

Supplementary Information (SI)

Acridinedione as Selective Fluoride ion Chemosensor: A Detailed Spectroscopic and Quantum Mechanical Investigation

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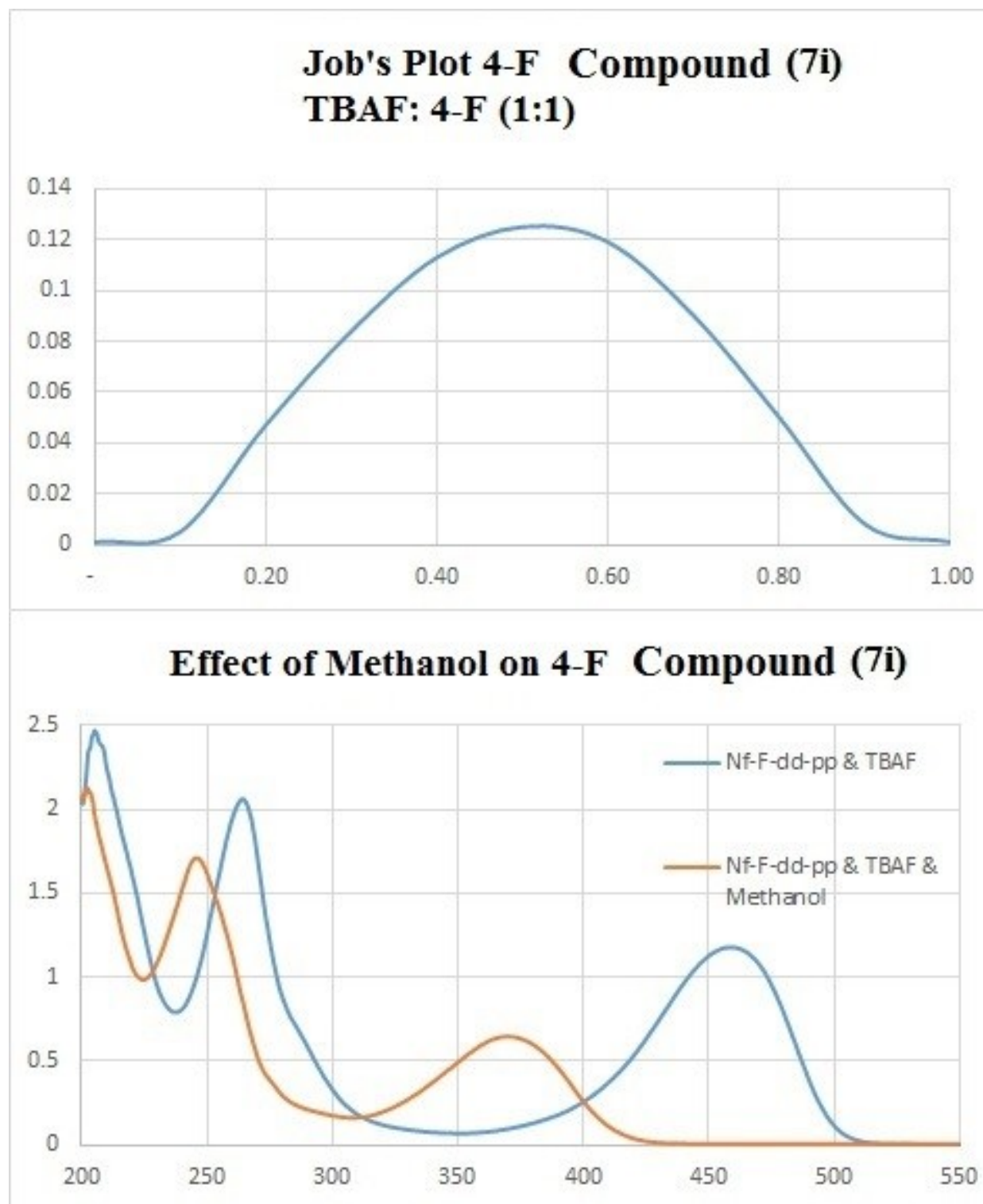


Figure-S1: Job's Plot and Effects of Methanol on 4-Fluoro substituted DHP (7i)

Limit of Detection and Binding constant

The detection limit was calculated from the calibration curve obtained by titrating prob **7i** with different concentration of fluoride sources in acetonitrile as shown in the Figure-S2. $R^2 = 0.99285$, slope (k) = 275.6138, standard deviation (SD) 0.004590. The data was obtained from Shimadzu UV-1800 UV-VIS Spectrophotometer. The detection limit was calculate from the following formula $[3.3 \times \text{SD}/k]$. The method was adopted for LOD of compound **7l** with LOD formula $[4.604 \times \text{SD}/k]$ Figure-S4.

Binding/association constants were calculated using Benesi Hilderbrand equation.

$$\frac{b}{\Delta A} = \frac{1}{S_t K_a \Delta \epsilon} \times \frac{1}{[L]} + \frac{1}{S_t \Delta \epsilon}$$

Equation-1: Benesi Hildebrand Equation

$\Delta A = A_{\text{substrate} + \text{anion}} - A_{\text{substrate}}$, S_t = Total concentration of substrate

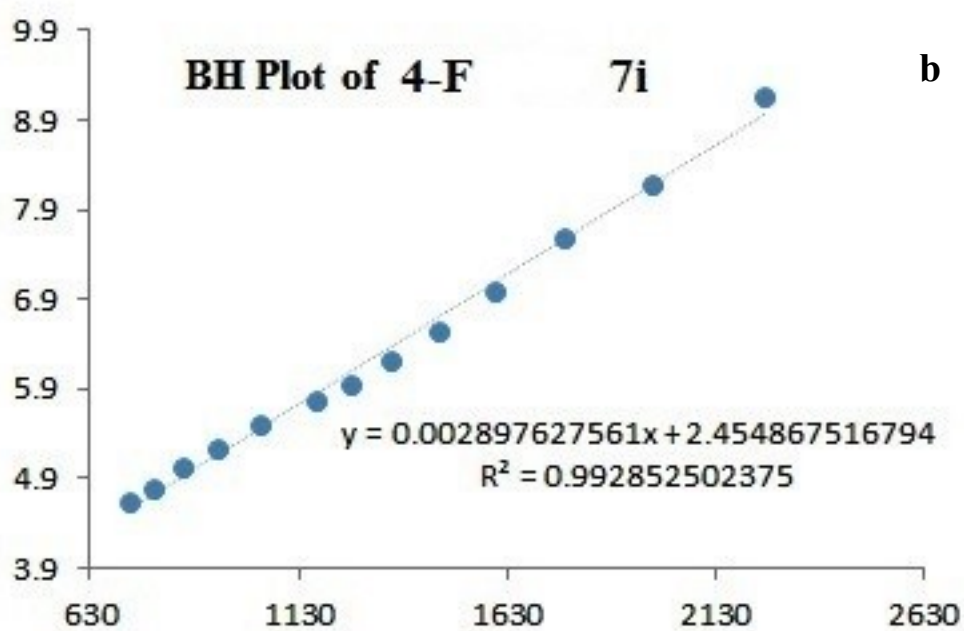
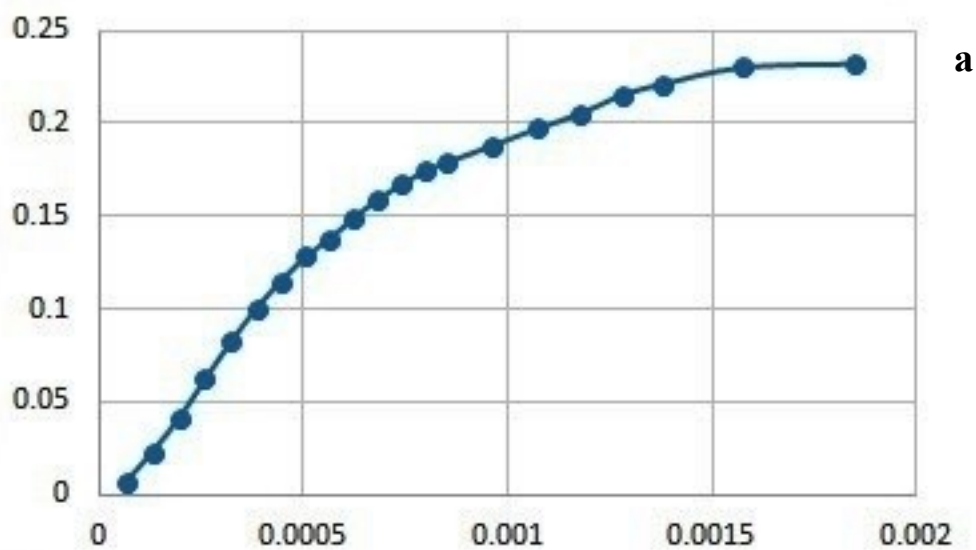
K_a = Binding /Association Constant

$\Delta \epsilon = \epsilon_{\text{substrate} + \text{anion}} - \epsilon_{\text{substrate}} - \epsilon_{\text{anion}}$.

Dividing the intercept with slope from BH Plot, K_a was calculated

	Acridinediones	
	7i	7l
Limit of detection (LOD)	$5.49 \times 10^{-5} \text{ M}$	$9.29 \times 10^{-5} \text{ M}$
Binding Constant	$8.47 \times 10^2 \text{ M}^{-1}$	$1.14 \times 10^3 \text{ M}^{-1}$

Calibration curve of 4-F Compound (7i)



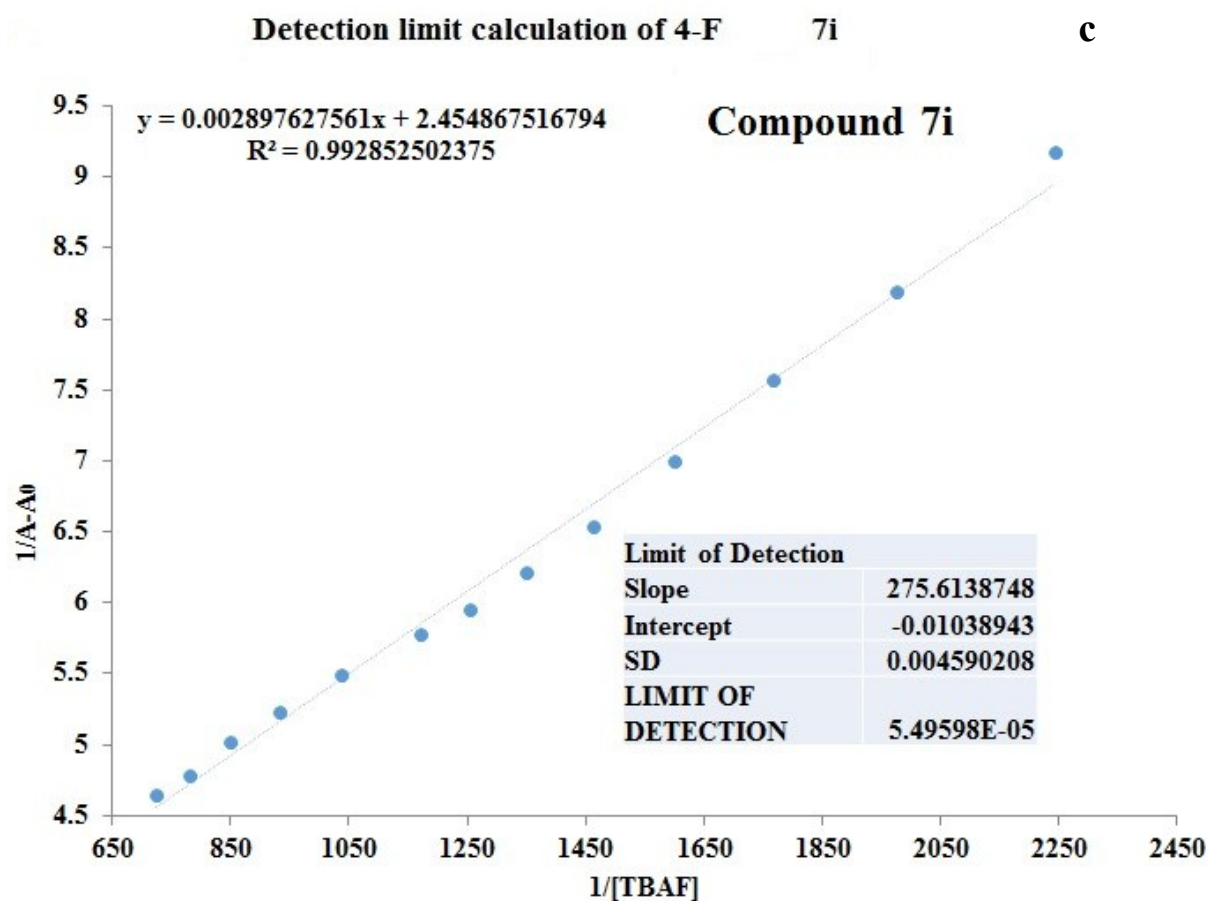


Figure-S2: Calibration Curve, BH plot and Detection Limit Calculations of **7i**

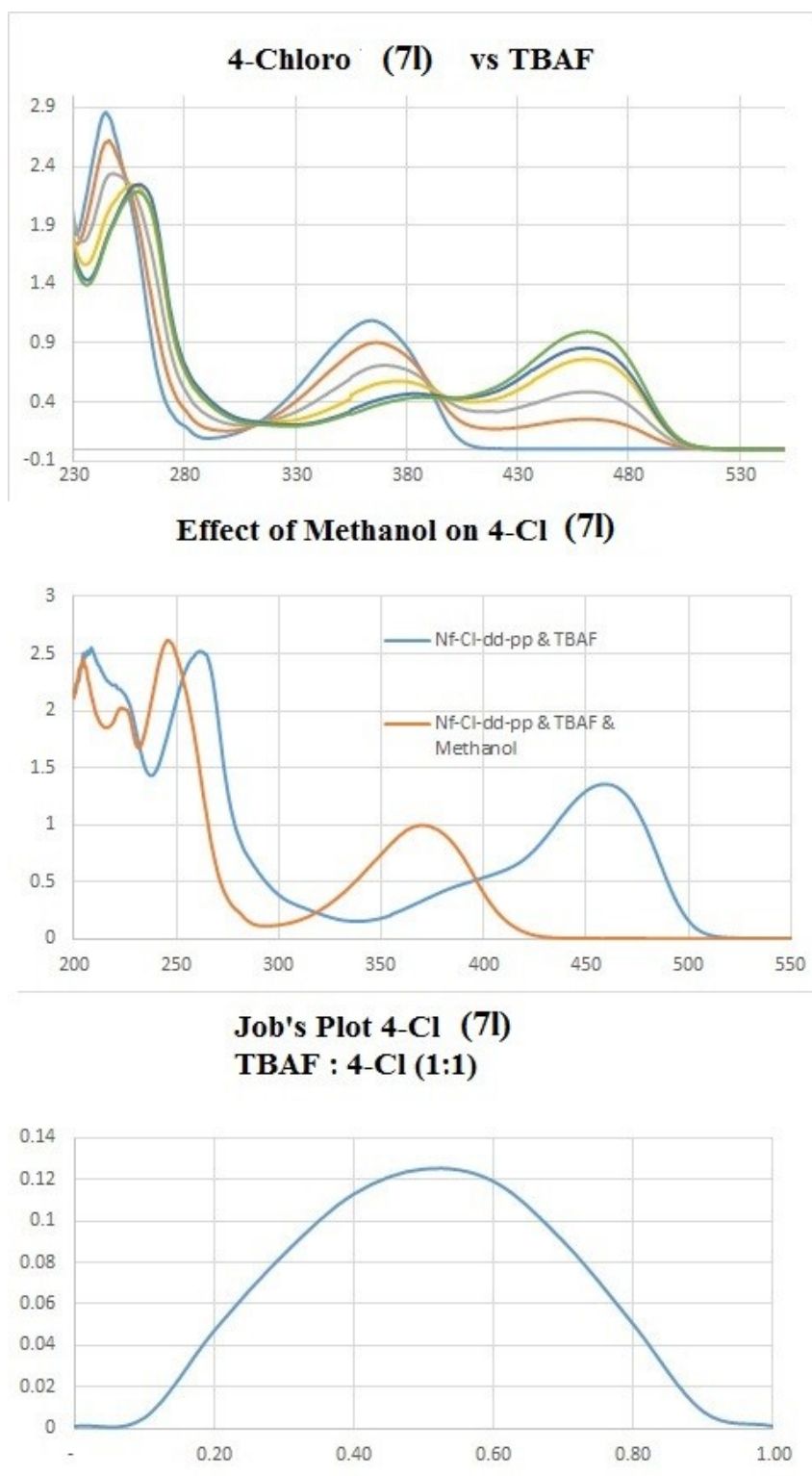
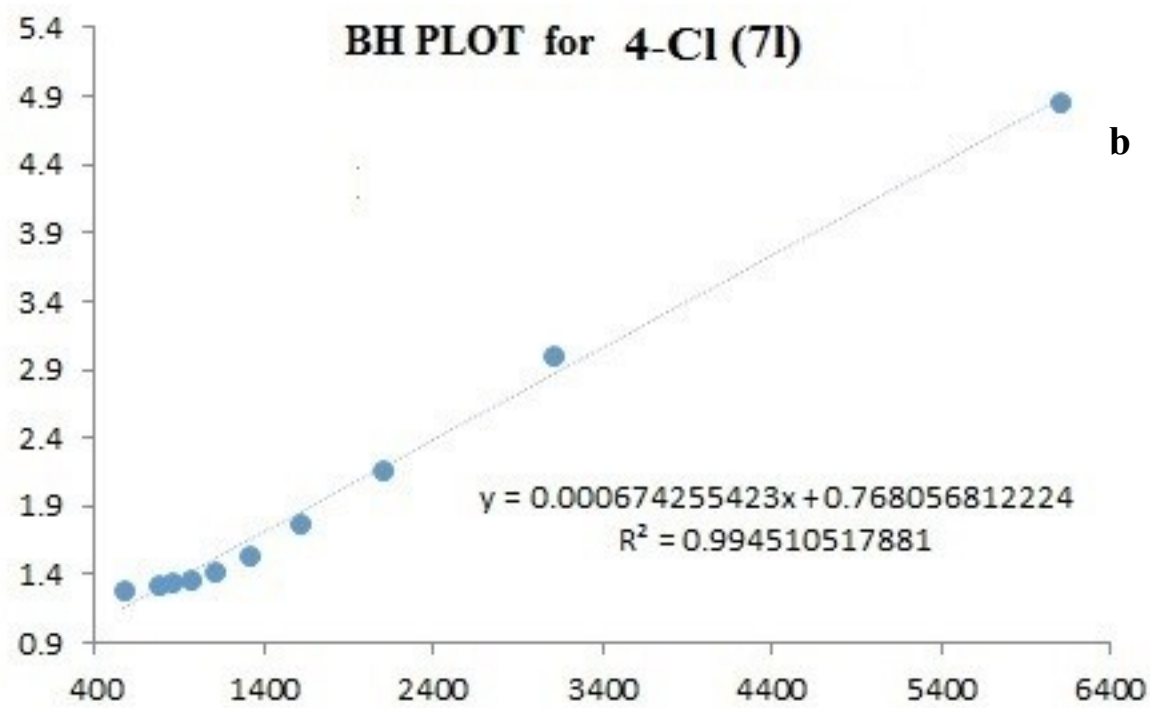
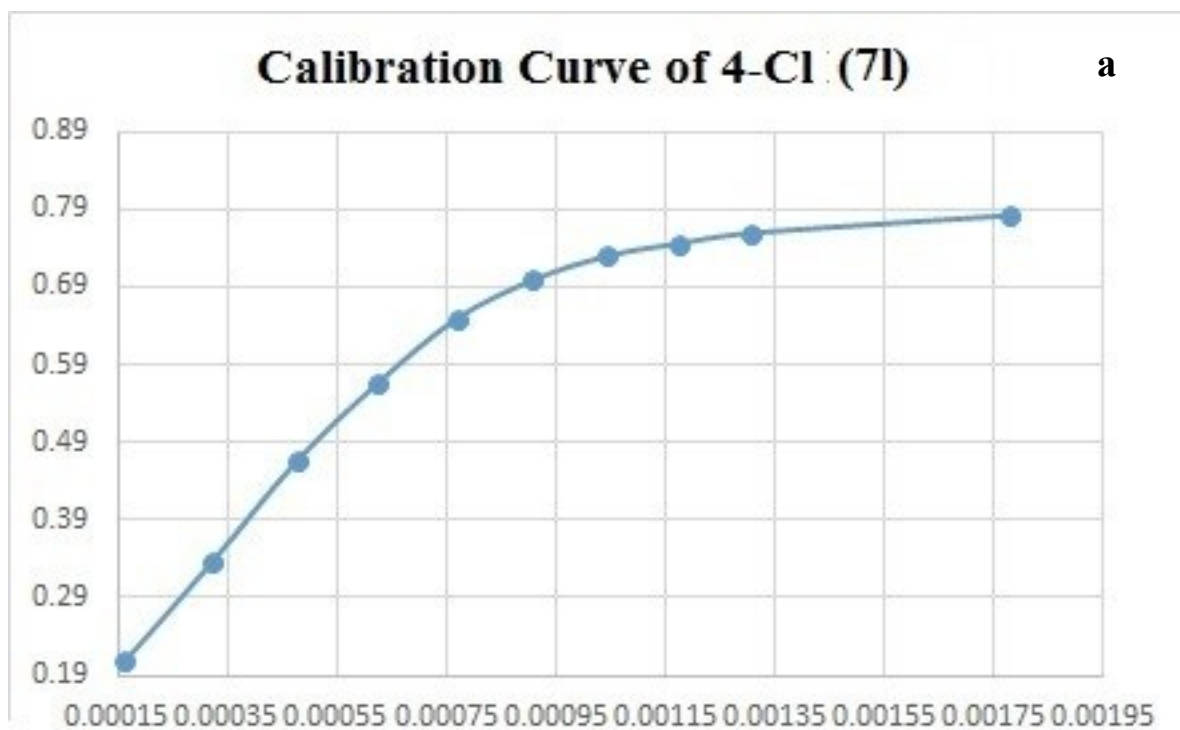


Figure-S3: 4-Chloro DHP vs TBAF, Job's Plot and Effects of Methanol on 4-Fluoro substituted DHP (7i)



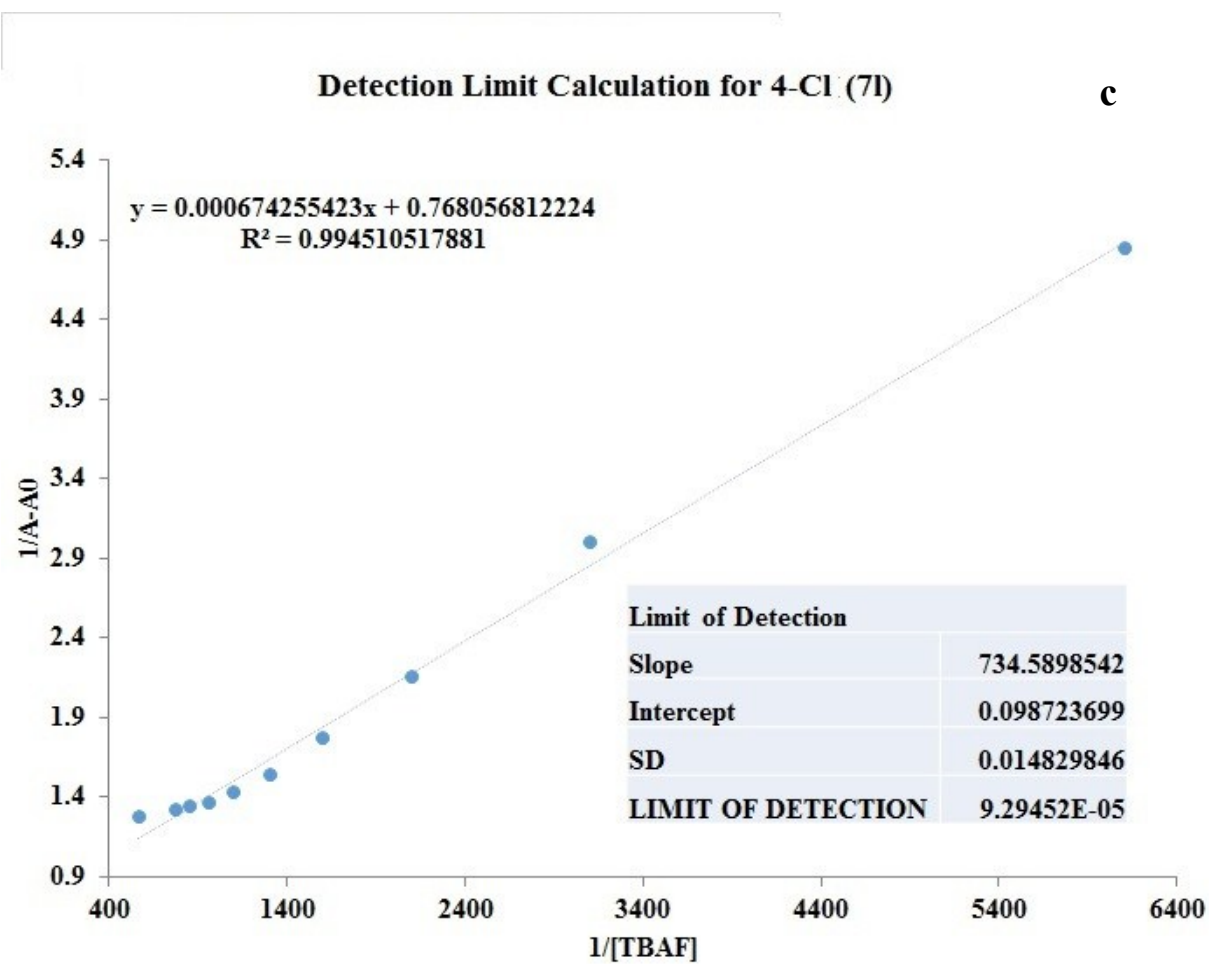


Figure S4: Calibration Curve, BH plot and Detection Limit Calculations of 7I

Thermal studies of IL (3)

In order to signify the catalytic efficiency of morpholinium-based ionic liquids in reactions demanding high temperatures, thermal studies of IL **3** (as model IL) were also carried out. Thermal stability and decomposition profile of **3** was studied *via* differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and derivative thermogravimetry (DTG) is given in.

Figure-S5a shows overlap of thermogravimetric analysis (TGA) and derivative thermogravimetric (DTG) data for compound **3**. Overlap of TGA and differential scanning calorimetry (DSC) for the IL **3** is given in Figure-S5b. In TGA of IL **3**, in the first step the compound gradually loses weight (16%) over the temperature range from ambient to 100 °C, this is probably due to loss of water. The accompanying DSC data in the same temperature range indicates an endothermic process. The first decomposition step appears from 100 °C to 190 °C, in which there is a loss of 20% weight, most likely due to the loss of alkyl chain. The DTG shows first decomposition temperature to be 135 °C. After 190 °C, all of the remaining weight (64%) is suddenly lost in next step in the temperature range 190 °C to 250 °C. According to DTG, the peak temperature for this second decomposition step is 225 °C. As can be seen from Figure-S5b, the last two weight loss steps also indicate an associated endothermic change.

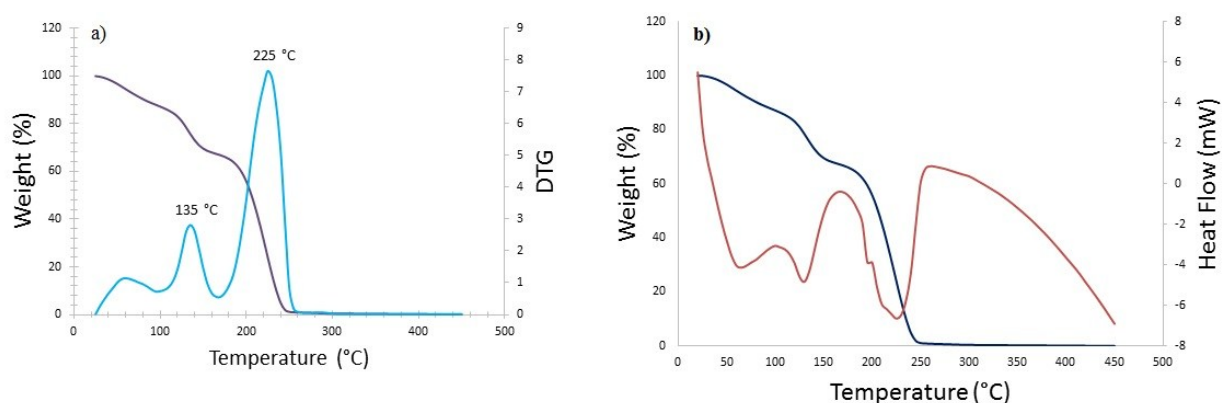
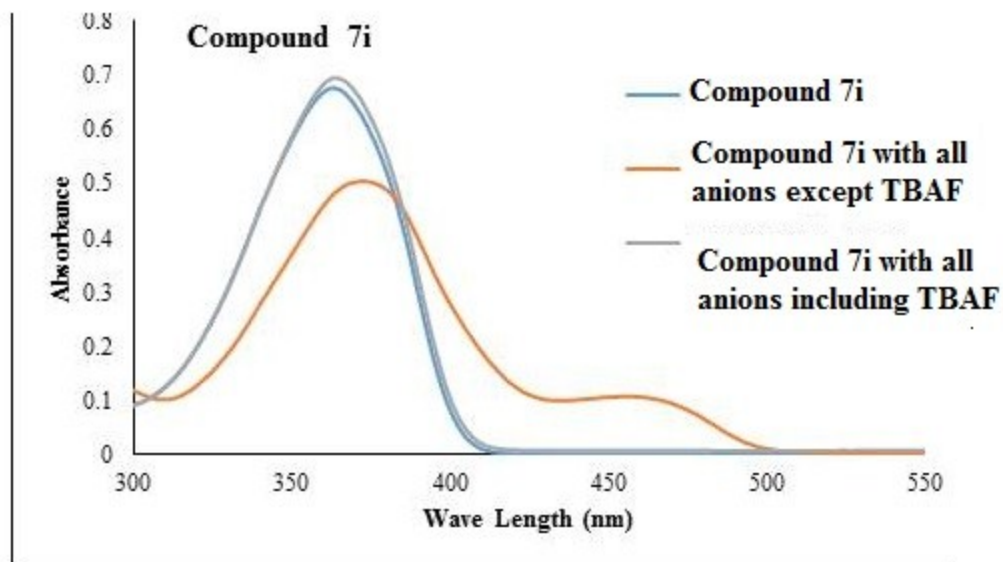


Figure-S5: a) Overlap of TGA and DTG for MoF **3**; b) Overlap of TGA and DSC data for IL **3**.



Figur-S6: Interference studies of compound **7i** in the presence and absence of TBAF

Cartesian coordinates of the optimized geometries and associated thermal correction data**7i**

HF=-1195.8863576

Zero-point correction =	0.417364	(Hartree/Particle)
Thermal correction to Energy =	0.442100	
Thermal correction to Enthalpy =	0.443045	
Thermal correction to Gibbs Free Energy =	0.363208	
Sum of electronic and zero-point Energies =	-1195.468993	
Sum of electronic and thermal Energies =	-1195.444257	
Sum of electronic and thermal Enthalpies =	-1195.443313	
Sum of electronic and thermal Free Energies =	-1195.523149	

C	-3.72574300	-1.88016400	-0.23615800
C	-2.37893100	-2.16630800	-0.84185900
C	-1.23394300	-1.48322400	-0.49172600
C	-1.26141700	-0.39865500	0.42562100
C	-2.52666700	0.08960900	0.94151600
C	-3.78702800	-0.41189500	0.24351400
C	-0.00009100	0.27635100	0.82668900
C	1.26082200	-0.39950000	0.42564800
C	1.23261000	-1.48403800	-0.49173200
C	2.37711400	-2.16796100	-0.84177900
H	2.30036100	-3.01903400	-1.51748300
C	3.72418700	-1.88269100	-0.23628100
C	3.78641700	-0.41455900	0.24369400
C	2.52639800	0.08758900	0.94184300
H	-2.30280700	-3.01723800	-1.51780400
H	-3.93434500	0.24071500	-0.62924600

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H	4.63697100	-0.25367900	0.91188300
H	3.93405800	0.23811000	-0.62896300
H	-0.00005800	0.40023300	1.91828700
H	-4.63744600	-0.25035800	0.91172300
O	2.59126700	0.91792000	1.85203900
O	-2.59095900	0.92044100	1.85128900
N	-0.00079500	-1.88005000	-1.02618000
C	3.92579600	-2.83748000	0.97441900
H	3.84087100	-3.88538200	0.66874900
H	4.92133100	-2.68932500	1.40771300
H	3.18040400	-2.64699500	1.75182300
C	4.83553600	-2.14775700	-1.27186600
H	5.81976200	-1.94240900	-0.83817700
H	4.82676600	-3.19280400	-1.60175600
H	4.71395300	-1.51184300	-2.15448100
C	-3.92767000	-2.83454500	0.97481900
H	-4.92303600	-2.68570700	1.40826400
H	-3.84341400	-3.88257000	0.66938400
H	-3.18201200	-2.64430000	1.75202500
C	-4.83743600	-2.14483300	-1.27145900
H	-4.82925700	-3.18994100	-1.60117600
H	-5.82147700	-1.93892800	-0.83761300
H	-4.71572100	-1.50913100	-2.15420800
C	0.00063200	1.73272100	0.26413100
C	0.00168300	2.82353300	1.13468700

Supplementary Information (SI)

C	0.00032700	1.95868000	-1.11815200
C	0.00240900	4.12846100	0.63753700
H	0.00195200	2.65785800	2.20520500
C	0.00105000	3.25501900	-1.62825300
H	-0.00049800	1.11775600	-1.80581700
C	0.00208500	4.32226800	-0.73601200
H	0.00319100	4.98536800	1.30213000
H	0.00081300	3.44653300	-2.69582700
F	0.00277400	5.58273400	-1.22545500
H	-0.00108400	-2.74180500	-1.55193600

7i-F

HF=-1295.7996339

Zero-point correction =	0.415831 (Hartree/Particle)
Thermal correction to Energy =	0.442449
Thermal correction to Enthalpy =	0.443393
Thermal correction to Gibbs Free Energy =	0.356293
Sum of electronic and zero-point Energies =	-1295.383803
Sum of electronic and thermal Energies =	-1295.357185
Sum of electronic and thermal Enthalpies =	-1295.356241
Sum of electronic and thermal Free Energies =	-1295.443341

C	3.67640200	-1.74679400	-0.00291300
C	2.32471700	-2.03898000	0.57463000
C	1.17779500	-1.31379900	0.25751500
C	1.26447200	-0.15199400	-0.57842700
C	2.52509600	0.35447300	-1.02286600
C	3.78030100	-0.25279700	-0.38110300
C	0.00531200	0.58373200	-0.93726900

Supplementary Information (SI)

C	-1.25950700	-0.14290700	-0.57954200
C	-1.18152500	-1.30512500	0.25643600
C	-2.33354500	-2.02306300	0.57244700
H	-2.19967400	-2.92137900	1.17255800
C	-3.68281300	-1.72105400	-0.00518000
C	-3.77618800	-0.22674300	-0.38481000
C	-2.51641200	0.37121600	-1.02612000
H	2.18576300	-2.93629100	1.17514600
H	3.97535500	0.33077200	0.53078400
H	-4.61982000	-0.04508000	-1.05955000
H	-3.96784900	0.35896400	0.52641000
H	0.00656200	0.79745300	-2.01443600
H	4.62568400	-0.07638900	-1.05506000
O	-2.63819200	1.31488100	-1.83005800
O	2.65413500	1.29863000	-1.82509300
N	-0.00394000	-1.82666300	0.72698200
C	-3.85918300	-2.59066300	-1.28358200
H	-3.74011000	-3.65536700	-1.05601100
H	-4.85889800	-2.43928300	-1.71067500
H	-3.11488100	-2.31624100	-2.03590300
C	-4.79191000	-2.09237600	1.00022400
H	-5.78265300	-1.88644000	0.57767200
H	-4.74885800	-3.15668100	1.25993500
H	-4.69093800	-1.51620200	1.92596600
C	3.84678300	-2.61631300	-1.28212100
H	4.84740000	-2.47141400	-1.70937600
H	3.72051500	-3.68044200	-1.05561200

Supplementary Information (SI)

H	3.10419000	-2.33613800	-2.03401000
C	4.78287100	-2.12660000	1.00217700
H	4.73266600	-3.19086100	1.26096000
H	5.77503900	-1.92718700	0.57986600
H	4.68587000	-1.55053700	1.92842200
C	0.00856300	1.96697100	-0.24374400
C	-0.00008800	3.14806200	-0.98956900
C	0.01870900	2.05830800	1.15535400
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C	0.02070200	3.29524000	1.79871700
H	0.02525300	1.14811600	1.74810300
C	0.01248900	4.44857100	1.02235300
H	-0.00429200	5.31939100	-0.93531600
H	0.02854900	3.37484500	2.88114400
F	0.01471900	5.66158900	1.64323600
H	-0.02281300	-3.10739400	1.48080000
F	-0.05063800	-3.99224100	1.96605000

7i-OAc

HF=-1424.4663668

Zero-point correction = 0.467251 (Hartree/Particle)

Thermal correction to Energy = 0.497792

Thermal correction to Enthalpy = 0.498737

Thermal correction to Gibbs Free Energy = 0.403250

Sum of electronic and zero-point Energies = -1423.999116

Sum of electronic and thermal Energies = -1423.968574

Sum of electronic and thermal Enthalpies = -1423.967630

Sum of electronic and thermal Free Energies = -1424.063117

C	-1.59183100	-3.42452500	-0.51392100
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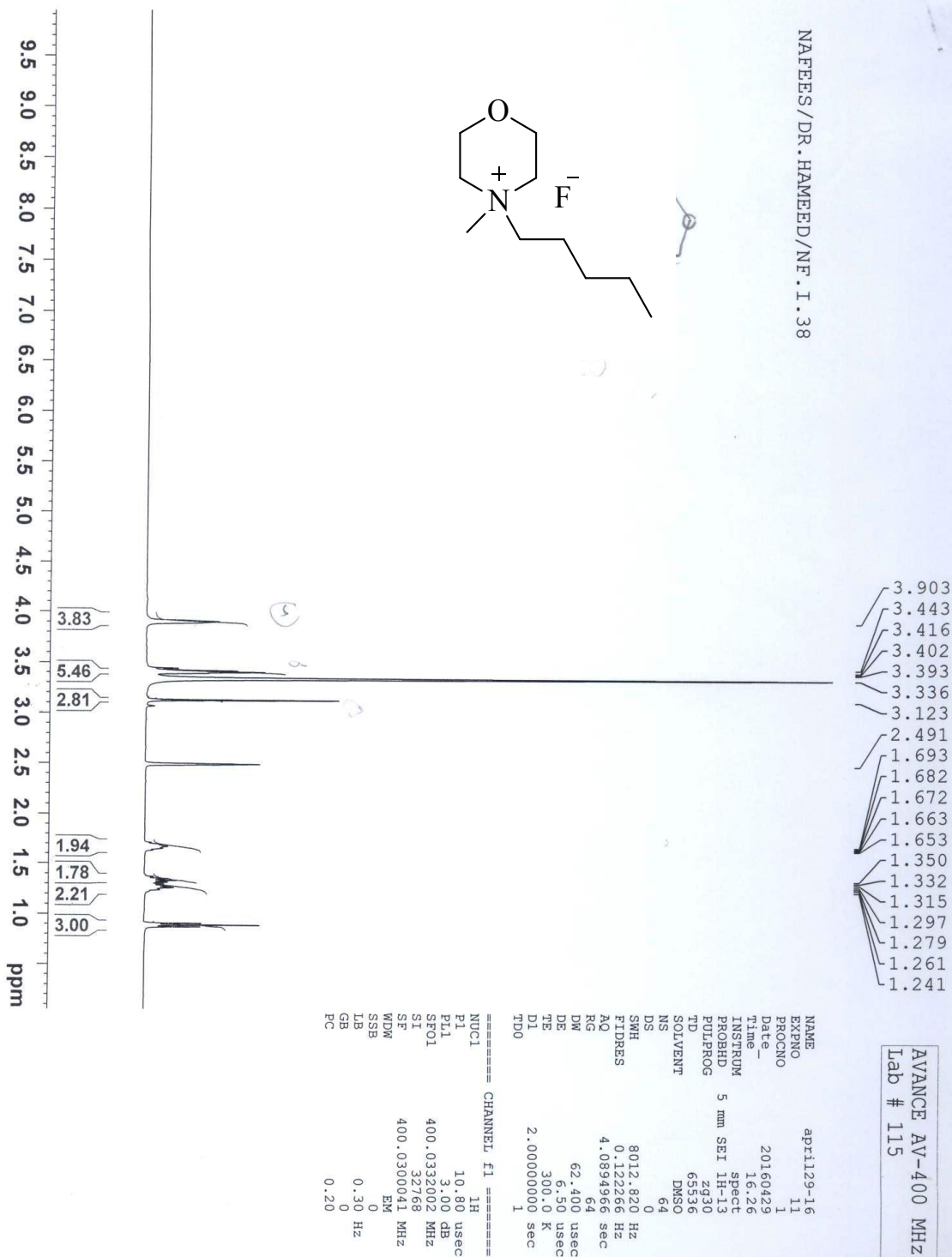
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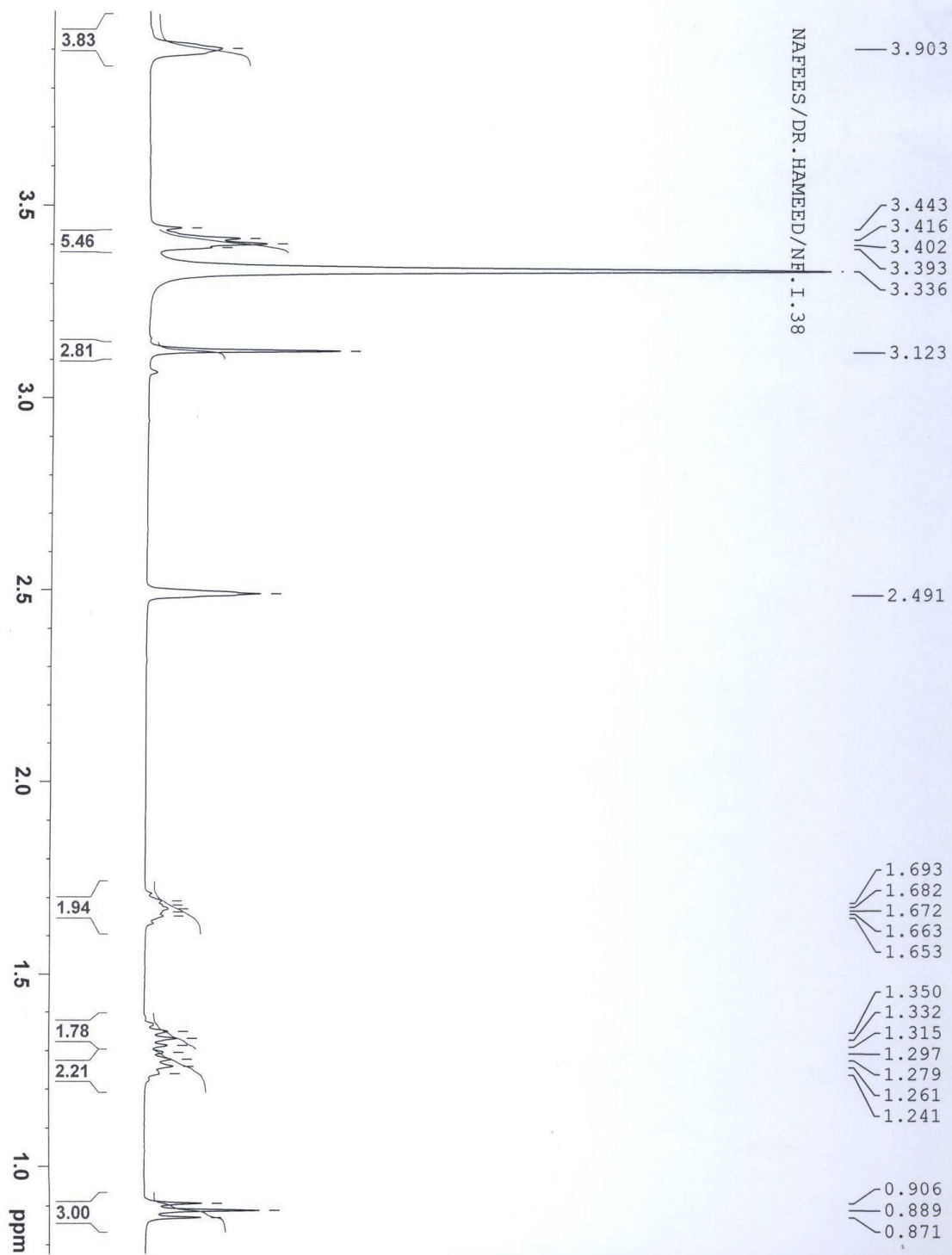
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C	0.76985100	-2.55031200	-1.14679600
C	-0.08141500	-3.71729700	-0.64354700
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C	0.69713900	1.27519800	-0.70362600
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C	-0.60672900	3.89713800	-0.39483000
C	0.93118900	3.77868700	-0.47931300
C	1.45761700	2.44744300	-1.02536500
H	-2.80854400	-1.81425100	0.45642000
H	0.31400600	-3.97829800	0.34929800
H	1.35579100	4.58676400	-1.08421700
H	1.35050800	3.88453200	0.53228000
H	1.68654100	-0.11367800	-1.97249200
H	0.10155100	-4.57931900	-1.29343000
O	2.53486900	2.42073300	-1.64481400
O	1.80183400	-2.77418300	-1.79938100
N	-1.29668300	0.24989700	0.26511500
C	-1.18492300	4.17446100	-1.81187000
H	-2.27888500	4.21328500	-1.78867600
H	-0.81372500	5.13461800	-2.19234800
H	-0.88667300	3.38749000	-2.51010000
C	-1.00189800	5.06137800	0.53590100
H	-0.58067900	6.00665600	0.17355400
H	-2.09107200	5.17216600	0.58617500
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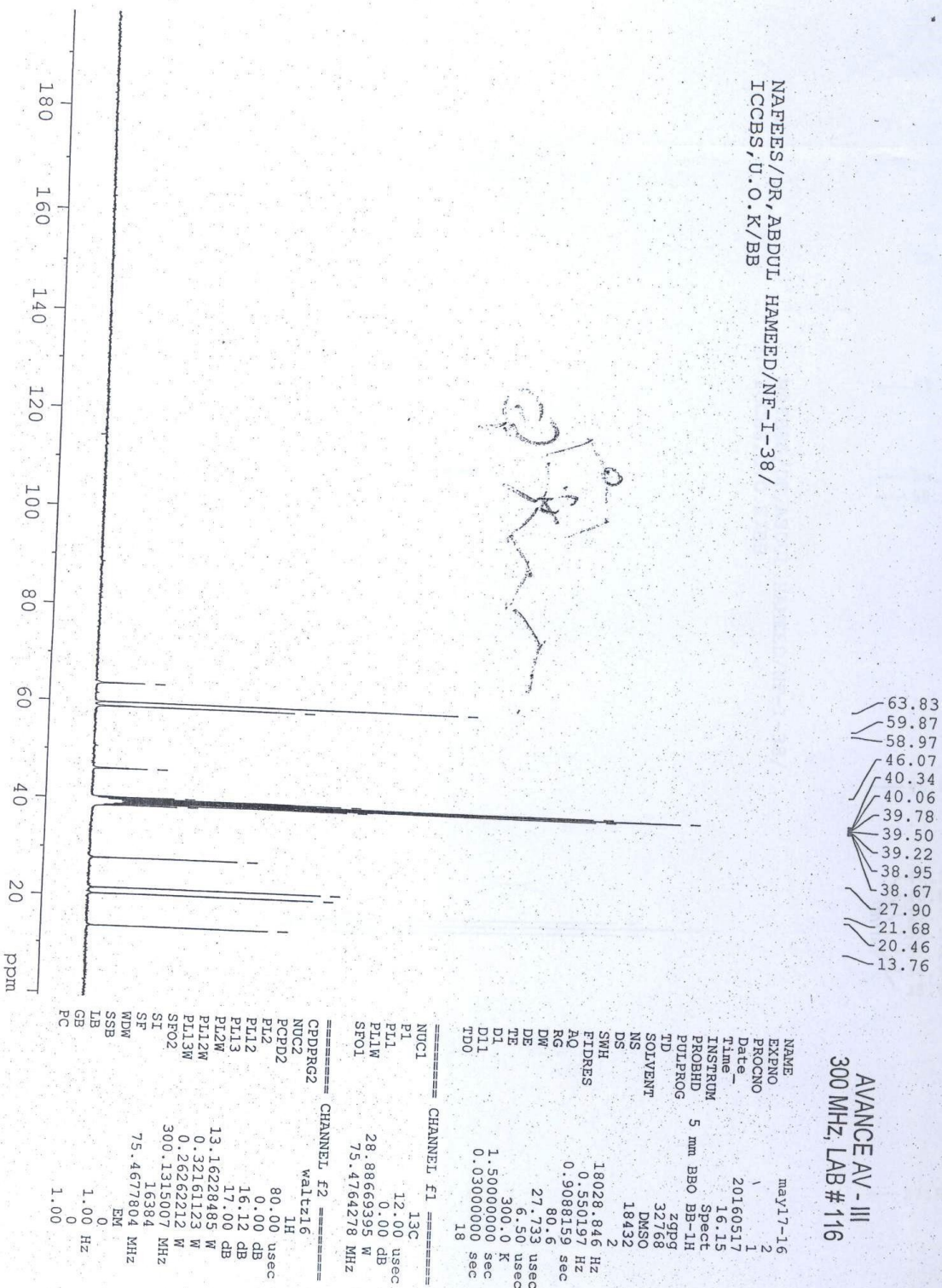
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C	-2.27092600	-4.46443000	0.40138600
H	-3.34230900	-4.25968400	0.49359300
H	-2.14225000	-5.47579200	-0.00260100
H	-1.83803900	-4.44258100	1.40699800
C	2.52516900	-0.27362800	-0.02792200
C	3.79528800	-0.49056500	-0.56680400
C	2.38205300	-0.24211600	1.36619700
C	4.90670900	-0.67083900	0.26081800
H	3.91634900	-0.52090900	-1.64319300
C	3.47917900	-0.42139300	2.20721900
H	1.40074900	-0.07342600	1.80029400
C	4.72857800	-0.63303500	1.63509600
H	5.89742100	-0.83775500	-0.14909800
H	3.37807700	-0.39874700	3.28739400
F	5.80475300	-0.80721600	2.44929000
H	-2.29315900	0.39799800	0.60785600
O	-3.74128900	0.92135600	1.09611200
C	-4.70255100	0.09167600	1.20530100
O	-4.66408900	-1.14439400	1.01463300
C	-6.04842400	0.71635800	1.62697300
H	-6.33946000	1.49185800	0.90945900
H	-6.83434400	-0.04028700	1.68792600
H	-5.93877100	1.20923400	2.59972100

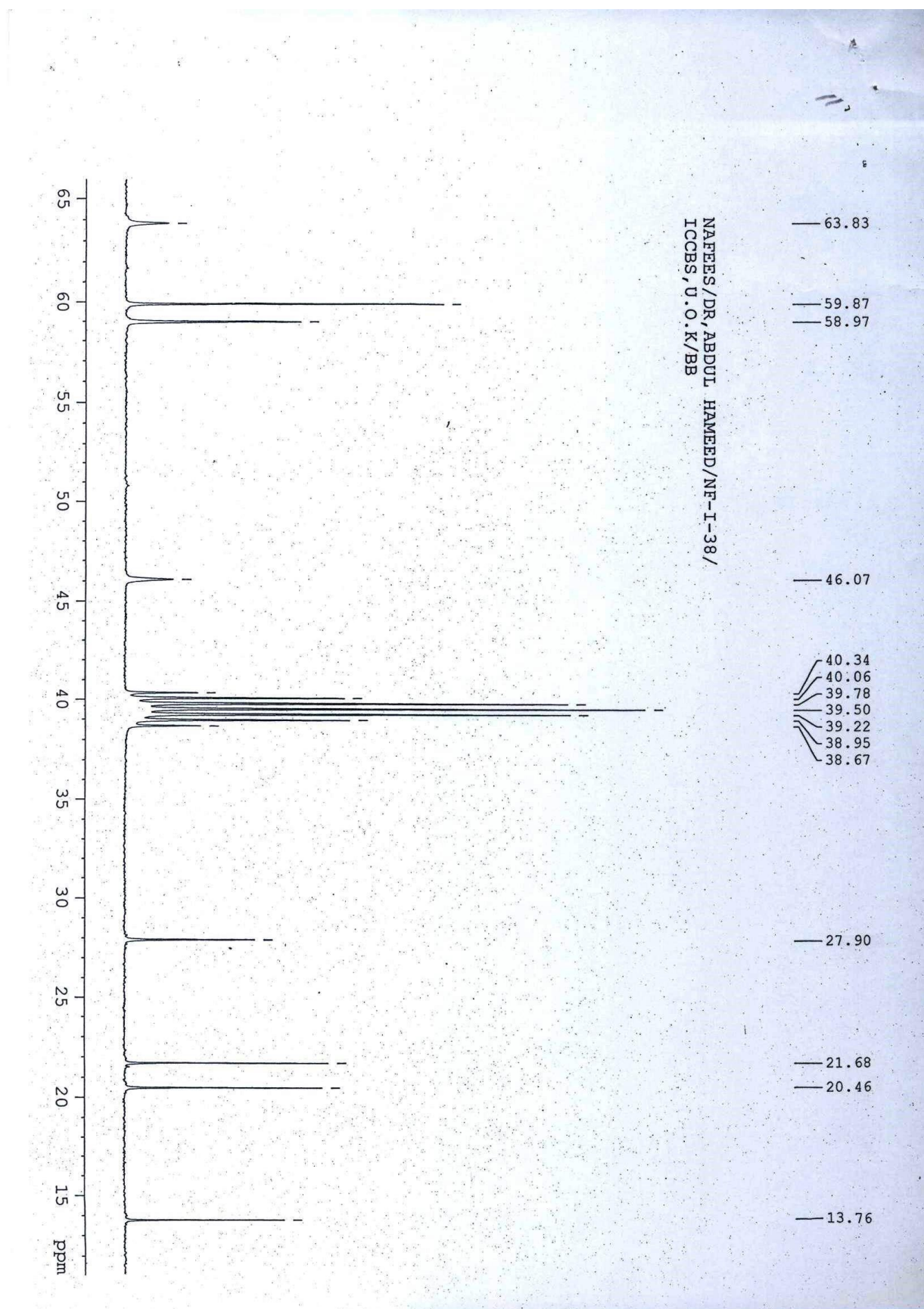
Spectral Data







Supplementary Information (SI)



Nafees / Dr. Iqbal / NF-1-38
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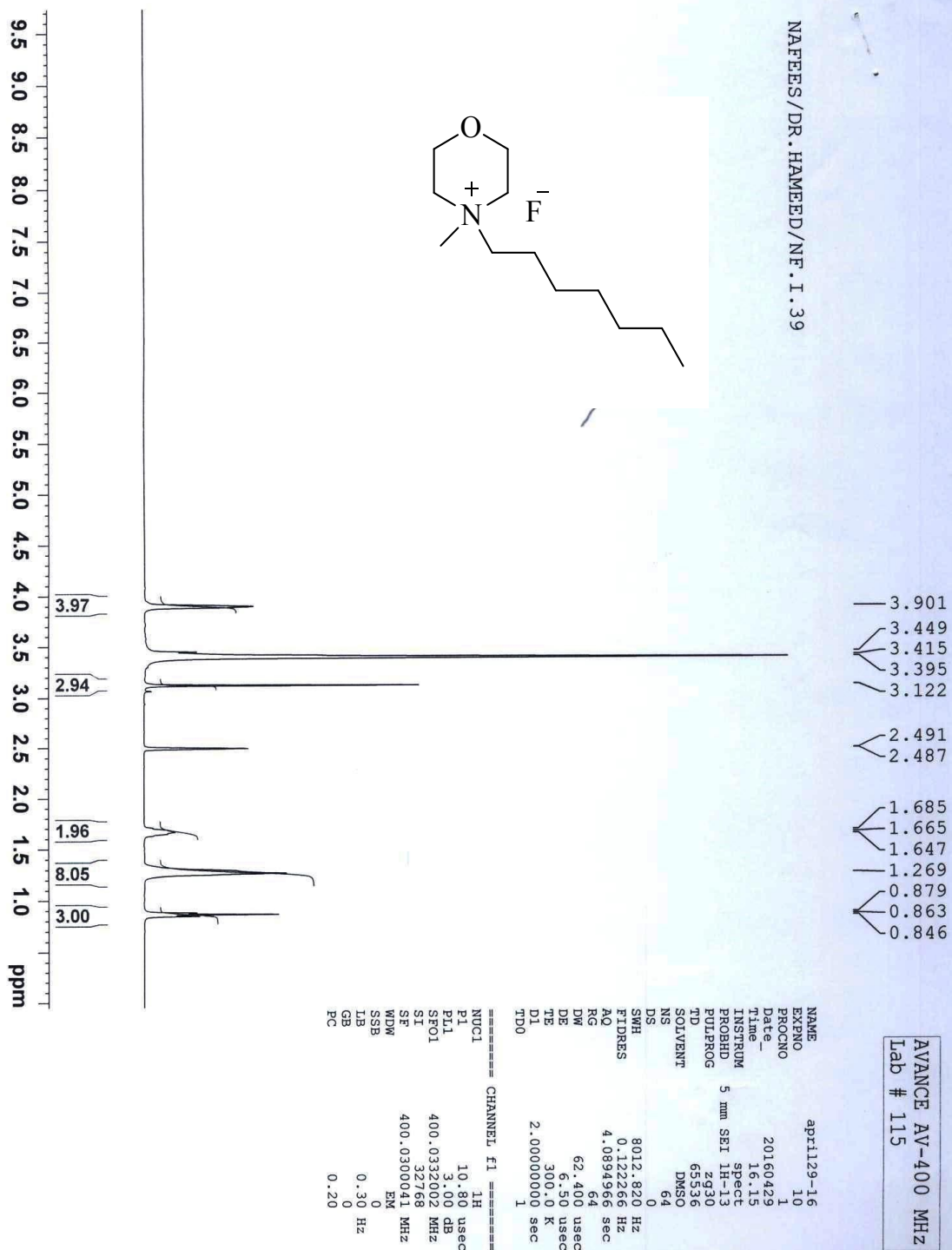
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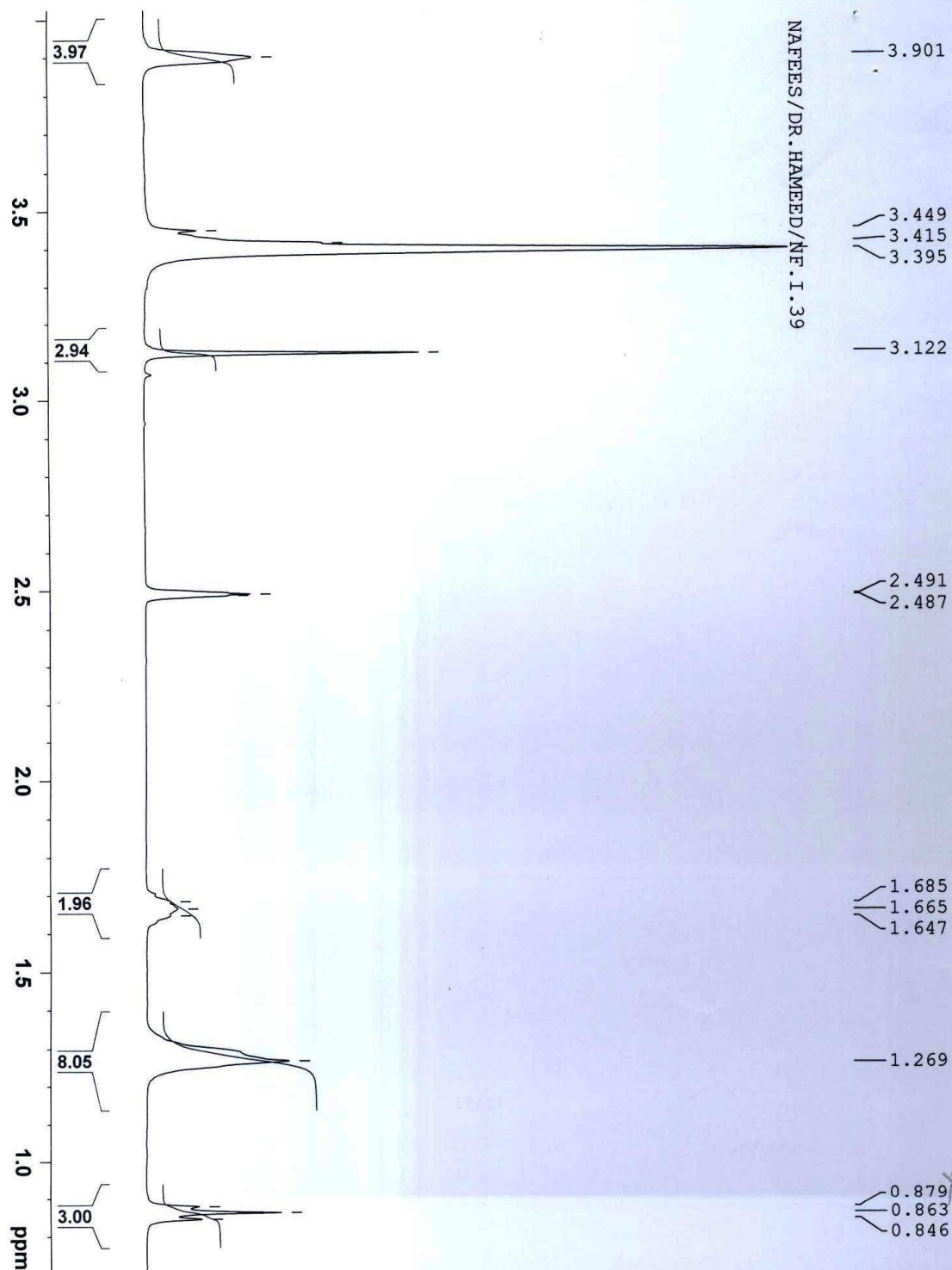
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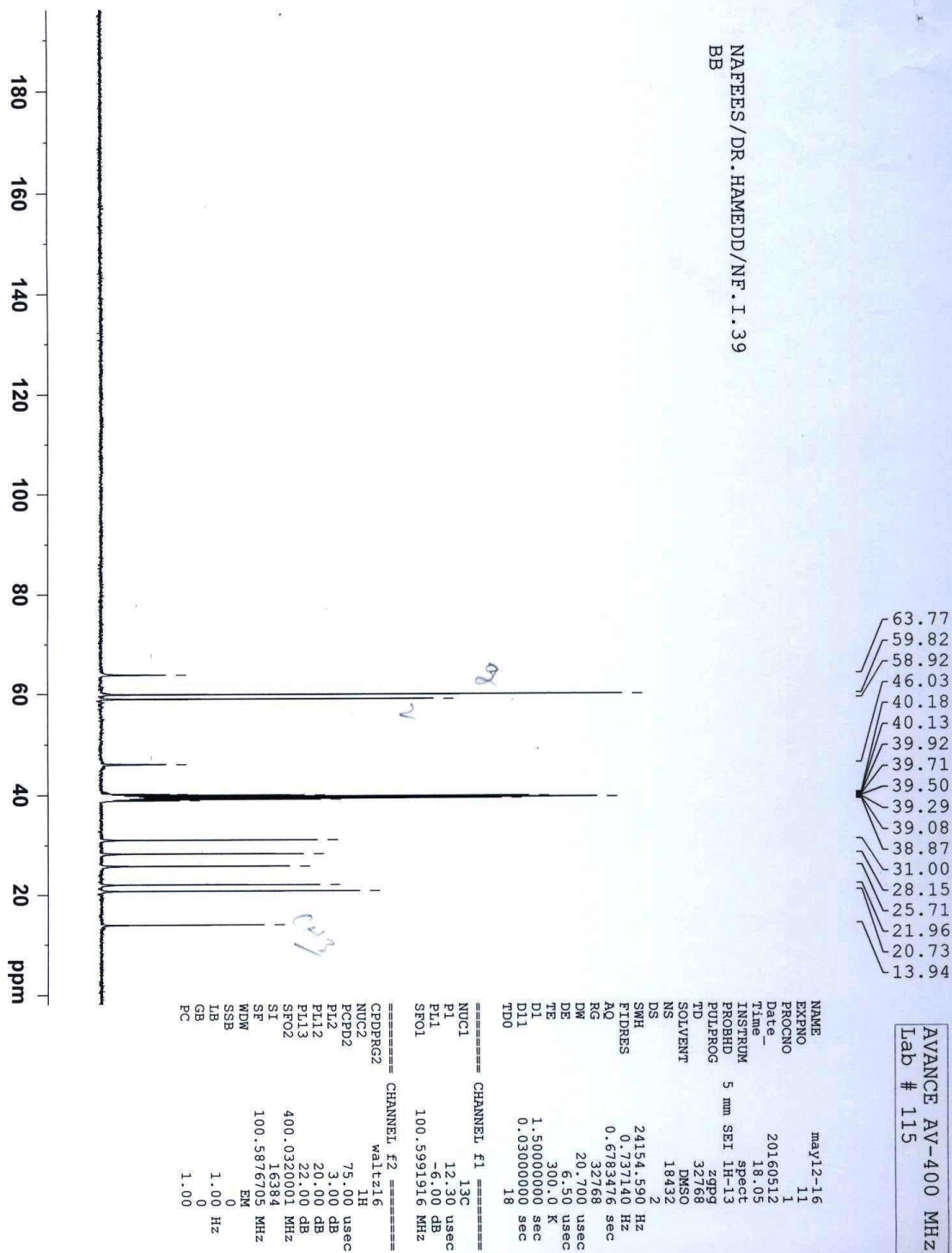
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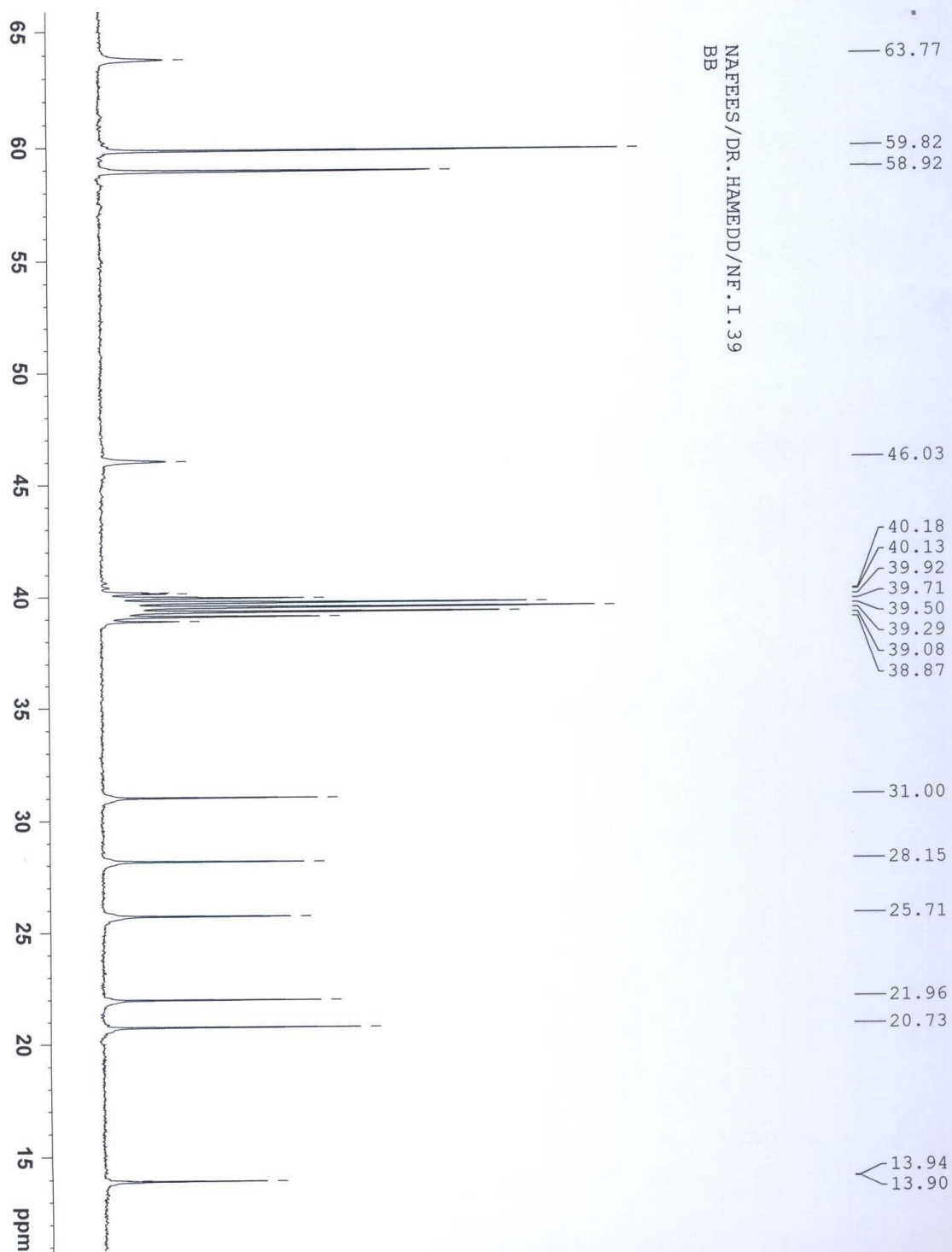


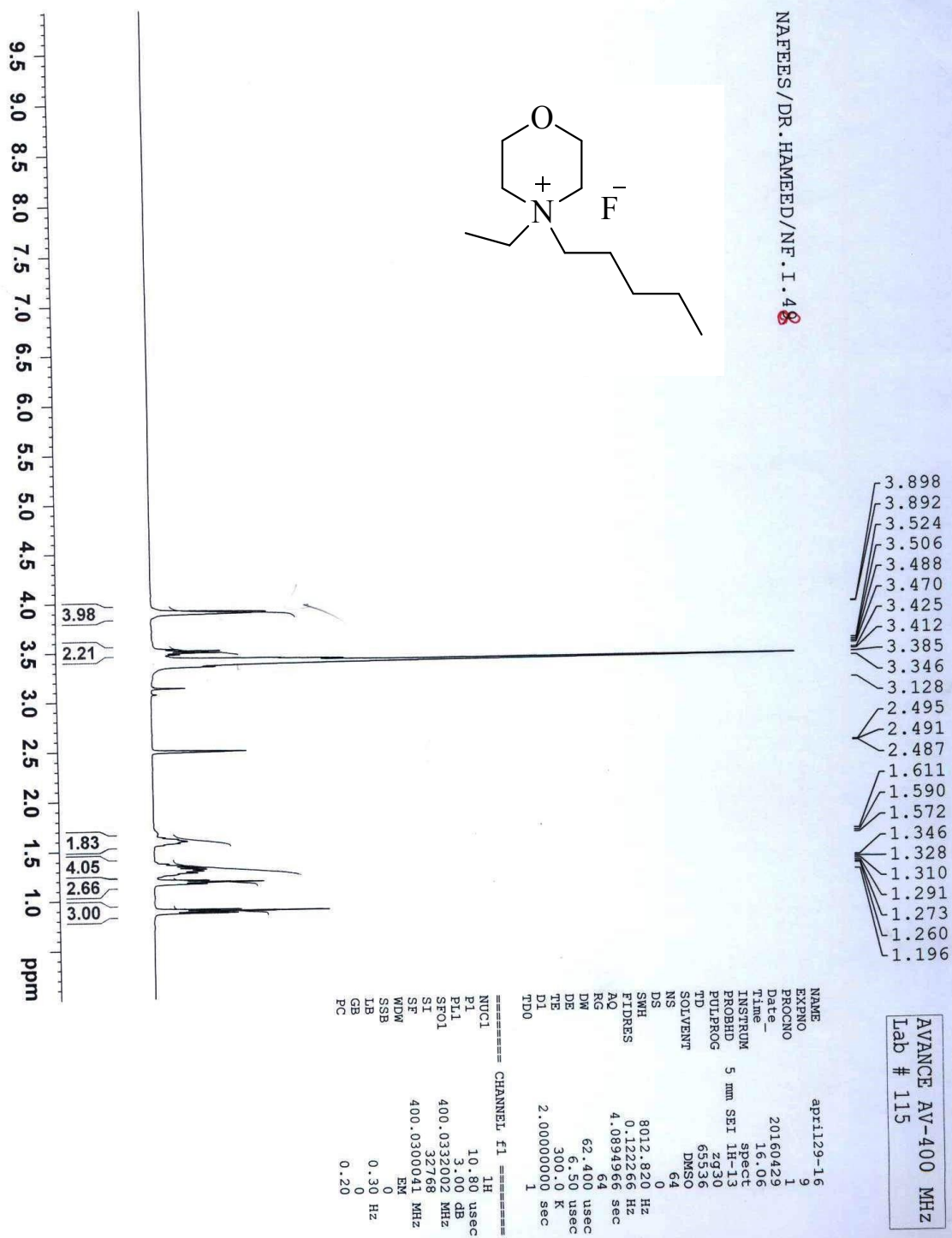


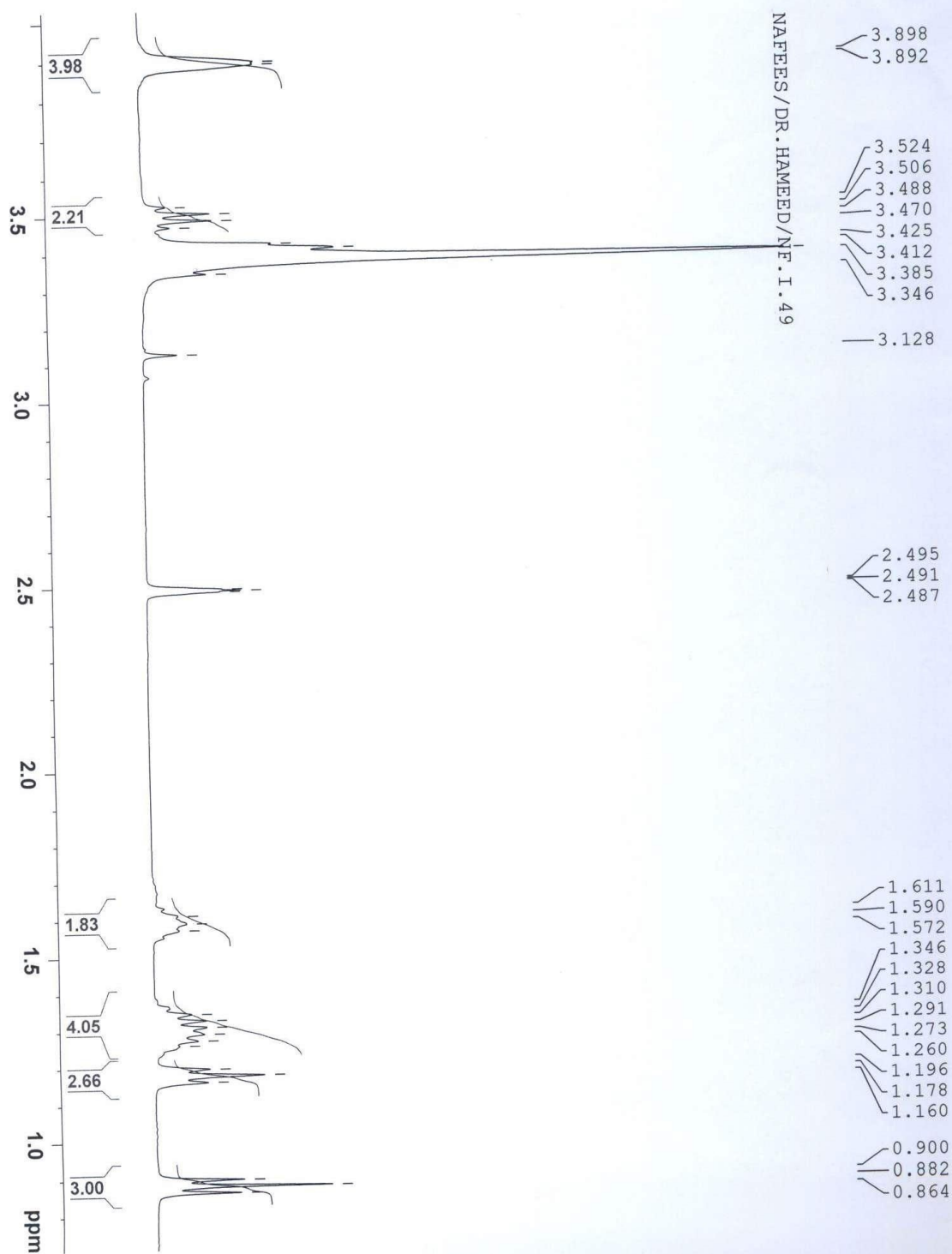


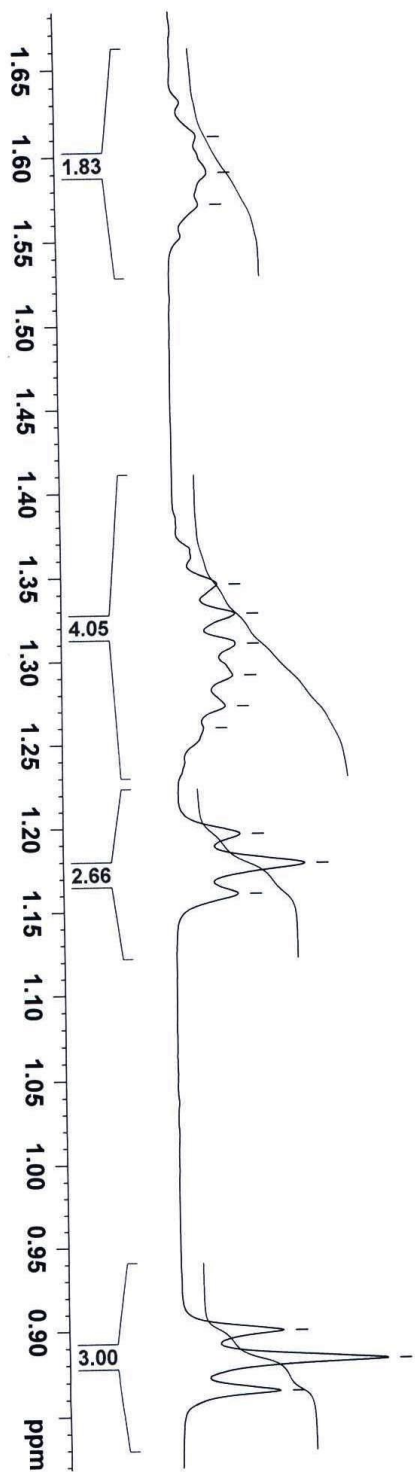


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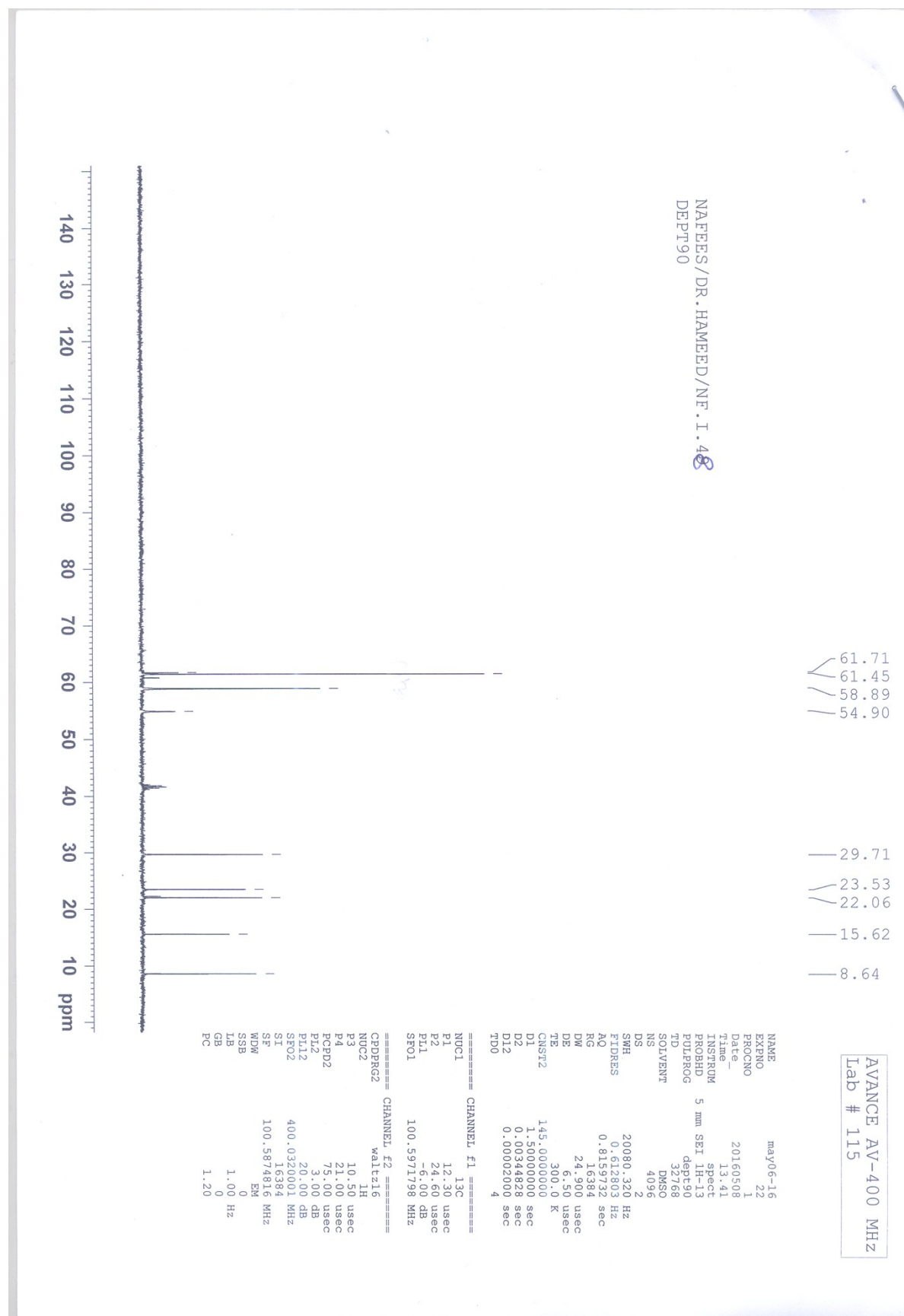
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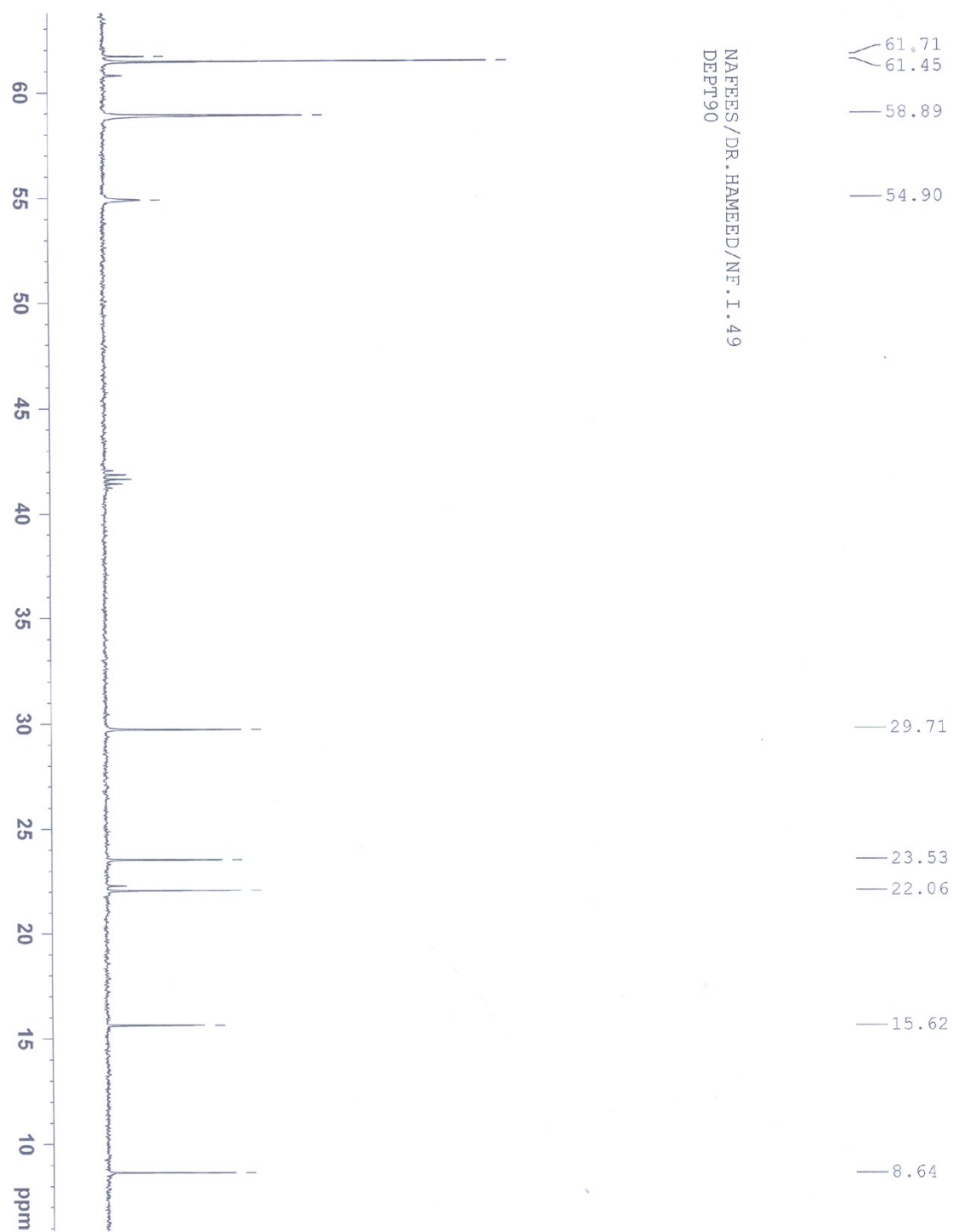
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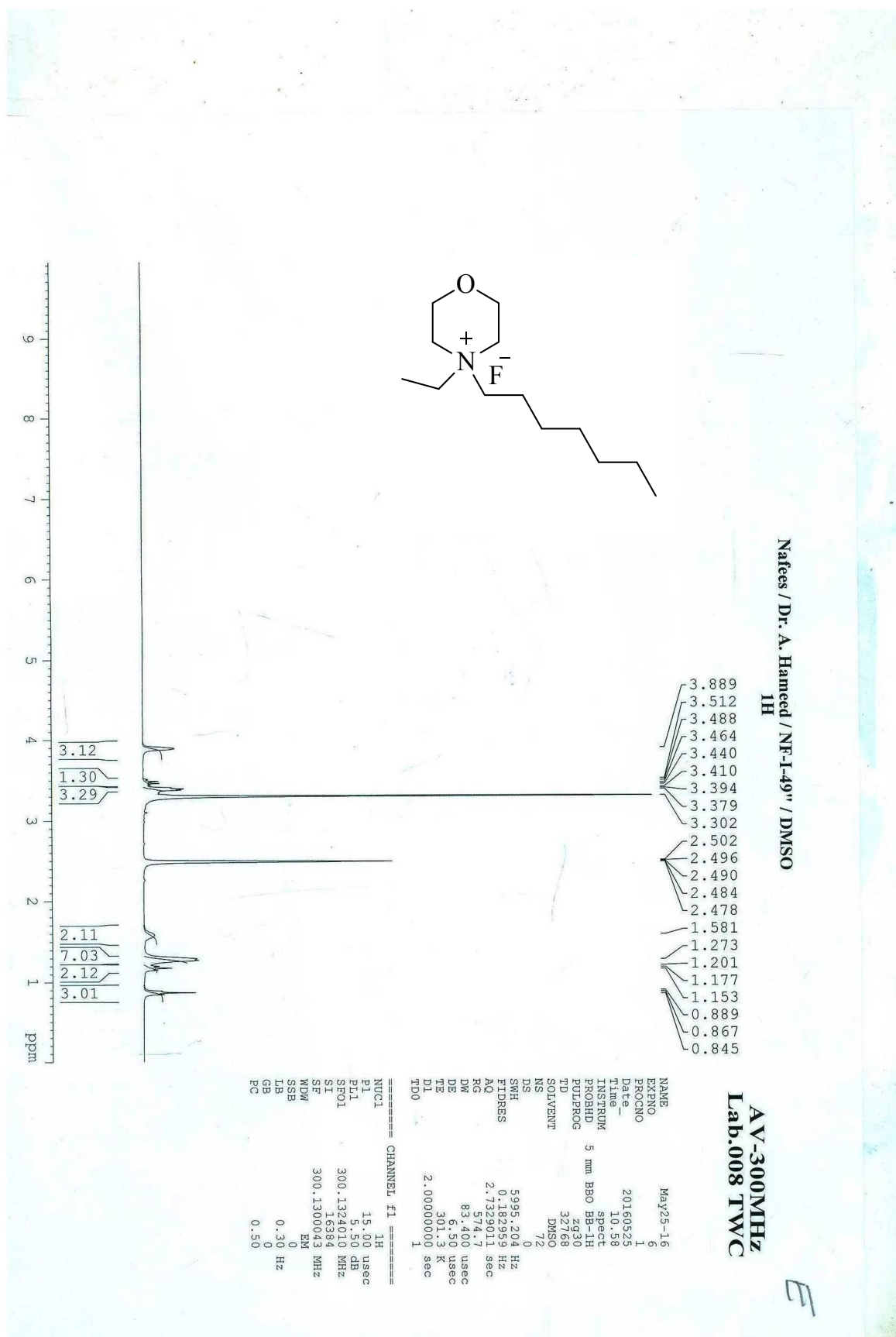
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— 0.882
— 0.864



Supplementary Information (SI)





Nafees / Dr. A. Hameed / NF-
F19-1H decoupled.



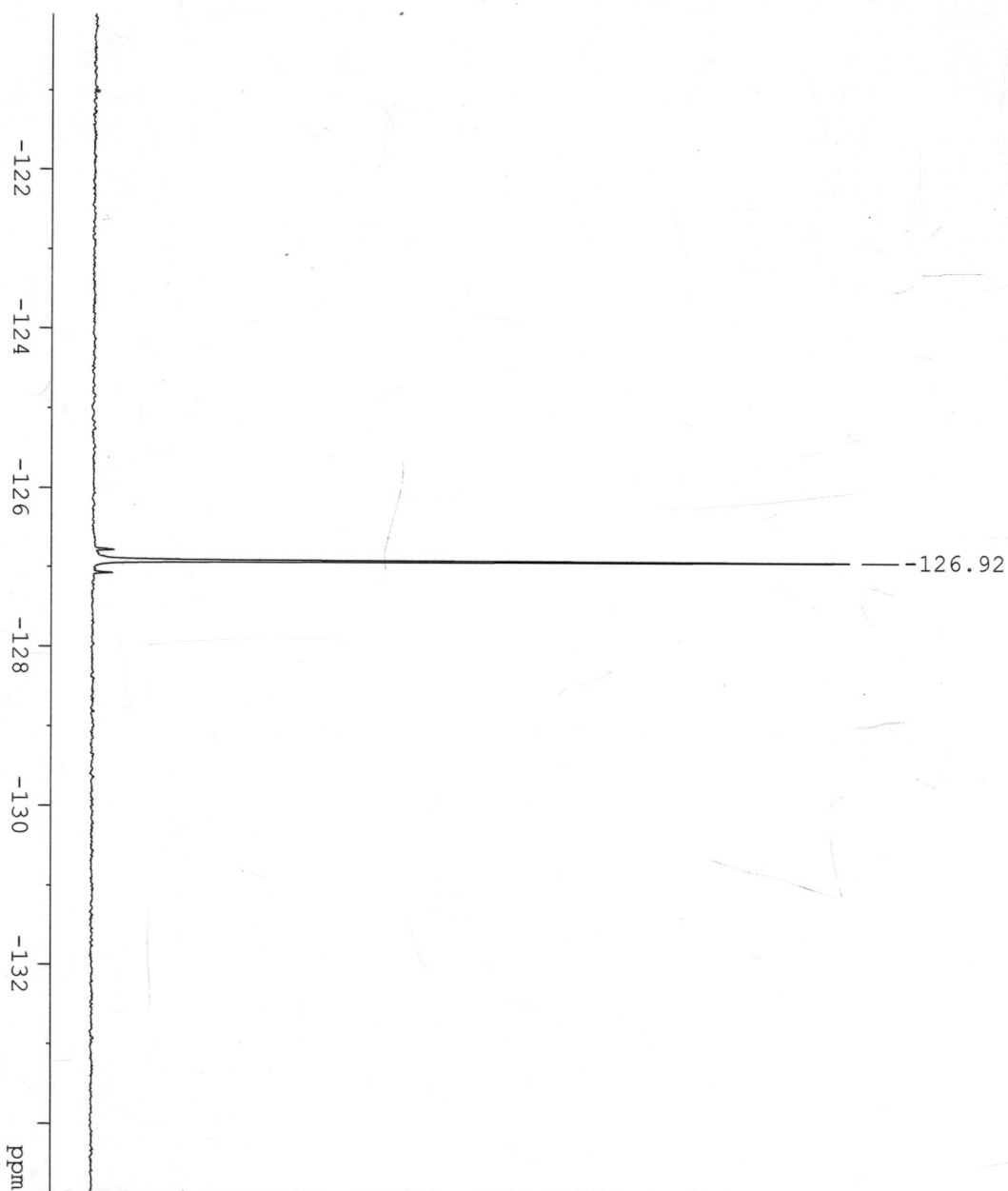
Current Data Parameters
NAME oct06-16
EXPNO 10
PROCNO 1

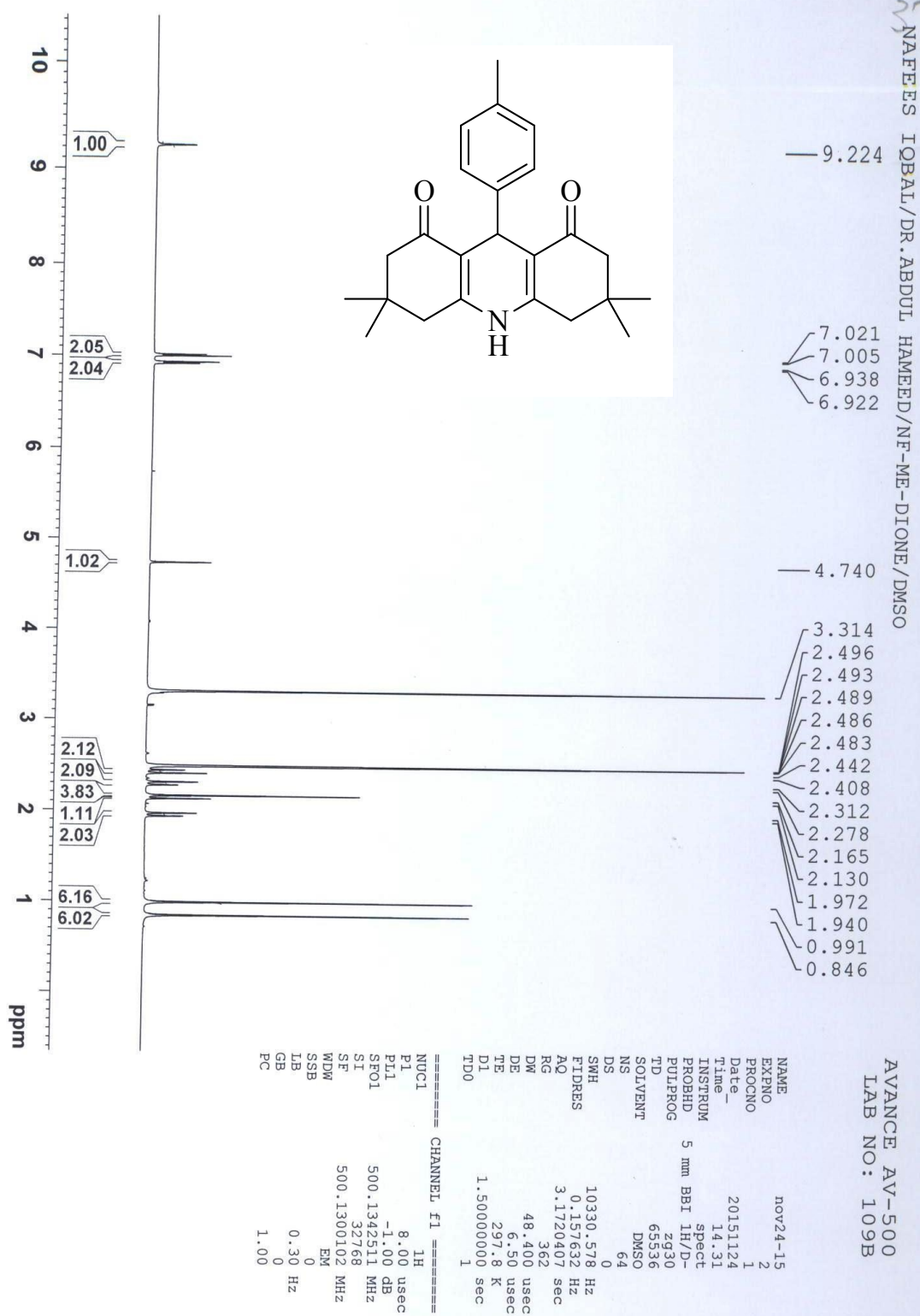
F2 - Acquisition Parameters
Date_ 20161006
Time_ 14.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgfgnq.2
TD 131072
SOLVENT CD3CN
NS 32
DS 0
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 196.51
DM 5.600 usec
DE 6.50 usec
TE 300.8 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

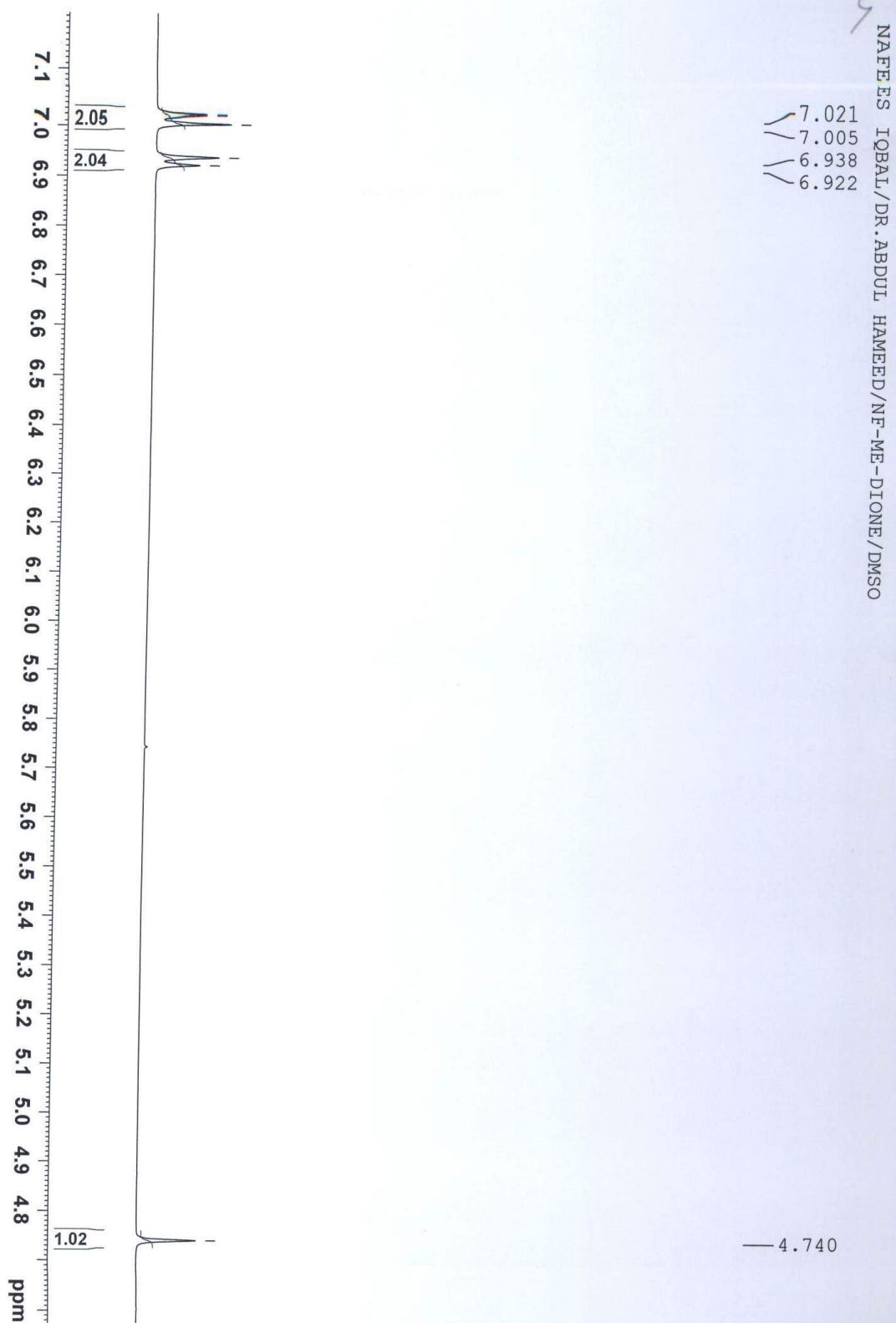
===== CHANNEL f1 =====
NUC1 19F
P1 13.80 usec
PLW1 26.00000000 W
SFO1 376.5548010 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 17.00000000 W
PLW12 0.19746999 W
SFO2 400.2316009 MHz

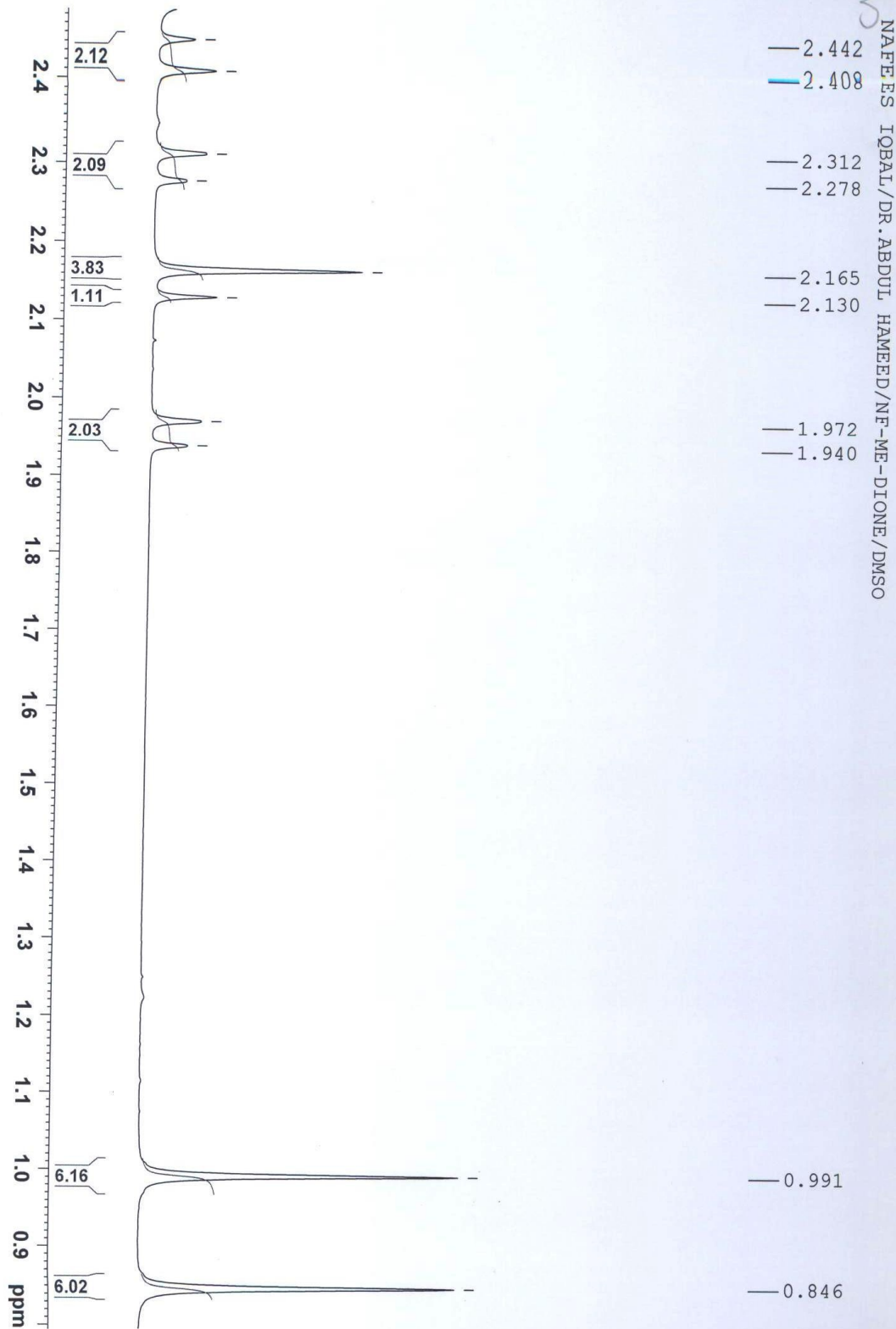
F2 - Processing parameters
SI 65536
SF 376.5924600 MHz
WDW EM
SSB 0
LB 0
GB 0
PC 1.00

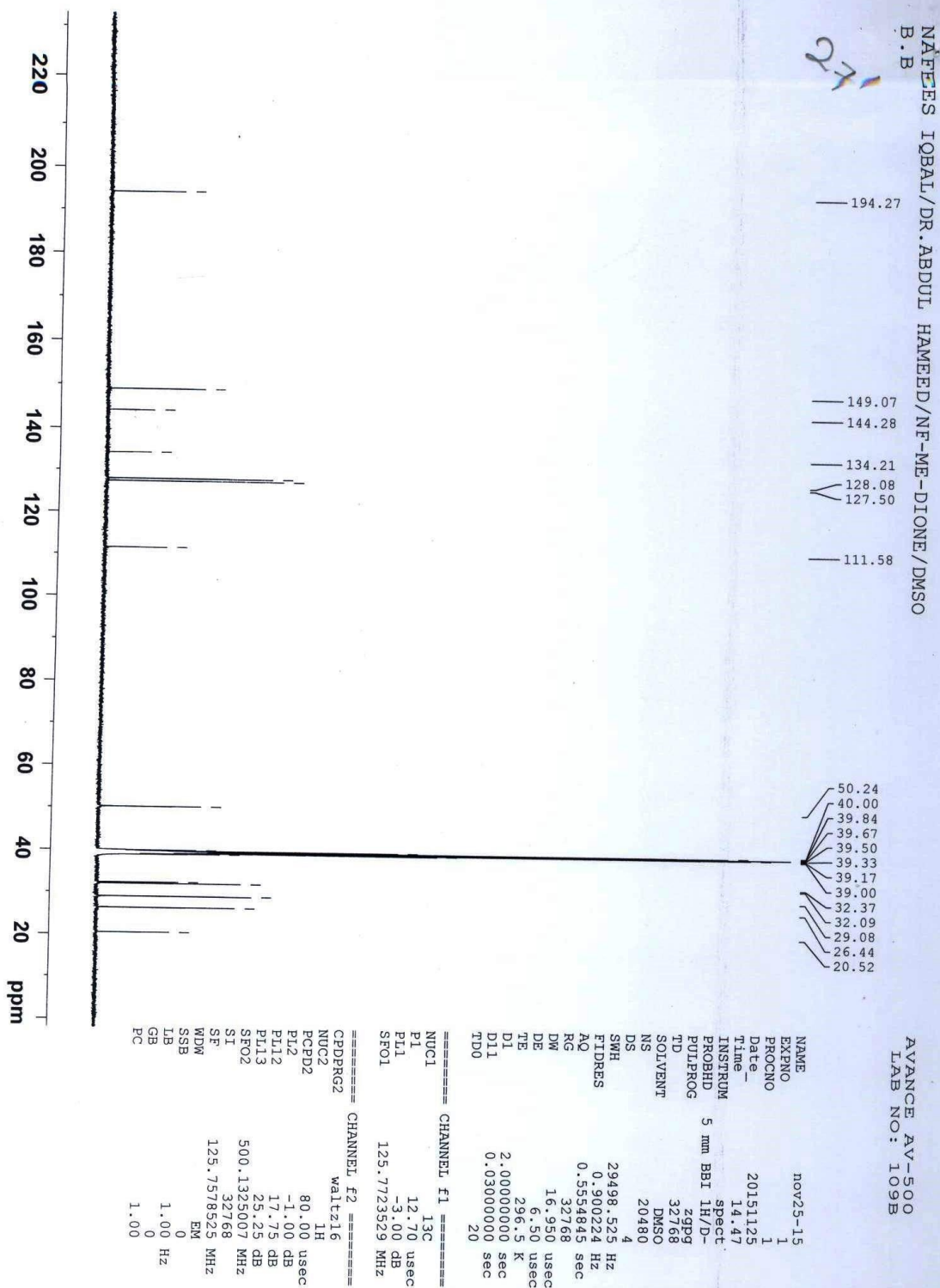


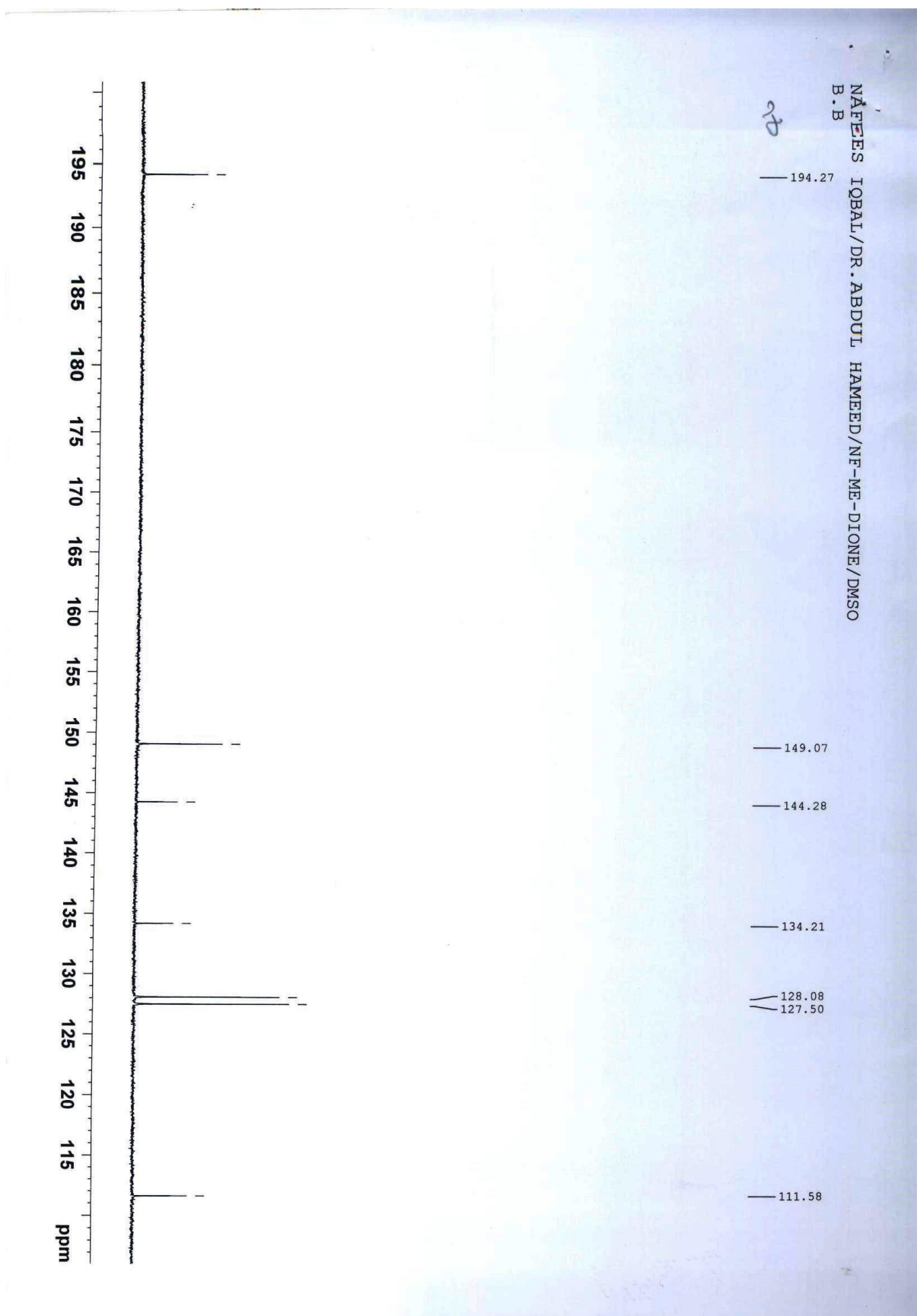


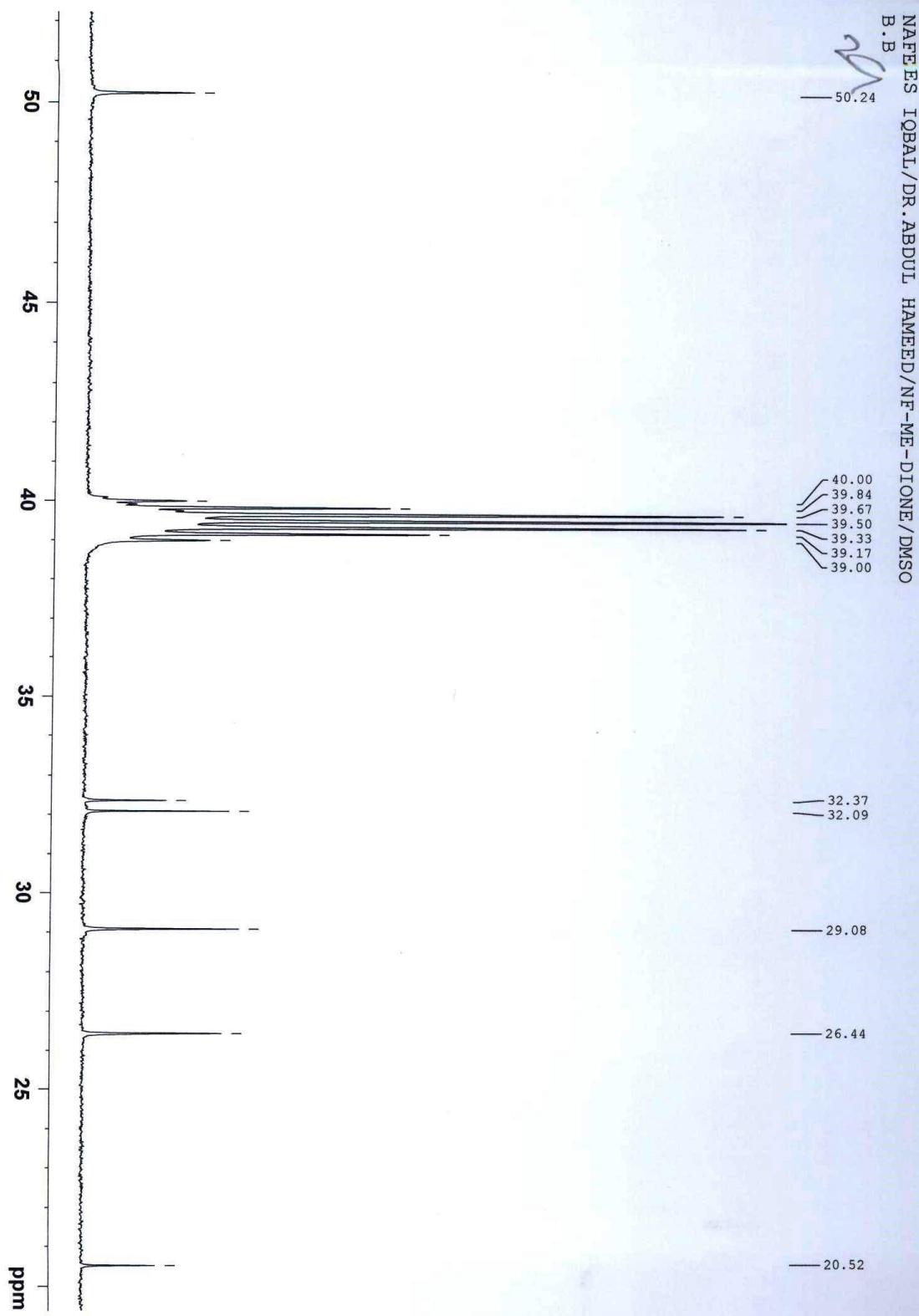


Supplementary Information (SI)

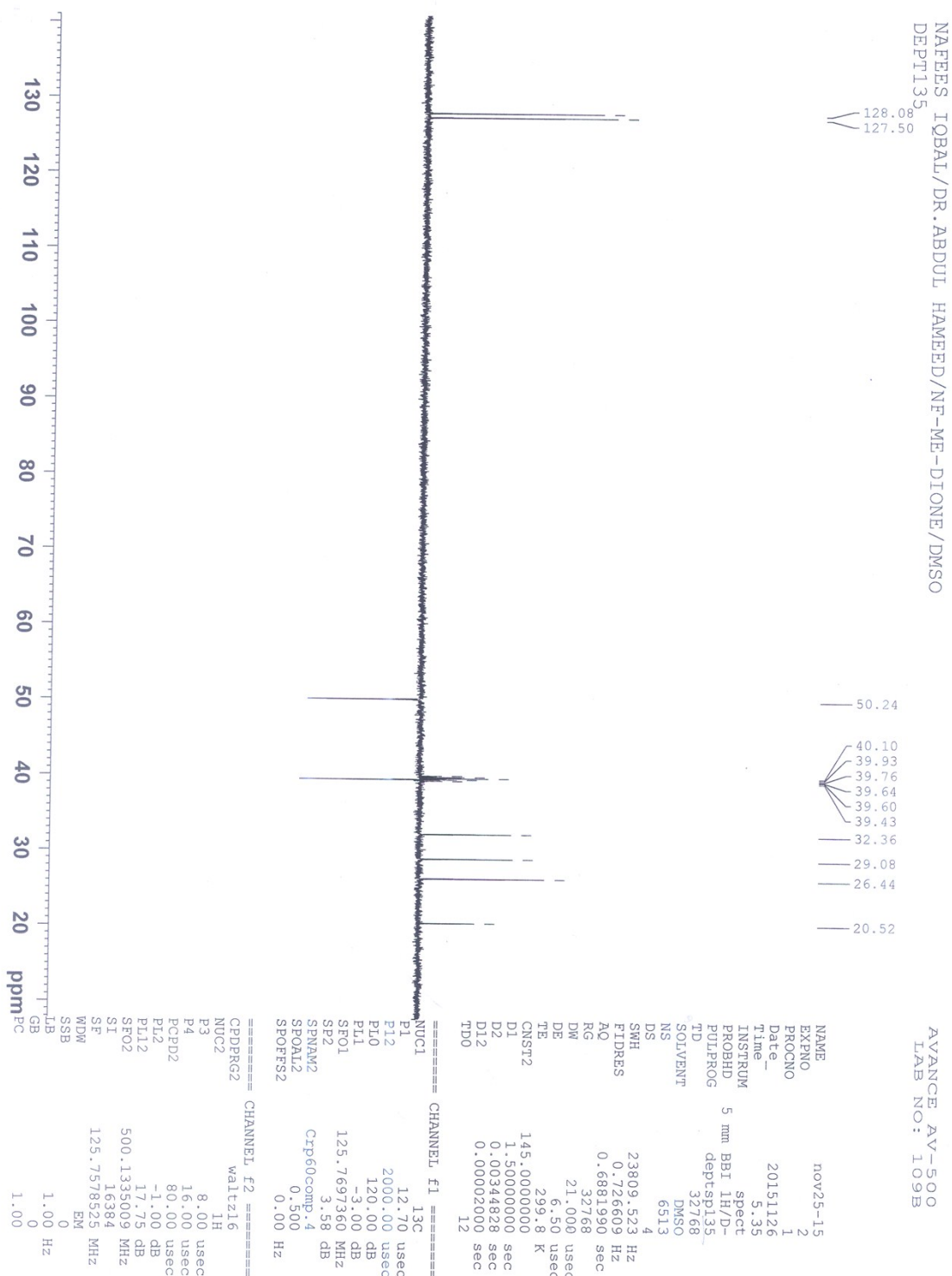


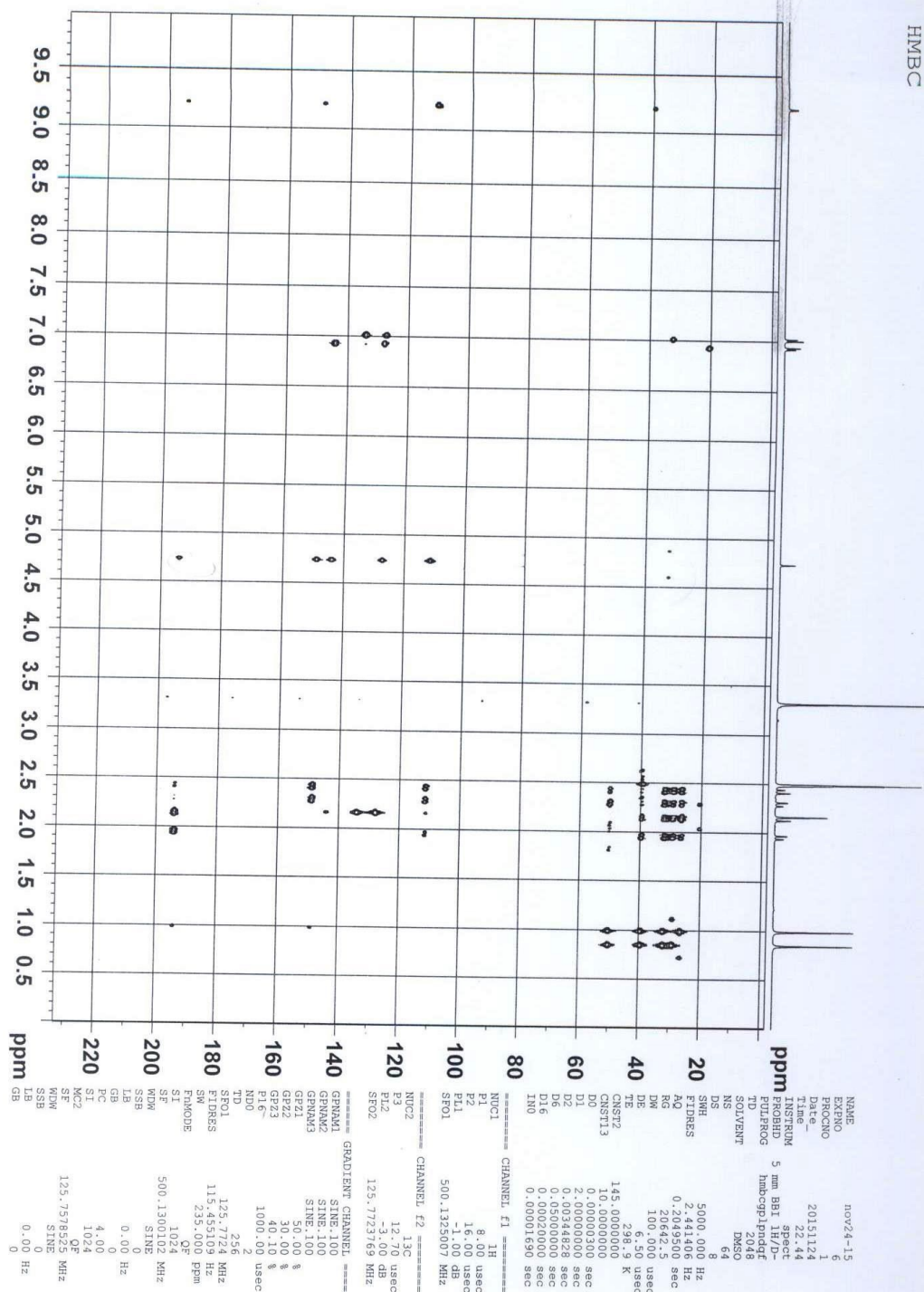






Supplementary Information (SI)

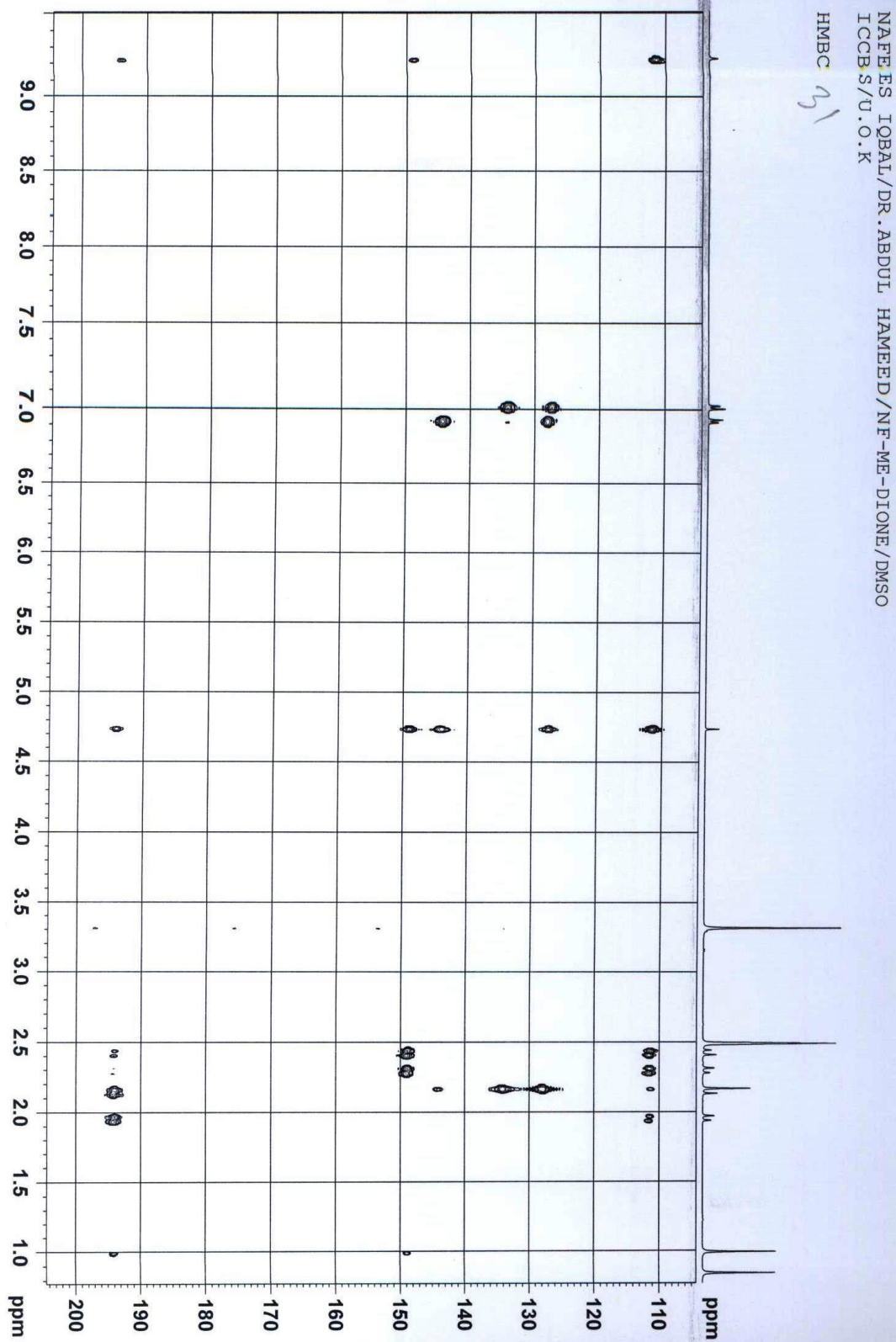


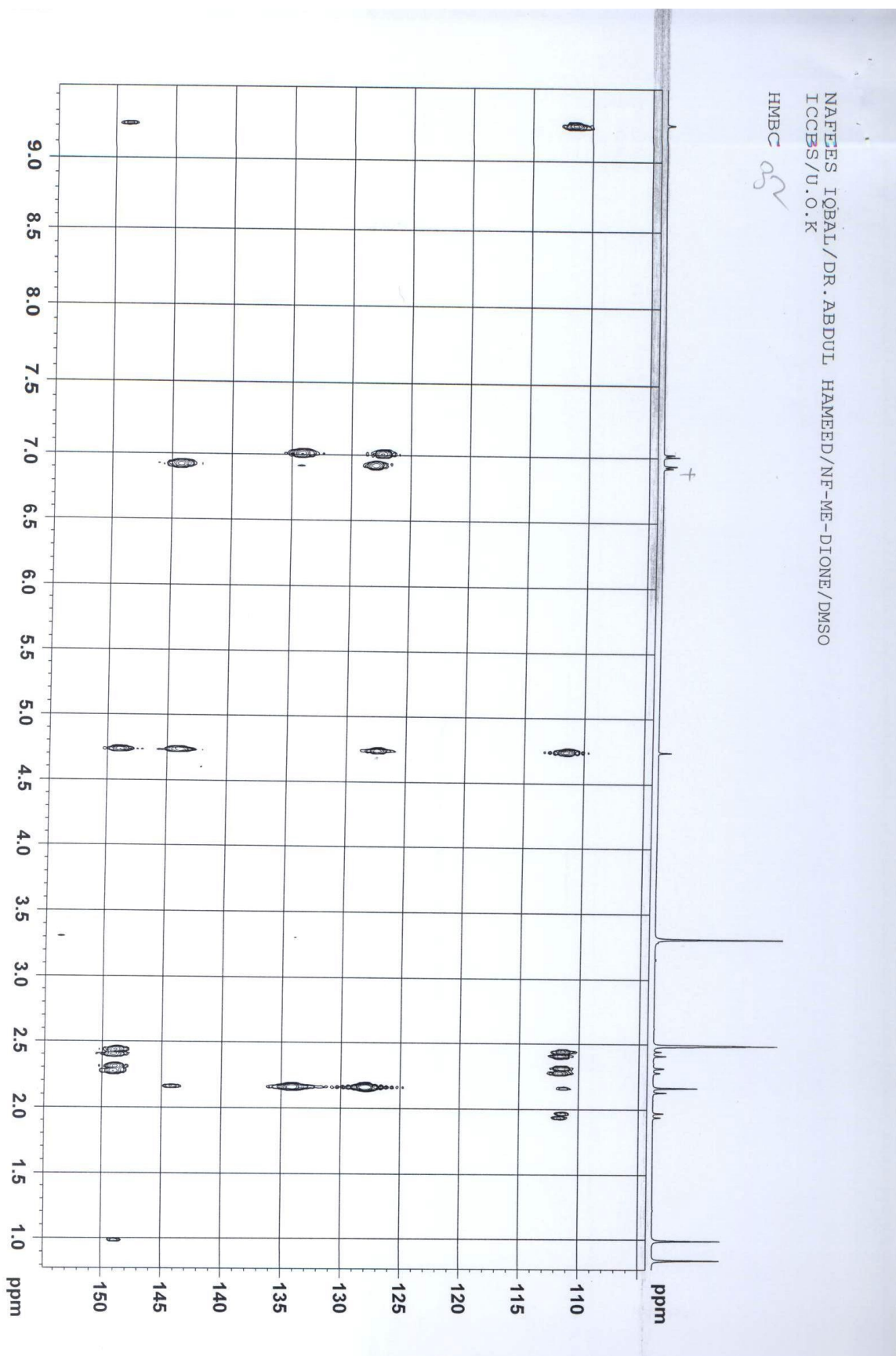


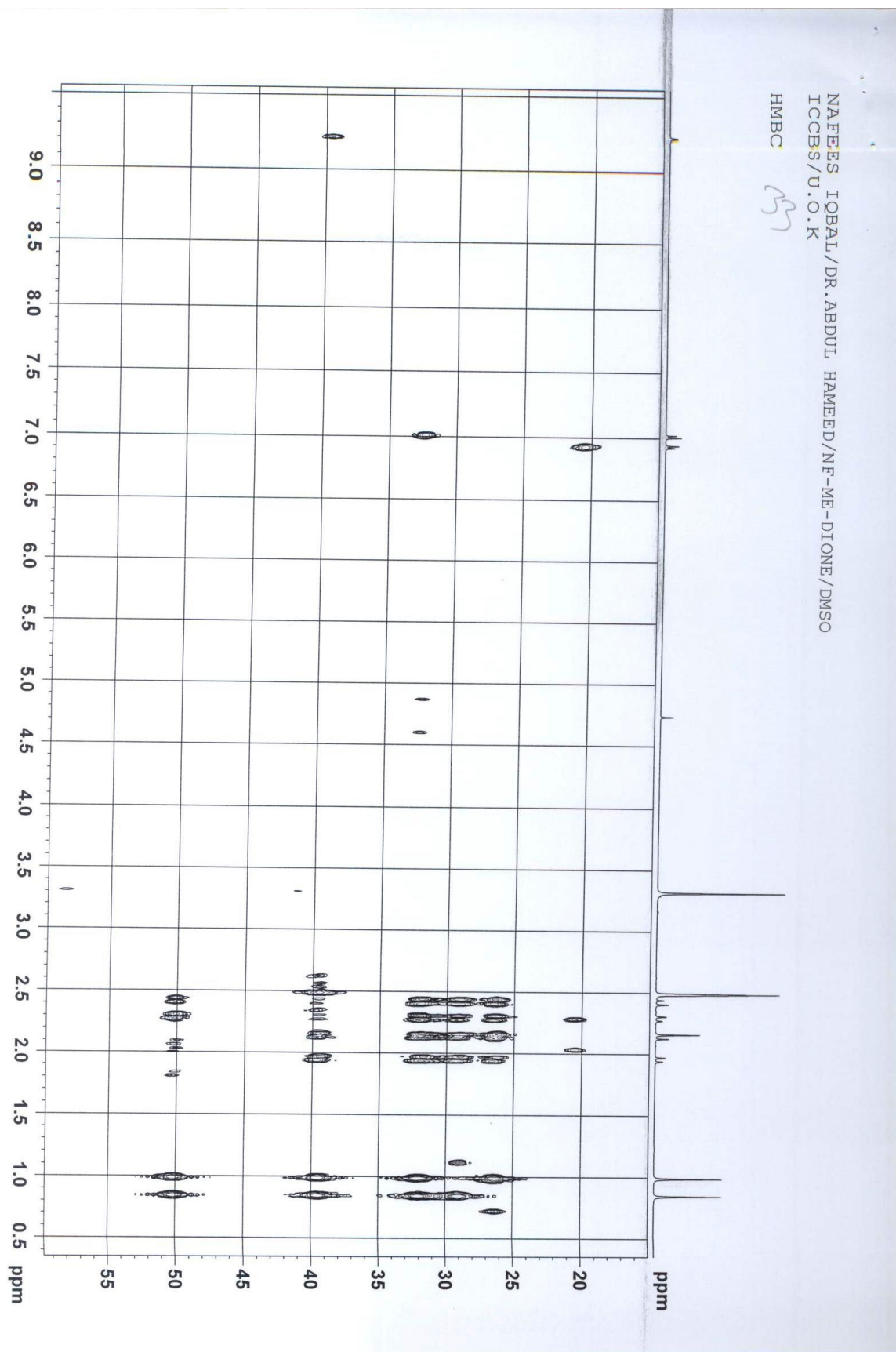
HMBC

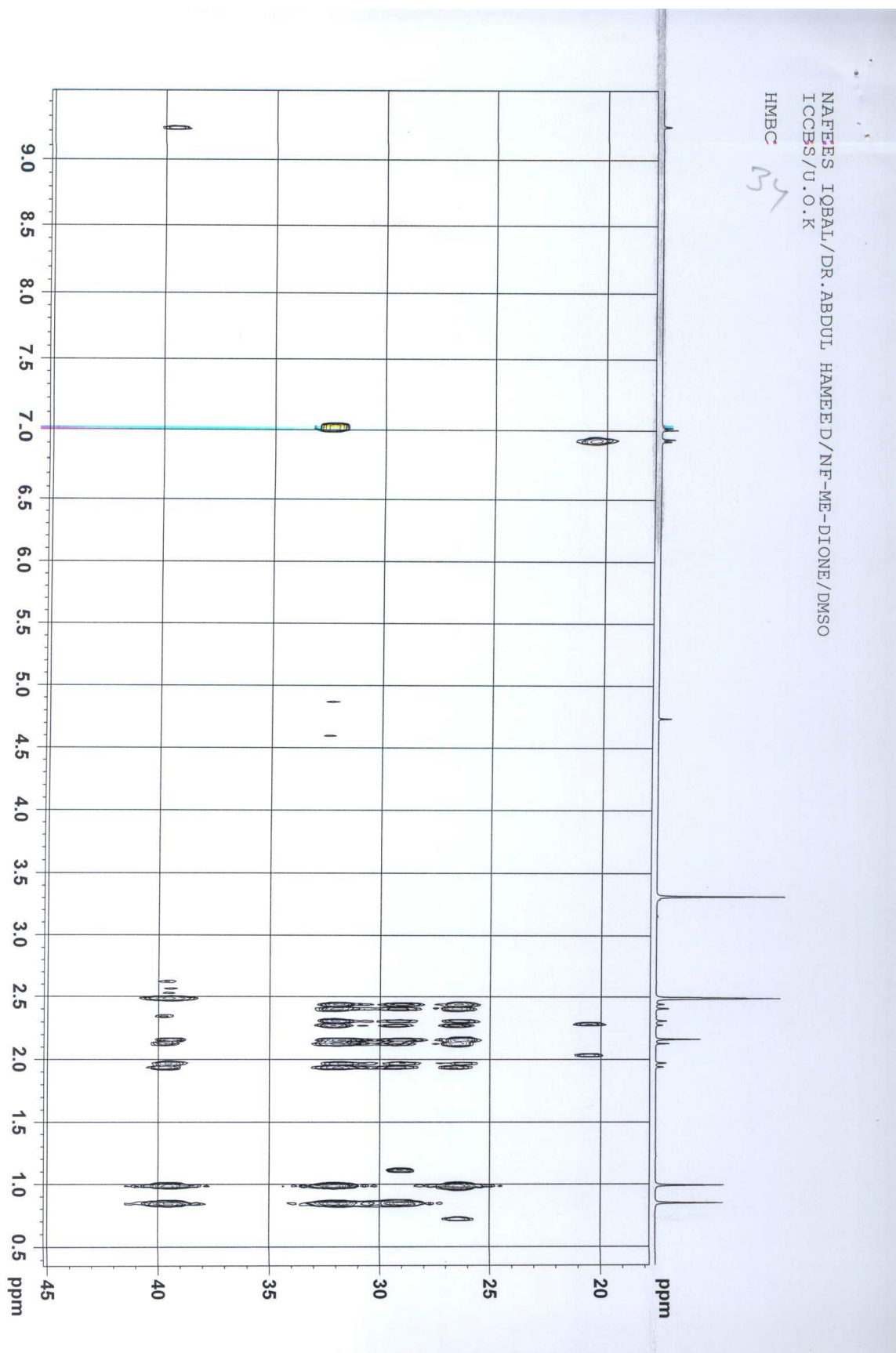
NAFEES IOBAL/DR.ABDUL HAMEED/NF-ME-DIONE/DMSO
ICCBS/U.O.K

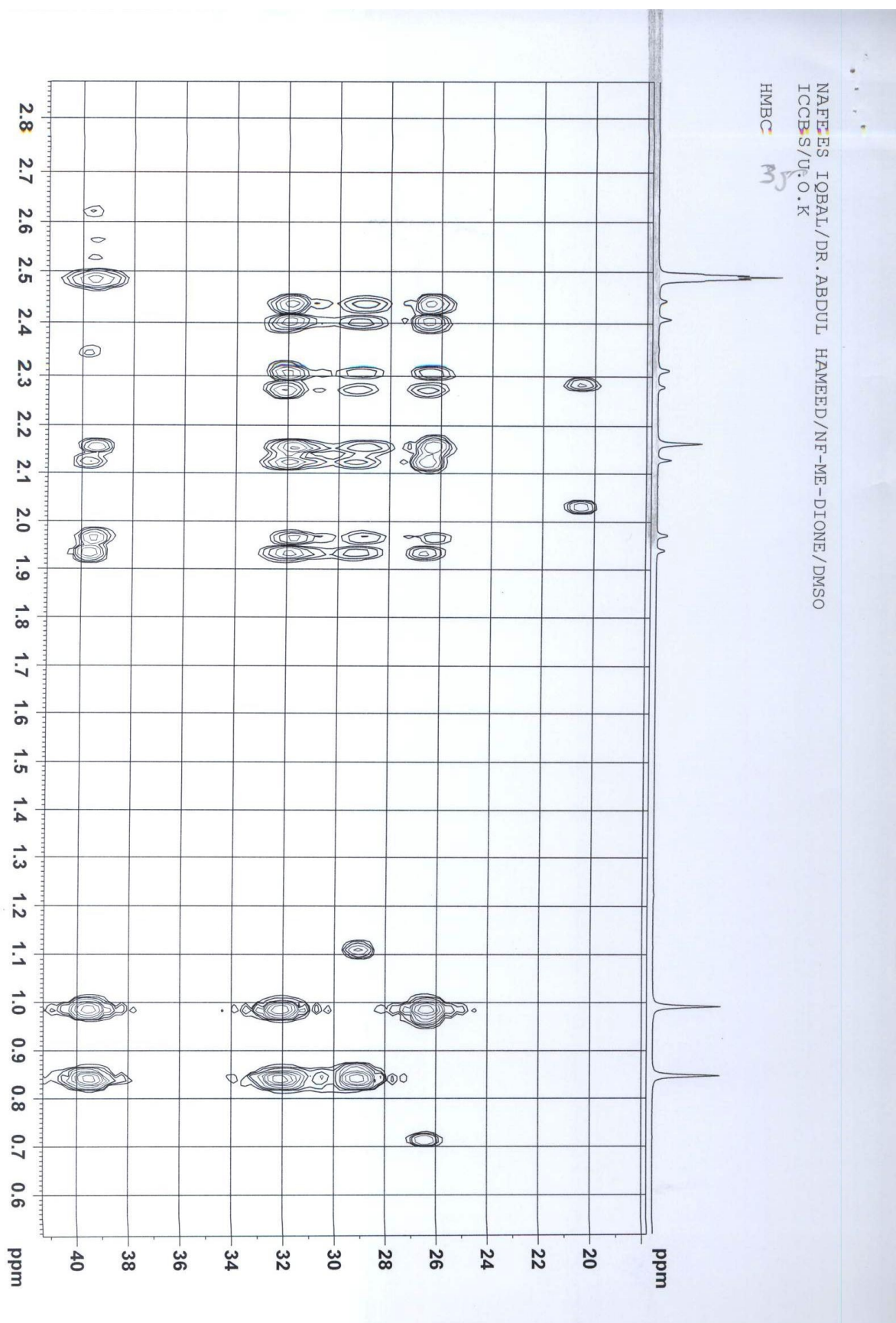
AVANCE AV-500
LAB NO: 109B



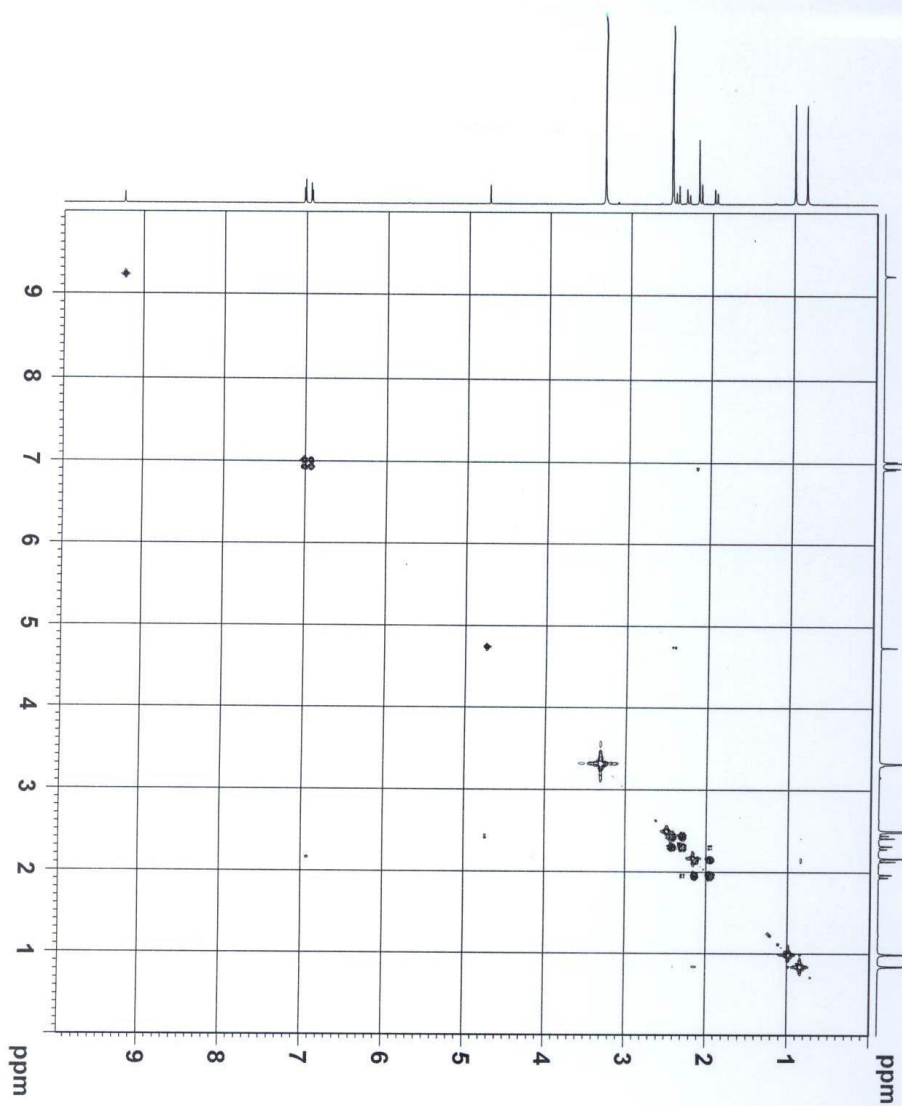








NAFEES IQBAL/DR. ABDUL HAMEED/NF-ME-DIONE/DMSO
ICCB S/U.O.K
COSY *nb*



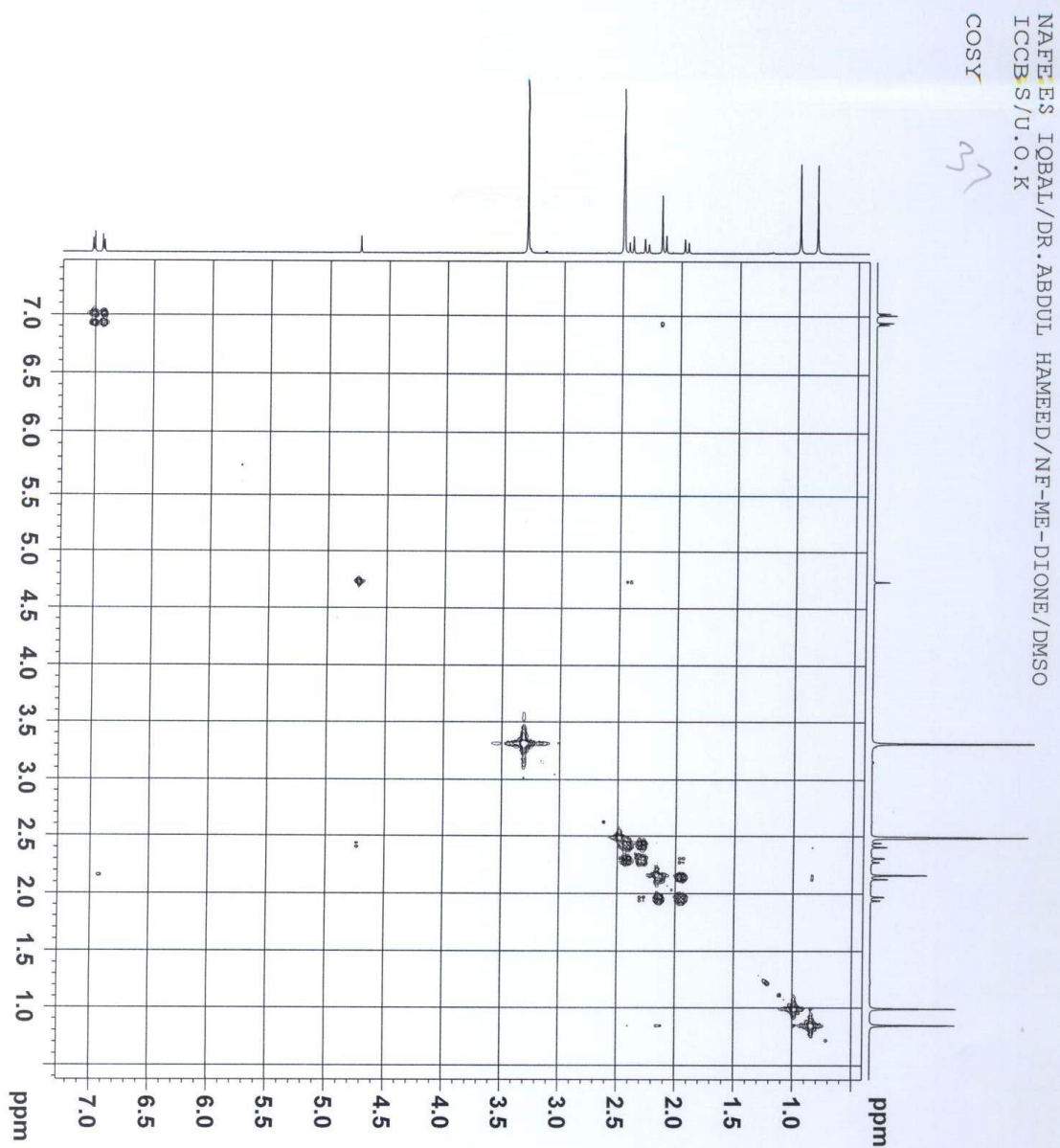
AVANCE AV-500
LAB NO: 109B

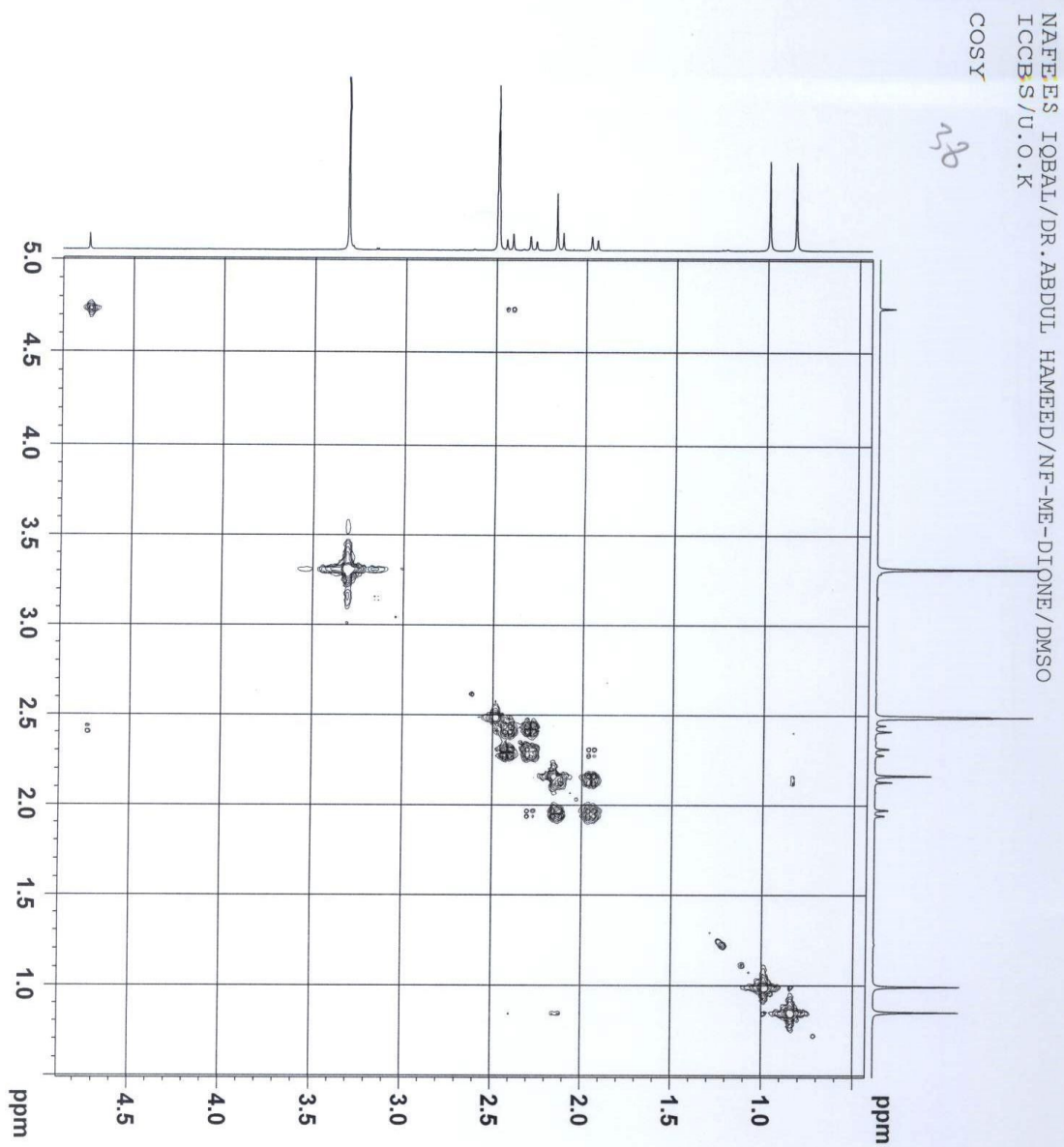
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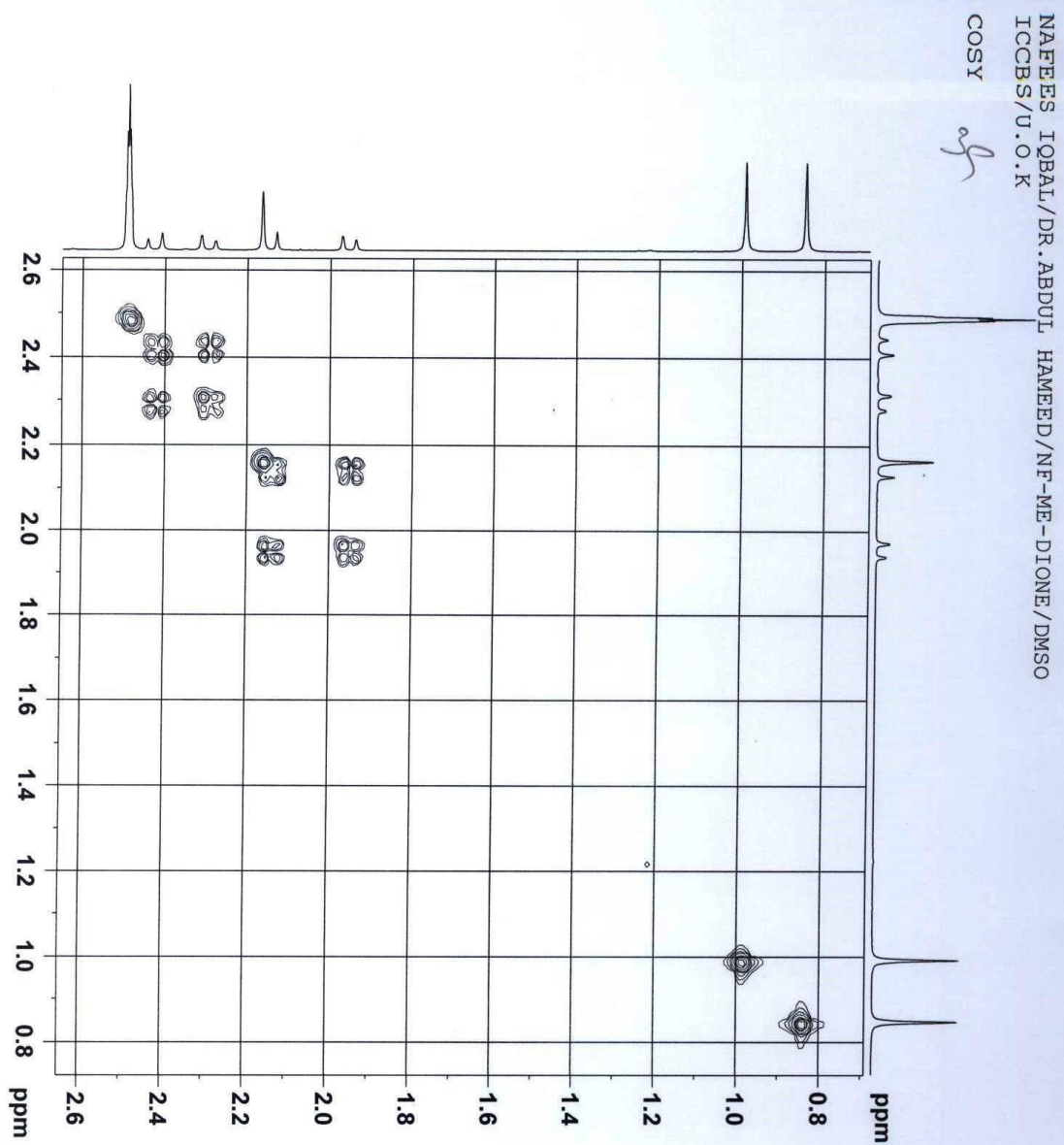
NAME nov24-15
EXPNO 3
PROCNO 1
Date_ 20151124
Time_ 14.34
INSTRUM spect
PROBHD 5 mm BBI 1H/D-
PULPROG cosygpgf
TD 2048
SOLVENT DMSO
NS 8
DS 8
SWH 5000.000 Hz
FIDRES 2.441406 Hz
AQ 0.2049500 sec
RG 362
DE 100.000 usec
TE 297.8 K
DO 0.00000300 sec
D1 1.50000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
INO 0.00020000 sec

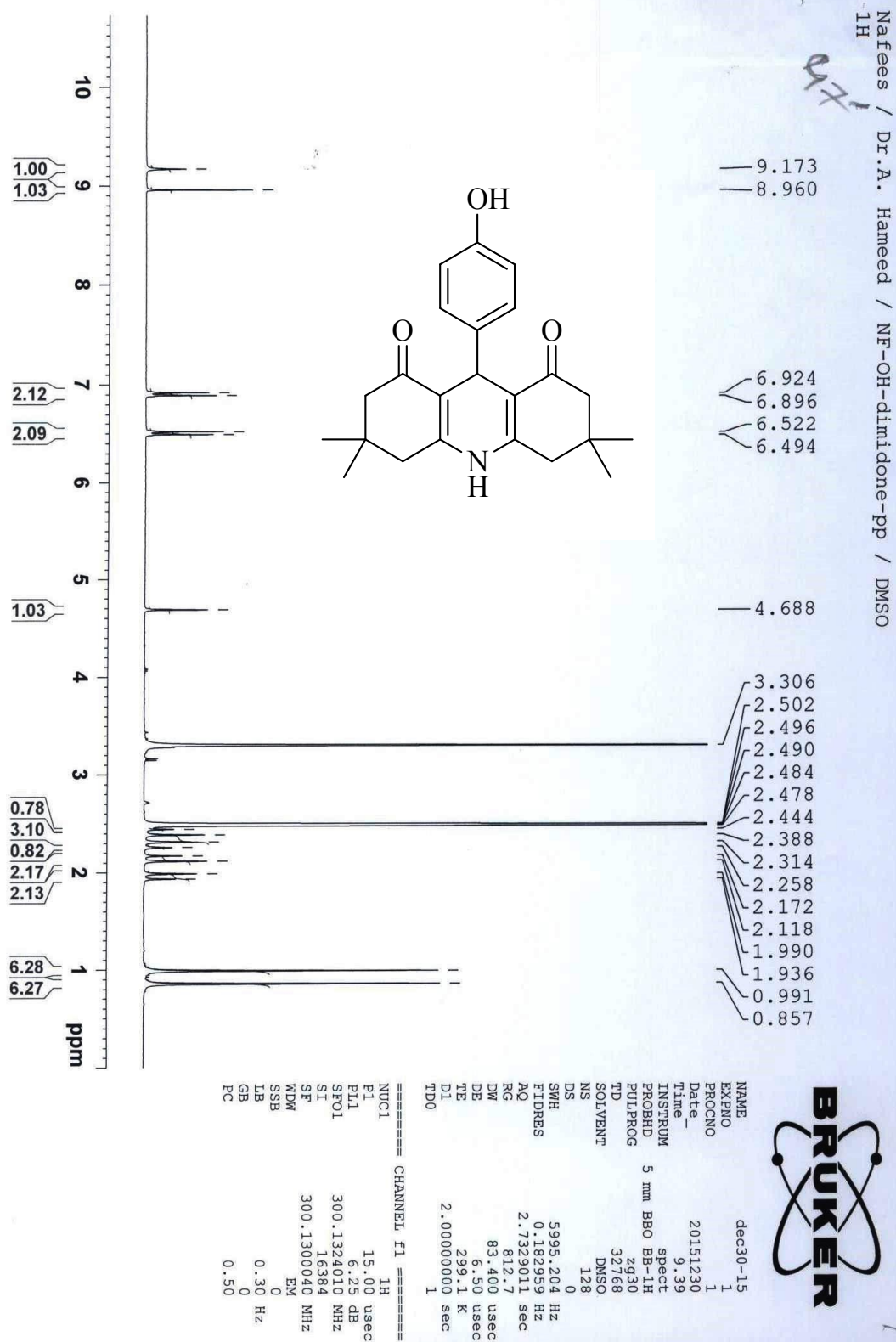
===== CHANNEL f1 =====
NUC1 1H
P0 8.00 usec
P1 8.00 usec
PL1 -1.00 dB
SFO1 500.1325007 MHz

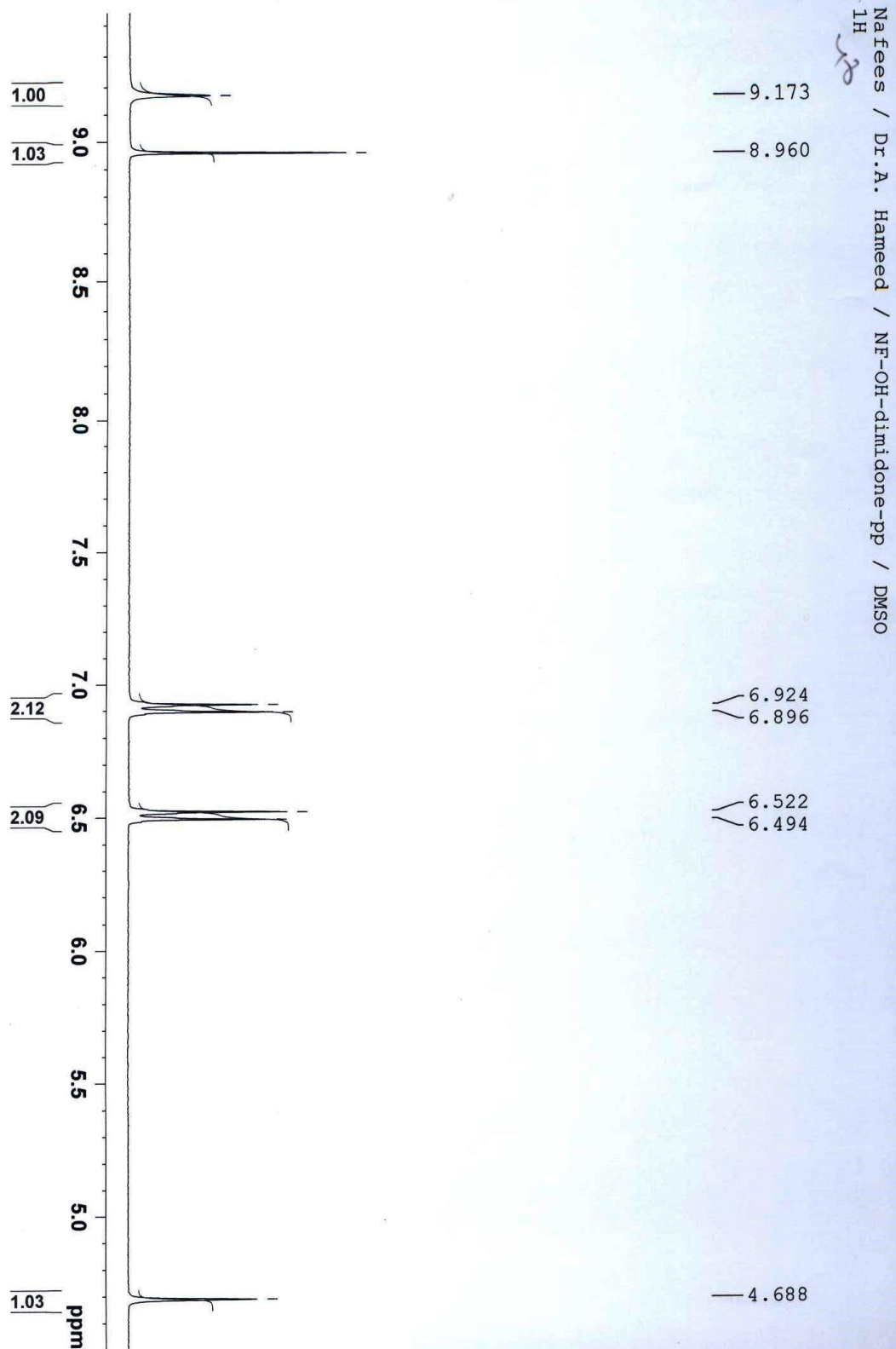
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPZ1 10.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 500.1325 MHz
FIDRES 19.531250 Hz
SW 9.997 ppm
FnmODE OF
SI 1024
SF 500.1300102 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
MC2 1024
OF 500.1300102 MHz
SF 500.1300102 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
  
```

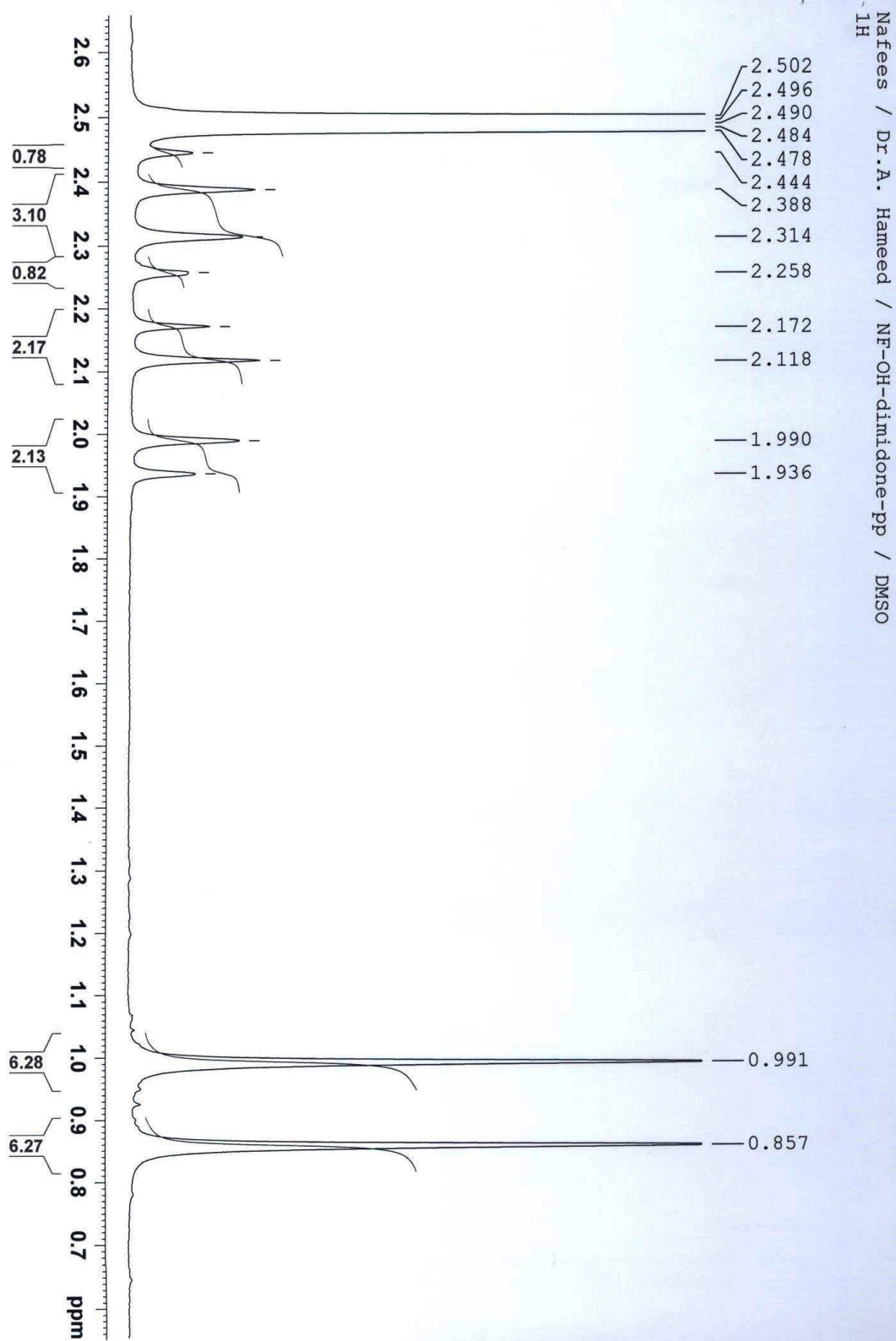



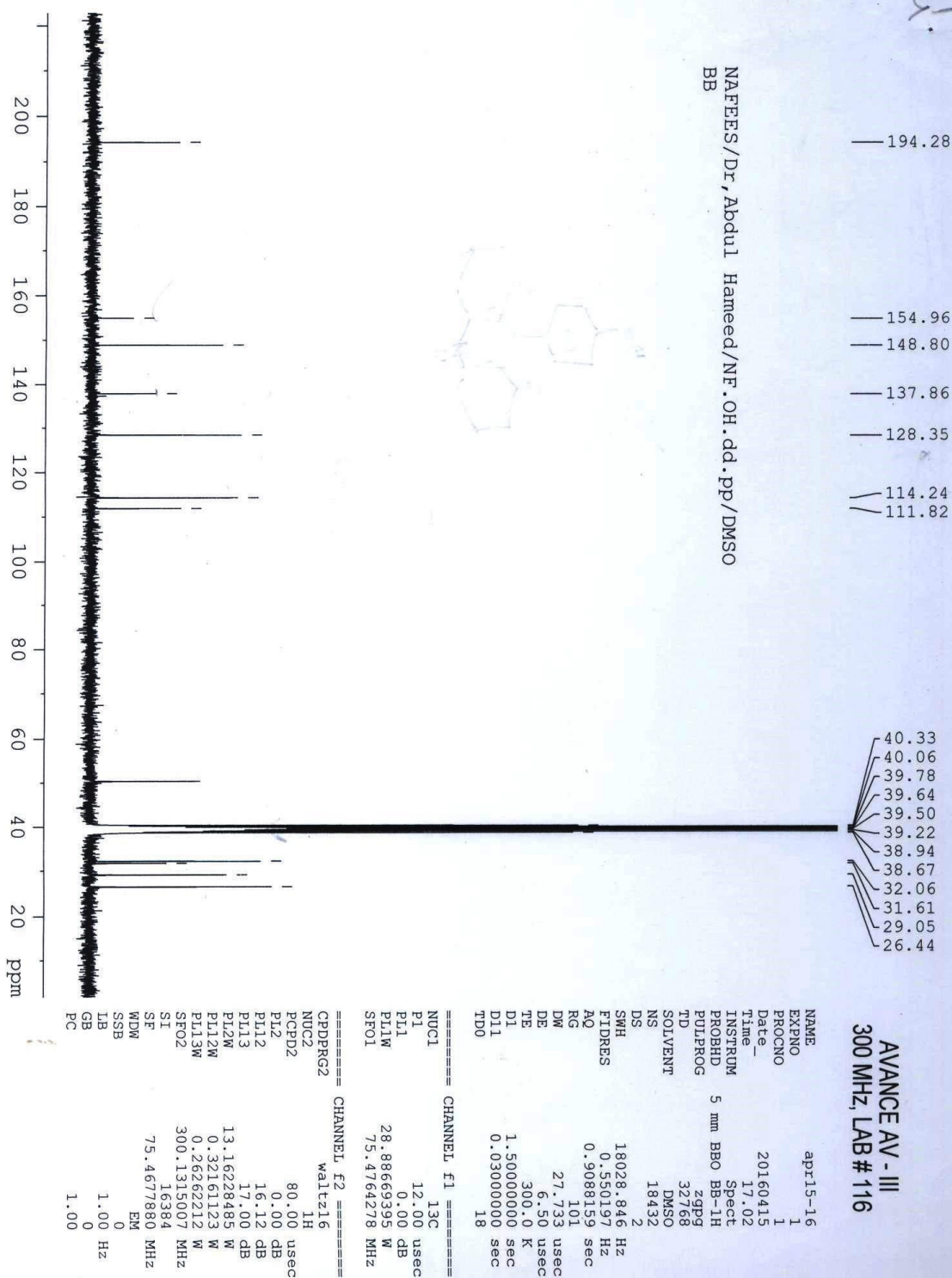


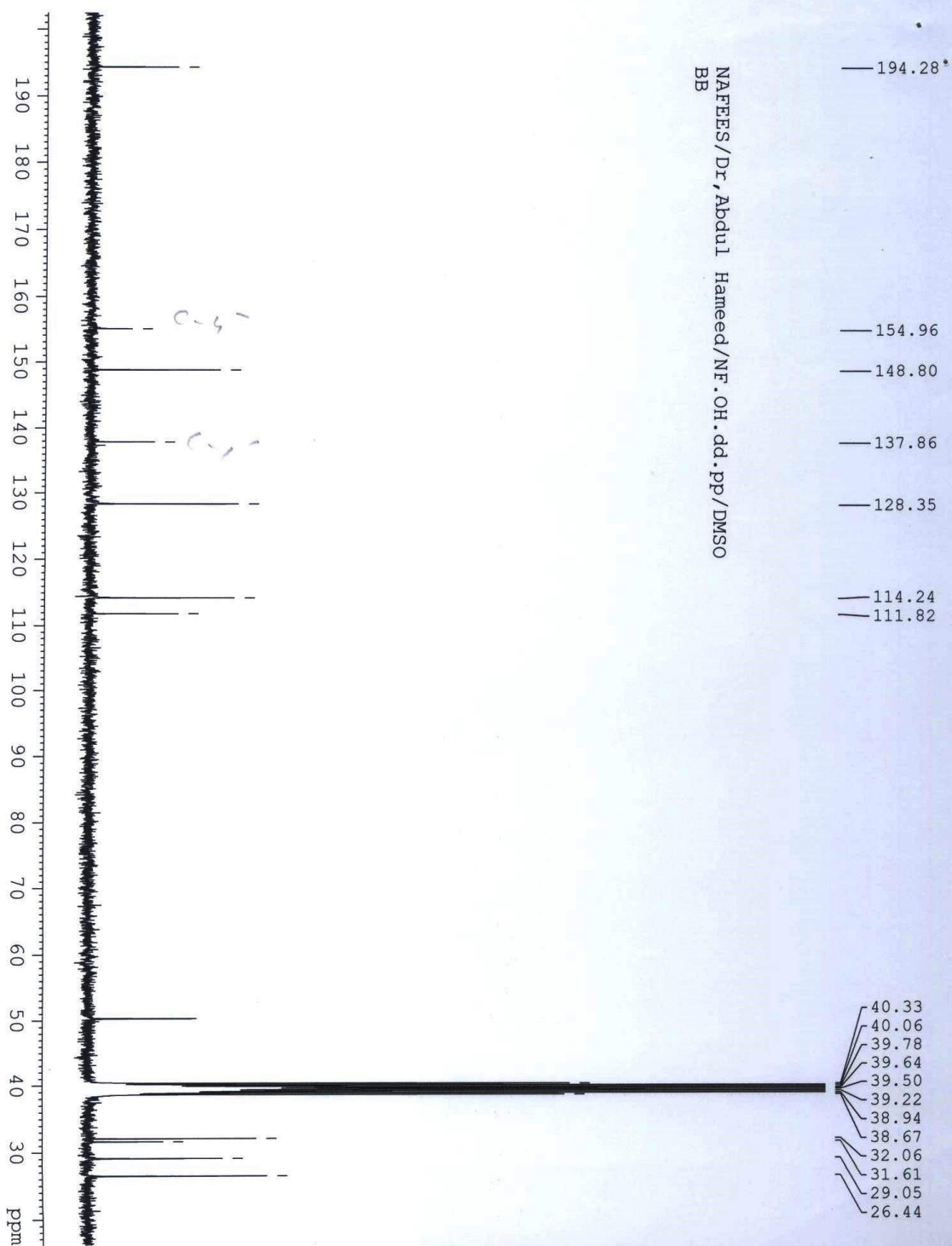


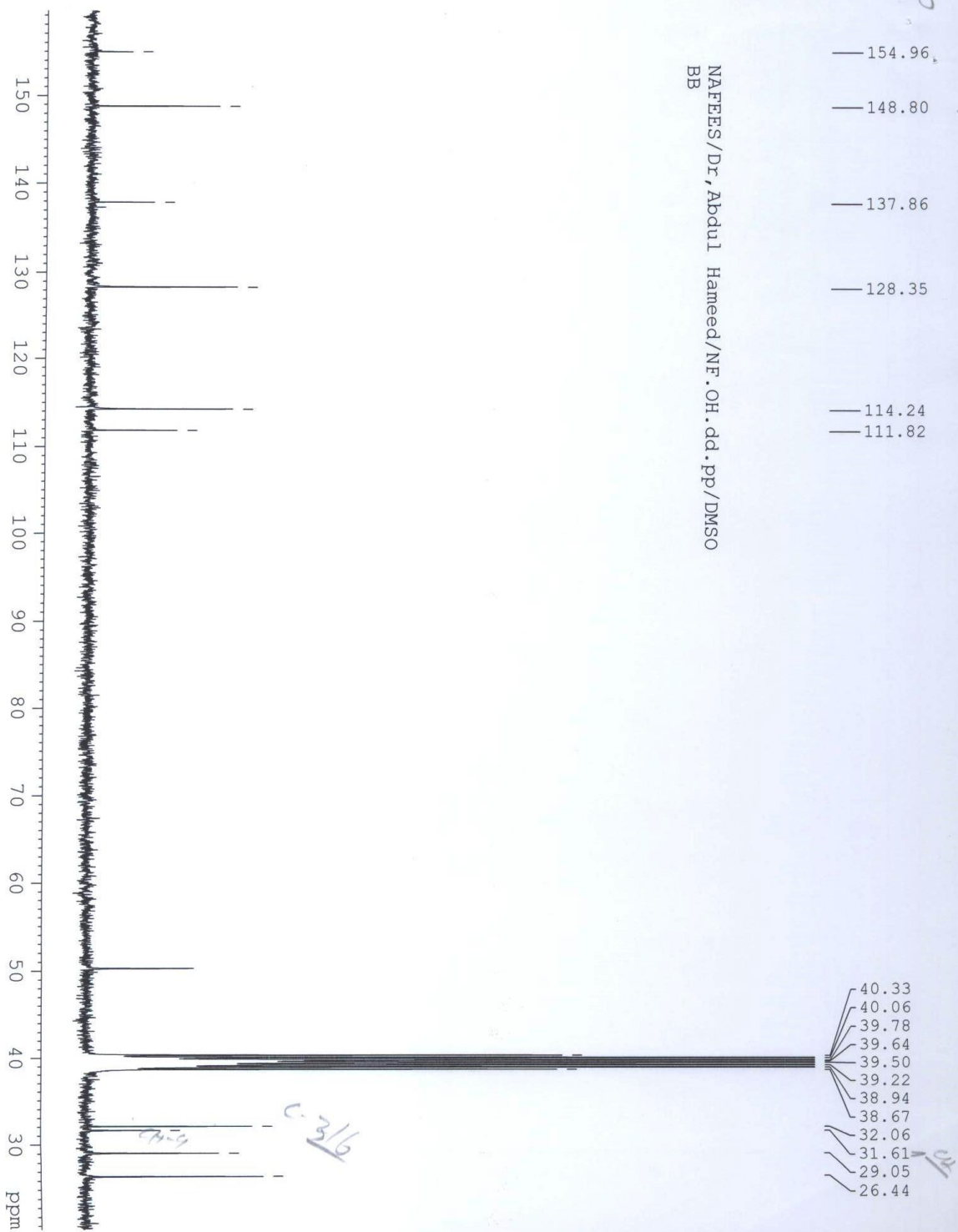


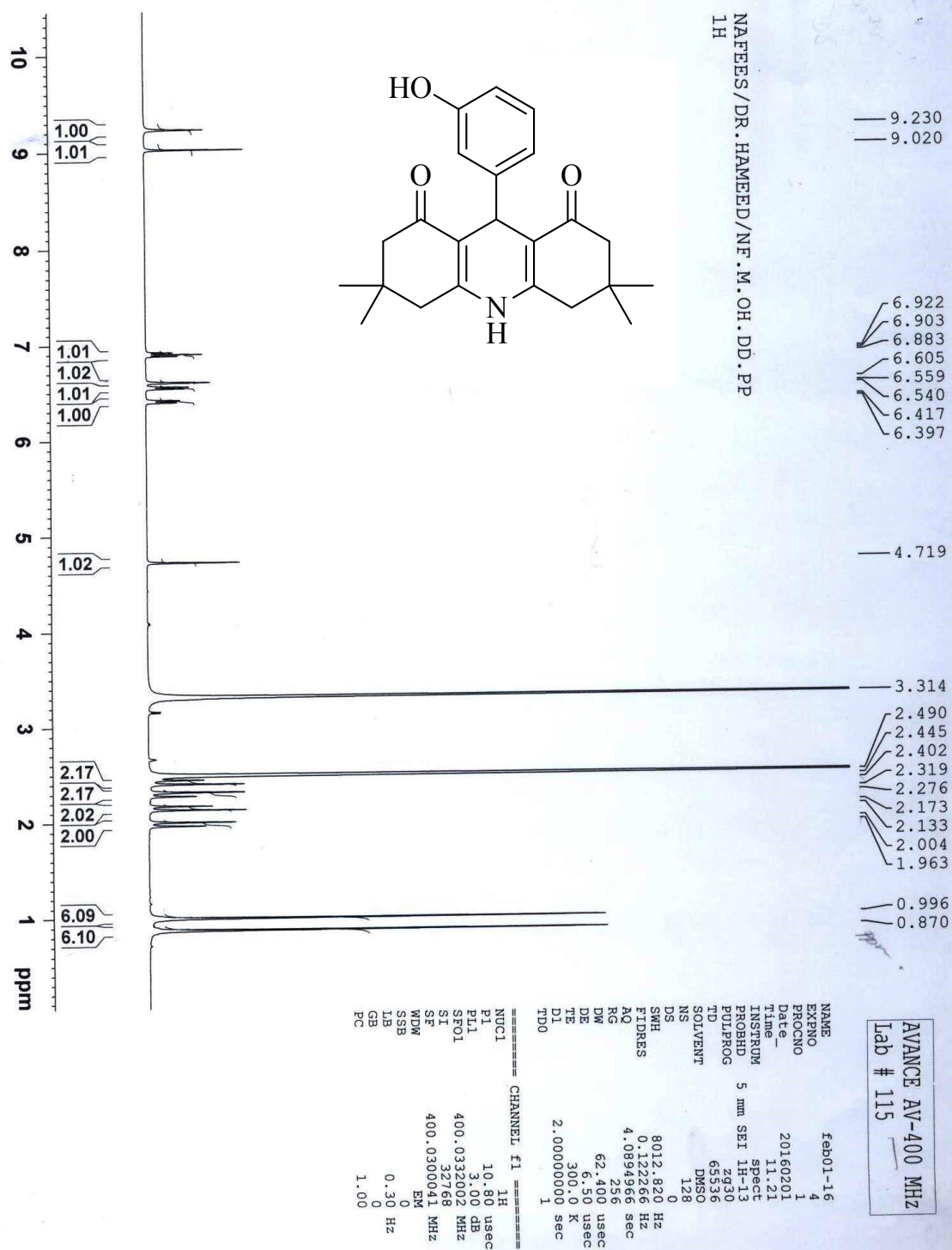


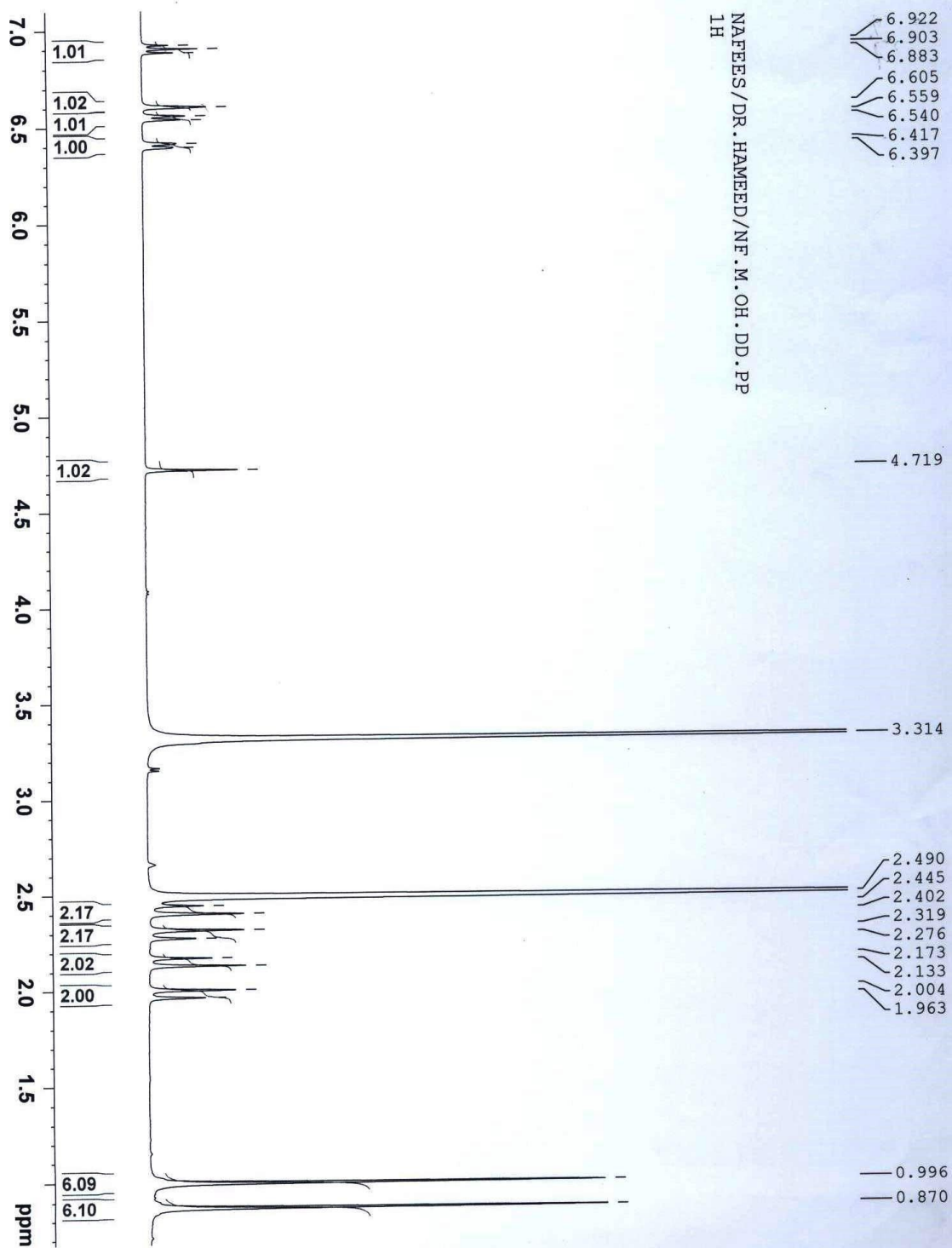


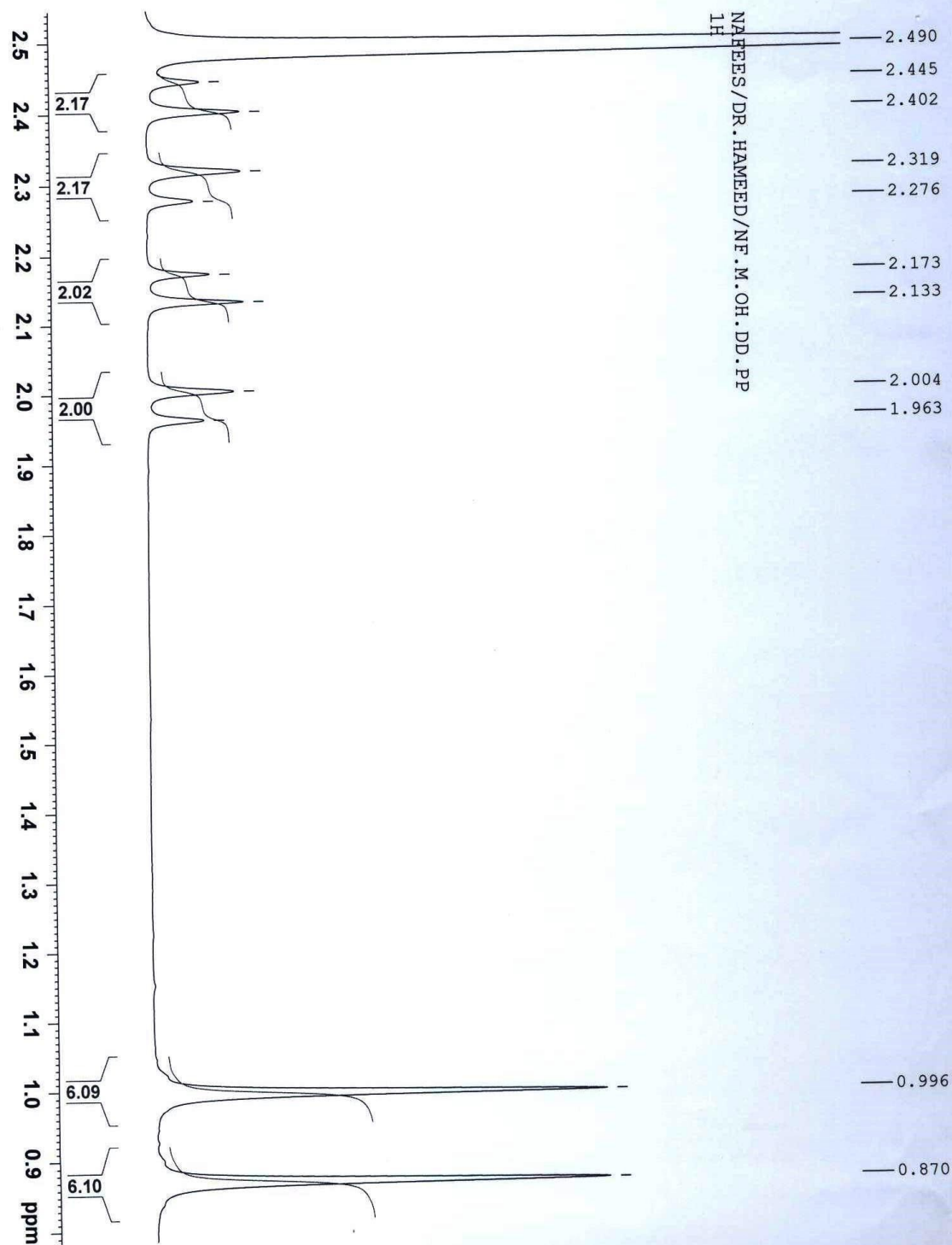


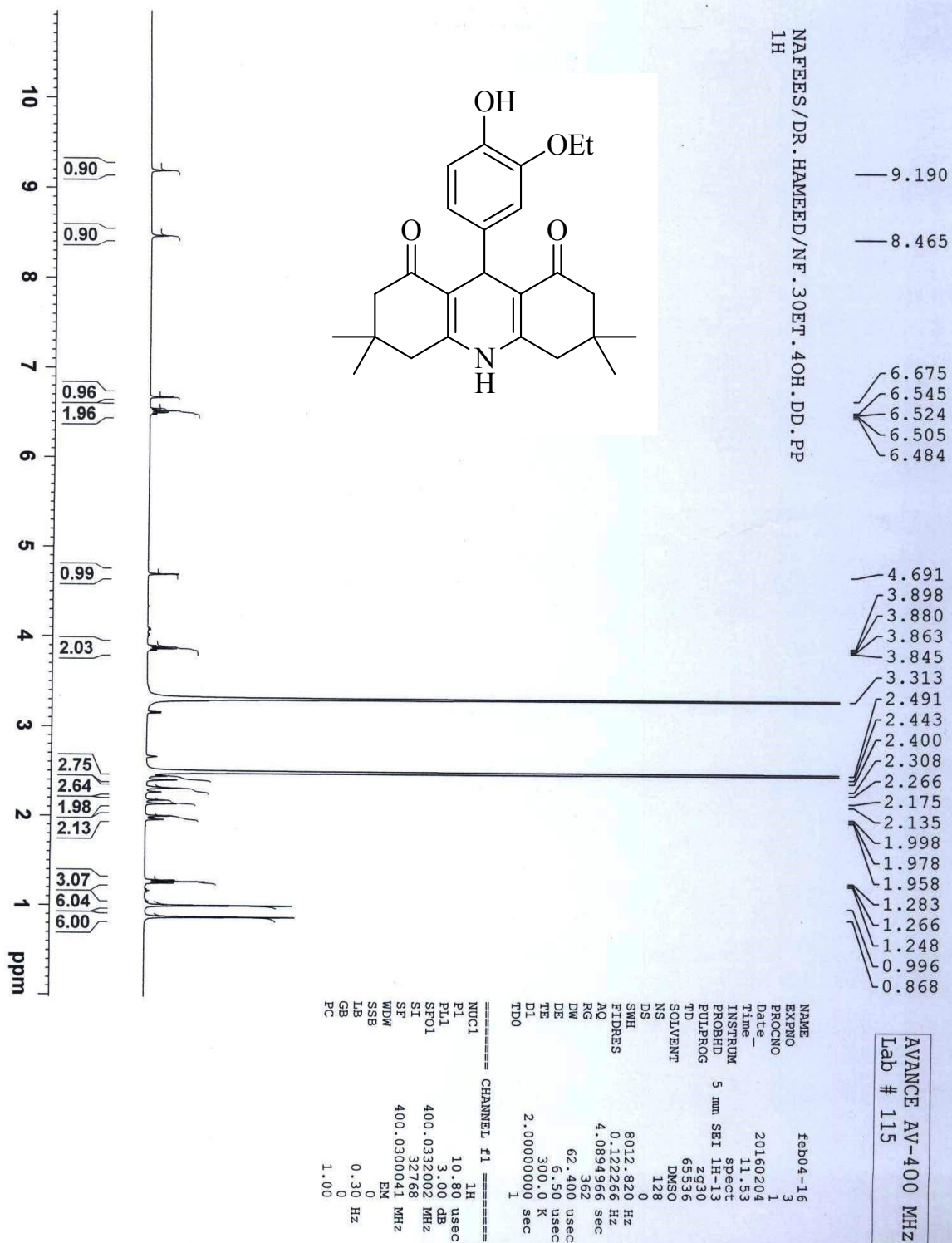


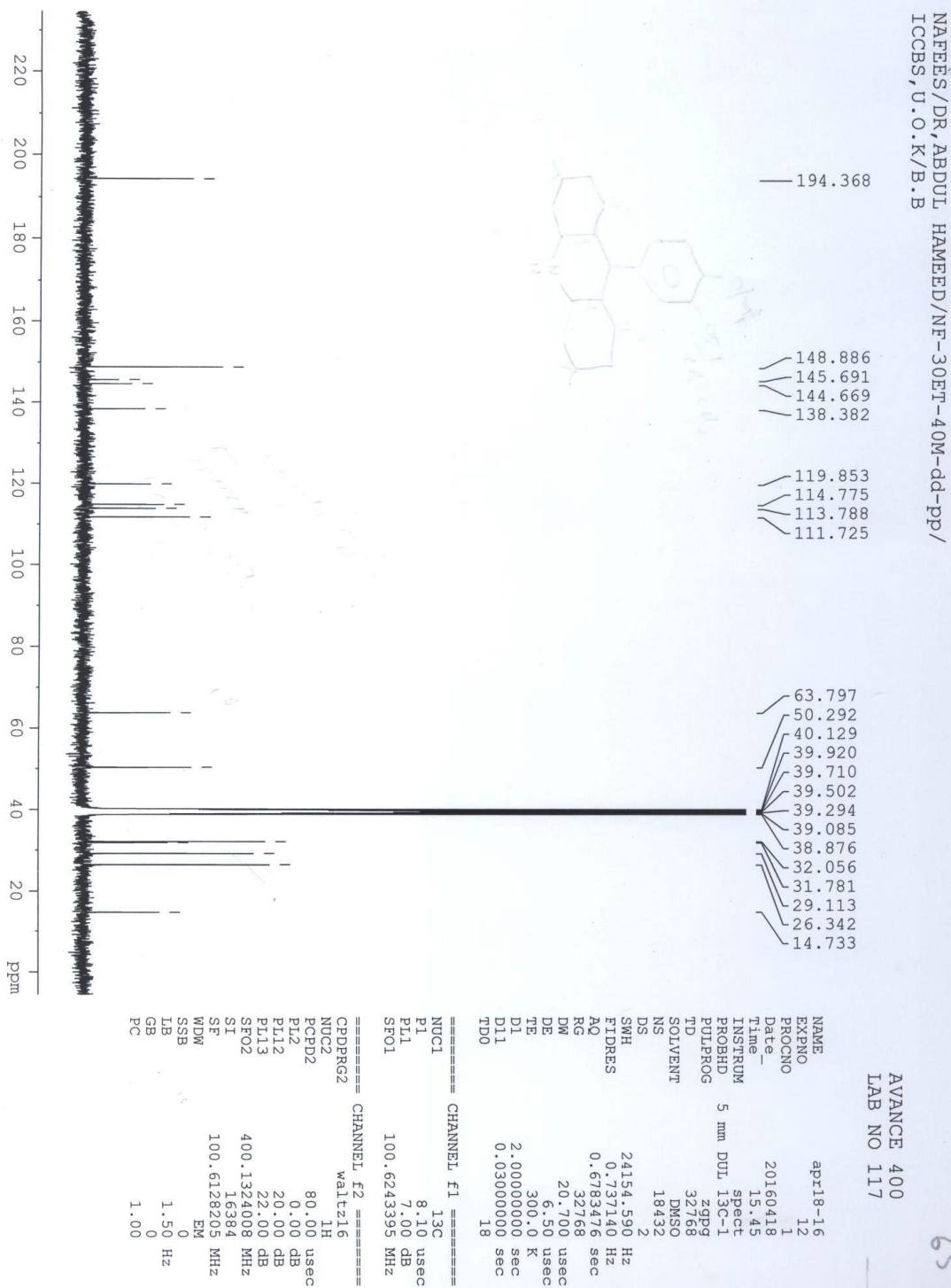


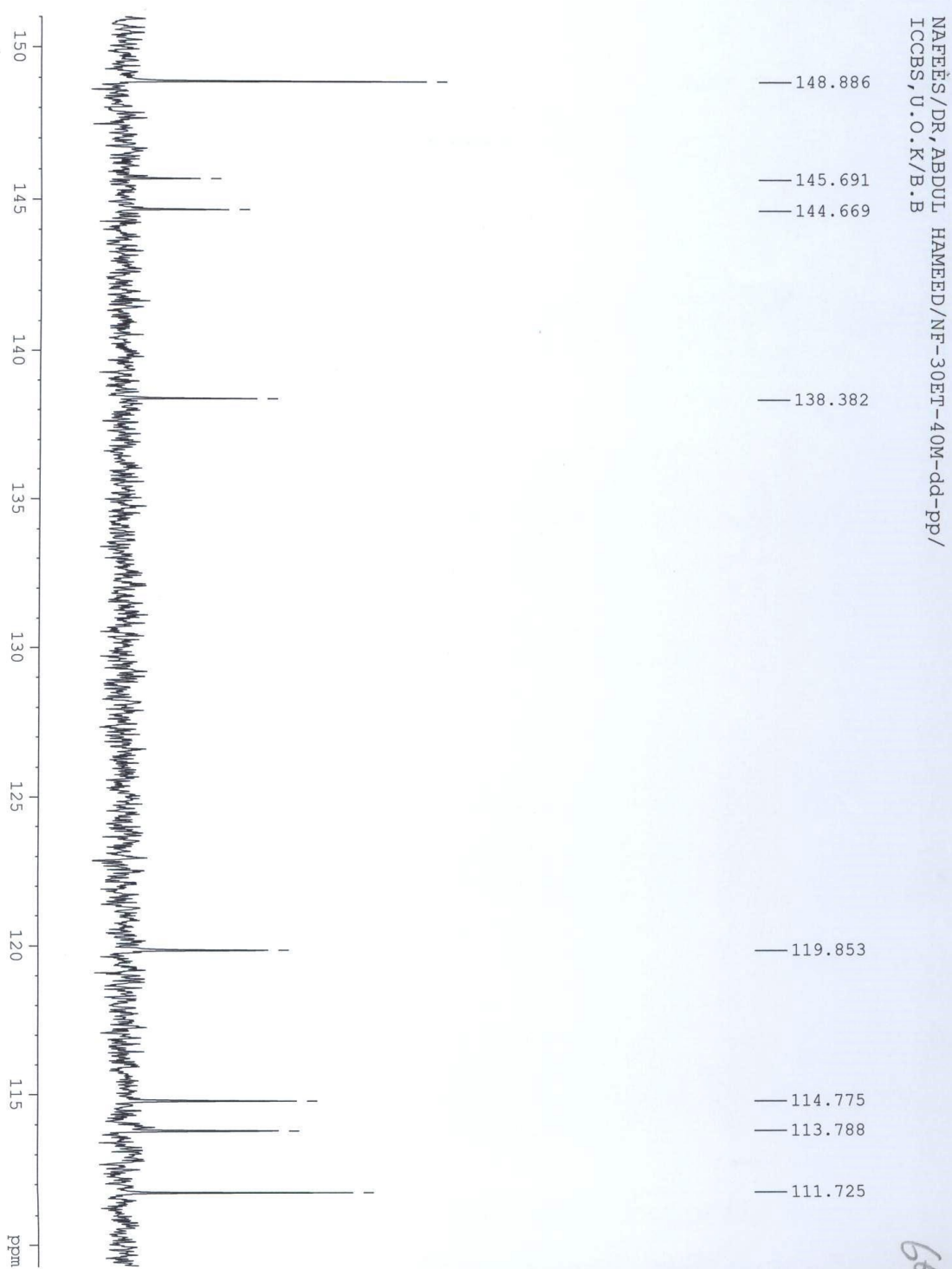


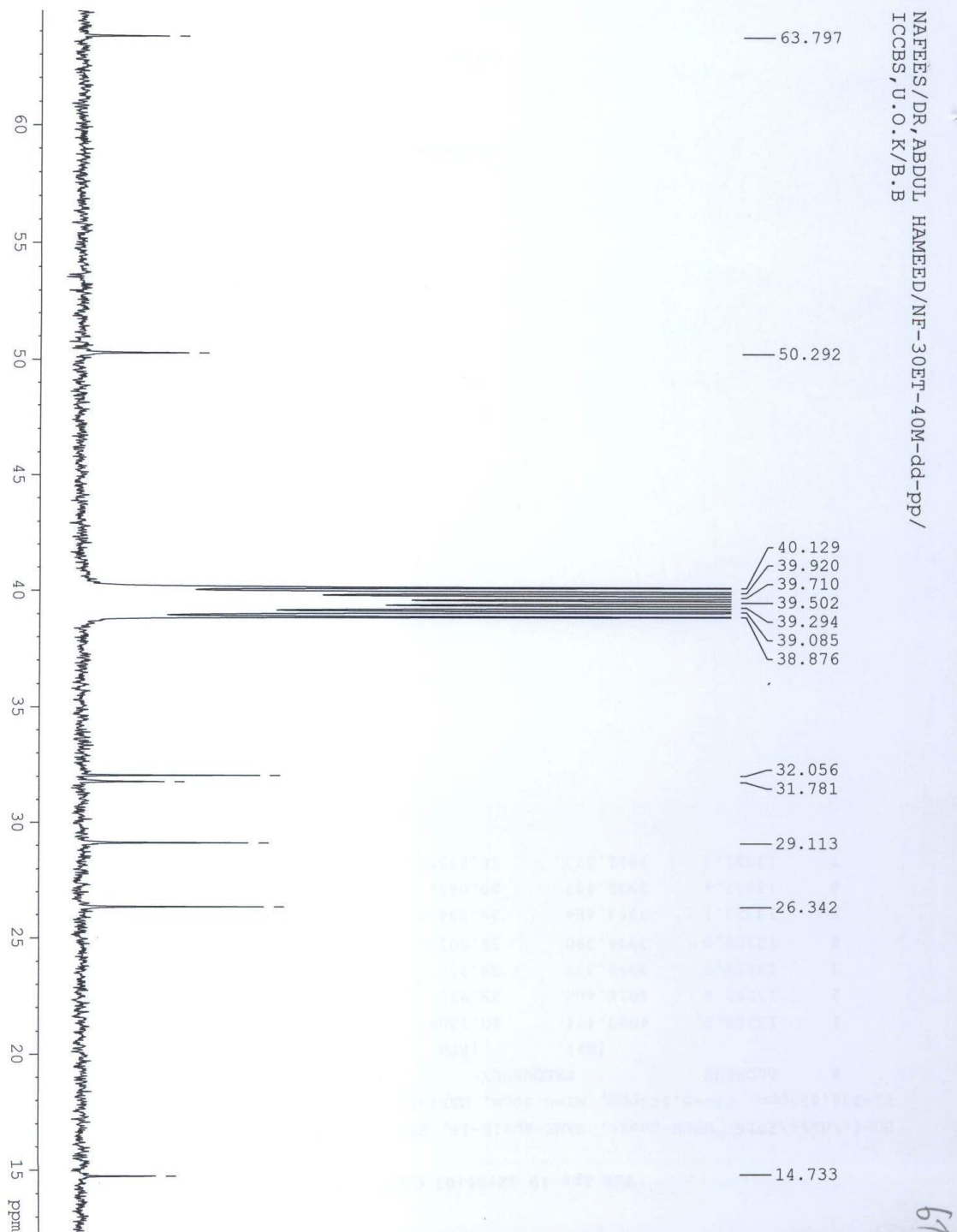


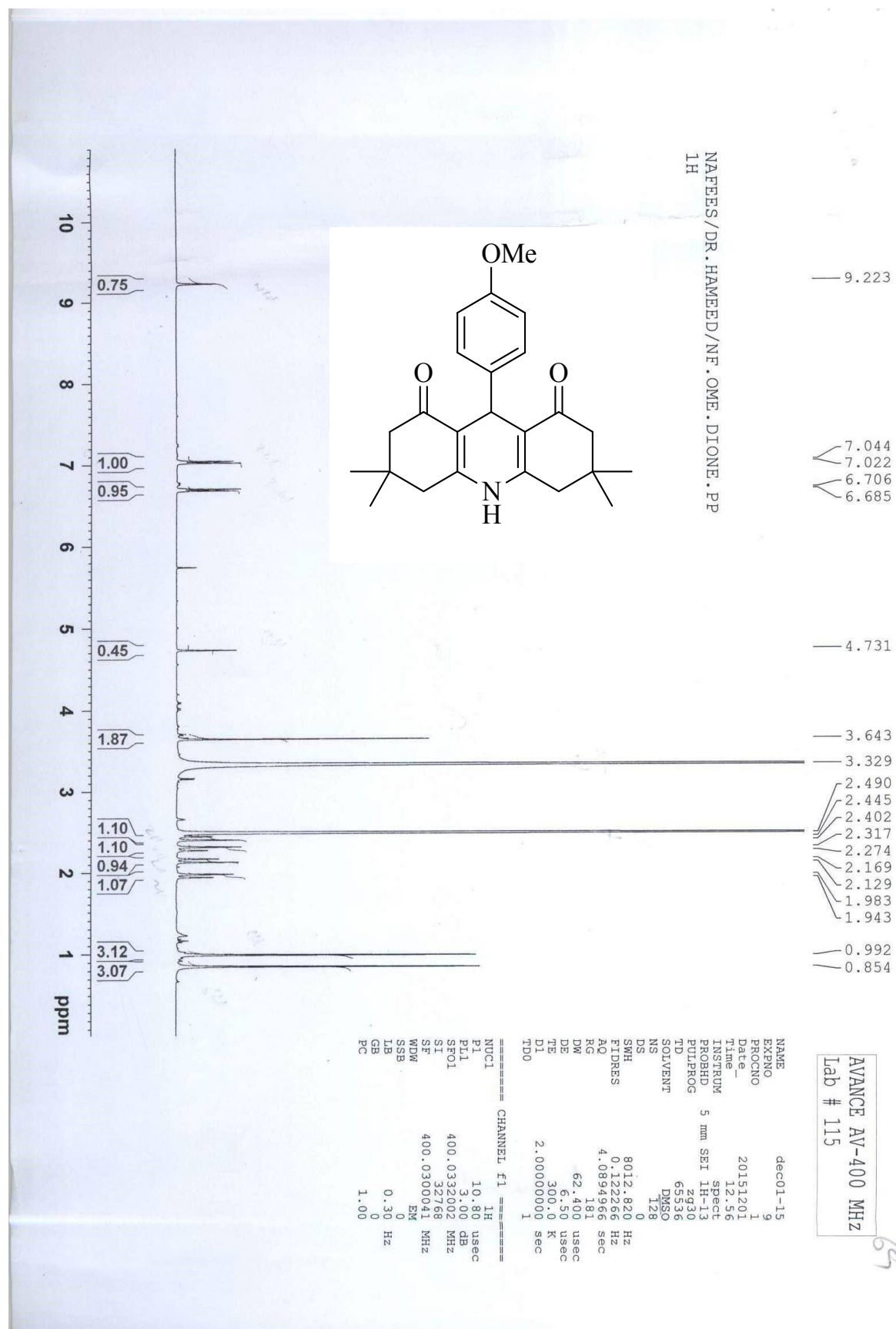




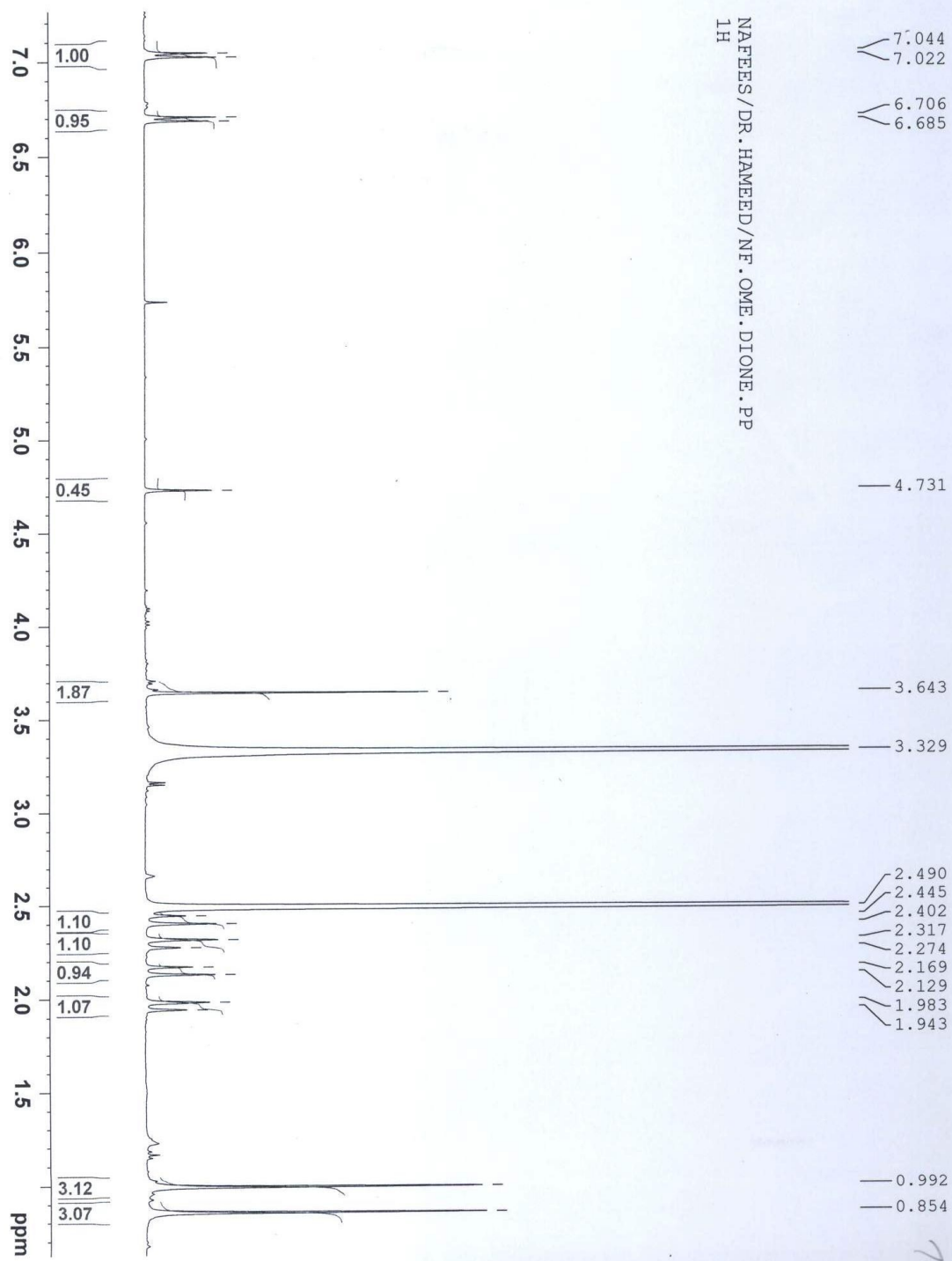


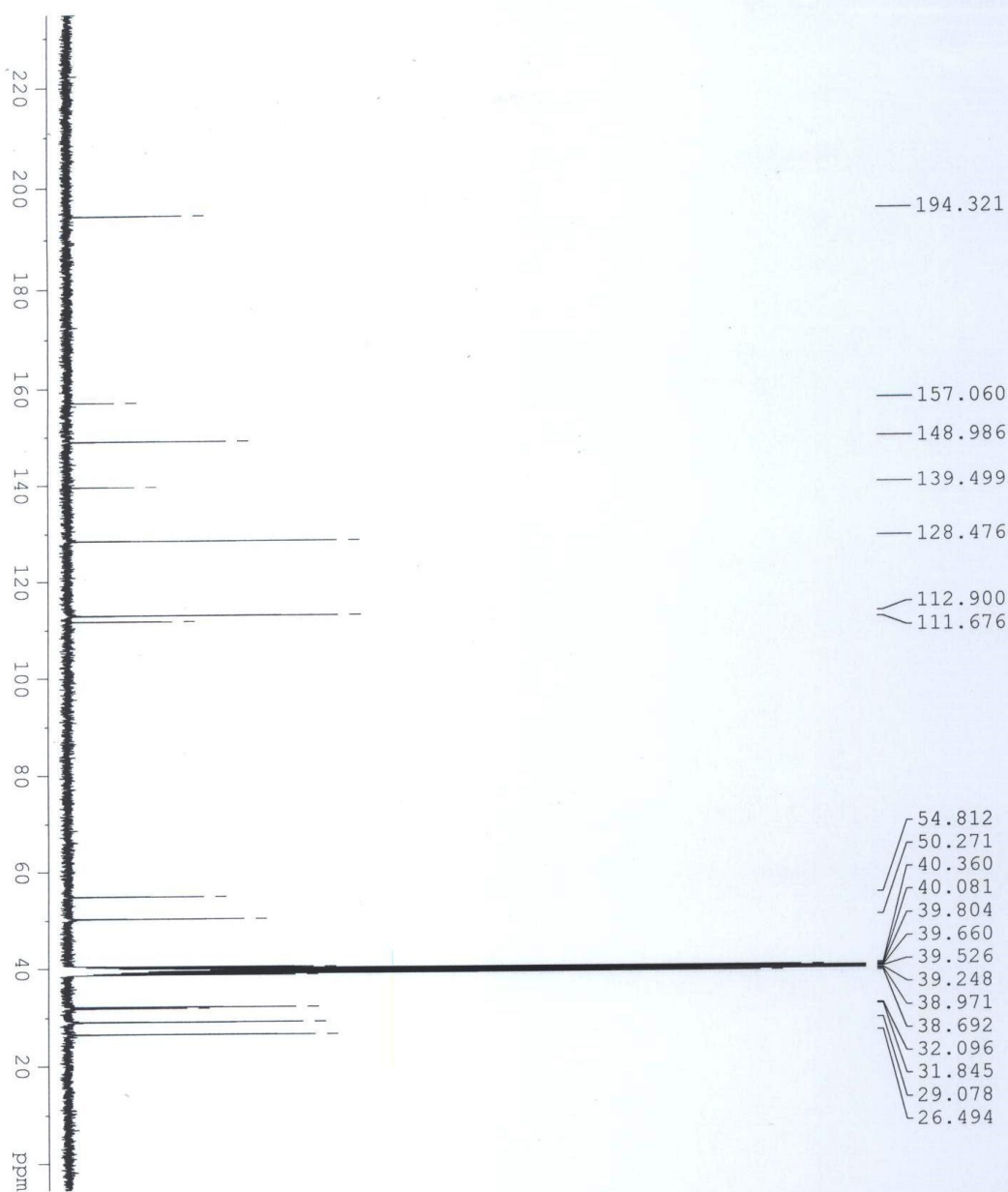






Supplementary Information (SI)





NAFEES/DR, ABDUL HAMEED/NF-OX7C-dd-pp/
BB/

AVANCE AV-300
LAB NO: 108

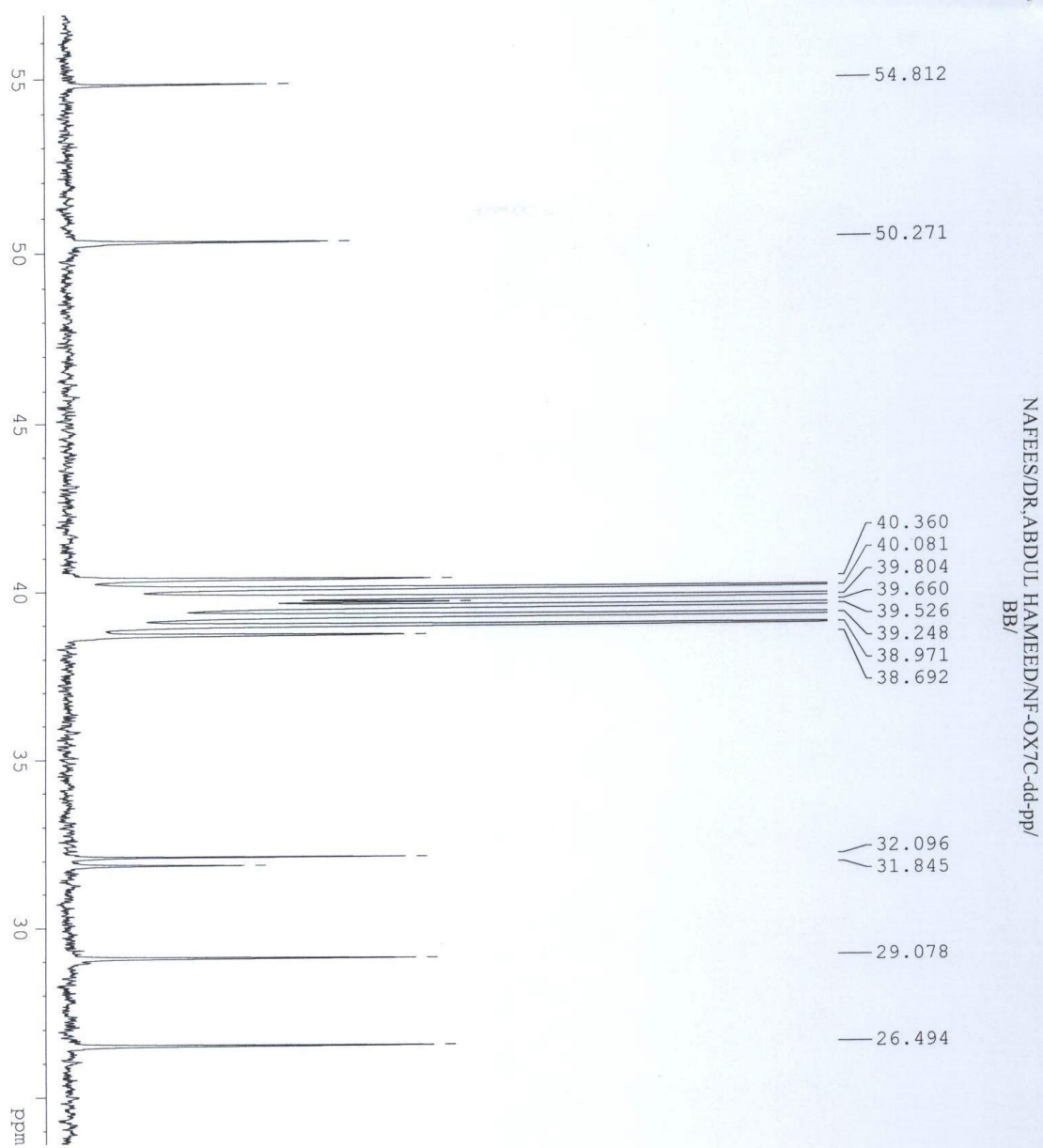
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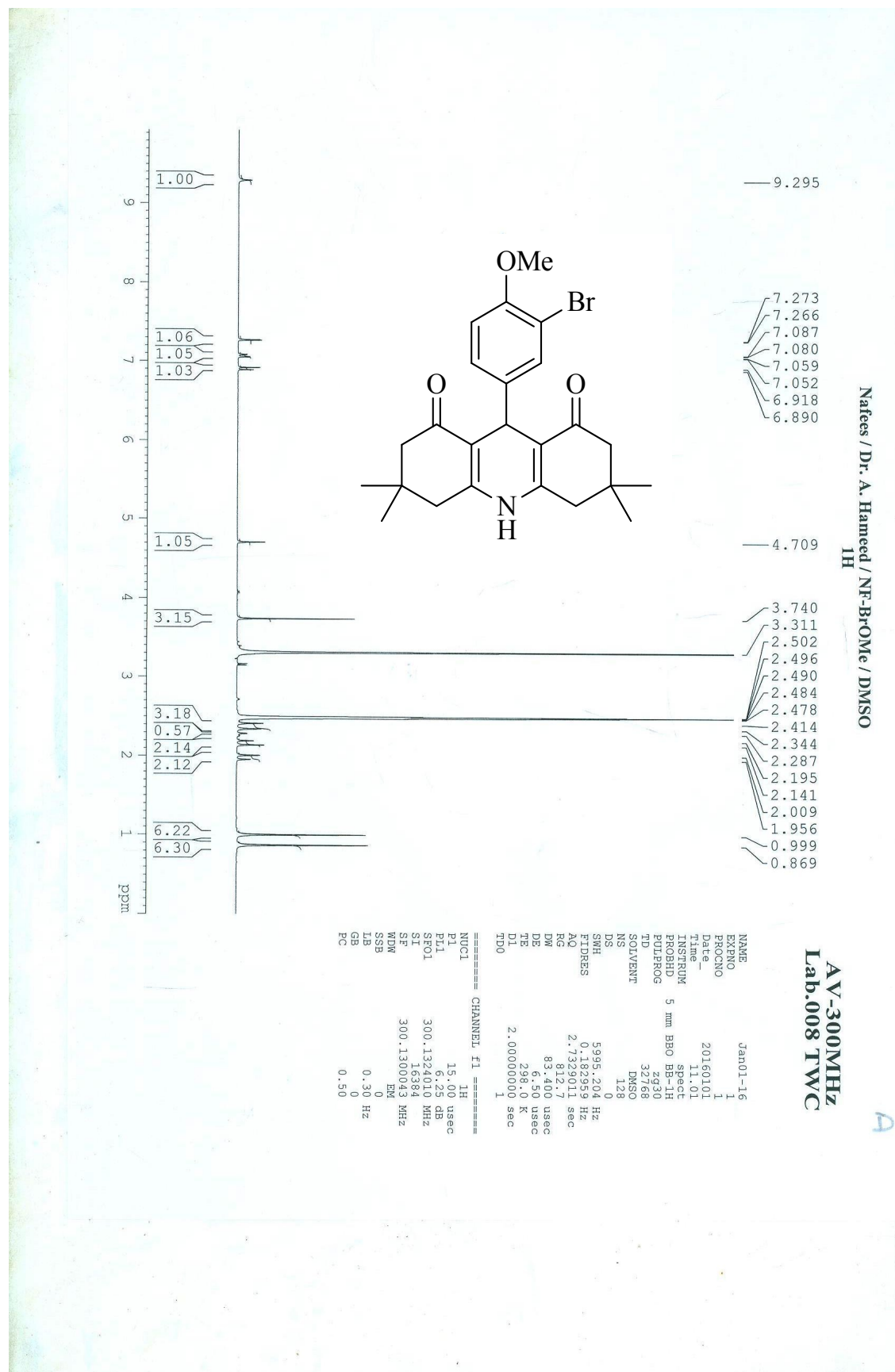
NAME          may12-16
EXPNO         1
PROCNO        1
Date_         20160512
Time_         13.45
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       zgpg
TD            32768
SOLVENT       DMSO
NS            18432
DS            2
SWH            18115.941 Hz
FIDRES        0.552855 Hz
AQ            0.9044468 sec
RG            32768
DW            27.600 usec
DE            6.50 usec
TE            300.0 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0           18

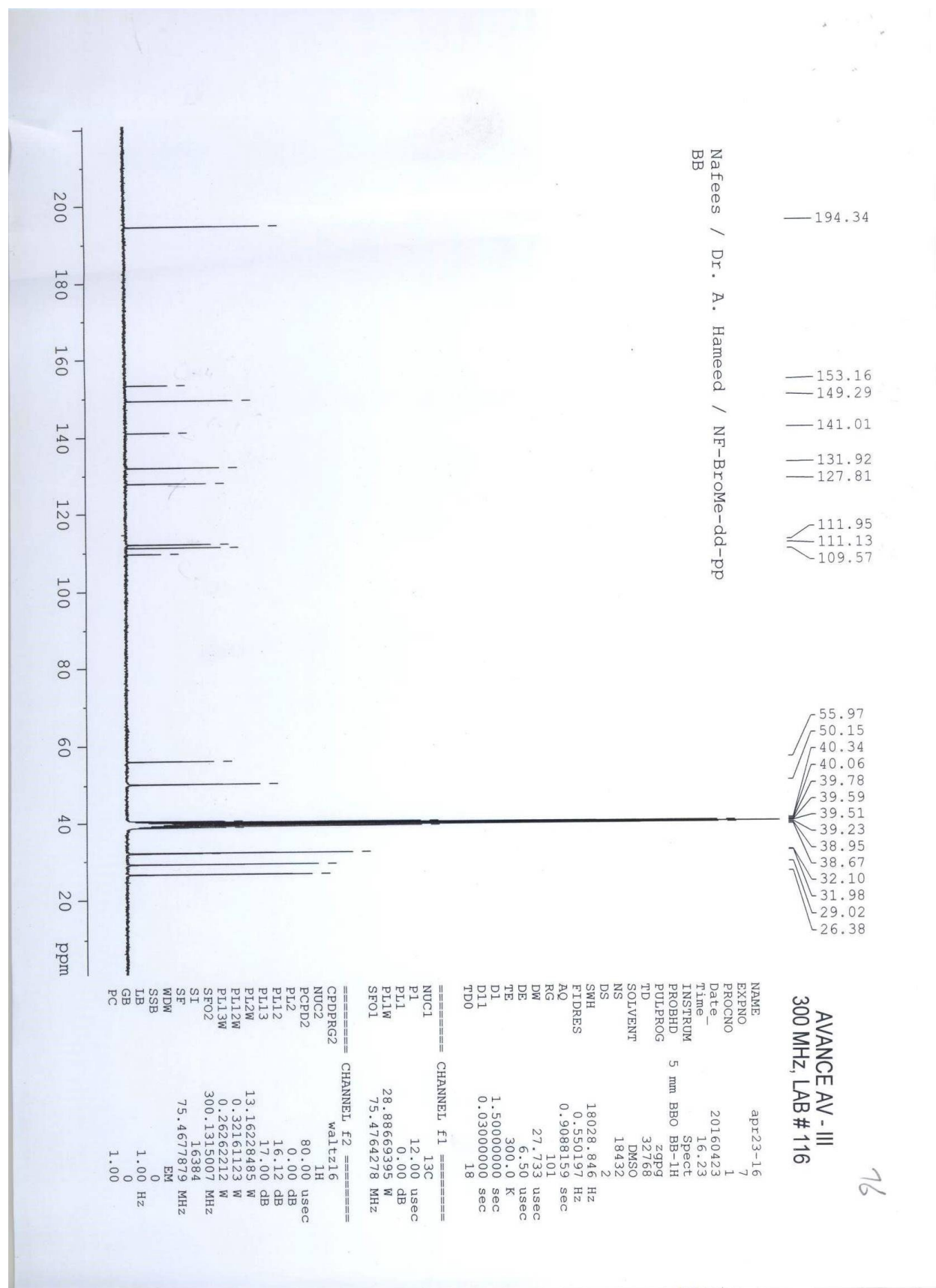
===== CHANNEL f1 =====
NUC1          13C
P1            10.10 usec
PL1           4.00 dB
SFO1          75.4764278 MHz

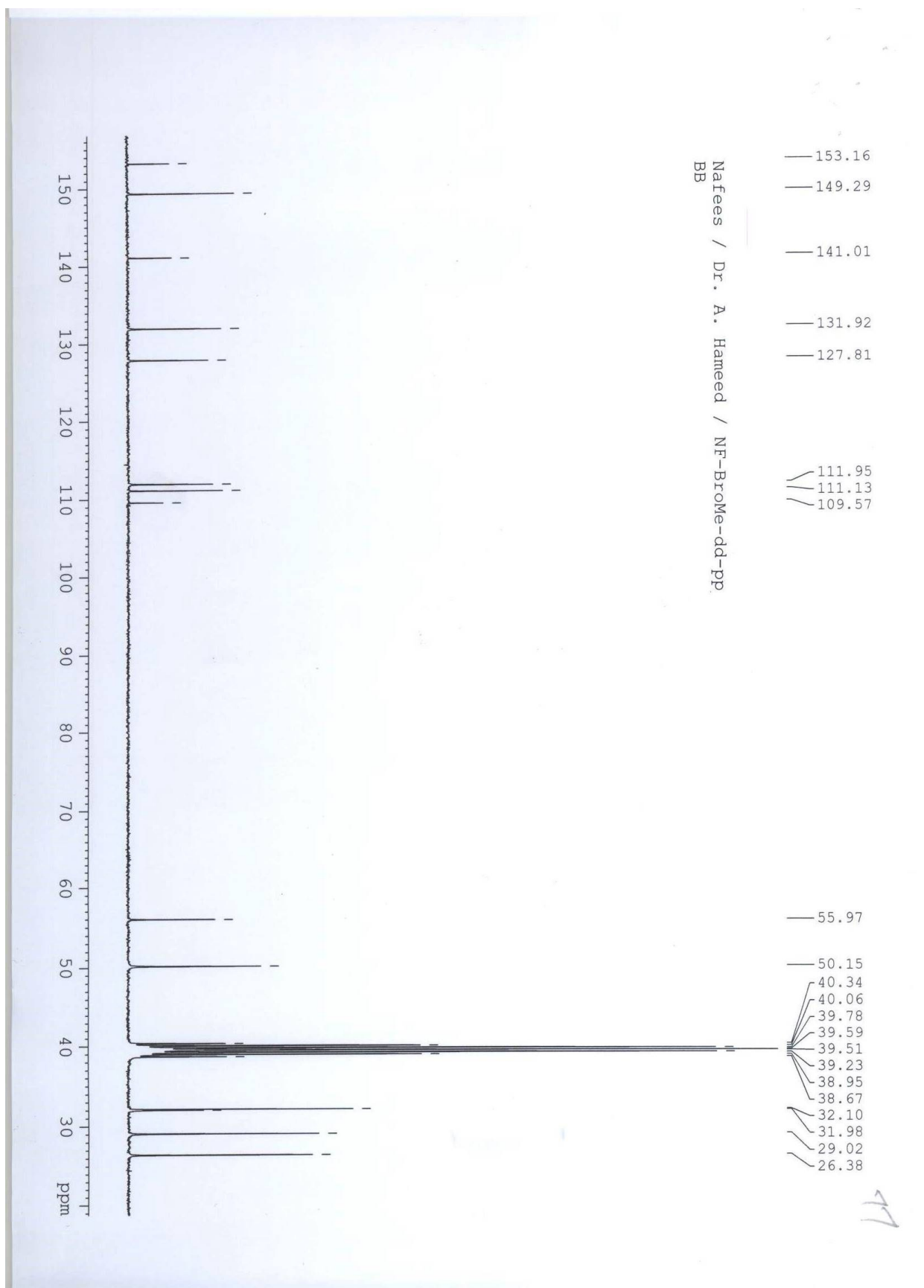
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           5.00 dB
PL12          20.92 dB
PL13          19.00 dB
SFO2          300.1318008 MHz
SI            32768
SF            75.4677856 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            0.10
  
```

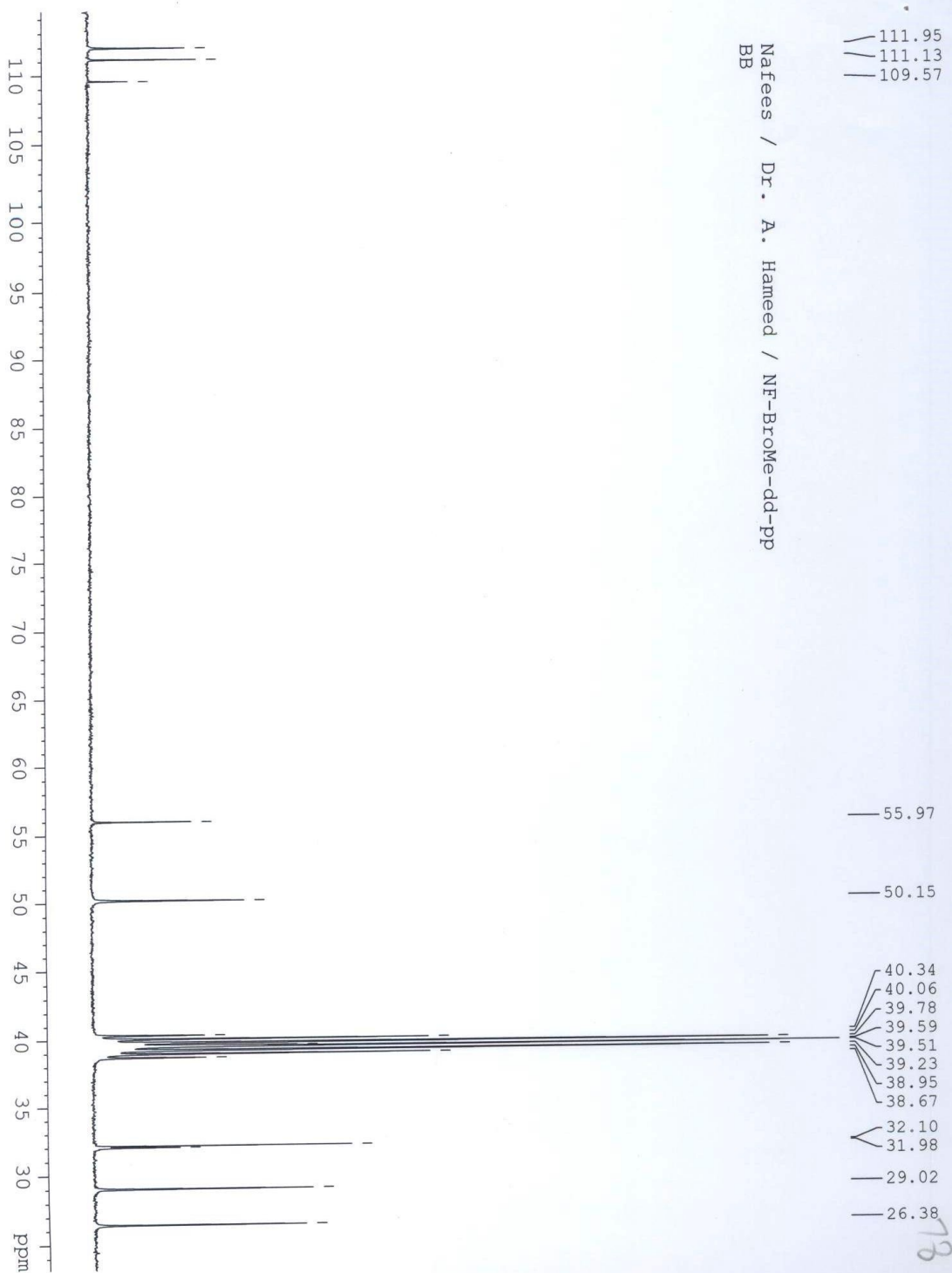
Supplementary Information (SI)

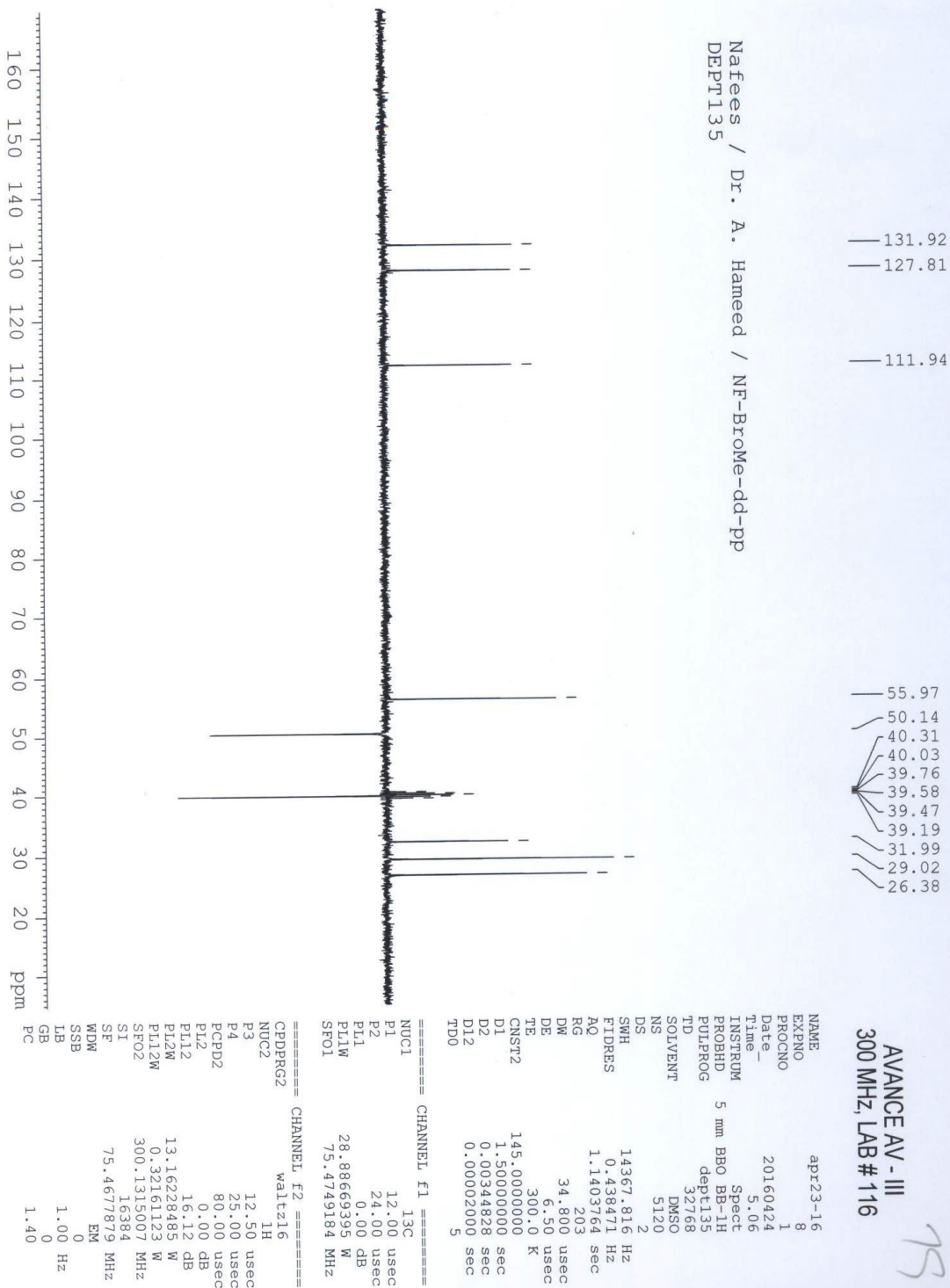


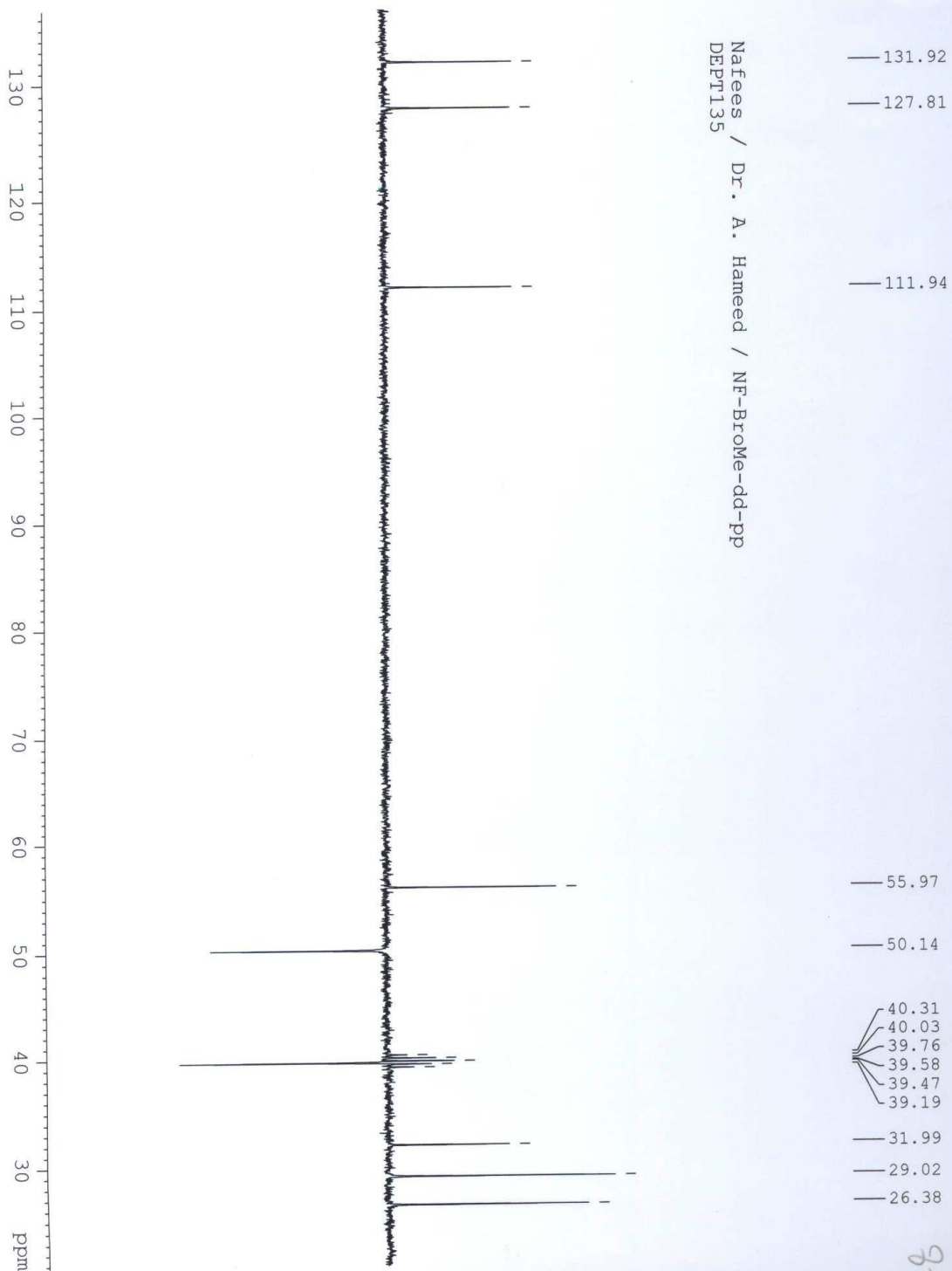


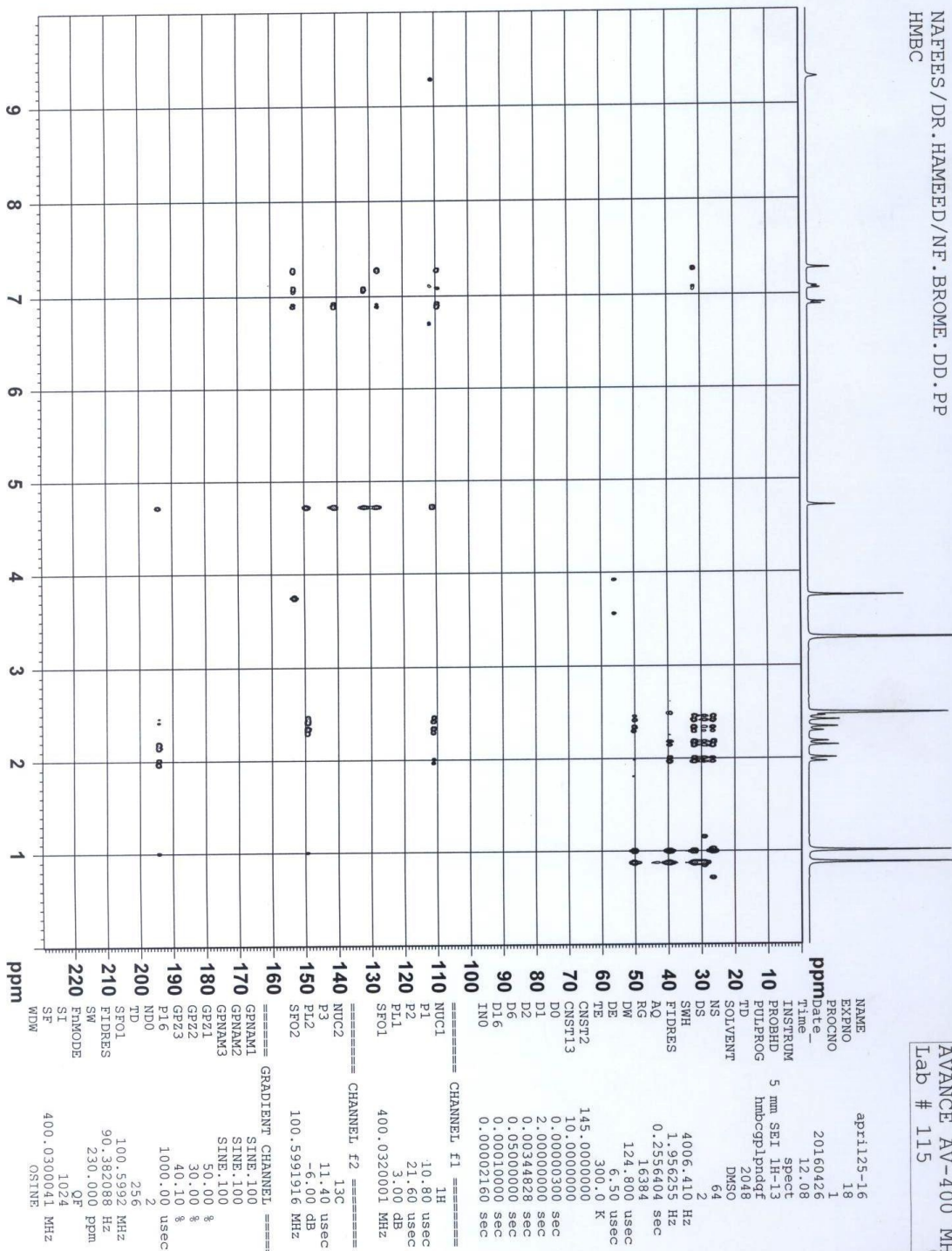




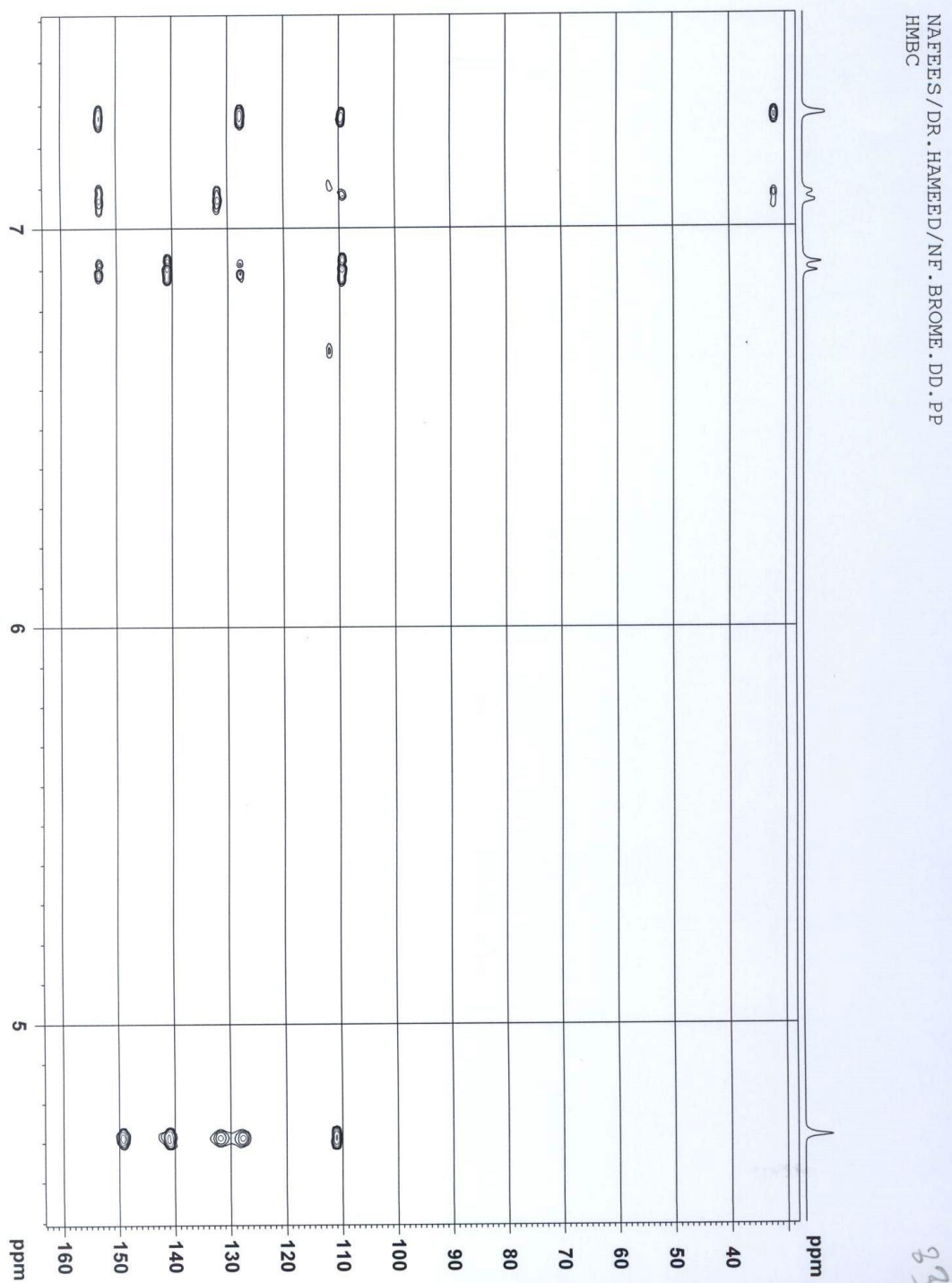


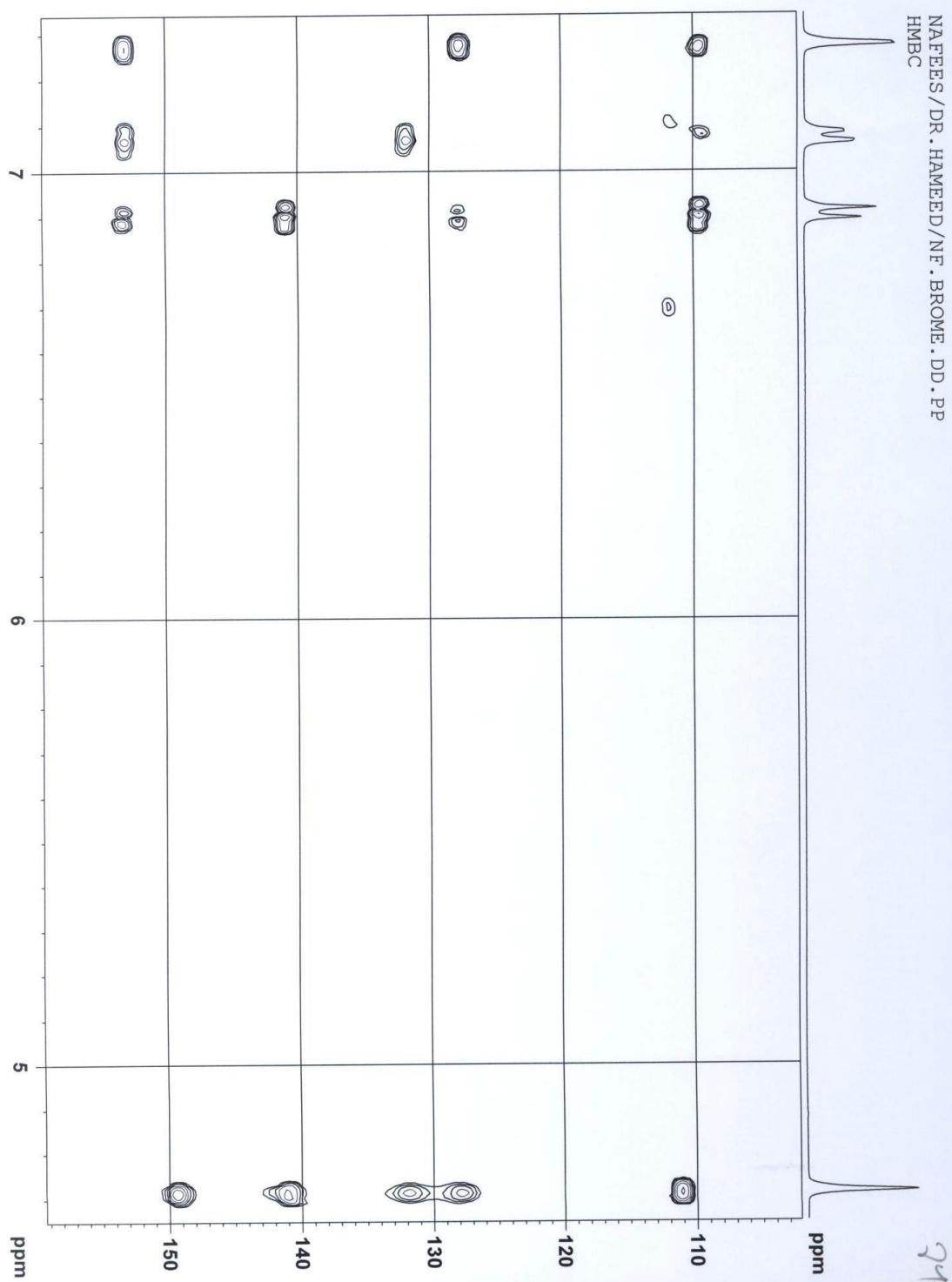


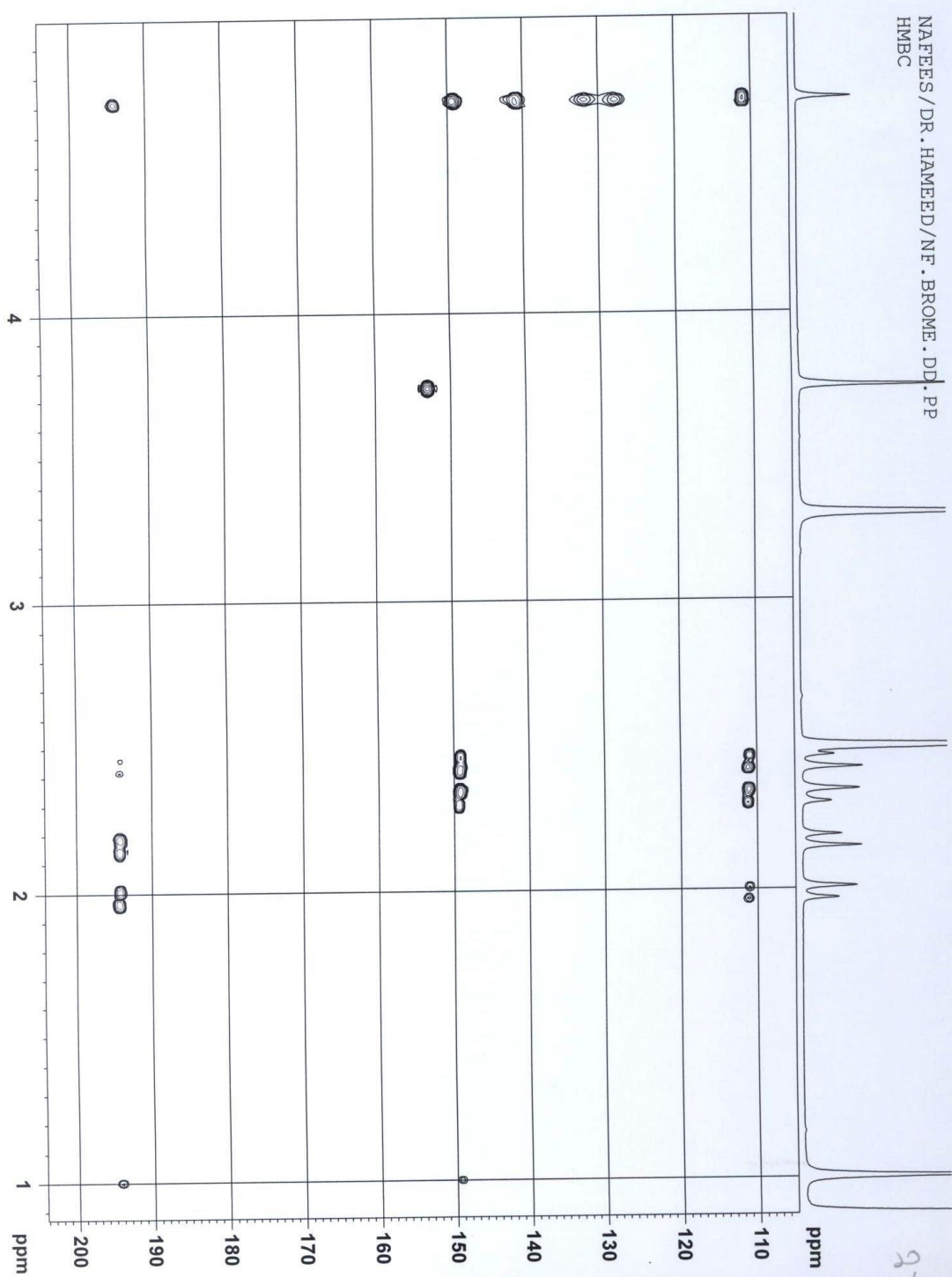


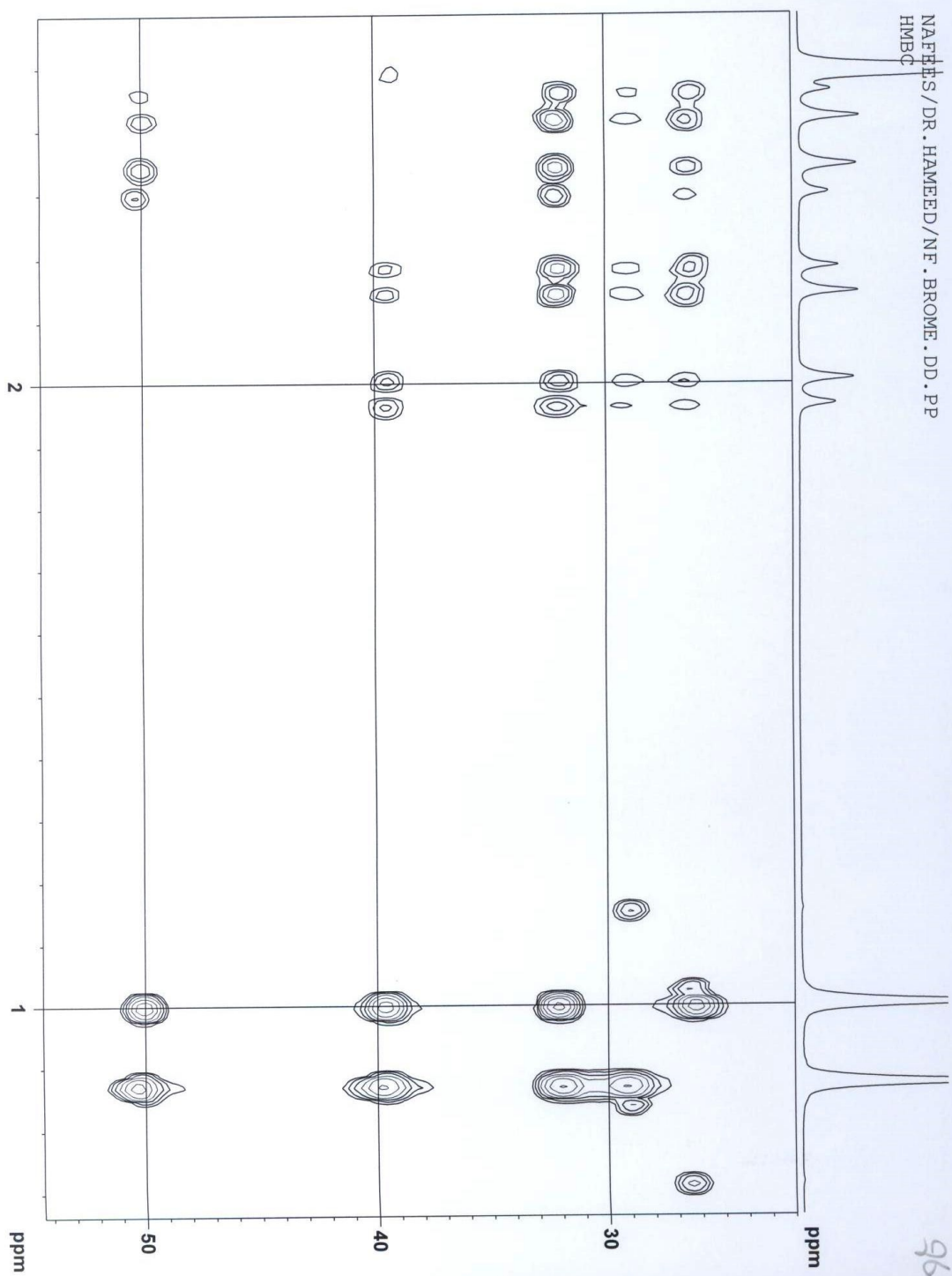


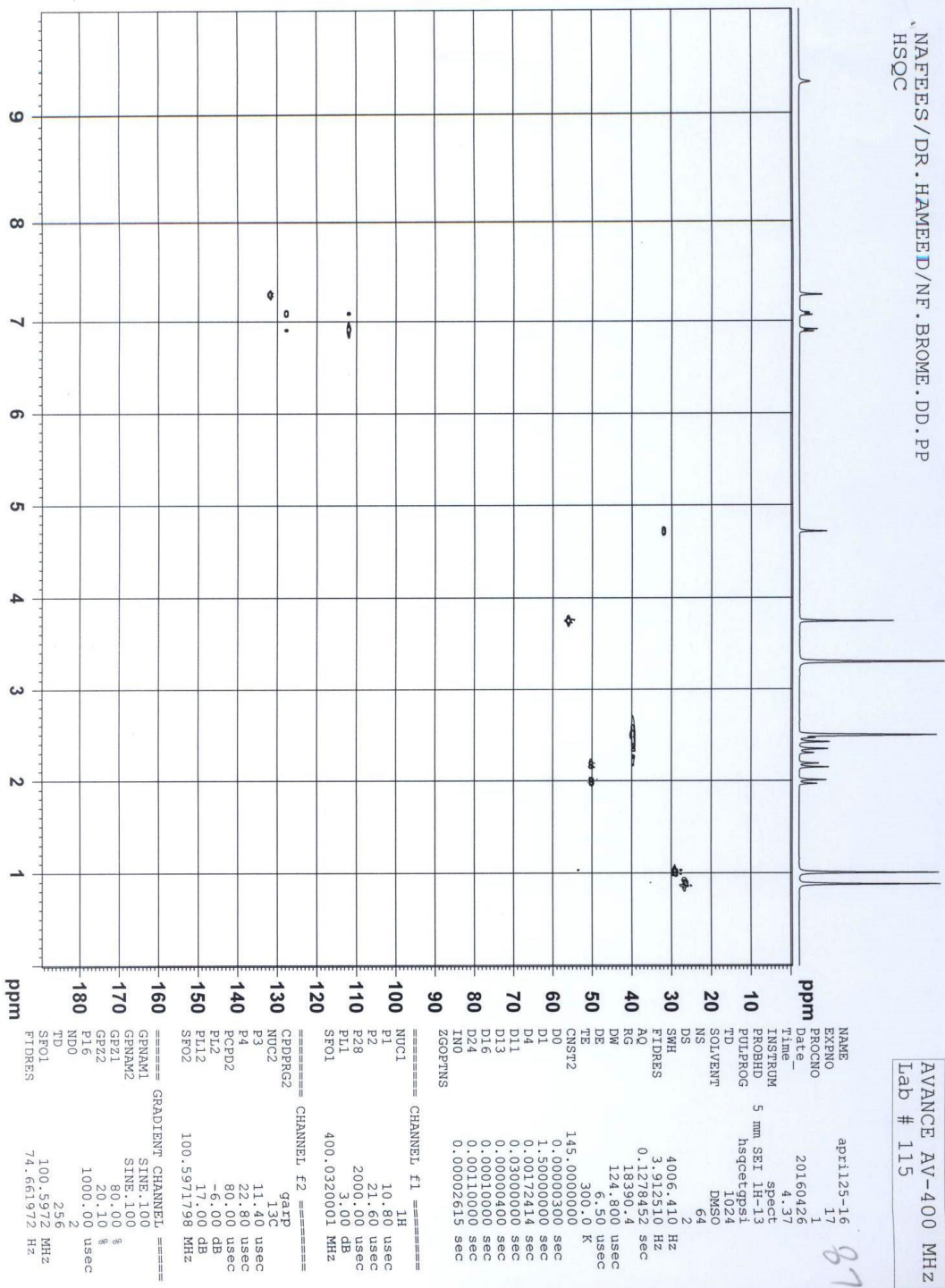


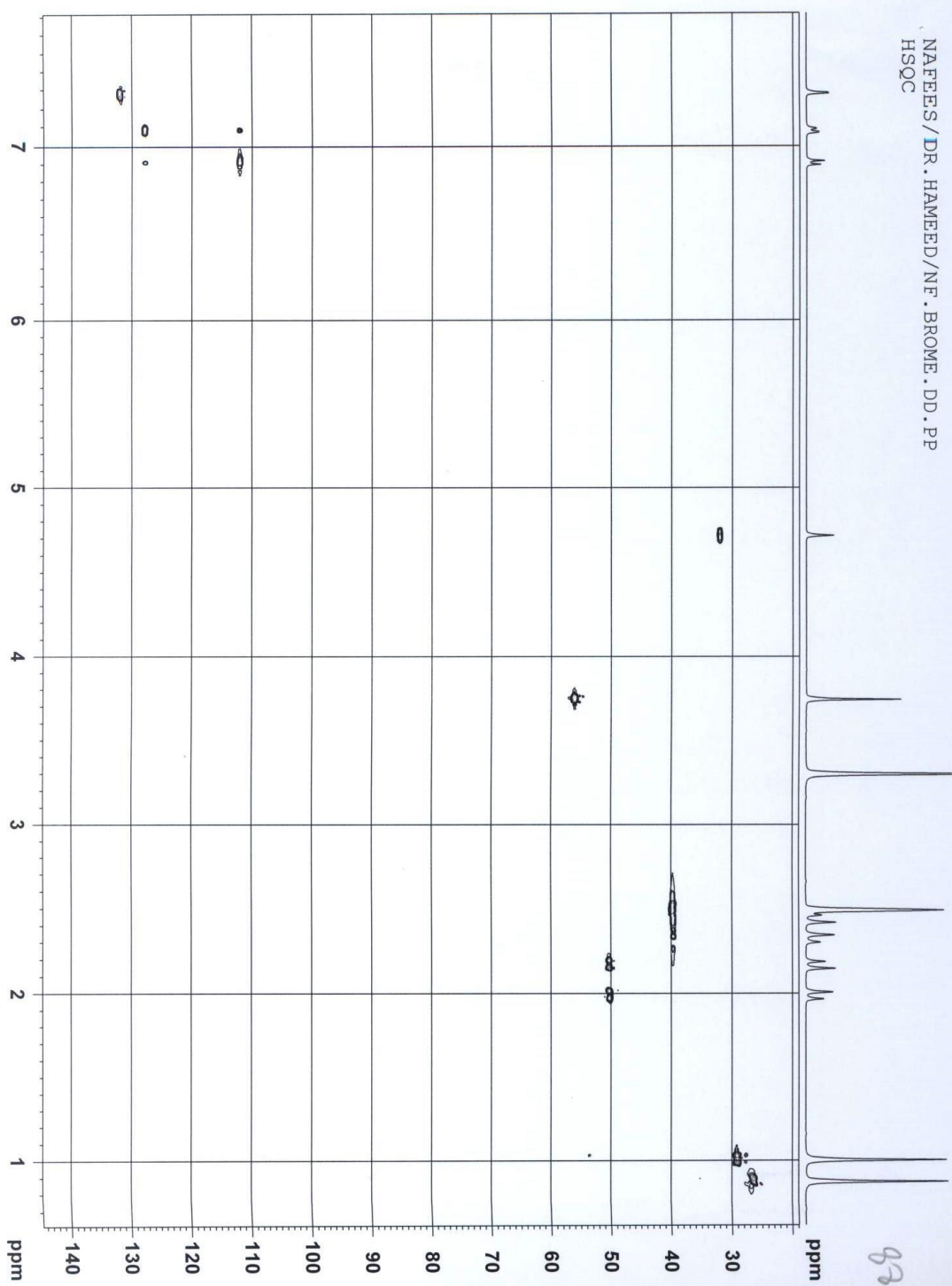




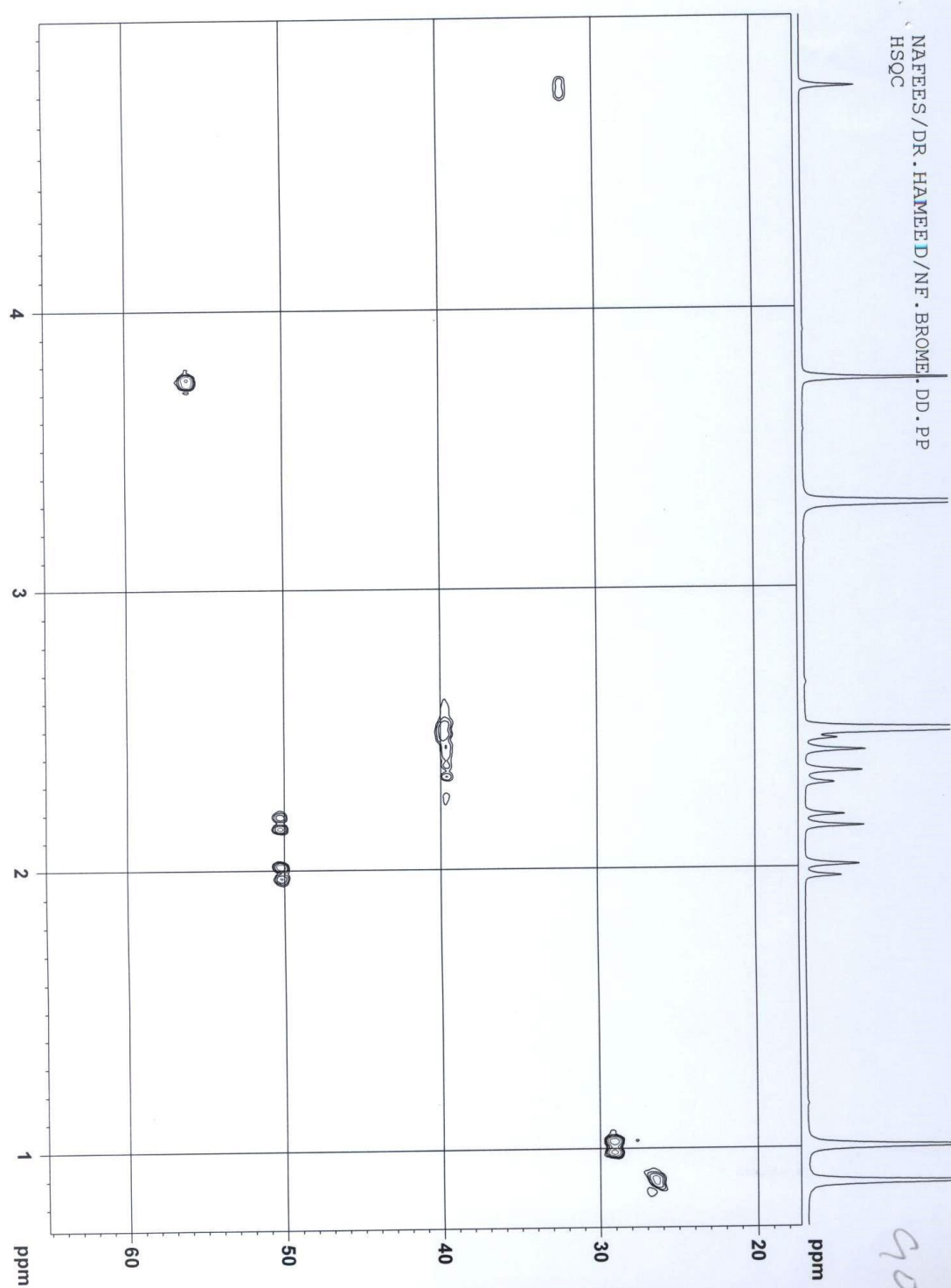


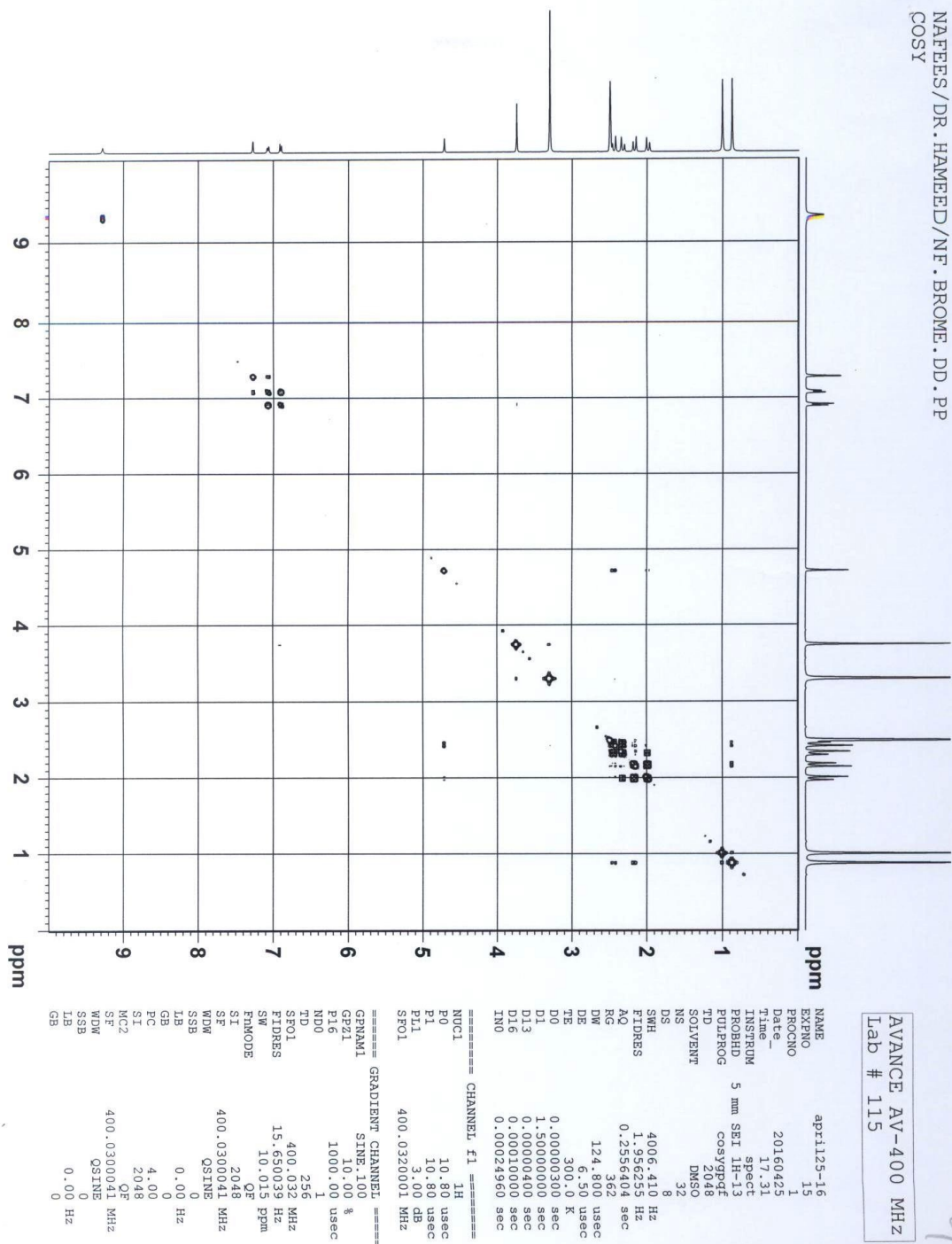


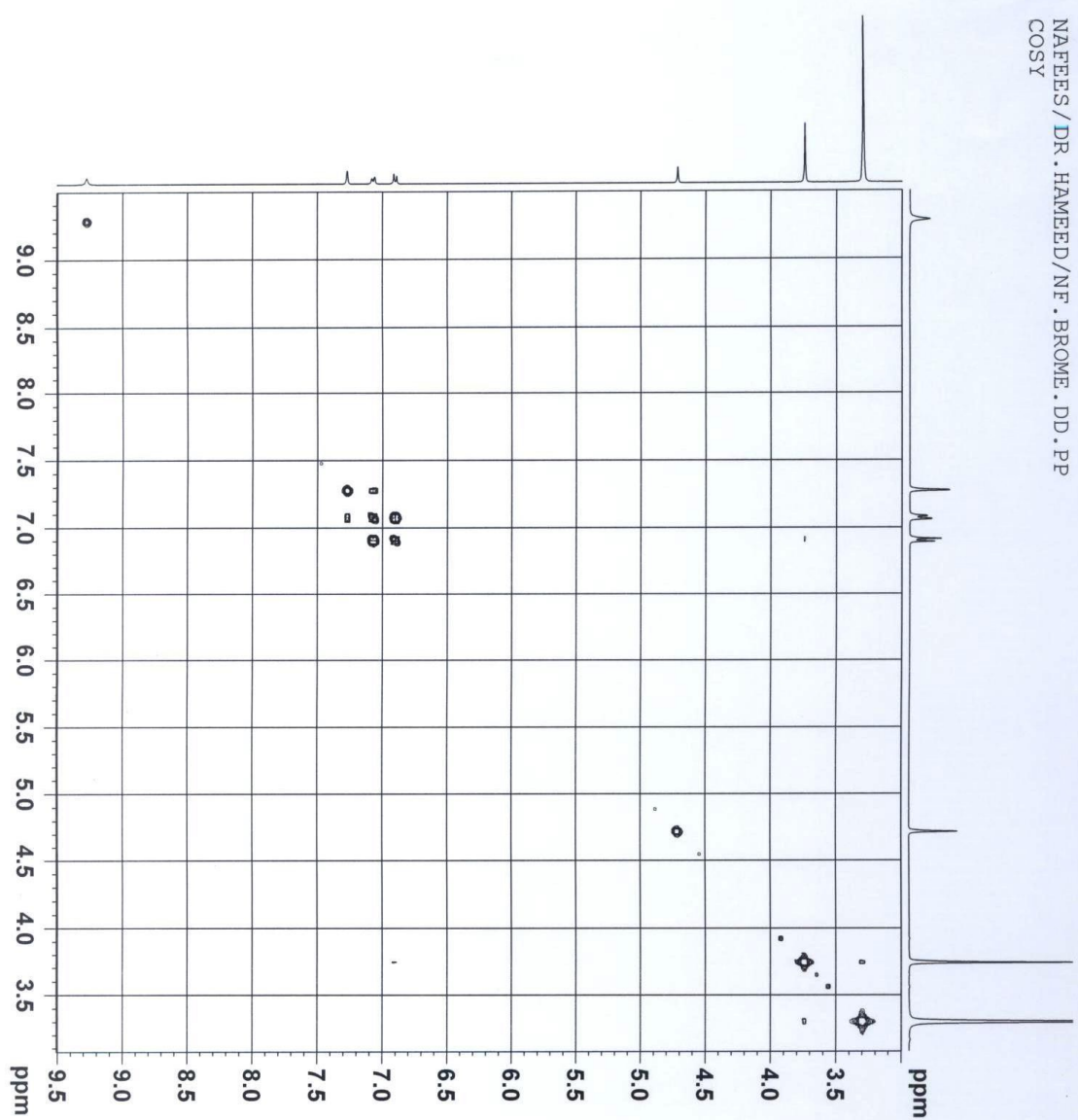




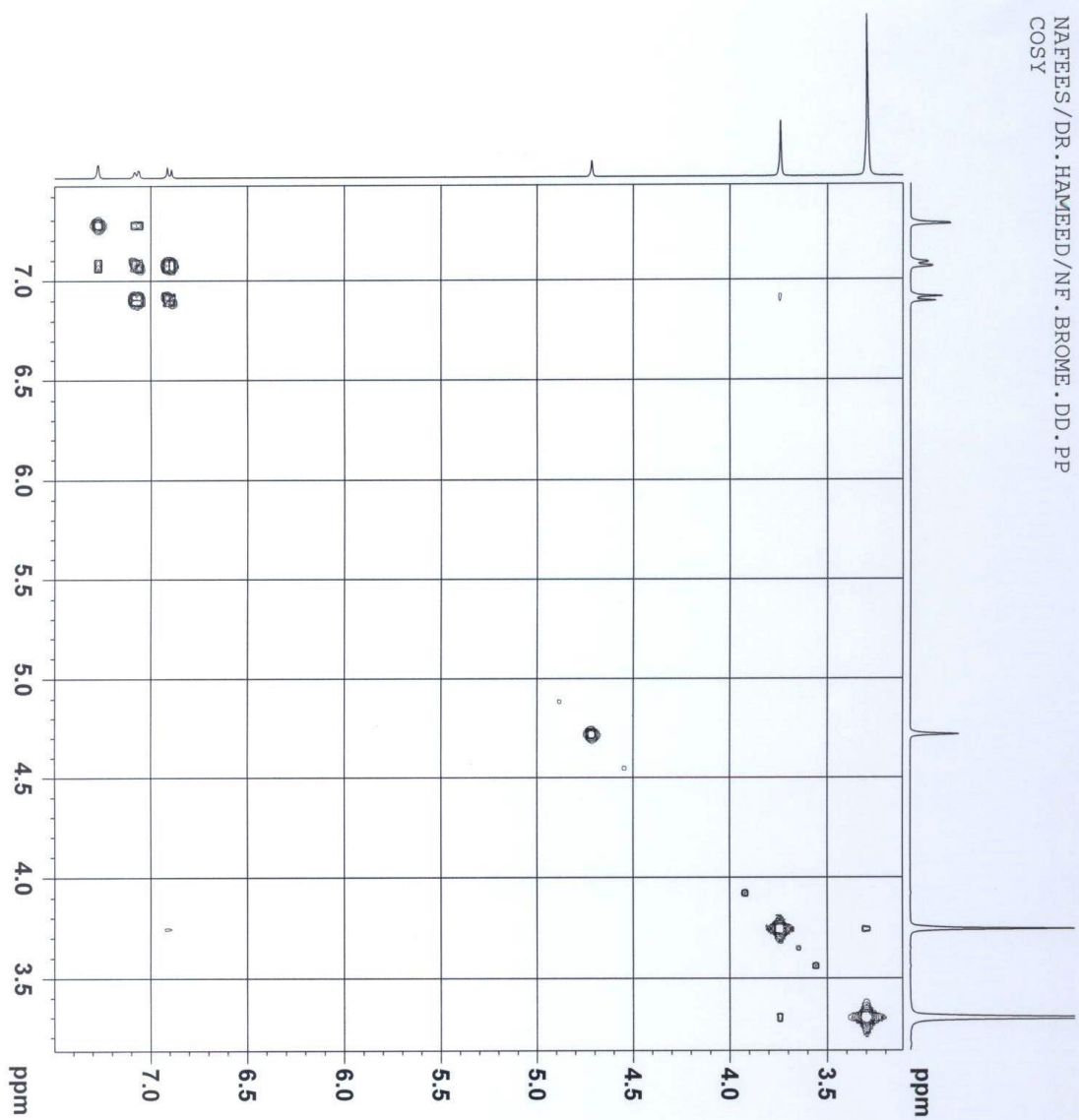




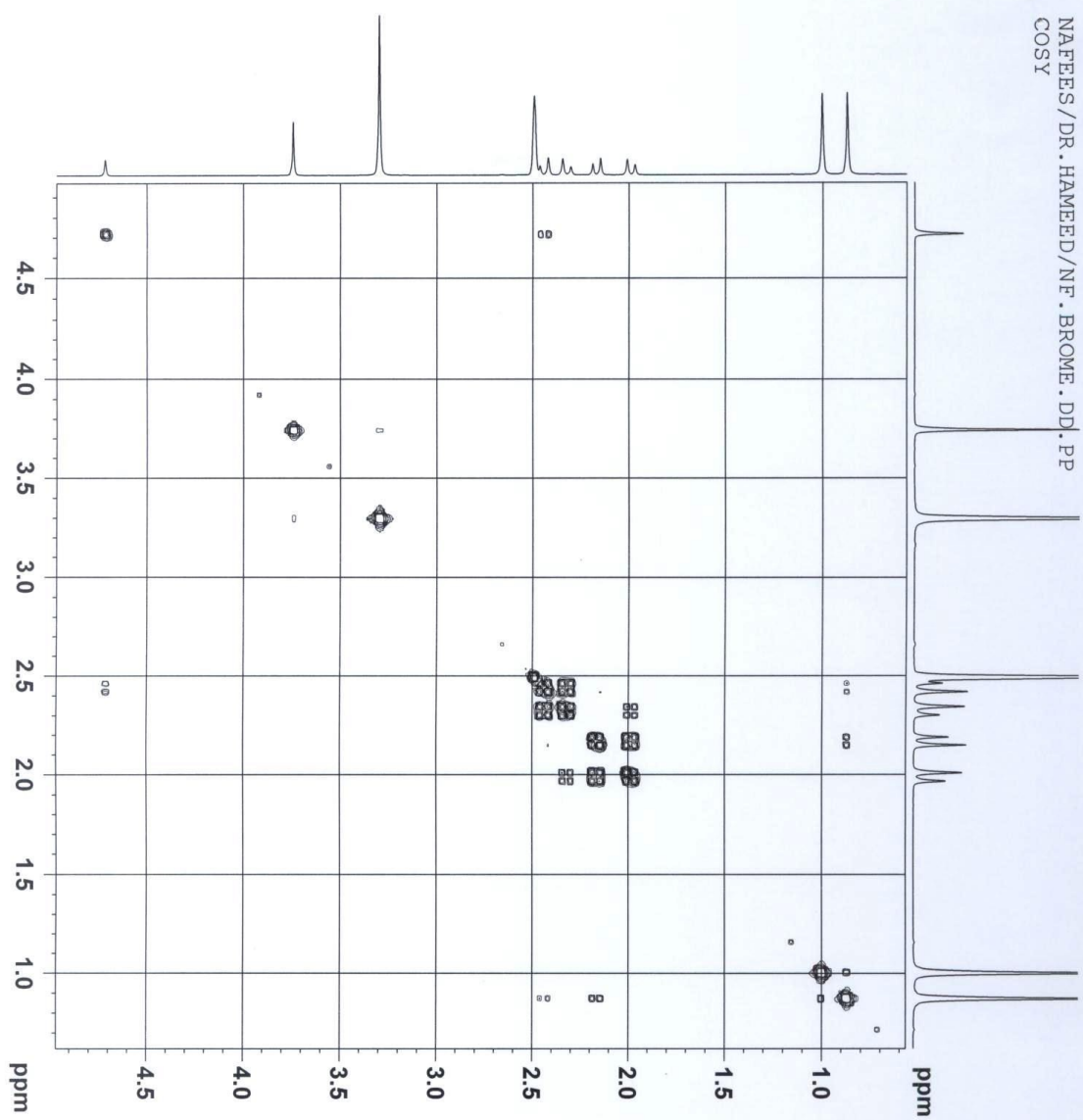


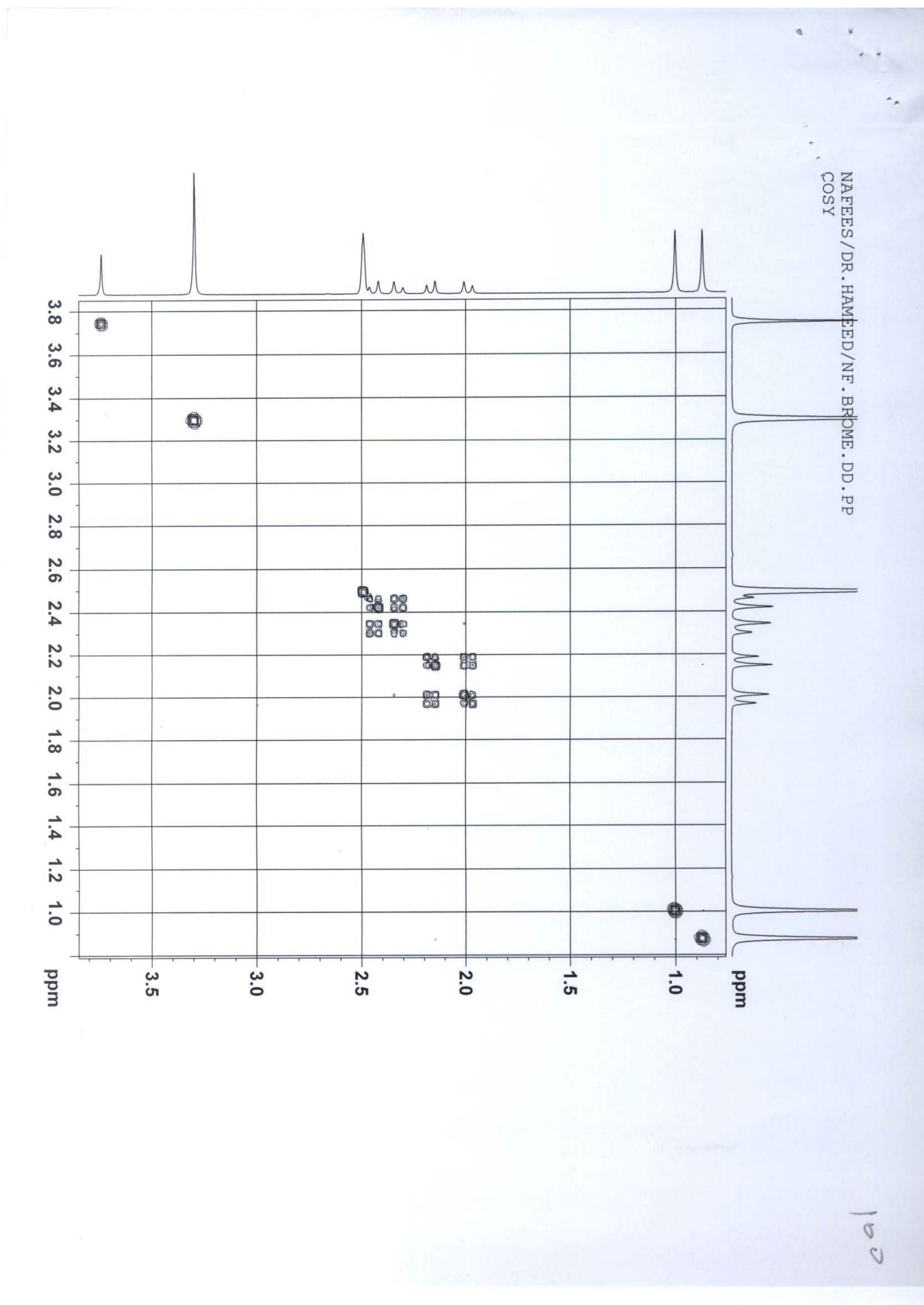


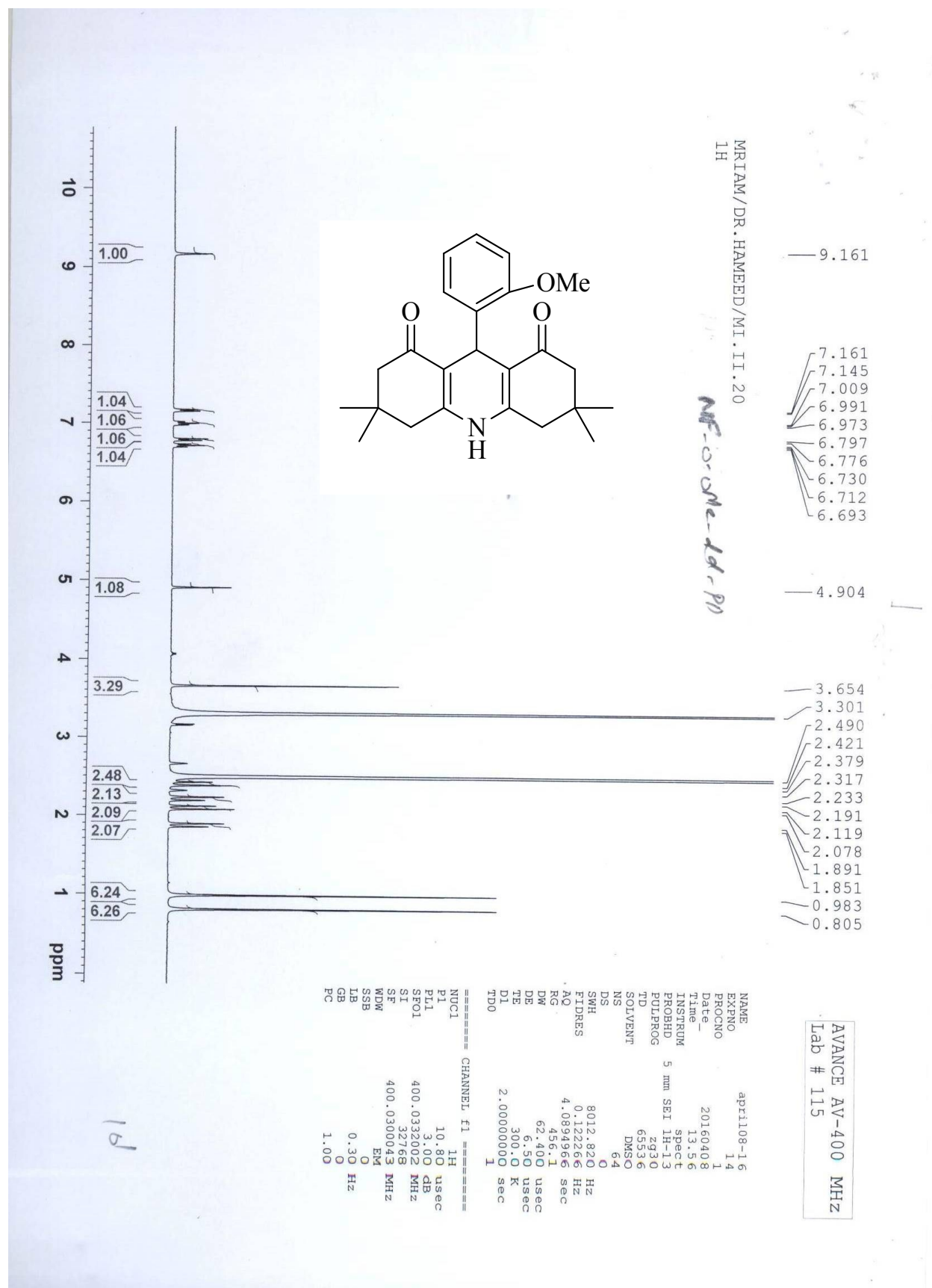
97



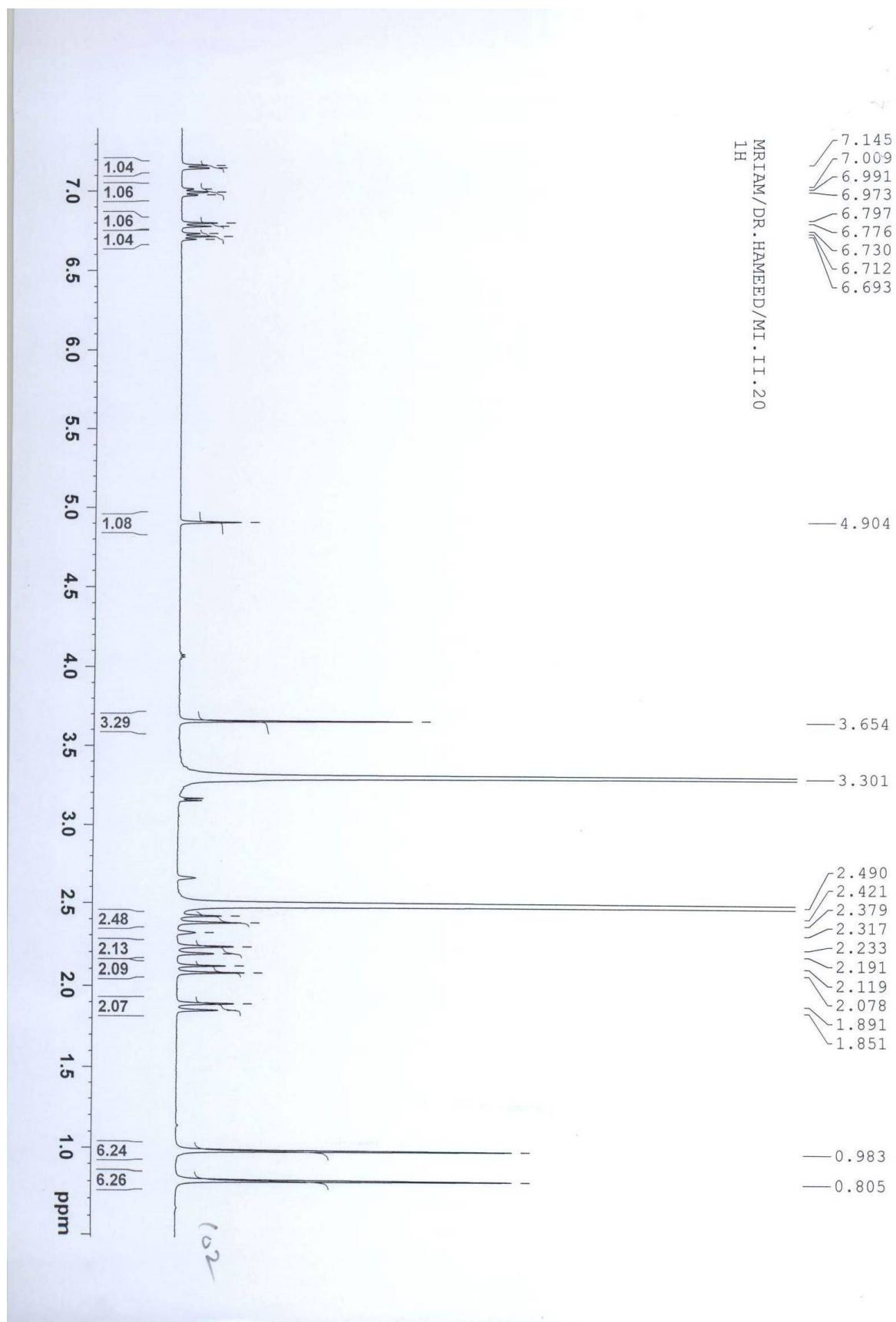
98



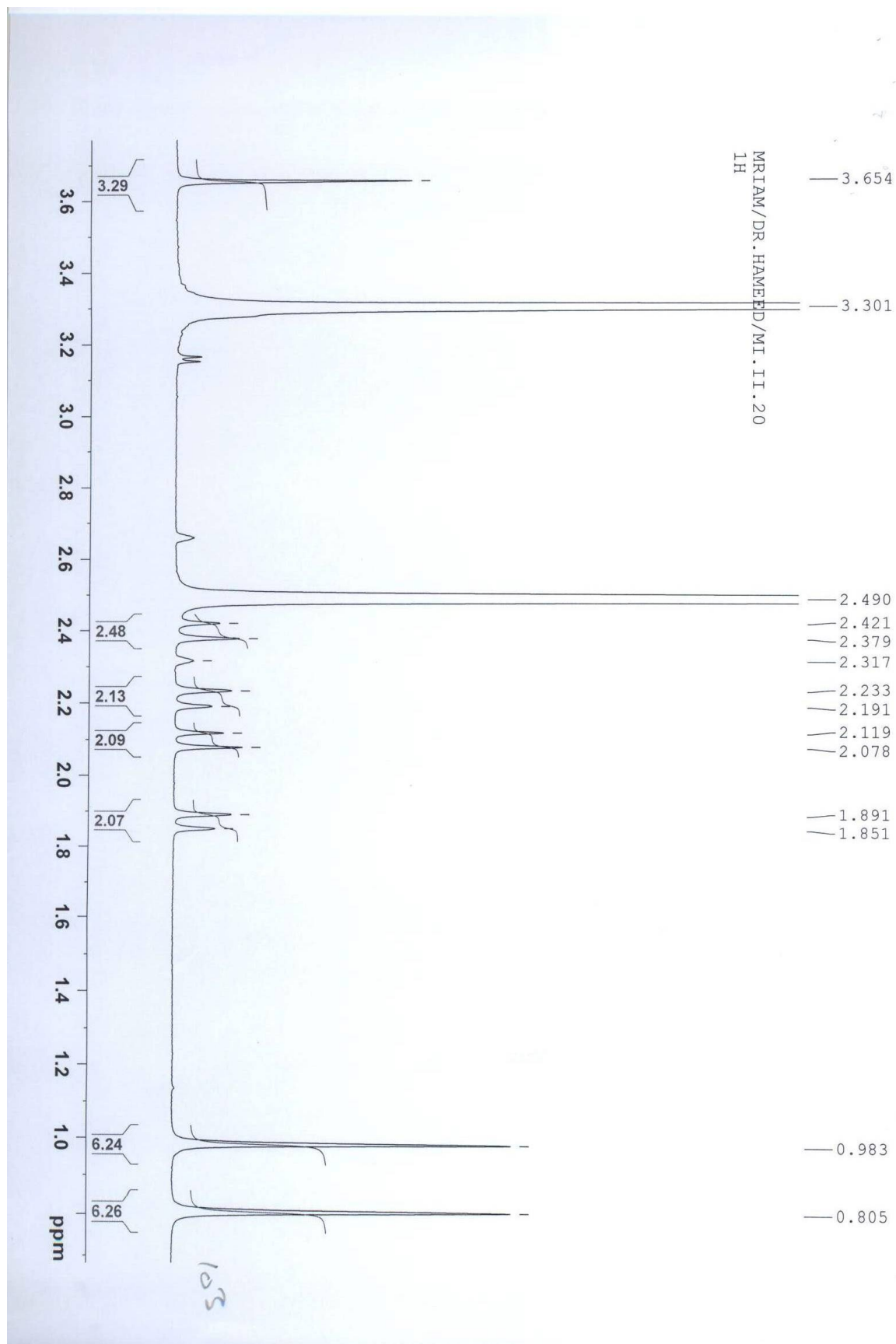




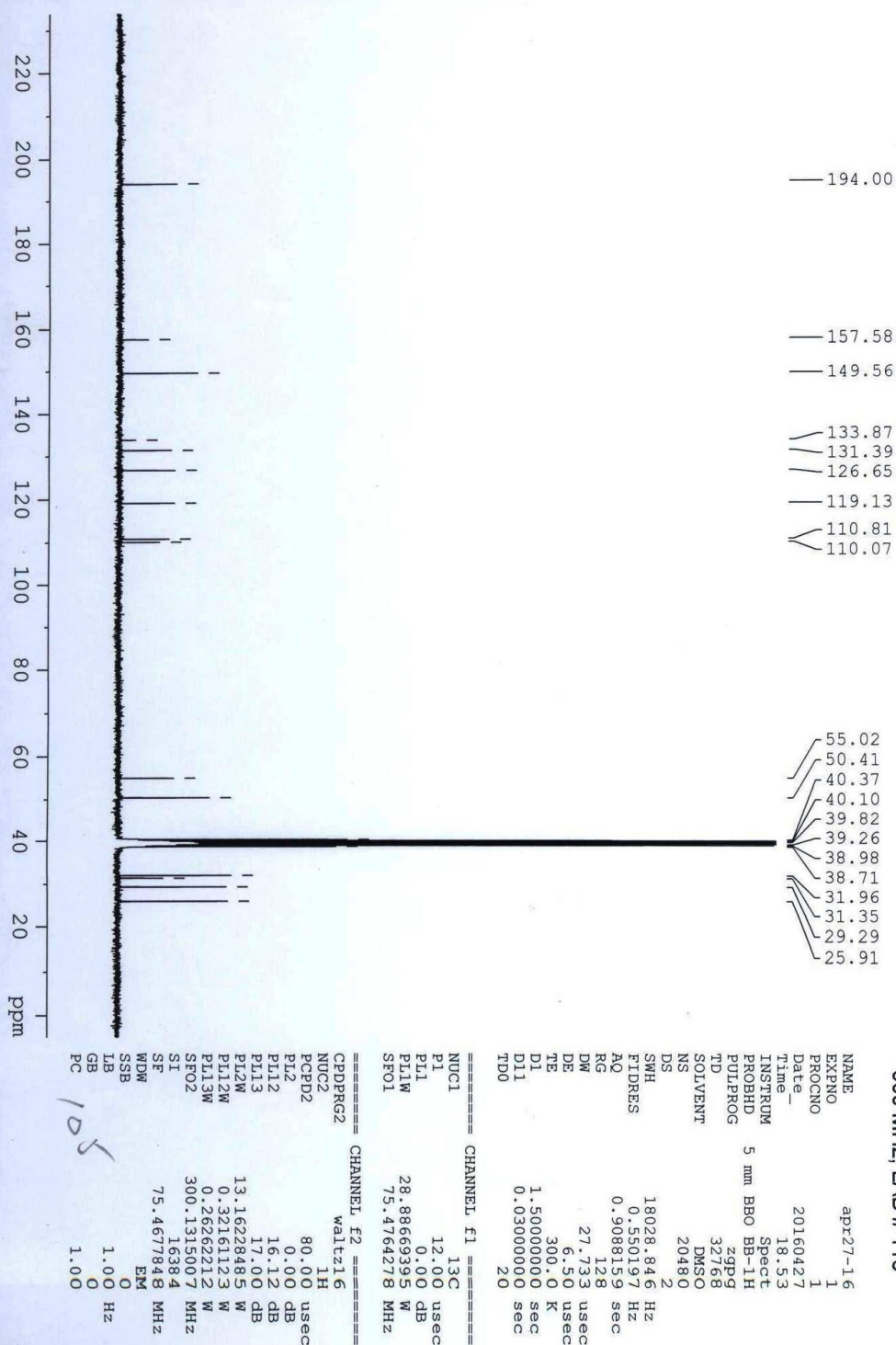
Supplementary Information (SI)

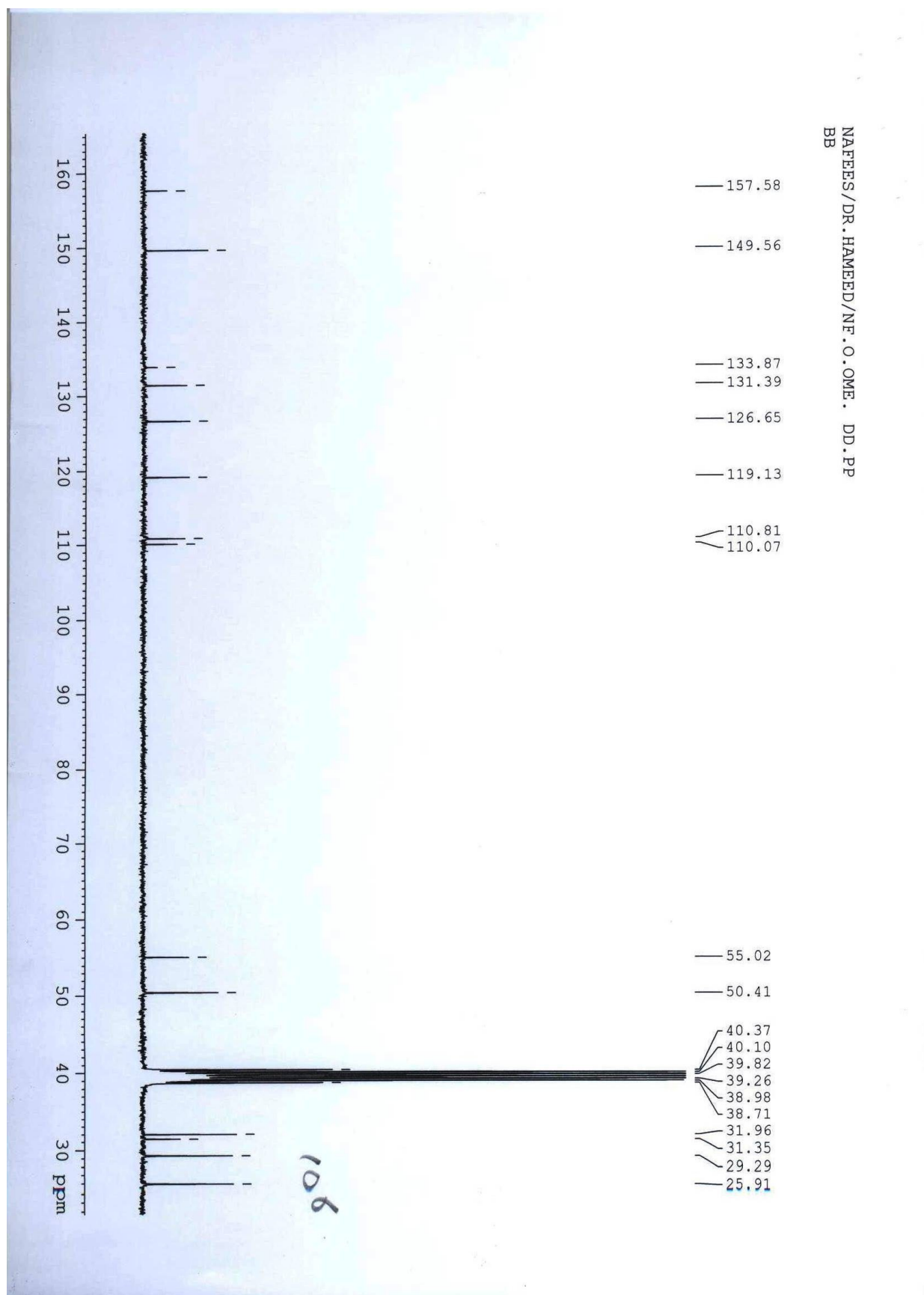


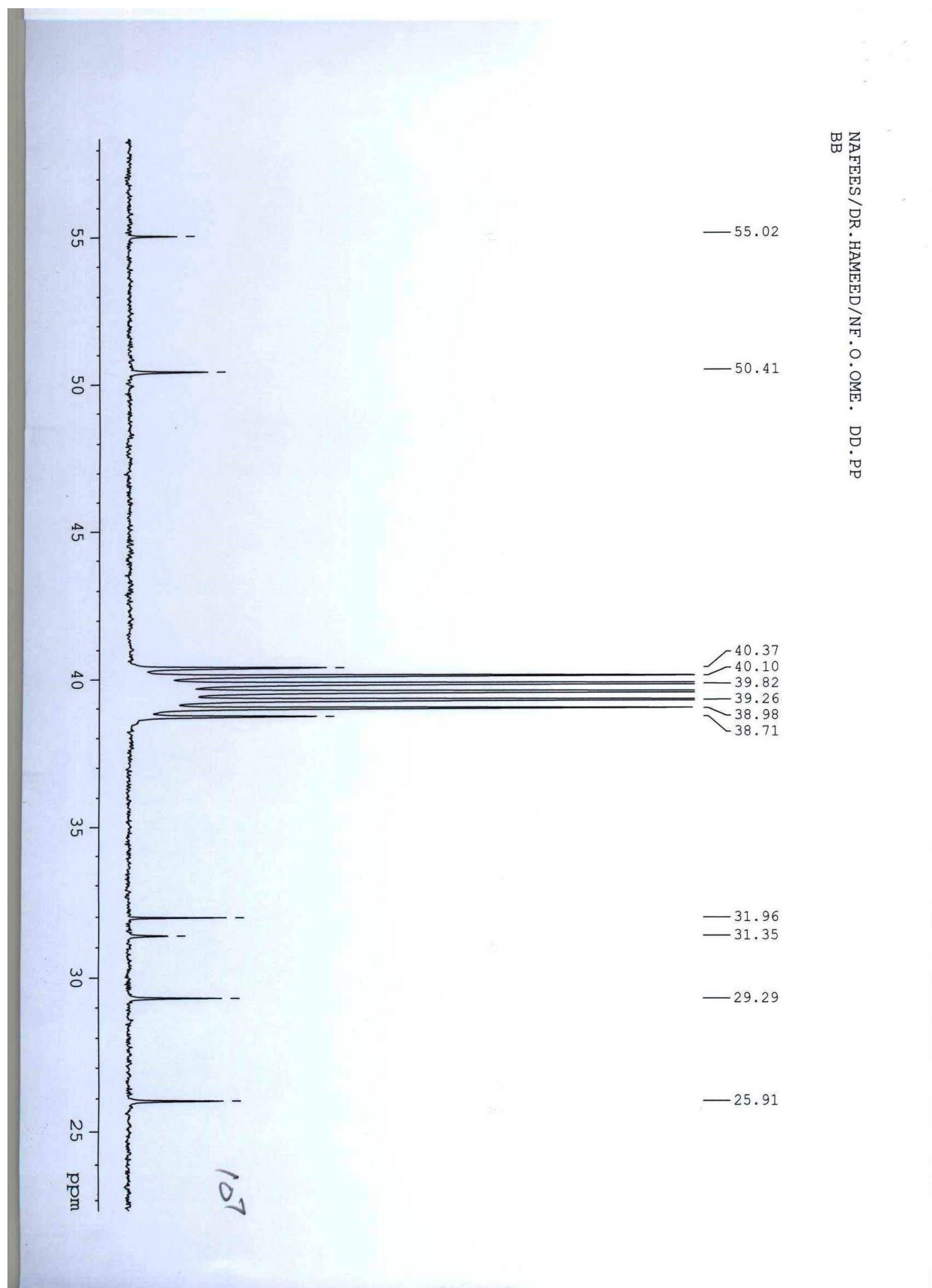
Supplementary Information (SI)

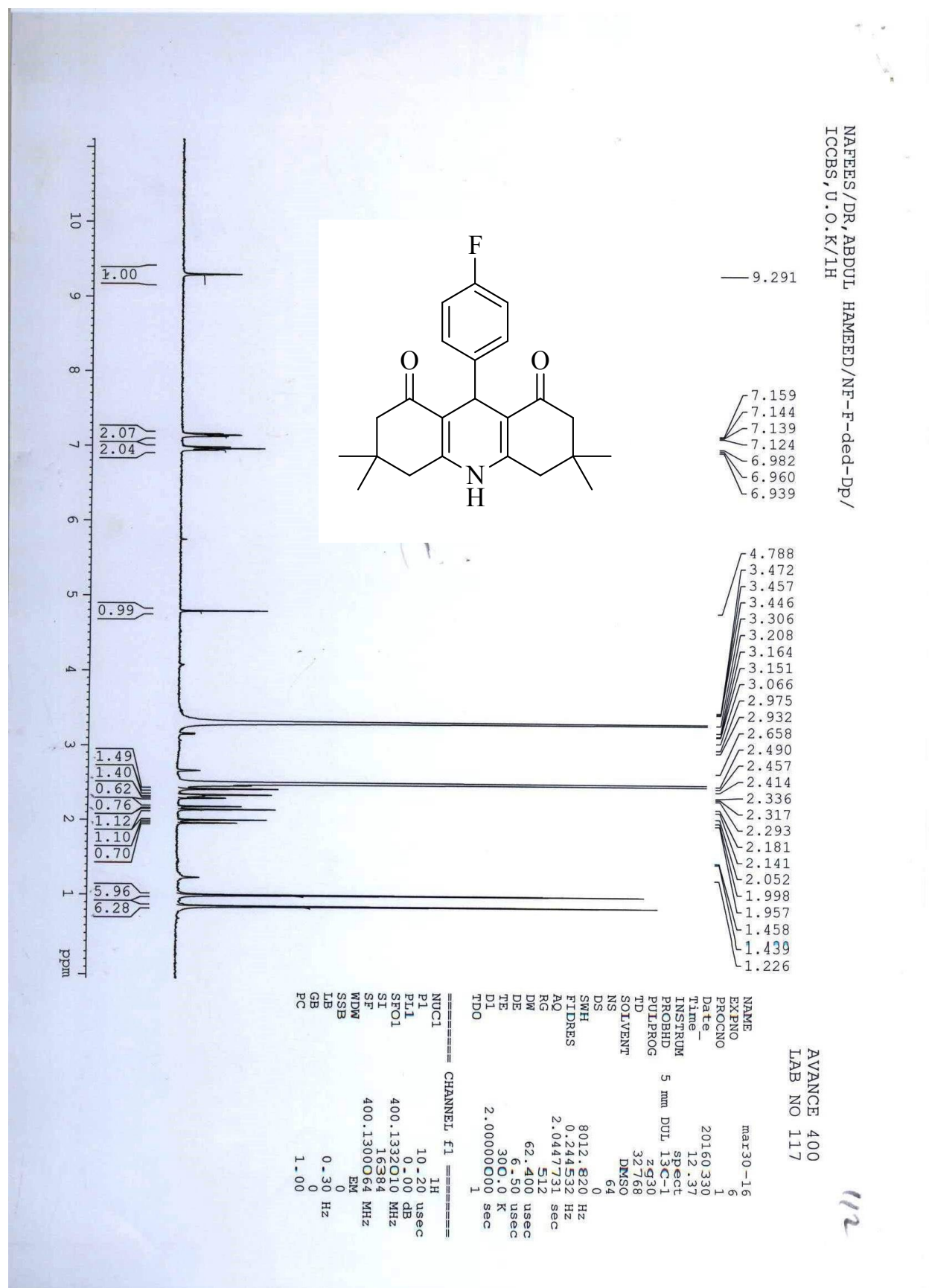


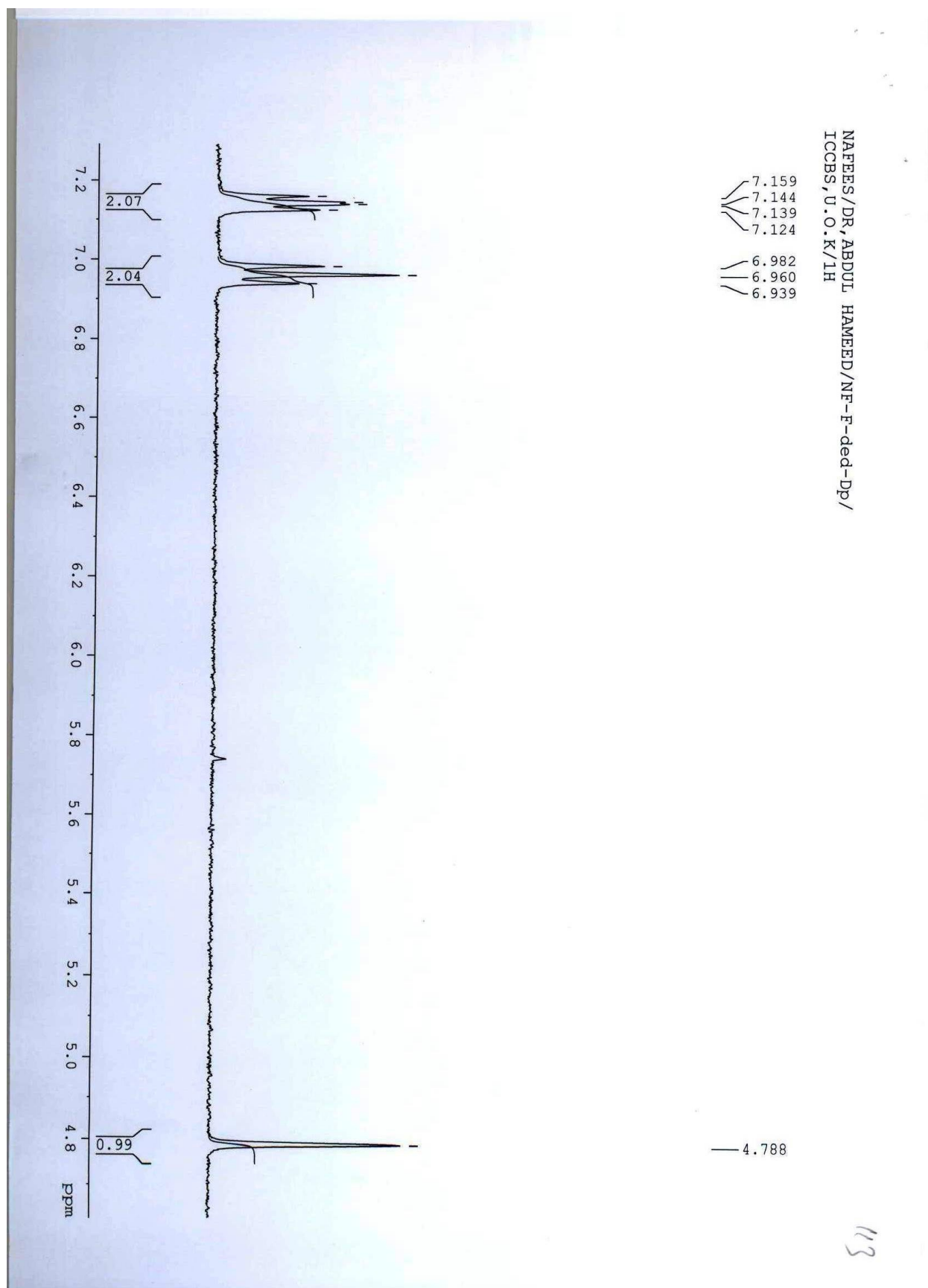
NAFEES/DR.HAMEED/NF.O.OME. DD.PP
BB

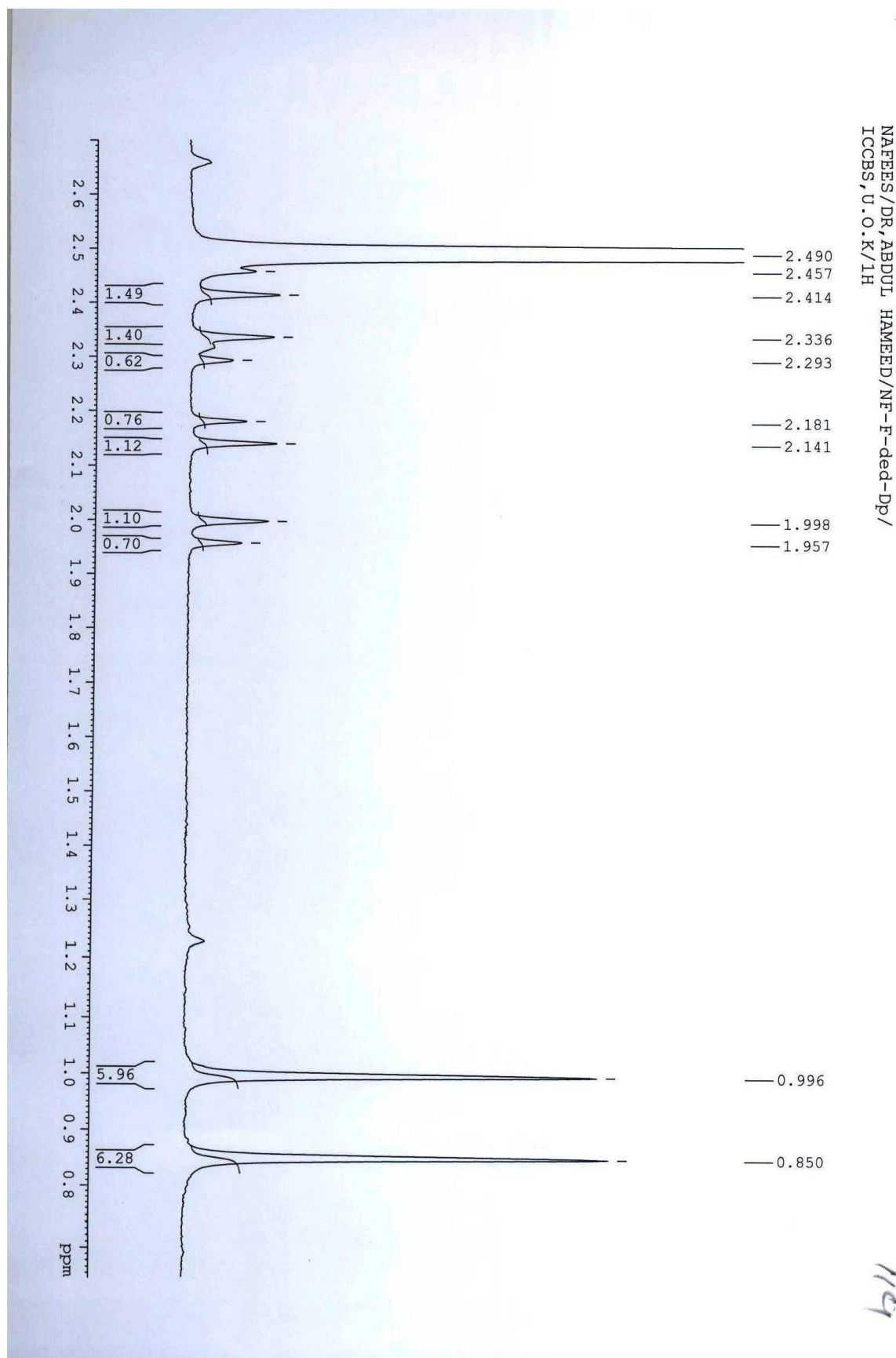


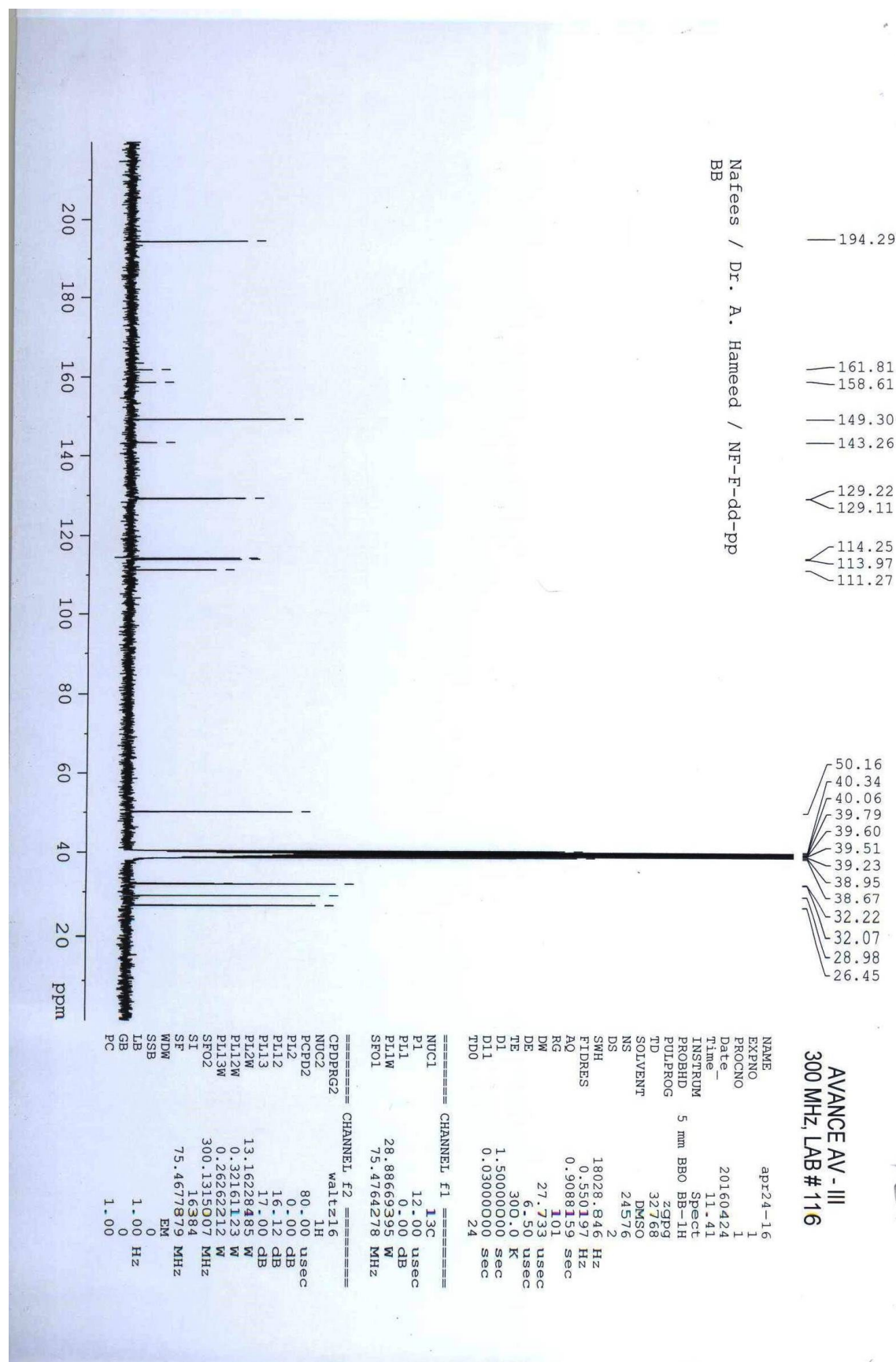


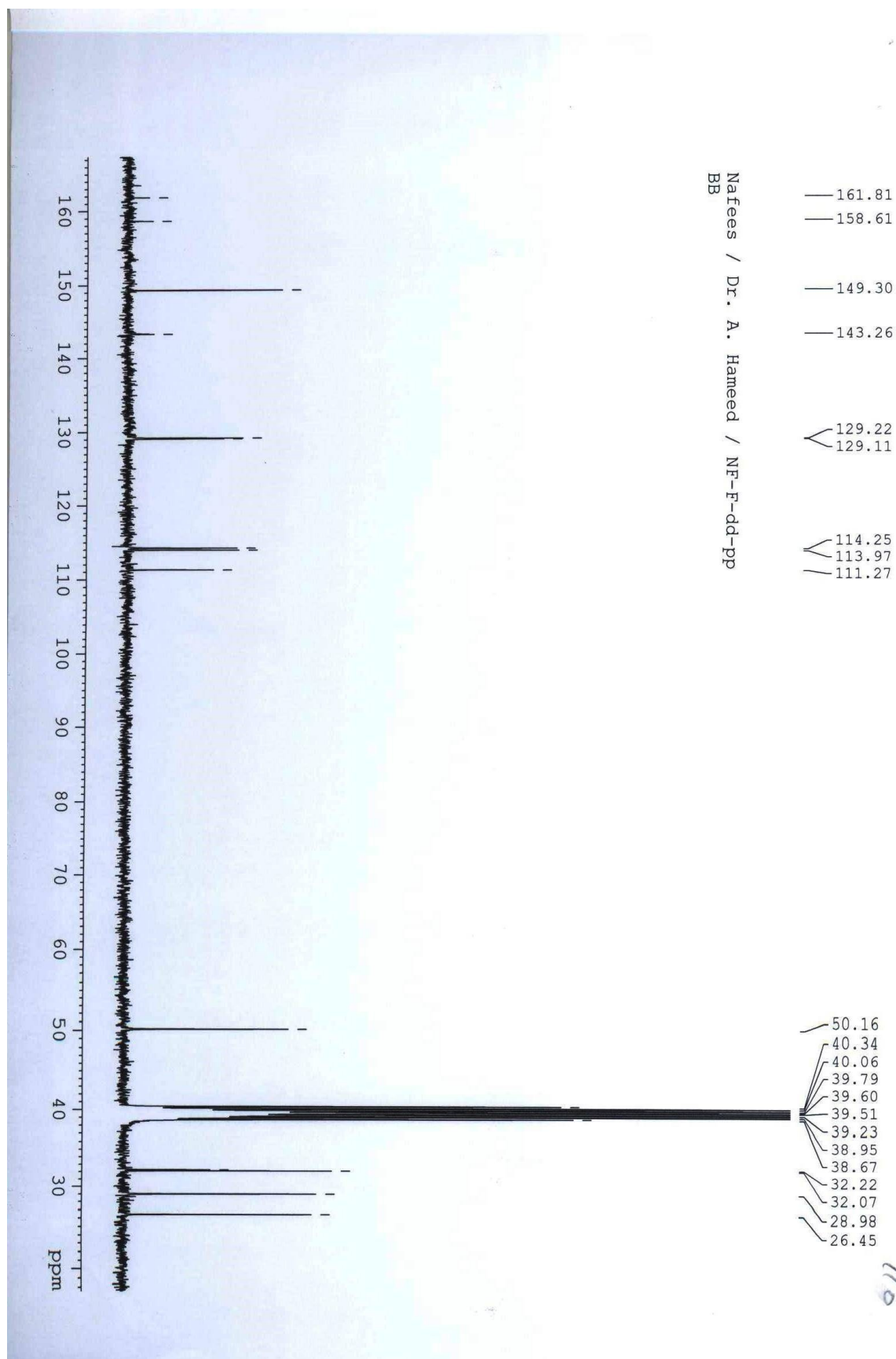


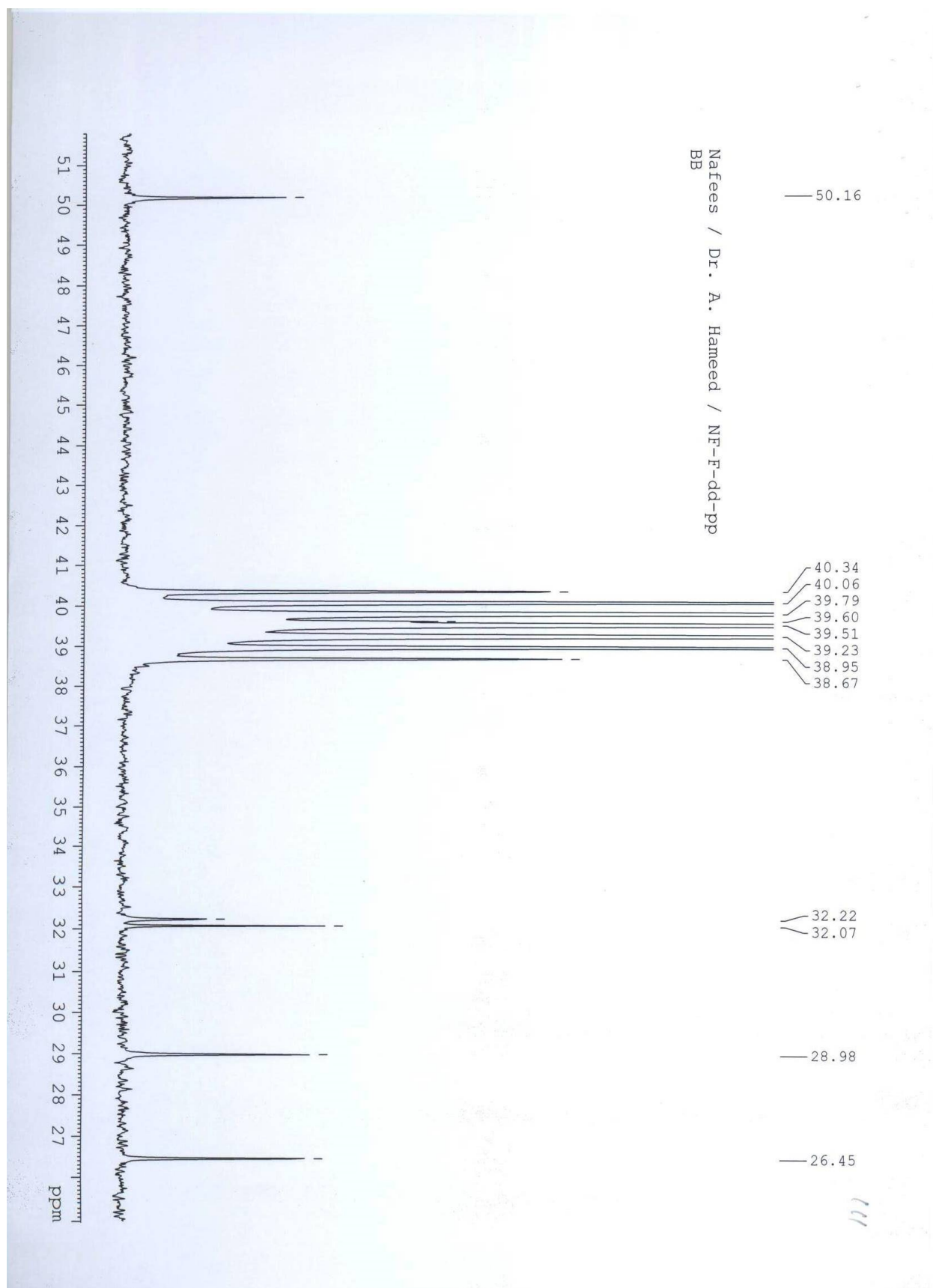


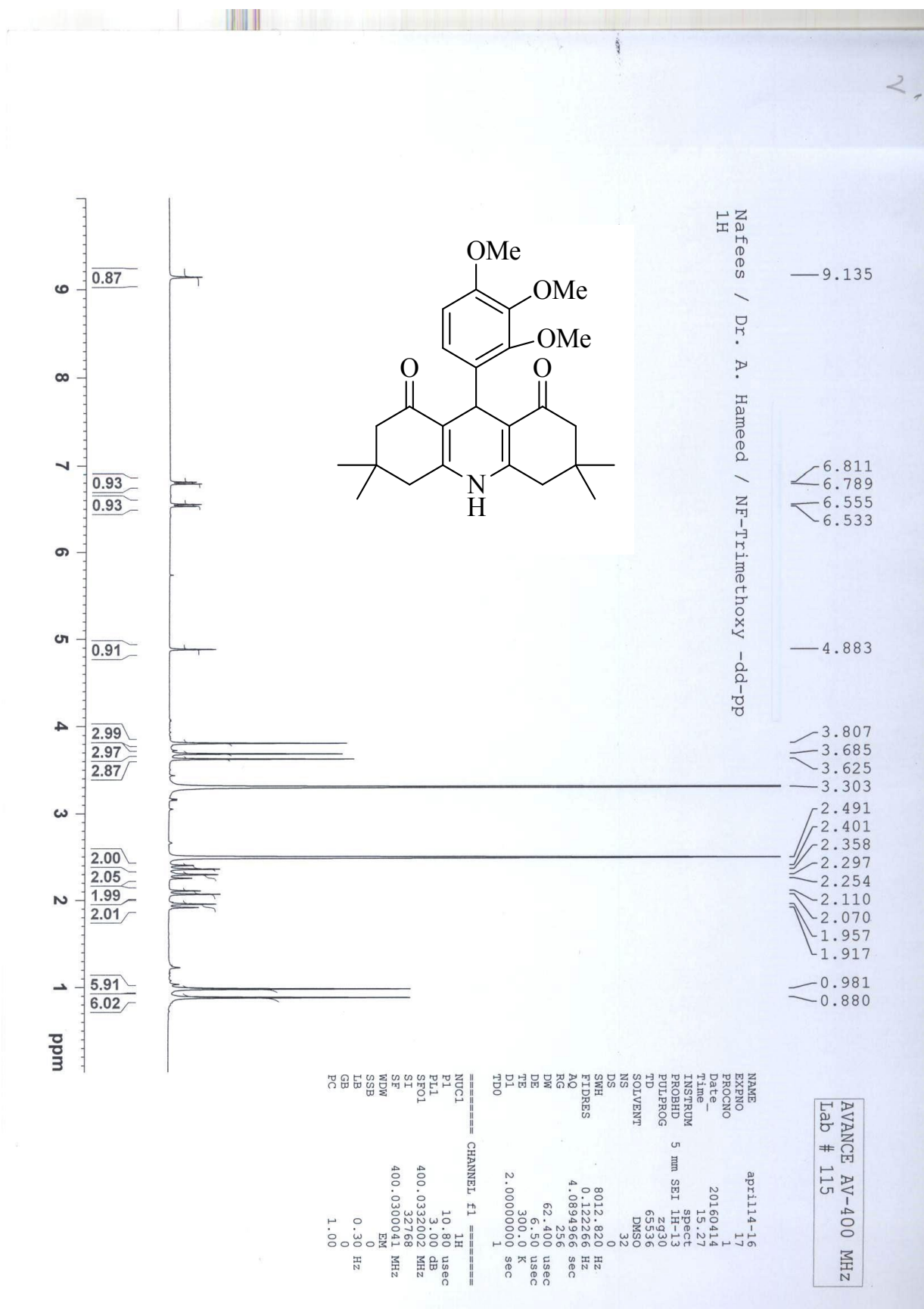


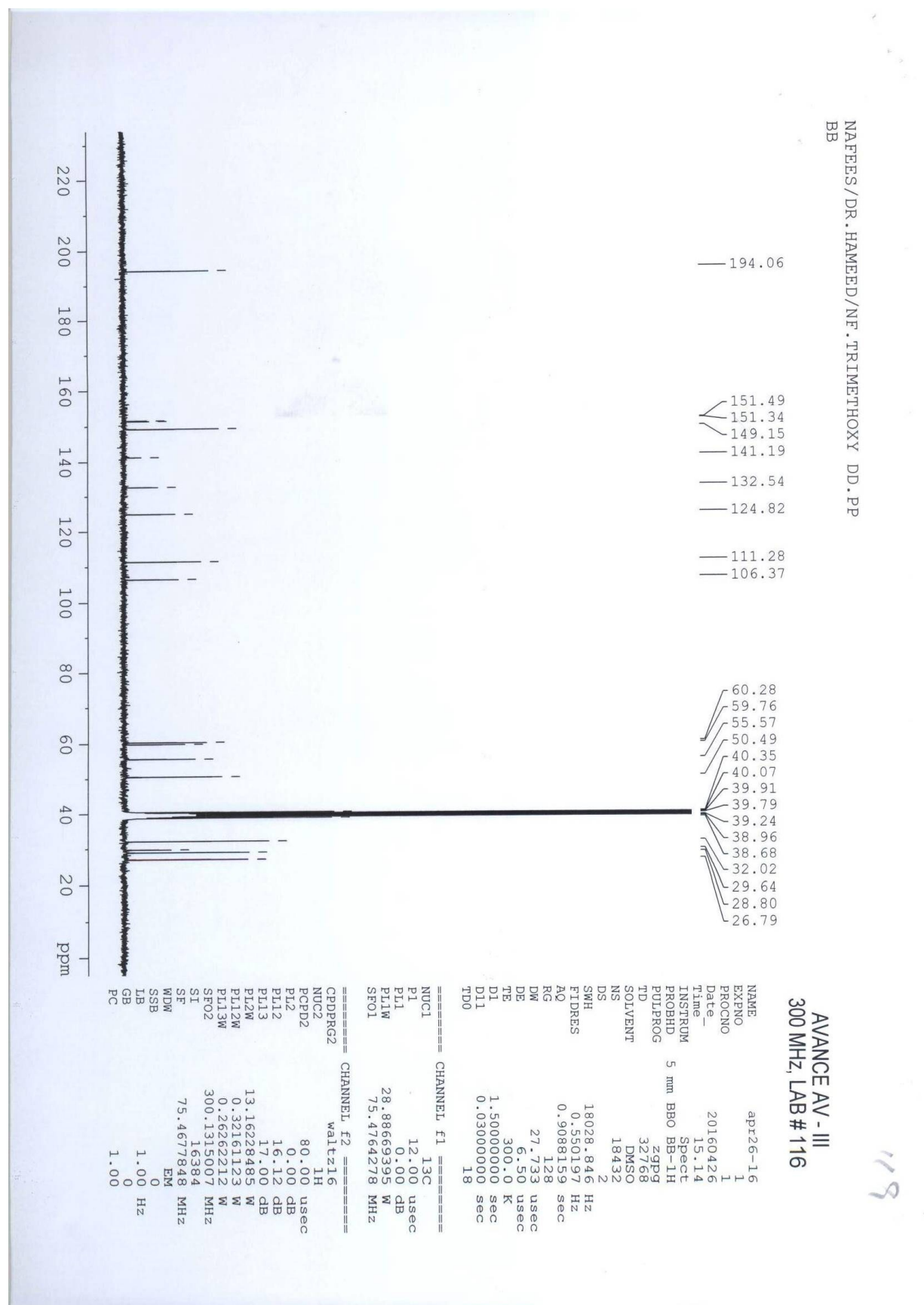


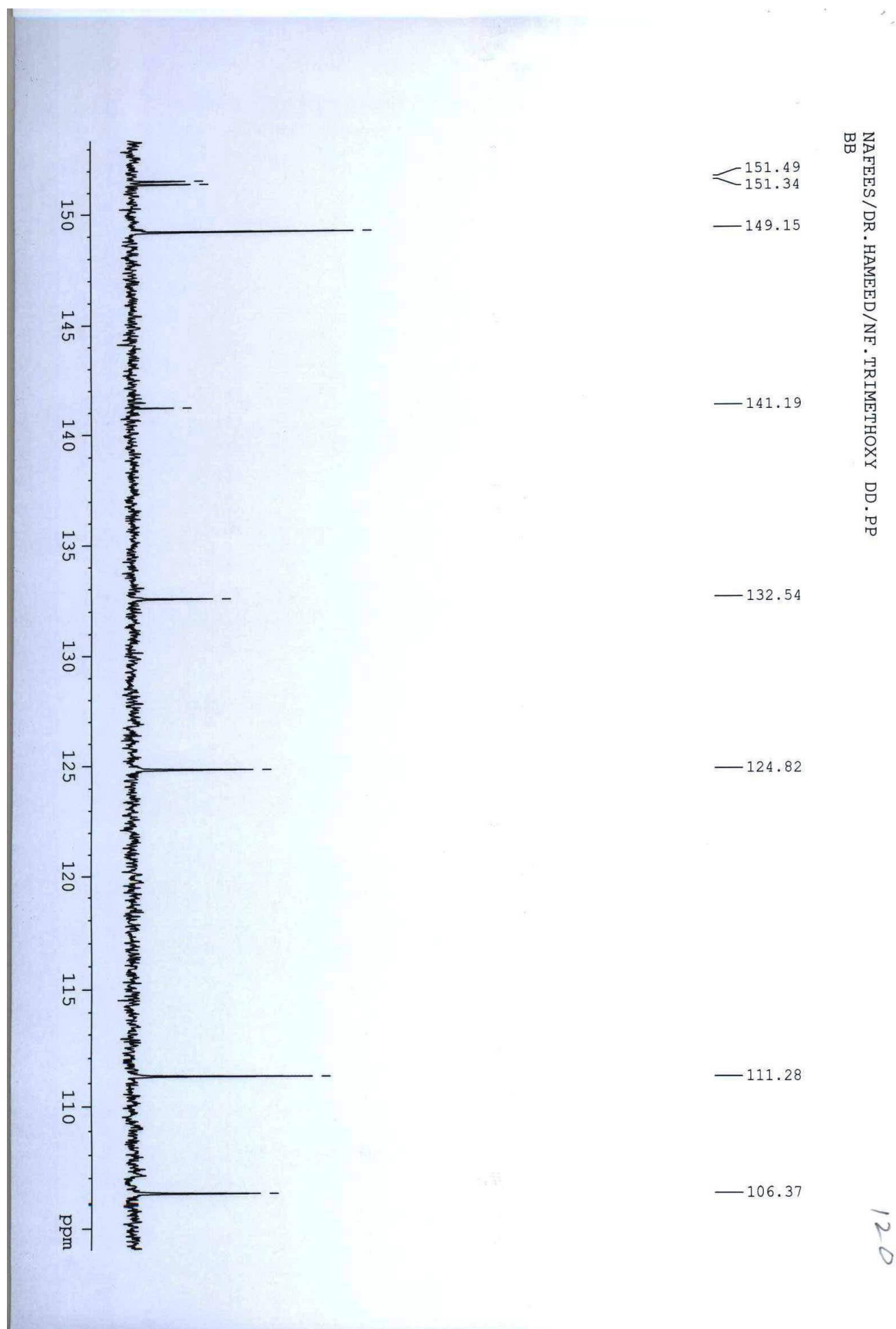


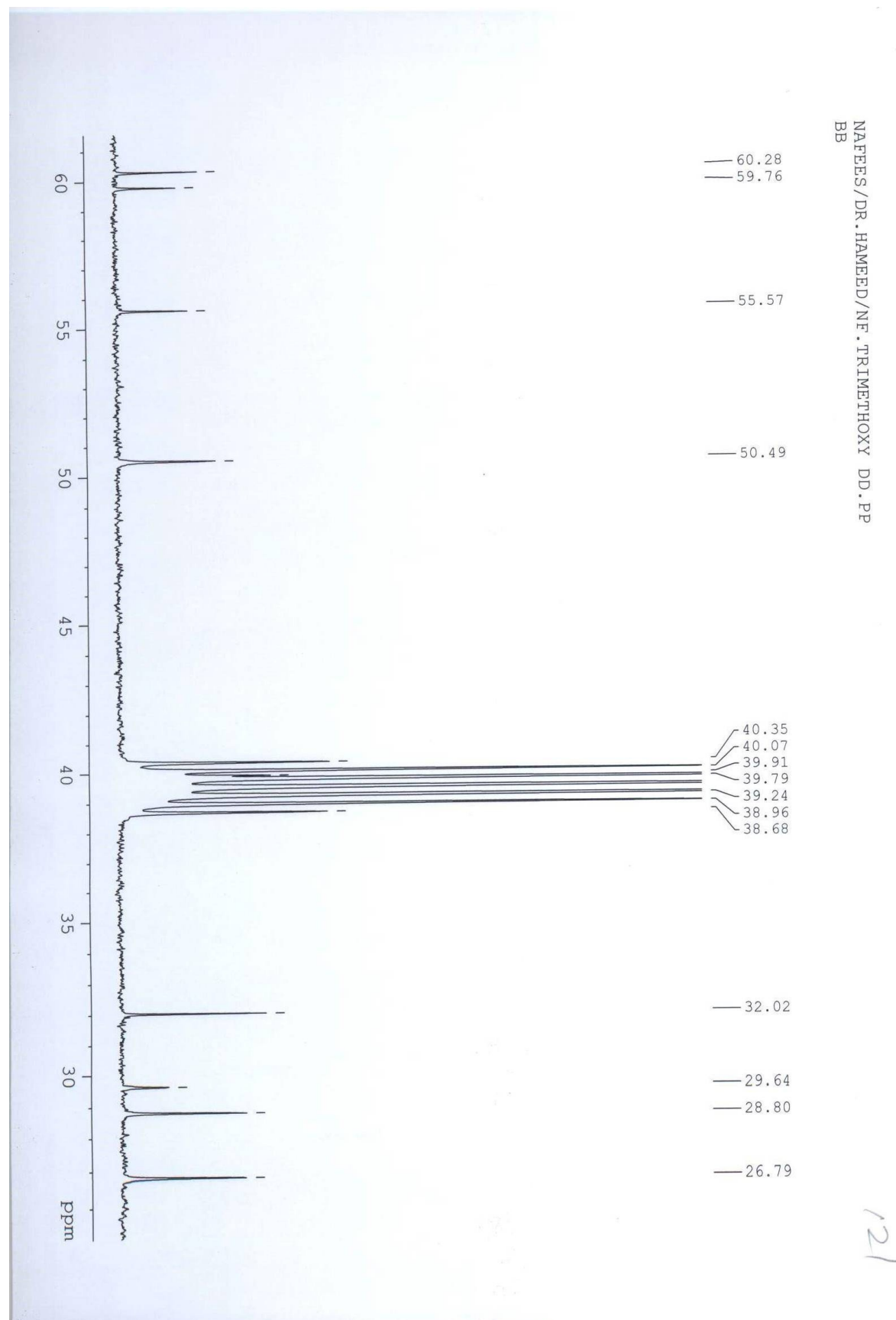


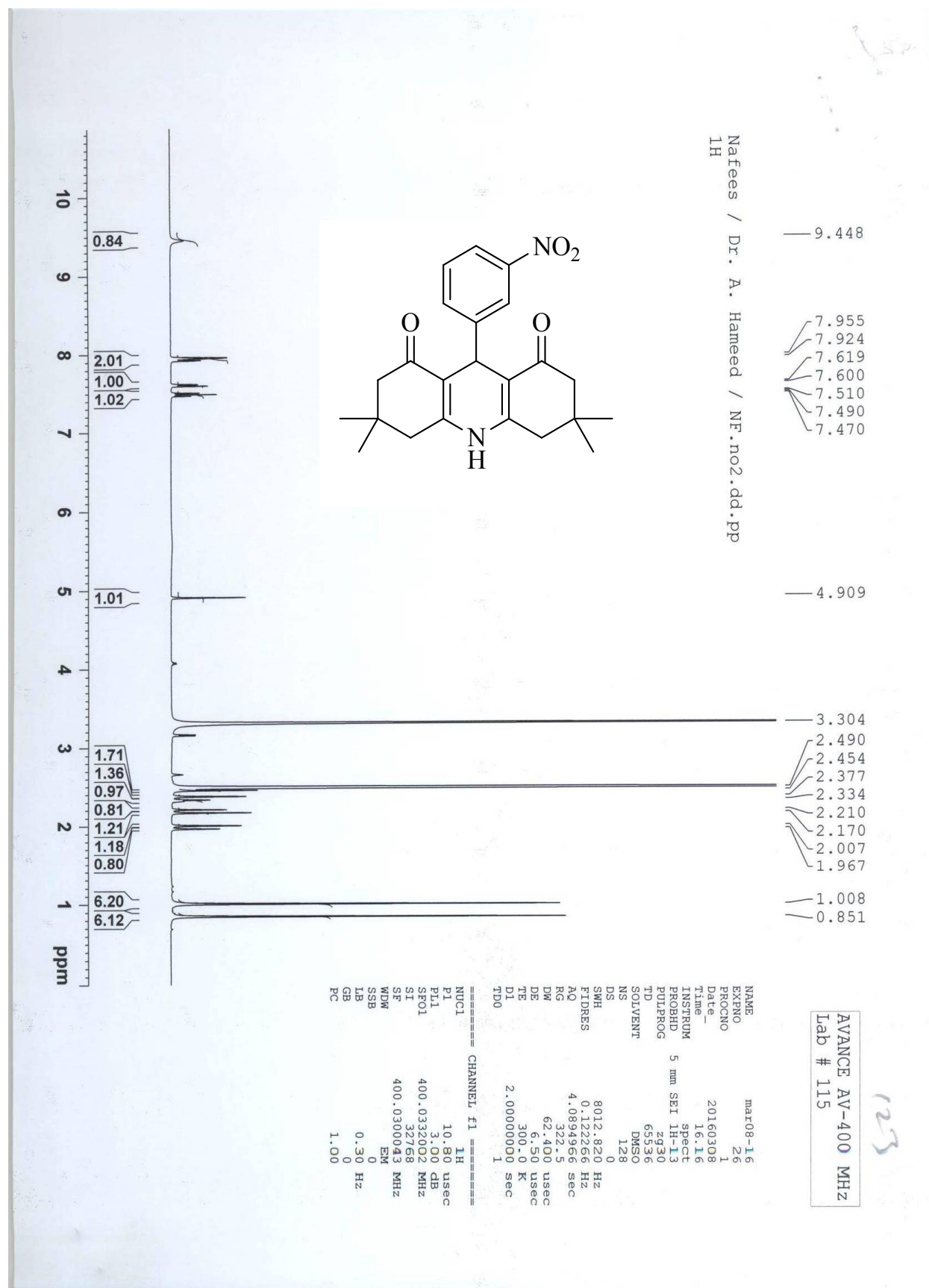


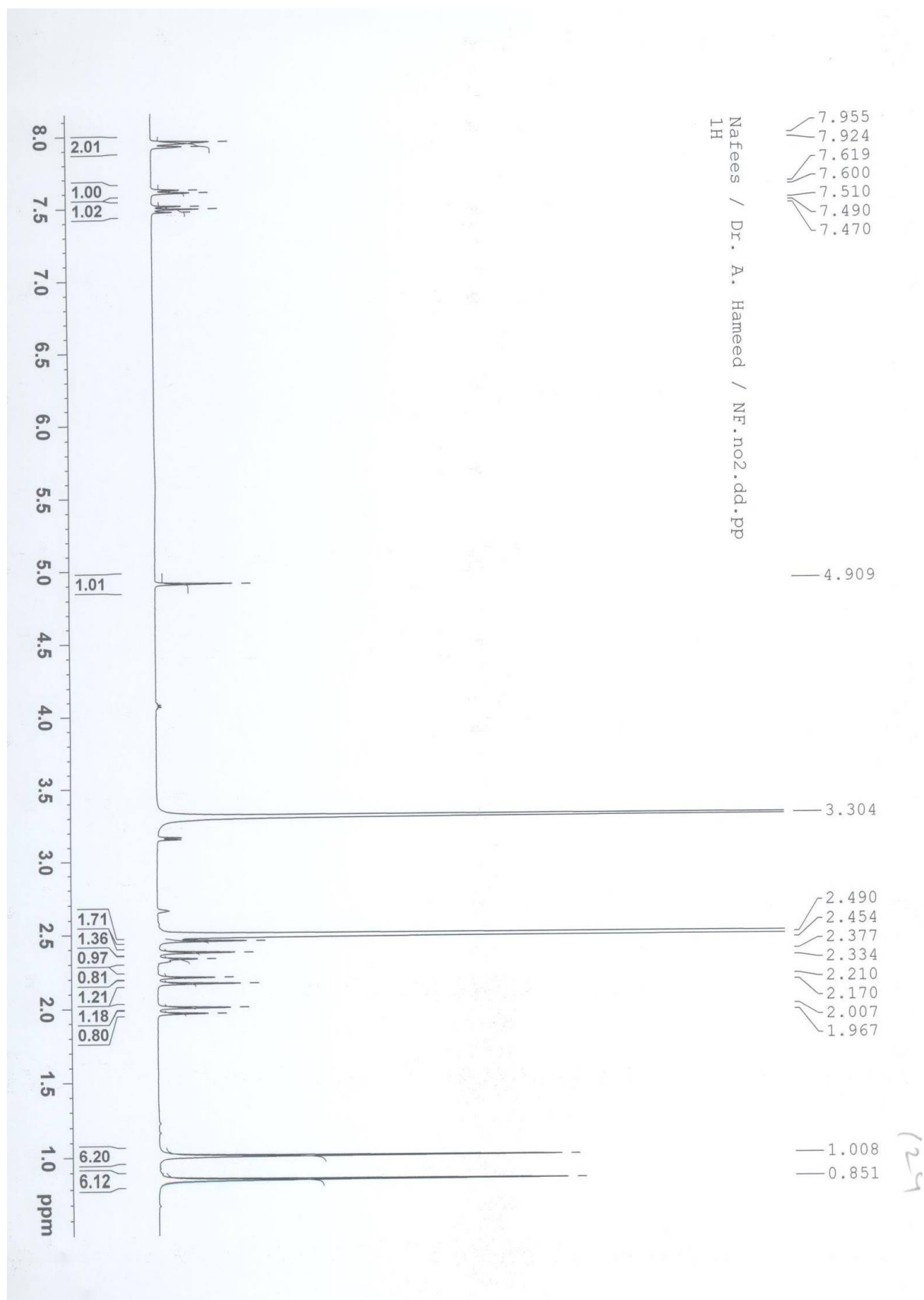




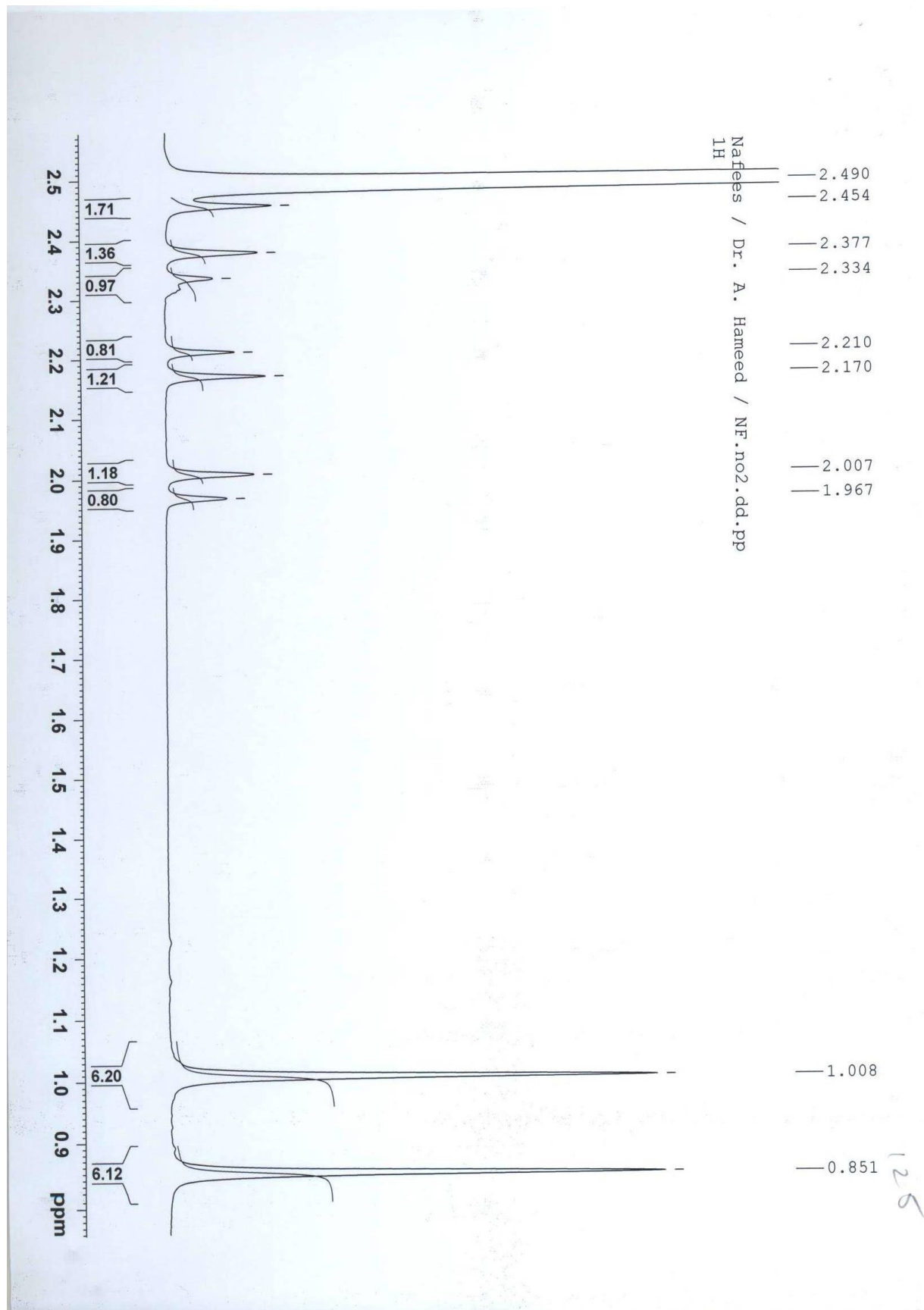


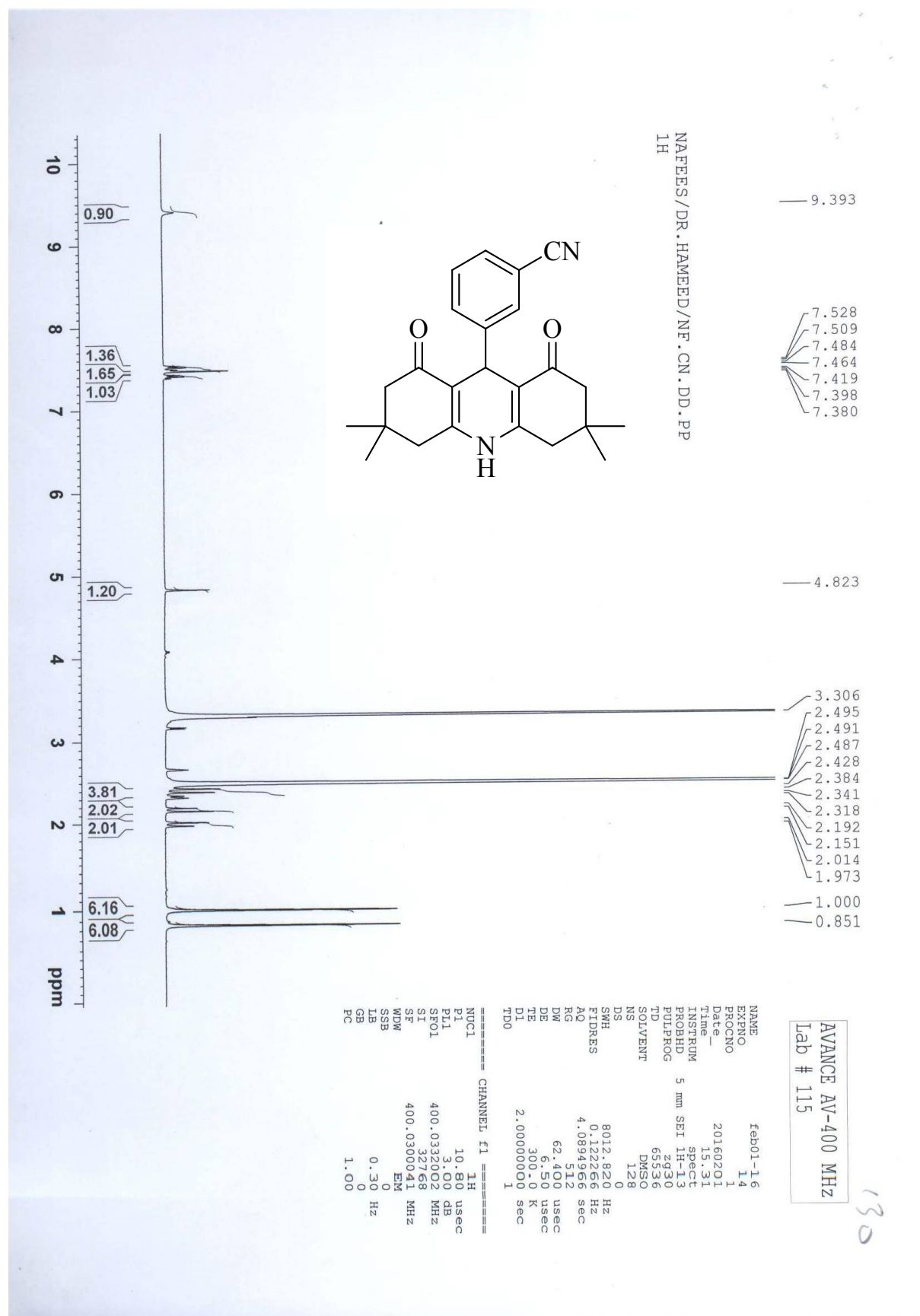


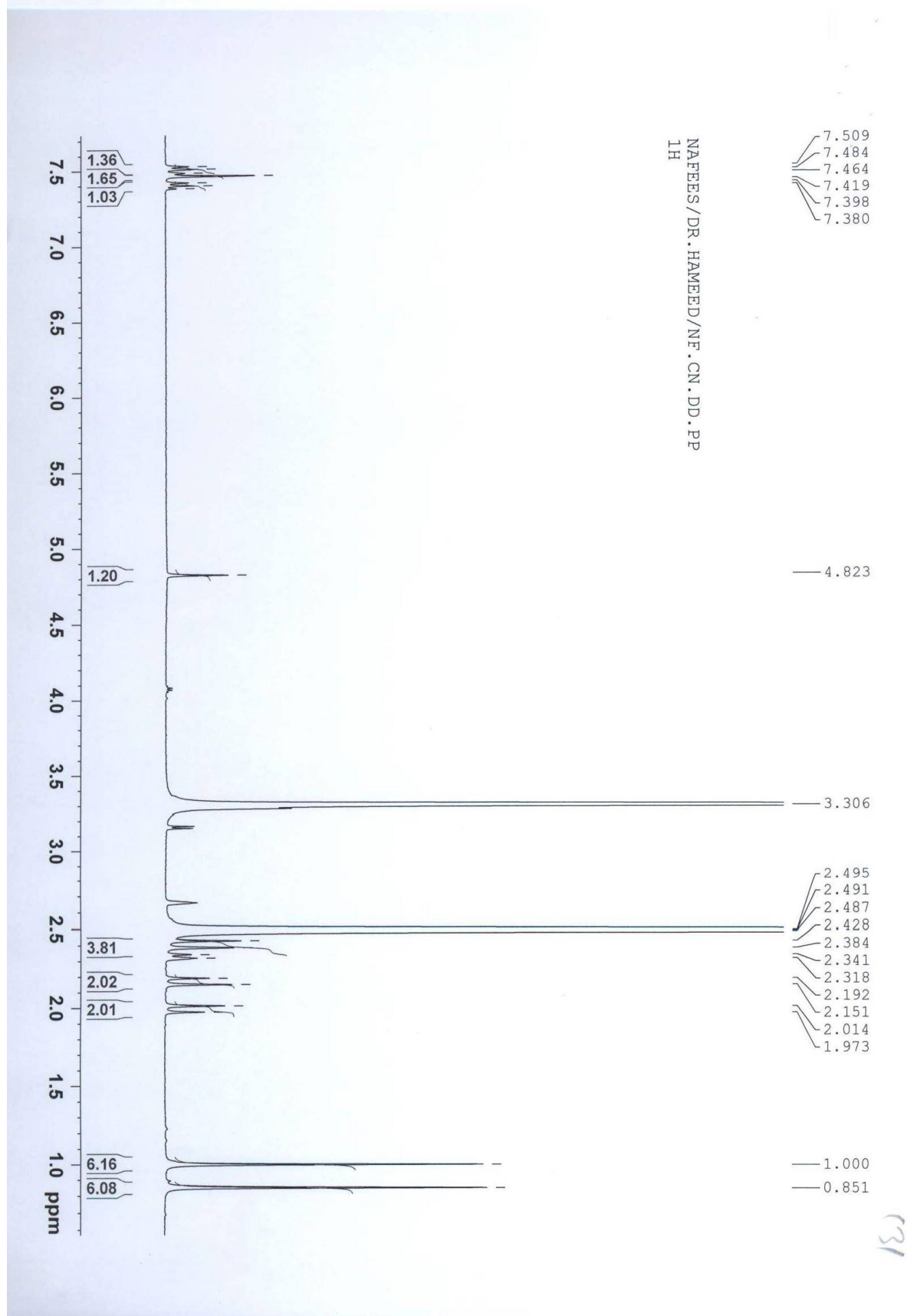




Supplementary Information (SI)







Supplementary Information (SI)

