

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

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Crystal Structure Compound **2c**:

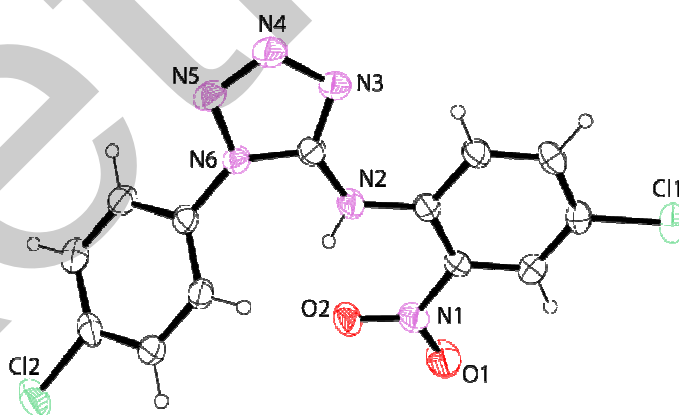


Figure 1: ORTEP diagram of *N*-(4-Chloro-2-nitrophenyl)-1-(4-chlorophenyl)-1*H*-tetrazol-5-amine **2c** with 50% ellipsoid.

Crystal Data and Structure Refinement for 2c at 296(2) K

Identification code	2c
Empirical formula	C ₁₃ H ₈ Cl ₂ N ₆ O ₂
Formula weight	351.15
Temperature	296(2)
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	$a = 6.4492(5)$ Å $\alpha(^{\circ}) = 101.507(7)$ $b = 7.6732(7)$ Å $\beta(^{\circ}) = 94.517(6)$ $c = 15.1467(11)$ Å $\gamma(^{\circ}) = 90.802(7)$
Volume	731.86(10) Å ³
Z	2
Density (calculated)	1.594 Mg/m ³
Absorption coefficient	0.463 mm ⁻¹
$F(000)$	356.0
Crystal size	0.26 x 0.22 x 0.18 mm
Theta range for data collection	25.00 °
Index ranges	-7 ≤ h ≤ 7, -9 ≤ k ≤ 9, -17 ≤ l ≤ 17
Reflections collected	2572
Independent reflections	1682
Completeness to theta = 27.66°	99.8 %
Absorption correction	Multi-scan
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters

2572/ 0 /212

Goodness-of-fit on F^2

1.228

Final R indices [$I > 2\sigma(I)$]

$R_I = 0.0450$, $wR_2 = 0.0604$

R indices (all data)

$R_I = 0.0784$, $wR_2 = 0.0722$

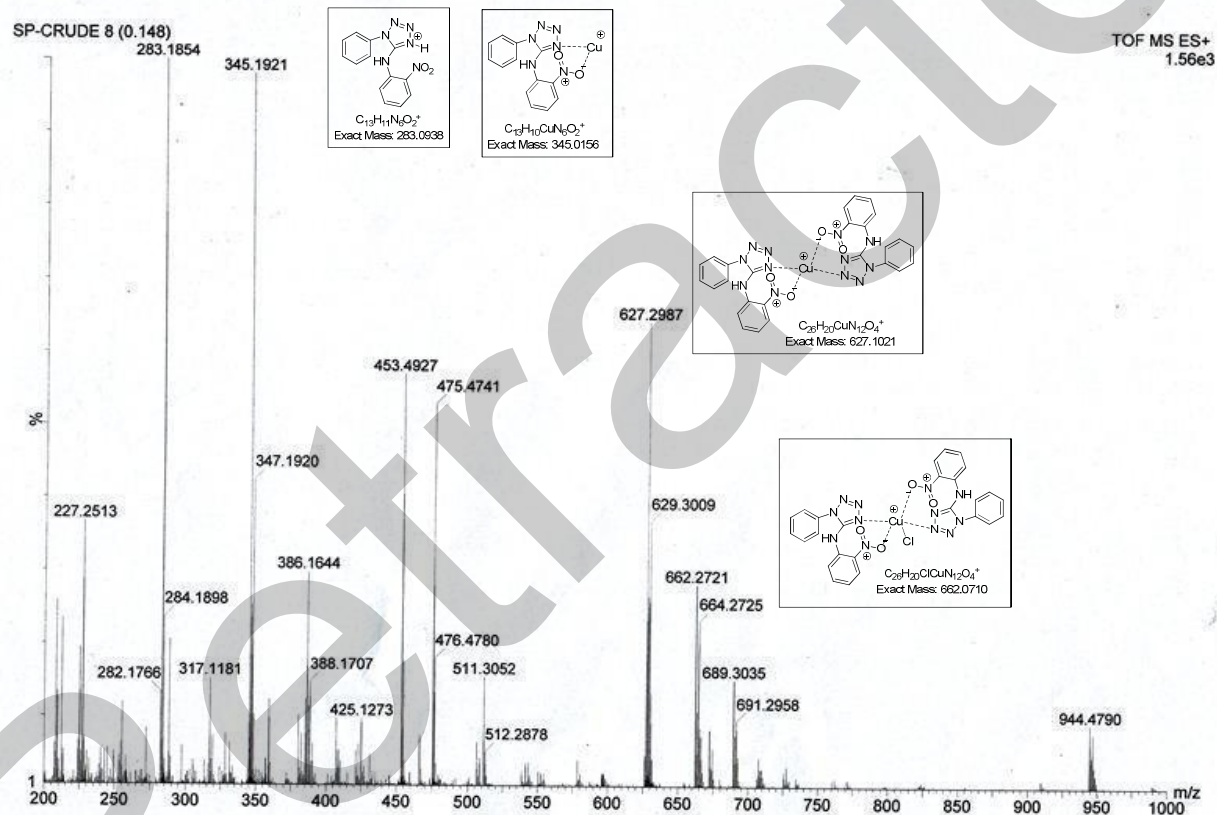
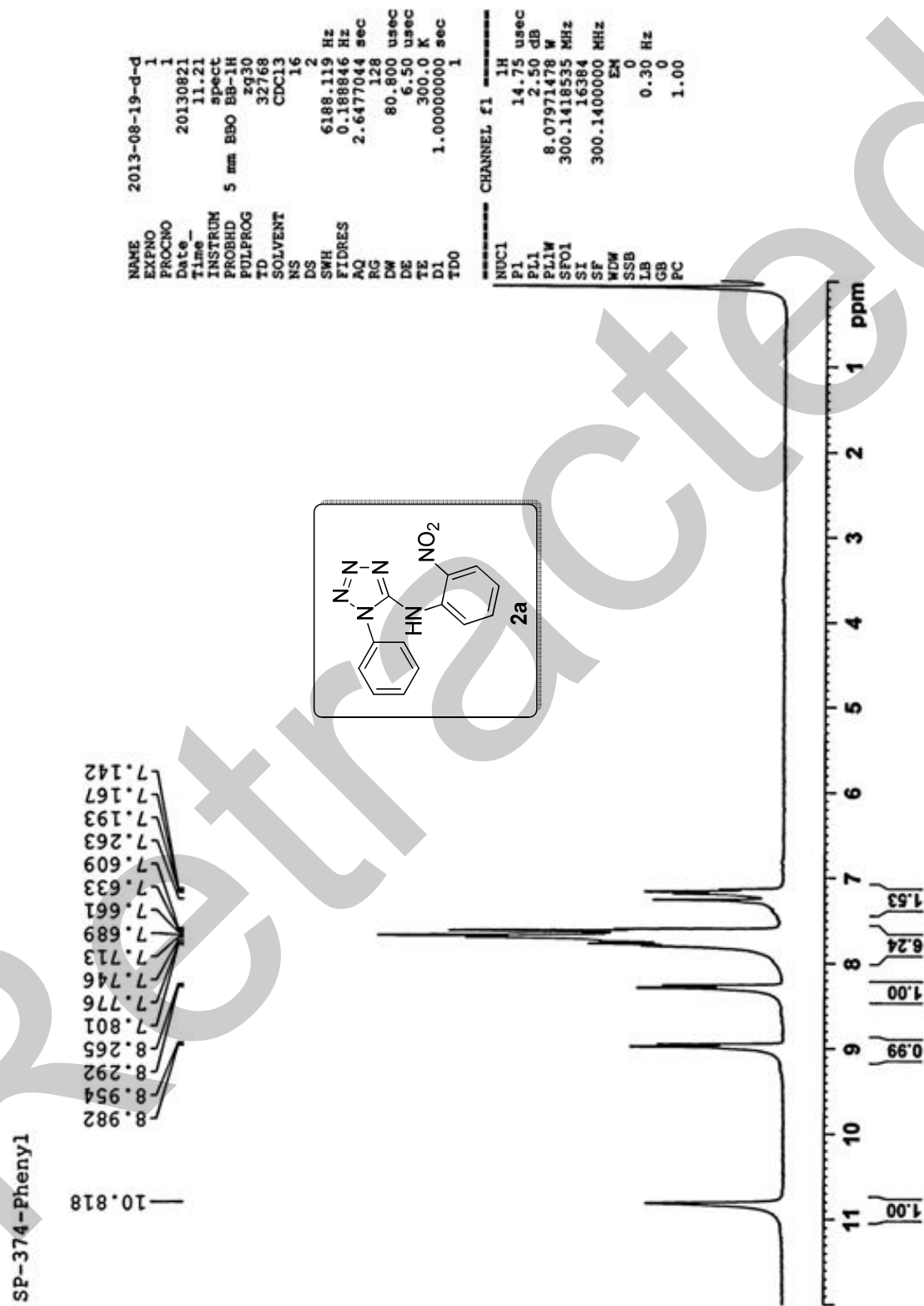


Figure S1. Mass spectra of reaction mixture **1a** prior to work up.

^1H and ^{13}C NMR Spectra of the Compounds 2a-v and 4a-c



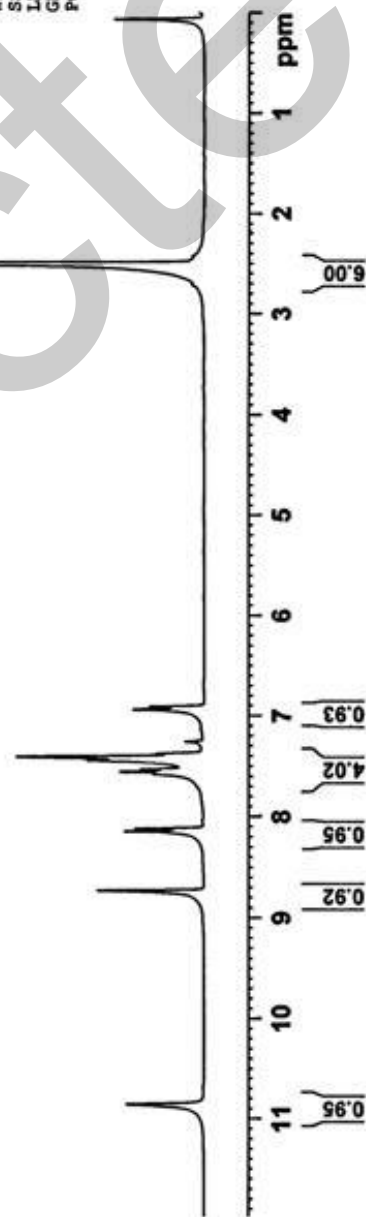
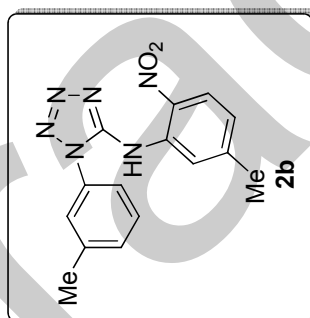


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8.152
8.123
7.585
7.561
7.536
7.449
7.413
7.384
6.944
6.916

2.505



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Time_	11.19
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PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	6188.119 Hz
FIDRES	0.188846 Hz
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TD0	1

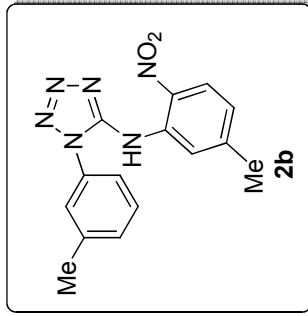
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SFO1	300.1418535 MHz
SI	16384
SF	300.1400000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

SP-386-3-Me

150.72
149.41
141.40
135.79
132.89
132.20
131.84
130.60
126.37
125.17
123.43
121.62
119.86

77.65
77.43
77.23
76.81

22.52
21.55



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PROCNO 1
Date_ 20130901
Time_ 0.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 3000
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 80.6
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PL1 -0.50 dB
PL1W 34.66611099 W
SFO1 75.4778101 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 2.50 dB
PL12 19.20 dB
PL13 23.00 dB
PL2W 8.07971478 W
PL12W 0.17274120 W
PL13W 0.07201053 W
SFO2 300.1412006 MHz
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SF 75.4702500 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

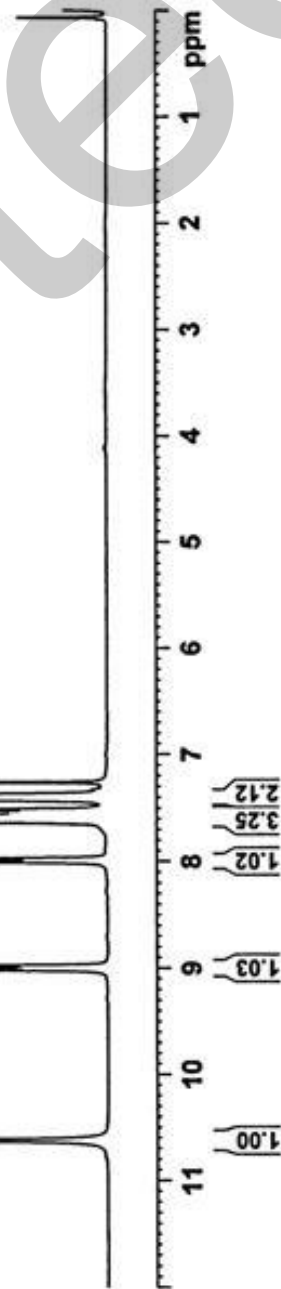
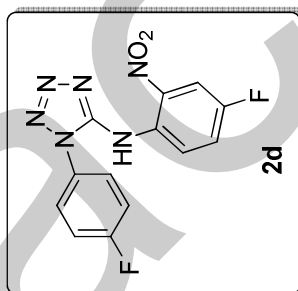


SP-389-F

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9.007
8.991
8.975
8.011
8.002
7.984
7.974
7.636
7.621
7.607
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7.565
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7.374
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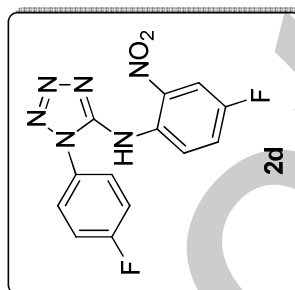
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TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.188846 Hz
AQ 2.6477044 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 14.75 usec
PL1 2.50 dB
PL1W 8.07971478 W
SFO1 300.1418535 MHz
SI 16384
SF 300.1400000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



SP-389-F

165.34
161.98
157.94
154.67
150.60
134.63
134.52
132.18
132.15
127.94
127.89
126.98
126.86
124.91
124.61
121.81
121.72
118.14
117.82
112.72
112.36
77.43
77.21
77.01
76.59



2d

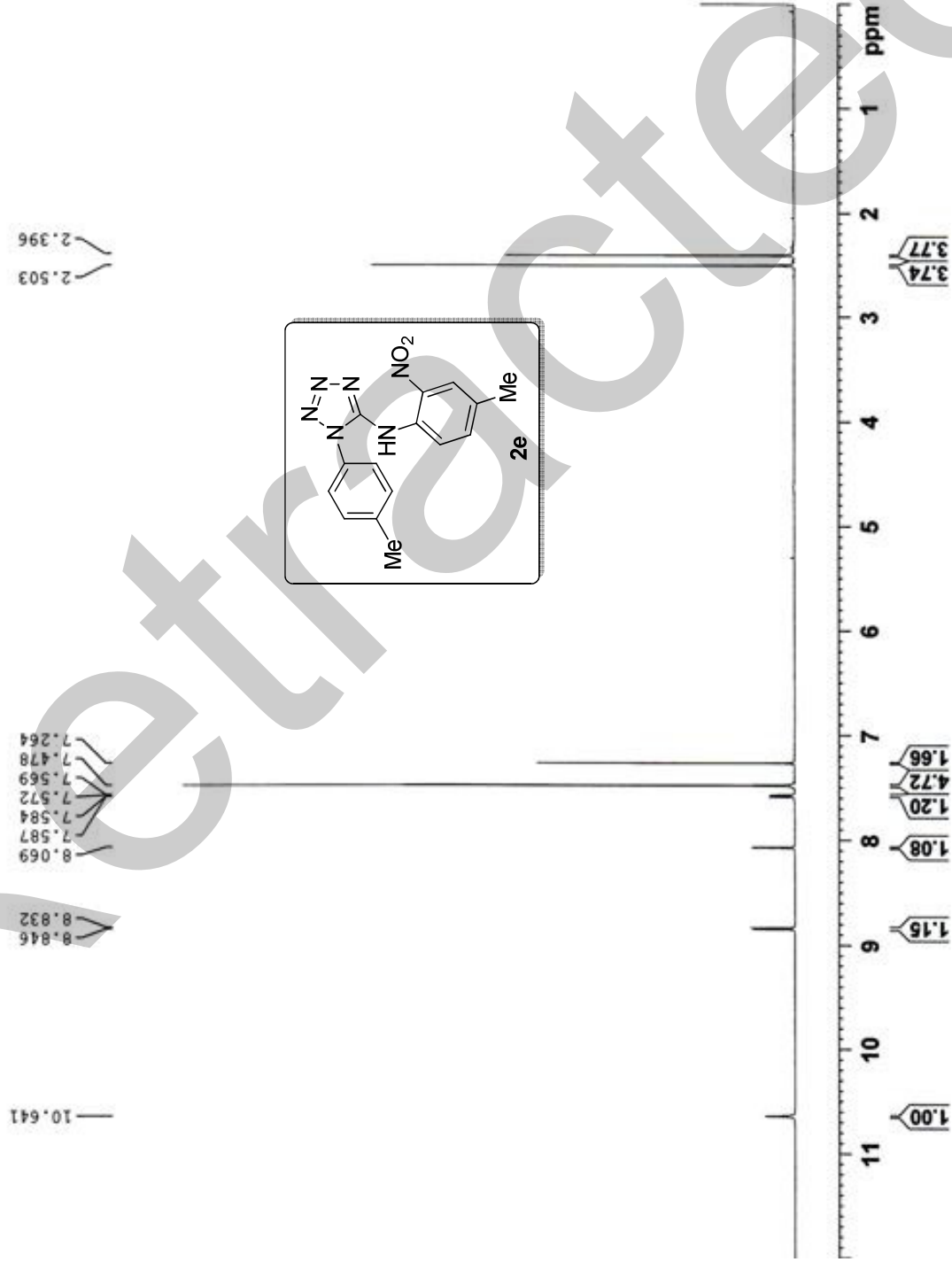
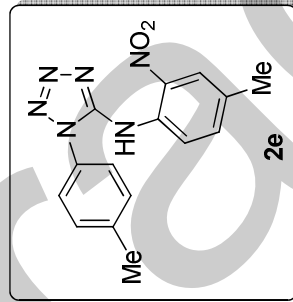
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TD 32768
SOLVENT CDCl3
NS 1566
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 80.6
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 9.80 usec
PL1 -0.50 dB
PL1W 34.66611099 W
SFO1 75.4778101 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 2.50 dB
PL12 19.20 dB
PL13 23.00 dB
PL2W 8.07971478 W
PL12W 0.17274120 W
PL13W 0.07201053 W
SFO2 300.1412006 MHz
SI 32768
SF 75.4702655 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

200 180 160 140 120 100 80 60 40 20 ppm

SP-4methyl-NO2_1H



```
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NAME      SP-40ethyl-NOP_1H
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20111114
Time      11.15
INSTRUM   spect
PROBHD    5 mm F4BBO BB/
PULPROG   zgpg30
TD        65536
AQ         1.96
RG          320
DS          4
SOLVENT   CDCl3
NS         16
DS         2
SWH         12019.230 Hz
FIDRES     0.346798 Hz
AQ         1.9631488 sec
RG          320
RG          143.33
DM          41.650 usec
DE         6.550 usec
TE         300.2 K
T2         398.2 K
T2RHO     0.00000000 sec
TDO        1

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NUC1       1H
P1         12.00 usec
PL1        21.000000000 W
PC         1.00

F2 - Processing parameters
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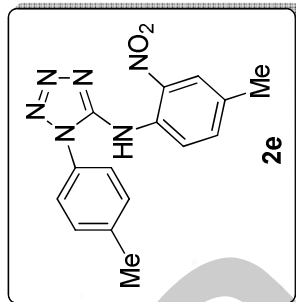
SP-P-ME-NO2-13C



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126.03
124.60
120.08

77.45
77.23
77.02

21.58
20.60



Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131115
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INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
DS 104
SHE 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543029 sec
RG 65.24
RG 13.610 usec
SHE 6.50 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD 1

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FPL1

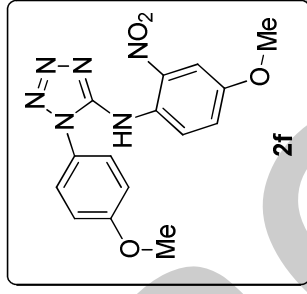
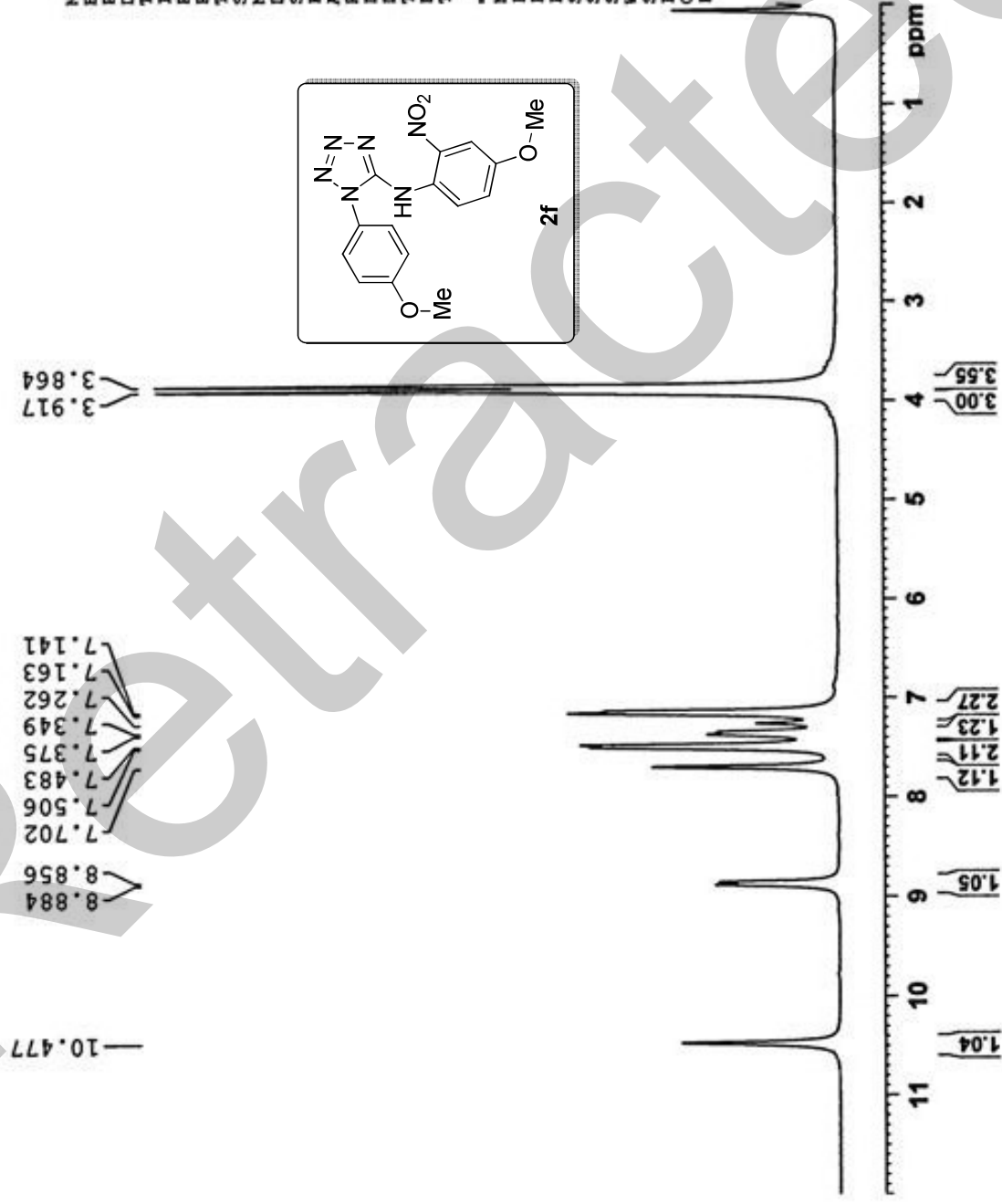
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PL2 0.00000000 W
FPL2

===== CHANNEL f3 =====
SFO3 21.00000000 MHz
NUC3 13C
P3 0.00000000 W
FPL3

F2 - Processing parameters
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WDW EM
SSB 0
GB 0
PC 1.40

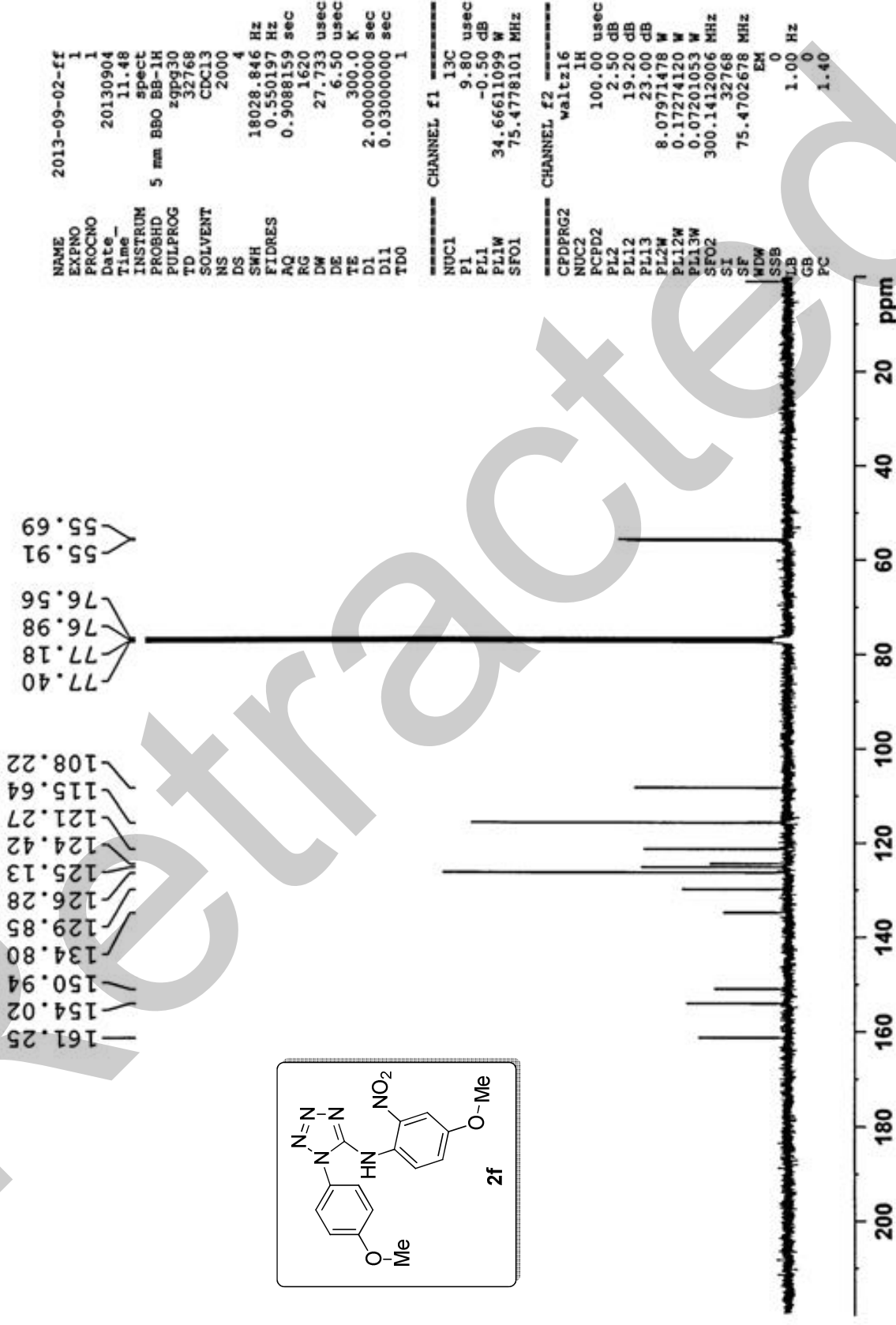
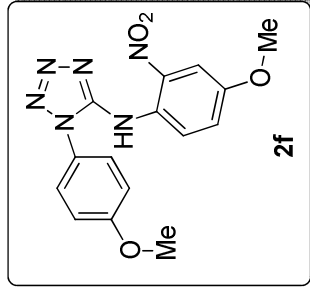
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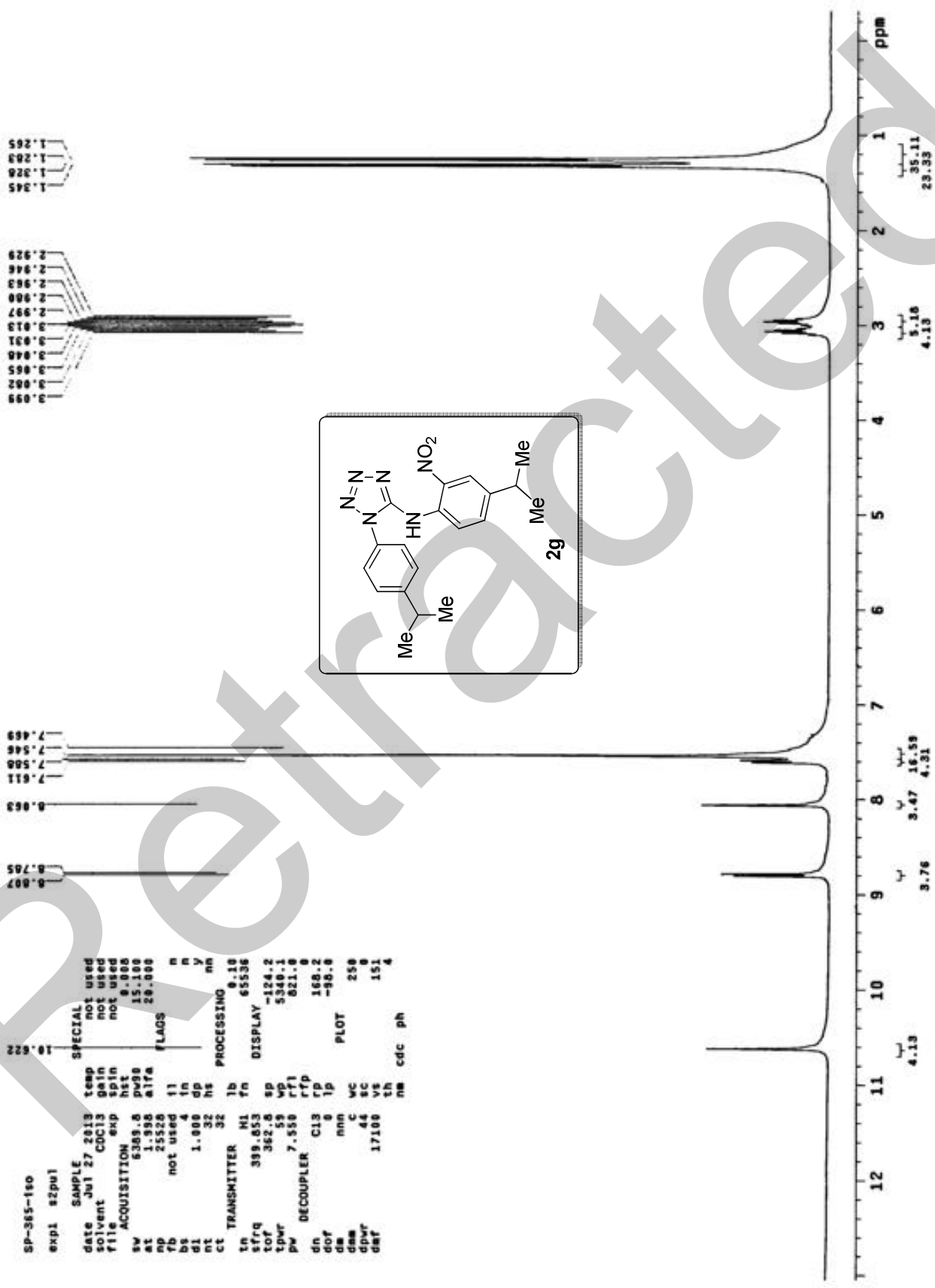
SP-390-OMe



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PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.188846 Hz
AQ 2.6477044 sec
RG 203
DM 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TDO 1
CHANNEL f1
NUC1 1H
P1 14.75 usec
PL1 2.50 dB
PL1W 8.07971478 W
SFO1 300.1418535 MHz
SI 16384
SF 300.1400000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

SP-390-OMe



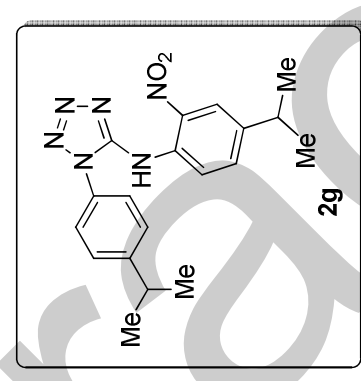


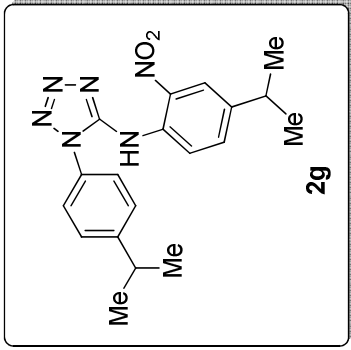
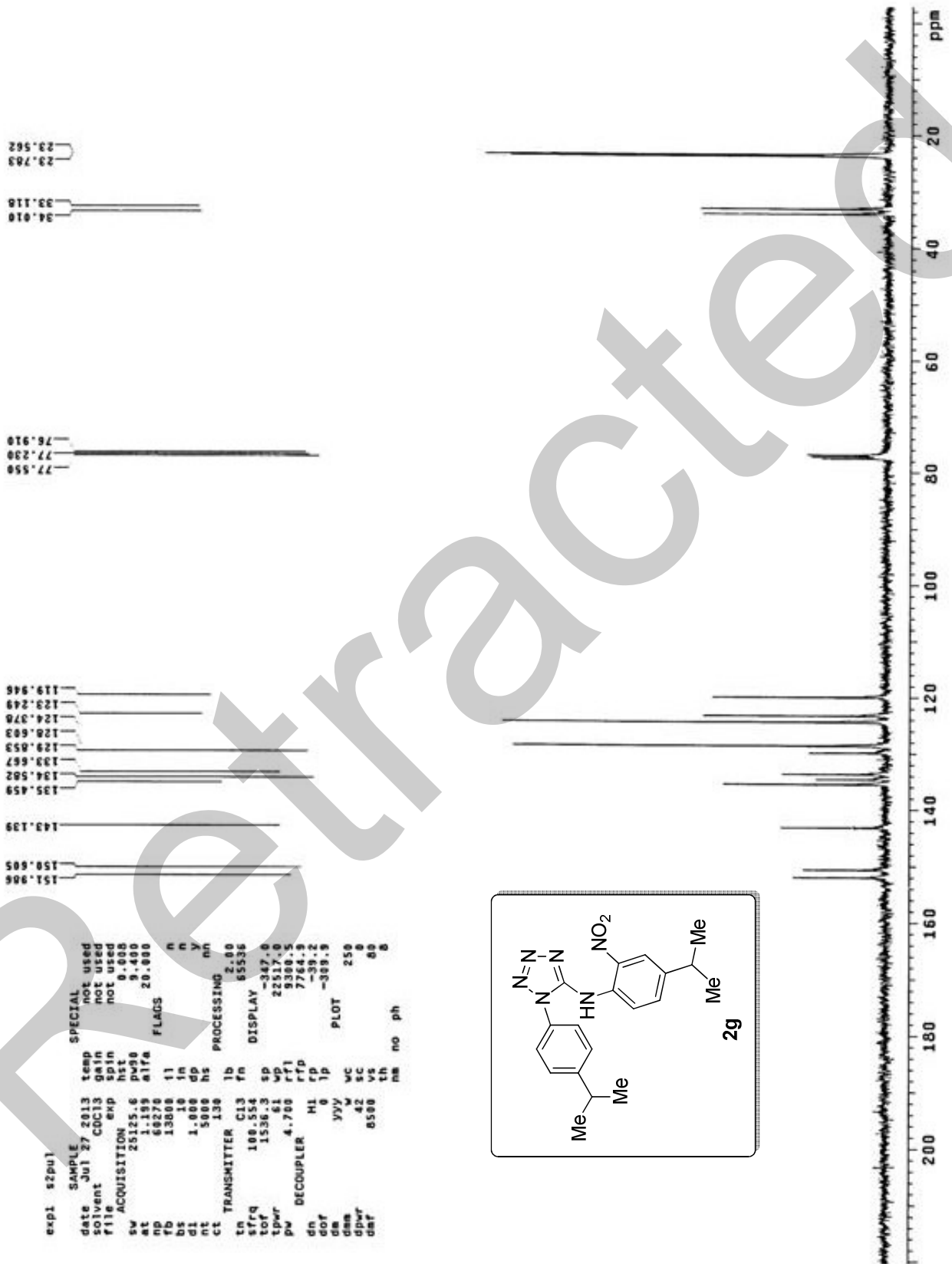
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2.963
2.980
2.997
3.013
3.031
3.048
3.065
3.082
3.099

7.469
7.546
7.568
7.611
8.693
8.705
8.807

SP-365-iso
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date Jul 27 2013 temp not used
solvent CDCl3 gain not used
file not used
ACQUISITION exp not used
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at 1.998 pw90 15.100
np 25528 alfa 20.000
fb not used 11
di 4 in n
nt 1.000 dp hs y
ct 32 hs
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 399.653
tof 362.8 sp
tpwr 59 wp 124.2
pw 7.550 rfl 5340.1
DECOUPLER C13 rfp 821.0
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dpr 44 sc 0
daf 17100 vs 151
nm cdc ph 4

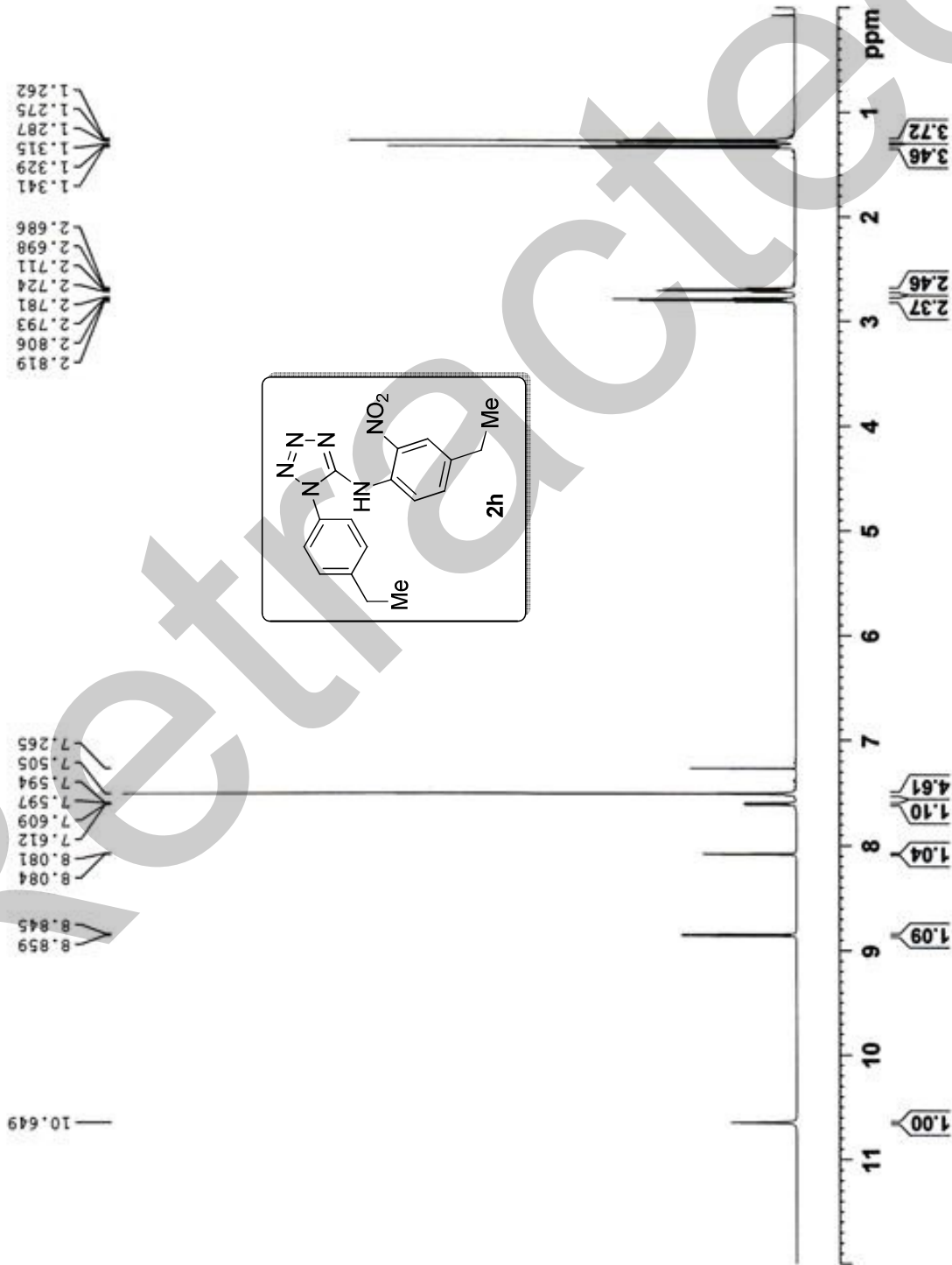






SP-Ethyl_1H

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Time_ 11:07
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PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 4
SW 12019.232 Hz
FIDRES 0.365798 Hz
AQ 1.3631488 sec
RG 54.94
DM 41.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
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SFO1 600.137043 MHz
NUC1 1H
P1 12.00 usec
PL1 21.00000000 W
F2 - Processing parameters
SI 16384
SF 600.1700115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



TK_ETHYL_NHOH_13C1



Current Data Parameters
 NAME TK_ETHYL_NHOH_13C1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 2011026
 Time 18:57
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 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 49
 DS 2
 SWH 36057.691 Hz
 FIDRES 1.100393 Hz
 AQ 0.4543629 sec
 RG 65.24
 DW 13.867 usec
 DE 6.50 usec
 TE 299.9 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 150.9279571 MHz
 NUC1 13C
 P1 10.50 usec
 PL1 95.0000000 W

===== CHANNEL f2 =====
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 PL13 0.3023999 W

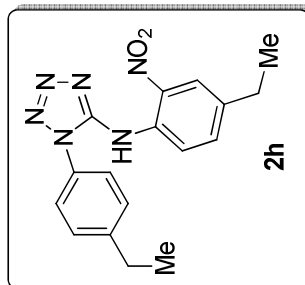
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15.22
15.34

27.97
28.79

77.44
77.23
77.02

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136.95
138.70
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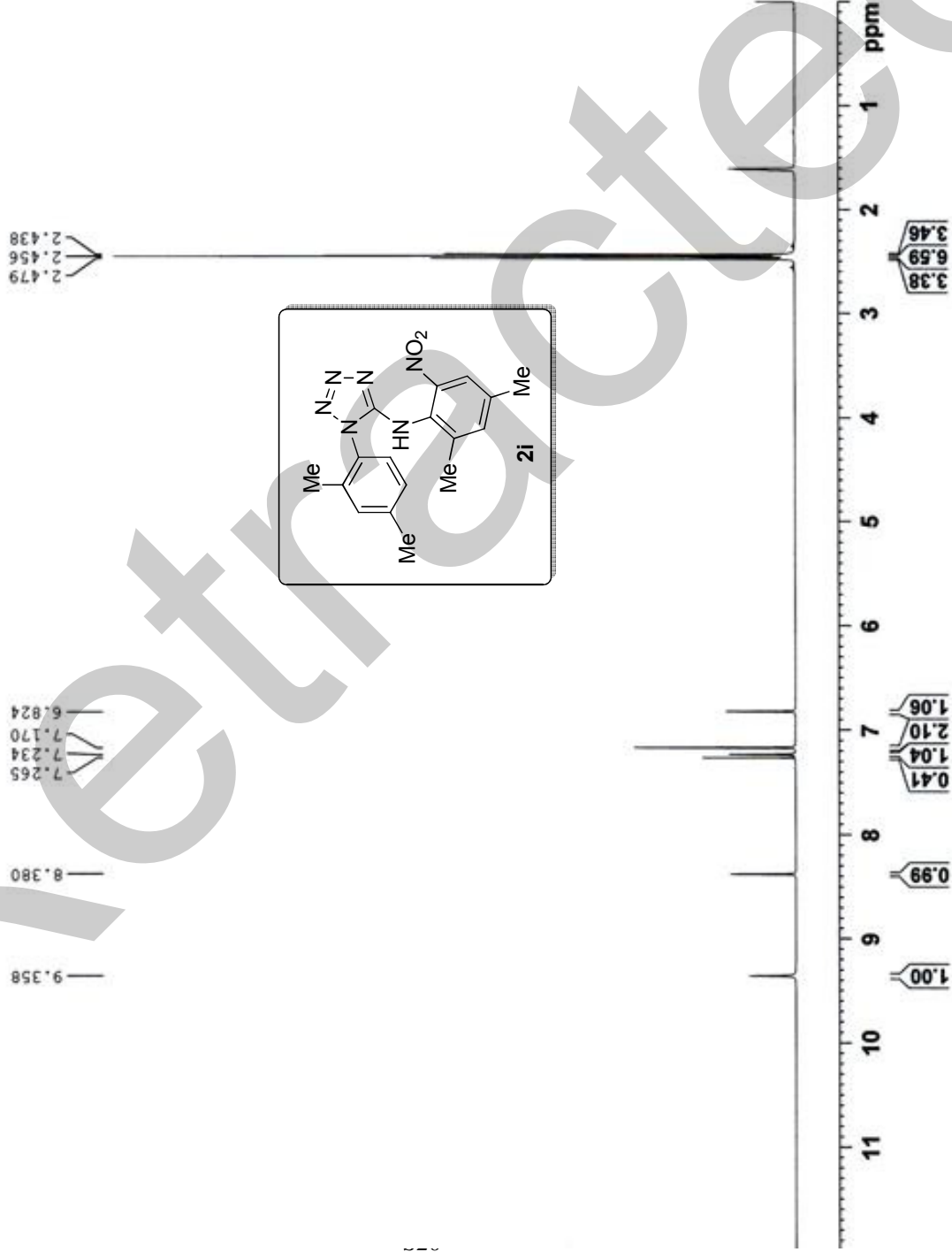


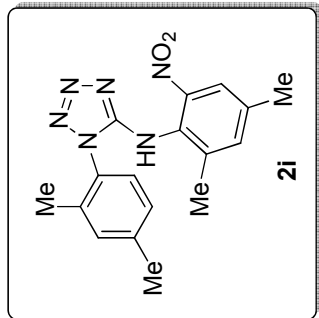
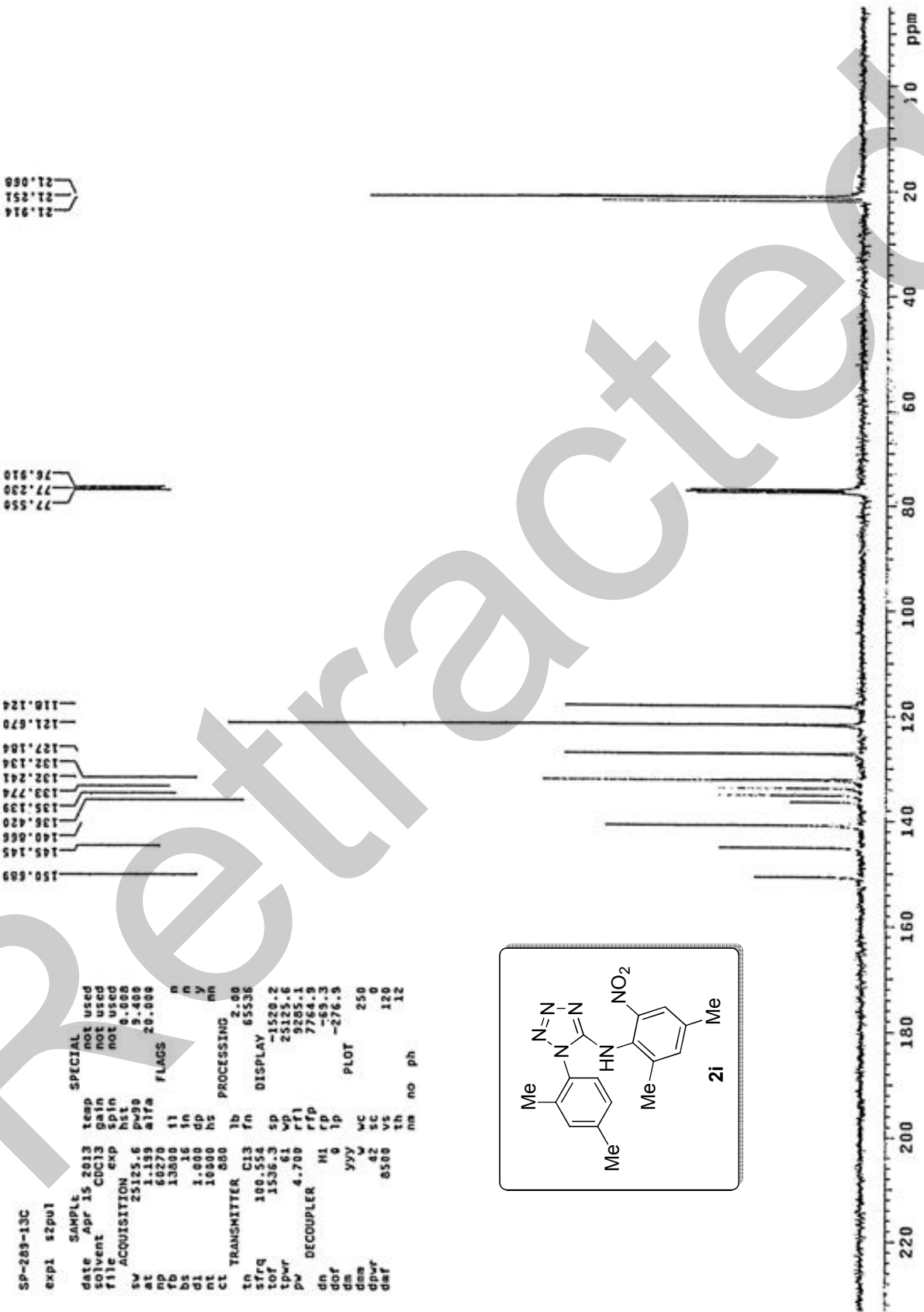
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SP-24-DIME 1H



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 PROCNO 1
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 Time 14.38
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 PROBED 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 15
 DS 2
 SFR 12019.230 Hz
 FIDRES 0.166798 Hz
 AQ 1.363188 sec
 RG 69.67
 DW 41.600 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.00000000 sec
 TDO 1
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 NUC1 1H
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 EQ 0
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 1.00
 PC



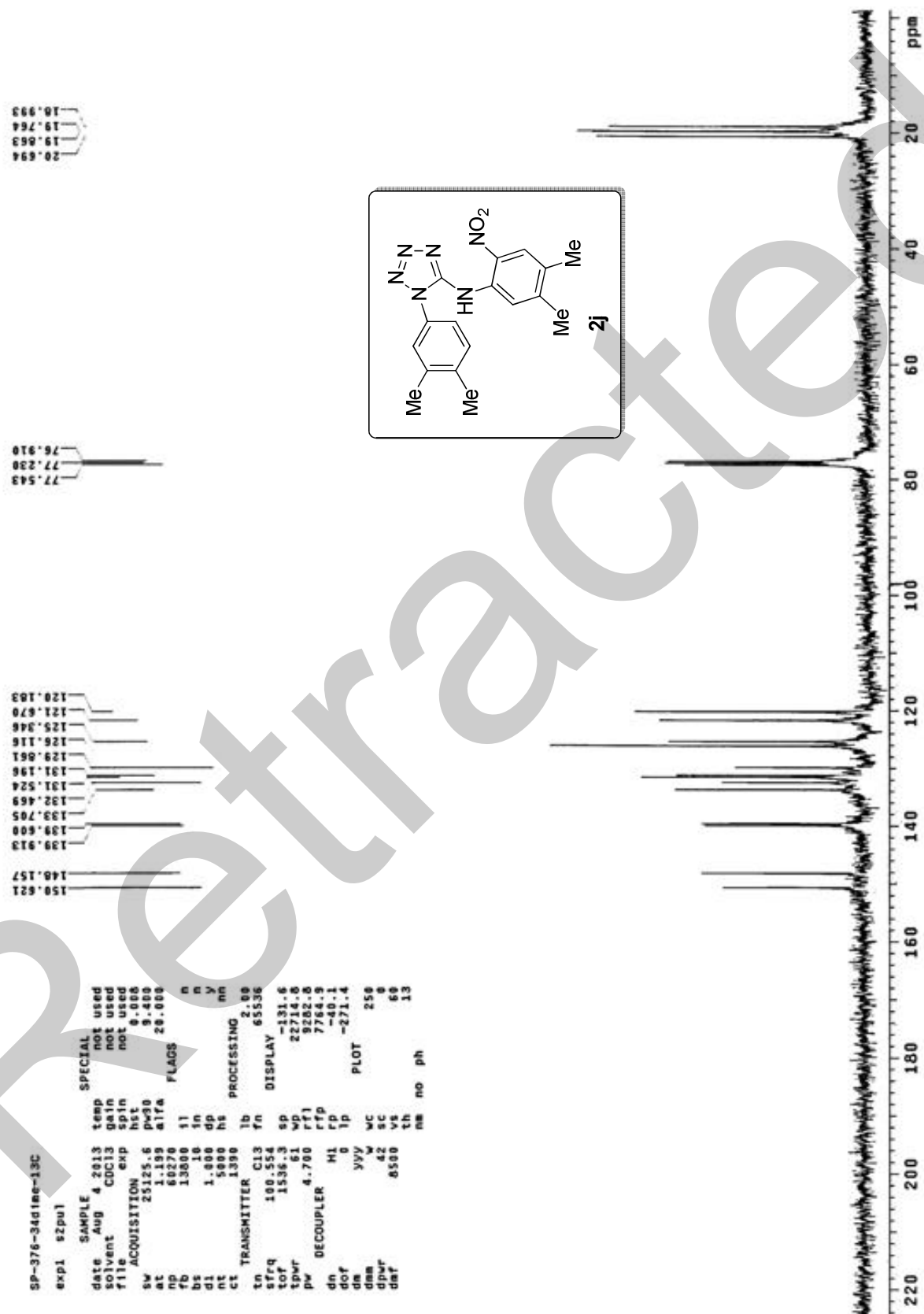


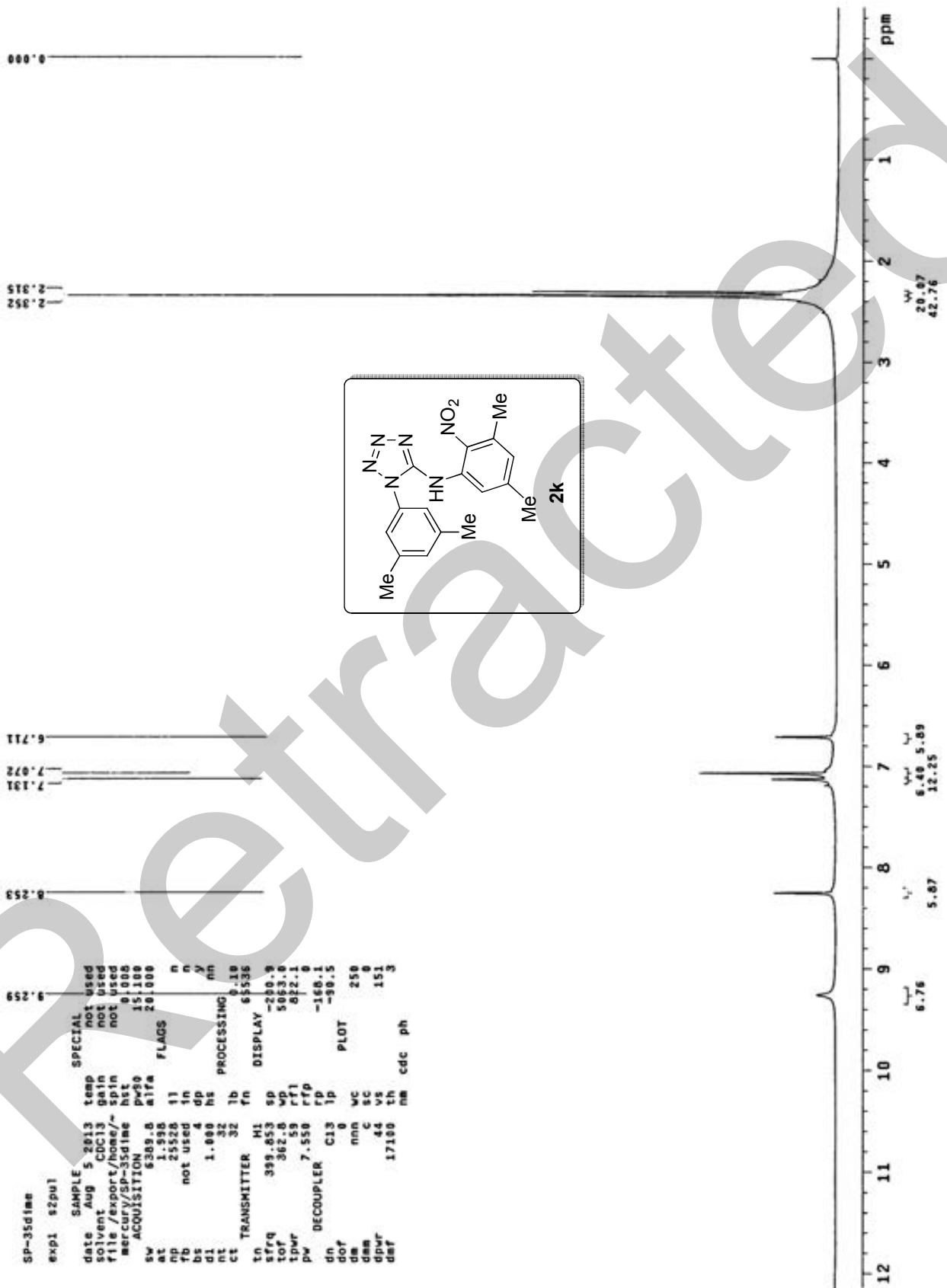
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 pw 4.709
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 daf 8500
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 21.251
 21.068

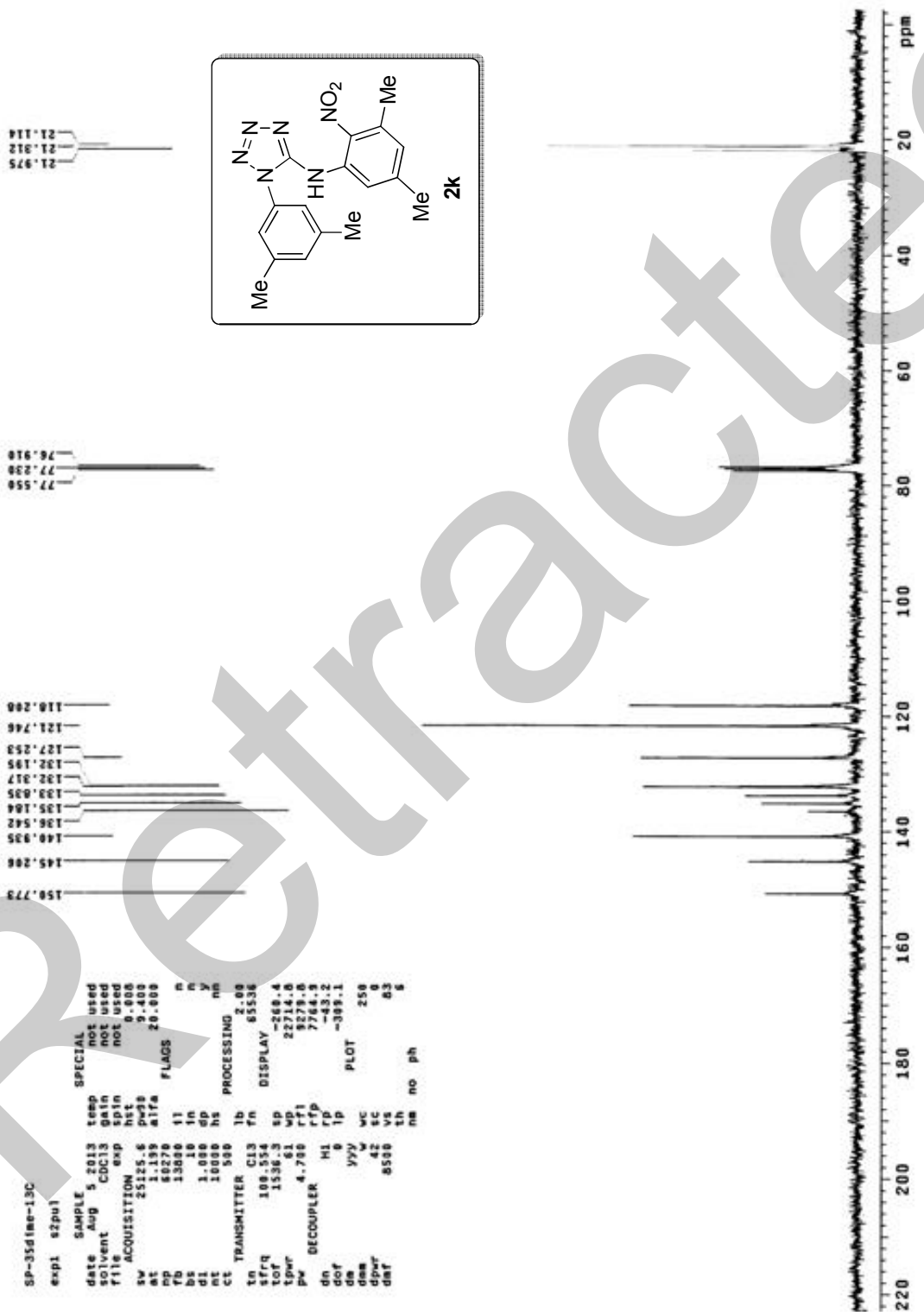
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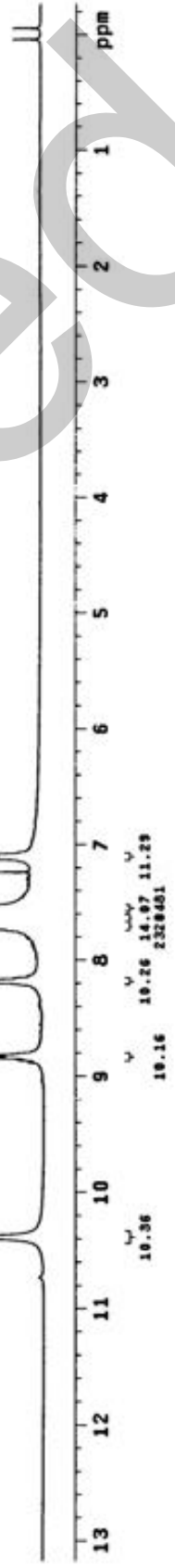
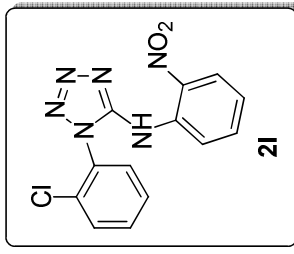
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date Aug 5 2013
solvent CDCl3
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NP 255.28
FB not used
BS 4
D1 1.000
CT 32
IN TRANSMITTER M1
SFRQ 399.853
TOR 362.0
TPR 59
PW 7.550
DN DECOUPLER C13
DOF 0
DM nnn
DMM C
DPR 44
DMF 17100
SPECIAL not used
temp not used
gain not used
spin not used
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PZ0 15.100
MIF 20.000
FLAGS
n n
n y
m n
0.10
6.538
DISPLAY
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5003.0
0.2.1
0
-160.1
-50.5
PLOT
250
0
151
3
nm cdc ph



```

SP-353-DMF
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solvent CDC13
temp not used
gain not used
file CDC13
spin not used
nst 8.005
wv ACQUISITION
at 6309.8
pp 2.998
pb 25520
ds not used
d1 1.092
ct TRANSMITTER
tn 399.853
tfq 362.8
tof 5373.5
tpw 7.558
pw DECOUPLER
dof 165.5
dm min
dwa 17100
dmf 44
th nm
cdc ph
SPECIAL
temp not used
gain not used
file CDC13
spin not used
nst 8.005
wv ACQUISITION
at 6309.8
pp 2.998
pb 25520
ds not used
d1 1.092
ct TRANSMITTER
tn 399.853
tfq 362.8
tof 5373.5
tpw 7.558
pw DECOUPLER
dof 165.5
dm min
dwa 17100
dmf 44
th nm
cdc ph
PROCESSING
n 8.18
y 45536
nm 5373.5
sp 3897.9
rf1 2884.9
rfp 165.5
lp -95.4
PLOT
259
44
SC
88
6

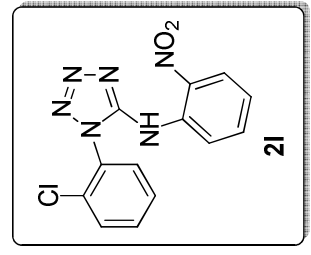
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SP-353-DMF-13C

exp1	s2pu1	SAMPLE		date	Jul 1 2013	temp	not used
		solvent	CDCl3	gain	not used		
		file	not used	spin	not used		
		ACQUISITION	exp	nsi	0.008		
		sv	25125.6	ps30	9.400		
		at	1.193	4176	20.000		FLAGS
		tp	60270			n	
		fb	13600	11		n	
		bl	10	fn		n	
		dl	1.000	dp		y	
		nt	10000	hs		nn	
		CT	TRANSMITTER	760	1b	PROCESSING	
		tn	100.554	fn	2.00		
		sfreq	153.813	sp	65536		
		tof	153.813	sp	230.5		
		tpwr	61	wp	2648.9		
		pw	4.700	rf1	3281.8		
		DECOUPLER	H1	rfp	7764.9		
		dn	0	tp	-19.6		
		dof	0	lp	-413.3		
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		dma	42	sc	0		
		dpr	42	vs	0		
		dst	8500	tn	no	ph	15

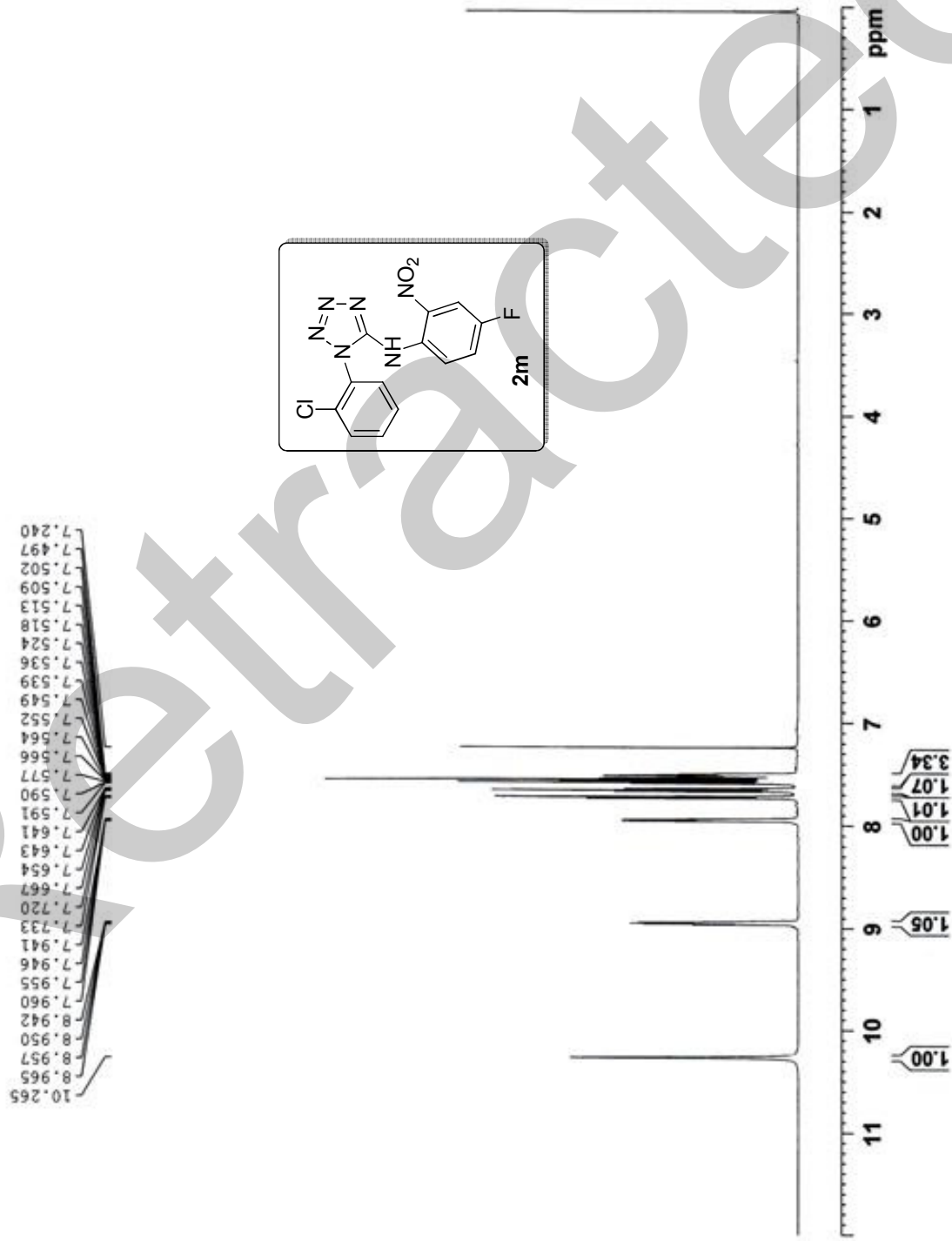
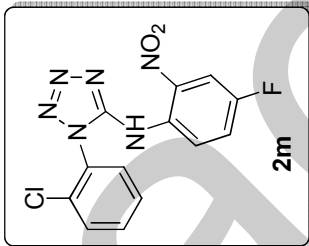
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134.757
133.399
131.703
131.547
129.449
129.327
129.904
126.216
122.295
119.848



SP-CLF_1H



Current Data Parameters
 NAME SP-CLF_1H
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20131119
 Time 14.30
 INSTRUM spect
 PROBRD 5 mm PABBO 88/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.366798 Hz
 AQ 1.363148 sec
 RG 327.68
 DM 41.600 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.00000000 sec
 TDO 1
 ===== CHANNEL f1 =====
 SFO1 600.1737043 MHz
 NUC1 1H
 P1 12.00 usec
 PL1 21.00000000 W
 F2 - Processing parameters
 SI 16384
 SF 600.1700268 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



SP-CL_F_13C

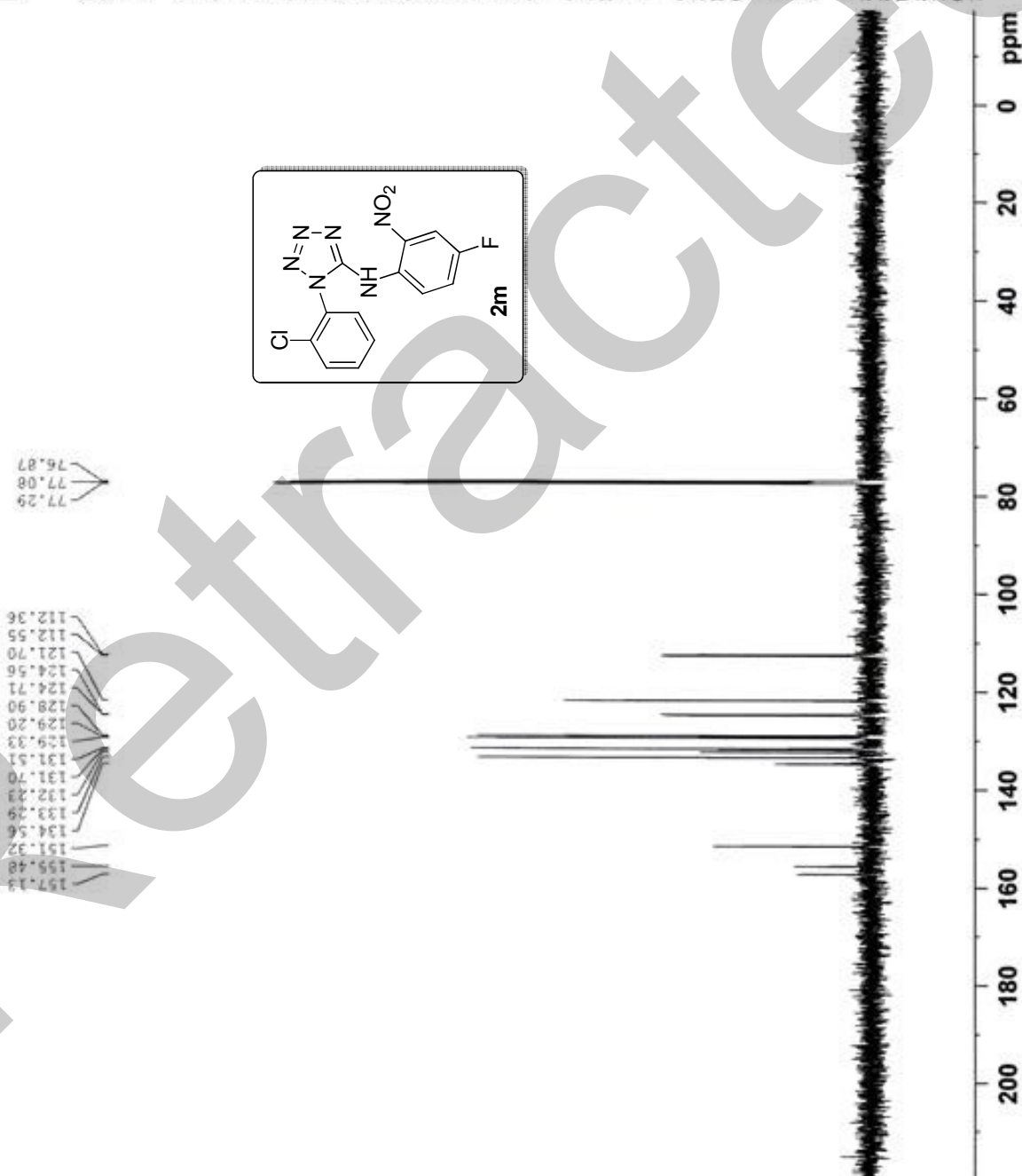
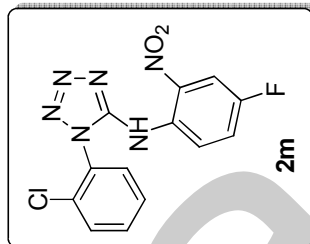


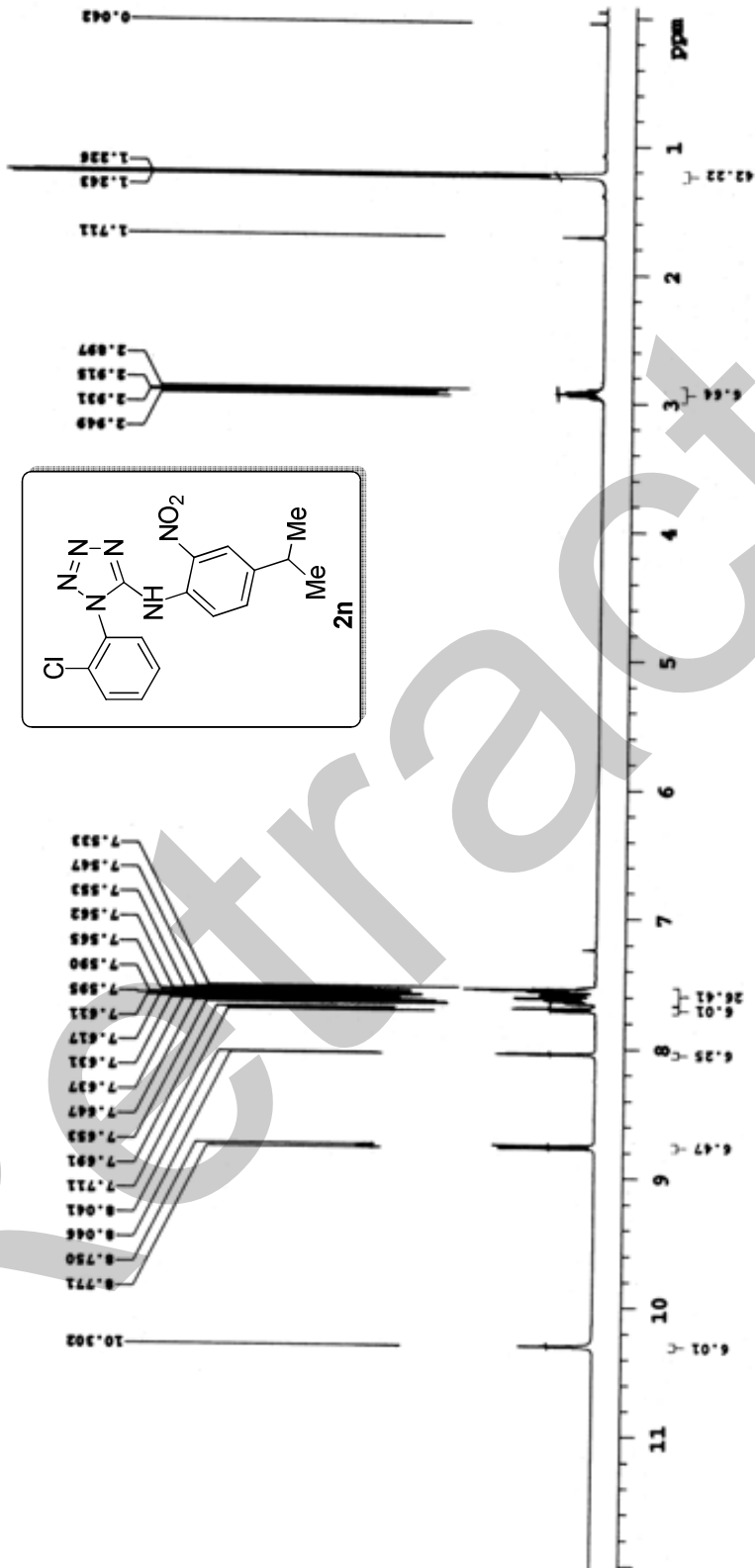
Current Data Parameters
NAME SP-CL_F_13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131021
Time 9.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 101
DS 2
SMH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 65.24
DW 13.867 usec
DE 6.50 usec
TE 301.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

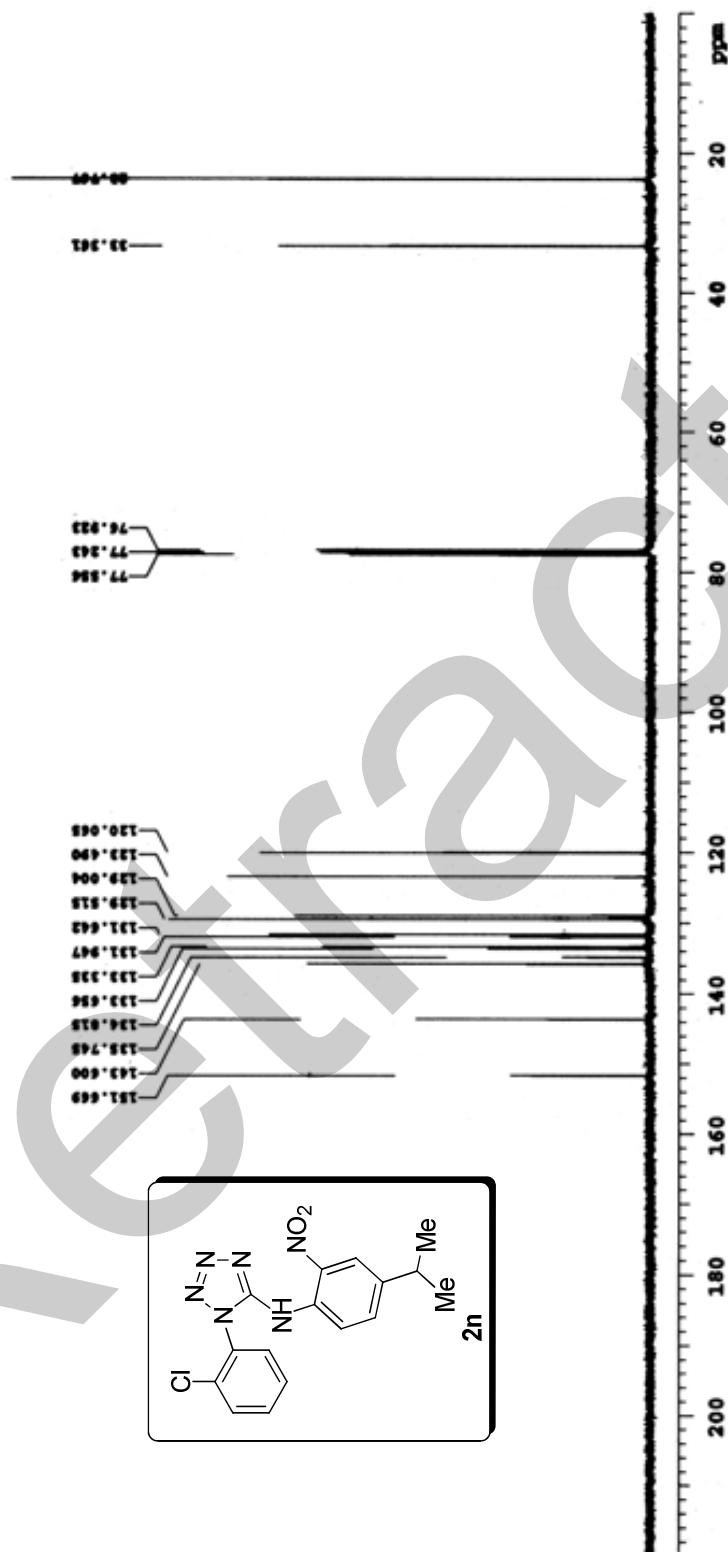
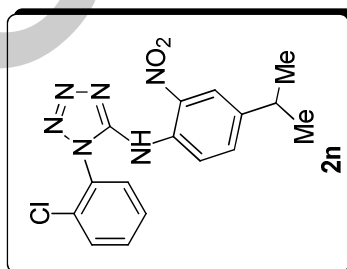
CHANNEL f1
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.00000000 W
CHANNEL f2
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.61714000 W
PLW13 0.30239999 W

F2 - Processing parameters
SI 16384
SF 150.9128434 MHz
WDW EM
SSB 0
LB 0
GB 0
PC 1.40





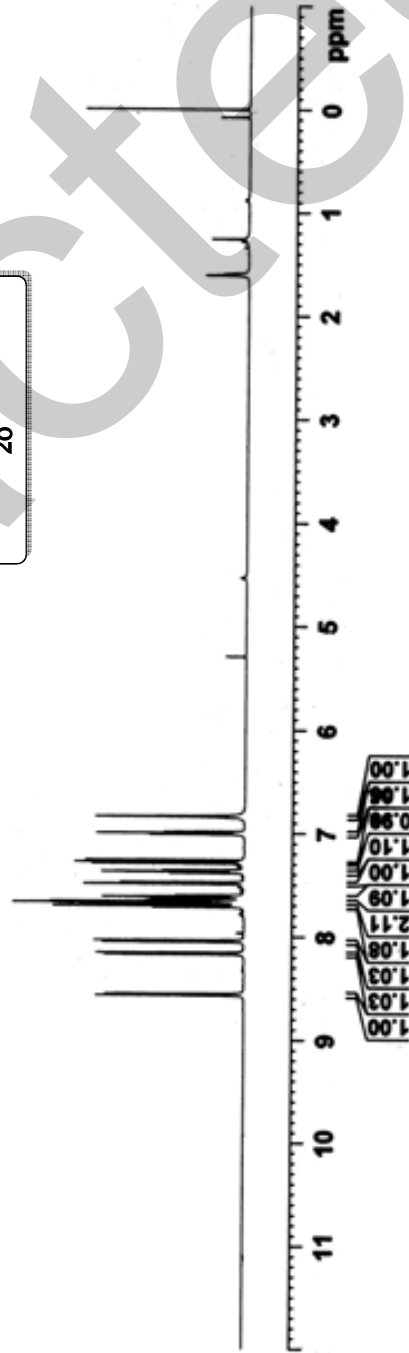
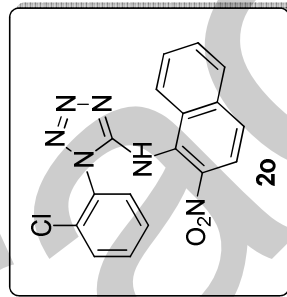
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	OBSERVE H1, 399.850721	DATA PROCESSING FT size 32768 Total time 1 minutes	89-01-1Pr Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chm Mercury-400 *H70-MM*
---	-------------------------------	---	---



PULSE SEQUENCE Solen. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.264 sec Width 25125.6 Hz 580 repetitions	CHANNELS C13, 100.625440 DECOUPLE H1, 399.852994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 22 minutes	SP-01-LPR Solvent: cdcl3 Temp: 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-MMR"
---	---	--	--

SP_Napthyl_1H

8.566
8.565
8.552
8.170
8.156
8.051
8.037
7.717
7.705
7.691
7.673
7.662
7.650
7.628
7.614
7.490
7.476
7.386
7.372
7.357
7.292
7.290
7.278
7.276
7.260
7.012
7.010
6.998
6.986
6.984
6.838



Current Data Parameters
NAME SP_Napthyl_1H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140124
Time 10.29
INSTRUM spect
PROBHD 5 mm PABBO MM/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 73.2
WDW 41.600 usec
SSB 0.50 usec
GB 0.0000000
PC 1.00000000 sec
TD0 1

CHANNEL F1
SPOL 600.1737943 MHz
NUC1 1H
P1 12.00 usec
PL1 21.00000000 dB
F2 - Processing parameters
SI 16384
SF 600.1700148 MHz
WDW 0
SSB 0
GB 0
PC 1.00

SP_NAPH_13C



Current Data Parameters
NAME SP_NAPH_13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131021
Time 9.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 100
DS 2
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 65.24
DW 13.867 usec
DE 6.50 usec
TE 301.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

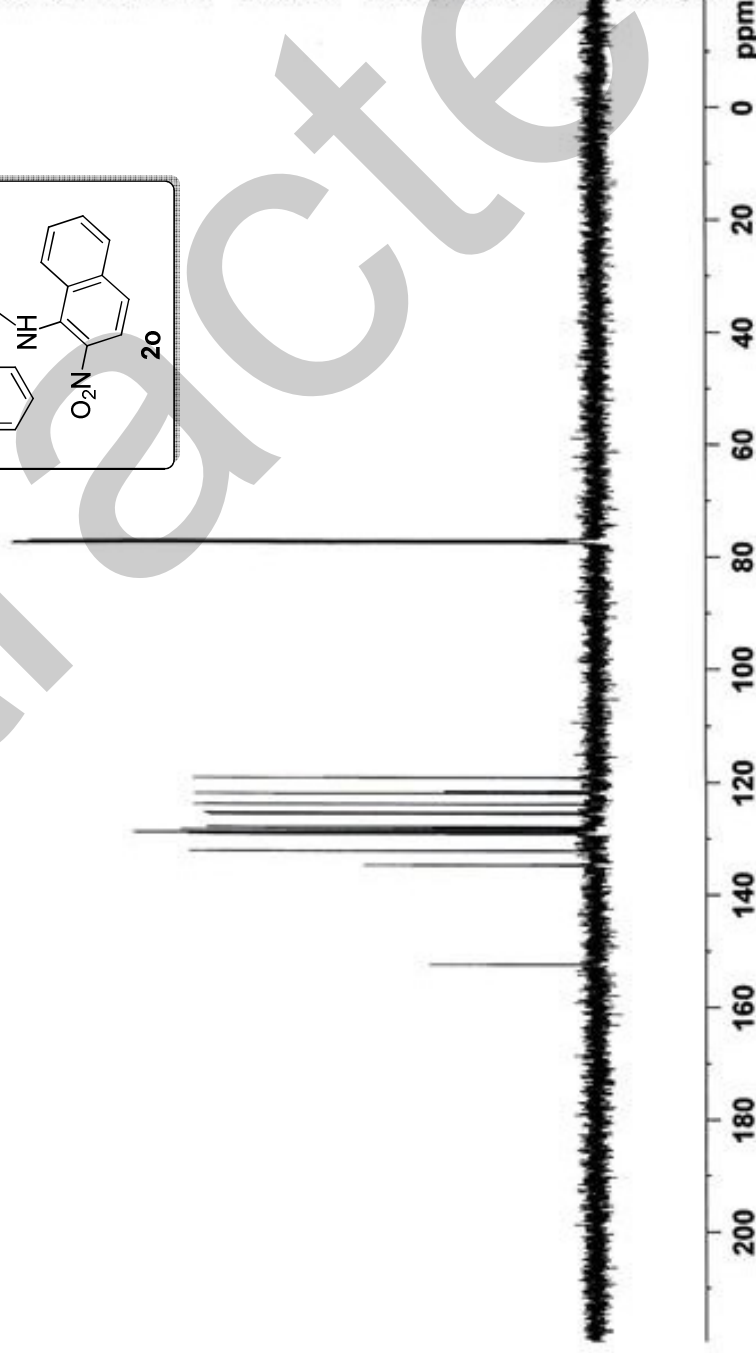
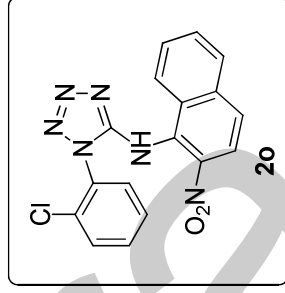
CHANNEL f1
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PL1 95.00000000 W

CHANNEL f2
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.61714000 W
PLW13 0.30239999 W

F2 - Processing parameters
SI 16384
SF 150.9128481 MHz
WDW EM
SSB 0
LB 0
GB 0
FC 1.40

152.41
134.74
132.21
129.16
128.90
128.85
128.36
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127.91
125.97
125.35
123.82
121.89
121.58
119.11

77.44
77.23
77.02

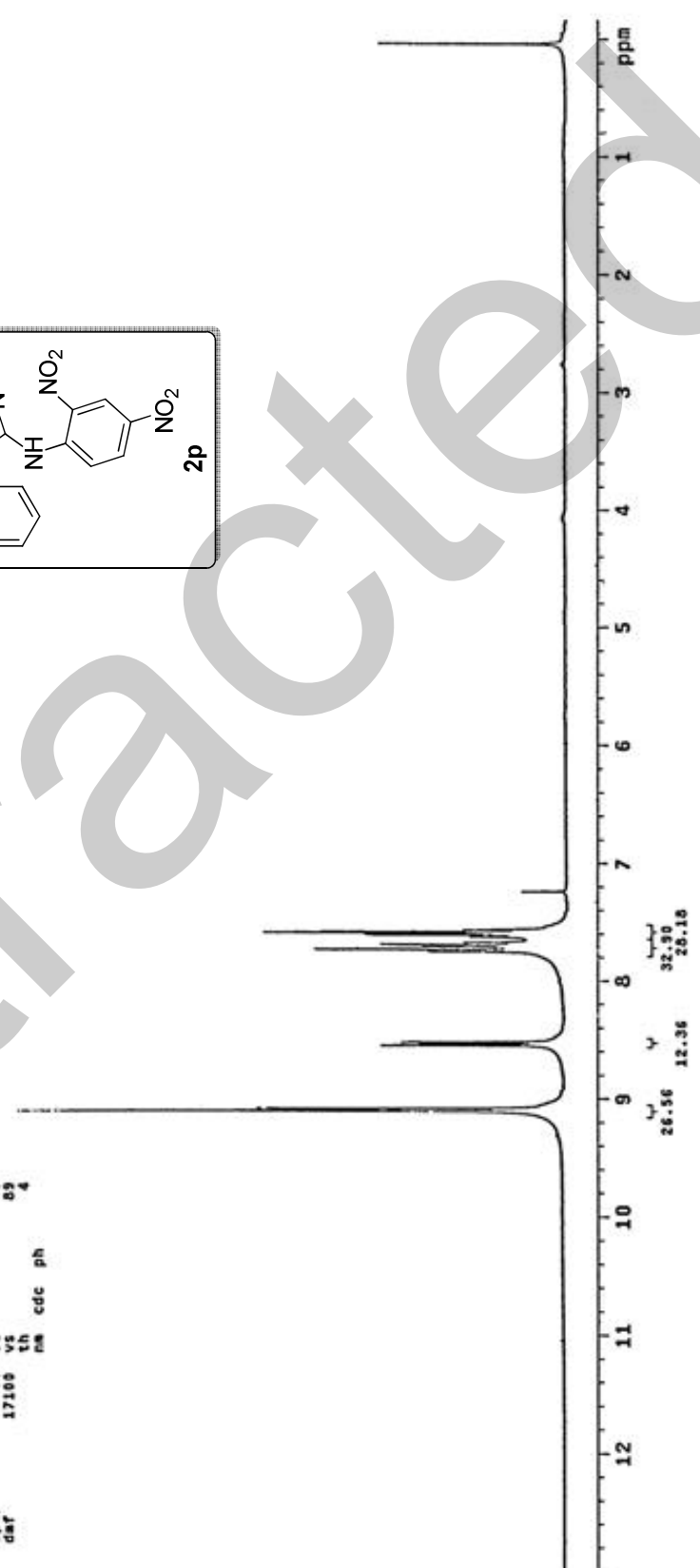
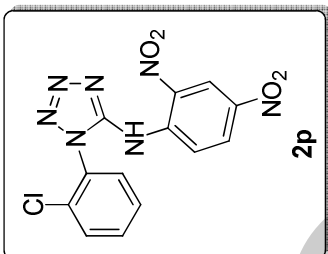


0.041

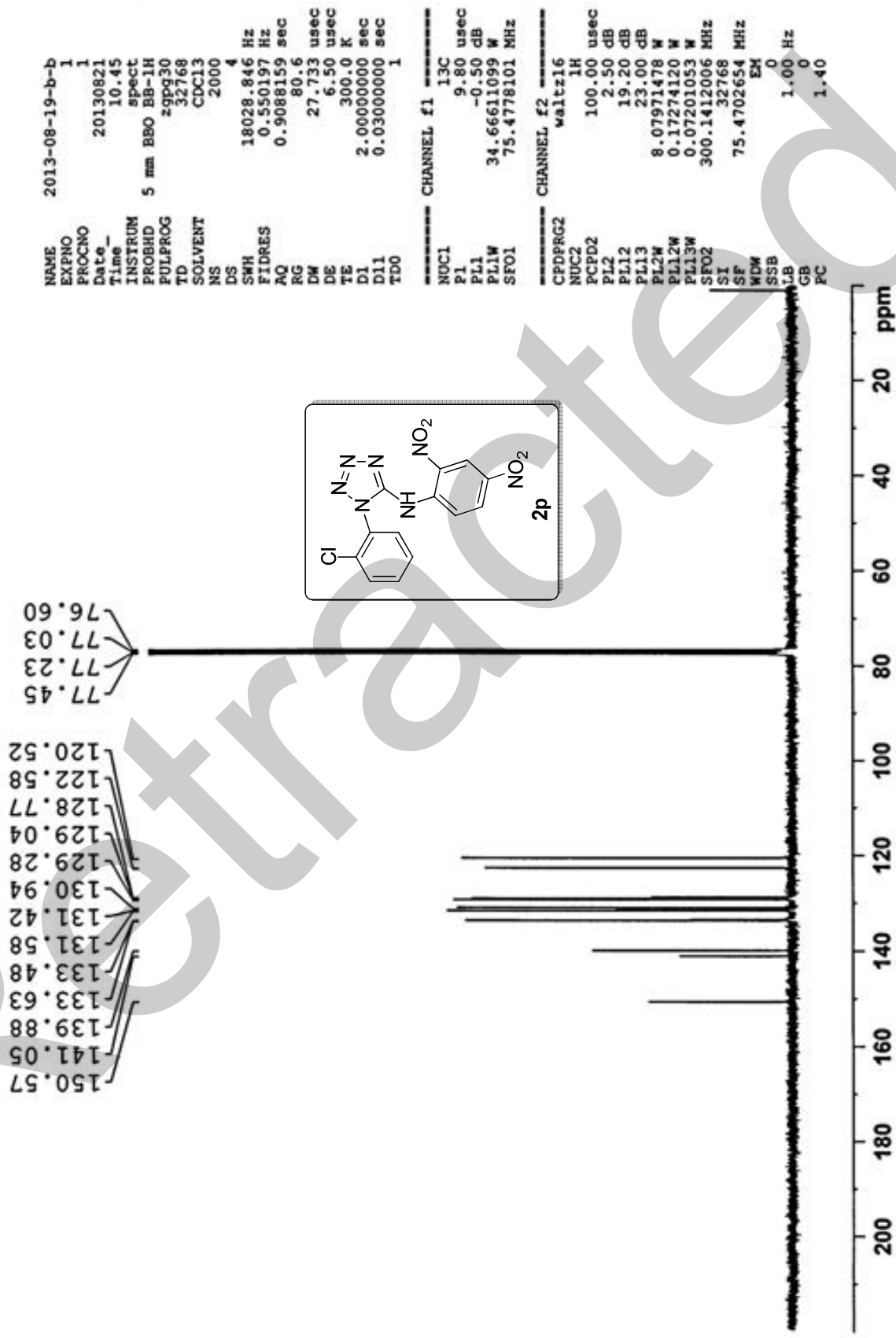
SP-375-NO2
exp1 stpu1

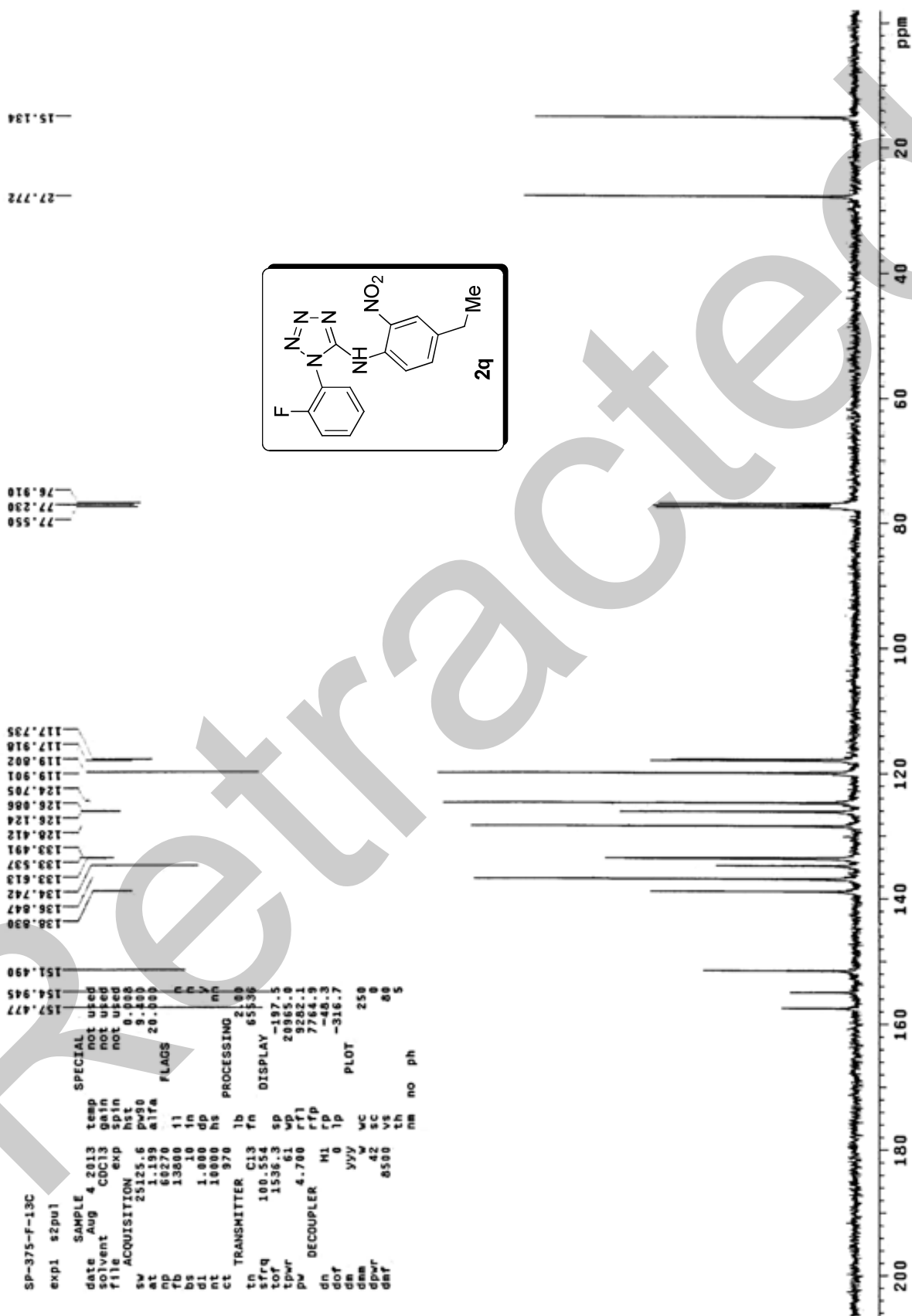
SAMPLE date Aug 6 2013 temp not used
solvent CDCl3 gain not used
file exp not used
ACQUISITION exp 0.000
SW 630.8 Hz
F2 1.978
F1 25328
alpha 20.000
flags
at not used 11 n
cp not used 11 n
pb not used 11 n
di 1.000 dp 32 y
nt 32 ns
CT TRANSMITTER . 32 1b
tn 6536
sfrq 399.653 fm DISPLAY
tof 362.8 sp
tpwr 53 vp
pw 7.550 rfp
DECOUPLER C13 rfp
dn -0 lp PLOT
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dm nnn wc 250
dms c sc 0
dpr 44 vs 0
dnt 17100 th 09
nm cdc ph 4

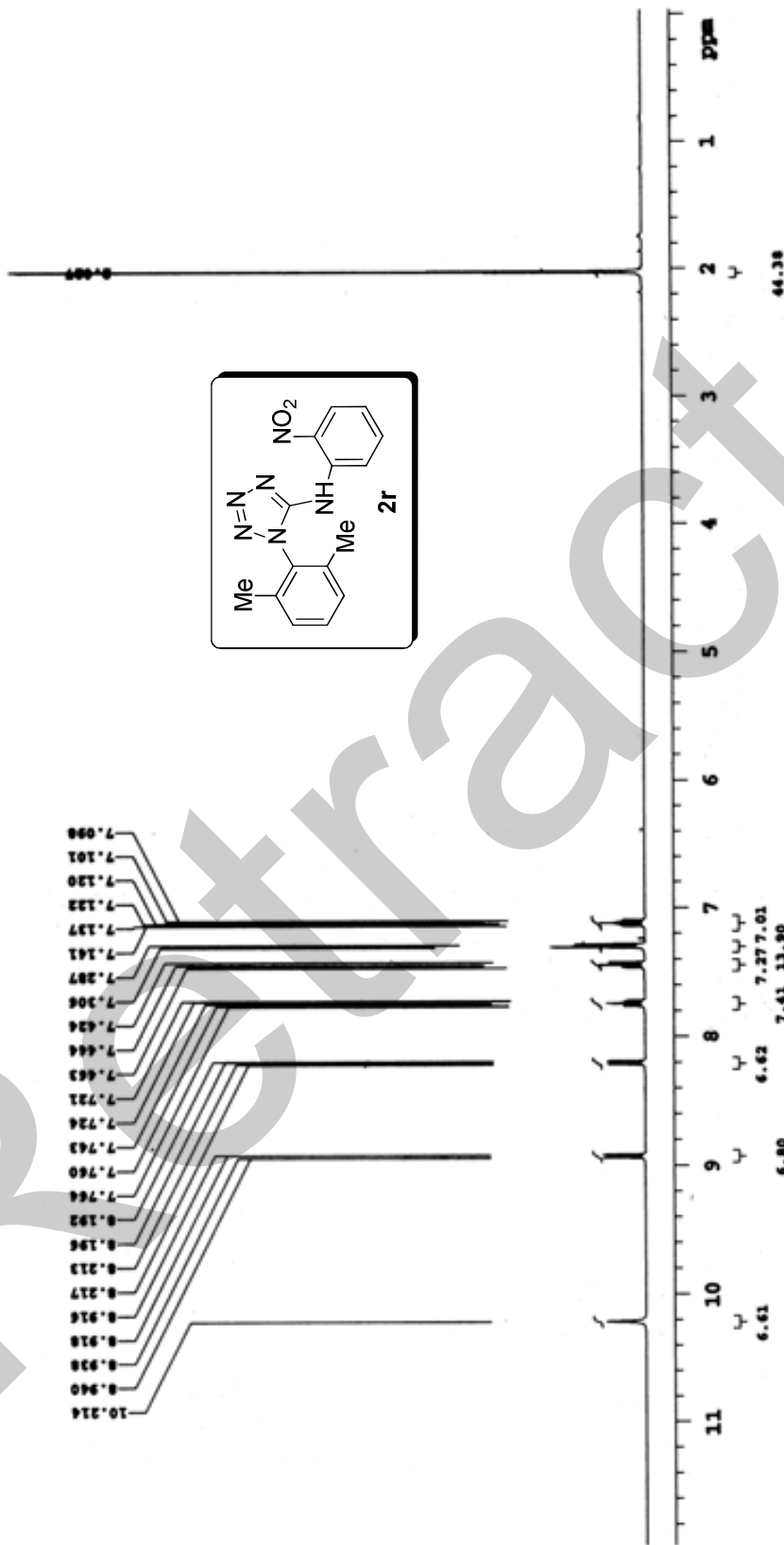
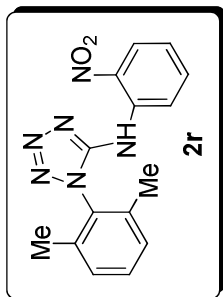
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7.675
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7.695
7.707
7.712
7.730
7.733
7.750
7.753
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SP-379-NO2





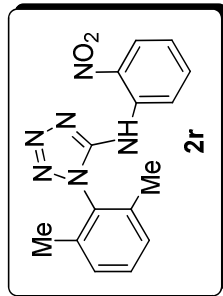


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	OBSERVE M1, 399.8509718	DATA PROCESSING FT size 32768 Total time 1 minutes	SP-26-M Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chen File: SP-26-M Mercury-400 "IITB-MEX"
---	-------------------------	--	--

17.866

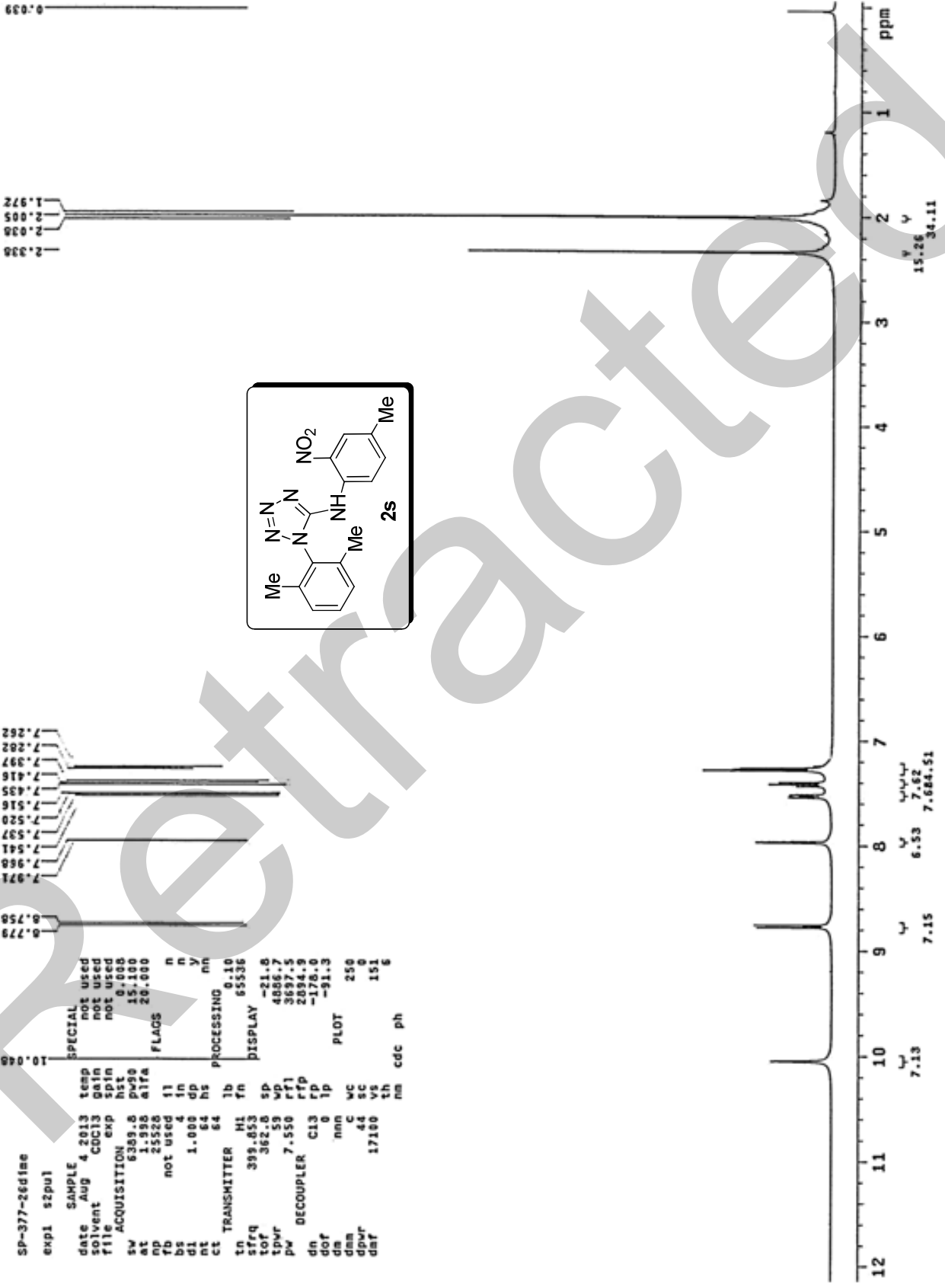
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151.447
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132.018
139.489
139.383
136.310
132.348
119.980



200 180 160 140 120 100 80 60 40 20 ppm

PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 200 repetitions	OSERVE C13, 100.5425912 DECOUPLE H1, 399.8232994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz PT size 65536 Total time 7 minutes	SP-24-K Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chm Mercury-400 *ITG-MM*
--	---	--	--



SP-377-26dme
exp1 szpul
SAMPLE
date Aug 4 2013
solvent COCl3
file
ACQUISITION
sw 6383.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 64
ct TRANSMITTER H1
tn 399.853
sfrq 362.8
tof 59
tpwr 7.550
pw DECOUPLER C13
dn 0
dof nnn
dm c
dam 44
dpr 0
dar 17100
nm cdc
ph 6

SPECIAL
temp not used
gain not used
spin not used
spt not used
hst 0.008
p490 15.100
a1ra 20.000
FLAGS
n n
n y
nn
lb 0.10
fb 65536
DISPLAY
-21.8
4886.7
3697.5
2894.9
-178.0
-91.3
PLOT
250
151

SP-377-26dme-13C

exp1 s2pul

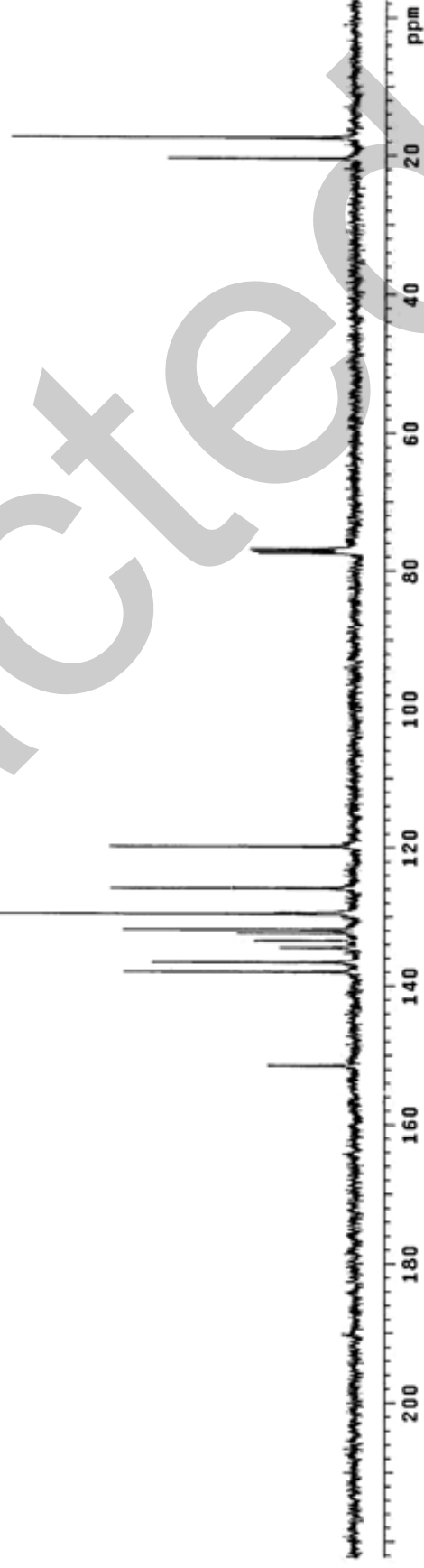
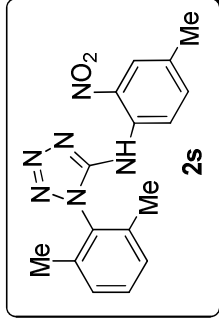
SAMPLE		SPECIAL	
date	Aug 4 2013	temp	not used
solvent	CDCl3	gain	not used
file		spn	not used
ACQUISITION		exp	0.000
sw	25125.6	hst	0.000
at	1.199	pw30	9.400
np	60270	alfr	20.000
fb	13800	fl	
bs	10	fn	n
dl	1.000	dp	y
nt	10000	hs	nn
ct	TRANSMITTER 230	PROCESSING	nn
tn	100.554	fb	2.00
sfrq	100.554	fn	65536
tof	1536.3	sp	DISPLAY
tpwr	61	wp	-263.5
pw	4.700	rf1	22615.9
DECOUPLER		rfp	9249.9
dn	H1	rfp	7764.9
dof	8	lp	-41.5
dm	yyv	PLOT	-300.4
dsm	42	vc	250
dpwr	8500	sc	0
daf		th	81
		nm	no ph
			6

137.960
136.595
134.460
133.430
132.399
131.075
129.594
129.396
125.065
119.009

151.490

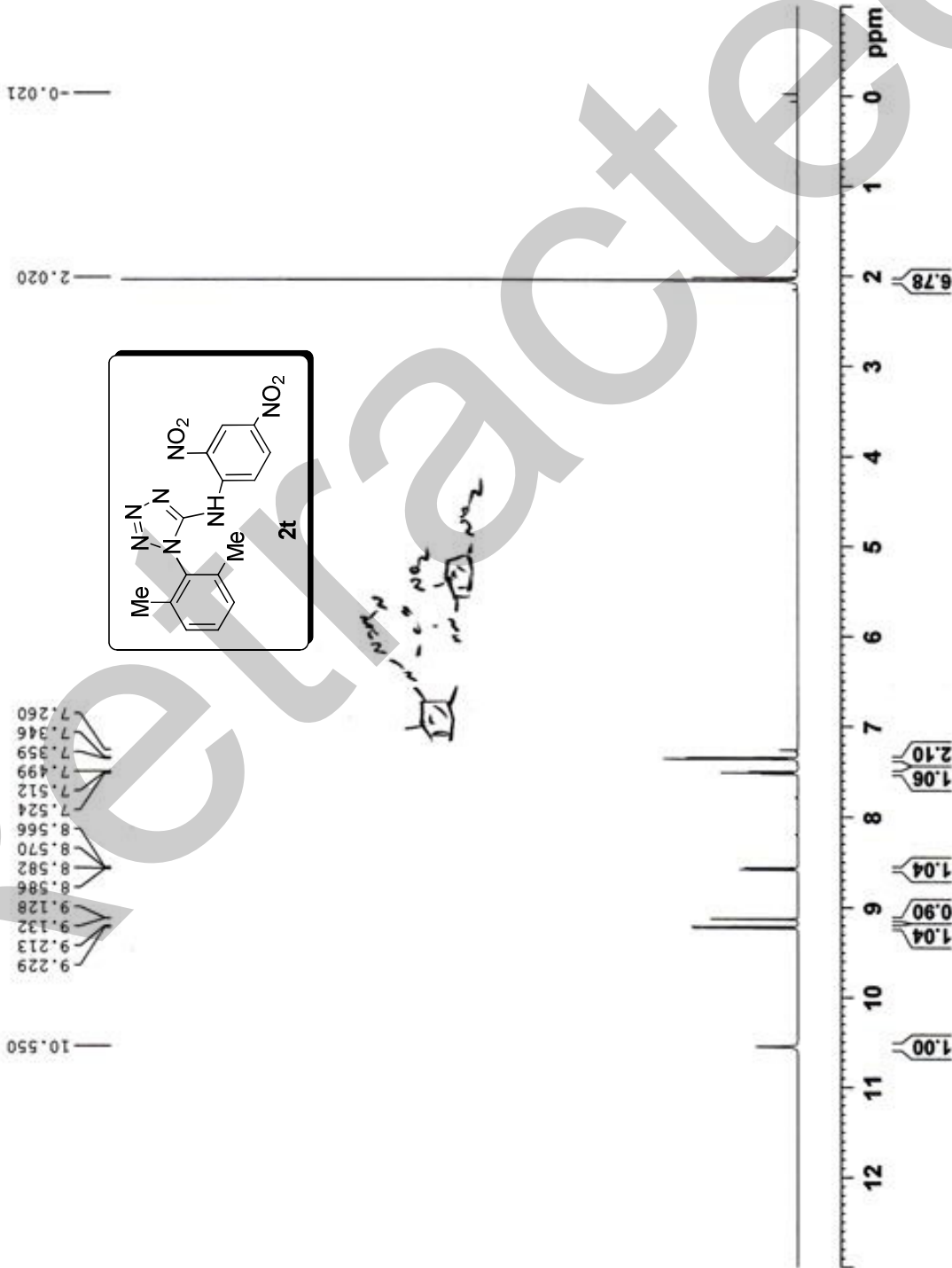
77.543
77.222
76.902

20.465
17.476





Current Data Parameters
NAME SP_15-11-13_1H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131115
Time 13.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.166786 Hz
AQ 1.303466 sec
RG 54.94
DM 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
===== CHANNEL f1 =====
SFO1 600.1737063 MHz
NUC1 1H
P1 12.00 usec
PL1 21.00000000 W
F2 - Processing parameters
SI 16384
SF 600.1700148 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



TK_ETHYL_NHOH_13C

2,6-dime, NO₂

Current Data Parameters
NAME TK_ETHYL_NHOH_13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131026
Time_ 18.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 52
DS 2
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 65.24
DW 13.867 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

CHANNEL f1

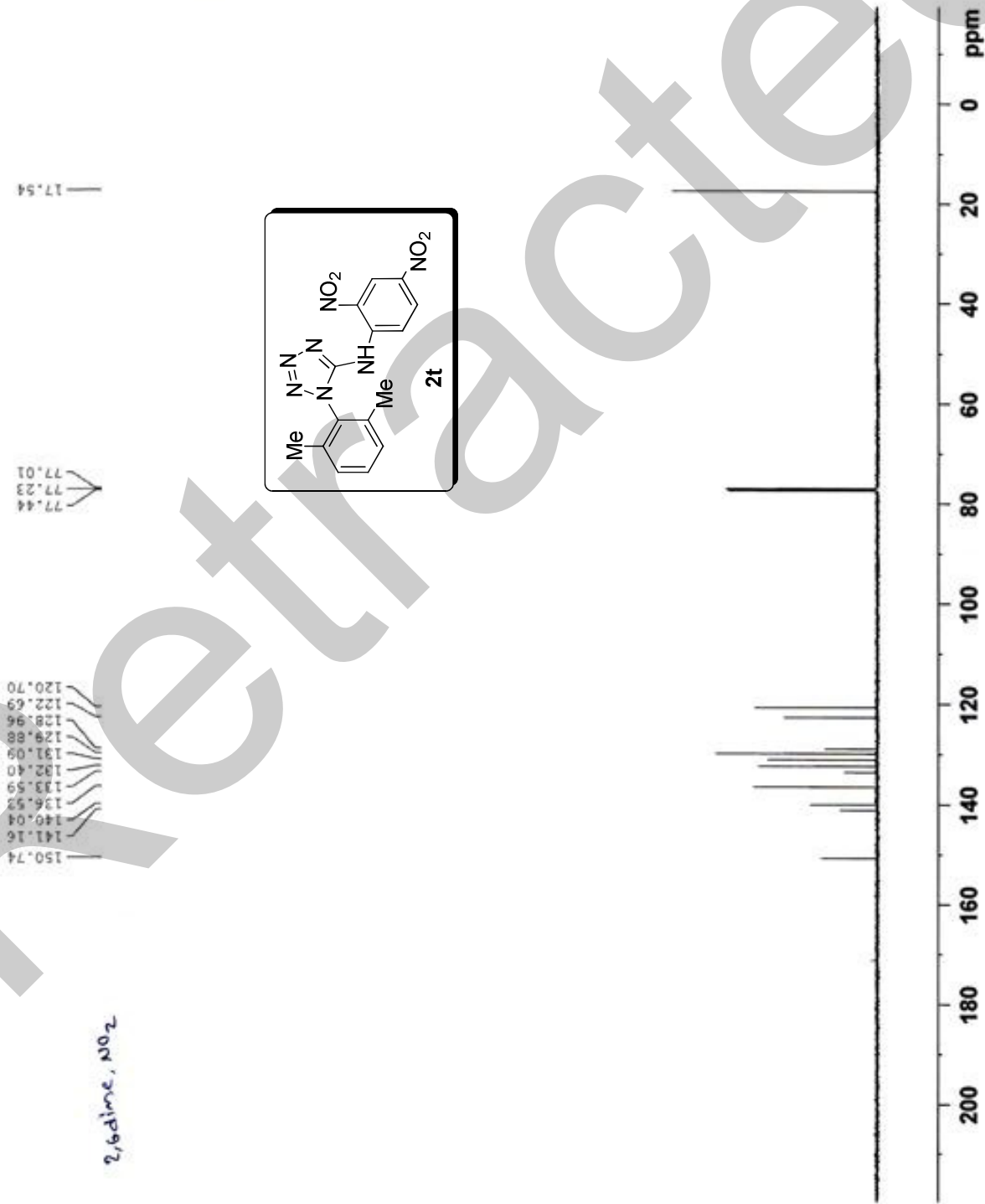
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.00000000 W

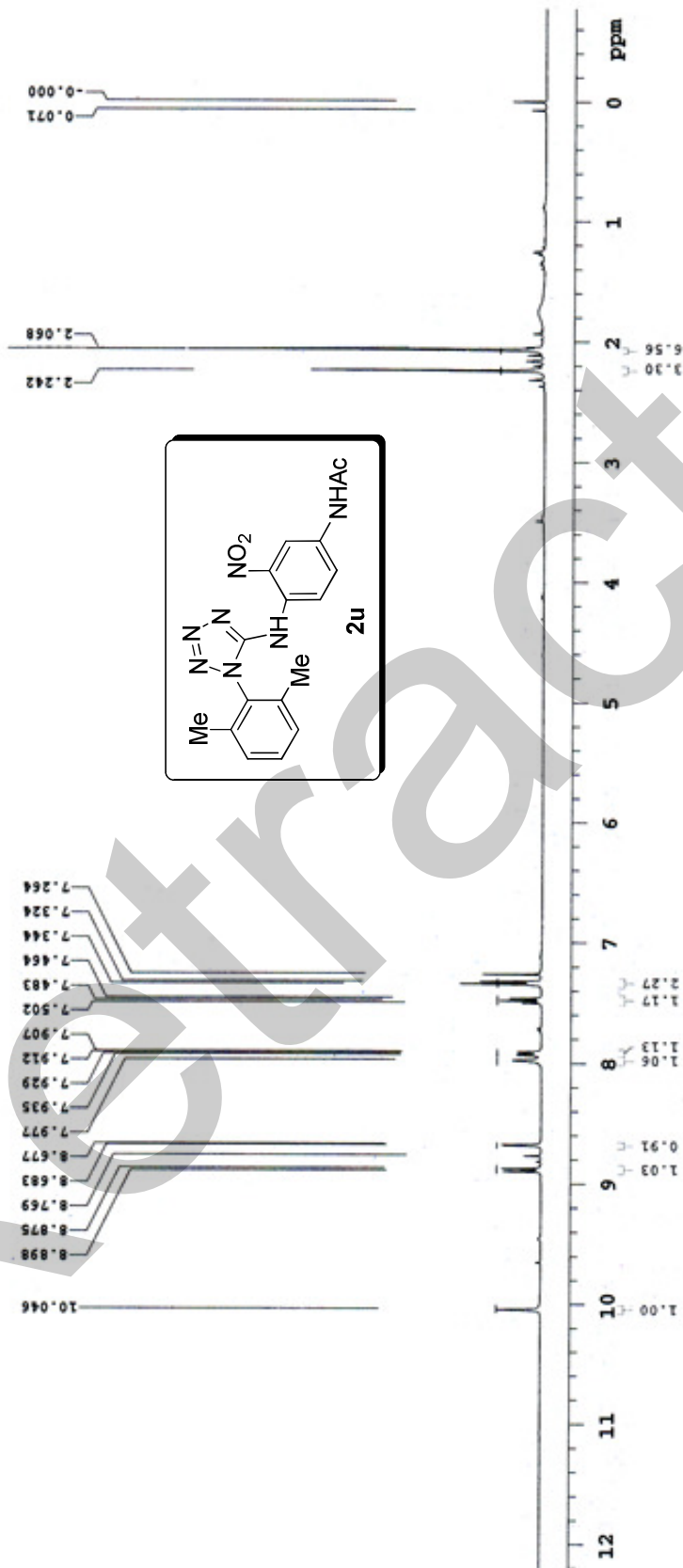
CHANNEL f2

SFO2 600.1724007 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.61714000 W
PLW13 0.30239999 W

F2 - Processing parameters

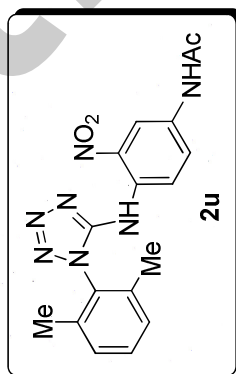
SI 16384
SF 150.9128457 MHz
WDW EM
SSB 0
LB 0
GB 0
PC 1.40





PULSE SEQUENCE Relax. delay 1.000 sec. Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	COSY 91, 399.8509602	DATA PROCESSING FT size 32768 Total time 1 minutes	SP-487-NHAC1 Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: SP-487-NHAC1 Mercury-400 -110-MHz
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SP-487_13C



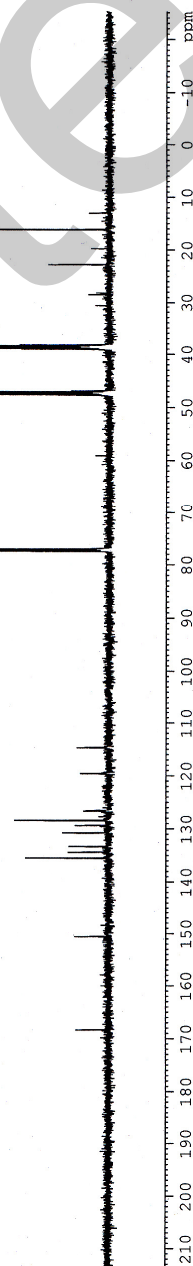
Current Data Parameters
NAME SP-487_13C
EXPNO 1
PROCNO 1

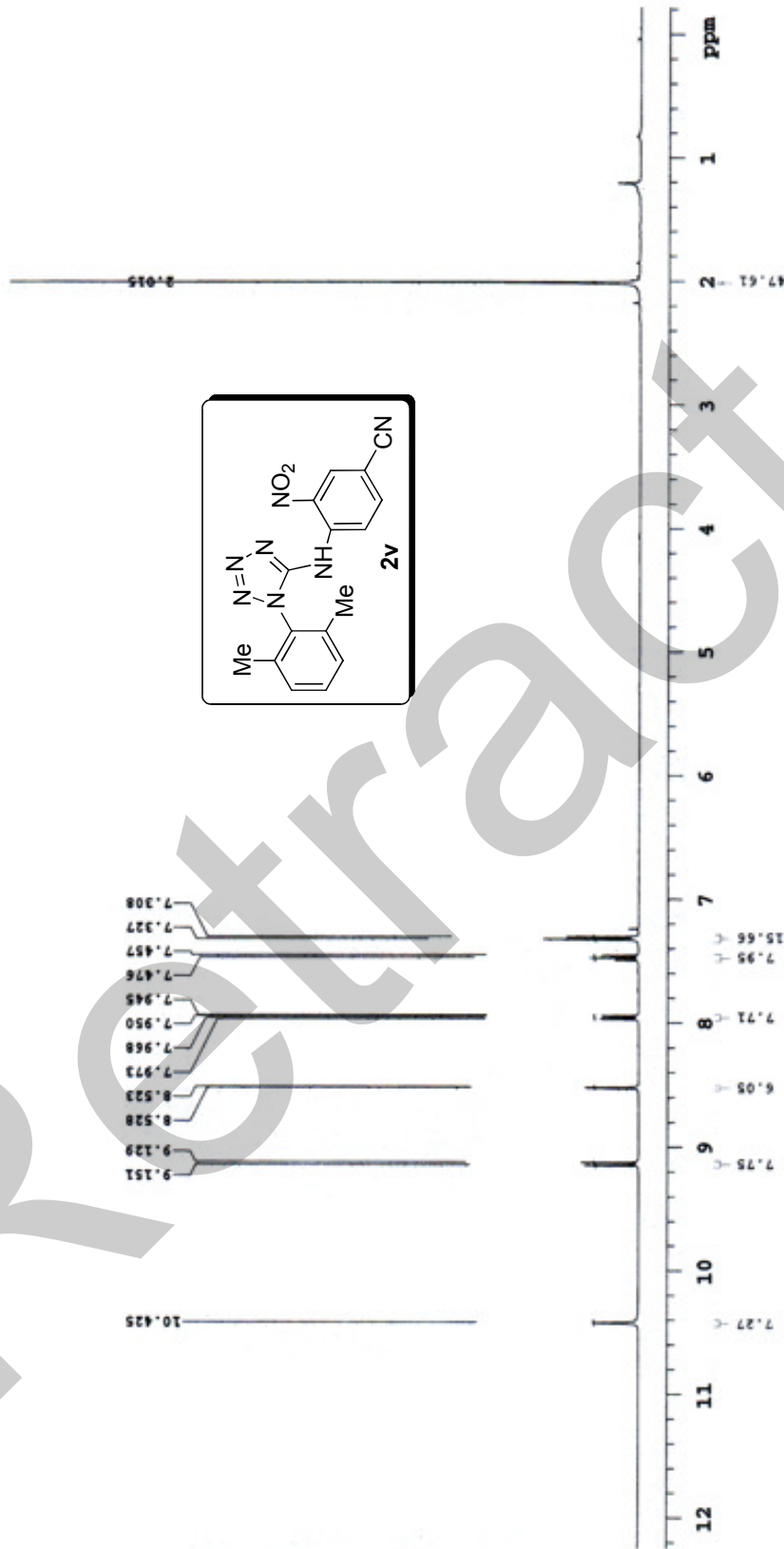
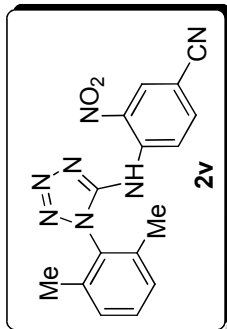
F2 - Acquisition Parameters
Date_ 20140319
Time 12.20
INSTRUM spect
PROBHD 5 mm FAPBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 443
DS 2
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 65.24
DW 13.867 usec
DE 6.50 usec
TE 301.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.00000000 W

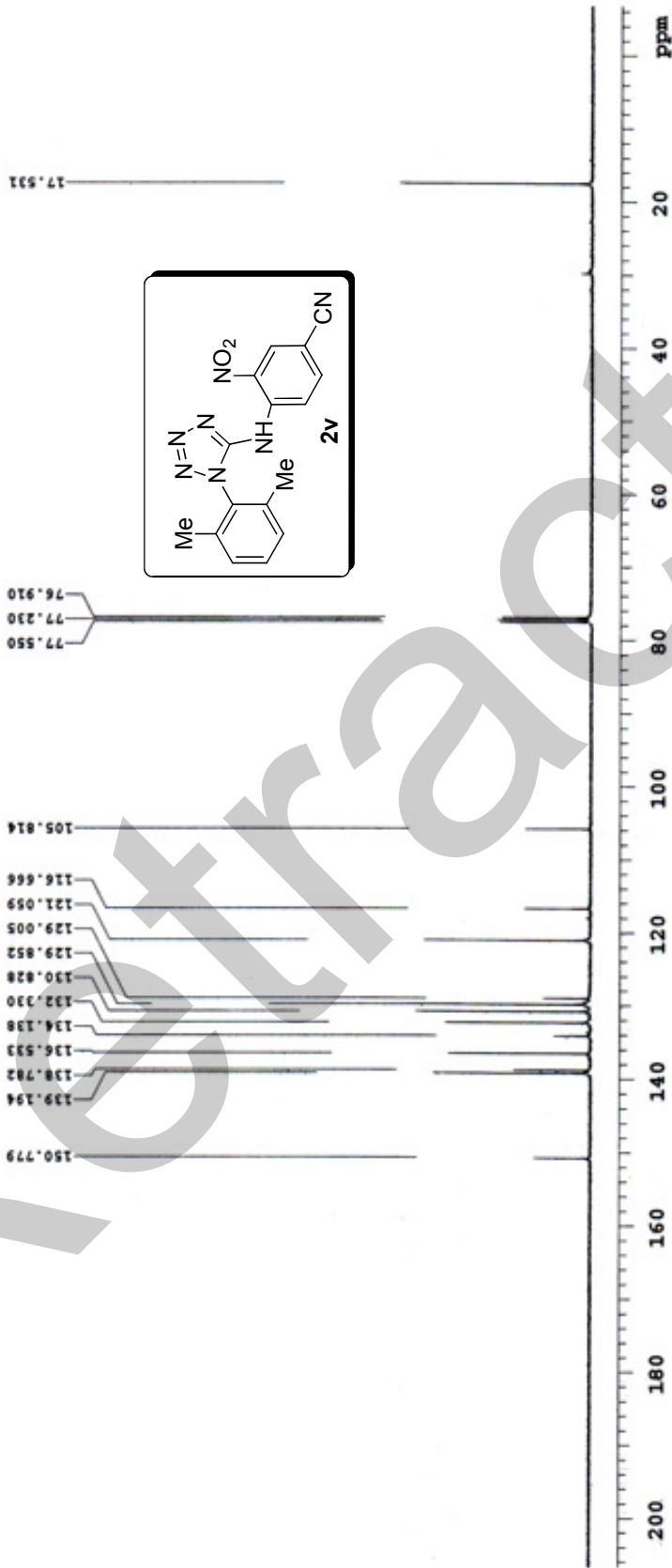
===== CHANNEL f2 =====
SFO2 600.1724007 MHz
NUC2 1H
PCPD2 waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.61714000 W
PLW13 0.30239999 W

F2 - Processing parameters
SI 16384
SF 150.9137348 MHz
WDW EM
SSB 0
LB 0
GB 0
PC 1.00 Hz
1.40





NAME: 2v EXP: 2v Solvent: cdcl3 Temp: 25.0 C / 298.1 K Operator: chm Mercury-400 1H/13C NMR	DATA PROCESSING FT size 32768 Total time 1 minutes	SEQUENCE: Relax: delay 1.000 sec Pulse: 45.0 degrees Acq: time 2.561 sec Width 6398.0 Hz 128 repetitions
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EXPERIMENTAL Relax: delay: 1.000 sec Pulse: 45.0 degree Acq: time: 1.304 sec Width: 25125.6 Hz 15470 repetitions	DATA PROCESSING OBSERVE: 101.37, 100.5425893 DECOUPLE: H1, 399.8529984 Power: 42 dB continuously on WALTZ-16 modulated	Line broadening 0.5 Hz FT size 65536 Total time 9.9 hours	NAME: CN-13C Solvent: cdcl3 Temp: 25.0 C / 298.1 K Operator: chem
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