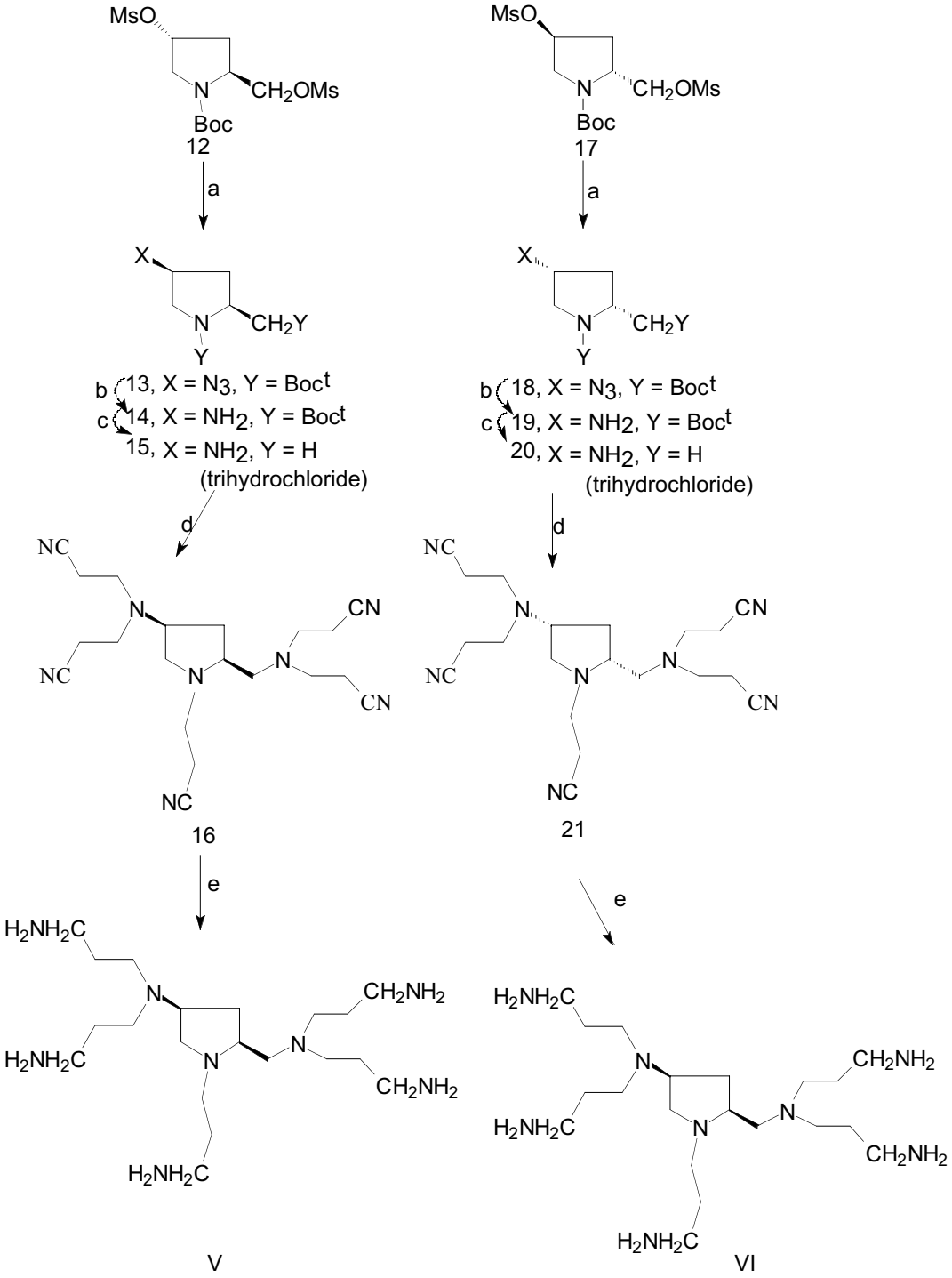
Supplementary Material

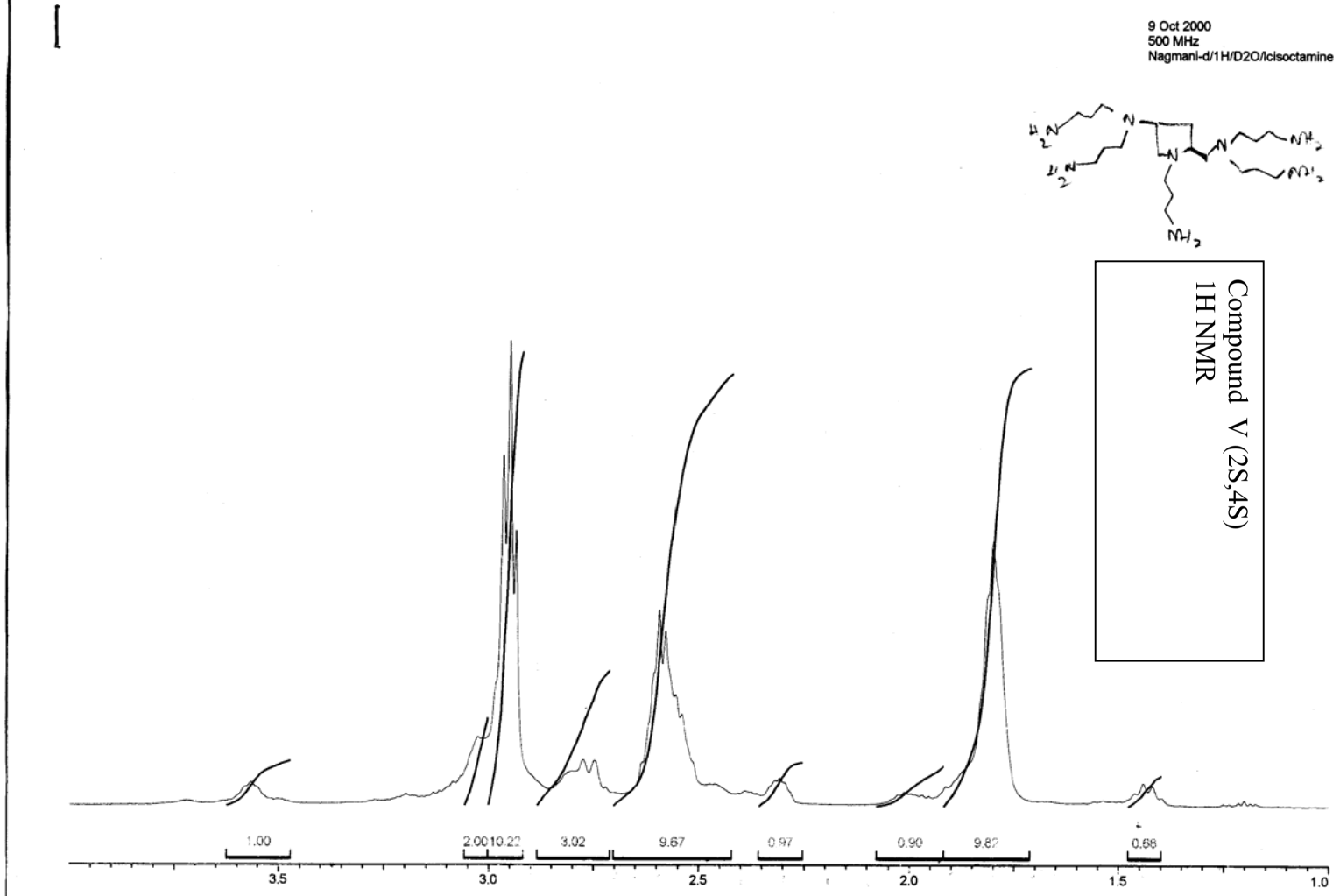
Scheme 2: Synthesis of V and VI
1H NMR of compounds III, IV, V, 6, 11, 16 and 23 (Scheme 2)
13C NMR of compounds V, 6, 11, 16, 21
FABMS of III, IV, V, VI, 6, 11, 16 and 21
Molecular modelling of III-IV
UV melting curves for V and VI
CD of polyamine-DNA complexes



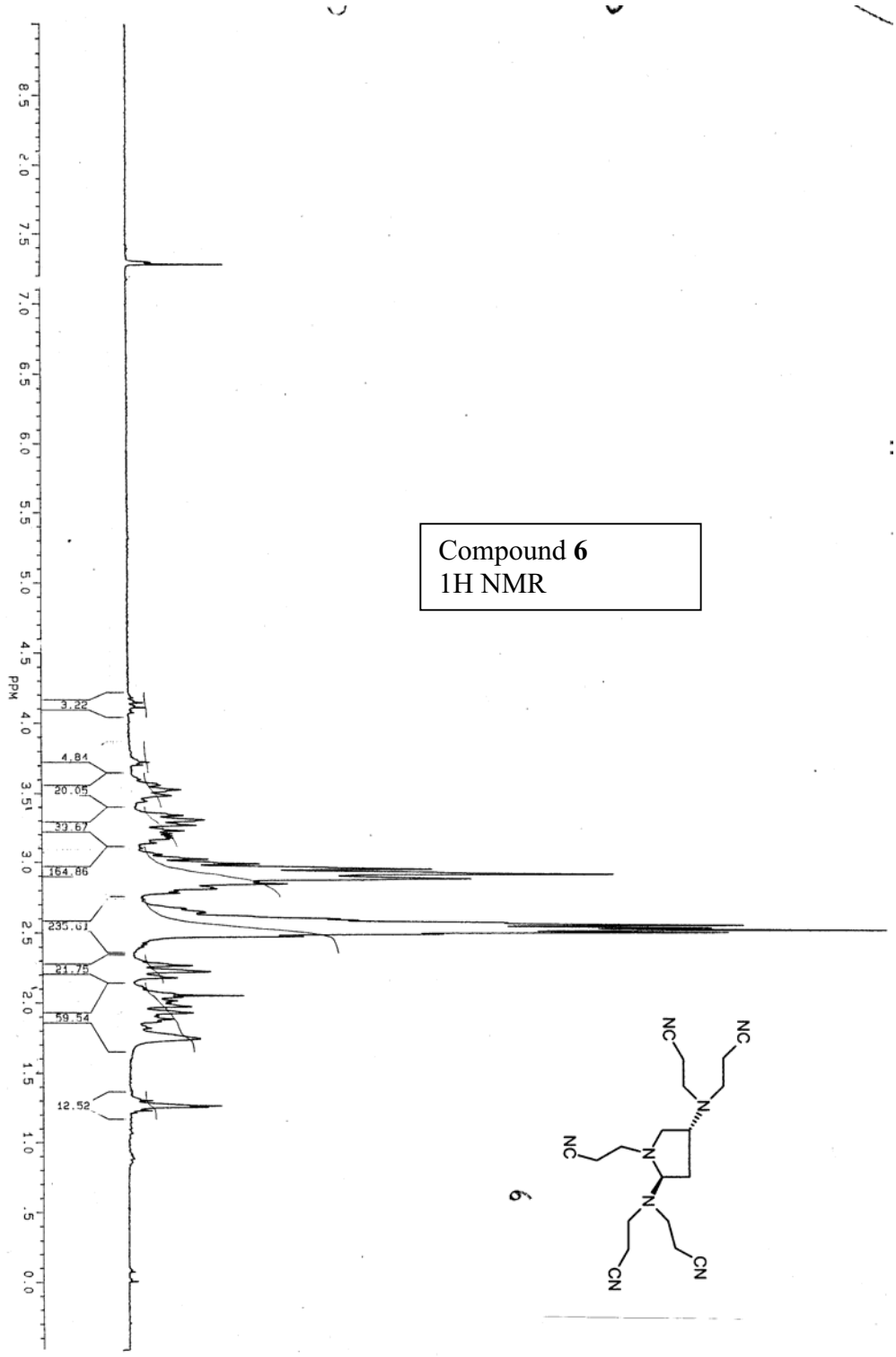
Scheme 2: **Reagents: a**. NaN_3-DMF; **b**. H_2/Pd-C/MeOH; **c**. 5M HCl; **d**, CH_2=CH-CN;

Compound **III (2S,4R)**
^{1}H NMR

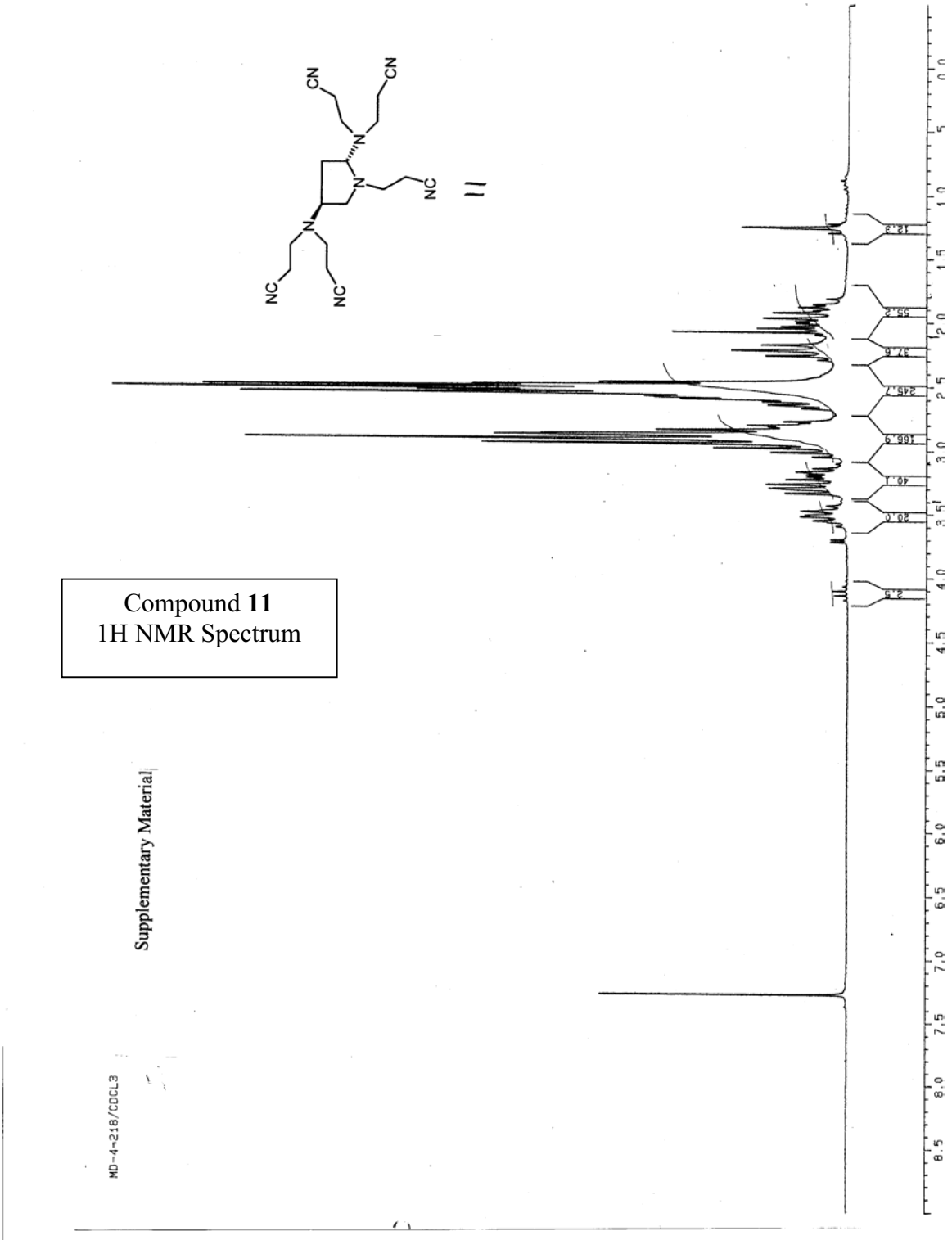
Compound **IV** (2R,4S)
1H NMR



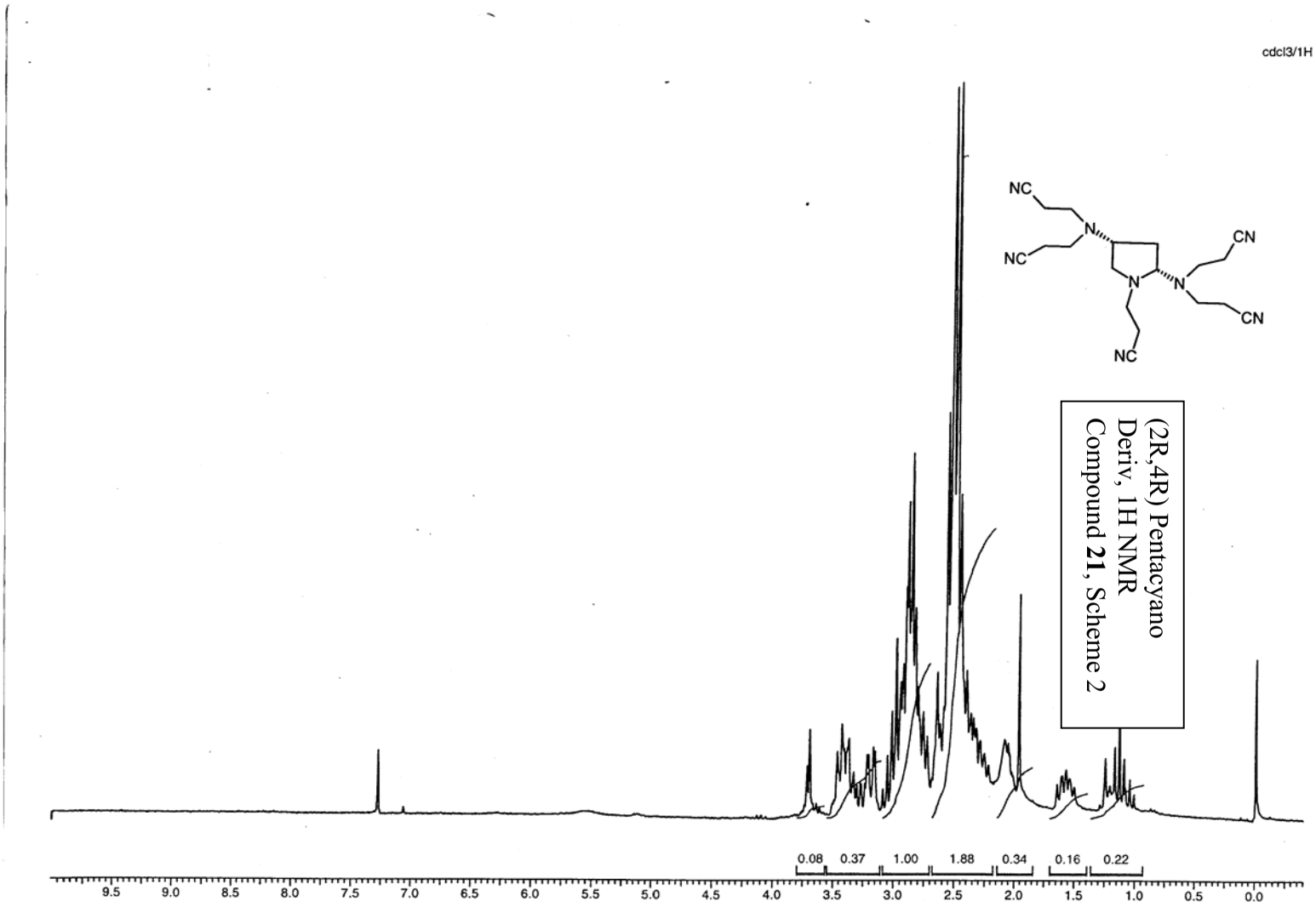
Compound V (2S,4S)
1H NMR



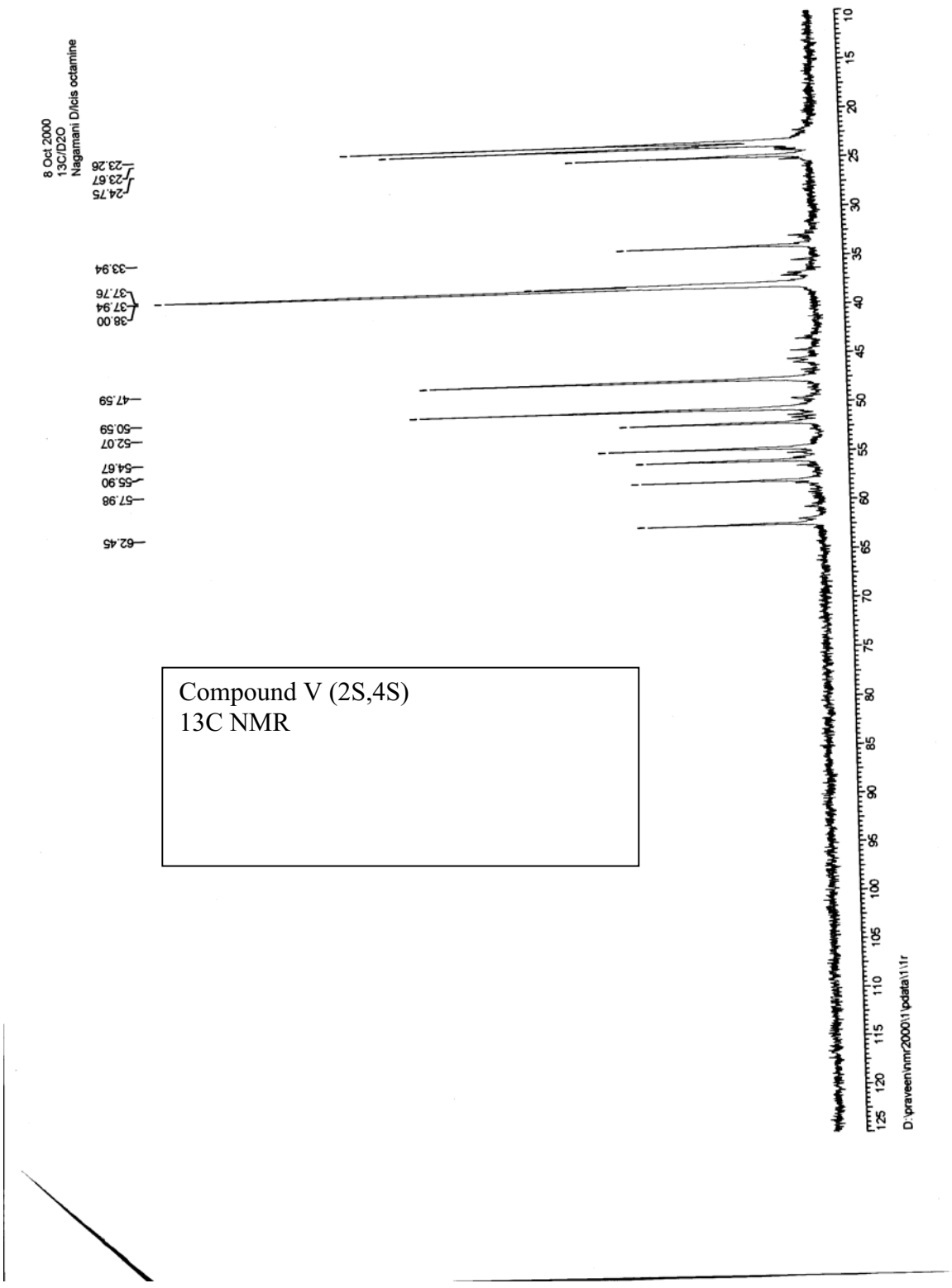
Compound **6**
1H NMR



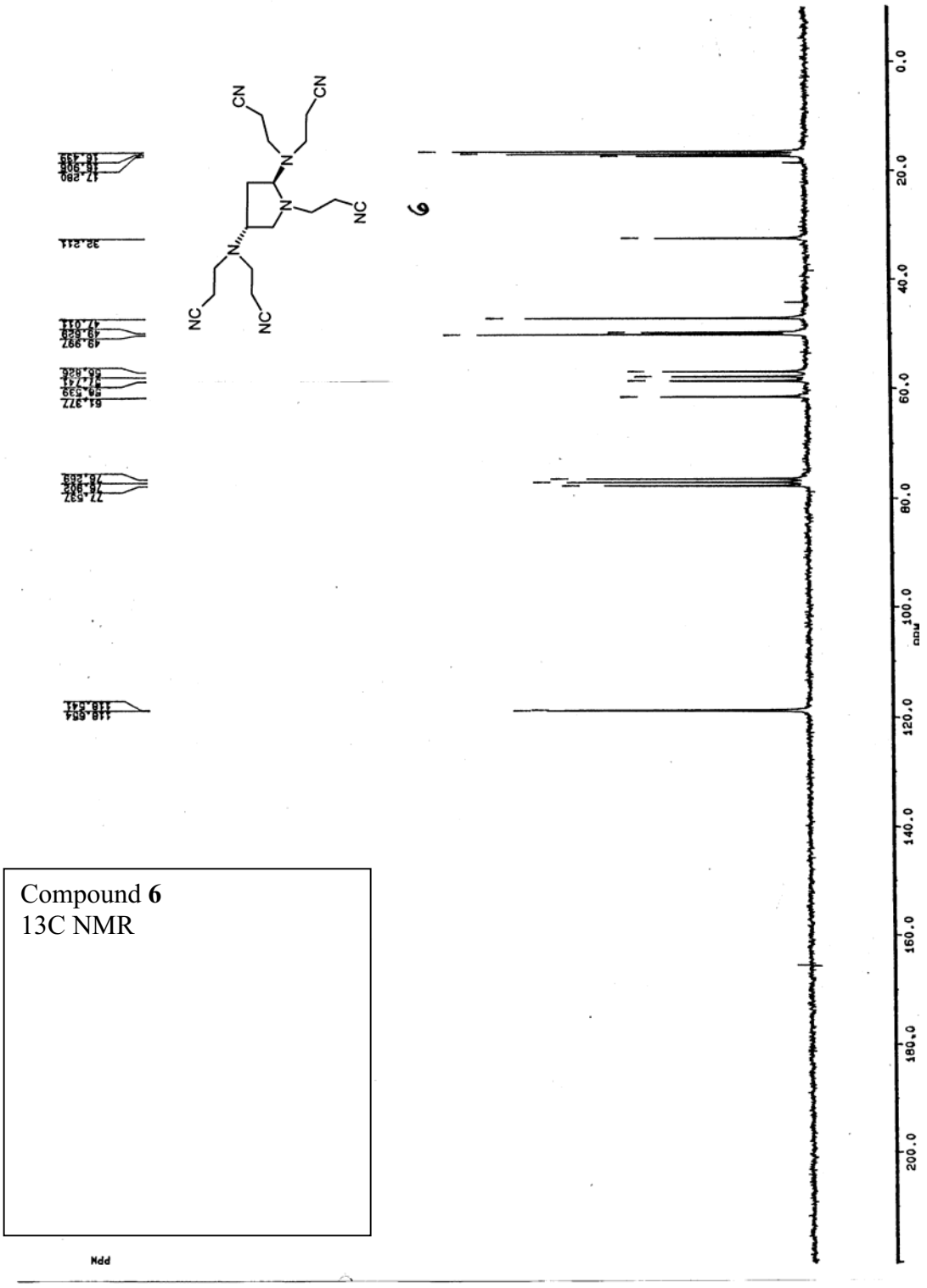
Compound **11**
1H NMR Spectrum



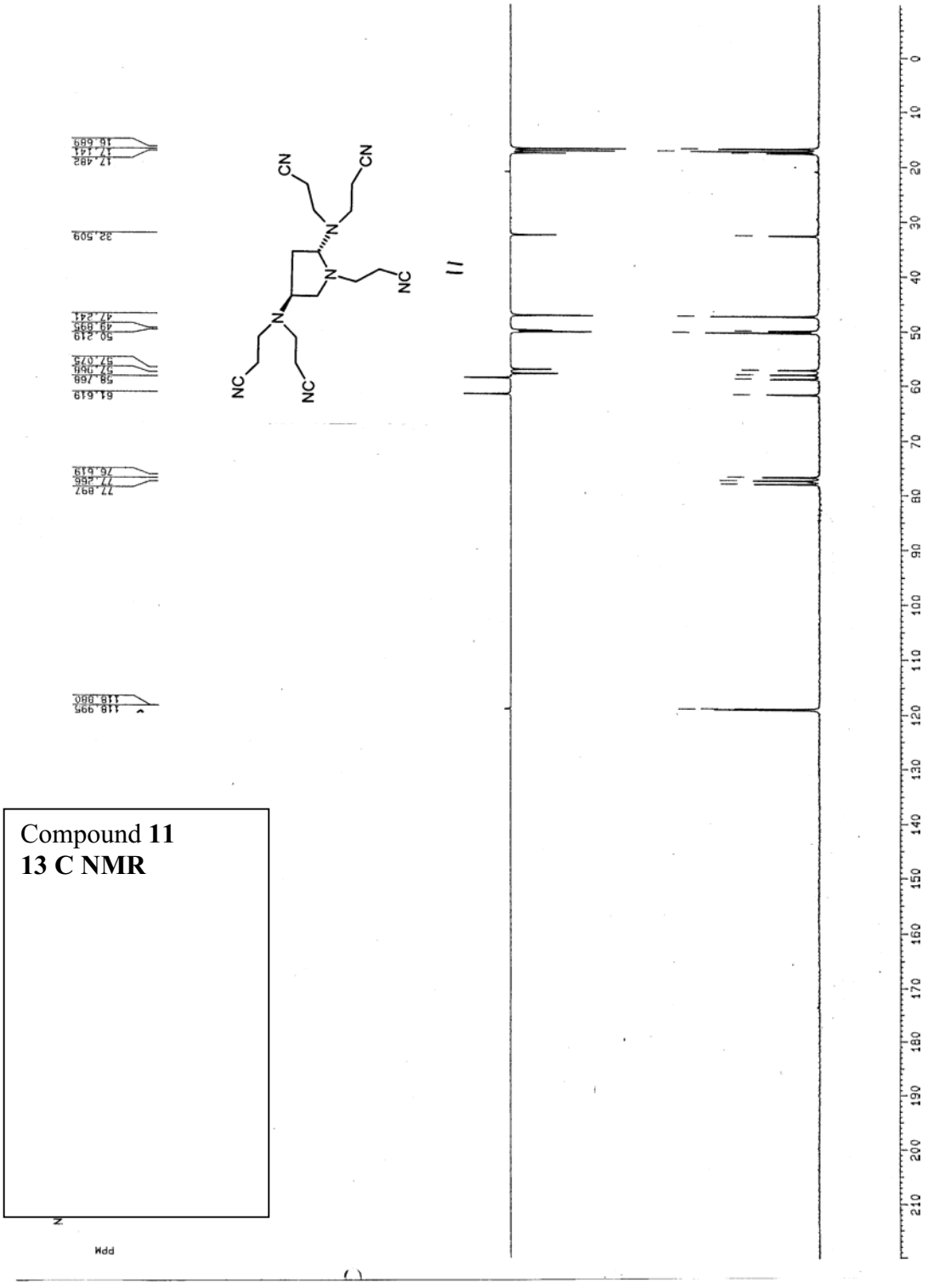
(2R,4R) Pentacyano Deriv, 1H NMR Compound **21**, Scheme 2



Compound V (2S,4S)
13C NMR



Compound **6**
13C NMR



Compound **11**
13 C NMR

NAGMANI/C13/ MD-IV-190/**SVT

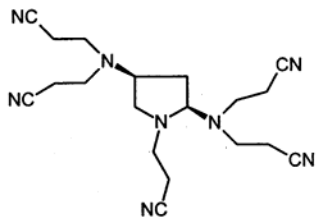
N	CURSOR	FREQUENCY	PPM	INTENSITY
1	4682	5990.887	119.0479	7.408
2	4687	5982.627	118.8838	7.009
3	5801	3921.472	77.9255	3.157
4	5819	3889.555	77.2913	3.256
5	5836	3857.051	76.6454	3.246
6	6247	3096.540	61.5329	5.383
7	6286	3024.832	60.1080	1.499
8	6344	2916.715	57.9595	4.850
9	6350	2906.643	57.7594	5.977
10	6356	2895.512	57.5382	5.319
11	6562	2513.893	49.9548	10.401
12	6575	2490.206	49.4841	5.098
13	6645	2361.509	46.9267	9.641
14	6999	1707.018	33.9210	4.396
15	7437	895.576	17.7964	11.743
16	7442	887.116	17.6283	6.445
17	7475	825.736	16.4086	12.979

Nagmani D.

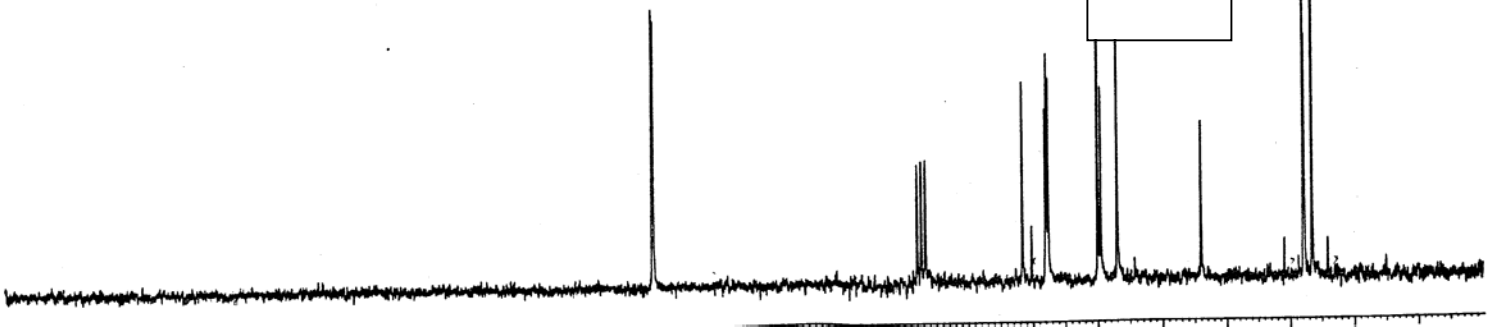
MD-IV-190 / CDCl3

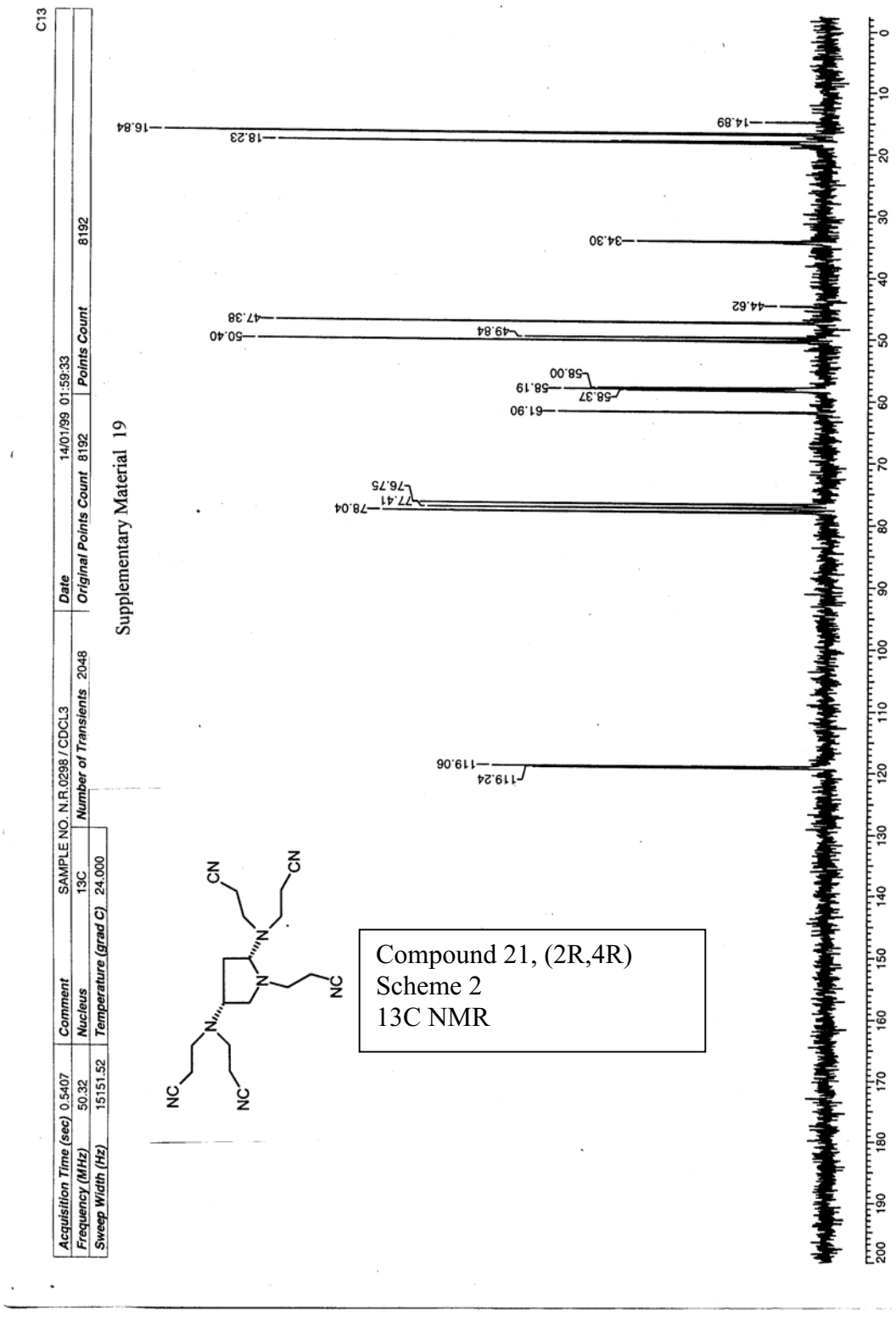
C13 /

17-10-92



Compound 16, (2S,4S)
Scheme 2
13C NMR

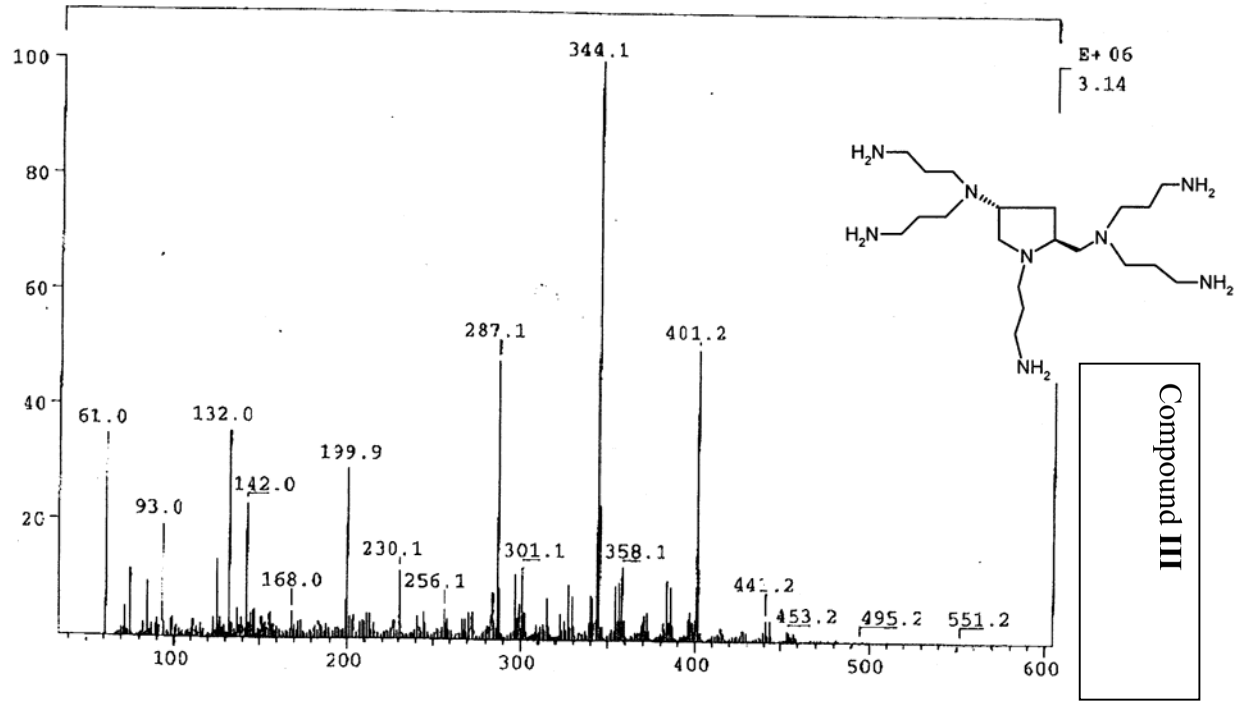



C13
Acquisition Time (sec) 0.5407
Comment
SAMPLE NO. N.R.0298 / CDCL3
Date
14/01/99 01:59:33
Frequency (MHz) 50.32
Nucleus
13C
Number of Transients 2048
Original Points Count 8192
Points Count 8192
Sweep Width (Hz) 15151.52
Temperature (grad C) 24.000
Supplementary Material 19
16.84
18.23
14.89
34.30
44.62
47.38
49.84
50.40
58.00
58.19
58.37
61.90
76.75
77.41
78.04
119.06
119.24
CN
CN
NC
NC
NC
Compound 21, (2R,4R)
Scheme 2
13C NMR

3153

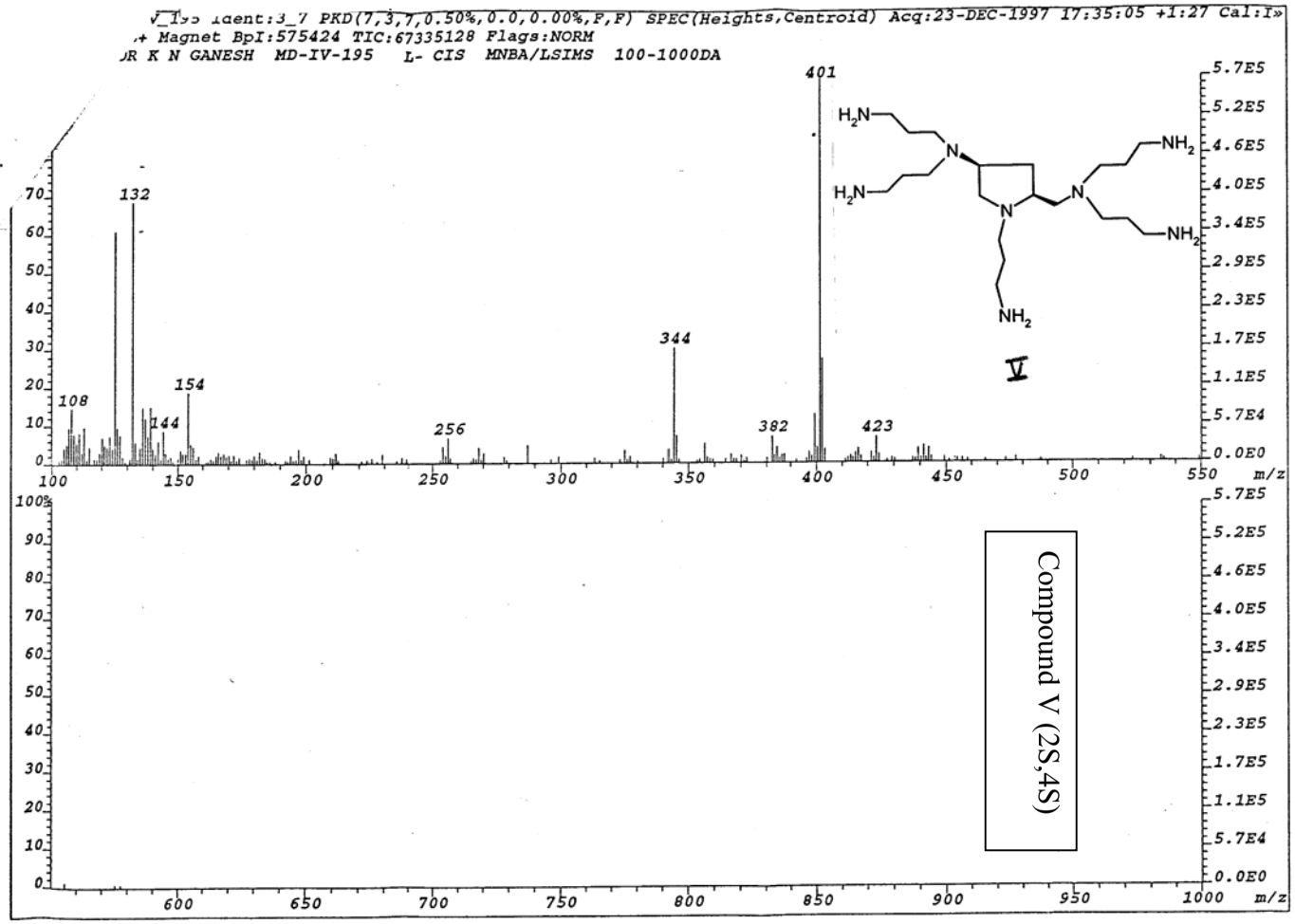
L trans

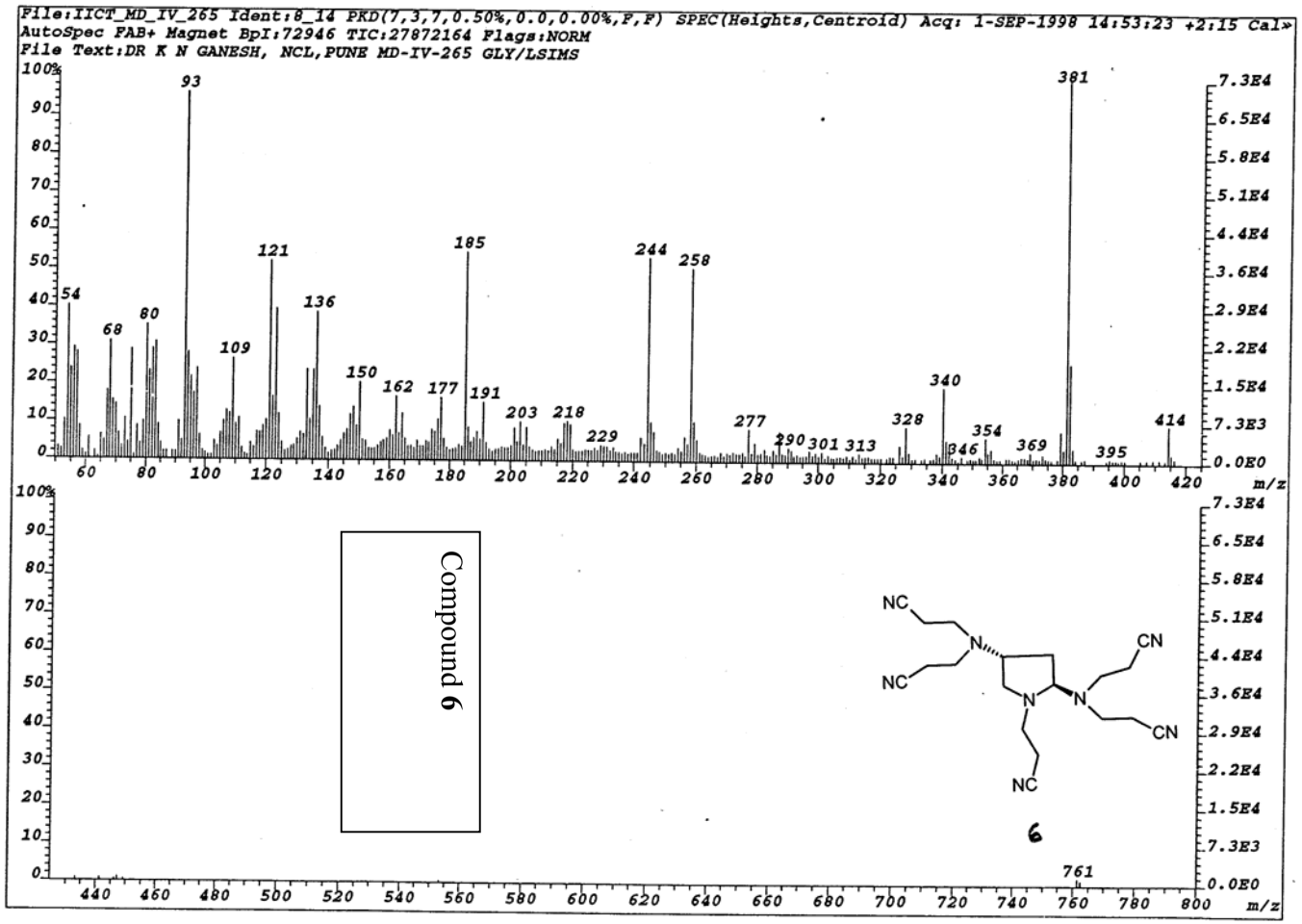
SPEC: 00mat156 28-Feb-00 Elapse: 04:43.2 69
Samp: MDV-267 Start : 15:30:43 98
Comm: LR/CI Spectrum @ 150eV/ isobutane
Mode: CI +VE +LMR BSCAN (EXP) UP LR Study : Med.Chem(Broom)
Oper: Wenchen Luo Client: K.G.Rajeev Inlet :
Base: 344.1 Inten : 3143583 Masses: 60 > 1000
Norm: 344.1 RIC : 35394253 #peaks: 512
Peak: 1000.00 mmu

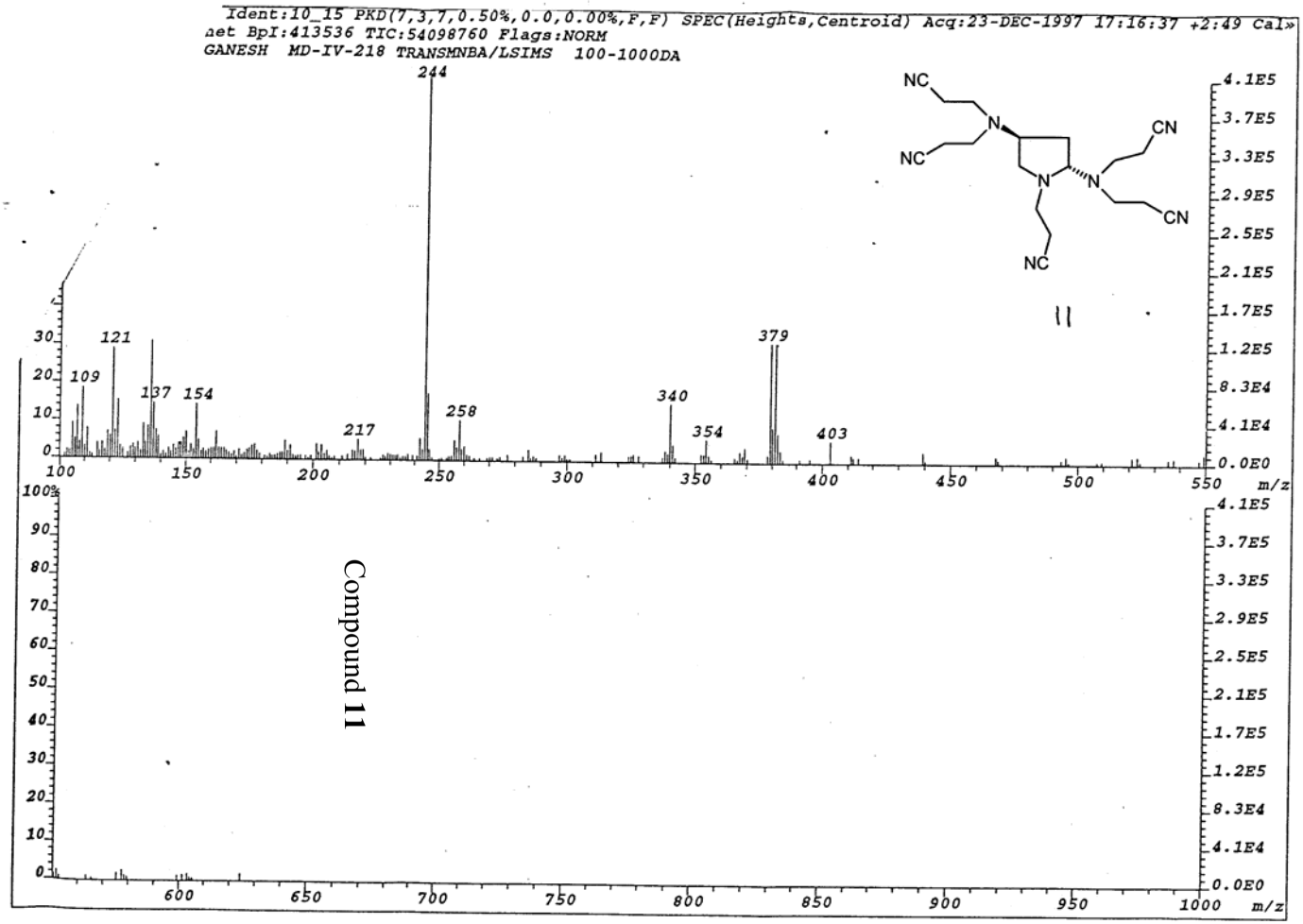


Compound III

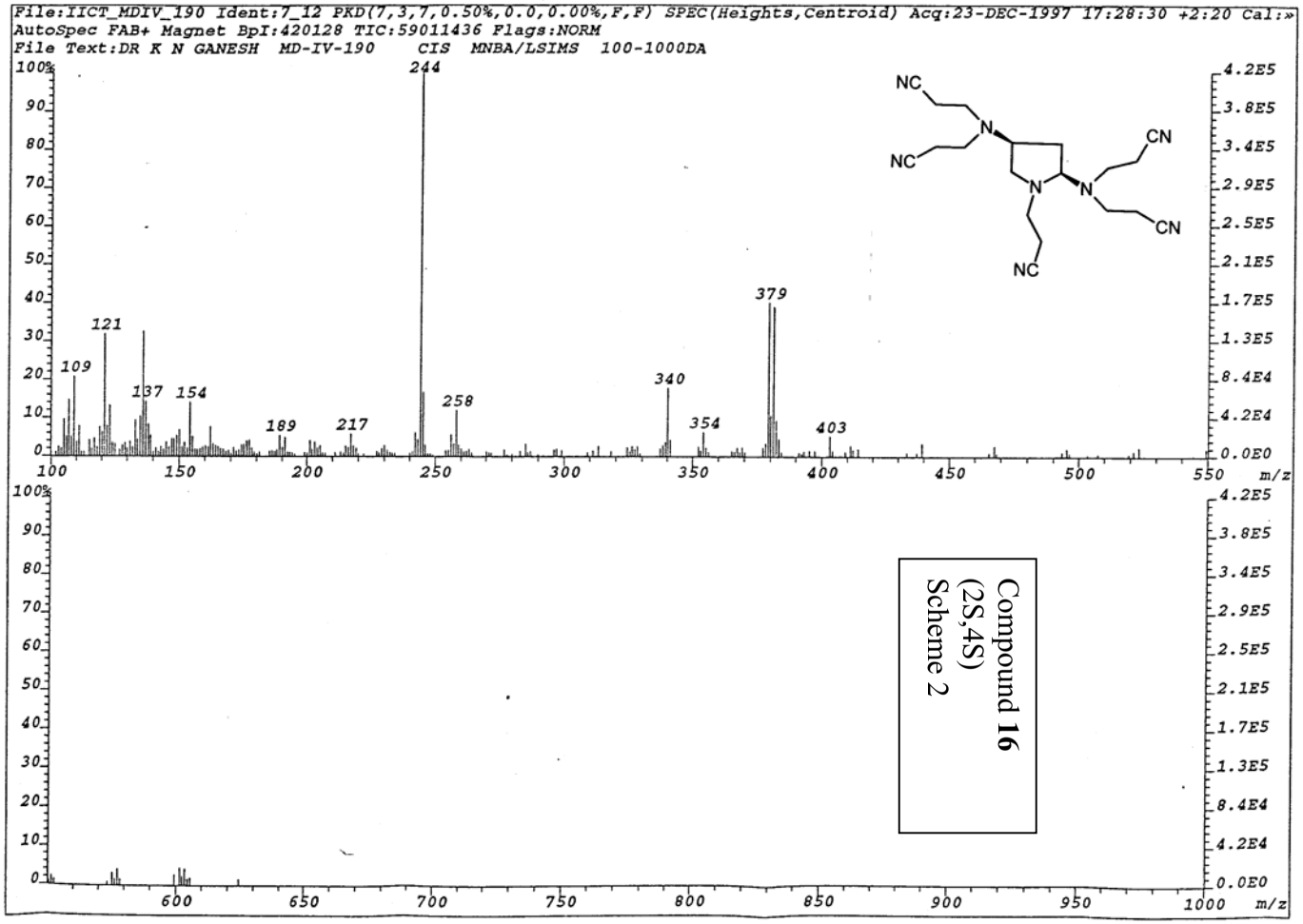
SPEC: 99mat1133
Samp: MDV-321
Comm: LR/Isobutane CI Spectrum @ 150eV
Mode: CI +VE +LMR BSCAN (EXP) UP LR
Oper: Wenchen Luo Client: K.G.Rajeev
Base: 132.1 Inten : 6012519
Norm: 132.1 RIC : 102183026
Peak: 1000.00 mmu
01-Dec-99
Elapse: 08:56.2 130
Start : 14:43:41 163
Study : Broom(Med.Chem)
Inlet :
Masses: 60 > 1000
#peaks: 584
E+06
6.01
Compound IV


PKD(7,3,7,0.50%,0.0,0.00%,F,F) SPEC(Heights,Centroid) Acq:23-DEC-1997 17:35:05 +1:27 Cal:I»
Magnet BpI:575424 TIC:67335128 Flags:NORM
K N GANESH MD-IV-195 L- CIS MNBA/LSIMS 100-1000DA
401
132
344
154
108
144
256
382
423
V
m/z
Compound V (2S,4S)


File:IICT_MD_IV_265 Ident:8_14 PKD(7,3,7,0.50%,0.0,0.00%,F,F) SPEC(Heights,Centroid) Acq: 1-SEP-1998 14:53:23 +2:15 Cal»
AutoSpec FAB+ Magnet BpI:72946 TIC:27872164 Flags:NORM
File Text:DR K N GANESH, NCL,PUNE MD-IV-265 GLY/LSIMS
Compound 6
NC
CN
6
m/z


Ident:10_15 PKD(7,3,7,0.50%,0.0,0.00%,F,F) SPEC(Heights,Centroid) Acq:23-DEC-1997 17:16:37 +2:49 Cal»
Net BpI:413536 TIC:54098760 Flags:NORM
GANESH MD-IV-218 TRANSMNBA/LSIMS 100-1000DA
244
121
109
137
154
217
258
340
354
379
403
NC
CN
m/z
11

Compound **11**



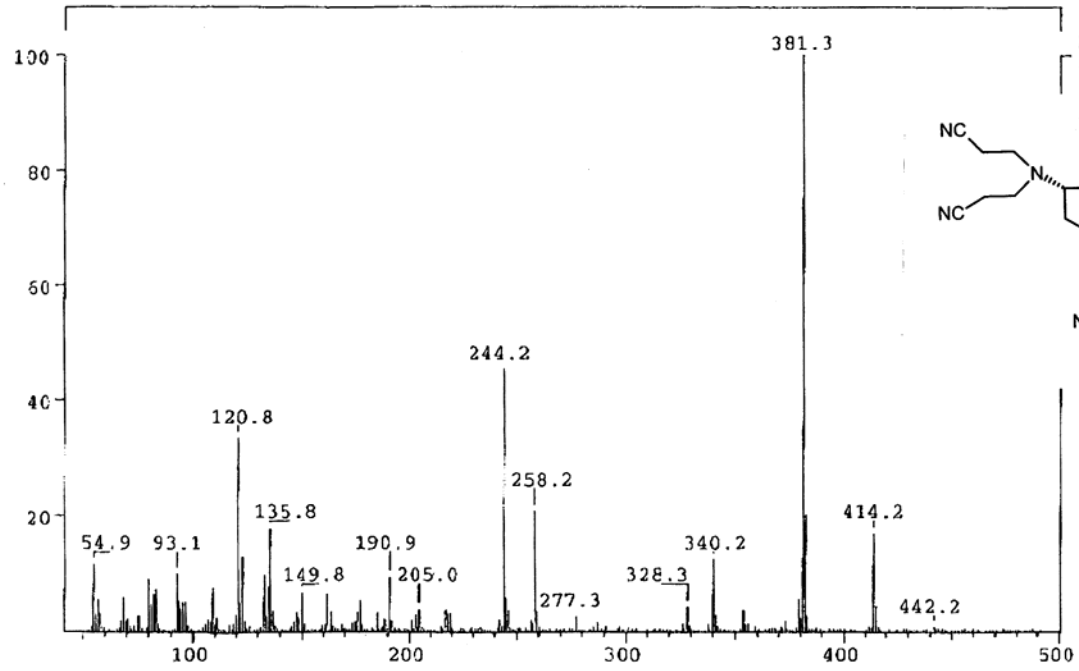
Compound **16**
(2S,4S)
Scheme 2

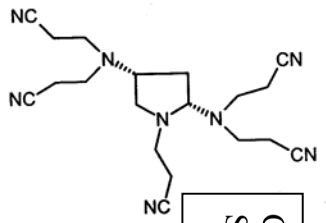
NOV-19-99 FRI 17:03 U OF U MED CHEM FAX NO. 8015859119 P.01

RANESH, K.N from RAJEEV

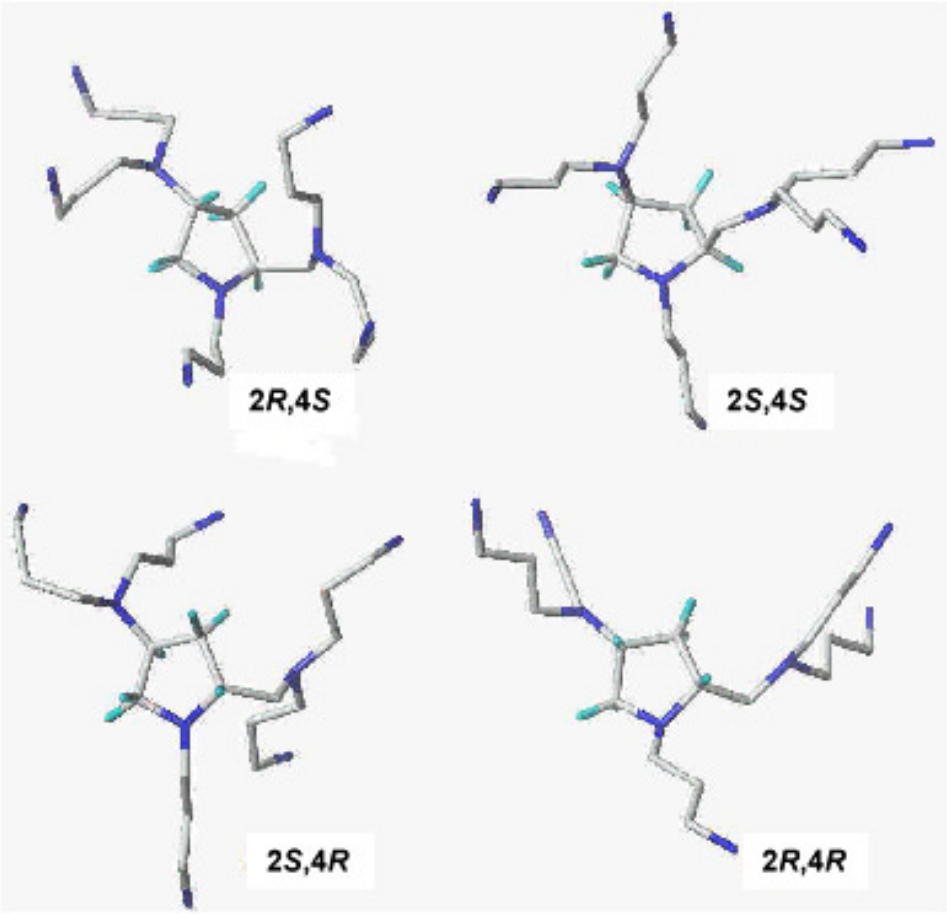
FAX 20 5.89 353

SPEC: 99mat1068 10-Nov-99 Elapse: 00:19.1 5
Samp: MDV-316 Start : 14:09:24 13
Comm: LR/FAB(+)/glycercl,MeOH,1%TFA
Mode: FAB +VE +LMR BSCAN (EXP) UP LR Study : Broom(Med.Chem)
Oper: Wenchen Luo Client: K.G.Rajeev Inlet :
Base: 381.3 Inten : 526133 Masses: 10 > 1000
Norm: 381.3 RIC : 3942144 #peaks: 654
Peak: 1000.00 mmu

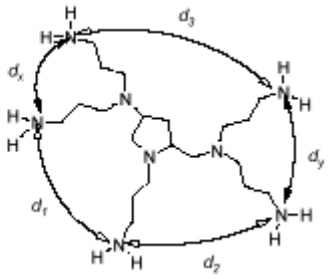




Compound 21 (2R,4R)
Scheme 2

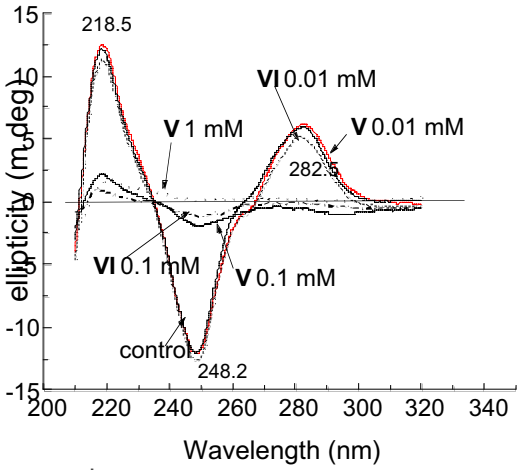


	d_1	d_2	d_3	d_x	d_y
(2*S*,4*S*)-*cis*	10.84	10.81	8.59	6.86	6.98
(2*R*,4*R*)-*cis*	11.67	11.01	11.34	7.10	6.92
(2*R*,4*S*)-*trans*	11.55	6.30	5.90	5.89	7.71
(2*S*,4*R*)-*trans*	6.74	5.19	8.50	5.58	6.24

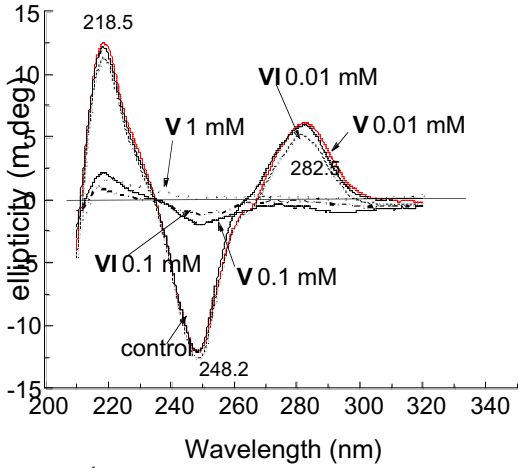


Preliminary molecular modeling was done on a Silicon Graphics computer using Tripos Sybyl software, version 6.1. The other details of energy minimization etc. will be reported later in a detailed paper.

CD data on Polyamine-DNA complexes



CD of duplexes: in 25 mM Tris at pH 7.3



CD of duplexes: in 25 mM Tris at pH 7.3

UV duplex melting curves of V and VI