

Ülesanne 2

TMR-katseklaasi kaaluti 128 mg vedelat ainet **B** ja lahustati see 0,6 mL deutereeritud kloroformis (99,8% deuteriumrikastusega CDCl_3 -s).

Aine **B** andmed:

Molekulivalem: $\text{C}_6\text{H}_6\text{F}_9\text{O}_3\text{P}$

Molekulmass: 328,07

Mõõdeti järgnevad TMR spektrid:

- 400,1 MHz ^1H ja $^1\text{H}\{^{31}\text{P}\}$ TMR spektrid;
- 100,6 MHz ^{13}C , DEPT-135, $^{13}\text{C}\{^1\text{H}\}$ TMR spektrid;
- 162,0 MHz ^{31}P ja $^{31}\text{P}\{^1\text{H}\}$ TMR spektrid;
- 54,2 MHz ^{17}O TMR spekter;
- 200,1 MHz $^1\text{H}\{^{19}\text{F}\}$ TMR spekter;
- 188,3 MHz ^{19}F ja $^{19}\text{F}\{^1\text{H}\}$ TMR spektrid.

Täiendavalt:

200 MHz spektromeeter oleks võimaldanud mõõta ka $^{13}\text{C}\{^{19}\text{F}\}$ ja $^{31}\text{P}\{^{19}\text{F}\}$ TMR spektreid, aga need jäid sellel korral mõõtmata, kuna neid saab mõõta vaid teise mõõtepeaga, mida oleks tulnud konkreetsete mõõtmiste jaoks ära vahetada. Oluliselt lihtsustavat infot poleks need spektrid siinkohal lisaks andnud.

Selgituseks:

$^{13}\text{C}\{^1\text{H}\}$ – tähendab seda, et mõõdetakse ^{13}C TMR spektrit, kus mõõtmise ajal kiiritatakse proovi ^1H sagedusega, mille tulemusena kaovad ^{13}C TMR spektrist ära $^nJ(^1\text{H}-^{13}\text{C})$ lõhenemised.

$^{31}\text{P}\{^1\text{H}\}$ – tähendab seda, et mõõdetakse ^{31}P TMR spektrit, kus mõõtmise ajal kiiritatakse proovi ^1H sagedusega, mille tulemusena kaovad ^{31}P TMR spektrist ära $^nJ(^1\text{H}-^{31}\text{P})$ lõhenemised.

$^1\text{H}\{^{19}\text{F}\}$ – tähendab seda, et mõõdetakse ^1H TMR spektrit, kus mõõtmise ajal kiiritatakse proovi ^{19}F sagedusega, mille tulemusena kaovad ^1H TMR spektrist ära $^nJ(^1\text{H}-^{19}\text{F})$ lõhenemised.

$^{19}\text{F}\{^1\text{H}\}$ – tähendab seda, et mõõdetakse ^{19}F TMR spektrit, kus mõõtmise ajal kiiritatakse proovi ^1H sagedusega, mille tulemusena kaovad ^{19}F TMR spektrist ära $^nJ(^1\text{H}-^{19}\text{F})$ lõhenemised.

^{13}C DEPT-135 TMR spektris on $\underline{\text{CH}_2}$ -le vastavad signaalid vastandfaasis võrreldes $\underline{\text{CH}}$ ja $\underline{\text{CH}_3}$ -le vastavate signaalidega ning protoneerimata süsinikud ei anna üldse signaali.

Lahenduskäik:

- Teil on kasutada ülalnimetatud spektrid ja TMR korrelatsioonitabelid. Lugege üle, mitu signaali 1D spektritesse tekkis, vaadake ka signaalide integraale, võrrelge molekuli-valemiga – selle põhjal saate öelda üht-teist molekuli sümmeetria ja asendajate ekvivalentsuse kohta.
- Leida, mis tüüpi multipllettidega [singlett (s), dublett (d), triplett (t), kvartett (q), kvintett (quin), dubleti dublett (dd), dubleti kvartett (dq), okteti heptett jne.] on tegemist.
Võtke arvesse seminaris mainitud valemit: $M=2nI+1$
- Mõõta ^1H , ^{13}C ja ^{19}F spektritest kõik lõhestumiskonstandid J (ühikuks hertsid, täpsusega 1 kümnendkoht).

Raportisse kirjutada:

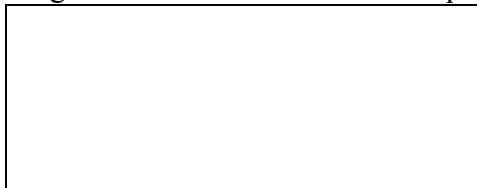
1. Leida toodud spektrite põhjal aine **B** struktuurivalem.

Struktuurivalemite joonistamiseks soovitan kasutada vabavaralist tarkvara ACD ChemSketch (<http://www.acdlabs.com/resources/freeware/chemsketch/>) või tasulist tarkvara CambridgeSoft ChemDraw (http://www.cambridgesoft.com/Ensemble_for_Chemistry/ChemDraw/).

2. Millele (mis aine ja mis isotopomeerile) vastab ^1H TMR spektris signaal 7,26 ppm juures? Joonistage struktuurivalem koos isotooptähistega:



3. Millele (mis aine ja mis isotopomeerile) vastab ^{13}C TMR spektris 1:1:1-kujuline tripleti signaal 77,00 ppm juures? Leidke sealt multiuletilt lõhestumiskonstant (ühikuks herts, täpsusega 1 kümnendkoht) ja täpsustage, milliste tuumade tõttu see signaalide lõhestumine tekib. Joonistage struktuurivalem koos isotooptähistega:



Tuletage meelde seminaris räägitut!

4. Esitage aine **B** täielik TMR spektriinfo (1D ^1H , ^{13}C , ^{17}O , ^{19}F ja ^{31}P TMR spektrite kohta) tekstiformaadis kujul nt:

Siia kirjutage aine B süstemaatiline nimetus:

^1H TMR (200,0 MHz, CDCl_3 , 25 °C) δ : 4,44 (s, 1H, OH); 3,18 (q, $^3J_{\text{HH}}=7,1$ Hz, 2H, CH_2); 0,74 (t, $^3J_{\text{HH}}=7,1$ Hz, 3H, CH_3).

^{13}C TMR (100,6 MHz, CDCl_3 , 25 °C) δ : 48,3 (q, $^1J_{\text{CH}} = 140,5$ Hz, $3\times\text{CH}_3$).

^{17}O TMR (54,2 MHz, CDCl_3 , 25 °C) δ : -33,2 ($3\times\text{OH}$).

^{19}F TMR (376,5 MHz, CDCl_3 , 25 °C) δ : -29,40 (q, $^3J_{\text{FH}} = 9,1$ Hz, 4F, $2\times\text{CF}_2$).

^{31}P TMR (162,0 MHz, CDCl_3 , 25 °C) δ : 110,0 (qt, $^3J_{\text{HP}}=4,5$ Hz, $^4J_{\text{FP}}=4,0$ Hz, P).

PS. Pange tähele, kui täpselt (mitme kümnendkohaga) keemilisi nihkeid ja lõhestumiskonstante märkida!

NB! Mõõtkite ära ja kirjutage raportisse kõik $^1J_{\text{CF}}$, $^1J_{\text{CH}}$, $^2J_{\text{CF}}$, $^2J_{\text{CH}}$, $^2J_{\text{CP}}$, $^3J_{\text{HF}}$, $^3J_{\text{CP}}$, $^3J_{\text{HP}}$ ja $^4J_{\text{FP}}$ lõhestumiskonstandid.

NB. Pange tähele, et lõhestumiskonstandid esinevad erinevate multiulettide juures paari-kaupa.

NB! Signaalide kirjelduste juurde kirjutage täpselt välja, millistele konkreetsetele tuumadele aines **B** TMR signaalid kuuluvad.

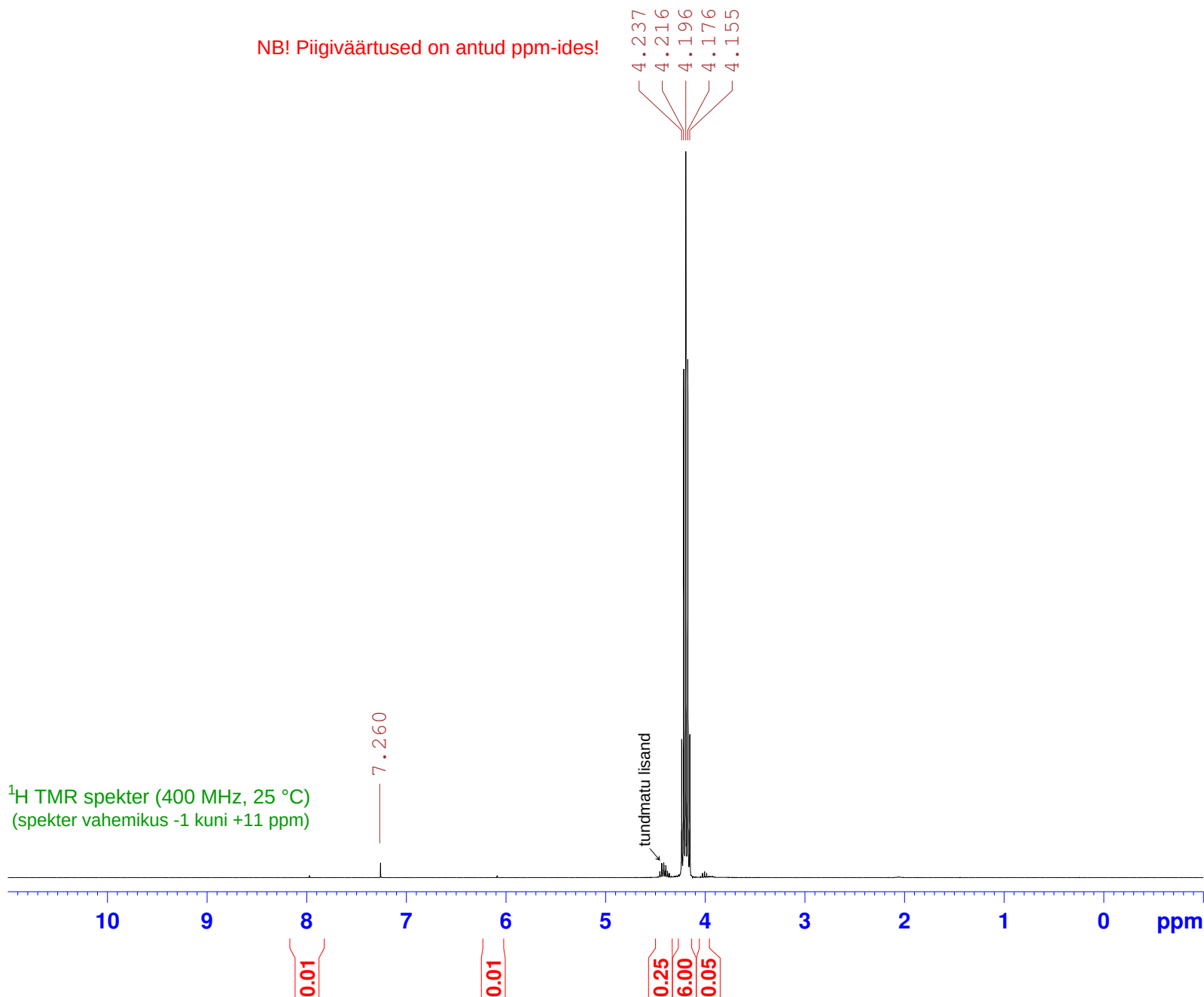
PS. Pange tähele, mis spektromeetri sagedusel konkreetset tuuma mõõdeti! Siin näites ei pruugi raporteeritud spektromeetri sagedus olla sama, mis teile antud spektritel kirjas on.

5. Kas oskate valemi $M=2nI+1$ abil öelda, mis tüüpi multiulett on ^{31}P TMR spektris 139,2 ppm juures?
6. Miks on ^1H , ^{13}C , ^{19}F ja ^{31}P spektrites ^{13}C -st tingitud signaalide lõhenemisi vähe (või pole üldse) näha?
7. Kuidas oleks saanud ^{13}C ja ^{17}O TMR spektrites signaal-müra suhet parandada (pakkuda välja vähemalt 3 varianti)?
8. Miks ^{17}O teiste molekulis olevate tuumade (^1H , ^{13}C , ^{19}F , ^{31}P) signaale ei lõhesta (2 pühjust)?

Ülesanne on kättesaadav PDF-formaadis aadressilt: <http://kodu.ut.ee/~laurit/AK2/>

Raportit soovin saada oma e-posti aadressile lauri.toom@ut.ee ainult PDF-formaadis.

Raporti 1. versiooni esitamise tähtaeg on 15. mai 2015 kell 17:00. Minupoolse tagasiside põhjal korrektselt parandatud lõpp-versiooni esitamise tähtaeg on 29. mai 2015 kell 17:00.



Current Data Parameters

```
EXPNO          1
PROCNO         1

F2 - Acquisition Parameters
Date_          20120321
Time           10.47
INSTRUM        spect
PROBHD         5 mm BBO BB-1H
PULPROG        zg30
TD             32768
SOLVENT        CDC13
NS             16
DS             4
SWH            7211.539 Hz
FIDRES         0.220079 Hz
AQ            2.2719646 sec
RG             80.6
DW            69.333 usec
DE             6.00 usec
TE            298.2 K
D1            3.00000000 sec
TD0            1
```

```
===== CHANNEL f1 =====
NUC1            1H
P1             14.35 usec
PL1            0.00 dB
SFO1          400.1324008 MHz
```

```
F2 - Processing parameters
SI            131072
SF          400.1300176 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```

NB! Piigiväärtused on antud ppm-ides!

4.237
4.216
4.196
4.176
4.155

Current Data Parameters

```
EXPNO          1
PROCNO         1

F2 - Acquisition Parameters
Date_          20120321
Time           10.47
INSTRUM        spect
PROBHD         5 mm BBO BB-1H
PULPROG        zg30
TD             32768
SOLVENT        CDC13
NS             16
DS             4
SWH            7211.539 Hz
FIDRES         0.220079 Hz
AQ            2.2719646 sec
RG             80.6
DW            69.333 usec
DE             6.00 usec
TE            298.2 K
D1            3.00000000 sec
TD0            1
```

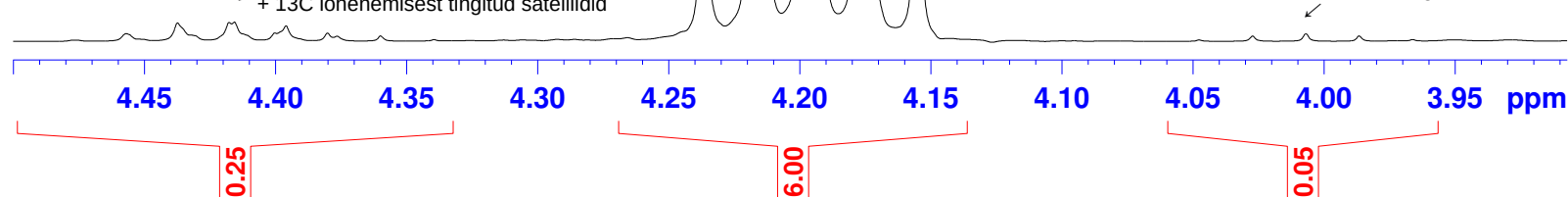
```
===== CHANNEL f1 =====
NUC1            1H
P1             14.35 usec
PL1            0.00 dB
SFO1          400.1324008 MHz
```

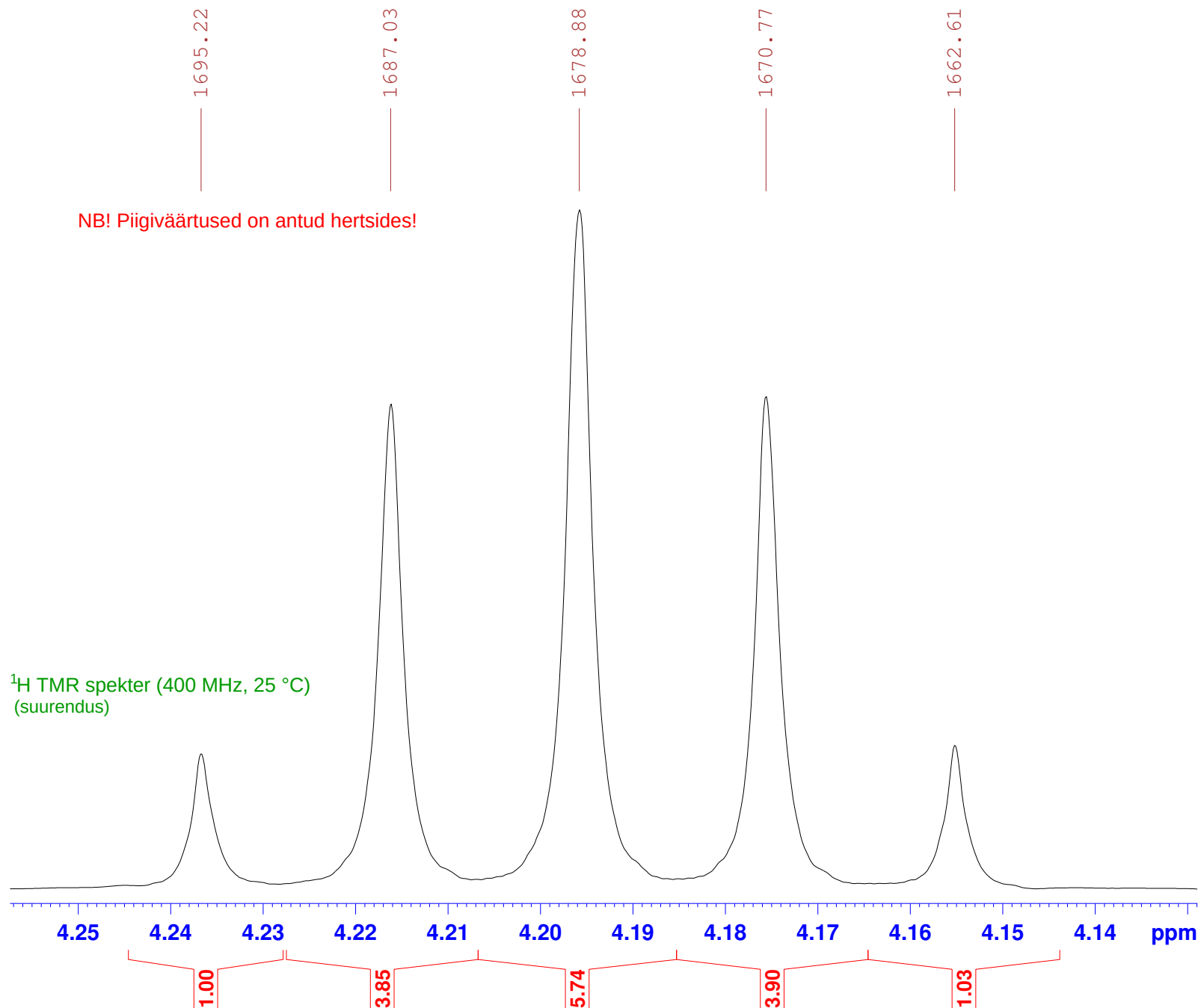
```
F2 - Processing parameters
SI             131072
SF            400.1300176 MHz
WDW            EM
SSB            0
LB             0.30 Hz
GB             0
PC             1.00
```

¹H TMR spekter (400 MHz, 25 °C)
(suurendus)

tundmatu lisand
+ ¹³C lõhenemisest tingitud satelliidid

¹³C lõhenemisest tingitud satelliidid





Current Data Parameters

EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

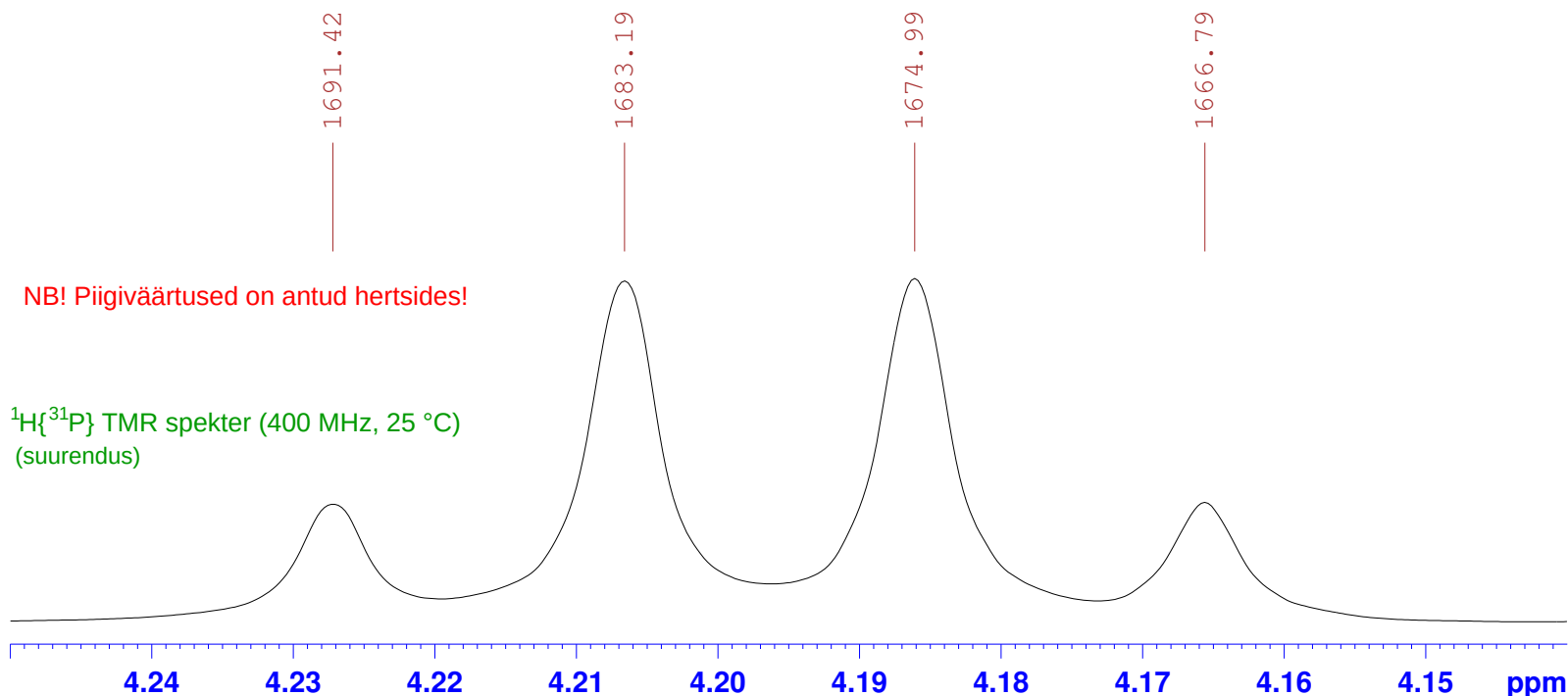
Date_ 20120321
Time 10.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 4
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719646 sec
RG 80.6
DW 69.333 usec
DE 6.00 usec
TE 298.2 K
D1 3.00000000 sec
TD0 1

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

NUC1 1H
P1 14.35 usec
PL1 0.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters

SI 131072
SF 400.1300176 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



Current Data Parameters

EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

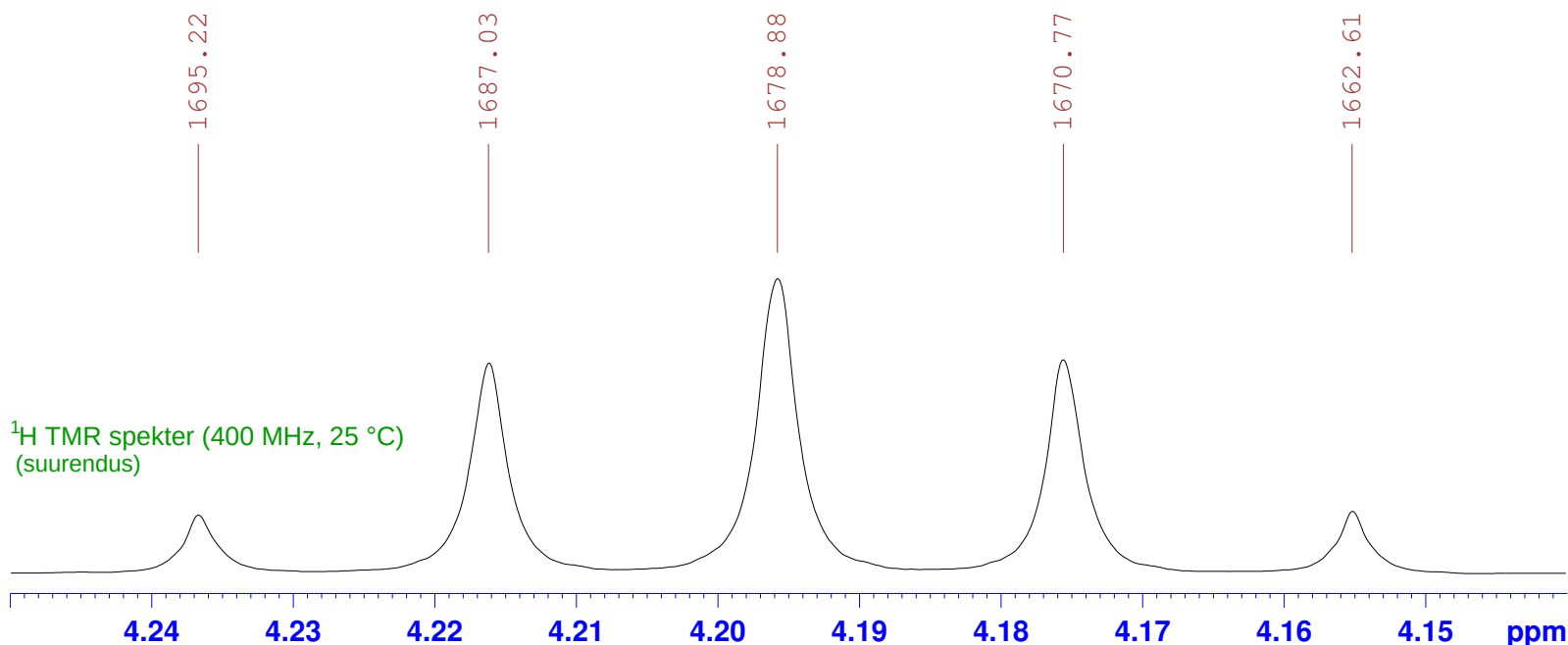
Date_ 20120321
Time 11.55
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgig30
TD 32768
SOLVENT CDC13
NS 16
DS 4
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5625076 sec
RG 80.6
DW 78.200 usec
DE 6.00 usec
TE 298.2 K
D1 5.00000000 sec
d11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 31P
PCPD2 100.00 usec
PL12 20.03 dB
PL2 0.00 dB
SFO2 161.9837299 MHz

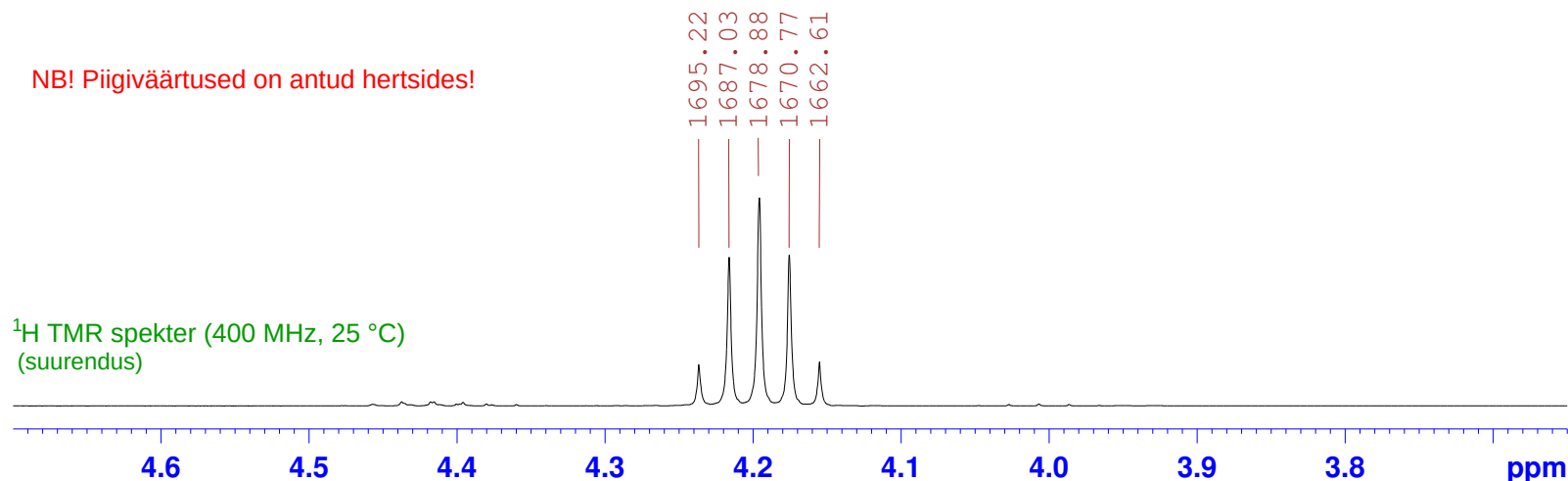
F2 - Processing parameters

SI 65536
SF 400.1300175 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

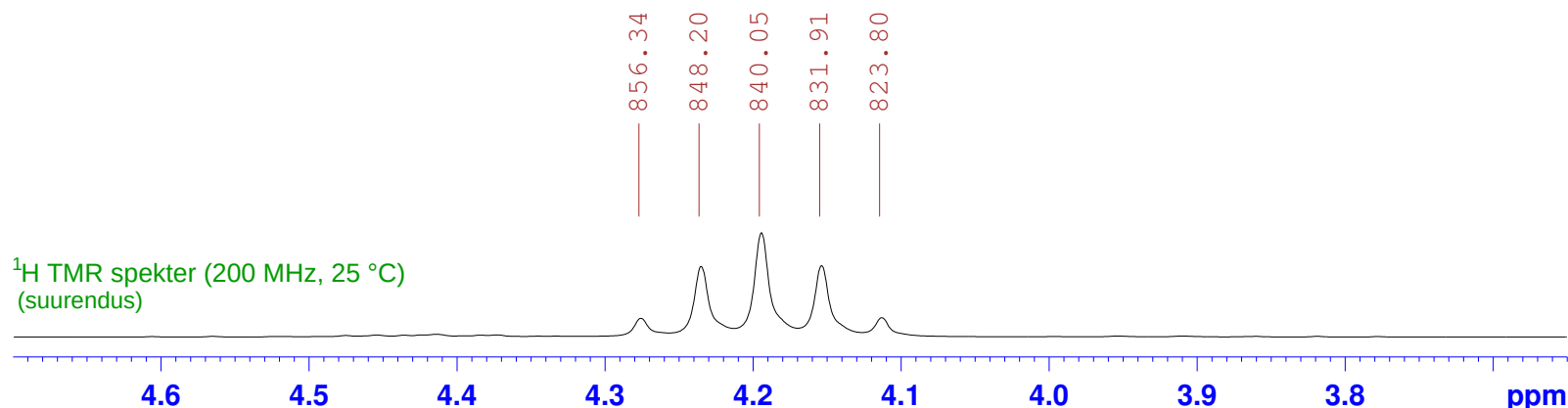


NB! Piigiväärtused on antud hertsides!

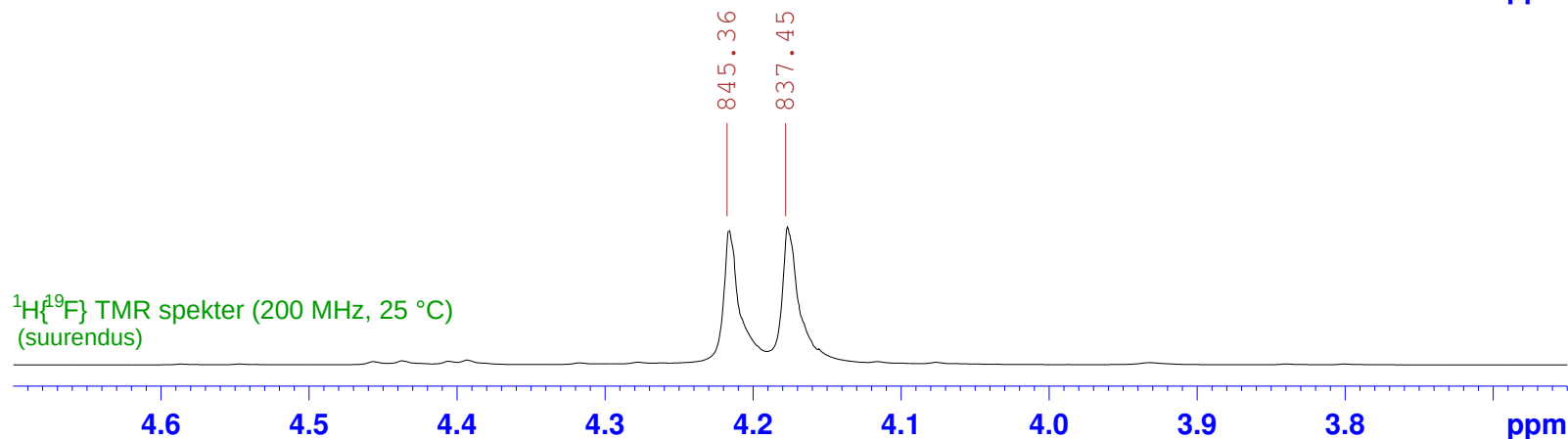
^1H TMR spekter (400 MHz, 25 °C)
(suurendus)



^1H TMR spekter (200 MHz, 25 °C)
(suurendus)



$^1\text{H}\{^{19}\text{F}\}$ TMR spekter (200 MHz, 25 °C)
(suurendus)



Current Data Parameters

EXPNO 24
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120409
Time 15.40
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgfhgqn
TD 524288
SOLVENT CDCl3
NS 17
DS 4
SWH 45454.547 Hz
FIDRES 0.086698 Hz
AQ 5.7672181 sec
RG 36
DW 11.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

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

NUC1 19F
P1 7.00 usec
PL1 0.00 dB
PL1W 14.06656361 W
SFO1 188.2926422 MHz

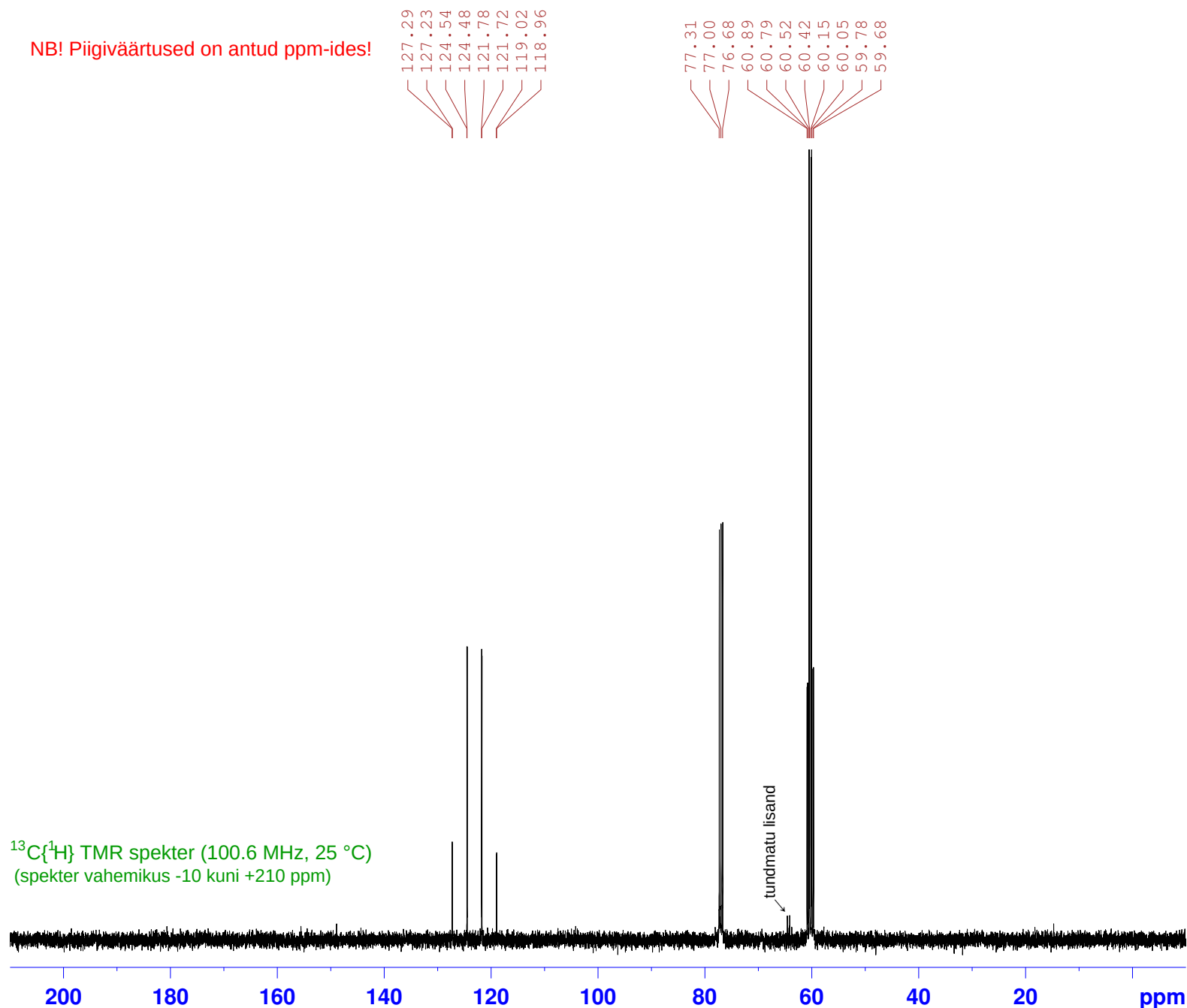
===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 55.00 dB
PL2W 14.31775284 W
PL12W 0.00004528 W
SFO2 200.1320005 MHz

F2 - Processing parameters

SI 524288
SF 188.3114730 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NB! Piigiväärtused on antud ppm-ides!



Current Data Parameters

EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120321
Time 10.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 32800
DW 20.800 usec
DE 6.00 usec
TE 298.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

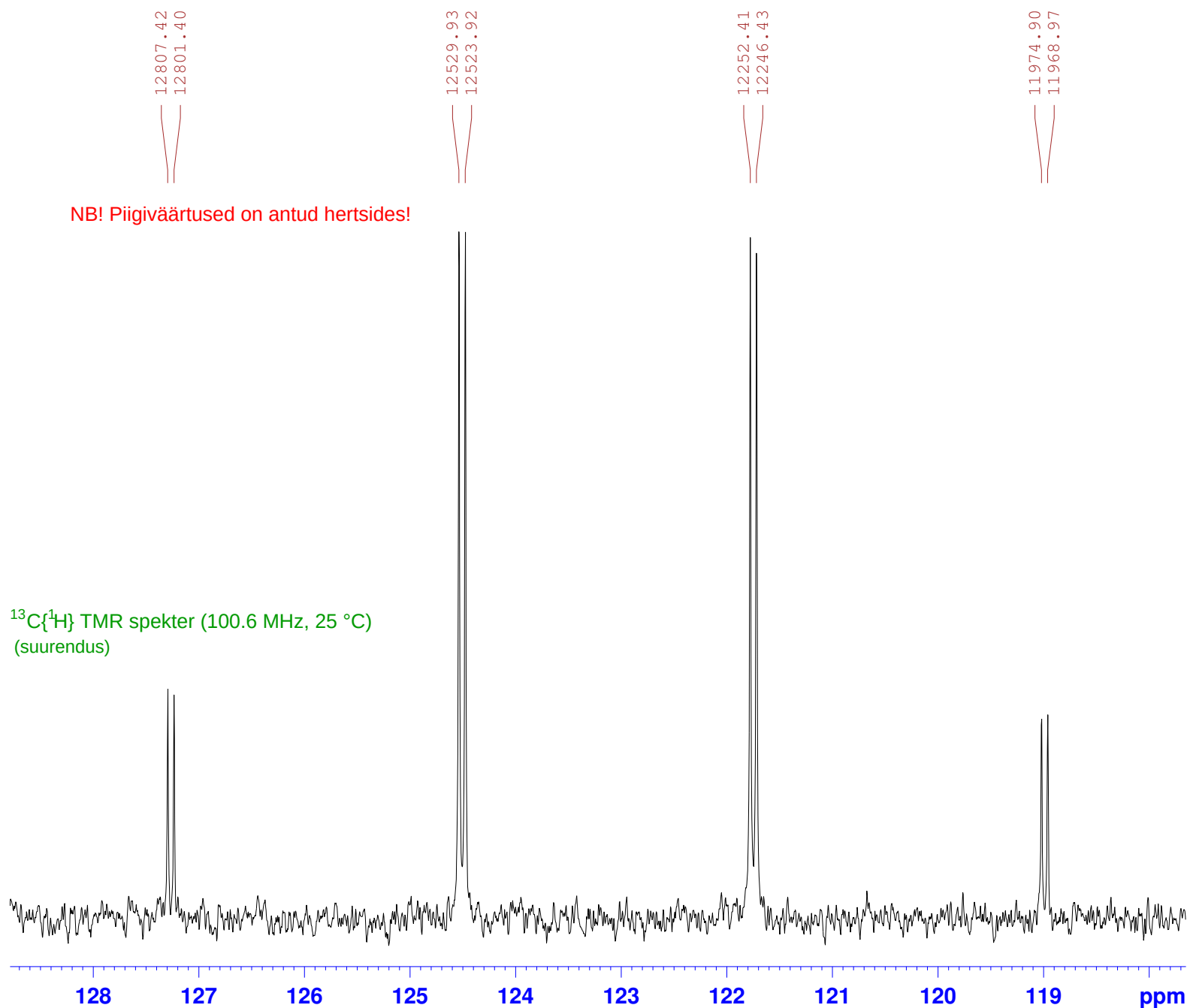
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

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

CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 13.76 dB
PL13 14.00 dB
PL2 0.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 65536
SF 100.6127601 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters

EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120321
Time 10.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 32800
DW 20.800 usec
DE 6.00 usec
TE 298.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

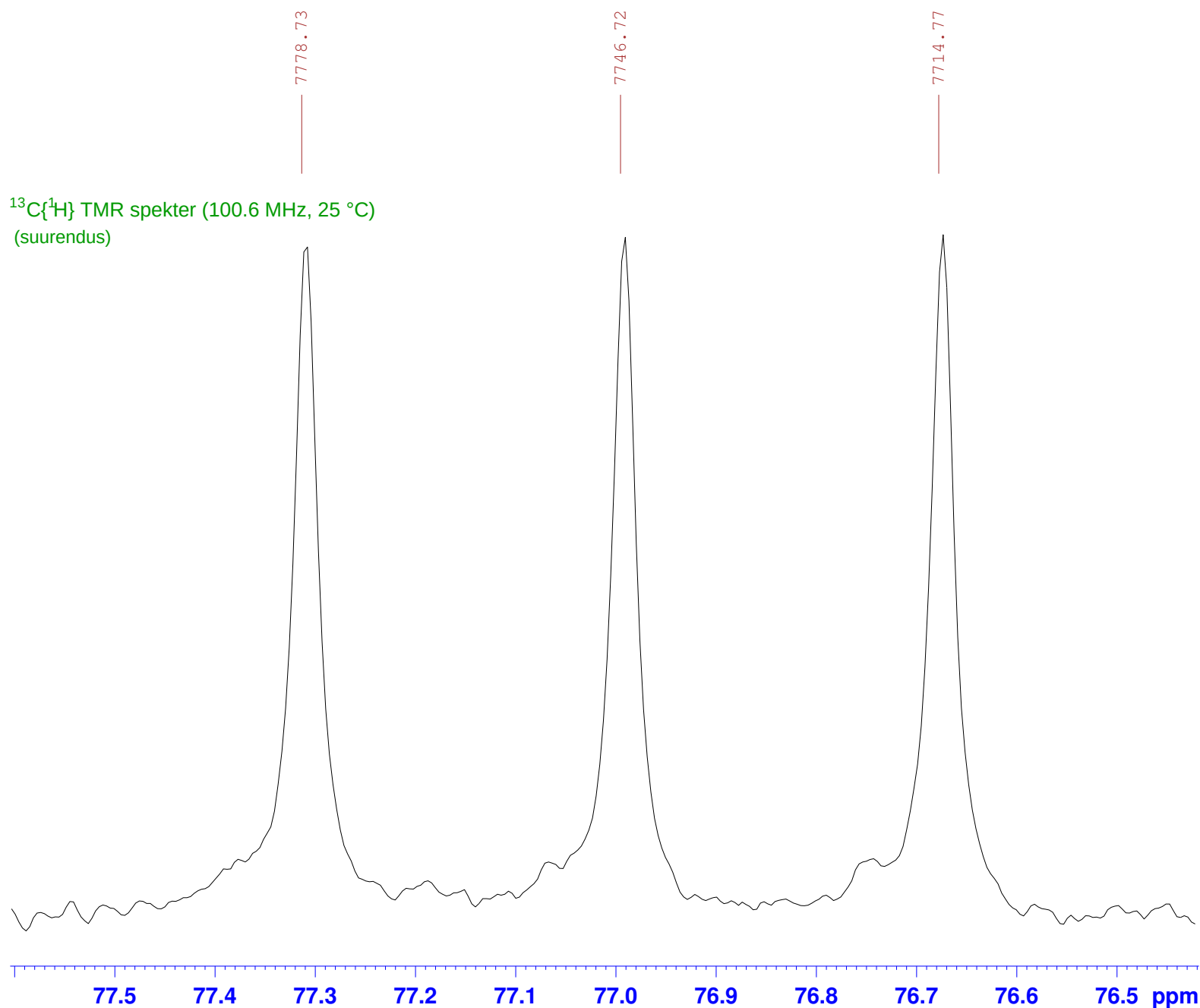
===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 13.76 dB
PL13 14.00 dB
PL2 0.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 65536
SF 100.6127601 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NB! Piigiväärtused on antud hertsides!



Current Data Parameters

EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120321
Time 10.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 32800
DW 20.800 usec
DE 6.00 usec
TE 298.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

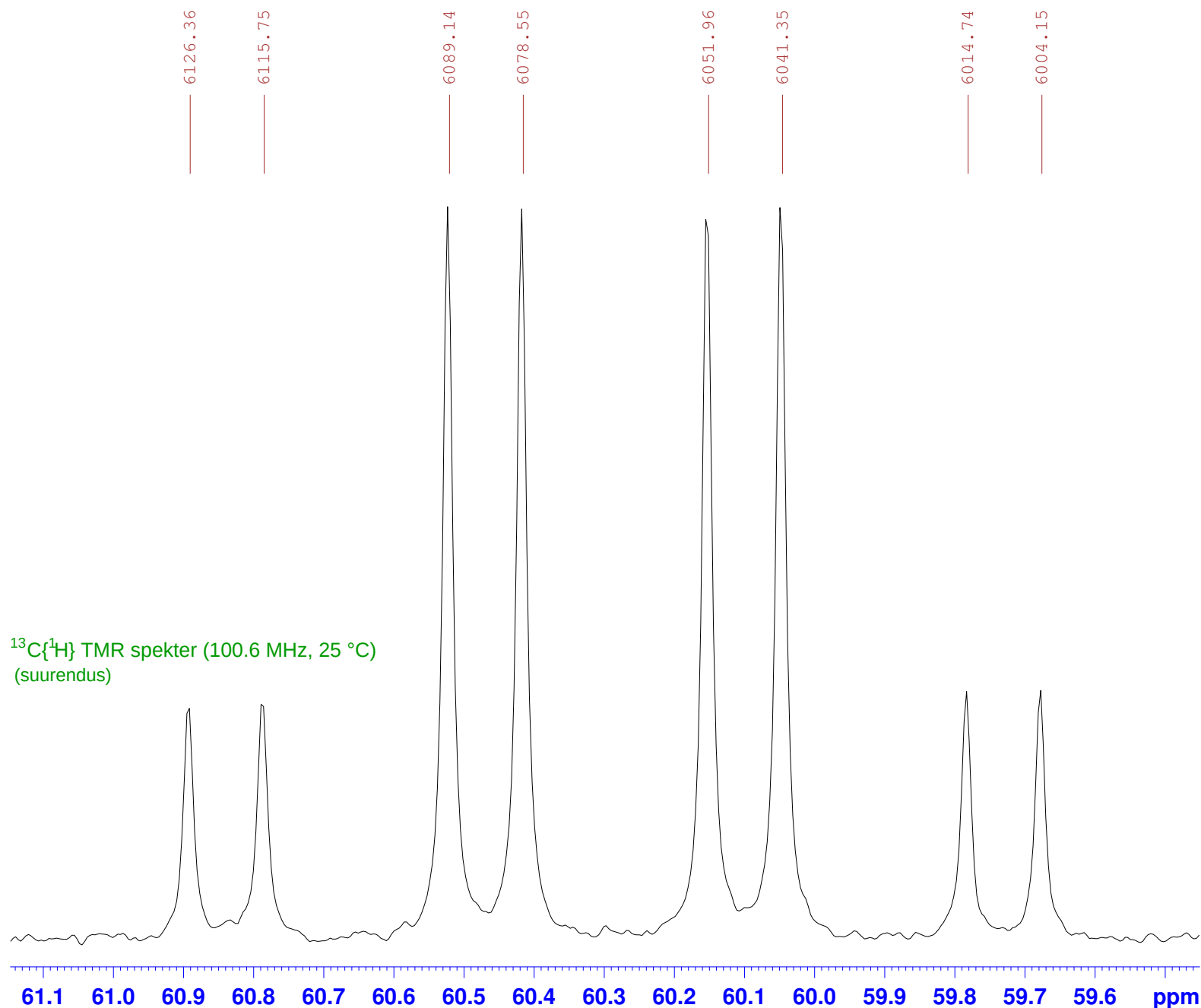
===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 13.76 dB
PL13 14.00 dB
PL2 0.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 65536
SF 100.6127601 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NB! Piigiväärtused on antud hertsides!



Current Data Parameters

EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120321
Time 10.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 32800
DW 20.800 usec
DE 6.00 usec
TE 298.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

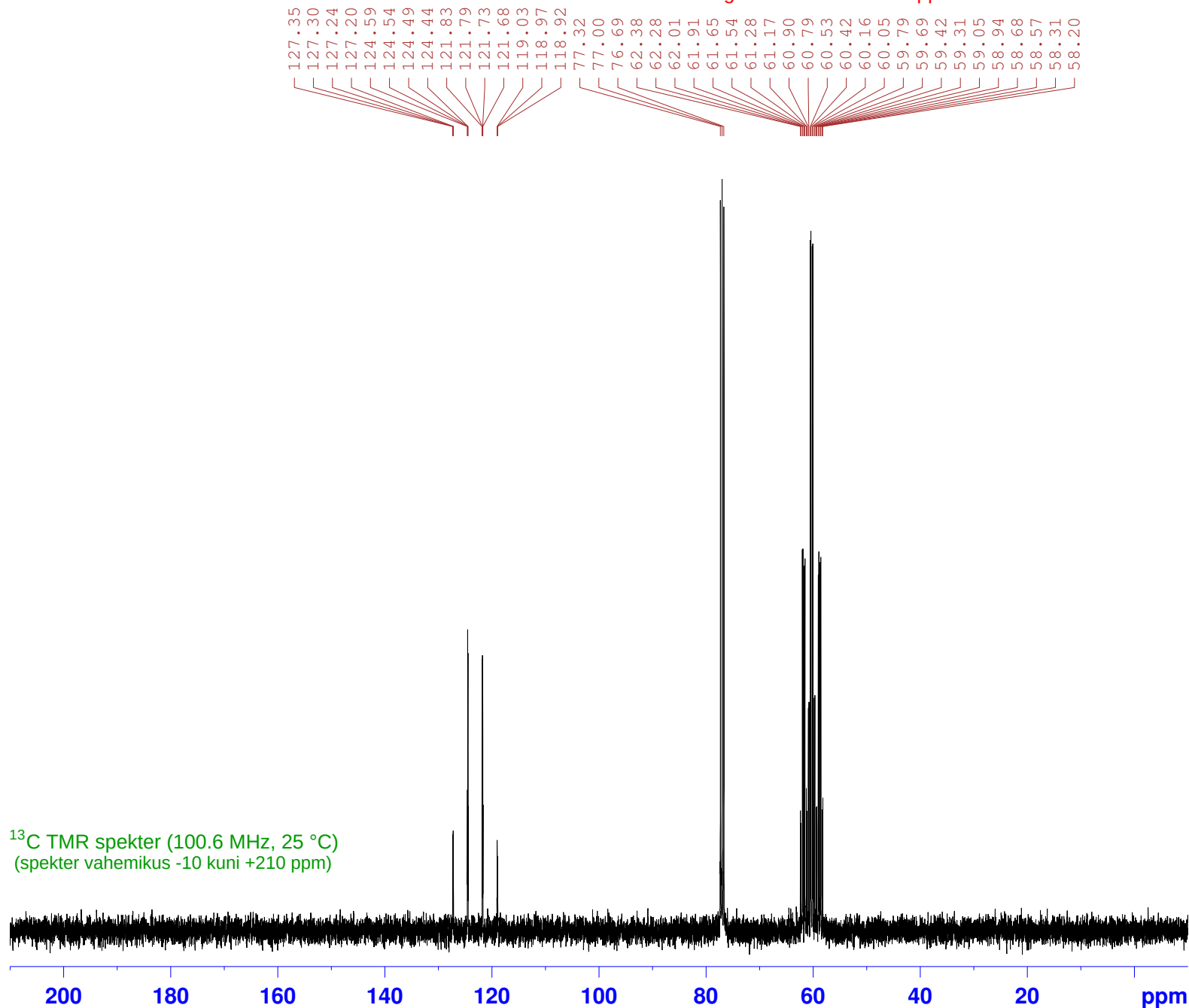
===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 13.76 dB
PL13 14.00 dB
PL2 0.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 65536
SF 100.6127601 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NB! Piigiväärtused on antud ppm-ides!



Current Data Parameters

EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120321
Time 11.00
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 16400
DW 20.800 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1

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

NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
SFO1 100.6228293 MHz

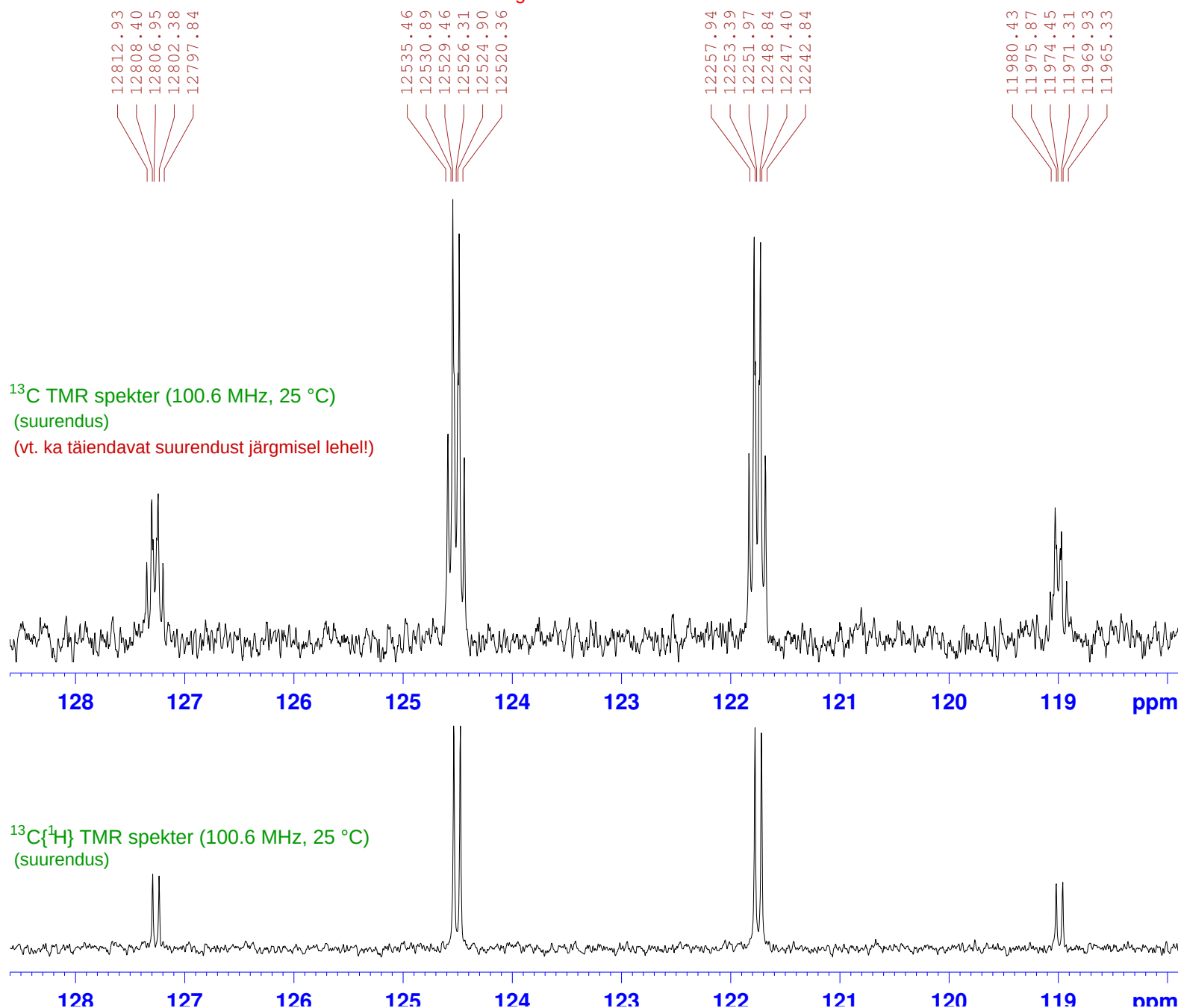
===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 13.76 dB
PL2 0.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 65536
SF 100.6127592 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NB! Piigiväärtused on antud hertsides!



Current Data Parameters

EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120321
Time 11.00
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 16400
DW 20.800 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1

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

NUC1 ^{13}C
P1 9.50 usec
PL1 -2.00 dB
SFO1 100.6228293 MHz

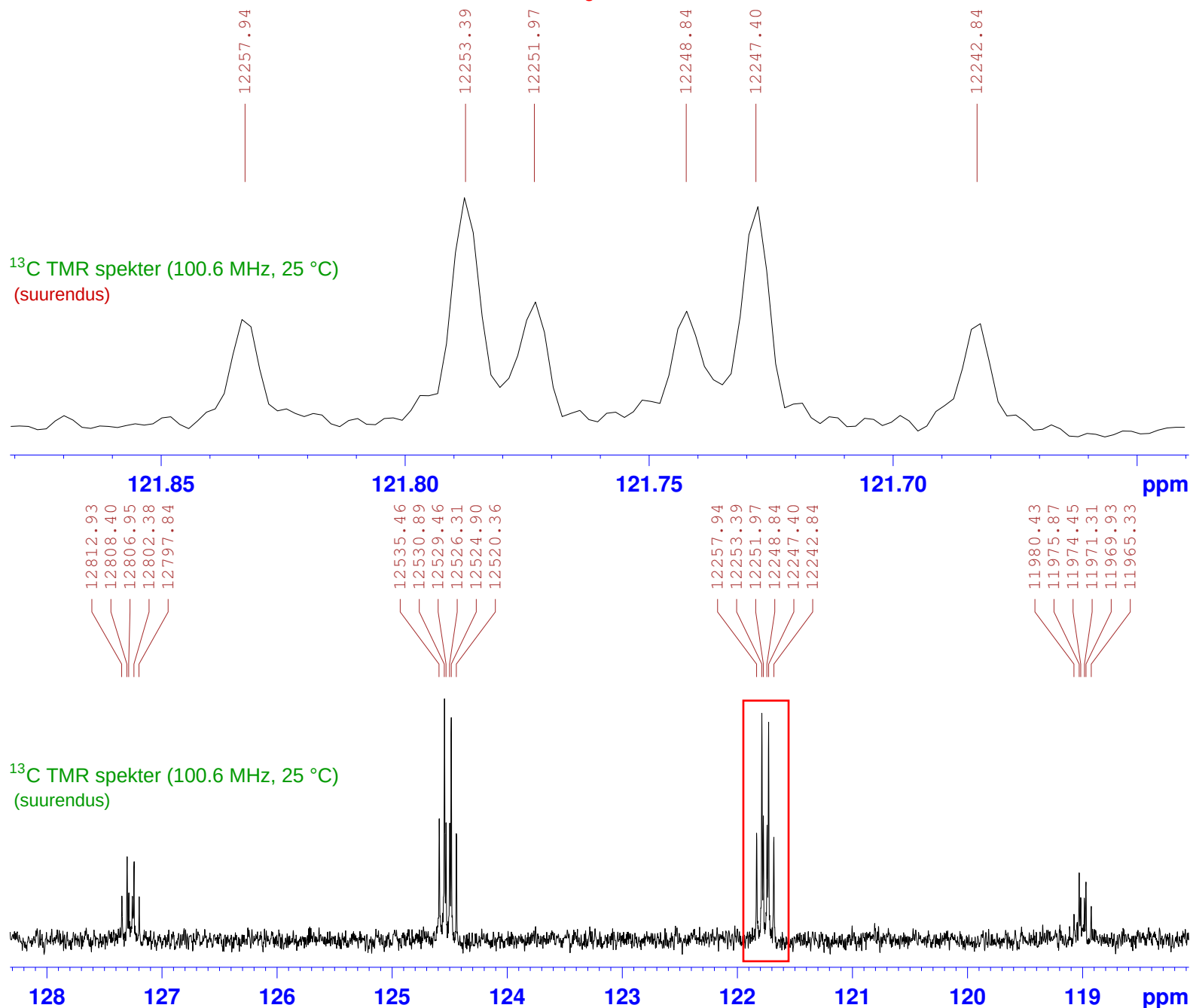
===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 ^1H
PCPD2 70.00 usec
PL12 13.76 dB
PL2 0.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 65536
SF 100.6127592 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NB! Piigiväärtused on antud hertsides!



Current Data Parameters

EXPNO 99
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120321
Time 11.00
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 16400
DW 20.800 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1

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

NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
SFO1 100.6228293 MHz

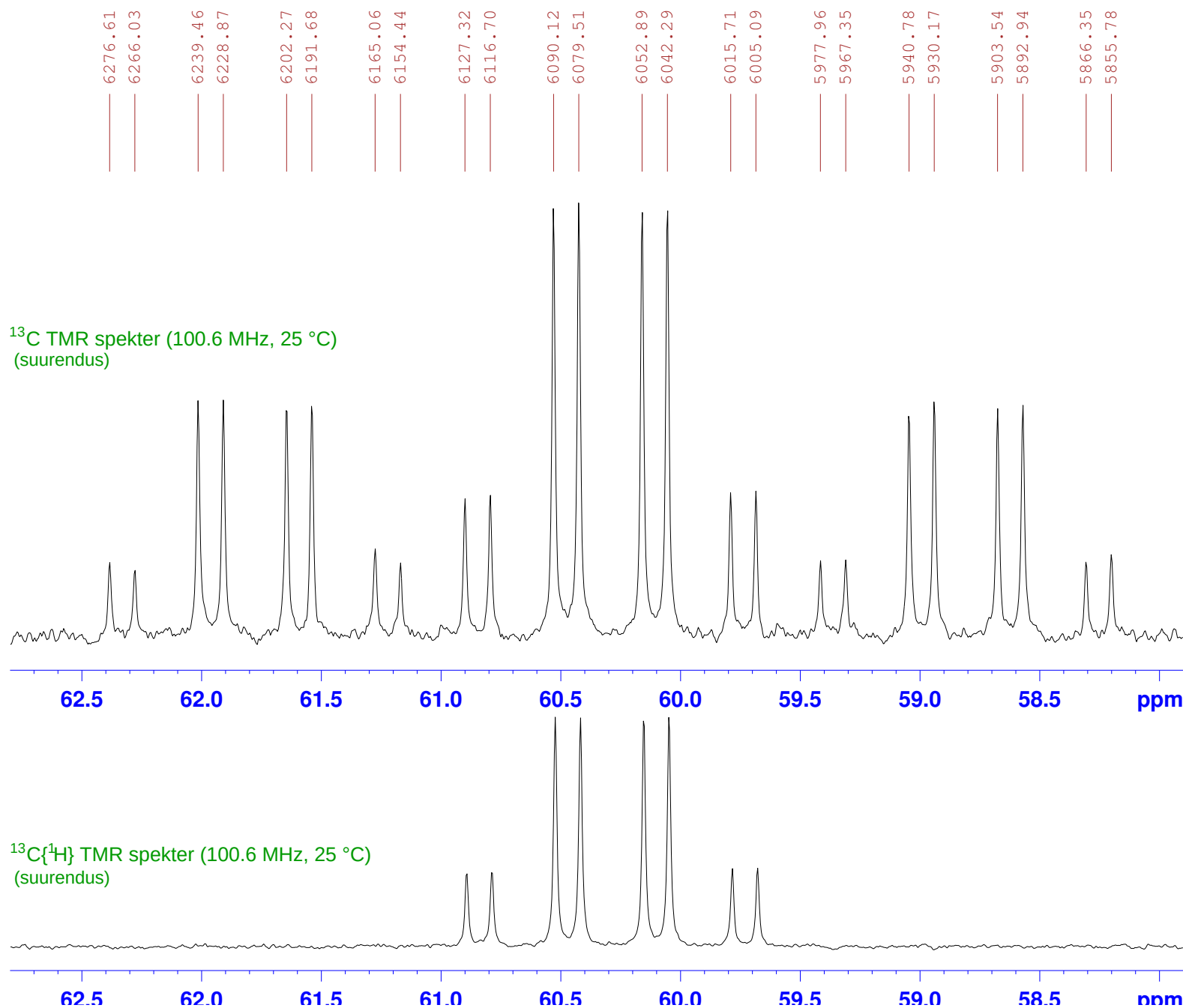
===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 13.76 dB
PL2 0.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 131072
SF 100.6127592 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.40

NB! Piigiväärtused on antud hertsides!



Current Data Parameters

EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120321
Time 11.00
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 16400
DW 20.800 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1

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

NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
SFO1 100.6228293 MHz

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

CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 13.76 dB
PL2 0.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

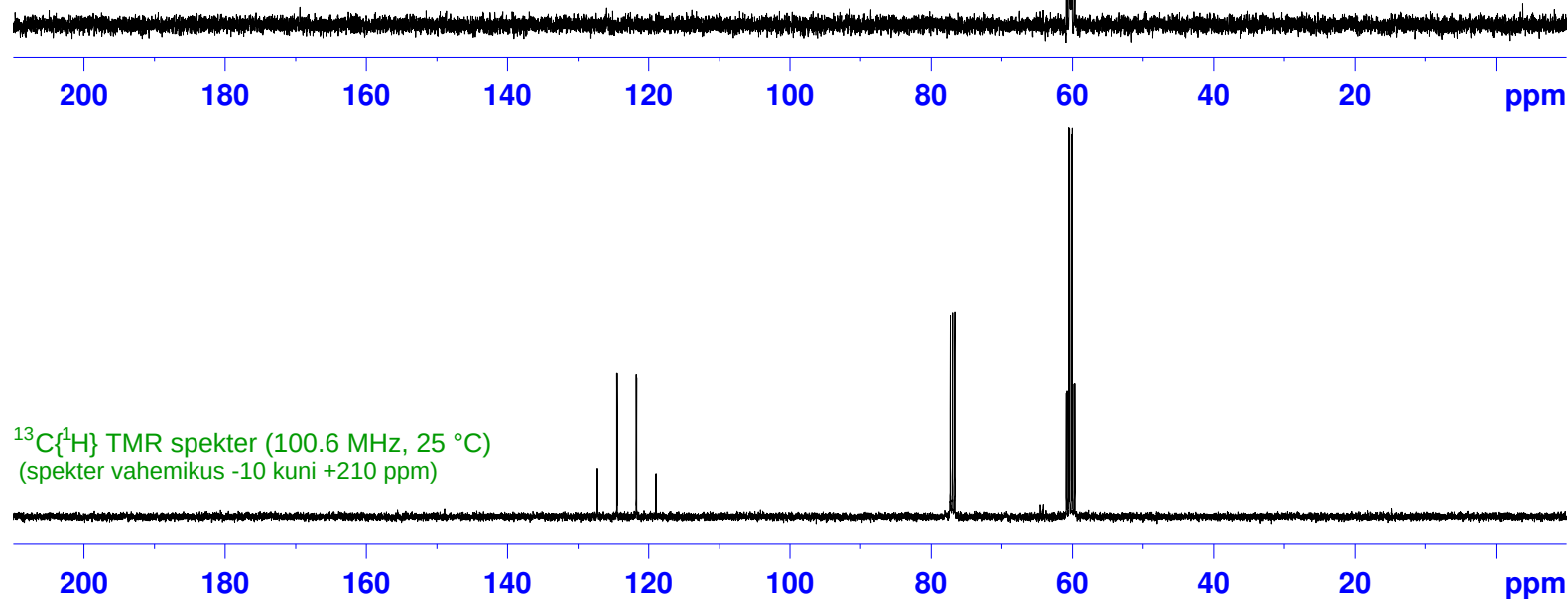
SI 65536
SF 100.6127592 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NB! Piigiväärtused on antud ppm-ides!

60.89
60.78
60.52
60.41
60.15
60.04
59.78
59.67

^{13}C DEPT-135 TMR spekter (100.6 MHz, 25 °C)

CH_2 ↑
 CH, CH_3 ↓



Current Data Parameters

```
EXPNO          5
PROCNO         1

F2 - Acquisition Parameters
Date_          20120321
Time           11.27
INSTRUM        spect
PROBHD         5 mm BBO BB-1H
PULPROG        dept135
TD             65536
SOLVENT        CDC13
NS             128
DS             4
SWH            24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG            16400
DW            20.800 usec
DE             6.00 usec
TE            298.1 K
CNST2         145.0000000
D1            2.00000000 sec
d12           0.00002000 sec
d2            0.00344828 sec
DELTA         0.00001210 sec
TD0           1
```

```
===== CHANNEL f1 =====
NUC1           13C
P1            9.50 usec
p2           19.00 usec
PL1           -2.00 dB
SFO1         100.6228298 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2        waltz16
NUC2           1H
P3           14.35 usec
p4           28.70 usec
PCPD2         70.00 usec
PL12          13.76 dB
PL2           0.00 dB
SFO2         400.1316005 MHz
```

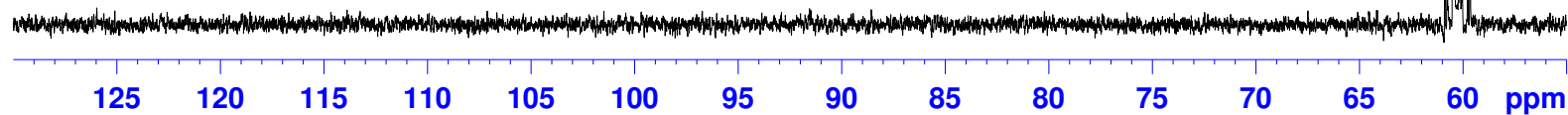
```
F2 - Processing parameters
SI            32768
SF           100.6127601 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```


NB! Piigiväärtused on antud ppm-ides!

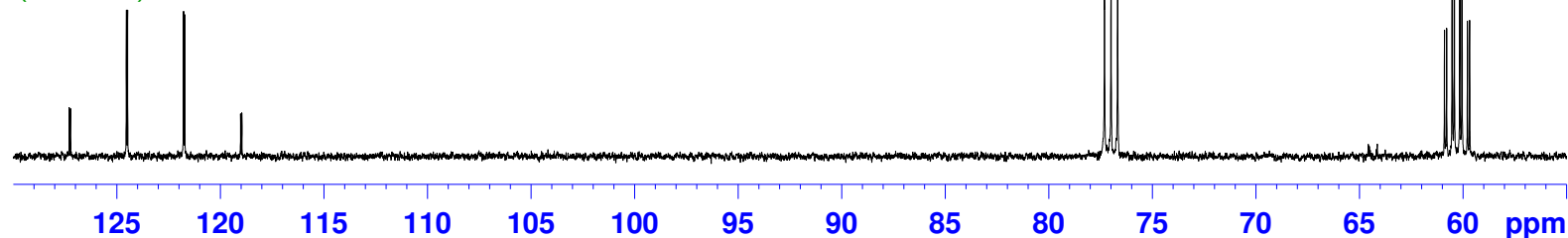
60.89
60.78
60.52
60.41
60.15
60.04
59.78
59.67

^{13}C DEPT-135 TMR spekter (100.6 MHz, 25 °C)

CH_2 ↑
 CH, CH_3 ↓



$^{13}\text{C}\{^1\text{H}\}$ TMR spekter (100.6 MHz, 25 °C)
(suurendus)



Current Data Parameters

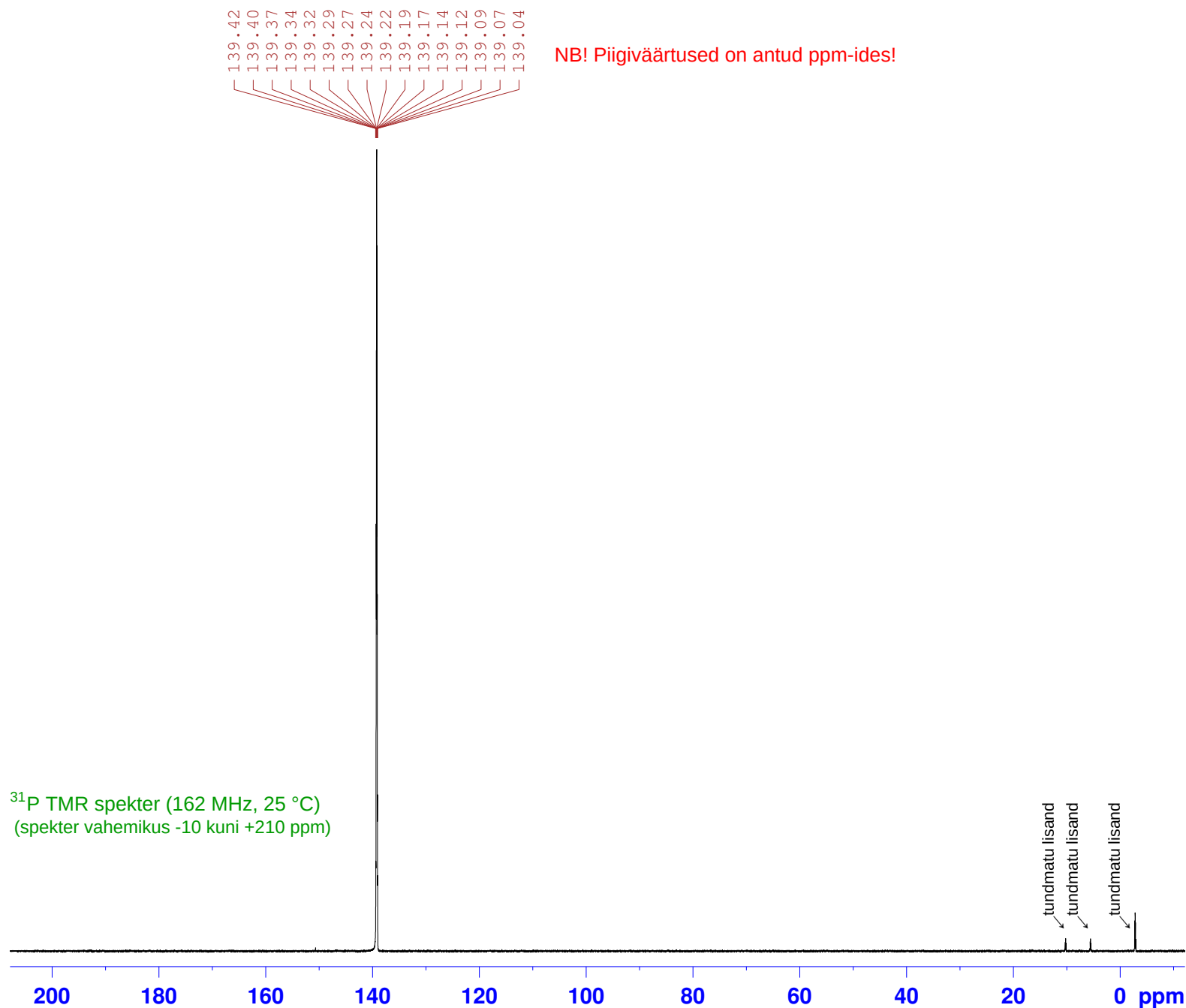
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120321
Time 11.27
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG dept135
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 16400
DW 20.800 usec
DE 6.00 usec
TE 298.1 K
CNST2 145.0000000
D1 2.00000000 sec
d12 0.00002000 sec
d2 0.00344828 sec
DELTA 0.00001210 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
p2 19.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 14.35 usec
p4 28.70 usec
PCPD2 70.00 usec
PL12 13.76 dB
PL2 0.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127601 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters

EXPNO 7
PROCNO 1

F2 - Acquisition Parameters

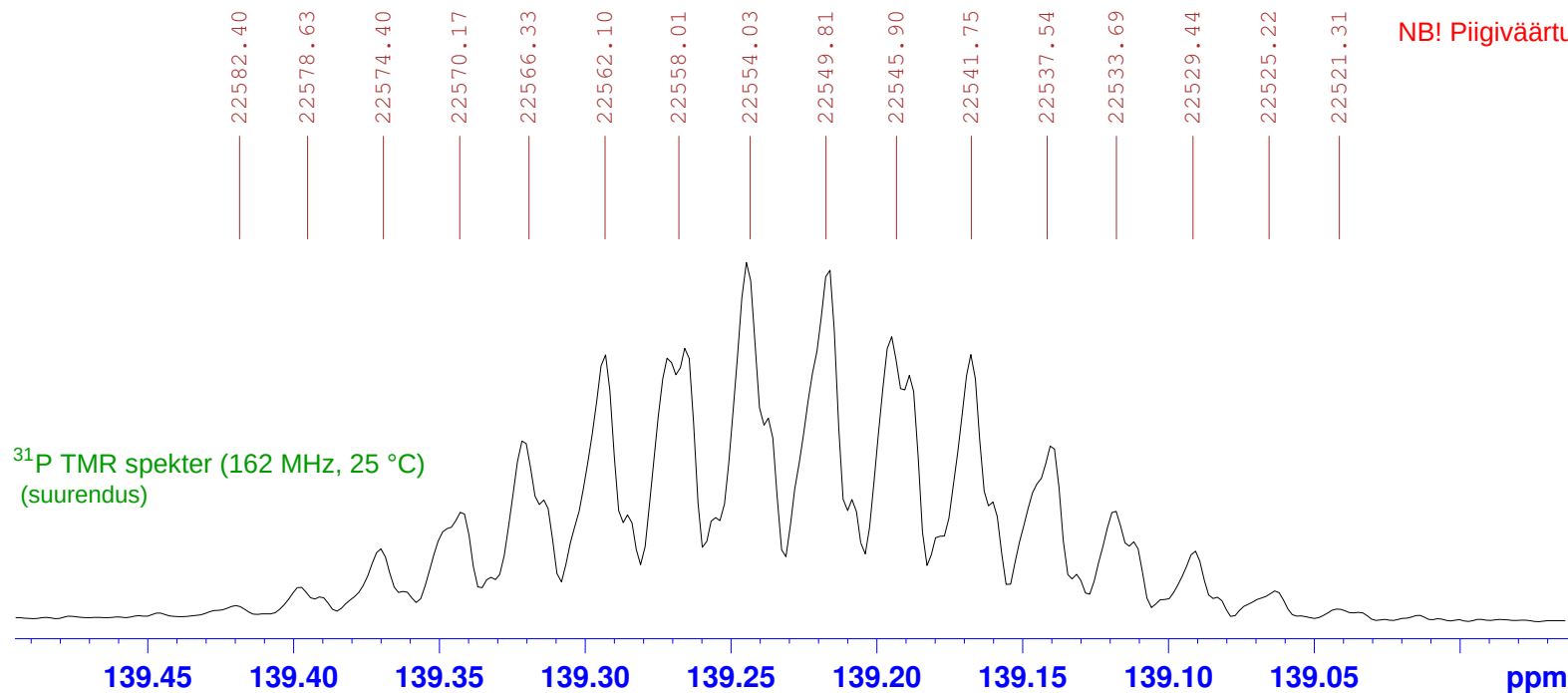
Date_ 20120321
Time 11.39
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 131072
SOLVENT CDC13
NS 64
DS 4
SWH 64102.562 Hz
FIDRES 0.489064 Hz
AQ 1.0224116 sec
RG 2890
DW 7.800 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1

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

NUC1 31P
P1 9.96 usec
PL1 0.00 dB
SFO1 161.9772128 MHz

F2 - Processing parameters

SI 131072
SF 161.9755930 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



NB! Piigiväärtused on antud hertsides!

Current Data Parameters

EXPNO 7
PROCNO 1

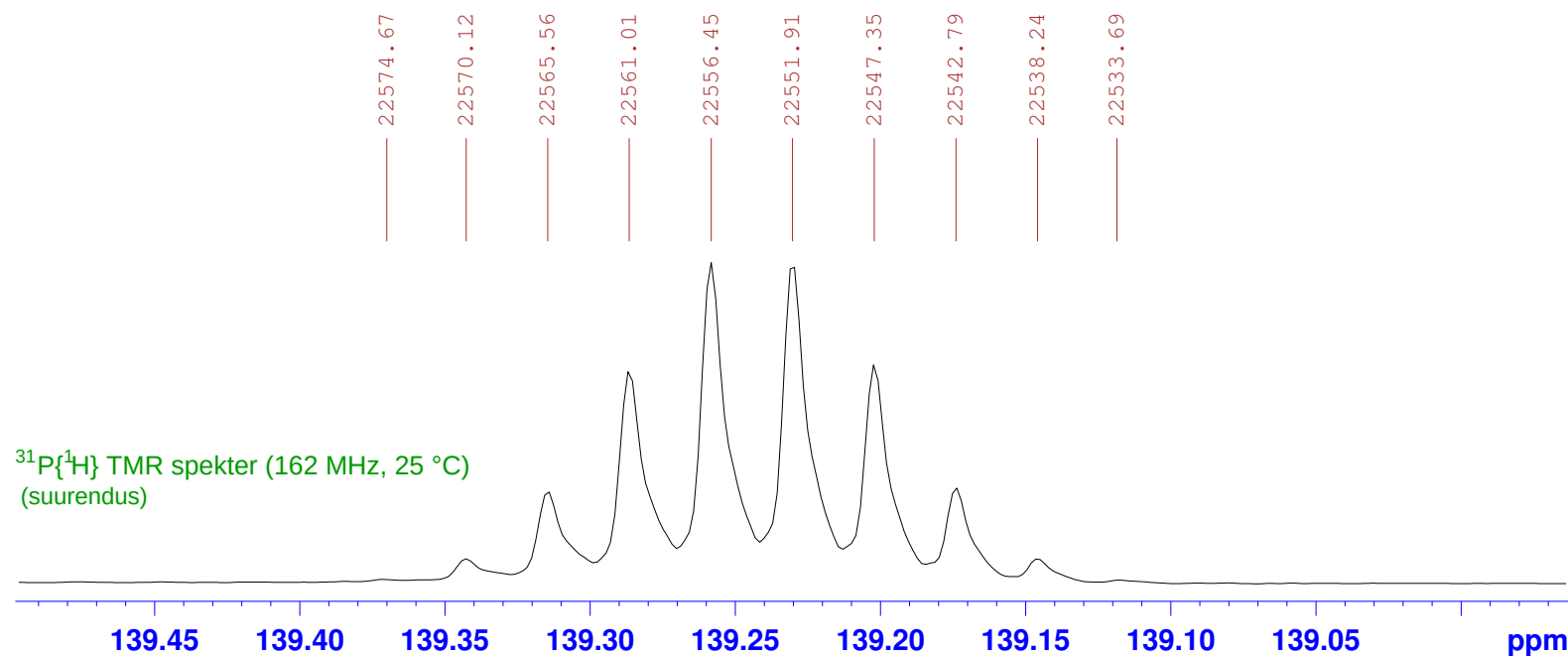
F2 - Acquisition Parameters

Date_ 20120321
Time 11.39
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 131072
SOLVENT CDC13
NS 64
DS 4
SWH 64102.562 Hz
FIDRES 0.489064 Hz
AQ 1.0224116 sec
RG 2890
DW 7.800 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 31P
P1 9.96 usec
PL1 0.00 dB
SFO1 161.9772128 MHz

F2 - Processing parameters

SI 131072
SF 161.9755930 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



NB! Piigiväärtused on antud ppm-ides!

-75.72
-75.75
-75.77
-75.79
-75.81
-75.83

Current Data Parameters

EXPNO 23
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120409
Time 15.32
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgflqn
TD 262144
SOLVENT CDCl3
NS 64
DS 4
SWH 45454.547 Hz
FIDRES 0.173395 Hz
AQ 2.8836341 sec
RG 90.5
DW 11.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

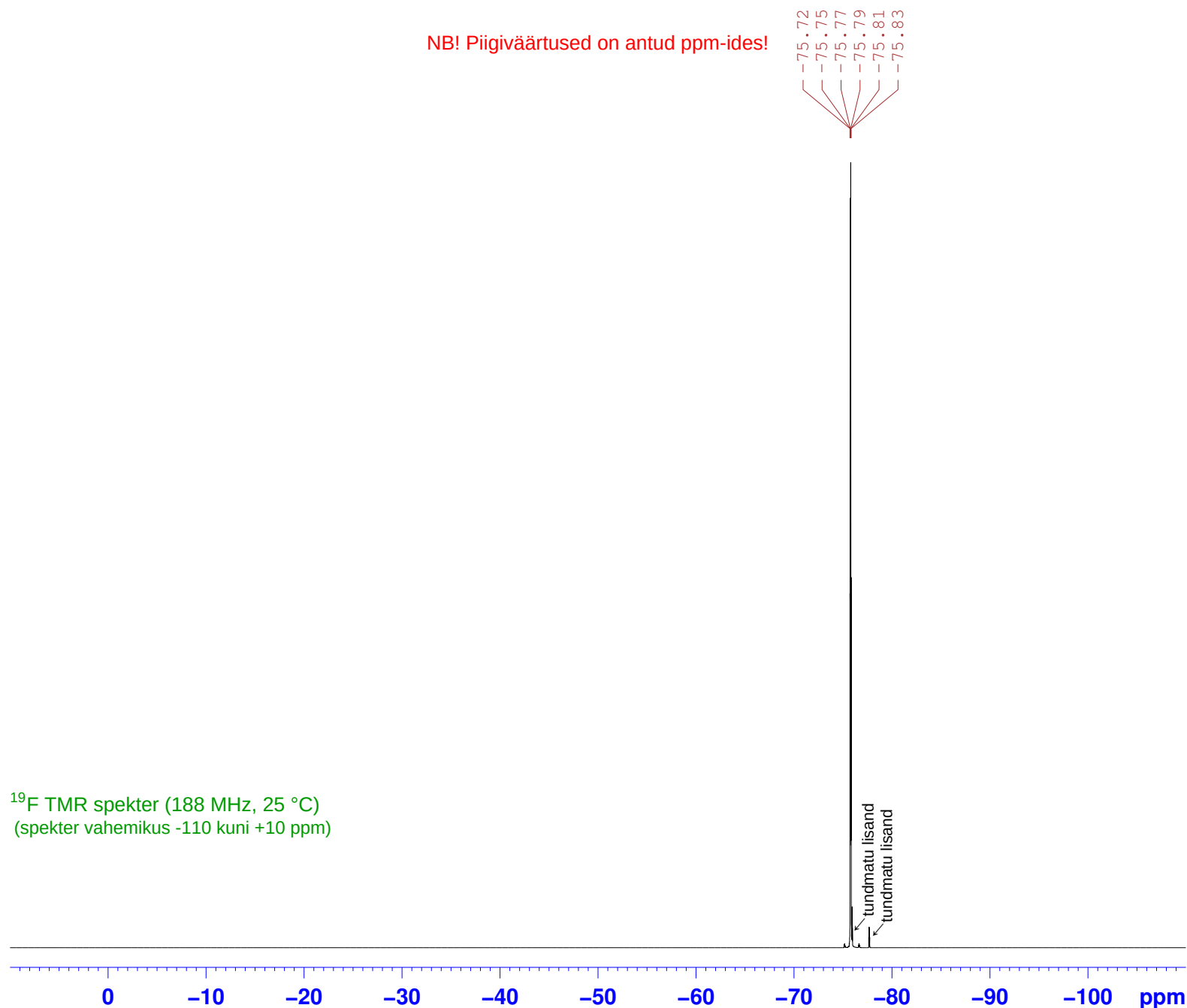
===== CHANNEL f1 =====

NUC1 19F
P1 7.00 usec
PL1 0.00 dB
PL1W 14.06656361 W
SFO1 188.2926422 MHz

F2 - Processing parameters

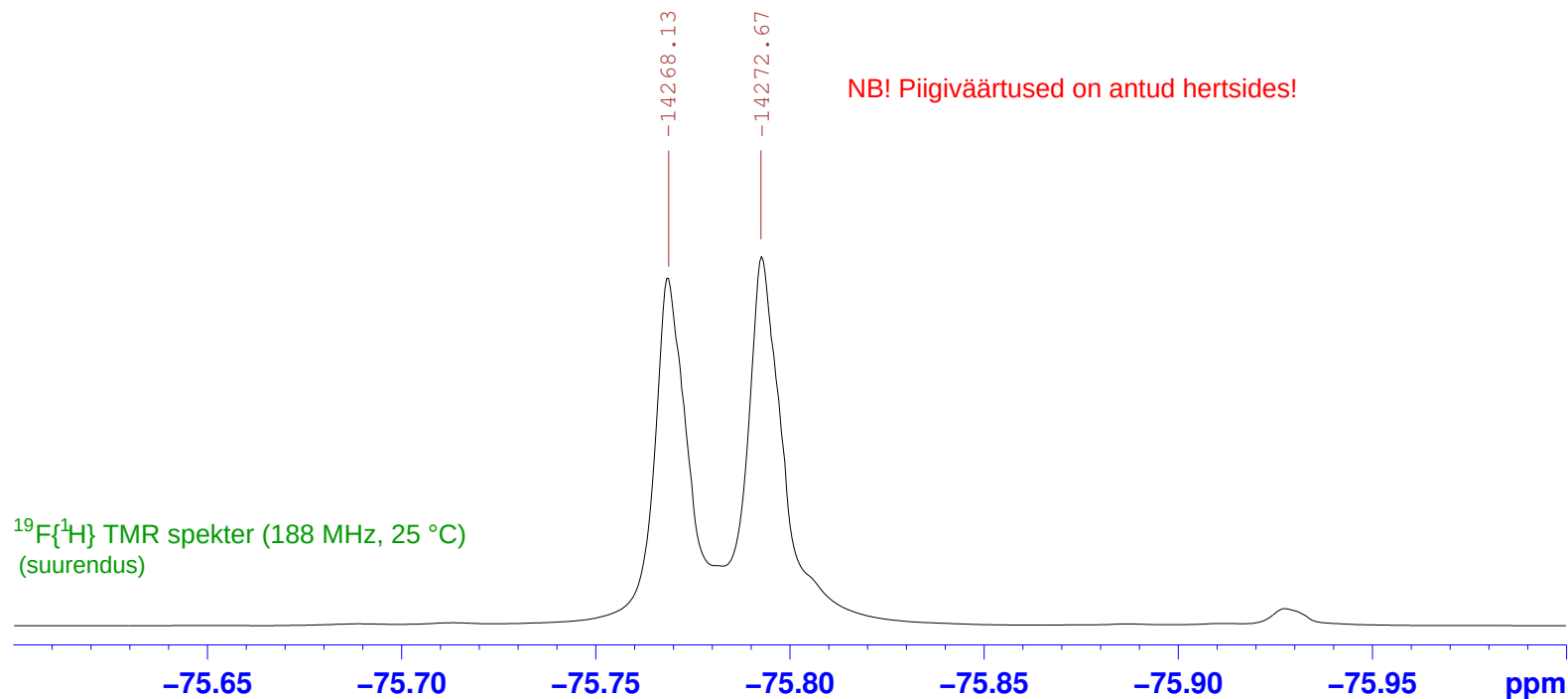
SI 131072
SF 188.3114730 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹⁹F TMR spekter (188 MHz, 25 °C)
(spekter vahemikus -110 kuni +10 ppm)

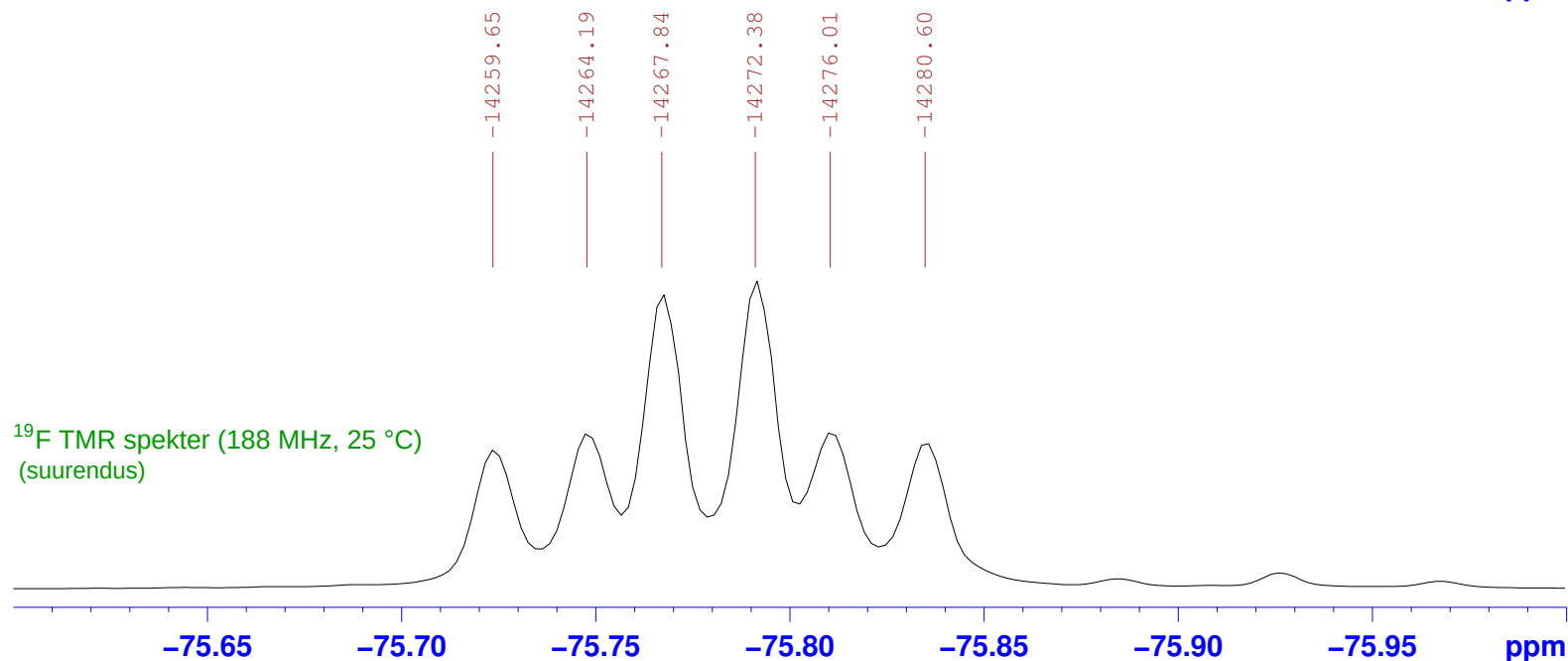


NB! Piigiväärtused on antud hertsides!

$^{19}\text{F}\{^1\text{H}\}$ TMR spekter (188 MHz, 25 °C)
(suurendus)



^{19}F TMR spekter (188 MHz, 25 °C)
(suurendus)



Current Data Parameters

EXPNO 23
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120409
Time 15.32
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgflqn
TD 262144
SOLVENT CDC13
NS 64
DS 4
SWH 45454.547 Hz
FIDRES 0.173395 Hz
AQ 2.8836341 sec
RG 90.5
DW 11.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

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

NUC1 19F
P1 7.00 usec
PL1 0.00 dB
PL1W 14.06656361 W
SFO1 188.2926422 MHz

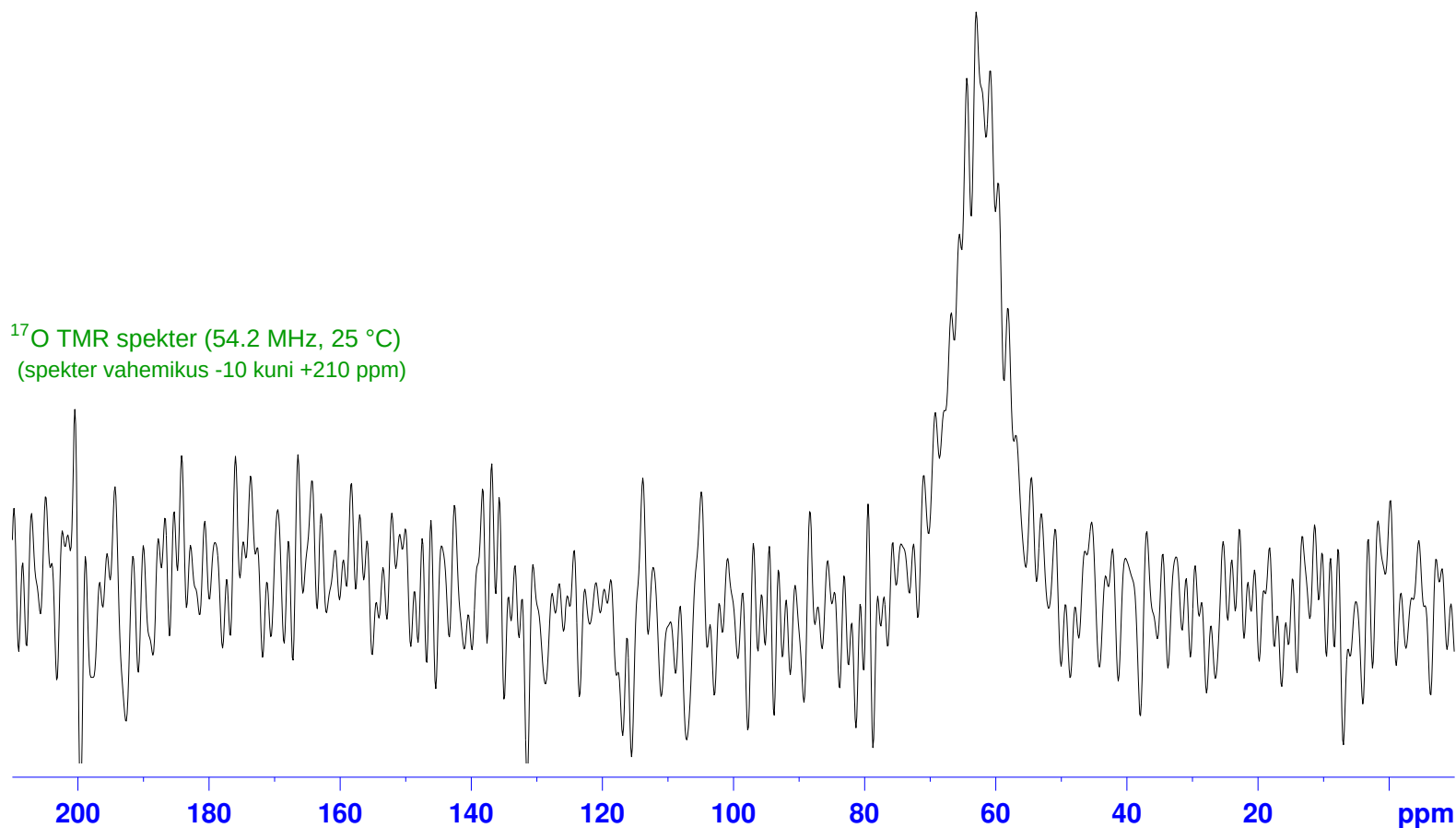
F2 - Processing parameters

SI 131072
SF 188.3114730 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NB! Piigiväärtus on antud ppm-ides!

62.97

¹⁷O TMR spekter (54.2 MHz, 25 °C)
(spekter vahemikus -10 kuni +210 ppm)



Current Data Parameters

EXPNO 11
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120321
Time 12.03
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 1024
SOLVENT CDC13
NS 49152
DS 32
SWH 27173.912 Hz
FIDRES 26.537024 Hz
AQ 0.0188916 sec
RG 16400
DW 18.400 usec
DE 6.00 usec
TE 298.2 K
D1 0.00200000 sec
TD0 1

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

NUC1 17O
P1 13.70 usec
PL1 0.00 dB
SFO1 54.2543001 MHz

F2 - Processing parameters

SI 4096
SF 54.2434510 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40