

Phospha-Michael Additions to Activated Internal Alkenes: Steric and Electronic Effects

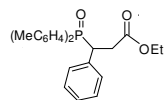
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^1H NMR spectrum (CDCl_3 , 25 $^\circ\text{C}$)

Ethyl 3-((4-methylphenyl)phosphoryl)-3-phenylpropanoate (1)

Std proton

File: home/ras/Desktop/600ras042111.010.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras042111.010

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 9615.4 Hz

Single scan

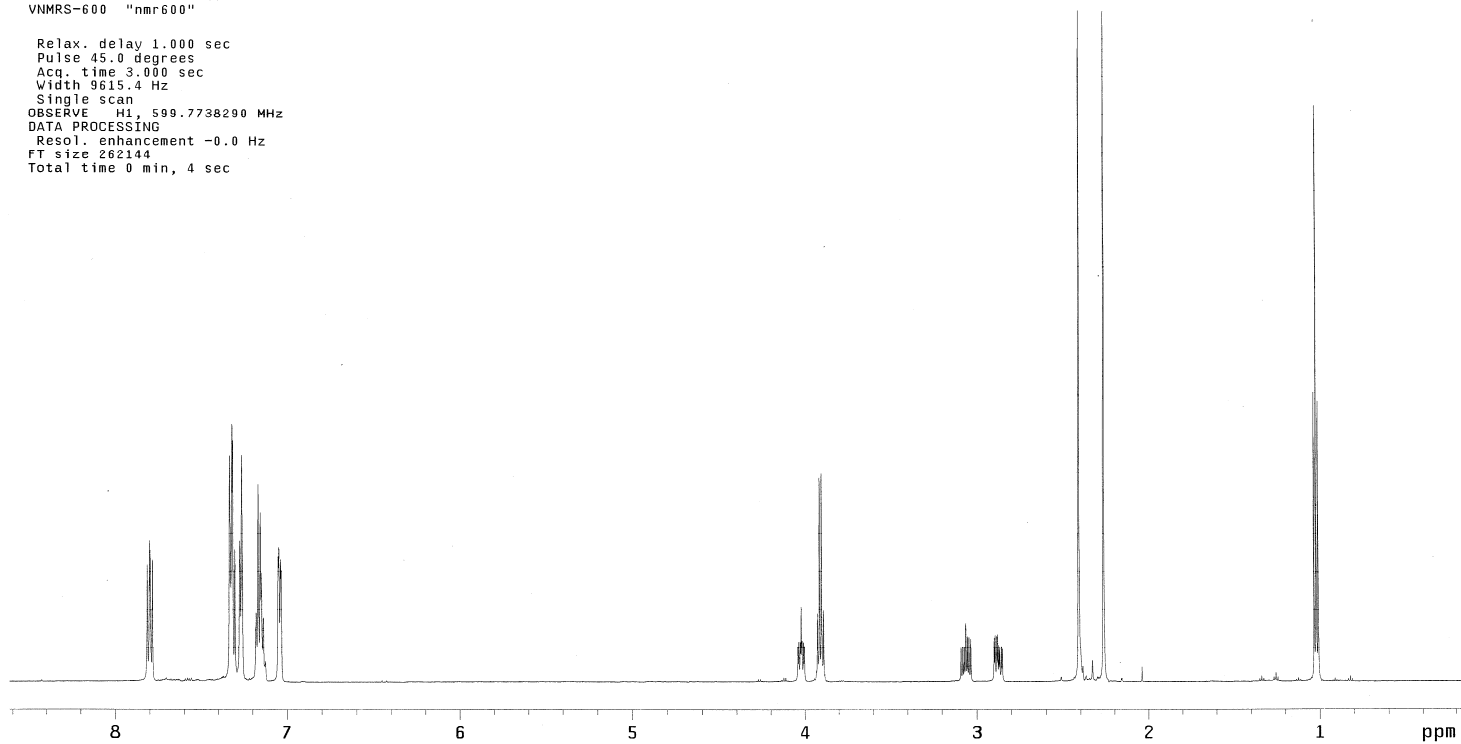
OBSERVE H1, 599.7738290 MHz

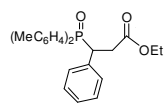
DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 262144

Total time 0 min, 4 sec





Ethyl 3-[bis(4-methylphenyl)phosphinyl]-3-phenylpropanoate (1)

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Probe tuning parameter

File: home/ras/Desktop/600ras042111.011.fid

Pulse Sequence: s2pul

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras042111.011

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

192 repetitions

OBSERVE C13, 150.8132467 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

Continuously on

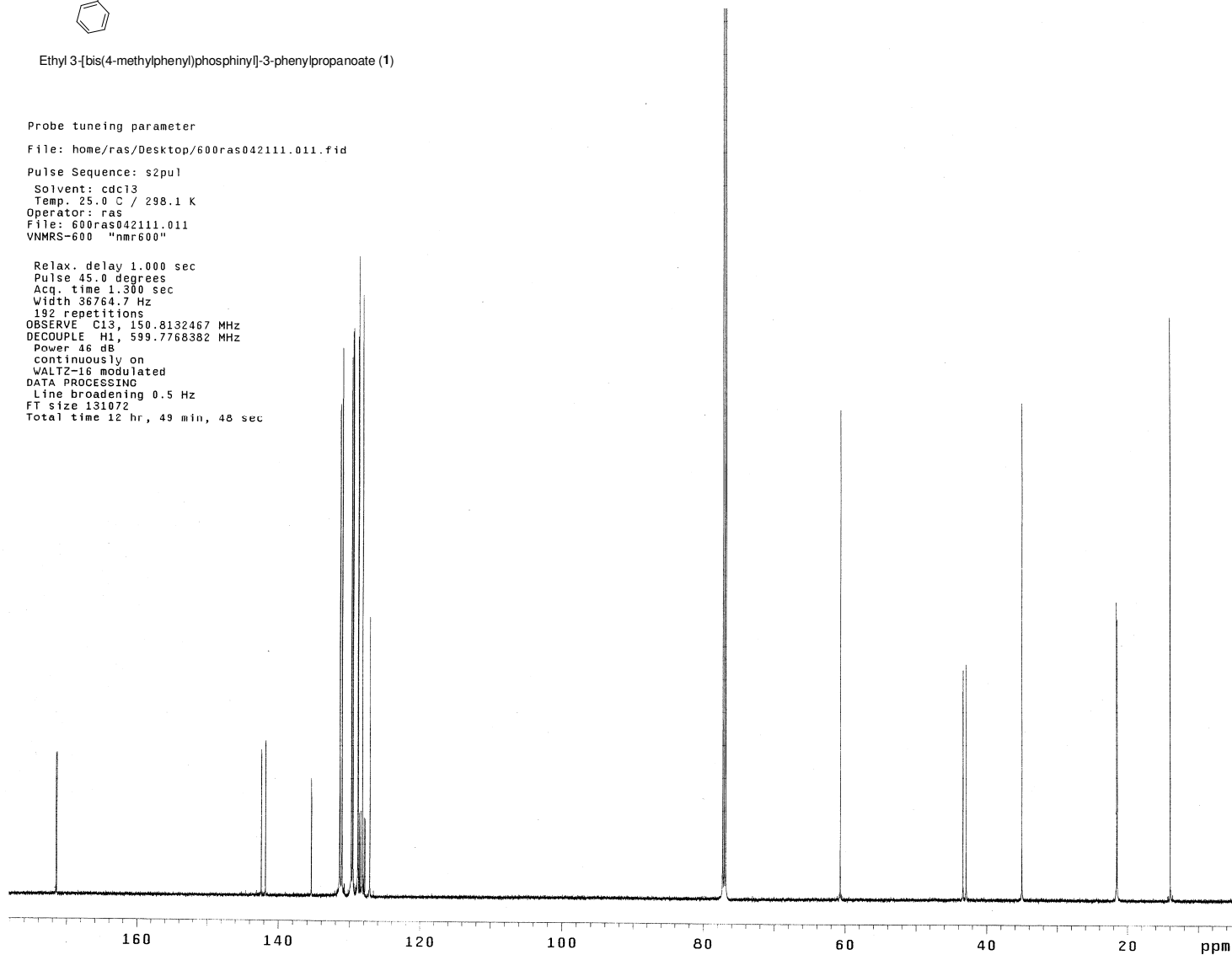
VALTZ-16 modulated

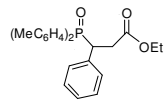
DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 12 hr, 49 min, 48 sec





$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Ethyl 3-[bis(4-methylphenyl)phosphiny]-3-phenylpropanoate (1)

Std phosphorus

File: home/ras/Desktop/600ras042311.001.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: ras

File: 600ras042311.001

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

12 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

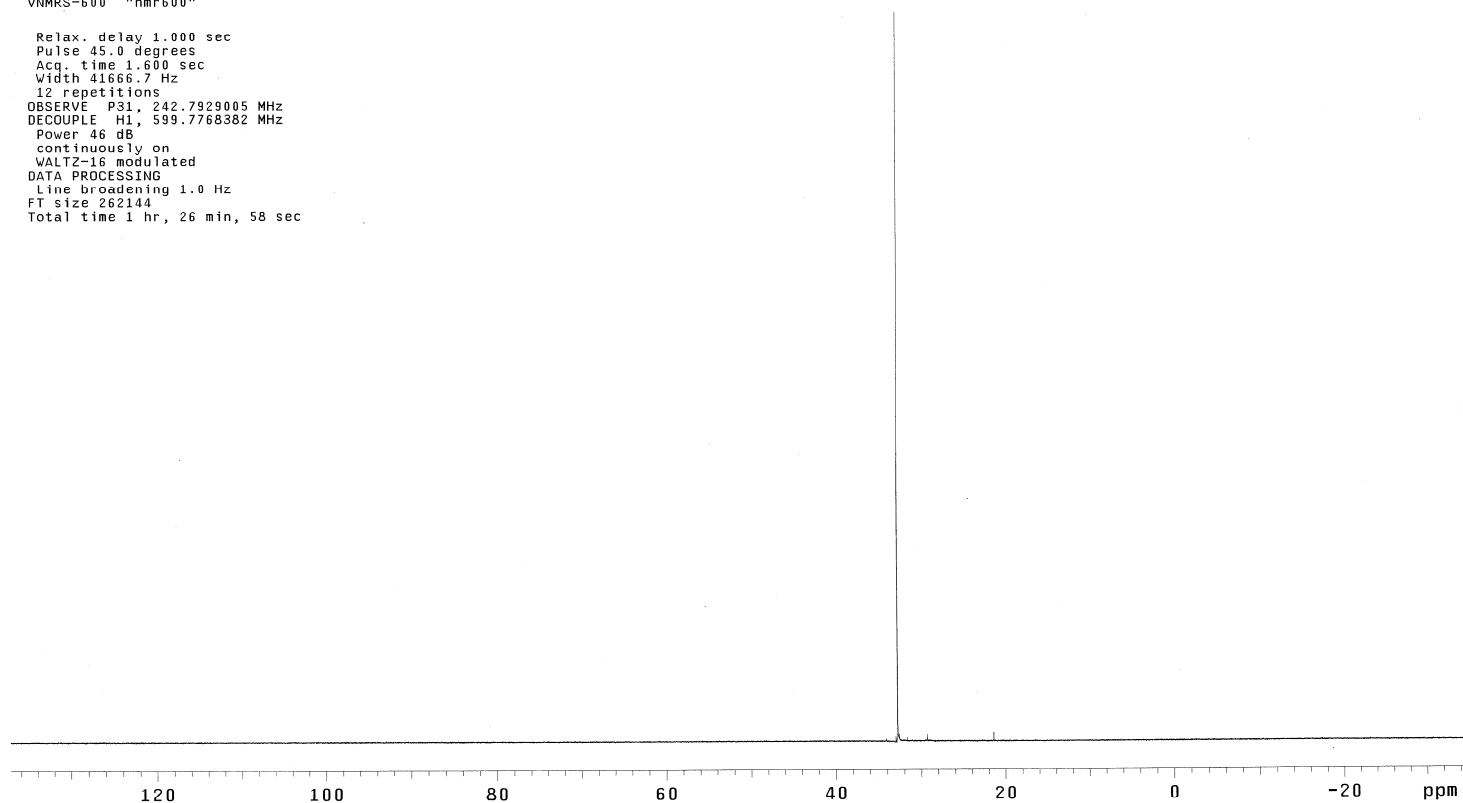
WALTZ-16 modulated

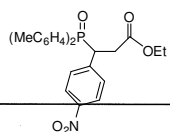
DATA PROCESSING

Line broadening 1.0 Hz

FT size 262144

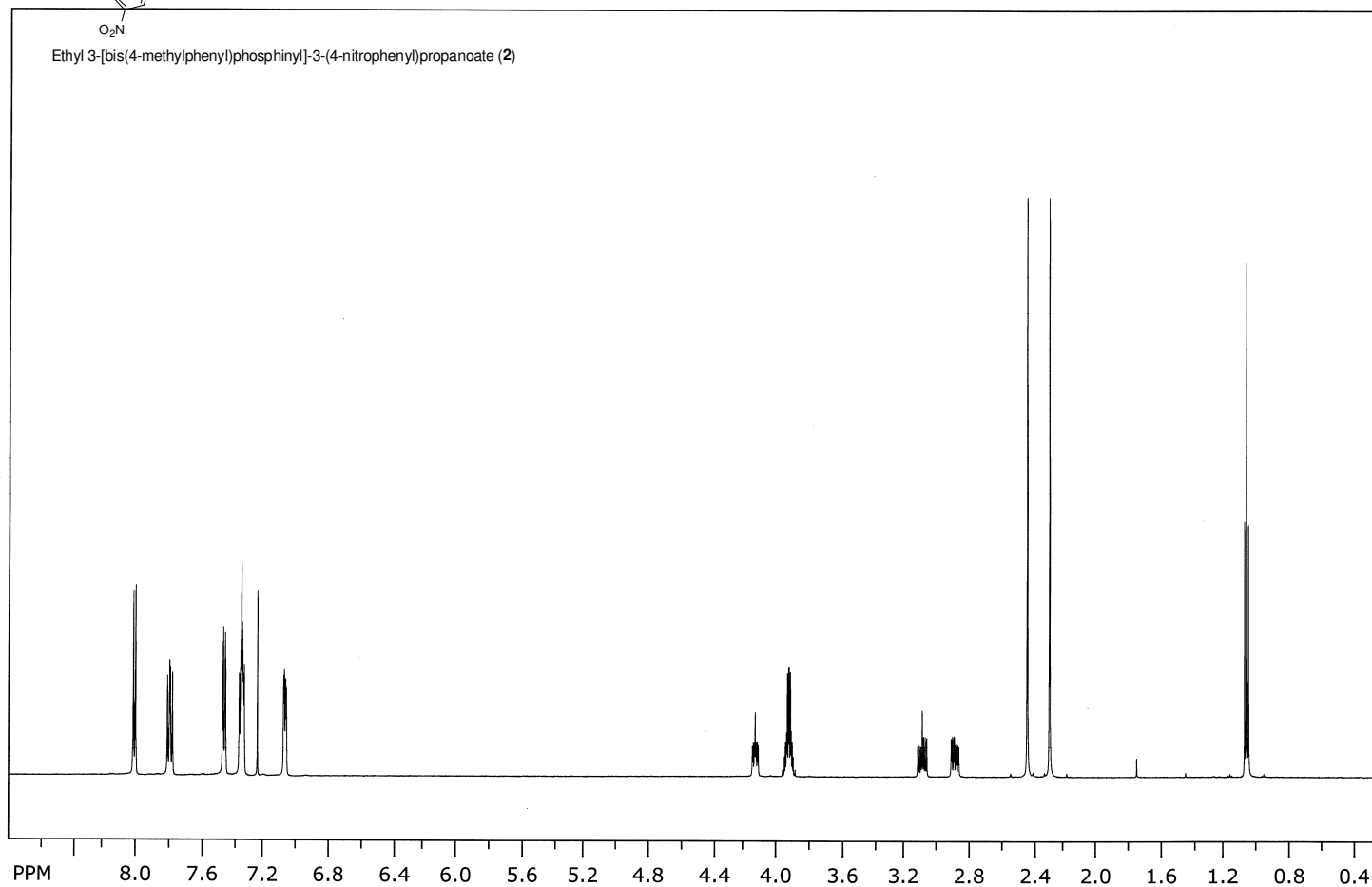
Total time 1 hr, 26 min, 58 sec





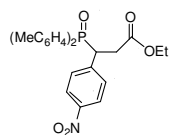
¹H NMR spectrum (CDCl₃, 25 °C)

Ethyl 3-[bis(4-methylphenyl)phosphinyl]-3-(4-nitrophenyl)propanoate (2)



file: ...-2011\600\600ras041411.001.fid\fid block# 1 expt: "s2pul"
 transmitter freq.: 599.777438 MHz
 time domain size: 39396 points
 width: 9615.38 Hz = 16.0316 ppm = 0.244070 Hz/pt
 number of scans: 1

freq. of 0 ppm: 599.773833 MHz
 processed size: 65536 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 206.974 ppm/cm: 0.34508



Ethyl 3-[bis(4-methylphenyl)phosphinyl]-3-(4-nitrophenyl)propanoate (2)

Probe tuning parameter

File: home/ras/Desktop/600ras041411.002.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras041411.002

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

20000 repetitions

OBSERVE C13, 150.8132455 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

WALTZ-16 modulated

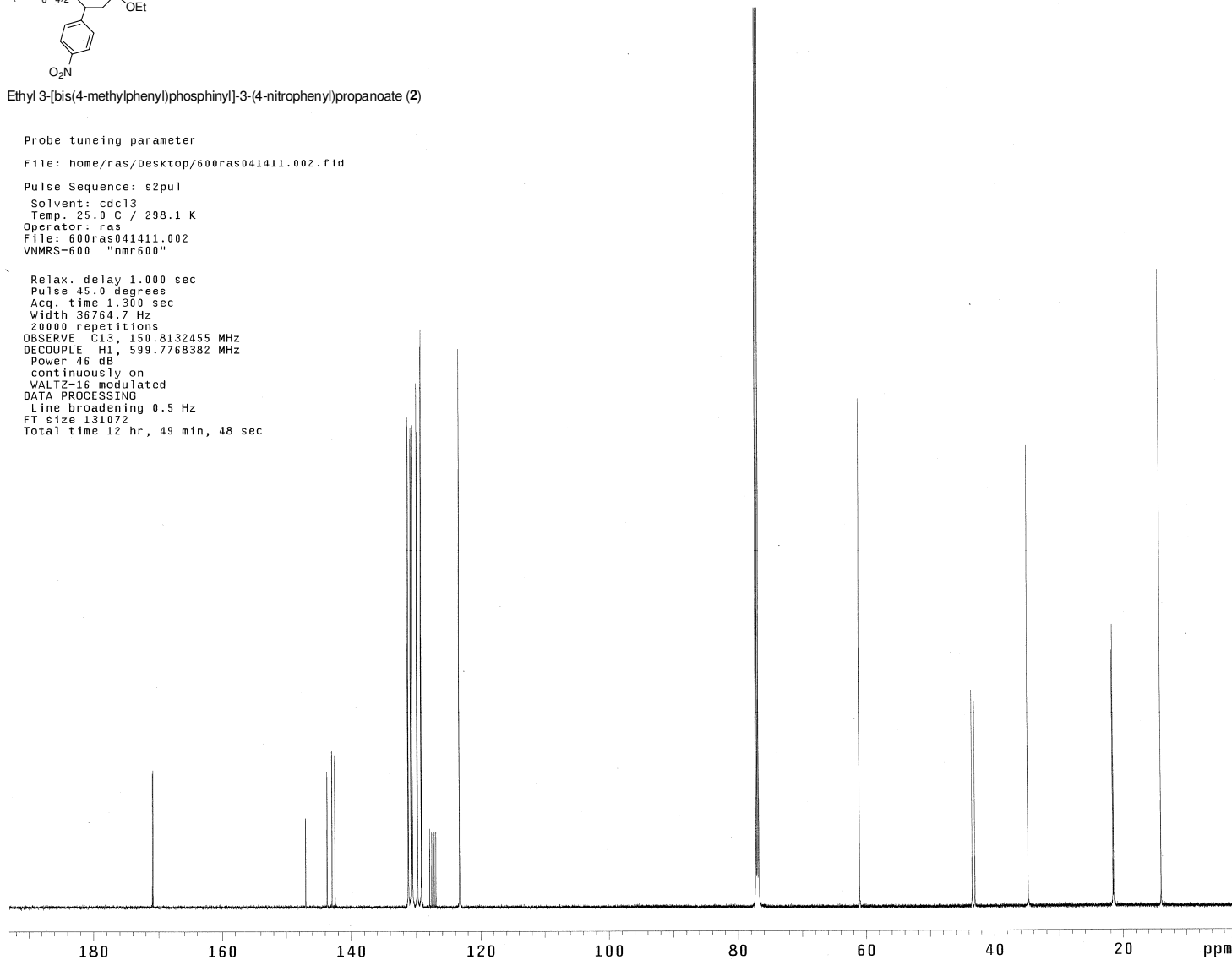
DATA PROCESSING

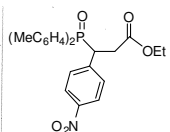
Line broadening 0.5 Hz

FT size 131072

Total time 12 hr, 49 min, 48 sec

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)





$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Ethyl 3-[[bis(4-methylphenyl)phosphoryl]-3-(4-nitrophenyl)propanoate (2)

Std phosphorus

File: home/ras/Desktop/600ras041811.004.fid

Pulse Sequence: s2pu1

Solvent: cdcl_3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras041811.004

VNMR-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

152 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

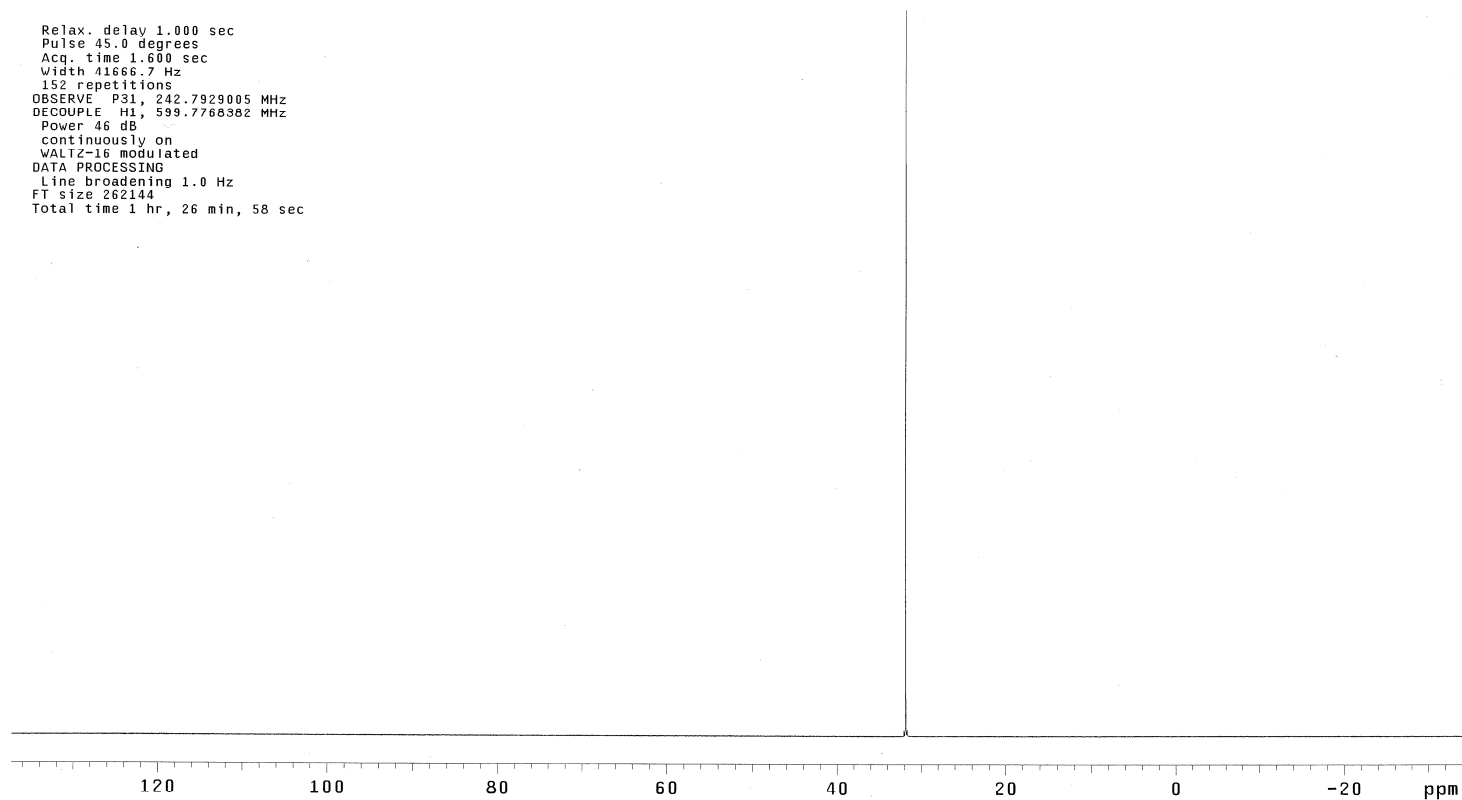
WALTZ-16 modulated

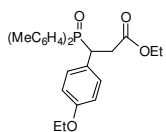
DATA PROCESSING

Line broadening 1.0 Hz

FT size 262144

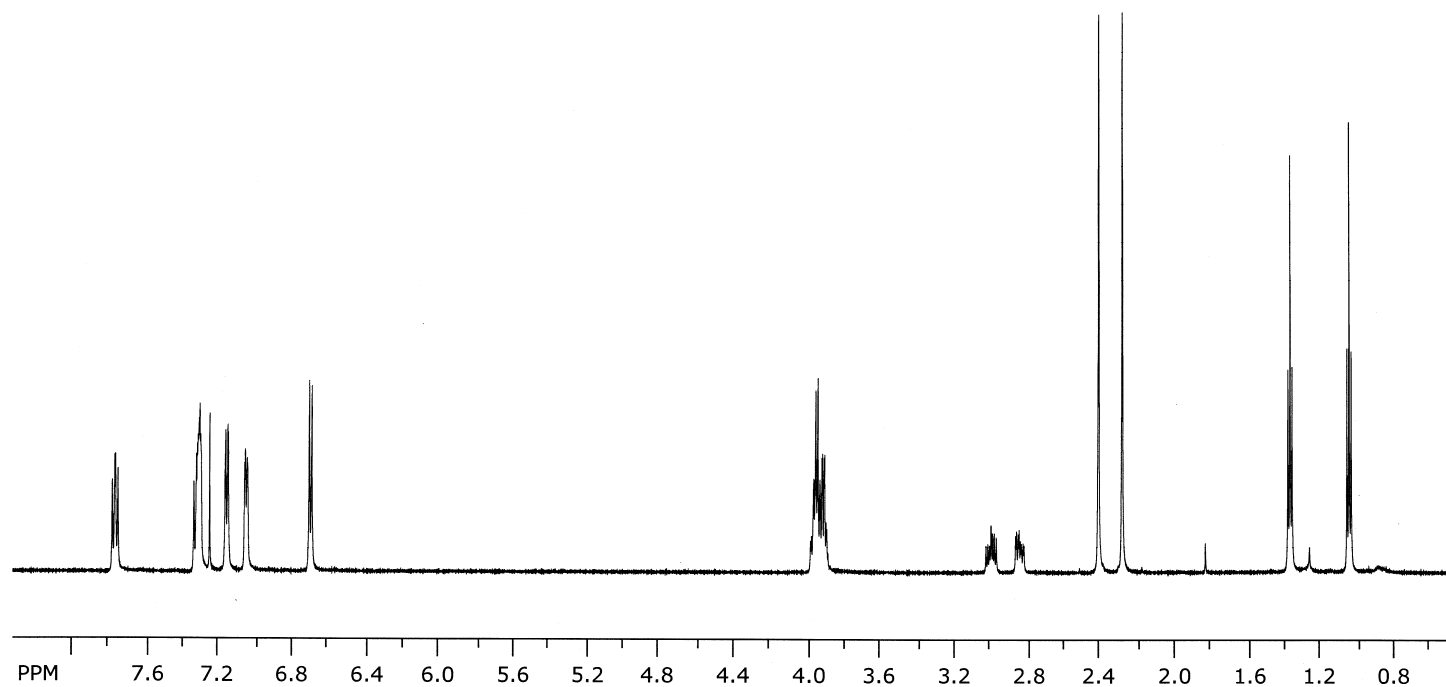
Total time 1 hr, 26 min, 58 sec





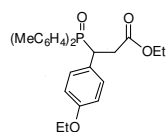
3-[Bis(4-methylphenyl)phosphiny]-3-(4-ethoxyphenyl)propanoate (**3**)

^1H NMR spectrum (CDCl_3 , 25 °C)



file: ...-2011\600\600ras070411.004.fid\fid block# 1 expt: "s2pul"
 transmitter freq.: 599.777438 MHz
 time domain size: 57692 points
 width: 9615.38 Hz = 16.0316 ppm = 0.166668 Hz/pt
 number of scans: 1

freq. of 0 ppm: 599.773832 MHz
 processed size: 131072 complex points
 LB: -0.200 GF: 0.0000
 Hz/cm: 189.177 ppm/cm: 0.31541



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

3-[Bis(4-methylphenyl)phosphinyl]-3-(4-ethoxyphenyl)propanoate (3)

Std carbon

File: home/ras/Desktop/600ras053111.005.fid

Pulse Sequence: s2pul

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras053111.005

VNMR-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

10000 repetitions

OBSERVE C13, 150.8132461 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

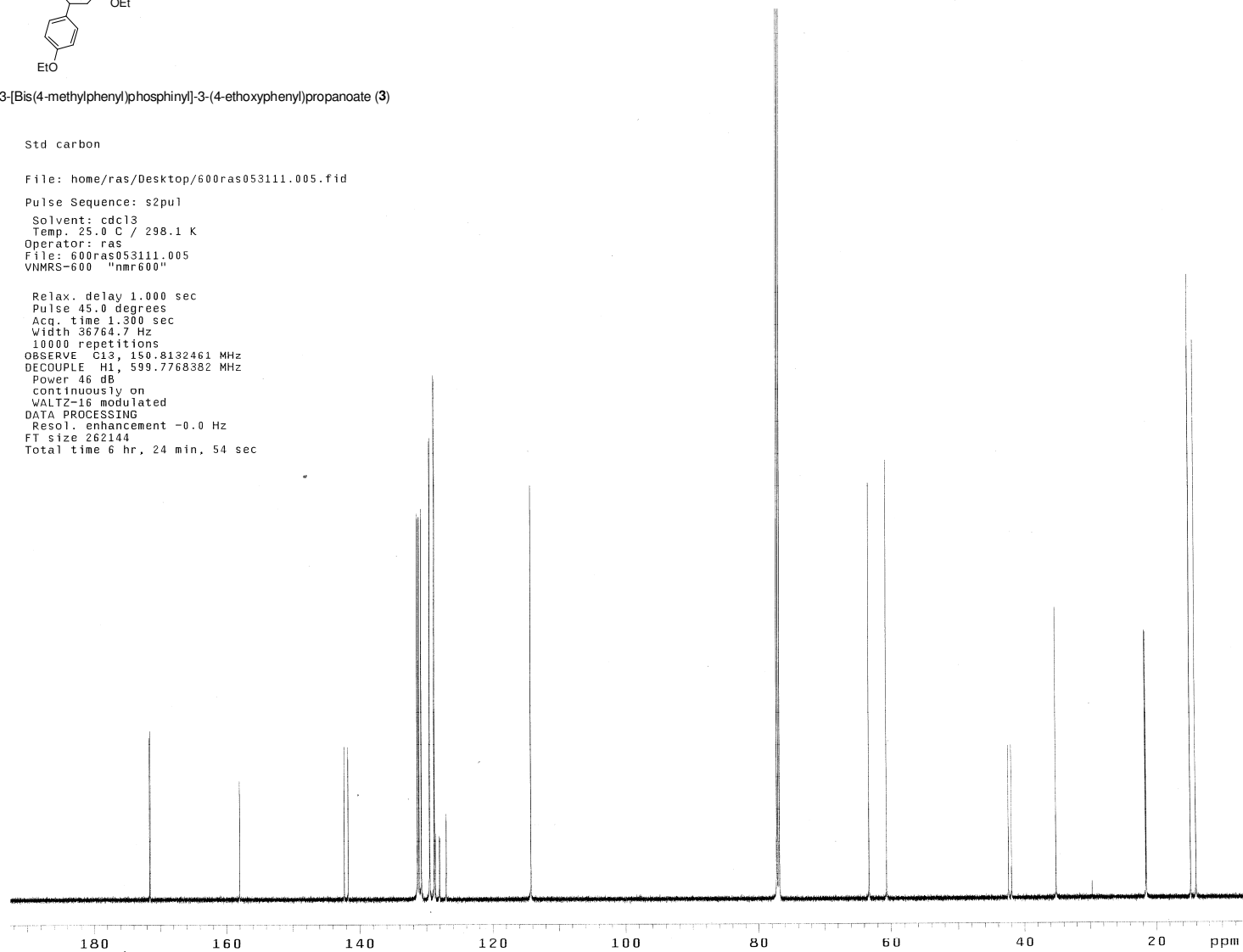
WALTZ-16 modulated

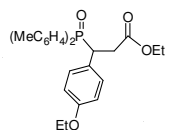
DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 262144

Total time 6 hr, 24 min, 54 sec





3-[Bis(4-methylphenyl)phosphinyl]-3-(4-ethoxyphenyl)propanoate (3)

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

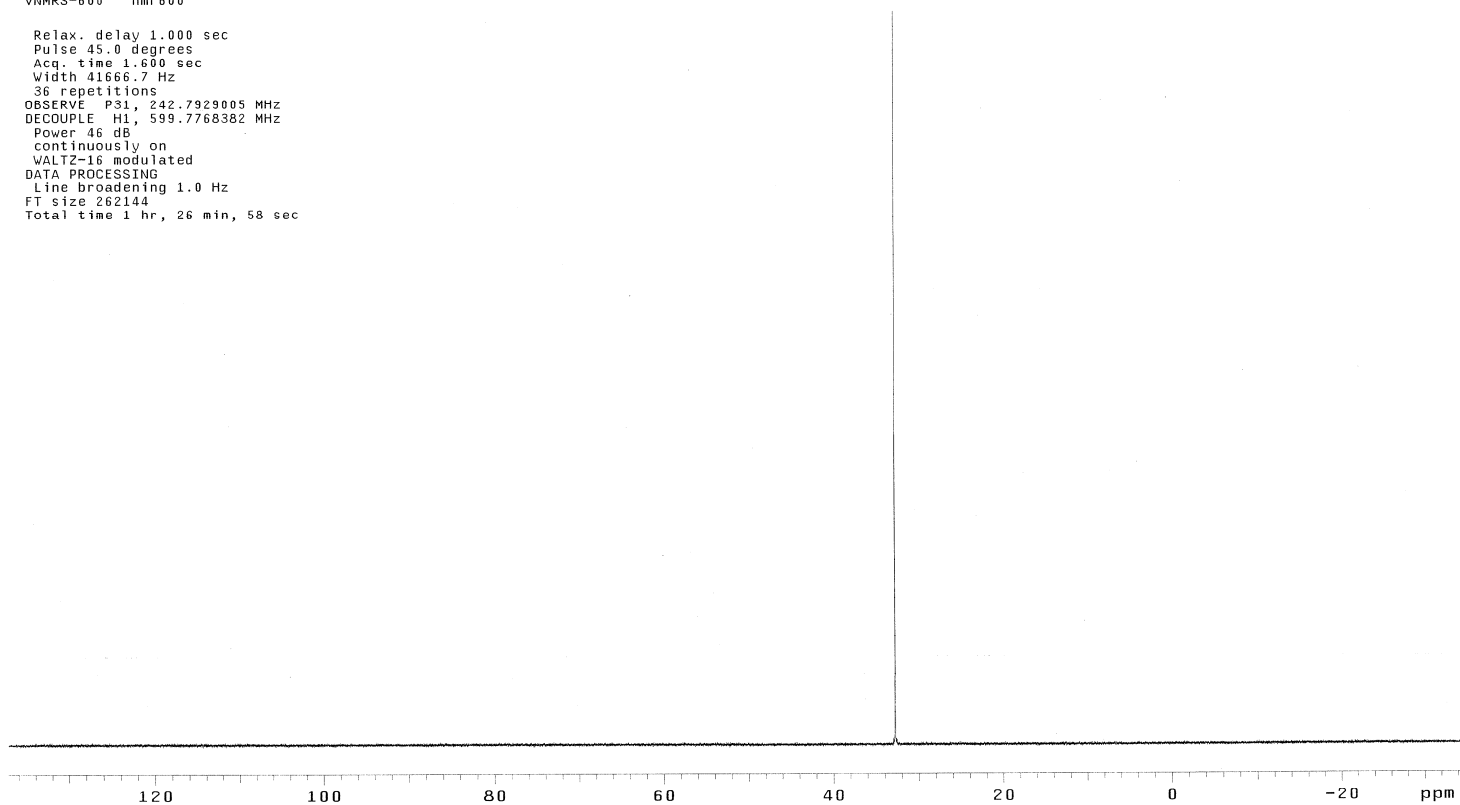
Std phosphorus

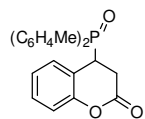
File: home/ras/Desktop/600ras070411.005.fid

Pulse Sequence: s2pu1

Solvent: cdcl_3
Temp. 25.0 C / 298.1 K
Operator: ras
File: 600ras070411.005
VNMR-600 "nmr600"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.600 sec
Width 41666.7 Hz
36 repetitions
OBSERVE P31, 242.7929005 MHz
DECOUPLE H1, 599.7768382 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 262144
Total time 1 hr, 26 min, 58 sec



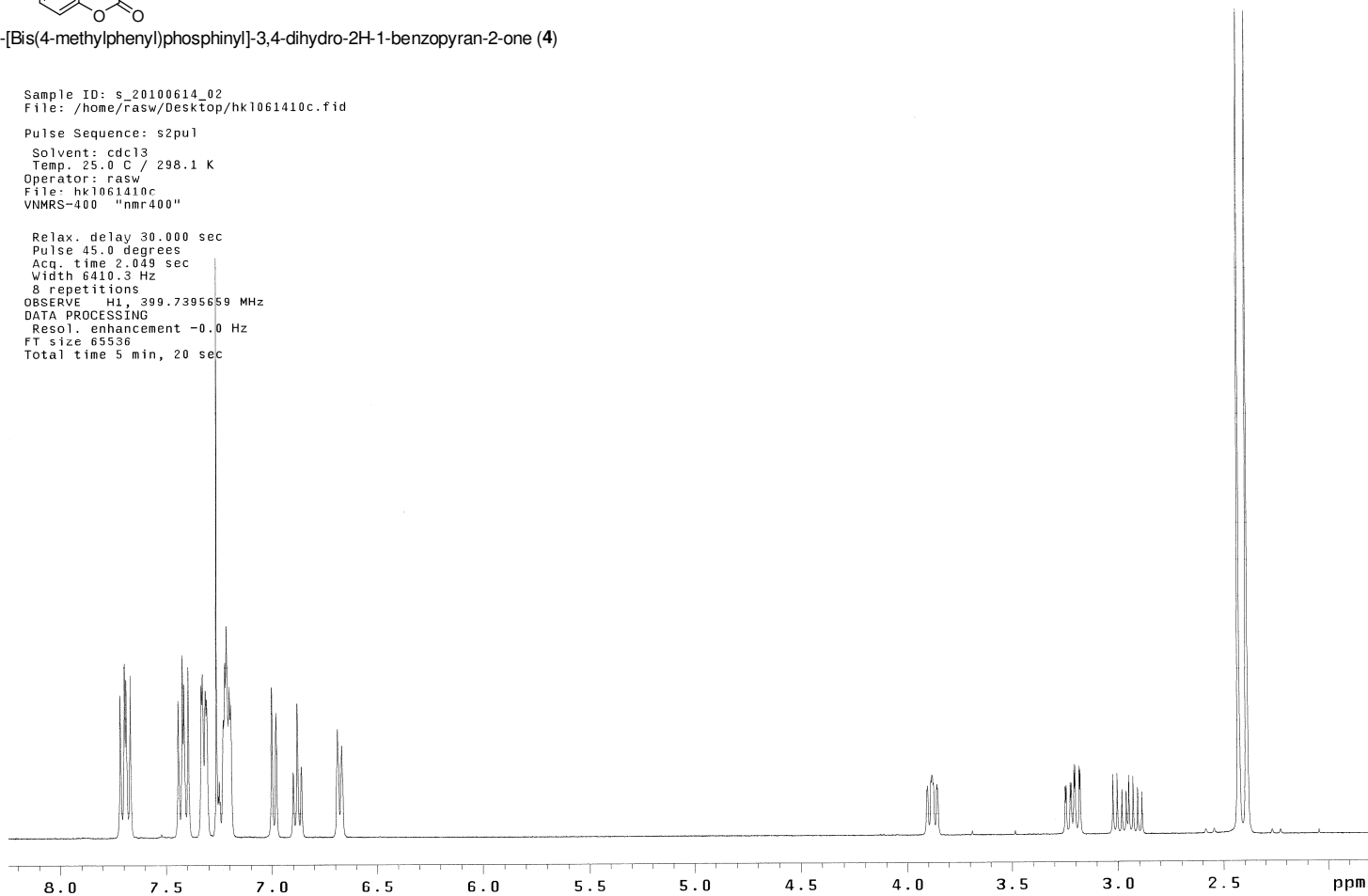


¹H NMR spectrum (CDCl₃, 25 °C)

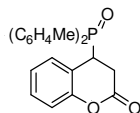
4-[Bis(4-methylphenyl)phosphinyl]-3,4-dihydro-2H-1-benzopyran-2-one (4)

Sample ID: s_20100614_02
File: /home/rasw/Desktop/hk1061410c.fid
Pulse Sequence: s2pu1
Solvent: cdcl3
Temp: 25.0 C / 298.1 K
Operator: rasw
File: hk1061410c
VNMR-400 "nmr400"

Relax. delay 30.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.7395659 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 65536
Total time 5 min, 20 sec



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



4-[Bis(4-methylphenyl)phosphinyl]-3,4-dihydro-2H-1-benzopyran-2-one (**4**)

Std carbon

File: home/ras/Desktop/600ras061510.001.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: ras

File: 600ras061510.001

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

21568 repetitions

OBSERVE C13, 150.8132467 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

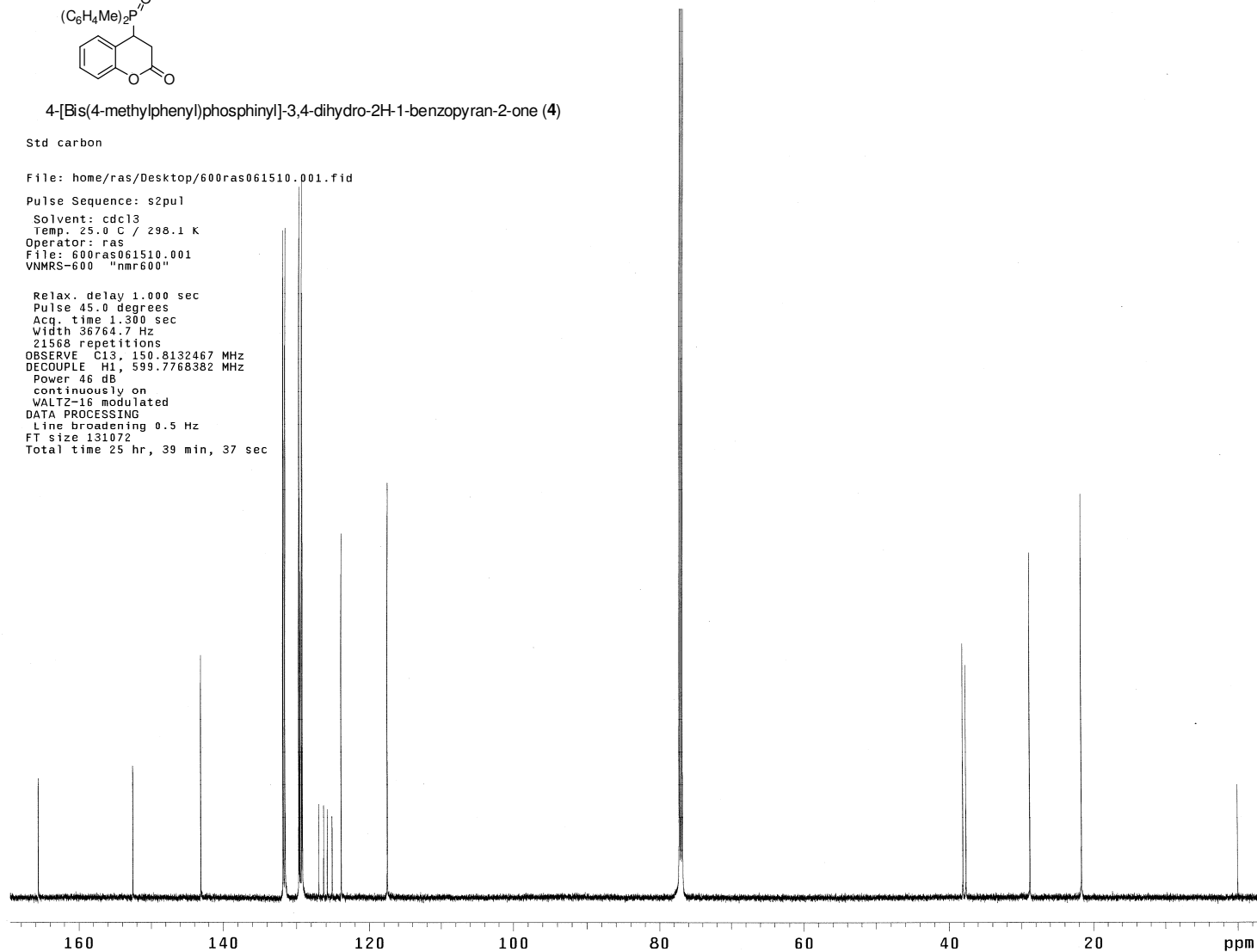
WALTZ-16 modulated

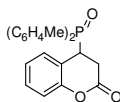
DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 25 hr, 39 min, 37 sec





$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

4-[Bis(4-methylphenyl)phosphinyl]-3,4-dihydro-2H-1-benzopyran-2-one (4)
Std phosphorus

File: home/ras/Desktop/600ras061510.002.fid

Pulse Sequence: s2pul

Solvent: cdc13

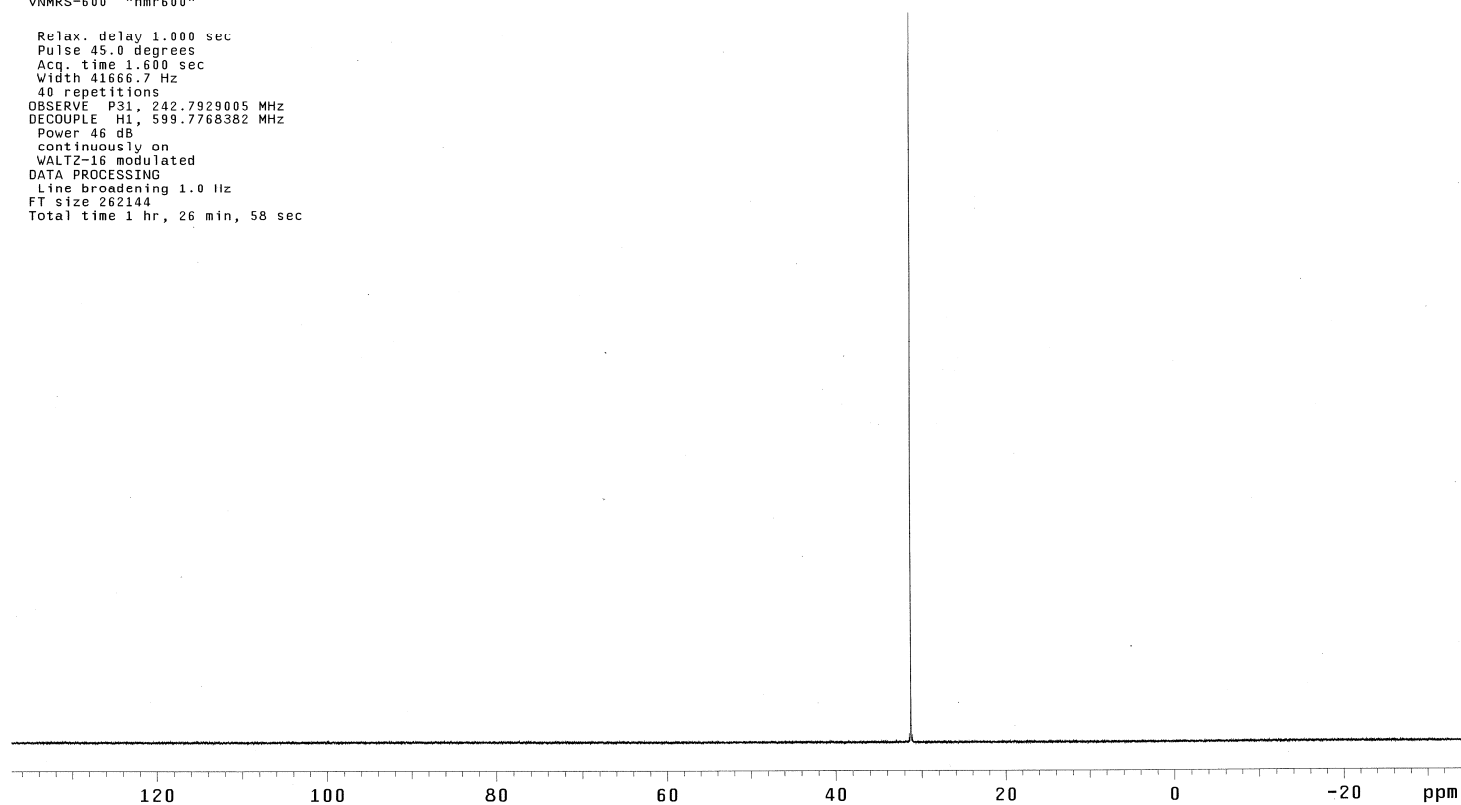
Temp. 25.0 C / 298.1 K

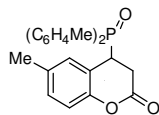
Operator: ras

File: 600ras061510.002

VNMR-600 "nmr600"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.600 sec
Width 41666.7 Hz
40 repetitions
OBSERVE P31, 242.7929005 MHz
DECOUPLE H1, 599.7768382 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 262144
Total time 1 hr, 26 min, 58 sec





^1H NMR spectrum (CDCl_3 , 25 °C)

6-Methyl-4-[bis(4-methylphenyl)phosphinyl]-3,4-dihydro-2H-1-benzopyran-2-one (5)

Std proton

File: home/ras/Desktop/600ras050311.005.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras050311.005

VNMR-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 9615.4 Hz

16 repetitions

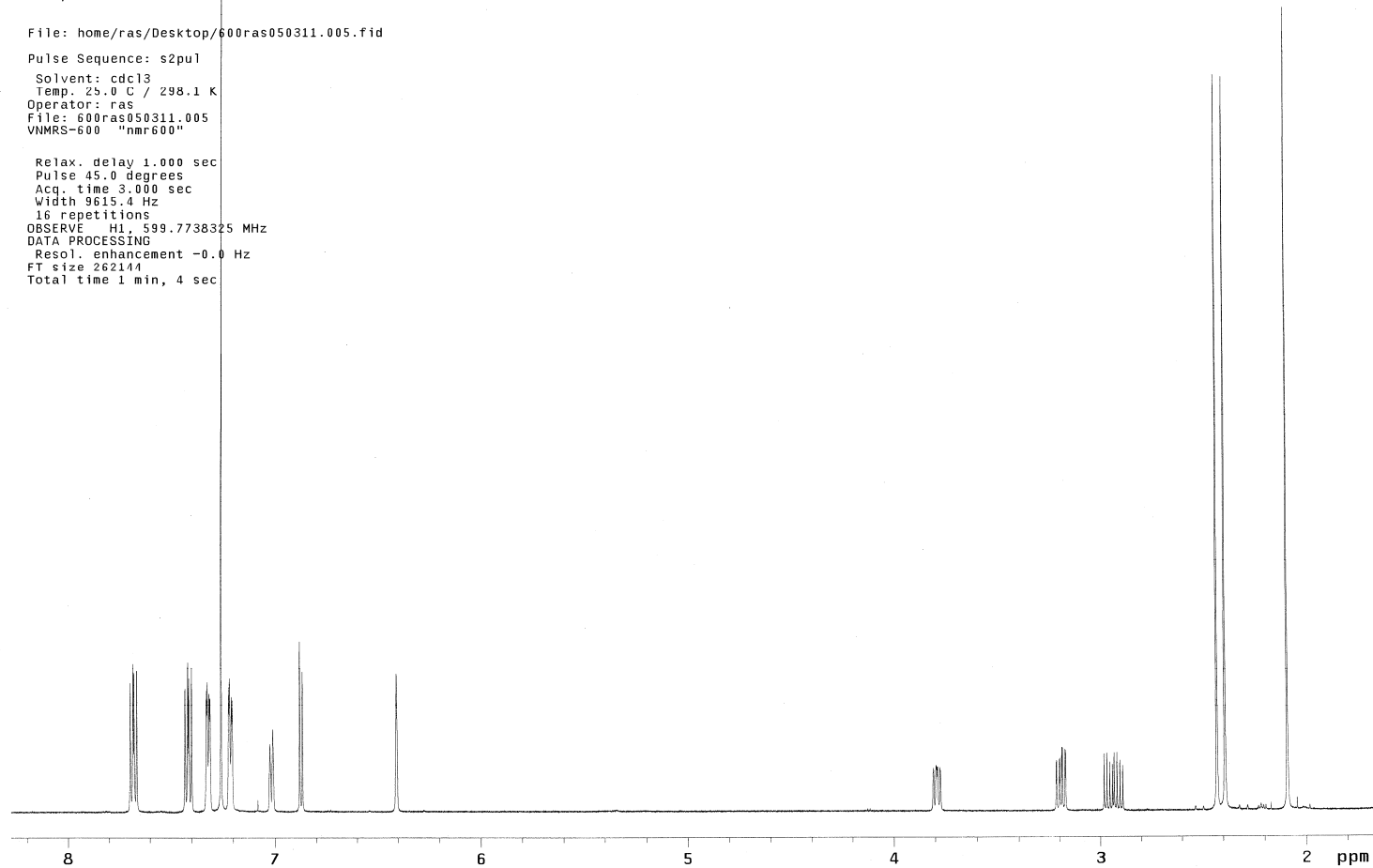
OBSERVE H1, 599.7738325 MHz

DATA PROCESSING

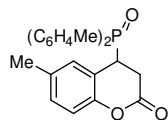
Resol. enhancement -0.0 Hz

FT size 262144

Total time 1 min, 4 sec



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



6-Methyl-4-[(4-methylphenyl)phosphinyl]-3,4-dihydro-2H-1-benzopyran-2-one (5)

Probe tuning parameter

File: home/ras/Desktop/600ras050311.006.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras050311.006

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

20000 repetitions

OBSERVE C13, 150.8132461 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

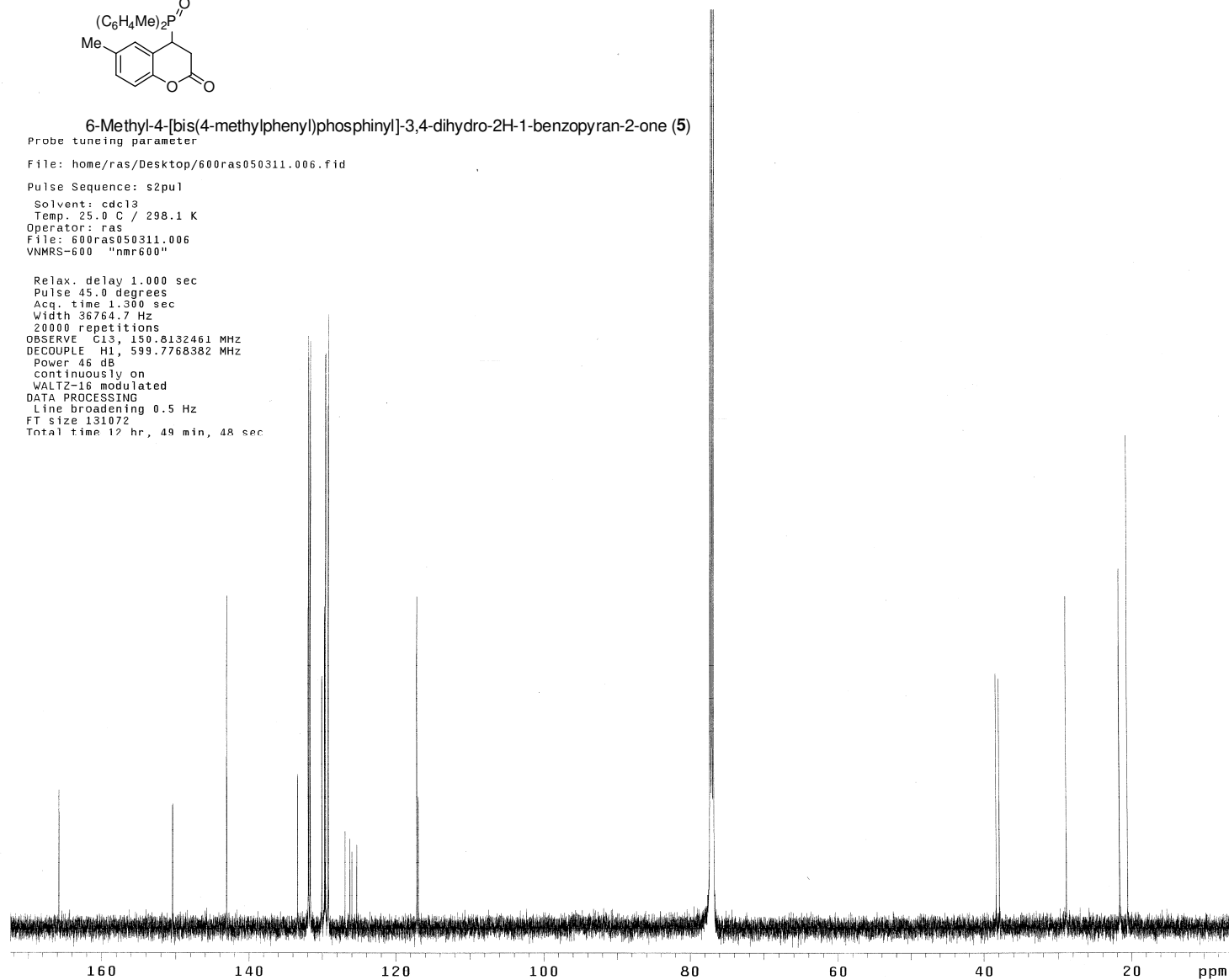
WALTZ-16 modulated

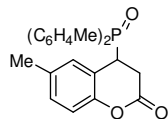
DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 12 hr, 49 min, 48 sec





$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

6-Methyl-4-[bis(4-methylphenyl)phosphinyl]-3,4-dihydro-2H-1-benzopyran-2-one (5)

Std phosphorus

File: home/ras/Desktop/600ras050411.004.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras050411.004

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

280 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

Continuously on

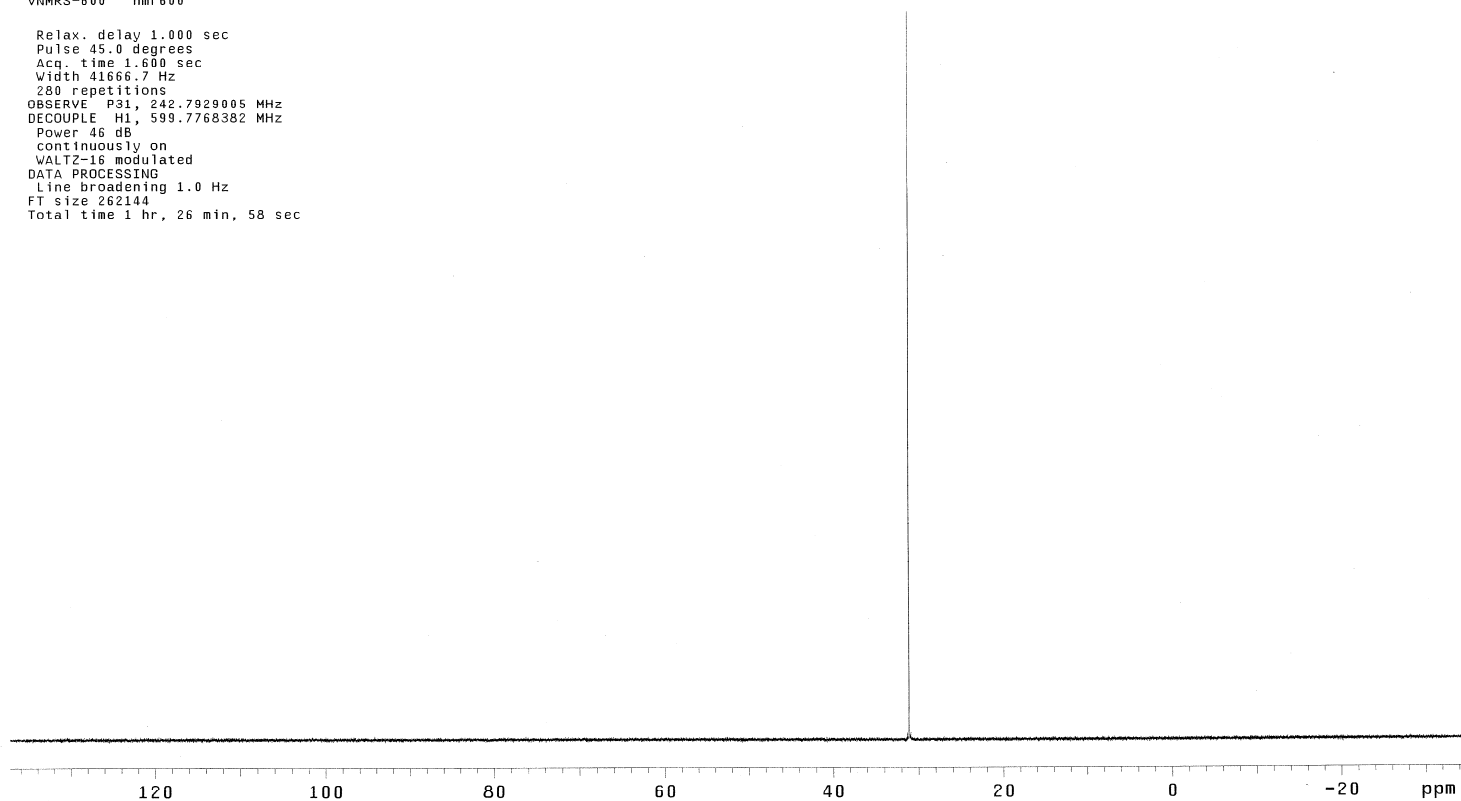
WALTZ-16 modulated

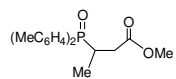
DATA PROCESSING

Line broadening 1.0 Hz

FT size 262144

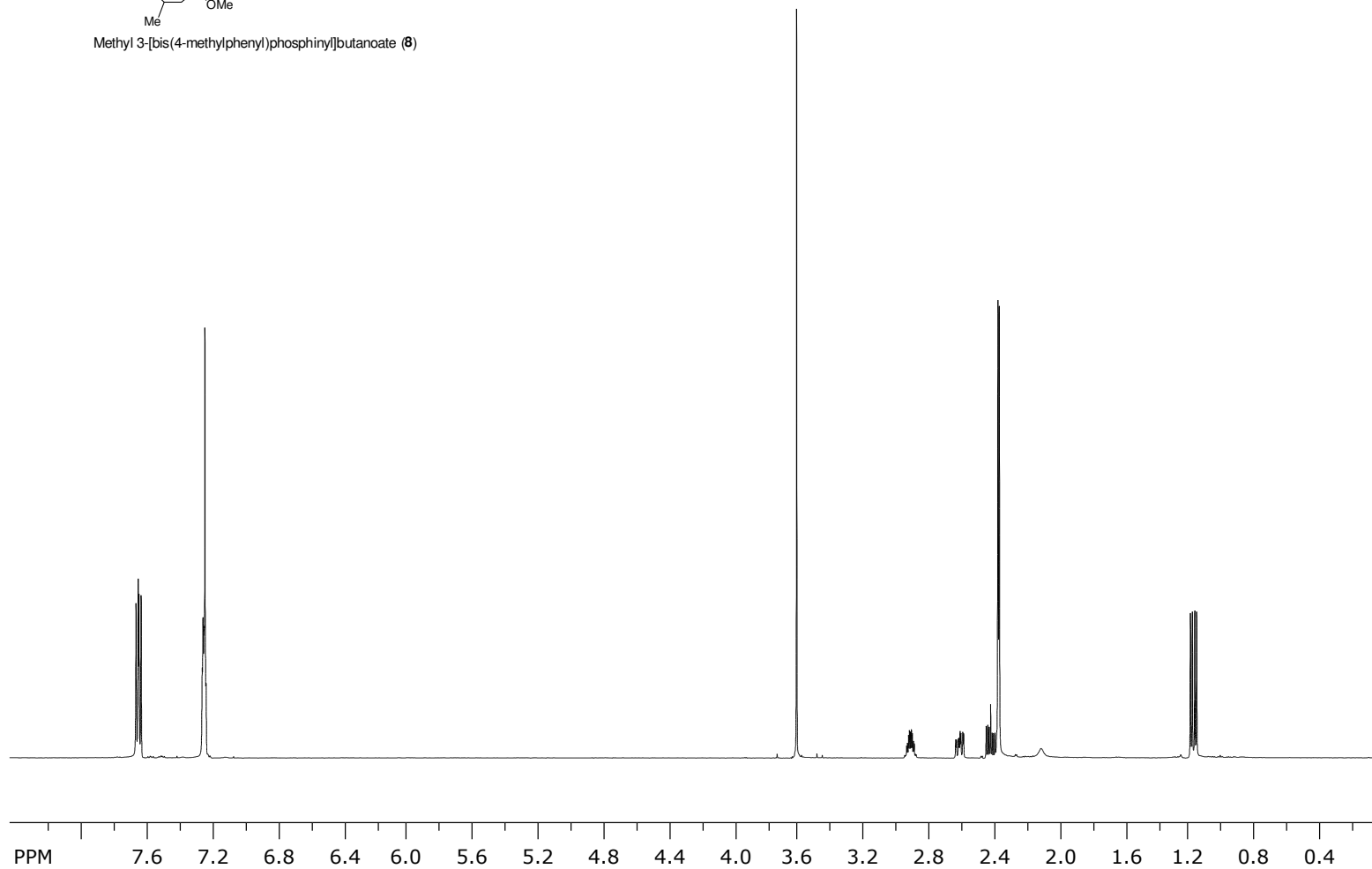
Total time 1 hr, 26 min, 58 sec





Methyl 3-[bis(4-methylphenyl)phosphinyl]butanoate (**8**)

^1H NMR spectrum (CDCl_3 , 25 °C)

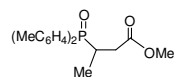


file: ...-2011\600\600ras051911.009.fid\fid block# 1 expt: "s2pul"
 transmitter freq.: 599.777438 MHz
 time domain size: 57692 points
 width: 9615.38 Hz = 16.0316 ppm = 0.166668 Hz/pt

freq. of 0 ppm: 599.773832 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 202.689 ppm/cm: 0.33794

S17

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



Methyl 3-[bis(4-methylphenyl)phosphiny]butanoate (**8**)

Probe tuning parameter

File: home/ras/Desktop/600ras051911.007.fid

Pulse Sequence: s2pul

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras051911.007

VNMR5-400 "nmr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

24600 repetitions

OBSERVE C13, 150.8132500 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

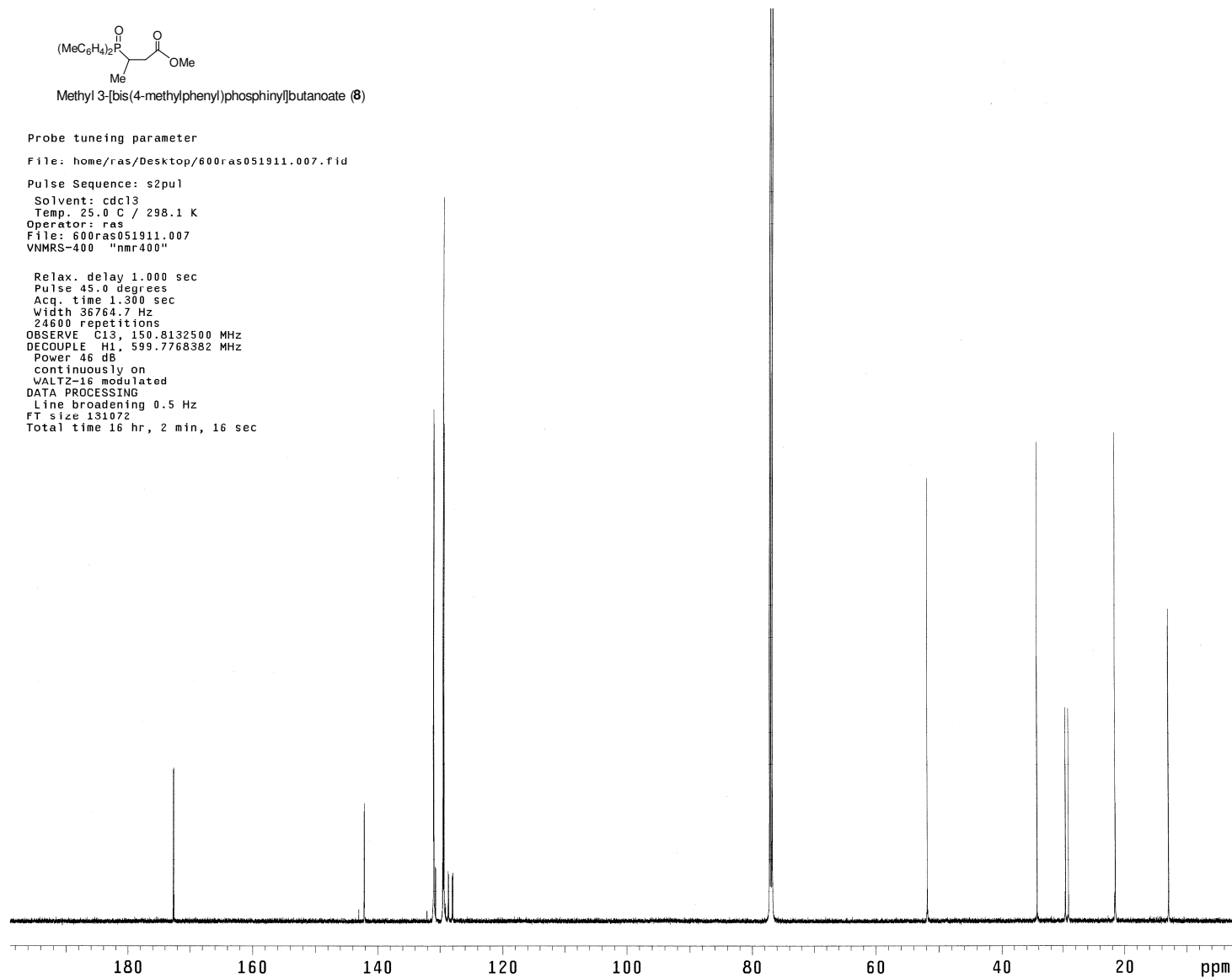
WALTZ-16 modulated

DATA PROCESSING

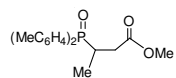
Line broadening 0.5 Hz

FT size 131072

Total time 16 hr, 2 min, 16 sec



$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



Methyl 3-[(4-methylphenyl)phosphinyl]butanoate (**8**)

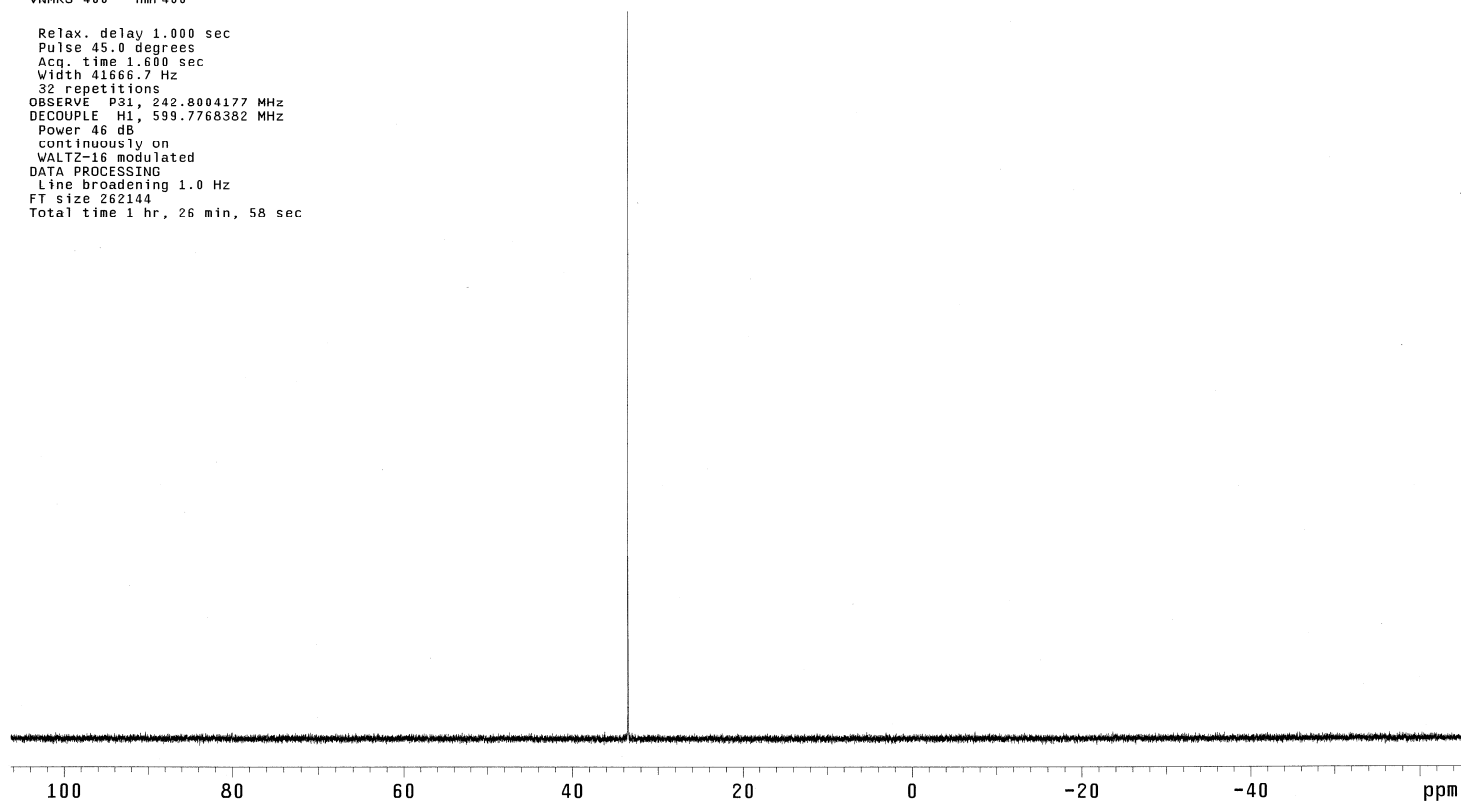
Std phosphorus

File: home/ras/Desktop/600ras030911.002.fid

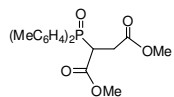
Pulse Sequence: s2pul

Solvent: cdc13
Temp. 25.0 C / 298.1 K
Operator: ras
File: 600ras030911.002
VNMR5-400 "nmr400"

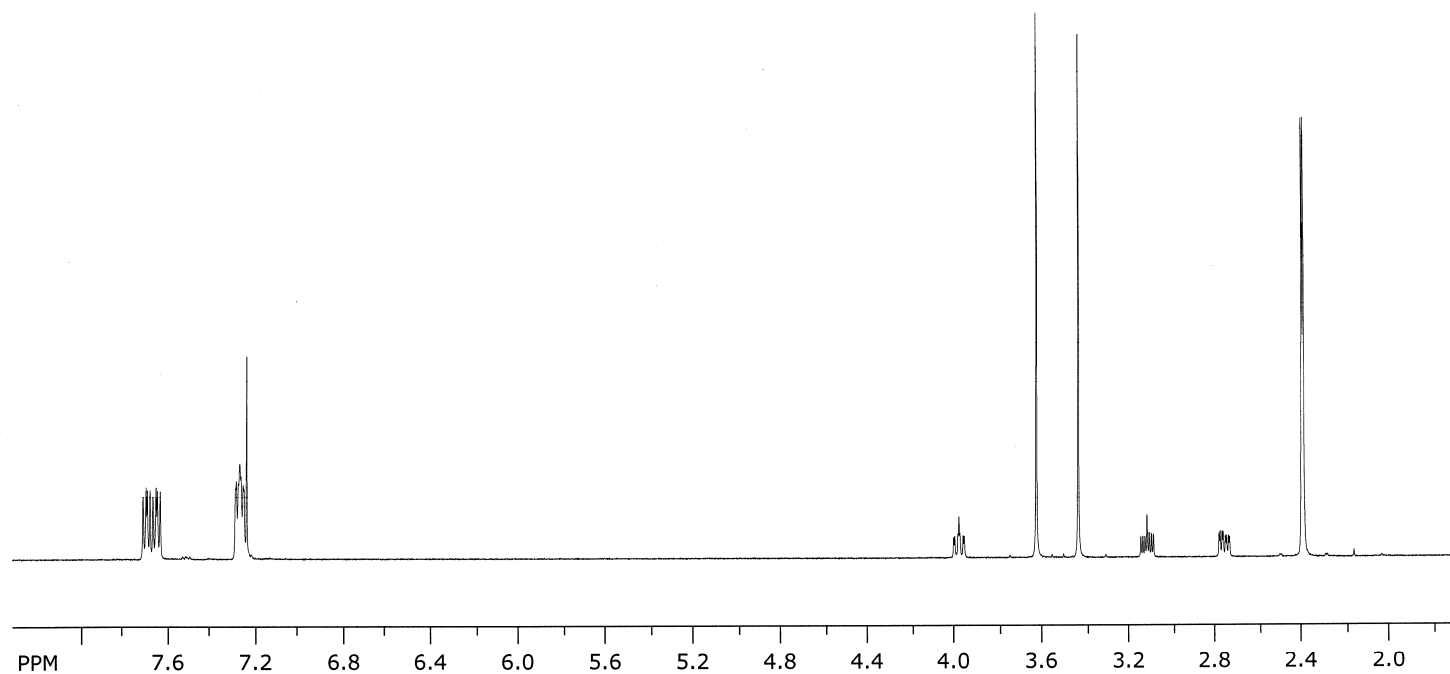
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.600 sec
Width 41666.7 Hz
32 repetitions
OBSERVE P31, 242.8004177 MHz
DECOUPLE H1, 599.7768382 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 262144
Total time 1 hr, 26 min, 58 sec



¹H NMR spectrum (CDCl₃, 25 °C)



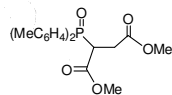
Dimethyl-2-[bis(4-methylphenyl)phosphiny]succinate (**9**)



file: ...2010\2010\600ras041310.012.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 599.777438 MHz
time domain size: 39396 points
width: 9615.38 Hz = 16.0316 ppm = 0.244070 Hz/pt
number of scans: 1

freq. of 0 ppm: 599.773839 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 159.515 ppm/cm: 0.26596

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



Dimethyl-2-[bis(4-methylphenyl)phosphiny]succinate (**9**)

Std carbon

File: home/ras/Desktop/600ras043010.005.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: ras

File: 600ras043010.005

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

32 repetitions

OBSERVE C13, 150.8132455 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

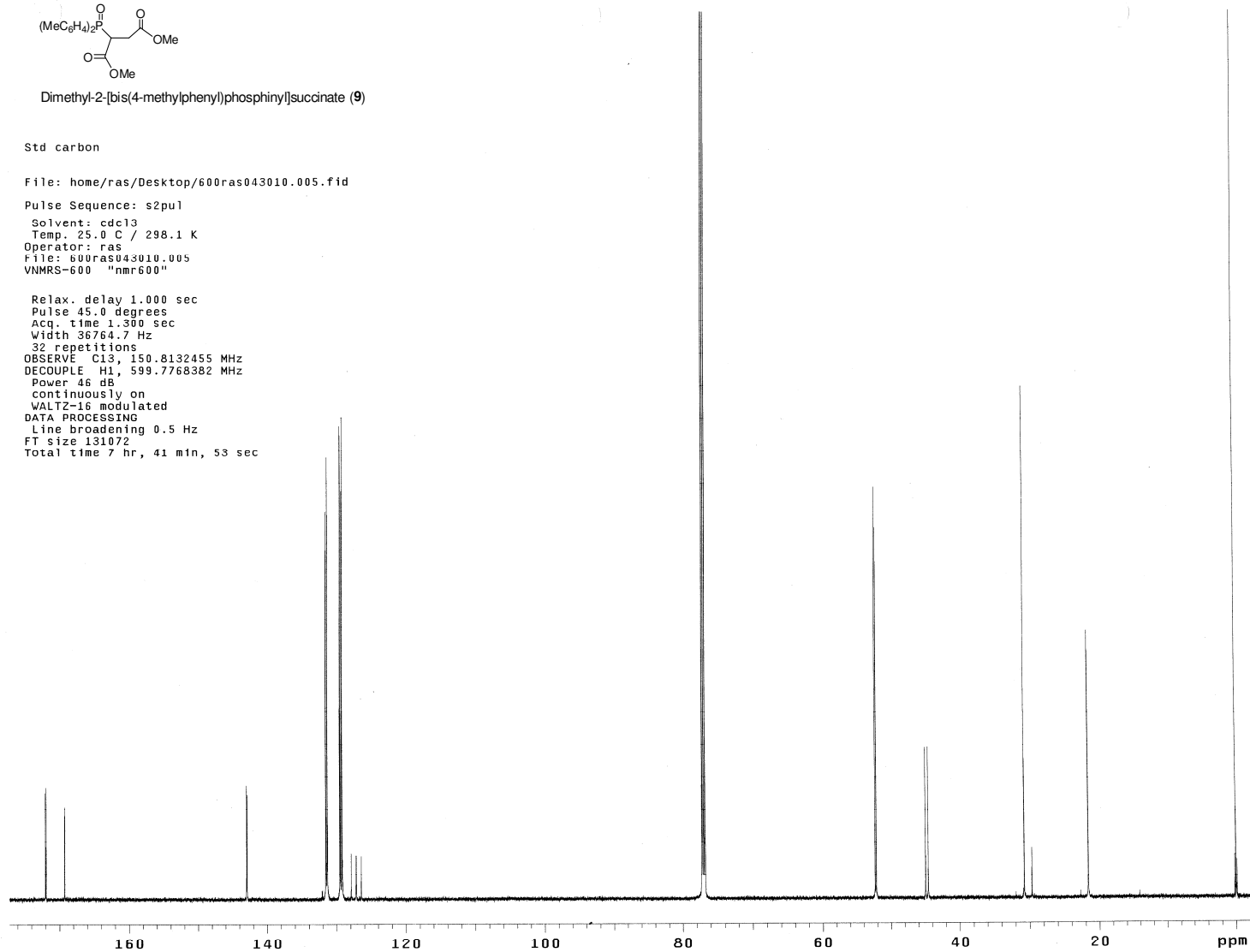
WALTZ-16 modulated

DATA PROCESSING

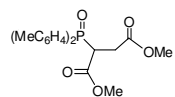
Line broadening 0.5 Hz

FT size 131072

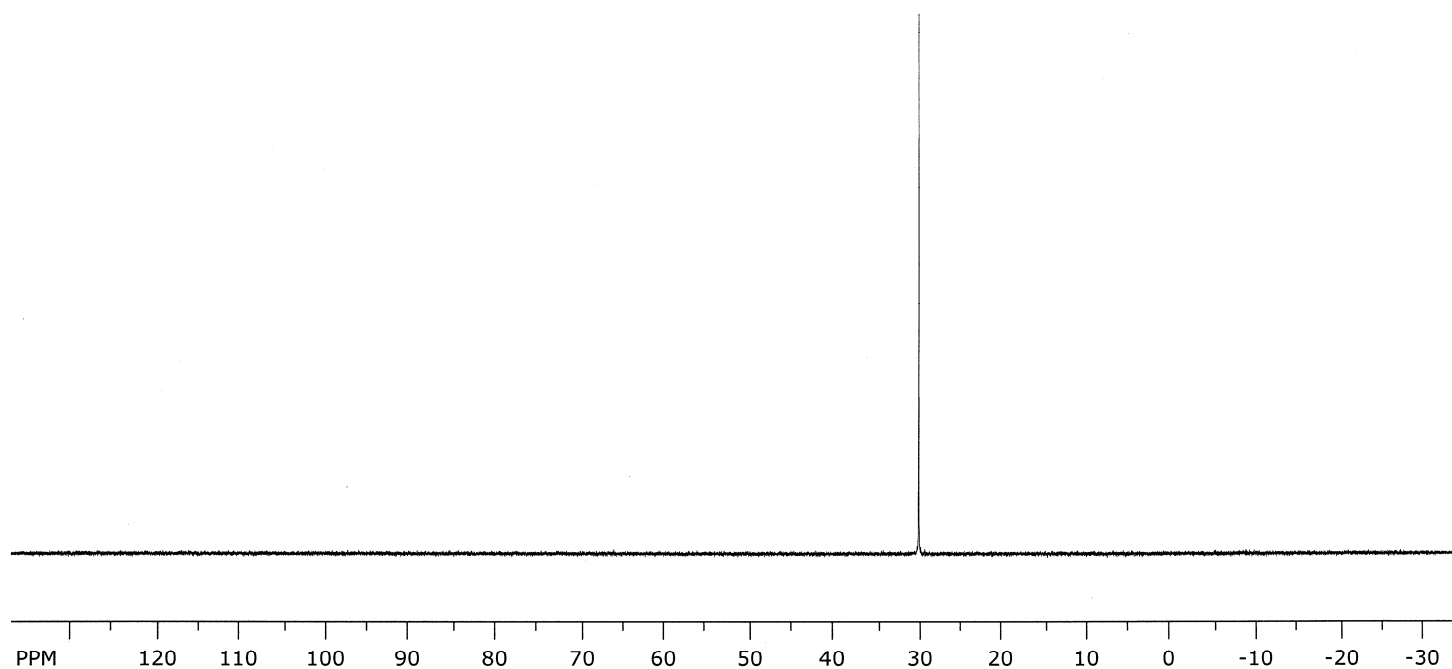
Total time 7 hr, 41 min, 53 sec



$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

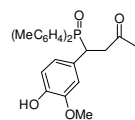


Dimethyl-2-[[bis(4-methylphenyl)phosphoryl]succinate (**9**)



file: ...2010\2010\600ras041310.011.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 242.805398 MHz
time domain size: 133336 points
width: 41666.67 Hz = 171.6052 ppm = 0.312494 Hz/pt
number of scans: 80

freq. of 0 ppm: 242.792900 MHz
processed size: 262144 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 1666.667 ppm/cm: 6.86421



^1H NMR spectrum (CDCl_3 , 25 °C)

4-[Bis(4-methylphenyl)phosphinyl]-4-[4-hydroxy-3-methoxyphenyl]butan-2-one (**10**)

Std proton

File: home/ras/Desktop/600ras051111.001.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras051111.001

VNMR5-400 "nmr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 9615.4 Hz

Single scan

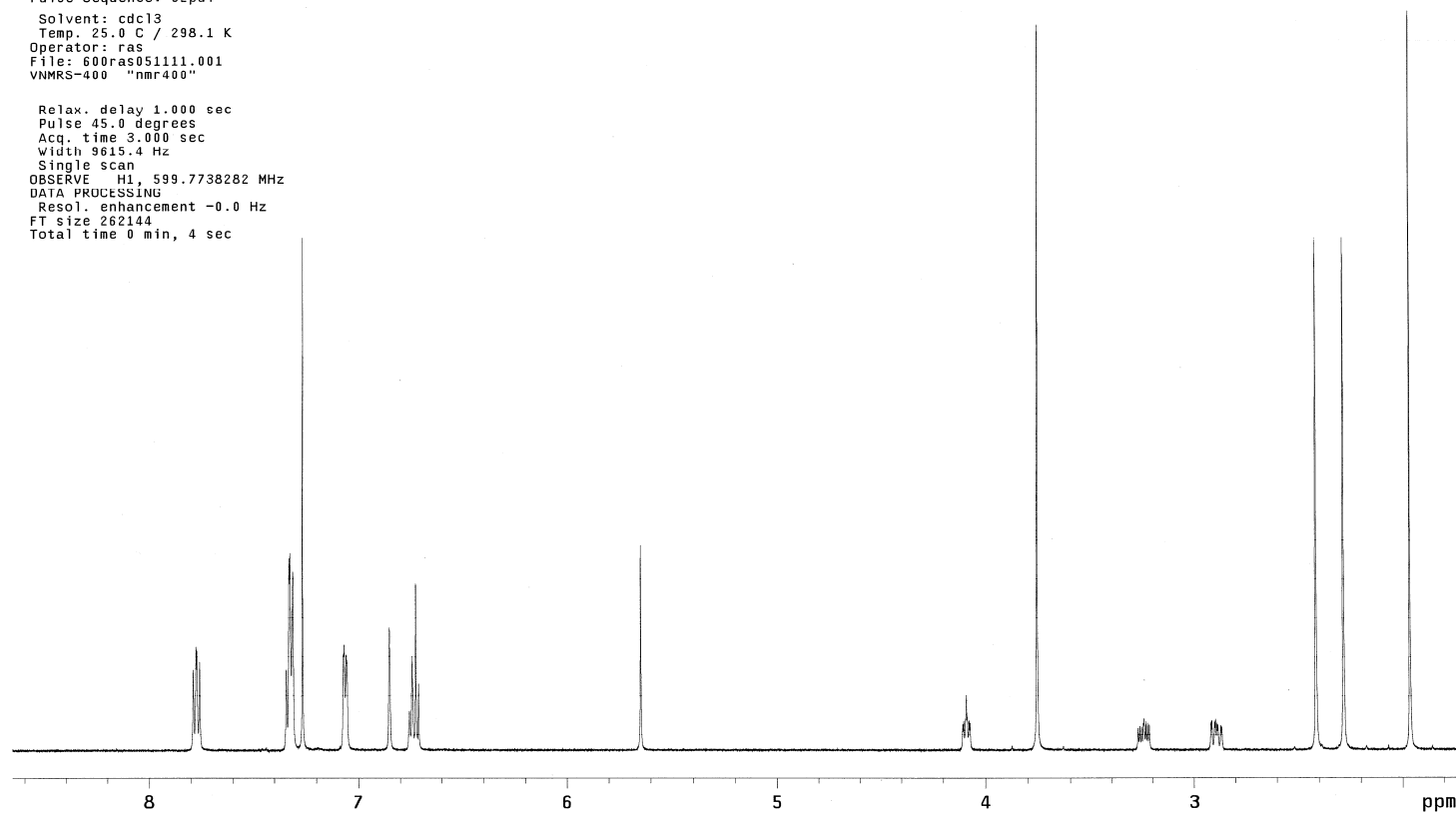
OBSERVE H1, 599.7738282 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 262144

Total time 0 min, 4 sec



CC(=O)CC(C(=O)OP(=O)(OC1=CC=C(C=C1)C=C1)C1=CC=C(C=C1)C=C1)C1=CC=C(C=C1)C=C1

Probe tuning parameter

File: home/ras/Desktop/600ras051111.002.f1d

Pulse Sequence: s2pu1

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras
File: 600res05

File: 600ras051111.002
VNMR5-400 "nmr400"

VNMR5-400 --HMF400--

Relax. delay 1.000 sec

Relax. delay 1.000
Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz
3488 repetitions

```
3488 repetitions
OBSERVE C13 150
```

OBSERVE C13, 150.8132463 MHz
DECOUPLE H1, 599.7768382 MHz

DECOUPLE H1, 599.7768382 MHz
Power 46 dB

continuously

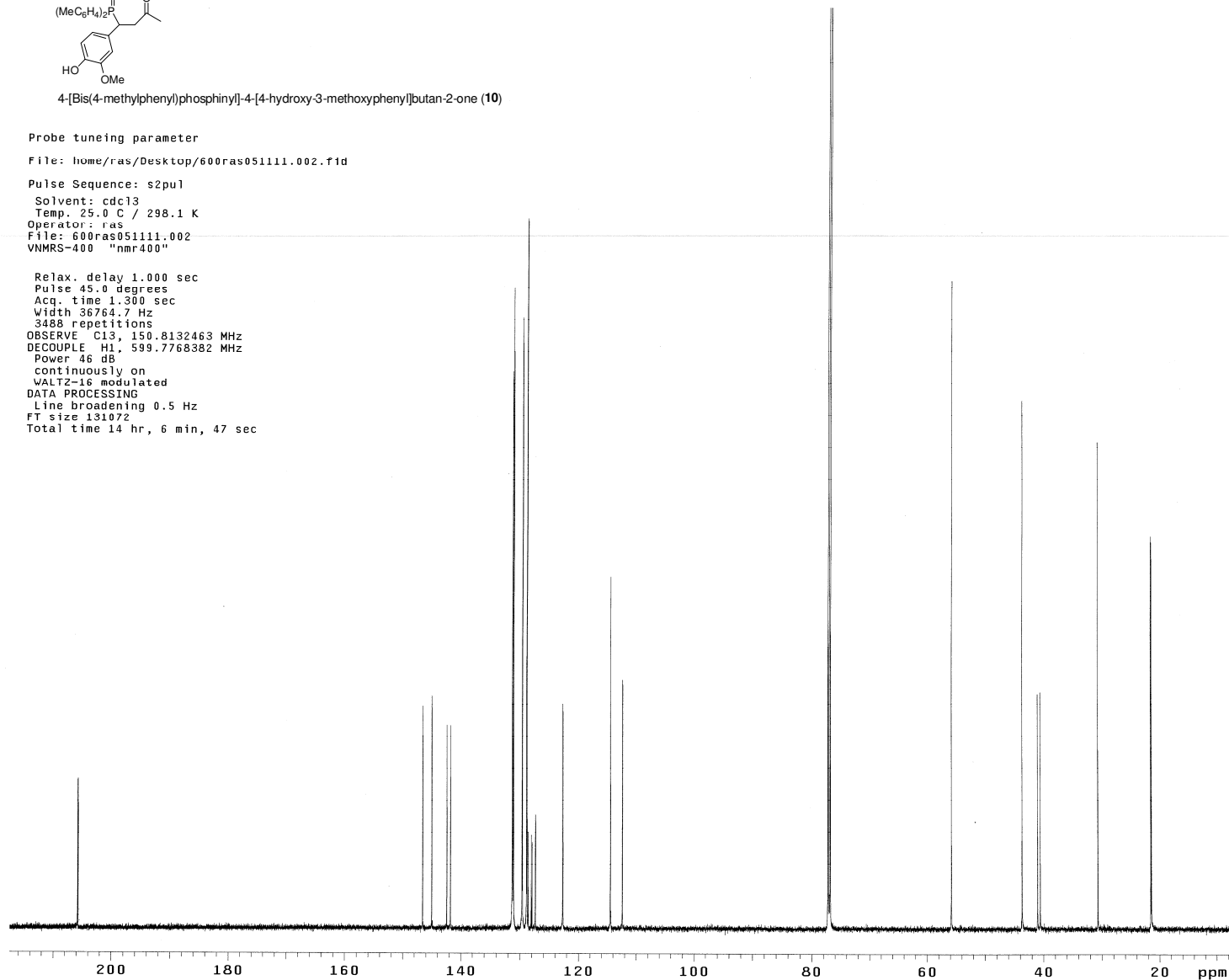
WALTZ-16 modulat
DATA PROCESSING

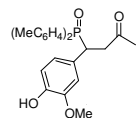
DATA PROCESSING
Line broadening

Line broadening 0.5 Hz
FT size 131072

FI size 131072
Total time 14 1

Total time 14 min, 6 min, 47 sec





$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

4-[Bis(4-methylphenyl)phosphinyl]-4-[4-hydroxy-3-methoxyphenyl]butan-2-one (**10**)

Std phosphorus

File: home/ras/Desktop/600ras051111.006.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp: 25.0 C / 298.1 K

Operator: ras

File: 600ras051111.006

VNMR-400 "nmr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

12 repetitions

OBSERVE P31, 242.7929129 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

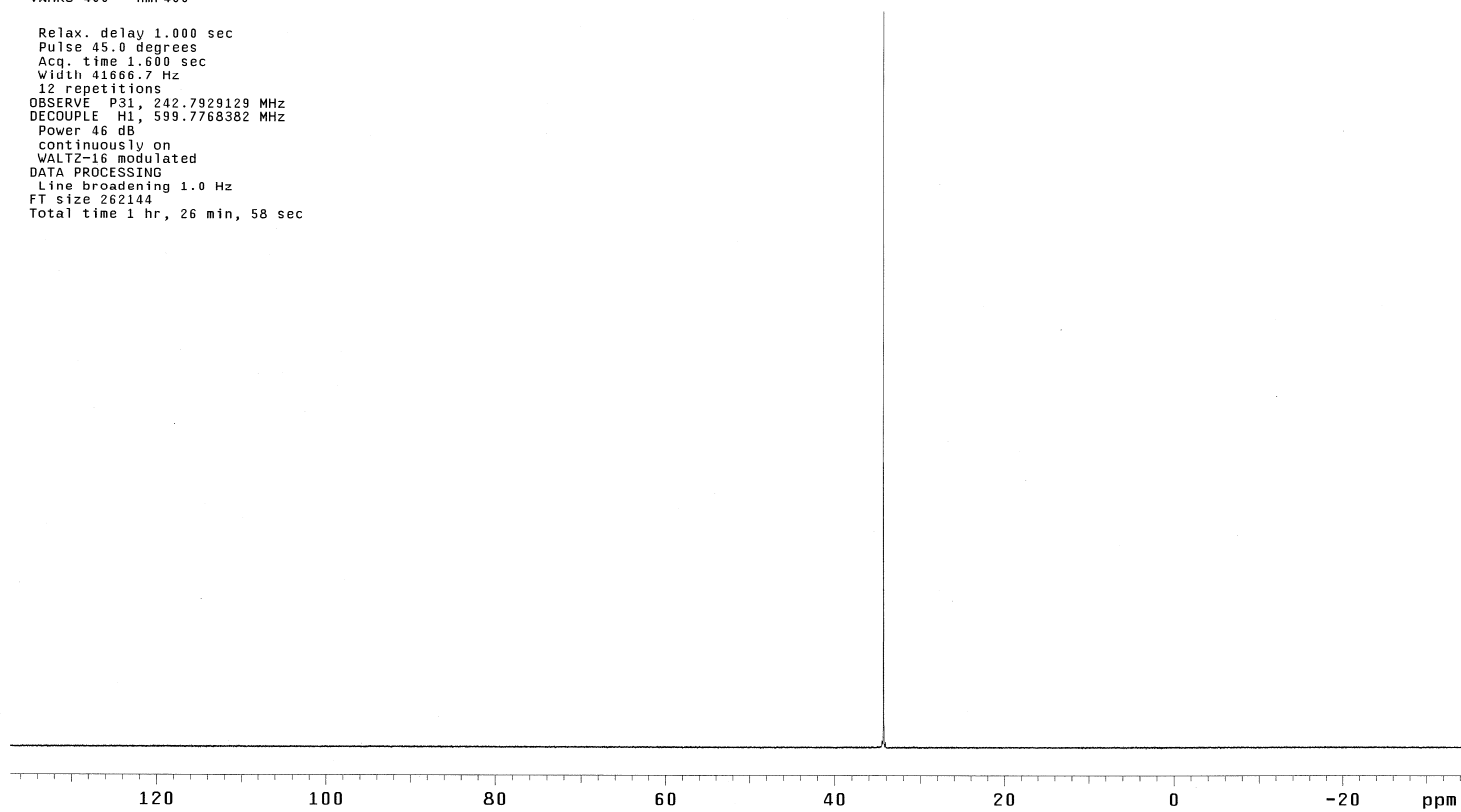
WALTZ-16 modulated

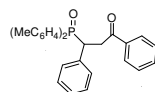
DATA PROCESSING

Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec





3-[Bis(4-methylphenyl)phosphiny]-1,3-diphenylpropan-1-one (11)
Std proton

File: home/ras/Desktop/600ras050411.001.fid

Pulse Sequence: s2pul

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras050411.001

VNMR-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 9615.4 Hz

Single scan

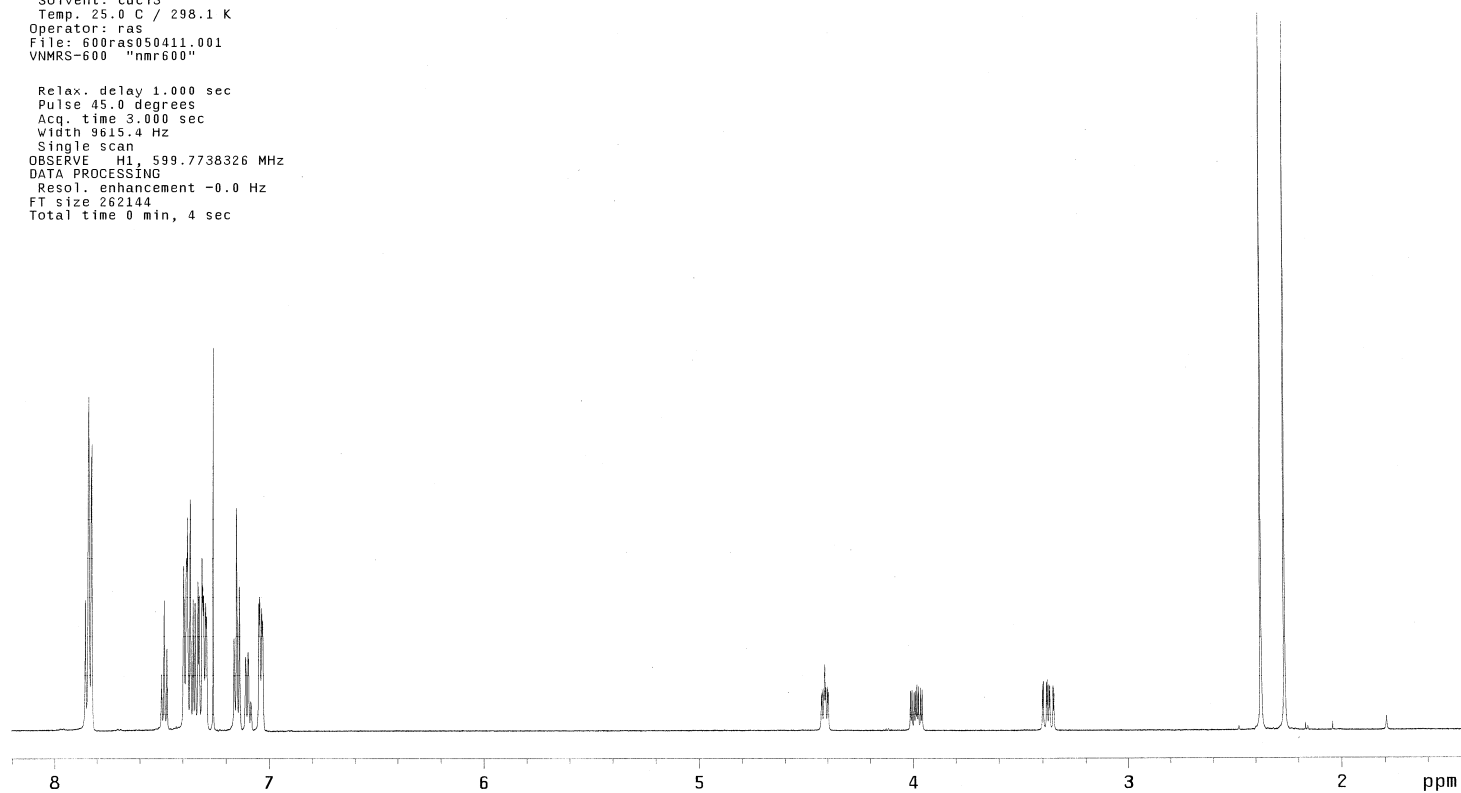
OBSERVE H1, 599.7738326 MHz

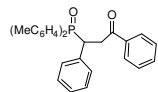
DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 262144

Total time 0 min, 4 sec





3-[Bis(4-methylphenyl)phosphinyl]-1,3-diphenylpropan-1-one (**11**)

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Probe tuning parameter

File: home/ras/Desktop/600ras050411.002.fid

Pulse Sequence: s2pul

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras050411.002

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

4616 repetitions

OBSERVE C13, 150.8132472 MHz

DECOUPLE H1, 599.7768382 MHz

Power 16 dB

continuously on

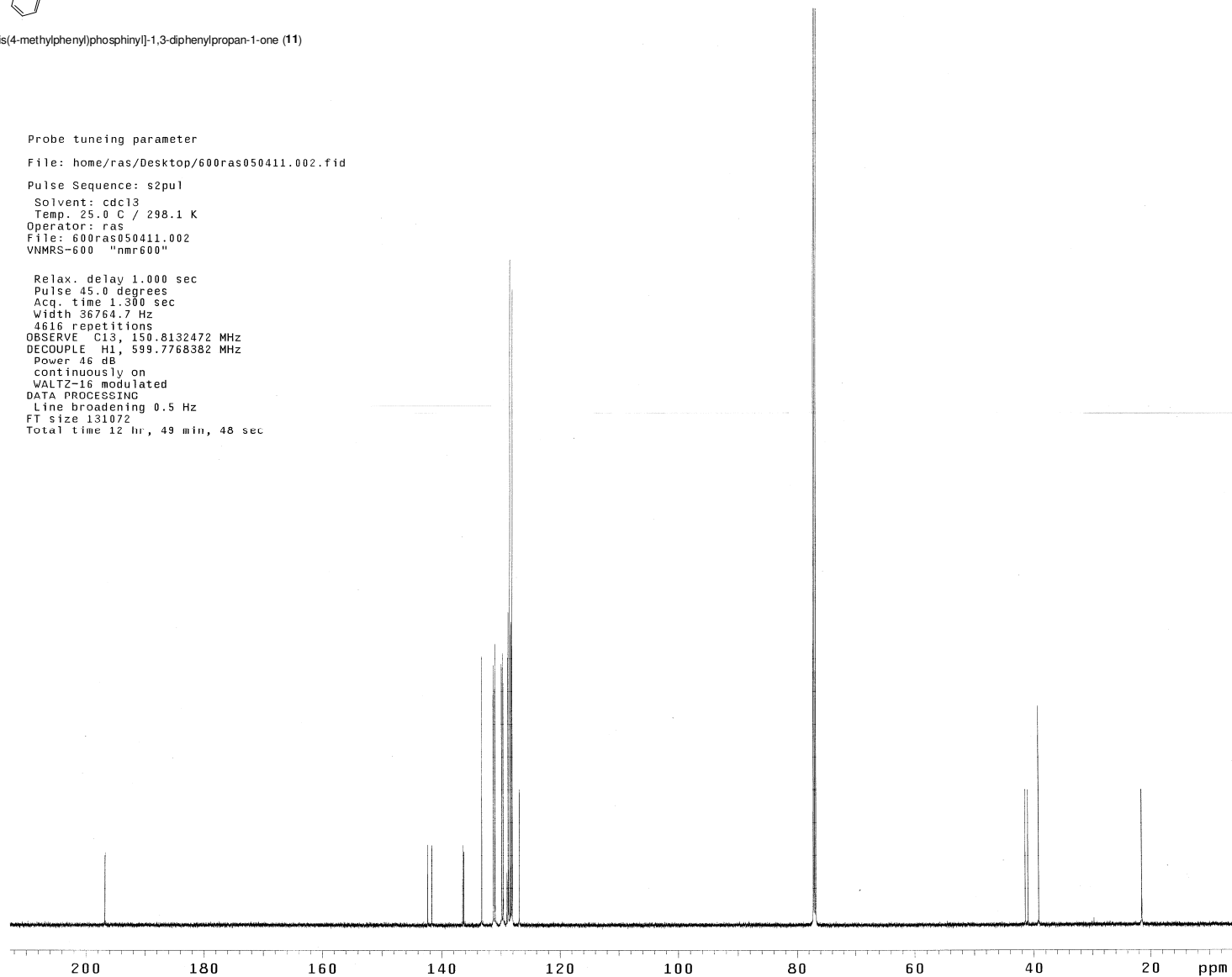
WALTZ-16 modulated

DATA PROCESSING

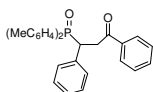
Line broadening 0.5 Hz

FT size 131072

Total time 12 hr, 49 min, 48 sec



$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



3-[Bis(4-methylphenyl)phosphiny]-1,3-diphenylpropan-1-one (**11**)

Std phosphorus

File: home/ras/Desktop/600ras050411.003.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras050411.003

VNMR-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

12 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

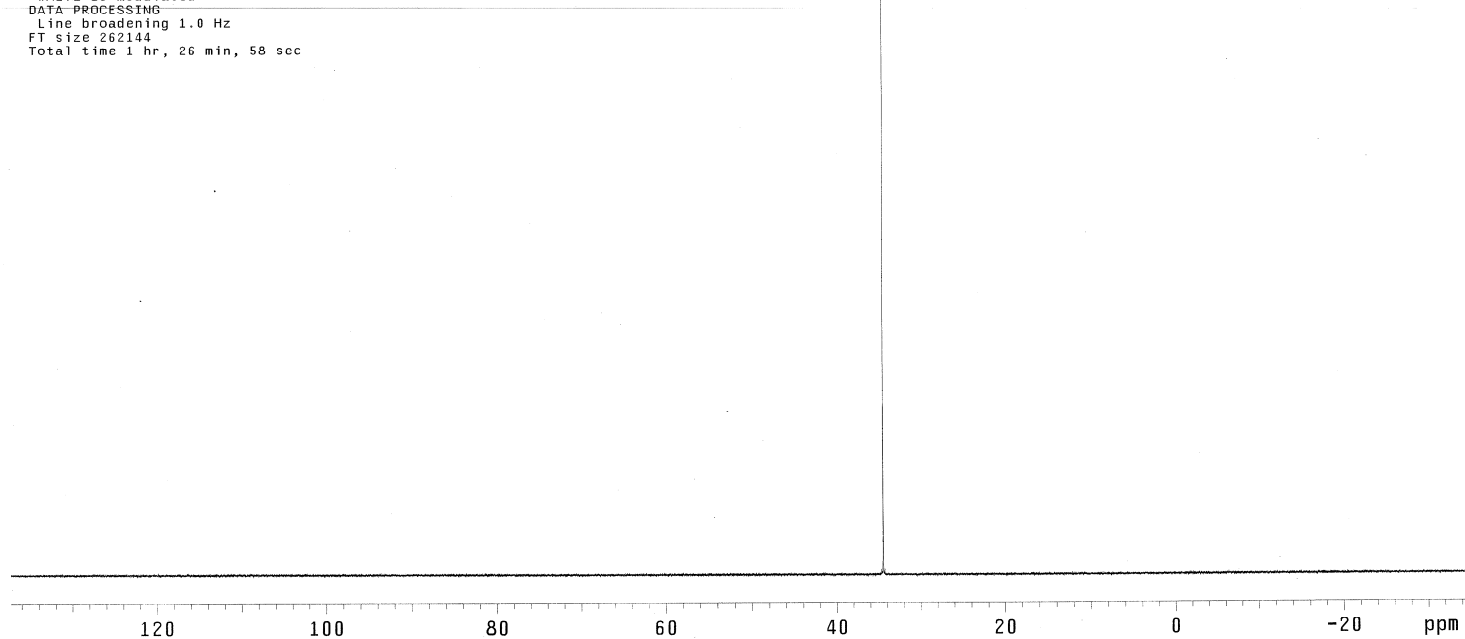
WALTZ-16 modulated

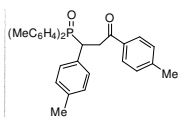
DATA PROCESSING

Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec





3-[bis(4-methylphenyl)phosphinyl]-1,3-bis(4-methylphenyl)propan-1-one (**12**)

^1H NMR spectrum (CDCl_3 , 25 °C)

Std proton

File: home/ras/Desktop/600ras042111.013.fid

Pulse Sequence: s2pul

Solvent: cdcl_3

Temp: 25.0 C / 298.1 K

Operator: ras

File: 600ras042111.013

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 9615.4 Hz

Single scan

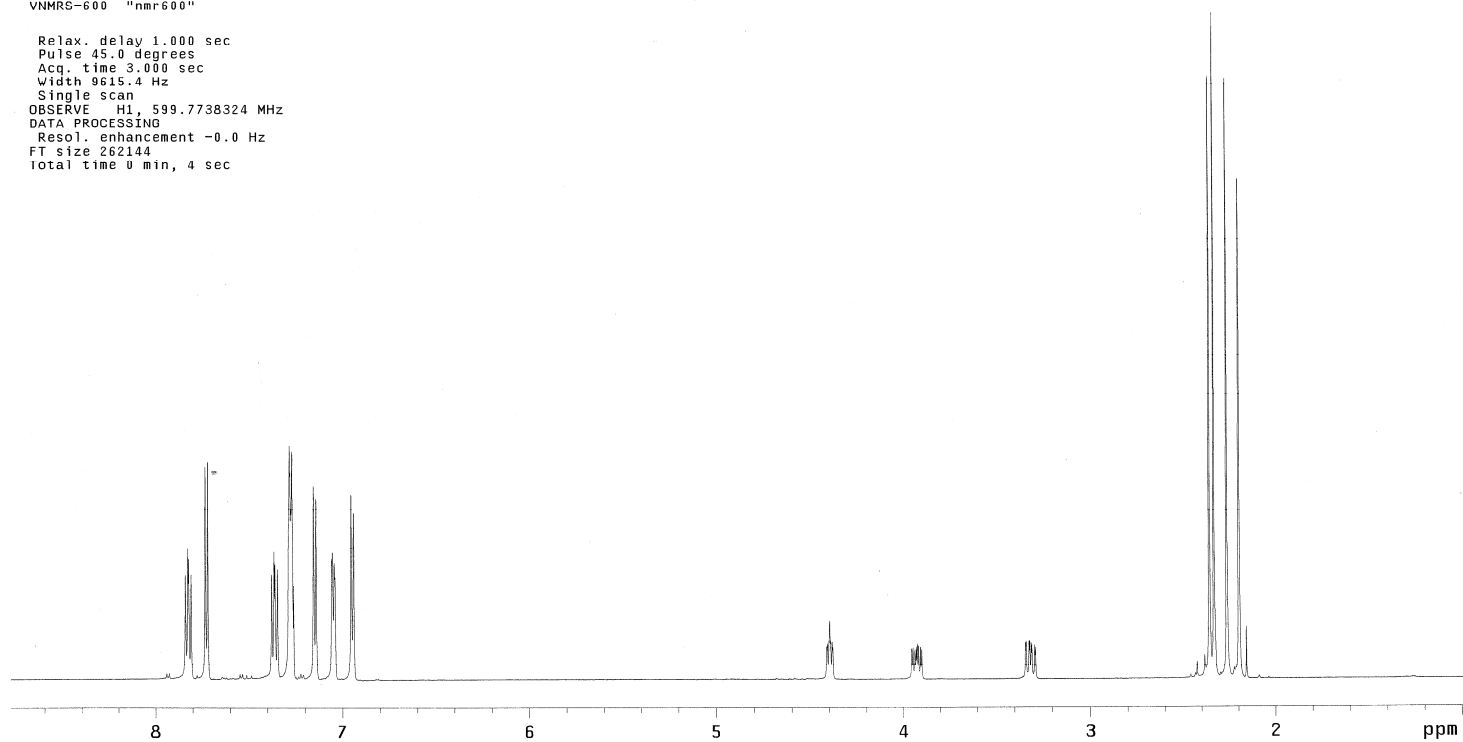
OBSERVE H1, 599.7738324 MHz

DATA PROCESSING

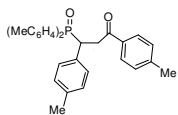
Resol. enhancement -0.0 Hz

FT size 262144

total time 0 min, 4 sec



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



3-[bis(4-methylphenyl)phosphinyl]-1,3-bis(4-methylphenyl)propan-1-one (**12**)

Probe tuning parameter

File: home/ras/Desktop/600ras042211.001.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

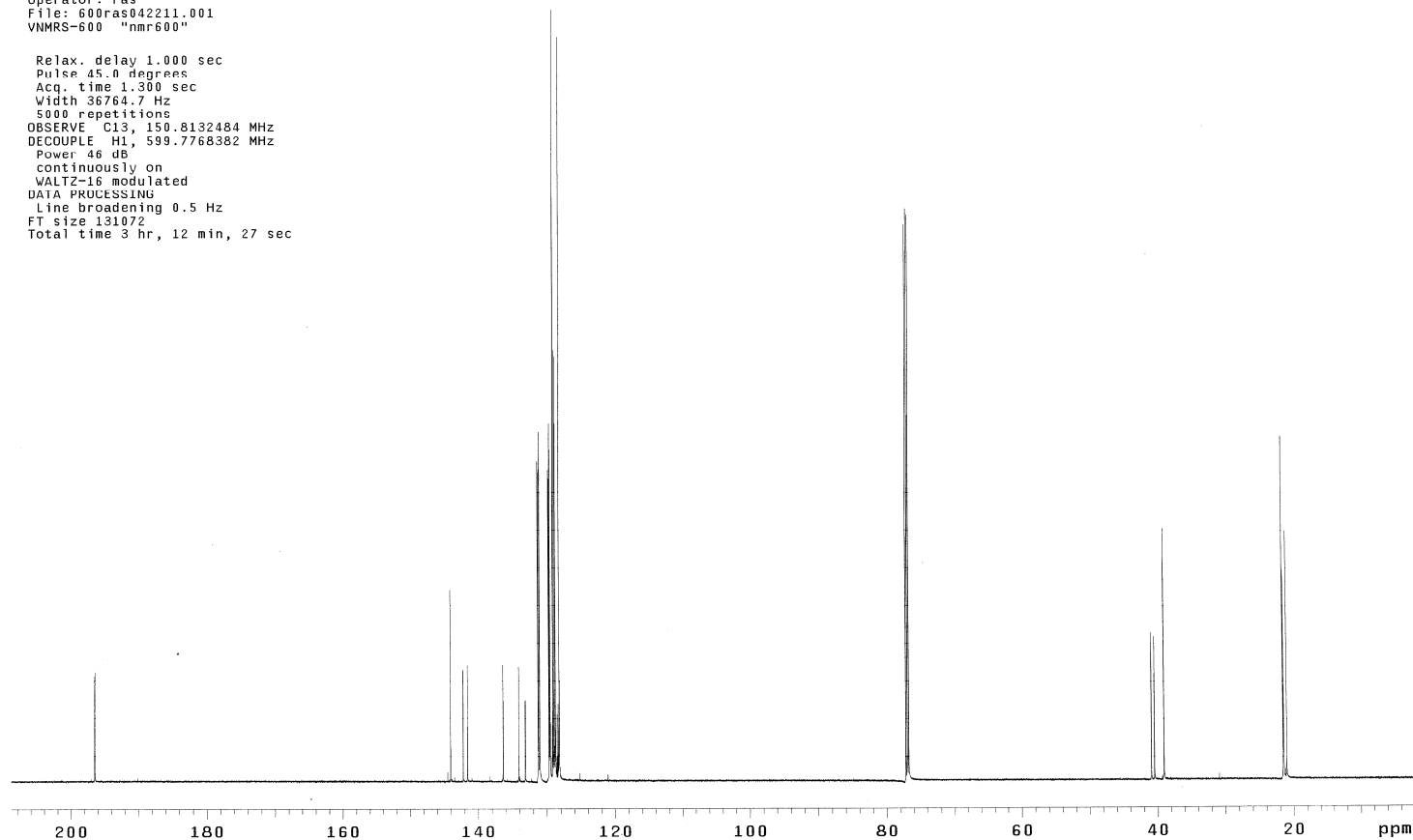
Temp. 25.0 C / 298.1 K

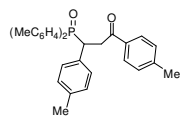
Operator: ras

File: 600ras042211.001

VNMR-600 "nmr600"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 36764.7 Hz
5000 repetitions
OBSERVE C13, 150.8132484 MHz
DECOUPLE H1, 599.7768382 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 3 hr, 12 min, 27 sec





3-[Bis(4-methylphenyl)phosphinyl]-1,3-bis(4-methylphenyl)propan-1-one (12)

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Std phosphorus

File: home/ras/Desktop/600ras042311.002.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras042311.002

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

8 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

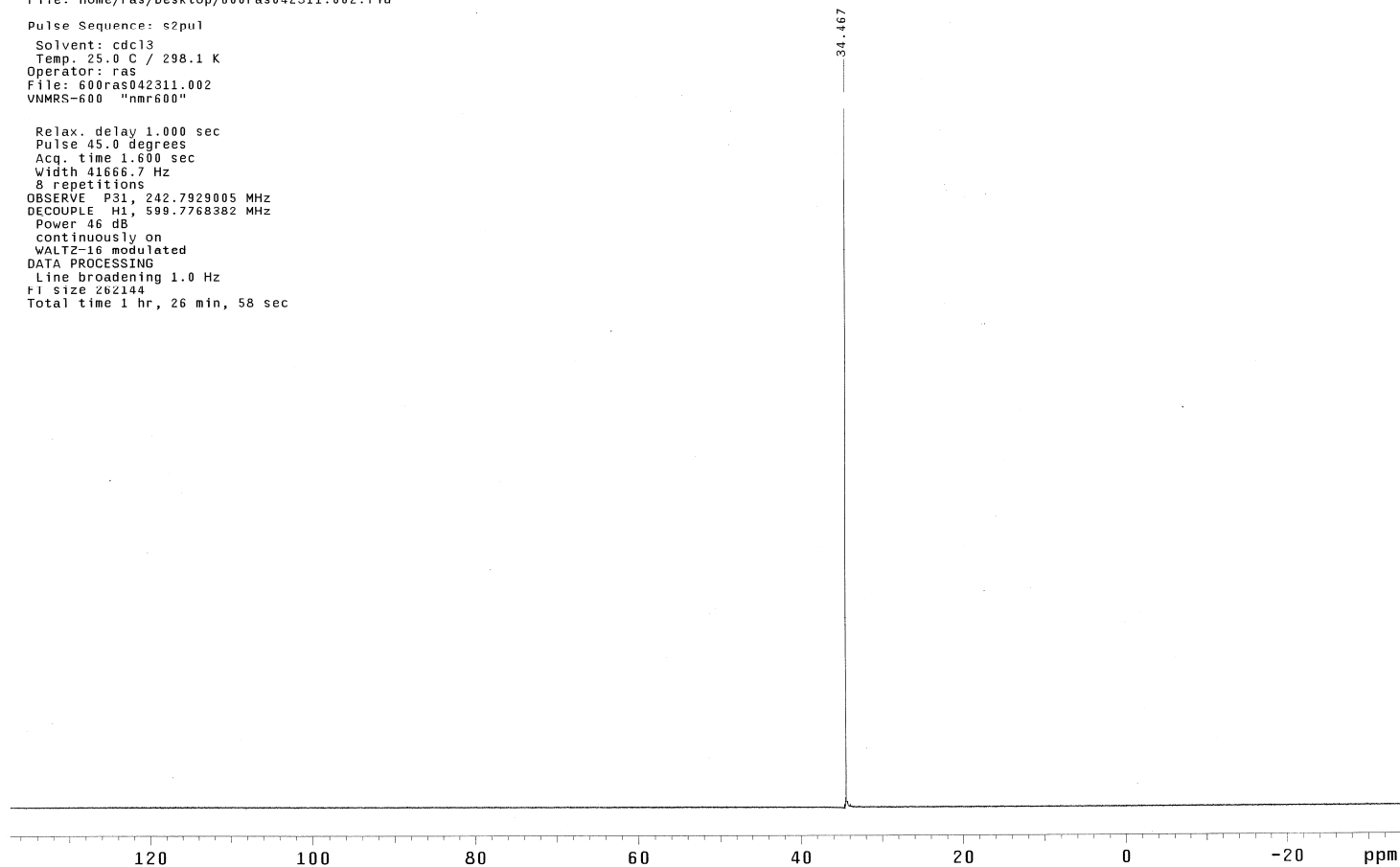
WALTZ-16 modulated

DATA PROCESSING

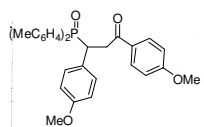
Line broadening 1.0 Hz

F1 size 262144

Total time 1 hr, 26 min, 58 sec



¹H NMR spectrum (CDCl₃, 25 °C)



3-[Bis(4-methylphenyl)phosphinyl]-1,3-bis(4-methoxyphenyl)propan-1-one (13)

Std proton

File: home/ras/Desktop/400ras051110.002.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 400ras051110.002

VNMR-400 "nmr400"

Relax. delay 30.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

8 repetitions

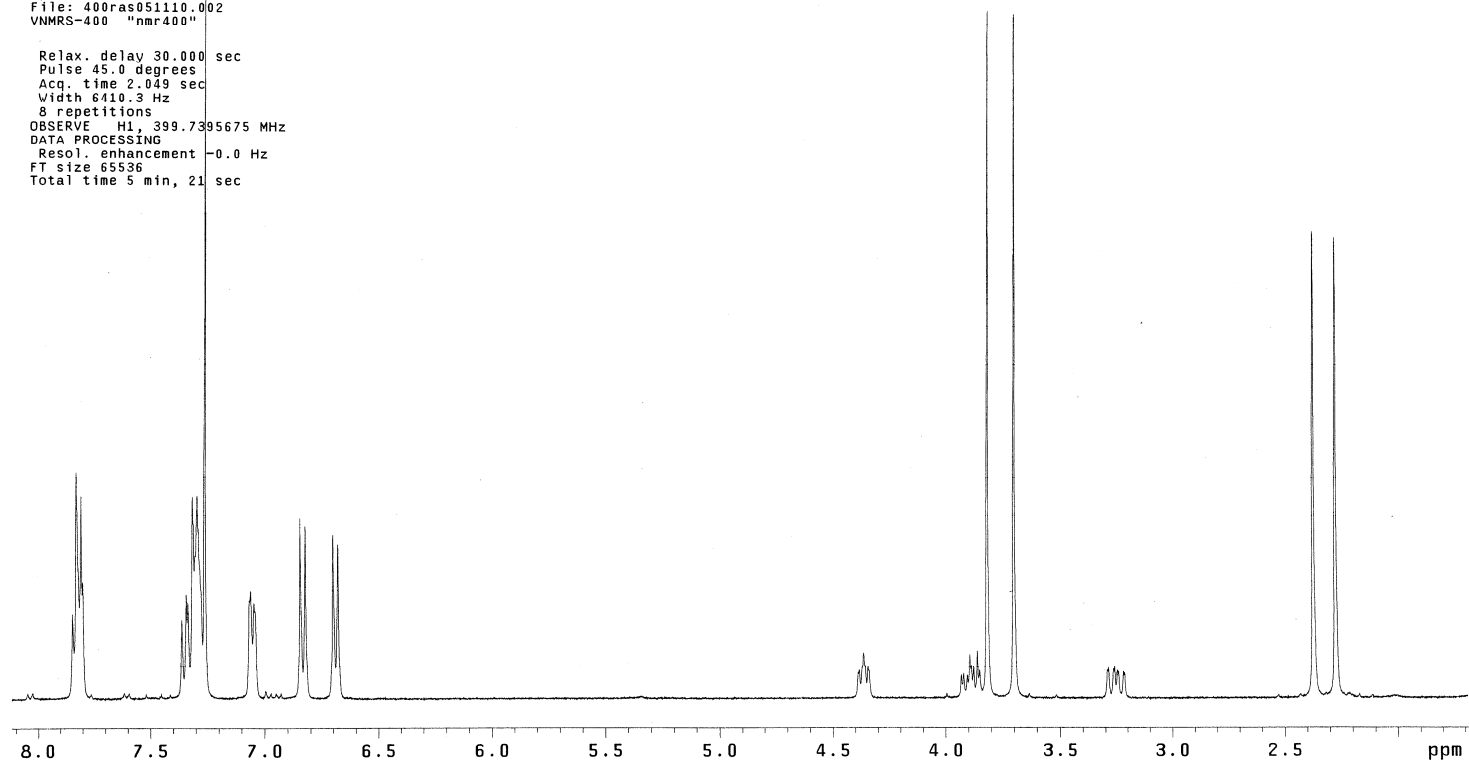
OBSERVE H1, 399.7395675 MHz

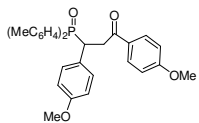
DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 65536

Total time 5 min, 21 sec





$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

3-[Bis(4-methylphenyl)phosphinyl]-1,3-bis(4-methoxyphenyl)propan-1-one (13)

Probe tuning parameter

File: home/ras/Desktop/600ras042511.001.fid

Pulse Sequence: s2pu1

Solvent: cdc13

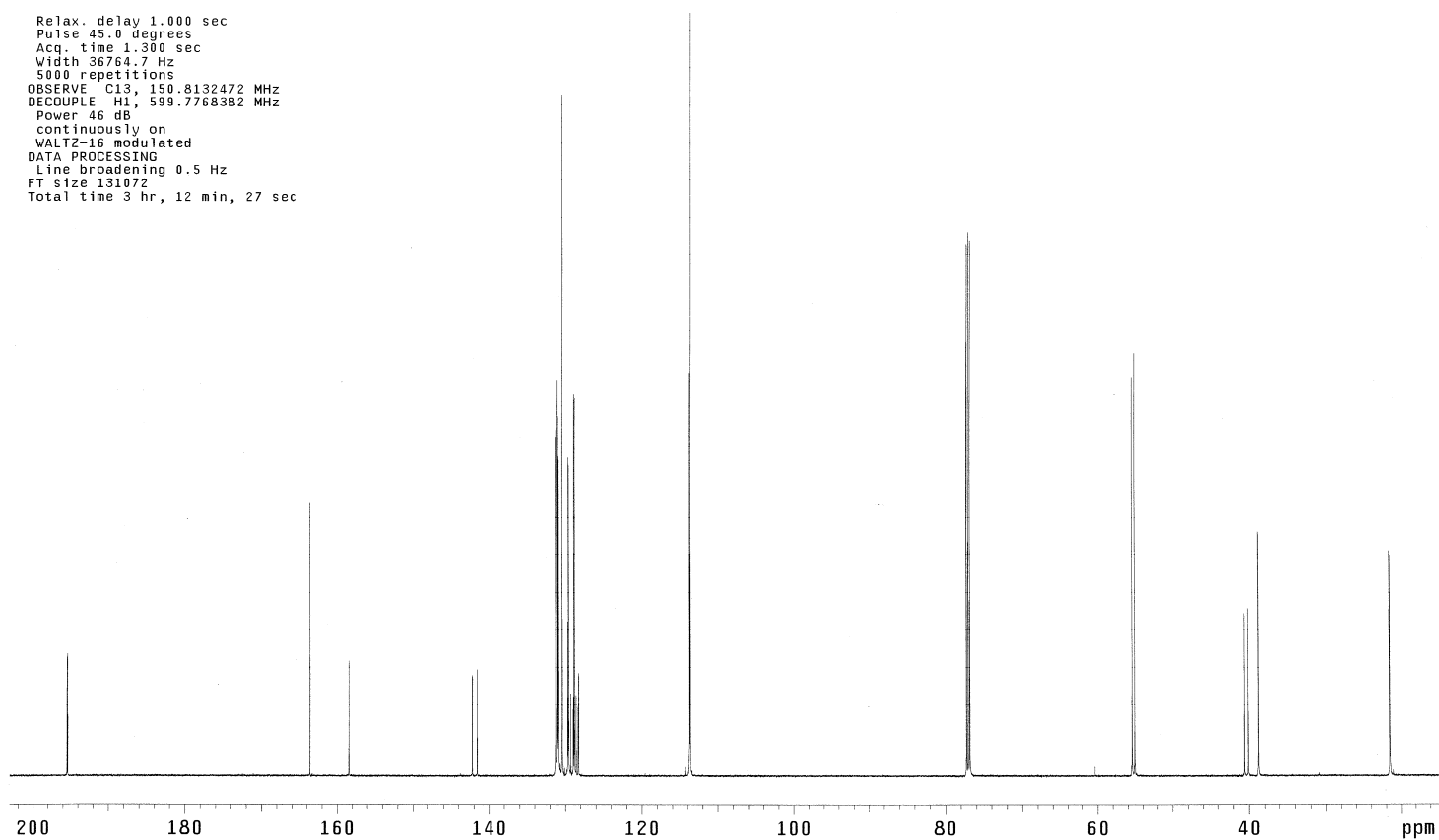
Temp. 25.0 C / 298.1 K

Operator: ras

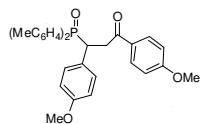
File: 600ras042511.001

VNMR5-600 "nmr600"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 36764.7 Hz
5000 repetitions
OBSERVE C13, 150.8132472 MHz
DECOUPLE H1, 599.7768382 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 3 hr, 12 min, 27 sec



S33

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)3-[Bis(4-methylphenyl)phosphinyl]-1,3-bis(4-methoxyphenyl)propan-1-one (**13**)

Std phosphorus

File: home/ras/Desktop/600ras060810.017.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras060810.017

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Relax. delay 1.000
Pulse 45.0 degrees

Pulse 45.0 degrees
Acq. time 1.600 sec

Width 41666.7 Hz

16 repetitions

OBSERVE P31, 242.7929005 MHz

OBSERVE P31, 242.7929005 MHz
DECOUPLE H1, 599.7768382 MHz

Power 46 dB

Power 46 dB
continuously on

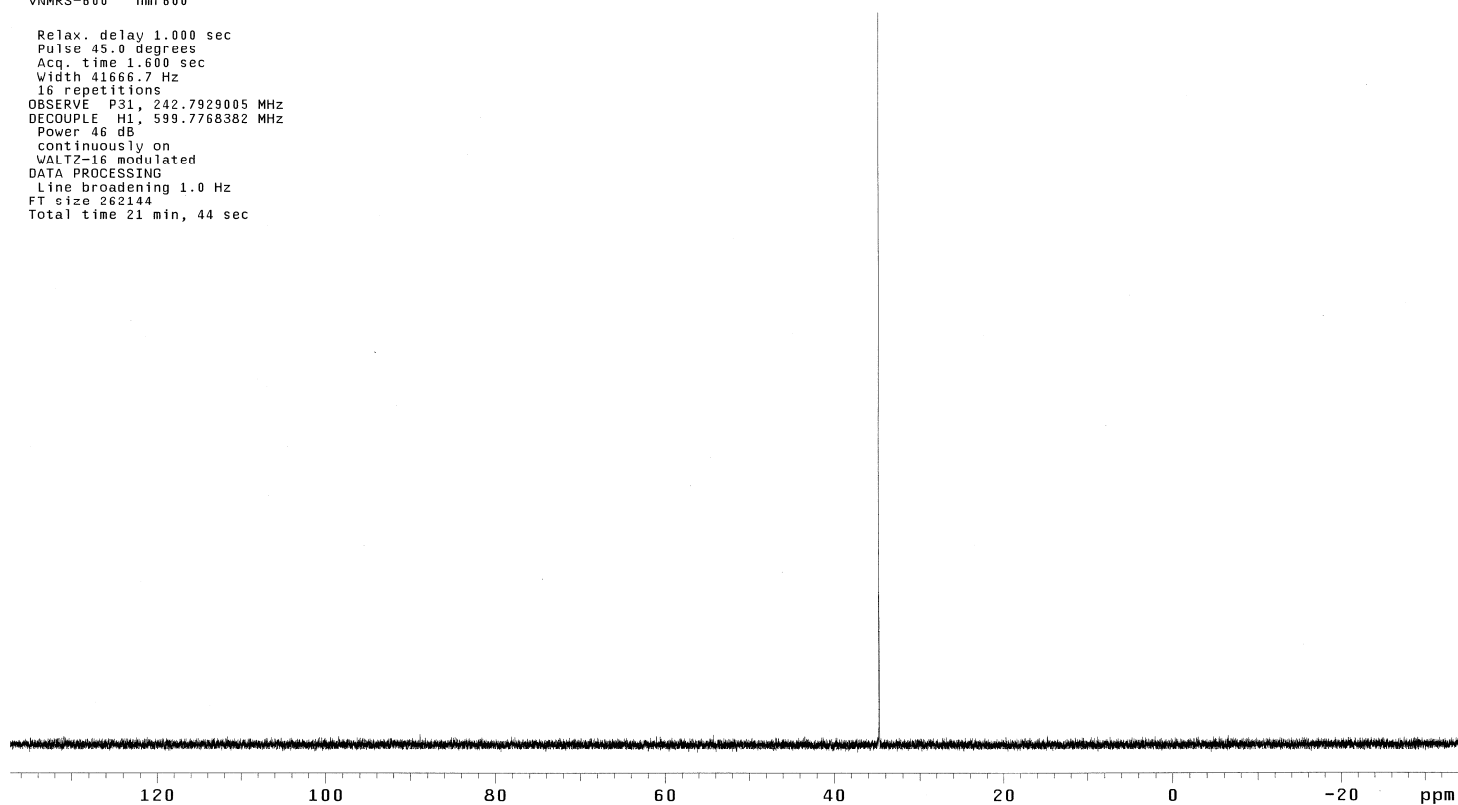
continuously on
WALTZ-16 modulated

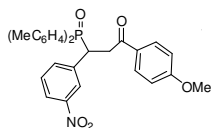
DATA PROCESSING

DATA PROCESSING
Line broadening 1.0 Hz

FT size 262144

Total time 21 min, 44 sec





^1H NMR spectrum (CDCl_3 , 25 °C)

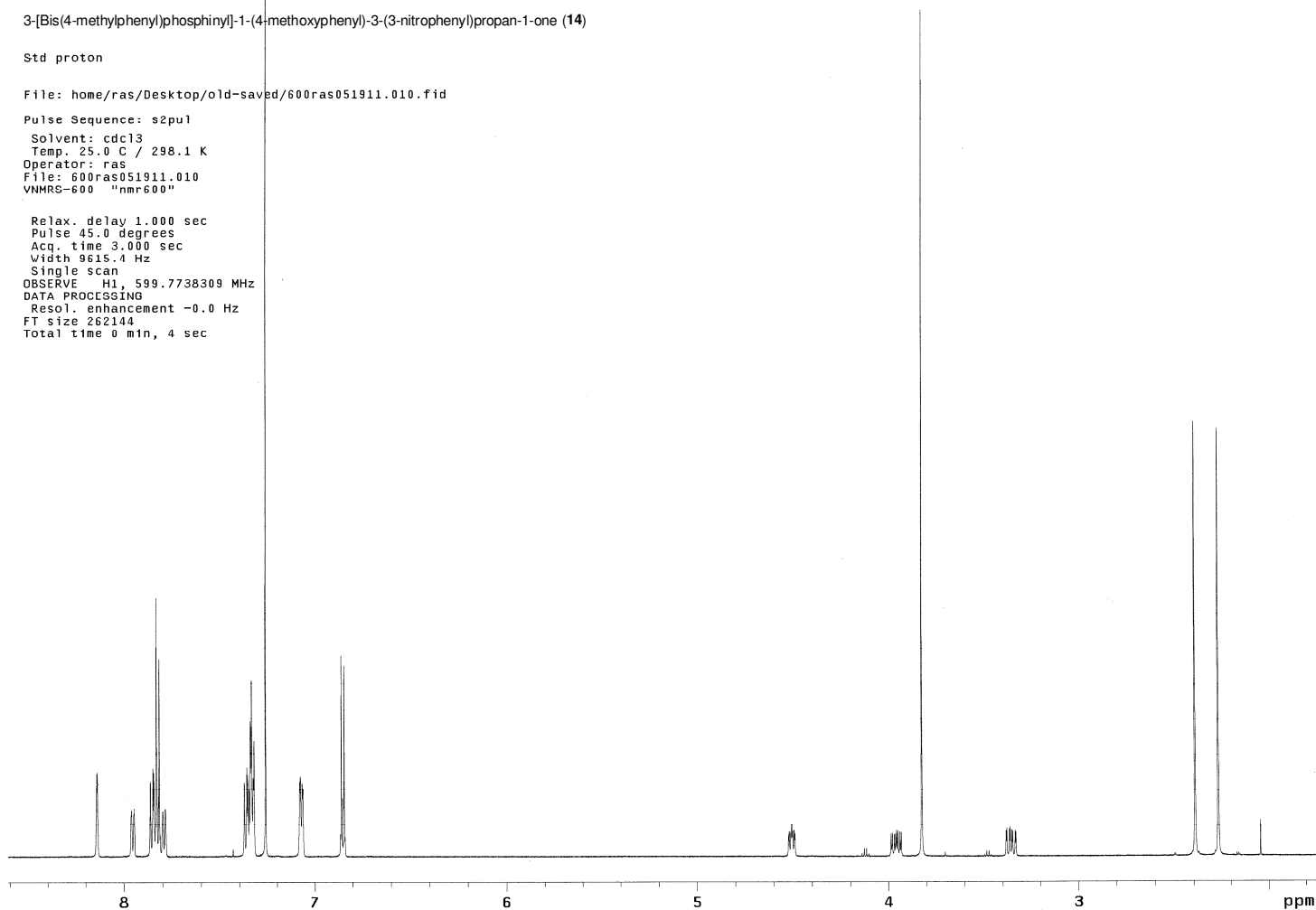
3-[Bis(4-methylphenyl)phosphinyl]-1-(4-methoxyphenyl)-3-(3-nitrophenyl)propan-1-one (14)

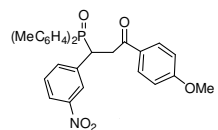
Std proton

File: home/ras/Desktop/old-saved/600ras051911.010.fid

Pulse Sequence: s2pu1
Solvent: cdc13
Temp. 25.0 C / 298.1 K
Operator: ras
File: 600ras051911.010
VNMR-600 "nmr600"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 9615.4 Hz
Single scan
OBSERVE H1, 599.7738309 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 262144
Total time 0 min, 4 sec





3-[Bis(4-methylphenyl)phosphinyl]-1-(4-methoxyphenyl)-3-(3-nitrophenyl)propan-1-one (**14**)

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

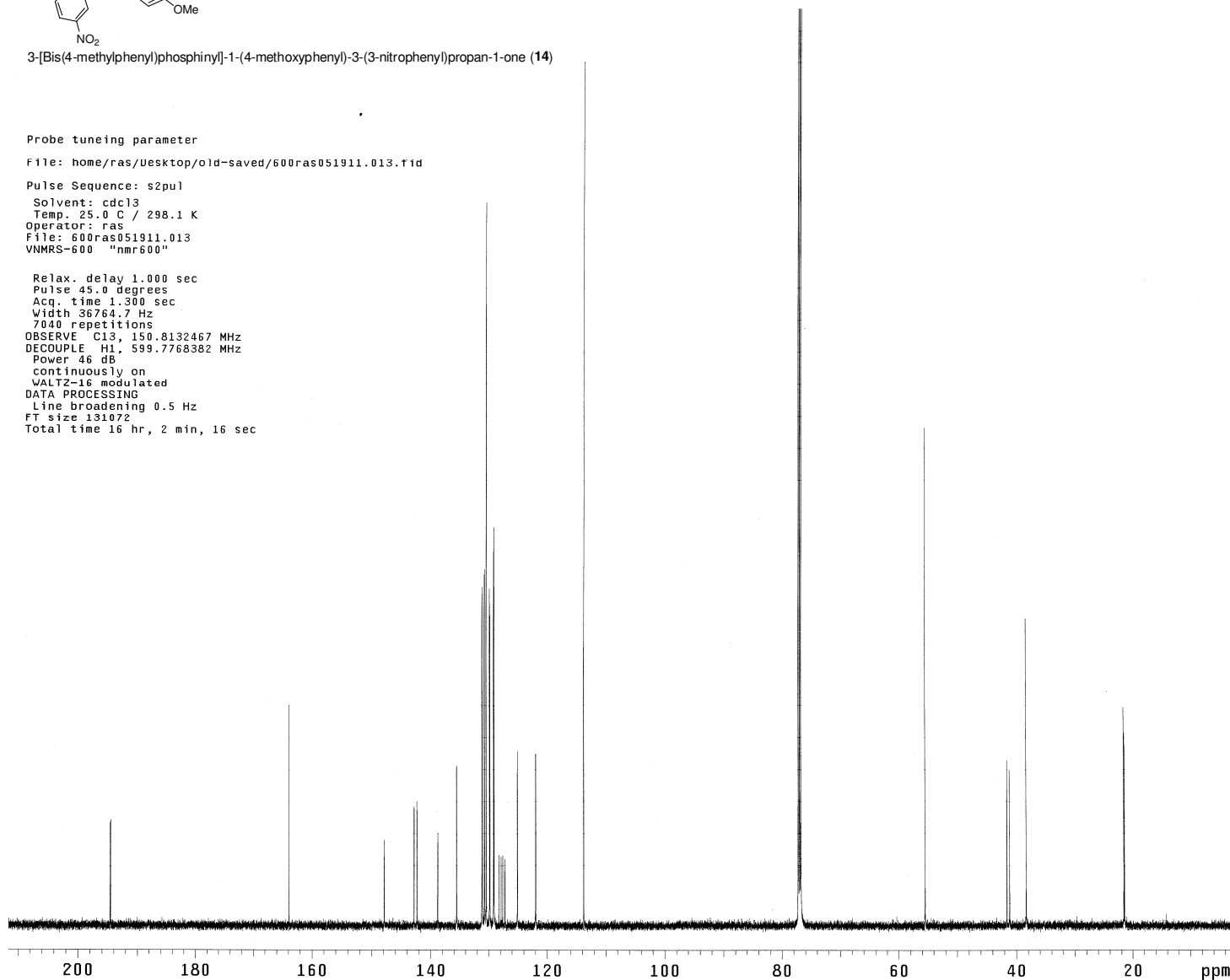
Probe tuning parameter

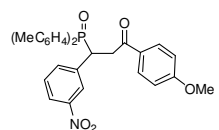
File: home/ras/Desktop/old-saved/600ras051911.013.fid

Pulse Sequence: s2pul

Solvent: cdcl_3
Temp. 25.0 C / 298.1 K
Operator: ras
File: 600ras051911.013
VNMR-600 "nmr600"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 36764.7 Hz
7040 repetitions
OBSERVE $\text{C}13$, 150.8132467 MHz
DECOUPLE $\text{H}1$, 599.7768382 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 16 hr, 2 min, 16 sec





3-[Bis(4-methylphenyl)phosphinyl]-1-(4-methoxyphenyl)-3-(3-nitrophenyl)propan-1-one (**14**)

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Std phosphorus

File: home/ras/Desktop/600ras120611.020.fid

Pulse Sequence: szpu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras120611.020

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

356 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

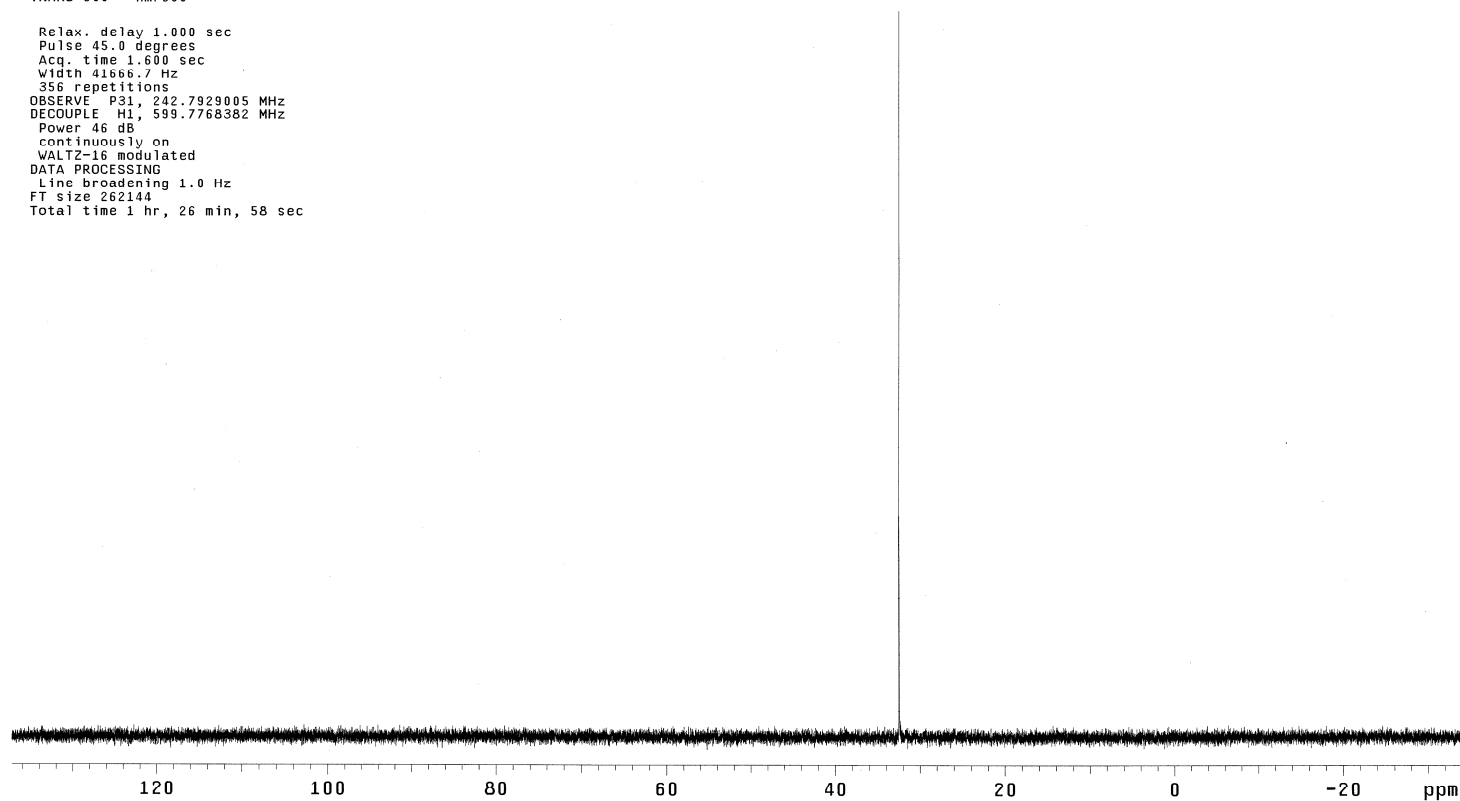
WALTZ-16 modulated

DATA PROCESSING

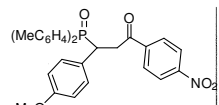
Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec



¹H NMR spectrum (CDCl₃, 25 °C)

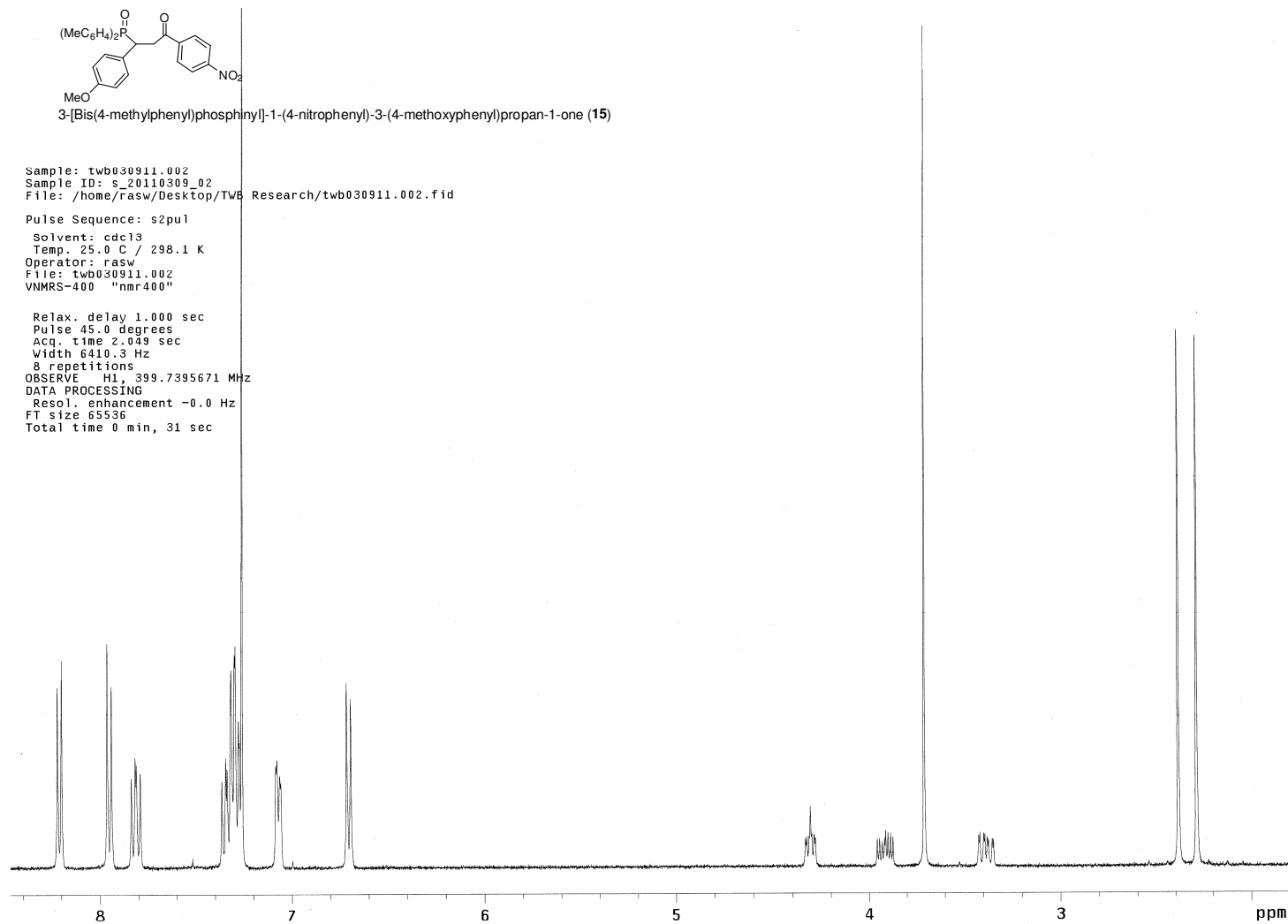


3-[Bis(4-methylphenyl)phosphinyl]-1-(4-nitrophenyl)-3-(4-methoxyphenyl)propan-1-one (**15**)

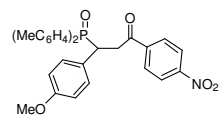
Sample: twb030911.002
Sample ID: s_20110309_02
File: /home/rasw/Desktop/TW6 Research/twb030911.002.fid

Pulse Sequence: s2pul
Solvent: cdc13
Temp. 25.0 C / 298.1 K
Operator: rasw
File: twb030911.002
VNMR-400 "nmr400"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.7395671 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 65536
Total time 0 min, 31 sec



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



3-[Bis(4-methylphenyl)phosphinyl]-1-(4-nitrophenyl)-3-(4-methoxyphenyl)propan-1-one (**15**)

Std carbon

File: home/ras/Desktop/600ras092711.001.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Ambient temperature

Operator: ras

File: 600ras092711.001

VNMR-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

30368 repetitions

OBSERVE C13, 150.8132484 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

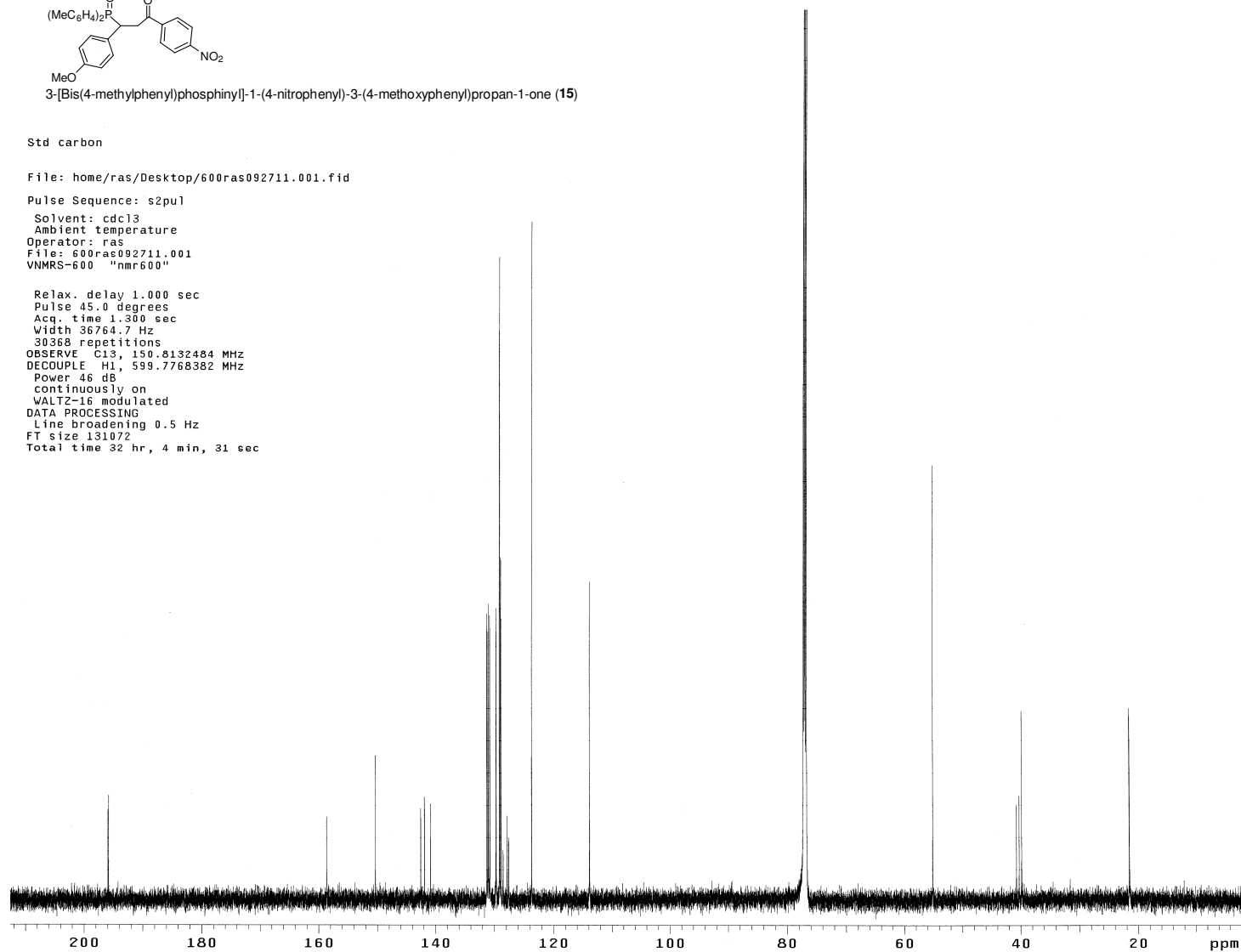
WALTZ-16 modulated

DATA PROCESSING

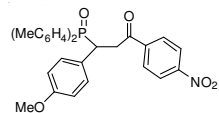
Line broadening 0.5 Hz

FT size 131072

Total time 32 hr, 4 min, 31 sec



$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



3-[Bis(4-methylphenyl)phosphinyl]-1-(4-nitrophenyl)-3-(4-methoxyphenyl)propan-1-one (**15**)

Std phosphorus

File: home/ras/Desktop/600ras032411.013.fid

Pulse Sequence: szpul

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras032411.013

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

8 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

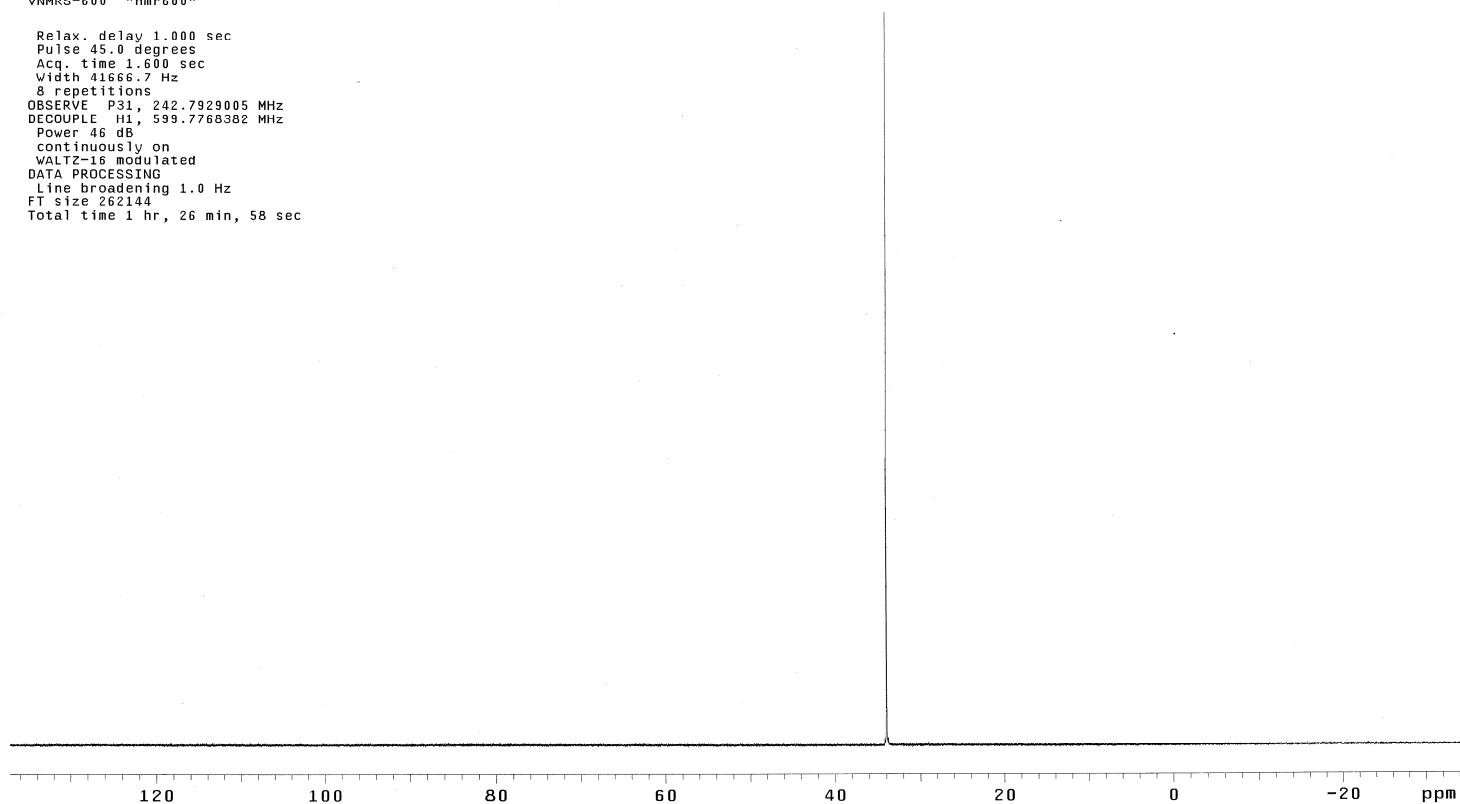
WALTZ-16 modulated

DATA PROCESSING

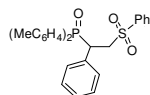
Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec



¹H NMR spectrum (CDCl₃, 25 °C)



Bis(4-methylphenyl)[1-phenyl-2-(phenylsulfonyl)ethane]phosphine oxide (**16**)

Std proton

File: home/ras/Desktop/old-saved/600ras051711.007.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras051711.007

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 9615.4 Hz

Single scan

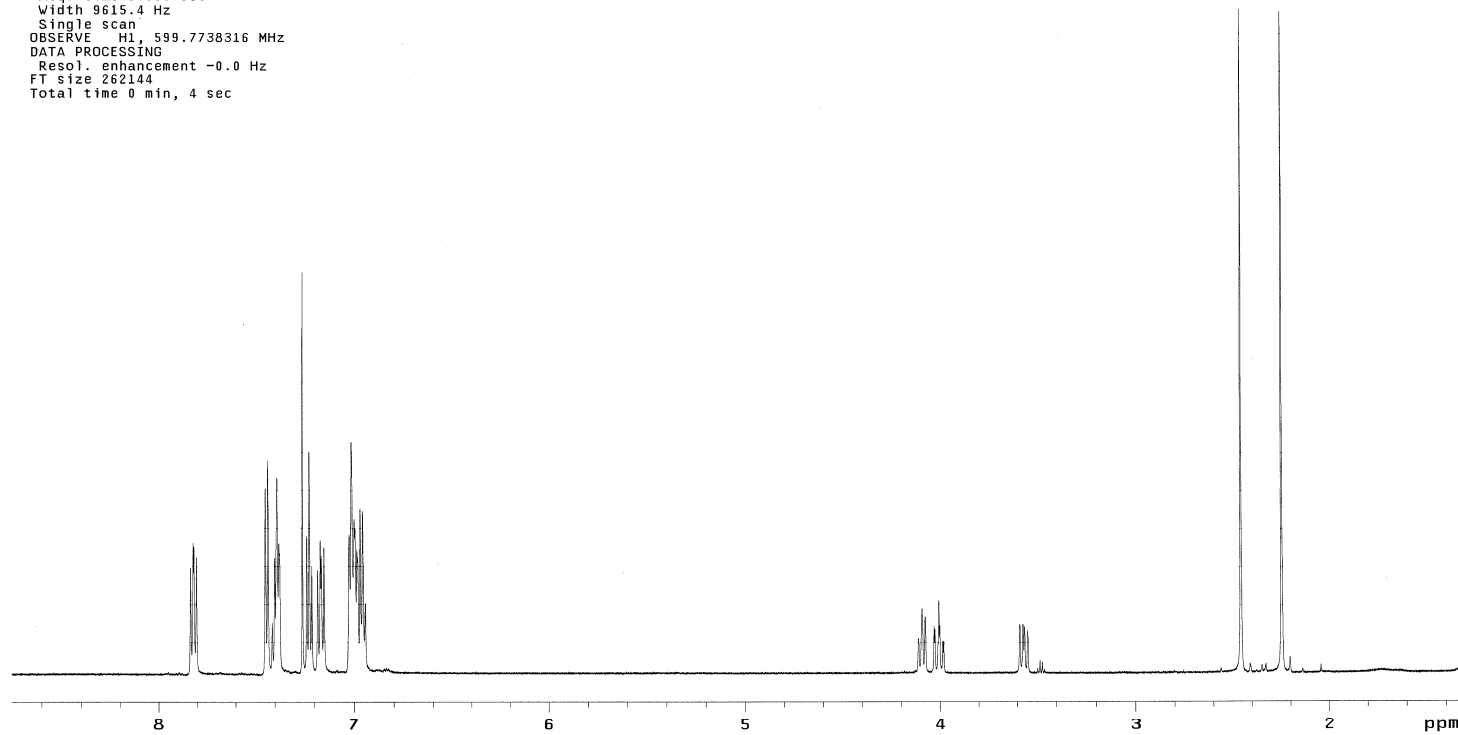
OBSERVE H1, 599.7738316 MHz

DATA PROCESSING

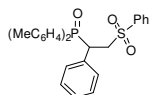
Resol. enhancement -0.0 Hz

FT size 262144

Total time 0 min, 4 sec



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



Bis(4-methylphenyl)[1-phenyl-2-(phenylsulfonyl)ethane]phosphine oxide (**16**)

Probe tuning parameter

File: home/ras/Desktop/Old-saved/600ras051711.008.fid

Pulse Sequence: s2pu1

Solvent: cdc13

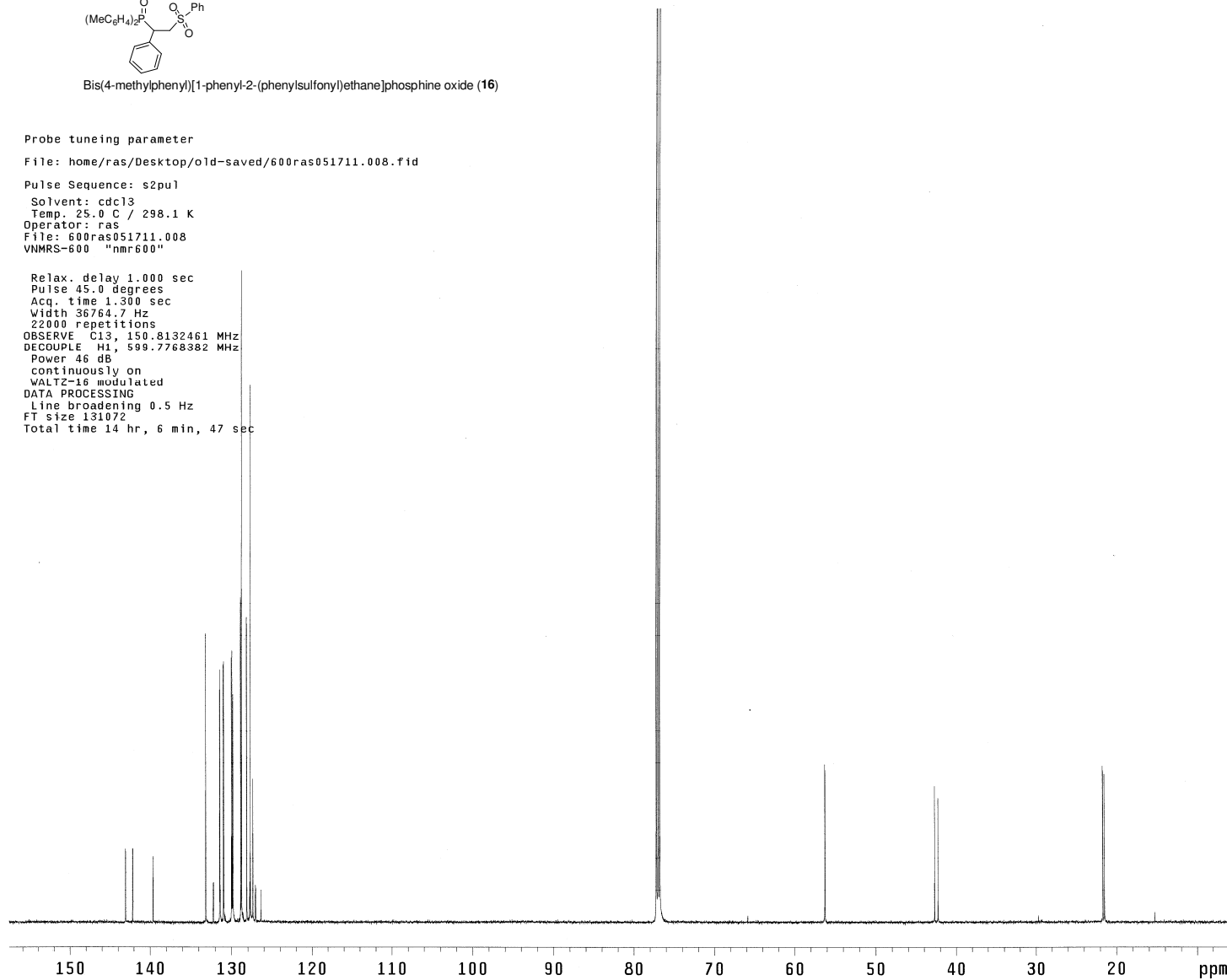
Temp. 25.0 C / 298.1 K

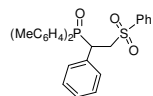
Operator: ras

File: 600ras051711.008

VNMR-600 "nmr600"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 36764.7 Hz
22000 repetitions
OBSERVE C13, 150.8132461 MHz
DECOUPLE H1, 599.7768382 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 14 hr, 6 min, 47 sec





Bis(4-methylphenyl)[1-phenyl-2-(phenylsulfonyl)ethane]phosphine oxide (**16**)

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Std phosphorus

File: home/ras/Desktop/old-saved/600ras051711.010.fid

Pulse Sequence: s2pul

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras051711.010

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

16 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

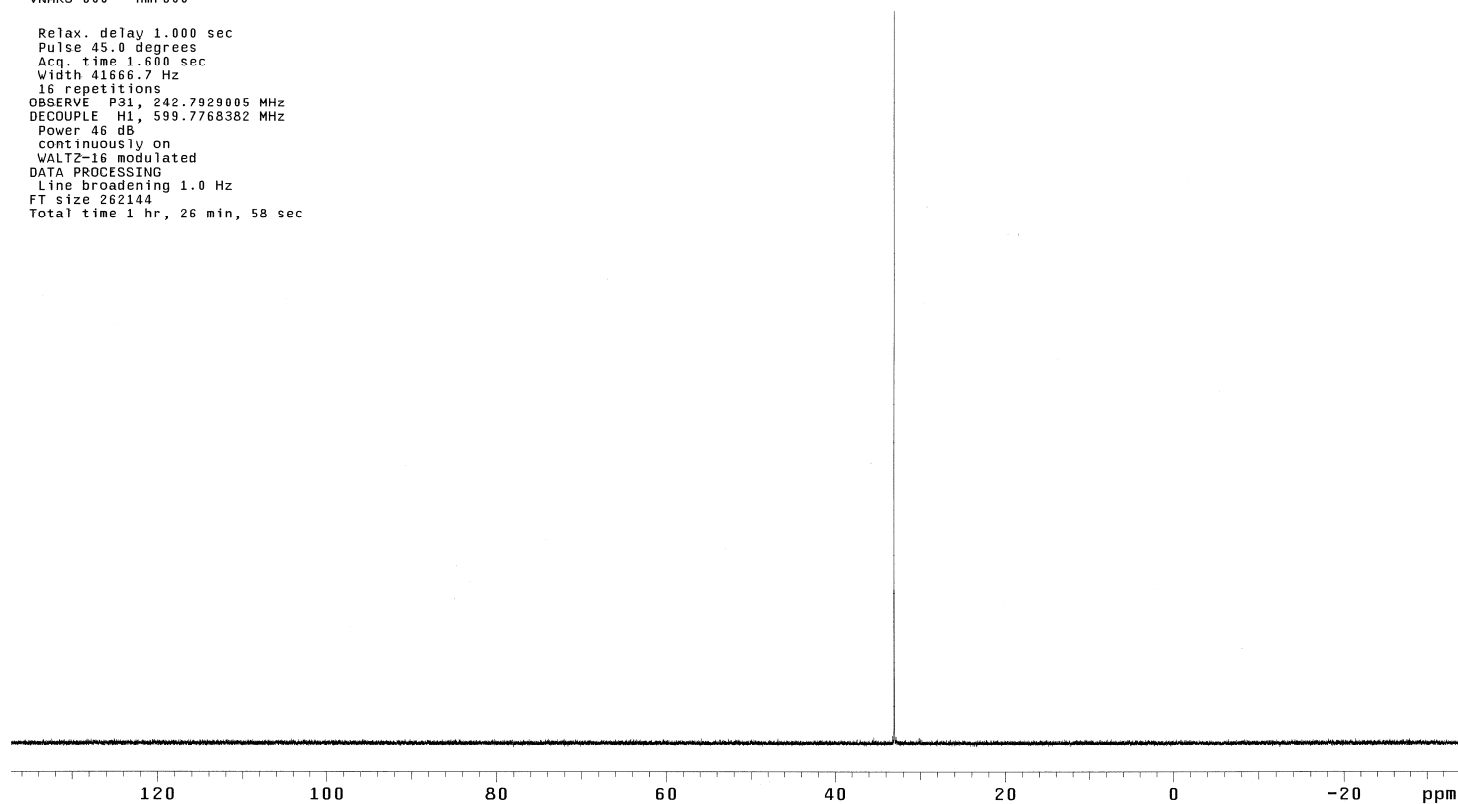
WALTZ-16 modulated

DATA PROCESSING

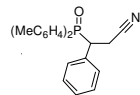
Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec



¹H NMR spectrum (CDCl₃, 25 °C)



3-[Bis(4-methylphenyl)phosphinyl]-3-phenylpropanenitrile (**17**)

Std proton

File: home/ras/Desktop/600ras051111.004.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras051111.004

VNMR5-400 "nmr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 9615.4 Hz

Single scan

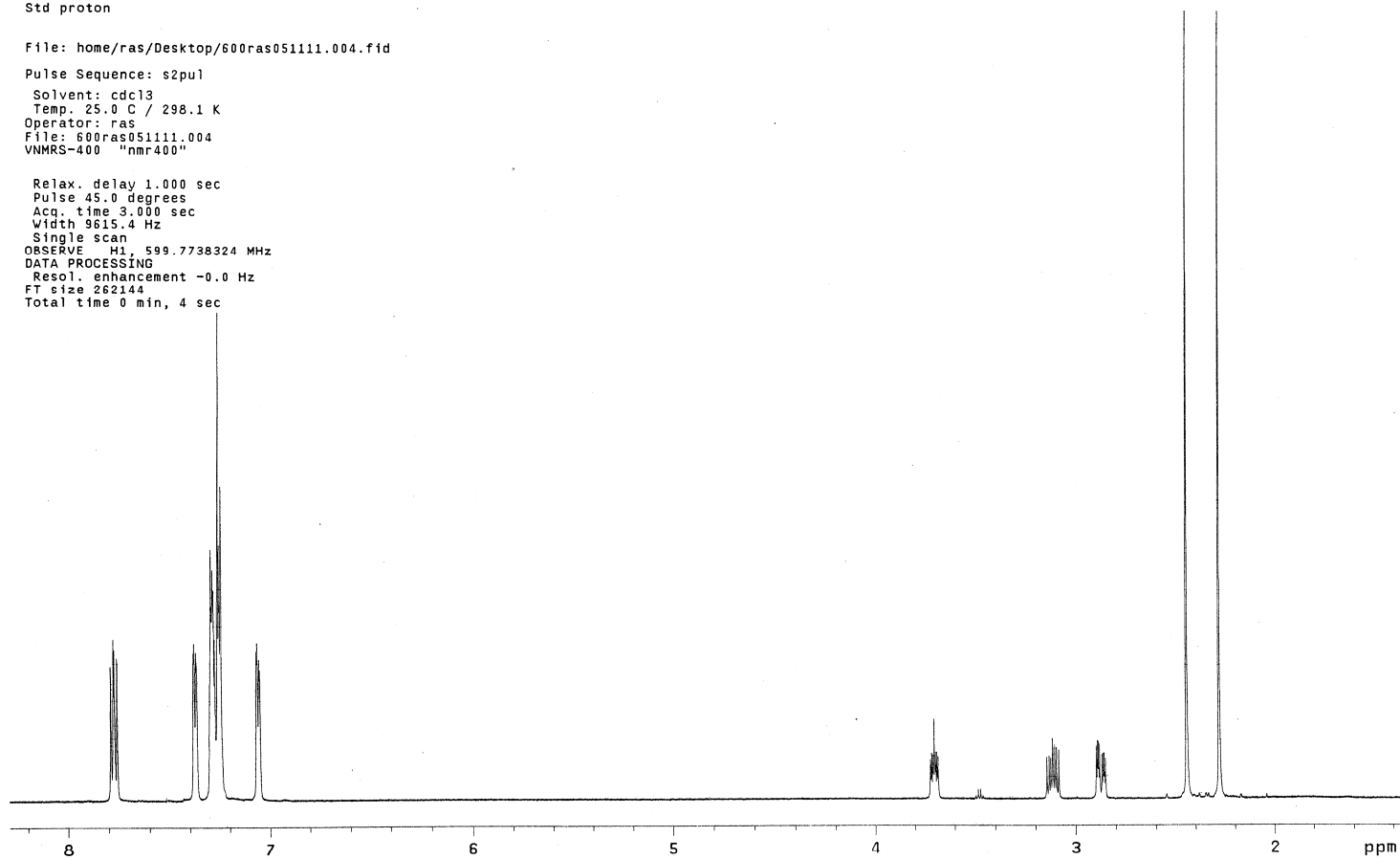
OBSERVE H1, 599.7738324 MHz

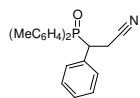
DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 262144

Total time 0 min, 4 sec





3-[Bis(4-methylphenyl)phosphinyl]-3-phenylpropanenitrile (17)

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Probe tuning parameter

File: home/ras/Desktop/old-saved/600ras051711.002.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras051711.002

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

22000 repetitions

OBSERVE C13, 150.8132467 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

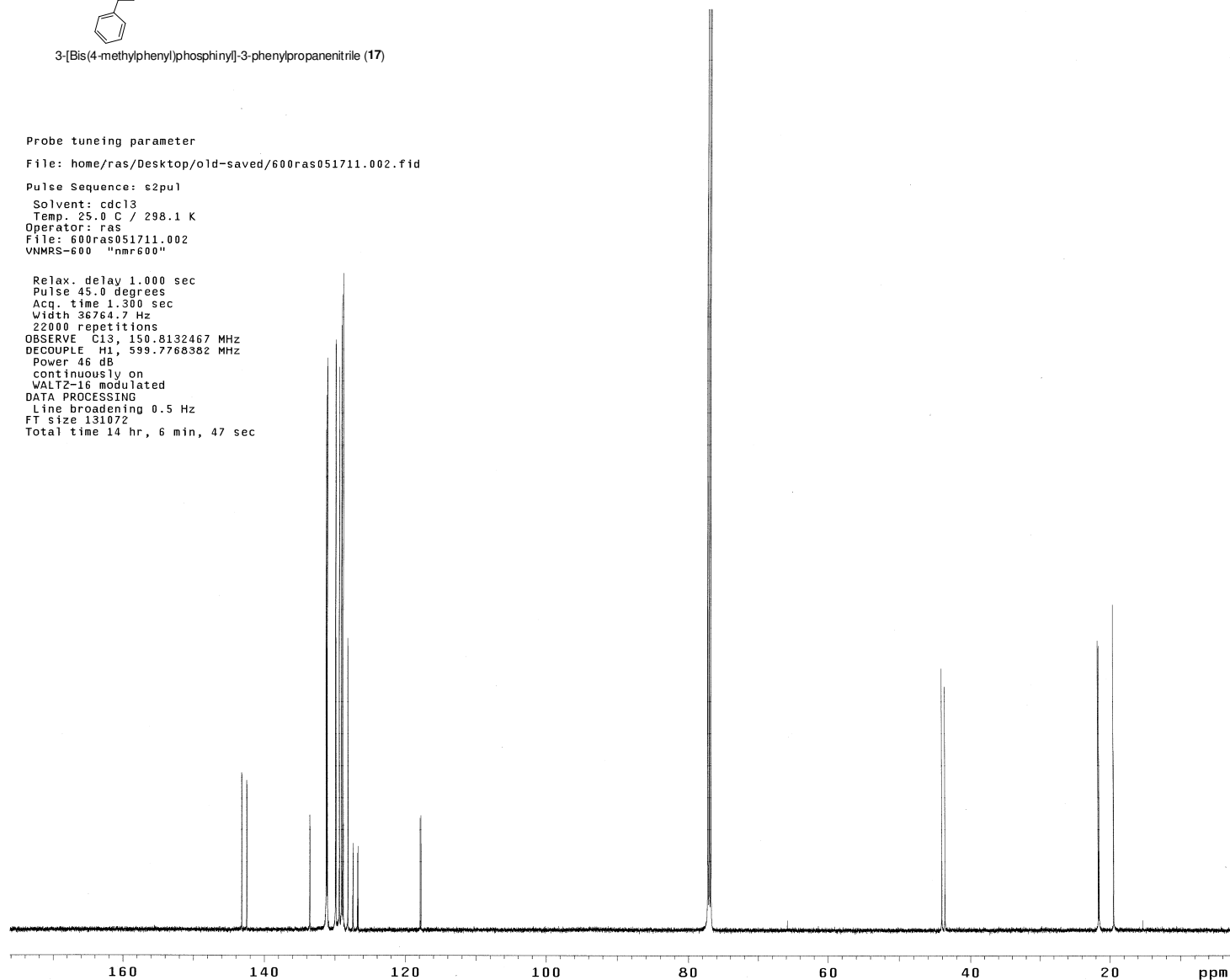
WALTZ-16 modulated

DATA PROCESSING

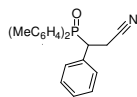
Line broadening 0.5 Hz

FT size 131072

Total time 14 hr, 6 min, 47 sec



S45



3-[Bis(4-methylphenyl)phosphinyl]-3-phenylpropanenitrile (17)

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Std phosphorus

File: home/ras/Desktop/old-saved/600ras051111.005.fid

Pulse Sequence: szpu1

Solvent: cdcl_3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras051111.005

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

32 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

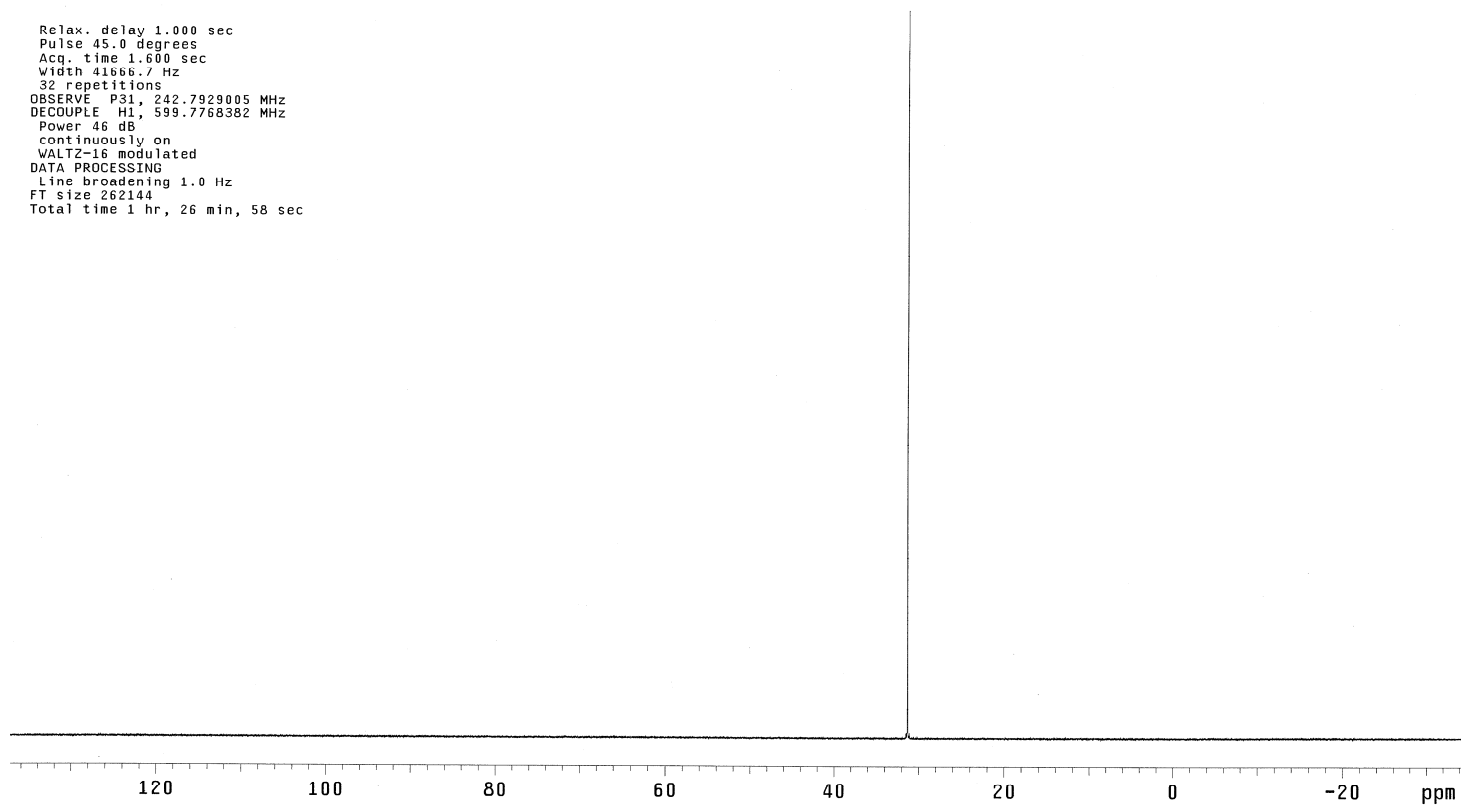
WALTZ-16 modulated

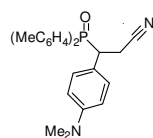
DATA PROCESSING

Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec





3-[Bis(4-methylphenyl)phosphinyl]-3-[(4-dimethylamino)phenyl]propanenitrile (**18**)

^1H NMR spectrum (CDCl_3 , 25 °C)

Std proton

File: home/ras/Desktop/old-saved/600ras070711.001.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras070711.001

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 9615.4 Hz

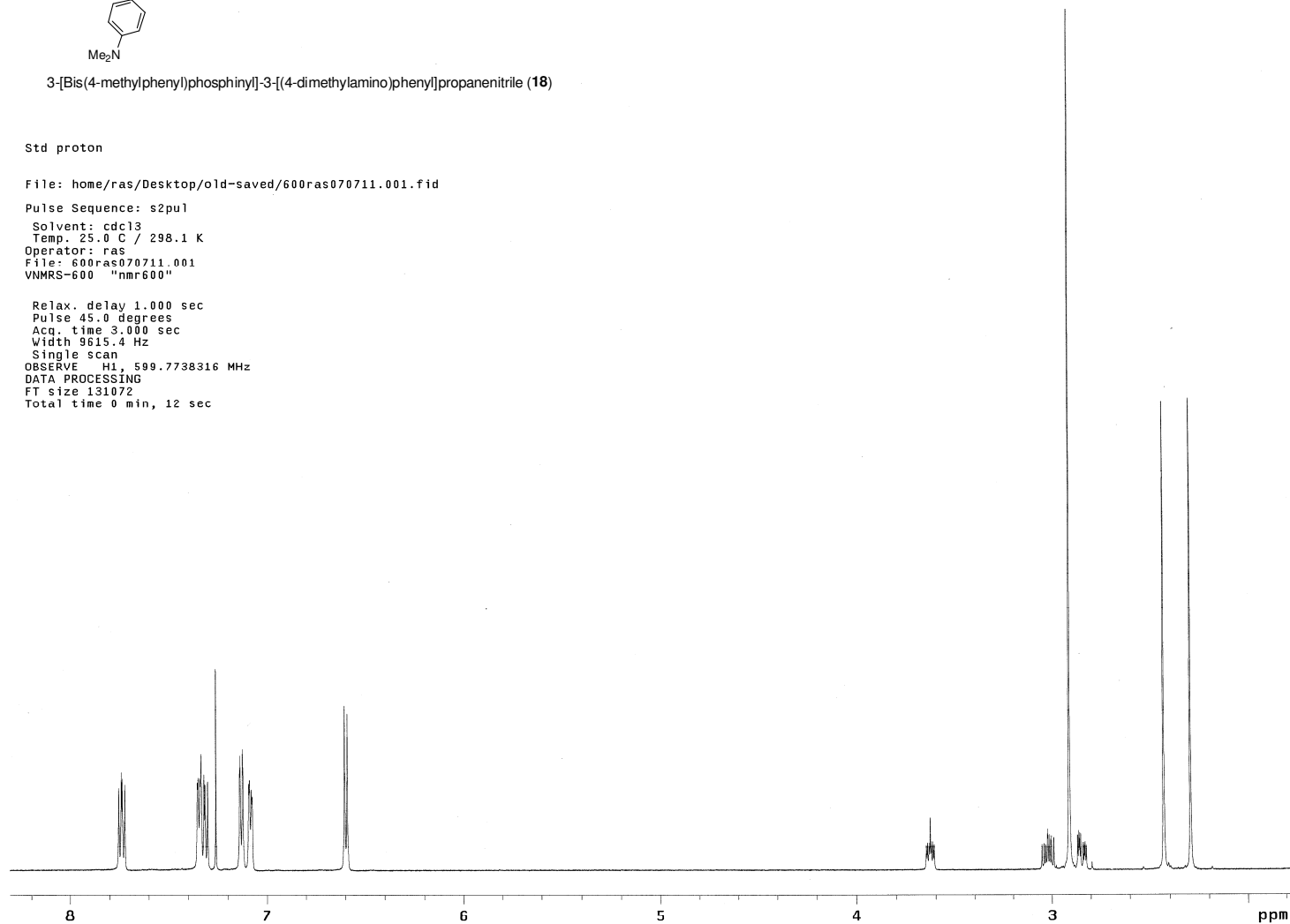
Single scan

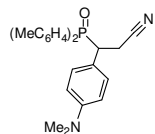
OBSERVE H1, 599.7738316 MHz

DATA PROCESSING

FT size 131072

Total time 0 min, 12 sec





3-[Bis(4-methylphenyl)phosphiny]-3-[(4-dimethylamino)phenyl]propanenitrile (**18**)

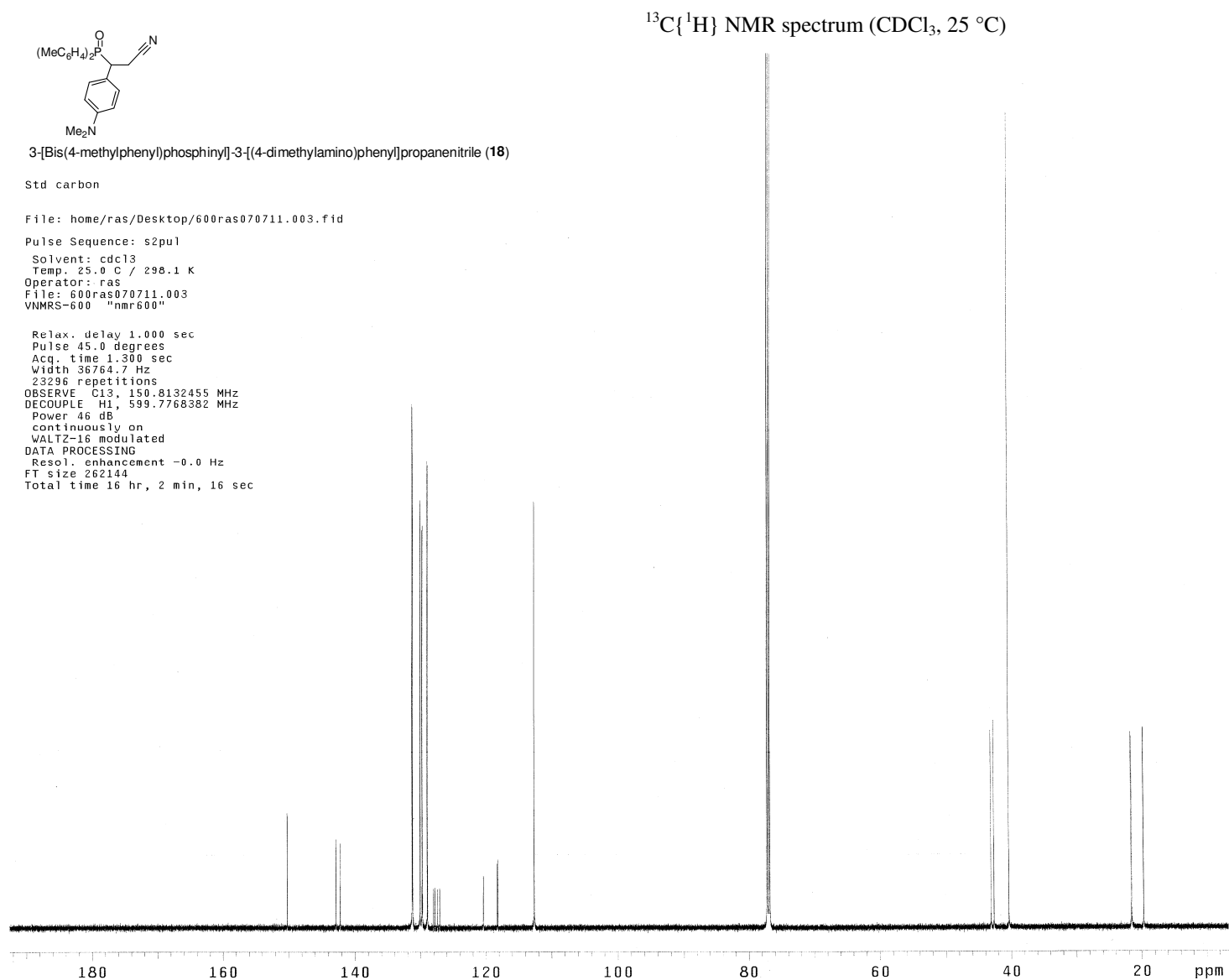
Std carbon

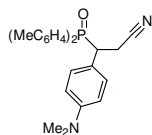
File: home/ras/Desktop/600ras070711.003.fid

Pulse Sequence: s2pul

Solvent: cdc13
Temp. 25.0 C / 298.1 K
Operator: ras
File: 600ras070711.003
VNMR-600 "nmr600"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 36764.7 Hz
23296 repetitions
OBSERVE C13, 150.8132455 MHz
DECOUPLE H1, 599.7768382 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 262144
Total time 16 hr, 2 min, 16 sec





3-[Bis(4-methylphenyl)phosphinyl]-3-[(4-dimethylamino)phenyl]propanenitrile (**18**)

Std phosphorus

File: home/ras/Desktop/600ras070711.002.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp: 25.0 C / 298.1 K

Operator: ras

File: 600ras070711.002

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

20 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

WALTZ-16 modulated

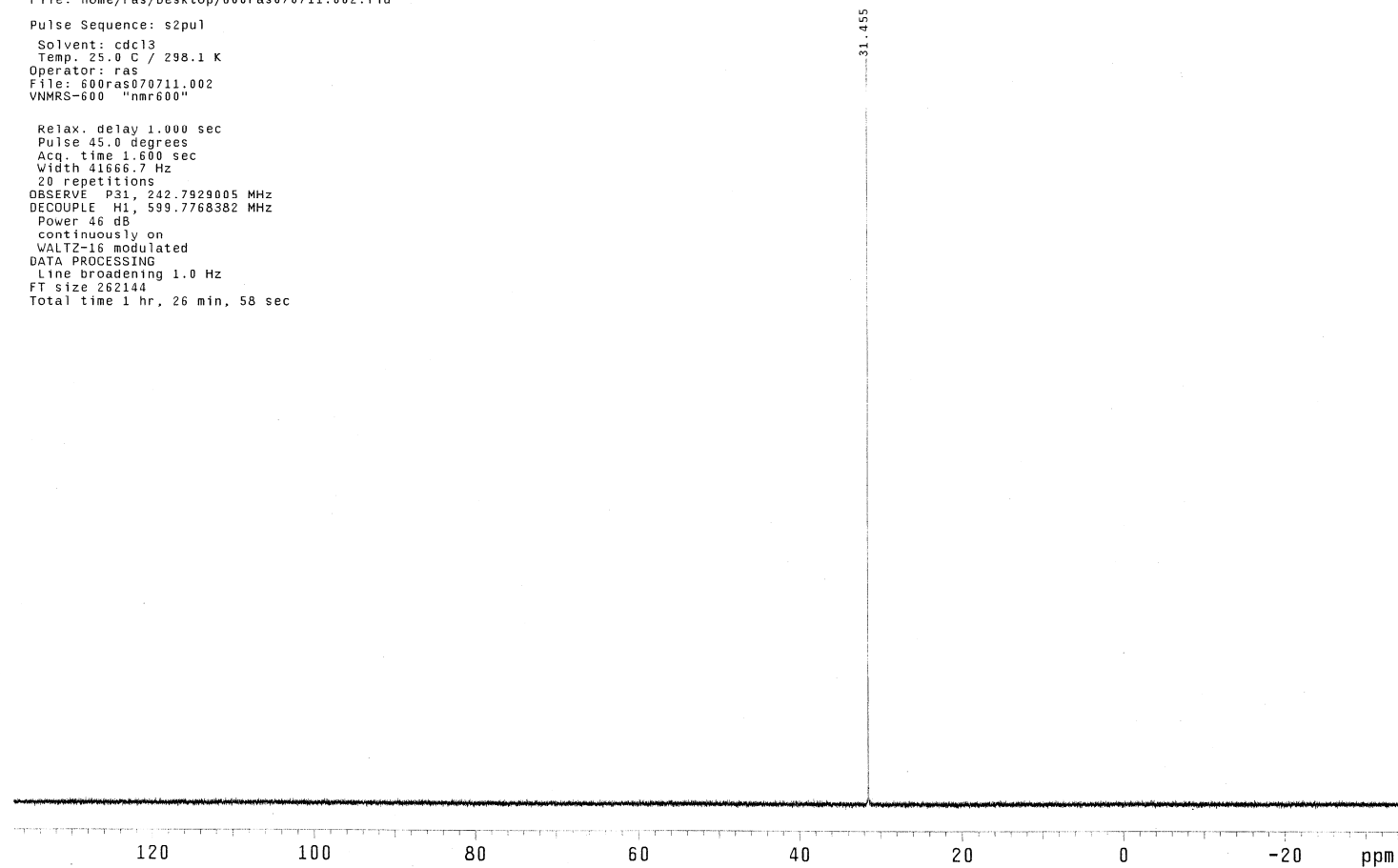
DATA PROCESSING

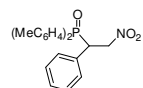
Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)





(2-Nitro-1-phenylethyl)-bis(4-methylphenyl)phosphine oxide (**19**)

Std proton

File: home/ras/Desktop/old-saved/600ras042611.003.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras042611.003

VNMR-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 9615.4 Hz

Single scan

OBSERVE H1, 599.7738311 MHz

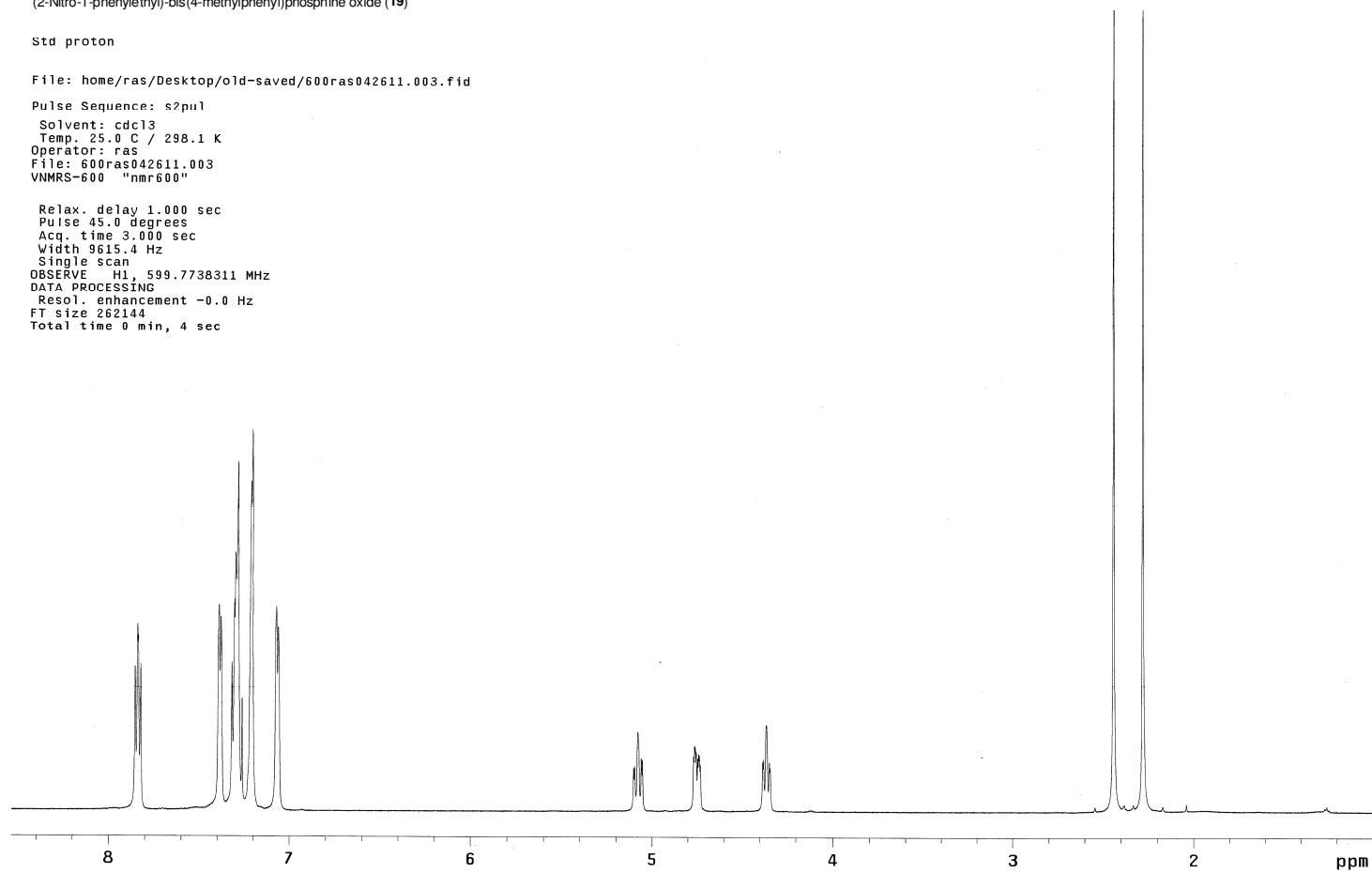
DATA PROCESSING

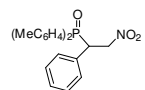
Resol. enhancement -0.0 Hz

FT size 262144

Total time 0 min, 4 sec

¹H NMR spectrum (CDCl₃, 25 °C)





(2-Nitro-1-phenylethyl)-bis(4-methylphenyl)phosphine oxide (**19**)

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Probe tuning parameter

File: home/ras/Desktop/old-saved/600ras042611.006.fid

Pulse Sequence: s2pu1

Solvent: cdcl_3

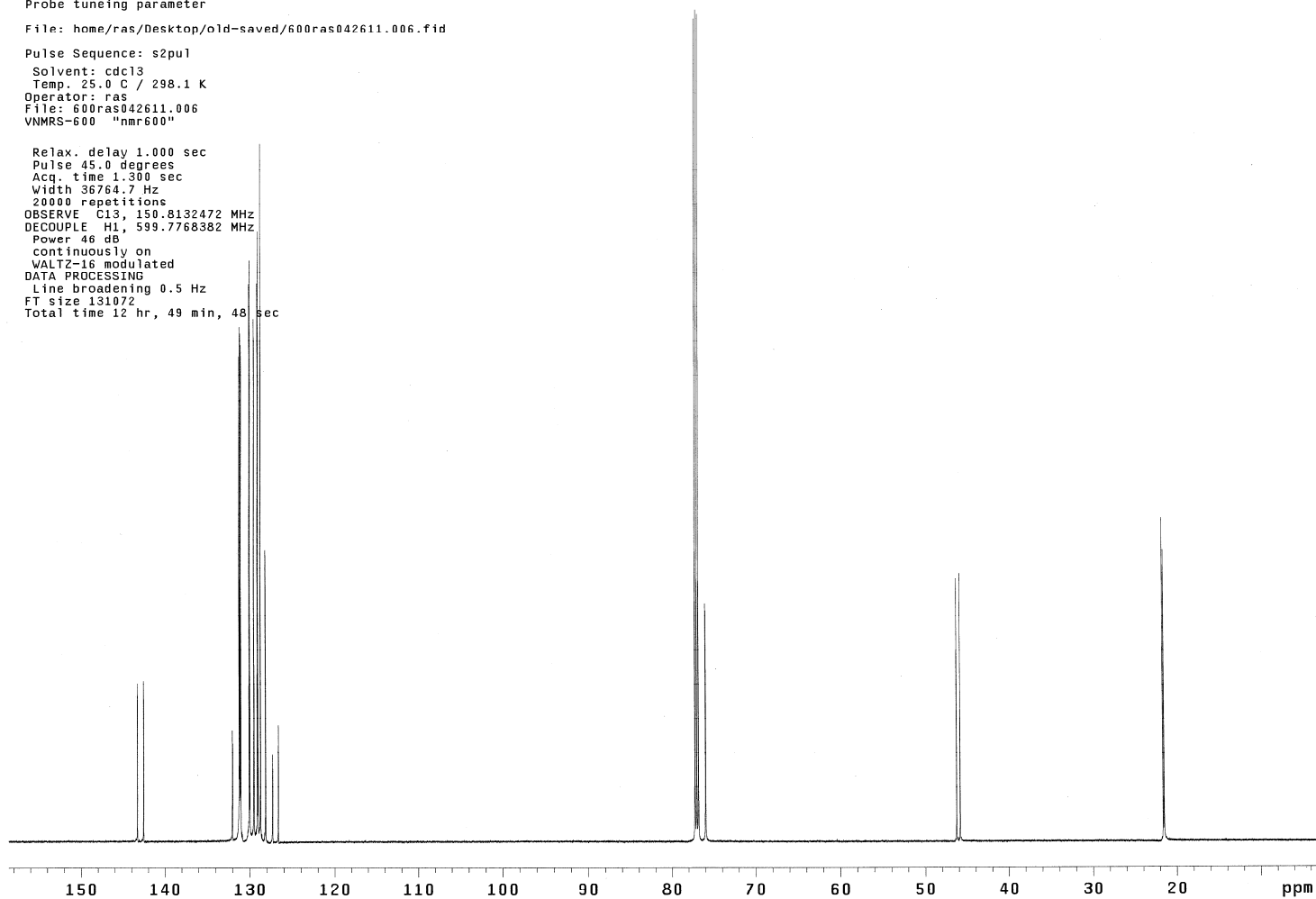
Temp. 25.0 C / 298.1 K

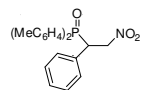
Operator: ras

File: 600ras042611.006

VNMRS-600 "nmr600"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 36764.7 Hz
20000 repetitions
OBSERVE C13, 150.8132472 MHz
DECOUPLE H1, 599.7768382 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 12 hr, 49 min, 48 sec





(2-Nitro-1-phenylethyl)-bis(4-methylphenyl)phosphine oxide (**19**)

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Std phosphorus

File: home/ras/Desktop/600ras042611.004.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras042611.004

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

2000 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

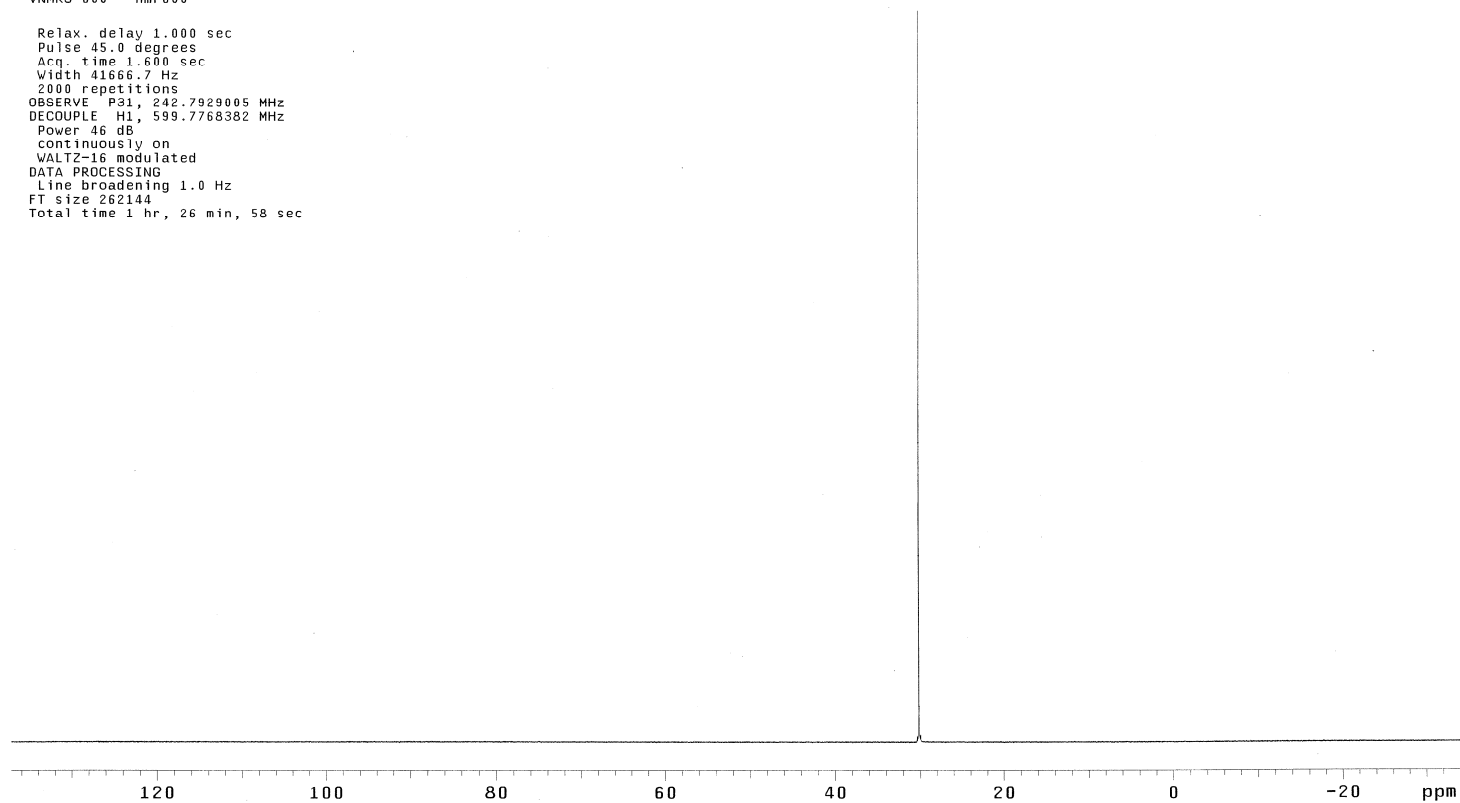
WALTZ-16 modulated

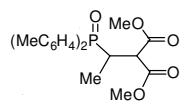
DATA PROCESSING

Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec





Dimethyl 2-(1-[bis(4-methylphenyl)phosphinyl]ethyl)malonate (**20**)

^1H NMR spectrum (CDCl_3 , 25 °C)

Std proton

File: home/ras/Desktop/600ras012511.016.fid

Pulse Sequence: s2pul

Solvent: cdcl_3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras012511.016

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 9615.4 Hz

Single scan

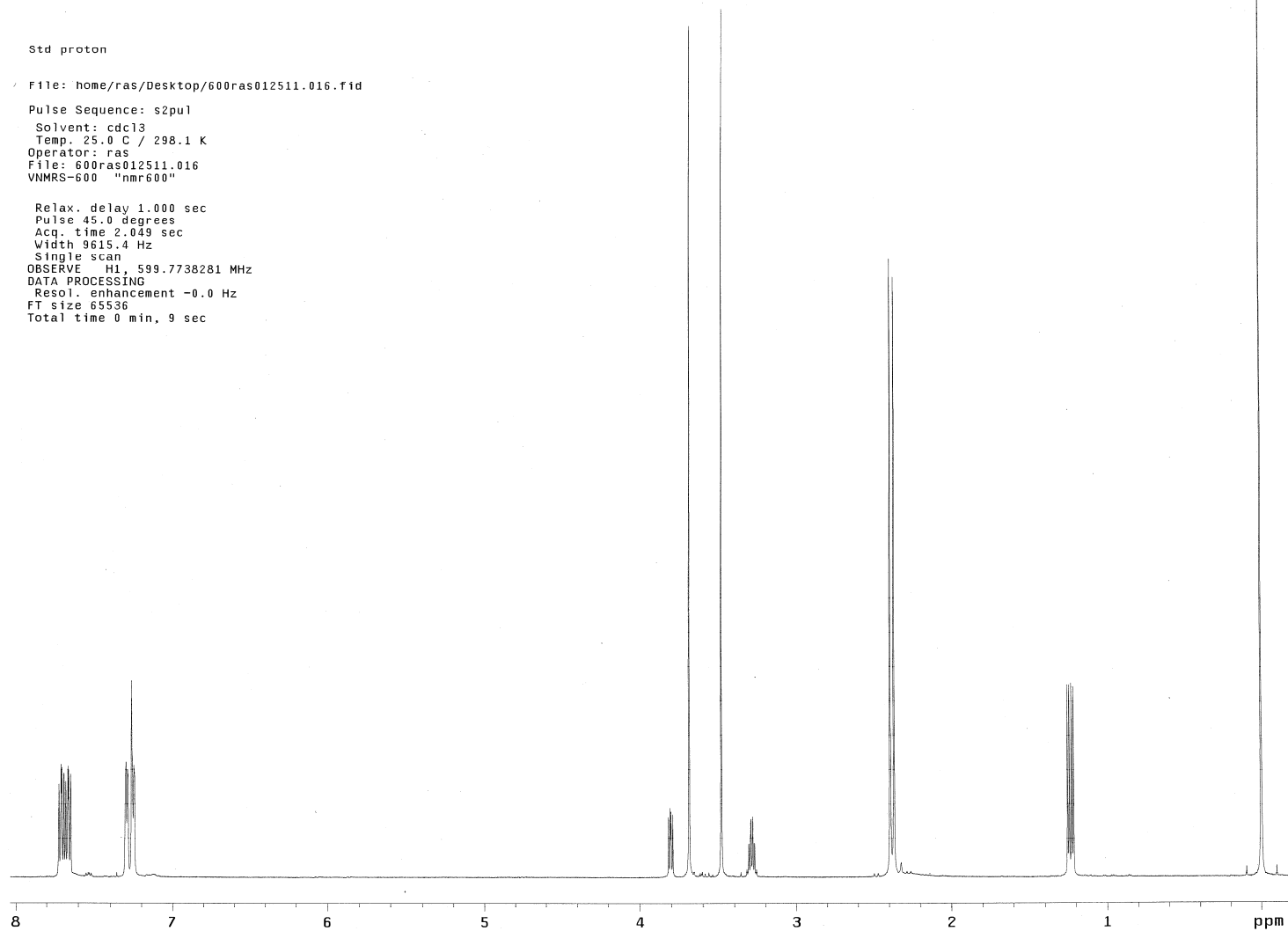
OBSERVE H1, 599.7738281 MHz

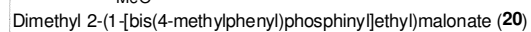
DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 65536

Total time 0 min, 9 sec





Probe tuning parameter

File: home/ras/Desktop/600ras012511.017.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp. 25.0 C / 298.1 K

```
Operator: ras
File: 0000000
```

```
File: 600ras012511.017
VNMRBS-600  "nmr600"
```

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz
18416 repetitions

```

18416 repetitions
OBSERVE C13 150

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OBSERVE   C13, 150.8132455 MHz
DECOUPLE  H1, 599.7768382 MHz
```

DECOUPLE H1, 599.7768382 MHz
Power 46 dBPower 46 dB
continuously

WALTZ-16 modulated

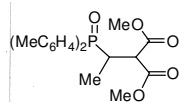
DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 12 hr, 49 min, 48 sec





Dimethyl 2-(1-[bis(4-methylphenyl)phosphinyl]ethyl)malonate (**20**)

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Std phosphorus

File: home/ras/Desktop/600ras012511.015.fid

Pulse Sequence: c2pu1

Solvent: cdcl_3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras012511.015

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

40 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

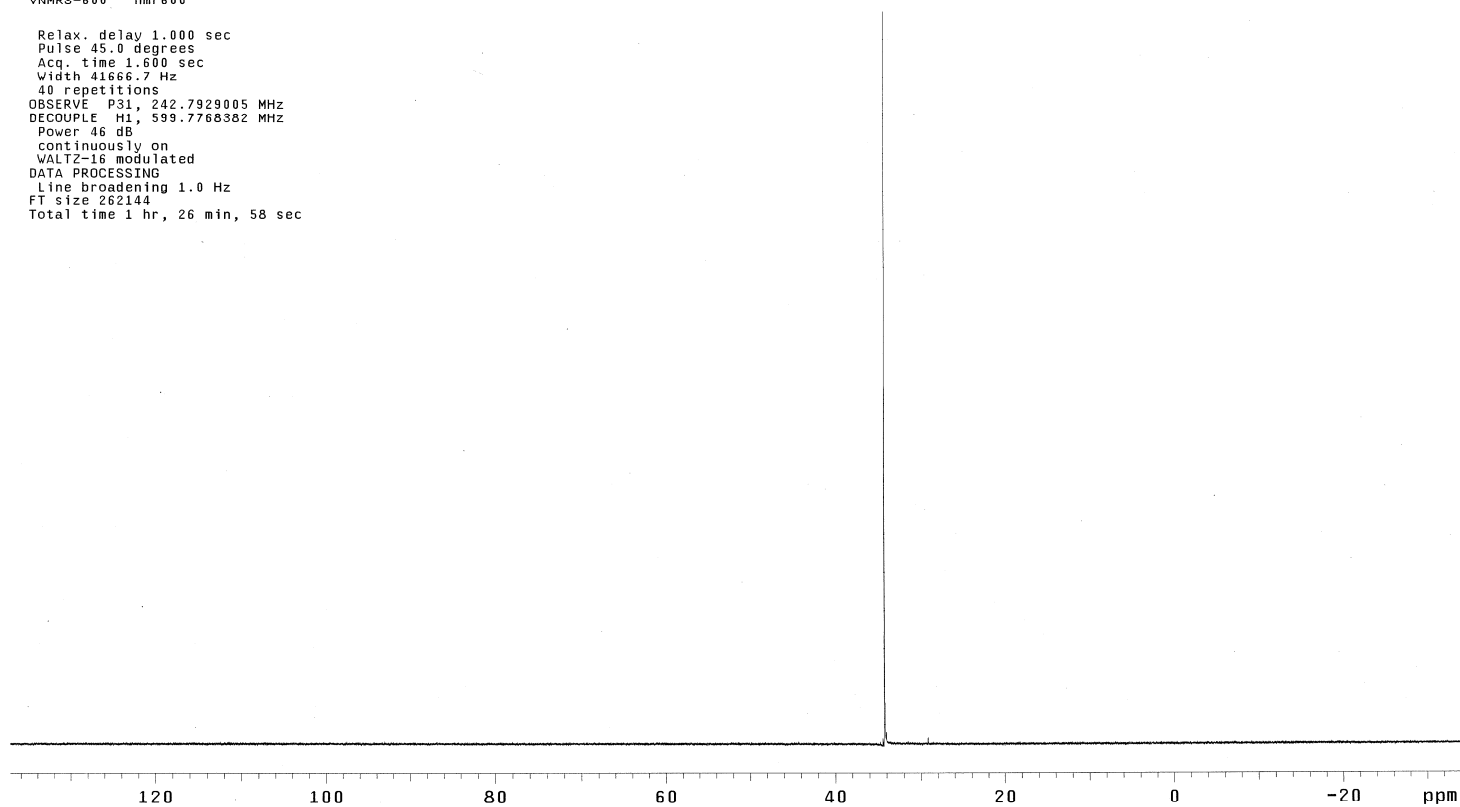
WALTZ-16 modulated

DATA PROCESSING

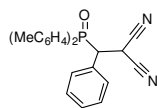
Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec



¹H NMR spectrum (CDCl₃, 25 °C)

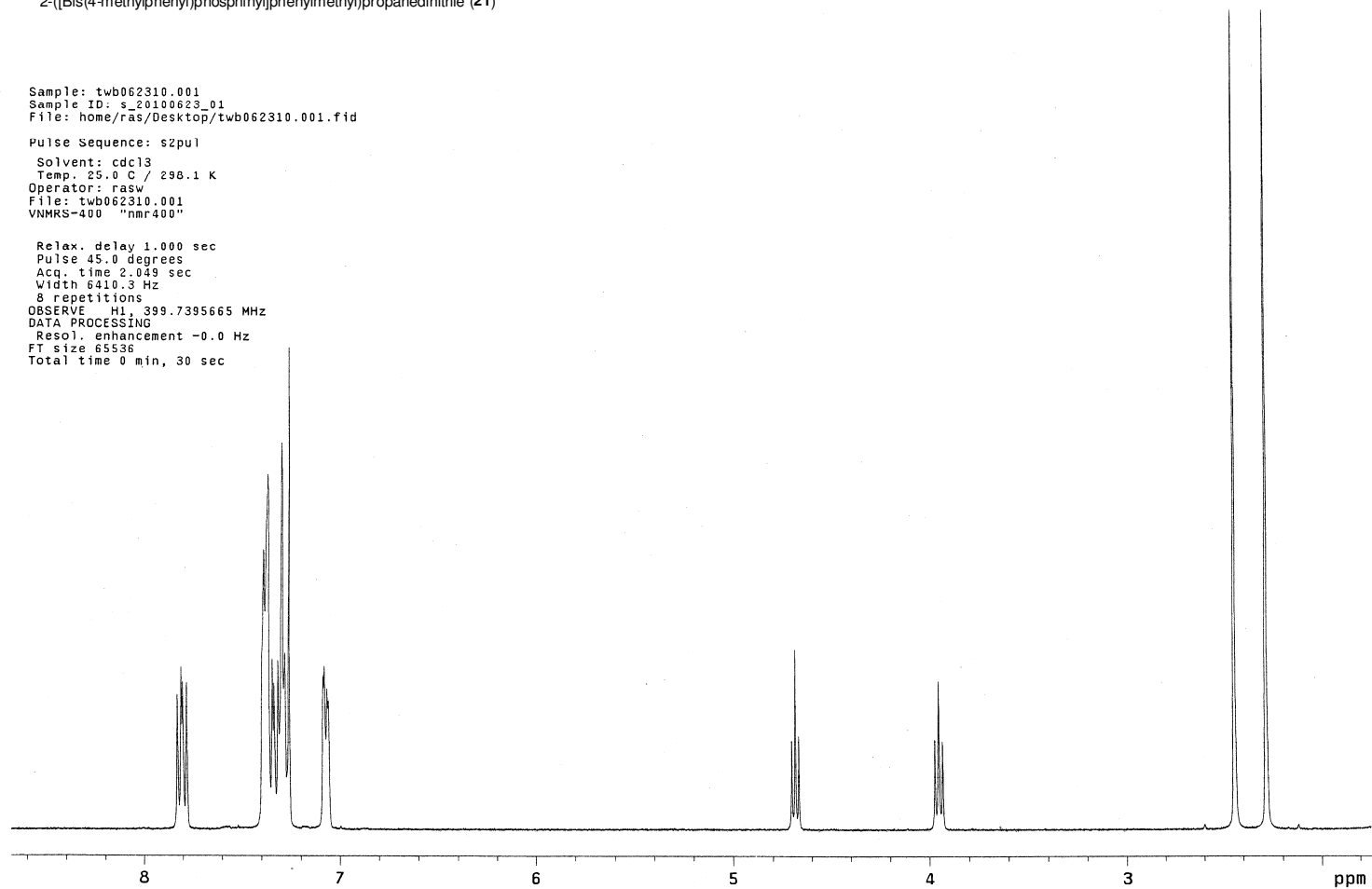


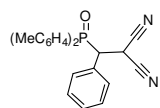
2-((Bis(4-methylphenyl)phosphinyl)phenylmethyl)propanedinitrile (**21**)

Sample: twb062310.001
Sample ID: s_20100623_01
File: home/ras/Desktop/twb062310.001.fid

Pulse Sequence: s2pul
Solvent: cdcl3
Temp: 25.0 C / 298.1 K
Operator: rasw
File: twb062310.001
VNMR-400 "nmr400"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.7395665 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 65536
Total time 0 min, 30 sec





2-([Bis(4-methylphenyl)phosphiny]phenylmethyl)propanedinitrile (**21**).

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Probe tuning parameter

File: home/ras/Desktop/600ras050411.007.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras050411.007

VNMR-400 "nmr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

3616 repetitions

OBSERVE C13, 150.8132475 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

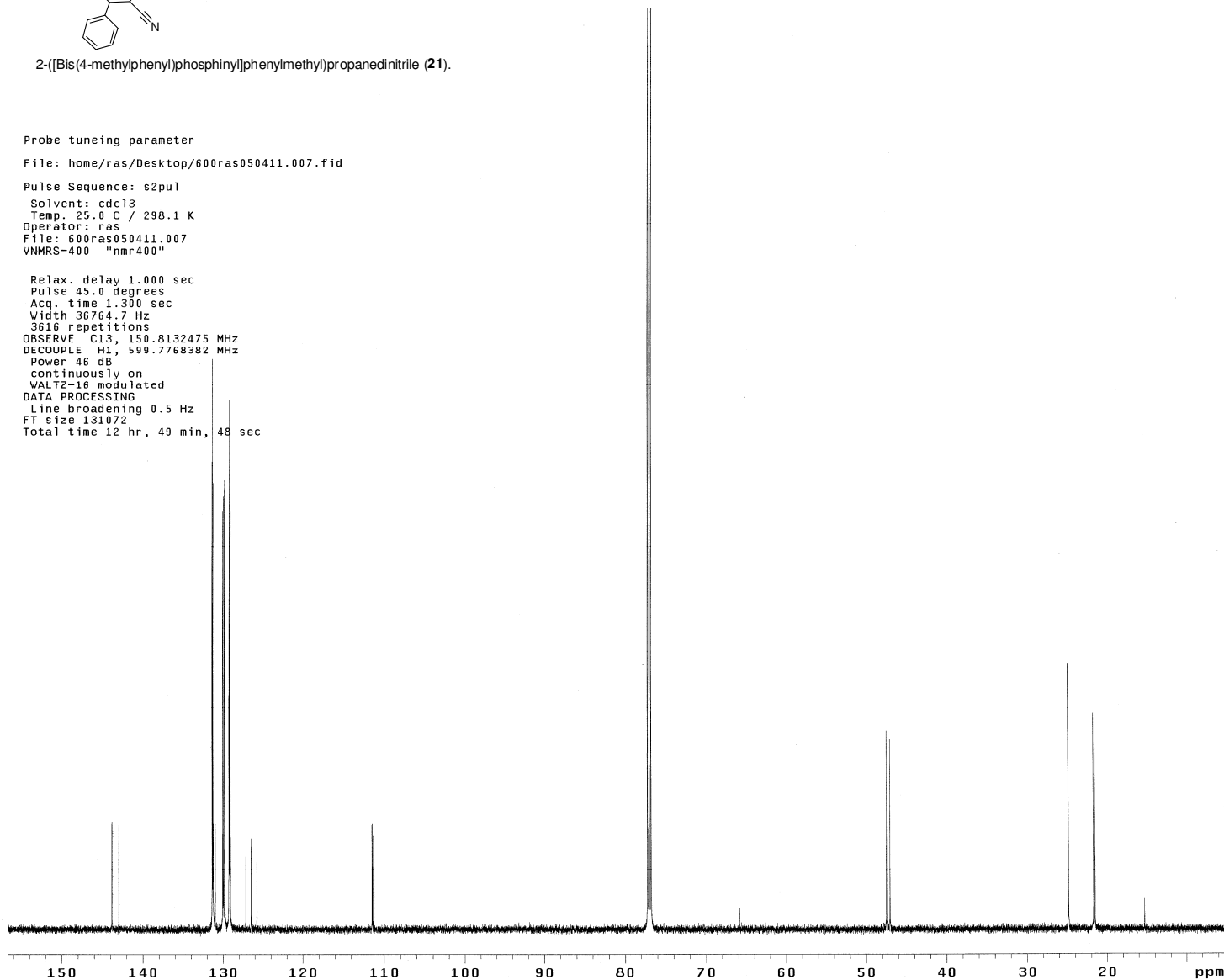
WALTZ-16 modulated

DATA PROCESSING

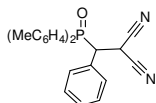
Line broadening 0.5 Hz

FT size 131072

Total time 12 hr, 49 min, 48 sec



$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



2-((Bis(4-methylphenyl)phosphinyl)phenylmethyl)propanedinitrile (**21**).

Std phosphorus

File: home/ras/Desktop/600ras050411.006.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras050411.006

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

2000 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

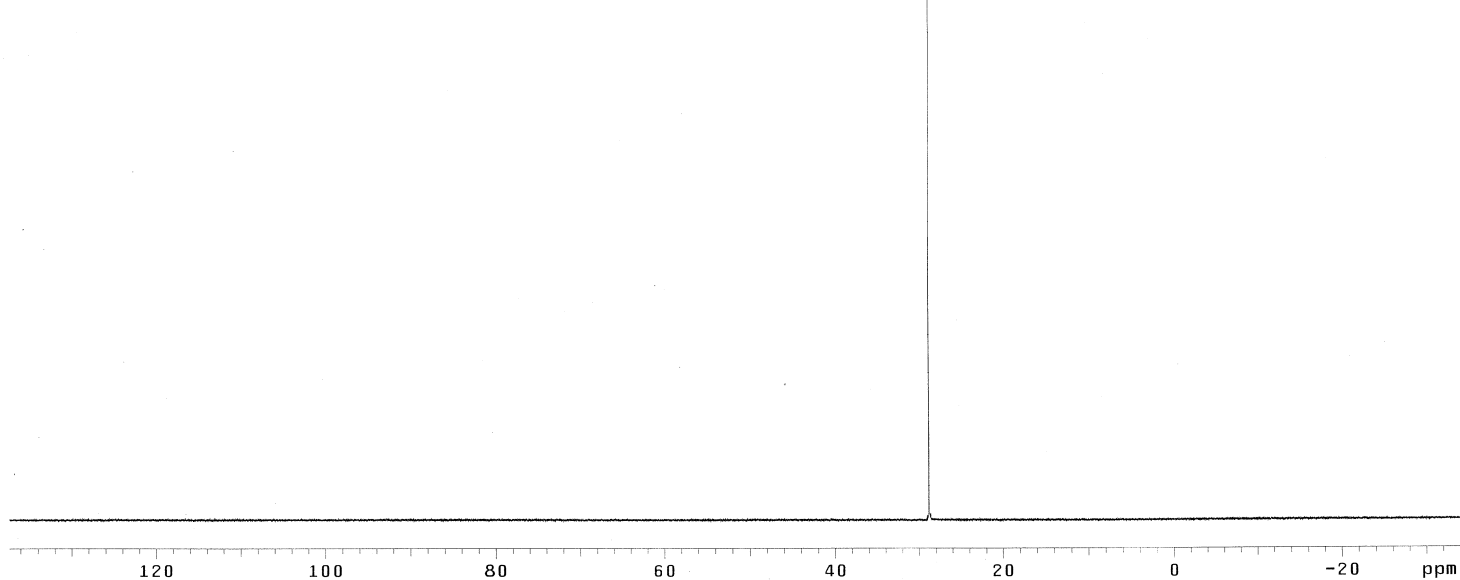
WALTZ-16 modulated

DATA PROCESSING

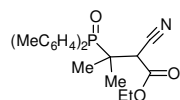
Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec



¹H NMR spectrum (CDCl₃, 25 °C)



Ethyl 2-cyano-3-[bis(4-methylphenyl)phosphinyl]-3-methylbutanoate (**22**)

Std proton

File: home/ras/Desktop/600ras051011.004.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras051011.004

VNMR-400 "nmr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 9615.4 Hz

Single scan

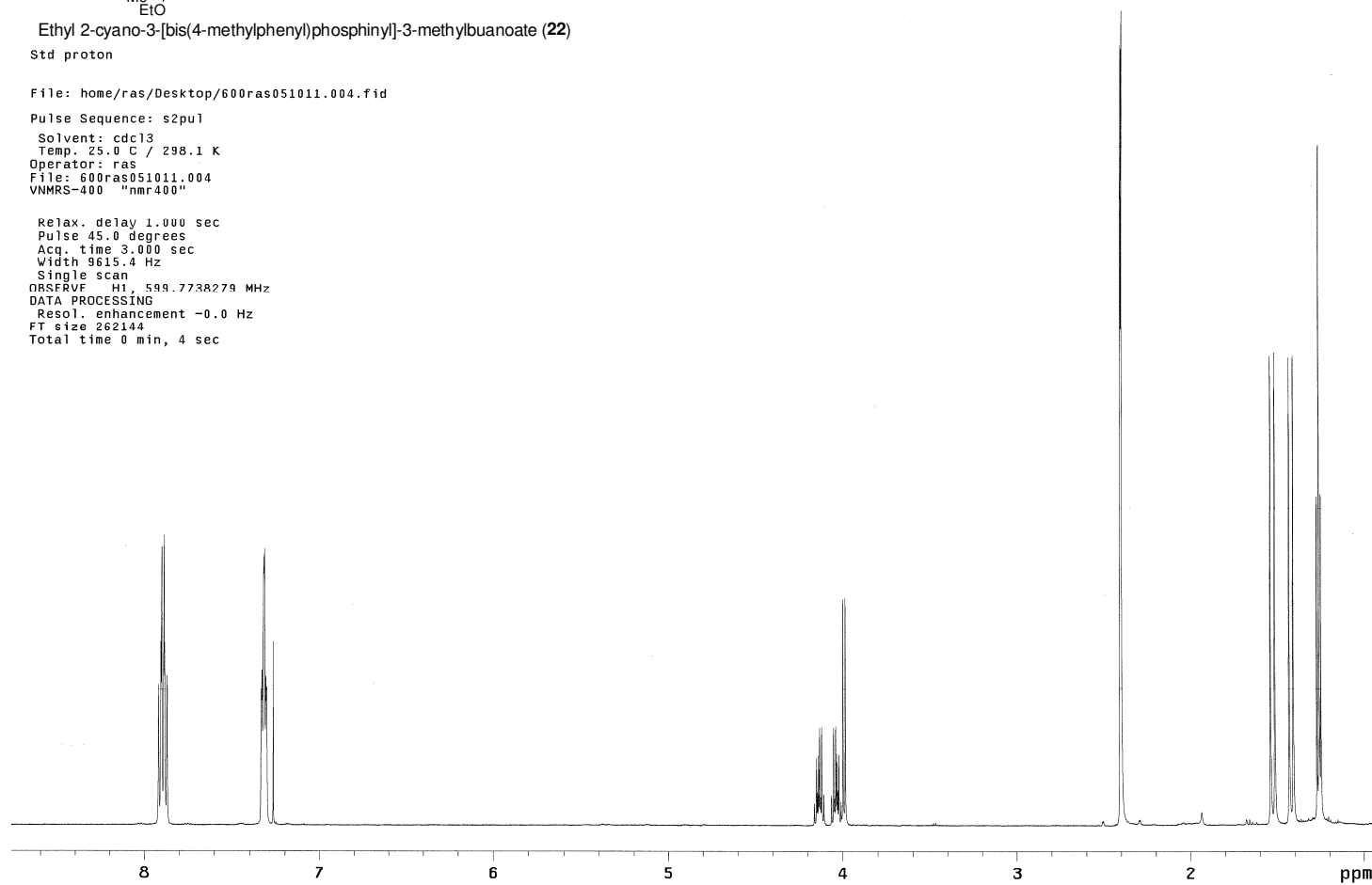
ORSERVF H1, 599.7738279 MHz

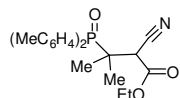
DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 262144

Total time 0 min, 4 sec





Ethyl 2-cyano-3-[bis(4-methylphenyl)phosphinyl]-3-methylbutanoate (**22**)

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Probe tuning parameter

File: home/ras/Desktop/600ras051011.005.fid

Pulse Sequence: s2pul

Solvent: cdc13

Temp: 25.0 C / 298.1 K

Operator: ras

File: 600ras051011.005

VNMRS-400 "nmr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

3040 repetitions

OBSERVE C13, 150.8132463 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

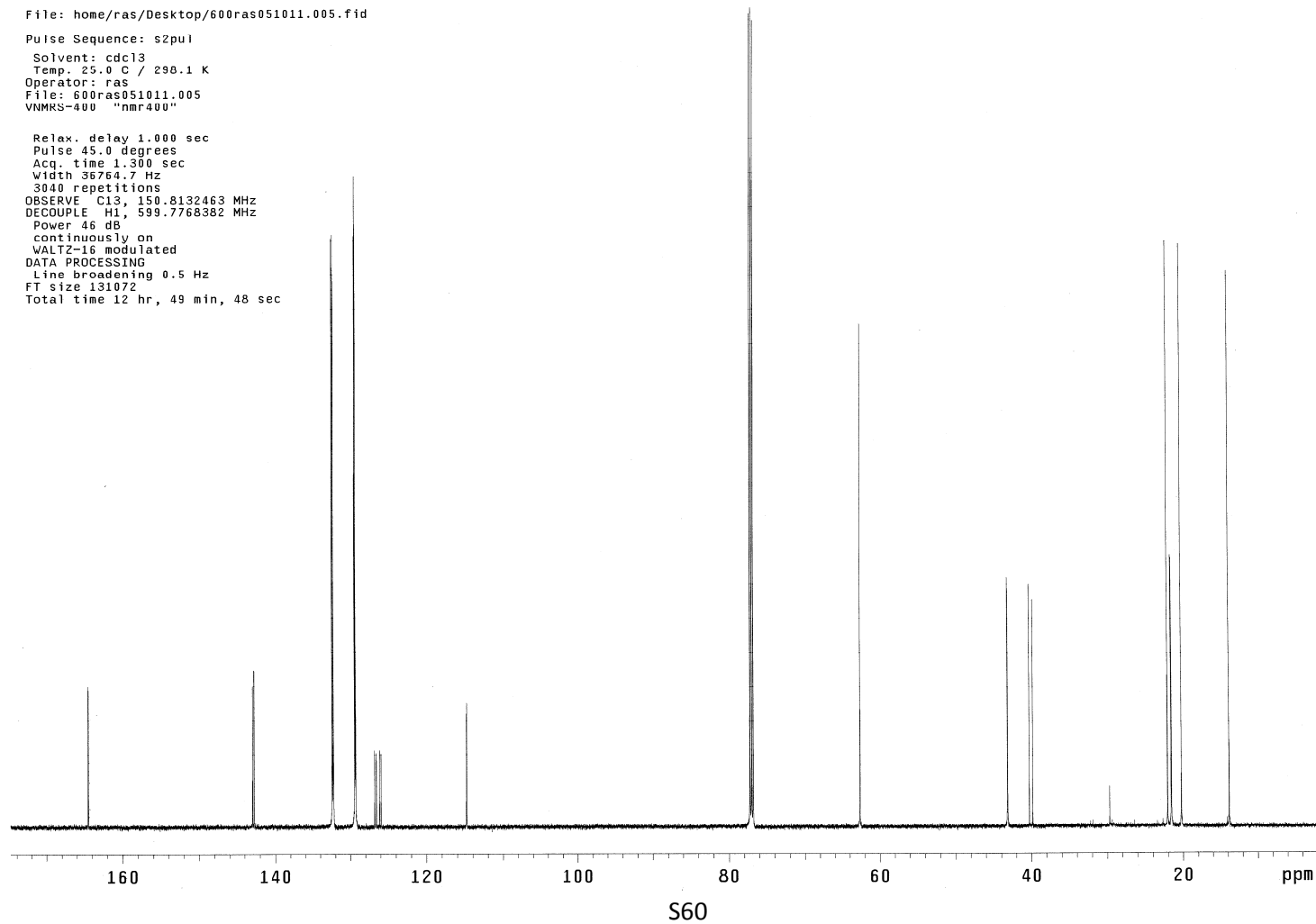
WALTZ-16 modulated

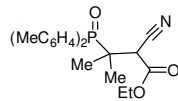
DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 12 hr, 49 min, 48 sec





Ethyl 2-cyano-3-[bis(4-methylphenyl)phosphinyl]-3-methylbutanoate (**22**)

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Std phosphorus

File: home/ras/Desktop/600ras051011.007.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras051011.007

VNMR5-400 "nmr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

20 repetitions

OBSERVE P31, 242.7929009 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

Continuously on

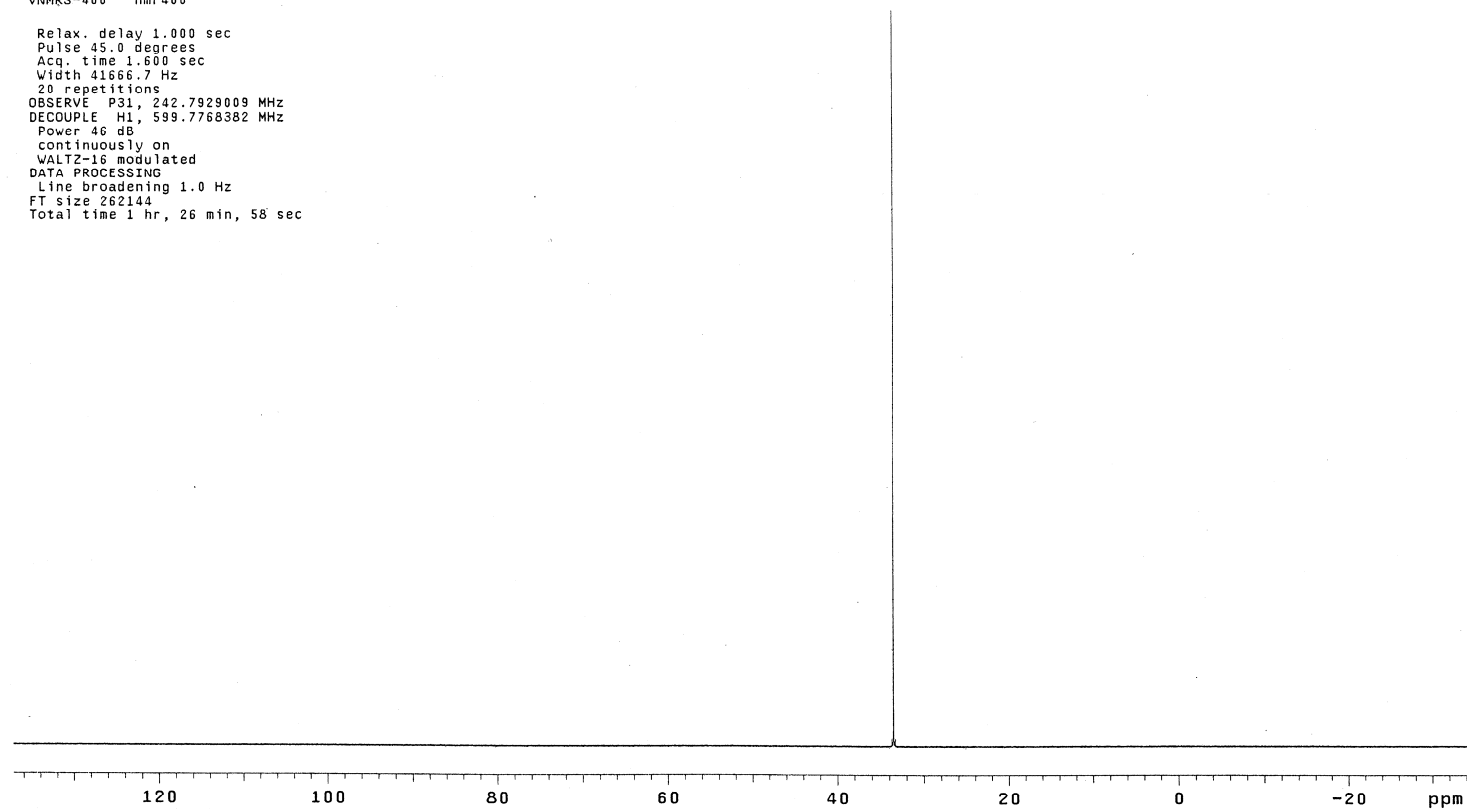
VALTZ-16 modulated

DATA PROCESSING

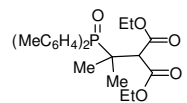
Line broadening 1.0 Hz

FT size 262144

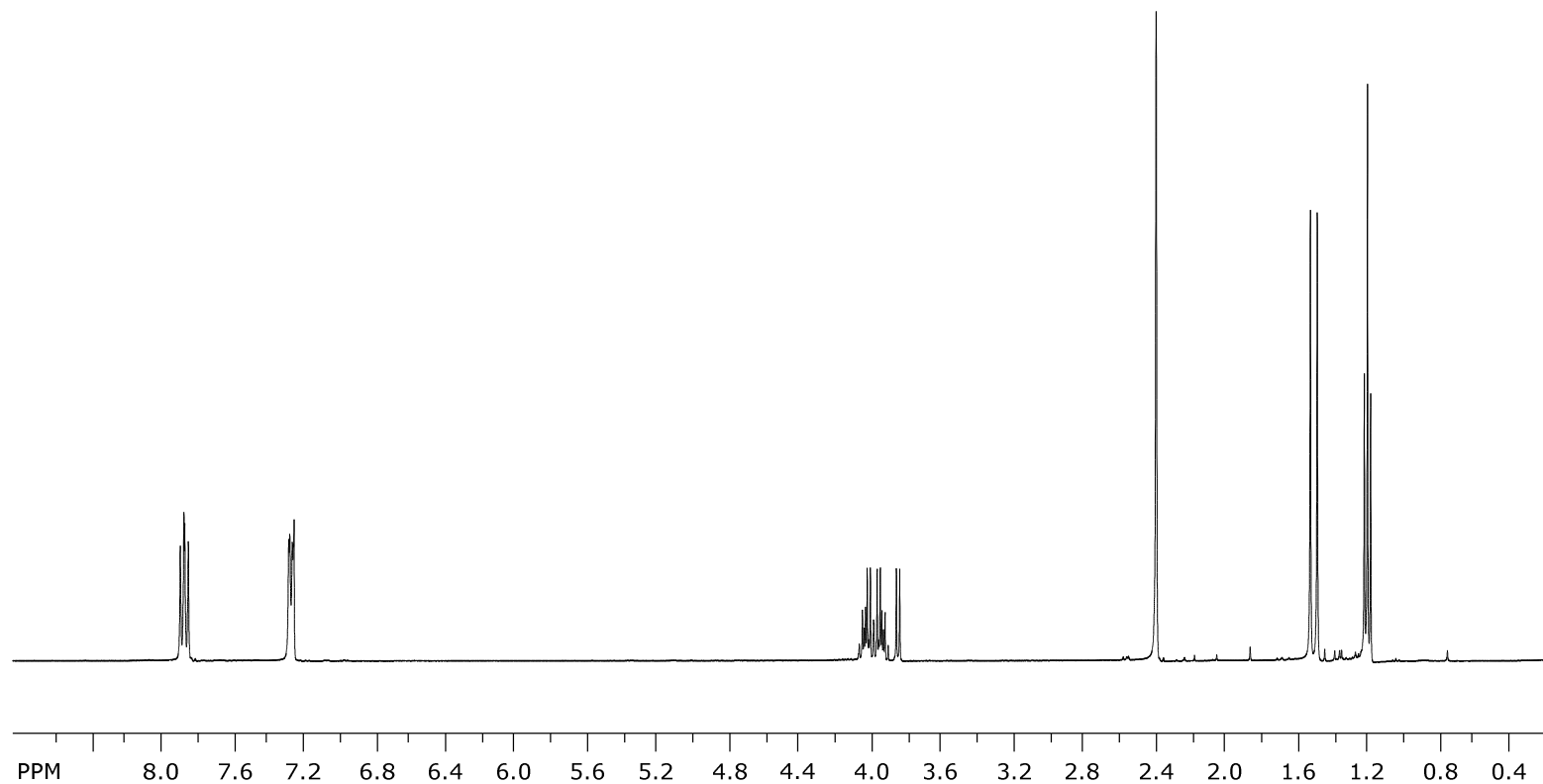
Total time 1 hr, 26 min, 58 sec



¹H NMR spectrum (CDCl₃, 25 °C)



Diethyl 2-(2-[bis(4-methylphenyl)phosphinyl]propan-2-yl)malonate (**23**)

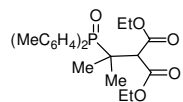


file: ...0\mer050310diethylisopureH.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.741966 MHz
time domain size: 26264 points
width: 6410.26 Hz = 16.0360 ppm = 0.244070 Hz/pt

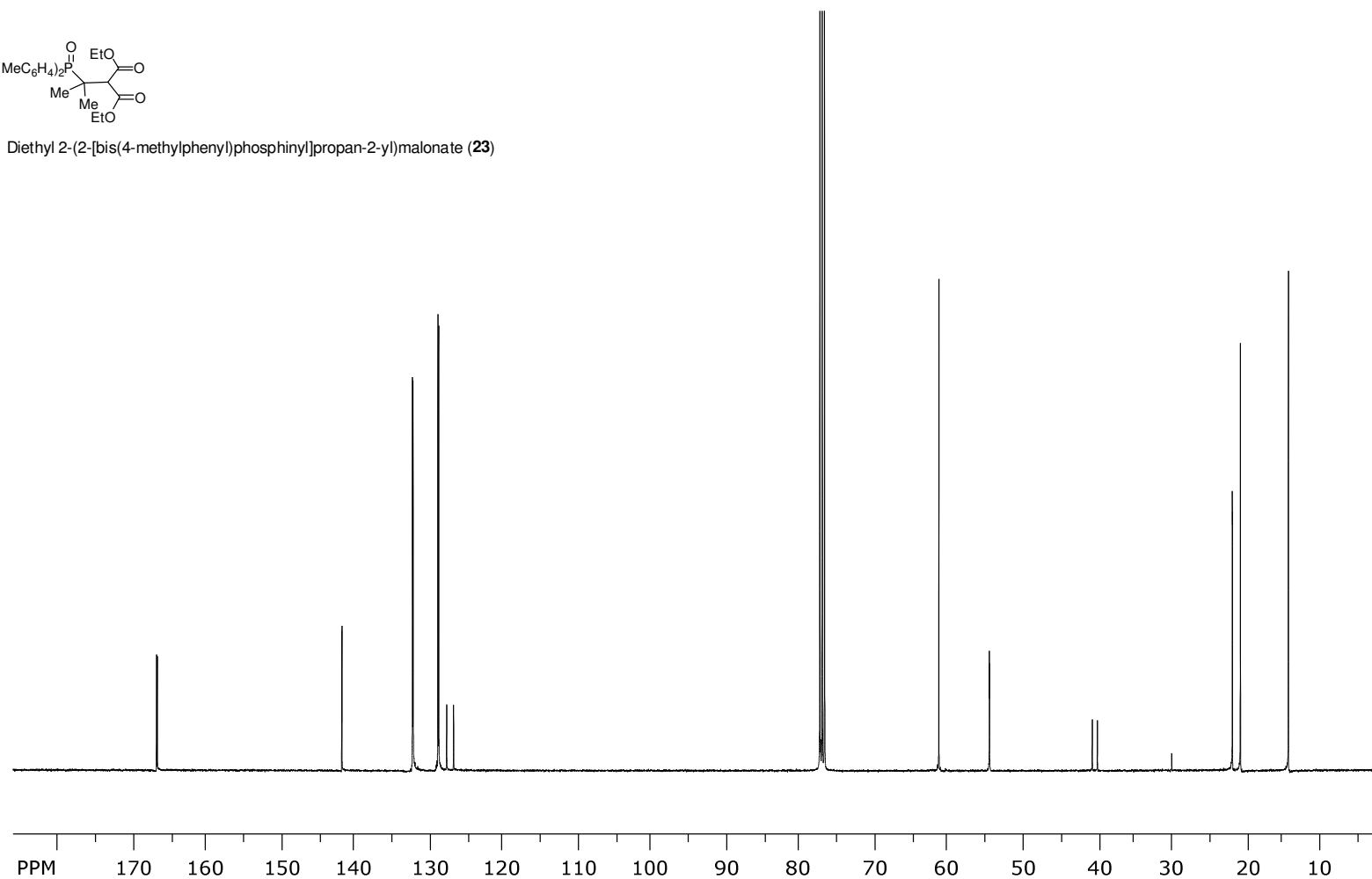
freq. of 0 ppm: 399.739565 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 139.301 ppm/cm: 0.34848

S62

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



Diethyl 2-(2-bis(4-methylphenyl)phosphinyl)propan-2-ylmalonate (**23**)

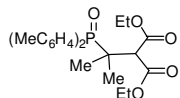


file: ...2010\mer033110diethylpureC.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.525148 MHz
time domain size: 63750 points
width: 24509.80 Hz = 243.8176 ppm = 0.384468 Hz/pt

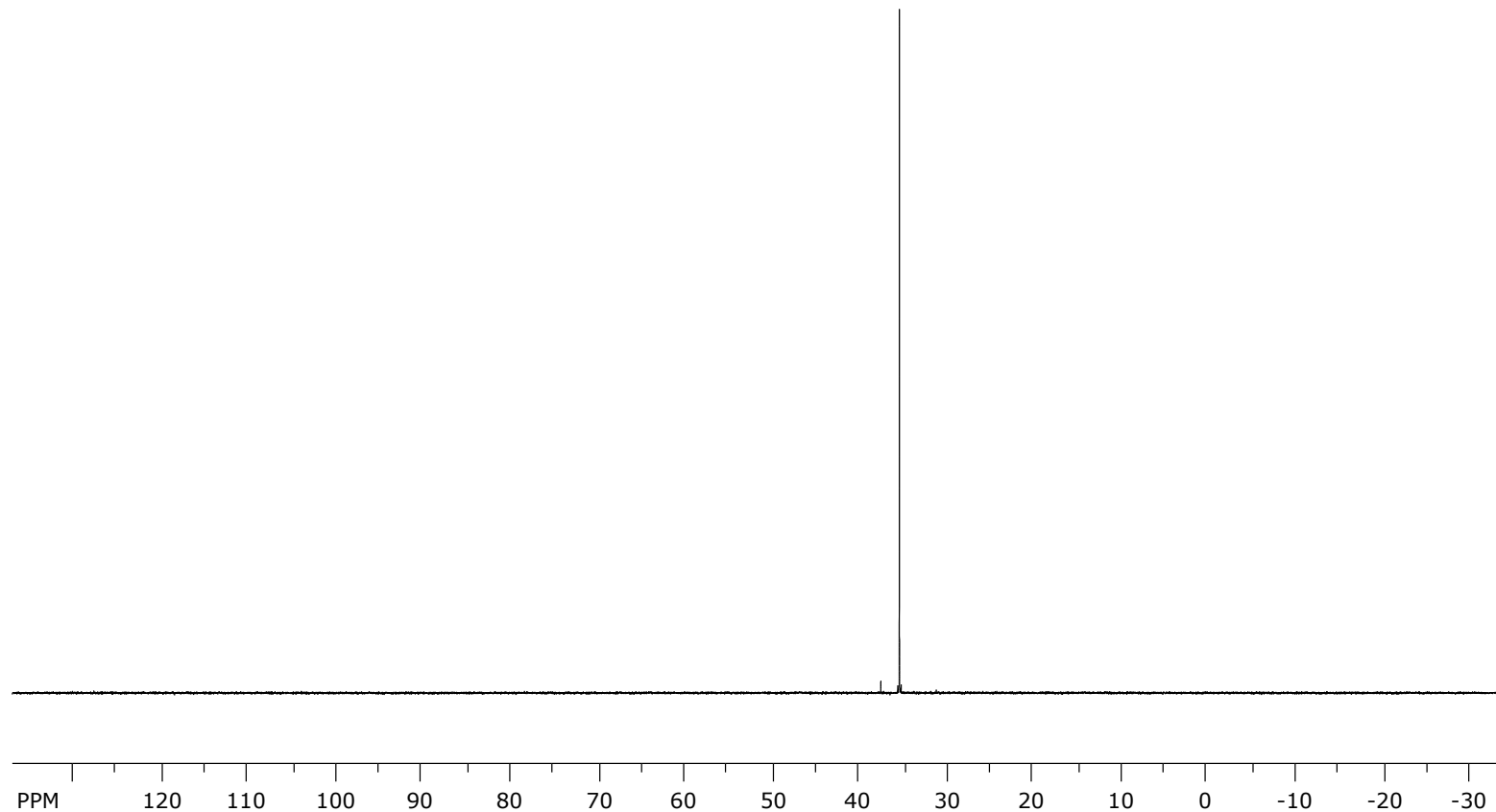
freq. of 0 ppm: 100.514591 MHz
processed size: 65536 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 744.325 ppm/cm: 7.40437

S63

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



Diethyl 2-(2-[bis(4-methylphenyl)phosphinyl]propan-2-yl)malonate (**23**)

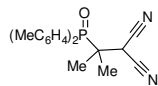


file: ...2010\2010\600ras050410.006.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 242.805398 MHz
time domain size: 133336 points
width: 41666.67 Hz = 171.6052 ppm = 0.312494 Hz/pt

freq. of 0 ppm: 242.792900 MHz
processed size: 262144 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 1666.667 ppm/cm: 6.86421

S64

¹H NMR spectrum (CDCl₃, 25 °C)



2-(2-[Bis(4-methylphenyl)phosphinyl]propan-2-yl)propanedinitrile (**24**)

Std proton

File: home/ras/Desktop/600ras051111.008.fid

Pulse Sequence: szpu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras051111.008

VNMRS-400 "nmr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 9615.4 Hz

16 repetitions

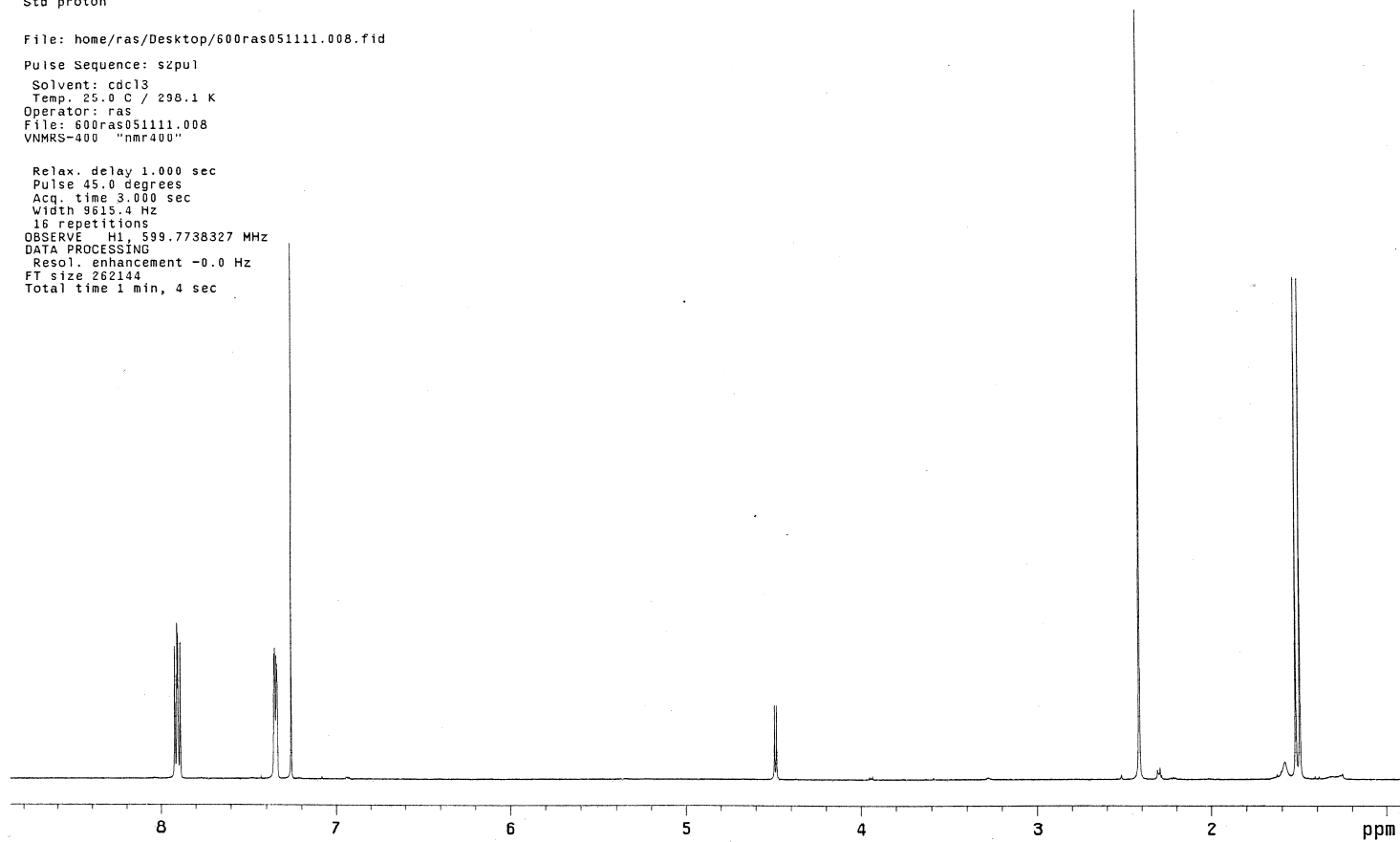
OBSERVE H1, 599.7738327 MHz

DATA PROCESSING

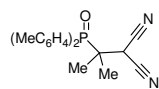
Resol. enhancement -0.0 Hz

FT size 262144

Total time 1 min, 4 sec



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



2-(2-[Bis(4-methylphenyl)phosphinyl]propan-2-yl)propanedinitrile (24)

Probe tuning parameter

File: home/ras/Desktop/600ras051011.009.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras051011.009

VNMRS-400 "nmr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

22000 repetitions

OBSERVE C13, 150.8132489 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

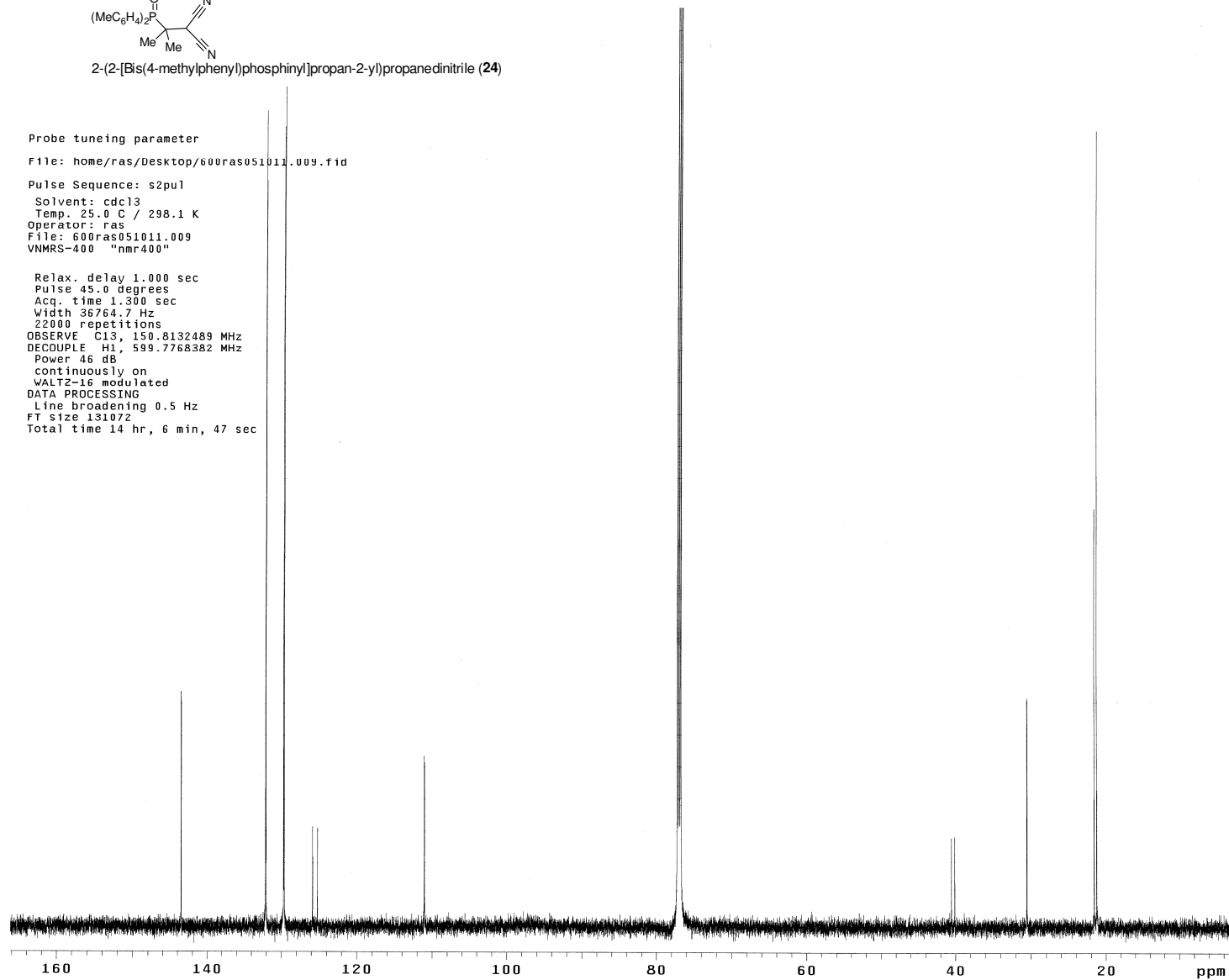
WALTZ-16 modulated

DATA PROCESSING

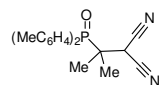
Line broadening 0.5 Hz

FT size 131072

Total time 14 hr, 6 min, 47 sec



$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



2-(2-[Bis(4-methylphenyl)phosphinyl]propan-2-yl)propanedinitrile (**24**)

Std phosphorus

File: home/ras/Desktop/600ras051111.007.fid

Pulse Sequence: s2pul

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras051111.007

VNMR-400 "nmr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

100 repetitions

OBSERVE P31, 242.7929103 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

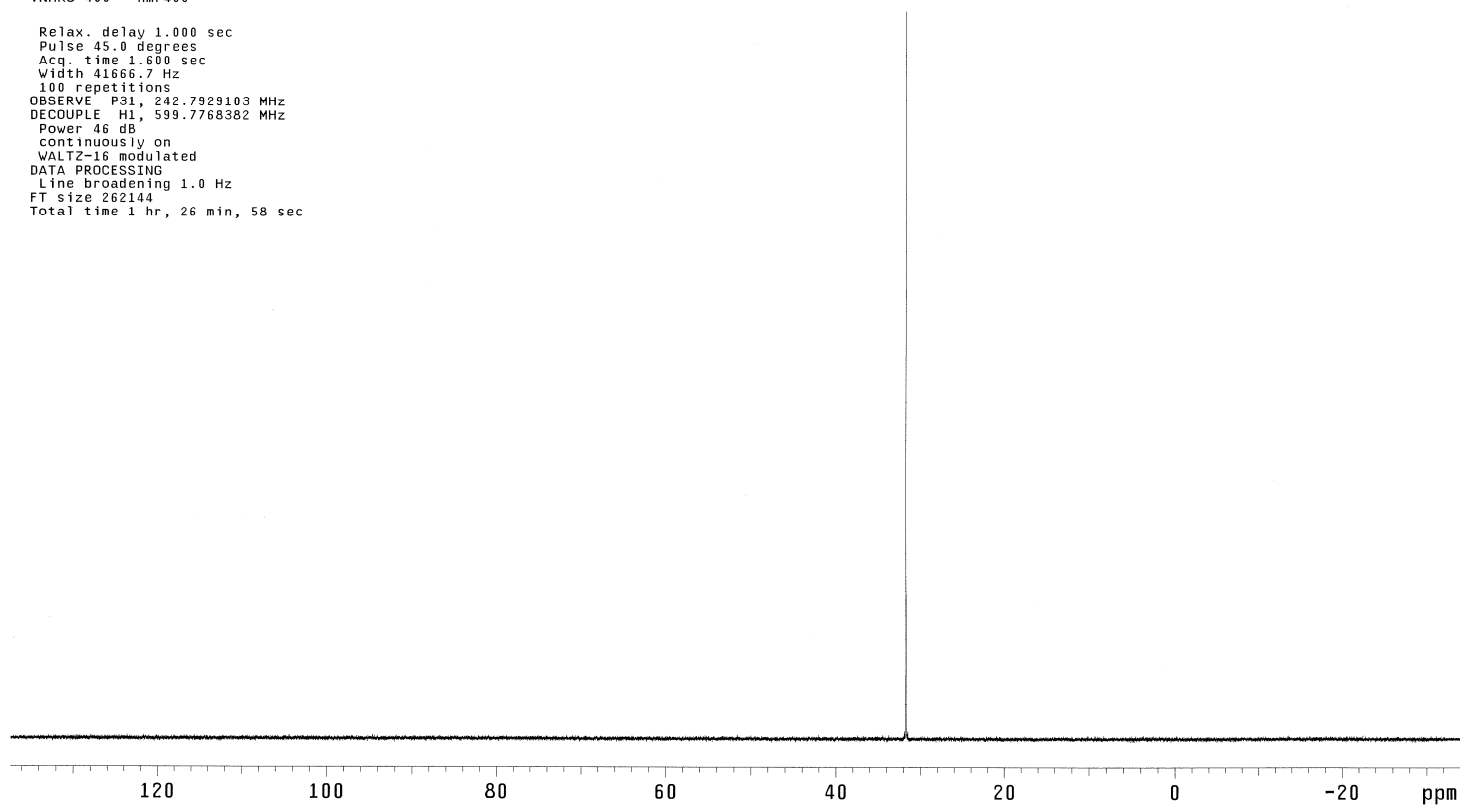
WALTZ-16 modulated

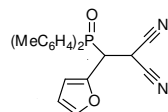
DATA PROCESSING

Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec





2-([Bis(4-methylphenyl)phosphinyl](furan-2-yl)methyl)propanedinitrile (25)

^1H NMR spectrum (CDCl_3 , 25 °C)

Std proton

File: home/ras/Desktop/2D600ras012511.005.fid

Pulse Sequence: s2pu1

Solvent: cdcl_3

Temp: 25.0 C / 298.1 K

Operator: ras

File: 2D600ras012511.005

VNMR5-600 "nmr 600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 9615.4 Hz

Single scan

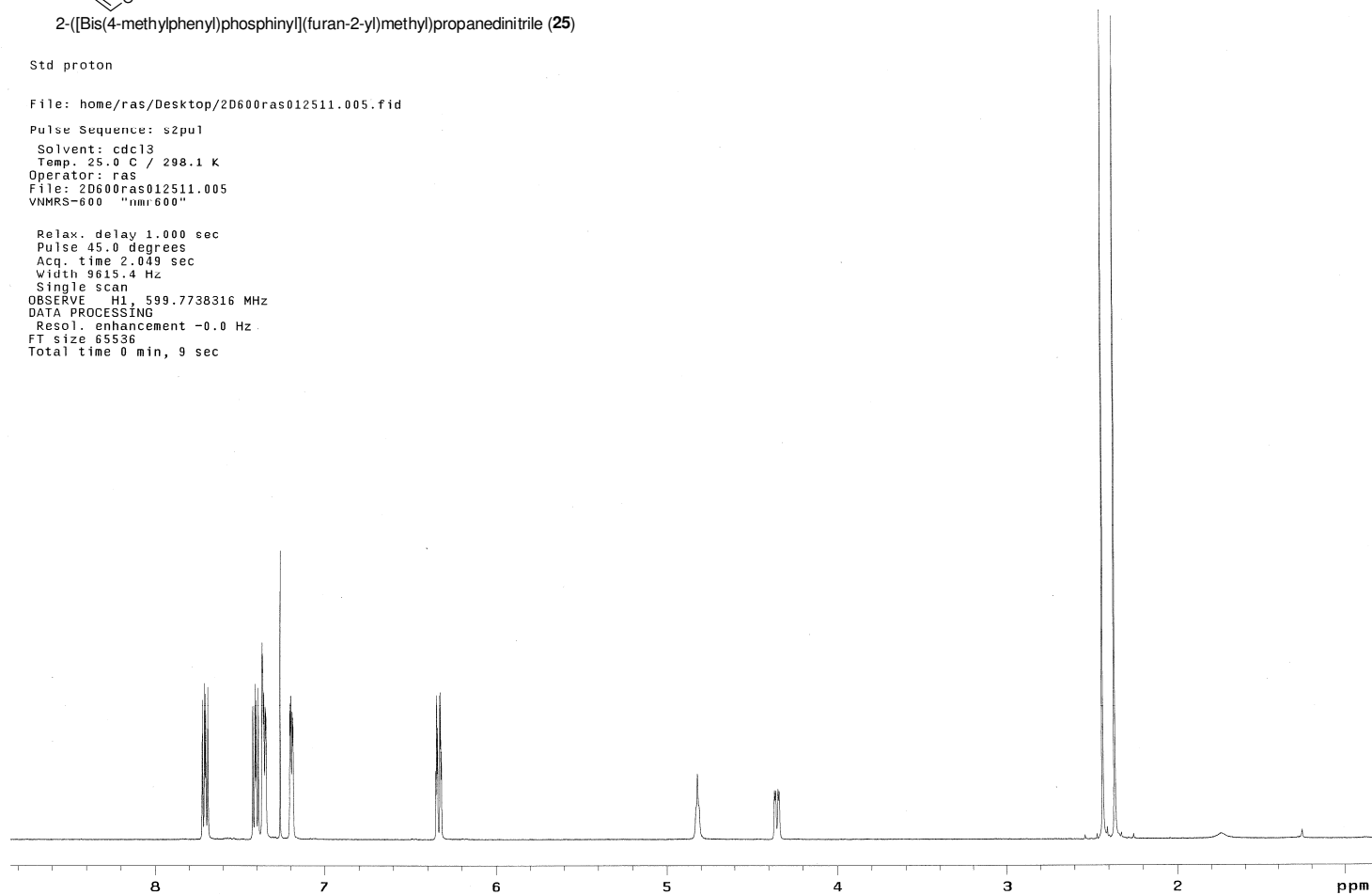
OBSERVE H1, 599.7738316 MHz

DATA PROCESSING

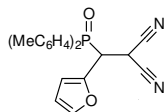
Resol. enhancement -0.0 Hz

FT size 65536

Total time 0 min, 9 sec



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



2-((Bis(4-methylphenyl)phosphinyl)(furan-2-yl)methyl)propanedinitrile (**25**)

Probe tuning parameter

File: home/ras/Desktop/600ras012511.007.fid

Pulse Sequence: szpu1

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: ras

File: 600ras012511.007

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

3464 repetitions

OBSERVE C13, 150.8132461 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

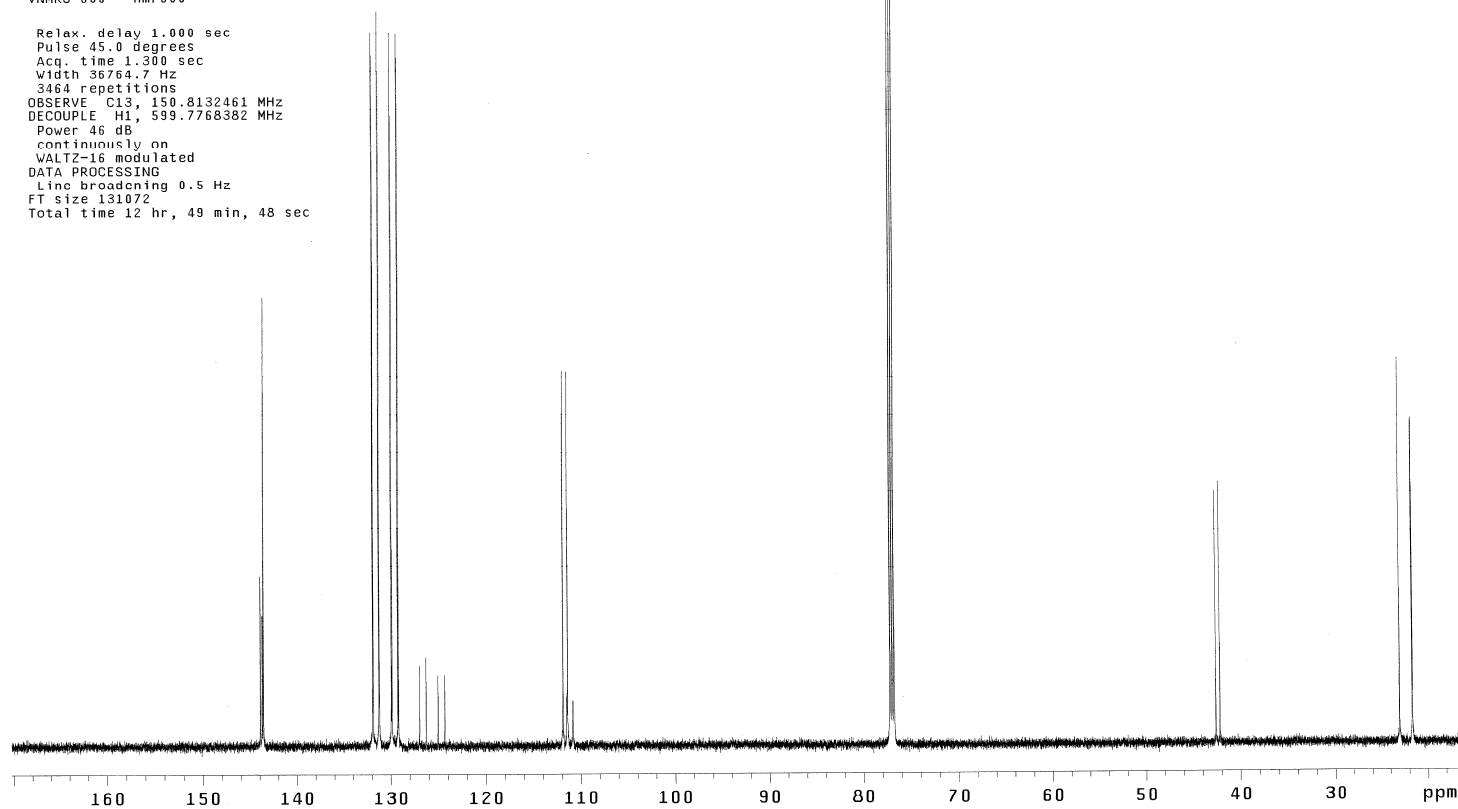
WALTZ-16 modulated

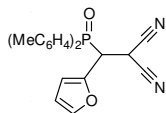
DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 12 hr, 49 min, 48 sec





2-([Bis(4-methylphenyl)phosphinyl](furan-2-yl)methyl)propanedinitrile (25)

Std phosphorus

File: home/ras/Desktop/2D600ras012511.006.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 2D600ras012511.006

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

40 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

WALTZ-16 modulated

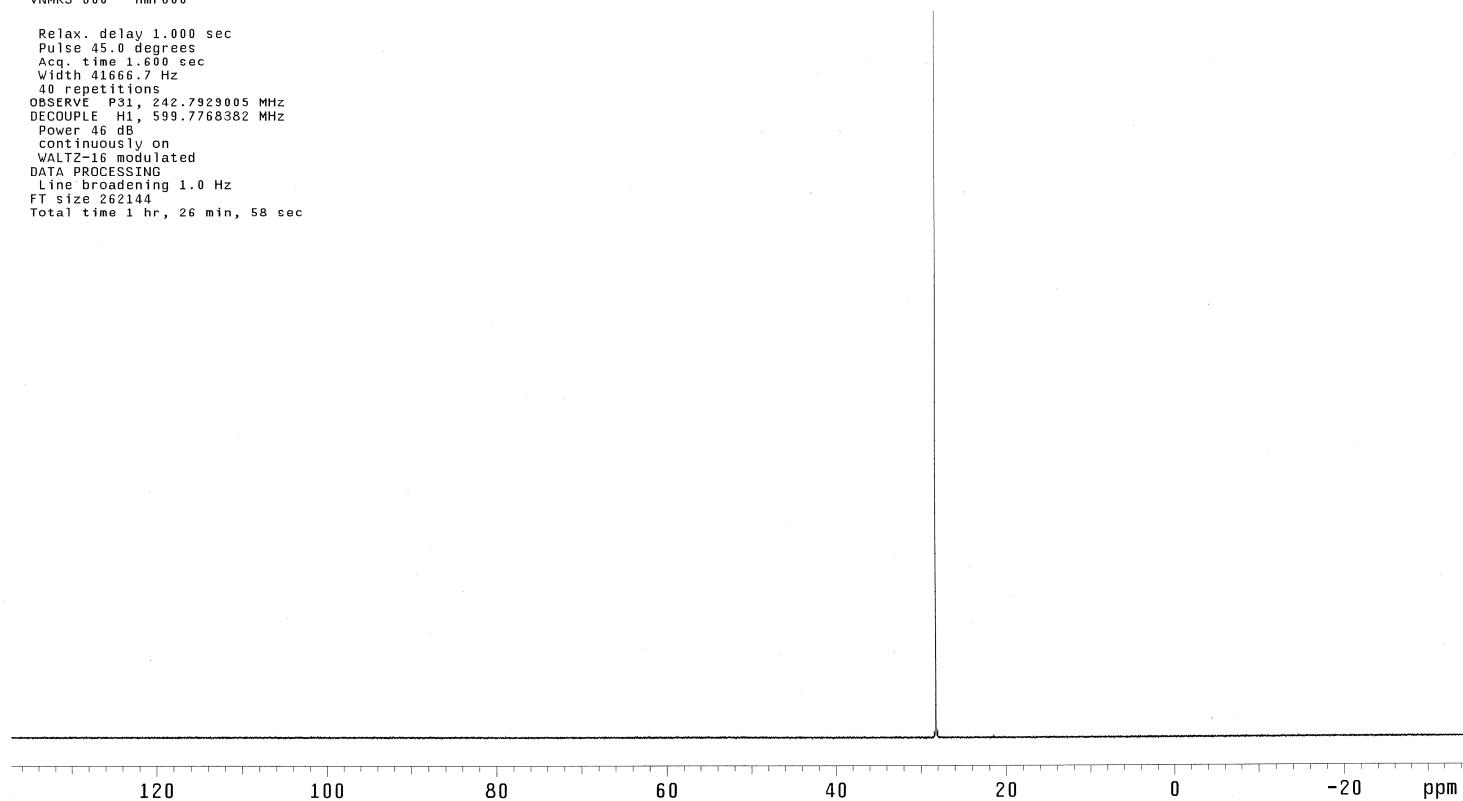
DATA PROCESSING

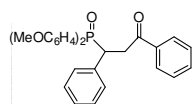
Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)





3-[Bis(4-methoxyphenyl)phosphiny]-1,3-diphenyl-1-propanone (**28**)

^1H NMR spectrum (CDCl_3 , 25 °C)

Std proton

File: home/ras/Desktop/600ras121511.009.fid

Pulse Sequence: szpu1

Solvent: cdc13

Temp: 25.0 C / 298.1 K

Operator: ras

File: 600ras121511.009

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 9615.4 Hz

8 repetitions

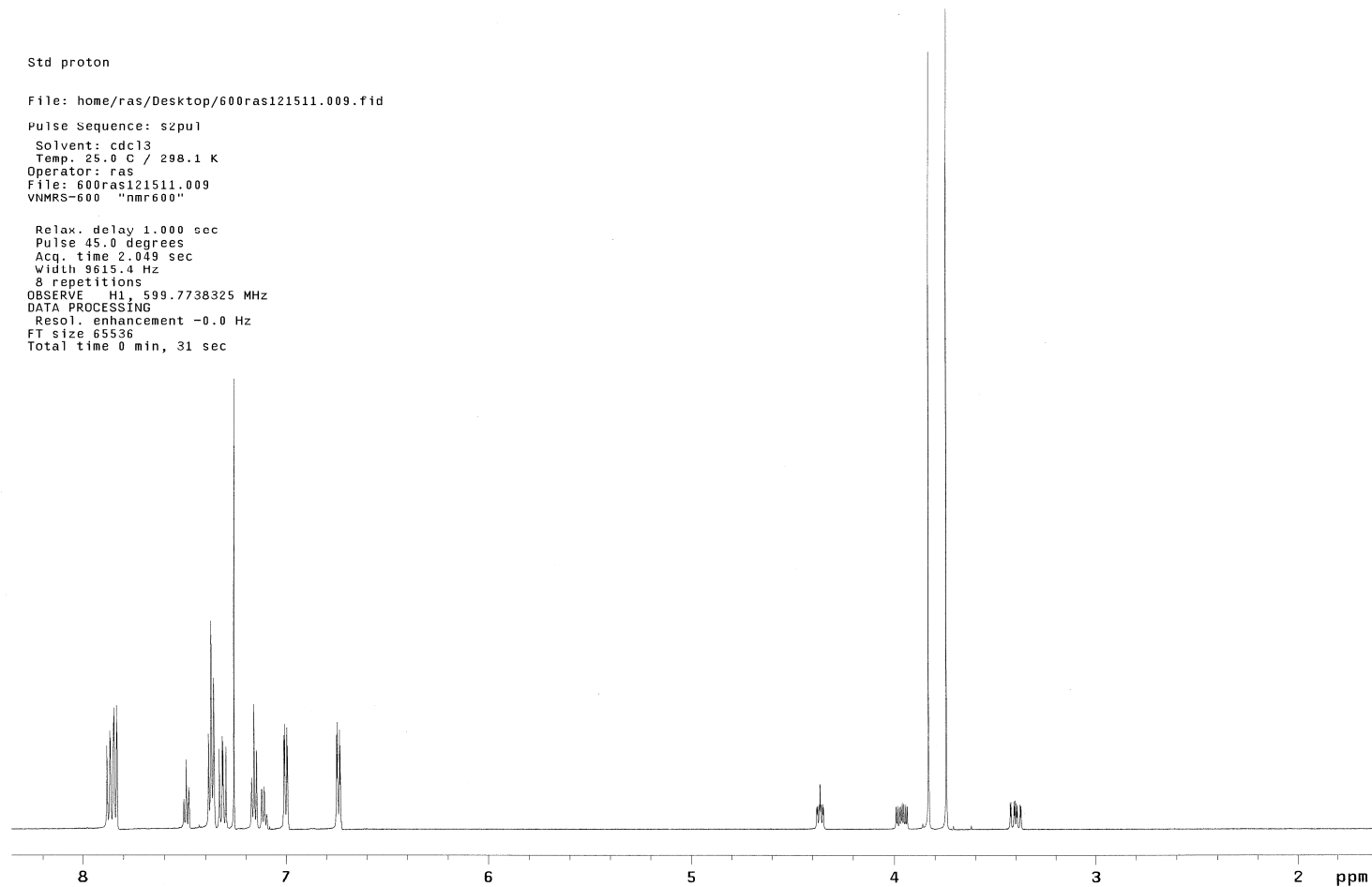
OBSERVE H1, 599.7738325 MHz

DATA PROCESSING

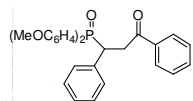
Resol. enhancement -0.0 Hz

FT size 65536

Total time 0 min, 31 sec



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



3-[Bis(4-methoxyphenyl)phosphiny]-1,3-diphenyl-1-propanone (28)

Std carbon

File: home/ras/Desktop/600ras120911.017.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras120911.017

VNMR-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

18880 repetitions

OBSERVE C13, 150.8132461 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

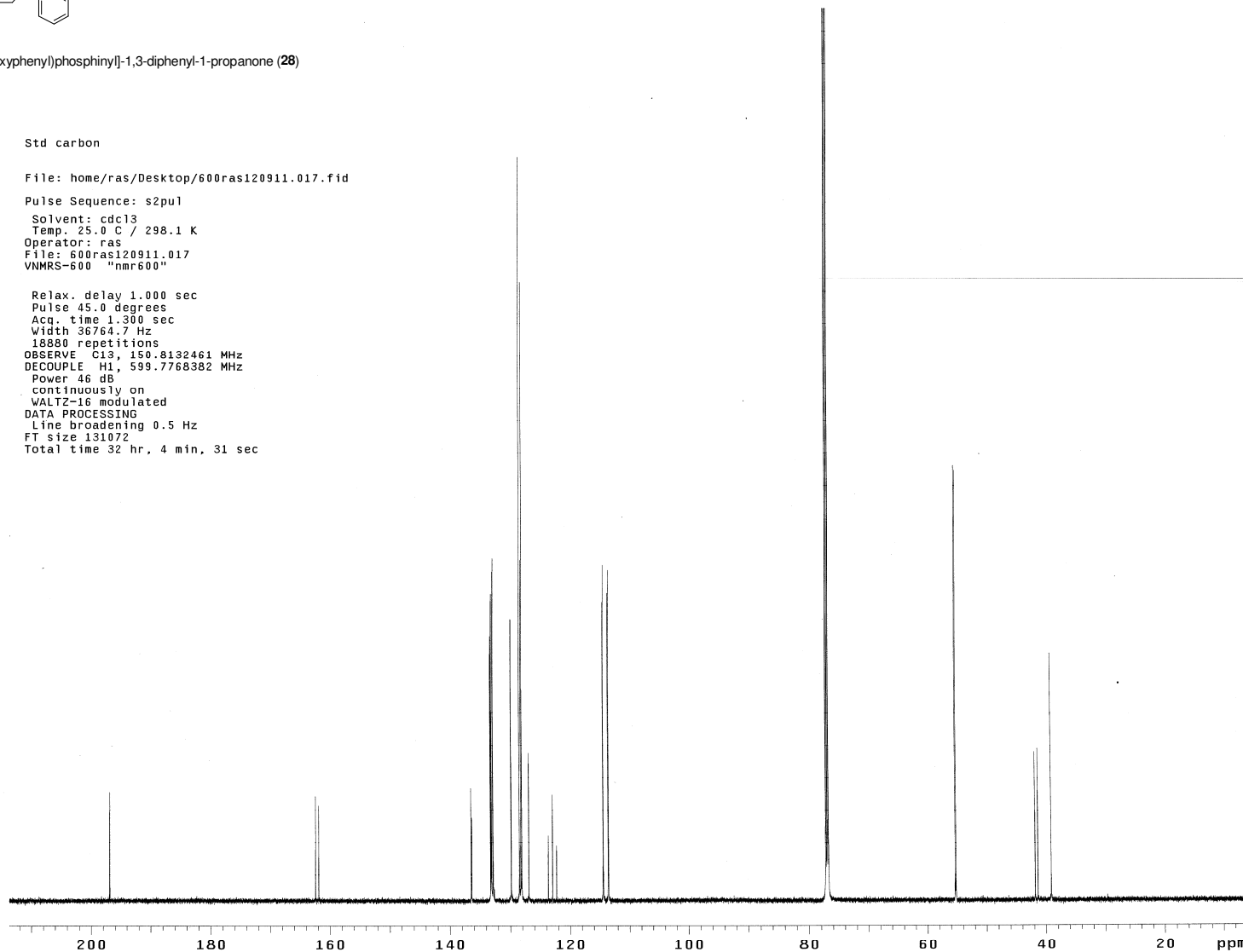
WALTZ-16 modulated

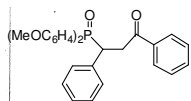
DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 32 hr, 4 min, 31 sec





3-[Bis(4-methoxyphenyl)phosphinyl]-1,3-diphenyl-1-propanone (**28**)

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

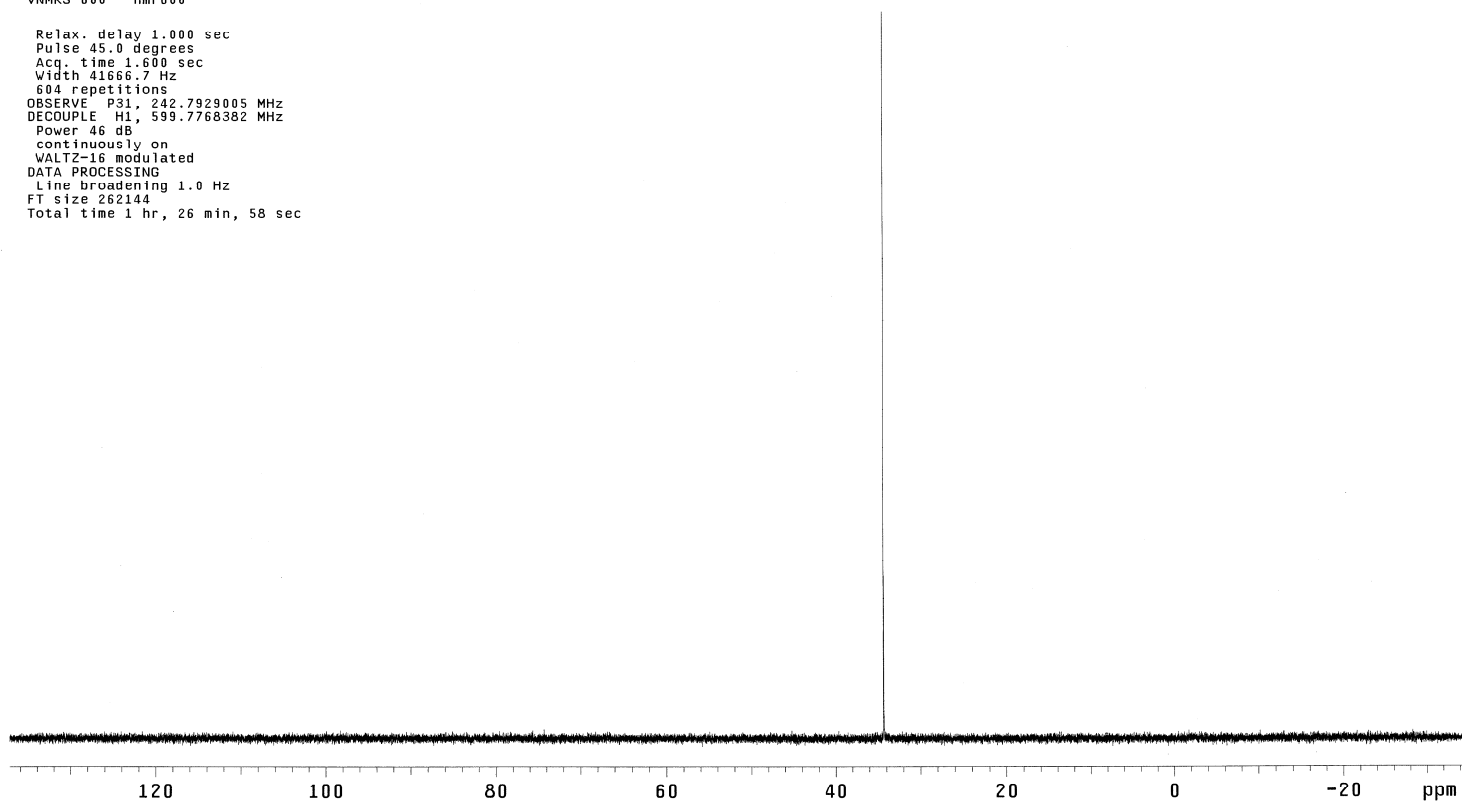
Std phosphorus

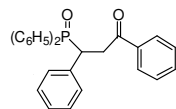
File: home/ras/Desktop/600ras120911.009.fid

Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: ras
File: 600ras120911.009
VNMR-600 "nmr600"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.600 sec
Width 41666.7 Hz
604 repetitions
OBSERVE P31, 242.7929005 MHz
DECOUPLE H1, 599.7768382 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 262144
Total time 1 hr, 26 min, 58 sec





3-(Diphenylphosphinyl)-1,3-diphenyl-1-propanone (29)

^1H NMR spectrum (CDCl_3 , 25 °C)

Std proton

File: home/ras/Desktop/600ras121511.012.fid

Pulse Sequence: s2pu1

Solvent: cdc13

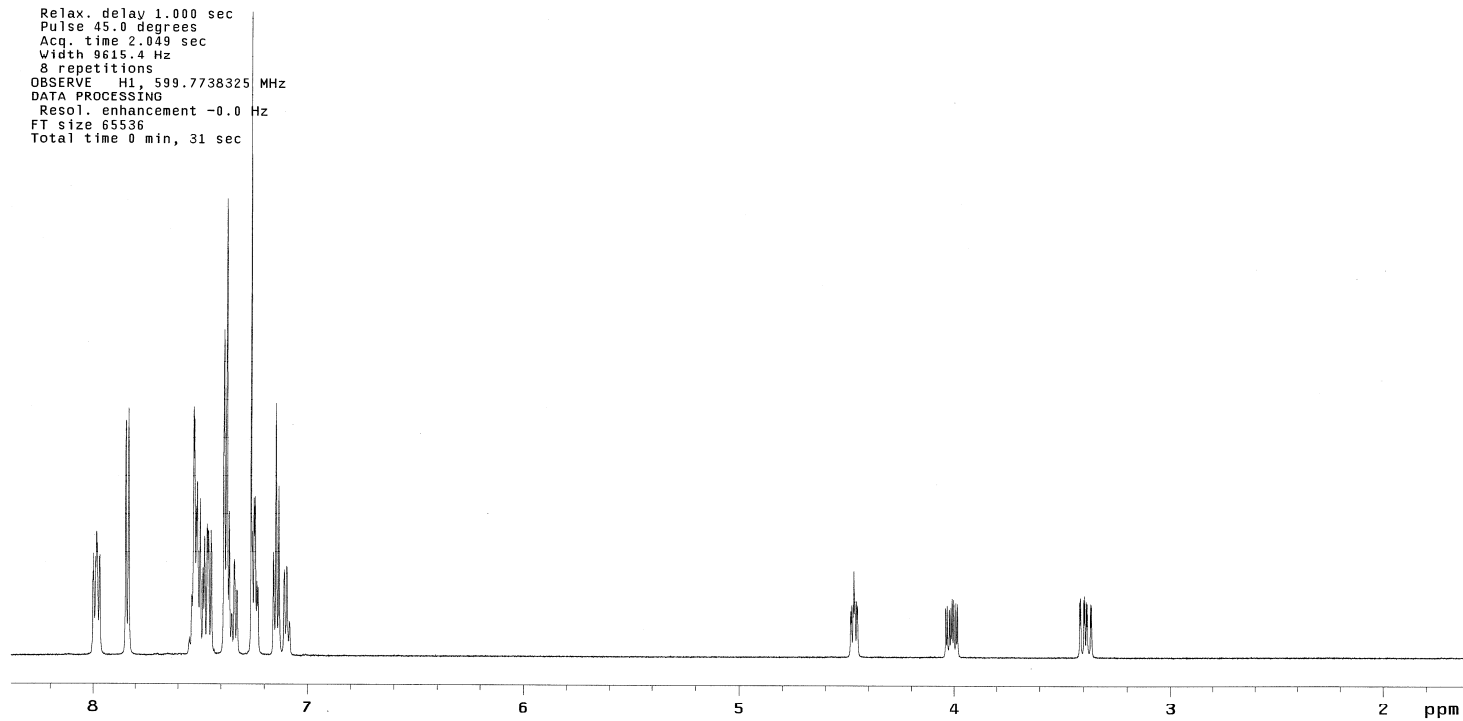
Temp. 25.0 C / 298.1 K

Operator: ras

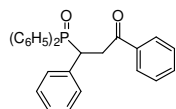
File: 600ras121511.012

VNMR-600 "nmr600"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 9615.4 Hz
8 repetitions
OBSERVE H1, 599.7738325 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 65536
Total time 0 min, 31 sec



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



3-(Diphenylphosphinyl)-1,3-diphenyl-1-propanone (29)

Std carbon

File: home/ras/Desktop/600ras121511.007.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras121511.007

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

27568 repetitions

OBSERVE C13, 150.8132472 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

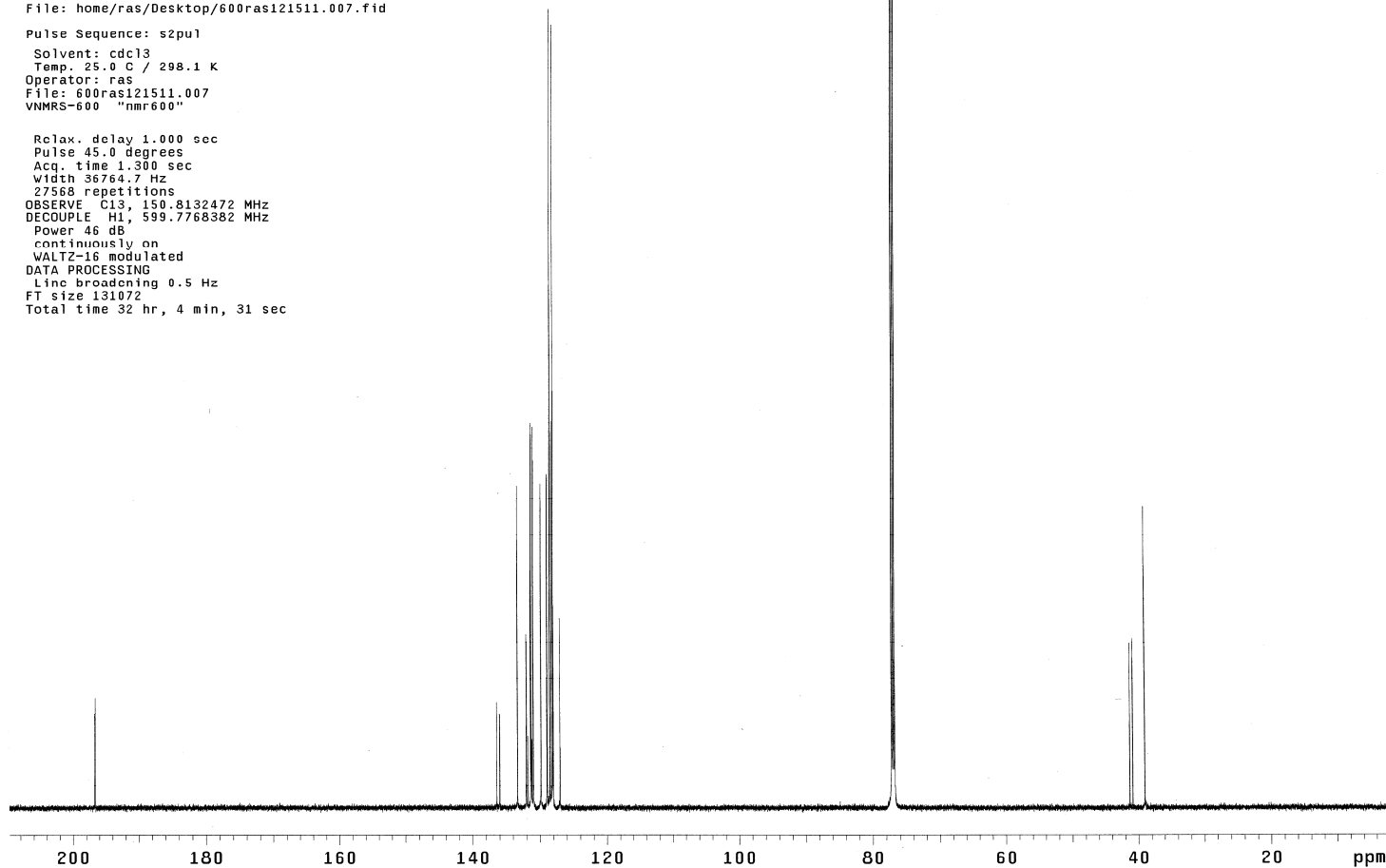
WALTZ-16 modulated

DATA PROCESSING

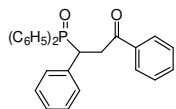
Line broadening 0.5 Hz

FT size 131072

Total time 32 hr, 4 min, 31 sec



$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



3-(Diphenylphosphinyl)-1,3-diphenyl-1-propanone (**29**)

Std phosphorus

File: home/ras/Desktop/600ras121511.008.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: ras

File: 600ras121511.008

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

60 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

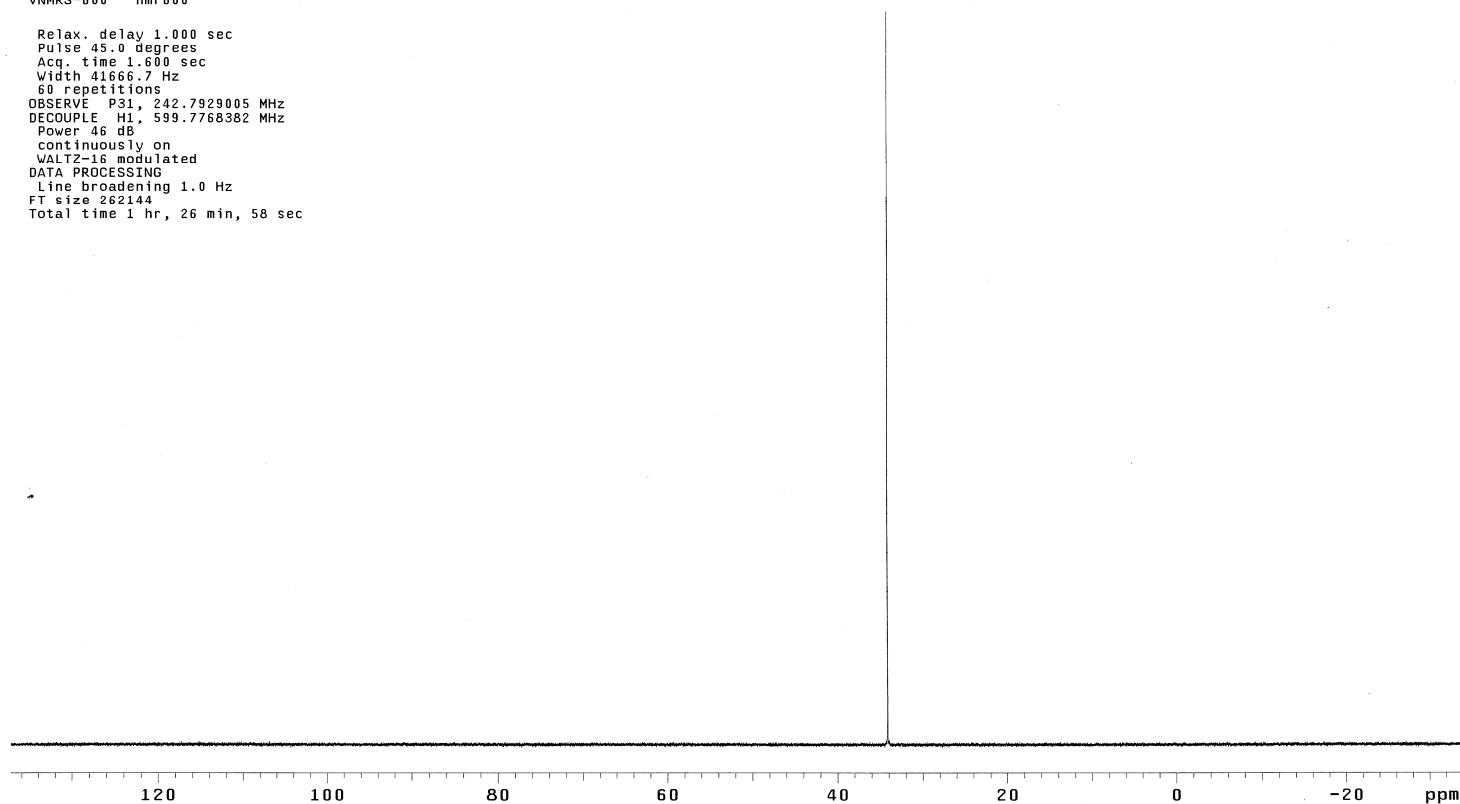
WALTZ-16 modulated

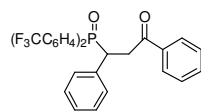
DATA PROCESSING

Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec





3-[Bis[(4-trifluoromethyl)phenyl]phosphoryl]-1,3-diphenyl-1-propanone (**30**)

^1H NMR spectrum (CDCl_3 , 25 °C)

Std proton

File: home/ras/Desktop/600ras121511.011.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras121511.011

VNMR-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 9615.4 Hz

8 repetitions

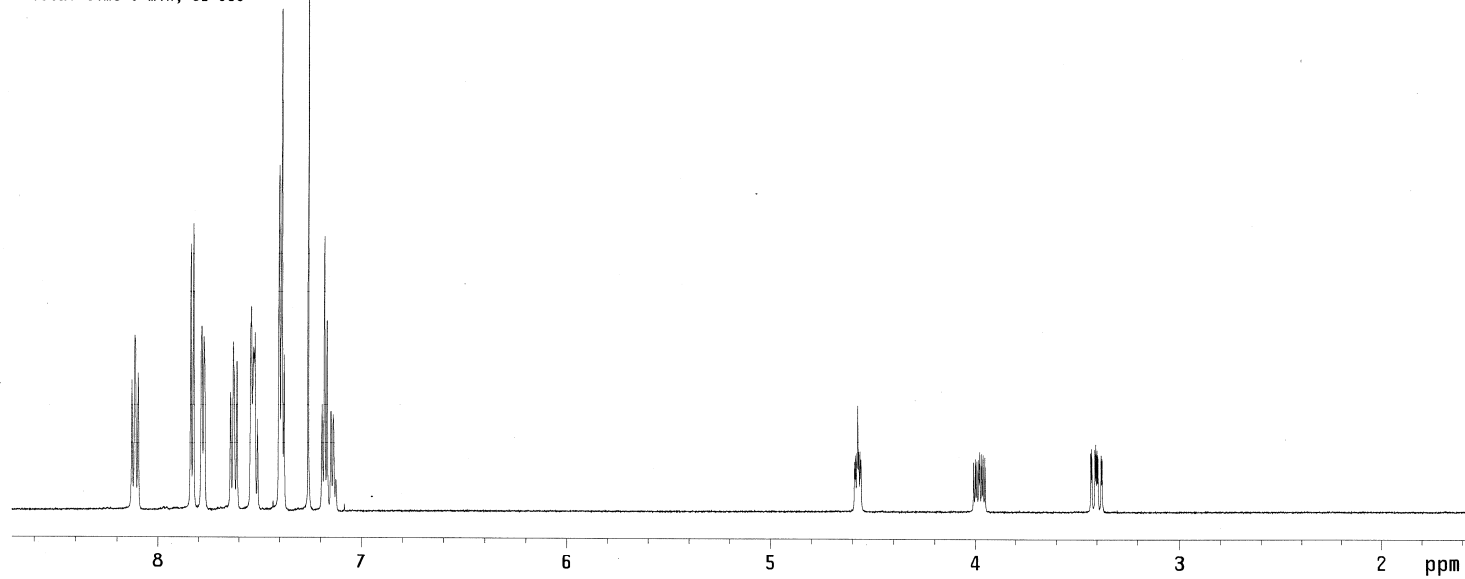
OBSERVE H1, 599.7738325 MHz

DATA PROCESSING

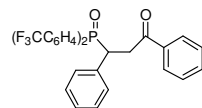
Resol. enhancement -0.0 Hz

FT size 65536

Total time 0 min, 31 sec



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)



3-[Bis[(4-trifluoromethyl)phenyl]phosphinyl]-1,3-diphenyl-1-propanone (**30**)

Std carbon

File: home/ras/Desktop/600ras120911.024.fid

Pulse Sequence: s2pu1

Solvent: cdc13

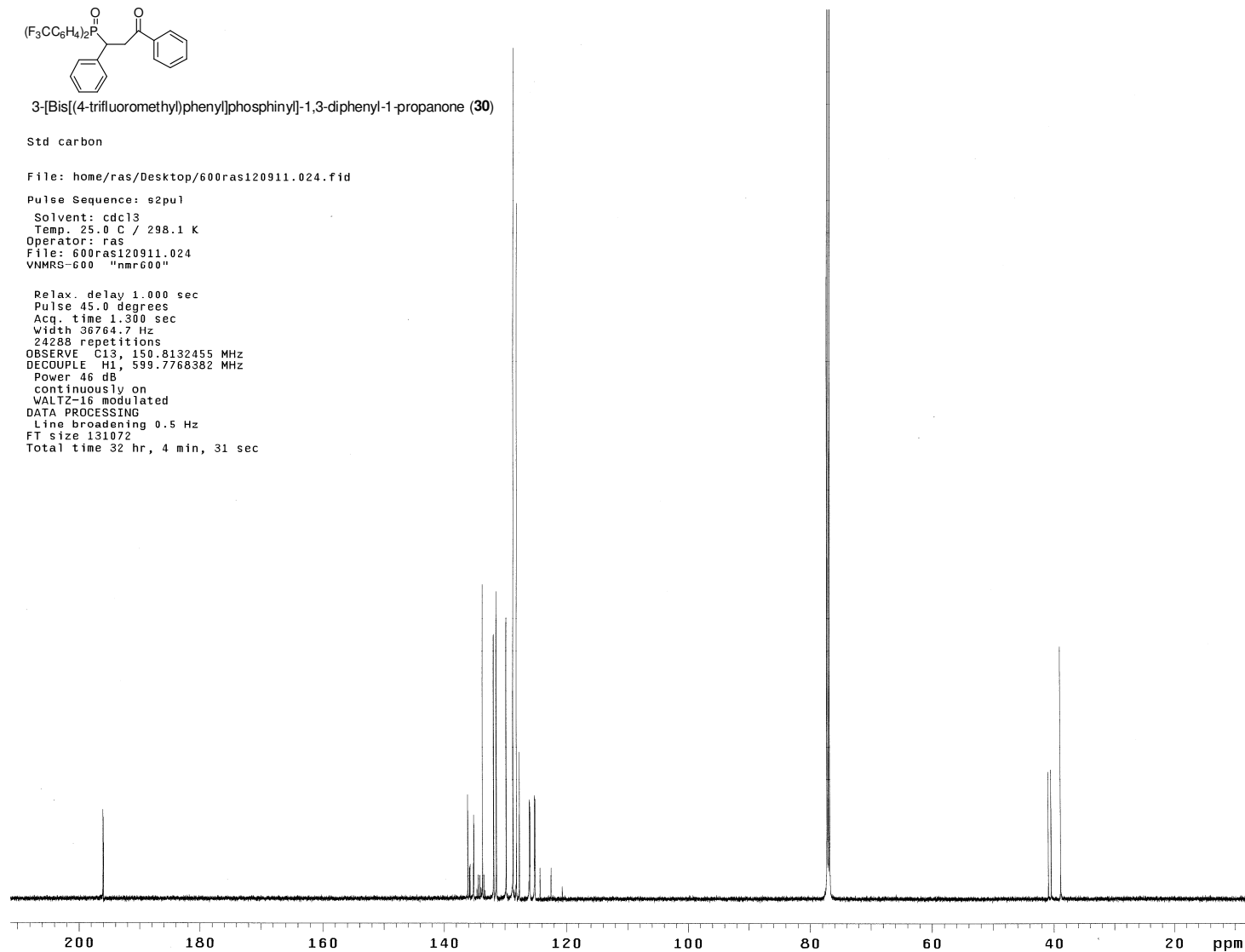
Temp. 25.0 C / 298.1 K

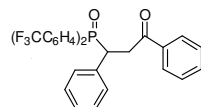
Operator: ras

File: 600ras120911.024

VNMR5-600 "nmr600"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 36764.7 Hz
24288 repetitions
OBSERVE C13, 150.8132455 MHz
DECOUPLE H1, 599.7768382 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 32 hr, 4 min, 31 sec





3-[Bis(4-trifluoromethyl)phenyl]phosphinyl]-1,3-diphenyl-1-propanone (30)

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Std phosphorus

File: home/ras/Desktop/600ras120911.011.fid

Pulse Sequence: s2pul

Solvent: cdcl_3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras120911.011

VNMRS-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

604 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

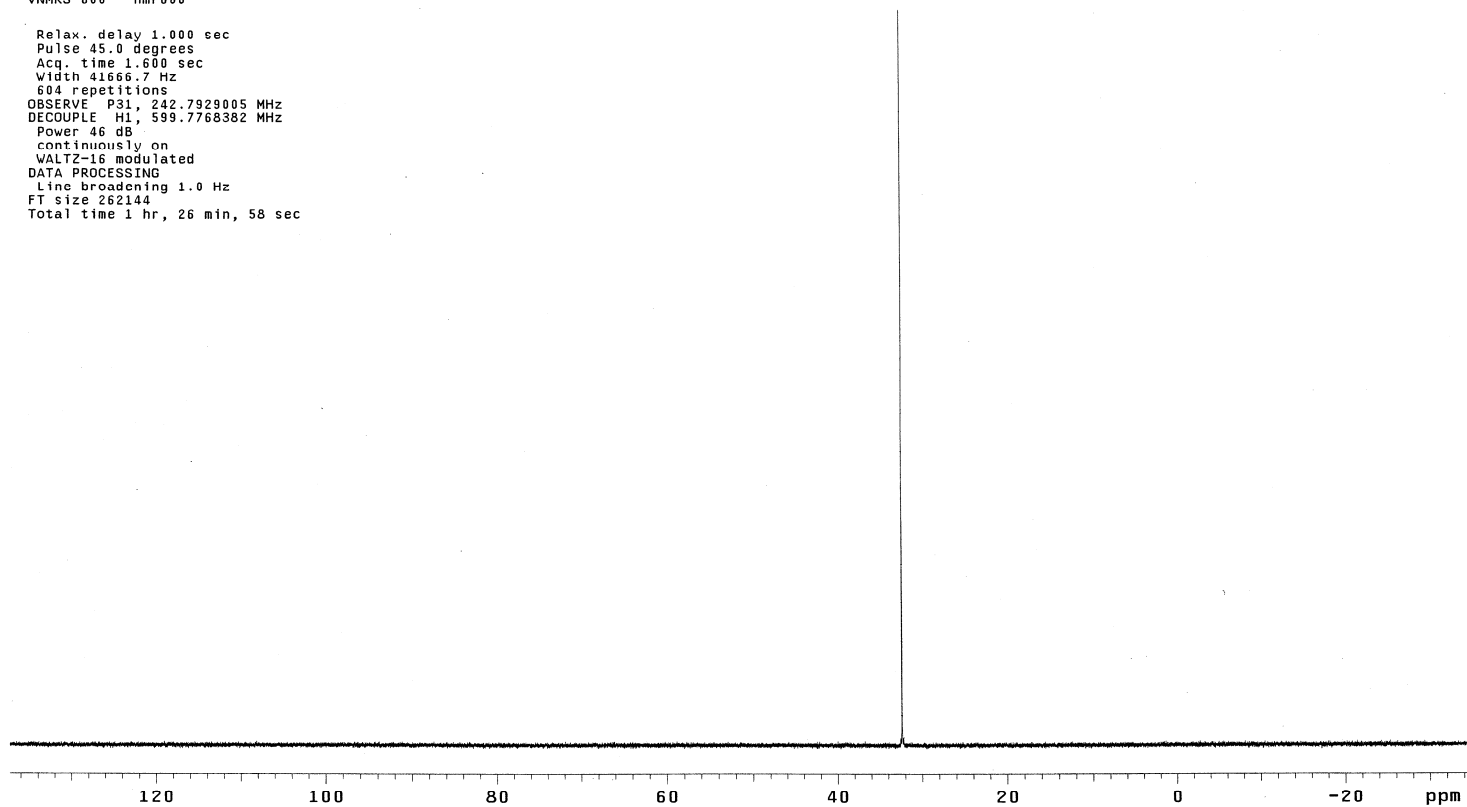
WALTZ-16 modulated

DATA PROCESSING

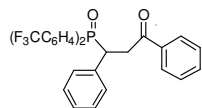
Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec



^{19}F NMR spectrum (CDCl_3 , 25 °C)



3-[Bis[(4-trifluoromethyl)phenyl]phosphinyl]-1,3-diphenyl-1-propanone (**30**)

Std Fluorine

File: home/ras/Desktop/600ras121511.003.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: ras

File: 600ras121511.003

VNMR-600 "nmr600"

Relax. delay 1.000 sec

Pulse 30.0 degrees

Acq. time 1.000 sec

Width 113.6 kHz

16 repetitions

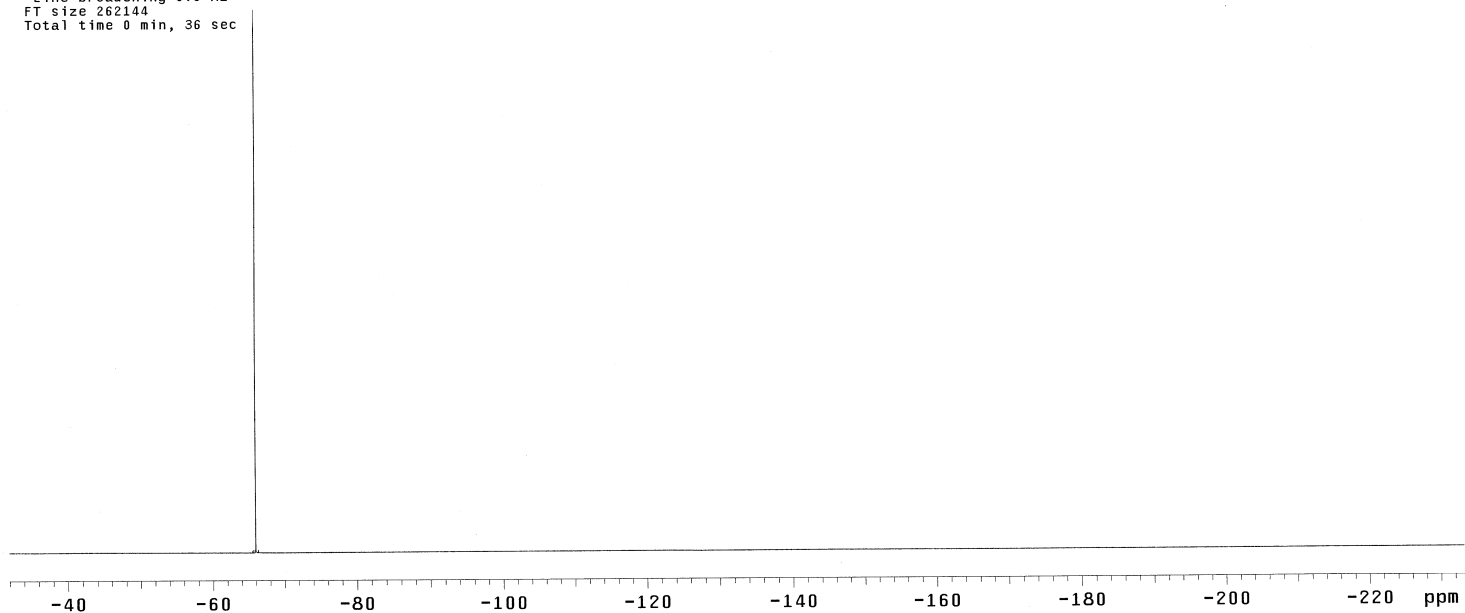
OBSERVE F19, 564.3527190 MHz

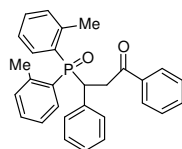
DATA PROCESSING

Line broadening 0.9 Hz

FT size 262144

Total time 0 min, 36 sec





3-[Bis(2-methylphenyl)phosphinyl]-1,3-diphenyl-1-propanone (**31**)

^1H NMR spectrum (CDCl_3 , 25 °C)

Std proton

File: xp

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 9615.4 Hz

16 repetitions

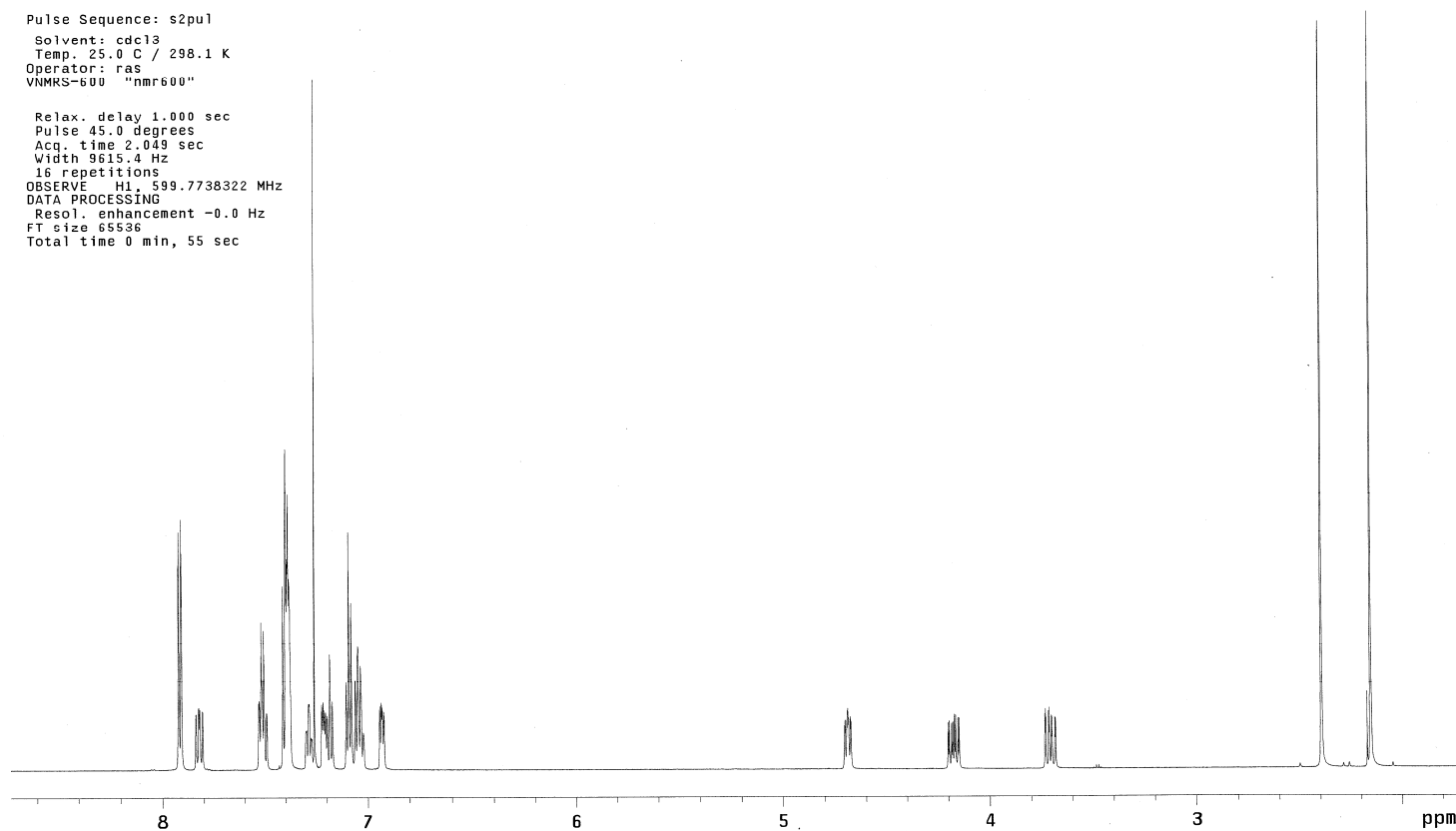
OBSERVE H1, 599.7738322 MHz

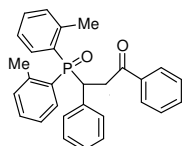
DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 65536

Total time 0 min, 55 sec





3-[Bis(2-methylphenyl)phosphinyl]-1,3-diphenyl-1-propanone (**31**)

Std carbon

File: home/ras/Desktop/600ras120611.028.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras120611.028

VNMR-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 36764.7 Hz

24704 repetitions

OBSERVE C13, 150.8132472 MHz

DECOUPLE H1, 599.7768382 MHz

Power 46 dB

continuously on

WALTZ-16 modulated

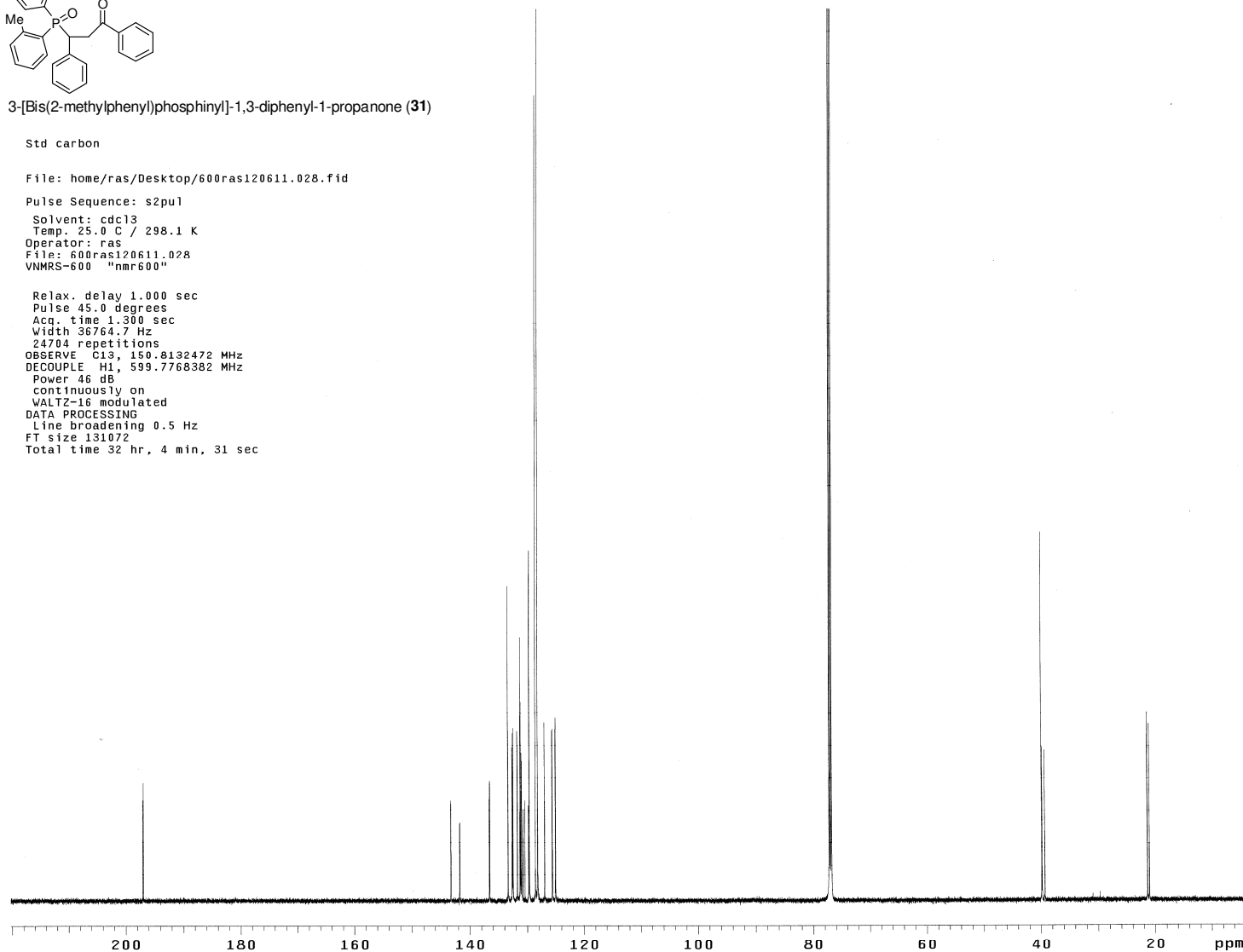
DATA PROCESSING

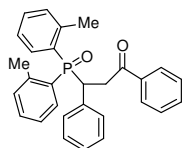
Line broadening 0.5 Hz

FT size 131072

Total time 32 hr, 4 min, 31 sec

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)





3-[Bis(2-methylphenyl)phosphinyl]-1,3-diphenyl-1-propanone (**31**)

$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3 , 25 °C)

Std phosphorus

File: home/ras/Desktop/600ras120611.012.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: ras

File: 600ras120611.012

VNMR5-600 "nmr600"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.600 sec

Width 41666.7 Hz

376 repetitions

OBSERVE P31, 242.7929005 MHz

DECOUPLE H1, 599.7768382 MHz

Power 45 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 262144

Total time 1 hr, 26 min, 58 sec

