

A third generation of Sansalvamide A derivatives: Design and synthesis of Hsp90 Inhibitors

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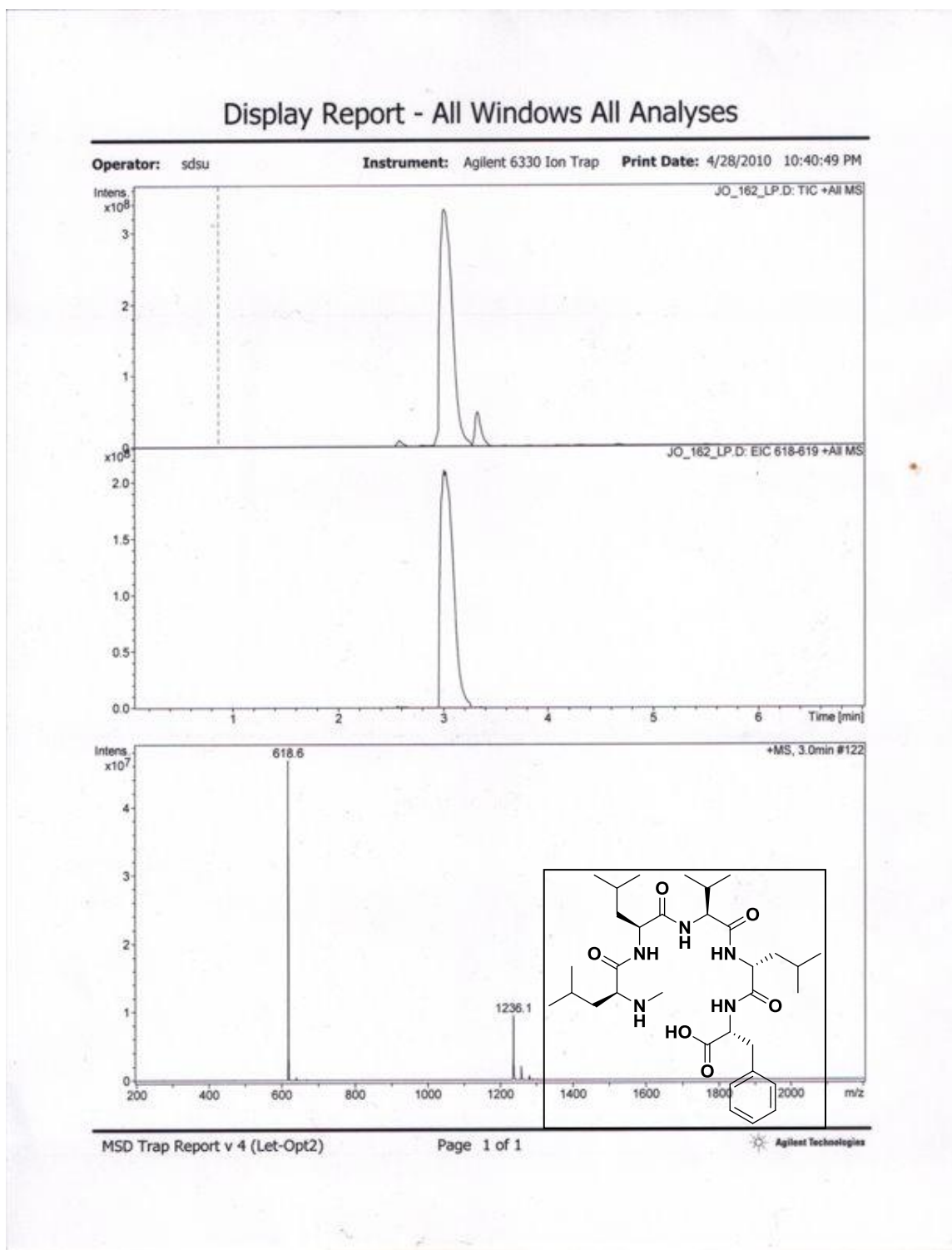
Compound 3 LCMS Double Deprotected Linear Pentapeptide HO-D-Phe-Leu-Leu-Val- <i>N</i> -Me-Leu-NH	S6
Compound 3 NMR Cyclized Pentapeptide D-Phe-D-Leu-Val-Leu- <i>N</i> -Me-Leu	S7
Compound 3 LCMS Cyclized Pentapeptide D-Phe-D-Leu-Val-Leu- <i>N</i> -Me-Leu	S8
Compound 3 HPLC Cyclized Pentapeptide D-Phe-D-Leu-Val-Leu- <i>N</i> -Me-Leu	S9
Compound 4 LCMS Double Deprotected Linear Pentapeptide HO- <i>N</i> -Me-Phe-D-Leu-D-Val-Leu-Leu-NH ₂	S10
Compound 4 NMR Cyclized Pentapeptide <i>N</i> -Me-Phe-D-Leu-D-Val-Leu-Leu	S11
Compound 4 LCMS Cyclized Pentapeptide <i>N</i> -Me-Phe-D-Leu-D-Val-Leu-Leu	S12
Compound 4 HPLC Cyclized Pentapeptide <i>N</i> -Me-Phe-D-Leu-D-Val-Leu-Leu	S13
Compound 5 LCMS Double Deprotected Linear Pentapeptide HO-Phe- <i>N</i> -Me-Leu-D-Val-D-Leu-Leu-NH ₂ Leu	S14
Compound 5 NMR Cyclized Pentapeptide Phe- <i>N</i> -Me-Leu-D-Val-D-Leu-Leu	S15
Compound 5 LCMS Cyclized Pentapeptide Phe- <i>N</i> -Me-Leu-D-Val-D-Leu-Leu	S16
Compound 5 HPLC Cyclized Pentapeptide Phe- <i>N</i> -Me-Leu-D-Val-D-Leu-Leu	S17
Compound 6 NMR Dipeptide MeO-D-Phe-Leu- NHBoc	S18
Compound 6 NMR Tripeptide MeO-D-Phe-Leu-Val-NHBoc	S19
Compound 6 NMR Dipeptide MeO-Leu-D-Leu-NHBoc	S20
Compound 6 NMR Linear Pentapeptide MeO-D-Phe-Leu-Val-Leu-D-Leu-NHBoc	S21
Compound 6 LCMS Linear Pentapeptide MeO-D-Phe-Leu-Val-Leu-D-Leu-NHBoc	S22
Compound 6 LCMS Double Deprotected Linear Pentapeptide HO-D-Phe-Leu-Val-Leu-D-Leu-NH ₂	S23
Compound 6 NMR Cyclized Pentapeptide D-Phe-Leu-Val-Leu-D-Leu	S24
Compound 6 LCMS Cyclized Pentapeptide D-Phe-Leu-Val-Leu-D-Leu	S25
Compound 6 HPLC Cyclized Pentapeptide D-Phe-Leu-Val-Leu-D-Leu	S26
Compound 7 NMR Dipeptide MeO-D-Phe-Leu-NHBoc	S27
Compound 7 NMR Tripeptide MeO-D-Phe-Leu- <i>N</i> -Me-Val-Boc	S28
Compound 7 NMR Tetrapeptide MeO-D-Phe-Leu- <i>N</i> -Me-Val- <i>N</i> -Me-D-Leu-NBoc	S29
Compound 7 NMR Linear Pentapeptide MeO-D-Phe-Leu- <i>N</i> -Me-Val- <i>N</i> -Me-D-Leu-D-Phe-NHBoc	S30
Compound 7 LCMS Double Deprotected Pentapeptide HO-D-Phe-Leu- <i>N</i> -Me-Val- <i>N</i> -Me-D-Leu-D-Phe-NH ₂	S31
Compound 7 NMR Cyclized Pentapeptide D-Phe-Leu- <i>N</i> -Me-Val- <i>N</i> -Me-D-Leu-D-Phe	S32
Compound 7 LCMS Cyclized Pentapeptide D-Phe-Leu- <i>N</i> -Me-Val- <i>N</i> -Me-D-Leu-D-Phe	S33
Compound 7 HPLC Cyclized Pentapeptide D-Phe-Leu- <i>N</i> -Me-Val- <i>N</i> -Me-D-Leu-D-Phe	S34
Compound 10 NMR Dipeptide MeO-D-Phe-D-Leu-NHBoc	S35
Compound 10 NMR Tripeptide MeO-D-Phe-D-Leu-Val-NHBoc	S36

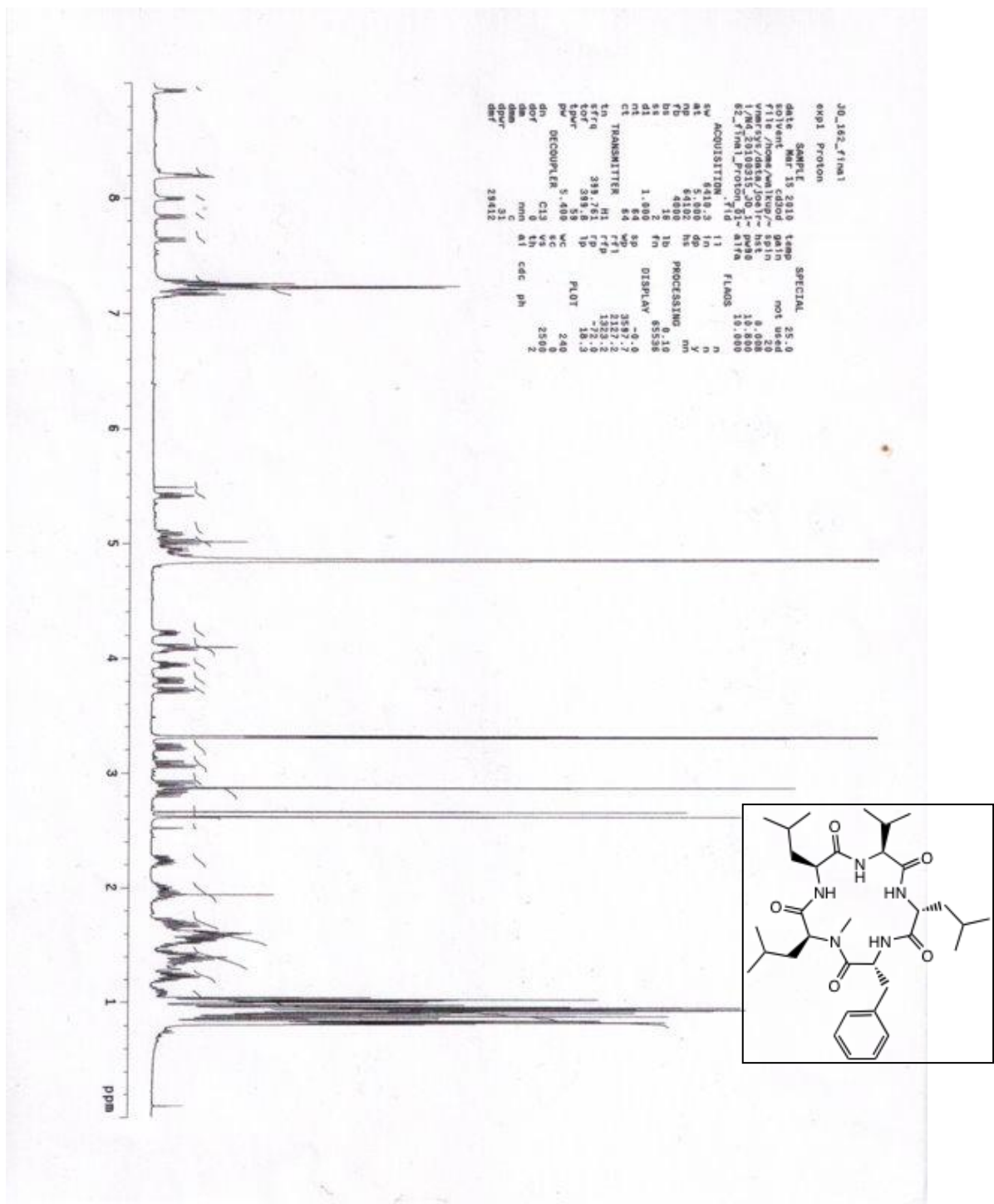
Compound 10 NMR Dipeptide MeO-Leu-Leu-NHBoc	S37
Compound 10 NMR Linear Pentapeptide MeO-D-Phe-D-Leu-Val-Leu-Leu-NHBoc	S38
Compound 10 LCMS Linear Pentapeptide MeO-D-Phe-D-Leu-Val-Leu-Leu-NHBoc	S39
Compound 10 LCMS Double Deprotected Linear Pentapeptide HO-D-Phe-D-Leu-Val-Leu-Leu-NH ₂	S40
Compound 10 NMR Cyclized Pentapeptide D-Phe-D-Leu-Val-Leu-Leu.....	S41
Compound 10 LCMS Cyclized Pentapeptide D-Phe-D-Leu-Val-Leu-Leu	S42
Compound 10 HPLC Cyclized Pentapeptide D-Phe-D-Leu-Val-Leu-Leu	S43
Compound 12 NMR Tripeptide MeO-Phe-Leu-Val-NHBoc	S44
Compound 12 NMR Dipeptide MeO-D-Leu-D-Phe-NHBoc.....	S45
Compound 12 NMR Linear Pentapeptide MeO-Phe-Leu-Val-D-Leu-D-Phe-NHBoc	S46
Compound 12 LCMS Linear Pentapeptide MeO-Phe-Leu-Val-D-Leu-D-Phe-NHBoc	S47
Compound 12 LCMS Double Deprotected Linear Pentapeptide HO-Phe-Leu-Val-D-Leu-D-Phe-NH ₂	S48
Compound 12 NMR Cyclized Pentapeptide Phe-Leu-Val-D-Leu-D-Phe.....	S49
Compound 12 LCMS Cyclized Pentapeptide Phe-Leu-Val-D-Leu-D-Phe	S50
Compound 12 HPLC Cyclized Pentapeptide Phe-Leu-Val-D-Leu-D-Phe.....	S51
Compound 15 NMR Dipeptide MeO-Phe- <i>N</i> -Me-D-Phe-Boc	S52
Compound 15 NMR Tripeptide MeO-Phe- <i>N</i> -Me-D-Phe-Val-NHBoc.....	S53
Compound 15 NMR Linear Pentapeptide MeO-Phe- <i>N</i> -Me-D-Phe-Val-Leu- <i>N</i> -Me-Leu-Boc	S54
Compound 15 LCMS Linear Pentapeptide MeO-Phe- <i>N</i> -Me-D-Phe-Val-Leu- <i>N</i> -Me-Leu-Boc	S55
Compound 15 LCMS Double Deprotected Linear Pentapeptide HO-Phe- <i>N</i> -Me-D-Phe-Val-Leu- <i>N</i> -Me- Leu-H	S56
Compound 15 NMR Cyclized Pentapeptide Phe- <i>N</i> -Me-D-Phe-Val-Leu- <i>N</i> -Me-Leu.....	S57
Compound 15 LCMS Cyclized Pentapeptide Phe- <i>N</i> -Me-D-Phe-Val-Leu- <i>N</i> -Me-Leu	S58
Compound 15 HPLC Cyclized Pentapeptide Phe- <i>N</i> -Me-D-Phe-Val-Leu- <i>N</i> -Me-Leu.....	S59
Compound 18 NMR Dipeptide MeO-Phe-D-Phe-NHBoc	S60
Compound 18 NMR Tripeptide MeO-Phe-D-Phe-D-Val-NHBoc	S61
Compound 18 NMR Dipeptide MeO-Leu-Leu-NHBoc	S62
Compound 18 NMR Linear Pentapeptide MeO-Phe-D-Phe-D-Val-Leu-Leu-NHBoc	S63
Compound 18 LCMS Linear Pentapeptide MeO-Phe-D-Phe-D-Val-Leu-Leu-NHBoc	S64
Compound 18 LCMS Double Deprotected Linear Pentapeptide HO-Phe-D-Phe-D-Val-Leu-Leu-NH ₂	S65
Compound 18 NMR Cyclized Pentapeptide Phe-D-Phe-D-Val-Leu-Leu	S66
Compound 18 LCMS Cyclized Pentapeptide Phe-D-Phe-D-Val-Leu-Leu	S67
Compound 18 HPLC Cyclized Pentapeptide Phe-D-Phe-D-Val-Leu-Leu.....	S68
Compound 20 LCMS Double Deprotected Linear Pentapeptide HO-D-Phe-D-Val-Cha-Ser(Bzl)-Phe- NH ₂	S69
Compound 20 NMR Cyclized Pentapeptide Phe-D-Phe-D-Val-Cha-Ser(Bzl)	S70
Compound 20 LCMS Cyclized Pentapeptide Phe-D-Phe-D-Val-Cha-Ser(Bzl)	S71
Compound 20 HPLC Cyclized Pentapeptide Phe-D-Phe-D-Val-Cha-Ser(Bzl)	S72
Compound 21 LCMS Double Deprotected Pentapeptide HO-Phe- <i>N</i> -Me-D-Phe-D-Val-Cha-Ser(Bzl)- NH ₂	S73
Compound 21 NMR Cyclized Protected Pentapeptide Phe- <i>N</i> -Me-D-Phe-D-Val-Cha-Ser(Bzl)	S74
Compound 21 NMR Cyclized Pentapeptide Phe- <i>N</i> -Me-D-Phe-D-Val-Cha-Ser.....	S75
Compound 21 LCMS Cyclized Pentapeptide Phe-<i>N</i>-Me-D-Phe-D-Val-Cha-Ser	S76
Compound 21 HPLC Cyclized Pentapeptide Phe- <i>N</i> -Me-D-Phe-D-Val-Cha-Ser.....	S77
Compound 23 NMR Dipeptide MeO-D-Tyr-Leu-NHBoc	S78
Compound 23 NMR Tripeptide MeO-D-Tyr-Leu-Val-NHBoc	S79
Compound 23 NMR Dipeptide MeO-Lys(Cbz)-Leu-NHBoc	S80
Compound 23 NMR Linear Pentapeptide MeO-D-Tyr-Leu-Val-Lys(Cbz)-Leu-NHBoc.....	S81

Compound 23 NMR Cyclized Pentapeptide D-Tyr-Leu-Val-Lys(Cbz)-Leu	S82
Compound 23 LCMS Cyclized Pentapeptide D-Tyr-Leu-Val-Lys(Cbz)-Leu	S83
Compound 24 NMR Dipeptide MeO-D-Tyr-Leu-NHBoc	S84
Compound 24 NMR Tripeptide MeO-D-Tyr-Leu-Val-NHBoc	S85
Compound 24 NMR Dipeptide MeO-Lys(Cbz)-Leu-NHBoc	S86
Compound 24 NMR Linear Pentapeptide MeO-D-Tyr-Leu-Val-Lys(Cbz)-Leu-NHBoc	S87
Compound 24 NMR Cyclized Pentapeptide D-Tyr-Leu-Val-Lys-Leu	S88
Compound 24 LCMS Cyclized Pentapeptide D-Tyr-Leu-Val-Lys-Leu	S89
Compound 26 NMR Dipeptide MeO-D-Trp-Leu-NHBoc	S90
Compound 26 NMR Tripeptide MeO-D-Trp-Leu-Val-NHBoc	S91
Compound 26 NMR Dipeptide MeO-Arg(2Cbz)-Leu-NHBoc	S92
Compound 26 NMR Linear Pentapeptide MeO-D-Trp-Leu-Val-Arg(2Cbz)-Leu-NHBoc.....	S93
Compound 26 NMR Cyclized Pentapeptide D-Trp-Leu-Val-Arg(2Cbz)-Leu	S94
Compound 26 LCMS Cyclized Pentapeptide D-Trp-Leu-Val-Arg(2Cbz)-Leu	S95
Compound 27 NMR Dipeptide MeO-D-Trp-Leu-NHBoc	S96
Compound 27 NMR Tripeptide MeO-D-Trp-Leu-Val-NHBoc	S97
Compound 27 NMR Dipeptide MeO-Arg(2Cbz)-Leu-NHBoc	S98
Compound 27 NMR Linear Pentapeptide MeO-D-Trp-Leu-Val-Arg(2Cbz)-Leu-NHBoc.....	S99
Compound 27 NMR Cyclized Pentapeptide D-Trp-Leu-Val-Arg-Leu	S100
Compound 27 LCMS Cyclized Pentapeptide D-Trp-Leu-Val-Arg-Leu	S101
Compound 28 NMR Dipeptide MeO-Phe- <i>N</i> -Me-D-Phe-NBoc	S102
Compound 28 NMR Tripeptide MeO-Phe- <i>N</i> -Me-D-Phe-Val-NHBoc.....	S103
Compound 28 NMR Dipeptide MeO-Leu-Lys(Cbz)-NHBoc	S104
Compound 28 NMR Linear Pentapeptide MeO-Phe- <i>N</i> -Me-D-Phe-Val-Leu-Lys(Cbz)-NHBoc	S105
Compound 28 LCMS Linear Pentapeptide MeO-Phe- <i>N</i> -Me-D-Phe-Val-Leu-Lys(Cbz)-NHBoc	S106
Compound 28 LCMS Double Deprotected Linear Pentapeptide HO-Phe- <i>N</i> -Me-D-Phe-Val-Leu- Lys(Cbz)-NH ₂	S107
Compound 28 NMR Cyclized Pentapeptide Phe- <i>N</i> -Me-D-Phe-Val-Leu-Lys(Cbz)	S108
Compound 28 LCMS Cyclized Pentapeptide Phe- <i>N</i> -Me-D-Phe-Val-Leu-Lys(Cbz)	S109
Compound 29 LCMS Double Deprotected Linear Pentapeptide HO-Phe- <i>N</i> -Me-D-Phe-Val-Leu- Lys(Boc)-NH ₂	S110
Compound 29 NMR Cyclized Pentapeptide Phe- <i>N</i> -Me-D-Phe-Val-Leu-Lys(Boc)	S111
Compound 29 LCMS Cyclized Pentapeptide Phe- <i>N</i> -Me-D-Phe-Val-Leu-Lys(Boc)	S112
Compound 29 HPLC Cyclized Pentapeptide Phe- <i>N</i> -Me-D-Phe-Val-Leu-Lys(Boc)	S113
Compound 30 NMR Dipeptide MeO-Phe- <i>N</i> -Me-D-Phe-NBoc	S114
Compound 30 NMR Tripeptide MeO-Phe- <i>N</i> -Me-D-Phe-Val-NHBoc.....	S115
Compound 30 NMR Dipeptide MeO-Leu-Lys(Cbz)-NHBoc	S116
Compound 30 NMR Linear Pentapeptide MeO-Phe- <i>N</i> -Me-D-Phe-Val-Leu-Lys(Cbz)-NHBoc	S117
Compound 30 LCMS Linear Pentapeptide MeO-Phe- <i>N</i> -Me-D-Phe-Val-Leu-Lys(Cbz)-NHBoc	S118
Compound 30 LCMS Double Deprotected Linear Pentapeptide HO-Phe- <i>N</i> -Me-D-Phe-Val-Leu- Lys(Cbz)-NH ₂	S119
Compound 30 NMR Cyclized Protected Pentapeptide Phe- <i>N</i> -Me-D-Phe-Val-Leu-Lys(Cbz)	S120
Compound 30 LCMS Cyclized Protected Pentapeptide Phe- <i>N</i> -Me-D-Phe-Val-Leu-Lys(Cbz)	S121
Compound 30 NMR Cyclized Pentapeptide Phe- <i>N</i> -Me-D-Phe-Val-Leu-Lys.....	S122
Compound 30 LCMS Cyclized Pentapeptide Phe- <i>N</i> -Me-D-Phe-Val-Leu-Lys.....	S123
Compound 30 HPLC Cyclized Pentapeptide Phe- <i>N</i> -Me-D-Phe-Val-Leu-Lys	S124
Compound 31 LCMS Double Deprotected Linear Pentapeptide HO-Phe-Leu-Val-Leu-Lys(Boc)-NH ₂	S125
Compound 31 NMR Cyclized Pentapeptide Phe-Leu-Val-Leu-Lys(Boc)	S126

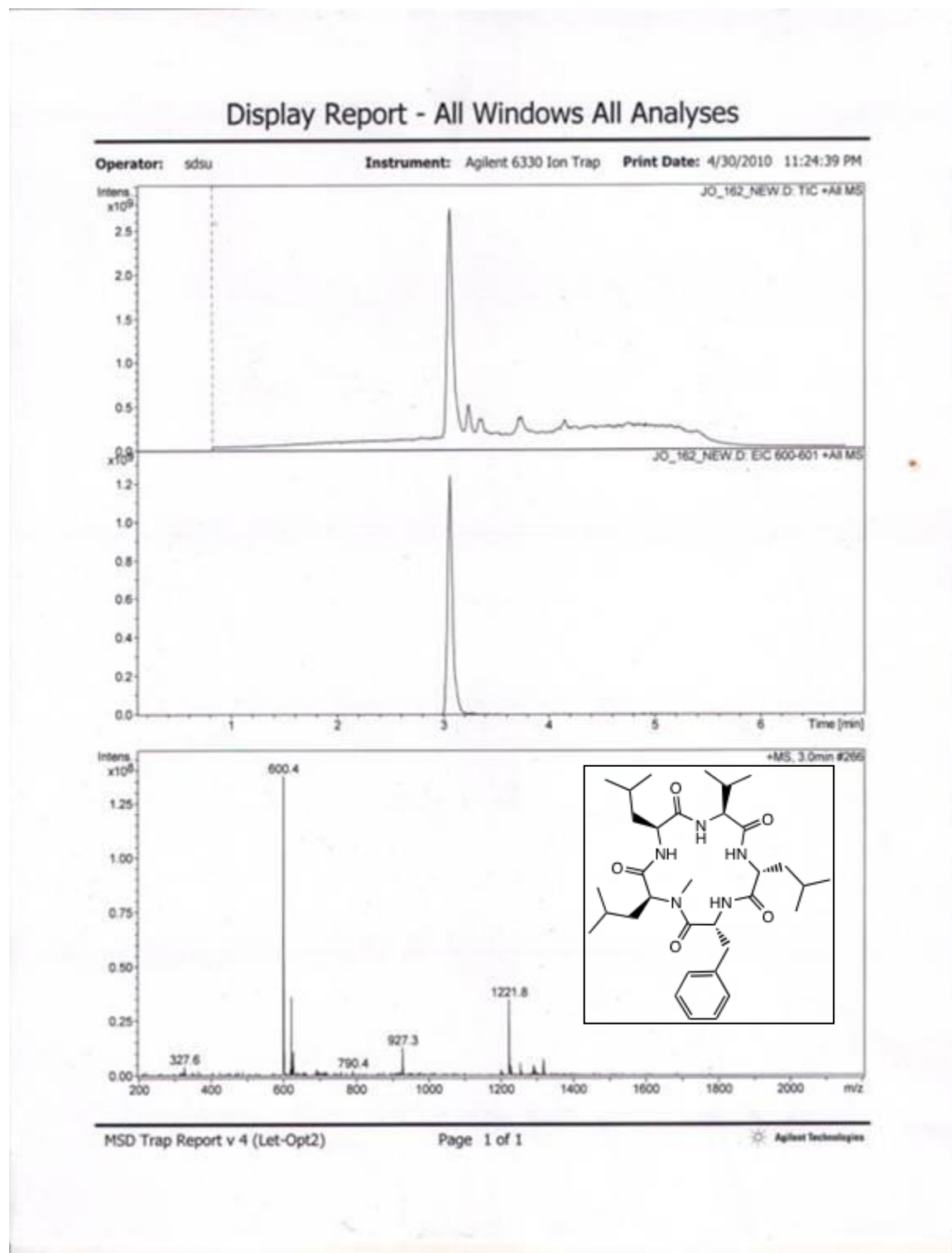
Compound 31 LCMS Cyclized Pentapeptide Phe-Leu-Val-Leu-Lys(Boc)	S127
Compound 32 LCMS Double Deprotected Linear Pentapeptide HO-Phe-Leu-Val-Leu-Lys(Boc)-NH ₂	S128
Compound 32 NMR Cyclized Pentapeptide Phe-Leu-Val-Leu-Lys	S129
Compound 32 LCMS Cyclized Pentapeptide Phe-Leu-Val-Leu-Lys	S130
Compound 34 LCMS Double Deprotected Linear Pentapeptide HO-Leu- <i>N</i> -Me-Lys(Boc)-Phe-Leu-Val- NH ₂	S131
Compound 34 NMR Cyclized Pentapeptide Phe-Leu-Val-Leu- <i>N</i> -Me-Lys(Boc)	S132
Compound 34 LCMS Cyclized Pentapeptide Phe-Leu-Val-Leu- <i>N</i> -Me-Lys(Boc)	S133
Compound 34 HPLC Cyclized Pentapeptide Phe-Leu-Val-Leu- <i>N</i> -Me-Lys(Boc)	S134
Compound 35 LCMS Double Deprotected Linear Pentapeptide HO-Leu- <i>N</i> -Me-Lys(Boc)-Phe-Leu-Val- NH ₂	S135
Compound 35 NMR Cyclized Pentapeptide Phe-Leu-Val-Leu- <i>N</i> -Me-Lys.....	S136
Compound 35 LCMS Cyclized Pentapeptide Phe-Leu-Val-Leu- <i>N</i> -Me-Lys	S137
Compound 35 HPLC Cyclized Pentapeptide Phe-Leu-Val-Leu- <i>N</i> -Me-Lys	S138
Compound 36 LCMS Double Deprotected Linear Pentapeptide HO-Leu-Lys(Boc)-Phe-Leu- <i>D</i> -Val-NH ₂	S139
Compound 36 NMR Cyclized Pentapeptide Phe-Leu- <i>D</i> -Val-Leu-Lys(Boc).....	S140
Compound 36 LCMS Cyclized Pentapeptide Phe-Leu- <i>D</i> -Val-Leu-Lys(Boc)	S141
Compound 36 HPLC Cyclized Pentapeptide Phe-Leu- <i>D</i> -Val-Leu-Lys(Boc).....	S142
Compound 37 LCMS Double Deprotected Linear Pentapeptide HO-Leu-Lys(Boc)-Phe-Leu- <i>D</i> -Val-NH ₂	S143
Compound 37 NMR Cyclized Pentapeptide Phe-Leu- <i>D</i> -Val-Leu-Lys	S144
Compound 37 LCMS Cyclized Pentapeptide Phe-Leu- <i>D</i> -Val-Leu-Lys	S145
Compound 37 HPLC Cyclized Pentapeptide Phe-Leu- <i>D</i> -Val-Leu-Lys.....	S146
Compound 39 LCMS Double Deprotected Linear Pentapeptide HO-Leu- <i>N</i> -Me-Val-Lys(2-Cl-Z)- <i>D</i> -Phe- Phe-NH ₂	S147
Compound 39 NMR Cyclized Pentapeptide Phe-Leu- <i>N</i> -Me-Val-Lys(2-Cl-Z)- <i>D</i> -Phe	S148
Compound 39 LCMS Cyclized Pentapeptide Phe-Leu- <i>N</i> -Me-Val-Lys(2-Cl-Z)- <i>D</i> -Phe	S149
Compound 39 HPLC Cyclized Pentapeptide Phe-Leu- <i>N</i> -Me-Val-Lys(2-Cl-Z)- <i>D</i> -Phe.....	S150
Compound 40 LCMS Double Deprotected Linear Pentapeptide HO-Leu- <i>N</i> -Me-Val- <i>D</i> -Lys(Cbz)- <i>D</i> -Phe- Phe-NH ₂	S151
Compound 40 NMR Cyclized Pentapeptide Phe-Leu- <i>N</i> -Me-Val- <i>D</i> -Lys(Cbz)- <i>D</i> -Phe	S152
Compound 40 LCMS Cyclized Pentapeptide Phe-Leu- <i>N</i> -Me-Val- <i>D</i> -Lys(Cbz)- <i>D</i> -Phe	S153
Compound 40 HPLC Cyclized Pentapeptide Phe-Leu- <i>N</i> -Me-Val- <i>D</i> -Lys(Cbz)- <i>D</i> -Phe.....	S154
Compound 41 LCMS Double Deprotected Linear Pentapeptide HO-Phe-Leu-Val- <i>N</i> -Me- <i>D</i> -Lys(2-Cl- Cbz)- <i>D</i> -Phe-NH ₂	S155
Compound 41 NMR Cyclized Pentapeptide Phe-Leu-Val- <i>N</i> -Me- <i>D</i> -Lys(2-Cl-Cbz)- <i>D</i> -Phe.....	S156
Compound 41 LCMS Cyclized Pentapeptide Phe-Leu-Val- <i>N</i> -Me- <i>D</i> -Lys(2-Cl-Cbz)- <i>D</i> -Phe	S157
Compound 41 HPLC Cyclized Pentapeptide Phe-Leu-Val- <i>N</i> -Me- <i>D</i> -Lys(2-Cl-Cbz)- <i>D</i> -Phe.....	S158
Compound 42 NMR Linear Pentapeptide MeO-Leu-Val- <i>D</i> -Lys(2-Cl-Z)- <i>N</i> -Me- <i>D</i> -Phe-Phe-NHBoc	S159
Compound 42 LCMS Linear Pentapeptide MeO-Leu-Val- <i>D</i> -Lys(2-Cl-Z)- <i>N</i> -Me- <i>D</i> -Phe-Phe-NHBoc	S160
Compound 42 LCMS Double Deprotected Linear Pentapeptide HO-Leu-Val- <i>D</i> -Lys(2-Cl-Z)- <i>N</i> -Me- <i>D</i> - Phe-Phe-NH ₂	S161
Compound 42 NMR Cyclized Pentapeptide Phe-Leu-Val- <i>D</i> -Lys(2-Cl-Z)- <i>N</i> -Me- <i>D</i> -Phe.....	S162
Compound 42 LCMS Cyclized Pentapeptide Phe-Leu-Val- <i>D</i> -Lys(2-Cl-Z)- <i>N</i> -Me- <i>D</i> -Phe	S163
Compound 42 HPLC Cyclized Pentapeptide Phe-Leu-Val- <i>D</i> -Lys(2-Cl-Z)- <i>N</i> -Me- <i>D</i> -Phe.....	S164

Compound 43 LCMS Double Deprotected Linear Pentapeptide HO-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe-β-OH-Phe-NH ₂	S165
Compound 43 NMR Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe.....	S166
Compound 43 ROESY NMR Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe. S167	
Compound 43 TOSCY NMR Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe. S168	
Compound 43 LCMS Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe	S169
Compound 43 HPLC Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe.....	S170
Compound 44 LCMS Double Deprotected Linear Pentapeptide HO-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe-β-OH-Phe-NH ₂	S171
Compound 44 NMR Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe.....	S172
Compound 44 ROESY NMR Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe. S173	
Compound 44 TOSCY NMR Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe. S174	
Compound 44 LCMS Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe	S175
Compound 44 HPLC Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe.....	S176
Compound 45 LCMS Double Deprotected Linear Pentapeptide HO-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe-β-OH-D-Phe-NH ₂	S177
Compound 45 NMR Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe.....	S178
Compound 45 LCMS Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe	S179
Compound 45 HPLC Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe.....	S180
Compound 46 LCMS Double Deprotected Linear Pentapeptide HO-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe-β-OH-Phe-NH ₂	S181
Compound 46 NMR Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe.....	S182
Compound 46 ROSEY NMR Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe. S183	
Compound 46 TOSCY NMR Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe. S184	
Compound 46 LCMS Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe	S185
Compound 46 HPLC Cyclized Pentapeptide β-benzyloxy-Phe-Leu- <i>N</i> -Me-Val-D-Leu-D-Phe.....	S186

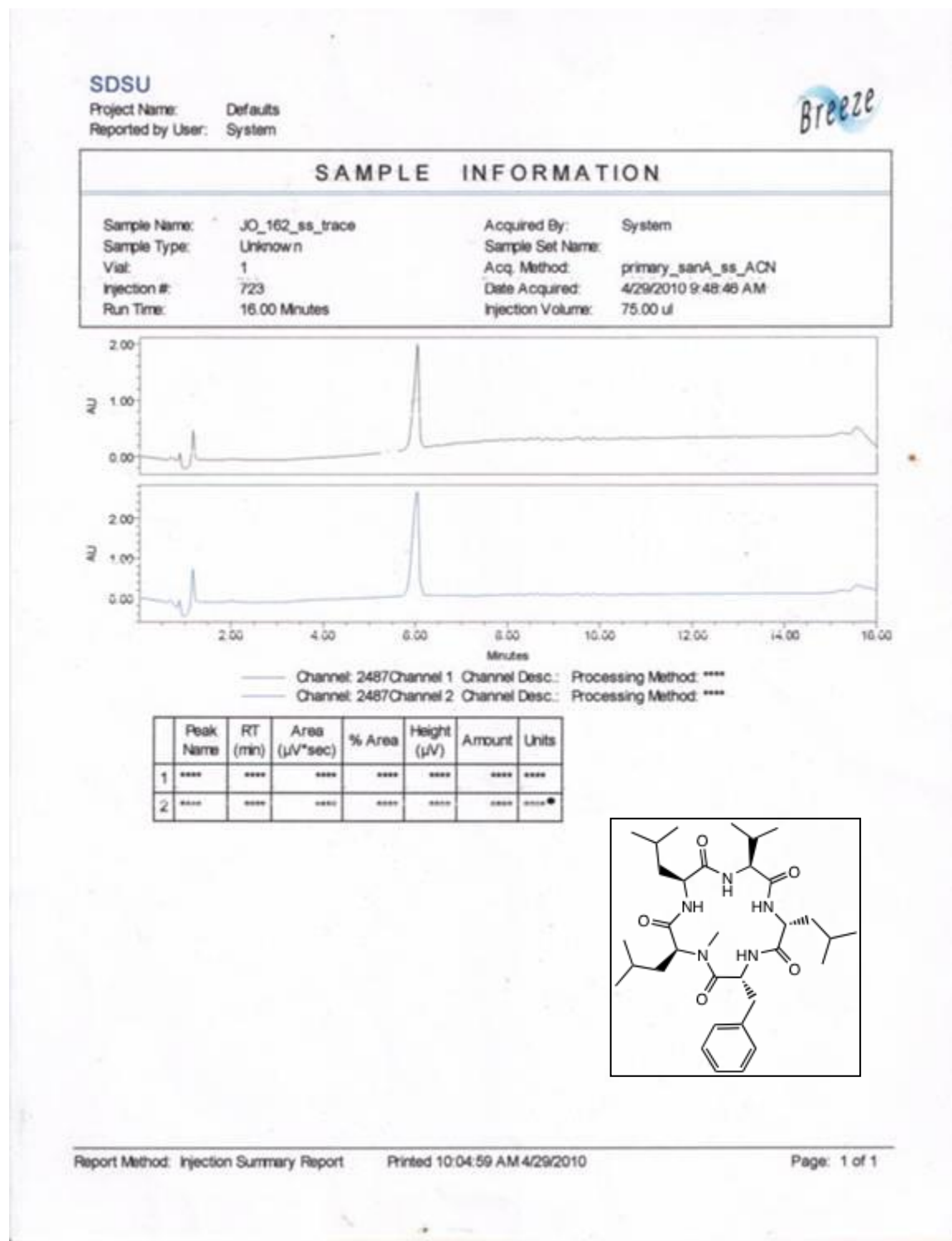




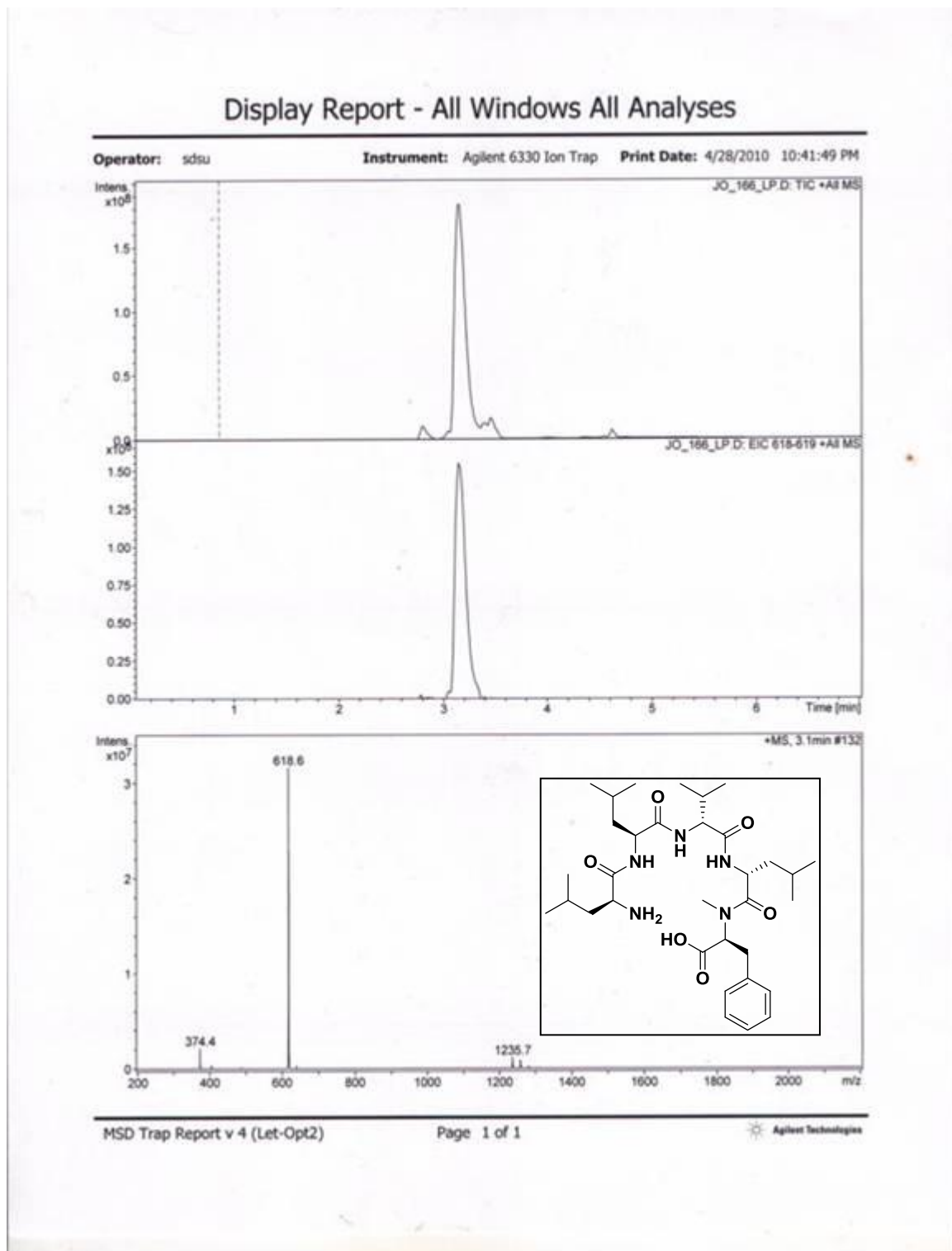
Compound 3 NMR Cyclized Pentapeptide D-Phe-D-Leu-Val-Leu-N-Me-Leu



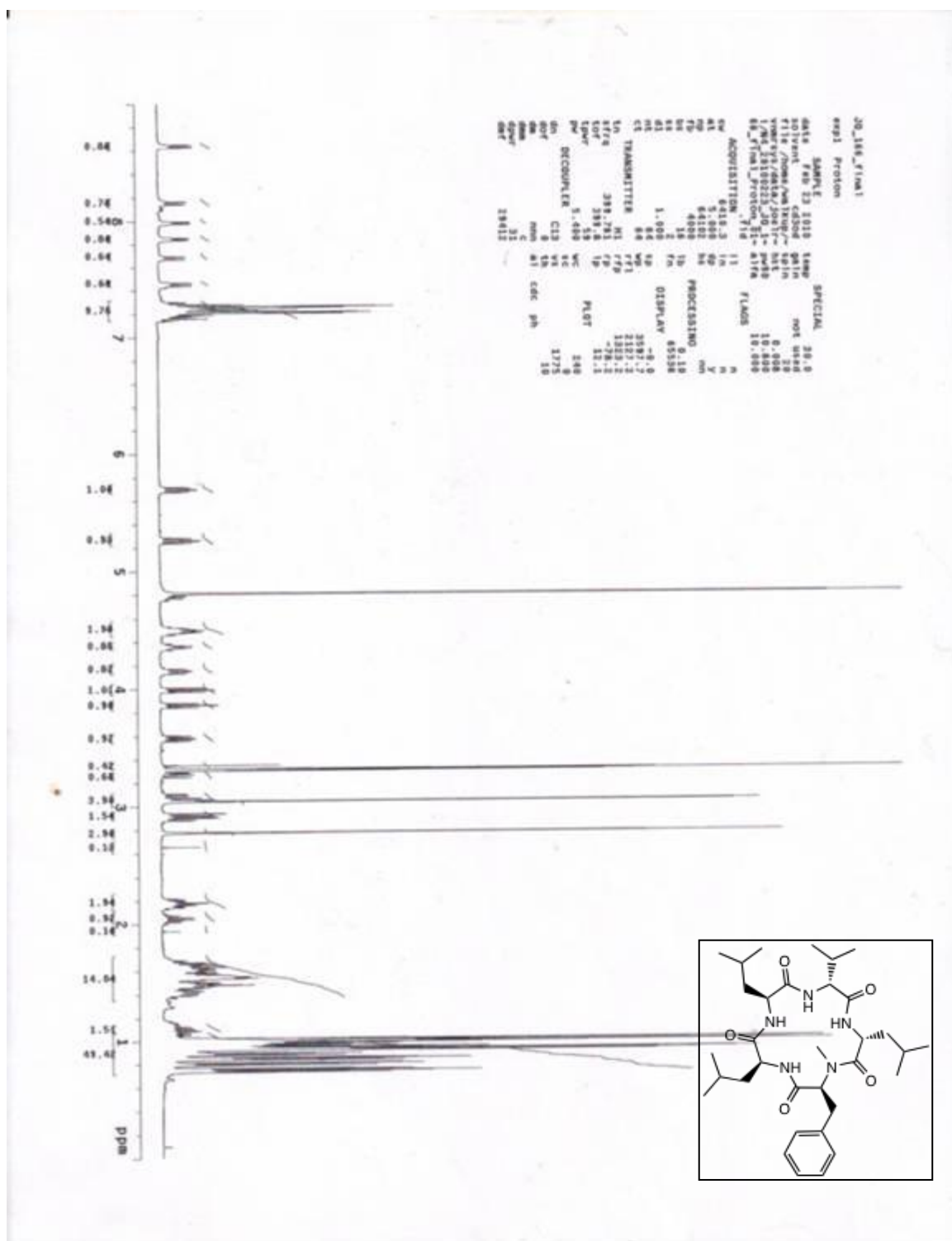
Compound 3 LCMS Cyclized Pentapeptide D-Phe-D-Leu-Val-Leu-N-Me-Leu (MW=600)

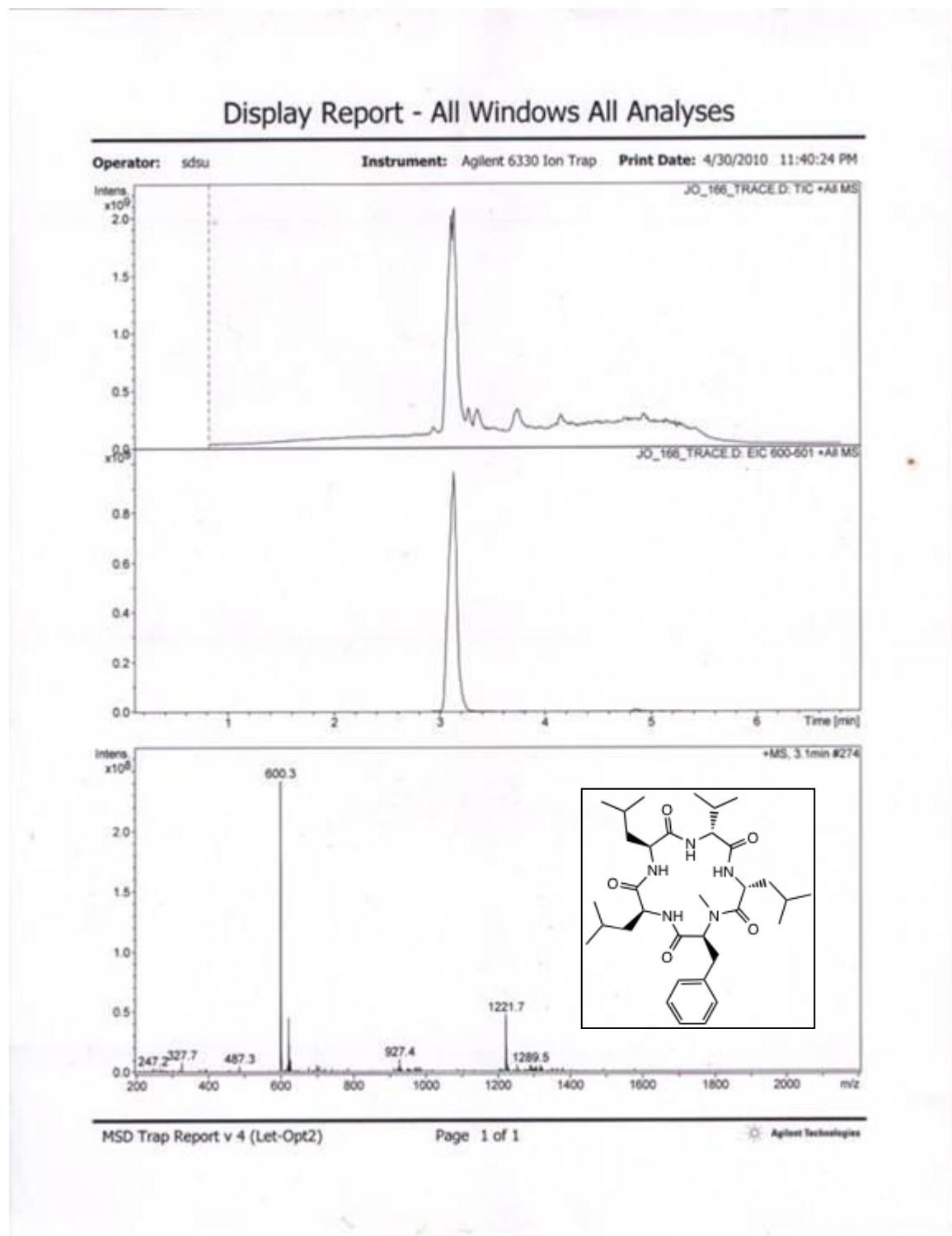


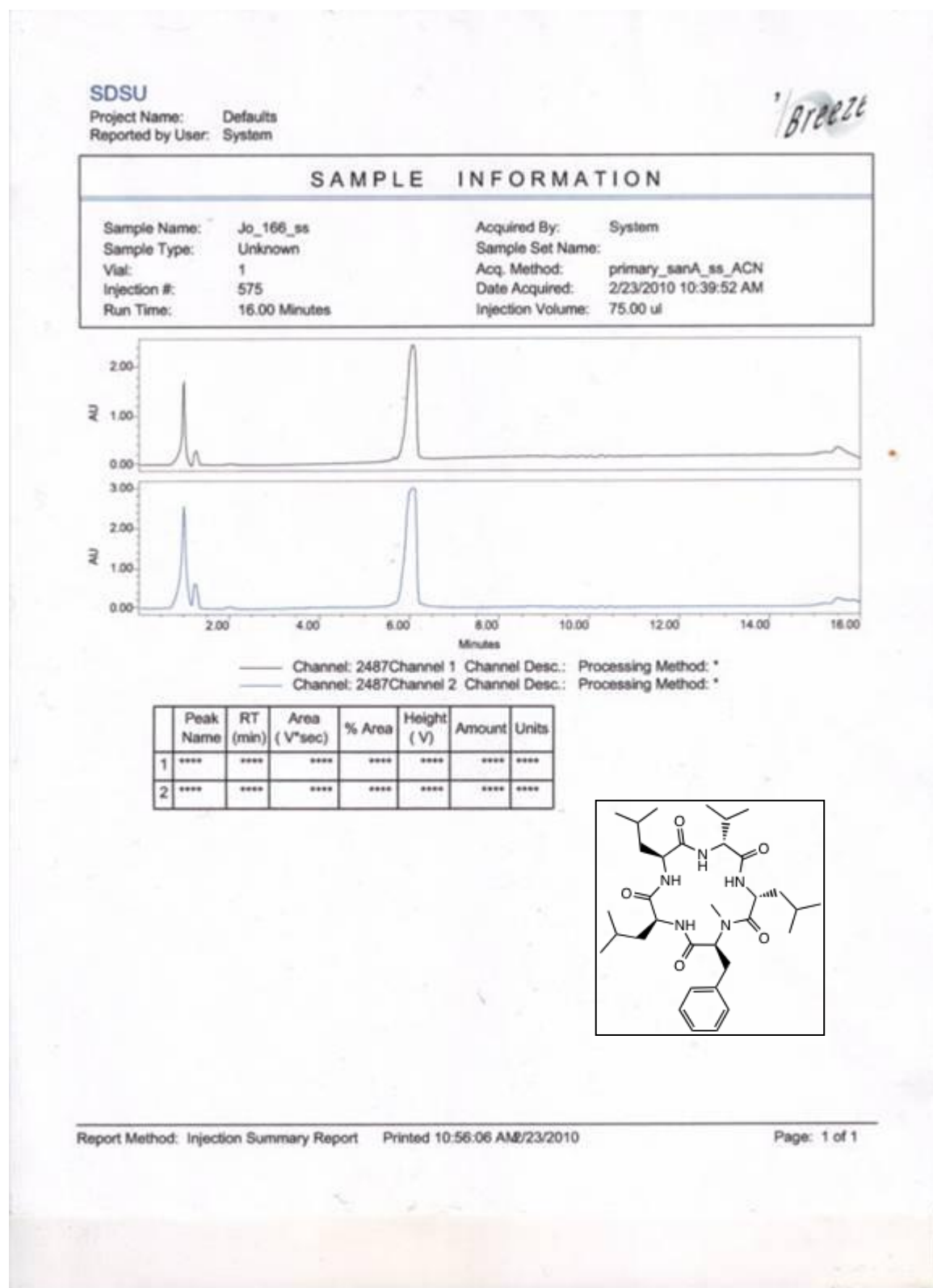
Compound 3 HPLC Cyclized Pentapeptide D-Phe-D-Leu-Val-Leu-N-Me-Leu

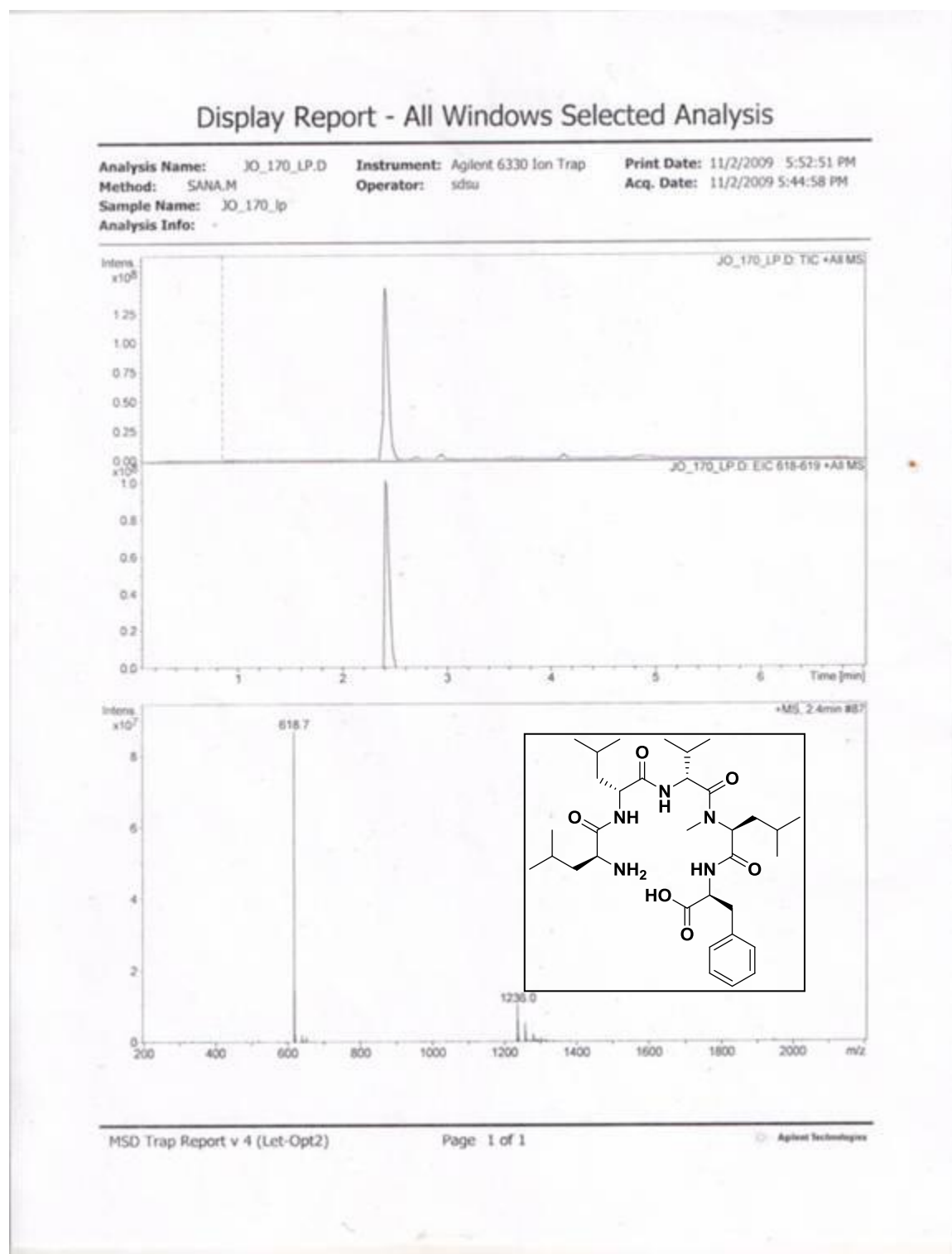


Compound 4 LCMS Double Deprotected Linear Pentapeptide HO-N-Me-Phe-D-Leu-D-Val-Leu-Leu-NH₂ (MW=618)

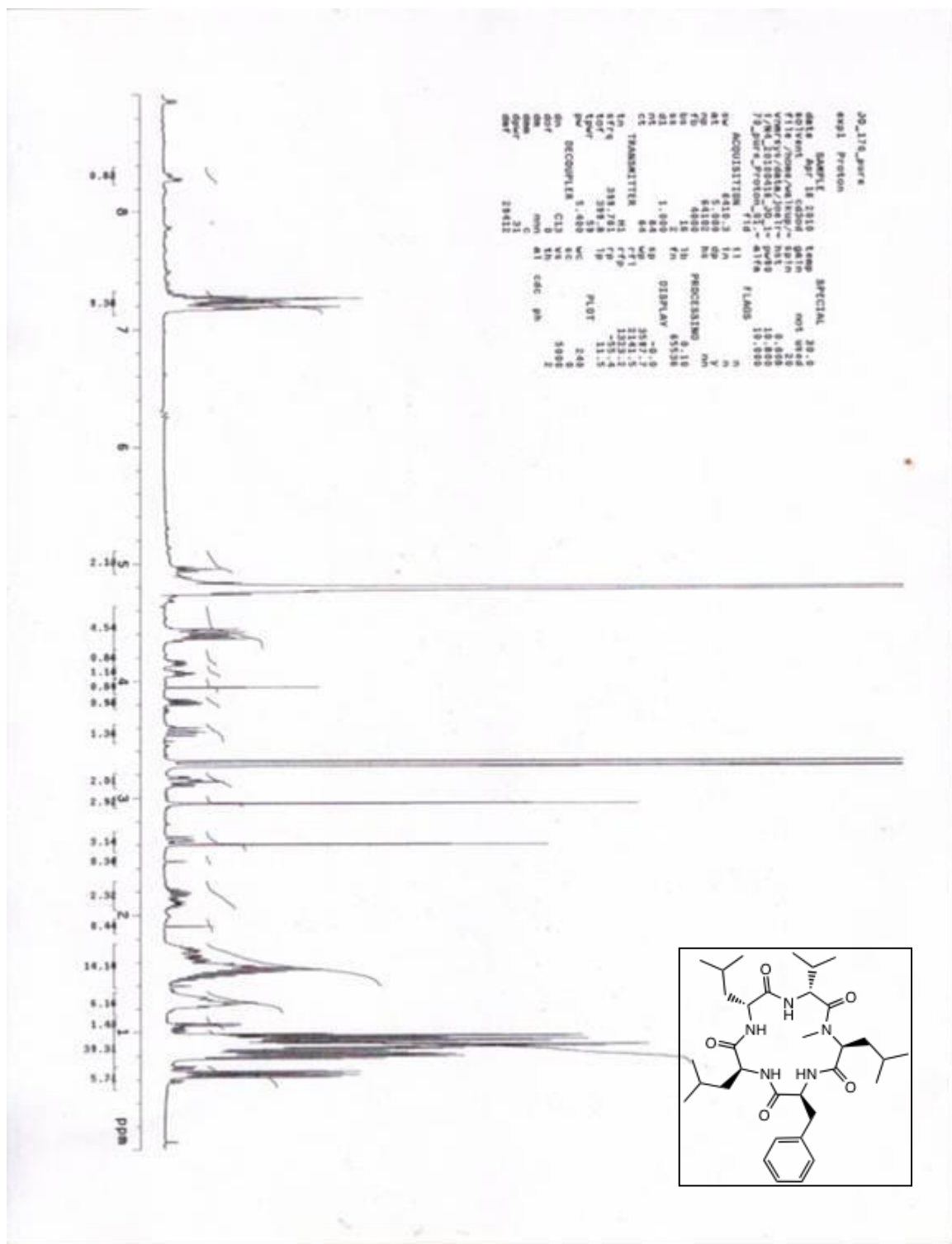
Compound 4 NMR Cyclized Pentapeptide *N*-Me-Phe-D-Leu-D-Val-Leu-Leu

Compound 4 LCMS Cyclized Pentapeptide *N*-Me-Phe-D-Leu-D-Val-Leu-Leu

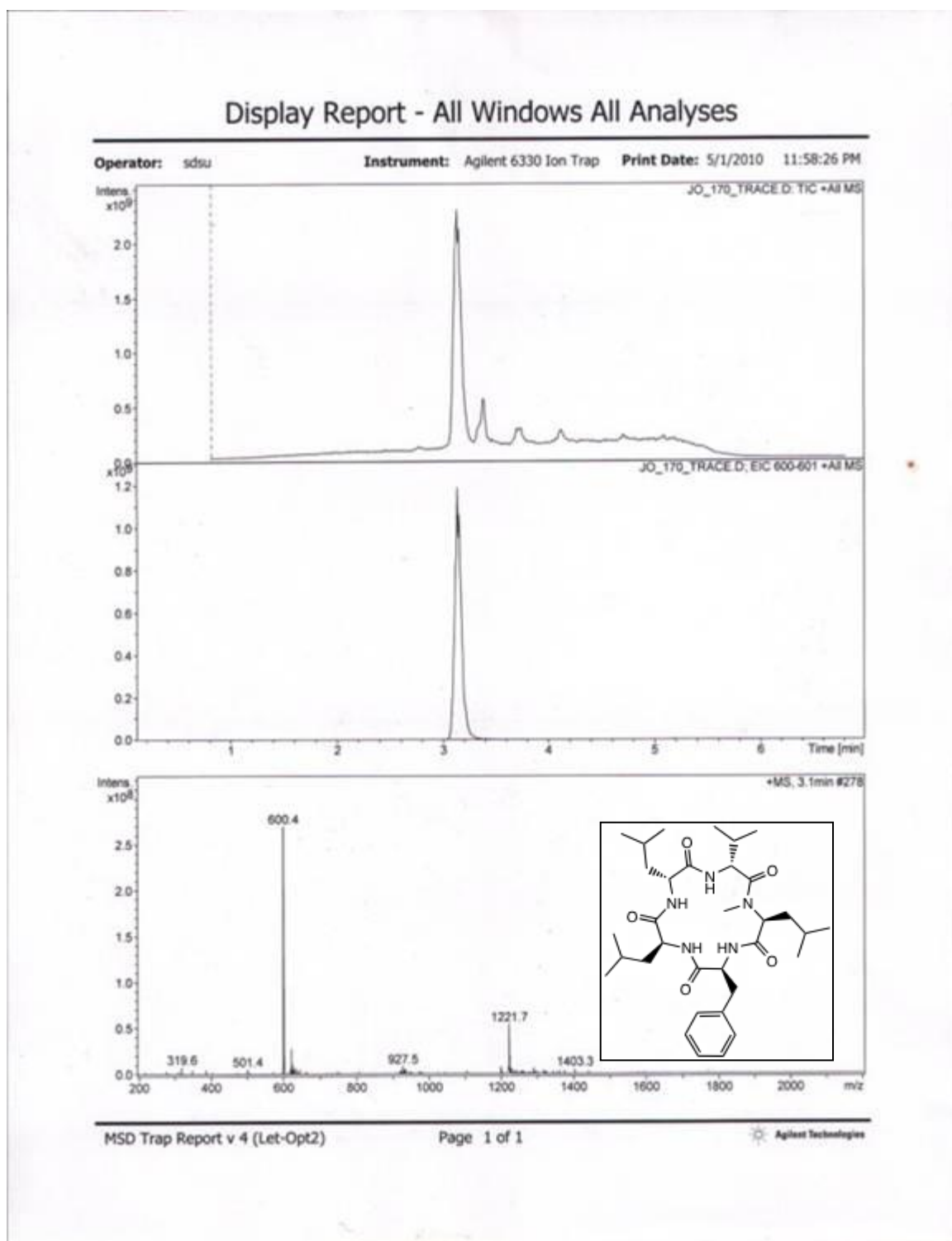
Compound 4 HPLC Cyclized Pentapeptide *N*-Me-Phe-D-Leu-D-Val-Leu-Leu



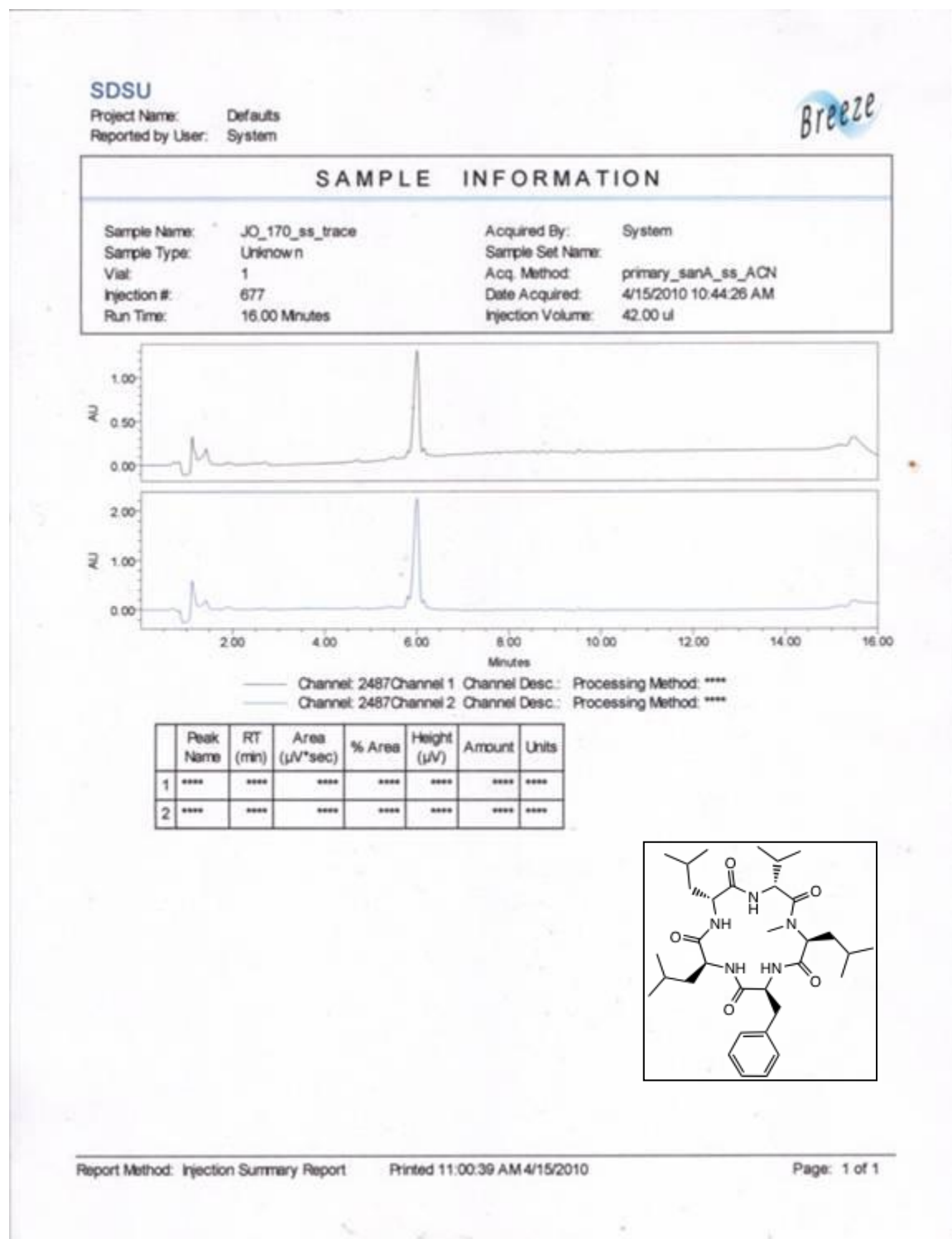
Compound 5 LCMS Double Deprotected Linear Pentapeptide HO-Phe-N-Me-Leu-D-Val-D-Leu-Leu-NH₂ Leu (MW=618)



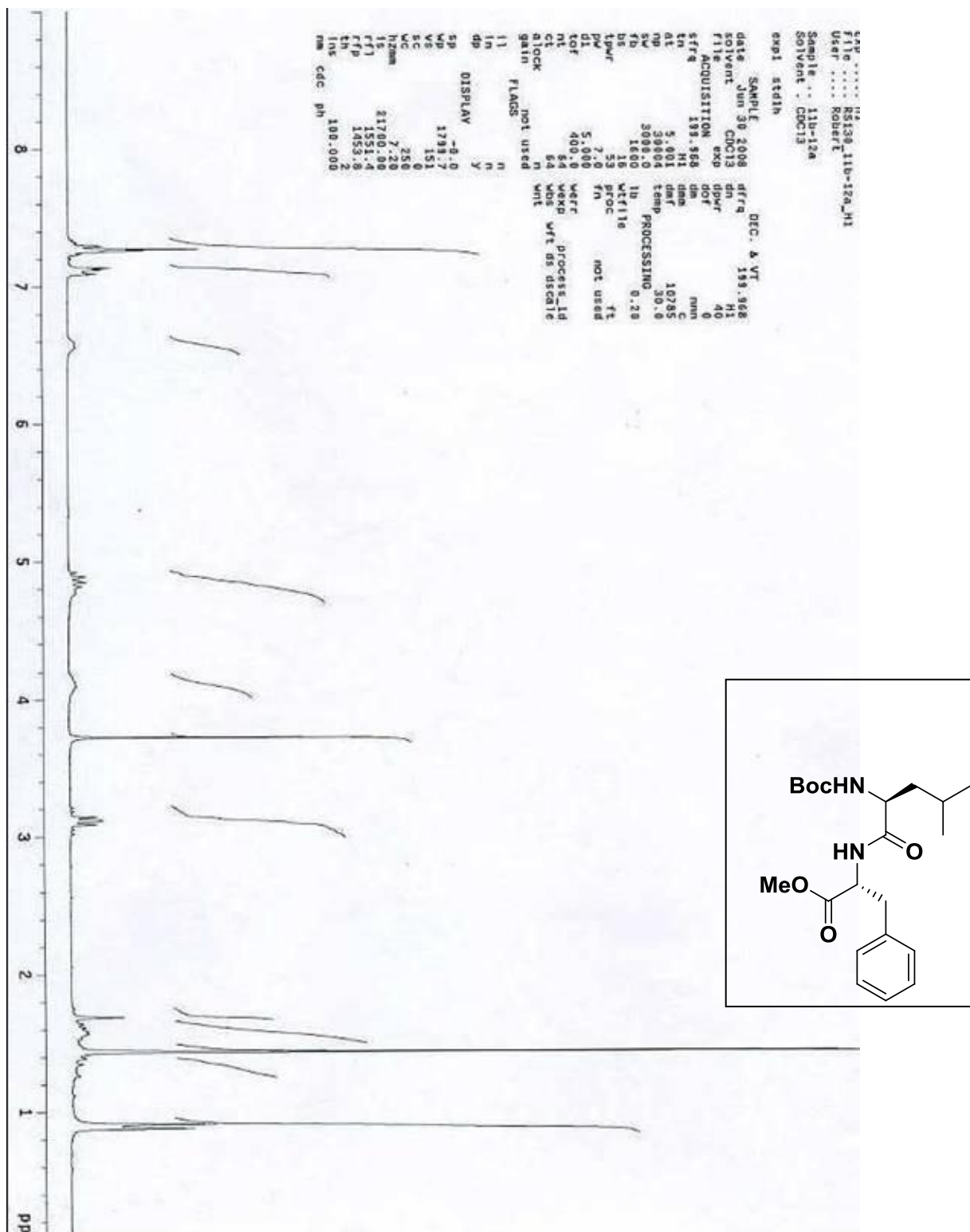
Compound 5 NMR Cyclized Pentapeptide Phe-N-Me-Leu-D-Val-D-Leu-Leu



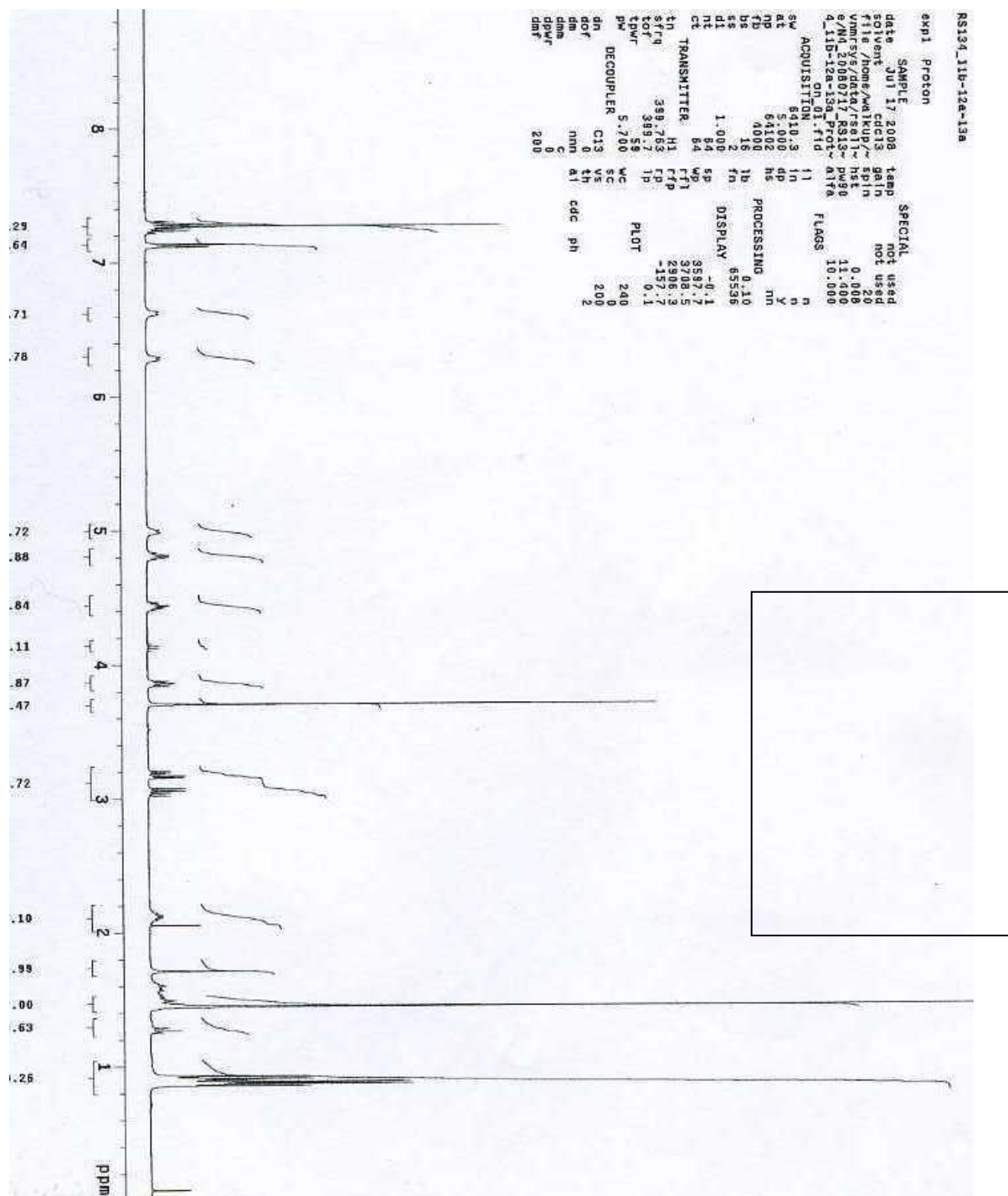
Compound 5 LCMS Cyclized Pentapeptide Phe-*N*-Me-Leu-*D*-Val-*D*-Leu-Leu (MW=600)



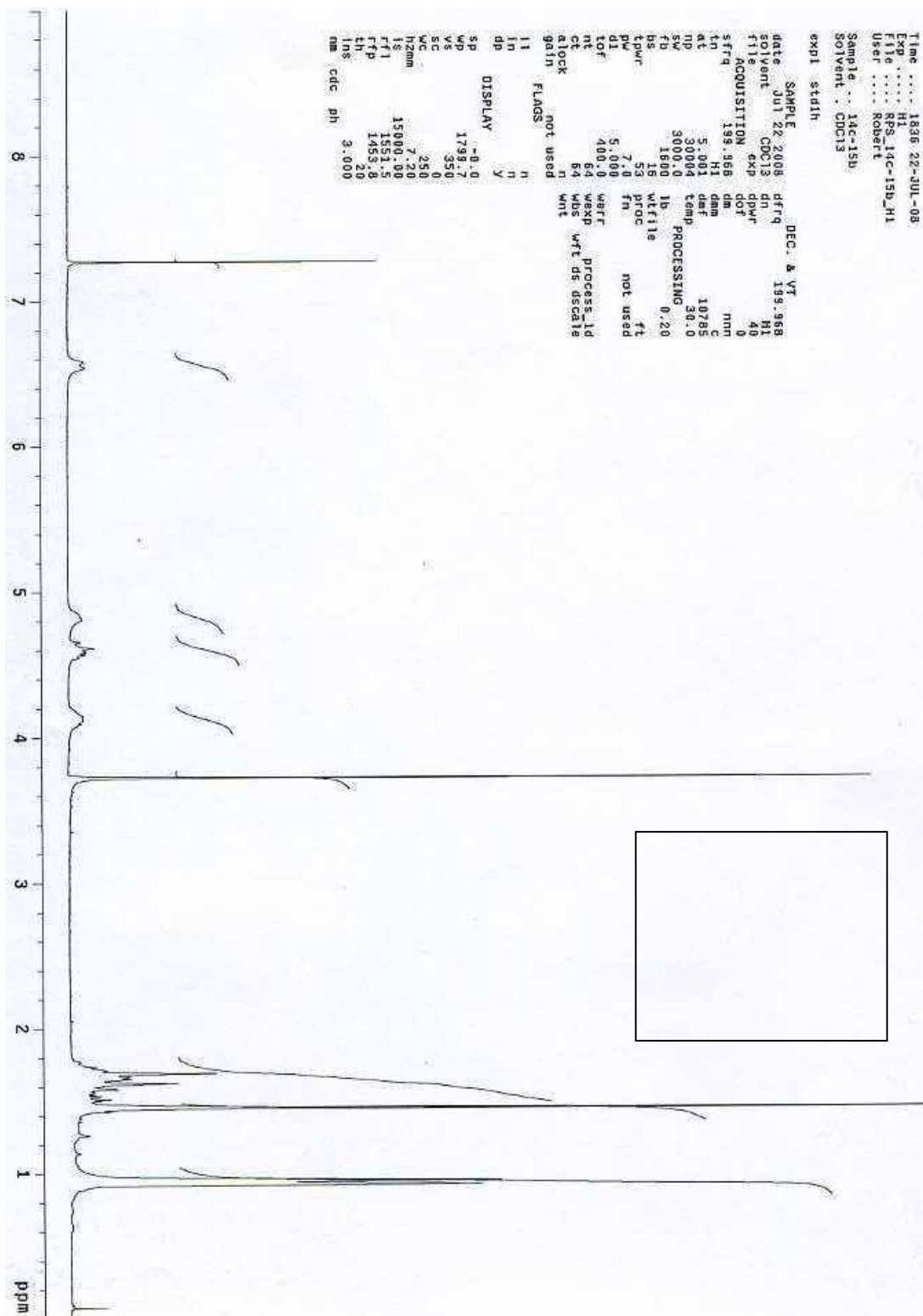
Compound 5 HPLC Cyclized Pentapeptide Phe-N-Me-Leu-D-Val-D-Leu-Leu



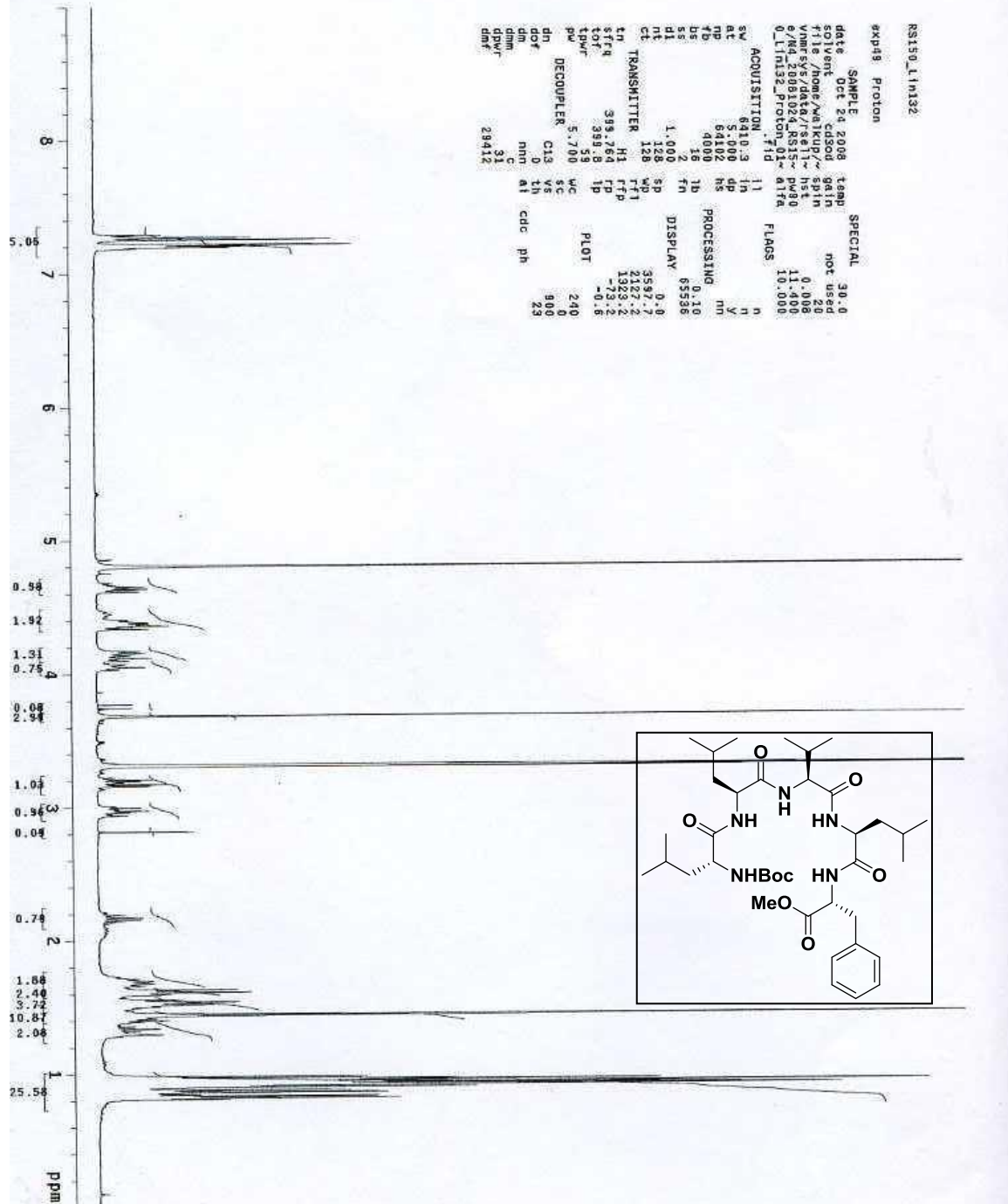
Compound 6 NMR Dipeptide MeO-D-Phe-Leu- NHBoc



Compound 6 NMR Tripeptide MeO-D-Phe-Leu-Val-NHBoc



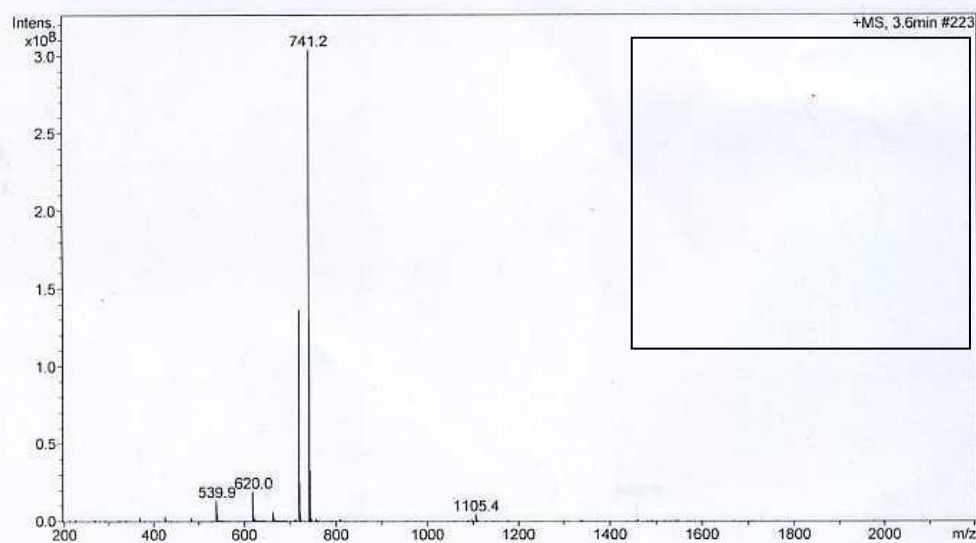
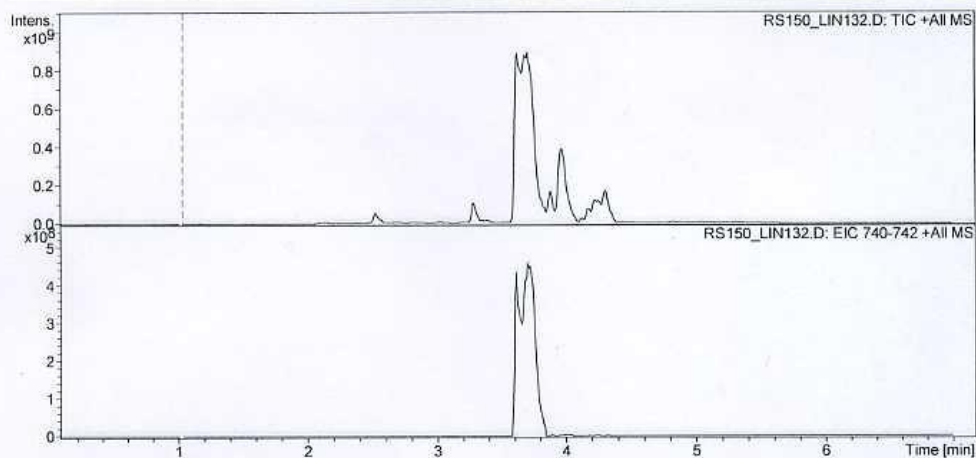
Compound 6 NMR Dipeptide MeO-Leu-D-Leu-NHBoc



Compound 6 NMR Linear Pentapeptide MeO-D-Phe-Leu-Val-Leu-D-Leu-NHBoc

Display Report - All Windows Selected Analysis

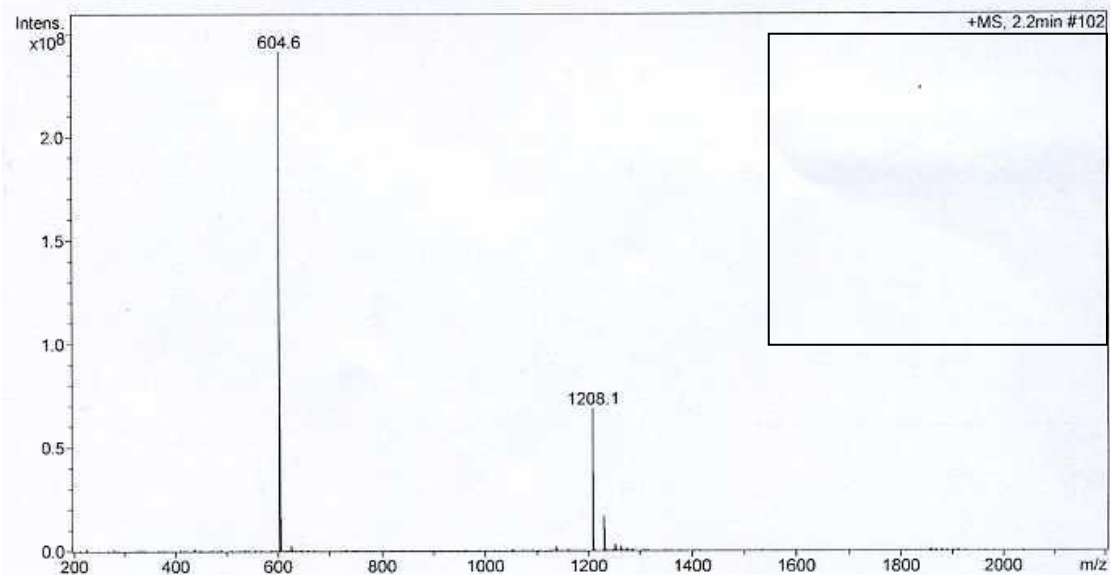
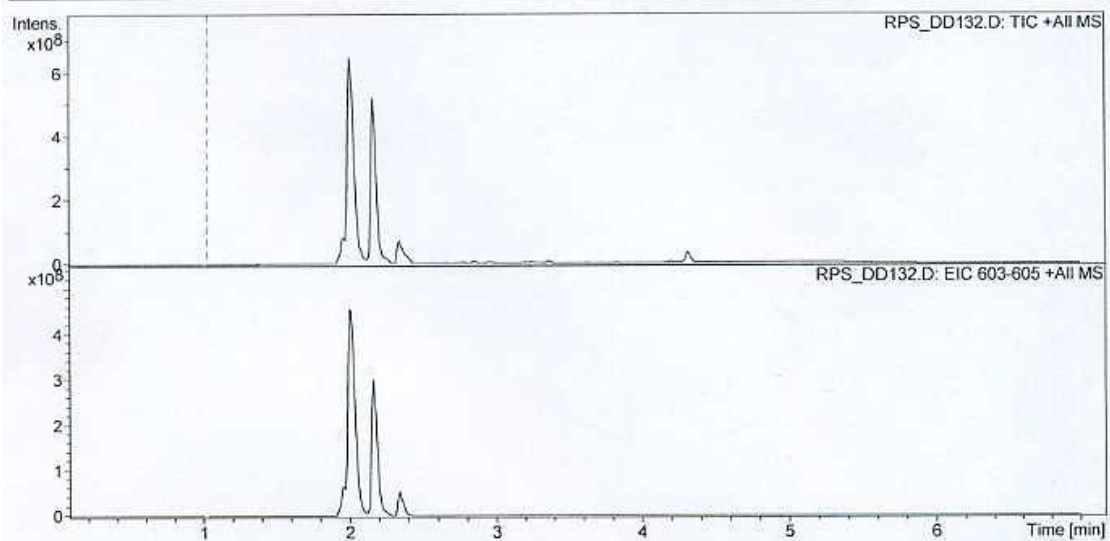
Analysis Name: RS150_LIN132.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 12/19/2008 2:47:40 PM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 10/24/2008 4:37:39 PM
Sample Name: RS150_Lin132
Analysis Info:



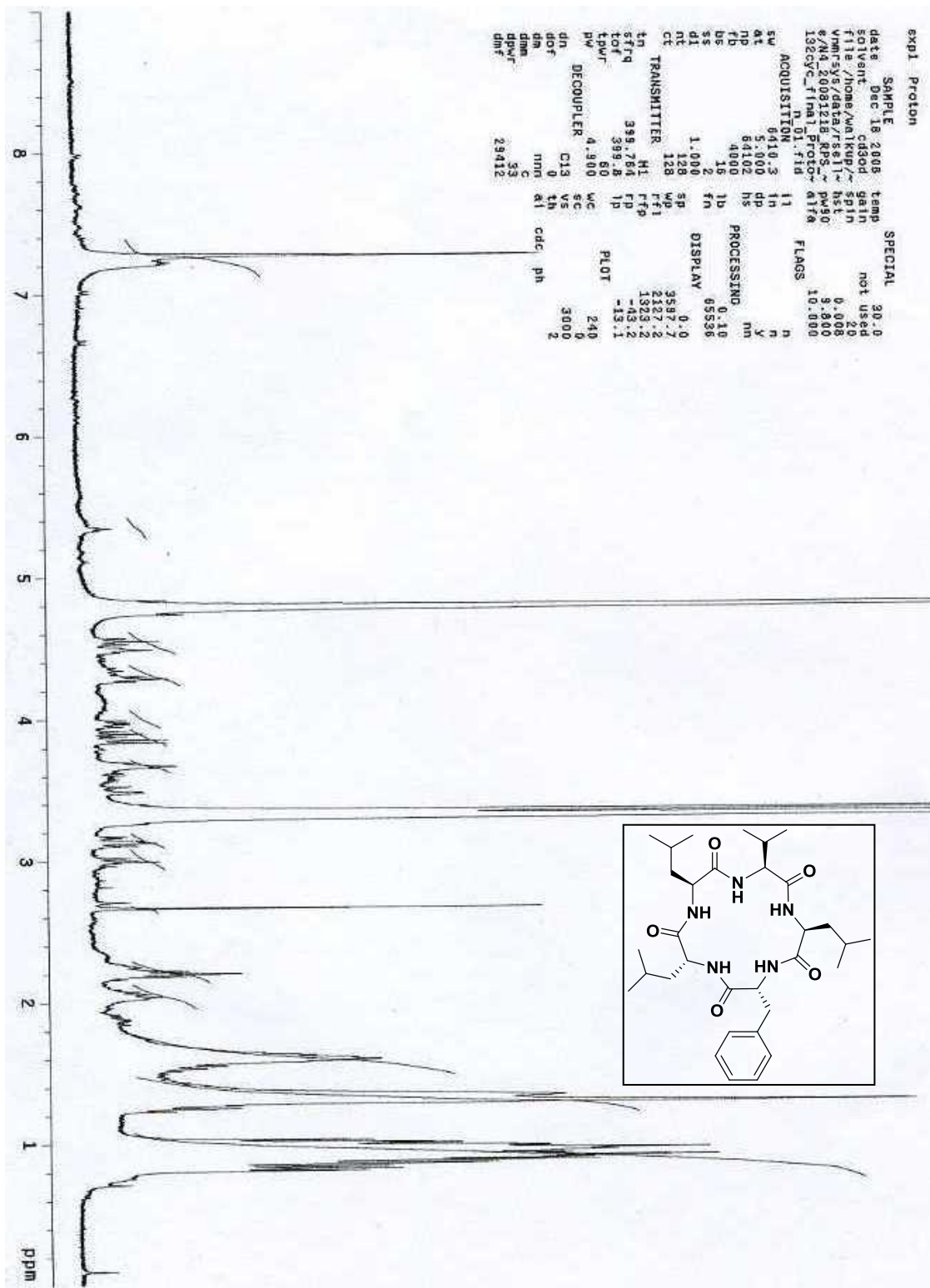
Compound 6 LCMS Linear Pentapeptide MeO-D-Phe-Leu-Val-Leu-D-Leu-NHBoc (MW = 717.9)

Display Report - All Windows Selected Analysis

Analysis Name: RPS_DD132.D Instrument: Agilent 6330 Ion Trap Print Date: 11/6/2008 3:44:40 AM
Method: SANA.M Operator: sdsu Acq. Date: 11/6/2008 2:46:26 AM
Sample Name: RPS_DD132
Analysis Info:



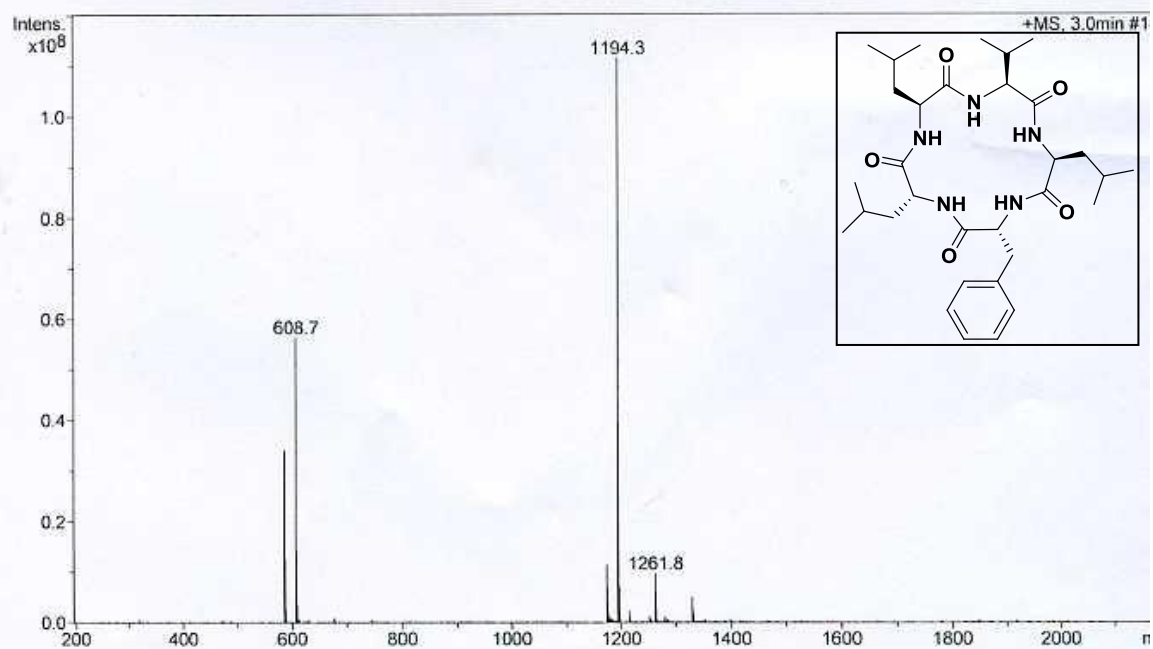
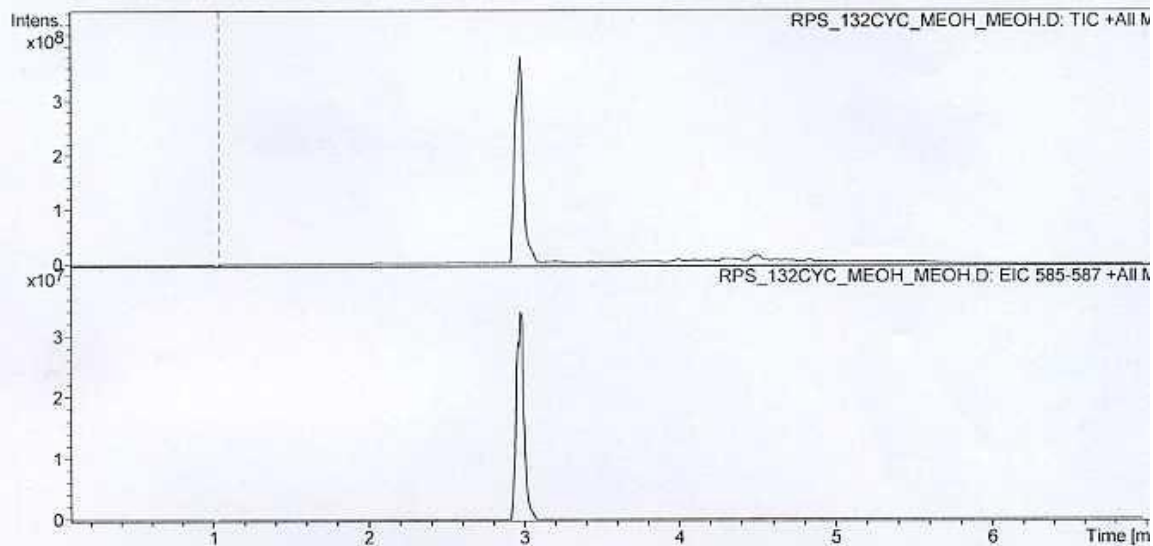
Compound 6 LCMS Double Deprotected Linear Pentapeptide HO-D-Phe-Leu-Val-Leu-D-Leu-NH₂ (MW = 603.8)



Compound 6 NMR Cyclized Pentapeptide D-Phe-Leu-Val-Leu-D-Leu

Display Report - All Windows Selected Analysis

Analysis Name: RPS_132CYC_ME **Instrument:** Agilent 6330 Ion Trap **Print Date:** 12/19/2008 1:30:49 PM
Method: SANA.M OH_MEOH.D **Operator:** sdsu **Acq. Date:** 12/18/2008 1:41:41 PM
Sample Name: RPS_132cyc_MeOH/MeOH
Analysis Info:



**Compound 6 LCMS Cyclized Pentapeptide D-Phe-Leu-Val-Leu-D-Leu
(MW = 585.8)**

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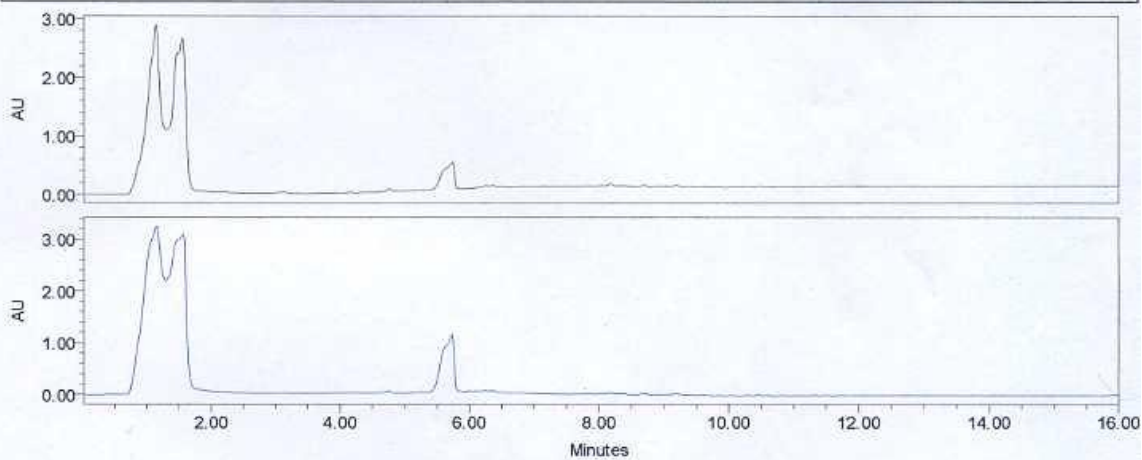
Project Name: Defaults

Reported by User: shelli

Breeze

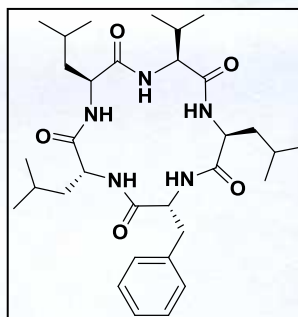
SAMPLE INFORMATION

Sample Name:	RFS_132	Acquired By:	shelli
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	PrimarySanA_SS_new
Injection #:	37	Date Acquired:	12/19/2008 4:28:05 AM
Run Time:	16.00 Minutes	Injection Volume:	100.00 ul

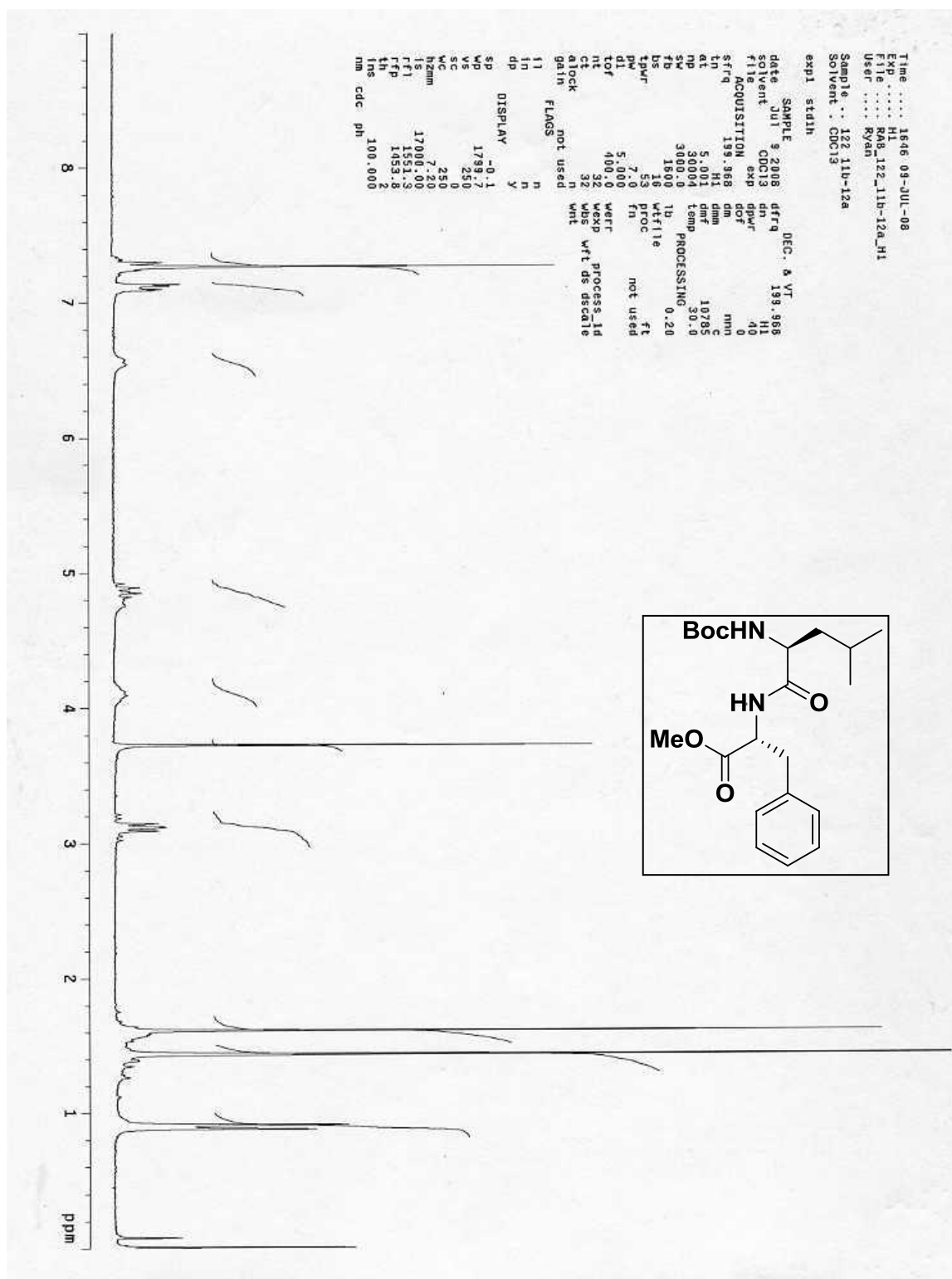


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 — Channel: 2487Channel 2 Channel Desc.: Processing Method: ****

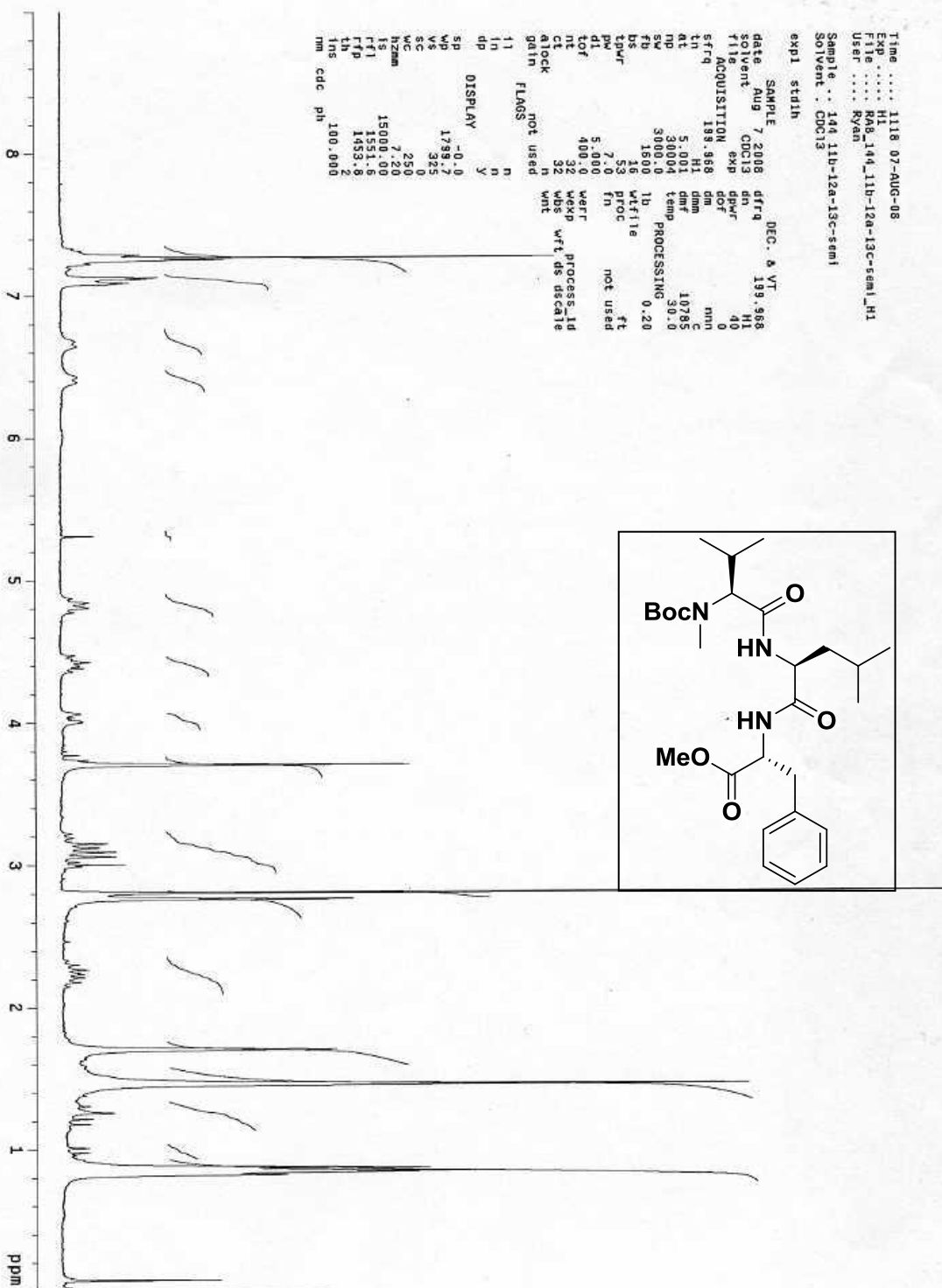
Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	Amount	Units
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2 ****	****	****	****	****	****	****



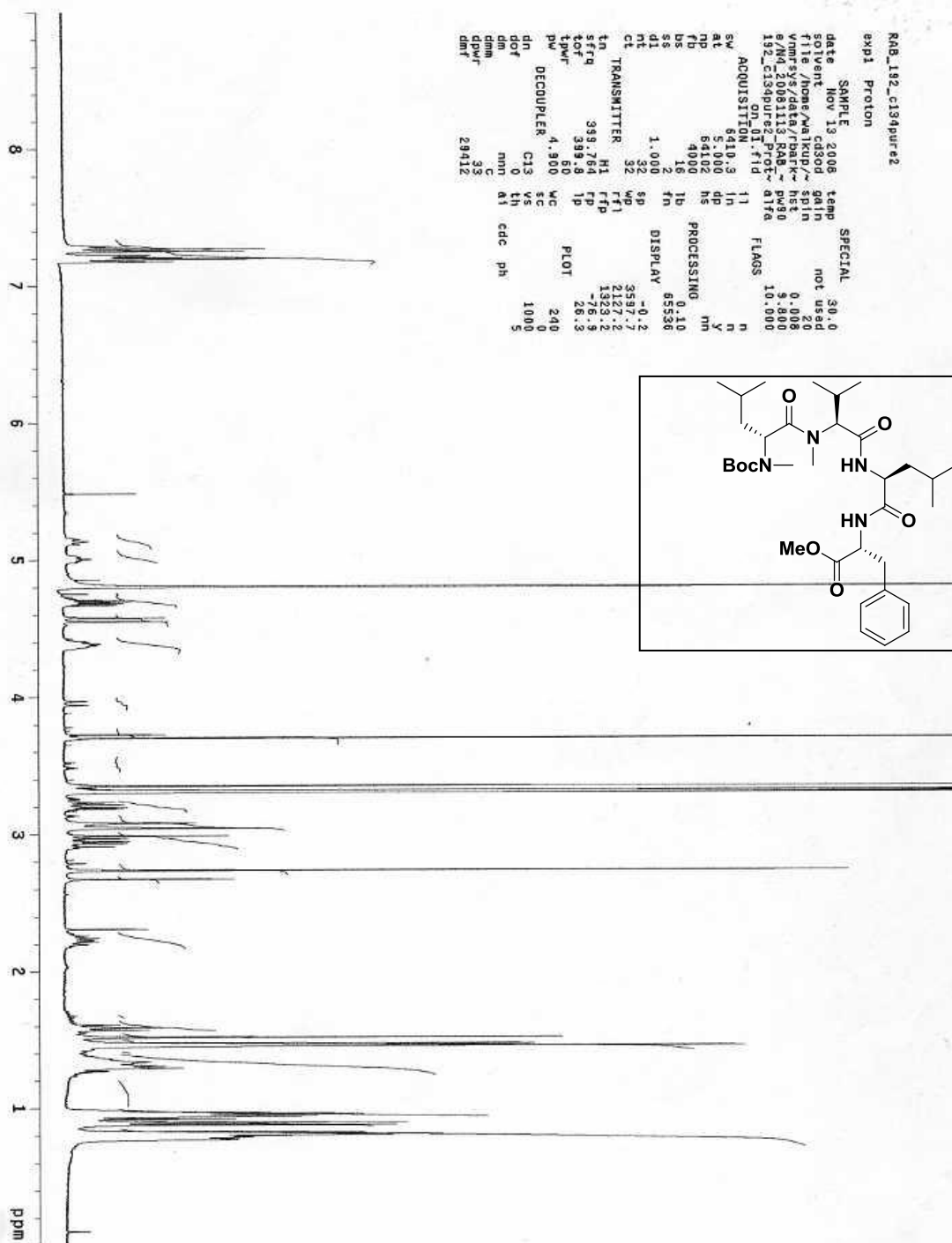
Compound 6 HPLC Cyclized Pentapeptide D-Phe-Leu-Val-Leu-D-Leu



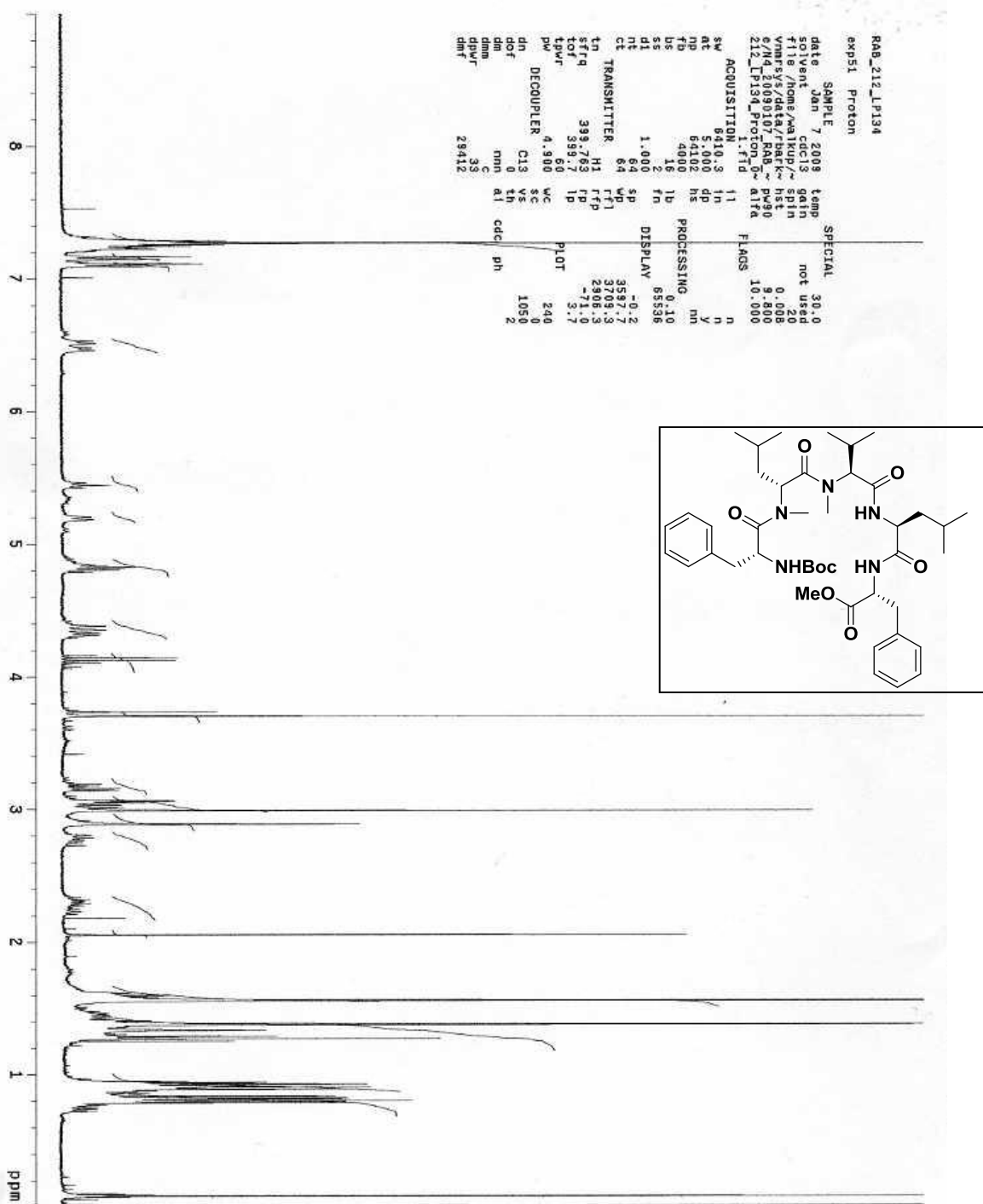
Compound 7 NMR Dipeptide MeO-D-Phe-Leu-NHBoc



Compound 7 NMR Tripeptide MeO-D-Phe-Leu-N-Me-Val-Boc



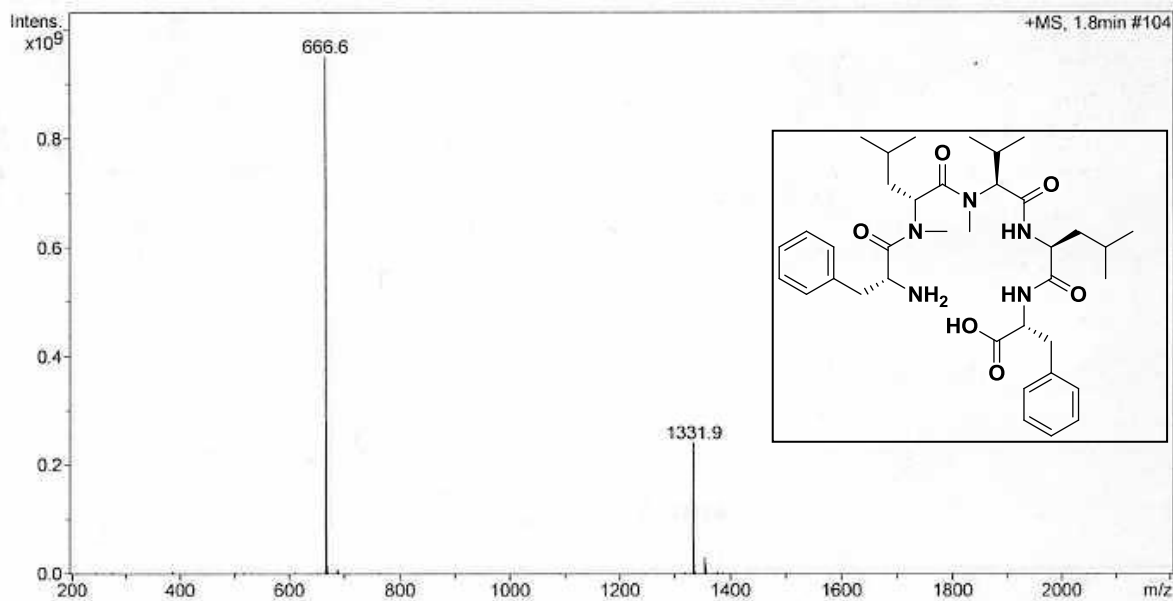
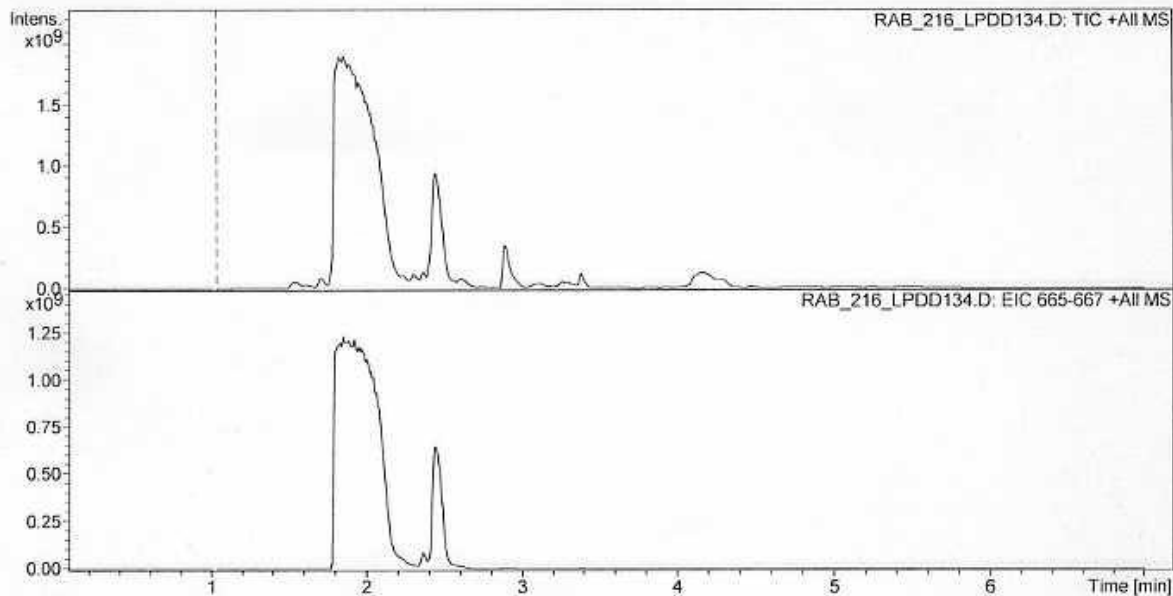
Compound 7 NMR Tetrapeptide MeO-D-Phe-Leu-N-Me-Val-N-Me-D-Leu-NBoc



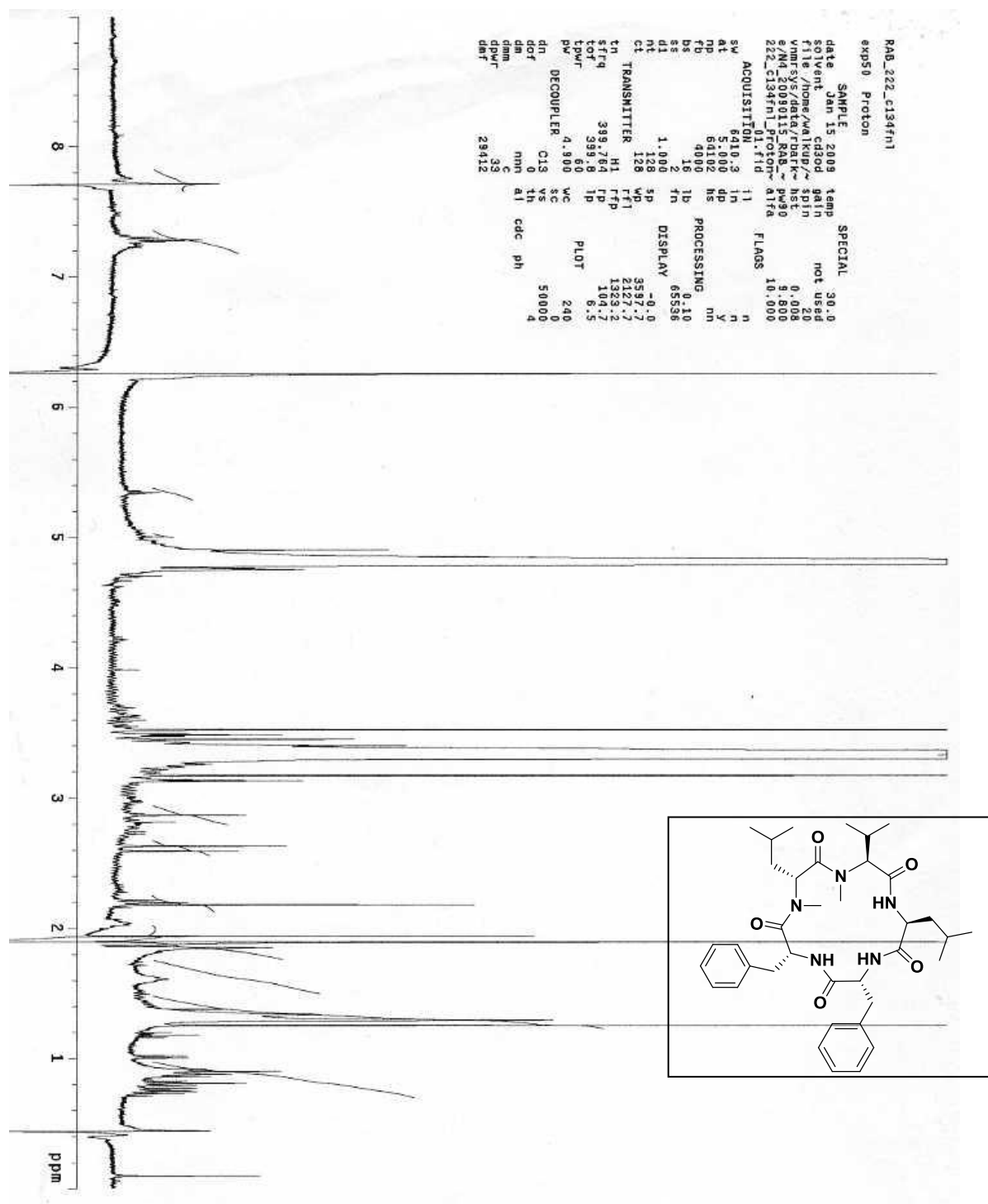
Compound 7 NMR Linear Pentapeptide MeO-D-Phe-Leu-N-Me-Val-N-Me-D-Leu-D-Phe-NHBoc

Display Report - All Windows Selected Analysis

Analysis Name: RAB_216_LPDD1 **Instrument:** Agilent 6330 Ion Trap **Print Date:** 1/12/2009 12:28:42 PM
Method: SANA.M 34.D **Operator:** sdsu **Acq. Date:** 1/12/2009 11:54:32 AM
Sample Name: RAB_216_LPdd134
Analysis Info:



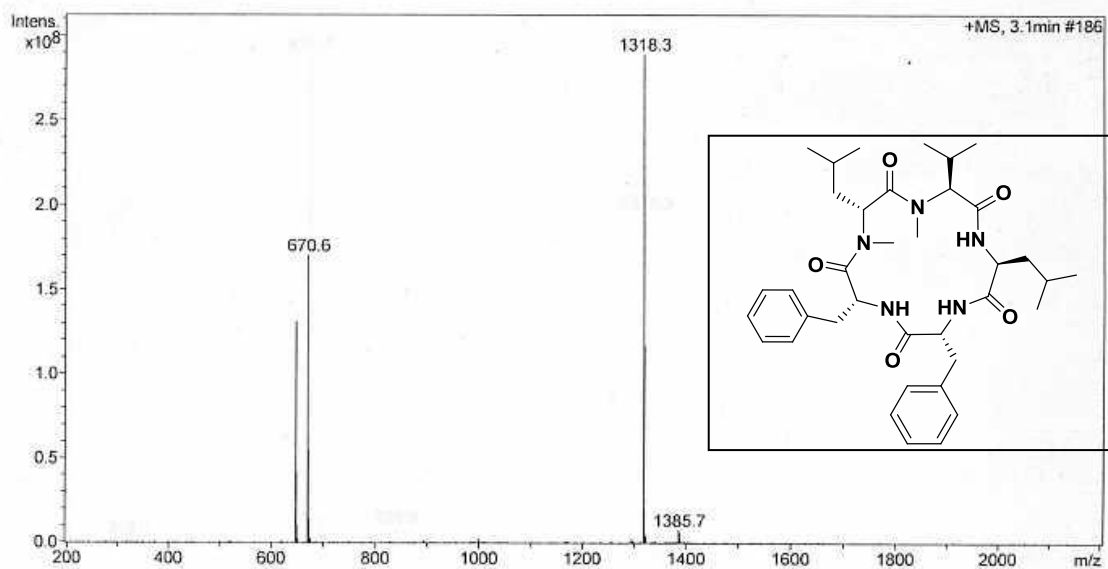
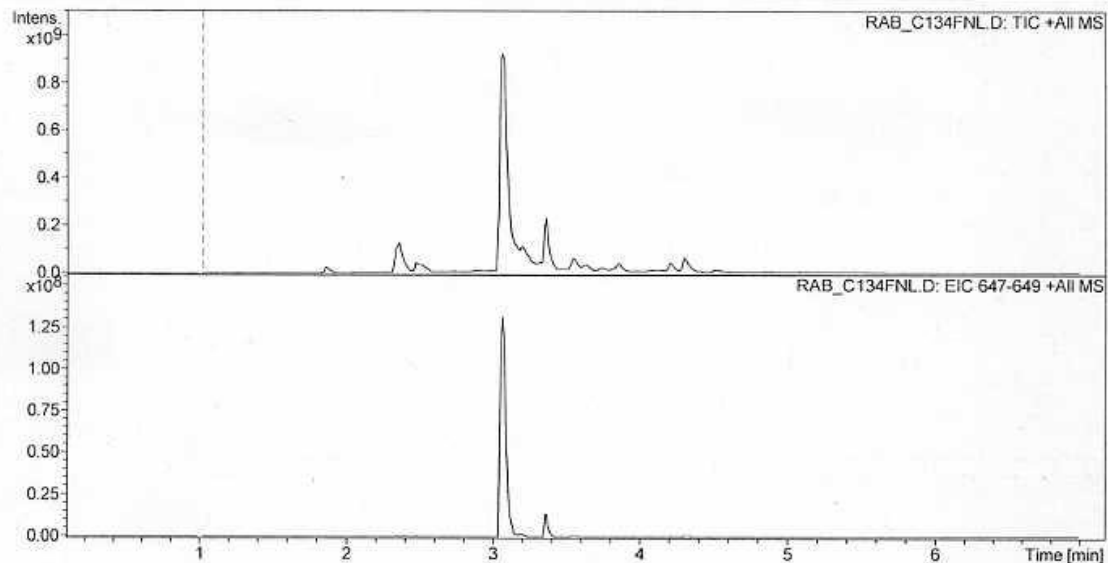
Compound 7 LCMS Double Deprotected Pentapeptide HO-D-Phe-Leu-N-Me-Val-N-Me-D-Leu-D-Phe-NH₂ (MW=665.86)



Compound 7 NMR Cyclized Pentapeptide D-Phe-Leu-N-Me-Val-N-Me-D-Leu-D-Phe

Display Report - All Windows Selected Analysis

Analysis Name: RAB_C134FNL.D Instrument: Agilent 6330 Ion Trap Print Date: 1/15/2009 2:18:22 PM
Method: SANA.M Operator: sdsu Acq. Date: 1/15/2009 2:09:31 PM
Sample Name: RAB_c134fni
Analysis Info:



Compound 7 LCMS Cyclized Pentapeptide D-Phe-Leu-N-Me-Val-N-Me-D-Leu-D-Phe (MW=647.8)

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Project Name: Defaults

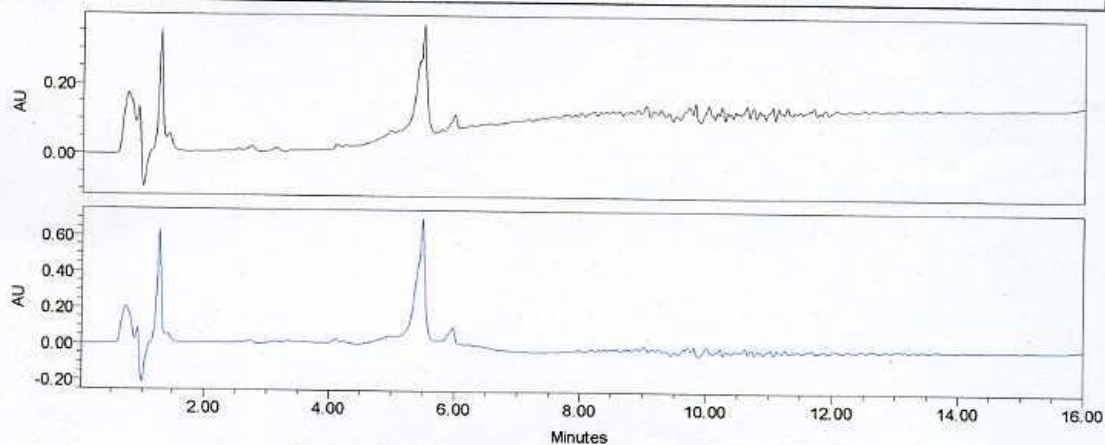
Reported by User: shelli

Breeze

SAMPLE INFORMATION

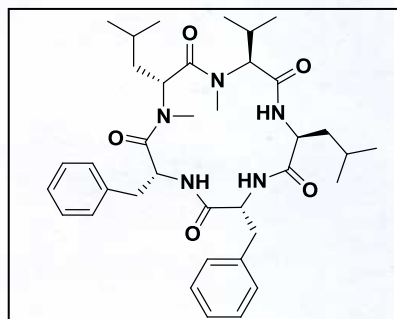
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 Sample Type: Unknown
 Vial: 1
 Injection #: 5
 Run Time: 16.00 Minutes

Acquired By: shelli
 Sample Set Name:
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 Date Acquired: 1/16/2009 12:51:27 AM
 Injection Volume: 50.00 ul

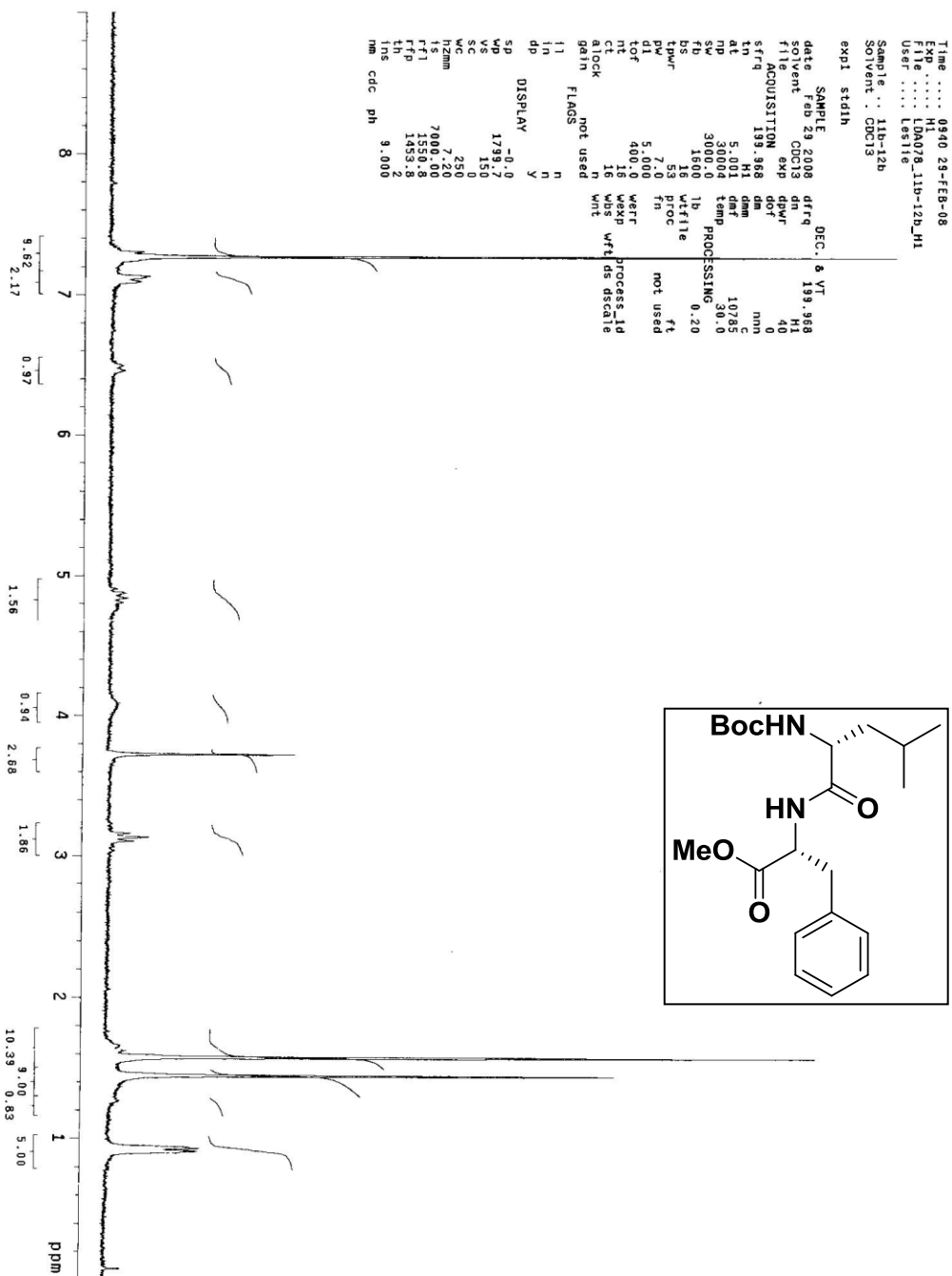


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 — Channel: 2487Channel 2 Channel Desc.: Processing Method: ****

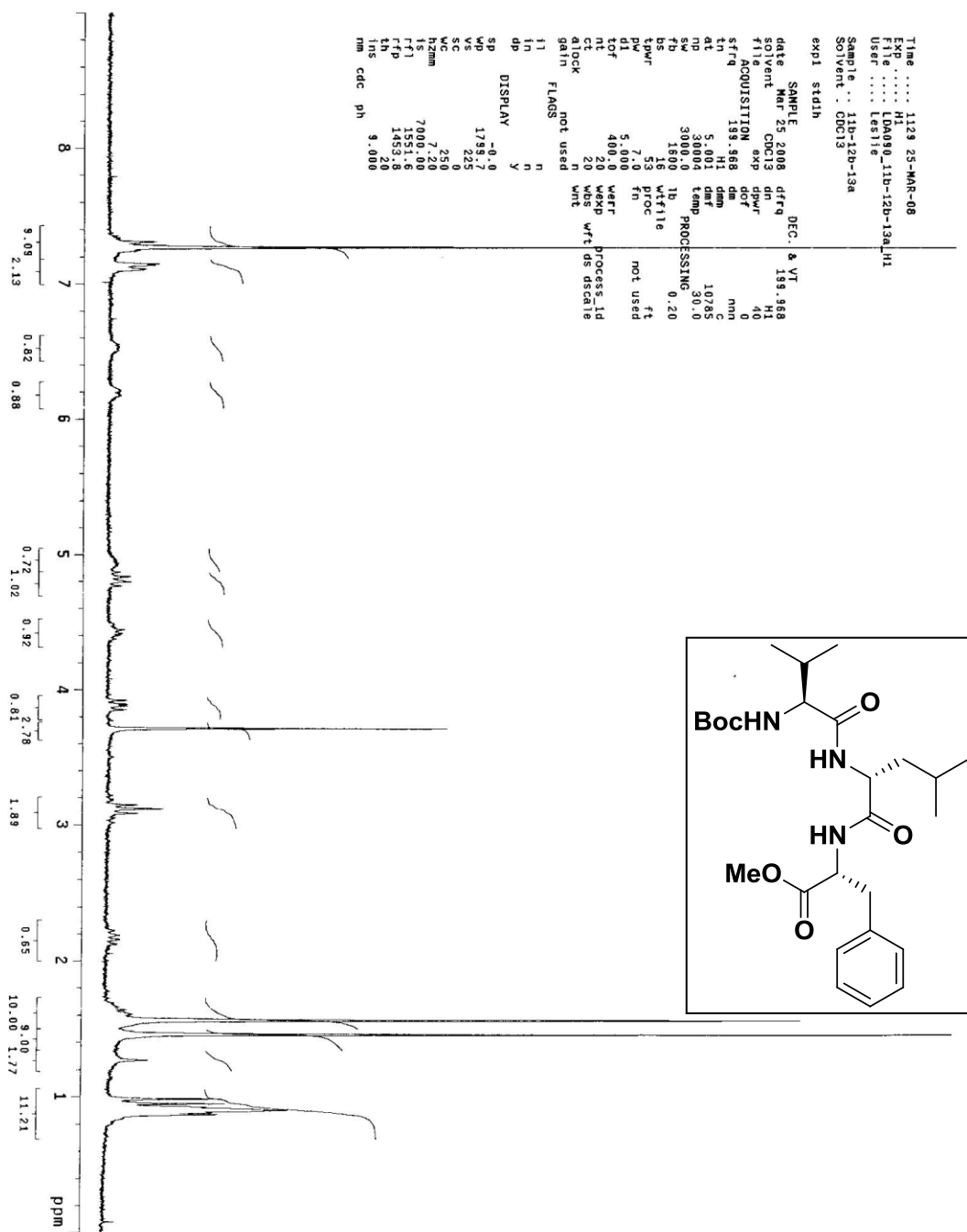
Peak Name	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	Amount	Units
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2	****	****	****	****	****	****



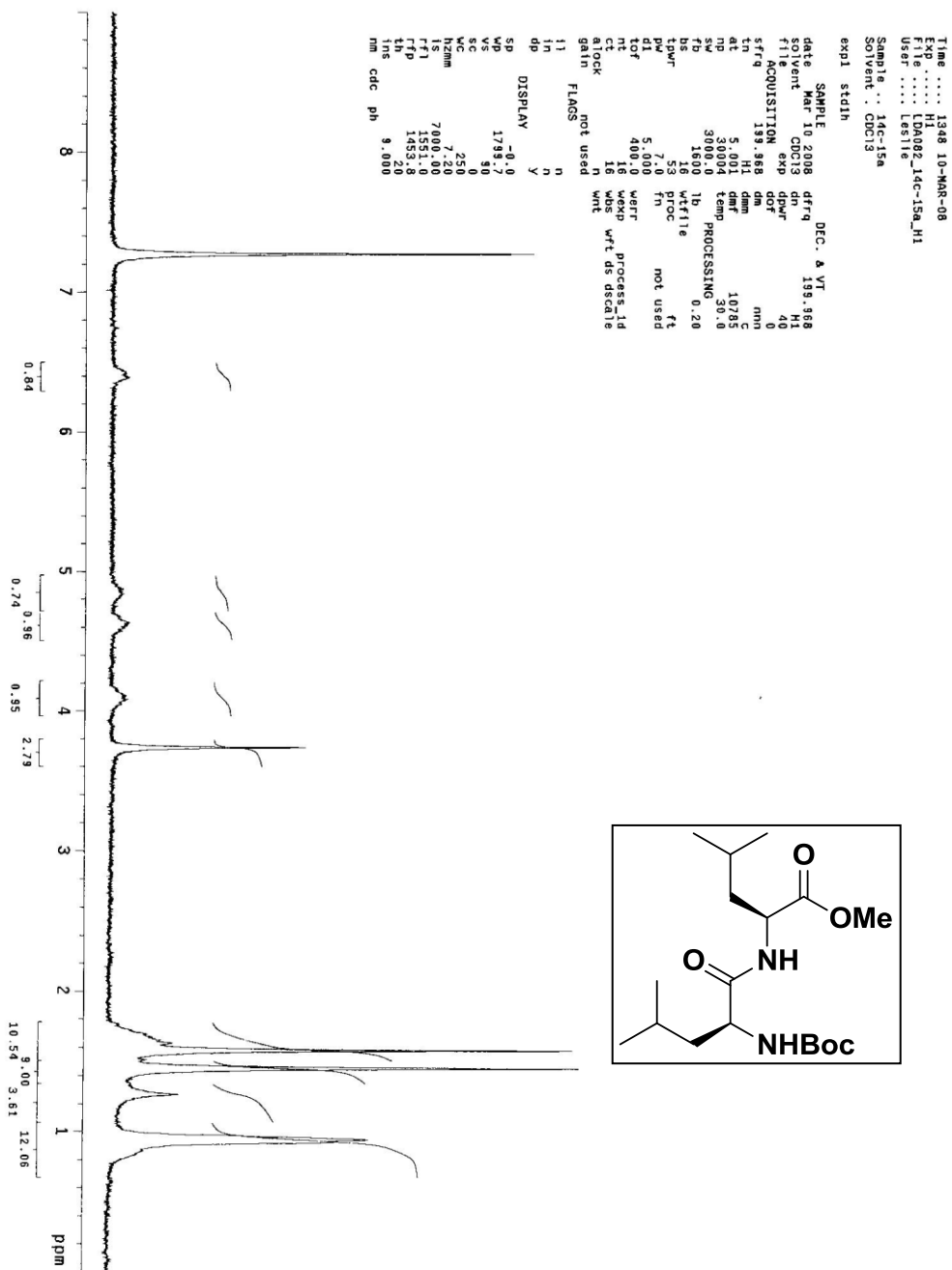
Compound 7 HPLC Cyclized Pentapeptide D-Phe-Leu-N-Me-Val-N-Me-D-Leu-D-Phe



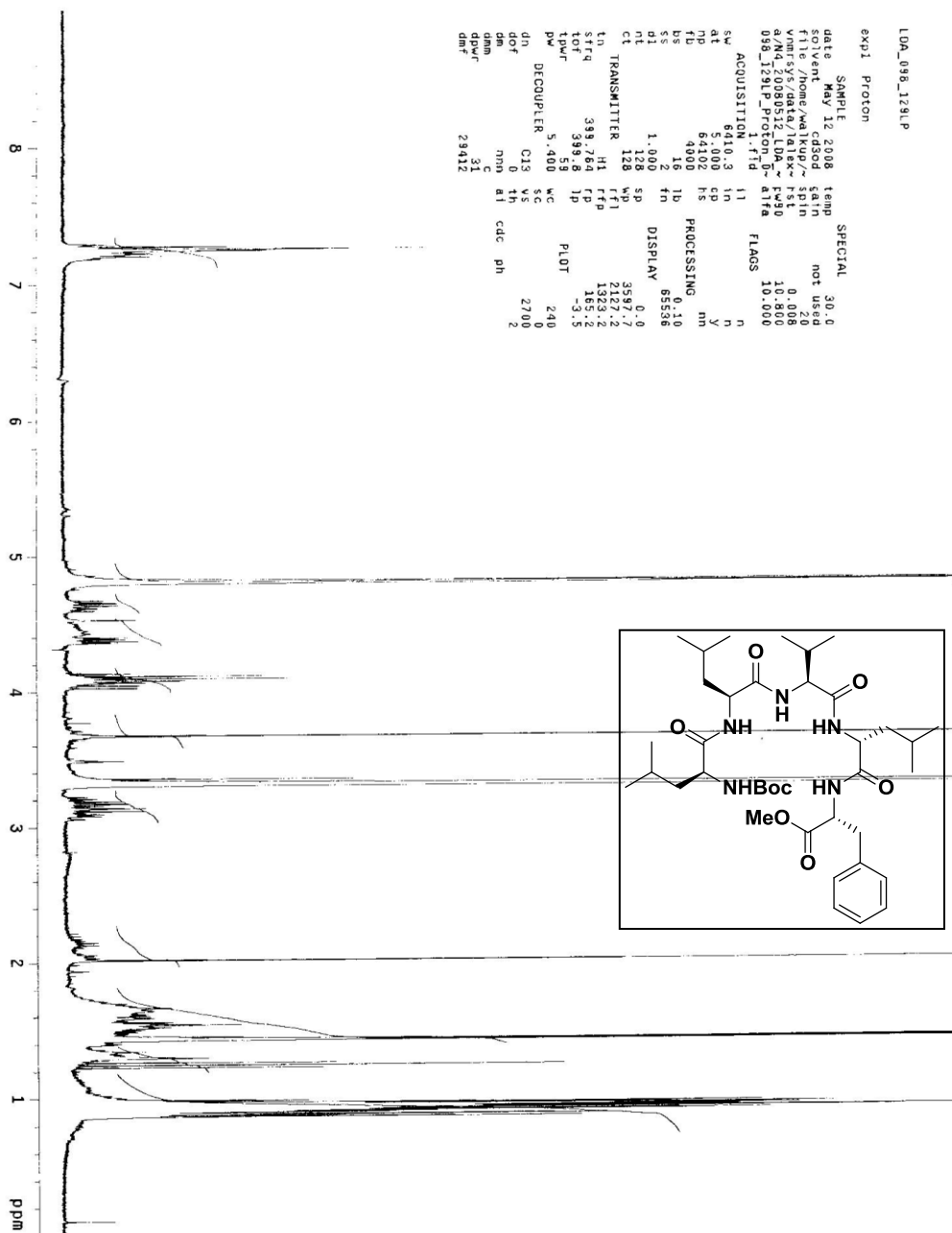
Compound 10 NMR Dipeptide MeO-D-Phe-D-Leu-NHBoc



Compound 10 NMR Tripeptide MeO-D-Phe-D-Leu-Val-NHBoc



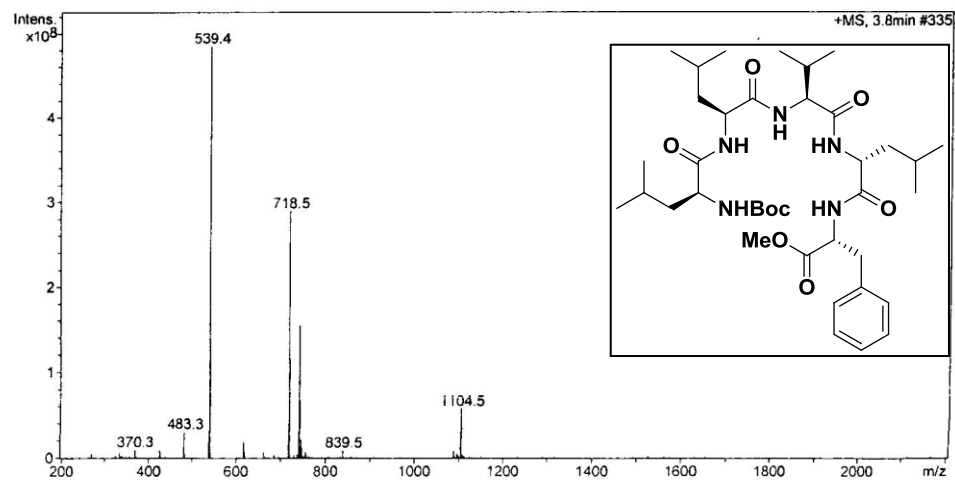
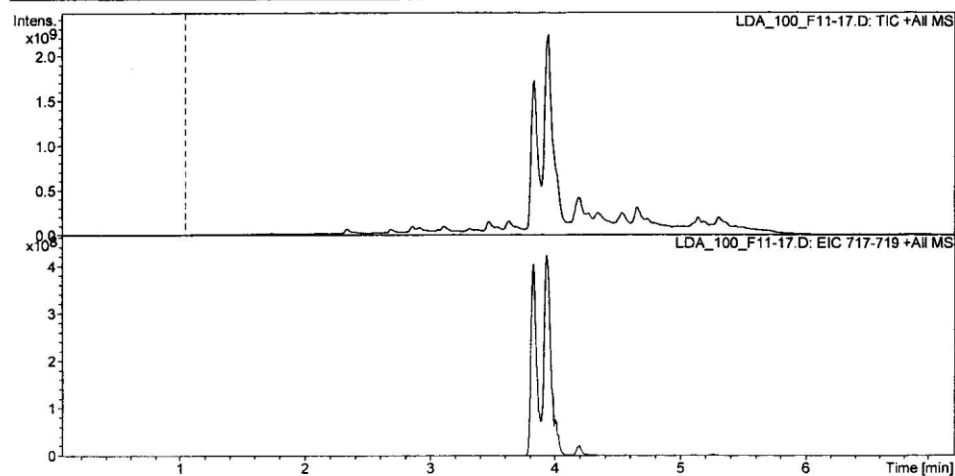
Compound 10 NMR Dipeptide MeO-Leu-Leu-NHBoc



Compound 10 NMR Linear Pentapeptide MeO-D-Phe-D-Leu-Val-Leu-Leu-NHBoc

Display Report - All Windows Selected Analysis

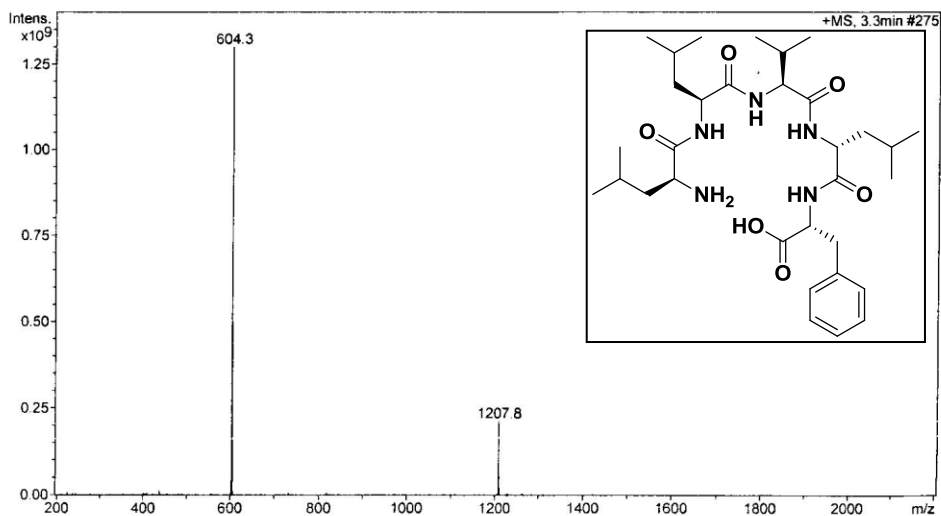
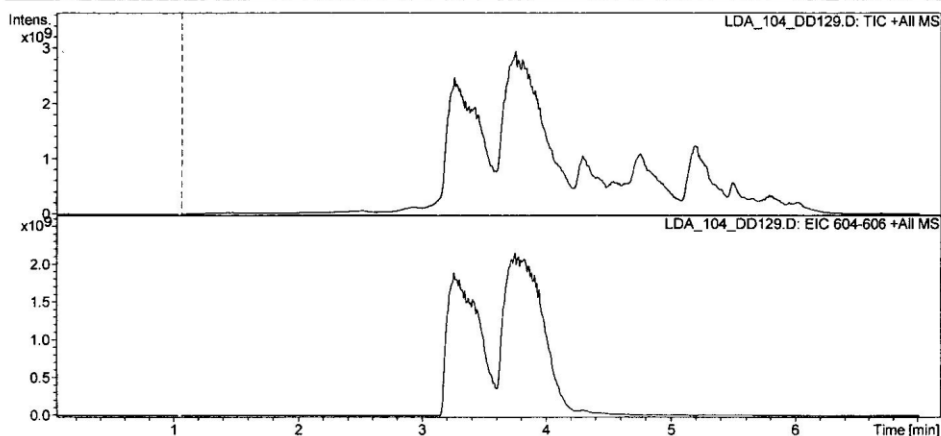
Analysis Name: LDA_100_F11-17 **Instrument:** Agilent 6330 Ion Trap **Print Date:** 5/12/2008 1:28:07 PM
Method: SANA.M.D **Operator:** sdsu **Acq. Date:** 5/12/2008 12:08:15 PM
Sample Name: LDA_100_f11-17
Analysis Info:



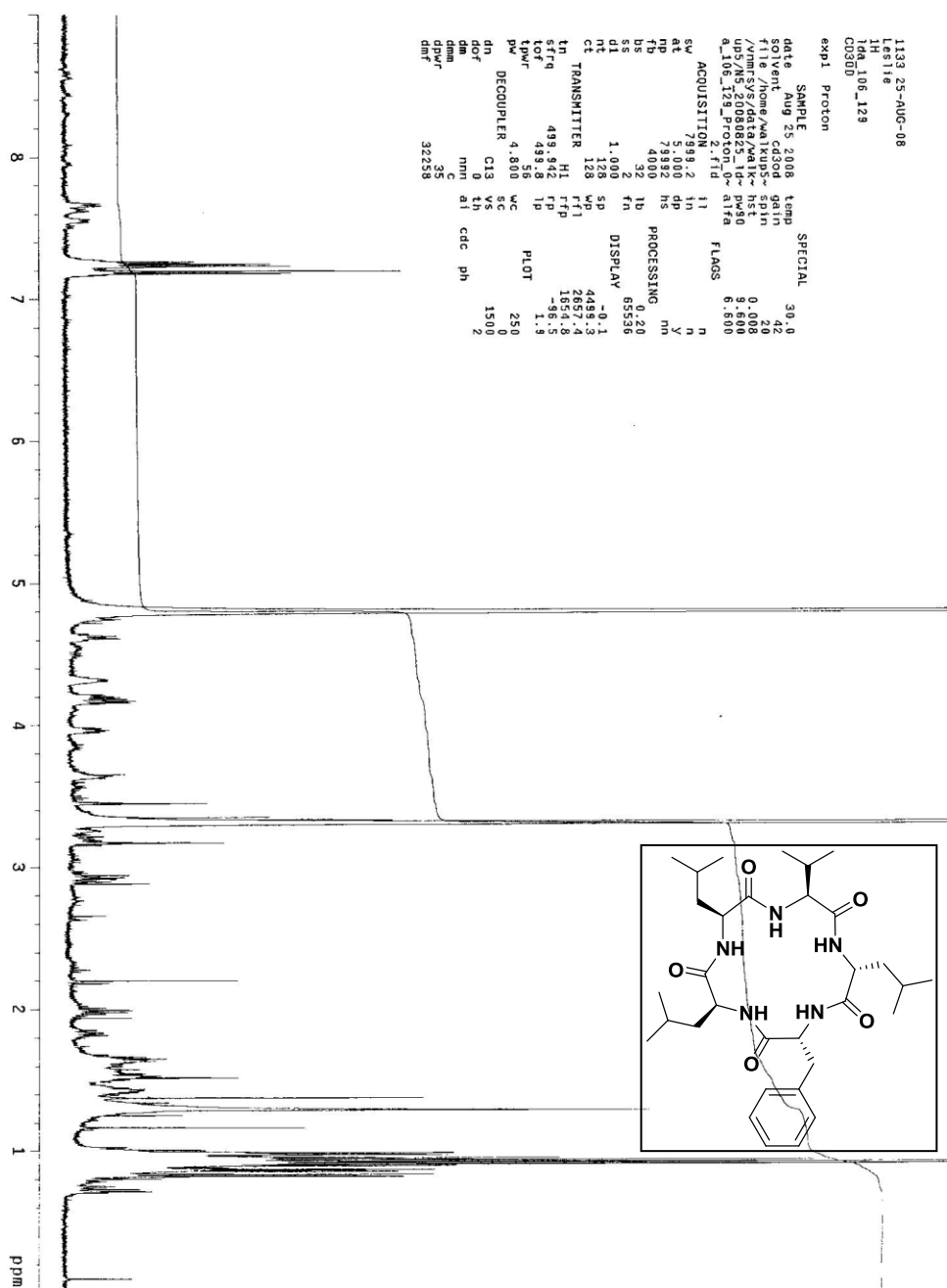
Compound 10 LCMS Linear Pentapeptide MeO-D-Phe-D-Leu-Val-Leu-Leu-NHBoc (MW=718)

Display Report - All Windows Selected Analysis

Analysis Name: LDA_104_DD129 **Instrument:** Agilent 6330 Ion Trap **Print Date:** 5/16/2008 12:17:03 PM
Method: SANA.M .D **Operator:** sdsu **Acq. Date:** 5/16/2008 12:08:41 PM
Sample Name: LDA_104_DD129
Analysis Info:



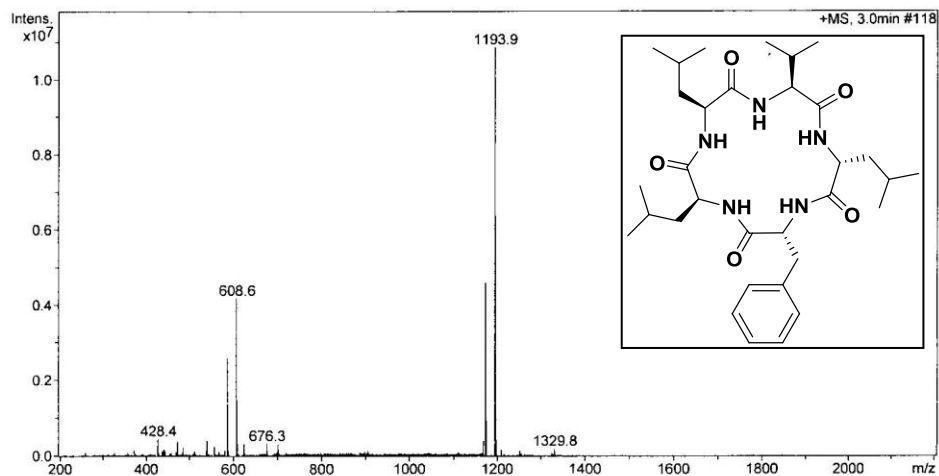
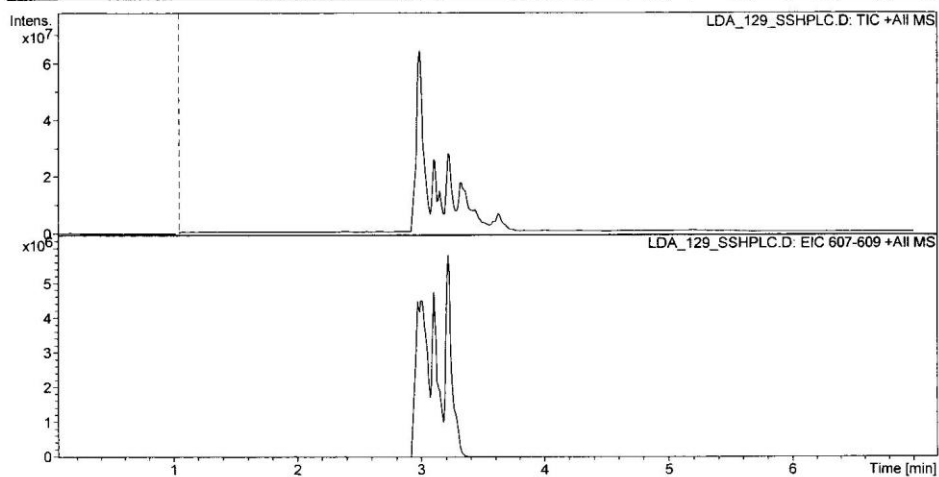
Compound 10 LCMS Double Deprotected Linear Pentapeptide HO-D-Phe-D-Leu-Val-Leu-Leu-NH₂ (MW=604)



Compound 10 NMR Cyclized Pentapeptide D-Phe-D-Leu-Val-Leu-Leu

Display Report - All Windows Selected Analysis

Analysis Name: LDA_129_SSHPL **Instrument:** Agilent 6330 Ion Trap **Print Date:** 9/2/2008 3:50:08 PM
Method: SANA.M C.D **Operator:** sdsu **Acq. Date:** 8/8/2008 10:58:40 AM
Sample Name: LDA_129_sshplc
Analysis Info:



Compound 10 LCMS Cyclized Pentapeptide D-Phe-D-Leu-Val-Leu-Leu (MW=586)

San Diego State University; Department of Chemis

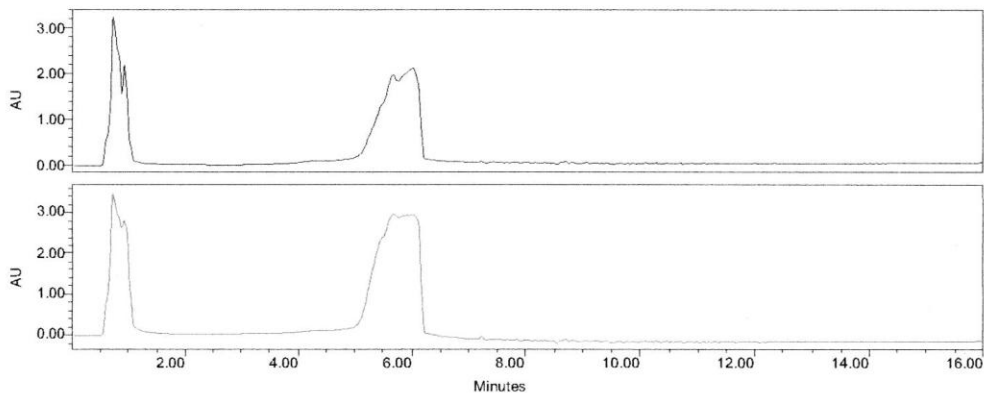
Project Name: Defaults

Reported by User: shelli

Breeze

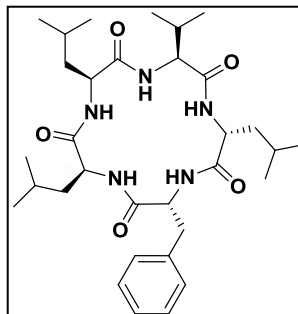
SAMPLE INFORMATION

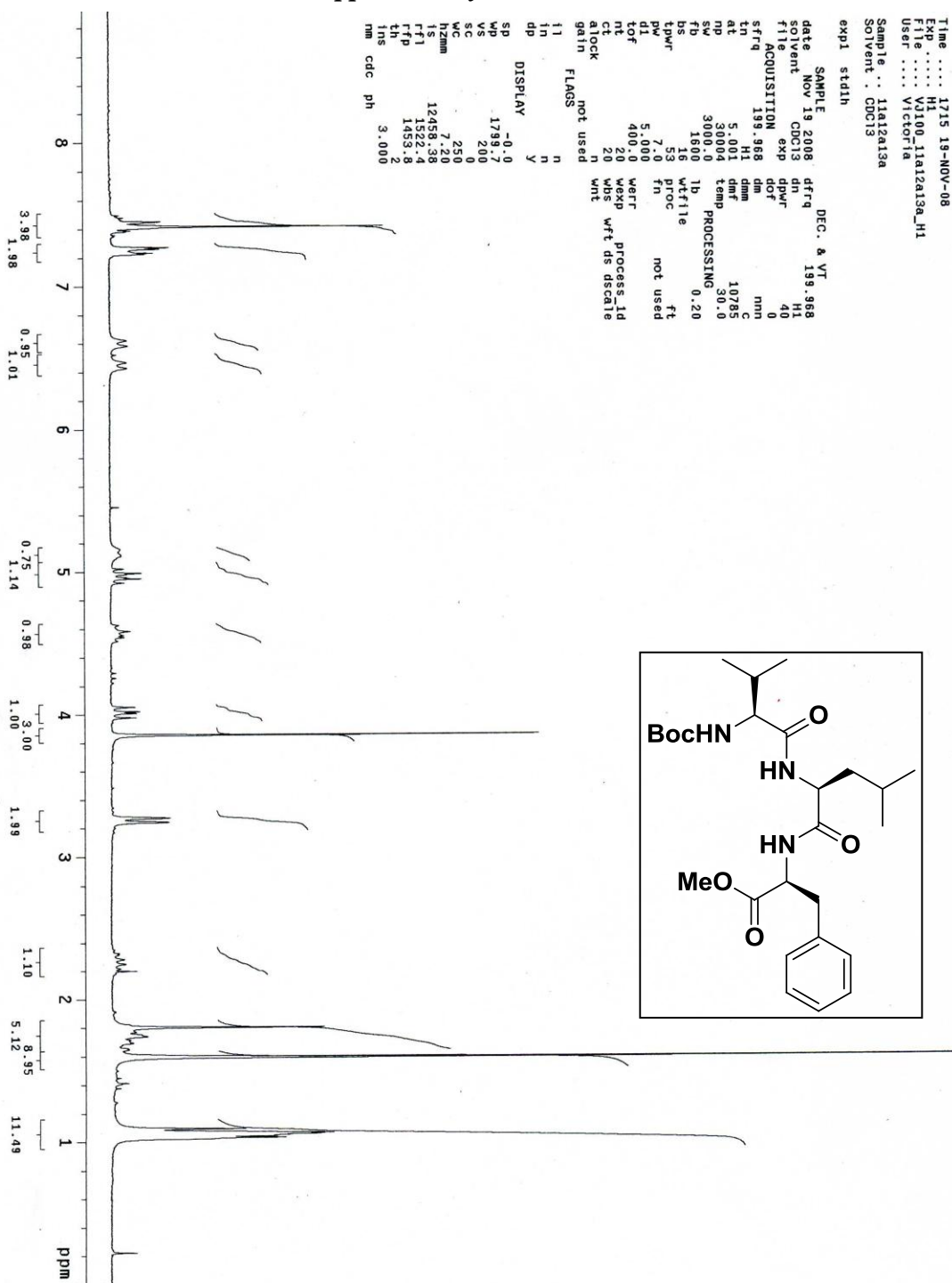
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Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	PrimarySanA_SS_new
Injection #:	5	Date Acquired:	8/6/2008 2:27:33 PM
Run Time:	16.00 Minutes	Injection Volume:	100.00 ul



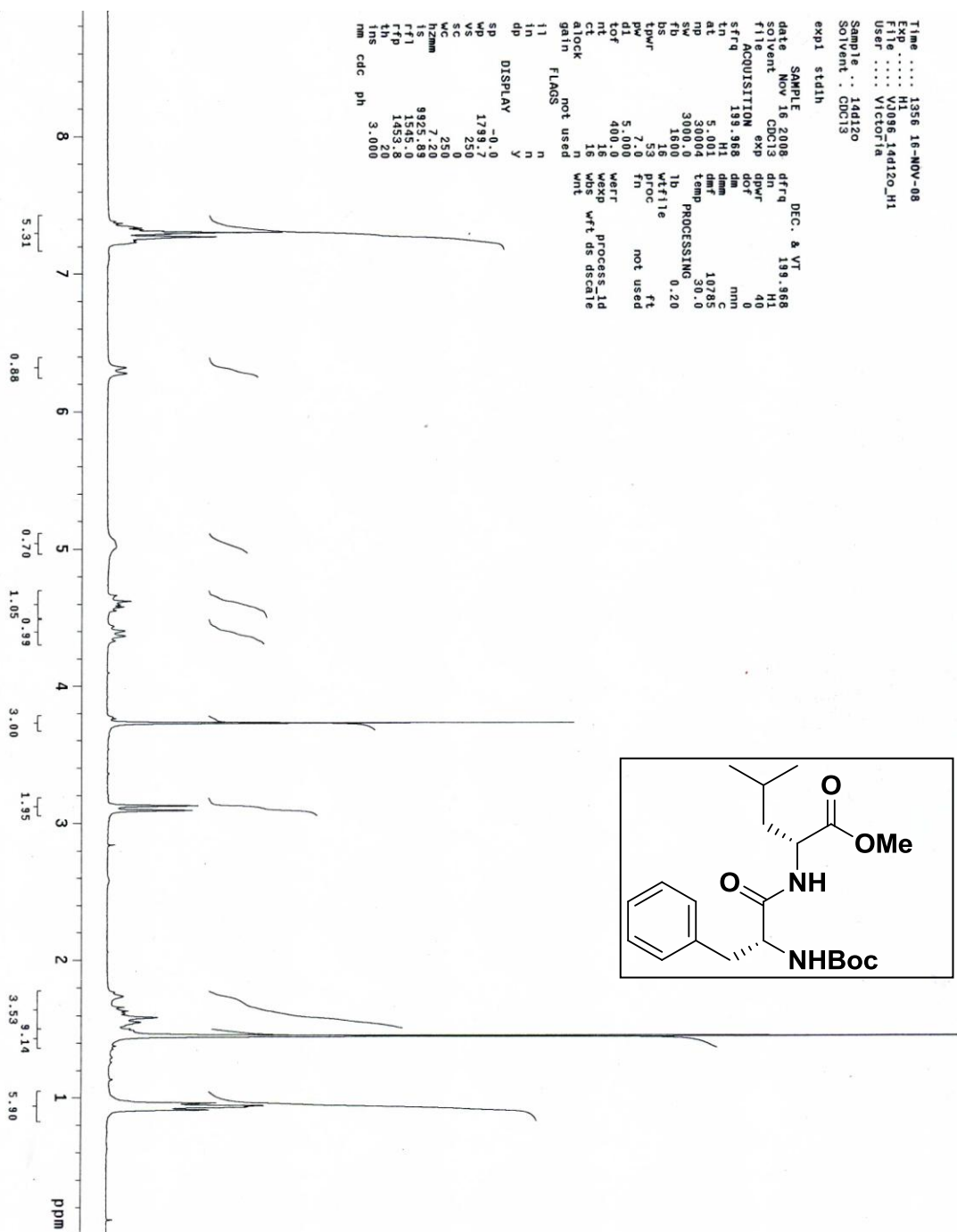
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 Channel: 2487Channel 2 Channel Desc.: Processing Method: *

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

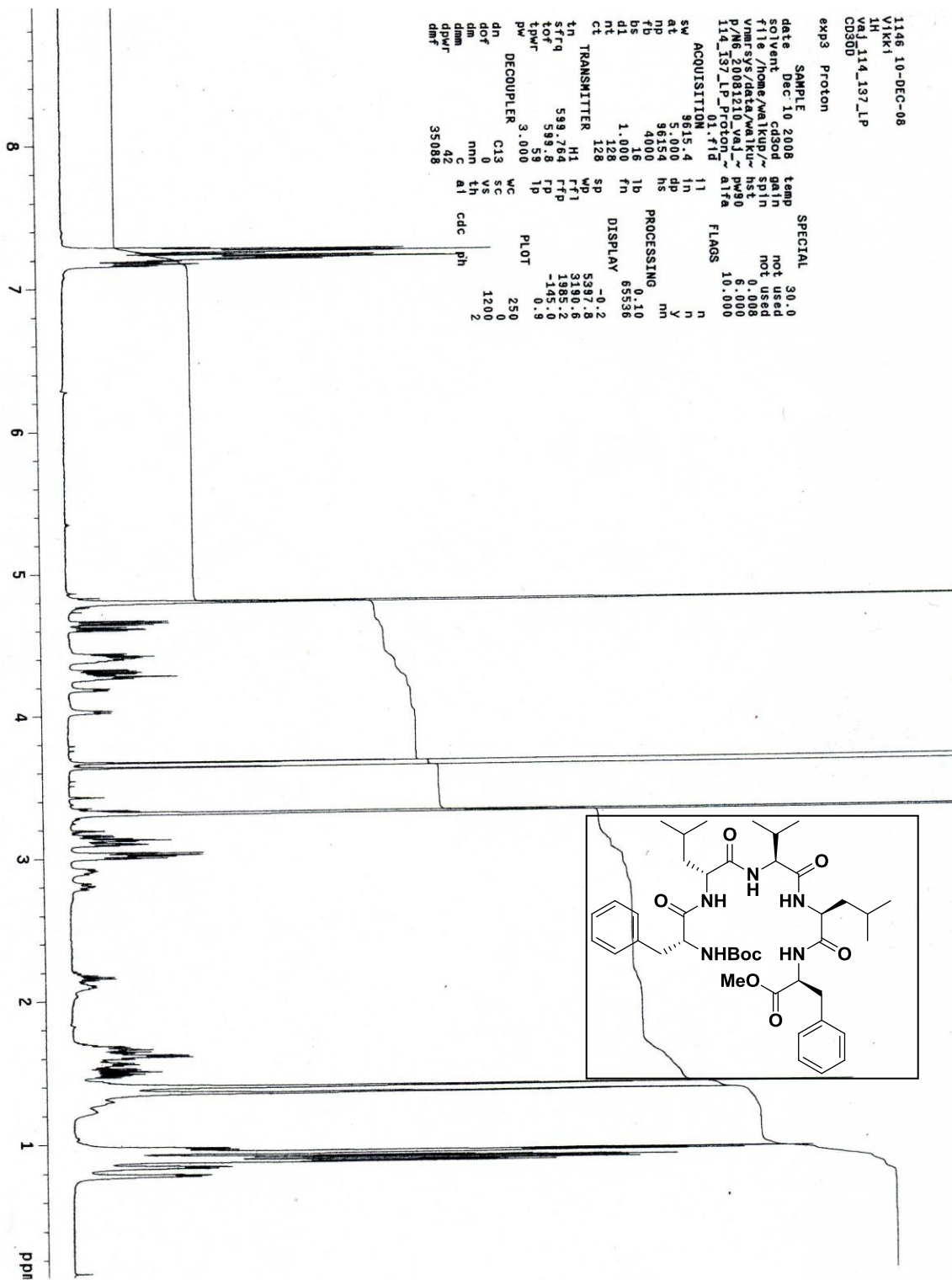




Compound 12 NMR Tripeptide MeO-Phe-Leu-Val-NHBoc



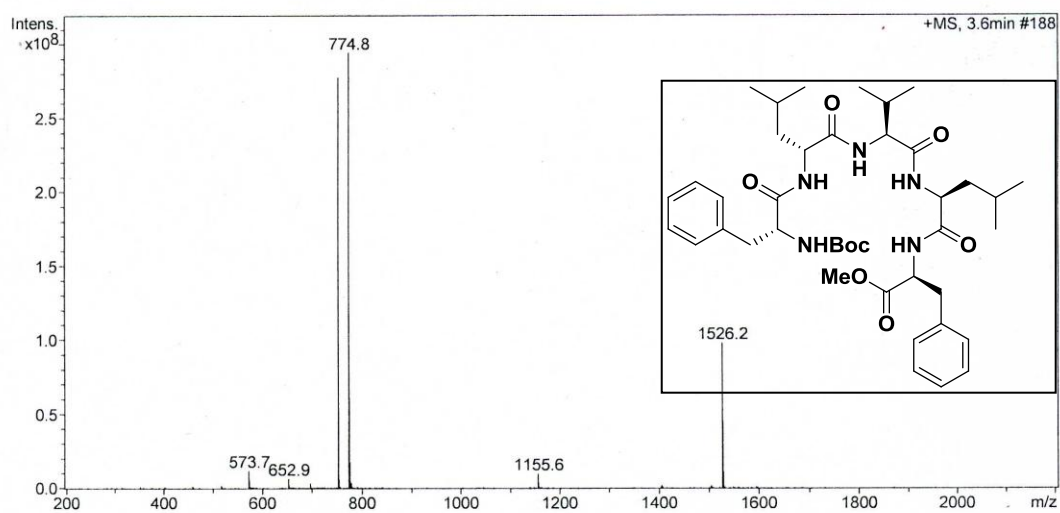
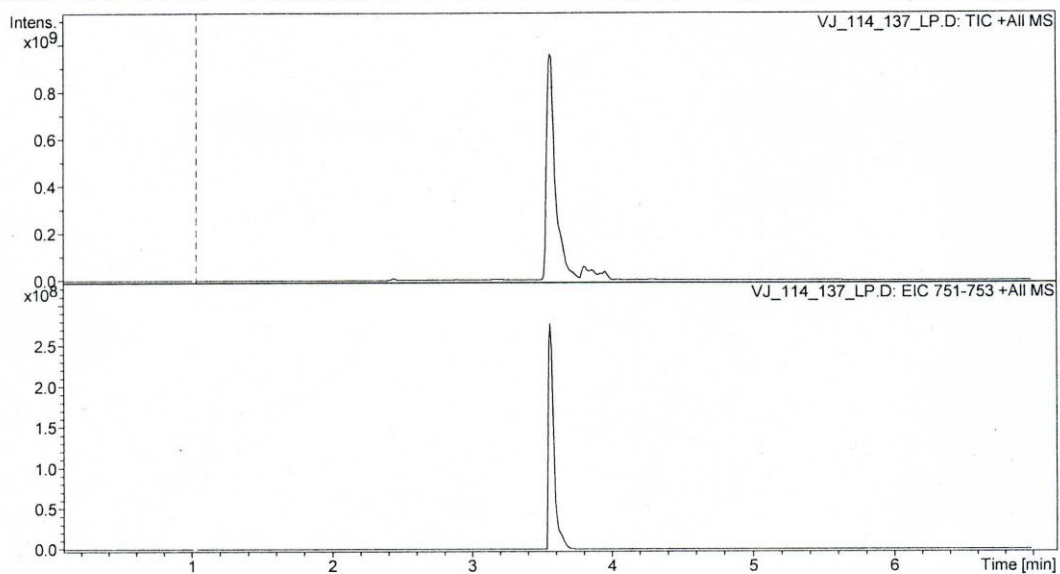
Compound 12 NMR Dipeptide MeO-D-Leu-D-Phe-NHBoc



Compound 12 NMR Linear Pentapeptide MeO-Phe-Leu-Val-D-Leu-D-Phe-NHBoc

Display Report - All Windows Selected Analysis

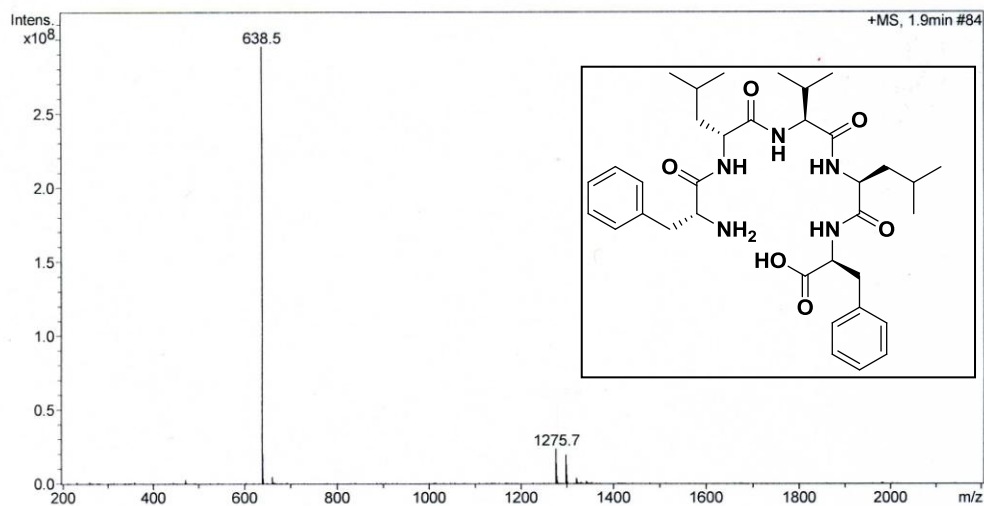
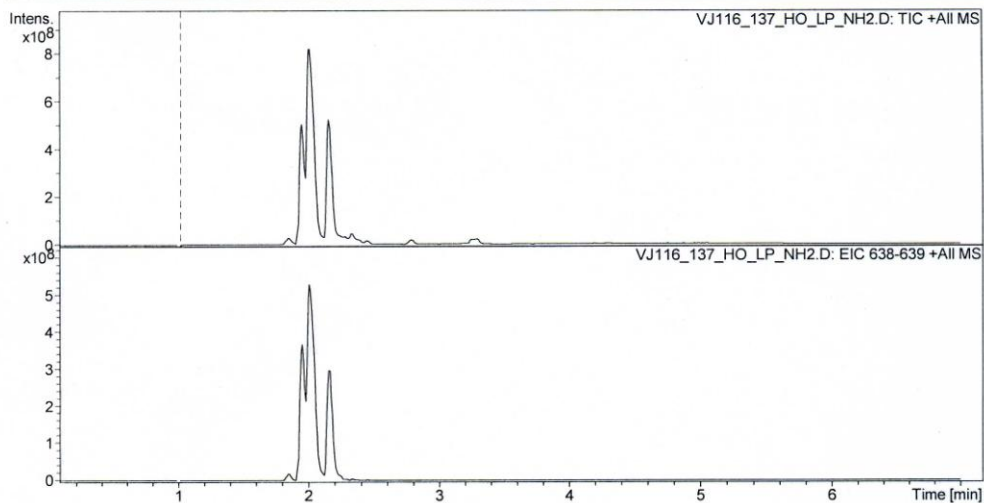
Analysis Name: VJ_114_137_LP. **Instrument:** Agilent 6330 Ion Trap **Print Date:** 12/9/2008 7:12:01 PM
Method: SANA.M D **Operator:** sdsu **Acq. Date:** 12/9/2008 7:02:09 PM
Sample Name: VJ_114_137_LP
Analysis Info:



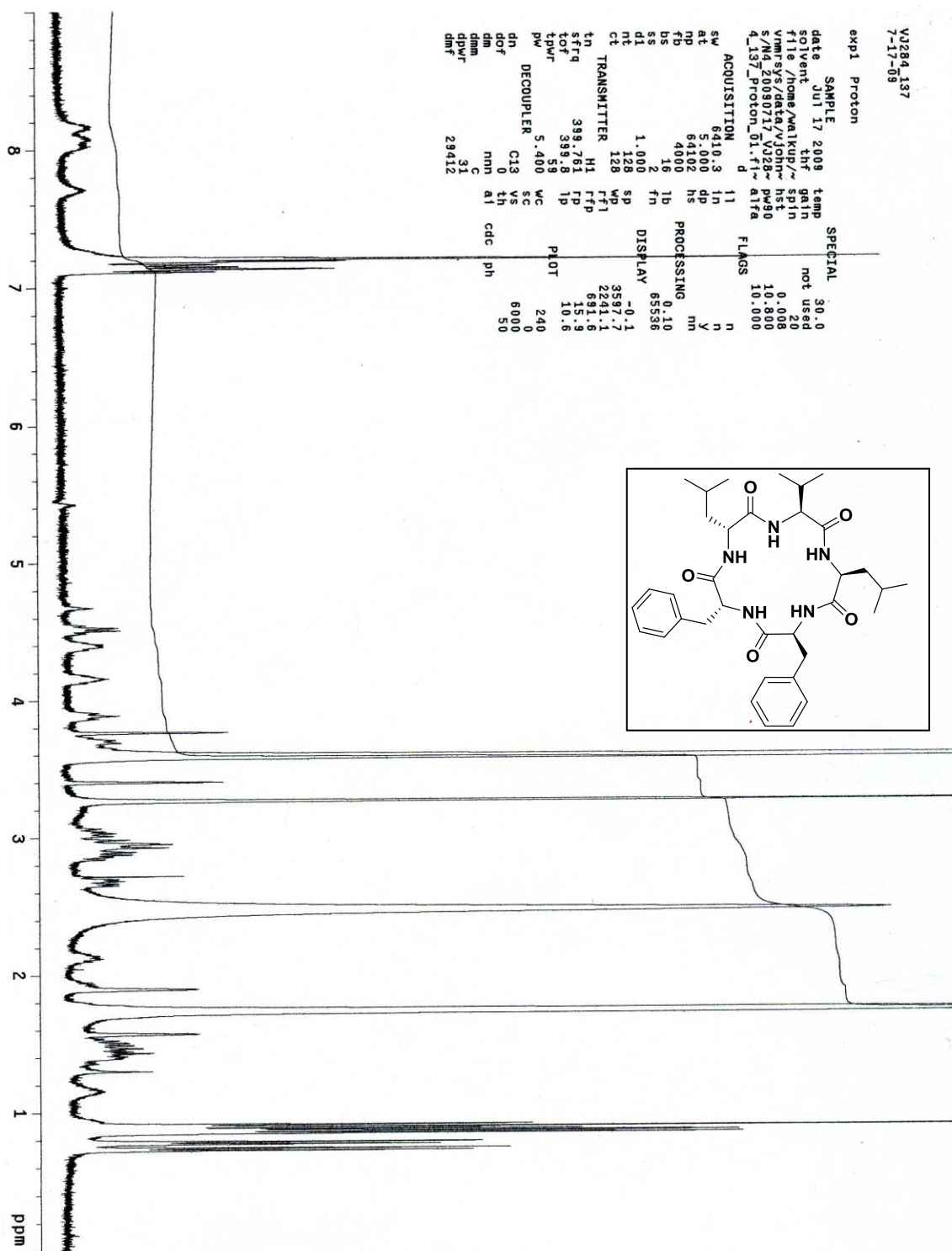
Compound 12 LCMS Linear Pentapeptide MeO-Phe-Leu-Val-D-Leu-D-Phe-NHBoc (MW=751)

Display Report - All Windows Selected Analysis

Analysis Name: VJ116_137_HO_ **Instrument:** Agilent 6330 Ion Trap **Print Date:** 7/23/2009 6:09:34 PM
Method: SANA.M LP_NH2.D **Operator:** sdsu **Acq. Date:** 1/7/2009 5:14:33 PM
Sample Name: VJ116_137_HO_LP_NH2
Analysis Info:



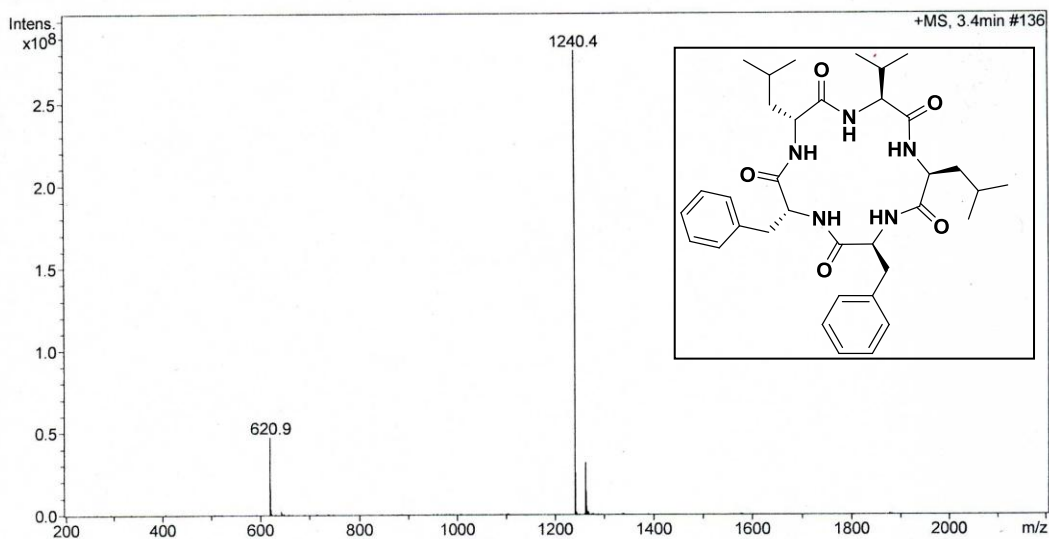
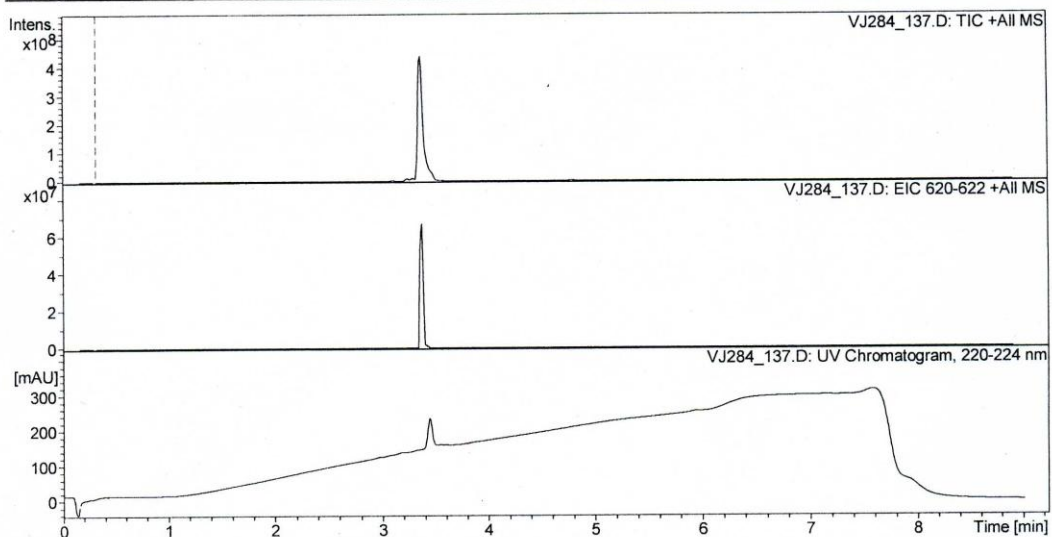
Compound 12 LCMS Double Deprotected Linear Pentapeptide HO-Phe-Leu-Val-D-Leu-D-Phe-NH₂ (MW=638)



Compound 12 NMR Cyclized Pentapeptide Phe-Leu-Val-D-Leu-D-Phe

Display Report - All Windows Selected Analysis

Analysis Name: VJ284_137.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 7/17/2009 1:22:58 PM
Method: SANA_LONG.M **Operator:** sdsu **Acq. Date:** 7/16/2009 8:11:40 PM
Sample Name: VJ284_137
Analysis Info:



Compound 12 LCMS Cyclized Pentapeptide Phe-Leu-Val-D-Leu-D-Phe (MW=620)

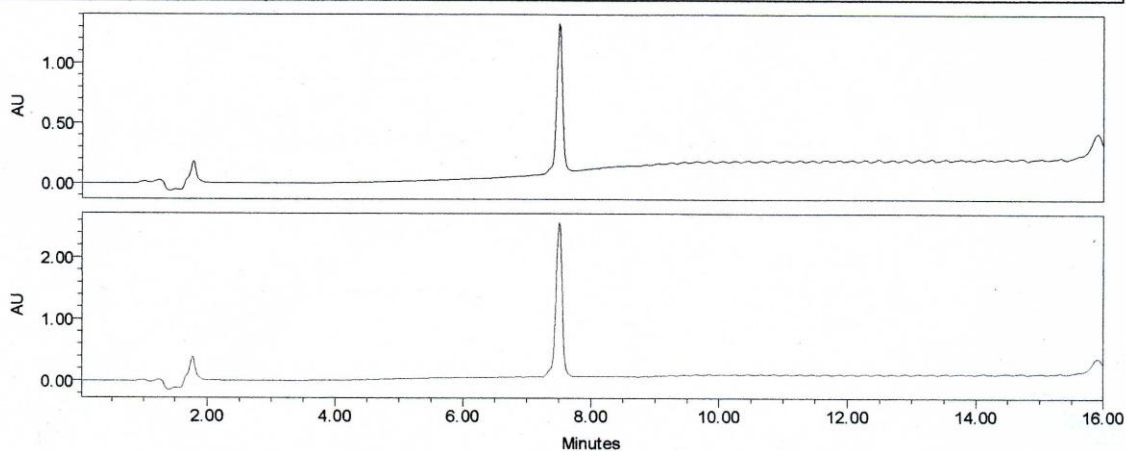
SDSU

Project Name: Defaults
Reported by User: System

Breeze

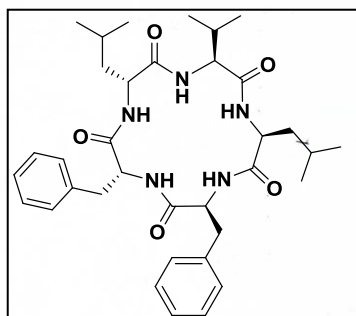
SAMPLE INFORMATION

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Sample Type:	Unknown	Sample Set Name:	
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Injection #:	40	Date Acquired:	7/16/2009 6:55:06 PM
Run Time:	16.00 Minutes	Injection Volume:	50.00 ul

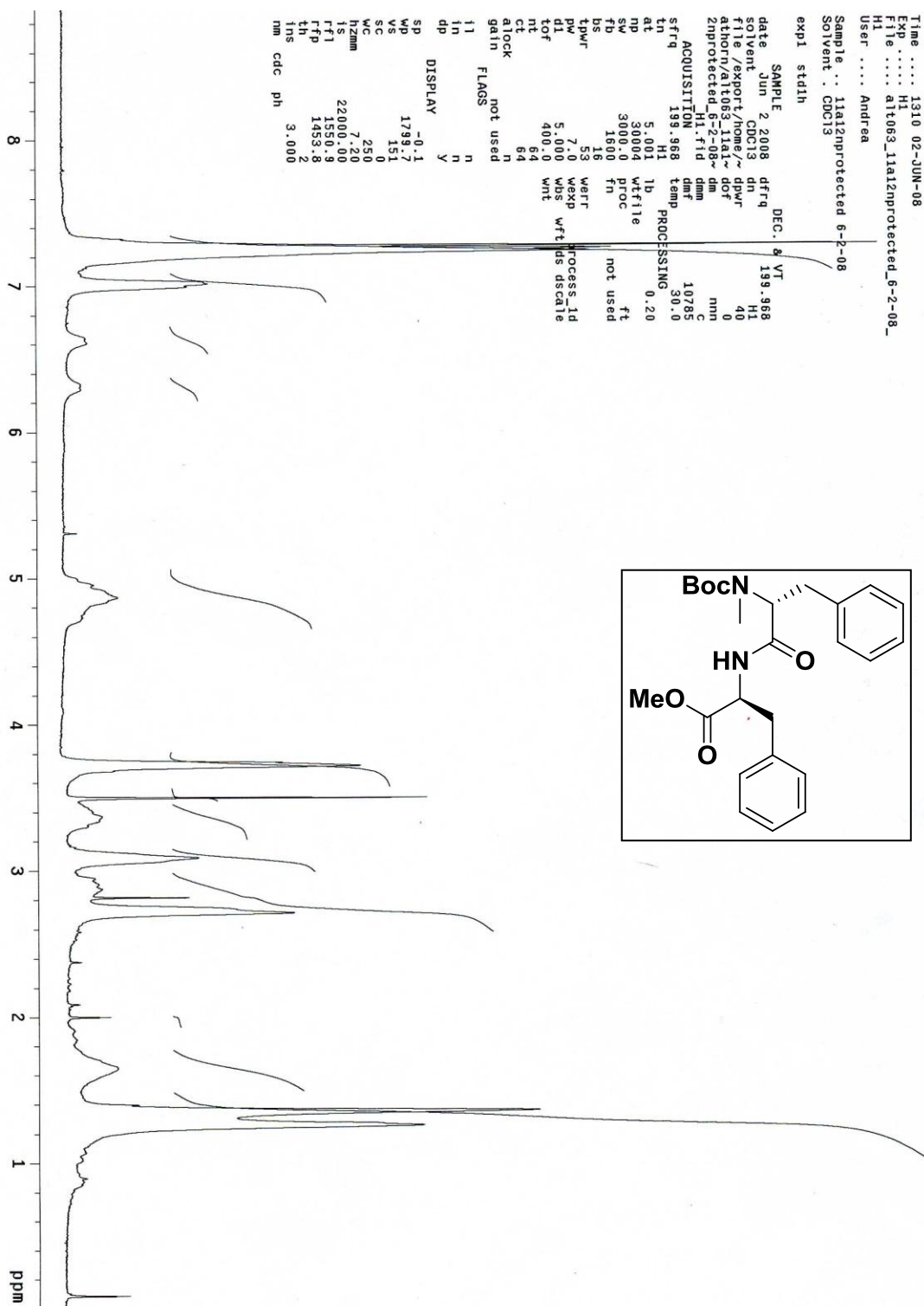


— Channel: 2487Channel 1 Channel Desc.: Processing Method: ****
 — Channel: 2487Channel 2 Channel Desc.: Processing Method: ****

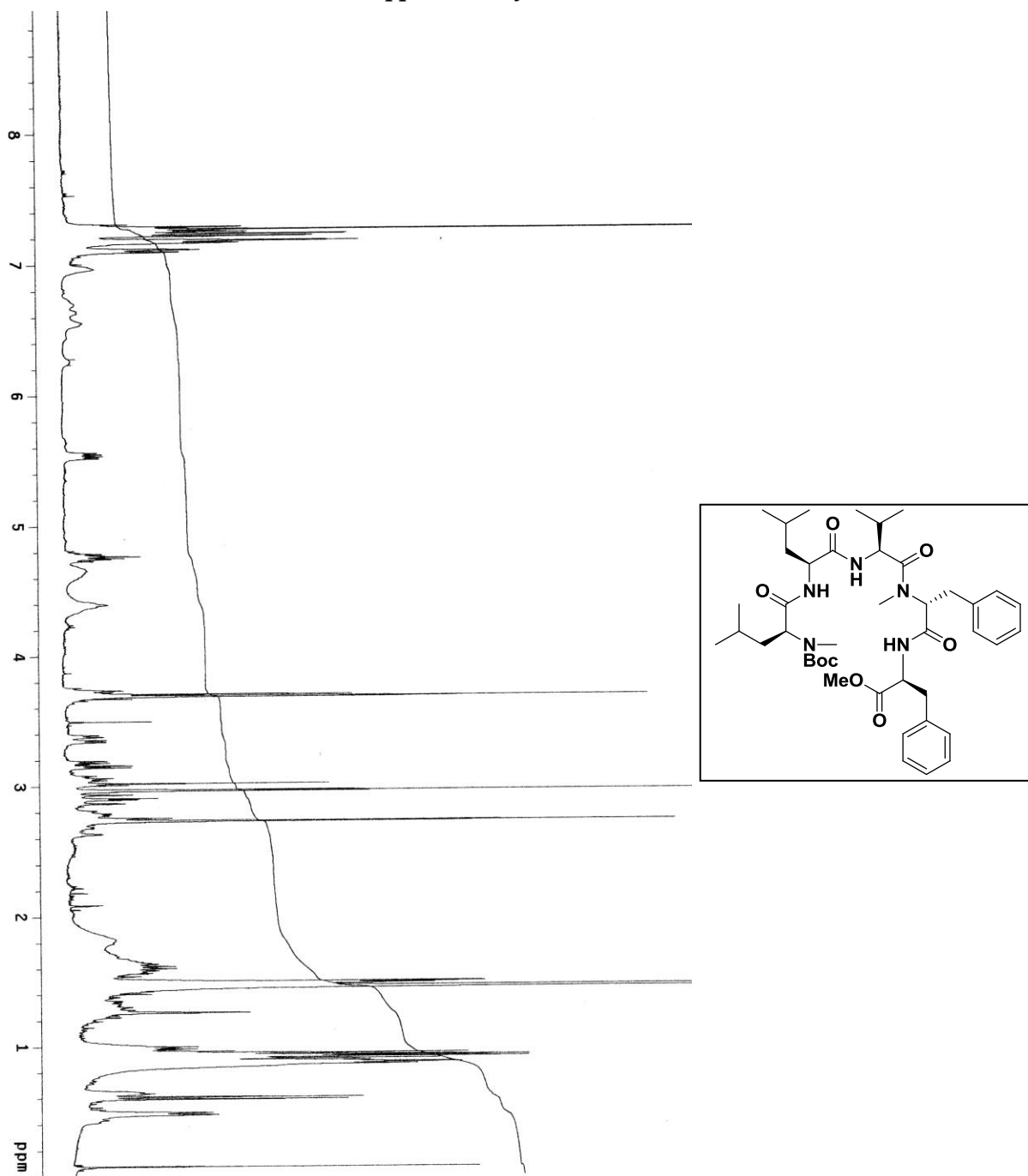
Peak Name	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	Amount	Units
1	****	****	****	****	****	****
2	****	****	****	****	****	****



Compound 12 HPLC Cyclized Pentapeptide Phe-Leu-Val-D-Leu-D-Phe

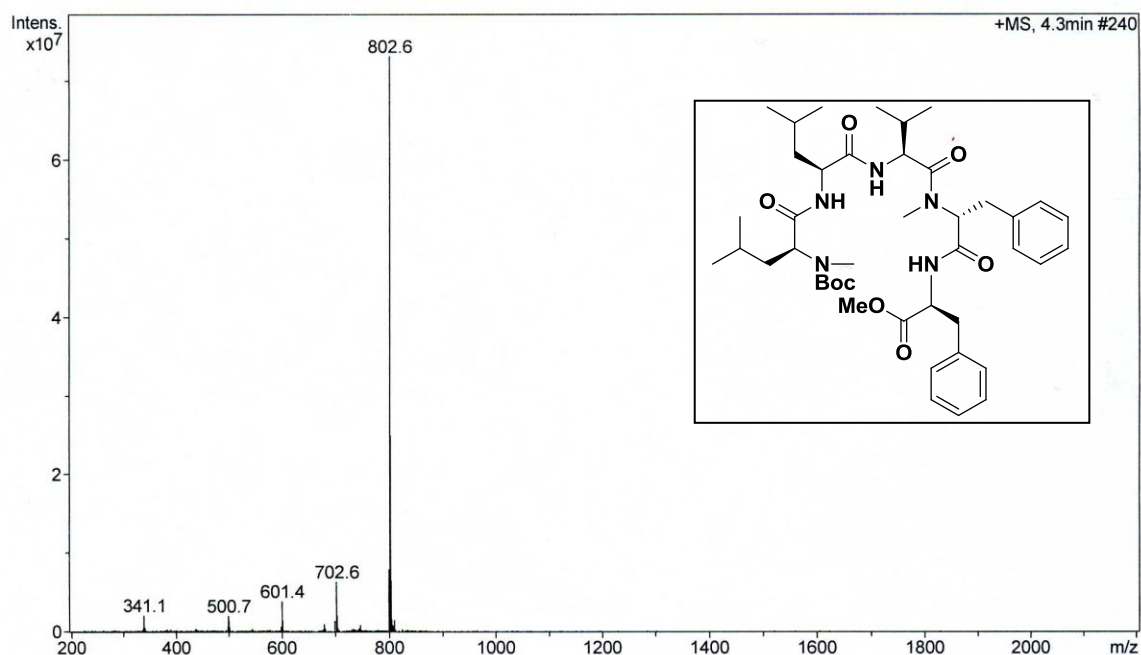
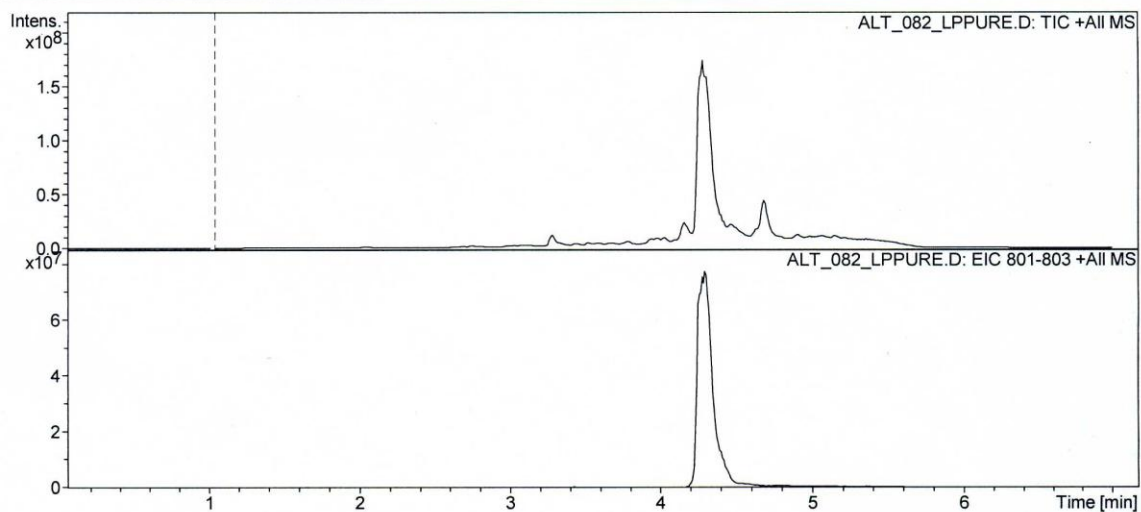


Compound 15 NMR Dipeptide MeO-Phe-N-Me-D-Phe-Boc



Display Report - All Windows Selected Analysis

Analysis Name: ALT_082_LPPUR **Instrument:** Agilent 6330 Ion Trap **Print Date:** 6/12/2008 1:15:31 PM
Method: SANA.M E.D **Operator:** sdsu **Acq. Date:** 6/12/2008 12:53:28 PM
Sample Name: ALT_082_LPpure
Analysis Info:



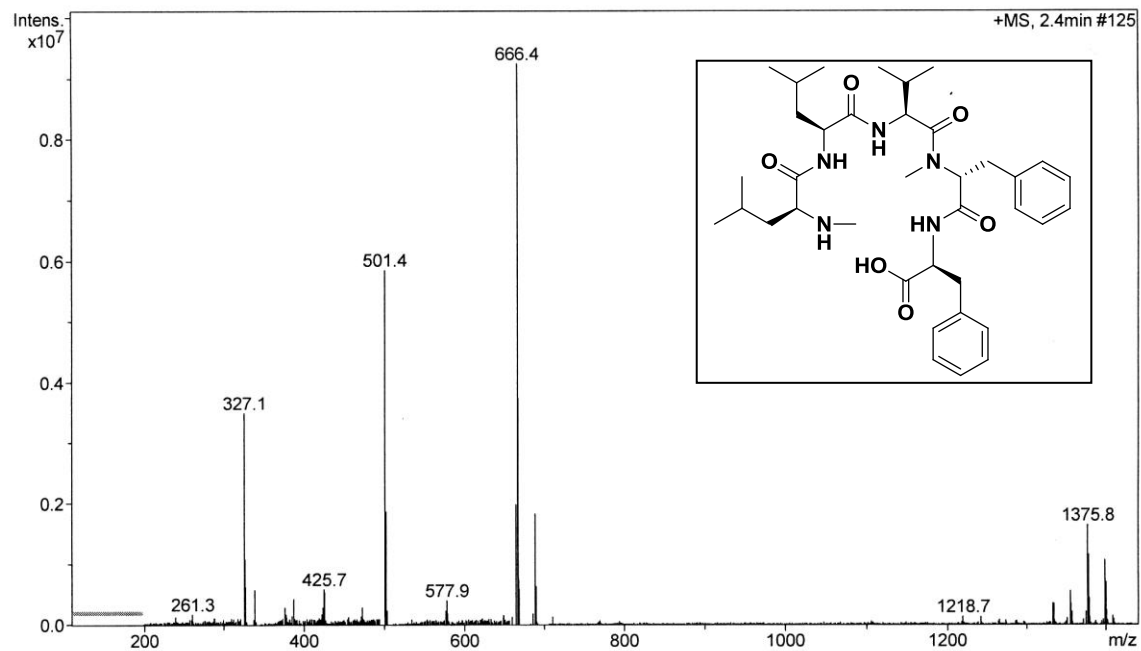
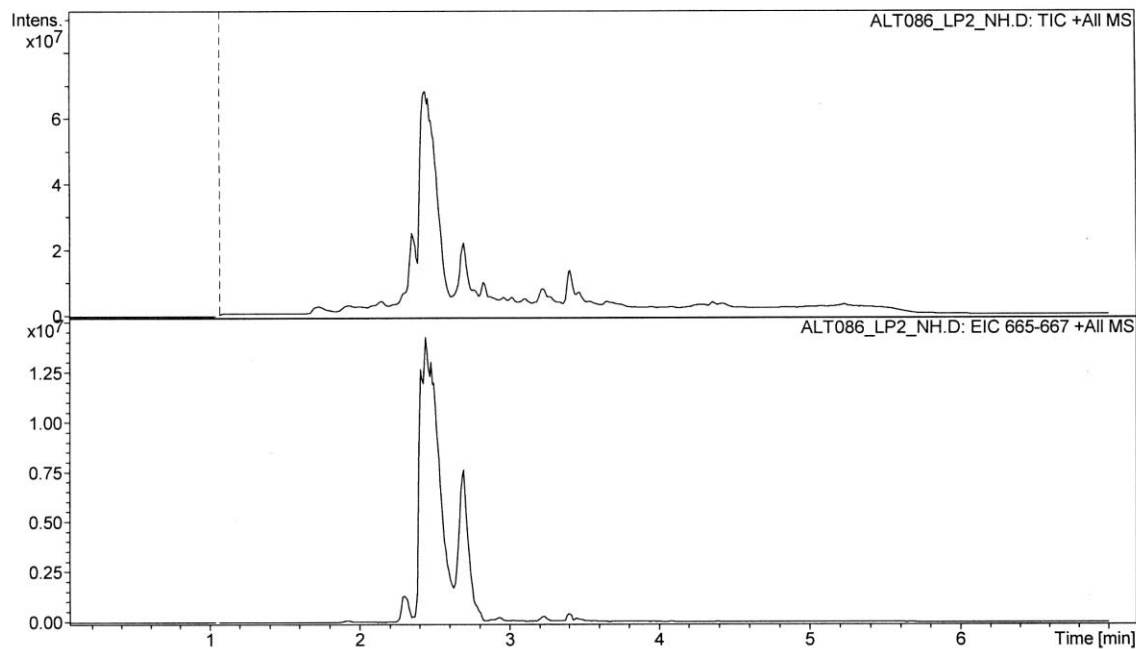
Compound 15 LCMS Linear Pentapeptide MeO-Phe-N-Me-D-Phe-Val-Leu-N-Me-Leu-Boc (MW=780)

Display Report - All Windows All Analyses

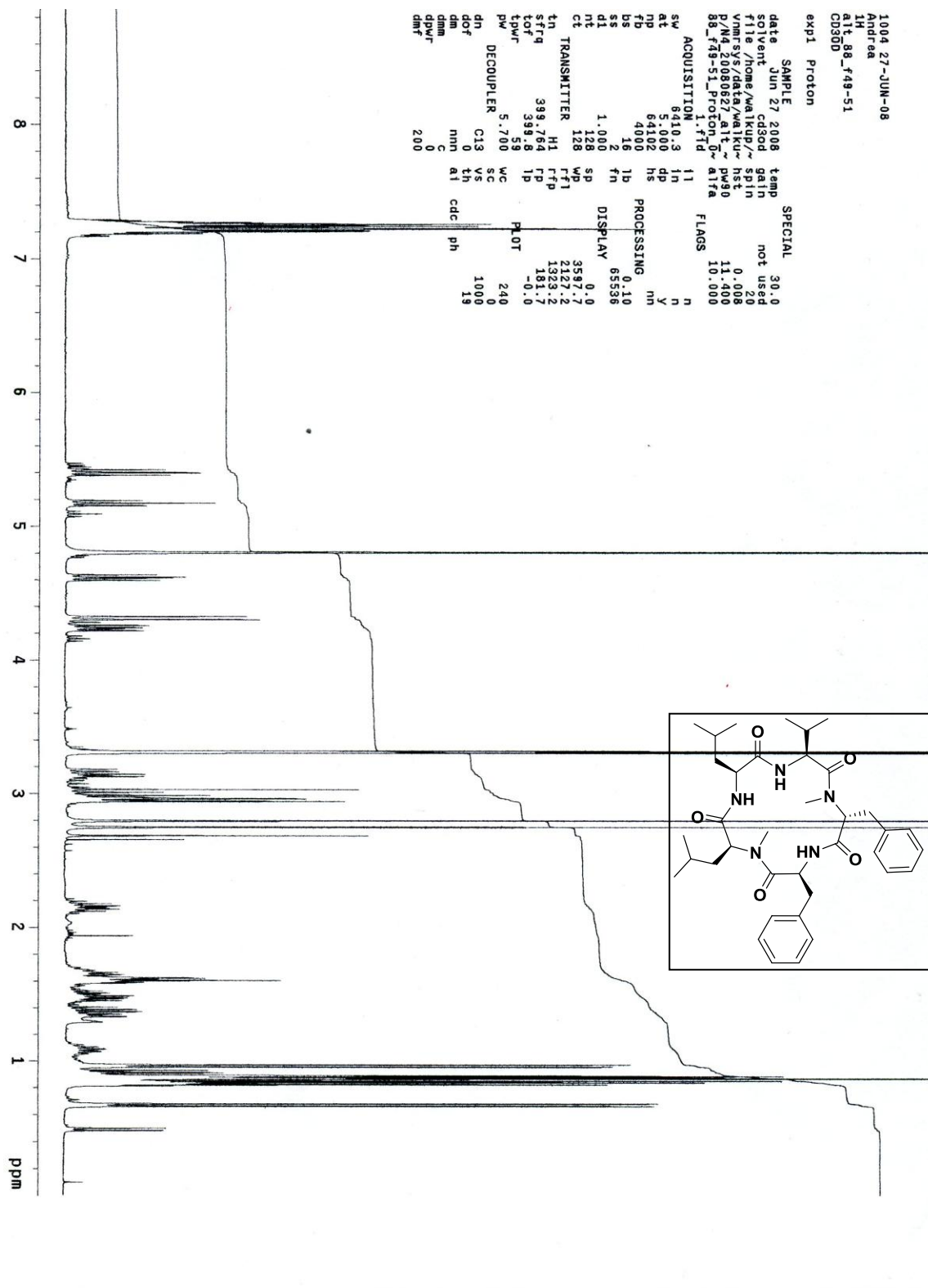
Operator: sdsu

Instrument: Agilent 6330 Ion Trap

Print Date: 6/19/2008 12:00:11 PM



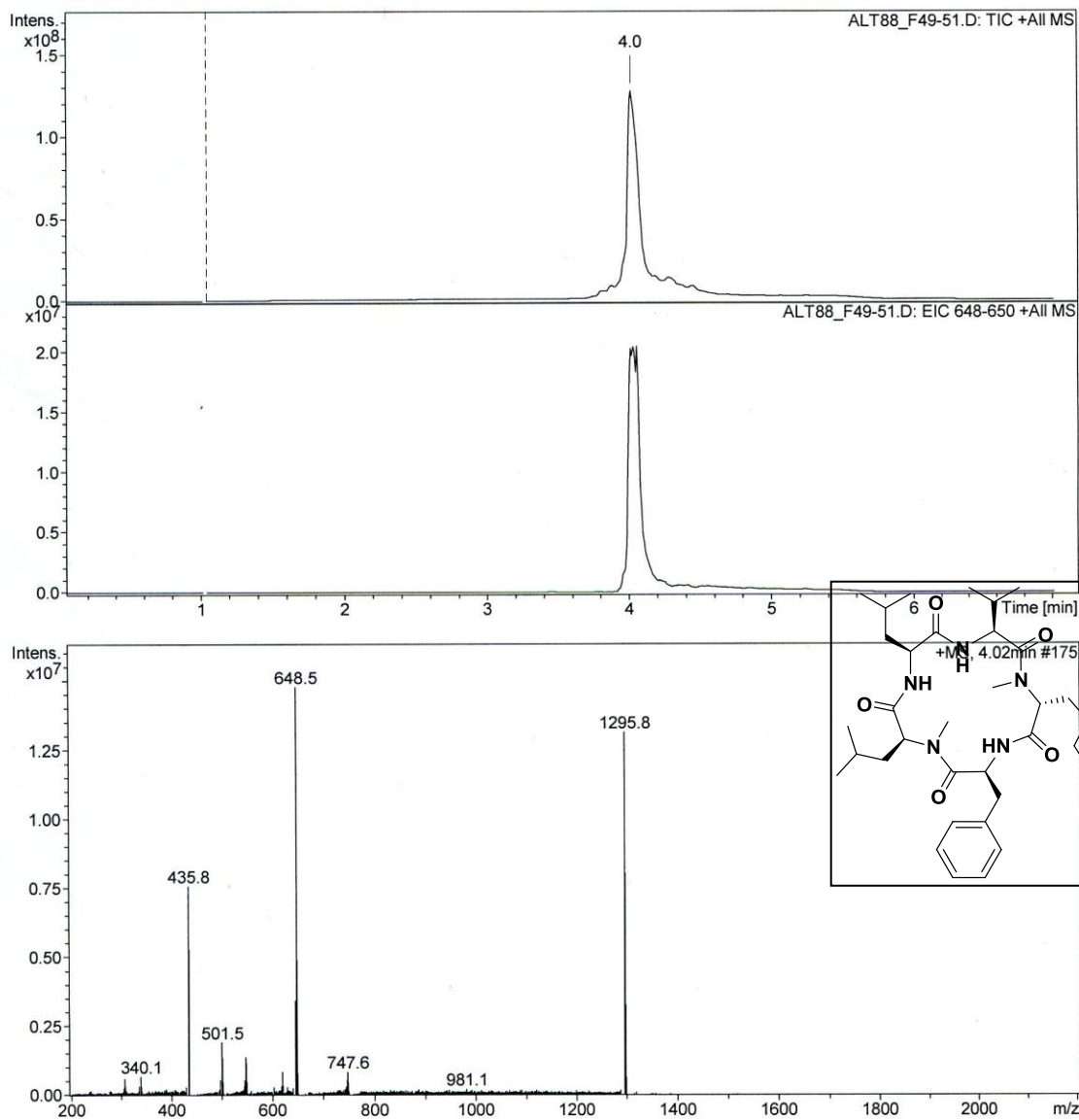
Compound 15 LCMS Double Deprotected Linear Pentapeptide HO-Phe-N-Me-D-Phe-Val-Leu-N-Me-Leu-H (MW=665.8)



Compound 15 NMR Cyclized Pentapeptide Phe-N-Me-D-Phe-Val-Leu-N-Me-Leu

Display Report - All Windows Selected Analysis

Analysis Name: ALT88_F49-51.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 6/25/2008 7:19:15 PM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 6/25/2008 7:09:38 PM
Sample Name: ALT88_f49-51
Analysis Info:



San Diego State University; Department of Chemis

Project Name: Defaults

Reported by User: shelli

Breeze

SAMPLE INFORMATION

Sample Name: alt_88_f-49-51

Sample Type: Unknown

Vial: 1

Injection #: 22

Run Time: 16.00 Minutes

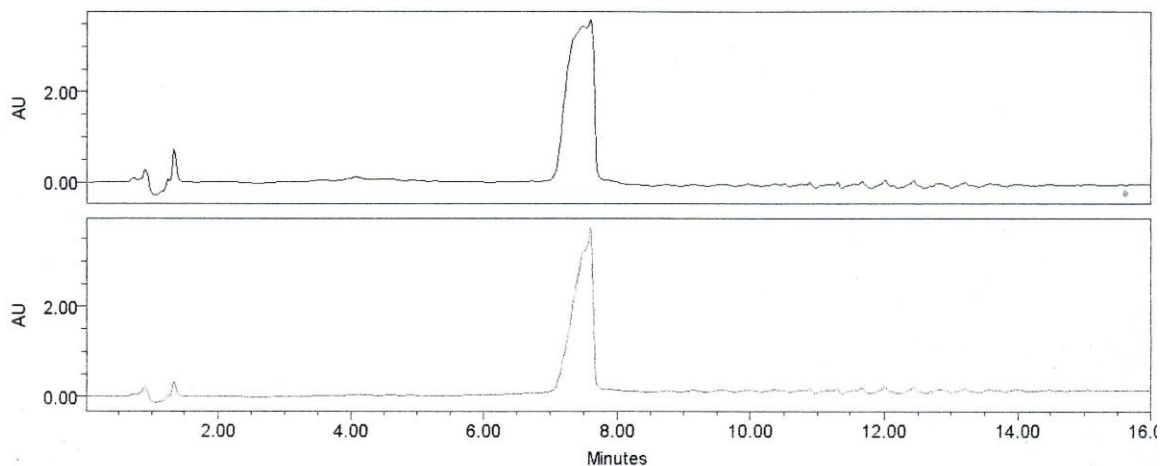
Acquired By: shelli

Sample Set Name:

Acq. Method: PrimarySanA_SS

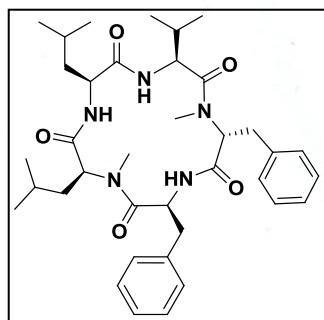
Date Acquired: 6/27/2008 4:10:05 PM

Injection Volume: 100.00 ul

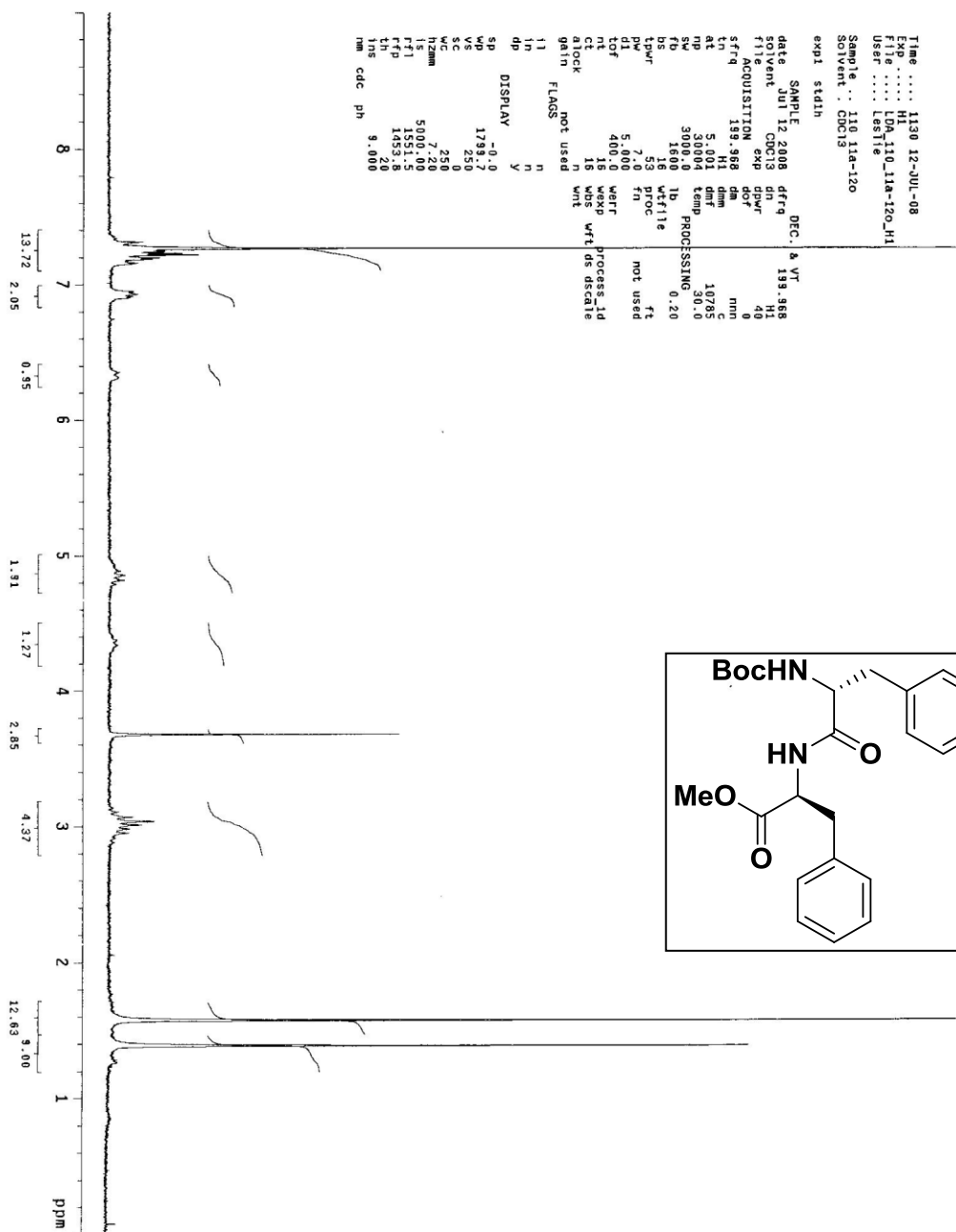


Channel: 2487Channel 1 Channel Desc.: Processing Method: ****
 Channel: 2487Channel 2 Channel Desc.: Processing Method: ****

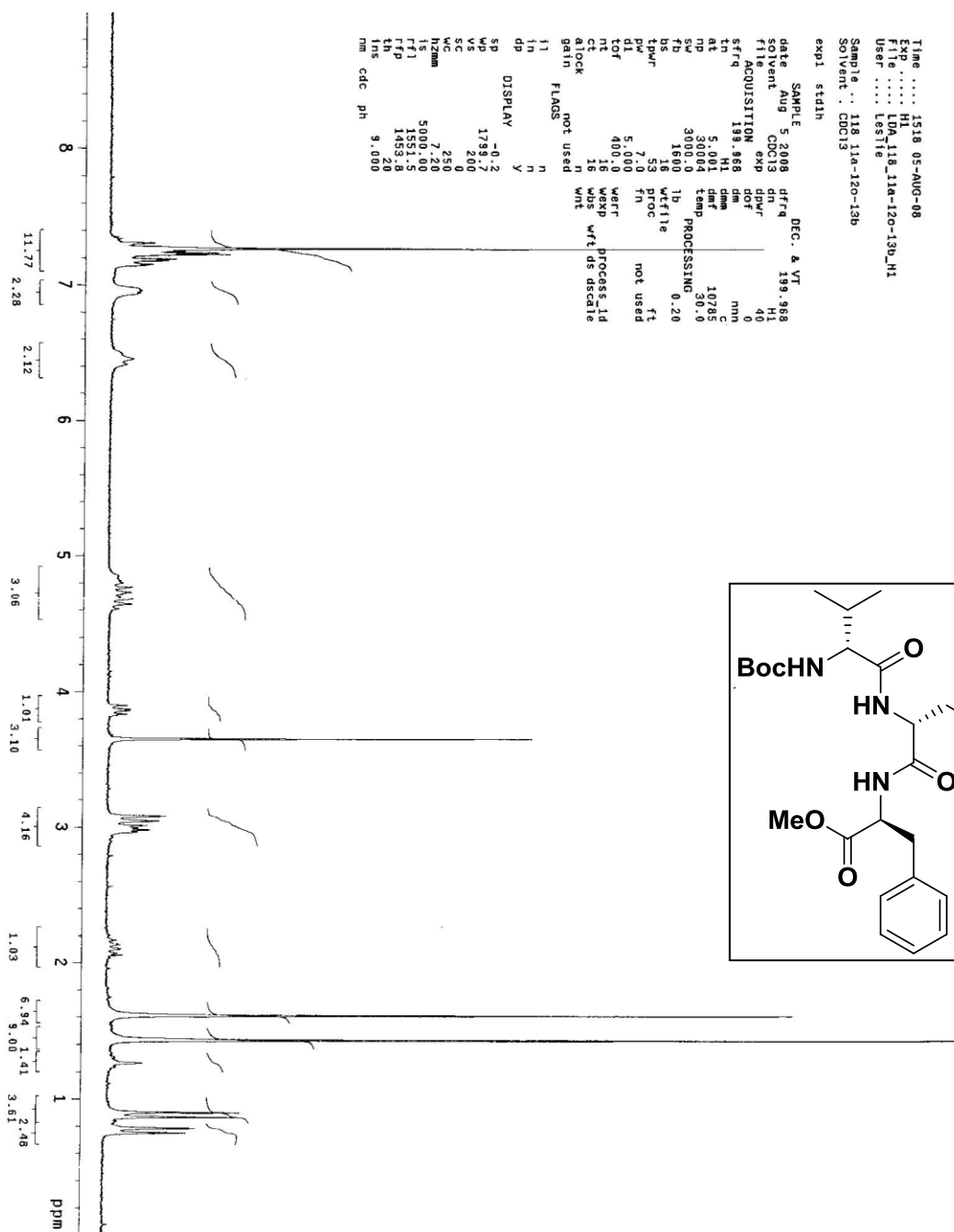
Peak Name	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	Amount	Units
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2 ****	****	****	****	****	****	****



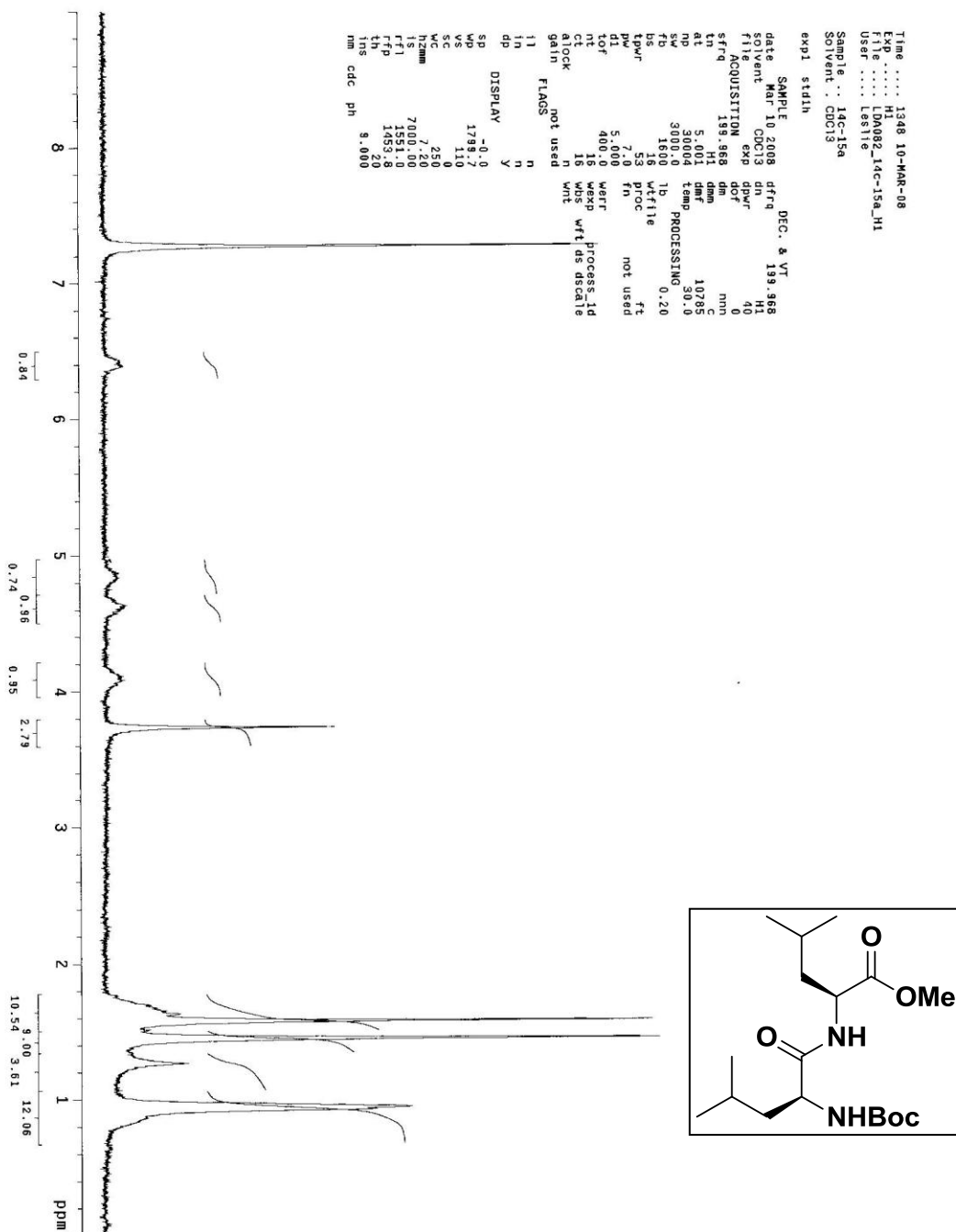
Compound 15 HPLC Cyclized Pentapeptide Phe-N-Me-D-Phe-Val-Leu-N-Me-Leu



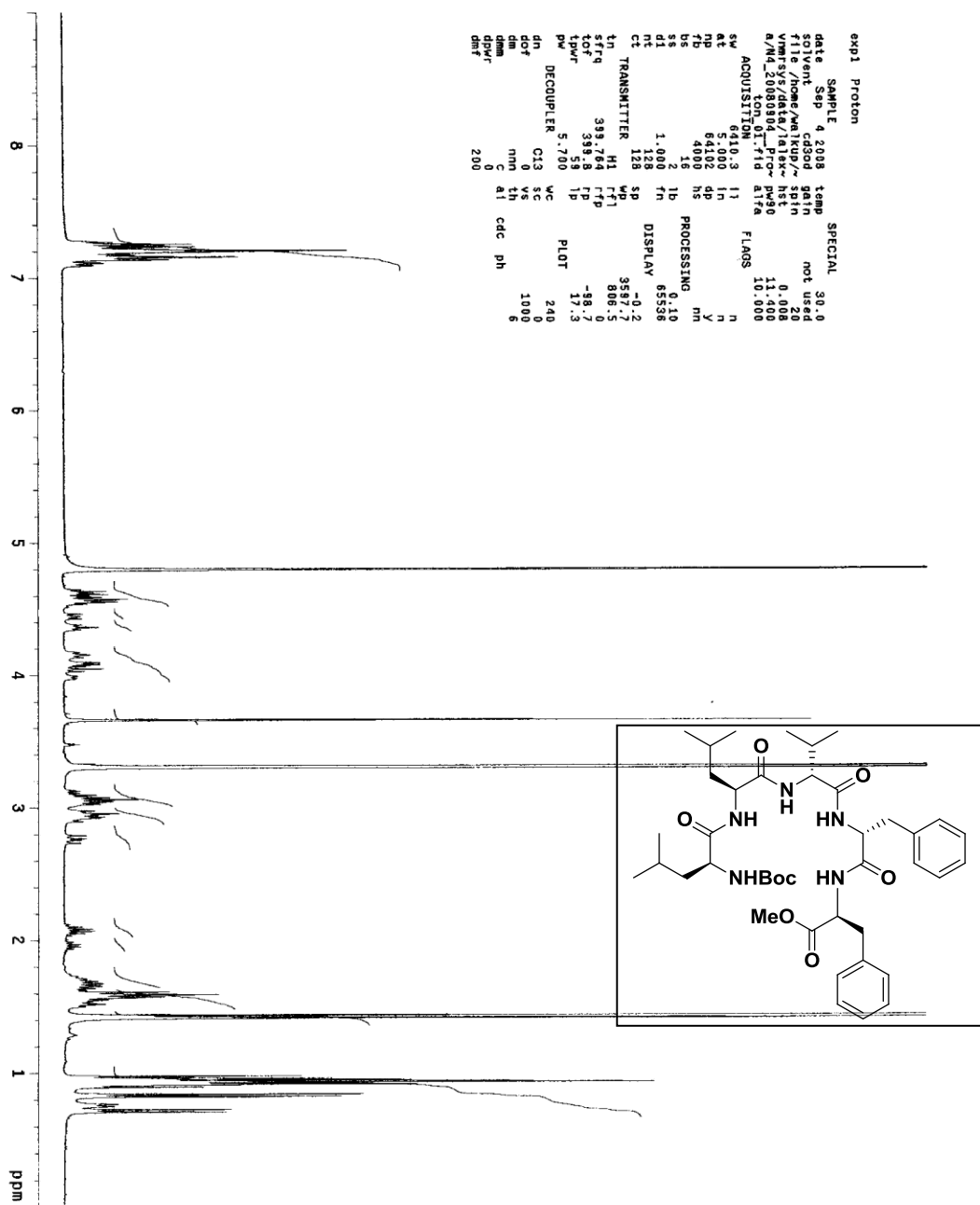
Compound 18 NMR Dipeptide MeO-Phe-D-Phe-NHBoc



Compound 18 NMR Tripeptide MeO-Phe-D-Phe-D-Val-NHBoc



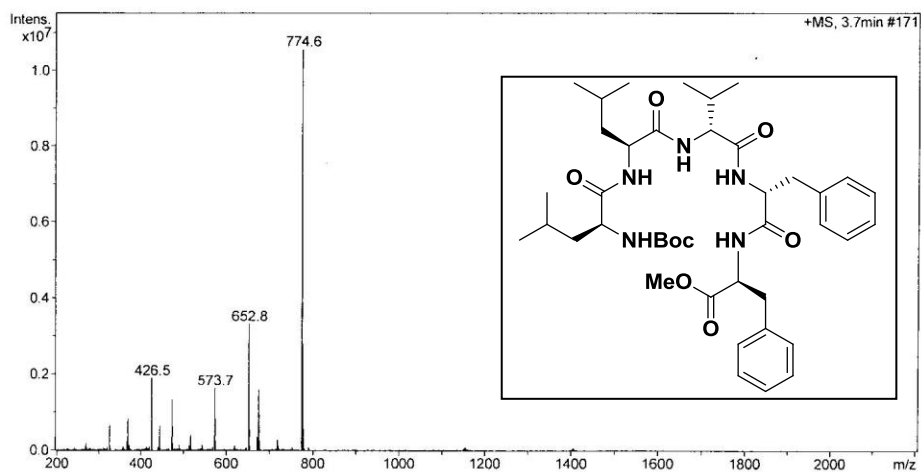
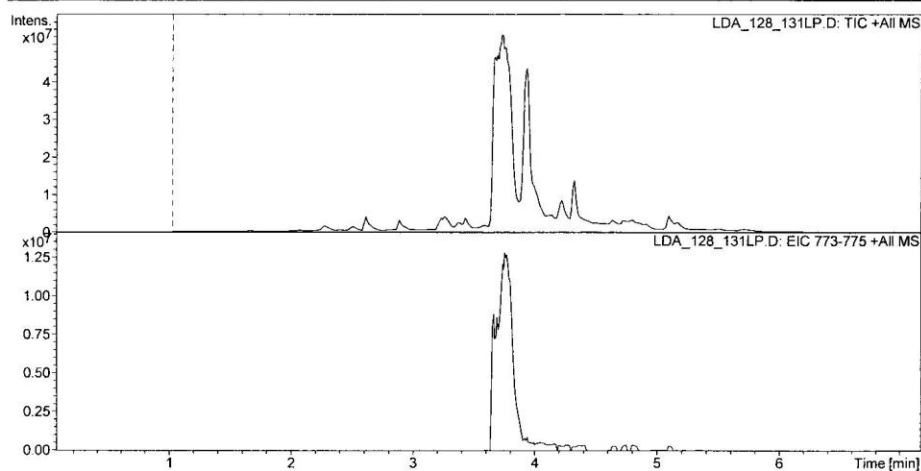
Compound 18 NMR Dipeptide MeO-Leu-Leu-NHBoc



Compound 18 NMR Linear Pentapeptide MeO-Phe-D-Phe-D-Val-Leu-Leu-NHBoc

Display Report - All Windows Selected Analysis

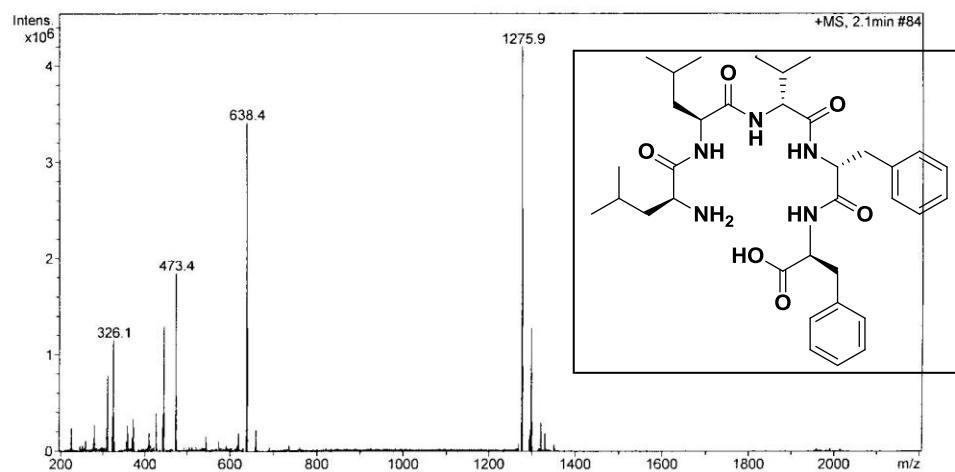
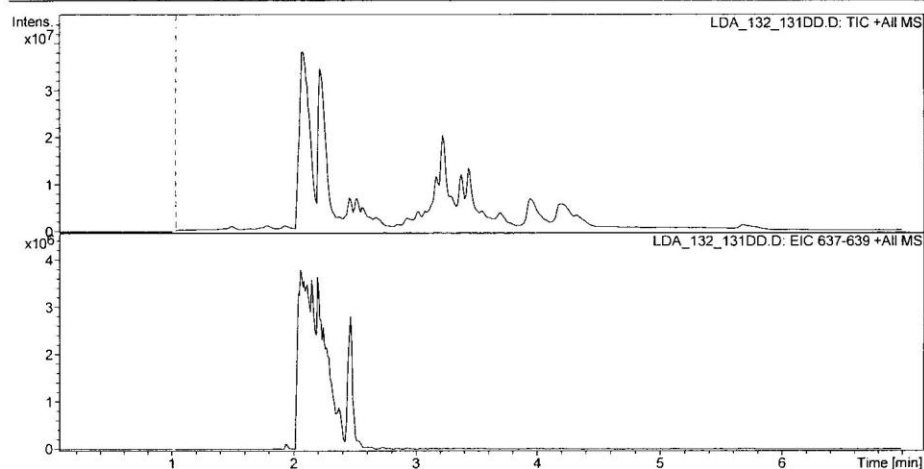
Analysis Name: LDA_128_131LP. Instrument: Agilent 6330 Ion Trap. Print Date: 9/10/2008 11:13:12 AM
Method: SANA.M D. Operator: sdsu. Acq. Date: 9/9/2008 7:19:49 PM
Sample Name: LDA_128_131lp
Analysis Info:



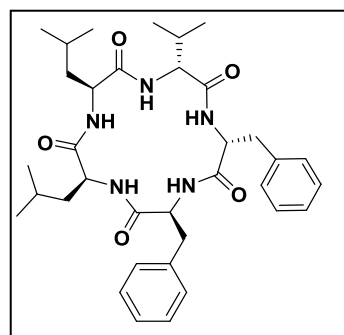
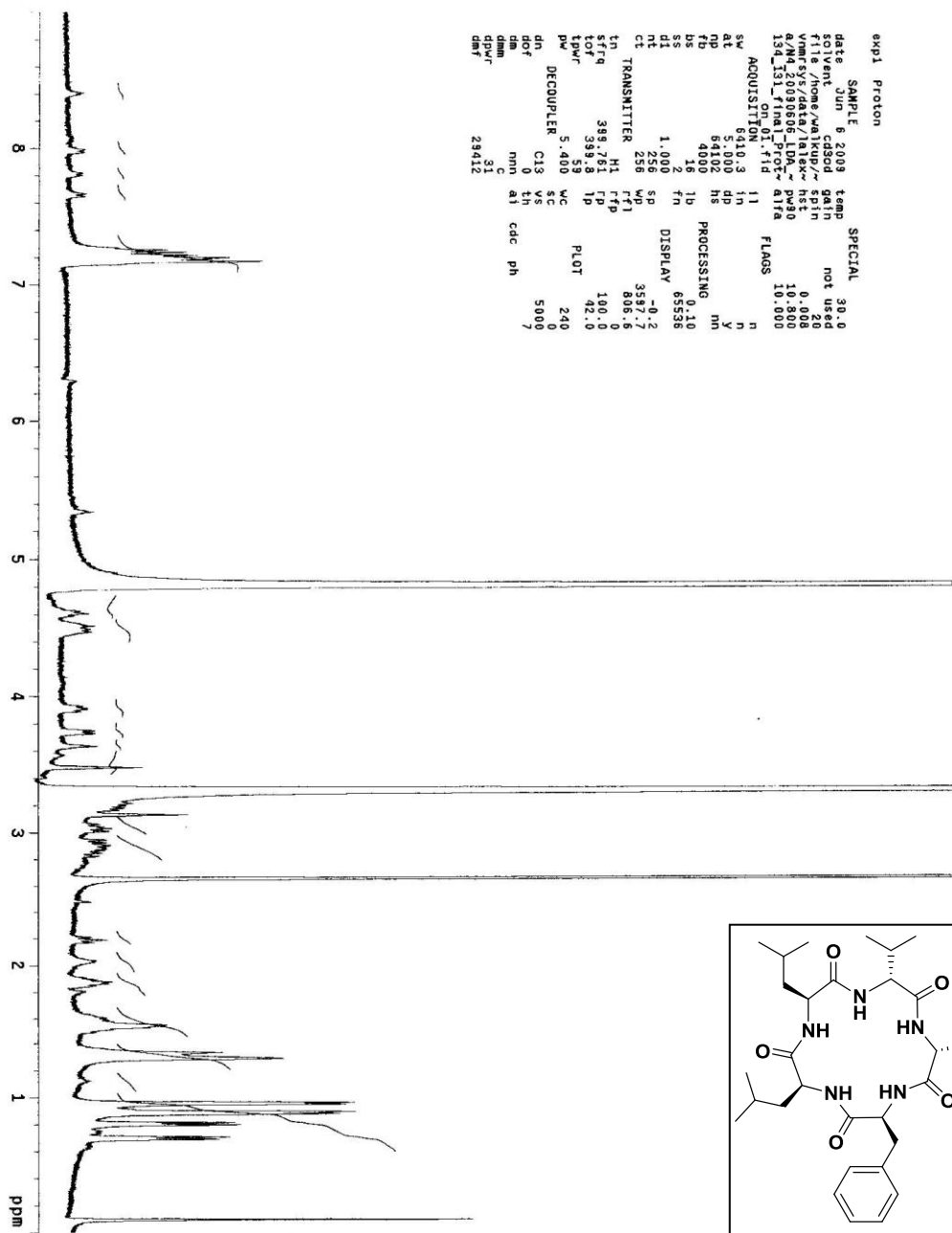
Compound 18 LCMS Linear Pentapeptide MeO-Phe-D-Phe-D-Val-Leu-Leu-NHBoc (MW=752)

Display Report - All Windows Selected Analysis

Analysis Name: LDA_132_131DD Instrument: Agilent 6330 Ion Trap Print Date: 9/9/2008 4:58:50 PM
Method: SANA.M.D Operator: sdsu Acq. Date: 9/9/2008 4:19:37 PM
Sample Name: LDA_132_131dd
Analysis Info:



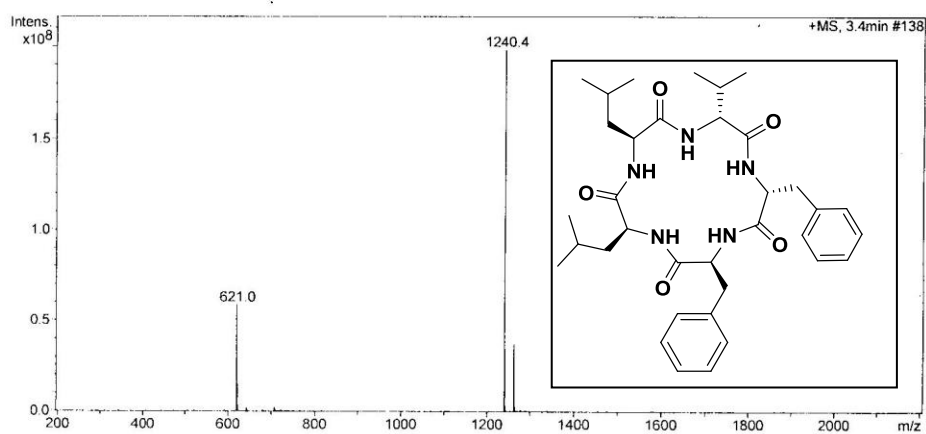
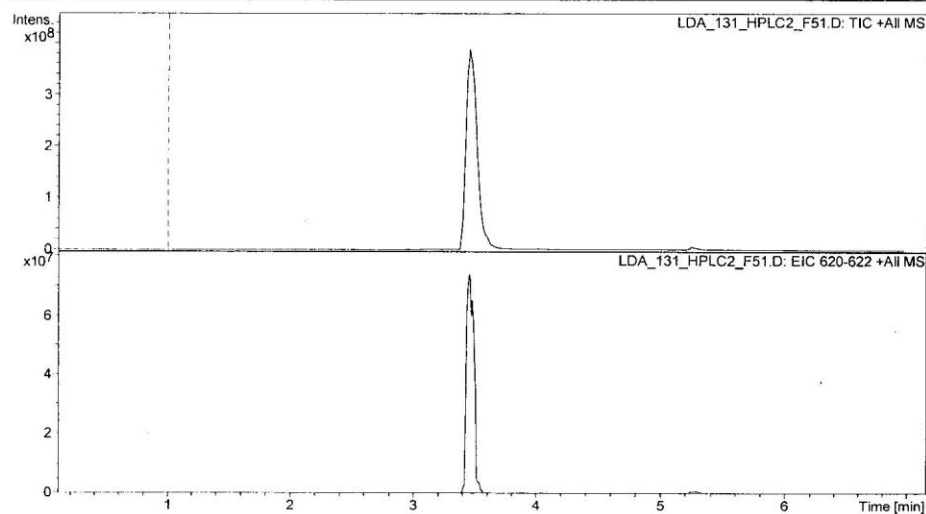
Compound 18 LCMS Double Deprotected Linear Pentapeptide HO-Phe-D-Phe-D-Val-Leu-Leu-NH₂ (MW=638)



Compound 18 NMR Cyclized Pentapeptide Phe-D-Phe-D-Val-Leu-Leu

Display Report - All Windows Selected Analysis

Analysis Name: LDA_131_HPLC2 **Instrument:** Agilent 6330 Ion Trap **Print Date:** 6/24/2009 2:54:13 PM
Method: SANA.M_F51.D **Operator:** sdsu **Acq. Date:** 5/9/2009 1:09:43 PM
Sample Name: LDA_131_hplc2_f51
Analysis Info:



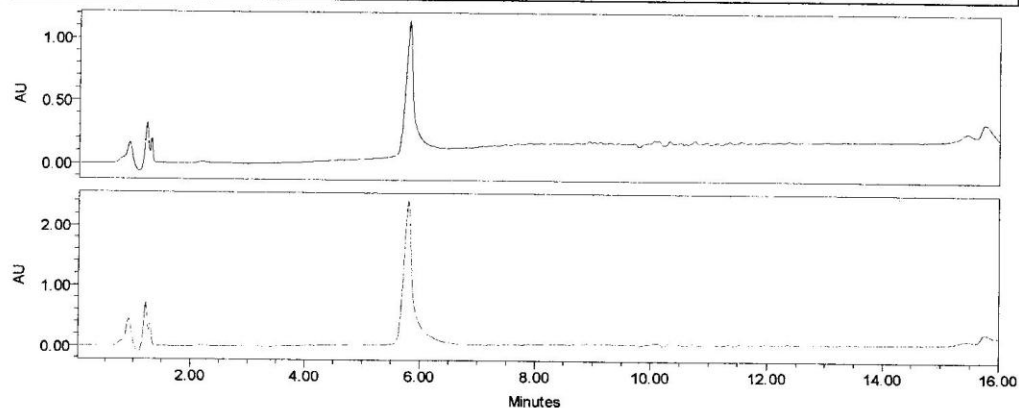
Compound 18 LCMS Cyclized Pentapeptide Phe-D-Phe-D-Val-Leu-Leu (MW=620)

SDSU

Project Name: Defaults
Reported by User: System

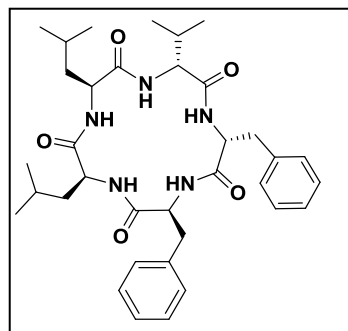
Breeze

SAMPLE INFORMATION			
Sample Name:	LDA_131_final	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	333	Date Acquired:	6/1/2009 11:08:15 AM
Run Time:	16.00 Minutes	Injection Volume:	30.00 ul



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

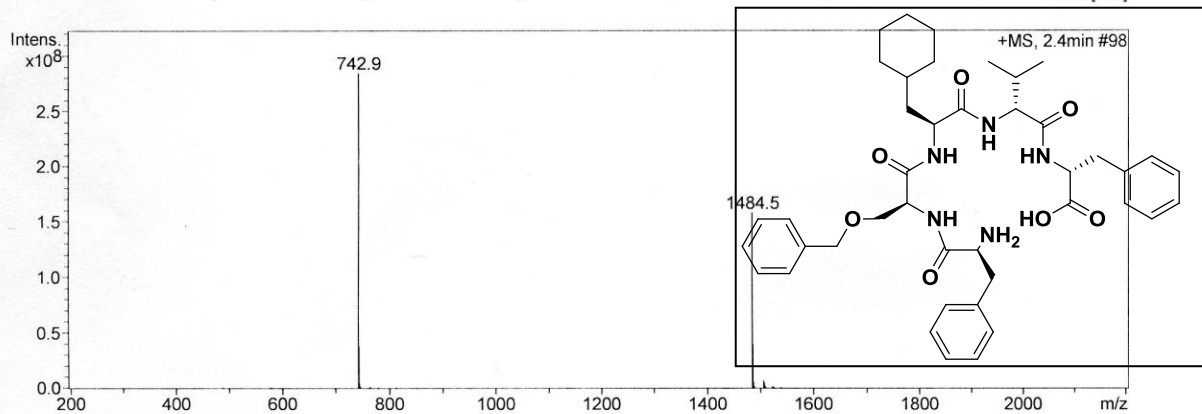
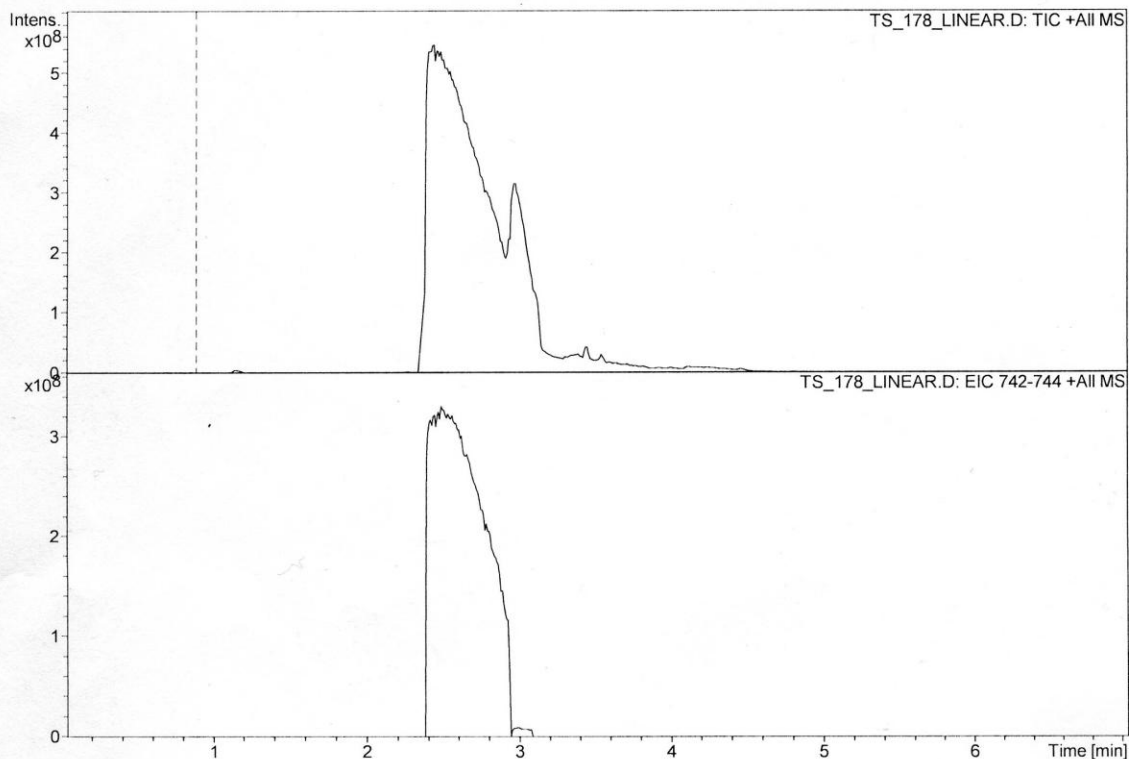
Peak Name	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	Amount	Units
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2 ****	****	****	****	****	****	****



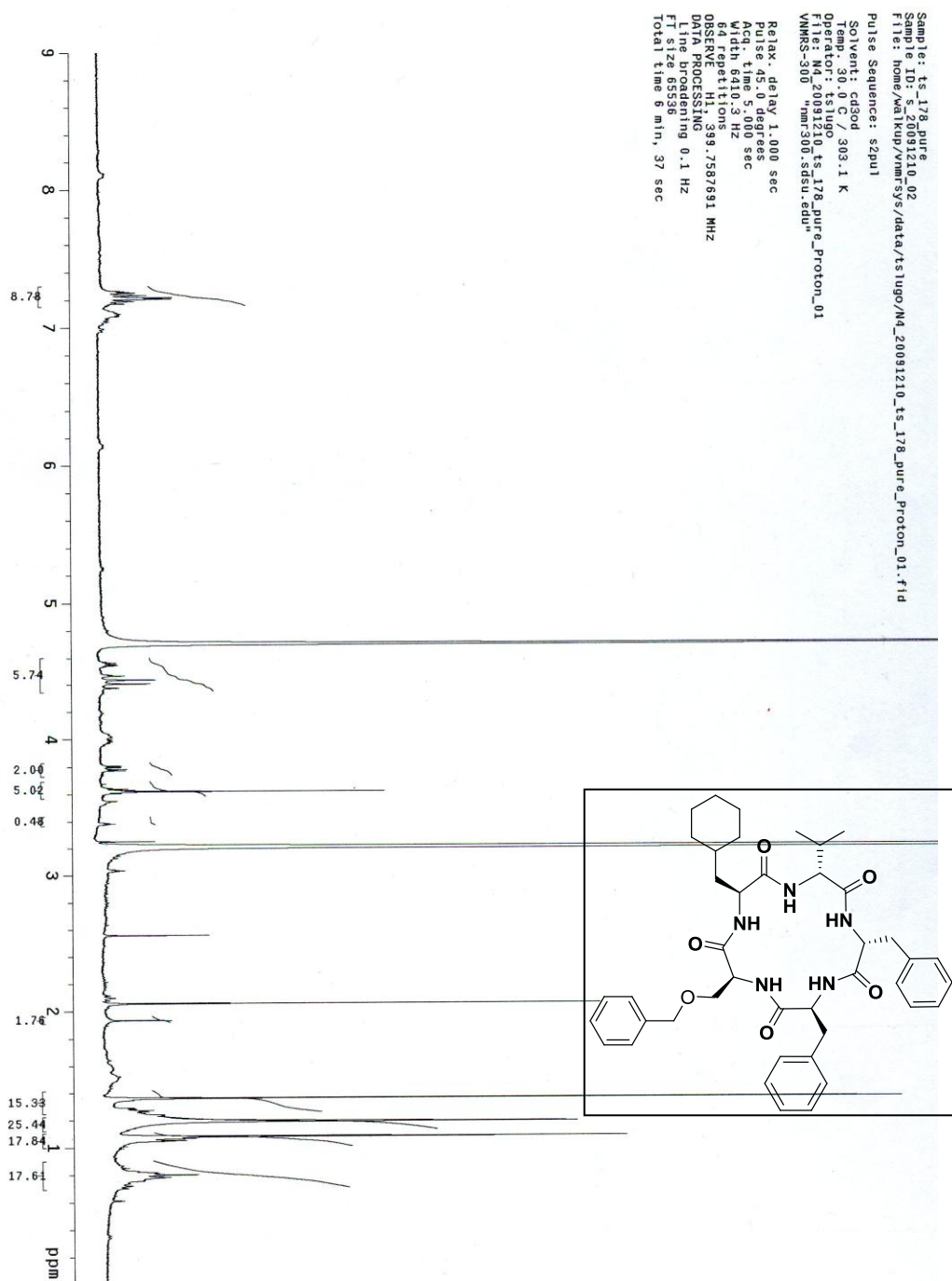
Compound 18 HPLC Cyclized Pentapeptide Phe-D-Phe-D-Val-Leu-Leu

Display Report - All Windows Selected Analysis

Analysis Name: TS_178_LINEAR. **Instrument:** Agilent 6330 Ion Trap **Print Date:** 9/24/2009 3:52:58 PM
Method: SANA.M D **Operator:** sdsu **Acq. Date:** 8/30/2009 11:43:55 AM
Sample Name: ts_178_linear
Analysis Info:



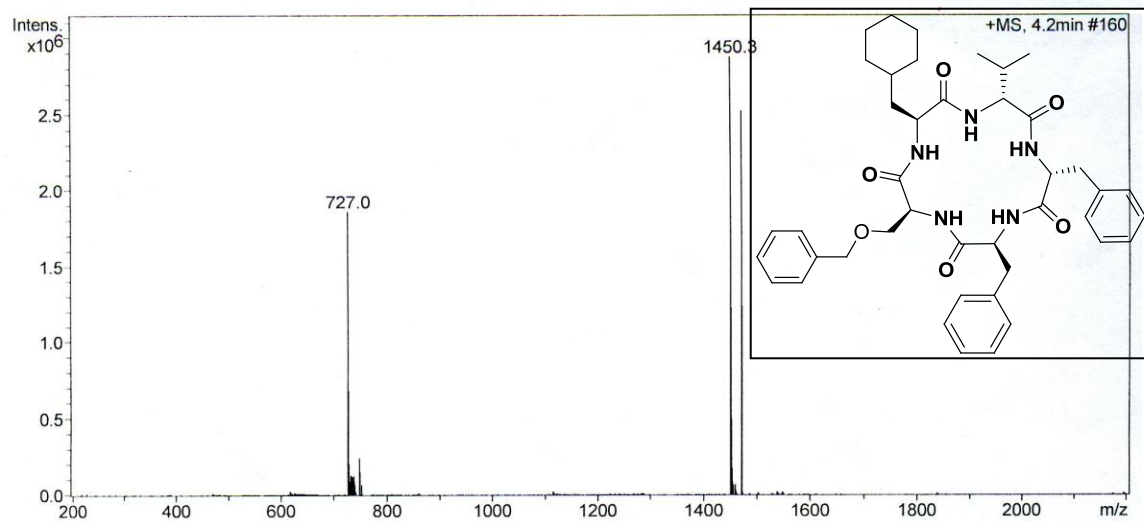
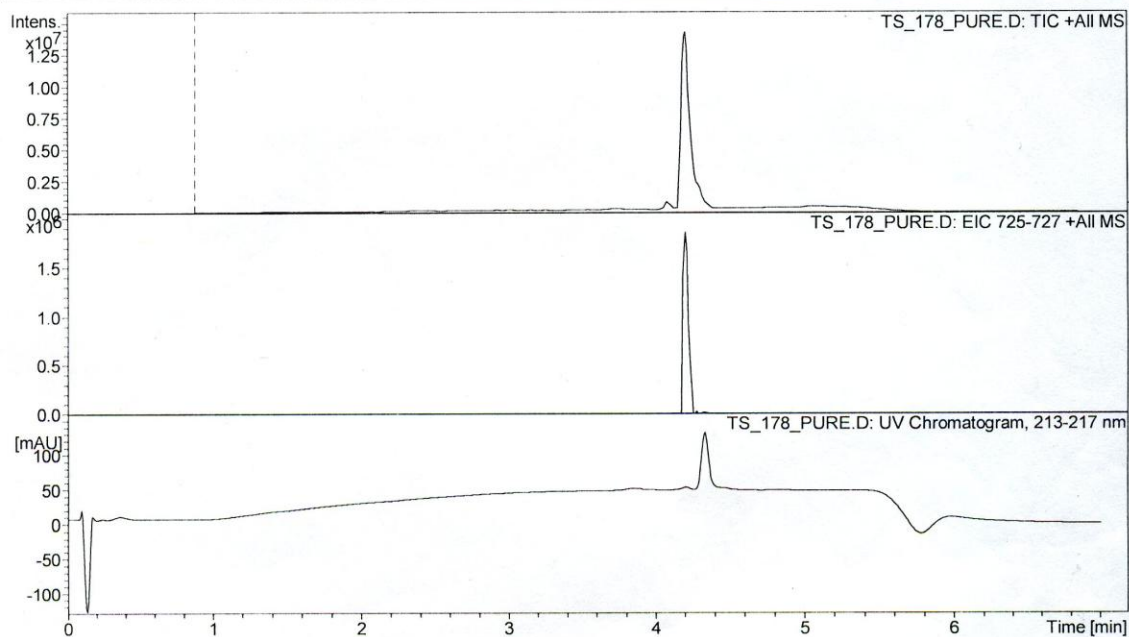
Compound 20 LCMS Double Deprotected Linear Pentapeptide HO-D-Phe-D-Val-Cha-Ser(Bzl)-Phe-NH₂ (MW=742)



Compound 20 NMR Cyclized Pentapeptide Phe-D-Phe-D-Val-Cha-Ser(Bzl)

Display Report - All Windows Selected Analysis

Analysis Name: TS_178_PURE.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 9/15/2009 3:54:16 PM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 9/15/2009 3:46:00 PM
Sample Name: ts_178_pure
Analysis Info:



Compound 20 LCMS Cyclized Pentapeptide Phe-D-Phe-D-Val-Cha-Ser(Bzl) (MW=726)

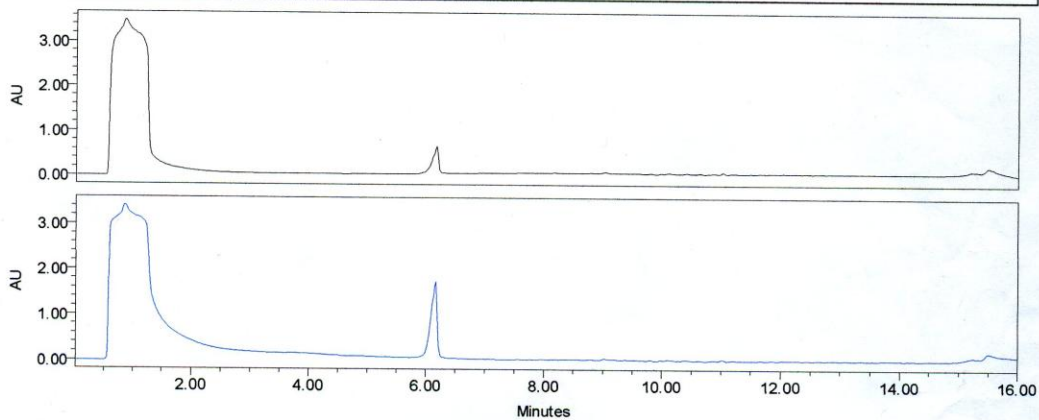
SDSU

Project Name: Defaults
Reported by User: System

Breeze

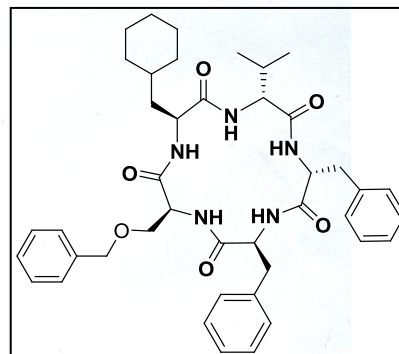
SAMPLE INFORMATION

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Injection #:	157	Date Acquired:	9/14/2009 2:43:44 PM
Run Time:	16.00 Minutes	Injection Volume:	90.00 ul



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

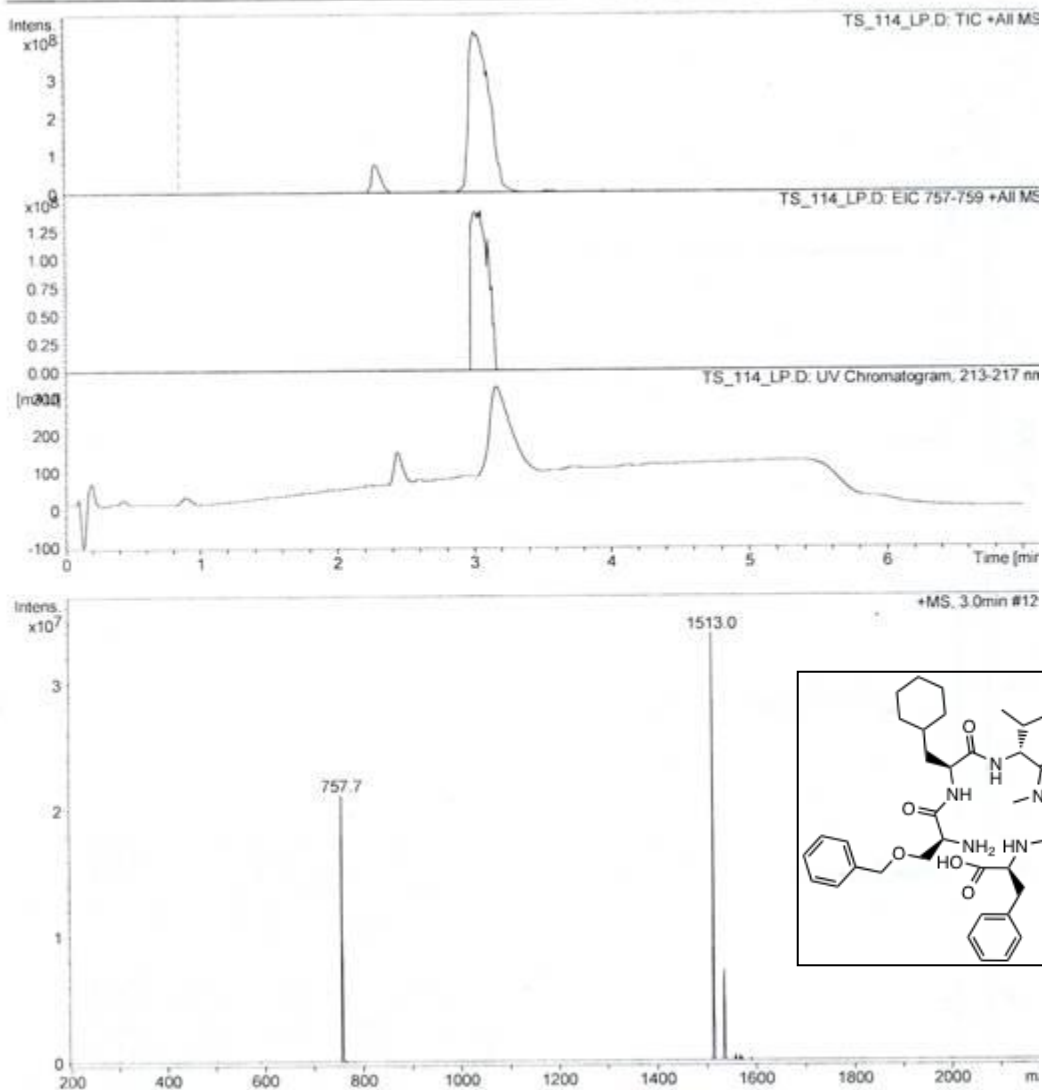
Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	Amount	Units
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2	****	****	****	****	****	****



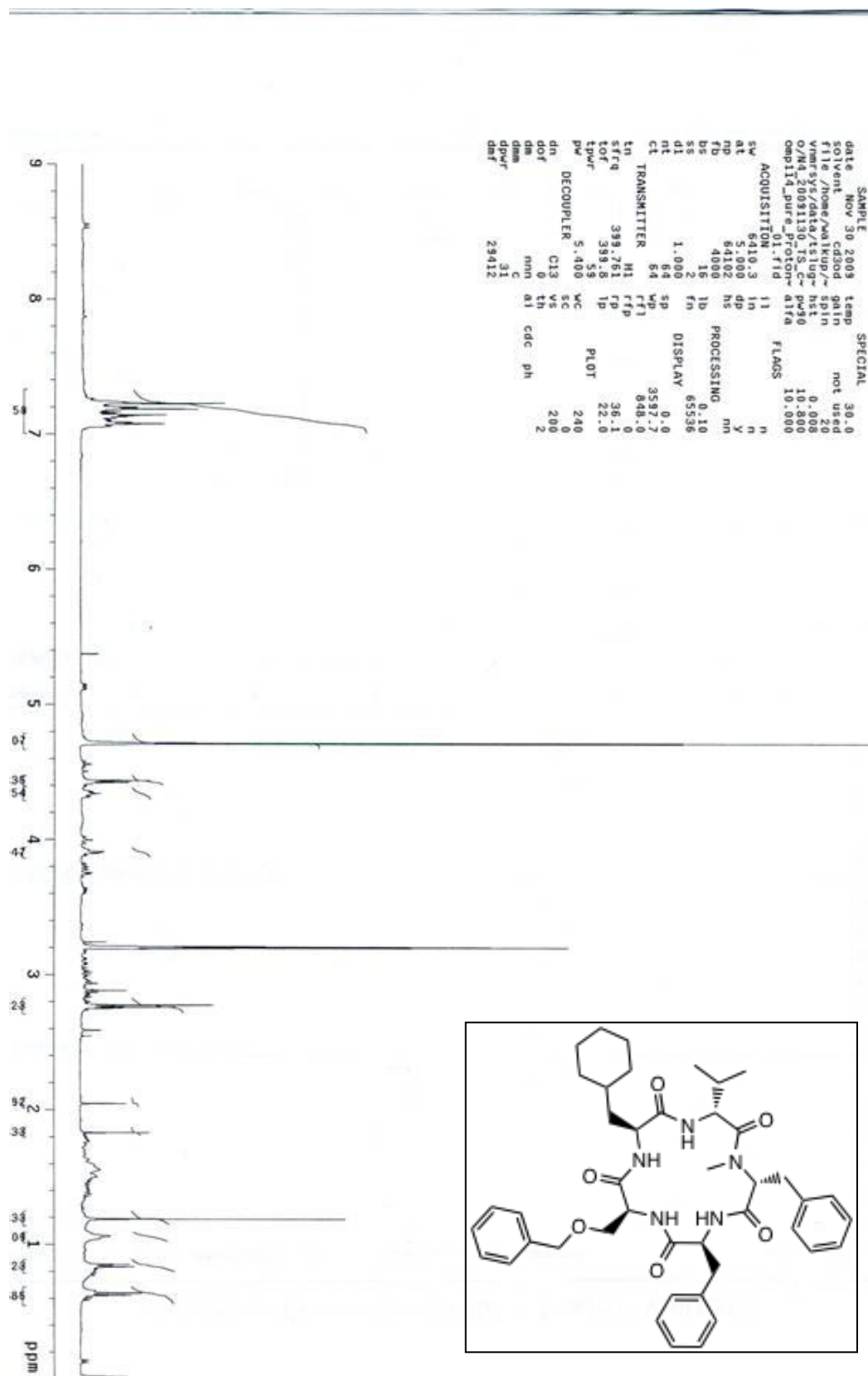
Compound 20 HPLC Cyclized Pentapeptide Phe-D-Phe-D-Val-Cha-Ser(Bzl)

Display Report - All Windows Selected Analysis

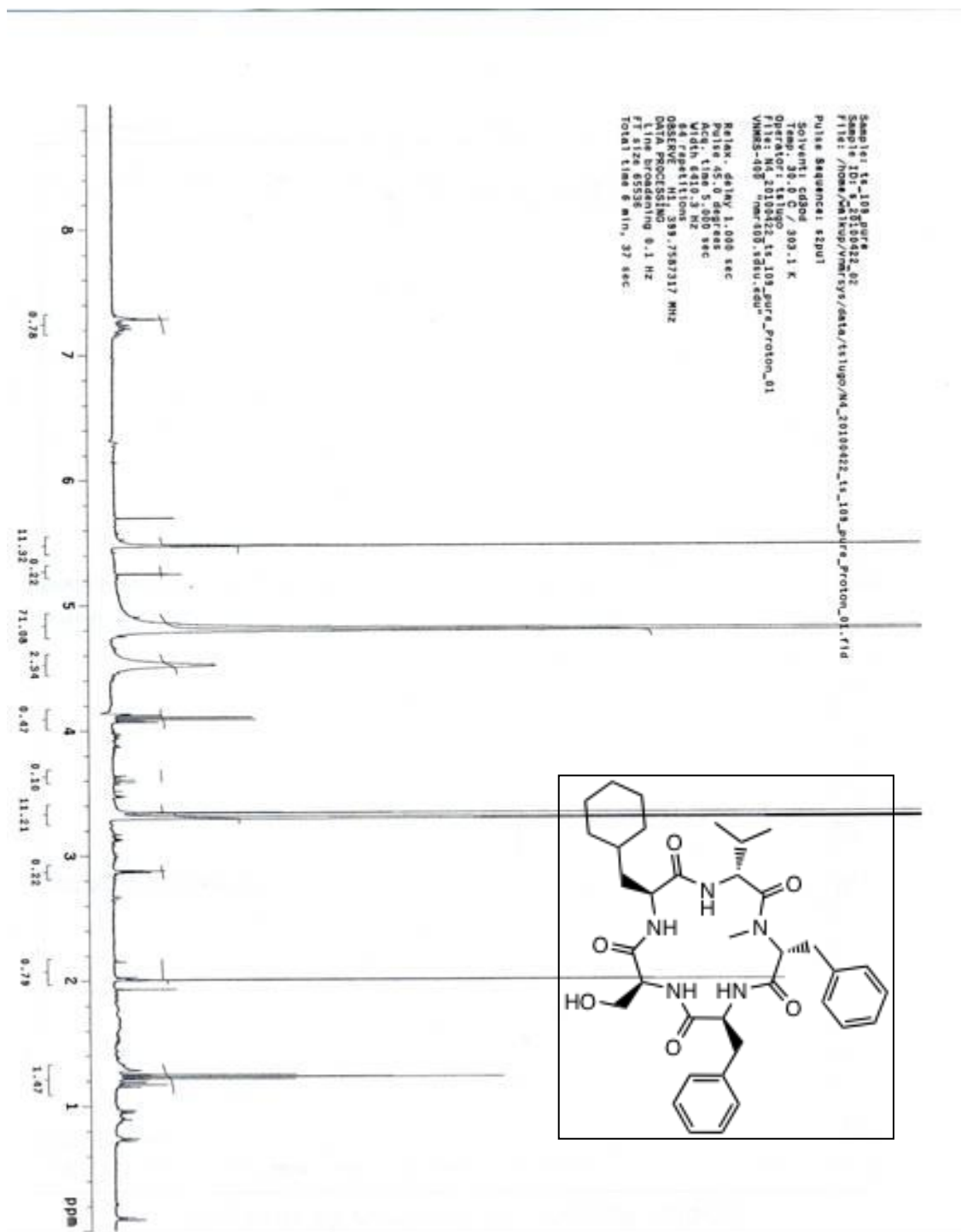
Analysis Name: TS_114_LP.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 11/30/2009 2:44:14 PM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 11/12/2009 3:20:28 PM
Sample Name: ts_114_LP
Analysis Info:



Compound 21 LCMS Double Deprotected Pentapeptide HO-Phe-N-Me-D-Phe-D-Val-Cha-Ser(Bzl)-NH₂ (MW=757)

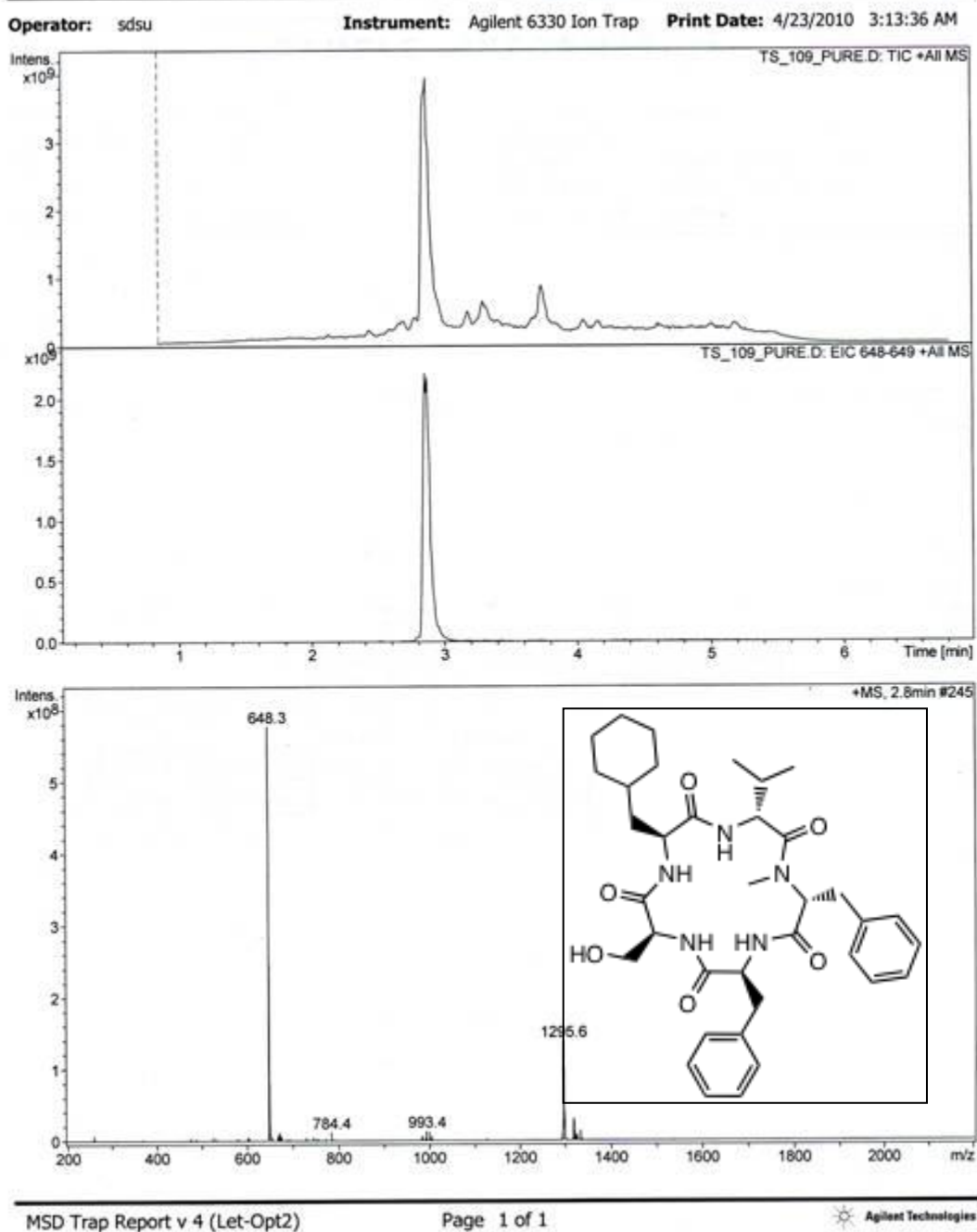


Compound 21 NMR Cyclized Protected Pentapeptide Phe-N-Me-D-Phe-D-Val-Cha-Ser(Bzl)



Compound 21 NMR Cyclized Pentapeptide Phe-N-Me-D-Phe-D-Val-Cha-Ser

Display Report - All Windows All Analyses



Compound 21 LCMS Cyclized Pentapeptide Phe-N-Me-D-Phe-D-Val-Cha-Ser

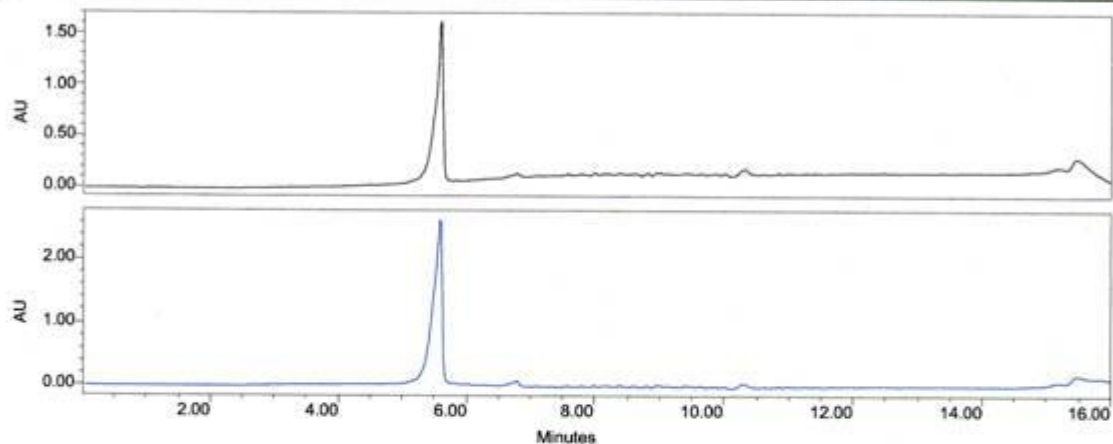
SDSU

Project Name: Defaults
Reported by User: System

Breeze

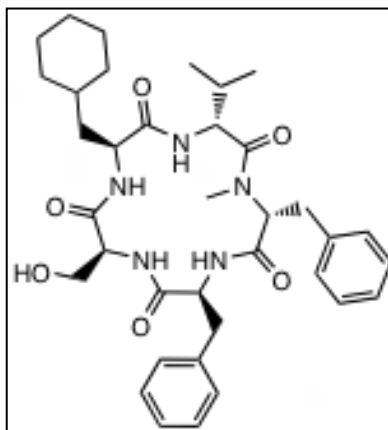
SAMPLE INFORMATION

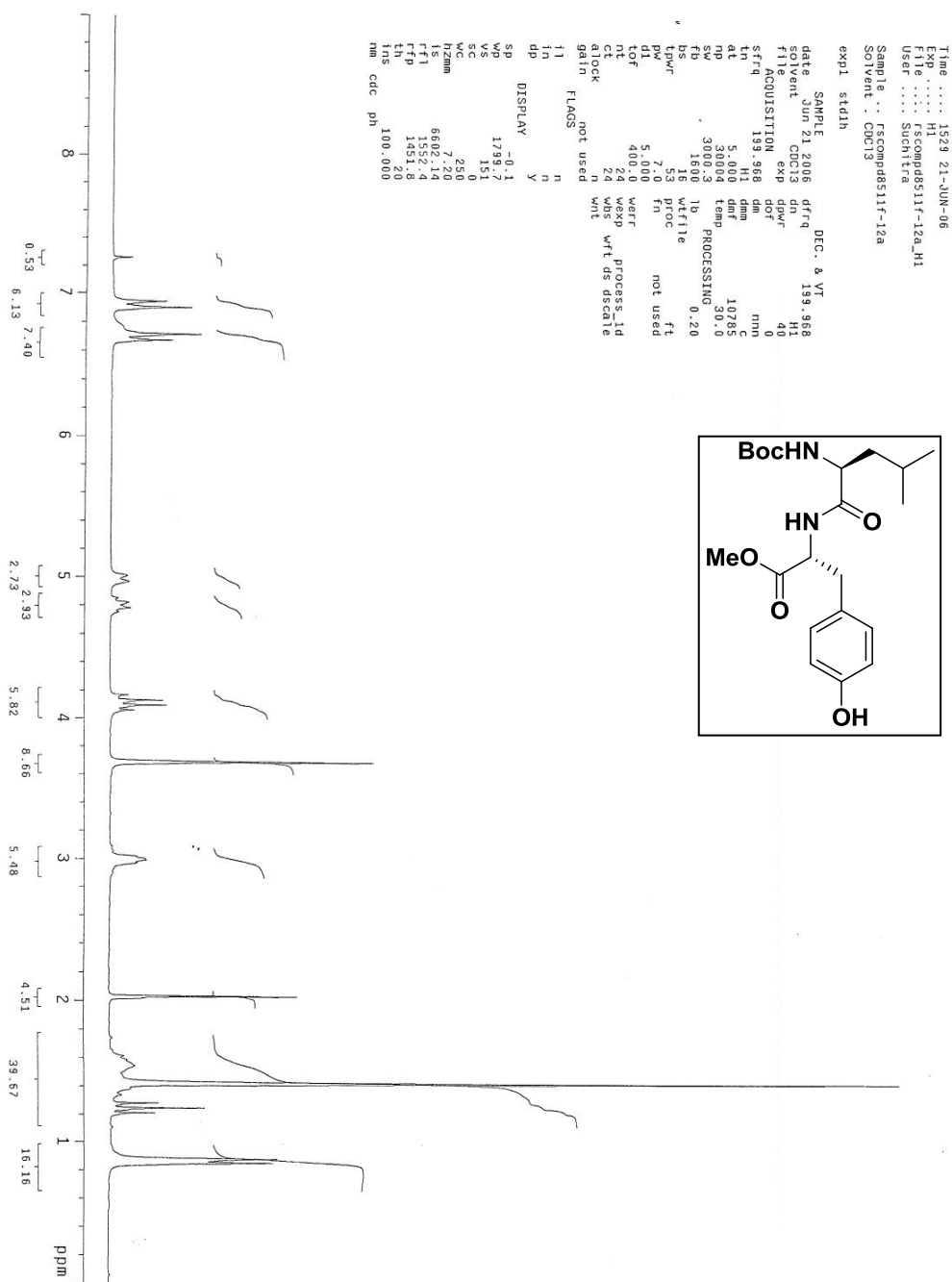
Sample Name:	ts_109_pure	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	702	Date Acquired:	4/20/2010 3:28:55 PM
Run Time:	16.00 Minutes	Injection Volume:	60.00 ul



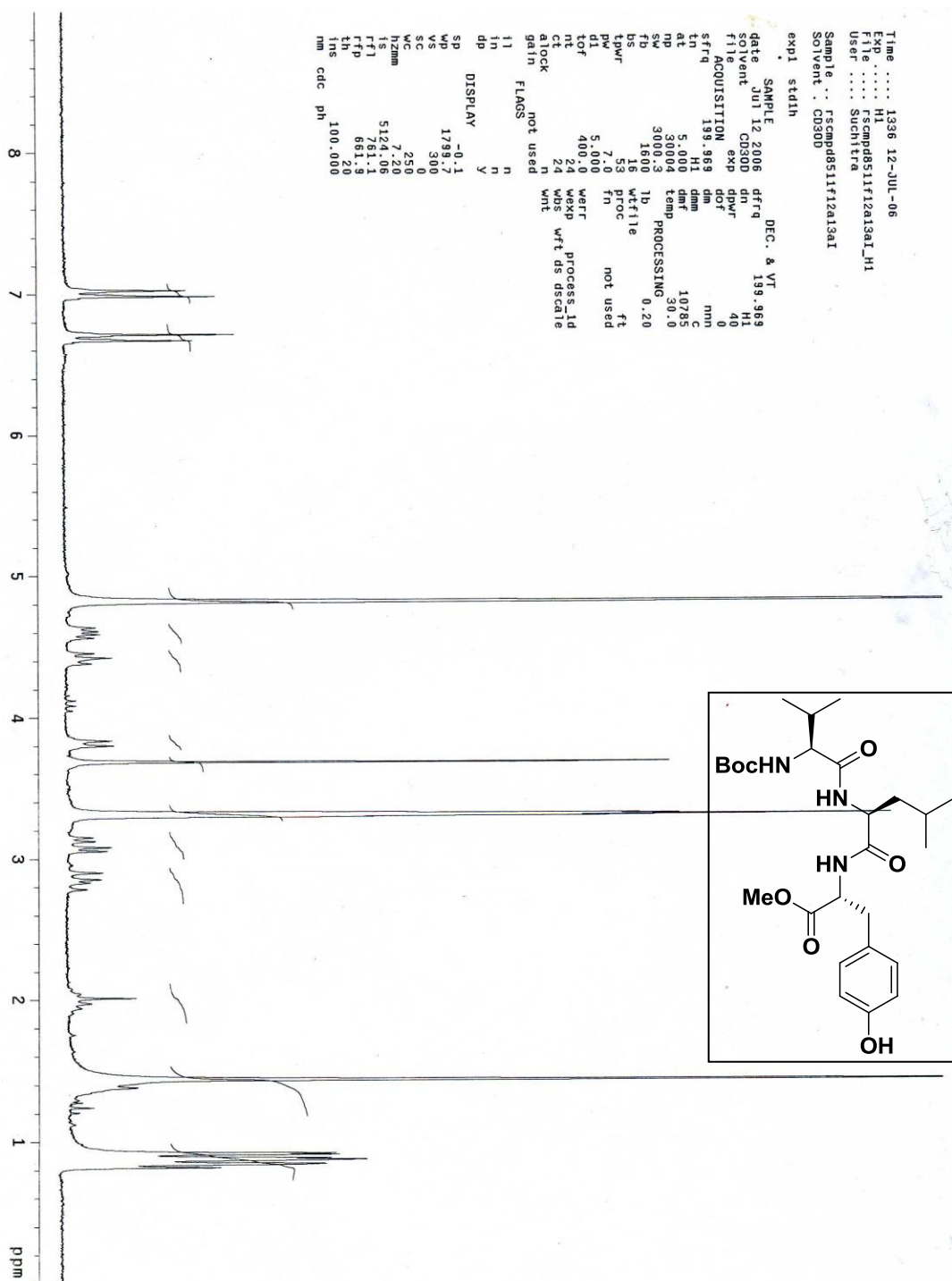
— Channel: 2487Channel 1 Channel Desc.: Processing Method: *
 — Channel: 2487Channel 2 Channel Desc.: Processing Method: *

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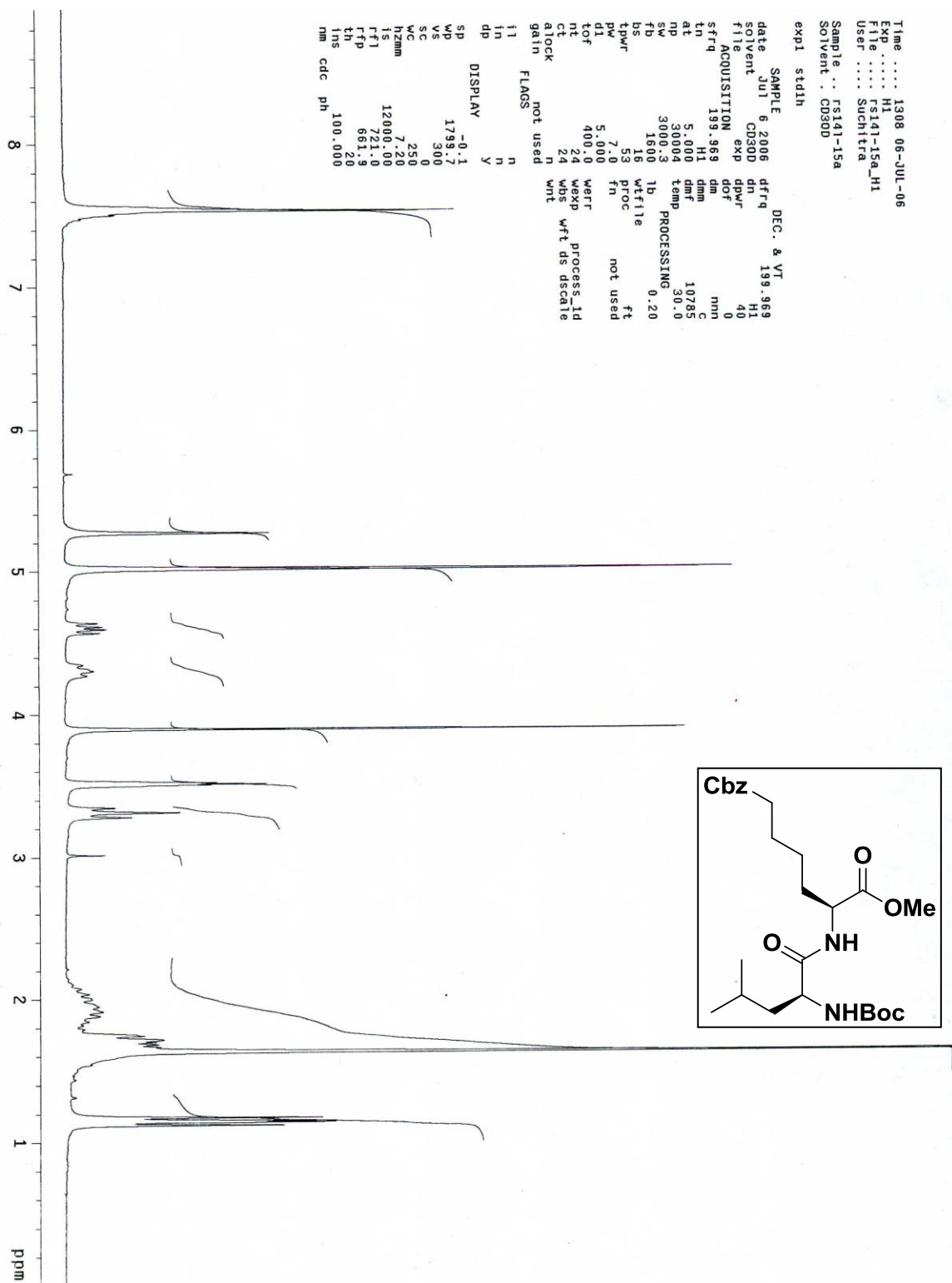




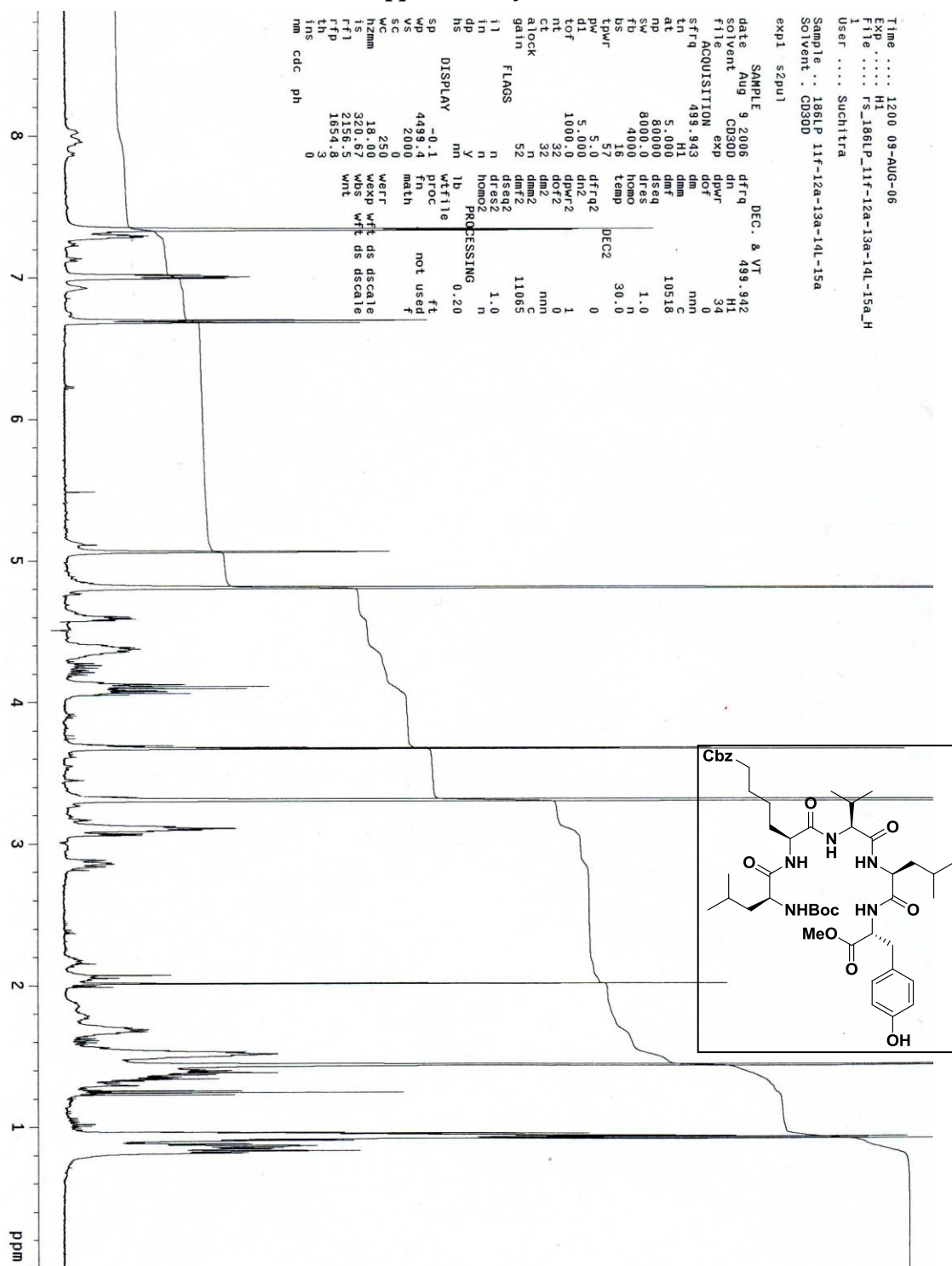
Compound 23 NMR Dipeptide MeO-D-Tyr-Leu-NHBoc



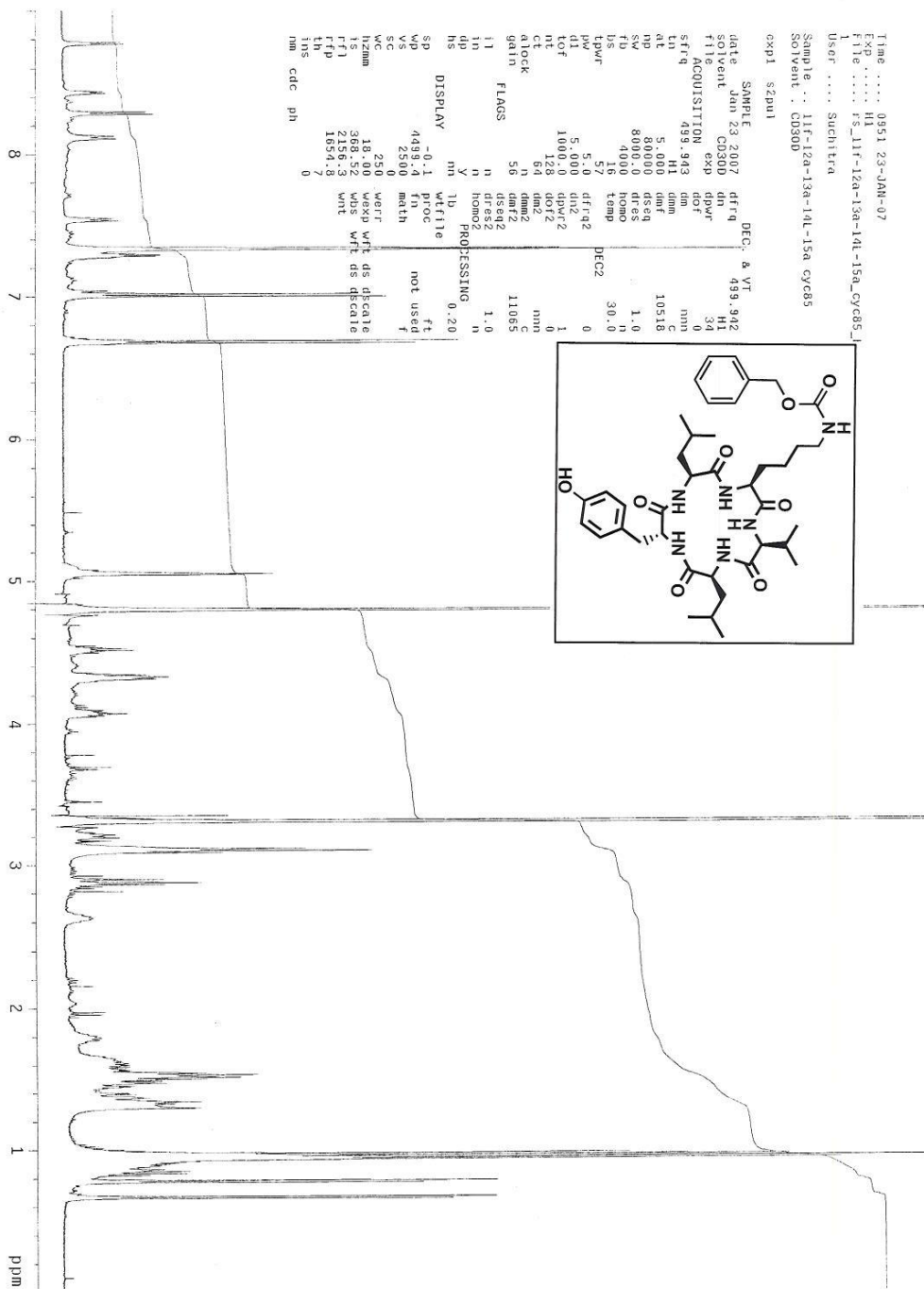
Compound 23 NMR Tripeptide MeO-D-Tyr-Leu-Val-NHBoc



Compound 23 NMR Dipeptide MeO-Lys(Cbz)-Leu-NHBoc



Compound 23 NMR Linear Pentapeptide MeO-D-Tyr-Leu-Val-Lys(Cbz)-Leu-NHBoc

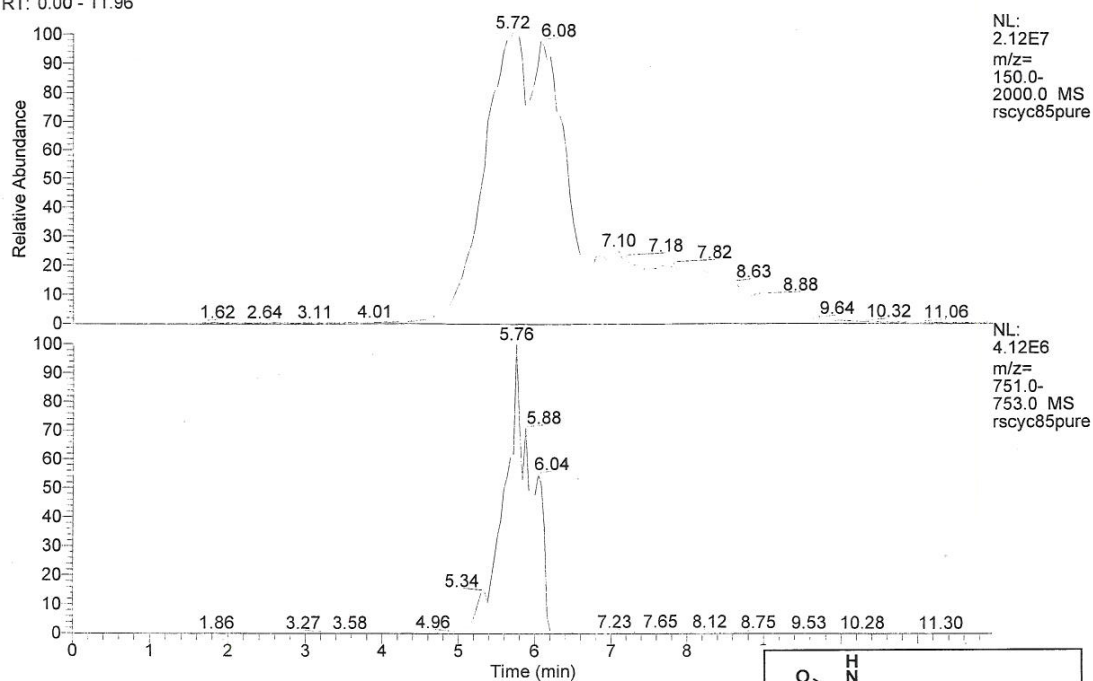
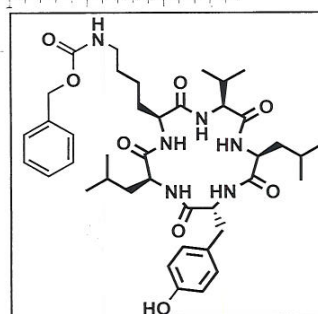
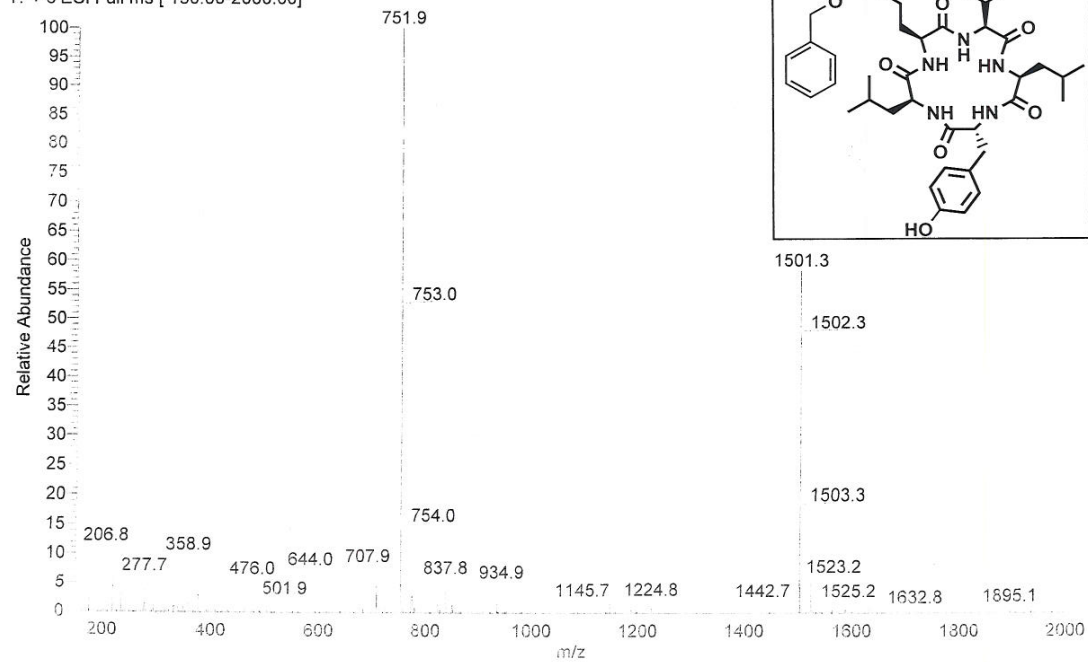


Compound 23 NMR Cyclized Pentapeptide D-Tyr-Leu-Val-Lys(Cbz)-Leu

D:\Department Results\...rscyc85pure
rscyc85pure

10/19/06 10:29:08 AM

RT: 0.00 - 11.96

rscyc85pure #111 RT: 5.88 AV: 1 NL: 1.92E6
T: + c ESI Full ms [150.00-2000.00]

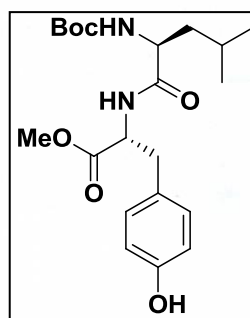
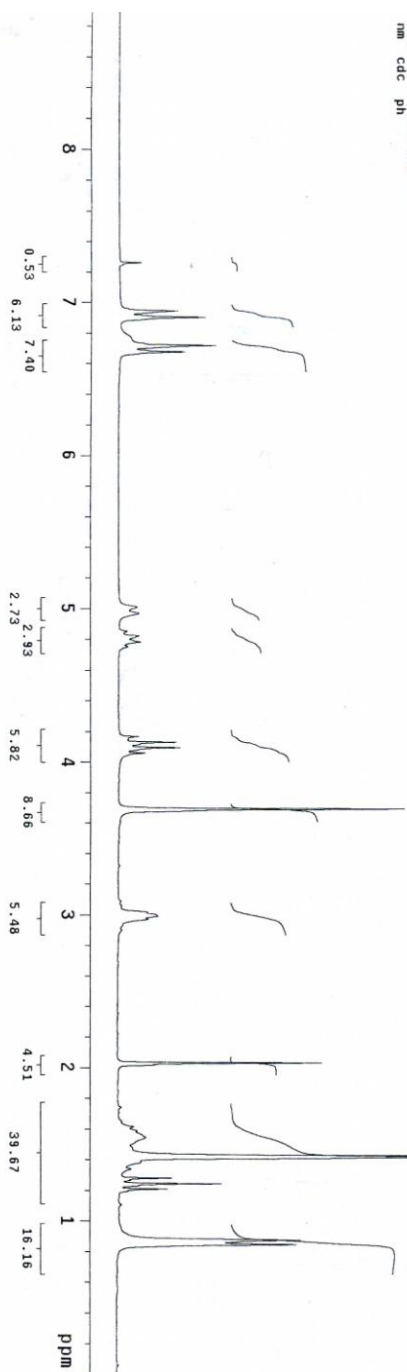
Compound 23 LCMS Cyclized Pentapeptide D-Tyr-Leu-Val-Lys(Cbz)-Leu (MW=751)


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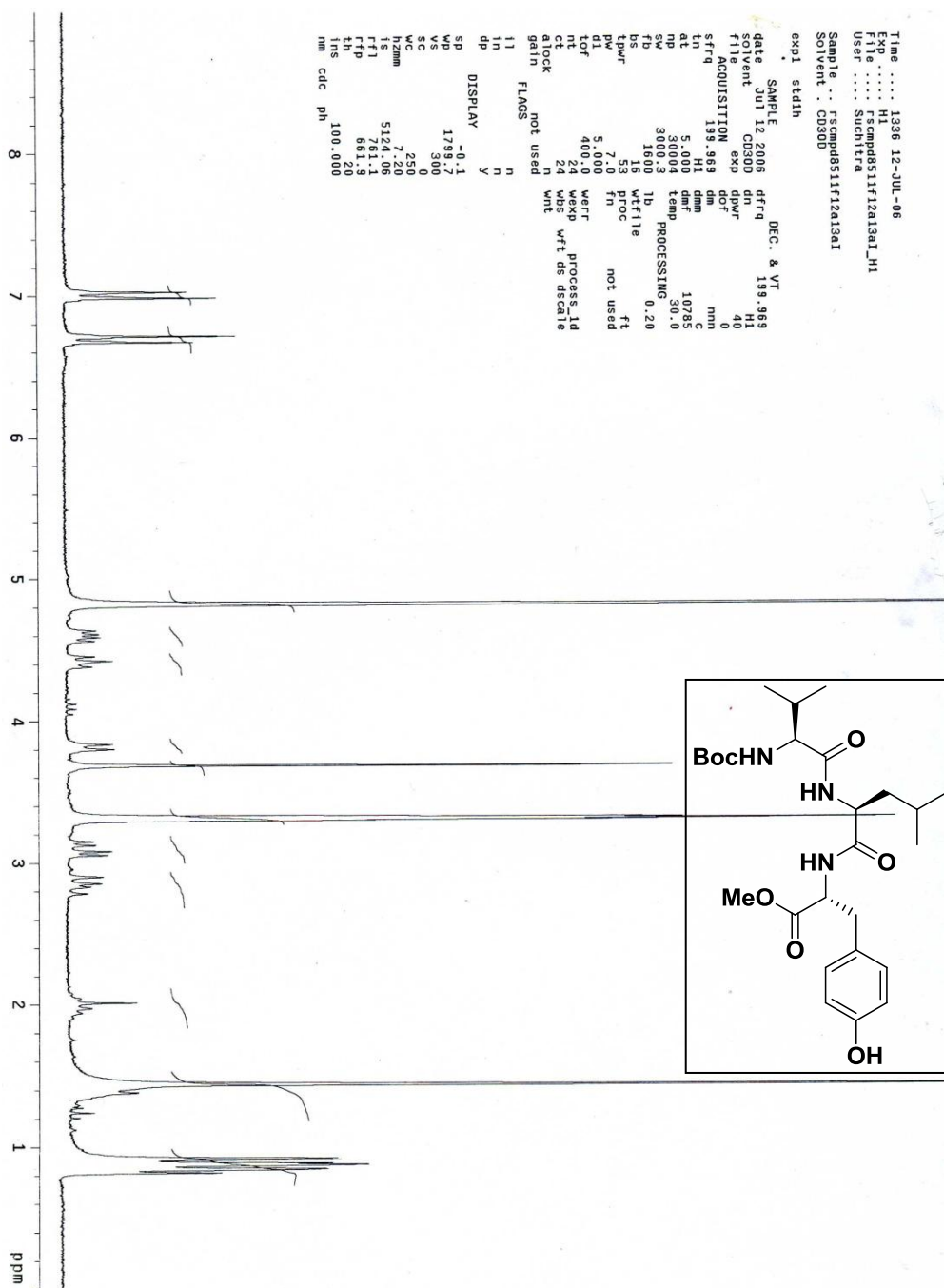
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User ..... Suchitra
Sample .. fscmpd511f-12a
Solvent .. CDCl3
expi stdin

SAMPLE          DEC. & VT
date            un 21 2006  dfrq 199.968
solvent         CDCl3  dn      H1
file           exp      dpr  40
ACQUISITION    dof      0
sfrq           199.968  dm      mm
IN             5.000    dm      10265
NS             30000    temp  30.0
SW             9000.3   PROCESsing 0.20
fb             1800    lb      wftt1e
bs             16      proc  ft
lpwr           7.0    fn      not used
pw            5.000   warr  400.0
tof           400.0   wexp  24
nt            24     wts  wft ds dscate
ct            24     wnt  not used
alock         n
gain         not used
ll           n
in           n
dp           y
DISPLAY      -0.1
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lns         100.000
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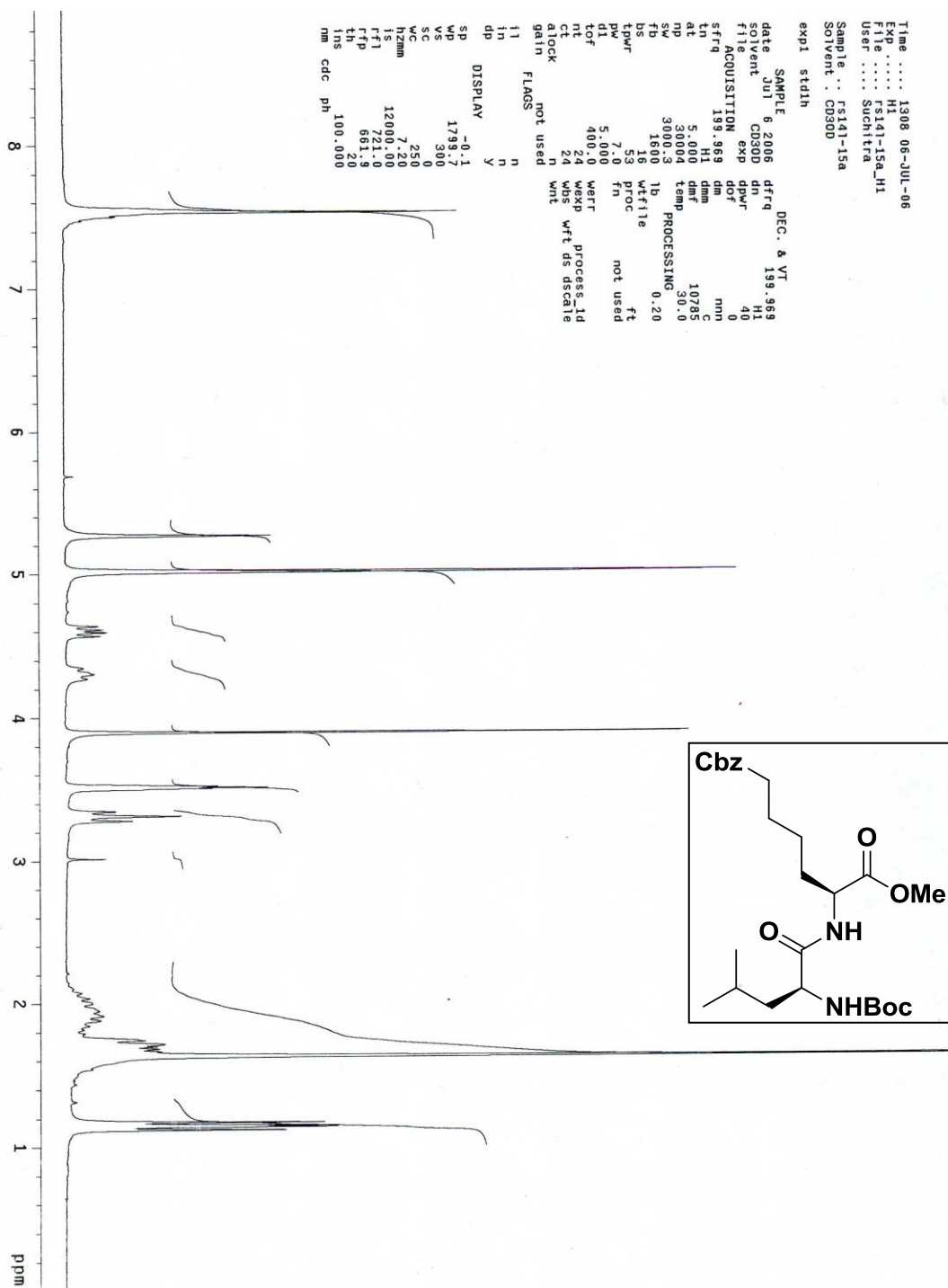
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Compound 24 NMR Dipeptide MeO-D-Tyr-Leu-NHBoc

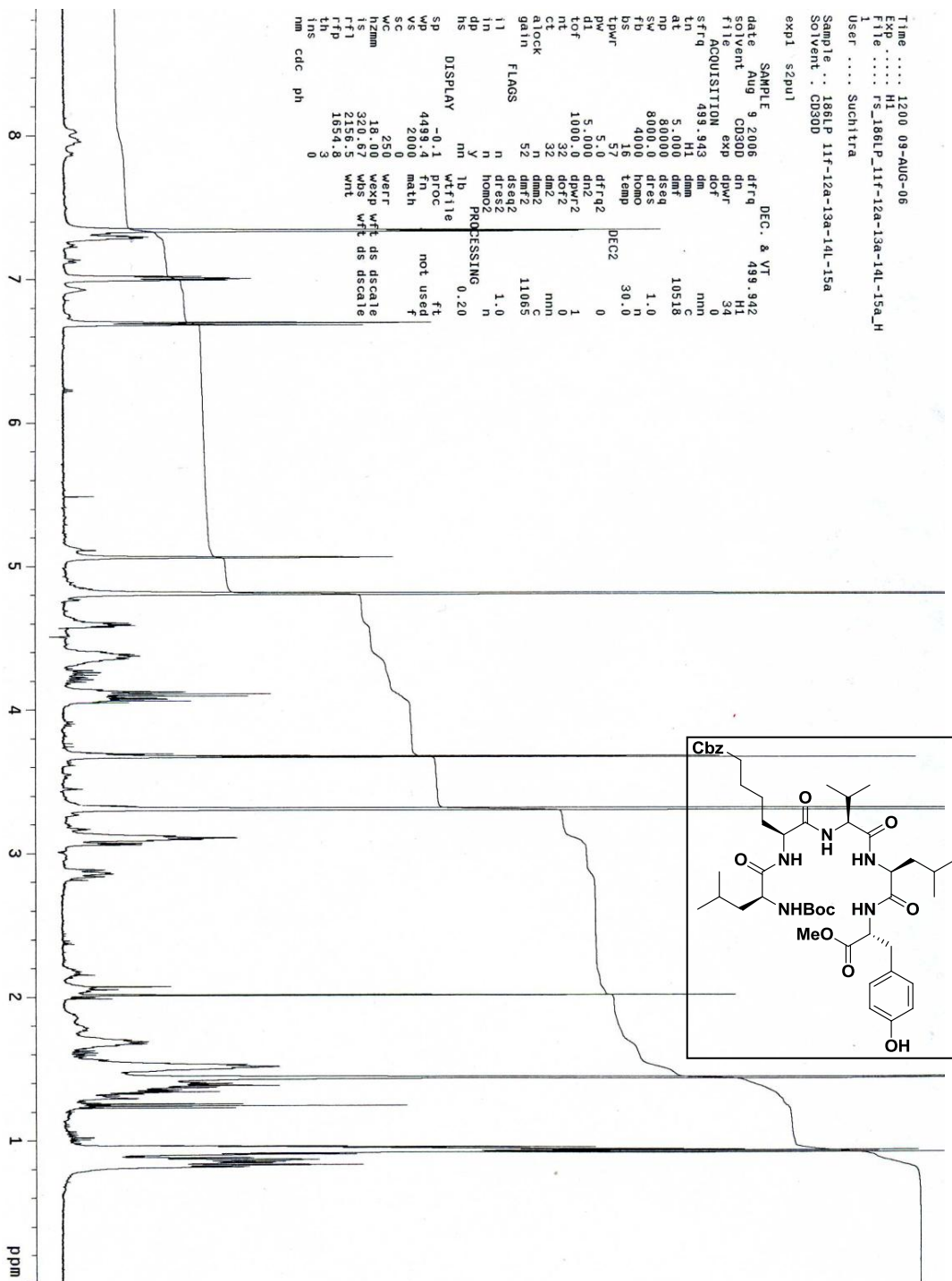


Compound 24 NMR Tripeptide MeO-D-Tyr-Leu-Val-NHBoc

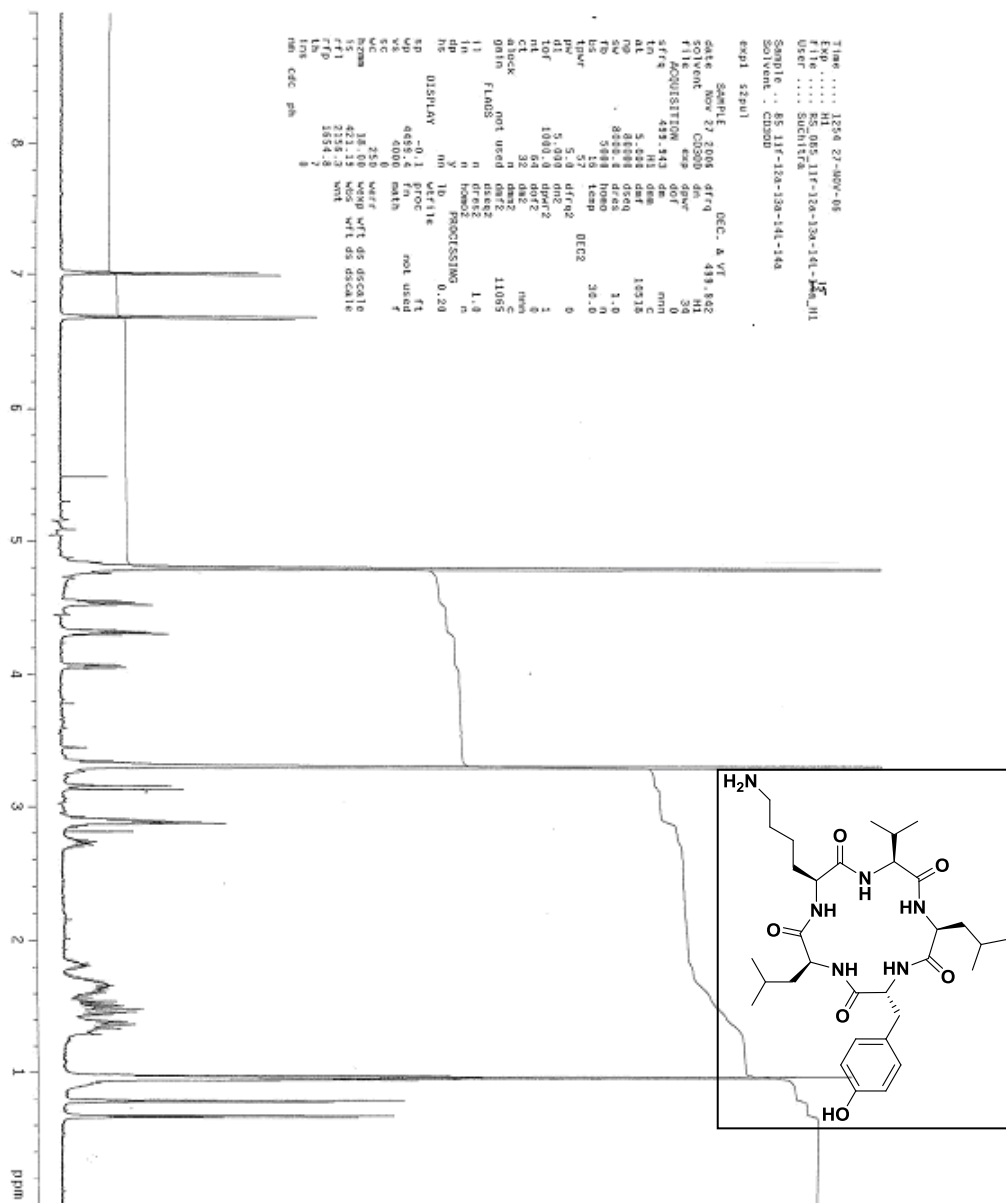


Compound 24 NMR Dipeptide MeO-Lys(Cbz)-Leu-NHBoc

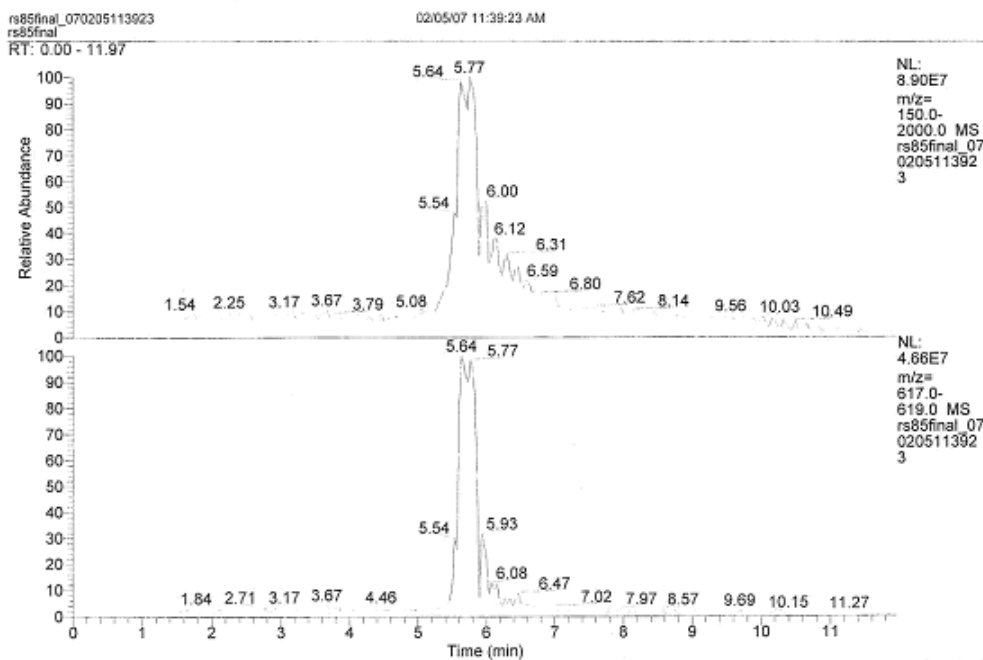
Supplementary Material



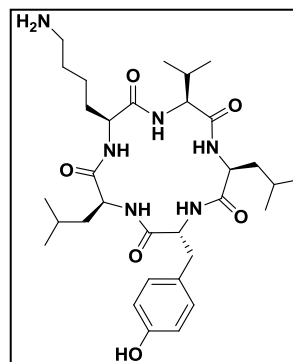
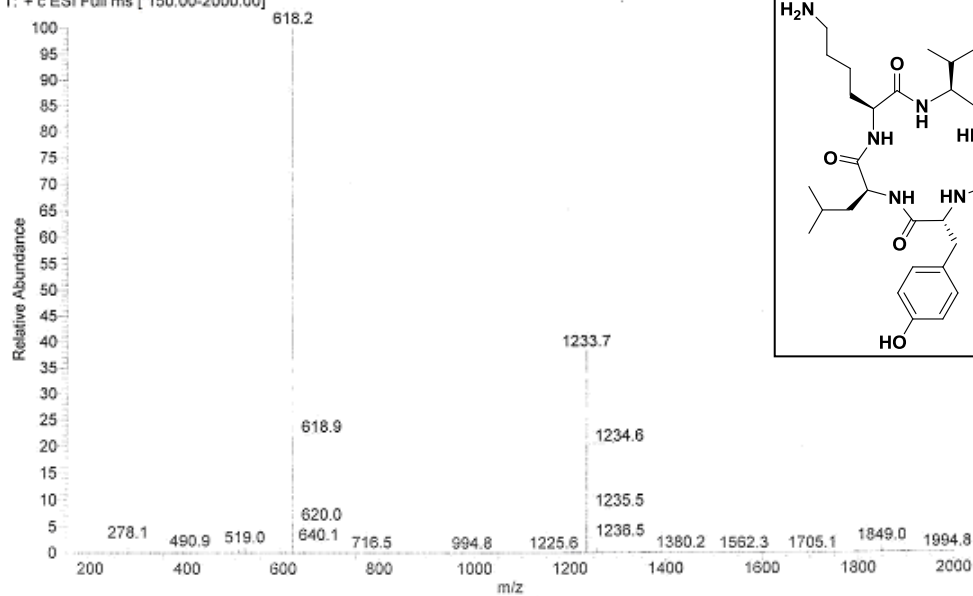
Compound 24 NMR Linear Pentapeptide MeO-D-Tyr-Leu-Val-Lys(Cbz)-Leu-NHBoc



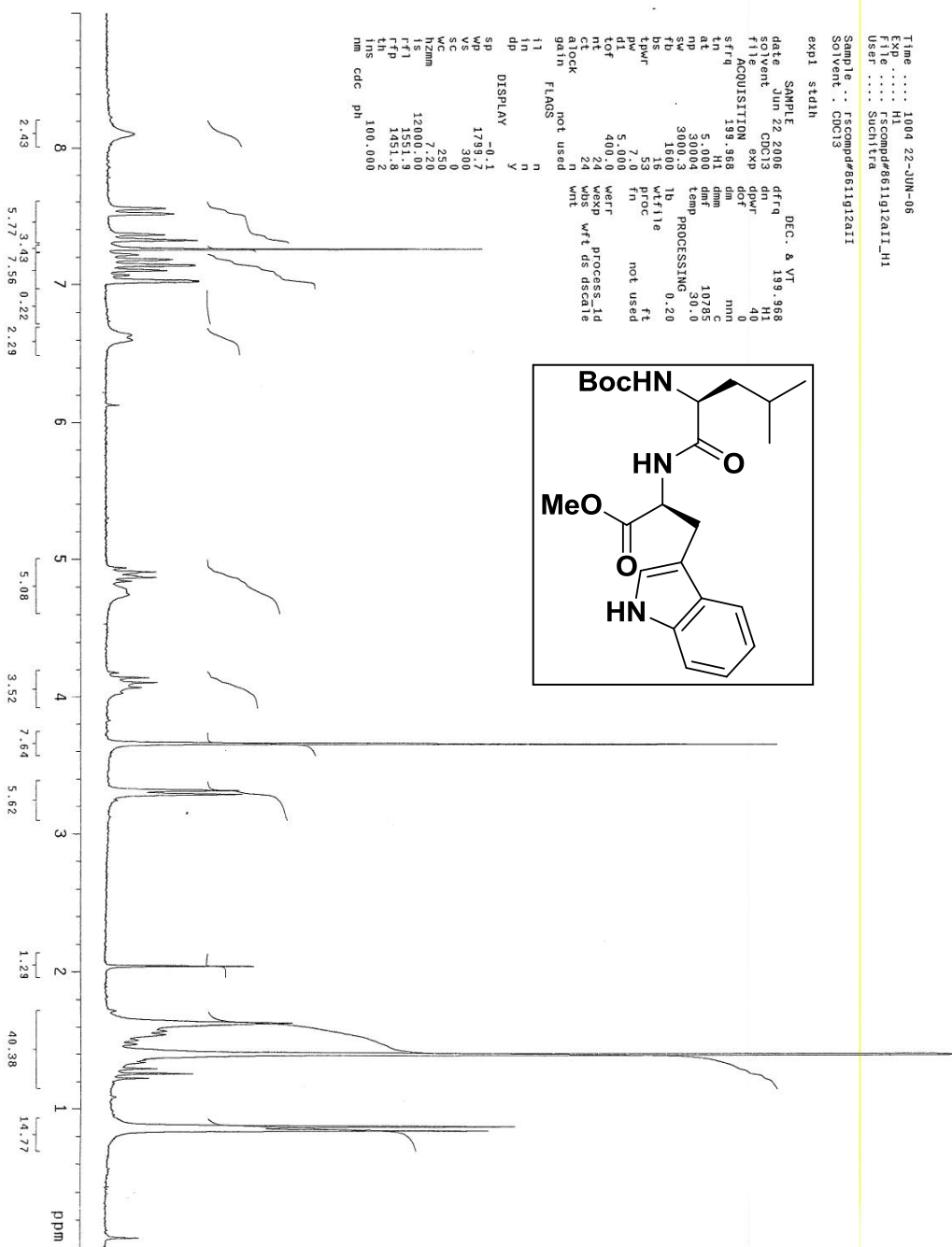
Compound 24 NMR Cyclized Pentapeptide D-Tyr-Leu-Val-Lys-Leu



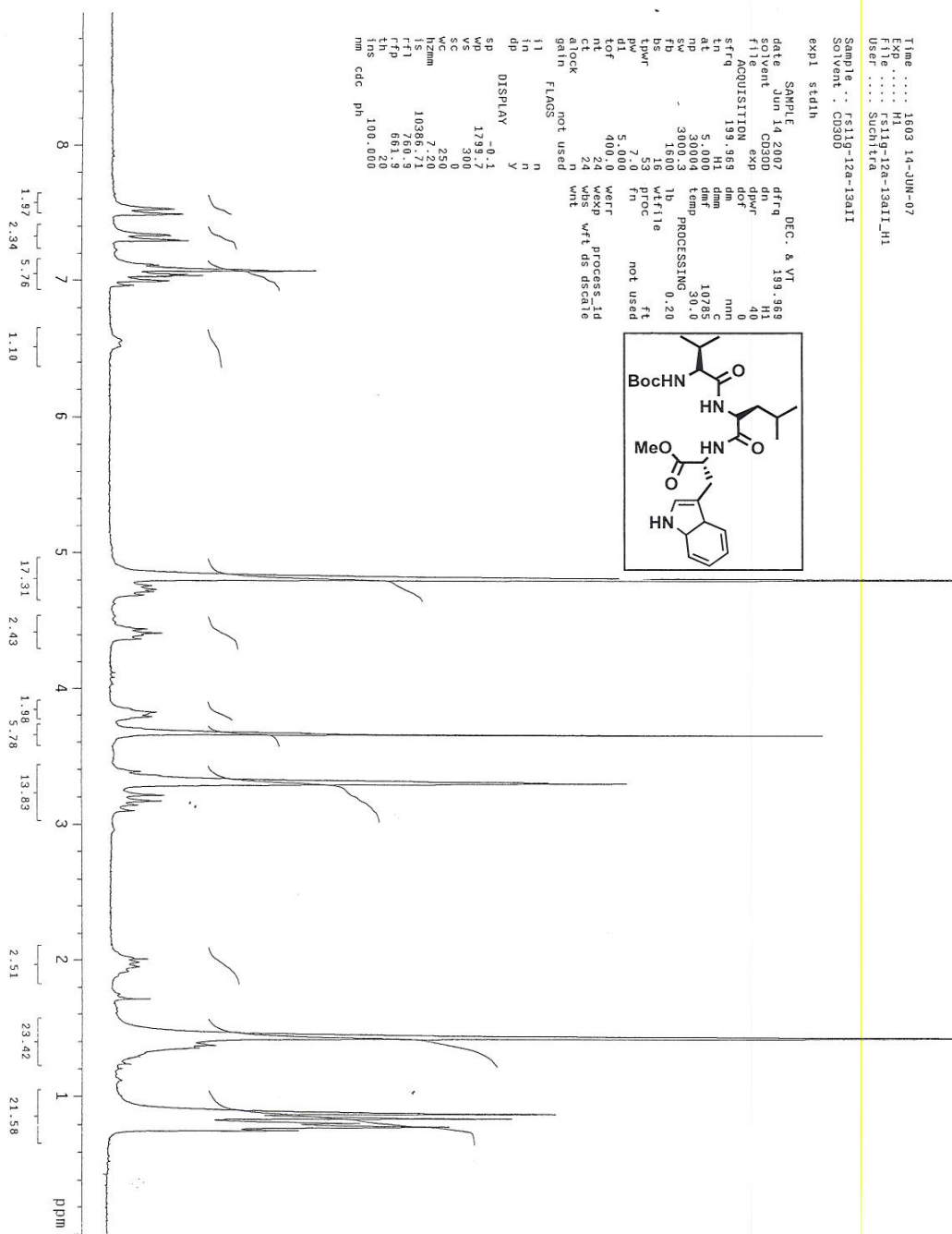
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T: + c ESI Full ms [150.00-2000.00]



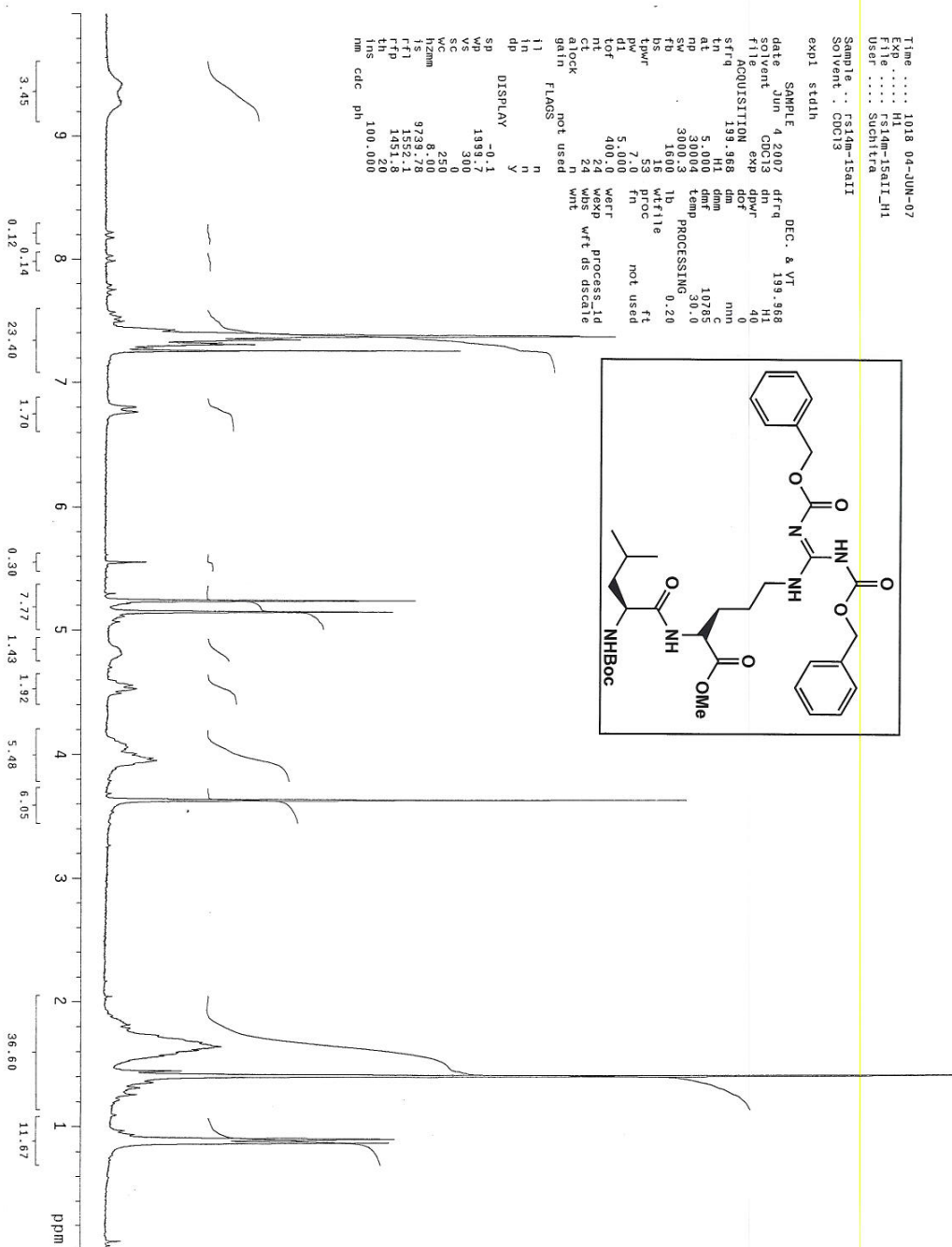
Compound 24 LCMS Cyclized Pentapeptide D-Tyr-Leu-Val-Lys-Leu (MW=616.8)



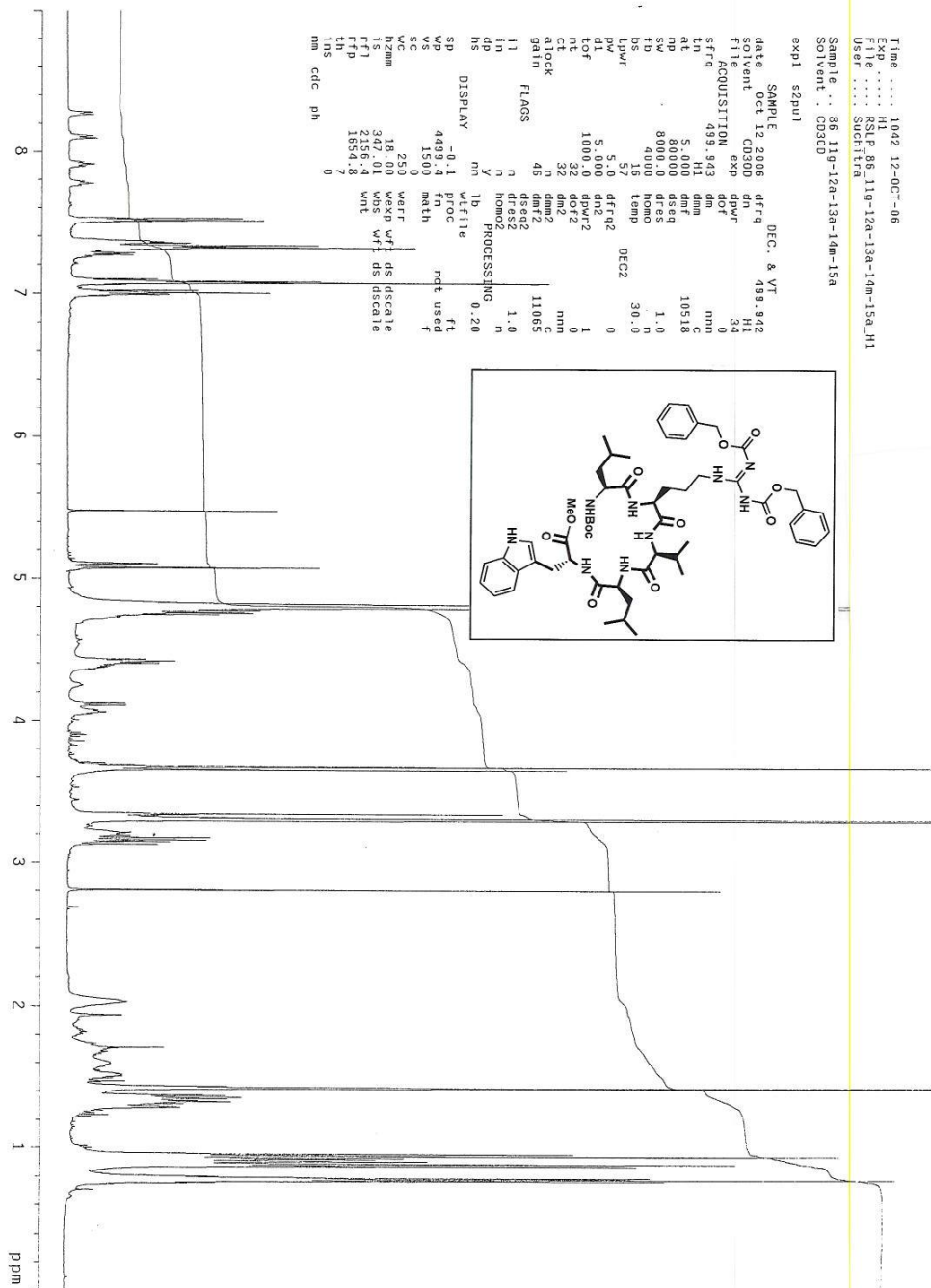
Compound 26 NMR Dipeptide MeO-D-Trp-Leu-NHBoc



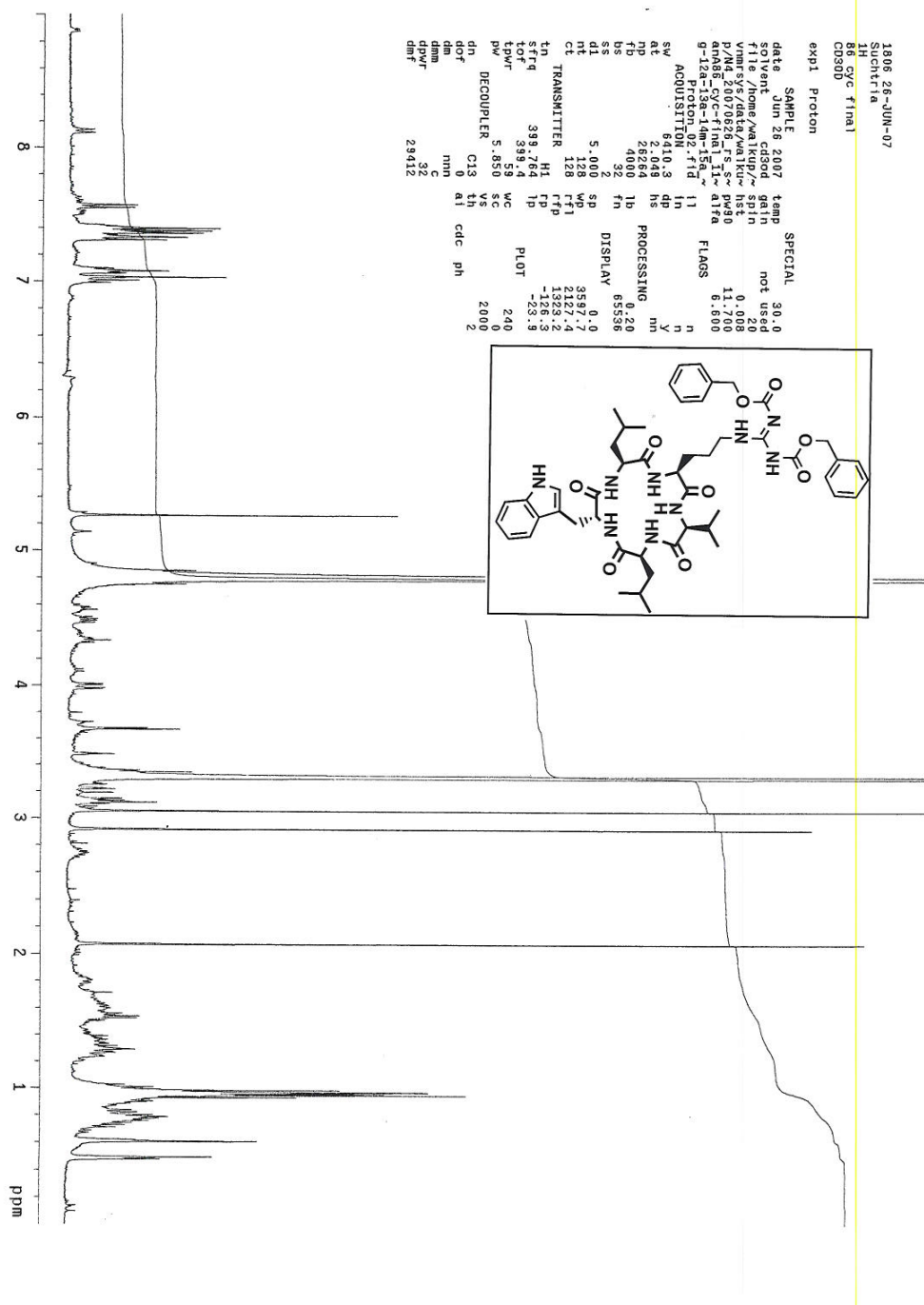
Compound 26 NMR Tripeptide MeO-D-Trp-Leu-Val-NHBoc



Compound 26 NMR Dipeptide MeO-Arg(2Cbz)-Leu-NHBoc



Compound 26 NMR Linear Pentapeptide MeO-D-Trp-Leu-Val-Arg(2Cbz)-Leu-NHBoc



Compound 26 NMR Cyclized Pentapeptide D-Trp-Leu-Val-Arg(2Cbz)-Leu

FractionLynx Report - srx

Sample: 1
File:srx326-1
Description:

Vial:5,1:30
Date:15-Nov-2007

ID:4330
Time:09:15:53

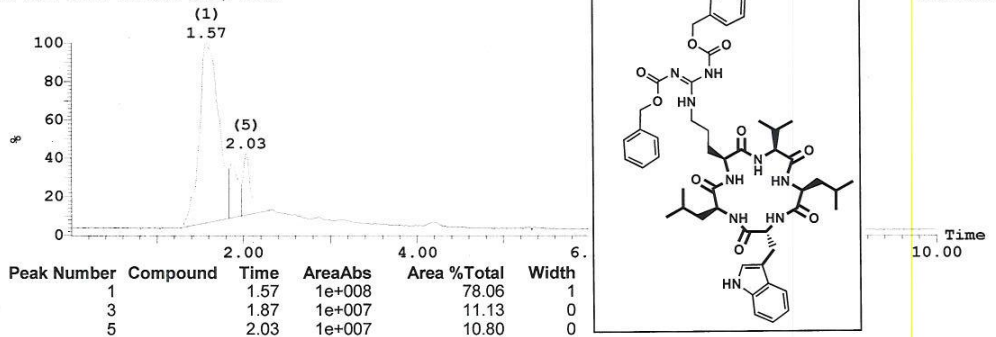
Page 1

Printed: Thu Nov 15 09:37:28 2007

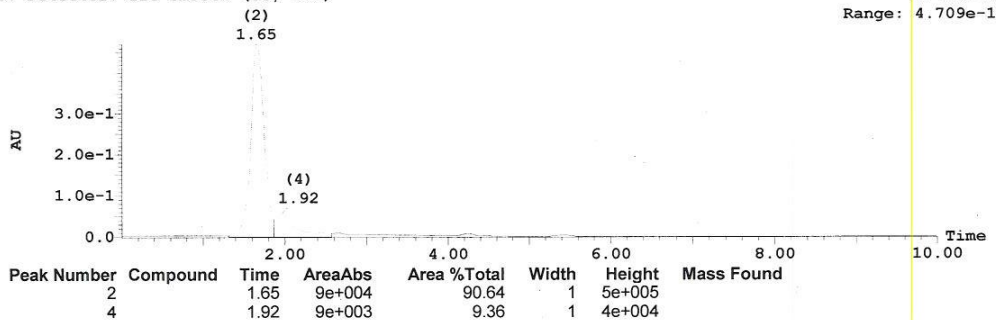
Sample Report:

Sample 1 Vial 5,1:30 ID 4330 File srx326-1 Date 15-Nov-2007 Time 09:15:53 Description

MS ES+ :TIC Smooth (SG, 2x2)



UV Detector: TIC Smooth (SG, 2x2)

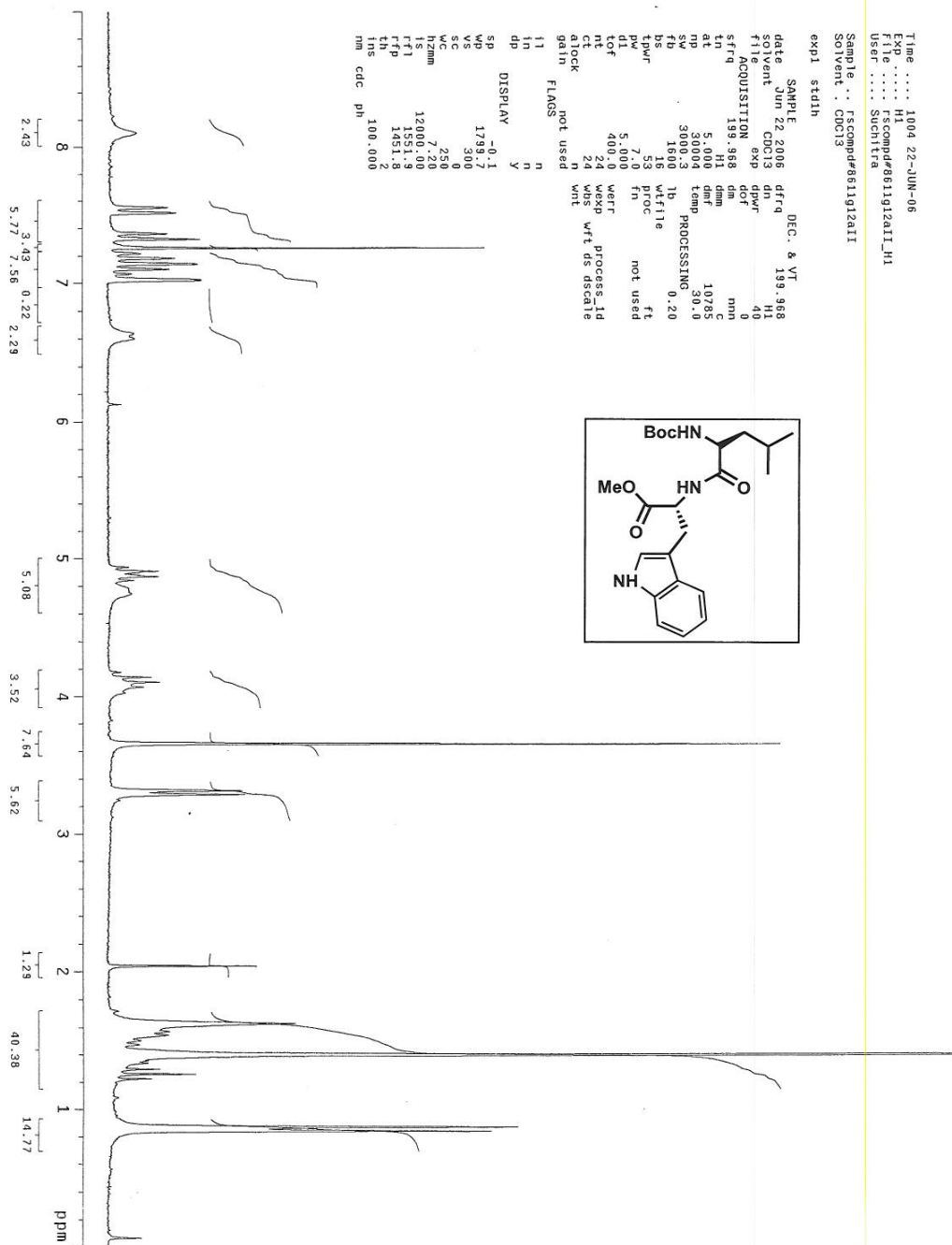


Peak ID	Compound	Time	Mass Found
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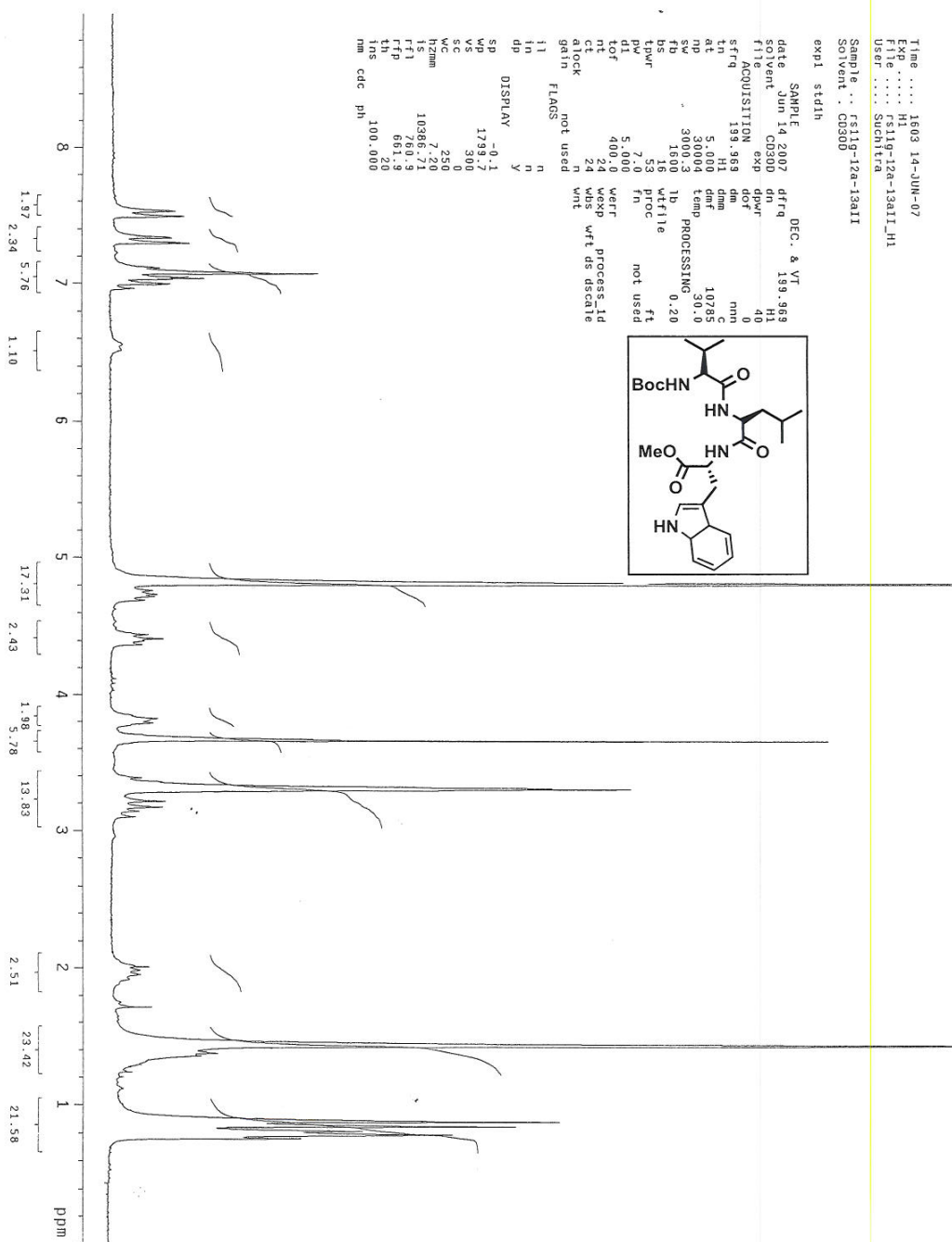
SAMPLE: 5,1:30 Combine (151:161-(70:75+231:236))



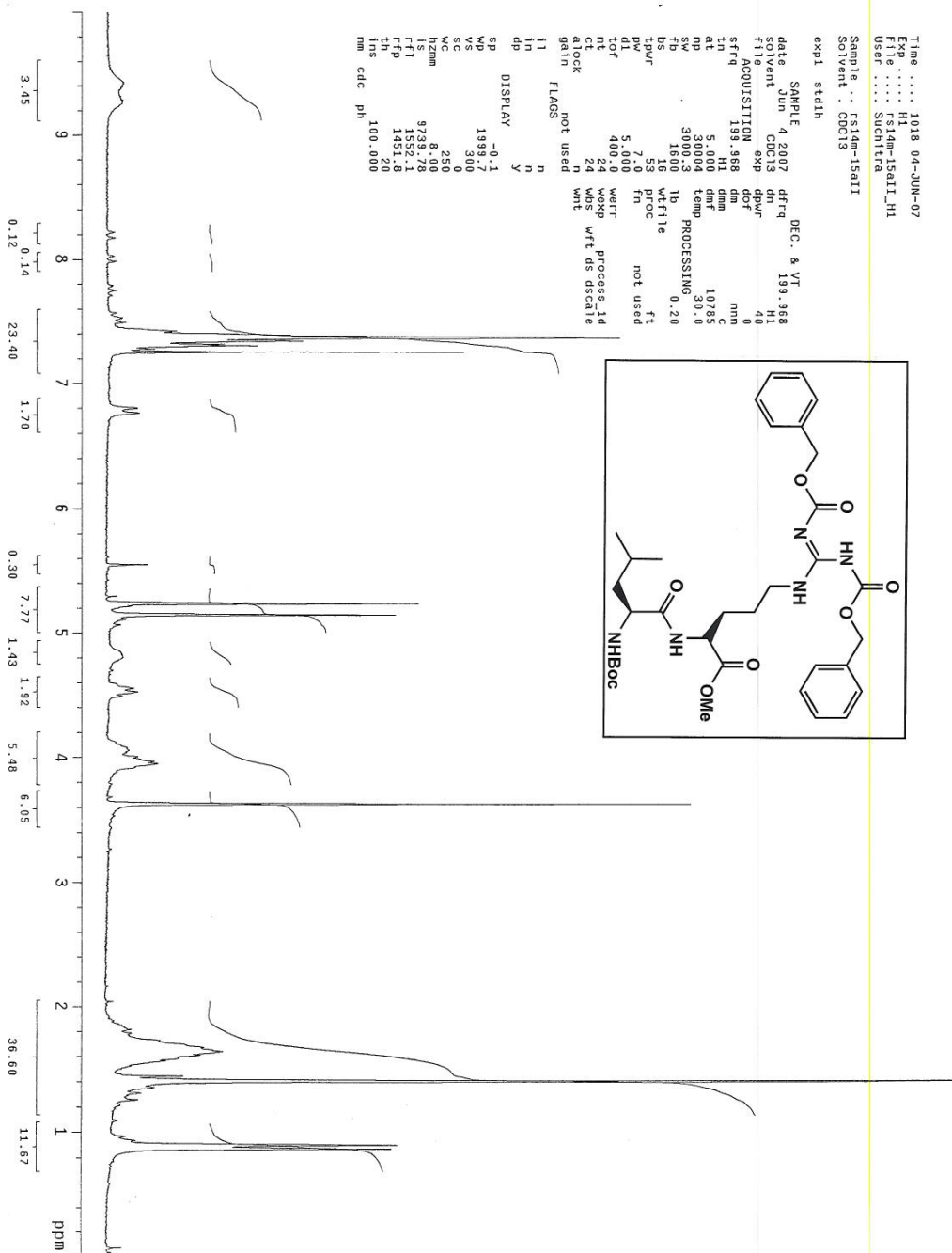
Compound 26 LCMS Cyclized Pentapeptide D-Trp-Leu-Val-Arg(2Cbz)-Leu (MW=802)



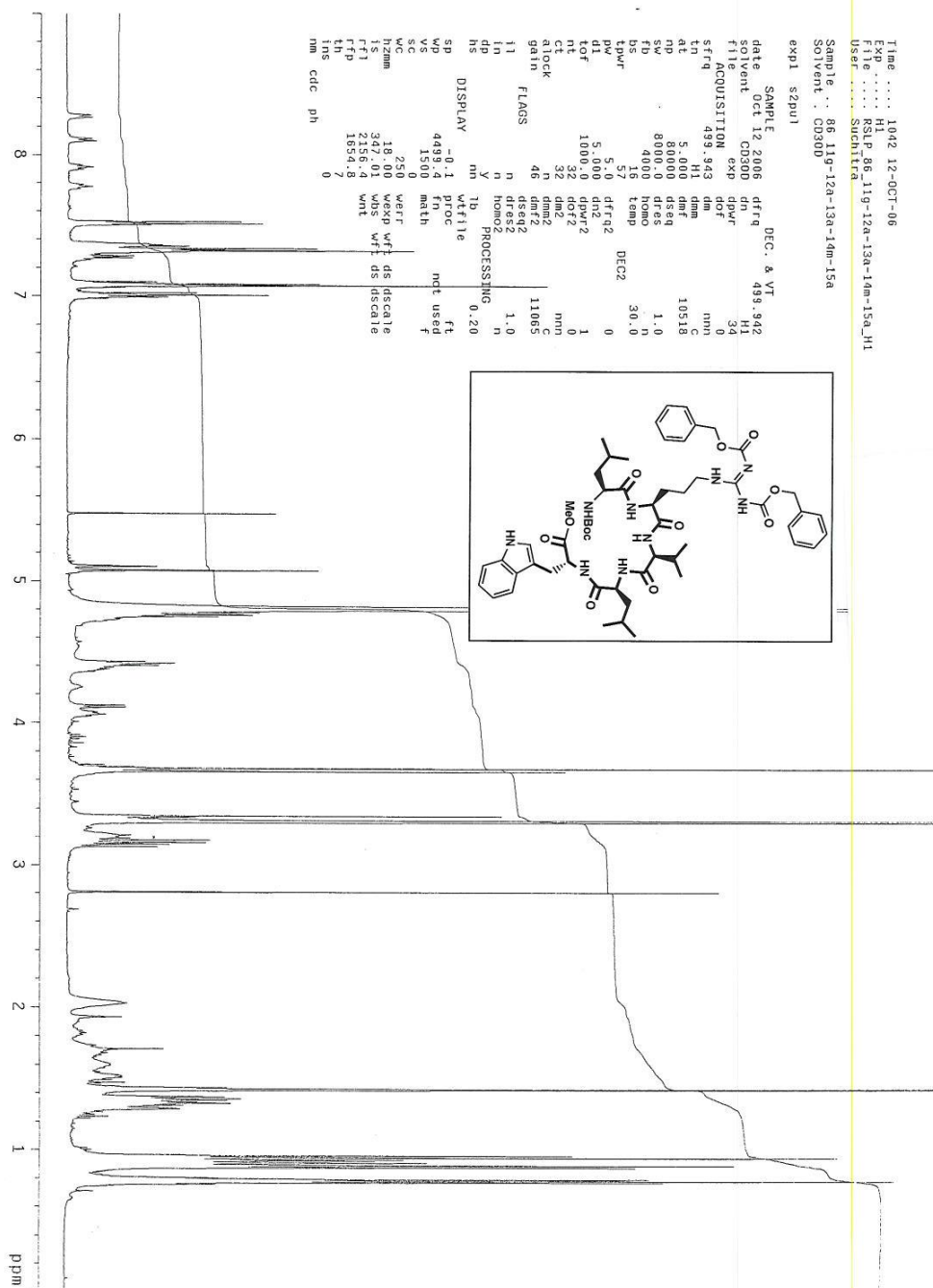
Compound 27 NMR Dipeptide MeO-D-Trp-Leu-NHBoc



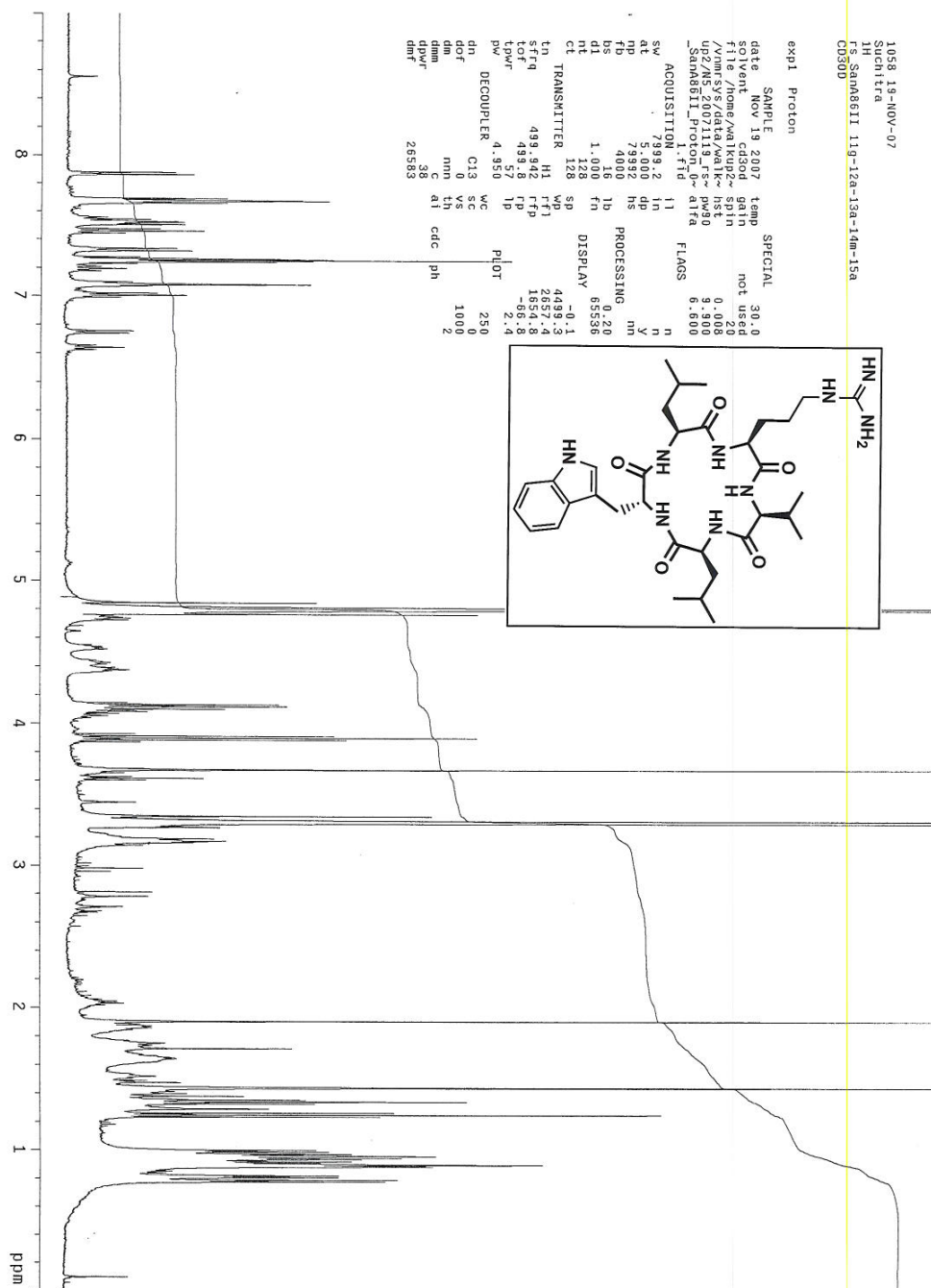
Compound 27 NMR Tripeptide MeO-D-Trp-Leu-Val-NHBoc



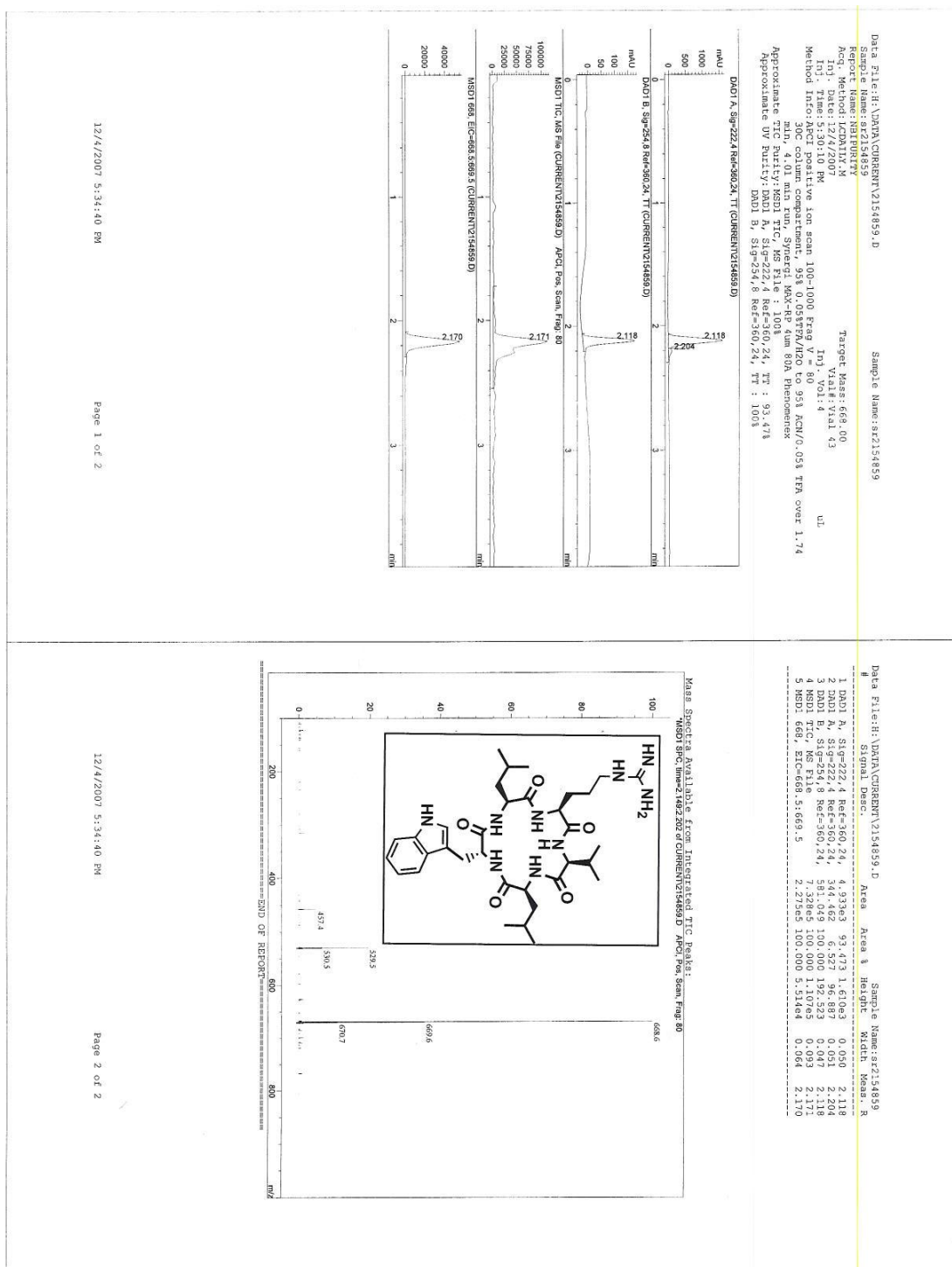
Compound 27 NMR Dipeptide MeO-Arg(2Cbz)-Leu-NHBoc



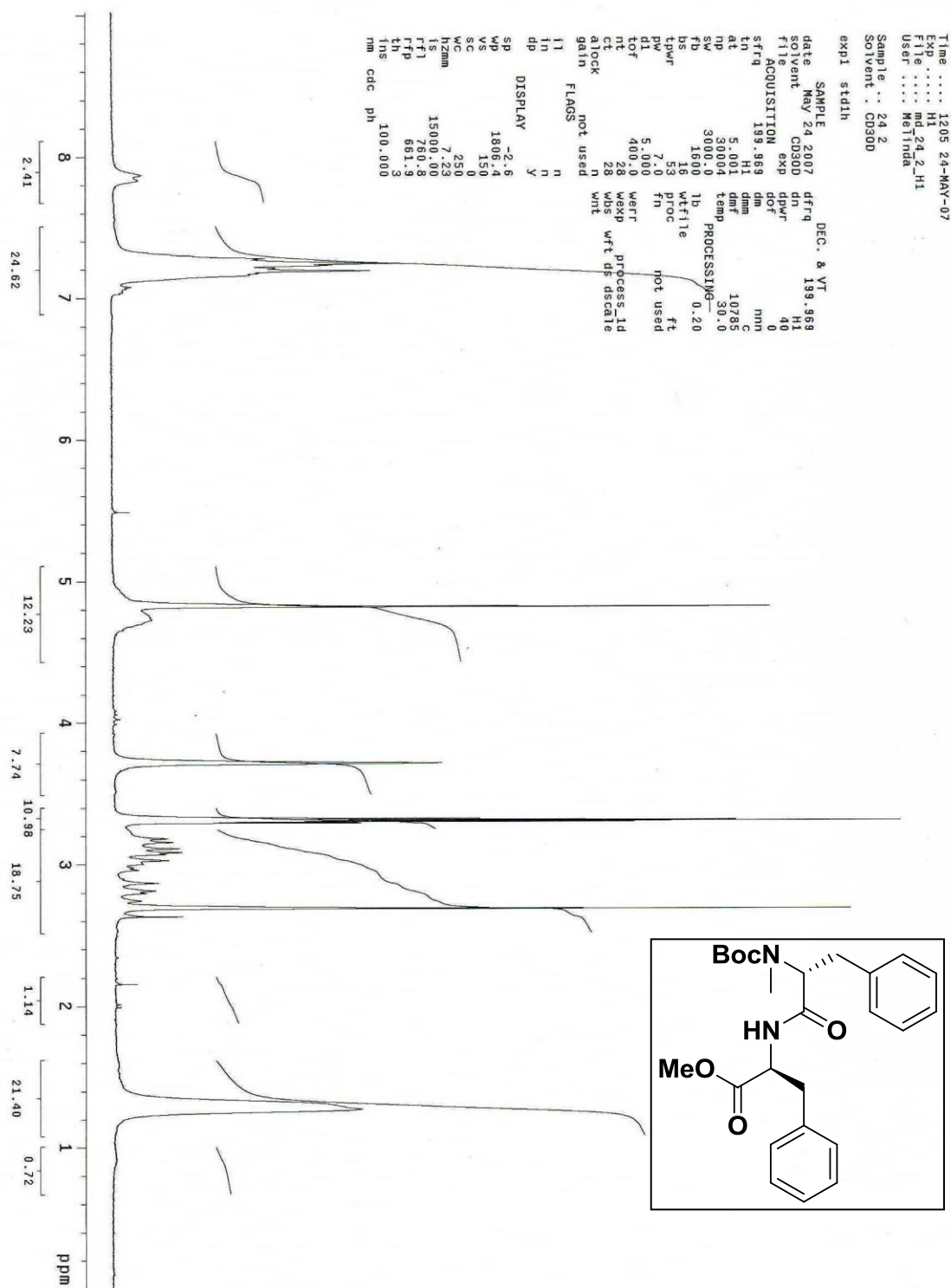
Compound 27 NMR Linear Pentapeptide MeO-D-Trp-Leu-Val-Arg(2Cbz)-Leu-NHBoc



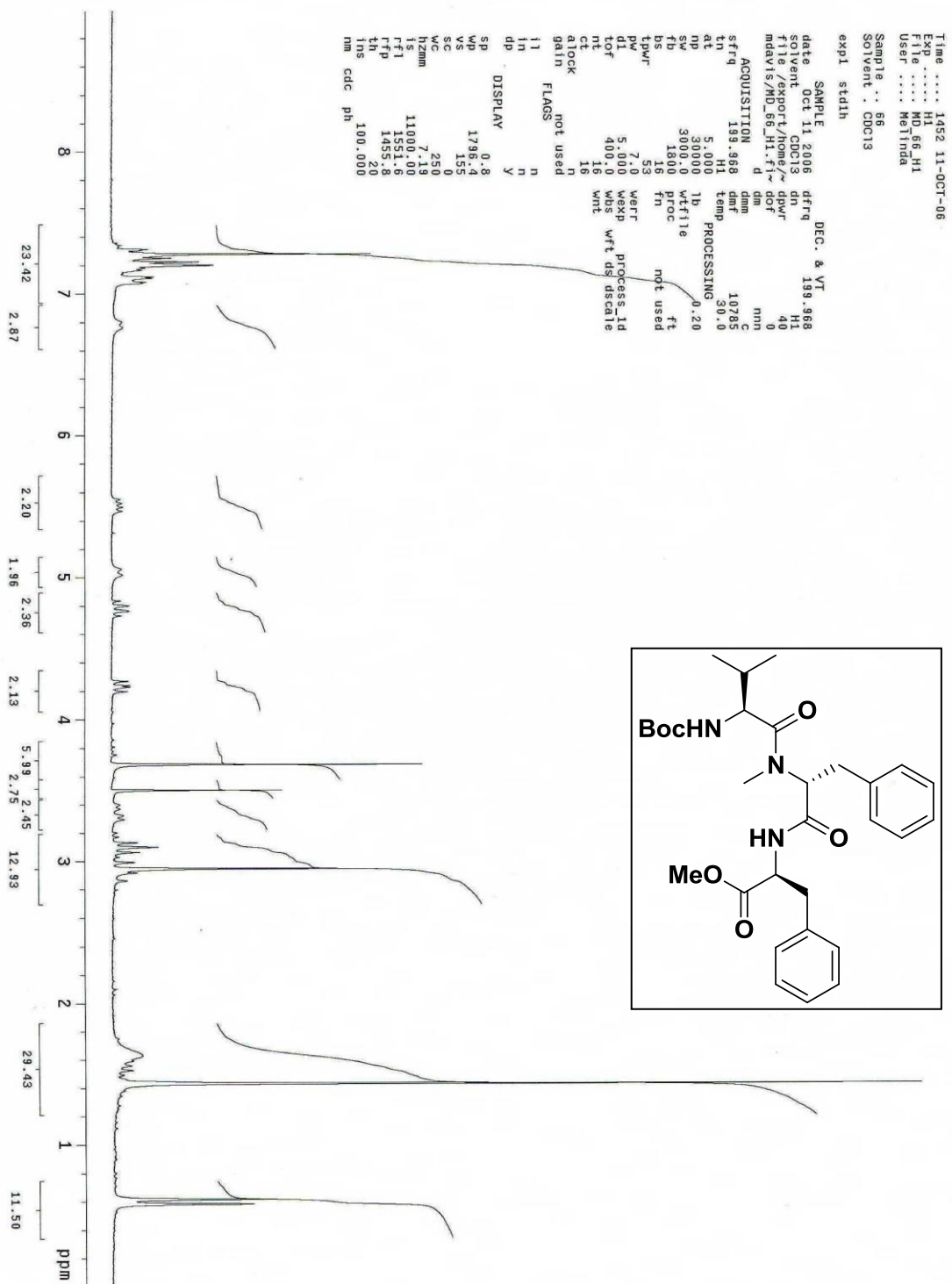
Compound 27 NMR Cyclized Pentapeptide D-Trp-Leu-Val-Arg-Leu



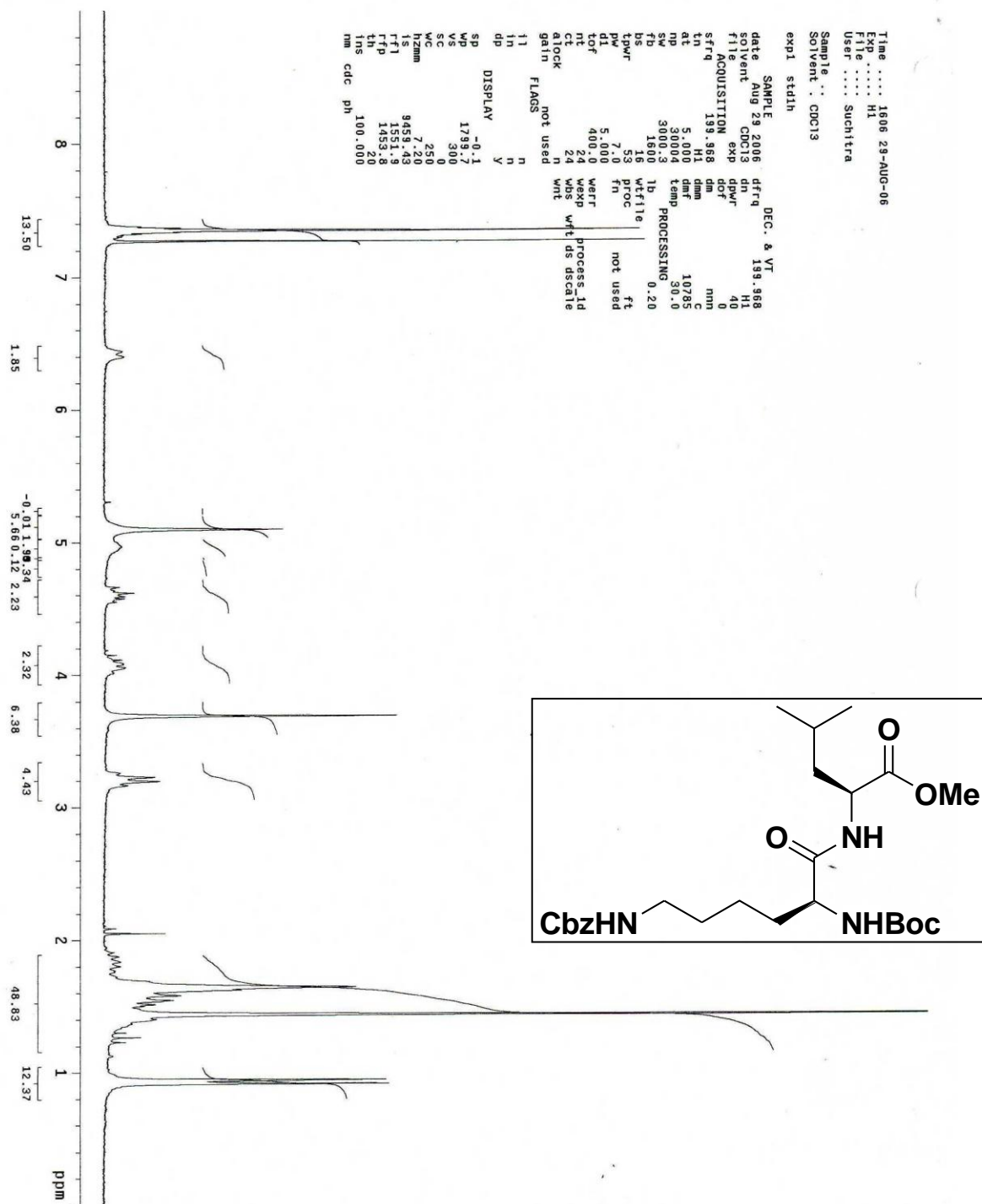
Compound 27 LCMS Cyclized Pentapeptide D-Trp-Leu-Val-Arg-Leu (MW=668)



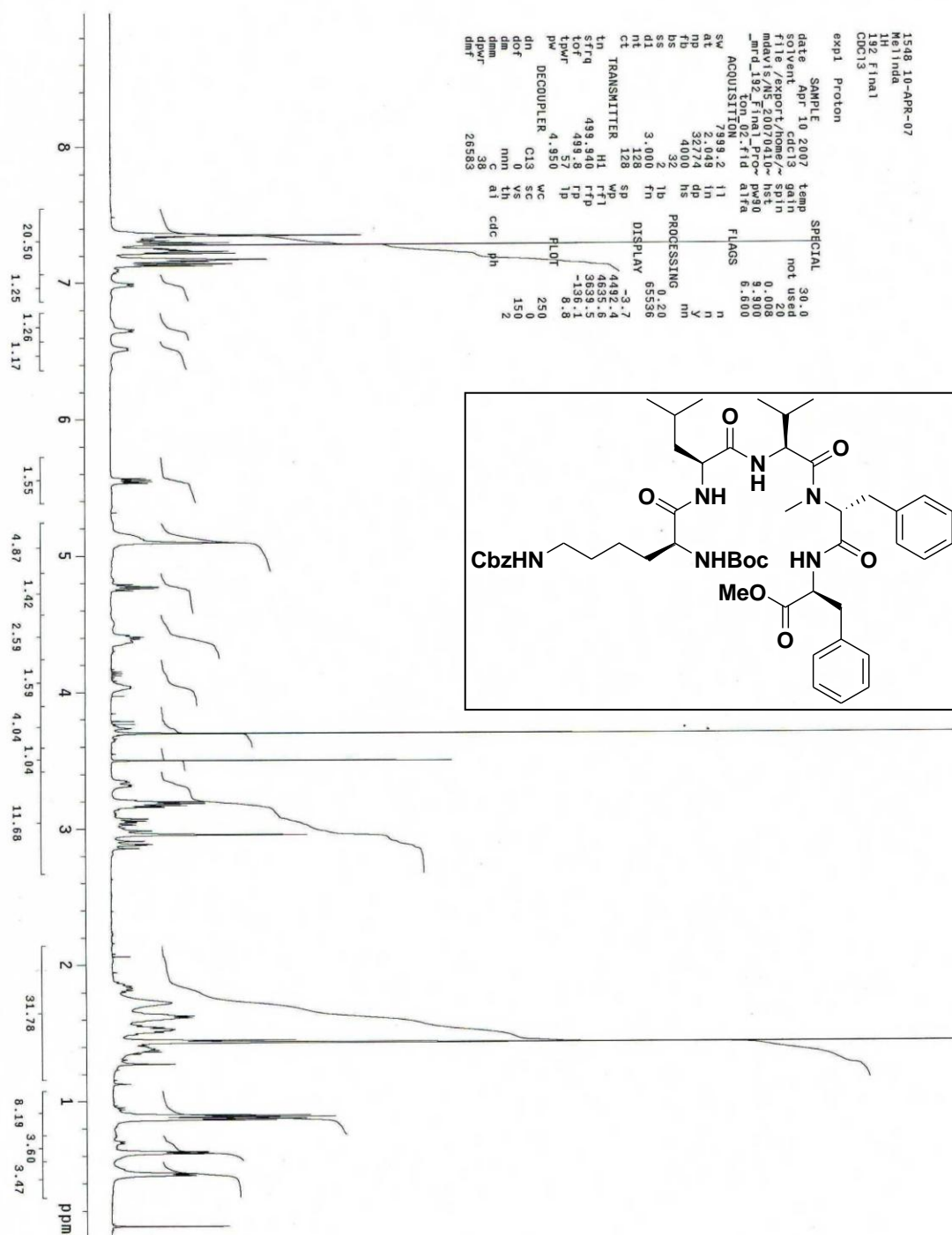
Compound 28 NMR Dipeptide MeO-Phe-N-Me-D-Phe-NBoc



Compound 28 NMR Tripeptide MeO-Phe-N-Me-D-Phe-Val-NHBoc



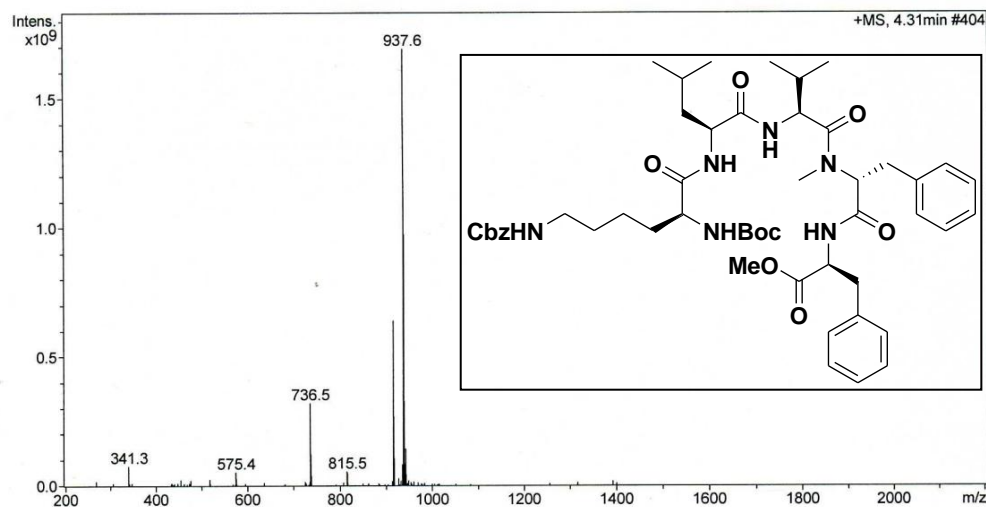
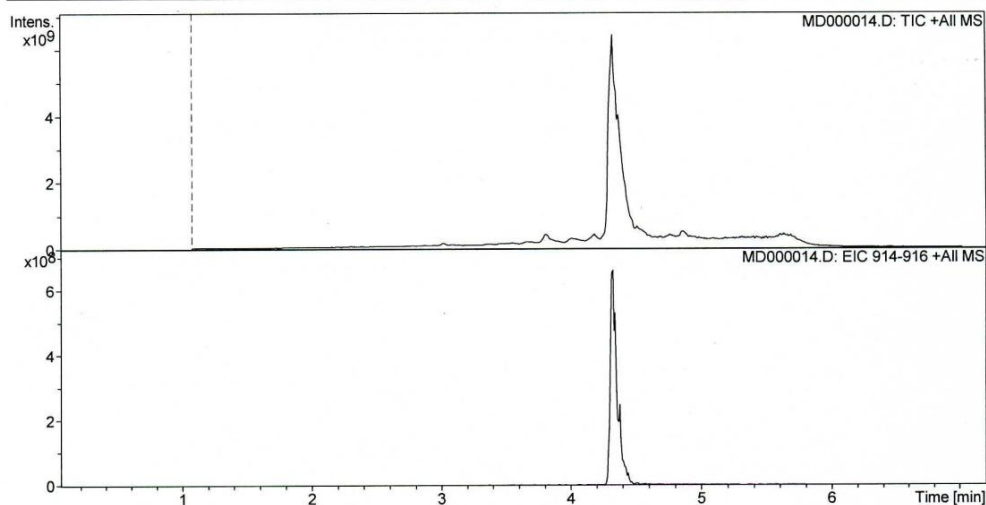
Compound 28 NMR Dipeptide MeO-Leu-Lys(Cbz)-NH-Boc



Compound 28 NMR Linear Pentapeptide MeO-Phe-N-Me-D-Phe-Val-Leu-Lys(Cbz)-NHBOC

Display Report - All Windows Selected Analysis

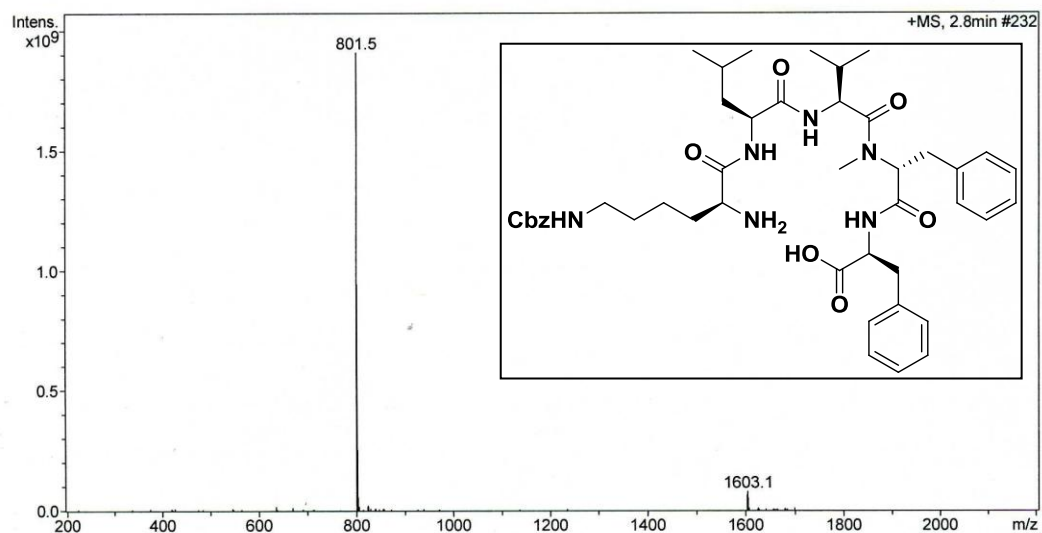
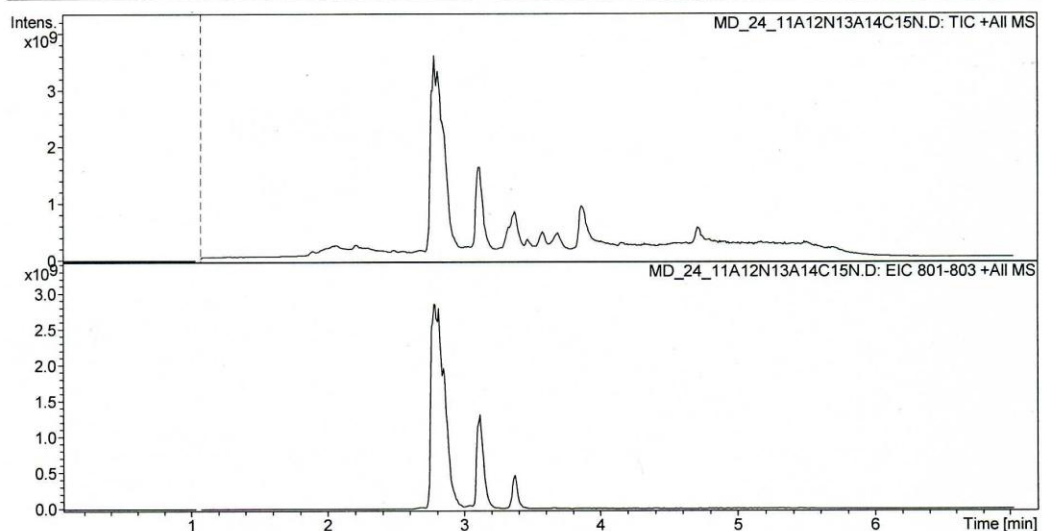
Analysis Name: MD000014.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 5/16/2008 5:28:06 PM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 2/28/2008 2:18:45 PM
Sample Name: md_122LP
Analysis Info:



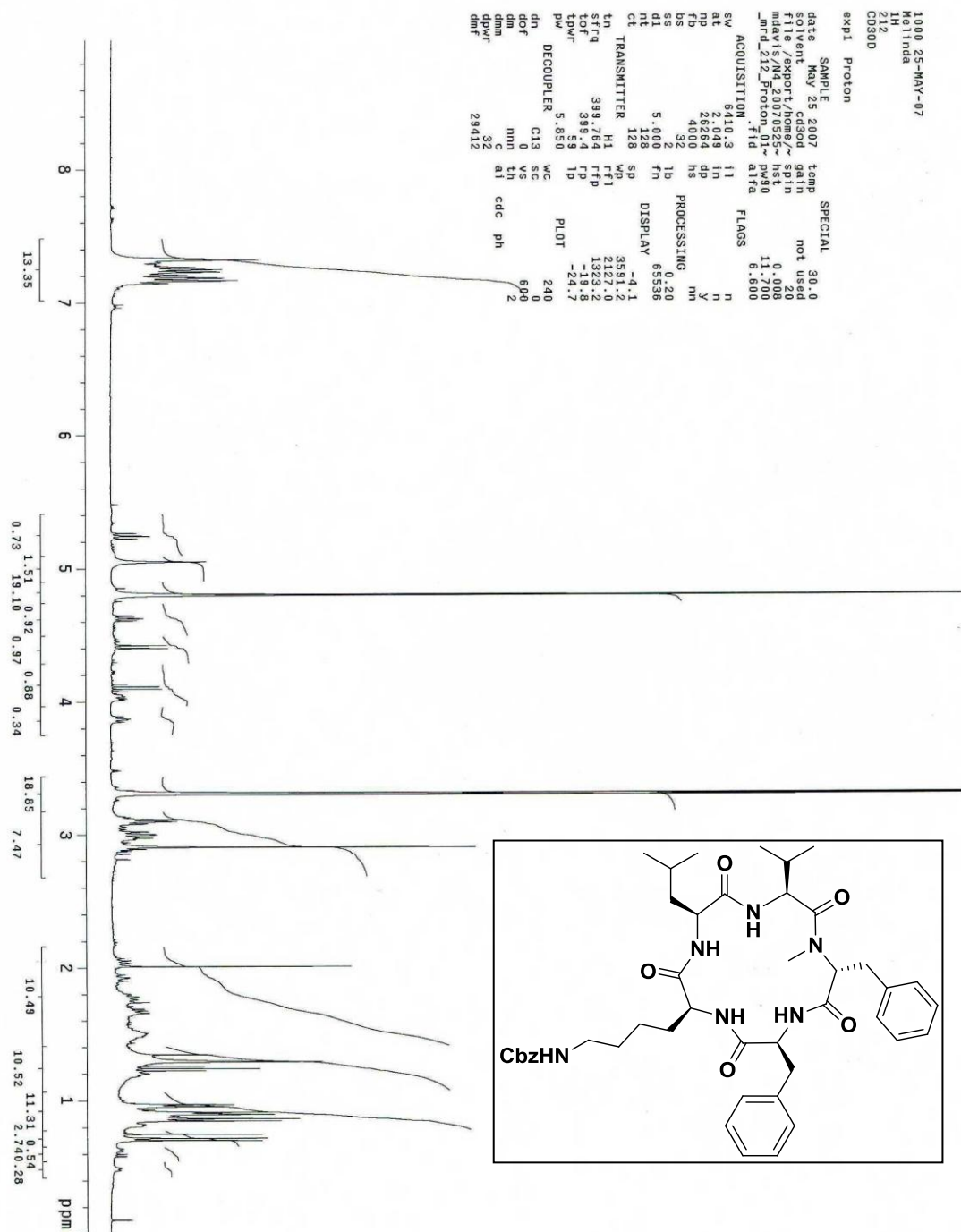
Compound 28 LCMS Linear Pentapeptide MeO-Phe-N-Me-D-Phe-Val-Leu-Lys(Cbz)-NH-Boc (MW=915.1)

Display Report - All Windows Selected Analysis

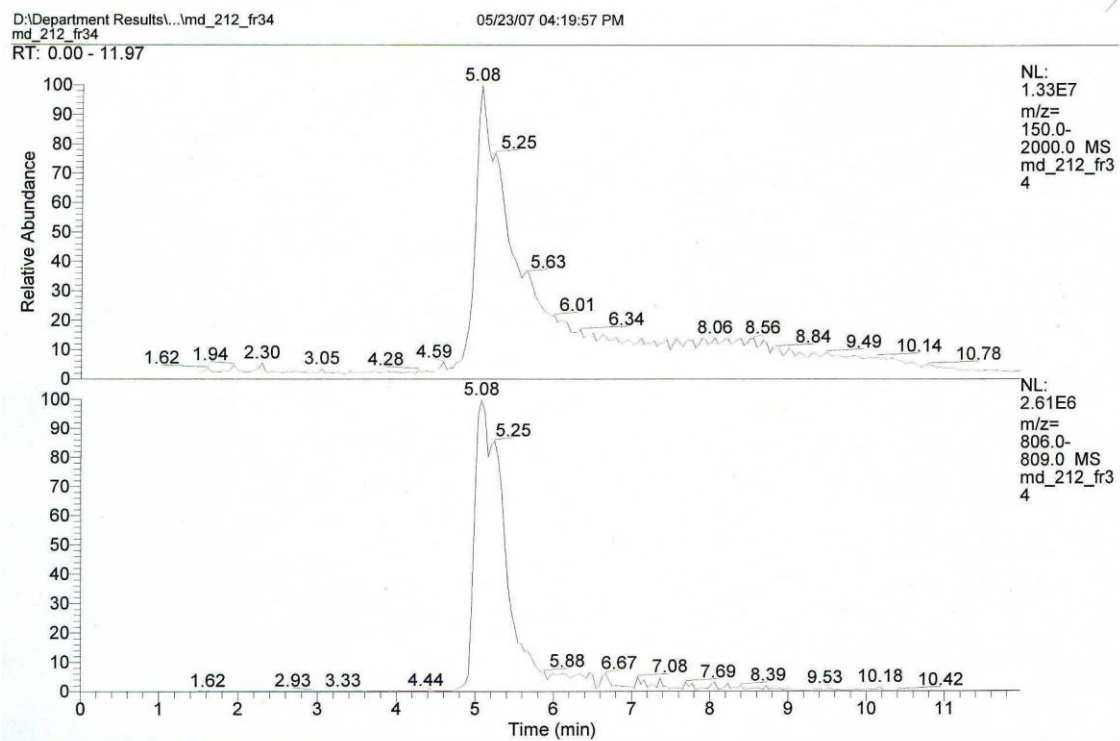
Analysis Name: MD_24_11A12N **Instrument:** Agilent 6330 Ion Trap **Print Date:** 5/16/2008 5:38:07 PM
Method: SANA.M 13A14C15N.D **Operator:** sdsu **Acq. Date:** 3/10/2008 1:37:49 PM
Sample Name: MD_24_11a12n13a14c15n
Analysis Info:



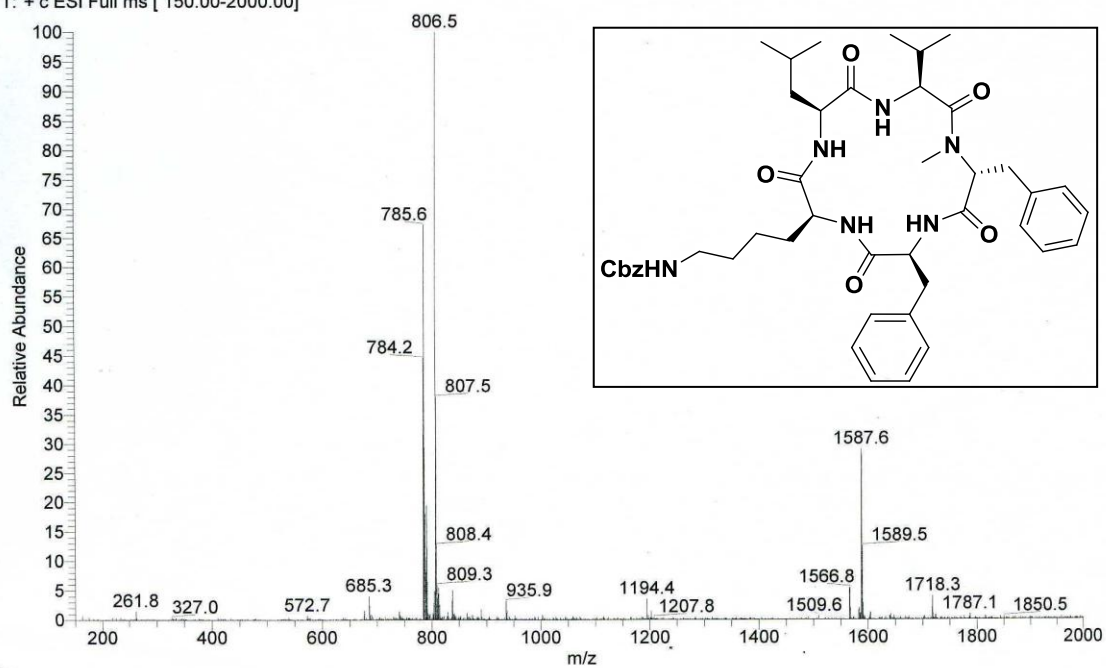
Compound 28 LCMS Double Deprotected Linear Pentapeptide HO-Phe-N-Me-D-Phe-Val-Leu-Lys(Cbz)-NH₂ (MW=801)



Compound 28 NMR Cyclized Pentapeptide Phe-N-Me-D-Phe-Val-Leu-Lys(Cbz)



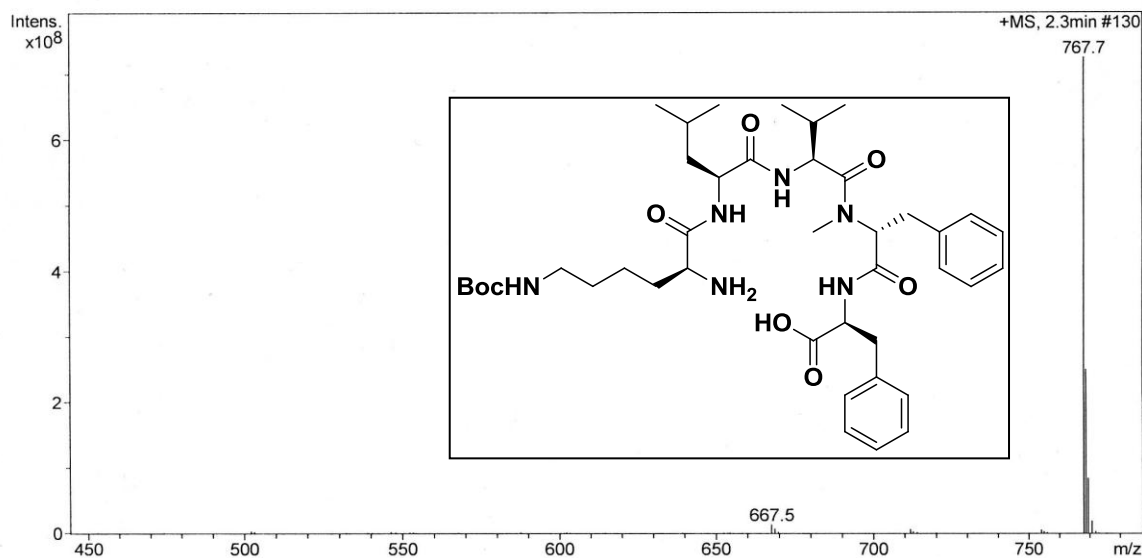
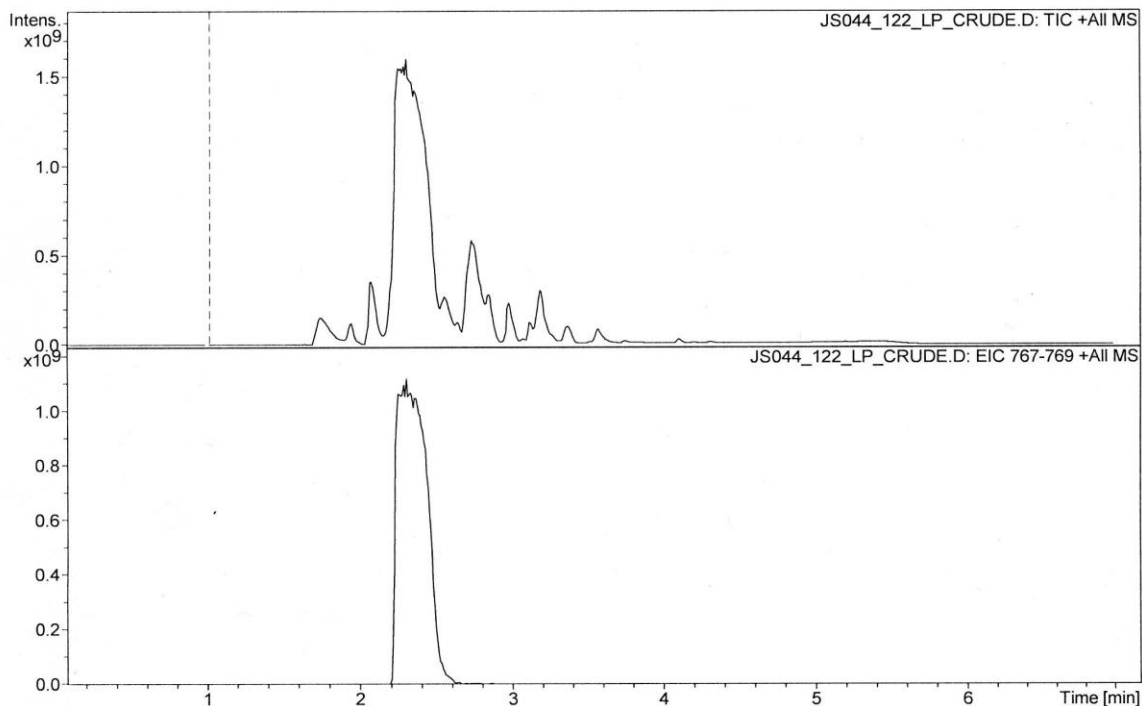
md_212_fr34 #91 RT: 5.08 AV: 1 NL: 1.73E6
T: + c ESI Full ms [150.00-2000.00]



Compound 28 LCMS Cyclized Pentapeptide Phe-*N*-Me-D-Phe-Val-Leu-Lys(Cbz) (MW=783)

Display Report - All Windows All Analyses

Operator: sdsu Instrument: Agilent 6330 Ion Trap Print Date: 7/1/2009 11:21:51 AM

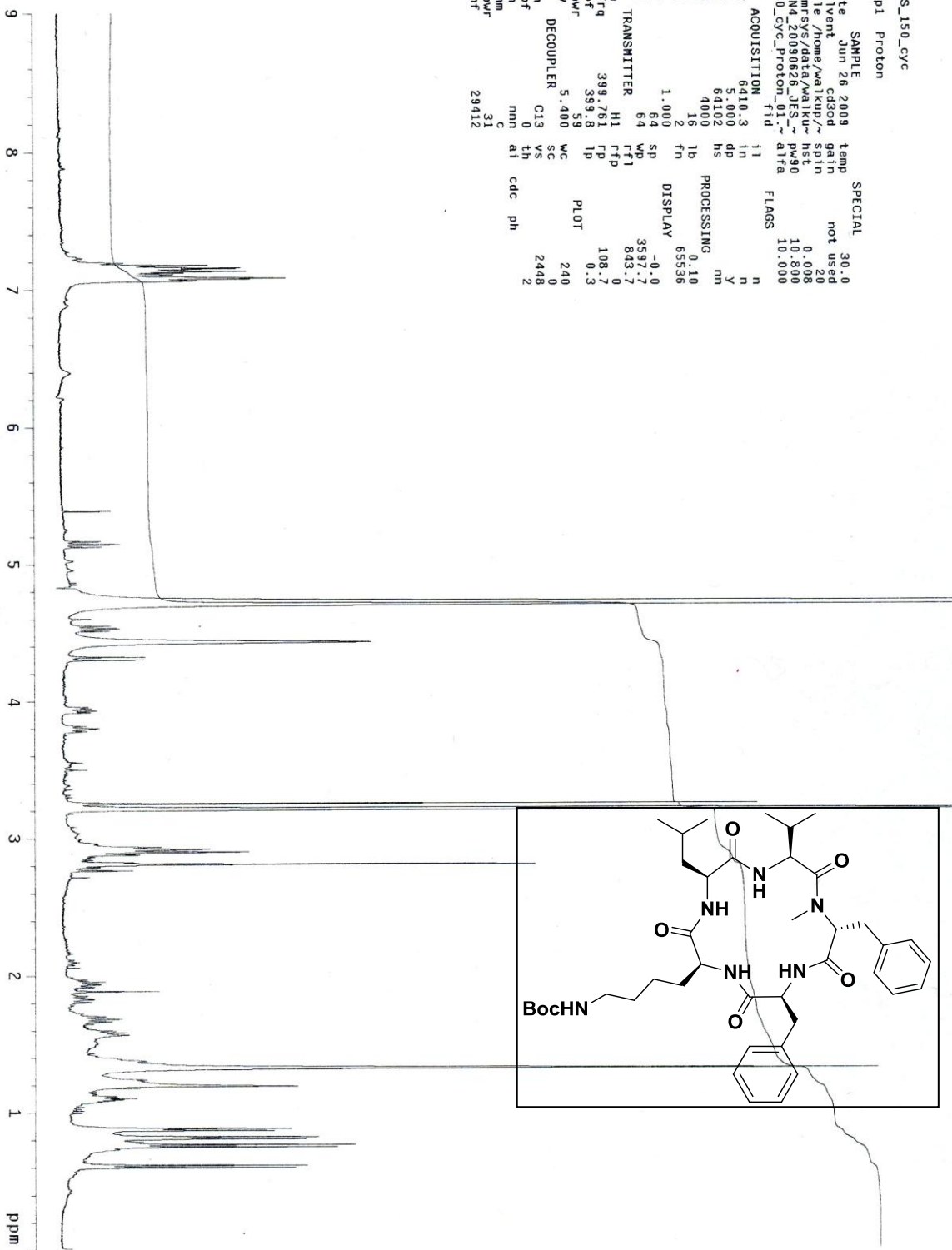


Compound 29 LCMS Double Deprotected Linear Pentapeptide HO-Phe-N-Me-D-Phe-Val-Leu-Lys(Boc)-NH₂ (MW = 767)

JES_150_cyc

expi Proton

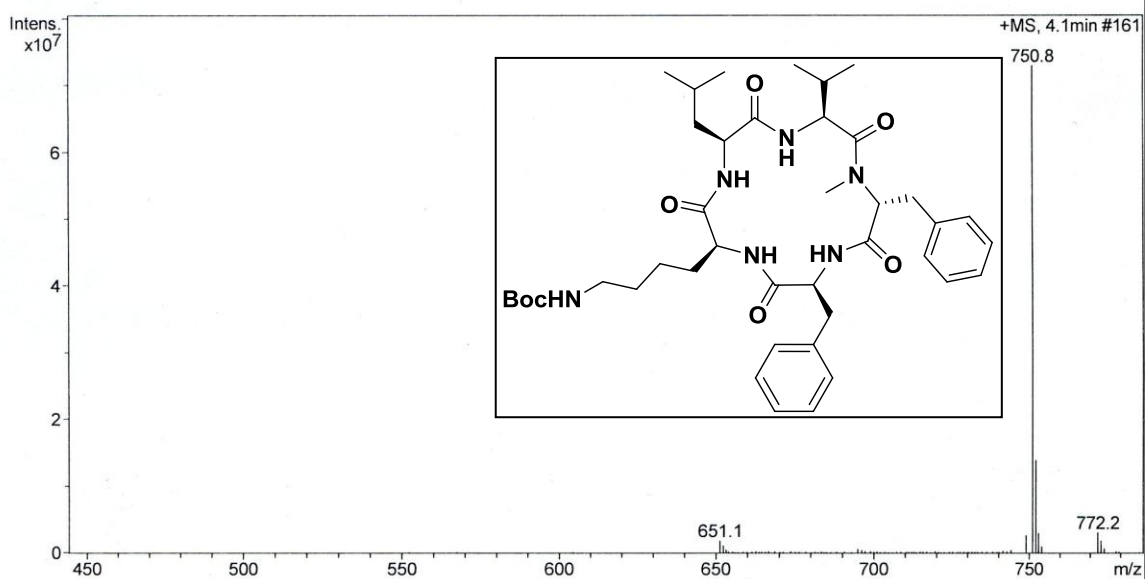
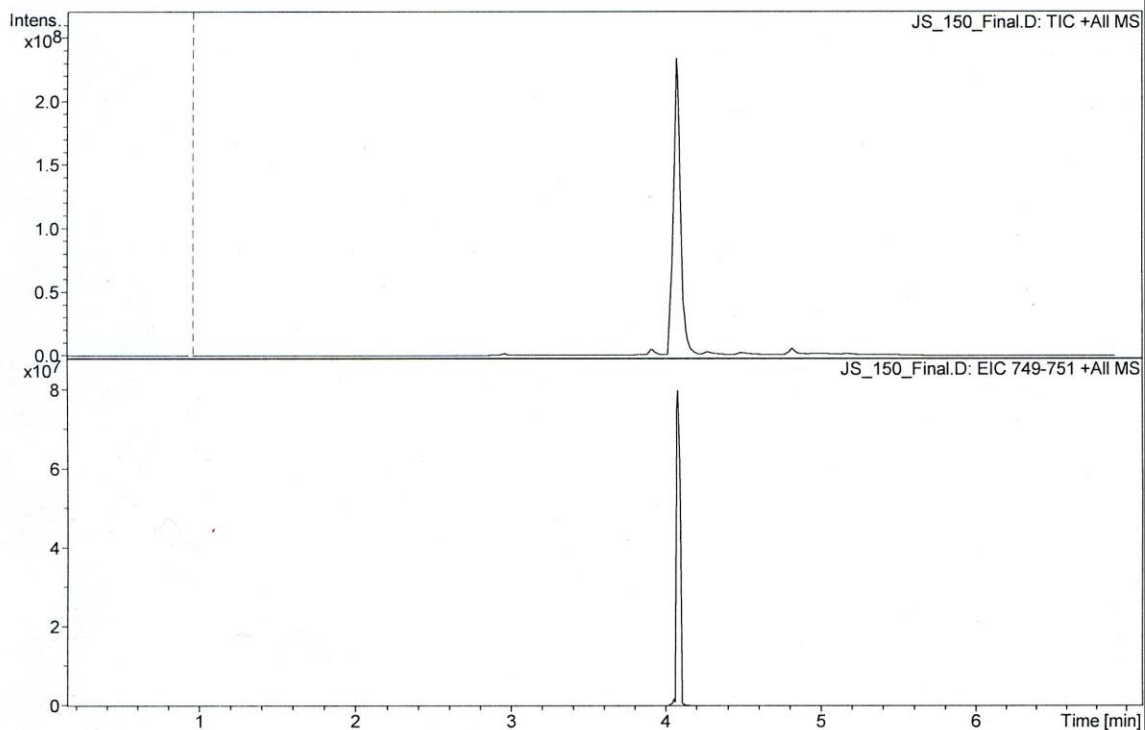
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vmrSYS/data/waikup/		hst	0.008		
P/N4_20090626_JES_~		pw90	10.800		
150_cyc_Proton_01.~		alfa	10.000	FLAGS	
f1d					
ACQUISITION	f1d	i1	n		
sw	6410.3	in	n		
at	3.000	dp	y		
mp	6410	hs	m	PROCESSING	
fd	4092	lb	m		
rs	18	fn	65536		
ds	1.000	sd	-0.0	DISPLAY	
dt	64	wd	3597.7		
nt	64	rf1	843.7		
ct			108.7		
tn	399.761	fp	0.3		
sfreq	399.761	lp	0.3	PL0T	
tof	399.8				
tpwr	59				
pw	5.400	WC	240		
DECOUPLER	C13	VS	2448		
dn		th	0		
dof	0	at	cdc	ph	
dm	0				
dmm	nmn				
dpwr	c				
dmf	31				
	29412				



Compound 29 NMR Cyclized Pentapeptide Phe-N-Me-D-Phe-Val-Leu-Lys(Boc)

Display Report - All Windows All Analyses

Operator: sdsu Instrument: Agilent 6330 Ion Trap Print Date: 7/1/2009 11:19:51 AM



Compound 29 LCMS Cyclized Pentapeptide Phe-N-Me-D-Phe-Val-Leu-Lys(Boc) (MW=749)

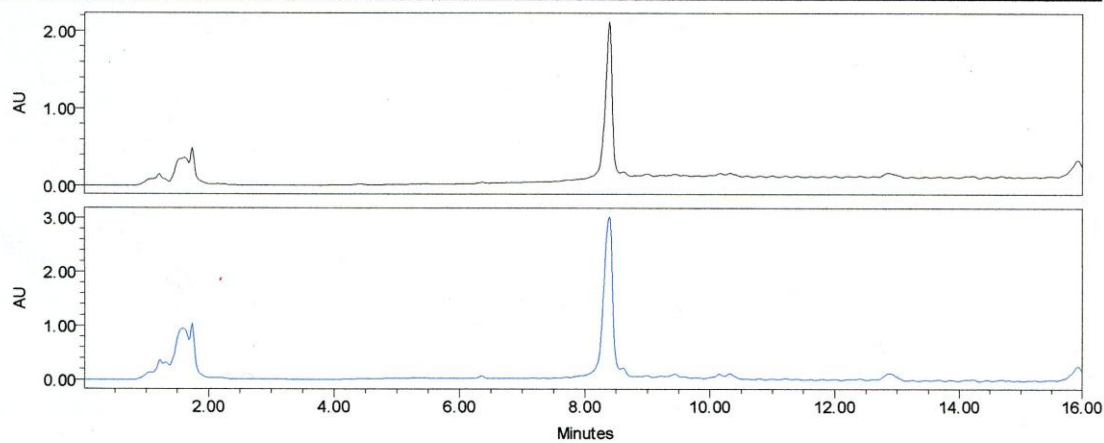
SDSU

Project Name: Defaults
Reported by User: System



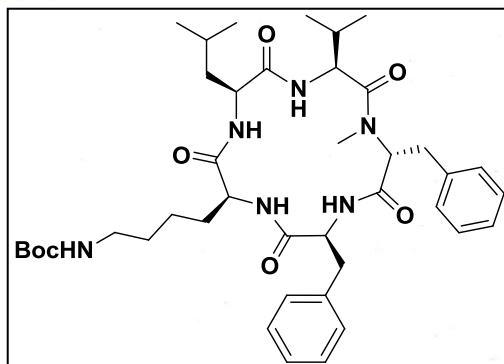
SAMPLE INFORMATION

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Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	582	Date Acquired:	7/1/2009 10:28:20 AM
Run Time:	16.00 Minutes	Injection Volume:	30.00 ul

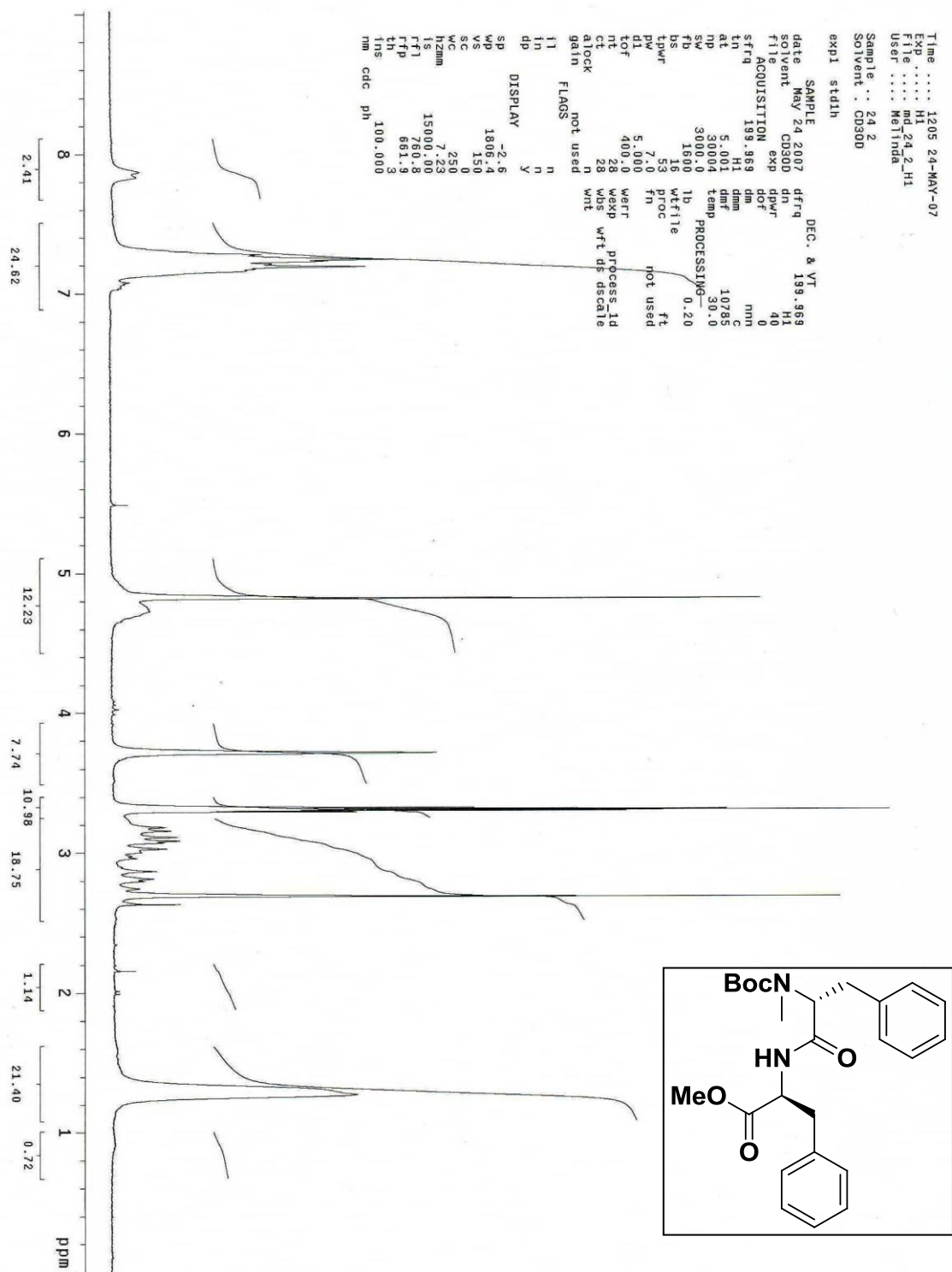


— Channel: 2487Channel 1 Channel Desc.: Processing Method: ****
— Channel: 2487Channel 2 Channel Desc.: Processing Method: ****

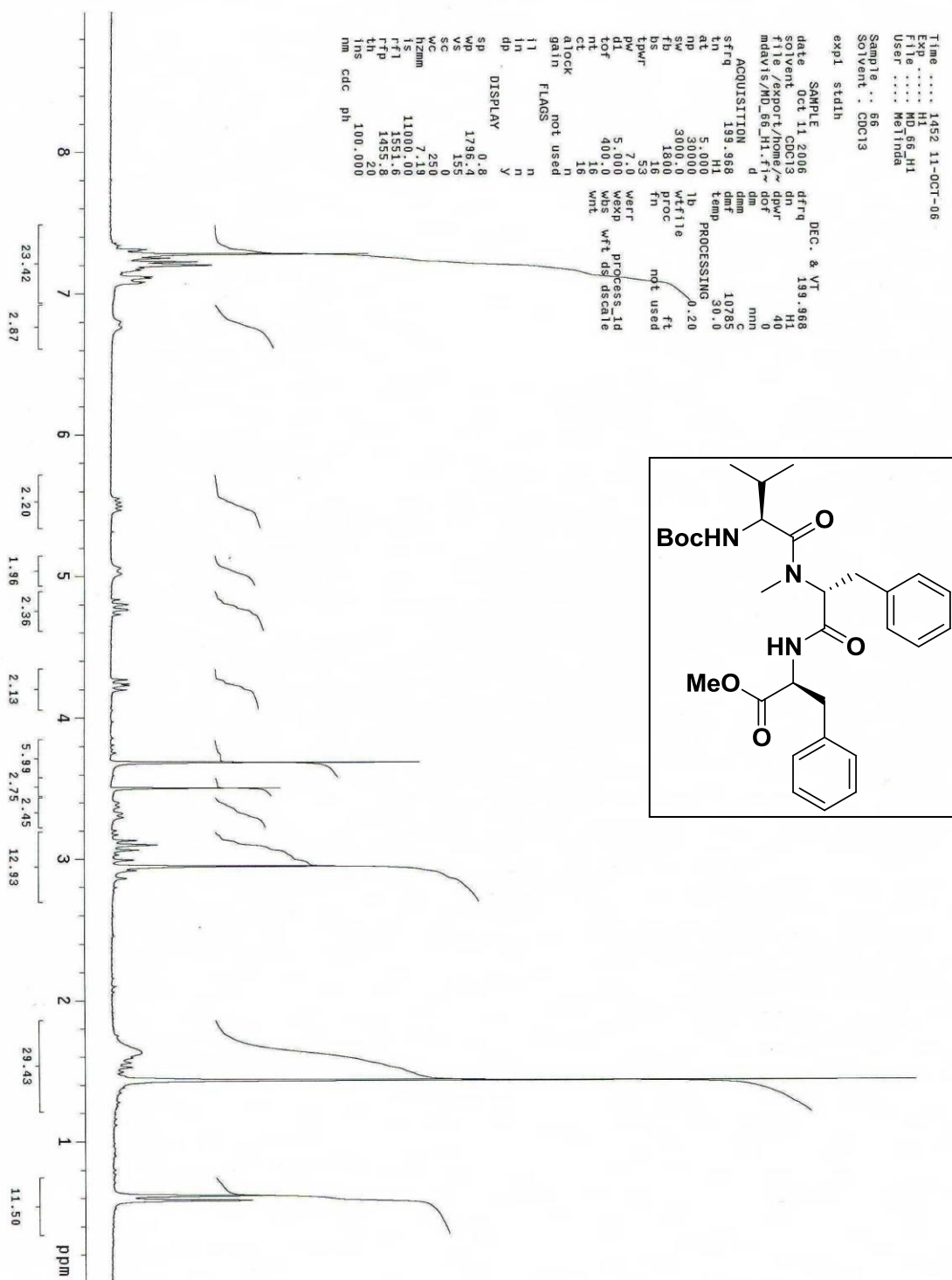
Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	Amount	Units
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2 ****	****	****	****	****	****	****



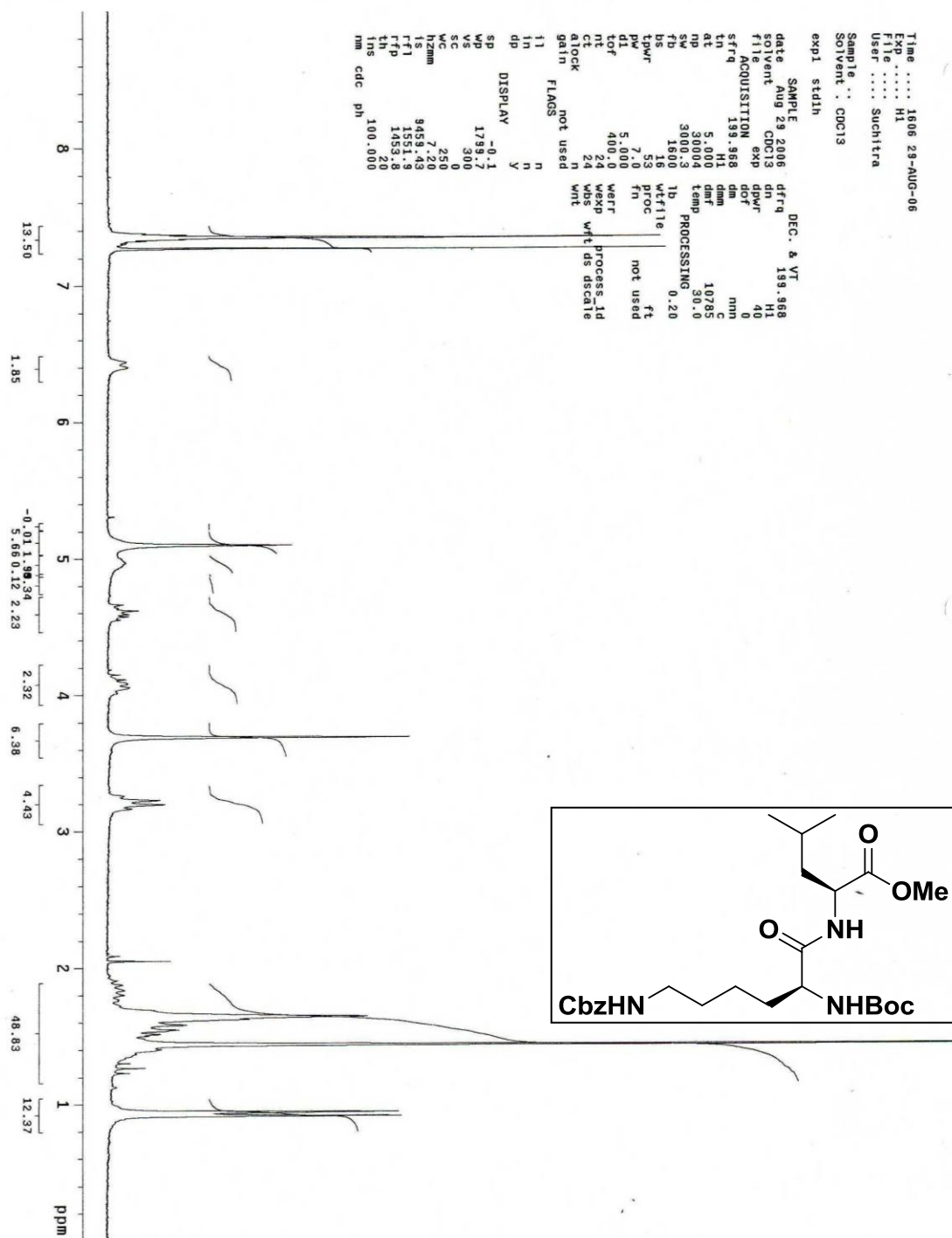
Compound 29 HPLC Cyclized Pentapeptide Phe-N-Me-D-Phe-Val-Leu-Lys(Boc)



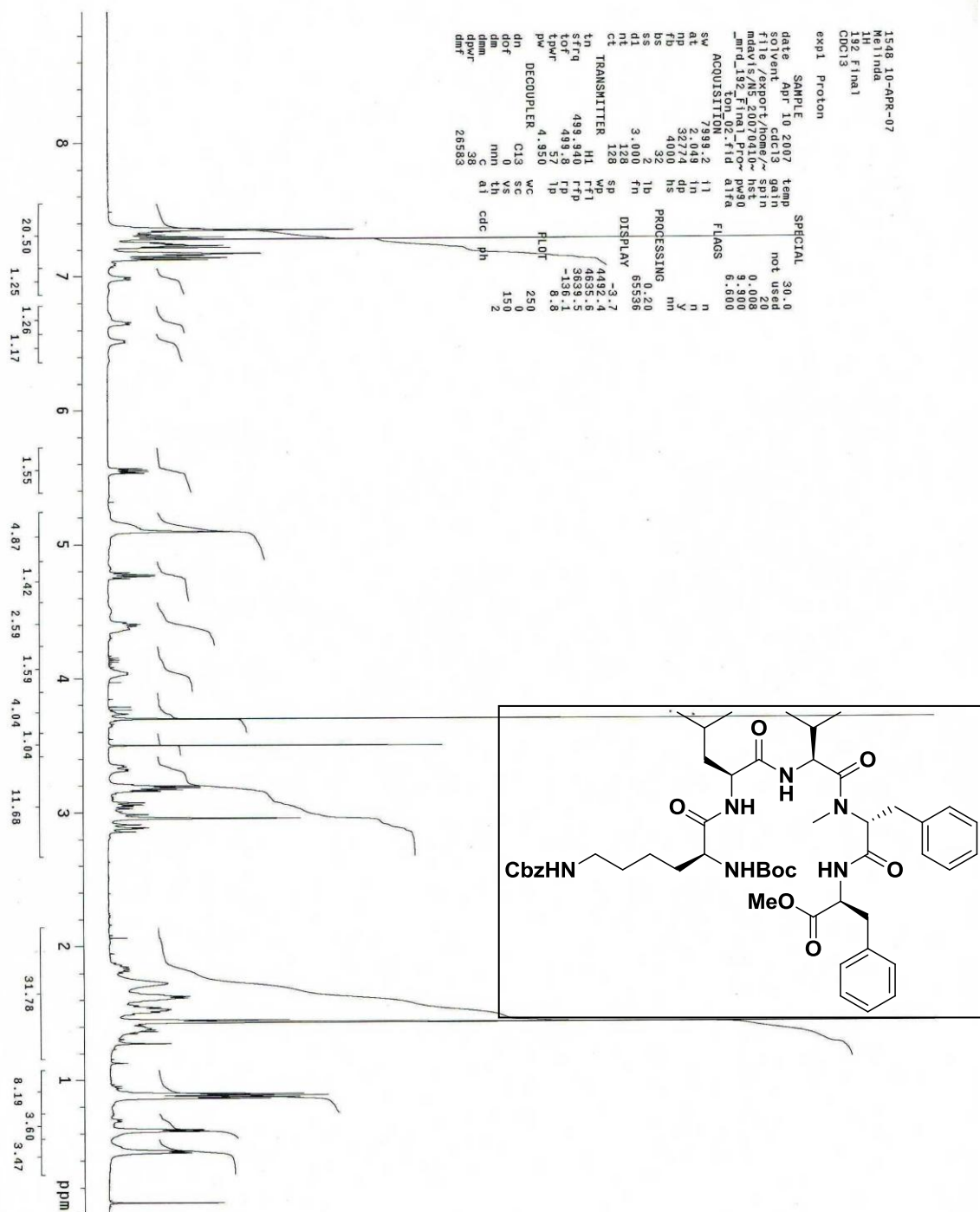
Compound 30 NMR Dipeptide MeO-Phe-N-Me-D-Phe-NBoc



Compound 30 NMR Tripeptide MeO-Phe-N-Me-D-Phe-Val-NHBoc



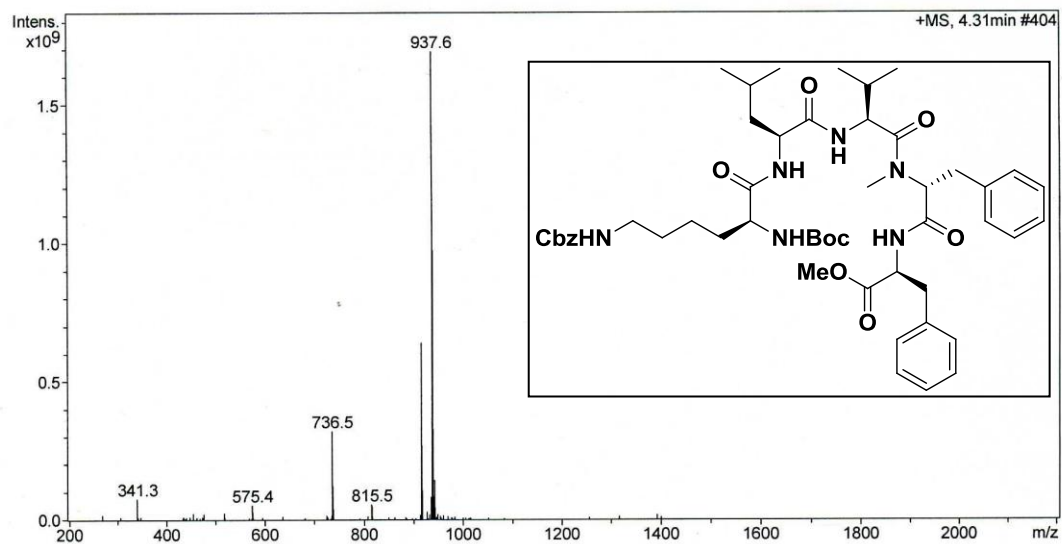
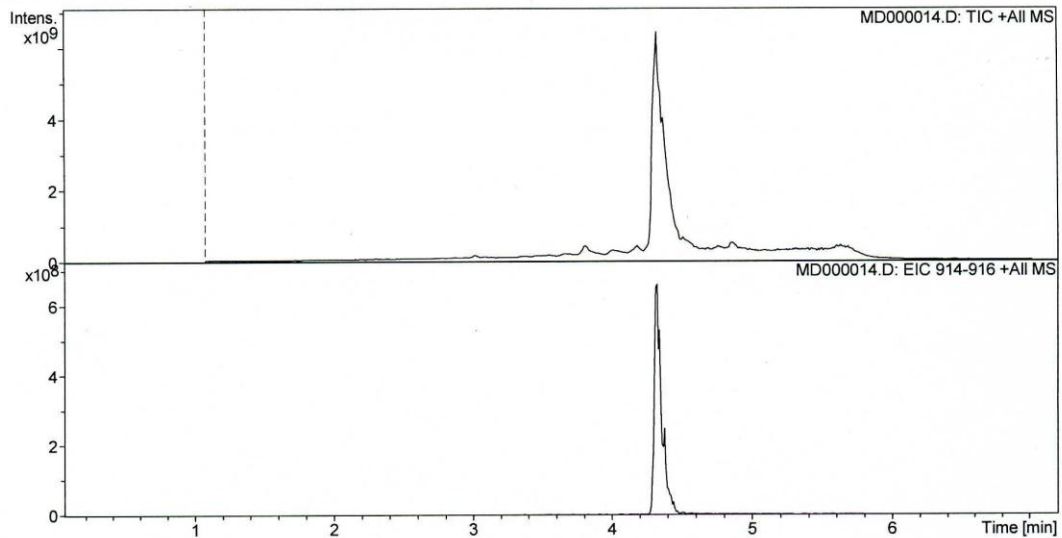
Compound 30 NMR Dipeptide MeO-Leu-Lys(Cbz)-NH-Boc



Compound 30 NMR Linear Pentapeptide MeO-Phe-N-Me-D-Phe-Val-Leu-Lys(Cbz)-NHBOC

Display Report - All Windows Selected Analysis

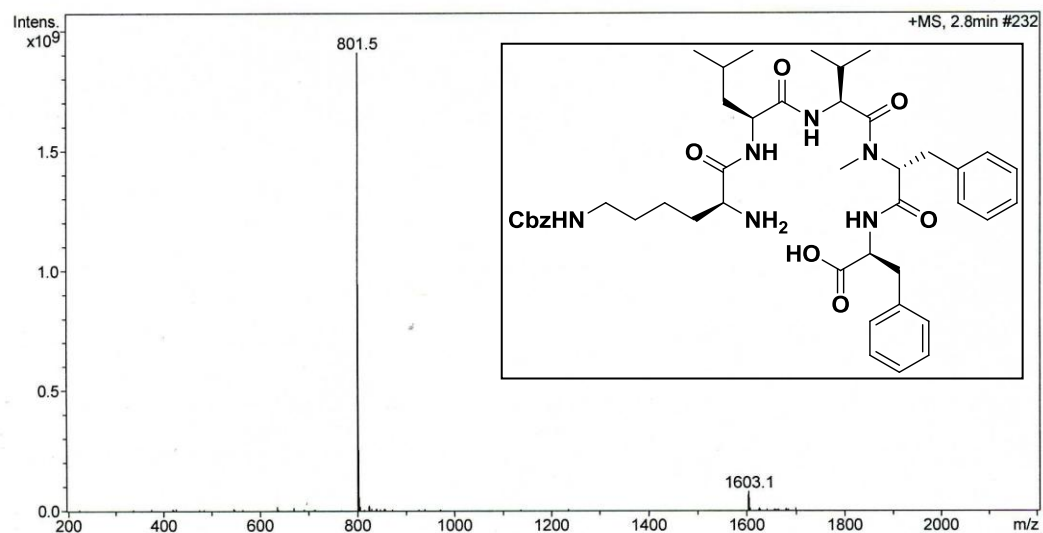
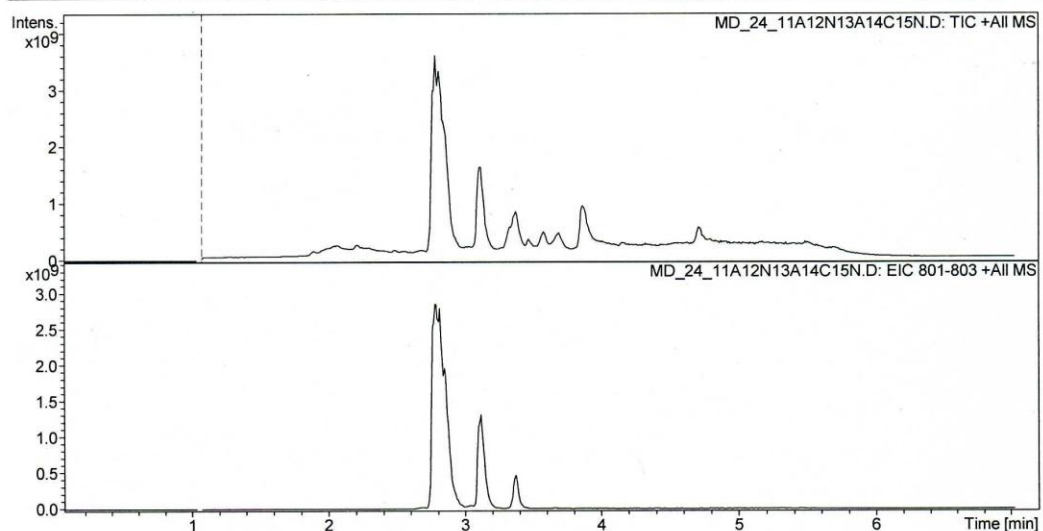
Analysis Name: MD000014.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 5/16/2008 5:28:06 PM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 2/28/2008 2:18:45 PM
Sample Name: md_122LP
Analysis Info:



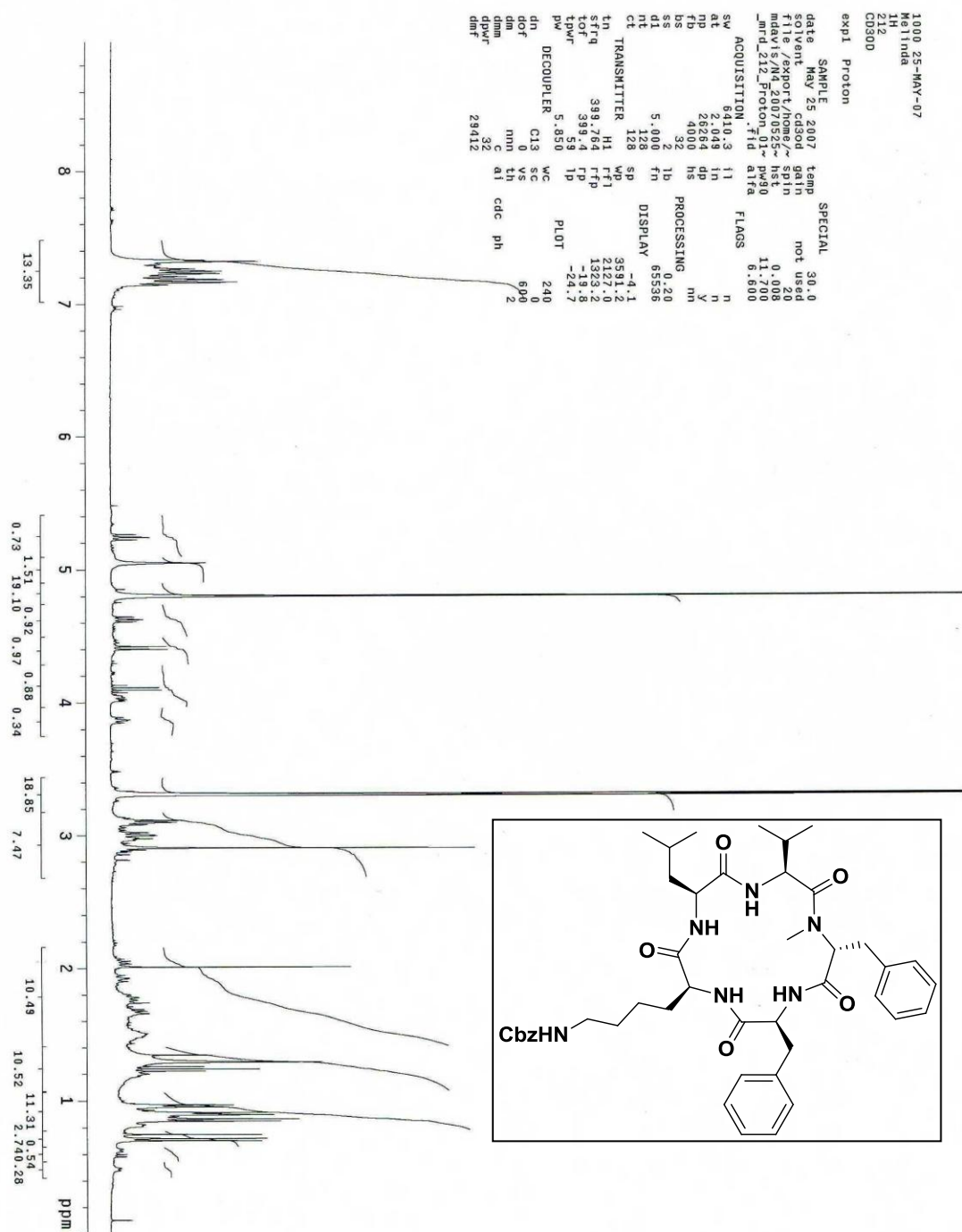
Compound 30 LCMS Linear Pentapeptide MeO-Phe-N-Me-D-Phe-Val-Leu-Lys(Cbz)-NHBoc (MW=915)

Display Report - All Windows Selected Analysis

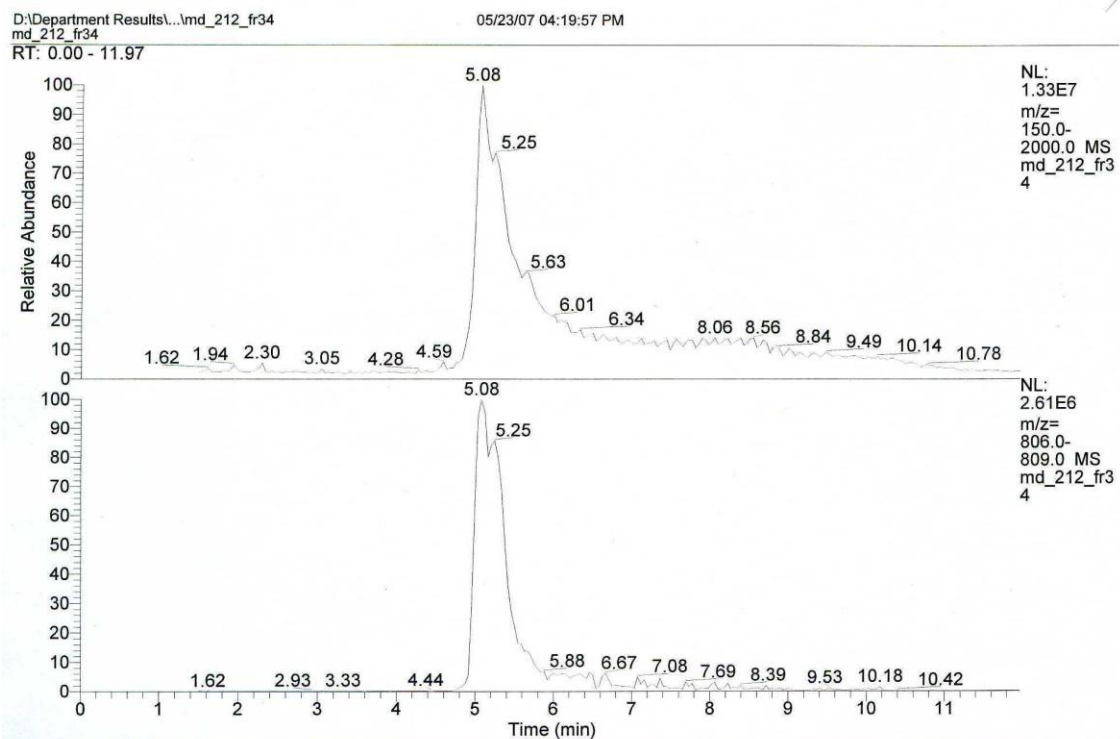
Analysis Name: MD_24_11A12N **Instrument:** Agilent 6330 Ion Trap **Print Date:** 5/16/2008 5:38:07 PM
Method: SANA.M 13A14C15N.D **Operator:** sdsu **Acq. Date:** 3/10/2008 1:37:49 PM
Sample Name: MD_24_11a12n13a14c15n
Analysis Info:



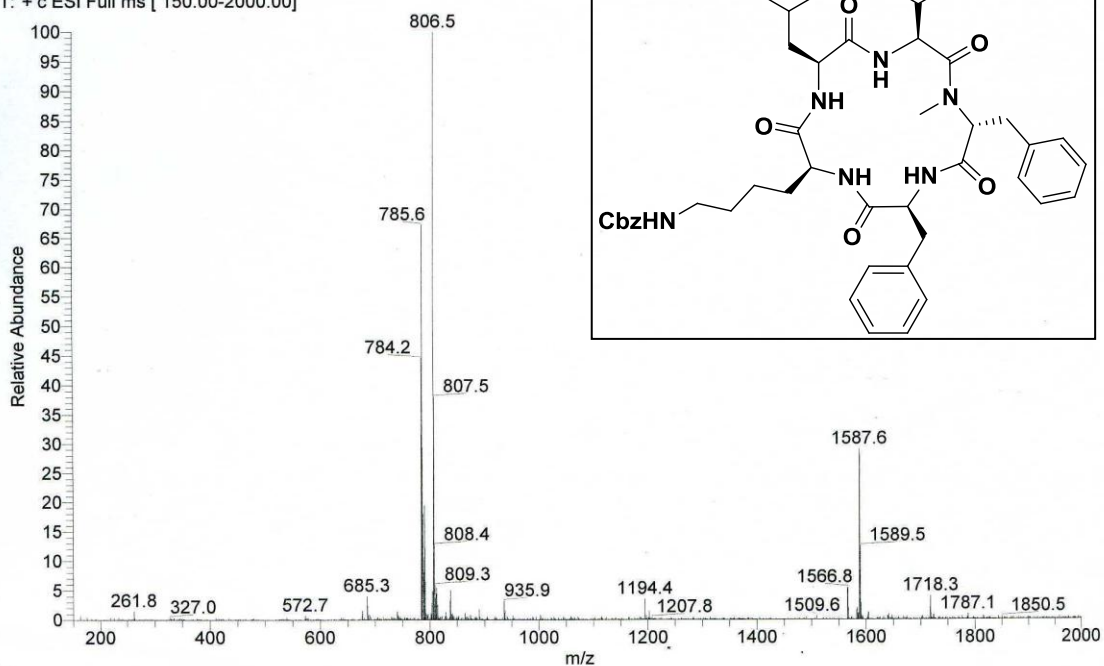
Compound 30 LCMS Double Deprotected Linear Pentapeptide HO-Phe-N-Me-D-Phe-Val-Leu-Lys(Cbz)-NH₂ (MW=801)



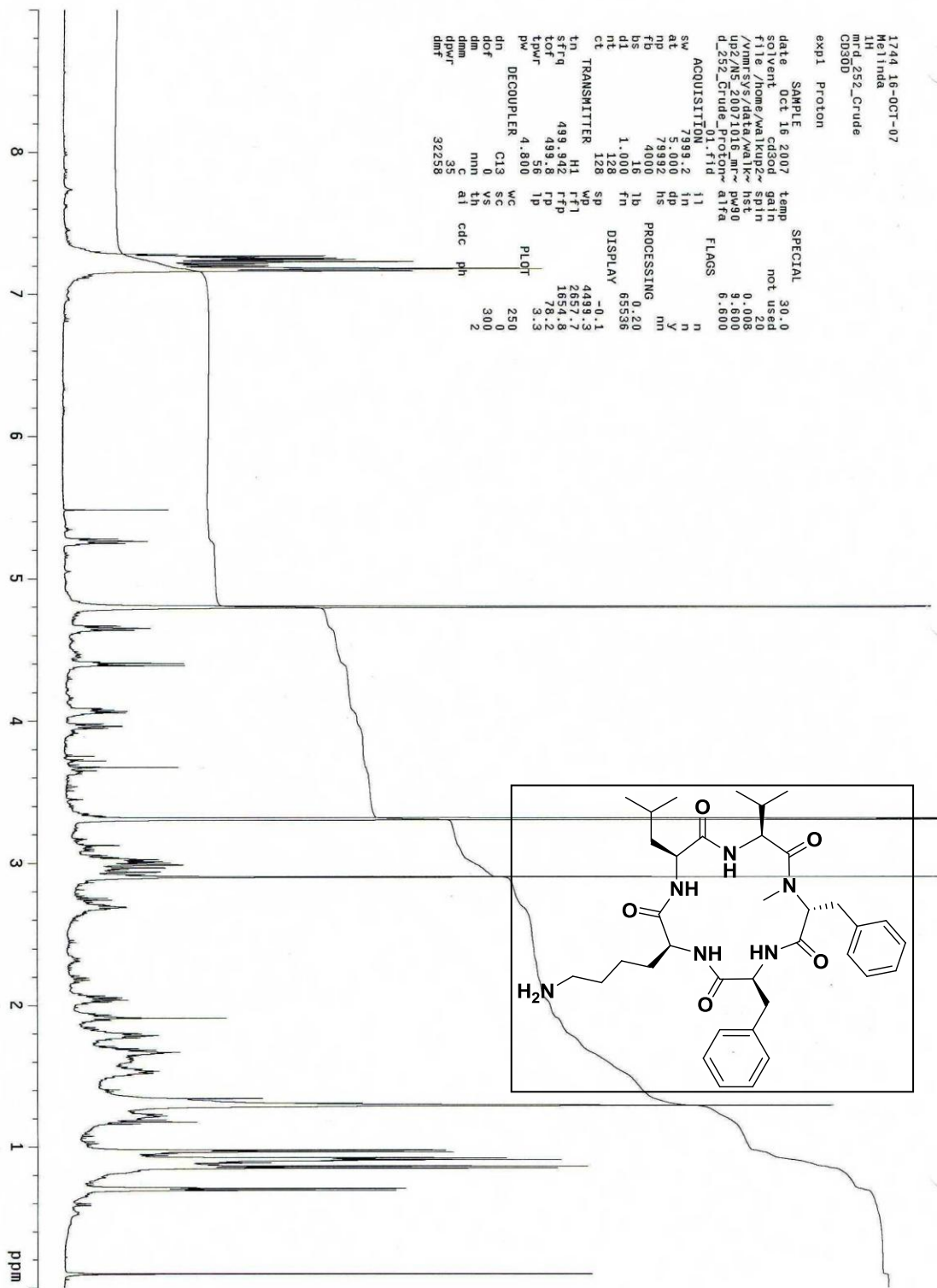
Compound 30 NMR Cyclized Protected Pentapeptide Phe-N-Me-D-Phe-Val-Leu-Lys(Cbz)



md_212_fr34 #91 RT: 5.08 AV: 1 NL: 1.73E6
T: + c ESI Full ms [150.00-2000.00]



Compound 30 LCMS Cyclized Protected Pentapeptide Phe-N-Me-D-Phe-Val-Leu-Lys(Cbz)
(MW=783)

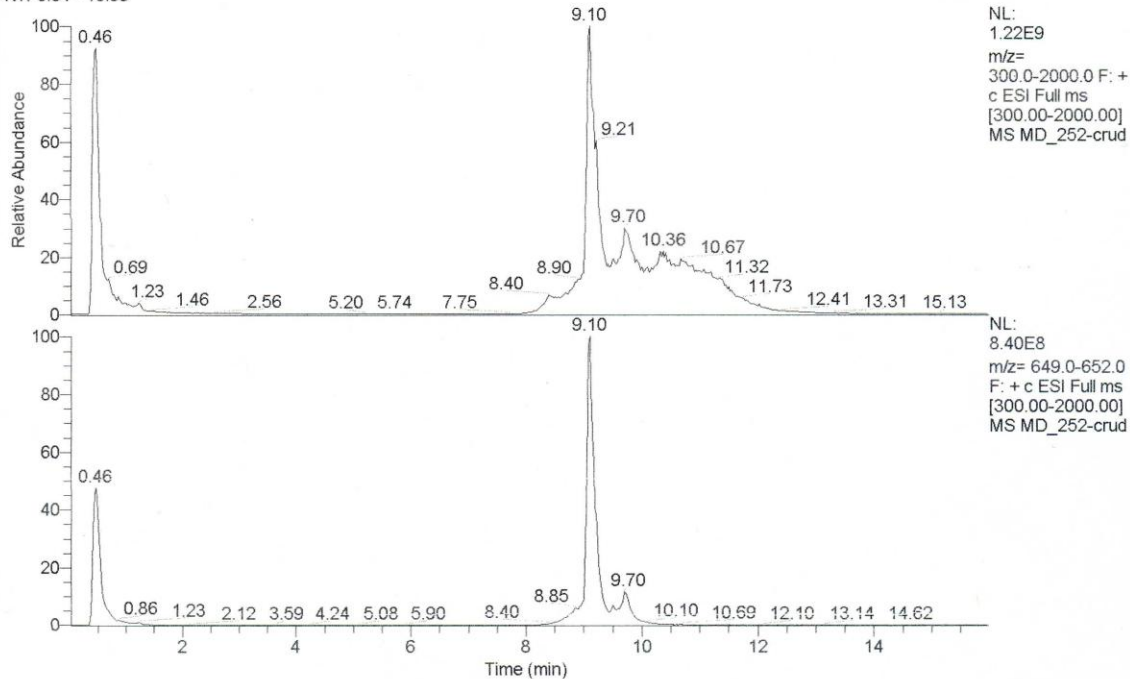
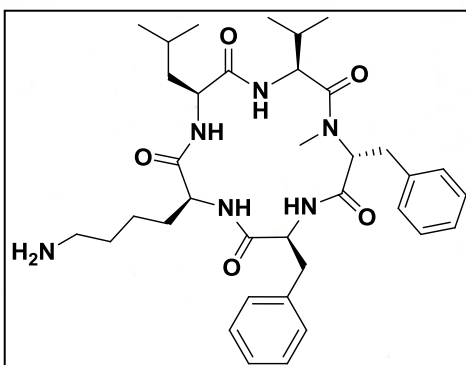
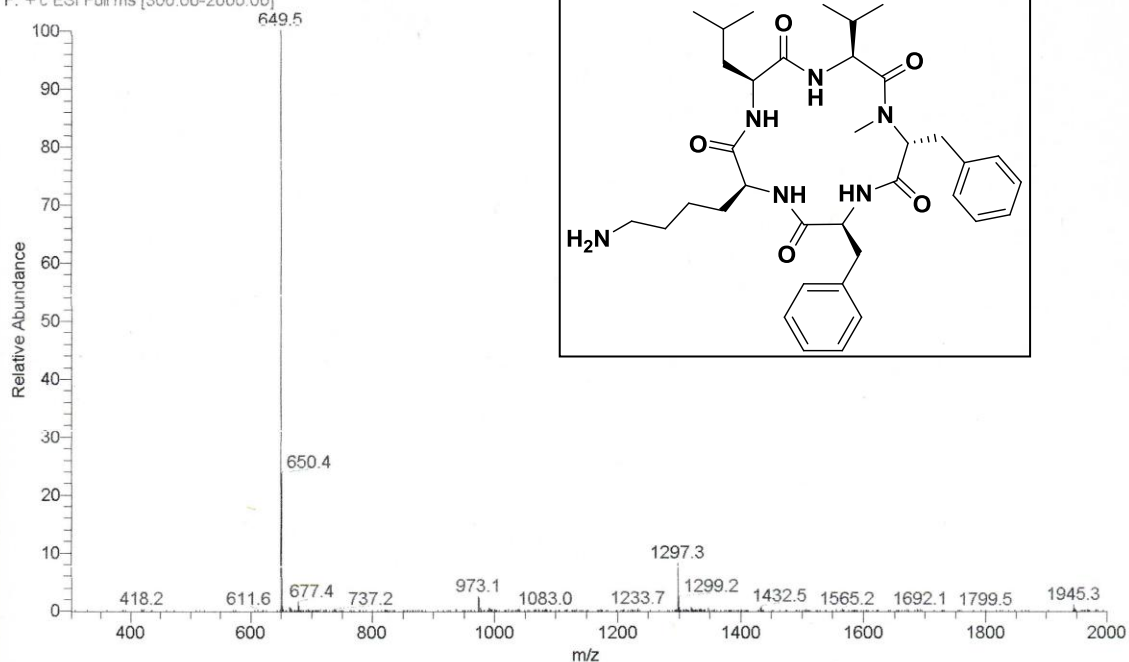


Compound 30 NMR Cyclized Pentapeptide Phe-N-Me-D-Phe-Val-Leu-Lys

MD_252-crud

10/18/2007 8:35:18 PM

RT: 0.01 - 15.99

MD_252-crud #375 RT: 9.10 AV: 1 NL: 6.48E8
F: + c ESI Full ms [300.00-2000.00]

Compound 30 LCMS Cyclized Pentapeptide Phe-N-Me-D-Phe-Val-Leu-Lys (MW=649)

San Diego State University; Department of Chemis

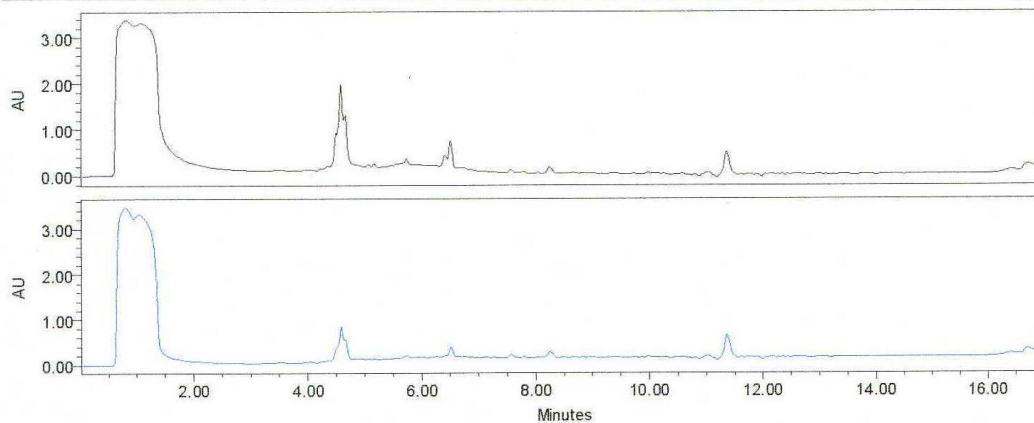
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Reported by User: shelli

Breeze

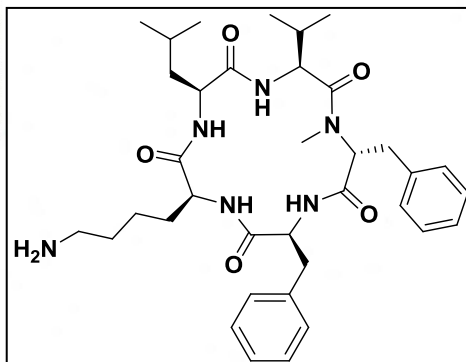
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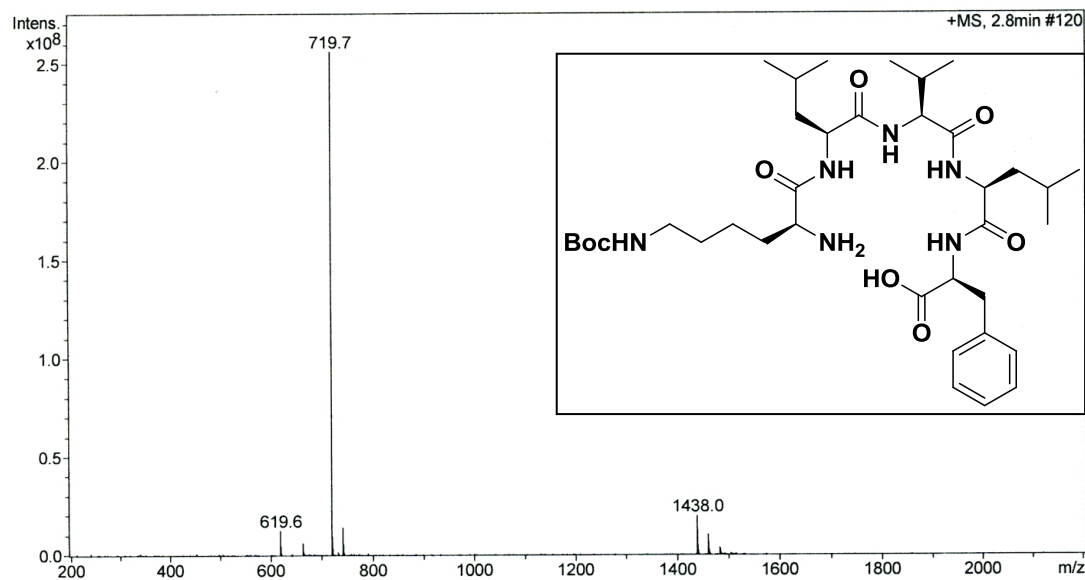
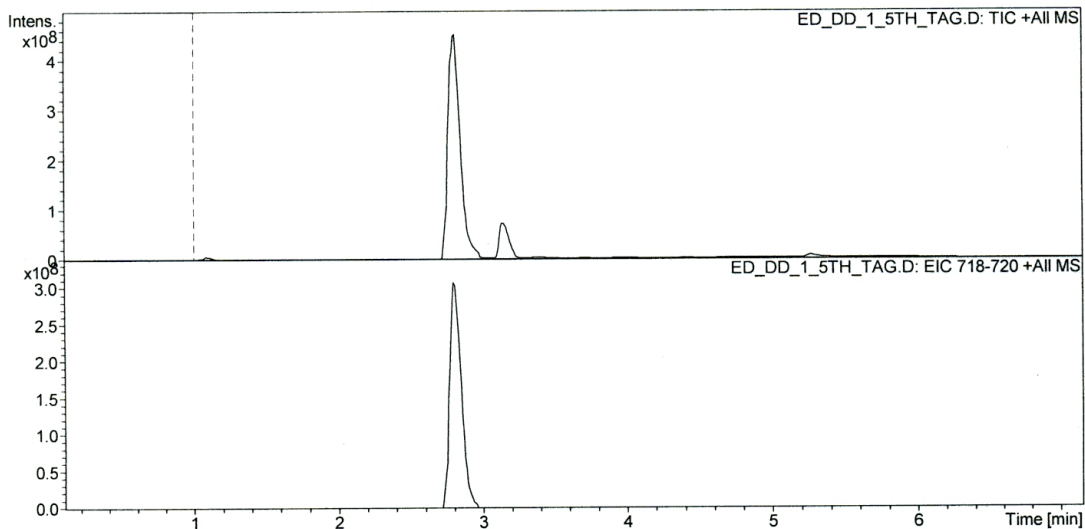
Peak Name	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	Amount	Units
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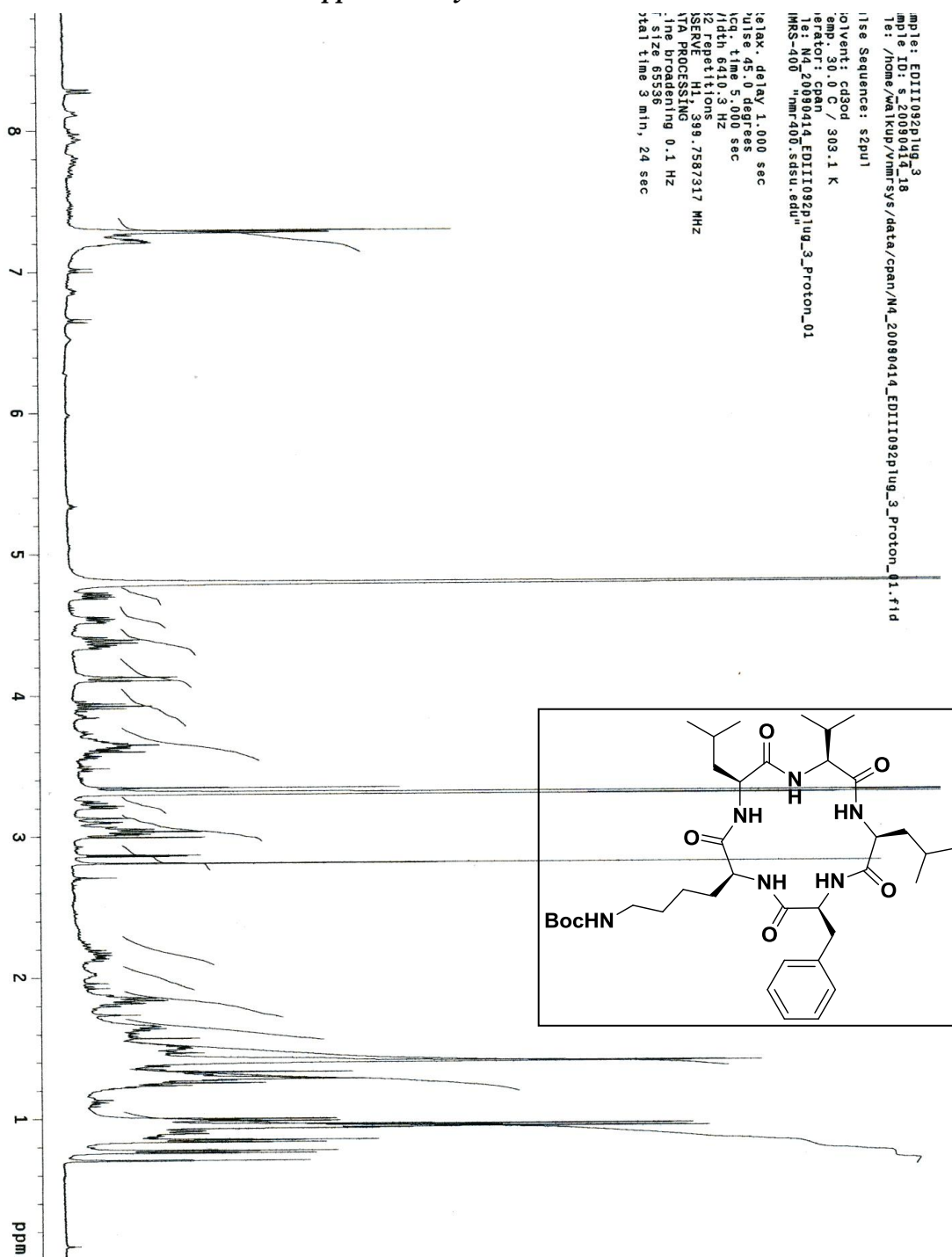
Compound 30 HPLC Cyclized Pentapeptide Phe-N-Me-D-Phe-Val-Leu-Lys

Display Report - All Windows Selected Analysis

Analysis Name: ED_DD_1_5TH_ **Instrument:** Agilent 6330 Ion Trap **Print Date:** 4/22/2009 1:51:45 PM
Method: SANA.M TAG.D **Operator:** sdsu **Acq. Date:** 3/30/2009 1:51:37 PM
Sample Name: ED_dd_1_5th_tag
Analysis Info:

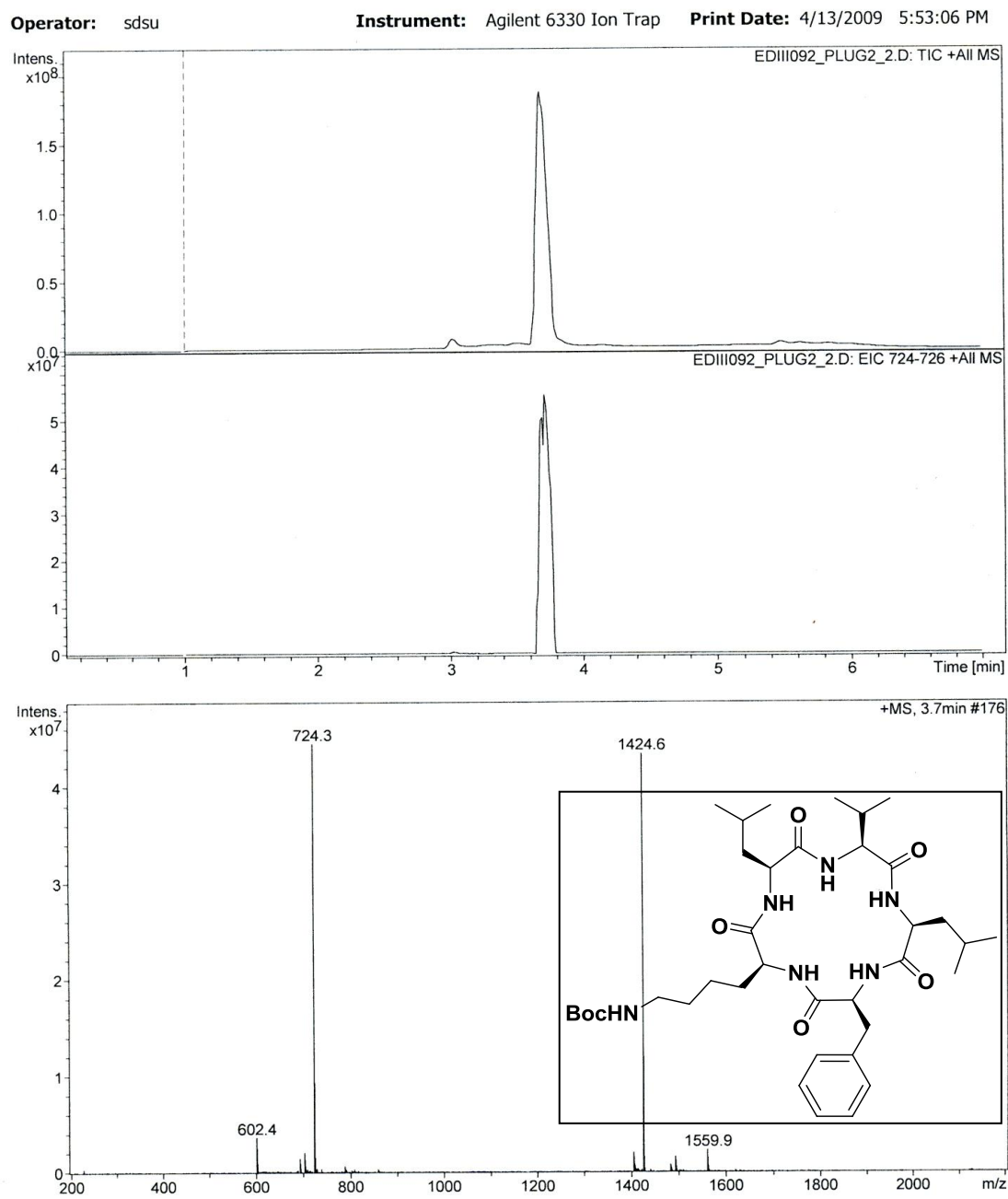


Compound 31 LCMS Double Deprotected Linear Pentapeptide HO-Phe-Leu-Val-Leu-Lys(Boc)-NH₂ (MW = 719)



Compound 31 NMR Cyclized Pentapeptide Phe-Leu-Val-Leu-Lys(Boc)

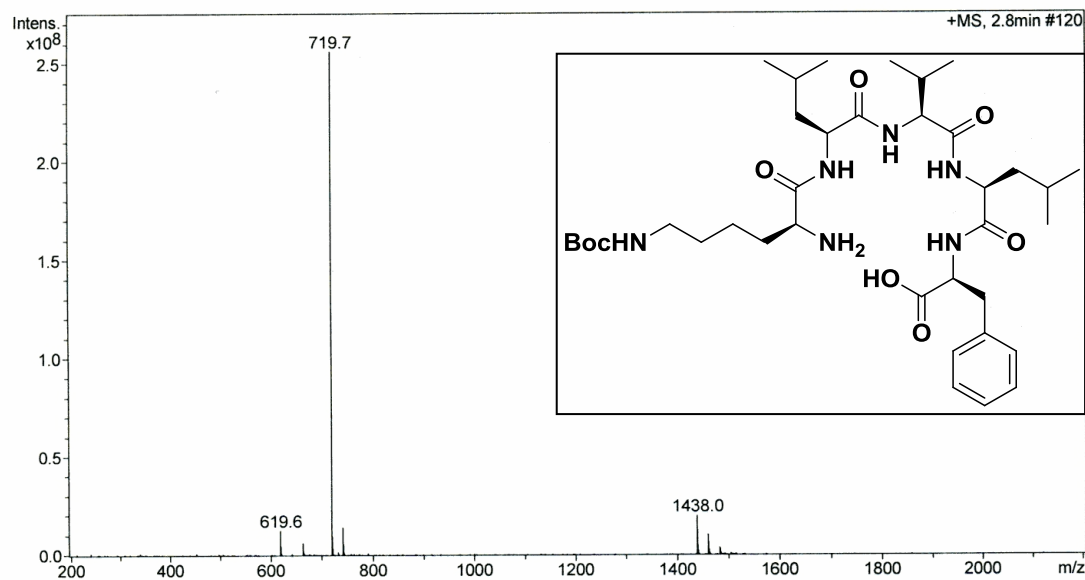
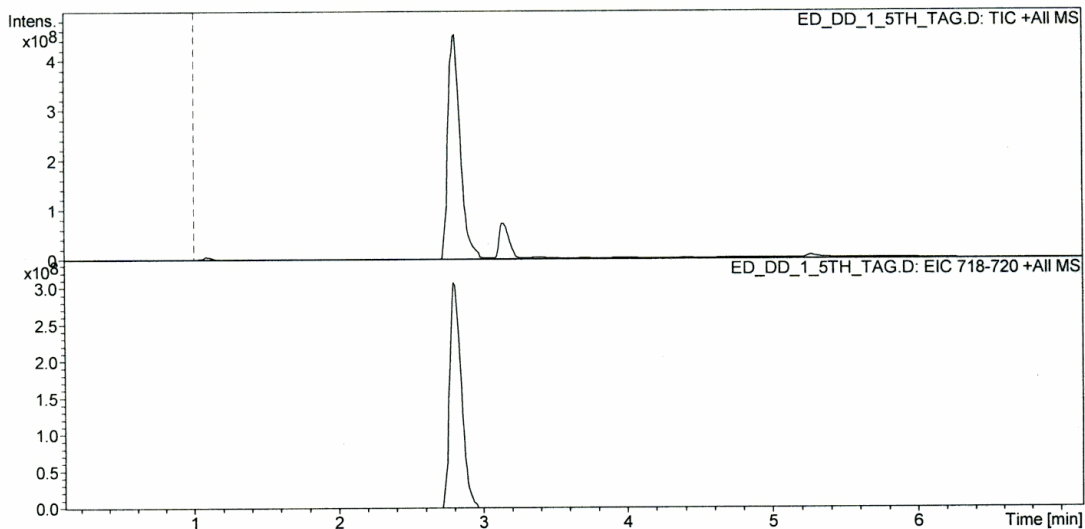
Display Report - All Windows All Analyses



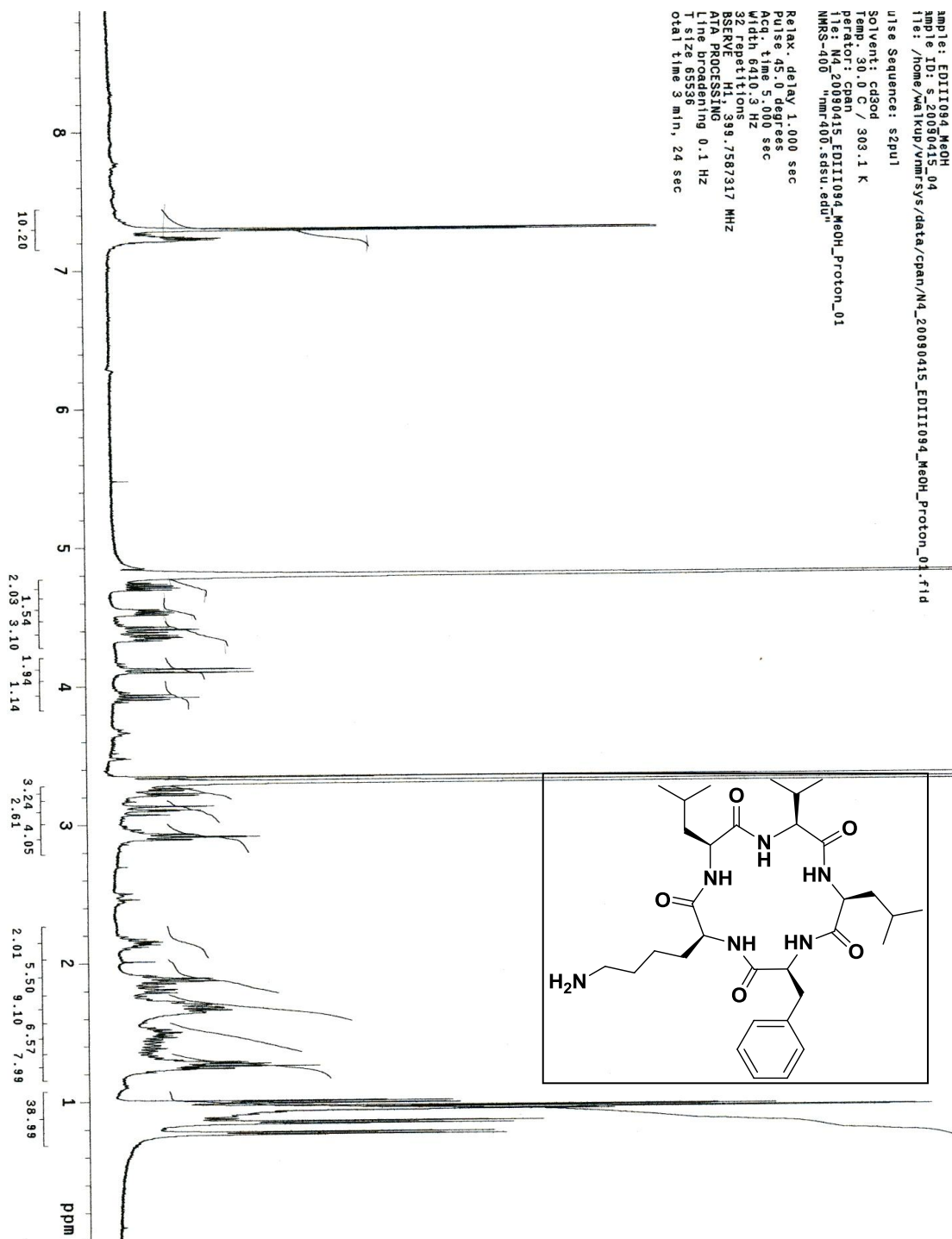
Compound 31 LCMS Cyclized Pentapeptide Phe-Leu-Val-Leu-Lys(Boc) (MW+Na=724.3)

Display Report - All Windows Selected Analysis

Analysis Name: ED_DD_1_5TH_ **Instrument:** Agilent 6330 Ion Trap **Print Date:** 4/22/2009 1:51:45 PM
Method: SANA.M TAG.D **Operator:** sdsu **Acq. Date:** 3/30/2009 1:51:37 PM
Sample Name: ED_dd_1_5th_tag
Analysis Info:



Compound 32 LCMS Double Deprotected Linear Pentapeptide HO-Phe-Leu-Val-Leu-Lys(Boc)-NH₂ (MW = 719)



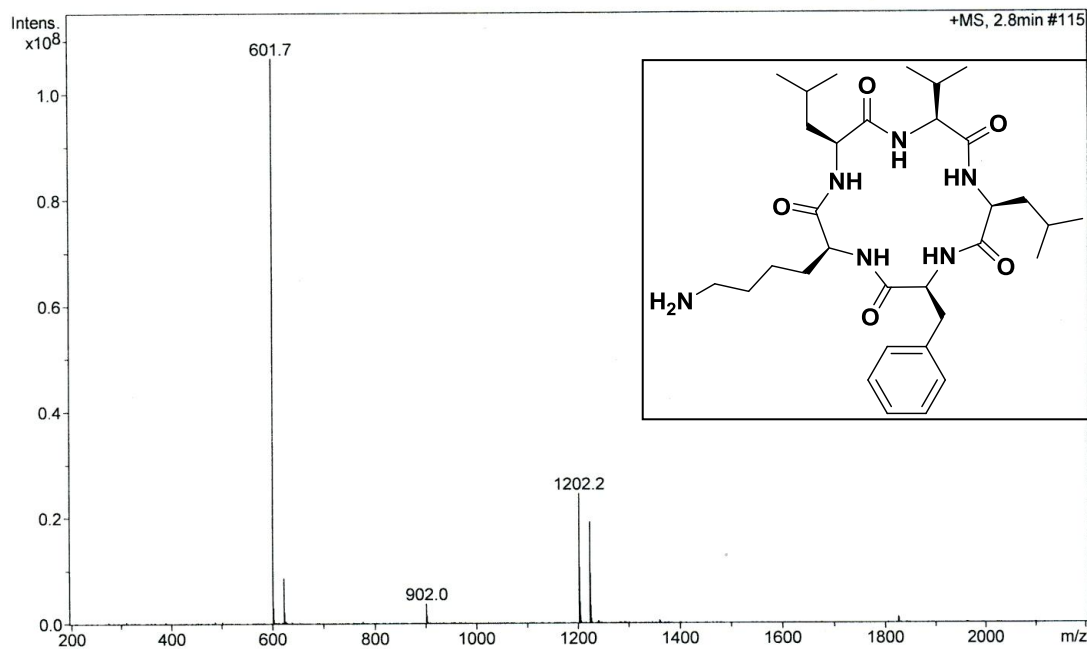
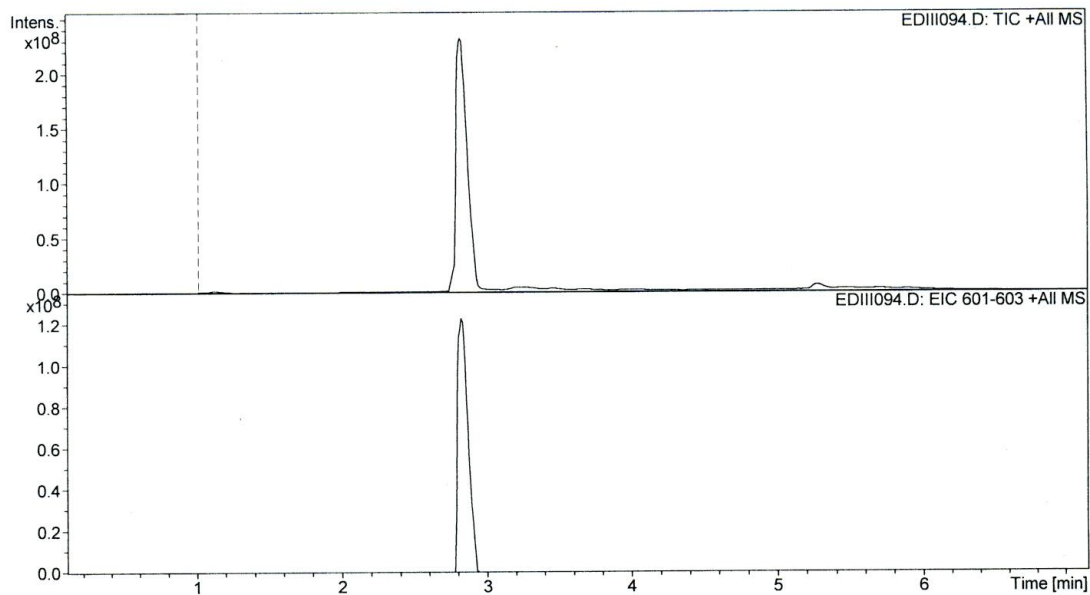
Compound 32 NMR Cyclized Pentapeptide Phe-Leu-Val-Leu-Lys

Display Report - All Windows All Analyses

Operator: sdsu

Instrument: Agilent 6330 Ion Trap

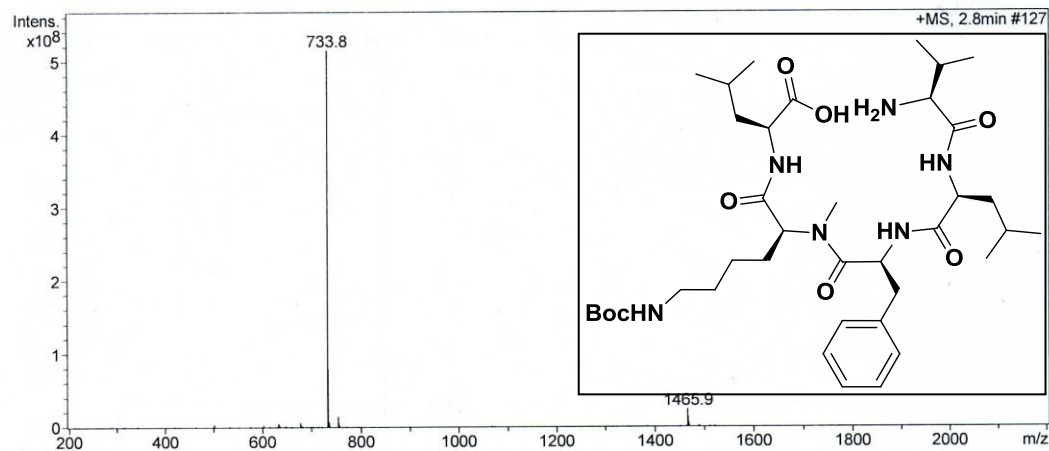
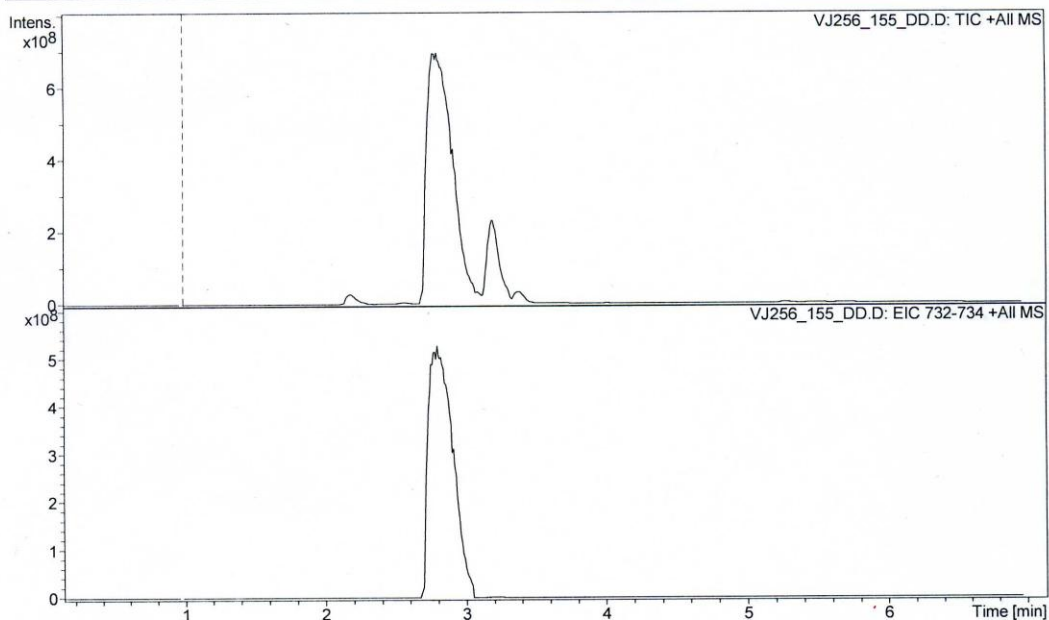
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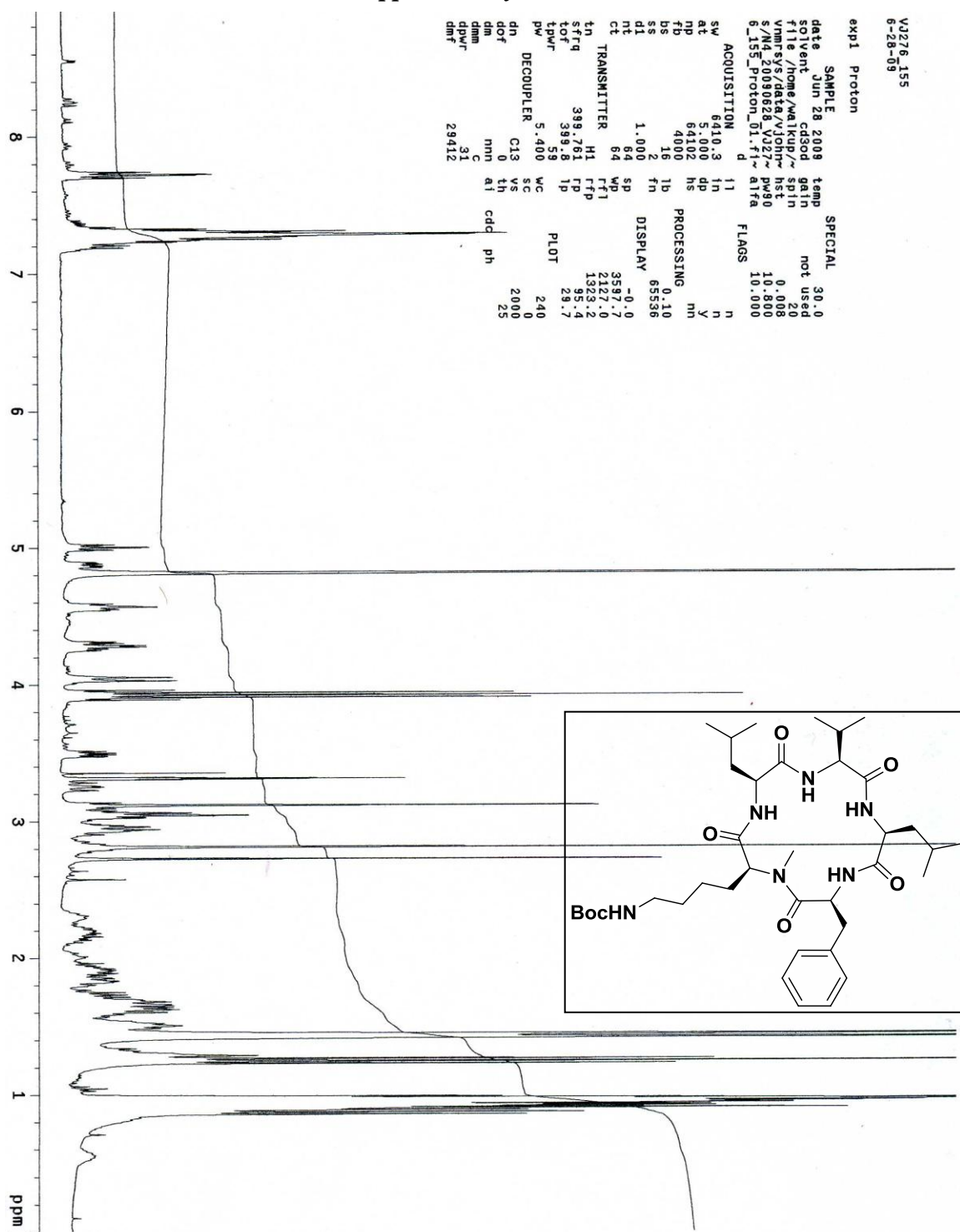
Compound 32 LCMS Cyclized Pentapeptide Phe-Leu-Val-Leu-Lys (MW=601.7)

Display Report - All Windows Selected Analysis

Analysis Name: VJ256_155_DD. **Instrument:** Agilent 6330 Ion Trap **Print Date:** 7/14/2009 1:07:22 PM
Method: SANA.M D **Operator:** sdsu **Acq. Date:** 5/21/2009 2:55:27 PM
Sample Name: VJ256_155_DD
Analysis Info:



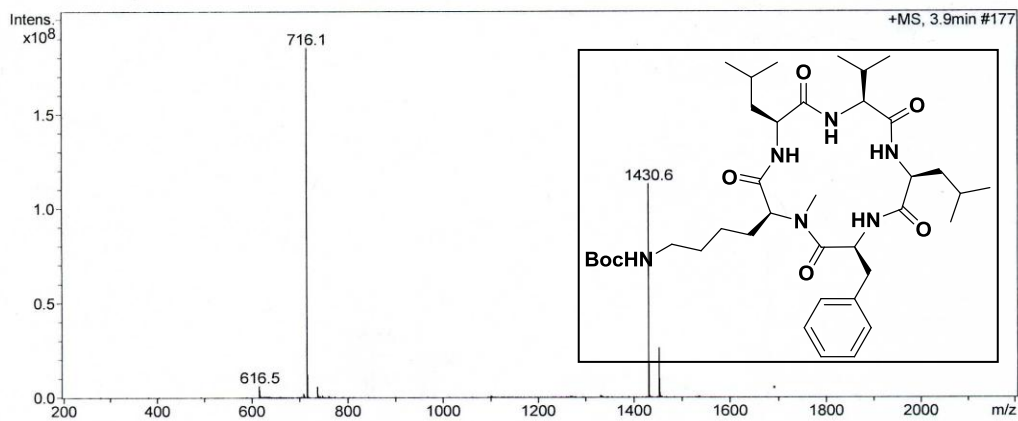
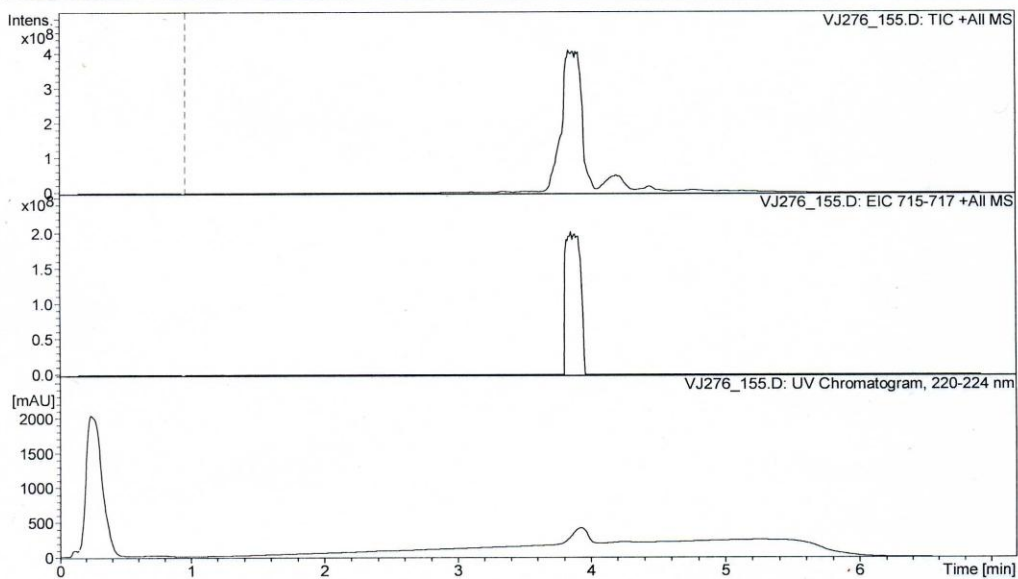
Compound 34 LCMS Double Deprotected Linear Pentapeptide HO-Leu-N-Me-Lys(Boc)-Phe-Leu-Val-NH₂ (MW = 719)



Compound 34 NMR Cyclized Pentapeptide Phe-Leu-Val-Leu-N-Me-Lys(Boc)

Display Report - All Windows Selected Analysis

Analysis Name: VJ276_155.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 7/14/2009 1:04:45 PM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 6/27/2009 5:34:13 PM
Sample Name: VJ276_155
Analysis Info:



Compound 34 LCMS Cyclized Pentapeptide Phe-Leu-Val-Leu-N-Me-Lys(Boc) (MW = 715)

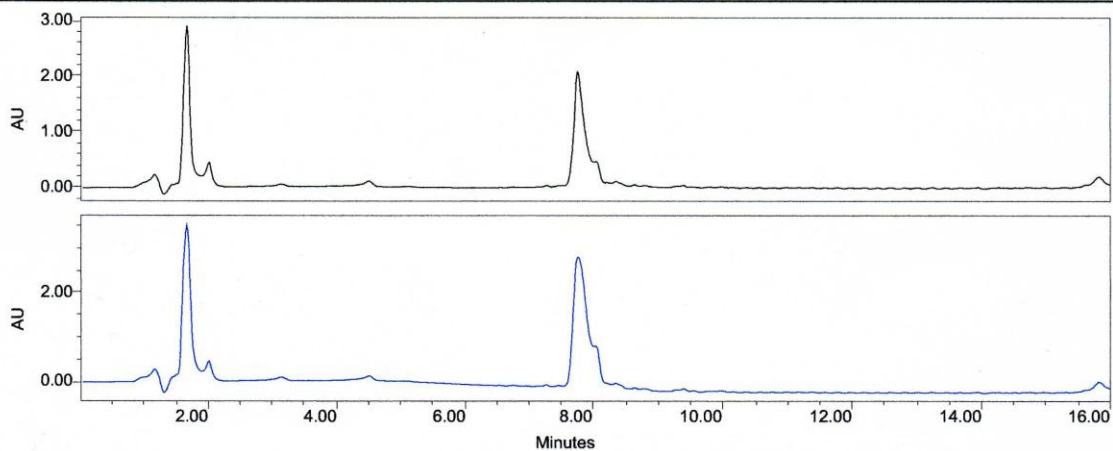
SDSU

Project Name: Defaults
Reported by User: System

Breeze

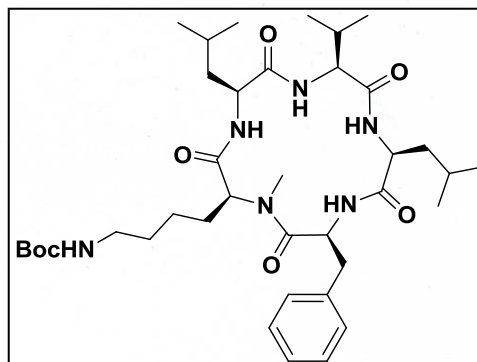
SAMPLE INFORMATION

Sample Name:	VJ276_155	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	557	Date Acquired:	6/27/2009 6:15:09 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: *

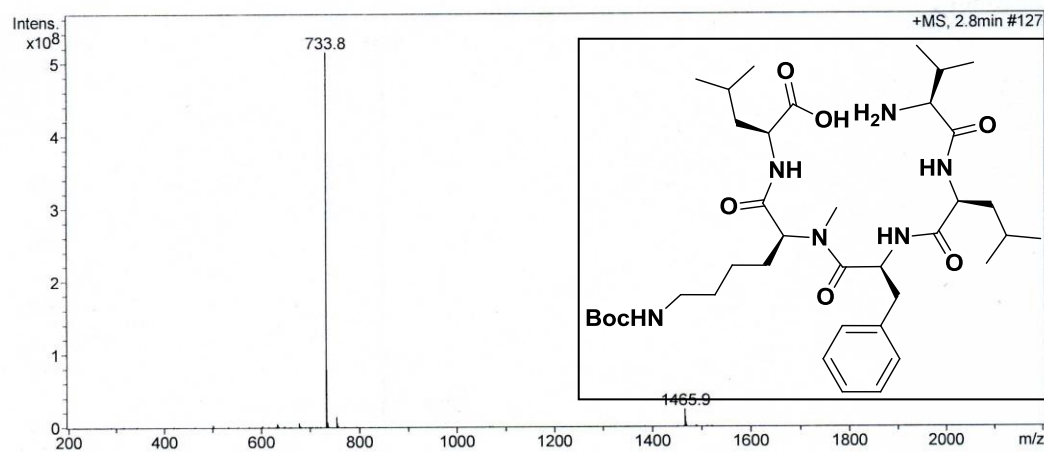
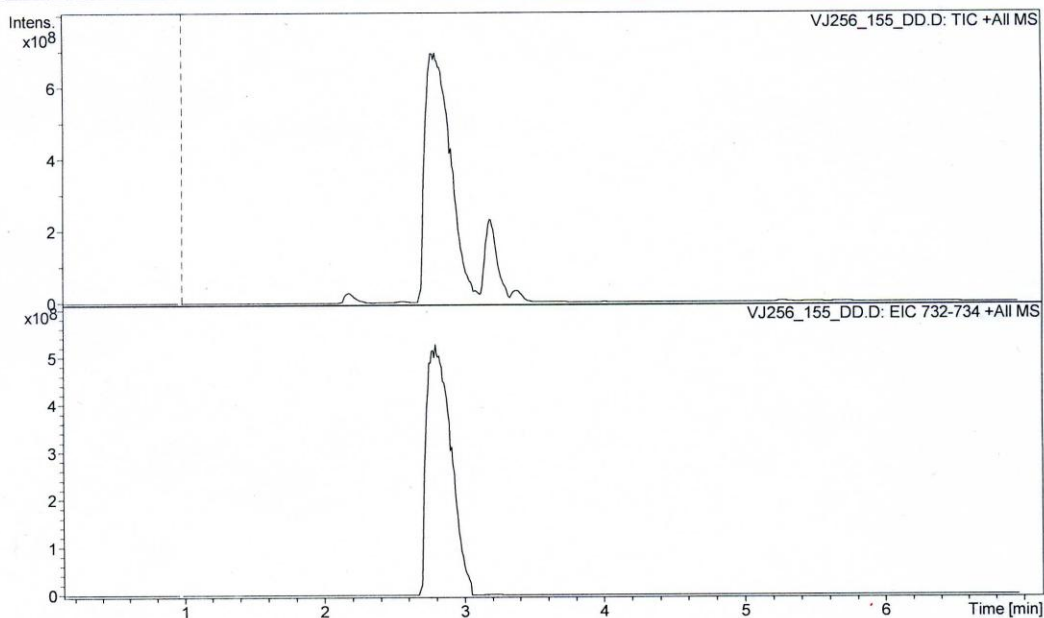
Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	Amount	Units
1	****	****	****	****	****	****
2	****	****	****	****	****	****



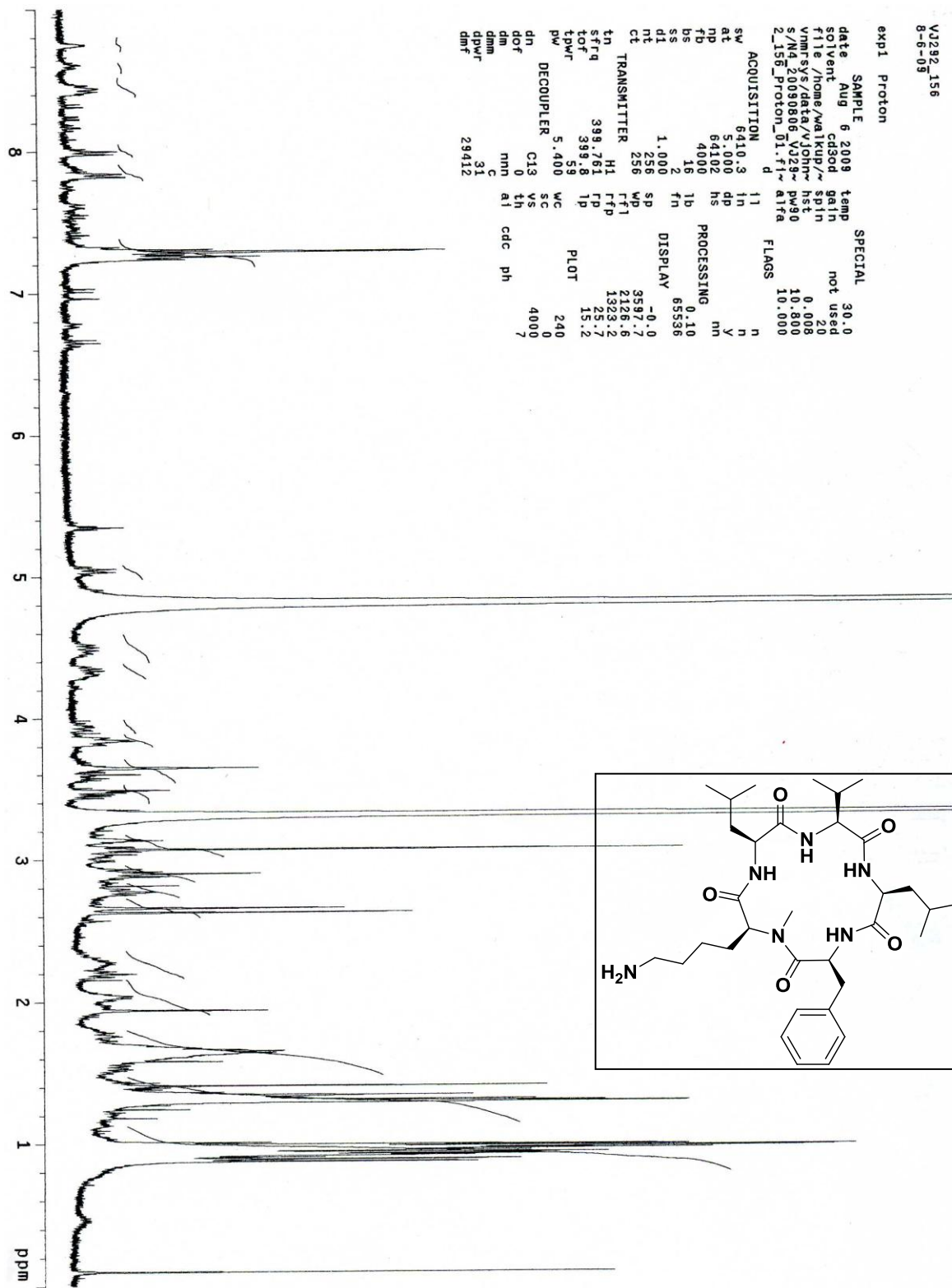
Compound 34 HPLC Cyclized Pentapeptide Phe-Leu-Val-Leu-N-Me-Lys(Boc)

Display Report - All Windows Selected Analysis

Analysis Name: VJ256_155_DD. **Instrument:** Agilent 6330 Ion Trap **Print Date:** 7/14/2009 1:07:22 PM
Method: SANA.M D **Operator:** sdsu **Acq. Date:** 5/21/2009 2:55:27 PM
Sample Name: VJ256_155_DD
Analysis Info:



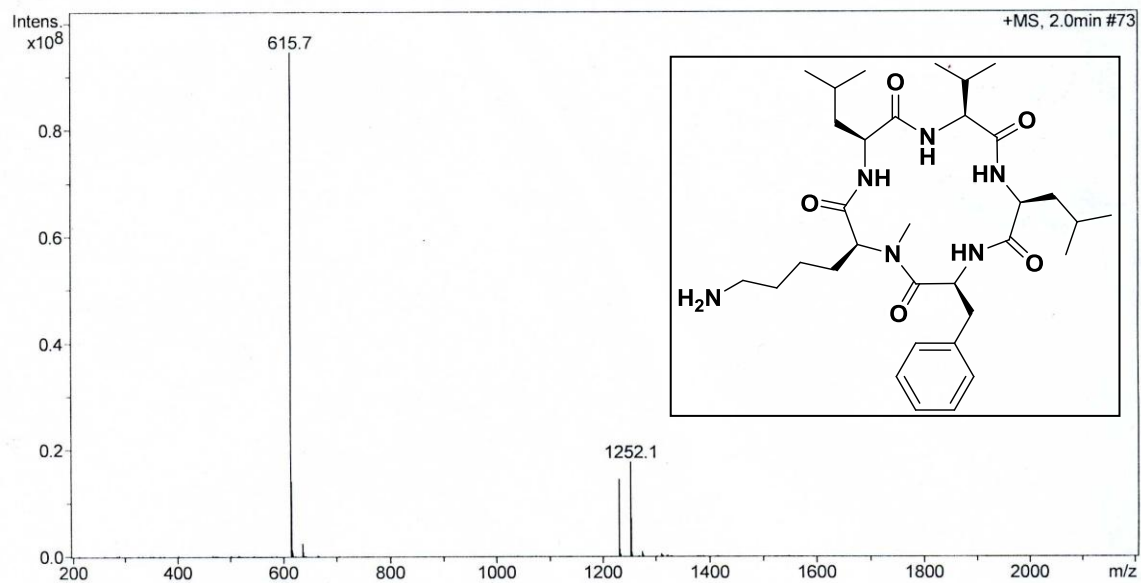
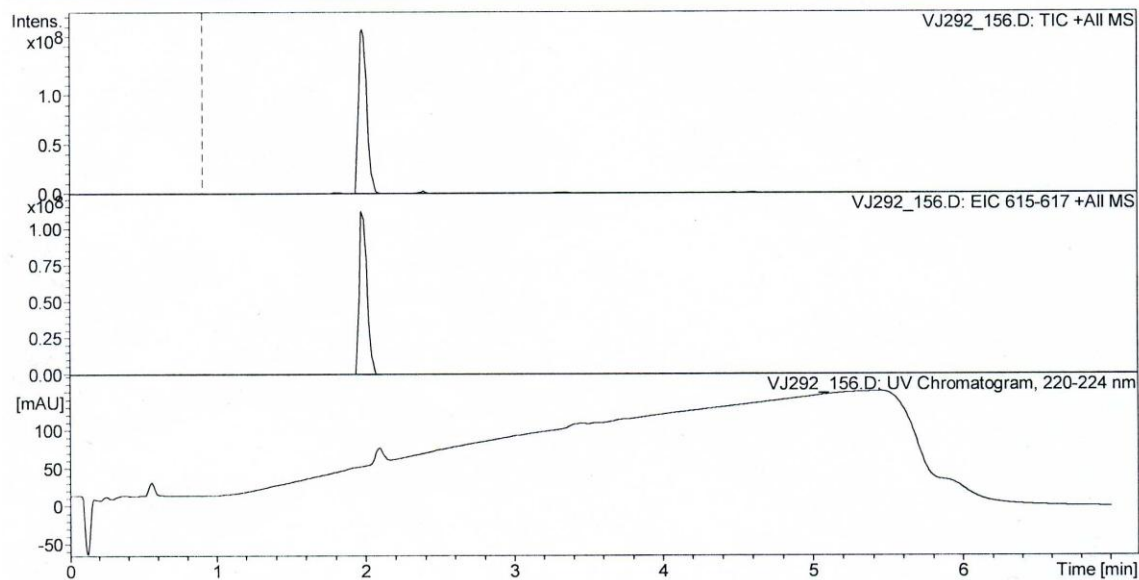
Compound 35 LCMS Double Deprotected Linear Pentapeptide HO-Leu-N-Me-Lys(Boc)-Phe-Leu-Val-NH₂ (MW = 719)



Compound 35 NMR Cyclized Pentapeptide Phe-Leu-Val-Leu-N-Me-Lys

Display Report - All Windows Selected Analysis

Analysis Name: VJ292_156.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 8/5/2009 8:40:02 PM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 8/5/2009 8:32:41 PM
Sample Name: VJ292_156
Analysis Info:



Compound 35 LCMS Cyclized Pentapeptide Phe-Leu-Val-Leu-N-Me-Lys (MW = 615)

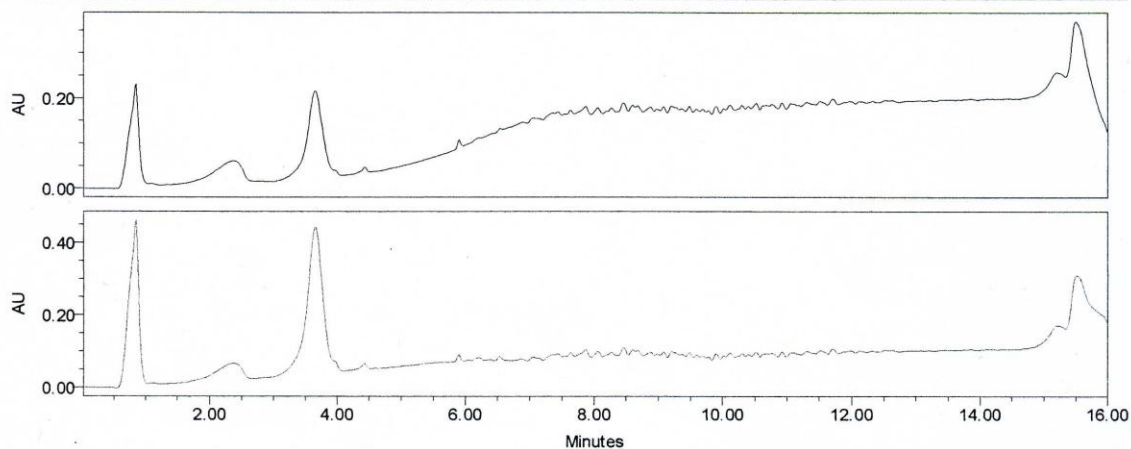
SDSU

Project Name: Defaults
Reported by User: System

Breeze

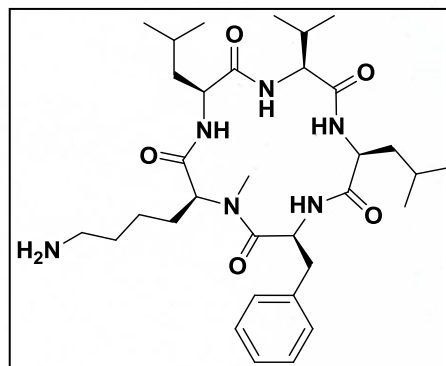
SAMPLE INFORMATION

Sample Name:	VJ292_156	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	207	Date Acquired:	8/5/2009 7:59:53 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: ****

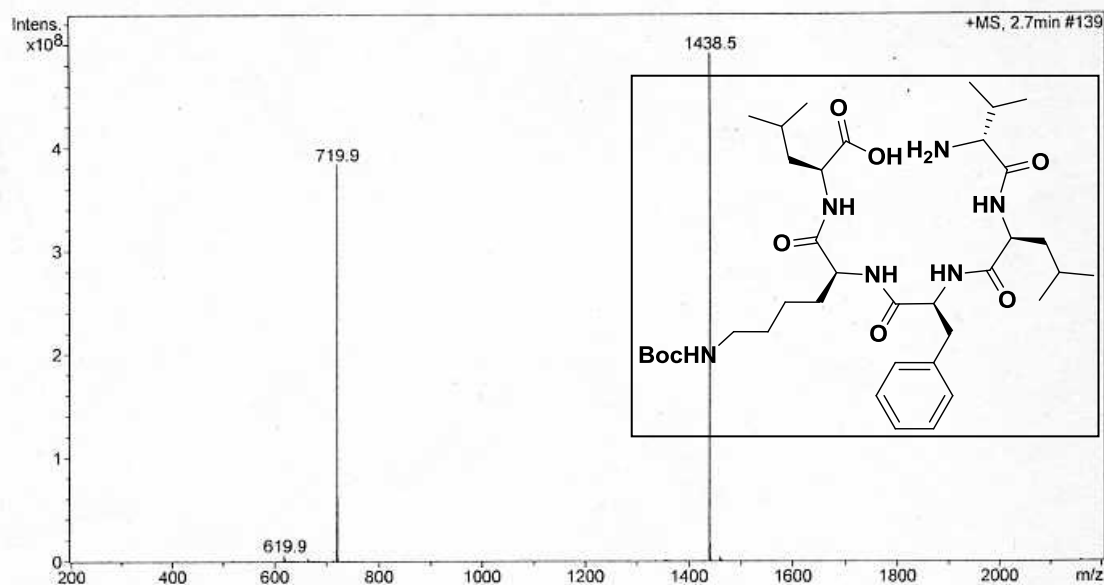
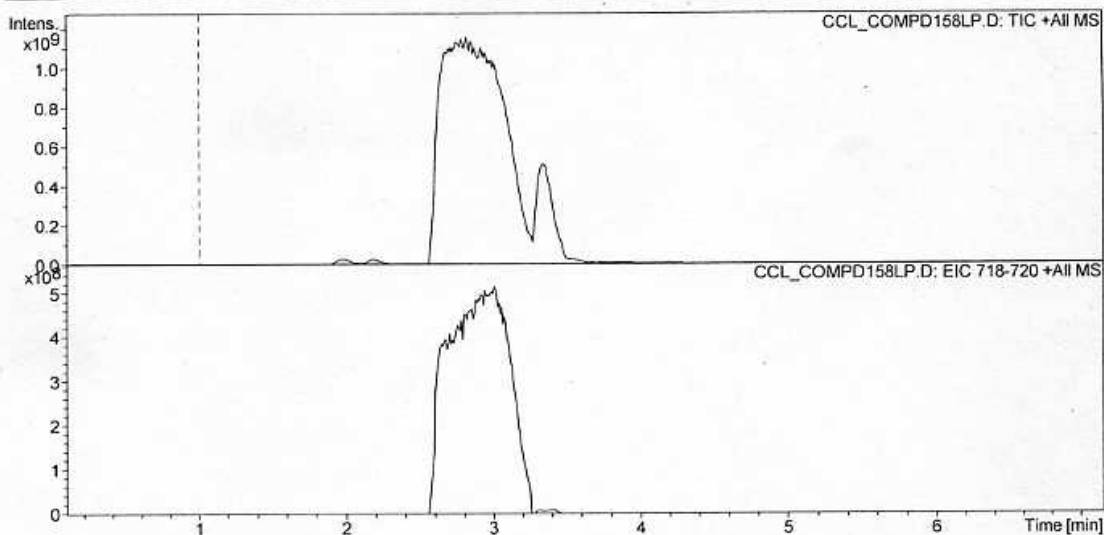
Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	Amount	Units
1	****	****	****	****	****	****
2	****	****	****	****	****	****



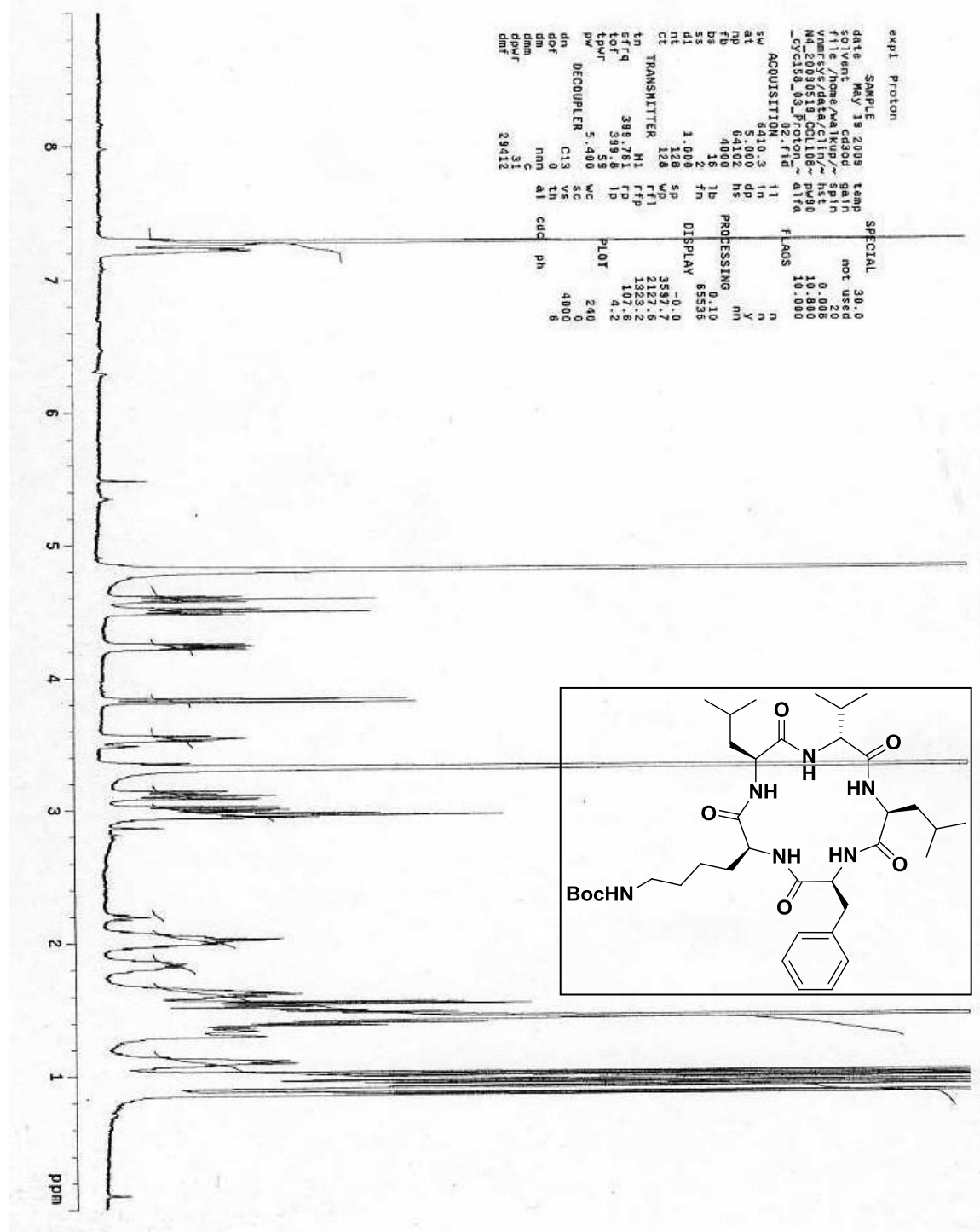
Compound 35 HPLC Cyclized Pentapeptide Phe-Leu-Val-Leu-N-Me-Lys

Display Report - All Windows Selected Analysis

Analysis Name: CCL_COMPD158 **Instrument:** Agilent 6330 Ion Trap **Print Date:** 4/22/2009 3:22:36 PM
Method: SANA.M LP.D **Operator:** sdsu **Acq. Date:** 4/21/2009 5:10:51 PM
Sample Name: CCL_comp158LP
Analysis Info:



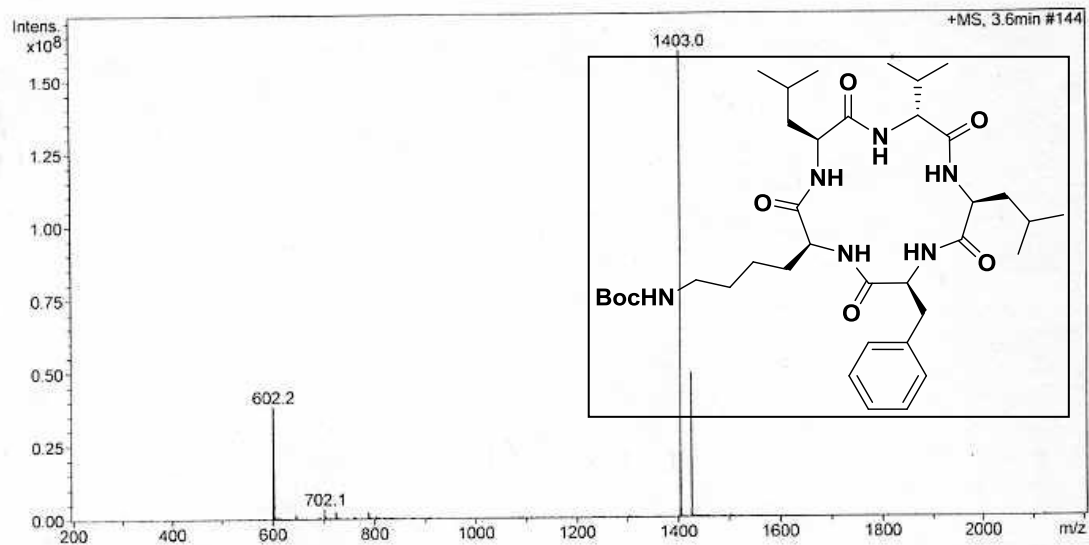
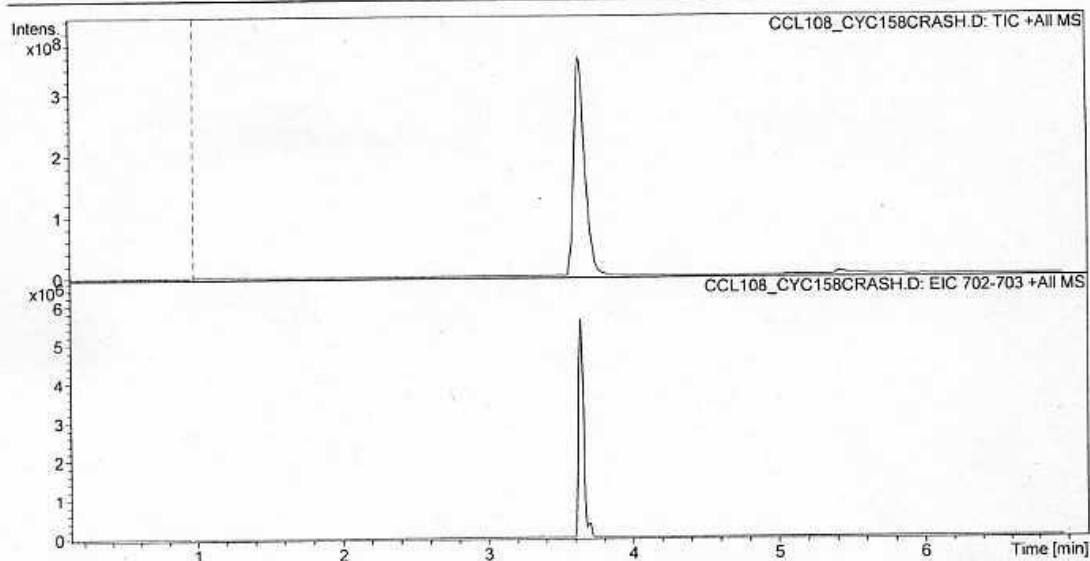
Compound 36 LCMS Double Deprotected Linear Pentapeptide HO-Leu-Lys(Boc)-Phe-Leu-D-Val-NH₂ (MW = 719)



Compound 36 NMR Cyclized Pentapeptide Phe-Leu-D-Val-Leu-Lys(Boc)

Display Report - All Windows Selected Analysis

Analysis Name: CCL108_CYC158 **Instrument:** Agilent 6330 Ion Trap **Print Date:** 5/19/2009 5:53:37 PM
Method: SANA.M CRASH.D **Operator:** sdsu **Acq. Date:** 5/12/2009 6:04:22 PM
Sample Name: CCL108_cyc158crash
Analysis Info:



Compound 36 LCMS Cyclized Pentapeptide Phe-Leu-D-Val-Leu-Lys(Boc) (MW = 702)

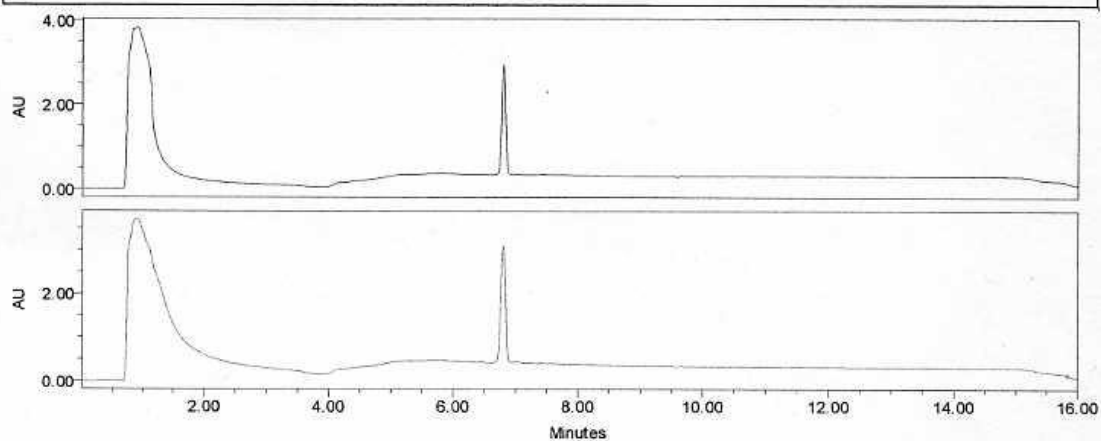
SDSU

Project Name: Defaults
Reported by User: System

Breeze

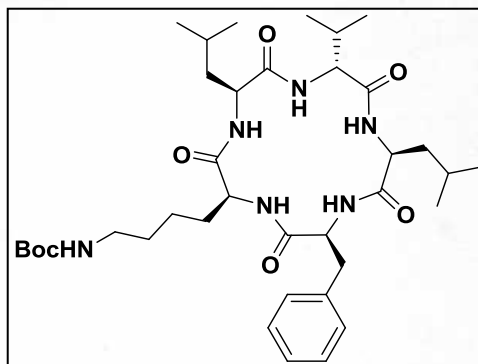
SAMPLE INFORMATION

Sample Name:	CCL108_cyc158_01	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss
Injection #:	228	Date Acquired:	5/18/2009 2:36:27 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: ****

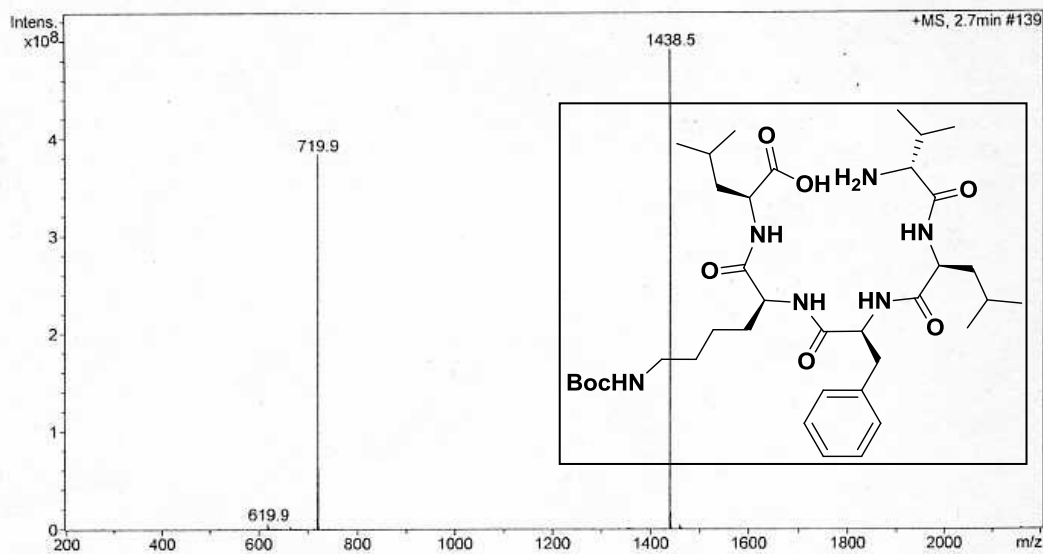
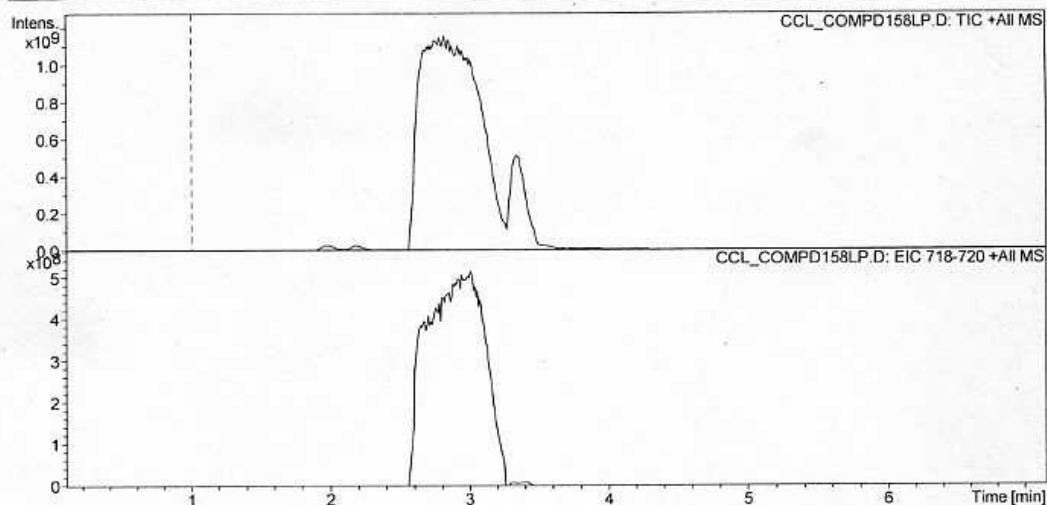
Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	Amount	Units
1 ****	****	****	****	****	****	****
2 ****	****	****	****	****	****	****



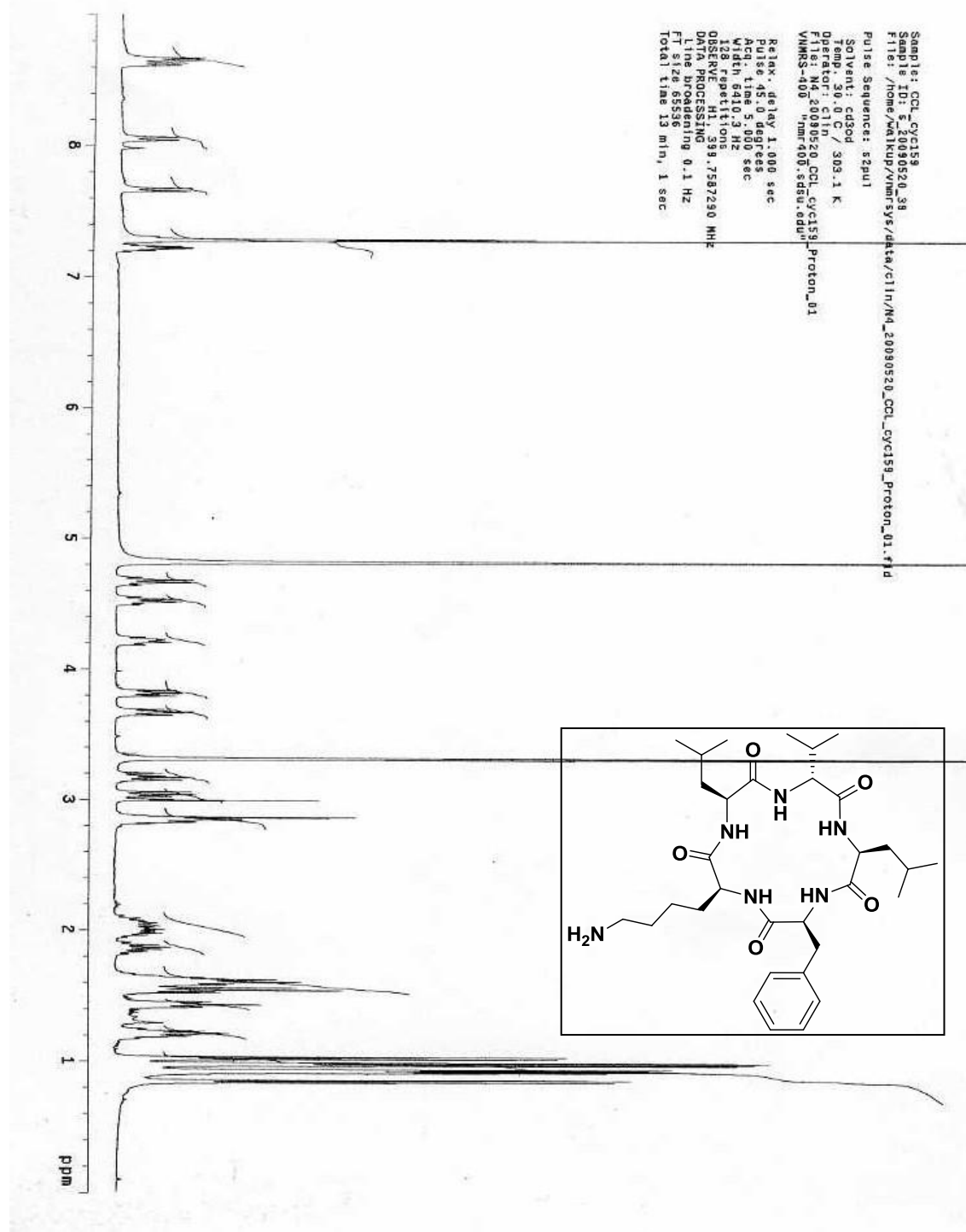
Compound 36 HPLC Cyclized Pentapeptide Phe-Leu-D-Val-Leu-Lys(Boc)

Display Report - All Windows Selected Analysis

Analysis Name: CCL_COMPD158 Instrument: Agilent 6330 Ion Trap Print Date: 4/22/2009 3:22:36 PM
Method: SANA.M LP.D Operator: sdsu Acq. Date: 4/21/2009 5:10:51 PM
Sample Name: CCL_comp158LP
Analysis Info:



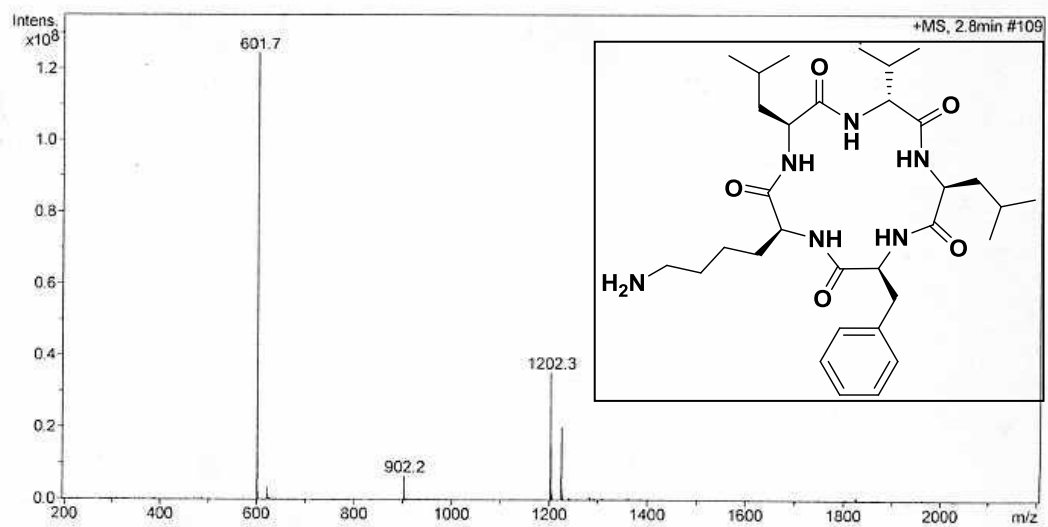
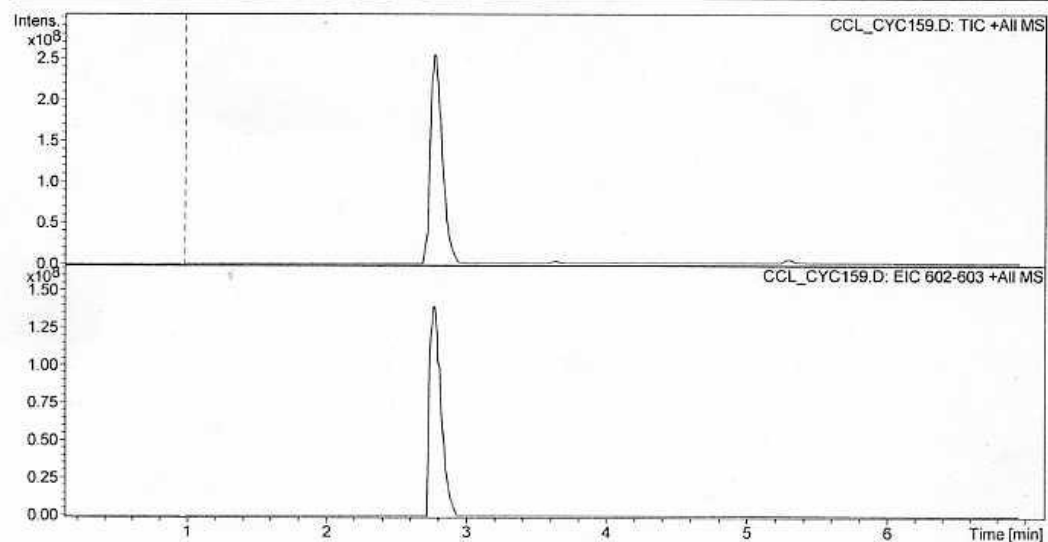
Compound 37 LCMS Double Deprotected Linear Pentapeptide HO-Leu-Lys(Boc)-Phe-Leu-D-Val-NH₂ (MW = 719)



Compound 37 NMR Cyclized Pentapeptide Phe-Leu-D-Val-Leu-Lys

Display Report - All Windows Selected Analysis

Analysis Name: CCL_CYC159.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 5/19/2009 9:41:42 PM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 5/19/2009 9:31:35 PM
Sample Name: CCL_cyc159
Analysis Info:



Compound 37 LCMS Cyclized Pentapeptide Phe-Leu-D-Val-Leu-Lys (MW = 602)

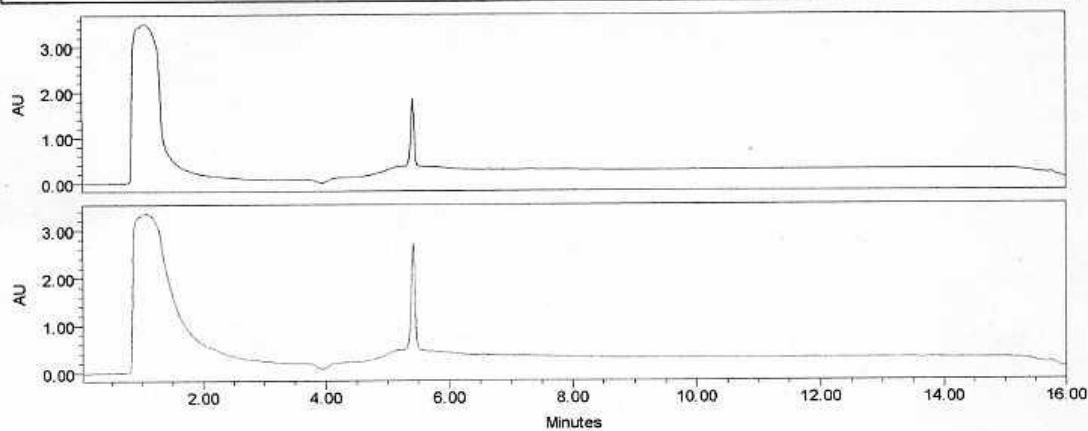
SDSU

Project Name: Defaults
Reported by User: System

Breeze

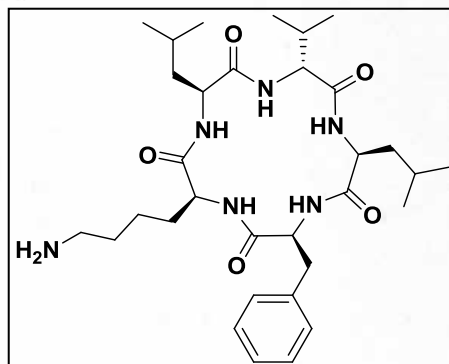
SAMPLE INFORMATION

Sample Name:	CCL112_cyc159_02	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss
Injection #:	247	Date Acquired:	5/19/2009 10:12:07 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: ****

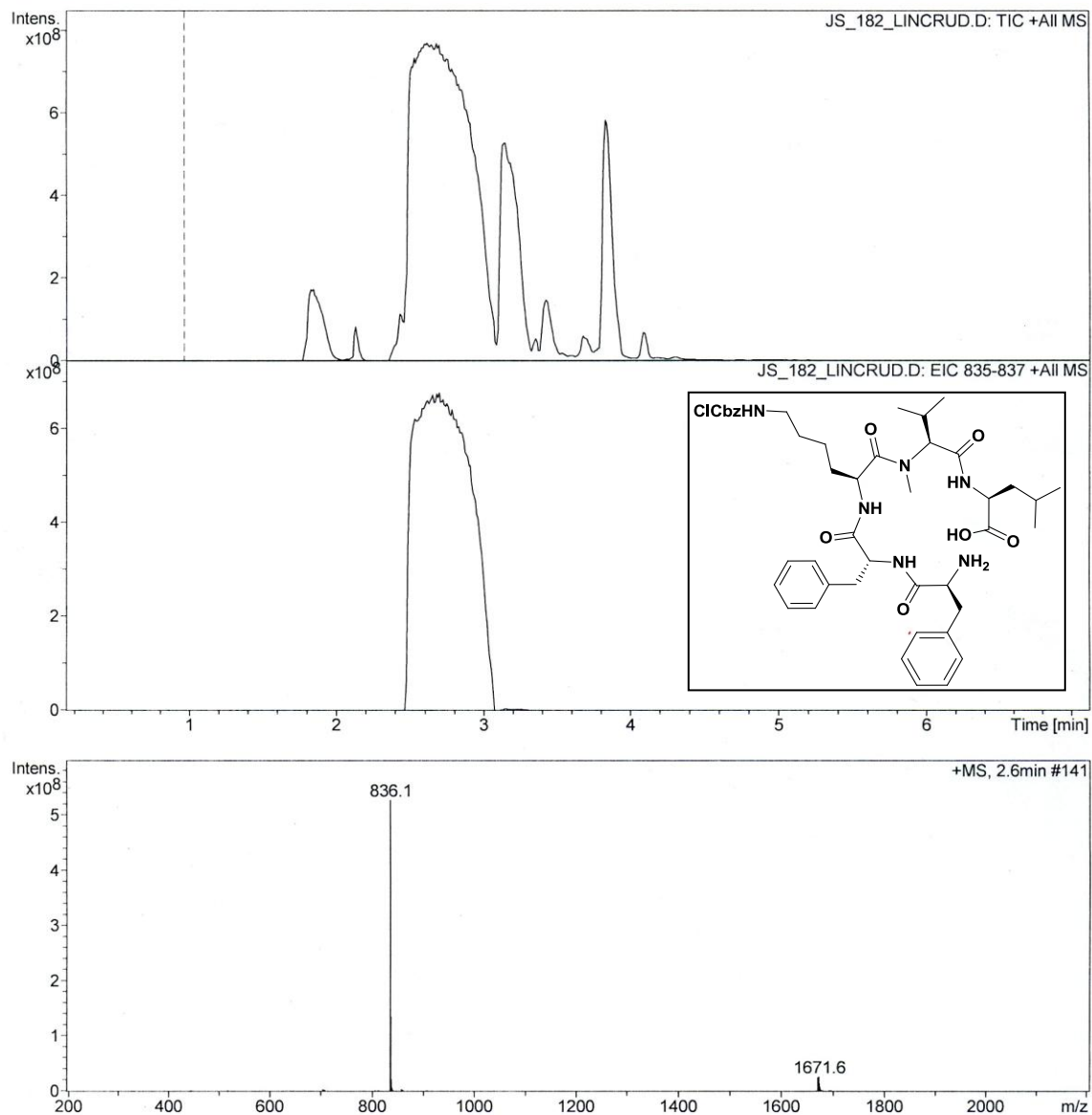
Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	Amount	Units
1 ****	****	****	****	****	****	****
2 ****	****	****	****	****	****	****



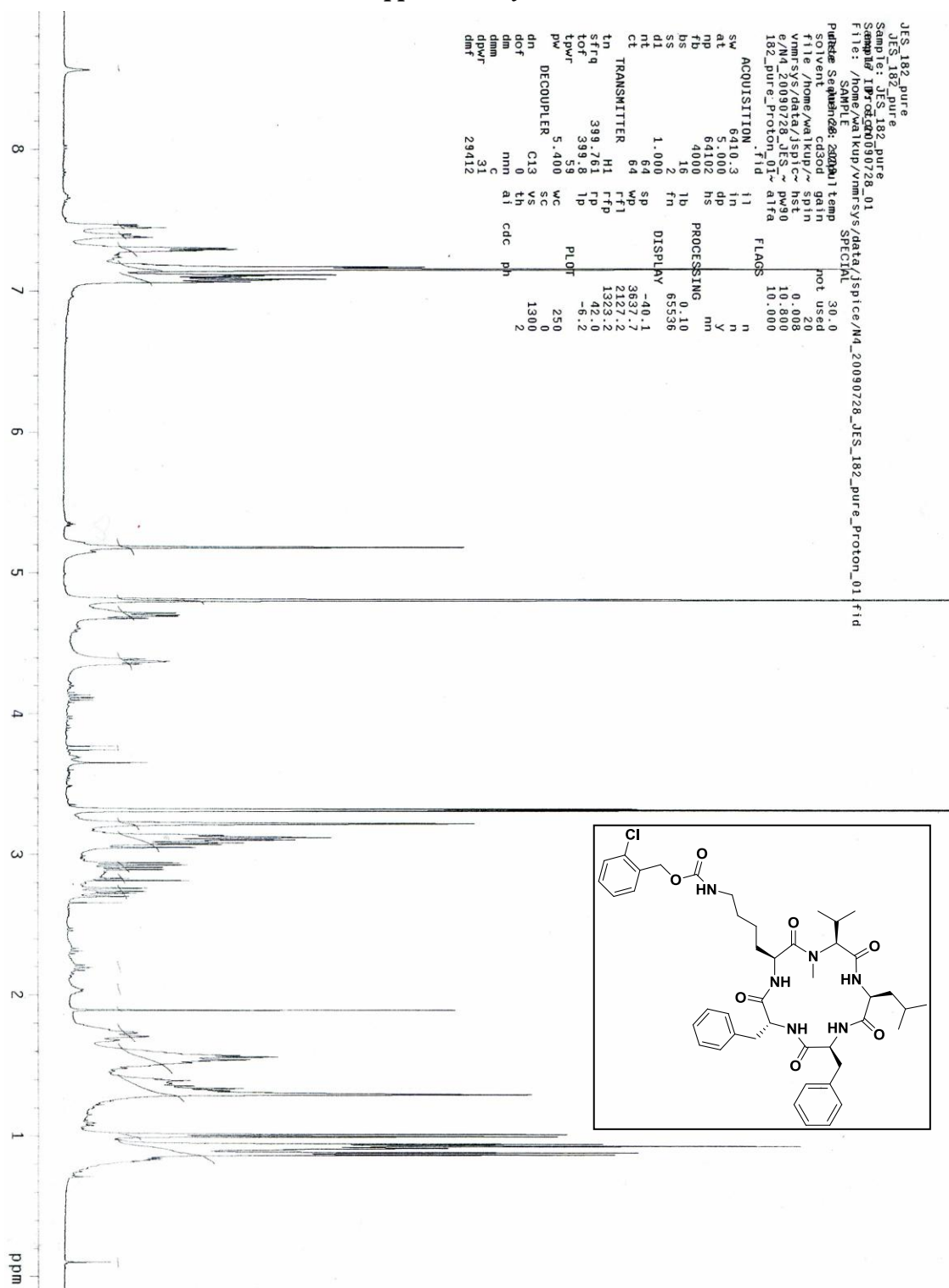
Compound 37 HPLC Cyclized Pentapeptide Phe-Leu-D-Val-Leu-Lys

Display Report - All Windows Selected Analysis

Analysis Name: JS_182_LINCRU **Instrument:** Agilent 6330 Ion Trap **Print Date:** 6/25/2009 9:20:24 AM
Method: SANA.M D.D **Operator:** sdsu **Acq. Date:** 6/24/2009 7:02:04 PM
Sample Name: JS_182_lincrud
Analysis Info:



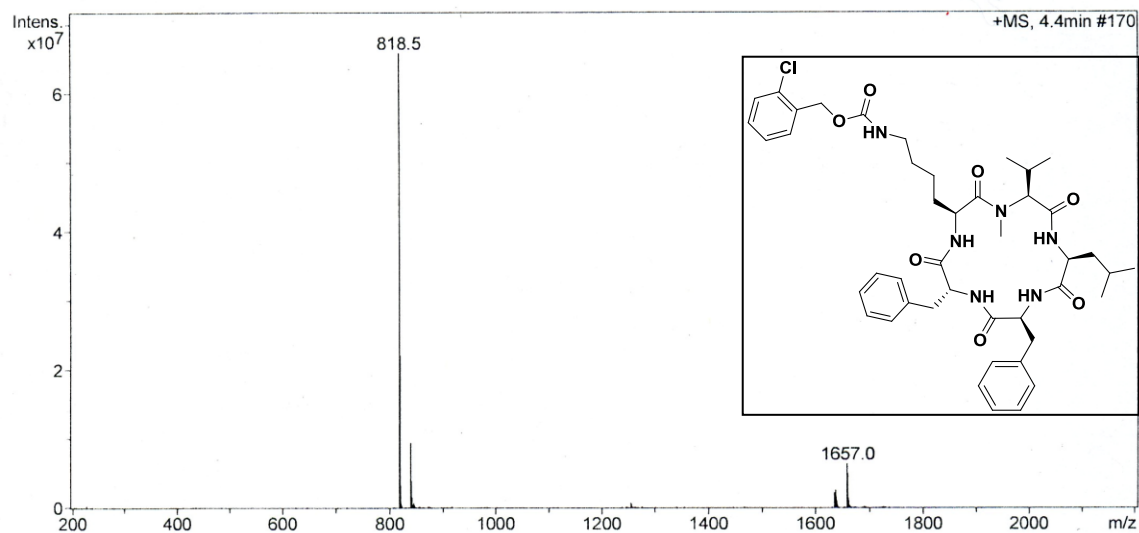
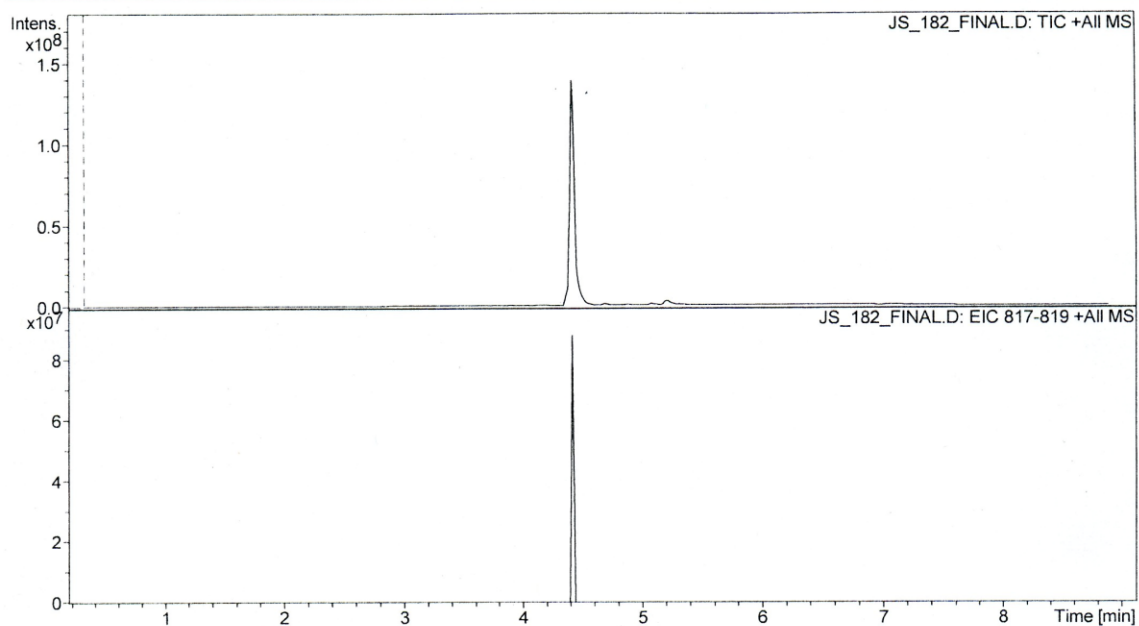
Compound 39 LCMS Double Deprotected Linear Pentapeptide HO-Leu-N-Me-Val-Lys(2-Cl-Z)-D-Phe-Phe-NH₂ (MW = 835.4)



Compound 39 NMR Cyclized Pentapeptide Phe-Leu-N-Me-Val-Lys(2-Cl-Z)-D-Phe

Display Report - All Windows Selected Analysis

Analysis Name: JS_182_FINAL.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 7/28/2009 12:18:35 PM
Method: SANA_LONG.M **Operator:** sdsu **Acq. Date:** 7/28/2009 12:09:13 PM
Sample Name: JS_182_final
Analysis Info:



Compound 39 LCMS Cyclized Pentapeptide Phe-Leu-N-Me-Val-Lys(2-Cl-Z)-D-Phe (MW=817.4)

SDSU

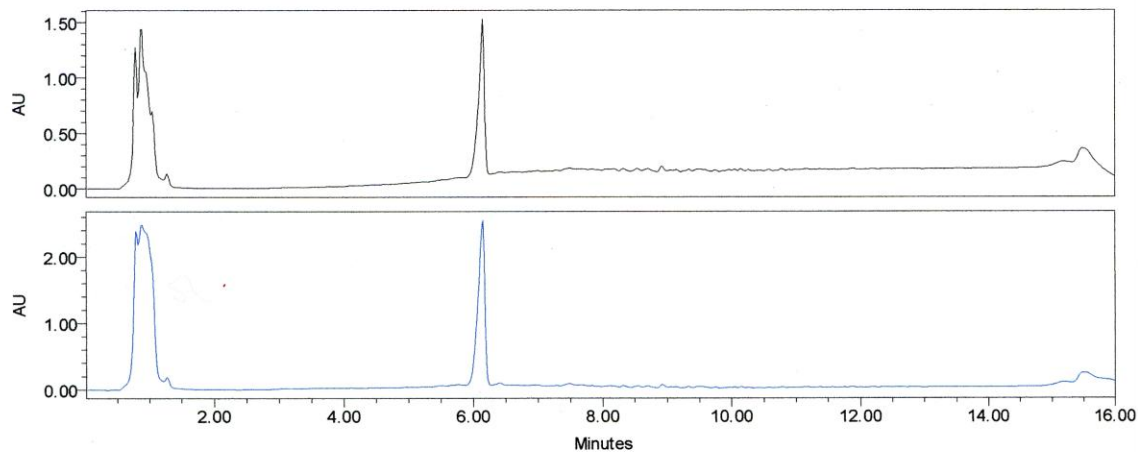
Project Name: Defaults
 Reported by User: System

Breeze

SAMPLE INFORMATION

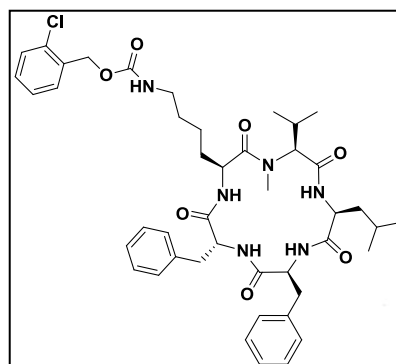
Sample Name: JS_182_ss_pure
 Sample Type: Unknown
 Vial: 1
 Injection #: 185
 Run Time: 16.00 Minutes

Acquired By: System
 Sample Set Name:
 Acq. Method: primary_sanA_ss_ACN
 Date Acquired: 7/31/2009 9:35:13 AM
 Injection Volume: 48.00 ul



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

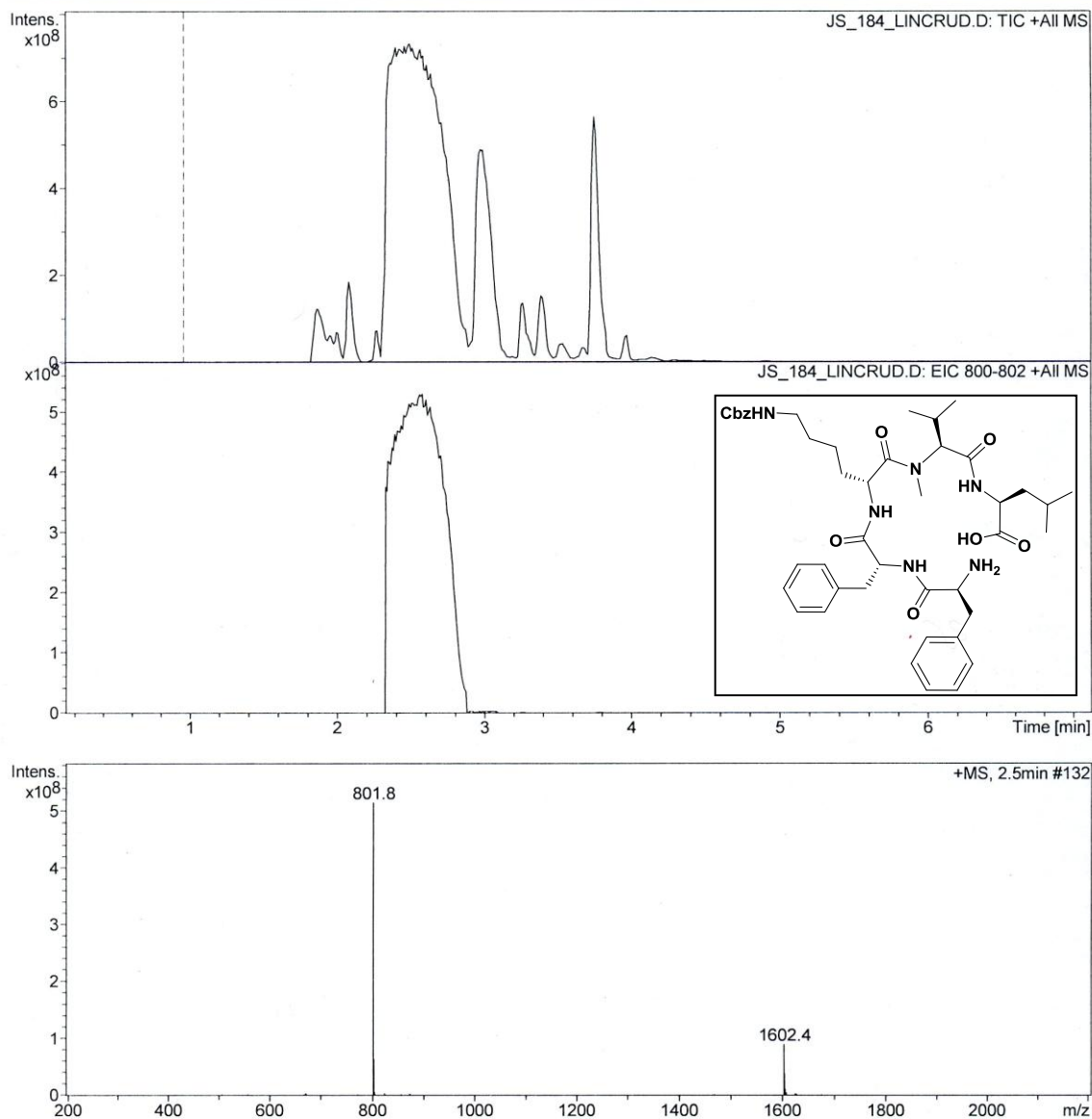
Peak Name	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	Amount	Units
1 ****	****	****	****	****	****	****
2 ****	****	****	****	****	****	****



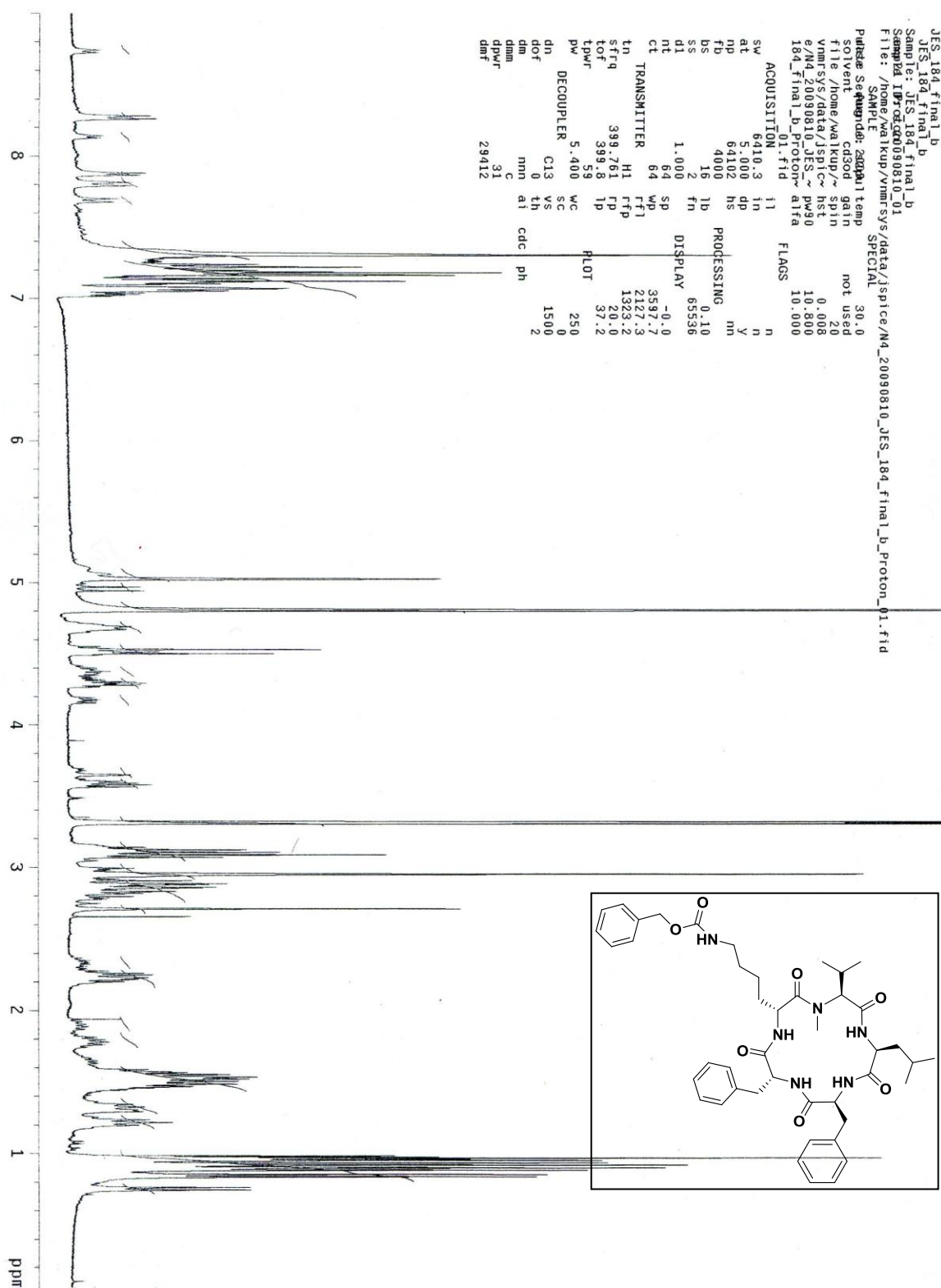
Compound 39 HPLC Cyclized Pentapeptide Phe-Leu-N-Me-Val-Lys(2-Cl-Z)-D-Phe

Display Report - All Windows Selected Analysis

Analysis Name: JS_184_LINCRU **Instrument:** Agilent 6330 Ion Trap **Print Date:** 6/25/2009 9:20:39 AM
Method: SANA.M D.D **Operator:** sdsu **Acq. Date:** 6/24/2009 7:11:02 PM
Sample Name: JS_184_lincrud
Analysis Info:



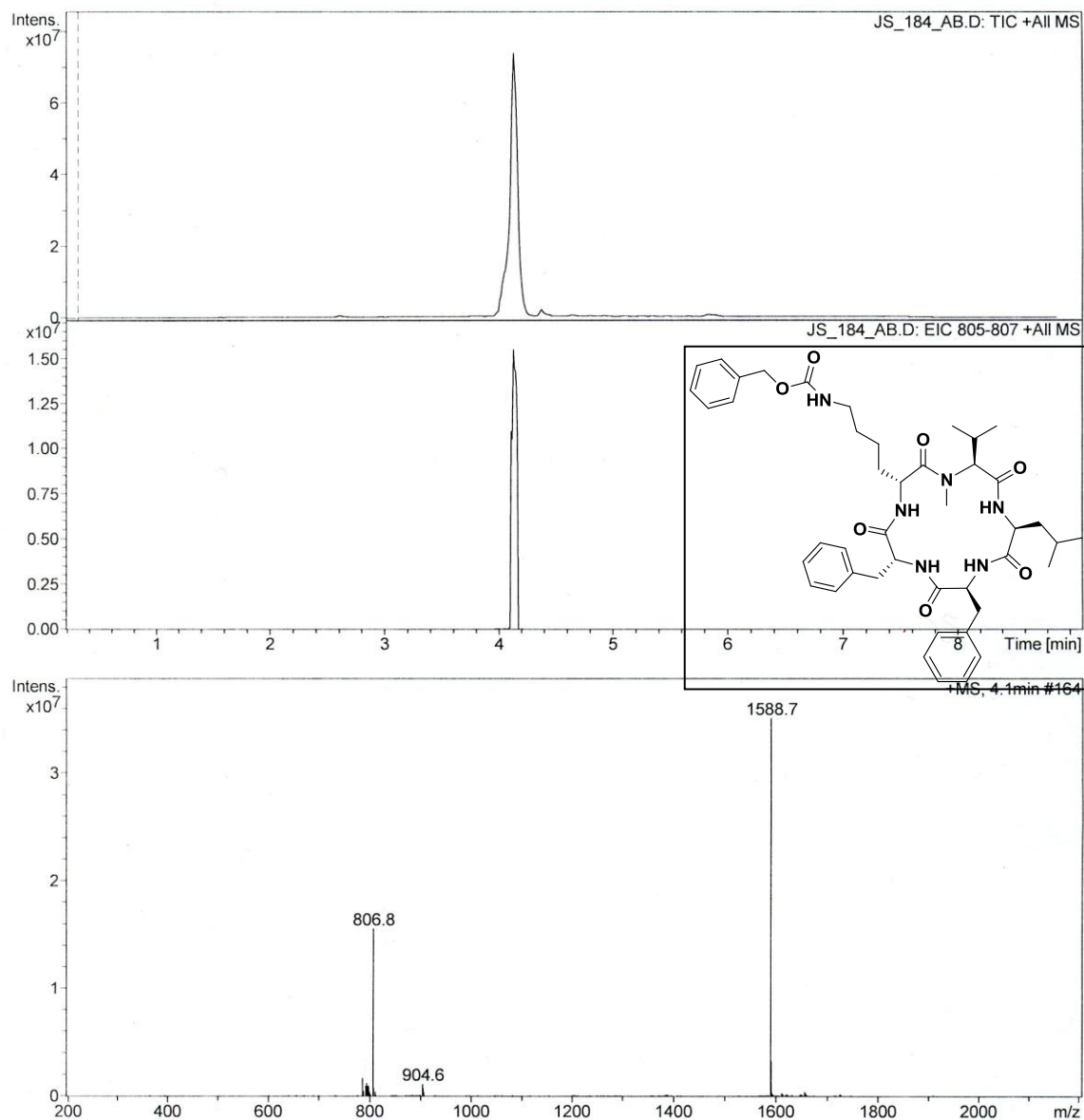
Compound 40 LCMS Double Deprotected Linear Pentapeptide HO-Leu-N-Me-Val-D-Lys(Cbz)-D-Phe-Phe-NH₂ (MW = 801)



Compound 40 NMR Cyclized Pentapeptide Phe-Leu-N-Me-Val-D-Lys(Cbz)-D-Phe

Display Report - All Windows Selected Analysis

Analysis Name: JS_184_AB.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 8/11/2009 11:58:37 AM
Method: SANA_LONG.M **Operator:** sdsu **Acq. Date:** 8/11/2009 11:43:34 AM
Sample Name: JS_184_AB
Analysis Info:



Compound 40 LCMS Cyclized Pentapeptide Phe-Leu-N-Me-Val-D-Lys(Cbz)-D-Phe (MW= 783)

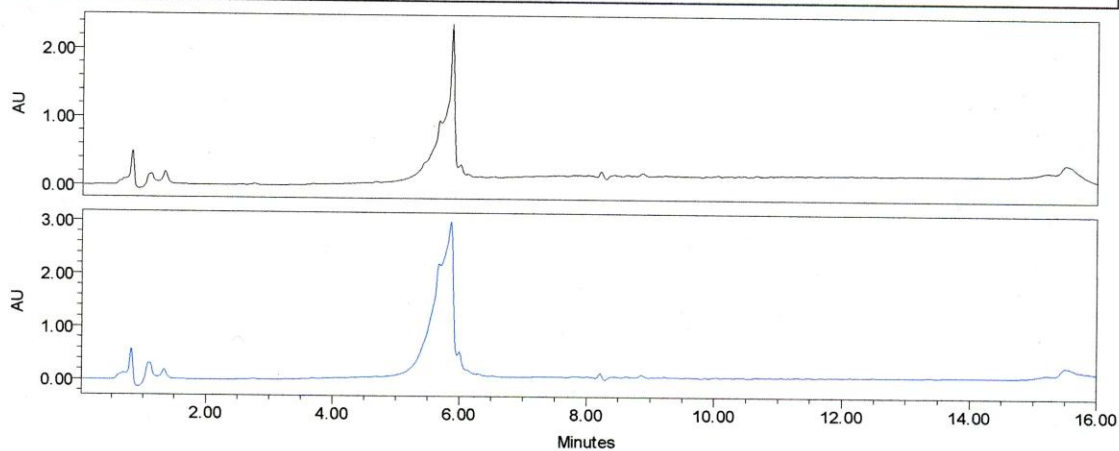
SDSU

Project Name: Defaults
Reported by User: System

Breeze

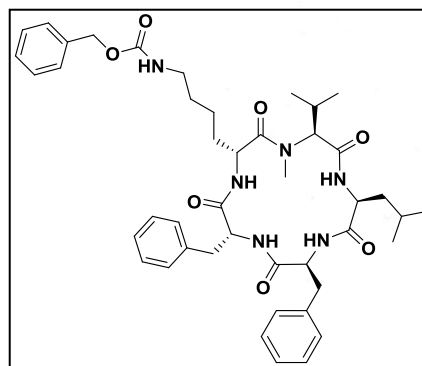
SAMPLE INFORMATION

Sample Name:	JS_184_ss_final	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	19	Date Acquired:	8/11/2009 8:57:01 AM
Run Time:	16.00 Minutes	Injection Volume:	80.00 ul



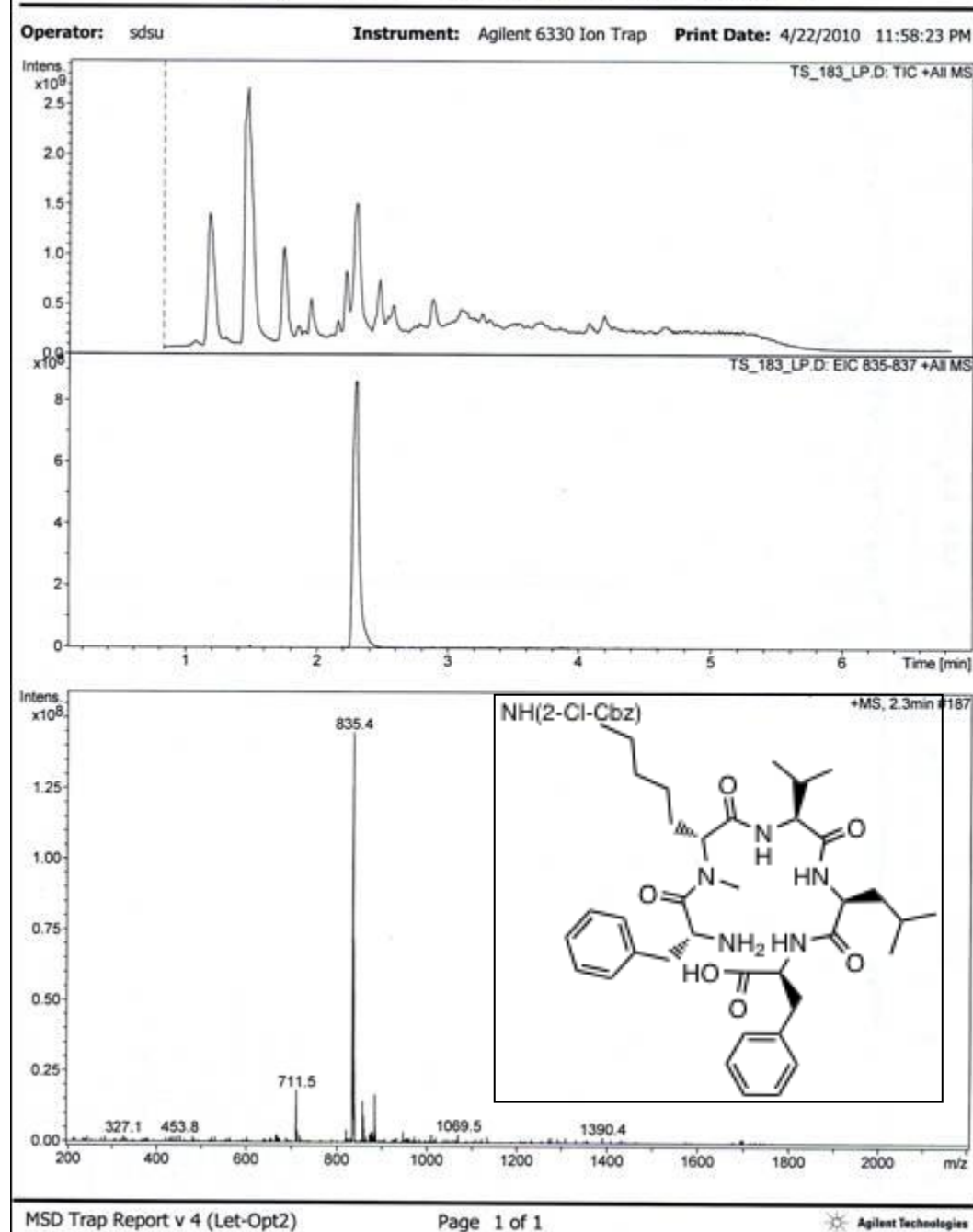
— Channel: 2487Channel 1 Channel Desc.: Processing Method: ****
 — Channel: 2487Channel 2 Channel Desc.: Processing Method: ****

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

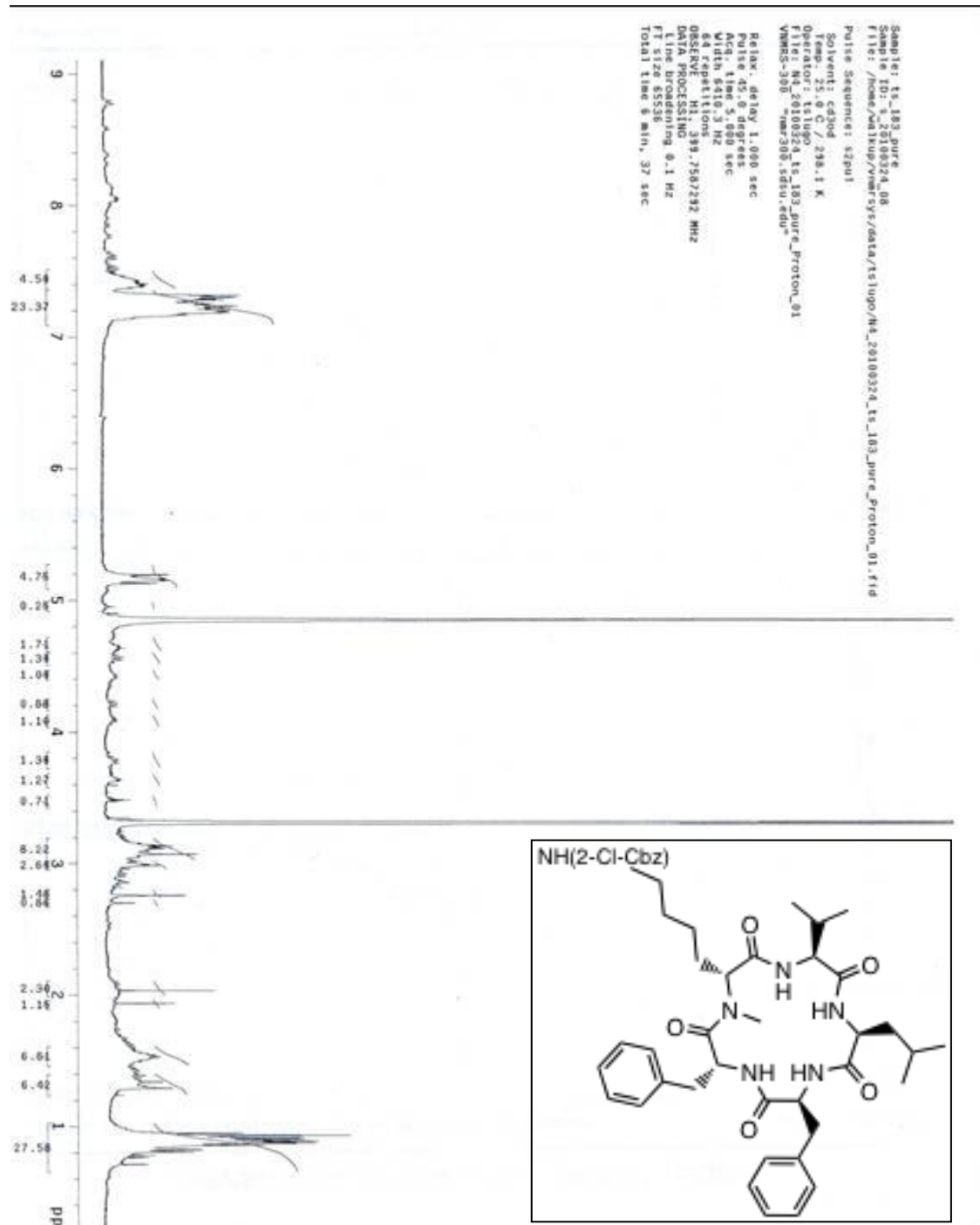


Compound 40 HPLC Cyclized Pentapeptide Phe-Leu-N-Me-Val-D-Lys(Cbz)-D-Phe

Display Report - All Windows All Analyses



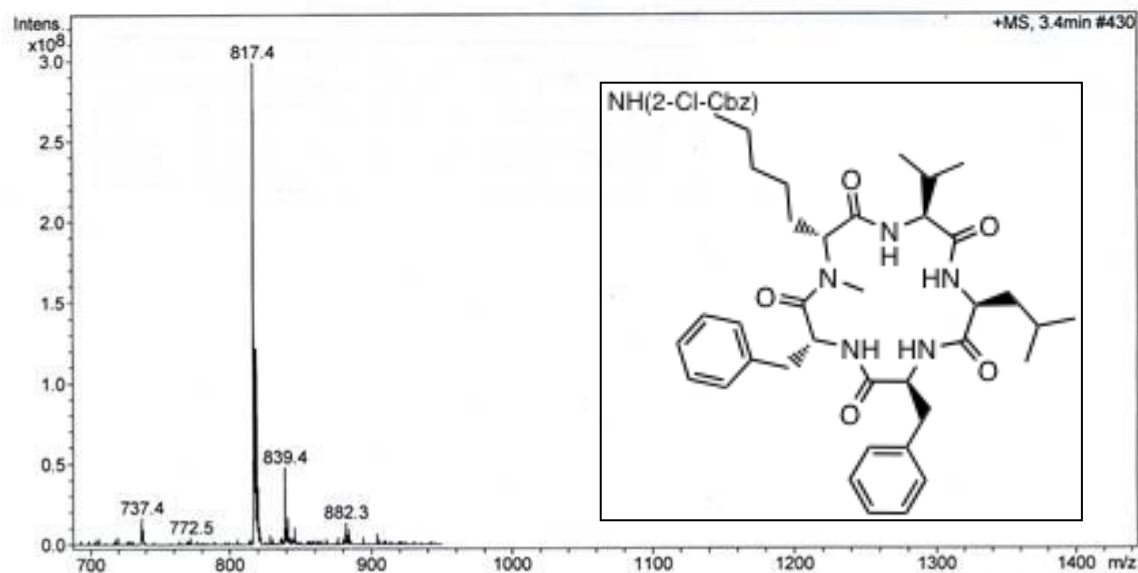
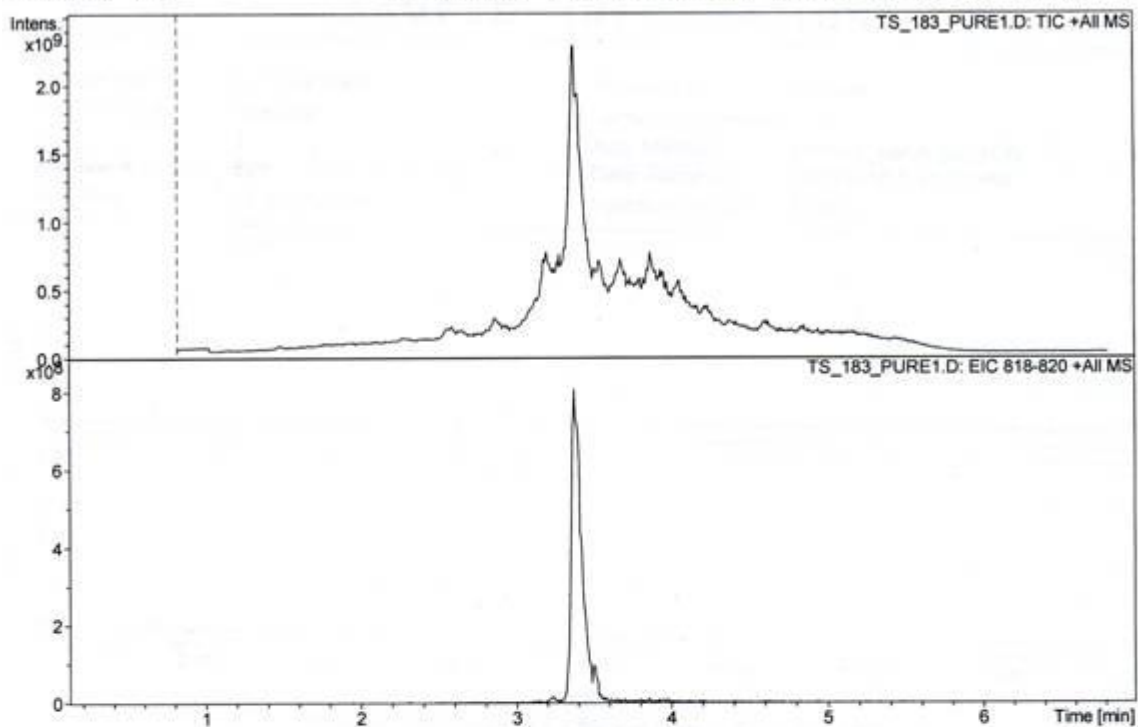
Compound 41 LCMS Double Deprotected Linear Pentapeptide HO-Phe-Leu-Val-N-Me-D-Lys(2-Cl-Cbz)-D-Phe-NH₂ (MW=835)



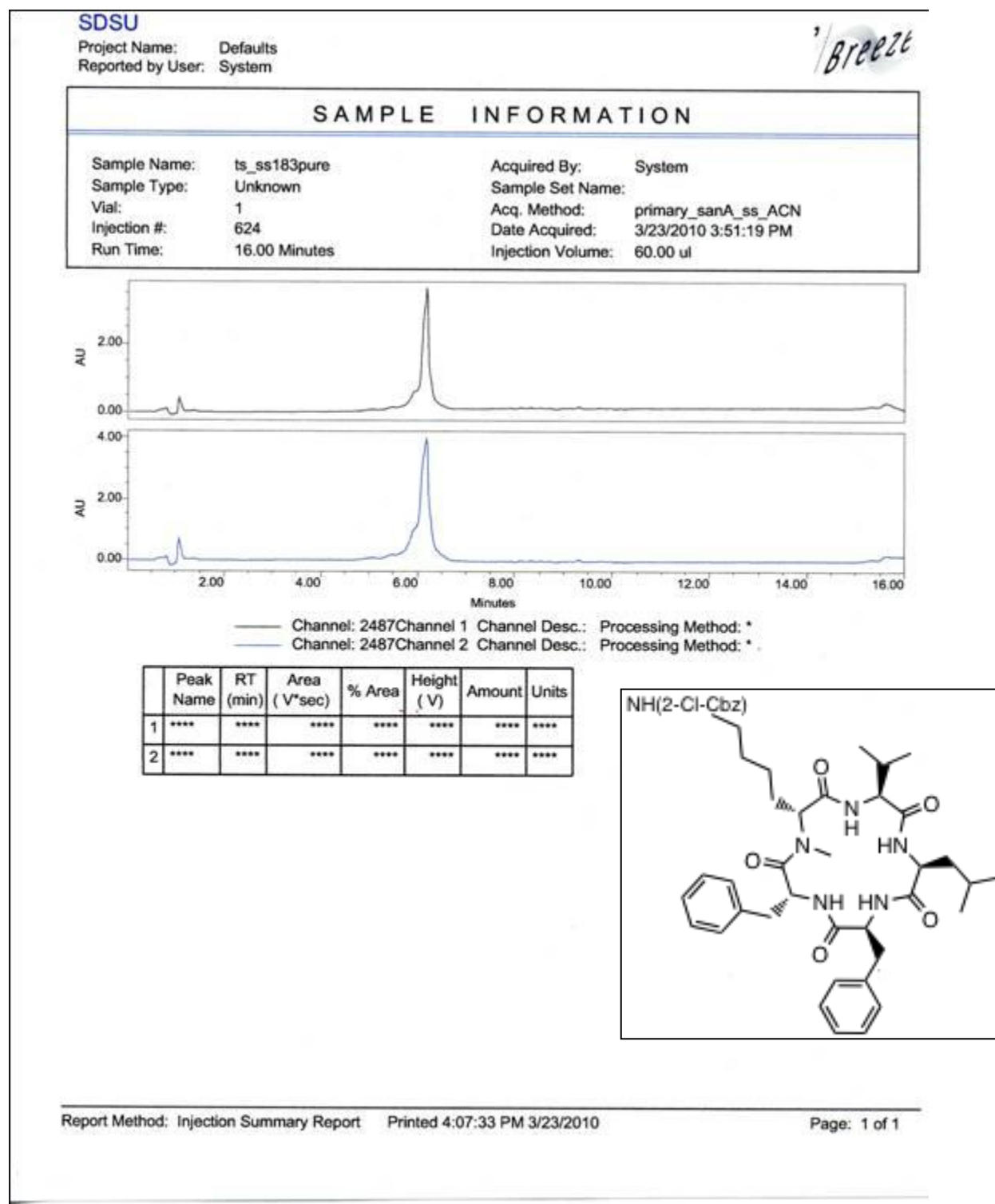
Compound 41 NMR Cyclized Pentapeptide Phe-Leu-Val-N-Me-D-Lys(2-Cl-Cbz)-D-Phe

Display Report - All Windows All Analyses

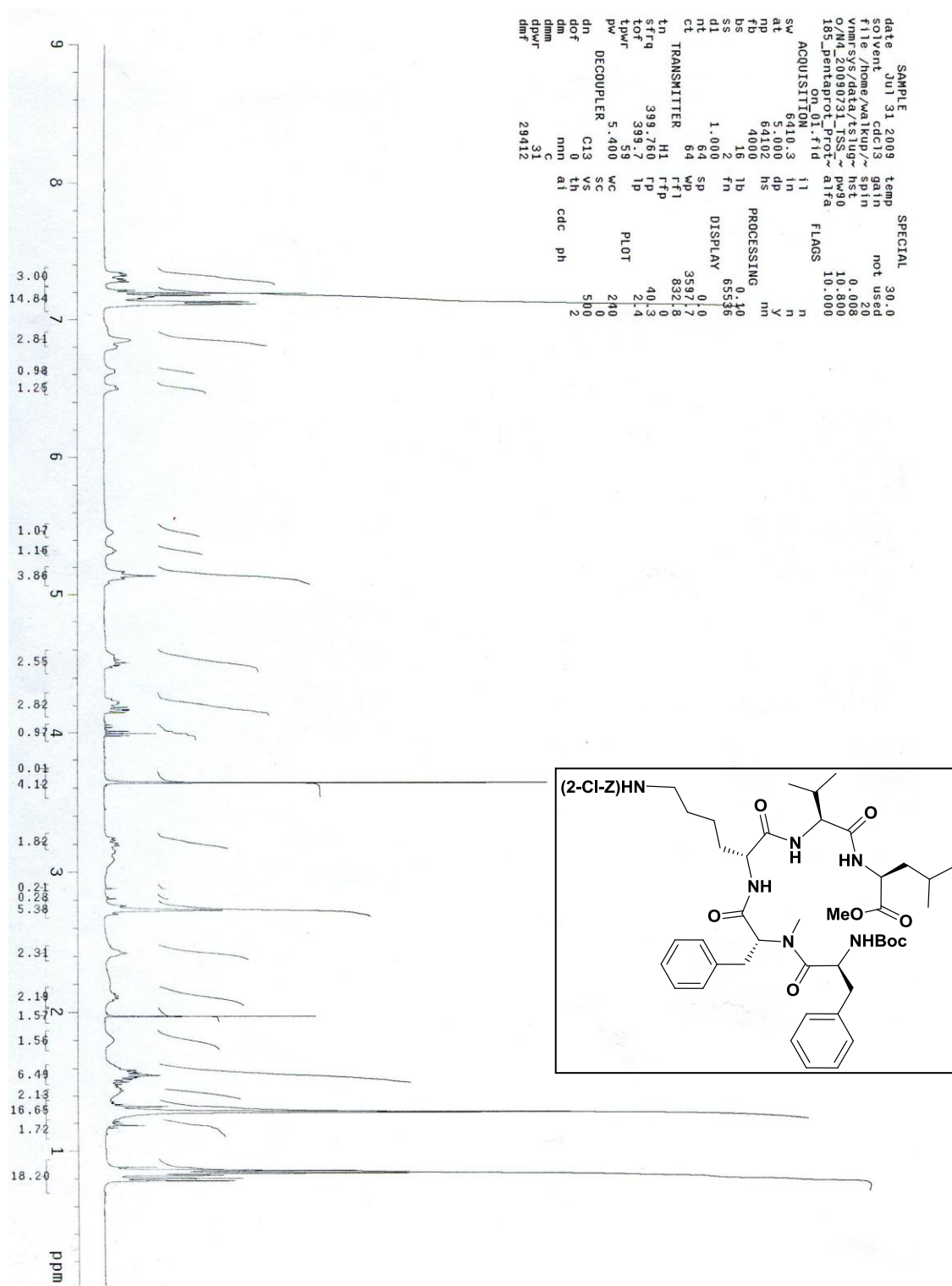
Operator: sdsu Instrument: Agilent 6330 Ion Trap Print Date: 4/23/2010 12:00:04 AM



Compound 41 LCMS Cyclized Pentapeptide Phe-Leu-Val-N-Me-D-Lys(2-Cl-Cbz)-D-Phe (MW=817)



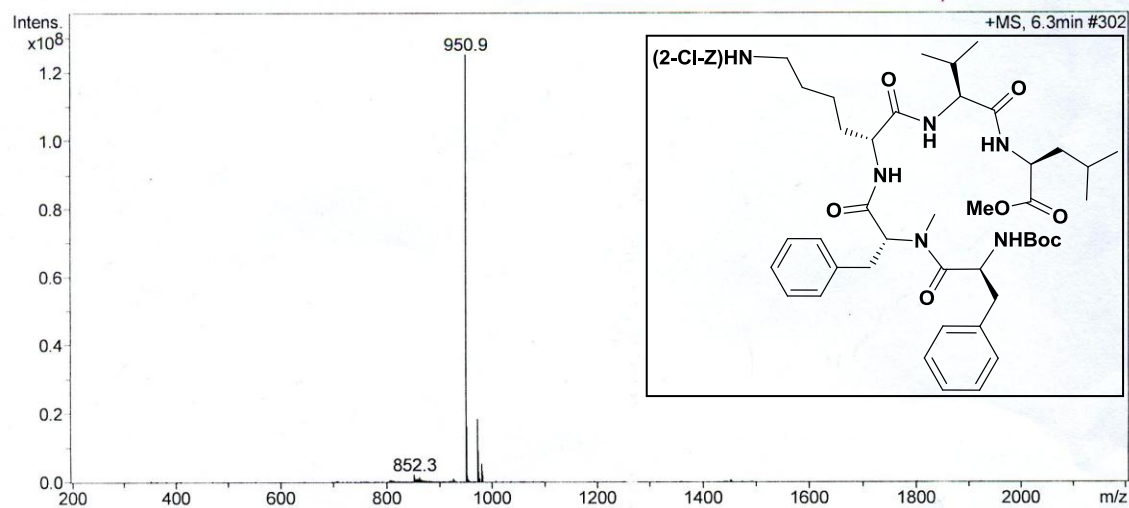
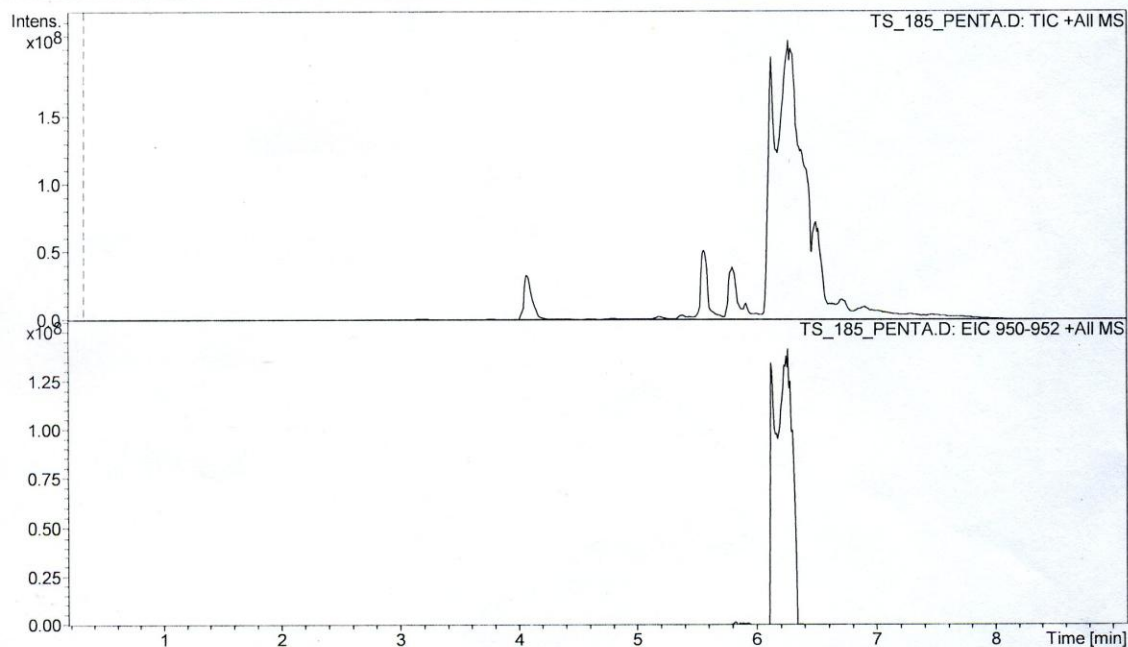
Compound 41 HPLC Cyclized Pentapeptide Phe-Leu-Val-N-Me-D-Lys(2-Cl-Cbz)-D-Phe



Compound 42 NMR Linear Pentapeptide MeO-Leu-Val-D-Lys(2-Cl-Z)-N-Me-D-Phe-Phe-NHBoc

Display Report - All Windows Selected Analysis

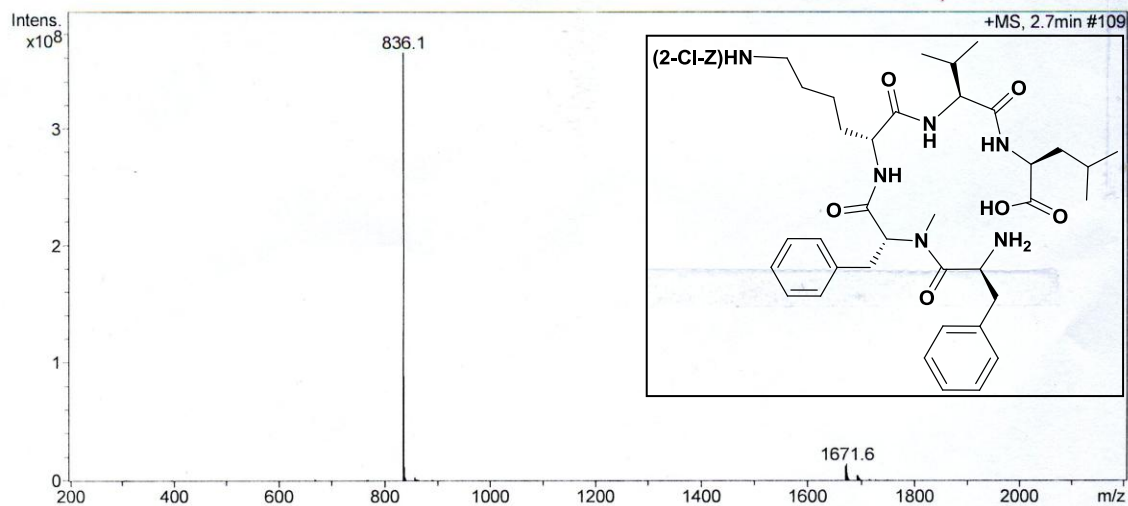
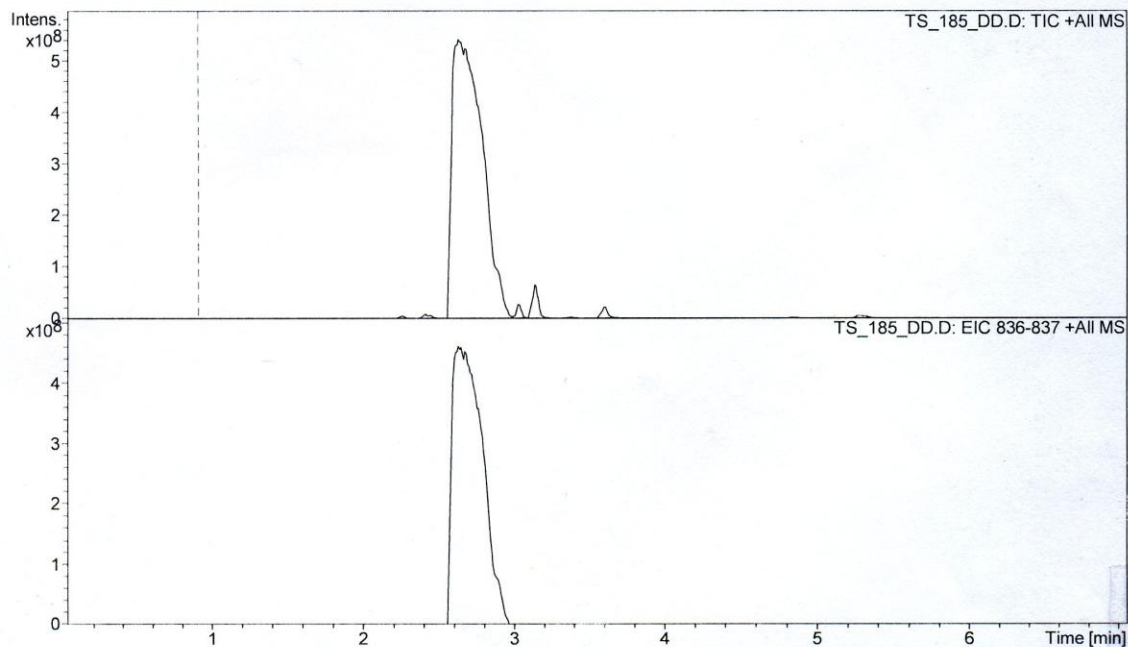
Analysis Name: TS_185_PENTA. **Instrument:** Agilent 6330 Ion Trap **Print Date:** 9/26/2009 1:01:11 PM
Method: SANA_LOW.G.M **Operator:** sdsu **Acq. Date:** 7/30/2009 4:59:22 PM
Sample Name: ts_185_penta
Analysis Info:



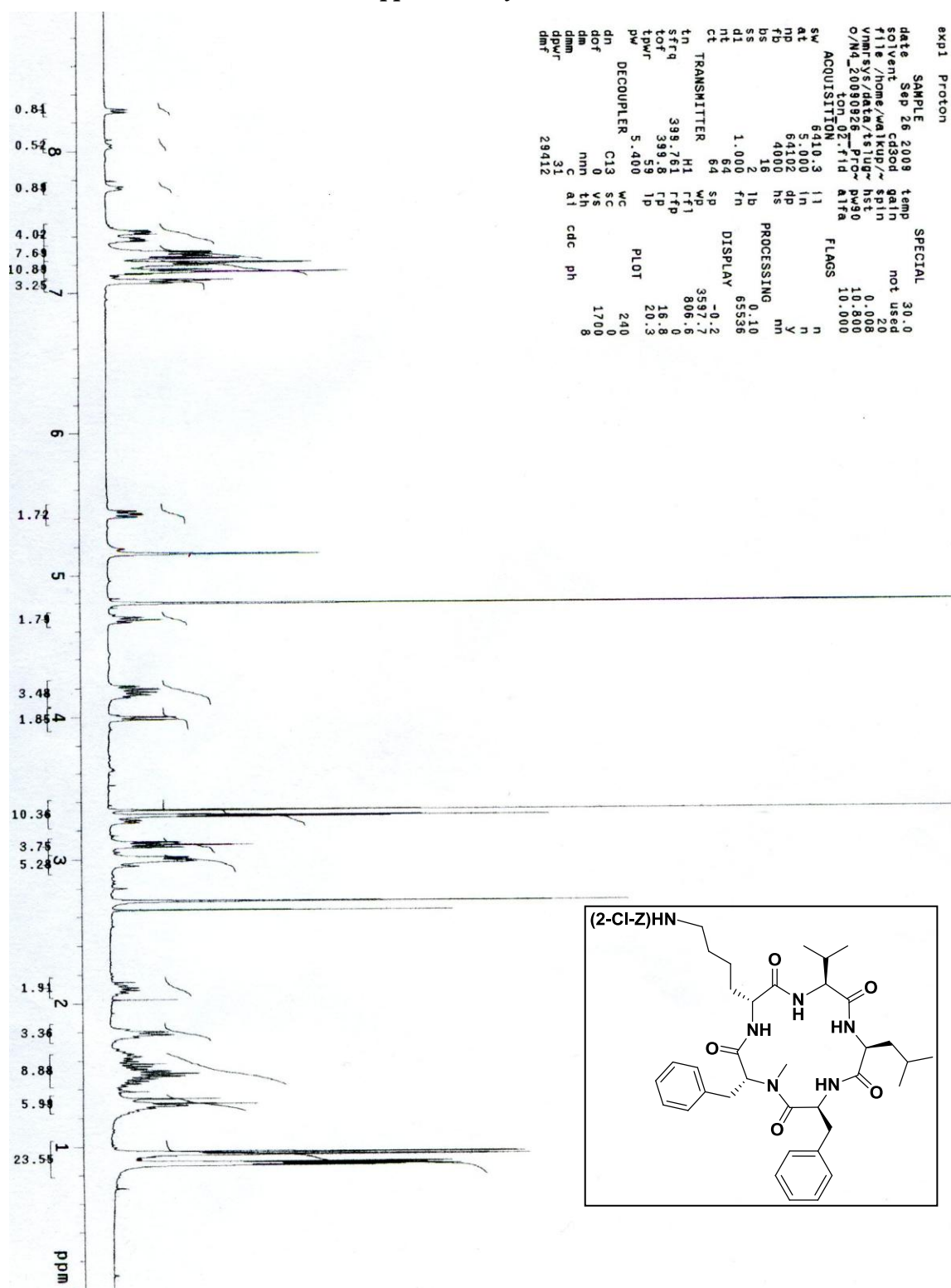
Compound 42 LCMS Linear Pentapeptide MeO-Leu-Val-D-Lys(2-Cl-Z)-N-Me-D-Phe-Phe-NHBoc (MW = 950)

Display Report - All Windows Selected Analysis

Analysis Name: TS_185_DD.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 9/26/2009 12:59:44 PM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 8/6/2009 1:58:10 PM
Sample Name: ts_185_dd
Analysis Info:



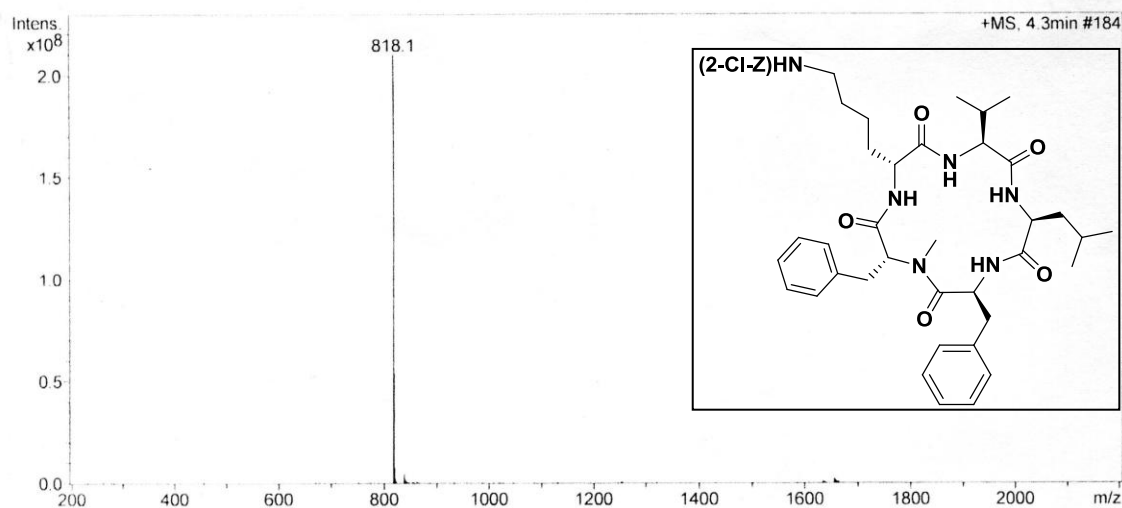
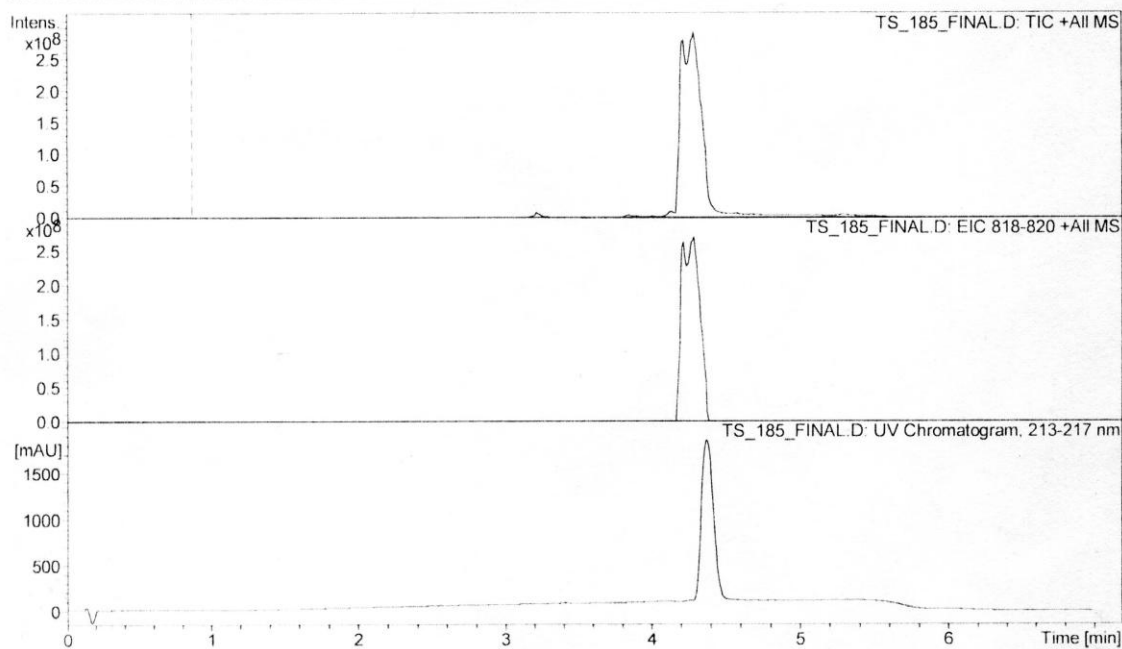
Compound 42 LCMS Double Deprotected Linear Pentapeptide HO-Leu-Val-D-Lys(2-Cl-Z)-N-Me-D-Phe-Phe-NH₂ (MW = 836)



Compound 42 NMR Cyclized Pentapeptide Phe-Leu-Val-D-Lys(2-Cl-Z)-N-Me-D-Phe

Display Report - All Windows Selected Analysis

Analysis Name: TS_185_FINAL.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 9/25/2009 3:53:57 PM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 9/25/2009 3:37:40 PM
Sample Name: ts_185_final
Analysis Info:



Compound 42 LCMS Cyclized Pentapeptide Phe-Leu-Val-D-Lys(2-Cl-Z)-N-Me-D-Phe (MW=818.4)

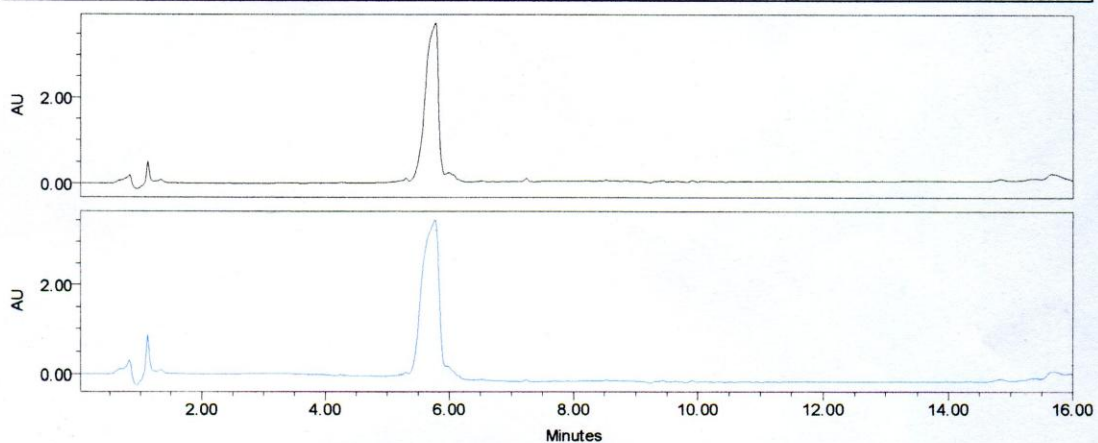
SDSU

Project Name: Defaults
Reported by User: System

Breeze

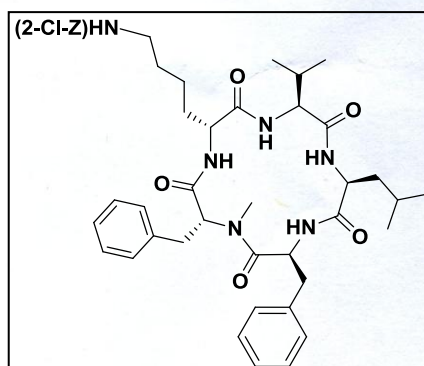
SAMPLE INFORMATION

Sample Name:	ts_185_ss	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	202	Date Acquired:	9/25/2009 2:41:51 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: ****

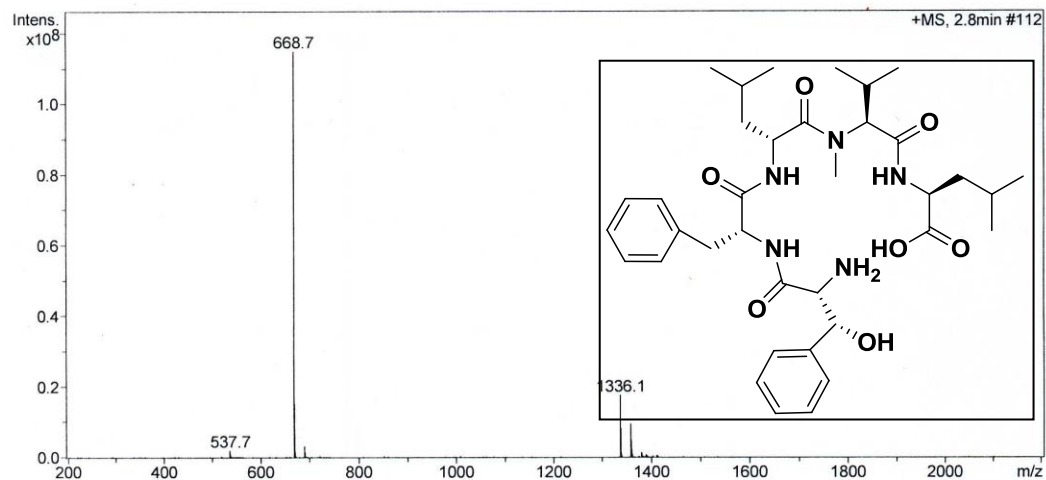
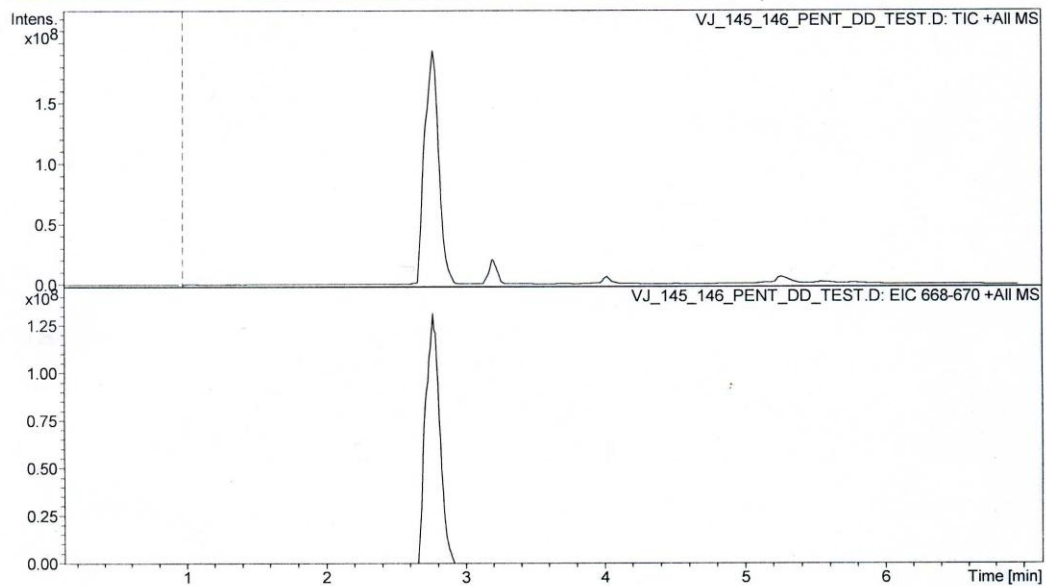
Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	Amount	Units
1 ****	****	****	****	****	****	****
2 ****	****	****	****	****	****	****



Compound 42 HPLC Cyclized Pentapeptide Phe-Leu-Val-D-Lys(2-Cl-Z)-N-Me-D-Phe

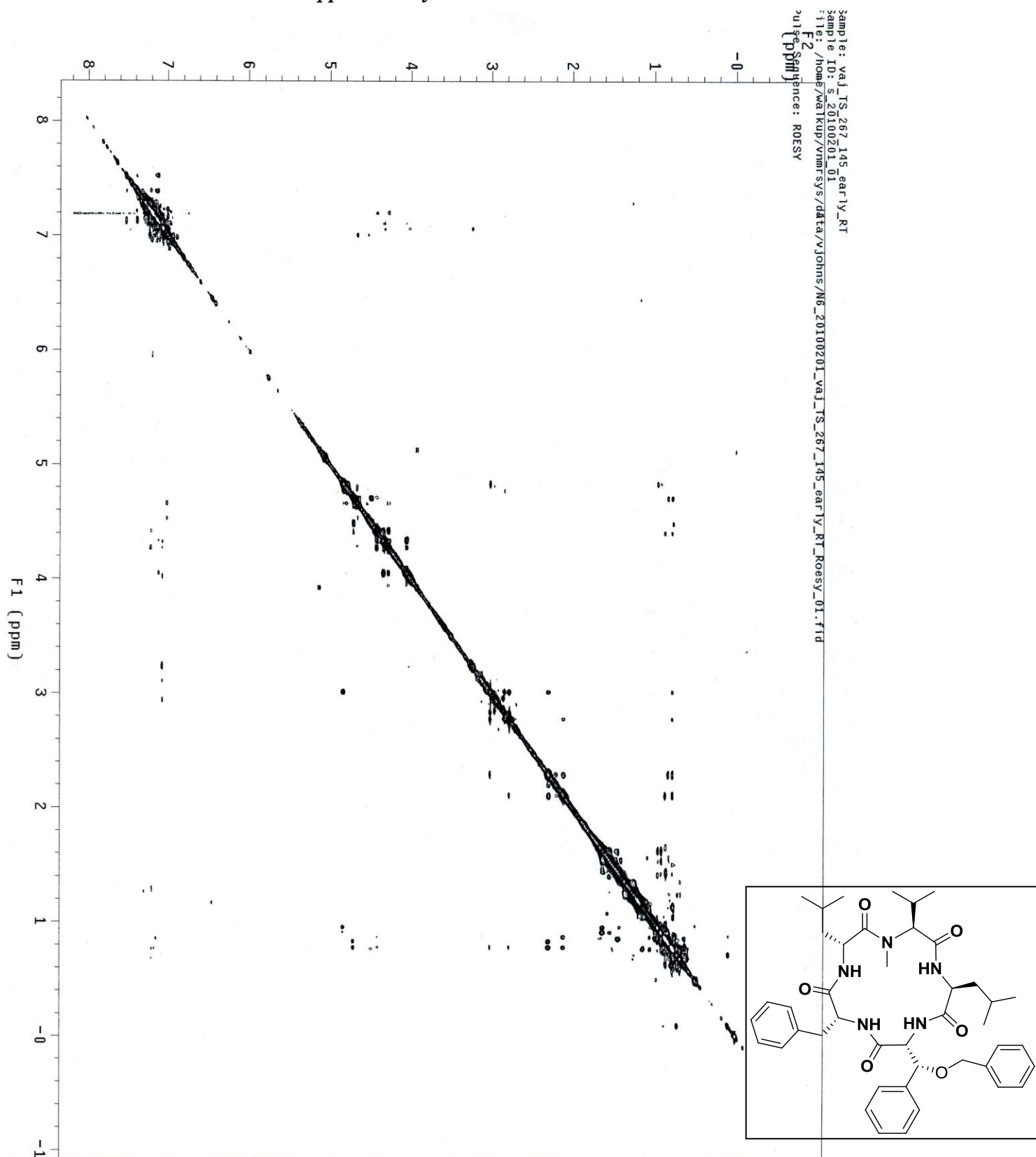
Display Report - All Windows Selected Analysis

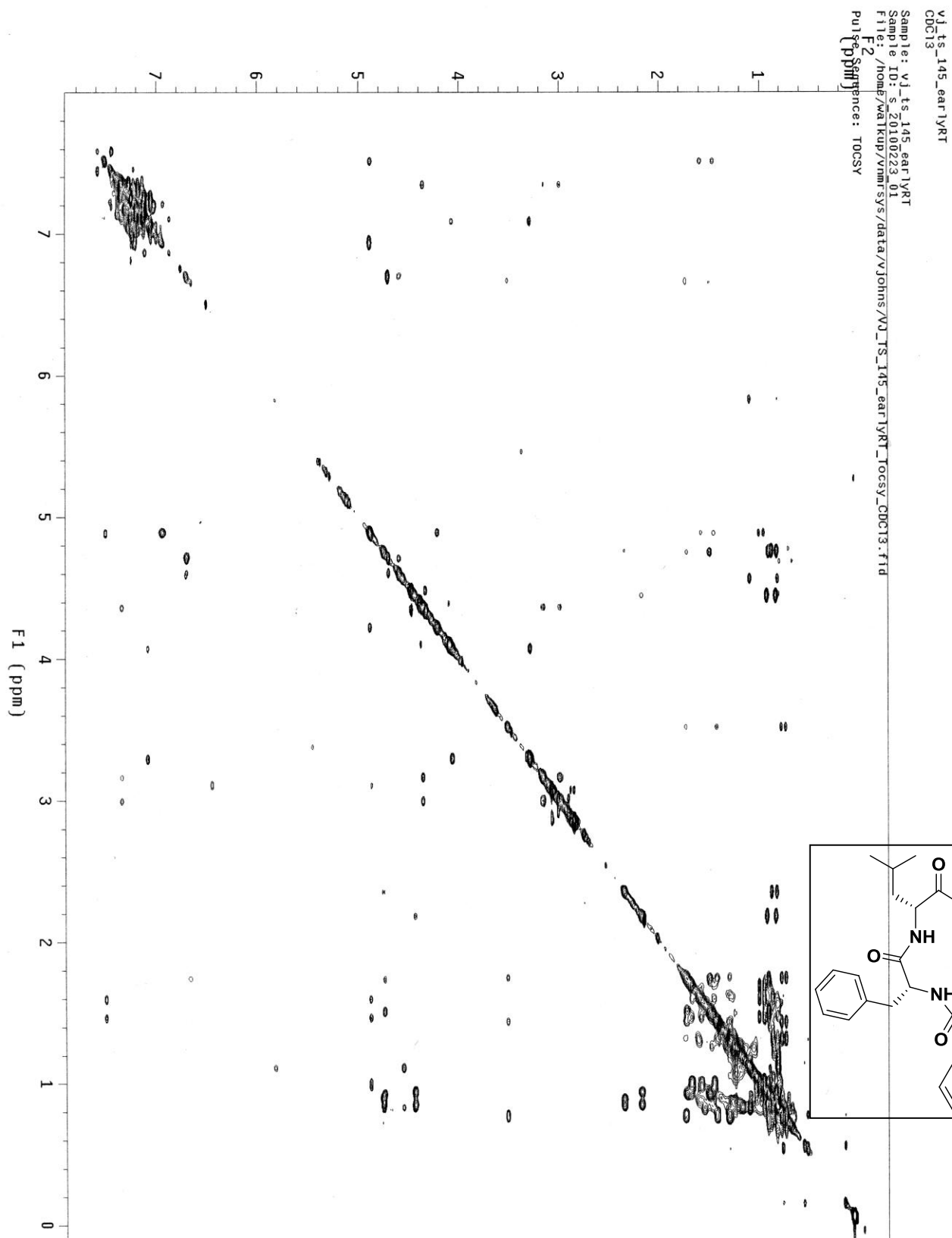
Analysis Name: VJ_145_146_PE **Instrument:** Agilent 6330 Ion Trap **Print Date:** 8/14/2009 3:08:02 PM
Method: SANA.M NT_DD_TEST.D **Operator:** sdsu **Acq. Date:** 5/14/2009 2:49:09 PM
Sample Name: VJ_145_146_pent_DD_test
Analysis Info:



Compound 43 LCMS Double Deprotected Linear Pentapeptide HO-Leu-N-Me-Val-D-Leu-D-Phe-β-OH-Phe-NH₂ (MW=668)

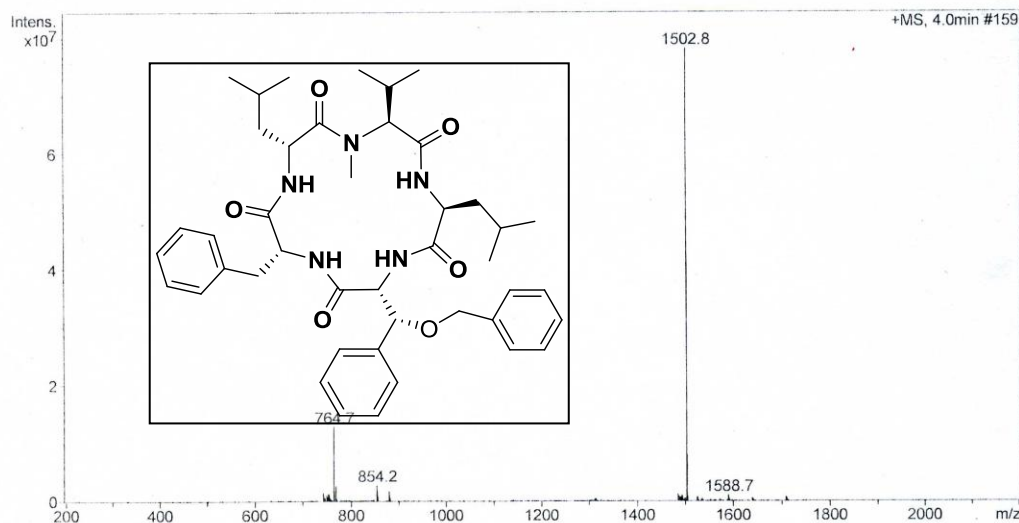
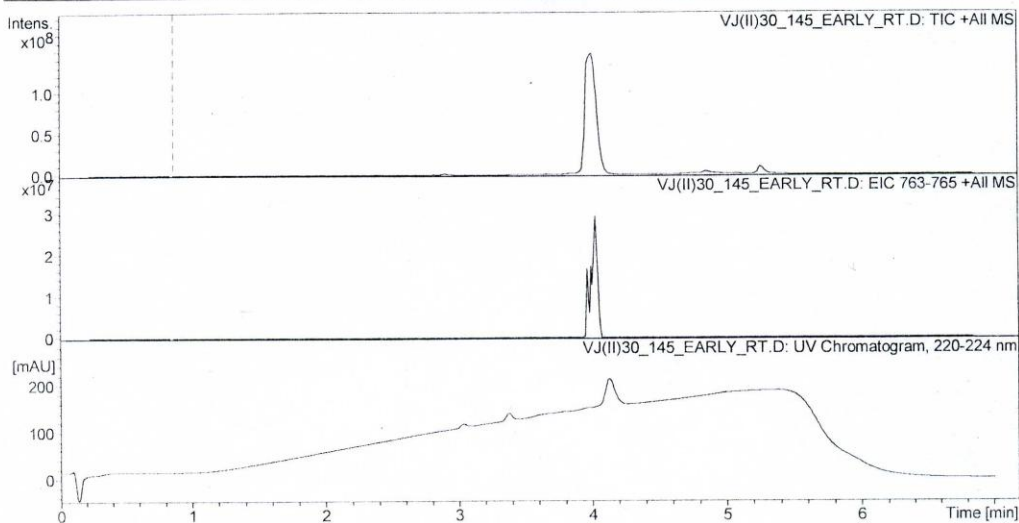
Compound 43 NMR Cyclized Pentapeptide β -benzyloxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe

**Compound 43 ROESY NMR Cyclized Pentapeptide β -benzoxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe**

Compound 43 TOCSY NMR Cyclized Pentapeptide β -benzoxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe

Display Report - All Windows Selected Analysis

Analysis Name: VJ(II)30_145_EA **Instrument:** Agilent 6330 Ion Trap **Print Date:** 10/14/2009 10:44:41 AM
Method: SANA.M RLY_RT.D **Operator:** sdsu **Acq. Date:** 9/28/2009 4:33:40 PM
Sample Name: VJ(II)30_145_Early_RT
Analysis Info:



Compound 43 LCMS Cyclized Pentapeptide β -benzoxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe (MW=740)

SDSU

Project Name: Defaults

Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: VJ(l)30_145_Early_RT

Acquired By: System

Sample Type: Unknown

Sample Set Name:

Vial: 1

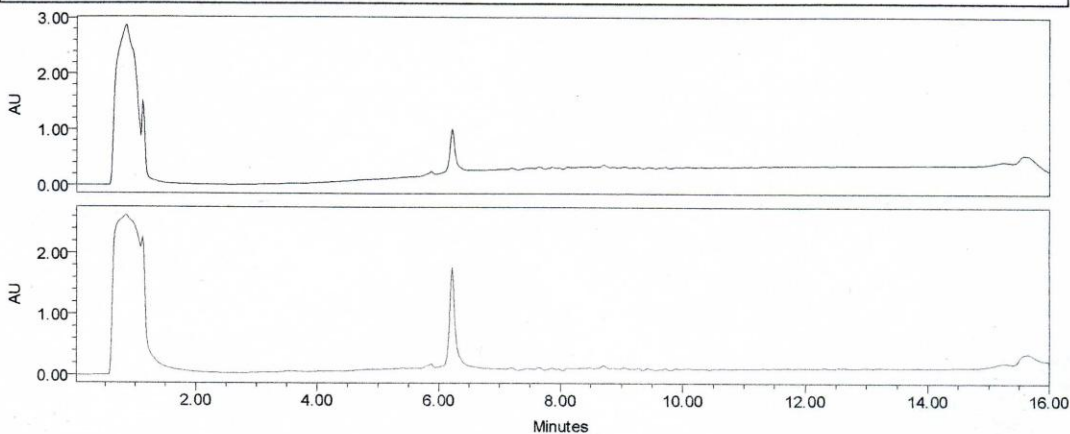
Acq. Method: primary_sanA_ss_ACN

Injection #: 245

Date Acquired: 10/13/2009 5:20:10 PM

Run Time: 16.00 Minutes

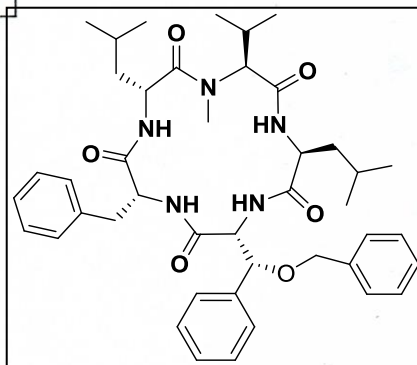
Injection Volume: 50.00 ul



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

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

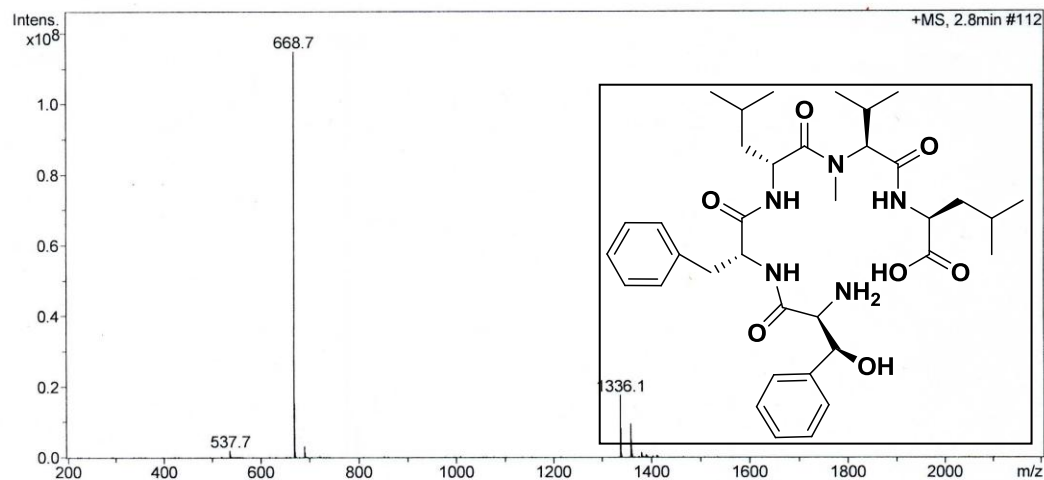
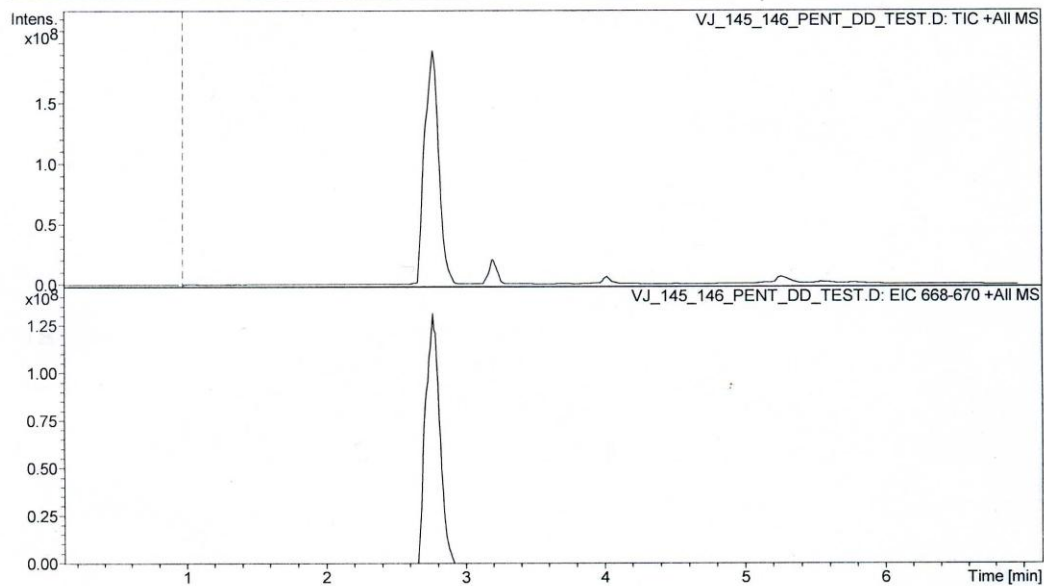
Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	Amount	Units
1 ****	****	****	****	****	****	****
2 ****	****	****	****	****	****	****



Compound 43 HPLC Cyclized Pentapeptide β-benzyloxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe

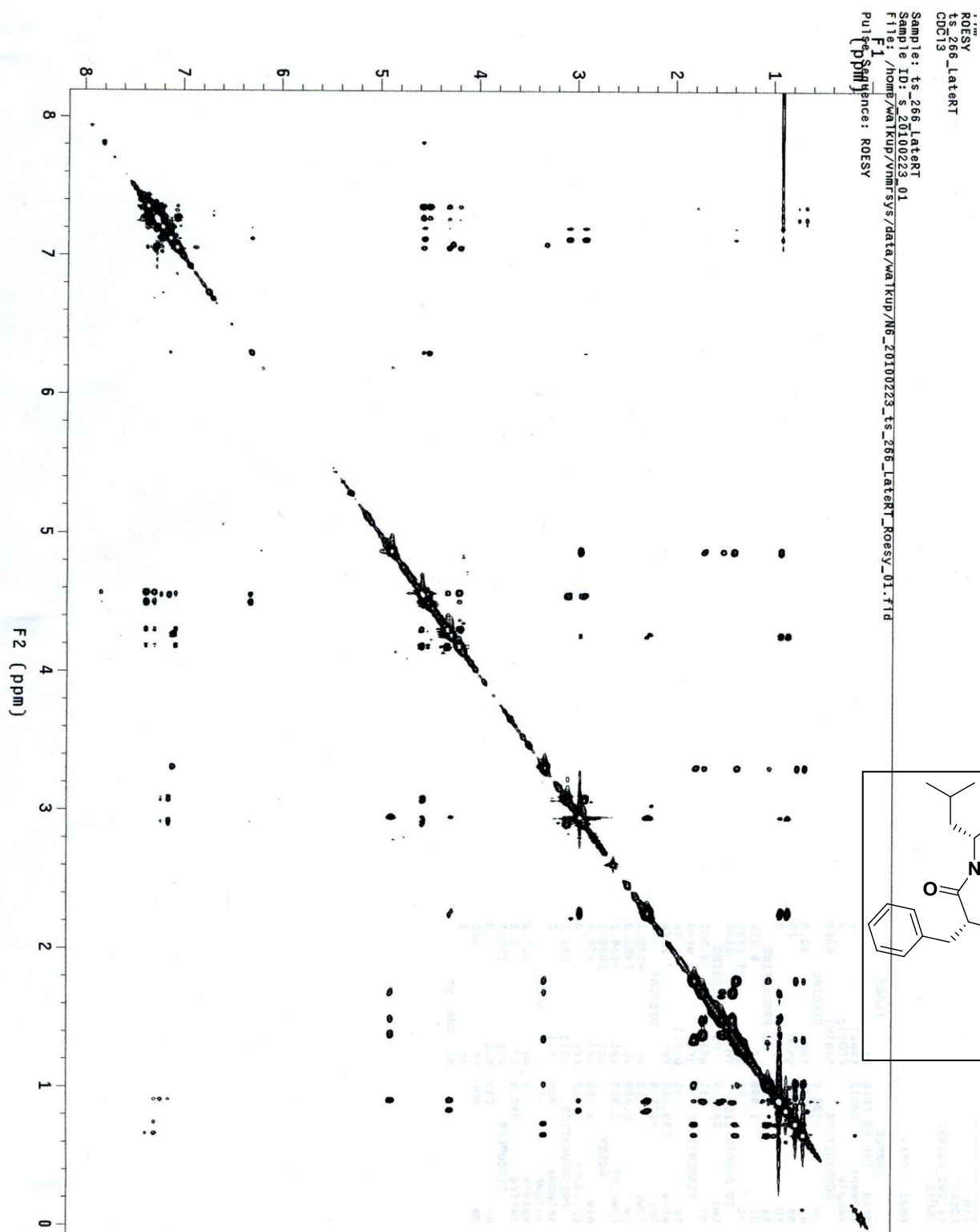
Display Report - All Windows Selected Analysis

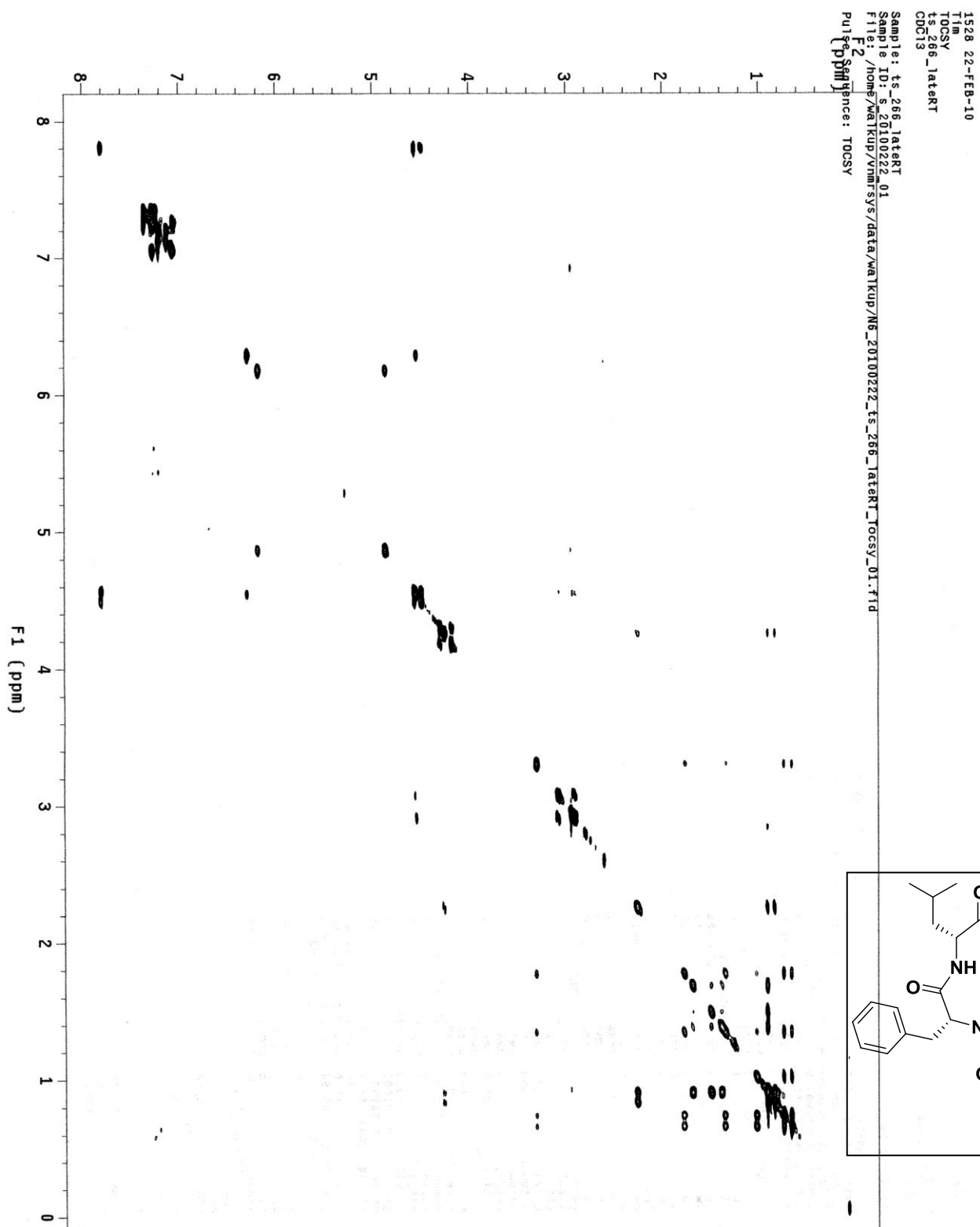
Analysis Name: VJ_145_146_PE **Instrument:** Agilent 6330 Ion Trap **Print Date:** 8/14/2009 3:08:02 PM
Method: SANA.M NT_DD_TEST.D **Operator:** sdsu **Acq. Date:** 5/14/2009 2:49:09 PM
Sample Name: VJ_145_146_pent_DD_test
Analysis Info:



Compound 44 LCMS Double Deprotected Linear Pentapeptide HO-Leu-N-Me-Val-D-Leu-D-Phe-β-OH-Phe-NH₂ (MW=668)

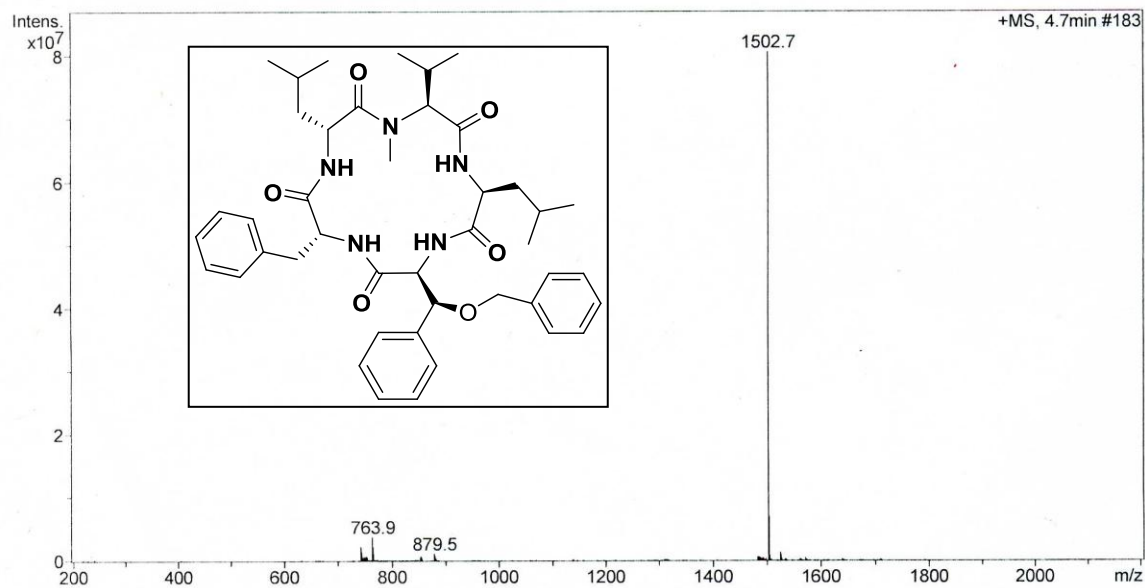
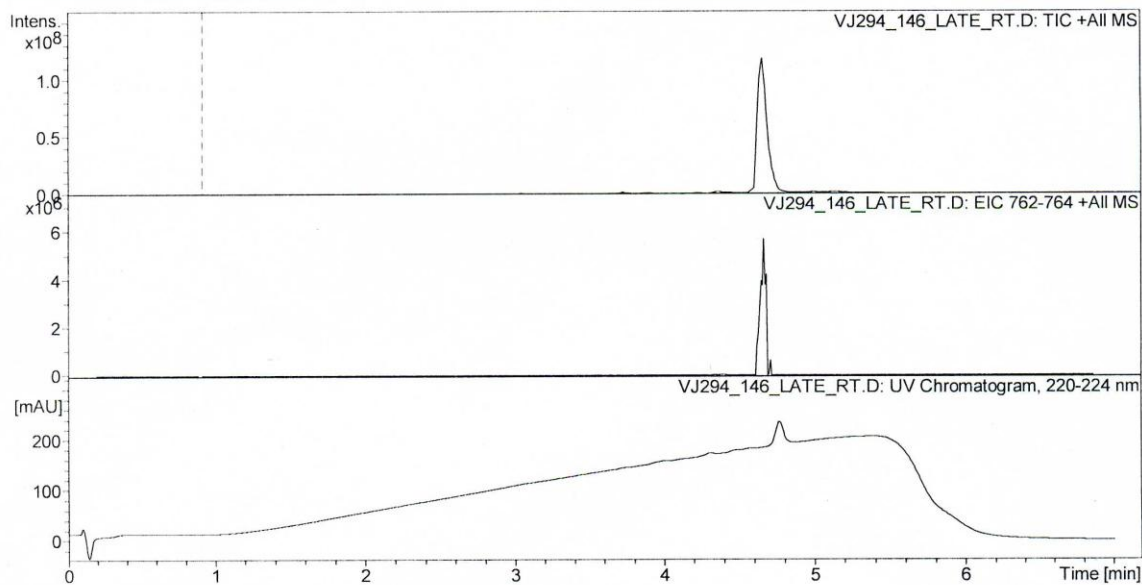
Compound 44 NMR Cyclized Pentapeptide β -benzoxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe

Compound 44 ROESY NMR Cyclized Pentapeptide β -benzoxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe

Compound 44 TOSCY NMR Cyclized Pentapeptide β -benzoxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe

Display Report - All Windows Selected Analysis

Analysis Name: VJ294_146_LATE **Instrument:** Agilent 6330 Ion Trap **Print Date:** 10/14/2009 10:43:12 AM
Method: SANA.M_RT.D **Operator:** sdsu **Acq. Date:** 8/18/2009 5:09:28 PM
Sample Name: VJ294_146_late_RT
Analysis Info:



Compound 44 LCMS Cyclized Pentapeptide β -benzoxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe (MW=740)

SDSU

Project Name: Defaults

Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: VJ_146_late_RT

Acquired By: System

Sample Type: Unknown

Sample Set Name:

Vial: 1

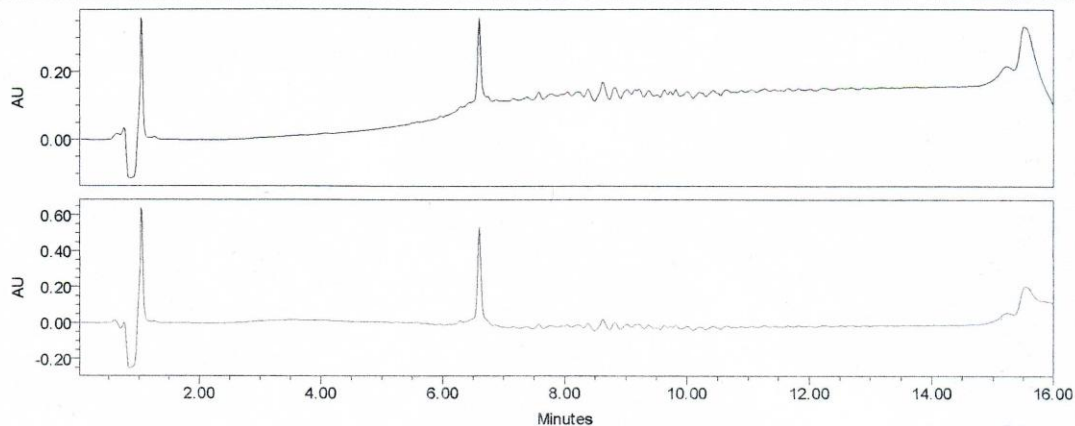
Acq. Method: primary_sanA_ss_ACN

Injection #: 37

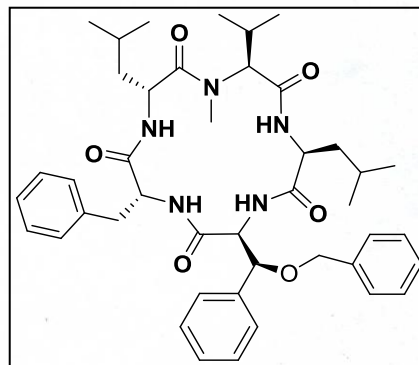
Date Acquired: 8/18/2009 5:31:33 PM

Run Time: 16.00 Minutes

Injection Volume: 50.00 ul

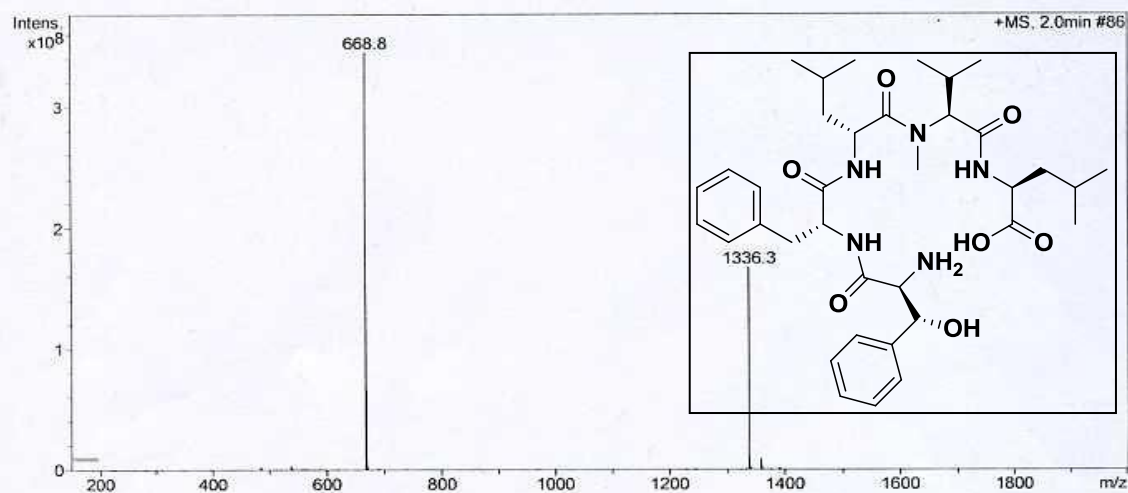
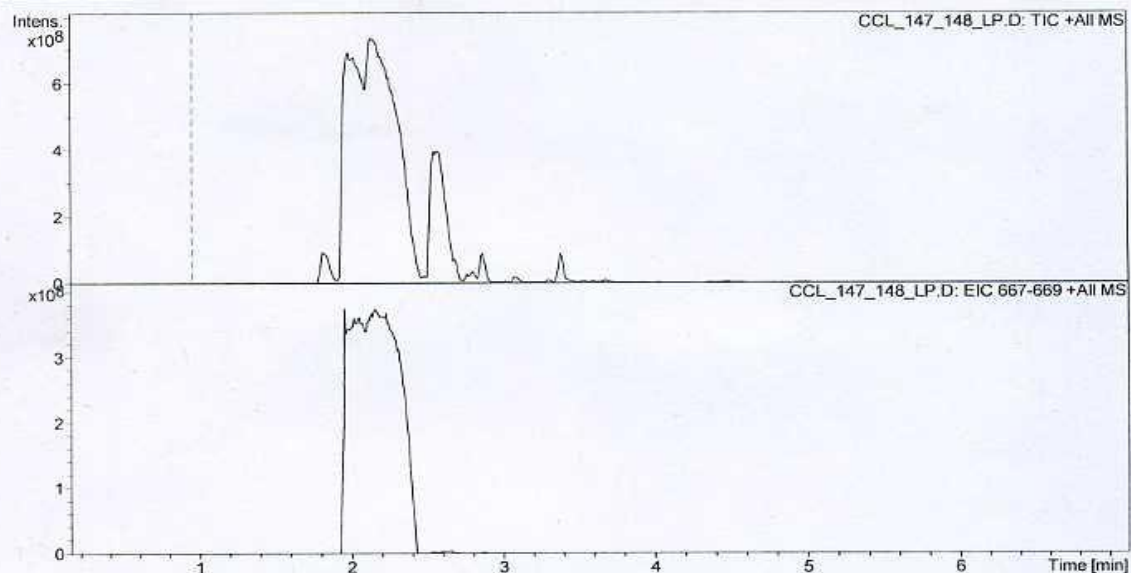


Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	Amount	Units
1 ****	****	****	****	****	****	****
2 ****	****	****	****	****	****	****

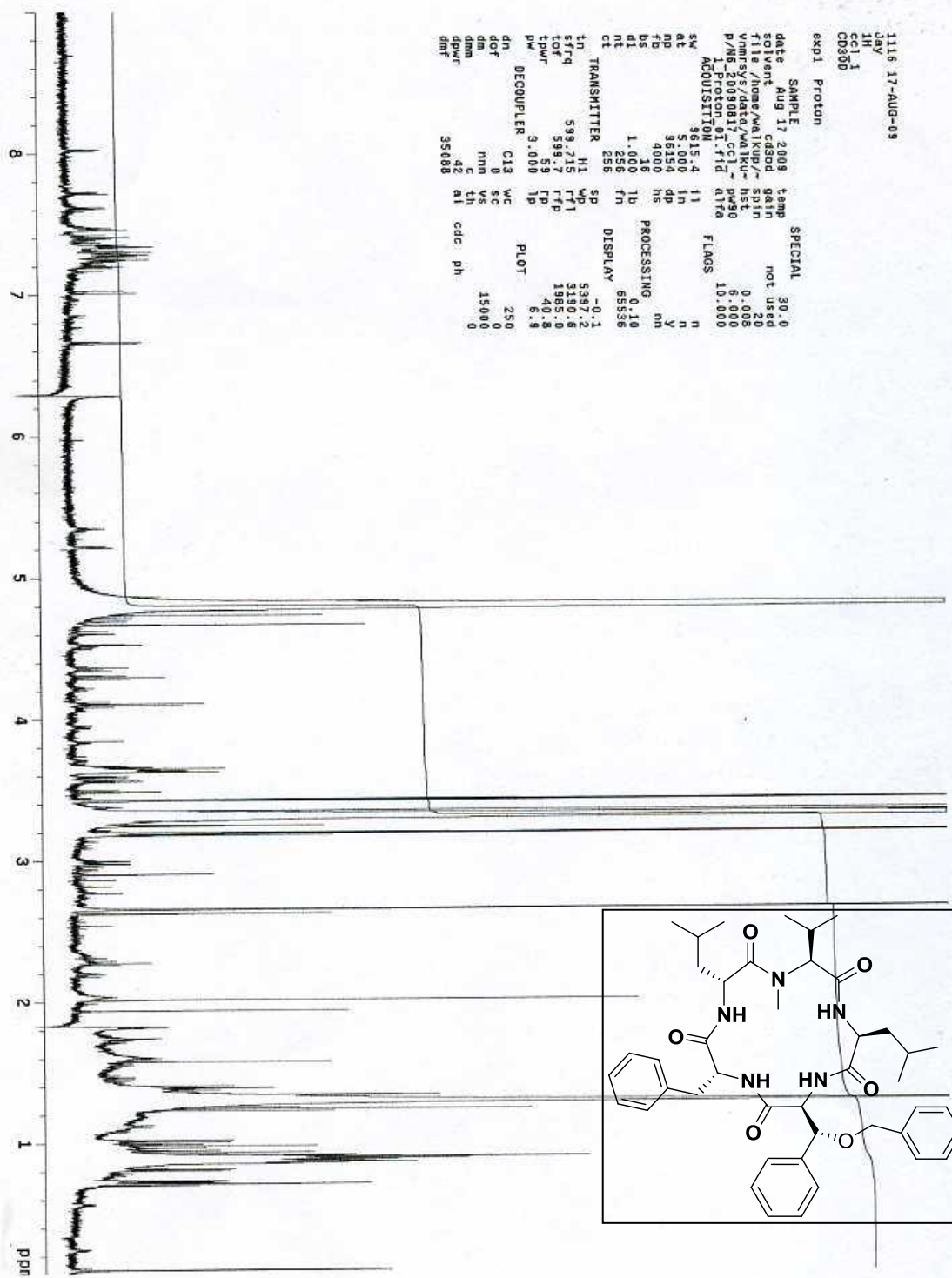
Compound 44 HPLC Cyclized Pentapeptide β -benzoxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe

Display Report - All Windows Selected Analysis

Analysis Name: CCL_147_148_L Instrument: Agilent 6330 Ion Trap Print Date: 8/17/2009 11:10:14 AM
Method: SANA.M P.D Operator: sdsu Acq. Date: 6/23/2009 11:58:06 PM
Sample Name: CCL_147_148_LP
Analysis Info:

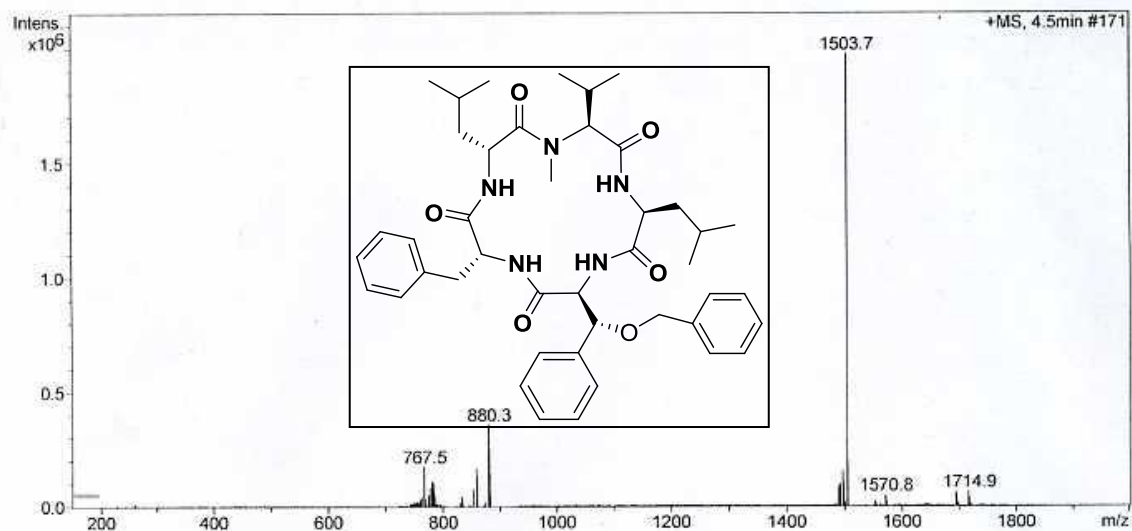
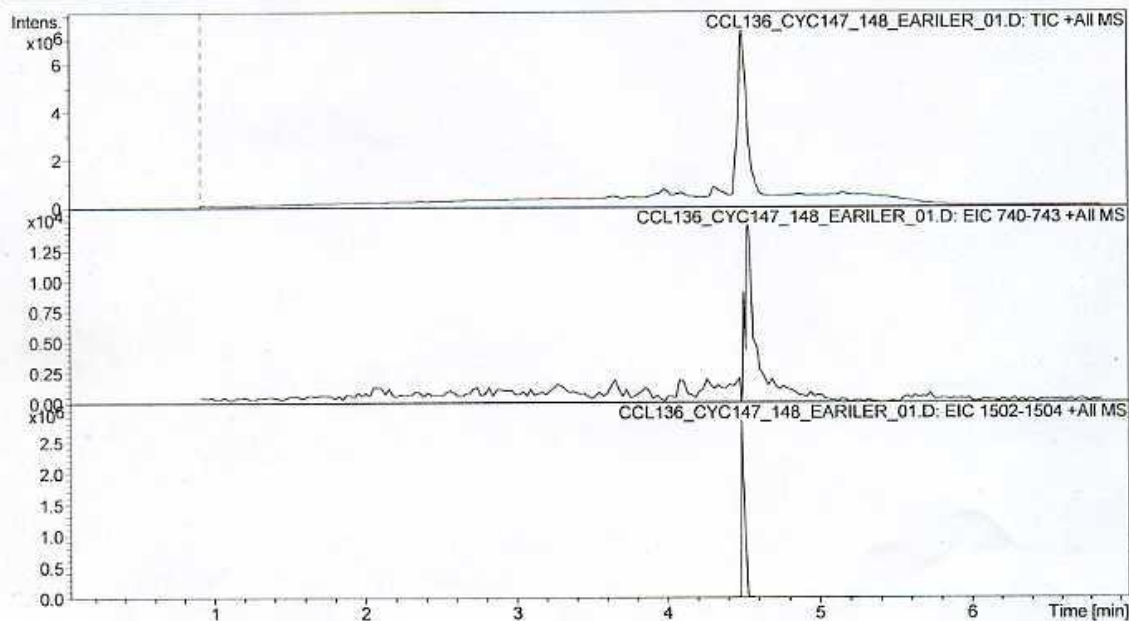


Compound 45 LCMS Double Deprotected Linear Pentapeptide HO-Leu-N-Me-Val-D-Leu-D-Phe-β-OH-D-Phe-NH₂ (MW=668)

Compound 45 NMR Cyclized Pentapeptide β -benzoxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe

Display Report - All Windows Selected Analysis

Analysis Name: CCL136_CYC147 **Instrument:** Agilent 6330 Ion Trap **Print Date:** 8/15/2009 8:16:24 PM
Method: SANA.M_148_EARILER_ **Operator:** sdsu **Acq. Date:** 8/15/2009 7:40:18 PM
Sample Name: CCL136_cyc147_148_eariler_01
Analysis Info:



Compound 45 LCMS Cyclized Pentapeptide β -benzoxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe (MW=740)

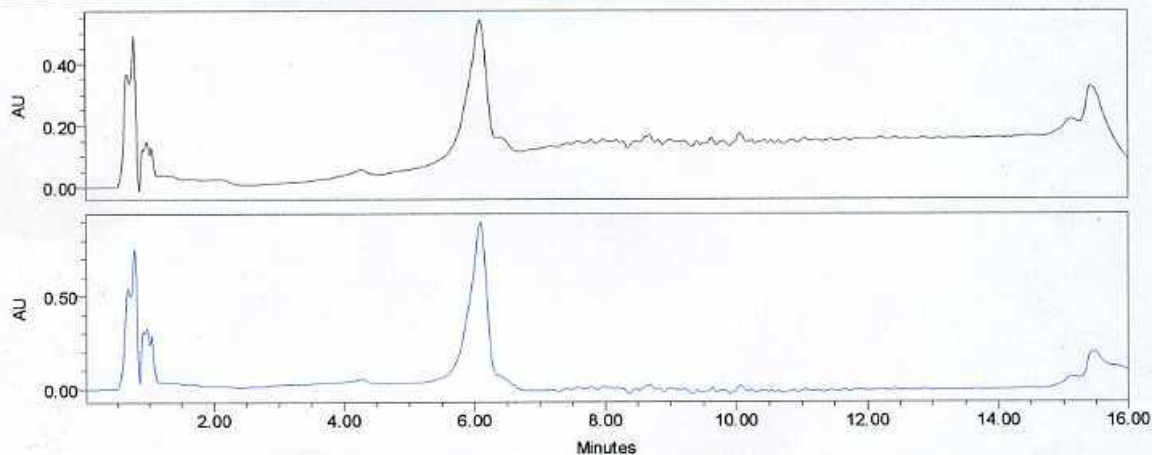
SDSU

Project Name: Defaults
Reported by User: System

Breeze

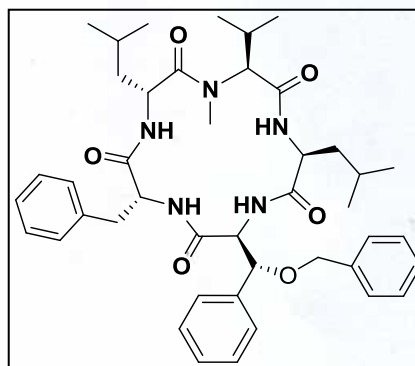
SAMPLE INFORMATION

Sample Name:	CCL136_cyc147_148_earlier_03	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	22	Date Acquired:	8/16/2009 5:58:09 PM
Run Time:	16.00 Minutes	Injection Volume:	50.00 ul



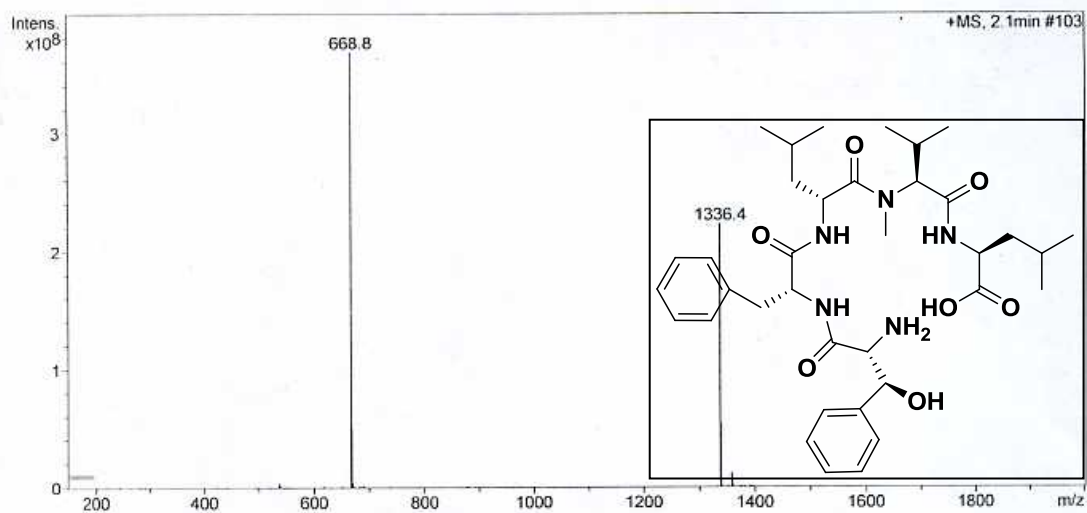
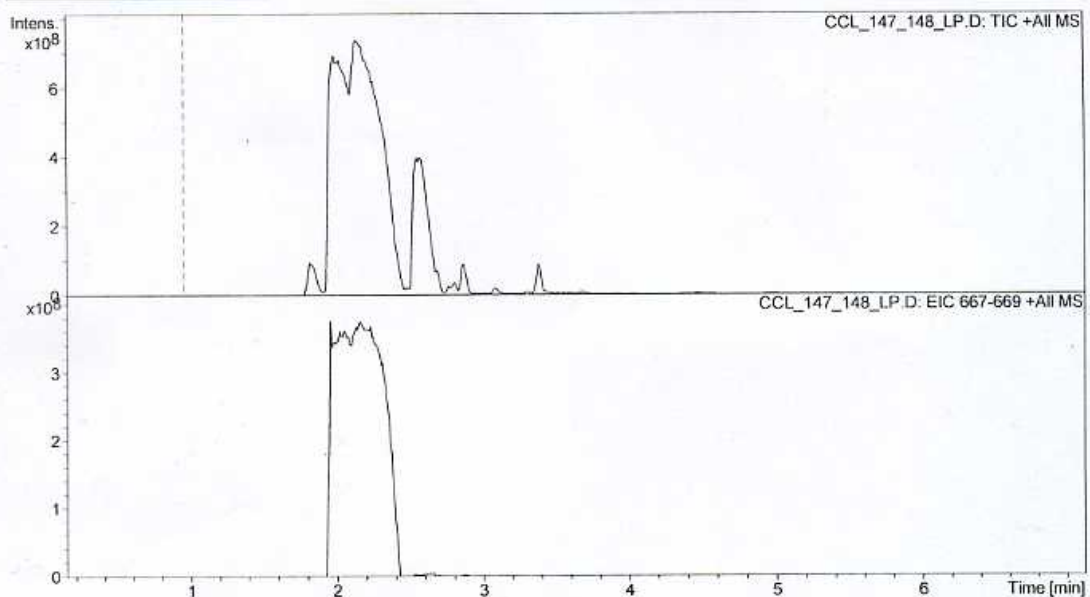
— Channel: 2487Channel 1 Channel Desc.: Processing Method: ****
 — Channel: 2487Channel 2 Channel Desc.: Processing Method: ****

Peak Name	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	Amount	Units
1	****	****	****	****	****	****
2	****	****	****	****	****	****

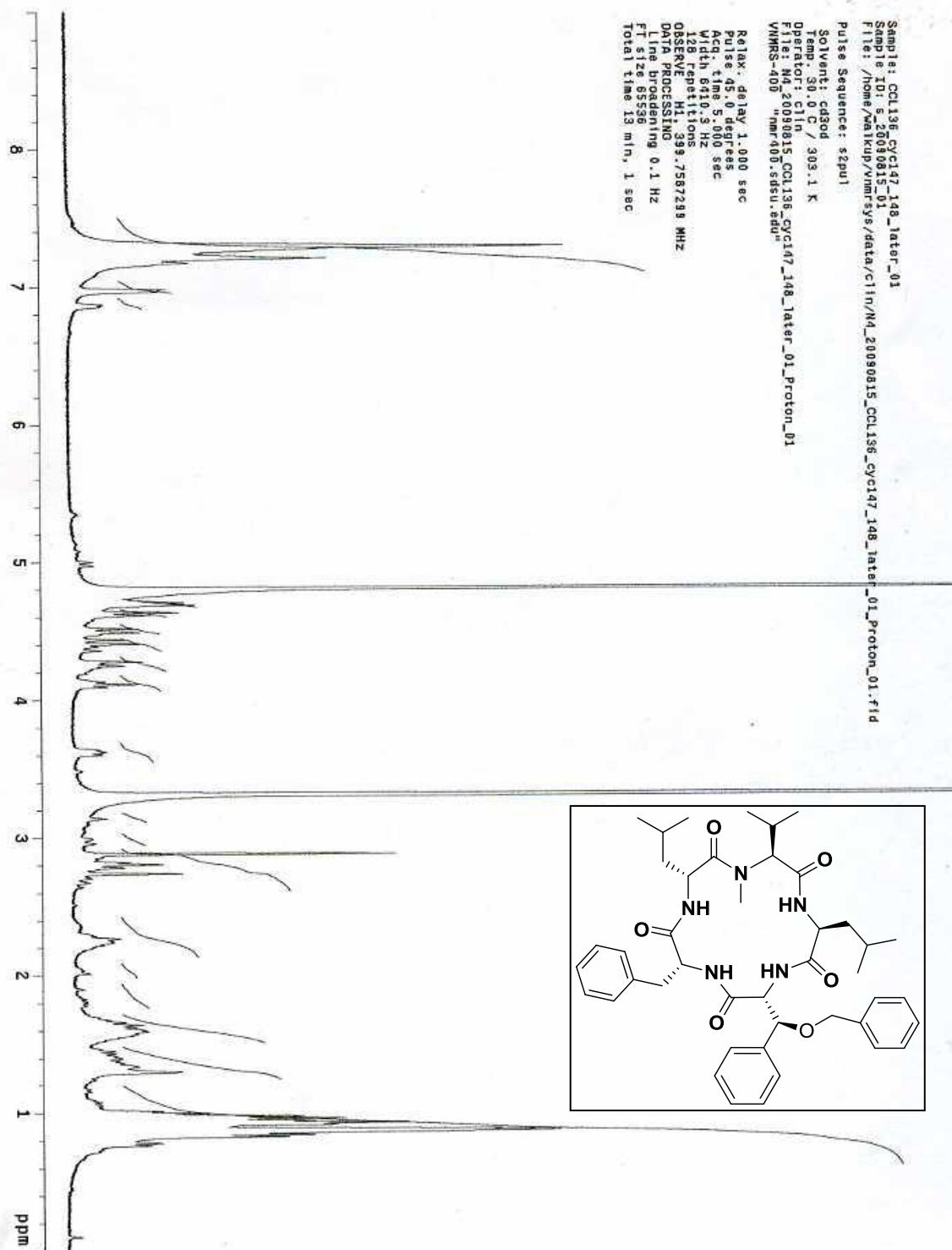


Display Report - All Windows Selected Analysis

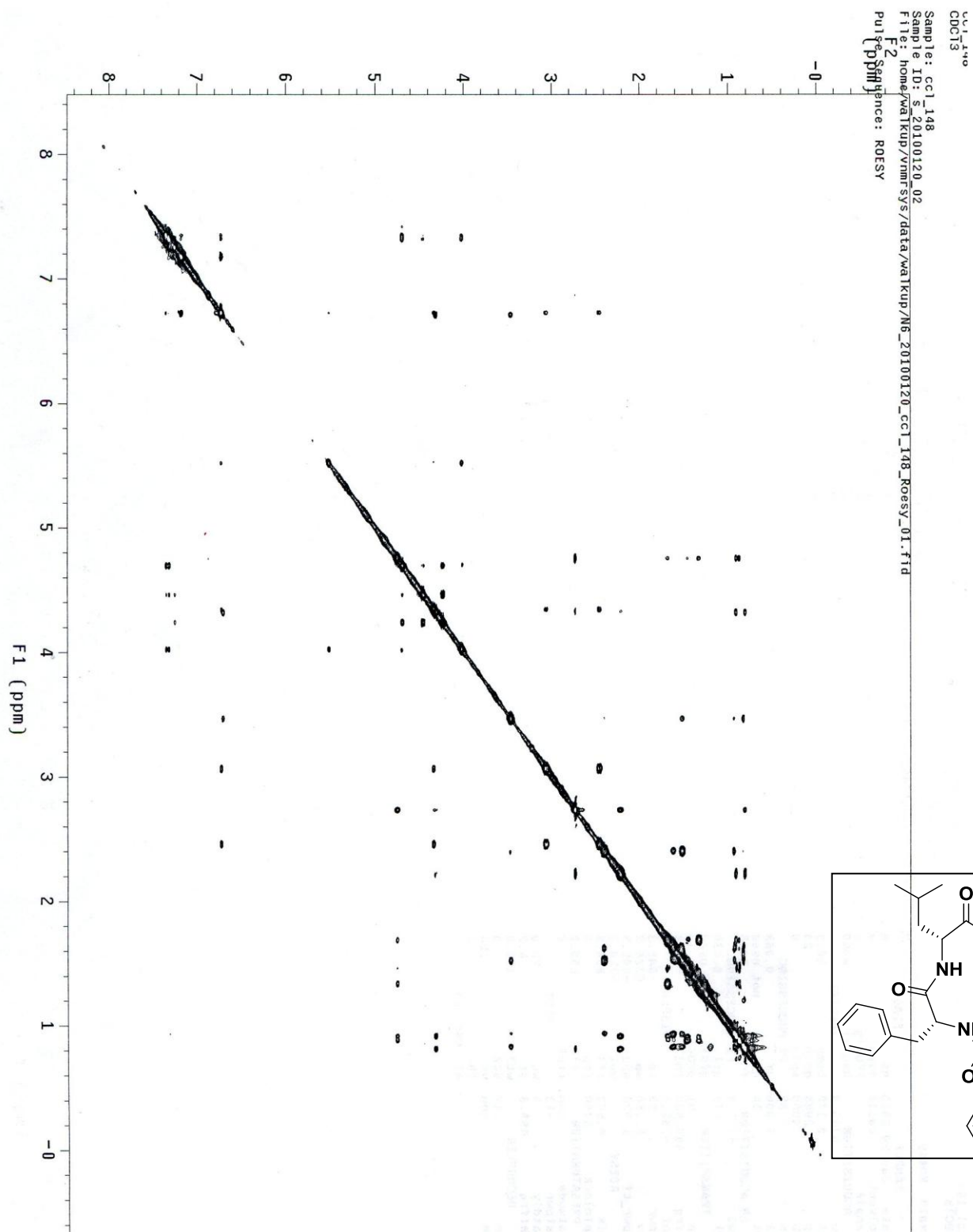
Analysis Name: CCL_147_148_L Instrument: Agilent 6330 Ion Trap Print Date: 8/17/2009 11:10:39 AM
Method: SANA.M P.D Operator: sdsu Acq. Date: 6/23/2009 11:58:06 PM
Sample Name: CCL_147_148_LP
Analysis Info:



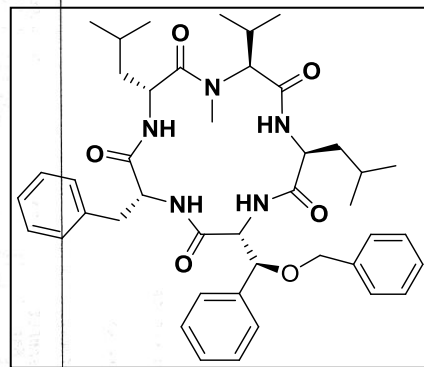
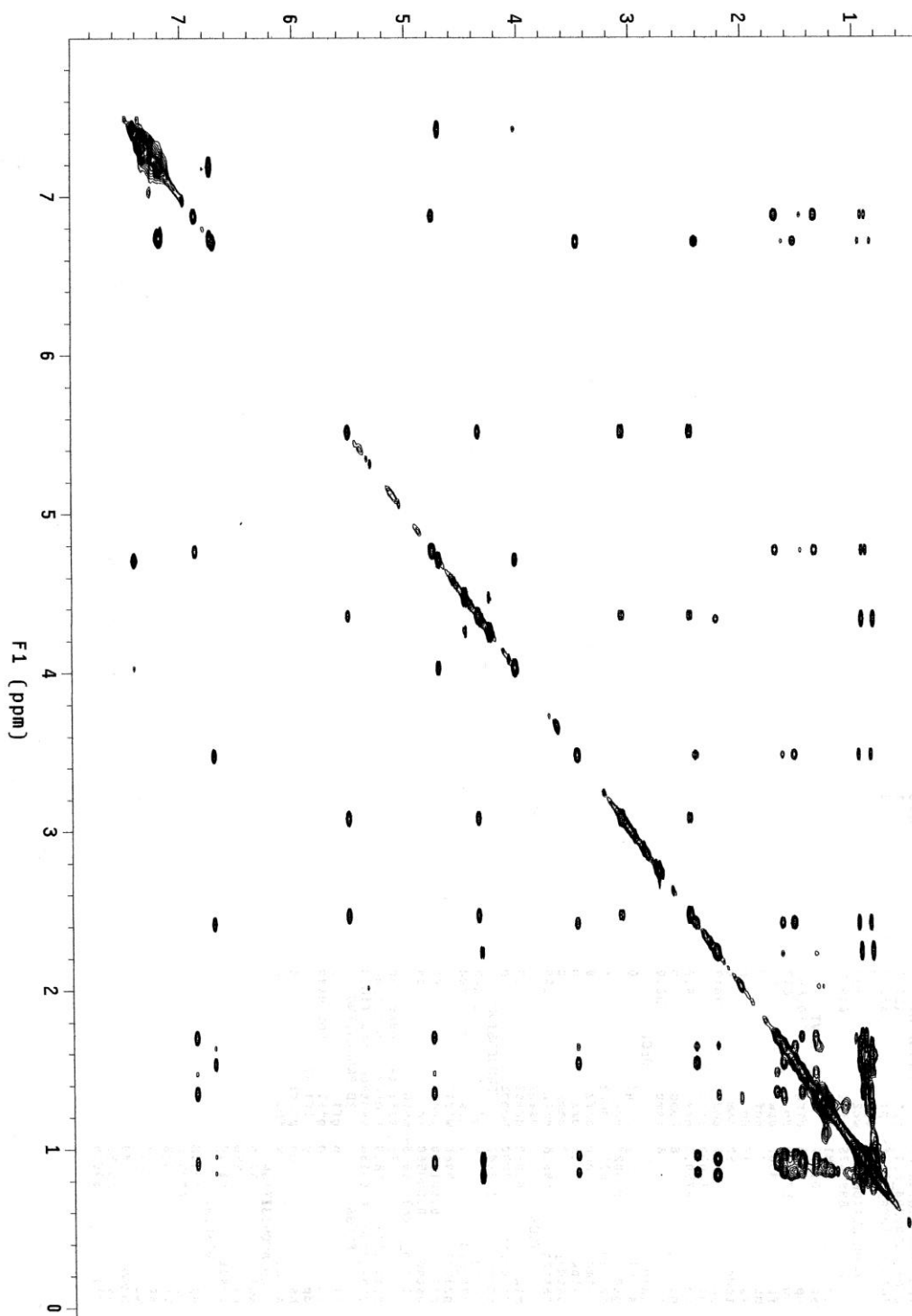
Compound 46 LCMS Double Deprotected Linear Pentapeptide HO-Leu-N-Me-Val-D-Leu-D-Phe-β-OH-Phe-NH₂ (MW=668)



Compound 46 NMR Cyclized Pentapeptide β -benzoxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe

Compound 46 ROSEY NMR Cyclized Pentapeptide β -benzoxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe

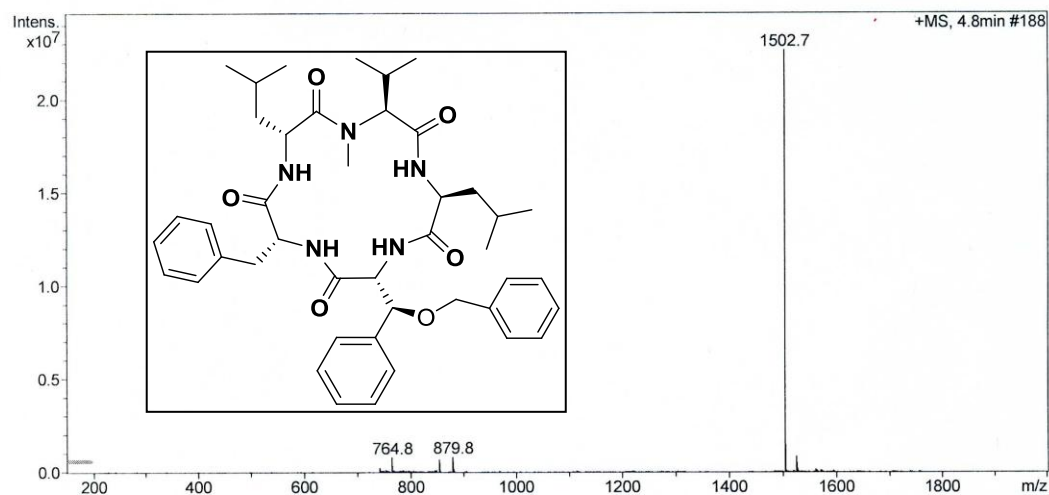
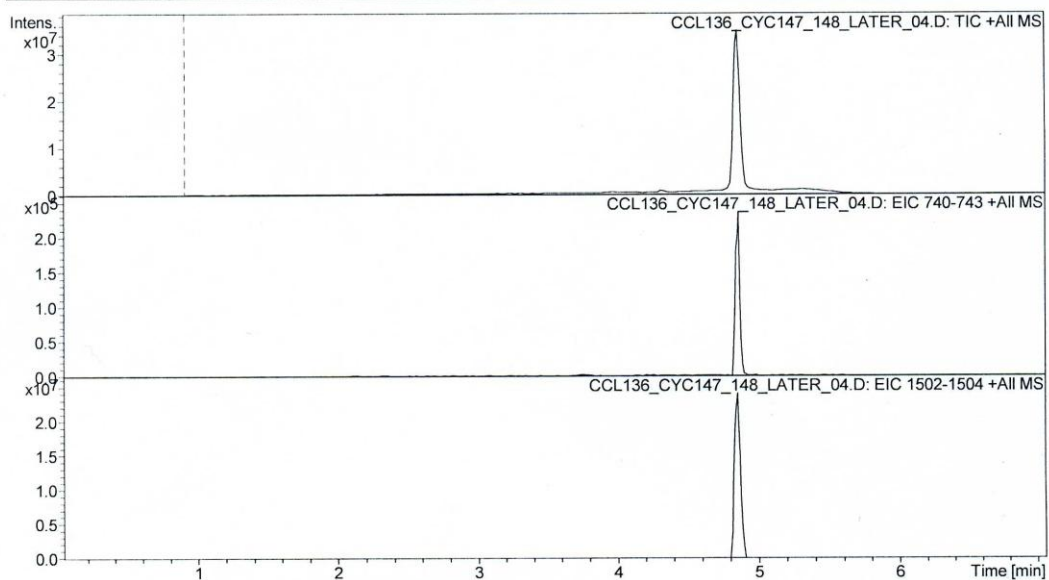
1318 04-MAR-10
131Y
TOSCY
ccl_tate_RT
CDCl3
Sample: ccl_tate_RT
Sample ID: S_20100304_01
File: /home/waikup/vnmrsvs/data/waikup/N6_20100304_ccl_tate_RT_toscy_01.fid
F2
Pulse Sequence: TOSCY
[ppm]



Compound 46 TOSCY NMR Cyclized Pentapeptide β -benzoxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe

Display Report - All Windows Selected Analysis

Analysis Name: CCL136_CYC147 **Instrument:** Agilent 6330 Ion Trap **Print Date:** 8/15/2009 9:30:37 PM
Method: SANA.M_148_LATER_04 **Operator:** sdsu **Acq. Date:** 8/15/2009 9:22:08 PM
Sample Name: CCL136_cyc147_148_later_04
Analysis Info:



Compound 46 LCMS Cyclized Pentapeptide β -benzoxy-Phe-Leu-N-Me-Val-D-Leu-D-Phe (MW=740)

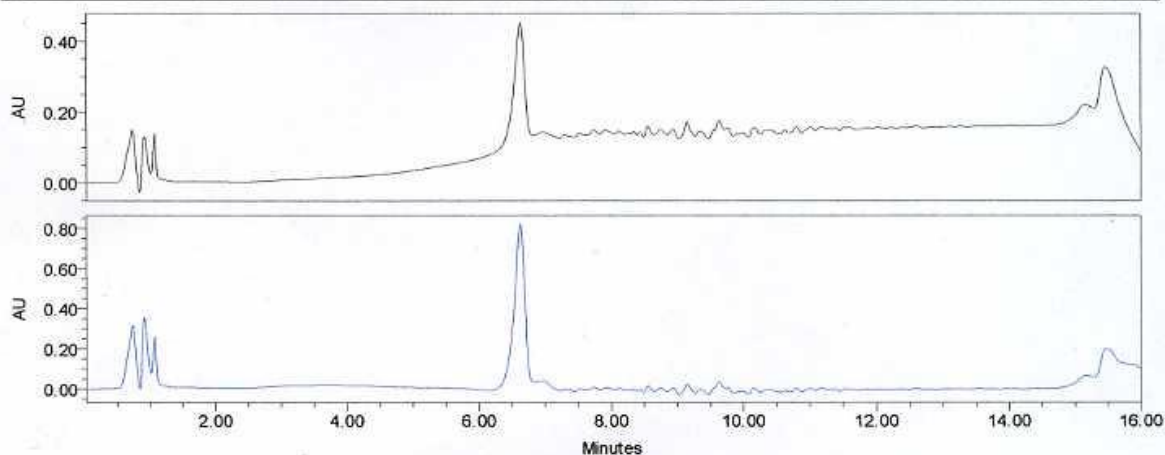
SDSU

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	CCL_cyc147_148_later	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	7	Date Acquired:	8/15/2009 2:59:51 PM
Run Time:	16.00 Minutes	Injection Volume:	40.00 ul



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

Peak Name	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	Amount	Units
1	****	****	****	****	****	****
2	****	****	****	****	****	****

