A New Entry to Polycyclic Indole Skeleton via Palladium-Catalyzed Intramolecular Heteroannulation

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Supporting Information

General Methods. All reactions were carried out under an atmosphere of argon in dry glassware with magnetic stirring. Commercially available anhydrous tetrahydrofuran, N-methylpyrrolidinone and N, N-dimethylformamide are received from Aldrich and used without any further purification. Column chromatography was performed on EM Science silica gel 60 (230-400 mesh). Thin layer chromatography was performed on EM Science 0.25 mm silica gel 60-F plates. Visualization was accomplished with UV light, KMnO₄, aqueous ceric ammonium molybdate, or bromocresol green dips followed by heating.

Melting points were measured with a MelTemp II melting point apparatus outfitted with a Fluke 51 thermocouple and are uncorrected. Infrared spectra were obtained on a NEXUS 670 FT-IR spectrometer. ¹H NMR and spectra were recorded on a Bruker 400 MHz spectrometer at ambient temperature. Data are reported as follows: chemical shift in parts per million (δ , ppm) from an internal standard [tetramethylsilane (TMS) or deuterated chloroform (CDCl₃)], multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, and m = multiplet), integration, and coupling constant (Hz). ¹³C NMR and spectra were recorded on a Bruker 400 MHz spectrometer at ambient temperature. Chemical shifts are reported in ppm from CDCl₃ taken as 77.0 ppm. Mass spectra were obtained on Fisons VG Autospec.

JL 6452-106

8.397
8.377
8.362
7.358
7.342
7.338
7.301
7.281
7.263
7.261
7.254
7.243
7.240
7.095
7.075
7.048
7.045
7.029
7.026
7.010
7.006

9

2.654
2.636
2.617
2.569
2.552
2.535
2.330
2.076
2.059
2.041
2.023
2.006
1.619

Current Data Parameters
NAME JL 6452-106
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040702
Time 16.51
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 90.5
DW 60.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 7.15 usec
PL1 3.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300119 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
 NAME JL 6452-106
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040703
 Time 2.25
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 10000
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 4096
 DW 20.850 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 15.00 usec
 PL1 -5.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 3.50 dB
 PL12 21.00 dB
 PL13 21.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127722 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME J1 6452-032
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20040630
 Time 18.18
 INSTRUM spect
 PROBD 5 mm BBI 1H-BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 90.5
 DW 60.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.15 usec
 PL1 3.50 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300088 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters
 NAME JL 6452-032
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040701
 Time 3.52
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 10000
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 10321.3
 DW 20.850 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 15.00 usec
 PL1 -5.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 3.50 dB
 PL12 21.00 dB
 PL13 21.00 dB
 SFO2 400.1316005 MHz

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

Current Data Parameters
 NAME JL 6452-134
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20040703
 Time 2.32
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 256
 DW 60.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 7.15 usec
 PL1 3.50 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300099 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

13

JL 6452-134

Current Data Parameters
NAME JL 6452-134
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040703
Time 12.07
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10000
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 4096
DW 20.850 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 15.00 usec
PL1 -5.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.50 dB
PL12 21.00 dB
PL13 21.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127700 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

13

180 160 140 120 100 80 60 40 20 ppm

JL 7317-024

Current Data Parameters
NAME JL 7317-024
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050512
Time_ 18.35
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 101.6
DW 60.400 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 7.15 usec
PL1 3.50 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

2.347
2.093
2.075
2.058
2.048
2.040
2.022
1.982
1.963
1.945
1.928
1.910
1.641
1.114
1.095
1.077
0.000

8.194
8.191
7.714
7.353
7.332
7.295
7.292
7.275
7.271
7.259
7.240
7.236
7.218
7.200
7.197
7.123
7.104
6.952
6.949
6.933
6.930
6.914
6.910
4.880

17

Current Data Parameters
 NAME JL 7317-024
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050513
 Time_ 4.09
 INSTRUM spect
 PROBD 5 mm BBI 1H-BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 10000
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQC 1.3664756 sec
 RG 2580.3
 DW 20.850 usec
 DE 6.50 usec
 TE 673.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 15.00 usec
 PL1 -5.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 3.50 dB
 PL12 21.00 dB
 PL13 21.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127715 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME JL Larock SM2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050510
 Time 17.52
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 80.6
 DW 60.400 usec
 DE 6.50 usec
 TE 673.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.15 usec
 PL1 3.50 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300066 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

19

Current Data Parameters
 NAME JL Larock SM2
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050511
 Time_ 3.27
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 10000
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 2580.3
 DW 20.850 usec
 DE 6.50 usec
 TE 673.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 15.00 usec
 PL1 -5.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 3.50 dB
 PL12 21.00 dB
 PL13 21.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127722 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

159.89
 154.05
 142.24
 139.37
 133.36
 128.47
 123.11
 114.15
 113.96
 87.79
 86.28
 77.32
 77.00
 76.68
 56.89
 55.28
 32.39
 8.81
 -0.04

19

180 160 140 120 100 80 60 40 20 ppm

Current Data Parameters
 NAME JL 7203-106
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date 20050315
 Time 19.09
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 114
 DW 60.400 usec
 DE 6.50 usec
 TE 673.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.15 usec
 PL1 3.40 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1299995 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

2.510
 2.506
 2.502
 2.104
 1.627
 1.614

3.355

8.185
 8.167
 8.164
 8.067
 7.410
 7.407
 7.394
 7.389
 7.386
 7.382
 7.373
 7.369
 7.362
 7.356
 7.353
 7.346
 7.314
 7.232
 6.963
 6.947
 6.944

21

JL 7203-106

Current Data Parameters
NAME JL 7203-106
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050315
Time_ 23.58
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 5000
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 3649.1
DW 20.850 usec
DE 6.50 usec
TE 673.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 15.00 usec
PL1 -5.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.40 dB
PL12 21.00 dB
PL13 21.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128209 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

212.62
153.16
136.58
131.25
129.01
128.53
128.13
127.37
122.77
122.33
120.91
120.53
116.27
92.97
82.18
66.97
50.84
40.12
39.91
39.70
39.50
39.29
39.08
38.87
36.93
25.08
24.86
22.10

21

JL 6452-120

Current Data Parameters
 NAME JL 6452-120
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040129
 Time 12.03
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 10000
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 2580.3
 DW 20.850 usec
 DE 6.00 usec
 TE 292.5 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 15.00 usec
 PL1 -5.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 20.98 dB
 PL13 120.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127781 MHz
 EM

WDW 0
 SSB 1.00 Hz
 LB 0
 GB 1.40
 PC

22.82
 21.30
 21.22

34.57

77.27
 77.16
 76.95
 76.64

136.81
 134.67
 133.74
 130.11
 129.49
 129.33
 129.12
 124.44
 124.00
 118.74
 118.37
 116.45

10

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

Current Data Parameters
NAME JL 6452-120
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040128
Time_ 14.19
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
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 291.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 7.15 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

0.000

1.581
2.046
2.061
2.077
2.093
2.109
2.432
2.822
2.839
2.854
3.037
3.053
3.068

7.254
7.262
7.264
7.280
7.283
7.293
7.298
7.302
7.313
7.320
7.320
7.337
7.340
7.340
7.355
7.358
7.378
7.383
7.398
7.569
7.571
7.589
8.529
8.549

10

JL 6452-120

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

2.18
3.22
2.17
2.17

6.64
1.09
0.99

Current Data Parameters	
NAME	JL 6452-117
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

```

Date_      20040206
Time       15.42
INSTRUM    spect
PROBHD     5 mm BBI 1H-BB
PULPROG    zg30
TD         65536
SOLVENT    CDCl3
NS         16
DS         2
SWH        8278.146 Hz
FIDRES     0.126314 Hz
AQ         3.9584243 sec
RG         128
DE         60.400 usec
TE         292.3 K
DD1
MCREST     1.00000000 sec
MCCWRK     0.00000000 sec
           0.01500000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         7.15 usec
PL1        0.00 dB
SF01       400.1324710 MHz

F2 - Processing parameters
SI         32768
SF         400.1300092 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
OC         1.00

```

Current Data Parameters
 NAME JL 6452-117
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040210
 Time_ 9.20
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 15030
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 4597.6
 DW 20.850 usec
 DE 6.00 usec
 TE 292.5 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 15.00 usec
 PL1 -5.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 20.98 dB
 PL13 120.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz

WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

21.41
17.16
14.44

77.36
77.05
76.73
67.00

135.22
129.79
128.10
124.40
123.55
118.59
118.39
115.45

148.26

12

200 180 160 140 120 100 80 60 40 20 ppm

Current Data Parameters
 NAME JL 6452-152
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040309
 Time_ 2.09
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 10000
 DS 2
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 5792.6
 DW 20.850 usec
 DE 6.00 usec
 TE 293.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 15.00 usec
 PL1 -5.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 20.98 dB
 PL13 120.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127732 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

14

Current Data Parameters
 NAME JL 6452-152
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040308
 Time 16.30
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 40.3
 DW 60.400 usec
 DE 6.00 usec
 TE 293.9 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.15 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300176 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters
 NAME JL 6450-098
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050428
 Time 17.22
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 57
 DW 60.400 usec
 DE 6.50 usec
 TE 673.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.15 usec
 PL1 3.50 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300149 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

2.426
 1.884
 1.865
 1.847
 1.829
 0.842
 0.823
 0.805
 0.001

8.037
 8.017
 7.540
 7.520
 7.345
 7.342
 7.337
 7.324
 7.322
 7.317
 7.307
 7.304
 7.272
 7.262
 7.259
 7.252
 7.244
 7.242
 7.224
 6.284

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Current Data Parameters
 NAME JL 6450-098
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050429
 Time 6.04
 INSTRUM spect
 PROBD 5 mm BBI 1H-BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 10000
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 2580.3
 DW 20.850 usec
 DE 6.50 usec
 TE 673.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 15.00 usec
 PL1 -5.00 dB
 SFO1 100.6228298 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 3.50 dB
 PL12 21.00 dB
 PL13 21.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127744 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

153.47
 138.19
 136.95
 133.42
 130.12
 129.93
 129.34
 129.12
 123.27
 122.55
 119.75
 113.63
 112.56
 77.32
 77.00
 76.68
 64.70
 32.54
 21.25
 8.07

18

ppm

Current Data Parameters
 NAME JL Larock 2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050506
 Time 18.53
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 181
 DW 60.400 usec
 DE 6.50 usec
 TE 673.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 7.15 usec
 PL1 3.50 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300063 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1.986
1.968
1.950
1.932
1.922
1.913
1.903
1.885
1.867
1.849
0.848
0.830
0.812
0.002

3.861

8.576
8.572
8.270
8.267
8.250
8.246
7.512
7.505
7.500
7.489
7.483
7.266
7.253
7.244
7.232
7.035
7.028
7.023
7.011
7.006
5.693

20

Current Data Parameters
 NAME JL Larock 2
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050507
 Time 8.16
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 14000
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 2896.3
 DW 20.850 usec
 DE 6.50 usec
 TE 673.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 15.00 usec
 PL1 -5.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 3.50 dB
 PL12 21.00 dB
 PL13 21.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127707 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME JL 7203-109
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050314
 Time 16.58

INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 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 6.50 usec
 TE 673.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.15 usec
 PL1 3.50 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300101 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

7.466
7.460
7.458
7.455
7.452
7.425
7.418
7.410
7.403
7.398
7.394
7.359
7.356
7.340
7.338
7.320
7.317
7.257
7.238
7.236
7.221
7.218
6.670
2.048
1.892
1.883
1.866
1.858
1.815
1.807
1.782
1.760
1.508
1.499
1.491
1.482
1.476
1.466
1.457
1.449
1.440
1.301
1.278

Current Data Parameters
 NAME JL 7203-109-S
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050319
 Time_ 14.10
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 20000
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 2580.3
 DW 20.850 usec
 DE 6.50 usec
 TE 295.3 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 15.00 usec
 PL1 -5.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 3.50 dB
 PL12 21.00 dB
 PL13 21.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127707 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

36.97
31.57
29.68
24.59
22.67
22.63
14.18
14.09

60.36
59.74

77.31
77.00
76.68

152.46
141.61
133.66
132.97
130.03
129.81
128.51
127.33
123.55
122.70
119.78
113.23
112.59