Identification of Bis Cyclic Guanidines as Antiplasmodial Compounds from Positional Scanning Mixture Based Libraries

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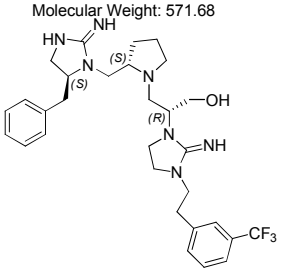
Supporting Information

	R1	R2	R3	R4
TPI-1955-1	Boc-Ala-OH	X	X	X
TPI-1955-2	Boc-Phe-OH	X	X	X
TPI-1955-3	Boc-Gly-OH	X	X	X
TPI-1955-4	Boc-Ile-OH·½H_2O	X	X	X
TPI-1955-5	Boc-Leu-OH·H_2O	X	X	X
TPI-1955-6	Boc-Ser(Bzl)-oh	X	X	X
TPI-1955-7	Boc-Thr(Bzl)-OH	X	X	X
TPI-1955-8	Boc-Val-OH	X	X	X
TPI-1955-9	Boc-Tyr(2-Br-Z)-OH	X	X	X
TPI-1955-10	Boc-D-Ala-OH	X	X	X
TPI-1955-11	Boc-D-Phe-OH	X	X	X
TPI-1955-12	Boc-D-Ile-OH	X	X	X
TPI-1955-13	Boc-D-Leu-OH·H_2O	X	X	X
TPI-1955-14	Boc-D-Ser(Bzl)-oh	X	X	X
TPI-1955-15	Boc-D-Thr(Bzl)-OH	X	X	X
TPI-1955-16	Boc-D-Val-OH	X	X	X
TPI-1955-17	Boc-D-Tyr(2-Br-Z)-OH	X	X	X
TPI-1955-18	Boc-Phg-OH	X	X	X
TPI-1955-19	Boc-Nva-OH	X	X	X
TPI-1955-20	Boc-D-Nva-OH	X	X	X
TPI-1955-21	Boc-Nle-OH	X	X	X
TPI-1955-22	Boc-D-Nle-OH	X	X	X
TPI-1955-23	Boc-Ala(2-naphthyl)-OH	X	X	X
TPI-1955-24	Boc-D-Ala(2-naphthyl)-OH	X	X	X
TPI-1955-25	Boc-Cha-OH	X	X	X
TPI-1955-26	Boc-D-Cha-OH	X	X	X
TPI-1955-27	X	Boc-Ala-OH	X	X
TPI-1955-28	X	Boc-Phe-OH	X	X
TPI-1955-29	X	Boc-Gly-OH	X	X
TPI-1955-30	X	Boc-Ile-OH·½H_2O	X	X
TPI-1955-31	X	Boc-Leu-OH·H_2O	X	X
TPI-1955-32	X	Boc-Ser(Bzl)-oh	X	X
TPI-1955-33	X	Boc-Thr(Bzl)-OH	X	X
TPI-1955-34	X	Boc-Val-OH	X	X
TPI-1955-35	X	Boc-Tyr(2-Br-Z)-OH	X	X
TPI-1955-36	X	Boc-D-Ala-OH	X	X
TPI-1955-37	X	Boc-D-Phe-OH	X	X
TPI-1955-38	X	Boc-D-Ile-OH	X	X
TPI-1955-39	X	Boc-D-Leu-OH·H_2O	X	X
TPI-1955-40	X	Boc-D-Ser(Bzl)-oh	X	X

TPI-1955-41	X	Boc-D-Thr(Bzl)-OH	X	X
TPI-1955-42	X	Boc-D-Val-OH	X	X
TPI-1955-43	X	Boc-D-Tyr(2-Br-Z)-OH	X	X
TPI-1955-44	X	Boc-Phg-OH	X	X
TPI-1955-45	X	Boc-Nva-OH	X	X
TPI-1955-46	X	Boc-D-Nva-OH	X	X
TPI-1955-47	X	Boc-Nle-OH	X	X
TPI-1955-48	X	Boc-D-Nle-OH	X	X
TPI-1955-49	X	Boc-Ala(2-naphthyl)-OH	X	X
TPI-1955-50	X	Boc-D-Ala(2-naphthyl)-OH	X	X
TPI-1955-51	X	Boc-Cha-OH	X	X
TPI-1955-52	X	Boc-D-Cha-OH	X	X
TPI-1955-53	X	X	Boc-Ala-OH	X
TPI-1955-54	X	X	Boc-Phe-OH	X
TPI-1955-55	X	X	Boc-Gly-OH	X
TPI-1955-56	X	X	Boc-Ile-OH·½H_2O	X
TPI-1955-57	X	X	Boc-Leu-OH·H_2O	X
TPI-1955-58	X	X	Boc-Ser(Bzl)-oh	X
TPI-1955-59	X	X	Boc-Thr(Bzl)-OH	X
TPI-1955-60	X	X	Boc-Val-OH	X
TPI-1955-61	X	X	Boc-Tyr(2-Br-Z)-OH	X
TPI-1955-62	X	X	Boc-D-Ala-OH	X
TPI-1955-63	X	X	Boc-D-Phe-OH	X
TPI-1955-64	X	X	Boc-D-Ile-OH	X
TPI-1955-65	X	X	Boc-D-Leu-OH·H_2O	X
TPI-1955-66	X	X	Boc-D-Ser(Bzl)-oh	X
TPI-1955-67	X	X	Boc-D-Thr(Bzl)-OH	X
TPI-1955-68	X	X	Boc-D-Val-OH	X
TPI-1955-69	X	X	Boc-D-Tyr(2-Br-Z)-OH	X
TPI-1955-70	X	X	Boc-Phg-OH	X
TPI-1955-71	X	X	Boc-Nva-OH	X
TPI-1955-72	X	X	Boc-D-Nva-OH	X
TPI-1955-73	X	X	Boc-Nle-OH	X
TPI-1955-74	X	X	Boc-D-Nle-OH	X
TPI-1955-75	X	X	Boc-Ala(2-naphthyl)-OH	X
TPI-1955-76	X	X	Boc-D-Ala(2-naphthyl)-OH	X
TPI-1955-77	X	X	Boc-Cha-OH	X
TPI-1955-78	X	X	Boc-D-Cha-OH	X
TPI-1955-79	X	X	X	1-phenyl-1-cyclopropanecarboxylic acid
TPI-1955-80	X	X	X	2-Phenylbutyric Acid
TPI-1955-81	X	X	X	3-Phenylbutyric Acid
TPI-1955-82	X	X	X	m-Tolylacetic acid

TPI-1955-83	X	X	X	3-Fluorophenylacetic Acid
TPI-1955-84	X	X	X	3-Bromophenylacetic Acid
TPI-1955-85	X	X	X	(α, α, α Trifluoro-m-Toly) acetic acid
TPI-1955-86	X	X	X	p-Tolylacetic acid
TPI-1955-87	X	X	X	4-Fluorophenylacetic acid
TPI-1955-88	X	X	X	3-Methoxyphenylacetic acid
TPI-1955-89	X	X	X	4-Bromophenylacetic acid
TPI-1955-90	X	X	X	4-Methoxyphenylacetic acid
TPI-1955-91	X	X	X	4-ethoxyphenylacetic acid
TPI-1955-92	X	X	X	4-isobutyl-alpha-Methylphenylacetic Acid
TPI-1955-93	X	X	X	3,4-Dichlorophenylacetic acid
TPI-1955-94	X	X	X	3,5-Bis(Trifluoromethyl)-Phenylacetic acid
TPI-1955-95	X	X	X	3-(3,4-Dimethoxyphenyl)-propionic Acid
TPI-1955-96	X	X	X	Phenylacetic acid
TPI-1955-97	X	X	X	3,4,5-Trimethoxybenzoic acid
TPI-1955-98	X	X	X	Butyric Acid
TPI-1955-99	X	X	X	Heptanoic Acid
TPI-1955-100	X	X	X	Isobutyric Acid
TPI-1955-101	X	X	X	2-Methylbutiric Acid
TPI-1955-102	X	X	X	Isovaleric acid
TPI-1955-103	X	X	X	3-Methylvaleric acid
TPI-1955-104	X	X	X	4-Methylvaleric acid
TPI-1955-105	X	X	X	p-Toluic Acid
TPI-1955-106	X	X	X	cyclopentanecarboxylic acid
TPI-1955-107	X	X	X	cyclohexanecarboxilic acid
TPI-1955-108	X	X	X	cyclohexylacetic acid
TPI-1955-109	X	X	X	cyclohexanebutyric acid
TPI-1955-110	X	X	X	cycloheptanecarboxylic acid
TPI-1955-111	X	X	X	2-Methylcyclopropanecarboxylic acid
TPI-1955-112	X	X	X	cyclobutanecarboxylic acid
TPI-1955-113	X	X	X	3-cyclopentylpropionic acid
TPI-1955-114	X	X	X	cyclohexanepropionic acid
TPI-1955-115	X	X	X	4-methyl-1-cyclohexancarboxylic acid
TPI-1955-116	X	X	X	4-tert-butyl-cyclohexancecarboxylic acid
TPI-1955-117	X	X	X	4-biphenylacetic acid
TPI-1955-118	X	X	X	1-Adamantancecarboxylic acid
TPI-1955-119	X	X	X	1-adamantaneacetic acid
TPI-1955-120	X	X	X	2-norbornaneacetic acid

2359-1
Molecular Weight: 571.68



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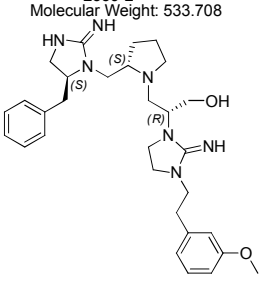
Molecular Weight: 533.708



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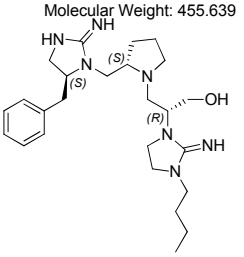

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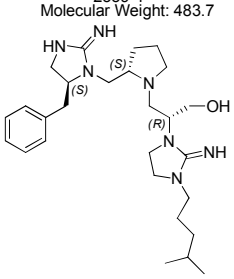
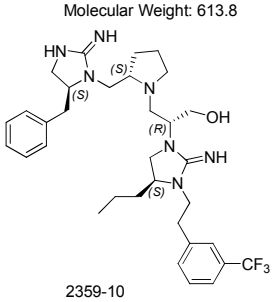


2359-5
Molecular Weight: 613.8



2359-6
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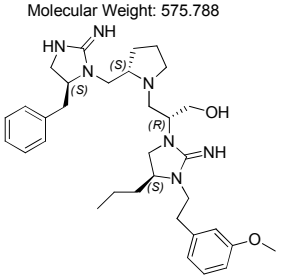

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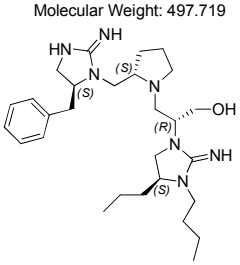
Molecular Weight: 497.719



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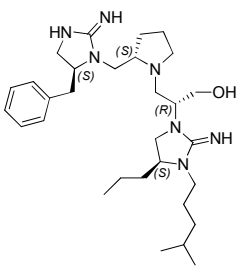
Molecular Weight: 525.772



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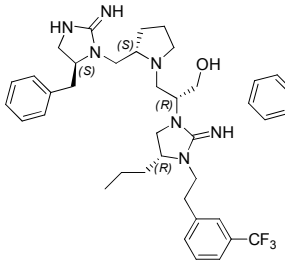
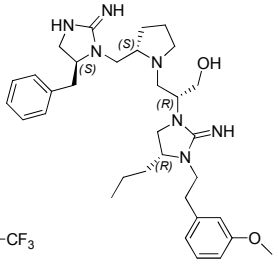
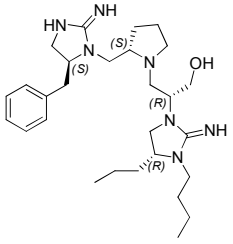


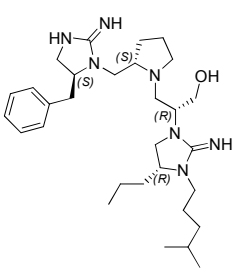
2359-10
Molecular Weight: 575.788



2359-11
Molecular Weight: 497.719



2359-12
Molecular Weight: 525.772



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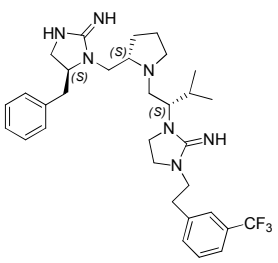
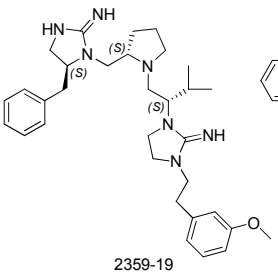
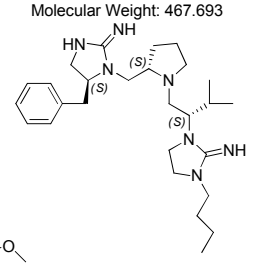
Molecular Weight: 583.734



2359-14
Molecular Weight: 545.762



2359-15
Molecular Weight: 467.693



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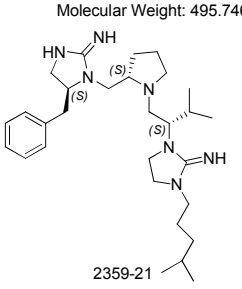
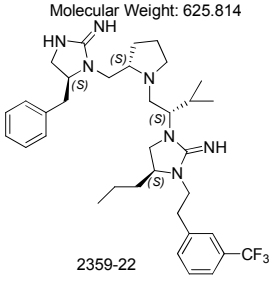
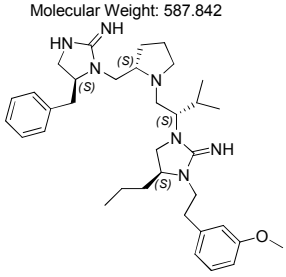
Molecular Weight: 495.746



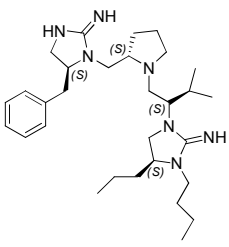
2359-17
Molecular Weight: 625.814



2359-18
Molecular Weight: 587.842



2359-19
Molecular Weight: 509.773



2359-20
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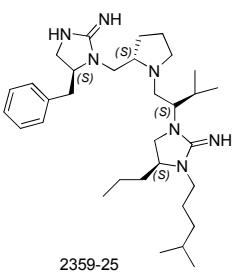

2359-21
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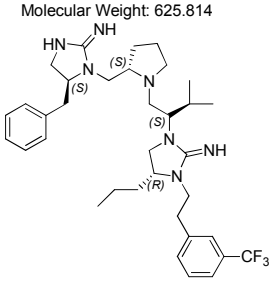
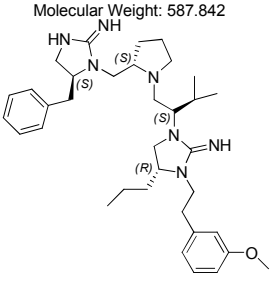
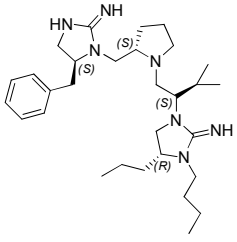


2359-22
Molecular Weight: 587.842



2359-23
Molecular Weight: 509.773



2359-24
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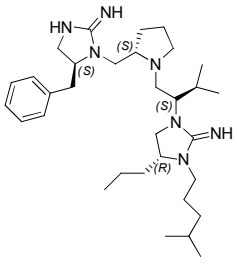

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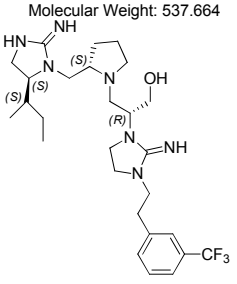
Molecular Weight: 537.664



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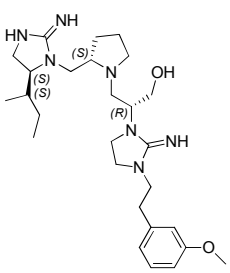

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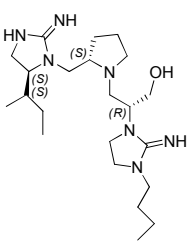

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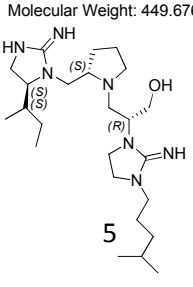

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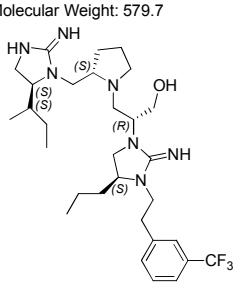

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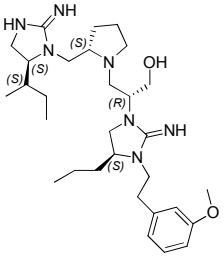
Molecular Weight: 541.8



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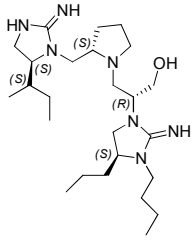
Molecular Weight: 463.703



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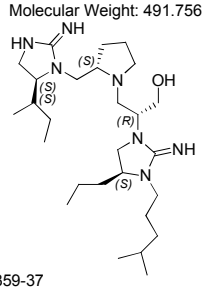

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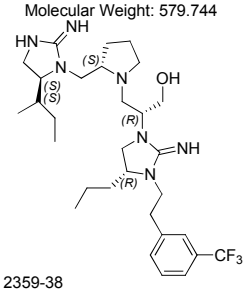

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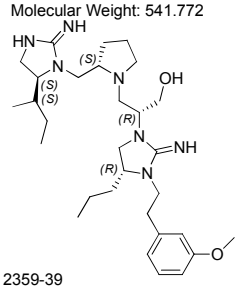
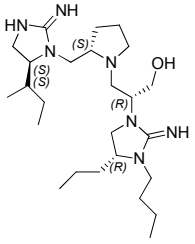
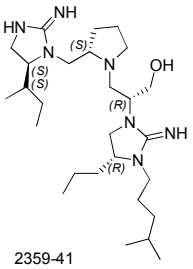


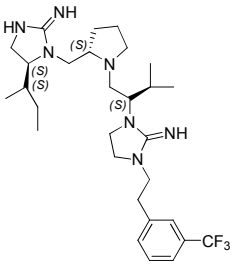
2359-35
Molecular Weight: 463.703



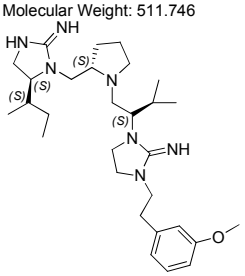
2359-36
Molecular Weight: 491.756



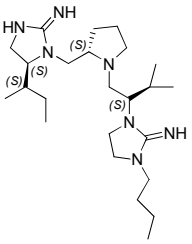
2359-37
Molecular Weight: 549.718



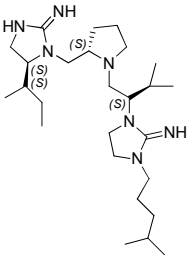
2359-38
Molecular Weight: 511.746



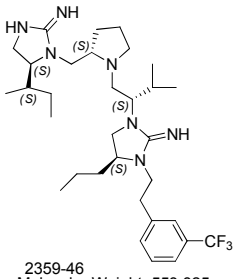
2359-39
Molecular Weight: 433.677



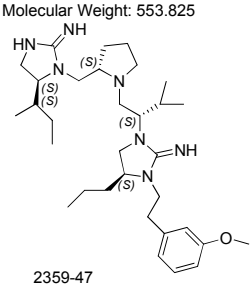
2359-40
Molecular Weight: 461.730



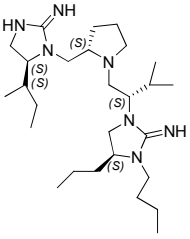
2359-41
Molecular Weight: 591.797



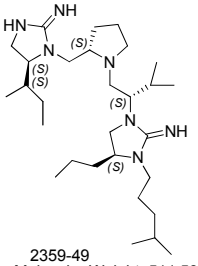
2359-42
Molecular Weight: 553.825



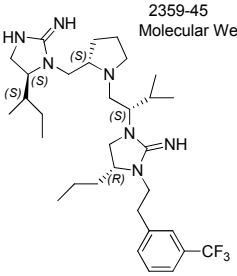
2359-43
Molecular Weight: 475.757



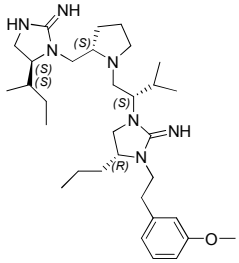
2359-44
Molecular Weight: 503.810



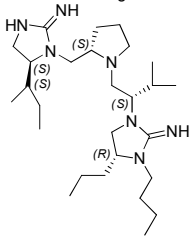
2359-45
Molecular Weight: 591.8



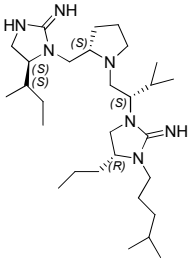
2359-46
Molecular Weight: 553.825



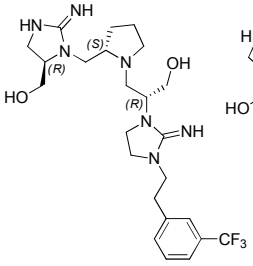
2359-47
Molecular Weight: 475.757



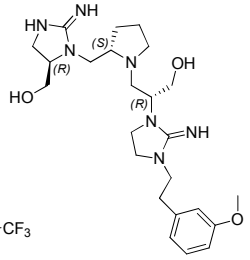
2359-48
Molecular Weight: 503.810



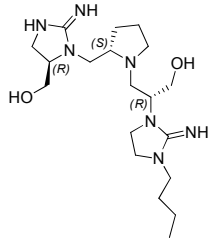
2359-49
Molecular Weight: 511.584



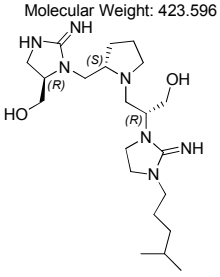
2359-50
Molecular Weight: 473.612



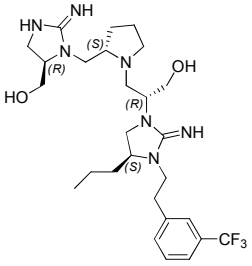
2359-51
Molecular Weight: 395.543



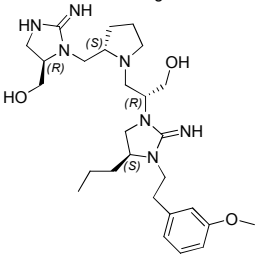
2359-52
Molecular Weight: 423.596



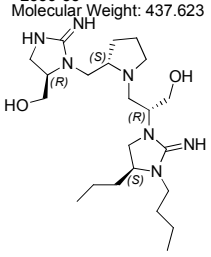
2359-53
Molecular Weight: 553.663



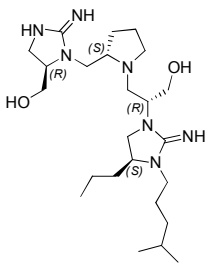
2359-54
Molecular Weight: 515.691



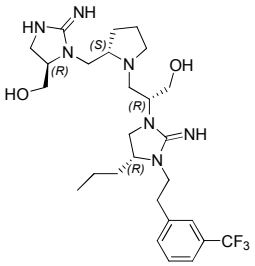
2359-55
Molecular Weight: 437.623



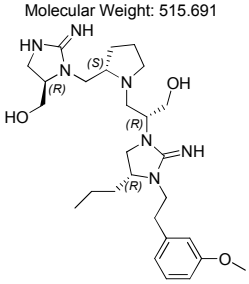
2359-56
Molecular Weight: 465.676



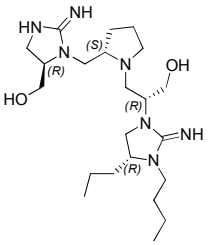
2359-57
Molecular Weight: 553.663



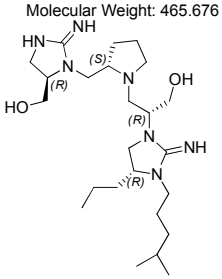
2359-58
Molecular Weight: 515.691



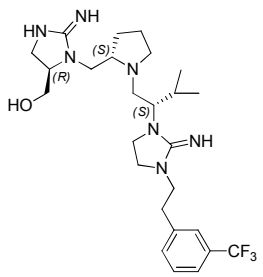
2359-59
Molecular Weight: 437.623



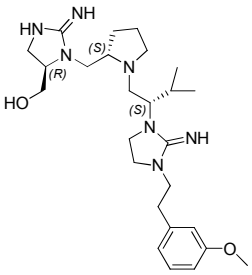
2359-60
Molecular Weight: 465.676



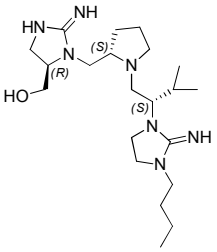
2359-61
Molecular Weight: 523.637



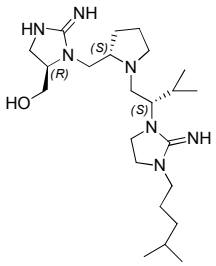
2359-62
Molecular Weight: 485.665



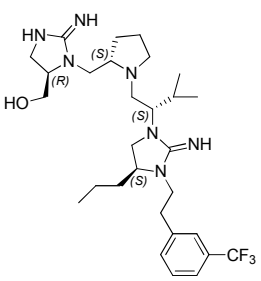
2359-63
Molecular Weight: 407.597



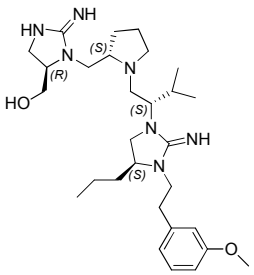
2359-64
Molecular Weight: 435.650



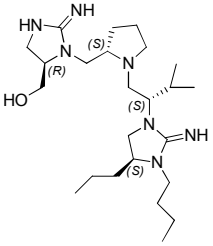
2359-65
Molecular Weight: 565.717



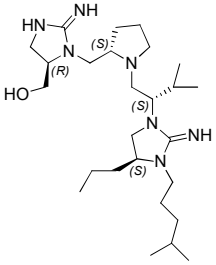
2359-66
Molecular Weight: 527.745



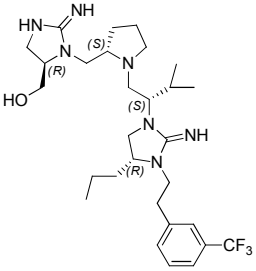
2359-67
Molecular Weight: 449.676



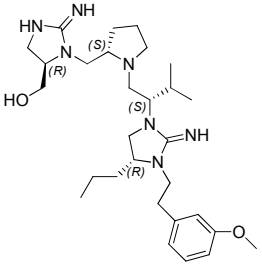
2359-68
Molecular Weight: 477.729



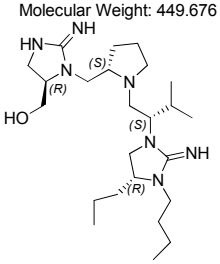
2359-69
Molecular Weight: 565.717



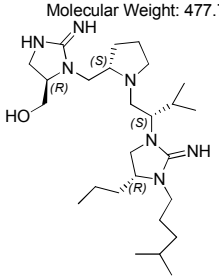
2359-70
Molecular Weight: 527.745



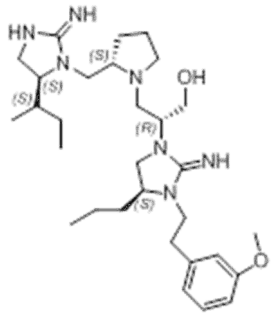
2359-71
Molecular Weight: 449.676

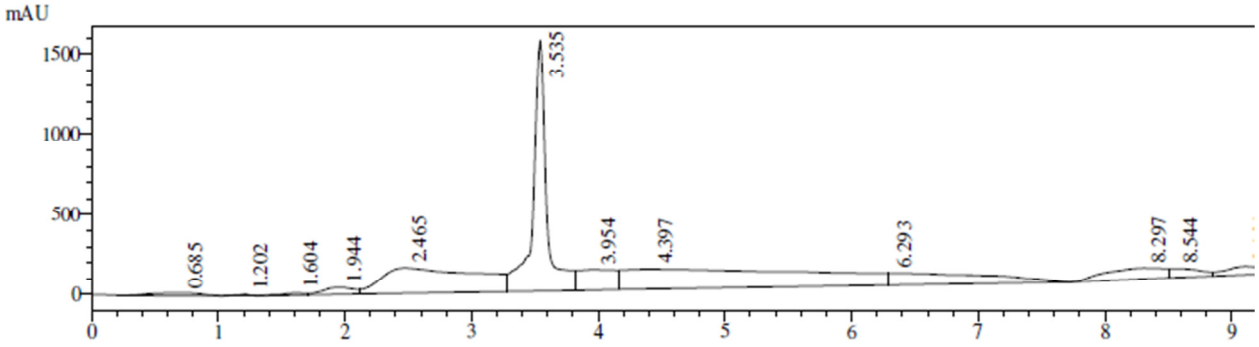


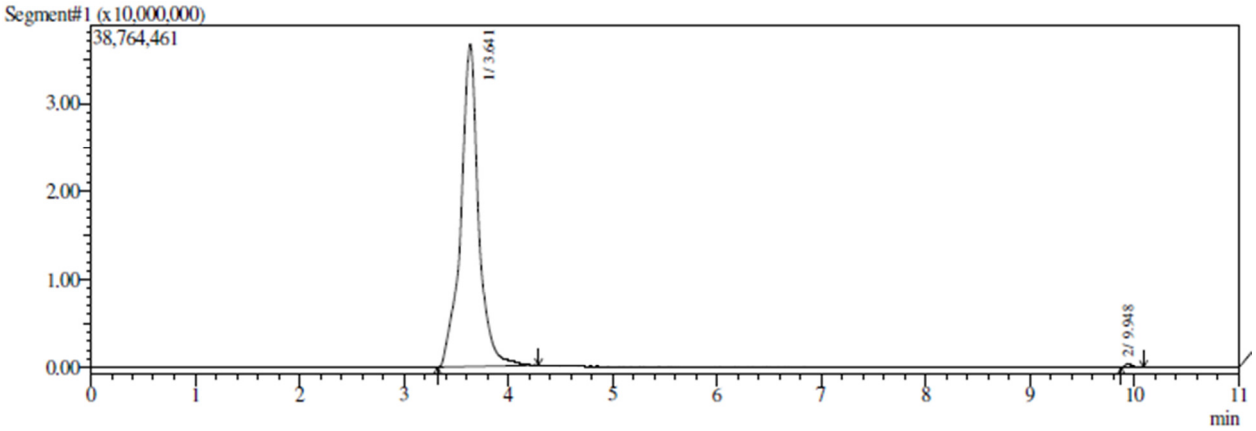
2359-72
Molecular Weight: 477.729



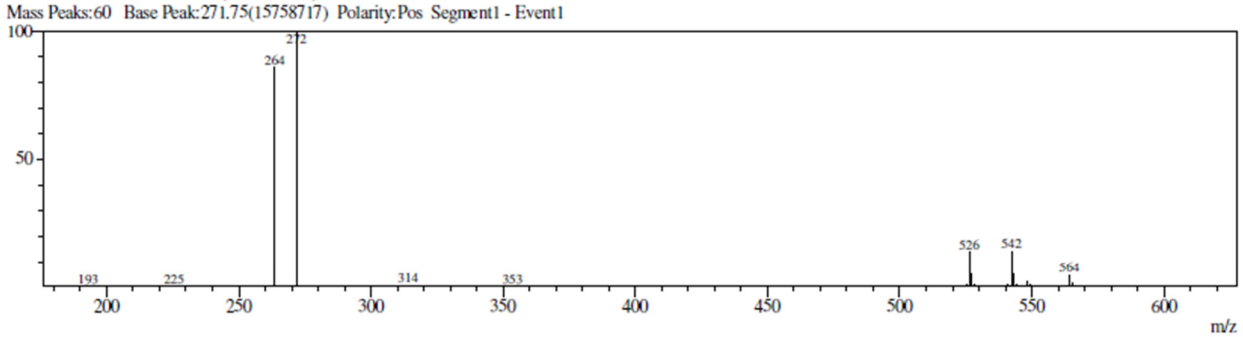
2359-30
Molecular Weight: 541.77



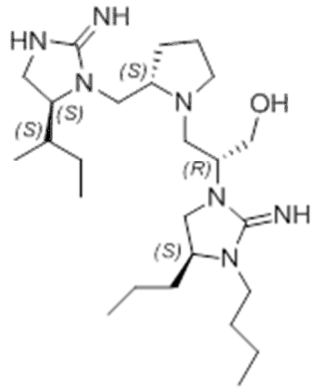


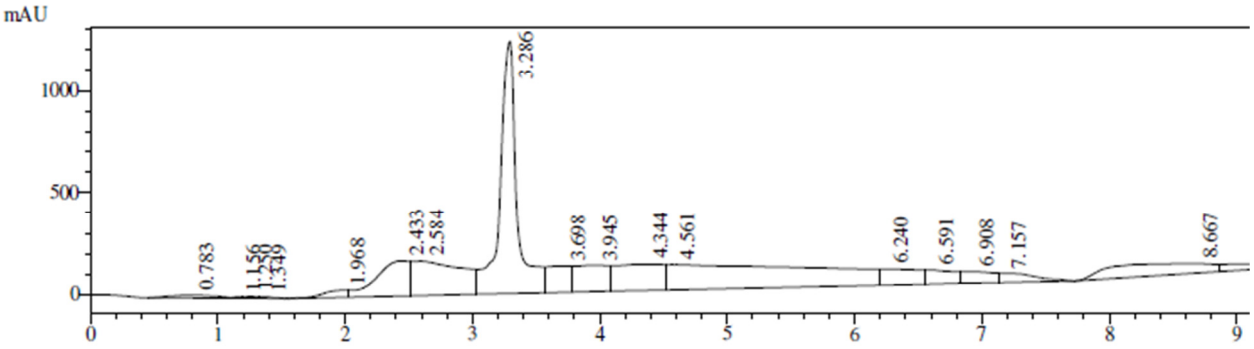


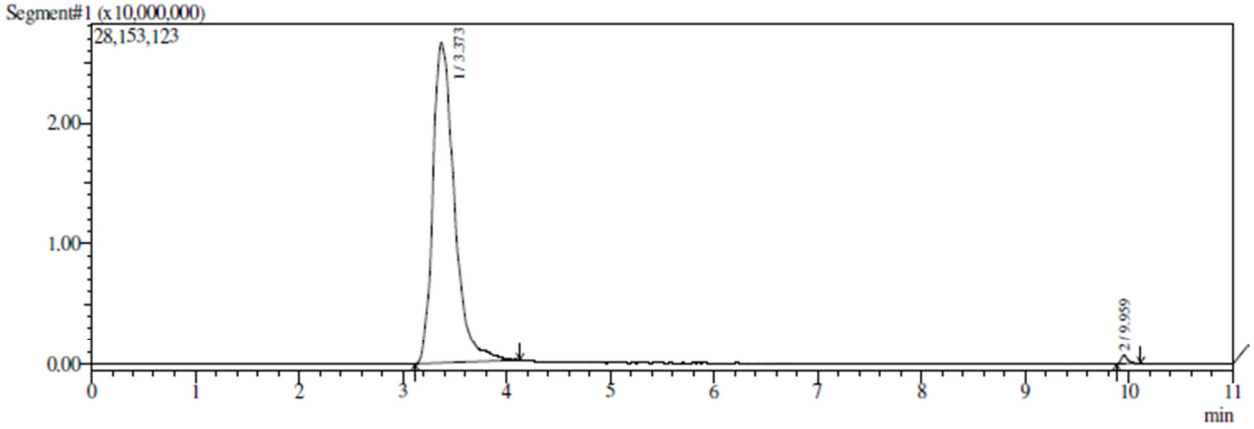
Peak#:1 Ret.Time:Averaged 3.637-3.643(Scan#:1092-1094)
BG Mode:Calc 3.320<->4.290(997<->1288)
Mass Peaks:60 Base Peak:271.75(15758717) Polarity:Pos Segment1 - Event1

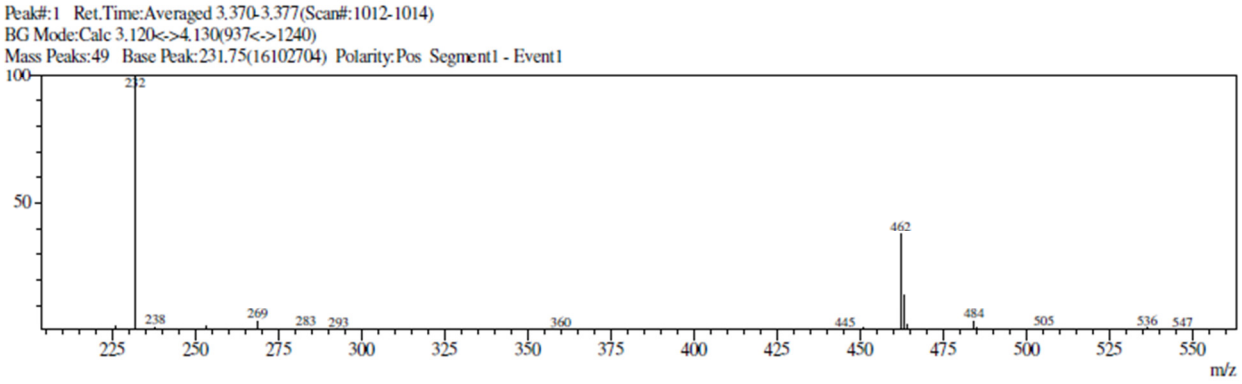


2359-31
Molecular Weight: 463.703



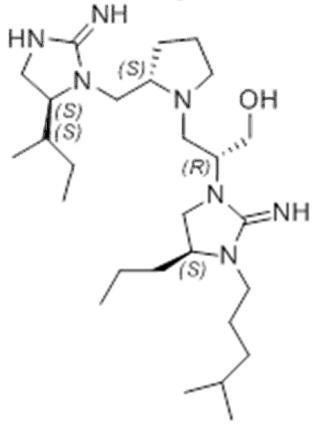


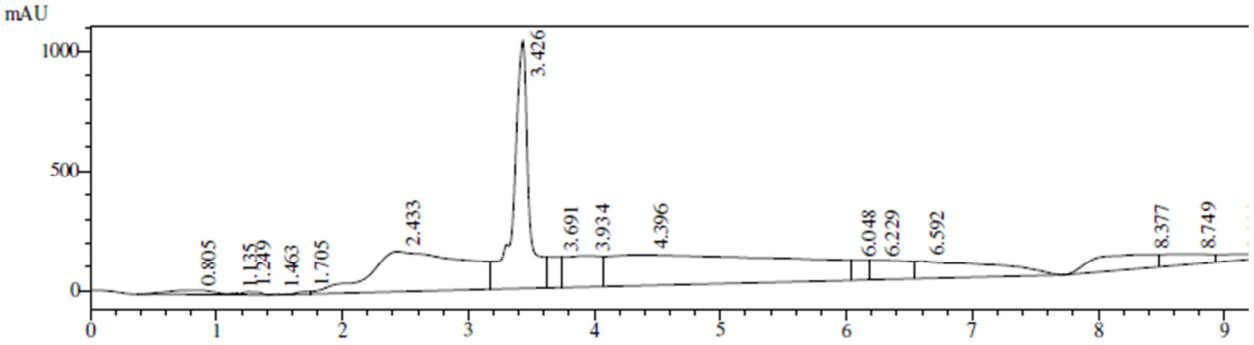


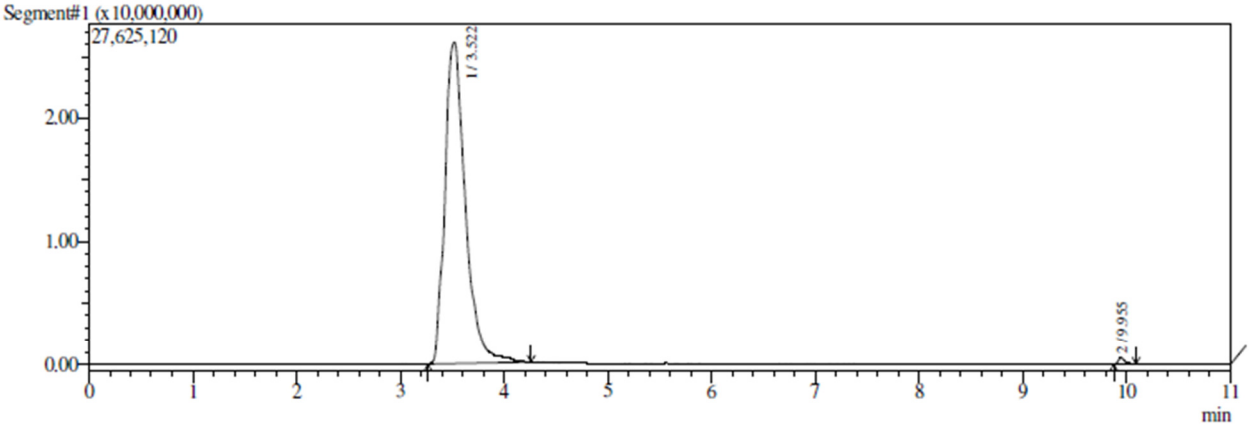


2359-32

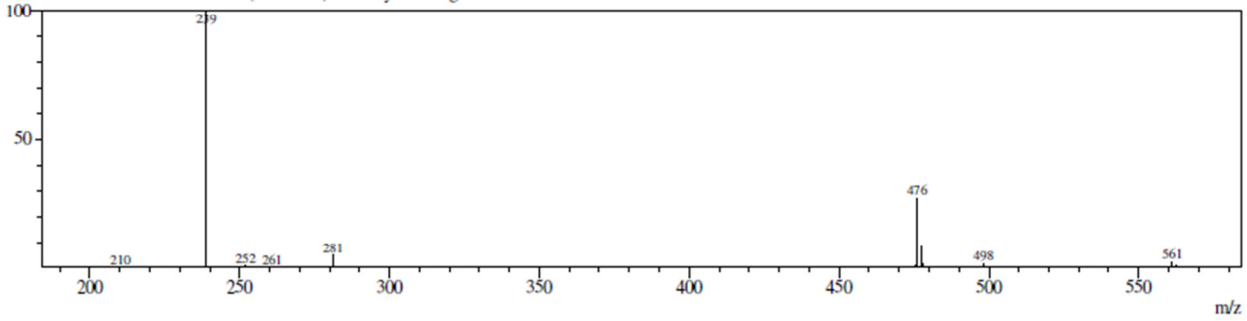
Molecular Weight: 491.756





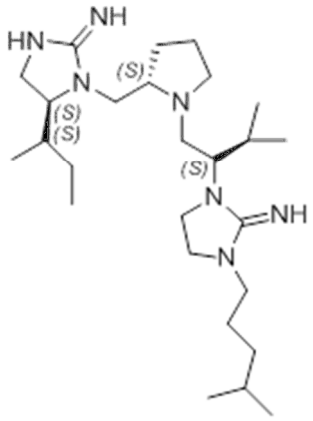


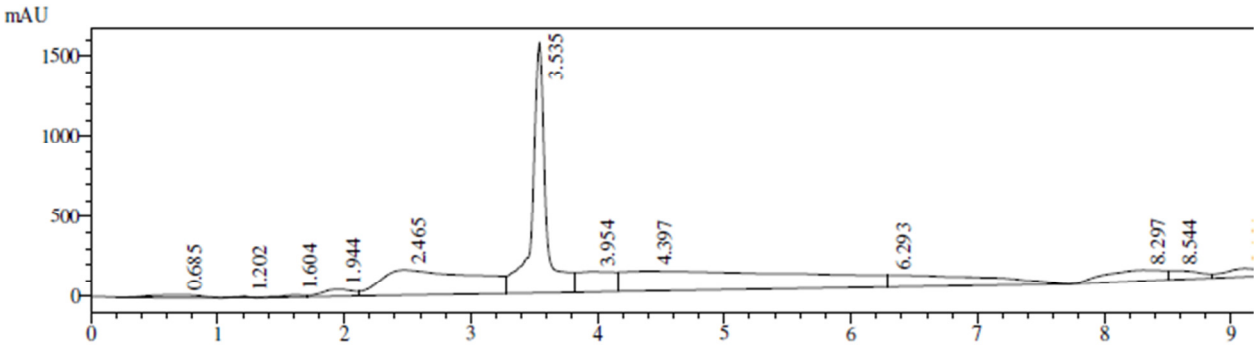
Peak#:1 Ret.Time:Averaged 3.520-3.527(Scan#:1057-1059)
BG Mode:Calc 3.267<->4.260(981<->1279)
Mass Peaks:35 Base Peak:238.75(17033442) Polarity:Pos Segment1 - Event1

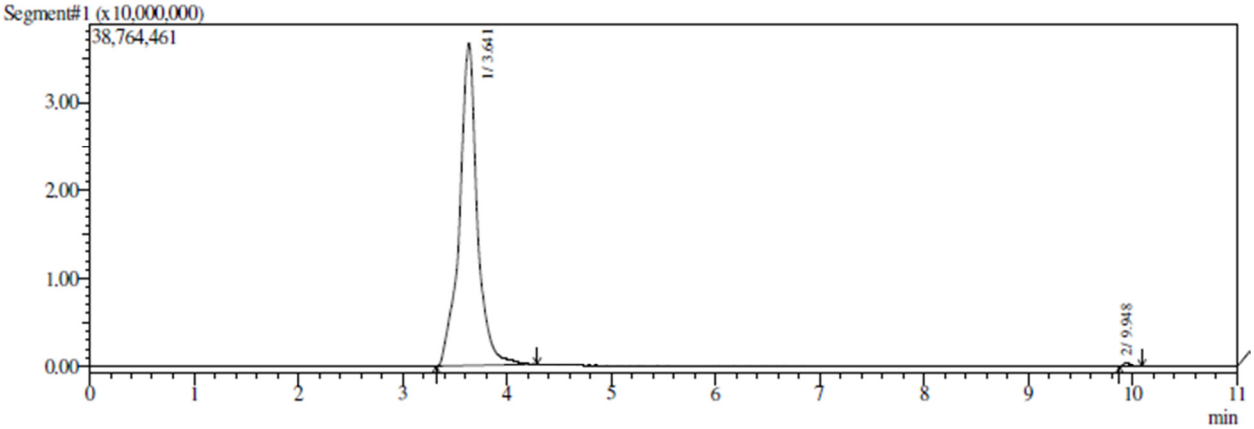


2359-40

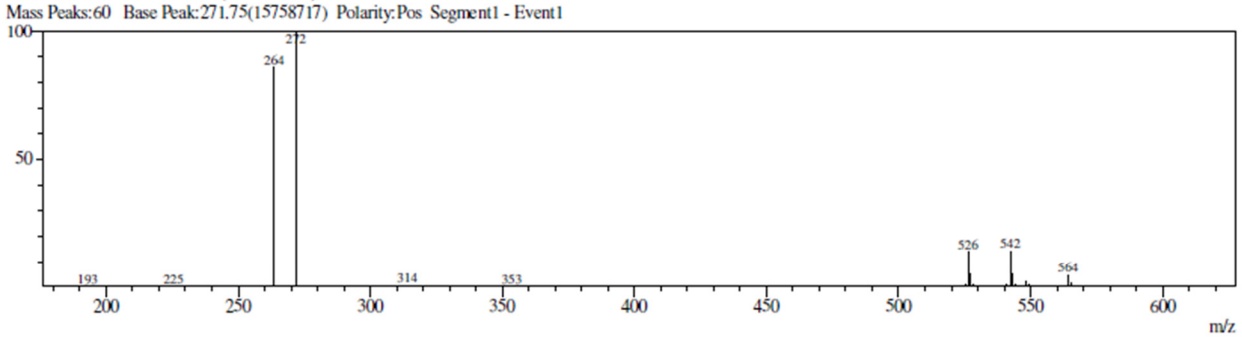
Molecular Weight: 461.730



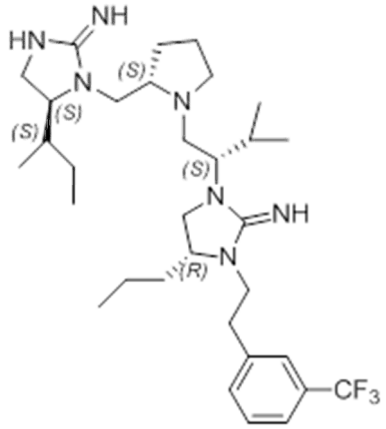


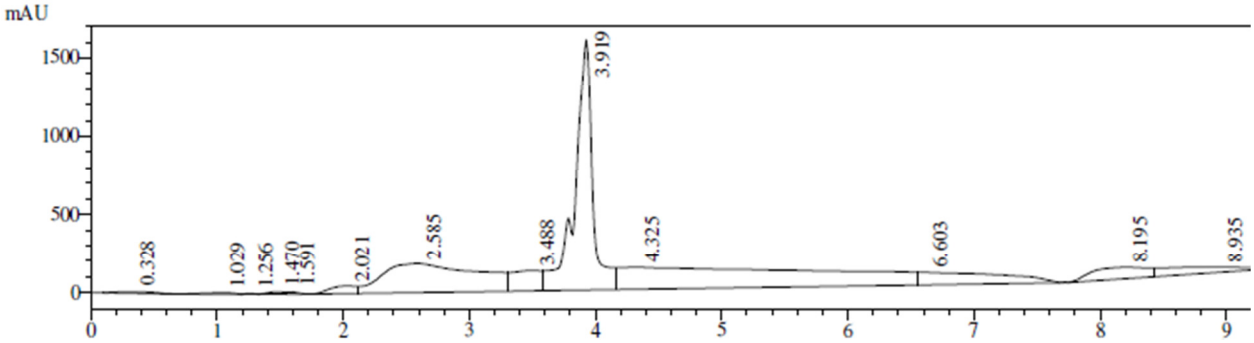


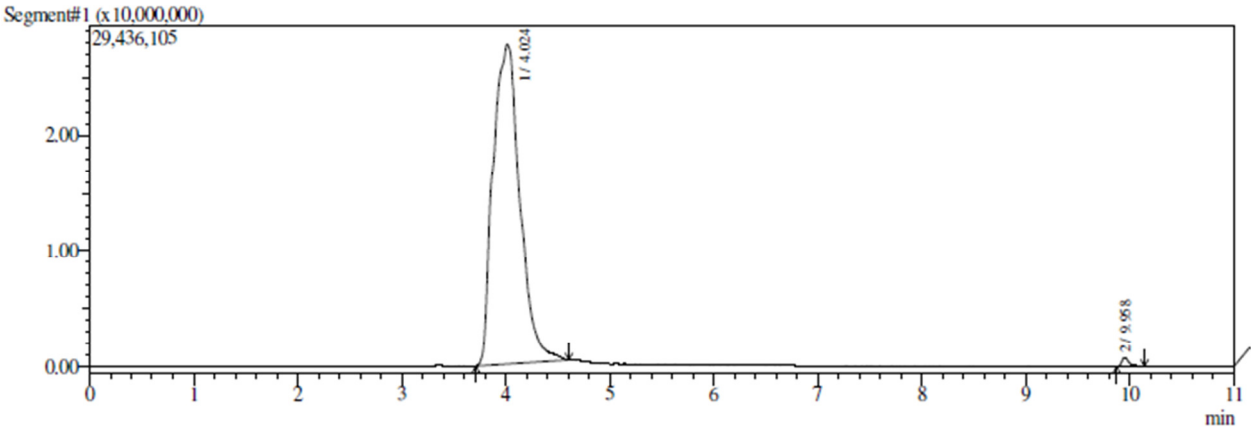
Peak#:1 Ret.Time:Averaged 3.637-3.643(Scan#:1092-1094)
BG Mode:Calc 3.320<->4.290(997<->1288)
Mass Peaks:60 Base Peak:271.75(15758717) Polarity:Pos Segment1 - Event1

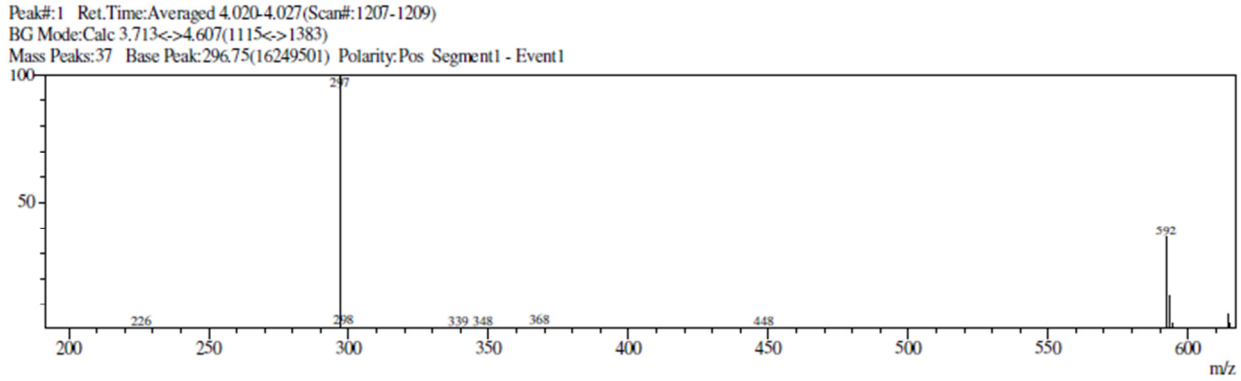


2359-45
Molecular Weight: 591.80



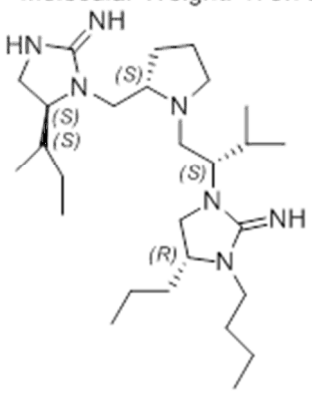


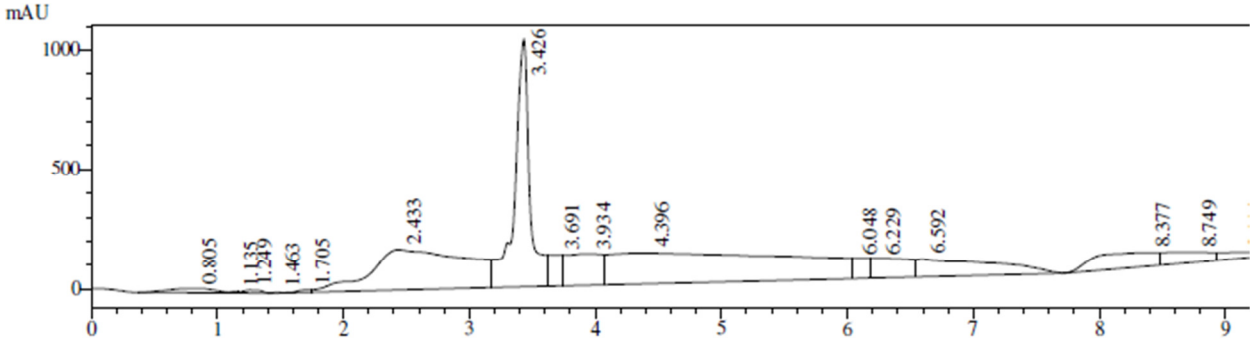


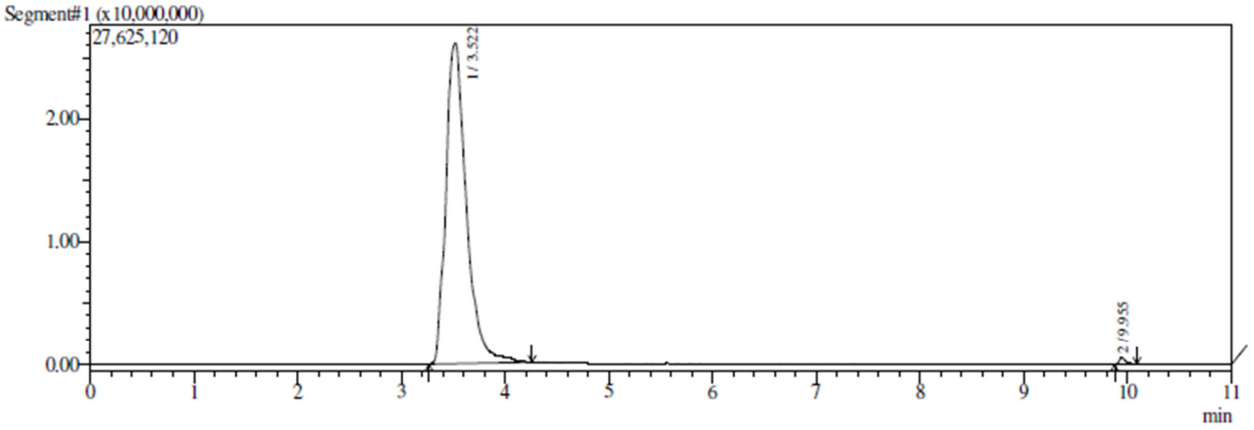


2359-47

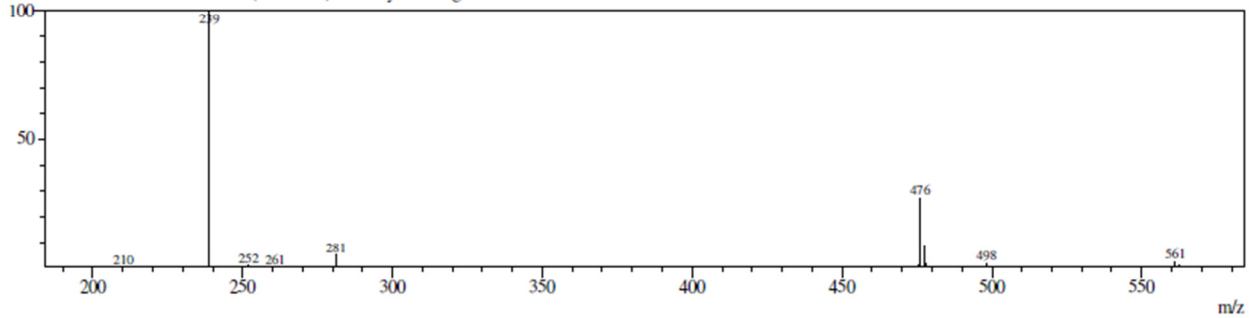
Molecular Weight: 475.757





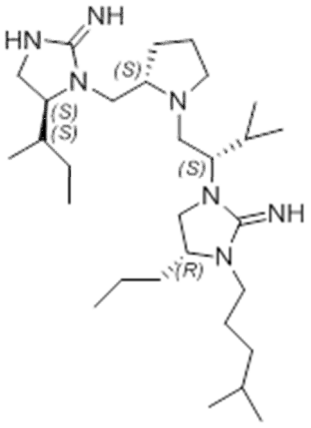


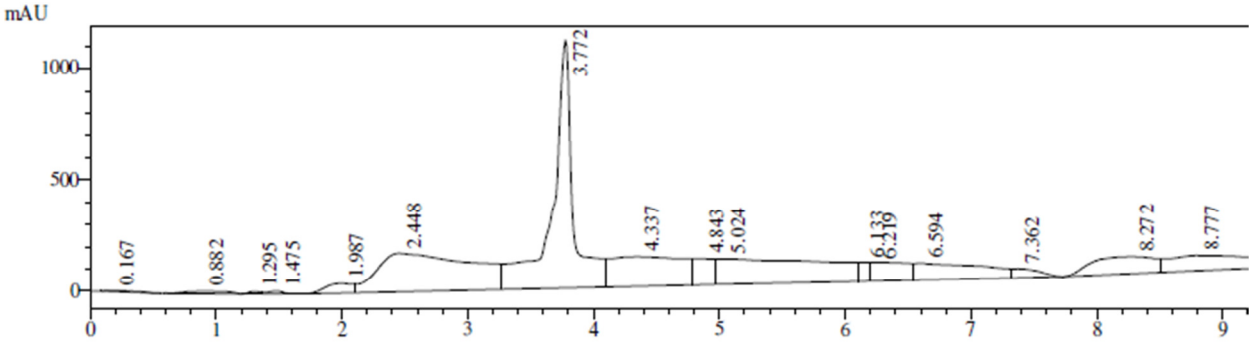
Peak#:1 Ret.Time:Averaged 3.520-3.527(Scan#:1057-1059)
BG Mode:Calc 3.267<->4.260(981<->1279)
Mass Peaks:35 Base Peak:238.75(17033442) Polarity:Pos Segment1 - Event1

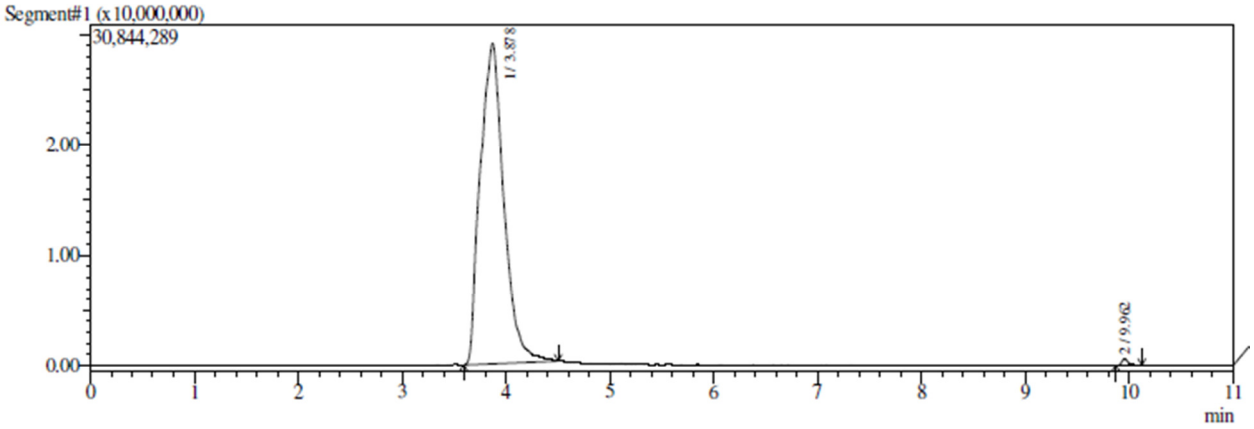


2359-48

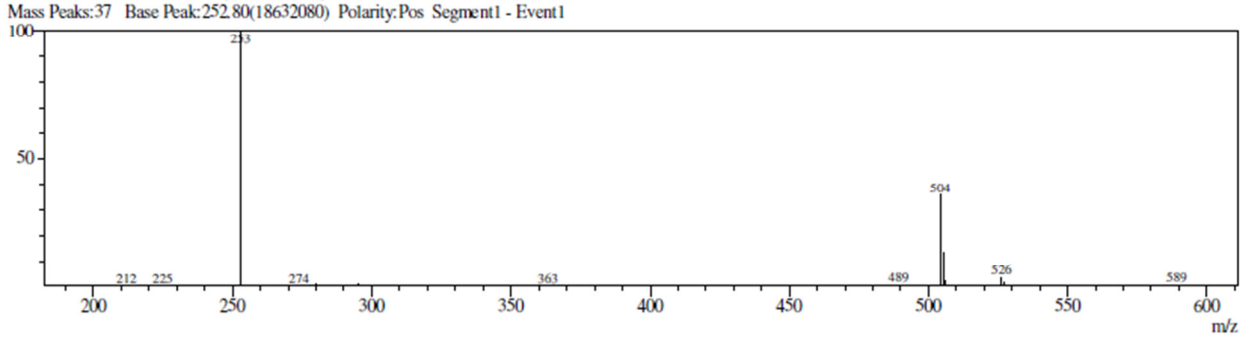
Molecular Weight: 503.810

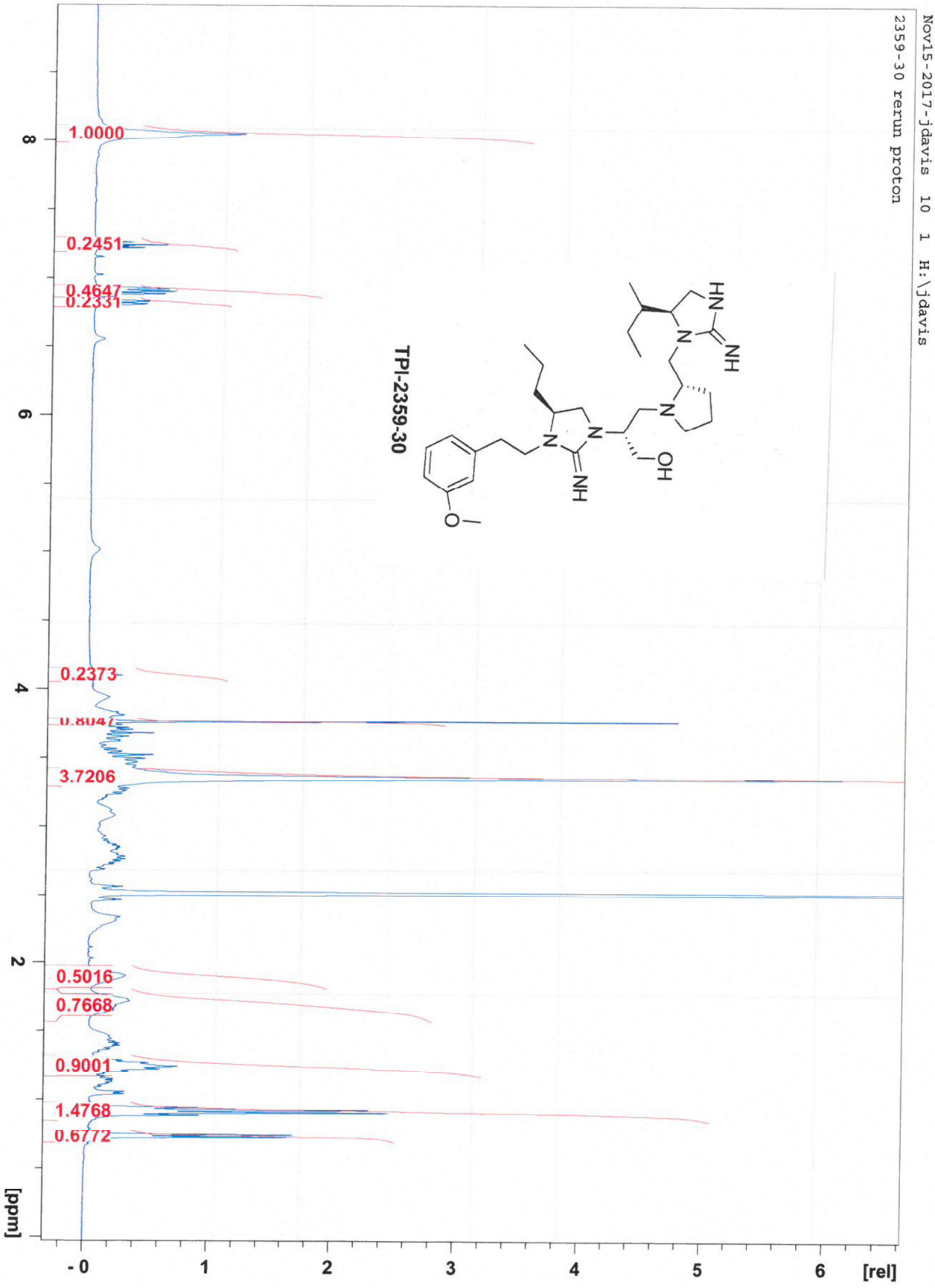




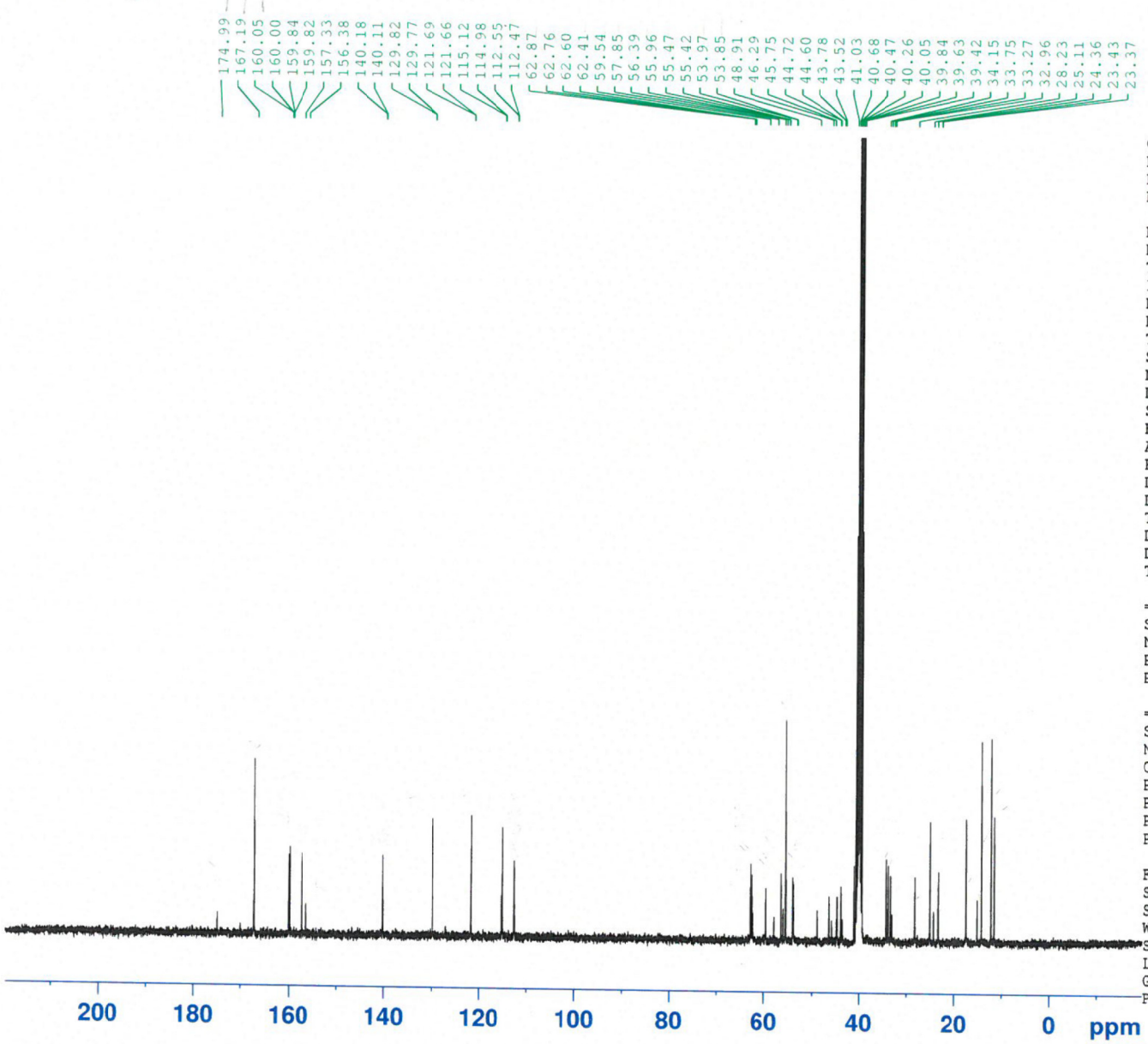


Peak#:1 Ret.Time:Averaged 3.873-3.880(Scan#:1163-1165)
BG Mode:Calc 3.593<->4.503(1079<->1352)
Mass Peaks:37 Base Peak:252.80(18632080) Polarity:Pos Segment1 - Event1

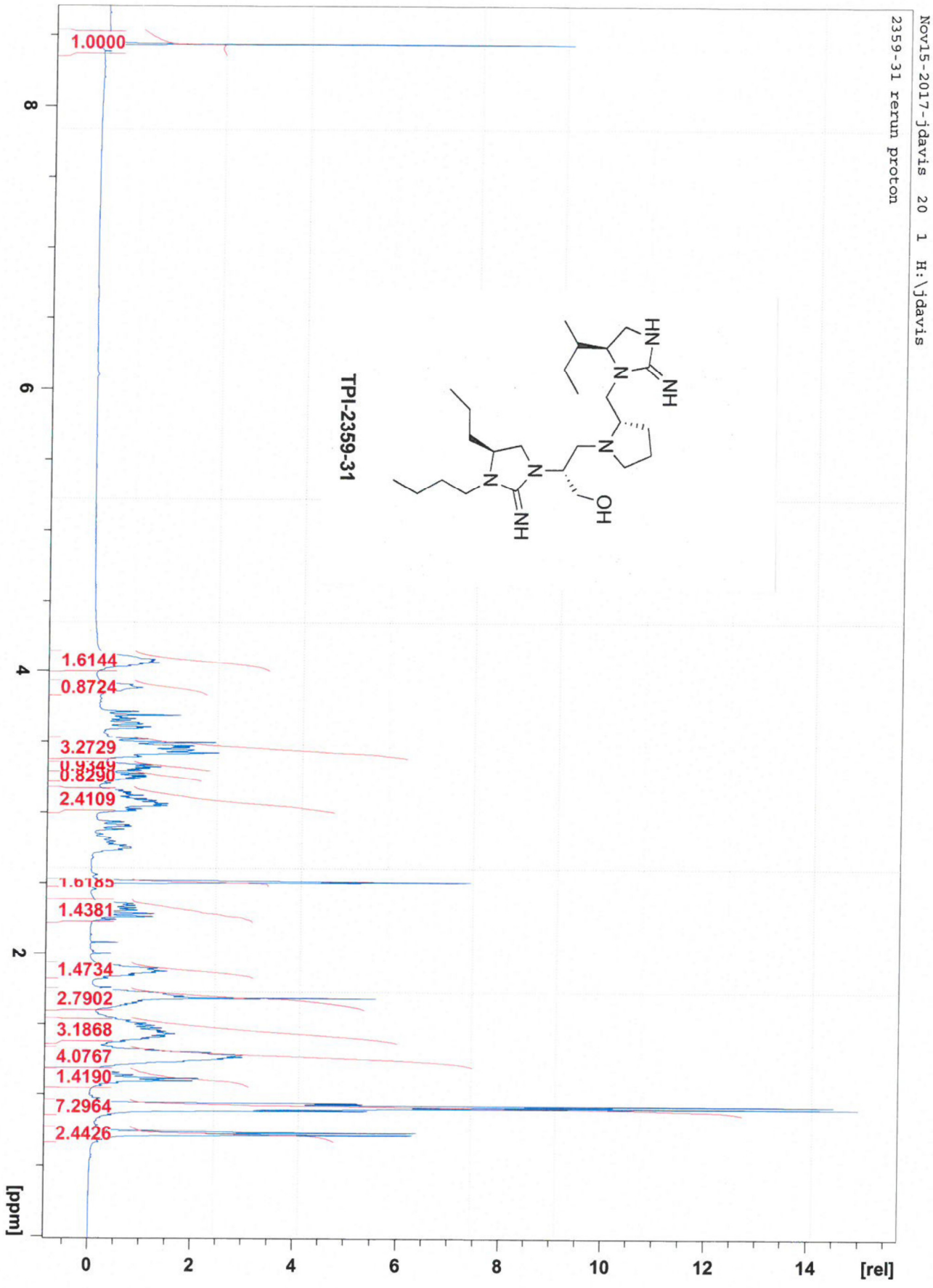



Nov15-2017-jdavis 10 1 H:\jdavis
2359-30 rerun proton
TPI-2359-30
1.0000
0.2451
0.4647
0.2331
0.2373
0.8047
3.7206
0.5016
0.7668
0.9001
1.4768
0.6772
[ppm]
[rel]

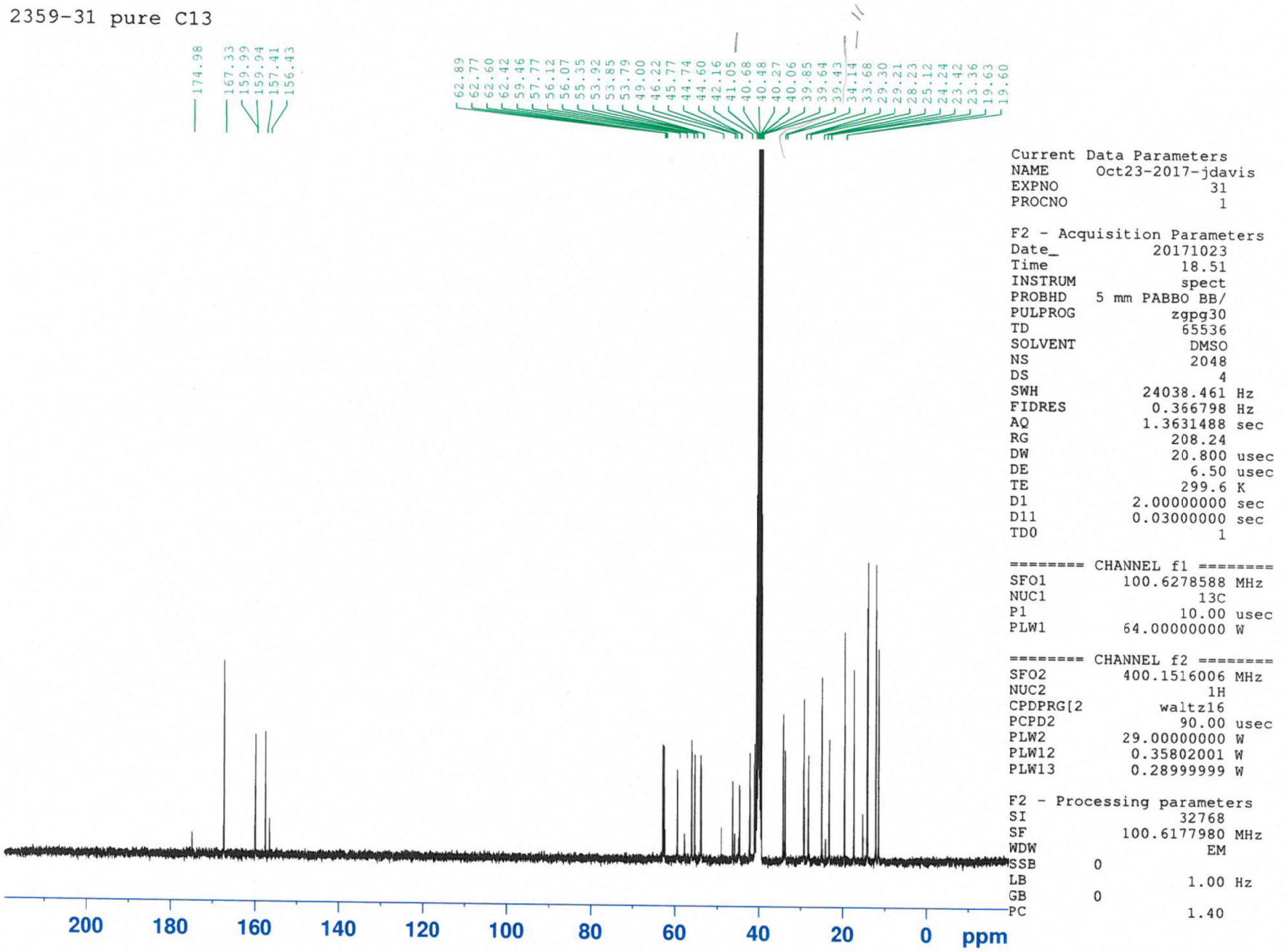
2359-30 pure C13



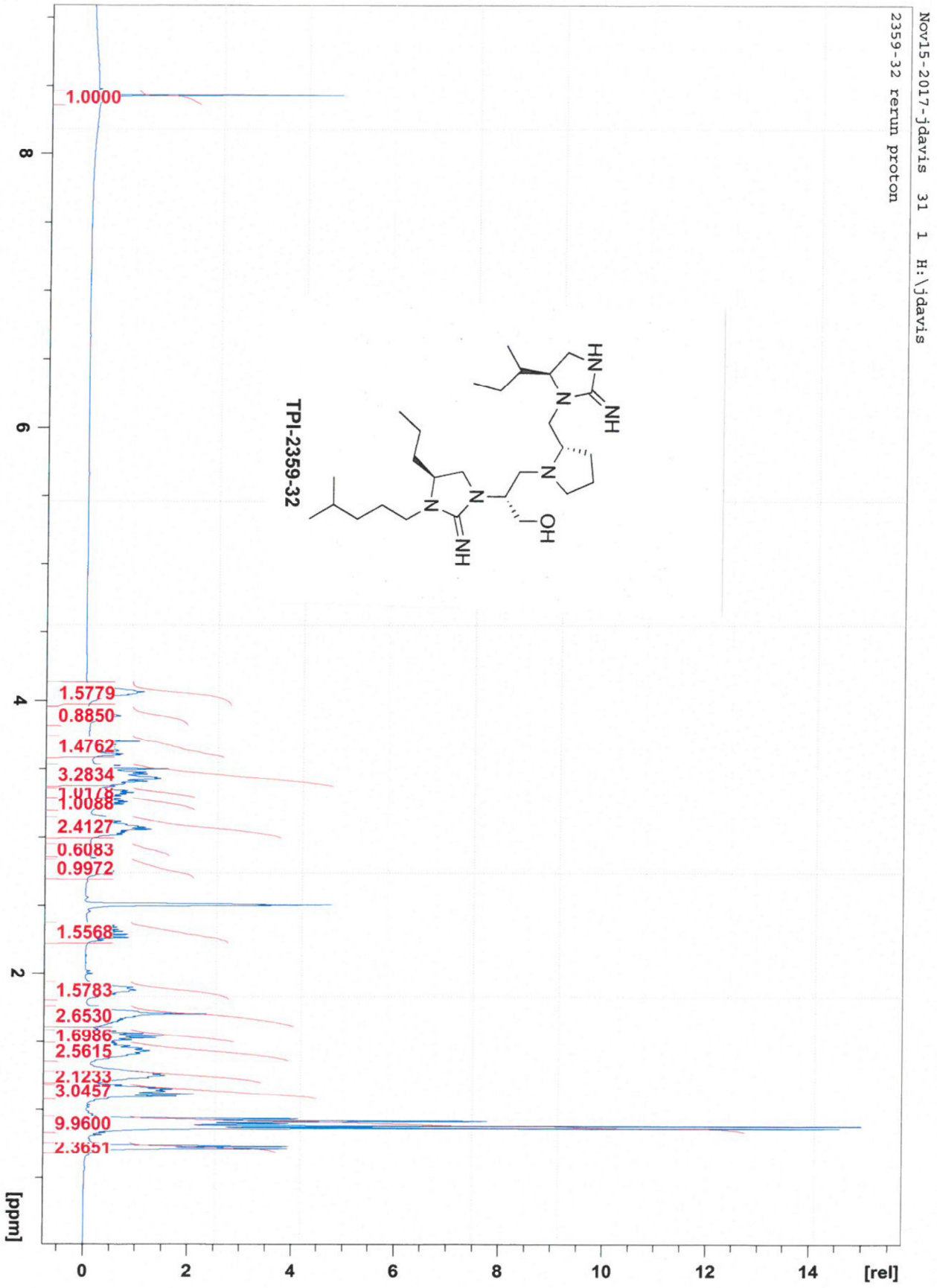

```
Current Data Parameters
NAME      Oct23-2017-jdavis
EXPNO                   21
PROCNO                   1

F2 - Acquisition Parameters
Date_              20171023
Time                  16.26
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                     2048
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    208.24
DW                    20.800 usec
DE                     6.50 usec
TE                    299.6 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           100.6278588 MHz
NUC1                    13C
P1                    10.00 usec
PLW1           64.00000000 W

======== CHANNEL f2 ========
SFO2           400.1516006 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                 90.00 usec
PLW2           29.00000000 W
PLW12           0.35802001 W
PLW13           0.28999999 W

F2 - Processing parameters
SI                    32768
SF             100.6177980 MHz
WDW                      EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```


Nov15-2017-jdavis 20 1 H:\jdavis
2359-31 rerun proton
TPI-2359-31
1.0000
1.6144
0.8724
3.2729
0.9349
0.8290
2.4109
1.6185
1.4381
1.4734
2.7902
3.1868
4.0767
1.4190
7.2964
2.4426
[ppm]
[rel]

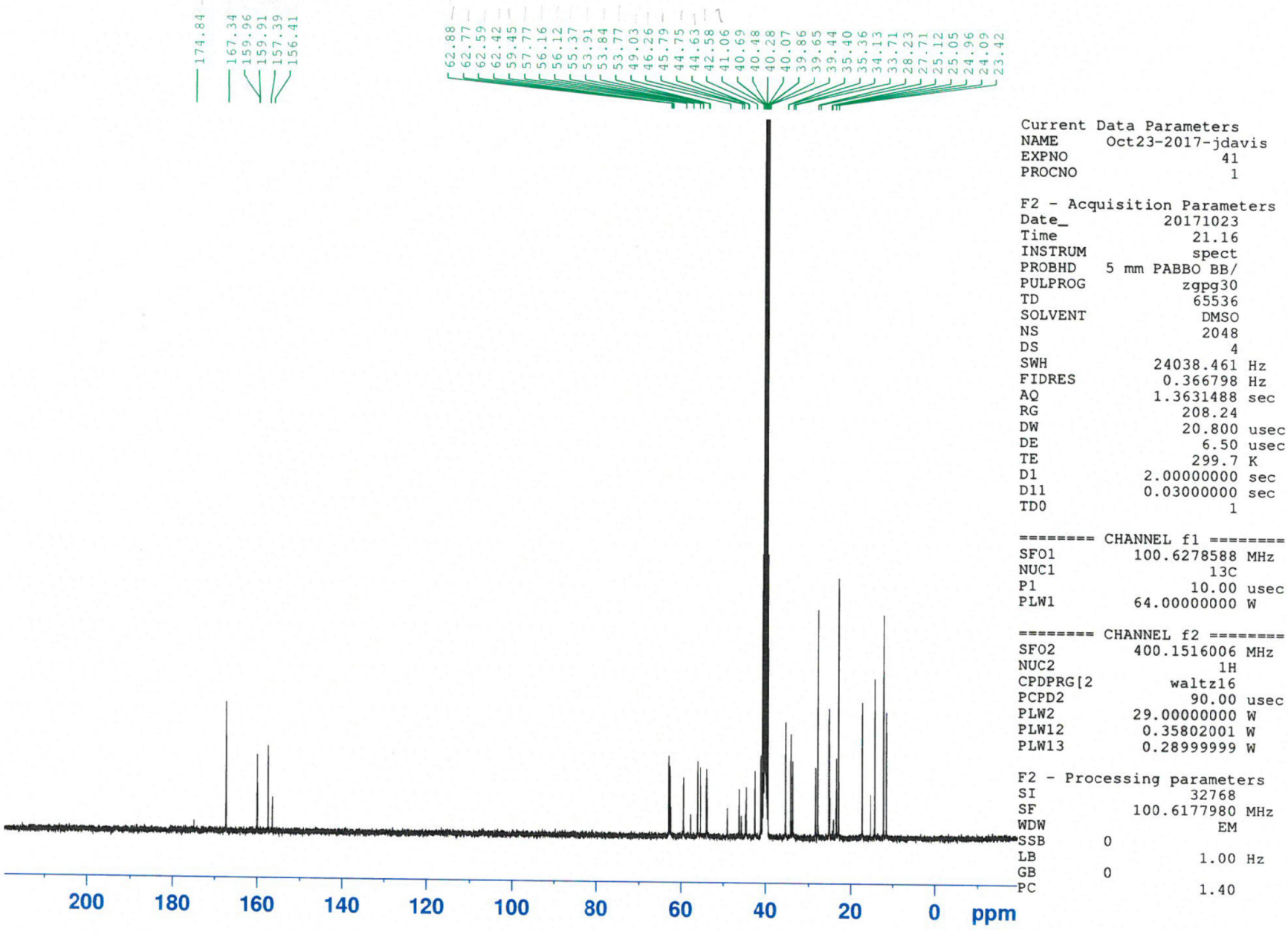
2359-31 pure C13



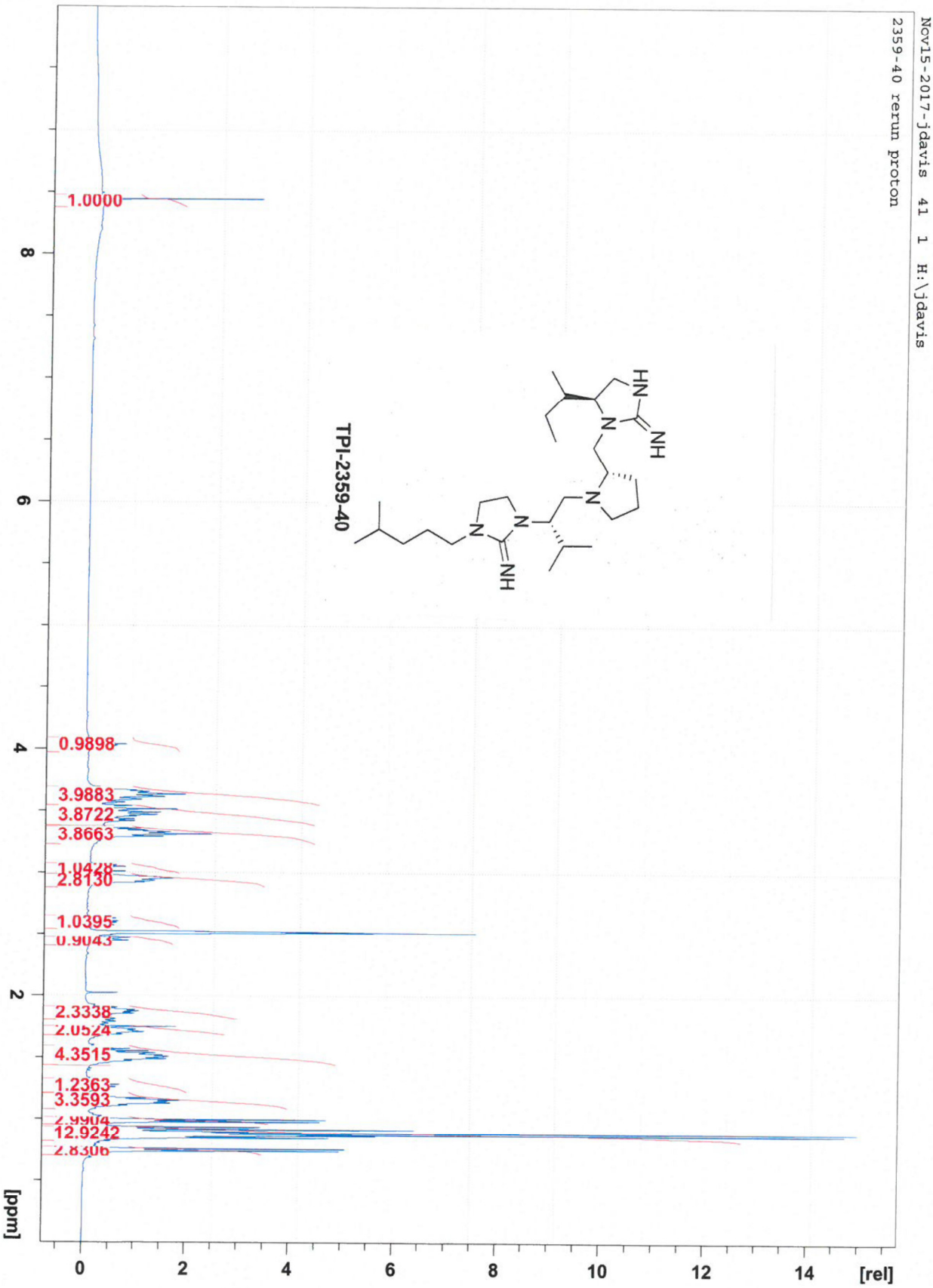

```
Current Data Parameters
NAME      Oct23-2017-jdavis
EXPNO                   31
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171023
Time               18.51
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 2048
DS                    4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ           1.3631488 sec
RG              208.24
DW              20.800 usec
DE               6.50 usec
TE              299.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1                13C
P1                10.00 usec
PLW1        64.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        29.00000000 W
PLW12        0.35802001 W
PLW13        0.28999999 W

F2 - Processing parameters
SI                32768
SF          100.6177980 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


Nov15-2017-jdavis 31 1 H:\jdavis
2359-32 rerun proton
TPI-2359-32
HN
NH
N
N
N
N
OH
NH
1.0000
1.5779
0.8850
1.4762
3.2834
1.0088
2.4127
0.6083
0.9972
1.5568
1.5783
2.6530
1.6986
2.5615
2.1233
3.0457
9.9600
2.3651
8
6
4
2
[ppm]
0
2
4
6
8
10
12
14
[rel]

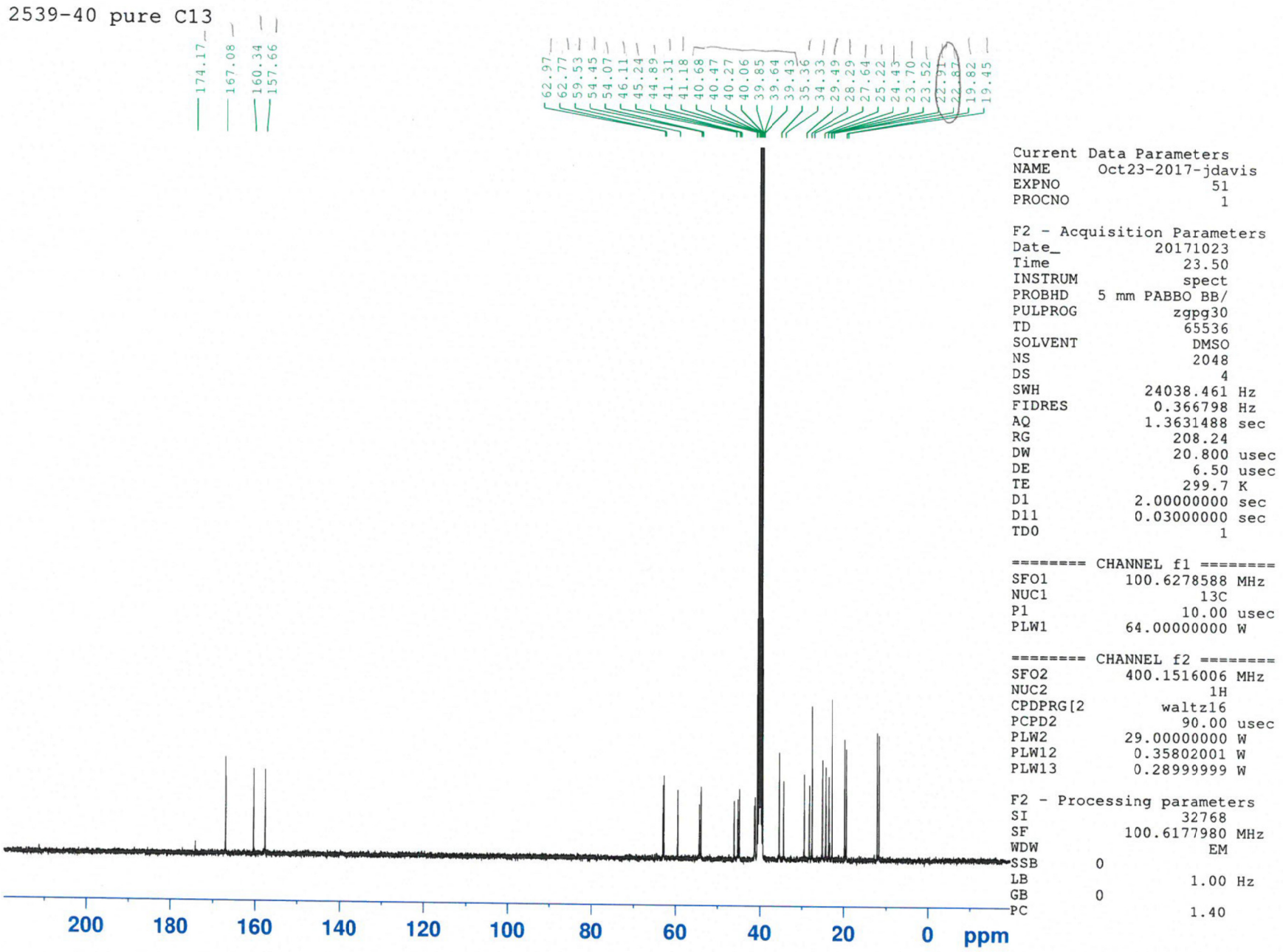
2359-32 pure C13



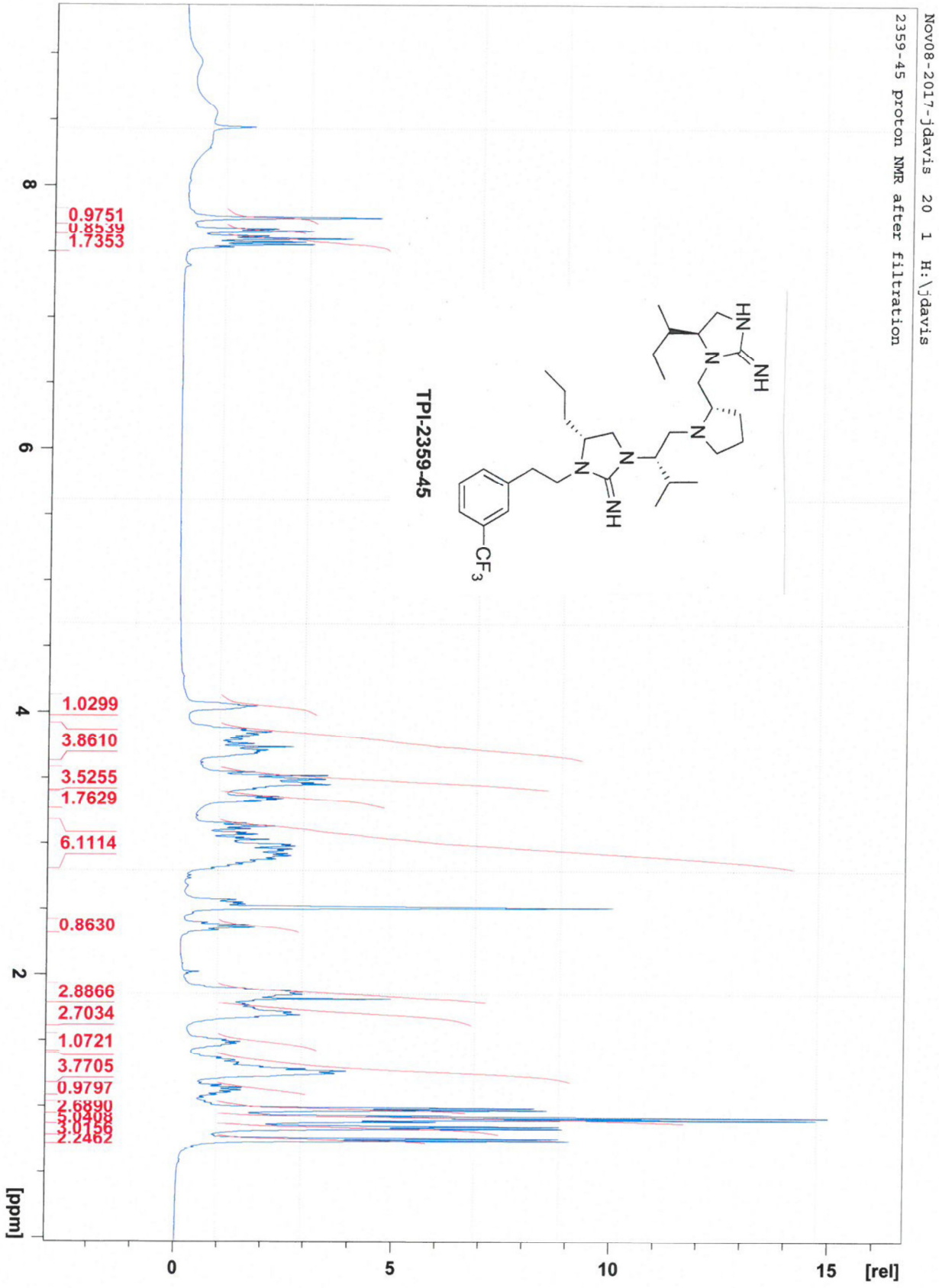

```
Current Data Parameters
NAME      Oct23-2017-jdavis
EXPNO                   41
PROCNO                   1

F2 - Acquisition Parameters
Date_            20171023
Time                21.16
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT              DMSO
NS                   2048
DS                      4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                208.24
DW                20.800 usec
DE                 6.50 usec
TE                299.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1                13C
P1                10.00 usec
PLW1         64.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2                 1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2         29.00000000 W
PLW12         0.35802001 W
PLW13         0.28999999 W

F2 - Processing parameters
SI                  32768
SF          100.6177980 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


Nov15-2017-jdavis 41 1 H:\jdavis
2359-40 rerun proton
TPI-2359-40
1.0000
0.9898
3.9883
3.8722
3.8663
2.8130
1.0395
2.3338
4.3515
1.2363
3.3593
12.9242
[ppm]
[rel]

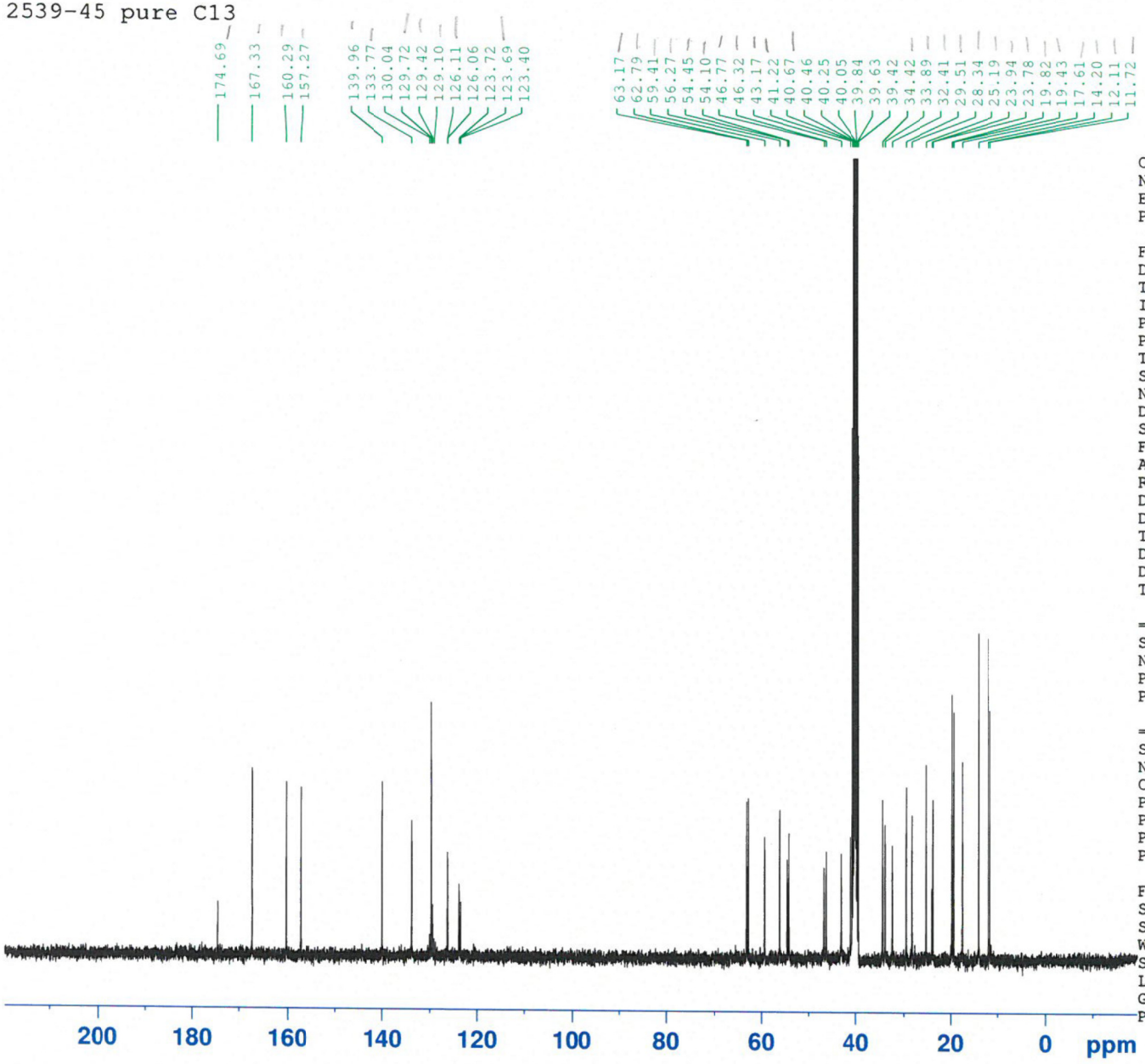
2539-40 pure C13



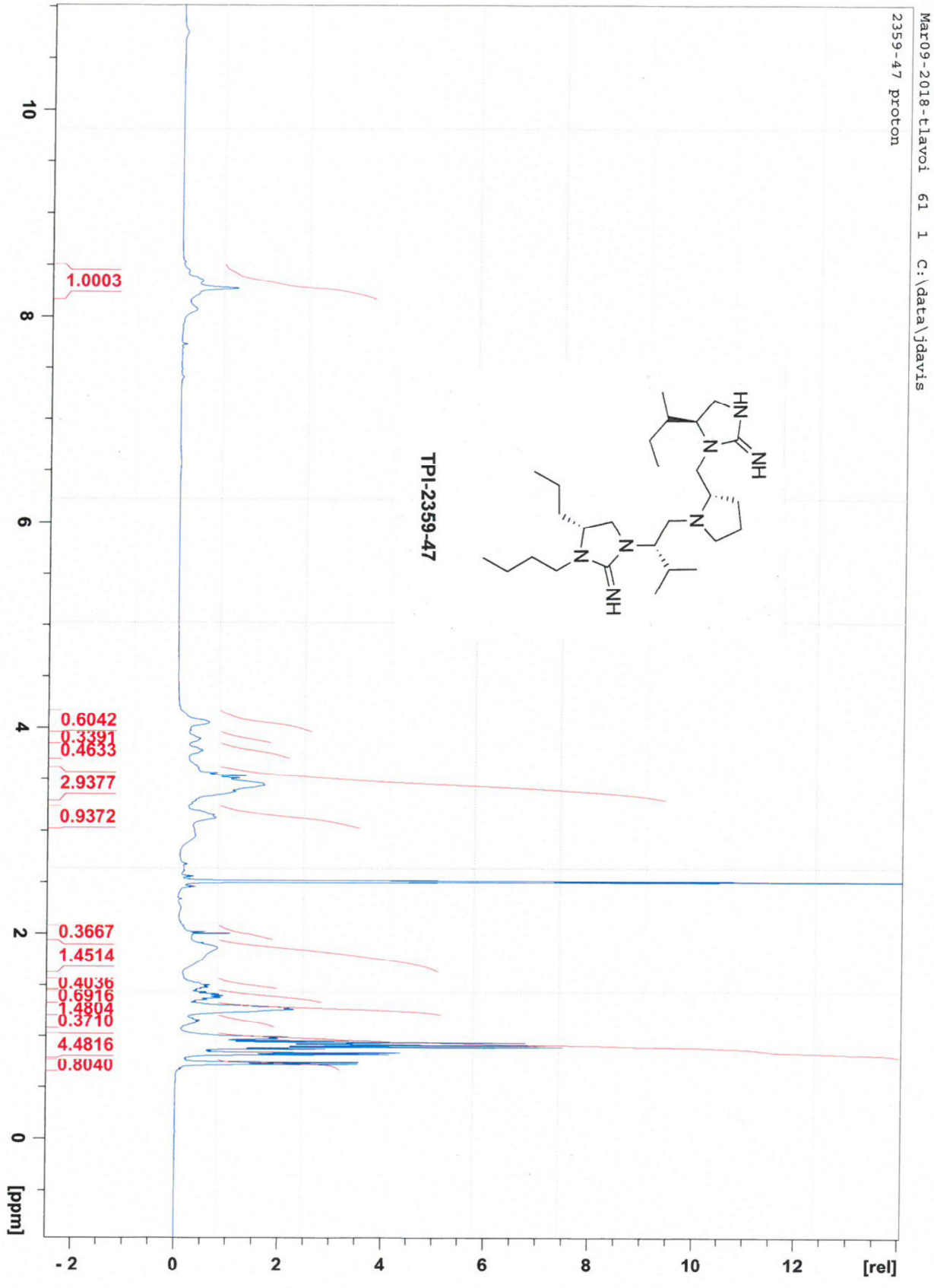

```
Current Data Parameters
NAME      Oct23-2017-jdavis
EXPNO                   51
PROCNO                   1

F2 - Acquisition Parameters
Date_             20171023
Time                 23.50
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                    2048
DS                       4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                 208.24
DW                 20.800 usec
DE                  6.50 usec
TE                 299.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          100.6278588 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          64.00000000 W

======== CHANNEL f2 ========
SFO2          400.1516006 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          29.00000000 W
PLW12          0.35802001 W
PLW13          0.28999999 W

F2 - Processing parameters
SI                    32768
SF            100.6177980 MHz
WDW                      EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```


Nov08-2017-jdavis 20 1 H:\jdavis
2359-45 proton NMR after filtration
TPI-2359-45
HN
NH
N
N
N
N
NH
CF3
0.9751
0.8539
1.7353
1.0299
3.8610
3.5255
1.7629
6.1114
0.8630
2.8866
2.7034
1.0721
3.7705
0.9797
2.6890
5.0408
3.0156
2.2462
8
6
4
2
[ppm]
0
5
10
15
[rel]

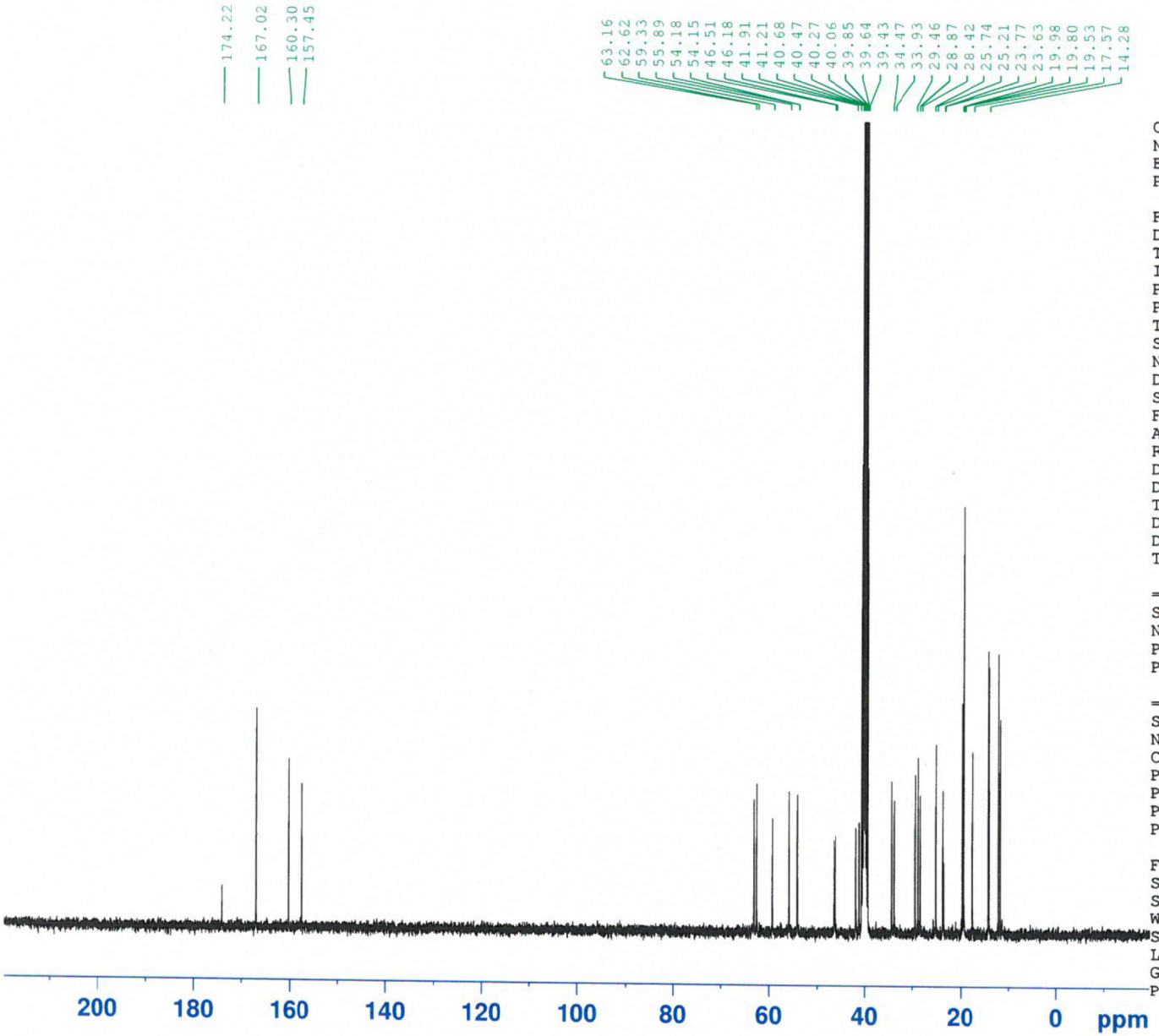
2539-45 pure C13



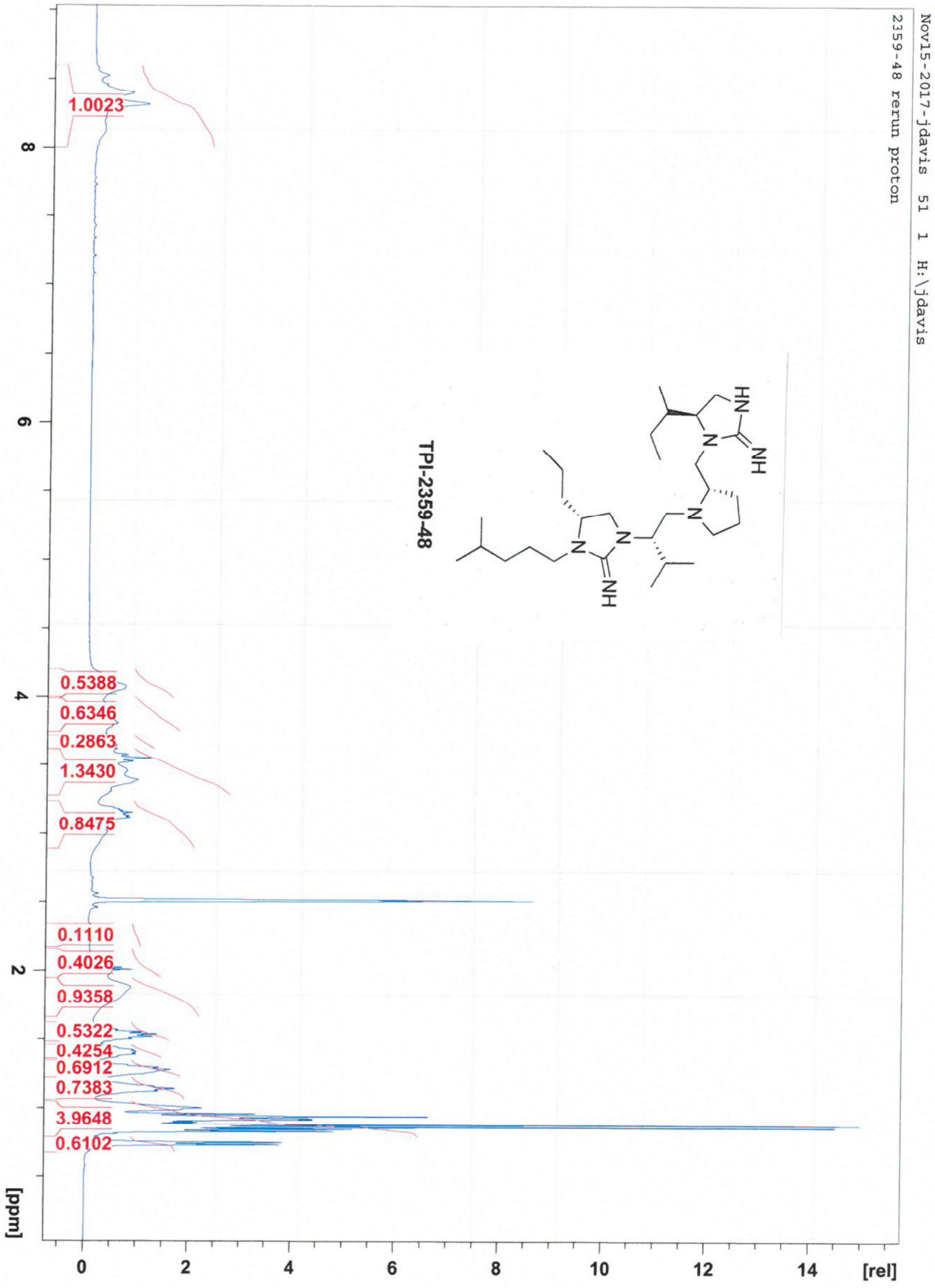

```
Current Data Parameters
NAME      Oct23-2017-jdavis
EXPNO                   61
PROCNO                   1

F2 - Acquisition Parameters
Date_              20171024
Time                  2.16
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    2048
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                  208.24
DW                  20.800 usec
DE                   6.50 usec
TE                  299.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          100.6278588 MHz
NUC1                  13C
P1                  10.00 usec
PLW1          64.00000000 W

======== CHANNEL f2 ========
SFO2          400.1516006 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2          29.00000000 W
PLW12          0.35802001 W
PLW13          0.28999999 W

F2 - Processing parameters
SI                   32768
SF            100.6177980 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```


Mar09-2018-tlavoi 61 1 C:\data\jdavis
2359-47 proton
TPI-2359-47
1.0003
0.6042
0.3391
0.4633
2.9377
0.9372
0.3667
1.4514
0.4036
0.6916
1.4804
0.3710
4.4816
0.8040
[ppm]
[rel]

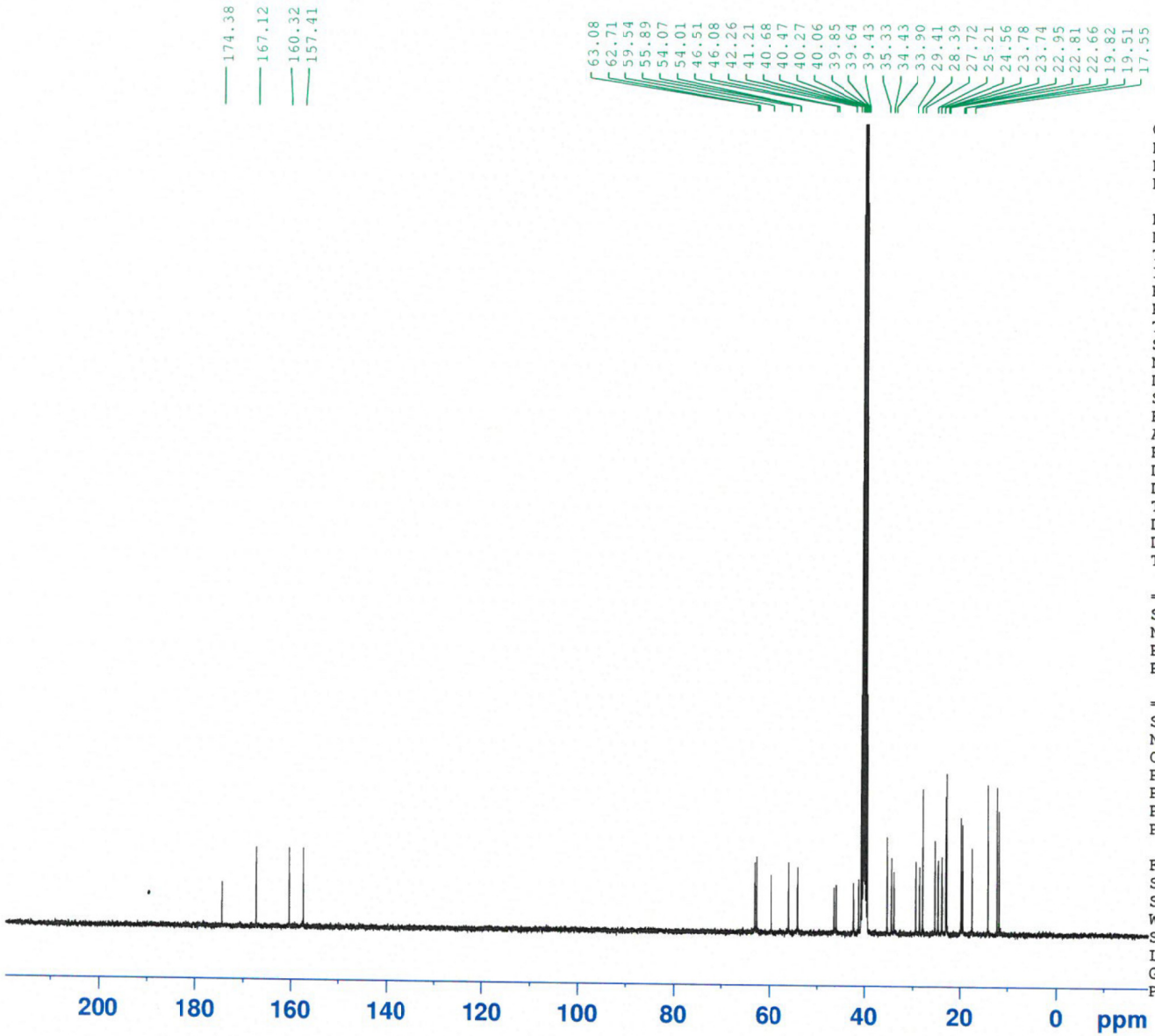
2539-47 pure C13




```
Current Data Parameters
NAME      Oct23-2017-jdavis
EXPNO                   71
PROCNO                   1

F2 - Acquisition Parameters
Date_              20171024
Time                   4.41
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     2048
DS                        4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                  208.24
DW                20.800 usec
DE                 6.50 usec
TE                299.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          100.6278588 MHz
NUC1                   13C
P1                 10.00 usec
PLW1          64.00000000 W

======== CHANNEL f2 ========
SFO2          400.1516006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2              90.00 usec
PLW2          29.00000000 W
PLW12          0.35802001 W
PLW13          0.28999999 W

F2 - Processing parameters
SI                     32768
SF            100.6177980 MHz
WDW                       EM
SSB       0
LB                  1.00 Hz
GB        0
PC                     1.40
```


Nov15-2017-jdavis 51 1 H:\jdavis
2359-48 rerun proton
TPI-2359-48
1.0023
0.5388
0.6346
0.2863
1.3430
0.8475
0.1110
0.4026
0.9358
0.5322
0.4254
0.6912
0.7383
3.9648
0.6102
[ppm]
[rel]

2539-48 pure C13



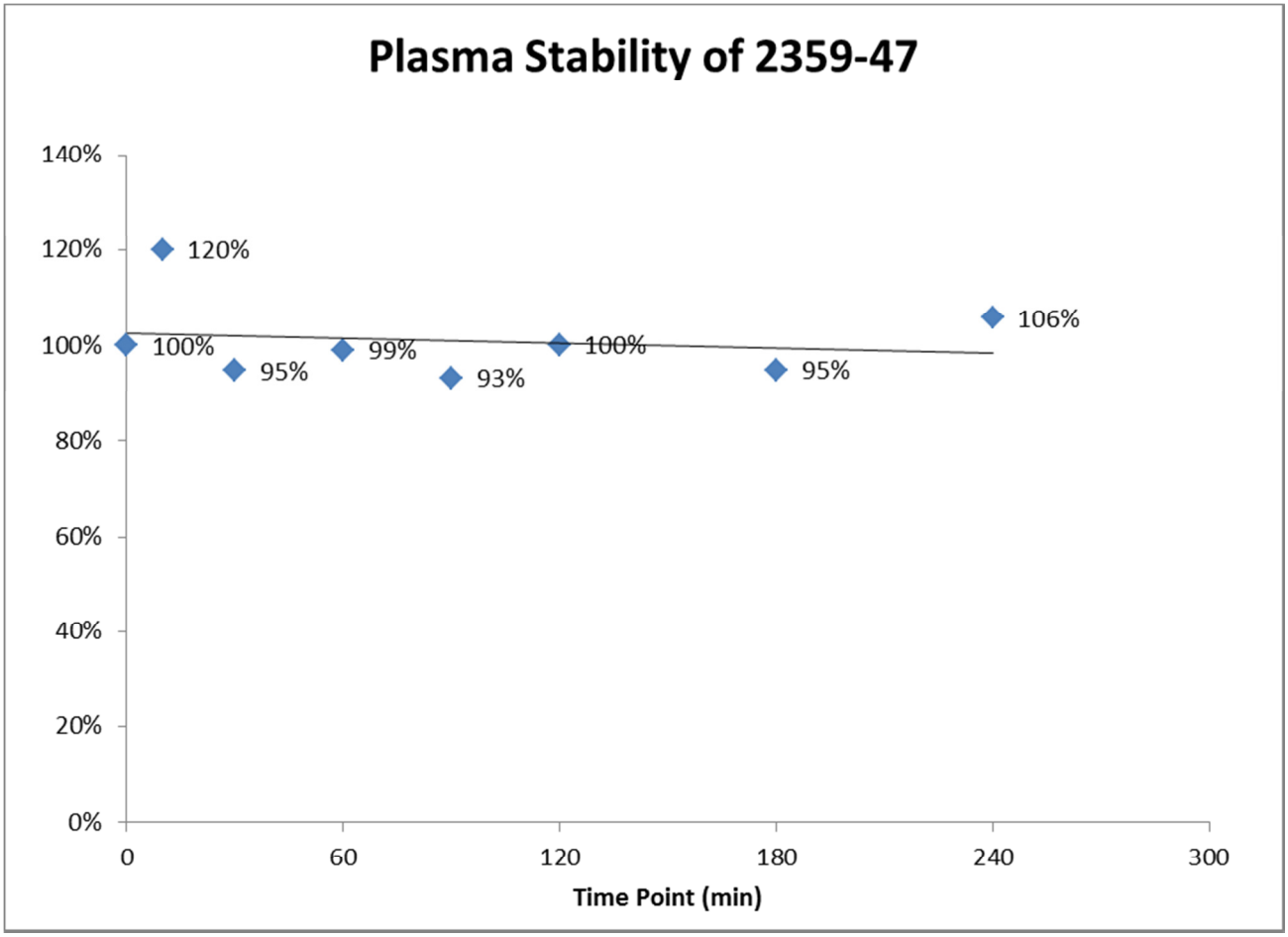
Current Data Parameters
NAME Oct23-2017-jdavis
EXPNO 81
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171024
Time 7.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 208.24
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 64.00000000 W

======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 29.00000000 W
PLW12 0.35802001 W
PLW13 0.28999999 W

F2 - Processing parameters
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



The percentage of analyte detected compared to time point zero.