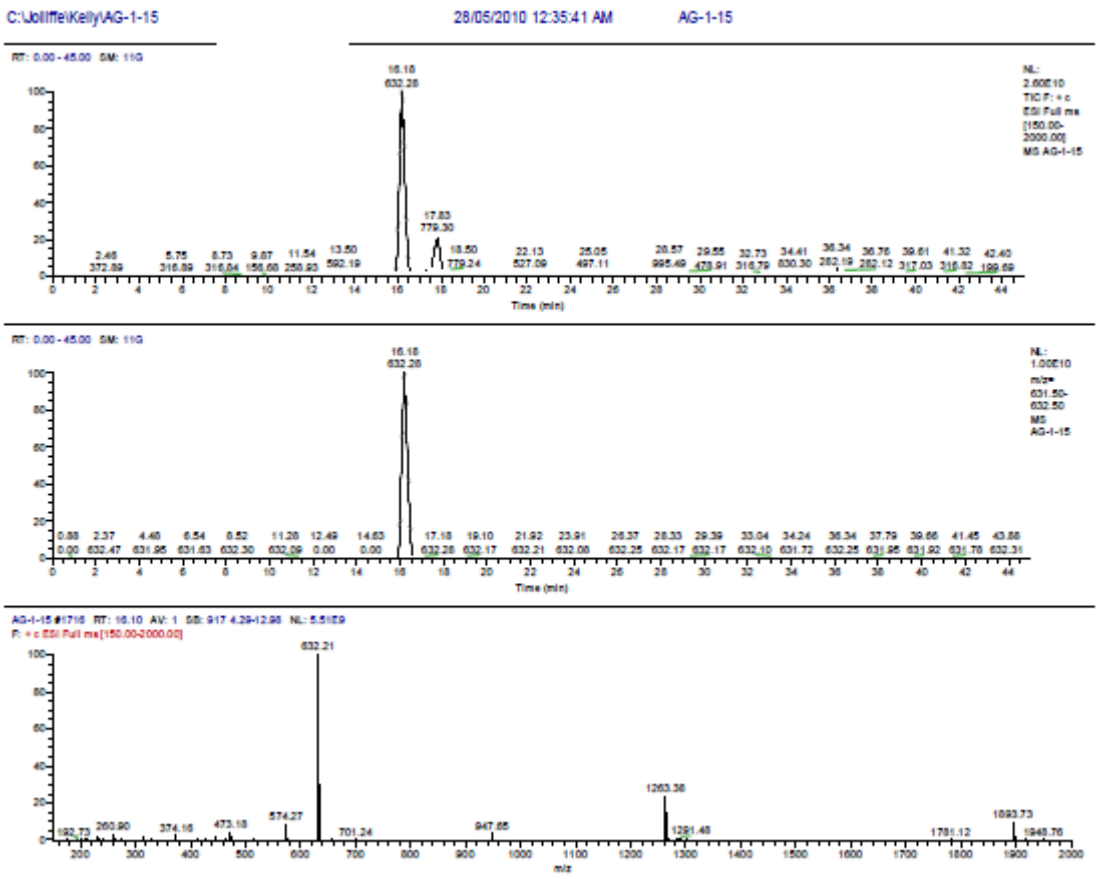
Compound 11: C-Th-III

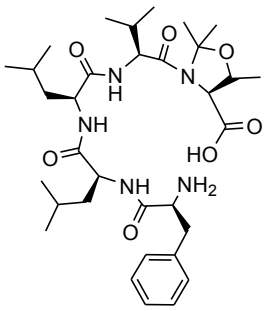
HPLC+LCMS Macrocycle Phe-D-Phe-N(Me)- Thiazole-Leu-Lys(Cbz) (11) (MW = 766)



Compound 11: C-Th-III

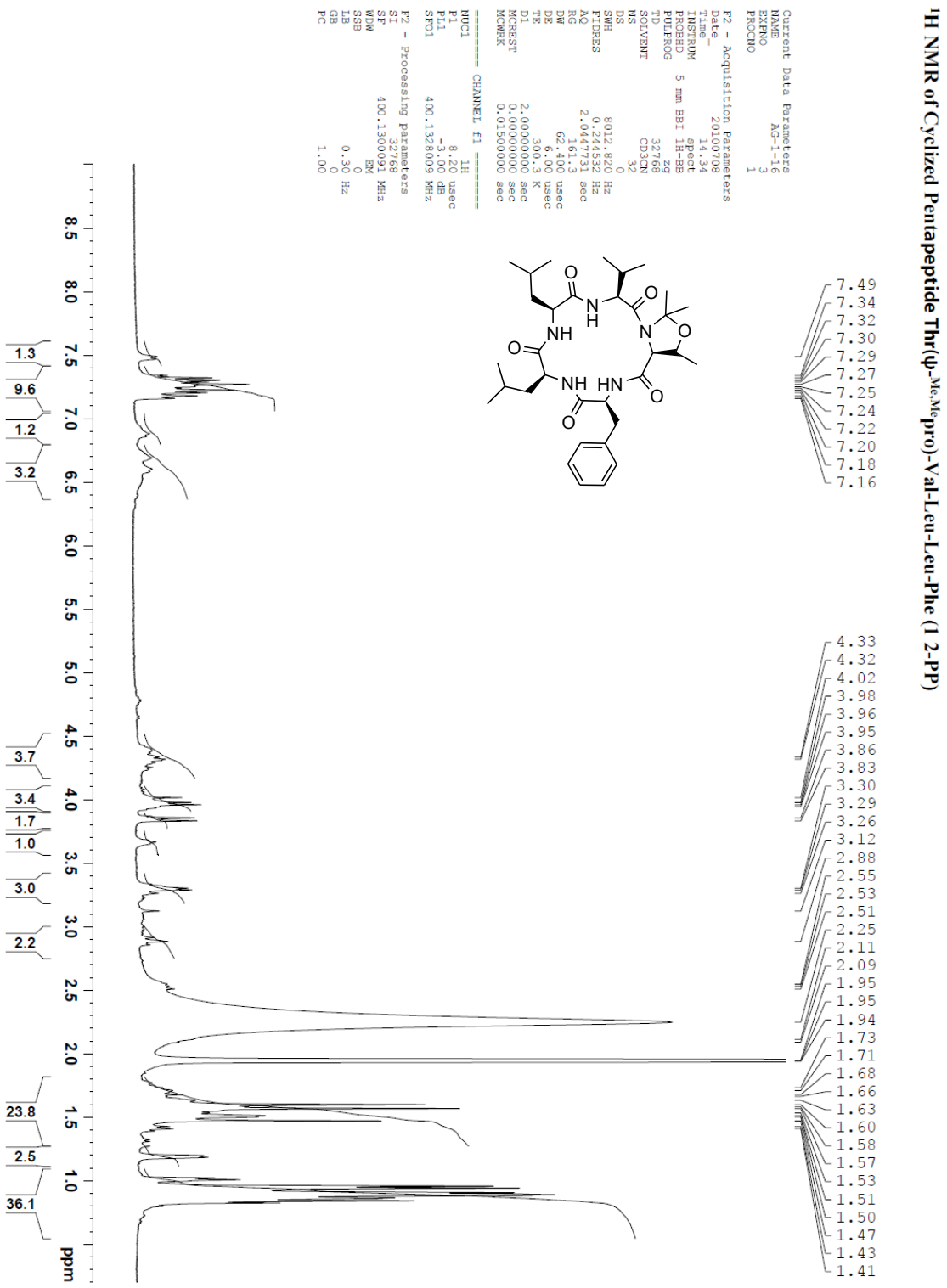
HRMS Macrocycle Phe-D-Phe-N(Me)- Thiazole-Leu-Lys(Cbz) (11) (MW = 767.3583)





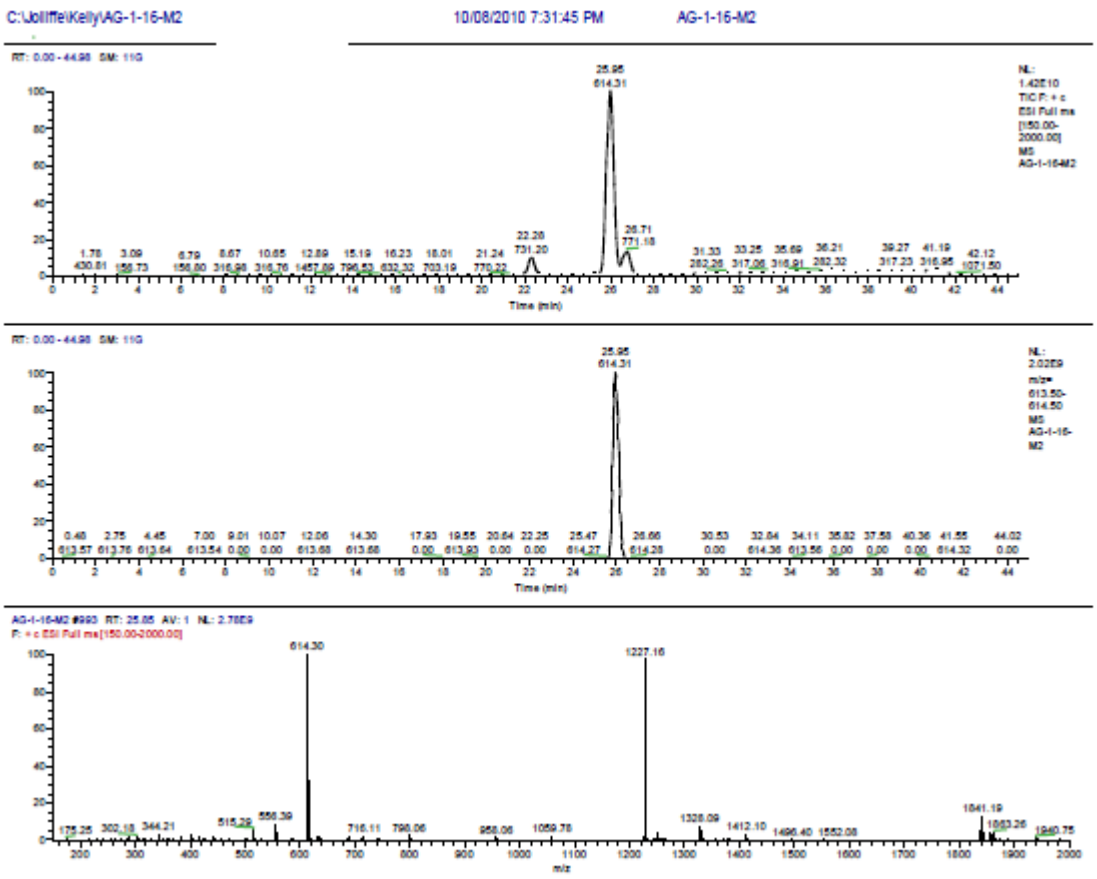
Compound 12: A-PP-II

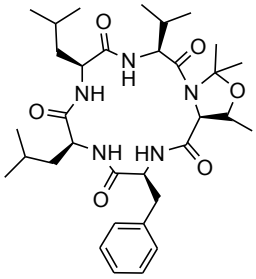
LCMS Deprotected Pentapeptide HO-Thr(ΨMe,Me-Pro)-Val-Leu-Leu-Phe-NH_2 (MW = 631)



Compound 12: A-PP-II

NMR Macrocycle Phe-Thr(ΨMe,Me-Pro)-Val-Leu-Leu (12)





Compound 12: A-PP-II

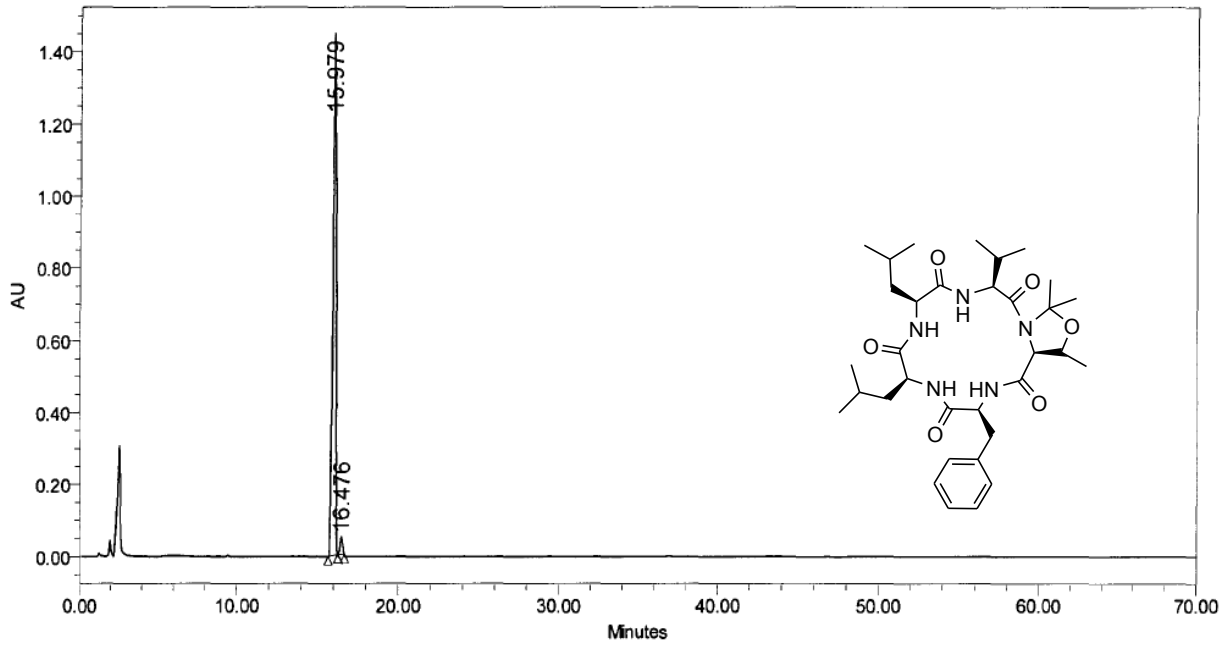
LCMS Macrocycle Phe-Thr(ΨMe,Me-Pro)-Val-Leu-Leu (MW = 613)

Empower

The University of Sydney, School of Chemistry

Single Channel Report

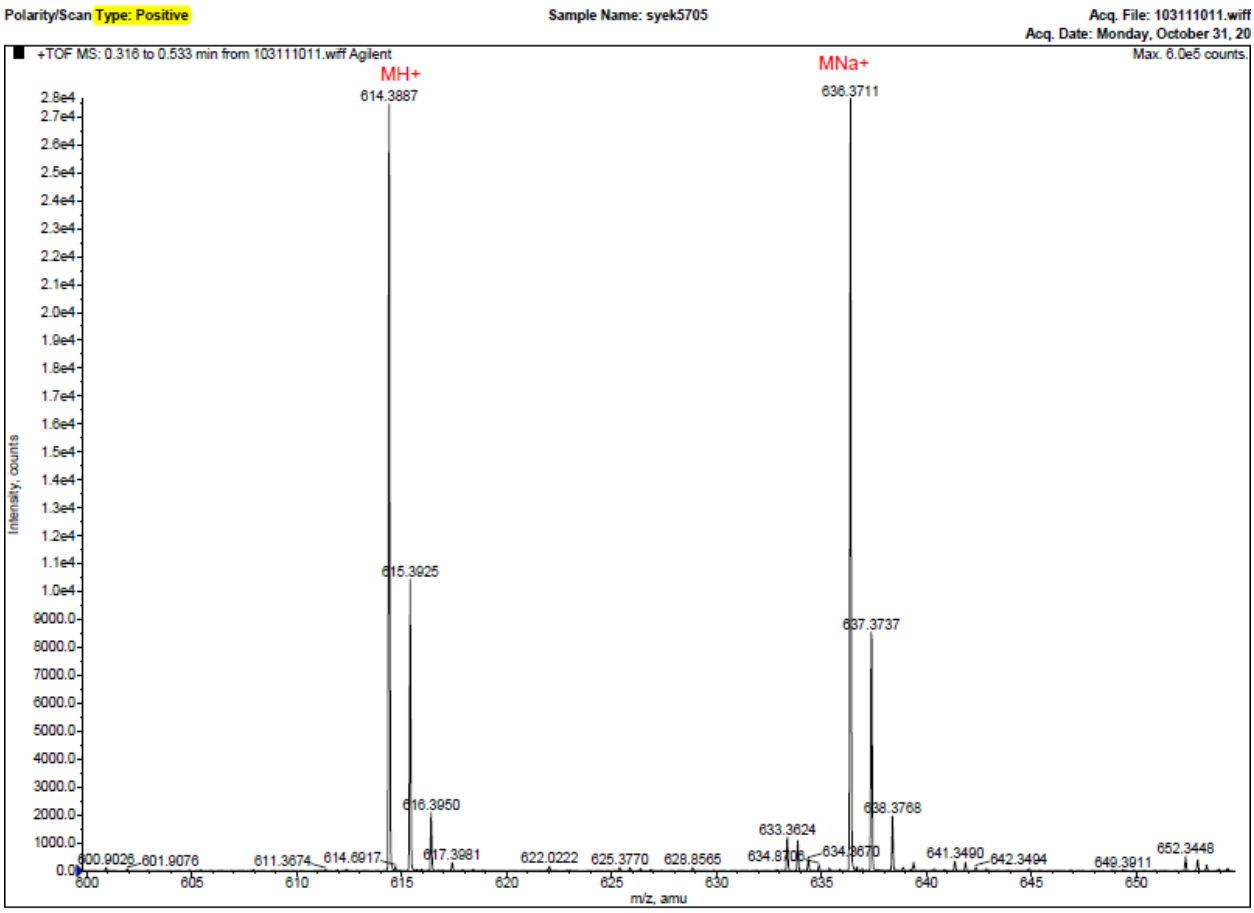
SAMPLE INFORMATION			
Project Name:	Payne	Acq. Method Set:	G_40to100ov30_B_D2ml
Sample Name:	AG-1-16M-2	Sample Set Name:	RJP_AFGPanalyt
Sample Type:	Unknown	Date Acquired:	9/08/2010 9:42:11 PM EST
Vial:	8	Proc. Method:	NoPeaks
Injection #:	1	Date Processed:	13/08/2010 1:49:27 PM EST
Injection Volume:	10.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	70.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0 nm)
Chromatogram_Info:	0t100%Bover40, A:H2O/TFA 100:0.1, B:ACN/TFA 100:0.1; SunFire C18-106 01;0.2 mL/min		



	RT	Area	% Area	Height
1	15.979	20121855	97.31	1447222
2	16.476	557241	2.69	48631

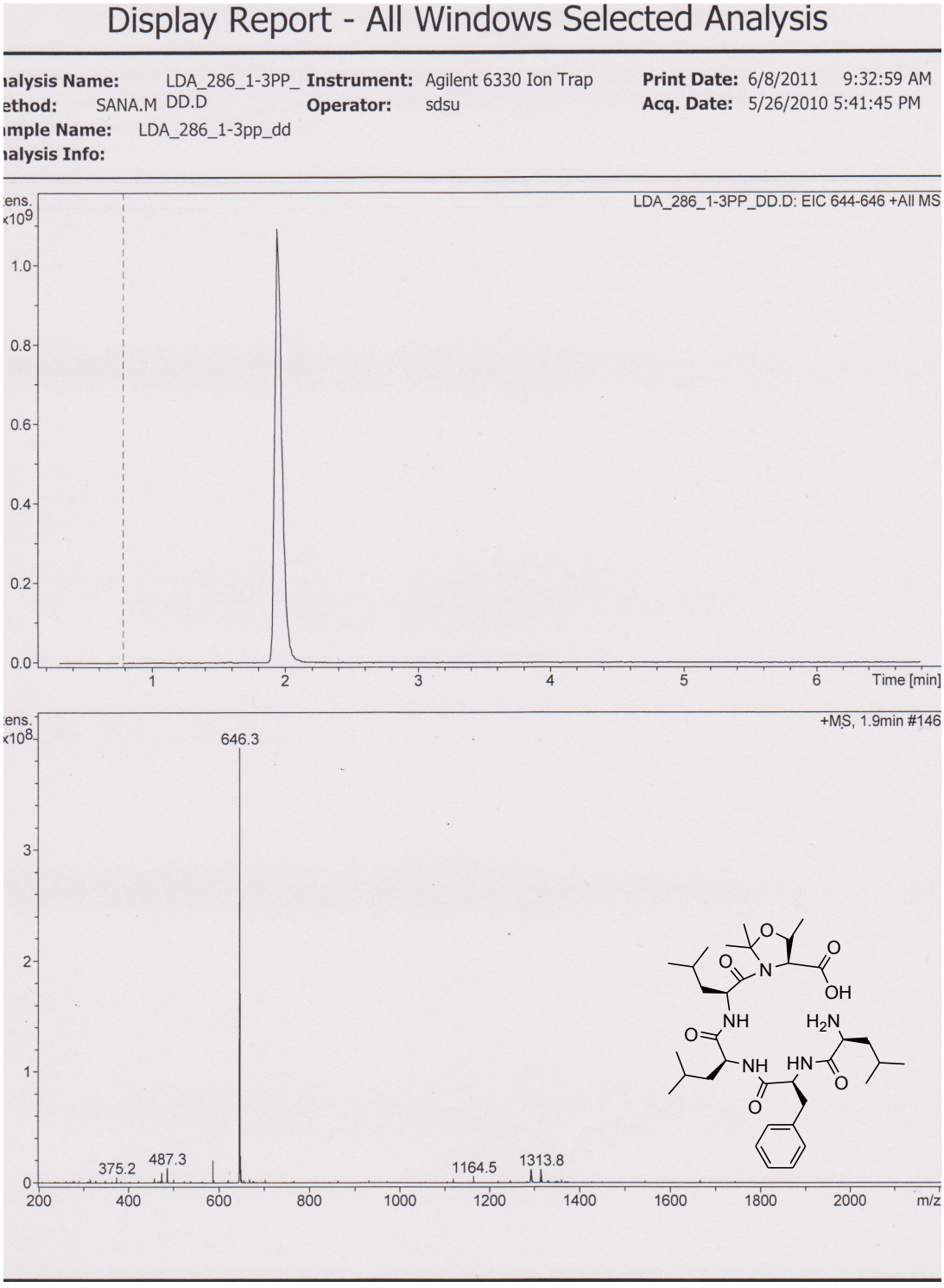
Compound 12: A-PP-II

HPLC Macrocycle Phe-Thr(ΨMe,Me-Pro)-Val-Leu-Leu (12)



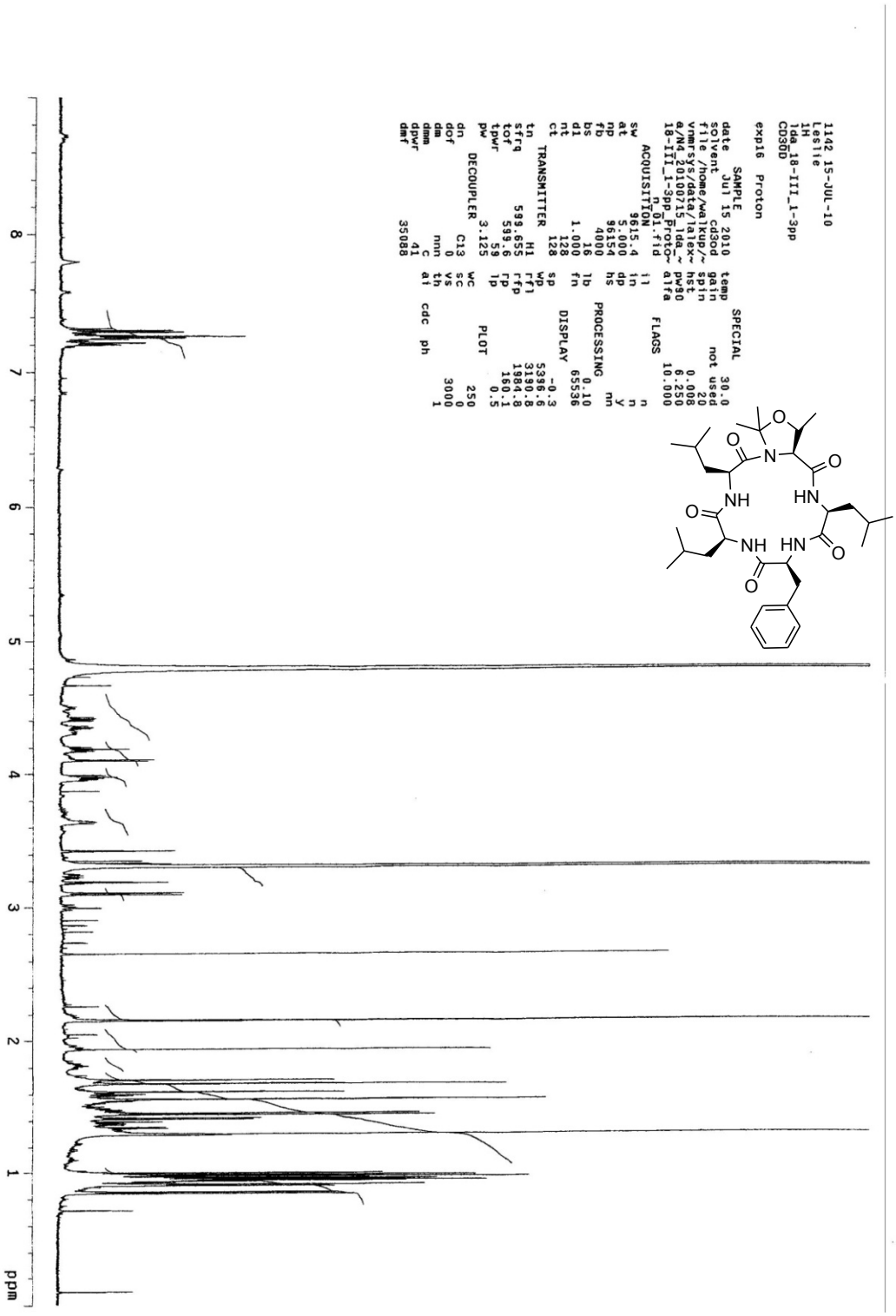
Compound 12: A-PP-II

HRMS Macrocycle Phe-Thr(ΨMe,Me-Pro)-Val-Leu-Leu (MW = 614.3887)



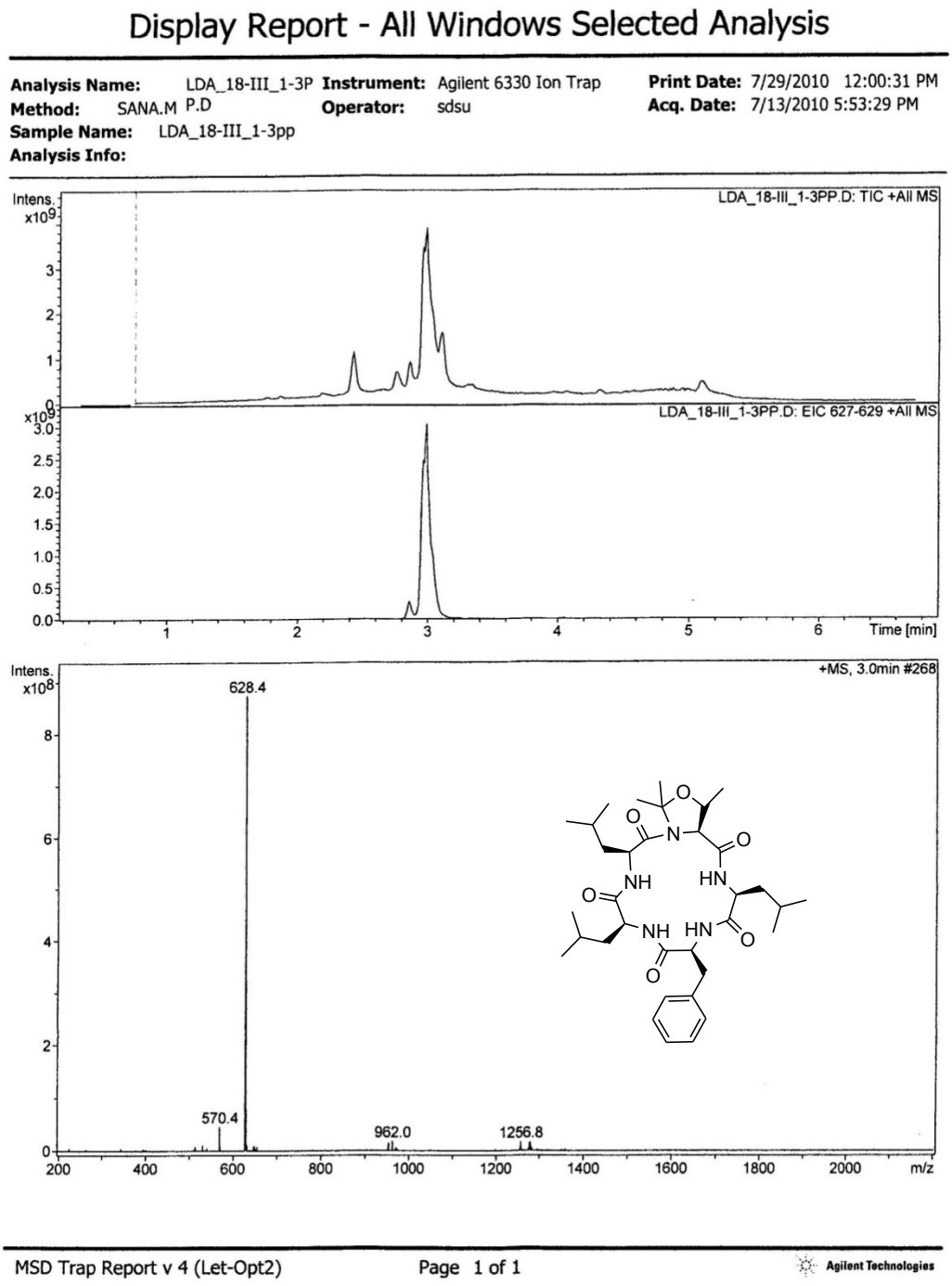
Compound 13: A-PP-III

LCMS Deprotected Pentapeptide HO-Thr(ΨMe,Me-Pro)-Leu-Leu-Phe-Leu-NH_2 (MW= 646)



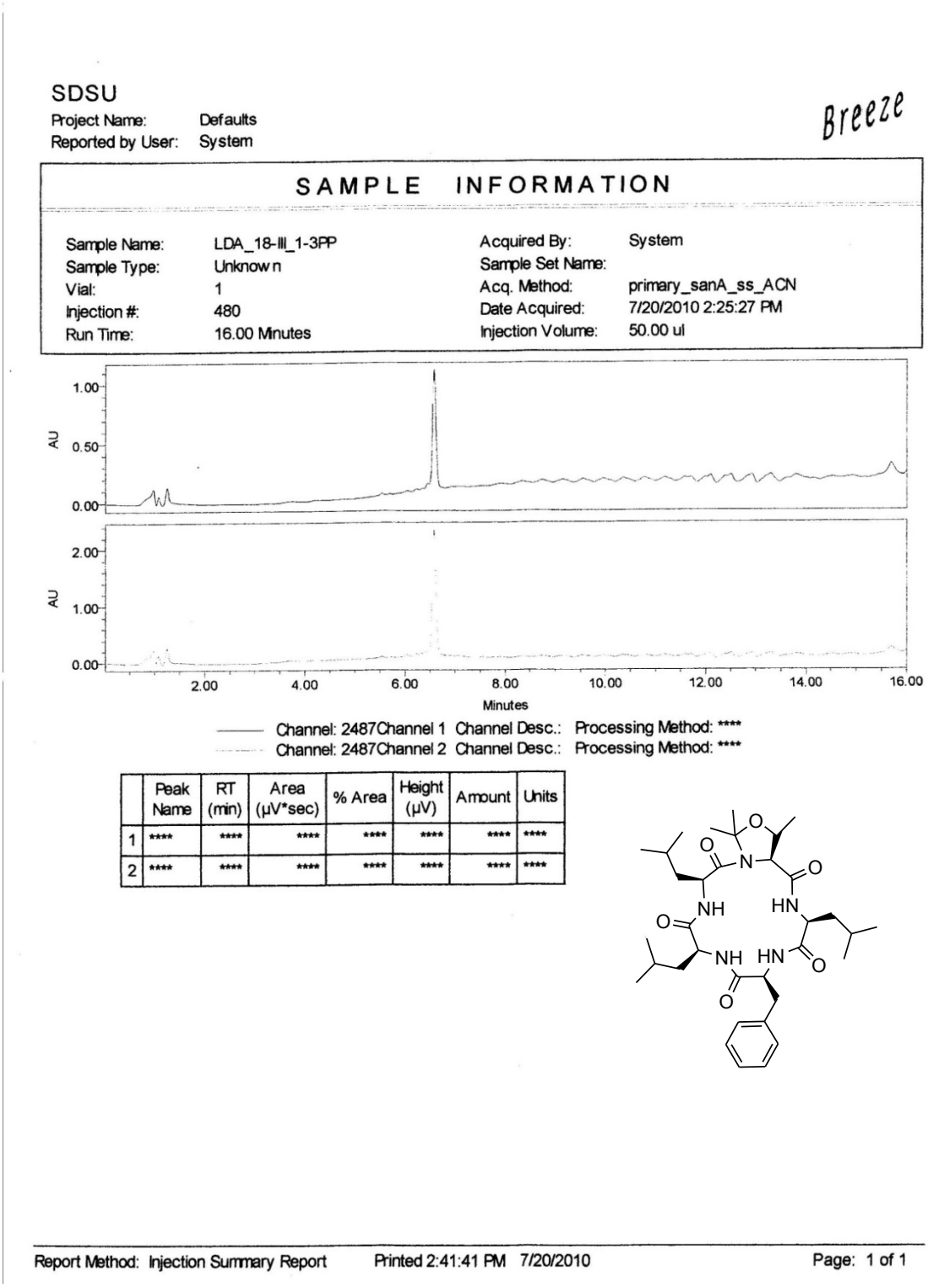
Compound 13: A-PP-III

NMR Macrocycle Phe-Leu-Thr(ΨMe,Me-Pro)-Leu-Leu (13)



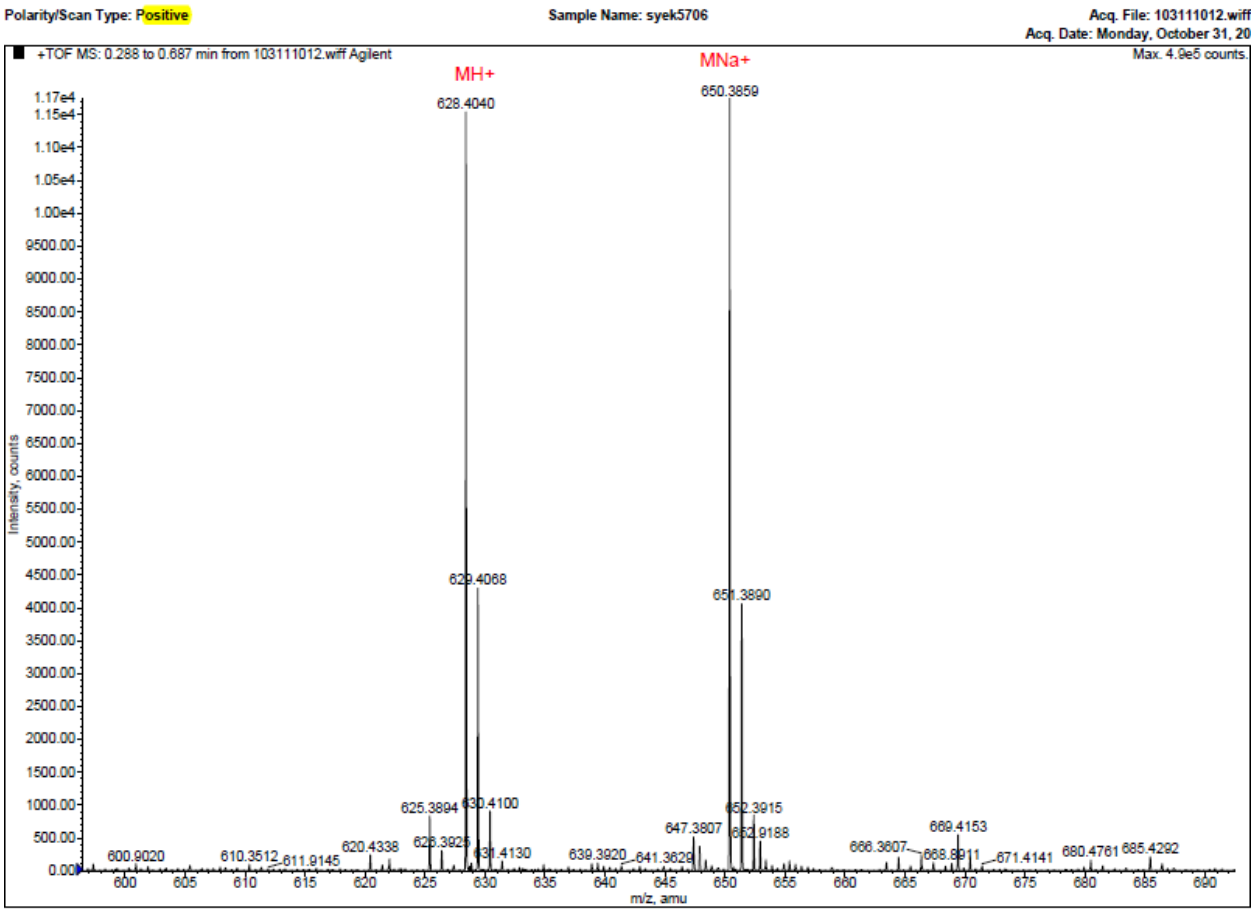
Compound 13: A-PP-III

LCMS Macrocycle Phe-Leu-Thr(ΨMe,Me-Pro)-Leu-Leu (13) (MW= 628)



Compound 13: A-PP-III

HPLC Macrocycle Phe-Leu-Thr(ΨMe,Me-Pro)-Leu-Leu (13)



Compound 13: A-PP-III

HRMS Macrocycle Phe-Leu-Thr(ΨMe,Me-Pro)-Leu-Leu (13) (MW= 628.4040)