Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Rhodium(I)-Catalyzed 1,4-Conjugate Arylation toward β-Fluoroalkylated Electron-Deficient Alkenes: A New Entry to a Construction of a Tertiary Carbon Center Possessing a Fluoroalkyl Group

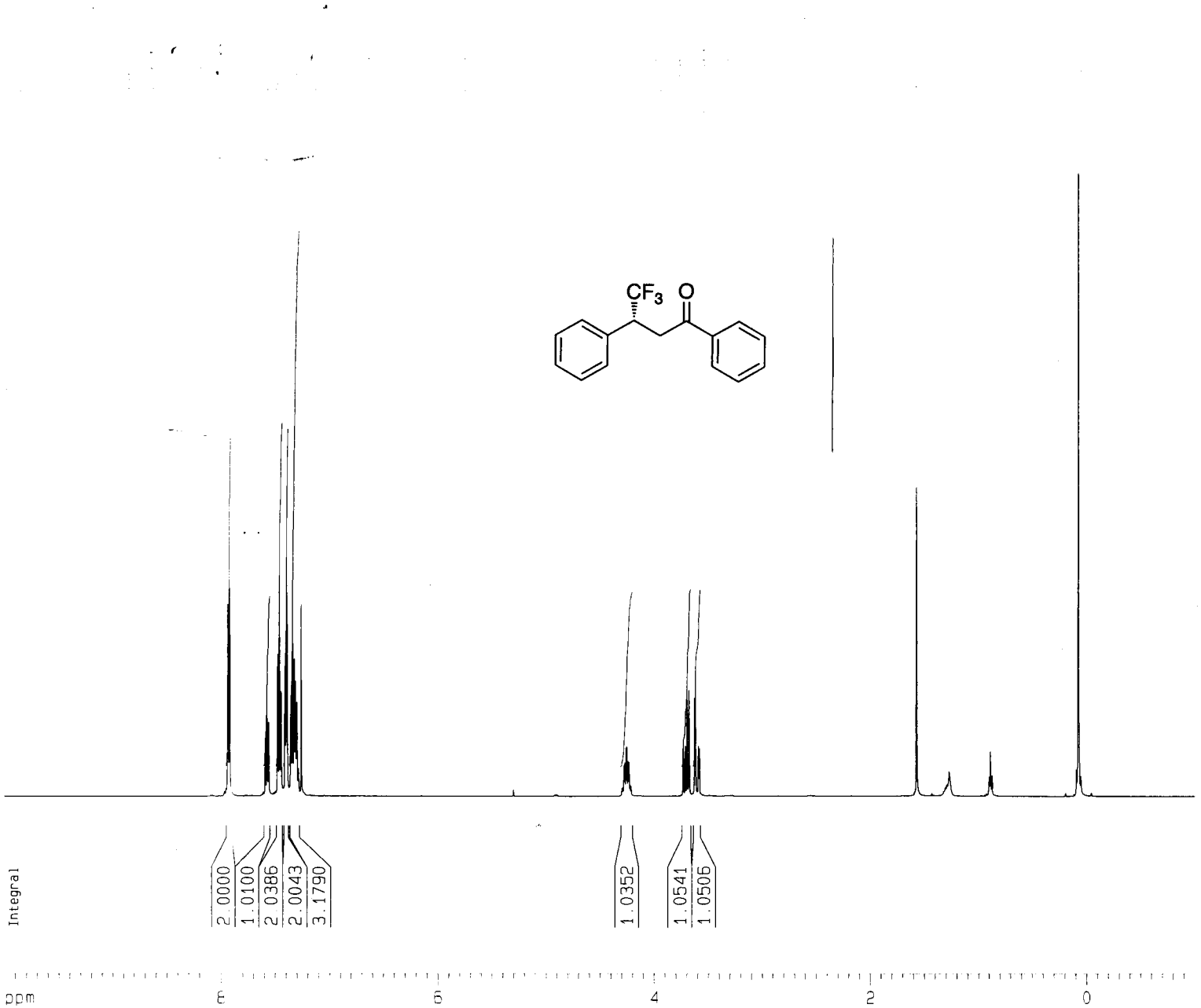
Atsunori Morigaki,[a] Tomoo Tanaka,[b]

Tomotsugu Miyabe,[b] Takashi Ishihara,[b] and Tsutomu Konno*[b]

a) Functional Materials Research Laboratories
Lion Corporation, 7-2-1 Hirai, Edogawa-ku, Tokyo 132-0035 (Japan)

b) Department of Chemistry and Materials Technology, Kyoto Institute of Technology
Matsugasaki, Sakyo-ku, Kyoto 606-0962 (Japan)
Fax: (+81) 75-724-7580, E-mail: konno@chem.kit.ac.jp (Japan)

sample



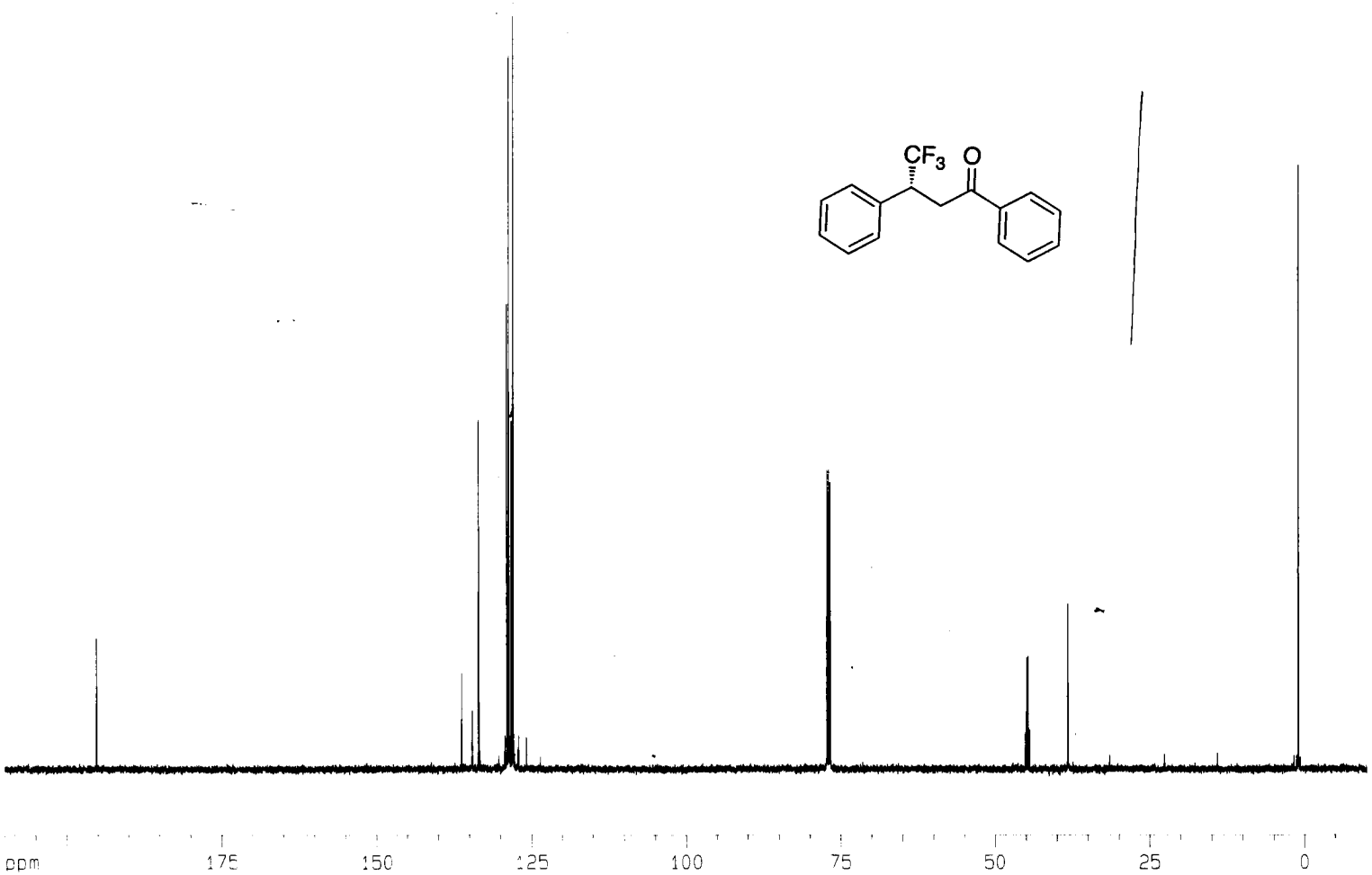
Current Data Parameters
NAME tanaka-12-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20031202
Time 19.35
INSTRUM drx500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 362
DW 48.400 usec
DE 6.00 usec
TE 295.5 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SFO1 500.1330885 MHz

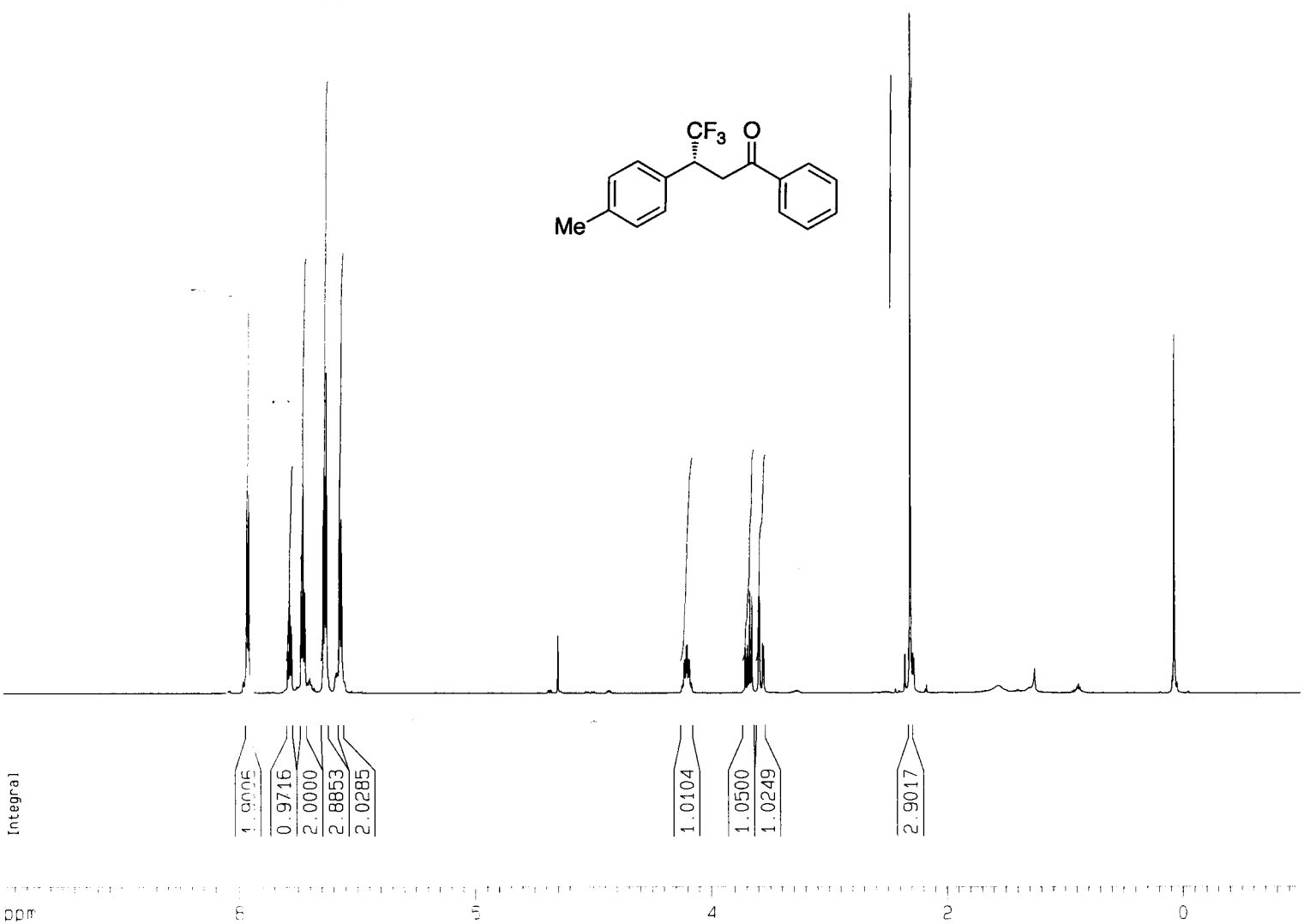
F2 - Processing parameters
SI 32768
SF 500.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 11.89 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

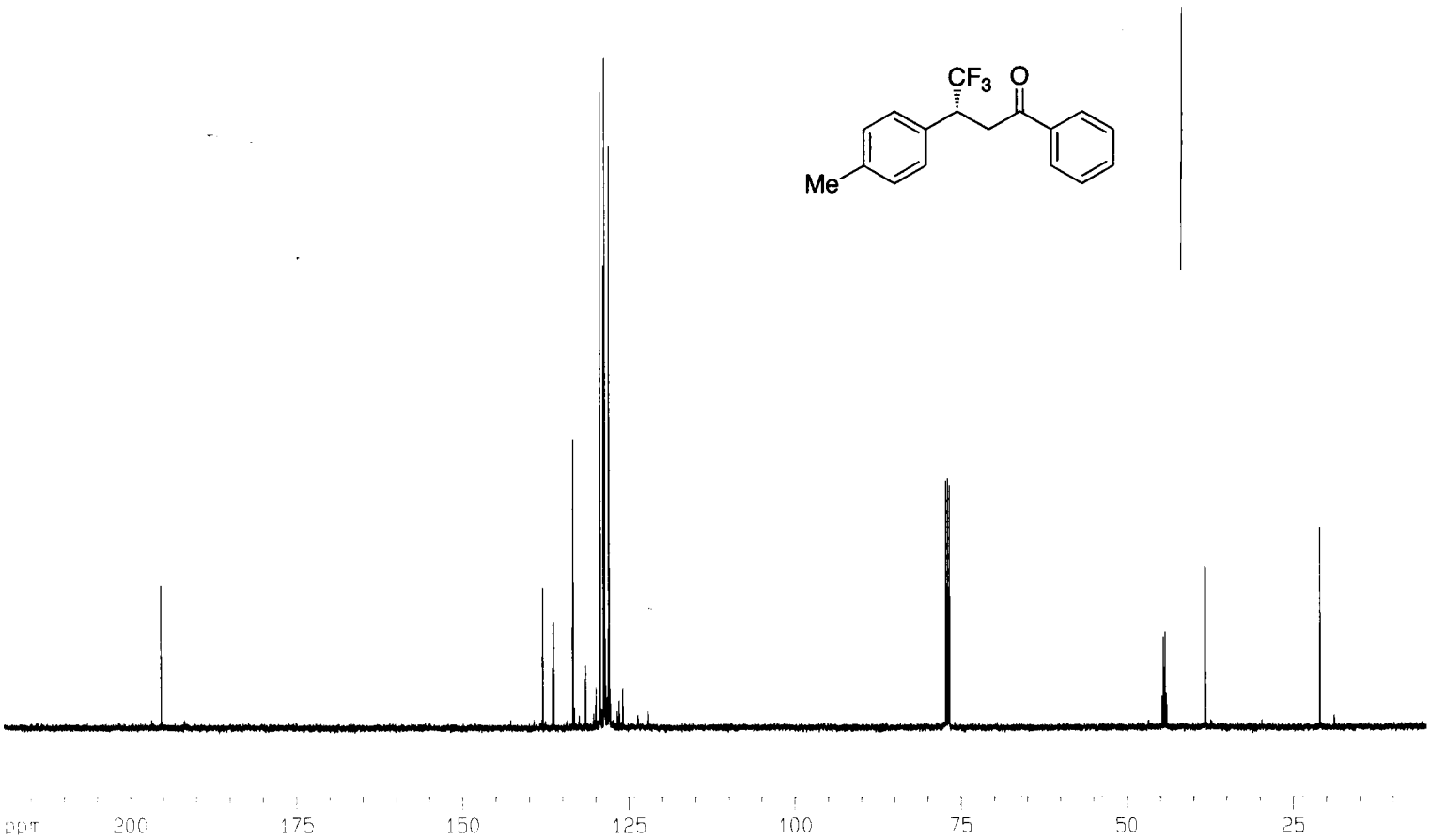



```
Current Data Parameters
NAME      tanaka-03.11.21
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20031121
Time               15.36
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    2
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912244 sec
RG               3649.1
DW               16.650 usec
DE                 6.00 usec
TE                296.5 K
D1           0.50000000 sec
D11          0.03000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 5.70 usec
PL1               -2.00 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            100.00 usec
PL2               -6.00 dB
PL12              13.74 dB
PL13              13.74 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577960 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 0.10

1D NMR plot parameters
CX                20.00 cm
CY                11.15 cm
F1P             210.000 ppm
F1            26409.14 Hz
F2P             -10.000 ppm
F2            -1257.58 Hz
PPMCM          11.00000 ppm/cm
HZCM         1383.33569 Hz/cm
```

ta.Rxn96 proton

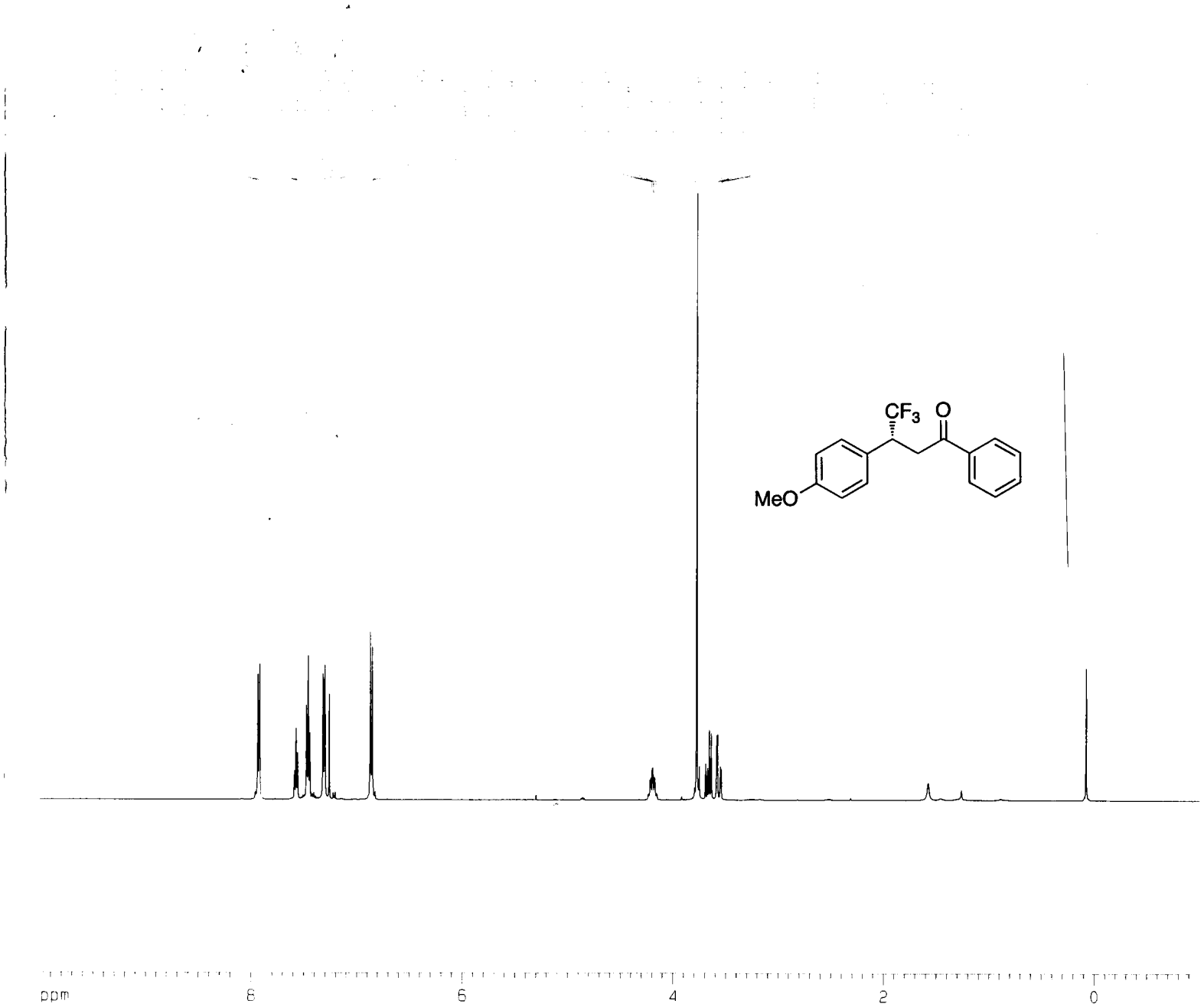



```
Current Data Parameters
NAME          tanaka-12-9
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20031209
Time               12.35
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719923 sec
RG                   512
DW                48.400 usec
DE                 6.00 usec
TE                295.4 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.30 usec
PL1               -6.00 dB
SFO1        500.1330885 MHz

F2 - Processing parameters
SI                 32768
SF          500.1300131 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 11.55 cm
F1P               10.000 ppm
F1               5001.30 Hz
F2P               -1.000 ppm
F2                -500.13 Hz
PPMCM             0.55000 ppm/cm
HZCM            275.07150 Hz/cm
```

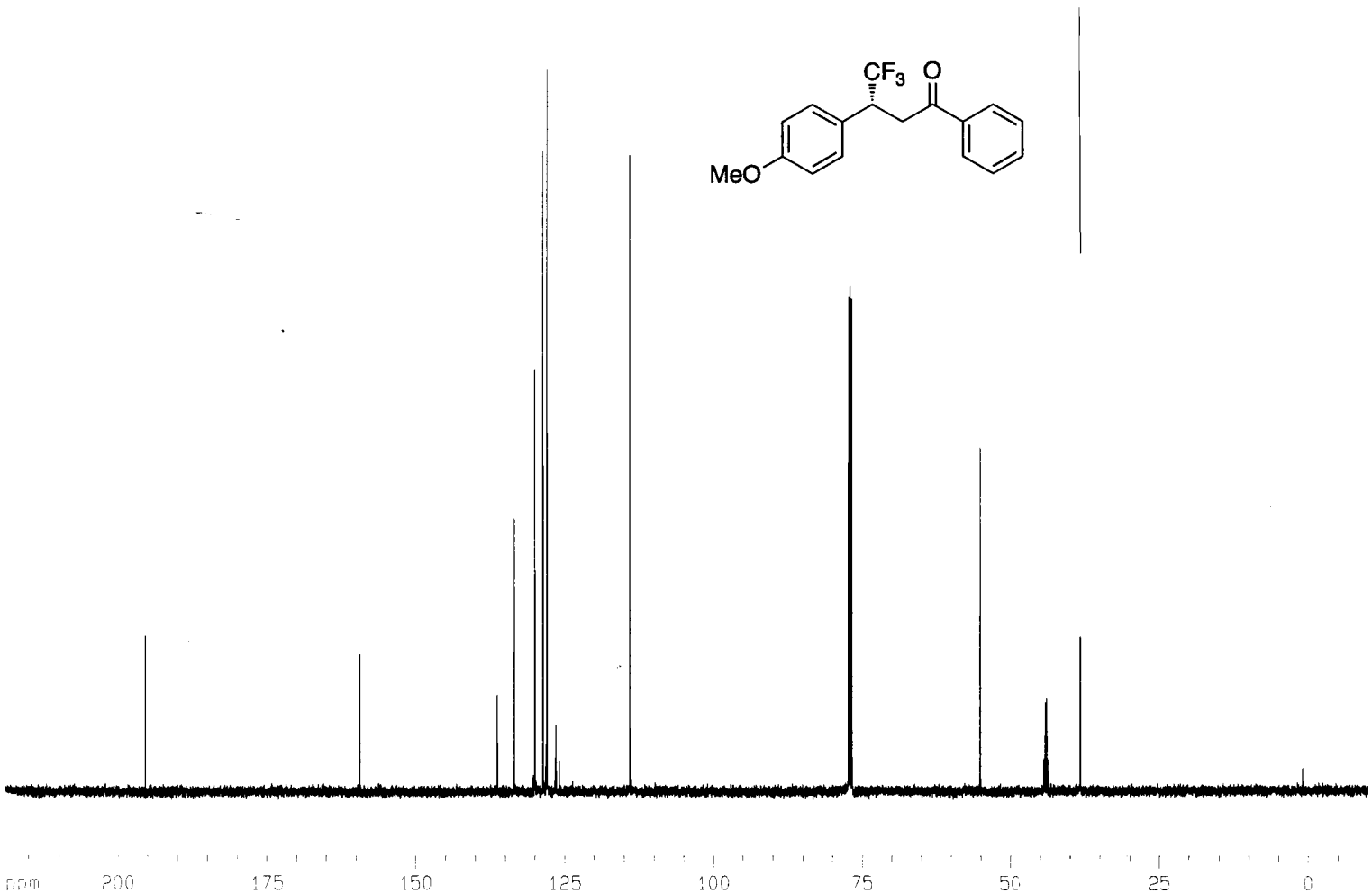



```
Current Data Parameters
NAME      tanaka-04.6.17
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_          20040617
Time              10.10
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    2
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912244 sec
RG               2896.3
DW               16.650 usec
DE                 6.00 usec
TE               298.1 K
D1           0.50000000 sec
d11          0.03000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 5.70 usec
PL1               -2.00 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2            100.00 usec
PL2               -6.00 dB
PL12              13.74 dB
PL13              13.74 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577978 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                 9.41 cm
F1P             219.000 ppm
F1            27540.96 Hz
F2P               5.000 ppm
F2              628.79 Hz
PPMCM          10.70000 ppm/cm
HZCM         1345.60840 Hz/cm
```

sample

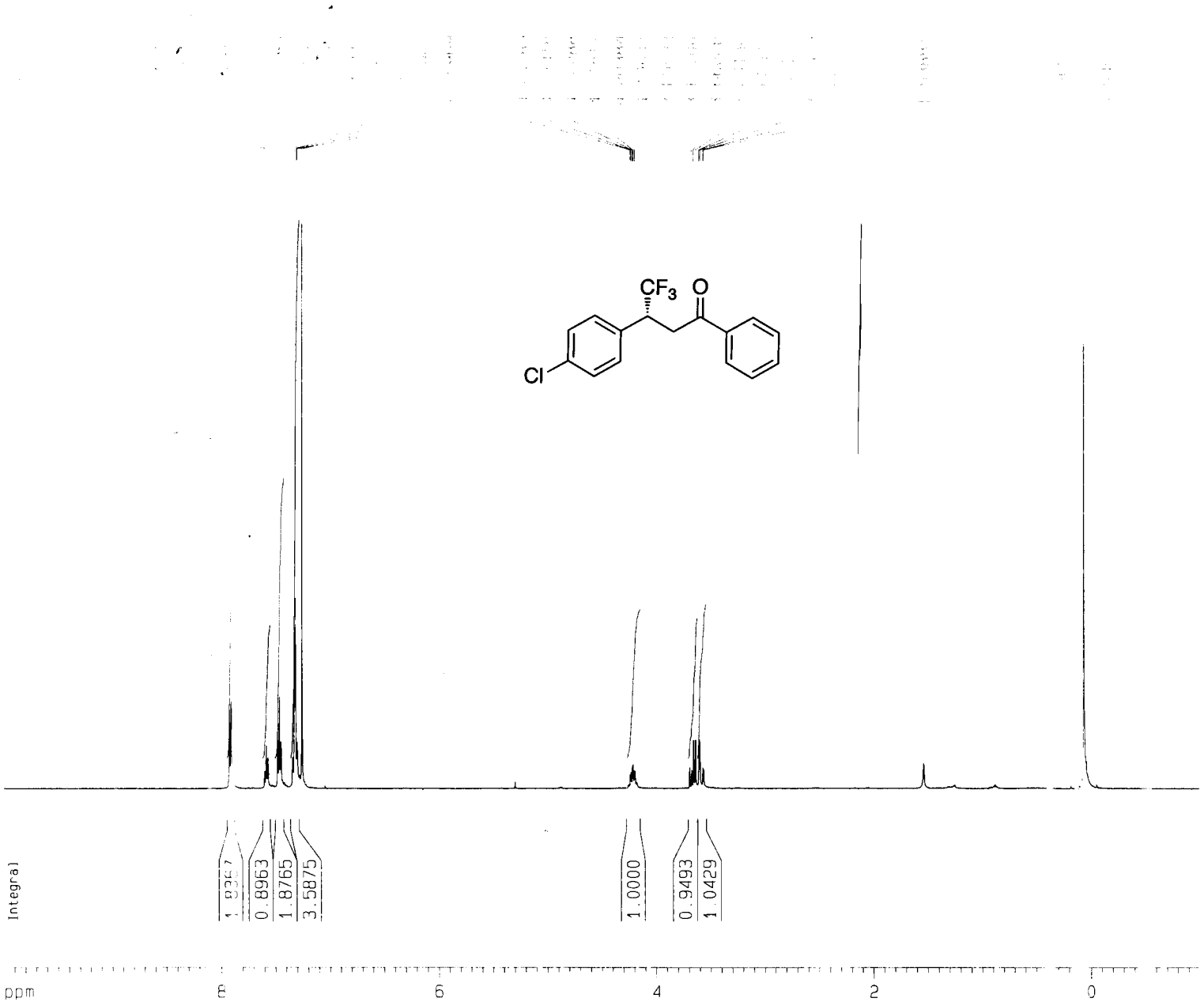



```
Current Data Parameters
NAME      tanaka-03.11.19
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20031119
Time               17.54
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719923 sec
RG                   362
DW                48.400 usec
DE                  6.00 usec
TE                 295.6 K
D1             1.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.30 usec
PL1                -6.00 dB
SFO1         500.1330885 MHz

F2 - Processing parameters
SI                 32768
SF           500.1300134 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 11.54 cm
F1P               10.000 ppm
F1               5001.30 Hz
F2P               -1.000 ppm
F2               -500.13 Hz
PPMCM            0.55000 ppm/cm
HZCM           275.07150 Hz/cm
```




```
Current Data Parameters
NAME      tanaka-04.6.15-yellow
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20040615
Time                       10.45
INSTRUM                   drx500
PROBHD   5 mm Multinucl
PULPROG                   zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                           256
DS                             2
SWH                   30030.029 Hz
FIDRES                 0.458222 Hz
AQ                    1.0912244 sec
RG                       3649.1
DW                       16.650 usec
DE                        6.00 usec
TE                       297.8 K
D1                   0.50000000 sec
d11                  0.03000000 sec
MCREST               0.00000000 sec
MCWRK                0.01500000 sec

======== CHANNEL f1 ========
NUC1                         13C
P1                          5.70 usec
PL1                        -2.00 dB
SFO1                 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                          1H
PCPD2                     100.00 usec
PL2                        -6.00 dB
PL12                       13.74 dB
PL13                       13.74 dB
SFO2                 500.1320005 MHz

F2 - Processing parameters
SI                          32768
SF                   125.7577951 MHz
WDW                            EM
SSB                             0
LB                           1.00 Hz
GB                              0
PC                           1.40

1D NMR plot parameters
CX                          20.00 cm
CY                          10.56 cm
F1P                       219.000 ppm
F1                       27540.96 Hz
F2P                      -10.000 ppm
F2                       -1257.58 Hz
PPMCM                    11.45000 ppm/cm
HZCM                  1439.92676 Hz/cm
```

sample



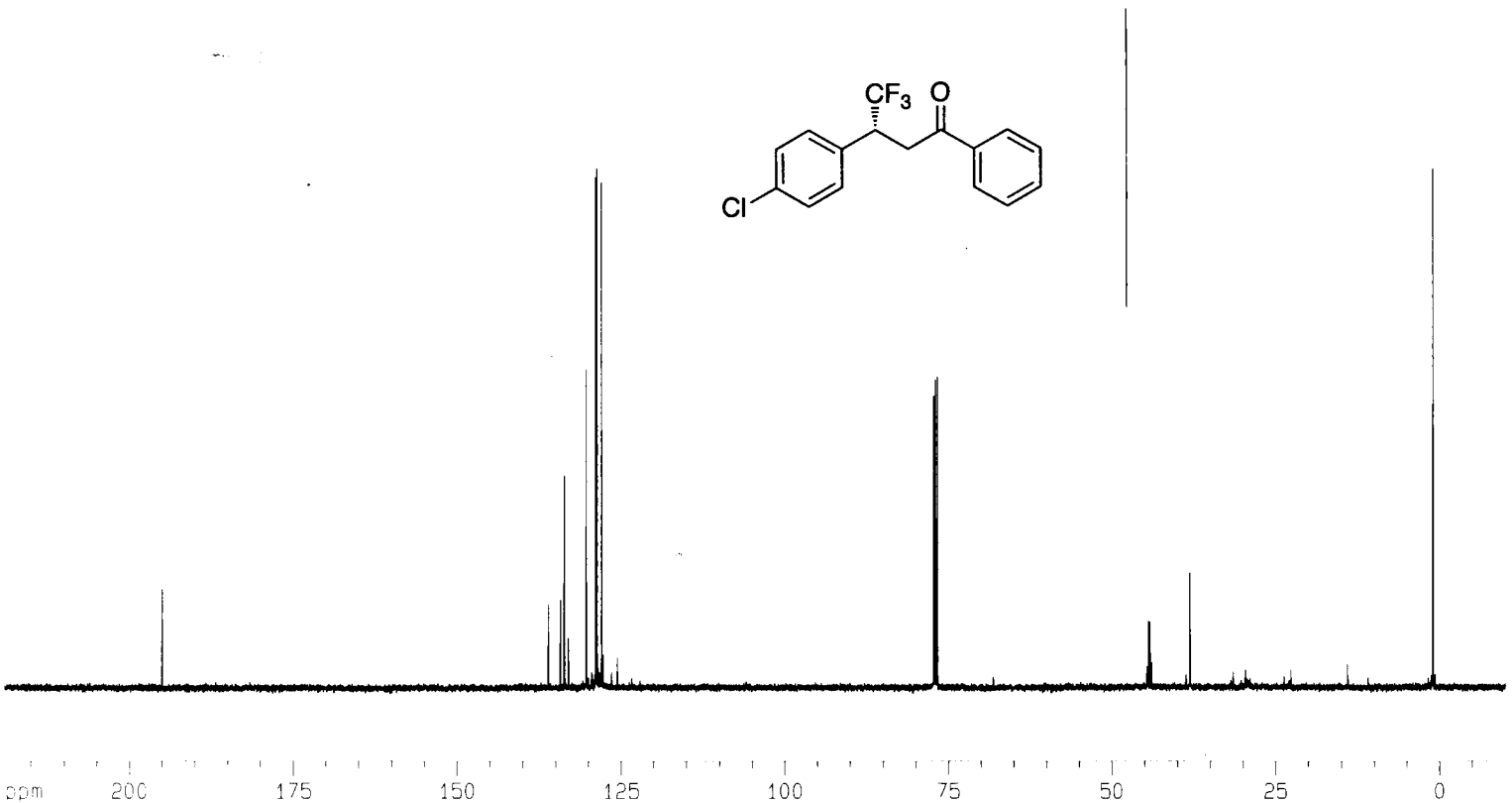
Current Data Parameters
NAME tanaka-p-Cl
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040213
Time 18.30
INSTRUM drx500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 912.3
DW 48.400 usec
DE 6.00 usec
TE 295.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.41 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm



Current Data Parameters
NAME tanaka-04.5.19-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040519
Time 19.15
INSTRUM drx500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 6502
DW 16.650 usec
DE 6.00 usec
TE 297.5 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 5.70 usec
PL1 -2.00 dB
SFO1 125.7703643 MHz

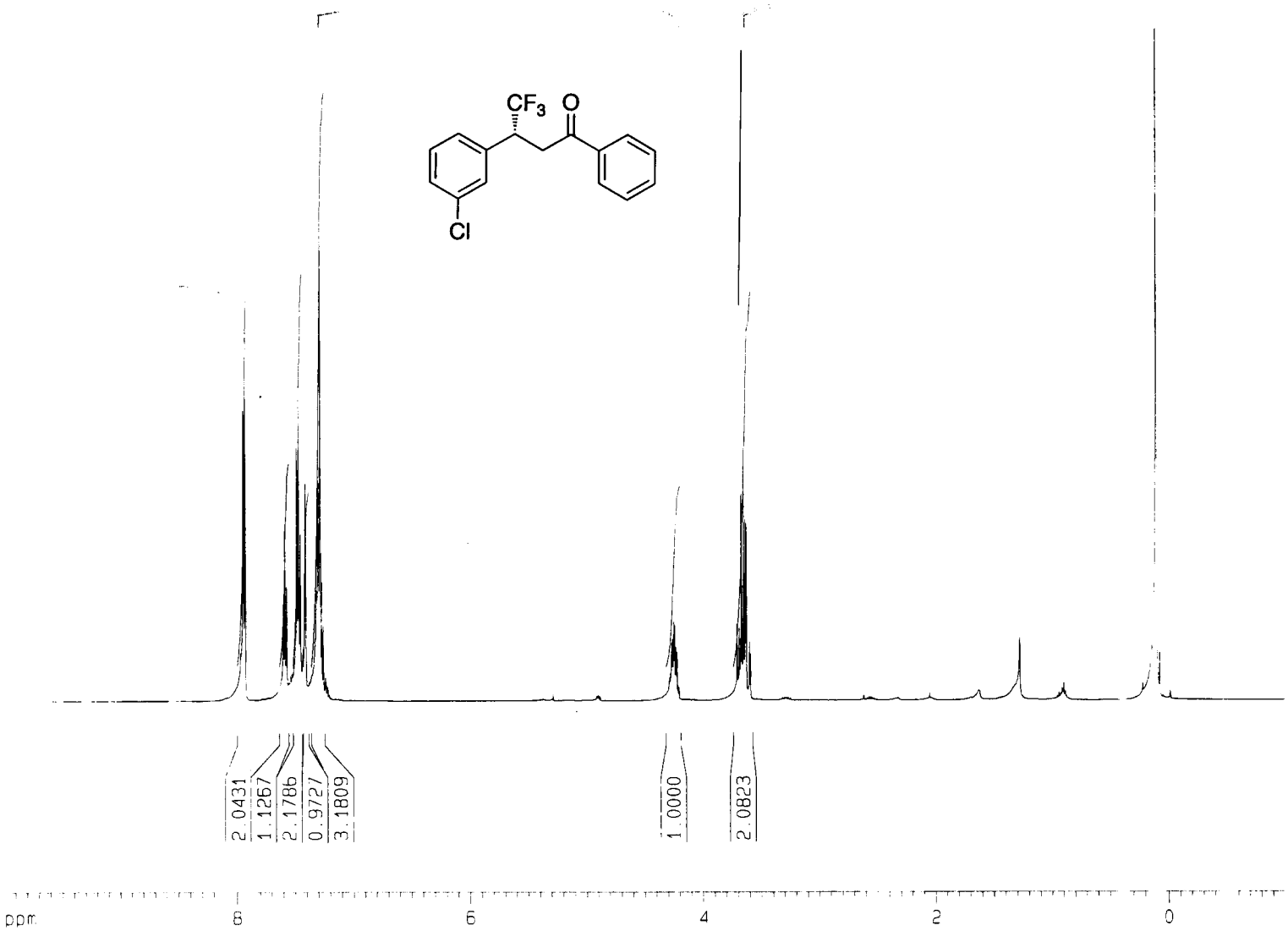
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 13.74 dB
PL13 13.74 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577951 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 6.97 cm
F1P 219.000 ppm
F1 27540.96 Hz
F2P -10.000 ppm
F2 -1257.58 Hz
PPMCM 11.45000 ppm/cm
HZCM 1439.92676 Hz/cm

(P) - α

sample



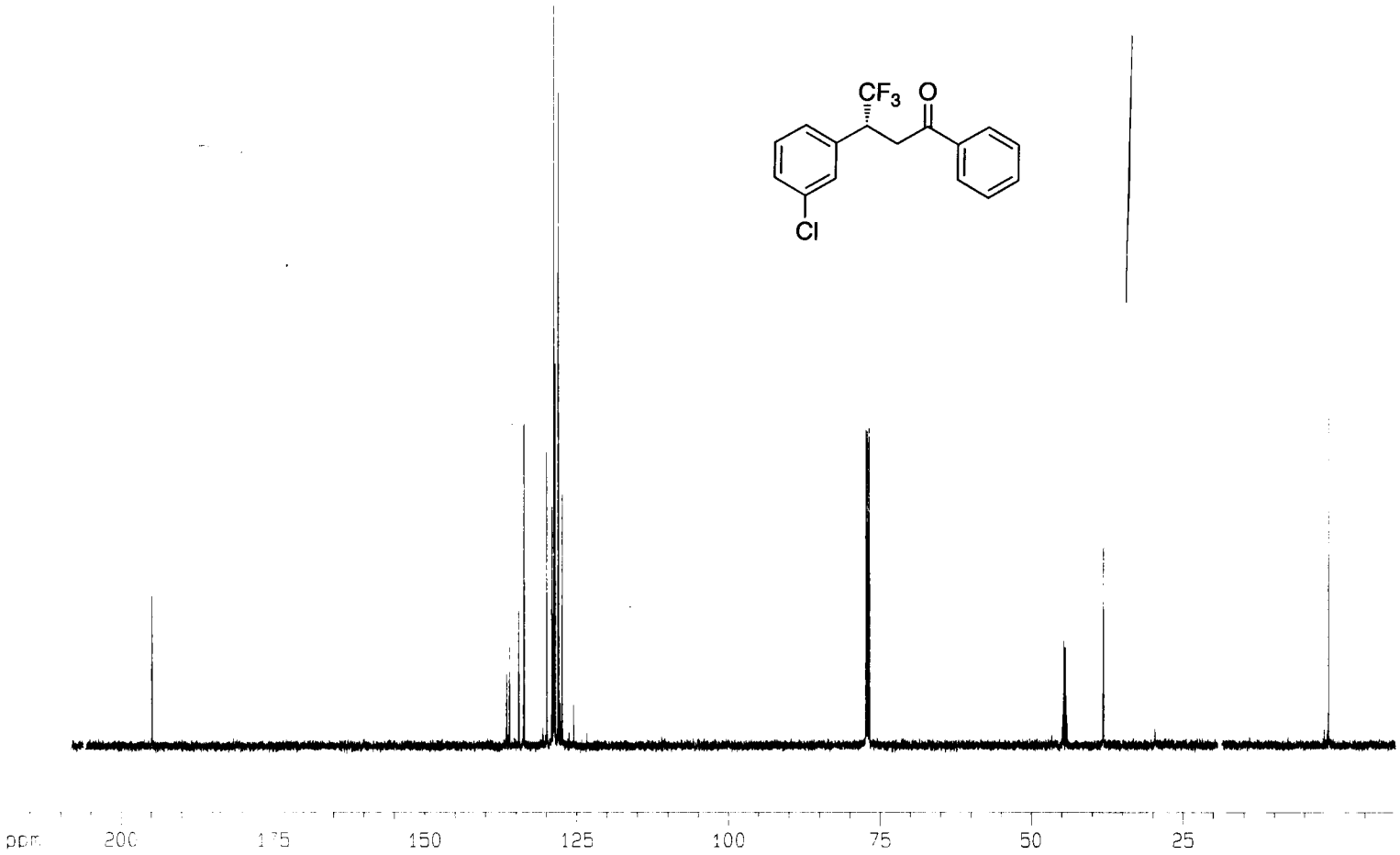
Current Data Parameters
NAME tanaka-04.4.8-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040408
Time 17 42
INSTRUM drx500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 57
DW 48.400 usec
DE 6.00 usec
TE 296.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300127 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

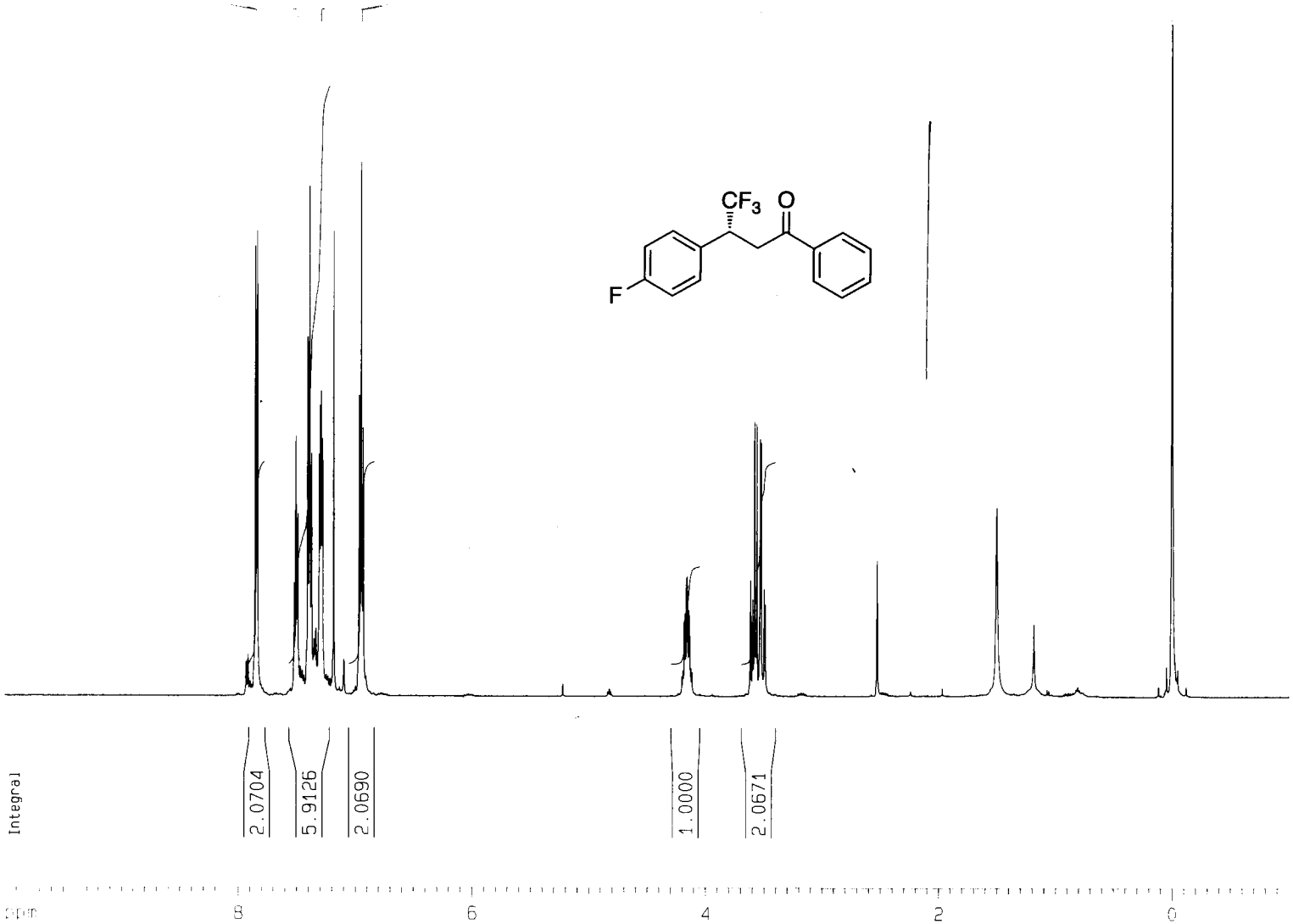
1D NMR plot parameters
CX 20.00 cm
CY 30.24 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm




```
Current Data Parameters
NAME      tsrgka- 4.4.8-2
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20040408
Time               17.51
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    2
SWH            30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0912244 sec
RG                3549.1
DW                16.650 usec
DE                 6.00 usec
TE                297.3 K
D1            0.50000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 5.70 usec
PL1               -2.00 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            100.00 usec
PL2               -6.00 dB
PL12              13.74 dB
PL13              13.74 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577969 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  0.10

1D NMR plot parameters
CX                 20.00 cm
CY                 10.78 cm
F1P             219.000 ppm
F1             27540.96 Hz
F2P             -10.000 ppm
F2             -1257.58 Hz
PPMCM           11.45000 ppm/cm
HZCM         1439.92676 Hz/cm
```

(m, - CF3

sample



Current Data Parameters

NAME	monof
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20040716
Time	10.46
INSTRUM	drx500
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	406.4
DW	48.400 usec
DE	6.00 usec
TE	298.7 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

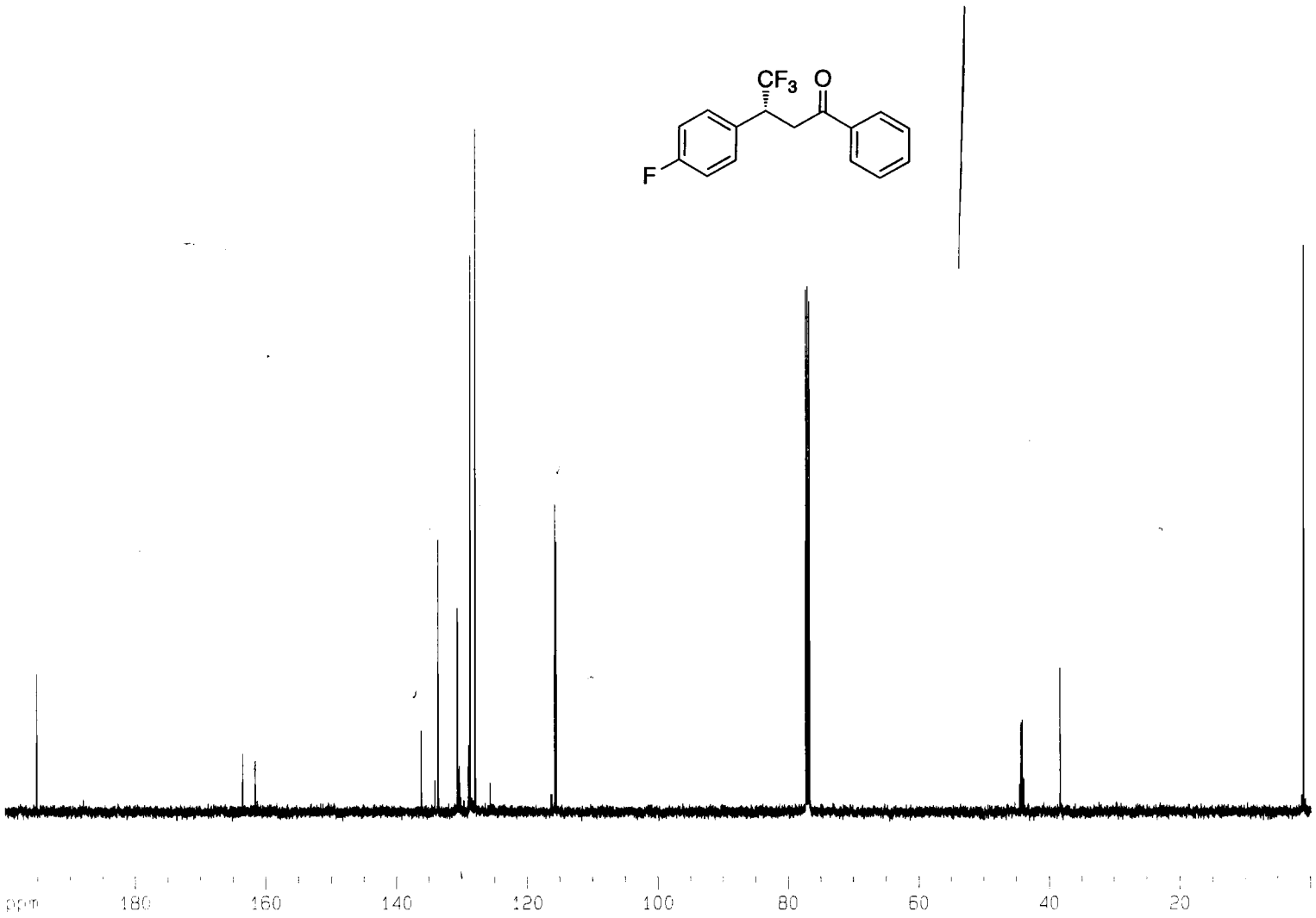
NUC1	1H
P1	10.30 usec
PL1	-6.00 dB
SFO1	500.1330885 MHz

F2 - Processing parameters

SI	32768
SF	500.1300512 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

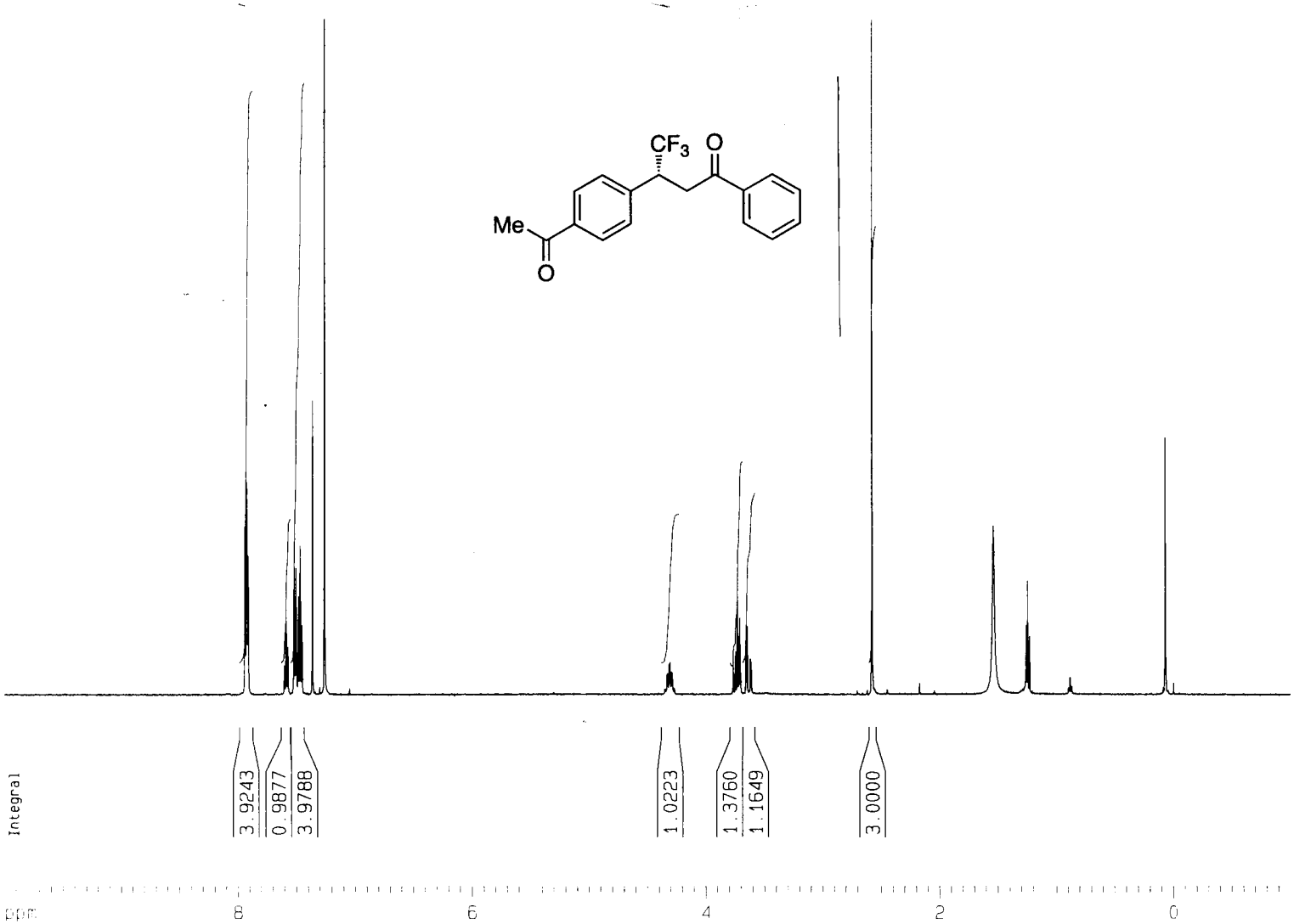
1D NMR plot parameters

CX	20.00 cm
CY	34.41 cm
F1P	10.000 ppm
F1	5001.30 Hz
F2P	-1.000 ppm
F2	-500.13 Hz
PPMCM	0.55000 ppm/cm
HZCM	275.07153 Hz/cm




```
Current Data Parameters
NAME              mono-f2
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20040727
Time               17.39
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    2
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912244 sec
RG               2896.3
DW               16.650 usec
DE                6.00 usec
TE                300.5 K
D1           0.50000000 sec
d11          0.03000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 5.70 usec
PL1               -2.00 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            100.00 usec
PL2               -6.00 dB
PL12              13.74 dB
PL13              13.74 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577932 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                10.50 cm
F1P              199.900 ppm
F1             25138.98 Hz
F2P              -0.100 ppm
F2              -12.58 Hz
PPMCM          10.00000 ppm/cm
HZCM         1257.57788 Hz/cm
```

sample



Current Data Parameters

NAME	acetyl
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20041210
Time	14.03
INSTRUM	drx500
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	1149.4
DW	48.400 usec
DE	6.00 usec
TE	297.6 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

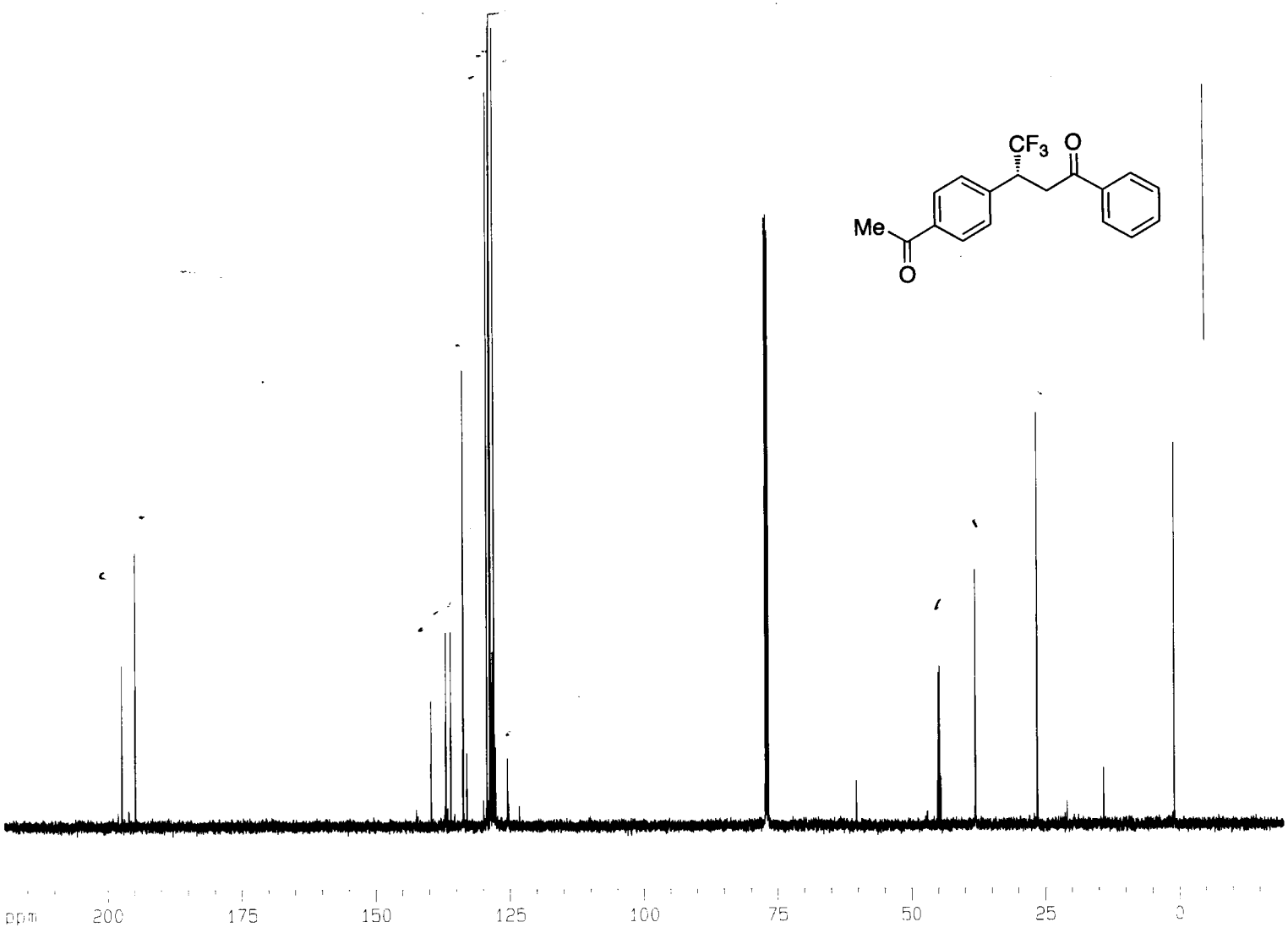
NUC1	1H
P1	10.30 usec
PL1	-6.00 dB
SFO1	500.1330885 MHz

F2 - Processing parameters

SI	32768
SF	500.1300129 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

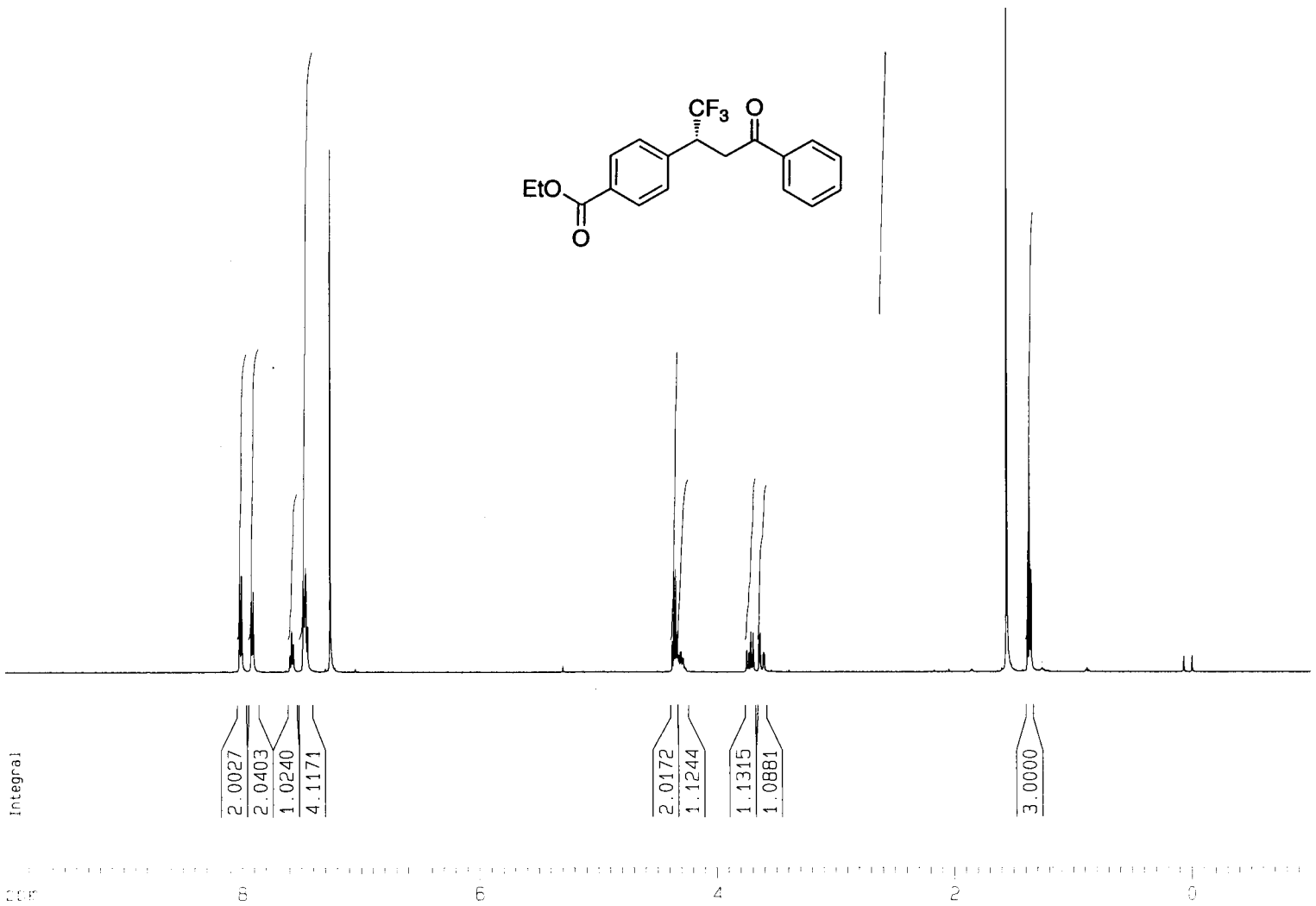
1D NMR plot parameters

CX	20.00 cm
CY	12.50 cm
F1P	10.000 ppm
F1	5001.30 Hz
F2P	-1.000 ppm
F2	-500.13 Hz
PPMCM	0.55000 ppm/cm
HZCM	275.07150 Hz/cm

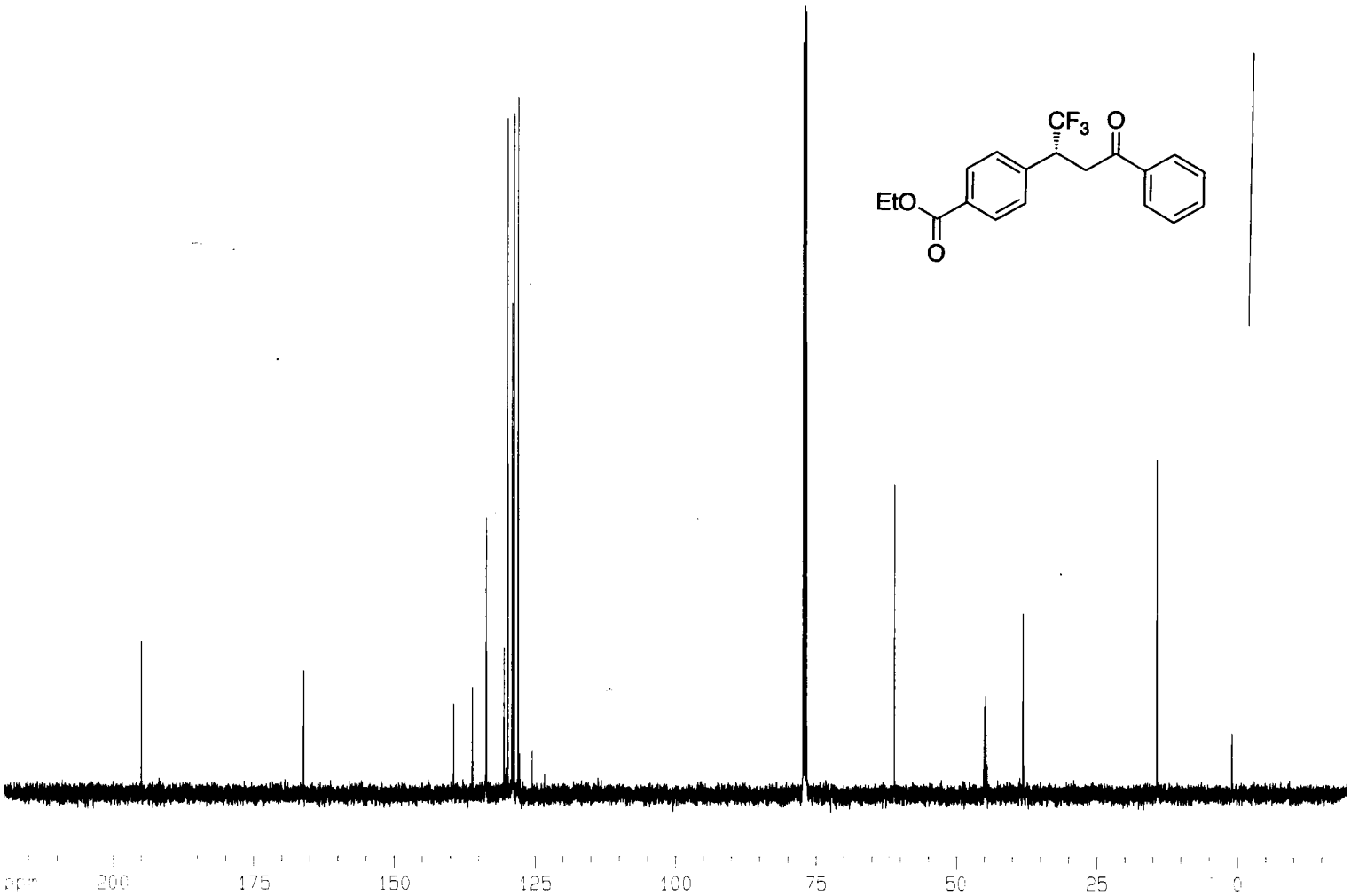



```
Current Data Parameters
NAME            acetyl-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20041014
Time               19.37
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    2
SWH            30030.029 Hz
FIDRES          0.458222 Hz
AQ             1.0912244 sec
RG                5160.6
DW                16.650 usec
DE                  6.00 usec
TE                298.2 K
D1            0.50000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                  5.70 usec
PL1                -2.00 dB
SFO1         125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             100.00 usec
PL2                -6.00 dB
PL12               13.74 dB
PL13               13.74 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF           125.7577997 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 17.10 cm
F1P               219.308 ppm
F1              27579.66 Hz
F2P              -19.485 ppm
F2              -2450.37 Hz
PPMCM            11.93963 ppm/cm
HZCM           1501.50159 Hz/cm
```

sample

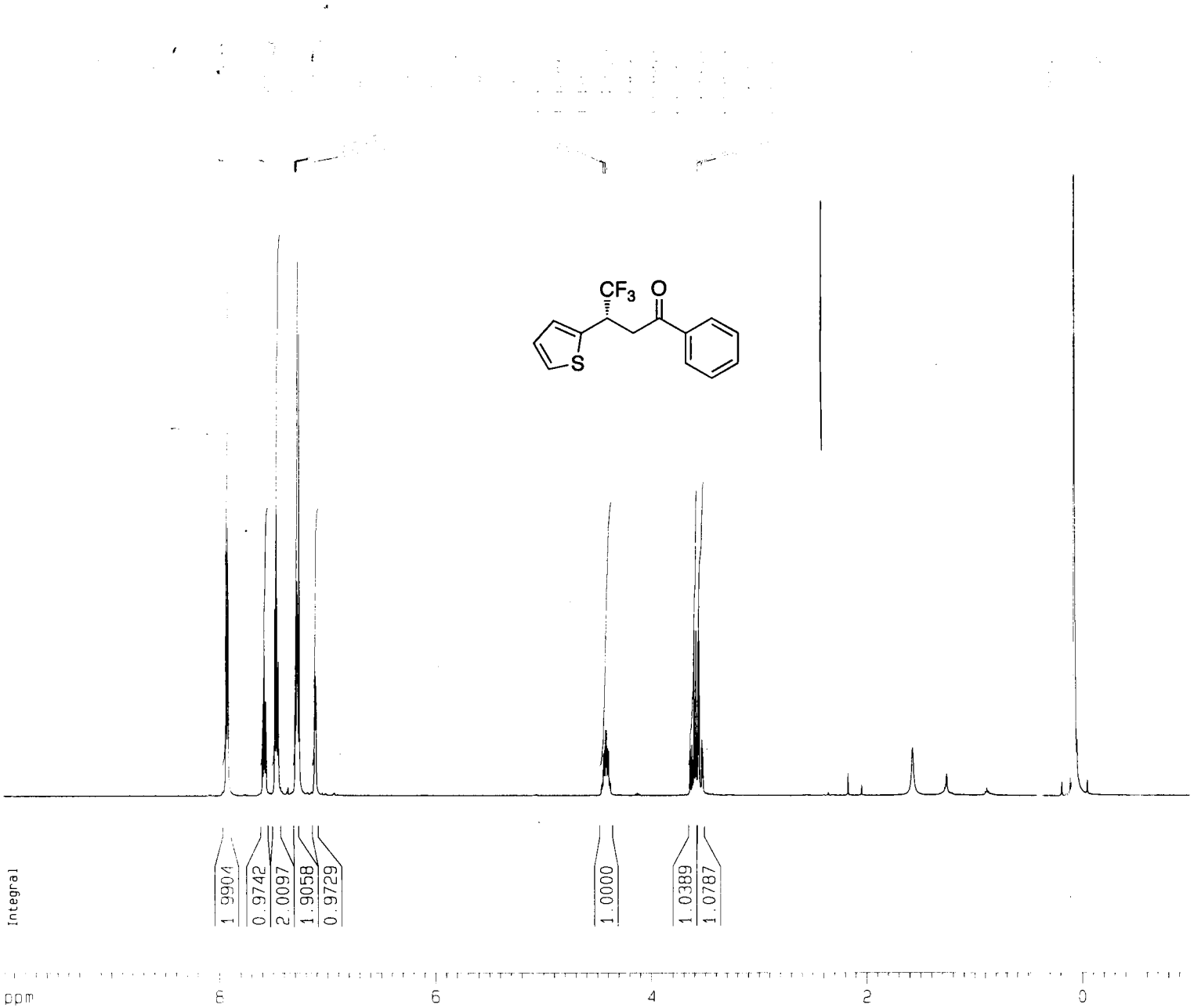



```
Current Data Parameters
NAME        tanaka-04.6.2
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20040602
Time                 9.13
INSTRUM           drx500
PROBHD   5 mm Multinucl
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719923 sec
RG                  1024
DW                48.400 usec
DE                 6.00 usec
TE                296.8 K
D1             1.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.30 usec
PL1               -6.00 dB
SFO1         500.1330885 MHz

F2 - Processing parameters
SI                 32768
SF           500.1300134 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.26 cm
F1P               10.000 ppm
F1               5001.30 Hz
F2P               -1.000 ppm
F2               -500.13 Hz
PPMCM            0.55000 ppm/cm
HZCM           275.07150 Hz/cm
```

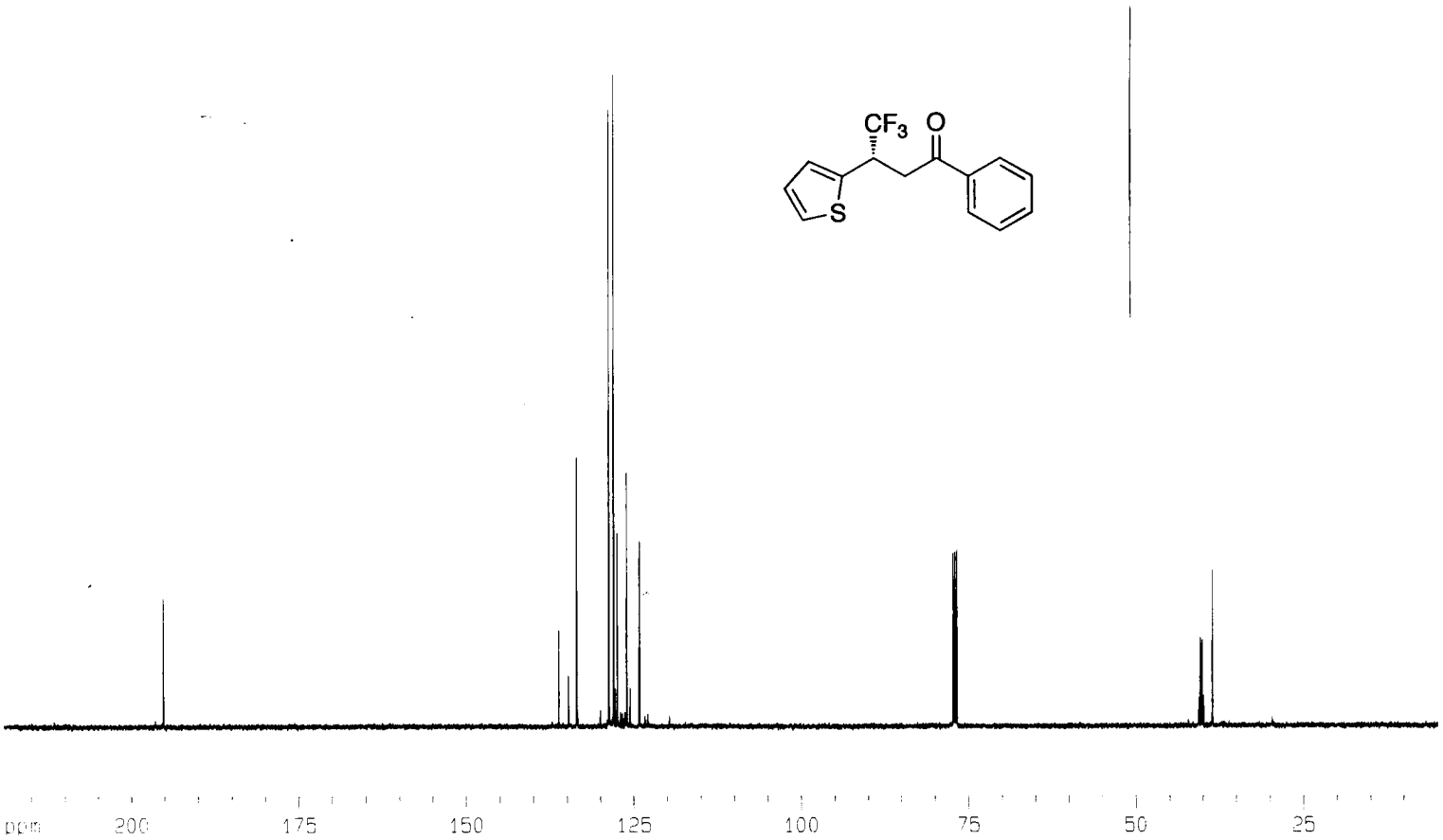



```
Current Data Parameters
NAME      ethoxycarbonyl
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20040831
Time              17.58
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    2
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912244 sec
RG               3649.1
DW               16.650 usec
DE                6.00 usec
TE               299.7 K
D1           0.50000000 sec
d11          0.03000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 5.70 usec
PL1               -2.00 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            100.00 usec
PL2               -6.00 dB
PL12              13.74 dB
PL13              13.74 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577932 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                11.98 cm
F1P             219.359 ppm
F1             27586.10 Hz
F2P             -19.434 ppm
F2             -2443.93 Hz
PPMCM          11.93963 ppm/cm
HZCM         1501.50146 Hz/cm
```

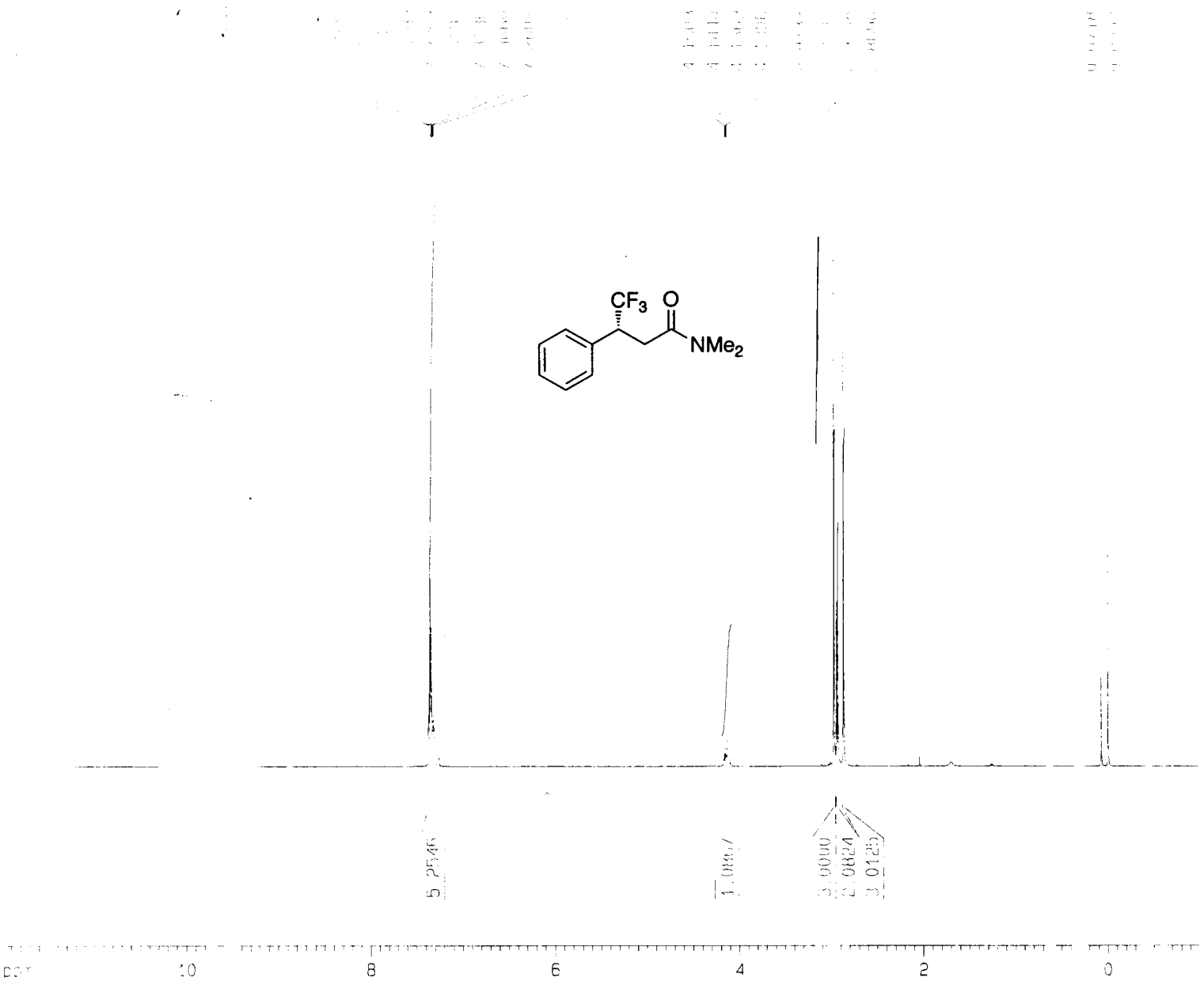
sample

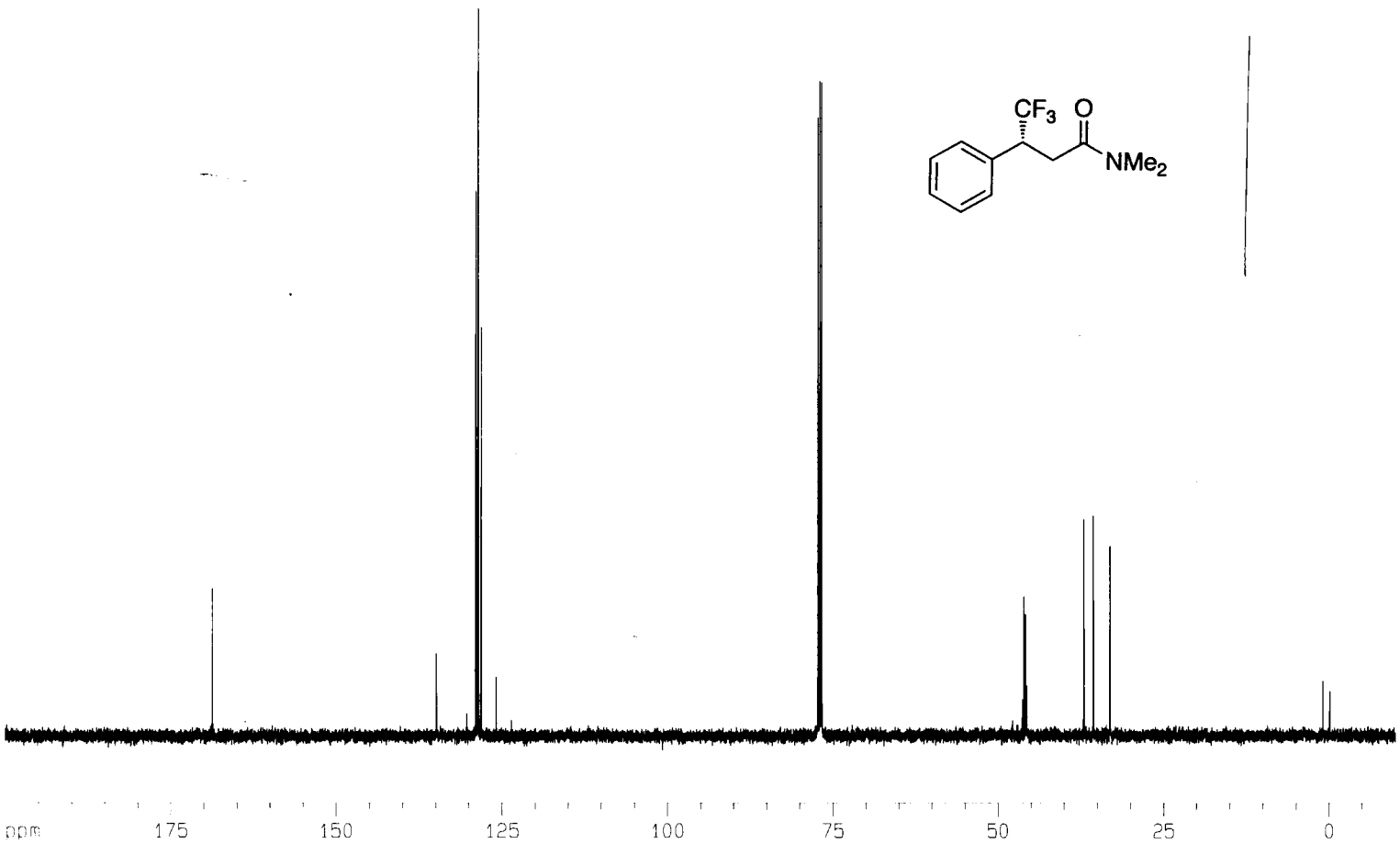



```
Current Data Parameters
NAME          tatsuki-f 12
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20040212
Time               17.22
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ            3.1719923 sec
RG                456.1
DW               48.400 usec
DE                6.00 usec
TE                295.8 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.30 usec
PL1               -6.00 dB
SFO1        500.1330885 MHz

F2 - Processing parameters
SI                32768
SF          500.1300131 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                50.62 cm
F1P              10.000 ppm
F1               5001.30 Hz
F2P              -1.000 ppm
F2               -500.13 Hz
PPMCM            0.55000 ppm/cm
HZCM           275.07150 Hz/cm
```



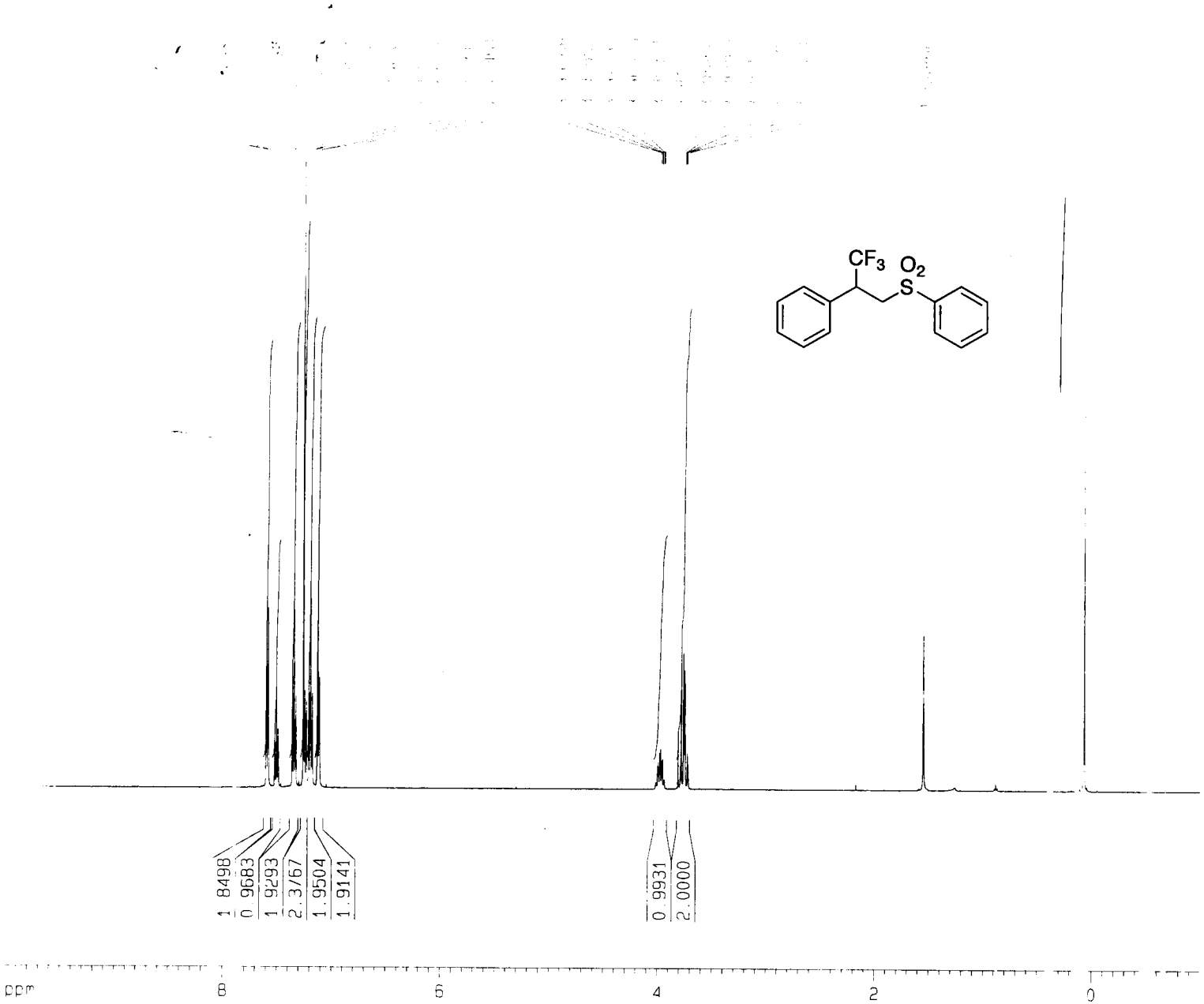

```
Current Data Parameters
NAME      tanaka-04.6.17
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20040617
Time               9.59
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    2
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912244 sec
RG               3649.1
DW               16.650 usec
DE                6.00 usec
TE               298.0 K
D1           0.50000000 sec
d11          0.03000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 5.70 usec
PL1               -2.00 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            100.00 usec
PL2               -6.00 dB
PL12              13.74 dB
PL13              13.74 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577978 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                12.68 cm
F1P            219.000 ppm
F1            27540.96 Hz
F2P              5.000 ppm
F2             628.79 Hz
PPMCM          10.70000 ppm/cm
HZCM         1345.60840 Hz/cm
```


CF3
O
NMe2
5.2545
1.0000
3.0000
2.0824
3.0125
10
8
6
4
2
0




```
Current Data Parameters
NAME      tanaka-04.5.14-2
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_            20040514
Time               11.50
INSTRUM           drx500
PROBHD   5 mm Multinucl
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    2
SWH            30030.029 Hz
FIDRES          0.458222 Hz
AQ             1.0912244 sec
RG                5160.6
DW                16.650 usec
DE                 6.00 usec
TE                297.6 K
D1            0.50000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                  5.70 usec
PL1                -2.00 dB
SFO1         125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             100.00 usec
PL2                -6.00 dB
PL12               13.74 dB
PL13               13.74 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF           125.7577960 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 10.84 cm
F1P             200.000 ppm
F1             25151.56 Hz
F2P             -10.000 ppm
F2             -1257.58 Hz
PPMCM          10.50000 ppm/cm
HZCM         1320.45679 Hz/cm
```

sample



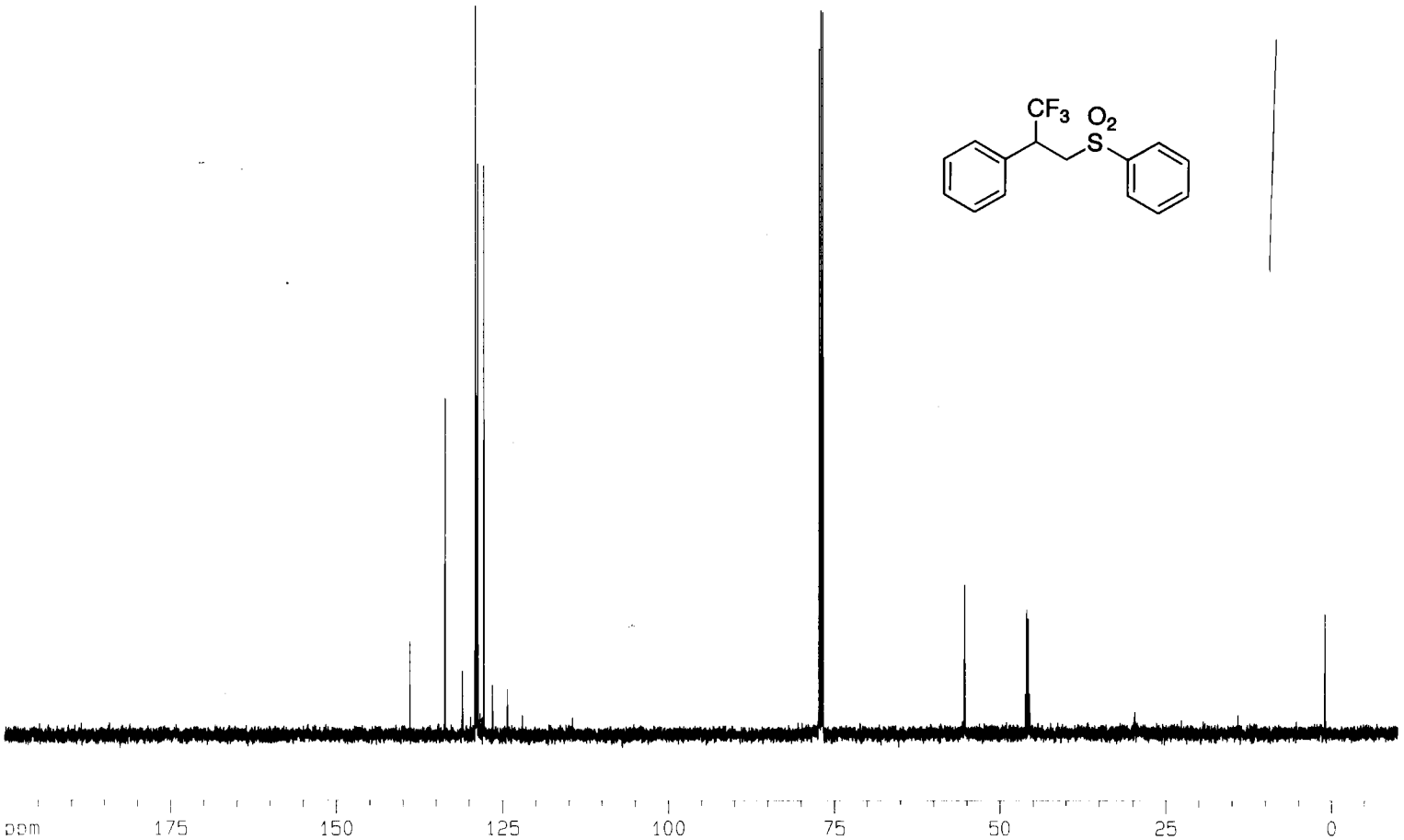
Current Data Parameters
NAME tanaka-3.10 -1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040310
Time 12.46
INSTRUM spx500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.575 Hz
FIDRES 0.157532 Hz
AQ 3.1719923 sec
RG 812.7
DW 48.400 usec
DE 6.00 usec
TE 295.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SFO1 500.1330885 MHz

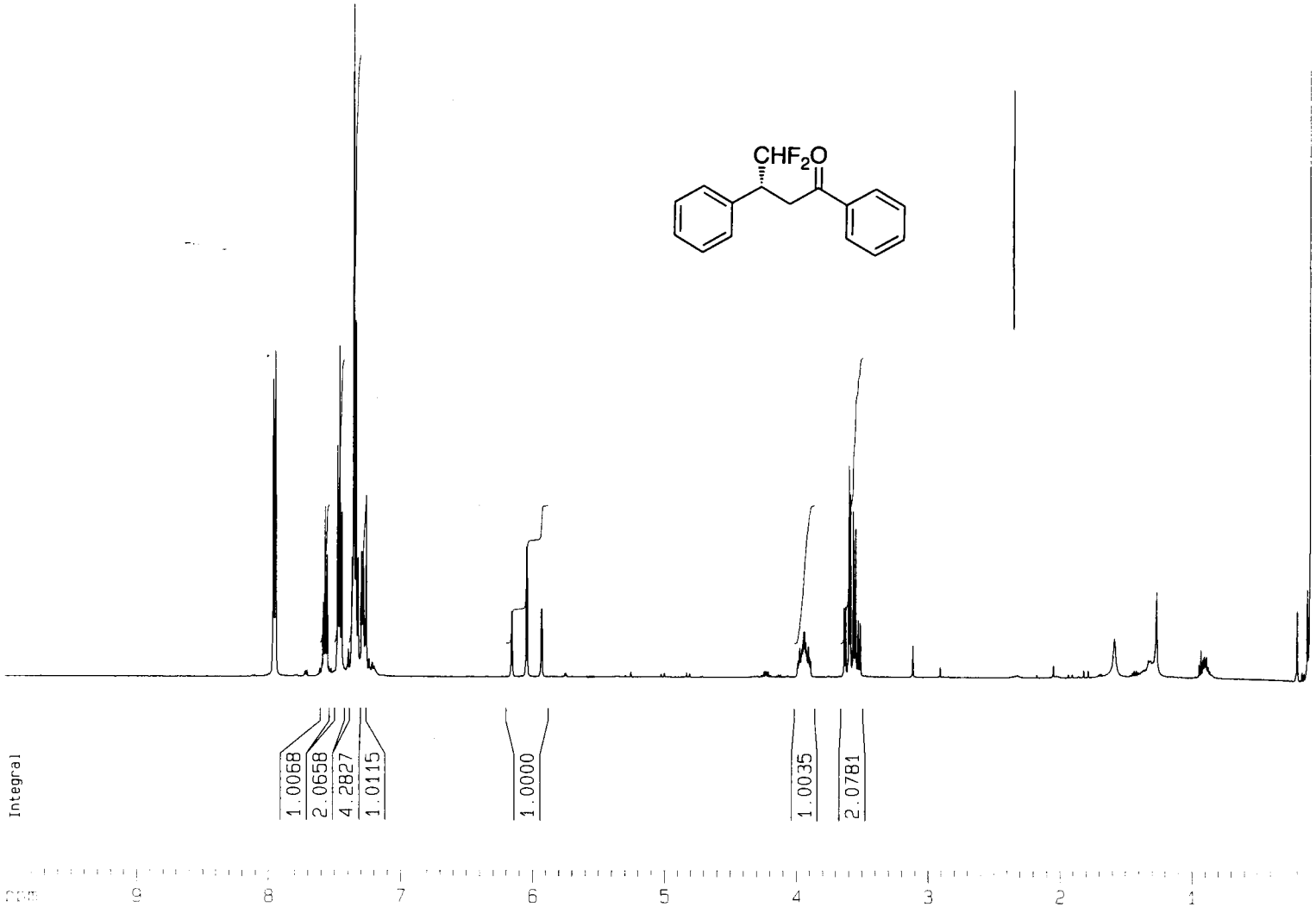
F2 - Processing parameters
SI 32768
SF 500.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 11.00 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

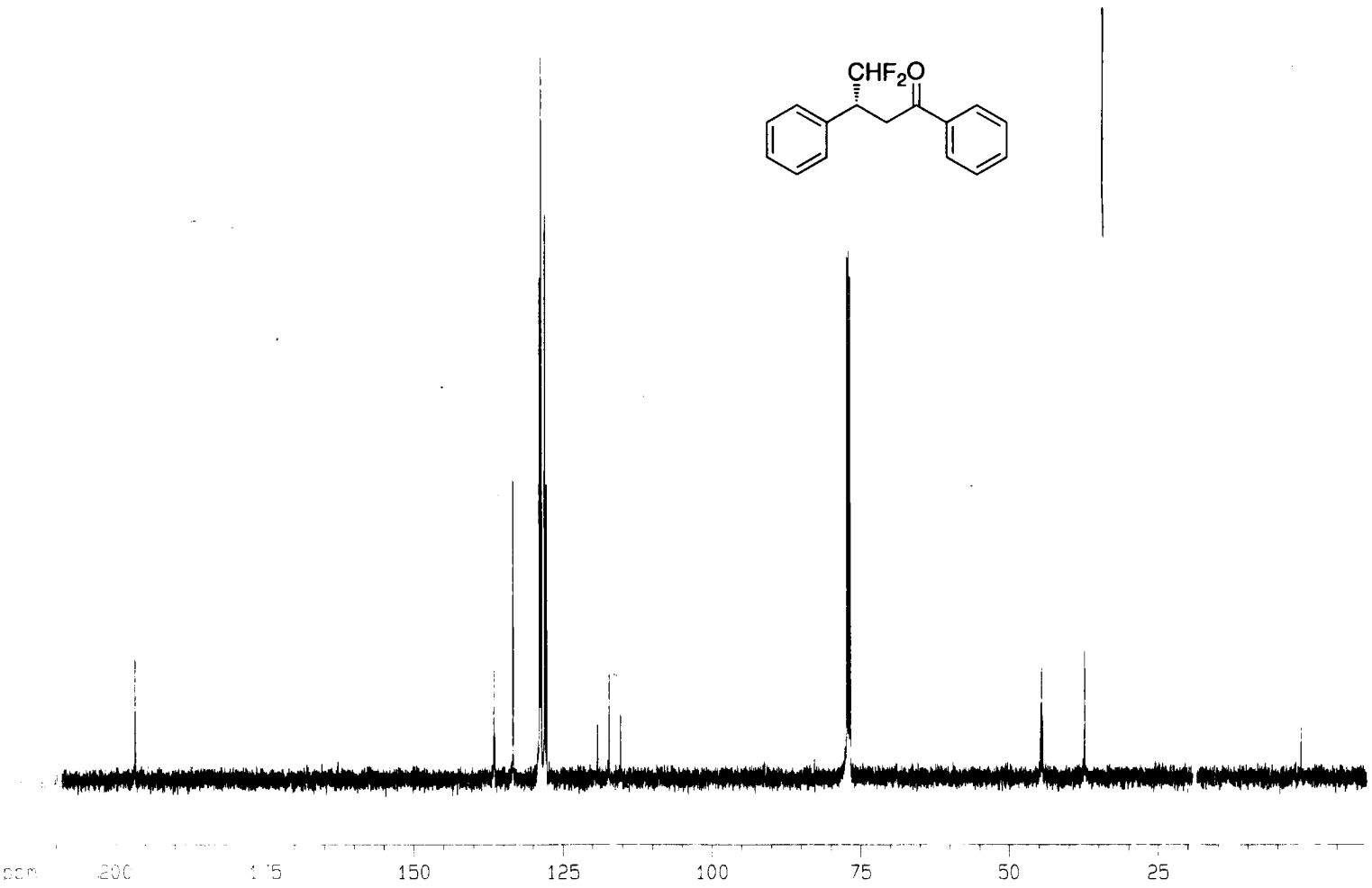



```
Current Data Parameters
NAME      tanaka-04.5.19-1
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20040519
Time               19.05
INSTRUM           drx500
PROBHD   5 mm Multinucl
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    2
SWH            30030.029 Hz
FIDRES          0.458222 Hz
AQ             1.0912244 sec
RG               2580.3
DW                16.650 usec
DE                 6.00 usec
TE                297.4 K
D1            0.50000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 5.70 usec
PL1               -2.00 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            100.00 usec
PL2               -6.00 dB
PL12              13.74 dB
PL13              13.74 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577951 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                10.60 cm
F1P              200.000 ppm
F1             25151.56 Hz
F2P             -10.000 ppm
F2             -1257.58 Hz
PPMCM           10.50000 ppm/cm
HZCM         1320.45679 Hz/cm
```

sample




```
Current Data Parameters
NAME                  f2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20041227
Time               15.54
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719923 sec
RG                   128
DW                48.400 usec
DE                 6.00 usec
TE                296.1 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.30 usec
PL1               -6.00 dB
SFO1         500.1330885 MHz

F2 - Processing parameters
SI                 32768
SF           500.1300129 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                225.49 cm
F1P               10.000 ppm
F1               5001.30 Hz
F2P                0.100 ppm
F2                 50.01 Hz
PPMCM            0.49500 ppm/cm
HZCM           247.56436 Hz/cm
```



[illegible]	[illegible]	sec
[illegible]	[illegible]	sec
ACQTIME	[illegible]	sec
PCPD1	[illegible]	sec

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

NUC1	13C	
P1	5.70	usec
PL1	-2.00	dB
SFO1	125.7703643	MHz

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

CPDPRG2	waltz16	
NUC2	1H	
PCPD2	100.00	usec
PL2	-6.00	dB
PL12	13.74	dB
PL13	13.74	dB
SFO2	500.1330005	MHz

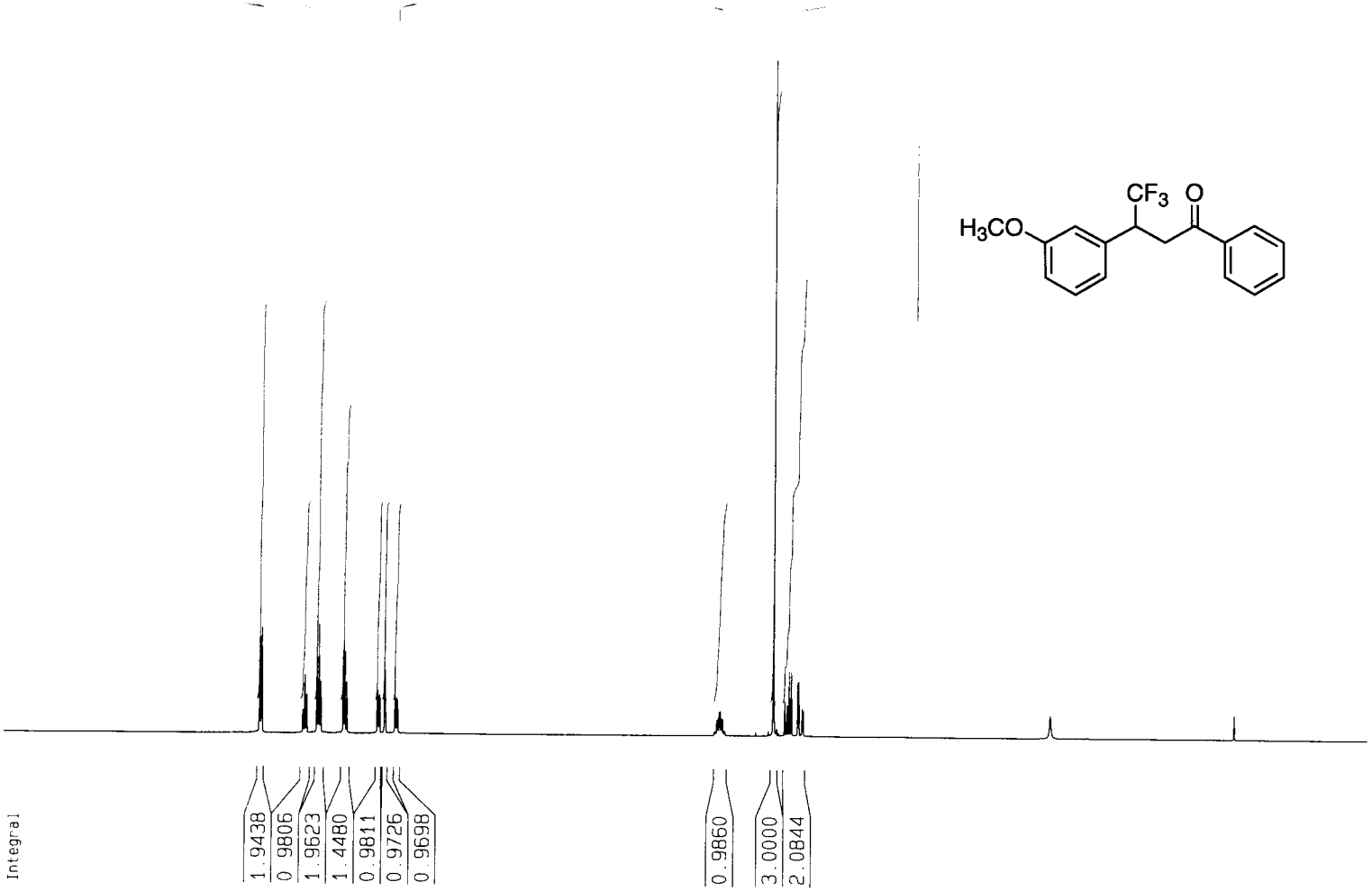
F2 - Processing parameters

SI	32768	
SF	125.7577969	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	0.10	

1D NMR plot parameters

CX	20.00	cm
CY	10.73	cm
F1P	219.000	ppm
F1	27540.96	Hz
F2P	-10.000	ppm
F2	-1257.58	Hz
PPMCM	11.45000	ppm/cm
HZCM	1439.92676	Hz/cm

sample



Current Data Parameters

NAME	morigaki060718
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20060718
Time	21.28
INSTRUM	drx500
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	645.1
DW	48.400 usec
DE	6.00 usec
TE	299.7 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

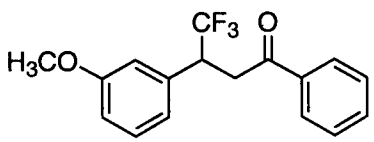
NUC1	1H
P1	10.00 usec
PL1	-6.00 dB
SFO1	500.1330885 MHz

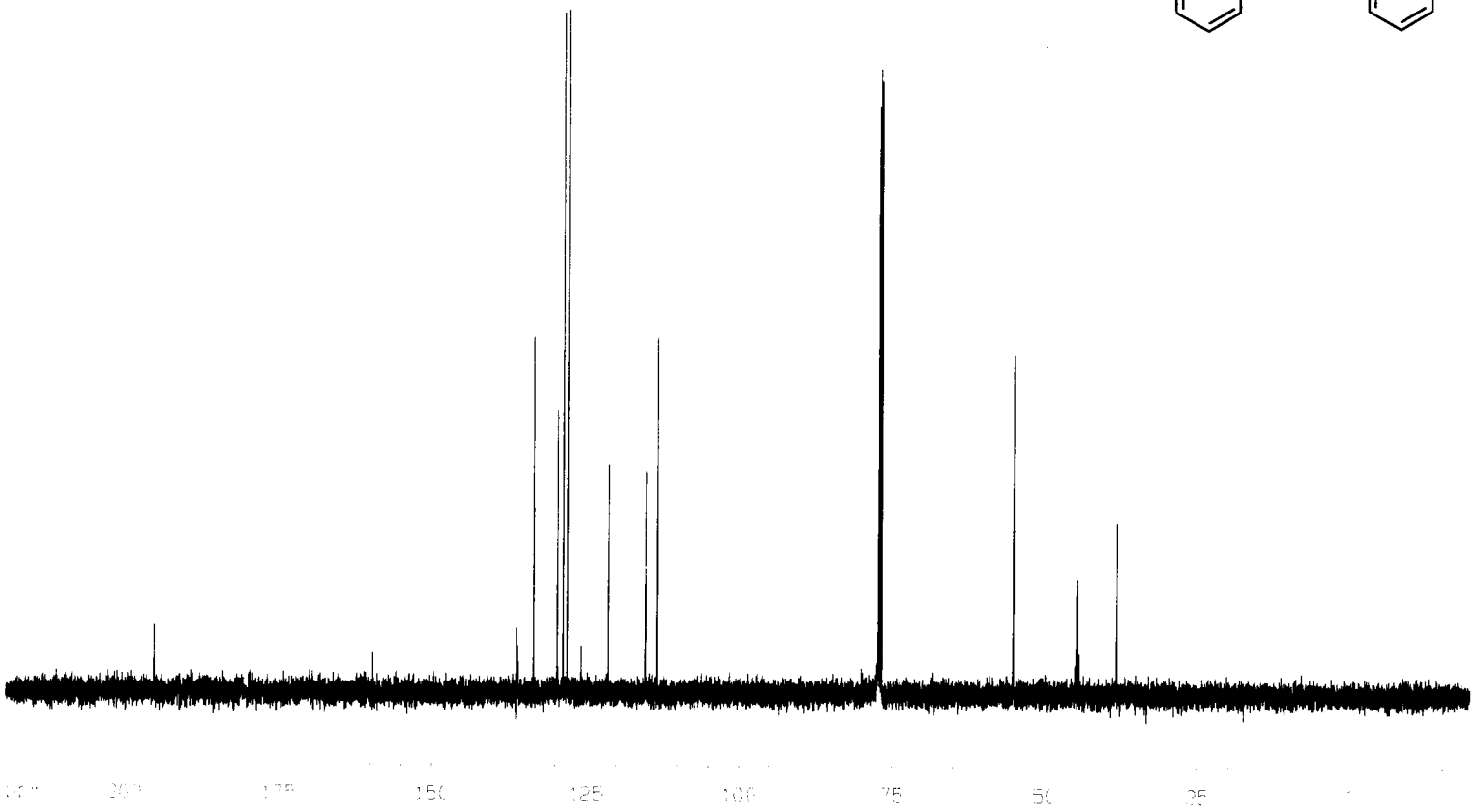
F2 - Processing parameters

SI	32768
SF	500.1300131 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

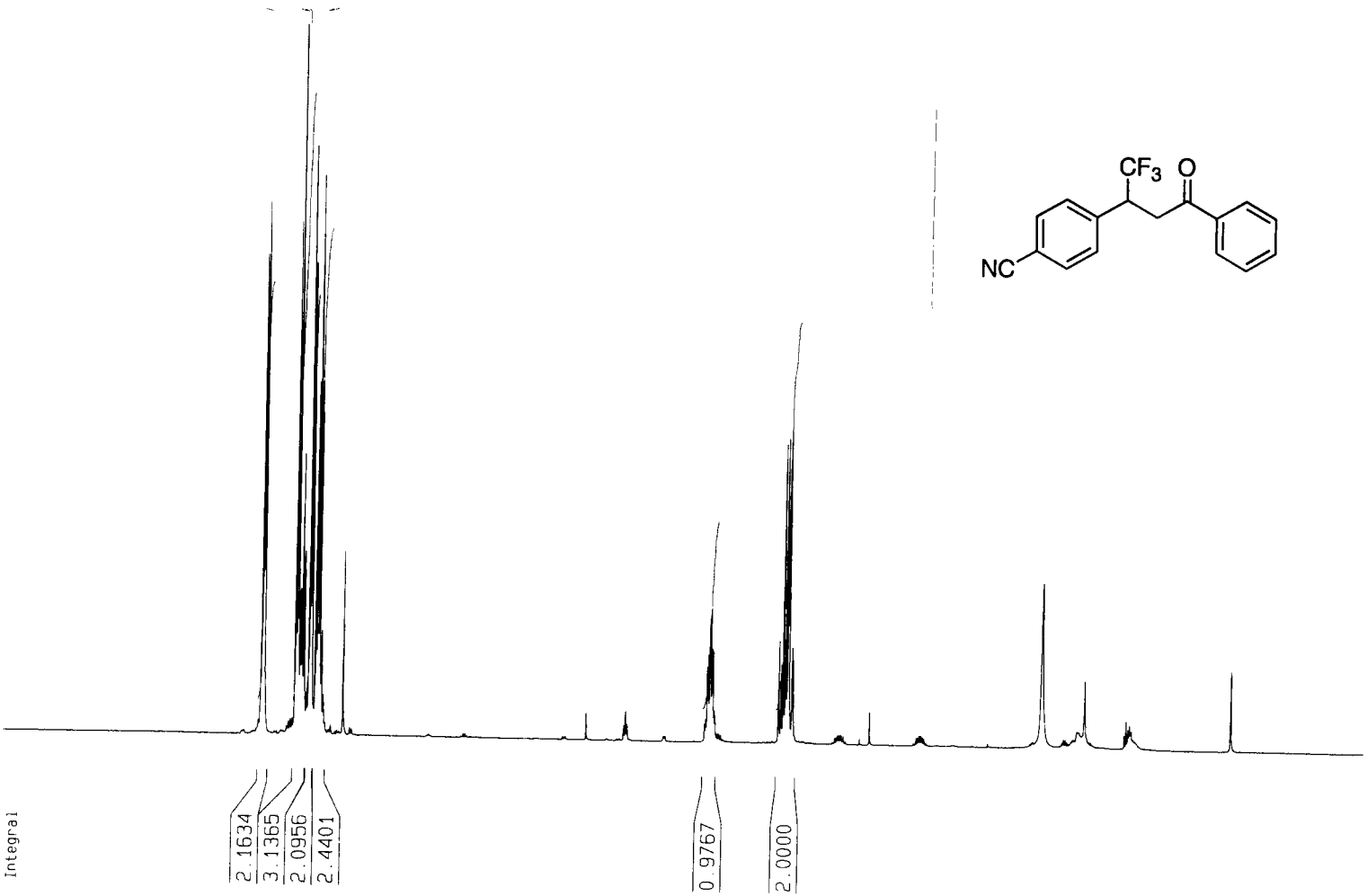
CX	20.00 cm
CY	10.03 cm
F1P	10.000 ppm
F1	5001.30 Hz
F2P	-1.000 ppm
F2	-500.13 Hz
PPMCM	0.55000 ppm/cm
HZCM	275.07150 Hz/cm






```
Current Data Parameters
NAME      morigaki060718
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20060718
Time               21.37
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    2
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912244 sec
RG               1824.6
DW               16.650 usec
DE                 6.00 usec
TE                300.0 K
D1           0.50000000 sec
d11          0.03000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                11.00 usec
PL1               -3.00 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2            100.00 usec
PL2               -6.00 dB
PL12              17.00 dB
PL13              19.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577914 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                 9.44 cm
F1P             219.373 ppm
F1             27587.91 Hz
F2P             -19.419 ppm
F2             -2442.12 Hz
PPMCM          11.93963 ppm/cm
HZCM         1501.50146 Hz/cm
```

sample



Current Data Parameters

NAME	gak1060711
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20060712
Time	21.15
INSTRUM	drx500
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	362
DW	48.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

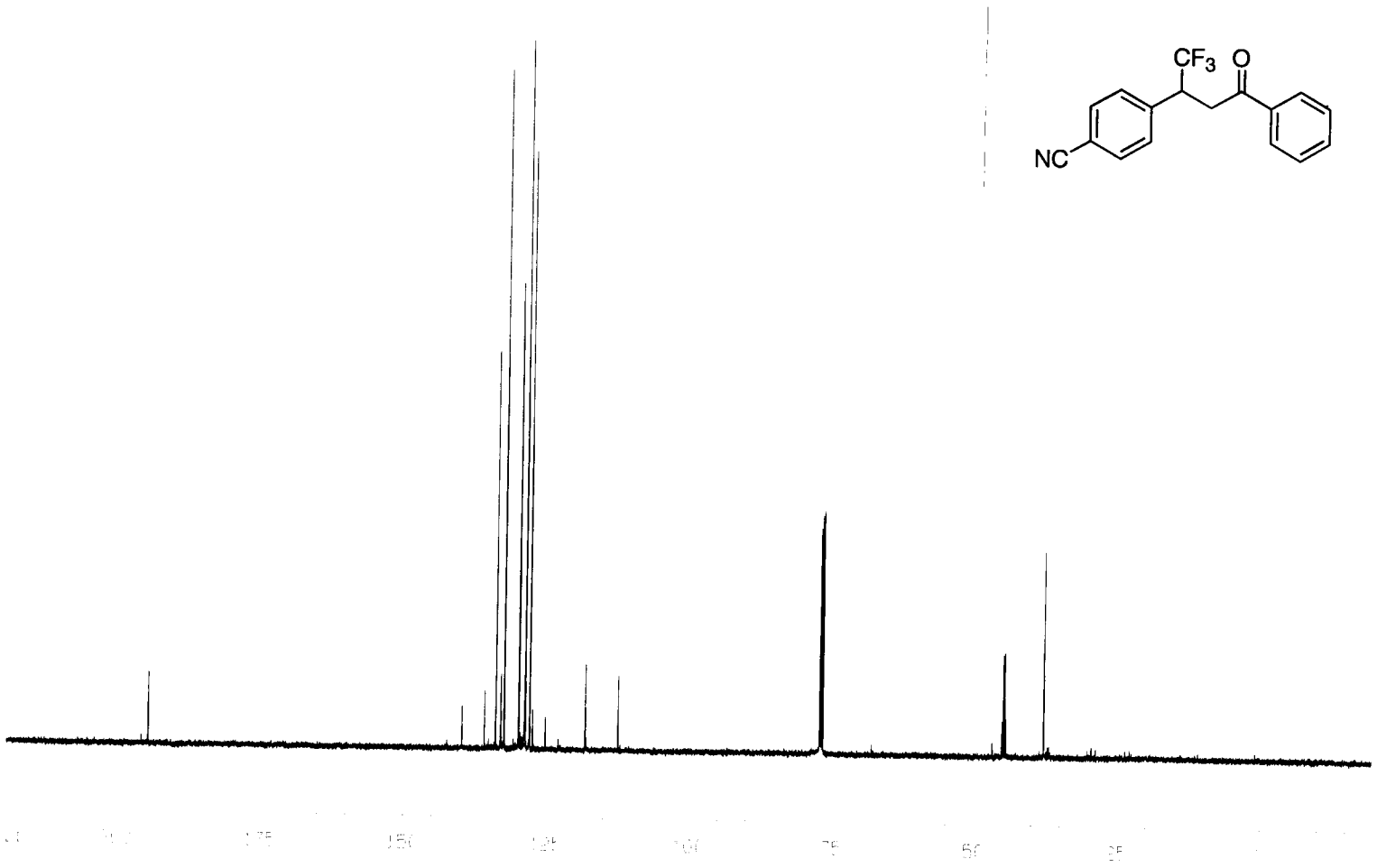
NUC1	1H
P1	10.00 usec
PL1	-6.00 dB
SFO1	500.1330885 MHz

F2 - Processing parameters

SI	32768
SF	500.1300131 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

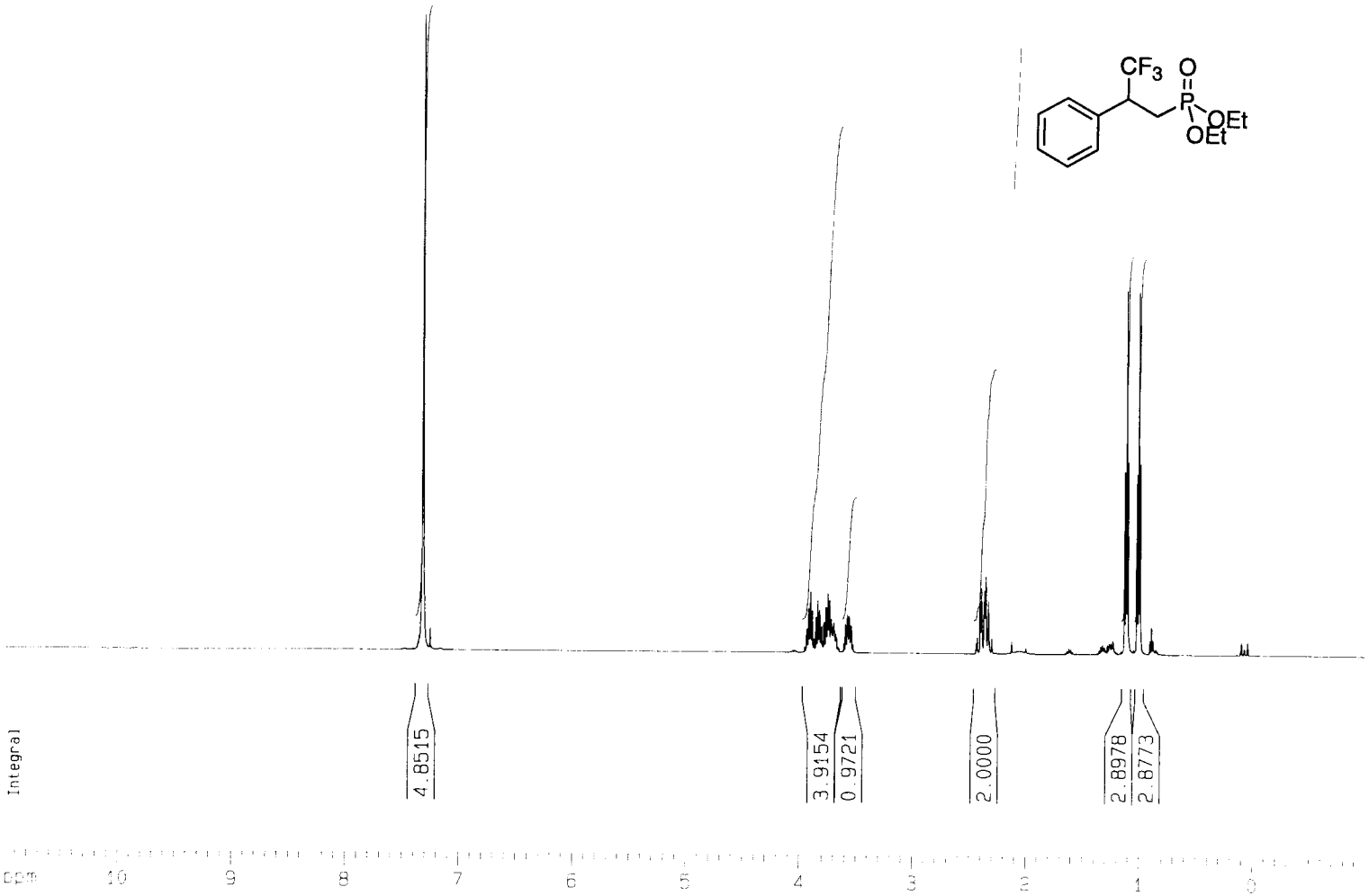
1D NMR plot parameters

CX	20.00 cm
CY	10.69 cm
F1P	10.000 ppm
F1	5001.30 Hz
F2P	-1.000 ppm
F2	-500.13 Hz
PPMCM	0.55000 ppm/cm
HZCM	275.07150 Hz/cm

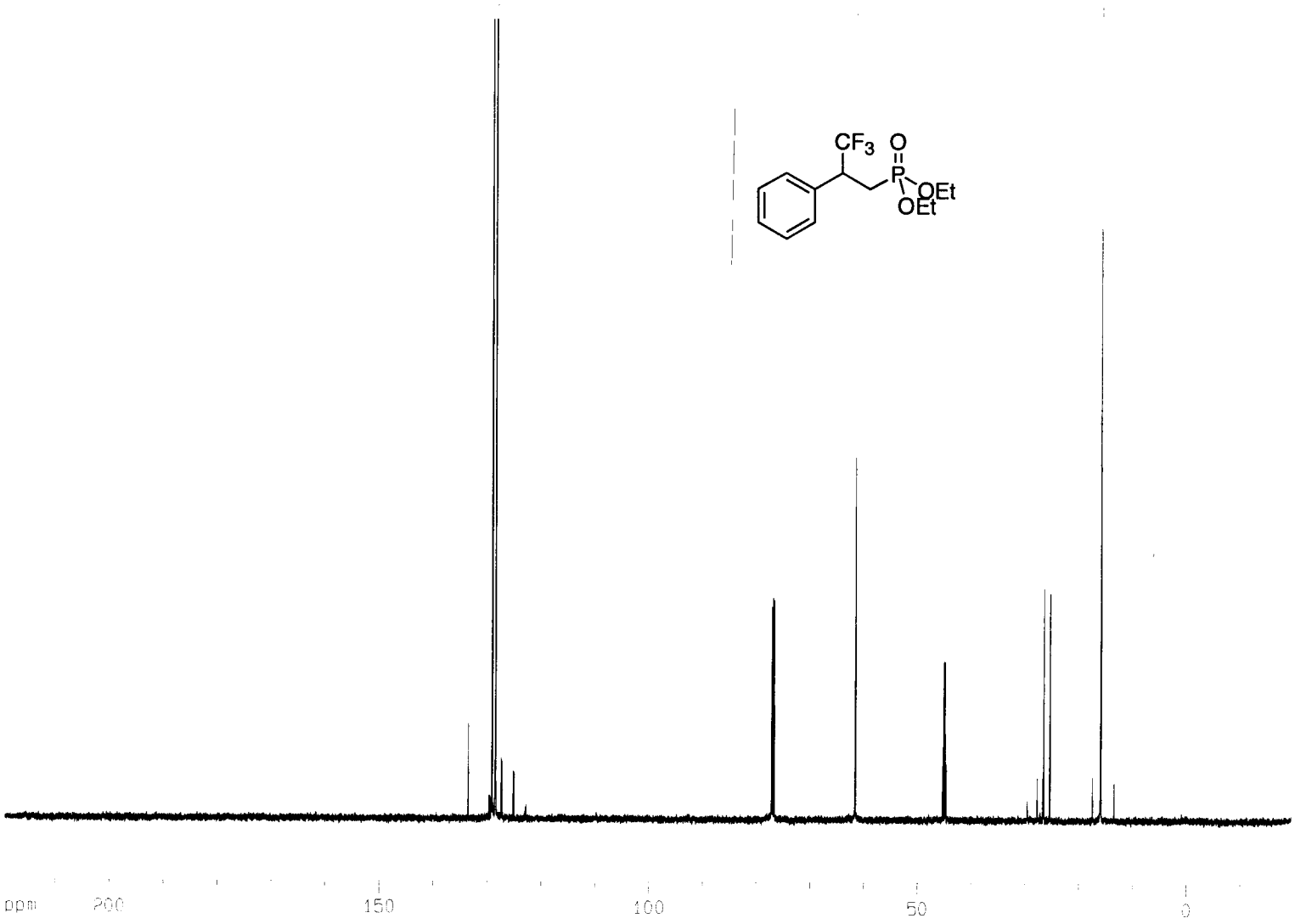



```
Current Data Parameters
NAME          gak1060711
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_          20060712
Time              21.52
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1280
DS                    2
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912244 sec
RG               1824.6
DW               16.650 usec
DE                6.00 usec
TE               300.6 K
D1            0.50000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                11.00 usec
PL1               -3.00 dB
SFO1         125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2               -6.00 dB
PL12              17.00 dB
PL13              19.00 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577932 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                10.43 cm
F1P            219.359 ppm
F1            27586.08 Hz
F2P            -19.434 ppm
F2            -2443.95 Hz
PPMCM          11.93963 ppm/cm
HZCM         1501.50146 Hz/cm
```

sample




```
Current Data Parameters
NAME      morigaki060807
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20060807
Time              21.59
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ            3.1719923 sec
RG                   57
DW               48.400 usec
DE                6.00 usec
TE               300.9 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.00 usec
PL1               -6.00 dB
SFO1        500.1330885 MHz

F2 - Processing parameters
SI                32768
SF          500.1300131 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                 9.40 cm
F1P               11.000 ppm
F1               5501.43 Hz
F2P               -1.000 ppm
F2               -500.13 Hz
PPMCM            0.60000 ppm/cm
HZCM           300.07800 Hz/cm
```




```
Current Data Parameters
NAME      morigaki060807
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20060807
Time               22.15
INSTRUM          drx500
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    2
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912244 sec
RG               1149.4
DW               16.650 usec
DE                 6.00 usec
TE                301.3 K
D1           0.50000000 sec
d11          0.03000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                11.00 usec
PL1               -3.00 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2            100.00 usec
PL2               -6.00 dB
PL12              17.00 dB
PL13              19.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577960 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  0.00

1D NMR plot parameters
CX                 20.00 cm
CY                 28.16 cm
F1P             219.337 ppm
F1             27583.33 Hz
F2P             -19.456 ppm
F2             -2446.70 Hz
PPMCM           11.93963 ppm/cm
HZCM          1501.50146 Hz/cm
```