

Supporting Information

A Study of the Scope and Regioselectivity of the Ruthenium-Catalyzed [3+2]-Cycloaddition of Azides with Internal Alkynes

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University Park, Pennsylvania 16802*

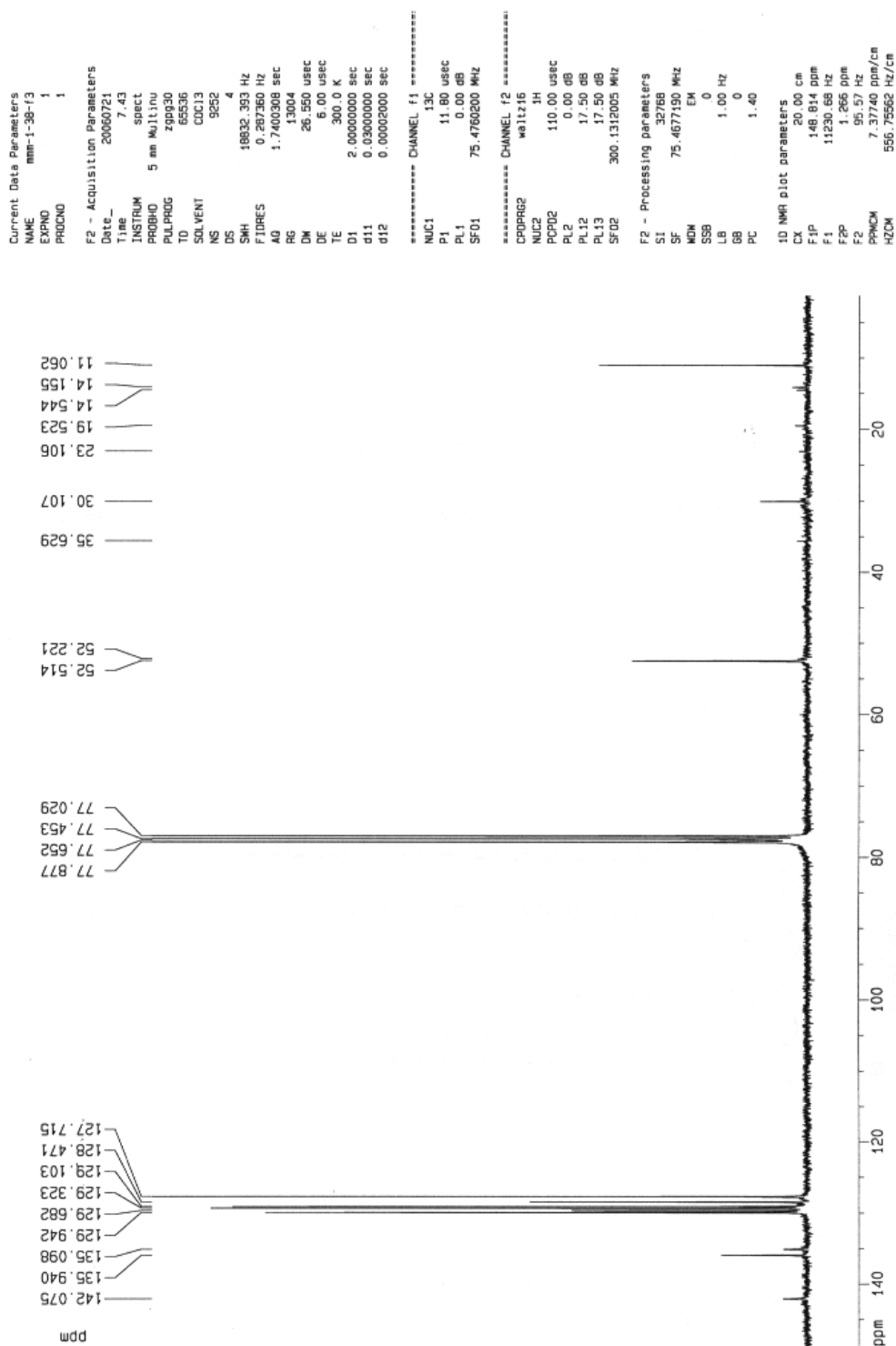
smw@chem.psu.edu

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1a





1a

Current Data Parameters
NAME 80t9-mm-1-3g
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters

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Time 10.55
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PULPROG zg30
TD 24690
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.250014 Hz
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RG 228.1
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DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

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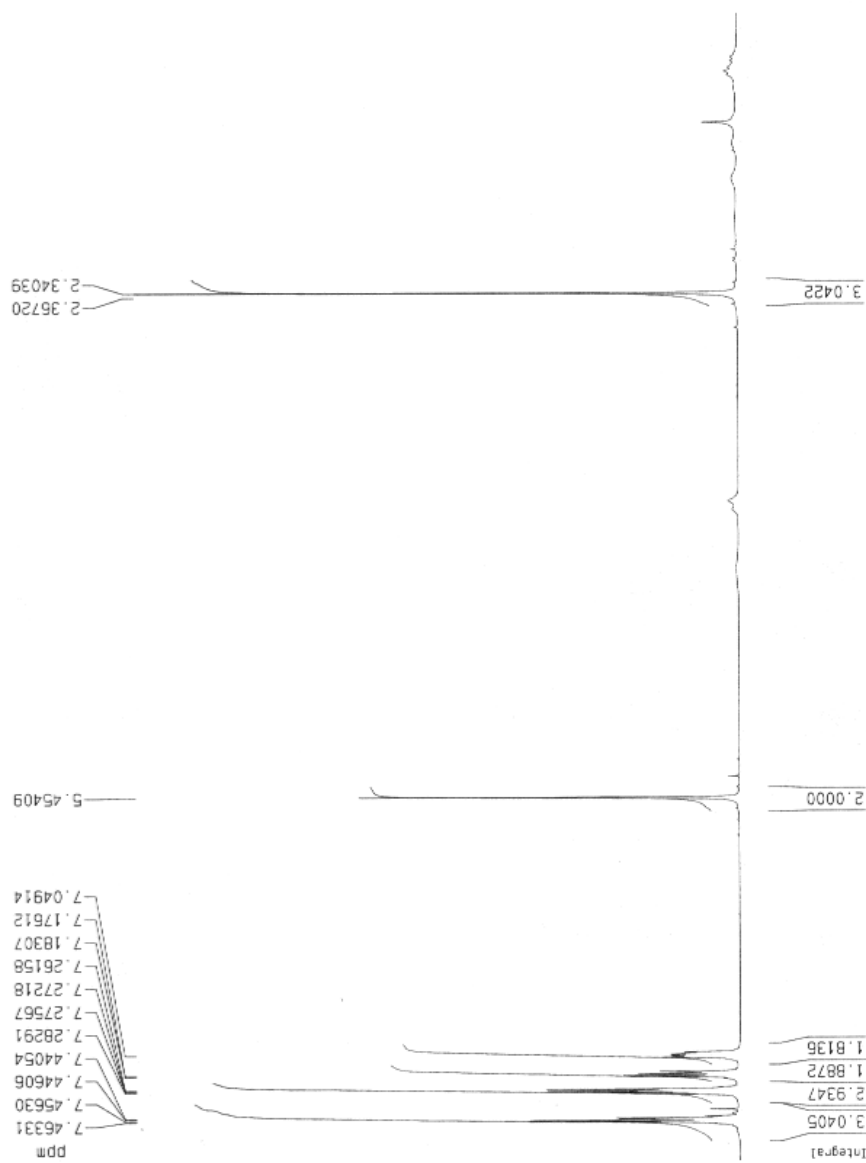
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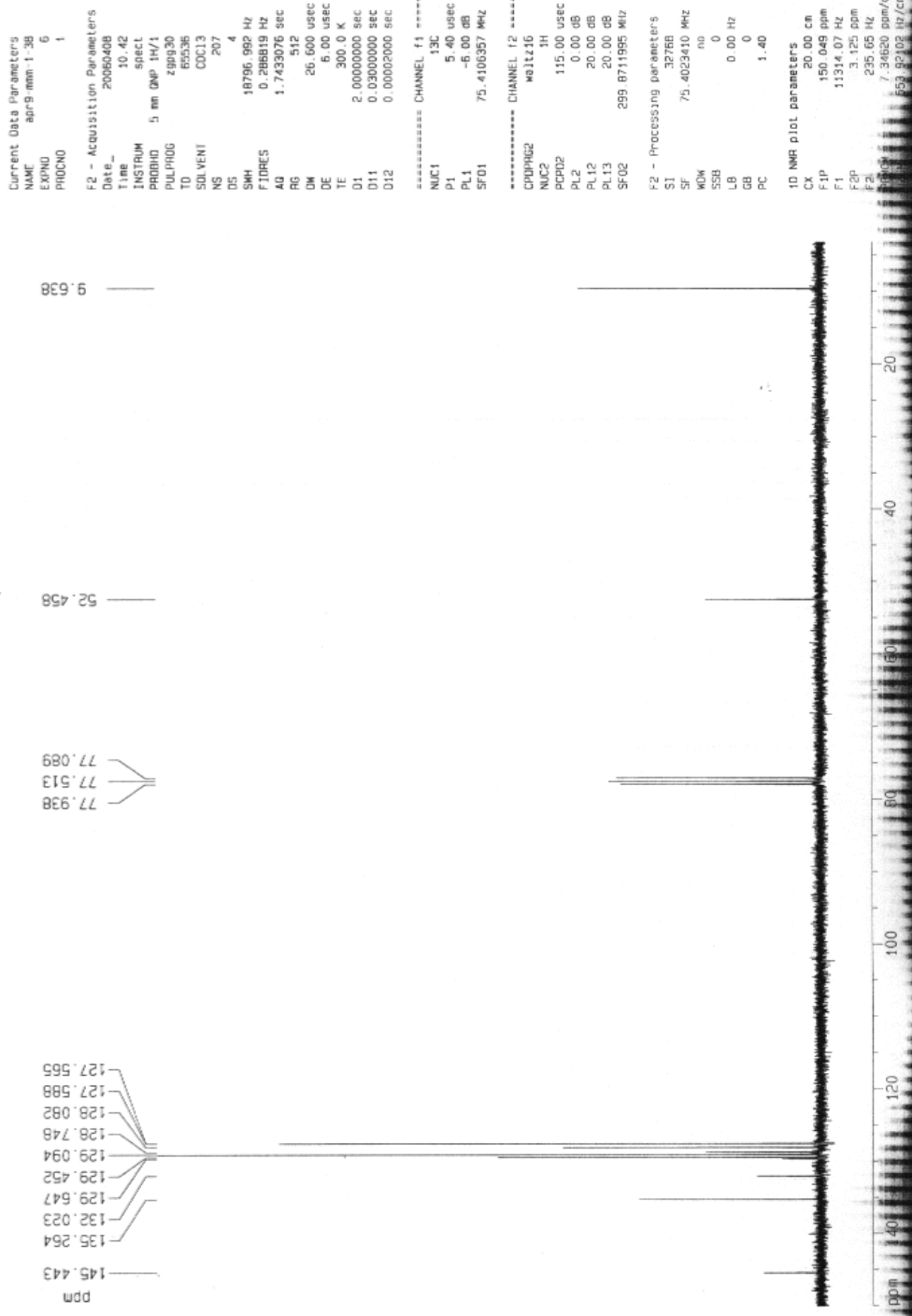
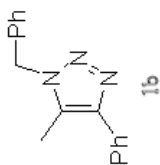
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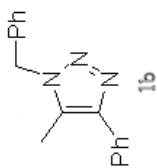
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WDW no
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GB 0
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10 NMR plot parameters

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F1 2310.04 Hz
F2 0.612 ppm
F2 183.50 Hz
PPMCM 0.35458 ppm/cm
HZCM 106.32729 Hz/cm







Current Data Parameters
 NAME apr-9-mm-1-3g
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

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 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TO 24690
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
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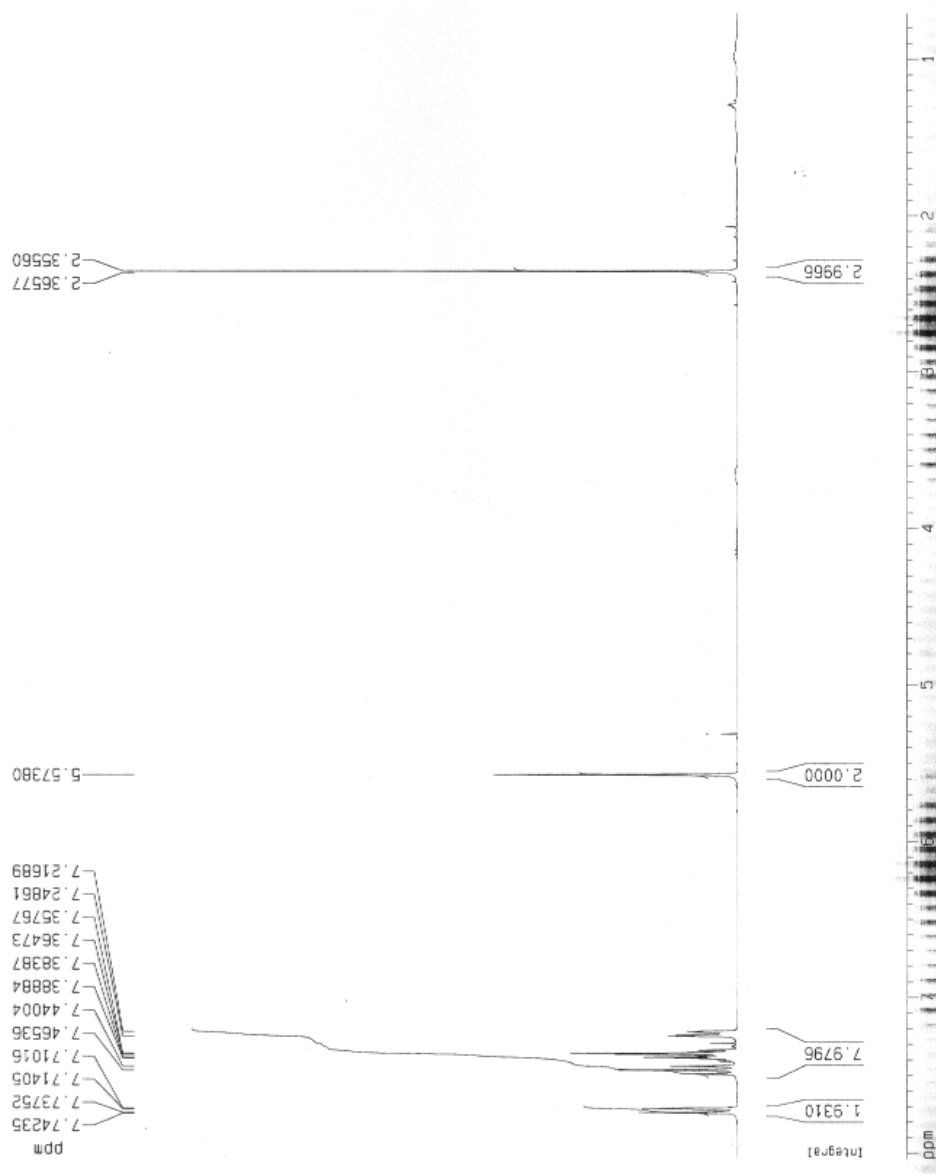
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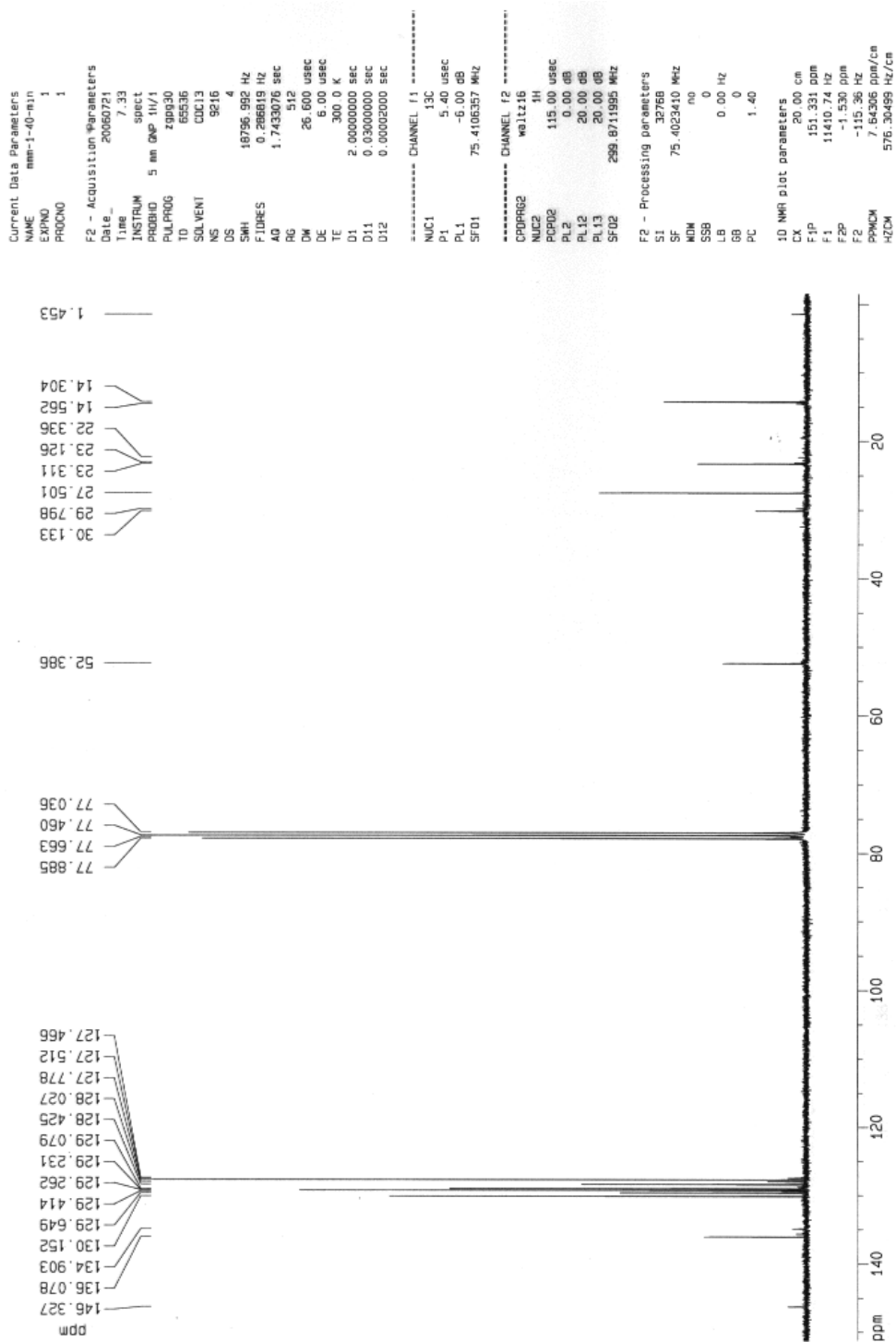
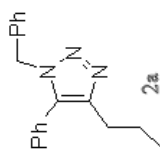
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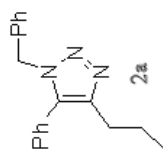
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1D NMR plot parameters

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 F2p 0.706 ppm
 F2 211.70 Hz
 PPMCM 0.36670 ppm/cm
 HZCM 109.96301 Hz/cm







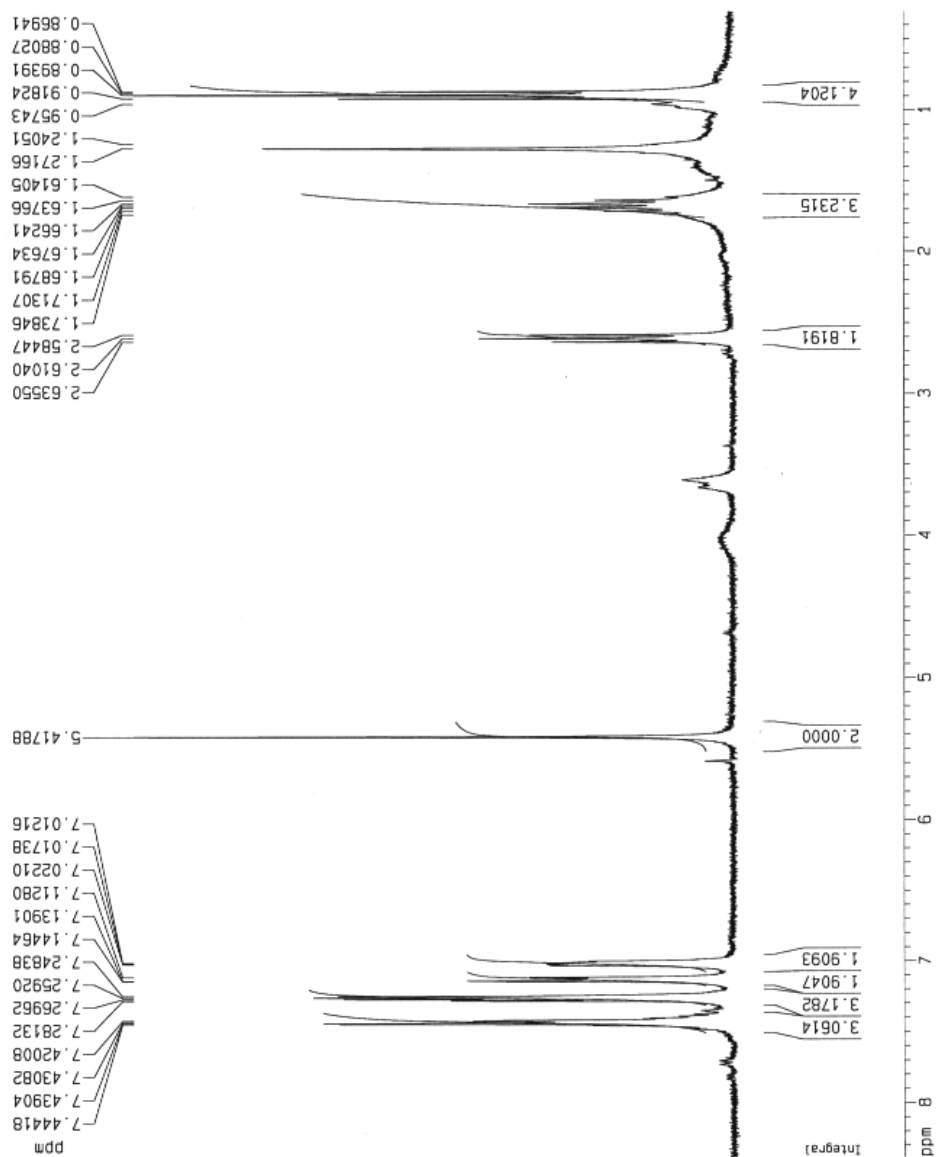
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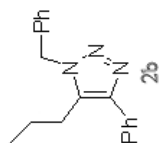
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 TO 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 406.4
 DM 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

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 NUC1 1H
 P1 9.60 usec
 PL1 -6.00 dB
 SF01 300.1318534 MHz

F2 - Processing parameters
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 SF 300.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
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 F1 2515.94 Hz
 F2P 0.307 ppm
 F2 92.13 Hz
 PPMCM 0.40379 ppm/cm
 HZCM 121.19061 Hz/cm





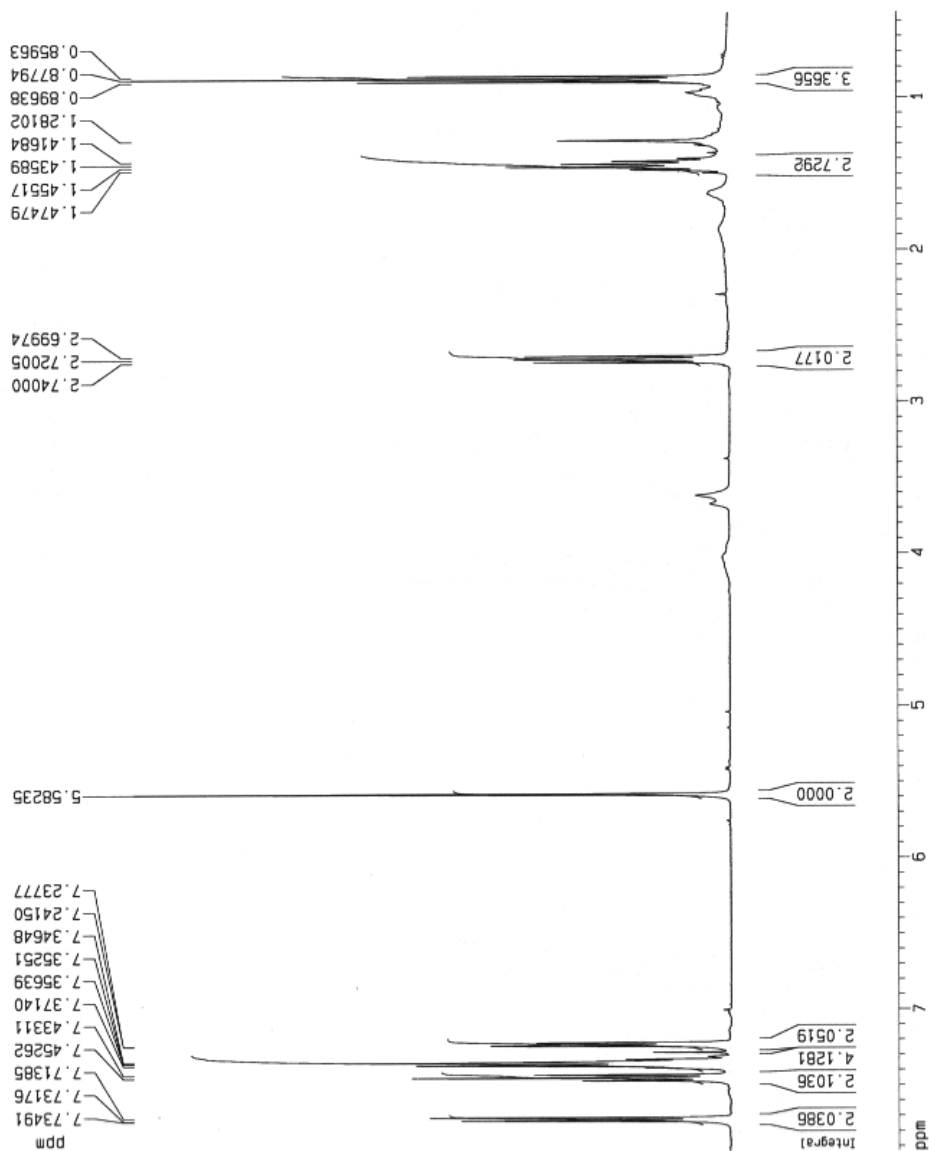
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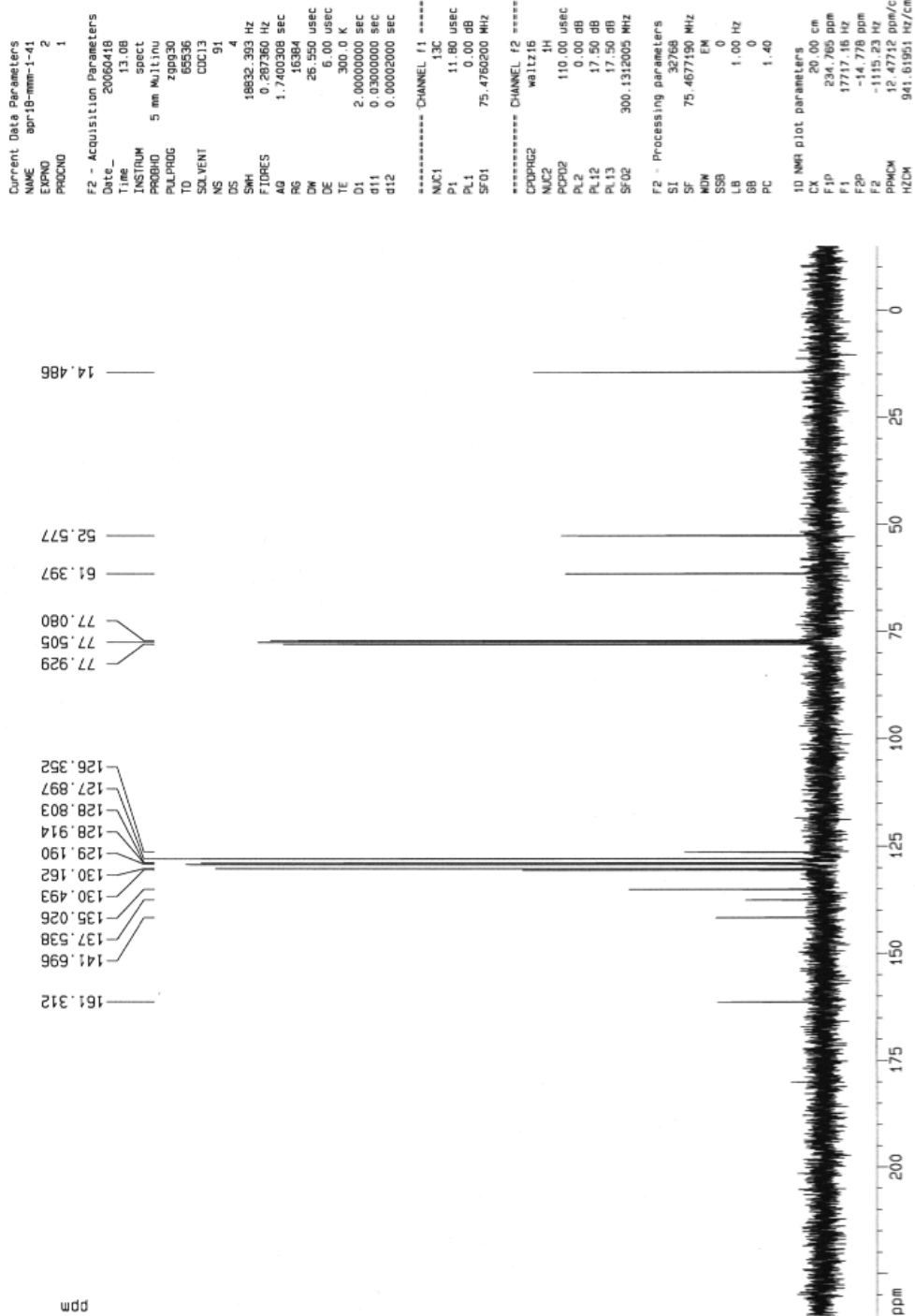
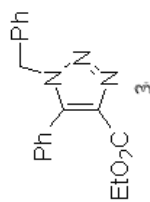
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 TD 65536
 SOLVENT CDCl3
 NS 1
 DS 0
 SWH 4401.409 Hz
 FIDRES 0.067160 Hz
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 RG 64
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 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

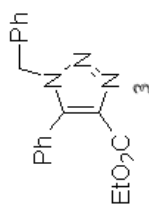
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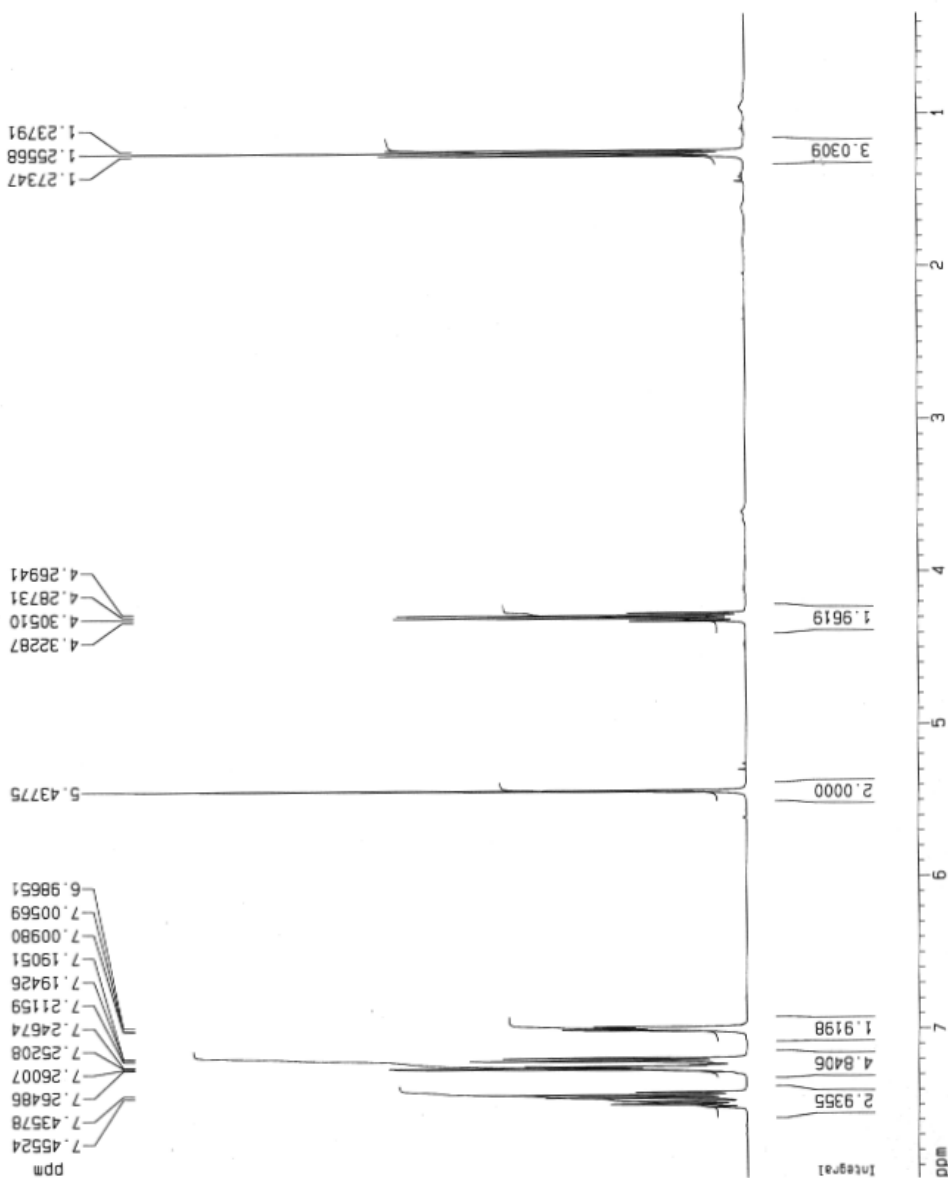
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 F2P 0.442 ppm
 F2 176.96 Hz
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 HZCM 149.81435 Hz/cm

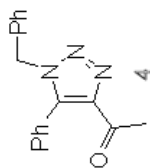






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 Time 9.14
 INSTRUM spect
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 PULPROG zg30
 TD 33110
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.250019 Hz
 AQ 1.9998940 sec
 RG 64
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CK 20.00 cm
 F1P 7.983 ppm
 F1 3194.15 Hz
 F2P 0.343 ppm
 F2 137.29 Hz
 PPM0M 0.30198 ppm/cm
 HZ0M 152.84308 Hz/cm





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EXPNO 1
PROCNO 1

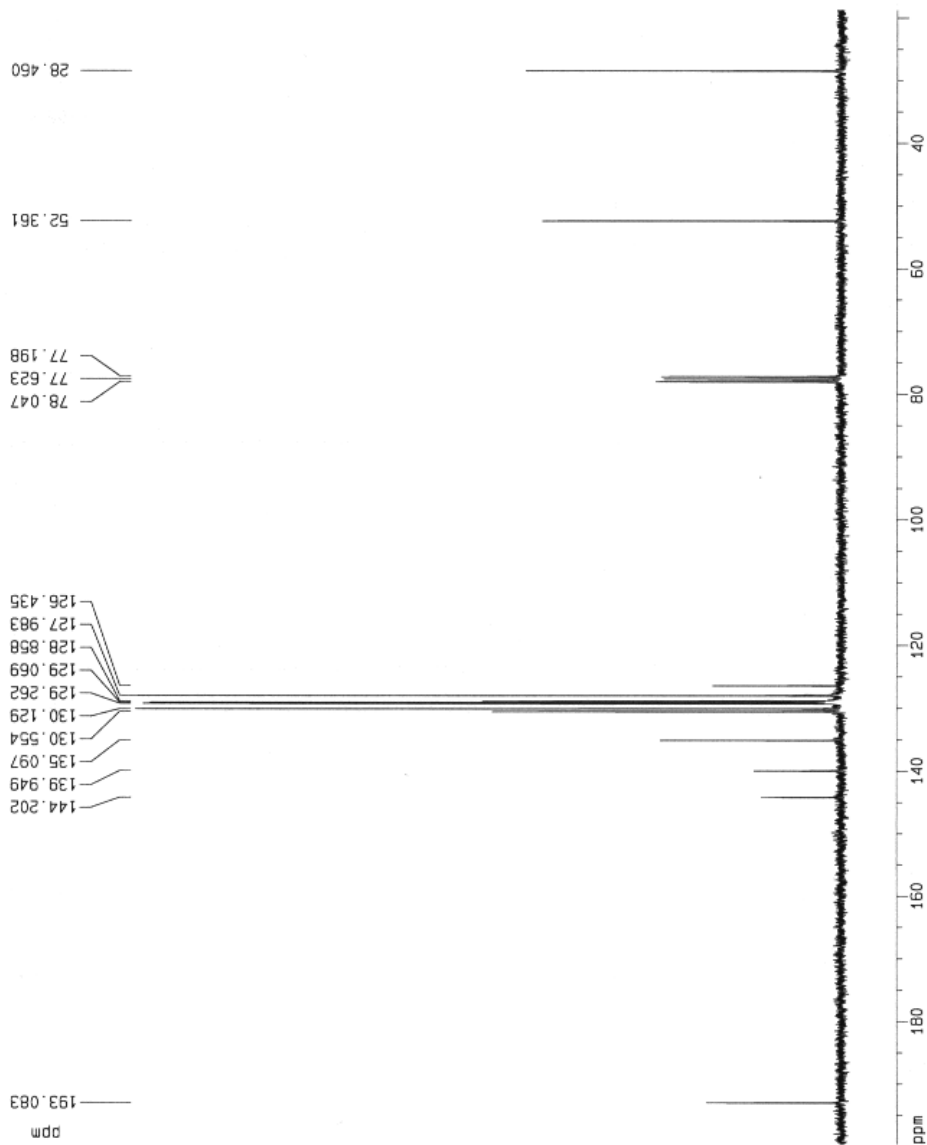
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Date_ 20060805
Time 15.07
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PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 101
DS 4
SWH 18796.992 Hz
FIDRES 0.288819 Hz
AQ 1.7433076 sec
RG 1625.5
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DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

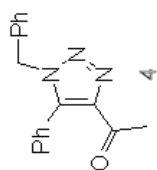
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NUC1 13C
P1 5.40 usec
PL1 -6.00 dB
SF01 75.4106357 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 0.00 dB
PL12 20.00 dB
PL13 20.00 dB
SF02 299.8711995 MHz

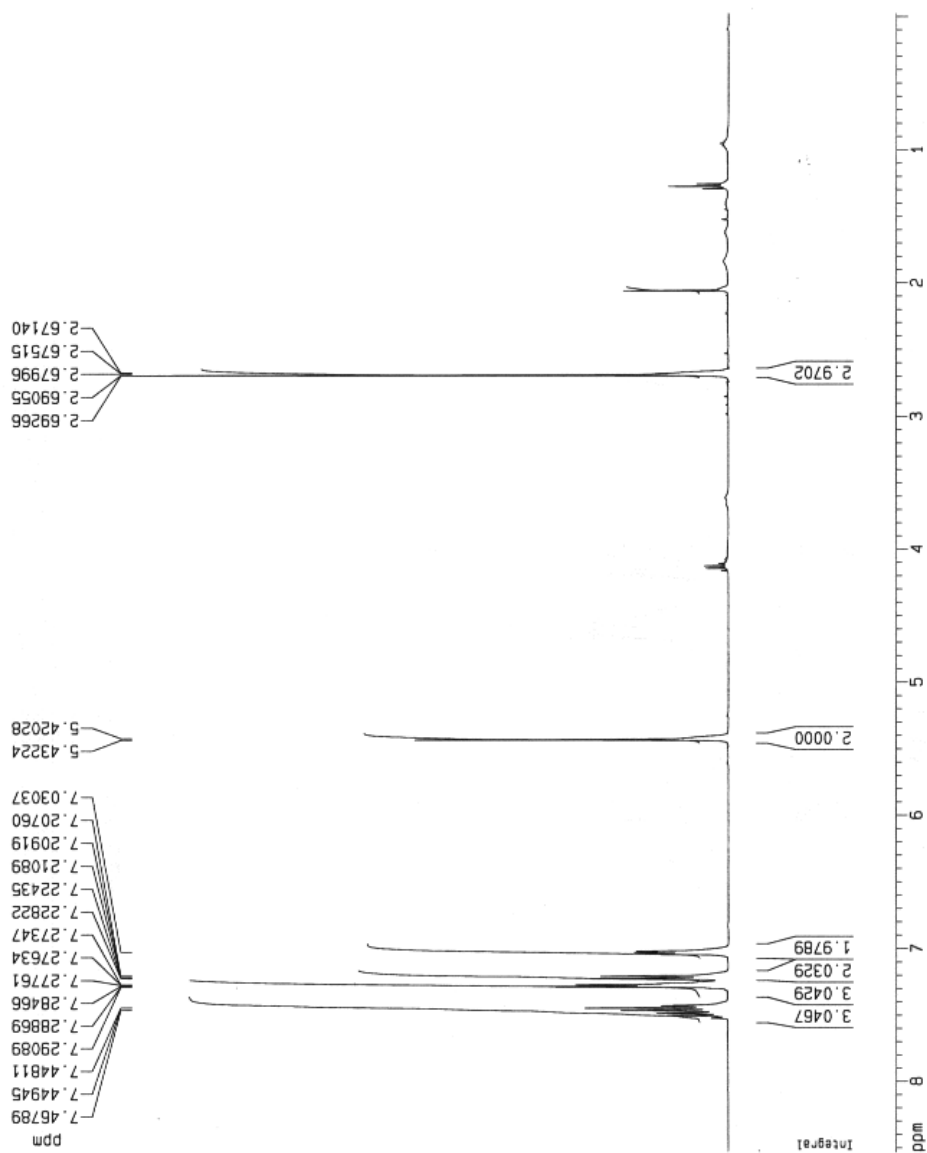
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

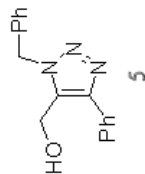
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F1 15054.46 Hz
F2P 18.752 ppm
F2 1413.95 Hz
PPMCM 9.04515 ppm/cm
HZCM 682.02515 Hz/cm





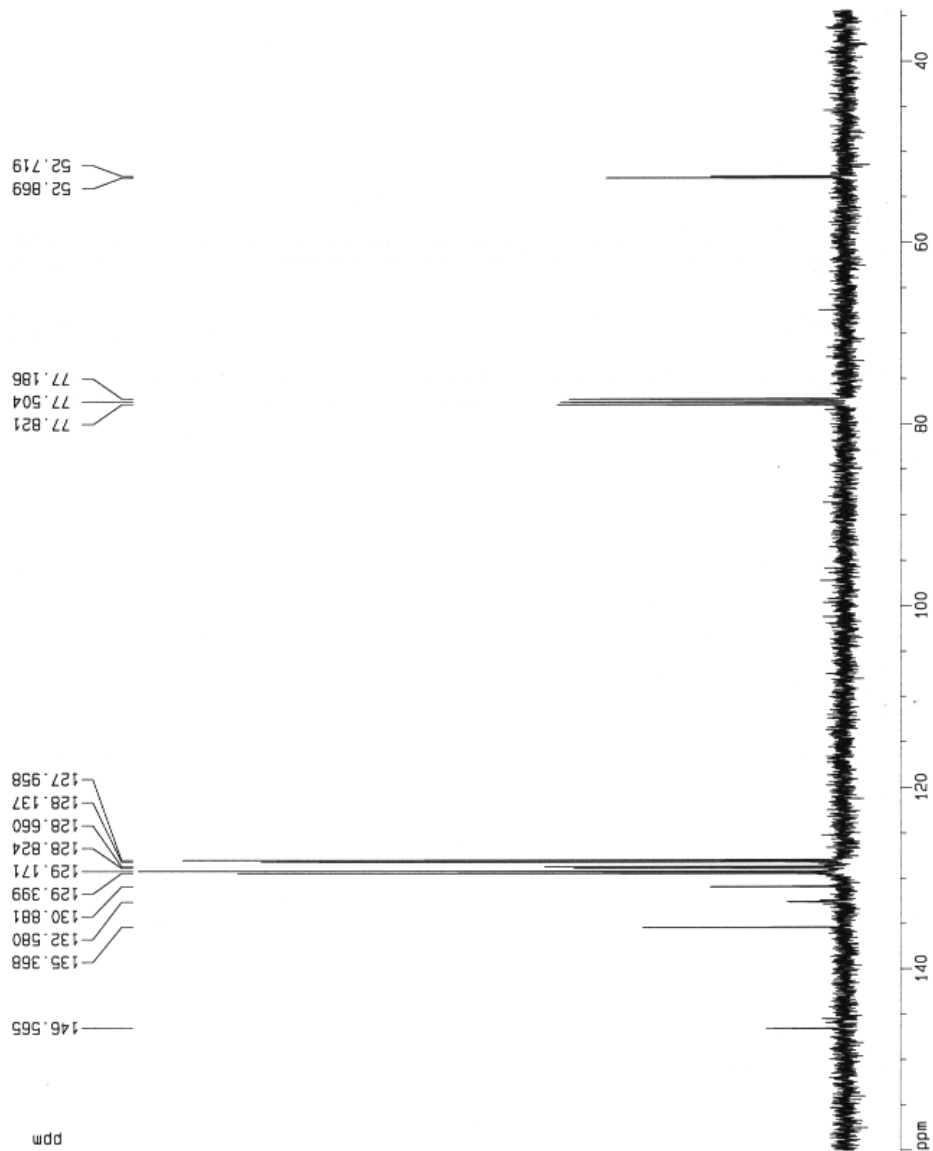
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 PROCNO 1
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 PULPROG zg30
 TD 33110
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.250019 Hz
 AQ 1.9998940 sec
 RG 203.2
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 20.00 cm
 FJP 8.531 ppm
 F1 3413.64 Hz
 F2P -0.026 ppm
 F2 -10.31 Hz
 PPMCM 0.42785 ppm/cm
 HZCM 171.19725 Hz/cm

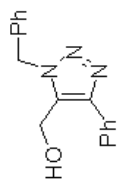




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Current Data Parameters
NAME 80r28-mm-1-44
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060426
Time 15.37
INSTRUM spect
PROBHD 5 mm BBI 1H-6
PULPROG zgpg30
TD 65536
SOLVENT CUC13
NS 105
DS 4
SWH 25125.629 Hz
FIDRES 0.363387 Hz
AQ 1.3042164 sec
RG 16384
DM 19.900 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 16.36 usec
PL1 -6.00 dB
SF01 100.6237959 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 114.00 usec
PL2 0.00 dB
PL12 24.00 dB
PL13 24.00 dB
SF02 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EN
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
FIP 160.032 ppm
F1 16101.22 Hz
F2P 34.408 ppm
F2 3461.89 Hz
PPMCM 6.28117 ppm/cm
HZCM 631.96619 Hz/cm





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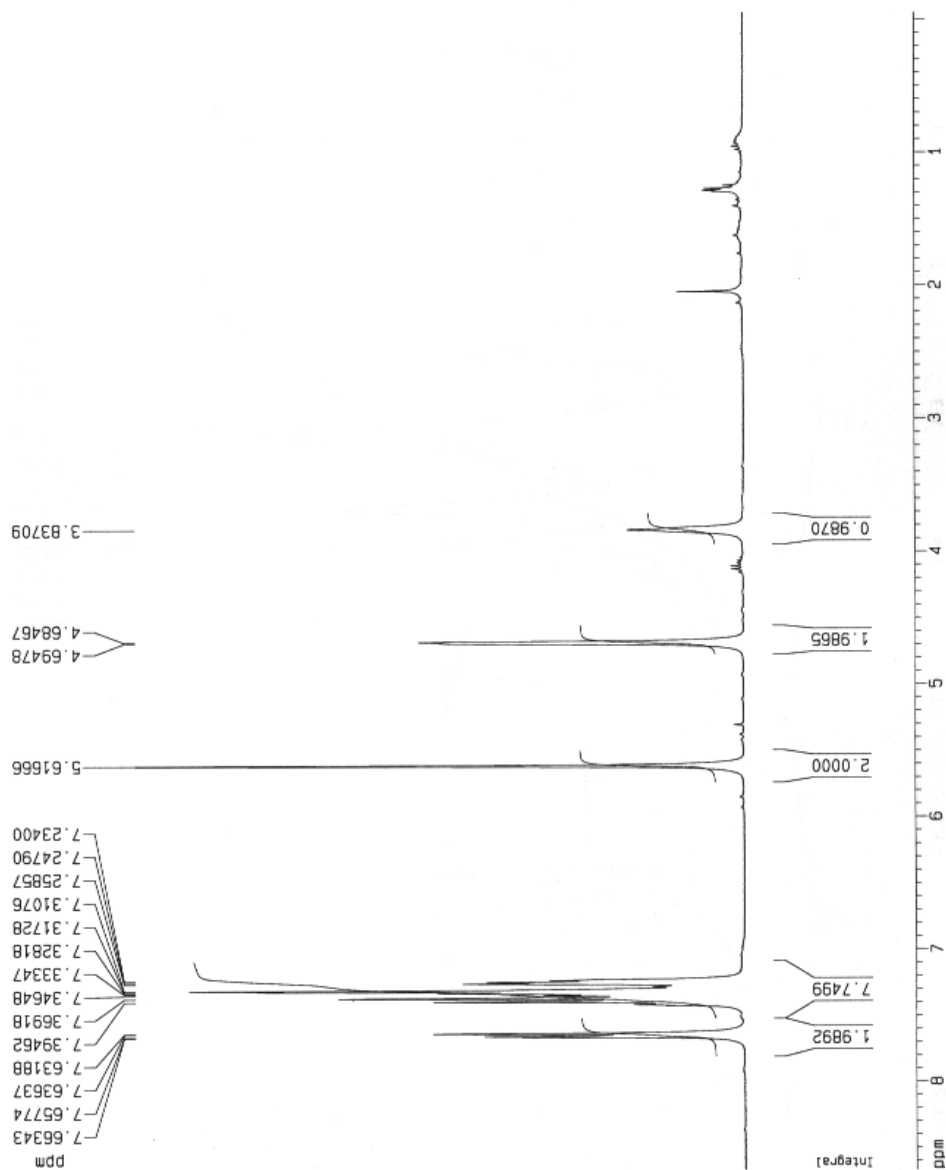
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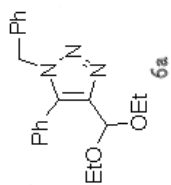
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Time 17.34
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PROBHD 5 mm Multinu
PULPROG zg30
TD 24690
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.250014 Hz
AQ 1.9999400 sec
RG 256
DM 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 ¹H
P1 9.60 usec
PL1 -6.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1p 8.667 ppm
F1 2501.20 Hz
F2p -0.053 ppm
F2 -15.02 Hz
PPMCM 0.43602 ppm/cm
HZCM 130.86127 Hz/cm





Current Data Parameters
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 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters

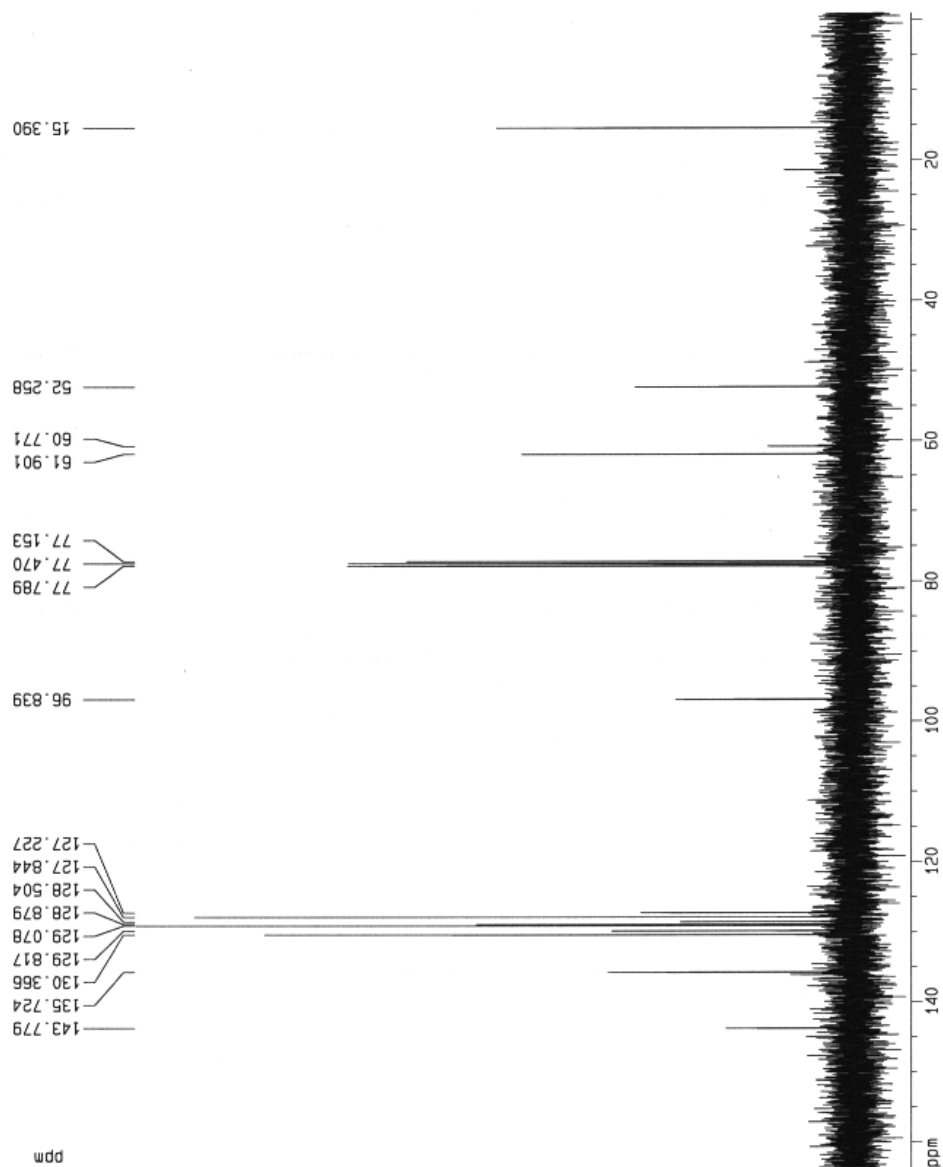
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 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 101
 DS 4
 SWH 25125.629 Hz
 AQ 1.3042164 sec
 RG 16384
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 DE 6.00 usec
 TE 300.0 K
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 d11 0.03000000 sec
 d12 0.00002000 sec

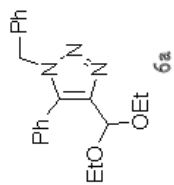
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 PL1 -6.00 dB
 SF01 100.6237959 MHz

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 PL2 0.00 dB
 PL12 24.00 dB
 PL13 24.00 dB
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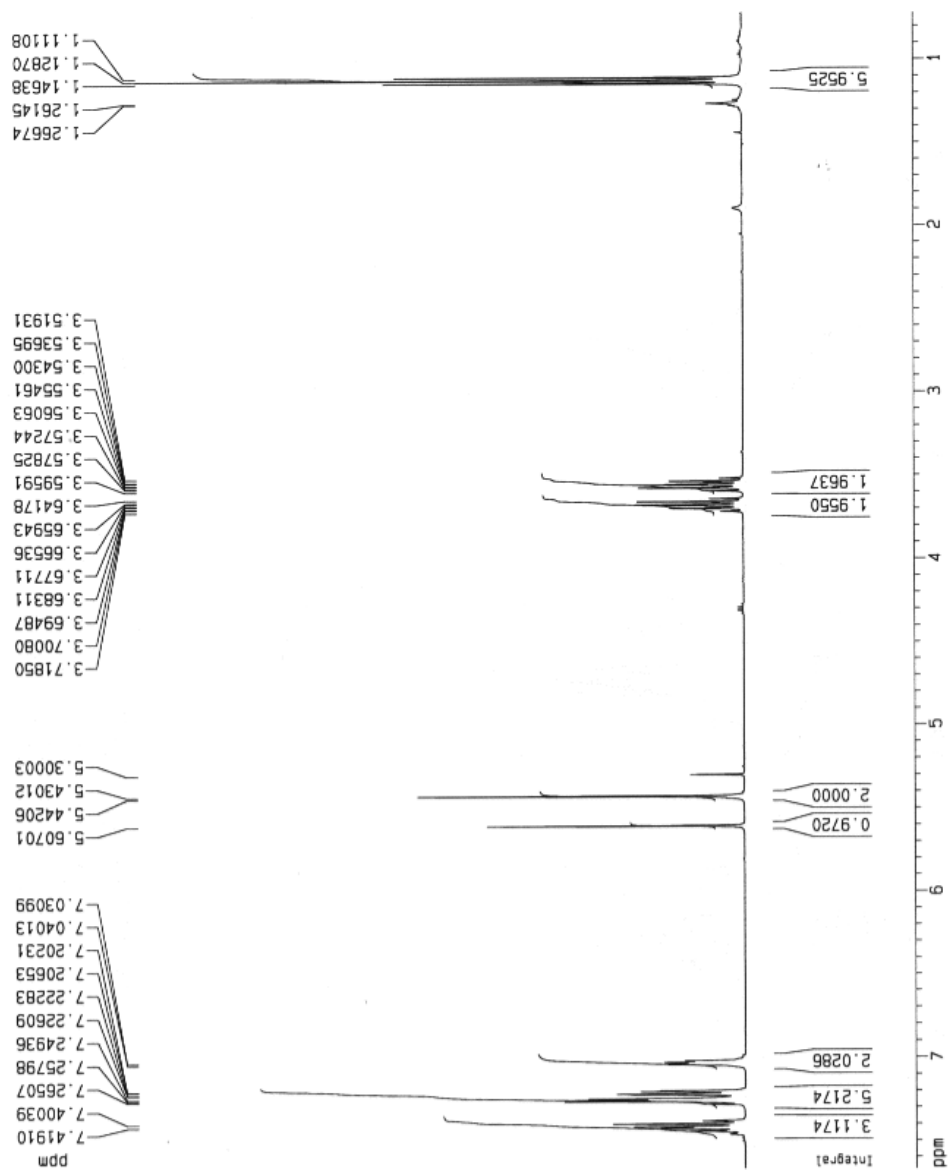
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1D NMR plot parameters
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 F1 16468.77 Hz
 F2 -0.943 ppm
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 HZCM 828.18666 Hz/cm



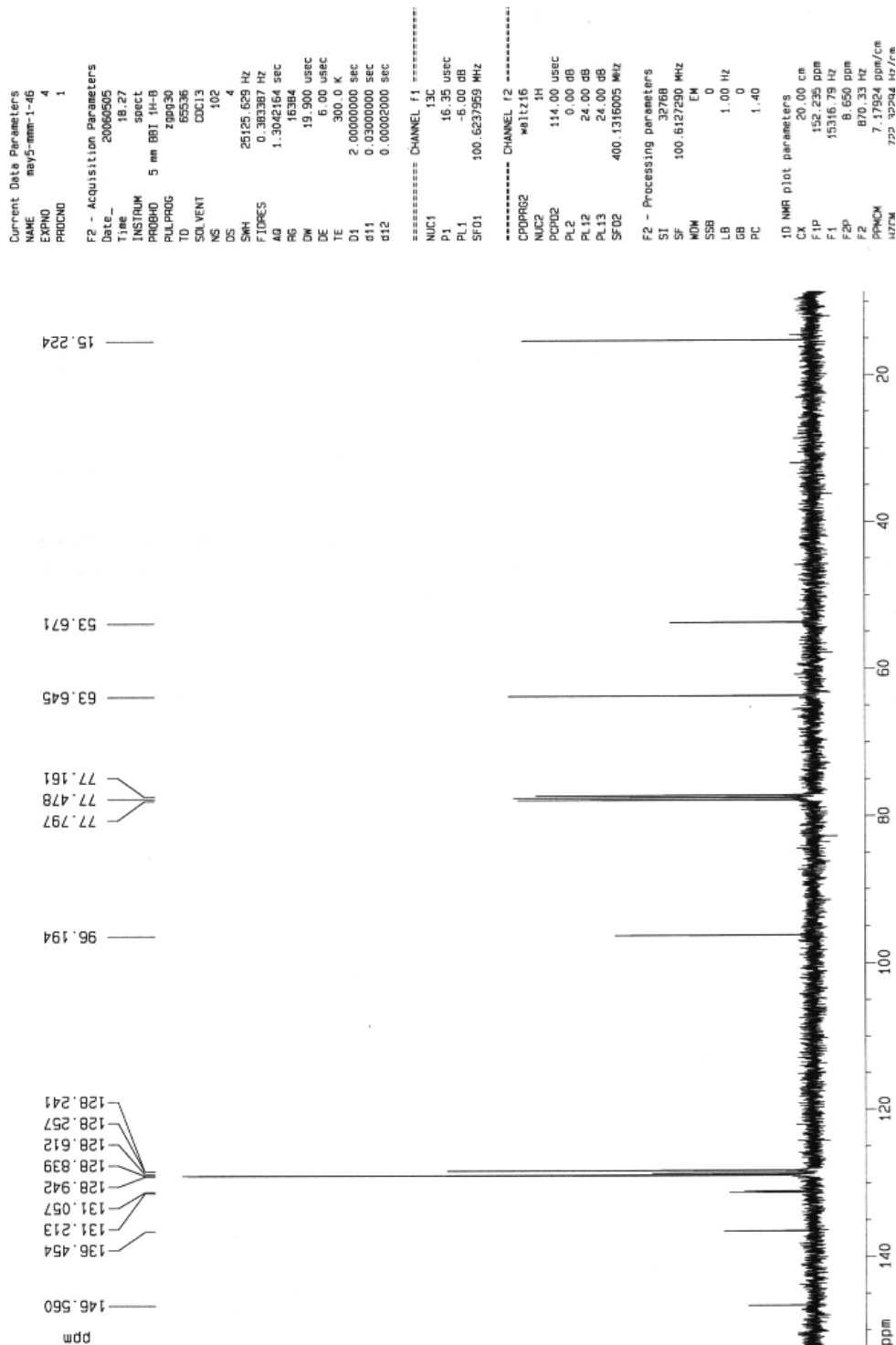


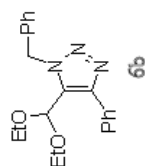
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Time 18.20
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PULPROG zg
TO 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 4222.973 Hz
FIDRES 0.064437 Hz
AQ 7.7595124 sec
RG 50.8
DM 118.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
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NUC1 1H
P1 7.26 usec
PL1 0.00 dB
SF01 400.1317043 MHz
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1p 7.670 ppm
F1 3066.67 Hz
F2p 0.720 ppm
F2 286.00 Hz
PPMCM 0.34750 ppm/cm
HZCM 139.04336 Hz/cm





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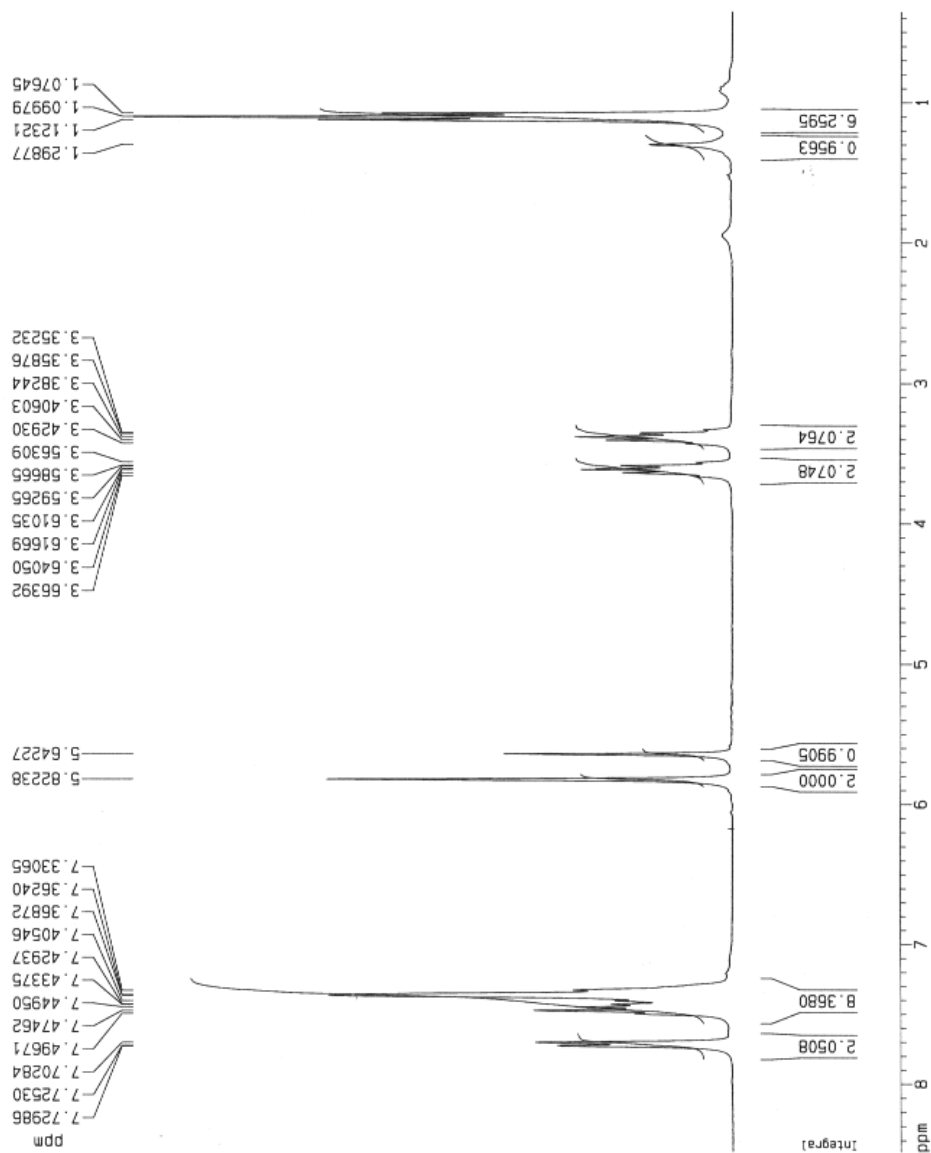
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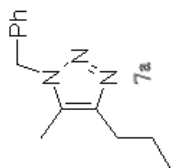
F2 - Acquisition Parameters
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 Time 17.39
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 PULPROG zgpg30
 TO 24690
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.250014 Hz
 AQ 1.9999400 sec
 RG 161.3
 DM 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.70 usec
 PL1 0.00 dB
 SF01 299.8718518 MHz

F2 - Processing parameters
 SI 32768
 SF 299.8700000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.484 ppm
 F1 2544.10 Hz
 F2P 0.356 ppm
 F2 106.70 Hz
 PPM0H 0.40641 ppm/cm
 HZ0H 121.87032 Hz/cm





Current Data Parameters
 NAME mm-1-55
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

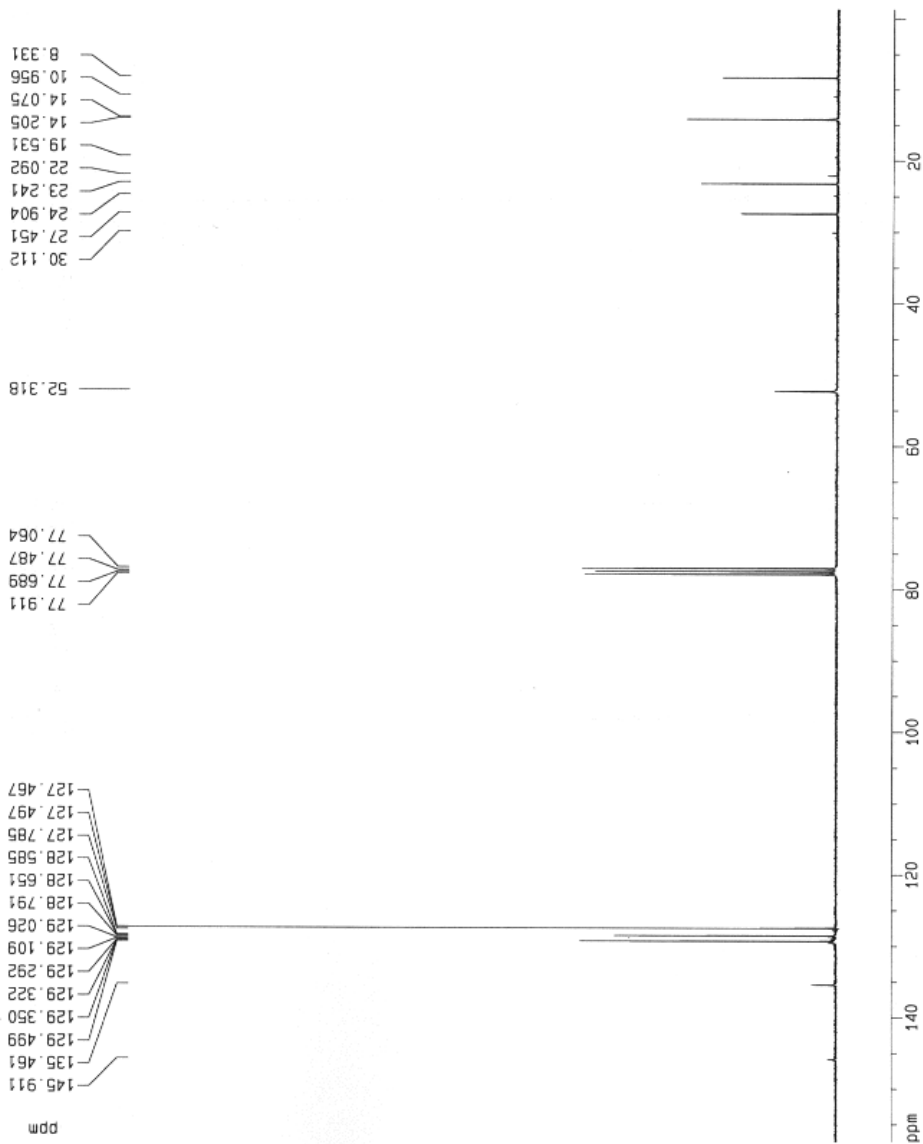
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 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 12595
 DS 4
 SWH 16736.952 Hz
 FIDRES 0.286819 Hz
 AQ 1.7433076 sec
 RG 8192
 DW 26.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.0002000 sec

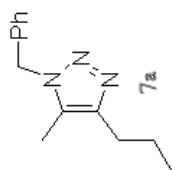
***** CHANNEL f1 *****
 NUC1 13C
 P1 5.40 usec
 PL1 -6.00 dB
 SF01 75.4106357 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 115.00 usec
 PL2 0.00 dB
 PL12 20.00 dB
 PL13 20.00 dB
 SF02 299.8711995 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4023410 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 157.476 ppm
 F1 11674.08 Hz
 F2P -1.242 ppm
 F2 -93.63 Hz
 PPMCM 7.93590 ppm/cm
 HZCM 588.38556 Hz/cm





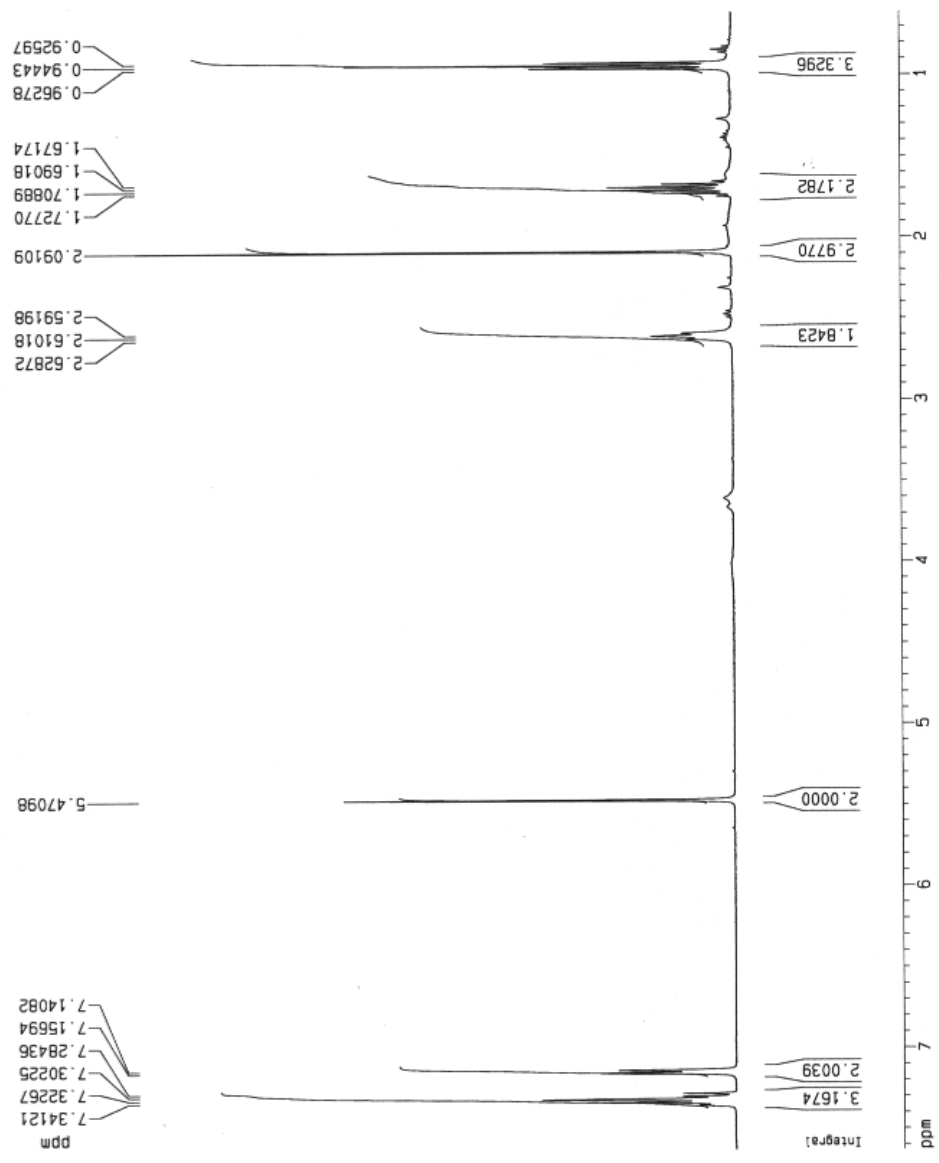
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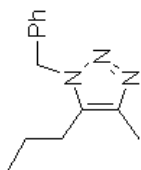
F2 - Acquisition Parameters
 Date_ 20060530
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 INSTRUM spect
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 1
 DS 2
 SNH 4194.631 Hz
 FIDRES 0.064005 Hz
 AQ 7.8119411 sec
 RG 32
 DM 119.200 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.16 usec
 PL1 0.00 dB
 SF01 400.1317125 MHz

F2 - Processing parameters
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 SF 400.1300000 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

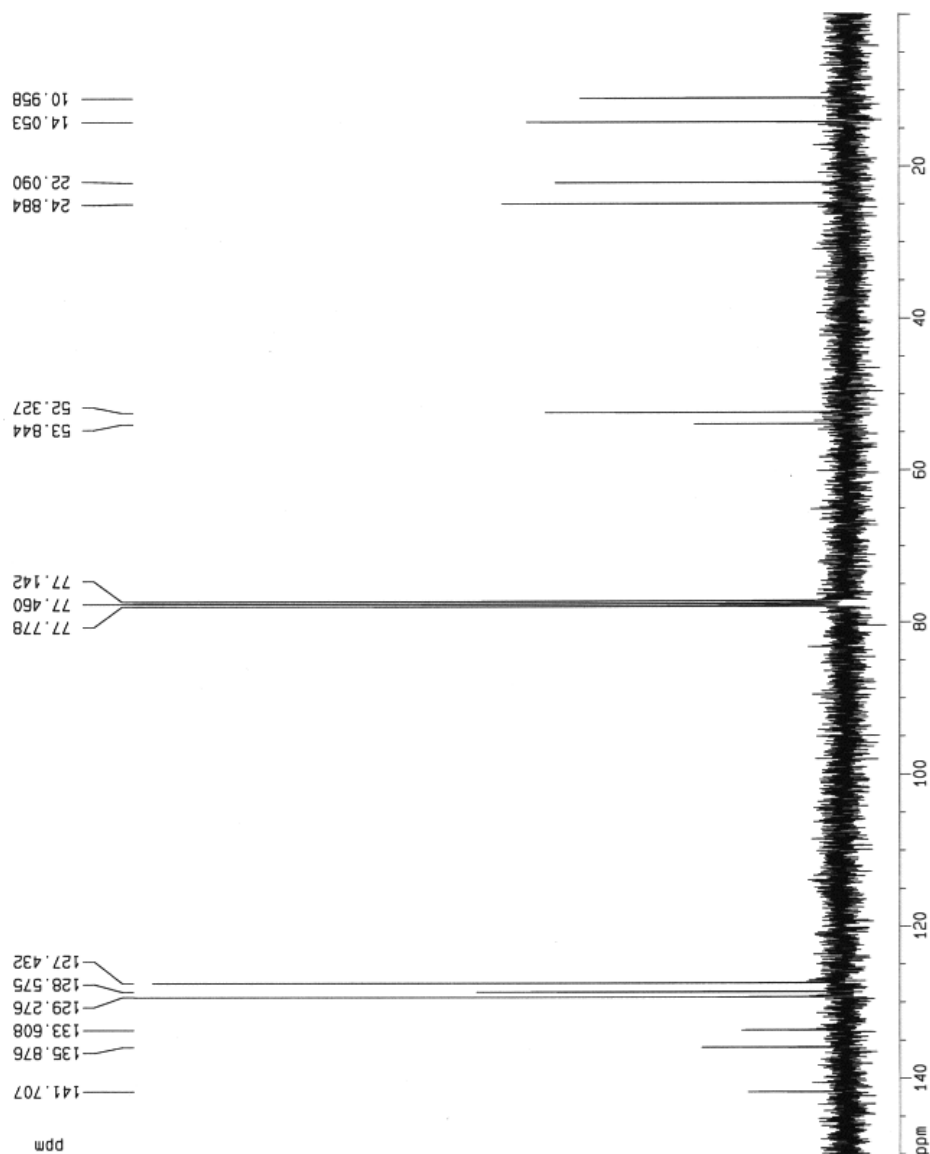
1D NMR plot parameters
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 F1P 7.632 ppm
 F1 3053.94 Hz
 F2P 0.612 ppm
 F2 245.08 Hz
 PPMCM 0.35099 ppm/cm
 HZCM 140.44315 Hz/cm

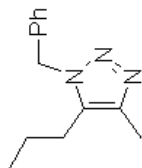




7b

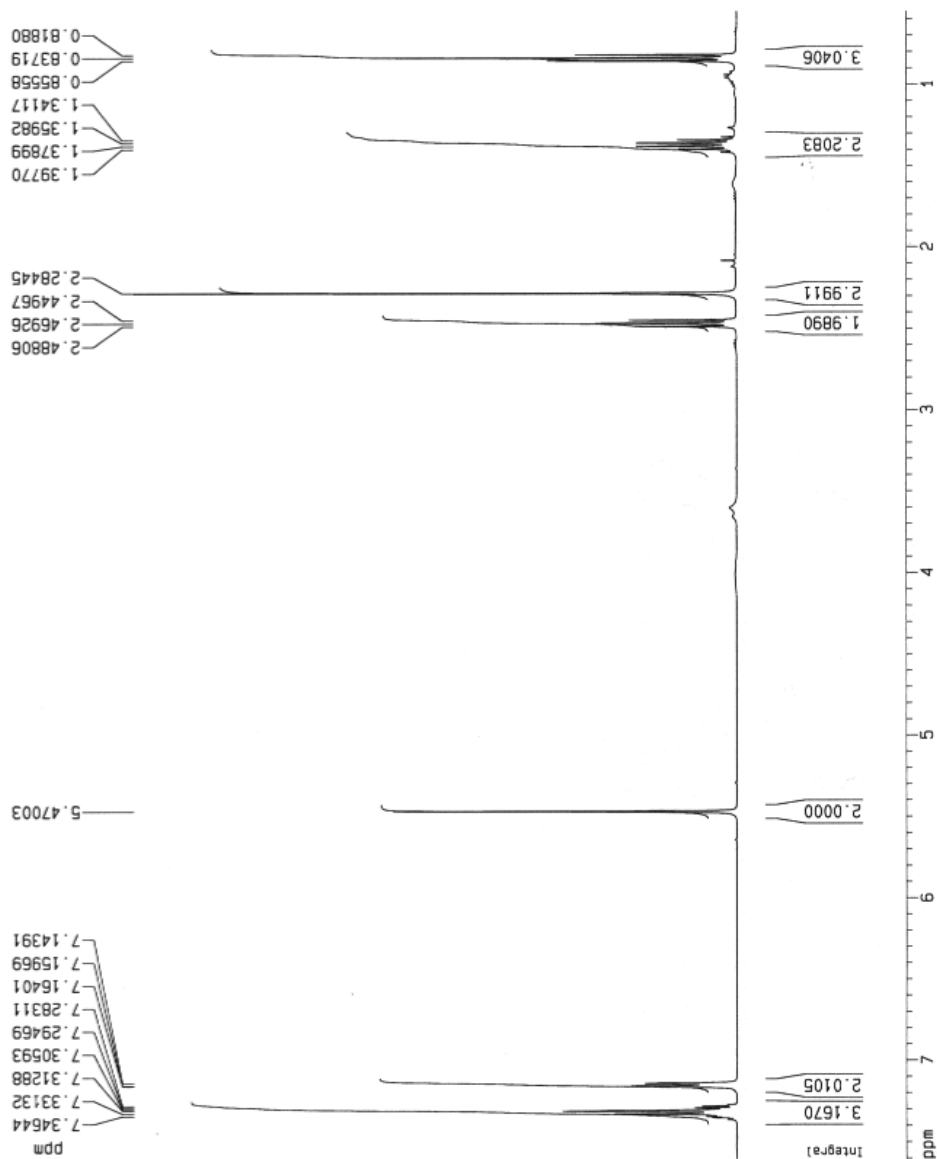
Current Data Parameters
 NAME may25-mm-1-56
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20060529
 Time 13.01
 INSTRUM spect
 PROBHD 5 mm BBI 1H-B
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 183
 DS 4
 SMH 25125.629 Hz
 FIDRES 0.383387 Hz
 AQ 1.3042164 sec
 RG 8192
 DM 19.900 usec
 DE 6.00 usec
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec
 ----- CHANNEL f1 -----
 NUC1 ¹³C
 P1 16.35 usec
 PL1 -6.00 dB
 SF01 100.6237959 MHz
 ----- CHANNEL f2 -----
 CPOPRG2 waltz16
 NUC2 ¹H
 PCPD2 114.00 usec
 PL2 0.00 dB
 PL12 24.00 dB
 PL13 24.00 dB
 SF02 400.1316005 MHz
 F2 - Processing parameters
 S1 32768
 SF 100.6127290 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 1D NMR plot parameters
 CA 20.00 cm
 F1P 150.184 ppm
 F1 1510.47 Hz
 F2P -0.142 ppm
 F2 -14.29 Hz
 PPMCM 7.51533 ppm/cm
 HZCM 756.23810 Hz/cm

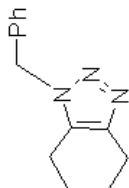




7b

Current Data Parameters
 NAME mm-1-5b-2
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20060524
 Time 18.46
 INSTRUM spect
 PROBHD 5 mm BBI 1H-B
 PULPROG zg
 TO 65536
 SOLVENT CDCl3
 NS 1
 DS 0
 SWH 4194.631 Hz
 FIDRES 0.064005 Hz
 AQ 7.8119411 sec
 RG 57
 DM 119.200 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 7.25 usec
 PL1 0.00 dB
 SF01 400.1316134 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 20.00 cm
 F1P 7.605 ppm
 F1 3043.54 Hz
 F2p 0.552 ppm
 F2 220.68 Hz
 PPMCM 0.35274 ppm/cm
 HZCM 141.14304 Hz/cm





8

Current Data Parameters
NAME Jun25-mm-1-77
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

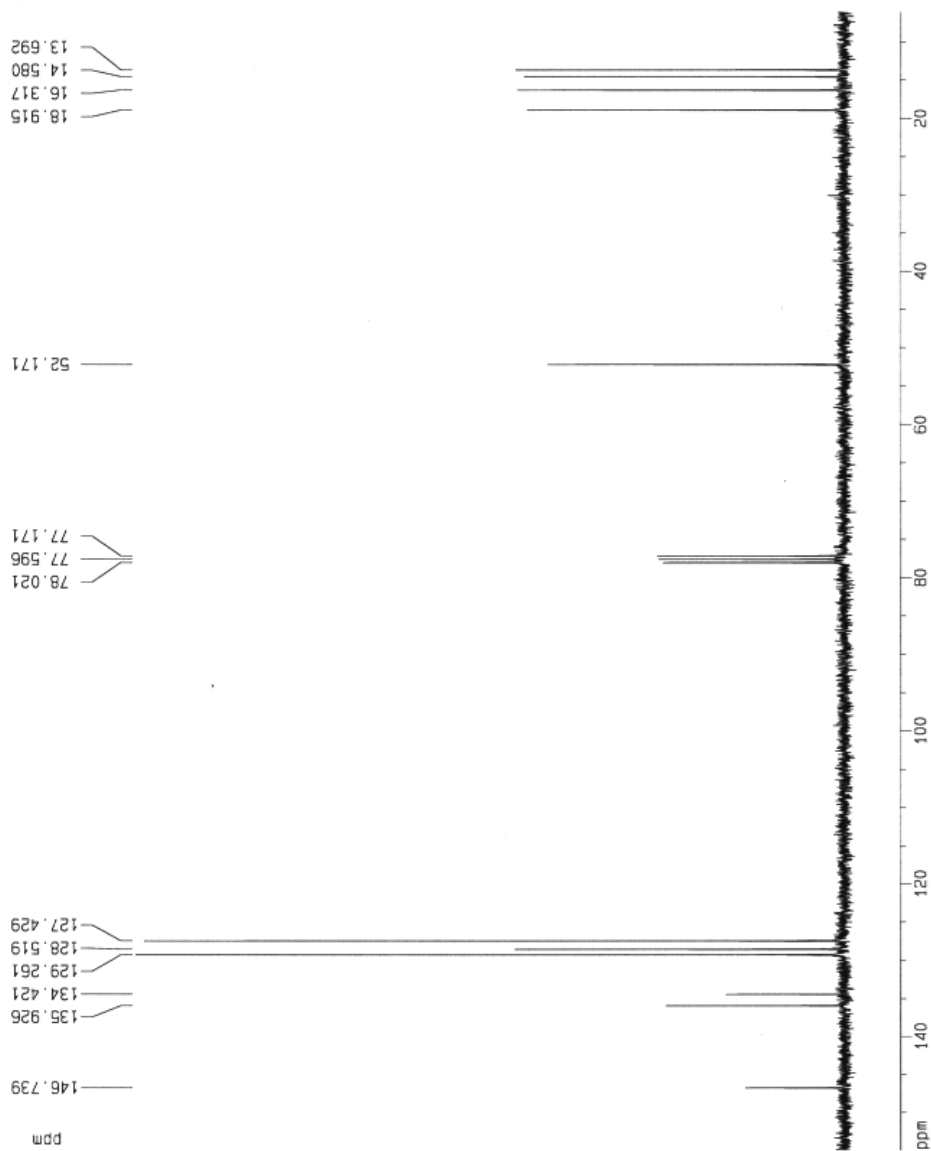
Date_ 20060629
Time 15.12
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 41
DS 4
SWH 18795.992 Hz
FIDRES 0.266819 Hz
AQ 1.7433076 sec
RG 1024
DM 26.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.0300000 sec
D12 0.0002000 sec

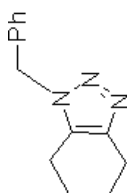
===== CHANNEL f1 =====
NUC1 13C
P1 5.40 usec
PL1 -6.00 dB
SF01 75.4106357 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 0.00 dB
PL12 20.00 dB
PL13 20.00 dB
SF02 299.8711995 MHz

F2 - Processing parameters
S1 32768
SF 75.4023410 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 154.932 DDM
F1 11681.49 Hz
F2P 6.105 DDM
F2 460.41 Hz
PPMCH 7.44680 ppm/cm
HZCH 561.05396 Hz/cm





8

Current Data Parameters

NAME Jun29-mm-1-77
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060629
Time 8.03
INSTRUM spect
PULPROG 5 mm GNP 1H/1
TD 2930
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 57
DM 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

----- CHANNEL f1 -----

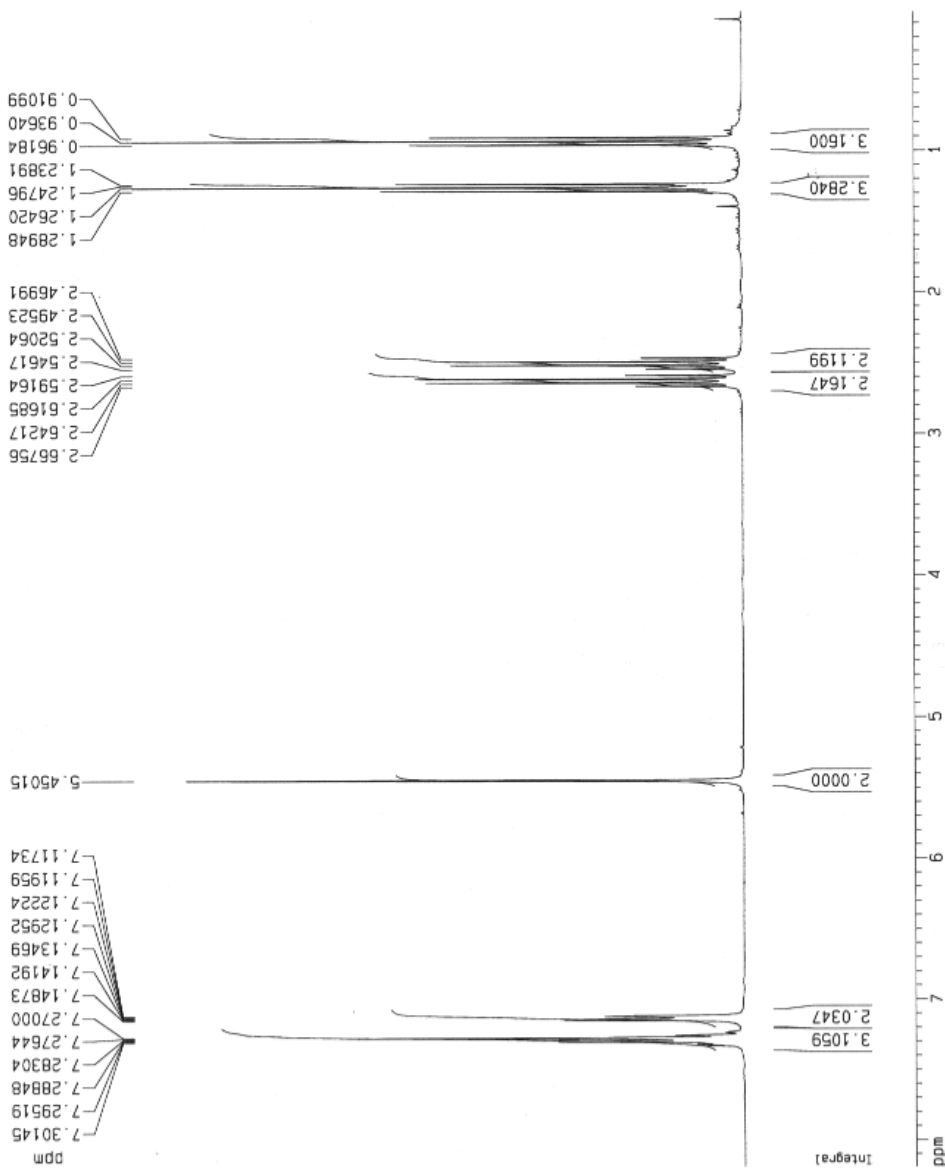
NUC1 1H
P1 11.70 usec
PL1 0.00 dB
SF01 299.8718518 MHz

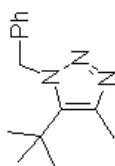
F2 - Processing parameters

SI 32768
SF 299.8700000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 8.192 ppm
F1 2456.54 Hz
F2P 0.021 ppm
F2 6.26 Hz
PPMCM 0.40856 ppm/cm
HZCM 122.51437 Hz/cm





9

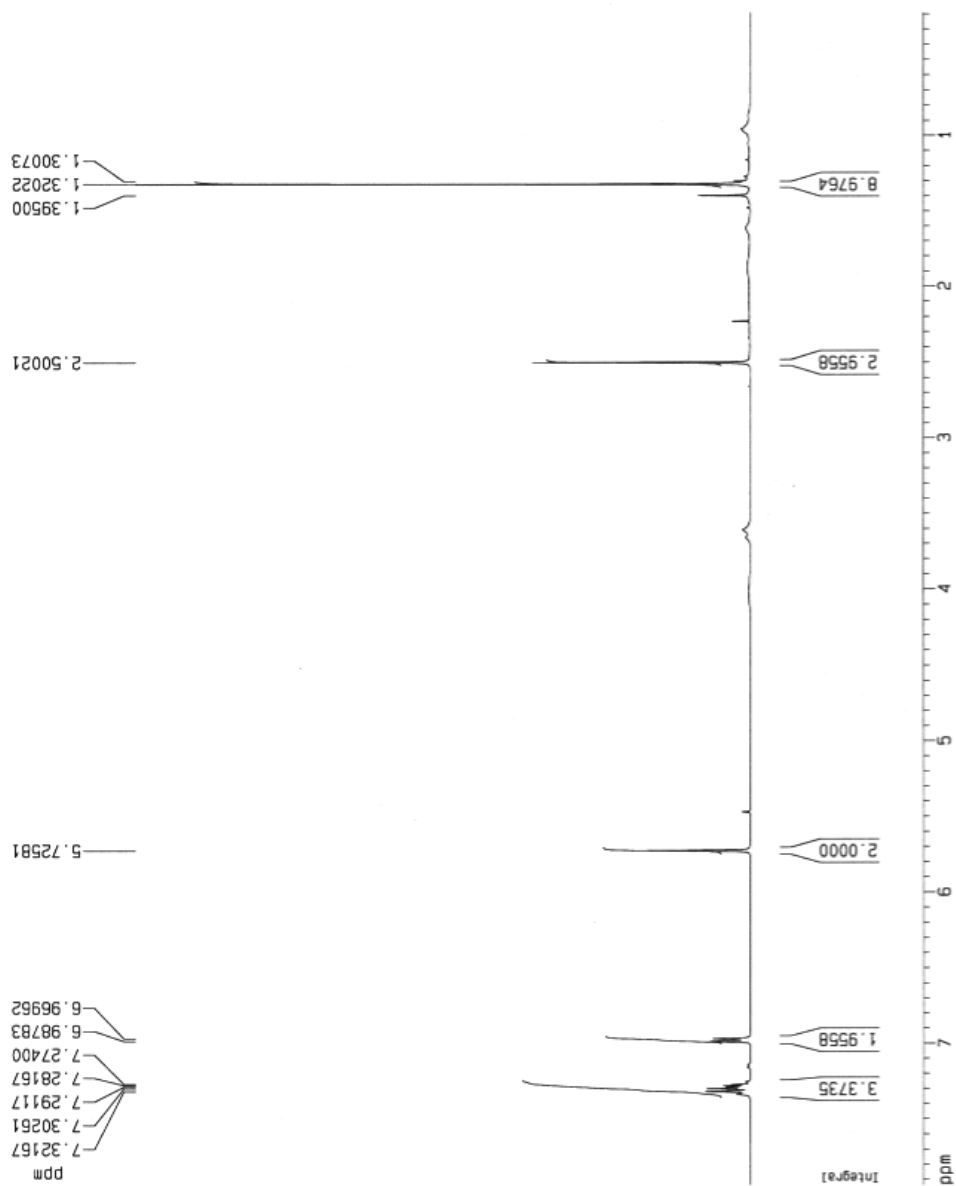
Current Data Parameters
NAME mm-1-86-1a
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060725
Time 21.46
INSTRUM spect
PROBHD 5 mm BBI 1H-B
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 128
DW 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec

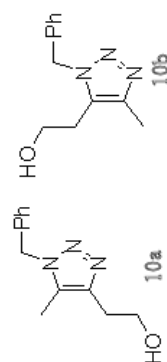
===== CHANNEL f1 =====
NUC1 1H
P1 6.45 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 7.936 ppm
F1 3175.26 Hz
F2P 0.191 ppm
F2 76.37 Hz
PPMCM 0.381723 ppm/cm
HZCM 154.94434 Hz/cm







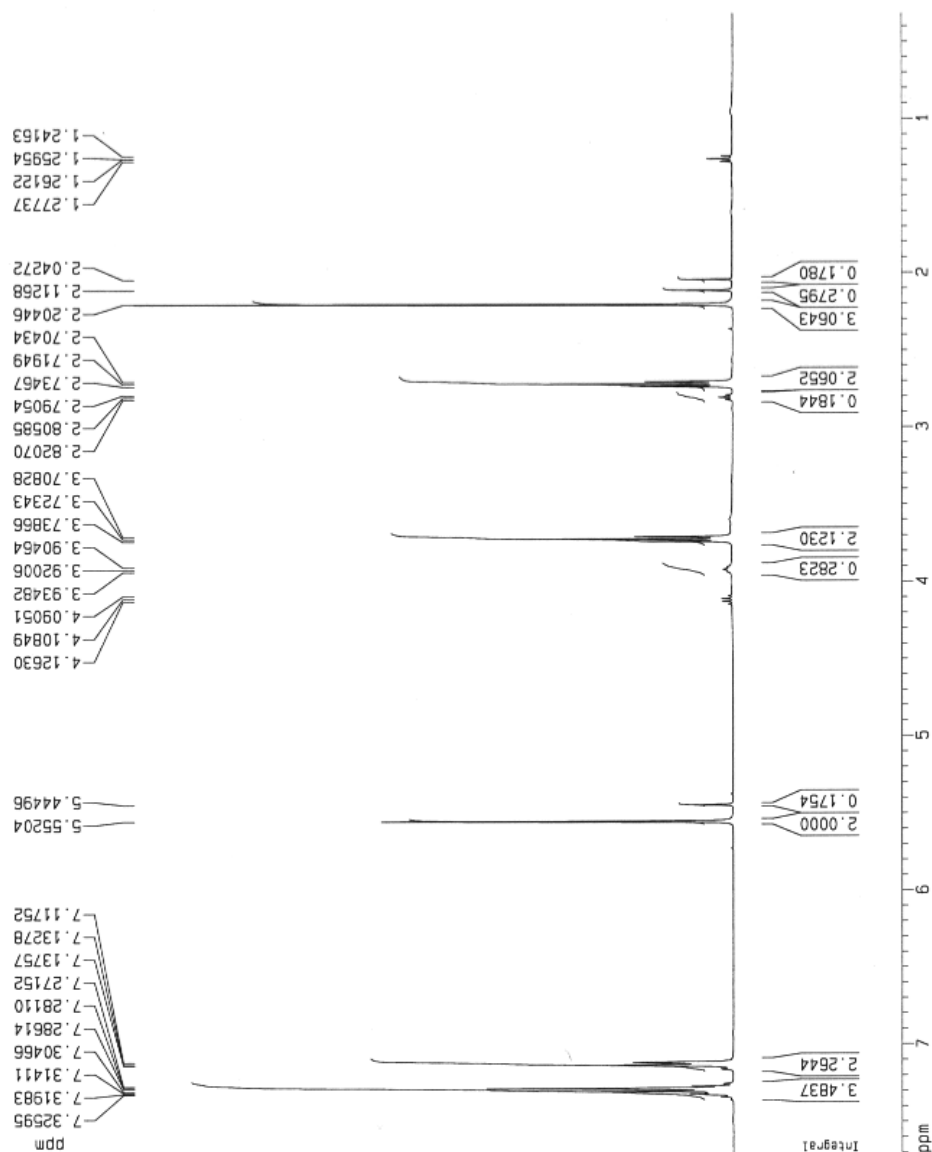
Current Data Parameters
NAME mm-1-8b-mix
EXPNO 1
PROCNO 1

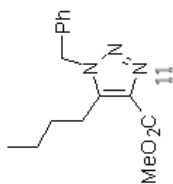
F2 - Acquisition Parameters
Date_ 20060731
Time 20.30
INSTRUM spect
PROBHD 5 mm BBI 1H-B
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 3634.356 Hz
FIDRES 0.058508 Hz
AQ 8.5459442 sec
RG 50.8
DM 130.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.63 usec
PL1 0.00 dB
SF01 400.1315728 MHz

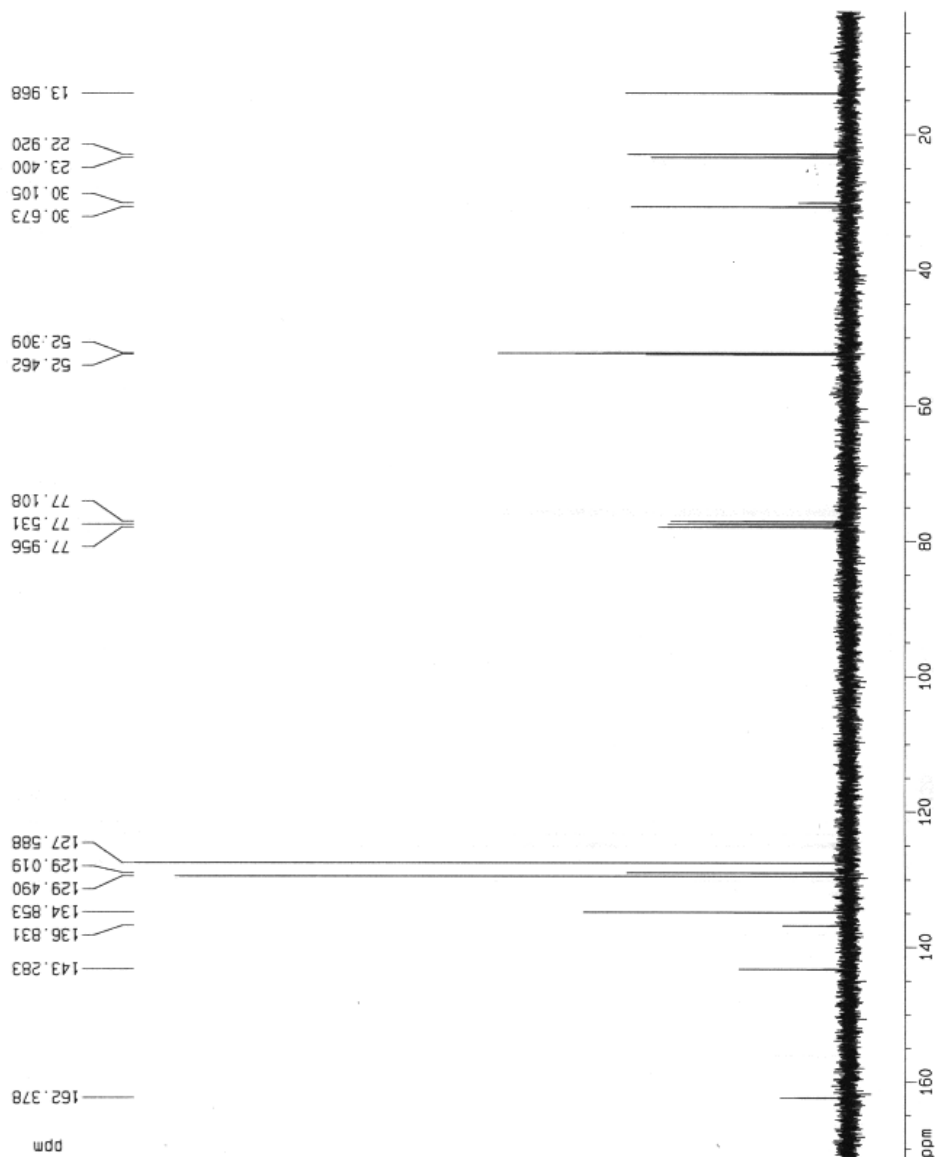
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

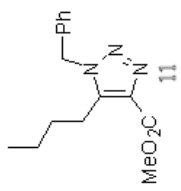
1D NMR plot parameters
CX 20.00 cm
F1P 7.710 ppm
F1 3084.98 Hz
F2P 0.317 ppm
F2 126.67 Hz
PPM0 0.3687 ppm/cm
HZCM 147.91545 Hz/cm





Current Data Parameters
NAME mmn-1-35
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060720
Time 21.37
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 49
DS 4
SWH 16796.992 Hz
FIDRES 0.286819 Hz
AQ 1.7433076 sec
RG 512
DM 26.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.0300000 sec
D12 0.0002000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 5.40 usec
PL1 -6.00 dB
SFO1 75.4106357 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 0.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 299.8711995 MHz
F2 - Processing parameters
SI 32768
SF 75.4023410 MHz
WDW ro
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
F1P 171.211 ppm
F1 12909.70 Hz
F2P 1.851 ppm
F2 139.55 Hz
PPHM 6.46801 ppm/cm
HZCM 638.50775 Hz/cm





Current Data Parameters

NAME MM-1-36
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060323
Time 16.59
INSTRUM spect
PQ08H0 5 mm BBI 1H-B
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 10
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 128
DM 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

----- CHANNEL f1 -----

NUC1 1H
P1 6.45 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters

SI 32768
SF 400.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 NMR plot parameters

CX 20.00 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.35000 ppm/cm
HZCM 220.07150 Hz/cm

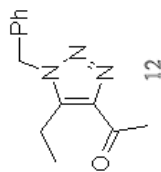
0.79803
0.81553
0.83266
1.22353
1.24202
1.25942
1.27554
1.28474
1.30837
2.82594
2.84502
2.86355
3.92121
5.53129
7.14791
7.16128
7.16692
7.27004
7.31037
7.32750
7.33640
7.34048

3.2965
2.1578
4.1106
2.0000
2.9796
2.0085
3.0439
2.0278

ppm

Integral





Current Data Parameters
 NAME jvl125-mm-1-87
 EXPNO 1
 PROCNO 1

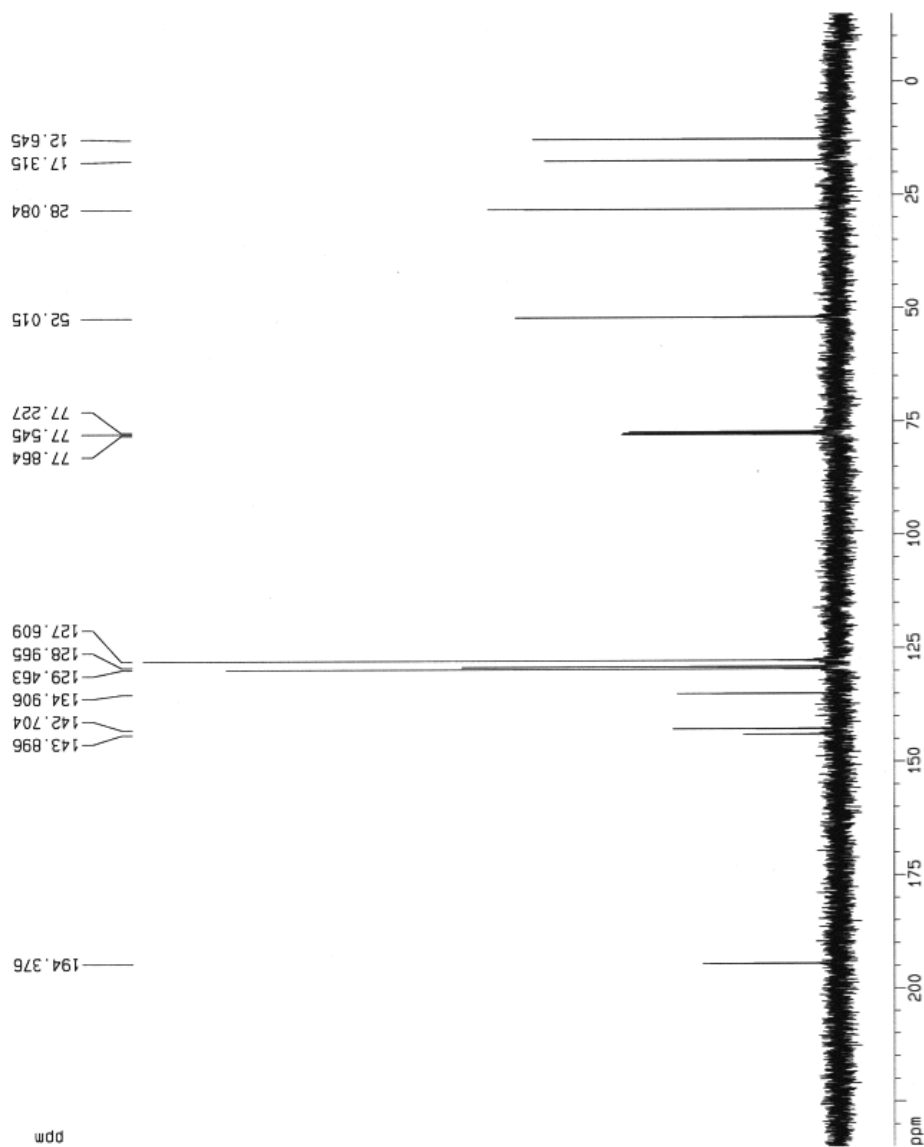
F2 - Acquisition Parameters
 Date_ 20060725
 Time 8.05
 INSTRUM spect
 PULPROG zgpg30
 TO 65336
 SOLVENT CDCl3
 NS 71
 DS 4
 SWH 25125.629 Hz
 FIDRES 0.363867 Hz
 AQ 1.3042184 sec
 RG 16384
 DM 19.900 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

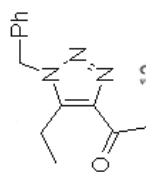
===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 16.35 usec
 PL1 -6.00 dB
 SF01 100.6237559 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCDP2 114.00 usec
 PL2 0.00 dB
 PL12 24.00 dB
 PL13 24.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127250 MHz
 WDM 0
 EQ 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 FIP 234.858 ppm
 F1 23629.72 Hz
 F2 -14.868 ppm
 F2 -1495.90 Hz
 PPMCM 12.48631 ppm/cm
 HZCM 1256.28137 Hz/cm





12

Current Data Parameters
NAME mm-1-B7
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060724
Time_ 18.47
INSTRUM spect
PROBHD 5 mm BBI 1H-5
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 32
DM 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec

***** CHANNEL f1 *****

NUC1 1H
P1 6.45 usec
PL1 0.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters

SI 32768
SF 400.1300000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 7.732 ppm
F1 3093.74 Hz
F2P 0.285 ppm
F2 113.59 Hz
PPMCM 0.37235 ppm/cm
HZCM 146.98746 Hz/cm

0.96780
0.94907
0.94797
0.93021

2.91728
2.89845
2.87958
2.86074
2.67111
2.66923

5.51433

7.32335
7.31033
7.30495
7.18285
7.18170
7.17985
7.17781
7.17697
7.16294
7.16127

3.1417

3.1518

2.1856

2.0000

2.1150

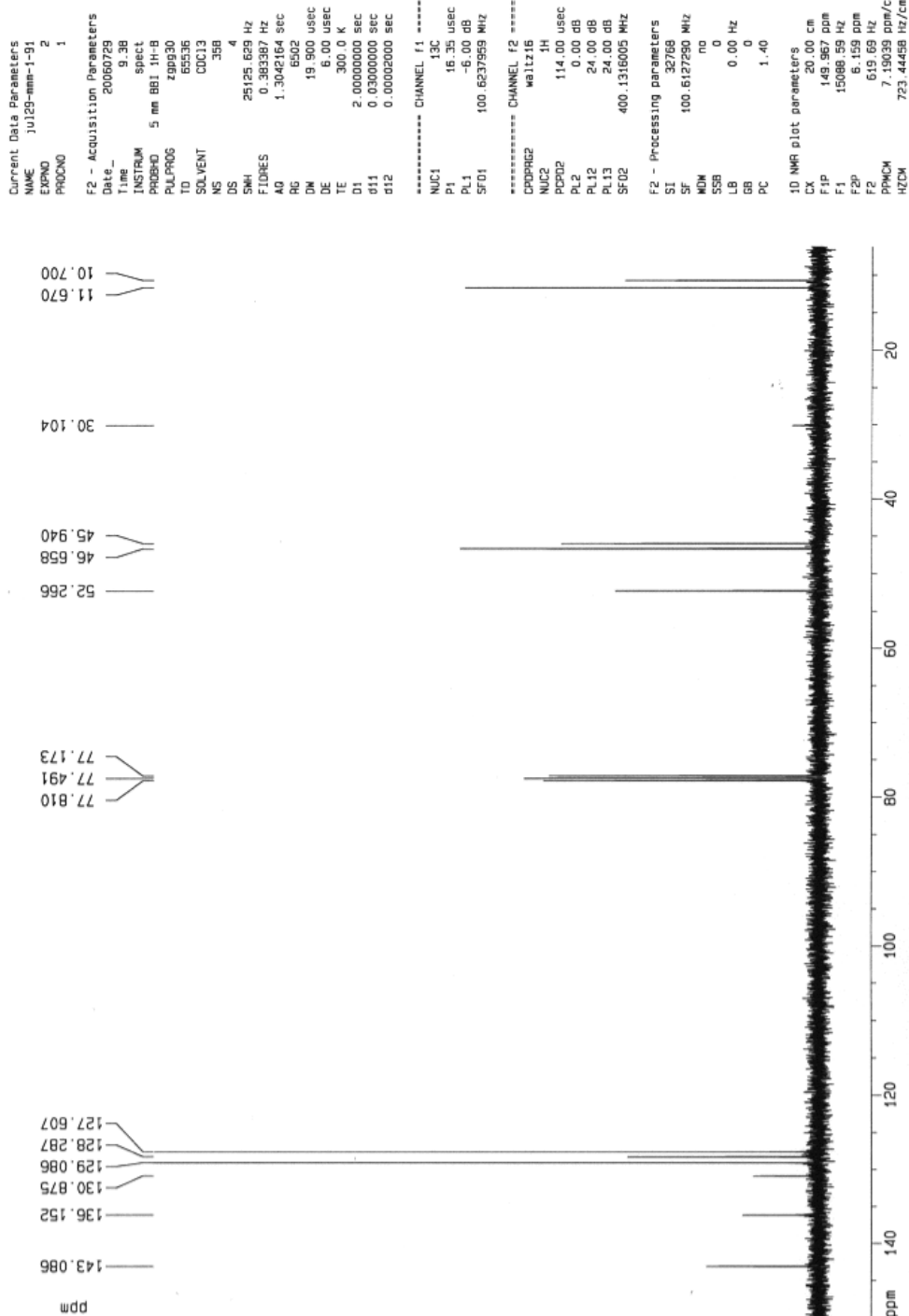
3.9974

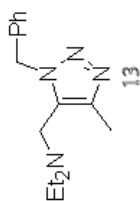
Integral



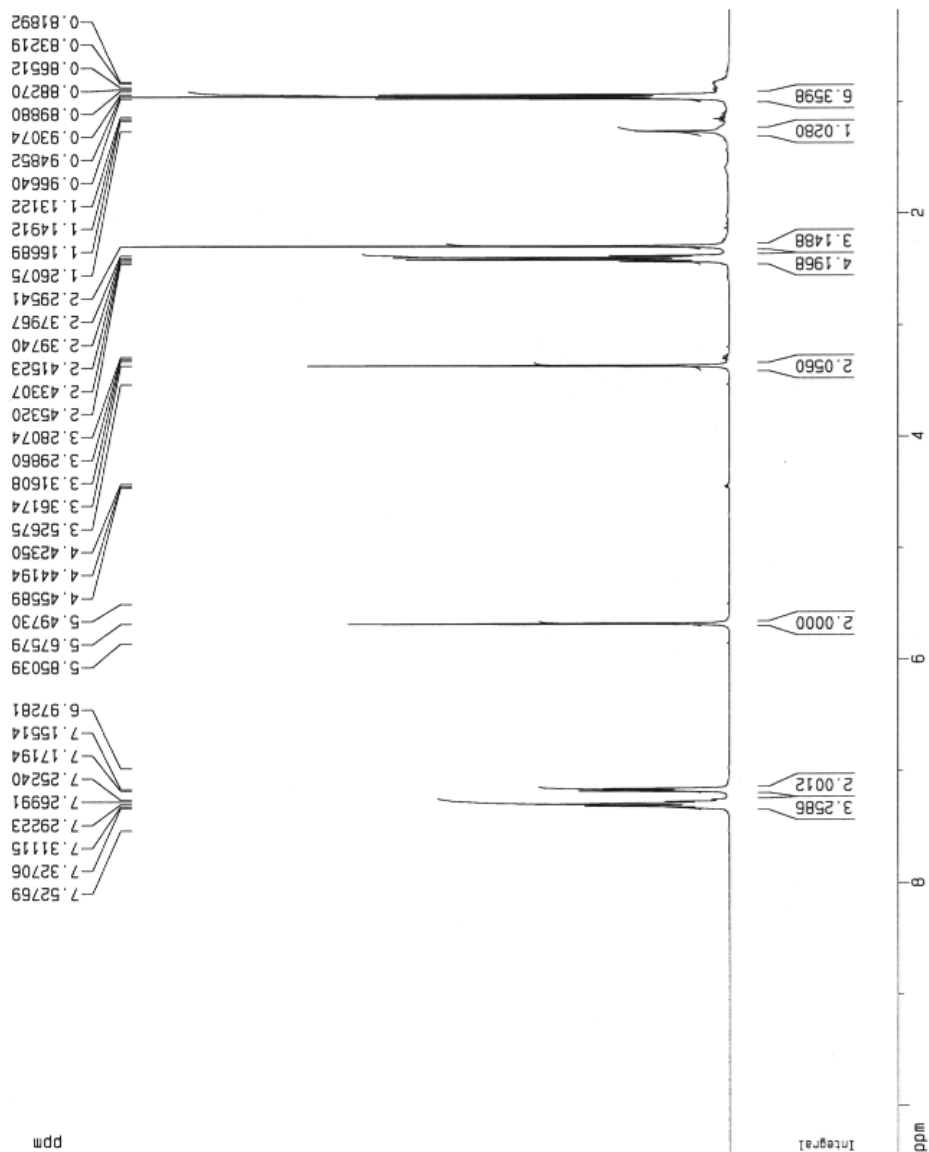


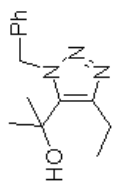
13





Current Data Parameters
 NAME j0129-mm-1-91
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20060729
 Time 8.56
 INSTRUM spect
 PULPROG 5 mm BBT 1H-8
 TO 2930
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8278.145 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 35.9
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 ***** CHANNEL f1 *****
 NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00
 ID NMR plot parameters
 CX 20.00 cm
 F1P 10.422 ppm
 F1 4170.05 Hz
 F2P 0.175 ppm
 F2 69.97 Hz
 PPMCM 0.51234 ppm/cm
 HZCM 205.00388 Hz/cm





14

Current Data Parameters
 NAME may17-mm-51
 EXPNO 3
 PROCNO 1

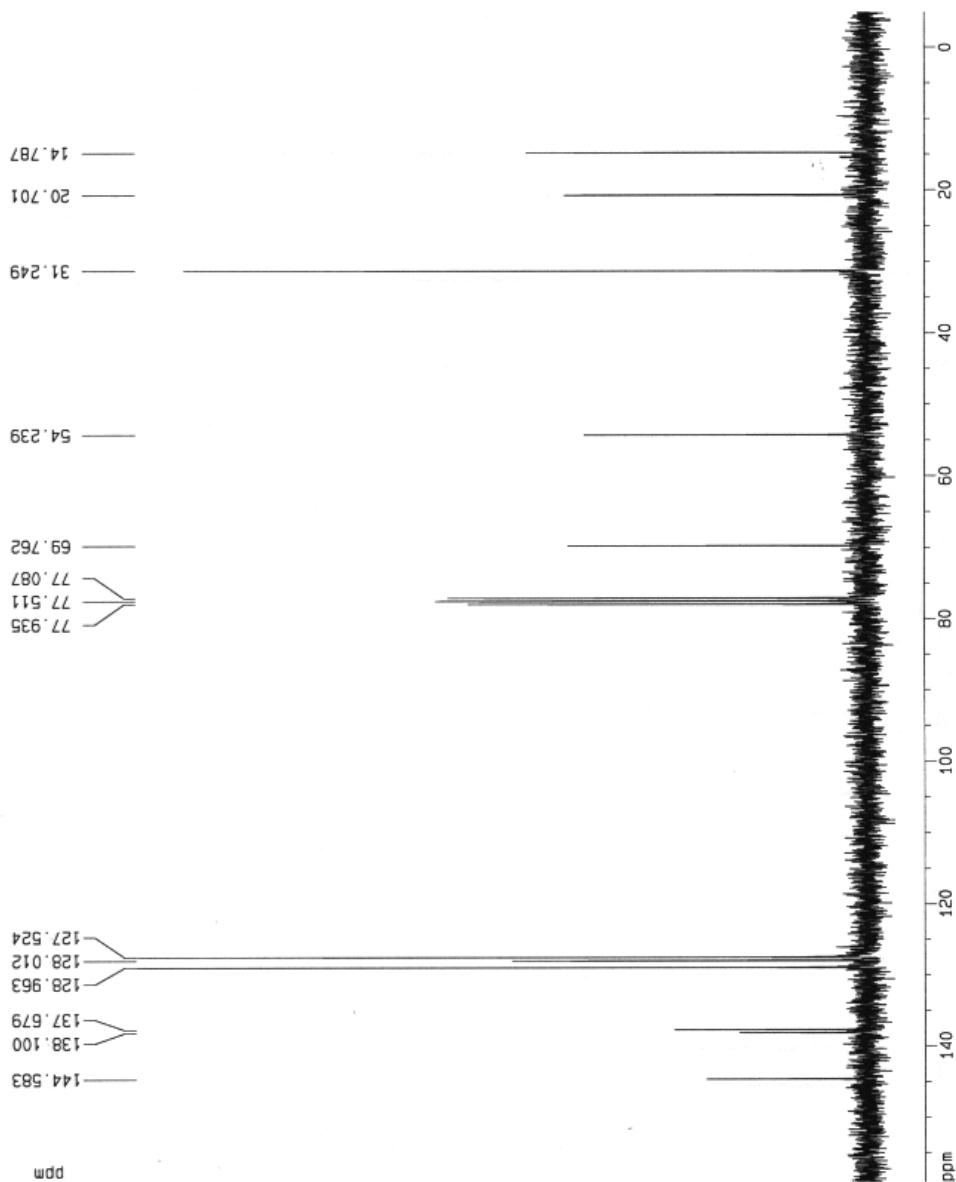
F2 - Acquisition Parameters
 Date_ 20060517
 Time 17 09
 INSTRUM spect
 PROBHD 5 mm Multinu
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 52
 DS 4
 SWH 18832.393 Hz
 FIDRES 0.267360 Hz
 AQ 1.7400308 sec
 RG 16384
 DM 26.550 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00020000 sec

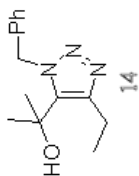
===== CHANNEL f1 =====
 NUC1 13C
 P1 11.80 usec
 PL1 0.00 dB
 SFO1 75.4750200 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 110.00 usec
 PL2 0.00 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677190 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 159.155 ppm
 F1 12011.05 Hz
 F2P -4.915 ppm
 F2 -370.96 Hz
 PPMQW 8.20852 ppm/cm
 HZQW 619.10077 Hz/cm





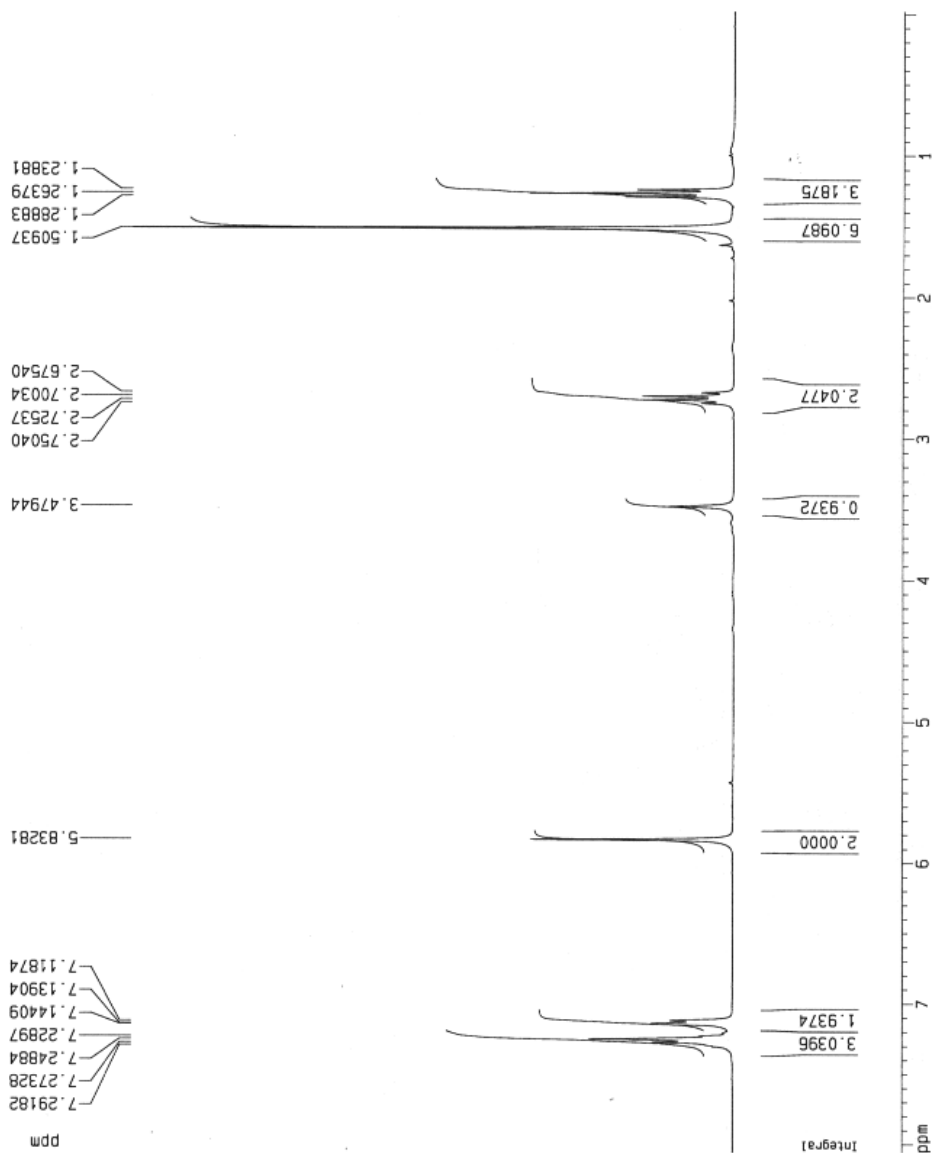
Current Data Parameters
 NAME may17-mm-5f
 EXPNO 2
 PROCNO 1

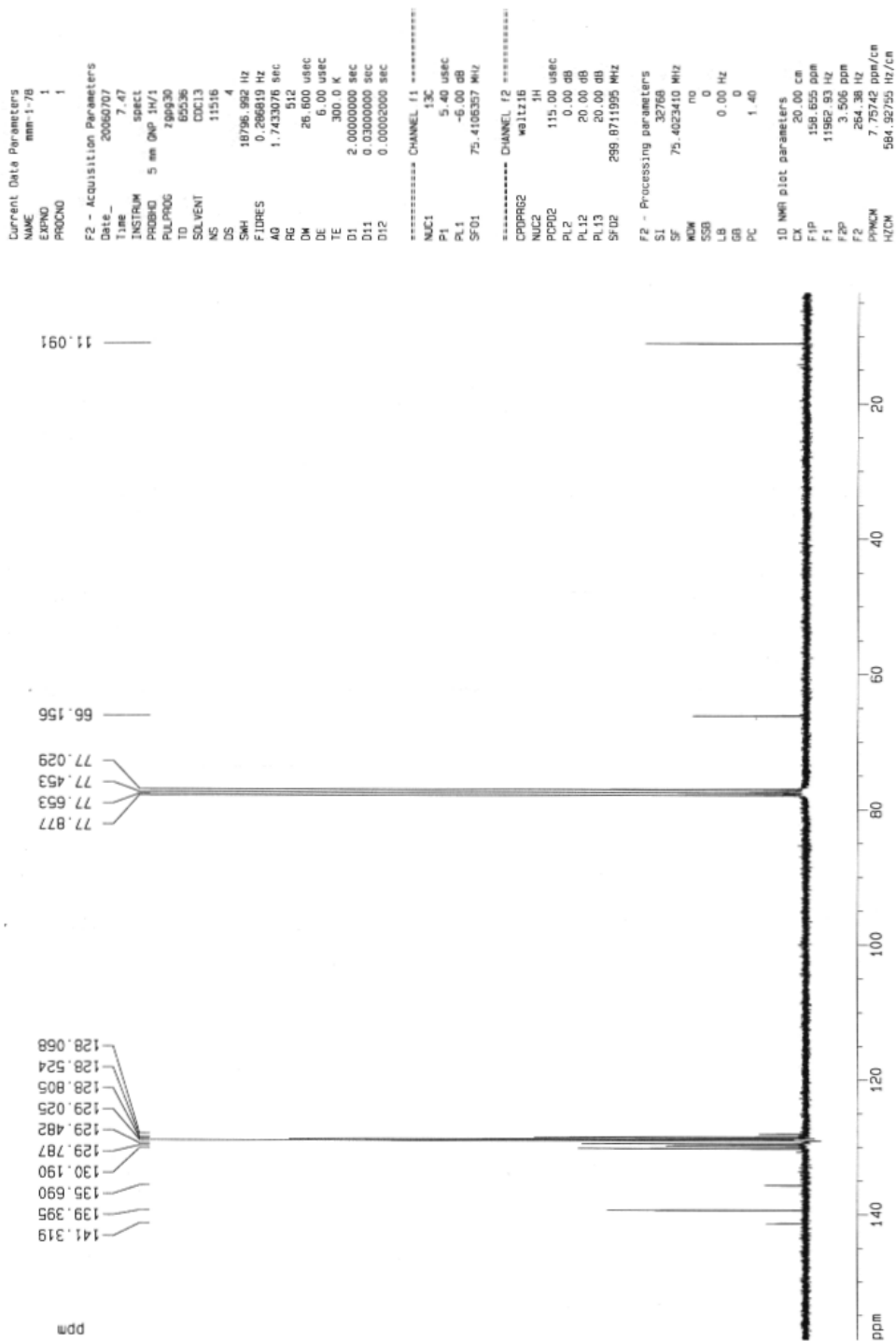
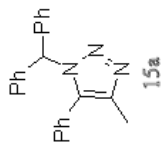
F2 - Acquisition Parameters
 Date_ 20060517
 Time 17.04
 INSTRUM spect
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 24690
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.250014 Hz
 AQ 1.9999400 sec
 RG 128
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

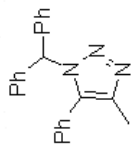
***** CHANNEL f1 *****
 NUC1 1H
 P1 9.60 usec
 PL1 -6.00 dB
 SF01 300.1316534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 FIP 8.060 ppm
 F1 2418.96 Hz
 F2P -0.019 ppm
 F2 -5.82 Hz
 PPMCM 0.40395 ppm/cm
 HZCM 121.23901 Hz/cm







15a

Current Data Parameters

NAME jul15-mm-1-7b
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060705
Time 17.24
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zg30
TD 24690
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.256014 Hz
AQ 1.9999400 sec
RG 512
DM 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====

NUC1 1H

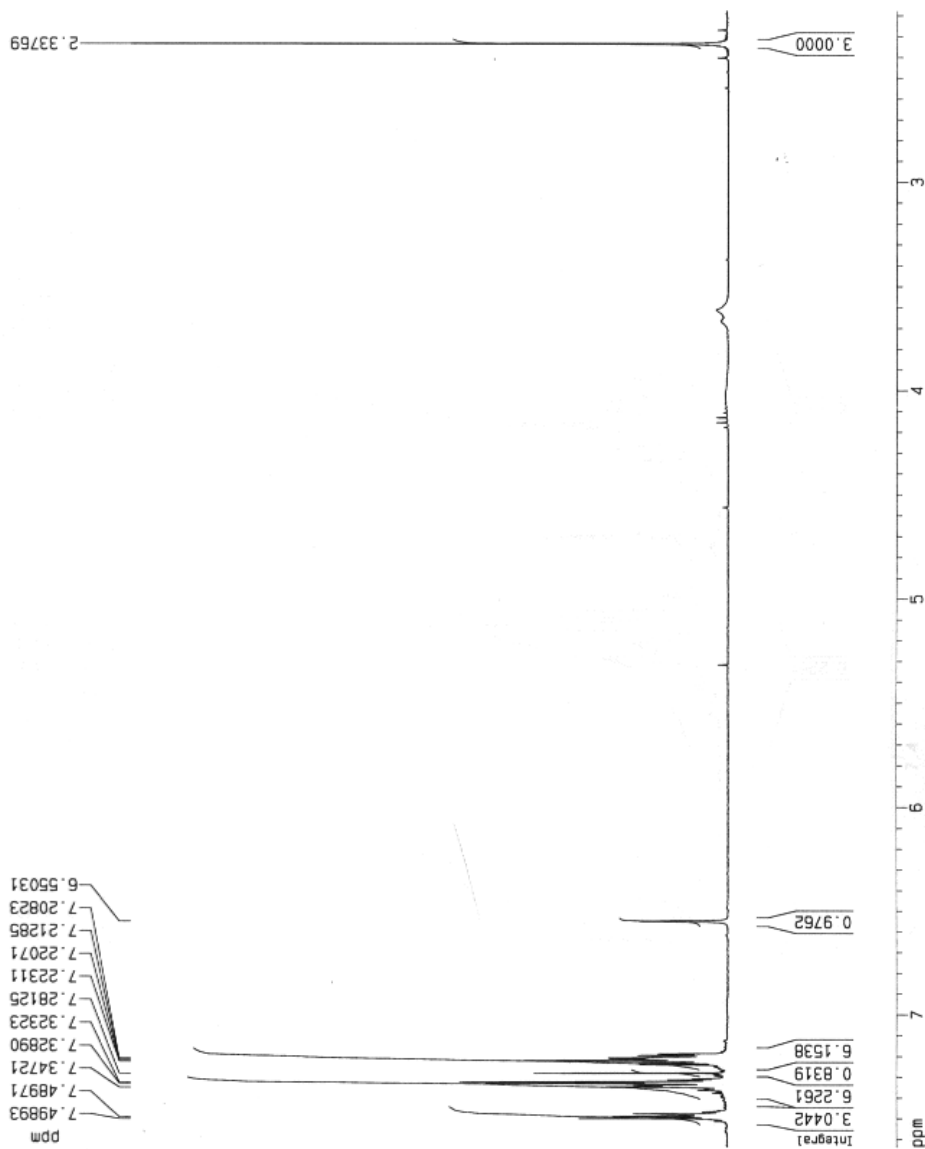
PL1 -6.00 dB
SF01 300.1318534 MHz

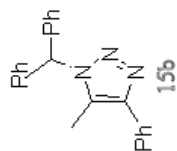
F2 - Processing parameters

SF 300.1300000 MHz
SI 32768
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 7.638 ppm
F1 2292.53 Hz
F2P 2.179 ppm
F2 6553.87 Hz
PPMCM 0.27289 ppm/cm
HZCM 81.93328 Hz/cm





Current Data Parameters
 NAME jun12-mm-1-66
 EXPNO 7
 PROCNO 1

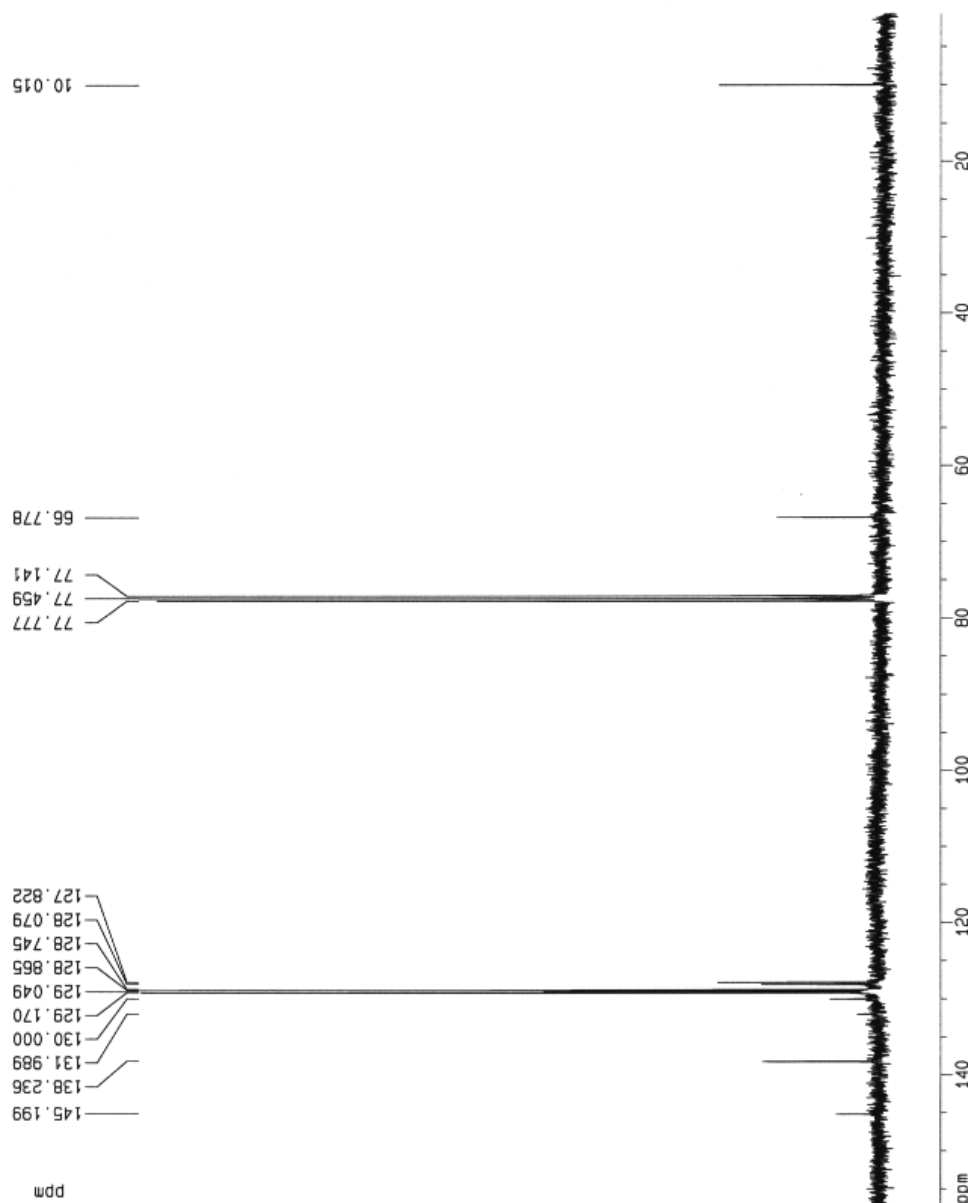
F2 - Acquisition Parameters
 Date_ 20060613
 Time 18.31
 INSTRUM spect
 PROBHD 5 mm BBI 1H-8
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 757
 DS 4
 SMH 25125.629 Hz
 FIDRES 0.383387 Hz
 AQ 1.3042164 sec
 RG 4597.6
 DW 19.900 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00020000 sec

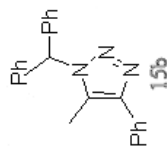
===== CHANNEL f1 =====
 NUC1 13C
 P1 16.35 usec
 PL1 -6.00 dB
 SF01 100.6237959 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 114.00 usec
 PL2 0.00 dB
 PL12 24.00 dB
 PL13 24.00 dB
 SF02 400.1315005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127290 MHz
 NQW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 FIP 156.990 ppm
 F1 15795.18 Hz
 F2P 0.645 ppm
 F2 64.88 Hz
 PPMCM 7.81725 ppm/cm





Current Data Parameters
 NAME 1UN12-mm-1-B8
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060613
 Time 18.05
 INSTRUM spect
 PROBHD 5 mm BBI 1H-B
 PULPROG zg30
 TO 33110
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 8278.146 Hz
 FIDRES 0.250019 Hz
 AQ 1.9998940 sec
 RG 128
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW na
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 FIP 8.455 ppm
 F1 3382.94 Hz
 F2P -0.132 ppm
 F2 -52.65 Hz
 PPMCM 0.42931 ppm/cm
 HZCM 171.77953 Hz/cm

1.28654
 0.99791
 0.99314
 0.97877
 0.97260

2.07254

2.39841

3.62316

6.85224
 7.25023
 7.26530
 7.27006
 7.36173
 7.37163
 7.37657
 7.38135
 7.38672
 7.39556
 7.44515
 7.46468
 7.71967
 7.73814

3.0721

1.0000

4.4456

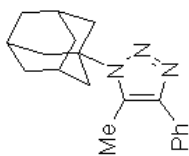
7.0731

2.0977

2.0049

Integral





16

Current Data Parameters

NAME mm-1-73
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060907
Time 7.40
INSTRUM spect
PROBHD 5 mm Multis
PULPROG zgpg30
TO 299930
F2 65536
SOLVENT CDCl3
NS 11776
DS 4
SWH 18832.393 Hz
FIDRES 0.267360 Hz
AQ 1.7400306 sec
RG 36384
BW 26.550 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec

===== CHANNEL f1 =====

NUC1 13C
P1 11.80 usec
PL1 0.00 dB
SFO1 75.4760200 MHz

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

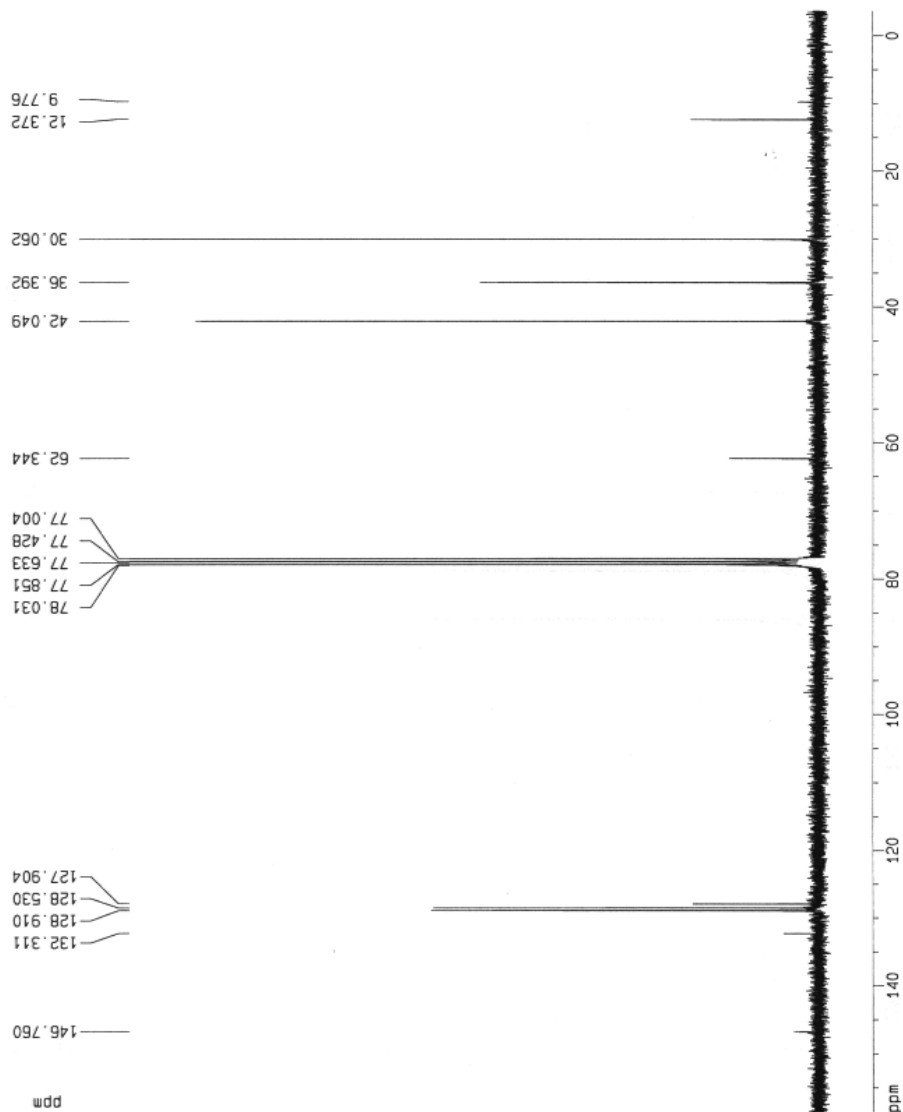
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 17.50 dB
PL13 17.50 dB
SFO2 300.1312005 MHz

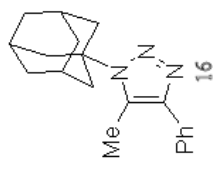
F2 - Processing parameters

SI 32768
SF 75.4677190 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

10 NMR plot parameters

CX 20.00 cm
FJP 156.638 ppm
F1 11972.05 Hz
F2P -3.609 ppm
F2 -272.33 Hz
PPMCM 8.11233 ppm/cm
HZCM 612.21912 Hz/cm





Current Data Parameters
 NAME mm-1-73
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060905
 Time 18.23
 INSTRUM spect
 PROBHD 5 mm BBI 1H-B
 PULPROG zg
 TO 65536
 SOLVENT CDCl3
 NS 1
 DS 0
 SWH 3881.988 Hz
 FIDRES 0.059234 Hz
 AQ 8.4410868 sec
 RG 228.1
 DM 128.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 7.25 usec
 PL1 0.00 dB
 SFO1 400.1317335 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
 F1P 7.991 ppm
 F1 3197.63 Hz
 F2P 0.439 ppm
 F2 175.83 Hz
 PPMCM 0.37760 ppm/cm
 HZCM 151.09000 Hz/cm

