SUPPLEMENTARY MATERIAL

Tripeptide Derivatives from Vietnamese Mangrove-Derived Fungus *Aspergillus terreus* LM.5.2

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Abstract: Three new tripeptide-derivatives containing in their structures a rare cinnamic acid residue asterripeptides A-C (1-3) were isolated from Vietnamese mangrove-derived fungus *Aspergillus terreus* LM 5.2. Structures of isolated compounds were determined by NMR and ESIMS techniques combination. Absolute configurations of all stereocenters were determined using the Murfey's method via determining of amino acids configuration. Cytotoxicity against several cancer cell lines and inhibition ability of sortase A from Staphylococcus aureus of asterripeptides A-C were investigated.

Keywords: marine-derived fungi, mangrove-derived fungi, secondary metabolites, diketopiperazines, tripeptide derivatives, cinnamic acid, sortase A, cytotoxicity

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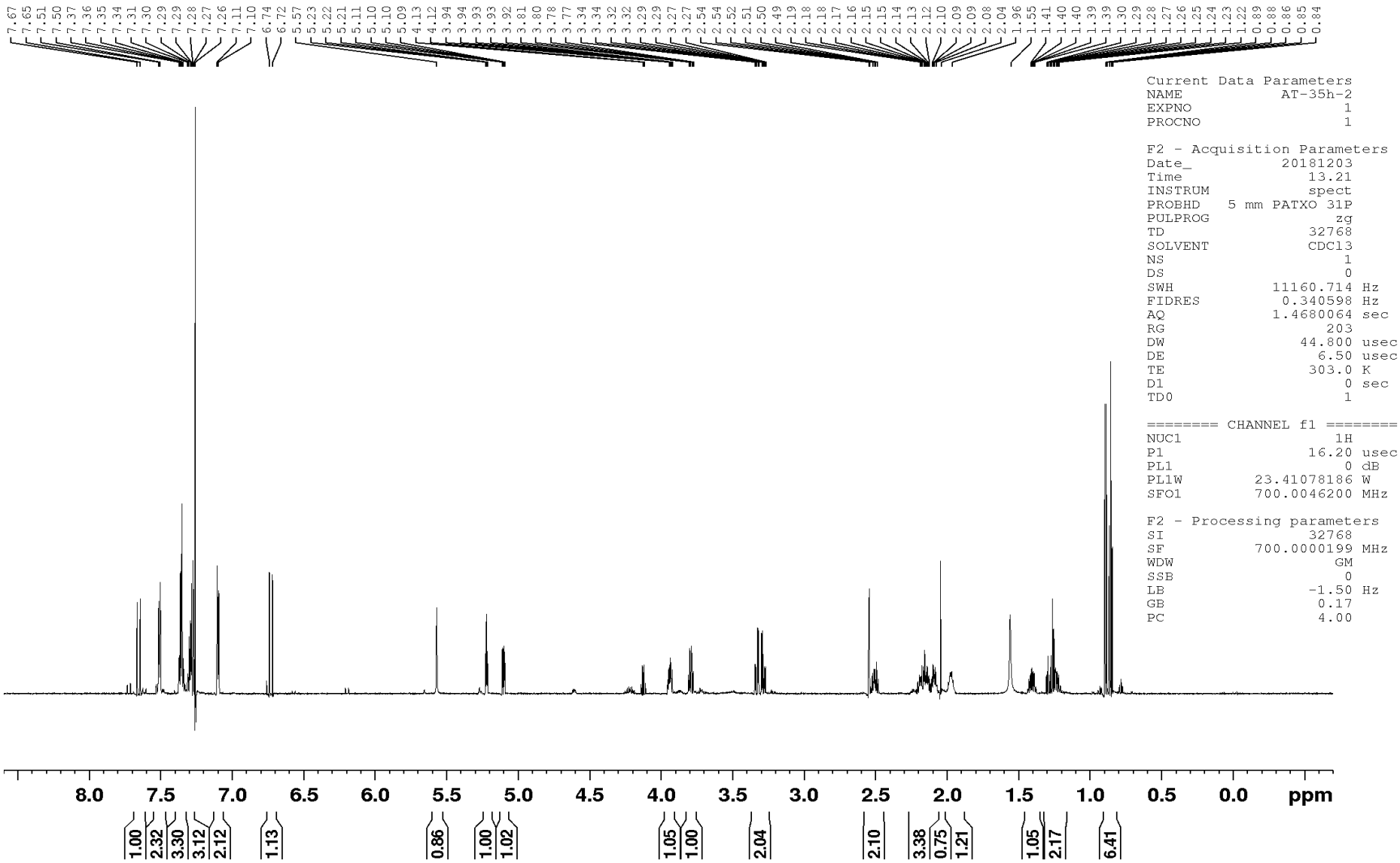
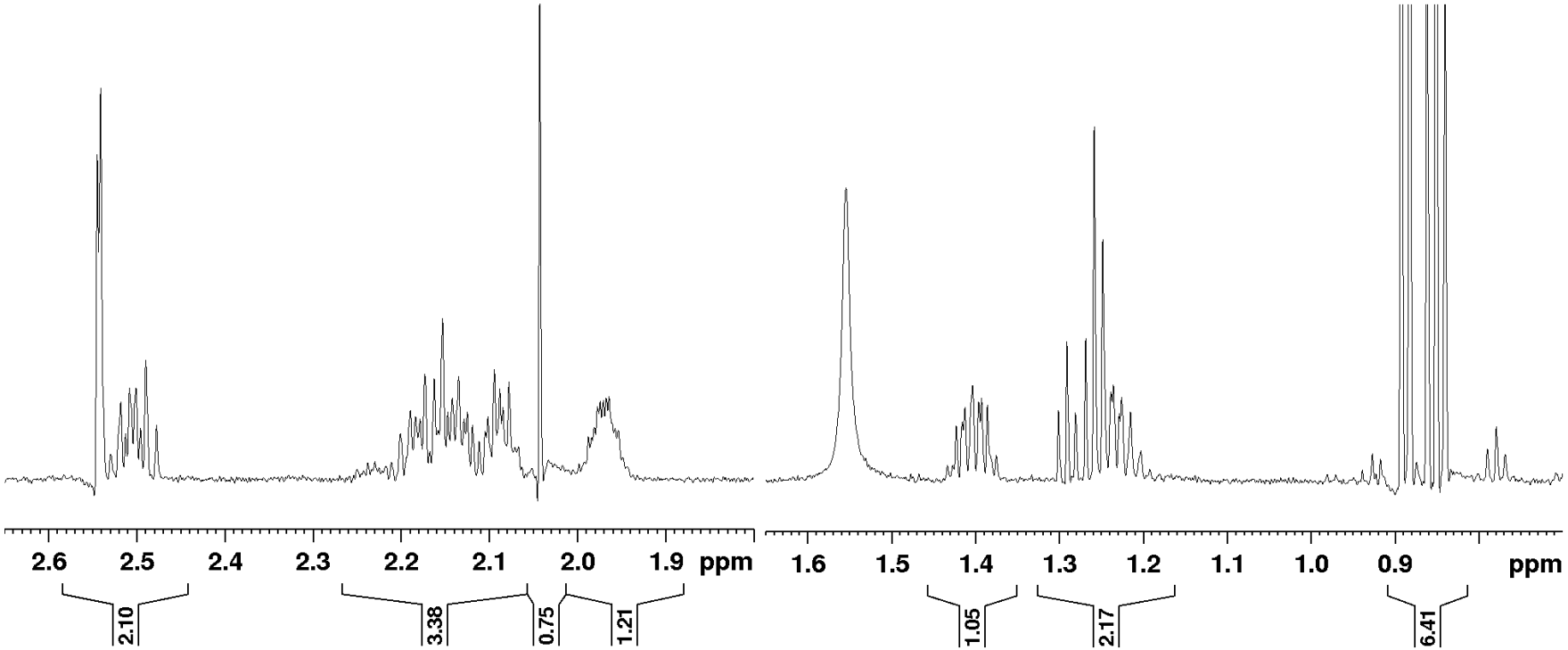
Figure S1. ^{1}H NMR spectrum of asterripeptide A (1)

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2.3
2.2
2.1
2.0
1.9
ppm
2.10
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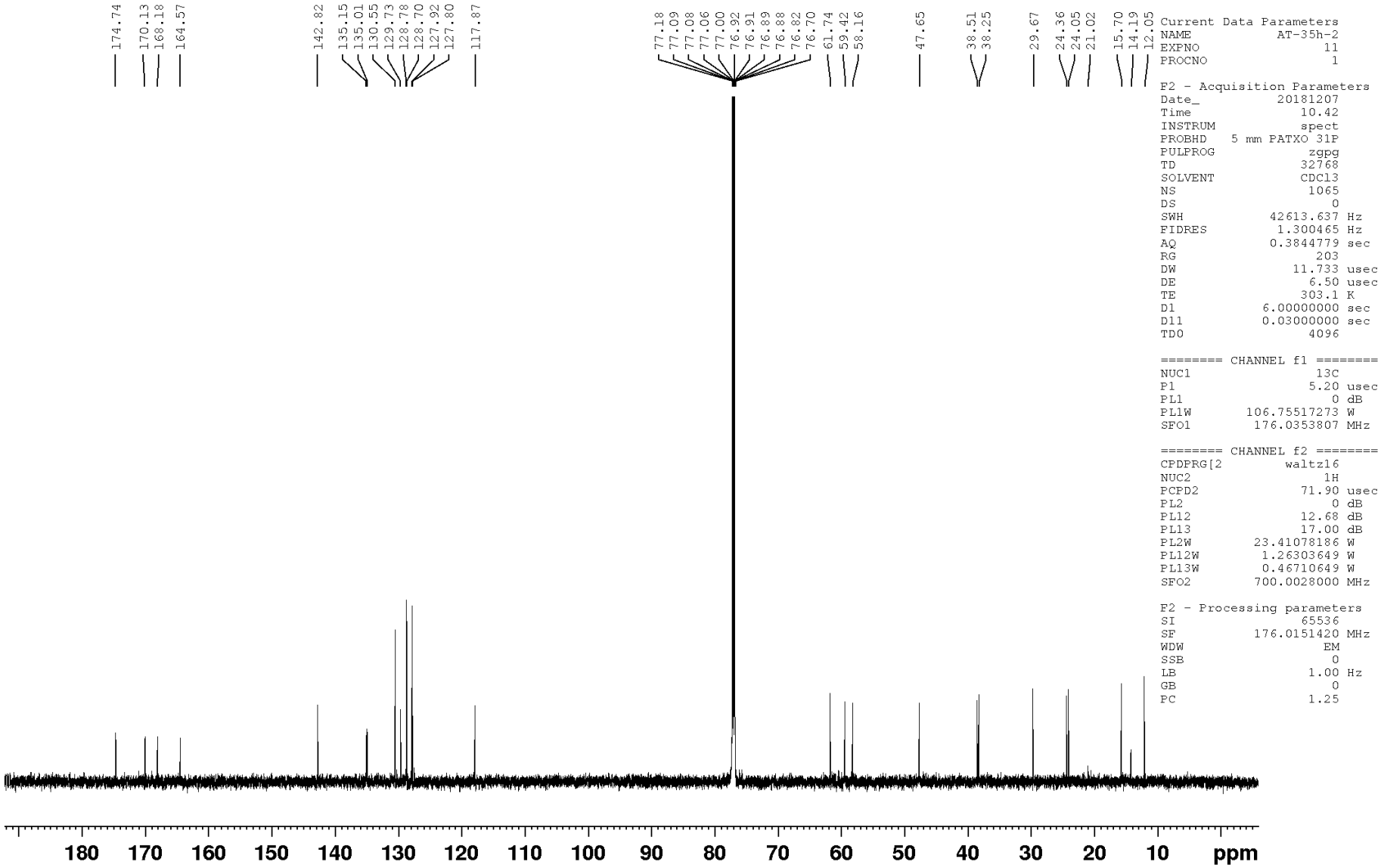
1.21
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
ppm
1.05
2.17
6.41

Figure S2. ^{13}C NMR spectrum of asterripeptide A (1)

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PULPROG                  zgpg
TD                      32768
SOLVENT                 CDCl3
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DS                          0
SWH                42613.637 Hz
FIDRES             1.300465 Hz
AQ                 0.3844779 sec
RG                        203
DW                   11.733 usec
DE                    6.50 usec
TE                    303.1 K
D1                 6.00000000 sec
D11                0.03000000 sec
TD0                       4096

======== CHANNEL f1 ========
NUC1                      13C
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PL1                         0 dB
PL1W          106.75517273 W
SFO1           176.0353807 MHz

======== CHANNEL f2 ========
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NUC2                      1H
PCPD2                71.90 usec
PL2                         0 dB
PL12                  12.68 dB
PL13                  17.00 dB
PL2W          23.41078186 W
PL12W          1.26303649 W
PL13W          0.46710649 W
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F2 - Processing parameters
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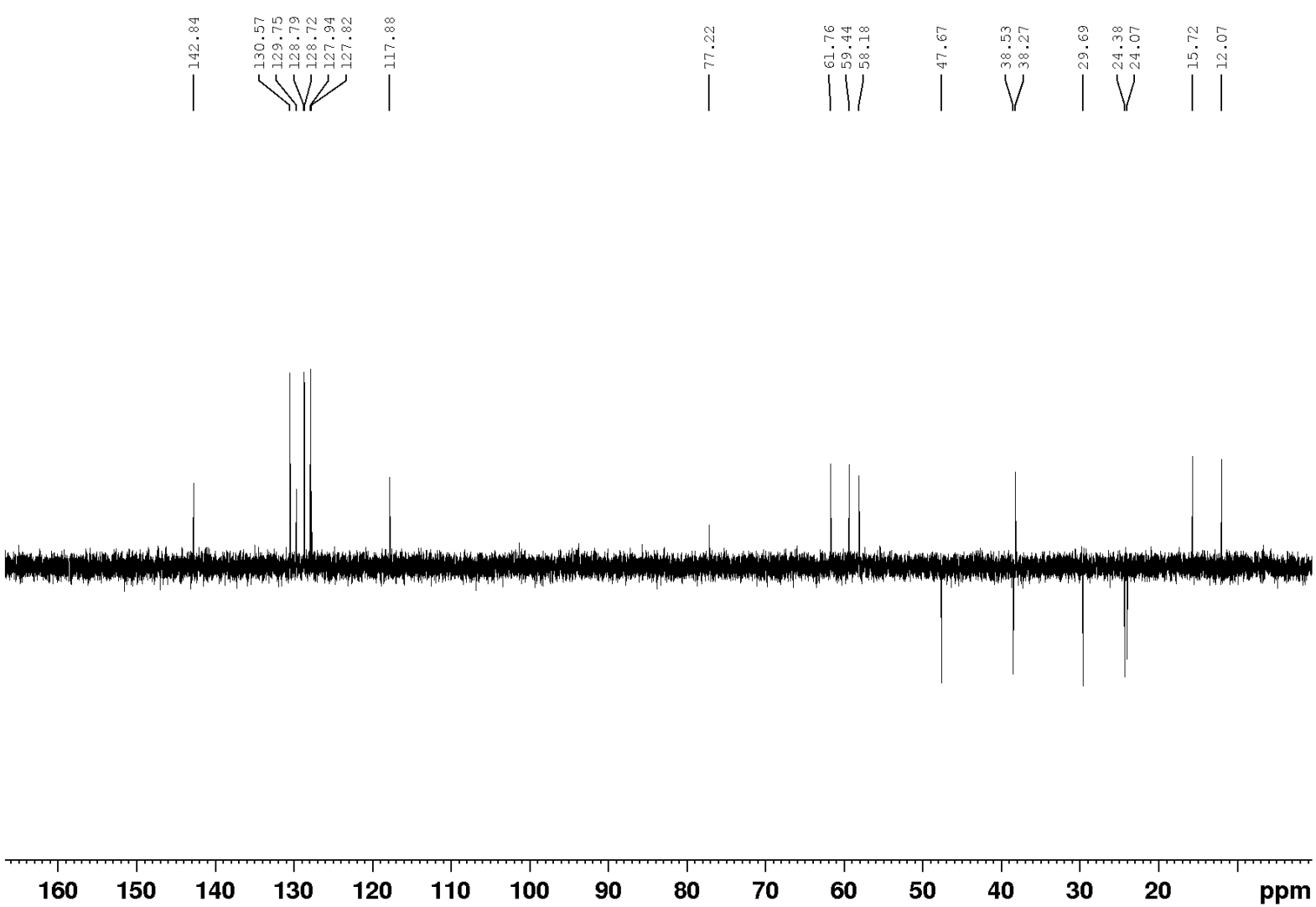
Figure S3. DEPT-135 spectrum of asterripeptide A (1)

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PROCNO                       1

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TD                       65536
SOLVENT                  CDCl3
NS                         165
DS                           2
SWH                  29761.904 Hz
FIDRES                0.454131 Hz
AQ                    1.1010048 sec
RG                         203
DW                      16.800 usec
DE                       6.50 usec
TE                      303.1 K
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D1                    2.00000000 sec
D2                    0.00344828 sec
D12                   0.00002000 sec
TD0                        4096

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NUC1                       13C
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P12                   2000.00 usec
PL0                    120.00 dB
PL1                         0 dB
PL0W                        0 W
PL1W               106.75517273 W
SFO1                176.0301003 MHz
SP2                      7.82 dB
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SPOFFS2                     0 Hz

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NUC2                       1H
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P4                      33.40 usec
PCPD2                   71.90 usec
PL2                         0 dB
PL12                    12.68 dB
PL2W               23.41078186 W
PL12W               1.26303649 W
SFO2                700.0028000 MHz

F2 - Processing parameters
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WDW                         EM
SSB                          0
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GB                           0
PC                        1.20
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Figure S4. ^{1}H-^{1}H COSY spectrum of asterripeptide A (1)

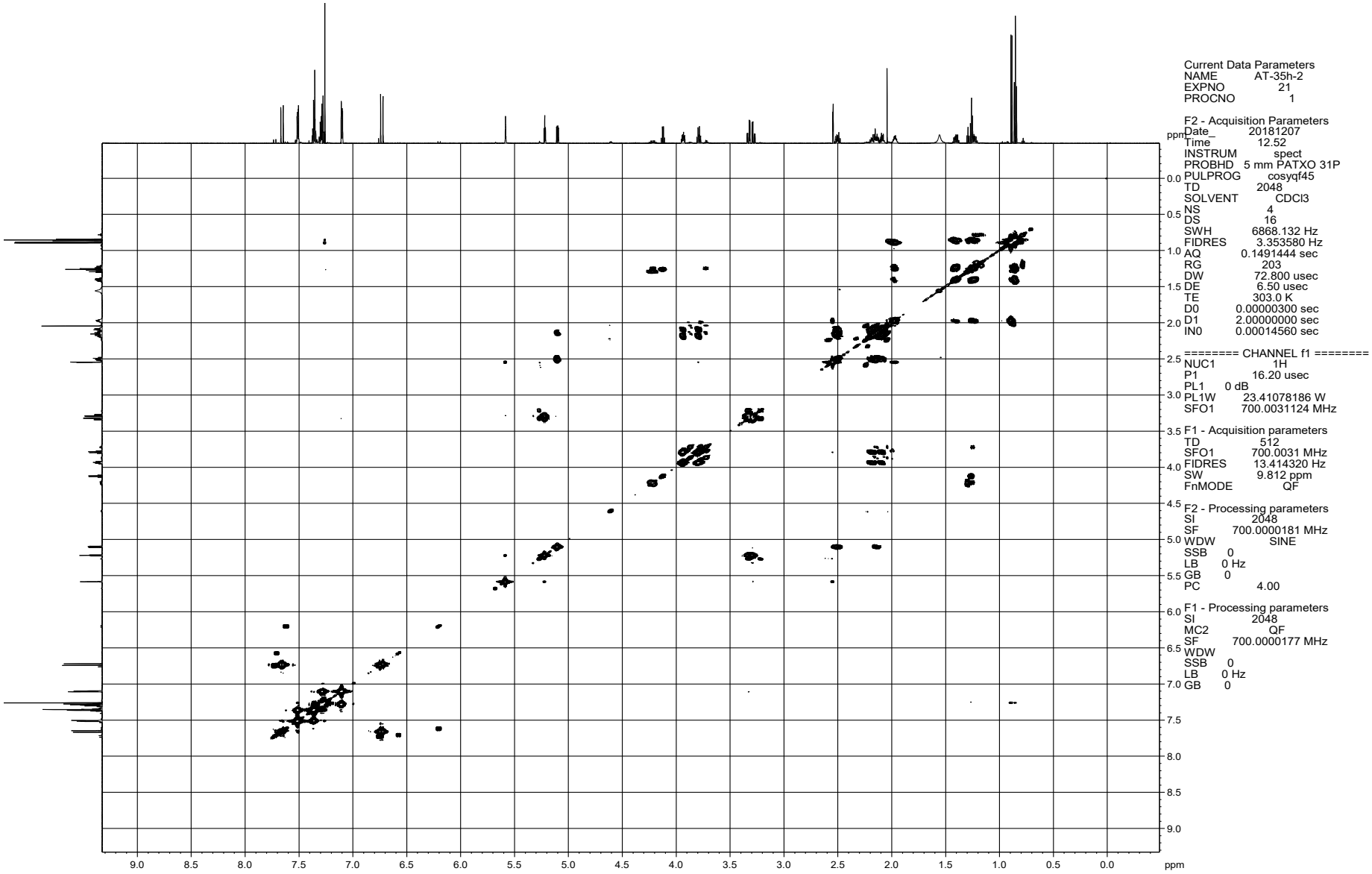


Figure S5. HMBC spectrum of asterripeptide A (1)

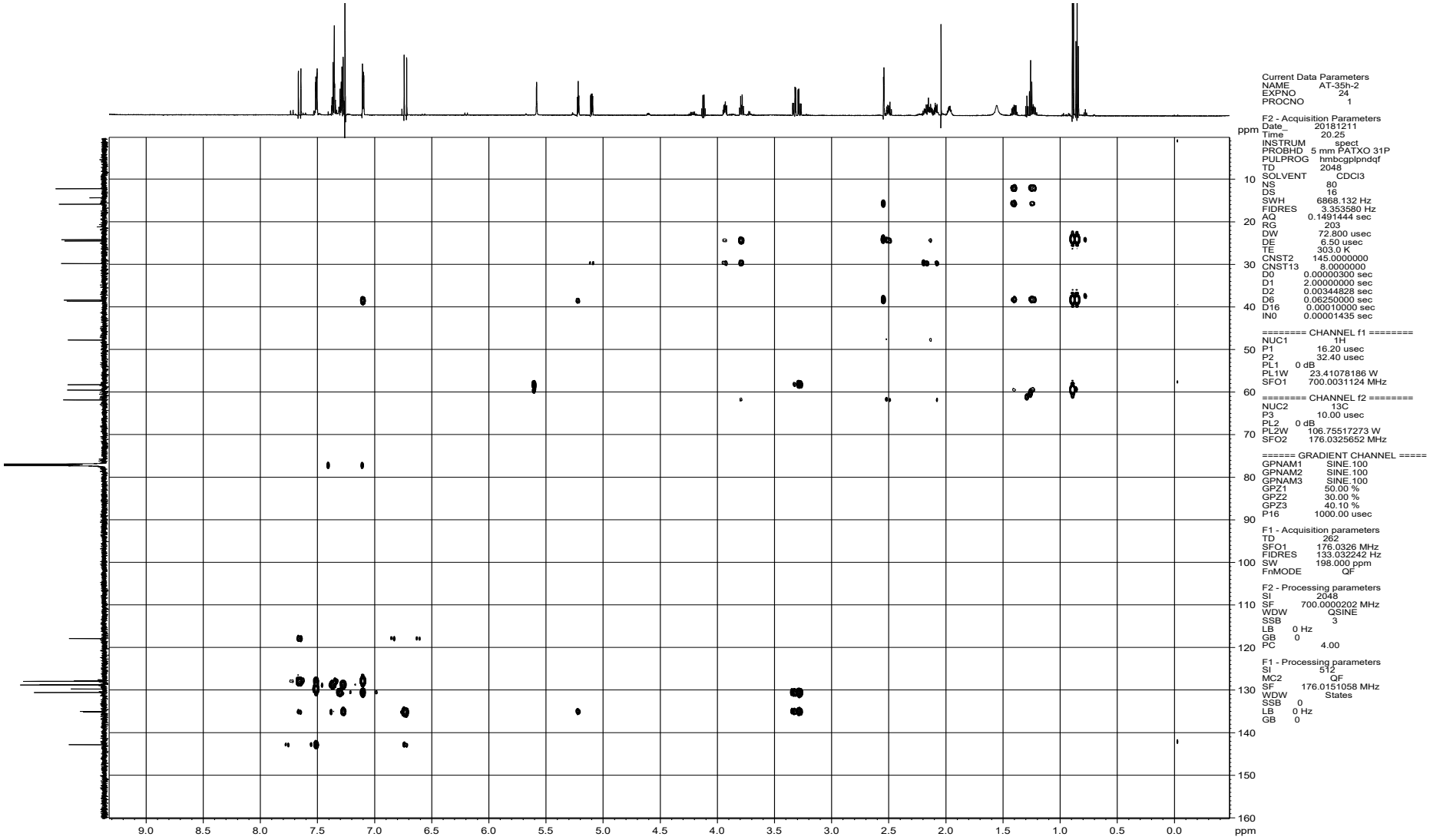


Figure S6. HSQC spectrum of asterripeptide A (1)

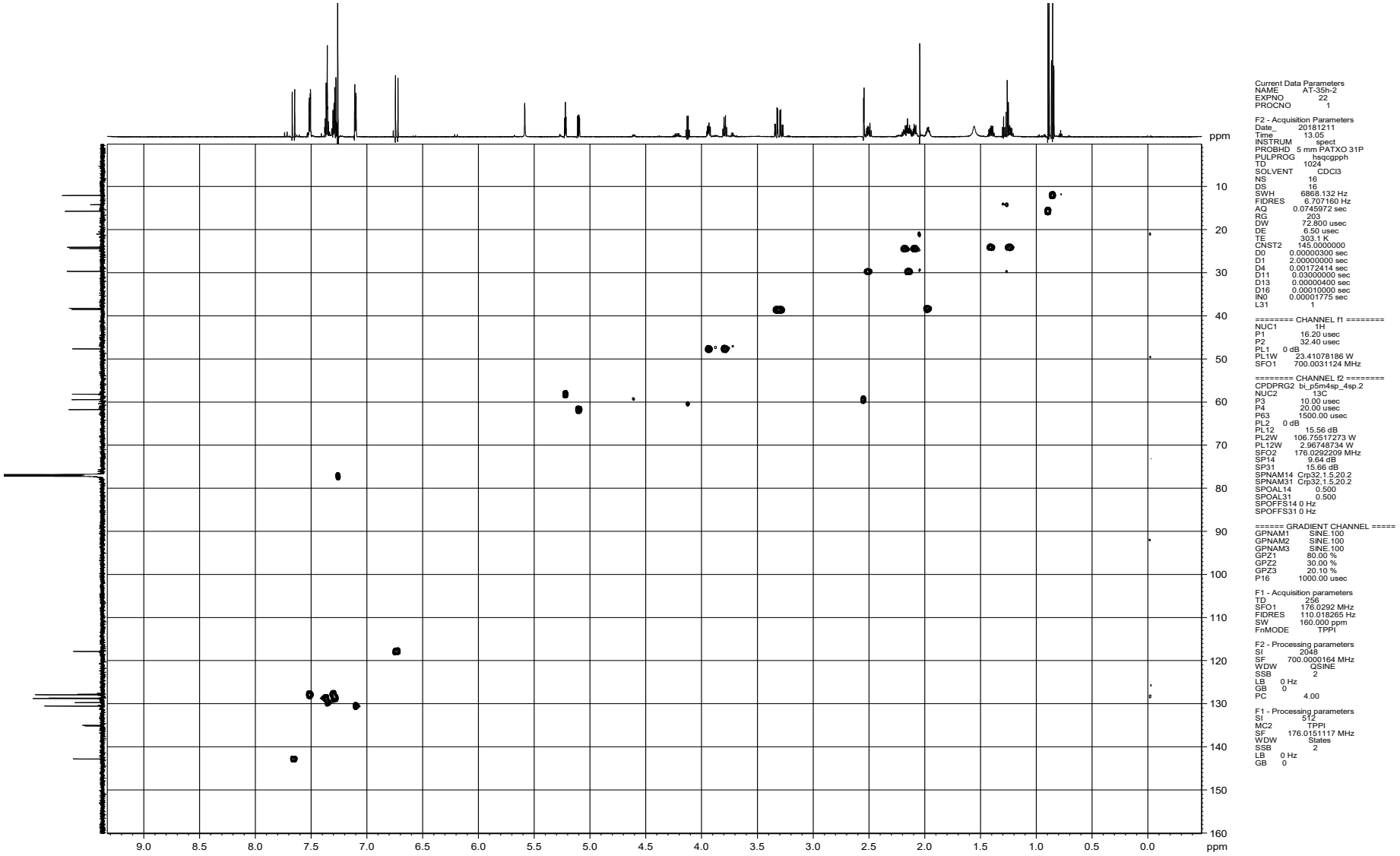
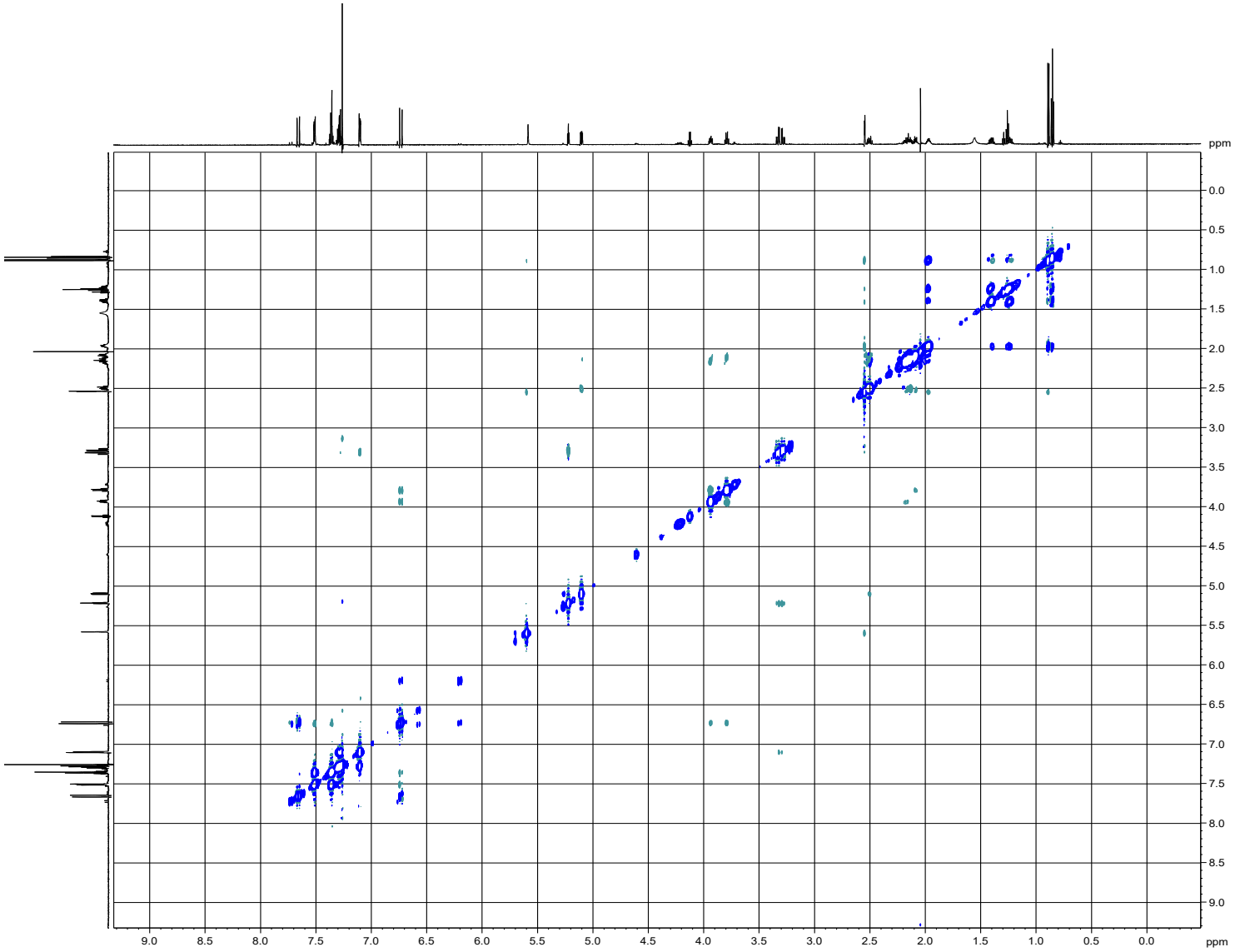


Figure S7. ROESY spectrum of asterripeptide A (1)



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PROCNO 1

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PULPROG roesyph.2
TD 2048
SOLVENT CDCl3
NS 24
DS 16
SWH 6868.132 Hz
FIDRES 3.353580 Hz
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RG 1.78
DW 72.800 usec
DE 6.50 usec
TE 303.0 K
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D1 2.00000000 sec
D12 0.00002000 sec
IN0 0.00014560 sec
L4 613
P15 270000.00 usec

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P25 220.00 usec
PL1 0 dB
PL27 16.64 dB
PL1W 23.41078186 W
PL27W 0.50747657 W
SFO1 700.0031124 MHz

F1 - Acquisition parameters
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SFO1 700.0031 MHz
FIDRES 26.828640 Hz
SW 9.812 ppm
FnMODE TPPI

F2 - Processing parameters
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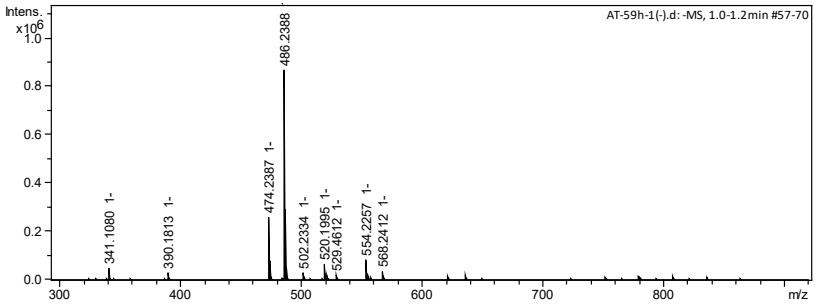
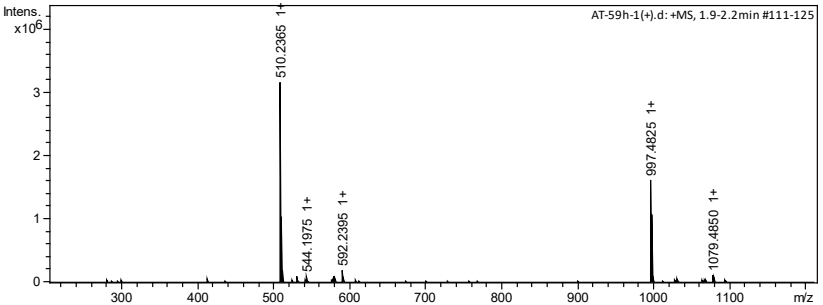
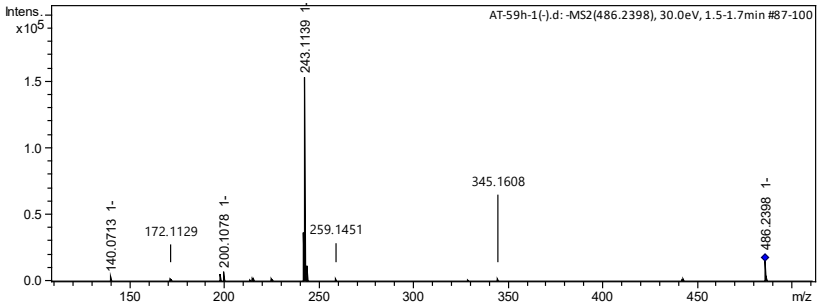
WDW SINE
SSB 2
LB 0 Hz
GB 0
PC 4.00

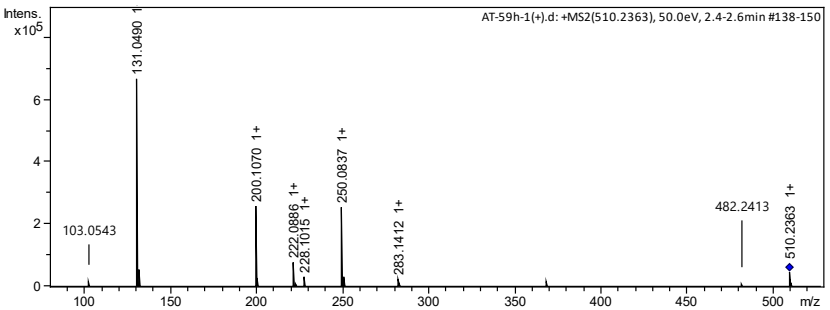
F1 - Processing parameters
SI 512
MC2 TPPI
SF 700.0000138 MHz
WDW States
SSB 2
LB 0 Hz
GB 0

Figure S8. MS and MS/MS data of asterripeptide A (1)



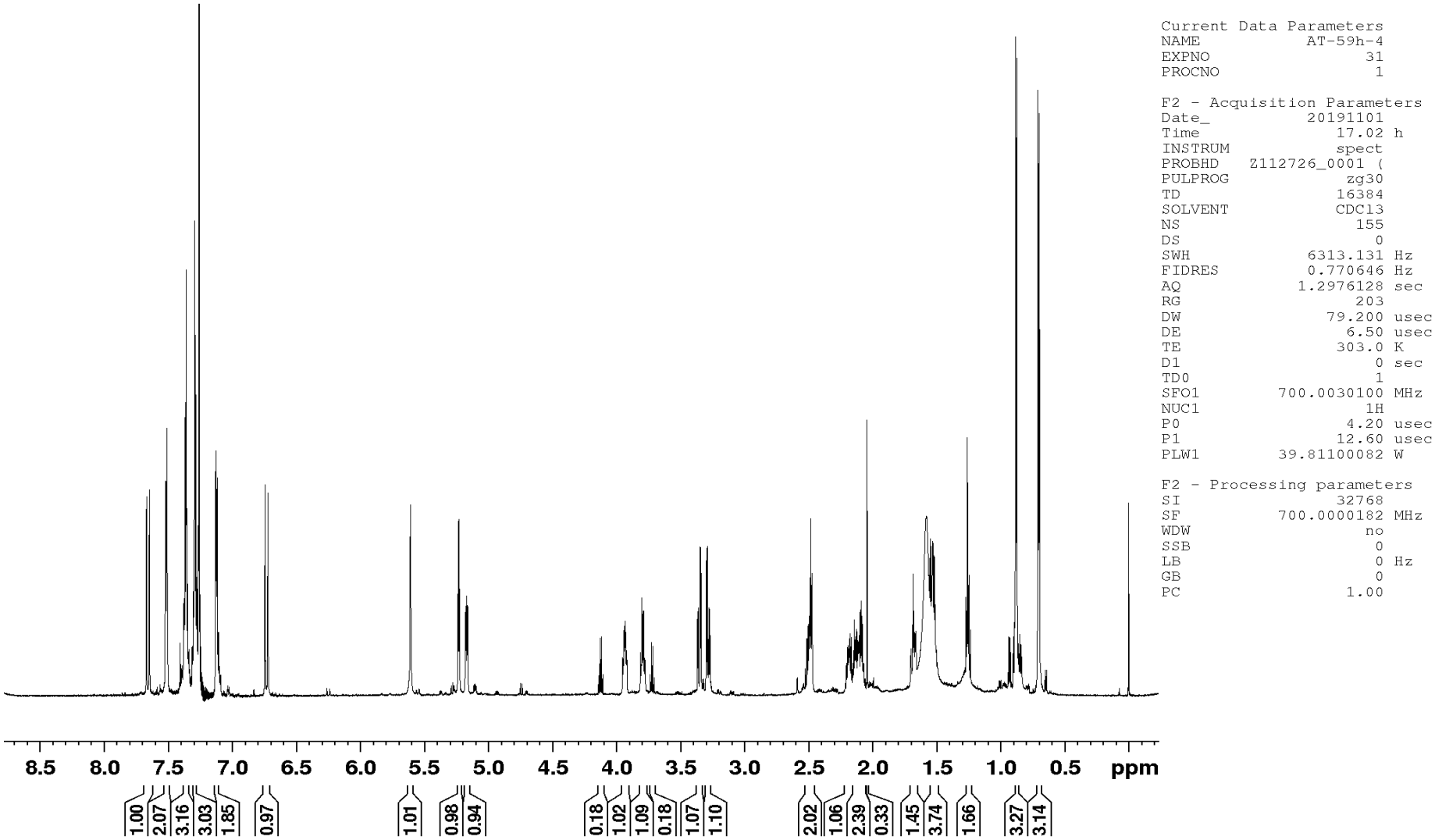






	meas.	calc.	Δ (ppm)
$[M-H]^-$	486,2387	486,2398	2,2
$[M+Na]^+$	510,2365	510,2363	-0,3

Figure S9. ^{1}H NMR data of asterripeptide B (2)

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PROCNO                      1

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PULPROG                 zg30
TD                     16384
SOLVENT                CDCl3
NS                       155
DS                         0
SWH                 6313.131 Hz
FIDRES              0.770646 Hz
AQ                 1.2976128 sec
RG                       203
DW                    79.200 usec
DE                     6.50 usec
TE                    303.0 K
D1                         0 sec
TD0                        1
SFO1           700.0030100 MHz
NUC1                      1H
P0                     4.20 usec
P1                    12.60 usec
PLW1           39.81100082 W

F2 - Processing parameters
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WDW                       no
SSB                        0
LB                         0 Hz
GB                         0
PC                      1.00
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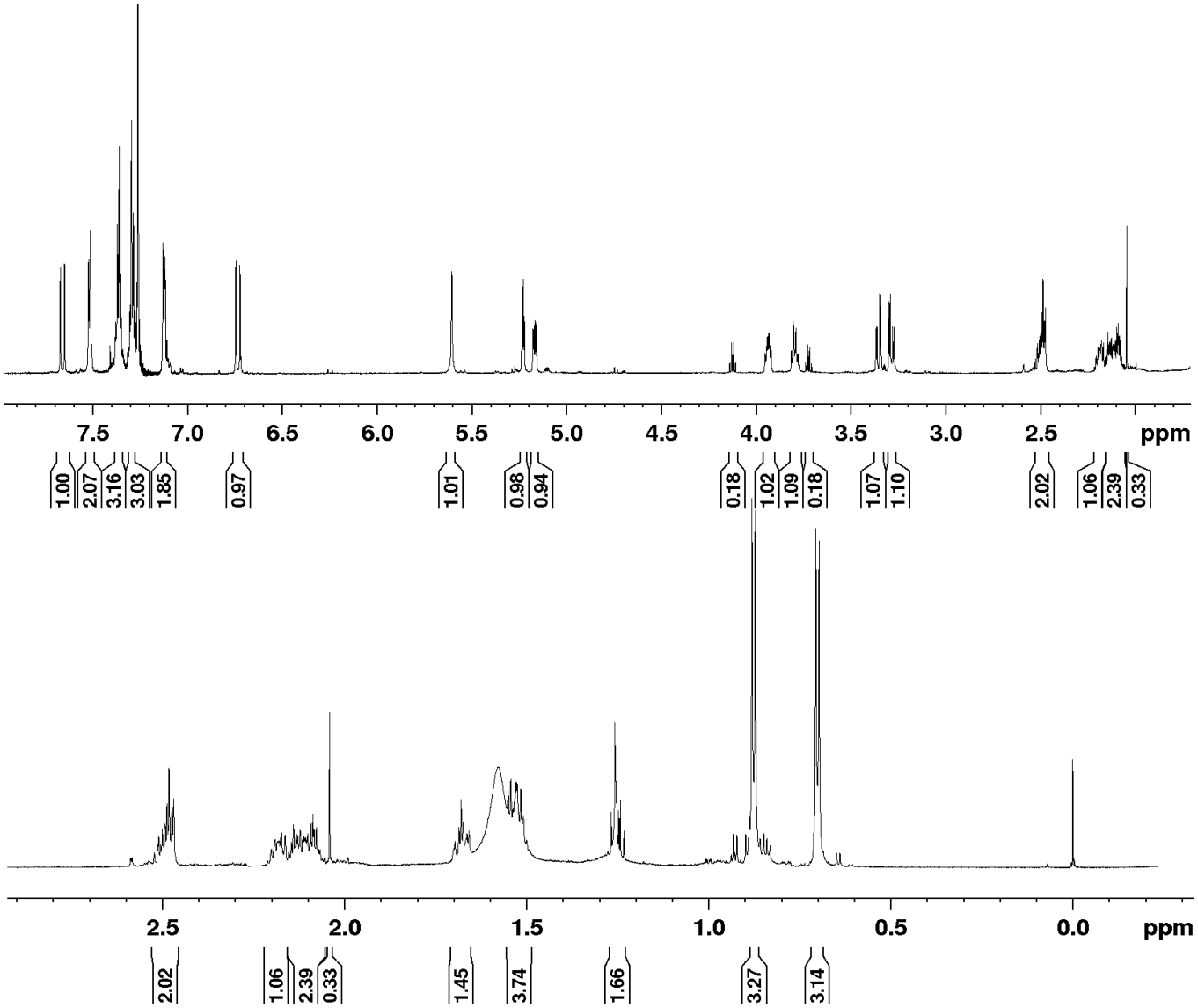


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EXPNO                       31
PROCNO                       1

F2 - Acquisition Parameters
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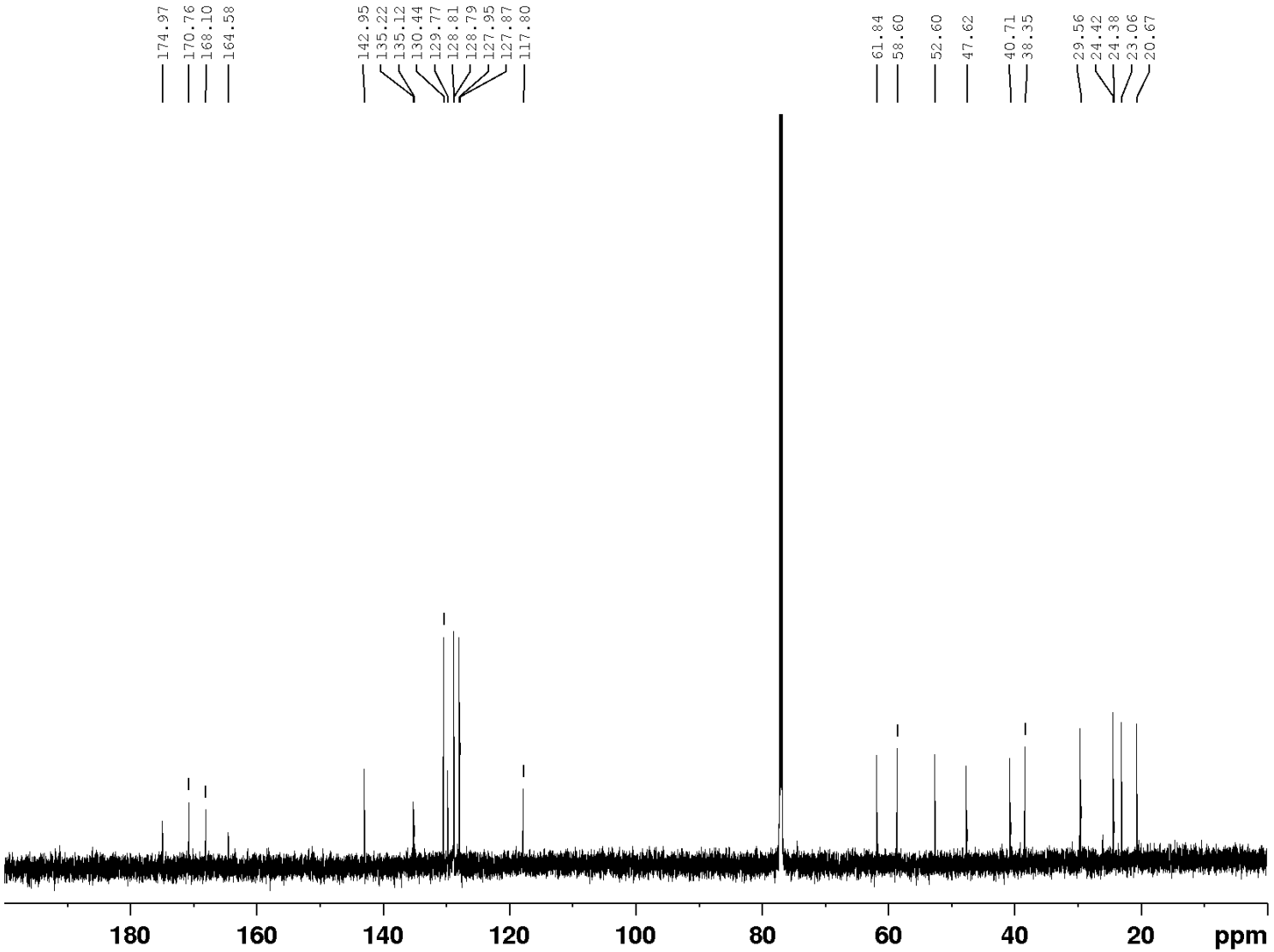
INSTRUM                  spect
PROBHD    Z112726_0001 (
PULPROG                   zg30
TD                       16384
SOLVENT                  CDCl3
NS                         155
DS                           0
SWH                   6313.131 Hz
FIDRES                0.770646 Hz
AQ                    1.2976128 sec
RG                         203
DW                       79.200 usec
DE                        6.50 usec
TE                       303.0 K
D1                           0 sec
TD0                          1
SFO1             700.0030100 MHz
NUC1                        1H
P0                        4.20 usec
P1                       12.60 usec
PLW1             39.81100082 W

F2 - Processing parameters
SI                       32768
SF               700.0000182 MHz
WDW                         no
SSB                          0
LB                           0 Hz
GB                           0
PC                        1.00
```

Figure S10. ^{13}C NMR spectrum of asterripeptide B (2)

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PROCNO                 1

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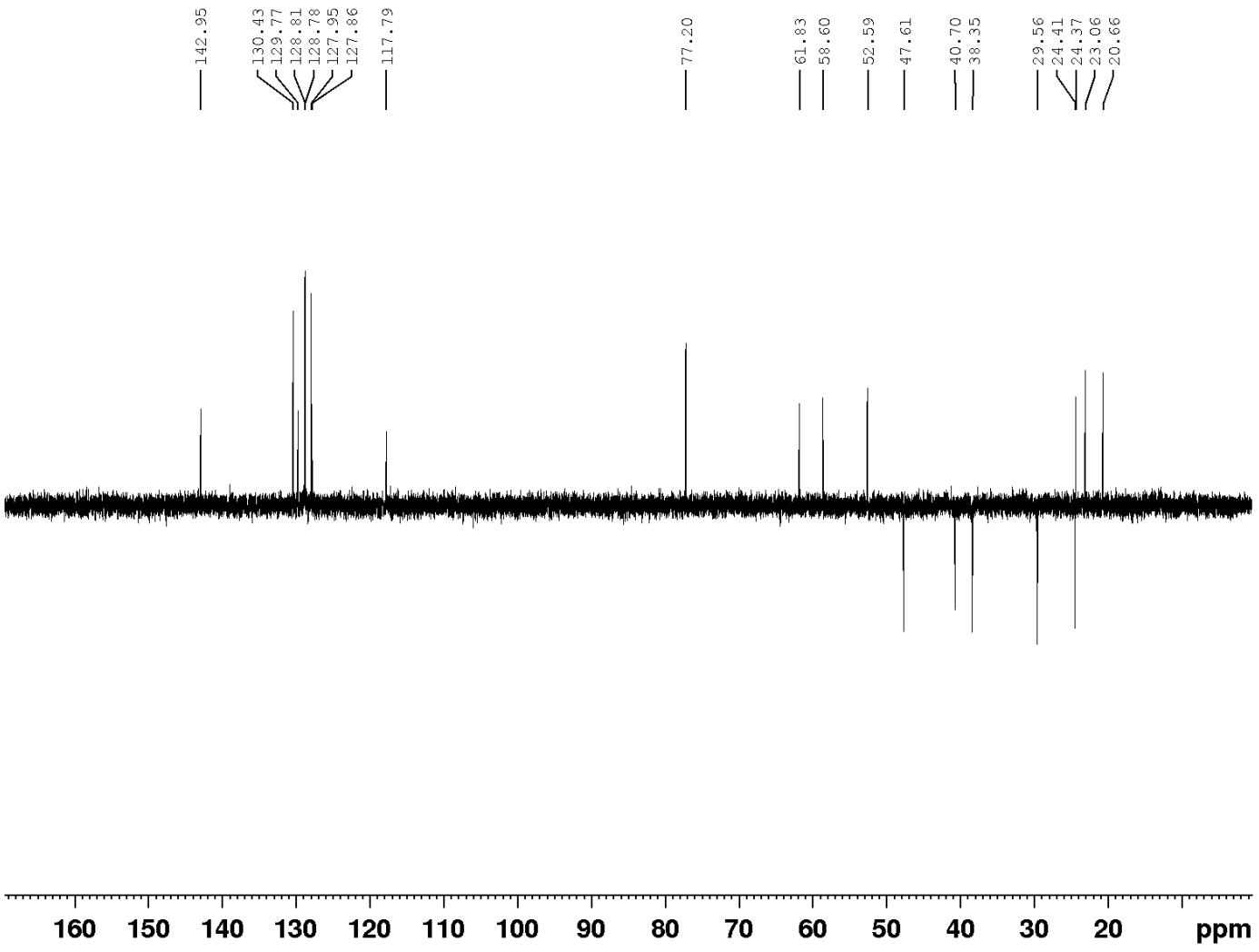
PULPROG          zgpg30
TD                 65536
SOLVENT            CDC13
NS                  3029
DS                     2
SWH            42613.637 Hz
FIDRES          1.300465 Hz
AQ             0.7689557 sec
RG                   203
DW                11.733 usec
DE                 6.50 usec
TE                303.8 K
D1           0.50000000 sec
D11          0.03000000 sec
TD0                 4096
SFO1        176.0353807 MHz
NUC1                13C
P0                 3.50 usec
P1                10.50 usec
PLW1        35.48099899 W
SFO2        700.0028000 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2        39.81100082 W
PLW12        1.43719995 W
PLW13        0.83929998 W

F2 - Processing parameters
SI                 65536
SF          176.0151407 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.00
```

Figure S11. DEPT NMR spectrum of asterripeptide B (2)

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PROCNO                       1

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PULPROG              deptsp135
TD                       65536
SOLVENT                  CDCl3
NS                        1024
DS                           2
SWH                  29761.904 Hz
FIDRES                0.908261 Hz
AQ                   1.1010048 sec
RG                         203
DW                      16.800 usec
DE                       6.50 usec
TE                       303.4 K
CNST2               145.0000000
D1                   2.00000000 sec
D2                   0.00344828 sec
D12                  0.00002000 sec
TD0                         64
SFO1                176.0301003 MHz
NUC1                        13C
P1                      10.50 usec
P13                   2000.00 usec
PLW0                         0 W
PLW1                35.48099899 W
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SPOFFS5                      0 Hz
SPW5                 7.96899986 W
SFO2                700.0028000 MHz
NUC2                        1H
CPDPRG[2                waltz16
P3                      13.30 usec
P4                      26.60 usec
PCPD2                   70.00 usec
PLW2                39.81100082 W
PLW12                1.43719995 W

F2 - Processing parameters
SI                       65536
SF                  176.0151418 MHz
WDW                         EM
SSB                          0
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GB                           0
PC                        1.40
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Figure S12. HSQC spectrum of asterripeptide B (2)

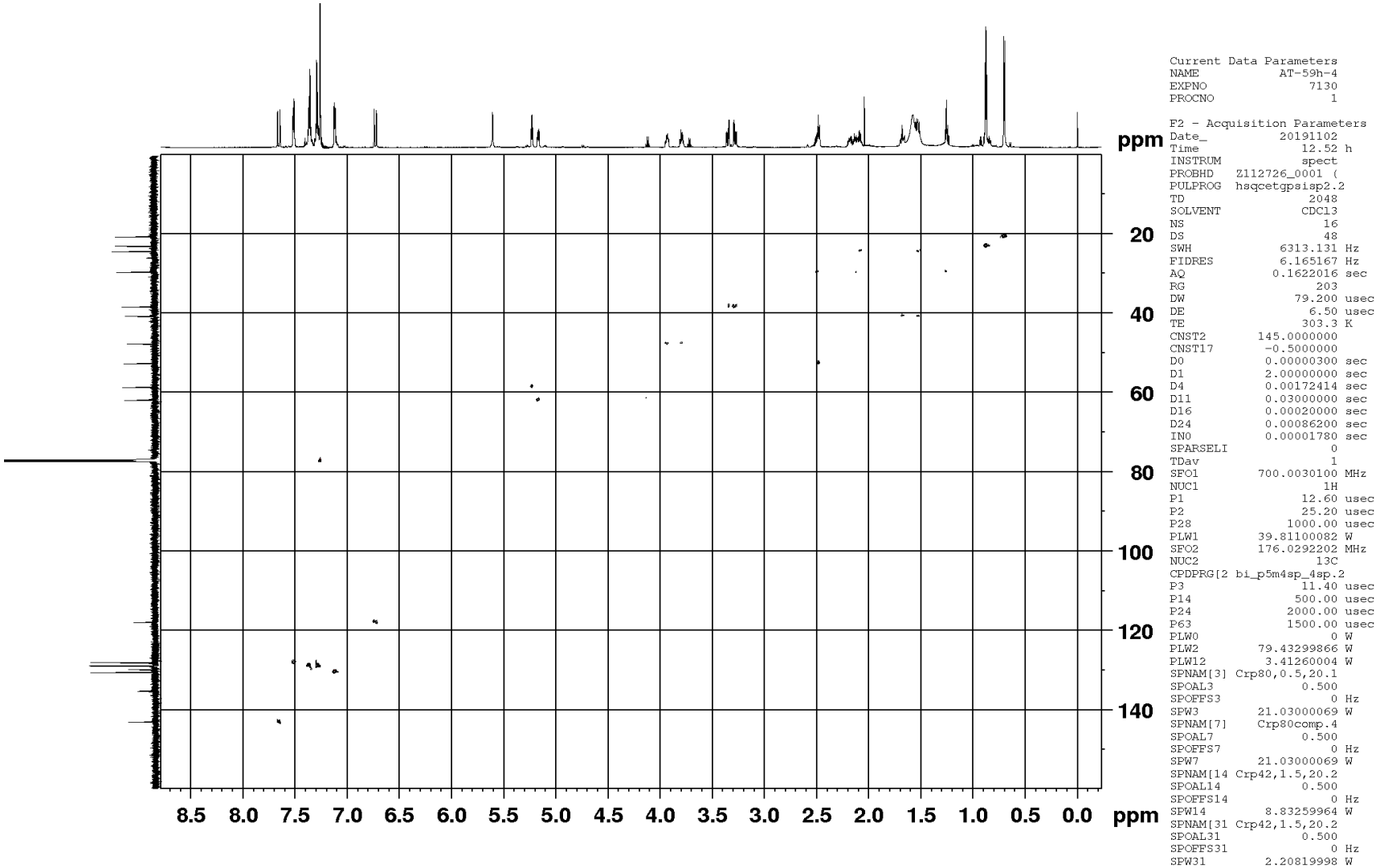
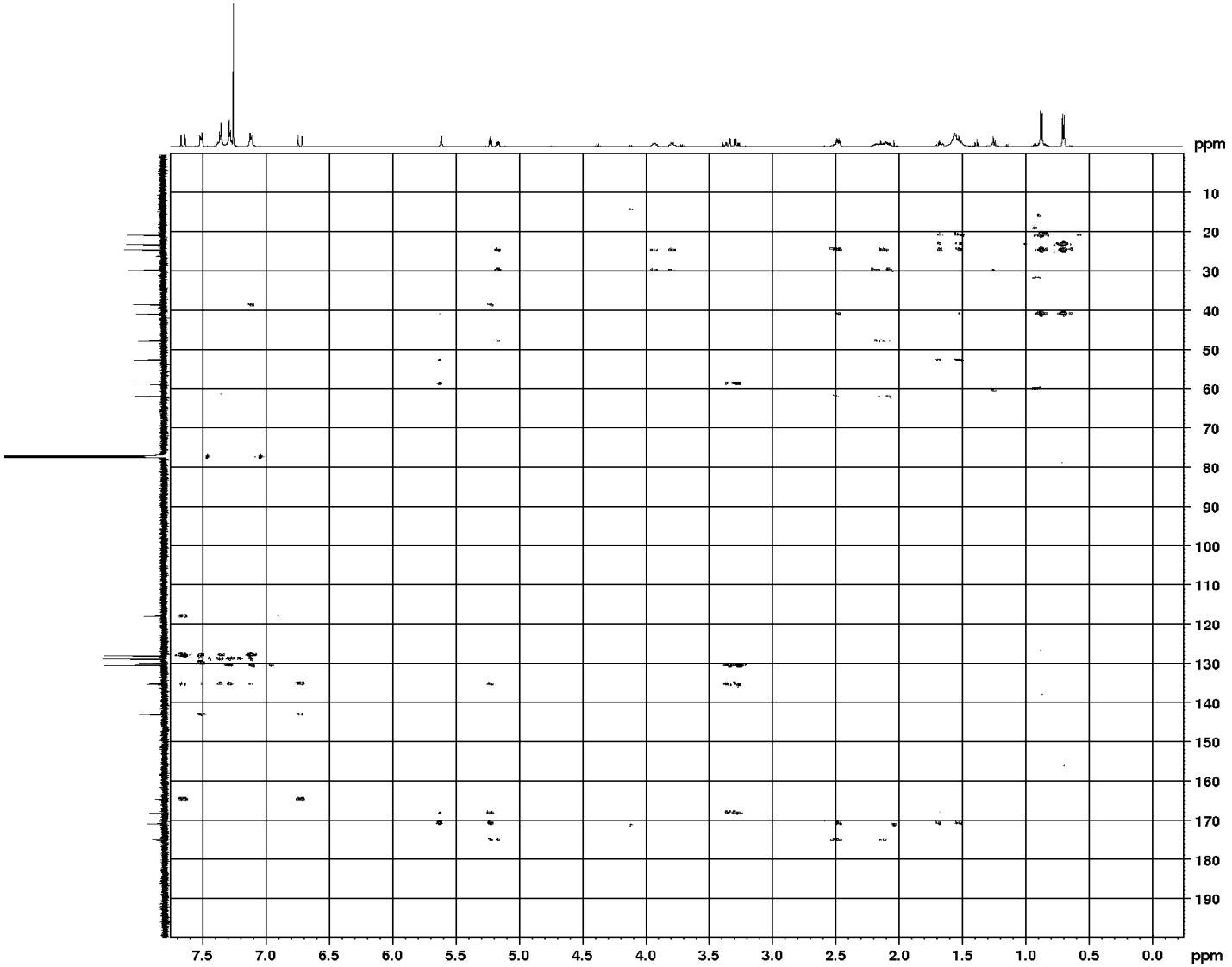


Figure S13. HMBC spectrum of asterripeptide B (2)

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PROCNO                   1

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PULPROG     hmbcgplpndqf
TD                    4096
SOLVENT              CDCl3
NS                     432
DS                      16
SWH               4000.000 Hz
FIDRES            1.953125 Hz
AQ                0.5120000 sec
RG                   196.84
DW                  125.000 usec
DE                    6.50 usec
TE                   303.1 K
CNST2           145.0000000
CNST13            8.0000000
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D1                1.50000000 sec
D2                0.00344828 sec
D6                0.06250000 sec
D16               0.00020000 sec
IN0               0.00001990 sec
SPARSELI                 0
TDav                     1
SFO1           500.1319005 MHz
NUC1                    1H
P1                   11.65 usec
P2                   23.30 usec
PLW1           15.84899998 W
SFO2           125.7703648 MHz
NUC2                   13C
P3                   12.10 usec
PLW2           79.43299866 W
GPNAM[1]       SMSQ10.100
GPZ1                 50.00 %
GPNAM[2]       SMSQ10.100
GPZ2                 30.00 %
GPNAM[3]       SMSQ10.100
GPZ3                 40.10 %
P16                1000.00 usec

F1 - Acquisition parameters
TD                      64
SFO1             125.7704 MHz
FIDRES           785.175903 Hz
SW                 199.774 ppm
FnMODE                  QF

F2 - Processing parameters
SI                    2048
SF             500.1300213 MHz
WDW                 QSINE
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LB                      0 Hz
GB                      0
PC                   1.00
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Figure S14. ^{1}H-^{1}H COSY spectrum of asterripeptide B (2)

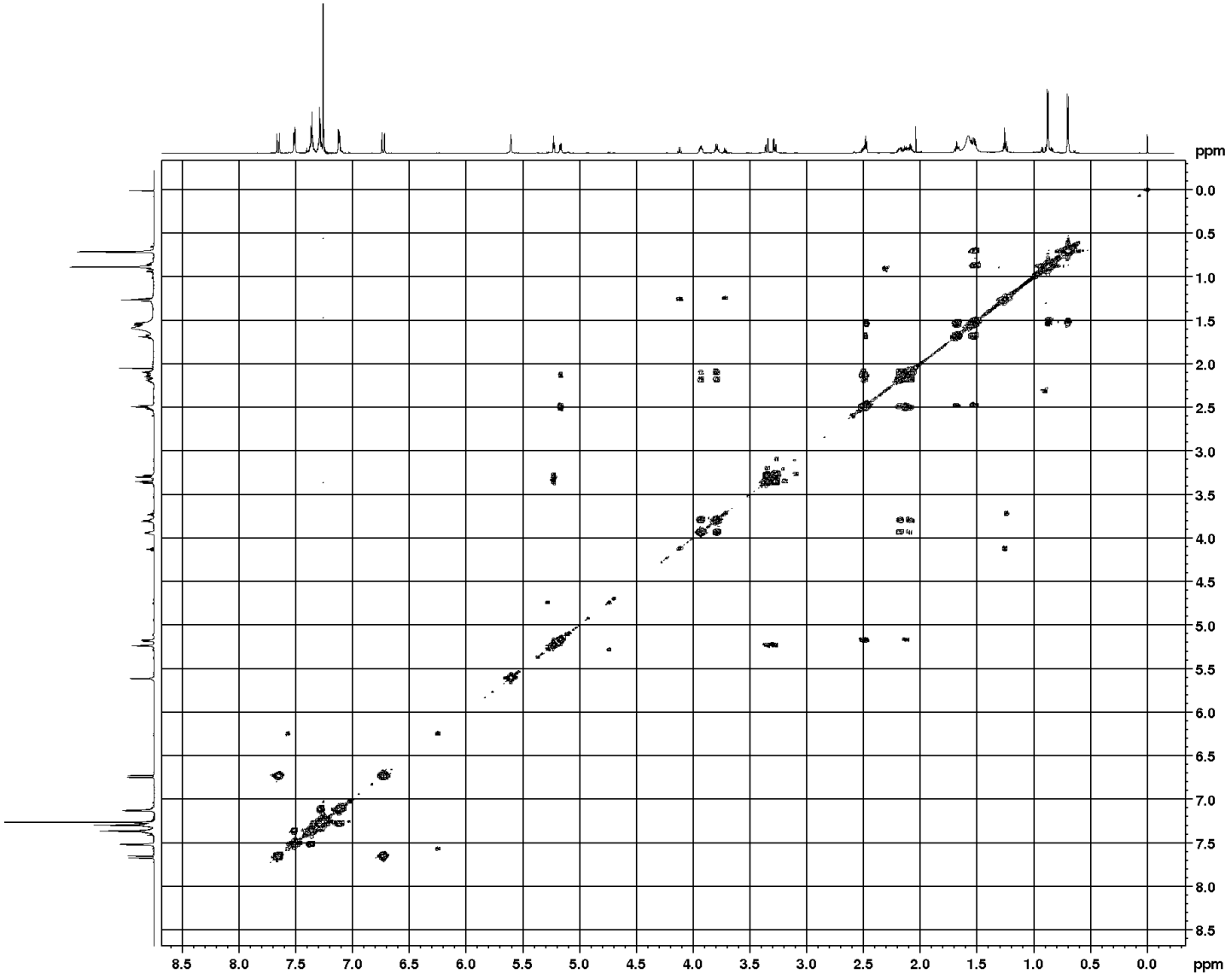
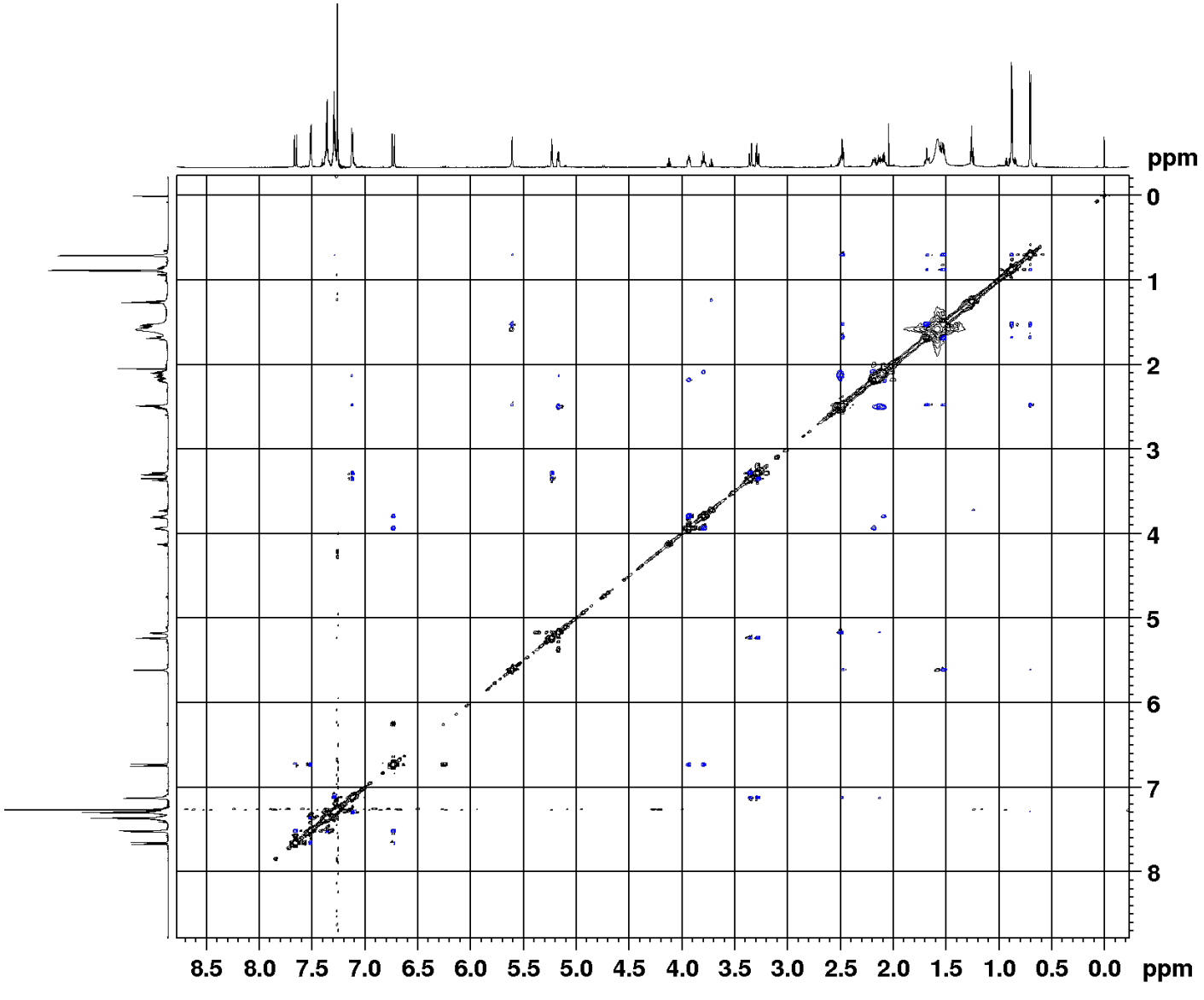


Figure S15. NOESY spectrum of asterripeptide B (2)

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Current Data Parameters
NAME                  AT-59h-4
EXPNO                     6030
PROCNO                       1

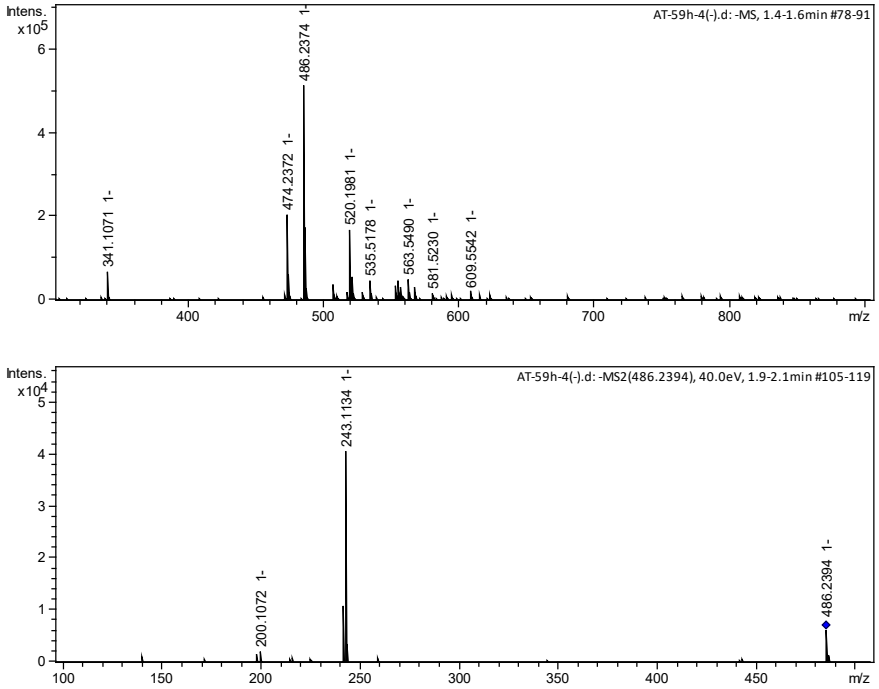
F2 - Acquisition Parameters
Date_                 20191101
Time                     17.28 h
INSTRUM                  spect
PROBHD    Z112726_0001 (
PULPROG             noesygpph
TD                        2048
SOLVENT                  CDCl3
NS                          16
DS                          16
SWH                   6313.131 Hz
FIDRES                6.165167 Hz
AQ                    0.1622016 sec
RG                          203
DW                       79.200 usec
DE                        6.50 usec
TE                       303.0 K
D0                    0.00006316 sec
D1                    1.00000000 sec
D8                    1.00000000 sec
D16                   0.00020000 sec
IN0                   0.00015840 sec
TDav                         1
SFO1               700.0030100 MHz
NUC1                        1H
P1                       12.60 usec
P2                       25.20 usec
PLW1              39.81100082 W
GPNAM[1]              SINE.100
GPZ1                     20.00 %
P16                    1000.00 usec

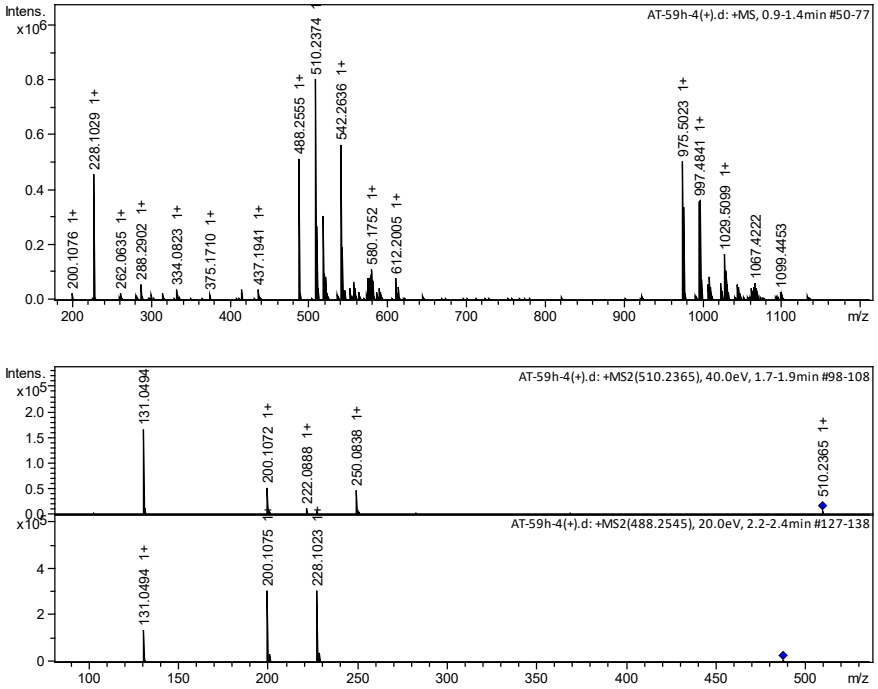
F1 - Acquisition parameters
TD                        256
SFO1                  700.003 MHz
FIDRES               49.321339 Hz
SW                        9.019 ppm
FnMODE                    TPPI

F2 - Processing parameters
SI                        2048
SF                 700.0000182 MHz
WDW                      QSINE
SSB                          2
LB                           0 Hz
GB                           0
PC                        1.00

F1 - Processing parameters
SI                        2048
MC2                       TPPI
SF                 700.0000168 MHz
```

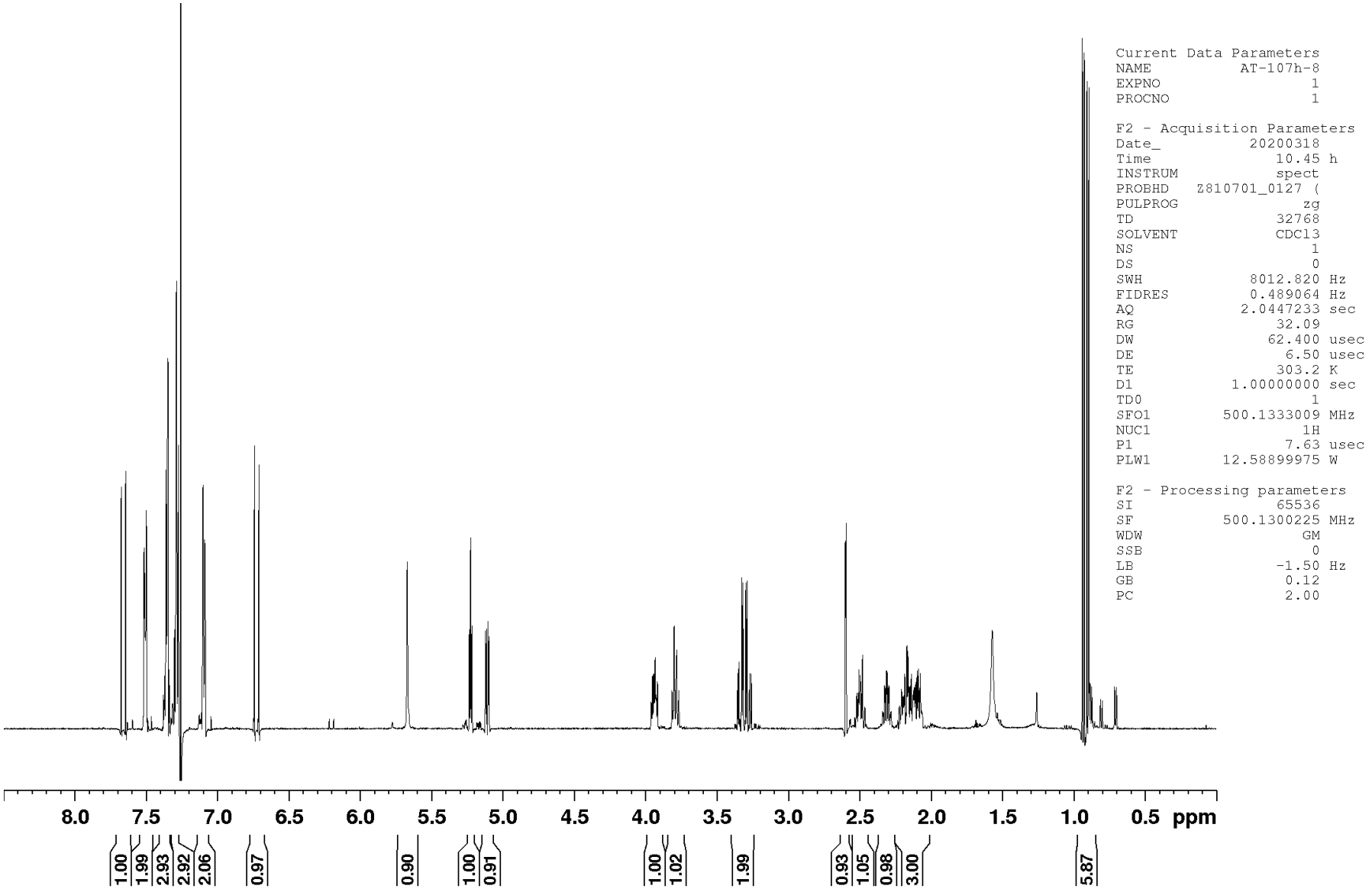
Figure S16. MS and MS/MS data of asterripeptide B (2)

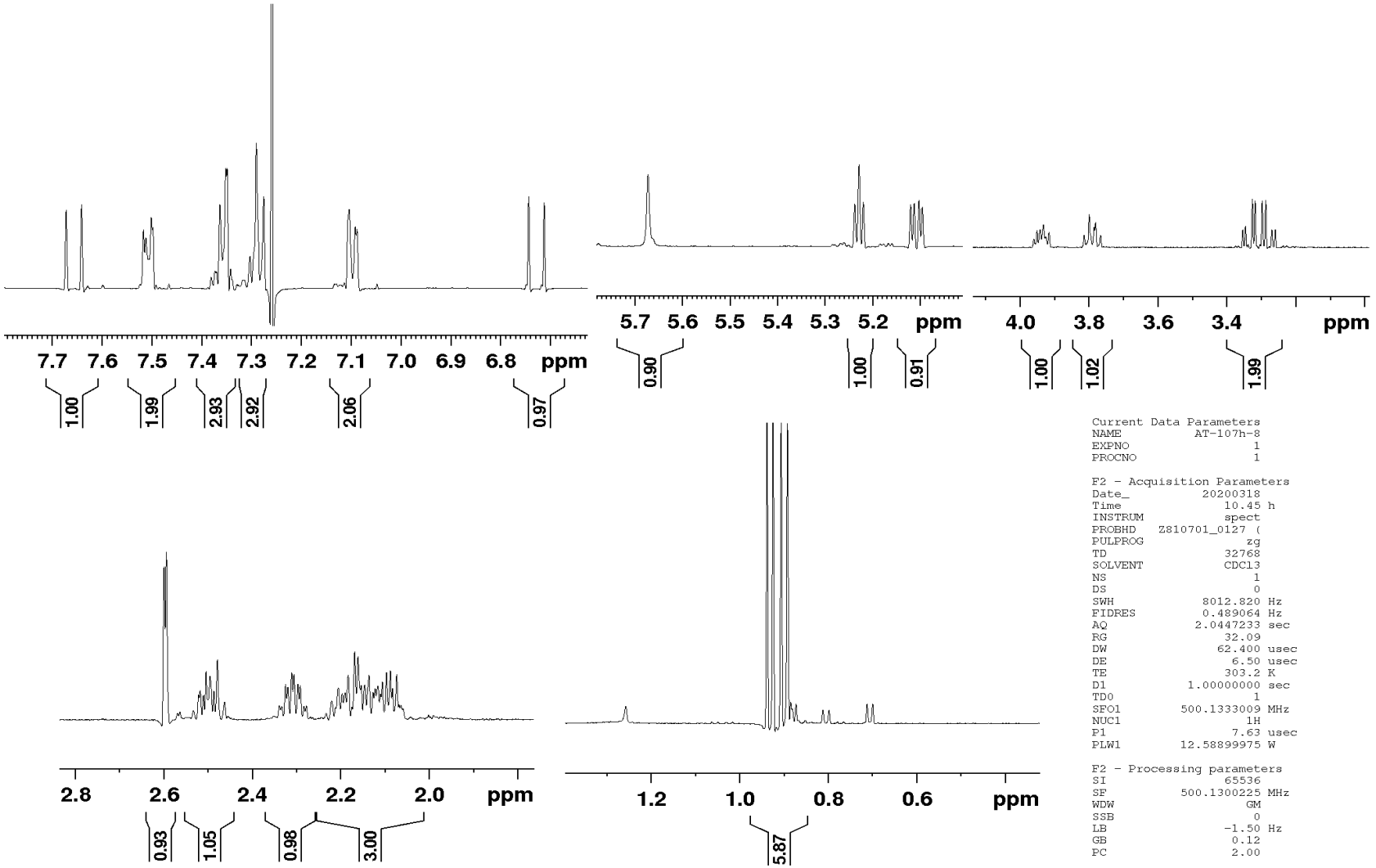




	meas.	calc.	Δ (ppm)
$[M-H]^-$	486,2374	486,2398	5,1
$[M+Na]^+$	510,2374	510,2363	-2,1

Figure S17. ^{1}H NMR spectrum of asterripeptide C (3)



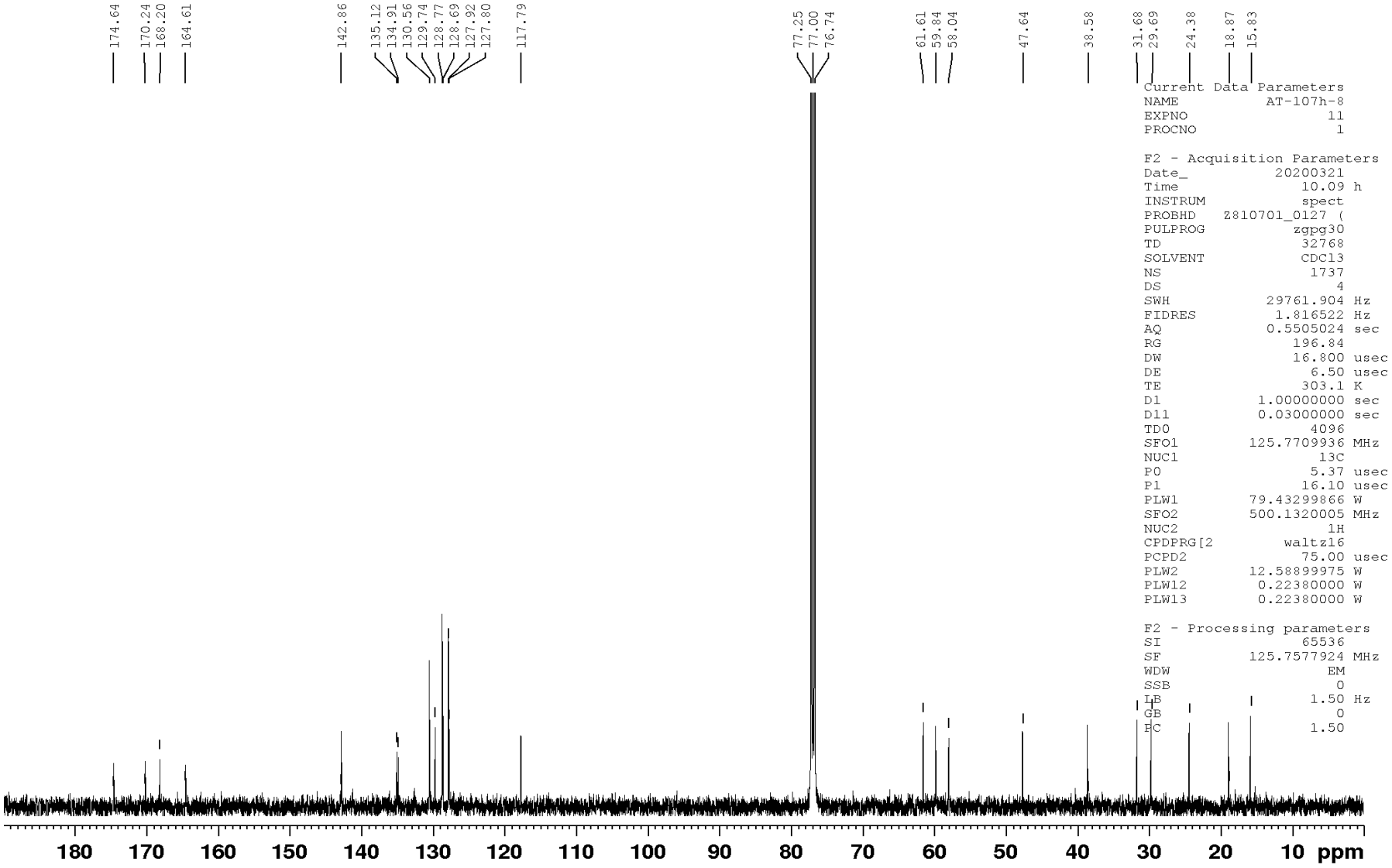



```
Current Data Parameters
NAME                 AT-107h-8
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20200318
Time                     10.45 h
INSTRUM                  spect
PROBHD    Z810701_0127 (
PULPROG                     zg
TD                       32768
SOLVENT                  CDCl3
NS                           1
DS                           0
SWH                   8012.820 Hz
FIDRES                0.489064 Hz
AQ                    2.0447233 sec
RG                       32.09
DW                       62.400 usec
DE                        6.50 usec
TE                       303.2 K
D1                 1.00000000 sec
TD0                          1
SFO1               500.1333009 MHz
NUC1                        1H
P1                        7.63 usec
PLW1               12.58899975 W

F2 - Processing parameters
SI                       65536
SF                 500.1300225 MHz
WDW                         GM
SSB                          0
LB                       -1.50 Hz
GB                        0.12
PC                        2.00
```

Figure S18. ^{13}C NMR spectrum of asterripeptide C (3)

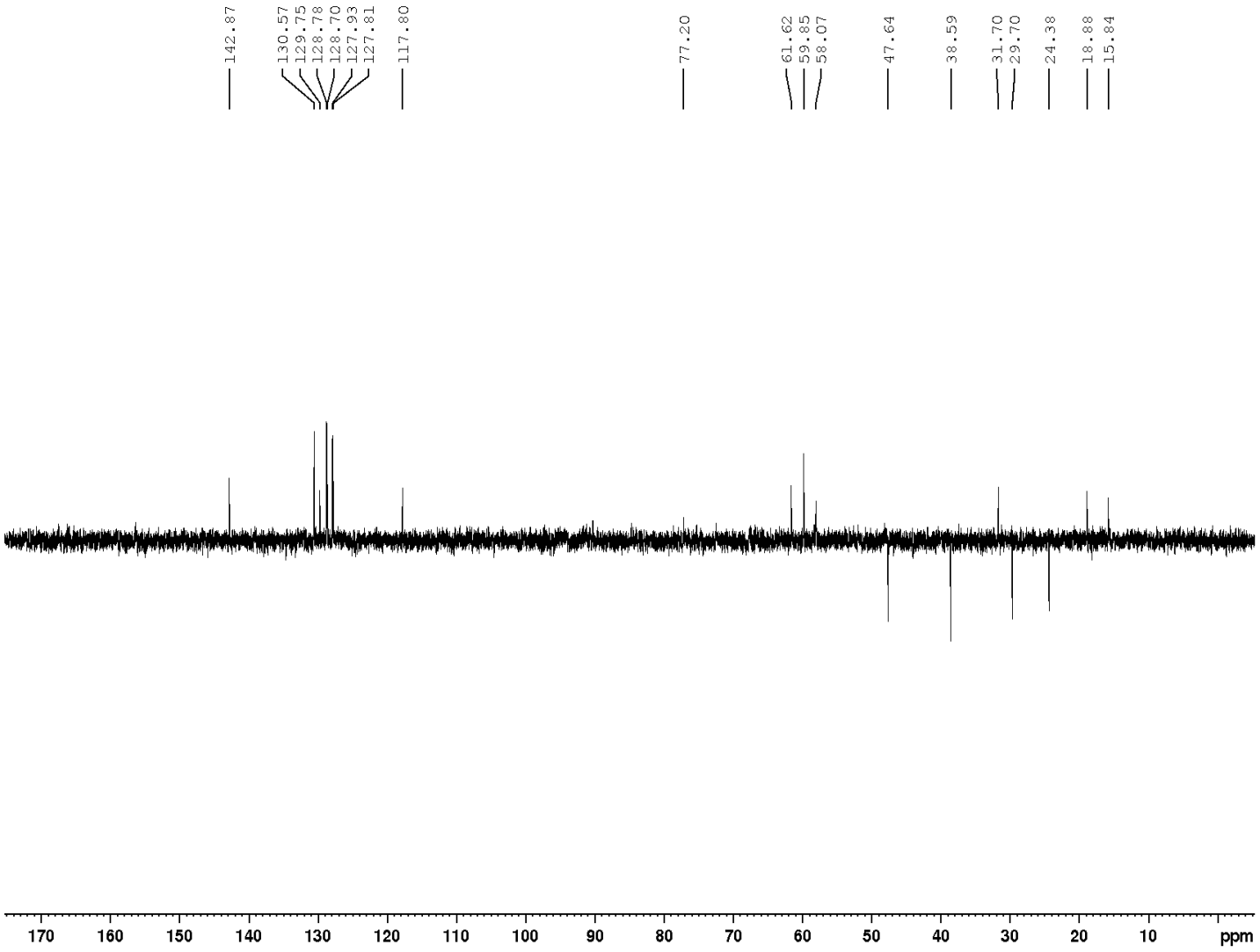



```
Current Data Parameters
NAME                  AT-107h-8
EXPNO                        11
PROCNO                        1

F2 - Acquisition Parameters
Date_                 20200321
Time                     10.09 h
INSTRUM                  spect
PROBHD    Z810701_0127 (
PULPROG                 zgpg30
TD                       32768
SOLVENT                  CDCl3
NS                        1737
DS                           4
SWH                  29761.904 Hz
FIDRES                1.816522 Hz
AQ                    0.5505024 sec
RG                       196.84
DW                       16.800 usec
DE                        6.50 usec
TE                       303.1 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                        4096
SFO1               125.7709936 MHz
NUC1                        13C
P0                        5.37 usec
P1                       16.10 usec
PLW1               79.43299866 W
SFO2               500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    75.00 usec
PLW2               12.58899975 W
PLW12               0.22380000 W
PLW13               0.22380000 W

F2 - Processing parameters
SI                         65536
SF                 125.7577924 MHz
WDW                           EM
SSB                            0
LB                         1.50 Hz
GB                             0
PC                         1.50
```

Figure S19. DEPT NMR spectrum of asterripeptide C (3)




```
Current Data Parameters
NAME                 AT-107h-8
EXPNO                       75
PROCNO                       1

F2 - Acquisition Parameters
Date_               20200322
Time                    7.53 h
INSTRUM                 spect
PROBHD   Z810701_0127 (
PULPROG             deptsp135
TD                      32768
SOLVENT                 CDCl3
NS                      26065
DS                          2
SWH                 22727.273 Hz
FIDRES               1.387163 Hz
AQ                  0.7208960 sec
RG                     196.84
DW                     22.000 usec
DE                      6.50 usec
TE                     303.2 K
CNST2              145.0000000
D1                  1.00000000 sec
D2                  0.00344828 sec
D12                 0.00002000 sec
TD0                      4096
SFO1               125.7684784 MHz
NUC1                       13C
P1                      16.10 usec
P13                   2000.00 usec
PLW0                        0 W
PLW1               79.43299866 W
SPNAM[5]           Crp60comp.4
SPOAL5                  0.500
SPOFFS5                     0 Hz
SPW5               31.45899963 W
SFO2               500.1320005 MHz
NUC2                       1H
CPDPRG[2               waltz16
P3                      10.50 usec
P4                      21.00 usec
PCPD2                   75.00 usec
PLW2               12.58899975 W
PLW12               0.24674000 W

F2 - Processing parameters
SI                      65536
SF                 125.7577911 MHz
WDW                        EM
SSB                         0
LB                      1.50 Hz
GB                          0
PC                      1.20
```

Figure S20. HSQC NMR spectrum of asterripeptide C (3)

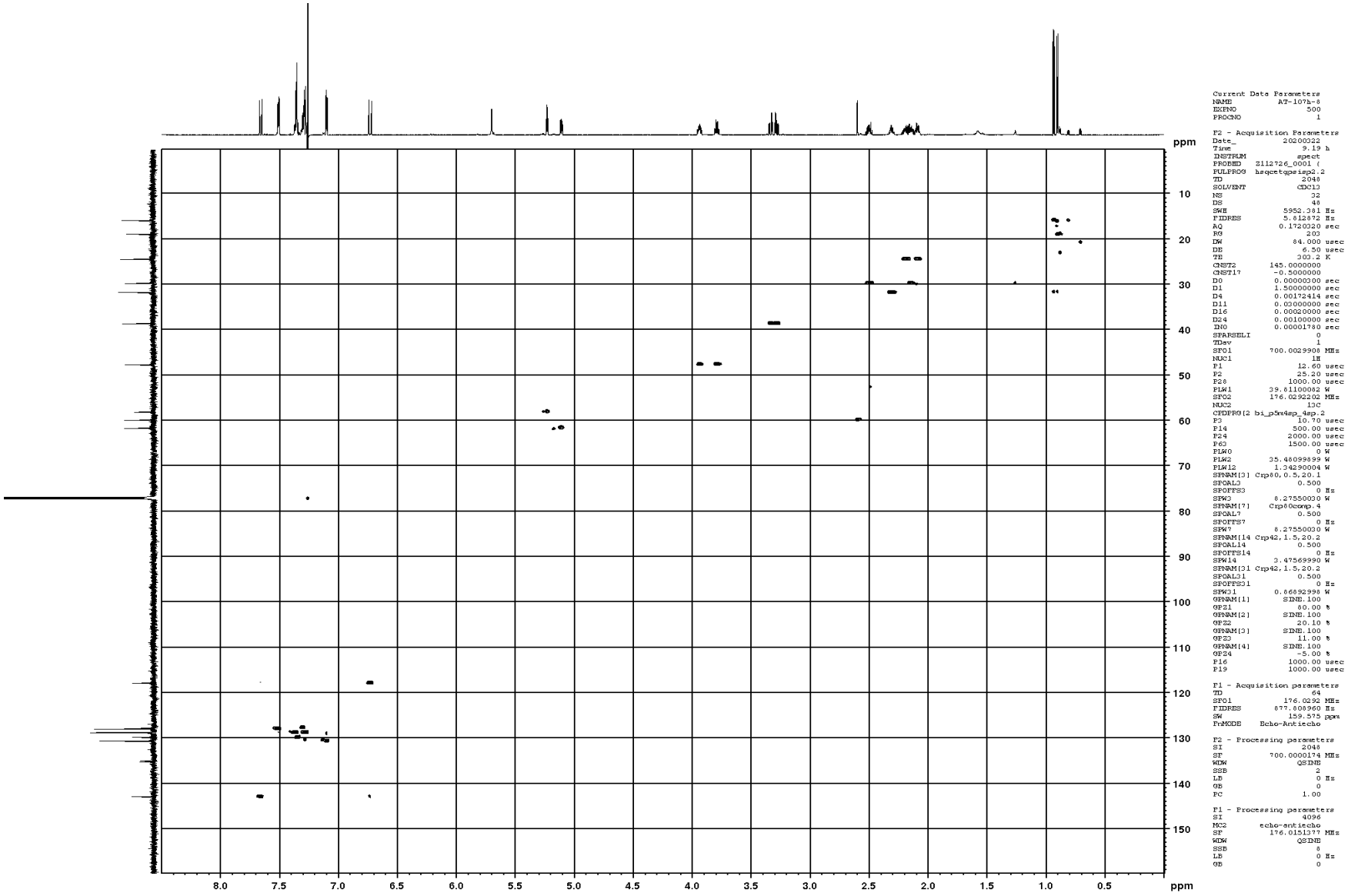
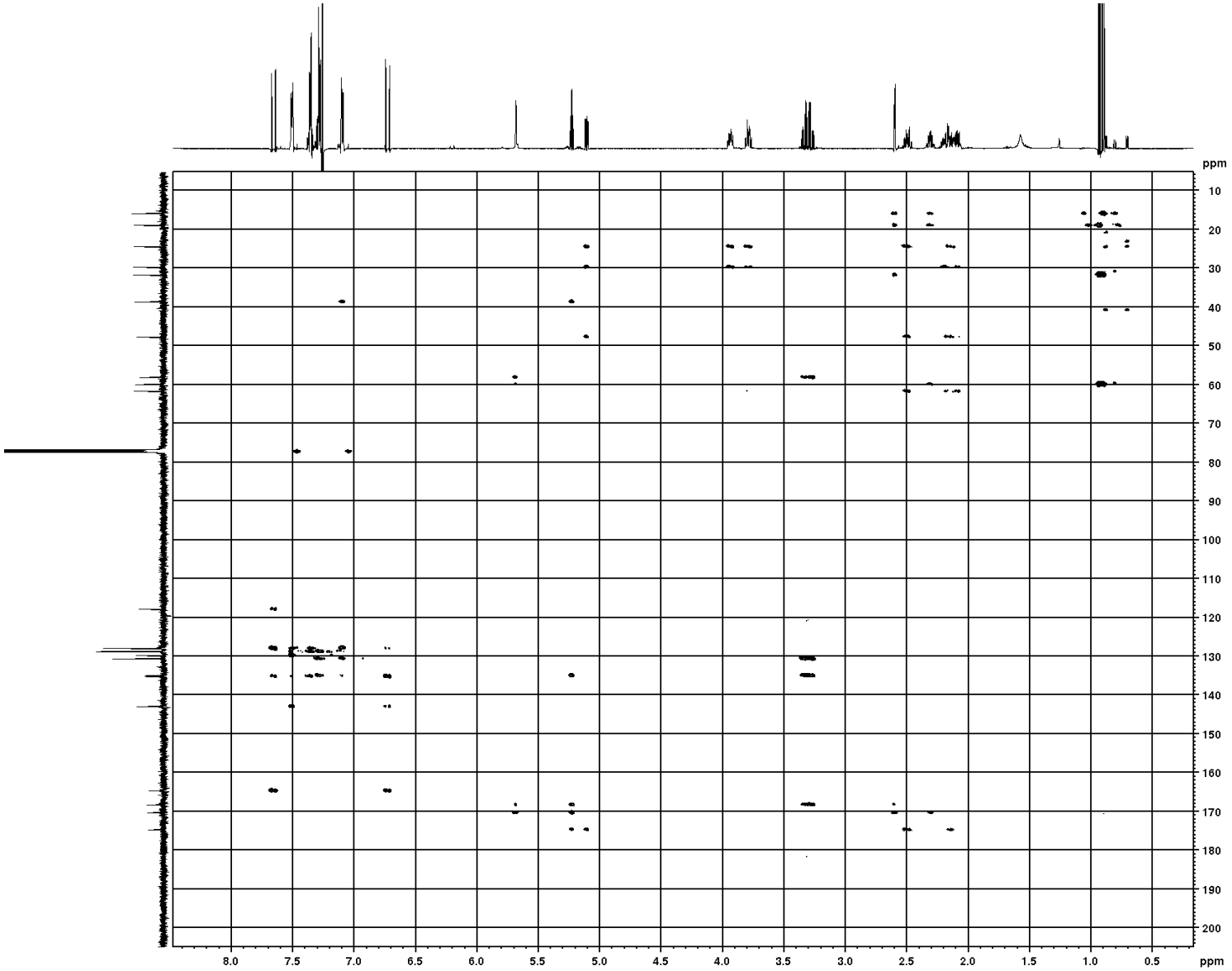


Figure S21. HMBC NMR spectrum of asterripeptide C (3)



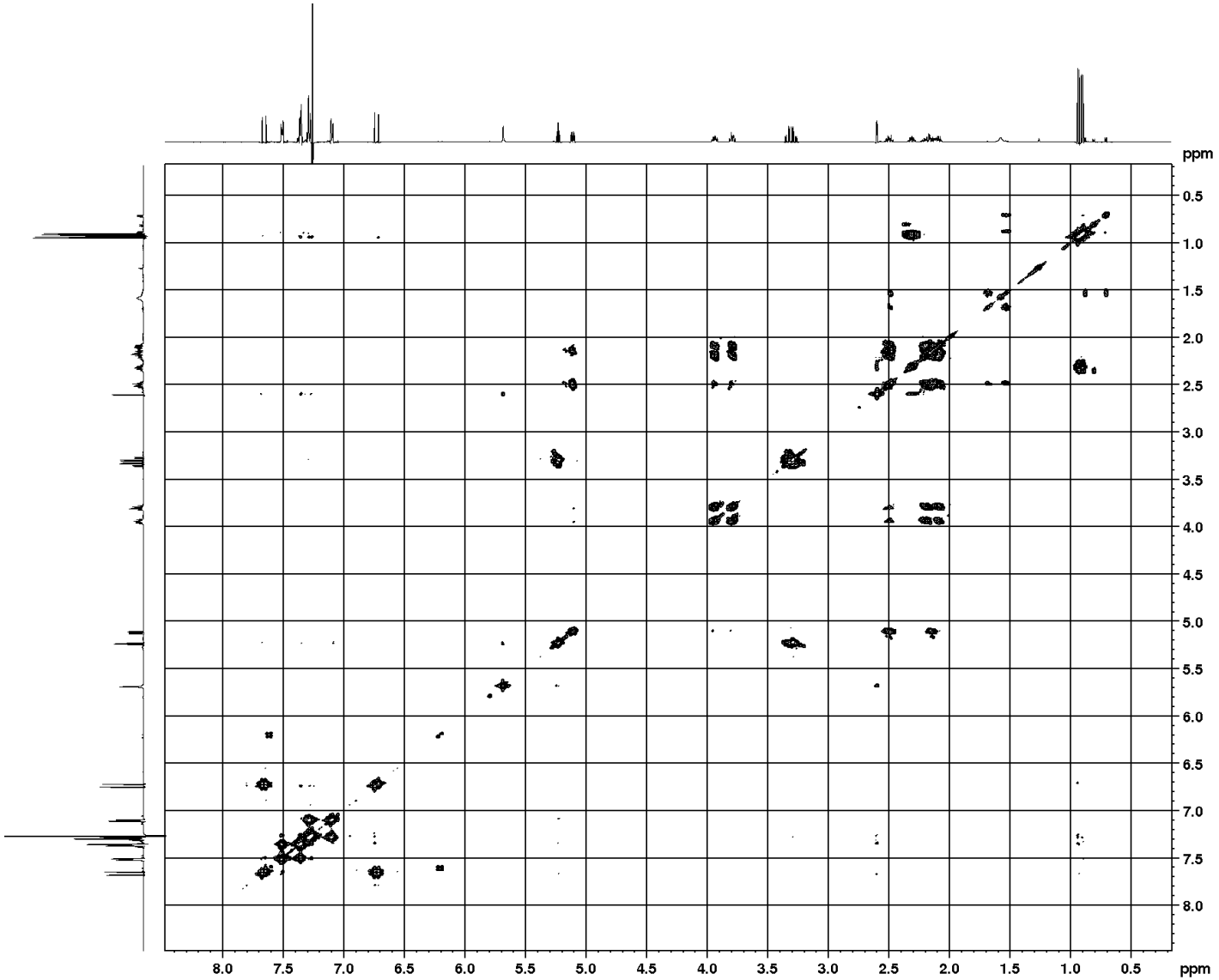

```
Current Data Parameters
NAME                 AT-107h-8
EXPNO                       24
PROCNO                       1

F2 - Acquisition Parameters
Date_               20200321
Time                    13.35 h
INSTRUM                  spect
PROBHD    Z810701_0127 (
PULPROG      hmbcgplpndqf
TD                       4096
SOLVENT                 CDCl3
NS                         32
DS                         16
SWH                 4157.428 Hz
FIDRES              2.029994 Hz
AQ                  0.4926123 sec
RG                     196.84
DW                    120.267 usec
DE                      6.50 usec
TE                     303.1 K
CNST2              145.0000000
CNST13               6.0000000
D0                  0.00000300 sec
D1                  1.50000000 sec
D2                  0.00344828 sec
D6                  0.08333334 sec
D16                 0.00010000 sec
IN0                 0.00001990 sec
SPARSELI                    0
TDav                        1
SFO1               500.1321834 MHz
NUC1                       1H
P1                       7.63 usec
P2                      15.26 usec
PLW1               12.58899975 W
SFO2               125.7709936 MHz
NUC2                       13C
P3                      17.80 usec
PLW2               79.43299866 W
GPNAM[1]            SMSQ10.100
GPZ1                    50.00 %
GPNAM[2]            SMSQ10.100
GPZ2                    30.00 %
GPNAM[3]            SMSQ10.100
GPZ3                    40.10 %
P16                   1000.00 usec

F1 - Acquisition parameters
TD                         73
SFO1                  125.771 MHz
FIDRES              688.373352 Hz
SW                    199.773 ppm
FnMODE                     QF

F2 - Processing parameters
SI                       2048
SF                 500.1300225 MHz
WDW                      SINE
SSB                         2
LB                          0 Hz
GB                          0
PC                       4.00
```

Figure S22. ^{1}H-^{1}H COSY NMR spectrum of asterripeptide C (3)

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Current Data Parameters
NAME            AT-107h-8
EXPNO                  21
PROCNO                  1

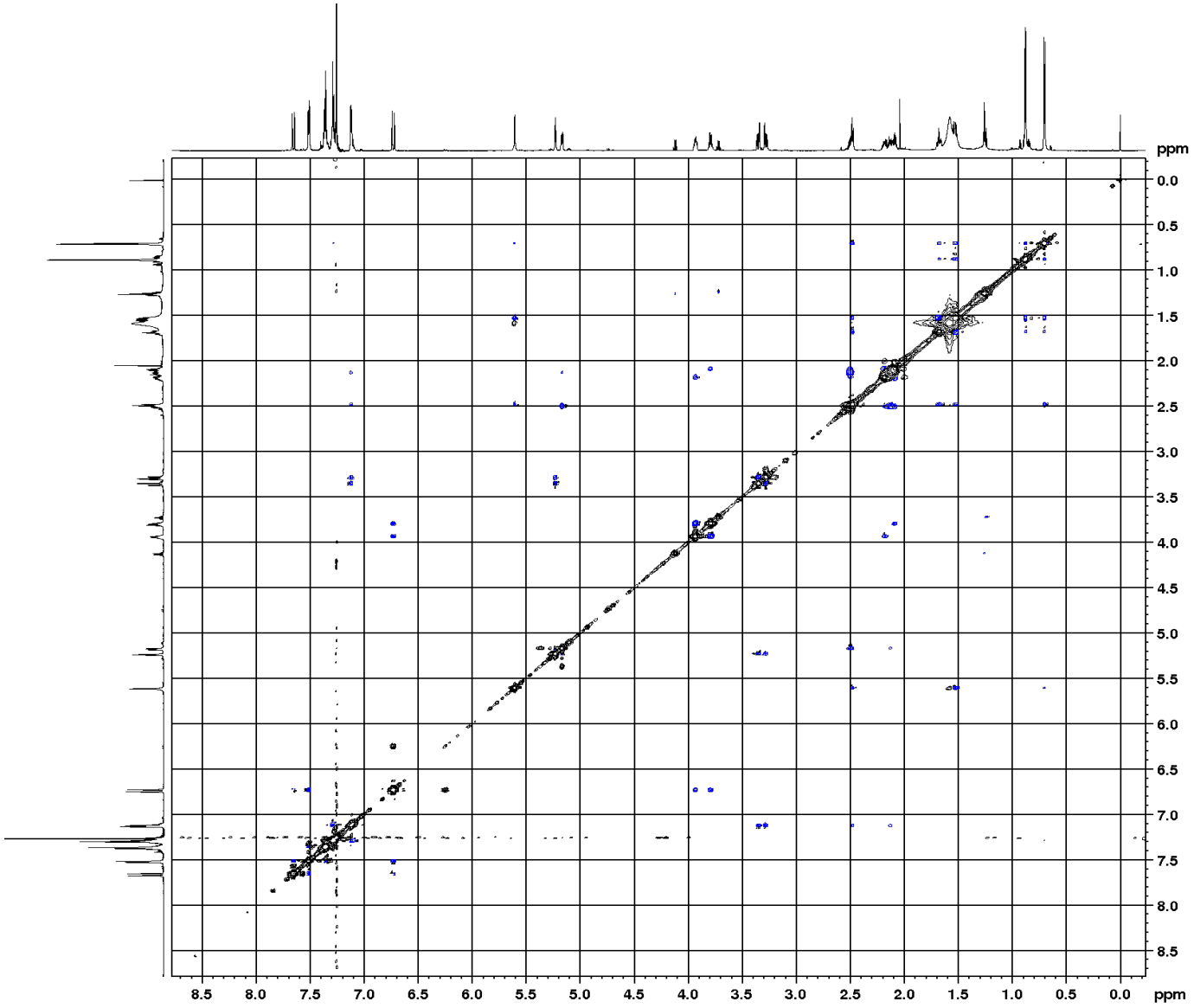
F2 - Acquisition Parameters
Date_            20200321
Time                10.43 h
INSTRUM              spect
PROBHD    Z810701_0127 (
PULPROG          cosygf45
TD                   2048
SOLVENT              CDCl3
NS                      4
DS                     16
SWH               4157.428 Hz
FIDRES            4.059988 Hz
AQ                0.2463061 sec
RG                   91.04
DW                 120.267 usec
DE                   6.50 usec
TE                  303.2 K
D0              0.00000300 sec
D1              2.00000000 sec
IN0             0.00024060 sec
SPARSELI                0
TDav                    1
SFO1          500.1321834 MHz
NUC1                   1H
P1                   7.63 usec
PLW1          12.58899975 W

F1 - Acquisition parameters
TD                    128
SFO1            500.1324 MHz
FIDRES          64.941811 Hz
SW                 8.310 ppm
FnMODE                 QF

F2 - Processing parameters
SI                   2048
SF            500.1300225 MHz
WDW                  SINE
SSB                     0
LB                      0 Hz
GB                      0
PC                   4.00

F1 - Processing parameters
SI                   2048
MC2                    QF
SF            500.1301891 MHz
WDW                  SINE
SSB                     0
LB                      0 Hz
GB                      0
```

Figure S23. ROESY NMR spectrum of asterripeptide C (3)

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Current Data Parameters
NAME                  AT-59h-4
EXPNO                     6030
PROCNO                       1

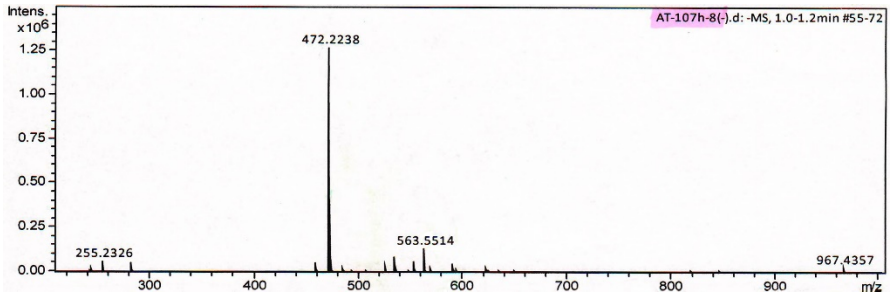
F2 - Acquisition Parameters
Date_                 20191101
Time                     17.28 h
INSTRUM                   spect
PROBHD    Z112726_0001 (
PULPROG              noesygpph
TD                        2048
SOLVENT                  CDCl3
NS                          16
DS                          16
SWH                   6313.131 Hz
FIDRES                6.165167 Hz
AQ                    0.1622016 sec
RG                          203
DW                       79.200 usec
DE                        6.50 usec
TE                       303.0 K
D0                    0.00006316 sec
D1                    1.00000000 sec
D8                    1.00000000 sec
D16                   0.00020000 sec
IN0                   0.00015840 sec
TDav                         1
SFO1               700.0030100 MHz
NUC1                        1H
P1                       12.60 usec
P2                       25.20 usec
PLW1              39.81100082 W
GPNAM[1]             SINE.100
GP21                     20.00 %
P16                    1000.00 usec

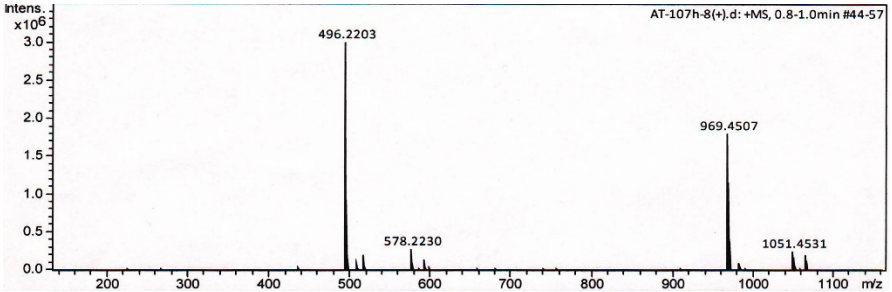
F1 - Acquisition parameters
TD                        256
SFO1                700.003 MHz
FIDRES             49.321339 Hz
SW                     9.019 ppm
FnMODE                  TPPI

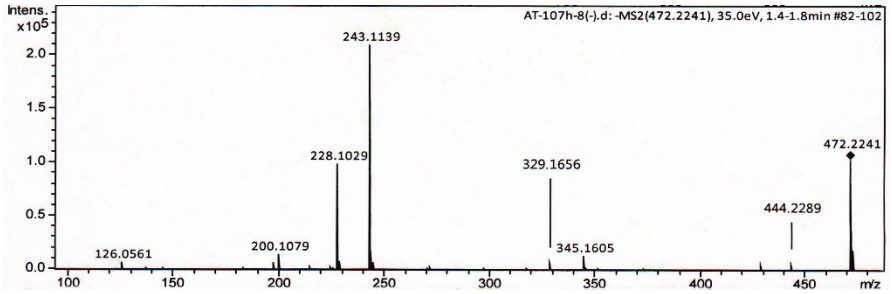
F2 - Processing parameters
SI                        2048
SF                 700.0000182 MHz
WDW                      QSINE
SSB                         2
LB                          0 Hz
GB                          0
PC                       1.00

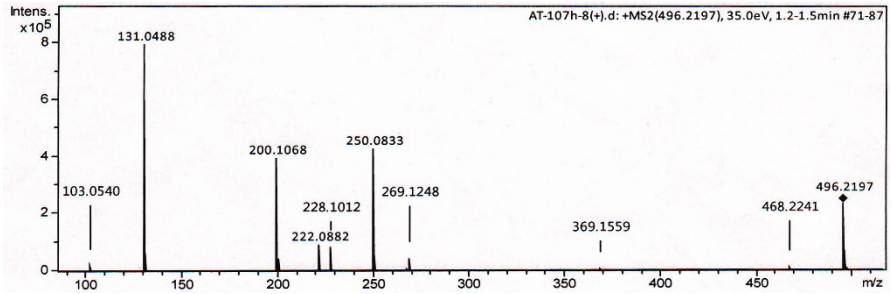
F1 - Processing parameters
SI                        2048
MC2                     TPPI
SF                 700.0000168 MHz
WDW                      QSINE
SSB                         2
LB                          0 Hz
GB                          0
```

Figure S24. MS and MS/MS data of asterripeptide C (3)



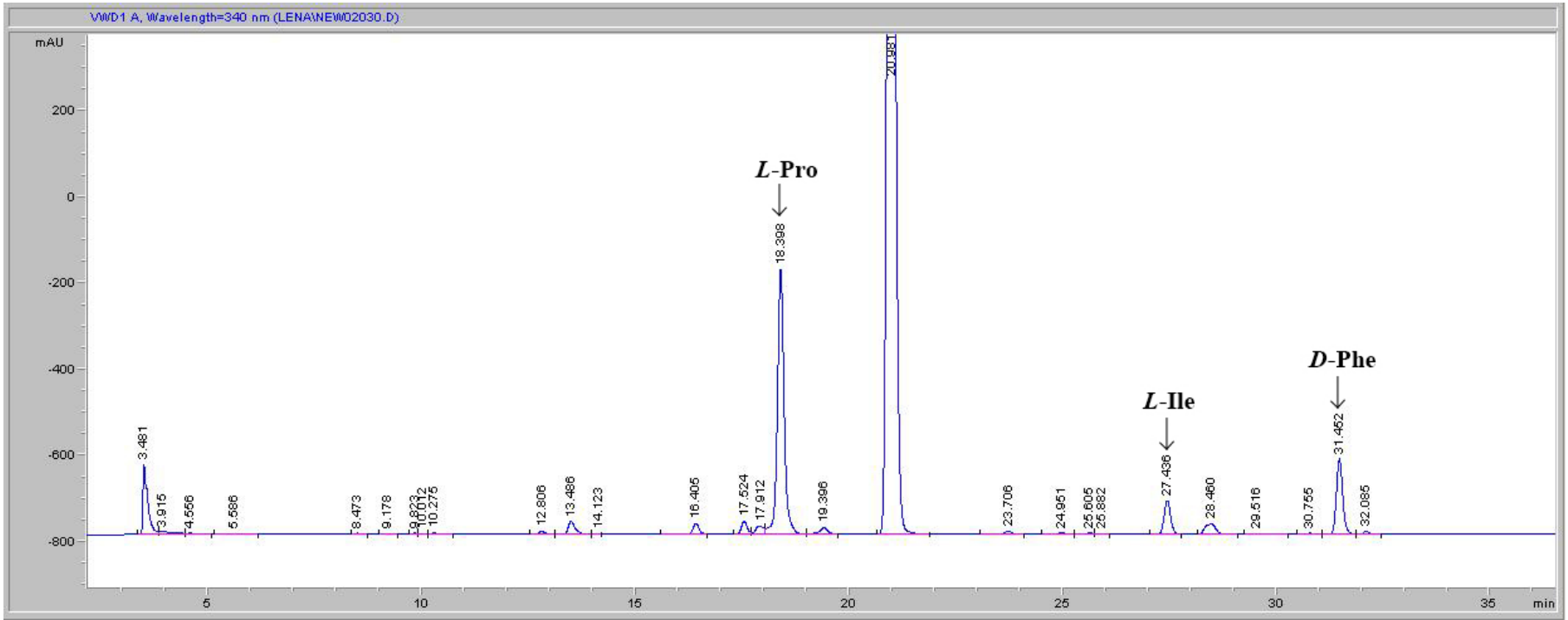






	meas.	calc.	Δ (ppm)
$[M-H]^-$	472.2238	472.2242	0.7
$[M+Na]^+$	496.2203	496.2207	0.8

Figure S25. HPLC profile of *L*-FDAA-derivatives of asterripeptide A (1) hydrolysis products (HP)



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File Path	C:\HPCHEM\1\DATA\LENA\
Date	23-Dec-21, 11:32:13
Sample	AT-59h-1
Sample Info	
Barcode	
Operator	Rimma
Method	MURFY.M
Analysis Time	54.983 min
Sampling Rate	0.0049 min (0.294 sec), 11330 datapoints

#	Time	Area	Height	Width	Symmetry
1	3.481	1447.8	163.6	0.1164	0.233
2	3.915	156.4	6.9	0.2819	0.145
3	4.556	60.8	3	0.2587	0.291
4	5.586	55.1	2	0.3406	1.728
5	8.473	20.1	2.4	0.1255	0.83
6	9.178	18.7	1.7	0.1573	0.622
7	9.823	25.1	3	0.1278	0.911
8	10.012	18.9	2.2	0.1262	0.869
9	10.275	43.2	3.9	0.1594	0.543
10	12.806	81.6	7.3	0.1604	1.062
11	13.486	340.7	29.9	0.1679	0.664
12	14.123	17.4	1.9	0.1321	0.968
13	16.405	273.3	25.9	0.1565	1.035
14	17.524	291.8	30.1	0.148	0.866
15	17.912	259	18.5	0.2083	1.191
16	18.398	6653	614.4	0.1627	0.918

Figure S26. HPLC profile of *L*-FDAA-derivatives of asterripeptide A (1) HP (a), asterripiptide A HP+*L*-Ile (b) and asterripiptide A HP+*D*,*L*-Ile (c)

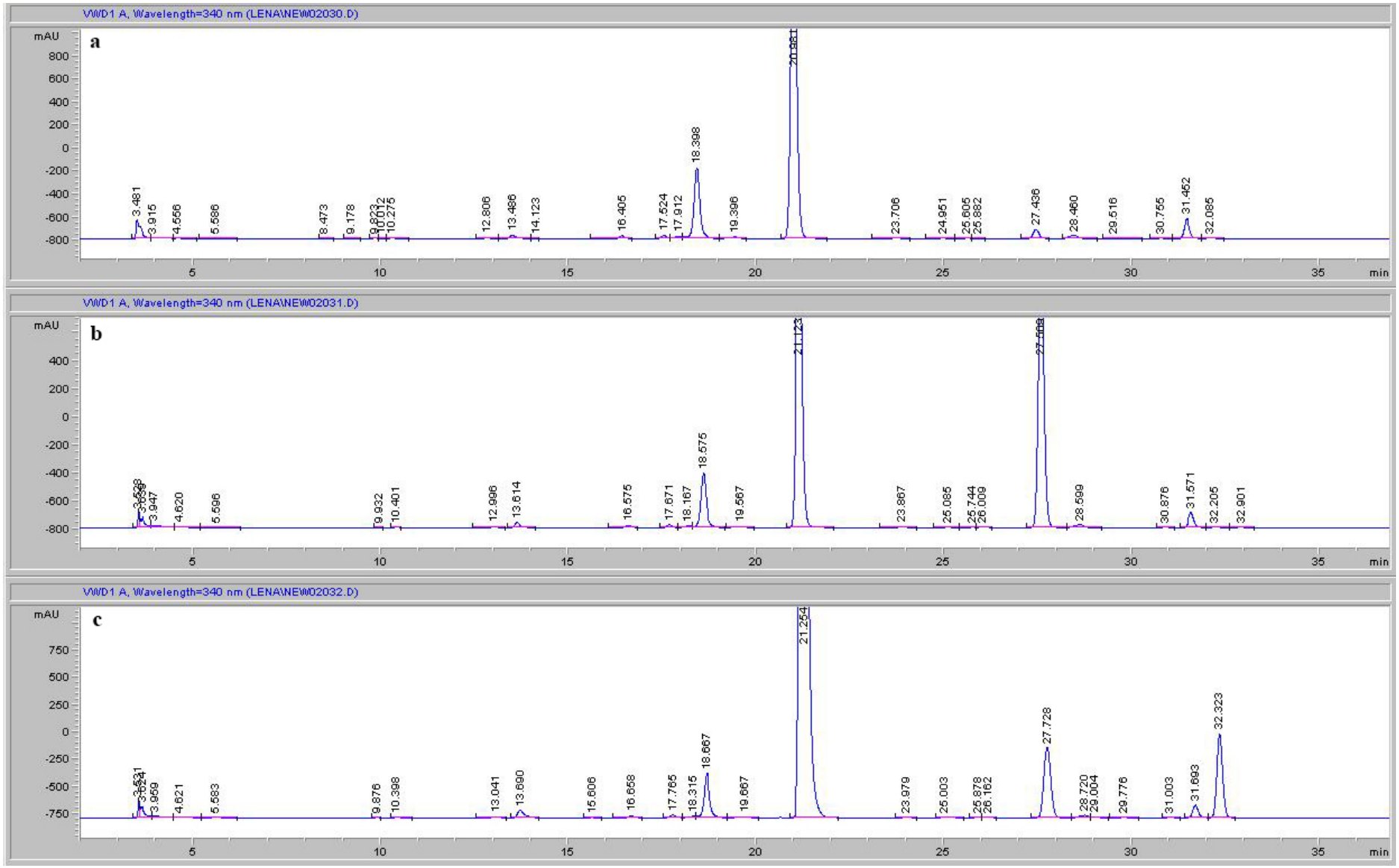


Figure S27. HPLC profile of *L*-FDAA-derivatives of asterripeptide A (1) HP, asterripiptide A HP+*L*-Phe and asterripiptide A HP+*D*,*L*-Phe

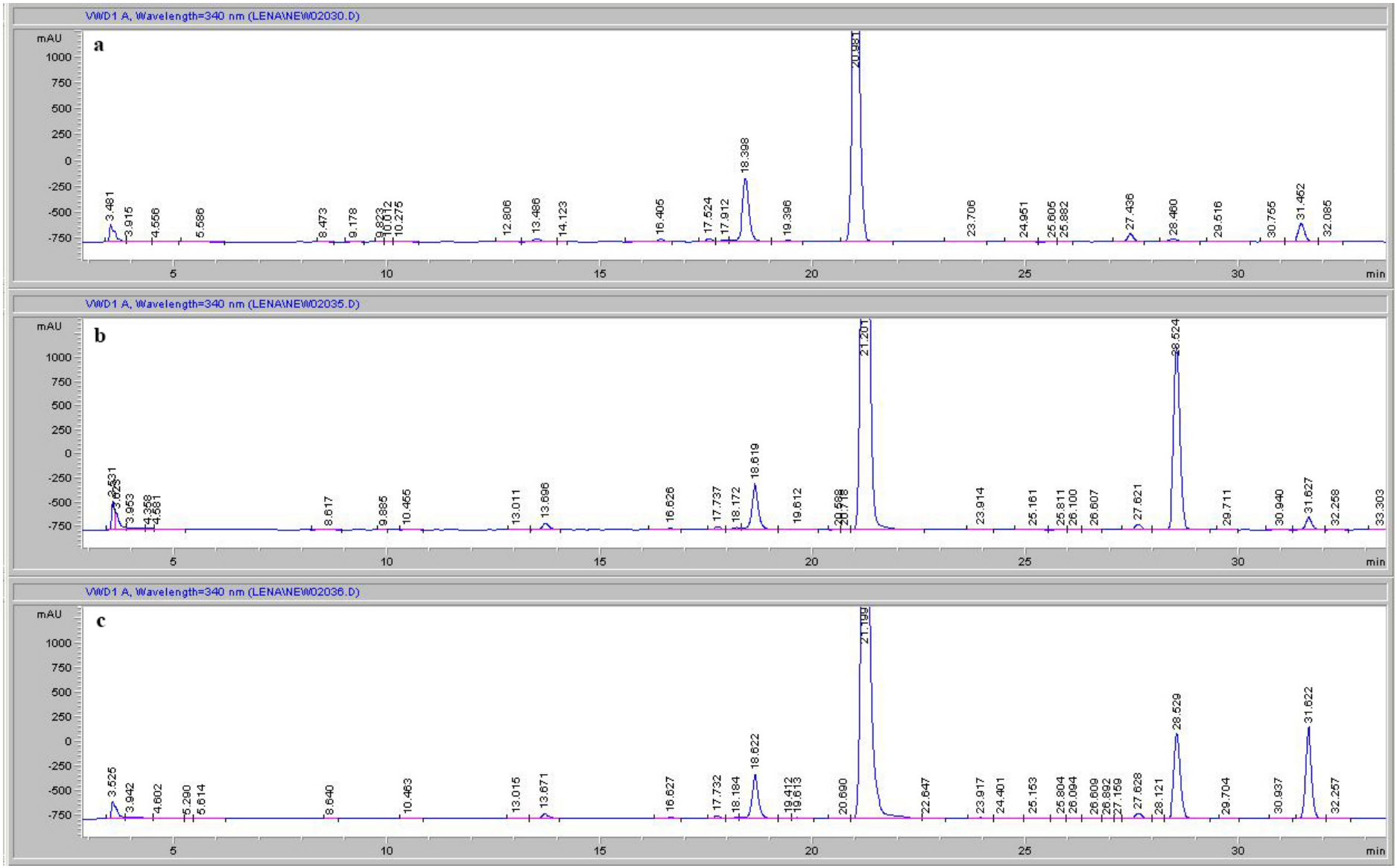


Figure S28. HPLC profile of *L*-FDAA-derivatives of asterripeptide A (1) HP, asterripiptide A HP+*D*,*L*-Pro and asterripiptide A HP+*L*-Pro

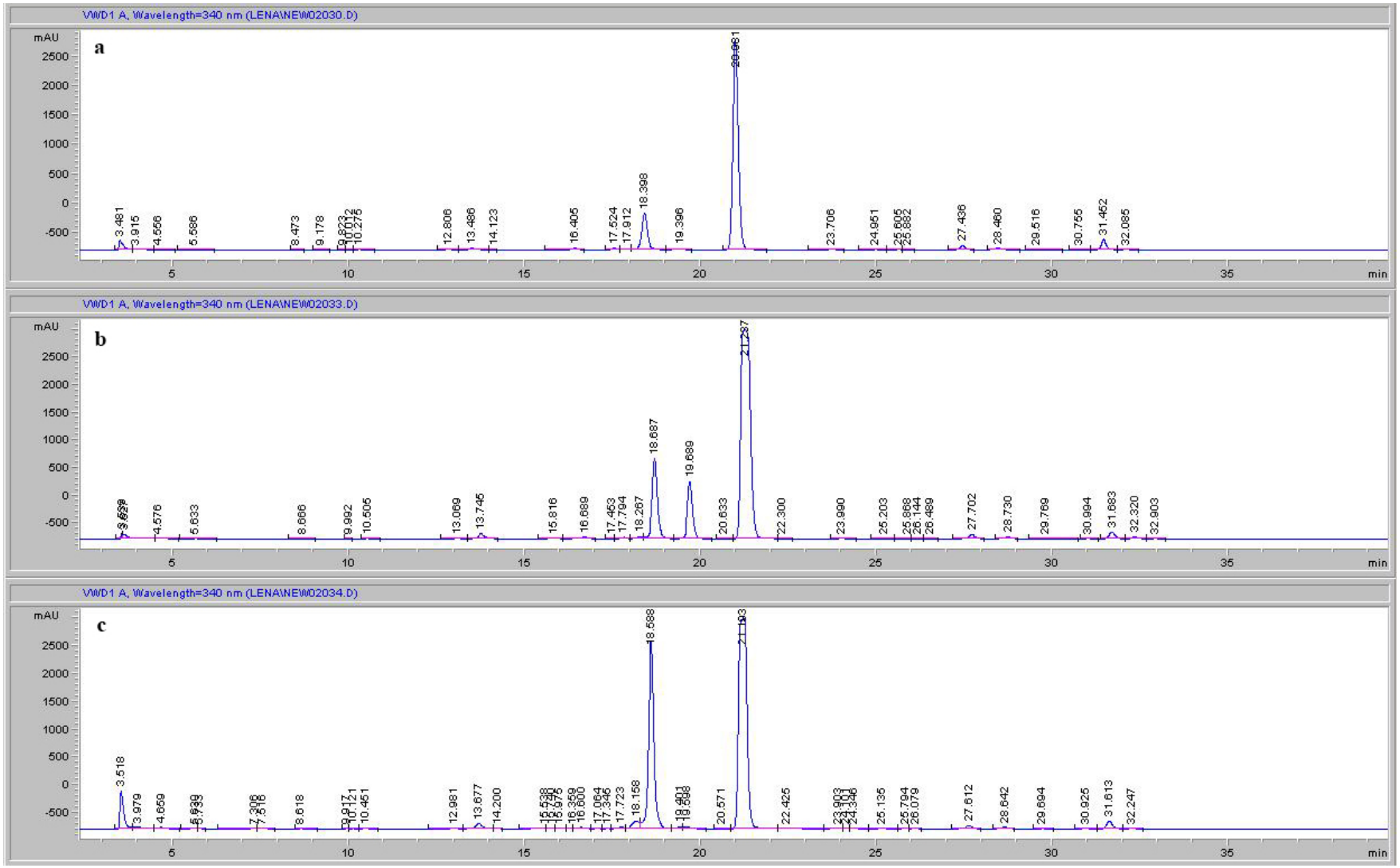
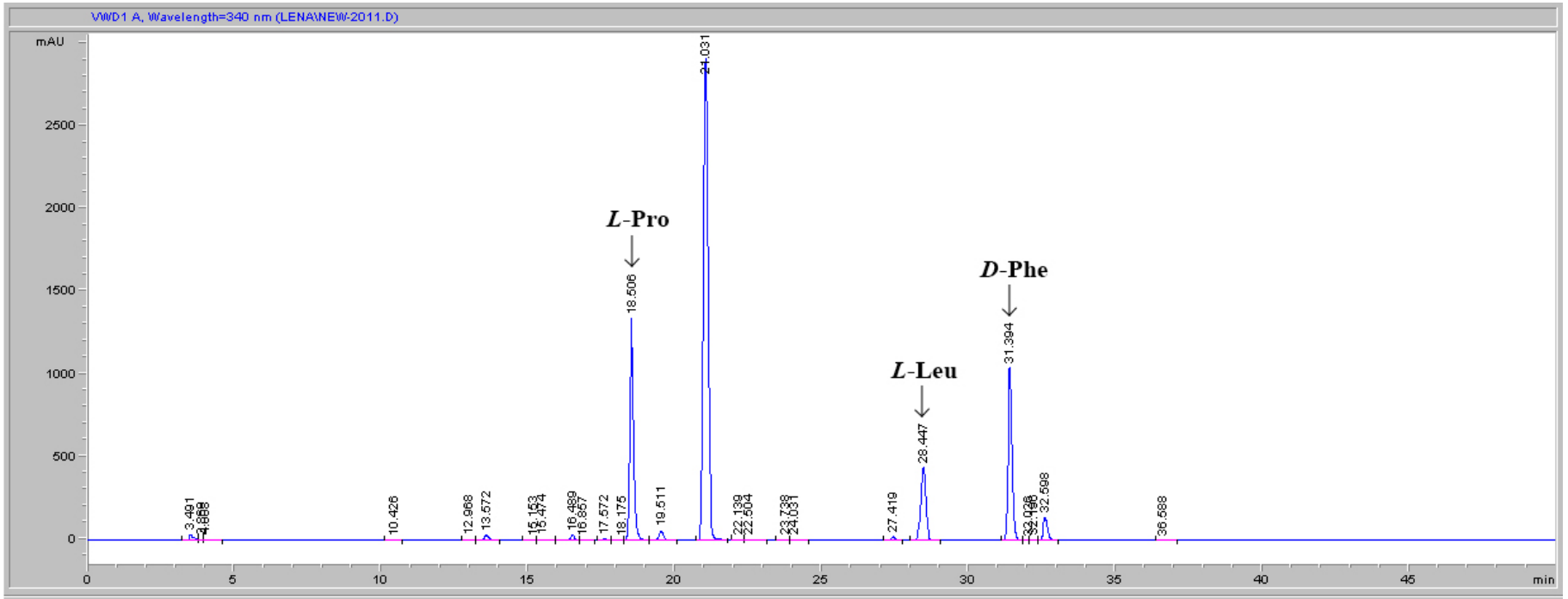


Figure S29. HPLC profile of *L*-FDAA-derivatives of asterripeptide B (2) HP



File Information	
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File Path	C:\HPCHEM\1\DATA\LENA\
Date	12-Oct-21, 13:02:18
Sample	Sample-1_new
Sample Info	
Barcode	
Operator	Rimma
Method	MURFY.M
Analysis Time	49.984 min
Sampling Rate	0.0049 min (0.294 sec), 10300 datapoints

#	Time	Area	Height	Width	Symmetry
1	3.491	332.2	37.8	0.1228	0.331
2	3.869	46.6	4.7	0.1361	1.175
3	4.008	88.4	4.2	0.2628	0.17
4	10.426	22.5	2.4	0.1365	1.089
5	12.968	61.6	4.8	0.2038	1.062
6	13.572	316.9	31.9	0.1478	0.789
7	15.153	34.9	2.1	0.2217	1.776
8	15.474	80.5	4.5	0.2431	0.472
9	16.489	312.9	30.9	0.1531	0.89
10	16.857	22.2	1.8	0.1771	0.686
11	17.572	87.1	8.6	0.1559	0.909
12	18.175	24.4	1.9	0.1834	2.265
13	18.506	12902.5	1341.3	0.1472	0.819
14	19.511	563.2	55.2	0.1524	0.892
15	21.031	30371.8	2920.2	0.1607	0.864

Figure S30. HPLC profiles of *L*-FDAA-derivatives of asterripeptide B (2) HP (a), asterripiptide B HP+*L*-Leu (b) and asterripiptide B HP+*D*,*L*-Leu (c)

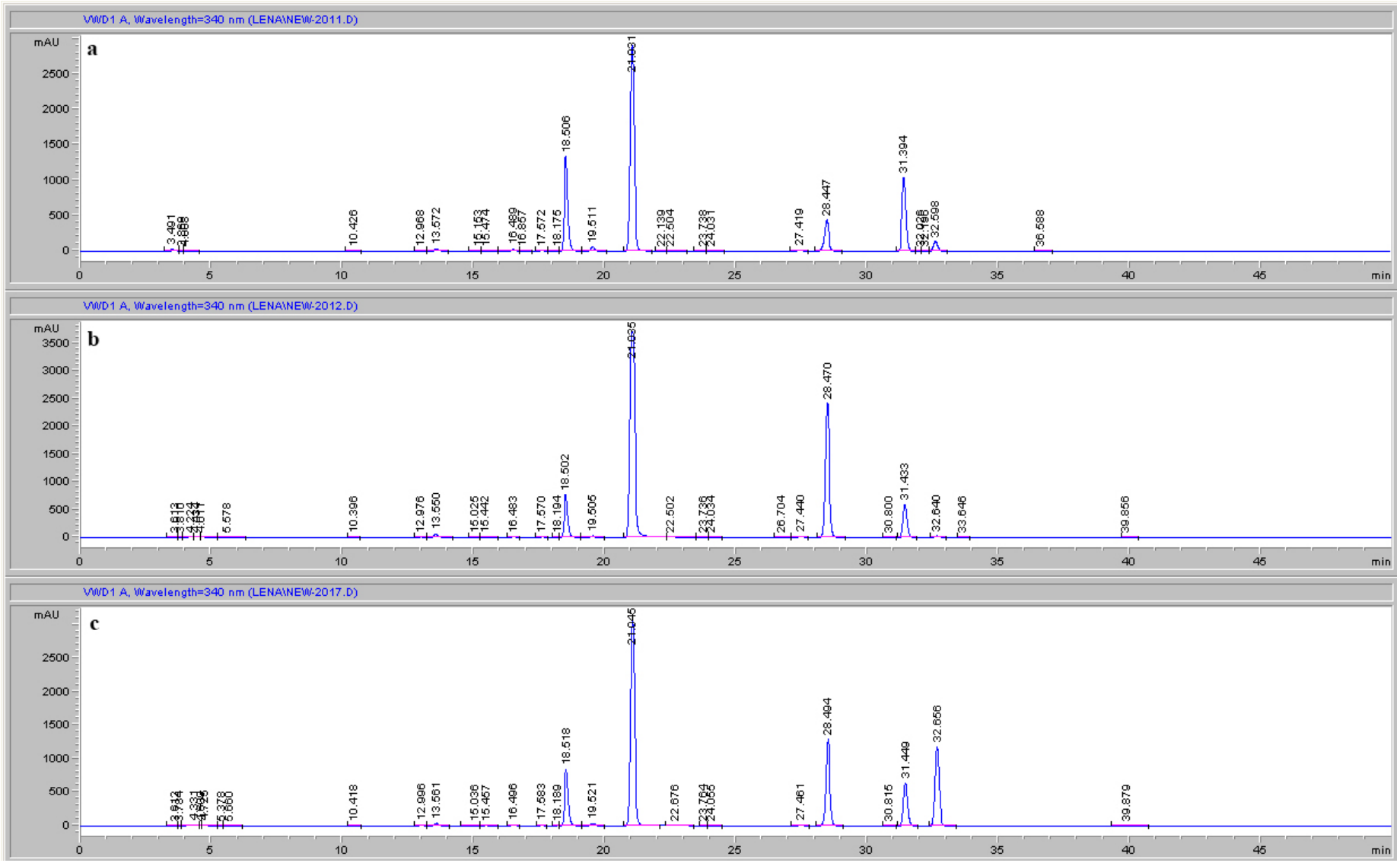


Figure S31. HPLC profiles of *L*-FDAA-derivatives of asterripeptide B (2) HP (a), asterripiptide B+ *D,L*-Pro (b) and asterripiptide B+ *L*-Pro (c)

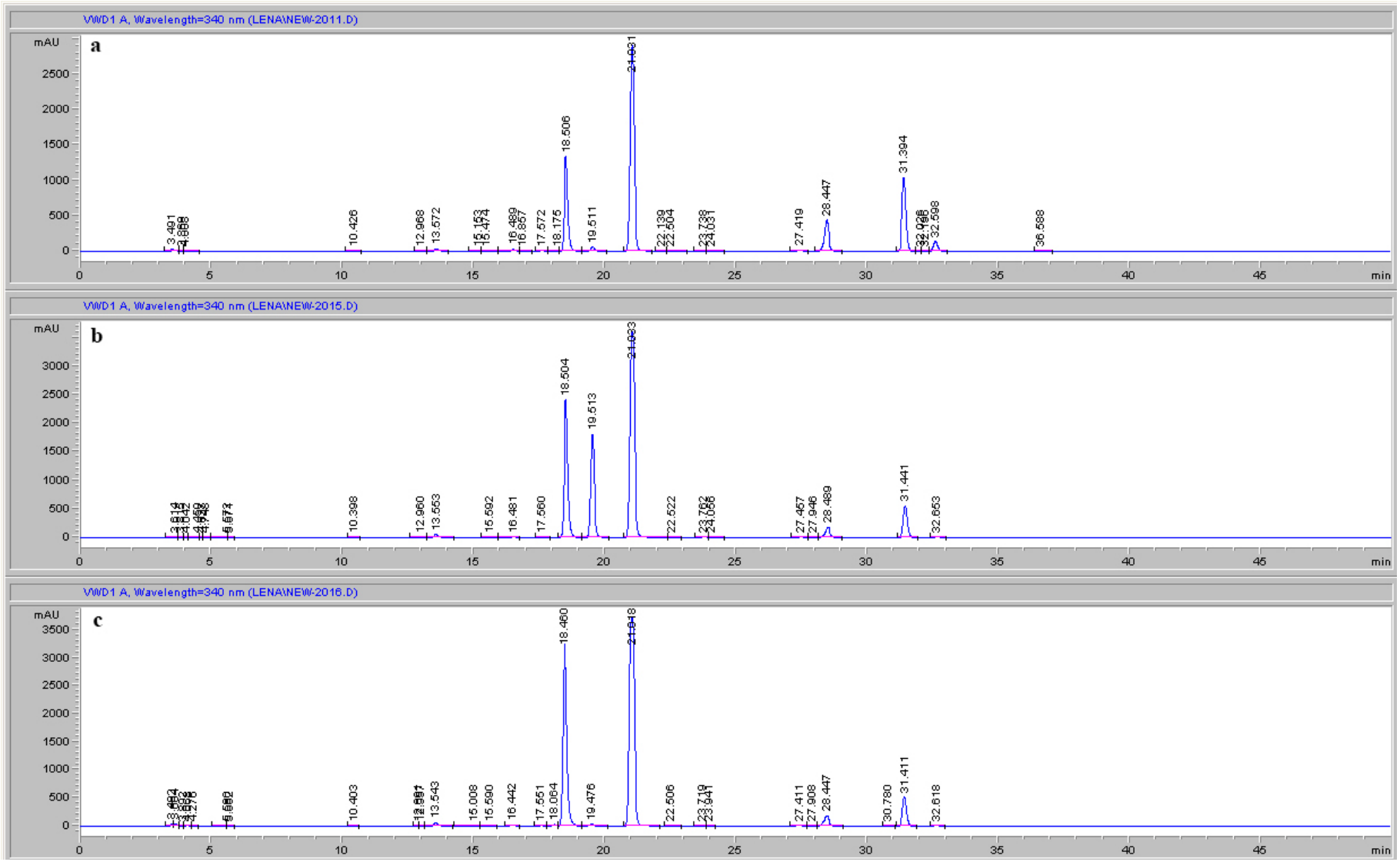


Figure S32. HPLC profiles of *L*-FDAA-derivatives of asterripeptide B (2) HP (a), asterripiptide B HP+ *L*-Phe (b) and asterripiptide B HP+ *D*,*L*-Phe (c)

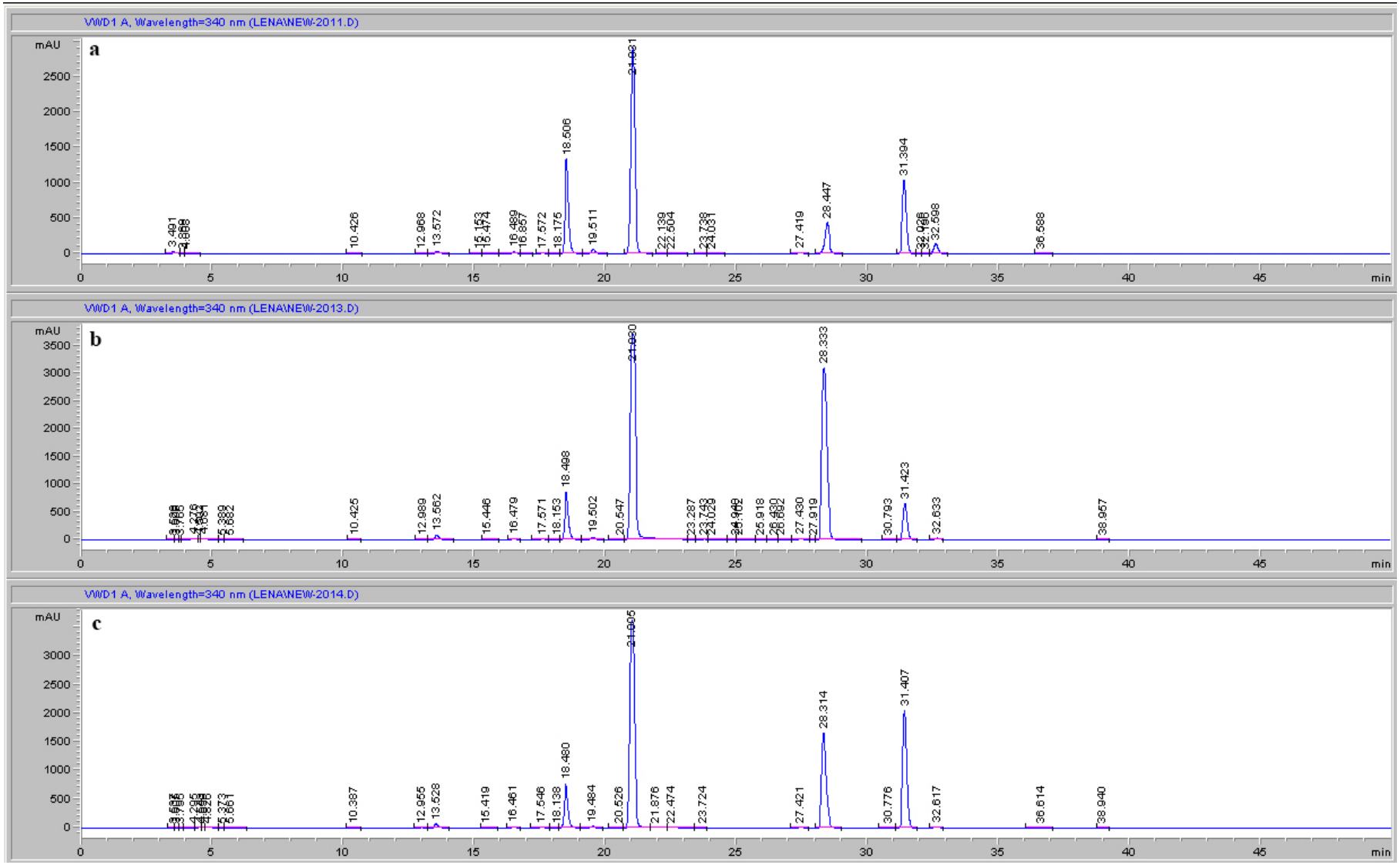
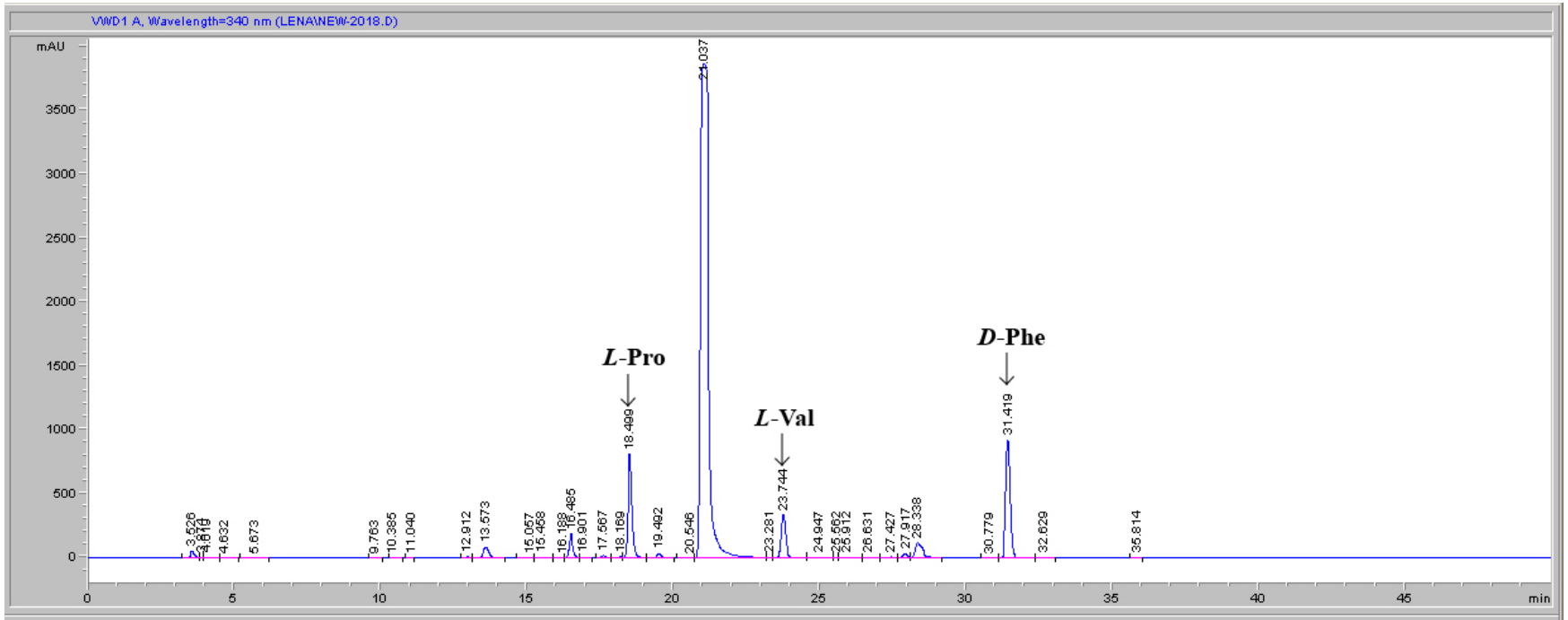


Figure S33. HPLC profile of *L*-FDAA-derivatives of asterripeptide C (3) HP



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Date	13-Oct-21, 11:26:27
Sample	Sample2_
Sample Info	
Barcode	
Operator	Rimma
Method	MURFY.M
Analysis Time	49.994 min
Sampling Rate	0.0049 min (0.294 sec), 10302 datapoints

#	Time	Area	Height	Width	Symmetry
1	3.526	523.7	57	0.1276	0.431
2	3.874	45.6	5.9	0.1049	0.59
3	4.019	134.9	5.4	0.3133	0.15
4	4.632	54.9	2.4	0.2965	0.402
5	5.673	61.1	2.6	0.2999	2.577
6	9.763	19.2	2.1	0.1411	0.833
7	10.385	28.6	3	0.1392	0.701
8	11.04	20.7	2.7	0.1183	0.812
9	12.912	109.7	9.7	0.1731	0.666
10	13.573	1097.4	87.5	0.1915	0.672
11	15.057	48.6	2.1	0.3354	1.417
12	15.458	114.7	7.8	0.2068	0.719
13	16.188	30.9	2.4	0.2014	2.018
14	16.485	1773.5	188.4	0.1448	0.805
15	16.901	57.3	5	0.1685	0.747

Figure S34. HPLC profiles of *L*-FDAA-derivatives of asterripeptide C (3) HP (a), asterripiptide C+*L*-Val H (b)P and asterripiptide C HP+*D*,*L*-Val (c)

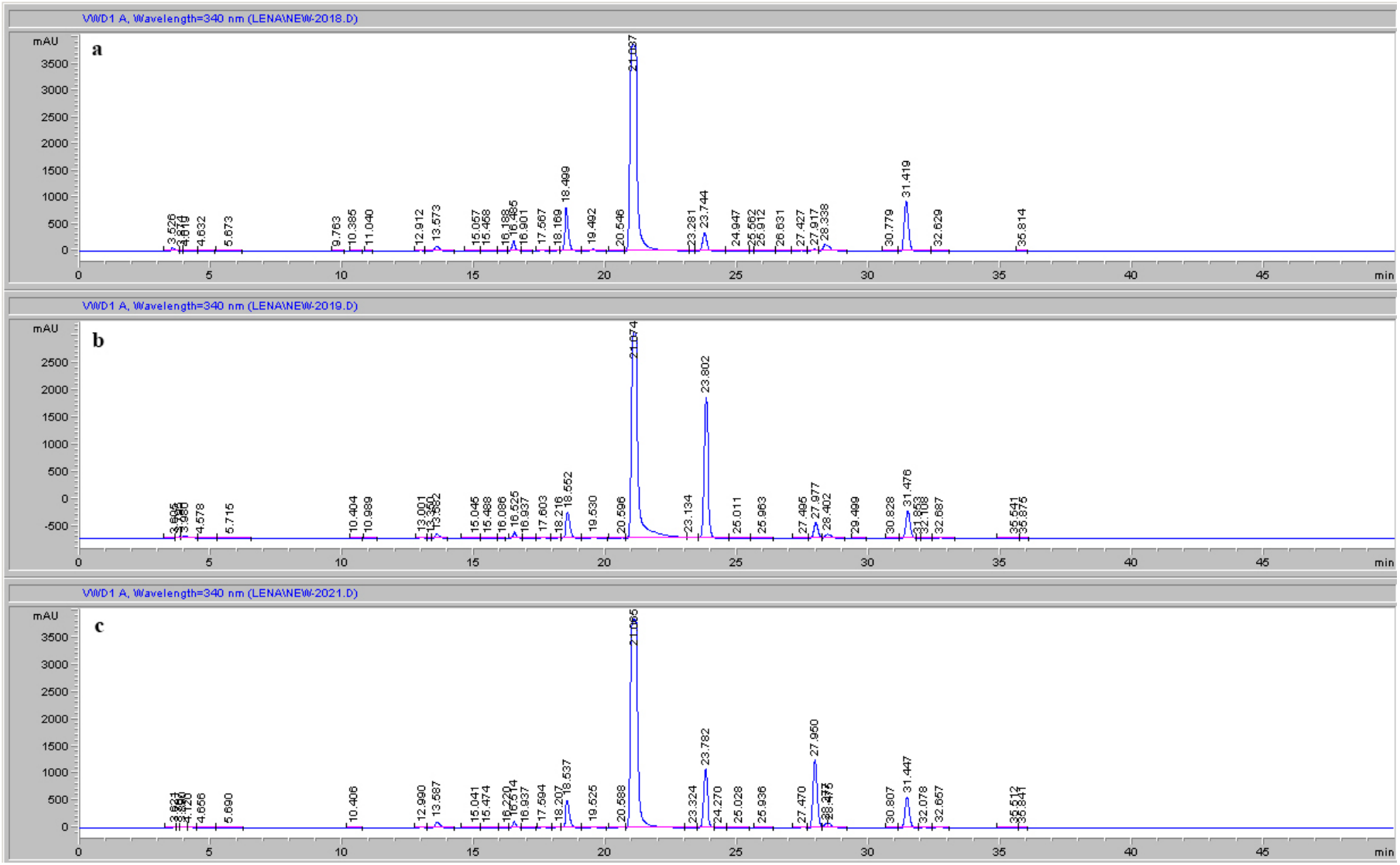

Figure S35. HPLC profiles of *L*-FDAA-derivatives of asterripeptide C (3) HP (a), asterripiptide C HP+*L*-Pro (b) and asterripiptide C HP+*D*,*L*-Pro (c)

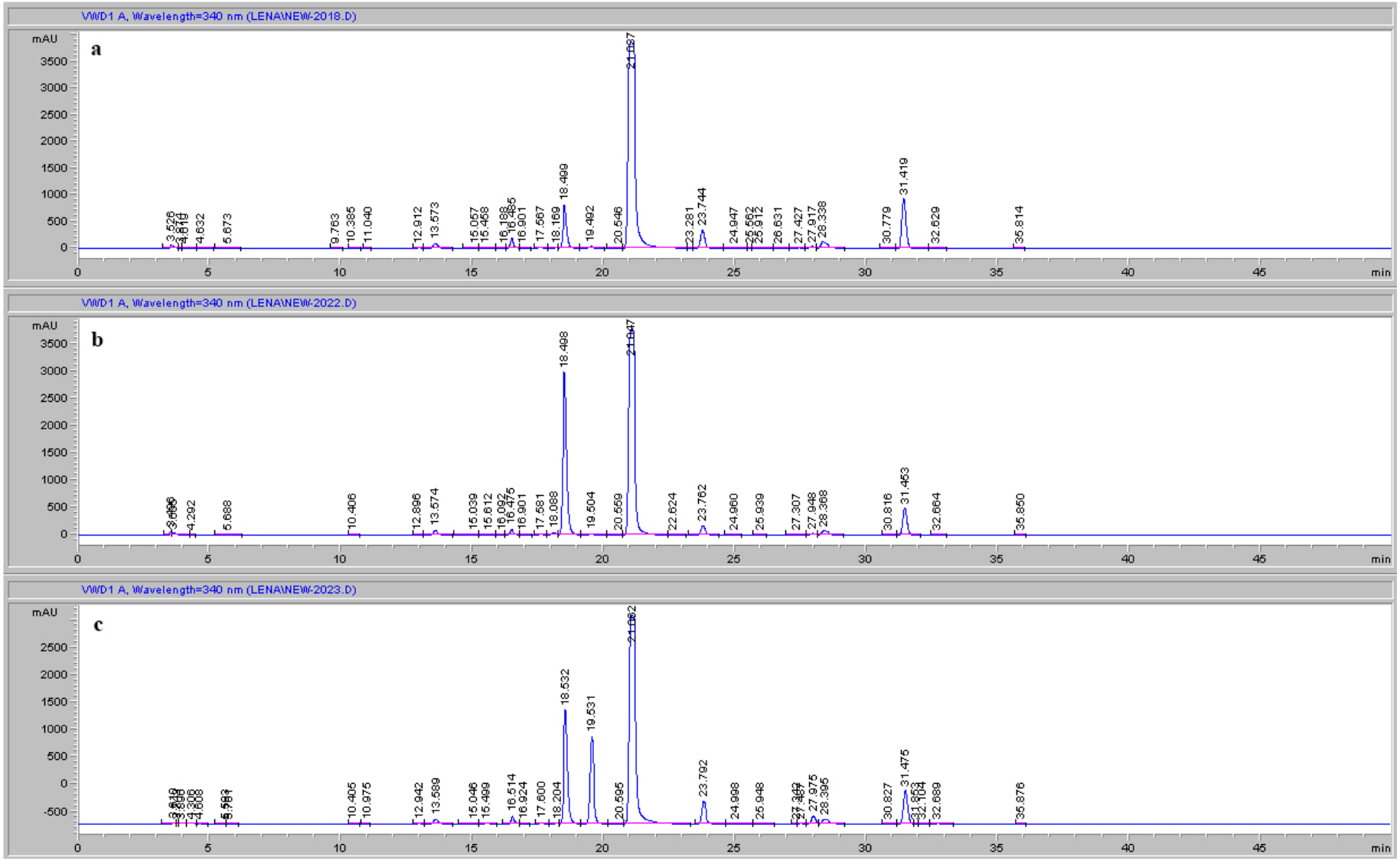

Figure S36. HPLC profiles of *L*-FDAA-derivatives of asterripeptide C (3) HP (a), asterripiptide C HP+ *D,L*-Phe (b) and asterripiptide C HP+*L*-Phe (c)