SUPPLEMENTARY INFORMATION 1

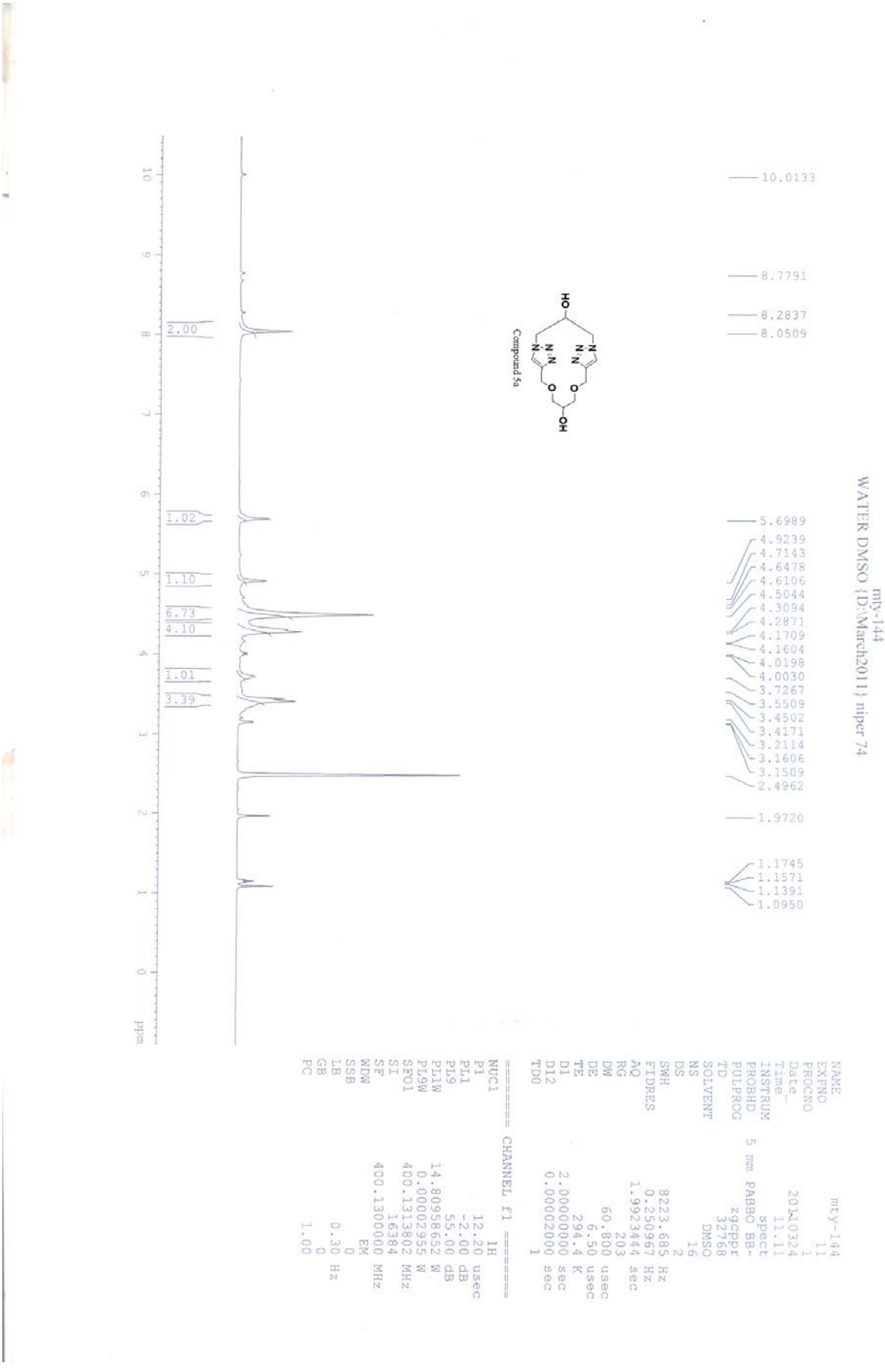
Synthesis of self-assembling glycerotriazolophanes

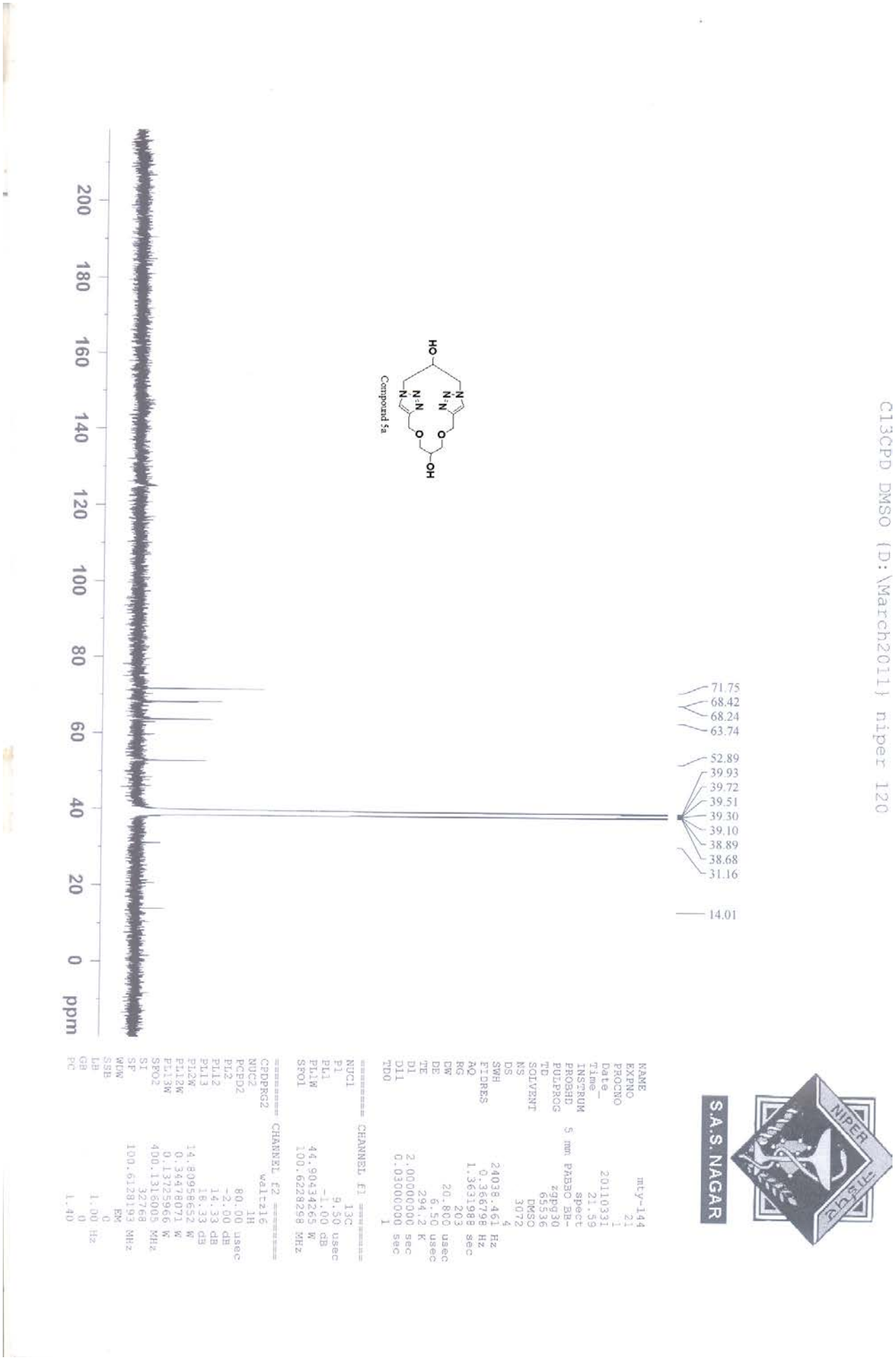
Mohit Tyagi, Nikhil Taxak, Prasad V. Bharatam, K. P. Ravindranathan Kartha*

Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research, SAS Nagar, Punjab 160062, India

*E-mail: rkartha@niper.ac.in

Table of Contents


mty-144
WATER DMSO (D:\March2011) niper 74
Compound 5a
10.0133
8.7791
8.2837
8.0509
5.6989
4.9239
4.7143
4.6478
4.6106
4.5044
4.3094
4.2871
4.1709
4.1604
4.0198
4.0030
3.7267
3.5509
3.4502
3.4171
3.2114
3.1606
3.1509
2.4962
1.9720
1.1745
1.1571
1.1391
1.0950
2.00
1.02
1.10
6.73
4.10
1.01
3.39
ppm
NAME mty-144
EXPNO 11
PROCNO 1
Date_ 20110324
Time 11.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgcppr
TD 32768
SOLVENT DMSO
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 294.4 K
D1 2.00000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -2.00 dB
PL9 55.00 dB
PL1W 14.80958652 W
PL9W 0.00002955 W
SFO1 400.1313802 MHz
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Mass Spectrum List Report

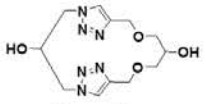
Analysis Info

Analysis Name	D:\Data\KARTHA\11-03-09-MTY-137.d	Acquisition Date	3/10/2011 3:35:54 PM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MTY-137	Instrument / Ser#	maXis 40
Comment			

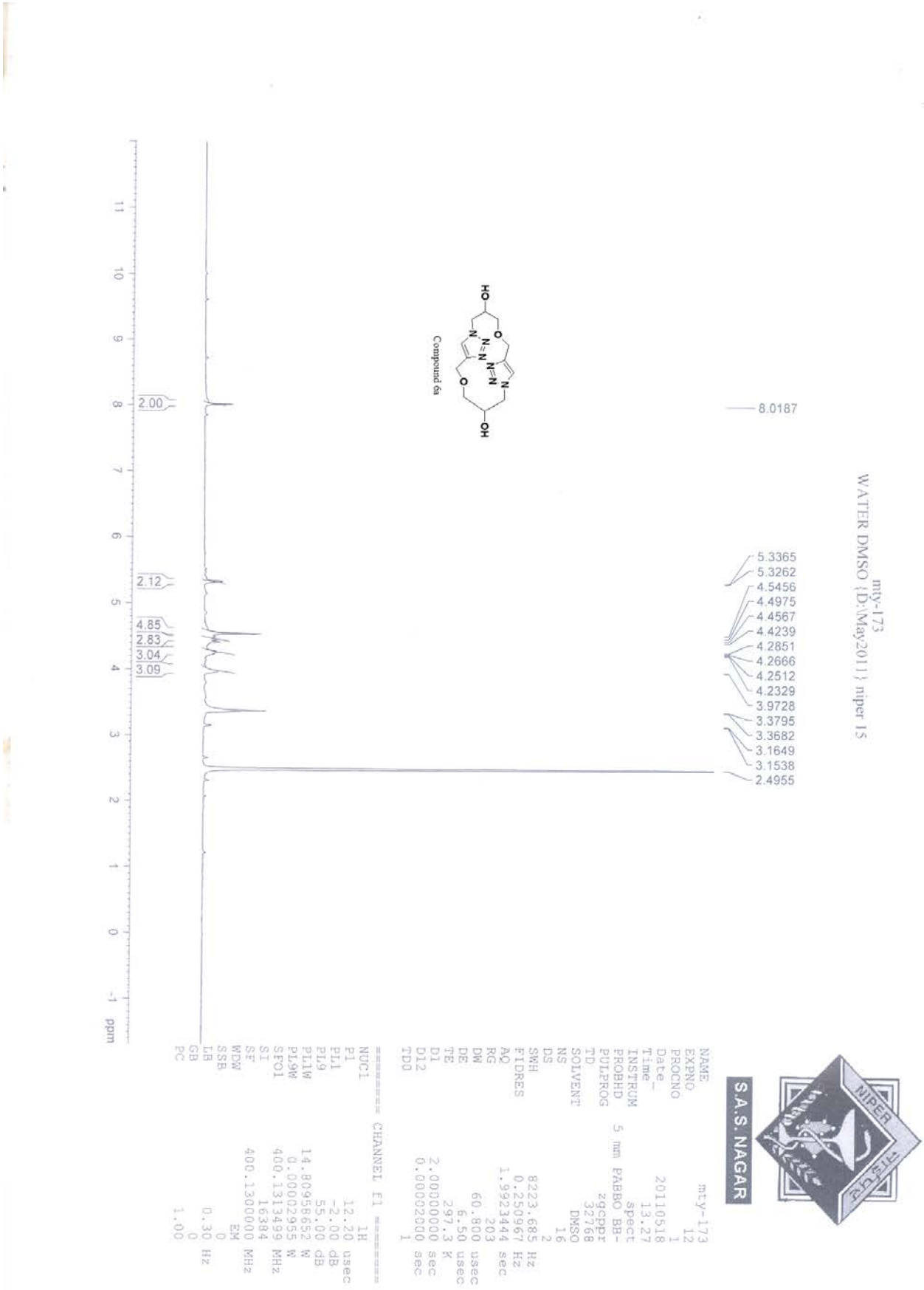
Acquisition Parameter

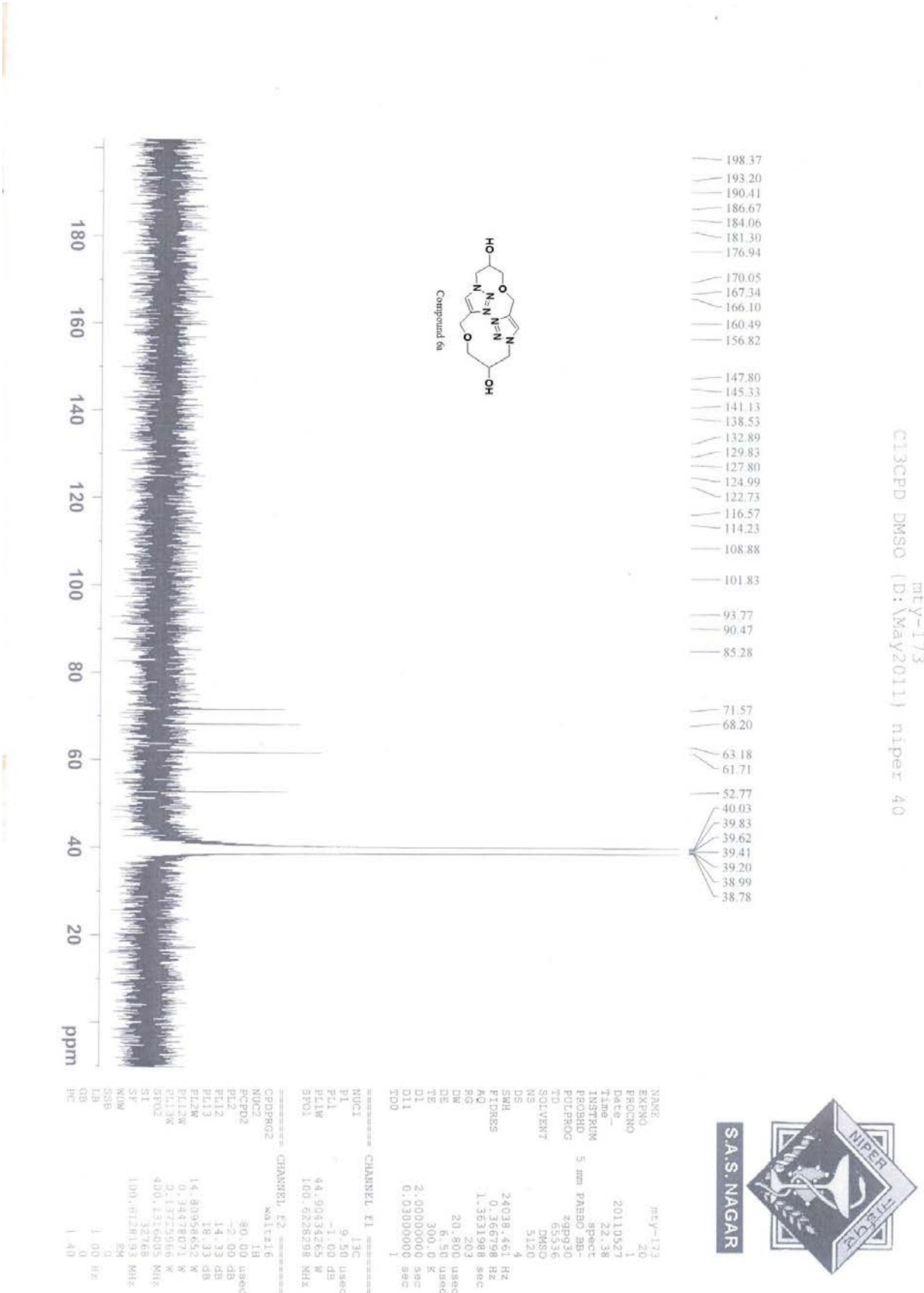
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

#	m/z	Res.	S/N	I	FWHM
1	261.0584	28898	568.9	7798	0.0090
2	274.2743	26857	1813.5	25638	0.0102
3	333.1290	20489	12286.3	220869	0.0163



Compound 5a


mty-173
WATER DMSO {D:\May2011} niper 15
Compound 6a
8.0187
5.3365
5.3262
4.5456
4.4975
4.4567
4.4239
4.2851
4.2666
4.2512
4.2329
3.9728
3.3795
3.3682
3.1649
3.1538
2.4955
2.00
2.12
4.85
2.83
3.04
3.09
ppm
NAME mty-173
EXPNO 12
PROCNO 1
Date_ 20110518
Time_ 13.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgcppr
TD 32768
SOLVENT DMSO
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -2.00 dB
PL9 55.00 dB
PL1W 14.80958652 W
PL9W 0.00002955 W
SFO1 400.1313499 MHz
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
S.A.S. NAGAR
NIPER


mty-173
C13CPD DMSO (D:\May2011) niper 40
Compound 6a
198.37
193.20
190.41
186.67
184.06
181.30
176.94
170.05
167.34
166.10
160.49
156.82
147.80
145.33
141.13
138.53
132.89
129.83
127.80
124.99
122.73
116.57
114.23
108.88
101.83
93.77
90.47
85.28
71.57
68.20
63.18
61.71
52.77
40.03
39.83
39.62
39.41
39.20
38.99
38.78
180
160
140
120
100
80
60
40
20
ppm
S.A.S. NAGAR
NIPER
Punjab

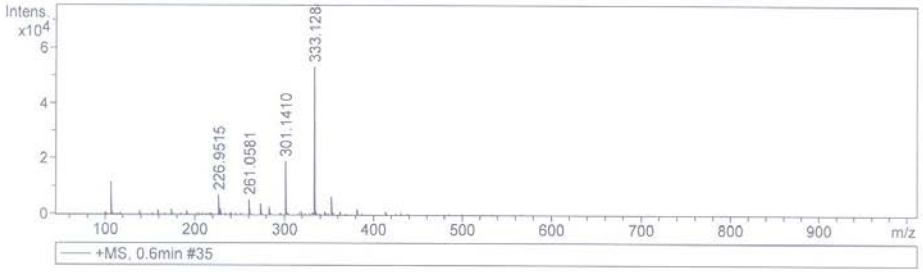
Mass Spectrum List Report

Analysis Info

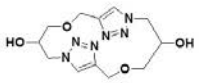
Analysis Name	D:\Data\KARTHA\11-03-09-MTY-136.d	Acquisition Date	3/10/2011 3:40:51 PM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MTY-136	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	226.9515	30261	368.9	7114	0.0075
2	229.0319	26280	98.5	1901	0.0087
3	261.0581	25098	283.8	5516	0.0104
4	301.1410	29044	923.3	18969	0.0104
5	333.1284	24894	2453.4	53092	0.0134



Compound 6a