

This paper was retracted on March 20, 2015 (*J. Org. Chem.* **2015**, DOI: 10.1021/acs.joc.5b00397).

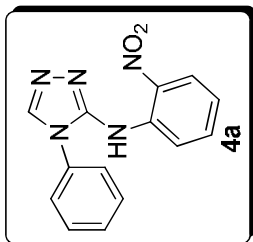
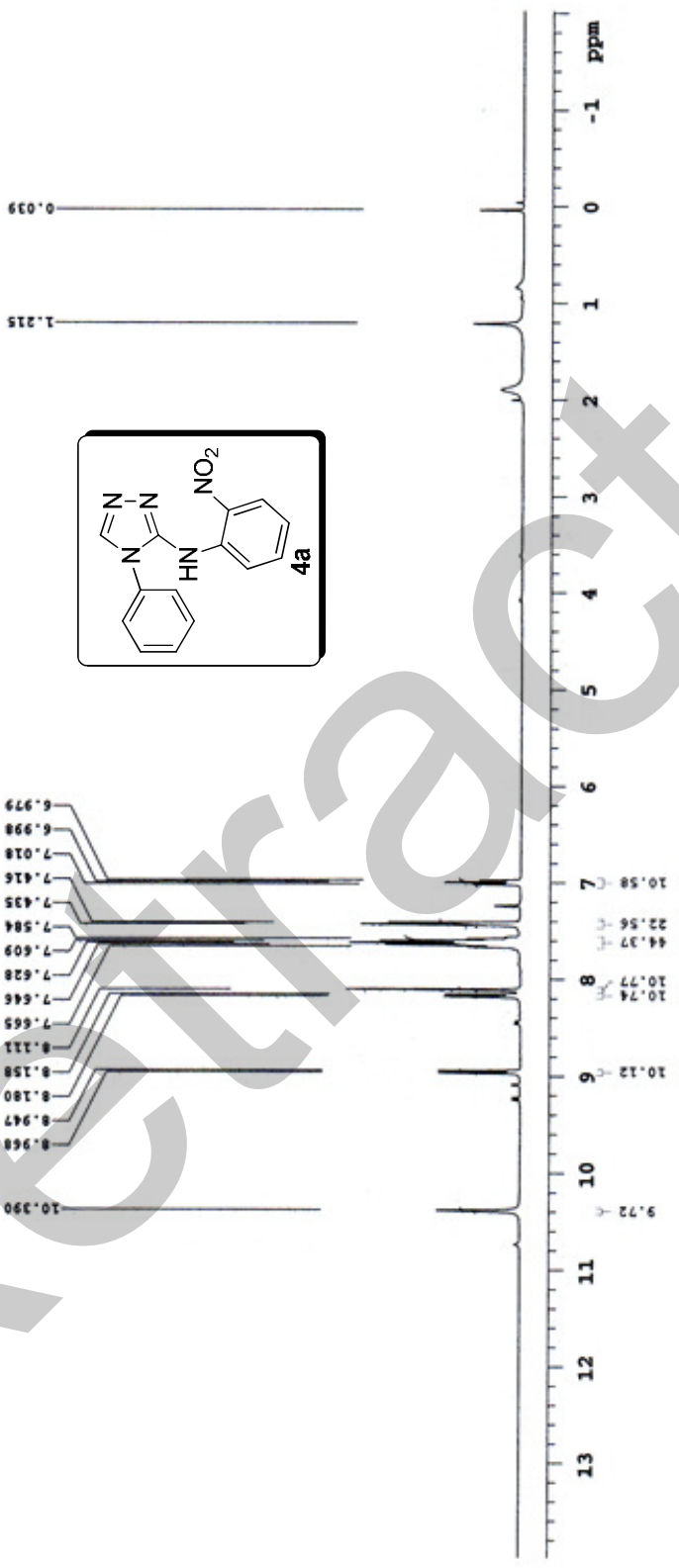
Room Temperature Cu(II)-Catalyzed Chemo- and Regioselective *Ortho*-Nitration of Arenes via C-H Functionalization

Pradeep Sadhu, Santhosh Kumar Alla and Tharmalingam Punniyamurthy*

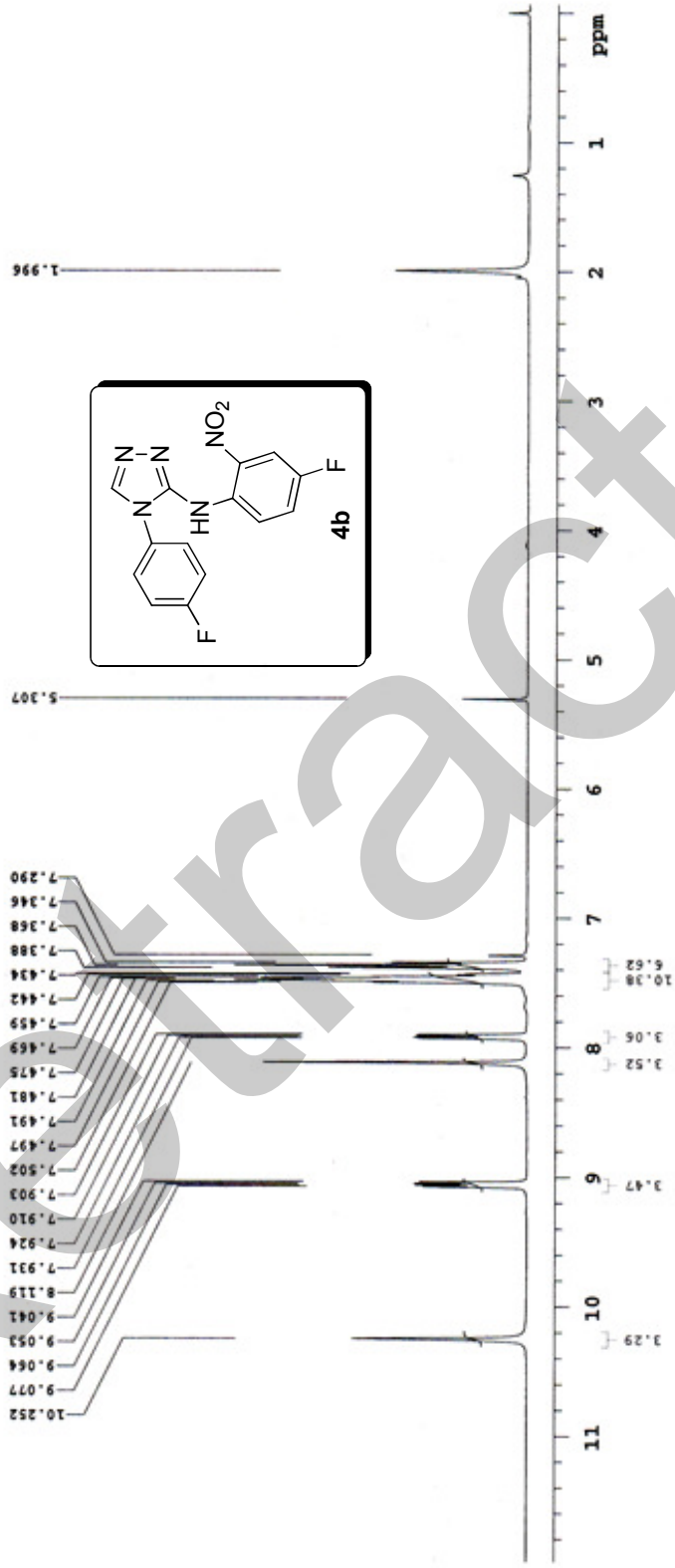
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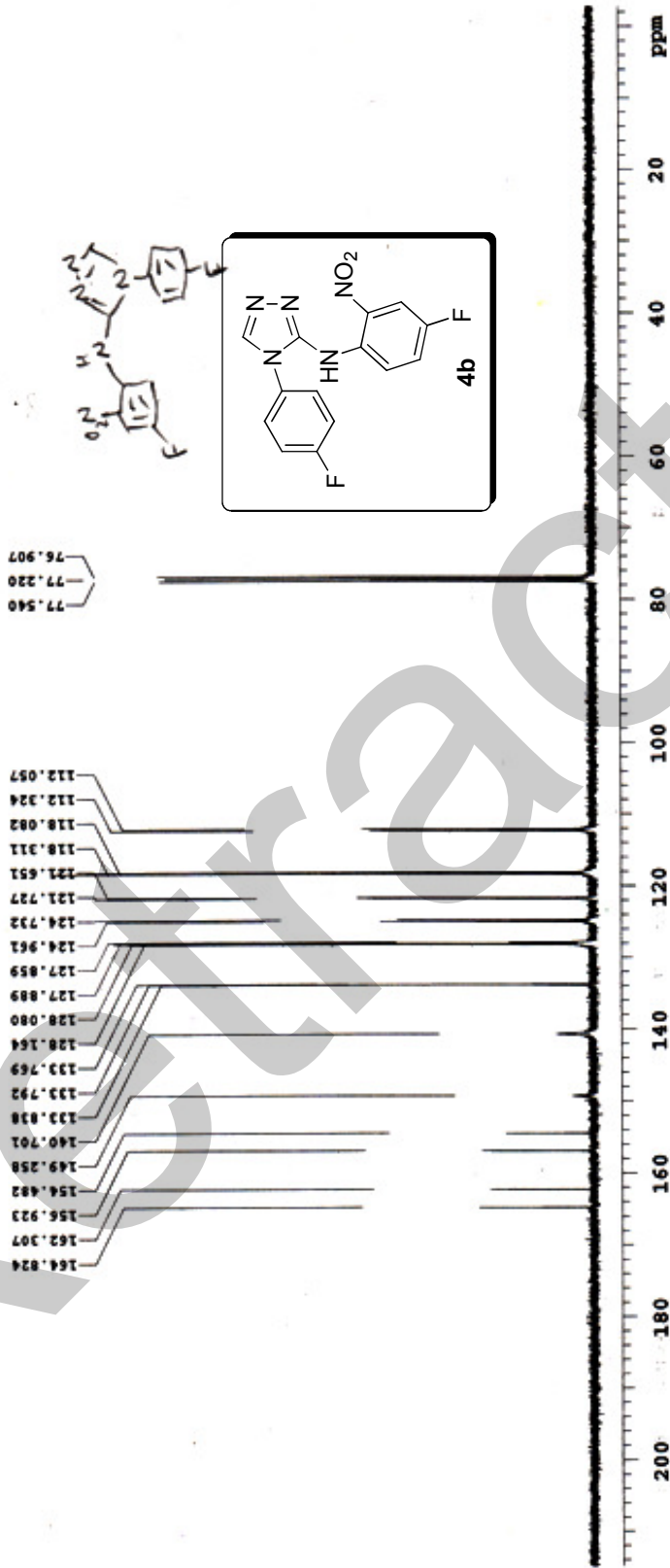
1. NMR (^1H and ^{13}C) Spectra of **4a-c**, **5a-b**, aniline- d_3 , **1r-d₃**, **2s-d** and **2r-d₂** S2-S15



<p>SEQUENCE</p> <p>Relax. delay 1.000 sec</p> <p>Pulse 45.0 degree</p> <p>Acq. time 2.561 sec</p> <p>Width 6398.0 Hz</p> <p>32 repetitions</p>	<p>OBSERVE: H1, 399.8509727</p>	<p>DATA PROCESSING</p> <p>FT size 32768</p> <p>Total time 1 minute</p>	<p>SP-552</p> <p>Solvent: cdcl3</p> <p>Temp. 25.0 C / 298.1 K</p> <p>Operator: chem</p> <p>Mercury-400 *HTR-800*</p>
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EXPERIMENT Relax-delay 1.000 sec Pulse: 45.0 degree Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	OBSERVE: 1H ; 399.8509523	DATA PROCESSING F2 size 32768 Total time 1 minutes	SP:399.850 Solvent: cdcl3 Temp: 25.0 C / 298.1 K Operator: chem File: SP-150214-F Mercury-400 *1H-399*
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SP-556-4-F

DATA PROCESSING SP-556-4-F

Relax delay 1.000 sec

Pulse 45.0 degrees

Acq time 1.304 sec

Width 25125.6 Hz

3090 repetitions

DECOUPLE H1, 399.8529994

Power 43 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING SP-556-4-F

Line broadening 0.5 Hz

FT size 65536

Total time 118 minutes

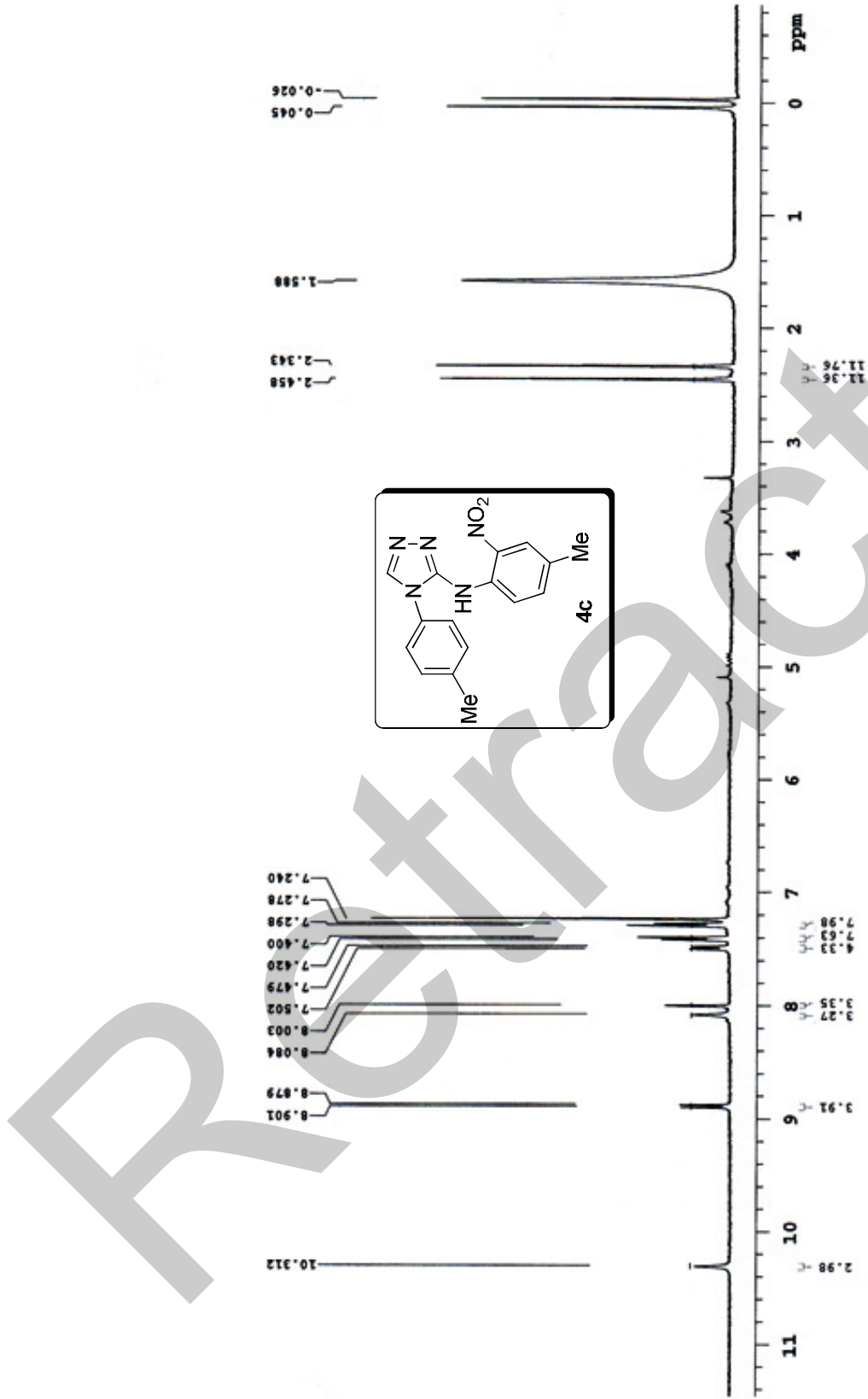
Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: chem

File: SP-556-4-F-13C

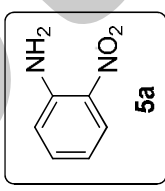
Mercury-400 "IITG-NMR"



SERIES SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degree Acq. time 2.561 sec Width 6398.0 Hz ff:repetitions	COSY/HSQC/NOE, 399.8509701	DATA PROCESSING FT size 32768 Total time 3:minutes	SAMP=8880
			140 MHz, 400 MHz Temp: 25.0 C / 298.1 K Operator: chem NS000014900 "1170-MMR"

SP-2NO2-B-21-8-14-1H

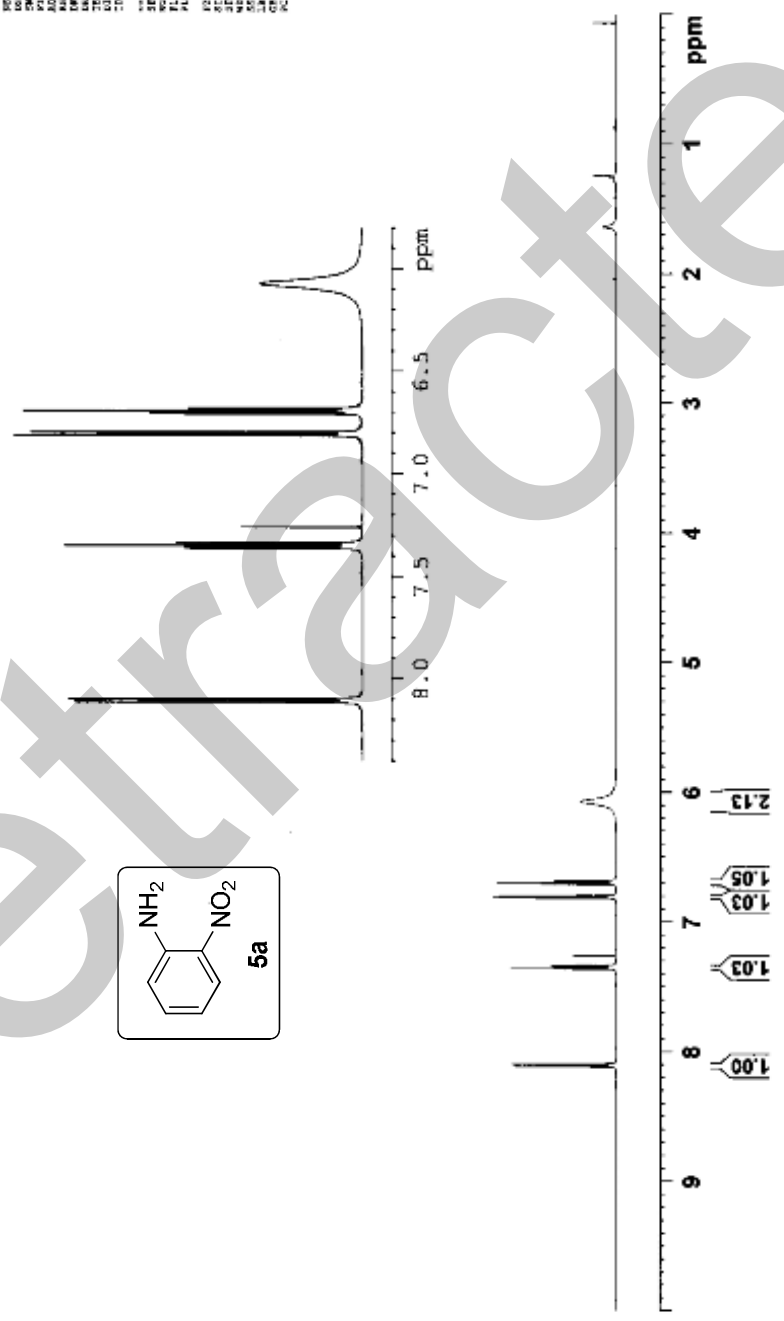
8.114
8.103
8.100
8.098
7.364
7.362
7.359
7.350
7.339
7.336
7.260
6.815
6.813
6.800
6.710
6.708
6.897
6.895
6.893
6.892
6.072



Date_ Time Parameters
NAME SP-2NO2-B-21-8-14-1H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
NAME SP-2NO2-B-21-8-14-1H
TIME 13.03
INSTRUM spect
PROBHD 5 mm ZB800 1H/1
PULPROG zgpg30
SFO 500.136060
SOLVENT H2O
NS 16
DS 4
SWH 12210.248 Hz
FIDRES 0.344788 Hz
AQ 1.363148 sec
RG 327.50
DQ 41.811 us
LQ 0.35 us
GZ 0.000000000000000000
CZ 1.018600000000000000
CZ0 0.000000000000000000

***** CHANNEL f1 *****
SFO2 610.171043 MHz
NUC1 15N
P1 12.00 us
PL1 0.000000000000000000
PL12 21.000000000000000000

F2 - Processing parameters
SI 32768
SF 610.171043 MHz
WDW 0
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



SP-2NO2-21-8-14-13C



Current Data Parameters
NAME SP-2NO2-21-8-14-13C
EXPNO 1
PROCNO 1

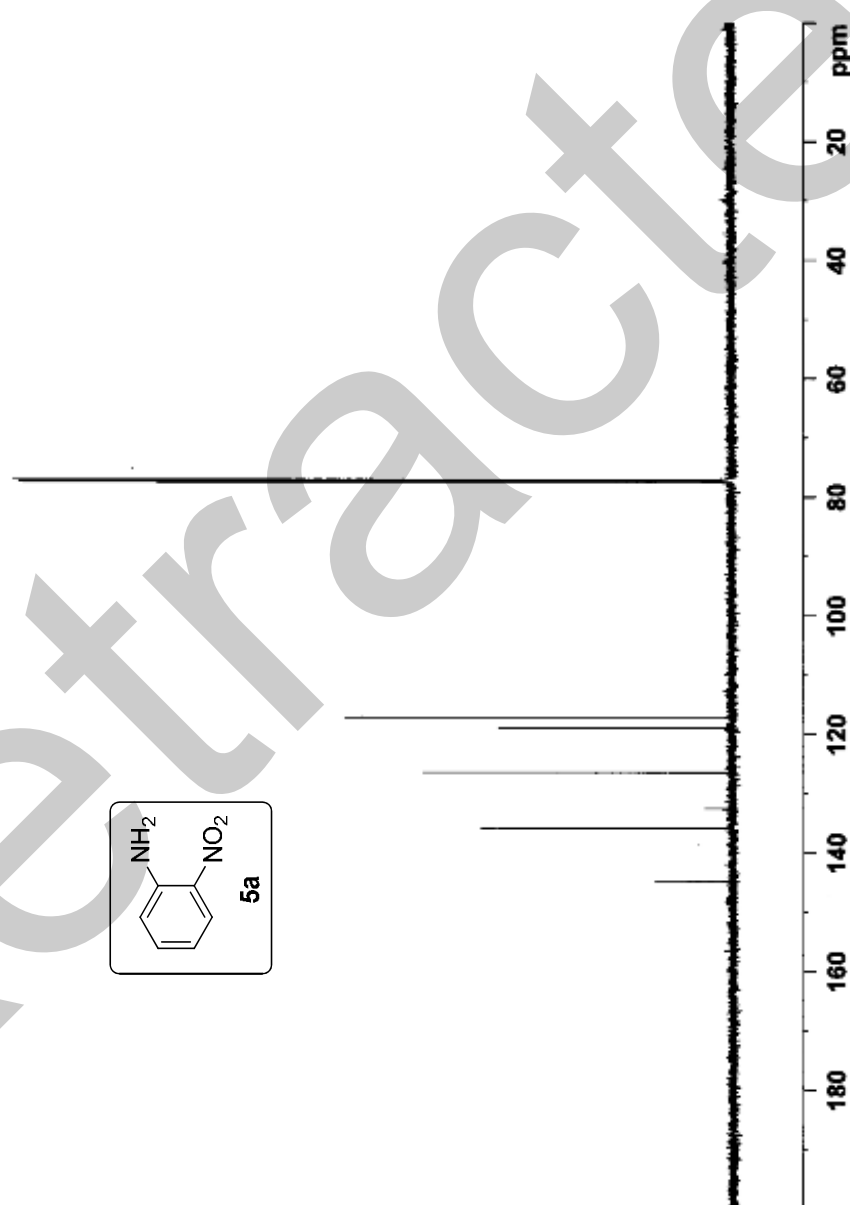
F2 - Acquisition Parameters
Date_ 20140821
Time 12.44
INSTRUM spect
PROBHD 5 mm RABBO DQ7
PULPROG zgpg30
TD 32768
SFO 400.146
CLOCK 300.135
GPR 17.2
DS 2
SWH 36057.697 Hz
FIDRES 1.100393 Hz
AQ 0.4543029 sec
RG 45.24
DQ 13.067 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.33000000 sec
TD0 1

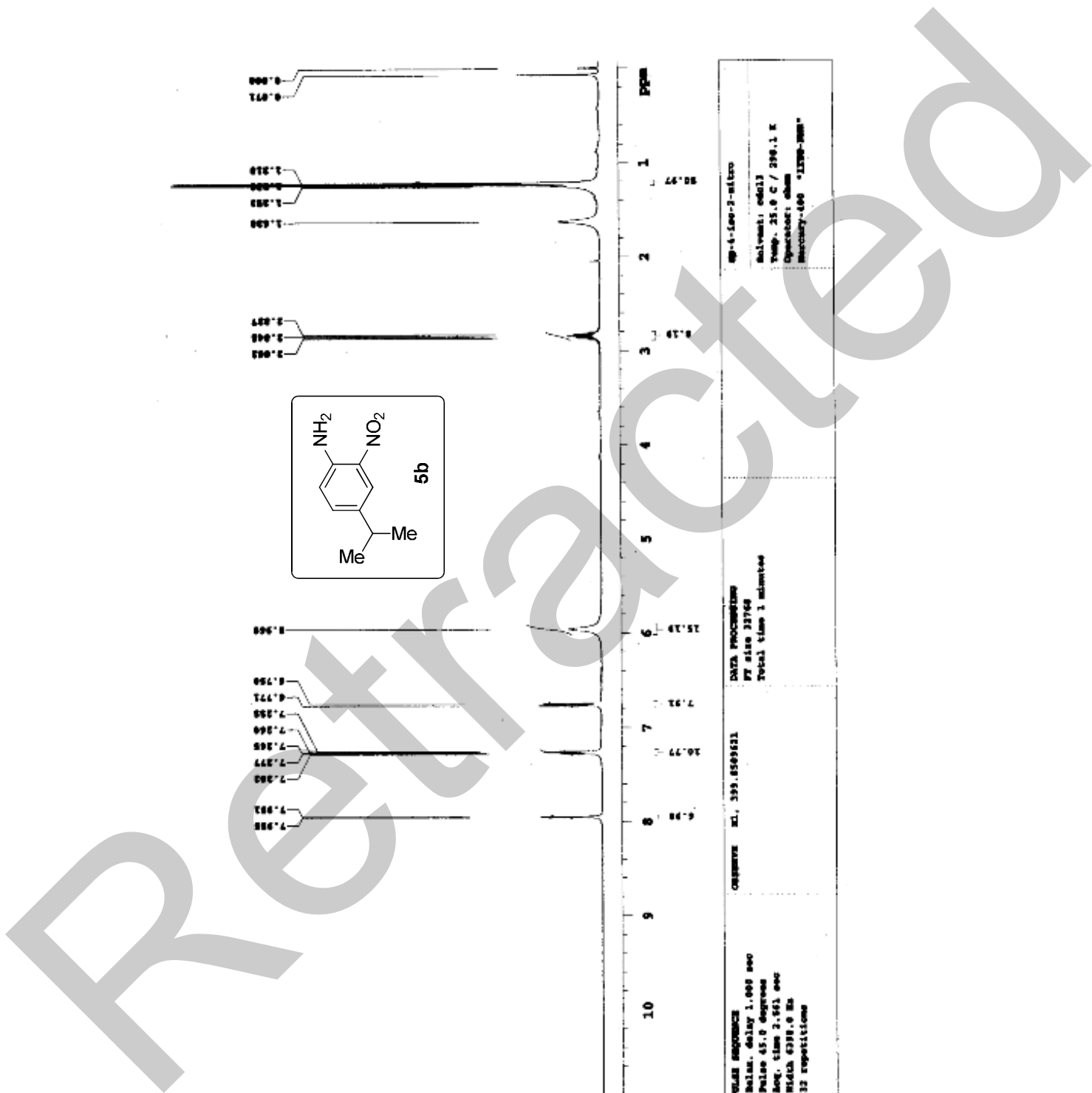
===== CHANNEL f1 =====
NUC1 150.9279571 MHz
P1 13C
SFO1 10.50 usec
PL1 95.00000000 W

===== CHANNEL f2 =====
NUC2 600.1704007 MHz
P2 1H
SFO2 10.50 usec
PL2 95.00000000 W

===== CHANNEL f3 =====
CPDPRG2 waltz16
PCPD2 70.00 usec
SFO3 21.00000000 MHz
PL3 0.61714000 W
PL13 0.30239999 W

F2 - Processing parameters
SI 16384
SF 150.9128301 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



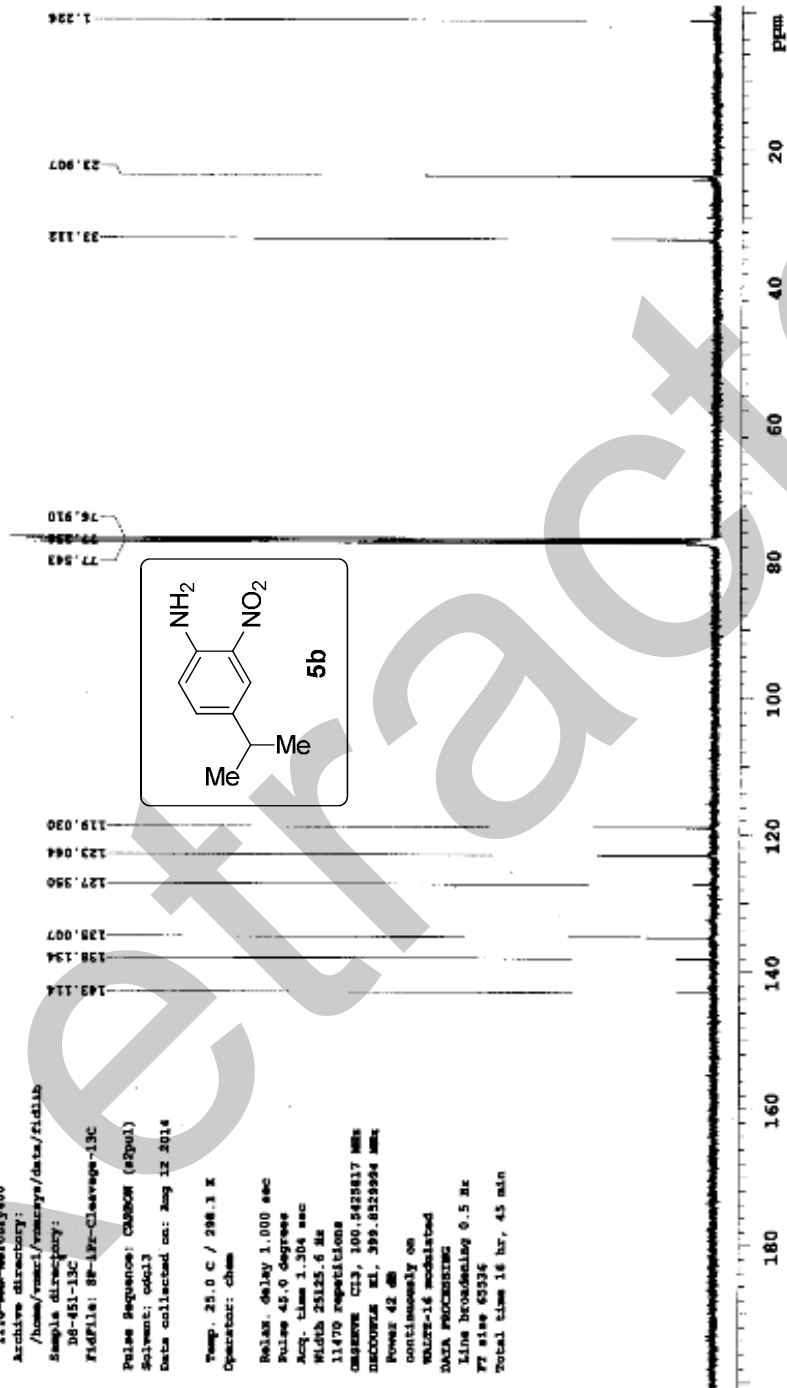


8F-13C-Cleavage-1R

Sample Name: 8F-13C-Cleavage-1R
Data Collected on: 11/10/98-mercury400
Archive directory: /home/rmci/rmcsys/data/fid11b
Sample directory: 30-451-13C
FIDFile: 8F-13C-Cleavage-13C
Pulse Sequence: CQSCOM (#2pul)
Solvent: cdcl3
Data collected on: Aug 12 2014

Temp: 25.0 C / 200.1 K
Operator: chem

Pulse delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.304 sec
Width 25125.6 Hz
11470 repetitions
current: 13, 100.5425817 MHz
recorder: 32, 399.0129954 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
F2 size 65536
Total time 16 hr, 45 min



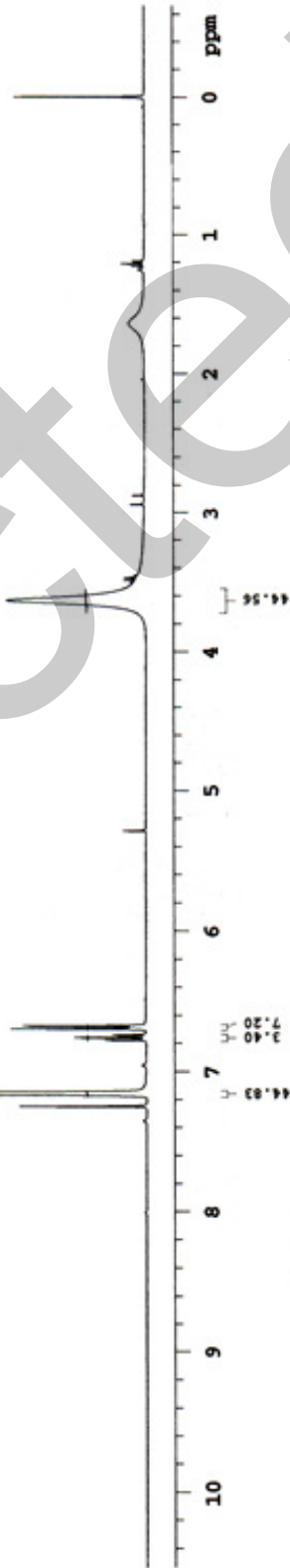
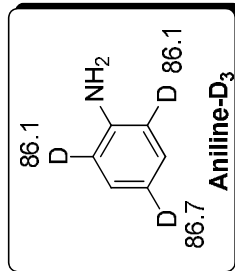
SP-ANILINE-D3
Sample Name:
SP-ANILINE-D3
Data Collected on:
IITG-NMR-mercury400
Archive directory:
/export/home/chempack/vmar/sy/data
Sample directory:

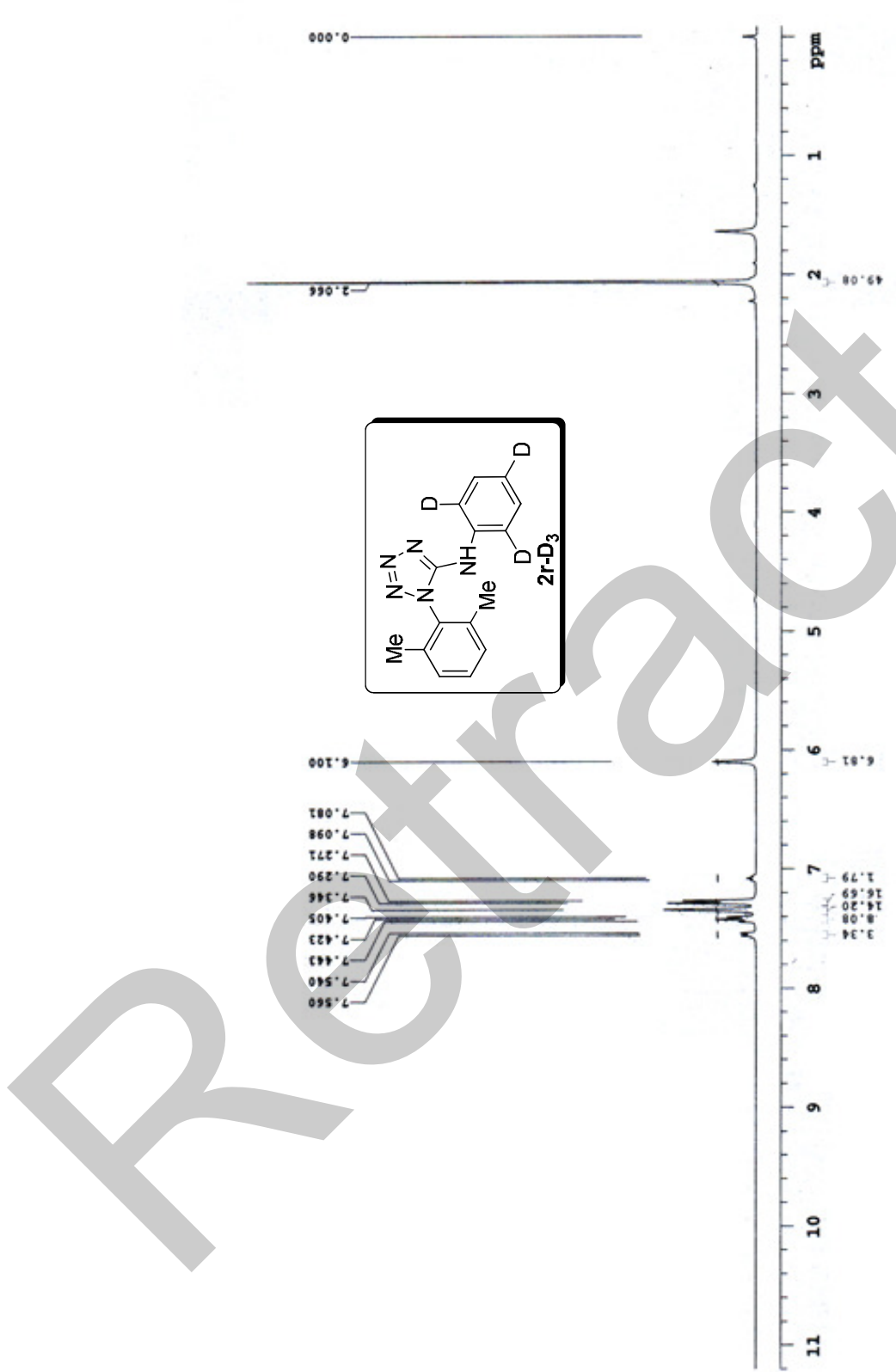
Fidfile: PROTON
Pulse Sequence: PROTON (e2pul)
Solvent: cdcl3
Data collected on: Jan 19 2014

Temp. 25.0 C / 298.1 K
Operator: chem

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.561 sec
Width 6398.0 Hz
32 repetitions

OBSERVE H1, 399.8509687 MHz
DATA PROCESSING
F1 size 32768
Total time 2 min 12 sec





<p>POWER SEQUENCE</p> <p>Relax. delay 1.000 sec</p> <p>Pulse 45.0 degrees</p> <p>Acq. time 2.561 sec</p> <p>Width 6396.0 Hz</p> <p>132 repetitions</p>	<p>DATA PROCESSING</p> <p>FT size 32768</p> <p>Total time: 1 minute</p>	<p>SP-DN-D3</p> <p>Solvent: cdcl3</p> <p>Temp. 25.0 C / 298.1 K</p> <p>Operator: cbeam</p> <p>Mercury-400 FTIR-MGR</p>
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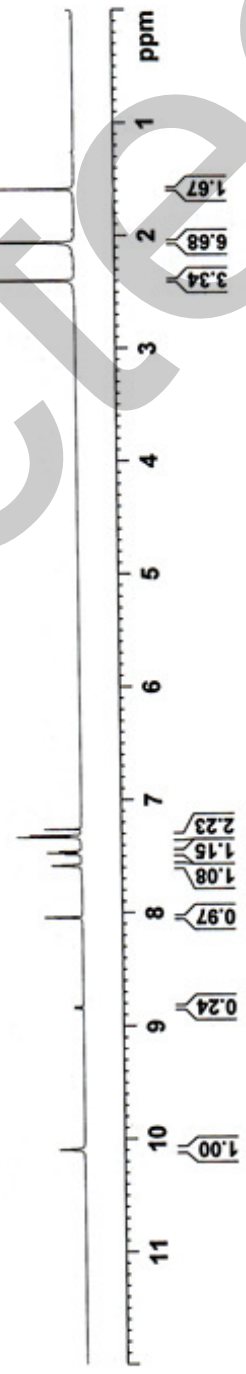
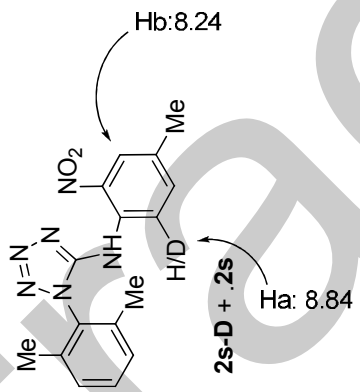
SP-564-D1-1H

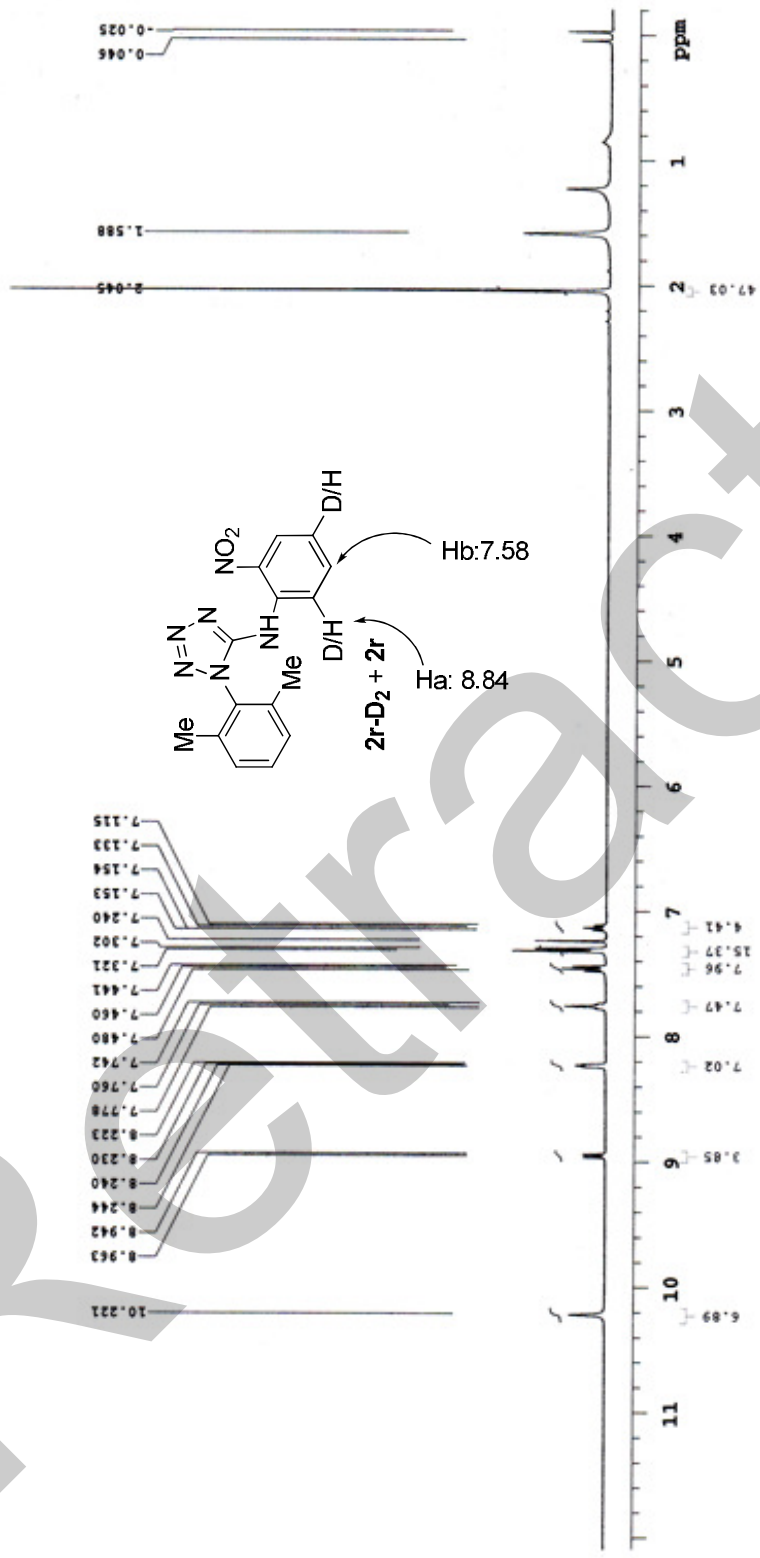
Current Data Parameters
NAME SP-564-D1-1H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160313
Time 11:33
INSTRUM spect
PROBHD 5 mm PABBO BBO
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 4
SWH 12019.220 MHz
FIDRES 0.366798 MHz
AQ 1.3631488 sec
RG 327.68
AQ 41.620 usec
DE 6.50 usec
TE 300.3 K
TD 1.0000000 sec
SFO 500.1363000 MHz
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 21.0000000 W
===== CHANNEL f2 =====
F2 - Processing parameters
SI 32768
SF 650.130148 MHz
WDW EM
SSB 0
LB 0.30 MHz
GB 0
PC 1.00

1.586
2.059
2.396

7.260
7.316
7.328
7.455
7.468
7.481
7.581
8.041
8.842
8.827

10.092





<p>EXPERIMENTAL</p> <p>Relax. delay 1.000 sec</p> <p>Pulse 45.0 degrees</p> <p>Acq. time 5.122 sec</p> <p>Width 6398.0 Hz</p> <p>32 repetitions</p>	<p>ORIGIN: FILE: 399.8509921</p> <p>DATA PROCESSING</p> <p>FT size 65536</p> <p>Total time 3 minute</p>	<p>EXP: 565-103</p> <p>SOVENT: CDCl₃</p> <p>Temp: 25.0 °C / 298.1 K</p> <p>Operator: cbm</p> <p>Machine: 400 *JITD-MMR*</p>
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