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שם גלמן דניאל (רב' א' בר' מלוס)

מחלקה _____ סמון החומר DG-8

היסודות שהחומר מכיל: C, H, N תכונות מיוחדות _____

נ.ר. או נ.ה. (ממס הגיבוש) _____

נא לקבוע: C, H, N מס' תקציב _____

נא לא למלא מס' אנליזה 0903 תאריך קבלה _____

	C	H	N	S	Cl, Br	O	F	P	
% מחושב	87.63	5.97	6.38						
% נמצא	87.33	6.25	6.48	*					

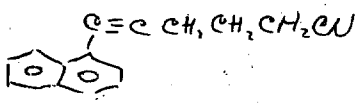
THE HEBREW UNIVERSITY JERUSALEM FACULTY OF SCIENCE
האוניברסיטה העברית בירושלים
המכון לכימיה

הערות

חומר חדש

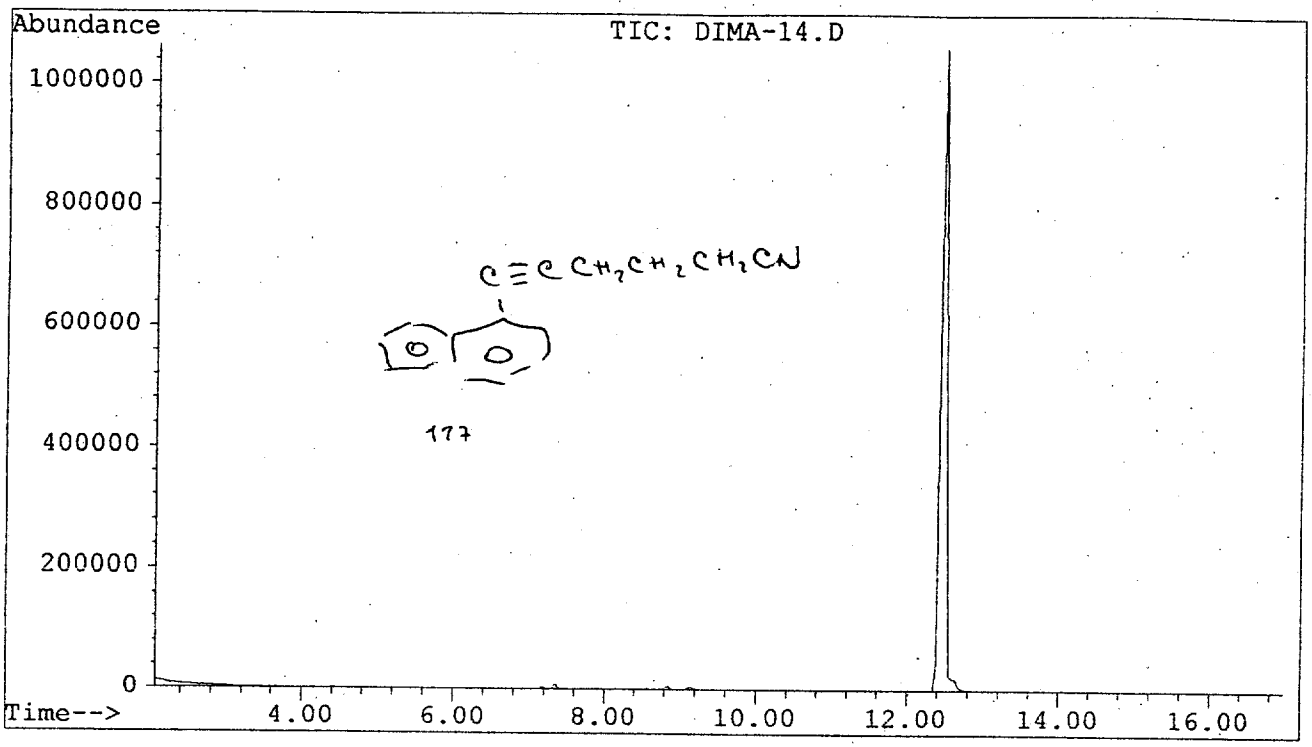
MW = 219.28116

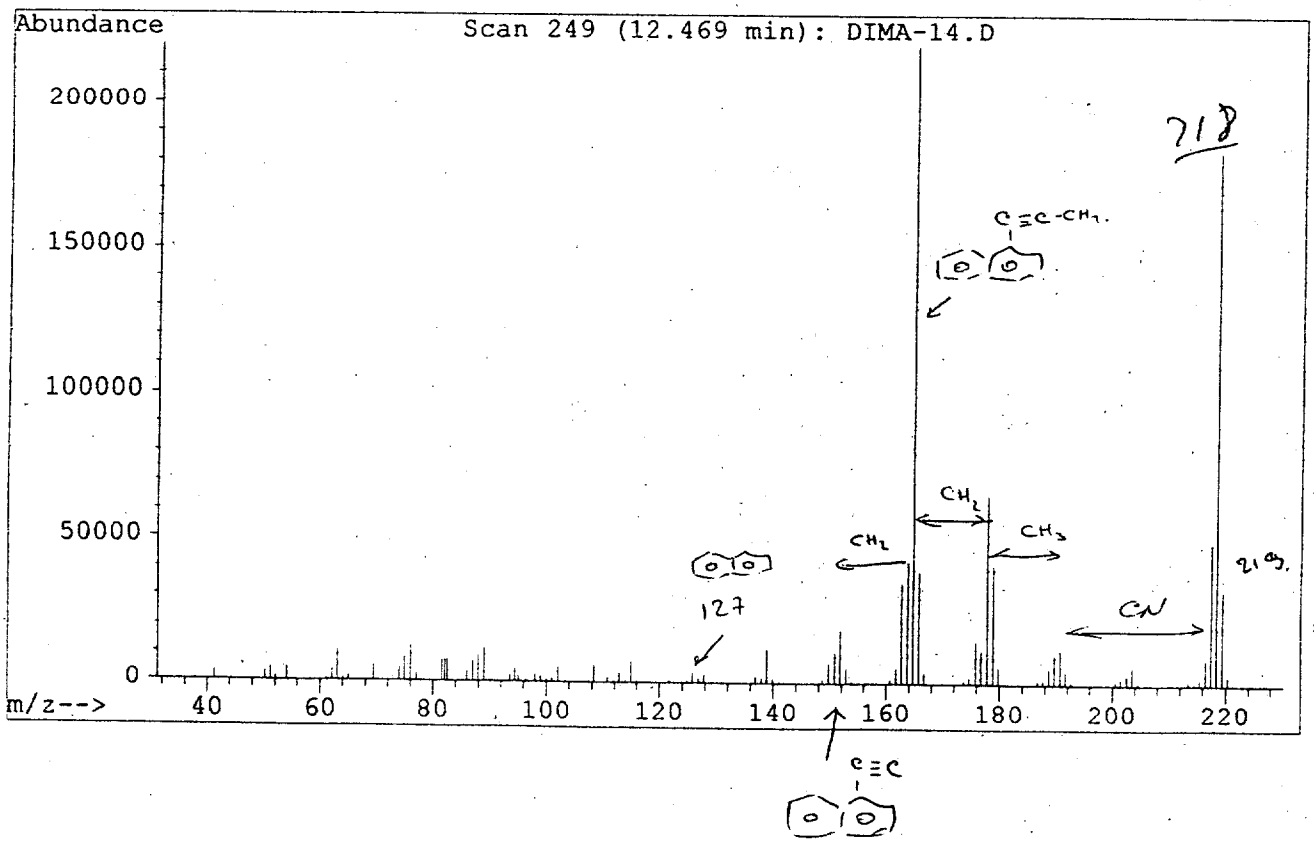
סוג החרכובת או נוסחת מבנה



$C_{16}H_{13}N$

File : C:\HPCHEM\1\DATA\DIMA-14.D
Operator :
Acquired : 28 Jan 102 1:19 pm using AcqMethod NOR
Instrument : 5989x - I
Sample Name: 14
Misc Info :
Vial Number: 1





14

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
41.20	3290	69.50	5524	87.95	9220	107.40	618
50.15	3312	74.00	5184	88.95	11784	108.40	5889
51.15	4715	75.00	8403	93.55	2089	110.80	1675
52.15	1566	76.00	12588	94.45	4580	111.90	617
54.15	4727	77.00	2768	95.05	1971	112.90	3103
55.15	546	81.50	7773	96.45	852	113.90	899
61.05	785	82.10	7907	97.95	2796	114.90	7602
62.05	3920	82.50	7919	98.95	2057	115.90	759
63.05	10975	85.00	661	99.95	1137	121.80	693
64.05	1003	86.00	3496	100.95	1596	124.85	954
65.05	1635	86.95	6930	101.95	5778	125.85	3602

Scan 249 (12.469 min): DIMA-14.D

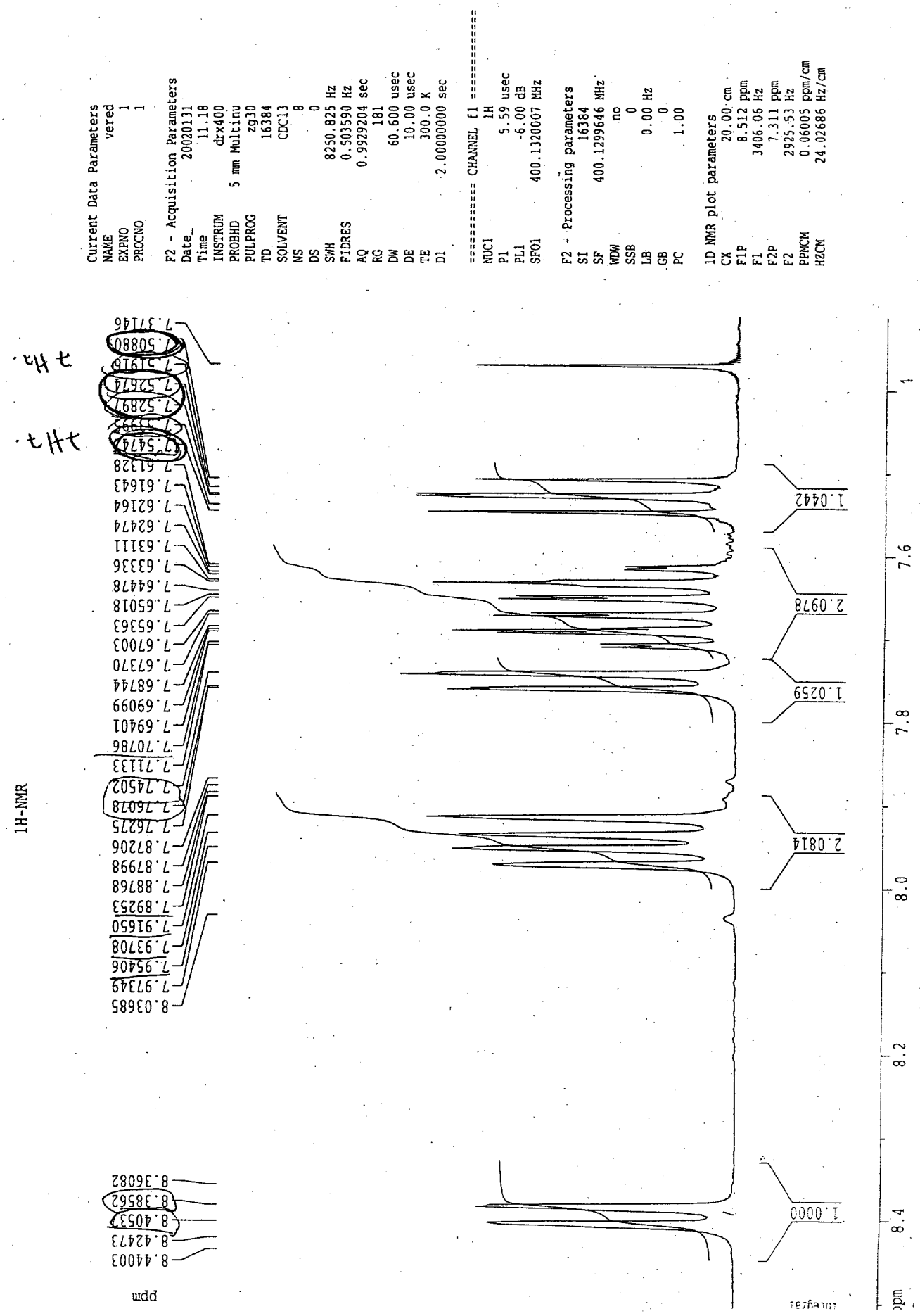
14

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
126.85	1761	152.80	5405	175.75	14937	192.60	974
127.85	2643	153.80	627	176.75	11763	200.55	1381
136.85	2318	160.70	1334	177.75	65720	201.55	2134
137.85	1793	161.70	5181	178.75	41168	202.55	3284
138.85	11965	162.65	34648	179.75	5711	203.55	6310
139.85	1669	163.75	42480	186.60	1168	204.55	1128
140.85	558	164.65	219840	187.60	1427	213.45	1345
148.70	1294	165.75	38752	188.60	5341	214.45	666
149.80	7025	166.65	3703	189.60	10409	215.45	1951
150.80	10992	173.65	1389	190.60	12121	216.45	8938
151.80	18704	174.65	2039	191.60	4641	217.45	49568

Scan 249 (12.469 min): DIMA-14.D

14

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
218.40	183936						
219.40	32592						
220.40	2926						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EXPNO 1
PROCNO 1
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Date_ 20020131
Time 11.18
INSTRUM drx400
PROBHD 5 mm Multinu
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 8
DS 0
SWH 8250.825 Hz
FIDRES 0.503590 Hz
AQ 0.9929204 sec
RG 181
DW 60.600 usec
DE 10.00 usec
TE 300.0 K
D1 2.00000000 sec
========== CHANNEL f1 ==========
NUC1 1H
P1 5.59 usec
PL1 -6.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1299646 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 8.512 ppm
F1 3406.06 Hz
F2P 7.311 ppm
F2 2925.53 Hz
PPMCM 0.06005 ppm/cm
HZCM 24.02686 Hz/cm
1H-NMR
ppm
integral
1.0000
2.0814
1.0259
2.0978
1.0442
1H
1H
8.44003
8.42473
8.40537
8.38562
8.36082
8.03685
7.97349
7.95406
7.93708
7.91650
7.89253
7.88768
7.87998
7.87206
7.76275
7.76078
7.74502
7.71133
7.70786
7.69401
7.69099
7.68744
7.67370
7.67003
7.65363
7.65018
7.64478
7.63336
7.63111
7.62474
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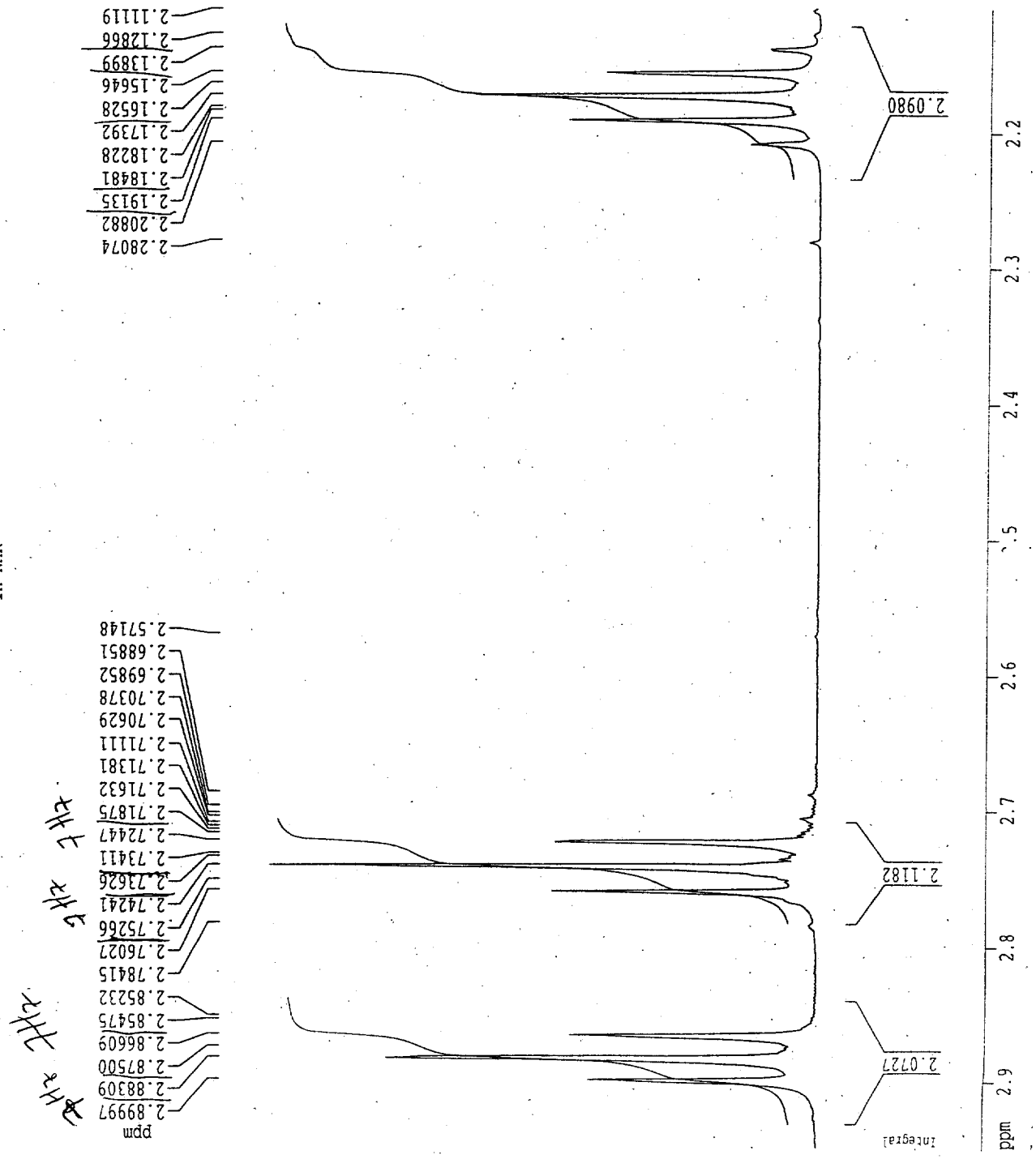
1H-NMR

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Current Data Parameters
NAME                 vered
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20020131
Time                 11.18
INSTRUM           drx400
PROBHD   5 mm Multinu
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8250.825 Hz
FIDRES          0.503590 Hz
AQ              0.9929204 sec
RG                   181
DW                60.600 usec
DE                10.00 usec
TE                 300.0 K
D1          2.00000000 sec

========== CHANNEL f1 ==========
NUC1                  1H
P1                  5.59 usec
PL1                -6.00 dB
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                 16384
SF          400.1299646 MHz
WDW                   no
SSB                    0
LB                0.00 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                20.00 cm
F1P                2.950 ppm
F1              1180.39 Hz
F2P                2.108 ppm
F2               843.59 Hz
PPMCM          0.04209 ppm/cm
HZCM           16.84003 Hz/cm
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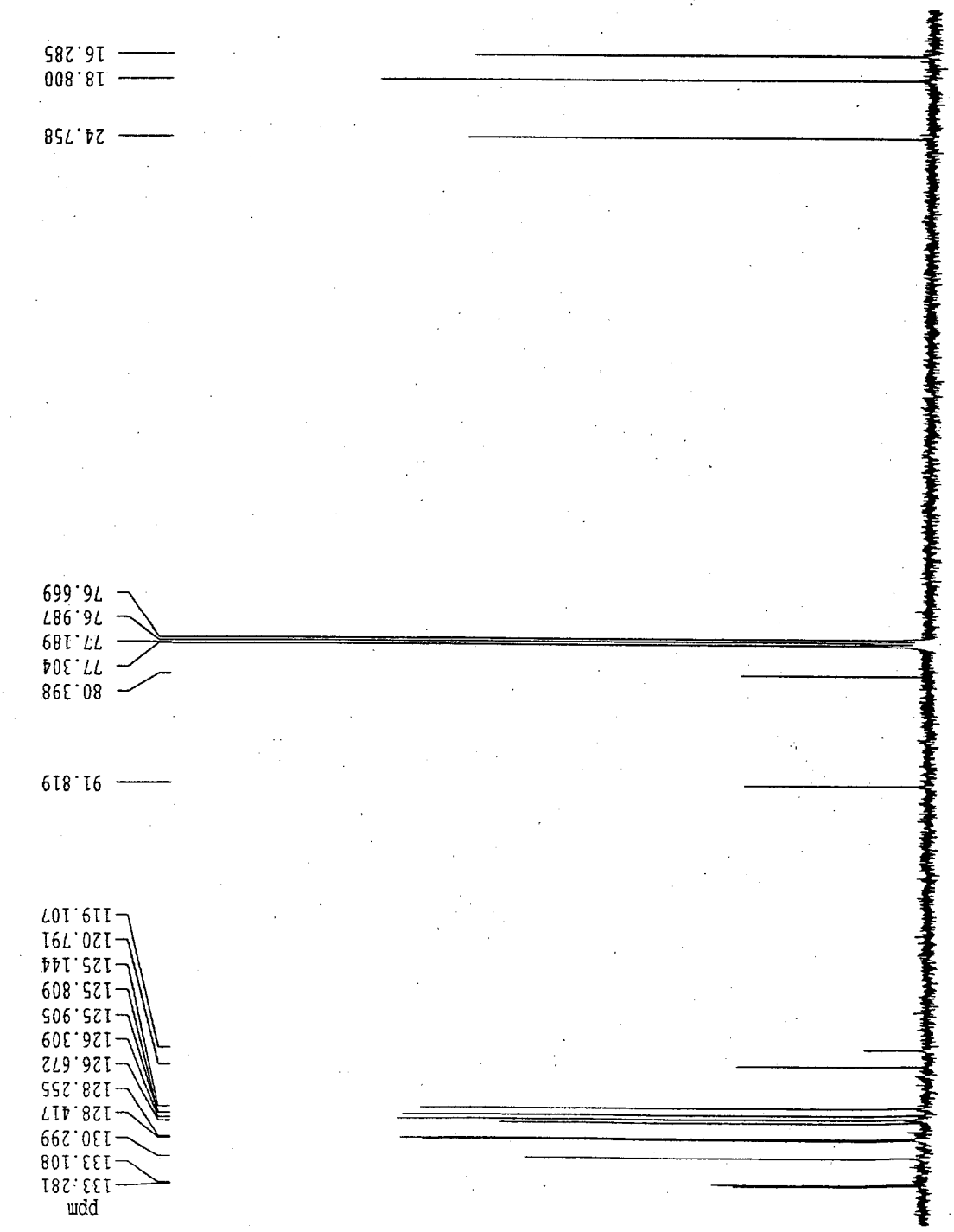
13C-NMR

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Current Data Parameters
NAME      cyanopentyne
EXPNO            1
PROCNO           1

F2 - Acquisition Parameters
Date_        20020131
Time            10.44
INSTRUM       drx400
PROBHD   5 mm Multinu
PULPROG      zgpg30
TD            65536
SOLVENT       CDCl3
NS              916
DS                2
SWH          31746.031 Hz
FIDRES        0.484406 Hz
AQ            1.0322419 sec
RG               8192
DW             15.750 usec
DE             30.00 usec
TE             300.0 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
========== CHANNEL f1 ==========
NUC1             13C
P1              7.19 usec
PL1            -6.00 dB
SFO1     100.6254358 MHz
========== CHANNEL f2 ==========
CPDPRG2      waltz16
NUC2              1H
PCPD2        100.00 usec
PL2           120.00 dB
PL12           15.60 dB
PL13           15.60 dB
SFO2     400.1316005 MHz

F2 - Processing parameters
SI               32768
SF       100.6127778 MHz
WDW              EM
SSB               0
LB             1.00 Hz
GB                0
PC             1.40

1D NMR plot parameters
CX             20.00 cm
F1P           137.271 ppm
F1            13811.19 Hz
F2P            11.393 ppm
F2             1146.33 Hz
PPMCM         6.29386 ppm/cm
HZCM         633.24323 Hz/cm
```

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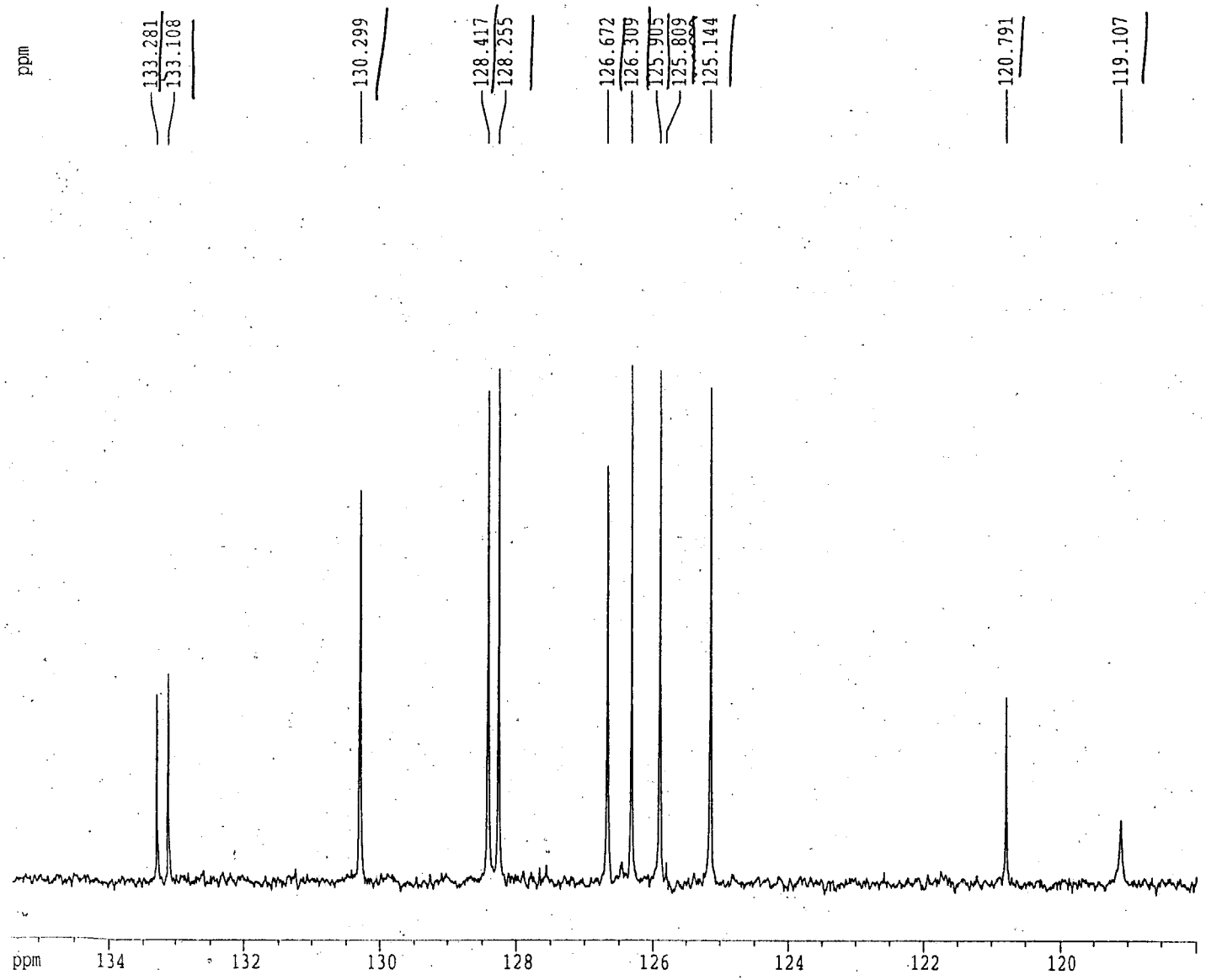
13C-NMR




```
Current Data Parameters
NAME        cyanopentyne
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20020131
Time                10.44
INSTRUM           drx400
PROBHD      5 mm Multinu
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   916
DS                     2
SWH            31746.031 Hz
FIDRES          0.484406 Hz
AQ             1.0322419 sec
RG                  8192
DW                15.750 usec
DE                 30.00 usec
TE                 300.0 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec

============ CHANNEL f1 =============
NUC1                 13C
P1                  7.19 usec
PL1                -6.00 dB
SFO1         100.6254358 MHz

============ CHANNEL f2 =============
CPDPRG2          waltz16
NUC2                  1H
PCPD2             100.00 usec
PL2               120.00 dB
PL12               15.60 dB
PL13               15.60 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127778 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                  20.00 cm
F1P                135.442 ppm
F1               13627.15 Hz
F2P                117.982 ppm
F2               11870.47 Hz
PPMCM             0.87299 ppm/cm
HZCM             87.83426 Hz/cm
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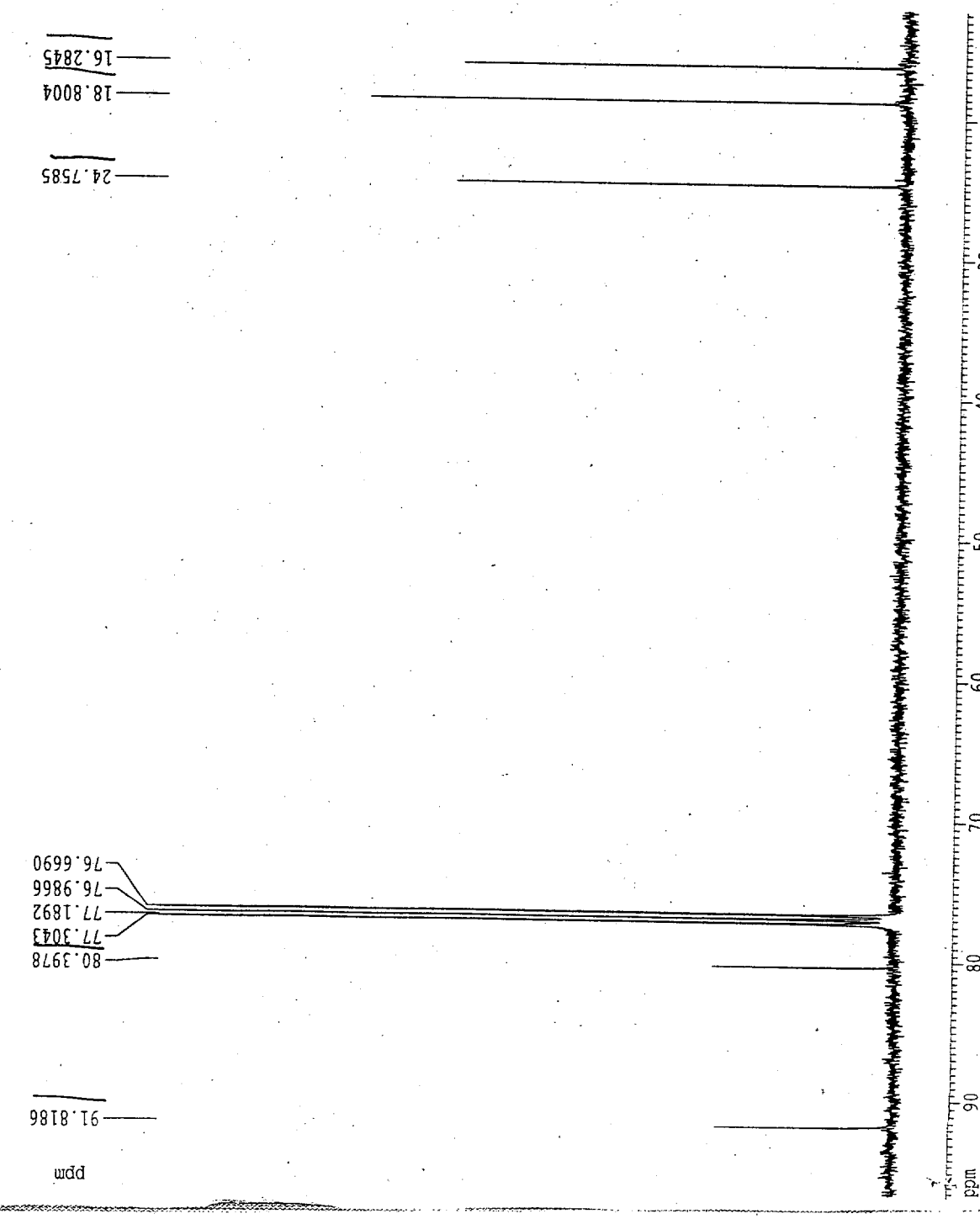
13C-NMR




```
Current Data Parameters
NAME        cyanopentyne
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20020131
Time              10.44
INSTRUM           drx400
PROBHD   5 mm Multinu
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 916
DS                   2
SWH           31746.031 Hz
FIDRES         0.484406 Hz
AQ           1.0322419 sec
RG                8192
DW              15.750 usec
DE              30.00 usec
TE               300.0 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
============ CHANNEL f1 ============
NUC1                13C
P1                 7.19 usec
PL1               -6.00 dB
SFO1        100.6254358 MHz
============ CHANNEL f2 ============
CPDPRG2          waltz16
NUC2                 1H
PCPD2           100.00 usec
PL2              120.00 dB
PL12              15.60 dB
PL13              15.60 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF          100.6127778 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                  20.00 cm
F1P                 96.840 ppm
F1                 9743.34 Hz
F2P                12.227 ppm
F2                 1230.20 Hz
PPMCM              4.23064 ppm/cm
HZCM             425.65686 Hz/cm
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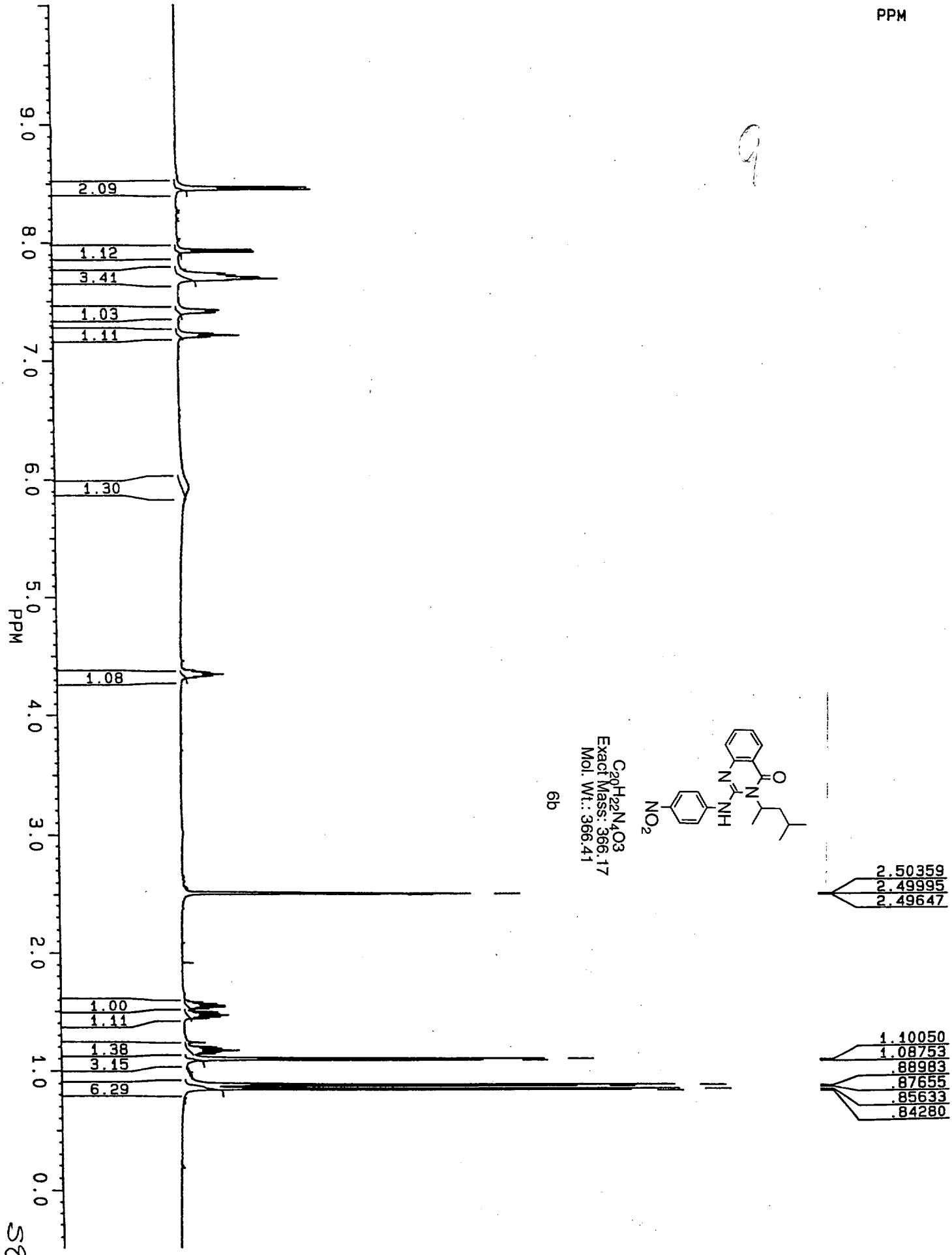
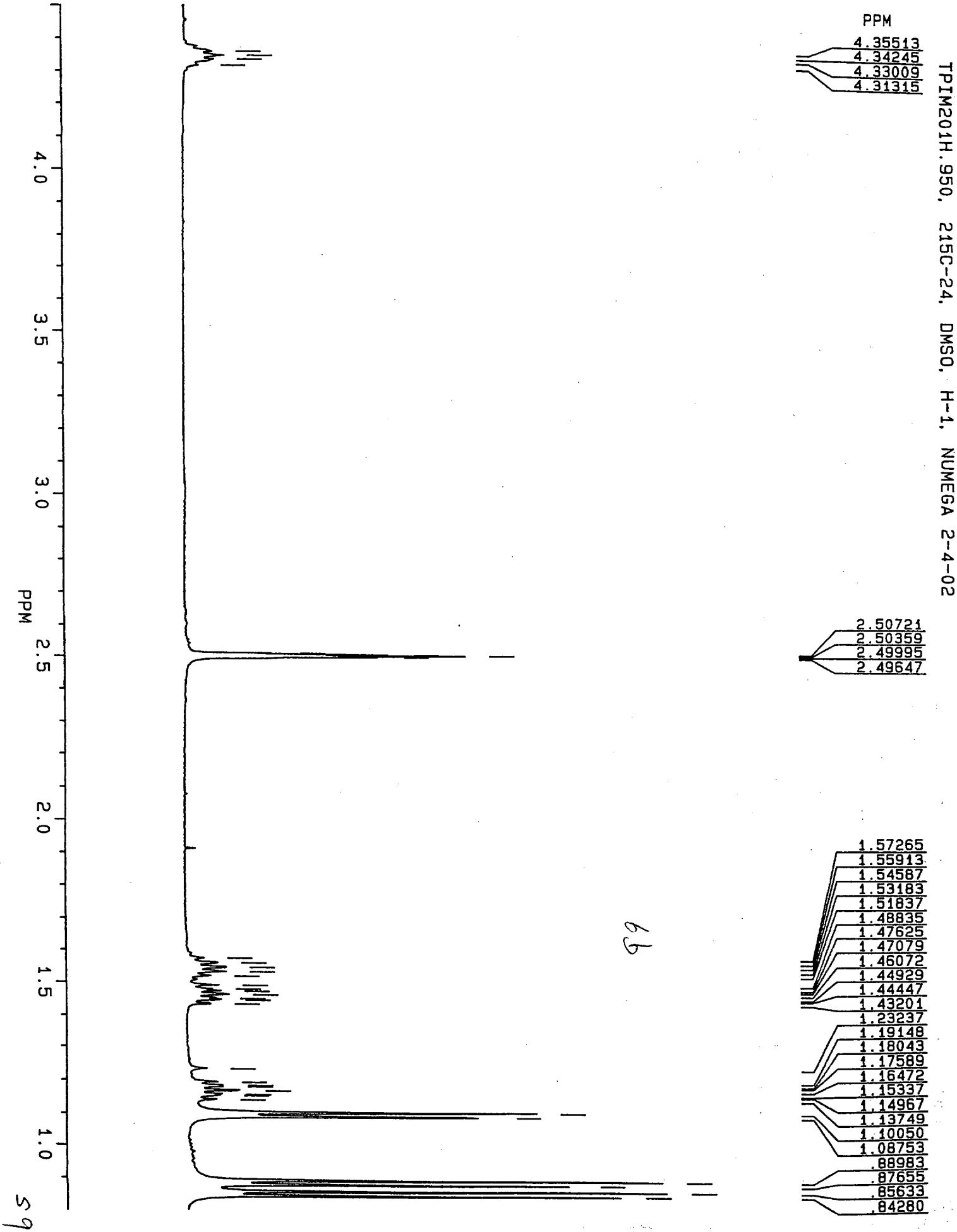

TPIM201H.950, 215C-24, DMSO, H-1, NUMEGA 2-4-02
PPM
9
$C_{20}H_{22}N_4O_3$
Exact Mass: 366.17
Mol. Wt.: 366.41
6b
NO_2
NH
N
N
O
2.50359
2.49995
2.49647
1.10050
1.08753
.88983
.87655
.85633
.84280
2.09
1.12
3.41
1.03
1.11
1.30
1.08
1.00
1.11
1.38
3.15
6.29
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
PPM


TPIM201H.950, 215C-24, DMSO, H-1, NUMEGA 2-4-02
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2.49995
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1.57265
1.55913
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1.53183
1.51837
1.48835
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1.47079
1.46072
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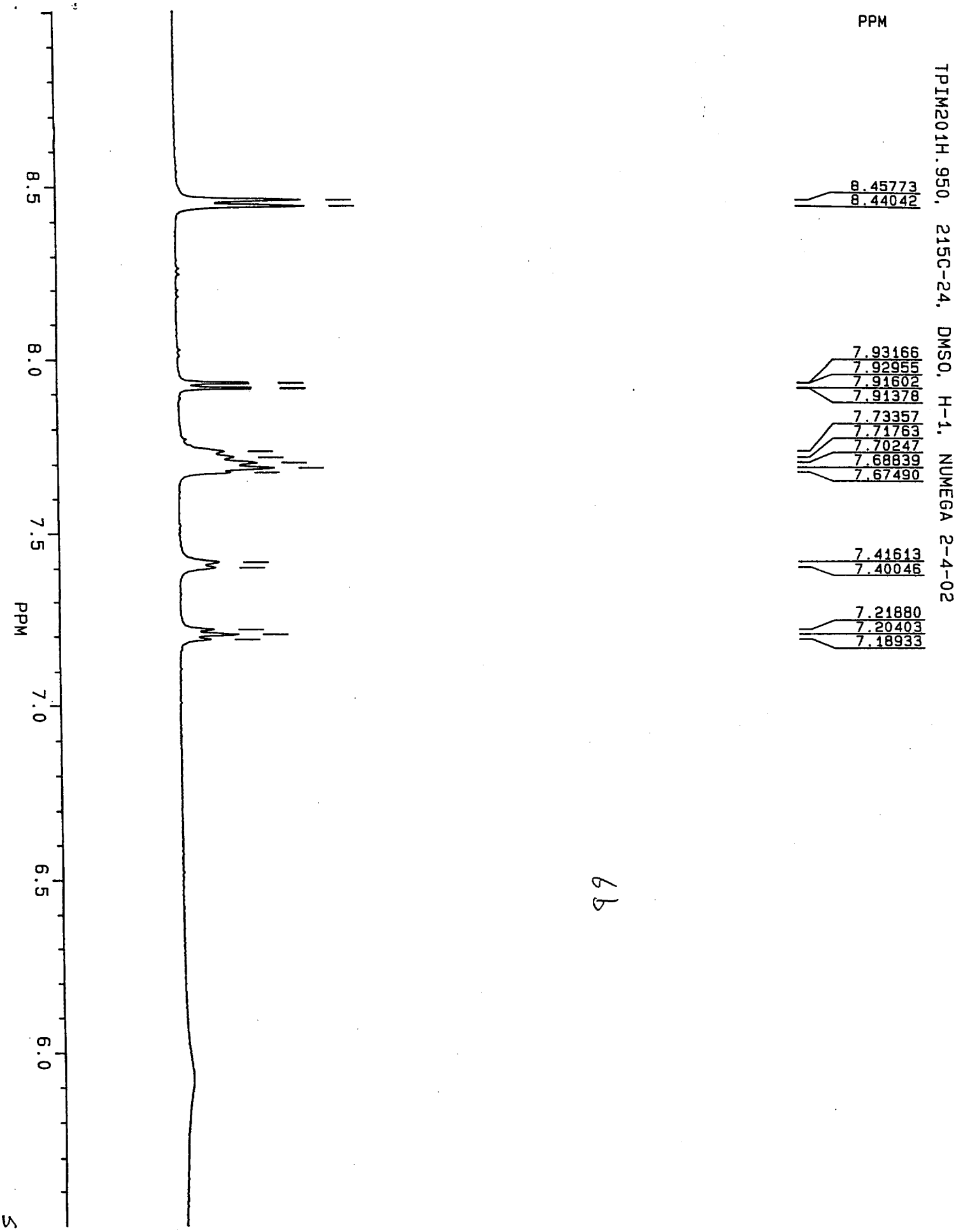
1.0
PPM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7.73357
7.71763
7.70247
7.68839
7.67490
7.41613
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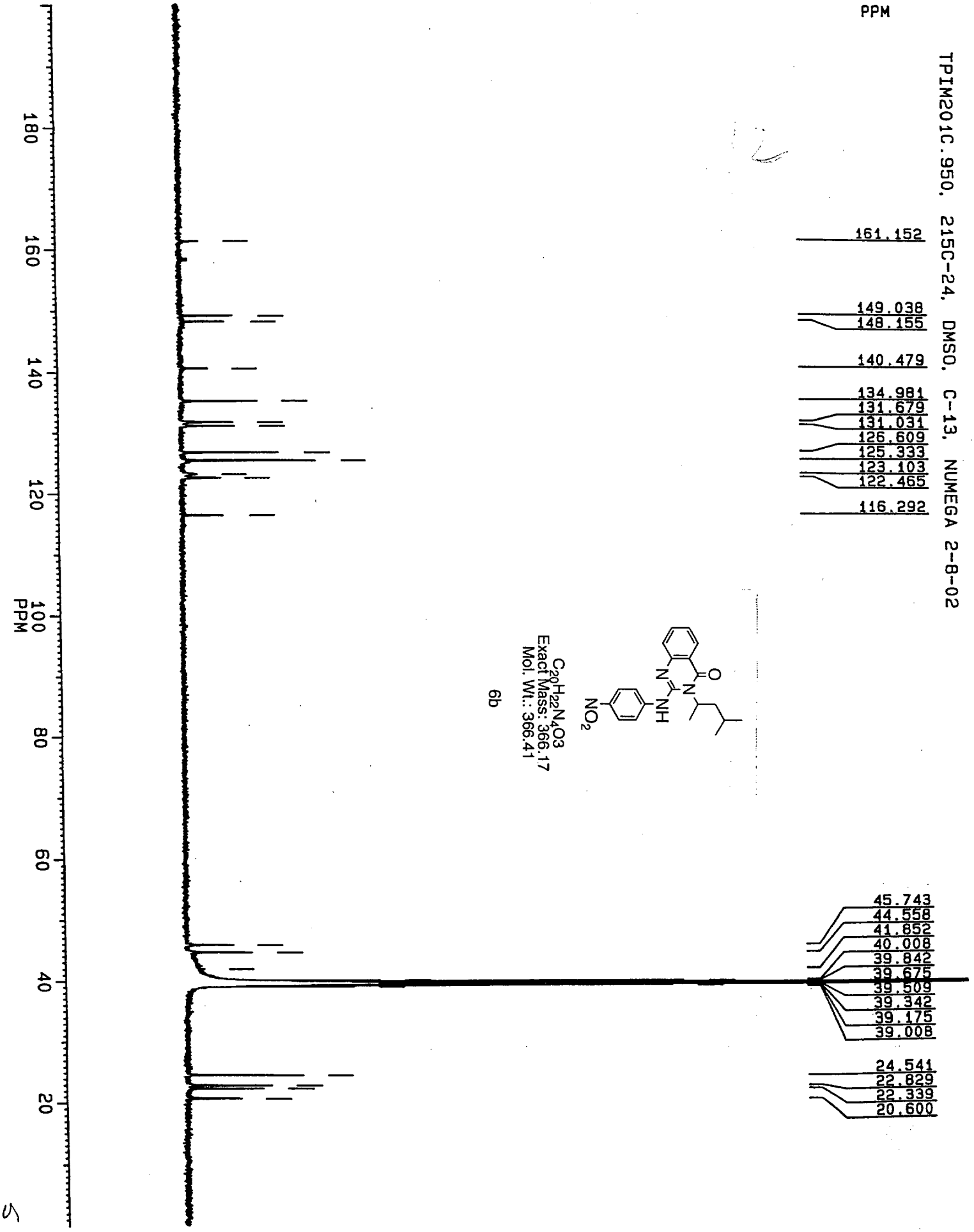
7.5
7.0
6.5
6.0
PPM


PPM
TPIM201C.950, 215C-24, DMSO, C-13, NUMEGA 2-8-02
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148.155
140.479
134.981
131.679
131.031
126.609
125.333
123.103
122.465
116.292
45.743
44.558
41.852
40.008
39.842
39.675
39.509
39.342
39.175
39.008
24.541
22.829
22.339
20.600
O
N
N
NH
NO2
C20H22N4O3
Exact Mass: 366.17
Mol. Wt.: 366.41
6b
180
160
140
120
100
PPM
80
60
40
20

S 11

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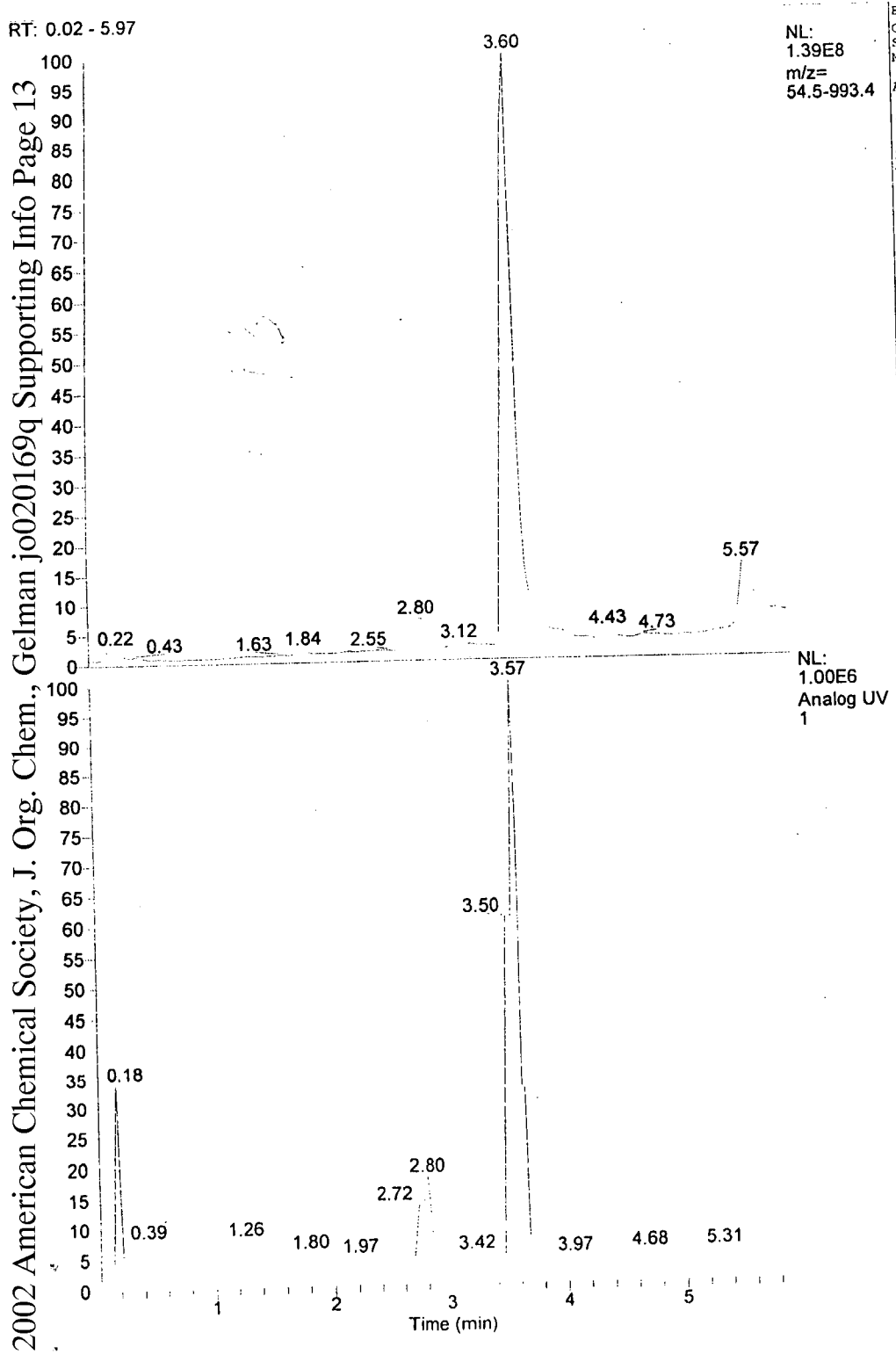

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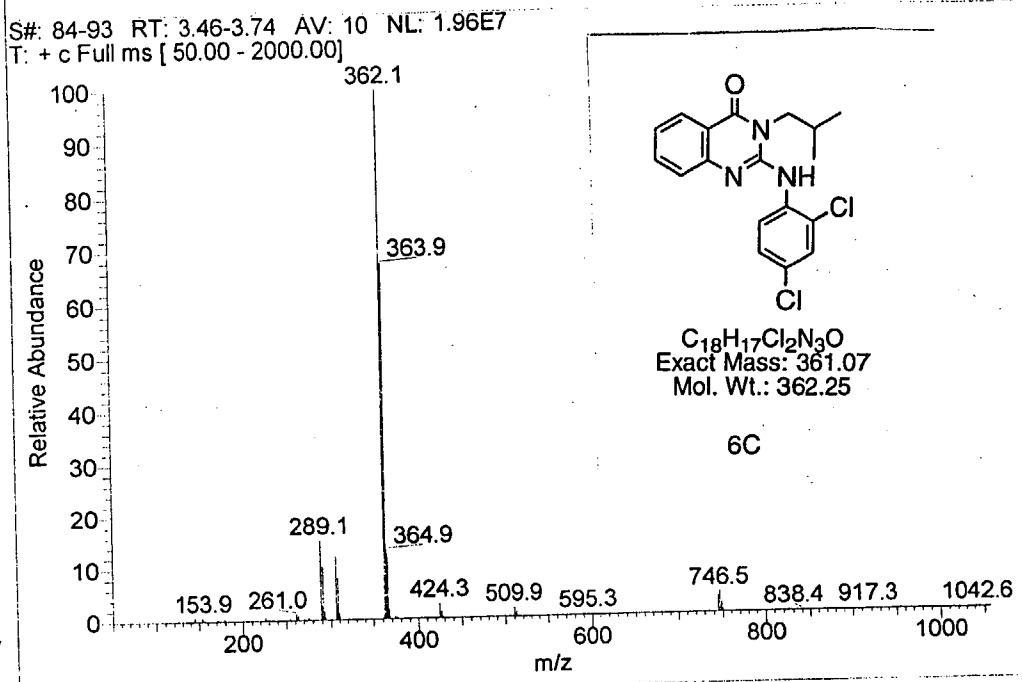
Summary: 5-95m8
MS Run Time (min): 6.00

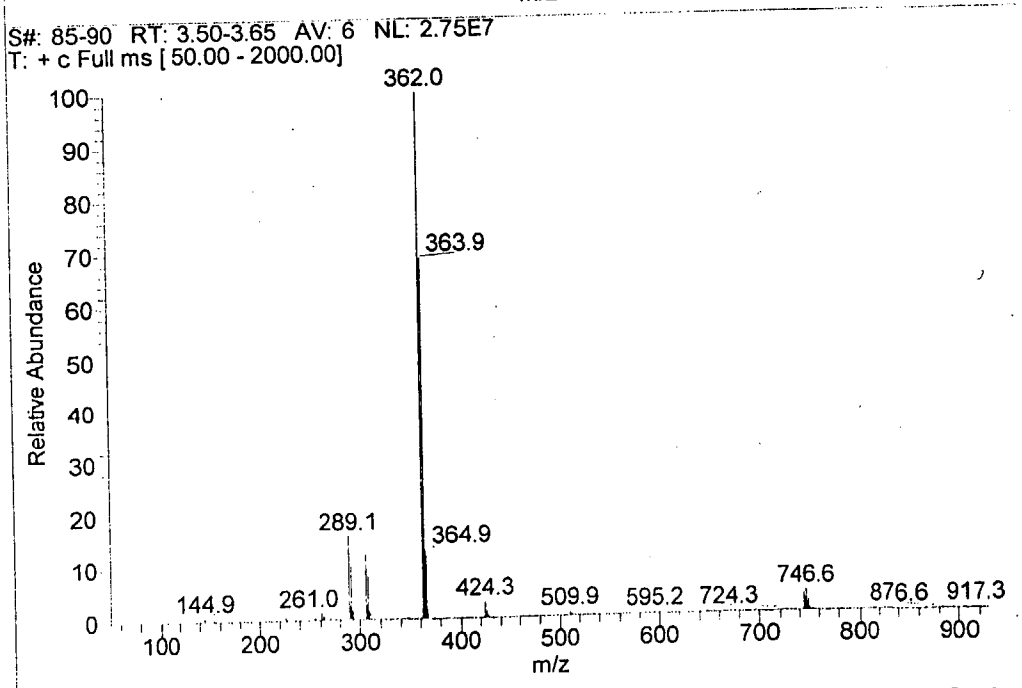
Autosampler Settings:

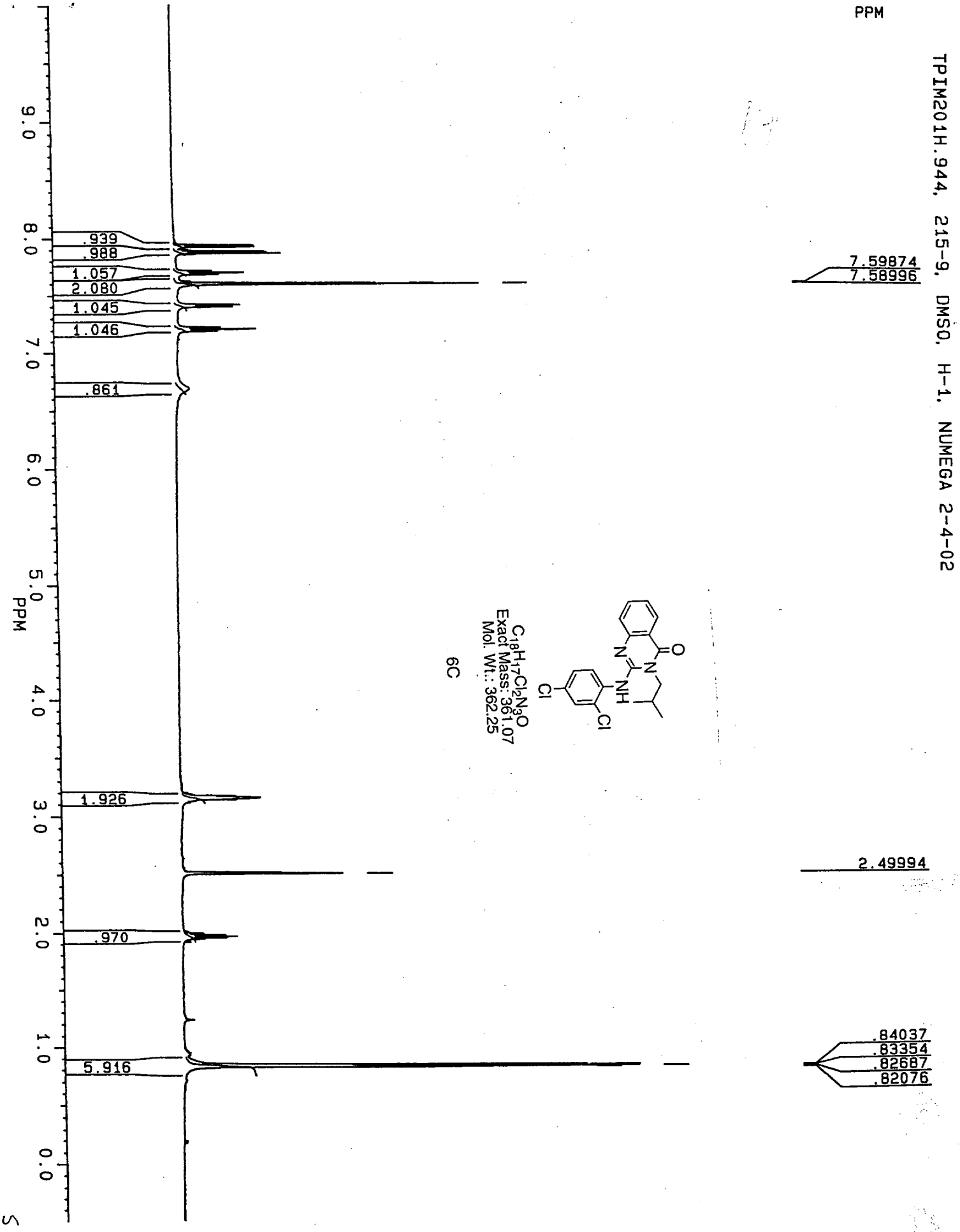
Injection Volume (µL): 20.0



$C_{18}H_{17}Cl_2N_3O$
Exact Mass: 361.07
Mol. Wt.: 362.25

6C

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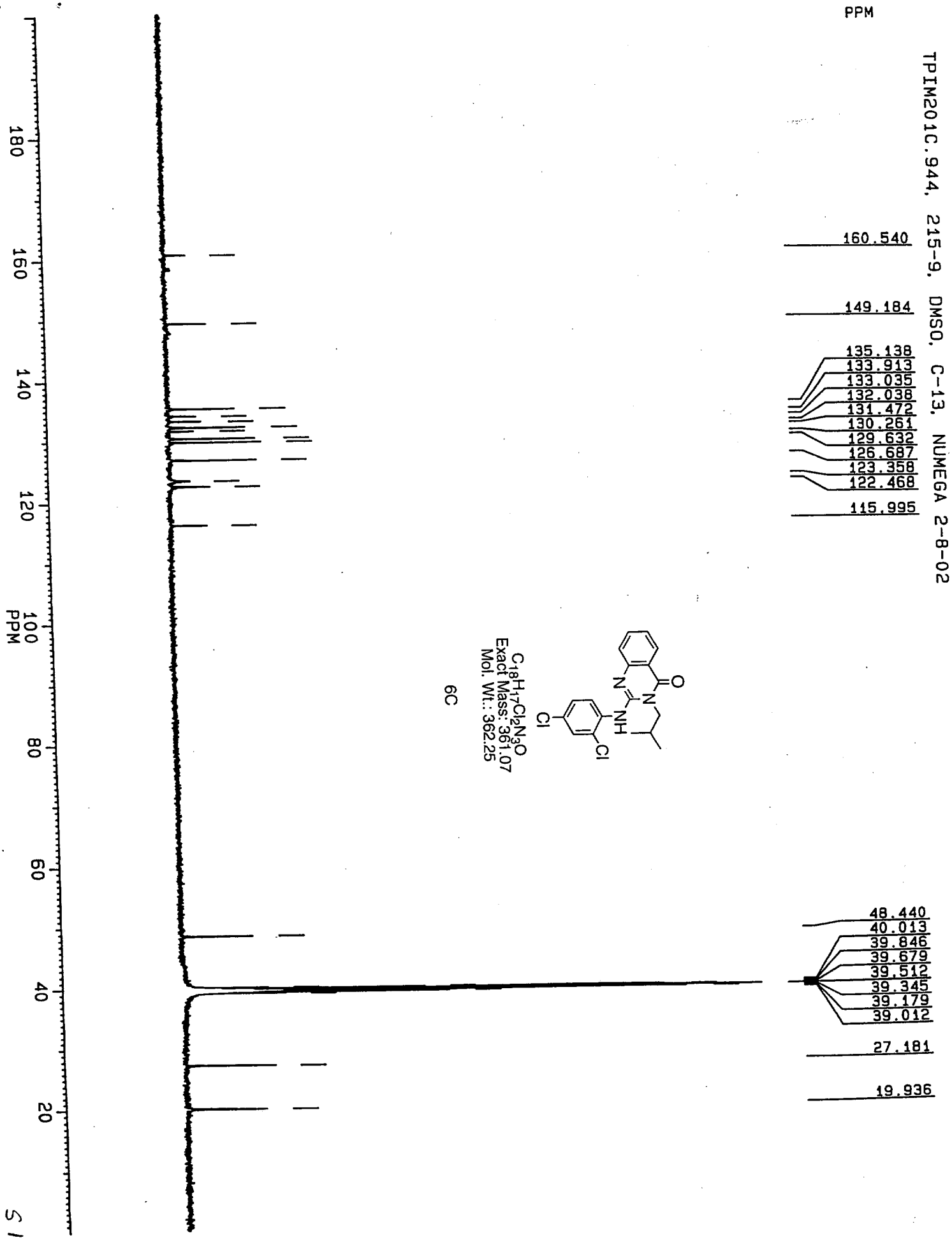
.861
1.926
.970
5.916
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
PPM
$C_{18}H_{17}Cl_2N_3O$
Exact Mass: 361.07
Mol. Wt.: 362.25
6C
Cl
Cl
NH
N
N
O

S13


PPM
TPIM201C.944, 215-9, DMSO, C-13, NUMEGA 2-8-02
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133.913
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132.038
131.472
130.261
129.632
126.687
123.358
122.468
115.995
48.440
40.013
39.846
39.679
39.512
39.345
39.179
39.012
27.181
19.936
180
160
140
120
100
80
60
40
20
PPM
O
N
N
NH
Cl
Cl
$C_{18}H_{17}Cl_2N_3O$
Exact Mass: 361.07
Mol. Wt.: 362.25
6C

S14

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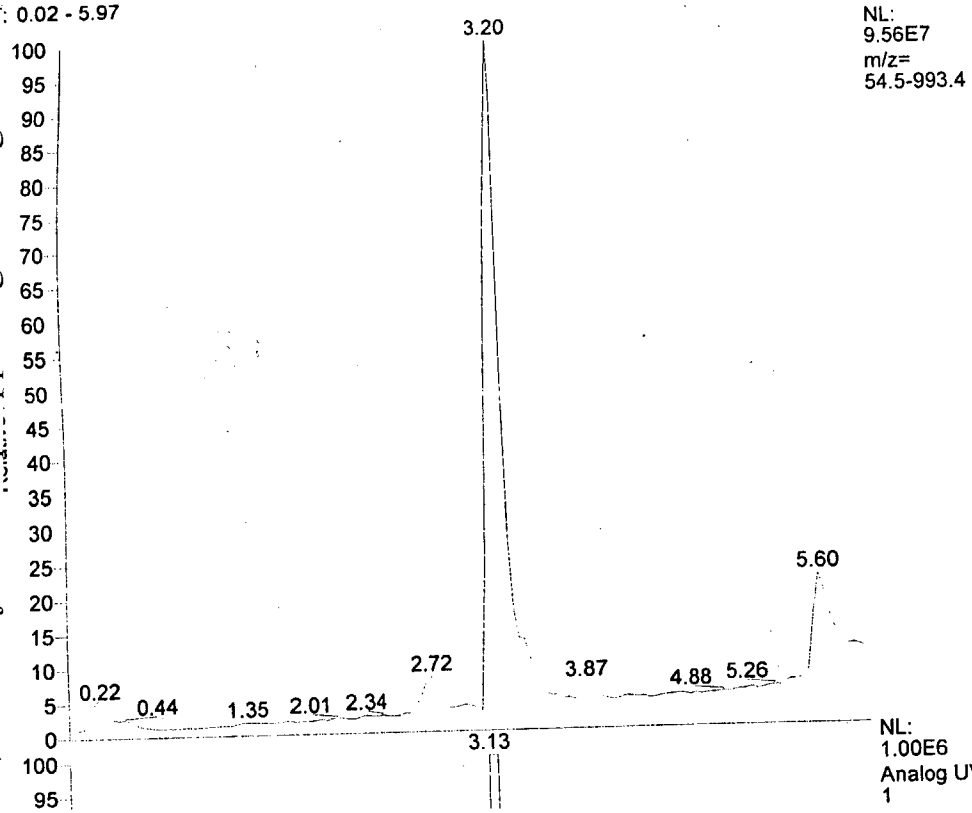

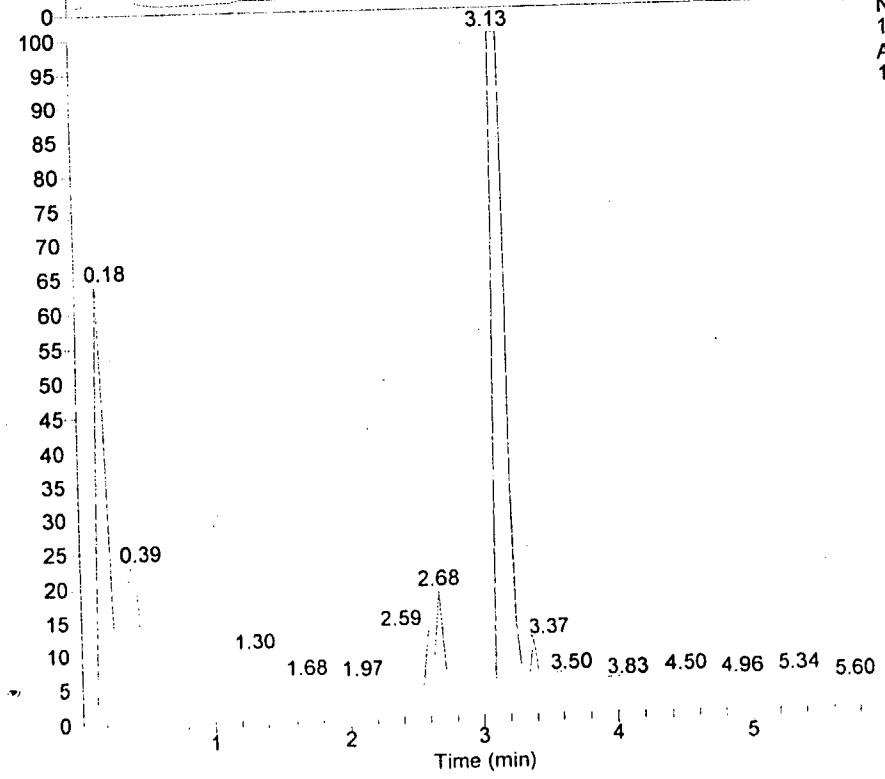

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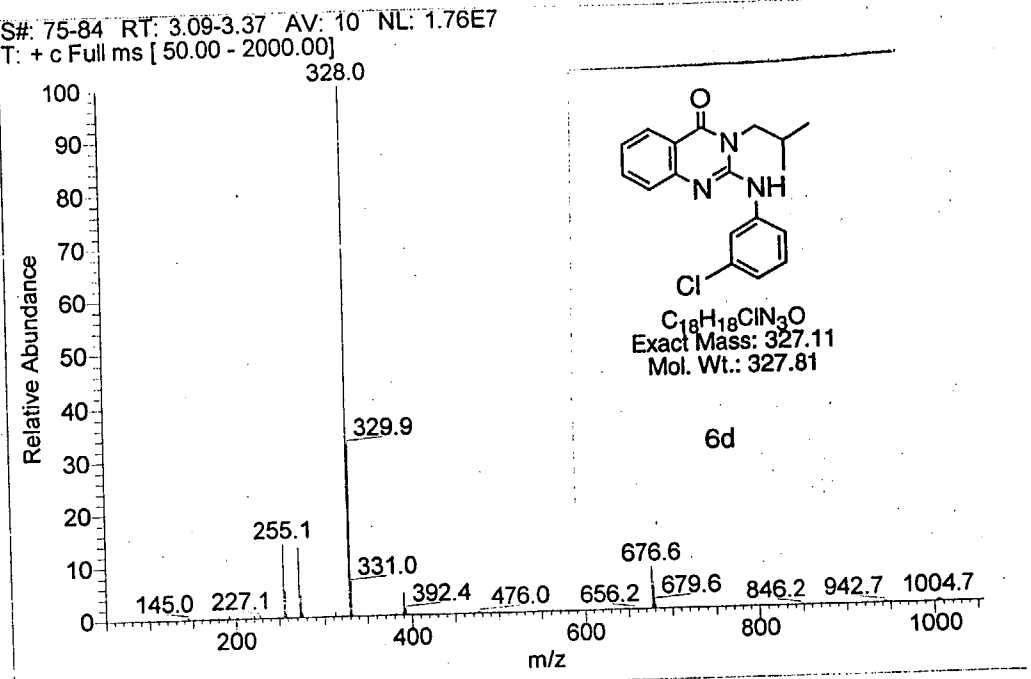
Creator: LCQ Last modified: 9/5/01 by lcq
Summary: 5-95m8
MS Run Time (min): 6.00

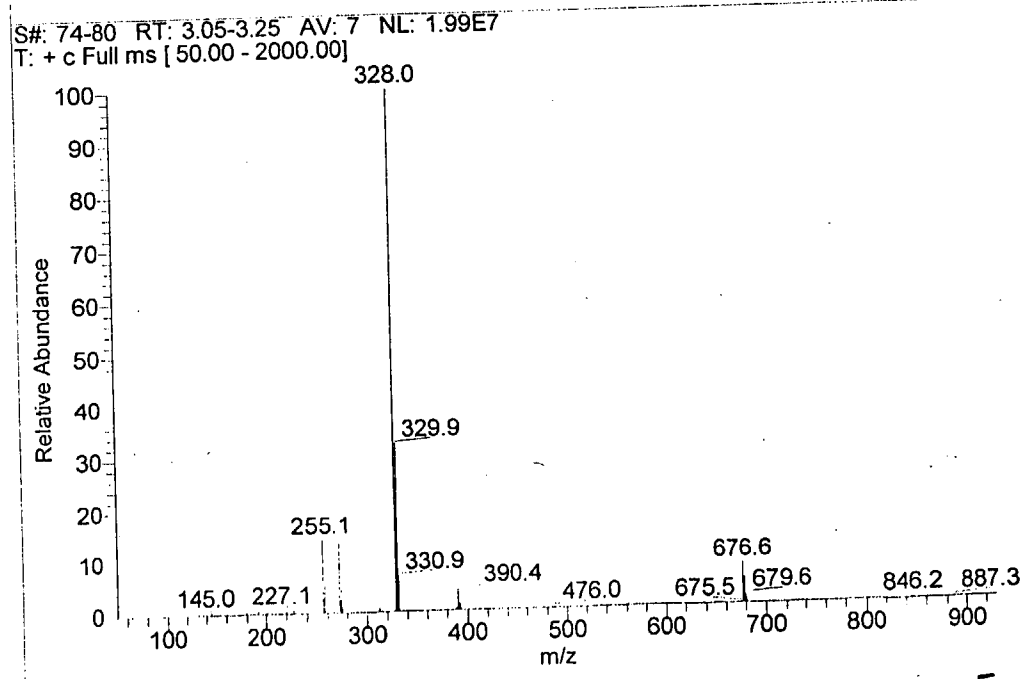
Autosampler Settings:

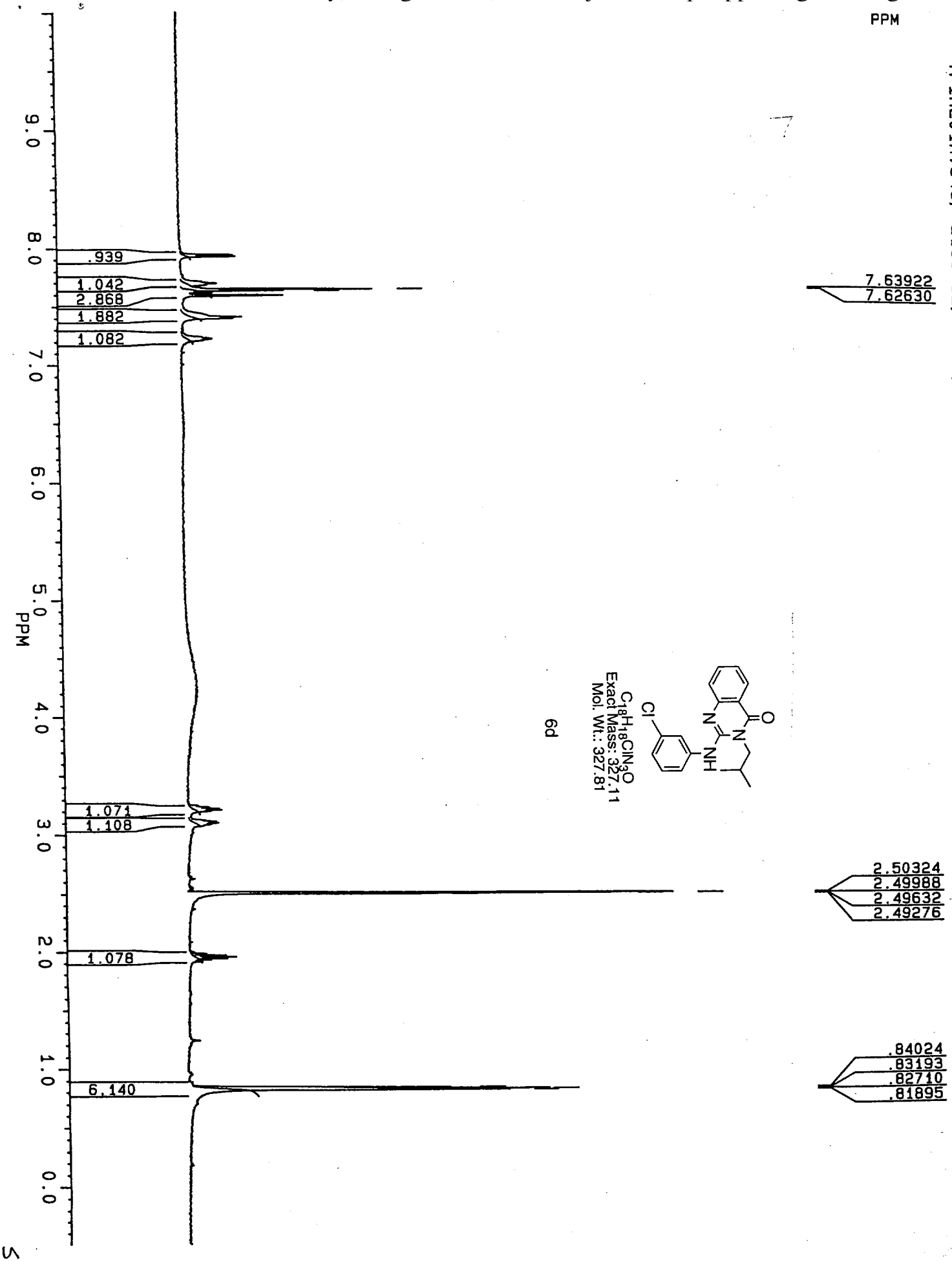
Injection Volume (µL): 20.0



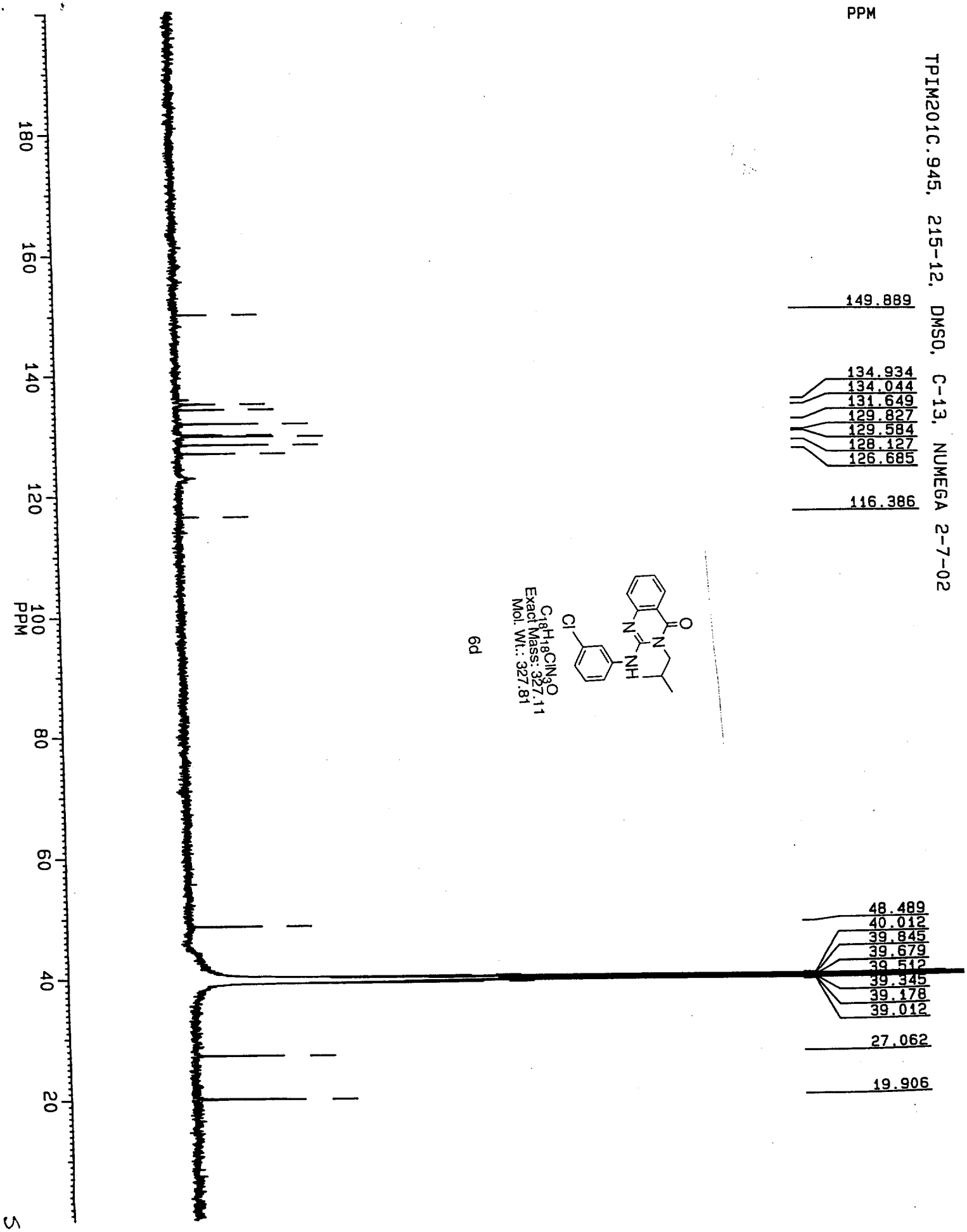
$C_{18}H_{18}ClN_3O$
Exact Mass: 327.11
Mol. Wt.: 327.81

6d




TPIM201H.945, 215C-12, DMSO, H-1, NUMEGA 2-4-02
PPM
7.63922
7.62630
2.50324
2.49988
2.49632
2.49276
.84024
.83193
.82710
.81895
.939
1.042
2.868
1.882
1.082
1.071
1.108
1.078
6.140
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
PPM
6d
$C_{18}H_{18}ClN_3O$
Exact Mass: 327.11
Mol. Wt.: 327.81
Cl
NH
N
N
O

S16


PPM
TPIM201C.945, 215-12, DMSO, C-13, NUMEGA 2-7-02
149.889
134.934
134.044
131.649
129.827
129.584
128.127
126.685
116.386
48.489
40.012
39.845
39.679
39.512
39.345
39.178
39.012
27.062
19.906
180
160
140
120
100
PPM
80
60
40
20
Cl
O
N
N
NH
$C_{18}H_{18}ClN_3O$
Exact Mass: 327.11
Mol. Wt.: 327.81
6d

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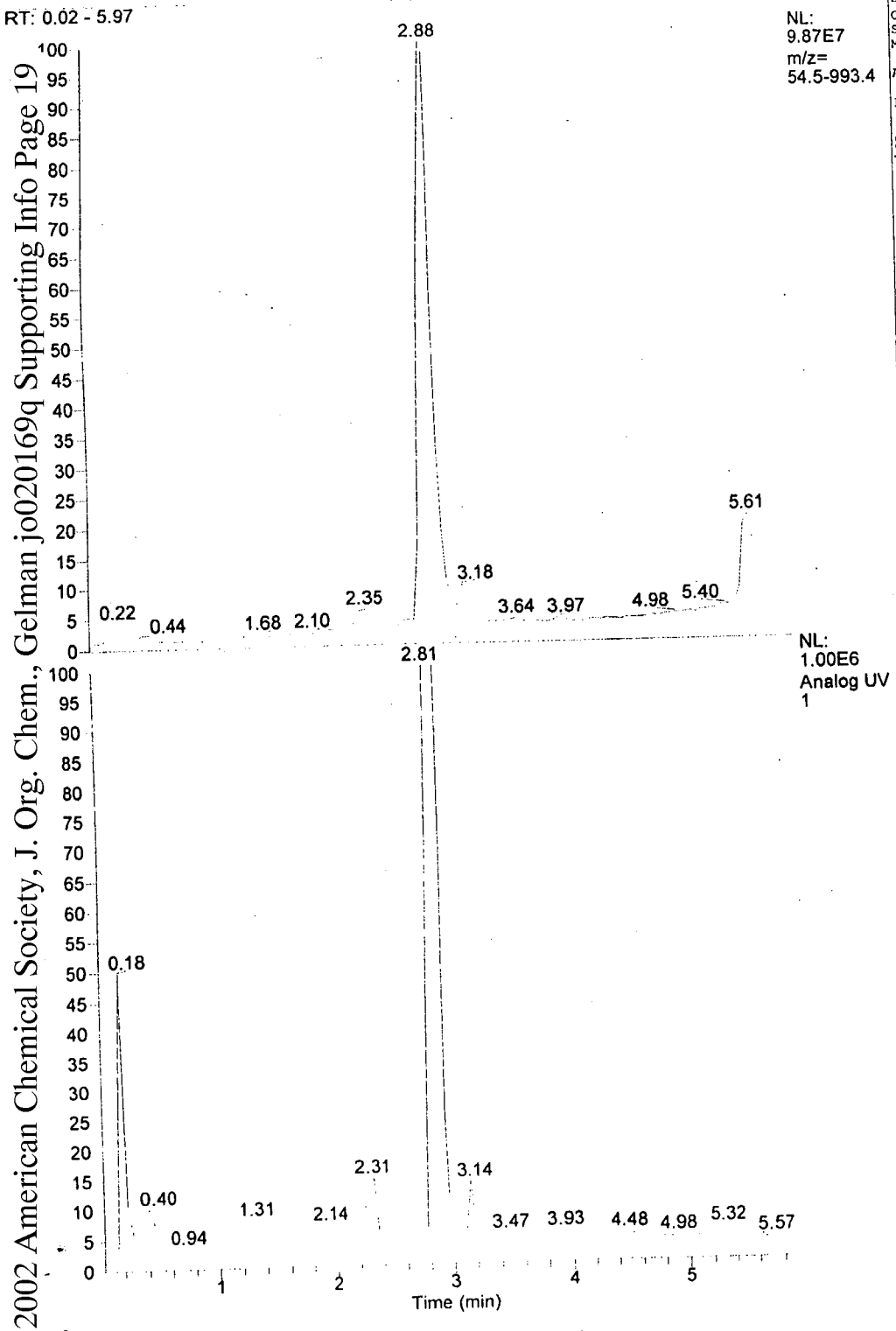
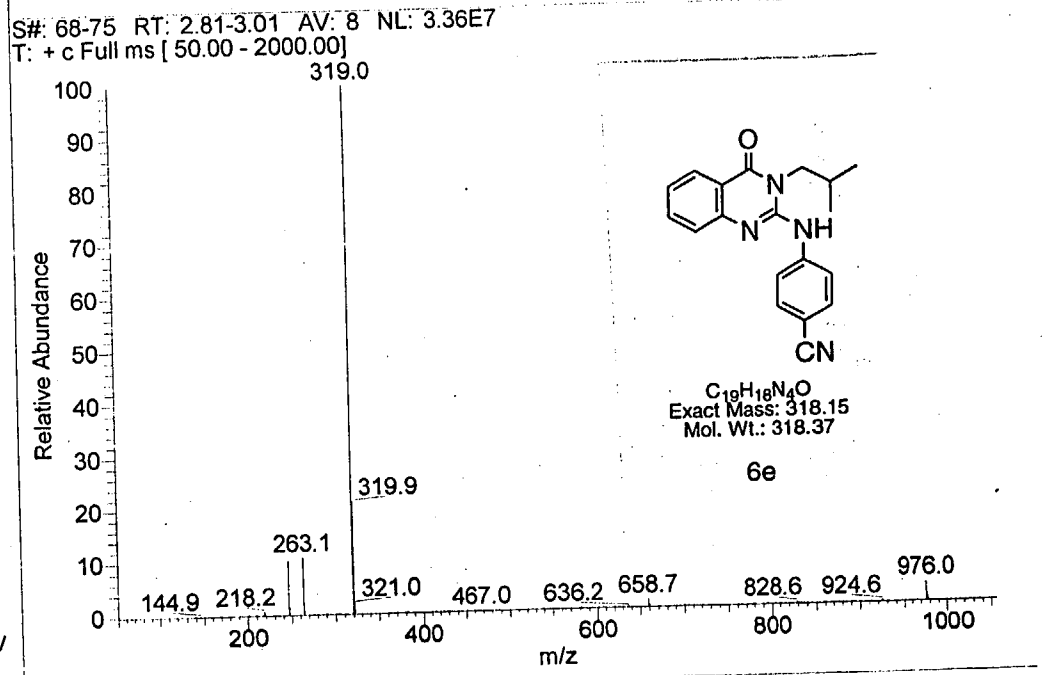
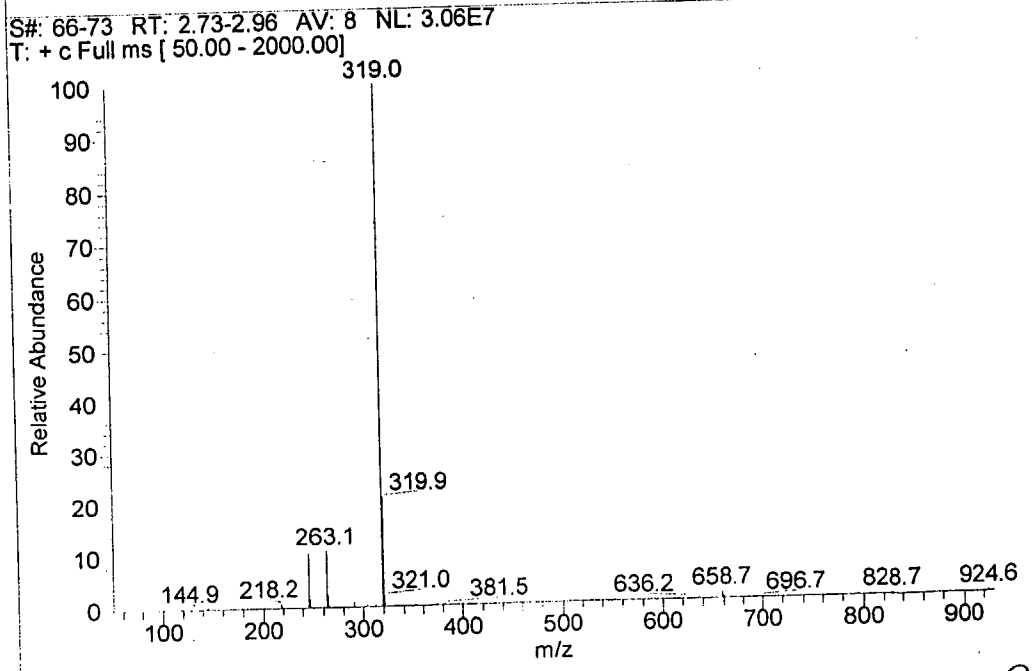


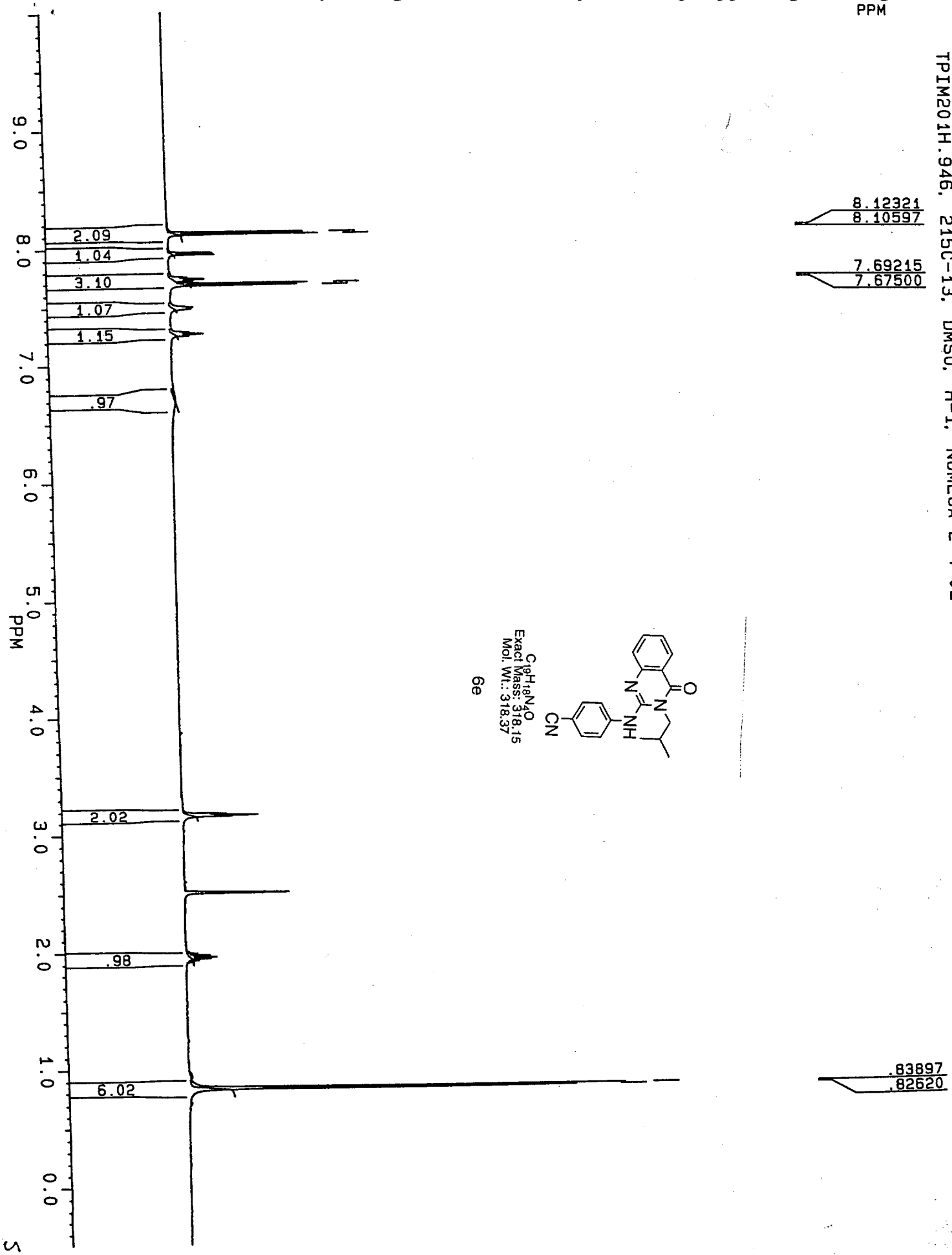
Experiment Method: C:\LCQ\Methods\ESI\Short-col\ESI5-95m0 Created: 11/11/9
Creator: LCQ Last modified: 9/5/01 by lcq
Summary: 5-95m0
MS Run Time (min): 6.00

Autosampler Settings:

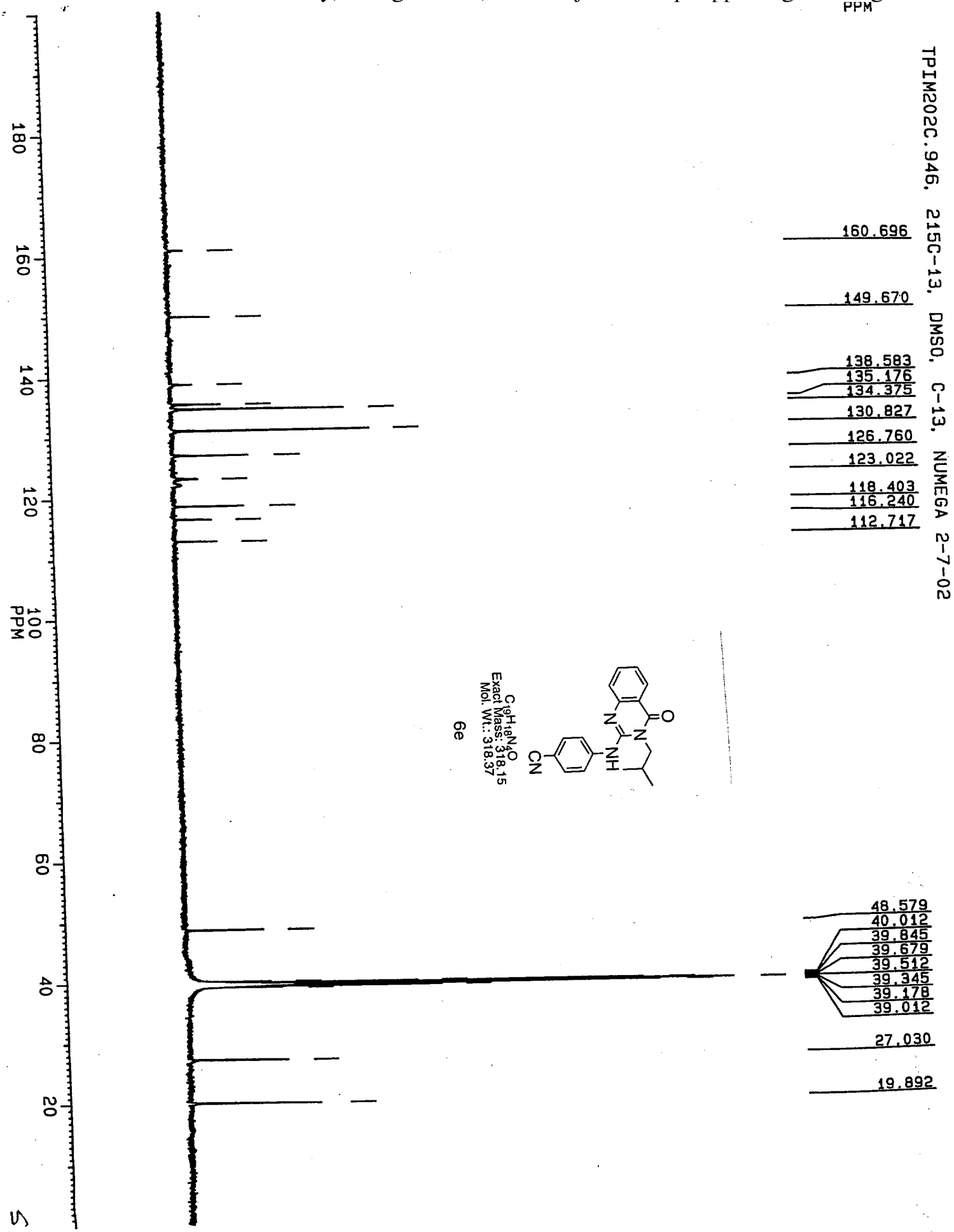
Injection Volume (µL): 20.0






PPM
TPIM201H.946, 215C-13, DMSO, H-1, NUMEGA 2-4-02
8.12321
8.10597
7.69215
7.67500
.83897
.82620
2.09
1.04
3.10
1.07
1.15
.97
2.02
.98
6.02
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
PPM
O
N
N
NH
CN
$C_{19}H_{18}N_4O$
Exact Mass: 318.15
Mol. Wt.: 318.37
6e

519


PPM
TPIM202C.946, 215C-13, DMSO, C-13, NUMEGA 2-7-02
160.696
149.670
138.583
135.176
134.375
130.827
126.760
123.022
118.403
116.240
112.717
48.579
40.012
39.845
39.679
39.512
39.345
39.178
39.012
27.030
19.892
180
160
140
120
100
PPM
80
60
40
20
O
N
N
NH
CN
$C_{19}H_{18}N_4O$
Exact Mass: 318.15
Mol. Wt.: 318.37
6e

S20

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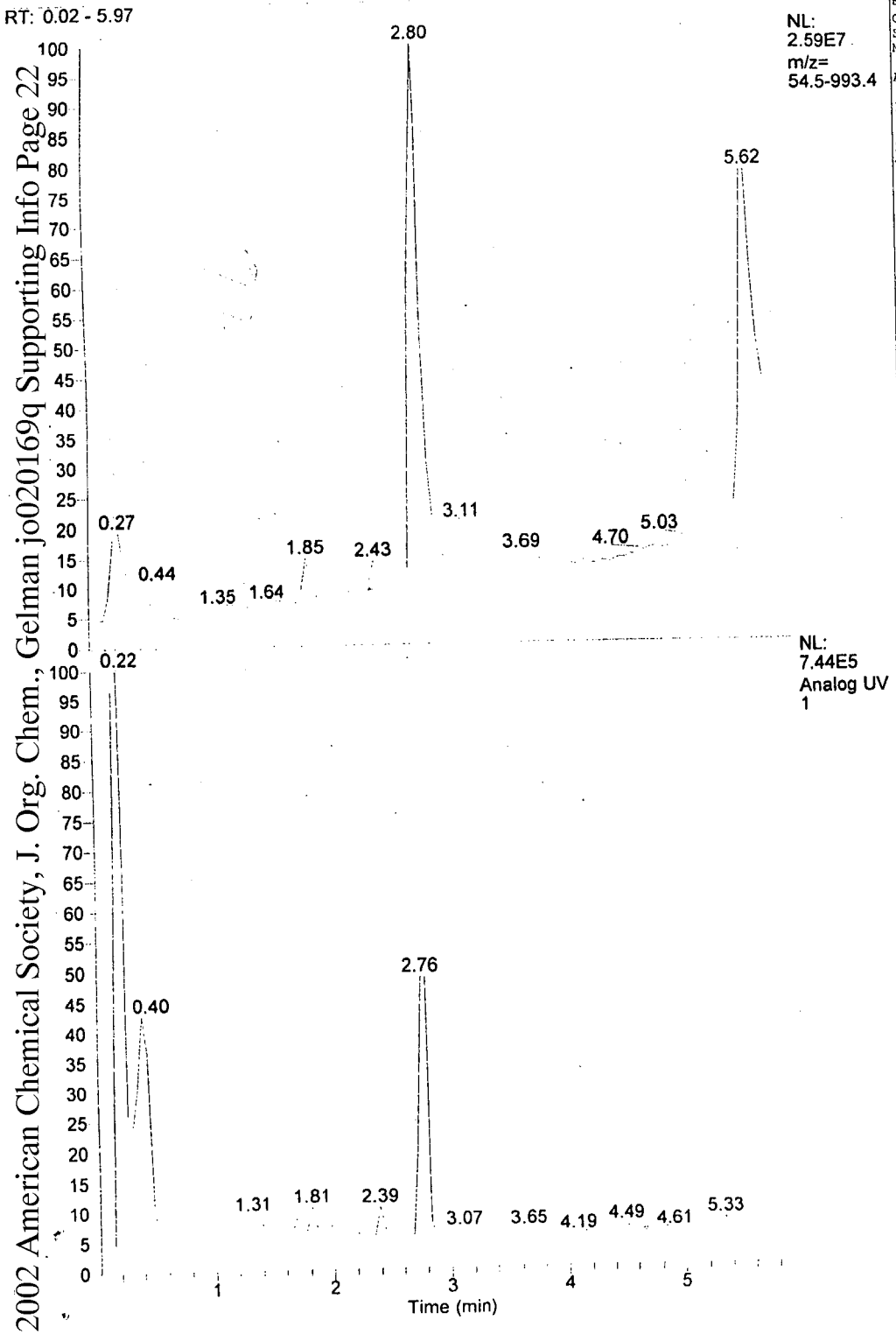
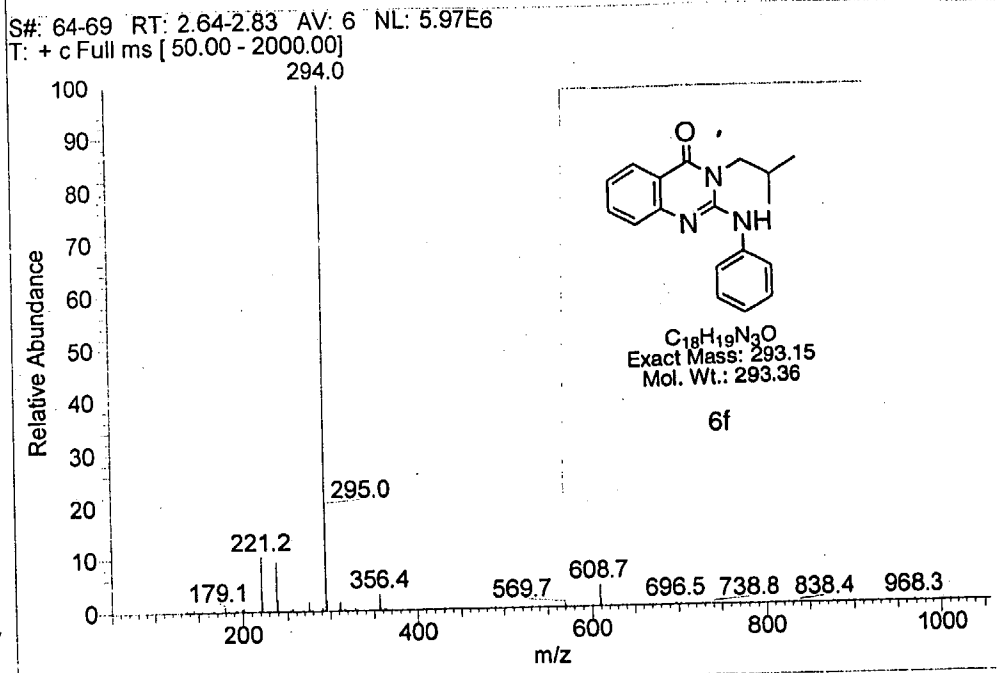
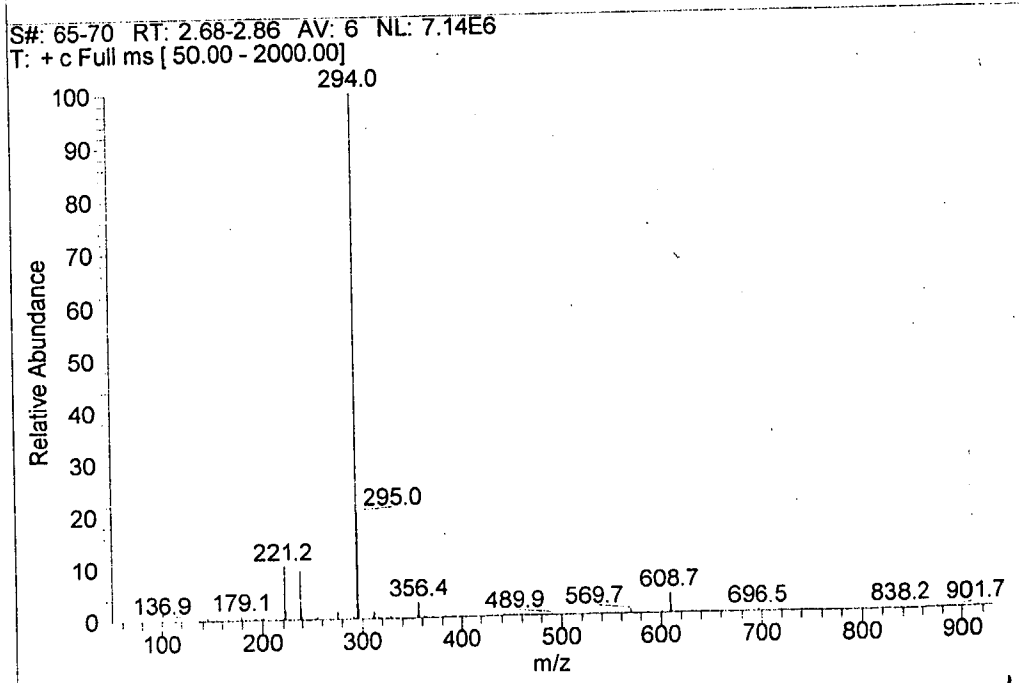


Experiment Method: C:\LCQ\Methods\ESI\Short-col\ESI5-95m8 Created: 11/11/97
Creator: LCQ Last modified: 9/5/01 by lcq
Summary: 5-95m8
MS Run Time (min): 6.00

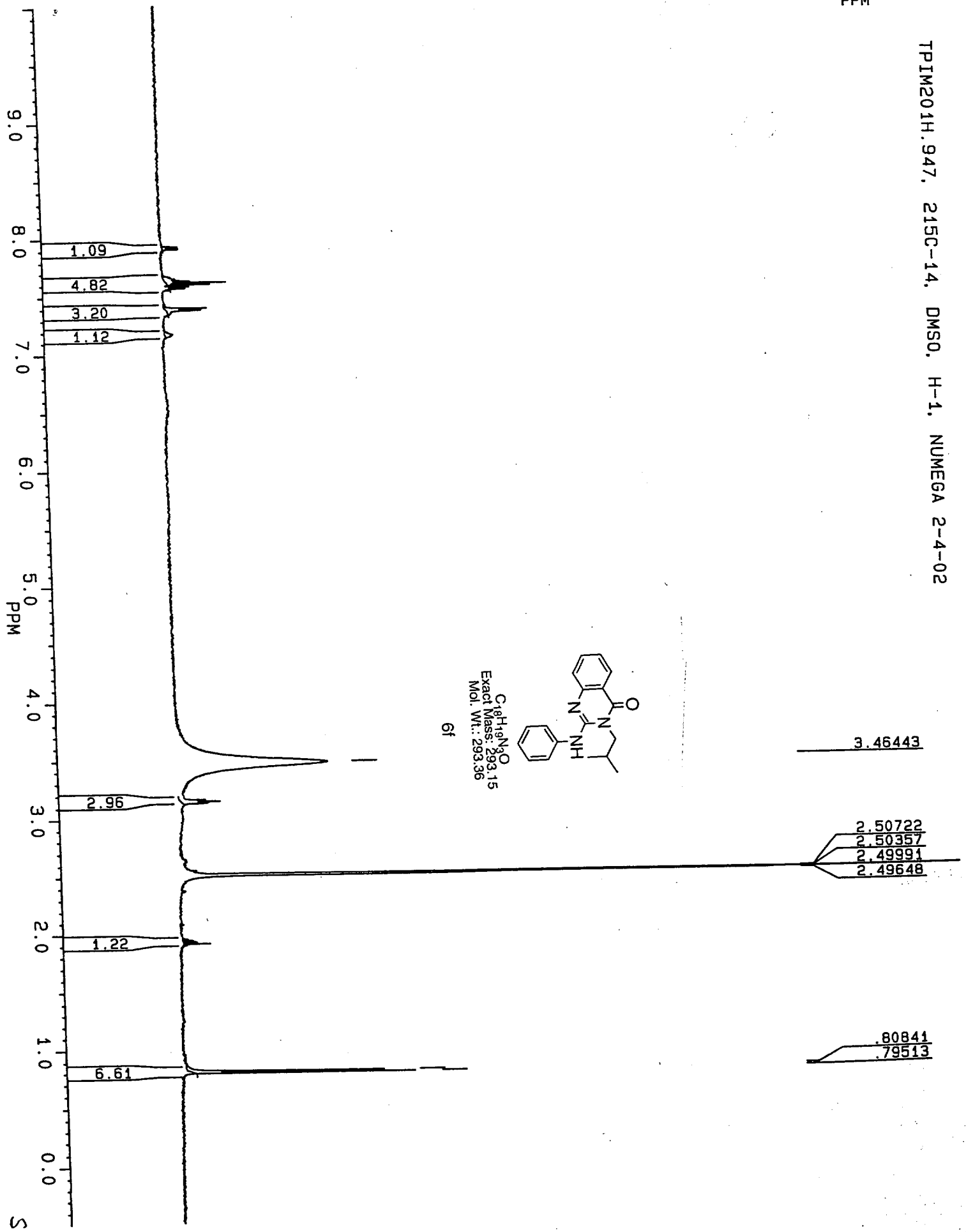
Autosampler Settings:

Injection Volume (µL): 20.0

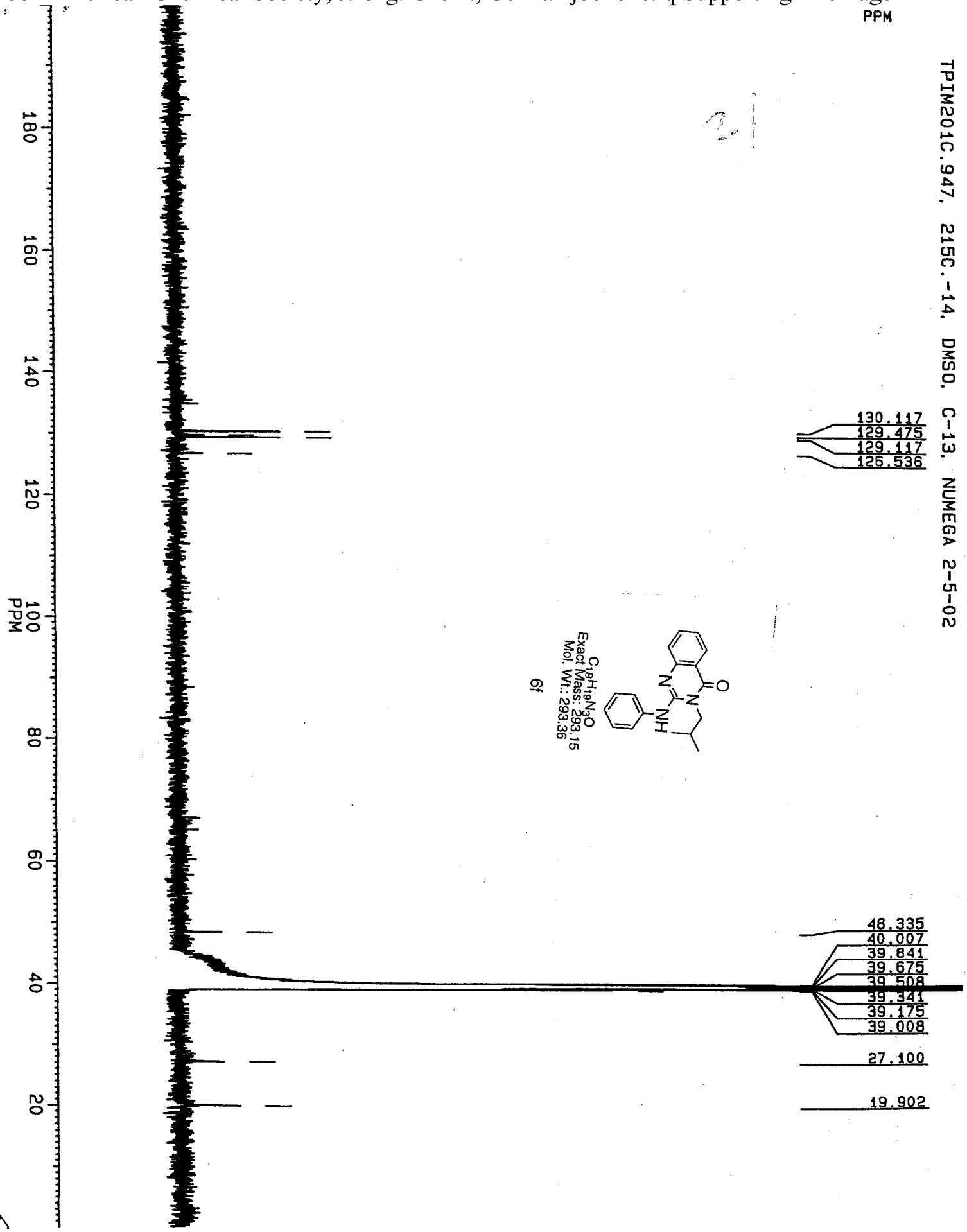




S21


TPIM201H.947, 215C-14, DMSO, H-1, NUMEGA 2-4-02
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.09
4.82
3.20
1.12
2.96
1.22
6.61
3.46443
2.50722
2.50357
2.49991
2.49648
.80841
.79513
C18H19N3O
Exact Mass: 293.15
Mol. Wt.: 293.36
6f

S22


PPM
TPIM201C.947, 215C.-14, DMSO, C-13, NUMEGA 2-5-02
130.117
129.475
129.117
126.536
48.335
40.007
39.841
39.675
39.508
39.341
39.175
39.008
27.100
19.902
O
N
N
NH
$C_{18}H_{19}N_3O$
Exact Mass: 293.15
Mol. Wt.: 293.36
6f
180
160
140
120
100
80
60
40
20
PPM

S23

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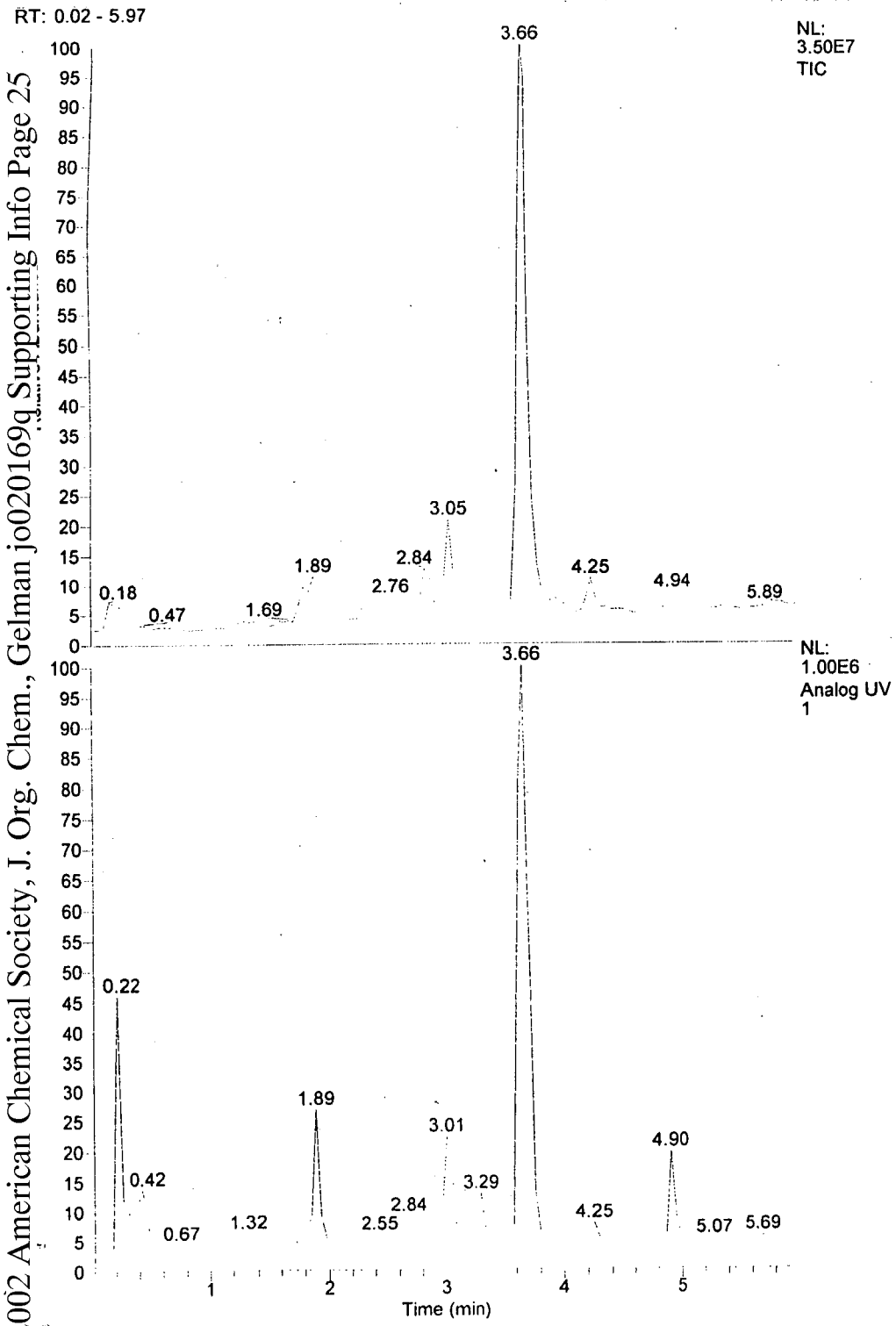
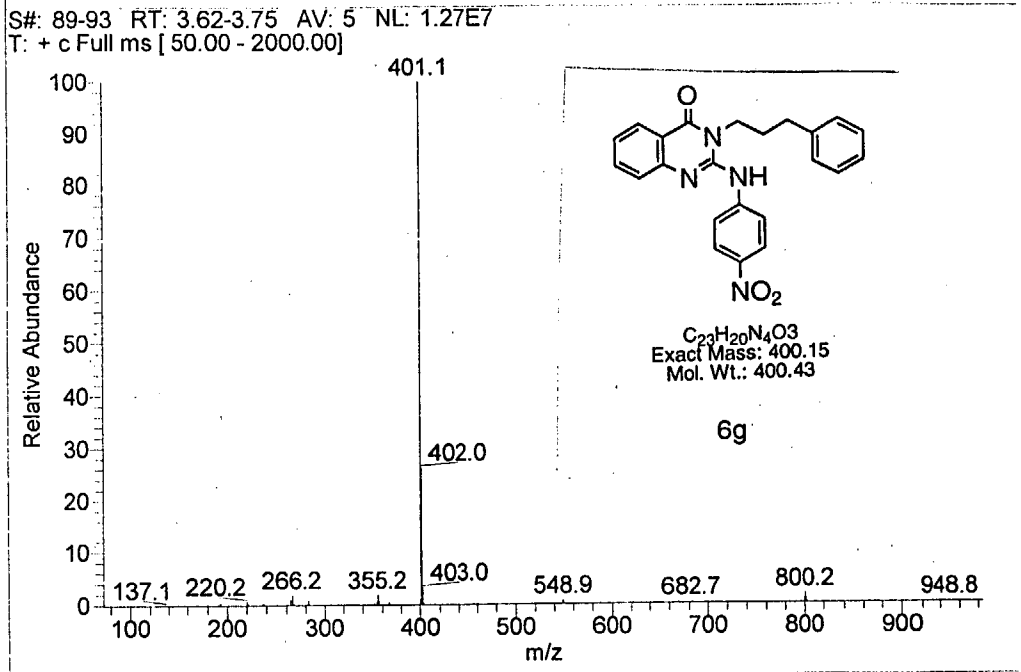
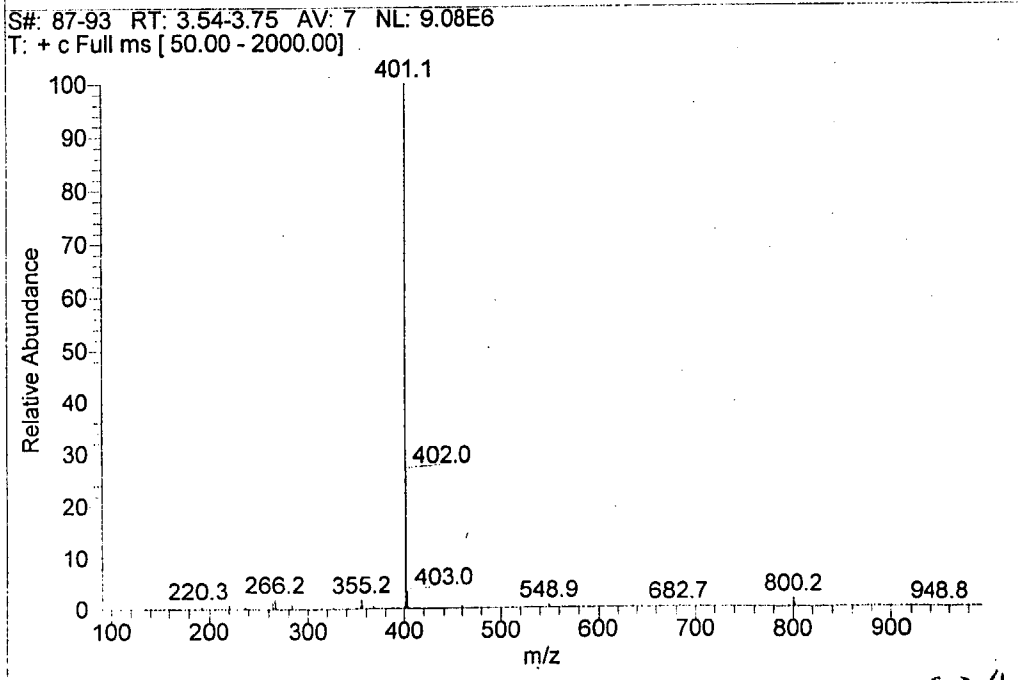


Experiment Method: C:\LCQ\Methods\ESI\Short-col\ESI5-95m8 Created: 11/11/97
Creator: LCQ Last modified: 1/5/01 by Administrator
Summary: 5-95m8
MS Run Time (min): 6.00

Autosampler Settings:

Injection Volume (µL): 20.0





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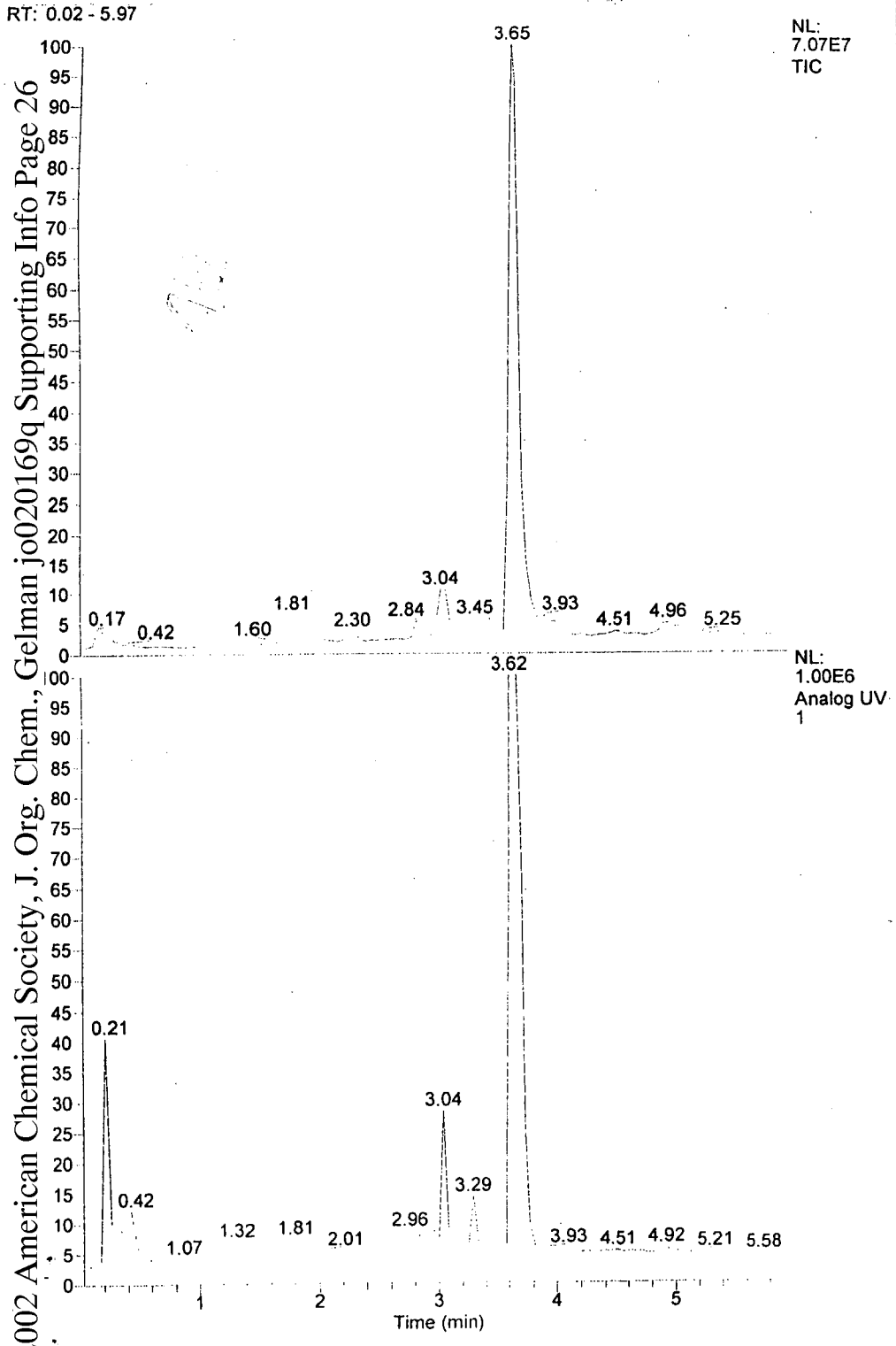
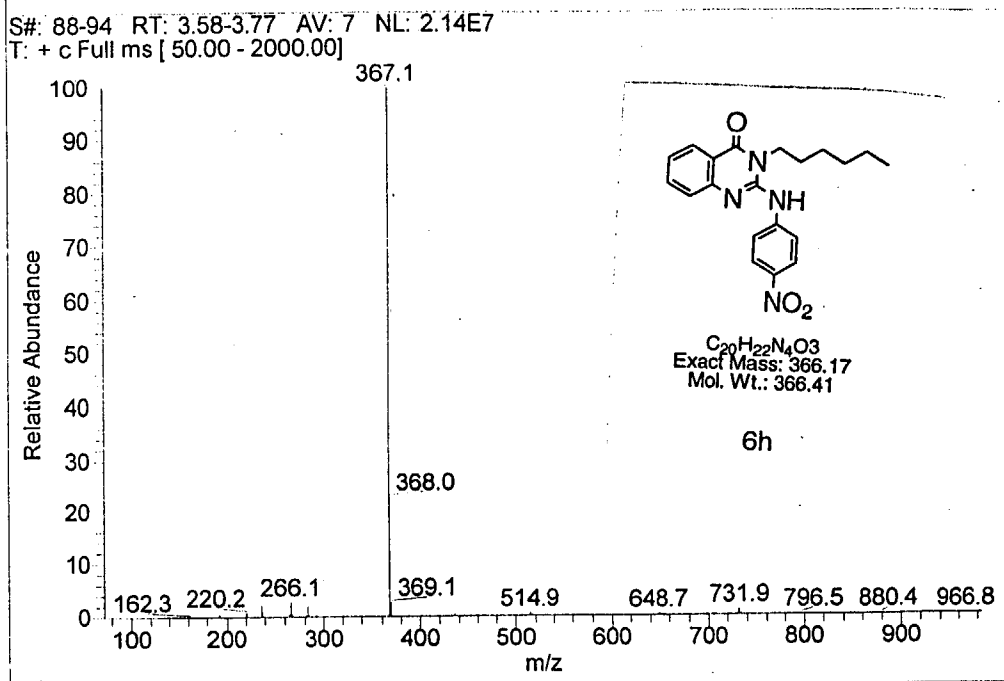
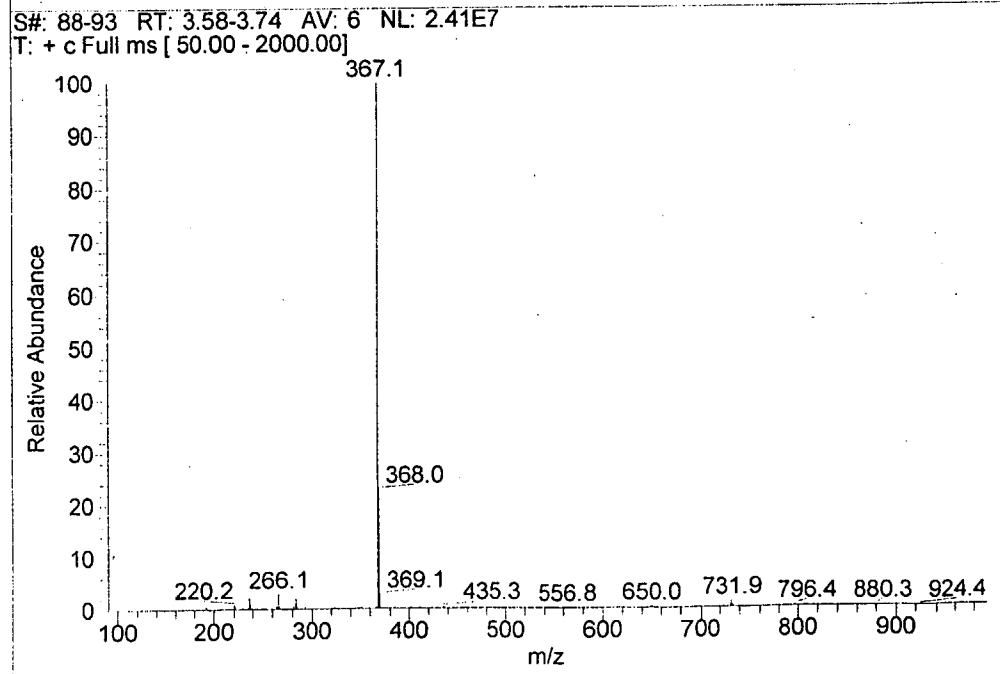


Experiment Method: C:\LCQ\Methods\ESI\Short-col\ESI5-95m8 Created: 11/11/97
Creator: LCQ Last modified: 1/5/01 by Administrator
Summary: 5-95m8
MS Run Time (min): 6.00

Autosampler Settings:

Injection Volume (µL): 20.0





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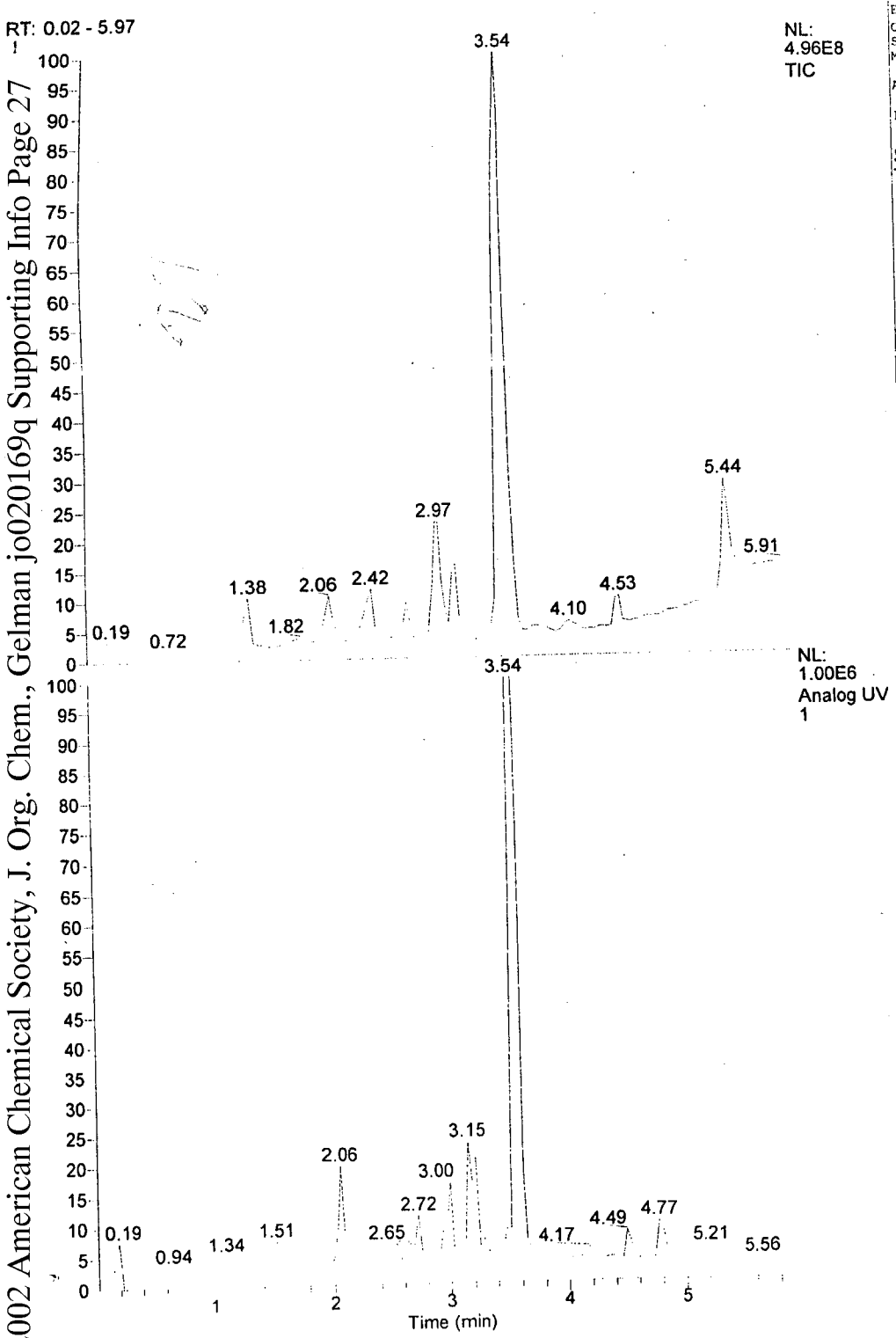
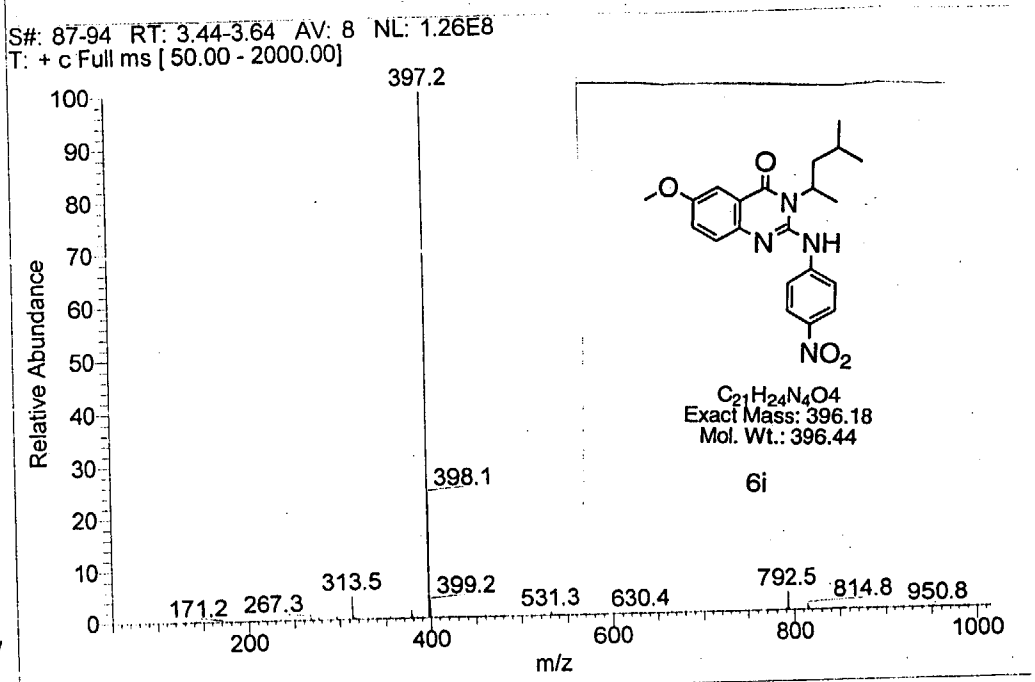
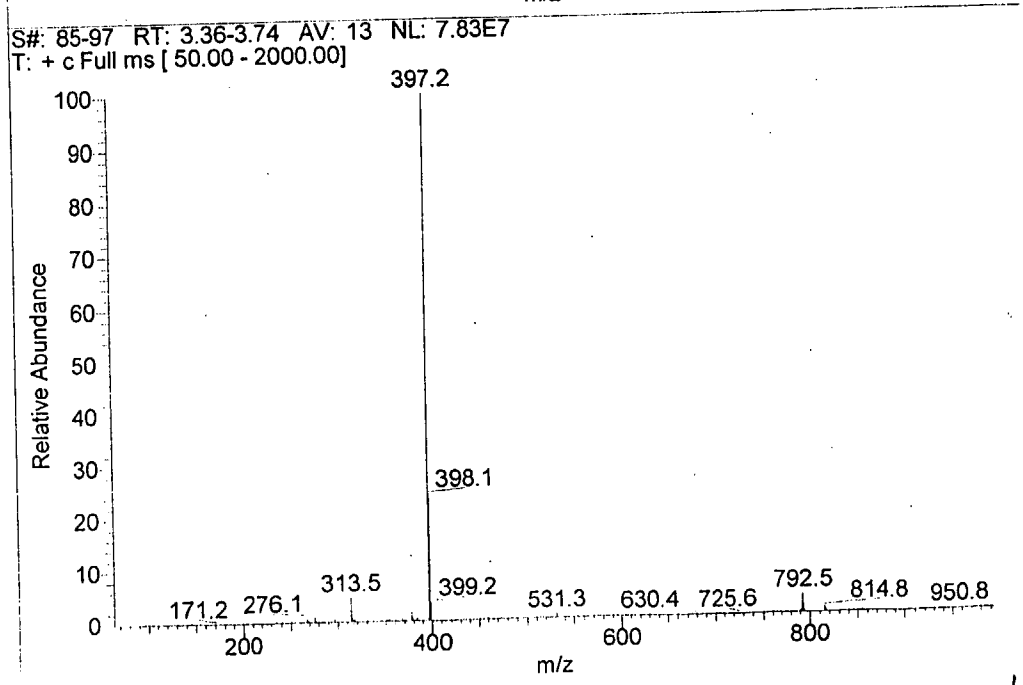


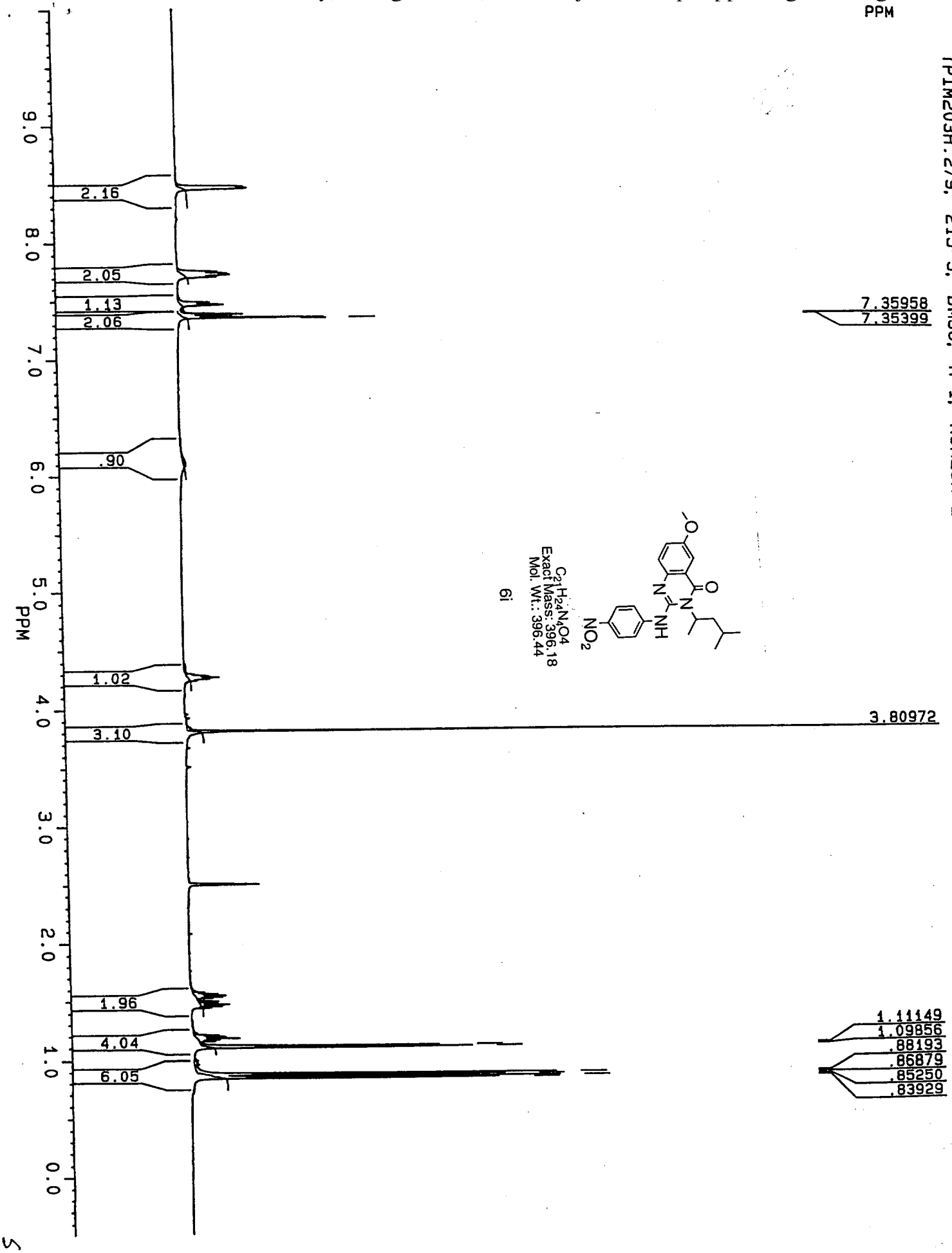
Experiment Method: C:\LCQ\Methods\ESI\Short-COI\ESI5-95m8 Created: 11/1/01
Last modified: 2/20/02 by lcq
Creator: LCQ
Summary: 5-95m8
MS Run Time (min): 6.00

Autosampler Settings:

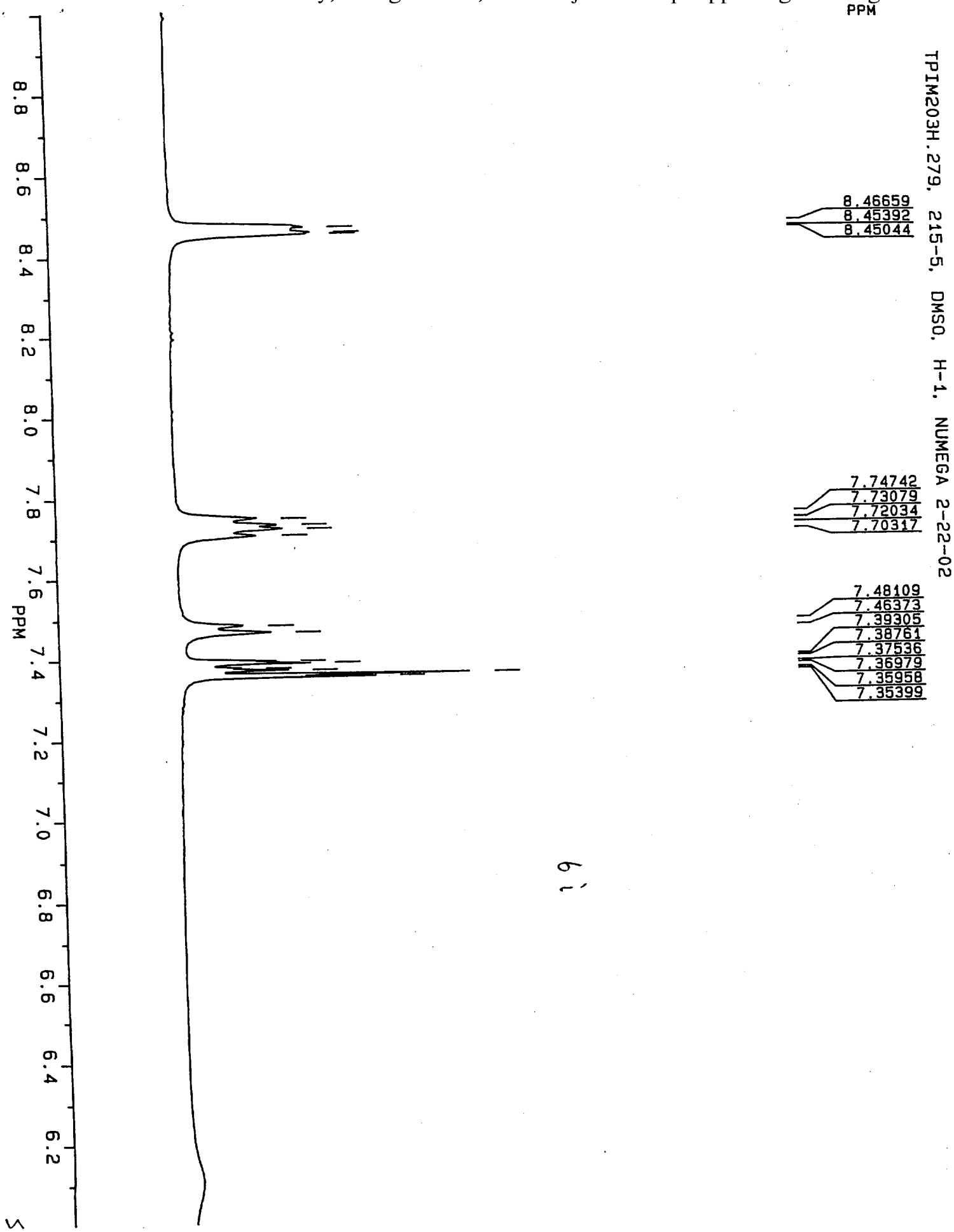
Injection Volume (µL): 20.0



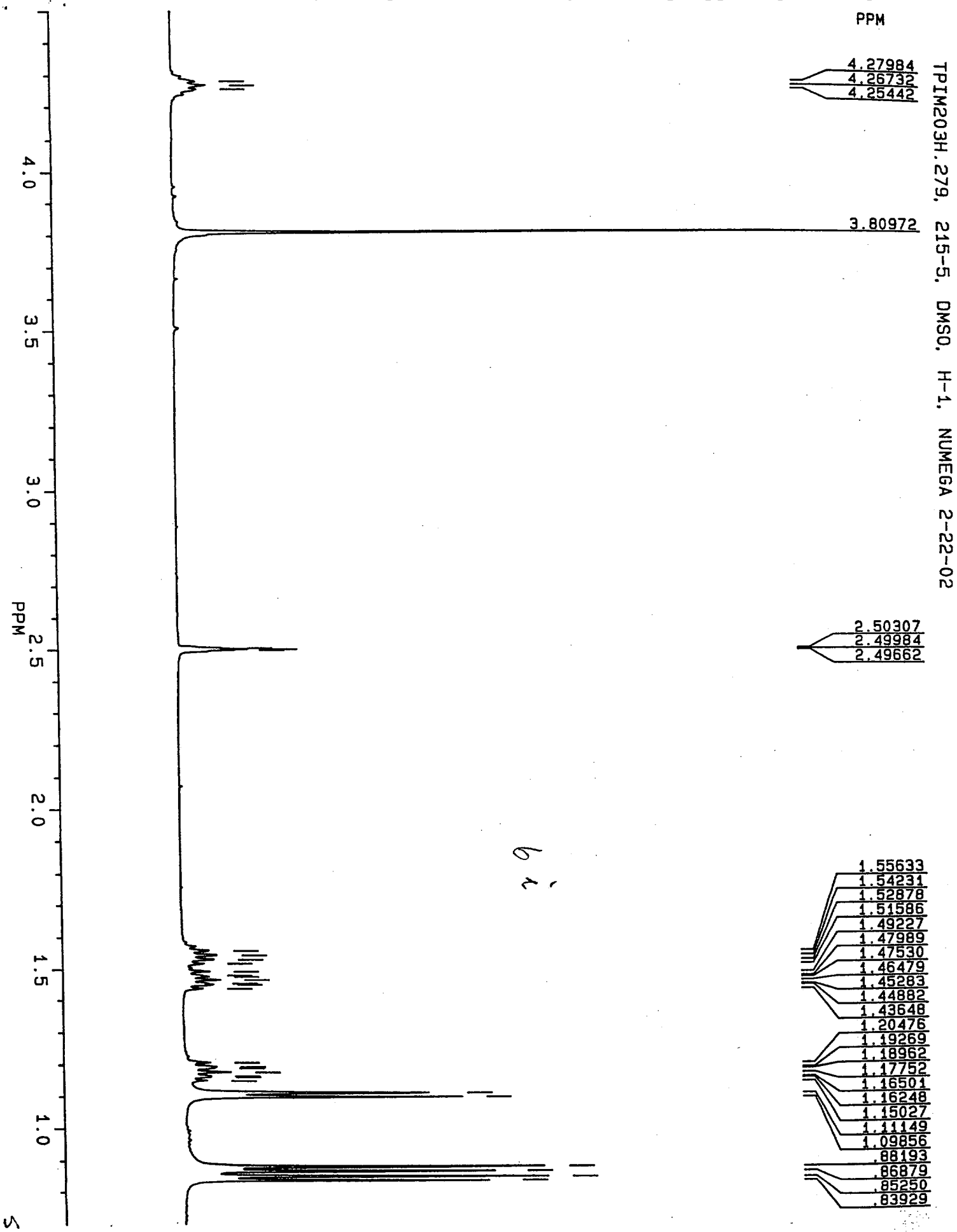



PPM
TPIM203H.279, 215-5, DMSO, H-1, NUMEGA 2-22-02
7.35958
7.35399
3.80972
1.11149
1.09856
.88193
.86879
.85250
.83929
2.16
2.05
1.13
2.06
.90
1.02
3.10
1.96
4.04
6.05
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
PPM
6i
$C_{21}H_{24}N_4O_4$
Exact Mass: 396.18
Mol. Wt.: 396.44
NH
N
N
O
O
NO_2

527

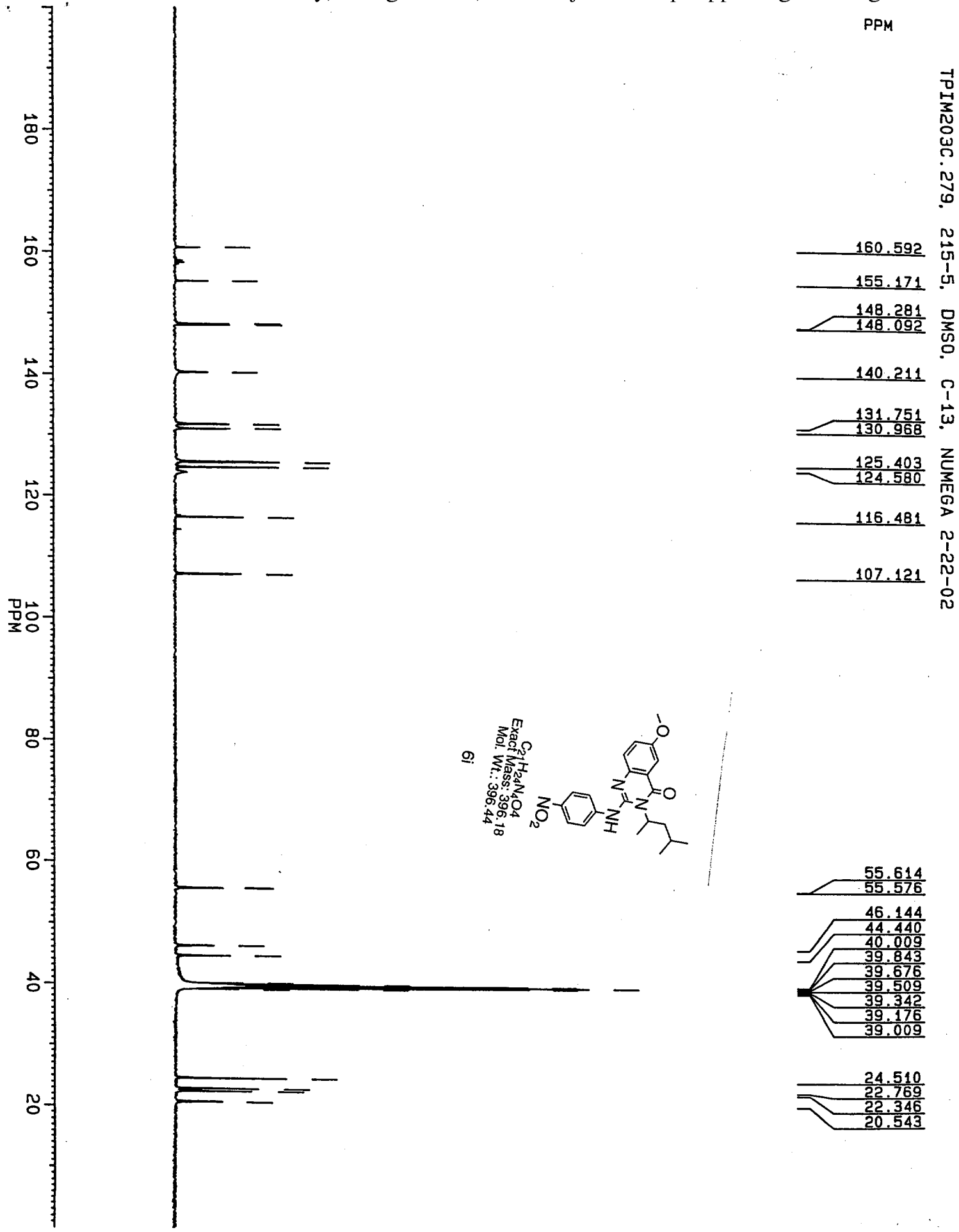

PPM
TPIM203H.279, 215-5, DMSO, H-1, NUMEGA 2-22-02
8.46659
8.45392
8.45044
7.74742
7.73079
7.72034
7.70317
7.48109
7.46373
7.39305
7.38761
7.37536
7.36979
7.35958
7.35399
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
PPM

S28


PPM
TPIM203H.279, 215-5, DMSO, H-1, NUMEGA 2-22-02
4.27984
4.26732
4.25442
3.80972
2.50307
2.49984
2.49662
1.55633
1.54231
1.52878
1.51586
1.49227
1.47989
1.47530
1.46479
1.45283
1.44882
1.43648
1.20476
1.19269
1.18962
1.17752
1.16501
1.16248
1.15027
1.11149
1.09856
.88193
.86879
.85250
.83929
4.0
3.5
3.0
2.5
2.0
1.5
1.0
PPM

6i

529


TPIM203C.279, 215-5, DMSO, C-13, NUMEGA 2-22-02
PPM
160.592
155.171
148.281
148.092
140.211
131.751
130.968
125.403
124.580
116.481
107.121
55.614
55.576
46.144
44.440
40.009
39.843
39.676
39.509
39.342
39.176
39.009
24.510
22.769
22.346
20.543
180
160
140
120
100
80
60
40
20
PPM
$C_{21}H_{24}N_4O_4$
Exact Mass: 396.18
Mol. Wt.: 396.44
6i

S30

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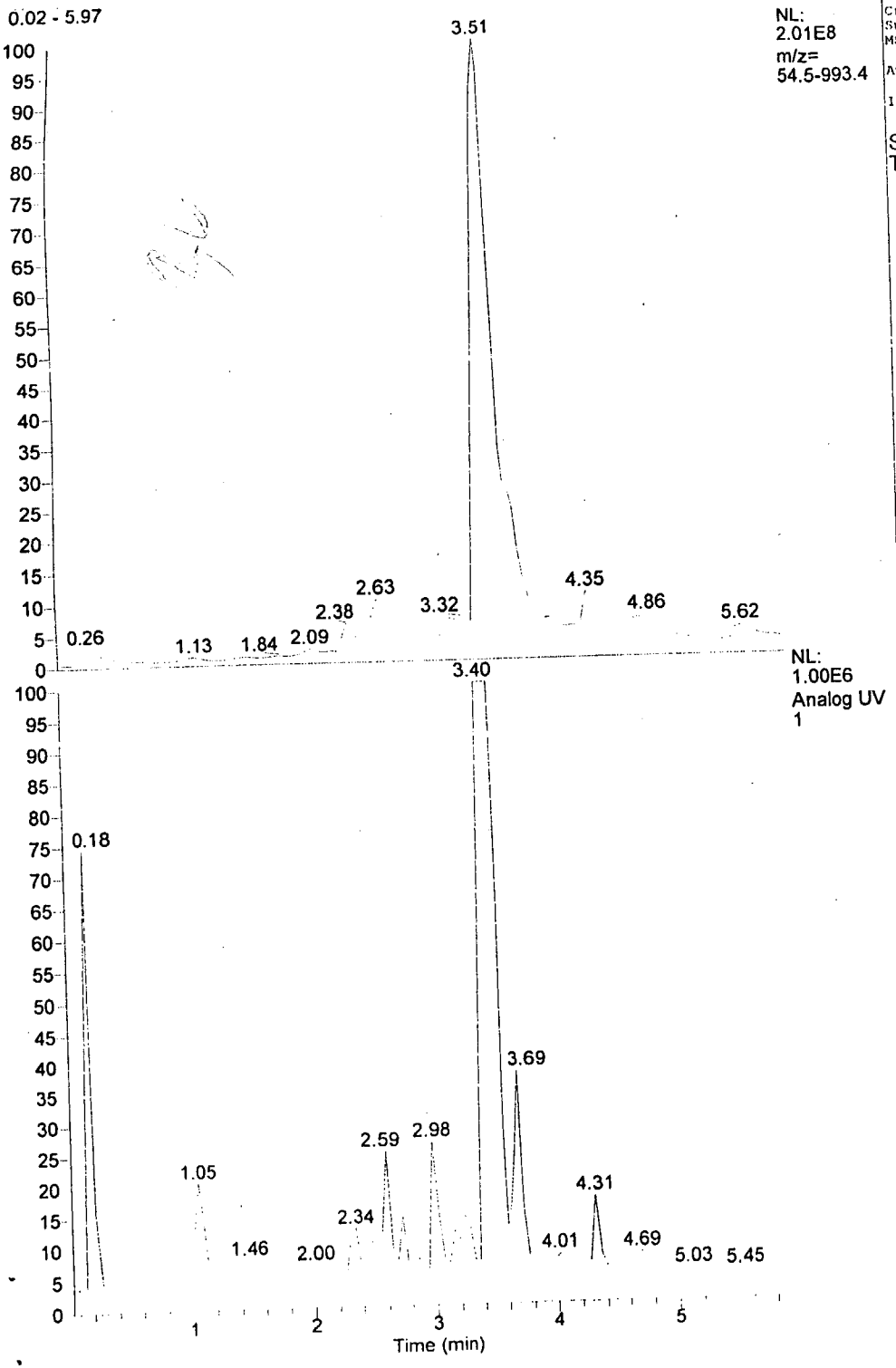
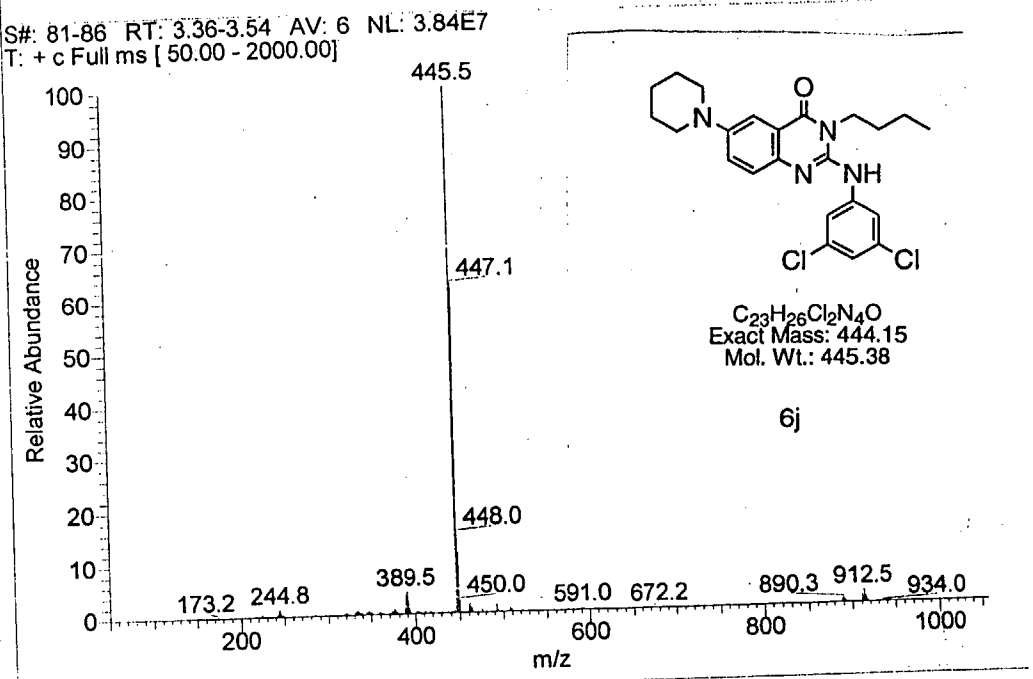


Experiment Method: C:\LCQ\Methods\ESI\Short-col\ESI5-95m8 Created: 11/11/97
Last modified: 9/22/01 by lcq
Creator: LCQ
Summary: 5-95m8
MS Run Time (min): 6.00

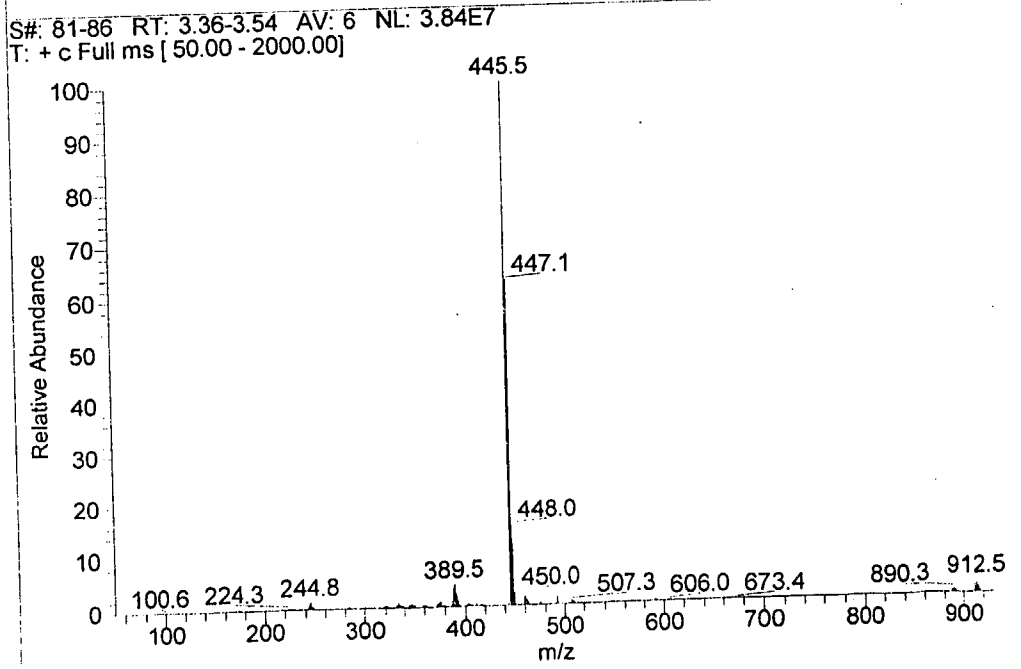
Autosampler Settings:

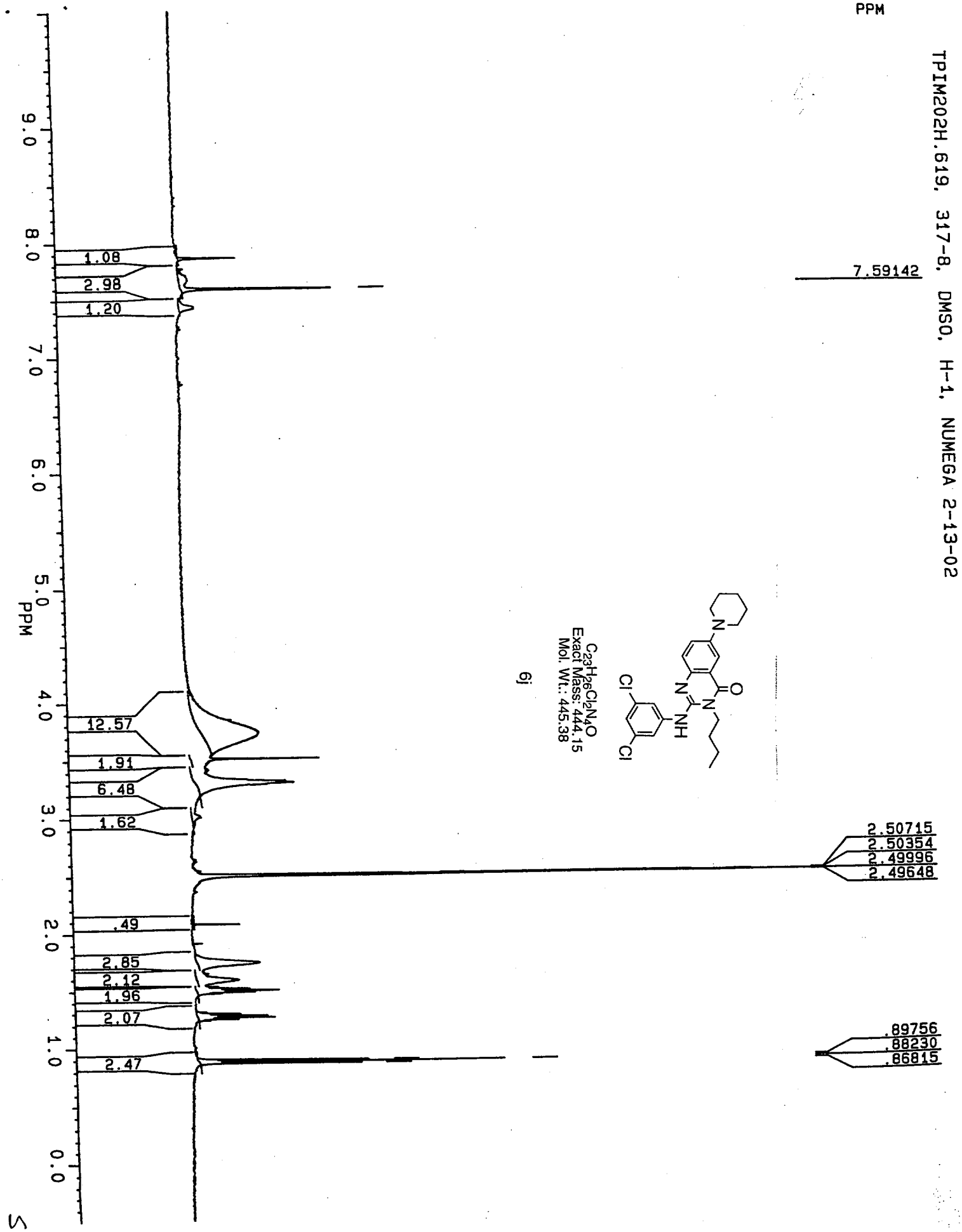
Injection Volume (µL): 20.0

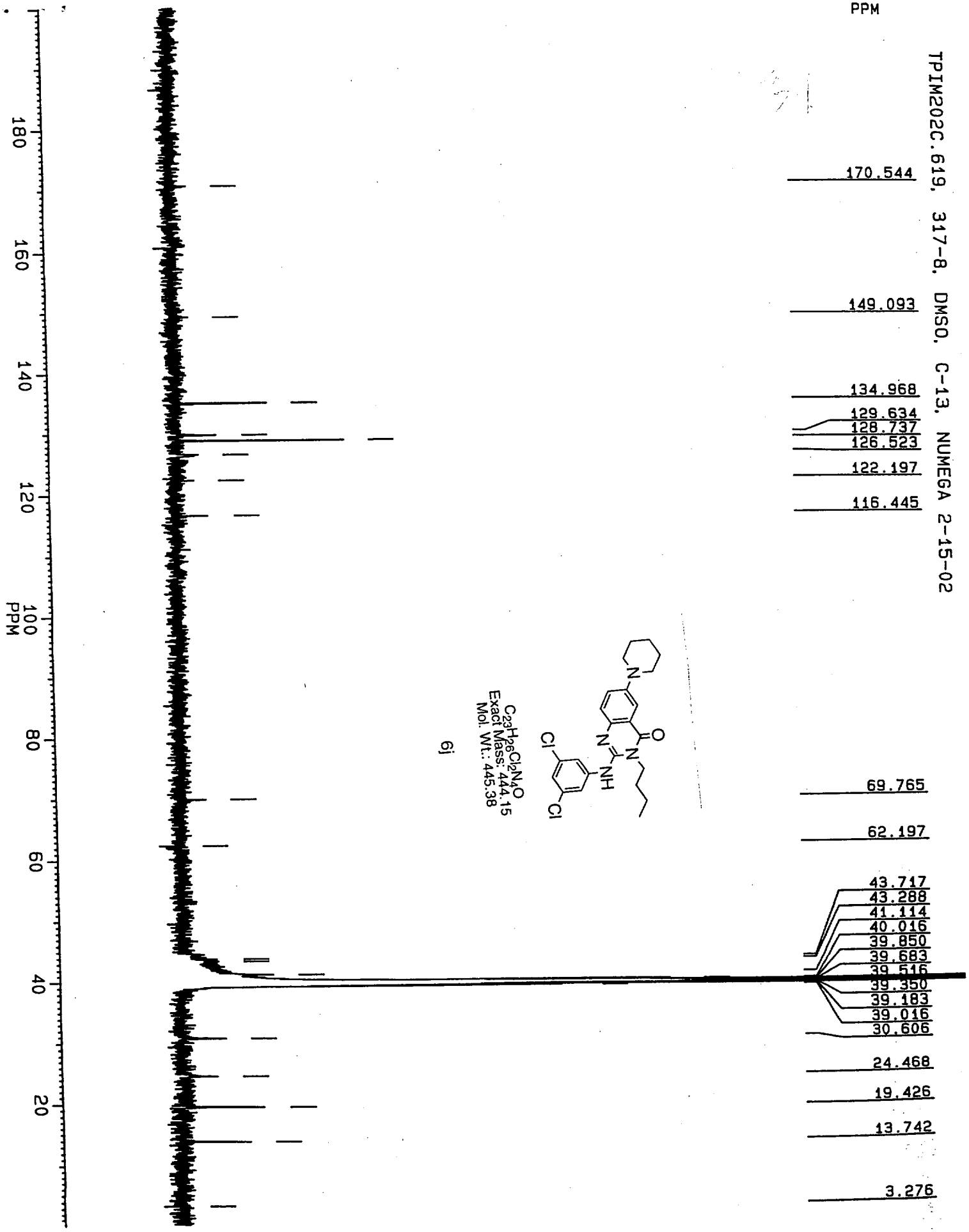


$C_{23}H_{26}Cl_2N_4O$
Exact Mass: 444.15
Mol. Wt.: 445.38

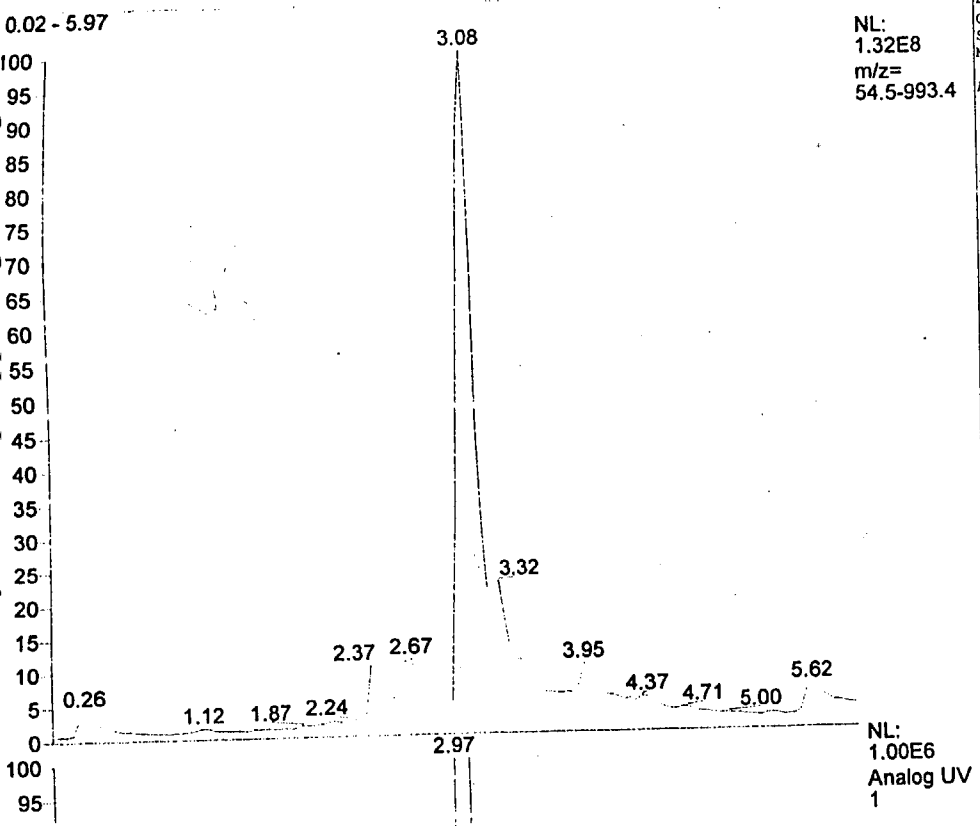
6j

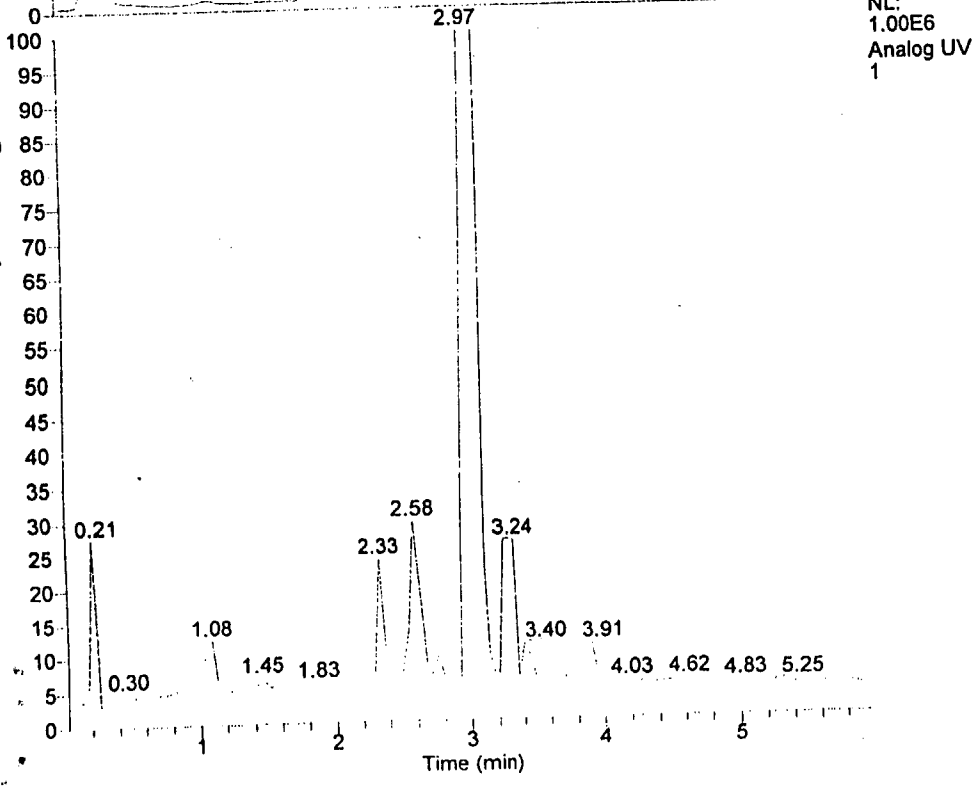



PPM
TPIM202H.619, 317-8, DMSO, H-1, NUMEGA 2-13-02
7.59142
2.50715
2.50354
2.49996
2.49648
.89756
.88230
.86815
1.08
2.98
1.20
12.57
1.91
6.48
1.62
.49
2.85
2.12
1.96
2.07
2.47
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
PPM
6j
$C_{23}H_{26}Cl_2N_4O$
Exact Mass: 444.15
Mol. Wt.: 445.38
Cl
Cl
NH
N
O
N
N


PPM
TPIM202C.619, 317-8, DMSO, C-13, NUMEGA 2-15-02
170.544
149.093
134.968
129.634
128.737
126.523
122.197
116.445
69.765
62.197
43.717
43.288
41.114
40.016
39.850
39.683
39.516
39.350
39.183
39.016
30.606
24.468
19.426
13.742
3.276
180
160
140
120
100
80
60
40
20
PPM
$C_{23}H_{26}Cl_2N_4O$
Exact Mass: 444.15
Mol. Wt.: 445.38
6j

E:\yongping\9-21-01--317--09

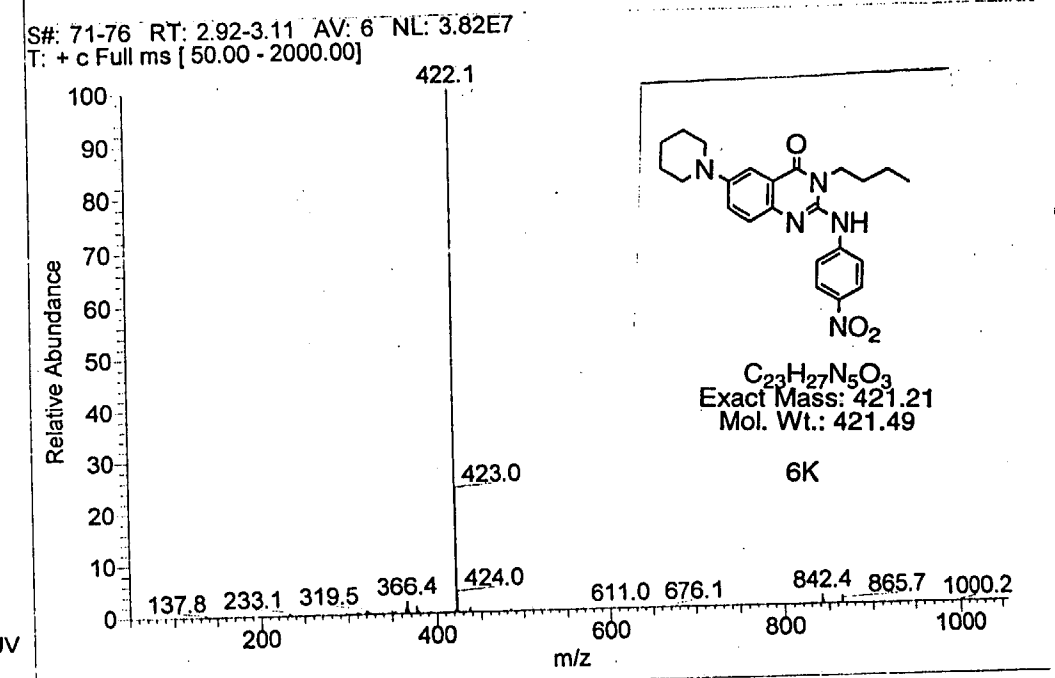


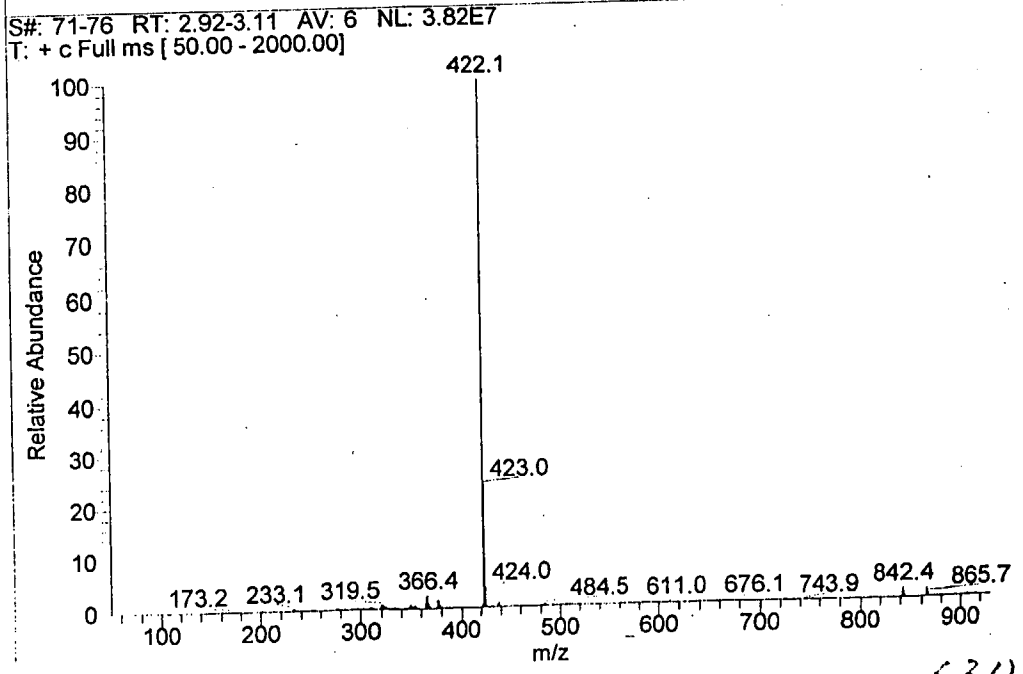


Experiment Method: C:\LCQ\Methods\ESI\Short-col\ESI5-95m8 Created: 11/11/97
Last modified: 9/22/01 by lcq
Creator: LCQ
Summary: 5-95m8
MS Run Time (min): 6.00

Autosampler Settings:

Injection Volume (µL): 20.0





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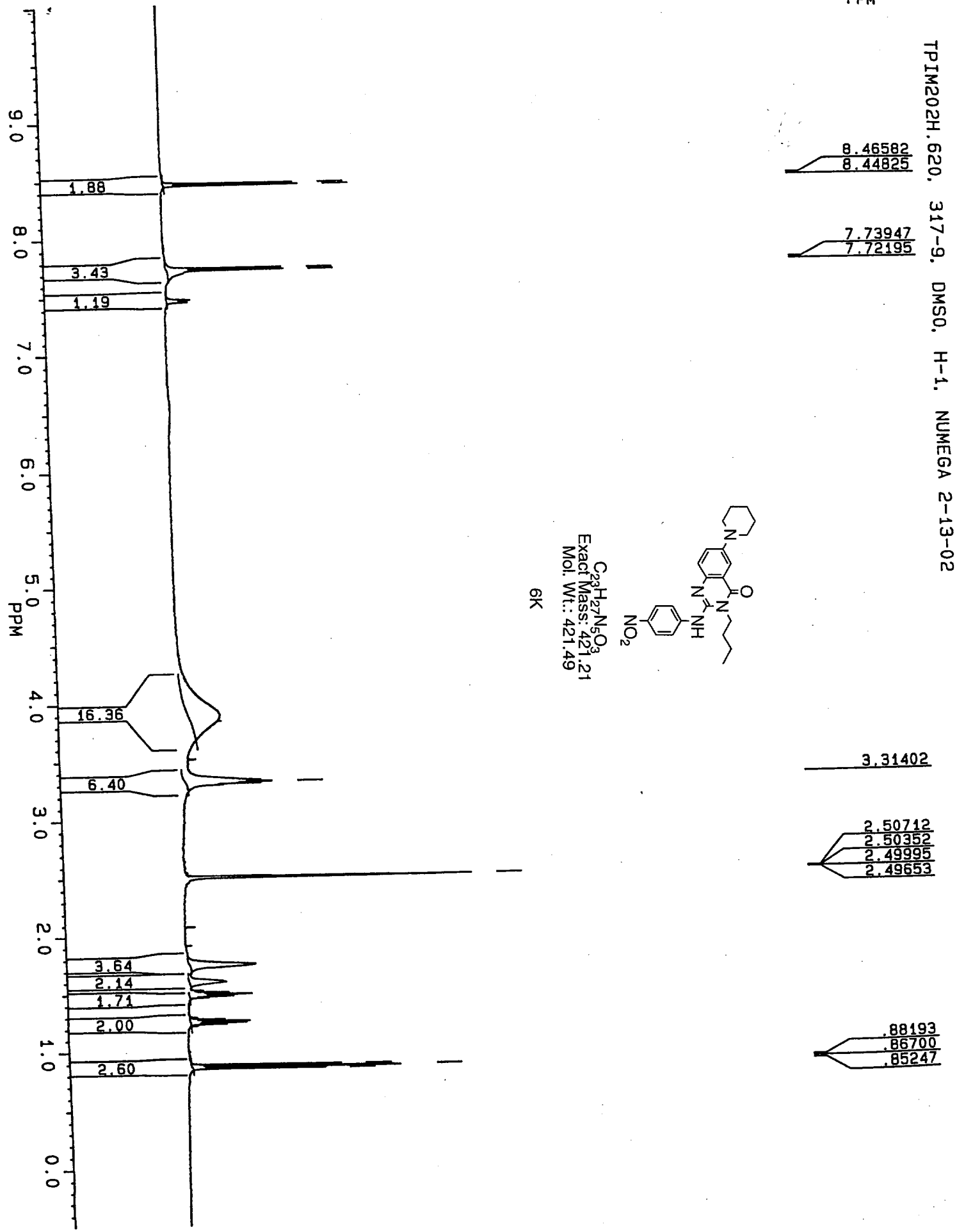
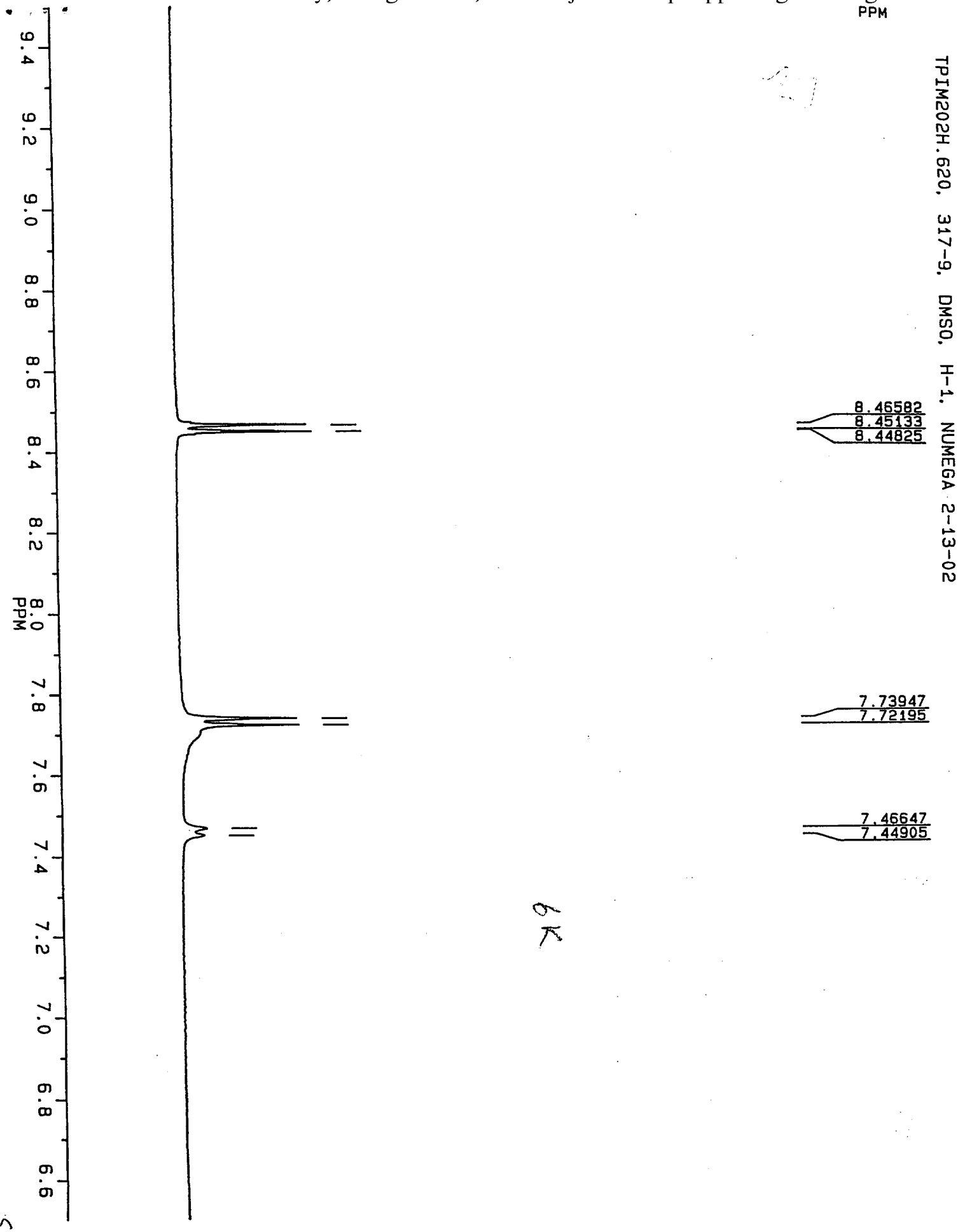

TPIM202H.620, 317-9, DMSO, H-1, NUMEGA 2-13-02
8.46582
8.44825
7.73947
7.72195
3.31402
2.50712
2.50352
2.49995
2.49653
.88193
.86700
.85247
$C_{23}H_{27}N_5O_3$
Exact Mass: 421.21
Mol. Wt.: 421.49
6K
1.88
3.43
1.19
16.36
6.40
3.64
2.14
1.71
2.00
2.60
PPM


PPM
TPIM202H.620, 317-9, DMSO, H-1, NUMEGA 2-13-02
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8.45133
8.44825
7.73947
7.72195
7.46647
7.44905
9.4
9.2
9.0
8.8
8.6
8.4
8.2
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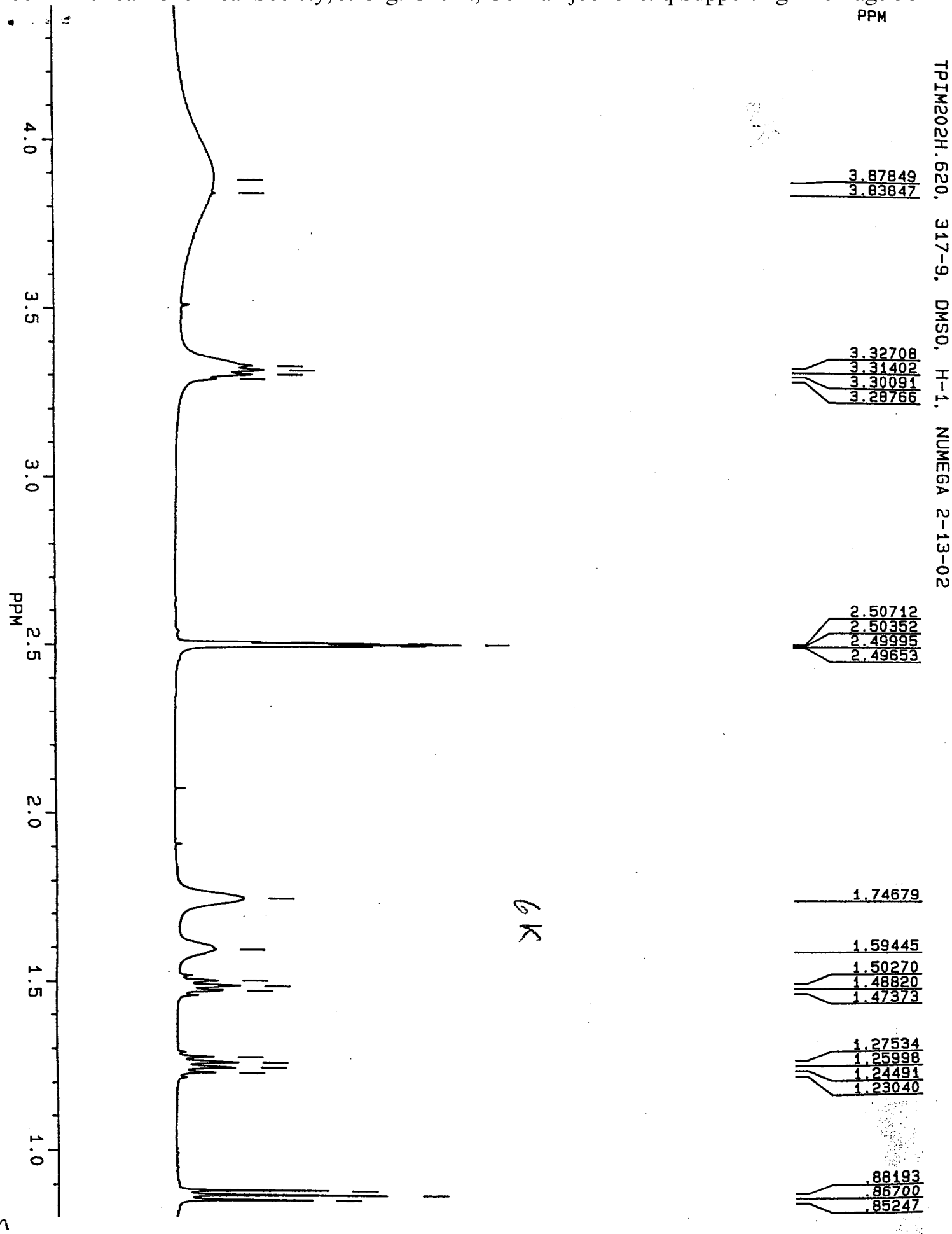
7.8
7.6
7.4
7.2
7.0
6.8
6.6
PPM

6K

S36.


PPM
TPIM202H.620, 317-9, DMSO, H-1, NUMEGA 2-13-02
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3.83847
3.32708
3.31402
3.30091
3.28766
2.50712
2.50352
2.49995
2.49653
1.74679
1.59445
1.50270
1.48820
1.47373
1.27534
1.25998
1.24491
1.23040
.88193
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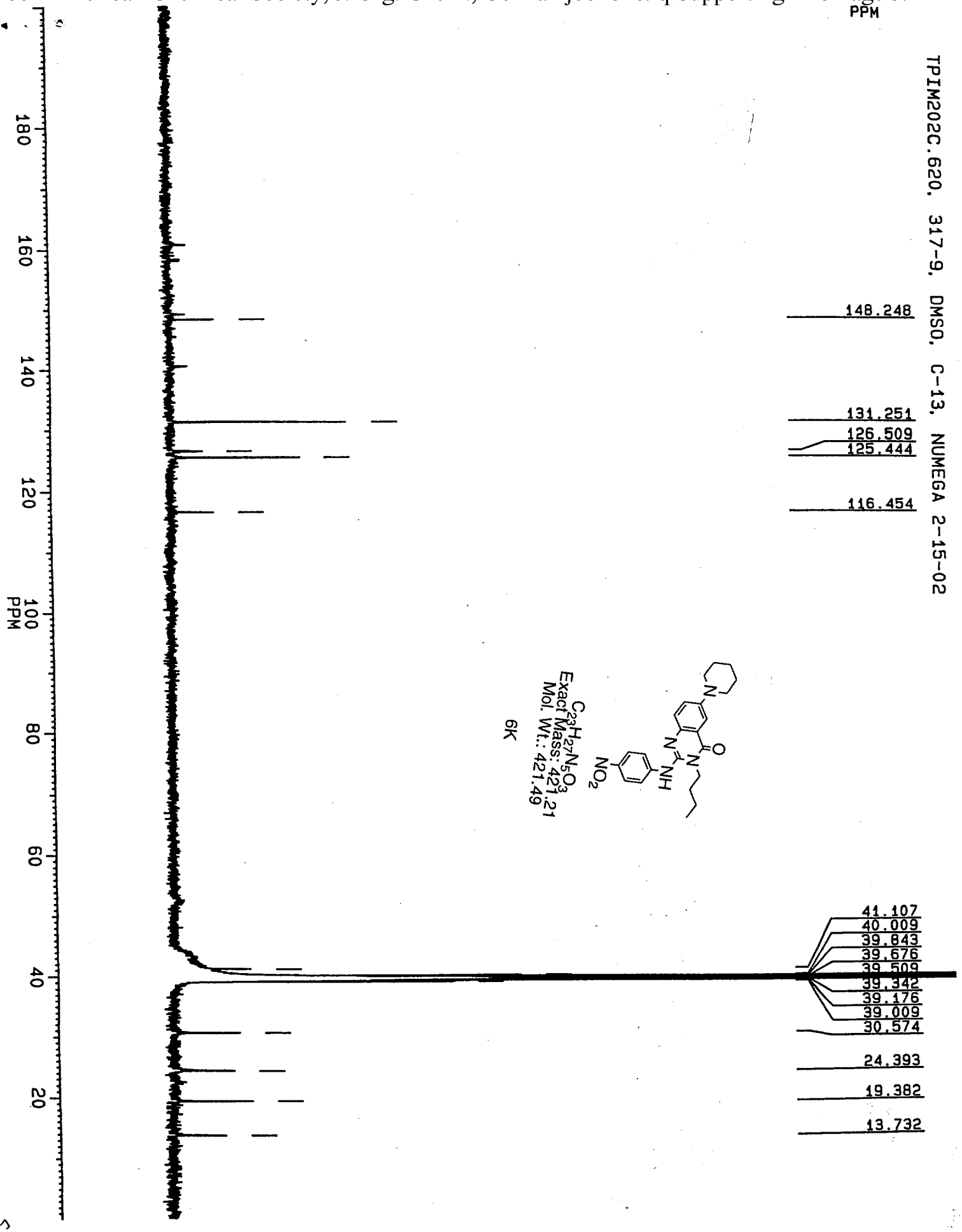
3.5
3.0
2.5
2.0
1.5
1.0
PPM

6K

S37


PPM
TPIM202C.620, 317-9, DMSO, C-13, NUMEGA 2-15-02
148.248
131.251
126.509
125.444
116.454
41.107
40.009
39.843
39.676
39.509
39.342
39.176
39.009
30.574
24.393
19.382
13.732
$C_{23}H_{27}N_5O_3$
Exact Mass: 421.21
Mol. Wt.: 421.49
6K
180
160
140
120
100
80
60
40
20
PPM

538