

7 Přílohy

7.1.1 NMR spektra sloučeniny **NPE25-F-51B**

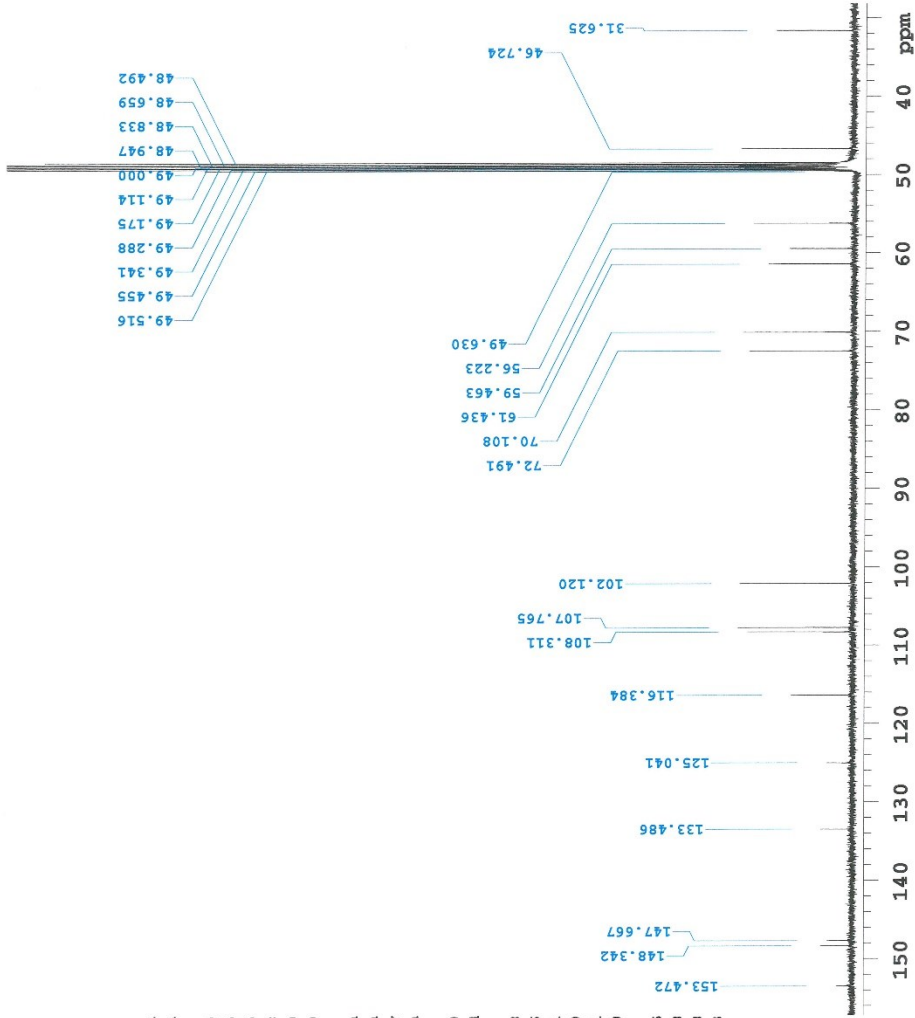
¹³C NMR

NPE25-F-51B

exp31 CARBON

```

SAMPLE PRESTURATION
date Dec 7 2016 satmode n
solvent cd3od wet n
file /home/vmxi/v~ SPECIAL
nmrSYS/data/lucie/~ temp 24.0
Narcissus/NPE-25-F~ gain 30
-51B/Methanol/NPE2~ spin 20
5-F-51B_C.fid hst 0.008
ACQUISITION pw90 11.300
sw 31250.0 alfa 10.000
at 1.049
np 65536 il n
fb 17000 in n
bs 1 dp y
dl 1.000 hs mn
nt 7000 PROCESSING
ct 7000 lb 0.50
TRANSMITTER fn not used
tn C13 DISPLAY
sfrq 125.705 sp 3545.8
tof 1913.9 wp 16209.6
tpwr 55 rfl 7779.1
pw 5.650 xfp 6158.9
DECOUPLER xp 46.1
dn H1 lp 0
dof 0 PLOT
dm YXY wc 175
decwave w sc 8
dpwr 41 vs 798
dmf 12346 th nm cdc ph
    
```

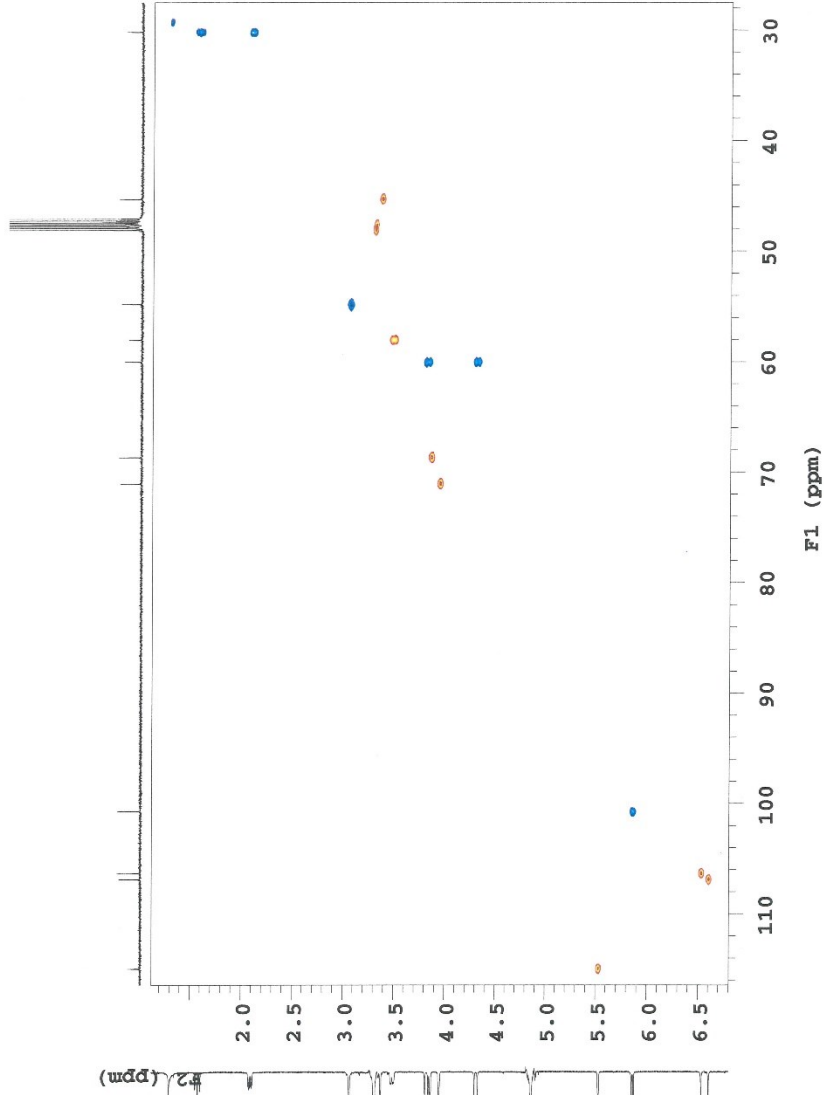


NPE25-F-51B

Sample Name:
OneNMR_W018_calib
Data Collected on:
vnmrs500.faf.cuni.cz-vnmrs500
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
OneNMR_W018_calib_20161101_01
FidFile: NPE25-F-51B_Het

Pulse Sequence: gHSQC
Solvent: cd3od
Data collected on: Dec 7 2016
Temp. 24.0 C / 297.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Acq. time 0.150 sec
Width 3125.0 Hz
2D Width 21367.5 Hz
8 repetitions
2 x 512 increments
OBSERVE H1, 499.8651827 MHz
DECOUPLE C13, 125.7006270 MHz
Power 37 dB
on during acquisition
off during delay
W40_OneNMR_W018 modulated
DATA PROCESSING
Gauss apodization 0.069 sec
F1 DATA PROCESSING
Gauss apodization 0.011 sec
Ft size 1024 x 4096
Total time 2 hr, 44 min

Agilent Technologies



gHSQC

NPE25-F-51B

Sample Name:
OneNMR_W018_calib
Data Collected on:
vmrs500.faf.cuni.cz-vmrs500
Archive directory:
/home/vmnr1/vmrs500/data
Sample directory:
OneNMR_W018_calib_20161101_01
FidFile: NPE25-F-51B_LR

Pulse Sequence: gHMBCAD
Solvent: cd3od
Data collected on: Dec 7 2016

Temp. 24.0 C / 297.1 K
Operator: vmnr1

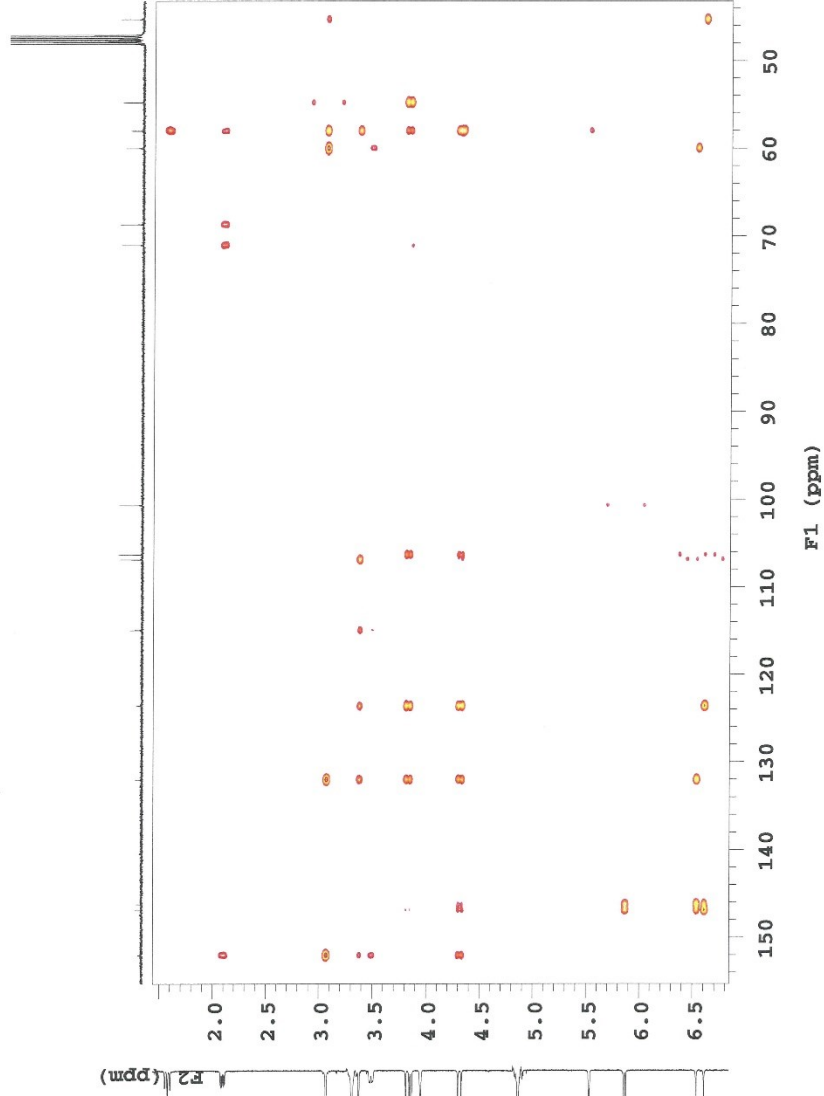
Relax. delay 1.000 sec
Acq. time 0.150 sec
Width 3125.0 Hz
2D Width 30165.9 Hz
16 repetitions

2 x 512 increments
OBSERVE H1, 499.8651827 MHz
DATA PROCESSING

Sq. sine bell 0.075 sec
F1 DATA PROCESSING
Gauss apodization 0.007-sec
FT size 1024 x 4096
Total time 5 hr, 39 min



gHMBC

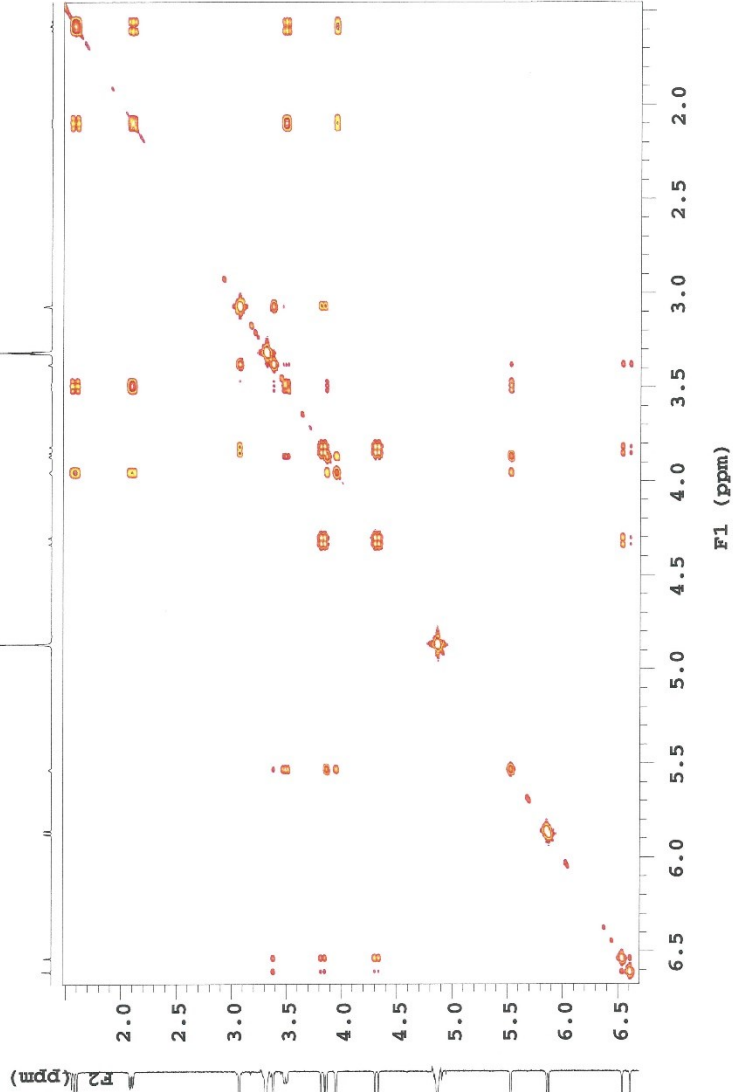


NPE25-F-51B



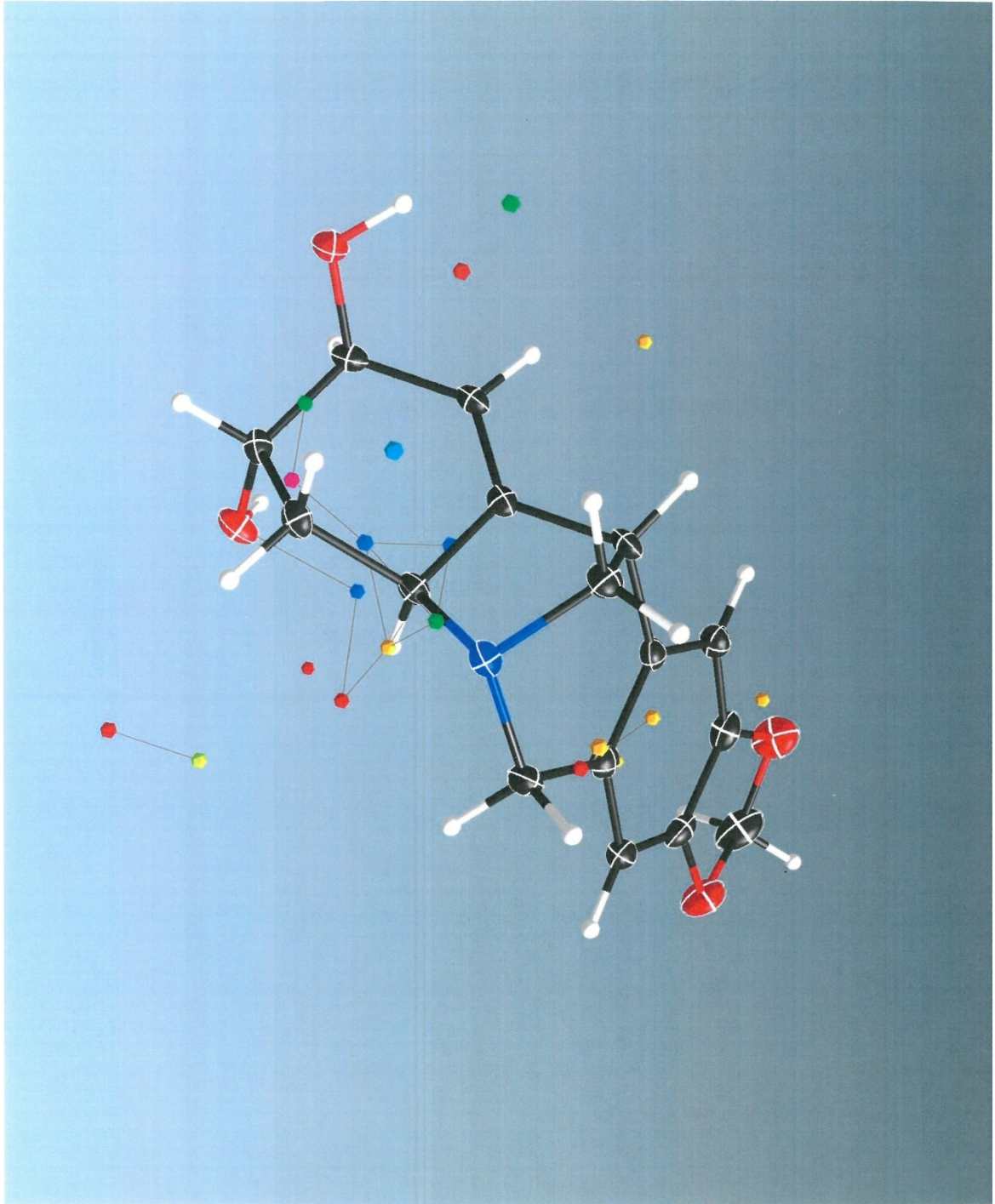
Sample Name:
OneNMR_W018_calib
Data Collected on:
vnmrs500.faf.cuni.cz-vnmrs500
Archive directory:
/home/vnmr1/vnmr5ys/data
Sample directory:
OneNMR_W018_calib_20161101_01
Fidfile: NPE25-F-51B_Cosy

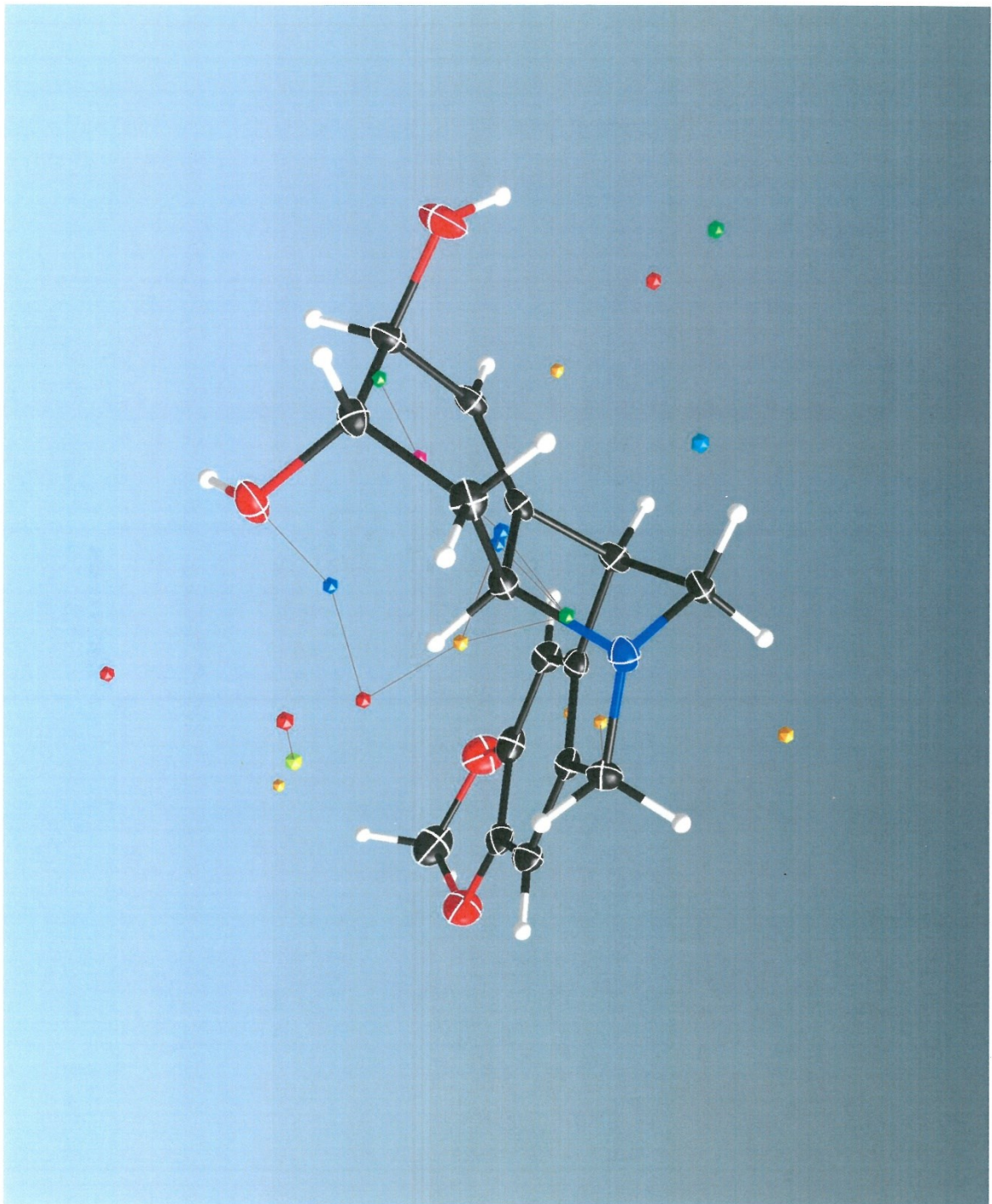
Pulse Sequence: gCOSY
Solvent: cd3od
Data collected on: Dec 7 2016
Temp. 24.0 C / 297.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Acq. time 0.150 sec
Width 3125.0 Hz
2D Width 3125.0 Hz
4 repetitions
512 increments
OBSERVE H1, 499.8651827 MHz
DATA PROCESSING
Sq. sine bell 0.075 sec
F1 DATA PROCESSING
Sq. sine bell 0.083 sec
Ft size 4096 x 4096
Total time 43 min



gCOSY

7.1.2 Strukturní rentgenová analýza sloučeniny **NPE25-F-51B**





7.2 NMR spektra sloučeniny **PR-75-97-2**

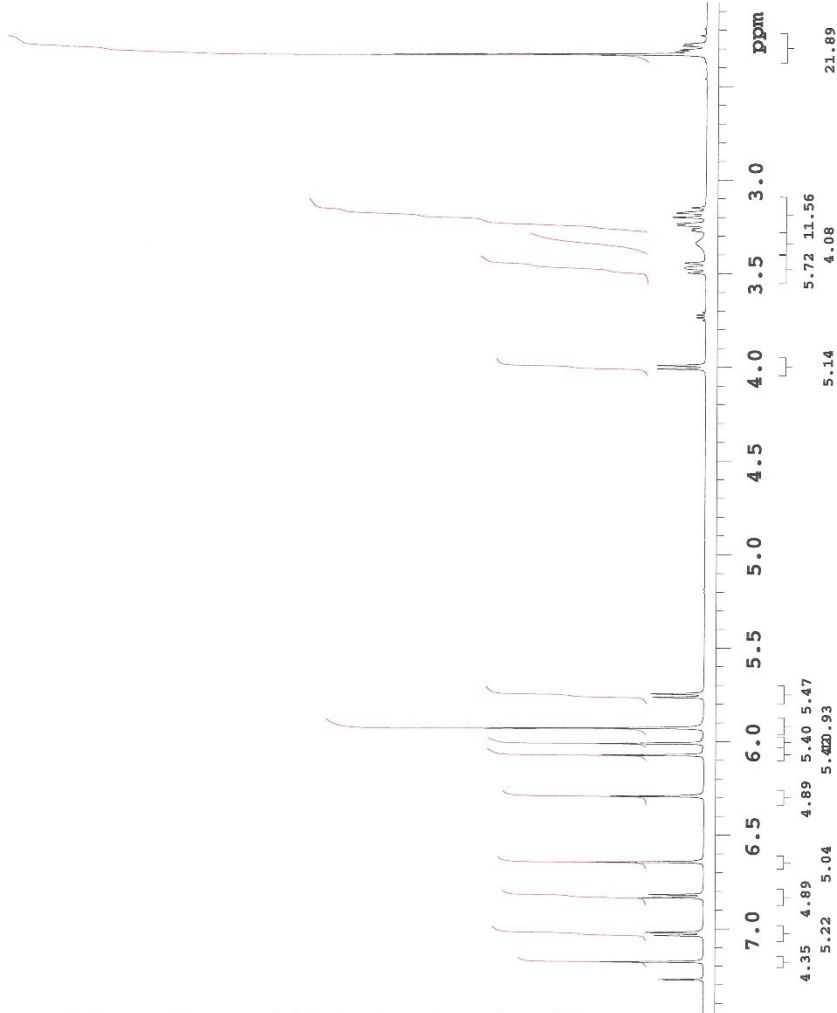
¹H NMR

PR-75-97-2

exp30 PROTON

```

SAMPLE PRESATURATION
date Apr 12 2016 satmode n
solvent cdcl3 wet n
file /home/vmnr1/v- SPECIAL
nmrSYS/data/Zalchy- temp 25.0
/2017/Lucie/Papave- gain 30
I_Rhoenag/PR-75-97- spin not used
2/PR-75-97-2_Hss.f- hst 0.008
id pw90 9.100
ACQUISITION alfa 10.000
sv 3289.5 FLAGS
at 2.490 il n
np 16384 in n
fb 4000 dp Y
bs 32 hs nn
di 1.000 PROCESSING
nt 8 fn not used
ct 8 DISPLAY
TRANSMITTER sp 1025.7
tn H1 wp 2702.4
sfrq 499.865 xfl -484.4
tof -370.2 xfp 0
tpwr 60 xp 114.1
pw 4.550 lp 0
DECOUPLER PLOT
dn C13 wc 175
dof 0 sc 8
dm nnn vs 142
decurve W40_OneNMR- th 7
dpwr _W018 ai cdc ph
dmf 37
32258
    
```



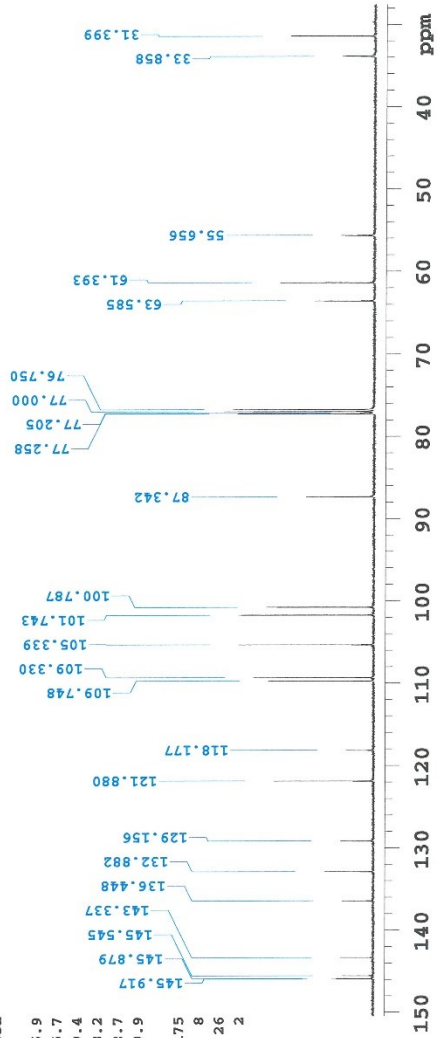
¹³C NMR

PR-75-97-2

exp31 CARBON

```

SAMPLE PRESATURATION
date Apr 12 2016 satmode n
solvent cdcl3 wet n
file /home/vmrl/V- SPECIAL
nmrSYS/data/Zalchy- temp 25.0
/2017/Lucie/Papave- gain 30
r_Rhoas/PR-75-97-2 not used
2/PR-75-97-2_C.Fid hst 0.008
ACQUISITION pw90 11.300
sw 31250.0 alfa 10.000
at 1.049 FLAGS
np 6536 il n
fb 17000 in n
bs 1 dp y
dl 1.000 hs nn
nt 5000 PROCESSING
ct 5000 lb 0.50
TRANSMITTER fn not used
DISPLAY
tn C13
sfrc 125.705 sp 3466.9
tof 1913.9 wp 15445.7
tpwr 55 rfl 11479.4
pw 5.650 xfp 9678.2
DECOUPLER xp -182.7
dn H1 lp 9.9
dof 0 PLOT
dm YYY wc 175
decwave w sc 8
dppwr 41 vs 26
dmf 12346 th nm cdc ph
    
```



PR-75-97-2

Sample Name:

Data Collected on:
vnmrs500-vnmrs500
Archive directory:

Sample directory:

File: PR-75-97-2_1et

Pulse Sequence: gHSQC

Solvent: cdcl3

Data collected on: Apr 12 2016

Temp. 25.0 C / 298.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Acq. time 0.150 sec
Width 3289.5 Hz
2D Width 21367.5 Hz
8 repetitions
2 x 512 increments

OBSERVE H1, 499.8632133 MHz
DECOUPLE C13, 125.7001318 MHz

Power 37 dB

on during acquisition

off during delay

W40_OneNMR_W018 modulated

DATA PROCESSING

Gauss apodization 0.069 sec

F1 DATA PROCESSING

Resol. enhancement 0.0 Hz

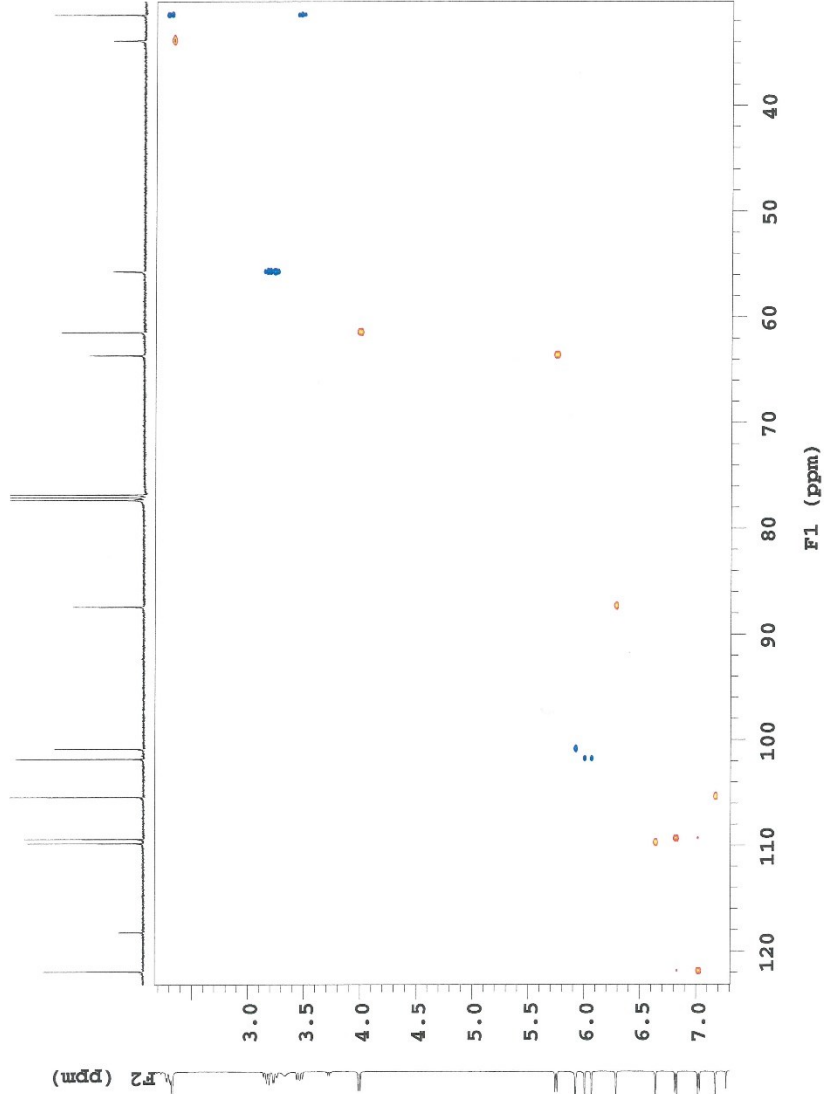
Gauss apodization 0.012 sec

FT size 4096 x 4096

Total time 2 hr, 44 min



gHSQC



PR-75-97-2

Sample Name:

Data Collected on:
vnmrs500-vnmrs500
Archive directory:

Sample directory:

F1File: PR-75-97-2_IR

Pulse Sequence: gHMBCAD

Solvent: cdcl3

Data collected on: Apr 12 2016

Temp. 25.0 C / 298.1 K

Operator: vnmr1

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 3289.5 Hz

2D Width 30165.9 Hz

16 repetitions

2 x 512 increments

OBSERVE HL, 499.8632133 MHz

DATA PROCESSING

Sq. sine bell 0.075 sec

F1 DATA PROCESSING

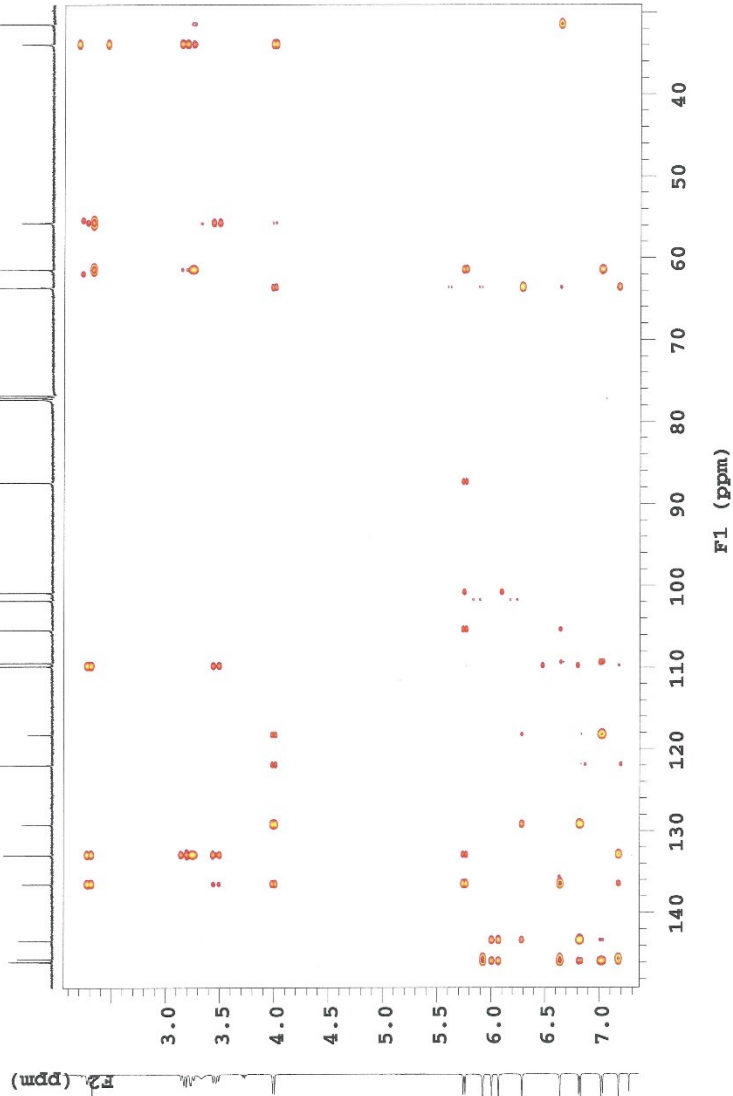
Gauss apodization 0.008 sec

Ft size 4096 x 4096

Total time 5 hr, 39 min



gHMBC



PR-75-97-2

Sample Name:

Data Collected on:
vnmrs500--vnmrs500
Archive directory:

Sample directory:

F1: PR-75-97-2_Cosy

Pulse Sequence: gCOSY

Solvent: cdc13

Data collected on: Apr 12 2016

Temp. 25.0 C / 298.1 K

Operator: vnmr1

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 3289.5 Hz

2D Width 3289.5 Hz

4 repetitions

512 increments

OBSERVE H1, 499.8632133 MHz

DATA PROCESSING

Sq. sine bell 0.075 sec

F1 DATA PROCESSING

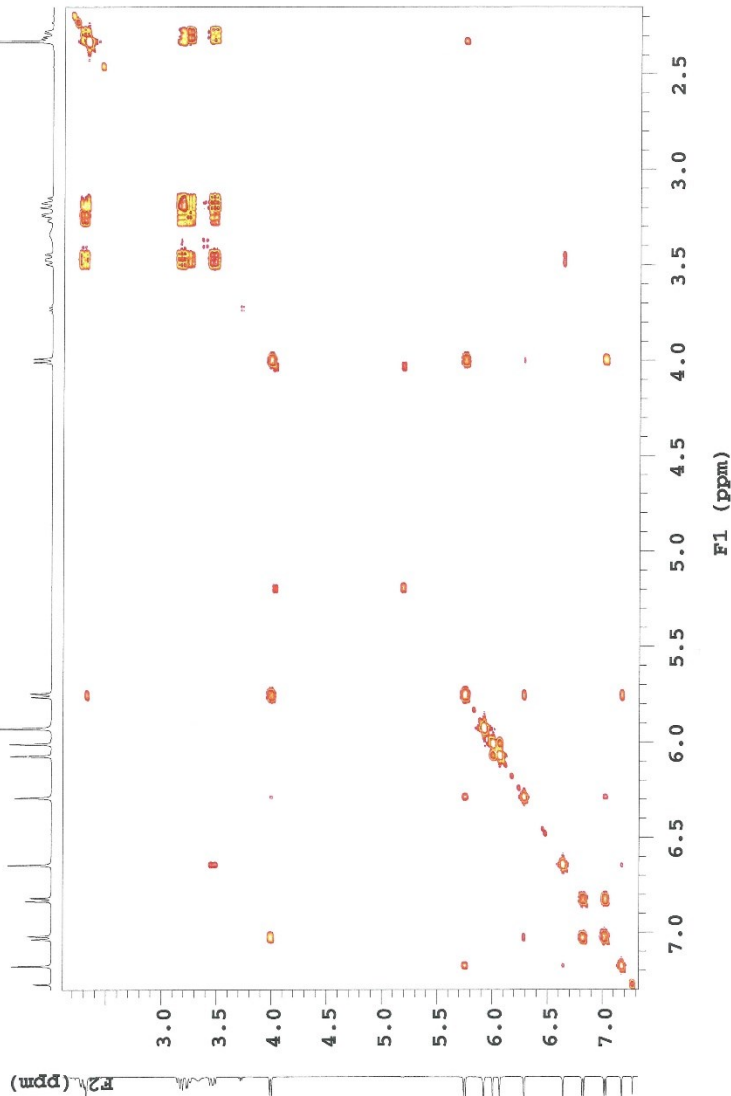
Sq. sine bell 0.077 sec

Ft size 4096 x 4096

Total time 43 min



gCOSY



7.3 NMR spektra sloučeniny **PR-Et2O-9-5-2**

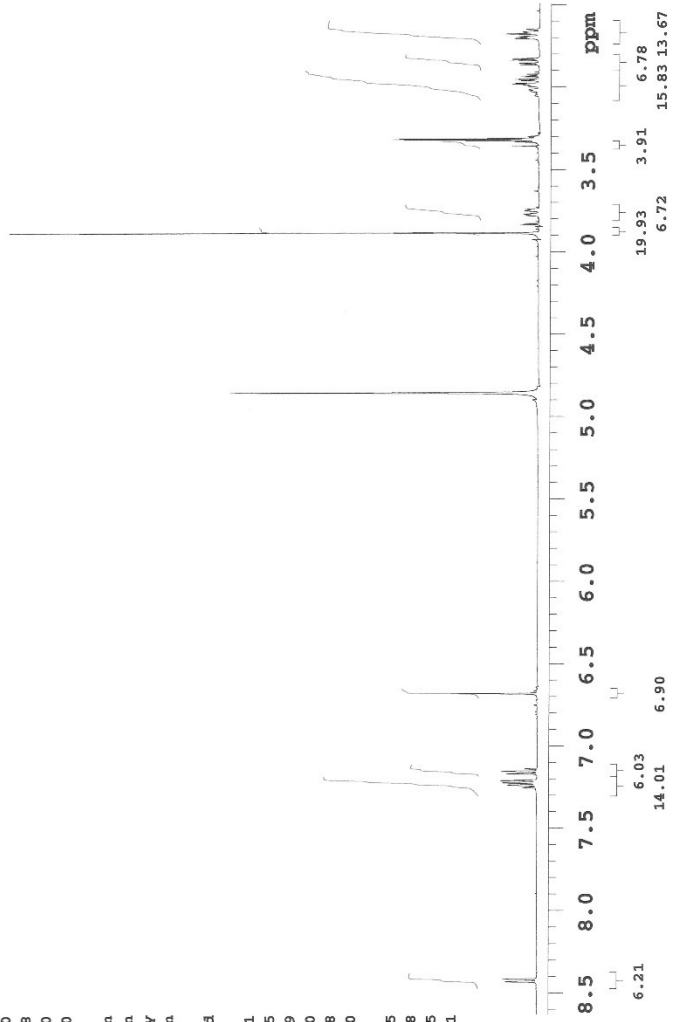
¹H NMR

PR-Et20-9-5-2

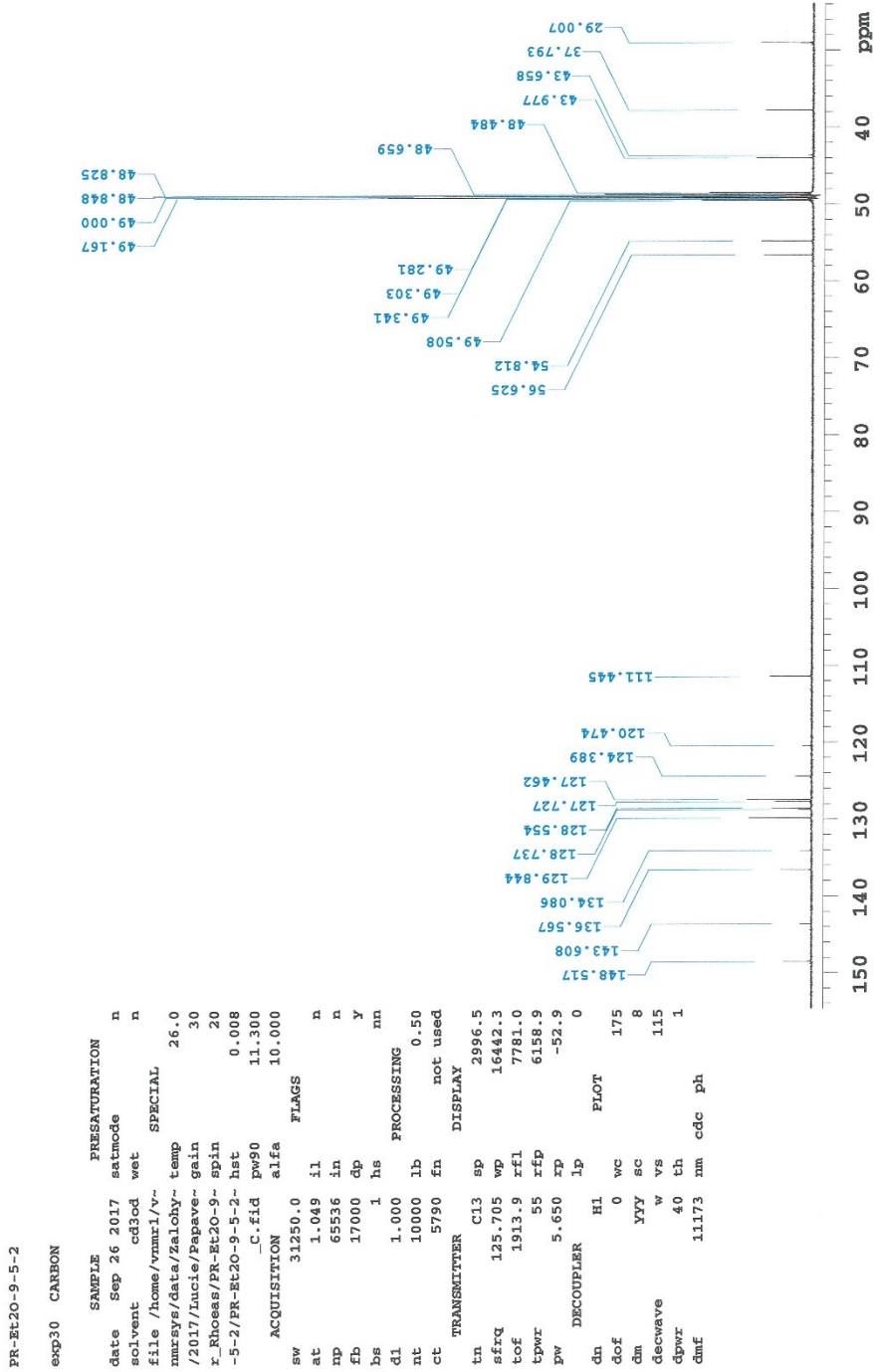
exp30 PROTON

```

SAMPLE          PRESATURATION
date   Sep 26 2017   satmode   n
solvent  cd3cd      wet       n
file  /home/vmmx1/v- SPECIAL
nmrSYS/data/Zalchyl- temp    26.0
/2017/Lucile/Papave- gain    38
x_Rhodes/PR-Et20-9- spIn    20
-5-2/PR-Et20-9-5-2- hst     0.008
_hss.fid pw90     9.100
ACQUISITION    alfa    10.000
sw    3811.0
at    2.150 il      n
np    16384 in     n
fb    4000 dp      Y
bs    32   hs     m
dl    1.000 PROCESSING
nt    8   fn     not used
ct    8   DISPLAY
TRANSMITTER    sp    1245.1
tn    H1 wp      3068.5
sfrq  499.868 rfl   -518.9
tof   -75.0 rfp    0
tpwr  60   tp     57.8
pw    4.550 lp     0
DECOUPLER      C13 wc    175
dn    0   sc     8
dof   0   vs     45
dm    mmn vs     45
decwave W40_OneNMR- th    11
_dpwr  _W018 ai   cdc ph
dmf    37
      32258
  
```



¹³C NMR



PR-ET20-9-5-2

Sample Name:

Data Collected on:
vnmrs500.faf.cuni.cz-vnmrs500
Archive directory:

Sample directory:

FidFile: PR-ET20-9-5-2_Het

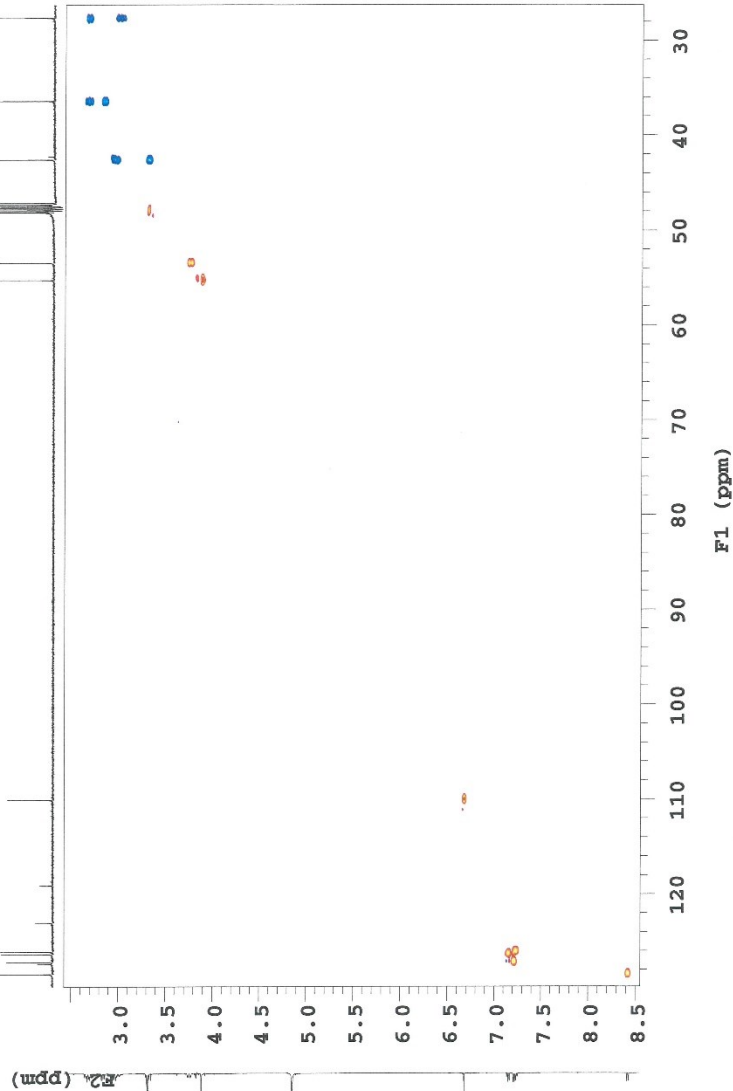
Pulse Sequence: gHSQCAD
Solvent: cd3od
Data collected on: Sep 26 2017

Temp. 26.0 C / 299.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Acq. time 0.450 sec
Width 3811.0 Hz
2D Width 25141.4 Hz
8 repetitions
2 x 512 increments
OBSERVE H1, 499.8651827 MHz
DECOUPLE C13, 125.7025124 MHz
Power 37 dB
on during acquisition
off during delay
W40_OneNMR_W018 modulated
DATA PROCESSING
Gauss apodization 0.069 sec
F1 DATA PROCESSING
Gauss apodization 0.009 sec
FT size 2048 x 4096
Total time 2 hr, 44 min



gHSQC



PR-Et20-9-5-2

Sample Name:

Data Collected on:
vnmrs500.faf.cuni.cz-vnmrs500
Archive directory:

Sample directory:

F1dFile: PR-Et20-9-5-2_LR

Pulse Sequence: gHMBCAD
Solvent: cd3od
Data collected on: Sep 26 2017

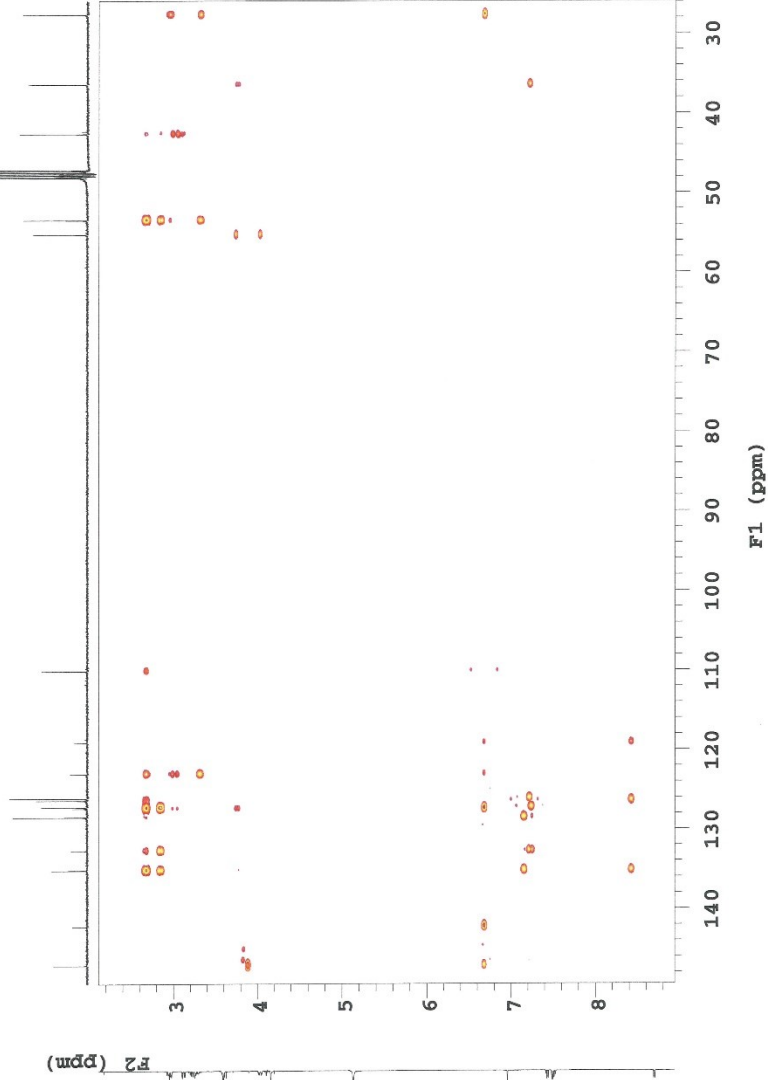
Temp. 26.0 C / 289.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Acq. time 0.150 sec
Width 8012.8 Hz
2D Width 30165.9 Hz
16 repetitions
2 x 512 increments

OBSERVE H1, 499.8651827 MHz
DATA PROCESSING
Sq. sine bell 0.075 sec
F1 DATA PROCESSING
Gauss apodization 0.007 sec
F1 size 4096 x 4096
Total time 5 hr, 39 min



gHMBC



PR-Et20-9-5-2

Sample Name:

Data Collected on:
vnmrs500.fsf.cuni.cz-vnmrs500
Archive directory:

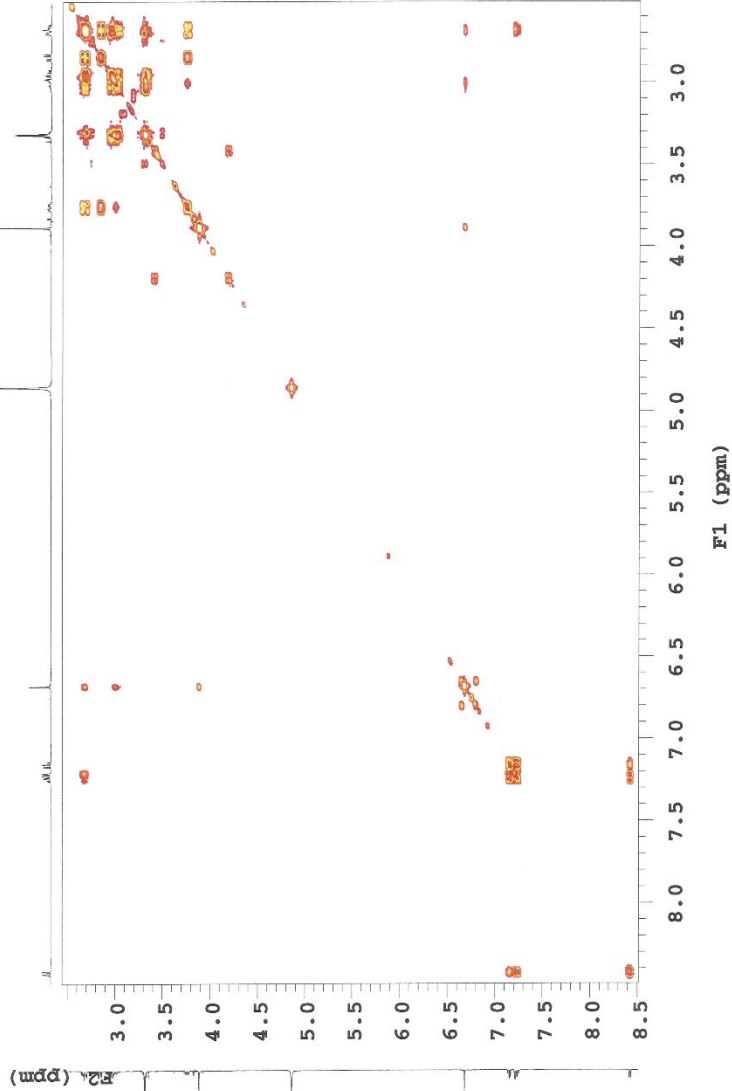
Sample directory:

File: PR-Et20-9-5-2_Cosy

Pulse Sequence: gCOSY
Solvent: cd3od
Data collected on: Sep 26 2017

Temp. 26.0 C / 299.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Acq. time 0.150 sec
Width 3811.0 Hz
2D Width 3811.0 Hz
4 repetitions
512 increments
OBSERVE F1, 499.8651827 MHz
DATA PROCESSING
Sq. sine bell 0.075 sec
F1 DATA PROCESSING
Sq. sine bell 0.068 sec
F1 size 4096 x 4096
Total time 43 min



gCOSY