***Supporting Information-----* NMR Spectra of Compounds**

Ruthenium-Catalyzed Cycloisomerization of *cis*-3-En-1-ynes to Cyclopentadiene and Related Derivatives Through a 1, 5-Sigmatropic Hydrogen Shift of Ruthenium-Vinylidene Intermediates.

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- (3) ¹H NOE Spectra of Compounds **3, 5, 37** and **39** S-8, S-9, S-16, S-17, S-84 and S-89~S-91.

sub-9
 expl std1h
 SAMPLE
 date Oct 10 2004 dfrq 400.454
 solvent CDC13 dn H1
 file exp dpwr 42
 ACQUISITION dof 0
 sfrq 400.455 dm nnn
 tn H1 dmm c
 at 2.664 dmf 8000
 np 32016
 sw 6009.6 lb
 fb 3400 wtfile
 bs 4 proc ft
 tpwr 58 fn not used
 pw 6.0
 d1 1.000 werr
 tof 500.0 wexp
 nt 100 wbs
 ct 36 wnt
 alock n
 gain not used
 FLAGS
 il n
 in n
 dp y
 DISPLAY
 sp -208.1
 wp 4204.5
 vs 200
 sc 0
 wc 250
 hzmm 1.61
 is 74.93
 rfl 3394.6
 rfp 2899.3
 th 4
 ins 10.000
 nm ph

DEC. & VT
 7.683
 7.681
 7.675
 7.404
 7.401
 7.397
 7.384
 7.380
 7.368
 7.365
 7.359
 7.333
 7.330
 7.326
 7.317
 7.311
 7.305
 7.296
 7.293
 7.289
 7.240
 7.192
 7.189
 7.173
 7.169

PROCESSING
 0.10
 wft aph

13C OBSERVE

exp3 std13c

SAMPLE DEC. & VT
 date Oct 9 2004 dfrq 400.454
 solvent CDC13 dn H1
 file exp dpwr 42
 ACQUISITION dof 0
 sfrq 100.705 dm yyy
 tn C13 dmm w
 at 0.635 dmf 8000
 np 32000
 sw 25188.9 lb 3.00
 fb 13800 wtfile
 bs 4 proc ft
 tpwr 58 fn not used
 pw 6.5
 d1 2.000 werr
 tof 2000.0 wexp
 nt 10000 wbs
 ct 180 wnt
 alock n
 gain not used
 FLAGS
 il n
 in n
 dp y
 DISPLAY
 sp -0.2
 wp 20138.2
 vs 60
 sc 0
 wc 250
 hzmm 80.56
 is 500.00
 rfl 8849.9
 rfp 7753.4
 th 8
 ins 100.000
 nm no ph

sub-8

expl stdih

SAMPLE DEC. & VT
 date Oct 10 2004 dfrq 400.454
 solvent CDC13 dn H1
 file exp dpwr 42
 ACQUISITION dof 0
 sfrq 400.455 dm nnn
 tn H1 dmm c
 at 2.664 dmf 8000
 np 32016 PROCESSING
 sw 6009.6 lb 0.10
 fb 3400 wtfile
 bs 4 proc ft
 tpwr 58 fn not used
 pw 6.0
 d1 1.000 werr
 tof 500.0 wexp
 nt 100 wbs
 ct 36 wnt
 alock n
 gain not used
 FLAGS
 il n
 in n
 dp y
 DISPLAY
 sp -208.1
 wp 4204.5
 vs 70
 sc 0
 wc 250
 hzmm 1.72
 is 74.93
 rfl 3394.9
 rfp 2899.3
 th 4
 ins 10.000
 nm ph

7.692
 7.671
 7.419
 7.416
 7.400
 7.398
 7.380
 7.355
 7.352
 7.335
 7.318
 7.316
 7.110
 7.097
 6.917
 6.907
 6.896
 6.789
 6.787
 6.784
 6.781

3.130
 3.118
 3.100
 3.093
 3.080
 3.063
 3.050
 3.003
 2.991
 2.972
 2.961
 2.954
 2.936
 2.924
 2.756
 2.754
 2.413
 2.400
 2.380
 2.368
 2.349
 2.337
 2.316
 2.304
 2.284
 2.272
 2.252
 2.240
 2.040
 2.038

sub-8

exp3 std13c

SAMPLE DEC. & VT
date Oct 5 2004 dfrq 400.454
solvent CDCl3 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 100.705 dm yyy
tn C13 dmm w
at 0.635 dmf 8000
np 32000
sw 25188.9 lb 3.00
fb 13800 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.5
d1 2.000 werr
tof 2000.0 wexp
nt 1000 wbs wft
ct 120 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -0.2
wp 20138.2
vs 70
sc 0
wc 250
hzmm 80.56
is 500.00
rfl 8857.6
rfp 7753.4
th 5
ins 100.000
nm ph

144.215
143.589

128.243
127.907
126.640
125.250
124.014
122.960

85.597

77.305
76.985
76.664
74.894
72.648

46.645

25.161

```

cch
expl stdlh
SAMPLE
date Mar 29 2005
solvent CDC13
file exp
ACQUISITION
sfrq 400.455
tn H1
at 2.664
np 32016
sw 6009.6
fb 3400
bs 4
tpwr 58
pw 6.0
dl 1.000
tof 500.0
nt 100
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.4
wp 4204.5
vs 100
sc 0
wc 250
hzmm 16.82
is 74.27
rfl 495.3
rfp 0
th 2
ins 10.000
nm ph
DEC. & VT
dfrq 400.454
dn H1
dpwr 42
dof 0
dm nnn
dmm c
dmf 8000
PROCESSING
lb 0.10
wtfile
proc ft
fn not used
werr
wexp
wbs wft aph
wnt

```

dehydration3c

exp3 std13c

SAMPLE DEC. & VT
date Mar 14 2005 dfrq 400.454
solvent CDCl3 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 100.705 dm yyy
tn C13 dmm w
at 0.635 dmf 8000
np 32000 PROCESSING
sw 25188.9 lb 3.00
fb 13800 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.5
d1 2.000 werr
tof 2000.0 wexp
nt 1000 wbs
ct 212 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1.7
wp 20138.2
vs 60
sc 0
wc 250
hzmm 1.73
is 500.00
rfl 8845.3
rfp 7753.4
th 4
ins 100.000
nm ph

157.254

138.061
137.618

129.877
128.289
127.953
127.556
125.937
122.792
120.547

110.271

83.092
80.955
77.321
77.000
76.679

55.318

31.880

dehyd3C

Pulse Sequence: s2pu1

dehyd3C

Pulse Sequence: s2pu1

d3
expl stdlh

SAMPLE		DEC. & VT	
date	Apr 6 2005	dfrq	400.454
solvent	CDCl3	dn	H1
file	exp	dpwr	42
ACQUISITION		dof	0
sfrq	400.455	dm	nnn
tn	H1	dmm	c
at	2.664	dmf	8000
np	32016	PROCESSING	
sw	6009.6	lb	0.10
fb	3400	wtfile	
bs	4	proc	ft
tpwr	58	fn	not used
pw	6.0		
d1	1.000	werr	
tof	500.0	wexp	
nt	100	wbs	wft aph
ct	32	wnt	
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-200.4		
wp	4204.5		
vs	100		
sc	0		
wc	250		
hzmm	1.89		
is	74.27		
rfl	3396.8		
rfp	2899.3		
th	5		
ins	10.000		
nm	ph		

7.632
7.612
7.348
7.331
7.311
7.277
7.274
7.258
7.240
7.224
7.222
7.205
7.202
6.931
6.913
6.891
6.870

d3
exp3 std13c

SAMPLE DEC. & VT
date Apr 6 2005 dfrq 400.454
solvent CDCl3 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 100.705 dm yyy
tn C13 dmm w
at 0.635 dmf 8000
np 32000 PROCESSING
sw 25188.9 lb 3.00
fb 13800 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.5
d1 2.000 werr
tof 2000.0 wexp
nt 10000 wbs
ct 768 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -0.2
wp 20138.2
vs 80
sc 0
wc 250
hzmm 80.56
is 500.00
rfl 8843.7
rfp 7753.4
th 3
ins 100.000
nm ph

dethio
expl stdlh

7.605
7.360
7.355
7.343
7.339
7.327
7.323
7.308
7.301
7.299
7.295
7.286
7.280
7.274
7.266
7.262
7.240
7.163
7.159
7.150
7.147
6.960
6.951
6.947
6.938
6.897

SAMPLE DEC. & VT
date Mar 22 2005 dfrq 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 400.455 dm nnn
tn H1 dmm c
at 2.664 dmf 8000
np 32016 PROCESSING
sw 6009.6 lb 0.10
fb 3400 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.0
dl 1.000 werr
tof 500.0 wexp
nt 100 wbs
ct 24 wnt
alock n
gain not used

FLAGS
il n
in n
dp y

DISPLAY
sp -200.4
wp 4204.5
vs 40
sc 0
wc 250
hzmm 2.43
is 54.03
rfl 3394.6
rfp 2899.3
th 4
ins 10.000
nm ph

Current Data Parameters
NAME Datta-dethio
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050327
Time 16.17
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT C6D6
NS 200
DS 0
SWH 37593.984 Hz
FIDRES 1.147277 Hz
AQ 0.4358644 sec
RG 2048
DW 13.300 usec
DE 6.50 usec
TE 296.3 K
D1 3.00000000 sec
d11 0.03000000 sec
DELTA 2.90000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.30 usec
PL1 0.00 dB
SFO1 150.7861246 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 11.30 dB
PL13 14.00 dB
SFO2 599.6029980 MHz

F2 - Processing parameters
SI 65536
SF 150.7695488 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 4.50 cm
F1P 200.000 ppm
F1 30153.91 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1507.69543 Hz/cm

pro4-Pdt-9
exp22 s2pu1

SAMPLE DEC. & VT
date Oct 11 2004 dfrq 499.838
solvent CDC13 dn H1
file /export/home/~ dpwr 38
opera/vnmrsvs/data~ dof 0
1/LIQU/liou1011.00~ dm nnn
4H.fid dmm c
ACQUISITION dmf 11299
sfrq 499.839 dseq
tn H1 dres 1.0
at 2.182 homo n
np 39276
sw 9000.9 wtfile
fb not used proc ft
bs 4 fn 32768
tpwr 55 math f
pw 5.5
dl 1.000 werr
tof 980.4 wexp
nt 16 wbs
ct 16 wnt
alock y
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -250.1
wp 5247.9
vs 131
sc 0
wc 250
hzmm 1.27
is 154.59
rf1 4658.4
rfp 3618.8
th 6
ins 100.000
nm ph

7.591
7.575
7.544
7.541
7.529
7.526
7.365
7.350
7.335
7.224
7.220
7.209
7.194
6.992
6.984
6.978
6.962
6.953
6.937

CH₃(OCH₃)
3.925
3.884

pro4-Pdt-9

exp23 s2pu1

SAMPLE DEC. & VT
date Oct 11 2004 dfrq 499.838
solvent CDCl3 dn H1
file /export/home/~ dpwr 38
opera/vnmrsys/data~ dof 0
1/LIOU/liou1011.00~ dm yyy
4C.fid dmm w
ACQUISITION dmf 11299
sfrq 125.700 dseq
tn C13 dres 1.0
at 0.508 homo n
np 37088
sw 36529.7 lb 3.00
fb not used wtfile
bs 4 proc ft
tpwr 55 fn not used
pw 5.0 math f
d1 2.000
tof 3769.1 werr
nt 1024 wexp
ct 308 wbs
alock y wnt
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -0.2
wp 27650.0
vs 76
sc 0
wc 250
hzmm 110.60
is 119.21
rfl 12275.4
rfp 9677.7
th 6
ins 100.000
nm ph

pro-4-pat-9

Pulse Sequence: s2pu1

Current Data Parameters
 NAME Datta-D-expt-1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050116
 Time 14.23
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.293438 Hz
 AQ 1.7039860 sec
 RG 128
 DW 52.000 usec
 DE 6.50 usec
 TE 0.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 599.6035976 MHz

F2 - Processing parameters
 SI 32768
 SF 599.6000312 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 0.50

1D NMR plot parameters
 CX 20.00 cm
 CY 12.00 cm
 FLP 9.500 ppm
 F1 5696.20 Hz
 F2P -0.500 ppm
 F2 -299.80 Hz
 PPMCM 0.50000 ppm/cm
 HZCM 299.80002 Hz/cm

Current Data Parameters
 NAME Datta-D-expt-1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20050112
 Time 16.11
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg
 TD 32768
 SOLVENT C6D6
 NS 500
 DS 0
 SWH 37593.984 Hz
 FIDRES 1.147277 Hz
 AQ 0.4358644 sec
 RG 2048
 DW 13.300 usec
 DE 6.50 usec
 TE 0.0 K
 D1 3.00000000 sec
 d11 0.03000000 sec
 DELTA 2.90000010 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 4.30 usec
 PL1 0.00 dB
 SFO1 150.7861246 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 92.00 usec
 PL2 120.00 dB
 PL12 11.30 dB
 PL13 14.00 dB
 SFO2 599.6029980 MHz

F2 - Processing parameters

SI 65536
 SF 150.7695500 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 0.50

1D NMR plot parameters

CX 20.00 cm
 CY 4.50 cm
 F1P 200.000 ppm
 F1 30153.91 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.00000 ppm/cm
 HZCM 1507.69543 Hz/cm

Current Data Parameters
NAME Datta-dethio-Pdt
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050323
Time 23.03
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9615.385 Hz
FIDRES 0.293438 Hz
AQ 1.7039860 sec
RG 128
DW 52.000 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 599.6030593 MHz

F2 - Processing parameters
SI 32768
SF 599.6000539 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 9.500 ppm
F1 5696.20 Hz
F2P -0.500 ppm
F2 -299.80 Hz
PPMCM 0.50000 ppm/cm
HZCM 299.80002 Hz/cm

Current Data Parameters
NAME Datta-dethio-Pdt
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050323
Time 23.05
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpgg
TD 32768
SOLVENT C6D6
NS 6144
DS 0
SWH 37593.984 Hz
FIDRES 1.147277 Hz
AQ 0.4358644 sec
RG 2048
DW 13.300 usec
DE 6.50 usec
TE 295.1 K
D1 3.00000000 sec
d11 0.03000000 sec
DELTA 2.90000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.30 usec
PL1 0.00 dB
SFO1 150.7861246 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 11.30 dB
PL13 14.00 dB
SFO2 599.6029980 MHz

F2 - Processing parameters
SI 65536
SF 150.7695534 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 200.000 ppm
F1 30153.91 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1507.69543 Hz/cm

phph
 exp1 stdih

SAMPLE
 date May 25 2005
 solvent CDC13
 file exp
 ACQUISITION
 sfrq 400.455
 tn H1
 at 2.664
 np 32016
 sw 6009.6
 fb 3400
 bs 4
 tpwr 58
 pw 6.0
 dl 1.000
 tof 500.0
 nt 100
 ct 64
 alock n
 gain not used

DEC. & VT
 400.454
 dn H1
 dpwr 42
 dof 0
 dm nnn
 dmm c
 dmf 8000
 lb 0.10
 wtfile
 proc ft
 fn not used
 werr
 wexp
 wbs
 wnt
 wft aph

FLAGS
 il n
 in n
 dp y

DISPLAY
 sp -200.4
 wp 4204.5
 vs 70
 sc 0
 wc 250
 hzmm 1.93
 is 87.95
 rfl 3394.6
 rfp 2899.3
 th 6
 ins 100.000
 nm ph

7.715
 7.712
 7.693
 7.686
 7.426
 7.421
 7.408
 7.387
 7.359
 7.345
 7.340
 7.334
 7.322
 7.302
 7.282
 7.274
 7.265
 7.240
 7.210
 7.198
 7.193
 7.178

2.914
 2.901
 2.881
 2.868
 2.850
 2.837
 2.788
 2.775
 2.766
 2.757
 2.745
 2.724
 2.711
 2.348
 2.336
 2.315
 2.302
 2.284
 2.272
 2.254
 2.241
 2.222
 2.211
 2.190
 2.177

phph
exp3 std13c

SAMPLE DEC. & VT
date May 25 2005 dfrq 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 100.705 dm yyy
tn C13 dmm w
at 0.635 dmf 8000
np 32000
sw 25188.9 lb 3.00
fb 13800 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.5
dl 2.000 werr
tof 2000.0 wexp
nt 1000 wbs
ct 280 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1.5
wp 20138.2
vs 100
sc 0
wc 250
hzmm 80.56
is 500.00
rfl 1062.4
rfp 0
th 5
ins 100.000
nm ph

144.263
141.866

128.658
128.581
128.184
126.138
125.650

86.362

77.644
77.323
77.002
74.819
73.323

47.167

31.317

Current Data Parameters
NAME Datta-Sub-5
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040909
Time 21.57
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2807028 sec
RG 32
DW 69.600 usec
DE 6.50 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 4.00 dB
SFO1 599.7029985 MHz

F2 - Processing parameters
SI 32768
SF 599.7000265 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 9.500 ppm
F1 5697.15 Hz
F2P -0.500 ppm
F2 -299.85 Hz
PPMCM 0.50000 ppm/cm
HZCM 299.85001 Hz/cm

sub-P-OMe
exp35 s2pu1

SAMPLE DEC. & VT
date Oct 4 2004 dfrq 499.838
solvent CDC13 dn H1
file /export/home/~ dpwr 38
opera/vnmrsys/data~ dof 0
1/LIOU/liou1004.00~ dm yyy
8C.fid dmm w
ACQUISITION dmf 11299
sfrq 125.700 dseq
tn C13 dres 1.0
at 0.508 homo n
np 37088
sw 36529.7 lb 3.00
fb not used wtfile
bs 4 proc ft
tpwr 55 fn not used
pw 5.0 math f
d1 2.000
tof 3769.1 werr
nt 1024 wexp
ct 52 wbs
alock y wnt
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -0.2
wp 27650.0
vs 90
sc 0
wc 250
hzmm 13.82
is 119.21
rfl 12279.9
rfp 9677.7
th 12
ins 100.000
nm ph

cf33csub

expl std1h

SAMPLE
date Apr 10 2005 dfrq 400.454
solvent CDCl3 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 400.455 dm nnn
tn H1 dmm c
at 2.664 dmf 8000
np 32016 PROCESSING
sw 6009.6 lb 0.10
fb 3400 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.0
dl 1.000 werr
tof 500.0 wexp
nt 100 wbs
ct 56 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.4
wp 4204.5
vs 50
sc 0
wc 250
hzmm 1.71
is 84.26
rfl 494.9
rfp 0
th 3
ins 10.000
nm ph

7.671
7.668
7.649
7.529
7.497
7.477
7.409
7.397
7.378
7.358
7.345
7.333
7.331
7.318
7.314
7.308
7.296
7.294
7.281
7.254
7.234

2.913
2.892
2.880
2.861
2.848
2.811
2.799
2.792
2.789
2.781
2.769
2.758
2.756
2.748
2.735
2.577
2.294
2.281
2.261
2.248
2.231
2.217
2.200
2.187
2.168
2.156
2.137

cf33csub

exp3 std13c

SAMPLE		DEC. & VT	
date	Apr 10 2005	dfrq	400.454
solvent	CDCl3	dn	H1
file	exp	dpwr	42
ACQUISITION		do	0
sfrq	100.705	dm	yyy
tn	C13	dmm	w
at	0.635	dmf	8000
np	32000	PROCESSING	
sw	25188.9	lb	3.00
fb	13800	wtfile	
bs	4	proc	ft
tpwr	58	fn	not used
pw	6.5		
d1	2.000	werr	
tof	2000.0	wexp	
nt	1000	wbs	wft
ct	204	wnt	
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-0.2		
wp	20138.2		
vs	70		
sc	0		
wc	250		
hzmm	80.56		
is	500.00		
rfl	8840.6		
rfp	7753.4		
th	5		
ins	100.000		
nm	ph		

145.726
143.726128.686
128.381
128.075
125.296

85.719

77.321
77.000
76.679
74.771
72.893

46.462

30.933

Current Data Parameters
NAME Datta-Pro-4-Sub-7
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040928
Time 18.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDC13
NS 16
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2807028 sec
RG 32
DW 69.600 usec
DE 6.50 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 4.00 dB
SFO1 599.7029985 MHz

F2 - Processing parameters
SI 32768
SF 599.7000265 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 9.500 ppm
F1 5697.15 Hz
F2P -0.500 ppm
F2 -299.85 Hz
PPMCM 0.50000 ppm/cm
HZCM 299.85001 Hz/cm

Current Data Parameters
NAME Datta-Pro-4-Sub-7
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040928
Time 18.49
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT C6D6
NS 19
DS 0
SWH 37878.789 Hz
FIDRES 1.155969 Hz
AQ 0.4325876 sec
RG 2048
DW 13.200 usec
DE 6.50 usec
TE 0.0 K
D1 4.00000000 sec
d11 0.03000000 sec
DELTA 3.90000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.50 usec
PL1 0.00 dB
SFO1 150.8112724 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 8.80 dB
PL13 10.00 dB
SFO2 599.7029985 MHz

F2 - Processing parameters
SI 65536
SF 150.7946992 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30158.94 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1507.94690 Hz/cm

Current Data Parameters
NAME Datta-Pro-4-Sub-12
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20041108
Time 12.47
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDC13
NS 16
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2807028 sec
RG 32
DW 69.600 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 4.00 dB
SFO1 599.6029980 MHz

F2 - Processing parameters
SI 32768
SF 599.6000000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 9.500 ppm
F1 5696.20 Hz
F2P -0.500 ppm
F2 -299.80 Hz
PPMCM 0.50000 ppm/cm
HZCM 299.79999 Hz/cm

Current Data Parameters
NAME Datta-Pro-4-Sub-12
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20041108
Time 12.55
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT C6D6
NS 100
DS 0
SWH 37878.789 Hz
FIDRES 1.155969 Hz
AQ 0.4325876 sec
RG 2048
DW 13.200 usec
DE 6.50 usec
TE 296.8 K
D1 4.00000000 sec
d11 0.03000000 sec
DELTA 3.90000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.30 usec
PL1 0.00 dB
SFO1 150.7861246 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 11.30 dB
PL13 14.00 dB
SFO2 599.6029980 MHz

F2 - Processing parameters

SI 65536
SF 150.7695598 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters

CX 20.00 cm
CY 4.50 cm
F1P 200.000 ppm
F1 30153.91 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1507.69556 Hz/cm

sub-13

expl std1h

SAMPLE
 date May 7 2004
 solvent CDC13
 file exp
 ACQUISITION
 sfrq 400.455
 tn H1
 at 2.664
 np 32016
 sw 6009.6
 fb 3400
 bs 4
 tpwr 58
 pw 6.0
 d1 1.000
 tof 500.0
 nt 100
 ct 0
 alock n
 gain not used
 FLAGS
 tl n
 in n
 dp y
 DISPLAY
 sp -200.4
 wp 4204.5
 vs 100
 sc 0
 wc 250
 hzmm 1.45
 is 60.40
 rfl 3395.7
 rfp 2899.3
 th 3
 ins 10.000
 nm ph

DEC. & VT
 dfrq 400.454
 dn H1
 dpwr 42
 dof 0
 dm nnn
 dmm c
 dmf 8000
 PROCESSING
 lb 0.10
 wtfile
 proc ft
 fn not used
 werr
 wexp
 wbs
 wnt
 wft aph

sub-13
exp5 std13c

SAMPLE DEC. & VT
date May 9 2004 dfrq 400.454
solvent CDCl3 dn H1
file /export/home/~ dpwr 42
chem/rs1/swarp/su~ dof 0
b-13.fid dm yyy
ACQUISITION dmm w
sfrq 100.705 dmf 8000
tn C13
at 0.635 lb PROCESSING 3.00
np 32000 wtfile
sw 25188.9 proc ft
fb 13800 fn not used
bs 4
tpwr 58 werr
pw 6.5 wexp
dl 2.000 wbs
tof 2000.0 wnt
nt 10000
ct 0
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -0.2
wp 20138.2
vs 70
sc 0
wc 250
hzmm 80.56
is 500.00
rfl 8849.9
rfp 7753.4
th 5
ins 100.000
nm ph

147.421
145.497
143.894

135.343

128.213
127.816
125.266
120.975

108.851
108.073

100.606

85.963

77.321
77.000
76.679
74.465
72.862

47.073

30.719

me
expt1 std1h

SAMPLE
date Jun 13 2004 dfrq 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 400.455 dm nnn
tn H1 dmm c
at 2.664 dmf 8000
np 32016
sw 6009.6 lb 0.10
fb 3400 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.0
dl 1.000 werr
tof 500.0 wexp
nt 100 wbs
ct 64 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.4
wp 4204.5
vs 100
sc 0
wc 250
hzmm 0.46
is 128.56
rfl 3394.2
rfp 2899.3
th 5
ins 10.000
nm ph

DEC. & VT
400.454
H1
42
0
nnn
c
8000
0.10
ft
not used
wft aph

S-34

```

me-sub
exp3 std13c
SAMPLE
date Jun 13 2004 dfrq 400.454
solvent CDCl3 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 100.705 dm yyy
tn C13 dmm w
at 0.635 dmf 8000
np 32000 PROCESSING
sw 25188.9 lb 3.00
fb 13800 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.5
dl 2.000 werr
tof 2000.0 wexp
nt 10000 wbs wft
ct 0 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -0.2
wp 20138.2
vs 60
sc 0
wc 250
hzmm 80.56
is 500.00
rfl 8837.6
rfp 7753.4
th 4
ins 100.000
nm ph

```

147.558
145.619

141.023
137.679

135.481
129.342

128.976
126.563
125.250

121.036
108.912
108.134

100.713

86.146

77.321
77.000
76.695
74.358
72.877

47.042

30.842

21.023

```

sub-cf3
expl stdih
SAMPLE
date Mar 2 2005 dfrq DEC. & VT 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 400.455 dm nnn
tn H1 dmm c
at 2.664 dmf 8000
np 32016 PROCESSING
sw 6009.6 lb 0.10
fb 3400 wtfile
bs 4 proc
tpwr 58 fn not used
pw 6.0
dl 1.000 werr
tof 500.0 wexp
nt 100 wbs
ct 24 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.4
wp 4204.5
vs 100
sc 0
wc 250
hzmm 1.75
ts 54.03
rfl 495.3
rfp 0
th 2
ins 10.000
nm ph

```

```

sub-cf3
exp3 std13c
SAMPLE
date Mar 2 2005 dfrq 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION
sfrq 100.705 dm 0
tn C13 dmm w
at 0.635 dmf 8000
np 32000 PROCESSING
sw 25188.9 lb 3.00
fb 13800 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.5
d1 2.000 werr
tof 2000.0 wexp
nt 1000 wbs
ct 168 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -0.2
wp 18124.1
vs 100
sc 0
wc 250
hzmm 72.50
is 500.00
rfl 8843.7
rfp 7753.4
th 4
ins 100.000
nm ph

```

unknown2
exp1 std1h

SAMPLE
date Apr 10 2005 dfrq 400.454
solvent CDCl3 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 400.455 dm nnn
tn H1 dmm c
at 2.664 dmf 8000
np 32016
sw 6009.6 lb 0.10
fb 3400 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.0
d1 1.000 werr
tof 500.0 wexp
nt 100 wbs
ct 52 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.4
wp 4204.5
vs 70
sc 0
wc 250
hzmm 2.31
is 84.26
rfl 3393.8
rfp 2899.3
th 3
ins 10.000
nm ph

phph4c

exp3 std13c

SAMPLE		DEC. & VT	
date	Apr 7 2005	dfrq	400.454
solvent	CDCl3	dn	H1
file	exp	dpwr	42
ACQUISITION		dof	0
sfrq	100.705	dm	yyy
tn	C13	dmm	w
at	0.635	dmf	8000
np	32000	PROCESSING	
sw	25188.9	lb	3.00
fb	13800	wtfile	
bs	4	proc	ft
tpwr	58	fn	not used
pw	6.5		
d1	2.000	werr	
tof	2000.0	wexp	
nt	1000	wbs	
ct	100	wnt	
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-0.2		
wp	20138.2		
vs	80		
sc	0		
wc	250		
hzmm	80.56		
is	500.00		
rfl	8854.5		
rfp	7753.4		
th	5		
ins	100.000		
nm	ph		

143.970
141.955

128.304
128.197
128.136
127.724
125.678
125.296

86.146

77.305
76.985
76.664
74.190
73.030

44.584

35.514

26.139

s
exp1 stdlh

7.607	7.604	7.586	7.351	7.334	7.318	7.314	7.288	7.270	7.251	7.243	7.237	7.160	7.156	7.140	7.137	7.121	7.117	7.072	6.856	6.838	6.820	6.808	6.787
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

SAMPLE
 date Dec 23 2004
 solvent CDCl3
 file exp
 ACQUISITION
 sfrq 400.455
 tn H1
 at 2.664
 np 32016
 sw 6009.6
 fb 3400
 bs 4
 tpwr 58
 pw 6.0
 dl 1.000
 tof 500.0
 nt 100
 ct 16
 alock n
 gain not used
 FLAGS
 il n
 in n
 dp y
 DISPLAY
 sp -200.4
 wp 4204.5
 vs 100
 sc 0
 wc 250
 hzmm 16.82
 is 25.07
 rfl 495.3
 rfp 0
 th 4
 ins 10.000
 nm ph

DEC. & VT
 dfrq 400.454
 dn H1
 dpwr 42
 dof 0
 dm nnn
 dmm c
 dmf 8000
 lb 0.10
 wtfile
 proc ft
 fn not used
 werr
 wexp
 wbs wft aph
 wnt

3.751
3.723
3.718

2.568
2.559
2.460

2.018
2.013
2.005
2.001
1.985
1.972
1.957
1.942
1.929
1.908
1.896
1.803
1.791
1.786
1.781
1.775
1.770
1.674
1.670
1.662
1.657
1.652
1.645
1.641

```

sub4c-ph
exp3 std13c
SAMPLE
date Dec 10 2004
solvent CDCl3
file exp
ACQUISITION
sfrq 100.705
tn C13
at 0.635
np 32000
sw 25188.9
fb 13800
bs 4
tpwr 58
pw 6.5
d1 2.000
tof 2000.0
nt 1000
ct 132
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1.7
wp 20138.2
vs 70
sc 0
wc 250
hzmm 80.56
is 500.00
rfl 8849.9
rfp 7753.4
th 6
ins 100.000
nm ph
DEC. & VT
dfrq 400.454
dn H1
dpwr 42
dof 0
dm vvy
dmm w
dmf 8000
PROCESSING
lb 3.00
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
wft

```

arjan

expl std1h

SAMPLE
date Apr 8 2005 dfrq 400.454
solvent CDCl3 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 400.455 dm nnn
tn H1 dmm C
at 2.664 dmf 8000
np 32016
sw 6009.6 lb 0.10
fb 3400 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.0
dl 1.000 werr
tof 500.0 wexp
nt 100 wbs
ct 32 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.4
wp 4004.2
vs 50
sc 0
wc 250
hzmm 8.79
is 167.14
rfl 495.3
rfp 0
th 9
ins 10.000
nm ph

DEC. & VT

PROCESSING

wft aph

7.281
7.266
7.263
7.245
7.239
7.228
7.211
7.196
7.179

3.628

3.045

2.225
1.951
1.936
1.586
1.579
1.571
1.559
1.546
1.529
1.524

final

exp2 std13c

SAMPLE		DEC. & VT	
date	Apr 8 2005	dfrq	400.454
solvent	CDC13	dn	H1
file	exp	dpwr	42
ACQUISITION			
sfrq	100.705	dm	yyy
tn	C13	dmm	w
at	0.635	dmf	8000
np	32000	PROCESSING	
sw	25188.9	lb	3.00
fb	13800	wtfile	
bs	4	proc	ft
tpwr	58	fn	not used
pw	6.5		
d1	2.000	werr	
tof	2000.0	wexp	
nt	10000	wbs	wft
ct	100	wnt	

alock n

gain not used

FLAGS

il n

in n

dp y

DISPLAY

sp -1.7

wp 20138.2

vs 50

sc 0

wc 250

hzmm 6.14

is 500.00

rfl 8852.9

rfp 7753.4

th 3

ins 100.000

nm no ph

145.879

139.909

128.671

128.243

125.983

114.883

84.696

78.542

77.305

76.985

76.679

42.080

29.880

28.444

22.276

naphthylamine cyc

exptl stdih

SAMPLE DEC. & VT
date Apr 23 2005 dfrq 400.454
solvent CDC13 dn H1
file /export/home/~ dpwr 42
chem/rs1/arjan/5-f~ dof 0
uran-23-04-2005.f1~ dm nnn
d dmm c

ACQUISITION 8000
sfrq 400.455 PROCESSING
tn H1 lb 0.10
at 2.664 wtfile
np 32016 proc ft
sw 6009.6 fn not used
fb 3400
bs 4 werr
tpwr 58 wexp
pw 6.0 wbs
d1 1.000 wnt
tof 500.0
nt 100
ct 20
alock n
gain not used

FLAGS
il n
in n
dp y

DISPLAY
sp -200.7
wp 3804.3
vs 150
sc 0
wc 250
hzmm 1.62
is 164.73
rfl 3394.9
rfp 2899.3
th 8
ins 10.000
nm ph

7.240

5.866
5.859
5.831
5.828
5.824
5.821

3.561
3.116

2.490
2.485
2.384
2.381
2.379
2.376
2.363
2.360
2.349
2.347
2.344
2.341
2.338
2.230
1.882
1.863
1.854
1.844
1.834
1.825
1.806
1.550
1.245

```

yui
expl std13c
SAMPLE
date Apr 2 2005 dfrq. 400.454
solvent CDCl3 dn H1
file /export/home/~ dpwr 42
chem/rs1/arjan/fur~ dof 0
an-C-02-04-2005.fi~ dm yyy
d dmm w
ACQUISITION dmf 8000
sfrq 100.705 PROCESSING
tn C13 lb 3.00
at 0.635 wtfile
np 32000 proc ft
sw , 25188.9 fn not used
fb 13800
bs 4 werr
tpwr 58 wexp
pw 6.5 wbs
dl 2.000 wnt
tof 2000.0
nt 1000
ct 0
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -0.2
wp 20138.2
vs 50
sc 0
wc 250
hzmm 1.69
is 500.00
rfl 8840.6
rfp 7753.4
th 6
ins 100.000
nm no ph

```

151.574
150.567

143.466

115.341

106.515
105.981

84.039
79.153
77.305
77.000
76.679

34.705

29.895
28.750

22.306
22.230

13.557

H-252-H

expl std1h

SAMPLE
date May 3 2005 dfrq 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 400.455 dm nnn
tn H1 dmm c
at 2.664 dmf 8000
np 32016
sw 6009.6 lb 0.10
fb 3400 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.0
d1 1.000 werr
tof 500.0 wexp
nt 100 wbs wft aph
ct 16 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.3
wp 4004.2
vs 100
sc 0
wc 250
hzmm 16.02
is 154.93
rfl 487.9
rfp 0
th 10
ins 10.000
nm ph

DEC. & VT
7.361
7.350
7.343
7.337
7.327
7.258
400.454
H1
42
0
nnn
c
8000
0.10
wtfile
ft
not used
werr
wexp
wbs
wnt
wft aph

3.894

3.192

1.701
1.557

B-252-C

exp3 std13c

```

SAMPLE          DEC. & VT
date  May  2 2005  dfrq    400.454
solvent  CDC13    dn      H1
file      exp     dpwr     42
              dof       0
ACQUISITION
sfrq    100.705   dm       yyy
tn       C13      dmm      w
at       0.635   dmf      8000
np       32000
sw       25188.9  lb       3.00
fb       13800   wtfile
bs        4      proc      ft
tpwr     58      fn       not used
pw        6.5
d1        2.000  werr
tof       2000.0  wexp
nt       10000   wbs      wft
ct        104   wnt
alock      n
gain      not used
              FLAGS
il         n
in         n
dp         y
              DISPLAY
sp        -0.2
wp       20138.2
vs        50
sc         0
wc        250
hzmm      80.56
is        500.00
rfl       1091.8
rfp        0
th         5
ins       100.000
nm no ph
```

—146.948

139.481
138.825129.144
128.793
128.457
128.136
127.098
126.30484.467
79.947
77.321
77.015
76.695

—43.454

—18.947

BRUKER
BRUKER PPM

7.29341
7.26861
7.24126
7.21285
7.18814
7.16703
7.15947

3.04770
2.90550
2.74718
2.72435
2.71040
2.69297
2.56903
2.53876
2.51482
2.15032
2.03729
1.58550
1.57455
1.56444
1.55419
1.53446

JUANG. 1H
DATE 13-4-5

SF 300.133
SY 299.0
Q1 4800.000
SI 8192
TD 8192
SW 4504.505
HZ/PT 1.100

PW 5.0
RD 0.0
AQ .909
RG 400
NS 48
TE 297

FW 5700
Q2 3200.000
DP 63L P0

LB .100
GB 0.0
CX 27.00
CY 0.0
F1 10.501P
F2 -.499P
HZ/CM 122.274
PPM/CM .407
SR 3373.75

... OBSERVE

exp8 std13c

SAMPLE		DEC. & VT	
date	Apr 12 2005	dfrq	400.454
solvent	CDCl3	dn	H1
file	exp	dpwr	42
ACQUISITION		PROCESSING	
sfrq	100.705	dm	yyy
tn	C13	dmm	w
at	0.635	dmf	8000
np	32000	lb	3.00
sw	25188.9	wtfile	
fb	13800	proc	ft
bs	4	fn	not used
tpwr	58		
pw	6.5		
d1	2.000	werr	
tof	2000.0	wexp	
nt	10000	wbs	wft
ct	0	wnt	
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-0.4		
wp	20138.2		
vs	50		
sc	0		
wc	250		
hzmm	80.56		
is	500.00		
rfl	8843.9		
rfp	7753.4		
th	5		
ins	100.000		
nm	no	ph	

146.865
142.121
128.638
128.379
128.241
125.890
125.752

84.251
79.029
77.334
77.013
76.693

38.108
34.321
29.740
29.389
22.411
22.319

B-257-H

expl std1h

SAMPLE

date May 24 2005 dfrg 400.454

solvent CDCl3 dn H1

file /export/home/~ dpwr 42

chem/rs1/arjan/B-2~ dof 0

57-H.fid dm nnn

ACQUISITION dmm c

sfrq 400.455 dmf 8000

tn H1 PROCESSING

at 2.664 lb 0.10

np 32016 wtfile

sw 6009.6 proc ft

fb 3400 fn not used

bs 4

tpwr 58 werr

pw 6.0 wexp

d1 1.000 wbs wft aph

tof 500.0 wnt

nt 1000

ct 32

alock n

gain not used

FLAGS

il n

in n

dp y

DISPLAY

sp -200.4

wp 4004.2

vs 60

sc 0

wc 250

hzmm 0.63

is 193.18

rfl 496.7

rfp 0

th 11

ins 10.000

nm ph

7.333
7.330
7.315
7.301
7.297
7.276
7.272
7.267
7.255
7.251
7.246
7.235
7.228

DEC. & VT

400.454

PROCESSING

0.10

wtfile

proc

ft

fn not used

werr

wexp

wbs

wnt

wft aph

3.128
2.647
2.632
2.617
2.218
2.204
2.188
2.175
1.689
1.674
1.660
1.613
1.600
1.592
1.585
1.577
1.569
1.556
1.545
1.530
1.516
1.501
1.486
1.239

13C OBSERVE

exp9 std13c

SAMPLE		DEC. & VT	
date	May 6 2005	dfrq	400.454
solvent	CDC13	dn	H1
file	exp	dpwr	42
ACQUISITION		dof	0
sfrq	100.705	dm	yyy
tn	C13	dmm	w
at	0.635	dmf	8000
np	32000	PROCESSING	
sw	25188.9	lb	3.00
fb	13800	wtfile	
bs	4	proc	ft
tpwr	58	fn	not used
pw	6.5		
d1	2.000	werr	
tof	2000.0	wexp	
nt	1000	wbs	wft
ct	144	wnt	
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-0.2		
wp	20138.2		
vs	100		
sc	0		
wc	250		
hzmm	80.56		
is	500.00		
rfl	8857.6		
rfp	7753.4		
th	6		
ins	100.000		
nm	no ph		

151.925

138.748

129.052

127.999

126.762

115.096

83.947

80.084

77.290

76.969

76.654

33.895

31.086

28.001

27.849

26.307

B-270-H

expt stdih

SAMPLE		DEC. & VT	
date	May 20 2005	dfrq	400.454
solvent	CDC13	dn	H1
file	exp	dpwr	42
ACQUISITION		PROCESSING	
sfrq	400.455	dof	0
tn	H1	dm	nnn
at	2.664	dmm	c
np	32016	dmf	8000
sw	6009.6	lb	0.10
fb	3400	wtfile	
bs	4	proc	ft
tpwr	58	fn	not used
pw	6.0		
dl	1.000	werr	
tof	500.0	wexp	
nt	1000	wbs	wft aph
ct	12	wnt	
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-200.4		
wp	4004.2		
vs	150		
sc	0		
wc	250		
hzmm	16.02		
is	324.44		
rfl	3394.6		
rfp	2899.3		
th	9		
ins	10.000		
nm	ph

13C OBSERVE

exp3 std13c

SAMPLE		DEC. & VT	
date	May 20 2005	dfrq	400.454
solvent	CDC13	dn	H1
file	exp	dpwr	42
ACQUISITION		dof	0
sfrq	100.705	dm	yyy
tn	C13	dmm	w
at	0.635	dmf	8000
np	32000	PROCESSING	
sw	25188.9	lb	3.00
fb	13800	wtfile	
bs	4	proc	ft
tpwr	58	fn	not used
pw	6.5		
d1	2.000	werr	
tof	2000.0	wexp	
nt	10000	wbs	wft
ct	312	wnt	
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-1062.6		
wp	20138.2		
vs	200		
sc	0		
wc	250		
hzmm	1.81		
is	500.00		
rfl	8840.6		
rfp	7753.4		
th	9		
ins	100.000		
nm	no ph

Current Data Parameters
NAME Datta-CH2CH2PH
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050510
Time 20.57
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2807028 sec
RG 32
DW 69.600 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 3.00 dB
SFO1 599.6024466 MHz

F2 - Processing parameters
SI 32768
SF 599.6000300 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 9.500 ppm
F1 5696.20 Hz
F2P -0.500 ppm
F2 -299.80 Hz
PPMCM 0.50000 ppm/cm
HZCM 299.80002 Hz/cm

Current Data Parameters
NAME Datta-CH2CH2PH
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050510
Time 21.00
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT C6D6
NS 46
DS 0
SWH 37593.984 Hz
FIDRES 1.147277 Hz
AQ 0.4358644 sec
RG 2048
DW 13.300 usec
DE 6.50 usec
TE 299.3 K
D1 3.00000000 sec
d11 0.03000000 sec
DELTA 2.90000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.30 usec
PL1 0.00 dB
SFO1 150.7861246 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 11.30 dB
PL13 14.00 dB
SFO2 599.6029980 MHz

F2 - Processing parameters
SI 65536
SF 150.7695563 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 4.50 cm
F1P 200.000 ppm
F1 30153.91 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1507.69556 Hz/cm

phph-³C-Pdt
 exp1 s2pu1

7.570
 7.554
 7.363
 7.348
 7.332
 7.240
 7.228
 7.213
 7.198
 6.943

— 3.783

SAMPLE DEC. & VT
 date Apr 12 2005 dfrq 499.832
 solvent CDC13 dn H1
 file /export/home/~ dpwr 38
 opera/vnmrsys/data~ dof 0
 1/LIOU/liou0412.00~ dm nnn
 2H.fid dmm c
 ACQUISITION dmf 11299
 sfrq 499.833 dseq
 tn H1 dres 1.0
 at 2.182 homo n
 np 39276
 sw 9000.9 wtfile
 fb not used proc ft
 bs 4 fn 32768
 tpwr 55 math f
 pw 5.5
 d1 1.000 werr
 tof 980.4 wexp
 nt 32 wbs wft
 ct 32 wnt wft
 alock y
 gain not used
 FLAGS
 il n
 in n
 dp y
 hs nn
 DISPLAY
 sp -250.1
 wp 5247.9
 vs 58
 sc 0
 wc 250
 hzmm 2.70
 is 114.74
 rfl 4663.9
 rfp 3618.8
 th 2
 ins 100.000
 nm ph

phph-4C-Pdt

exp2 s2pu1

SAMPLE		DEC. & VT	
date	Apr 12 2005	dfrq	499.832
solvent	CDC13	dn	H1
file	exp	dpwr	38
ACQUISITION		dof	0
sfrq	125.698	dm	yyy
tn	C13	dmm	w
at	0.508	dmf	11299
np	37088	dseq	
sw	36529.7	dres	1.0
fb	not used	homo	n
bs	4	PROCESSING	
tpwr	55	lb	3.00
pw	5.0	wtfile	
d1	2.000	proc	ft
tof	3769.1	fn	not used
nt	1024	math	f
ct	1024		
alock	y	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-0.3		
wp	27650.0		
vs	95		
sc	0		
wc	250		
hzmm	110.60		
is	119.21		
rfl	12270.9		
rfp	9677.5		
th	3		
ins	100.000		
nm	ph

Current Data Parameters
NAME Datta-pdt-5-3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040919
Time 22.10
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT MeOD
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 4.00 dB
SFO1 599.7027179 MHz

F2 - Processing parameters
SI 32768
SF 599.7000269 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
FLP 9.500 ppm
F1 5697.15 Hz
F2P -0.500 ppm
F2 -299.85 Hz
PPMCM 0.50000 ppm/cm
HZCM 299.85001 Hz/cm

Current Data Parameters
NAME Datta-Pdt-OME
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20050308
Time 18.07
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT C6D6
NS 200
DS 0
SWH 37593.984 Hz
FIDRES 1.147277 Hz
AQ 0.4358644 sec
RG 2048
DW 13.300 usec
DE 6.50 usec
TE 293.4 K
D1 3.00000000 sec
d11 0.03000000 sec
DELTA 2.90000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.30 usec
PL1 0.00 dB
SFO1 150.7861246 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 11.30 dB
PL13 14.00 dB
SFO2 599.6029980 MHz

F2 - Processing parameters

SI 65536
SF 150.7695477 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters

CX 20.00 cm
CY 3.50 cm
F1P 195.000 ppm
F1 29400.06 Hz
F2P -5.000 ppm
F2 -753.85 Hz
PPMCM 10.00000 ppm/cm
HZCM 1507.69556 Hz/cm

Current Data Parameters
NAME Datta-CF3-3C-Pdt
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050413
Time 17.37
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9259.259 Hz
FIDRES 0.282570 Hz
AQ 1.7695220 sec
RG 64
DW 54.000 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 4.00 dB
SFO1 599.6030610 MHz

F2 - Processing parameters
SI 32768
SF 599.6000934 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 9.500 ppm
F1 5696.20 Hz
F2P -0.500 ppm
F2 -299.80 Hz
PPMCM 0.50000 ppm/cm
HZCM 299.80005 Hz/cm

Current Data Parameters
NAME Datta-CP3-3C-Pdt
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050413
Time 18.53
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT C6D6
NS 1523
DS 0
SWH 37593.984 Hz
FIDRES 1.147277 Hz
AQ 0.4358644 sec
RG 2048
DW 13.300 usec
DE 6.50 usec
TE 296.2 K
D1 3.00000000 sec
d11 0.03000000 sec
DELTA 2.90000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.30 usec
PL1 0.00 dB
SFO1 150.7861246 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 11.30 dB
PL13 14.00 dB
SFO2 599.6029980 MHz

F2 - Processing parameters
SI 65536
SF 150.7695465 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 200.000 ppm
F1 30153.91 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1507.69543 Hz/cm

pro-4-Pdt-7-1

exp55 s2pu1

SAMPLE DEC. & VT
date Oct 1 2004 dfrq 499.838
solvent CDCl3 dn H1
file /export/home/~ dpwr 38
opera/vnmrsys/data~ dof 0
1/LIOU/liou1001.01~ dm nnn
0.fid dmm c

ACQUISITION
sfrq 499.839 dseq
tn H1 dres 1.0
at 2.182 homo n

PROCESSING
np 39276 wtfile
sw 9000.9 proc ft
fb not used fn 32768
bs 4 math f

tpwr 55
pw 5.5
d1 1.000 werr
tof 980.4 wexp
nt 32 wbs
ct 32 wnt wft

alock y
gain not used

FLAGS
il n
in n
dp y
hs nn

DISPLAY
sp -250.1
wp 5247.9
vs 88
sc 0
wc 250
hzmm 8.38
is 404.32
rfl 4656.2
rfp 3618.8
th 8
ins 100.000
nm ph

7.517
7.502
7.353
7.350
7.328
7.313
7.297
7.240
7.195
7.180
7.165
6.881
6.764
6.408
6.404
6.401
6.398
6.363
6.356

3.712

0.051

Current Data Parameters
NAME Datta-Pro-4-Pdt-7
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041011
Time 22.37
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT C6D6
NS 6144
DS 0
SWH 42372.883 Hz
FIDRES 1.293118 Hz
AQ 0.3867124 sec
RG 2048
OW 11.800 usec
DE 6.50 usec
TE 0.0 K
D1 4.00000000 sec
d11 0.03000000 sec
DELTA 3.90000010 sec
ACREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.50 usec
PL1 0.00 dB
SFO1 150.8112724 MHz

===== CHANNEL f2 =====
PCPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 8.80 dB
PL13 10.00 dB
SFO2 599.7029985 MHz

F2 - Processing parameters
SI 65536
SF 150.7946872 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 200.000 ppm
F1 30158.94 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1507.94690 Hz/cm

Current Data Parameters
NAME Datta-Pdt-13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041111
Time 16.16
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 32
DW 59.600 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 4.00 dB
SFO1 599.6023984 MHz

F2 - Processing parameters
SI 32768
SF 599.6000322 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 12.00 cm
F1P 9.500 ppm
F1 5696.20 Hz
F2P -0.500 ppm
F2 -299.80 Hz
PPMCM 0.50000 ppm/cm
HZCM 299.80002 Hz/cm

Current Data Parameters
NAME Datta-Pdt-13
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041111
Time 16.18
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT C6D6
NS 400
DS 0
SWH 37593.984 Hz
FIDRES 1.147277 Hz
AQ 0.4358644 sec
RG 2048
DW 13.300 usec
DE 6.50 usec
TE 299.4 K
D1 4.00000000 sec
d11 0.03000000 sec
DELTA 3.90000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.30 usec
PL1 0.00 dB
SFO1 150.7861246 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 11.30 dB
PL13 14.00 dB
SFO2 599.6029980 MHz

F2 - Processing parameters
SI 65536
SF 150.7695488 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 4.50 cm
F1P 200.000 ppm
F1 30153.91 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1507.69543 Hz/cm

exp1 s2pu1

SAMPLE DEC. & VT
date May 13 2004 dfrq 499.838
solvent CDC13 dn H1
file /export/home/~ dpwr 38
opera/vnmrsys/data~ dof 0
1/LIOU/liou0513.00~ dm nnn
5H.fid dmm c

ACQUISITION
sfrq 499.839 dseq
tn H1 dres 1.0
at 2.182 homo n
np 39276
sw 9000.9 wtfle
fb not used proc ft
bs 4 fn 32768
tpwr 55 math f
pw 5.5
d1 1.000 werr
tof 980.4 wexp
nt 32 wbs wft
ct 32 wnt wft
alock y
gain not used

PROCESSING
wtfile
proc ft
fn 32768
math f
werr
wexp
wbs wft
wnt wft

FLAGS
il n
in n
dp y
hs nn

DISPLAY
sp -250.1
wp 5247.9
vs 87
sc 0
wc 250
hzmm 8.42
is 404.32
rf1 1039.0
rfp 0
th 2
ins 100.000
nm ph

S-66

exp62 DEPT

SAMPLE
date May 13 2004
solvent CDCl3
file /export/home/~
opera/vnmrsvs/data~
1/LIOU/liou0513.00~
50.fid

ACQUISITION
sw 31446.5
at 0.507
np 31902
bs 16
ss -4
dl 1.000
nt 6400
ct 336

TRANSMITTER
tn C13
tof 2537.3
tpwr 55
pw 8.400

DECOUPLER
dn H1
dof 0
dpwr 38
dm nny
dmf 11299
pplvl 57
pp 14.300

DEPT
j1xh 140.0

SPECIAL
temp not used
gain 54
spin not used

PROCESSING
lb 3.00
fn not used

SPECTRUM
wp 31446.5
sp -1278.6
rp -56.1
lp 177.0
nm ph

REFERENCE
rf1 1278.6

PLOT

wc 250
sc 0
vs 20
hzmm 120.66
th 30

147.985
146.534
145.389
144.732
135.950
130.636
128.620
128.131
126.909
126.619
124.741
119.525
108.430
105.238
100.993

77.260
77.000
76.740

40.958

P0260 PA-ND

exp1 s2pu1

SAMPLE		DEC. & VT	
date	Jun 14 2004	dfrq	499.838
solvent	CDC13	dn	H1
file	/export/home/~	dpwr	38
opera	/vnmr/sys/data/~	dof	0
1/LIQU	11000614.00~	dm	n
	1H.fid	dmm	c
ACQUISITION		dmf	11299
sfrq	499.839	dseq	
tn	H1	dres	1.0
at	2.182	homo	n
np	39276	PROCESSING	
sw	9000.9	wtfile	
fb	not used	proc	ft
bs	4	fn	32768
tpwr	55	math	f
pw	5.5		
d1	1.000	werr	
tof	980.4	wexp	
nt	32	wbs	wft
ct	32	wnt	wft
alock	y		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.1		
wp	5247.9		
vs	54		
sc	0		
wc	250		
hzmm	2.62		
is	75.69		
rfl	4657.9		
rfp	3618.8		
th	4		
ins	100.000		
nm	ph		

7.428
7.411
7.240
7.140
7.125
7.031
7.012
6.833
6.785
6.768
6.755

5.942

3.683

exp3 DEPT

SAMPLE
date Jun 14 2004
solvent CDCl3
file /export/home/~
opera/vnmrsys/data~
1/LIU0614.00~
30.fid

ACQUISITION
sw 36529.7
at 0.508
np 37088
bs 4
ss -4
dl 1.000
nt 2048
ct 336

TRANSMITTER
tn C13
tof 3769.1
tpwr 55
pw 12.500

DECOUPLER
dn H1
dof 0
dpwr 38
dm npv
dmf 11299
pplvl 57
pp 13.400

DEPT
j1xh 140.0

SPECIAL
temp not used
gain 54
spin not used

PROCESSING
lb 3.00
fn not used

SPECTRUM
wp 27650.0
sp -0.3
rp -133.3
lp 248.2
nm ph

REFERENCE
rfl 17473.9

PLOT
wc 250
sc 0
vs 20
hzmm 110.60
th 14

147.961
146.426
144.848

136.394
133.254
130.753
129.307
127.249
126.948
124.668

118.423

108.409
105.189
100.958

77.257
77.000
76.752

40.978

21.163

Pdt-CF3

exp1 s2pu1

SAMPLE DEC. & VT
date Mar 8 2005 dfrq 499.832
solvent CDC13 dn H1
file /export/home/~ dpwr 38
opera/vnmrsys/data~ dof 0
1/LIU0/liou0308.00~ dm nnn
3H.fid dmm c
ACQUISITION dmf 11299
sfrq 499.833 dseq
tn H1 dres 1.0
at 2.182 homo n
np 39276
sw 9000.9 wtfile
fb not used proc ft
bs 4 fn 32768
tpwr 55 math f
pw 5.5
d1 1.000 werr
tof 980.4 wexp
nt 32 wbs wft
ct 32 wnt wft
alock y
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -250.1
wp 5247.9
vs 127
sc 0
wc 250
hzmm 1.57
is 107.82
rf1 1044.6
rfp 0
th 4
ins 100.000
nm ph

7.592
7.575
7.554
7.537
7.520
7.500
7.487
7.471
7.451
7.437
7.432
7.429
7.400
7.395
6.778
5.956
5.901

3.717

S-70

Current Data Parameters
 NAME Datta-Pdt-CF3
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20050320
 Time 21.51
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg
 TD 32768
 SOLVENT C6D6
 NS 6144
 DS 0
 SWH 37593.984 Hz
 FIDRES 1.147277 Hz
 AQ 0.4358644 sec
 RG 2048
 DW 13.300 usec
 DE 6.50 usec
 TE 296.5 K
 D1 3.00000000 sec
 d11 0.03000000 sec
 DELTA 2.90000010 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

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

NUC1 13C
 P1 4.30 usec
 PL1 0.00 dB
 SFO1 150.7861246 MHz

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

CPDPRG2 waltz16
 NUC2 1H
 PCPD2 92.00 usec
 PL2 120.00 dB
 PL12 11.30 dB
 PL13 14.00 dB
 SFO2 599.6029980 MHz

F2 - Processing parameters

SI 65536
 SF 150.7695471 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 0.50

1D NMR plot parameters

CX 20.00 cm
 CY 6.00 cm
 F1P 200.000 ppm
 F1 30153.91 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.00000 ppm/cm
 HZCM 1507.69543 Hz/cm

phph-A-C-Pdt

exp1 /s2pu1

SAMPLE DEC. & VT
date Apr 12 2005 dfrq 499.832
solvent CDC13 dn H1
file /export/home/~ dpwr 38
opera/vnmr/sys/data~ dof 0
1/LIU0412.00~ dm nnn
3H.fid dmm c
ACQUISITION dmf 11299
sfrq 499.833 dseq
tn H1 dres 1.0
at 2.182 homo n
np 39276
sw 9000.9 wtfile
fb not used proc ft
bs 4 fn 32768
tpwr 55 math f
pw 5.5
d1 1.000 werr
tof 980.4 wexp
nt 32 wbs
ct 32 wnt
alock y
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -250.1
wp 5247.9
vs 61
sc 0
wc 250
hzmm 7.95
is 114.74
rfl 1045.1
rfp 0
th 3
ins 100.000
nm ph

7.527
7.510
7.399
7.384
7.363
7.348
7.331
7.315
7.275
7.261
7.239
7.172
7.158
7.143
6.779
6.458

3.051
3.046
3.036
3.024
3.007

phph-~~3~~C-Pdt

exp2 s2pu1

```

SAMPLE
date Apr 12 2005 dfrq 499.832
solvent CDC13 dn H1
file /export/home/~ dpwr 38
opera/vnmrsys/data~ dof 0
1/LI0U/liou0412.00~ dm yyy
3C.fid dmm w
ACQUISITION dmf 11299
sfrq 125.698 dseq
tn C13 dres 1.0
at 0.508 homo n
np 37088
sw 36529.7 lb 3.00
fb not used wtfile
bs 4 proc ft
tpwr 55 fn not used
pw 5.0 math f
d1 2.000
tof 3769.1 werr
nt 1024 wexp
ct 788 wbs
alock y wnt
gain not used

FLAGS
il n
in n
dp y
hs nn

DISPLAY
sp -0.3
wp 27650.0
vs 95
sc 0
wc 250
hzmm 18.75
is 119.21
rfl 12267.6
rfp 9677.5
th 7
ins 100.000
nm ph
```

DEC. & VT

PROCESSING

149.807
147.989

138.763
135.898
131.605
128.474
128.394
127.897
127.782
125.698
120.322

77.257
77.000
76.752

33.101
29.393

Pdt-6-mem-ph

exp43 s2pu1

SAMPLE DEC. & VT
date Jan 3 2005 dfrq 499.838
solvent CDC13 dn H1
file /export/home/~ dpwr 38
opera/vnmrsys/data~ dof 0
1/LIOU/liou0103.00~ dm nnn
1H.fid dmm c
ACQUISITION dmf 11299
sfrq 499.839 dseq
tn H1 dres 1.0
at 2.182 homo n
np 39276
sw 9000.9 wtfile
fb not used proc ft
bs 4 fn 32768
tpwr 55 math f
pw 5.5
d1 1.000 werr
tof 980.4 wexp
nt 32 wbs wft
ct 32 wnt wft
alock y
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -250.1
wp 5247.9
vs 126
sc 0
wc 250
hzmm 3.25
is 103.43
rfl 4656.8
rfp 3618.8
th 5
ins 100.000
nm ph

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Pdt-6-mem-ph

exp45 DEPT

SAMPLE

date Jan 3 2005
solvent CDC13
file /export/home/~
opera/vnmr/sys/data/~
1/LIOU/liou0103.00~

10.fid

ACQUISITION

sw 36529.7
at 0.508
np 37088
bs 8
ss -4
dl 1.000
nt 2048
ct 216

TRANSMITTER

tn C13
tof 3769.1
tpwr 54
pw 9.400

DECOUPLER

dn H1
dof 0
dpwr 38
dm nny
dmm ccw
dmf 11111
pplvl 57
pp 13.000

DEPT

j1xh 140.0

SPECIAL

temp not used
gain 54
spin not used

PROCESSING

lb 3.00
fn not used

SPECTRUM

wp 27650.0
sp -0.2
rp -46.7
lp 177.0

nm ph

REFERENCE

rfl 18732.5
rfp 16139.2

PLOT

wc 250
sc 0
vs 20
hzmm 110.60
th 4

156.565

149.620

147.464

136.066

131.924

128.411

127.648

127.604

126.974

125.635

120.286

113.962

110.423

77.257

77.000

76.743

55.472

32.862

29.190

STANDARD 1H OBSERVED

exp4 std1h

SAMPLE
date Apr 12 2005 dfrq
solvent CD2Cl2 dn
file exp dpwr
ACQUISITION dof
sfrq 400.456 dm nnn
tn H1 dmm c
at 2.664 dmf 8000
np 32016
sw 6009.6 lb 0.10
fb 3400 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.0
d1 1.000 werr
tof 500.0 wexp
nt 100 wbs
ct 0 wnt
aLOCK n
gain not used

FLAGS
il n
in n
dp y

DISPLAY
sp -205.5
wp 4204.5
vs 100
sc 0
wc 250
hzmm 16.82
is 269.37
rfl 2623.5
rfp 2130.4
th 15
ins 10.000
nm ph

DEG. & VT
400.455
H1
42
0
nnn
c
8000
0.10
ft
not used
wft aph

7.256
7.253
7.447
7.436
7.432
7.428
7.415
7.412
7.392
7.387
7.373
7.369
7.357
7.353
7.349
7.338
7.266
7.262
7.258
7.249
7.245
7.239
7.226

2.818
2.816
2.814
2.672
2.666
2.651
2.641
2.634
2.630
2.617
2.611
2.605
2.596
2.589
2.583
2.579
2.574
2.567
2.214
2.206
2.196
2.192
2.190
2.184
2.182
2.178
1.727
1.719

13C OBSERVE

exp5 std13c

SAMPLE DEC. & VT
date Apr 10 2005 dfrq 400.455
solvent cd2cl2 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 100.705 dm yyy
tn C13 dmm w
at 0.635 dmf 8000
np 32000
sw 25188.9 lb 3.00
fb 13800 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.5
d1 2.000 werr
tof 2000.0 wexp
nt 1000 wbs
ct 108 wnt
a lock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -0.8
wp 20138.2
vs 40
sc 0
wc 250
hzmm 80.56
is 500.00
rfl 6462.1
rfp 5417.3
th 4
ins 100.000
nm no ph

147.476

138.421

138.330

137.413

128.466

127.733

126.817

116.907

54.060

53.800

53.525

33.614

27.537

26.010

25.461

23.216

B

expl std1h

SAMPLE		DEC. & VT	
date	Apr 4 2005	dfrq	400.454
solvent	CDC13	dn	H1
file	exp	dpwr	42
ACQUISITION		dof	0
sfrq	400.455	dm	nnn
tn	H1	dmm	c
at	2.664	dmf	8000
np	32016	PROCESSING	
sw	6009.6	lb	0.10
fb	3400	wtfile	
bs	4	proc	ft
tpwr	58	fn	not used
pw	6.0		
d1	1.000	werr	
tof	500.0	wexp	
nt	1000	wbs	wft aph
ct	24	wnt	
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-0.8		
wp	4004.2		
vs	100		
sc	0		
wc	250		
hzmm	16.02		
is	130.16		
rfl	487.9		
rfp	0		
th	14		
ins	10.000		
nm	ph		

6.171
6.163

```

yu1
exp1 std13c
SAMPLE
date Apr 4 2005 dfrq 400.454
solvent CDC13 dn H1
file /export/home/~ dpwr 42
chem/rs1/arjan/fur~ dof 0
an-product-04-04-2~ dm yyy
005.fid dmm w
ACQUISITION dmf 8000
sfrq 100.705 PROCESSING
tn C13 3.00
at 0.635 wtfile
np 32000 proc
sw 25188.9 fn not used
fb 13800
bs 4 werr
tpwr 58 wexp
pw 6.5 wbs
di 2.000 wnt
tof 2000.0
nt 1000
ct 0
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -0.2
wp 20138.2
vs 50
sc 0
wc 250
hzmm 80.56
is 500.00
rfl 8839.1
rfp 7753.4
th 9
ins 100.000
nm no ph

```

132.032

116.135

108.454
107.202

77.305
76.985
76.679

30.674
27.009
25.039
24.963
22.489

13.740

B-255-H

exp5 stdin

date May 3 2005

solvent cd2c12

file exp

ACQUISITION

sfrq 400.456

tn H1

at 2.664

np 32016

sw 6009.6

fb 3400

bs 4

tpwr 58

pw 6.0

d1 1.000

tof 500.0

nt 1000

ct 32

alock n

gain not used

FLAGS

il n

in n

dp y

DISPLAY

sp -200.3

wp 4004.2

vs 150

sc 0

wc 250

hzmm 4.95

is 328.36

rfl 487.9

rfp 0

th 10

ins 10.000

nm ph

DEF. & VT

400.456

H1

AZ

0

nnn

c

8000

PROCESSING

lb 0.10

wtfile

proc ft

fn not used

werr

wexp

wbs

wnt

wft aph

S-80

B-255-C

exp6 std13c

SAMPLE		DEC. & VT	
date	May 3 2005	dfrq	400.455
solvent	cd2cl2	dn	H1
file	exp	dpwr	42
ACQUISITION		PROCESSING	
sfrq	100.705	dm	yyy
tn	C13	dmm	w
at	0.635	dmf	8000
np	32000	lb	3.00
sw	25188.9	wf	not used
fb	13800	proc	ft
bs	4	fn	not used
tpwr	58		
pw	6.5		
d1	2.000	werr	
tof	2000.0	wexp	
nt	10000	wbs	wft
ct	312	wnt	
alock	n		
gain	not used		

FLAGS

dp	y
DISPLAY	
sp	-0.8
wp	20138.2
vs	50
sc	0
wc	250
hzmm	80.56
is	500.00
rfl	6465.2
rfp	5417.3
th	10
ins	100.000
nm	no ph

129.168
128.985
128.664
128.573
128.481
128.221
127.382
127.076
126.740
126.435

54.273
53.998
53.724
53.464
53.189

43.081

14.375

STANDARD 1H OBSERVE

exp3 std1h

SAMPLE DEC. & VT
 date Apr 14 2005 dfrq 400.455
 solvent cd2cl2 dn H1
 file /export/home/~ dpwr 42
 chem/rs1/arjan/ben~ dof 0
 zyl-P-14-04-2005.f~ dm nnn
 id dmm c
 dmfm 8000
 ACQUISITION
 sfrq 400.456
 tn H1 lb 0.10
 at 2.664 wtfile
 np 32016 proc ft
 sw 6009.6 fn not used
 fb 3400
 bs 4 werr
 tpwr 58 wexp
 pw 6.0 wbs
 dl 1.000 wnt
 tof 500.0
 nt 100
 ct 0
 alock n
 gain not used
 FLAGS
 il n
 in n
 dp y
 DISPLAY
 sp -200.4
 wp 4004.2
 vs 100
 sc 0
 wc 250
 hzmm 1.09
 is 190.20
 rfl 2623.5
 rfp 2130.4
 th 18
 ins 10.000
 nm ph

7.403
7.385
7.334
7.316
7.300
7.296
7.145
7.126

6.110

2.887
2.881
2.873
2.867
2.860
2.854
2.498
2.495
2.490
2.485
2.184
2.180
1.737
1.731
1.724
1.715
1.708
1.530

13C OBSERVE

exp5 std13c

SAMPLE		DEC. & VT	
date	Apr 16 2005	dfrq	400.455
solvent	cd2cl2	dn	H1
file	exp	dpwr	42
ACQUISITION			
sfrq	100.705	dm	yyy
tn	C13	dmm	w
at	0.635	dmf	8000
np	32000	PROCESSING	
sw	25188.9	lb	3.00
fb	13800	wtfile	
bs	4	proc	ft
tpwr	58	fn	not used
pw	6.5		
d1	2.000	werr	
tof	2000.0	wexp	
nt	10000	wbs	
ct	616	wnt	
glock	0		
gain	not used		

FLAGS	
il	n
in	n
dp	y
DISPLAY	
sp	-0.8
wp	20138.2
vs	45
sc	0
wc	250
hzmm	80.56
is	500.00
rfl	6465.2
rfp	5417.3
th	4
ins	100.000
nm	no ph

150.545
147.460
139.673
137.597
128.771
128.603
128.130
125.381
114.388

54.304
54.029
53.769
53.495
53.220

35.248
29.629
27.232
23.308
22.895
22.621

B-270-H

exp1 std1h

SAMPLE DEC. & VT
date May 21 2005 dfrq 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 400.455 dm nnn
tn H1 dmm c
at 2.664 dmf 8000
np 32016
sw 6009.6 lb 0.10
fb 3400 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.0
dl 1.000 werr
tof 500.0 wexp
nt 1000 wbs
ct 12 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -201.8
wp 4004.2
vs 400
sc 0
wc 250
hzmm 1.89
is 193.18
rfl 3396.0
rfp 2899.3
th 5
ins 10.000
nm ph

5.508

B-271-C

exp3 std13c

SAMPLE		DEC.	B	VT
date	May 21 2005	dfrq	400.454	
solvent	CDC13	dn	H1	
file	exp	dpwr	42	
ACQUISITION		dof	0	
sfrq	100.705	dm	yyy	
tn	C13	dmm	w	
at	0.635	dmf	8000	
np	32000	PROCESSING		
sw	25188.9	lb	3.00	
fb	13800	wtfile		
bs	4	proc	ft	
tpwr	58	fn	not used	
pw	6.5			
di	2.000	werr		
tof	2000.0	wexp		
nt	10000	wbs		wft
ct	416	wnt		
alock	n			
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
DISPLAY				
sp	-1084.1			
wp	20138.2			
vs	100			
sc	0			
wc	250			
hzmm	80.56			
is	500.00			
rfl	8837.6			
rfp	7753.4			
th	5			
ins	100.000			
nm	no ph

Pdt-CH2CH2Ph

exp21 s2pu1

SAMPLE DEC. & VT
date May 25 2005 dfrq 499.833
solvent CD2C12 dn H1
file /export/home/~ dpwr 38
opera/vnmrsys/data~ dof 0
1/LIOU/liou0525.00~ dm nnn
1H.fid dmm c
ACQUISITION dmf 11299
sfrq 499.834 dseq
tn H1 dres 1.0
at 2.182 homo n
np 39258
sw 8996.9 wtfile
fb 5000 proc ft
bs 4 fn 32768
tpwr 55 math f
pw 5.5
d1 1.000 werr
tof 980.4 wexp
nt 32 wbs
ct 32 wnt wft
alock y
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -250.5
wp 5247.8
vs 156
sc 0
wc 250
hzmm 2.50
is 404.32
rf1 3698.6
rfp 2649.1
th 5
ins 100.000
nm ph

Pdt-CH₂CH₂Ph

exp22 s2pu1

```

SAMPLE          DEC. & VT
date May 25 2005 dfrq      499.833
solvent CD2CL2  dn        H1
file /export/home/~ dpwr    38
opera/vnmrsys/data~ dof     0
1/LIOU/liou0525.00~ dm      yyy
                  1C.fid    dmm    w
ACQUISITION      dmf      11299
sfrq      125.698 dseq
tn         C13 dres      1.0
at         0.508 homo    n
np         37088
sw         36529.7 lb     3.00
fb         20000 wtfile
bs         16 proc      ft
tpwr       55 fn       not used
pw         5.0 math      f
d1         2.000
tof        3769.1 werr
nt         10000 wexp
ct         8640 wbs
alock      y wnt
gain      not used

FLAGS
il         n
in         n
dp         y
hs         nn

DISPLAY
sp         -0.9
wp         27650.0
vs         463
sc         0
wc         250
hzmm       18.02
is         119.21
rfl        9301.0
rfp        6761.7
th         4
ins        100.000
nm         ph

```

149.040
142.893
139.158
136.879
134.067
128.736
128.399
127.680
127.476
126.811
125.959
123.456
117.462

54.235
54.013
53.800
53.578
53.365

30.338
29.975
28.742
21.193

S-89

S-90