

Supplementary Information (SI)

Solvent-Free Click Chemistry for Tetrazole Synthesis from 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-Based Fluorinated Ionic Liquids, their Micellization, and Density Functional Theory Studies

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Corresponding author:

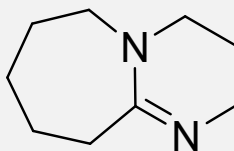
** A.H., Tel.: +92-219-9261701-2; Fax: +92-213-4819018

Email: abdul.hameed@iccs.edu / abdul_hameed8@hotmail.com

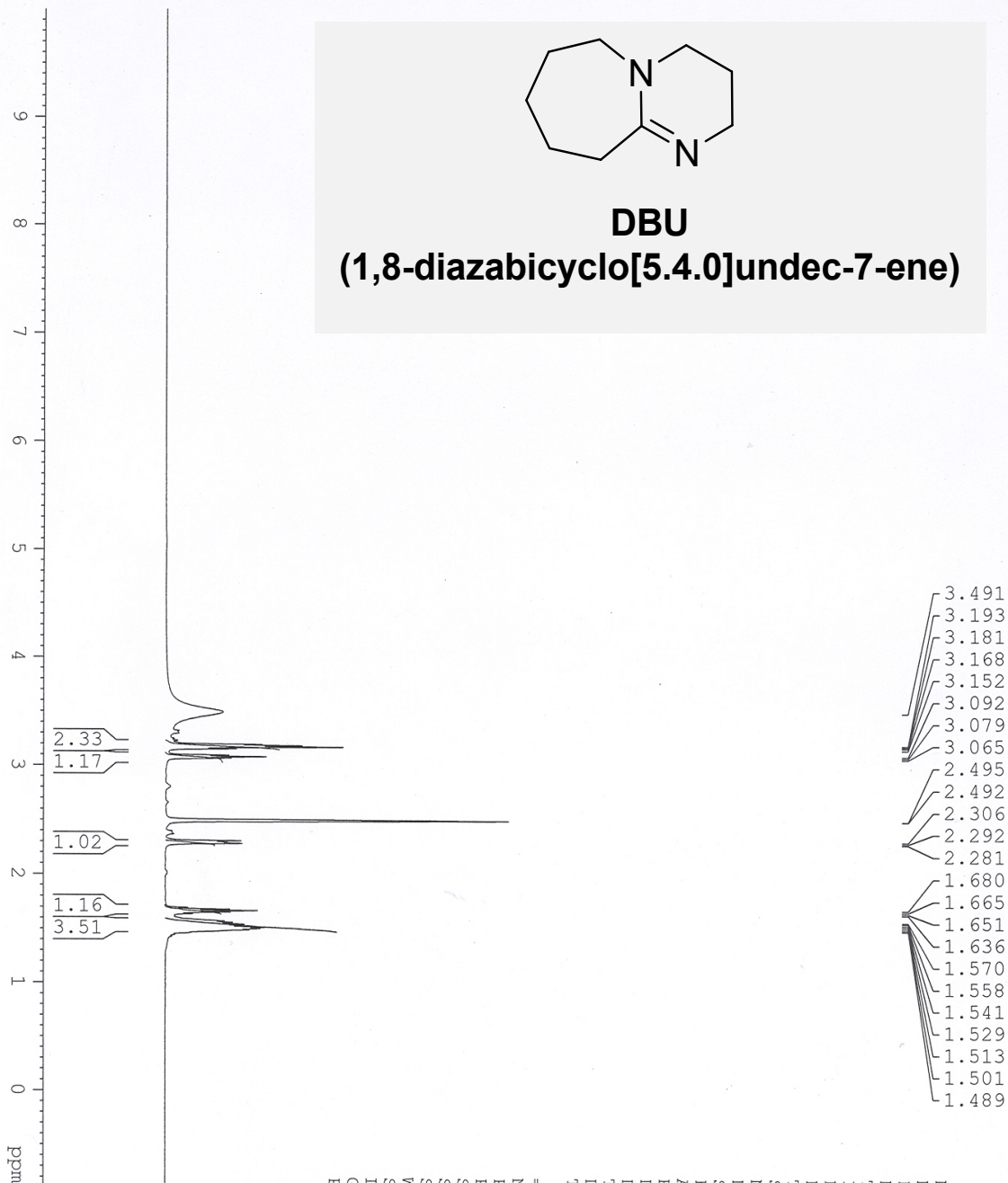
* M.I.M., Email: m.imran.malik1@gmail.com / mimran.malik@iccs.edu

Spectral Data

ALI ANUS/DR, FATIMA .B/DBU/ICCBS, U.O.K/
¹H



DBU
(1,8-diazabicyclo[5.4.0]undec-7-ene)



- 3.491
- 3.193
- 3.181
- 3.168
- 3.152
- 3.092
- 3.079
- 3.065
- 2.495
- 2.492
- 2.306
- 2.292
- 2.281
- 1.680
- 1.665
- 1.651
- 1.636
- 1.570
- 1.558
- 1.541
- 1.529
- 1.513
- 1.501
- 1.489

AVANCE 400
 LAB NO 117

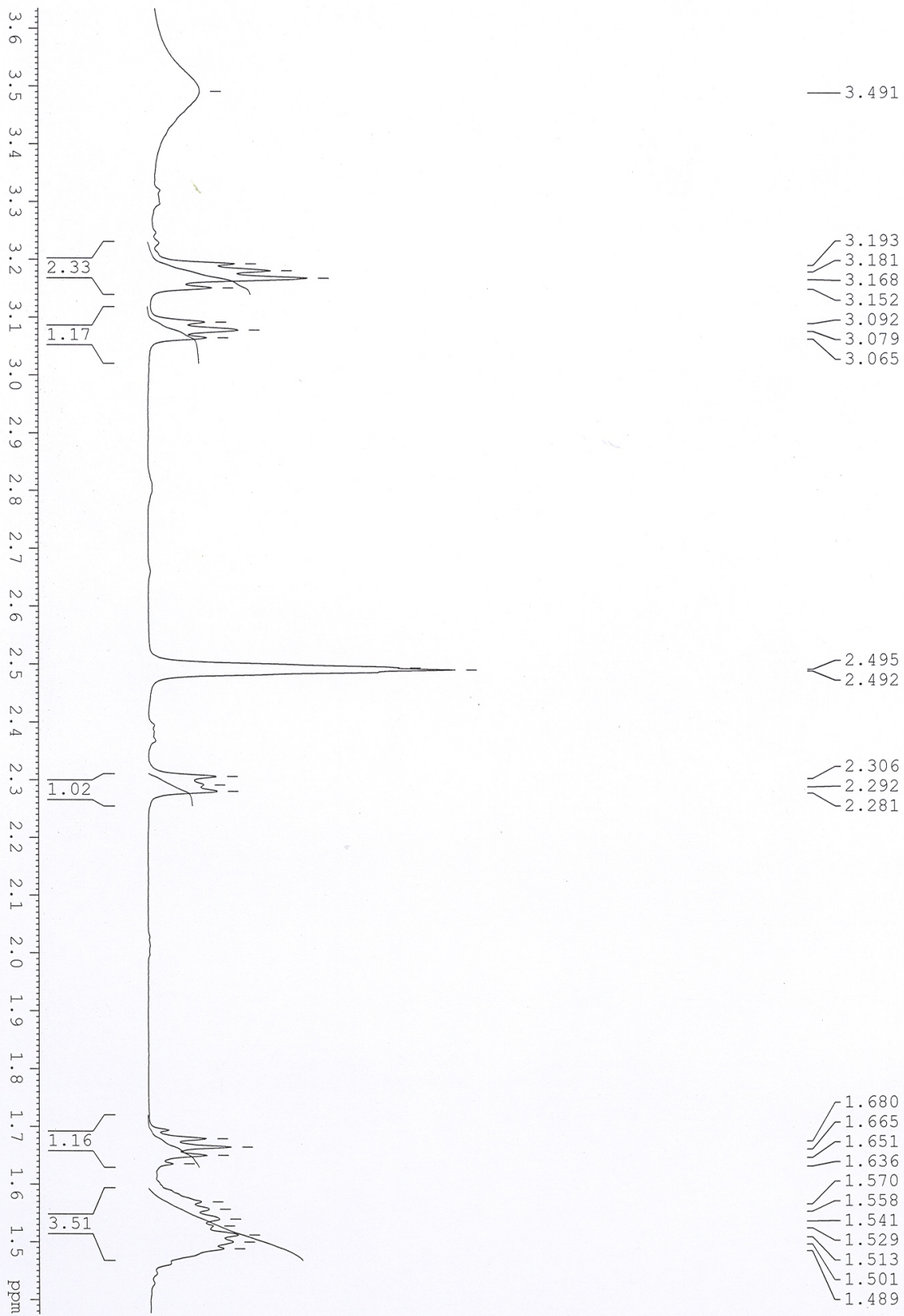
```

NAME          mar19-14
EXPNO         3
PROCNO        1
Date_         20140319
Time_         11.18
INSTRUM       5 mm DUL
PROBHD        13C-1
PULPROG       zg30
TD            32768
SOLVENT       DMSO
NS            64
DS            0
SWH           8012.820 Hz
FIDRES       0.244532 Hz
AQ           2.0447731 sec
RG           2048
DW           62.400 usec
DE           6.50 usec
TE           300.0 K
D1           2.000000000 sec
TD0          1

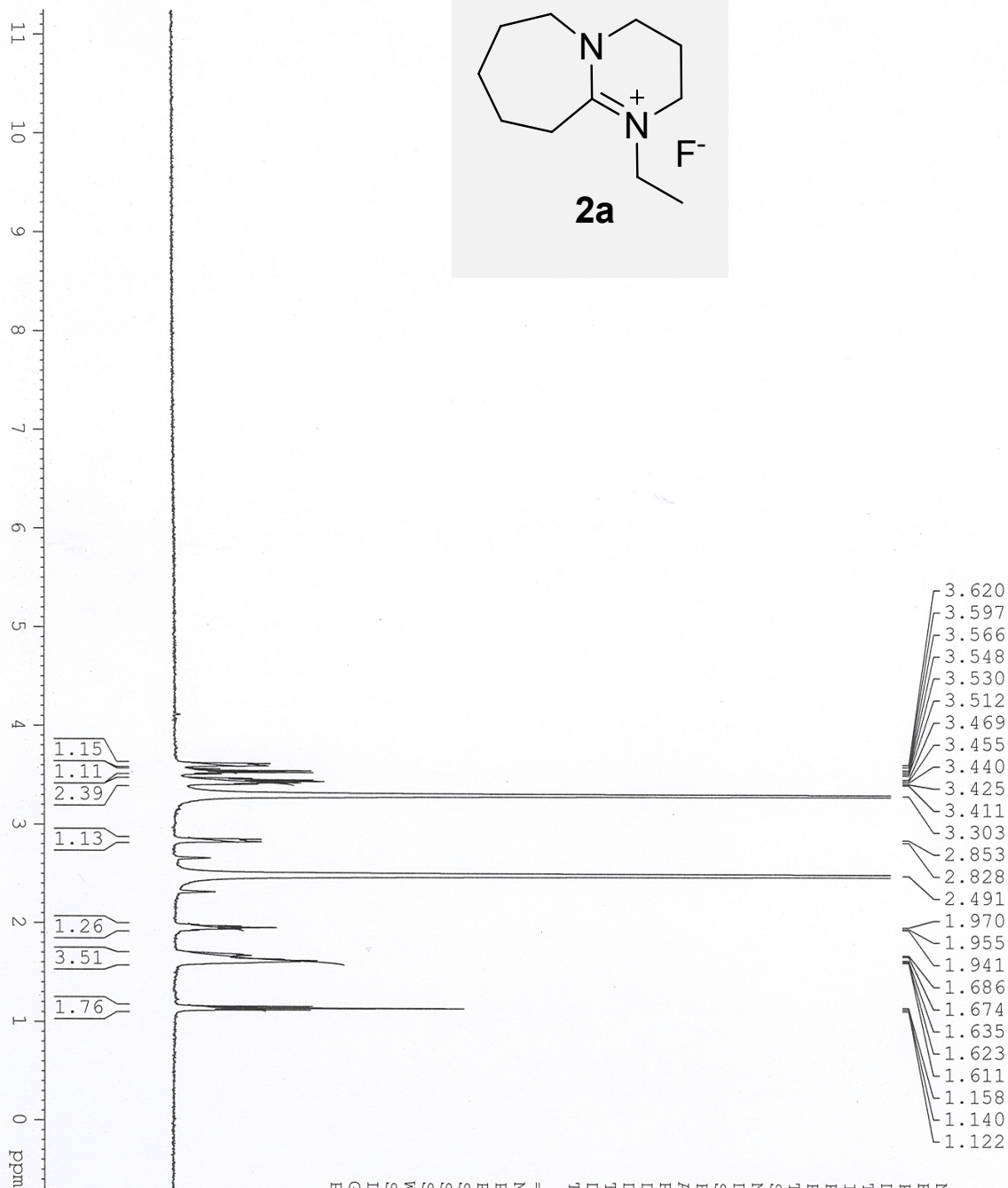
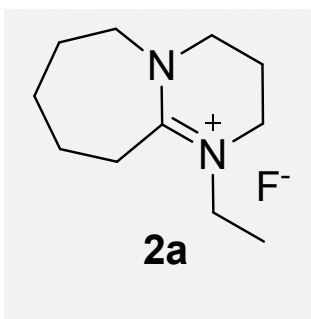
===== CHANNEL f1 =====
NUC1          1H
P1           10.20 usec
PL1          0.00 dB
SFO1         400.1332010 MHz
SI           16384
SF           400.1300064 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
    
```

Supplementary Information (SI)

ALI ANUS/DR, FATIMA .B/DBU/ICCBS, U.O.K/
¹H



ALI ANUS/DR, FATIMA B/AA-23/ICCBS. U.O.K/



AVANCE 400
LAB NO 117

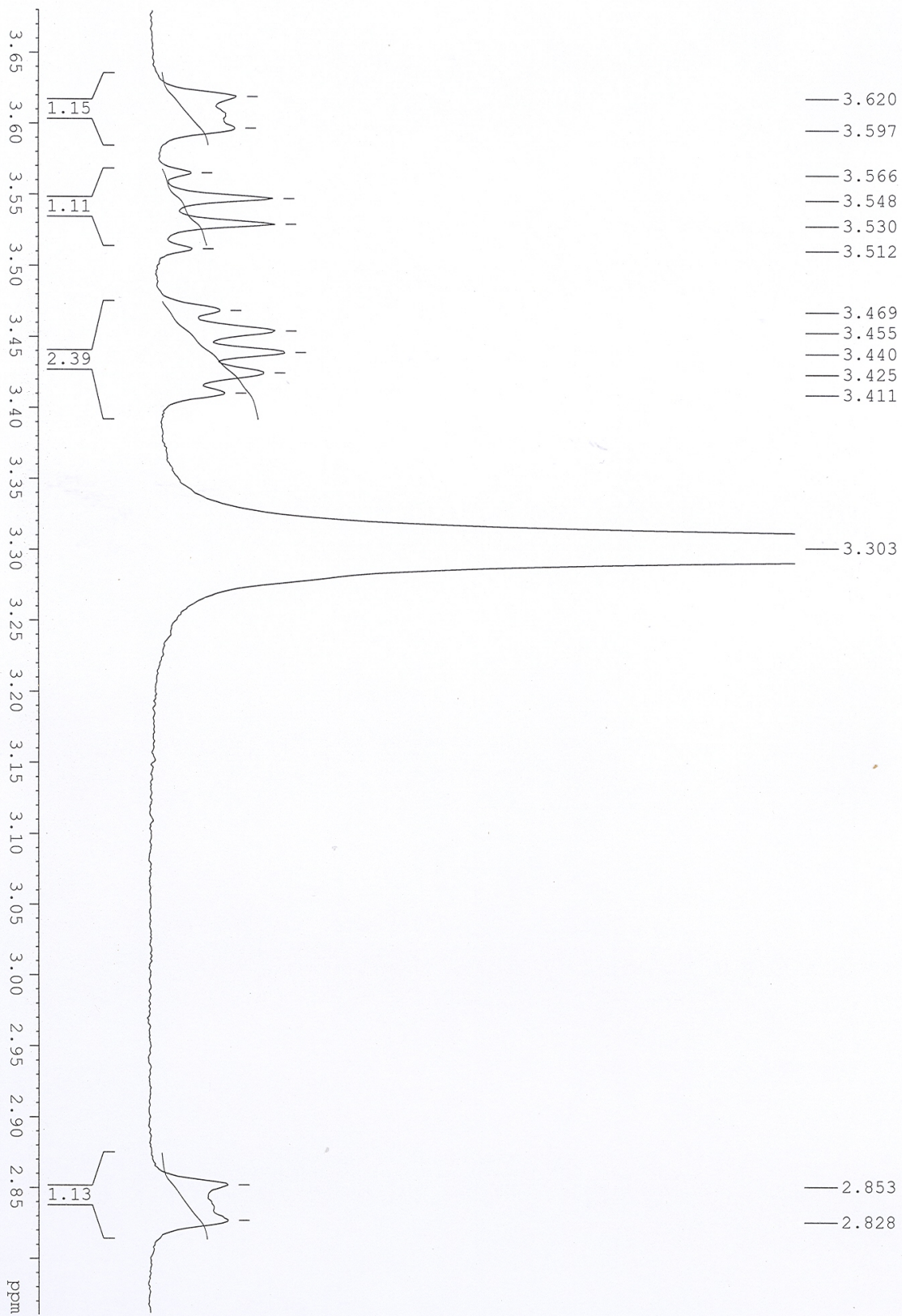
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EXPNO         2
PROCNO        1
Date_         20140313
Time_         8.39
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       zg30
TD            32768
SOLVENT       DMSO
NS            64
DS            0
SMH           8012.820 Hz
FIDRES        0.244532 Hz
AQ            2.0447731 sec
RG            2048
DE            62.400 usec
TE            300.0 K
D1            2.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            10.20 usec
PL1           0.00 dB
SFO1          400.1332010 MHz
SI            16384
SF            400.1300063 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
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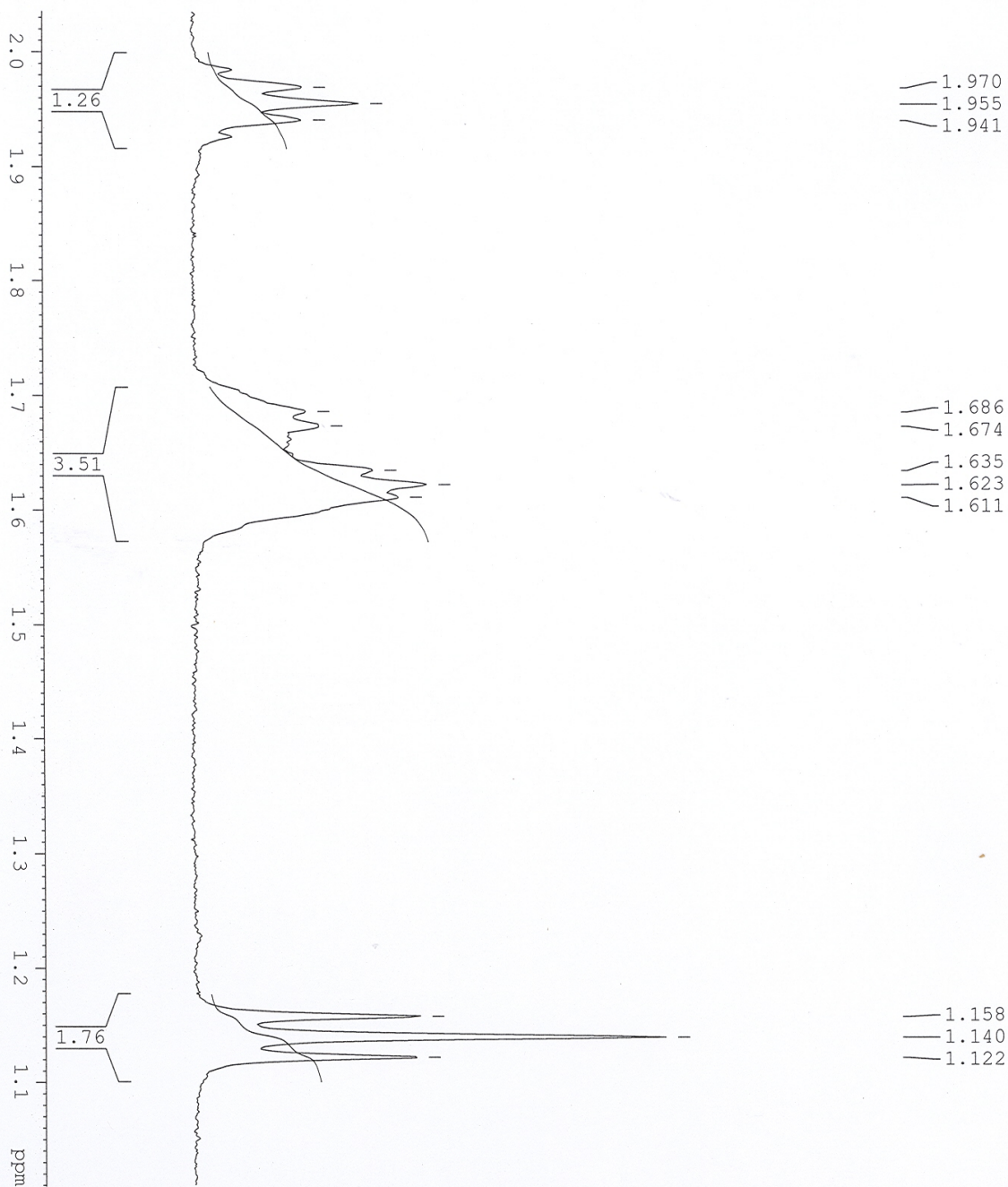

Supplementary Information (SI)

ALI ANUS/DR, FATIMA B/AA-23/ICCBS.U.O.K/



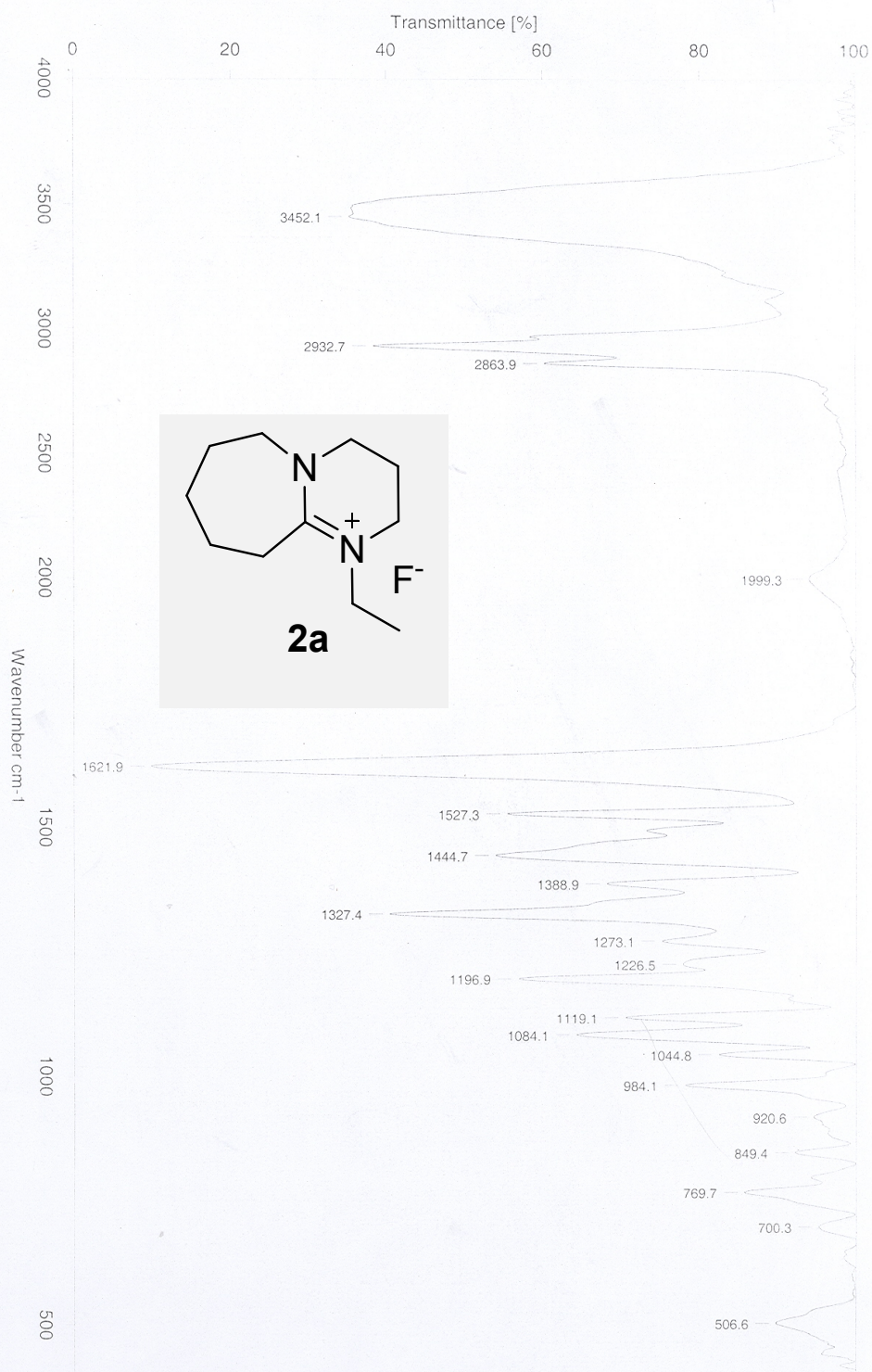
Supplementary Information (SI)

ALI ANUS/DR, FATIMA B/AA-23/ICCBS. U.O.K/

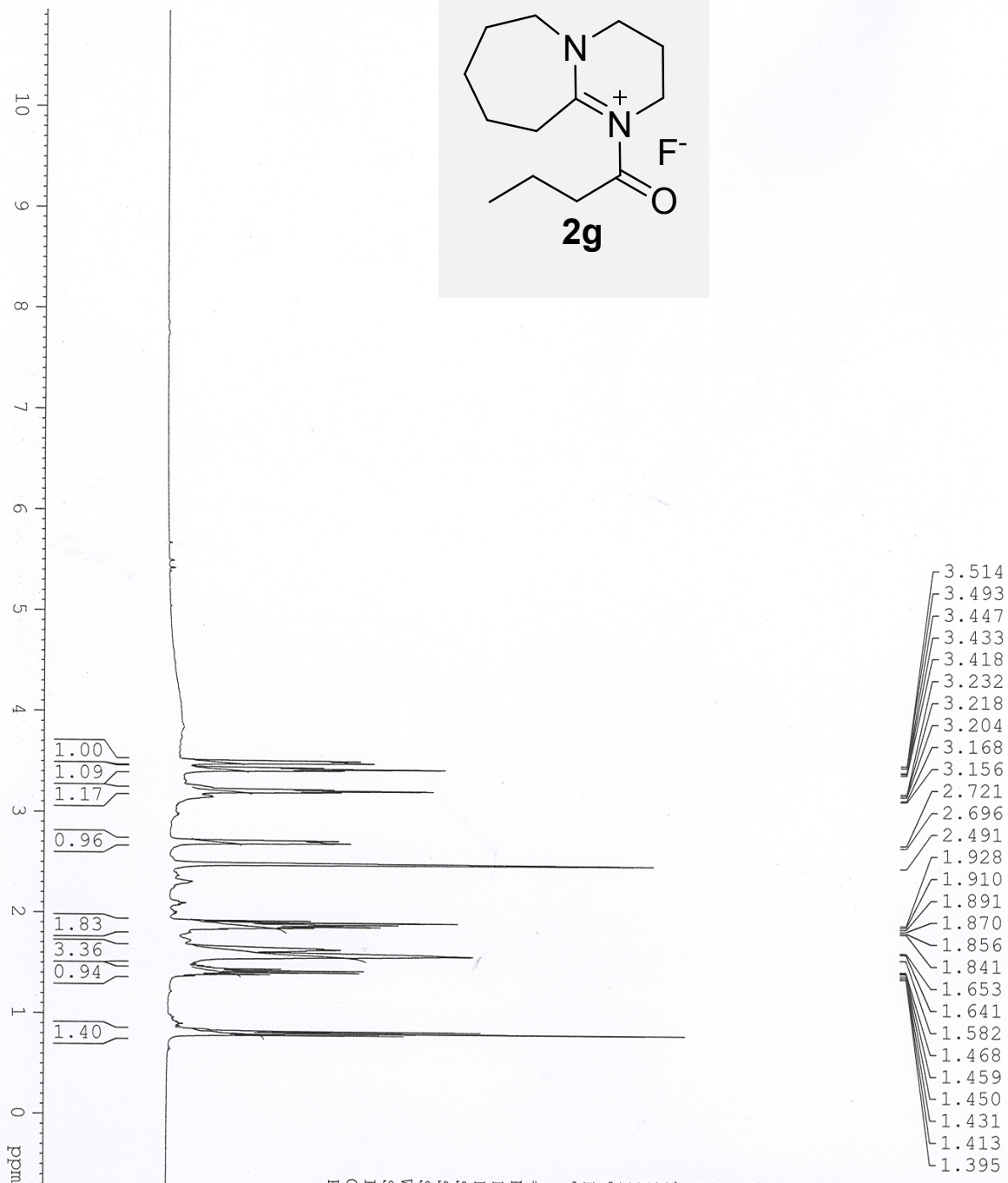
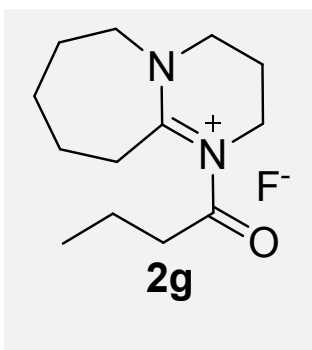


Supplementary Information (SI)

Sample : 1\ Ali Anus
Measured : 18/07/2014 on VECTOR22
Resolution : 4 cm⁻¹ (10 scans)
Spectrum : 1.5 (in D:\RSTUDENT)
Technic : SOLID
Qualifyst : ZURBIR/JANSHED



ALI ANUS/DR, FATIMA B/AA-25A/ICCBS.U.O.K/



AVANCE 400
LAB NO 117

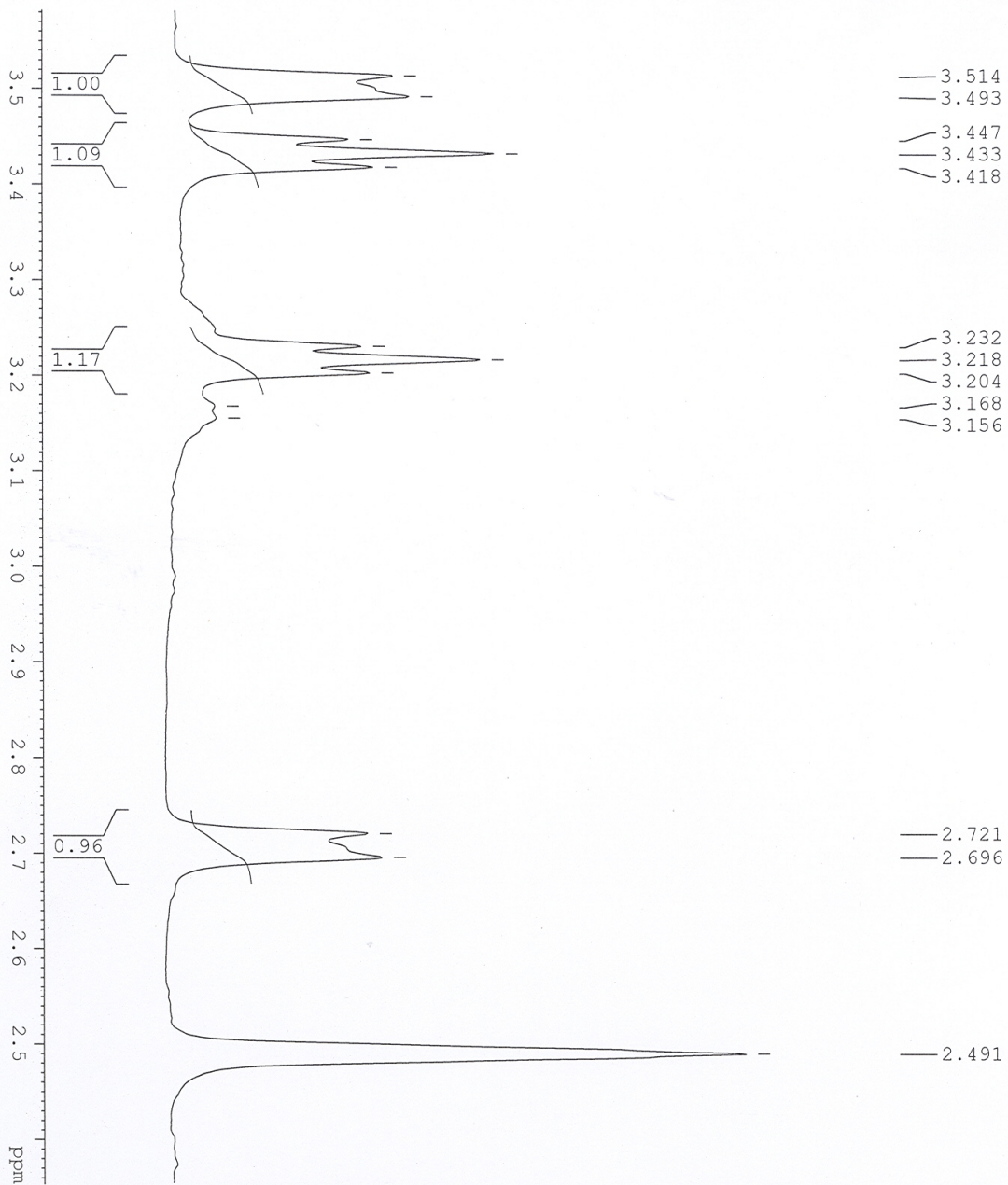
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NAME          mar13-14
EXPNO         1
PROCNO        1
Date_         20140313
Time          8.28
INSTRUM       5 mm DUL 13C-1
PROBHD        zg30
PULPROG       32768
TD            DMSO
SOLVENT       DMSO
NS            32
DS            0
SWH           8012.820 Hz
FIDRES       0.244532 Hz
AQ           2.0447731 sec
RG           2048
DW           62.400 usec
DE           6.50 usec
TE           300.0 K
D1           2.000000000 sec
TD0          1

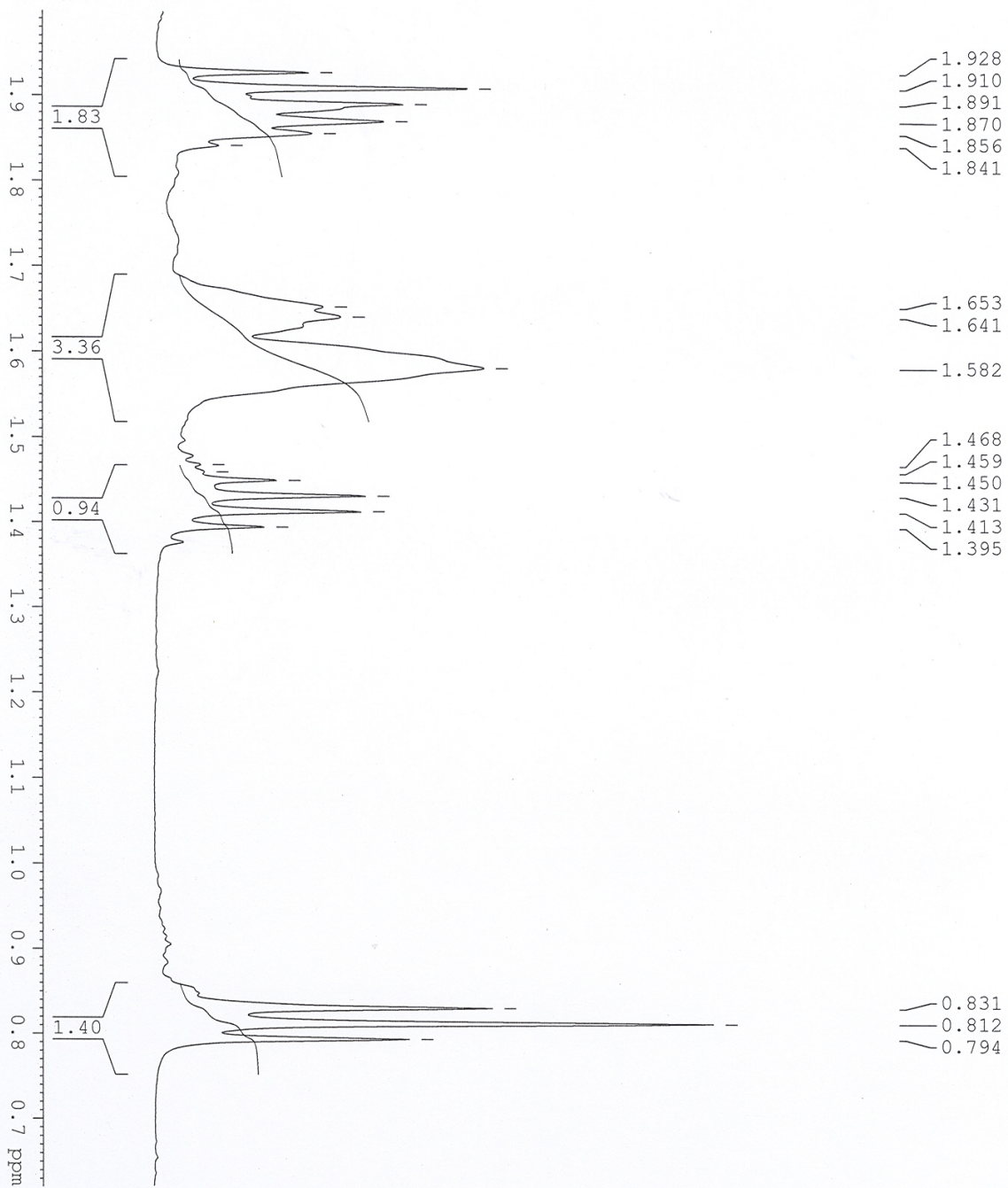
===== CHANNEL f1 =====
NUC1          1H
P1           10.20 usec
PL1          0.00 dB
SF01         400.1332010 MHz
SI           16384
SE           400.1300063 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
    
```

Supplementary Information (SI)

ALI ANUS/DR, FATIMA B/AA-25A/ICCBS. U. O. K/

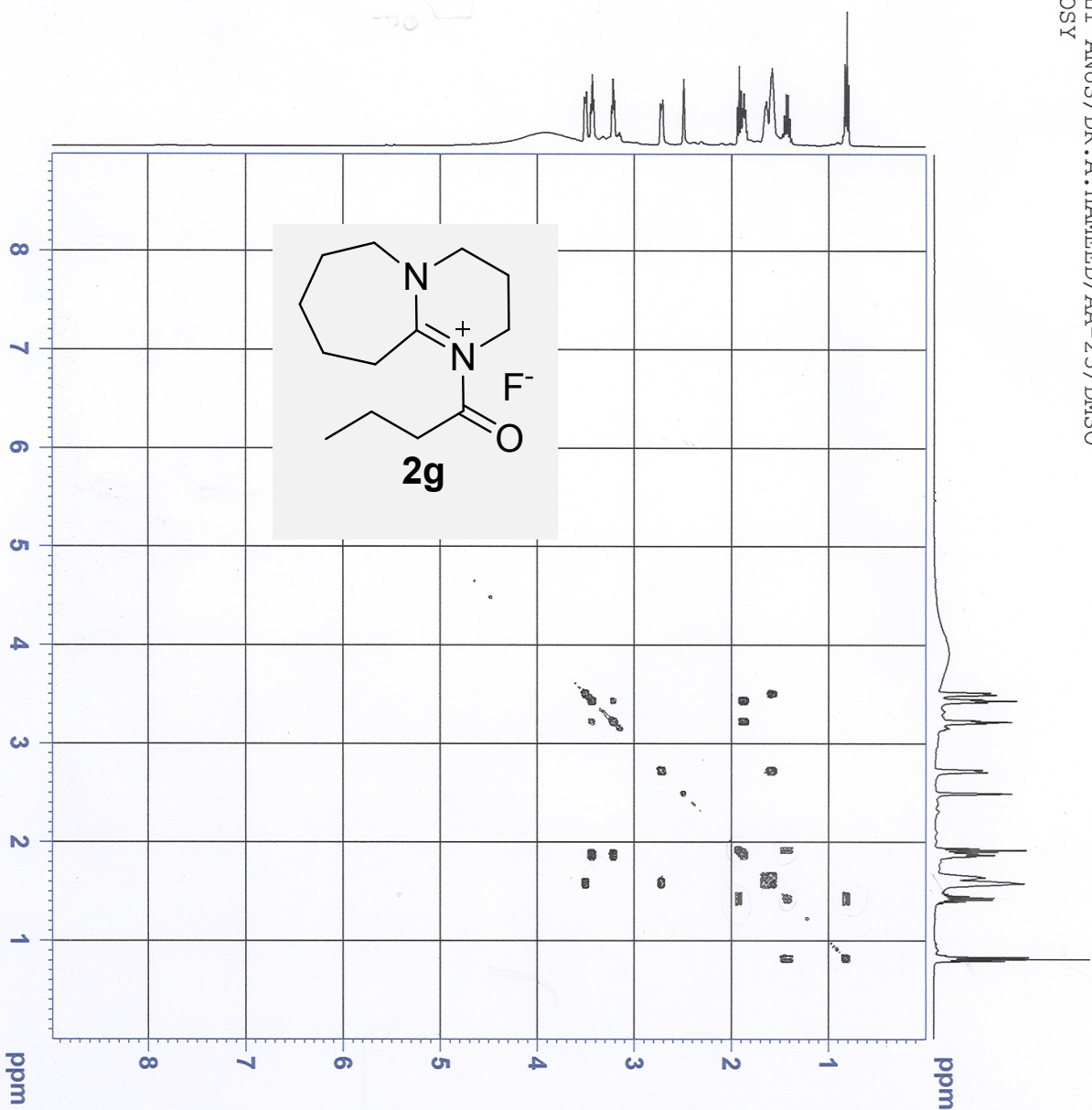


Supplementary Information (SI)



ALI ANUS/DR, FATIMA B/AA-25A/ICCBS. U.O.K/

ALI ANUS/DR.A.HAMEED/AA-23/DMSO
COSY



AVANCE AV-400 MHz
Lab # 115

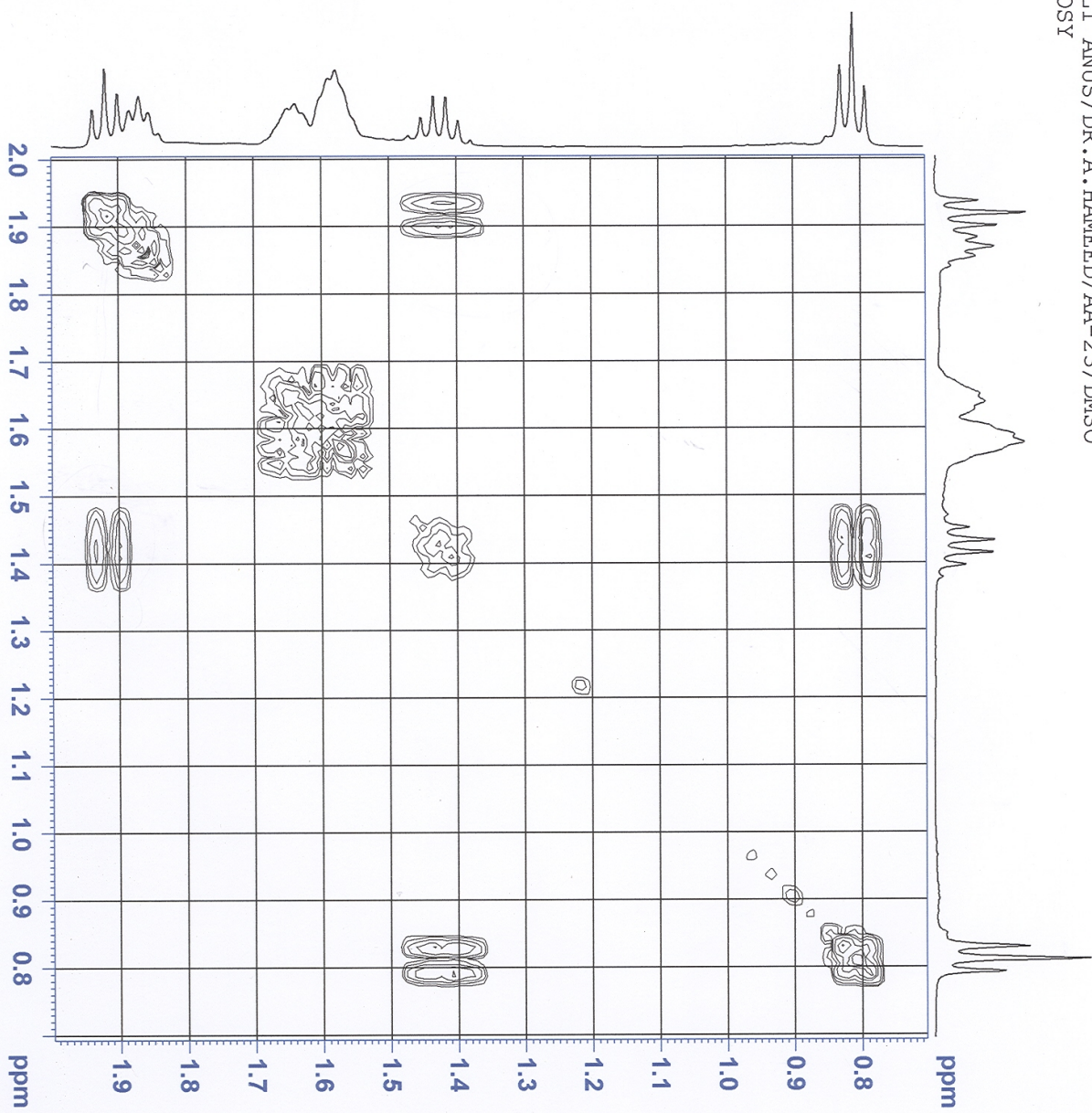
```

NAME          July02-14
EXPNO         7
PROCNO       1
Date_        20140702
Time         13.31
INSTRUM      spect
PROBHD       5 mm SEI 1H-13
PULPROG      cosyppdf
TD           2048
SOLVENT      DMSO
NS           32
DS           8
SMH          3591.954 Hz
FIDRES       1.753884 Hz
AQ           0.2851316 sec
RG           90.5
DM           139.200 usec
DE           6.50 usec
TE           301.5 K
DO           0.00000300 sec
D1           1.50000000 sec
D13          0.00000400 sec
D16          0.00010000 sec
INO          0.00027840 sec

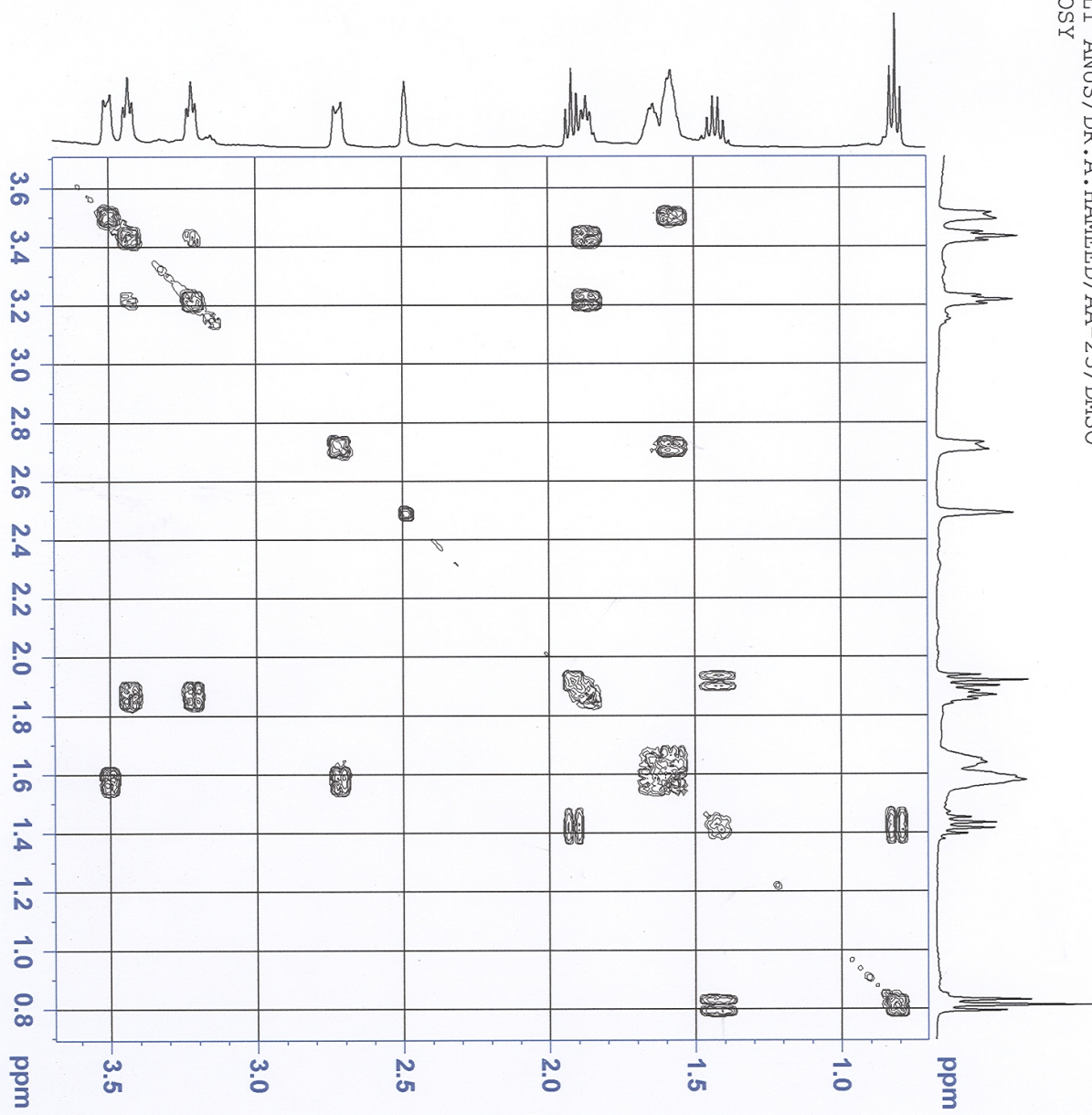
===== CHANNEL f1 =====
NUC1          1H
P0            10.80 usec
P1            10.80 usec
PL1           3.00 dB
SFO1         400.0318001 MHz

===== GRADIENT CHANNEL =====
GPNAM1       SINE.100
GPZ1         10.00 %
P16          1000.00 usec
NDO          1
TD           1
SFO1         400.0318 MHz
FIDRES       14.031071 Hz
SW           8.979 ppm
FnmODE       QF
SI           1024
SE           400.0300041 MHz
WDW          QSINE
SSB          0
LB           0.00 Hz
GB           0
PC           4.00
SI           1024
MC2          QF
SF           400.0300041 MHz
WDW          QSINE
SSB          0
LB           0.00 Hz
GB           0
    
```

ALI ANUS/DR.A.HAMEED/AA-23/DMSO
COSY



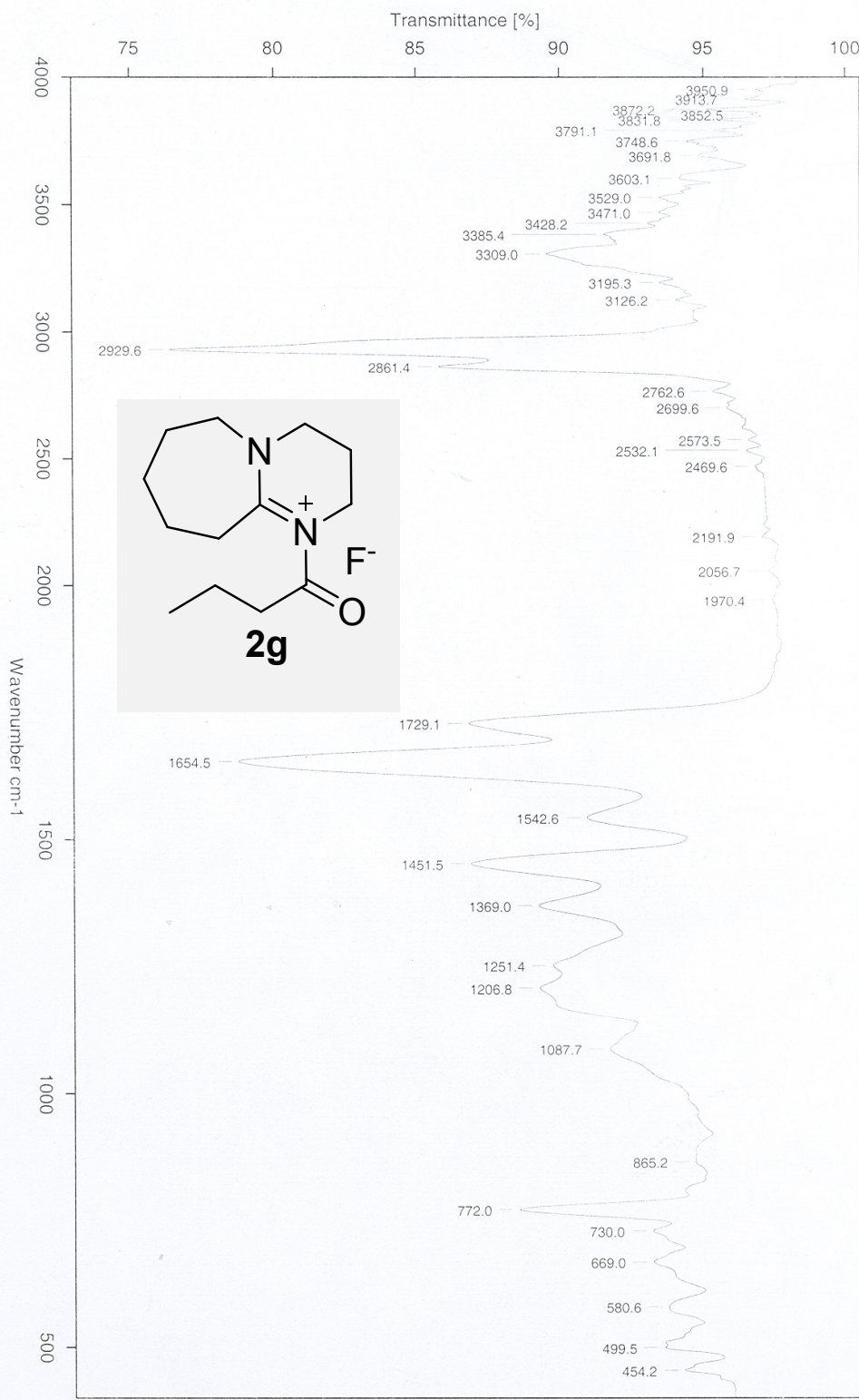
ALI ANUS / DR. A. HAMEED / AA-23 / DMSO
COSY

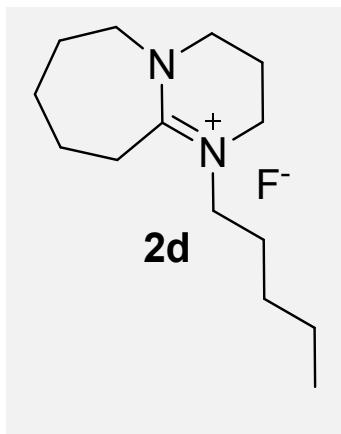


Supplementary Information (SI)

Sample : 4/ALI Anus
Measured : 24/07/2014 on VECTOR22
Resolution : 4 cm⁻¹ (10 scans)

Spectrum : 4:6 (in D:\FRSTUDENT)
Technic : SOLID
Analyst : ZAR/JAM





3.622
3.600
3.498
3.477
3.460
3.446
3.434
3.420
3.344
2.857
2.833
2.490
1.977
1.963
1.948
1.934
1.919
1.678
1.666
1.655
1.612
1.546
1.528
1.510
1.331

TAZEEN/DR. A. HAMED/DBD-C5-F/DMSO
1H

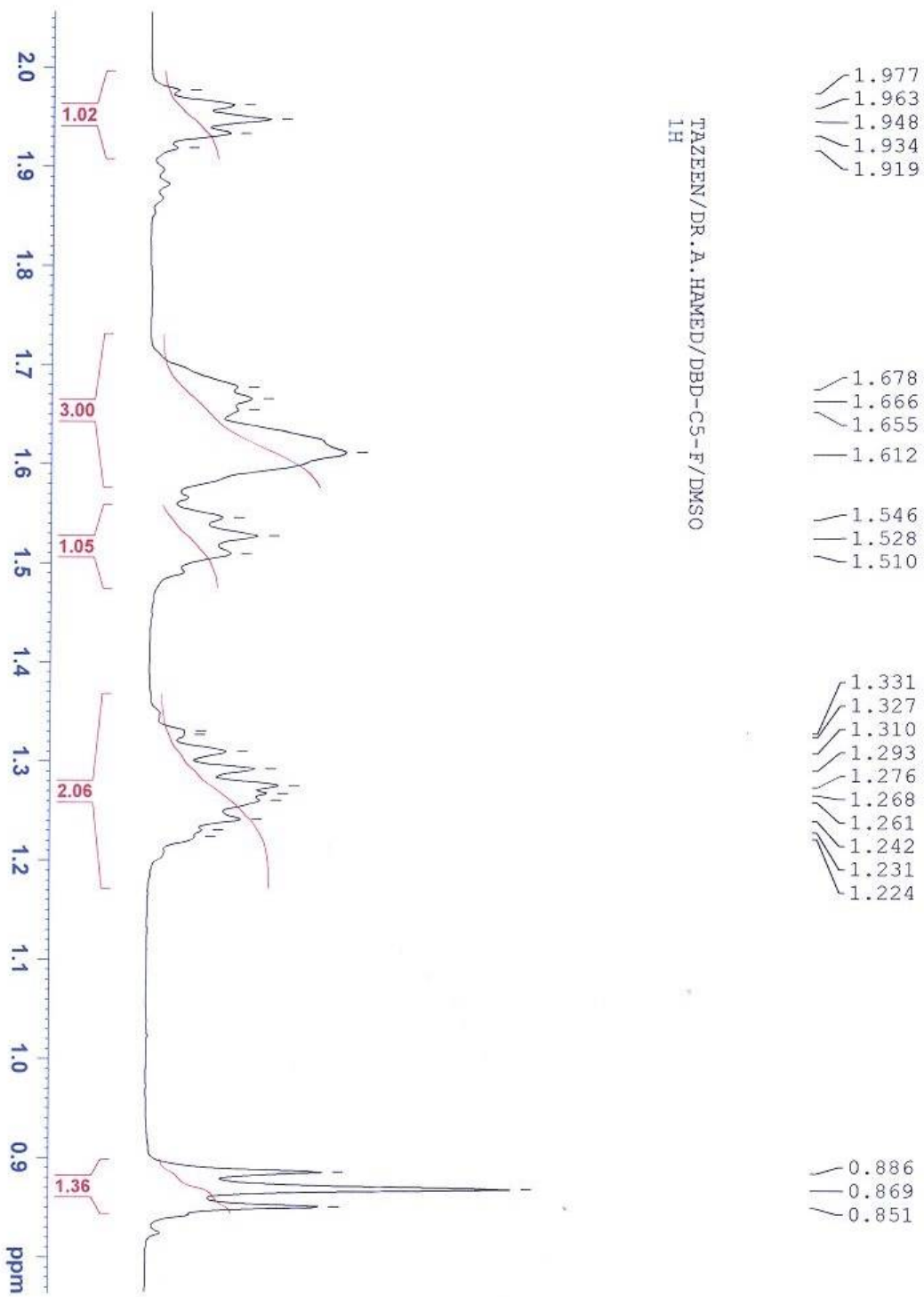


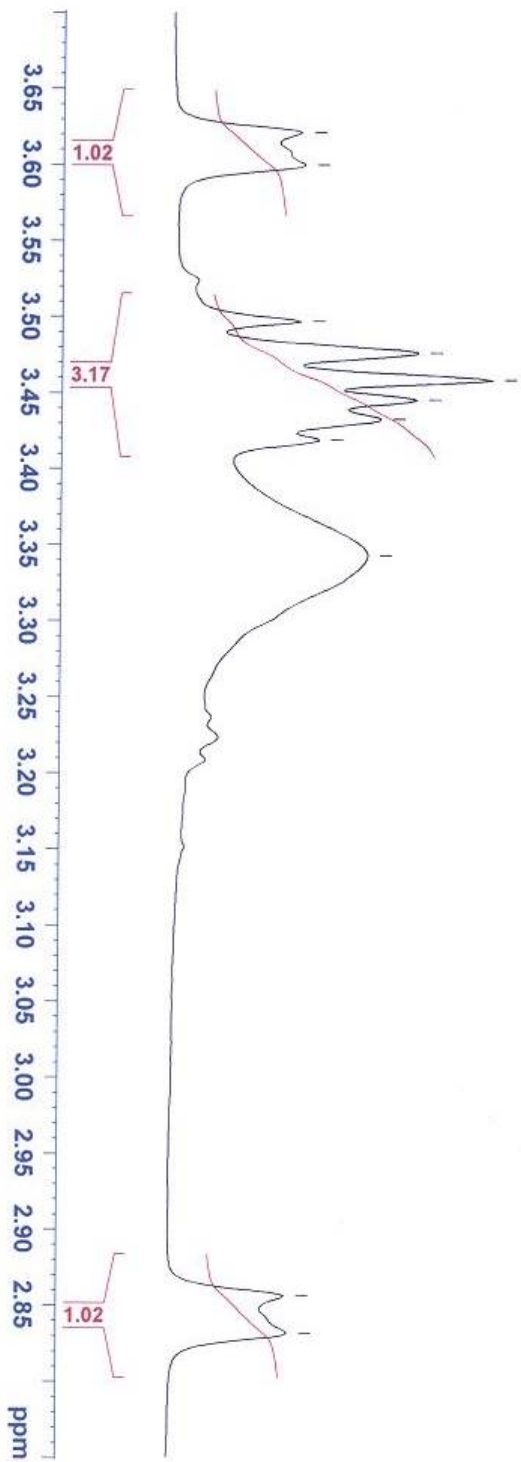
AVANCE AV-400 MHZ
Lab # 115

```

NAME      oct28-14
EXPNO     8
PROCNO    1
Date_     20141028
Time      10.52
INSTRUM   spect
PROBHD    5 mm SEI 1H-13
PULPROG   zg30
TD        32768
SOLVENT   DMSO
NS        32
DS        0
SMH       8012.820 Hz
FIDRES    0.244532 Hz
AQ        2.0447731 sec
RG        71.8
DM        62.400 usec
DE        6.50 usec
TE        300.0 K
D1        2.00000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      1H
P1        10.80 usec
PL1       3.00 dB
SFO1      400.0332002 MHz
SI        16384
SF        400.0300041 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```





TAZEEN/DR. A. HAMED/DBD-C5-F/DMSO
1H

— 3.622
— 3.600

— 3.498
— 3.477
— 3.460
— 3.446
— 3.434
— 3.420

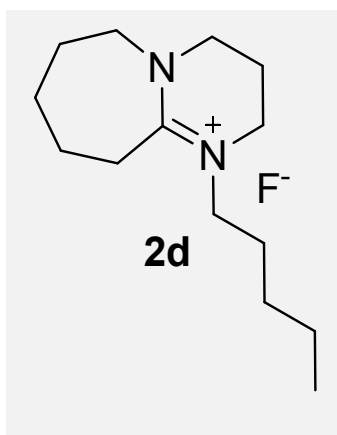
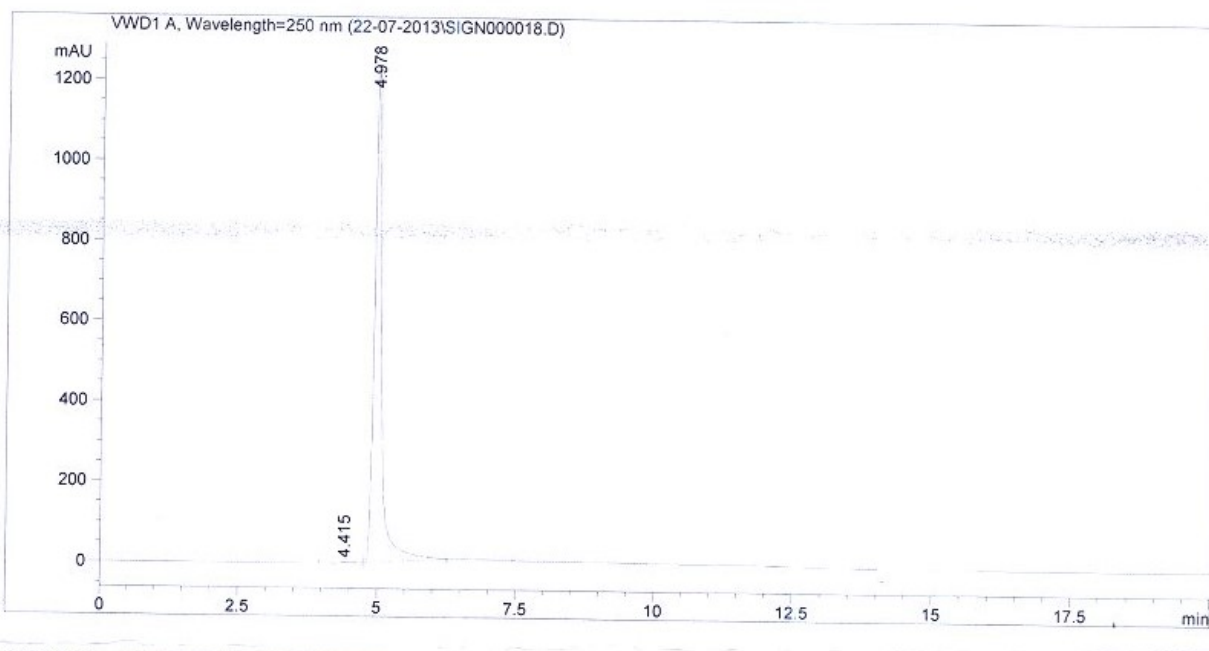
— 3.344

— 2.857
— 2.833

Supplementary Information (SI)

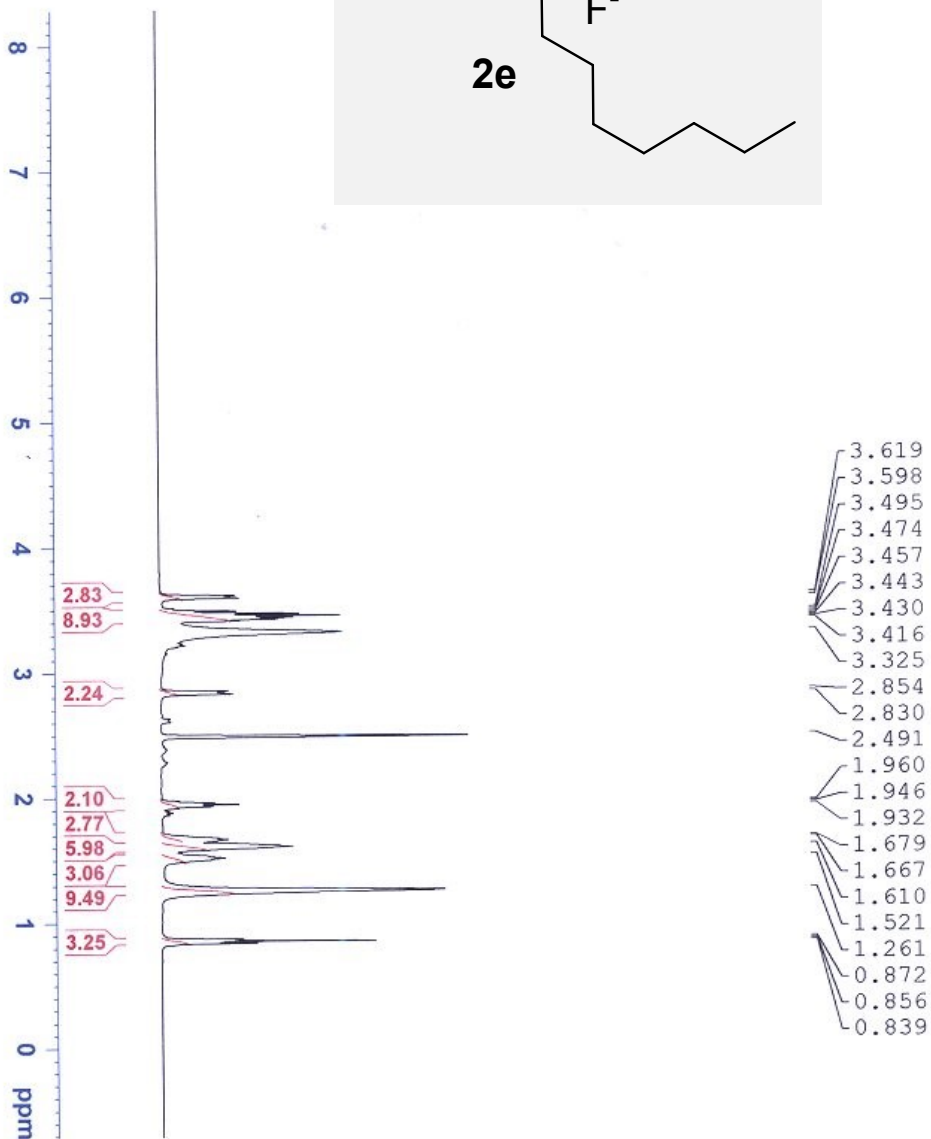
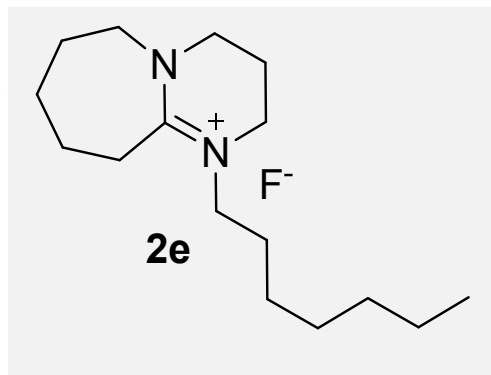
Data File C:\CHEM32\1\DATA\22-07-2013\SIGN000018.D
Sample Name: DBU_C5_

```
=====
Acq. Operator   : hameed
Acq. Instrument : Instrument 1                Location : Vial 1
Injection Date  : 10/28/2014 9:59:14 AM      Inj Volume : 1.000 µl
Acq. Method     : C:\CHEM32\1\METHODS\KINETIC.M
Last changed    : 10/28/2014 9:57:24 AM by hameed
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\KINETIC.M
Last changed    : 10/28/2014 10:19:18 AM by hameed
                  (modified after loading)
Method Info     : IONICLIQUIDS
Sample Info     : DBU_C5_
=====
```



TAZEEN/DR.A.HAMEED/AAC7F/DMSO
¹H

AVANCE AV-400 MHZ
 Lab # 115

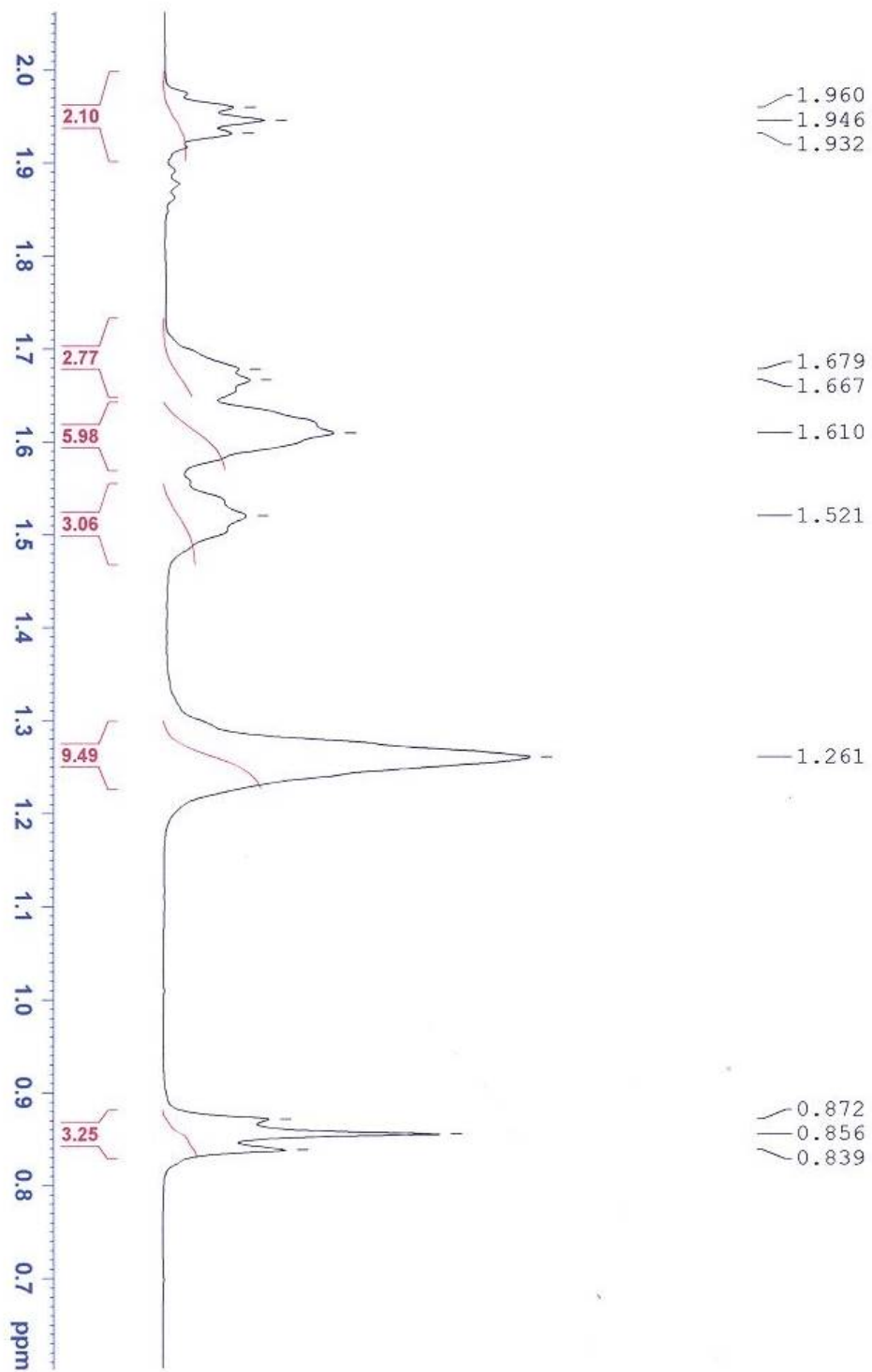


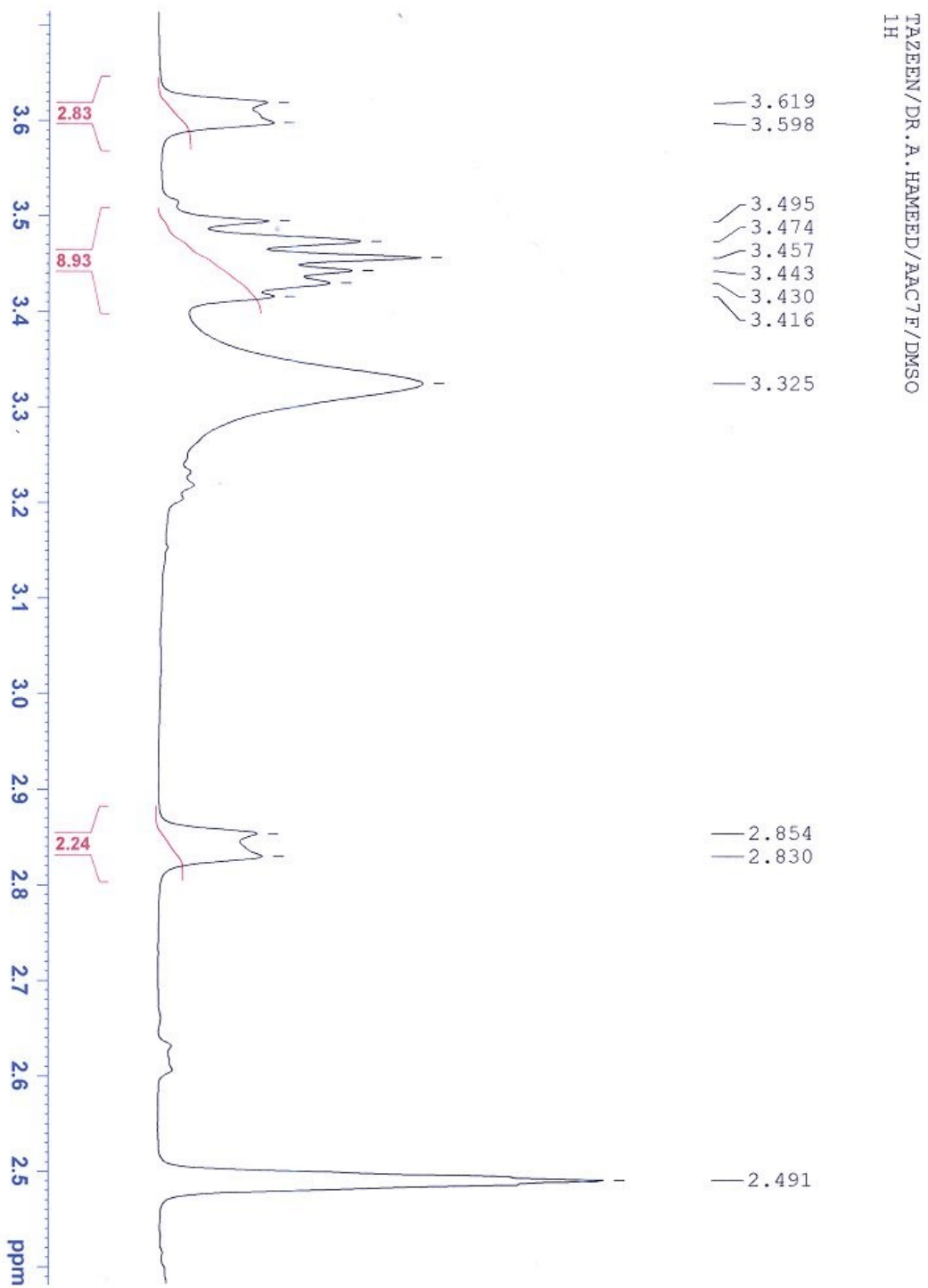
```

NAME          oct24-14
EXPNO         2
PROCNO        1
Date_         20141024
Time          11.31
INSTRUM       spect
PROBHD        5 mm SEI 1H-13
PULPROG       zg30
TD            32768
SOLVENT       DMSO
NS            32
DS            0
SWH            8012.820 Hz
FIDRES        0.244532 Hz
AQ            2.0447731 sec
RG            90.5
DE            62.400 usec
TE            300.0 K
D1            1.50000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            10.80 usec
PL1           3.00 dB
SFO1          400.032002 KHz
SI            16384
SF            400.0300041 KHz
WDW           EM
SSB           0
GB            0
PC            0.30 Hz
  
```


Supplementary Information (SI)

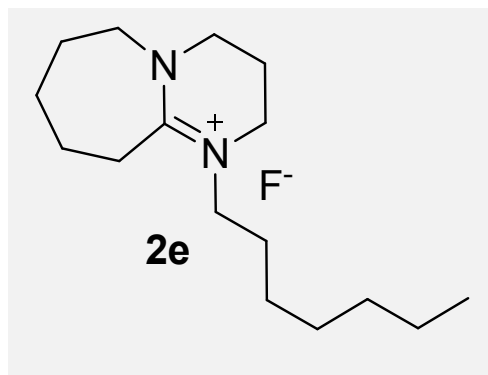
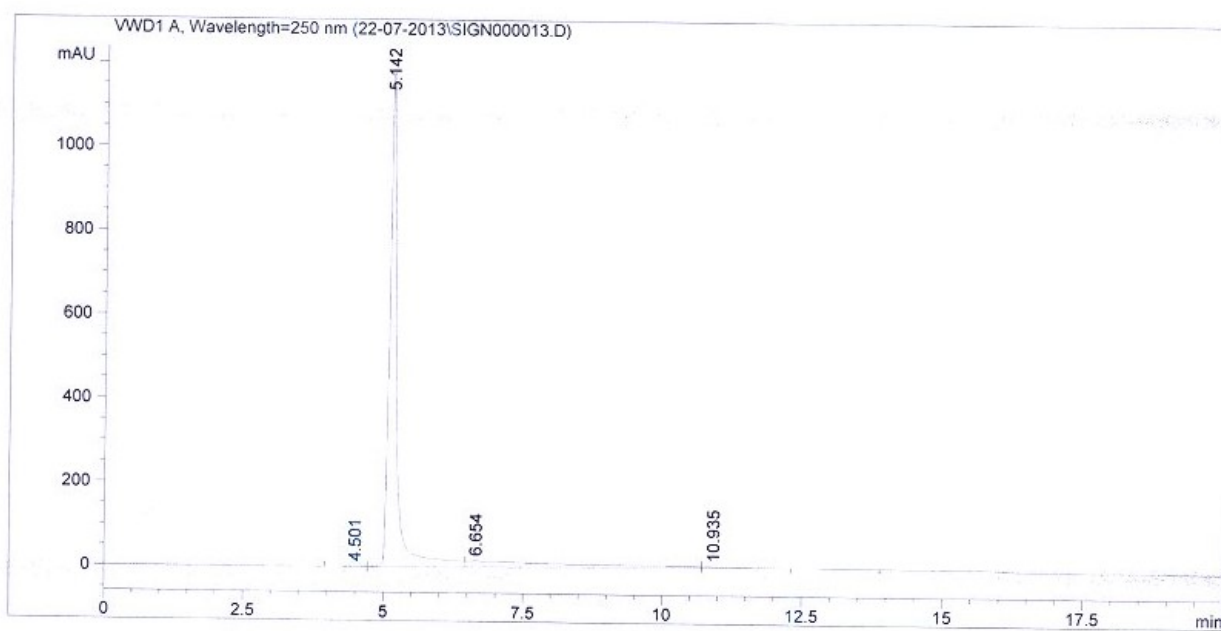


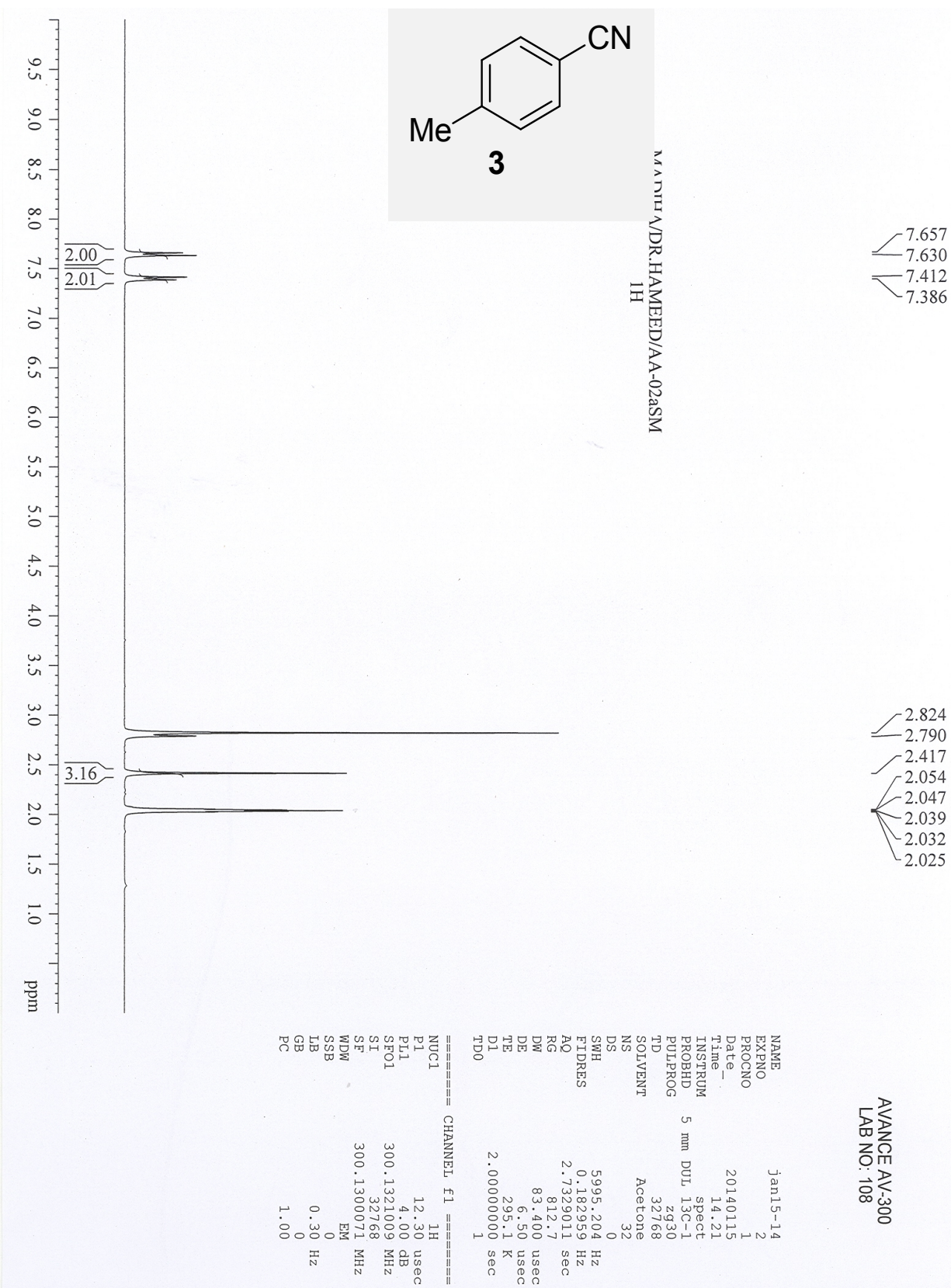


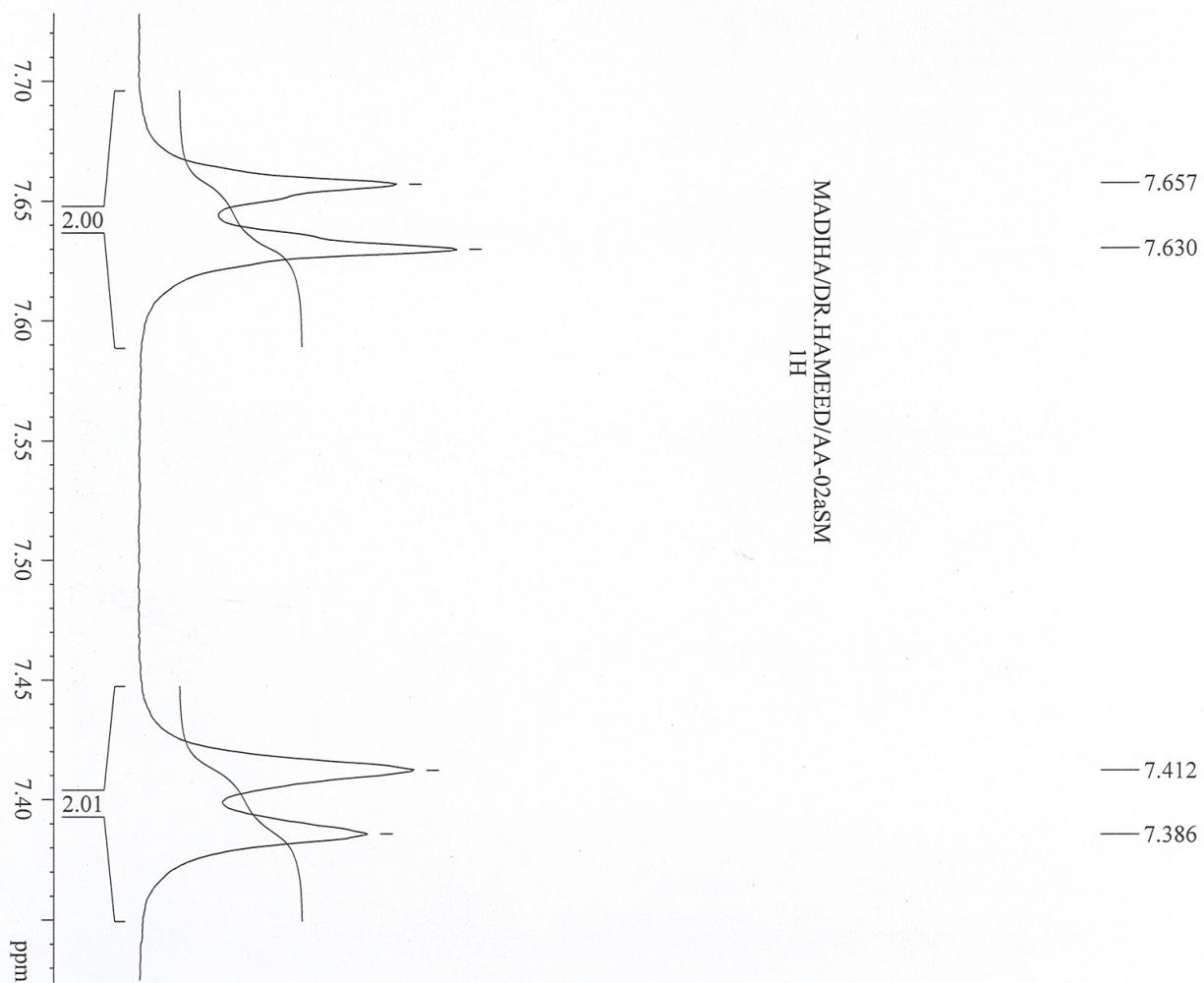
Supplementary Information (SI)

Data File C:\CHEM32\1\DATA\22-07-2013\SIGN000013.D
Sample Name: DBU_C7

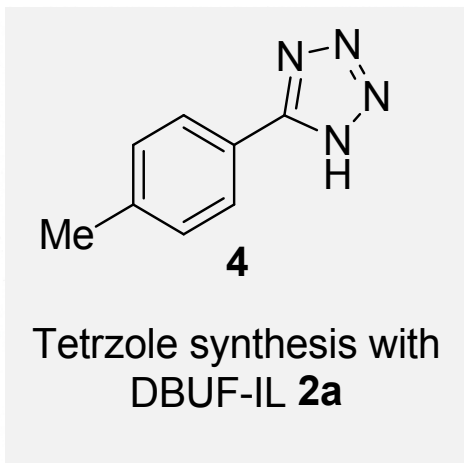
=====
Acq. Operator : hameed
Acq. Instrument : Instrument 1 Location : Vial 1
Injection Date : 10/24/2014 3:36:37 PM Inj Volume : 1.000 µl
Acq. Method : C:\CHEM32\1\METHODS\KINETIC.M
Last changed : 10/24/2014 3:34:10 PM by hameed
(modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\KINETIC.M
Last changed : 10/24/2014 3:56:42 PM by hameed
(modified after loading)
Method Info : IONICLIQUIDS
Sample Info : C-7_DBU



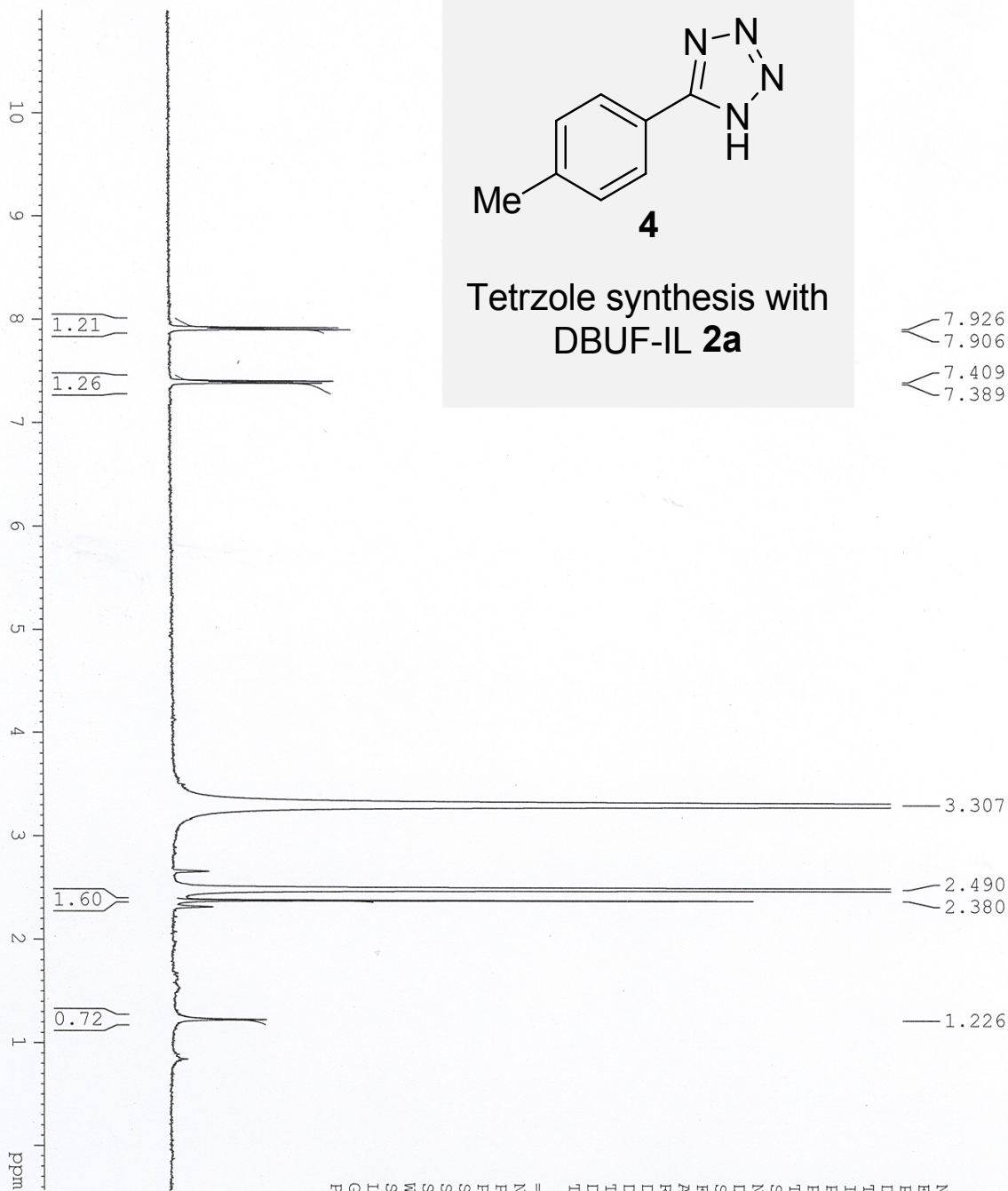




ALI ANUS/DR, FATIMA B/AA-40A/ICCBS U.O.K/



7.926
 7.906
 7.409
 7.389



```

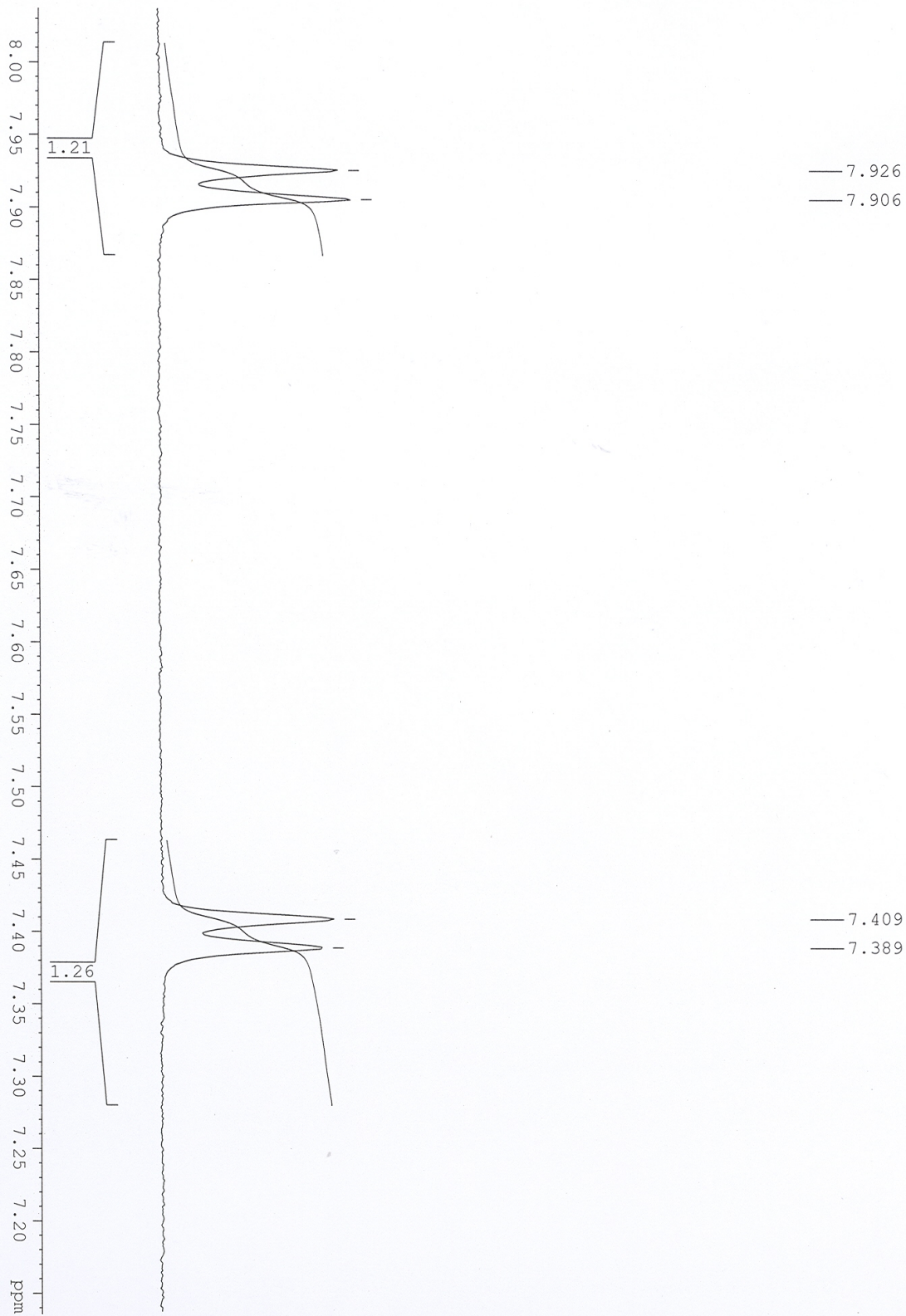
===== CHANNEL F1 =====
NAME          may21-14
EXPNO         1
PROCNO        1
Date_         20140521
Time_         11.58
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       zg30
TD            32768
SOLVENT       DMSO
NS            64
DS            0
SWH           8012.820 Hz
FIDRES        0.244532 Hz
AQ            2.0447731 sec
RG            2048
DE            62.400 usec
TE            300.0 K
D1            2.000000000 sec
TD0           1

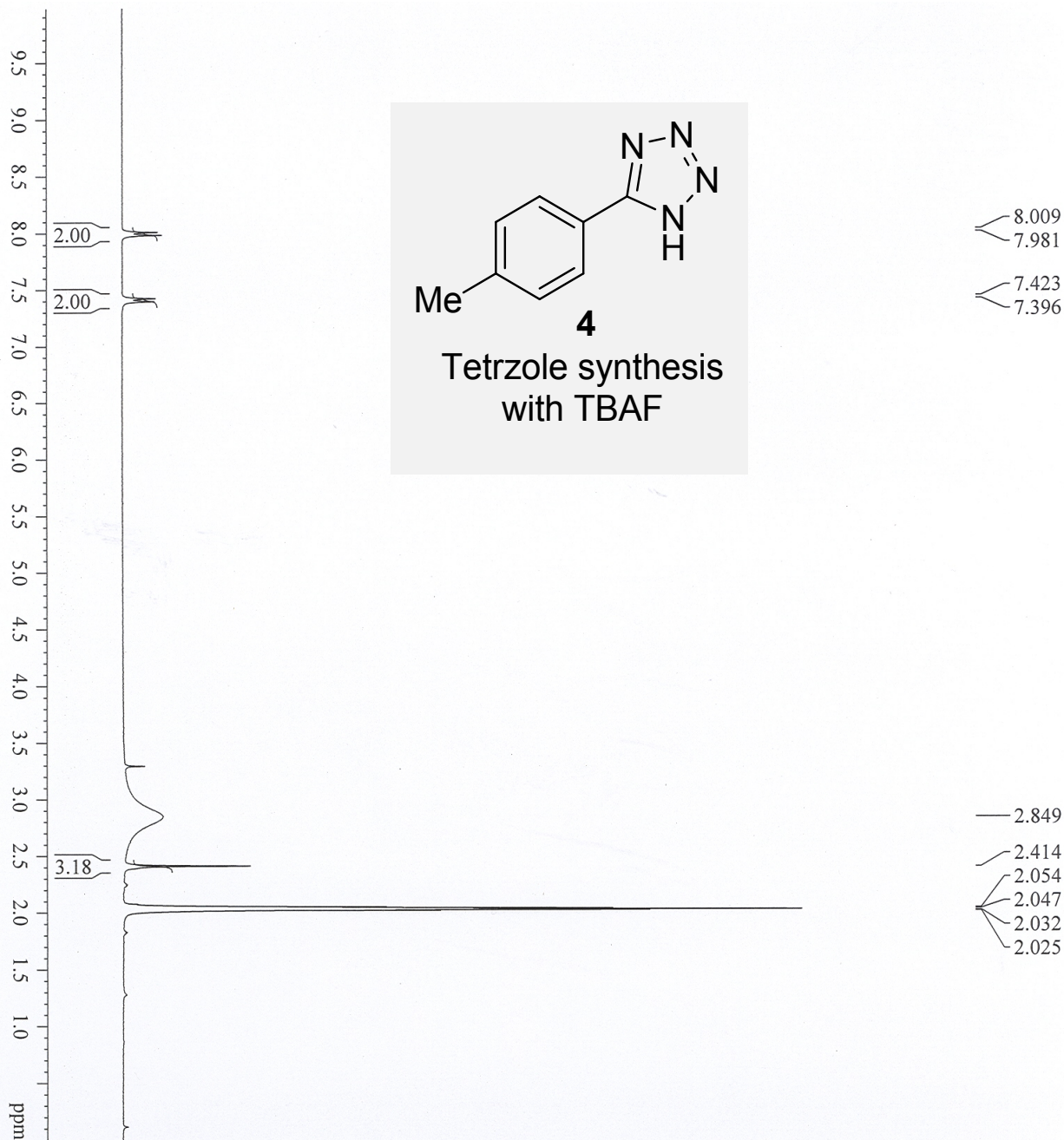
===== CHANNEL F1 =====
NUC1          1H
P1            10.20 usec
PL1           0.00 dB
SFO1          400.1332010 MHz
SI            16384
SF            400.1300064 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

AVANCE 400
 LAB NO 117

Supplementary Information (SI)

ALI ANUS/DR, FATIMA B/AA-40A/ICCBS U.O.K/





8.009
7.981
7.423
7.396

2.849
2.414
2.054
2.047
2.032
2.025

AVANCE AV-300
LAB NO: 108

```

===== CHANNEL f1 =====
NAME          Jan15-14
EXPNO         3
PROCNO        1
Date_         20140115
Time         14.34
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       zgpg30
TD            2930
SOLVENT       Acetone
NS            64
DS            0
SWH           5995.204 Hz
FIDRES        0.182959 Hz
AQ            2.7329011 sec
RG            812.7
DE            6.50 usec
TE            295.1 K
D1            2.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            12.30 usec
PL1           4.00 dB
SFO1          300.1321009 MHz
SI            32768
SF            300.1300071 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```