

Supporting Information

Discovery and Structure Activity Relationship Analysis of *Staphylococcus aureus* Sortase A Inhibitors

Nuttee Suree^{a,b}, Sung Wook Yi^a, William Thieu^a, Melanie Marohn^a, Robert Damoiseaux^c, Albert Chan^{a,b}, Michael E. Jung^{a*}, Robert T. Clubb^{a,b,d,*}

^aDepartment of Chemistry & Biochemistry, ^bMolecular Biology Institute, ^cMolecular Screening Shared Resource, University of California, Los Angeles, California 90095-1570, ^dUCLA-Department of Energy Institute for Genomics and Proteomics, University of California, Los Angeles, California 90095-1570

* Corresponding authors. RTC (Tel.: +1 310 206 2334; fax: +1 310 206 4779; e-mail: rclubb@mbi.ucla.edu) and MEJ (Tel.: +1 310 825 7954; fax: +1 310 206 3722; e-mail: jung@chem.ucla.edu)

Table of Contents

I. Observed Melting Points	Page 4~5
II. 1D-NMR Spectra	Page 6~80
2-42	6, 7
2-43	8, 9
2-44	10, 11
2-45	12, 13
2-46	14, 15
2-47	16, 17
2-48	18, 19
2-22	20, 21
2-23	22, 23
2-24	24, 25
2-25	26, 27
2-26	28, 29
2-27	30, 31
2-28	32, 33
2-29	34, 35
2-30	36, 37
2-31	38, 39
2-32	40, 41
2-33	42, 43
2-34	44, 45
2-35	46
2-36	47
2-37	48, 49
2-38	50, 51

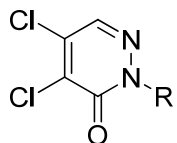
2-39	52, 53
2-40	54
2-41	55, 56
2-10	57, 58
2-11	59
2-12	60, 61
2-13	62, 63
2-14	64, 65
2-15	66, 67
2-16	68, 69
2-18	70
2-19	71
2-20	72, 73
2-21	74
2-17	75, 76
2-49	77, 78
2-50	79, 80

III. 2D-NMR Spectra

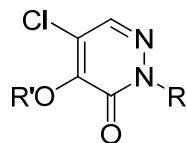
Page 81~82

NOESY for 2-10	81
NOESY for 2-18	82

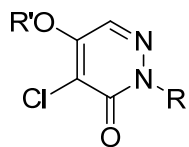
1. Observed Melting Points (mp)



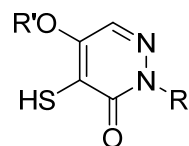
2-42 , R = Ph	mp 158 °C
2-43 , R = 4-nitrophenyl	mp 221 °C
2-44 , R = 3-bromophenyl	mp 194 °C
2-45 , R = 3-Fluorophenyl	mp 192 °C
2-46 , R = 3-methylphenyl (m-tolyl)	mp 117 °C
2-47 , R = 3,5-dichlorophenyl	mp 87 °C
2-48 , R = cyclohexyl	mp 157 °C



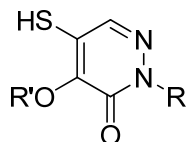
2-22 , R = Ph, R' = Me	
2-23 , R = 3-bromophenyl, R' = Me	
2-24 , R = 3-Fluorophenyl, R' = Me	
2-25 , R = 3-methylphenyl (m-tolyl), R' = Me	
2-26 , R = 3,5-dichlorophenyl, R' = Me	
2-27 , R = cyclohexyl, R' = Me	
2-28 , R = Ph, R' = Et	mp 78°C
2-29 , R = 4-nitrophenyl, R' = Et	mp 127°C
2-30 , R = 3-bromophenyl, R' = Et	mp 98°C
2-31 , R = 3-Fluorophenyl, R' = Et	mp 101°C
2-32 , R = 3-methylphenyl (m-tolyl), R' = Et	mp 84°C
2-33 , R = 3,5-dichlorophenyl, R' = Et	mp 124°C
2-34 , R = cyclohexyl, R' = Et	



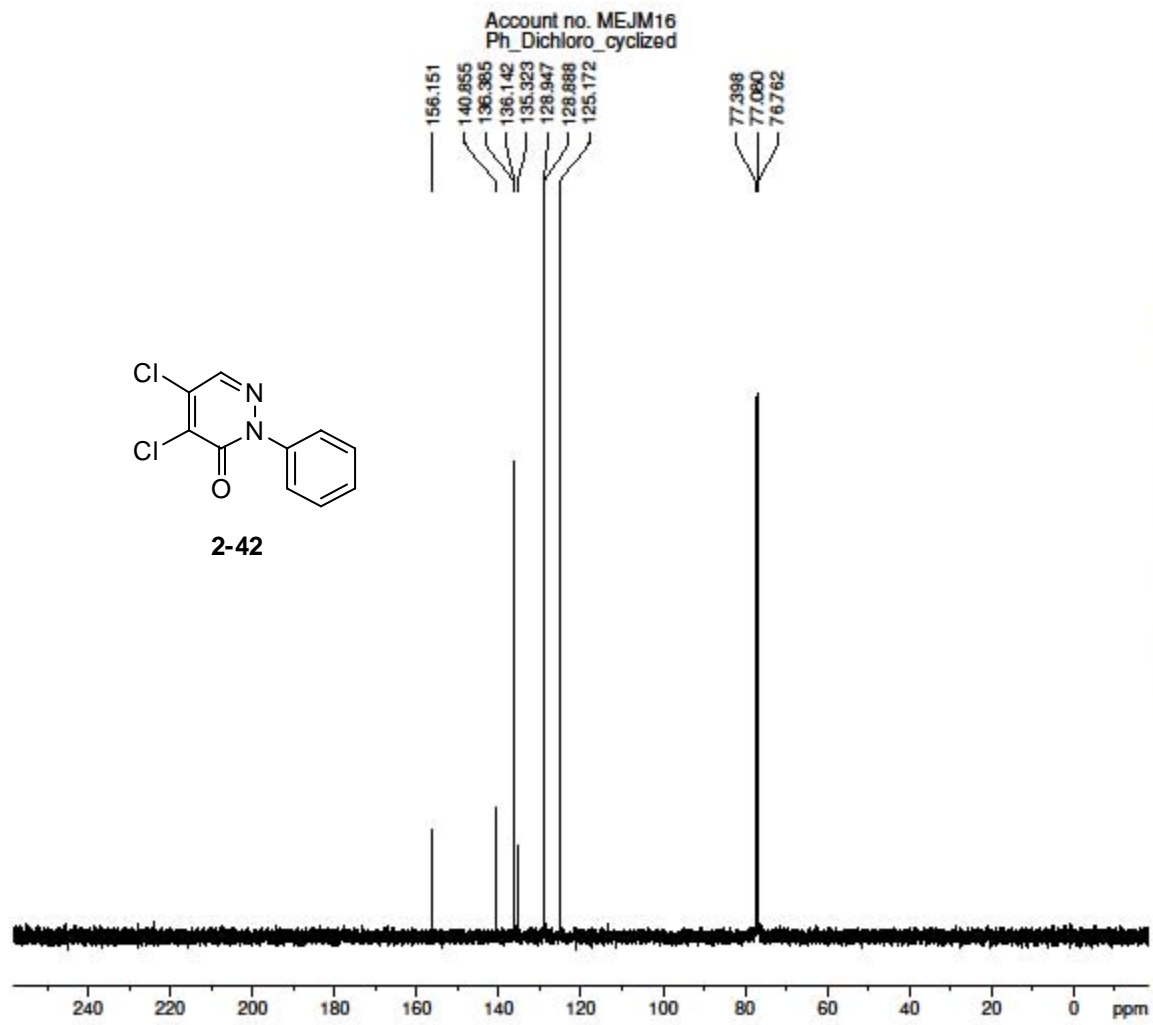
- 2-35**, R = Ph, R' = Et mp 110°C
2-36, R = 4-nitrophenyl, R' = Et
2-37, R = 3-bromophenyl, R' = Et mp 147°C
2-38, R = 3-Fluorophenyl, R' = Et mp 138°C
2-39, R = 3-methylphenyl (m-tolyl), R' = Et mp 122°C
2-40, R = 3,5-dichlorophenyl, R' = Et
2-41, R = cyclohexyl, R' = Et mp 141°C



- 2-18**, R = Ph, R' = Et
2-19, R = 3-Fluorophenyl, R' = Et
2-20, R = 3-methylphenyl (m-tolyl), R' = Et
2-21, R = 3,5-dichlorophenyl, R' = Et



- 2-10**, R = Ph, R' = Et mp 101°C
2-11, R = 4-nitrophenyl, R' = Et
2-12, R = 3-bromophenyl, R' = Et
2-13, R = 3-Fluorophenyl, R' = Et
2-14, R = 3-methylphenyl (m-tolyl), R' = Et
2-15, R = 3,5-dichlorophenyl, R' = Et
2-16, R = cyclohexyl, R' = Et

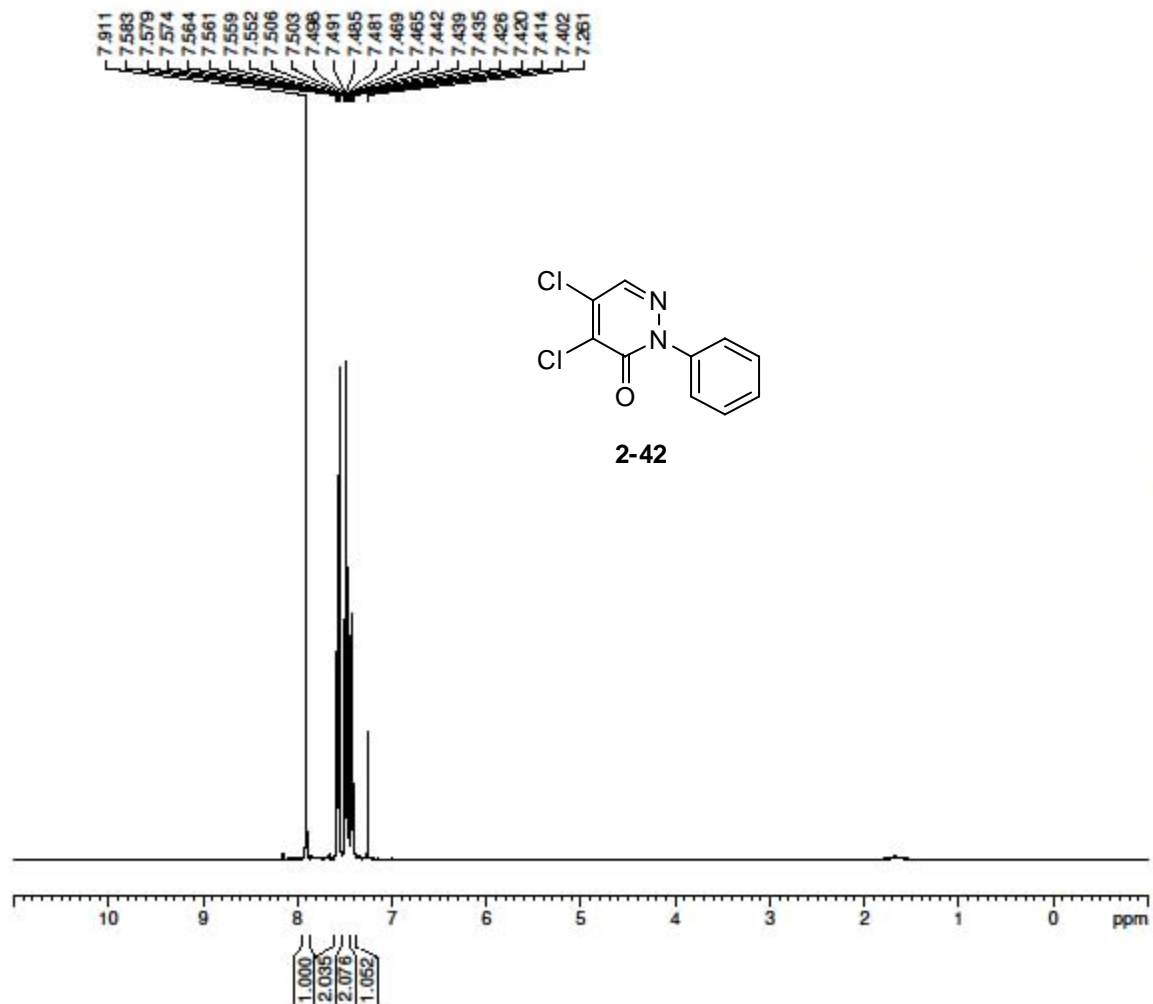


Current Data Parameters
 NAME 100708
 EXPNO 261
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081007
 Time 16.56
 INSTRUM arx400
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 200
 DS 0
 SWH 27777.777 Hz
 FIDRES 0.423855 Hz
 AQ 1.1796980 sec
 RG 32768
 DW 18.000 usec
 DE 25.71 usec
 TE 300.0 K
 D12 0.0000200 sec
 DL5 23.50 dB
 CPDPRG waltz16
 P31 100.00 usec
 D1 2.0000000 sec
 P1 8.25 usec
 SFO1 100.6248445 MHz
 NUCLEUS 13C
 D11 0.0300000 sec

F2 - Processing parameters
 SI 65536
 SF 100.6127710 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Account no. MEJM16
Ph_Dichloro_cyclized



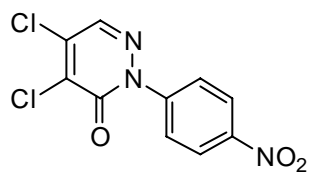
Current Data Parameters
NAME 100708
EXPNO 260
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081007
Time 16.45
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 715
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.0000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

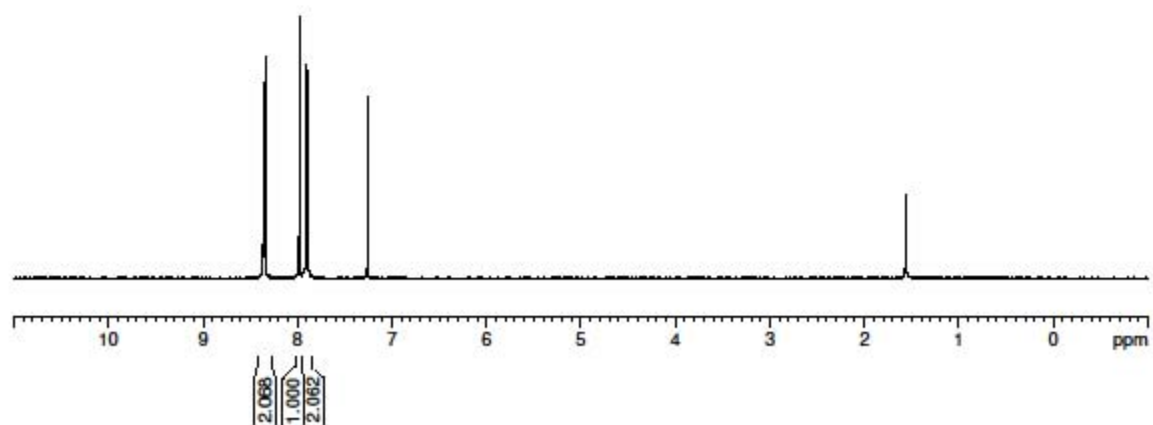
F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

default proton parameters

8.367
8.361
8.357
8.347
8.343
8.338
8.321
7.982
7.942
7.912
7.907
7.903
7.893
7.889
7.883
7.867
7.260



2-43



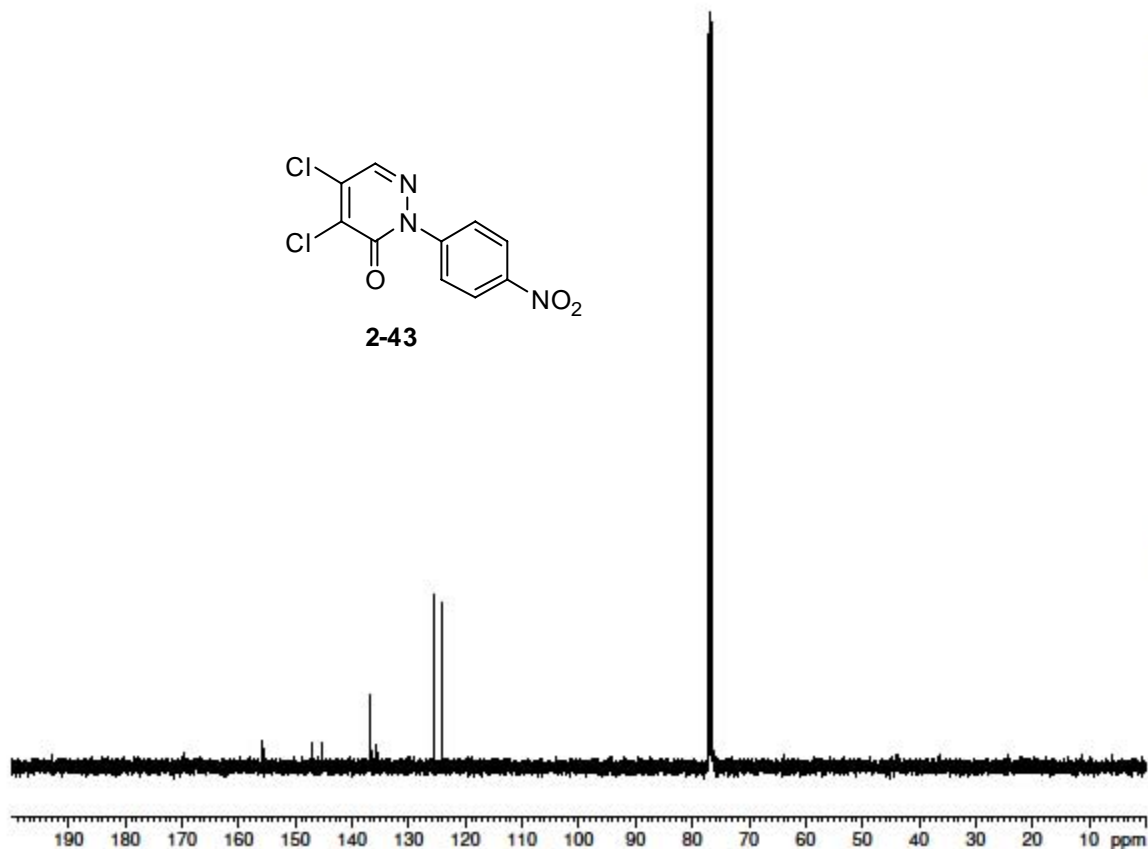
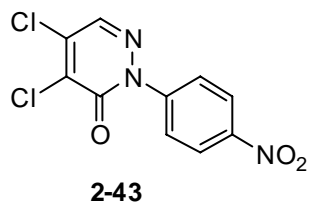
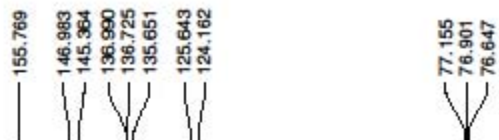
Current Data Parameters
NAME W1-YJ43
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090728
Time 11.13
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 2
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 322.5
DW 50.000 usec
DE 6.00 usec
TE 296.1 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 500.3330020 MHz

F2 - Processing parameters
SI 32768
SF 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

default carbon parameters (proton decoupled)



Current Data Parameters
NAME W1-YJ43
EXPNO 2
PROCNO 1

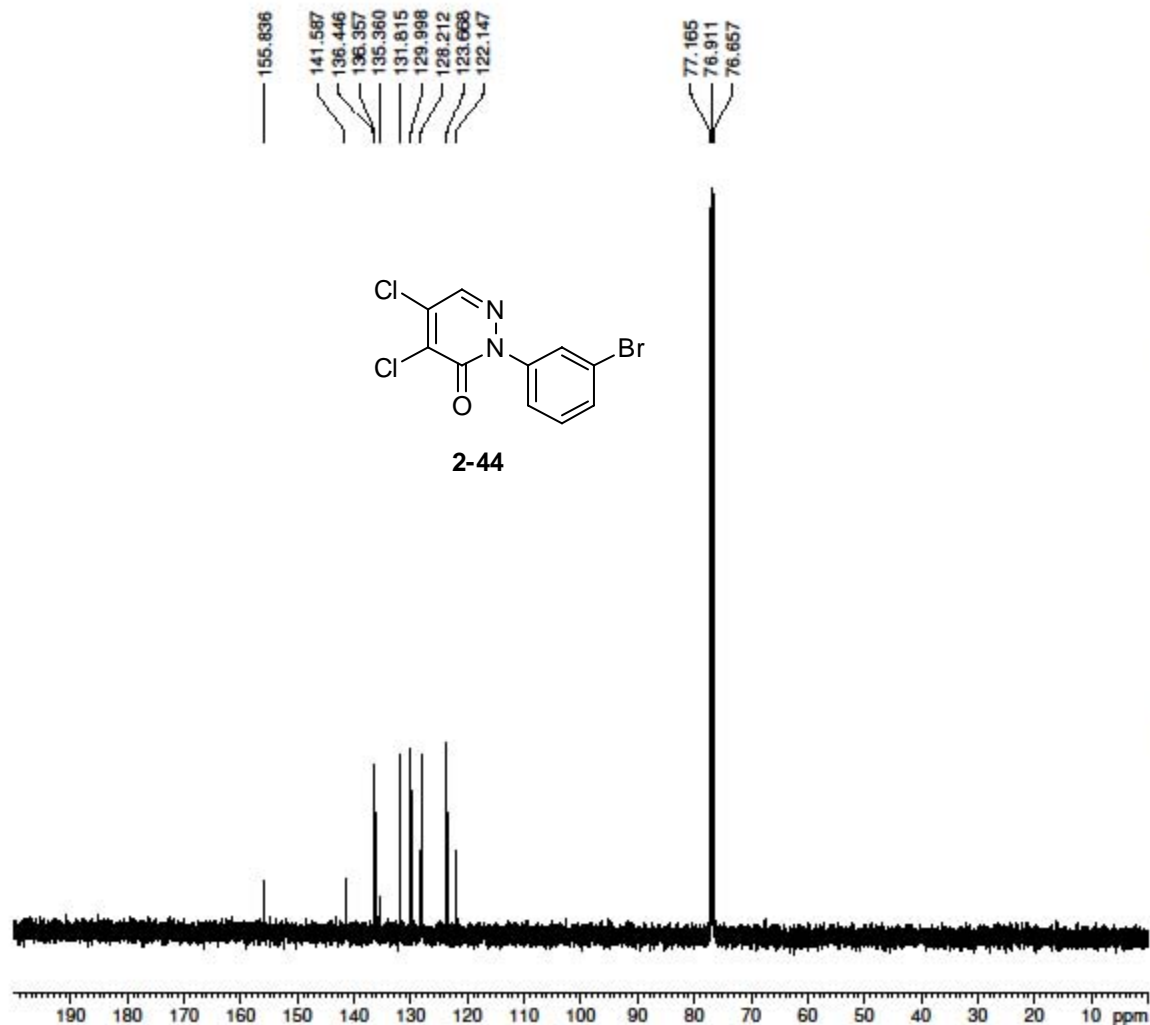
F2 - Acquisition Parameters
Date_ 20090728
Time 11.19
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 203
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 2298.8
DW 15.300 usec
DE 6.00 usec
TE 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.25 usec
PL1 0.00 dB
SFO1 125.8231939 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz

F2 - Processing parameters
SI 65536
SF 125.8080969 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

default carbon parameters (proton decoupled)



Current Data Parameters
NAME W1-YJ2-44
EXPNO 2
PROCNO 1

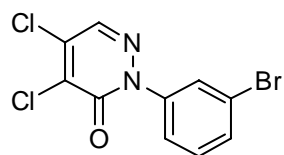
F2 - Acquisition Parameters
Date_ 20090728
Time 11.34
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 95
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 1448.2
DW 15.300 usec
DE 6.00 usec
TE 296.6 K
D1 2.0000000 sec
d11 0.0300000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.25 usec
PL1 0.00 dB
SFO1 125.8231939 MHz

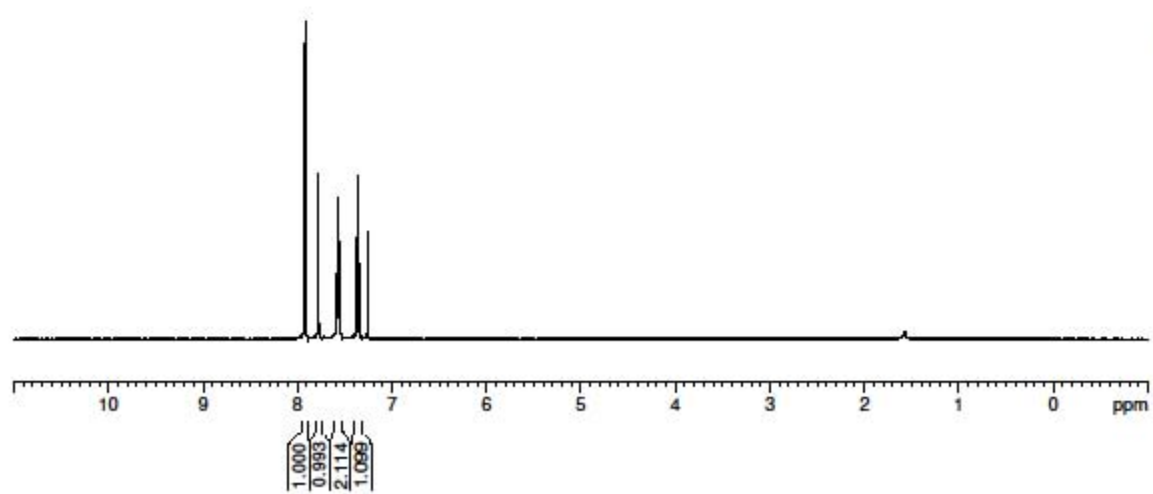
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz

F2 - Processing parameters
SI 65536
SF 125.8080969 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

default proton parameters



2-44



Current Data Parameters
NAME W1-YJ2-44
EXPNO 1
PROCNO 1

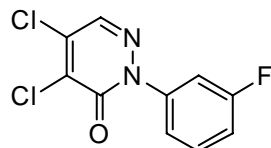
F2 - Acquisition Parameters
Date_ 20090728
Time 11.31
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 2
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 256
DW 50.000 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 500.3330020 MHz

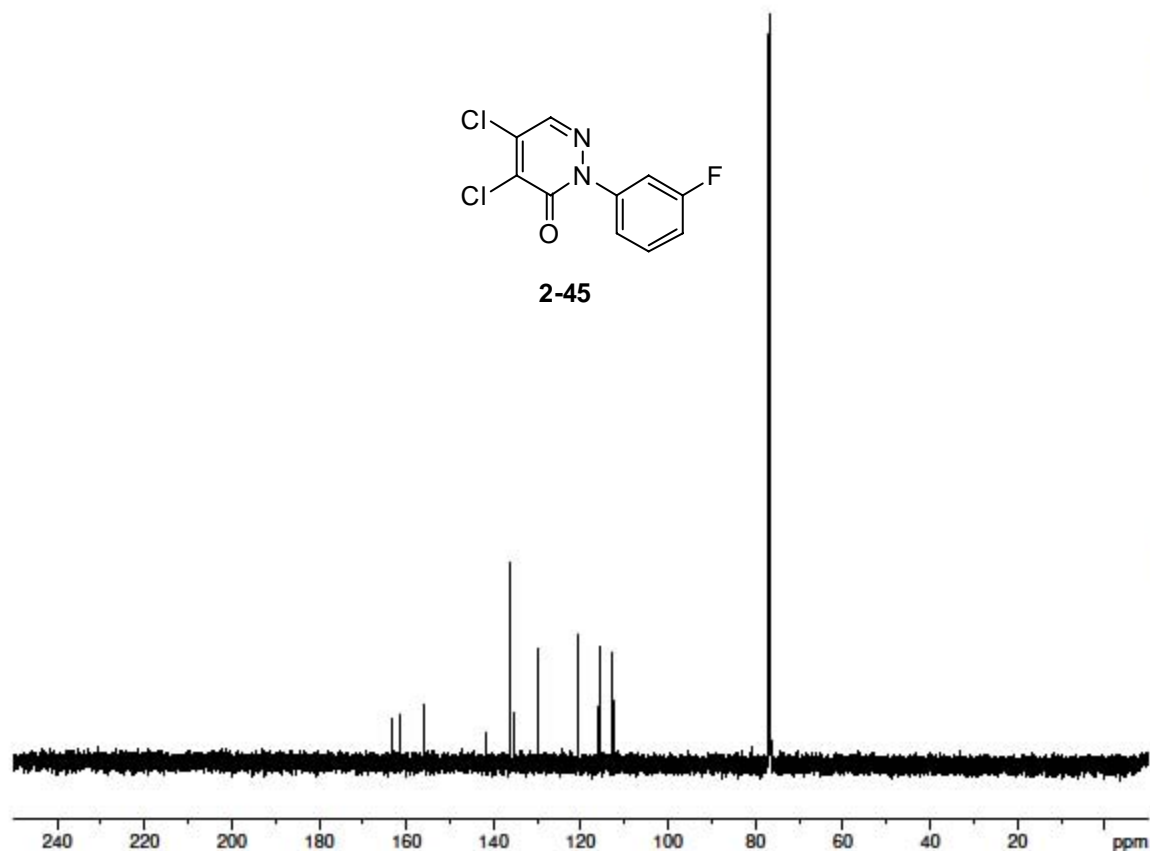
F2 - Processing parameters
SI 32768
SF 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

default carbon parameters (proton decoupled)

163.280
161.313
155.835
141.816
141.749
136.397
136.303
135.388
129.994
129.924
120.688
120.662
115.858
115.690
112.909
112.707
77.167
76.913
76.659



2-45



Current Data Parameters
NAME W1-YJ2-45
EXPNO 2
PROCNO 1

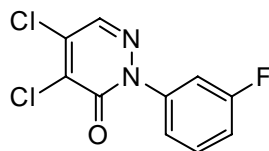
F2 - Acquisition Parameters
Date_ 20090728
Time 11.42
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 3251
DW 15.300 usec
DE 6.00 usec
TE 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.25 usec
PL1 0.00 dB
SFO1 125.8231939 MHz

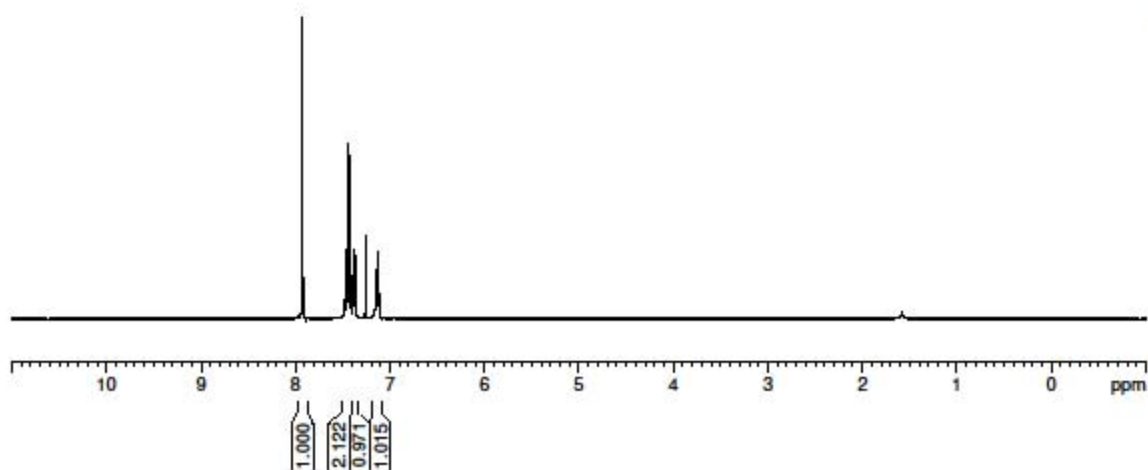
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz

F2 - Processing parameters
SI 65536
SF 125.8080969 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

default proton parameters



2-45



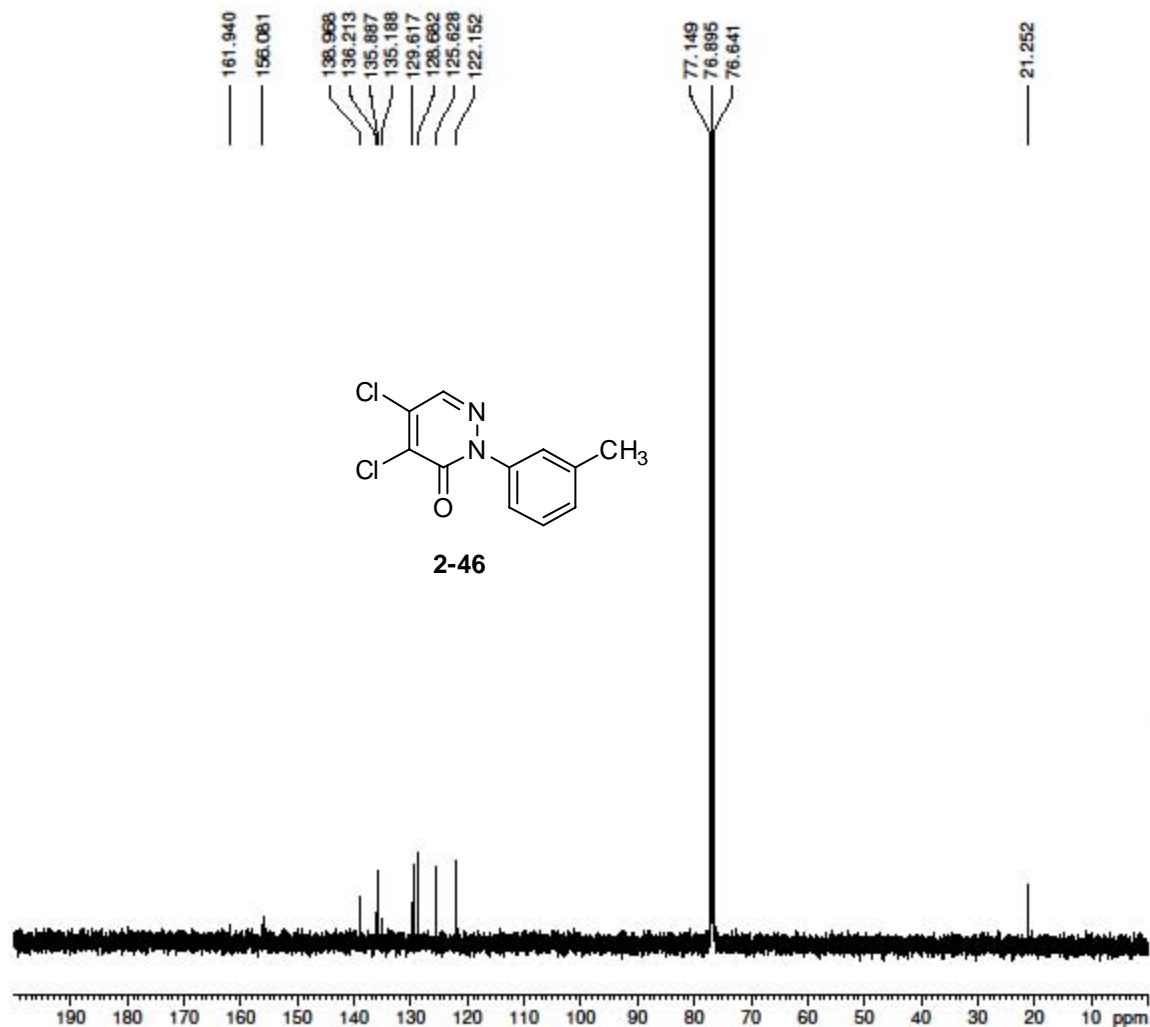
Current Data Parameters
NAME W1-YJ2-45
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090728
Time 11.40
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 2
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 256
DW 50.000 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 500.3330020 MHz

F2 - Processing parameters
SI 32768
SF 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

default carbon parameters (proton decoupled)



Current Data Parameters
NAME W1-YJ2-46
EXPNO 2
PROCNO 1

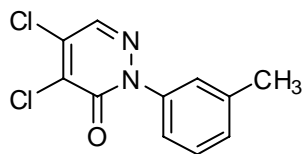
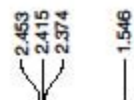
F2 - Acquisition Parameters
Date_ 20090728
Time 11.52
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 7298.2
DW 15.300 usec
DE 6.00 usec
TE 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.25 usec
PL1 0.00 dB
SFO1 125.8231939 MHz

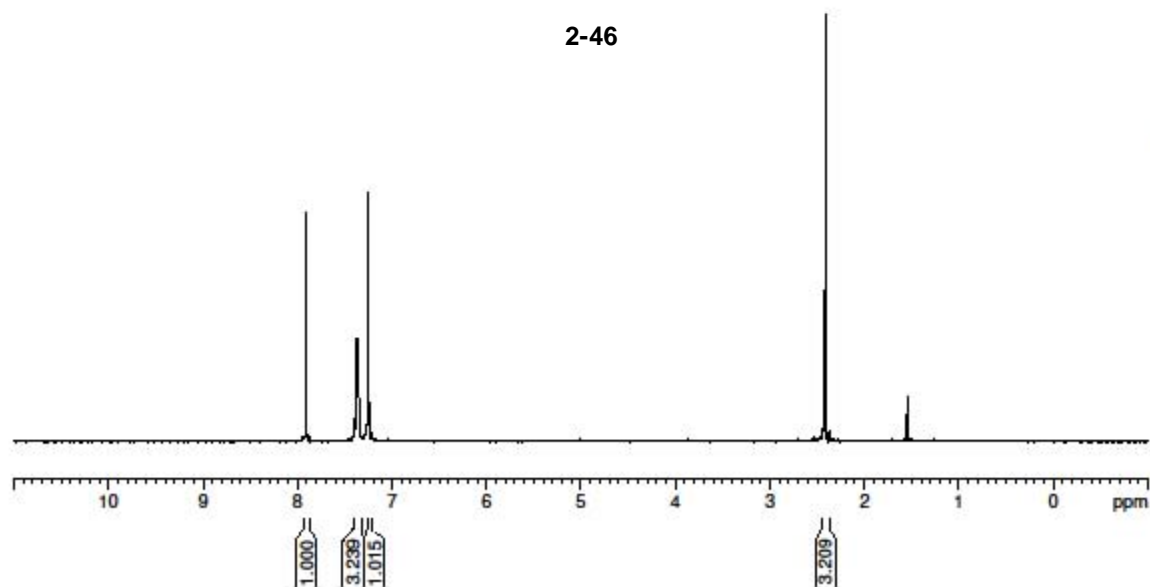
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz

F2 - Processing parameters
SI 65536
SF 125.8080969 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

default proton parameters



2-46



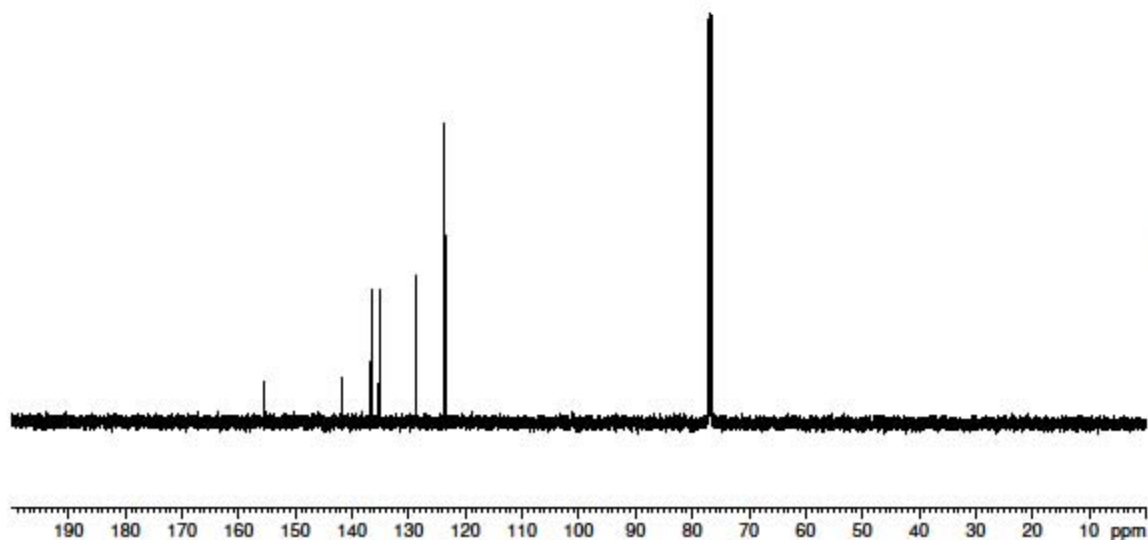
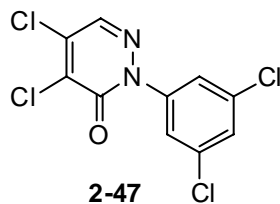
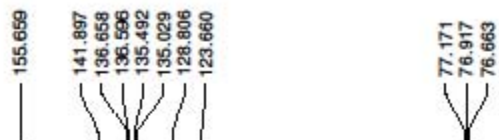
Current Data Parameters
NAME W1-YJ2-46
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090728
Time 11.50
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 2
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 181
DW 50.000 usec
DE 6.00 usec
TE 296.3 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 500.3330020 MHz

F2 - Processing parameters
SI 32768
SF 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

default carbon parameters (proton decoupled)



Current Data Parameters
 NAME W1-YJ2-47
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090728
 Time 12.08
 INSTRUM avance500
 PROBHD 5 mm bb-Z 2800
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 0
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 4096
 DW 15.300 usec
 DE 6.00 usec
 TE 296.7 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

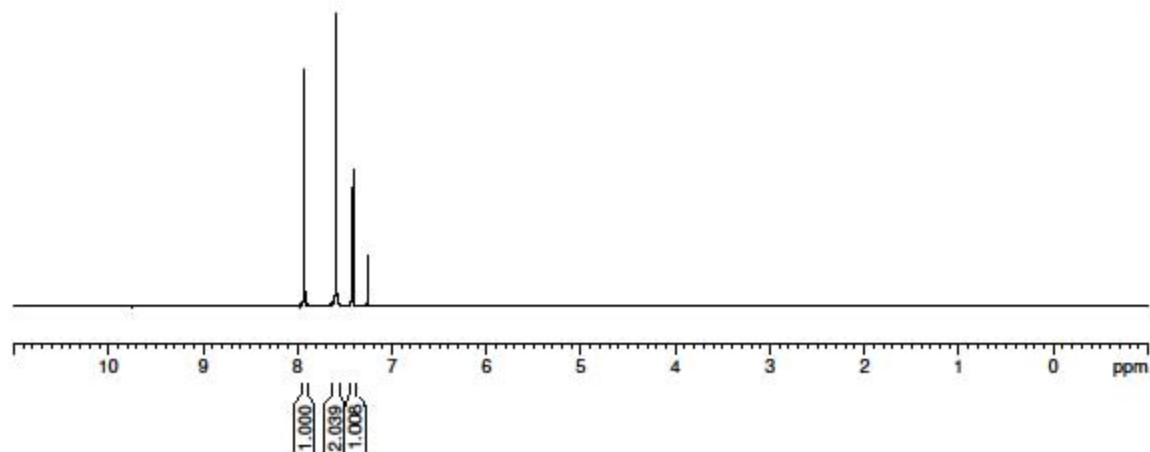
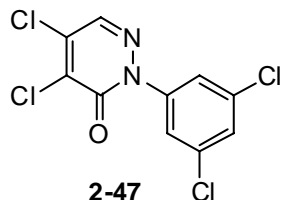
----- CHANNEL f1 -----
 NUC1 13C
 P1 5.25 usec
 PL1 0.00 dB
 SFO1 125.8231939 MHz

----- CHANNEL f2 -----
 CPDPRG2 waitz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 16.10 dB
 SFO2 500.3320013 MHz

F2 - Processing parameters
 SI 65536
 SF 125.8080969 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

default proton parameters

7.926
7.629
7.593
7.589
7.416
7.413
7.409
7.259



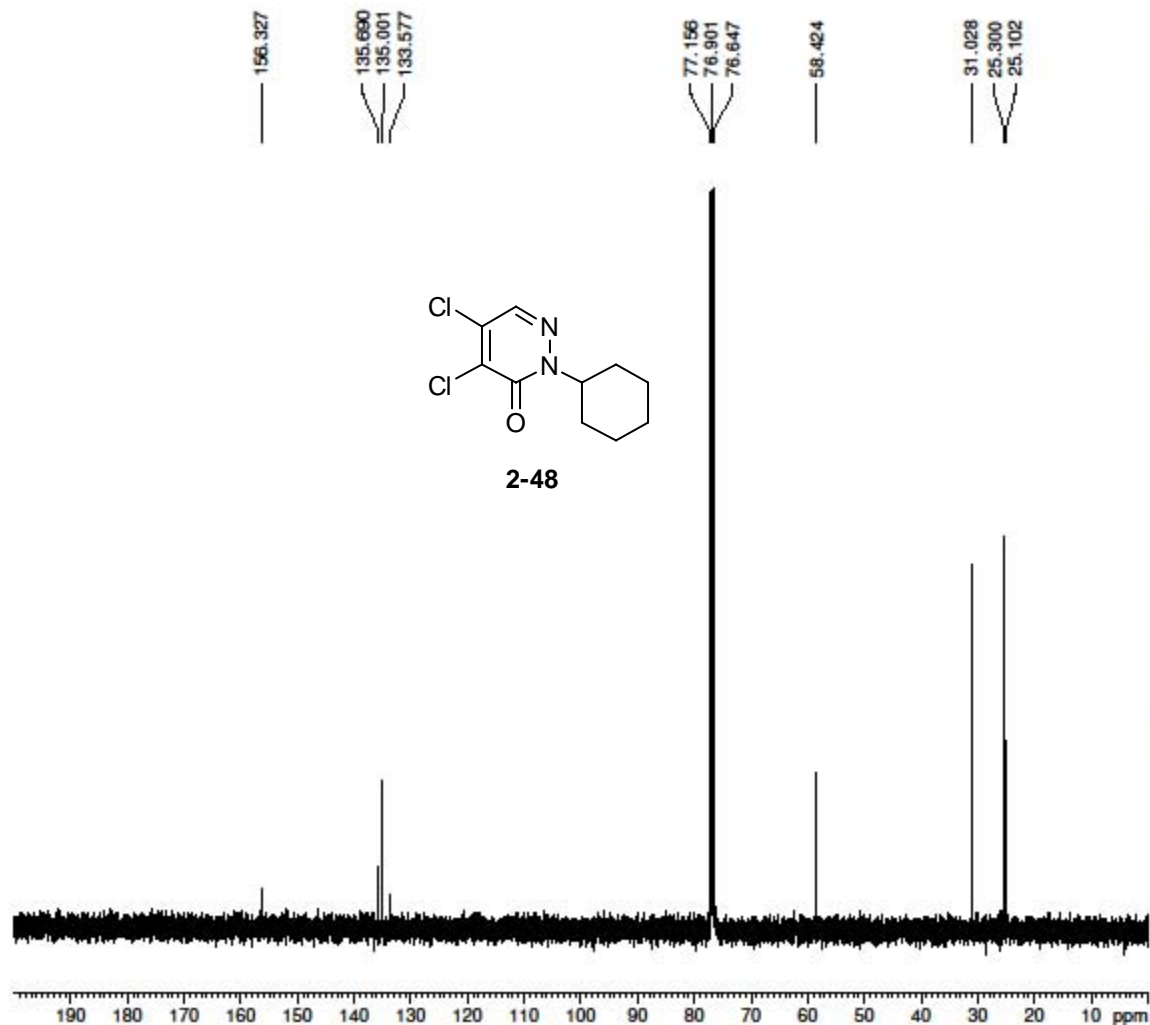
Current Data Parameters
NAME W1-YJ2-47
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090728
Time 12.06
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 2
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 1024
DW 50.000 usec
DE 6.00 usec
TE 296.4 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 500.3330020 MHz

F2 - Processing parameters
SI 32768
SF 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

default carbon parameters (proton decoupled)



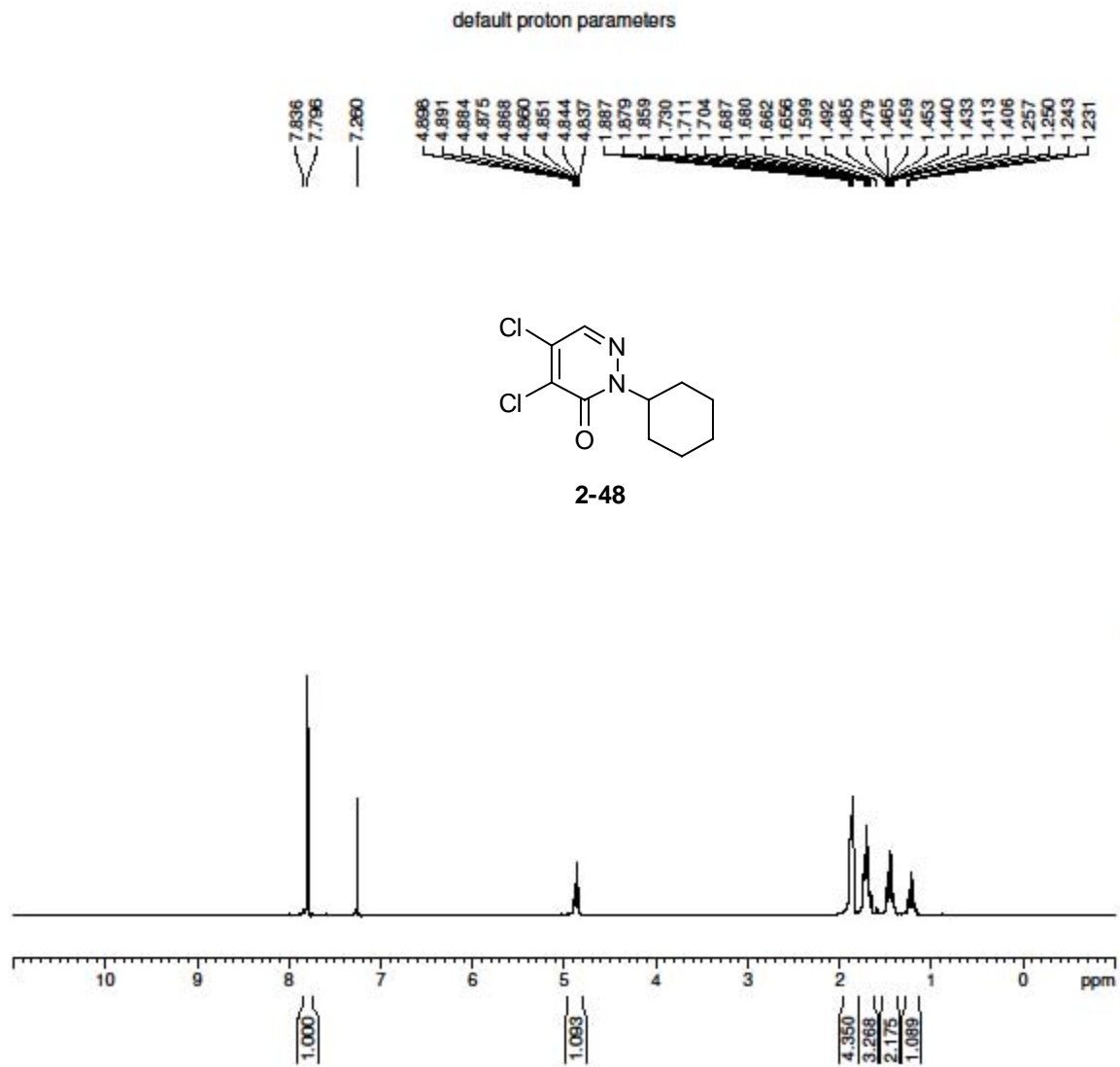
Current Data Parameters
NAME W1-YJ2-48
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090728
Time 12.14
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 296.5 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.25 usec
PL1 0.00 dB
SFO1 125.8231939 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz

F2 - Processing parameters
SI 65536
SF 125.8080969 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



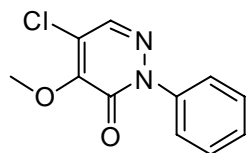
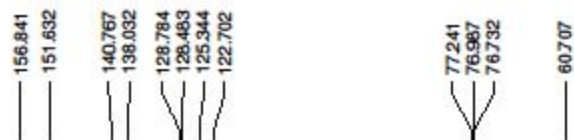
Current Data Parameters
 NAME W1-YJ2-48
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090728
 Time 12.13
 INSTRUM avance500
 PROBHD 5 mm bb-Z 2800
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 2
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2769001 sec
 RG 128
 DW 50.000 usec
 DE 6.00 usec
 TE 296.3 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

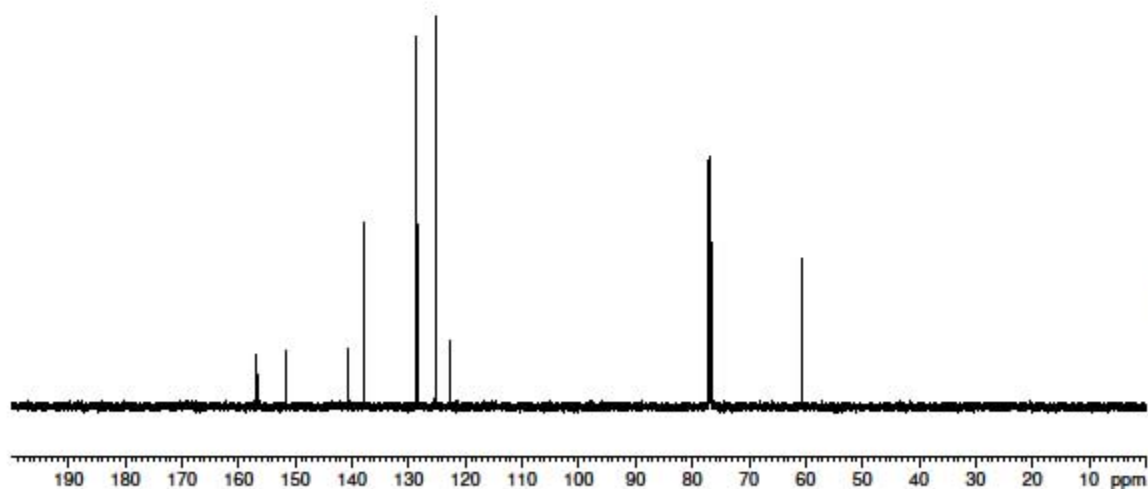
----- CHANNEL f1 -----
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 500.3330020 MHz

F2 - Processing parameters
 SI 32768
 SF 500.3300220 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

default carbon parameters (proton decoupled)



2-22



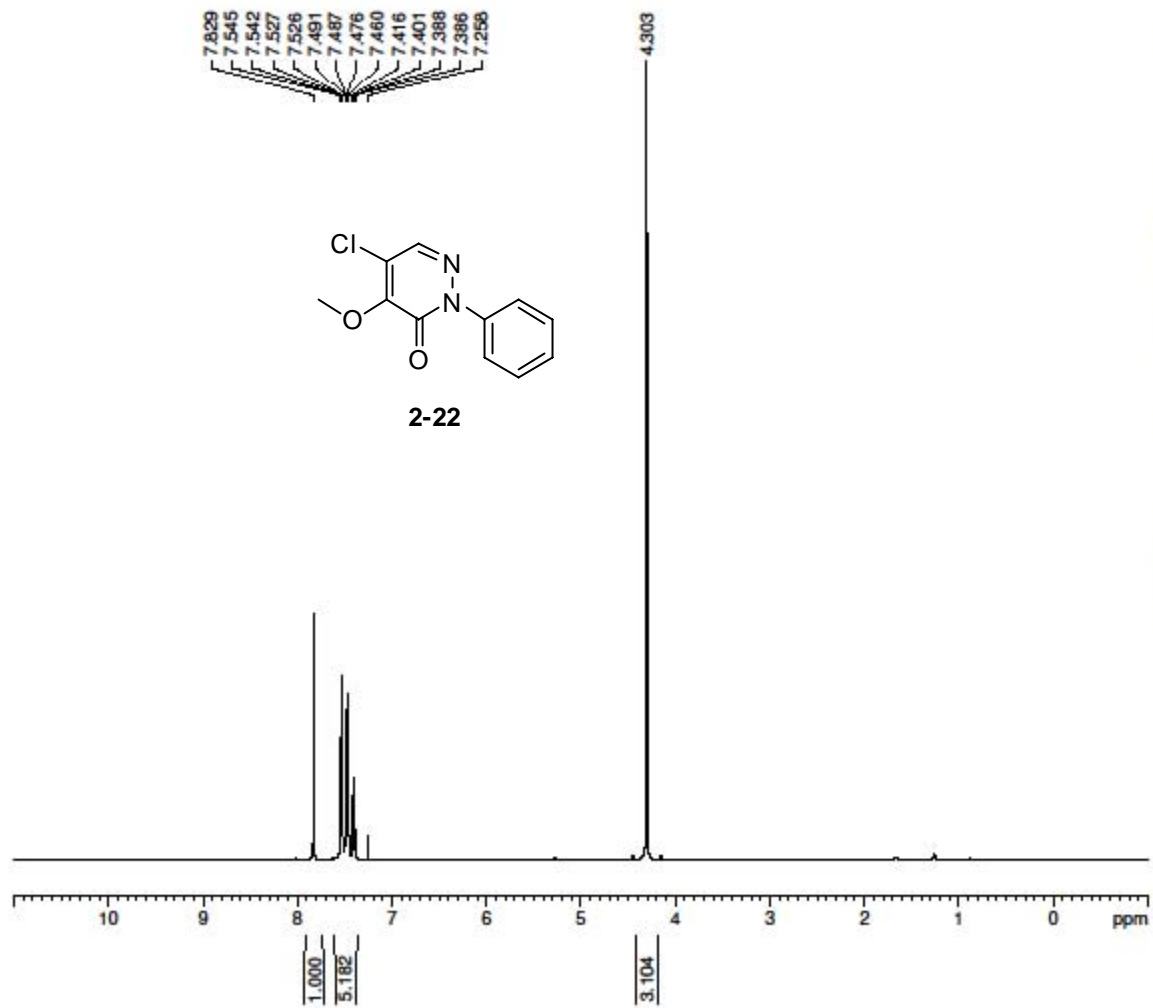
Current Data Parameters
NAME Ph_OMe_A_re
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081030
Time 11.14
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 36
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 295.4 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.25 usec
PL1 0.00 dB
SFO1 125.8231939 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 120.00 dB
PL12 19.00 dB
SFO2 500.3320013 MHz

F2 - Processing parameters
SI 65536
SF 125.8080969 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

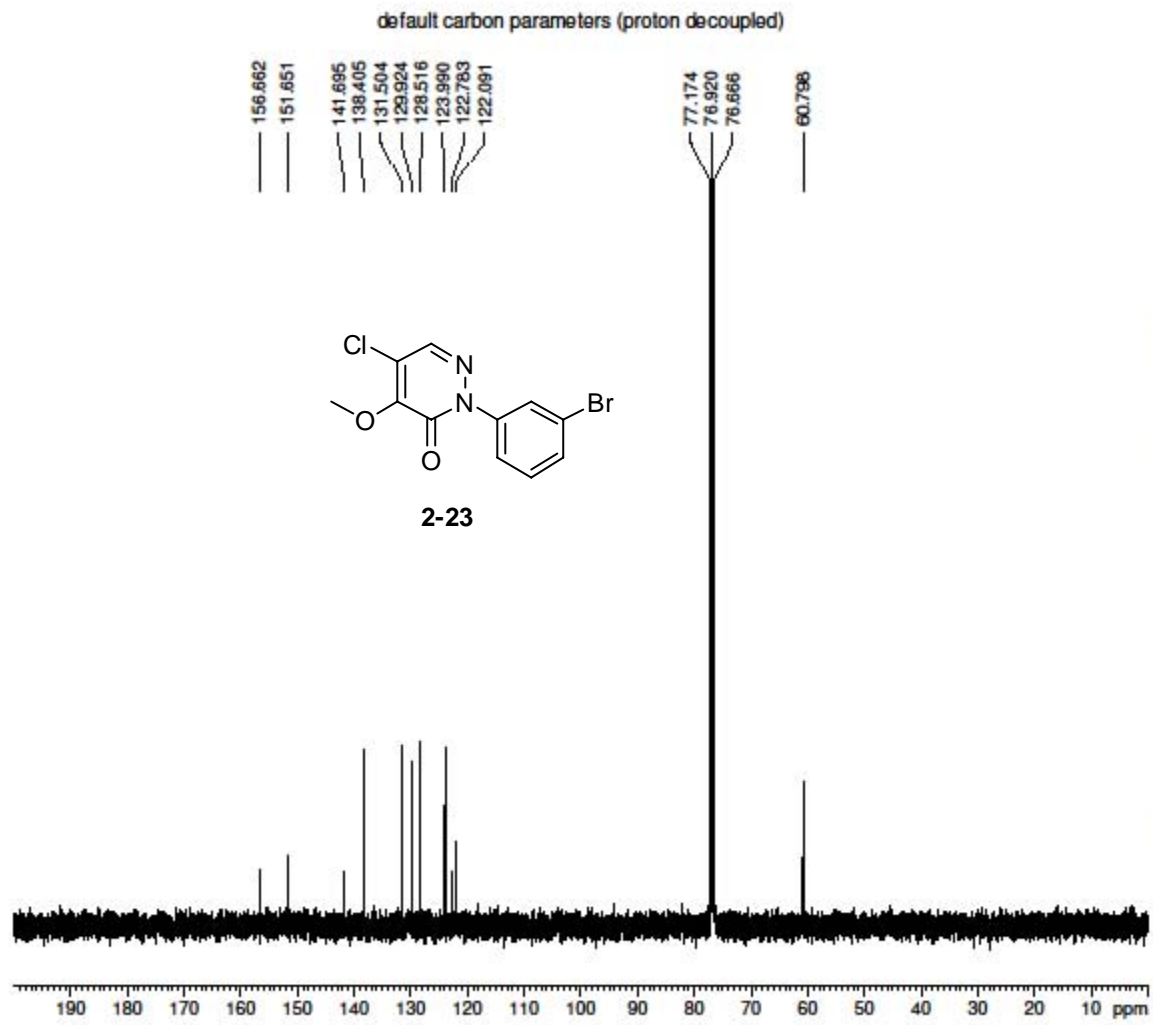


Current Data Parameters
 NAME Ph_OMe_A_re
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081030
 Time 11.12
 INSTRUM avance500
 PROBHD 5 mm bb-Z 2800
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6385000 sec
 RG 71.8
 DW 50.000 usec
 DE 6.00 usec
 TE 295.3 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

CHANNEL f1
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 500.3330020 MHz

F2 - Processing parameters
 SI 32768
 SF 500.3300220 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 3BrPh_OMe_A
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081030
 Time 11.21
 INSTRUM avance500
 PROBHD 5 mm bb-Z 2800
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 47
 DS 0
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 13004
 DW 15.300 usec
 DE 6.00 usec
 TE 295.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 5.25 usec
 PL1 0.00 dB
 SFO1 125.8231939 MHz

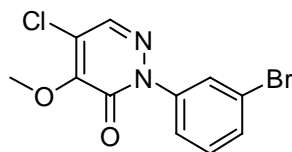
----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 105.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SFO2 500.3320013 MHz

F2 - Processing parameters
 SI 65536
 SF 125.8080969 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

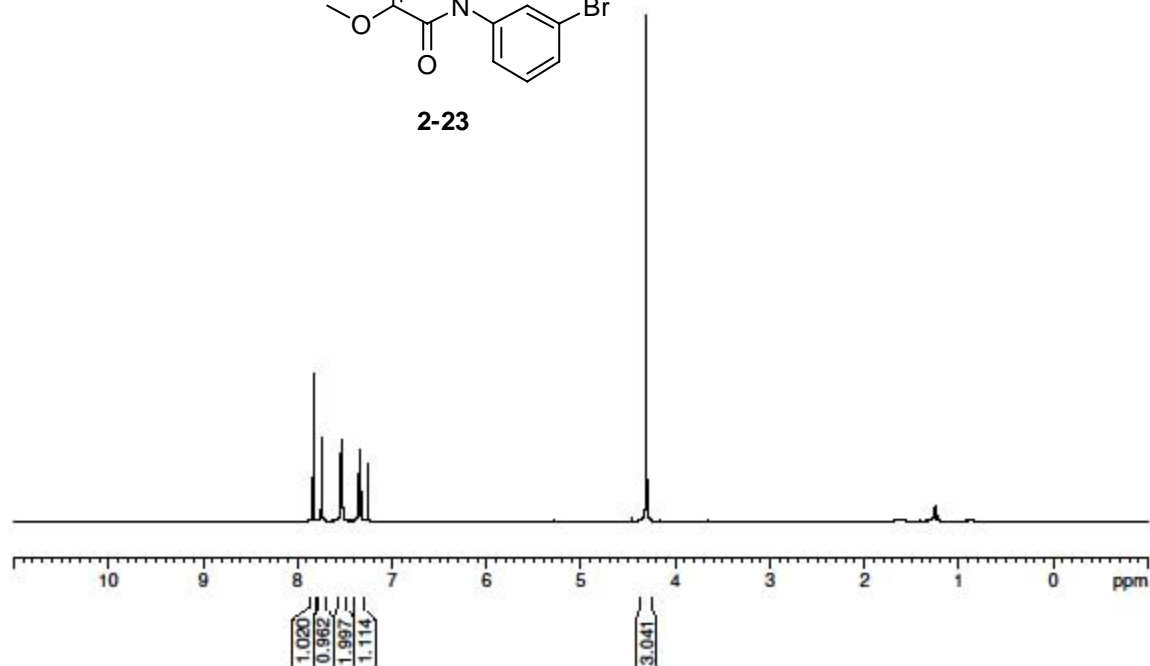
default proton parameters

7.835
7.749
7.745
7.742
7.544
7.542
7.530
7.528
7.527
7.362
7.346
7.330
7.258

4.307



2-23



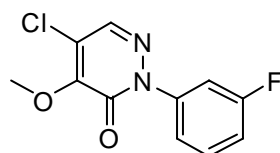
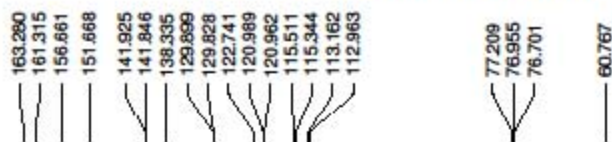
Current Data Parameters
NAME 3BrPh_OMe_A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081030
Time 11.19
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6385000 sec
RG 128
DW 50.000 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

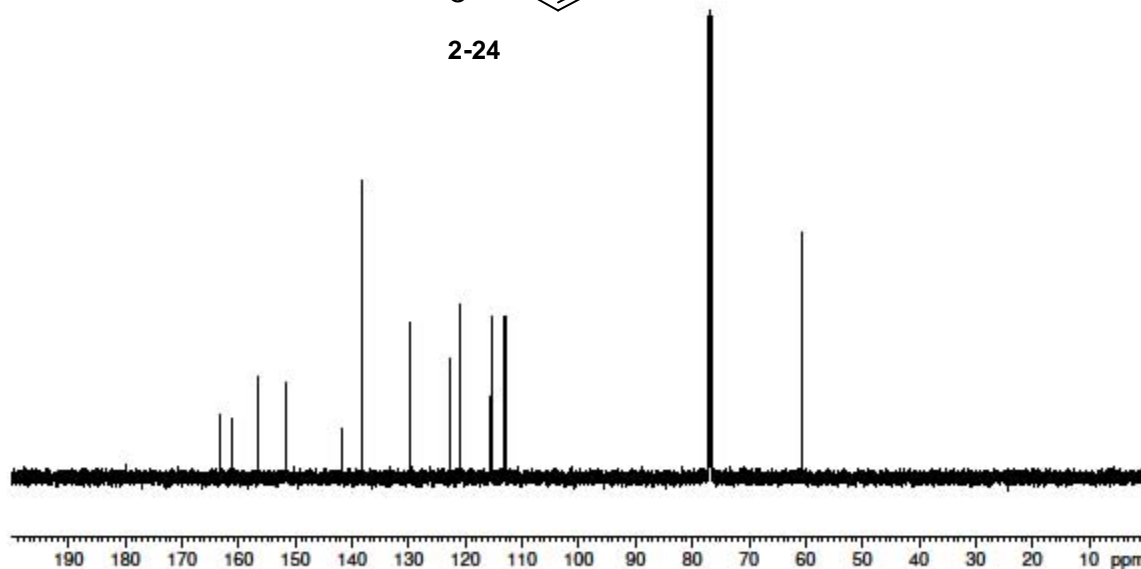
CHANNEL f1
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 500.3330020 MHz

F2 - Processing parameters
SI 32768
SF 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

default carbon parameters (proton decoupled)



2-24



Current Data Parameters
NAME 3F-Ph_OMe_A
EXPNO 2
PROCNO 1

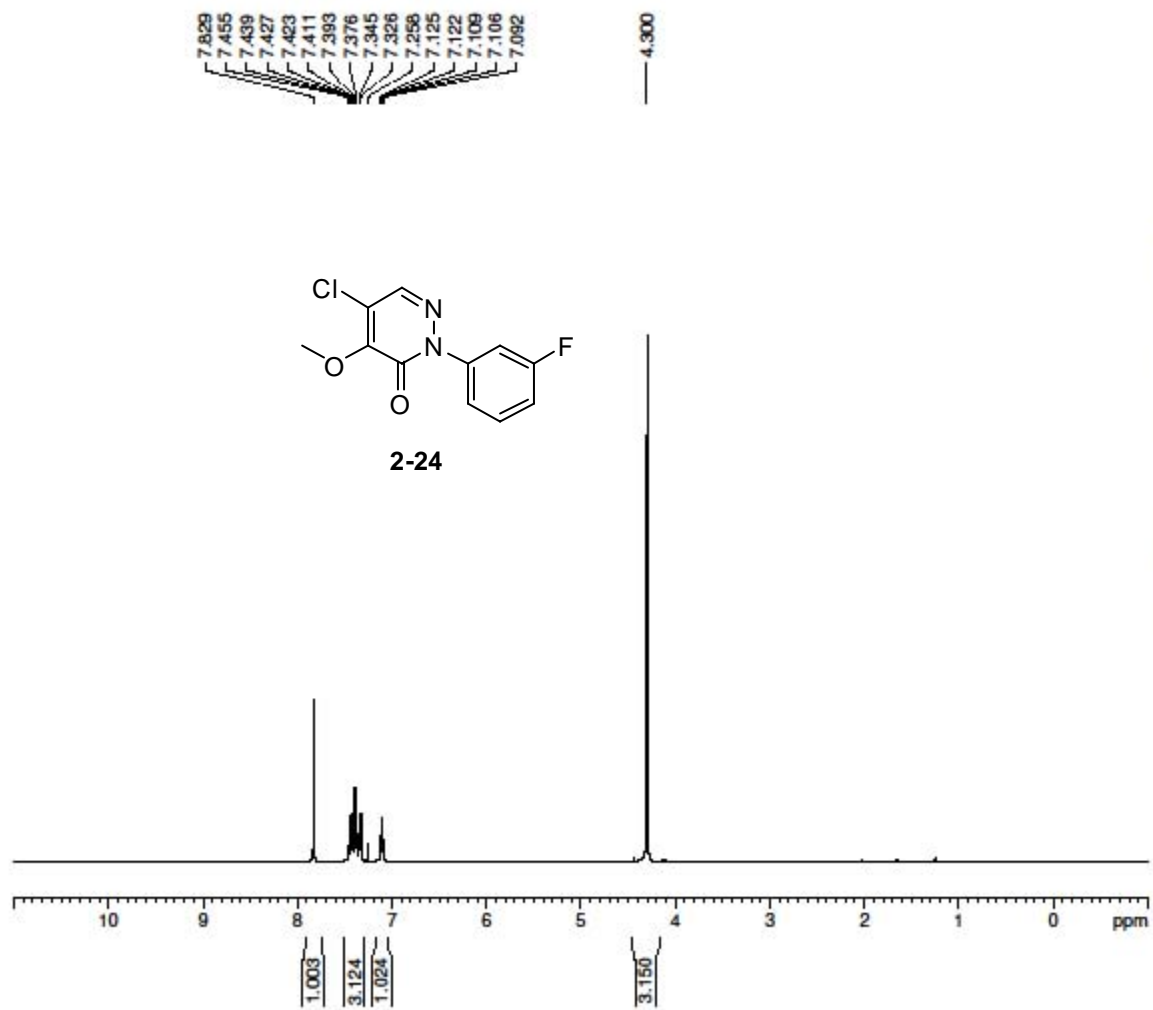
F2 - Acquisition Parameters
Date_ 20081030
Time 11.27
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 45
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 295.4 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.25 usec
PL1 0.00 dB
SFO1 125.8231939 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 120.00 dB
PL12 19.00 dB
SFO2 500.3320013 MHz

F2 - Processing parameters
SI 65536
SF 125.8080969 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

default proton parameters



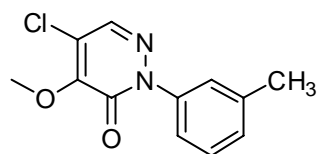
Current Data Parameters
NAME 3F-Ph_OMe_A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081030
Time 11.25
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6385000 sec
RG 90.5
DW 50.000 usec
DE 6.00 usec
TE 295.3 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

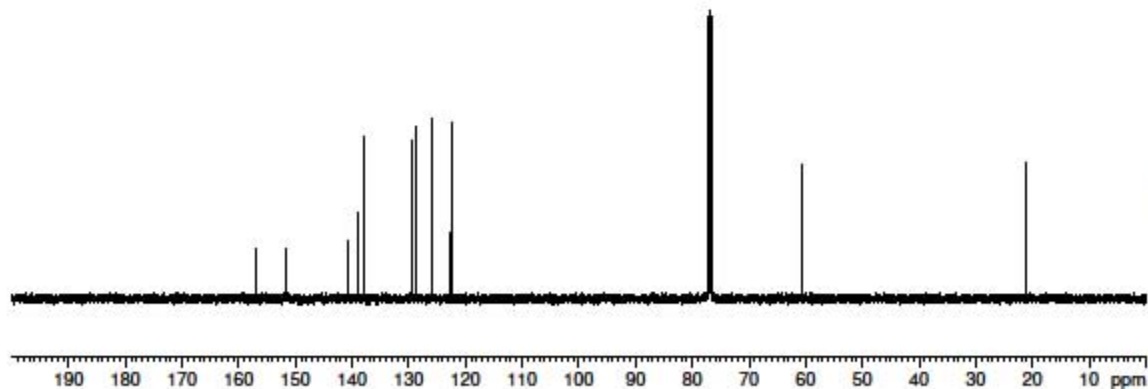
CHANNEL f1
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 500.3330020 MHz

F2 - Processing parameters
SI 32768
SF 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

default carbon parameters (proton decoupled)



2-25



Current Data Parameters
NAME 3Tolyl_OMe_A
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081030
Time 10.29
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 78
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 4096
DW 15.300 usec
DE 6.00 usec
TE 295.4 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.25 usec
PL1 0.00 dB
SFO1 125.8231939 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 120.00 dB
PL12 19.00 dB
SFO2 500.3320013 MHz

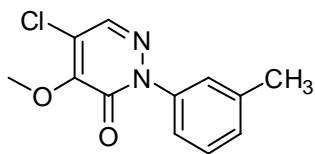
F2 - Processing parameters
SI 65536
SF 125.8080969 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

default proton parameters

7.822
7.379
7.364
7.349
7.329
7.305
7.258
7.228
7.213

4.306

2.408



2-25

10 9 8 7 6 5 4 3 2 1 0 ppm

1.004
3.224
0.998

3.207

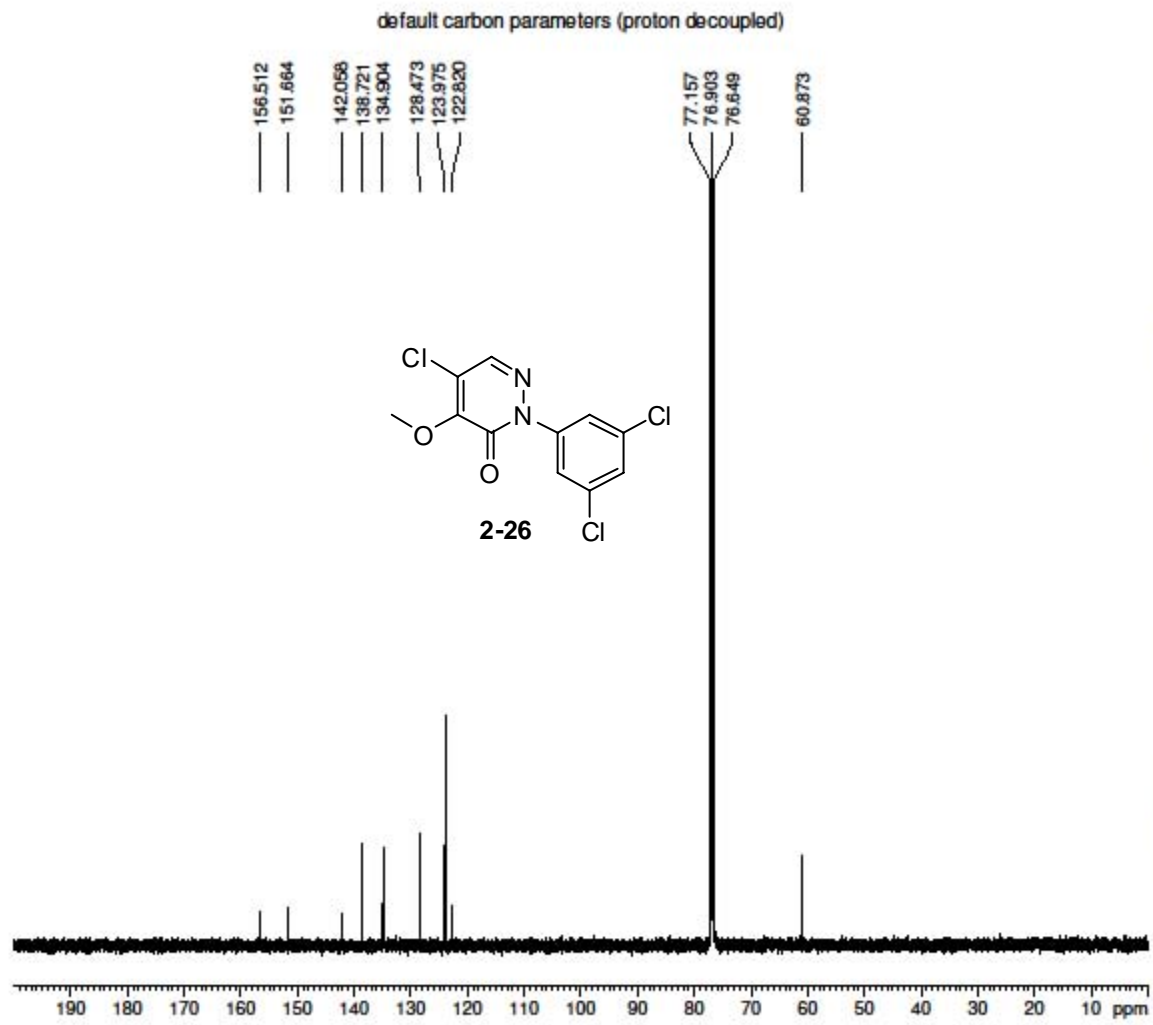
3.266

Current Data Parameters
NAME 3Tolyl_OMe_A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081030
Time 10.25
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6385000 sec
RG 90.5
DW 50.000 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 500.3330020 MHz

F2 - Processing parameters
SI 32768
SF 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME 3,5-Dichloro_OMe_A
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081030
 Time 10.44
 INSTRUM avance500
 PROBHD 5 mm bb-Z 2800
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 496
 DS 0
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 4096
 DW 15.300 usec
 DE 6.00 usec
 TE 295.3 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 5.25 usec
 PL1 0.00 dB
 SFO1 125.8231939 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 105.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SFO2 500.3320013 MHz

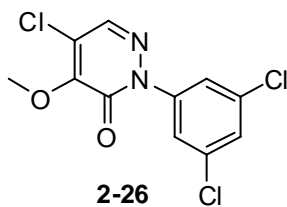
F2 - Processing parameters
 SI 65536
 SF 125.8080969 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

default proton parameters

7.840
7.561
7.557
7.400
7.397
7.384
7.258

4.311

1.554
1.250

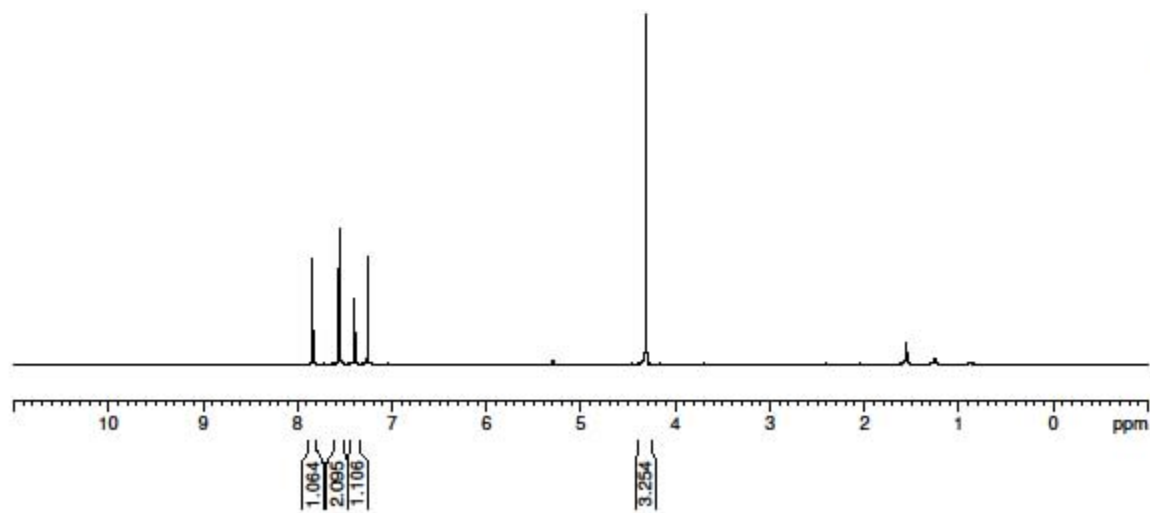


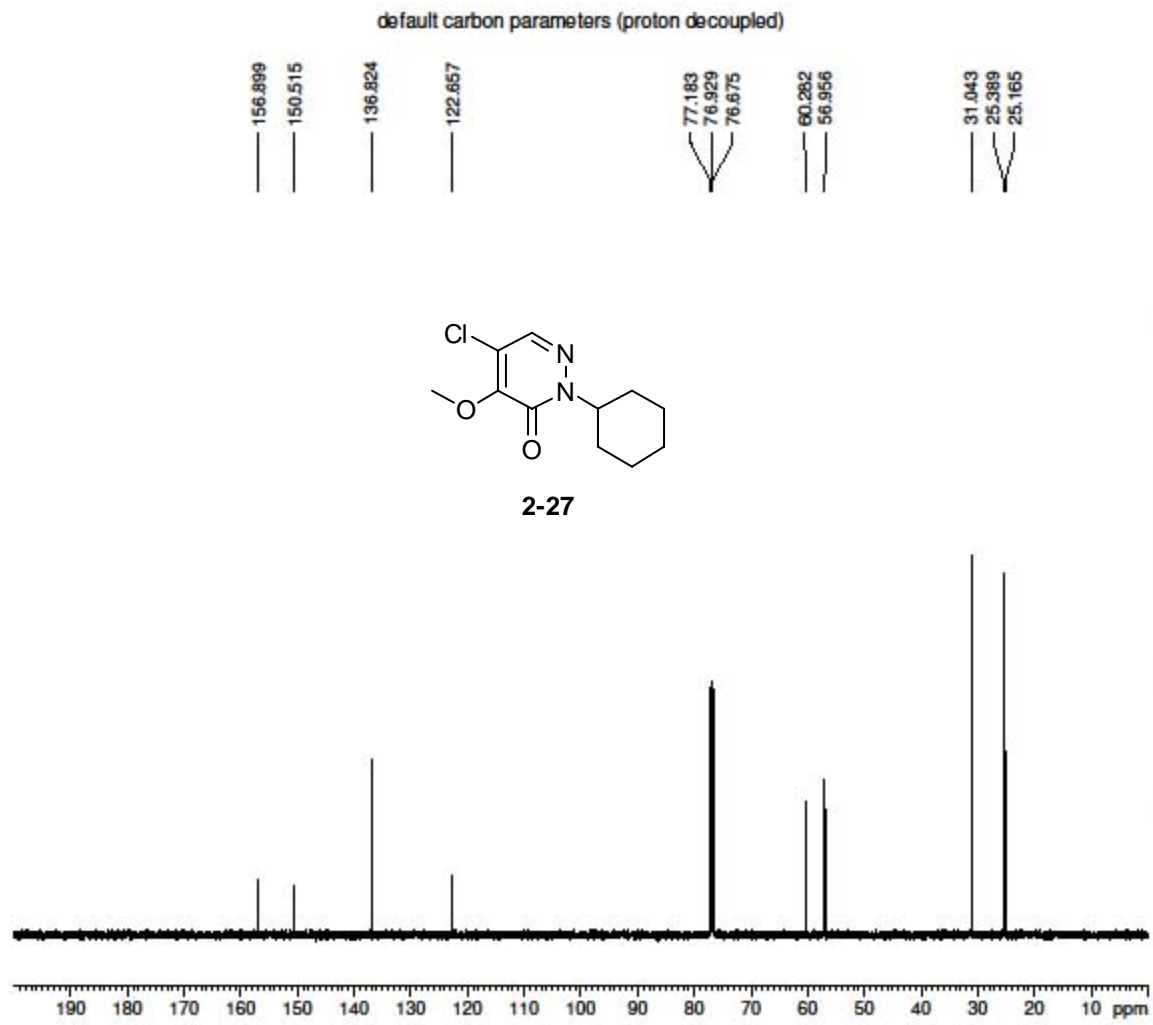
Current Data Parameters
NAME 3,5-Dichloro_OMe_A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081030
Time 10.42
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6385000 sec
RG 181
DW 50.000 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 500.3330020 MHz

F2 - Processing parameters
SI 32768
SF 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





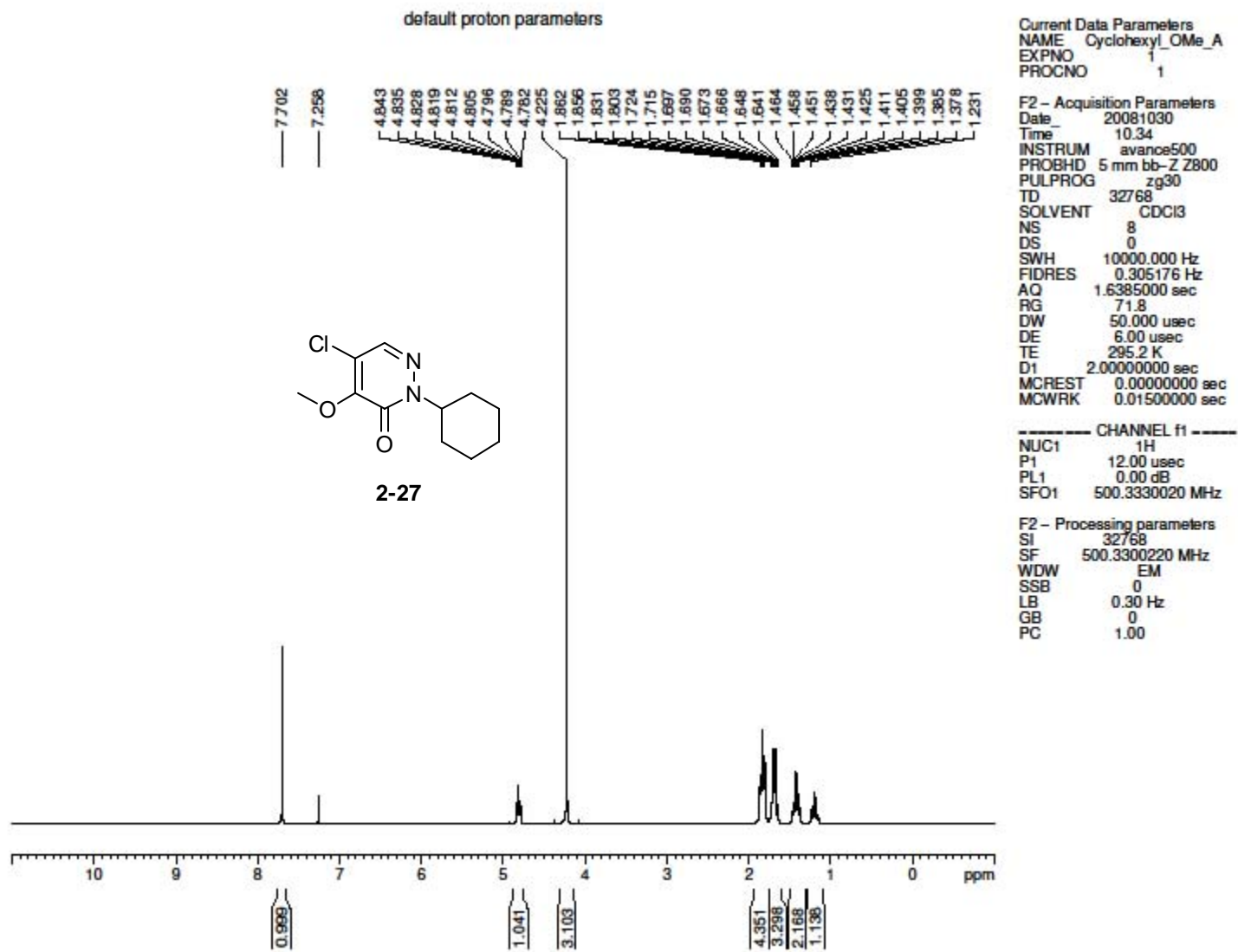
Current Data Parameters
 NAME Cyclohexyl_OMe_A
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081030
 Time 10.37
 INSTRUM avance500
 PROBHD 5 mm bb-Z 2800
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 62
 DS 0
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 4096
 DW 15.300 usec
 DE 6.00 usec
 TE 295.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

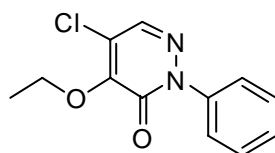
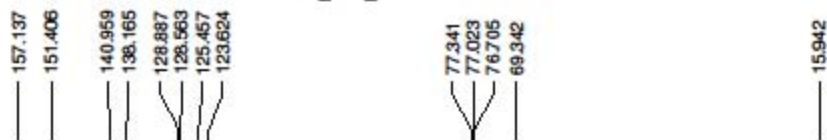
----- CHANNEL f1 -----
 NUC1 13C
 P1 5.25 usec
 PL1 0.00 dB
 SFO1 125.8231939 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 105.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SFO2 500.3320013 MHz

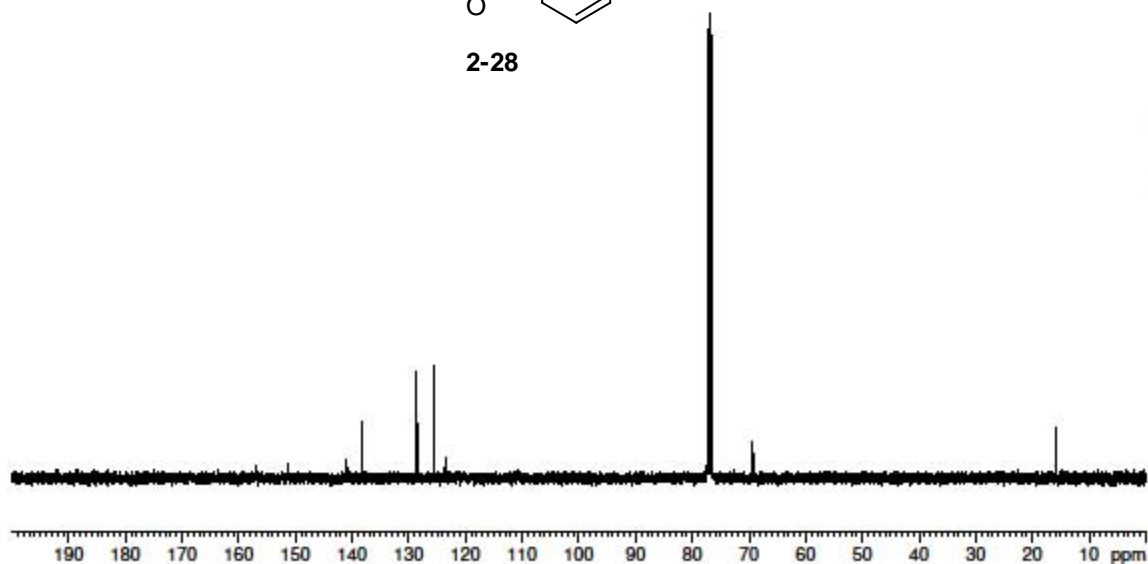
F2 - Processing parameters
 SI 65536
 SF 125.8080969 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Account no. MEJM16
Ph_OEt_A



2-28



Current Data Parameters
NAME 101608
EXPNO 121
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081016
Time 13.07
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

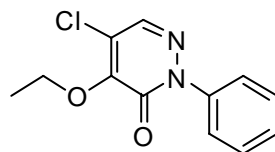
F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Account no. MEJM16
Ph_OEt_A

Current Data Parameters
NAME 101608
EXPNO 120
PROCNO 1

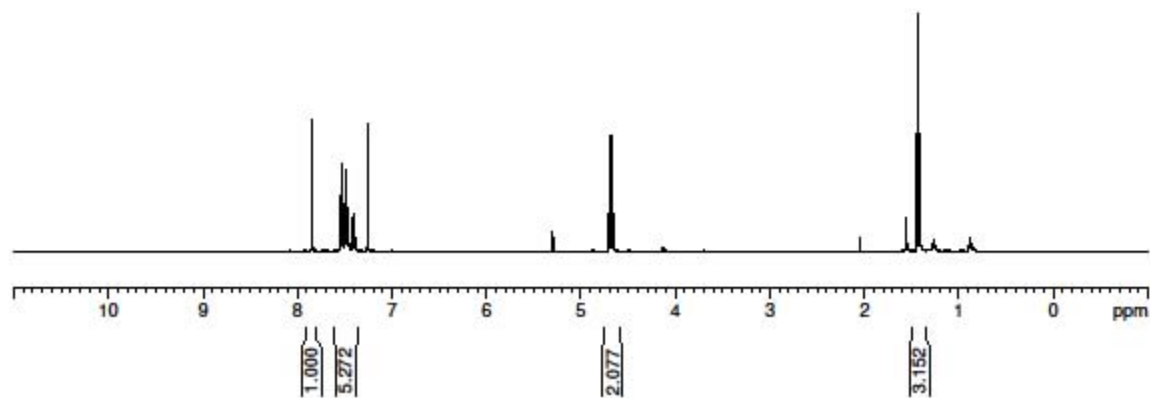


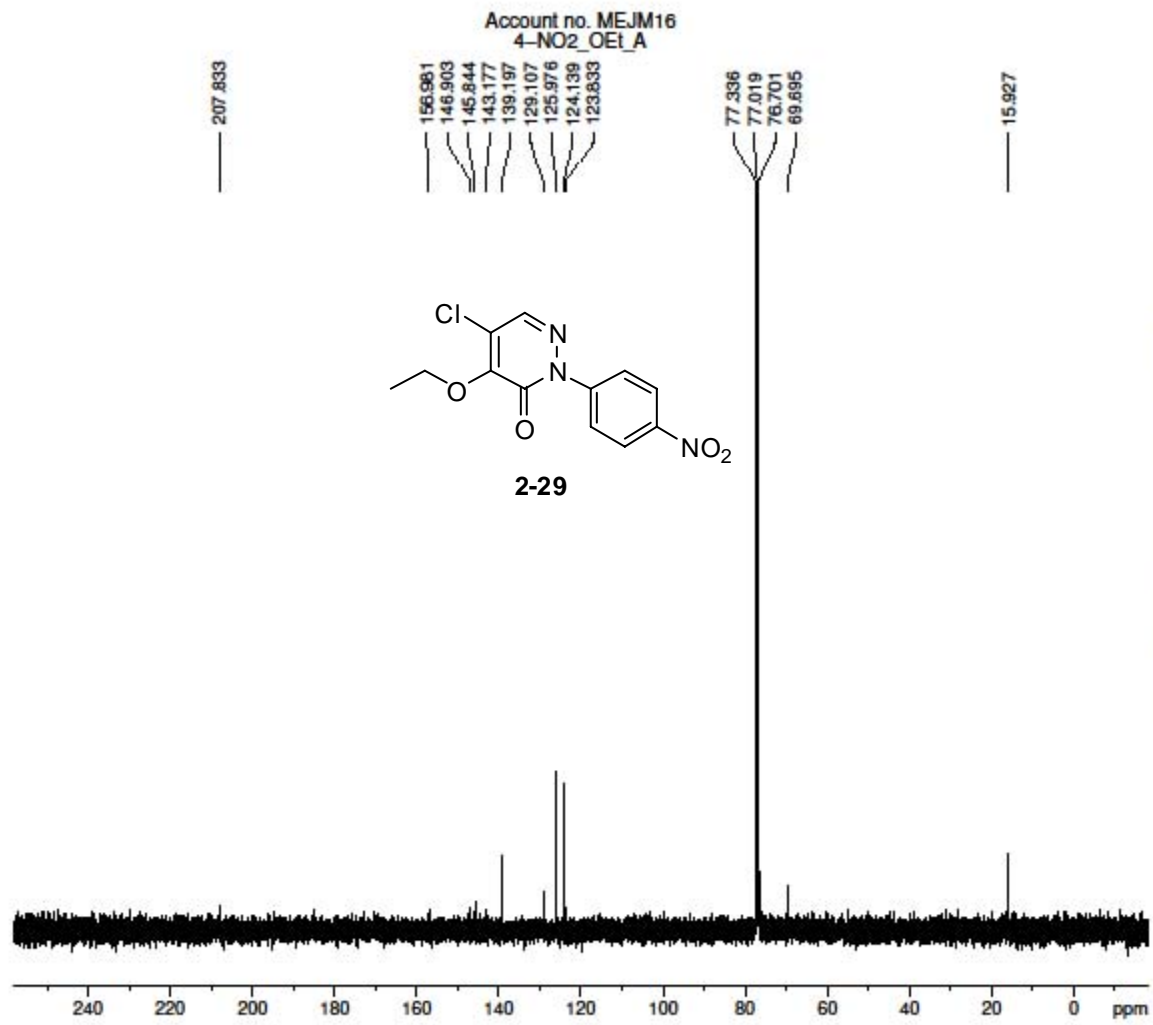
F2 - Acquisition Parameters
Date_ 20081016
Time 12.53
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 2048
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.0000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H



2-28

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



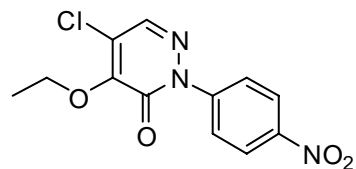
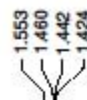


Current Data Parameters
 NAME 102108
 EXPNO 81
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081021
 Time 15.33
 INSTRUM arx400
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 0
 SWH 27777.777 Hz
 FIDRES 0.423855 Hz
 AQ 1.1796980 sec
 RG 32768
 DW 18.000 usec
 DE 25.71 usec
 TE 300.0 K
 D12 0.0000200 sec
 DL5 23.50 dB
 CPDPRG waltz16
 P31 100.00 usec
 D1 2.0000000 sec
 P1 8.25 usec
 SFO1 100.6248445 MHz
 NUCLEUS 13C
 D11 0.0300000 sec

F2 - Processing parameters
 SI 65536
 SF 100.6127710 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Account no. MEJM16
4-NO₂_OEt_A

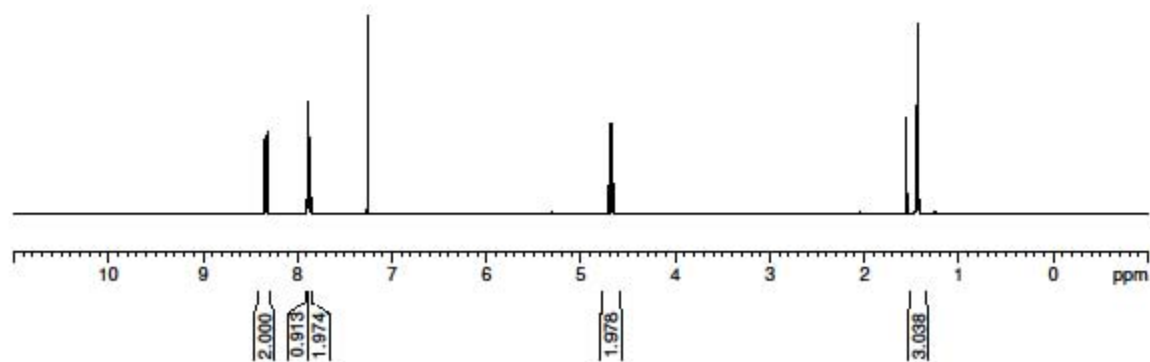


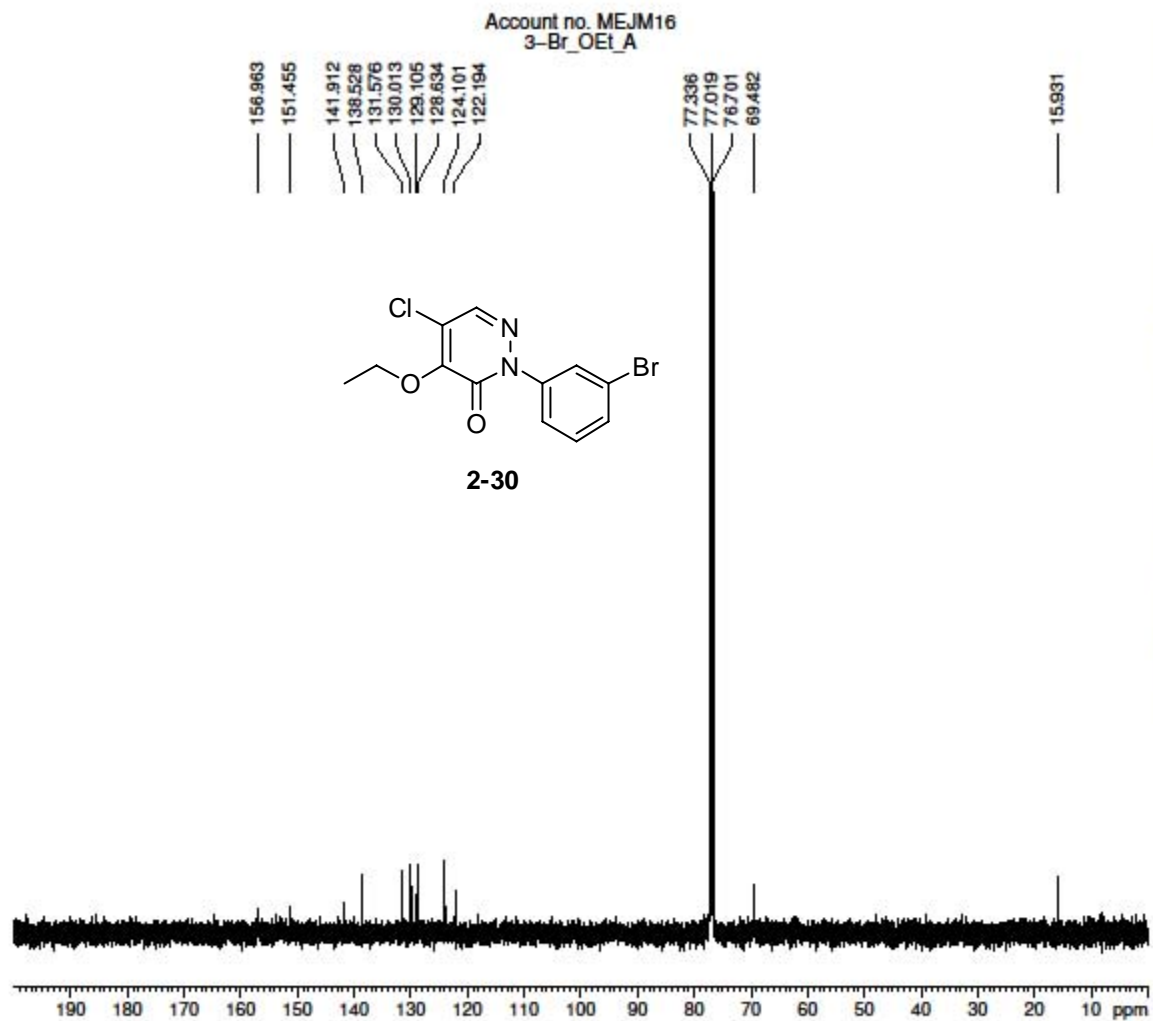
2-29

Current Data Parameters
NAME 102108
EXPNO 80
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081021
Time 15.19
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 8
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 4096
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.0000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





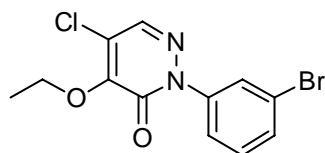
Current Data Parameters
NAME 102108
EXPNO 91
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081021
Time 15.54
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Account no. MEJM16
3-Br_OEt_A

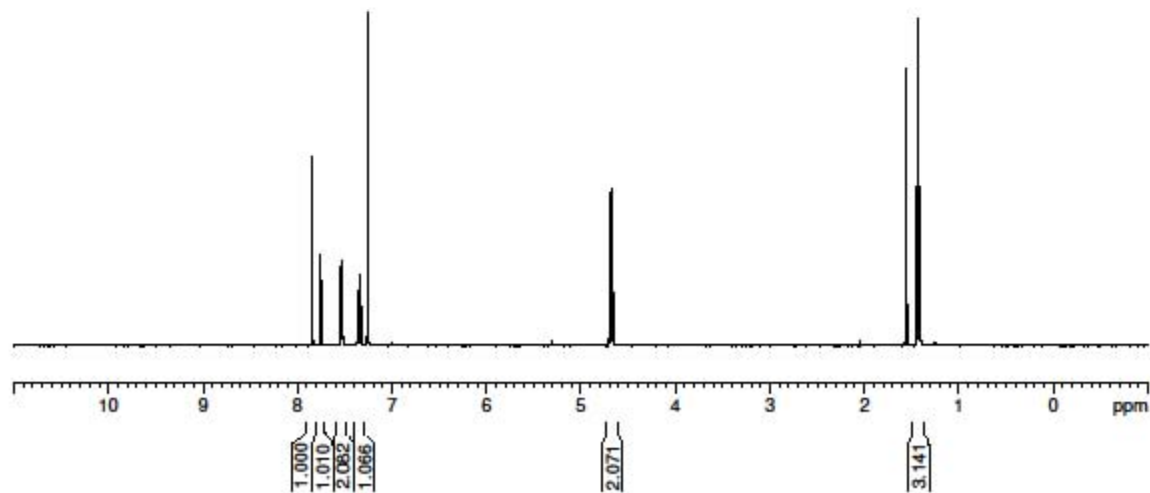
Current Data Parameters
NAME 102108
EXPNO 90
PROCNO 1

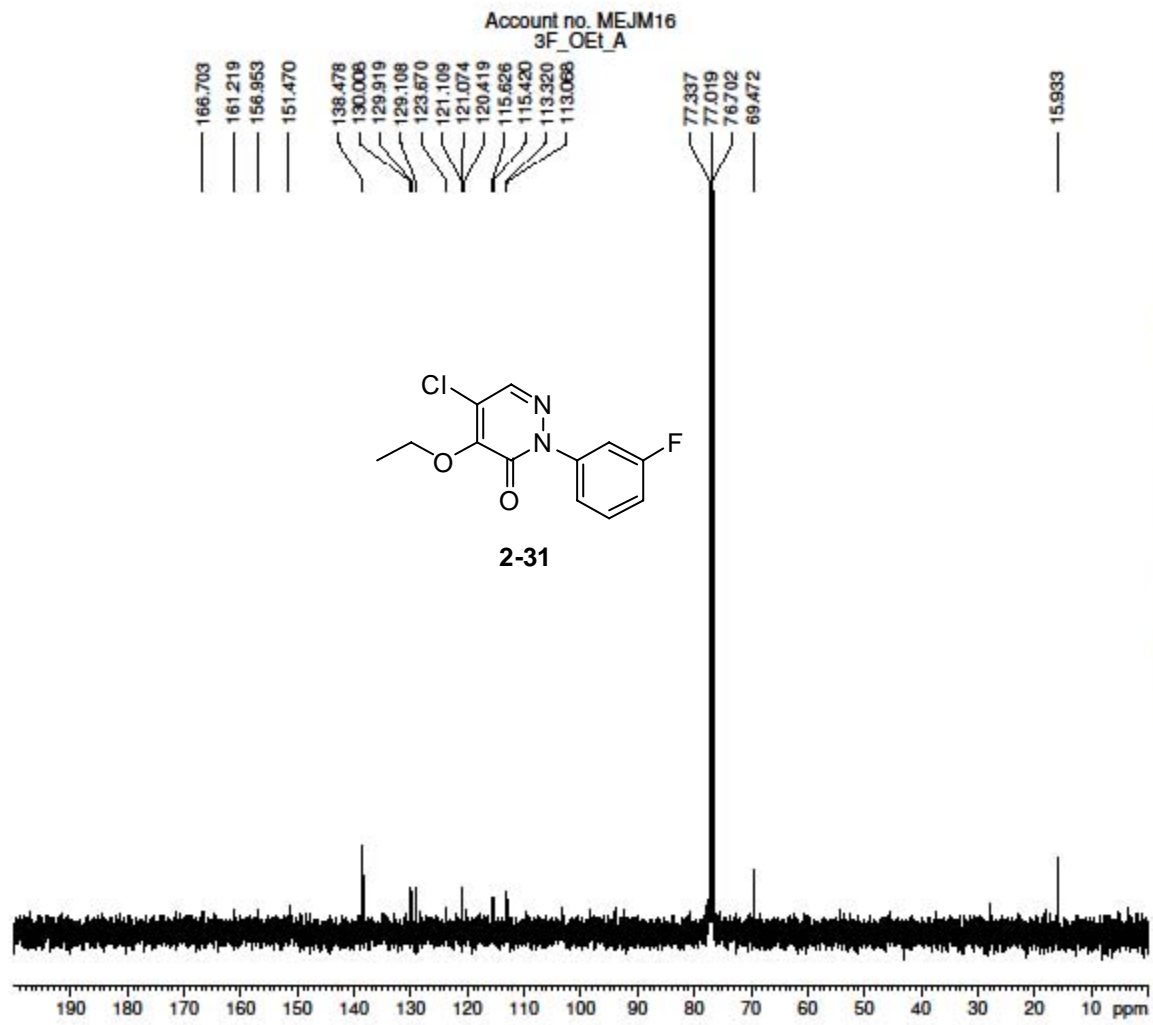


2-30

F2 - Acquisition Parameters
Date_ 20081021
Time 15.40
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 4096
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.0000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



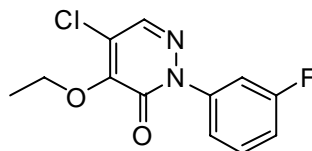


Current Data Parameters
NAME 102108
EXPNO 301
PROCNO 1

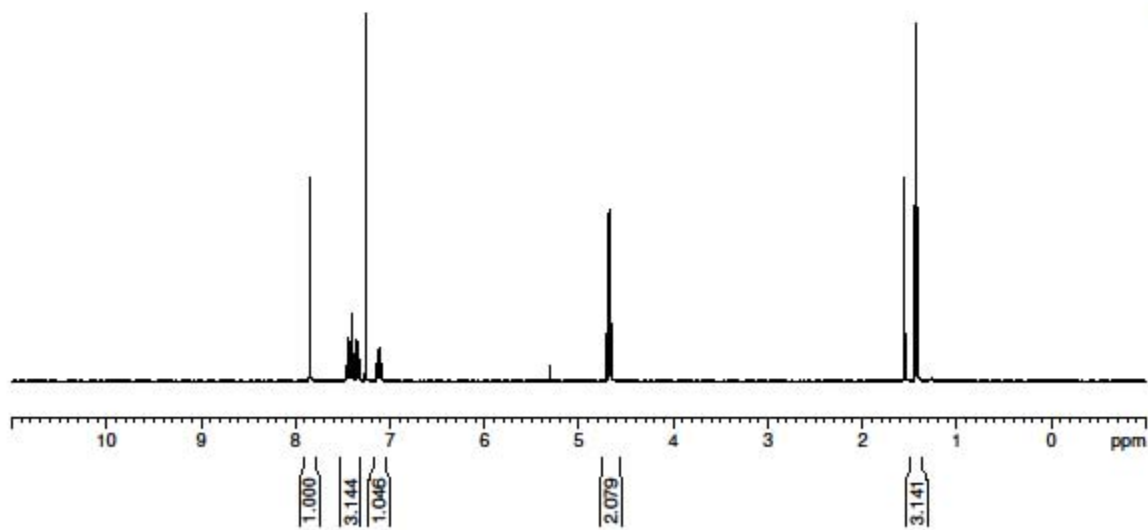
F2 - Acquisition Parameters
Date_ 20081020
Time 23.53
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Account no. MEJM16
3F_OEt_A



2-31



Current Data Parameters
NAME 102108
EXPNO 300
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081020
Time 23.39
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 4096
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

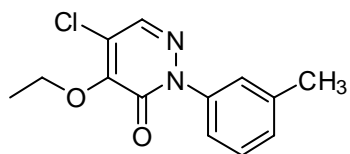
F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDB EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Account no. MEJM16
3Toly_OEt_A

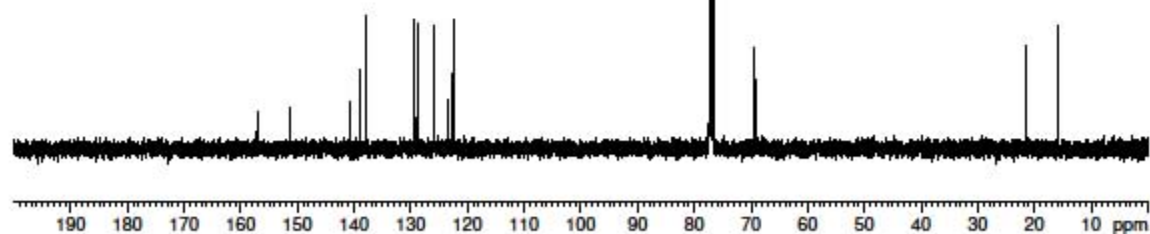
157.149
151.366
140.881
139.011
138.043
129.418
129.101
128.742
126.095
123.595
122.573

77.349
77.031
76.713
69.315

21.377
15.943



2-32



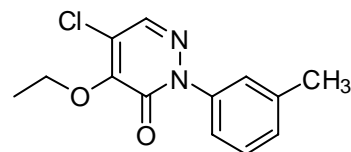
Current Data Parameters
NAME 102108
EXPNO 311
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081021
Time 0.14
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Account no. MEJM16
3Toly_OEL_A

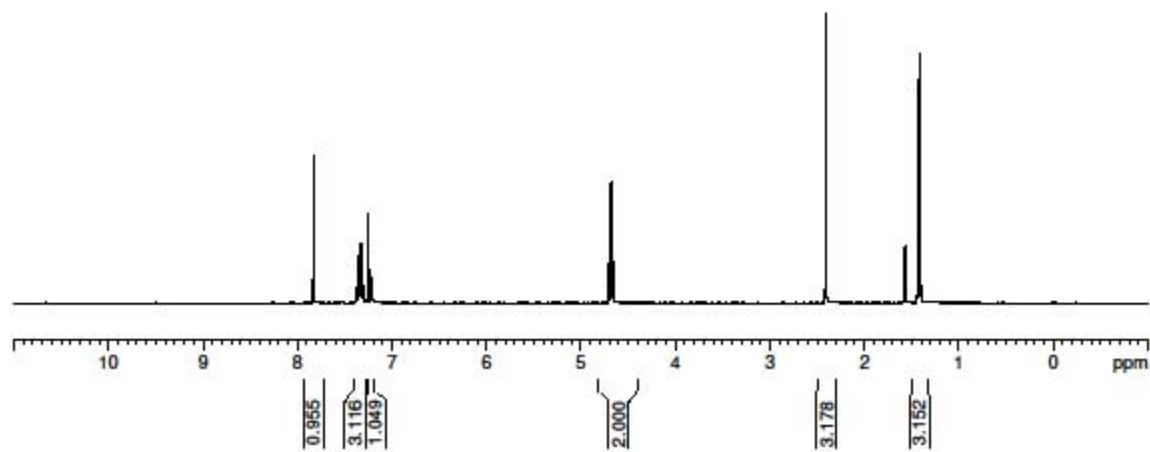
Current Data Parameters
NAME 102108
EXPNO 310
PROCNO 1



2-32

F2 - Acquisition Parameters
Date_ 20081021
Time 0.00
INSTRUM anx400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 2048
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

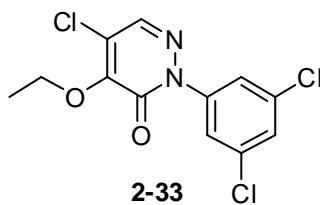


Account no. MEJM16
3,5-dichloro_OEt_A

163.740
156.797
151.436
142.258
138.848
136.000
129.100
128.540
124.065
123.740

77.339
77.022
76.704
69.606

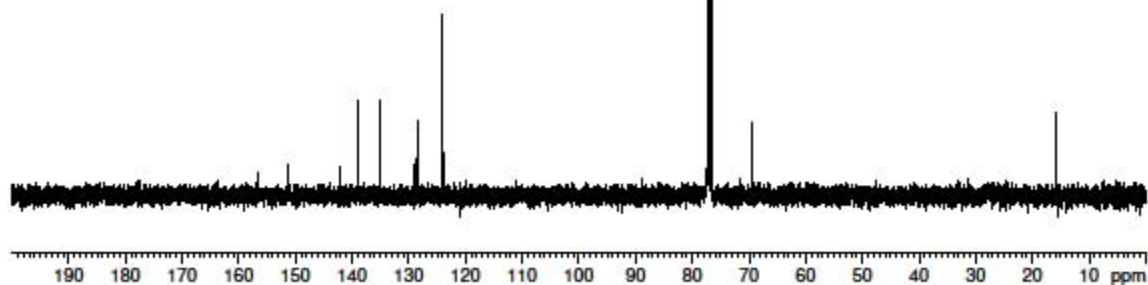
15.922



Current Data Parameters
NAME 102108
EXPNO 331
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081021
Time 0.56
INSTRUM anx400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



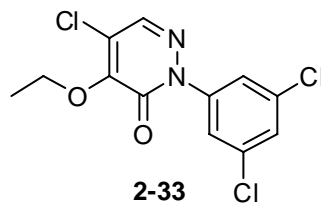
Account no. MEJM16
3,5-dichloro_OEt_A

Current Data Parameters
NAME 102108
EXPNO 330
PROCNO 1

7.849
7.568
7.563
7.394
7.261

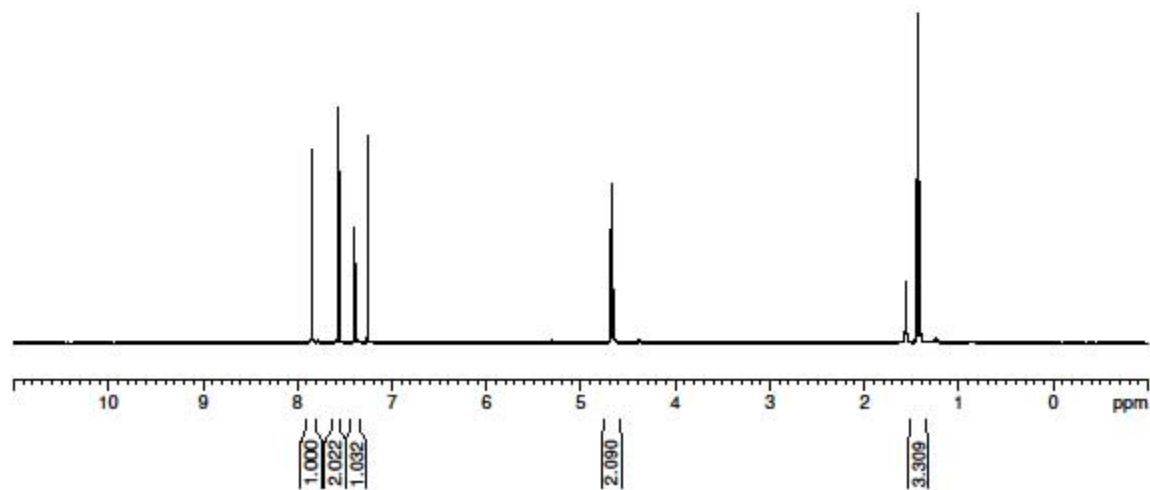
4.681
4.664

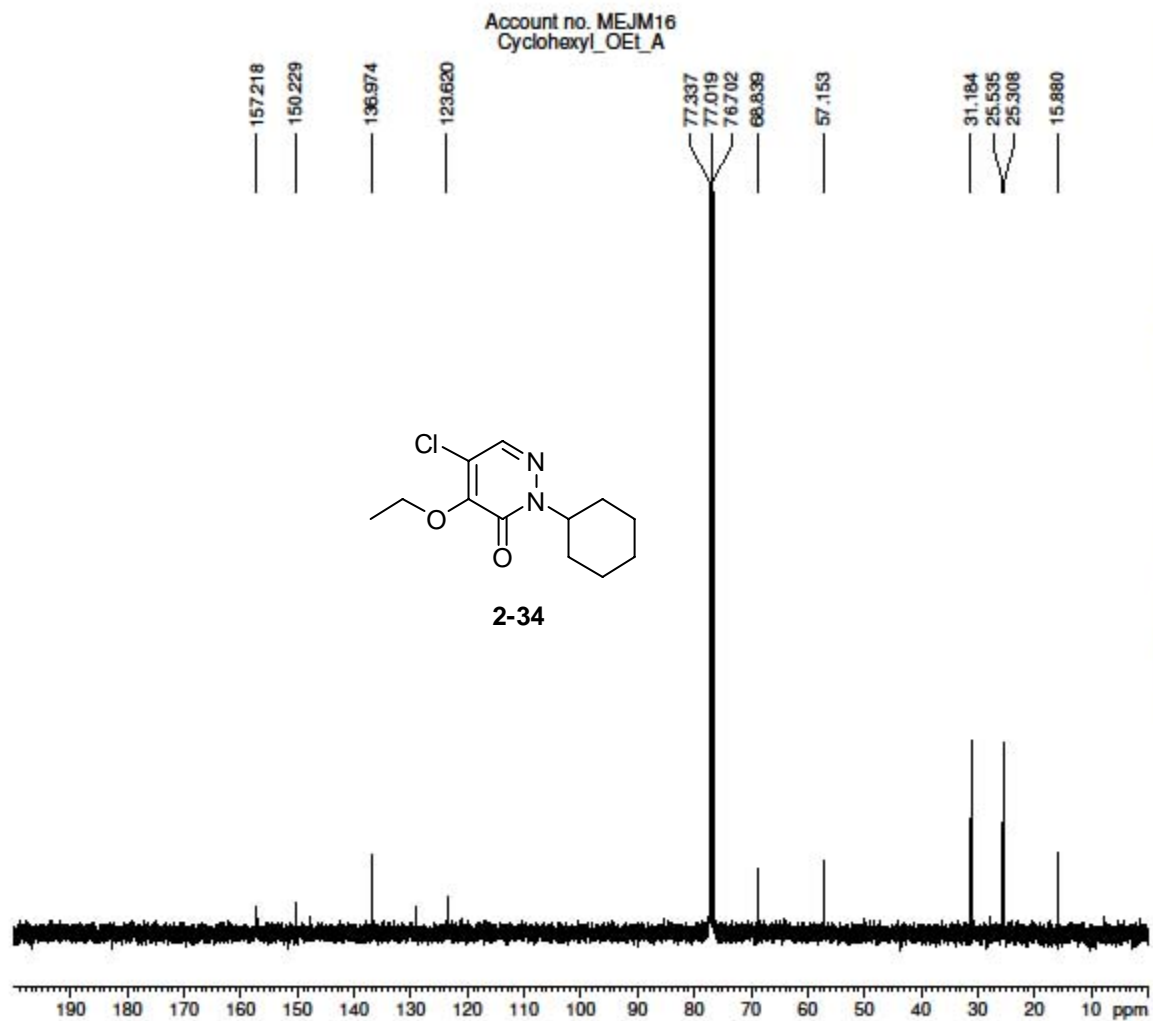
1.446
1.429
1.411



F2 - Acquisition Parameters
Date_ 20081021
Time 0.42
INSTRUM anx400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 2860
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





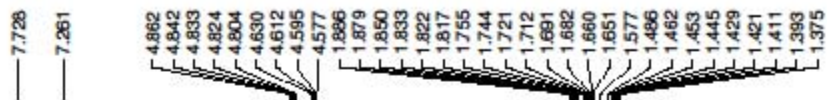
Current Data Parameters
NAME 102108
EXPNO 321
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081021
Time 0.35
INSTRUM anx400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

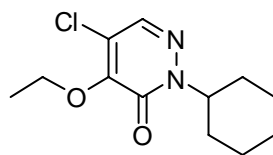
F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Account no. MEJM16
Cyclohexyl_OEt_A

Current Data Parameters
NAME 102108
EXPNO 320
PROCNO 1

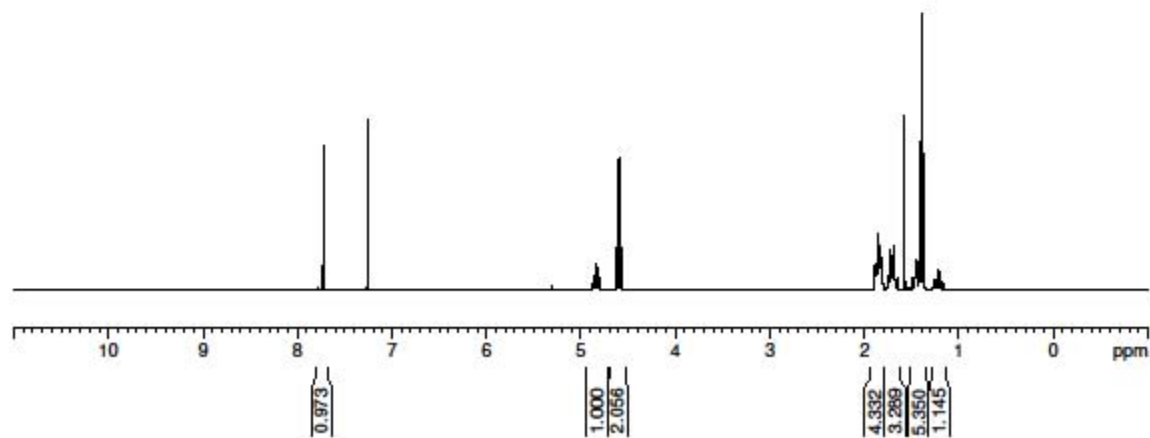


F2 - Acquisition Parameters
Date_ 20081021
Time 0.21
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 2048
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

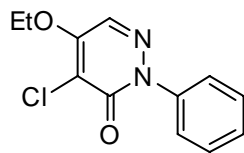
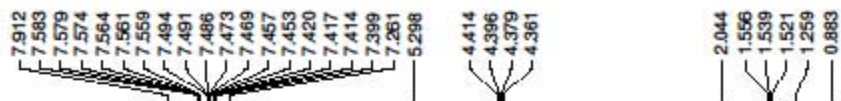


2-34

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Account no. MEJM16
Ph_OEt_B

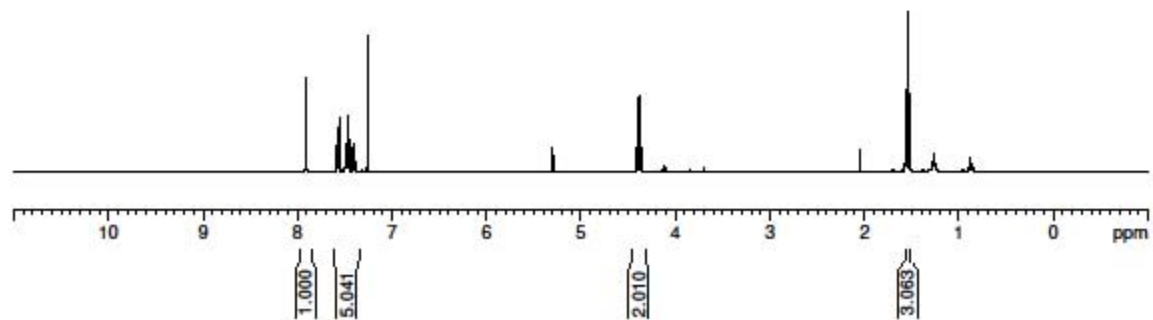


2-35

Current Data Parameters
NAME 101608
EXPNO 130
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081016
Time 13.14
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 2860
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Account no. MEJM16
4-NO2_OET_B

Current Data Parameters
NAME 102208
EXPNO 370
PROCNO 1

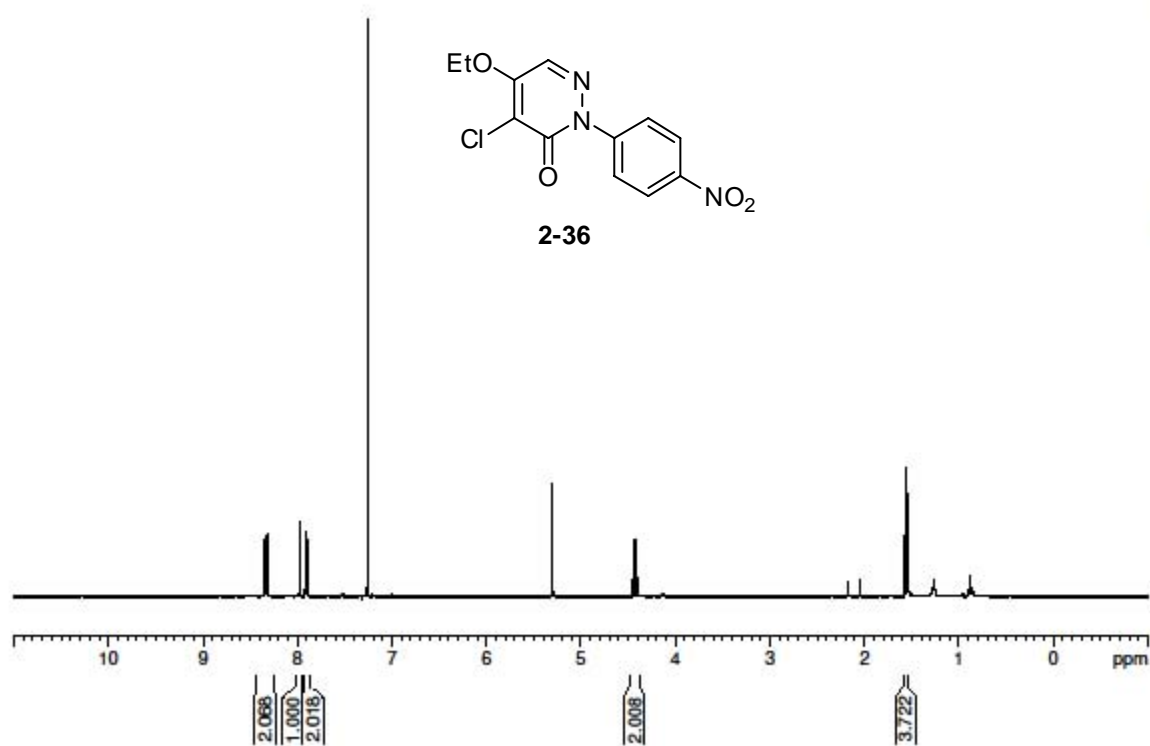
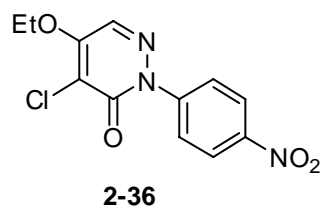
8.347
8.324
7.980
7.917
7.894
7.261

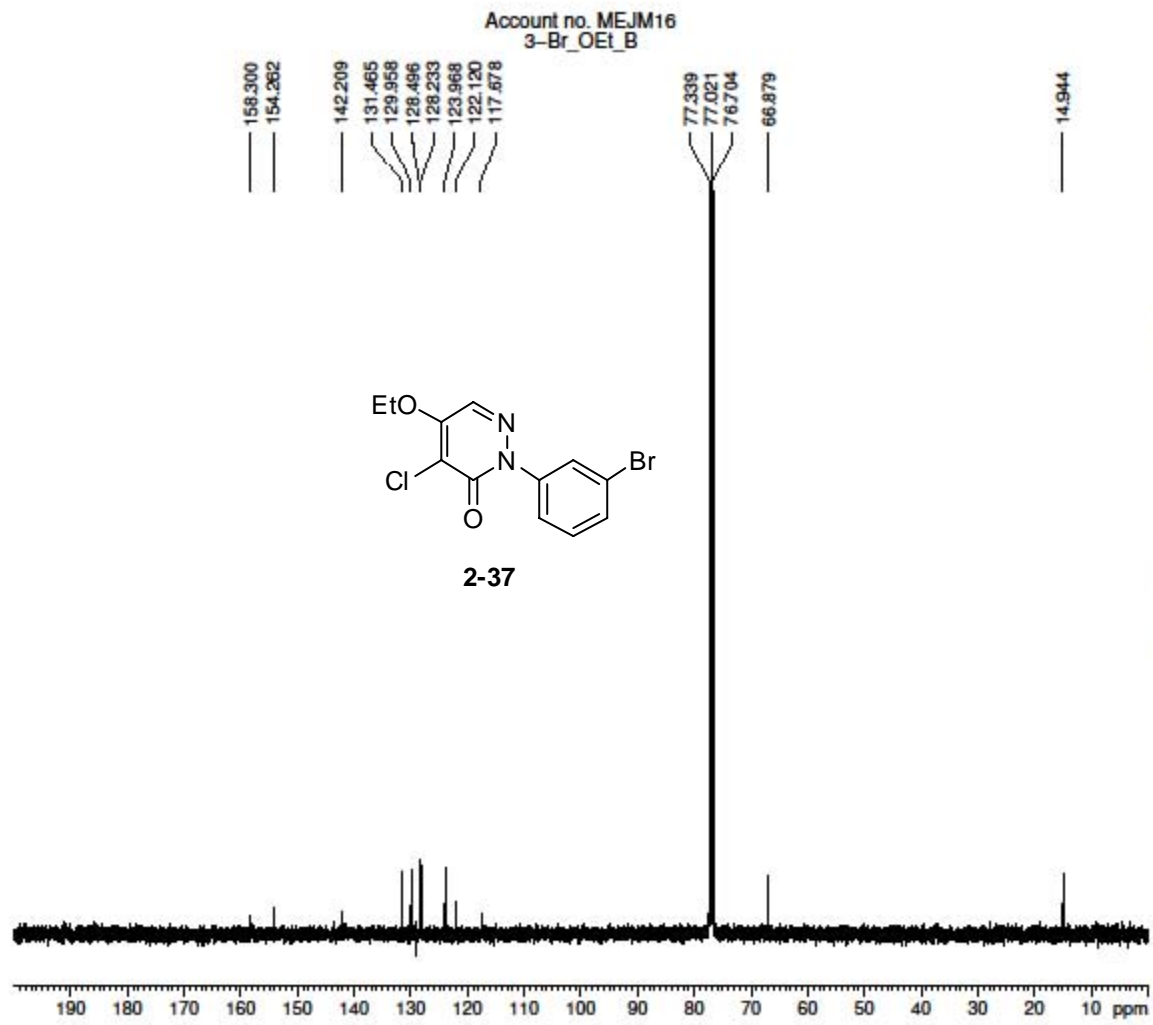
5.300
4.435
4.417

1.575
1.558
1.544
1.540
0.883

F2 - Acquisition Parameters
Date_ 20081022
Time 18.37
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 11400
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.0000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



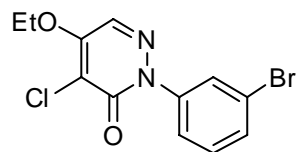
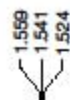


Current Data Parameters
NAME 102208
EXPNO 381
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081022
Time 19.42
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Account no. MEJM16
3-Br_OEt_B

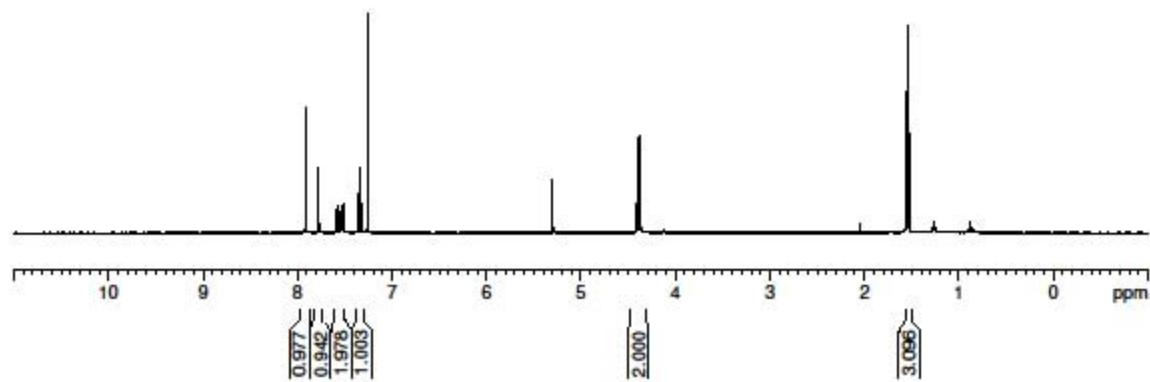


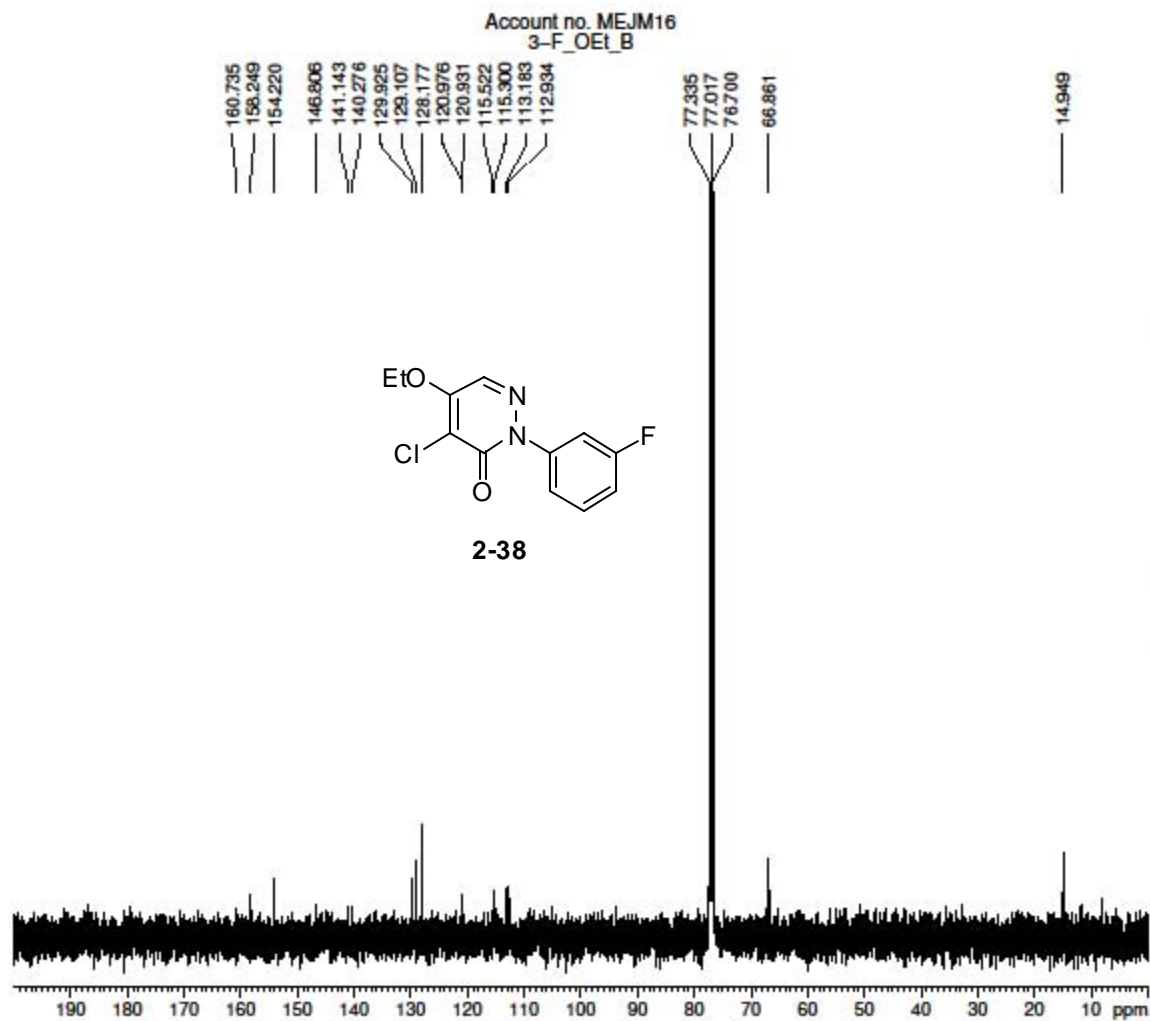
2-37

Current Data Parameters
NAME 102208
EXPNO 380
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081022
Time 19.14
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 4096
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



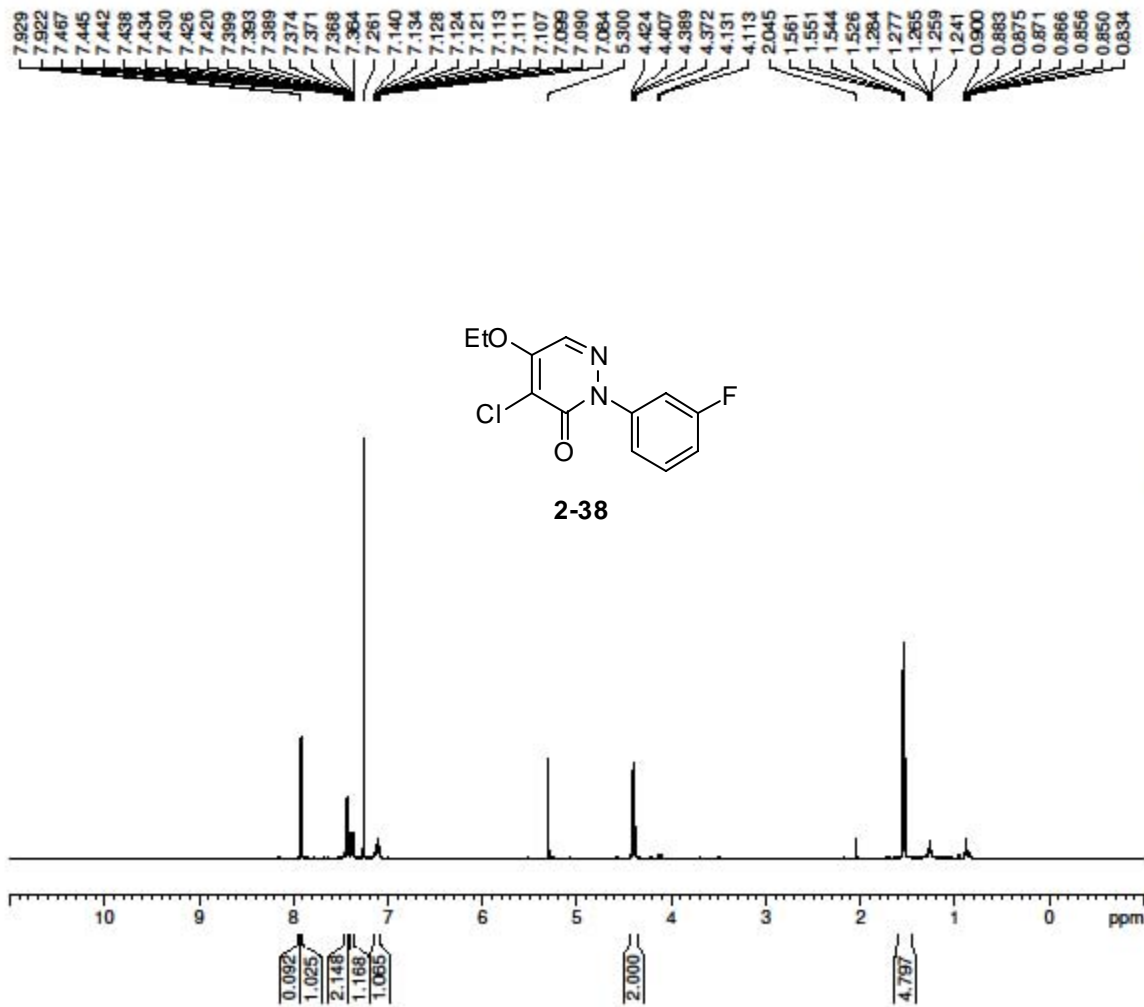


Current Data Parameters
NAME 102208
EXPNO 391
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081022
Time 20.19
INSTRUM anx400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Account no. MEJM16
3-F_OEt_B

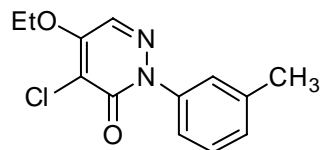
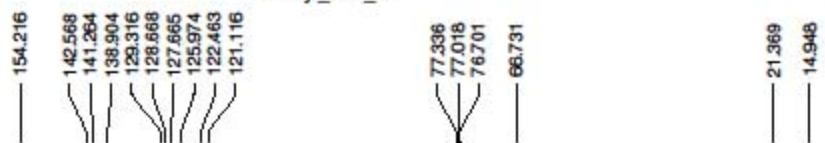


Current Data Parameters
NAME 102208
EXPNO 390
PROCNO 1

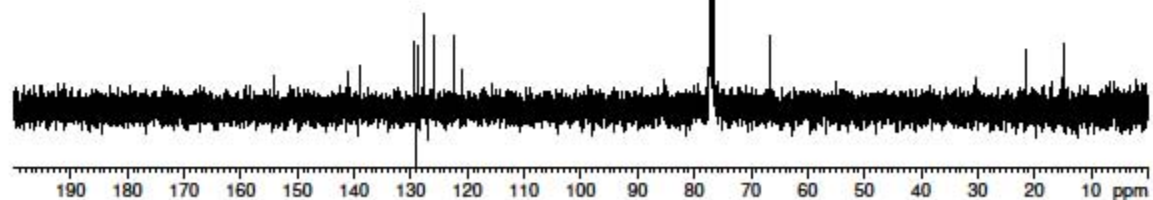
F2 - Acquisition Parameters
Date_ 20081022
Time 19.51
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 5700
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Account no. MEJM16
3Tolyl_OEt_B



2-39



Current Data Parameters
NAME 102208
EXPNO 401
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081022
Time 20.55
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

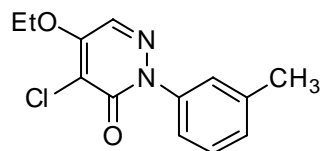
F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Account no. MEJM16
3Tolyl_OEL_B

Current Data Parameters
NAME 102208
EXPNO 400
PROCNO 1

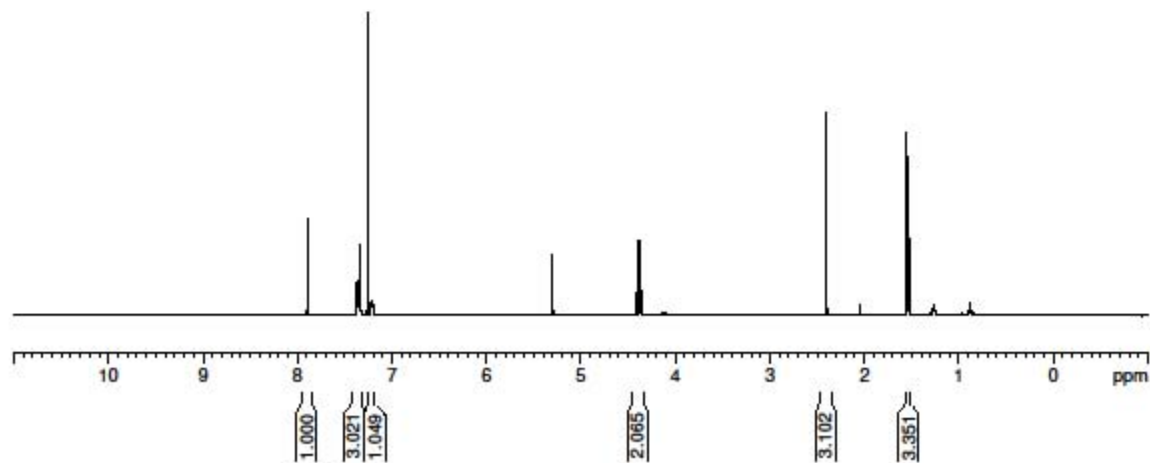


F2 - Acquisition Parameters
Date_ 20081022
Time 20.27
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 5700
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H



2-39

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

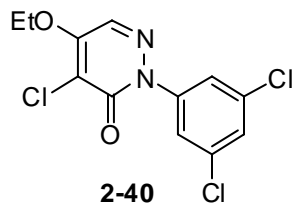


Account no. MEJM16
3,5-DiCl_OEL_B_re

7.923
7.605
7.601
7.391
7.387
7.382
7.260

5.299
4.428
4.411
4.393
4.376

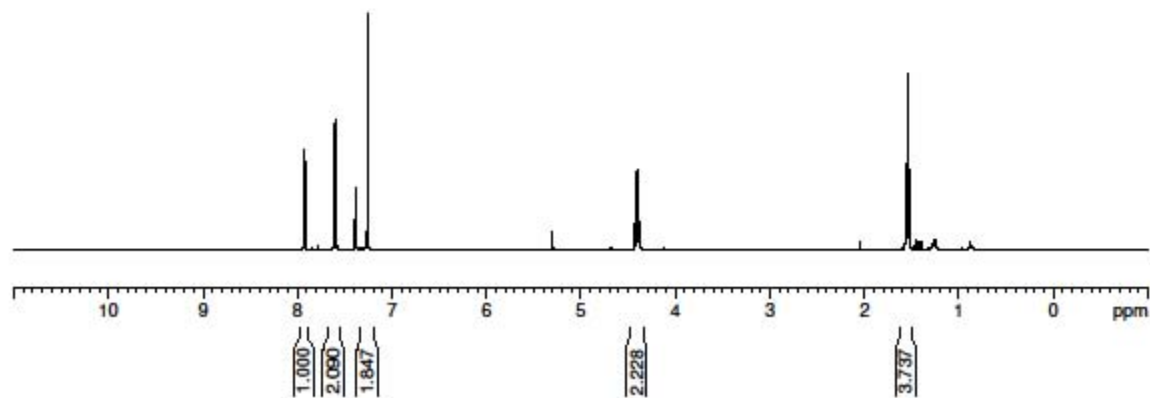
1.562
1.544
1.527



Current Data Parameters
NAME 102308
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081023
Time 10.02
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 5700
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Account no. MEJM16
Cyclohexyl_OMe_1

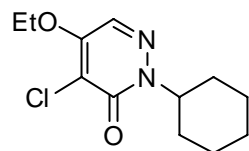
158.401
154.284

125.592
116.309

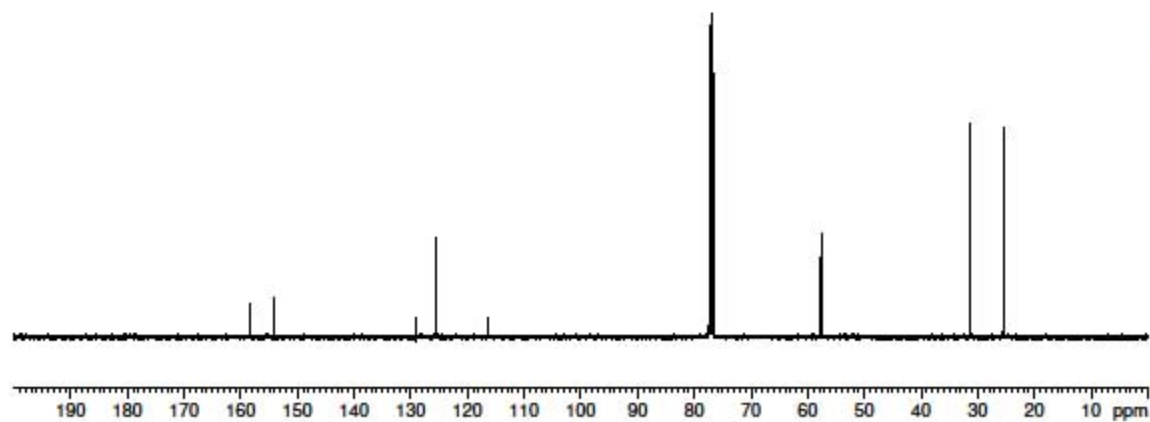
77.354
77.087
76.719

57.907
57.469

31.286
25.478
25.326



2-41



Current Data Parameters
NAME 091808
EXPNO 531
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080919
Time 2.15
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

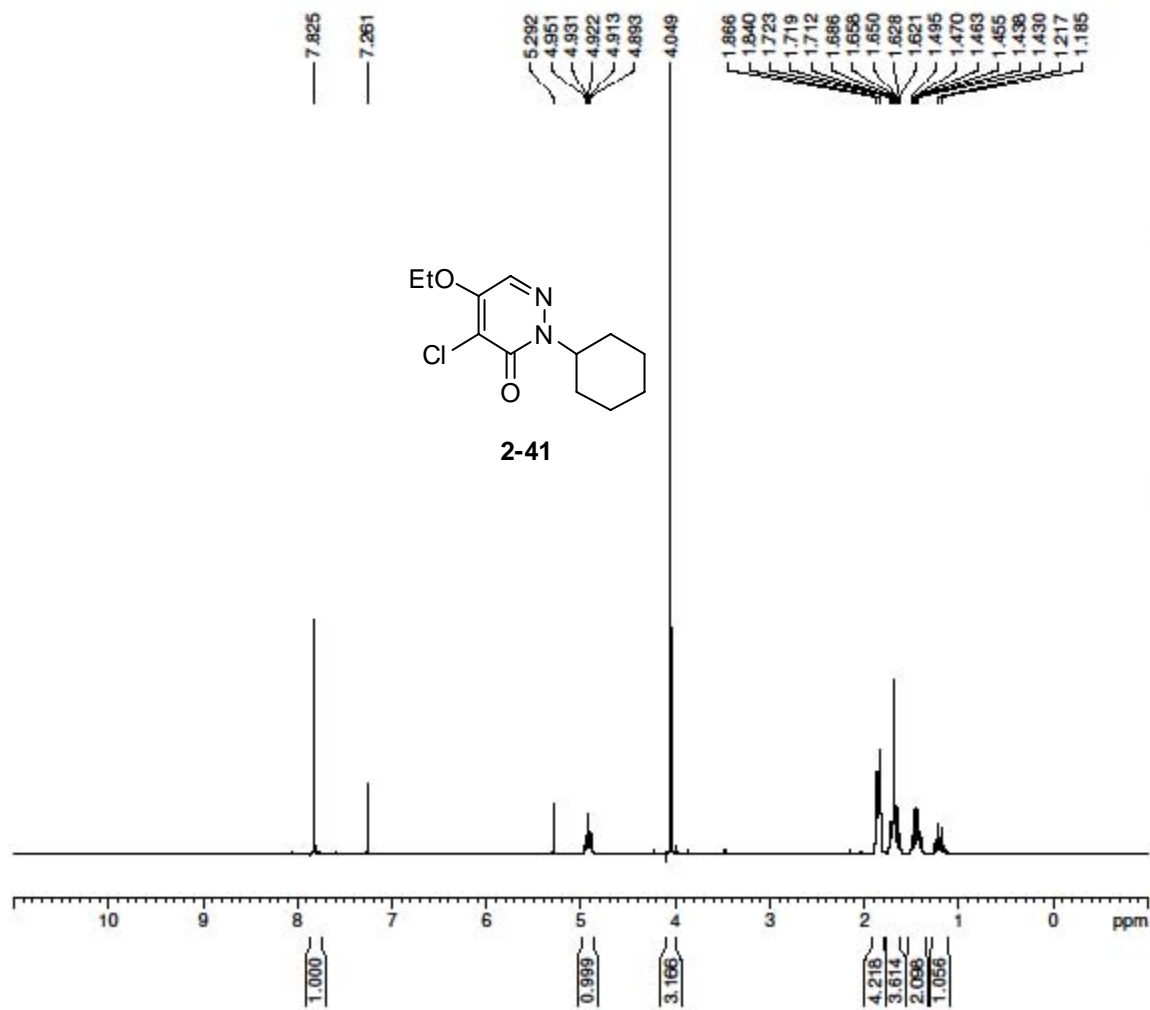
F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Account no. MEJM16
Cyclohexyl_OMe_1

Current Data Parameters
NAME 091808
EXPNO 530
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080919
Time 1.38
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 1024
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

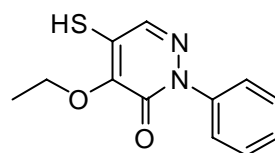


Account no. MEJM16
Ph_OEt_SH_Woogie_re

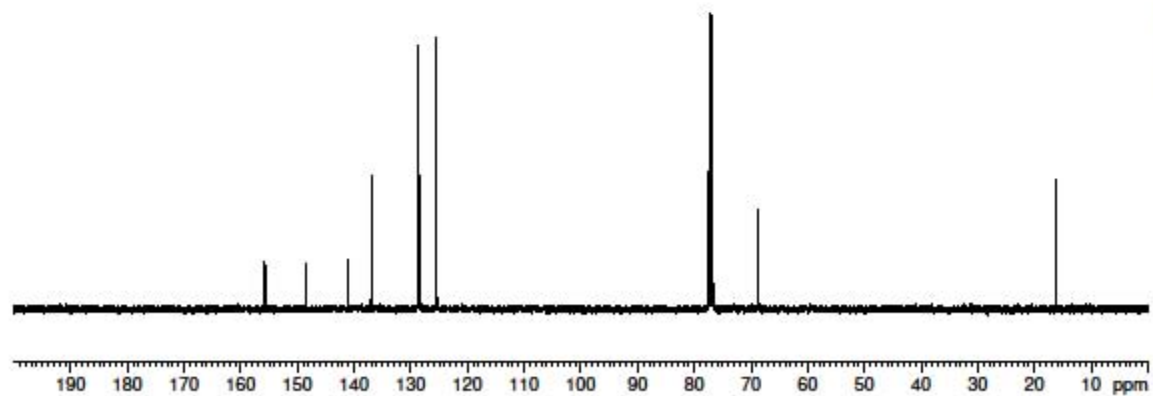
155.755
148.544
141.164
137.017
128.796
128.301
125.506
125.467

77.390
77.072
76.754
68.727

16.116



2-10

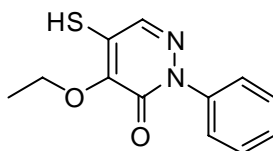
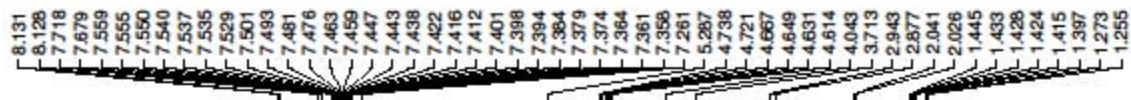


Current Data Parameters
NAME 101608
EXPNO 621
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081017
Time 0.42
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Account no. MEJM16
Ph_OEt_SH_Woogie_re

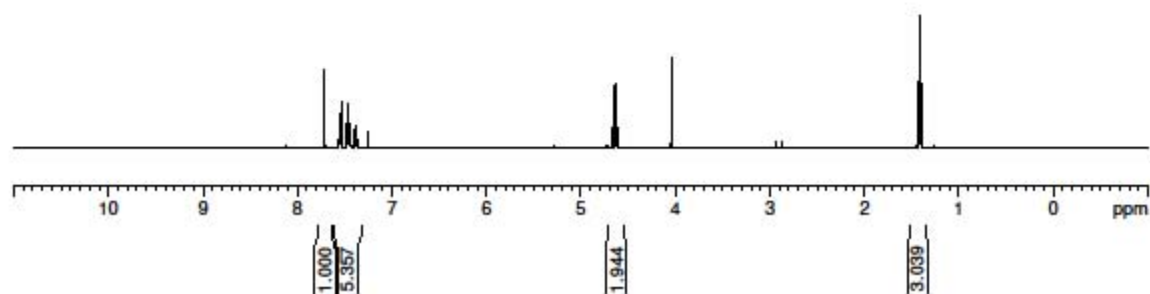


2-10

Current Data Parameters
NAME 101608
EXPNO 620
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081017
Time 0.28
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 512
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

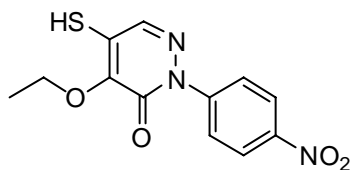


default proton parameters

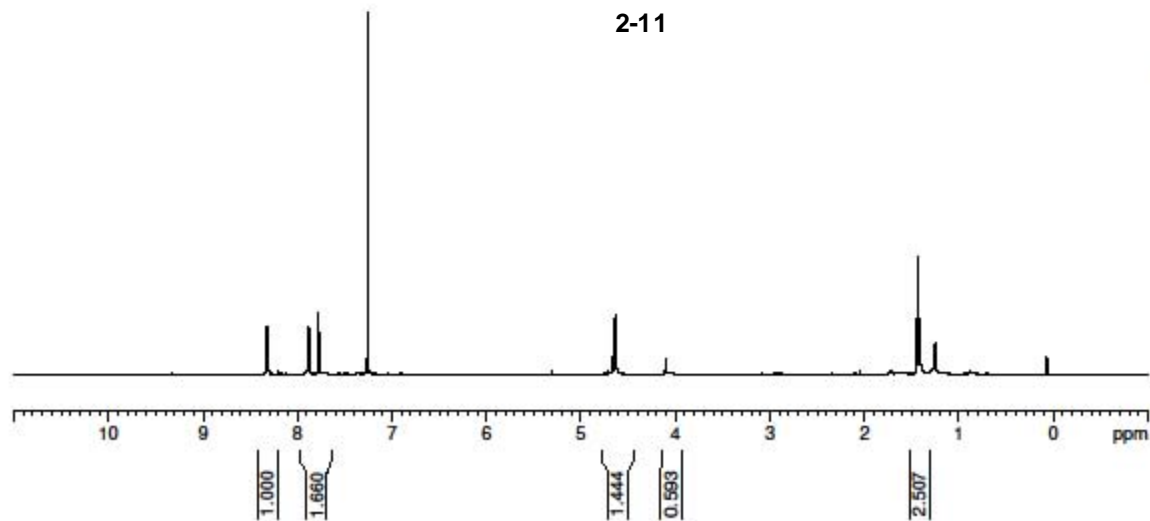
8.329
8.325
8.315
8.311
7.893
7.888
7.878
7.874
7.775
7.260

4.665
4.651
4.636
4.622
4.103

1.450
1.440
1.436
1.430
1.426
1.414
1.251
0.068



2-11

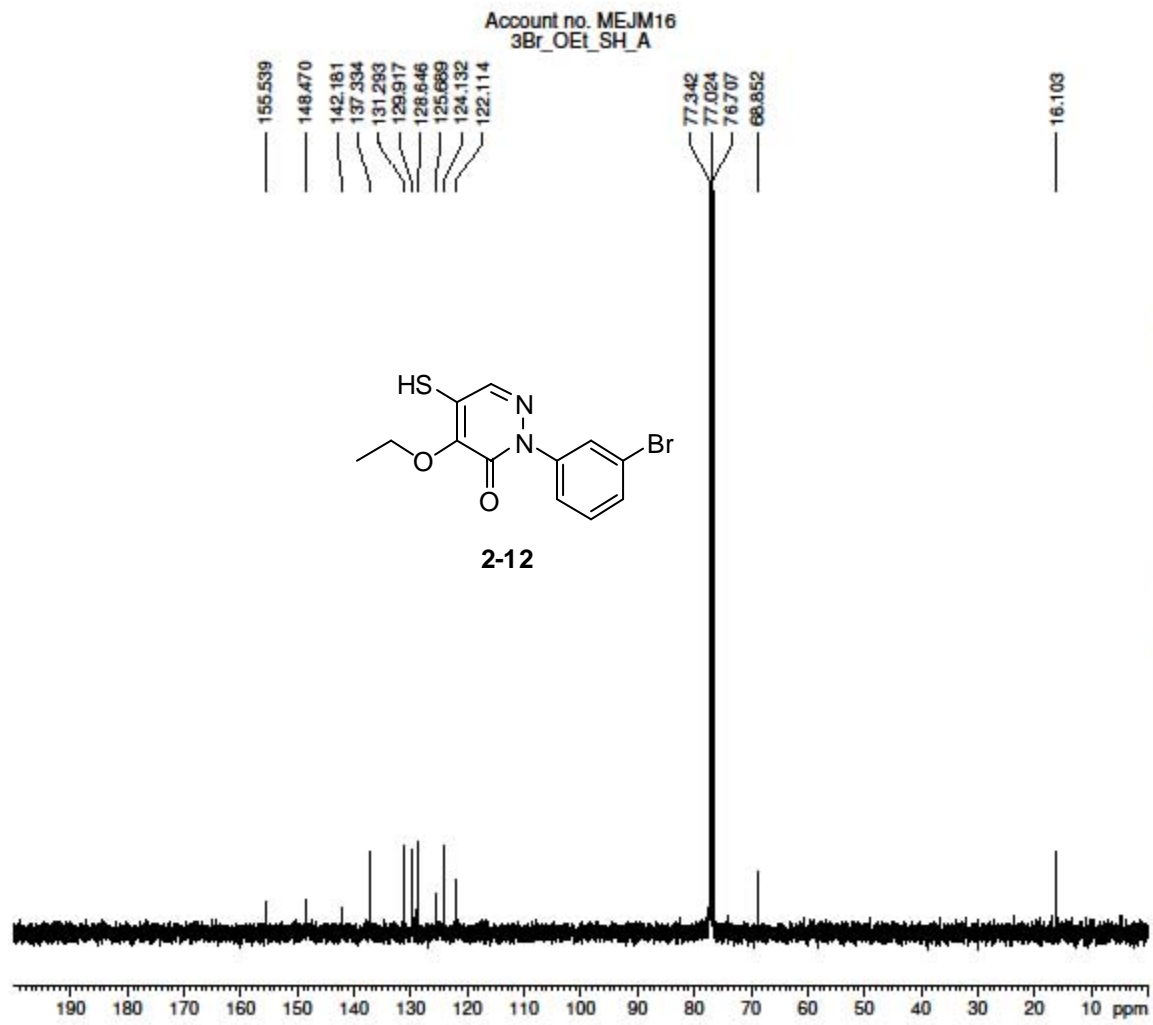


Current Data Parameters
NAME 4NO2_OEt_SH_A_re
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081024
Time 8.06
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6385000 sec
RG 322.5
DW 50.000 usec
DE 6.00 usec
TE 295.6 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 500.3330020 MHz

F2 - Processing parameters
SI 32768
SF 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 102408
EXPNO 70
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081024
Time 10.16
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

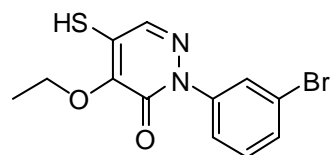
F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Account no. MEJM16
3Br_OEt_SH_A



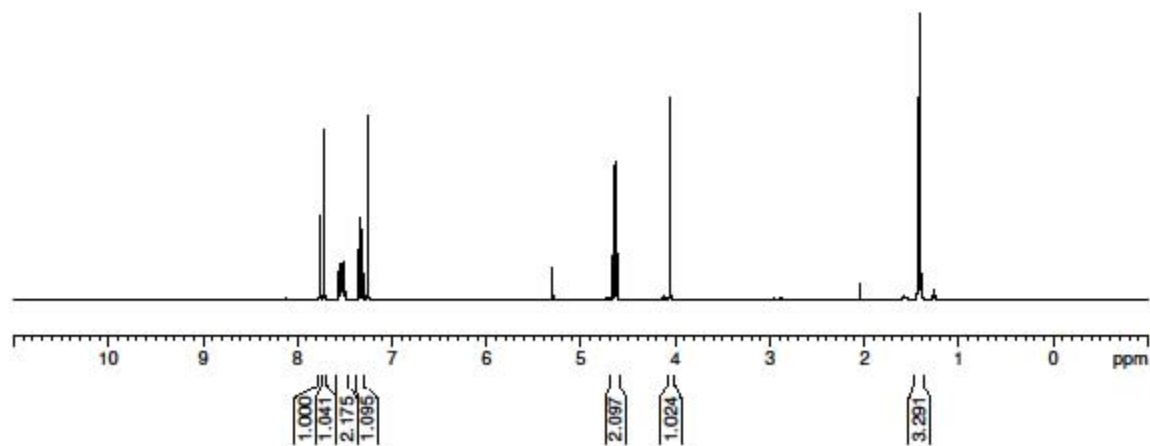
Current Data Parameters
NAME 102308
EXPNO 270
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081023
Time 18.34
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 2048
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

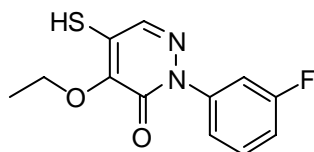


2-12

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Account no. MEJM16
3F_OEL_SH_A



2-13

Current Data Parameters
NAME 102308
EXPNO 290
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081023
Time 19.16
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

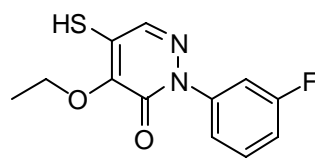
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Account no. MEJM16
3F_OEL_SH_A

7.724
7.415
7.410
7.406
7.403
7.261

4.666
4.648
4.631
4.613
4.057

1.440
1.422
1.405

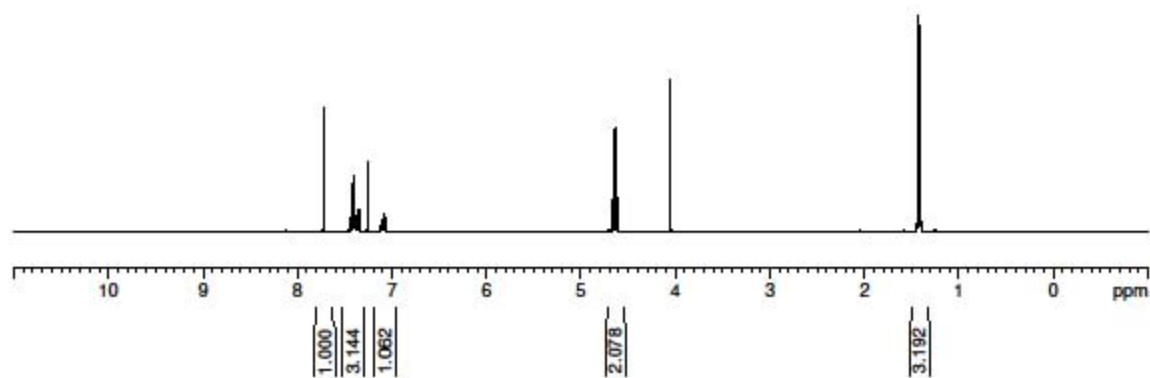


2-13

Current Data Parameters
NAME 102308
EXPNO 240
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081023
Time 17.39
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 2048
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

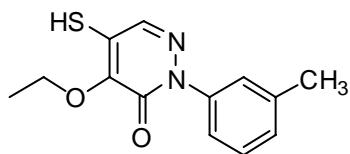


Account no. MEJM16
3Tolyl_OEt_SH_A

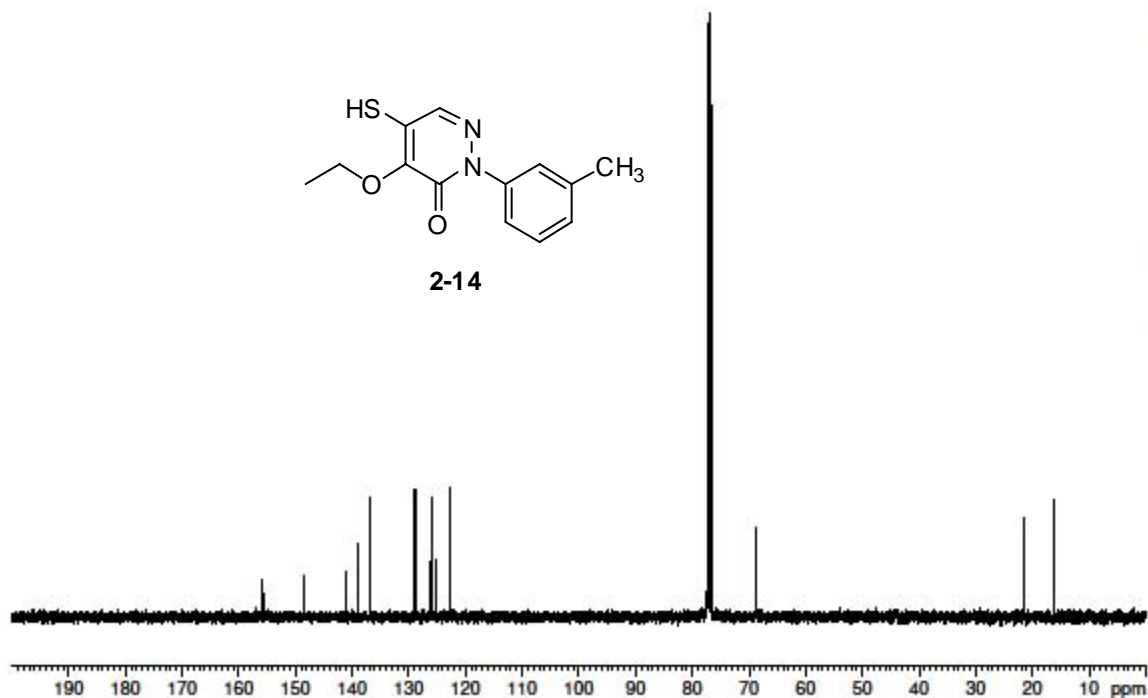
155.779
148.532
141.081
138.882
136.877
129.164
128.655
126.090
125.349
122.630

77.353
77.035
76.718
68.713

21.381
16.111



2-14

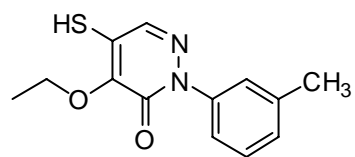
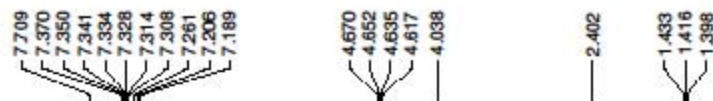


Current Data Parameters
NAME 102308
EXPNO 381
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081023
Time 21.49
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Account no. MEJM16
3Tolyl_OEt_SH_A

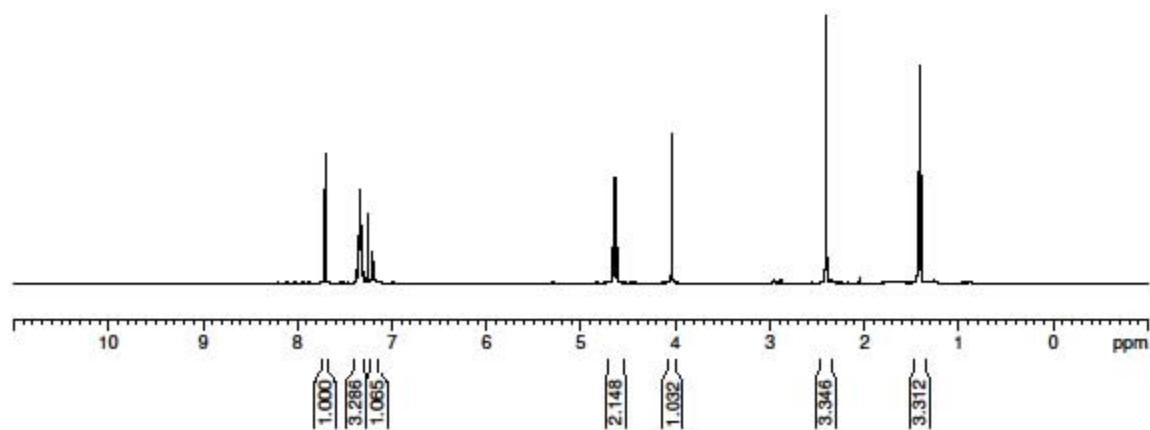


2-14

Current Data Parameters
NAME 102308
EXPNO 380
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081023
Time 21.21
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 1024
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDSW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

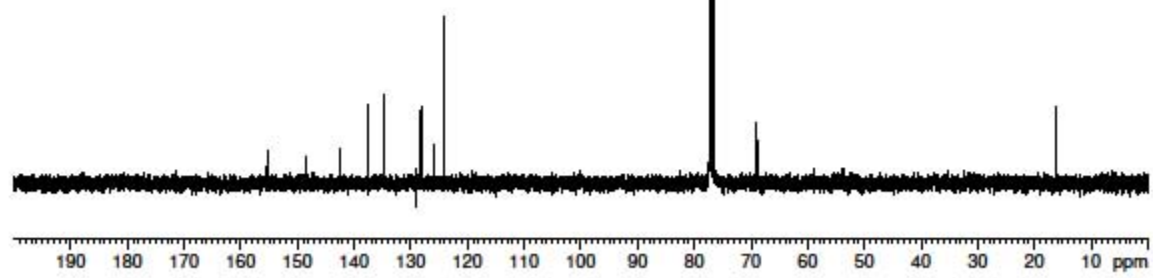
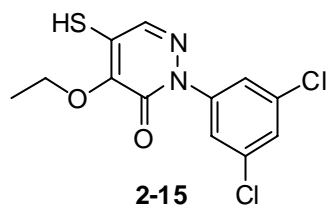


Account no. MEJM16
3,5-Dichloro_OEt_SH_A

155.375
148.414
142.509
137.634
134.876
128.231
125.896
124.075

77.337
77.020
76.702
68.960

16.092



Current Data Parameters
NAME 102308
EXPNO 401
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081023
Time 23.08
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
DL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

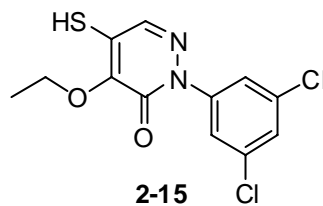
F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Account no. MEJM16
3,5-Dichloro_OEt_SH_A

7.724
7.582
7.577
7.376
7.371
7.366
7.261

4.662
4.644
4.627
4.609
4.071

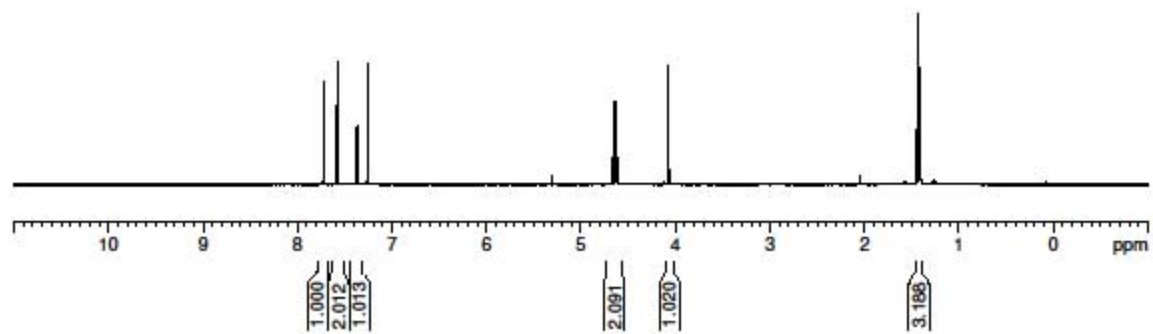
1.442
1.424
1.407

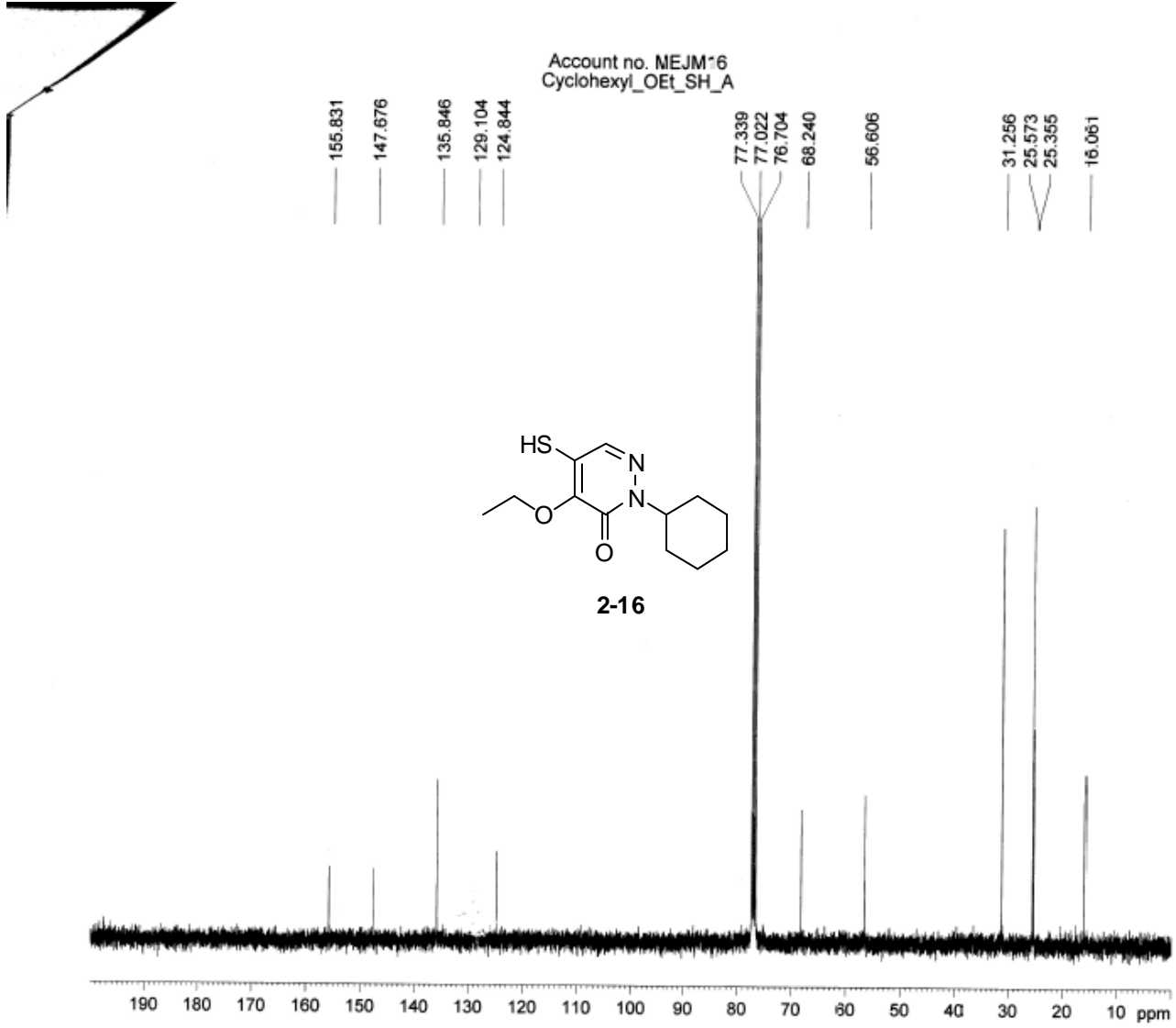


Current Data Parameters
NAME 102308
EXPNO 400
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081023
Time 22.40
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 4096
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





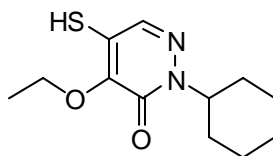
Current Data Parameters
NAME 102308
EXPNO 391
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081023
Time 22.29
INSTRUM arx400
PROBHD 5 mm QNP 1H
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 27777.777 Hz
FIDRES 0.423855 Hz
AQ 1.1796980 sec
RG 32768
DW 18.000 usec
DE 25.71 usec
TE 300.0 K
D12 0.0000200 sec
CL5 23.50 dB
CPDPRG waltz16
P31 100.00 usec
C1 2.0000000 sec
P1 8.25 usec
SFO1 100.6248445 MHz
NUCLEUS 13C
D11 0.0300000 sec

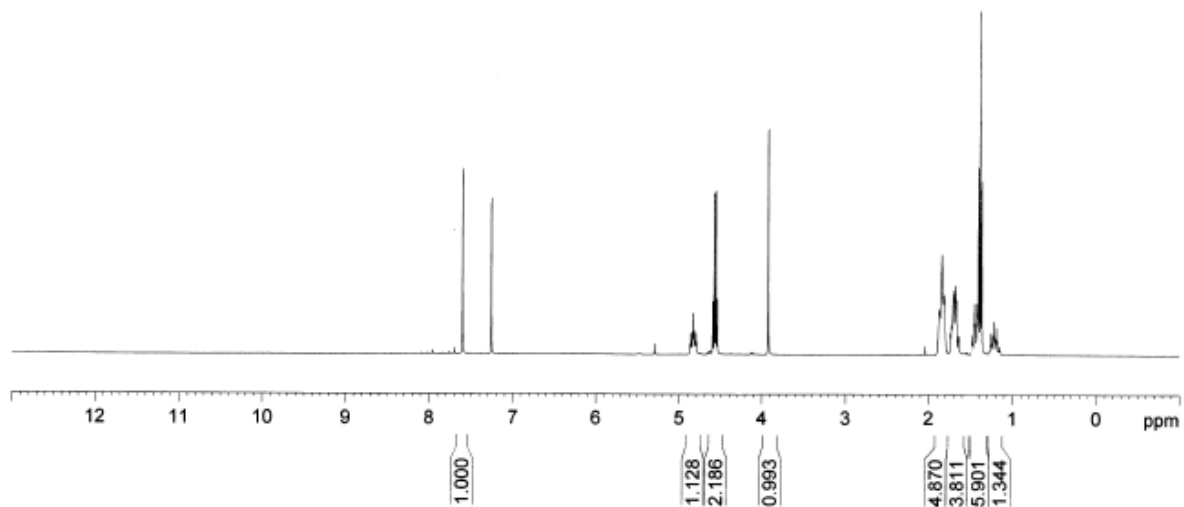
F2 - Processing parameters
SI 65536
SF 100.6127710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Account no. MEJM16
Cyclohexyl_OEt_SH_A

7.607
7.261
4.863
4.854
4.843
4.834
4.825
4.814
4.805
4.604
4.586
4.568
4.551
3.925
1.875
1.868
1.841
1.816
1.740
1.728
1.706
1.698
1.677
1.668
1.645
1.637
1.490
1.481
1.457
1.449
1.440
1.425
1.416
1.405



2-16

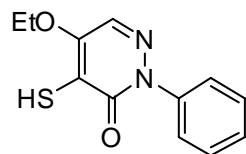
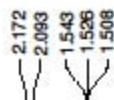


Current Data Parameters
NAME 102308
EXPNO 390
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081C23
Time 22.00
INSTRUM arx400
PROBHD 5 mm QNP 1H
PU_PROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 1024
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.00000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WCW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Account no. MEJM16
Ph_OEt_SH_pure

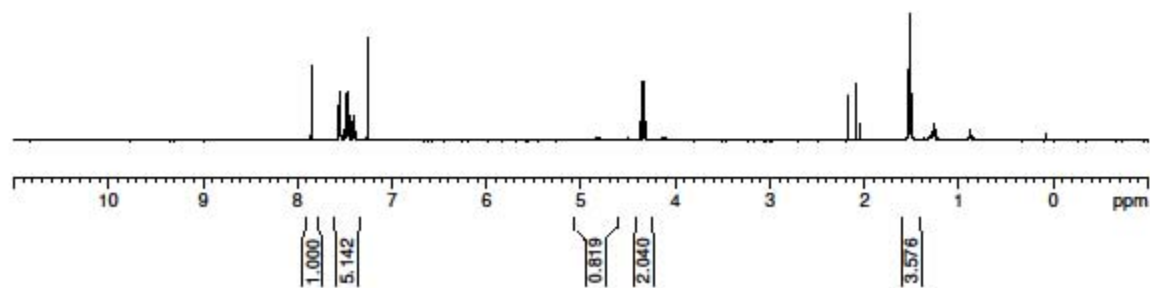


2-18

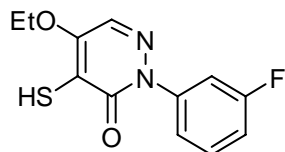
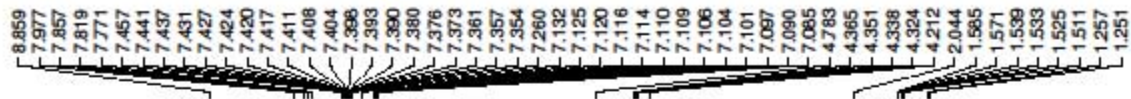
Current Data Parameters
NAME 092708
EXPNO 70
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080927
Time 16.14
INSTRUM ax400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8064.516 Hz
FIDRES 0.123055 Hz
AQ 4.0632820 sec
RG 2860
DW 62.000 usec
DE 88.57 usec
TE 300.0 K
D1 2.0000000 sec
P1 7.50 usec
SFO1 400.1324008 MHz
NUCLEUS 1H

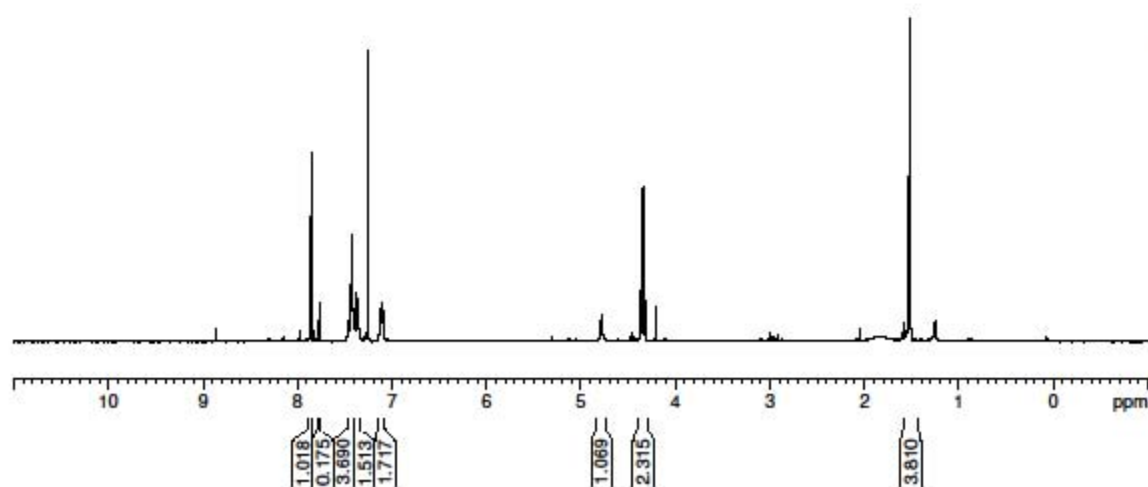
F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



default proton parameters



2-19

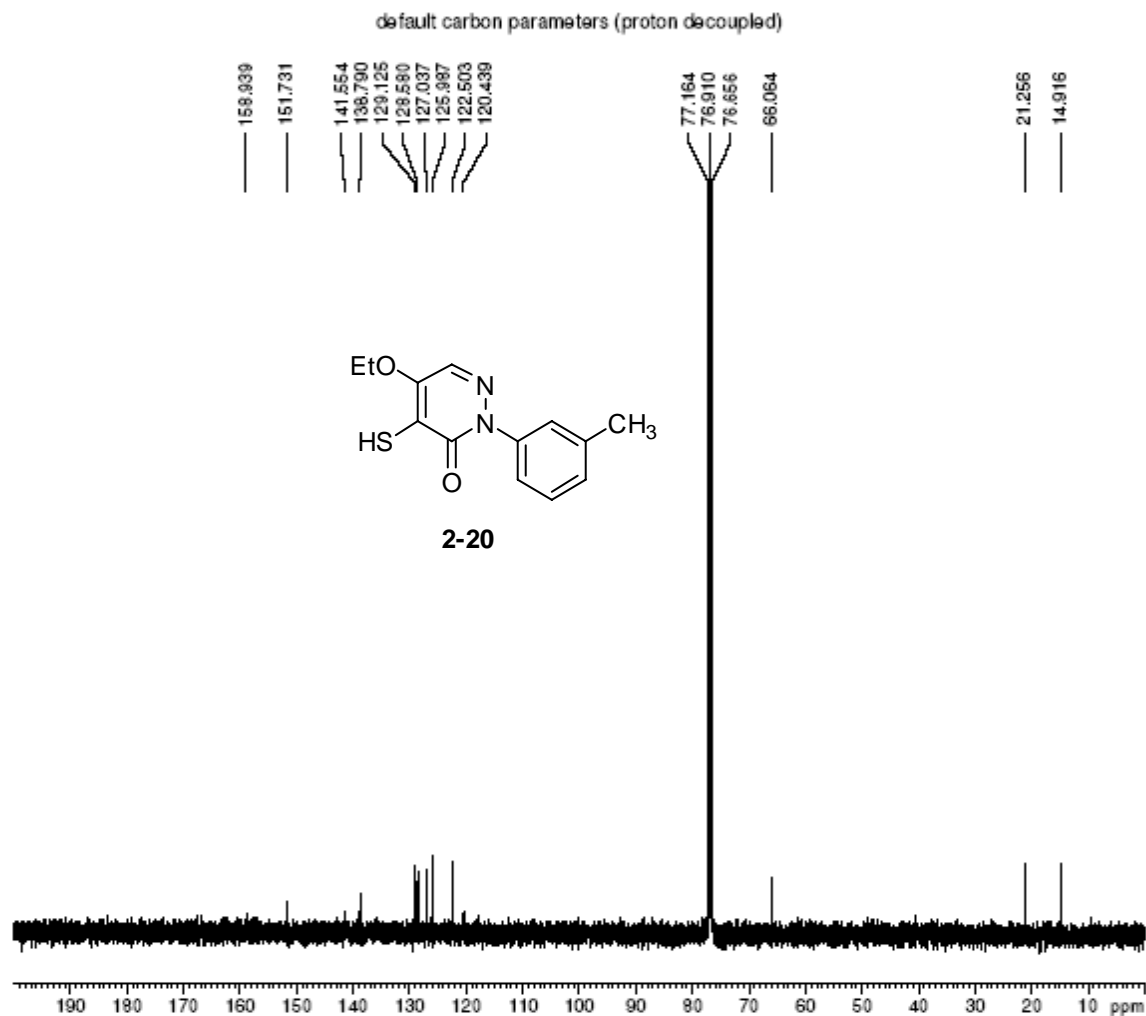


Current Data Parameters
NAME 3Php_OEt_SH_B_re
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081104
Time 8.06
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6385000 sec
RG 1024
DW 50.000 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 500.3330020 MHz

F2 - Processing parameters
SI 32768
SF 500.3300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



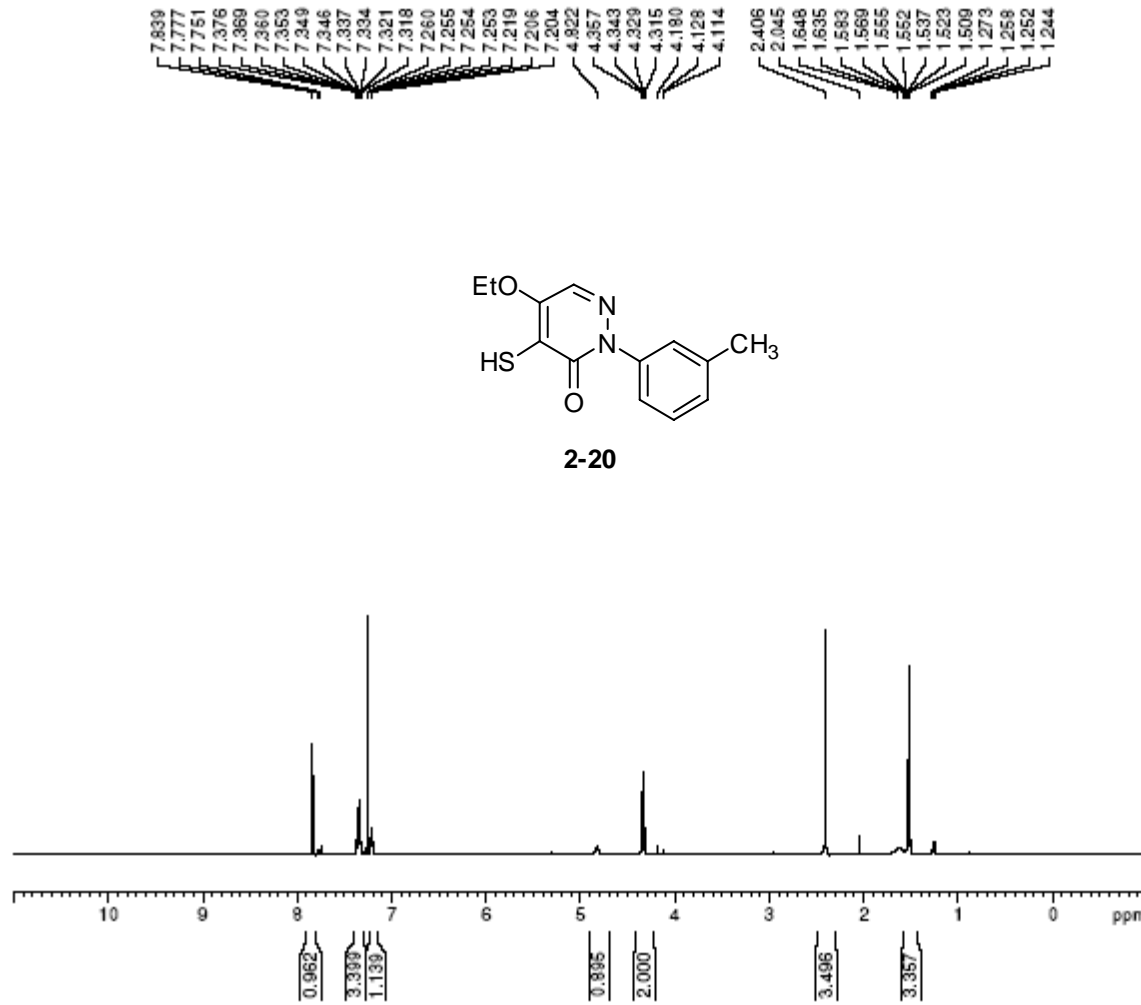
Current Data Parameters
 NAME 3Tolyl_OEt_SH_B_re
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081104
 Time 8.15
 INSTRUM avance500
 PROBHD 5 mm bb-Z Z800
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 128
 DS 0
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 4096
 DW 15.300 usec
 DE 6.00 usec
 TE 295.5 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 5.25 usec
 PL1 0.00 dB
 SFO1 125.8231939 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 P-CPD2 105.00 usec
 PL2 120.00 dB
 PL12 19.00 dB
 SFO2 500.3320013 MHz

F2 - Processing parameters
 SI 65536
 SF 125.8080969 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

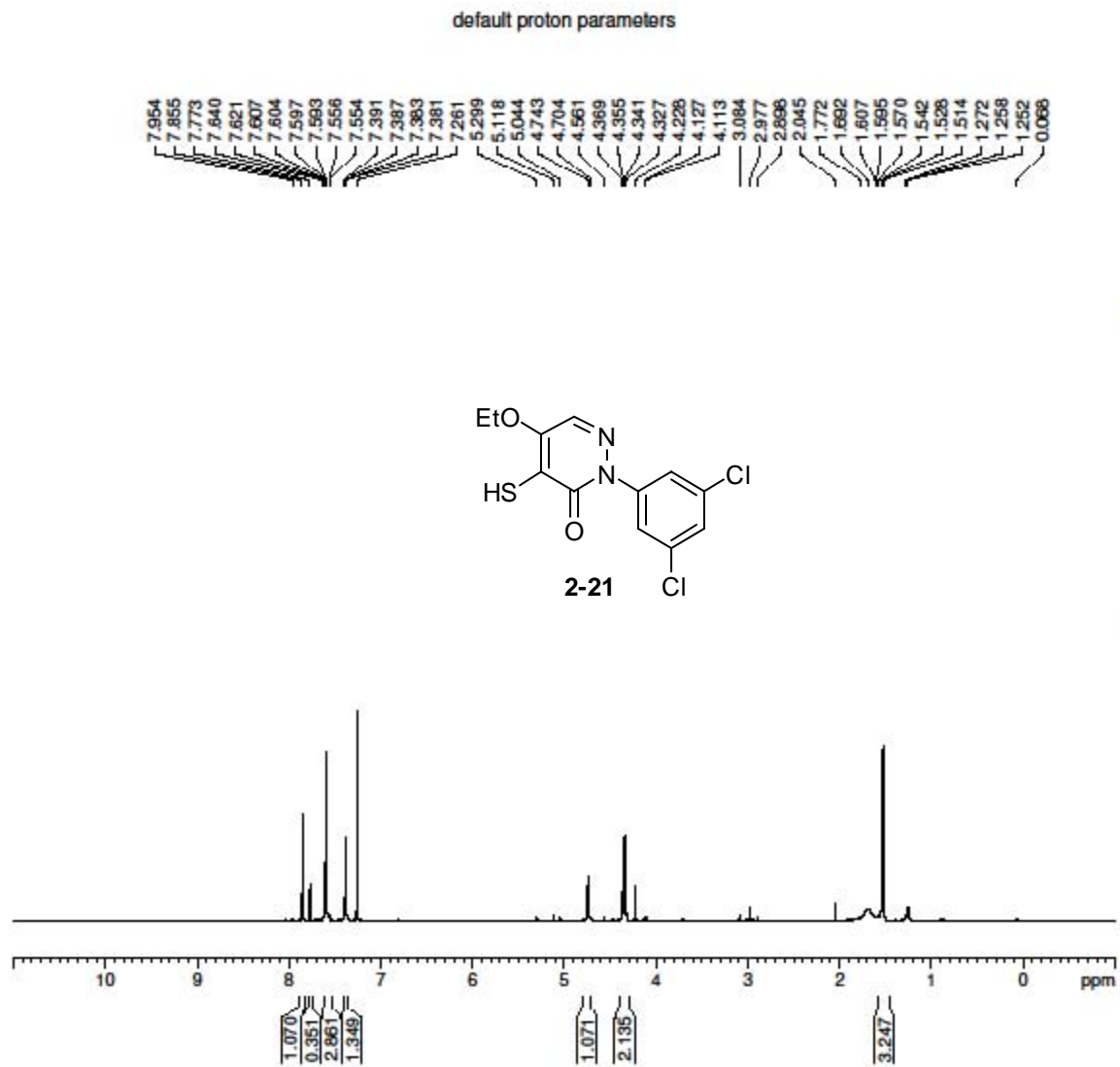


Current Data Parameters
 NAME 3Tolyl_OEt_SH_B_re
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081104
 Time 8.11
 INSTRUM avance500
 PROBHD 5 mm bb-Z Z800
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6385000 sec
 RG 1024
 DW 50.000 usec
 DE 6.00 usec
 TE 295.2 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 500.3330020 MHz

F2 - Processing parameters
 SI 32768
 SF 500.33300220 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

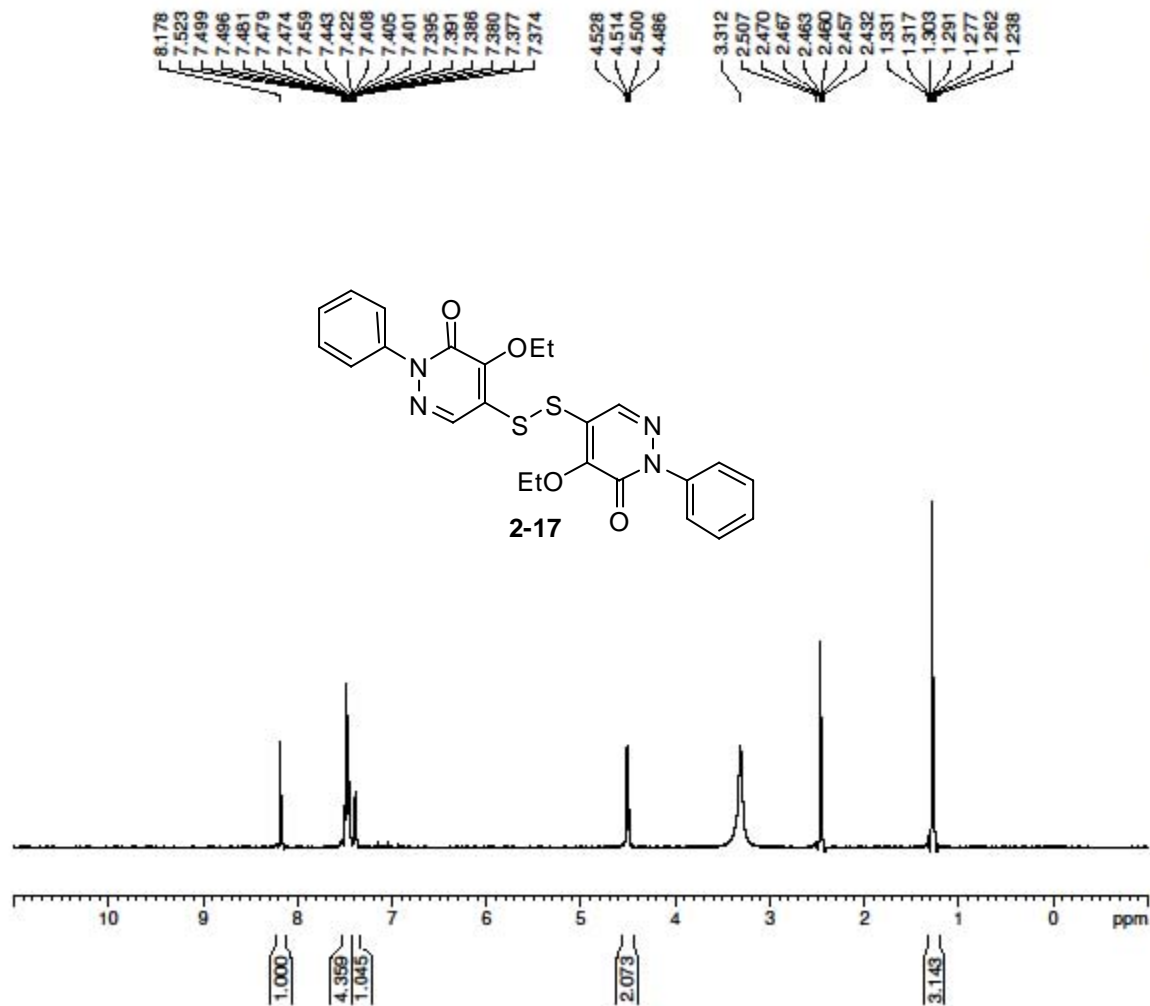


Current Data Parameters
 NAME 3,5-dichloroPh_OEt_1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081104
 Time 8.30
 INSTRUM avance500
 PROBHD 5 mm bb-Z 2800
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6385000 sec
 RG 1024
 DW 50.000 usec
 DE 6.00 usec
 TE 295.3 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 500.3330020 MHz

F2 - Processing parameters
 SI 32768
 SF 500.3300220 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

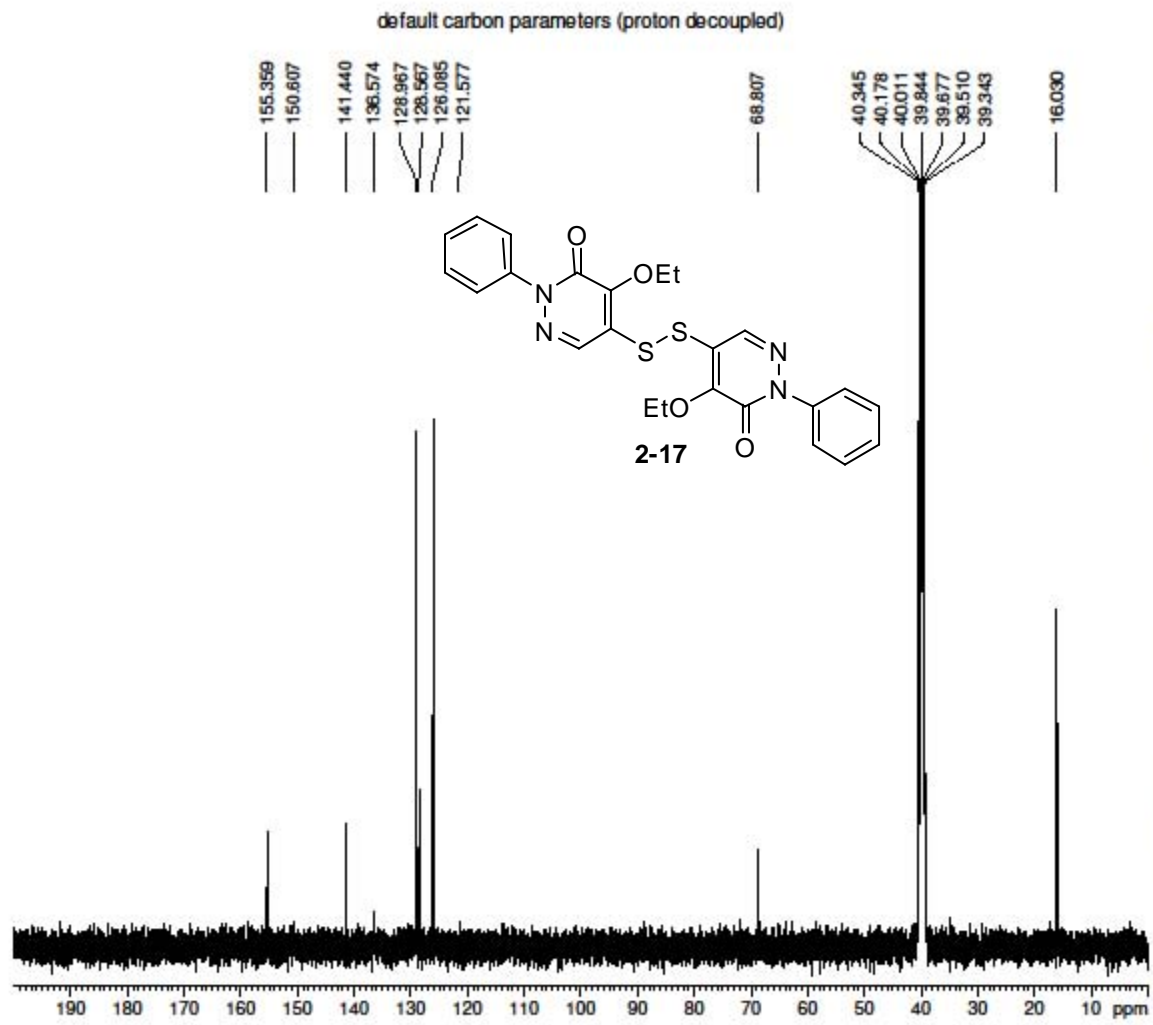


Current Data Parameters
 NAME W1-YJ2-17-re
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090729
 Time 9.18
 INSTRUM avance500
 PROBHD 5 mm bb-Z 2800
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 2
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2769001 sec
 RG 1024
 DW 50.000 usec
 DE 6.00 usec
 TE 296.2 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

CHANNEL f1
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 500.3330020 MHz

F2 - Processing parameters
 SI 32768
 SF 500.3300220 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



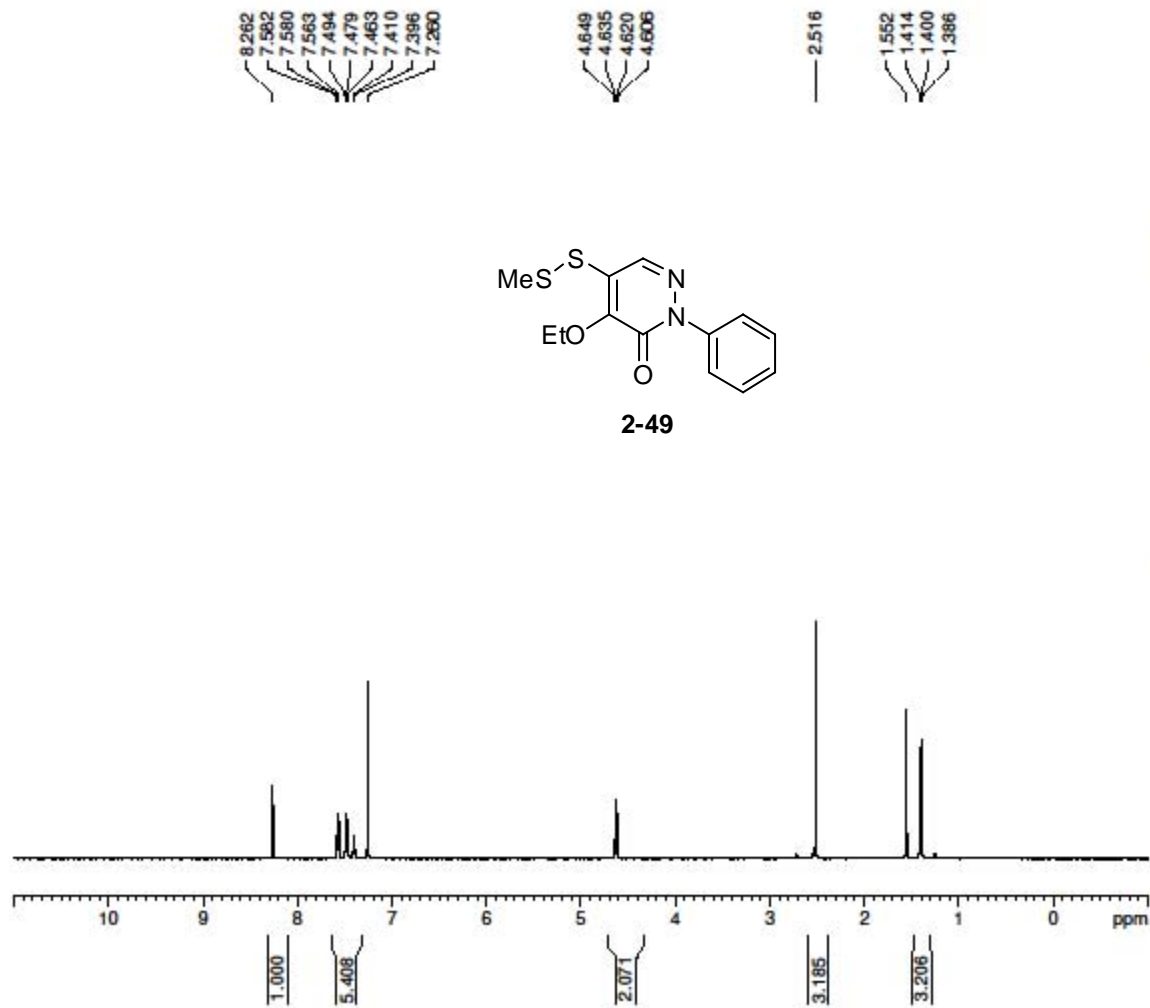
Current Data Parameters
 NAME W1-YJ2-17-re
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090729
 Time 9.23
 INSTRUM avance500
 PROBHD 5 mm bb-Z 2800
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 640
 DS 0
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 4096
 DW 15.300 usec
 DE 6.00 usec
 TE 296.6 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 5.25 usec
 PL1 0.00 dB
 SFO1 125.8231939 MHz

----- CHANNEL f2 -----
 CPDPRG2 waitz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 16.10 dB
 SFO2 500.3320013 MHz

F2 - Processing parameters
 SI 65536
 SF 125.8080969 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



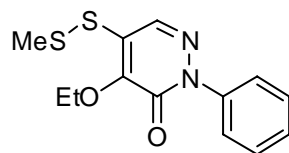
Current Data Parameters
 NAME PhePh_OEt_SSMe_A
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081209
 Time 10.45
 INSTRUM avance500
 PROBHD 5 mm bb-Z 2800
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6385000 sec
 RG 1024
 DW 50.000 usec
 DE 6.00 usec
 TE 294.7 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

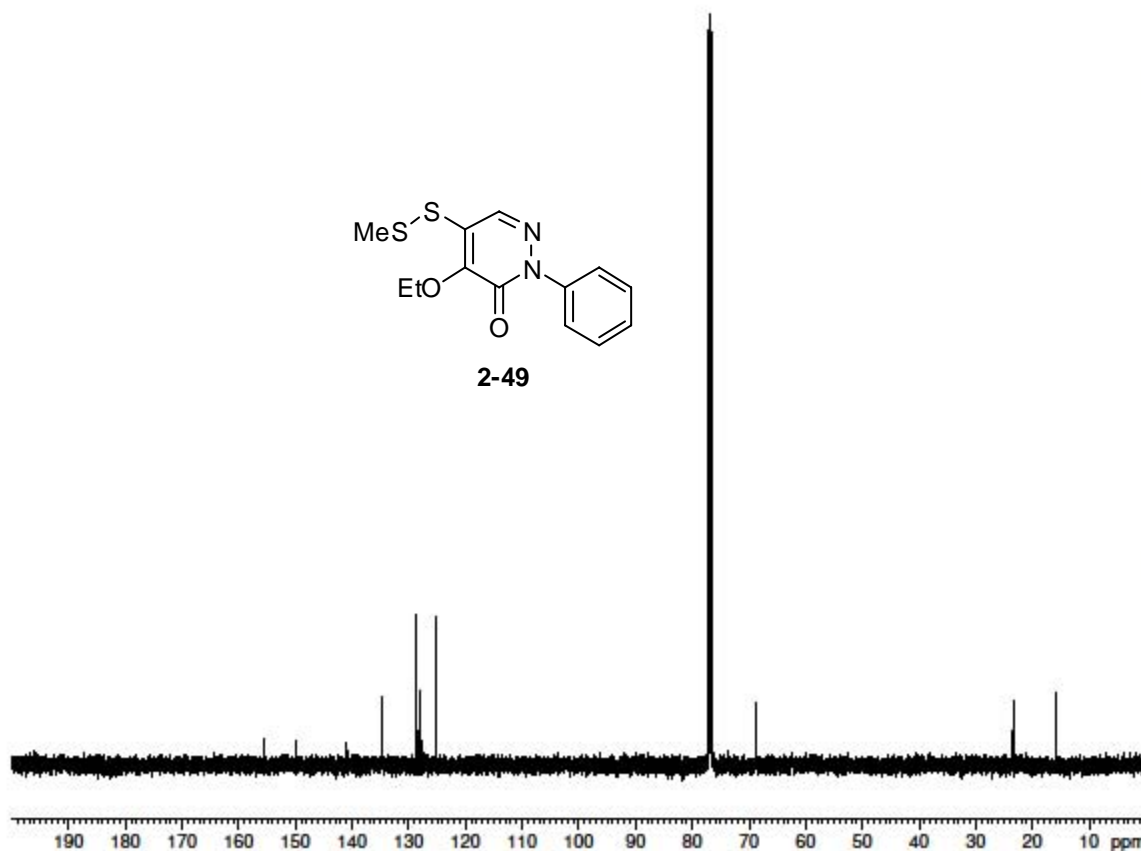
----- CHANNEL f1 -----
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 500.3330020 MHz

F2 - Processing parameters
 SI 32768
 SF 500.3300220 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

default carbon parameters (proton decoupled)



2-49



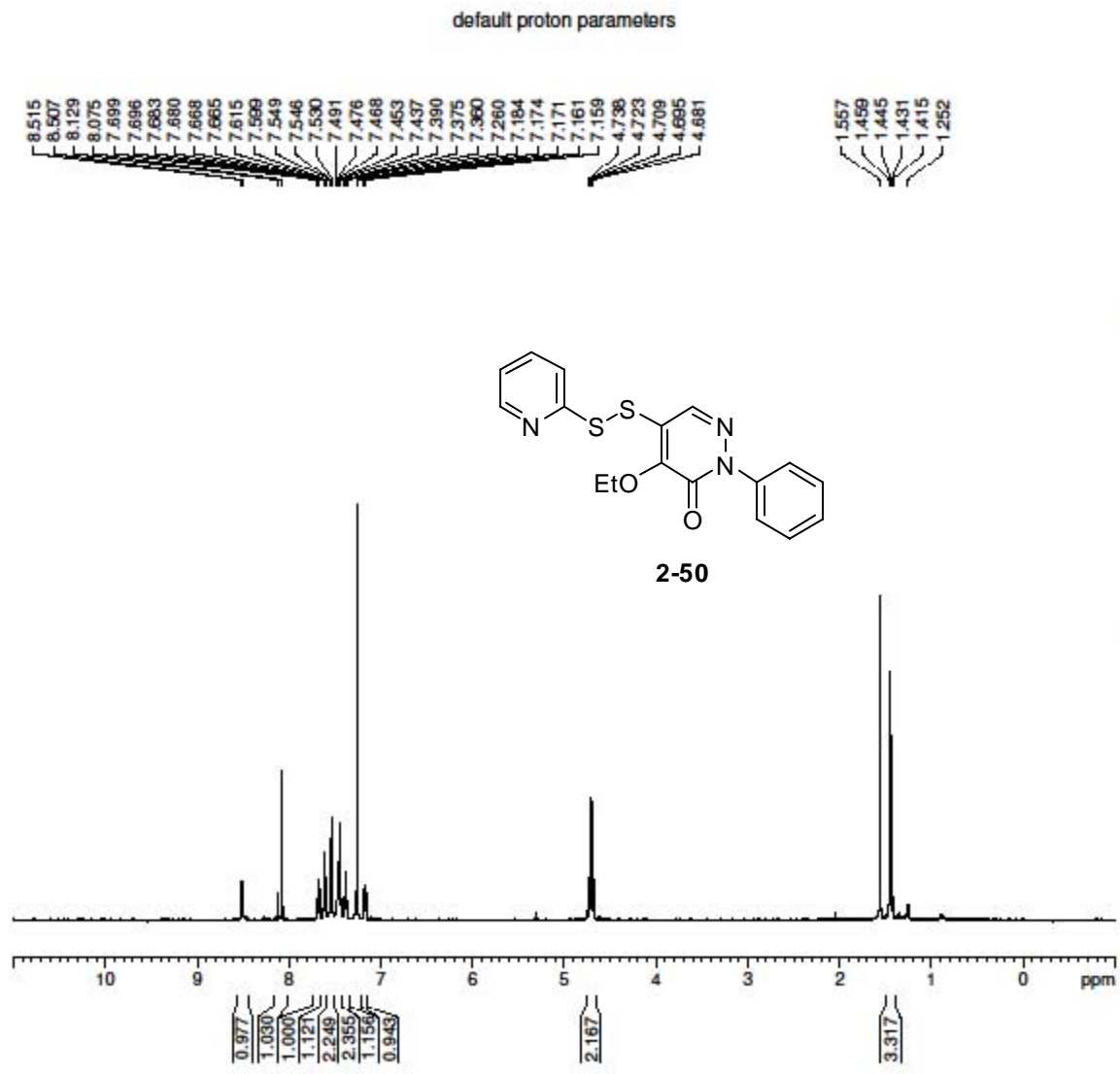
Current Data Parameters
NAME W1-YJ2-49
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090729
Time 12.37
INSTRUM avance500
PROBHD 5 mm bb-Z 2800
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 8192
DW 15.300 usec
DE 6.00 usec
TE 296.5 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.25 usec
PL1 0.00 dB
SFO1 125.8231939 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.10 dB
SFO2 500.3320013 MHz

F2 - Processing parameters
SI 65536
SF 125.8080969 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

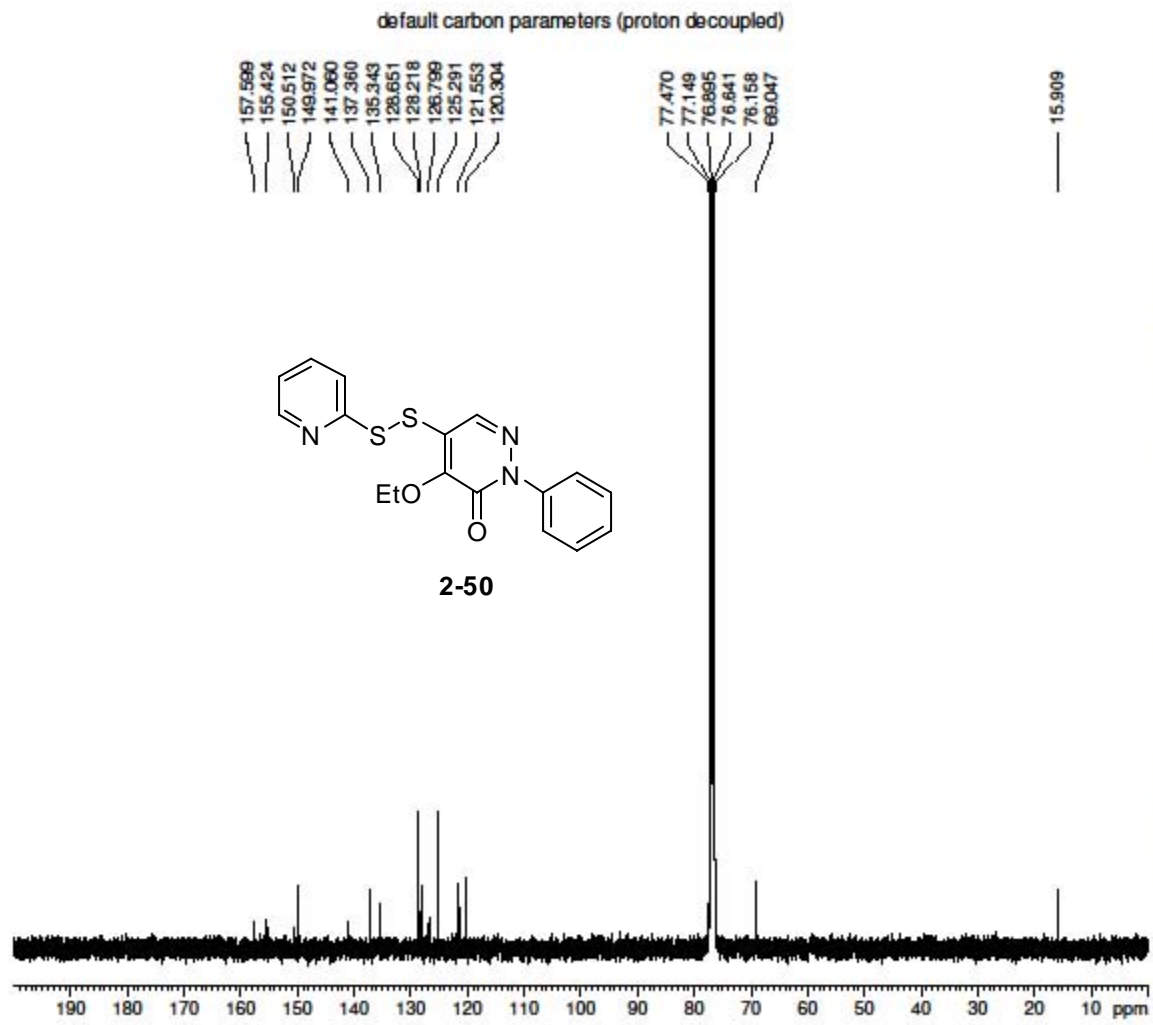


Current Data Parameters
 NAME Ph_OEt_SSPyr_A_bo
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081209
 Time 13.02
 INSTRUM avance500
 PROBHD 5 mm bb-Z 2800
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6385000 sec
 RG 1024
 DW 50.000 usec
 DE 6.00 usec
 TE 294.7 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 500.3330020 MHz

F2 - Processing parameters
 SI 32768
 SF 500.3300220 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



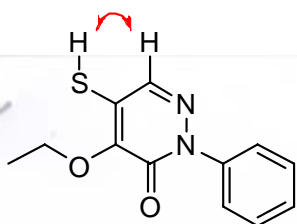
Current Data Parameters
 NAME Woogie
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090729
 Time 19.20
 INSTRUM avance500
 PROBHD 5 mm bb-Z 2800
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 10000
 DS 0
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 4096
 DW 15.300 usec
 DE 6.00 usec
 TE 296.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

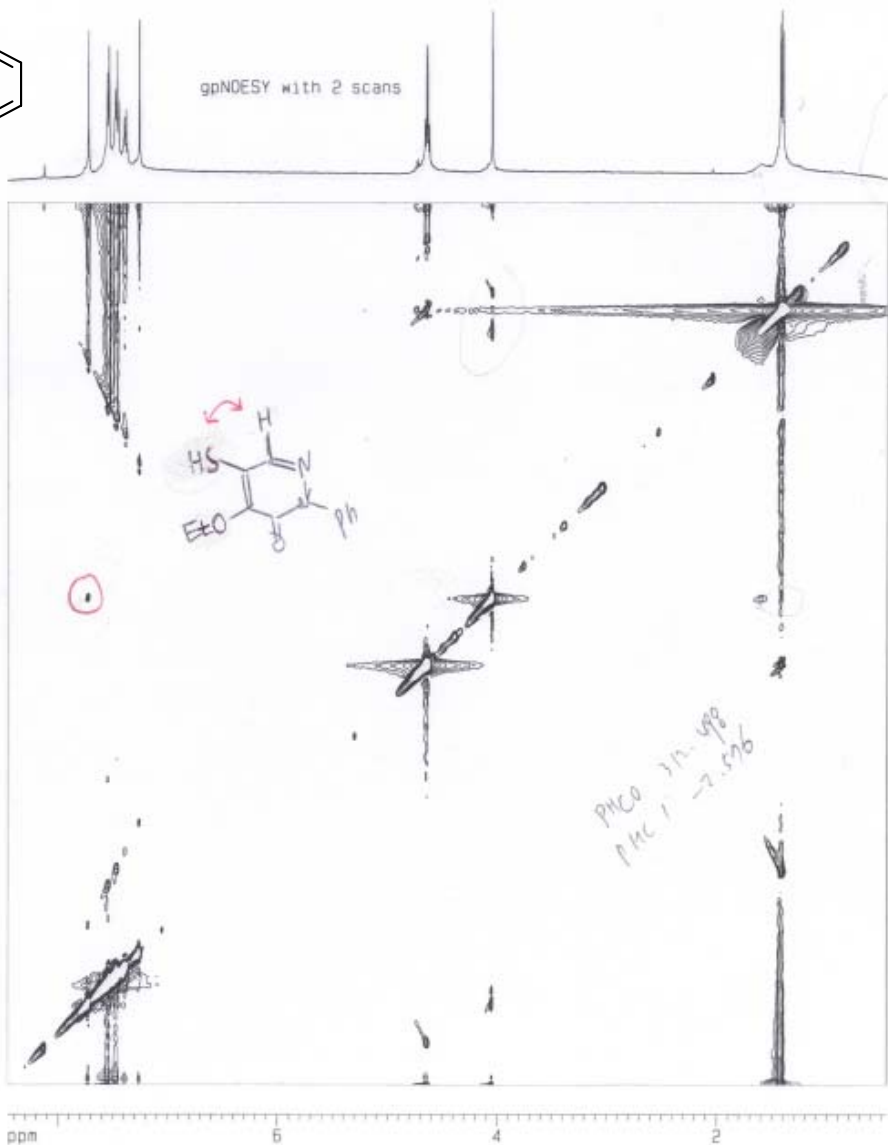
----- CHANNEL f1 -----
 NUC1 13C
 P1 5.25 usec
 PL1 0.00 dB
 SFO1 125.8231939 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 16.10 dB
 SFO2 500.3320013 MHz

F2 - Processing parameters
 SI 65536
 SF 125.8080969 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



2-10



```

Current Data Parameters
NAME      NMR3_3-1_1r0101
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20081012
Time     8:44
INSTRUM  avance300
PROBHD   5 mm cpz-1300
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        16
SWH       4000.410 Hz
FIDRES    3.912510 Hz
AQ         0.1272100 sec
RG         181
DM         124.000 usec
DE         5.00 usec
TE         295.3 K
AQ         0.0000000 sec
D1         2.0000000 sec
D8         0.7500000 sec
d11        0.0300000 sec
D15        0.0010000 sec
G20        0.3740000 sec
IN0        0.0052460 sec
L3         128

----- CHANNEL f1 -----
NUC1      1H
P1         12.75 usec
P2         29.50 usec
PL1        0.00 dB
PL2        0.00 dB
SFO1      500.330515 MHz

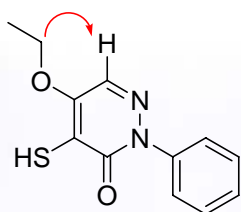
----- GRADIENT CHANNEL -----
SPARE1    SINE 100
SPARE2    SINE 100
GPR1      0.10 %
GPR2      0.10 %
GPR3      0.00 %
GPR4      0.10 %
GPR5      0.10 %
GPR6      40.00 %
GPR7      -40.10 %
P15       1500.00 usec

F1 - Acquisition parameters
RG          1
TD          65536
SFO1        500.330515 MHz
FIDRES      15.850040 Hz
SW           5.001 GHz
FWDRES      undefined

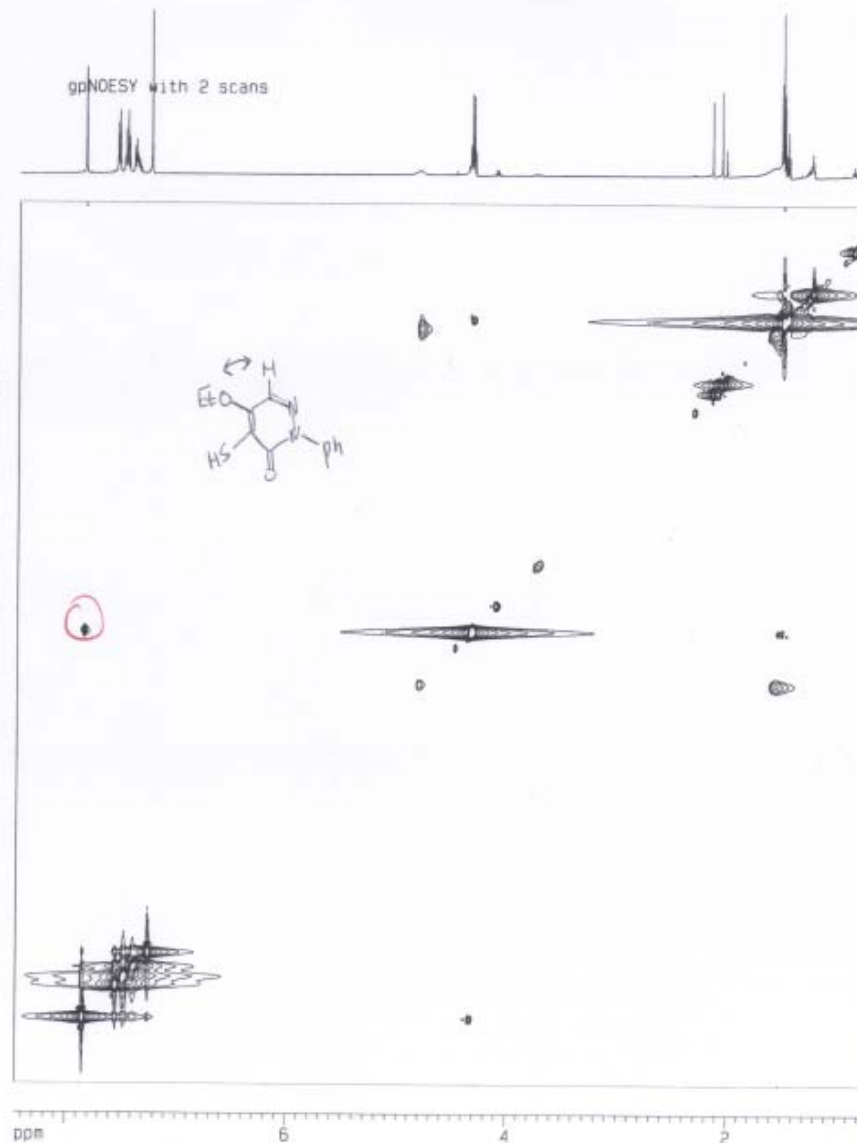
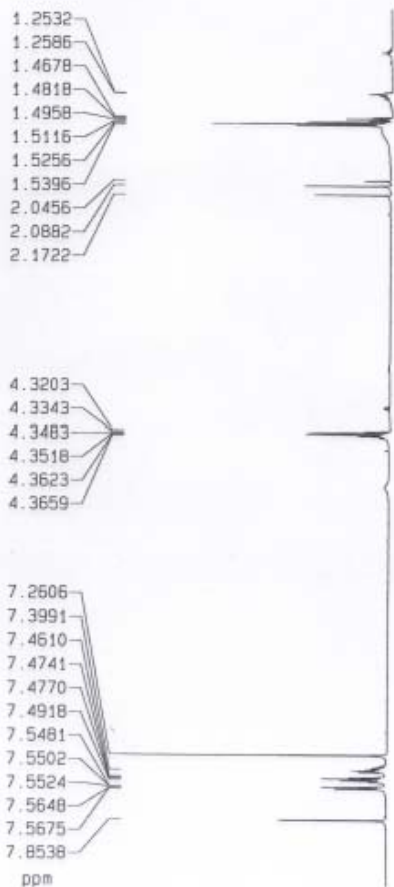
F2 - Processing parameters
SI          65536
SF          500.330515 MHz
GFM         0.00 Hz
L8          0
PC          1.00

F1 - Processing parameters
SI          65536
SF          500.330515 MHz
GFM         0.00 Hz
L8          0

2D NMR plot parameters
CX2         15.00 cm
CY1         15.00 cm
F2PL2      0.450 ppm
F2L0        4232.00 Hz
F2H1        0.450 ppm
F2H0        206.27 Hz
F1P1        0.496 ppm
F1L0        4040.57 Hz
F1H1        0.473 ppm
F1H0        259.58 Hz
F2PRNCK    0.52394 ppm/Hz
F2D1CK     257.00300 Hz/cm
F1PRNCK    0.52394 ppm/Hz
F1D1CK     257.00300 Hz/cm
  
```



2-18



Current Data Parameters
NAME: gqNOESY_01_01_01_01_01_01
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_ : 20081010
Time : 14.28
INSTRUM : avance500
PROBHD : 5 mm ssb-z BBOO
PULPROG : zgpg30
TD : 1674
SOLVENT : CDCl3
NS : 8
DS : 16
SWH : 4008.410 Hz
FIDRES : 0.312512 Hz
AQ : 0.127500 sec
RG : 521
IN : 174.800 usec
TE : 0.00 usec
IC : 295.0 K
CO : 0.0000000 sec
HI : 2.0000000 sec
HO : 0.7000000 sec
H1 : 0.0000000 sec
H11 : 0.0001000 sec
H2 : 0.0000000 sec
H3 : 0.0000000 sec
H4 : 0.0000000 sec
H5 : 0.0000000 sec
H6 : 0.0000000 sec
H7 : 0.0000000 sec
H8 : 0.0000000 sec
H9 : 0.0000000 sec
H10 : 0.0000000 sec
H11 : 0.0000000 sec
H12 : 0.0000000 sec
H13 : 0.0000000 sec
H14 : 0.0000000 sec
H15 : 0.0000000 sec
H16 : 0.0000000 sec
H17 : 0.0000000 sec
H18 : 0.0000000 sec
H19 : 0.0000000 sec
H20 : 0.0000000 sec
H21 : 0.0000000 sec
H22 : 0.0000000 sec
H23 : 0.0000000 sec
H24 : 0.0000000 sec
H25 : 0.0000000 sec
H26 : 0.0000000 sec
H27 : 0.0000000 sec
H28 : 0.0000000 sec
H29 : 0.0000000 sec
H30 : 0.0000000 sec
H31 : 0.0000000 sec
H32 : 0.0000000 sec
H33 : 0.0000000 sec
H34 : 0.0000000 sec
H35 : 0.0000000 sec
H36 : 0.0000000 sec
H37 : 0.0000000 sec
H38 : 0.0000000 sec
H39 : 0.0000000 sec
H40 : 0.0000000 sec
H41 : 0.0000000 sec
H42 : 0.0000000 sec
H43 : 0.0000000 sec
H44 : 0.0000000 sec
H45 : 0.0000000 sec
H46 : 0.0000000 sec
H47 : 0.0000000 sec
H48 : 0.0000000 sec
H49 : 0.0000000 sec
H50 : 0.0000000 sec
H51 : 0.0000000 sec
H52 : 0.0000000 sec
H53 : 0.0000000 sec
H54 : 0.0000000 sec
H55 : 0.0000000 sec
H56 : 0.0000000 sec
H57 : 0.0000000 sec
H58 : 0.0000000 sec
H59 : 0.0000000 sec
H60 : 0.0000000 sec
H61 : 0.0000000 sec
H62 : 0.0000000 sec
H63 : 0.0000000 sec
H64 : 0.0000000 sec
H65 : 0.0000000 sec
H66 : 0.0000000 sec
H67 : 0.0000000 sec
H68 : 0.0000000 sec
H69 : 0.0000000 sec
H70 : 0.0000000 sec
H71 : 0.0000000 sec
H72 : 0.0000000 sec
H73 : 0.0000000 sec
H74 : 0.0000000 sec
H75 : 0.0000000 sec
H76 : 0.0000000 sec
H77 : 0.0000000 sec
H78 : 0.0000000 sec
H79 : 0.0000000 sec
H80 : 0.0000000 sec
H81 : 0.0000000 sec
H82 : 0.0000000 sec
H83 : 0.0000000 sec
H84 : 0.0000000 sec
H85 : 0.0000000 sec
H86 : 0.0000000 sec
H87 : 0.0000000 sec
H88 : 0.0000000 sec
H89 : 0.0000000 sec
H90 : 0.0000000 sec
H91 : 0.0000000 sec
H92 : 0.0000000 sec
H93 : 0.0000000 sec
H94 : 0.0000000 sec
H95 : 0.0000000 sec
H96 : 0.0000000 sec
H97 : 0.0000000 sec
H98 : 0.0000000 sec
H99 : 0.0000000 sec
H100 : 0.0000000 sec