This paper was retracted on March 20, 2015 (*J. Org.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

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Crystal Structure Compound 2c:

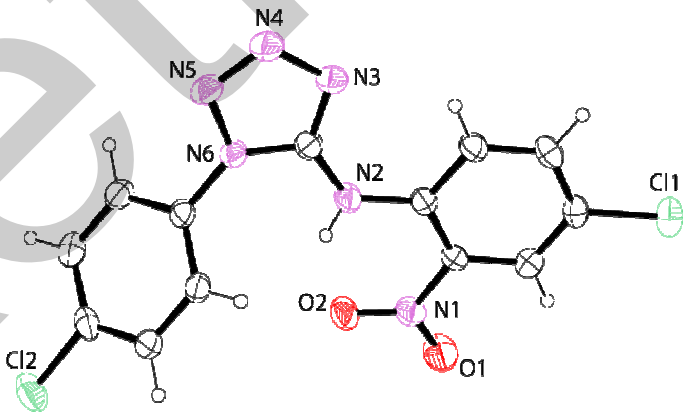


Figure 1: ORTEP diagram of *N*-(4-Chloro-2-nitrophenyl)-1-(4-chlorophenyl)-1*H*-tetrazol-5-amine **2c** with 50% ellipsoid.

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

Identification code	**2c**
Empirical formula	$C_{13}H_8Cl_2N_6O_2$
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 α(°) = 101.507(7)
	b = 7.6732(7) Å β(°) = 94.517(6)
	c = 15.1467(11) Å γ(°) = 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>2sigma (I)]	*R1* = 0.0450, *wR2* = 0.0604
R indices (all data)	*R1* = 0.0784, *wR2* = 0.0722

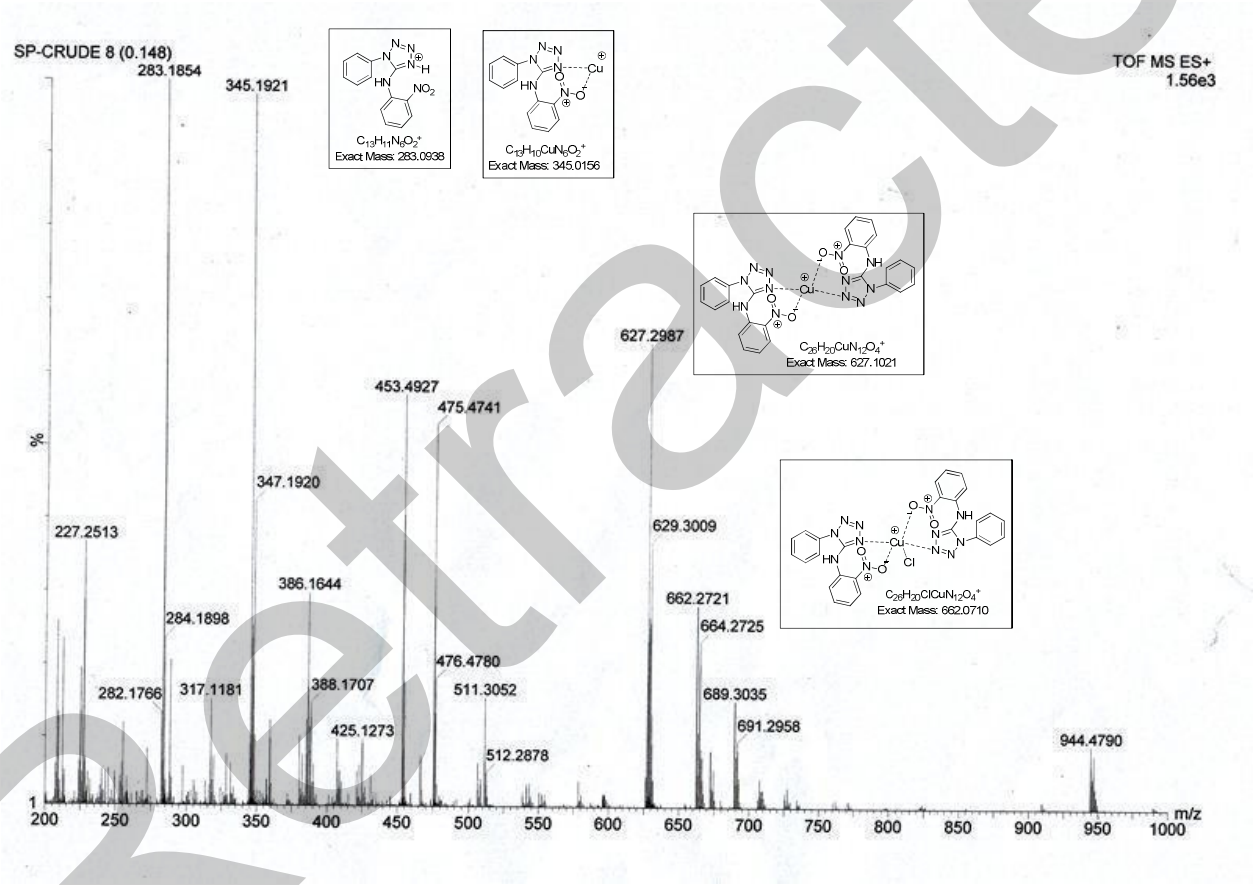
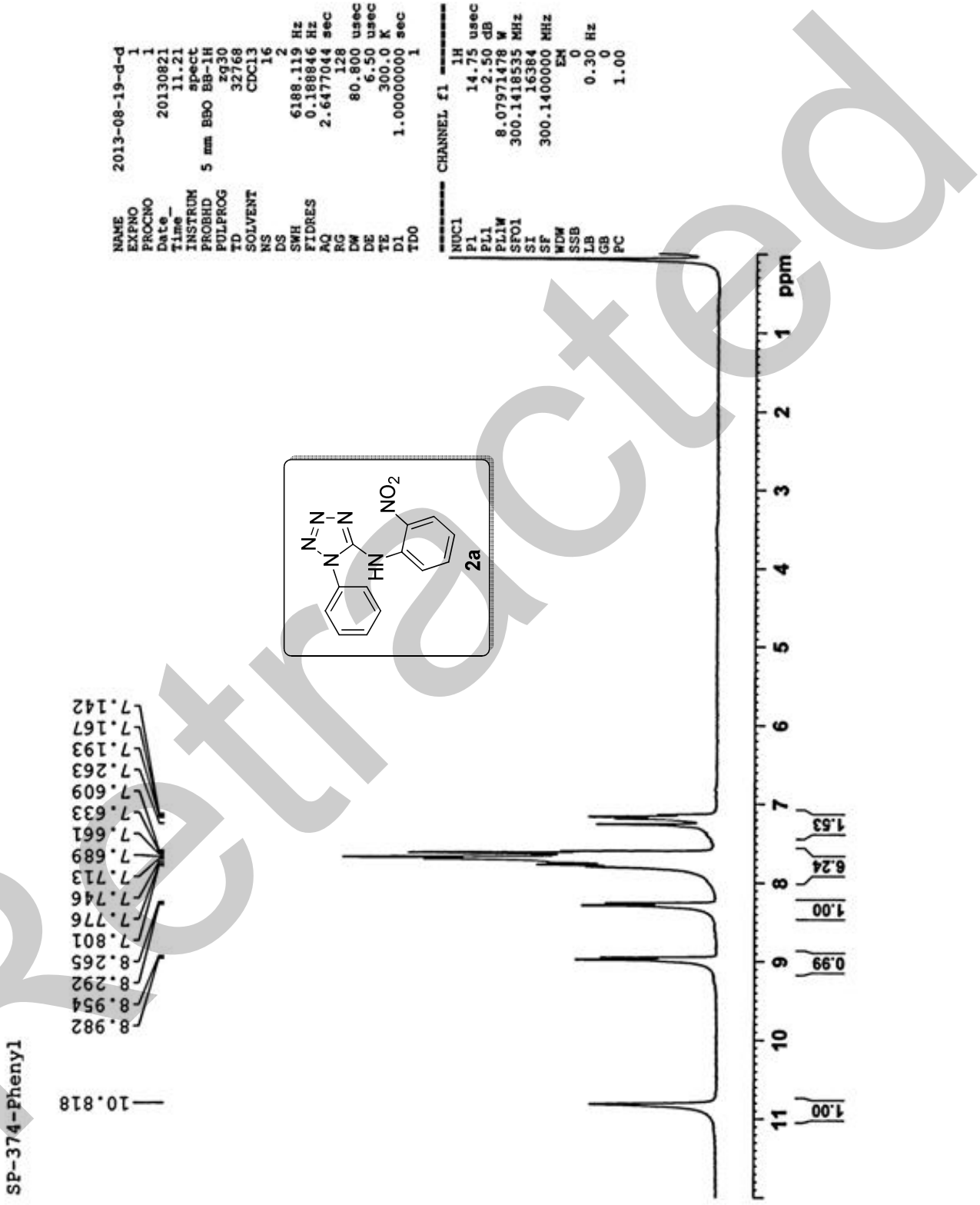
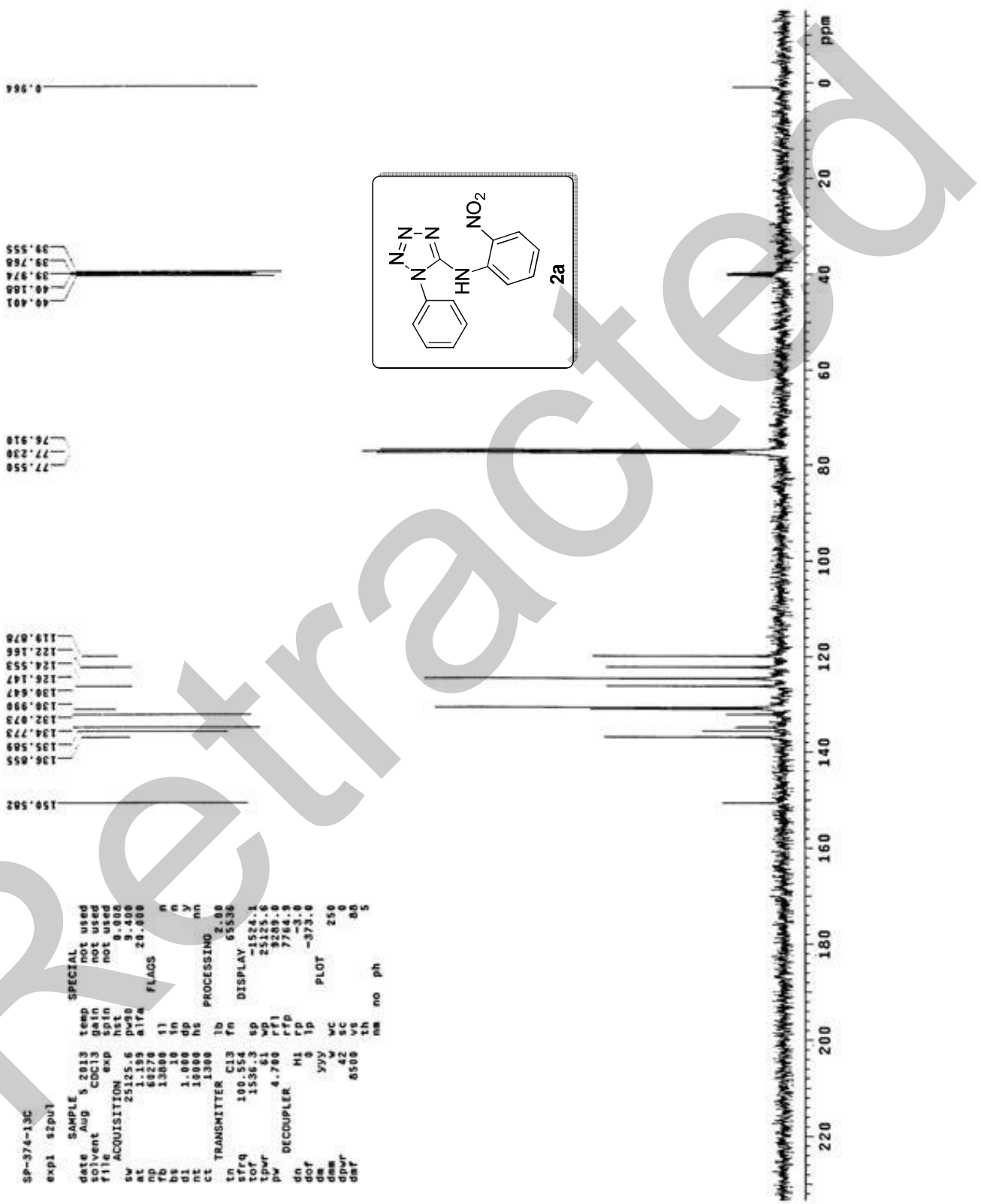


Figure S1. Mass spectra of reaction mixture **1a** prior to work up.

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

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nt 10000
ct 1300
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sfrq 100.554
tof 1536.3
tpwr 61
pw 4.700
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8500
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gain not used
spin not used
hst 0.008
pw90 9.400
alfa 20.000
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fn n
dp y
hs nn
PROCESSING
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fn 65536
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wp 25125.6
rfl 9289.0
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rp -3.0
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sc 0
vs 86
th 5
nm no ph
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39.768
39.974
40.186
40.401
76.910
77.230
77.550
119.078
122.166
124.553
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130.990
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134.773
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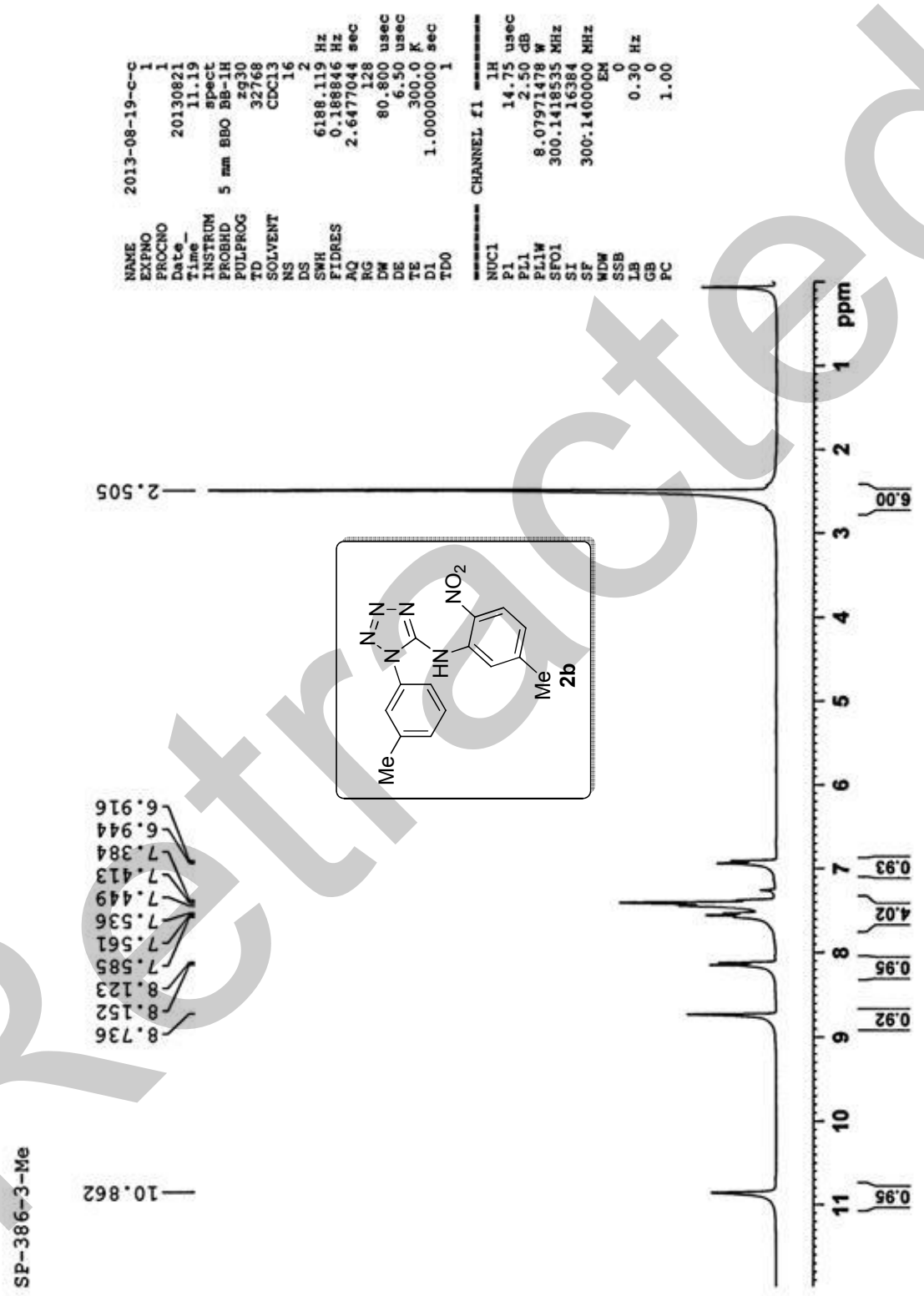
2a
ppm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6.916
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RG 128
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TE 300.0 K
D1 1.00000000 sec
TD0 1
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PL1 2.50 dB
PL1W 8.07971478 W
SFO1 300.1418535 MHz
SI 16384
SF 300.1400000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
HN
NO2
Me
2b
ppm
1
2
3
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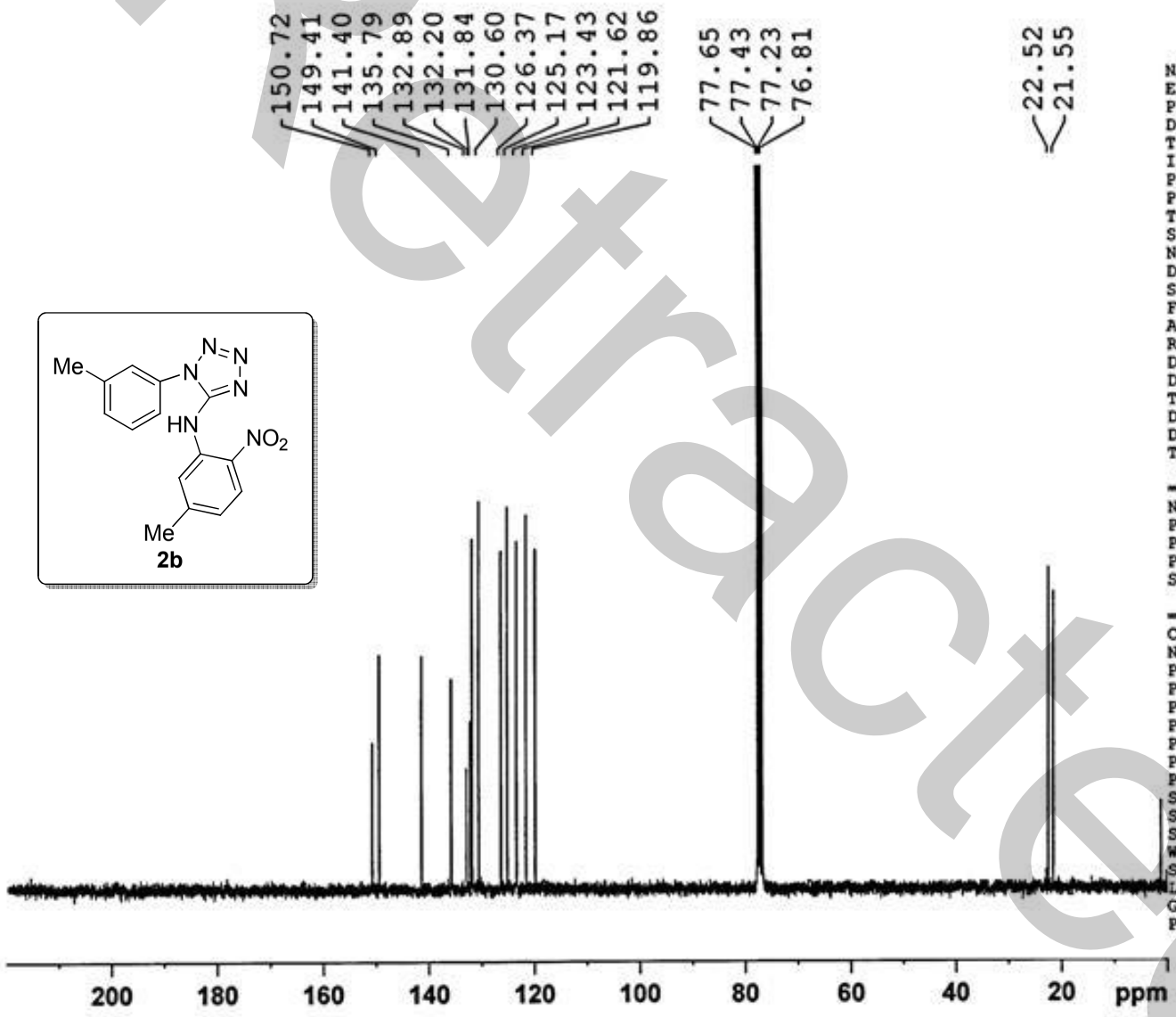

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P1	9.80 usec
PL1	-0.50 dB
PL1W	34.66611099 W
SFO1	75.4778101 MHz
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CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	2.50 dB
PL12	19.20 dB
PL13	23.00 dB
PL2W	8.07971478 W
PL12W	0.17274120 W
PL13W	0.07201053 W
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SI	32768
SF	75.4702500 MHz
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date Jul 27 2013
solvent CDCl3
file exp
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nt 20000
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sfrq 100.554
tof 1536.3
tpwr 61
pw 4.700
DECOUPLER
dn H1
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dmm y
dpwr 42
dmf 8500
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gain not used
spin not used
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120
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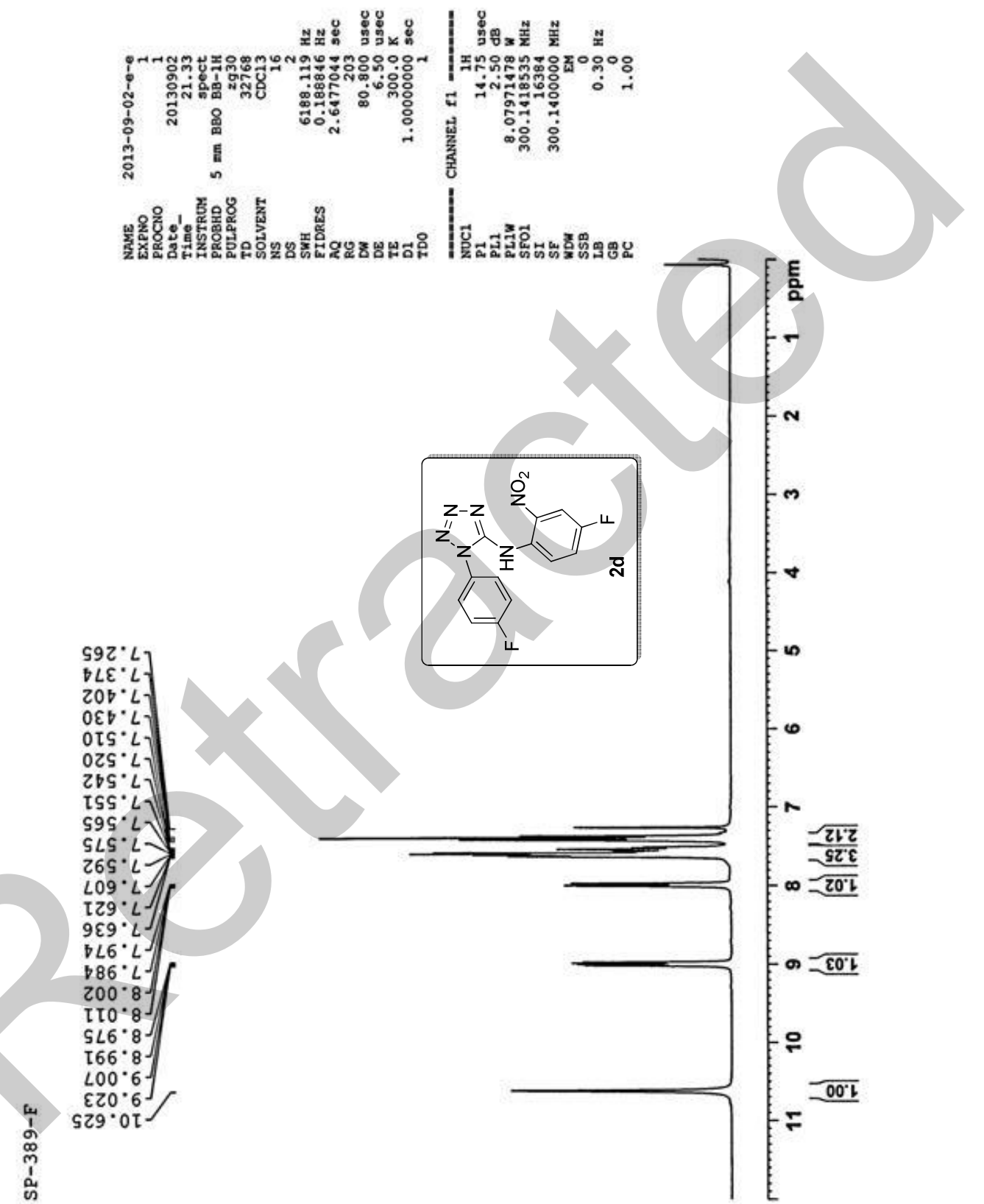
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8.975
8.011
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7.621
7.607
7.592
7.575
7.565
7.551
7.542
7.520
7.510
7.430
7.402
7.374
7.265
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EXPNO 1
PROCNO 1
Date_ 20130902
Time 21.33
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PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.188846 Hz
AQ 2.6477044 sec
RG 203
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
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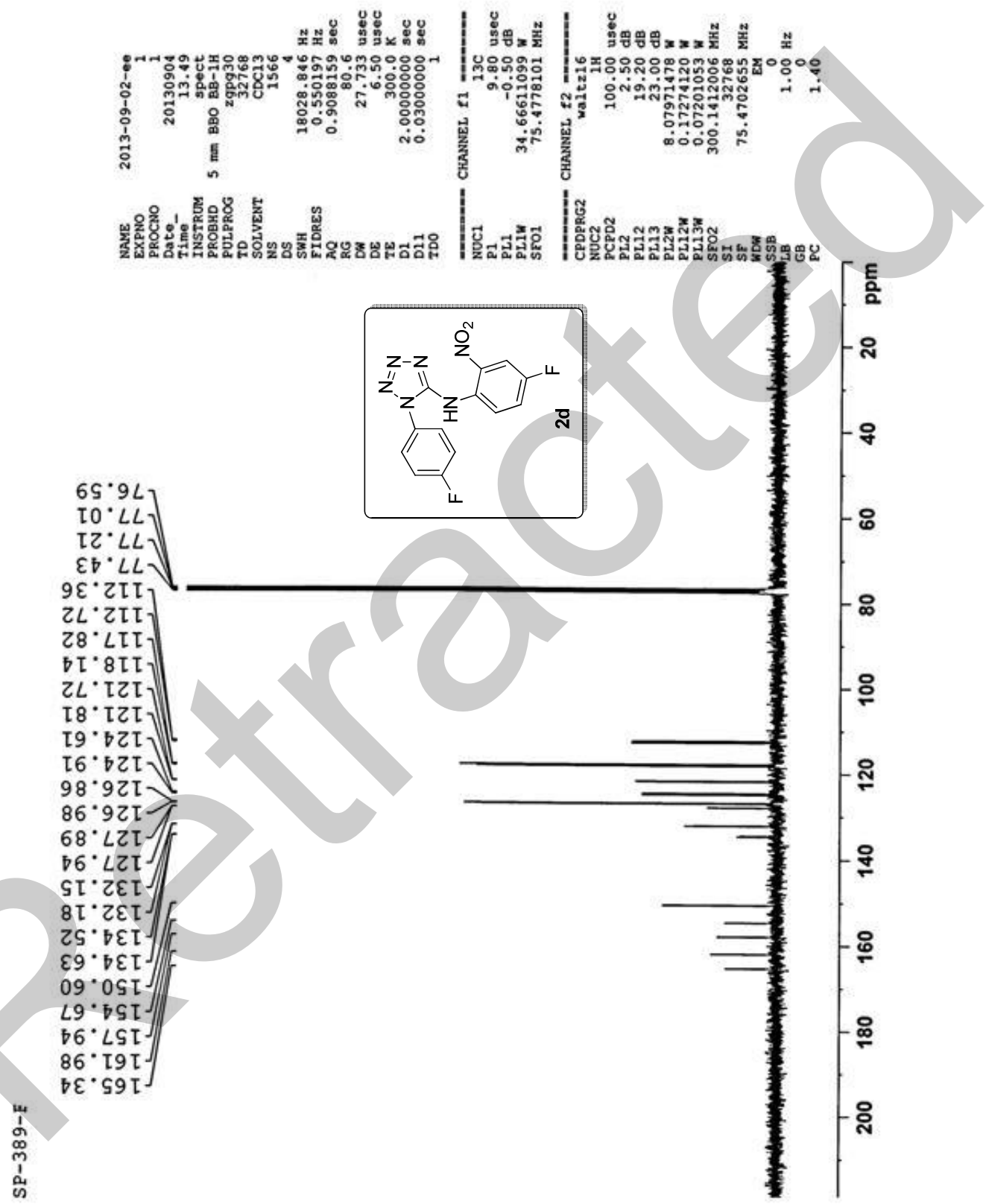
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121.72
118.14
117.82
112.72
112.36
77.43
77.21
77.01
76.59
2d
NO2
F
HN
F
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PROCNO 1
Date_ 20130904
Time 13.49
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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
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FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 80.6
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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
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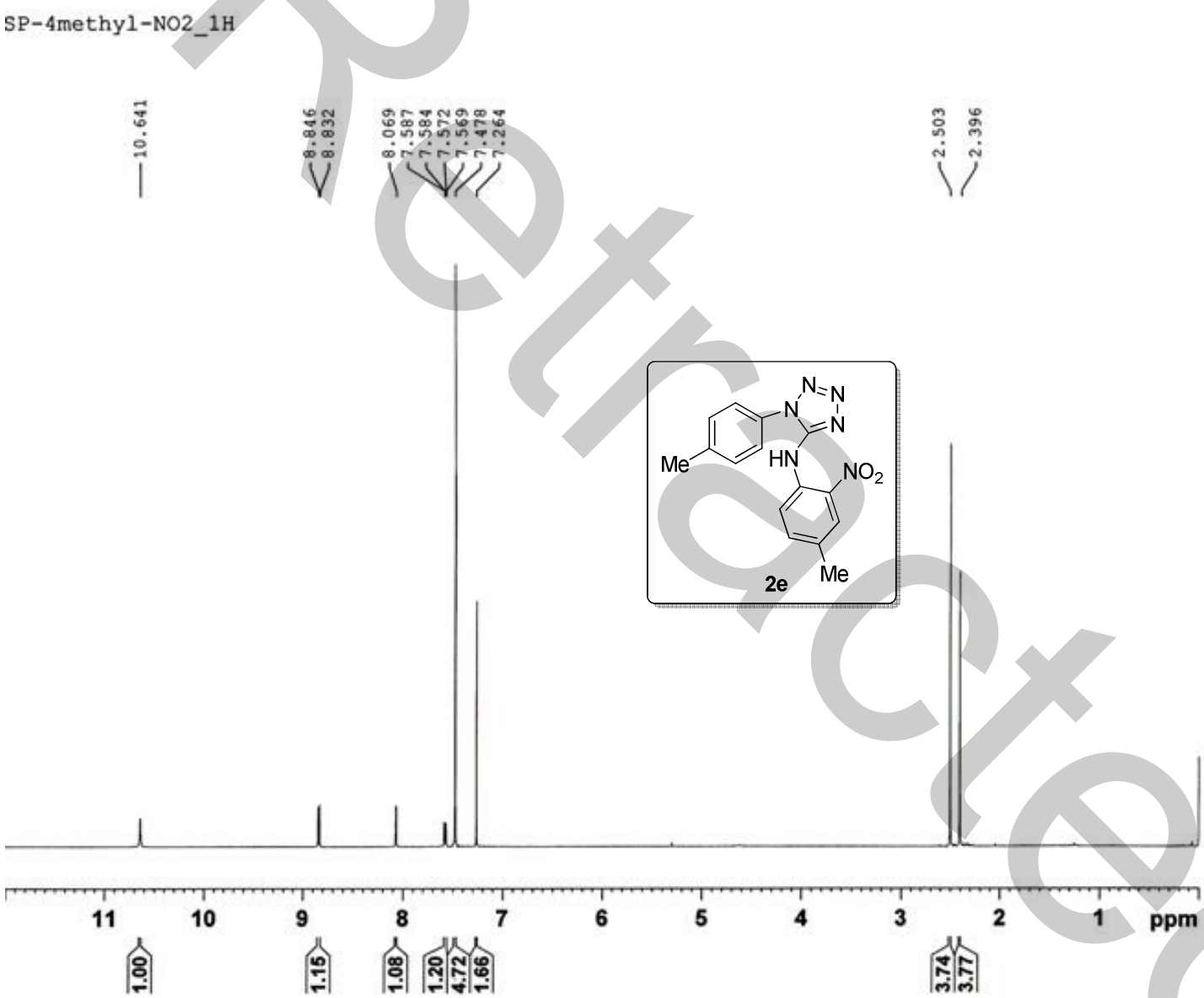
20
ppm

SP-4methyl-NO2_1H



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PROCNO                    1

F2 - Acquisition Parameters
Date_              20131114
Time                  11.15
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               12019.230 Hz
FIDRES            0.366798 Hz
AQ                1.36314688 sec
RG                   143.33
DW                  41.600 usec
DE                   6.50 usec
TE                  298.2 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           600.1737063 MHz
NUC1                     1H
P1                    12.00 usec
PLW1          21.00000000 W

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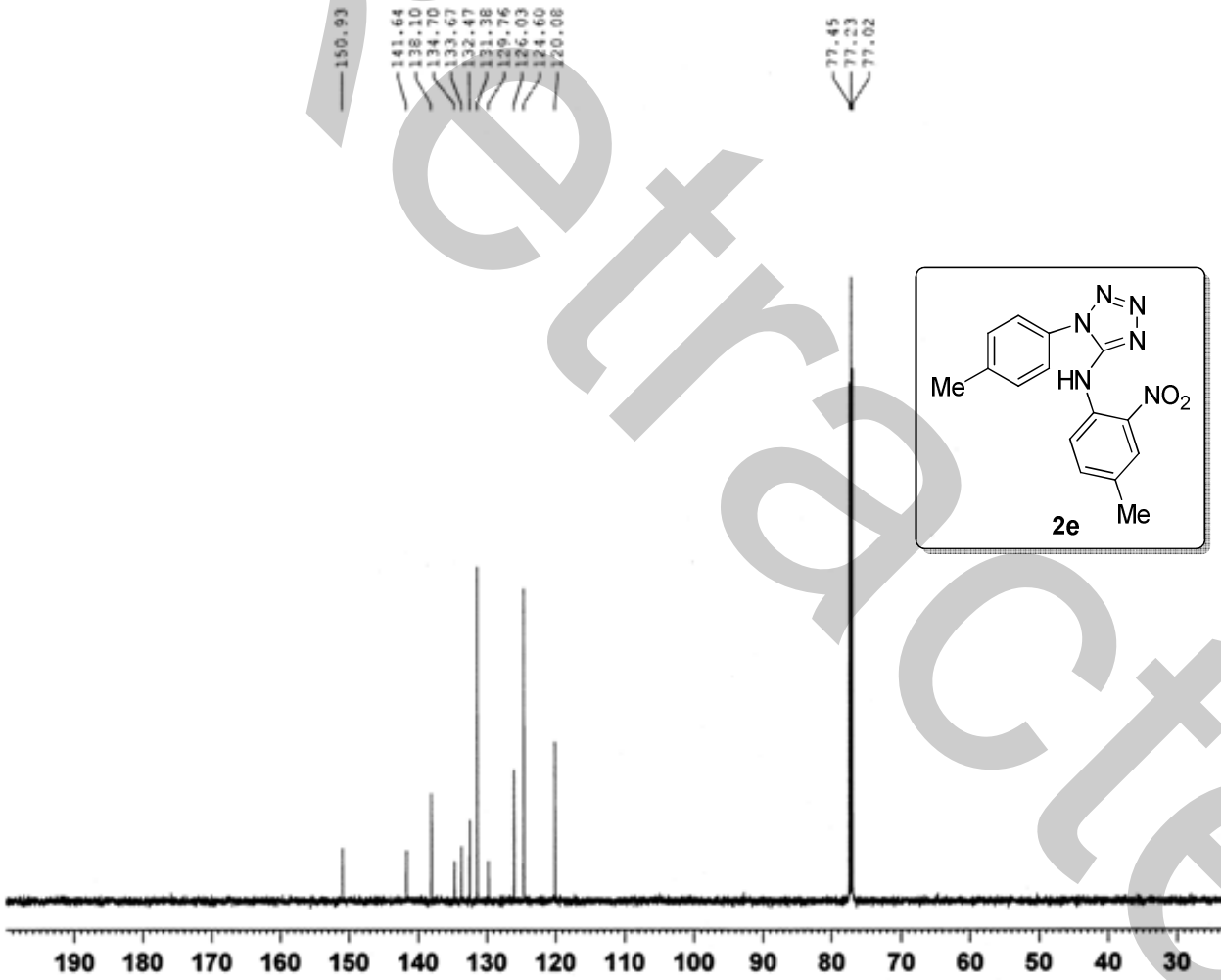
SP-P-ME-NO2-13C



BRUKER

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PROCNO                  1

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INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  104
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               298.7 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
CPDPRG[2          waltz16
PCPD2              70.00 usec
PLW2         21.00000000 W
PLW12         0.61714000 W
PLW13         0.30239999 W

F2 - Processing parameters
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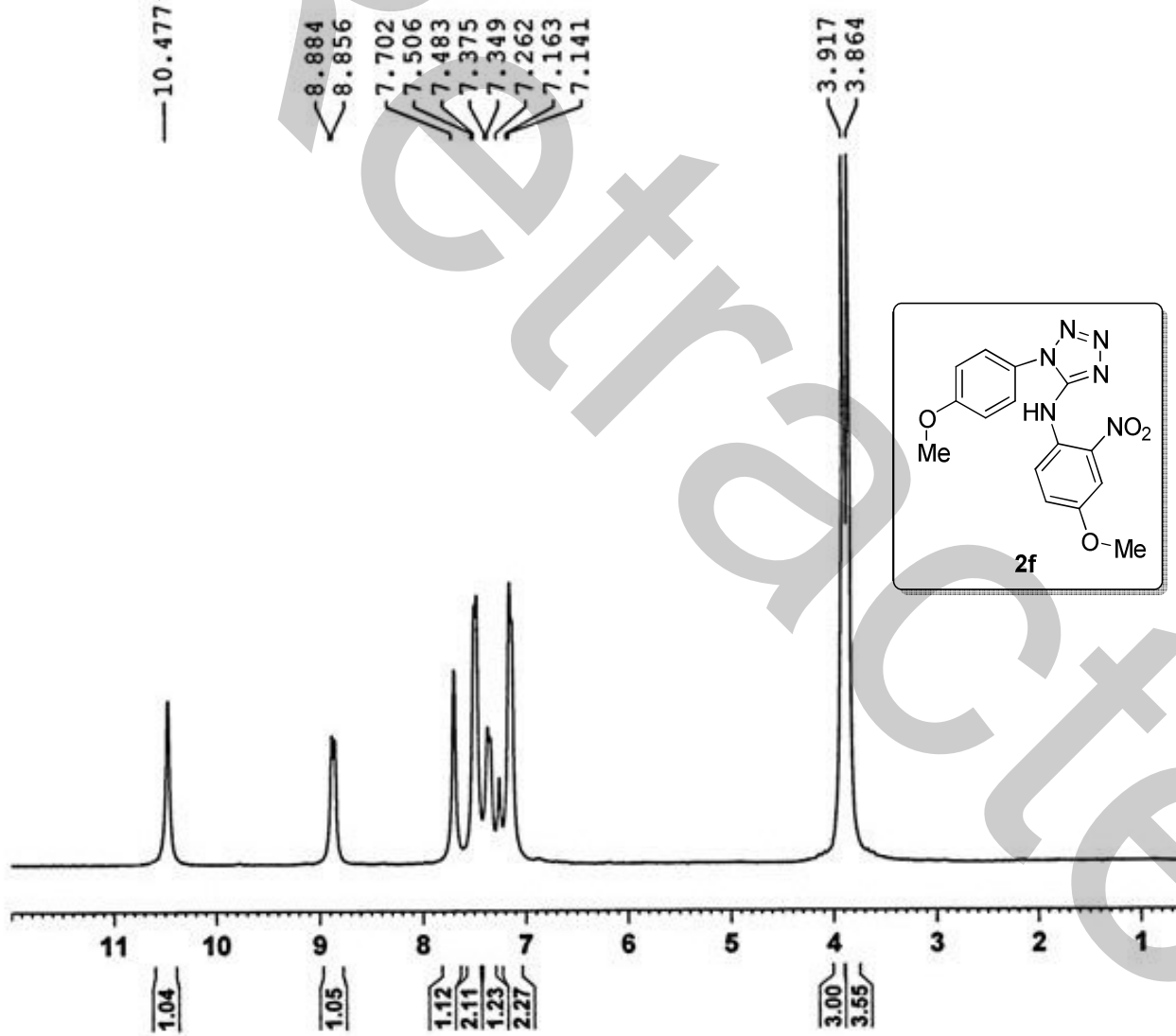
SP-390-OMe



2f

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PROCNO	1
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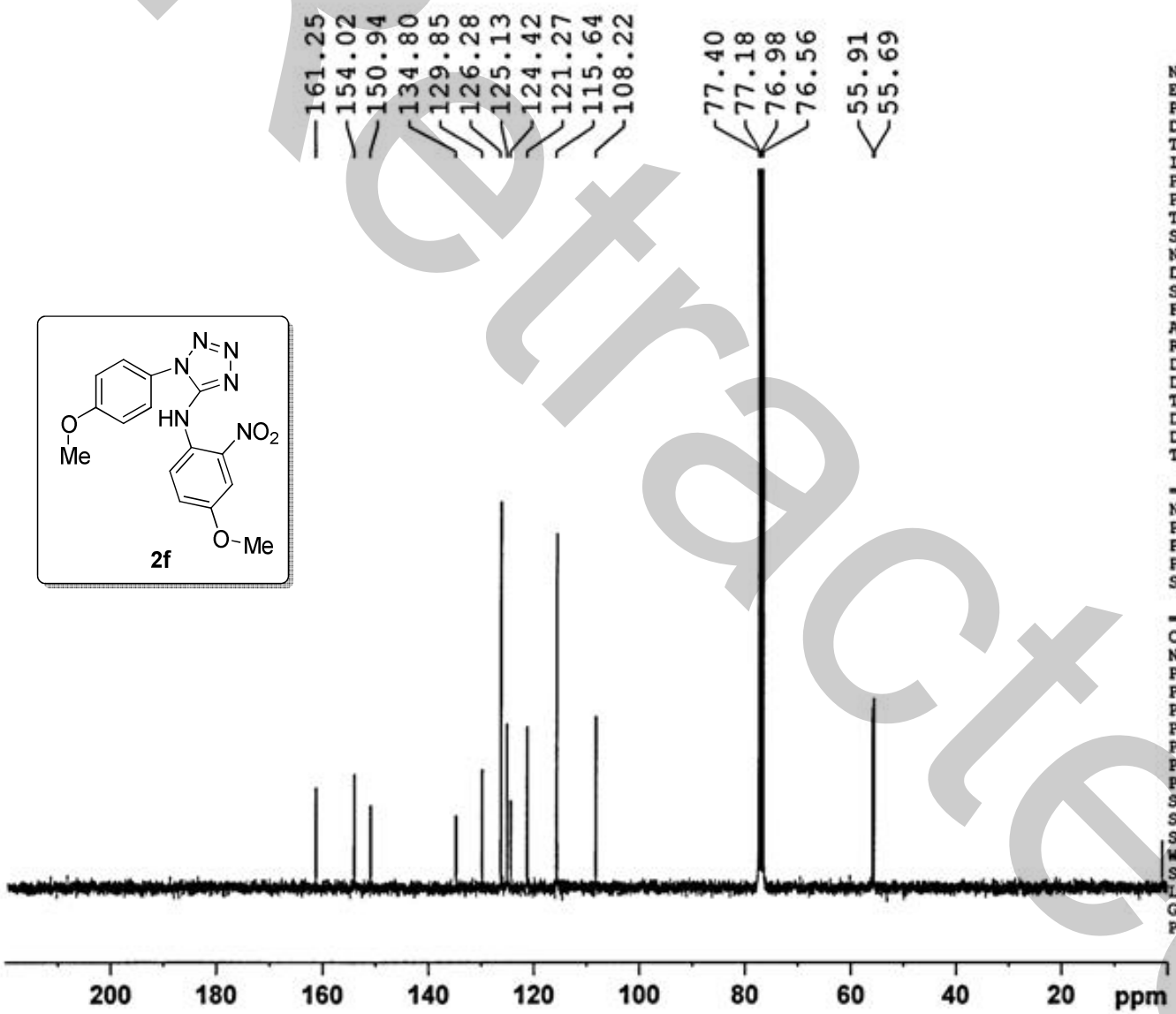
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	6188.119 Hz
FIDRES	0.188846 Hz
AQ	2.6477044 sec
RG	203
DW	80.800 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.75 usec
PL1	2.50 dB
PL1W	8.07971478 W
SFO1	300.1418535 MHz
SI	16384
SF	300.1400000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

SP-390-OMe



2f

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PROCNO	1
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PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	2000
DS	4
SWH	18028.846 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	1620
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
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GB	0
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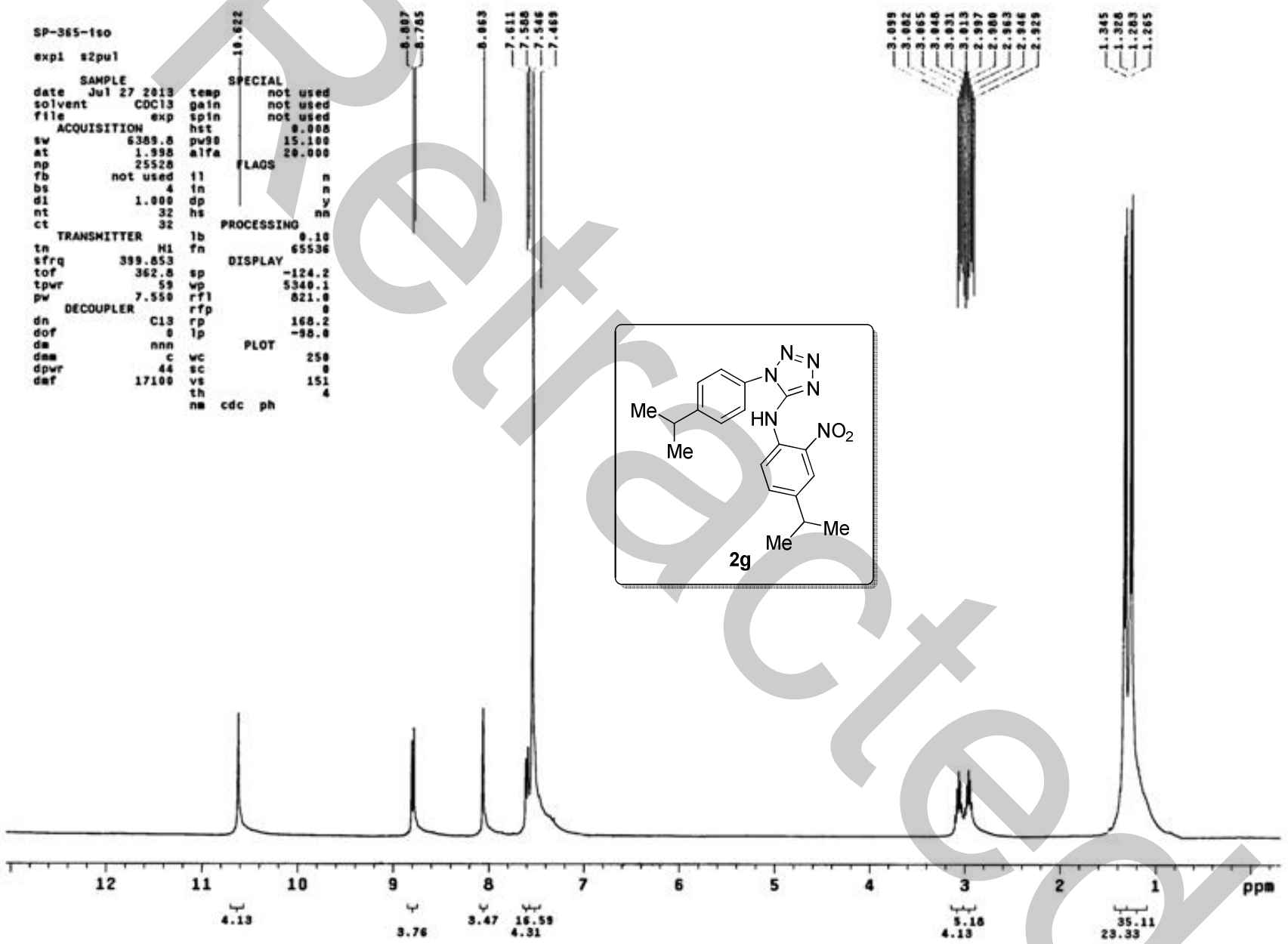
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solvent CDCl3
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ct 32
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sfrq 399.853
tof 362.8
tpwr 59
pw 7.550
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 44
dmf 17100
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 15.100
alfa 20.000
FLAGS
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in n
dp y
hs nn
PROCESSING
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fn 65536
DISPLAY
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wp 5340.1
rfl 821.0
rfp 0
rp 168.2
lp -98.6
PLOT
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sc 0
vs 151
th 4
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3.048
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3.013
2.997
2.980
2.963
2.946
2.929
1.345
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1.283
1.265
Me
Me
HN
N
N
N
NO2
Me
Me
2g
12
11
10
9
8
7
6
5
4
3
2
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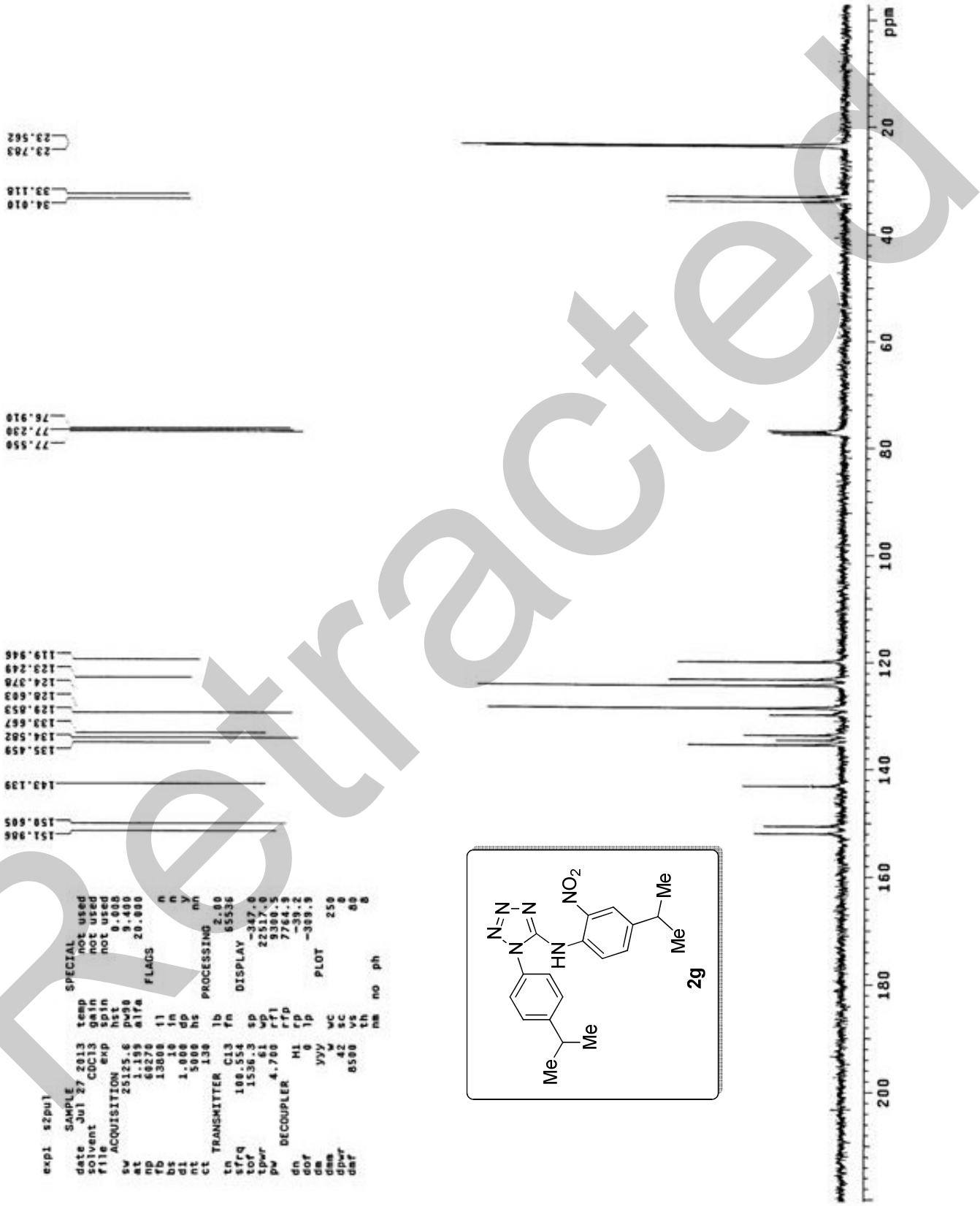
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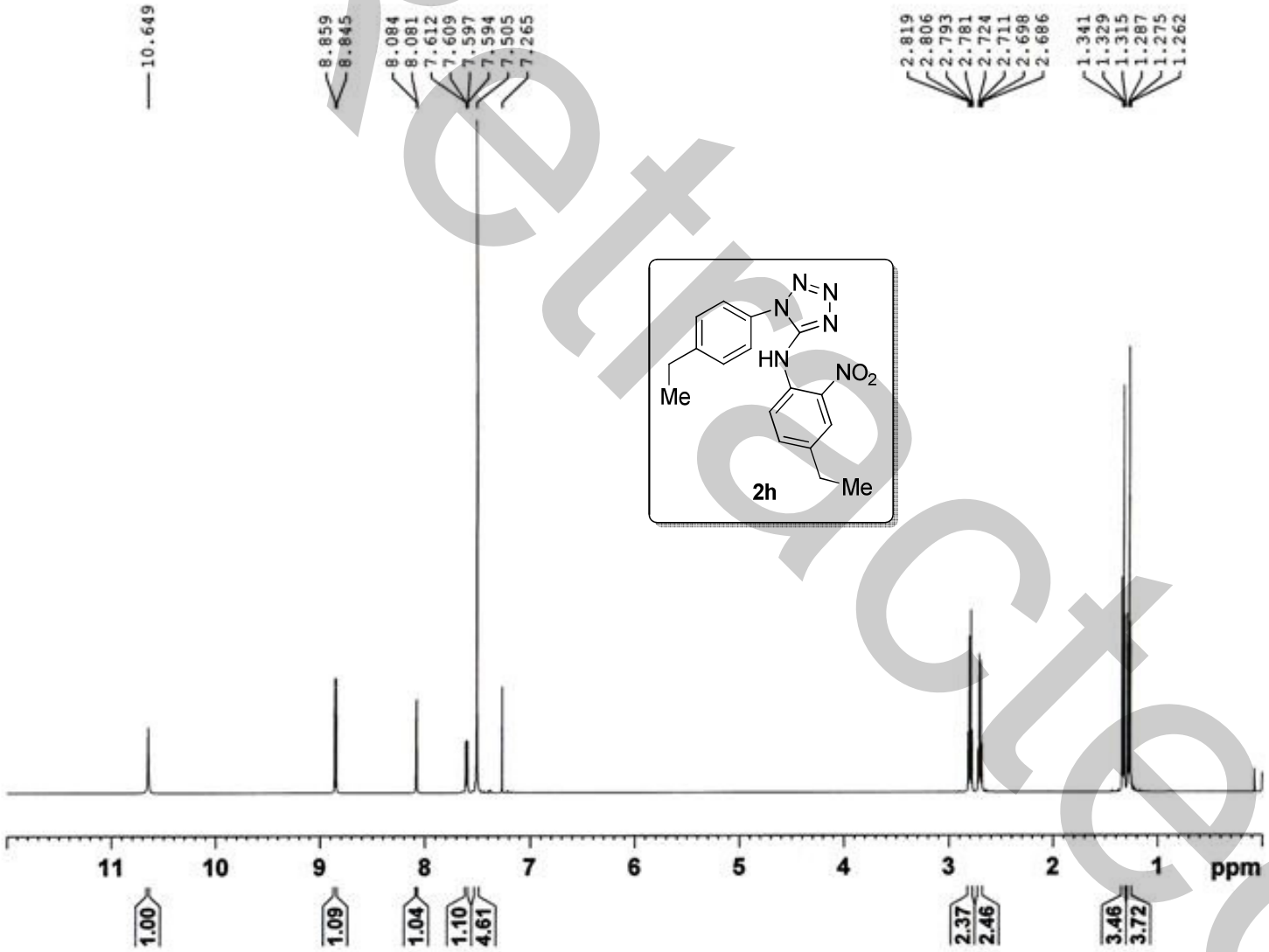
ppm

SP-Ethyl_1H

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PROCNO                  1

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Time                 11.07
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PULPROG              zg30
TD                  32768
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              12019.230 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                   54.94
DW                  41.600 usec
DE                   6.50 usec
TE                  298.2 K
D1               1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1            600.1737063 MHz
NUC1                    1H
P1                   12.00 usec
PLW1            21.00000000 W

F2 - Processing parameters
SI                      16384
SF              600.1700115 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
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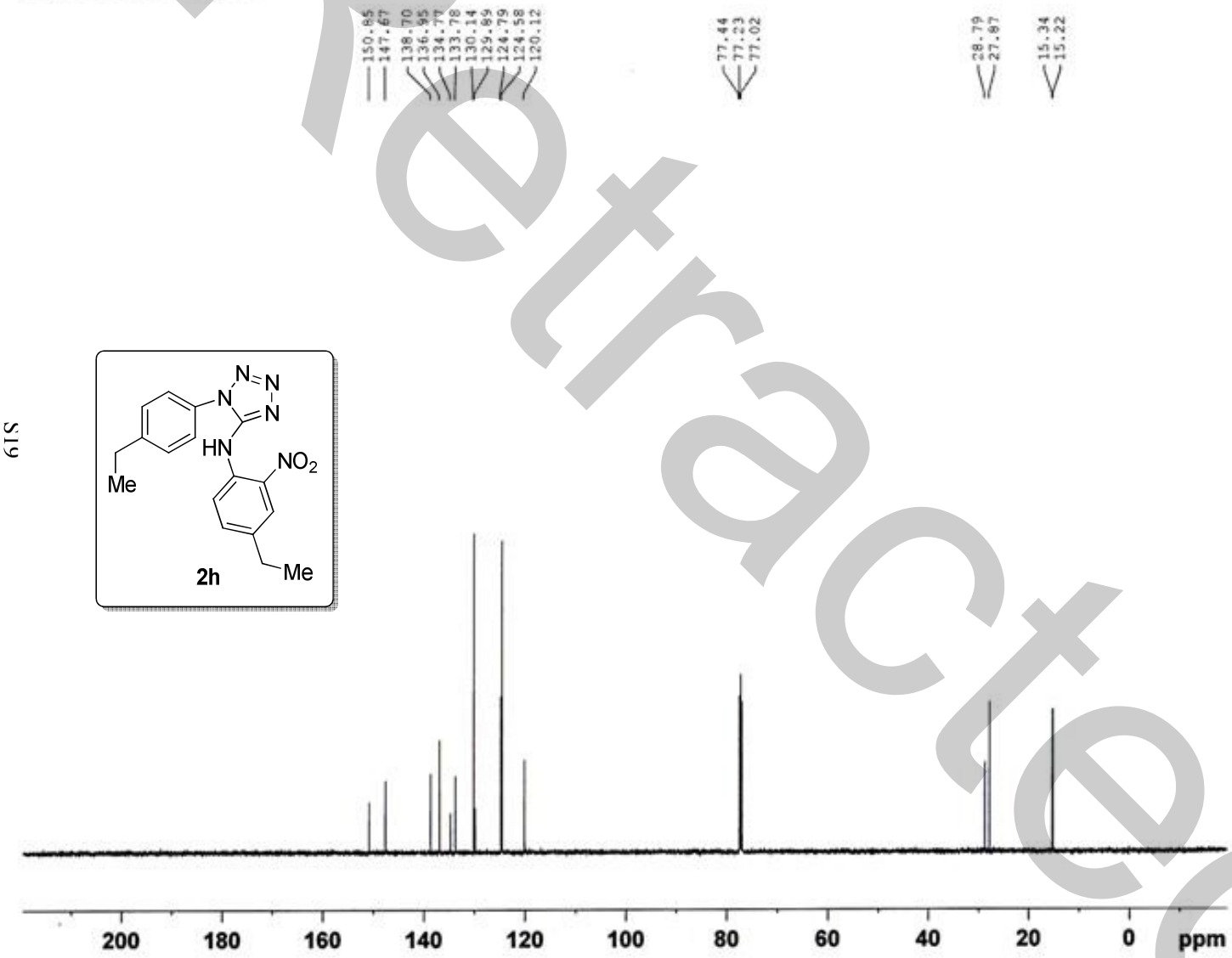
PC                    1.00
```

TK_ETHYL_NHOH_13C1



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PROCNO                     1

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INSTRUM               spect
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PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                      49
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                   299.9 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
CPDPRG[2           waltz16
PCPD2                70.00 usec
PLW2          21.00000000 W
PLW12          0.61714000 W
PLW13          0.30239999 W

F2 - Processing parameters
SI                   16384
SF           150.9128456 MHz
WDW                     EM
SSB      0
LB                    1.00 Hz
GB       0
PC                    1.40
```
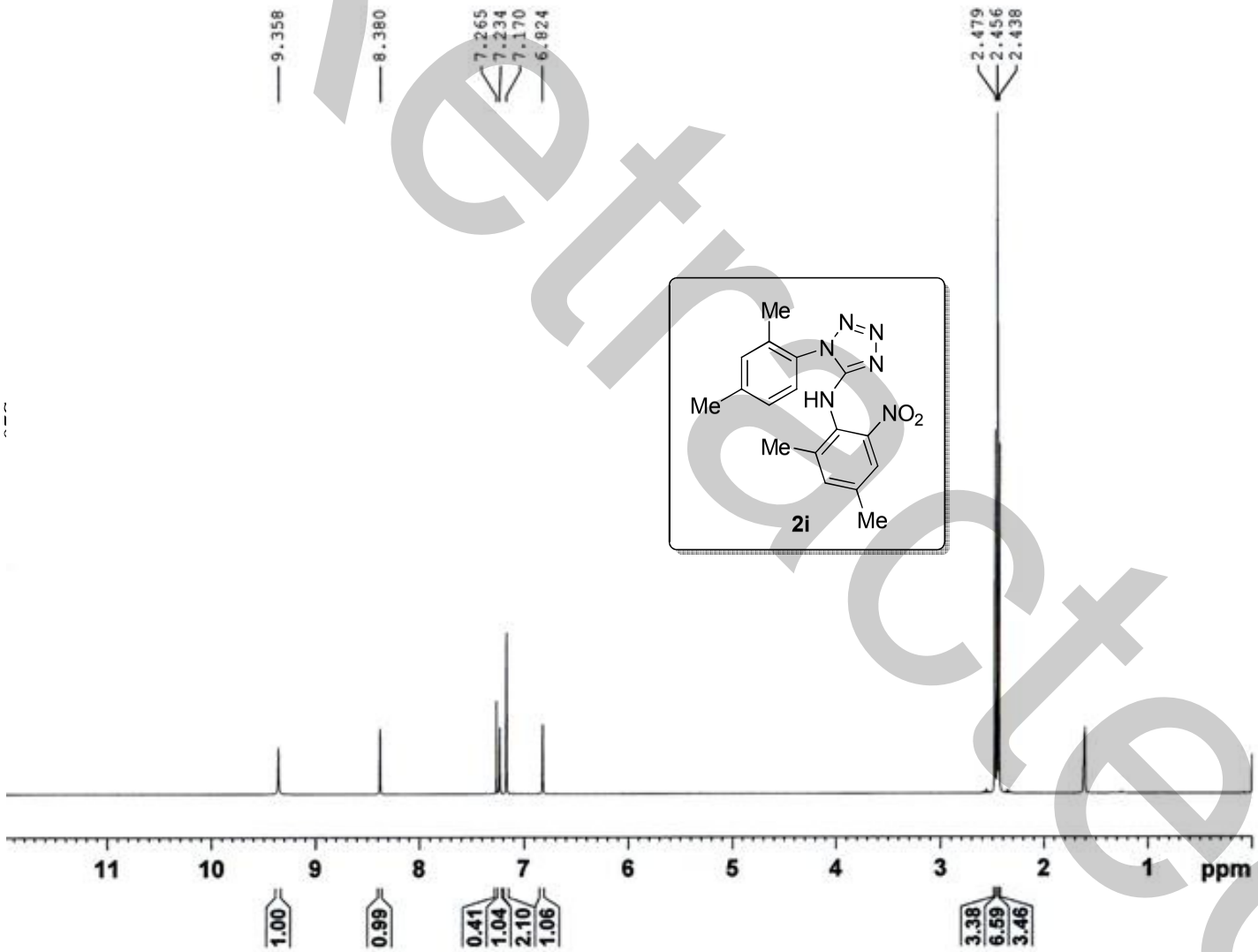
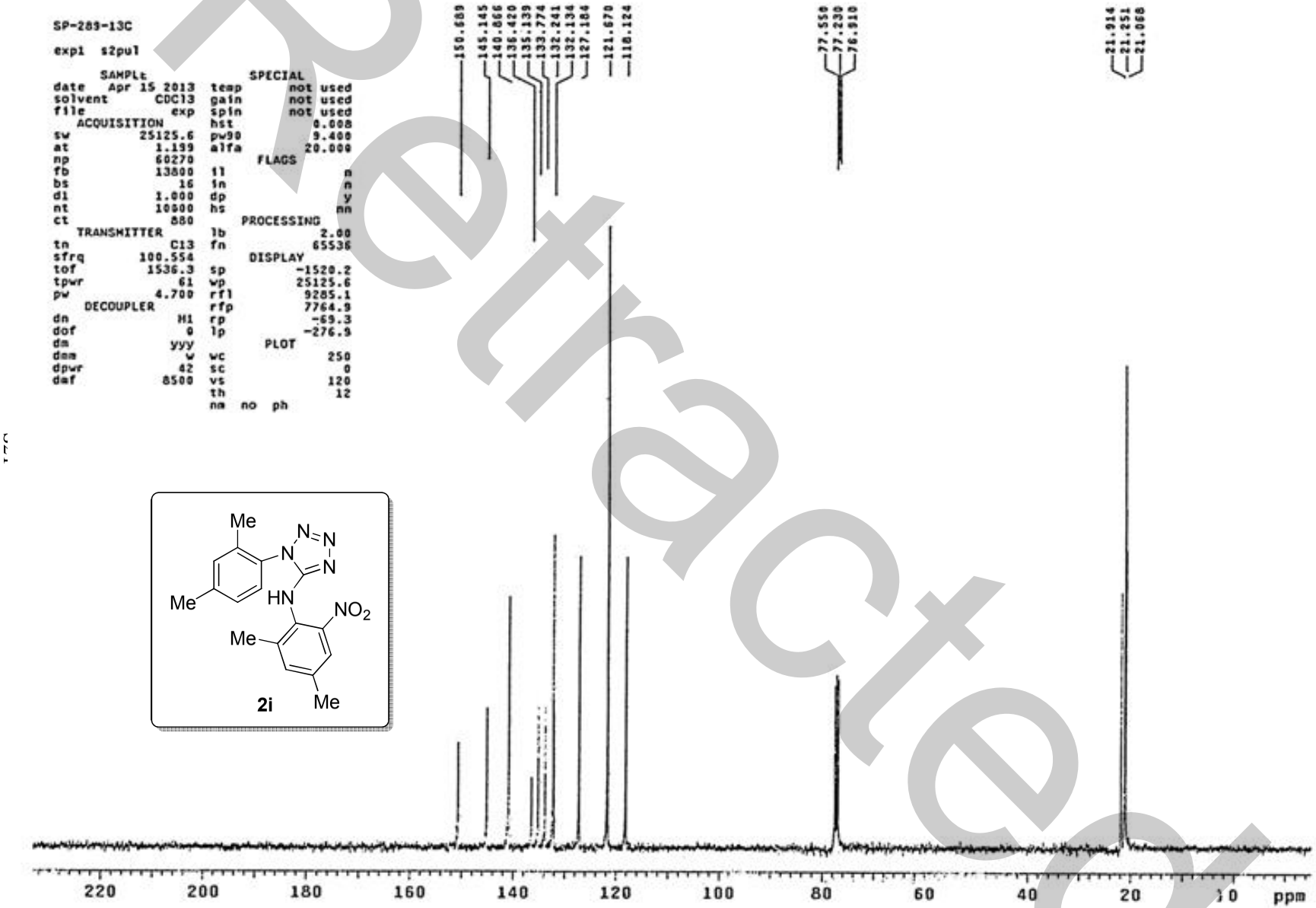
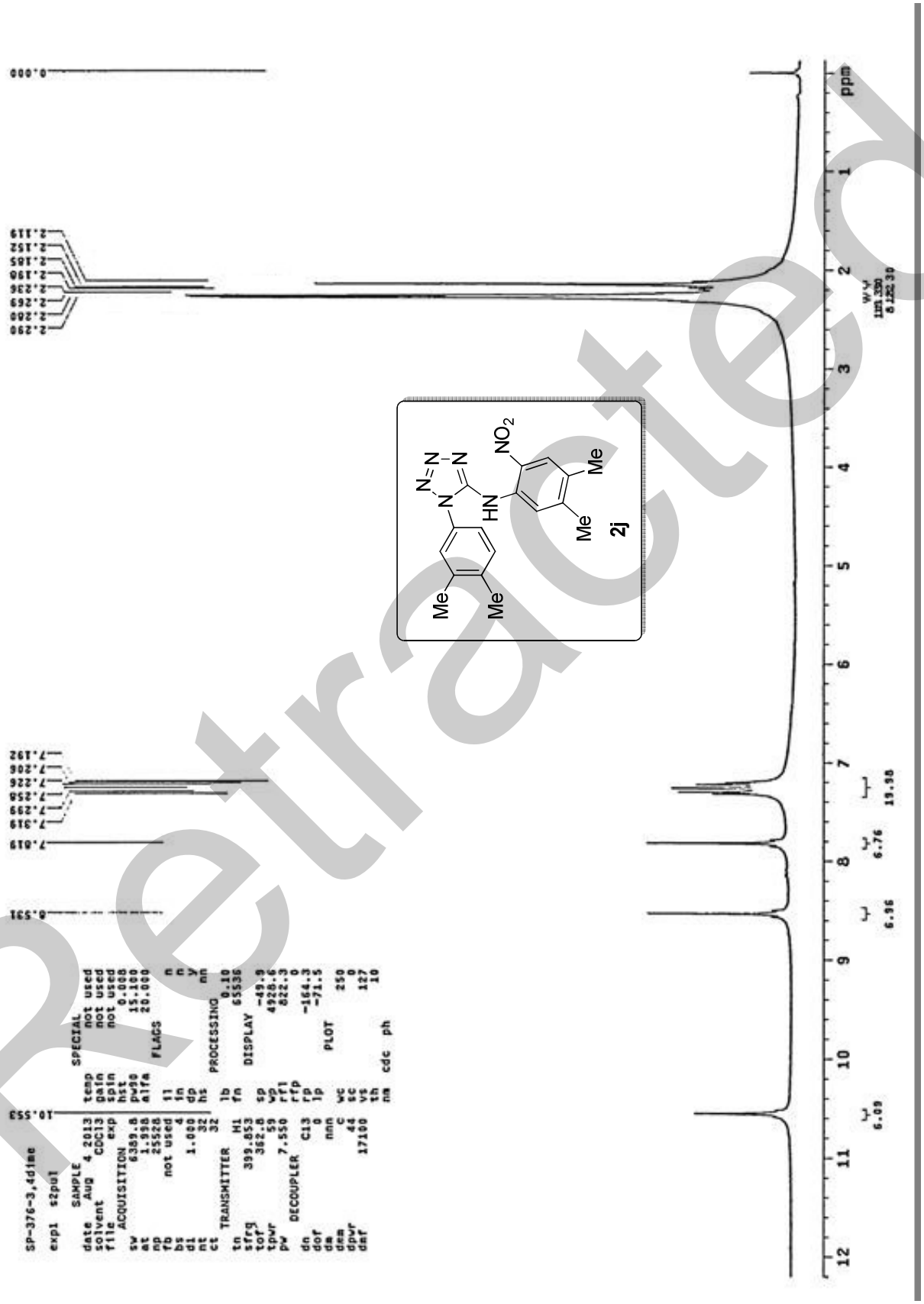

SP-24-DIME 1H

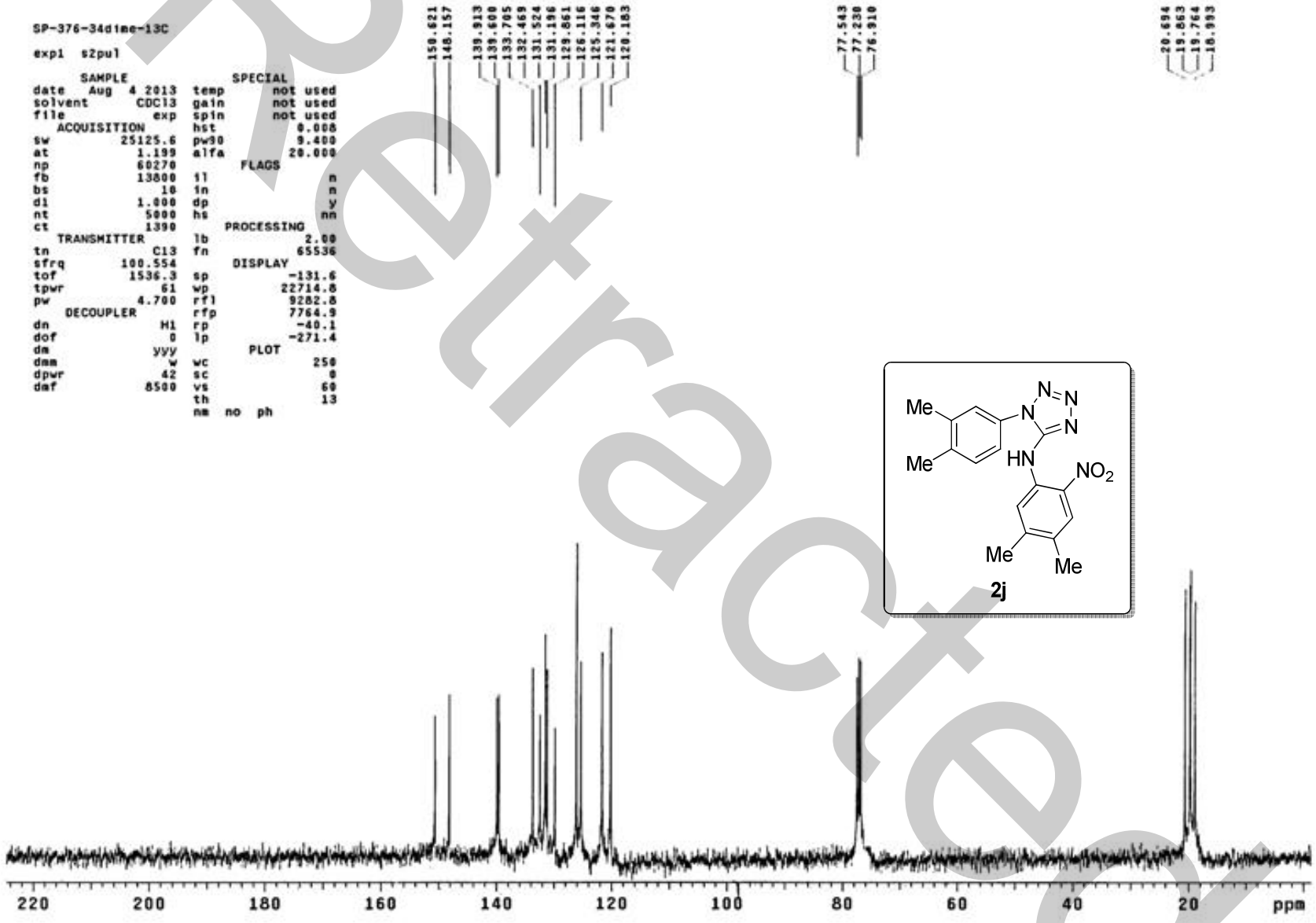


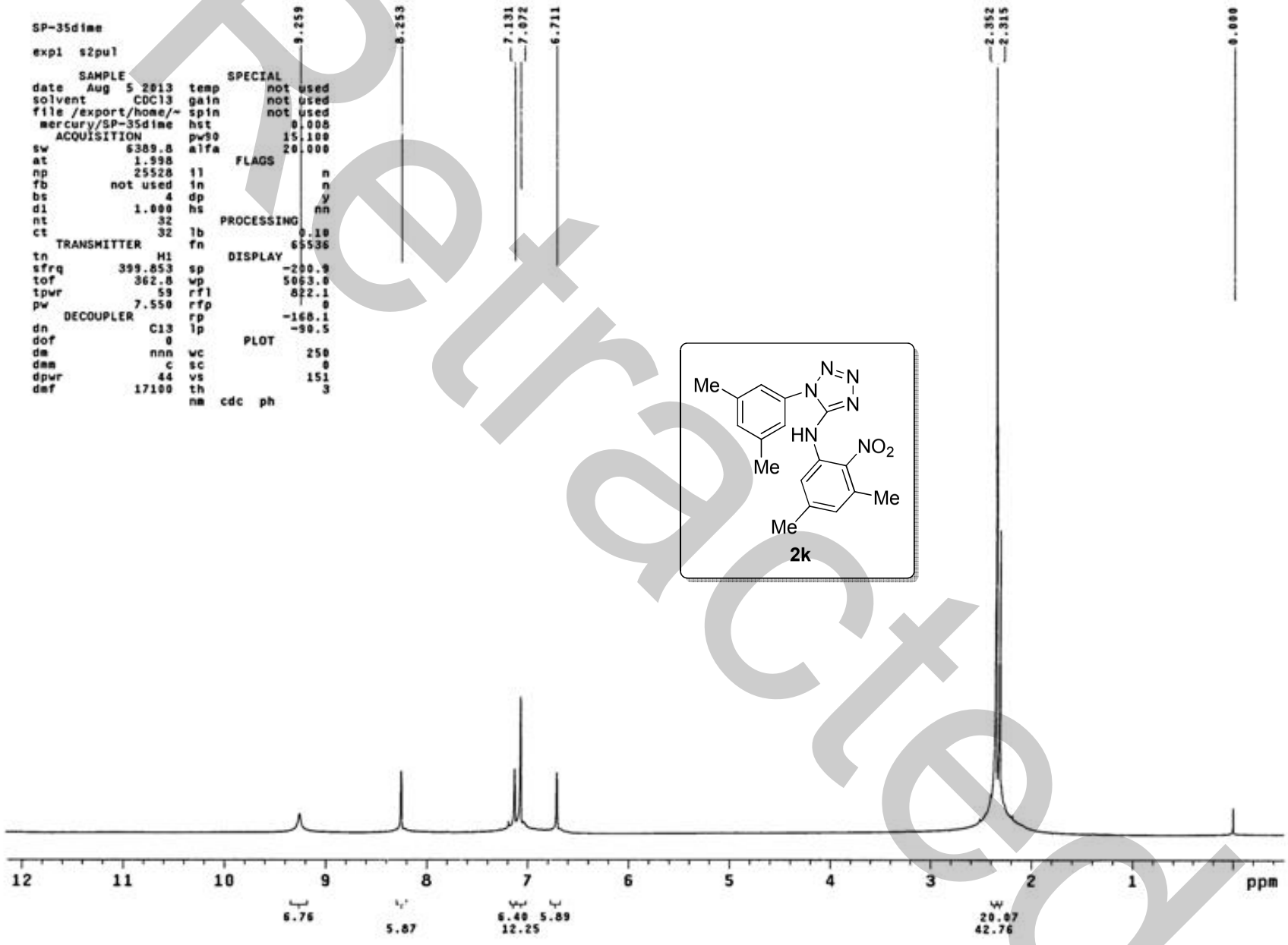
BRUKER

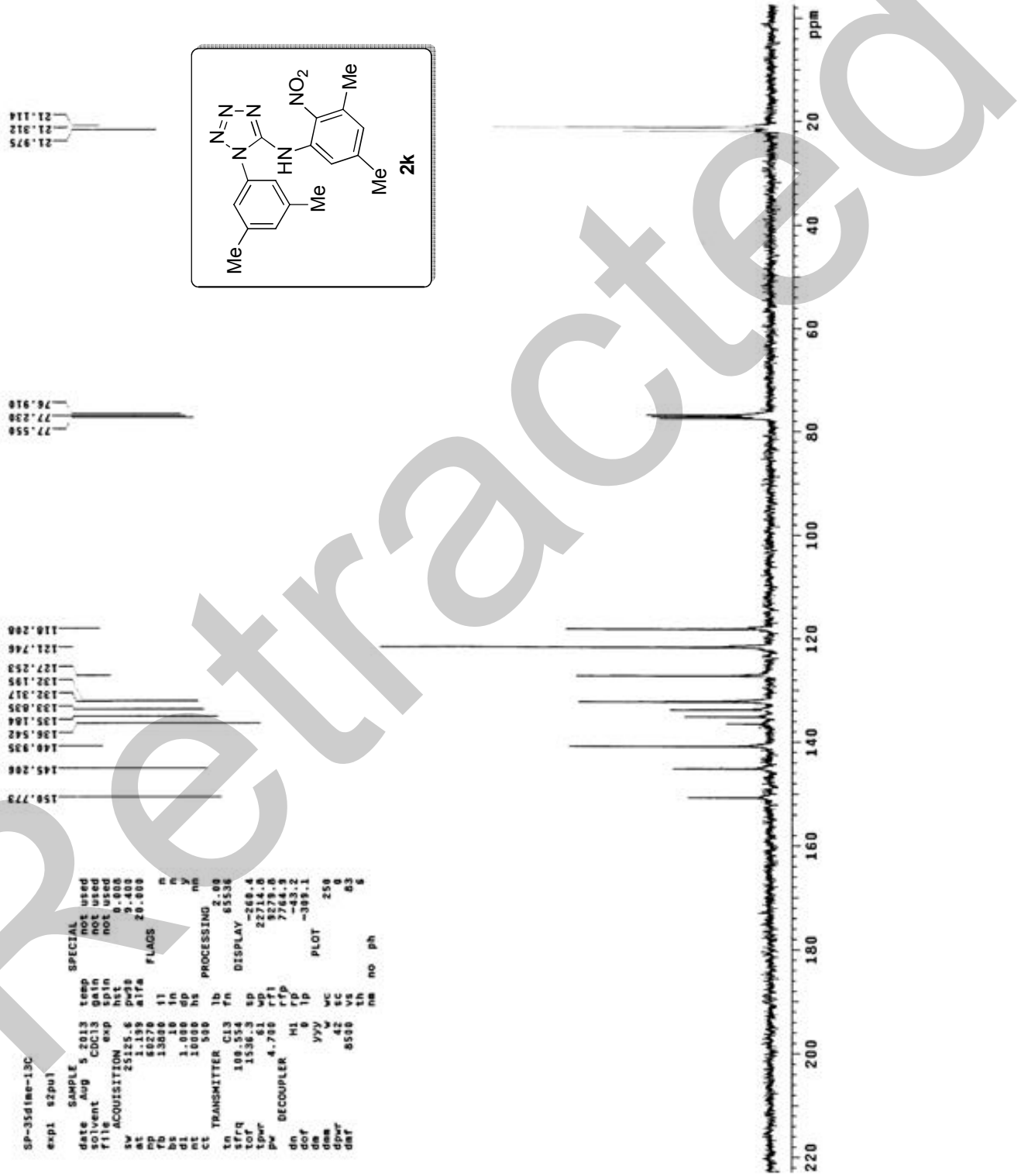
```
Current Data Parameters
NAME        SP-24-DIME_1H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20131119
Time              14.38
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          12019.230 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG                89.67
DW               41.600 usec
DE                6.50 usec
TE               297.2 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        600.1737063 MHz
NUC1              1H
P1               12.00 usec
PLW1        21.00000000 W

F2 - Processing parameters
SI               16384
SF          600.1700117 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

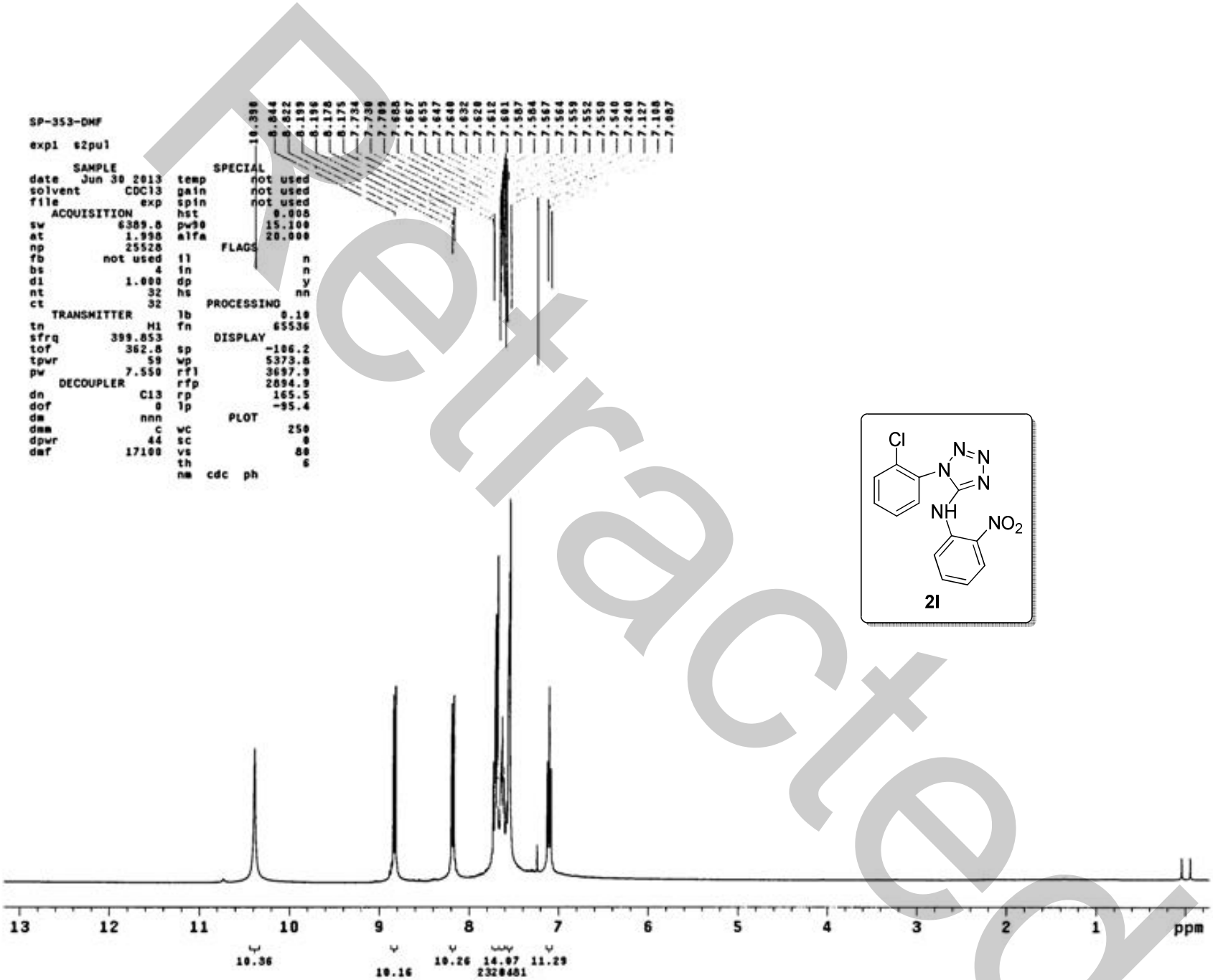

SP-289-13C
expl s2pul
SAMPLE
date Apr 15 2013
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
d1 1.000
nt 10800
ct 880
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 4.700
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8500
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 9.400
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1520.2
wp 25125.6
rfl 9285.1
rfp 7764.9
rp -69.3
lp -276.9
PLOT
wc 250
sc 0
vs 120
th 12
nm no ph
150.689
145.145
140.866
136.420
135.139
133.774
132.241
132.134
127.184
121.670
118.124
77.550
77.230
76.910
21.914
21.251
21.068
Me
N
N
N
HN
NO2
Me
Me
Me
2i
220
200
180
160
140
120
100
80
60
40
20
0
ppm

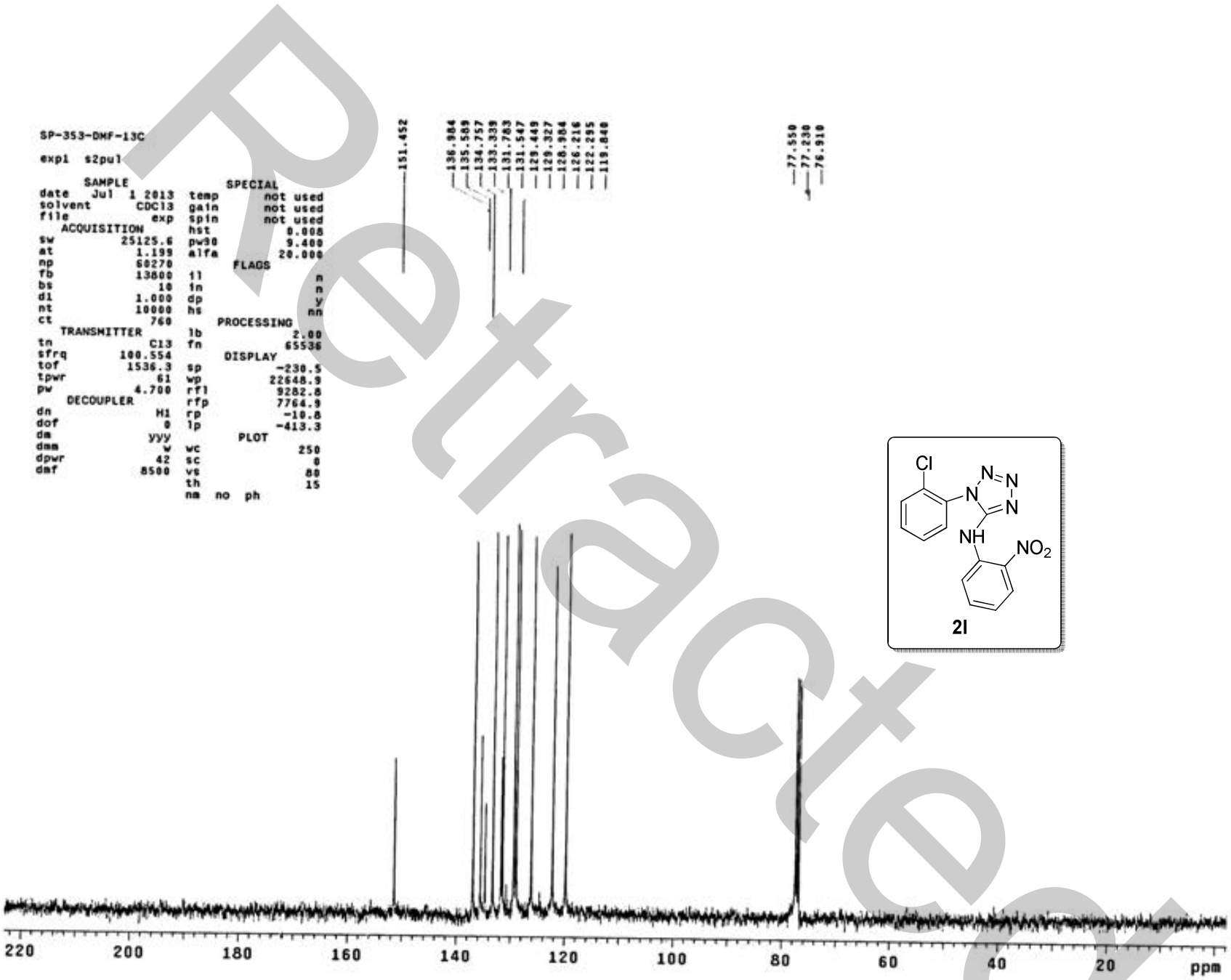



SP-376-34dime-13C
exp1 s2pul
SAMPLE
date Aug 4 2013
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 10
d1 1.000
nt 5000
ct 1390
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 4.700
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8500
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 9.400
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -131.6
wp 22714.8
rf1 9282.8
rfp 7764.9
rp -40.1
lp -271.4
PLOT
wc 250
sc 0
vs 60
th 13
nm no ph
150.621
148.157
139.913
139.600
133.705
132.469
131.524
131.196
129.861
126.116
125.346
121.670
120.183
77.543
77.230
76.910
20.694
19.863
19.764
18.993
Me
Me
N
N
N
HN
NO2
Me
Me
2j
220
200
180
160
140
120
100
80
60
40
20
ppm

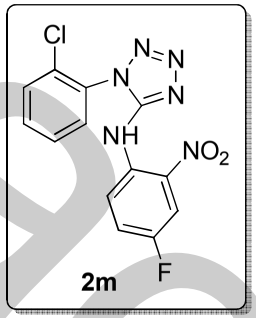

SP-35dime
expl s2pul
SAMPLE
date Aug 5 2013
solvent CDCl3
file /export/home/~
mercury/SP-35dime
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 59
pw 7.550
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 44
dmf 17100
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 15.100
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -200.9
wp 5063.6
rfl 822.1
rfp 0
rp -168.1
lp -90.5
PLOT
wc 250
sc 0
vs 151
th 3
nm cdc ph
9.259
8.253
7.131
7.072
6.711
2.352
2.315
0.000
Me
N
N
N
HN
NO2
Me
Me
Me
2k
12
11
10
9
8
7
6
5
4
3
2
1
ppm
6.76
5.87
6.40
12.25
5.89
20.07
42.76


2k
Me
Me
Me
NO2
HN
N
N
N
21.114
21.312
21.975
77.230
76.918
118.286
121.746
127.253
132.195
132.317
133.835
135.164
136.542
140.935
145.286
150.773
ppm


SP-353-DMF
exp1 s2pul
SAMPLE
date Jun 30 2013
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 59
pw 7.550
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 44
dmf 17100
SPECIAL
temp not used
gain not used
spin not used
hst 0.005
pw90 15.100
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -106.2
wp 5373.8
rf1 3697.9
rf2 2894.9
rp 165.5
lp -95.4
PLOT
wc 250
sc 0
vs 80
th 6
nm cdc ph
10.398
8.844
8.822
8.199
8.196
8.178
8.175
7.734
7.730
7.709
7.688
7.667
7.655
7.647
7.640
7.632
7.628
7.612
7.601
7.587
7.584
7.567
7.564
7.559
7.552
7.550
7.540
7.240
7.127
7.108
7.087
Cl
N
N
N
NH
NO2
2l
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
10.36
10.16
10.26
14.07
2328481
11.29


SP-353-DMF-13C
expl s2pul
SAMPLE
date Jul 1 2013
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 10
d1 1.000
nt 10000
ct 760
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 4.700
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8500
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 9.480
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -230.5
wp 22648.9
rfl 9282.8
rfp 7764.9
rp -10.8
lp -413.3
PLOT
wc 250
sc 0
vs 80
th 15
nm no ph
151.452
136.984
135.589
134.757
133.339
131.783
131.547
129.449
129.327
128.984
126.216
122.295
119.848
77.550
77.230
76.910
Cl
N
N
N
NH
NO2
2l
220
200
180
160
140
120
100
80
60
40
20
ppm

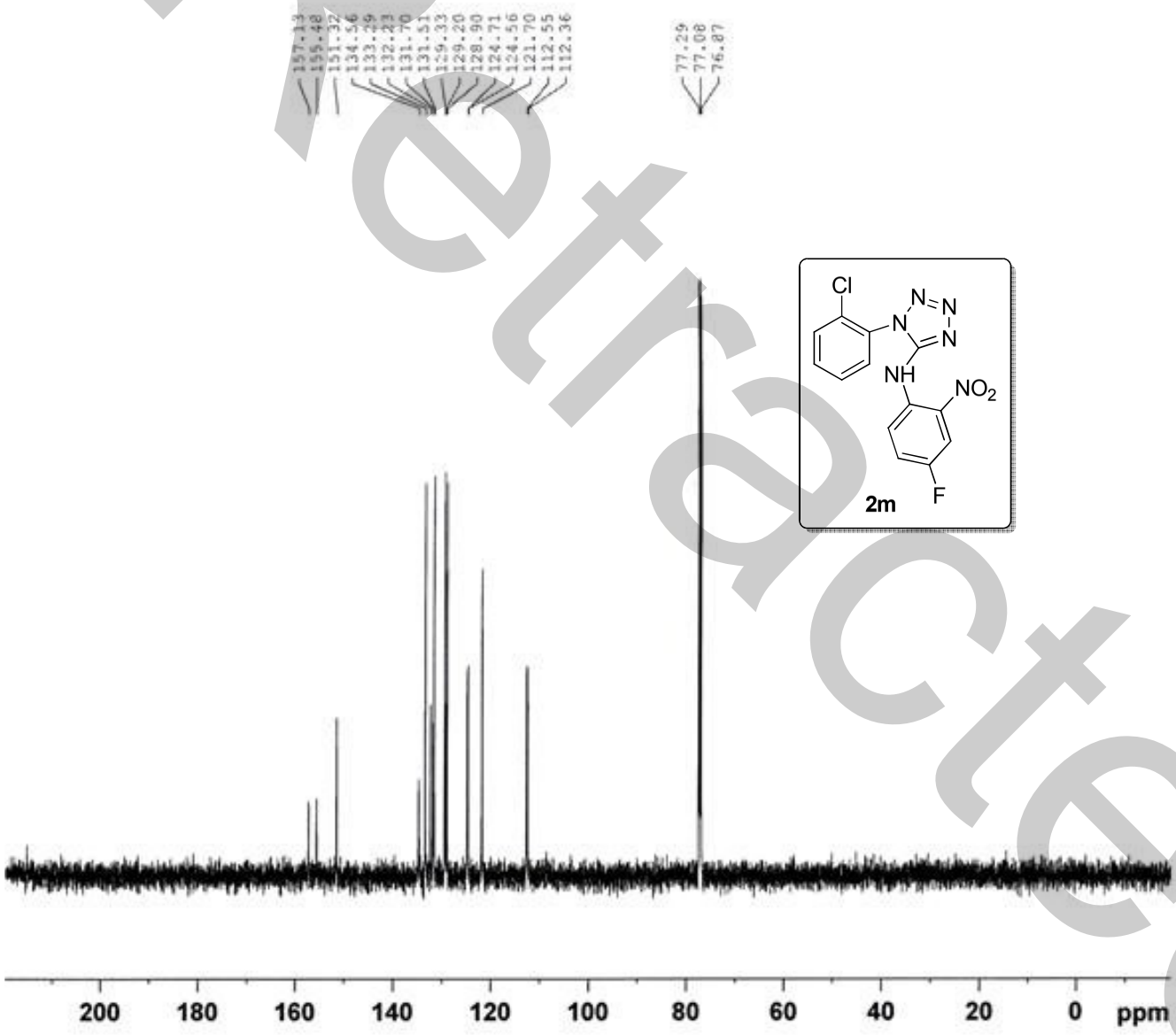
SP-CLF_1H



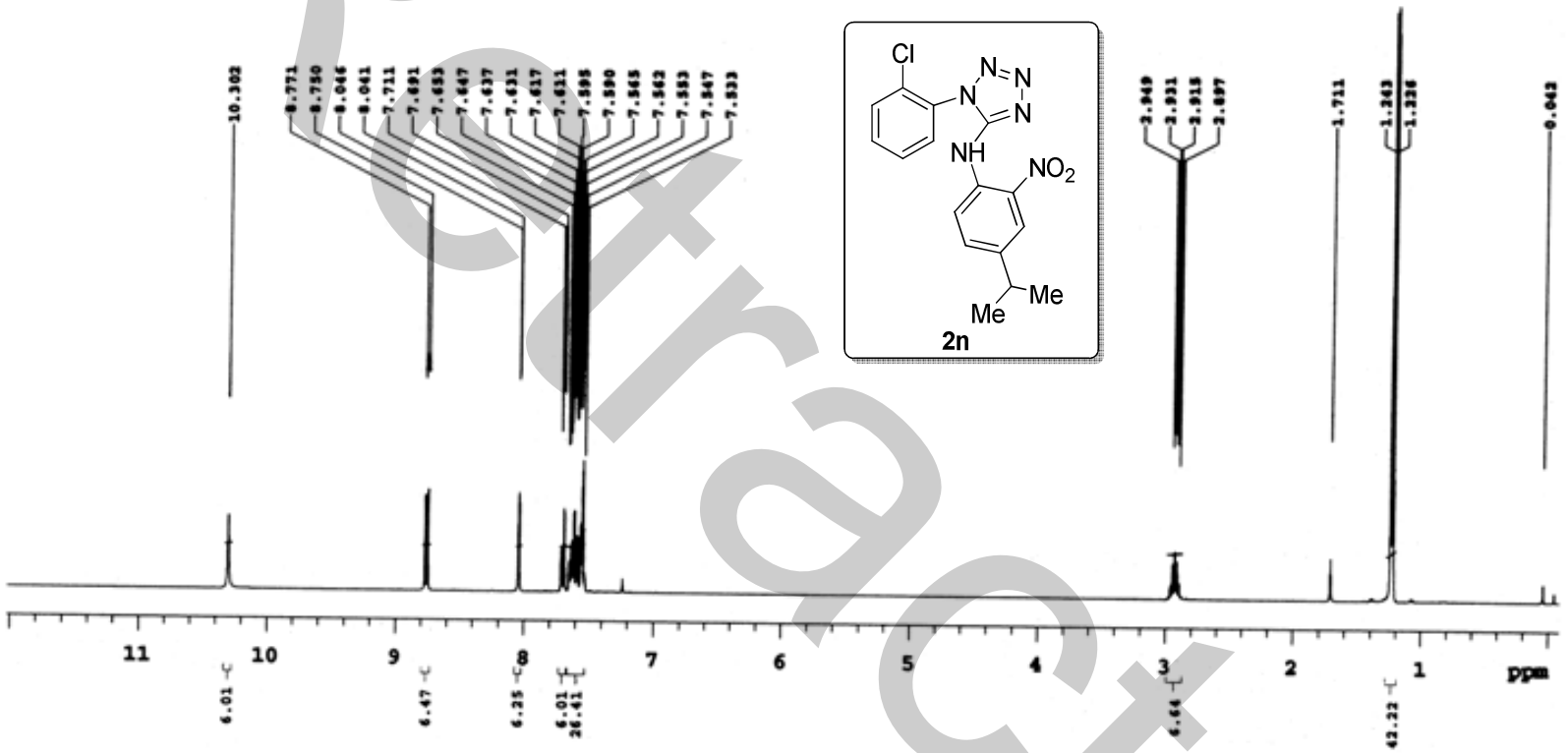
BRUKER

```
Current Data Parameters
NAME                  SP-CLF_1H
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20131119
Time                    14.30
INSTRUM                 spect
PROBHD   5 mm PABBO BB/
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         2
SWH               12019.230 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                     99.36
DW                   41.600 usec
DE                    6.50 usec
TE                   297.2 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1           600.1737063 MHz
NUC1                     1H
P1                    12.00 usec
PLW1          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
```

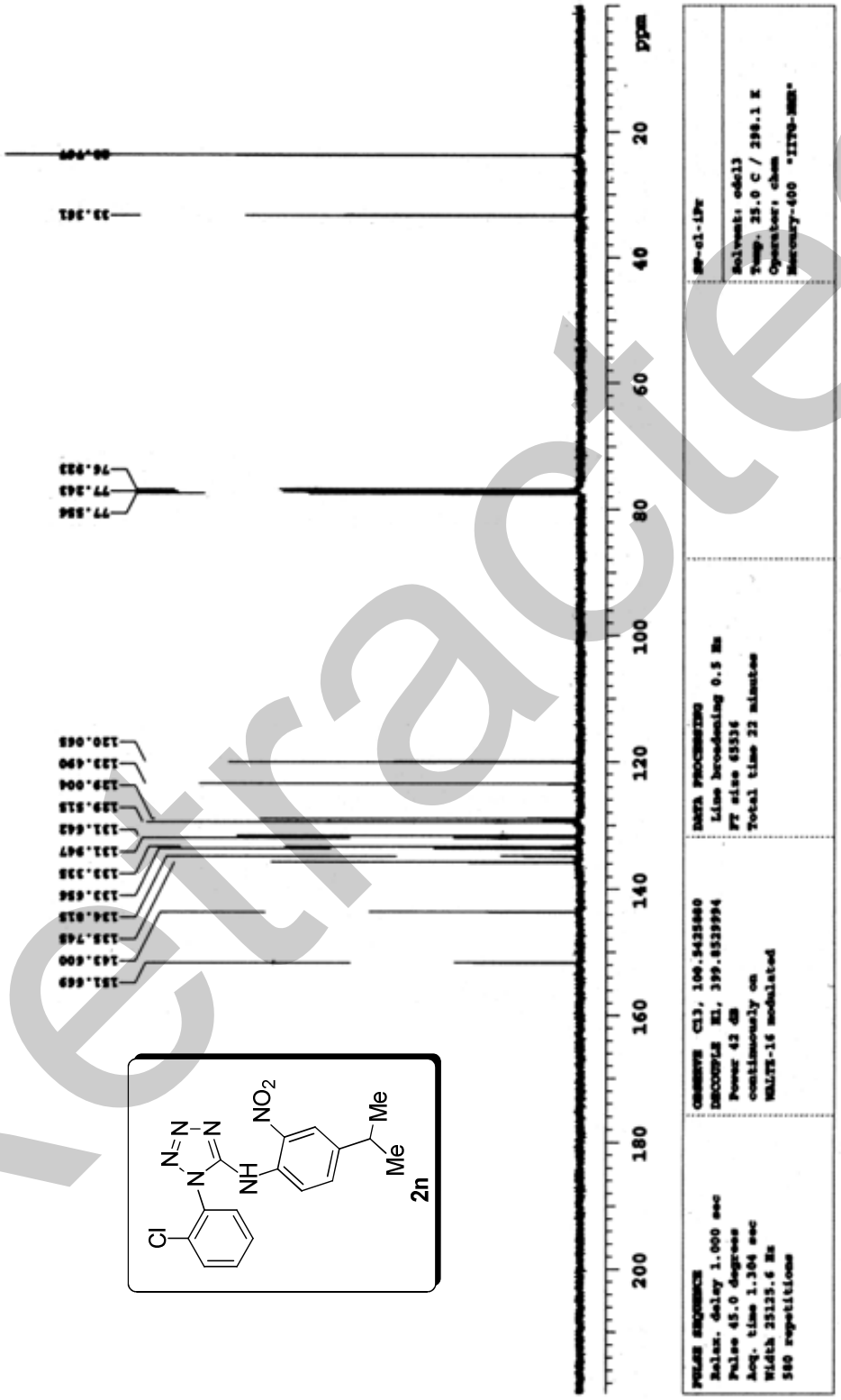
SP-CL_F_13C



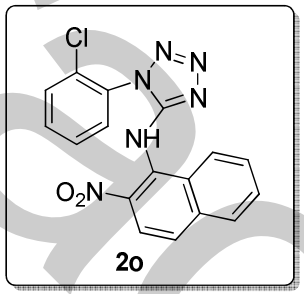

```
Current Data Parameters
NAME          SP-CL_F_13C
EXPNO                   1
PROCNO                  1

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
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ            0.4543829 sec
RG                65.24
DW               13.867 usec
DE                6.50 usec
TE               301.0 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
CPDPRG[2        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             1.00 Hz
GB           0
PC             1.40
```



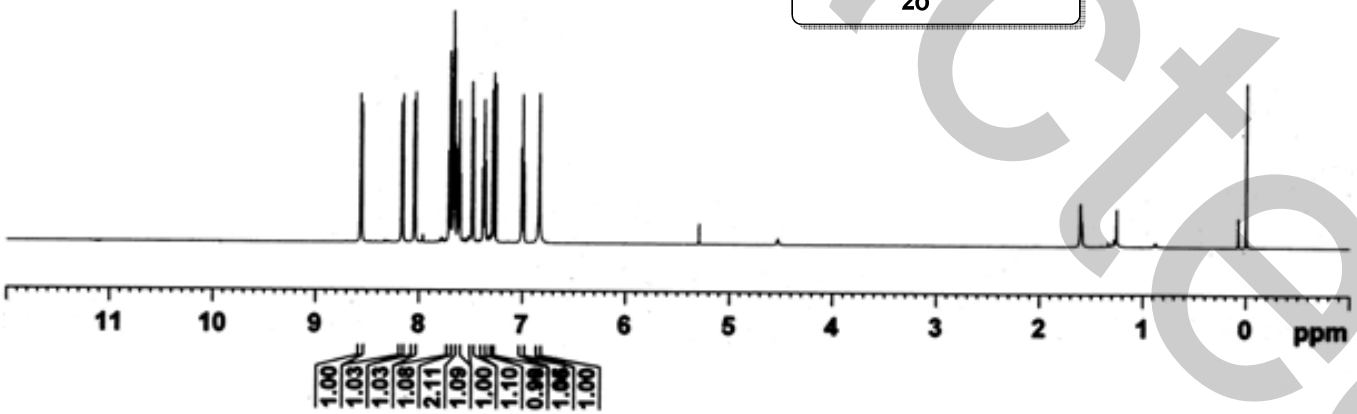
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	OBSERVE H1, 399.8509721	DATA PROCESSING FT size 32768 Total time 1 minutes		SP-cl-iPr Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*


151.669
143.600
138.748
136.815
133.654
133.338
131.947
131.643
129.515
129.004
123.490
120.063
77.584
77.343
76.923
33.361
00.909
200
180
160
140
120
100
80
60
40
20
ppm
2n
Cl
NH
NO2
Me
Me

SP_Napthyl_1H

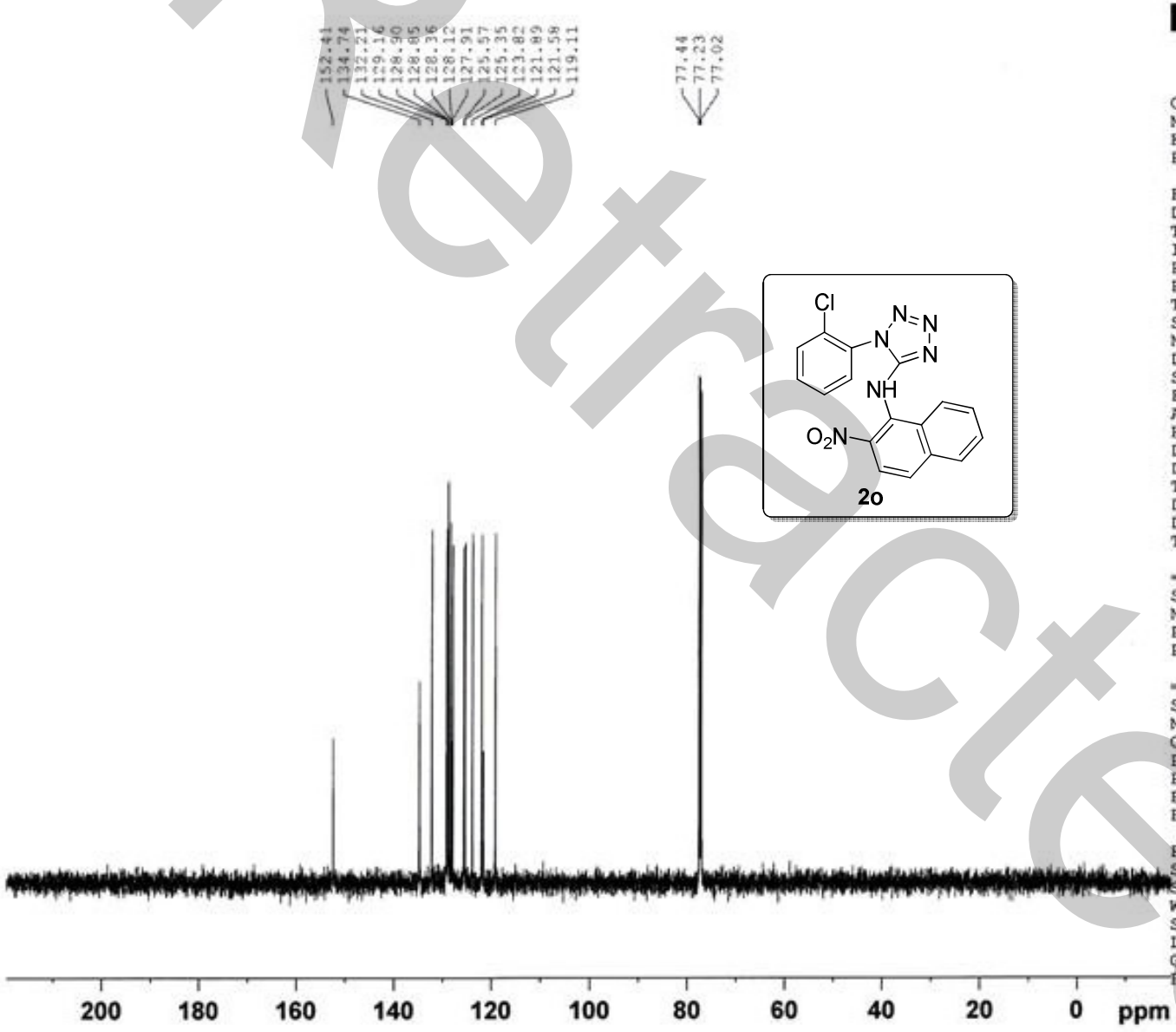


2o




```
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 BB/
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
DW                41.600 usec
DE                 6.50 usec
TE                298.8 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1        600.1737063 MHz
NUC1                   1H
P1                 12.00 usec
PLW1        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
```

SP_NAPH_13C



2o

BRUKER

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 ========

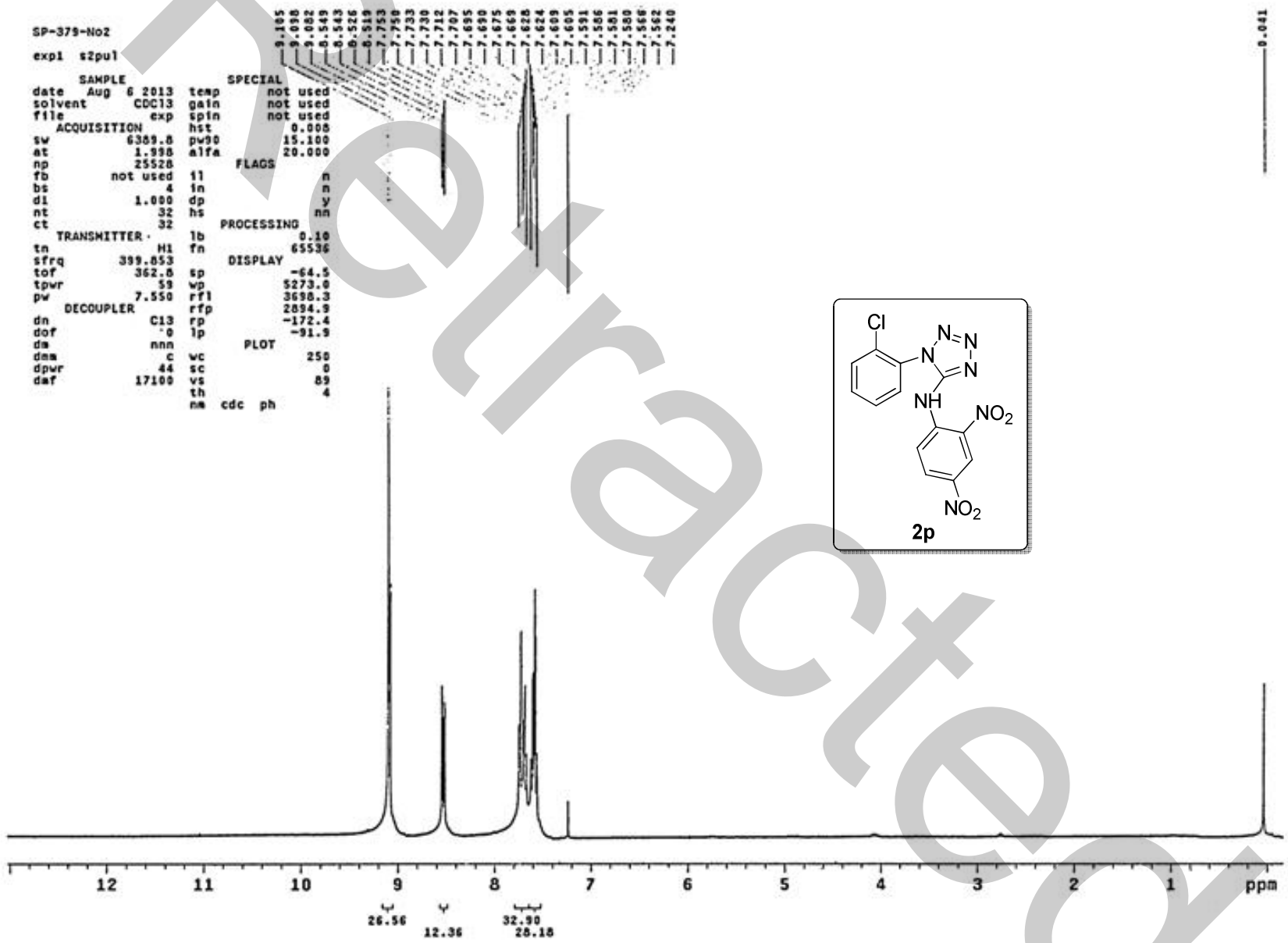
SFO1	150.9279571	MHz
NUC1	13C	
P1	10.50	usec
PLW1	95.00000000	W

======== CHANNEL f2 ========

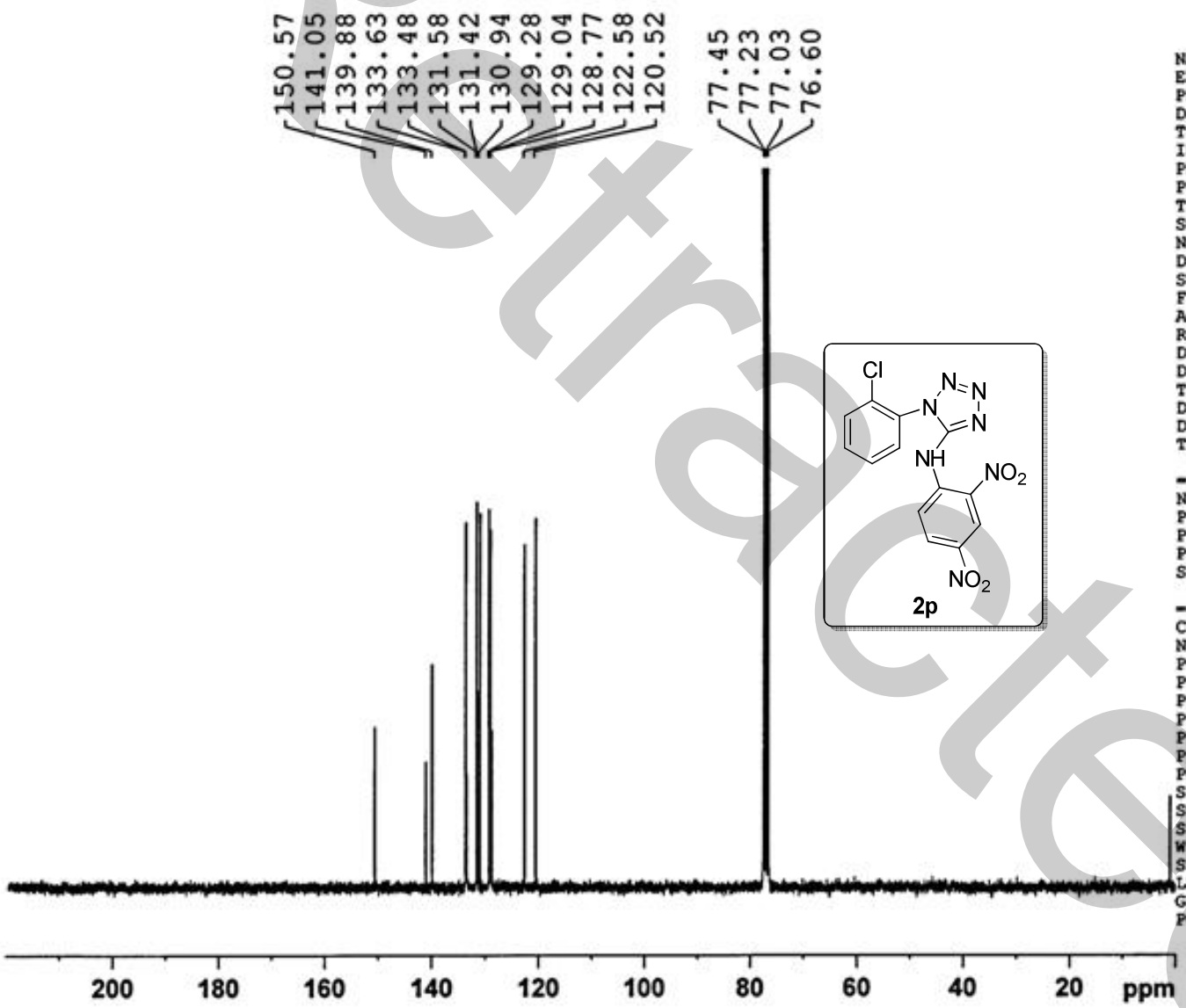
SFO2	600.1724007	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	70.00	usec
PLW2	21.00000000	W
PLW12	0.61714000	W
PLW13	0.30239999	W

F2 - Processing parameters

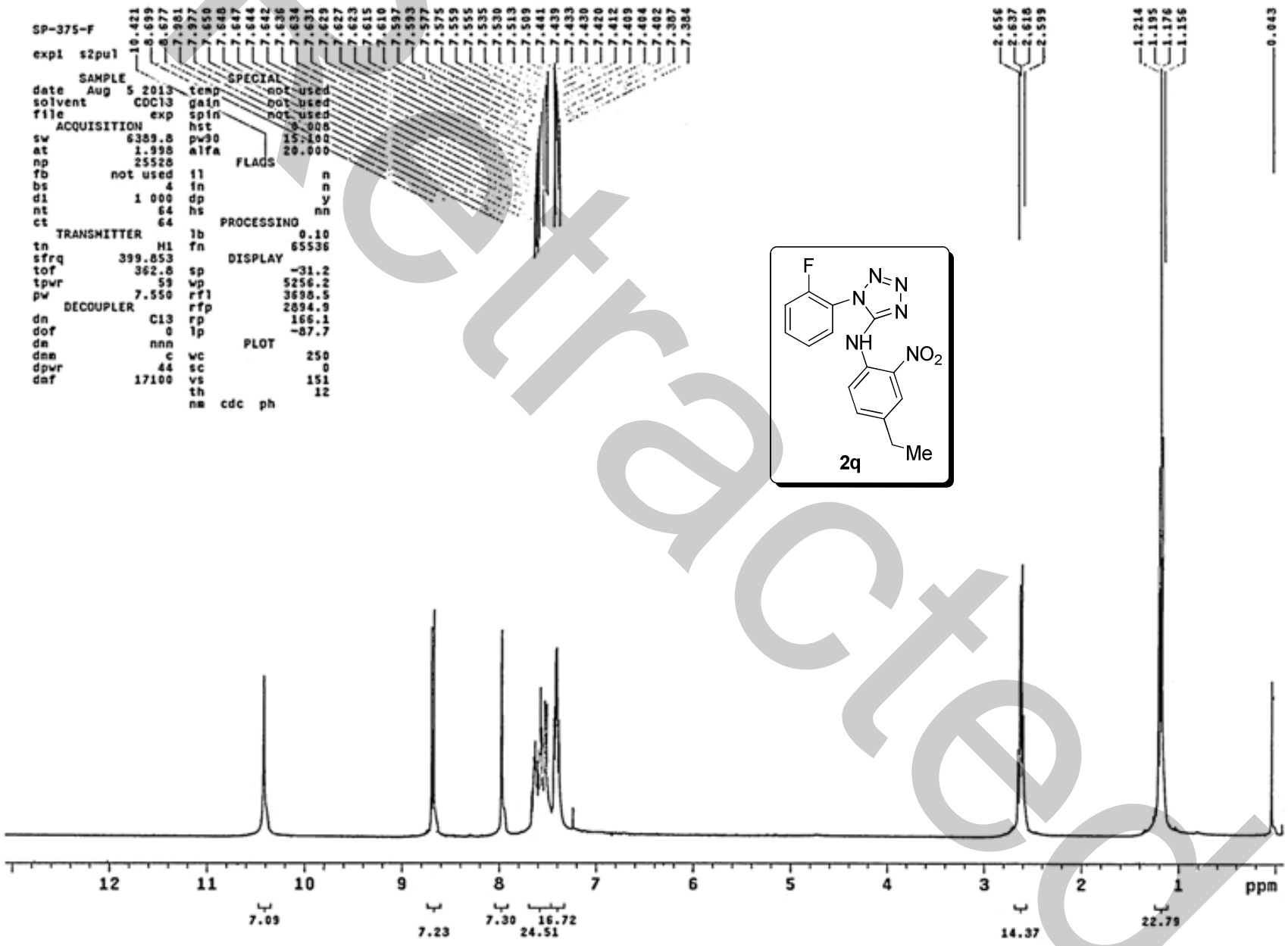
SI	16384	
SF	150.9128481	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	


SP-379-No2
exp1 s2pul
SAMPLE
date Aug 6 2013
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 59
pw 7.550
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 44
dmf 17100
SPECIAL
temp not used
gain not used
spin not used
hst 0.005
pw90 15.100
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -64.5
wp 5273.8
rf1 3698.3
rfp 2894.9
rp -172.4
lp -91.9
PLOT
wc 250
sc 0
vs 89
th 4
nm cdc ph
9.185
9.098
9.082
8.549
8.543
8.526
8.518
7.753
7.750
7.733
7.730
7.712
7.707
7.695
7.690
7.675
7.669
7.628
7.624
7.609
7.605
7.591
7.586
7.581
7.580
7.566
7.562
7.240
0.041
Cl
N
N
N
NH
NO2
NO2
2p
12
11
10
9
8
7
6
5
4
3
2
1
ppm
26.56
12.36
32.90
25.18

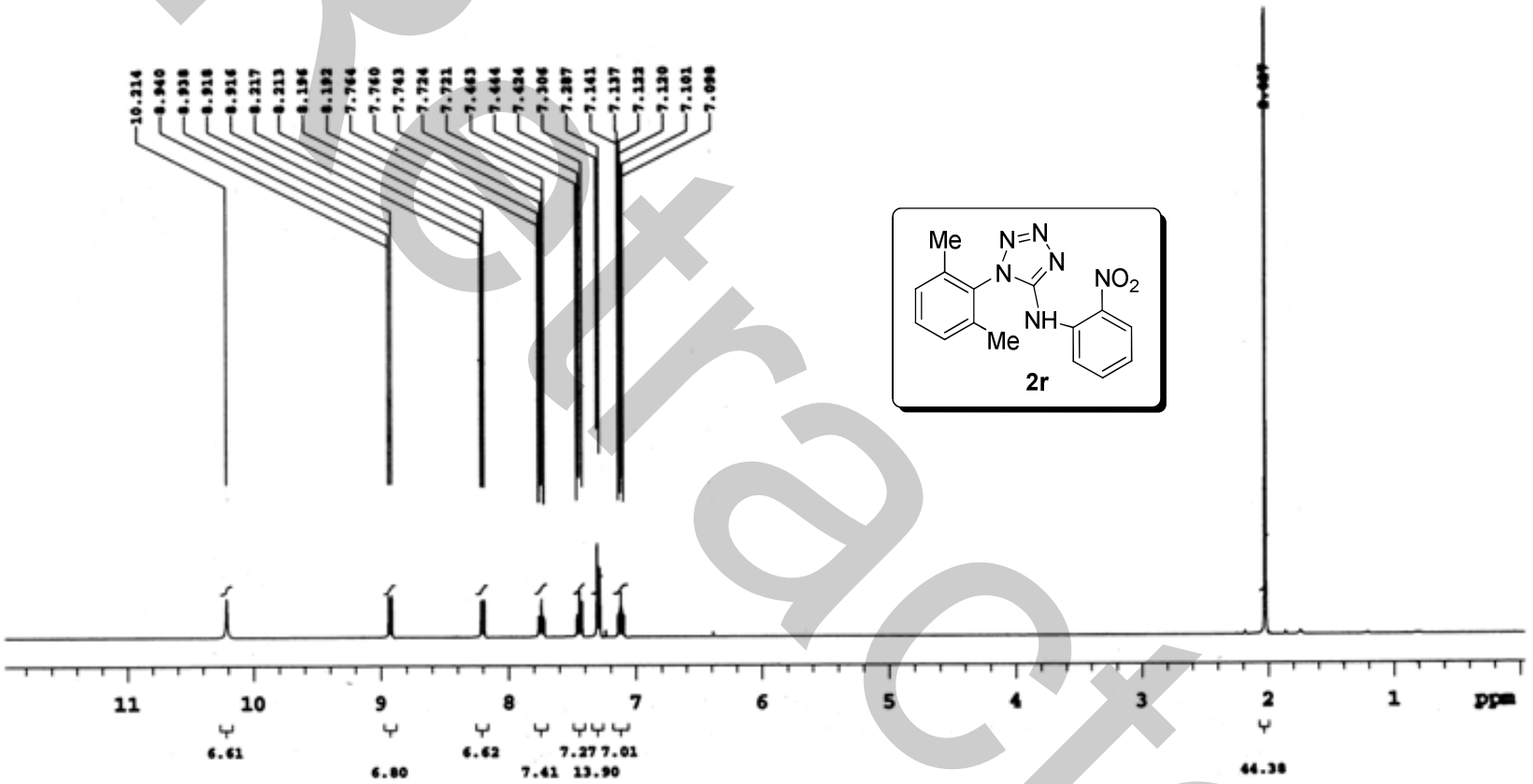
SP-379-NO2



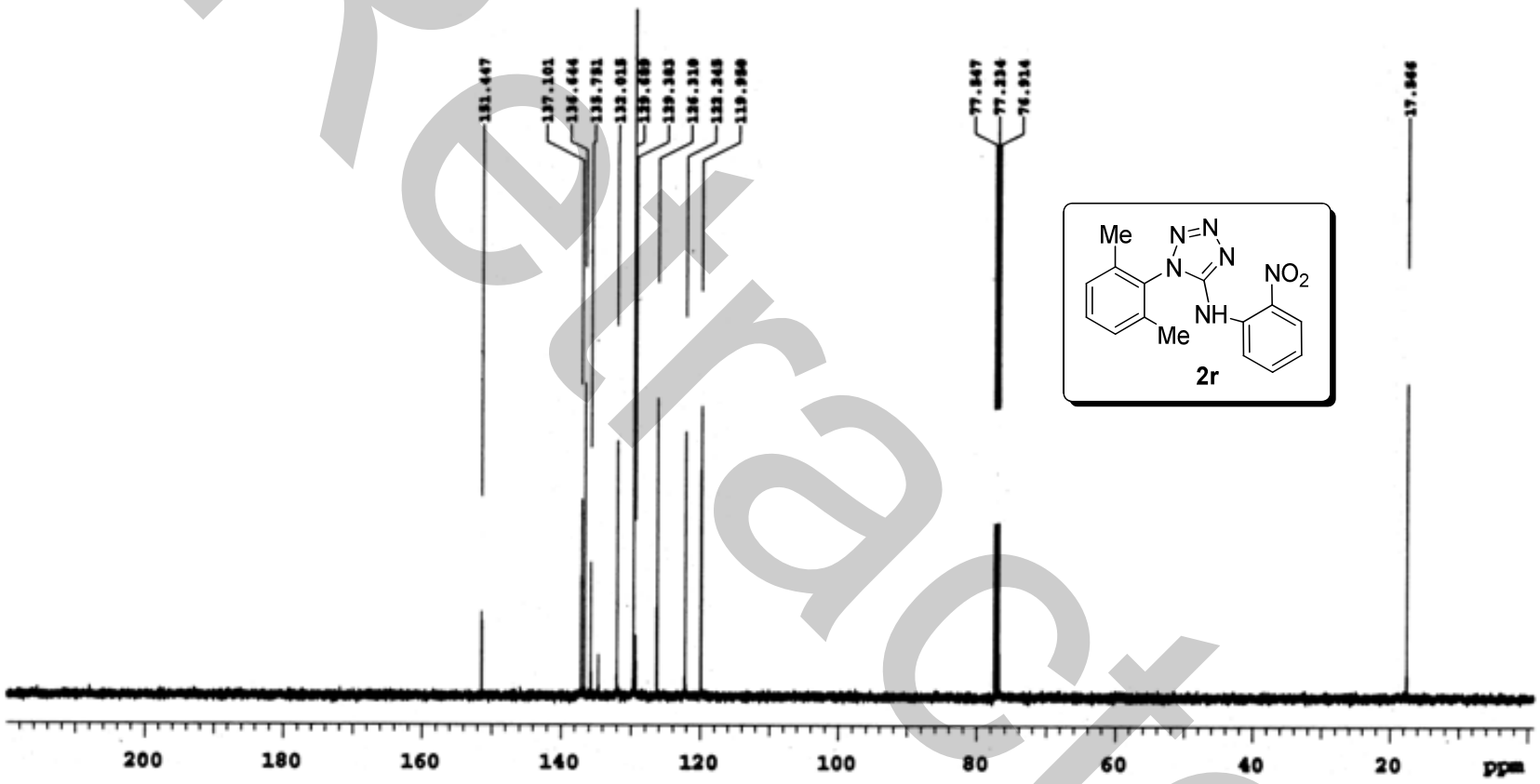
NAME	2013-08-19-b-b
EXPNO	1
PROCNO	1
Date_	20130821
Time	10.45
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	2000
DS	4
SWH	18028.846 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	80.6
DW	27.733 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
-------- 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	75.4702654 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


SP-375-F
expl s2pul
SAMPLE
date Aug 5 2013
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 64
ct 64
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 59
pw 7.550
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 44
dmf 17100
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 15.100
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -31.2
wp 5256.2
rf1 3698.5
rfp 2894.9
rp 166.1
lp -87.7
PLOT
wc 250
sc 0
vs 151
th 12
nm cdc ph
10.421
8.699
8.677
8.081
7.377
7.650
7.648
7.647
7.644
7.642
7.636
7.634
7.631
7.629
7.627
7.623
7.615
7.610
7.597
7.593
7.577
7.575
7.559
7.555
7.535
7.530
7.513
7.509
7.441
7.439
7.433
7.430
7.420
7.412
7.409
7.404
7.402
7.387
7.384
2.656
2.637
2.618
2.599
1.214
1.195
1.176
1.156
0.043
F
N
N
N
N
NH
NO2
Me
2q
12
11
10
9
8
7
6
5
4
3
2
1
ppm
7.09
7.23
7.30
16.72
24.51
14.37
22.79

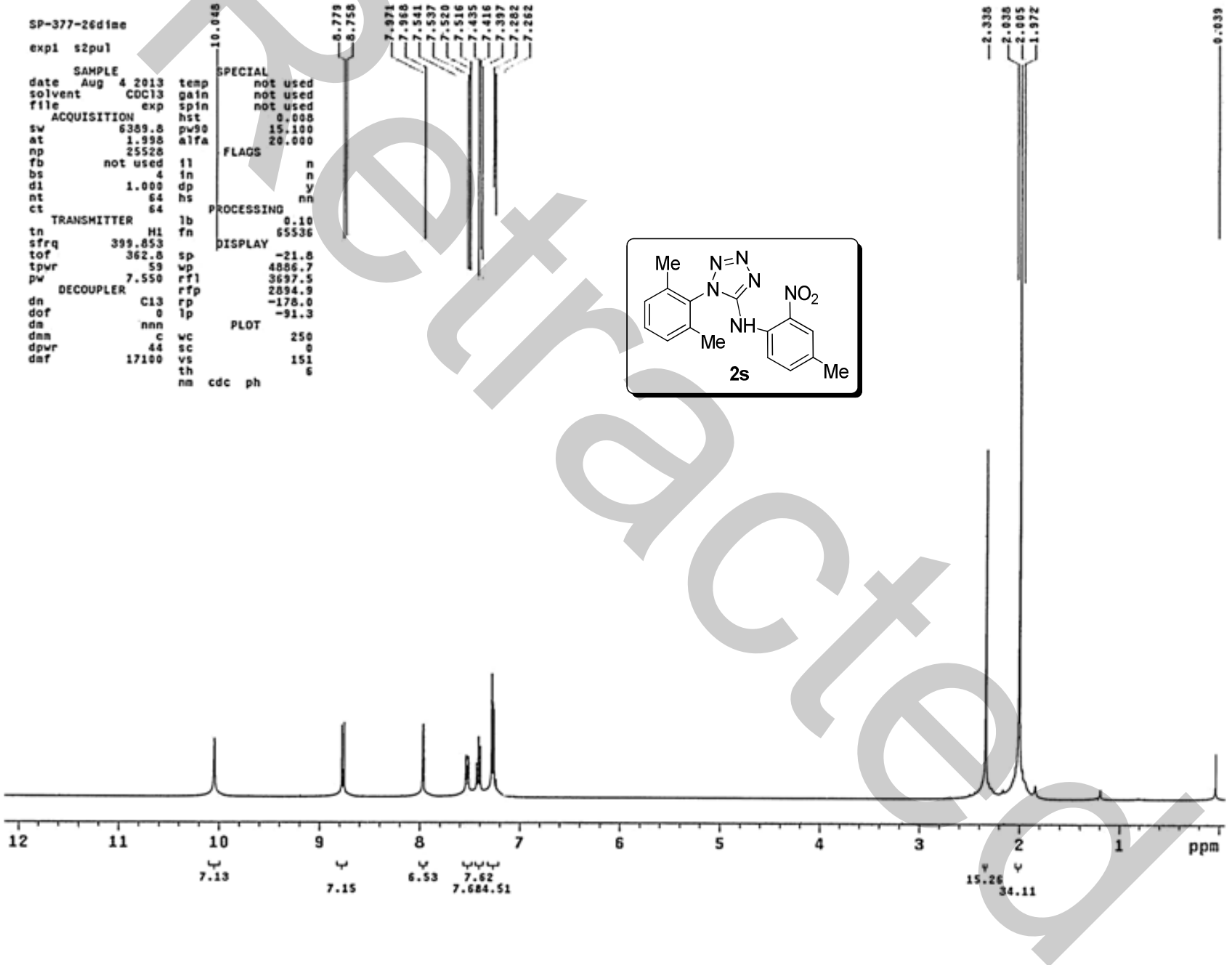
SP-375-f-13C
expl s2pul
SAMPLE
date Aug 4 2013
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 10
dl 1.000
nt 10000
ct 970
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 4.700
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8500
SPECIAL not used
not used
not used
0.000
9.480
20.000
FLAGS
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -197.5
wp 20965.8
rfl 9282.1
rfp 7764.9
rp -48.3
lp -316.7
PLOT
wc 250
sc 0
vs 80
th 5
nm no ph
2q
ppm

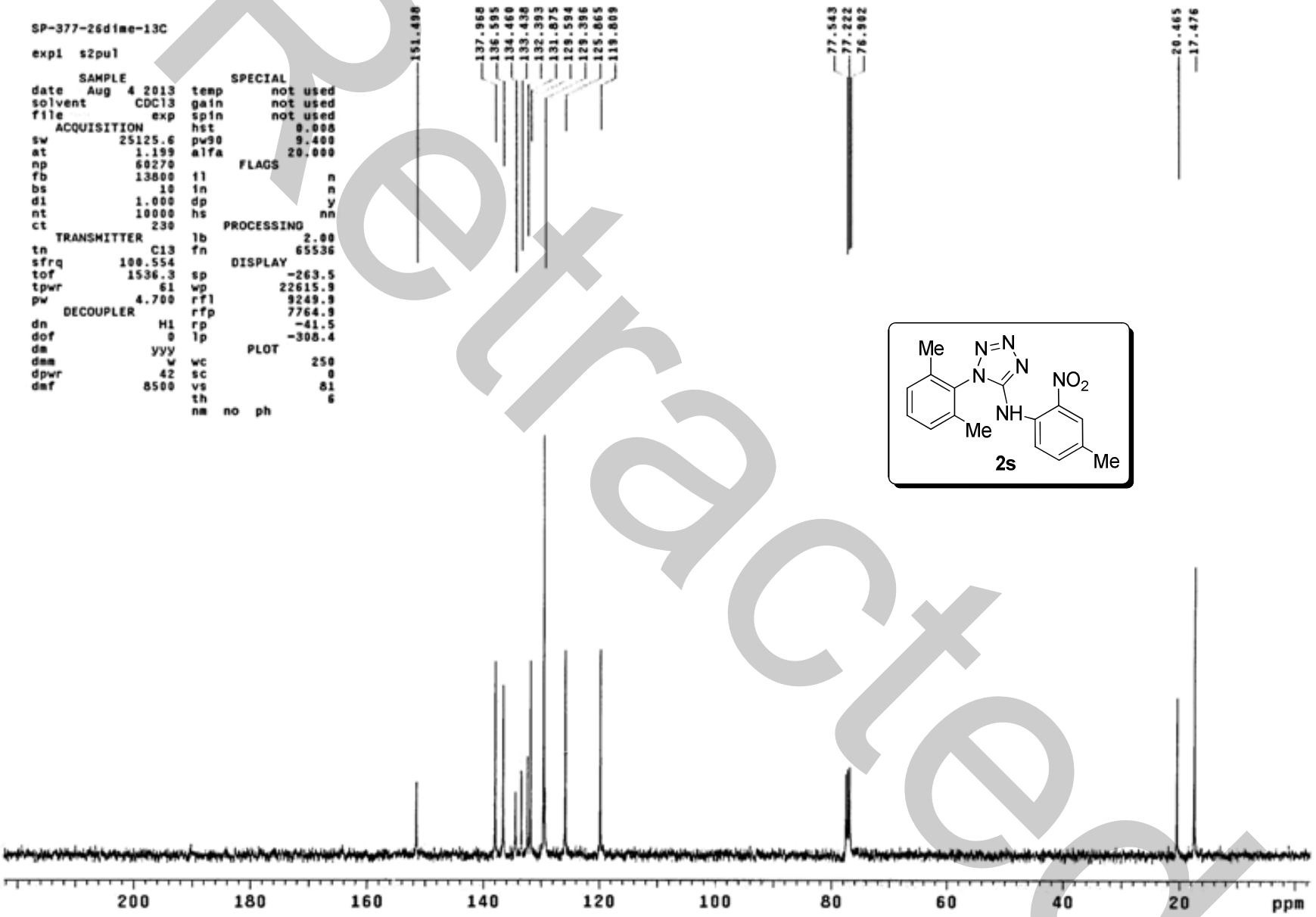


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	OBSERVE H1, 399.8509718	DATA PROCESSING FT size 32768 Total time 1 minutes		SP-26-H Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: SP-26-H Mercury-400 "IITG-NMR"

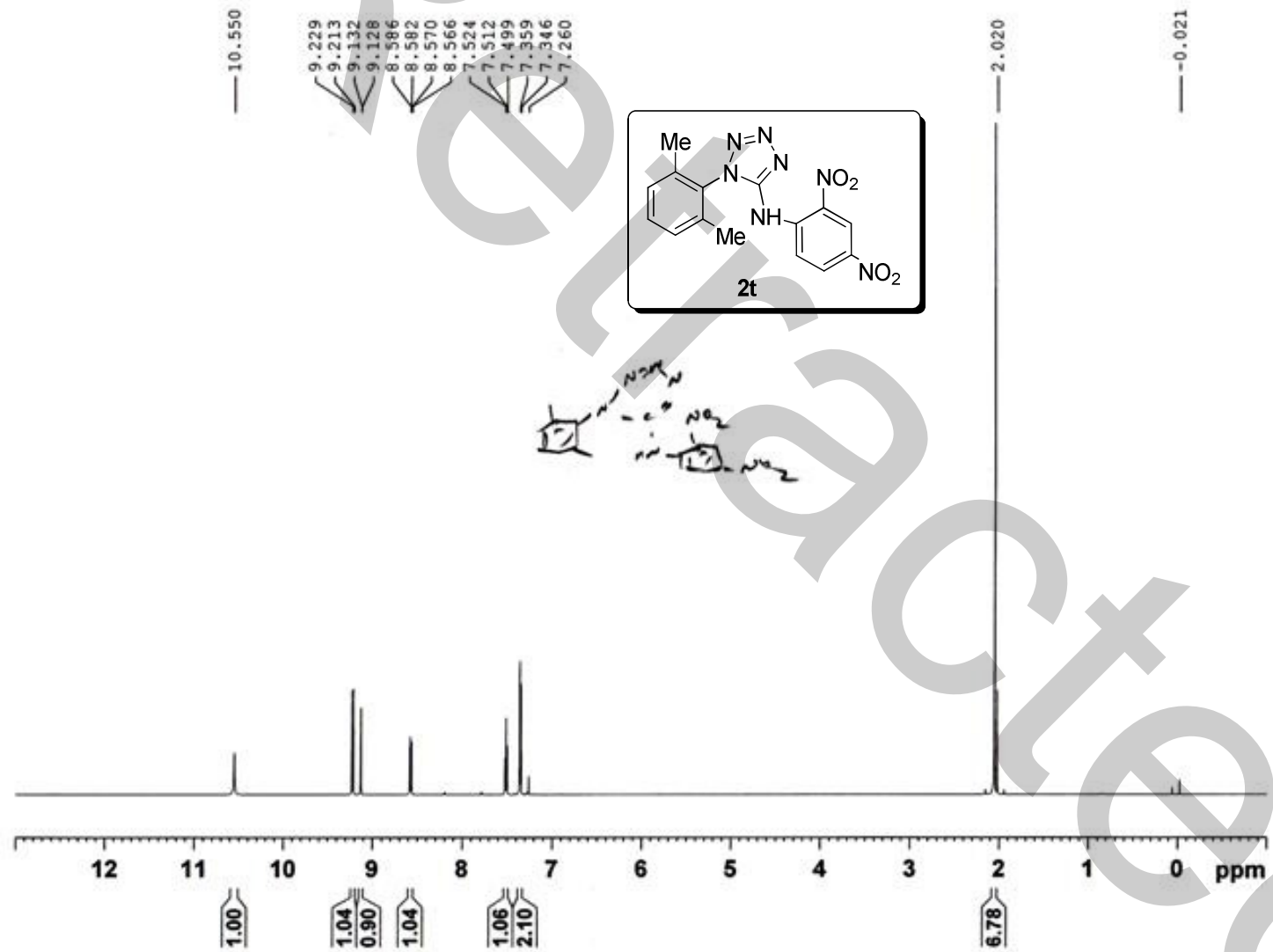


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 200 repetitions	OBSERVE C13, 100.5425912 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 7 minutes		SP-26-K Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR"


SP-377-26dime
exp1 s2pul
SAMPLE
date Aug 4 2013
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 64
ct 64
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 59
pw 7.550
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 44
dmf 17100
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 15.100
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -21.8
wp 4886.7
rfl 3697.5
rfp 2894.9
rp -178.0
lp -91.3
PLOT
wc 250
sc 0
vs 151
th 6
nm cdc ph
10.048
8.779
8.758
7.971
7.968
7.541
7.537
7.520
7.516
7.435
7.416
7.397
7.282
7.262
2.338
2.038
2.005
1.972
0.039
Me
N=N
N
N
NH
NO2
Me
Me
2s
12
11
10
9
8
7
6
5
4
3
2
1
ppm
7.13
7.15
6.53
7.62
7.68
4.51
15.26
34.11


SP-377-26dime-13C
expl s2pul
SAMPLE
date Aug 4 2013
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 10
d1 1.000
nt 10000
ct 230
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 4.700
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8500
SPECIAL
temp not used
gain not used
spin not used
hst 8.008
pw90 9.400
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -263.5
wp 22615.9
rfl 9249.9
rfp 7764.9
rp -41.5
lp -308.4
PLOT
wc 250
sc 0
vs 81
th 6
nm no ph
151.498
137.968
136.595
134.460
133.438
132.393
131.875
129.594
129.396
125.865
119.809
77.543
77.222
76.902
20.465
17.476
Me
N=N
N
N
NO2
NH
Me
Me
2s
200
180
160
140
120
100
80
60
40
20
ppm

SP_15-11-13_1H

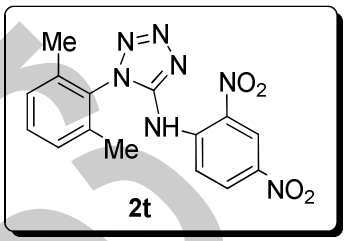


BRUKER

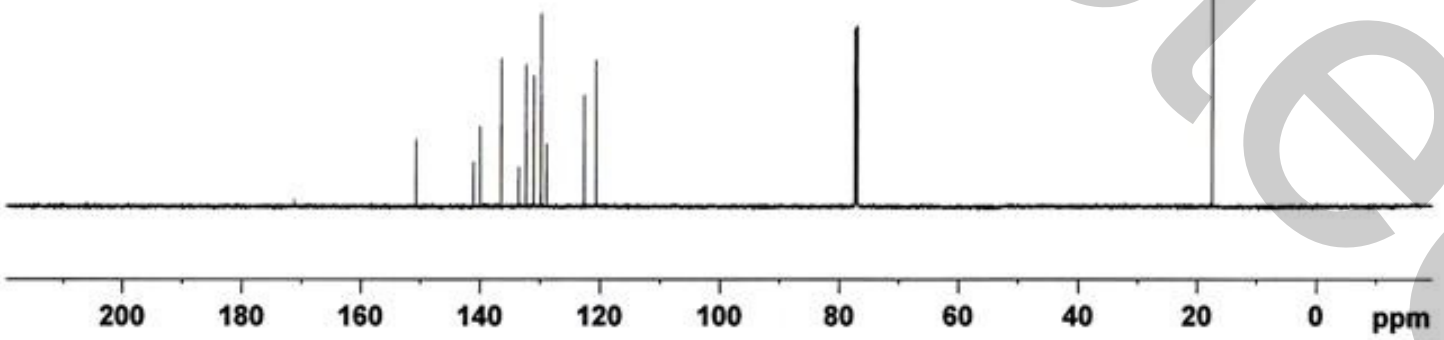
```
Current Data Parameters
NAME      SP_15-11-13_1H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20131115
Time              13.31
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          12019.230 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG                54.94
DW               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
PLW1       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

2,6dime, NO_2



2t



BRUKER

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 ========

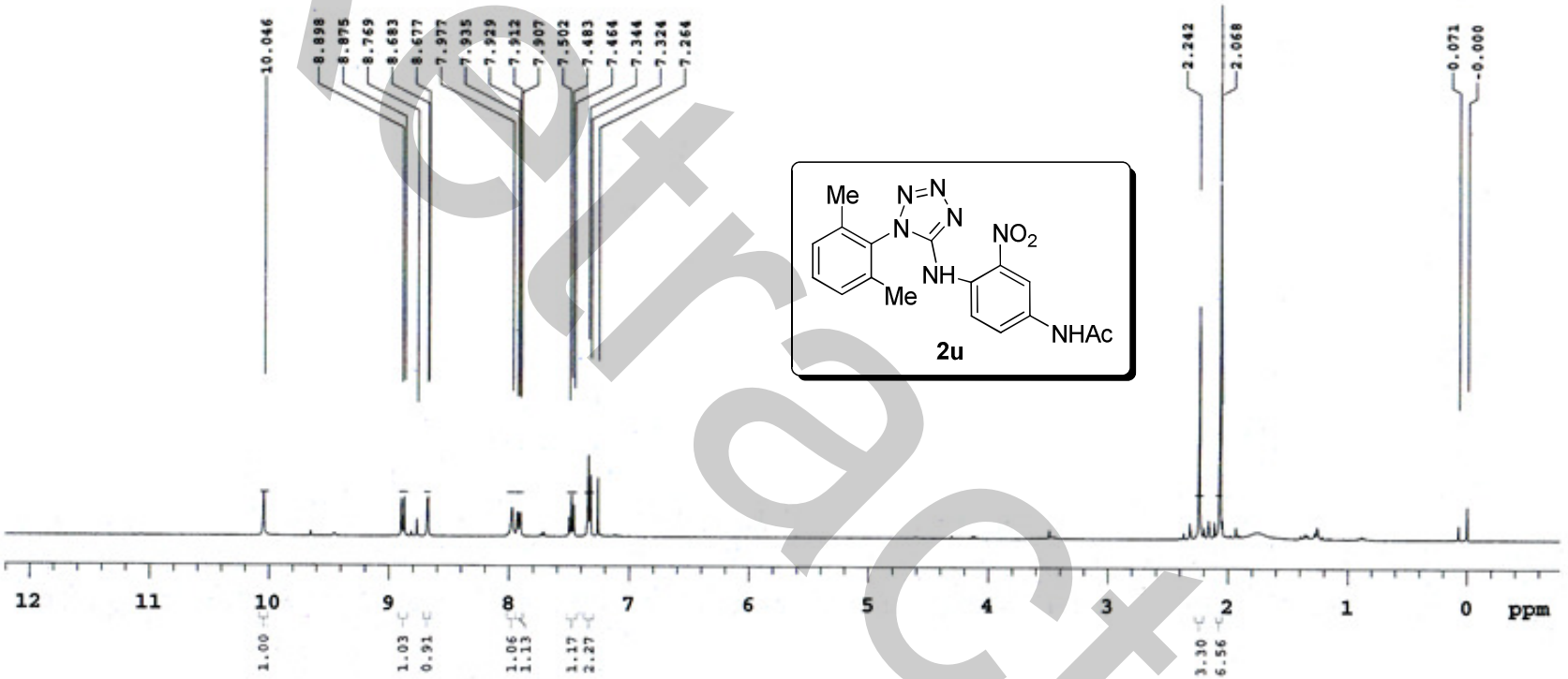
SFO1	150.9279571 MHz
NUC1	13C
P1	10.50 usec
PLW1	95.00000000 W

======== CHANNEL f2 ========

SFO2	600.1724007 MHz
NUC2	1H
CPDPRG[2	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	1.00 Hz
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

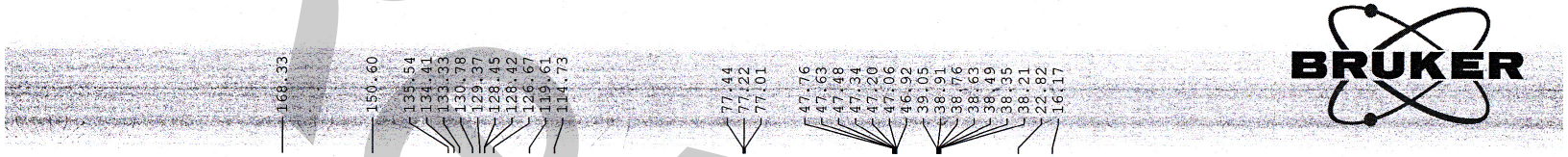
OBSERVE H1, 399.8509602

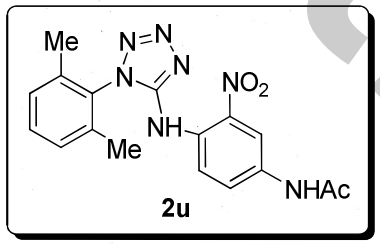
DATA PROCESSING
FT size 32768
Total time 1 minutes

SP-487-NHAC1

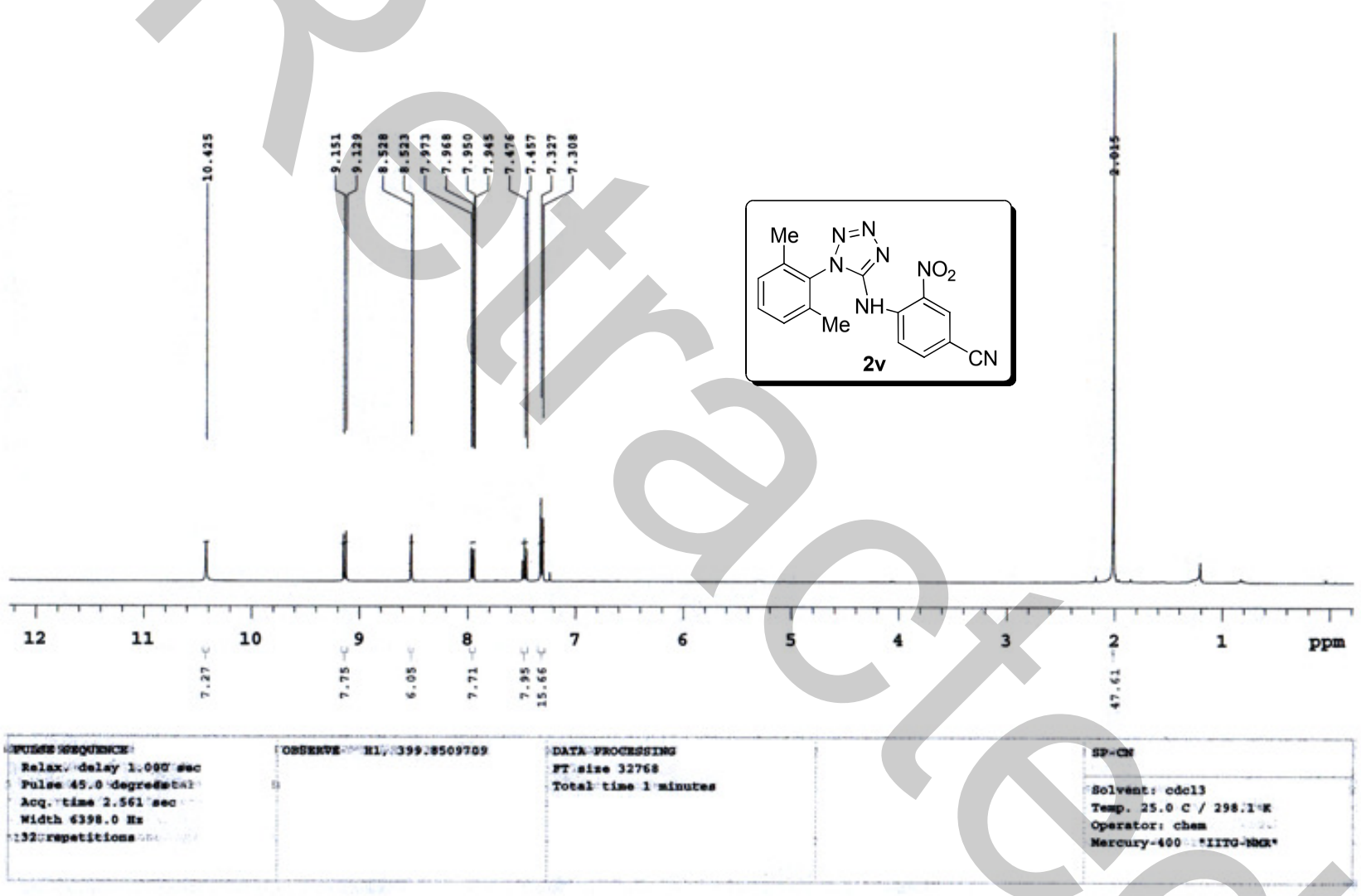
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: chem
File: SP-487-NHAC1
Mercury-400 "IITG-NMR"

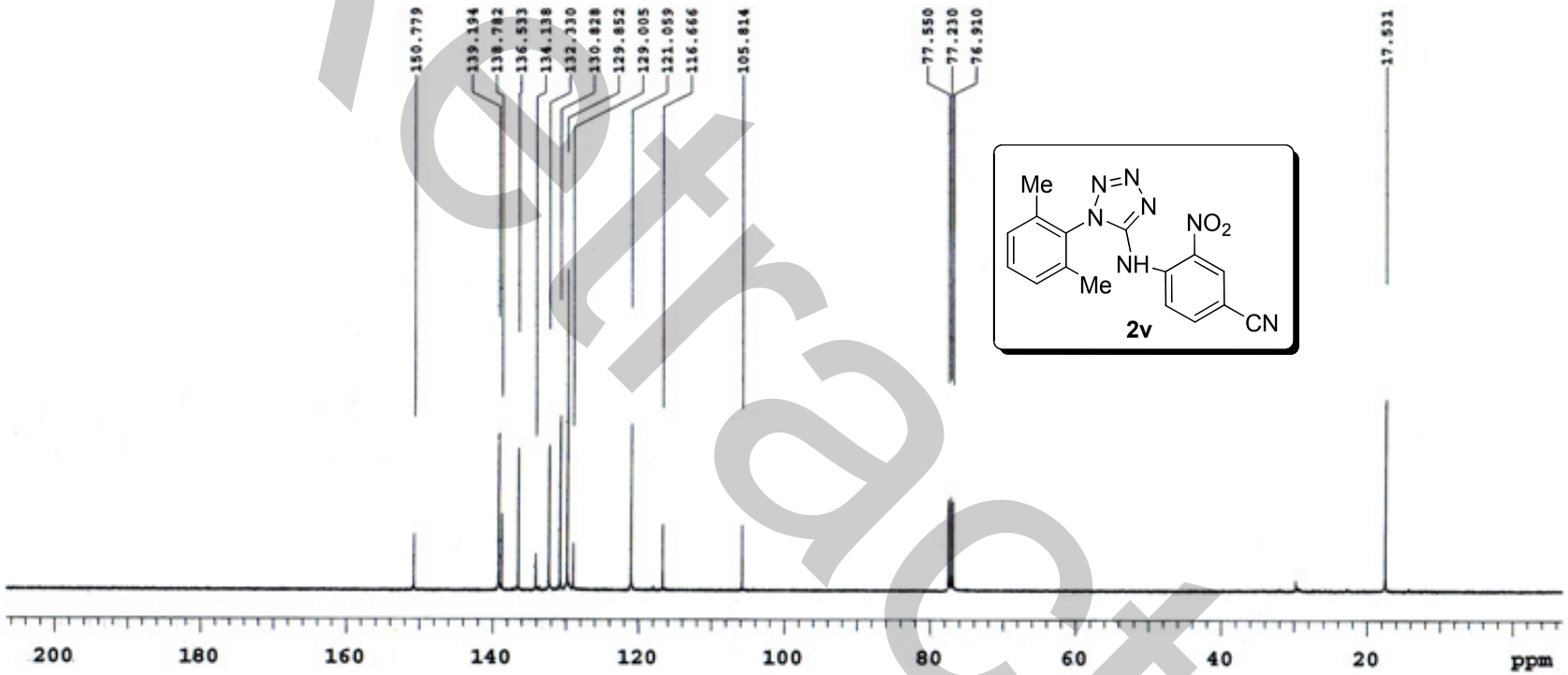
SP-487_13C






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

F2 - Acquisition Parameters
Date_           20140319
Time_              12.20
INSTRUM            spect
PROBHD   5 mm PABBO 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
CPDPRG[2         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                1.00 Hz
GB        0
PC                1.40
```


10.425
9.151
9.129
8.528
8.523
7.973
7.968
7.950
7.945
7.476
7.457
7.327
7.308
2.015
Me
N=N
N
N
NH
NO2
Me
CN
2v
12
11
10
9
8
7
6
5
4
3
2
1
ppm
7.27
7.75
6.05
7.71
7.95
15.66
47.61
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.561 sec
Width 6398.0 Hz
32 repetitions
OBSERVE H1, 399.8509709
DATA PROCESSING
FT size 32768
Total time 1 minutes
SP-CN
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: chem
Mercury-400 *IITG-NMR*



PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degree
Acq. time 1.304 sec
Width 25125.6 Hz
15470 repetitions

OBSERVE C13, 100.5425833
DECOUPLE H1, 399.8529994
Power 42 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 9.9 hours

SP-CN-13C

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: chem