Supporting information belonging to the paper

Dendrimers Functionalized with Palladium Complexes of N-, N,N-, and N,N,N-Ligands

Quentin Vanbellingen, Paul Servin, Anaïs Coinaud, Sonia Mallet-Ladeira, Régis Laurent, Anne-Marie Caminade*

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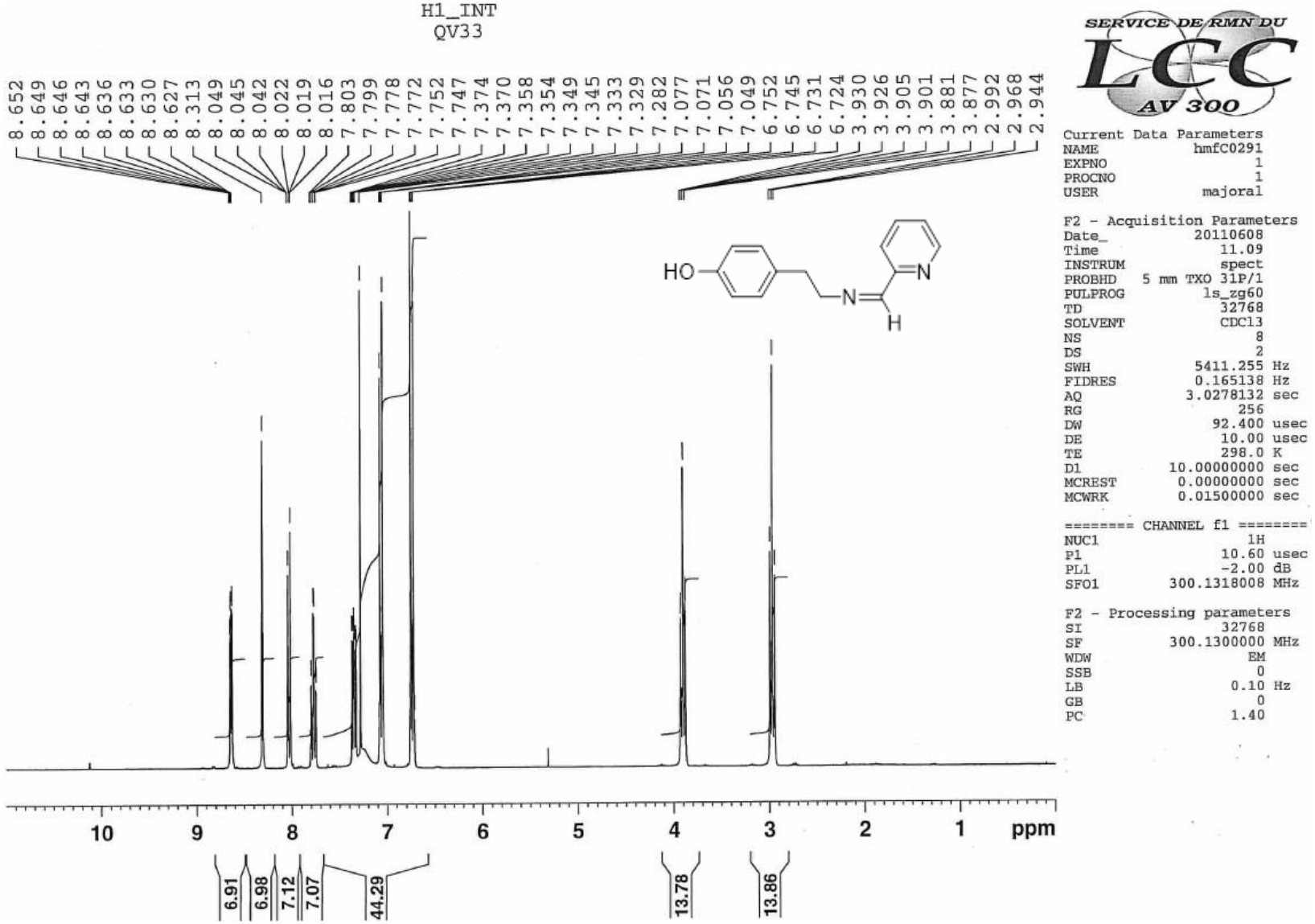
^{1}H NMR of Compound 2

1



SERVICE DE RMN DU LCC AV 300

Current Data Parameters
NAME hmfC0291
EXPNO 1
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20110608
Time 11.09
INSTRUM spect
PROBHD 5 mm TXO 31P/1
PULPROG ls_zg60
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5411.255 Hz
FIDRES 0.165138 Hz
AQ 3.0278132 sec
RG 256
DW 92.400 usec
DE 10.00 usec
TE 298.0 K
D1 10.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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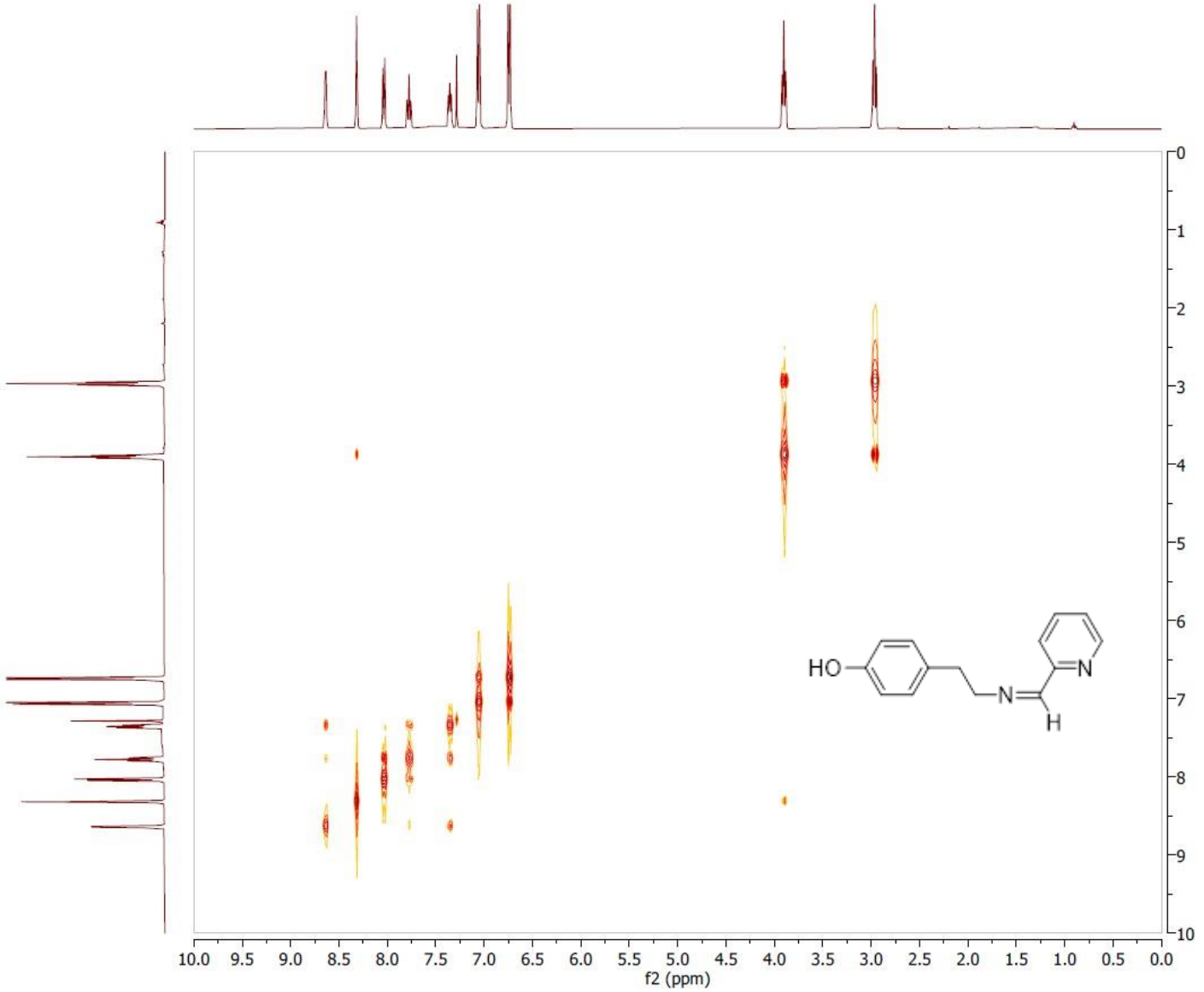
NUC1 1H
P1 10.60 usec
PL1 -2.00 dB
SFO1 300.1318008 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.40

^{1}H COSY NMR of Compound 2

1



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NAME ltrD0113
EXPNO 8
PROCNO 1
USER majoral

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Date_ 20110515
Time 6.01
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PULPROG ls_cosygpqf
TD 4096
SOLVENT CDCl3
NS 2
DS 8
SWH 5208.333 Hz
FIDRES 1.271566 Hz
AQ 0.3932660 sec
RG 114
DW 96.000 usec
DE 10.00 usec
TE 298.0 K
d0 0.00000300 sec
D1 2.00000000 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00019225 sec
MCREST 0.00000000 sec
MCWRK 2.00000000 sec

======== CHANNEL f1 ===
NUC1 1H
P0 9.70 usec
P1 9.70 usec
PL1 -1.00 dB
SFO1 400.1322007 MHz

====== GRADIENT CHANNEL
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 10.00 %
GPZ2 10.00 %
P16 1000.00 usec

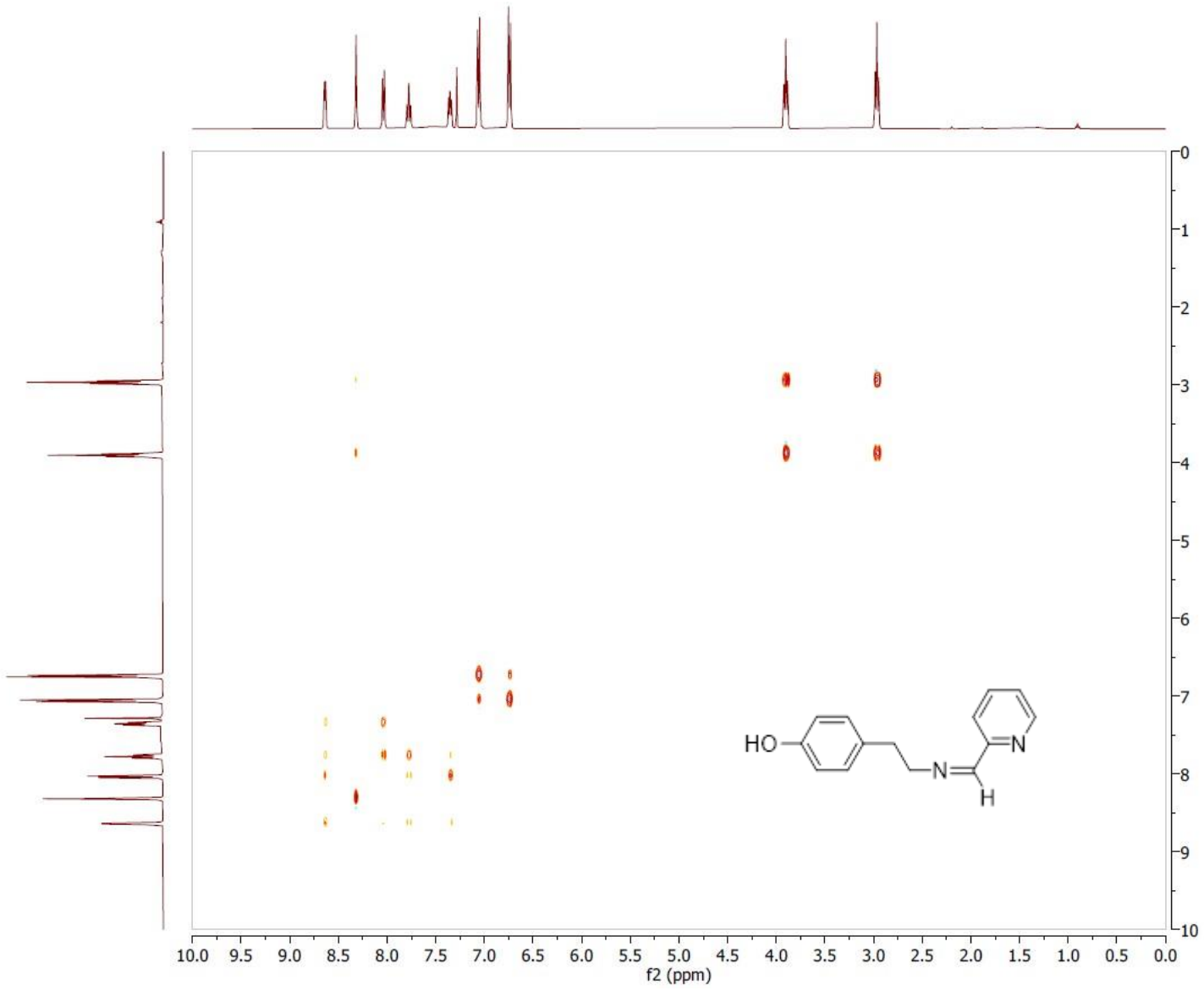
F1 - Acquisition parameters
ND0 1
TD 256
SFO1 400.1322 MHz
FIDRES 20.318596 Hz
SW 13.000 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 QF
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

^{1}H TOCSY NMR of Compound 2

1



Current Data Parameters
NAME ltrD0113
EXPNO 10
PROCNO 1
USER majoral

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Time 7.19
INSTRUM spect
PROBHD 5 mm BBO BB/2H
PULPROG ls_mlevph
TD 4096
SOLVENT CDCl3
NS 8
DS 16
SWH 5208.333 Hz
FIDRES 1.271566 Hz
AQ 0.3932660 sec
RG 256
DW 96.000 usec
DE 10.00 usec
TE 298.0 K
d0 0.00008595 sec
D1 0.20000000 sec
D9 0.06000000 sec
d12 0.00002000 sec
FACTOR1 4
IN0 0.00019225 sec
I1 24
MCREST 0.00000000 sec
MCWRK 0.10000000 sec
SCALEF 6
ST1CNT 128

======== CHANNEL f1 ==
NUC1 1H
P1 9.70 usec
p5 23.34 usec
P6 35.00 usec
p7 70.00 usec
P17 2500.00 usec
PL1 -1.00 dB
PL10 10.15 dB
SFO1 400.1322007 MHz

F1 - Acquisition parameters
ND0 1
TD 256
SFO1 400.1322 MHz
FIDRES 20.318596 Hz
SW 13.000 ppm
FnMODE States-TPPI

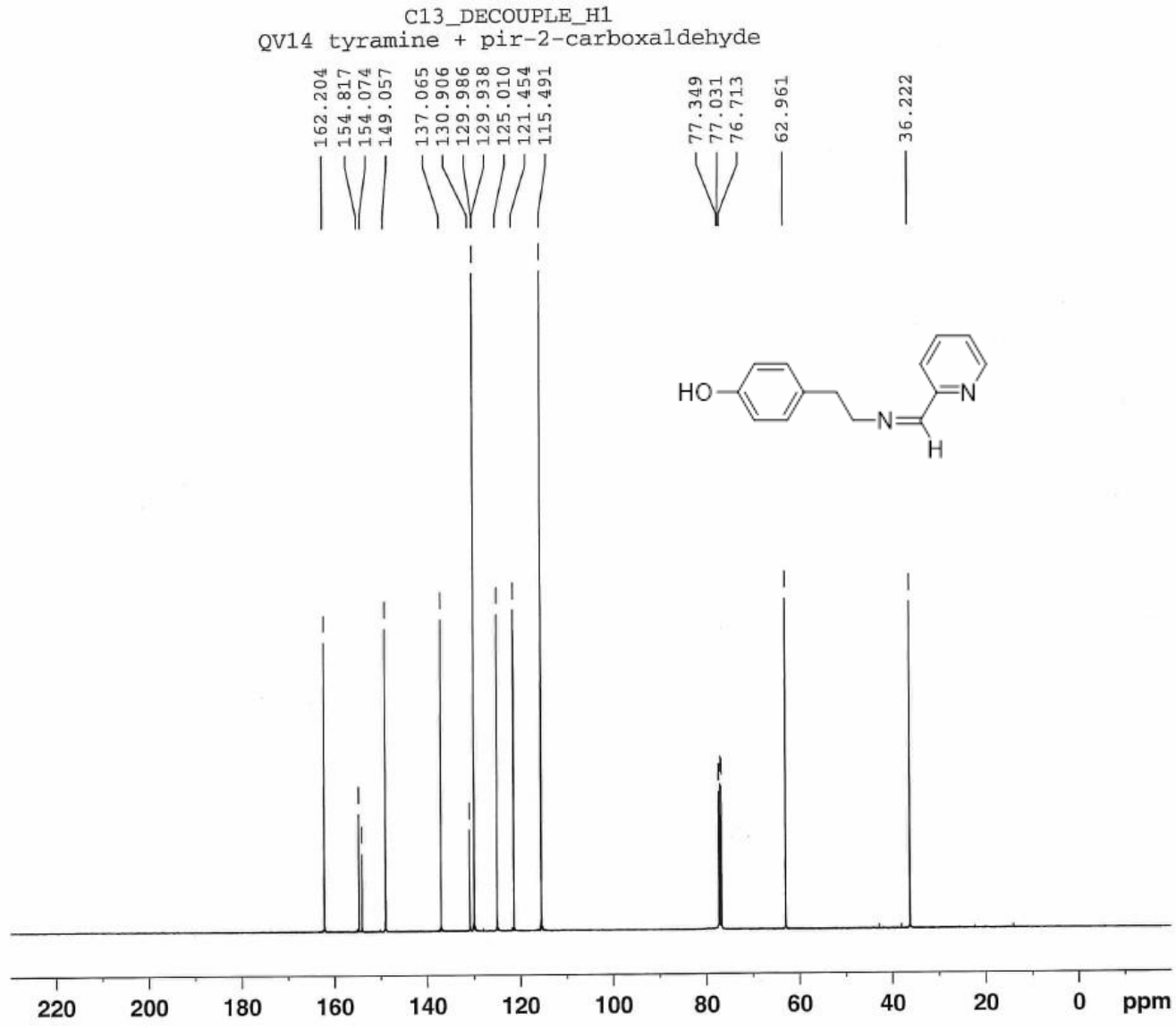
F2 - Processing parameters
SI 4096
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 States-TPPI
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

^{13}C

{^{1}H} NMR of Compound 2

^{13}C



SERVICE DE RMN DU LCC AV 400 Liq

Current Data Parameters
NAME 1trD0113
EXPNO 3
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20110515
Time 2.24
INSTRUM spect
PROBHD 5 mm BBO BB/2H
PULPROG ls_zg60dc
TD 32768
SOLVENT CDCl3
NS 26000
DS 4
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 36780.8
DW 19.900 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 7.30 usec
PL1 0.00 dB
SFO1 100.6233333 MHz

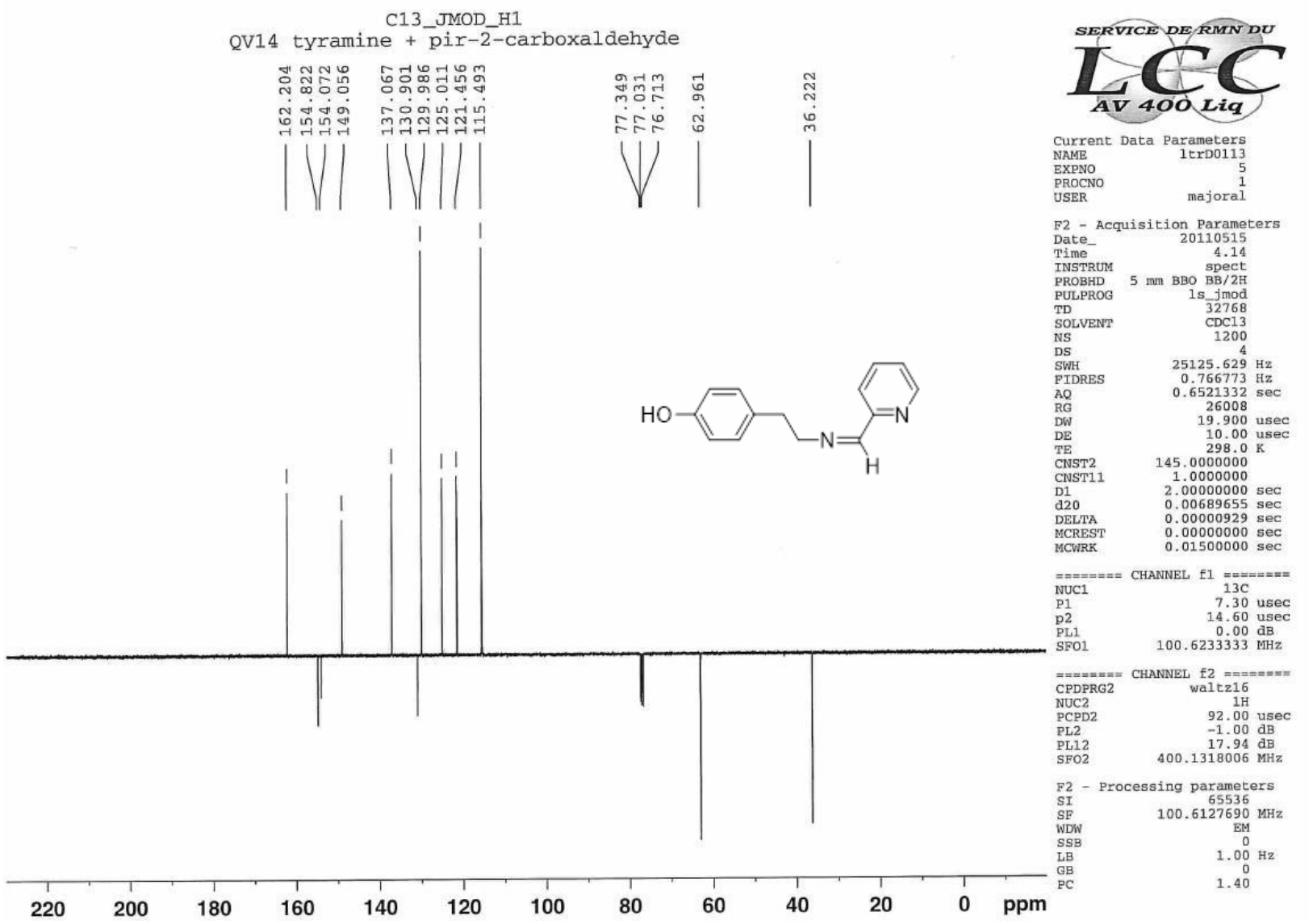
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 -1.00 dB
PL12 17.94 dB
SFO2 400.1318006 MHz

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.30

^{13}C

JMOD NMR of Compound 2

^{13}C



SERVICE DE RMN DU LCC AV 400 Liq

Current Data Parameters
NAME 1trD0113
EXPNO 5
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20110515
Time 4.14
INSTRUM spect
PROBHD 5 mm BBO BB/2H
PULPROG ls_jmod
TD 32768
SOLVENT CDCl3
NS 1200
DS 4
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 26008
DW 19.900 usec
DE 10.00 usec
TE 298.0 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
d20 0.00689655 sec
DELTA 0.00000929 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 7.30 usec
p2 14.60 usec
PL1 0.00 dB
SFO1 100.6233333 MHz

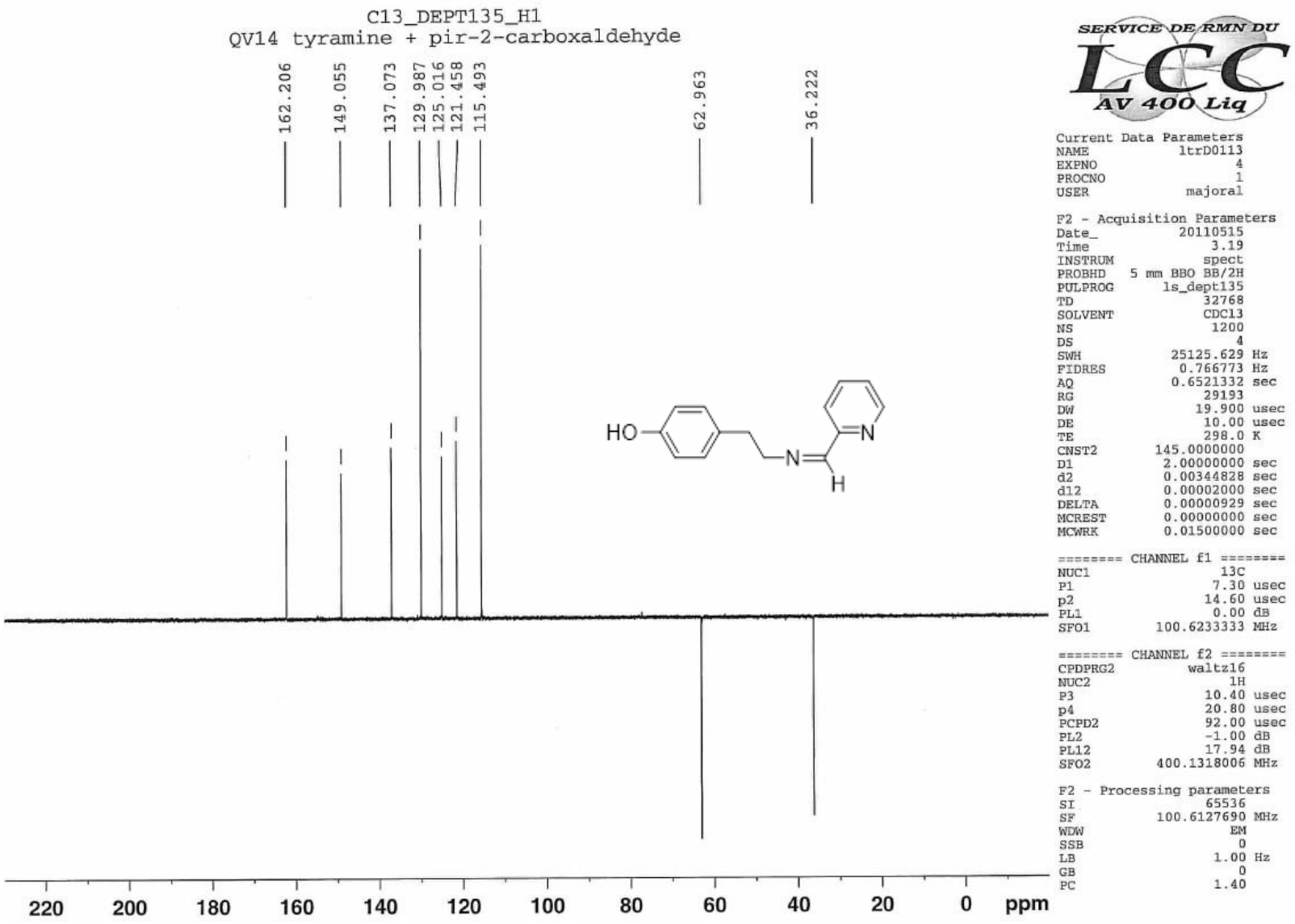
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 -1.00 dB
PL12 17.94 dB
SFO2 400.1318006 MHz

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{13}C

DEPT NMR of Compound 2

^{13}C



SERVICE DE RMN DU LCC AV 400 Liq

Current Data Parameters
NAME 1trD0113
EXPNO 4
PROCNO 1
USER majoral

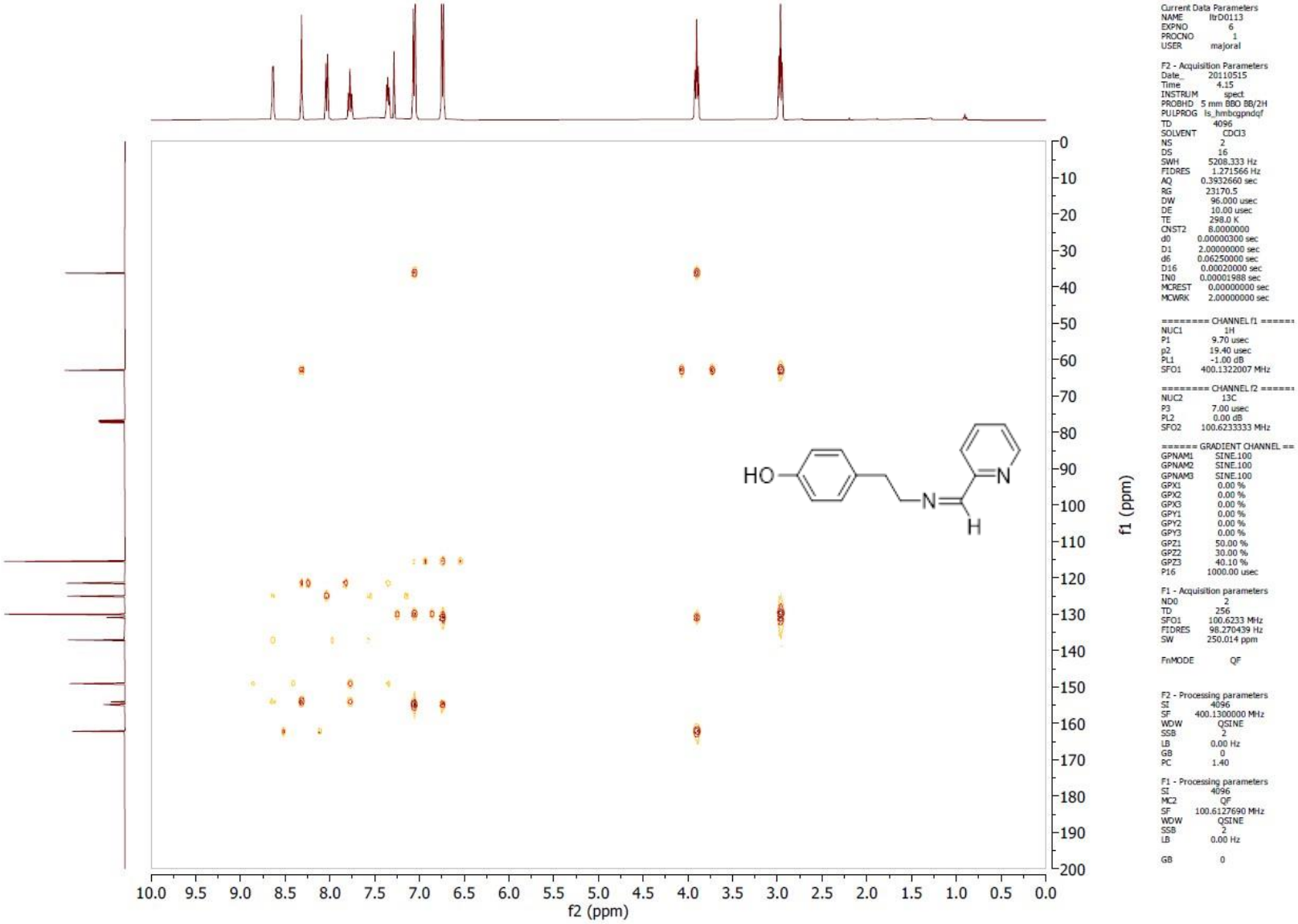
F2 - Acquisition Parameters
Date_ 20110515
Time 3.19
INSTRUM spect
PROBHD 5 mm BBO BB/2H
PULPROG 1s_dept135
TD 32768
SOLVENT CDCl3
NS 1200
DS 4
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 29193
DW 19.900 usec
DE 10.00 usec
TE 298.0 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00000929 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 7.30 usec
p2 14.60 usec
PL1 0.00 dB
SFO1 100.6233333 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 10.40 usec
p4 20.80 usec
PCPD2 92.00 usec
PL2 -1.00 dB
PL12 17.94 dB
SFO2 400.1318006 MHz

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{13}C HMBC NMR of Compound 2



Current Data Parameters
NAME ltrD0113
EXPNO 6
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20110515
Time 4.15
INSTRUM spect
PROBHD 5 mm BBO BB/2H
PULPROG ls_hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 2
DS 16
SWH 5208.333 Hz
FIDRES 1.271566 Hz
AQ 0.3932660 sec
RG 23170.5
DW 96.000 usec
DE 10.00 usec
TE 298.0 K
CNST2 8.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001988 sec
MCREST 0.00000000 sec
MCWRK 2.00000000 sec

======== CHANNEL f1 ======
NUC1 1H
P1 9.70 usec
p2 19.40 usec
PL1 -1.00 dB
SFO1 400.1322007 MHz

======== CHANNEL f2 ======
NUC2 13C
P3 7.00 usec
PL2 0.00 dB
SFO2 100.6233333 MHz

====== GRADIENT CHANNEL ==
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 100.6233 MHz
FIDRES 98.270439 Hz
SW 250.014 ppm

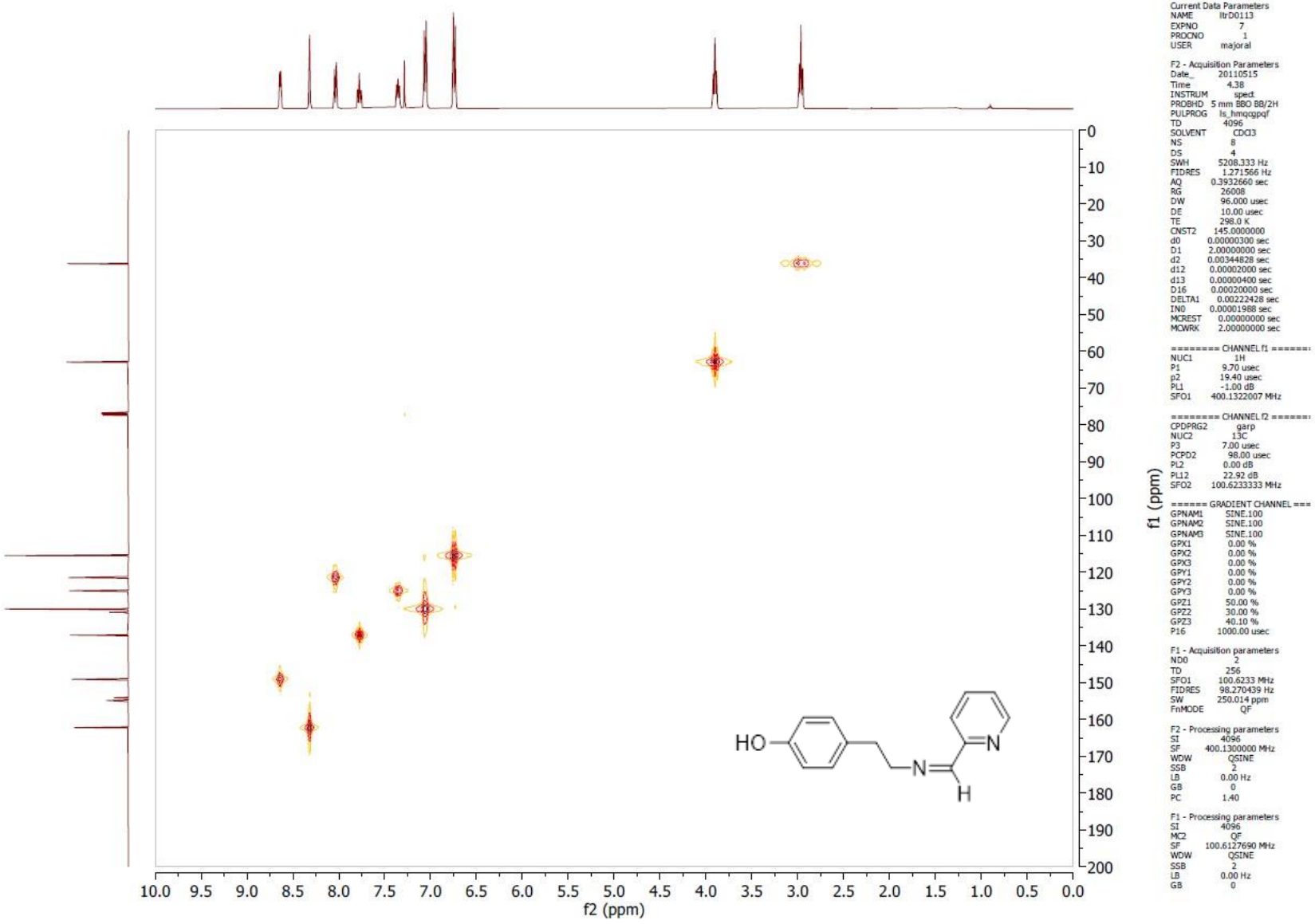
FnMODE QF

F2 - Processing parameters
SI 4096
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

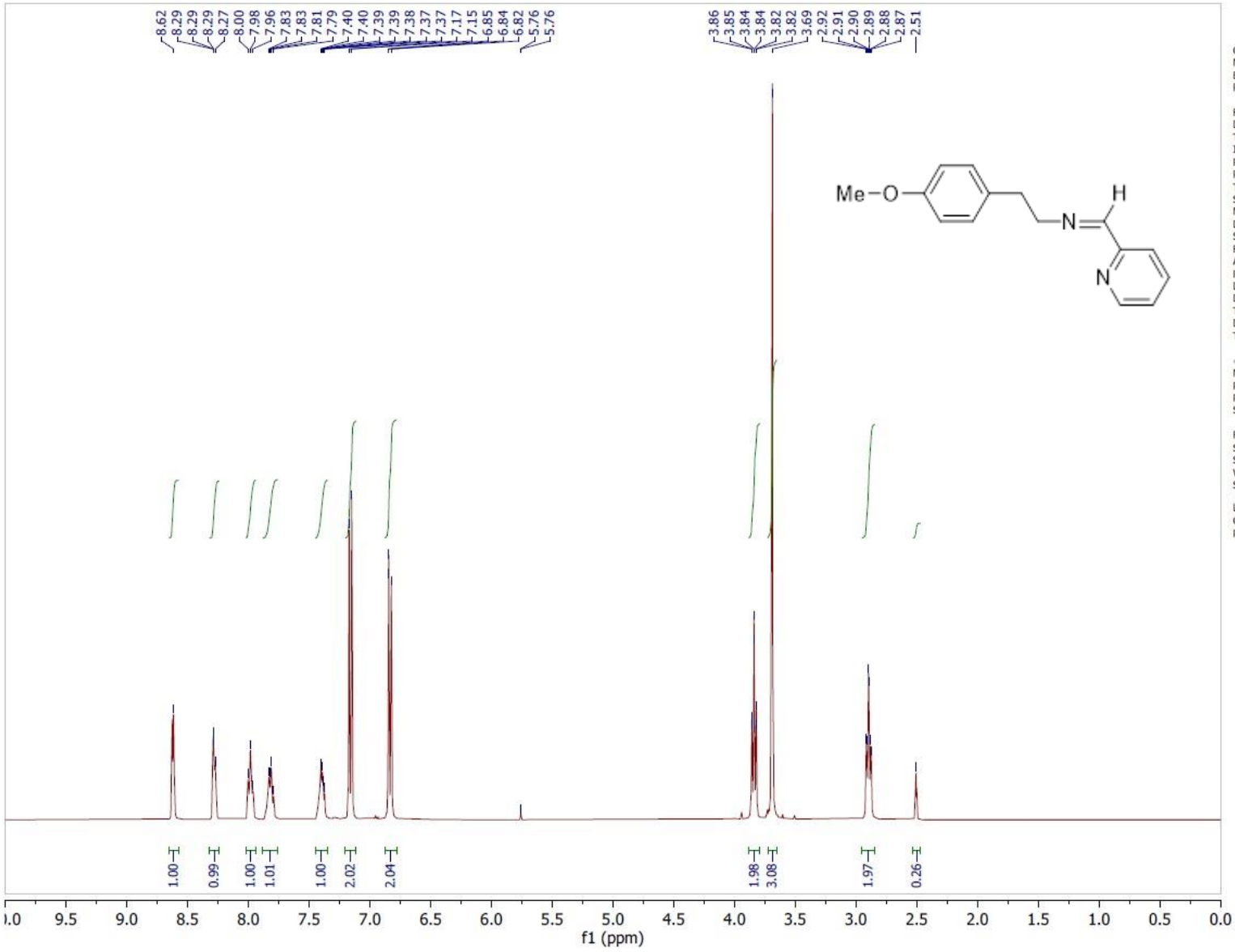
F1 - Processing parameters
SI 4096
MC2 QF
SF 100.6127690 MHz
WDW QSINE
SSB 2
LB 0.00 Hz

GB 0

C HMQC NMR of Compound 2



^{1}H NMR of Compound 2a



Current Data Parameters
NAME hmfG0252
EXPNO 1
PROCNO 1

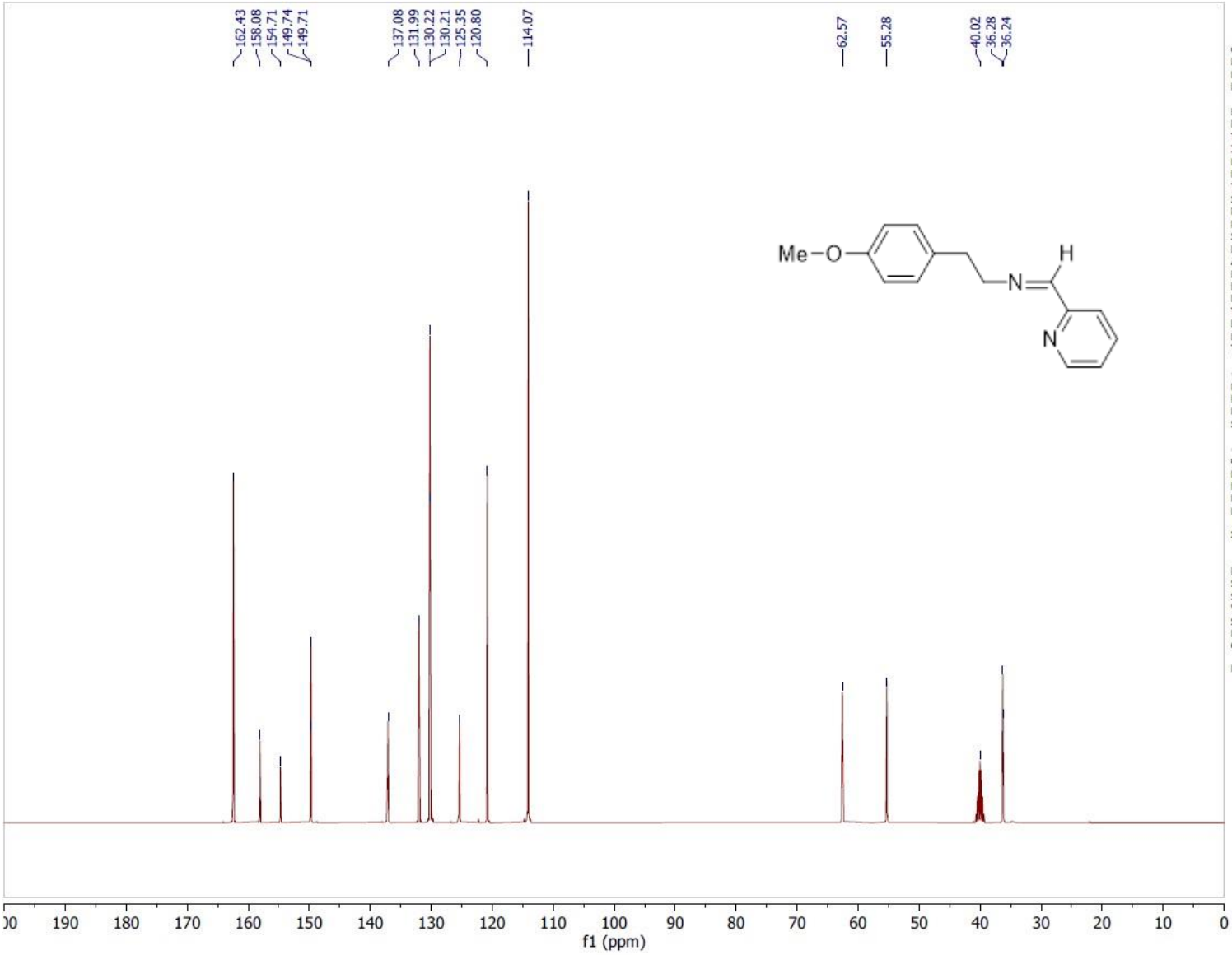
F2 - Acquisition Parameters
Date_ 20200722
Time 21.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG ls_zg60
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 7211.539 Hz
FIDRES 0.110039 Hz
AQ 4.5438795 sec
RG 10
DW 69.333 usec
DE 6.50 usec
TE 298.0 K
D1 20.00000000 sec
TD0 1

======== CHANNEL f1 ==
NUC1 1H
P1 14.00 usec
PLW1 17.00000000 W
SFO1 400.1628011 MHz

F2 - Processing parameters
SI 131072
SF 400.1600000 MHz
WDW EM
SSB 0

LB 0.10 Hz
GB 0
PC 1.50

C {^{1}H} NMR of Compound 2a



Current Data Parameters
NAME hmfG0252
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200723
Time 0.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG ls_zgdc60
TD 65536
SOLVENT DMSO
NS 3000
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 2050
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ==
NUC1 13C
P1 9.30 usec
PLW1 70.00000000 W
SFO1 100.6308781 MHz

======== CHANNEL f2 ==
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 17.00000000 W
PLW12 0.41136000 W

SFO2 400.1616006 MHz

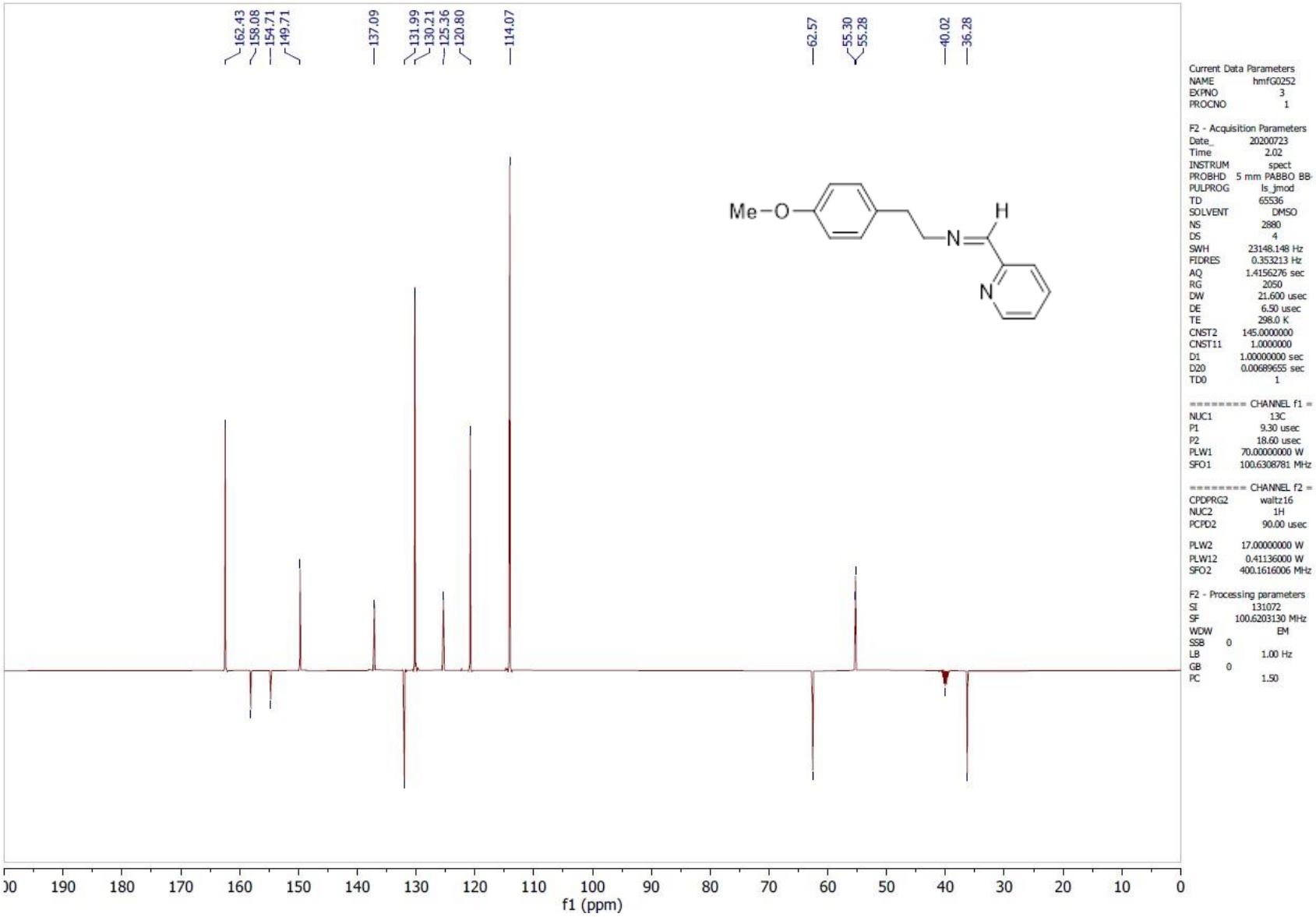
F2 - Processing parameters
SI 131072
SF 100.6203130 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0

PC 1.50

13

C JMOD NMR of Compound 2a

13



Current Data Parameters
NAME hmfG0252
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200723
Time 2.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG ls_jmod
TD 65536
SOLVENT DMSO
NS 2880
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 2050
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
CNST11 1.0000000
D1 1.00000000 sec
D20 0.00689655 sec
TD0 1

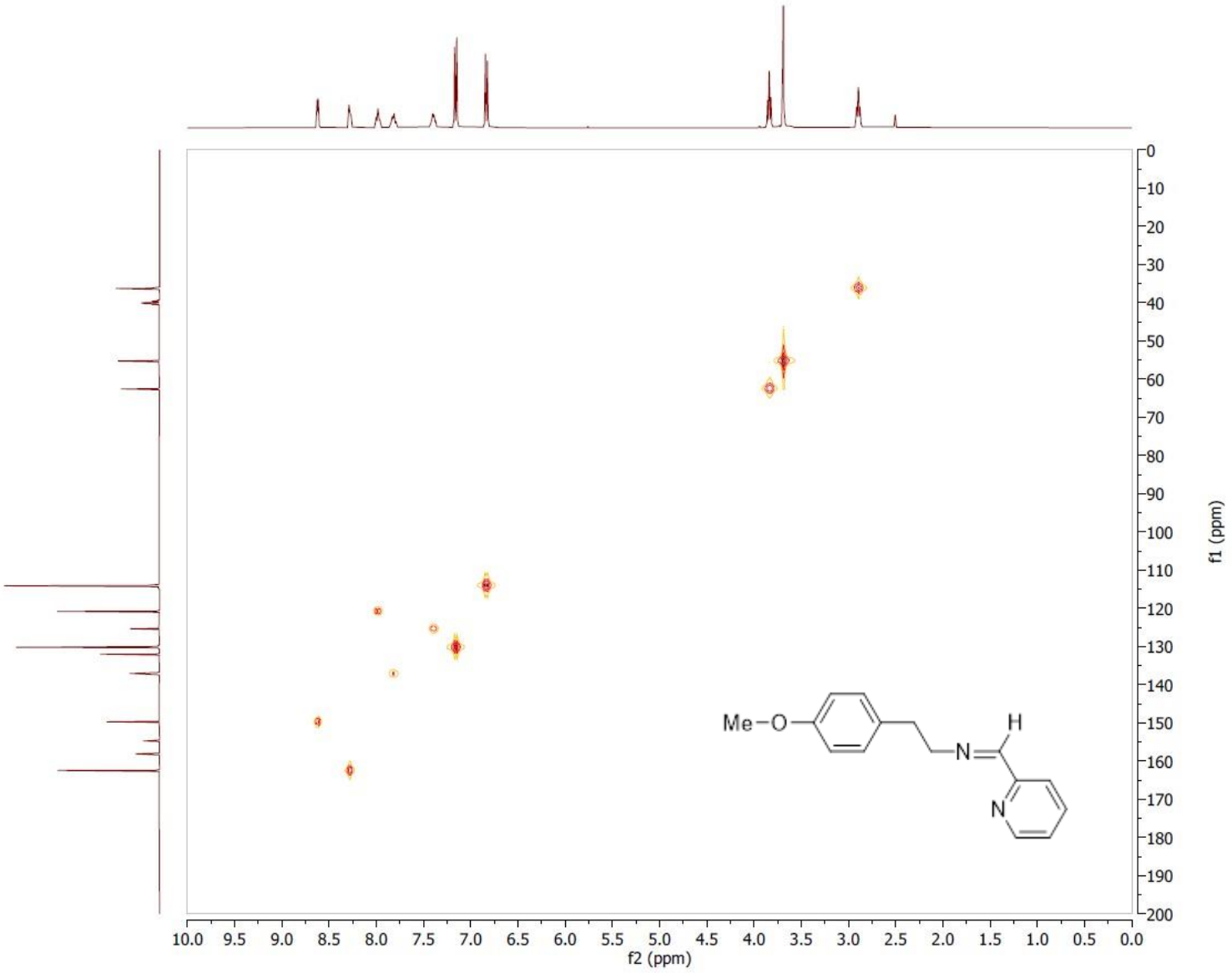
======== CHANNEL f1 =
NUC1 13C
P1 9.30 usec
P2 18.60 usec
PLW1 70.00000000 W
SFO1 100.6308781 MHz

======== CHANNEL f2 =
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec

PLW2 17.00000000 W
PLW12 0.41136000 W
SFO2 400.1616006 MHz

F2 - Processing parameters
SI 131072
SF 100.6203130 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.50

C HMQC NMR of Compound 2a



NAME hmfl0093
EXPNO 3
PROCNO 1
USER eq_m

F2 - Acquisition Parameters
Date_ 20200723
Time 15.20
INSTRUM spect
PROBHD 5 mm TBO BB-1H
PULPROG ls_hmqcgpqf
TD 4096
SOLVENT DMSO
NS 8
DS 16
SWH 7183.908 Hz
FIDRES 1.753884 Hz
AQ 0.2851316 sec
RG 5160.6
DW 69.600 usec
DE 10.00 usec
TE 297.9 K
CNST2 145.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000400 sec
D16 0.00020000 sec
DELTA1 0.00222428 sec
IN0 0.00001988 sec
MCREST 0.00000000 sec

MCWRK 2.00000000 sec

======== CHANNEL f1 ====
NUC1 1H
P1 9.50 usec
p2 19.00 usec
PL1 -1.00 dB
SFO1 400.1328009 MHz

======== CHANNEL f2 ====
CPDPRG2 garp
NUC2 13C
P3 10.00 usec
PCPD2 90.00 usec
PL2 2.00 dB
PL12 21.08 dB
SFO2 100.6233333 MHz

====== GRADIENT CHANNEL
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %

P16 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 100.6233 MHz
FIDRES 98.270439 Hz
SW 250.014 ppm
FnMODE QF

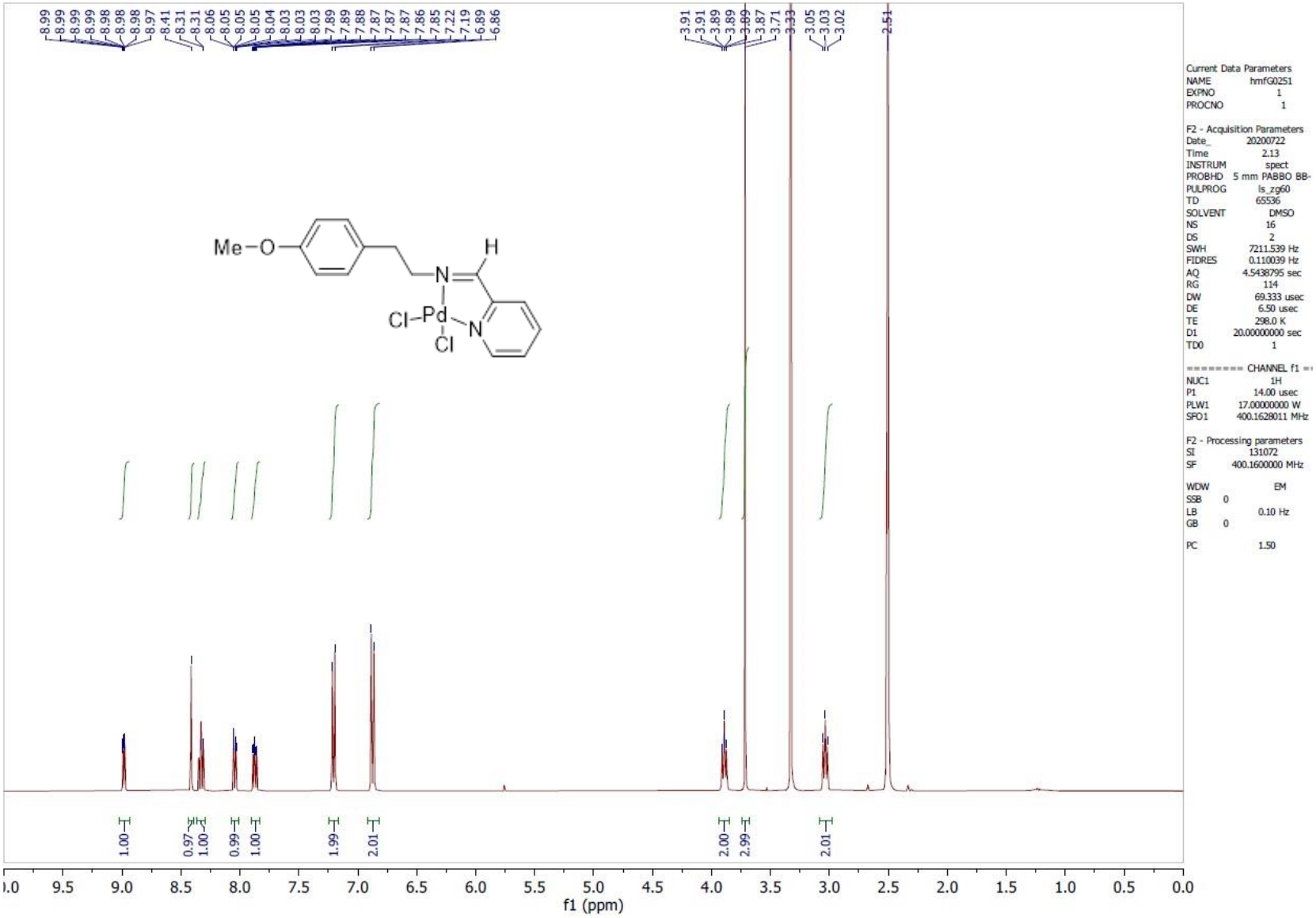
F2 - Processing parameters
SI 4096
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 QF
SF 100.6127690 MHz
WDW QSINE

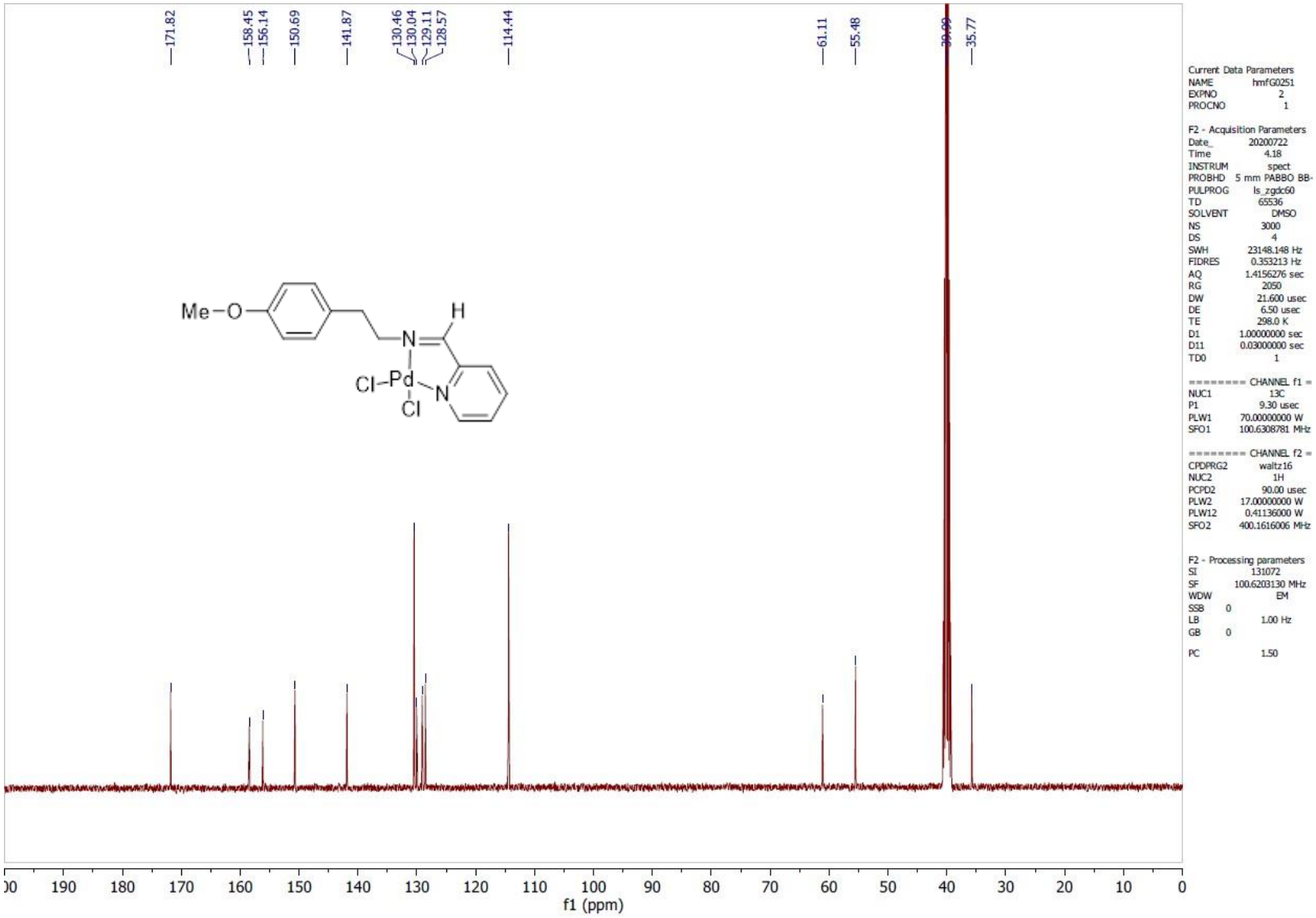
SSB 2
LB 0.00 Hz

GB 0

^{1}H NMR of Compound 2a-Pd



C {^{1}H} NMR of Compound 2a-Pd



Current Data Parameters
NAME hmfG0251
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200722
Time 4.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG ls_zgdc60
TD 65536
SOLVENT DMSO
NS 3000
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 2050
DW 21.600 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

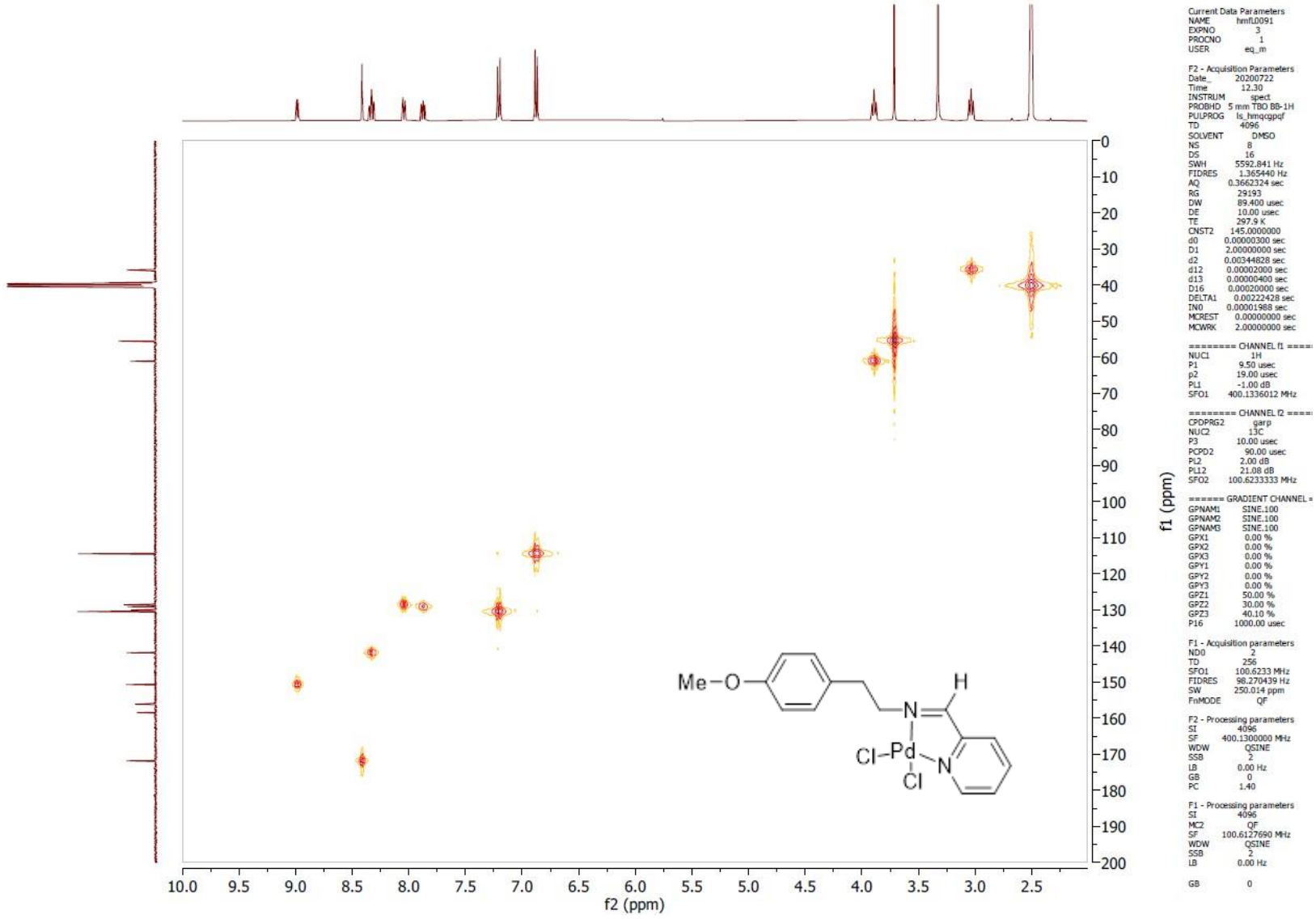
======== CHANNEL f1 =
NUC1 13C
P1 9.30 usec
PLW1 70.00000000 W
SFO1 100.6308781 MHz

======== CHANNEL f2 =
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 17.00000000 W
PLW12 0.41136000 W
SFO2 400.1616006 MHz

F2 - Processing parameters
SI 131072
SF 100.6203130 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0

PC 1.50

^{13}C HMQC NMR of Compound 2a-Pd



Current Data Parameters
NAME hmfl0091
EXPNO 3
PROCNO 1
USER eq_m

F2 - Acquisition Parameters
Date_ 20200722
Time 12.30
INSTRUM spect
PROBHD 5 mm TBO BB-1H
PULPROG ls_hmqcgpqf
TD 4096
SOLVENT DMSO
NS 8
DS 16
SWH 5592.841 Hz
FIDRES 1.365440 Hz
AQ 0.3662324 sec
RG 29193
DW 89.400 usec
DE 10.00 usec
TE 297.9 K
CNST2 145.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000400 sec
D16 0.00020000 sec
DELTA1 0.00222428 sec
IN0 0.00001988 sec
MCREST 0.00000000 sec
MCWRK 2.00000000 sec

======== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
p2 19.00 usec
PL1 -1.00 dB
SFO1 400.1336012 MHz

======== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 10.00 usec
PCPD2 90.00 usec
PL2 2.00 dB
PL12 21.08 dB
SFO2 100.6233333 MHz

======= GRADIENT CHANNEL =
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 100.6233 MHz
FIDRES 98.270439 Hz
SW 250.014 ppm
FnMODE QF

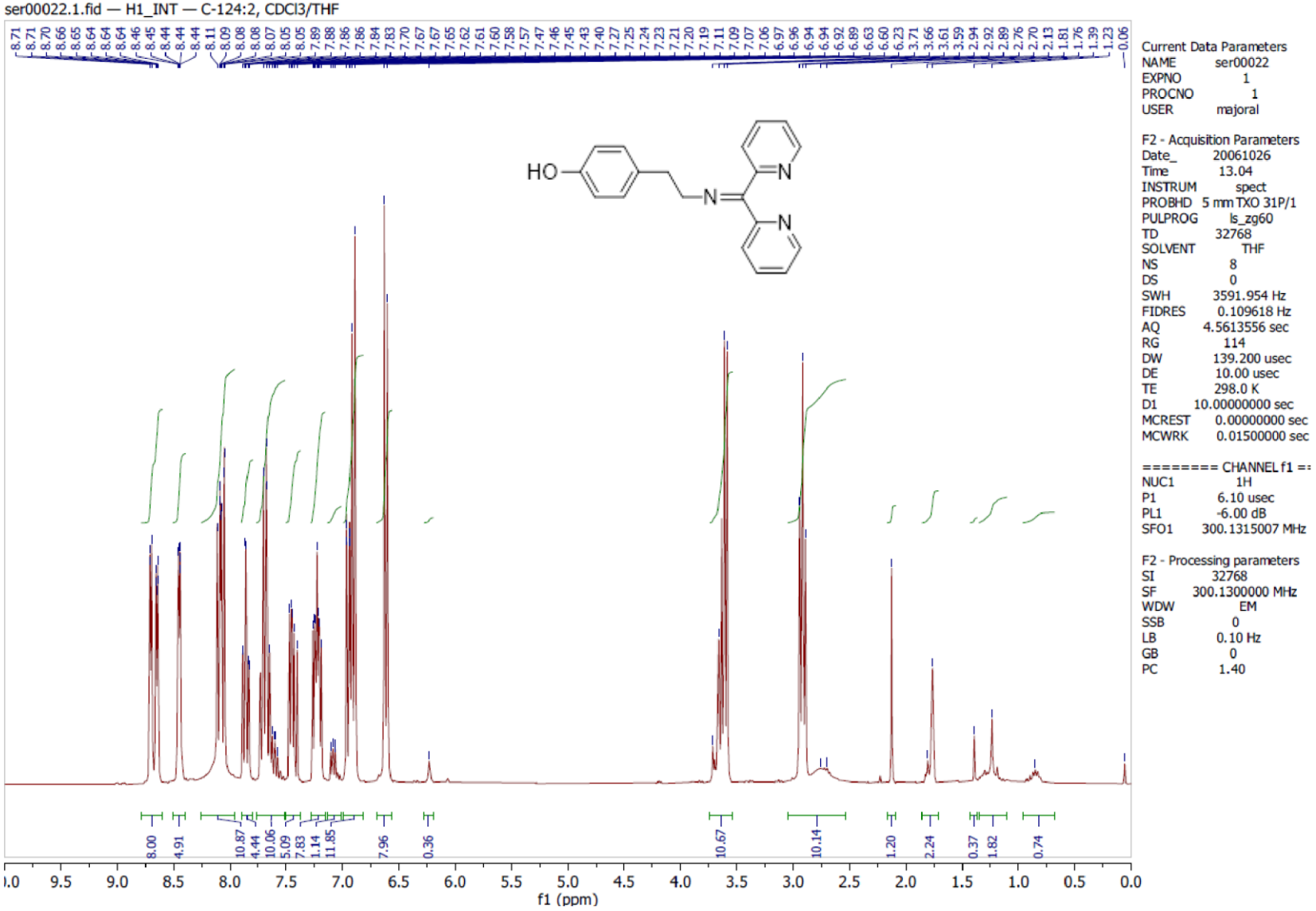
F2 - Processing parameters
SI 4096
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 QF
SF 100.6127690 MHz
WDW QSINE
SSB 2
LB 0.00 Hz

GB 0

^{1}H NMR of Compound 3

1



Current Data Parameters
NAME ser00022
EXPNO 1
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20061026
Time 13.04
INSTRUM spect
PROBHD 5 mm TXO 31P/1
PULPROG ls_zg60
TD 32768
SOLVENT THF
NS 8
DS 0
SWH 3591.954 Hz
FIDRES 0.109618 Hz
AQ 4.5613556 sec
RG 114
DW 139.200 usec
DE 10.00 usec
TE 298.0 K
D1 10.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

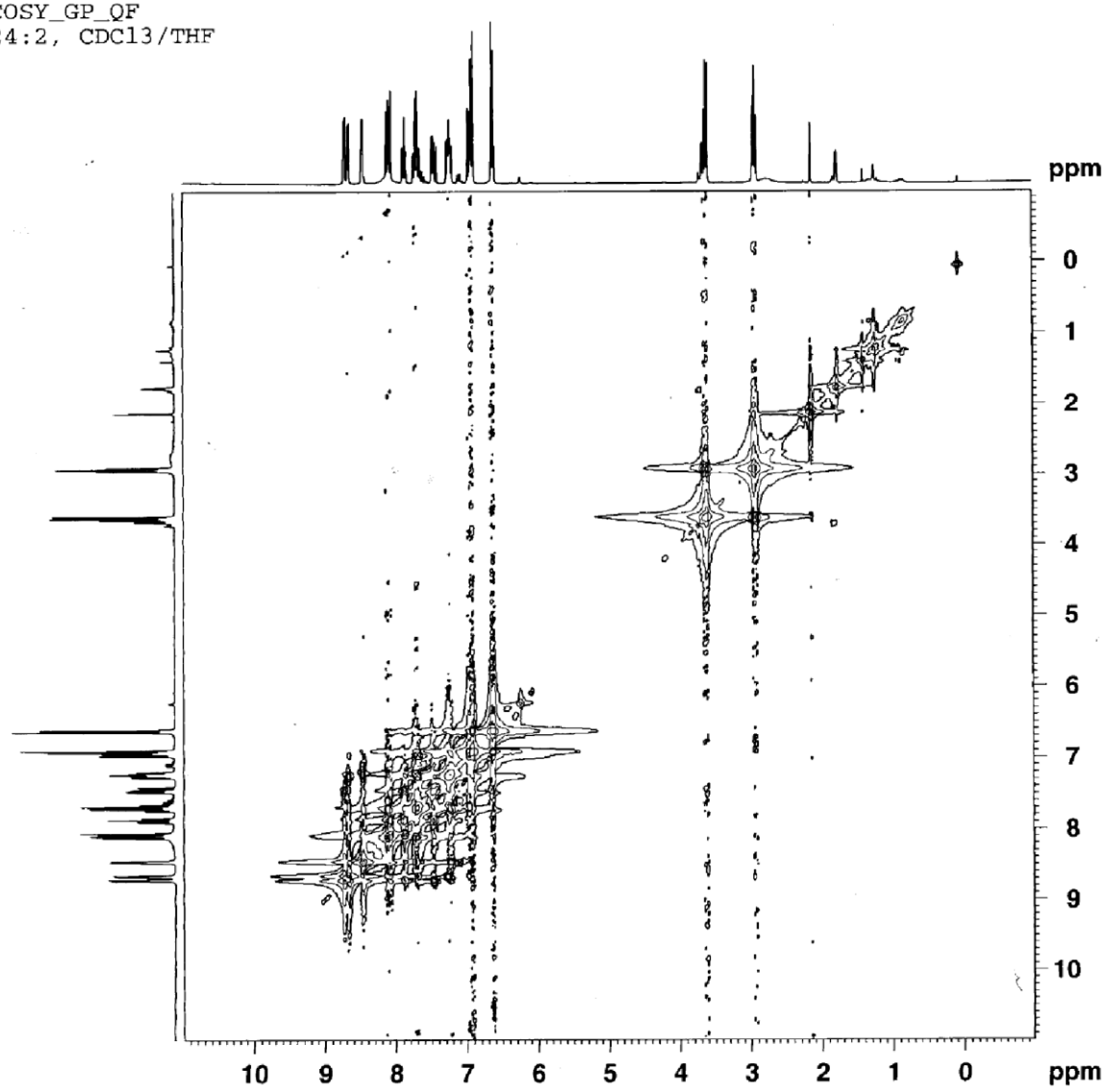
======== CHANNEL f1 ==
NUC1 1H
P1 6.10 usec
PL1 -6.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.40

^{1}H COSY NMR of Compound 3

1

H1_COSY_GP_QF
C-124:2, CDCl3/THF



SERVICE DE RMN DU
LCC
AV 300

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Current Data Parameters
NAME                 ser00022
EXPNO                       5
PROCNO                      1
USER                 majoral

F2 - Acquisition Parameters
Date_              20061026
Time                   13.52
INSTRUM                spect
PROBHD    5 mm TXO 31P/1
PULPROG      ls_cosygpqf
TD                       4096
SOLVENT                   THF
NS                          2
DS                          0
SWH                3591.954 Hz
FIDRES            0.876942 Hz
AQ                0.5702132 sec
RG                        128
DW                  139.200 usec
DE                   10.00 usec
TE                   298.0 K
d0                0.00000300 sec
D1                2.00000000 sec
d13               0.00008400 sec
D16               0.00020000 sec
IN0               0.00027840 sec
MCREST            0.00000000 sec
MCWRK             2.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P0                   6.10 usec
P1                   6.10 usec
PL1                 -6.00 dB
SFO1          300.1315007 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                10.00 %
GPZ2                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
ND0                         1
TD                        256
SFO1          300.1315 MHz
FIDRES        14.031071 Hz
SW                 11.968 ppm
FnMODE                   QF

F2 - Processing parameters
SI                       4096
SF            300.1300000 MHz
WDW                   QSINE
SSB                         2
LB                   0.00 Hz
GB                          0
PC                   1.40

F1 - Processing parameters
SI                       4096
MC2                      QF
SF            300.1300000 MHz
WDW                   QSINE
SSB                         2
LB                   0.00 Hz
GB                          0
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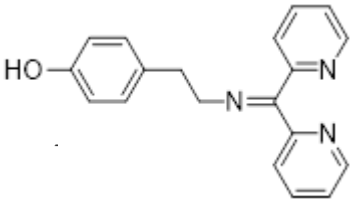
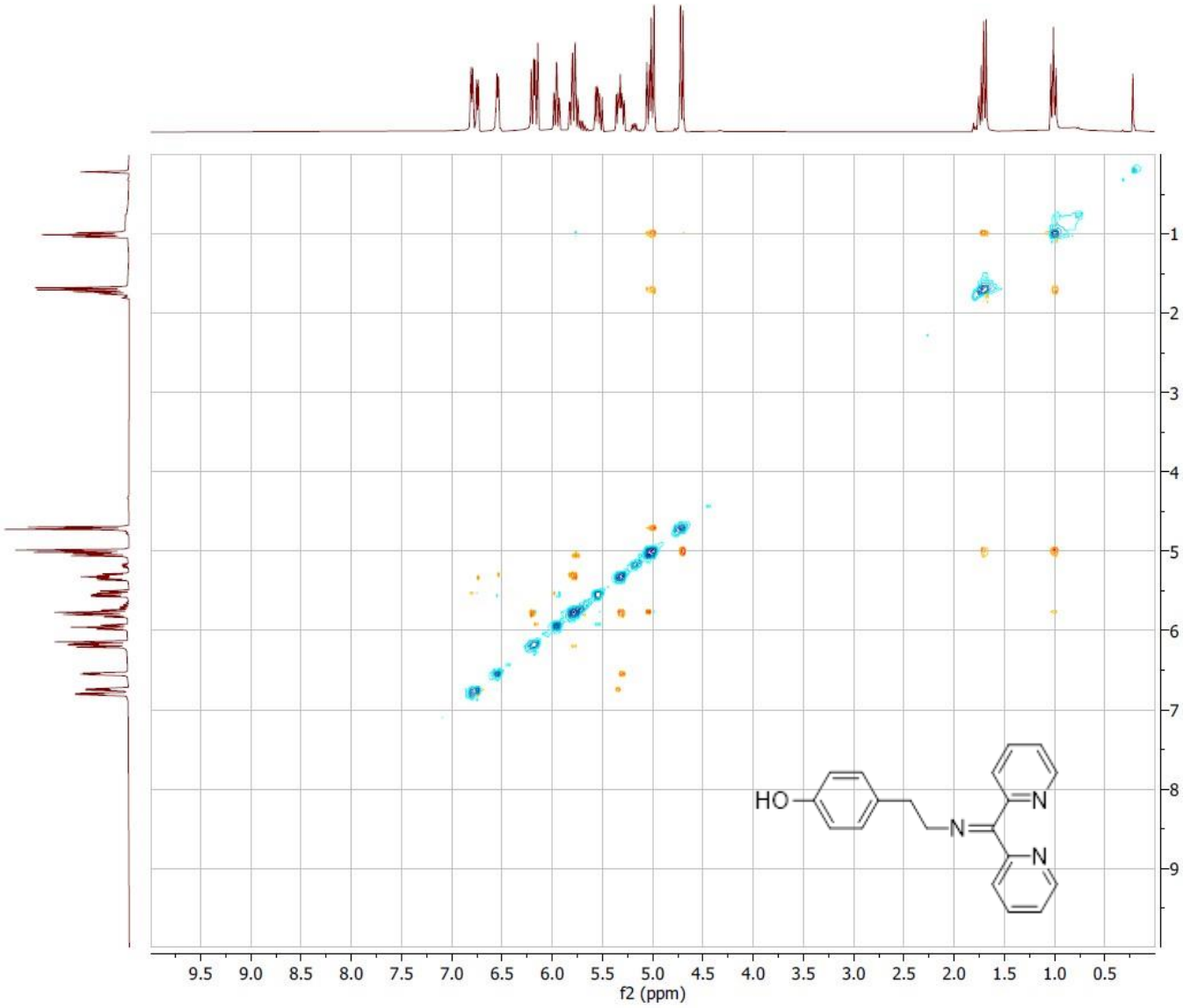


^{1}H NOESY NMR of Compound 3

1



Current Data Parameters
NAME ser00024
EXPNO 3
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20061028
Time 10.14
INSTRUM spect
PROBHD 5 mm TXO 31P/1
PULPROG ls_noesy phrv
TD 4096
SOLVENT THF
NS 8
DS 0
SWH 2997.602 Hz
FIDRES 0.731836 Hz
AQ 0.6832628 sec
RG 128
DW 166.800 usec
DE 10.00 usec
TE 298.0 K
d0 0.00015903 sec
D1 1.00000000 sec
D8 1.00000000 sec
IN0 0.00033360 sec
MCREST 0.00000000 sec
MCWRK 1.00000000 sec

======== CHANNEL f1 ==
NUC1 1H
P1 6.10 usec
PL1 -6.00 dB
SFO1 300.1315007 MHz

F1 - Acquisition parameters
ND0 1
TD 248
SFO1 300.1315 MHz
FIDRES 12.087105 Hz
SW 9.988 ppm
FnMODE TPPI

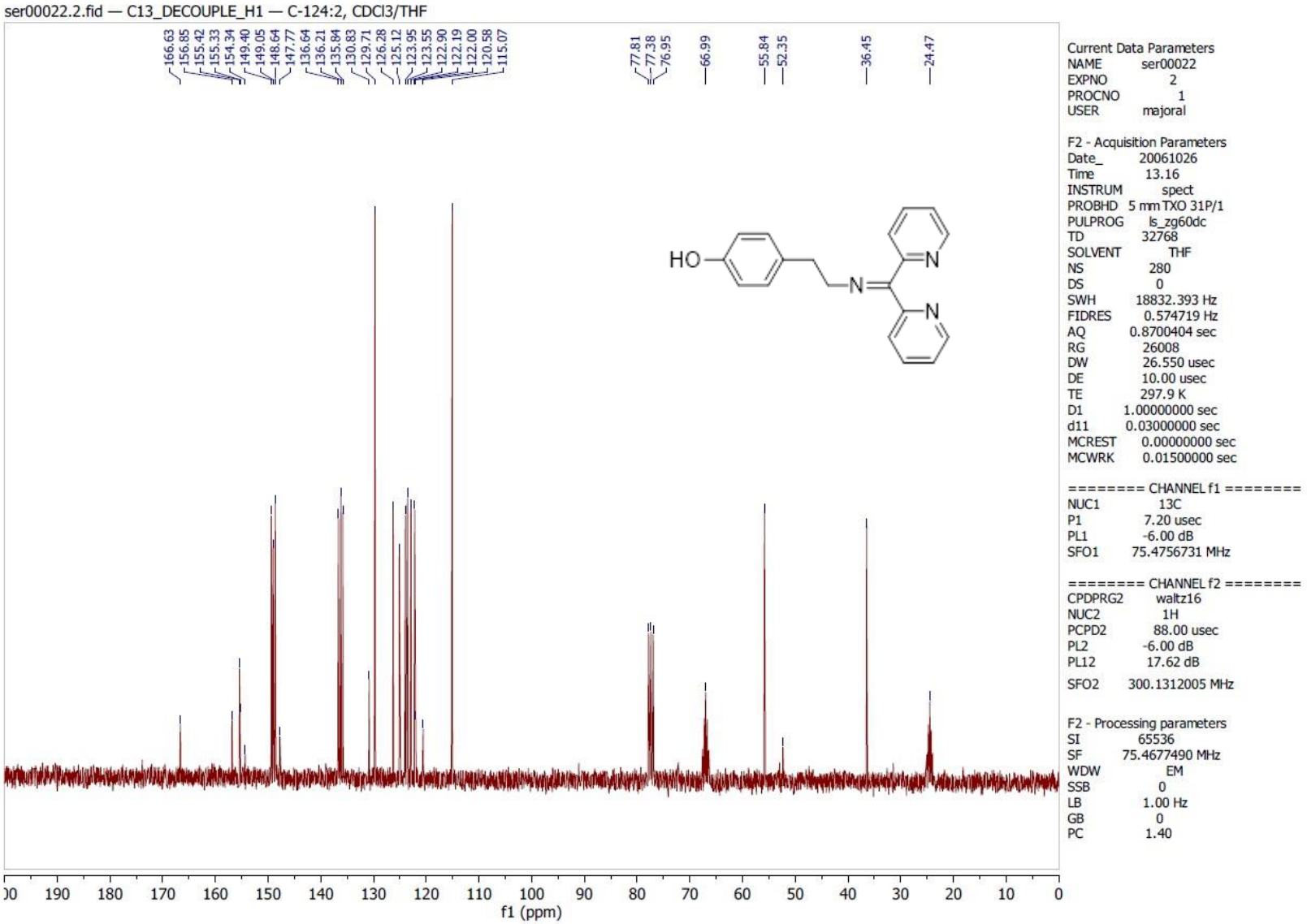
F2 - Processing parameters
SI 4096
SF 300.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 TPPI
SF 300.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

^{13}C

{^{1}H} NMR of Compound 3

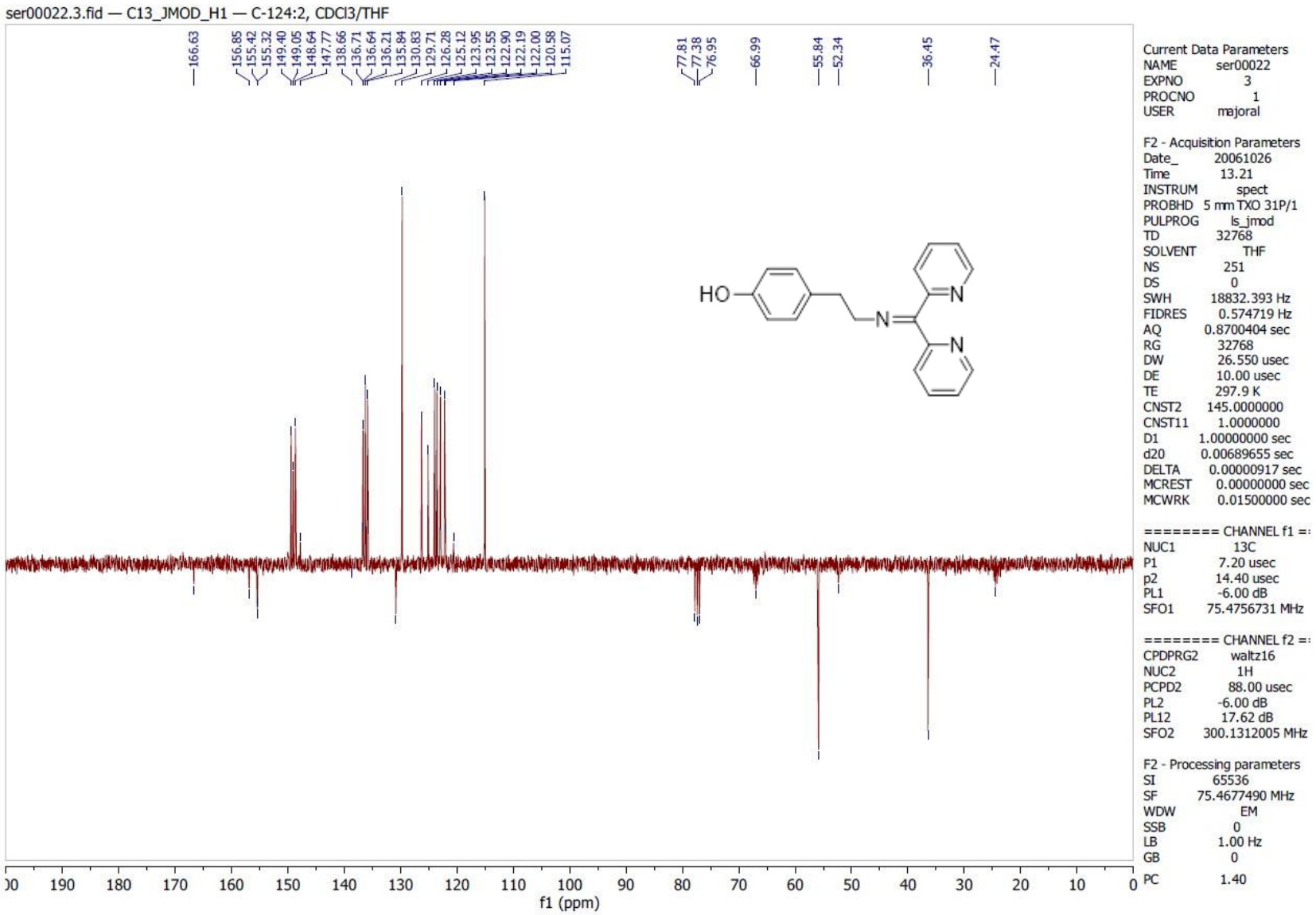
^{13}C


ser00022.2.fid — C13_DECOUPLE_H1 — C-124:2, CDCl3/THF
166.63
156.85
155.42
155.33
154.34
149.40
149.05
148.64
147.77
136.64
136.21
135.84
130.83
129.71
126.28
125.12
123.95
123.55
122.90
122.19
122.00
120.58
115.07
77.81
77.38
76.95
66.99
55.84
52.35
36.45
24.47
HO
N
N
N
f1 (ppm)
Current Data Parameters
NAME ser00022
EXPNO 2
PROCNO 1
USER majoral
F2 - Acquisition Parameters
Date_ 20061026
Time 13.16
INSTRUM spect
PROBHD 5 mm TXO 31P/1
PULPROG ls_zg60dc
TD 32768
SOLVENT THF
NS 280
DS 0
SWH 18832.393 Hz
FIDRES 0.574719 Hz
AQ 0.8700404 sec
RG 26008
DW 26.550 usec
DE 10.00 usec
TE 297.9 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.20 usec
PL1 -6.00 dB
SFO1 75.4756731 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00 usec
PL2 -6.00 dB
PL12 17.62 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{13}C

JMOD NMR of Compound 3

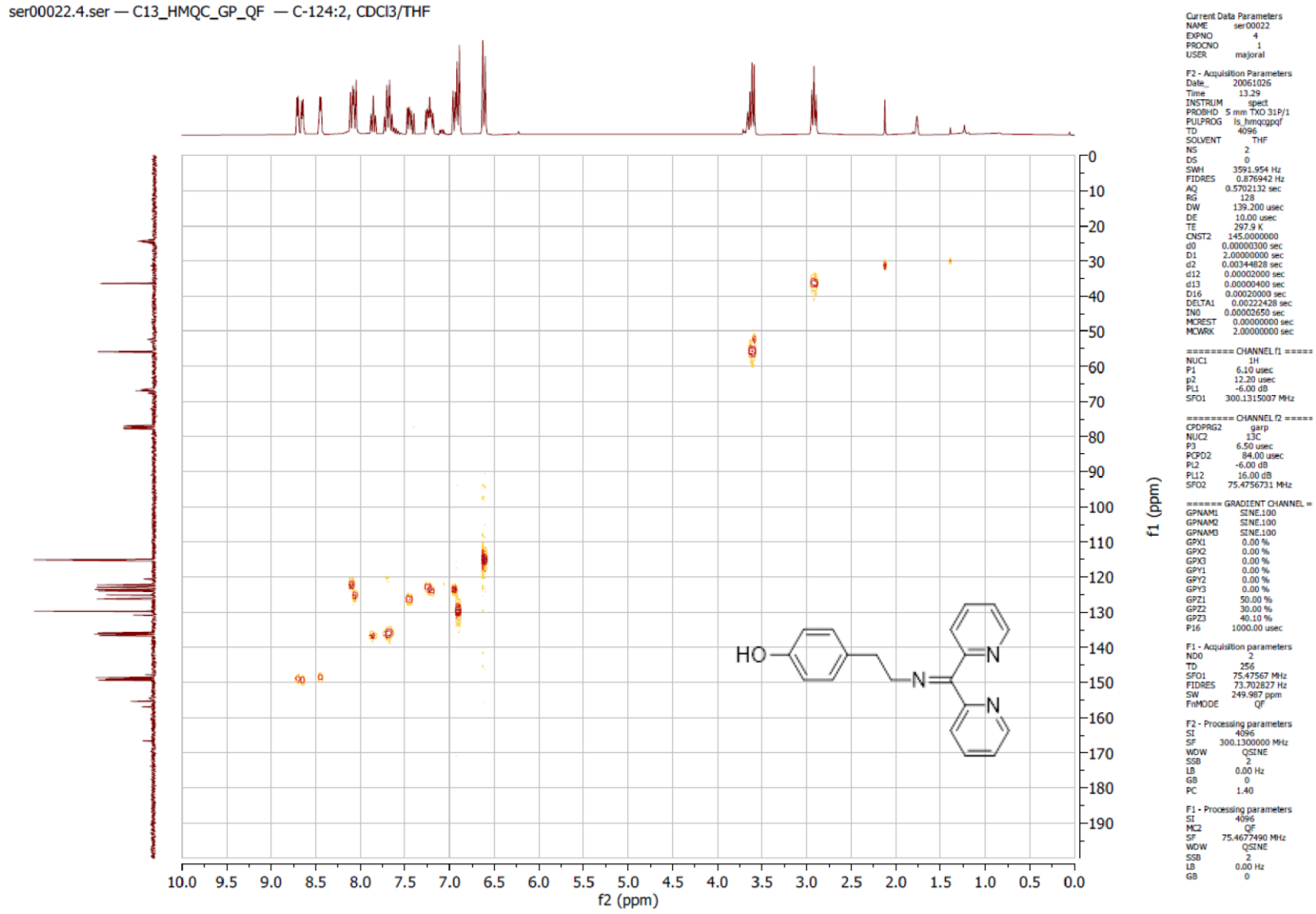
^{13}C


ser00022.3.fid — C13_JMOD_H1 — C-124:2, CDCl3/THF
166.63
156.85
155.42
155.32
149.40
149.05
148.64
147.77
138.66
136.71
136.64
136.21
135.84
130.83
129.71
126.28
125.12
123.95
123.55
122.90
122.19
122.00
120.58
115.07
77.81
77.38
76.95
66.99
55.84
52.34
36.45
24.47
HO
N
N
N
f1 (ppm)
Current Data Parameters
NAME ser00022
EXPNO 3
PROCNO 1
USER majoral
F2 - Acquisition Parameters
Date_ 20061026
Time 13.21
INSTRUM spect
PROBHD 5 mm TXO 31P/1
PULPROG ls_jmod
TD 32768
SOLVENT THF
NS 251
DS 0
SWH 18832.393 Hz
FIDRES 0.574719 Hz
AQ 0.8700404 sec
RG 32768
DW 26.550 usec
DE 10.00 usec
TE 297.9 K
CNST2 145.0000000
CNST11 1.0000000
D1 1.00000000 sec
d20 0.00689655 sec
DELTA 0.00000917 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 =
NUC1 13C
P1 7.20 usec
p2 14.40 usec
PL1 -6.00 dB
SFO1 75.4756731 MHz
======== CHANNEL f2 =
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00 usec
PL2 -6.00 dB
PL12 17.62 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{13}C

HMQC NMR of Compound 3

^{13}C



Current Data Parameters
NAME ser00022
EXPNO 4
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20061026
Time 13.29
INSTRUM spect
PROBHD 5 mm TXO 31P/1
PULPROG ls_hmqcgpqf
TD 4096
SOLVENT THF
NS 2
DS 0
SWH 3591.954 Hz
FIDRES 0.876942 Hz
AQ 0.5702132 sec
RG 128
DW 139.200 usec
DE 10.00 usec
TE 297.9 K
CNST2 145.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000400 sec
D16 0.00020000 sec
DELTA1 0.00222428 sec
IN0 0.00002650 sec
MCREST 0.00000000 sec
MCWRK 2.00000000 sec

======== CHANNEL f1 =====
NUC1 1H
P1 6.10 usec
p2 12.20 usec
PL1 -6.00 dB
SFO1 300.1315007 MHz

======== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 6.50 usec
PCPD2 84.00 usec
PL2 -6.00 dB
PL12 16.00 dB
SFO2 75.4756731 MHz

====== GRADIENT CHANNEL =
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 75.47567 MHz
FIDRES 73.702827 Hz
SW 249.987 ppm
FnMODE QF

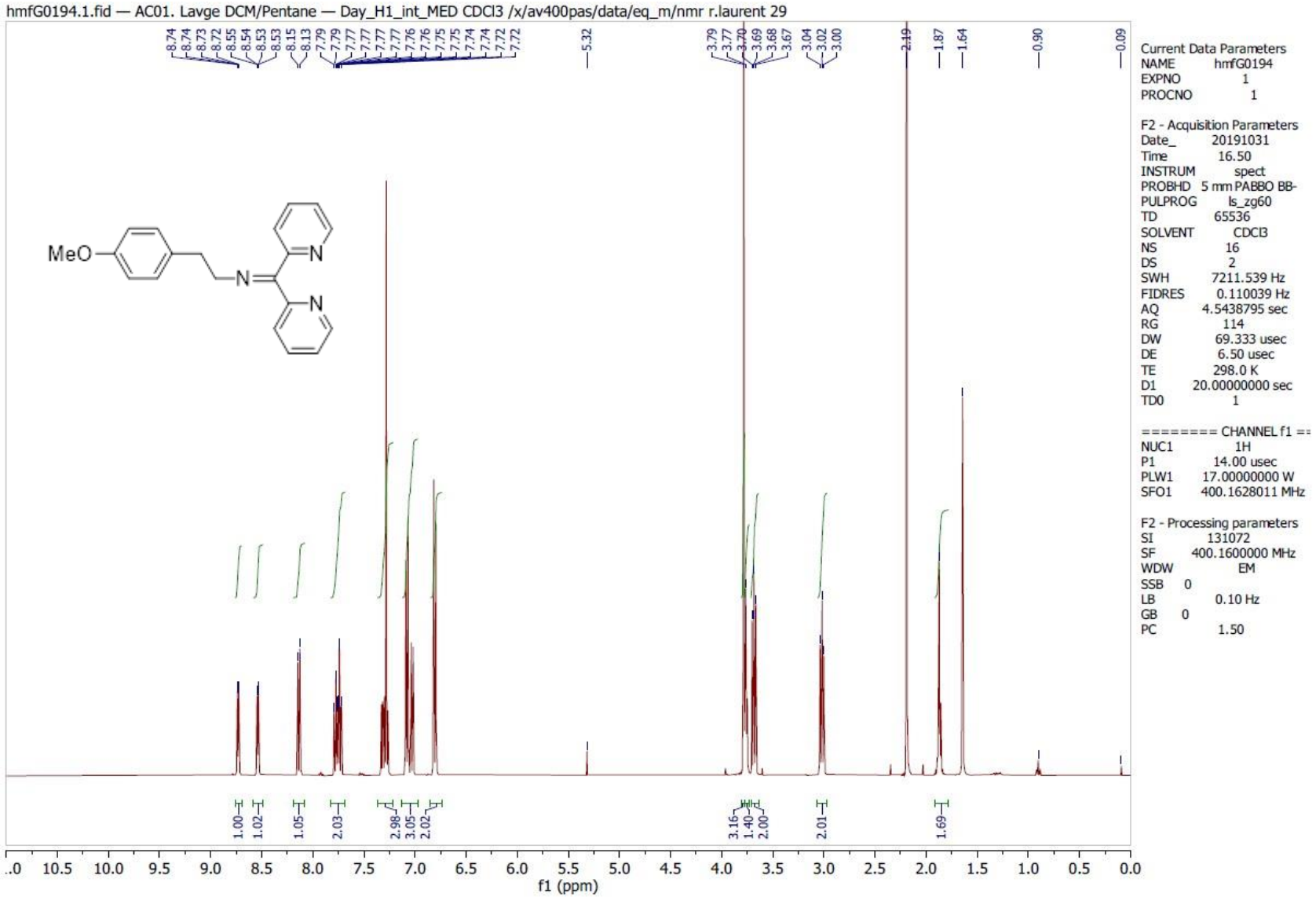
F2 - Processing parameters
SI 4096
SF 300.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 QF
SF 75.4677490 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

$^{13}C\{^{1}H\}$ NMR of Compound 3

a

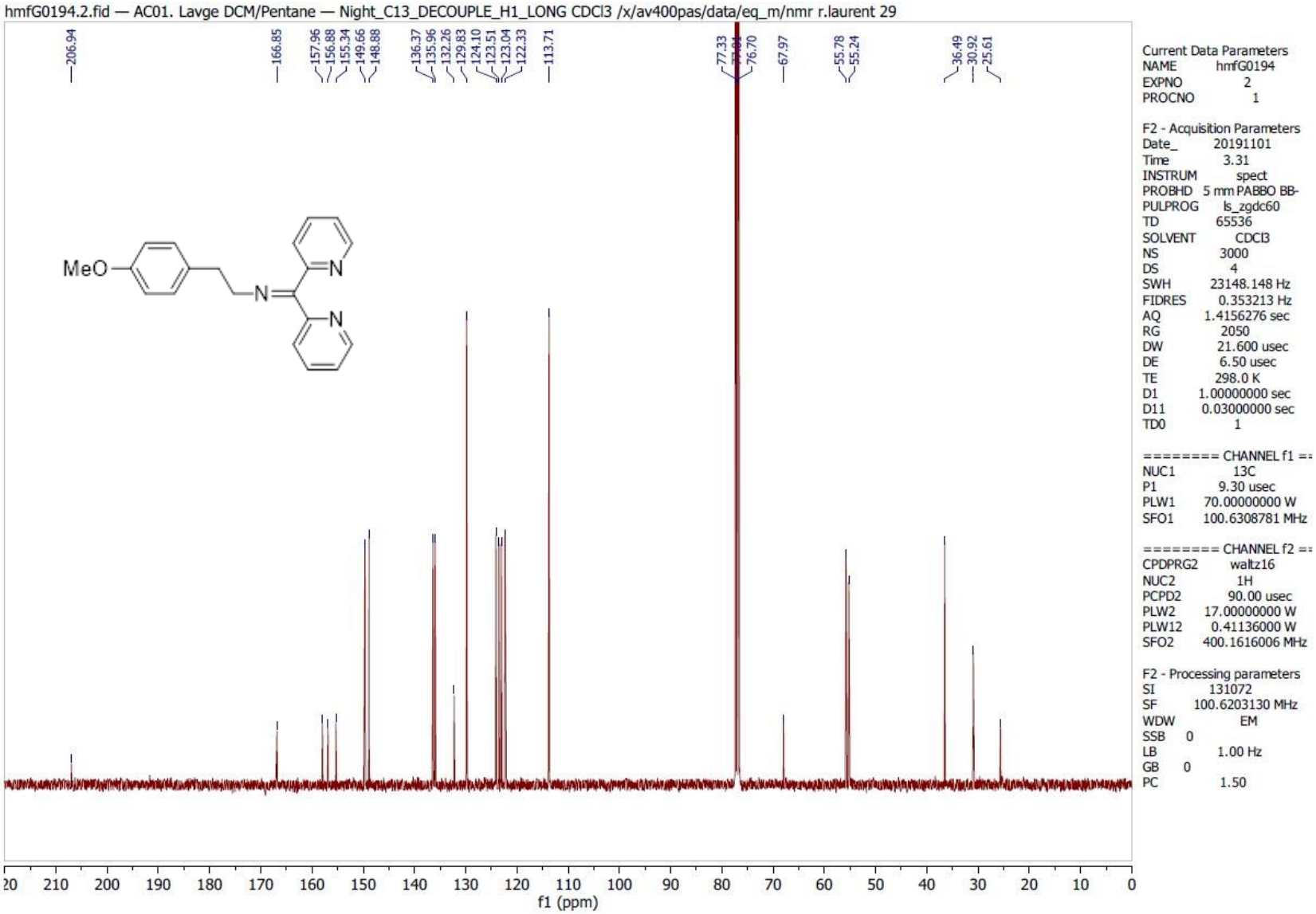
^{1}H NMR of Compound 3



$^{13}C\{^{1}H\}$ NMR of Compound 3

a

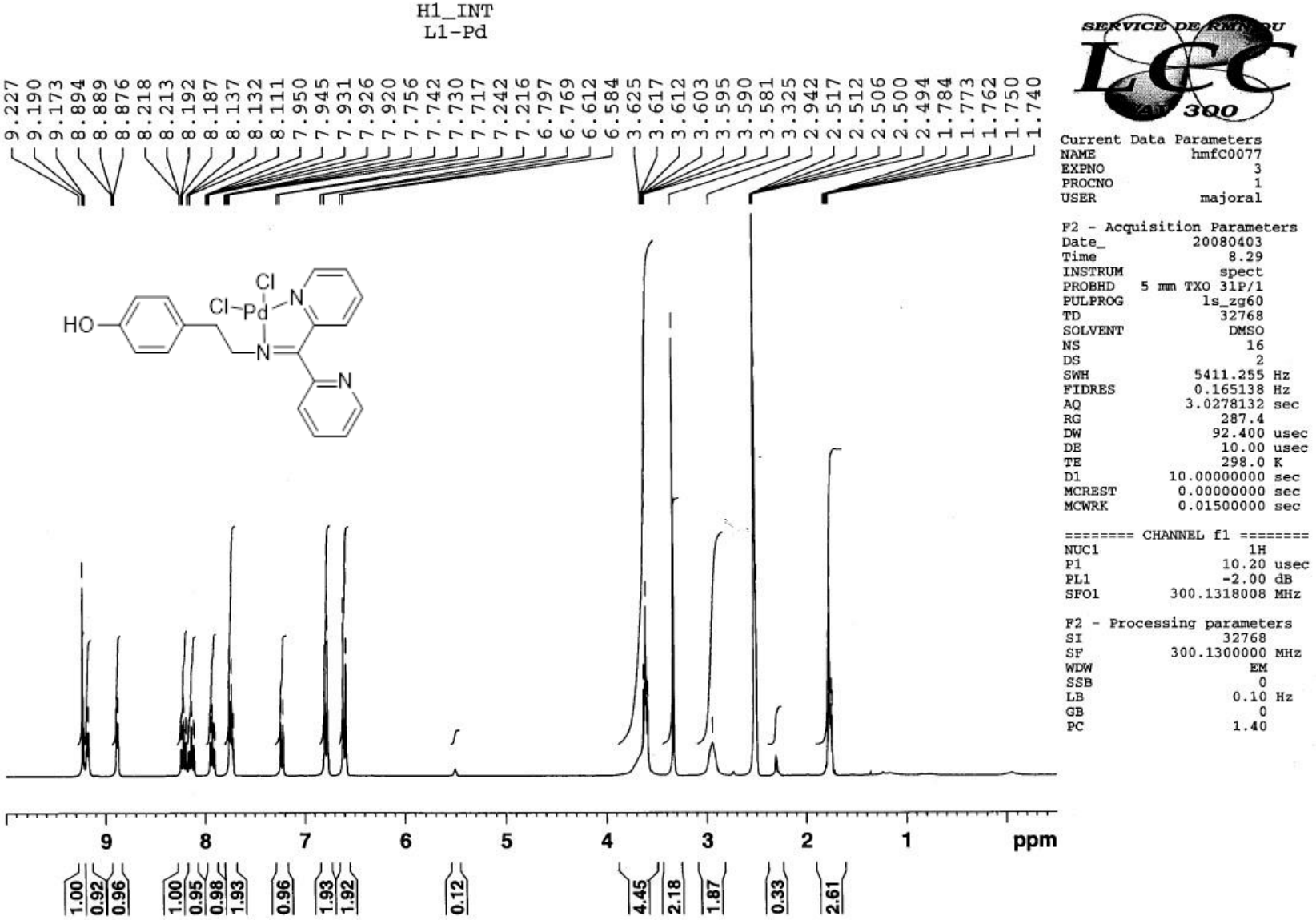
[1]H NMR of Compound 3



$^{13}C\{^{1}H\}$ NMR of Compound 3

-Pd

^{1}H NMR of Compound 3

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Current Data Parameters
NAME                 hmfC0077
EXPNO                       3
PROCNO                      1
USER                 majoral

F2 - Acquisition Parameters
Date_               20080403
Time                    8.29
INSTRUM                spect
PROBHD   5 mm TXO 31P/1
PULPROG             ls_zg60
TD                    32768
SOLVENT                DMSO
NS                       16
DS                        2
SWH                5411.255 Hz
FIDRES            0.165138 Hz
AQ                3.0278132 sec
RG                    287.4
DW                 92.400 usec
DE                 10.00 usec
TE                   298.0 K
D1                10.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

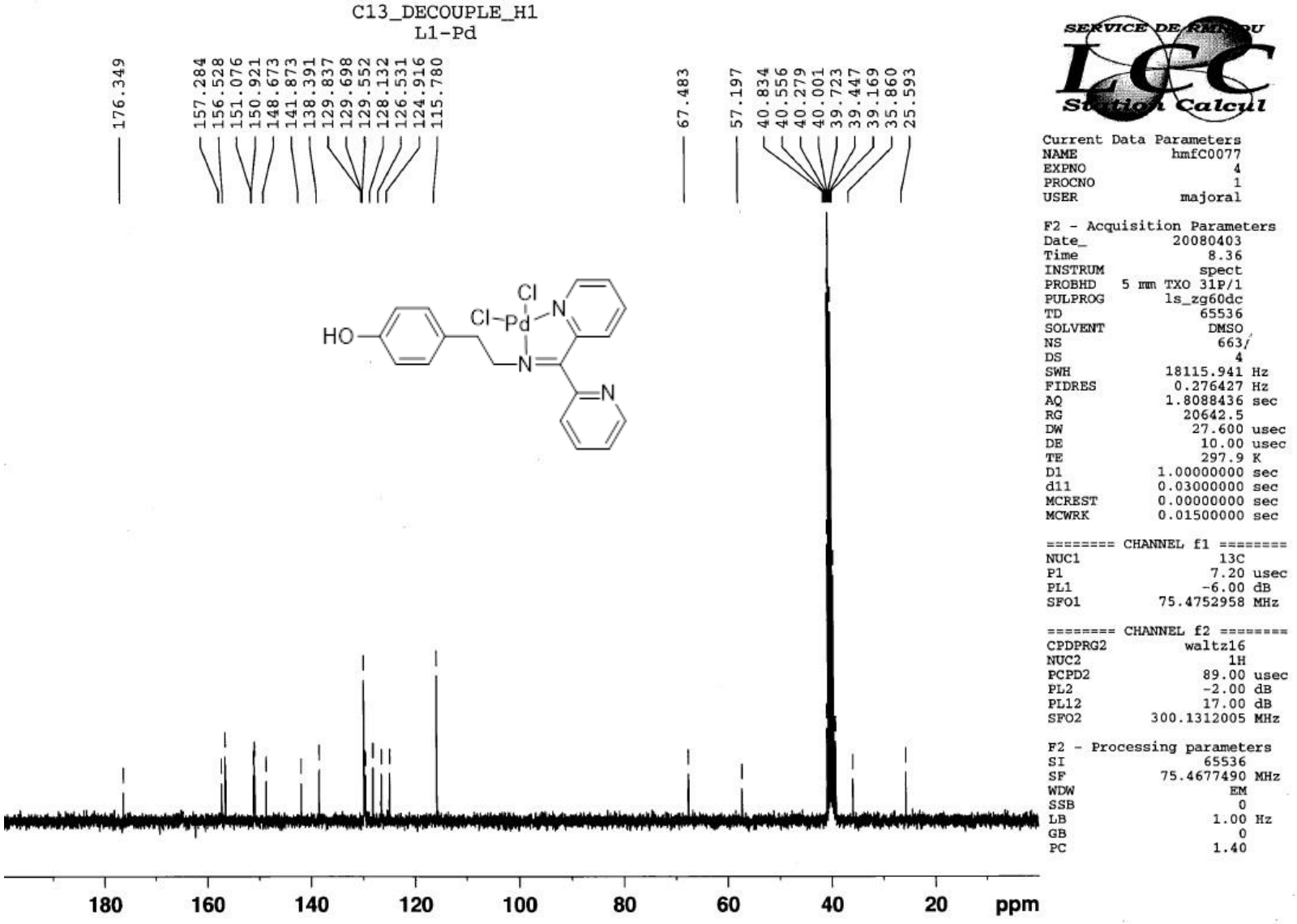
======== CHANNEL f1 ========
NUC1                      1H
P1                 10.20 usec
PL1                 -2.00 dB
SFO1          300.1318008 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300000 MHz
WDW                      EM
SSB                       0
LB                 0.10 Hz
GB                        0
PC                     1.40
```

$^{13}C\{^{1}H\}$ NMR of Compound 3

-Pd

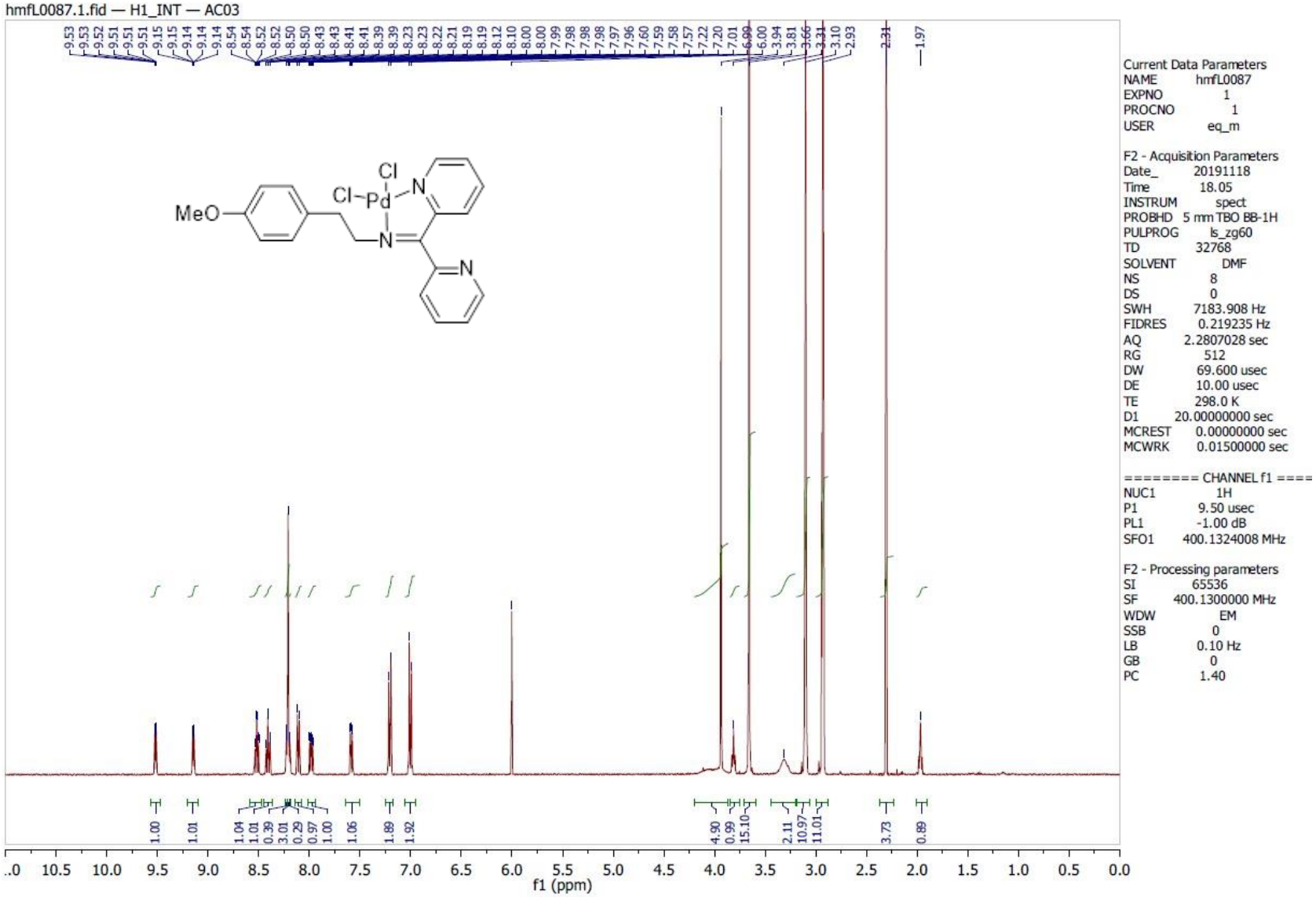
^{1}H NMR of Compound 3



$^{13}C\{^{1}H\}$ NMR of Compound 3

a-Pd

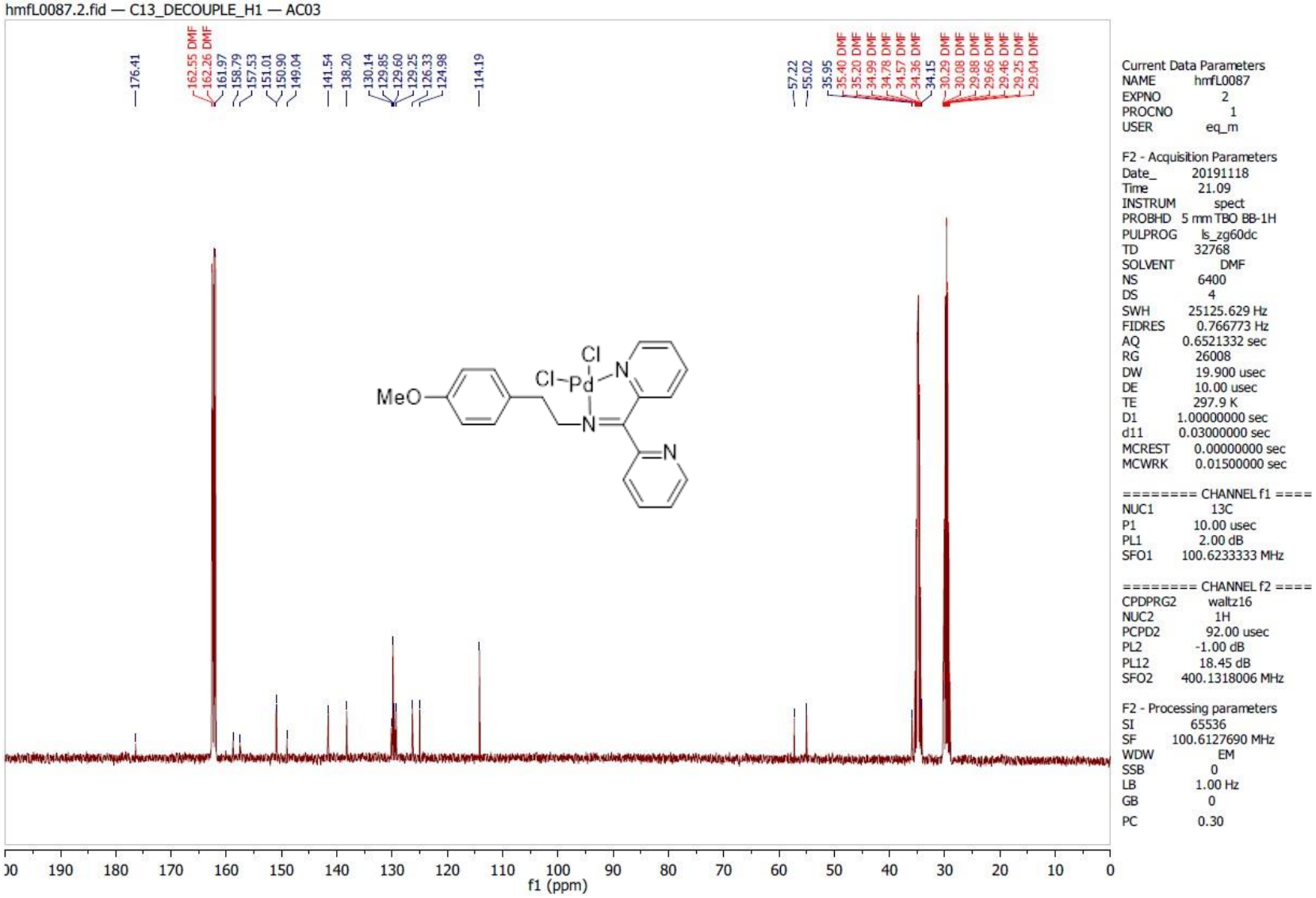
^{1}H NMR of Compound 3



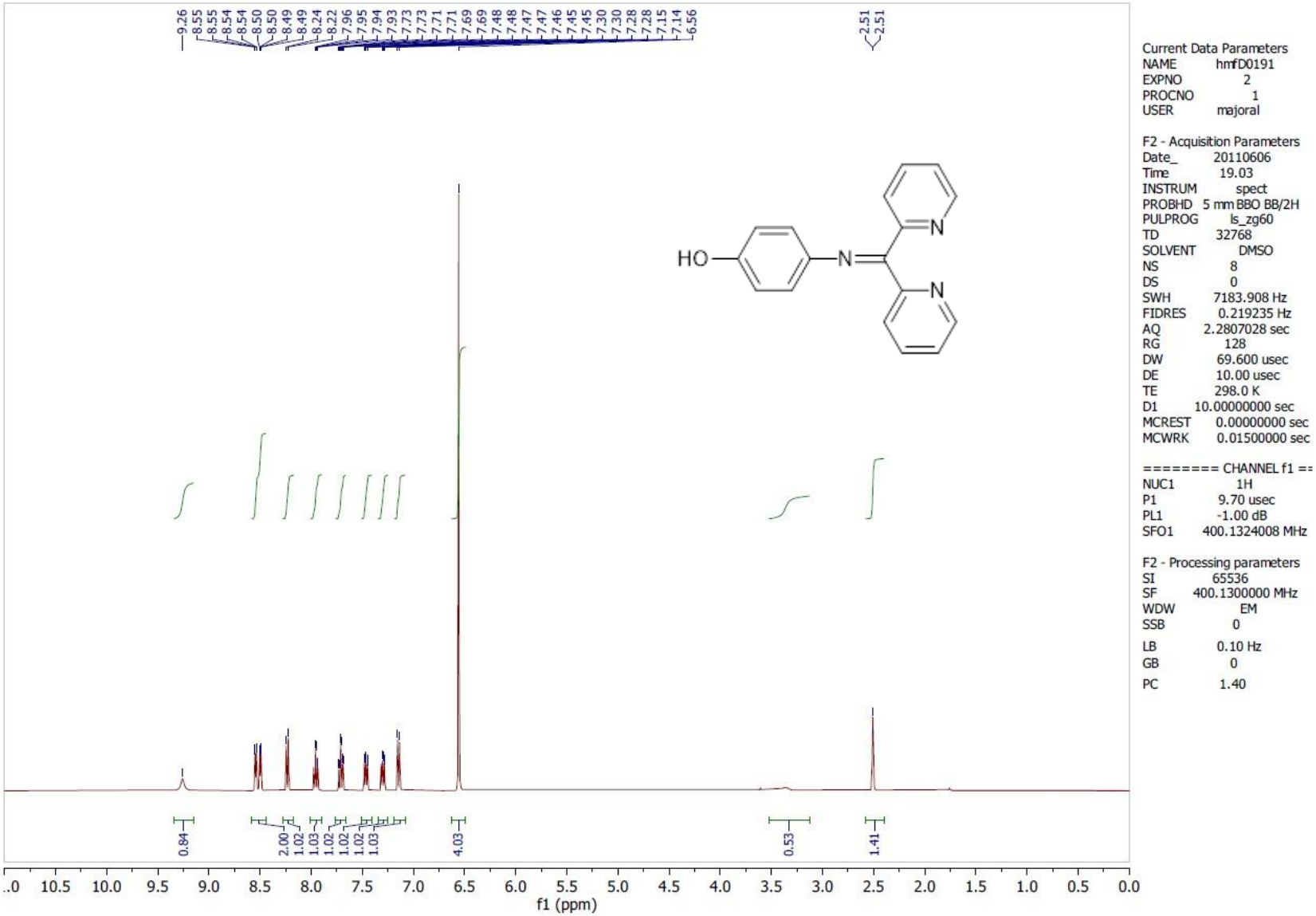
$^{13}C\{^{1}H\}$ NMR of Compound 3

a-Pd

^{1}H NMR of Compound 3



H NMR of Compound 4



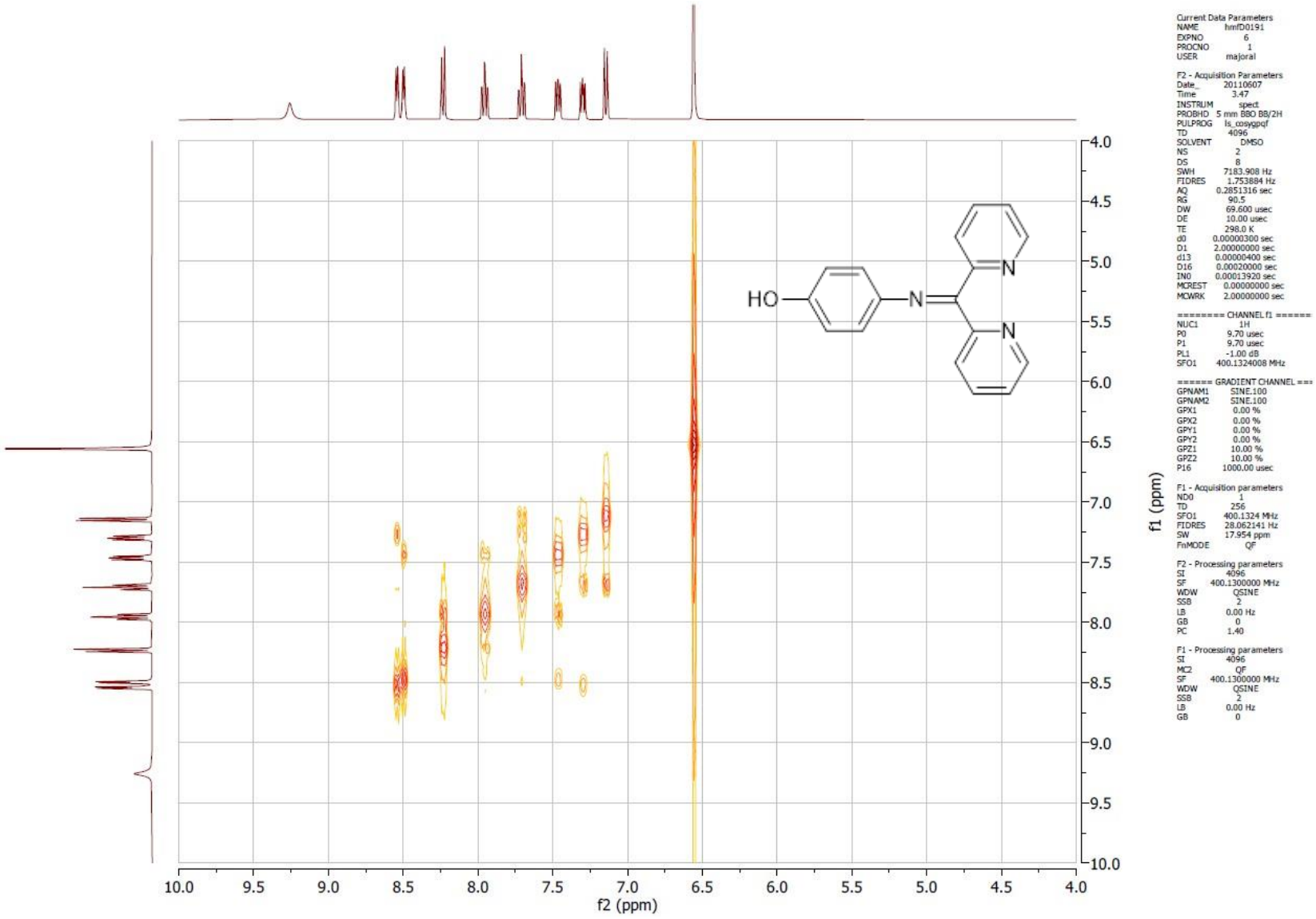
Current Data Parameters
NAME hmfD0191
EXPNO 2
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20110606
Time 19.03
INSTRUM spect
PROBHD 5 mm BBO BB/2H
PULPROG ls_zg60
TD 32768
SOLVENT DMSO
NS 8
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2807028 sec
RG 128
DW 69.600 usec
DE 10.00 usec
TE 298.0 K
D1 10.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ==
NUC1 1H
P1 9.70 usec
PL1 -1.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.40

^{1}H COSY NMR of Compound 4



Current Data Parameters
NAME hmfD0191
EXPNO 6
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20110607
Time 3.47
INSTRUM spect
PROBHD 5 mm BBO BB/2H
PULPROG ls_cosygpqf
TD 4096
SOLVENT DMSO
NS 2
DS 8
SWH 7183.908 Hz
FIDRES 1.753884 Hz
AQ 0.2851316 sec
RG 90.5
DW 69.600 usec
DE 10.00 usec
TE 298.0 K
d0 0.00000300 sec
D1 2.00000000 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00013920 sec
MCREST 0.00000000 sec
MCWRK 2.00000000 sec

======== CHANNEL f1 ======
NUC1 1H
P0 9.70 usec
P1 9.70 usec
PL1 -1.00 dB
SFO1 400.1324008 MHz

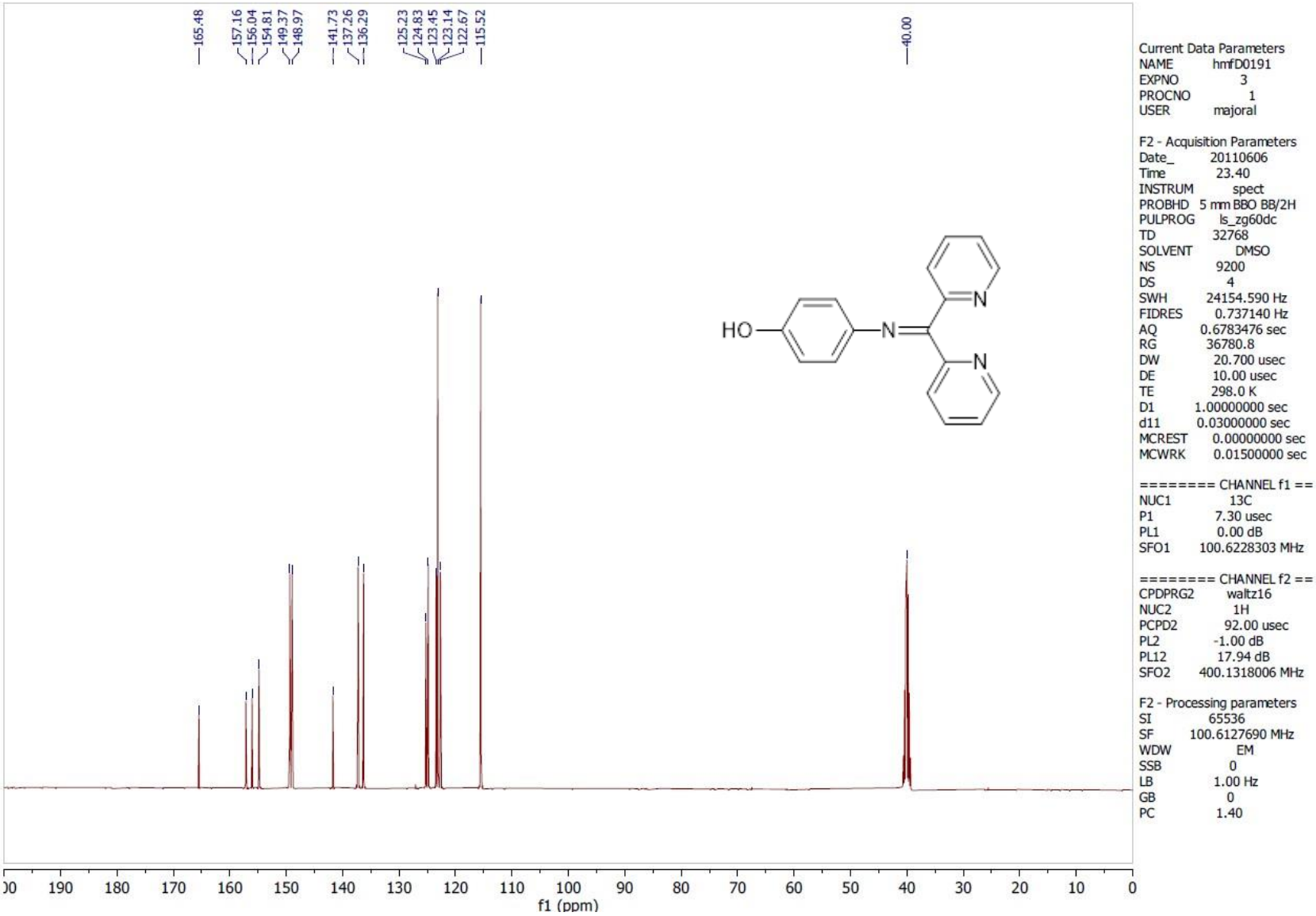
====== GRADIENT CHANNEL ===
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 10.00 %
GPZ2 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 256
SFO1 400.1324 MHz
FIDRES 28.062141 Hz
SW 17.954 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 QF
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

$^{13}C\{^{1}H\}$ NMR of Compound 4



Current Data Parameters
NAME hmfD0191
EXPNO 3
PROCNO 1
USER majoral

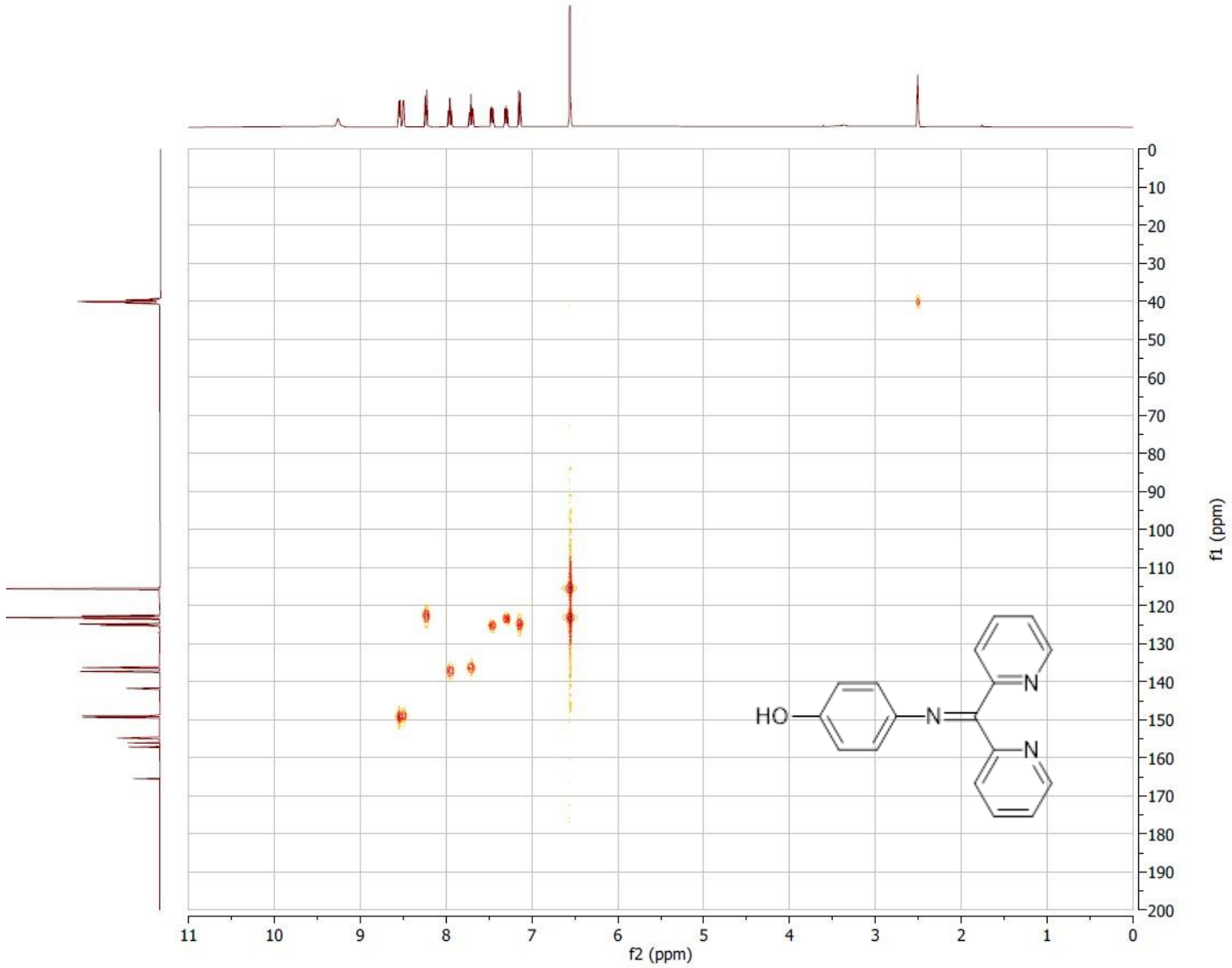
F2 - Acquisition Parameters
Date_ 20110606
Time 23.40
INSTRUM spect
PROBHD 5 mm BBO BB/2H
PULPROG ls_zg60dc
TD 32768
SOLVENT DMSO
NS 9200
DS 4
SWH 24154.590 Hz
FIDRES 0.737140 Hz
AQ 0.6783476 sec
RG 36780.8
DW 20.700 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ==
NUC1 13C
P1 7.30 usec
PL1 0.00 dB
SFO1 100.6228303 MHz

======== CHANNEL f2 ==
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 -1.00 dB
PL12 17.94 dB
SFO2 400.1318006 MHz

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{13}C HMQC NMR of Compound 4



Current Data Parameters
NAME hmfD0191
EXPNO 4
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20110606
Time 23.42
INSTRUM spect
PROBHD 5 mm BBO BB/2H
PULPROG ls_hmqcgpqf
TD 4096
SOLVENT DMSO
NS 8
DS 16
SWH 7183.908 Hz
FIDRES 1.753884 Hz
AQ 0.2851316 sec
RG 20642.5
DW 69.600 usec
DE 10.00 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000400 sec
D16 0.00020000 sec
DELTA1 0.00222428 sec
IN0 0.00002070 sec
MCREST 0.00000000 sec
MCWRK 2.00000000 sec

======== CHANNEL f1 ===
NUC1 1H
P1 9.70 usec
p2 19.40 usec
PL1 -1.00 dB
SFO1 400.1324008 MHz

======== CHANNEL f2 ===
CPDPRG2 garp
NUC2 13C
P3 7.00 usec
PCPD2 98.00 usec
PL2 0.00 dB
PL12 22.92 dB
SFO2 100.6228303 MHz

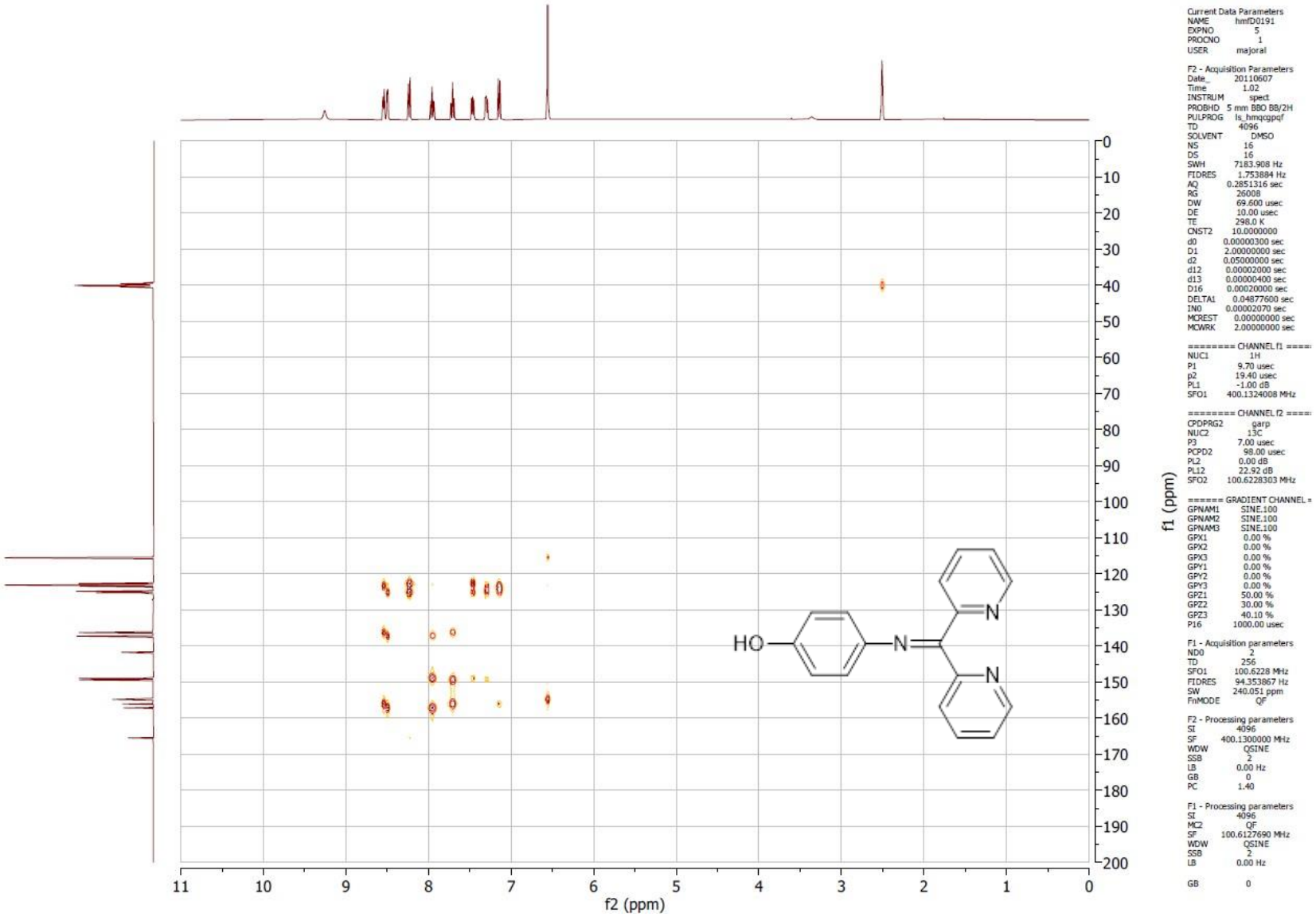
====== GRADIENT CHANNE
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 100.6228 MHz
FIDRES 94.353867 Hz
SW 240.051 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 QF
SF 100.6127690 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

^{13}C HMQC long range NMR of Compound 4



Current Data Parameters
NAME hmfD0191
EXPNO 5
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20110607
Time 1.02
INSTRUM spect
PROBHD 5 mm BBO BB/2H
PULPROG ls_hmqcgpqf
TD 4096
SOLVENT DMSO
NS 16
DS 16
SWH 7183.908 Hz
FIDRES 1.753884 Hz
AQ 0.2851316 sec
RG 26008
DW 69.600 usec
DE 10.00 usec
TE 298.0 K
CNST2 10.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d2 0.05000000 sec
d12 0.00002000 sec
d13 0.00000400 sec
D16 0.00020000 sec
DELTA1 0.04877600 sec
IN0 0.00002070 sec
MCREST 0.00000000 sec
MCWRK 2.00000000 sec

======== CHANNEL f1 =====
NUC1 1H
P1 9.70 usec
p2 19.40 usec
PL1 -1.00 dB
SFO1 400.1324008 MHz

======== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 7.00 usec
PCPD2 98.00 usec
PL2 0.00 dB
PL12 22.92 dB
SFO2 100.6228303 MHz

====== GRADIENT CHANNEL =
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

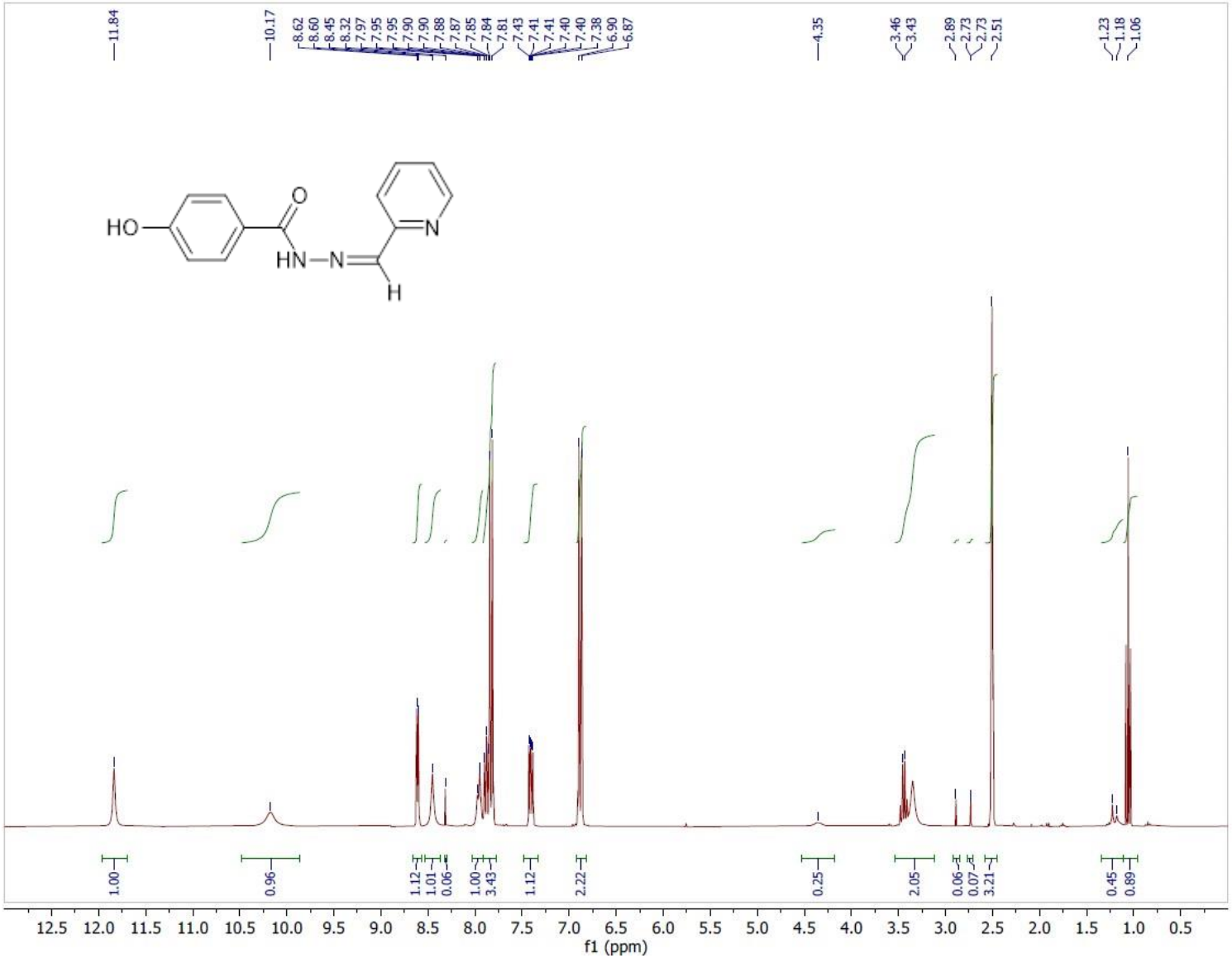
F1 - Acquisition parameters
ND0 2
TD 256
SFO1 100.6228 MHz
FIDRES 94.353867 Hz
SW 240.051 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 QF
SF 100.6127690 MHz
WDW QSINE
SSB 2
LB 0.00 Hz

GB 0

[1]H NMR of Compound 5



Current Data Parameters
NAME ahaC0471
EXPNO 1
PROCNO 1
USER majoral

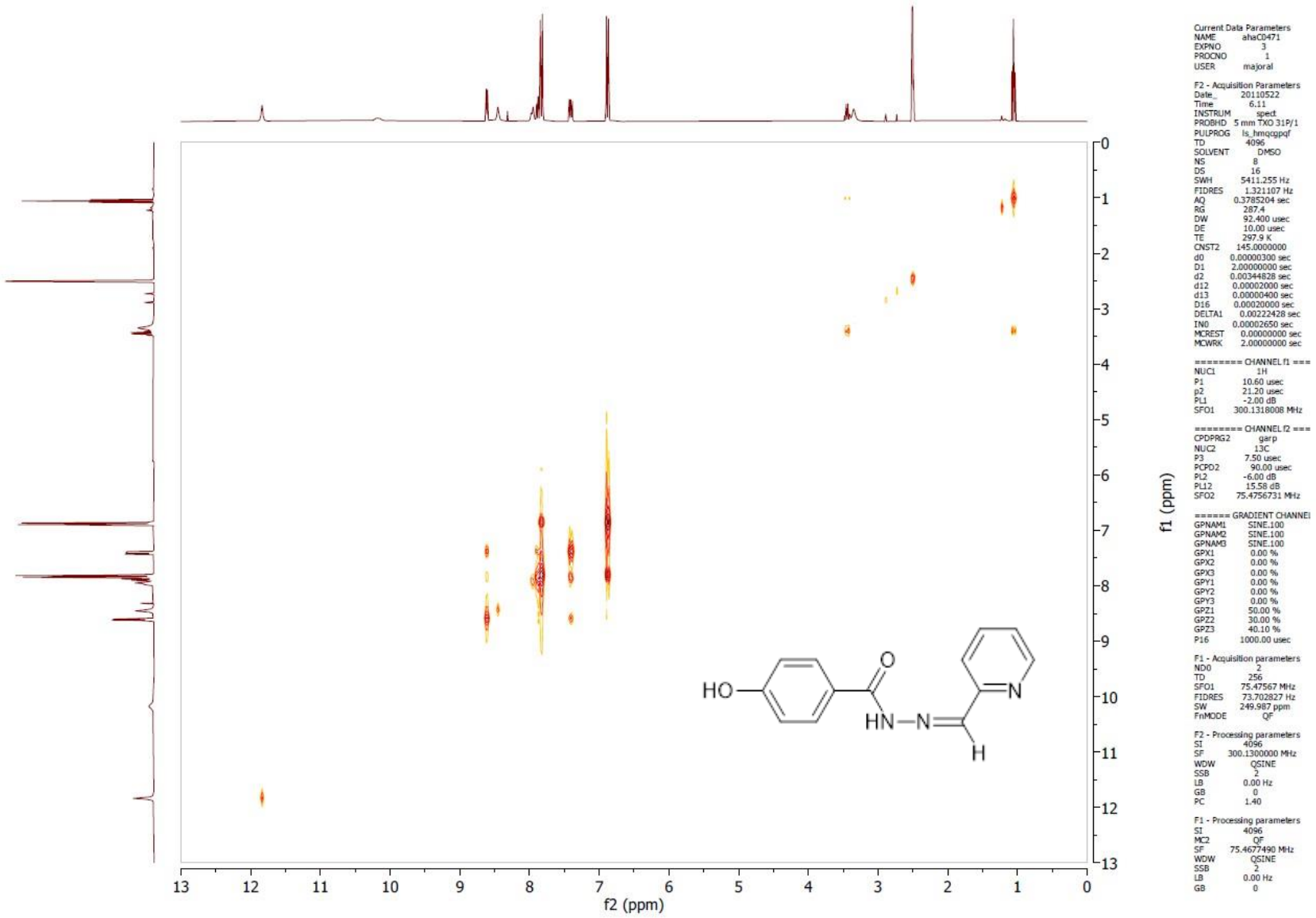
F2 - Acquisition Parameters
Date_ 20110521
Time 14.18
INSTRUM spect
PROBHD 5 mm TXO 31P/1
PULPROG ls_zg60
TD 32768
SOLVENT DMSO
NS 8
DS 2
SWH 5411.255 Hz
FIDRES 0.165138 Hz
AQ 3.0278132 sec
RG 228.1
DW 92.400 usec
DE 10.00 usec
TE 298.0 K
D1 30.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ==
NUC1 1H
P1 10.60 usec
PL1 -2.00 dB
SFO1 300.1318008 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0

PC 1.40

^{1}H COSY NMR of Compound 5



Current Data Parameters
NAME ahaC0471
EXPNO 3
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20110522
Time 6.11
INSTRUM spect
PROBHD 5 mm TXO 31P/1
PULPROG ls_hmqcgpqf
TD 4096
SOLVENT DMSO
NS 8
DS 16
SWH 5411.255 Hz
FIDRES 1.321107 Hz
AQ 0.3785204 sec
RG 287.4
DW 92.400 usec
DE 10.00 usec
TE 297.9 K
CNST2 145.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000400 sec
D16 0.00020000 sec
DELTA1 0.00222428 sec
IN0 0.00002650 sec
MCREST 0.00000000 sec
MCWRK 2.00000000 sec

======== CHANNEL f1 ===
NUC1 1H
P1 10.60 usec
p2 21.20 usec
PL1 -2.00 dB
SFO1 300.1318008 MHz

======== CHANNEL f2 ===
CPDPRG2 garp
NUC2 13C
P3 7.50 usec
PCPD2 90.00 usec
PL2 -6.00 dB
PL12 15.58 dB
SFO2 75.4756731 MHz

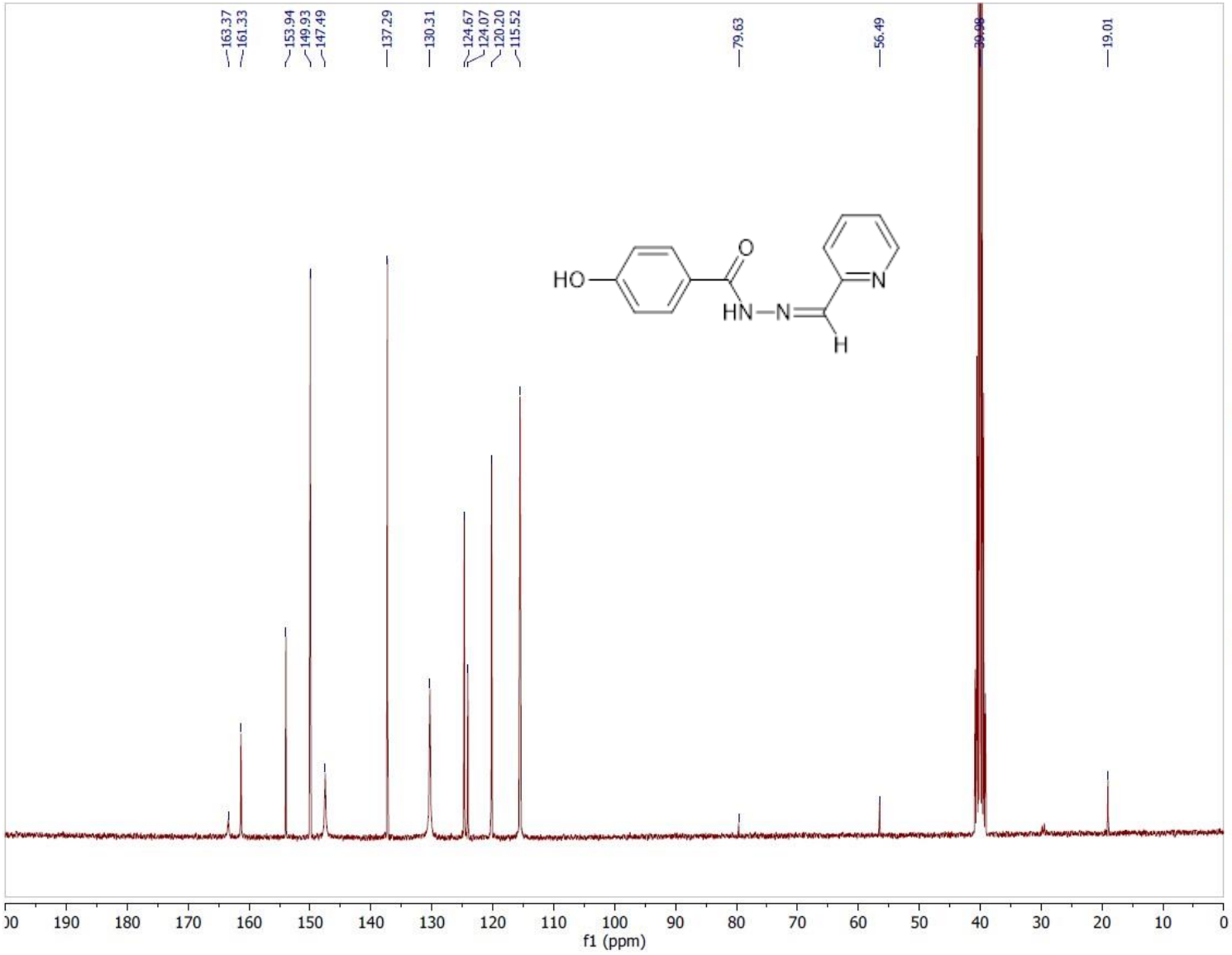
====== GRADIENT CHANNEL
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 75.47567 MHz
FIDRES 73.702827 Hz
SW 249.987 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 300.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 QF
SF 75.4677490 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

$^{13}C\{^{1}H\}$ NMR of Compound 5



Current Data Parameters
NAME ahaC0471
EXPNO 2
PROCNO 1
USER majoral

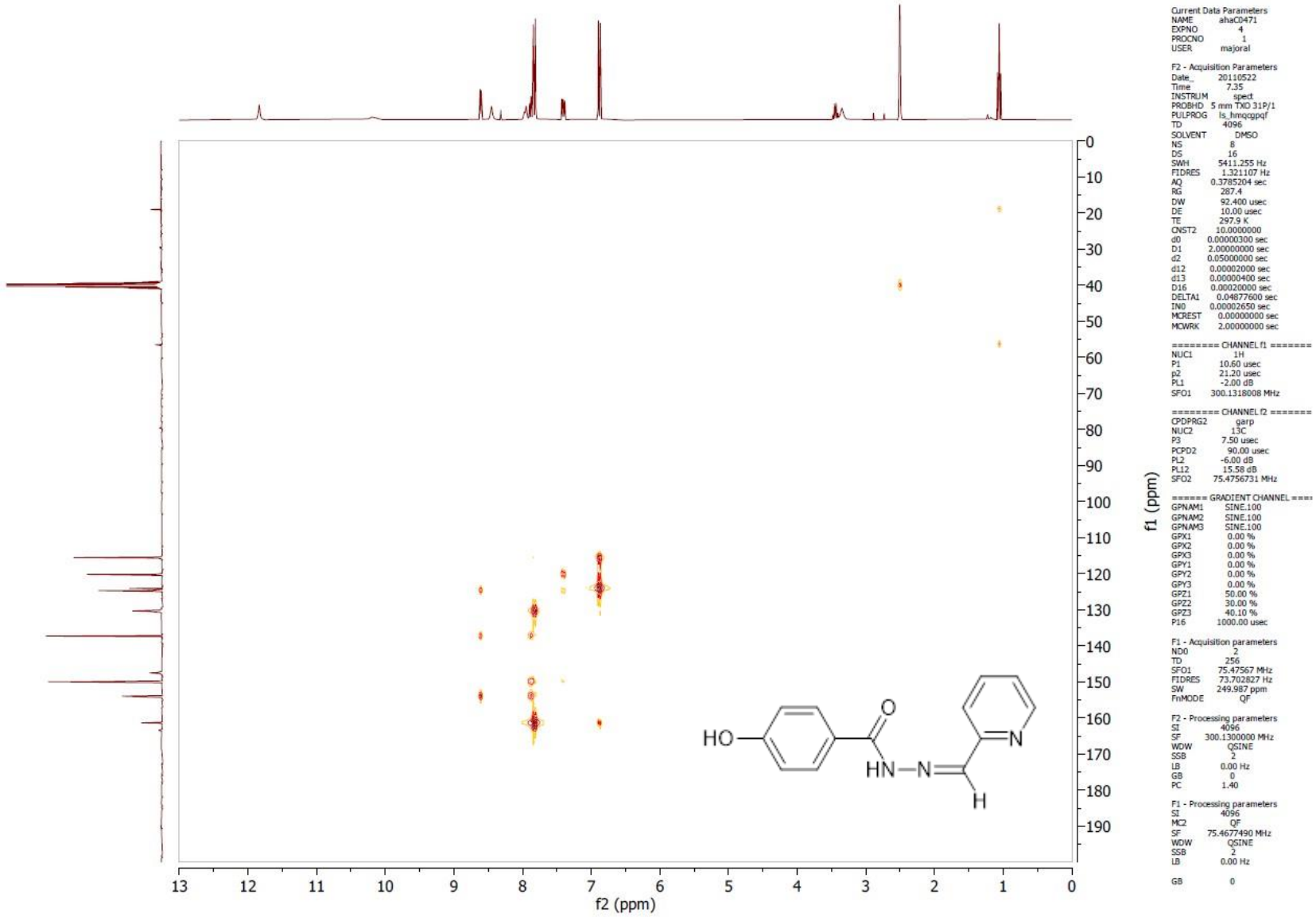
F2 - Acquisition Parameters
Date_ 20110522
Time 6.09
INSTRUM spect
PROBHD 5 mm TXO 31P/1
PULPROG ls_zg60dc
TD 32768
SOLVENT DMSO
NS 30000
DS 4
SWH 19607.844 Hz
FIDRES 0.598384 Hz
AQ 0.8356340 sec
RG 23170.5
DW 25.500 usec
DE 10.00 usec
TE 297.9 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 -6.00 dB
SFO1 75.4760505 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 16.66 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

^{13}C HMBC NMR of Compound 5



Current Data Parameters
NAME ahaCD471
EXPNO 4
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20110522
Time 7.35
INSTRUM spect
PROBHD 5 mm TXO 31P/1
PULPROG ls_hmqcgpqf
TD 4096
SOLVENT DMSO
NS 8
DS 16
SWH 5411.255 Hz
FIDRES 1.321107 Hz
AQ 0.3785204 sec
RG 287.4
DW 92.400 usec
DE 10.00 usec
TE 297.9 K
CNST2 10.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d2 0.05000000 sec
d12 0.00002000 sec
d13 0.00000400 sec
D16 0.00020000 sec
DELTA1 0.04877600 sec
IN0 0.00002650 sec
MCREST 0.00000000 sec
MCWRK 2.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.60 usec
p2 21.20 usec
PL1 -2.00 dB
SFO1 300.1318008 MHz

======== CHANNEL f2 ========
CPDPRG2 garp
NUC2 13C
P3 7.50 usec
PCPD2 90.00 usec
PL2 -6.00 dB
PL12 15.58 dB
SFO2 75.4756731 MHz

====== GRADIENT CHANNEL ====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

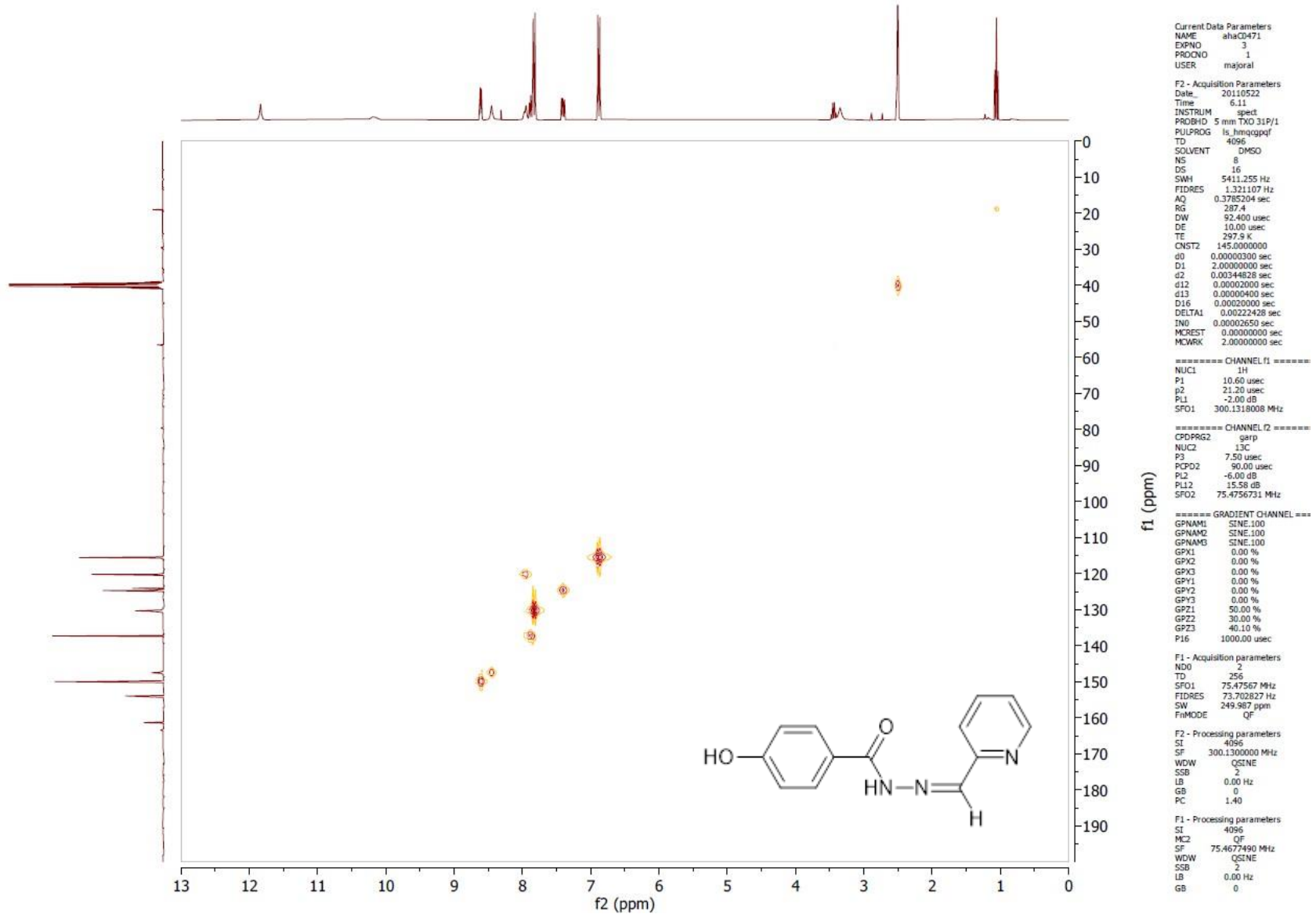
F1 - Acquisition parameters
ND0 2
TD 256
SFO1 75.47567 MHz
FIDRES 73.702827 Hz
SW 249.987 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 300.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 QF
SF 75.4677490 MHz
WDW QSINE
SSB 2
LB 0.00 Hz

GB 0

^{13}C HMQC NMR of Compound 5



Current Data Parameters
NAME ahaCD471
EXPNO 3
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20110522
Time 6.11
INSTRUM spect
PROBHD 5 mm TXO 31P/1
PULPROG ls_hmqcgpqf
TD 4096
SOLVENT DMSO
NS 8
DS 16
SWH 5411.255 Hz
FIDRES 1.321107 Hz
AQ 0.3785204 sec
RG 287.4
DW 92.400 usec
DE 10.00 usec
TE 297.9 K
CNST2 145.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000400 sec
D16 0.00020000 sec
DELTA1 0.00222428 sec
IN0 0.00002650 sec
MCREST 0.00000000 sec
MCWRK 2.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.60 usec
p2 21.20 usec
PL1 -2.00 dB
SFO1 300.1318008 MHz

======== CHANNEL f2 ========
CPDPRG2 garp
NUC2 13C
P3 7.50 usec
PCPD2 90.00 usec
PL2 -6.00 dB
PL12 15.58 dB
SFO2 75.4756731 MHz

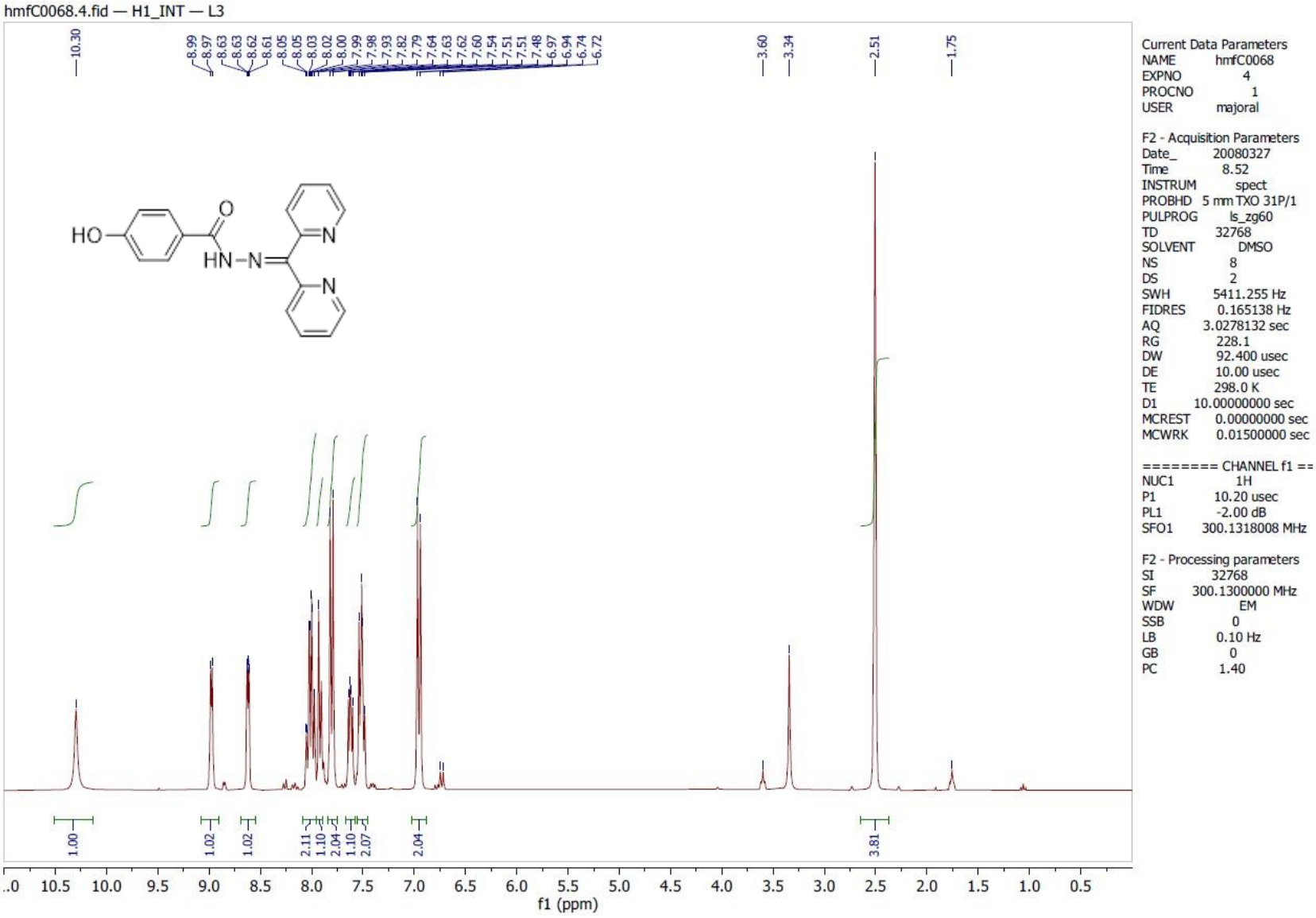
====== GRADIENT CHANNEL ===
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 75.47567 MHz
FIDRES 73.702827 Hz
SW 249.987 ppm
FnMODE QF

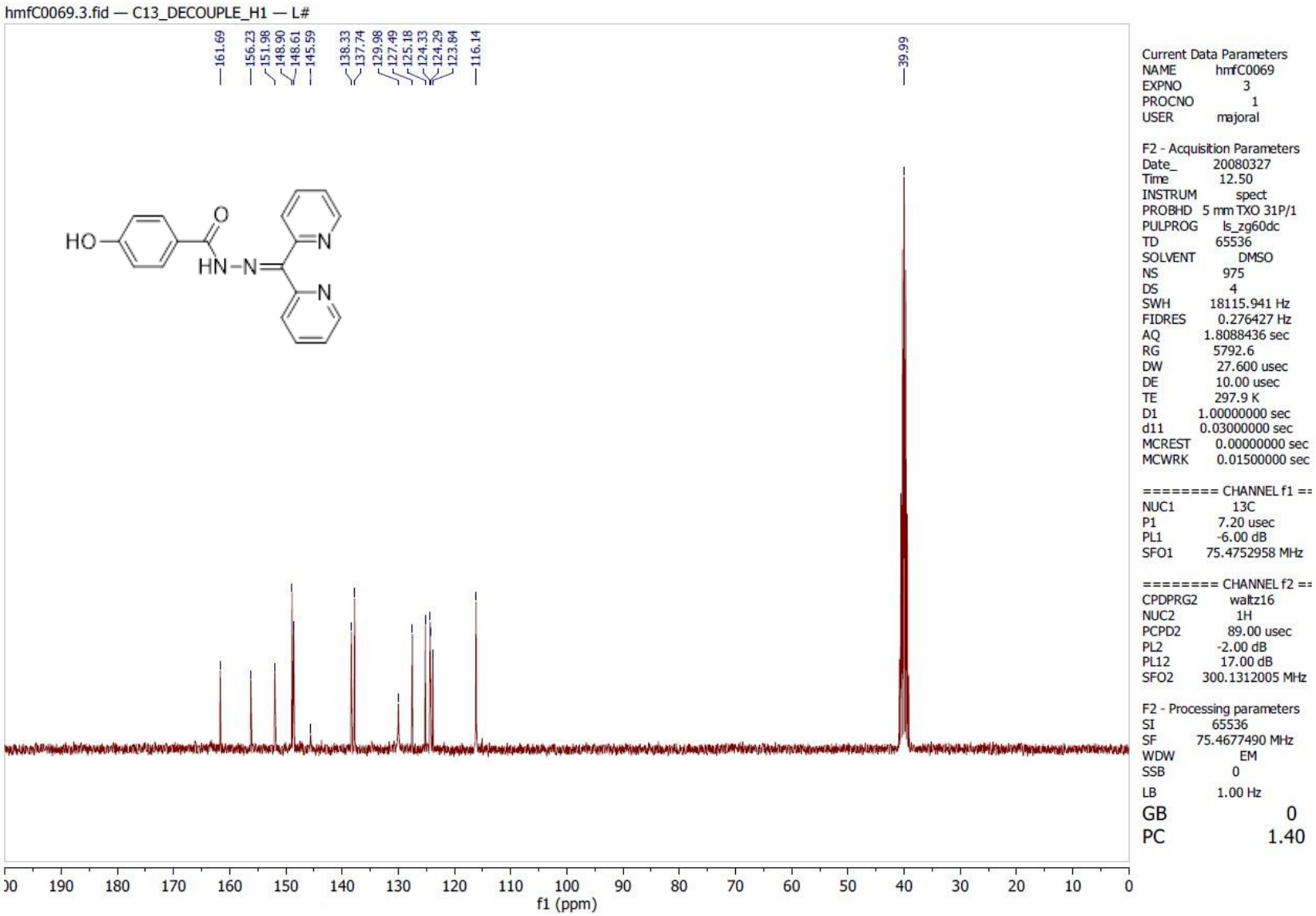
F2 - Processing parameters
SI 4096
SF 300.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 QF
SF 75.4677490 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

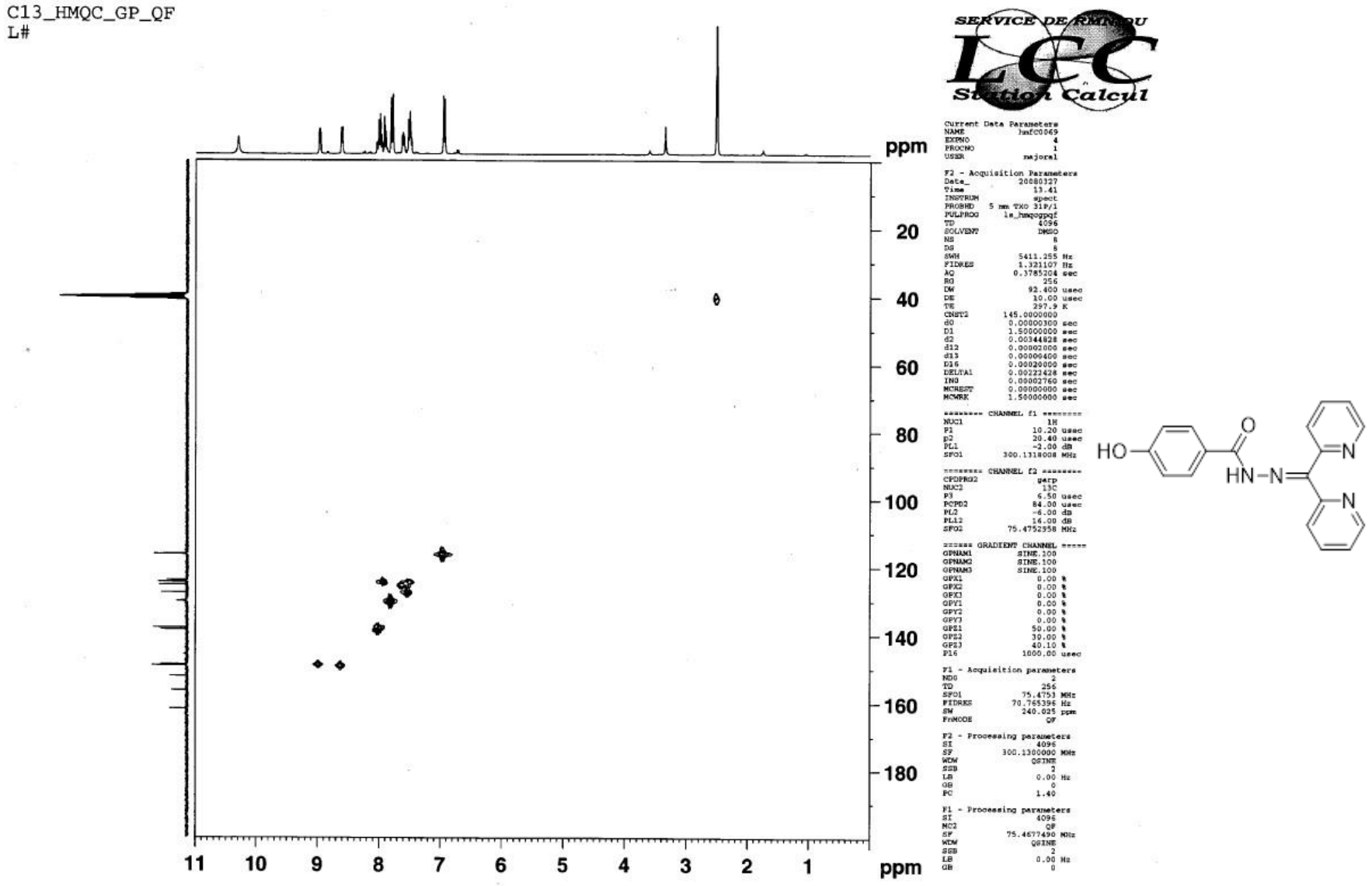
^{1}H NMR of Compound 6



$^{13}C\{^{1}H\}$ NMR of Compound 6

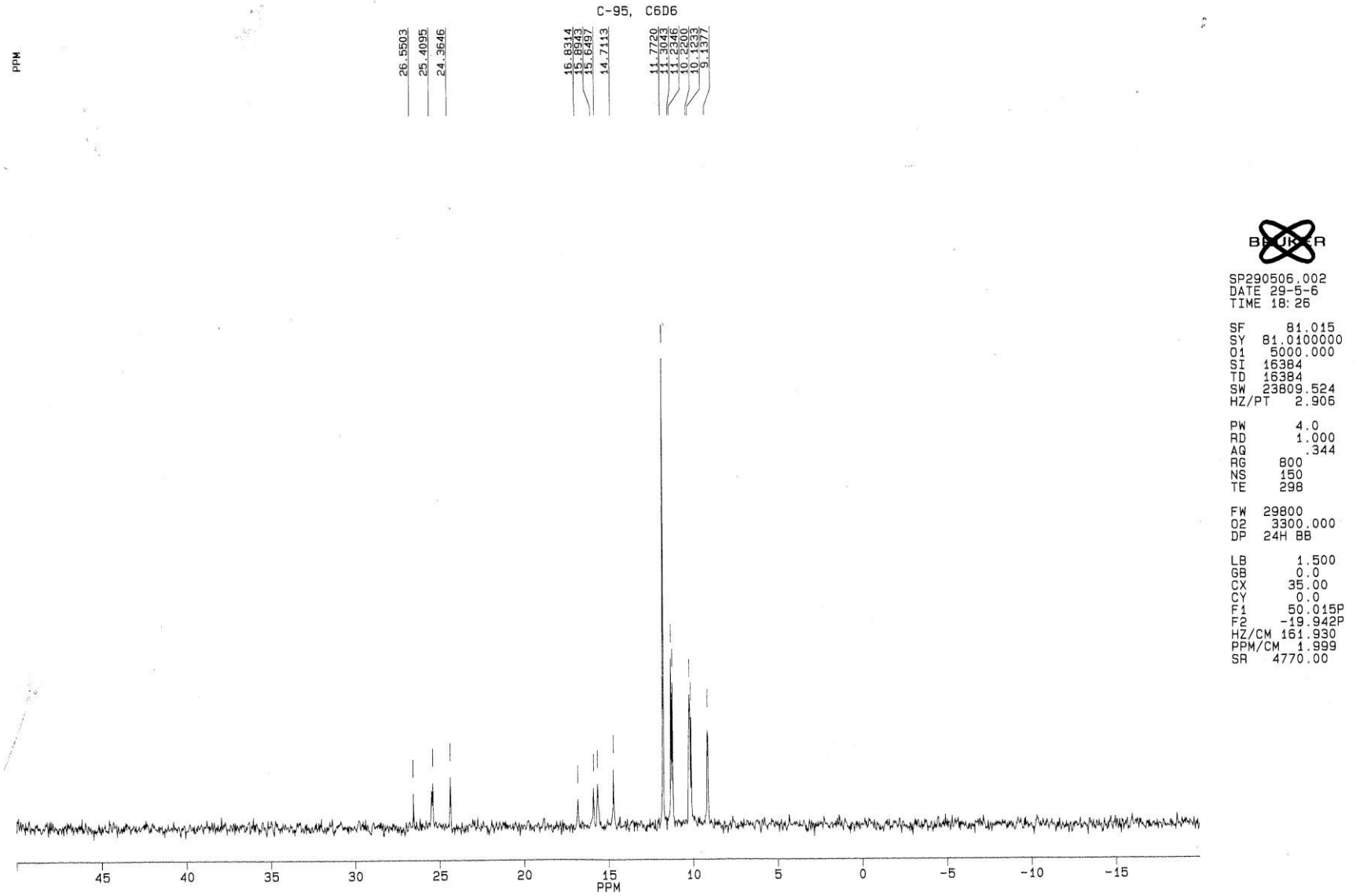


^{13}C HMQC of Compound 6



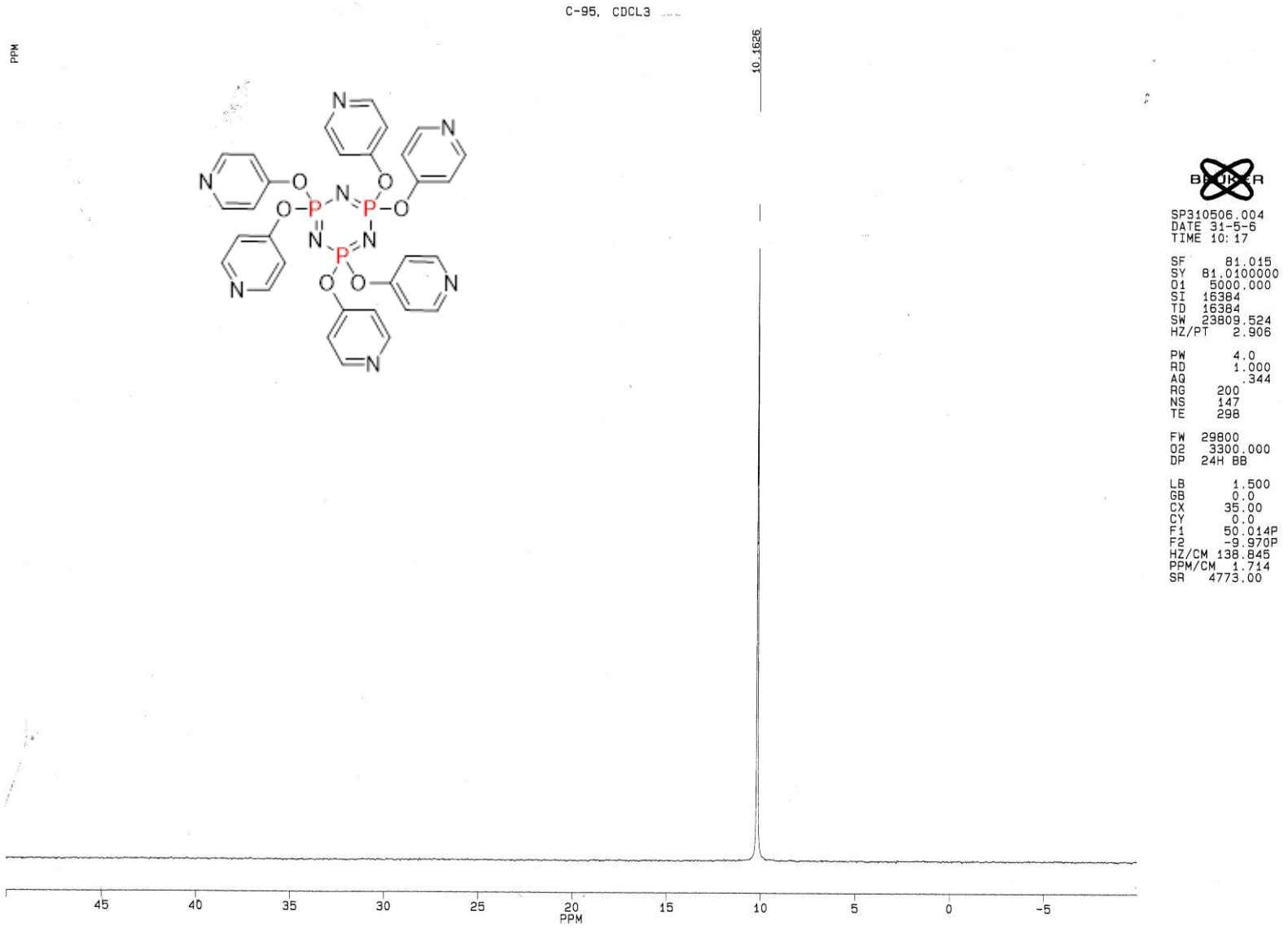
$^{31}P\{^{1}H\}$ NMR during the course of the synthesis of 1-G_0

$^{31}P\{^{1}$


C-95, C6D6
PPM
26.5503
25.4095
24.3646
16.8314
15.8943
15.6497
14.7113
11.7720
11.3643
11.2346
10.2200
10.1233
9.1377
45
40
35
30
25
20
15
10
5
0
-5
-10
-15
PPM
SP290506.002
DATE 29-5-6
TIME 18:26
SF 81.015
SY 81.0100000
O1 5000.000
SI 16384
TD 16384
SW 23809.524
HZ/PT 2.906
PW 4.0
RD 1.000
AQ .344
RG 800
NS 150
TE 298
FW 29800
O2 3300.000
DP 24H BB
LB 1.500
GB 0.0
CX 35.00
CY 0.0
F1 50.015P
F2 -19.942P
HZ/CM 161.930
PPM/CM 1.999
SR 4770.00

$^{31}P\{^{1}H\}$ NMR of 1-G_0

^{31}P {^{1}

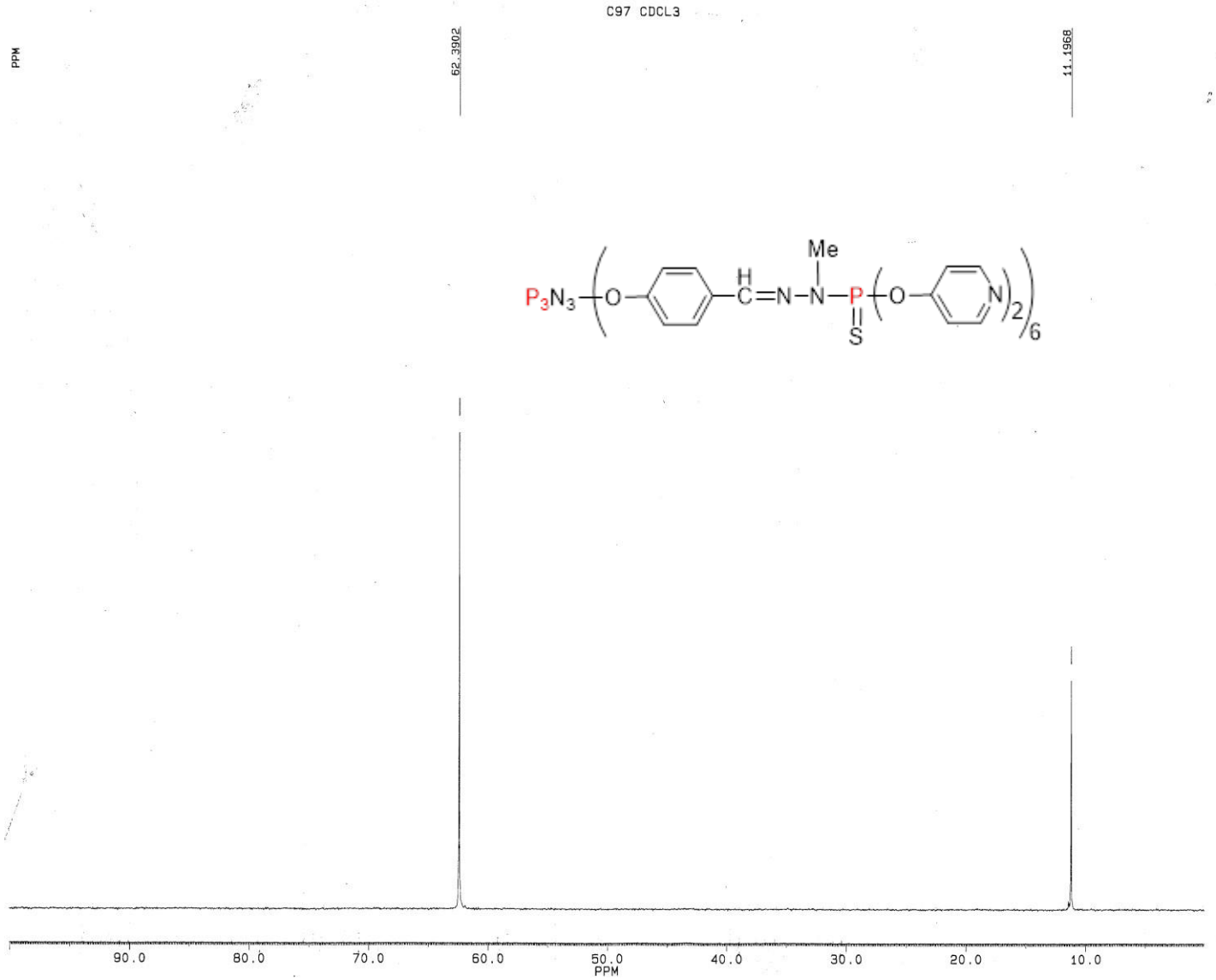


SP310506.004
DATE 31-5-6
TIME 10:17

SF	81.015
SY	81.0100000
O1	5000.000
SI	16384
TD	16384
SW	23809.524
HZ/PT	2.906
PW	4.0
RD	1.000
AQ	.344
RG	200
NS	147
TE	298
FW	29800
O2	3300.000
DP	24H BB
LB	1.500
GB	0.0
CX	35.00
CY	0.0
F1	50.014P
F2	-9.970P
HZ/CM	138.845
PPM/CM	1.714
SR	4773.00

$^{31}P\{^{1}H\}$ NMR of dendrimer 1-G_1

$^{31}P\{^{1}$



SP010606.002
DATE 1-6-6
TIME 10:59

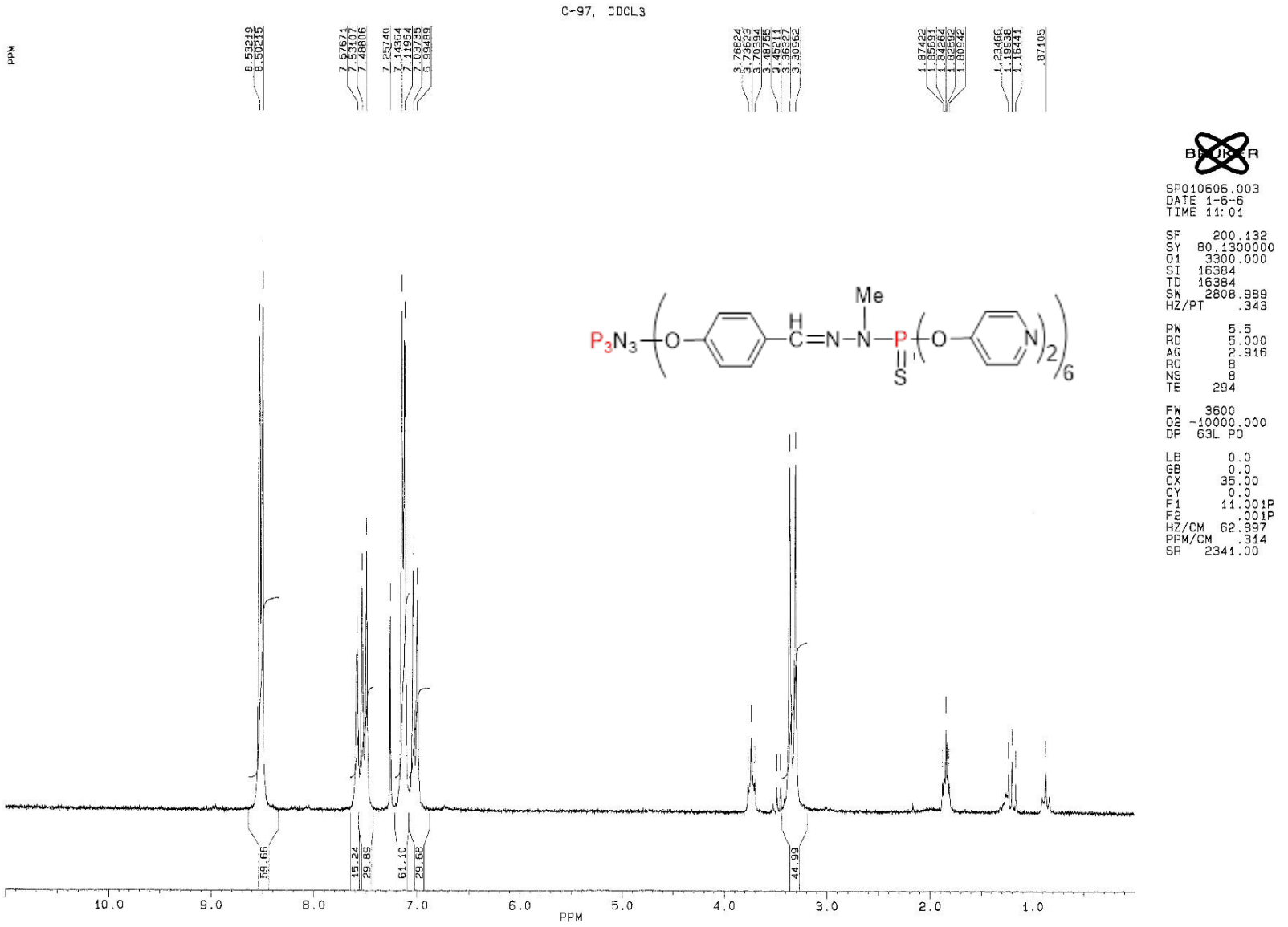
SF 81.015
SY 81.0100000
O1 5000.000
SI 16384
TD 16384
SW 23809.524
HZ/PT 2.906

PW 4.0
RD 1.000
AQ .344
RG 800
NS 137
TE 298

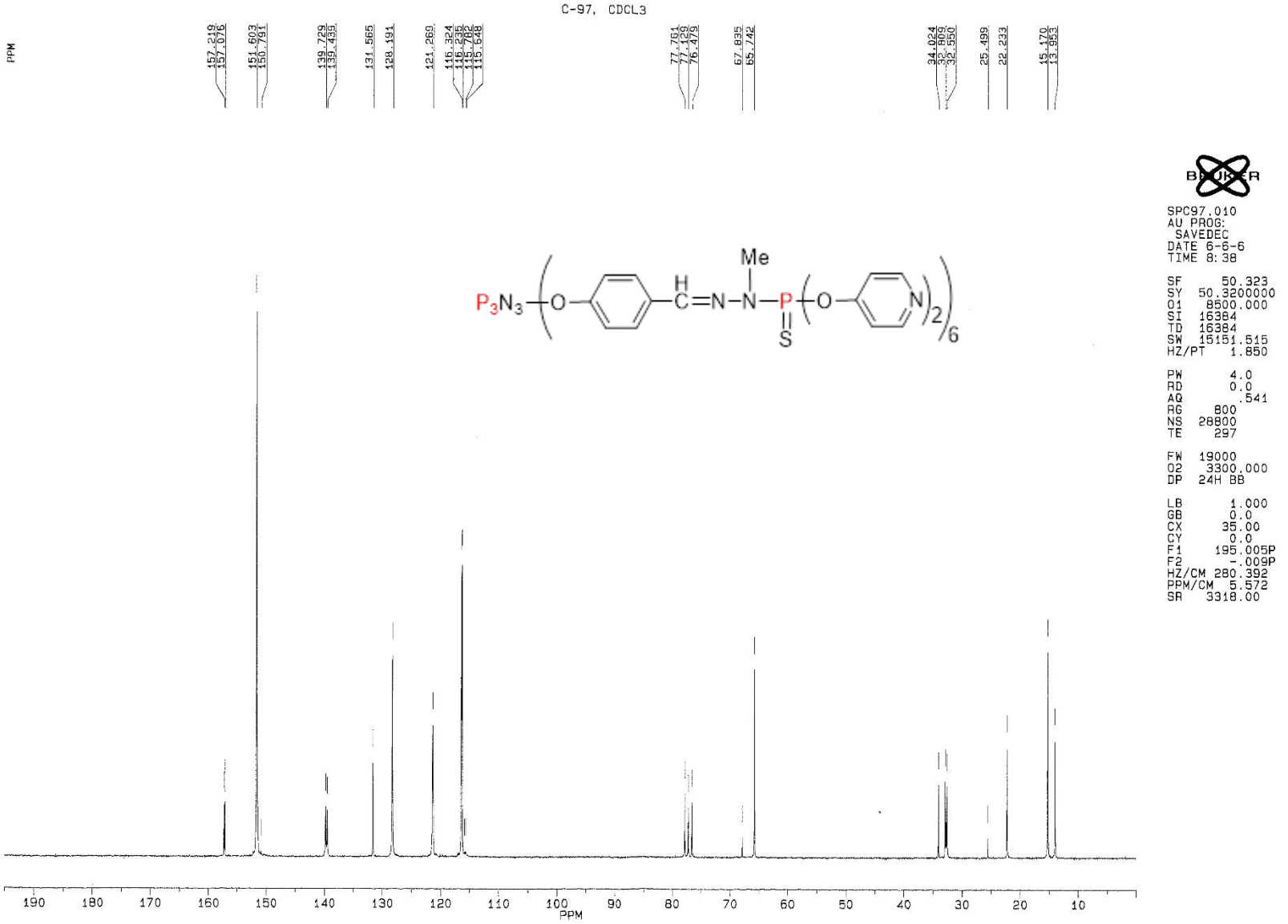
FW 29800
O2 3300.000
DP 24H BB

LB 1.500
GB 0.0
CX 35.00
CY 0.0
F1 100.024P
F2 .040P
HZ/CM 231.435
PPM/CM 2.857
SR 4773.00

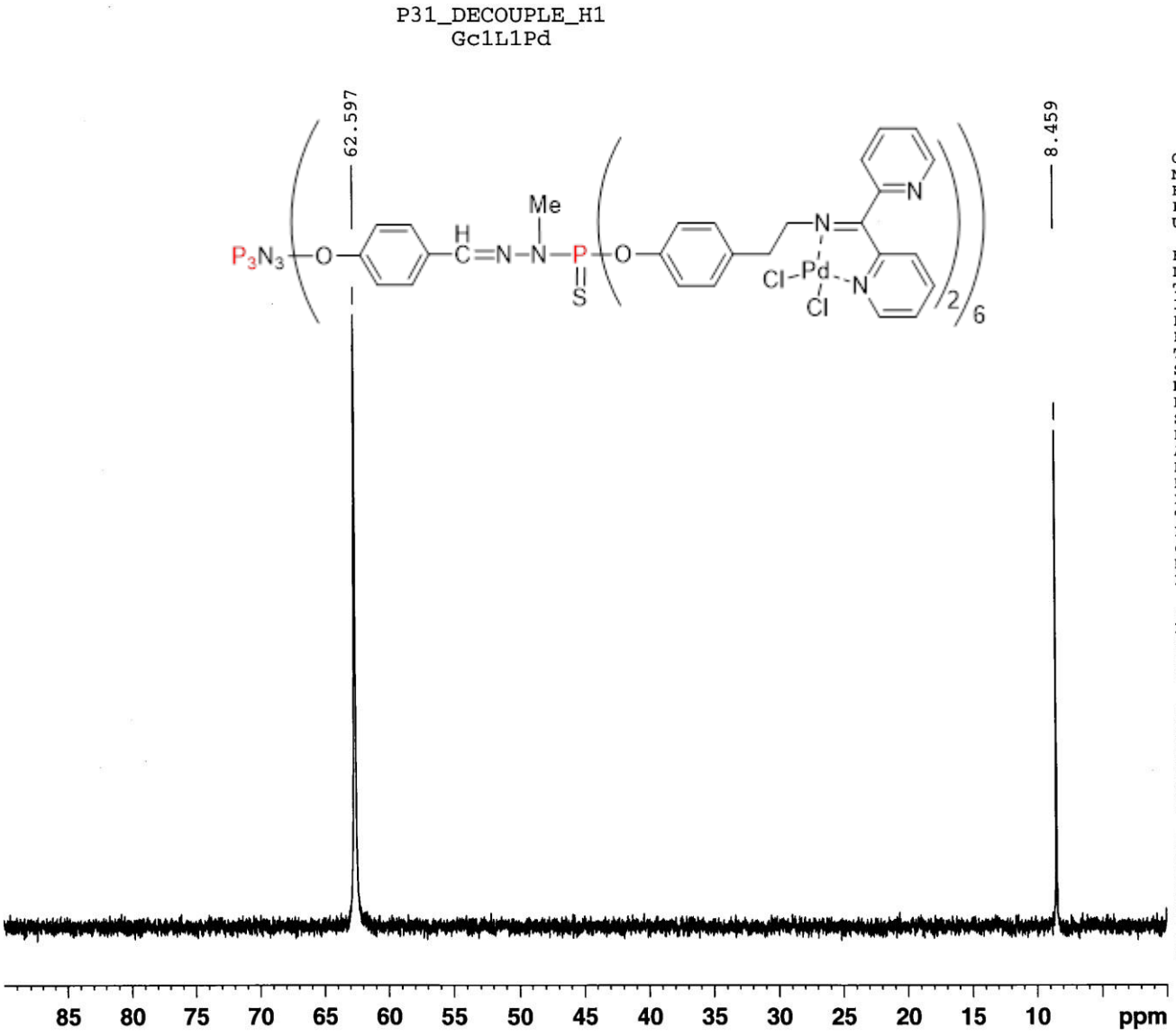
^{1}H NMR of dendrimer 1-G$_1$


C-97, CDCL3
PPM
8.53619
8.50215
7.57671
7.53107
7.48806
7.25740
7.14364
7.11954
7.03735
6.99489
3.76824
3.73623
3.70394
3.48755
3.45211
3.36327
3.30962
1.87422
1.85691
1.84264
1.82524
1.80942
1.23466
1.19938
1.16441
.87105
Me
H
C=N-N-P
O
N
S
2
6
59.66
15.24
29.89
61.10
29.68
44.99
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
PPM
SP010606.003
DATE 1-6-6
TIME 11:01
SF 200.132
SY 80.1300000
O1 3300.000
SI 16384
TD 16384
SW 2808.989
HZ/PT .343
PW 5.5
RD 5.000
AQ 2.916
RG 8
NS 8
TE 294
FW 3600
O2 -10000.000
DP 63L PO
LB 0.0
GB 0.0
CX 35.00
CY 0.0
F1 11.001P
F2 .001P
HZ/CM 62.897
PPM/CM .314
SR 2341.00

^{13}C {^{1}H} NMR of dendrimer 1-G_1



$^{31}P\{^{1}H\}$ NMR of dendrimer 3-G_1-Pd_{12}



SERVICE DE RMN DU
LCC
Station Calcul

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Current Data Parameters
NAME                 hmfC0096
EXPNO                       3
PROCNO                      1
USER                 majoral

F2 - Acquisition Parameters
Date_               20080429
Time                   18.56
INSTRUM                spect
PROBHD     5 mm TXO 31P/1
PULPROG           ls_zg60dc
TD                     65536
SOLVENT                DMSO
NS                       400
DS                         4
SWH                36496.352 Hz
FIDRES             0.556890 Hz
AQ                 0.8978932 sec
RG                   41285.1
DW                    13.700 usec
DE                    10.00 usec
TE                    297.9 K
D1                1.00000000 sec
d11               0.03000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     31P
P1                      8.80 usec
PL1                     0.00 dB
SFO1           121.4948510 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                 89.00 usec
PL2                   -2.00 dB
PL12                  17.00 dB
SFO2           300.1312005 MHz

F2 - Processing parameters
SI                     65536
SF             121.4948510 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```
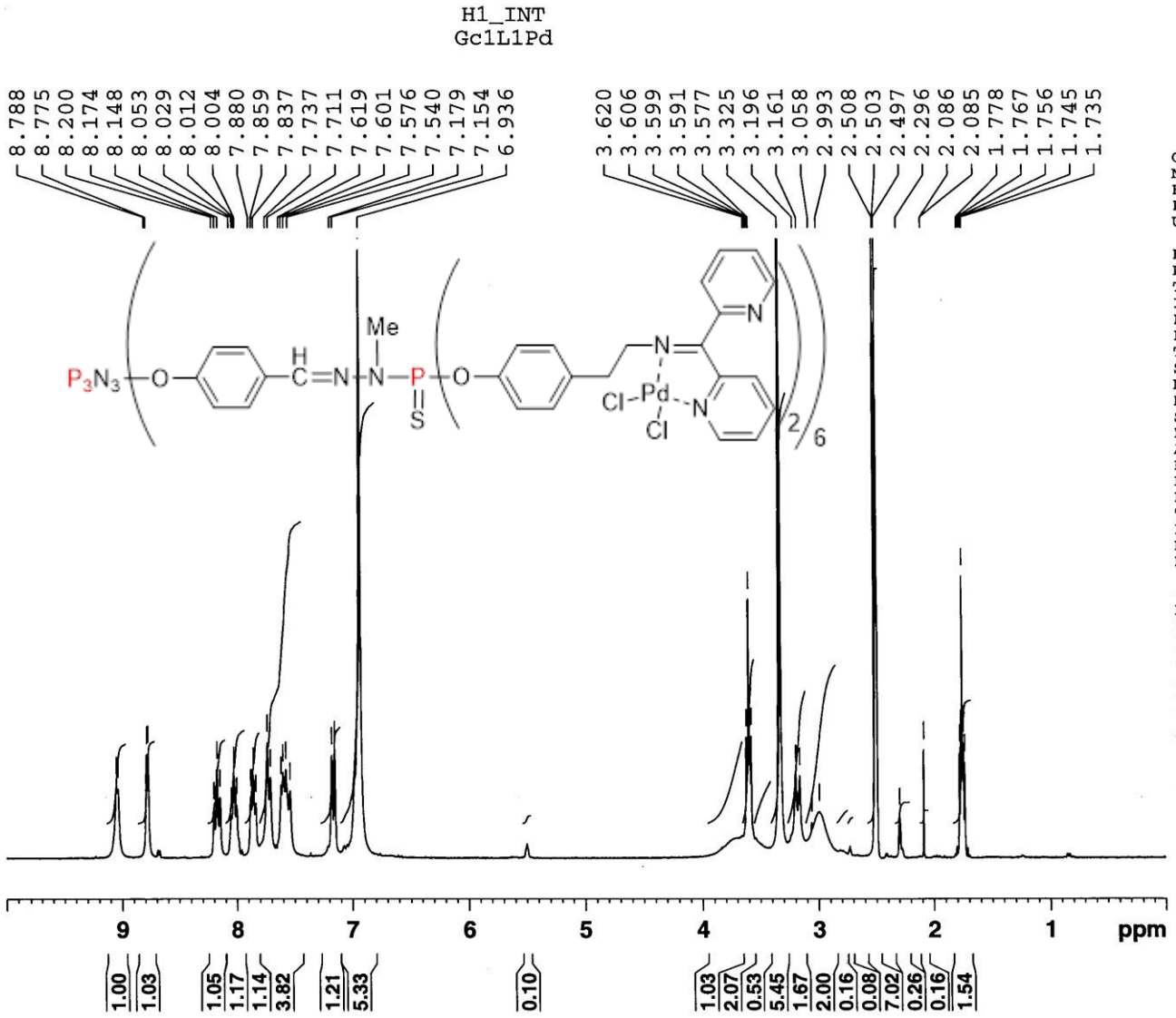

^{1}H NMR of dendrimer 3-G_1-Pd_{12}

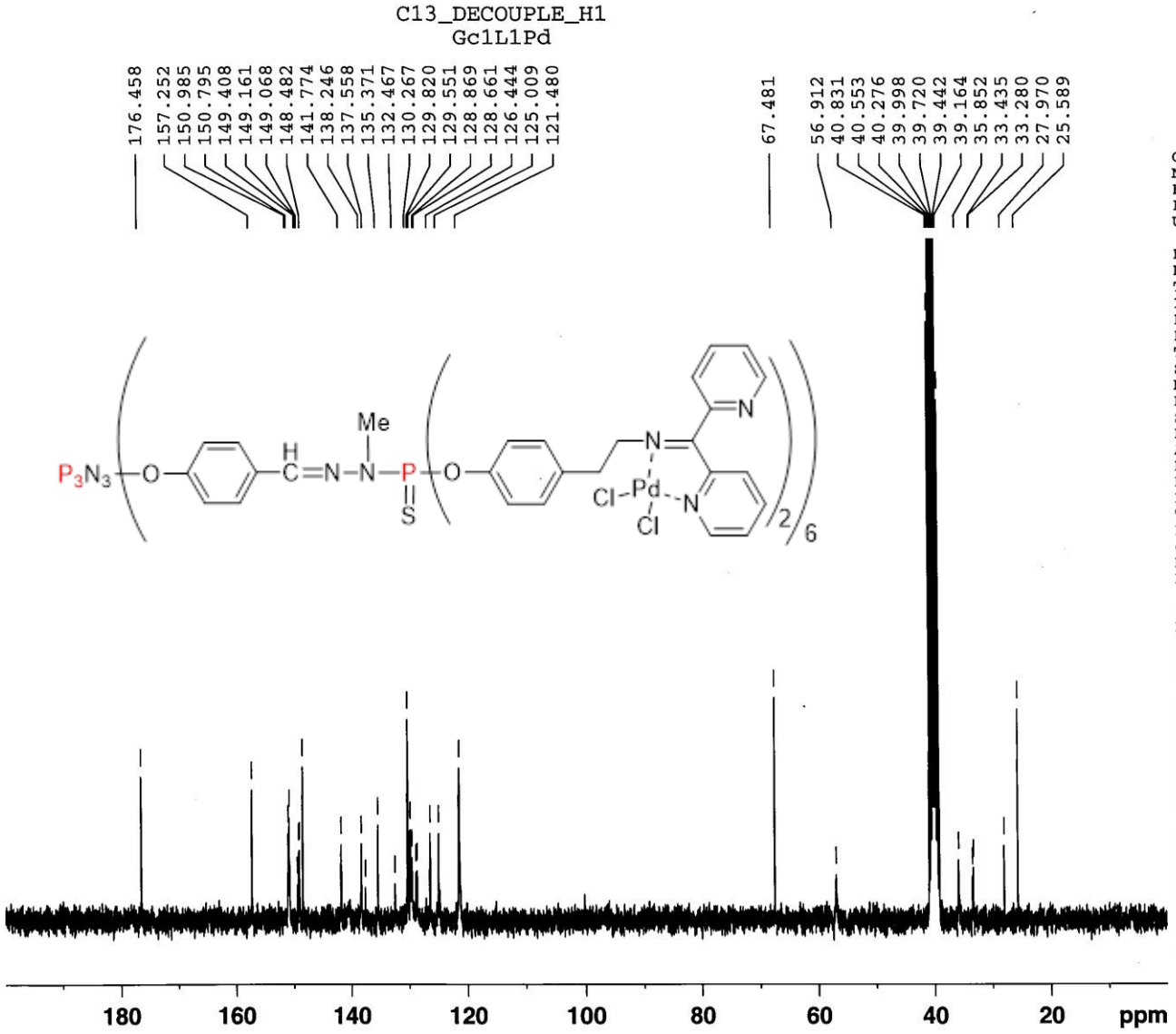


SERVICE DE RMN DU LCC Station Calcul

```
Current Data Parameters
NAME                  hmfC0096
EXPNO                        2
PROCNO                       1
USER                  majoral

F2 - Acquisition Parameters
Date_                 20080429
Time                     18.42
INSTRUM                  spect
PROBHD    5 mm TXO 31P/1
PULPROG                ls_zg60
TD                        32768
SOLVENT                   DMSO
NS                           16
DS                            2
SWH                  5411.255 Hz
FIDRES               0.165138 Hz
AQ                 3.0278132 sec
RG                        228.1
DW                    92.400 usec
DE                    10.00 usec
TE                    298.0 K
D1                10.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                         1H
P1                    10.20 usec
PL1                   -2.00 dB
SFO1              300.1318008 MHz

F2 - Processing parameters
SI                        32768
SF                300.1300000 MHz
WDW                         EM
SSB                          0
LB                    0.10 Hz
GB                           0
PC                        1.40
```

$^{13}C\{^{1}H\}$ NMR of dendrimer 3-G_1-Pd_{12}

13

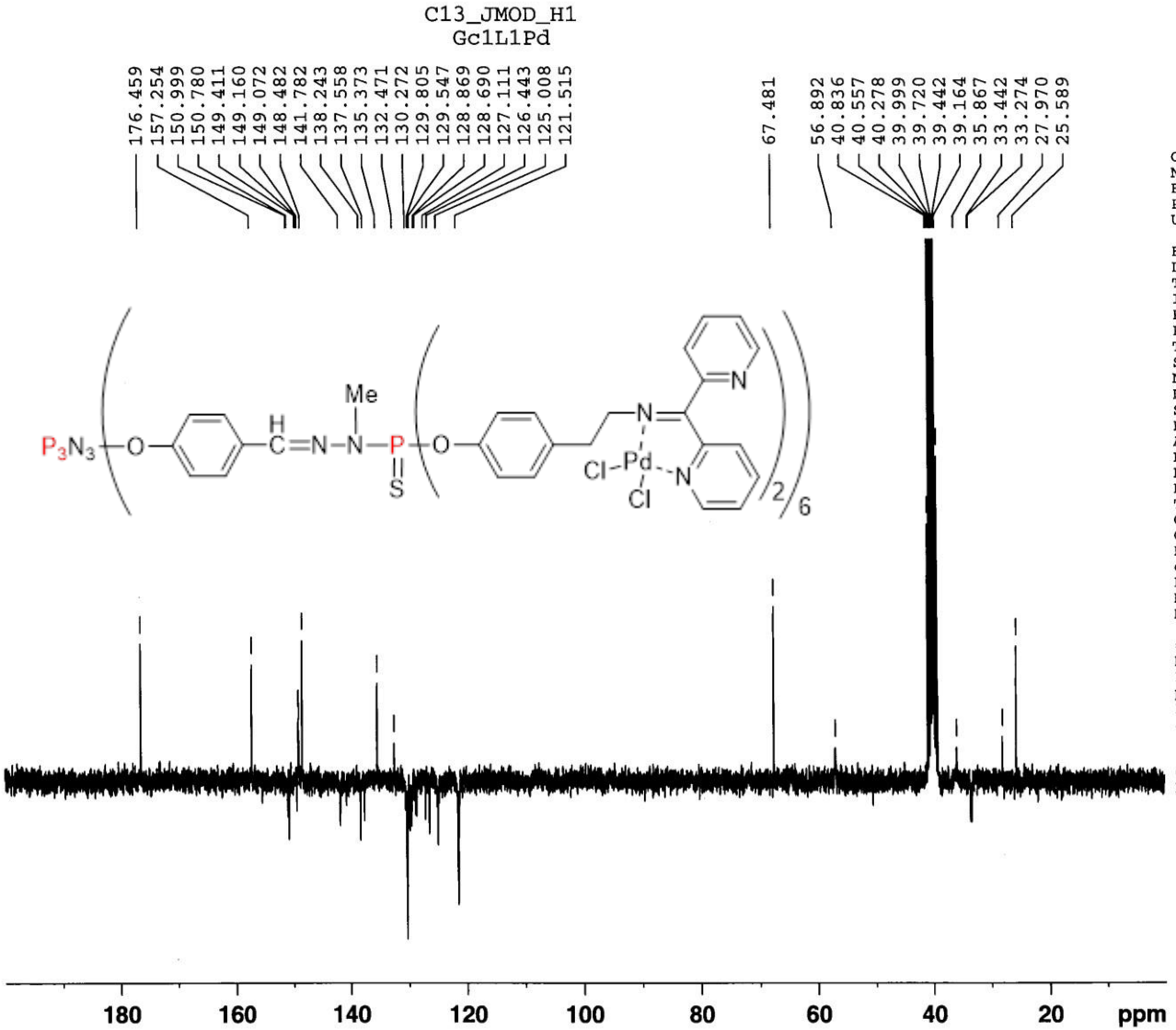


SERVICE DE RMN DU
LCC
Station Calcul

```
Current Data Parameters
NAME                  hmfC0096
EXPNO                        4
PROCNO                       1
USER                   majoral

F2 - Acquisition Parameters
Date_                 20080430
Time                      0.04
INSTRUM                  spect
PROBHD     5 mm TXO 31P/1
PULPROG              ls_zg60dc
TD                       65536
SOLVENT                  DMSO
NS                       6400
DS                          4
SWH                  18115.941 Hz
FIDRES                0.276427 Hz
AQ                    1.8088436 sec
RG                       26008
DW                      27.600 usec
DE                      10.00 usec
TE                        297.9 K
D1                   1.00000000 sec
d11                  0.03000000 sec
MCREST               0.00000000 sec
MCWRK                0.01500000 sec

======== CHANNEL f1 ========
NUC1                        13C
P1                         7.20 usec
PL1                       -6.00 dB
SFO1                 75.4752958 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     89.00 usec
PL2                       -2.00 dB
PL12                      17.00 dB
SFO2                300.1312005 MHz

F2 - Processing parameters
SI                       65536
SF                  75.4677490 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

^{13}C JMOD NMR of dendrimer 3-G_1-Pd_{12}

13

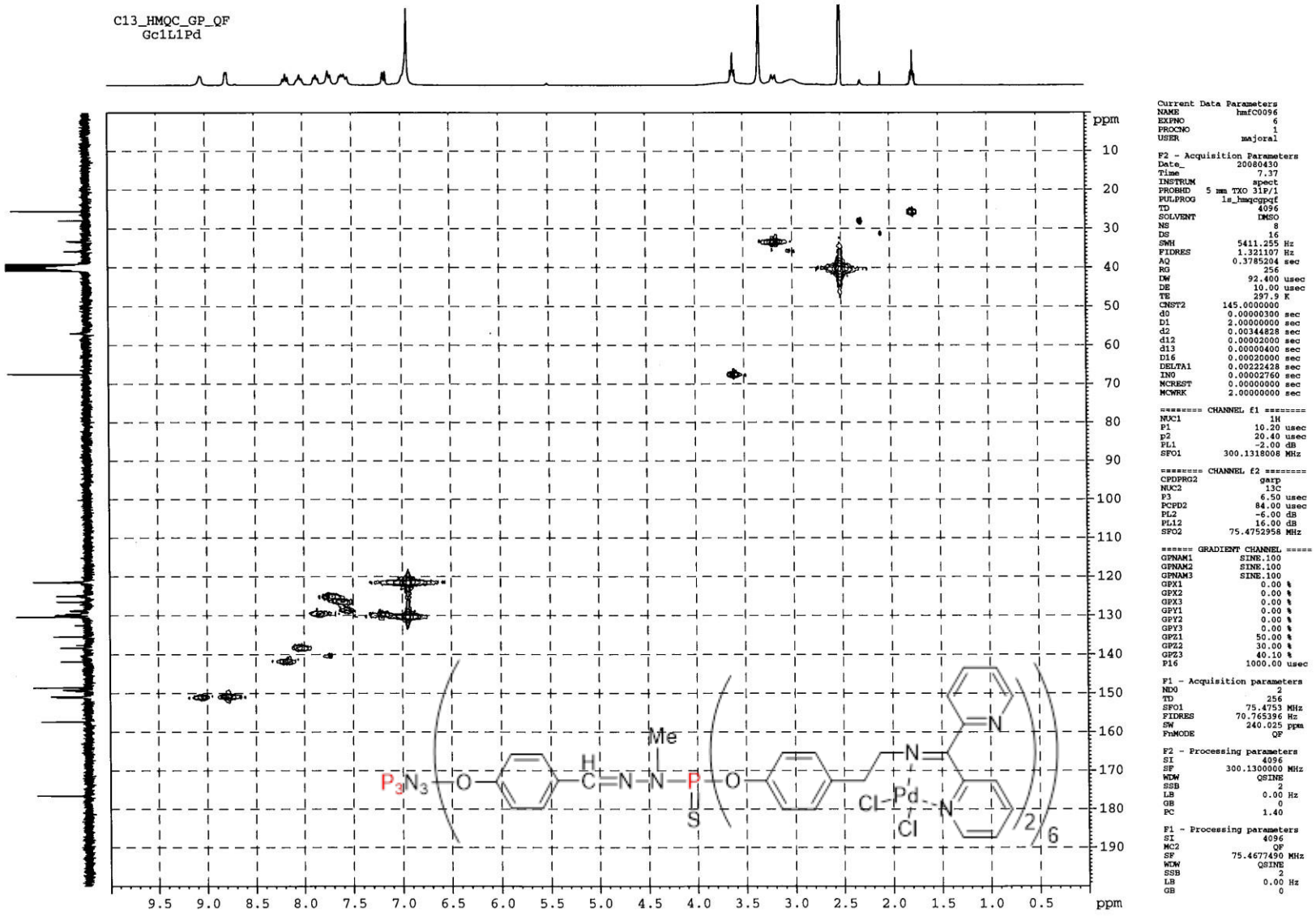


SERVICE DE RMN DU
LCC
Station Calcul

```
Current Data Parameters
NAME                 hmfC0096
EXPNO                       5
PROCNO                      1
USER                 majoral

F2 - Acquisition Parameters
Date_               20080430
Time                    7.35
INSTRUM                spect
PROBHD    5 mm TXO 31P/1
PULPROG              ls_jmod
TD                     65536
SOLVENT                DMSO
NS                      7000
DS                         4
SWH              18115.941 Hz
FIDRES            0.276427 Hz
AQ                1.8088436 sec
RG                     29193
DW                    27.600 usec
DE                    10.00 usec
TE                    297.9 K
CNST2            145.0000000
CNST11             1.0000000
D1                 2.00000000 sec
d20                0.00689655 sec
DELTA              0.00000917 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     7.20 usec
p2                    14.40 usec
PL1                   -6.00 dB
SFO1             75.4752958 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                 89.00 usec
PL2                   -2.00 dB
PL12                  17.00 dB
SFO2            300.1312005 MHz

F2 - Processing parameters
SI                     65536
SF               75.4677490 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

^{13}C HMQC NMR of dendrimer 3-G_1-Pd_{12}

13



Current Data Parameters
NAME hmfC0096
EXPNO 6
PROCNO 1
USER majoral

F2 - Acquisition Parameters
Date_ 20080430
Time 7.37
INSTRUM spect
PROBHD 5 mm TXO 31P/1
PULPROG 1s_hmqcgpqf
TD 4096
SOLVENT DMSO
NS 8
DS 16
SWH 5411.255 Hz
FIDRES 1.321107 Hz
AQ 0.3785204 sec
RG 256
DW 92.400 usec
DE 10.00 usec
TE 297.9 K
CNST2 145.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000400 sec
D16 0.00020000 sec
DELTA1 0.00222428 sec
IN0 0.00002760 sec
MCREST 0.00000000 sec
MCWRK 2.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.20 usec
p2 20.40 usec
PL1 -2.00 dB
SFO1 300.1318008 MHz

======== CHANNEL f2 ========
CPDPRG2 garp
NUC2 13C
P3 6.50 usec
PCPD2 84.00 usec
PL2 -6.00 dB
PL12 16.00 dB
SFO2 75.4752958 MHz

====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

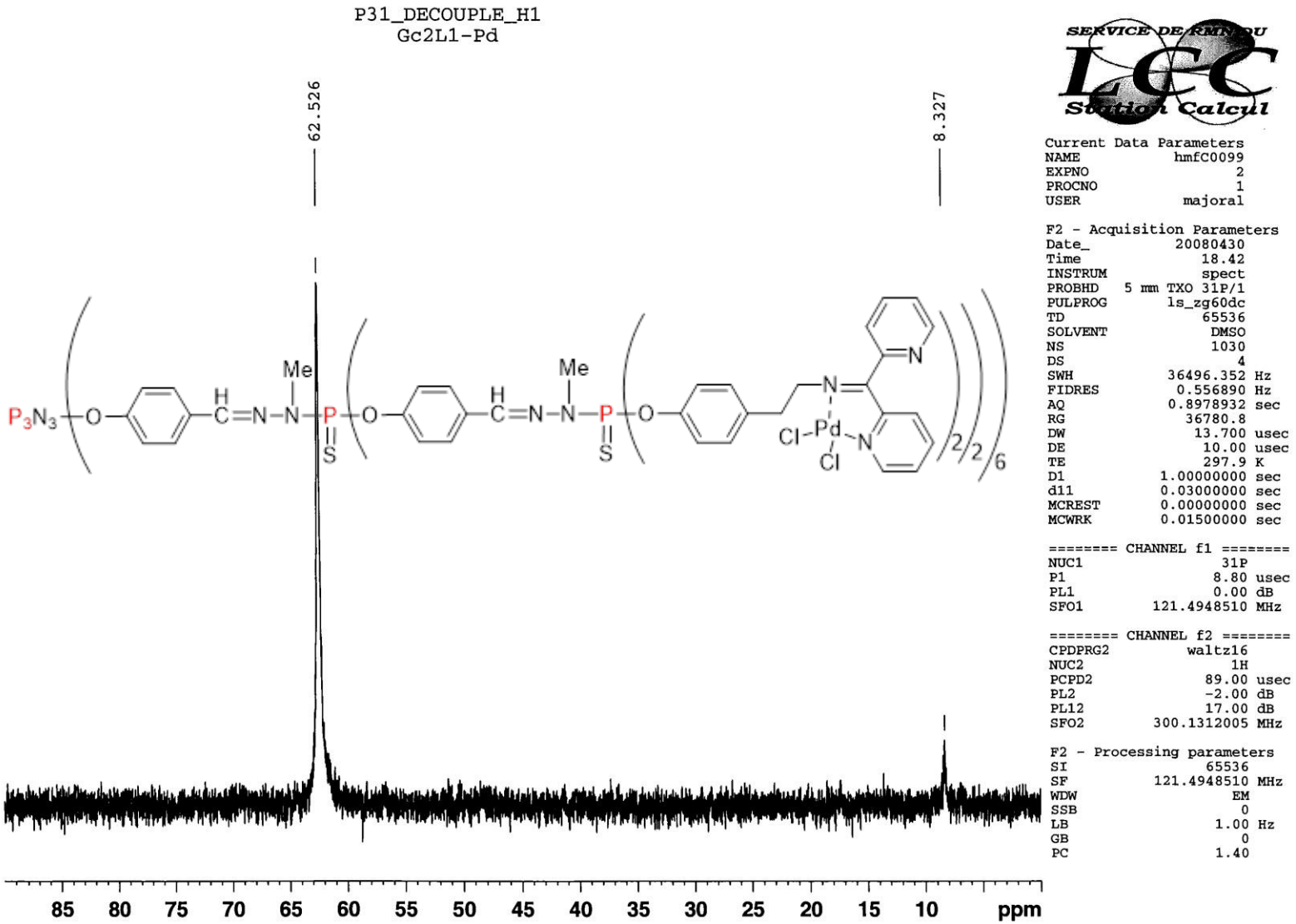
F1 - Acquisition parameters
ND0 2
TD 256
SFO1 75.4753 MHz
FIDRES 70.765396 Hz
SW 240.025 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 300.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 QF
SF 75.4677490 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

{^{1}H} NMR of dendrimer 3

^{31}P -G$_2$-Pd$_{24}$

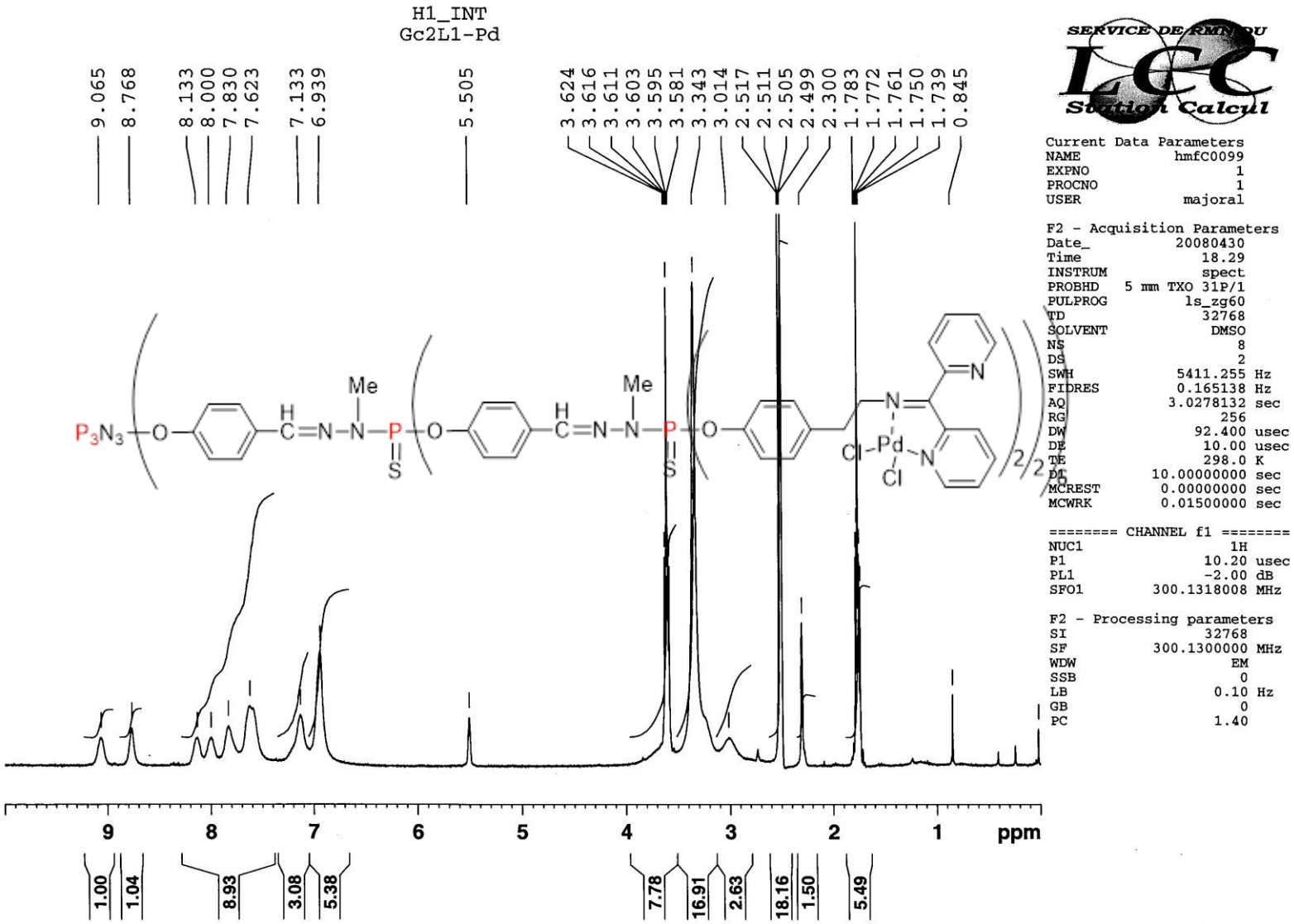


SERVICE DE RMN DU LCC Station Calcul

```
Current Data Parameters
NAME                 hmfC0099
EXPNO                       2
PROCNO                      1
USER                 majoral

F2 - Acquisition Parameters
Date_               20080430
Time                   18.42
INSTRUM                spect
PROBHD     5 mm TXO 31P/1
PULPROG           ls_zg60dc
TD                     65536
SOLVENT                DMSO
NS                      1030
DS                         4
SWH                36496.352 Hz
FIDRES             0.556890 Hz
AQ                 0.8978932 sec
RG                   36780.8
DW                    13.700 usec
DE                    10.00 usec
TE                    297.9 K
D1                 1.00000000 sec
d11                0.03000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      31P
P1                       8.80 usec
PL1                      0.00 dB
SFO1             121.4948510 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                 89.00 usec
PL2                     -2.00 dB
PL12                    17.00 dB
SFO2             300.1312005 MHz

F2 - Processing parameters
SI                     65536
SF               121.4948510 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

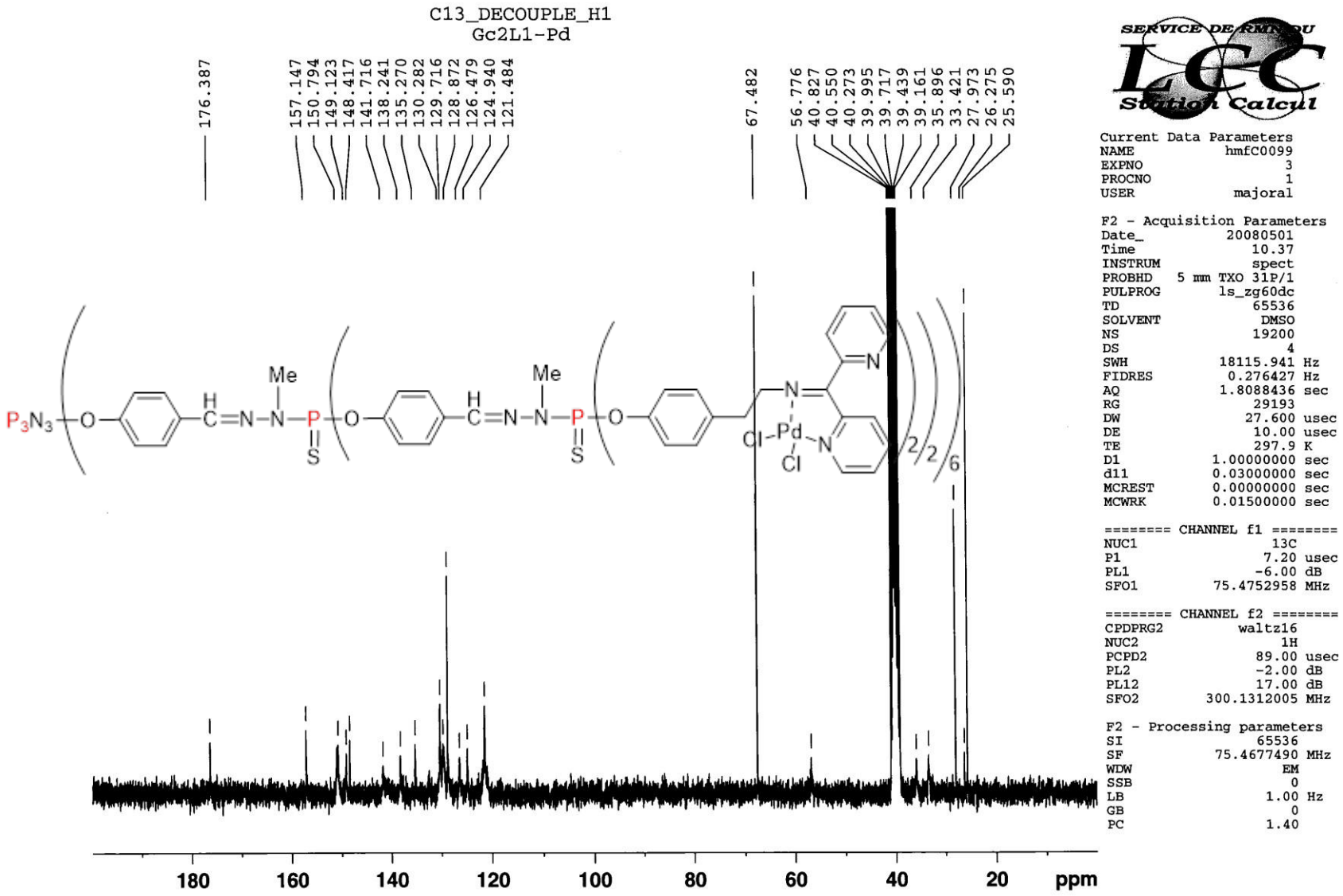
^{1}H NMR of dendrimer 3-G_2-Pd_{24}

{^{1}H} NMR of dendrimer 3



$_{13}$C -G$_2$-Pd$_{24}$

{^{1}H} NMR of dendrimer 3

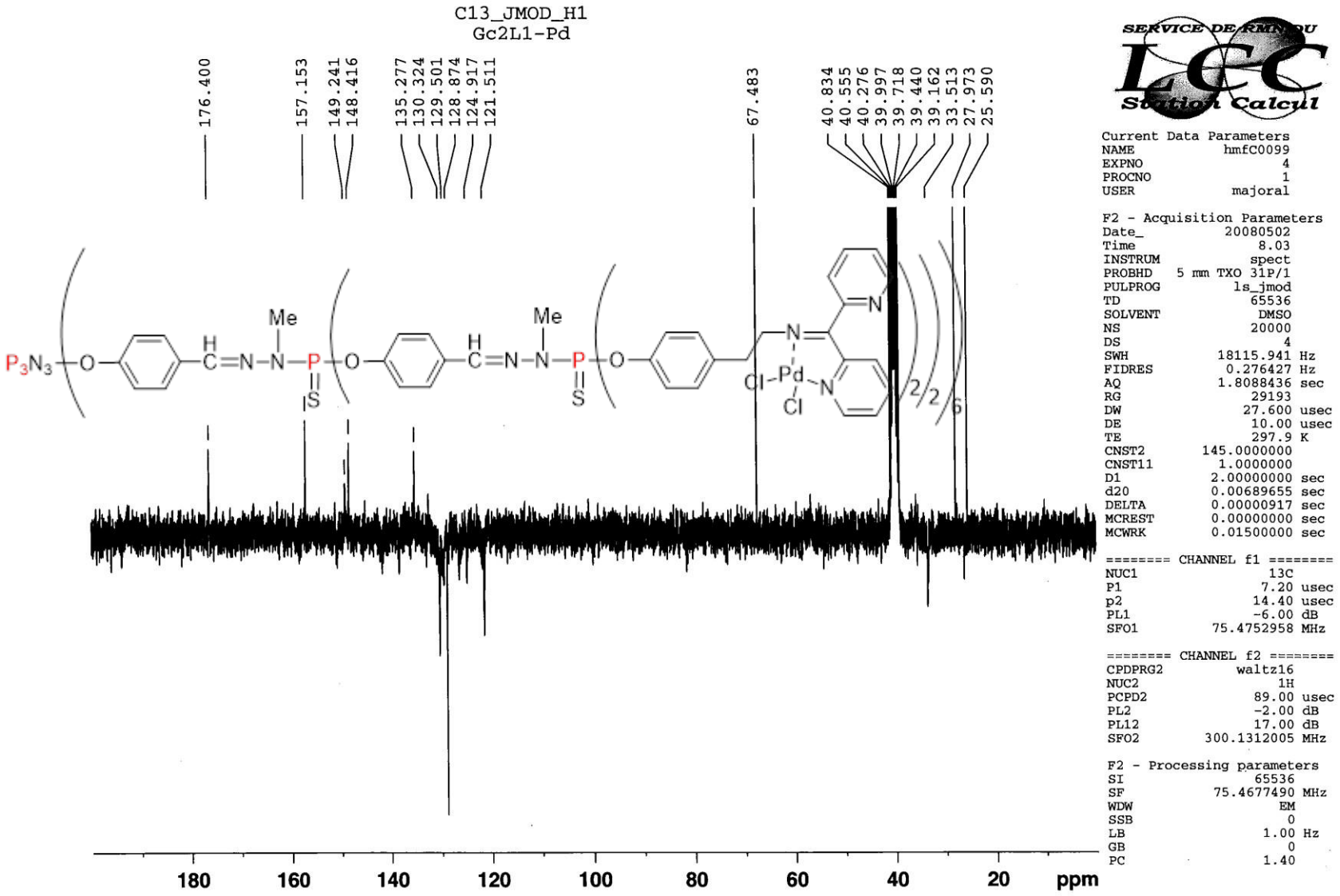


SERVICE DE RMN DU LCC Station Calcul

```
Current Data Parameters
NAME                  hmfC0099
EXPNO                        3
PROCNO                       1
USER                  majoral

F2 - Acquisition Parameters
Date_                20080501
Time                    10.37
INSTRUM                 spect
PROBHD    5 mm TXO 31P/1
PULPROG              ls_zg60dc
TD                       65536
SOLVENT                  DMSO
NS                       19200
DS                           4
SWH                18115.941 Hz
FIDRES              0.276427 Hz
AQ                  1.8088436 sec
RG                       29193
DW                    27.600 usec
DE                    10.00 usec
TE                    297.9 K
D1                  1.00000000 sec
d11                 0.03000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                     7.20 usec
PL1                   -6.00 dB
SFO1               75.4752958 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                 89.00 usec
PL2                   -2.00 dB
PL12                  17.00 dB
SFO2              300.1312005 MHz

F2 - Processing parameters
SI                       65536
SF                 75.4677490 MHz
WDW                         EM
SSB                          0
LB                    1.00 Hz
GB                           0
PC                    1.40
```

^{13}C JMOD NMR of dendrimer 3-G_2-Pd_{24}

{^{1}H} NMR of dendrimer 3

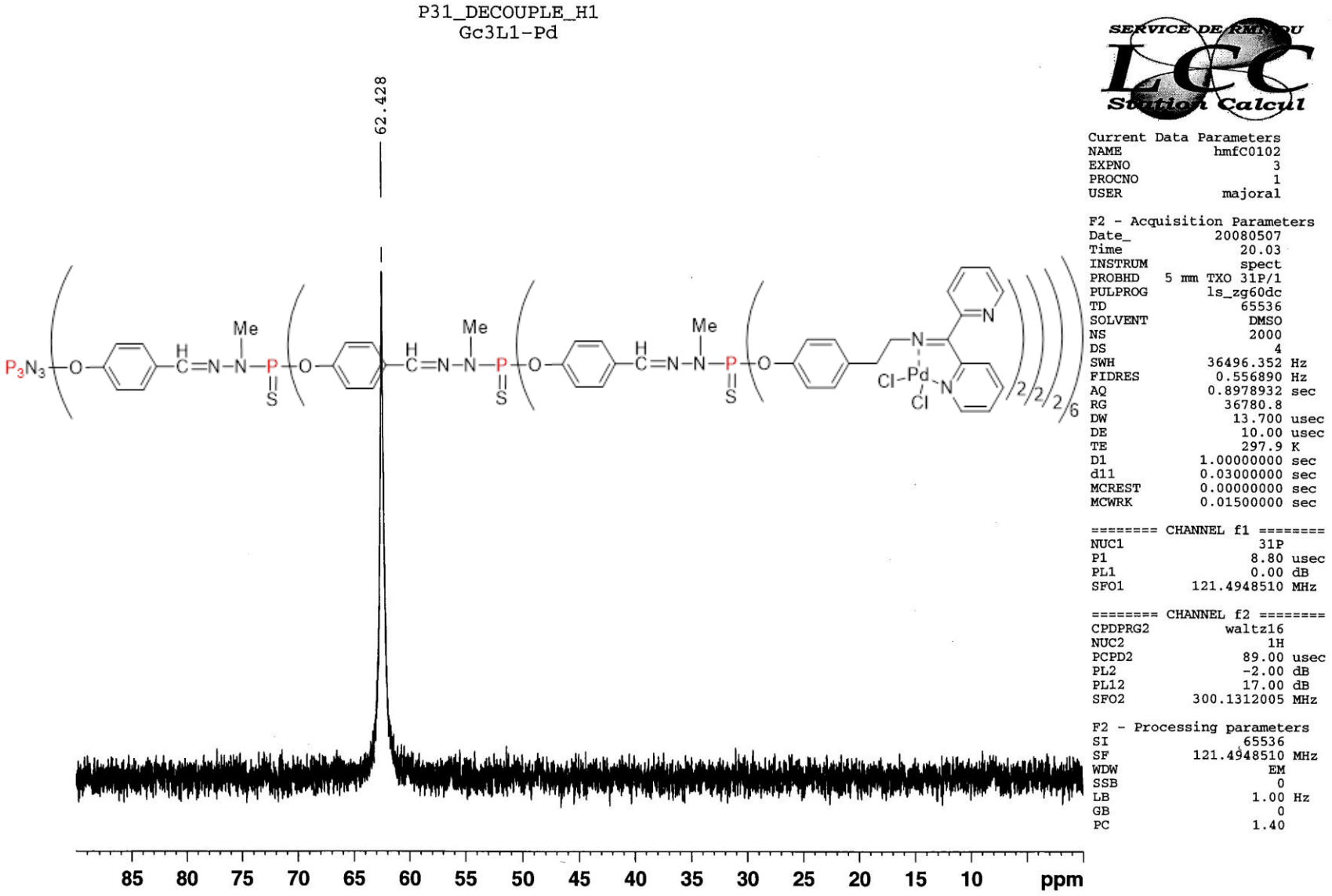


SERVICE DE RMN DU LCC Station Calcul

```
Current Data Parameters
NAME                  hmfC0099
EXPNO                        4
PROCNO                       1
USER                  majoral

F2 - Acquisition Parameters
Date_                 20080502
Time                      8.03
INSTRUM                  spect
PROBHD    5 mm TXO 31P/1
PULPROG                ls_jmod
TD                       65536
SOLVENT                  DMSO
NS                       20000
DS                           4
SWH                 18115.941 Hz
FIDRES                0.276427 Hz
AQ                    1.8088436 sec
RG                       29193
DW                      27.600 usec
DE                      10.00 usec
TE                      297.9 K
CNST2                145.0000000
CNST11                 1.0000000
D1                    2.00000000 sec
d20                   0.00689655 sec
DELTA                 0.00000917 sec
MCREST                0.00000000 sec
MCWRK                 0.01500000 sec

======== CHANNEL f1 ========
NUC1                        13C
P1                         7.20 usec
p2                        14.40 usec
PL1                       -6.00 dB
SFO1                 75.4752958 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                     89.00 usec
PL2                       -2.00 dB
PL12                      17.00 dB
SFO2                300.1312005 MHz

F2 - Processing parameters
SI                       65536
SF                  75.4677490 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

$_{31}$**P** **-G$_{3}$-Pd$_{48}$**

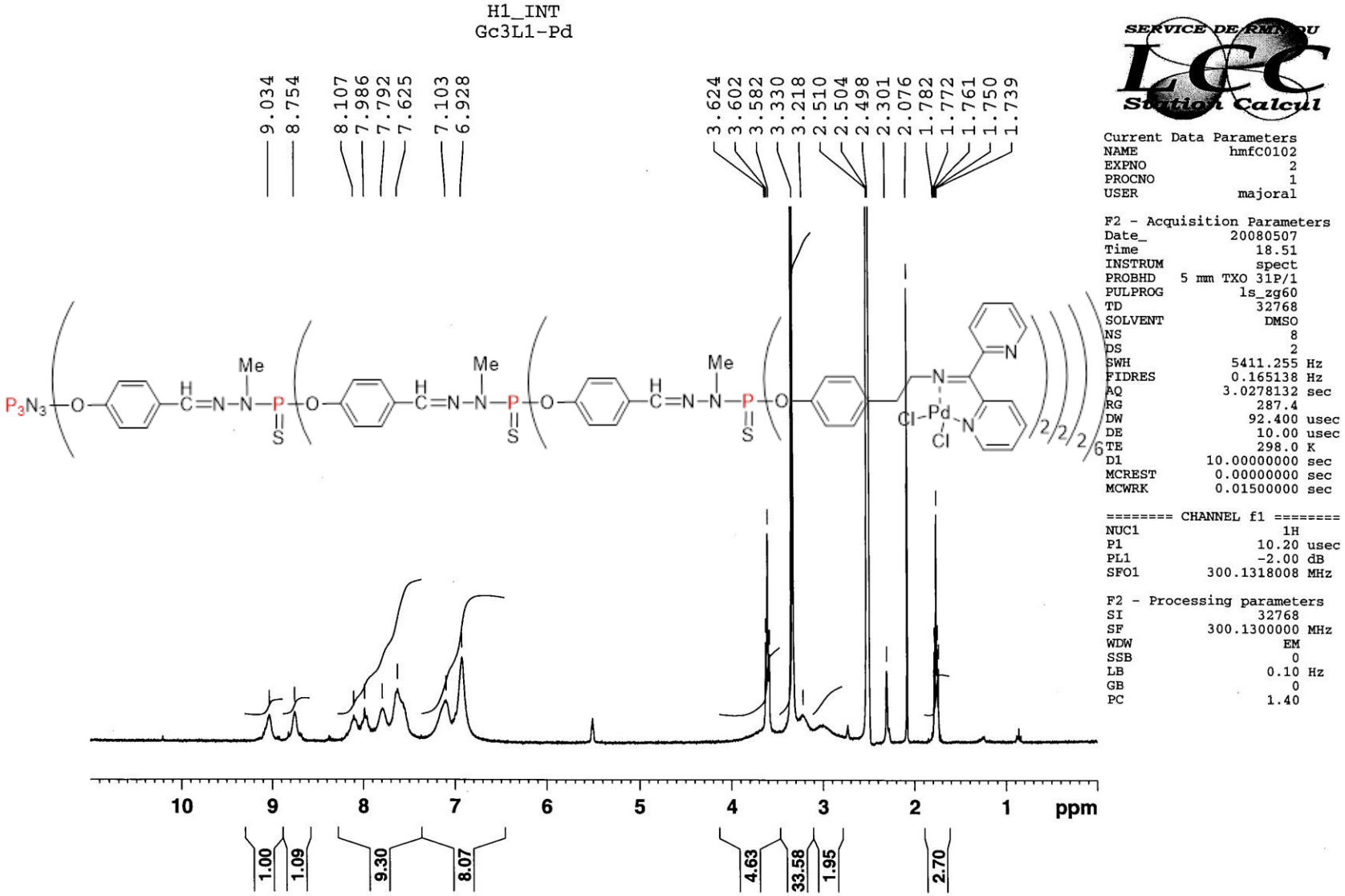
{^{1}H} NMR of dendrimer 3




```
Current Data Parameters
NAME                  hmfC0102
EXPNO                        3
PROCNO                       1
USER                  majoral

F2 - Acquisition Parameters
Date_                 20080507
Time                     20.03
INSTRUM                  spect
PROBHD    5 mm TXO 31P/1
PULPROG              ls_zg60dc
TD                       65536
SOLVENT                    DMSO
NS                         2000
DS                            4
SWH                  36496.352 Hz
FIDRES                0.556890 Hz
AQ                    0.8978932 sec
RG                      36780.8
DW                       13.700 usec
DE                       10.00 usec
TE                       297.9 K
D1                   1.00000000 sec
d11                  0.03000000 sec
MCREST               0.00000000 sec
MCWRK                0.01500000 sec

======== CHANNEL f1 ========
NUC1                        31P
P1                         8.80 usec
PL1                        0.00 dB
SFO1                121.4948510 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     89.00 usec
PL2                       -2.00 dB
PL12                      17.00 dB
SFO2                300.1312005 MHz

F2 - Processing parameters
SI                         65536
SF                  121.4948510 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40
```

^{1}H NMR of dendrimer 3-G_3-Pd_{48}

{^{1}H} NMR of dendrimer 3



Current Data Parameters
NAME hmfC0102
EXPNO 2
PROCNO 1
USER majoral

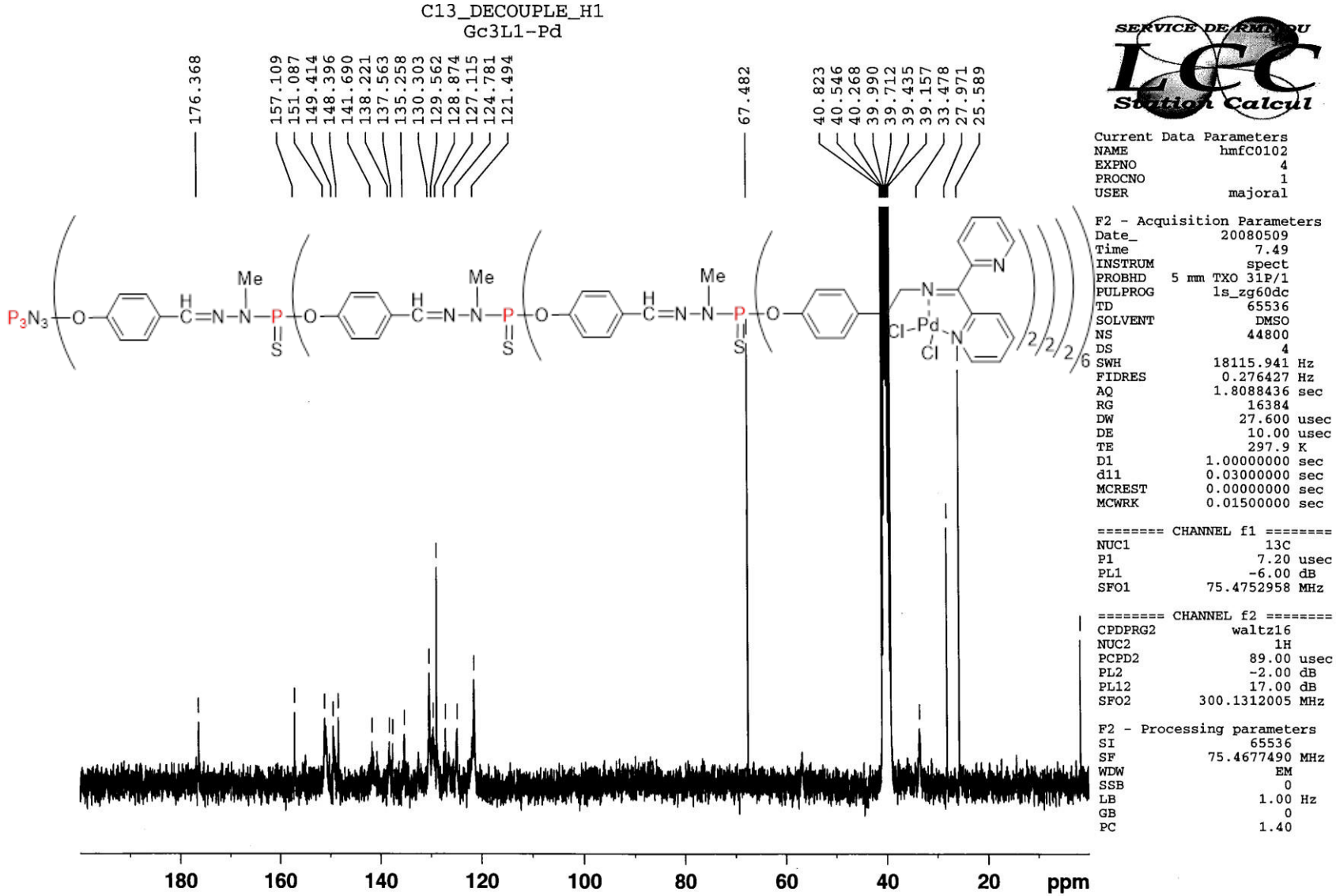
F2 - Acquisition Parameters
Date_ 20080507
Time 18.51
INSTRUM spect
PROBHD 5 mm TXO 31P/1
PULPROG ls_zg60
TD 32768
SOLVENT DMSO
NS 8
DS 2
SWH 5411.255 Hz
FIDRES 0.165138 Hz
AQ 3.0278132 sec
RG 287.4
DW 92.400 usec
DE 10.00 usec
TE 298.0 K
D1 10.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.20 usec
PL1 -2.00 dB
SFO1 300.1318008 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.40

$^{13}C\{^{1}H\}$ NMR of dendrimer 3-G_3-Pd_{48}

{^{1}H} NMR of


C13_DECOUPLE_H1
Gc3L1-Pd
176.368
157.109
151.087
149.414
148.396
141.690
138.221
137.563
135.258
130.303
129.562
128.874
127.115
124.781
121.494
67.482
40.823
40.546
40.268
39.990
39.712
39.435
39.157
33.478
27.971
25.589
Current Data Parameters
NAME hmfC0102
EXPNO 4
PROCNO 1
USER majoral
F2 - Acquisition Parameters
Date_ 20080509
Time 7.49
INSTRUM spect
PROBHD 5 mm TXO 31P/1
PULPROG 1s_zg60dc
TD 65536
SOLVENT DMSO
NS 44800
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 16384
DW 27.600 usec
DE 10.00 usec
TE 297.9 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.20 usec
PL1 -6.00 dB
SFO1 75.4752958 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 89.00 usec
PL2 -2.00 dB
PL12 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
160
140
120
100
80
60
40
20
ppm