Supporting Information

Highly Efficient 1,4-Addition of 1,3-Diesters to Conjugated

Enones by In/TMSCl

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^1H and ^{13}C NMR spectra of the compound **3a-3o**, **5**, **6**

S2-S35

SMD-170-2

H₂

2910.56

1694.51
1690.56
1689.51
1683.52
1682.30
1676.41
1675.22
1669.33
1668.17
1664.35

1026.51
1019.35
1012.05
932.63
872.70
865.39
858.30
850.84

663.24
515.35
508.18
501.04
493.89

0.00

Current Data Parameters
NAME mar-02
EXPNO 146
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020323
Time 10:58
INSTRUM spect
PROBHD 5 mm Dui1 13
PULPROG zgpg30
TO 32768
SOLVENT CDCl3
NS 16
DS 1
SWH 8223.595 Hz
FIDRES 0.450967 Hz
AQ 1.992344 sec
RG 181
DW 60.800 usec
DE 5.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 ¹H
P1 10.80 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300033 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 NMR plot parameters
CX 30.00 cm
CP 8.000 ppm
F1 3301.04 kHz
F2 -40.01 Hz
PRCK 0.27000 ppm/cm
HZCM 108.03510 Hz/cm

SMD-170-2

SMD-169-1

Current Data Parameters
NAME mar-02
EXPNO 121
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020320
Time 10.00
INSTRUM spect
PROBHD 5 mm Dui1 13
PULPROG zg30
TO 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.695 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 256
RW 60.800 uspc
DE 6.00 uspc
TE 300.0 K
D1 1.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.80 uspc
PL1 -2.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.130056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPHOM 0.27333 ppm/cm
HZCM 103.36988 Hz/cm

SMD-169-1

Current Data Parameters
NAME mar-02
EXPNO 123
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020320
Time 12.44
INSTRUM spect
PROBHD 5 mm Dui 13
PULPROG zgpg30
TO 65535
SOLVENT CDCl3
NS 3072
DS 2
SMH 31847.133 Hz
FIDRES 0.465949 Hz
AQ 1.026562 sec
RG 655.3
DM 15.700 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.0300000 sec
D12 0.0000200 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SF01 100.6254556 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SF02 400.1324708 MHz

F2 - Processing parameters
SI 32768
SF 100.6127055 MHz
WDW EM
SSB 0
GB 1.00 Hz
PC 1.40

1D NMR plot parameters
CX 30.00 cm
F1P 240.000 ppm
F1 2447.06 Hz
F2P -5.000 ppm
F2 -503.07 Hz
PPMCH 8.1667 ppm/cm
HZCH 821.67096 Hz/cm

SMD-168-1

H₂

2907.31

1584.41
1583.27
1677.29
1676.19
1670.20
1668.98
1663.11
1661.90
1414.71
1409.19
1110.39
1105.17
1093.16
1087.98
1077.92
1071.92
1065.97
1016.99
1010.42
999.76
993.23
856.65
636.04
634.87
553.99
547.54
545.51
538.51
531.60
524.53
514.23
512.84
507.12
505.84
502.32
500.19
498.87
354.82
348.33
341.37
68.79
0.00

Current Data Parameters
NAME: muf-02
EXPNO: 79
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20020314
Time: 3:34
INSTRUM: spect
PROBHD: 5 mm QNP 1H
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl₃
NS: 16
DS: 0
SWH: 8223.685 Hz
FIDRES: 0.250657 Hz
AQ: 1.9923444 sec
RG: 181
DM: 60.800 usec
DE: 6.00 usec
TE: 300.0 K
D1: 1.00000000 sec
===== CHANNEL f1 =====
NUC1: 1H
P1: 10.80 usec
PL1: -2.00 dB
SFO1: 400.1324710 MHz
F2 - Processing parameters
SI: 16384
SF: 400.130066 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
1D NMR plot parameters
CY: 30.00 cm
F1P: 8.100 ppm
F1: 3241.05 Hz
F2P: -40.100 ppm
F2: -40.01 Hz
PPM0: 0.27233 ppm/cm
HZCM: 109.36688 Hz/cm

SMD-166-1

Current Data Parameters

NAME	mar-02
EXPNO	103
PROCNO	1

F2 - Acquisition Parameters

Date_	20020315
Time	12.18
INSTRUM	spect
PROBHD	5 mm Dui1 13
PULPROG	zgpg30
TO	65536
SOLVENT	CDCl3
NS	3072
DS	2
SWH	31847.133 Hz
FIDRES	0.465949 Hz
AQ	1.028952 sec
RG	1623.3
DM	19.700 usec
DE	6.00 usec
TE	300.2 K
D1	2.0000000 sec
D11	0.0300000 sec
D12	0.0002000 sec

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

NUC1	13C
P1	10.50 usec
PL1	-1.00 dB
SFO1	100.6254399 MHz

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

CPDPRG2	waltz16
NUC2 <td>1H</td>	1H
PCPD2 <td>105.00 usec</td>	105.00 usec
PL2 <td>-2.00 dB</td>	-2.00 dB
PL12 <td>18.00 dB</td>	18.00 dB
PL13 <td>20.00 dB</td>	20.00 dB
SFO2 <td>400.1324708 MHz</td>	400.1324708 MHz

F2 - Processing parameters

SI	32768
SF <td>100.6127662 MHz</td>	100.6127662 MHz
WDW <td>EM</td>	EM
SSB <td>0</td>	0
LB <td>1.00 Hz</td>	1.00 Hz
GB <td>0</td>	0
PC <td>1.40</td>	1.40

1D NMR plot parameters

CH	30.00 cm
F1P <td>240.000 ppm</td>	240.000 ppm
F1 <td>244.706 Hz</td>	244.706 Hz
F2P <td>-5.000 ppm</td>	-5.000 ppm
F2 <td>-503.07 Hz</td>	-503.07 Hz
PPMCH <td>8.16667 ppm/cm</td>	8.16667 ppm/cm
HZCM <td>821.67090 Hz/cm</td>	821.67090 Hz/cm

SMO-179-1

Current Data Parameters
NAME apr-02
EXPNO 52
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020404
Time 17:41
INSTRUM spect
PROBHD 5 mm DUA1 13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.250957 Hz
AQ 1.9523444 sec
RG 512
DM 60.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 13H
P1 10.80 usec
PL1 -2.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 36384
SF 400.130063 MHz
WDW Hanning
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
F1P 8.100 DPM
F1 3241.05 Hz
F2P -40.01 DPM
F2 -40.01 Hz
PPHMC 0.27333 DPM/cm
HZCM 109.36688 Hz/cm

SMD-179-1

Current Data Parameters
 NAME apr-02
 EPRNO 53
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20020404
 Time 19.44
 INSTRUM spect
 PROBRD 5 mm QNP 13
 PULPROG zgpg30
 ID zgpg30
 SOLVENT CDCl3
 NS 2471
 DS 2
 SM 310.713 Hz
 FIDRES 0.465043 Hz
 AQ 1.029852 sec
 RG 3280.3
 INVM 15.700 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 10.50 usec
 PL1 -1.00 dB
 SF01 100.6254556 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 105.00 usec
 PL2 -2.00 dB
 PL12 18.00 dB
 PL13 20.00 dB
 SF02 400.1324700 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.6127676 MHz
 MW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 1D NMR plot parameters
 CX 30.00 cm
 F1P 220.000 ppm
 F1 2213.81 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCH 7.50000 ppm/cm
 HZCH 754.59570 Hz/cm

Integral

198.80

100.00

201.76

538.49

318.05

201.97

100.63

218.34

321.23

302.22

Current Data Parameters

NAME: 3e

EXPNO: 333

PROCNO: 1

F2 - Acquisition Parameters

Date_: 20000429

Time: 18.42

INSTRUM: spect

PROBHD: 5 mm Dui 13

PULPROG: zg30

TD: 32768

SOLVENT: CDCl3

NS: 16

DS: 0

SWH: 8223.685 Hz

FIDRES: 0.250967 Hz

AQ: 1.3923444 sec

RG: 362

DW: 60.800 usec

DE: 6.00 usec

TE: 300.0 K

D1: 1.00000000 sec

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

NUC1: 13C

P1: 10.00 usec

PL1: -2.00 dB

SFO1: 400.1324710 MHz

F2 - Processing parameters

SF: 400.1300087 MHz

WIDW: 16384

SSB: 0

LB: 0.30 Hz

GB: 0

PC: 1.00

ID NMR plot parameters

CX: 30.00 cm

F1P: 8.100 ppm

F1: 3241.05 Hz

F2P: -40.10 Hz

F2: 0.27333 ppm/cm

PPMCM: 109.36888 Hz/cm

HZCM:

SMD-195-P

Current Data Parameters

NAME	gbr-32
EXPNO	334
PROCNO	1

F2 - Acquisition Parameters

Date_	20030429
Time	20.31
INSTRUM	gpcr1
PROBHD	5 mm QNP 1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2048
DS	2
SWH	31847.133 Hz
FIDRES	0.485949 Hz
AQ	1.0289652 sec
RG	2298.8
DW	15.700 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	10.50 usec
PL1	-1.00 dB
SFO1	100.625459 MHz

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

CPDPRG2	waltz16
NUC2	1H
P2	105.00 usec
PL2	-2.00 dB
PL12	18.00 dB
PL13	20.00 dB
SFO2	400.1324708 MHz

F2 - Processing parameters

SI	32768
SF	100.6127579 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	30.00 cm
F1P	220.000 ppm
F1	22134.81 Hz
F2P	-503.06 ppm
F2	-738006.00 Hz/cm
PPMCK	734.55370 Hz/cm

SMD-194-5

Current Data Parameters
 NAME: SMD-194-5
 EXPNO: 302
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20030426
 Time: 11.13
 INSTRUM: spect
 PROBRD: 5 mm Dual 13
 PULPROG: zgpg30
 TO: 32768
 SOLVENT: CDCl3
 NS: 16
 DS: 0
 SWH: 8223.665 Hz
 FIDRES: 0.250967 Hz
 AQ: 1.3923444 sec
 RG: 256
 DW: 60.800 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec
 ===== CHANNEL f1 =====
 NUC1: 1H
 P1: 10.80 usec
 PL1: -2.00 dB
 SF01: 400.1324710 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 400.130075 MHz
 KW: EM
 SSF: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00
 ID NMR plot parameters:
 CX: 30.00 cm
 F1P: 8.100 ppm
 F1: 3241.05 Hz
 F2P: -0.100 ppm
 F2: -40.01 Hz
 PPMCH: 0.27333 ppm/cm
 HZCH: 109.35888 Hz/cm

SMD-194-P

Current Data Parameters
NAME: smp-02
EXPNO: 332
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20020429
Time: 17.29
INSTRUM: spect
PROBHD: 5 mm Dui1 13
PULPROG: zgpg30
TO: 65536
SOLVENT: CDCl3
NS: 2048
DS: 2
SWH: 31847.133 Hz
FIDRES: 0.465949 Hz
AQ: 1.028552 sec
RG: 15.700 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: 10.50 usec
PL1: -1.00 dB
SFO1: 100.6254359 MHz

===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 105.00 usec
PL2: -2.00 dB
PL12: 18.00 dB
PL13: 20.00 dB
SFO2: 400.1324708 MHz

F2 - Processing parameters
SF: 32768
SE: 100.6127673 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

1D NMR plot parameters
CX: 30.00 cm
F1P: 220.000 ppm
F1: 223.4181 Hz
F2P: -5.000 ppm
F2: -503.06 Hz
PPMCH: 754.59570 Hz/cm
HZCH:

SMD-174-1

Current Data Parameters
NAME: mbr-02
EXPNO: 178
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20030327
Time: 3.47
INSTRUM: spect
PROBHD: 5 mm DUA13
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 16
DS: 0
SWH: 8223.685 Hz
FIDRES: 0.250967 Hz
AQ: 1.9923444 sec
RG: 181
DE: 60.800 usec
TE: 300.0 K
D1: 1.00000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 10.80 usec
PL1: -2.00 dB
SFO1: 400.1324710 MHz

F2 - Processing parameters
SI: 65594
SF: 400.130093 MHz
RG: 0
SSB: 0
SB: 0
PC: 1.00

1D NMR plot parameters
CX: 30.00 cm
F1P: 8.100 ppm
F1: 3241.05 Hz
F2P: -40.01 Hz
F2: 0.27333 ppm/cm
PPMCH: 109.36888 Hz/cm
HZCM

SMD-174-1

Current Data Parameters
 NAME mar-02
 EXPNO 179
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20020327
 Time 14.51
 INSTRUM spect
 PROBHD 5 mm QNP1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2524
 DS 2
 SWH 31847.133 Hz
 FIDRES 0.485949 Hz
 AQ 1.0289652 sec
 RG 1824.6
 DW 15.700 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 10.50 usec
 PL1 -1.00 dB
 SFO1 100.625359 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 105.00 usec
 PL2 -2.00 dB
 PL12 18.00 dB
 PL13 20.00 dB
 SFO2 400.1324708 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127652 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

ID NMR plot parameters
 CX 30.00 cm
 F1P 230.000 ppm
 F1 23140.94 Hz
 F2P -5.000 ppm
 F2 -501.06 Hz
 PPMCH 7.8333 ppm/cm
 HZCH 788.1330 Hz/cm

Y6-53-1

Current Data Parameters
NAME: mar-02
EXPNO: 105
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20080315
Time: 19.36
INSTRUM: spect
PROBHD: 5 mm Dual 13
PULPROG: zgpg30
TO: 65536
SOLVENT: CDCl3
NS: 3296
DS: 2
SWH: 31847.133 Hz
FIDRES: 0.485949 Hz
AQ: 1.028552 sec
RG: 2048
DM: 15.700 usec
DE: 6.00 usec
TE: 300.0 K
D1: 2.0000000 sec
D11: 0.0300000 sec
D12: 0.0000000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 10.50 usec
PL1: -1.00 dB
SFO1: 100.6254559 MHz

===== CHANNEL f2 =====
CPOBPG2: waltz16
NUC2: 1H
PCPD2: 105.00 usec
PL2: -2.00 dB
PL12: 18.00 dB
PL13: 20.00 dB
SFO2: 400.1324708 MHz

F2 - Processing Parameters
SI: 32768
SF: 100.6127067 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

10 MHz plot parameters
CY: 30.00 cm
F1P: 240.000 ppm
F1: 244.706 Hz
F2P: -5.000 ppm
F2: -503.07 Hz
PPHMC: 8.16567 ppm/cm
HZCM: 821.67096 Hz/cm

SMD-171-1

Current Data Parameters
NAME mar-02
EXPNO 147
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020223
Time 11:02
INSTRUM spect
PROBHD 5 mm Data 11
PULPROG zgpg30
TD 32768
SOLVENT DMS
DS 16
NS 0
SMH 8223.665 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 181
RG 50.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.130059 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 MHz plot parameters
CX 30.00 cm
FIP 6.100 ppm
F1 3241.05 Hz
F2 -40.01 Hz
PPMCH 0.27233 ppm/cm
HZCH 109.36888 Hz/cm

SMD-171-1

YG-53-1

Hz

1697.43
1693.53
1690.35
1686.44
1683.24
1679.33
1676.13
1672.22

1323.81
1315.91
1012.23
990.21
988.33
976.01
974.16
971.97
956.78
924.83
911.58
901.94
898.91
829.02
825.48
779.56
682.51
669.64
636.83
613.36
610.48
598.27
518.90
517.45
511.61
510.15
504.70
503.15

0.00

Current Data Parameters
NAME mar-02
EXPNO 82
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020314

Time 10.11
INSTRUM spect
PROBHD 5 mm Dui1 13
PULPROG zg30
10 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.665 Hz
FIDRES 0.23067 Hz
AQ 1.392344 sec
RG 655
RW 60.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

***** CHANNEL f1 *****
NUC1 ¹H
P1 10.80 usec
PL1 -2.00 dB
SF01 400.1324710 MHz

F2 - Processing Parameters
SI 16384
SF 400.130065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 NMR plot parameters
CX 30.00 cm
FID 8100 ppm
F1 3244.05 Hz
F2 -40.01 Hz
PPMCK 0.2733 ppm/cm
HZCM 109.36888 Hz/cm

YG-53-1

Current Data Parameters
 NAME mar-02
 EXPNO 104
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20020315
 Time 14.26
 INSTRUM spect
 PROBHD 5 mm Dual 13
 PULPROG zgpg30
 TD 65536
 TO 65536
 SOLVENT CDCl3
 NS 3365
 DS 2
 SMH 31847.133 Hz
 FIDRES 0.485949 Hz
 AQ 1.028952 sec
 RG 3649.1
 DW 15.700 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 10.50 usec
 PL1 1.00 dB
 SFO1 100.6254359 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 105.00 usec
 PL2 -2.00 dB
 SFO2 400.1324708 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.6127659 MHz
 MDW EN
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 10 MHz plot parameters
 DX 30.00 cm
 FFP 240.000 ppm
 F1 24147.06 Hz
 F2P 53.000 ppm
 F2 53100.18 Hz
 FPPCHK 8.16567 ppm/cm
 HZCHK 821.67095 Hz/cm

Y6-59-P

Current Data Parameters
NAME: mer-02
EXPNO: 173
PROCNO: 1

F2 - Acquisition Parameters

Date_: 20030327
Time: 11.03
INSTRUM: spect
PROBHD: 5 mm Dui1 13
PULPROG: zg30
TD: 32768
SOLVENT: CDCl3
NS: 16
DS: 0
SWH: 8223.665 Hz
FIDRES: 0.25067 Hz
AQ: 1.9923444 sec
RG: 574.7
RW: 60.800 usec
DE: 6.00 usec
TE: 300.0 K
D1: 1.00000000 sec

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

NUC1: 13C
P1: 10.80 usec
PL1: -2.00 dB
SFO1: 400.1324710 MHz

F2 - Processing parameters

SI: 16384
SF: 400.1300072 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

ID NMR plot parameters

CX: 30.00 cm
F1P: 8.100 ppm
F1: 3241.05 Hz
F2P: -40.10 ppm
F2: -40.01 Hz
PPMCM: 0.27353 ppm/cm
HZCM: 109.36888 Hz/cm

Y6-59-P

Current Data Parameters
 NAME mar-02
 EXPNO 174
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20020327
 Time 13.23
 INSTRUM spect
 PROBN 5 mm DAI 13
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 2697
 US 2
 SMH 31647.133 Hz
 FIDRES 0.465949 Hz
 AQ 1.028562 sec
 RG 32768
 IN 15.700 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 10.50 usec
 PL1 -1.00 dB
 SFO1 100.6254358 MHz
 ***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 105.00 usec
 PL2 -2.00 dB
 PL12 18.00 dB
 PL13 20.00 dB
 SFO2 400.1324708 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.6127570 MHz
 NM 63
 DS 0
 SSB 0
 GB 1.00 Hz
 PC 1.40
 1D NMR Plot Parameters
 CX 30.00 cm
 F1P 240.000 ppm
 F1 244.4706 Hz
 F2P -5.000 ppm
 F2 -503.07 Hz
 PPMCH 8.16567 ppm/cm
 HZCH 821.67096 Hz/cm

SMD-173-2

Hz

2907.71

Current Data Parameters
NAME mar-02
EXPNO 165
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020326
Time 14.21

INSTRUM spect
PROBHD 5 mm Duij 13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 10
SWH 8233.695 Hz
FIDRES 0.280667 Hz
AQ 1.9823444 sec
RG 382
DM 60.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 -2.00 dB
SFO1 400.1364710 MHz

F2 - Processing parameters
SI 16384
SF 400.130063 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
EX 30.00 cm
FID 8.100 ppm
F1 3241.05 Hz
F2 -40.01 Hz

PPMCH 0.27333 ppm/cm
HZCM 109.36688 Hz/cm

SMD-173-2

Y6-57

SMO-189-R1

Current Data Parameters
NAME apr-02
EXPNO 199
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020416
Time 18.15
INSTRUM spect
PROBHD 5 mm Dui1 13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.865 Hz
FIDRES 0.250567 Hz
AQ 1.592344 sec
RG 620.4
DM 60.800 usec
DE 300.0 usec
TE 300.0 K
D1 1.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.80 usec
PL1 -2.00 dB
SFO1 400.132710 MHz

F2 - Processing parameters
SI 16384
SF 400.130070 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -0.100 ppm
F2 -40.01 Hz
P1PCN 0.2353 ppm/cm
N1CN 109.3688 Hz/cm

SMD-189-P

SMD-188-3

Current Data Parameters
NAME apr-02
EXPNO 146
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020412
Time 11:11
INSTRUM spect
PROBHD 5 mm Dui1 13
PULPROG zgpg30
TO 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.669 Hz
FIDRES 0.22369 Hz
AQ 1.59244 sec
RG 655.1
DS 60.800 usec
DE 5.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300062 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 NMR plot parameters
CX 30.00 cm
FIP 6140.000 Hz
F1 324.06 Hz
F2 40.100 Hz
F3 -40.01 Hz
PRCK 0.27333 ppm/cm
HZCM 109.36888 Hz/cm

SMD-188-3

Current Data Parameters
NAME SMD-02
EXPNO 131
PROCNO 1
Date_ 20030412
Time 13.14
INSTRUM spect
PROBHD 5 mm QNP 13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 2
SMH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 1625.5
DW 15.700 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 10.50 usec
PL1 -1.00 dB
SFO1 100.6254589 MHz

===== CHANNEL f2 =====
CROSSP2 waltz16
NUC2 1H
PCPRG2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz

F2 - Processing parameters.
SI 32768
SF 100.6127689 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters.
CX 30.00 cm
F1P 240.000 ppm
F1 244.4700 Hz
F2P -400.46 ppm
F2 -400.46 Hz
NUC1 13C
NUC2 1H
MAG 8.1333 ppm/cm
HZCM 818.31720 Hz/cm

SMD-202-1

Current Data Parameters
NAME may-02
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020508
Time 15:07
INSTRUM spect
PROBHD 5 mm Du1 13
PULPROG zg30
TO 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.669 Hz
FIDRES 0.220567 Hz
AQ 1.352344 sec
RG 654
RW 60.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 ¹H
P1 10.80 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300699 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
FIP 8.100 ppm
F1 324.15 Hz
F2 100.00 cm
CZ -40.01 Hz
PCPD 0.27333 ppm/cm
HZCM 109.36888 Hz/cm

SMD-202-1

Current Data Parameters
 NAME may-02
 EXPNO 89
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020511
 Time 11.07
 INSTRUM spect
 PROBHD 5 mm Dui1 13
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 2020
 DS 2
 SMH 31947.133 Hz
 FIDRES 0.465949 Hz
 AQ 1.028952 sec
 RG 3849.1
 DM 15120.0 usec
 DE 15.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00020000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 -1.00 dB
 SF01 100.6254558 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 105.00 usec
 PL2 -2.00 dB
 PL12 18.00 dB
 PL13 20.00 dB
 SF02 400.1324709 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6126520 MHz
 SM FM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 30.00 cm
 F1P 220.000 ppm
 F1 2234.81 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPM1H 7.50000 ppm/cm
 HZCM 754.59570 Hz/cm

SMD-200-P

Hz

2907.53

1688.67
1686.58
1681.54
1679.61
1674.44
1672.60
1667.38
1661.52

1009.43
959.39
957.43
953.68
937.16
935.53
933.74
909.60
905.16
896.31
891.25
882.82
831.43
771.41
758.53
667.75
654.46
636.55
599.41
596.14
587.06
583.69
563.18
509.84
502.73
495.60

0.00

373.48

95.60
198.54
199.22
101.92
100.00
86.54
41.03
103.11
293.09
580.52

Current Data Parameters
NAME may-02
EXPNO 51
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020508
Time 15.12
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zgpg30
TO 32768
SOLVENT CDCl3
NS 16
DS 4
SWH 8233.695 Hz
FIDRES 0.240967 Hz
AQ 1.9823444 sec
RG 456.1
DM 60.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.80 usec
PL1 -2.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.130065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 NMR plot parameters
CX 30.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -40.01 Hz
F2 0.27233 ppm/cm
PNUCH 109.36888 Hz/cm

SMD-200-P

Current Data Parameters
NAME may-02
EXPNO 52
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020908
Time 15:35
INSTRUM spect
PROBHD 5 mm DASH-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 883
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0286652 sec
RG 1625.5
DM 15.700 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 10.50 usec
PL1 -1.00 dB
SFO1 100.6254558 MHz

===== CHANNEL f2 =====
CROSSP2 wait16
NUC2 13C
P2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz

F2 - Processing parameters
SI 32768
SF 100.6127659 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

10 NMR plot parameters
CX 30.00 cm
F1P 230.000 ppm
F1 23140.94 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCK 7.63333 ppm/cm
HZCK 788.1335 Hz/cm