

Supporting Information

Synthesis of Optically Pure (S)-2-Amino-5-arylpent-4-ynoic acids by Sonogashira Reactions and their Potential Use as Highly Selective Potent Inhibitors of Aldose Reductase

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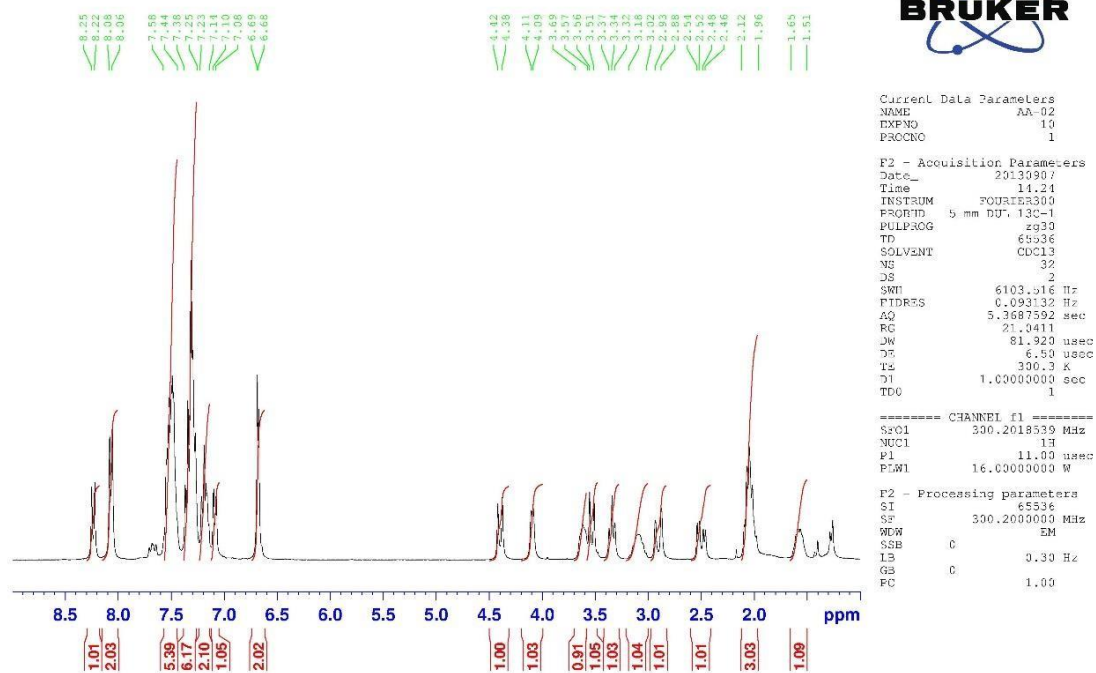
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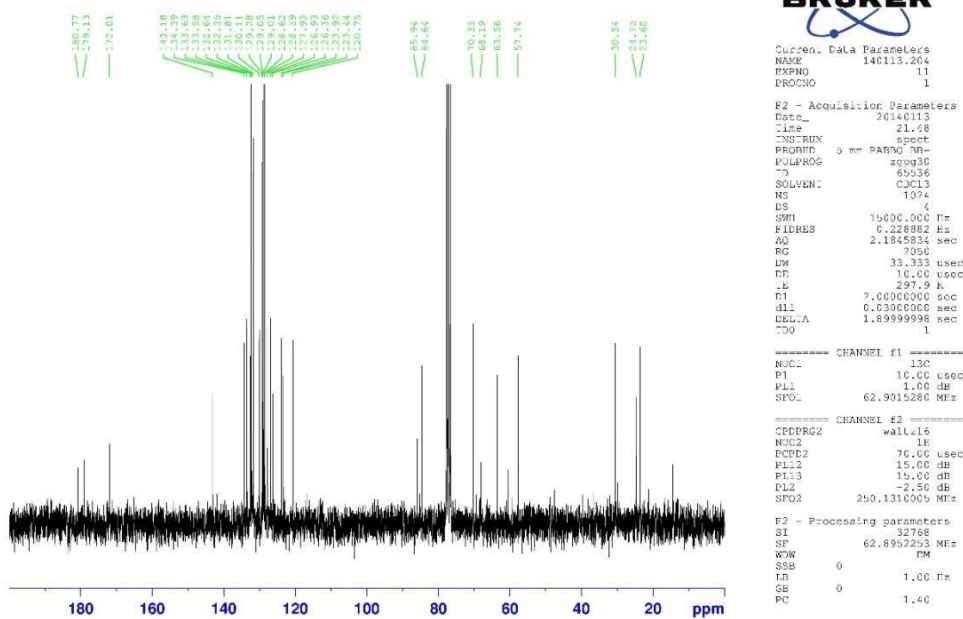
1 NMR spectras

1.1 (S)-2-Amino-5-[phenyl]pent-4-insäure-Ni-(S)-BPBP (2a):

Petrosyan, AA-02, CDCl₃

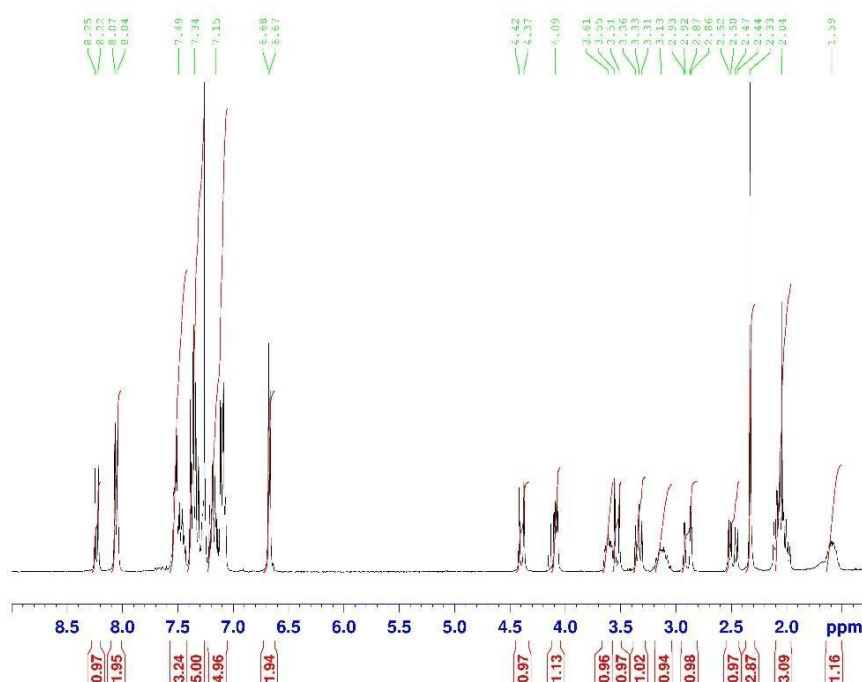


Pargapart Sp111 13C CDCl₃



1.2 (S)-2-Amino-5-[4-tolyl]pent-4-insäure-Ni-(S)-BPBP (2b):

Parpart ISP118.2 1H CDCl3



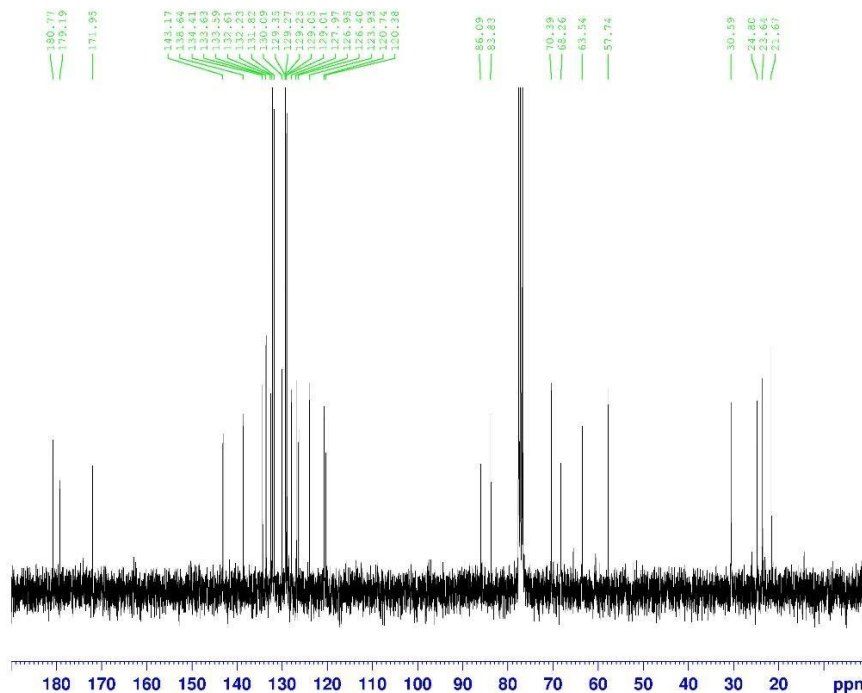
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PROCNO 1

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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094473 Hz
AQ 5.2933567 sec
RG 144
DM 80.800 usec
DE 15.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

CHANNEL F1 1H
NUC1 1H
P1 12.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1302105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Parpart ISP118.2 13C CDCl3



Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140123
Time 18.39
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 7050
DM 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 3.0000000 sec
D11 0.0300000 sec
TD0 1

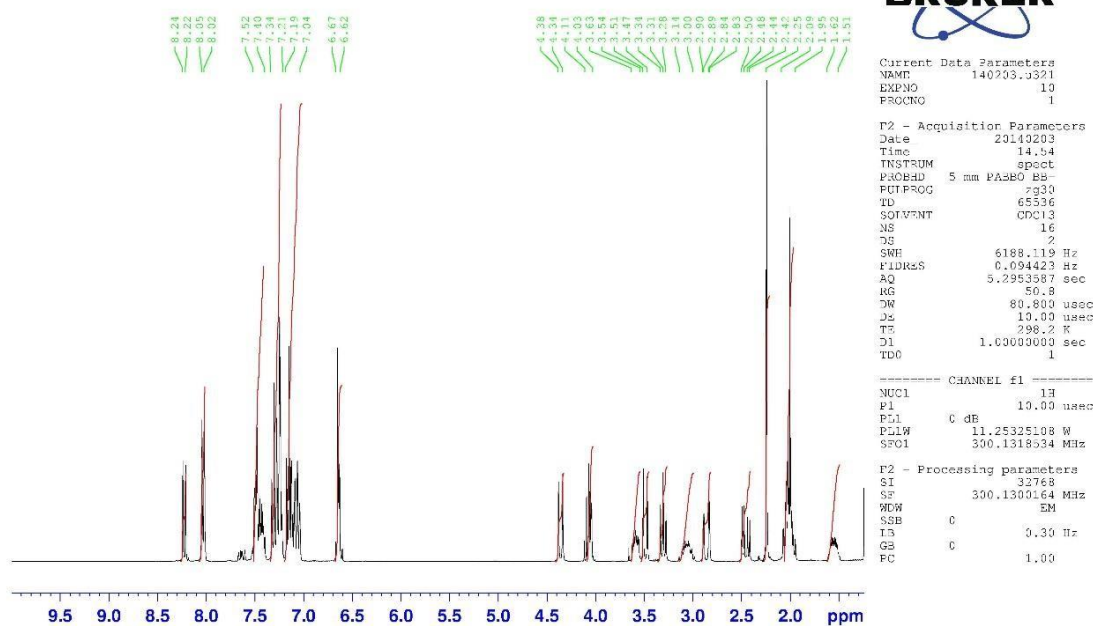
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NUC1 13C
P 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

CHANNEL F2 1H
CPDPRG2 waltz16
NUC2 1H
P2 12.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL1W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

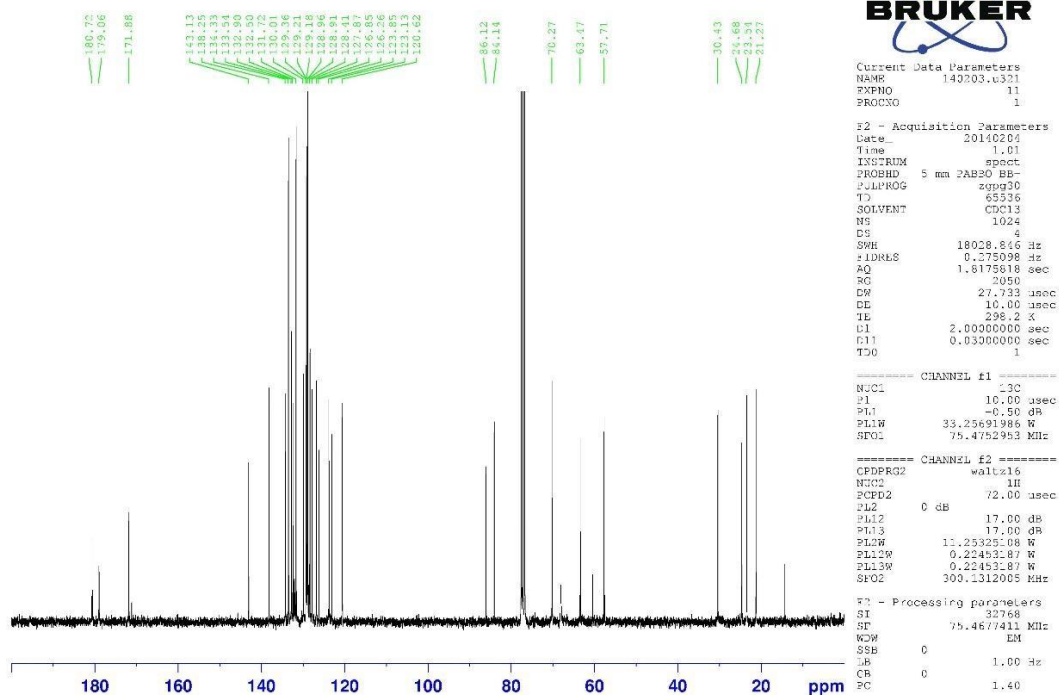
F2 - Processing parameters
SI 32768
SF 75.4677342 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1.3 (S)-2-Amino-5-[3-tolyl]pent-4-insäure-Ni-(S)-BPBP (2c):

Parpart SP123.1 1H CDC13

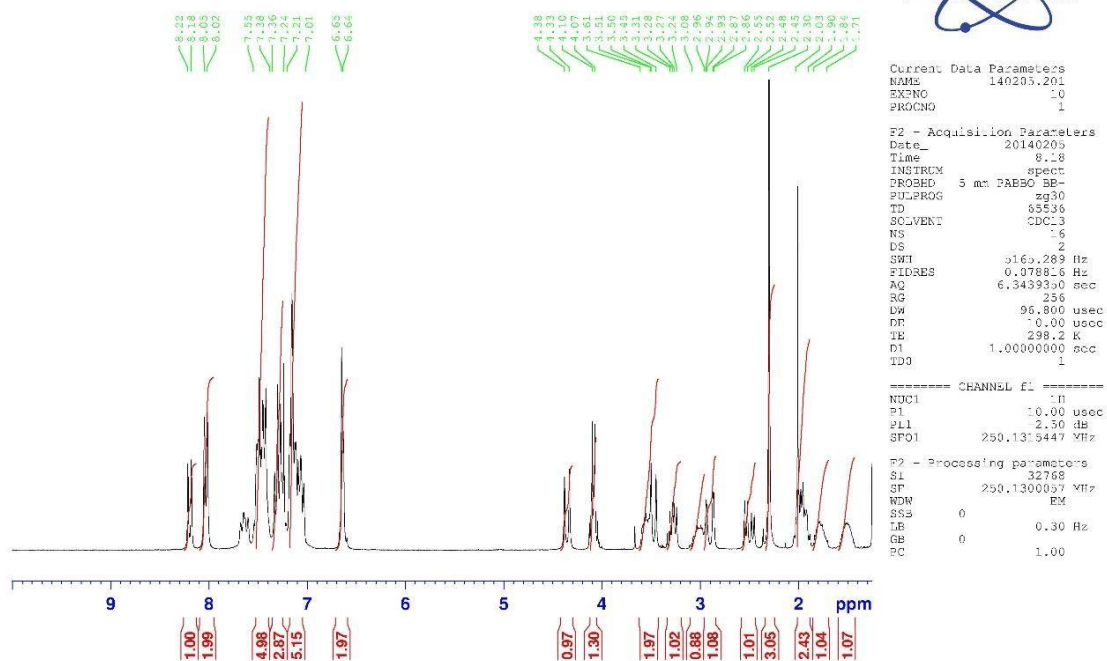


Parpart SP123.1 13C CDC13

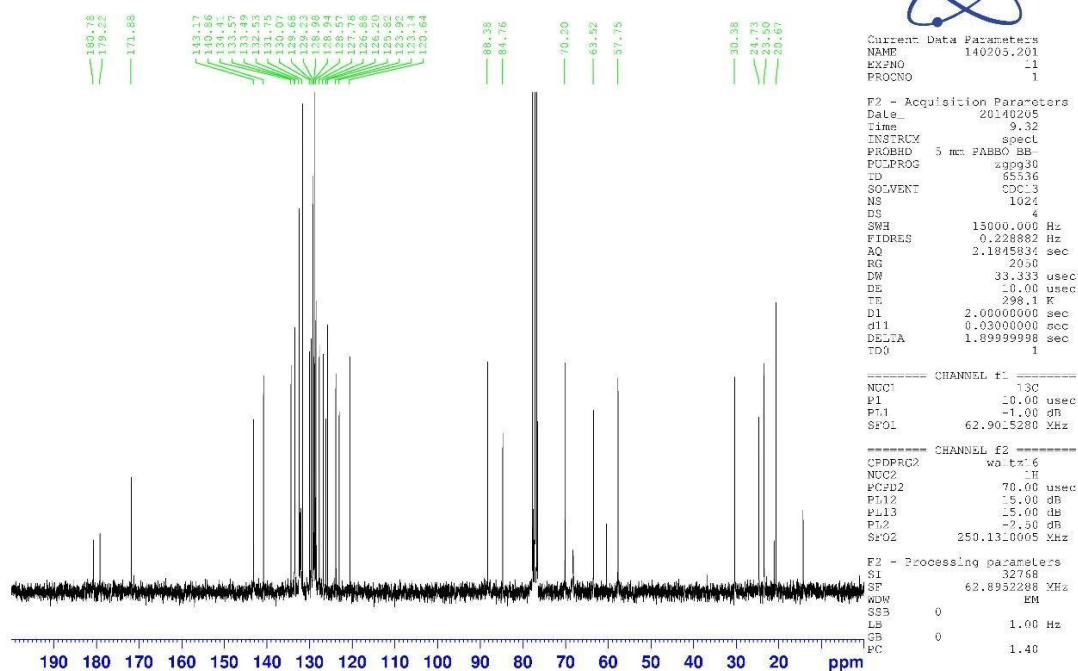


1.4 (S)-2-Amino-5-[2-tolyl]pent-4-insäure-Ni-(S)-BPBP (2d):

Parpart SP124 1H CDCl3

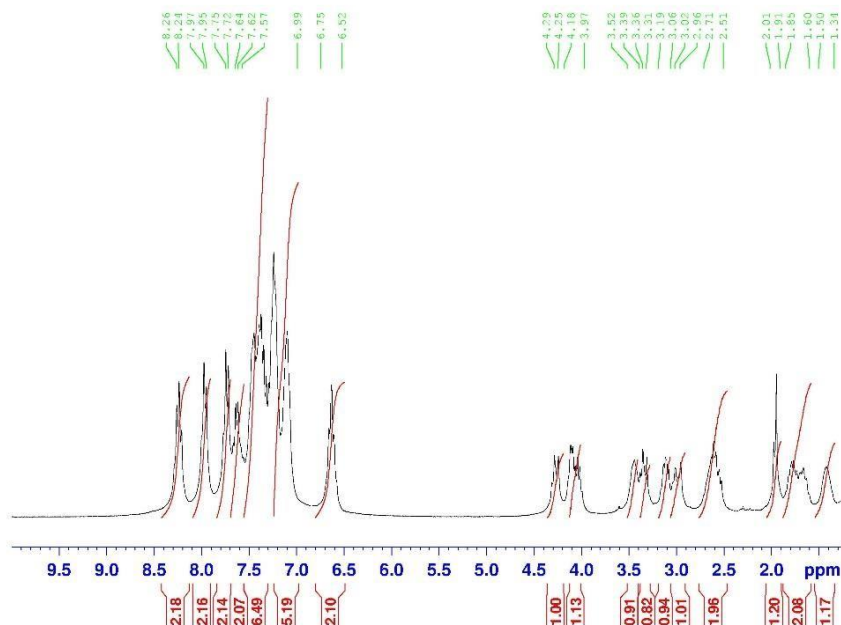


Parpart SP124 13C CDCl3



1.5 (S)-2-Amino-5-[naphth-1-yl]pent-4-ensäure-Ni-(S)-BPBP (2e):

Parpart SP 125 1H CDC13



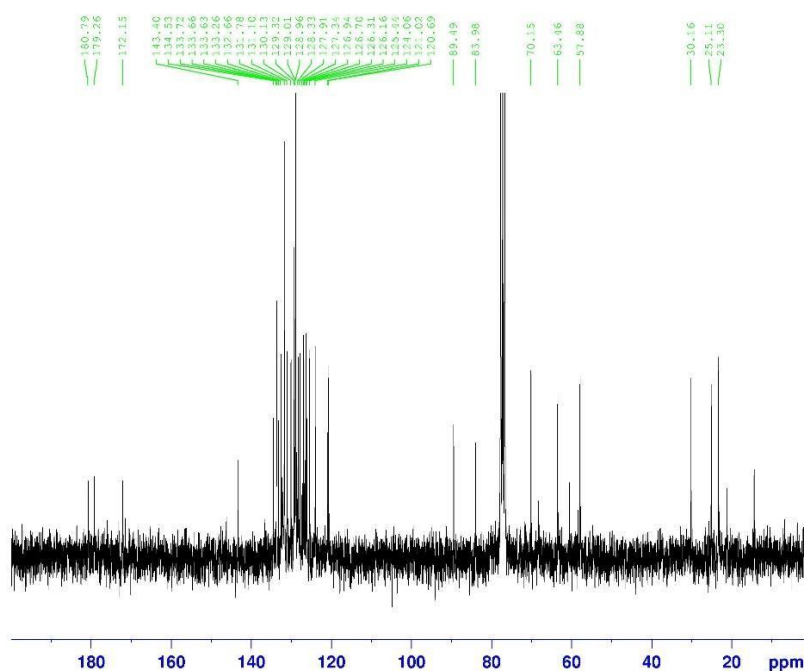
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F2 - Acquisition Parameters
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INSTRUM spect
PROBHD 5 mm PABBO ES-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 50.3
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.3000000 sec
TDC 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
PLW 11.25325108 W
SFO1 300.1318534 Mhz

F2 - Processing parameters
SI 32768
SF 300.1300400 Mhz
WDW FM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Parpart SP125 13C CDC13



Current Data Parameters
NAME 140212.205
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140212
Time 20.02
INSTRUM spect
PROBHD 5 mm PABBO RR-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1643834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999998 sec
TDC 1

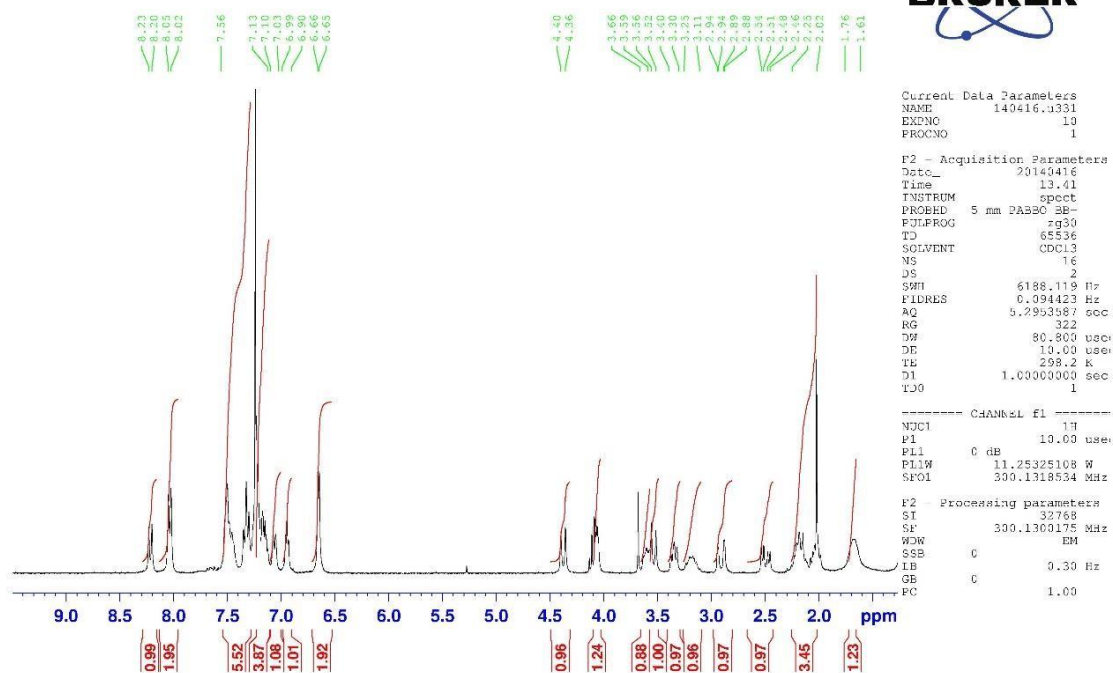
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SFO1 62.9015280 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310000 MHz

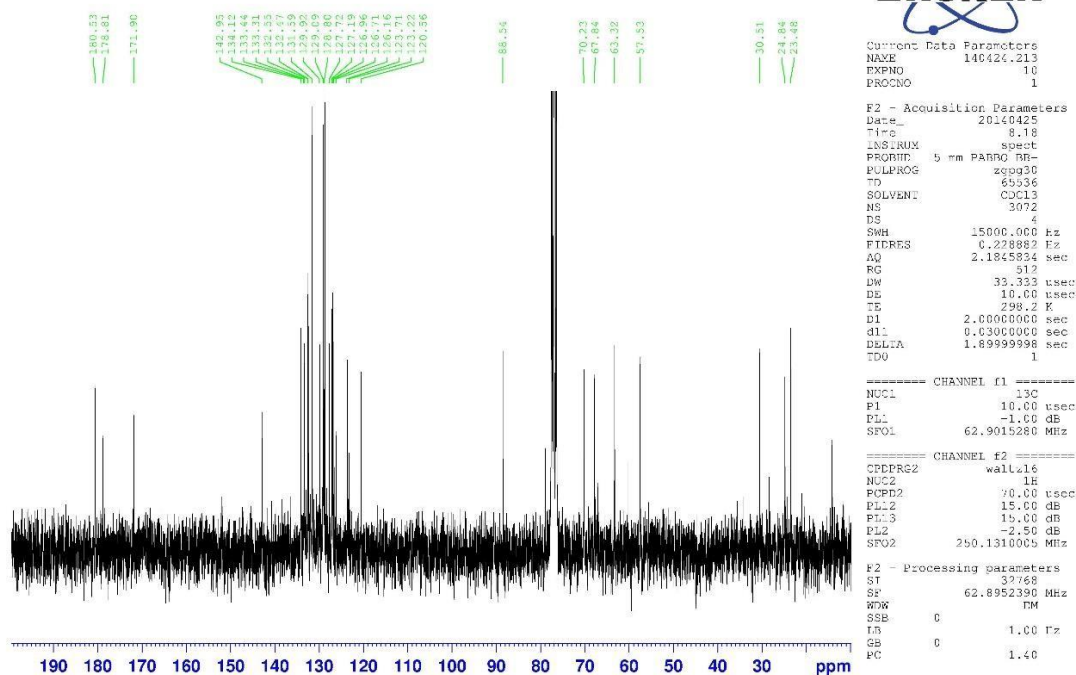
F2 - Processing parameters
SI 32768
SF 62.895262 MHz
WDW FM
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

1.6 (S)-2-Amino-5-[thiophene-2-yl]pent-4-ensäure-Ni-(S)-BPBP (2f):

Parpart SP161 1H CDCl3

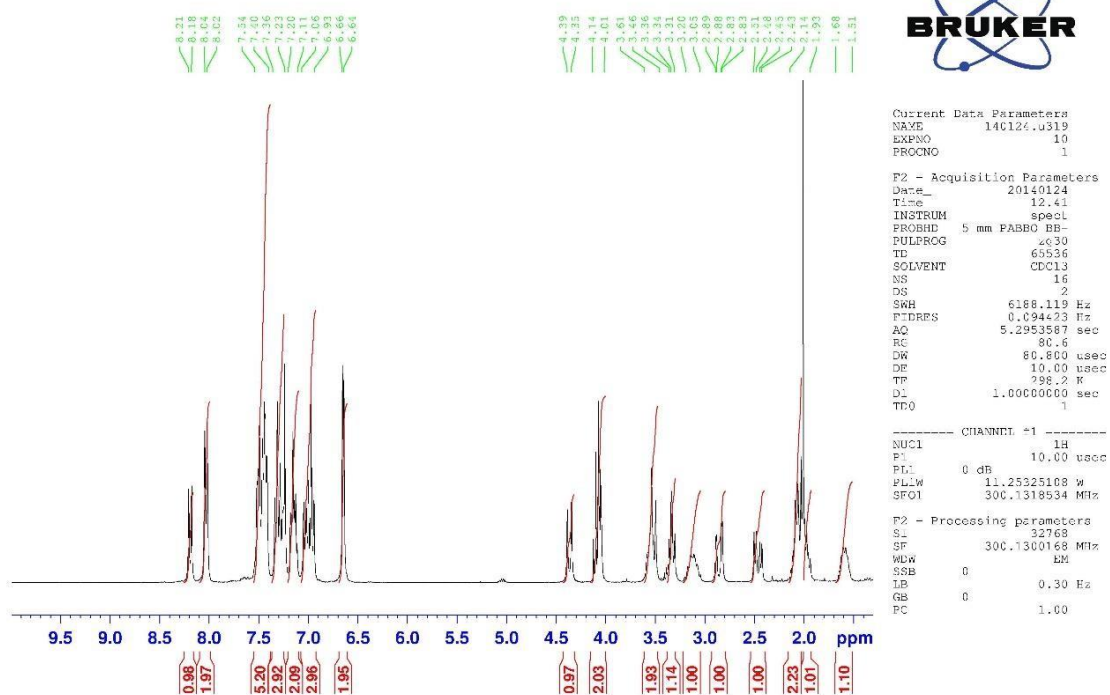


Parpart SP-161 13C CDCl3

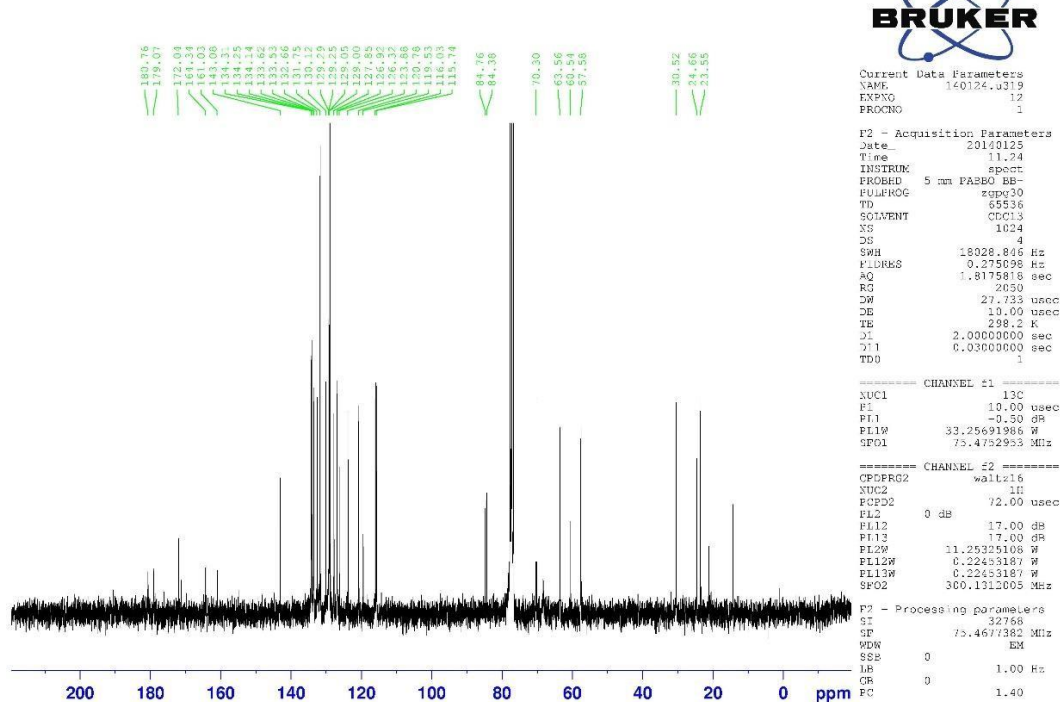


1.7 (S)-2-Amino-5-[4-fluorophenyl]pent-4-insäure-Ni-(S)-BPBP (2g):

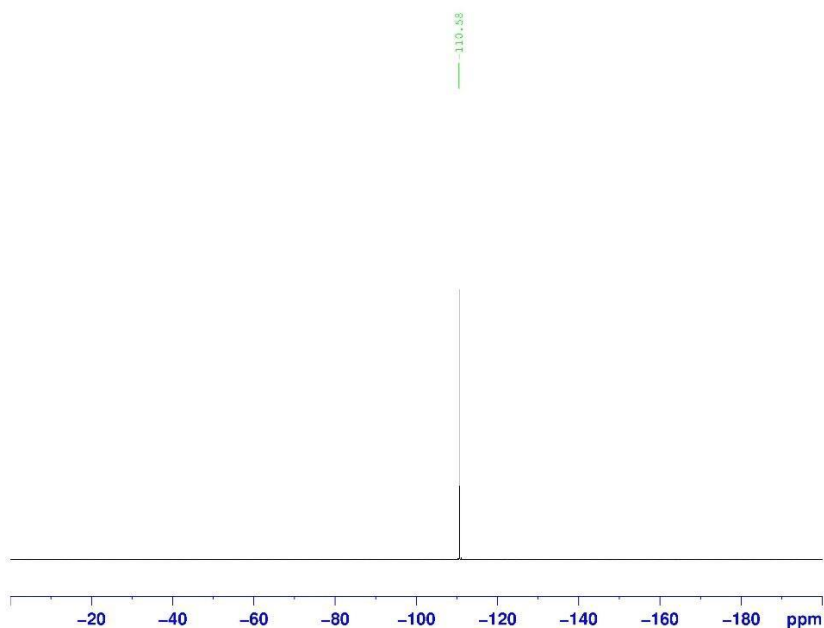
Parpart Spl119.1 1H CDC13



Parpart Spl119.1 13C CDC13



Farpart Sp119.1 19F CDC13



Current Data Parameters
NAME 140124.0319
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140124
Time 12.44
INSTRUM spect
PROBHD 5 mm PABBO 3H-
PULPROG zgpg30
TD 131072
SOLVENT CDC13
NS 64
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9787210 sec
RG 2050
DW 7.467 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00000000 sec
TD0 -

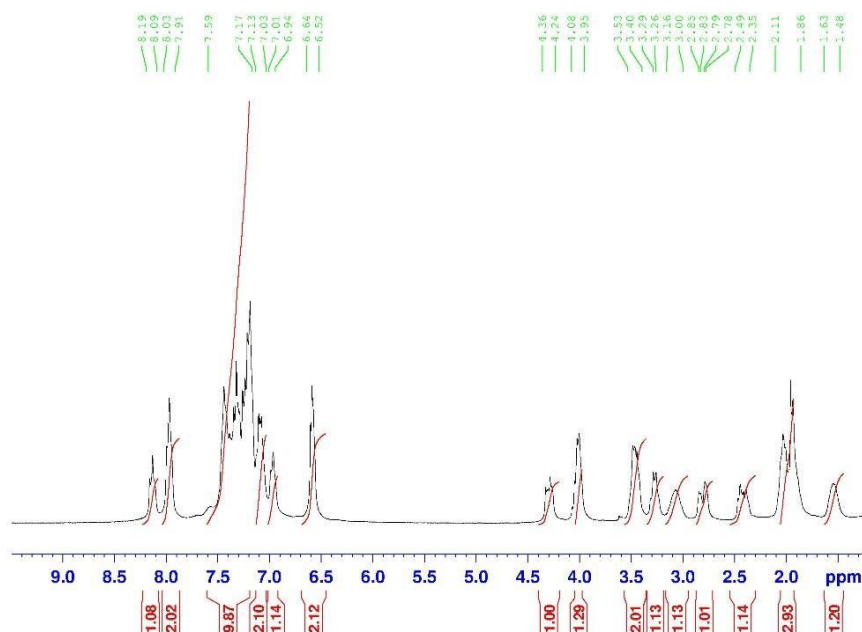
===== CHANNEL f1 =====
NUC1 19F
P1 10.00 usec
PL1 -3.00 dB
PL1W 15.53680420 W
SFO1 282.376148 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL1W 11.25325108 W
PL12W 0.22455187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
GB 0.30 Hz
CB 0
PC 1.00

1.8 (S)-2-Amino-5-[4-chlorophenyl]pent-4-ensäure-Ni-(S)-BPBP (2h):

Parpart SP 126 1H CDCl3



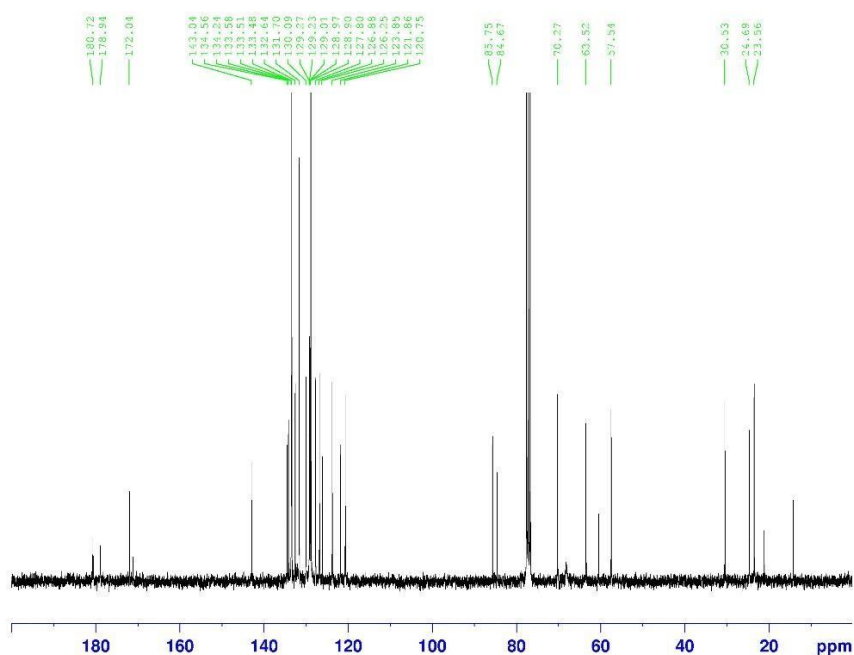
Current Data Parameters
NAME 140207.1334
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140209
Time 10.15
INSTRUM spect
PROBHD 5 mm DABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 50.8
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 Processing parameters
SI 32768
SF 300.1303403 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Parpart SP 126 13C CDCl3



Current Data Parameters
NAME 140207.1334
EXPNO 12
PROCNO 1

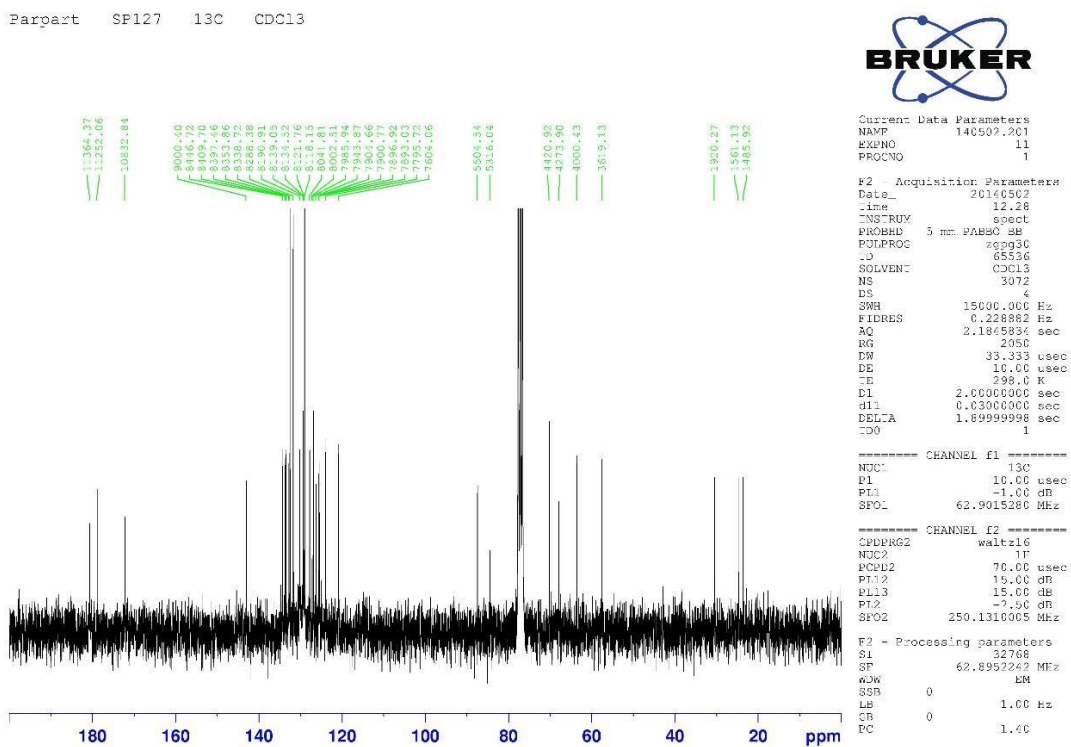
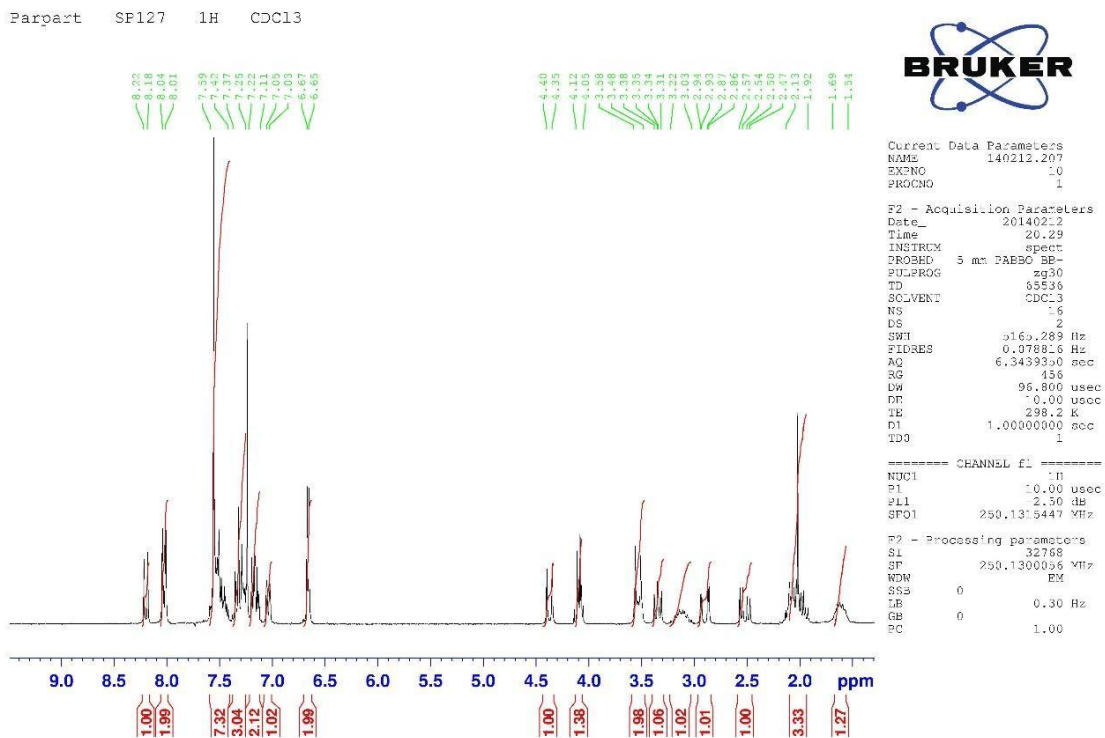
F2 - Acquisition Parameters
Date_ 20140209
Time 11.43
INSTRUM spect
PROBHD 5 mm DABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2040
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 10.00 usec
PL1 0.50 dB
PL1W 33.23691986 W
SFO1 75.4752953 MHz

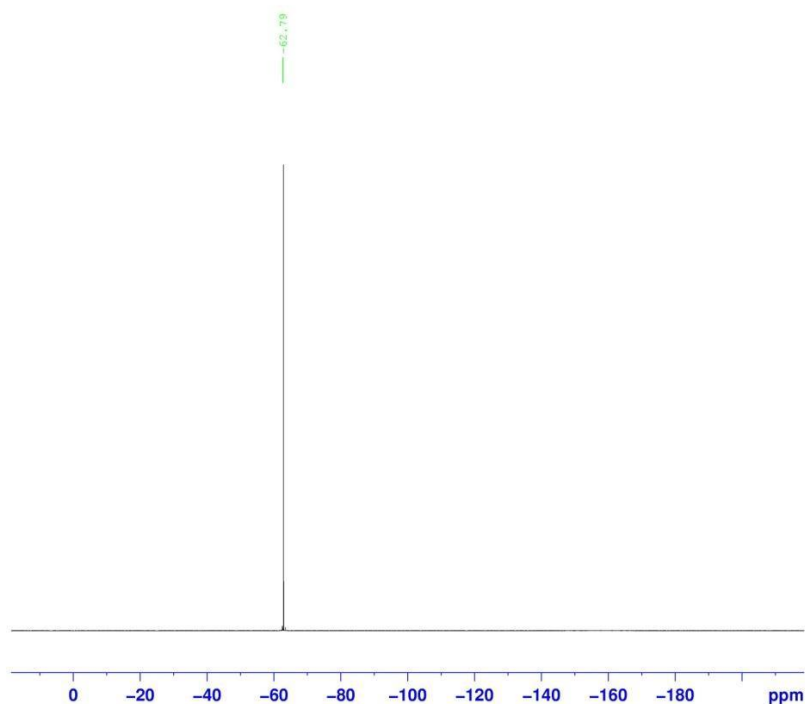
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CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
P12 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL12W 11.25325108 W
PL13W 0.22452187 W
PL13W 0.22452187 W
SFO2 300.1317005 MHz

F2 Processing parameters
SI 32768
SF 75.4677407 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1.9 (S)-2-Amino-5-[4-trifluormethylphenyl]pent-4-insäure-Ni-(S)-BPBP (2i):



Parpart SP127 19F CDC13



Current Data Parameters
NAME 140213.u301
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140213
Time 9.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhiggn
TD 131072
SOLVENT CDC13
NS 64
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9787210 sec
RG 2050
DW 7.467 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

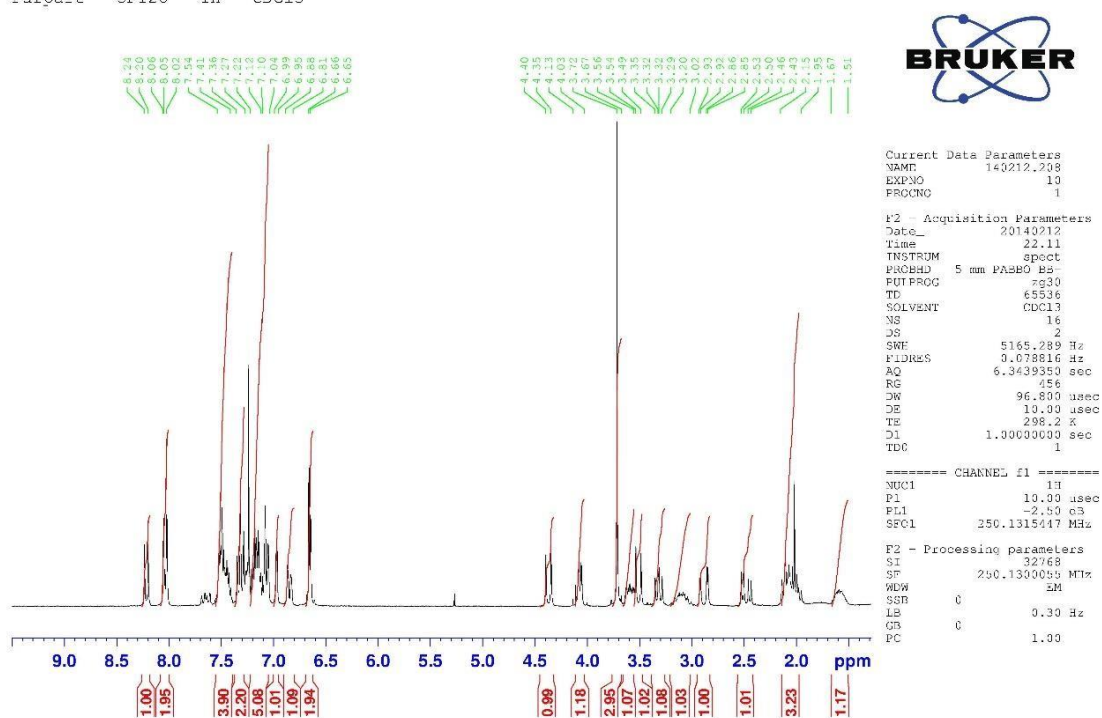
===== CHANNEL f1 =====
NUC1 19F
P1 10.00 usec
PL1 -3.00 dB
PL1W 15.53680420 W
SFO1 282.3761148 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
SFO2 300.1312005 MHz

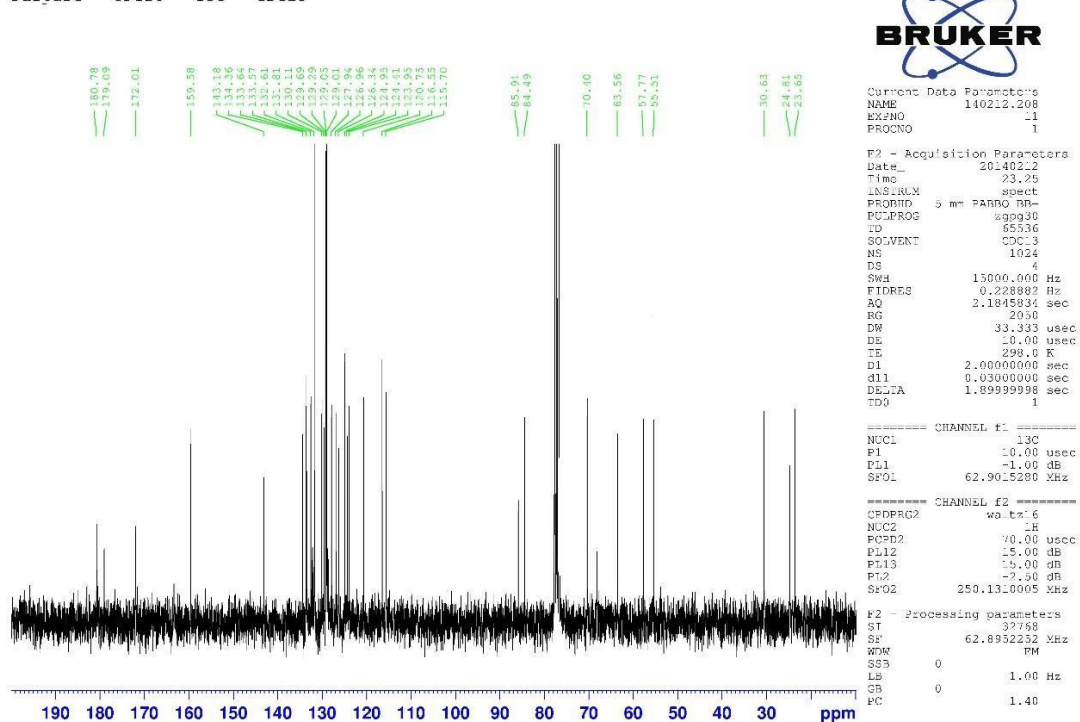
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1.10 (S)-2-Amino-5-[3-methoxyphenyl]pent-4-ensäure-Ni-(S)-BPBP (2j):

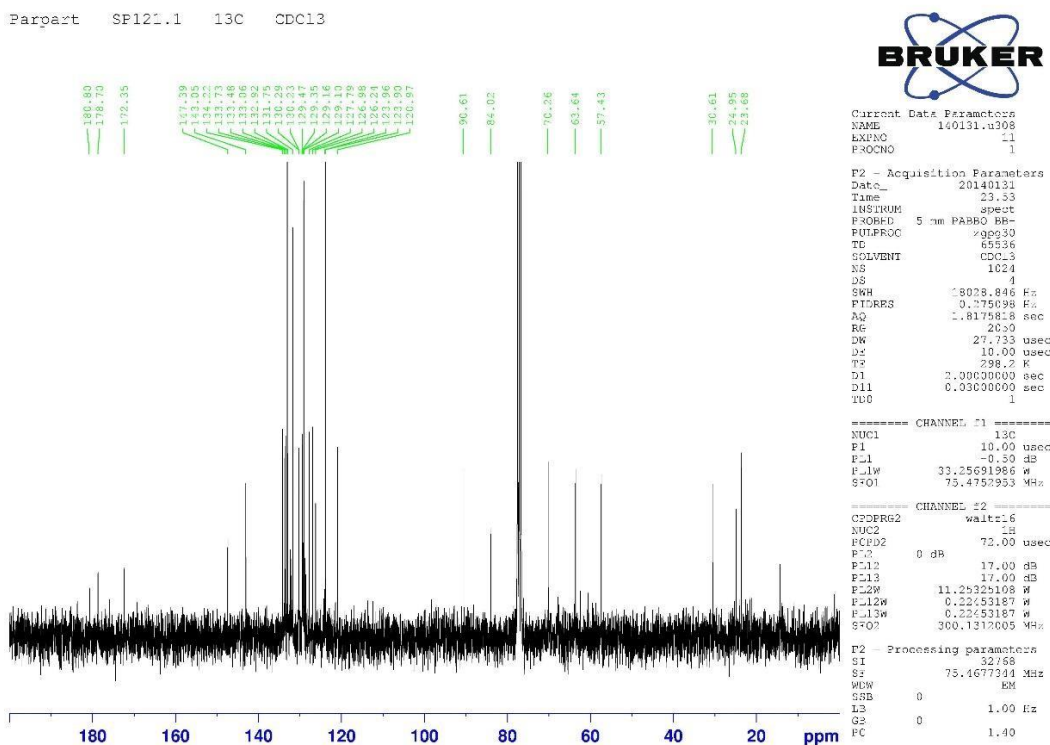
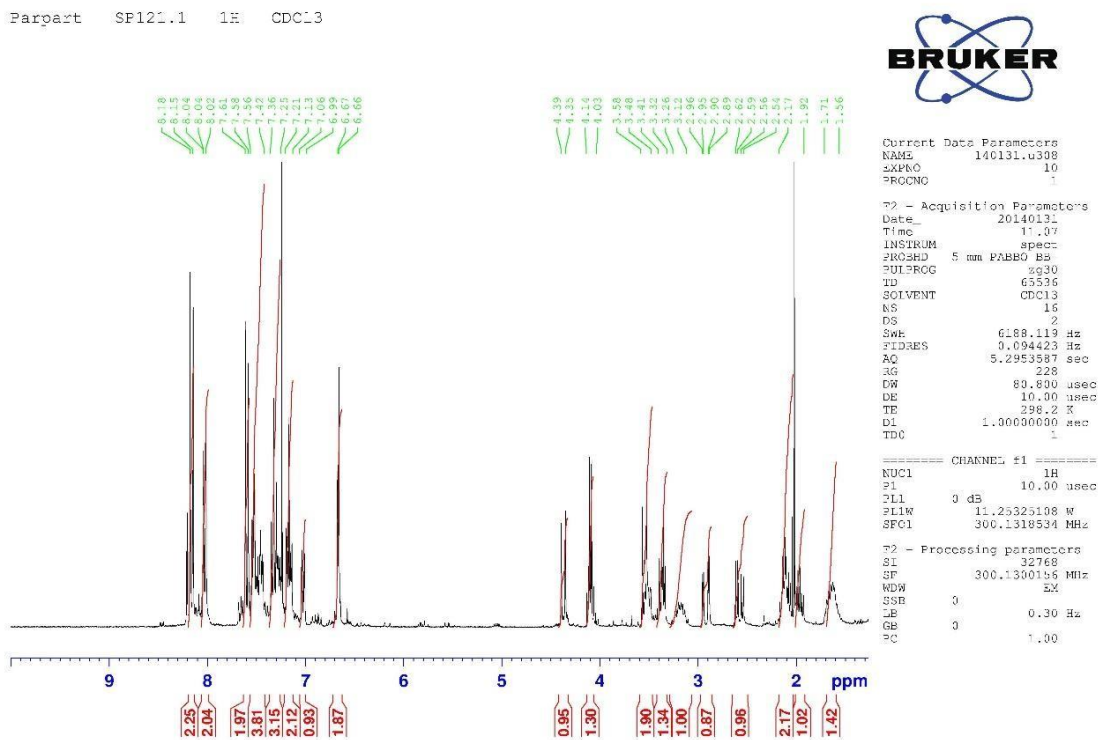
Parpart SP128 1H CDCl3



Parpart SP128 13C CDCl3

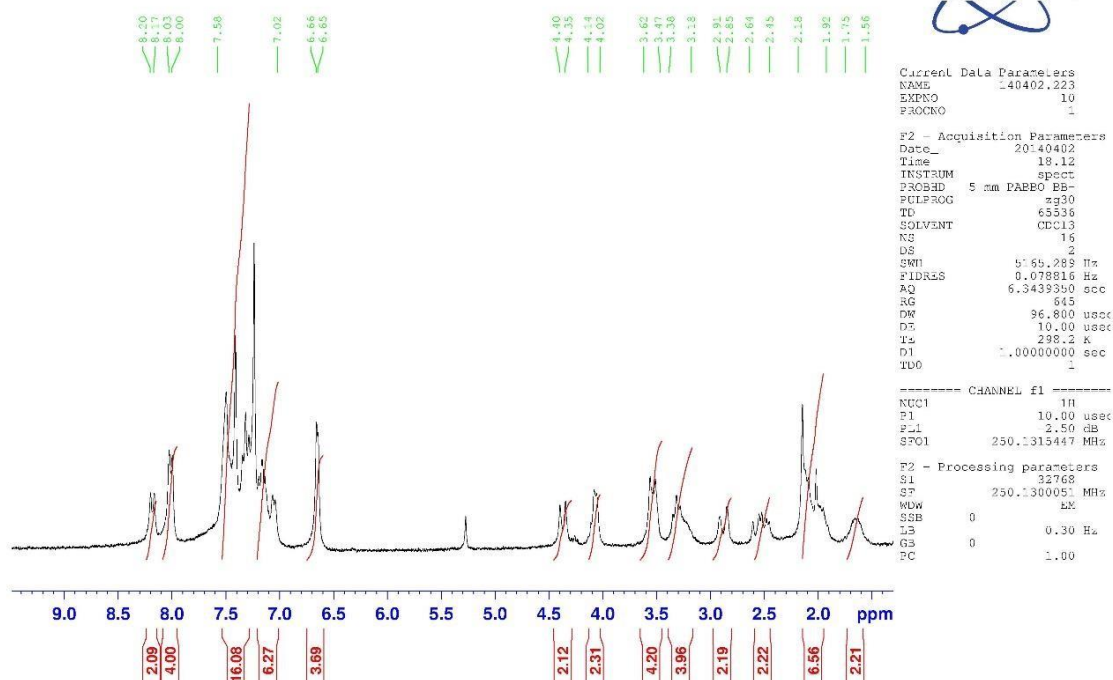


1.11 (S)-2-Amino-5-[4-nitrophenyl]pent-4-insäure-Ni-(S)-BPBP (2k):

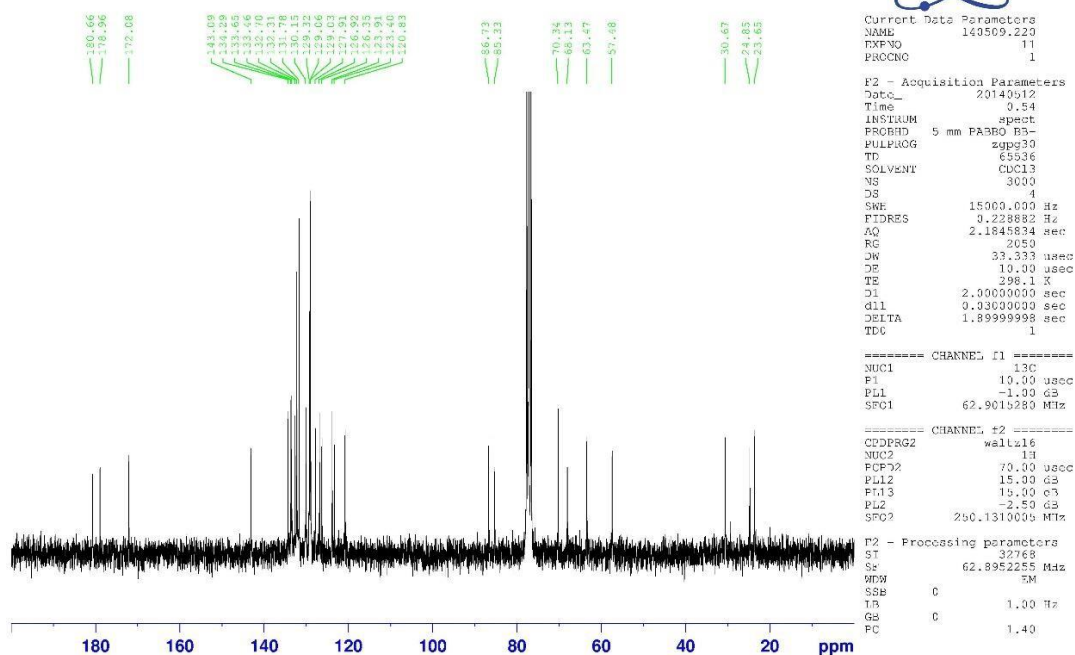


1.12 5,5'-[1,4-Phenyl]bis((S)-2-aminopent-4-ensäure-Ni-(S)-BPBP) (2I):

Parpart SP155 1H CDCl3

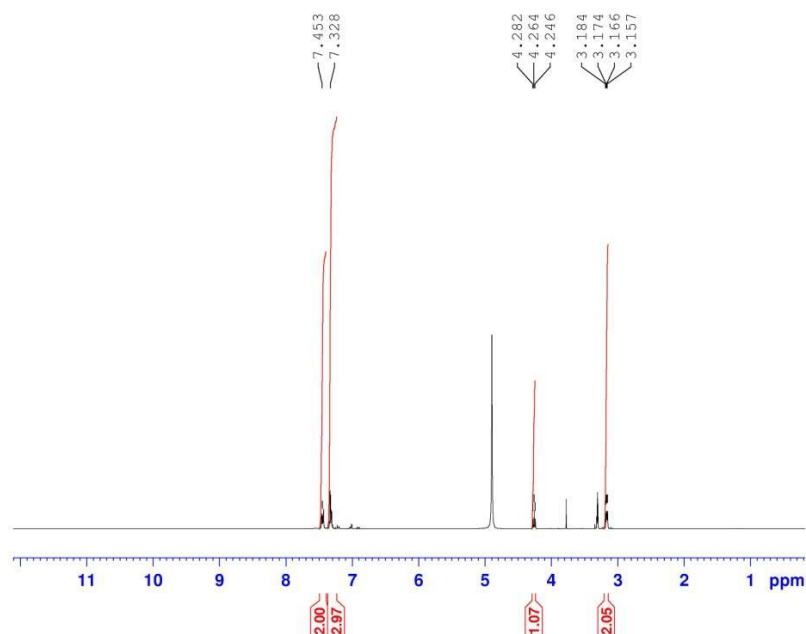


Parpart SP155 13C CDCl3



1.13 (S)-2-Amino-5-[phenyl]pent-4-insäure (3a):

Parpart SP 158 1H CD3OD/H2O



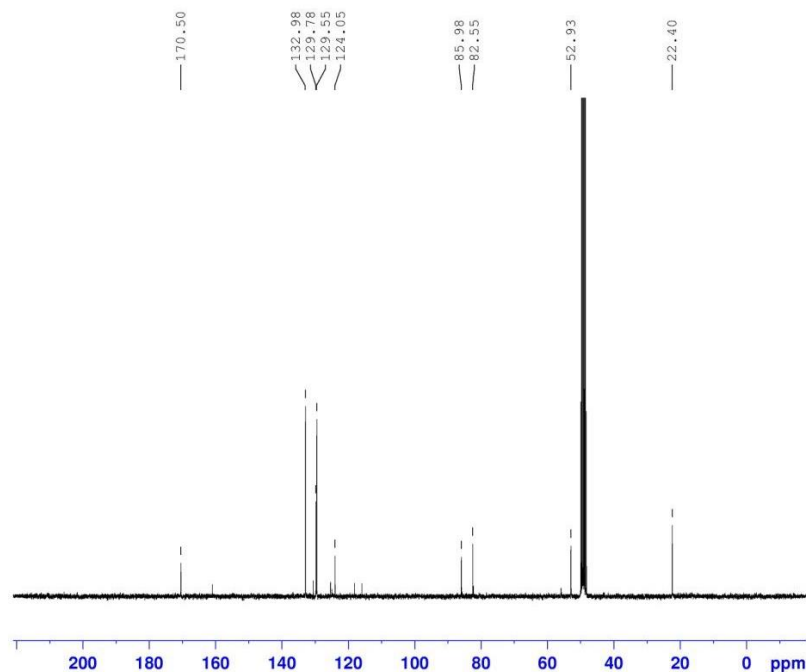
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NAME 140410.u320
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140410
Time 13.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 101
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Parpart SP 158 13C CD3OD



Current Data Parameters
NAME 140410.u320
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140410
Time 20.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

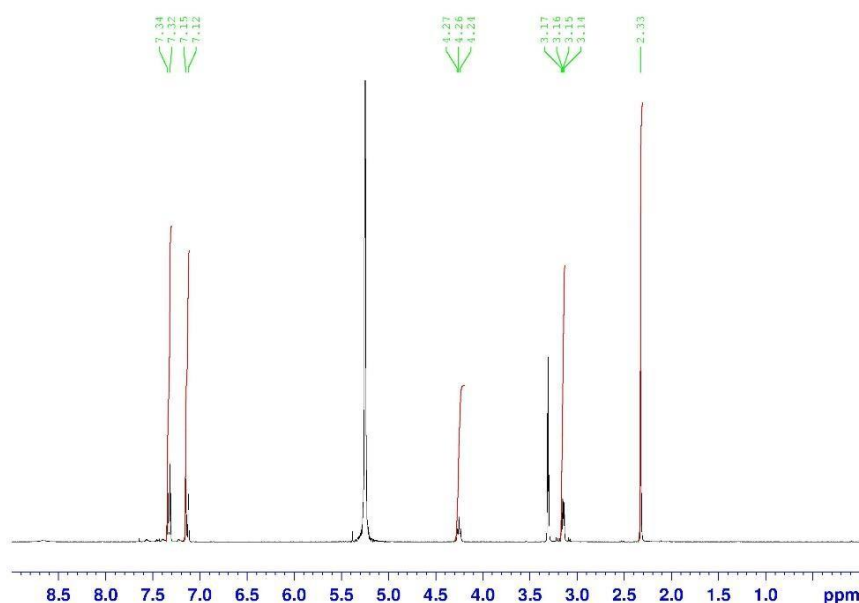
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4676332 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1.14 (S)-2-Amino-5-[4-tolyl]pent-4-insäure (3b):

Pargpart SP144 1H CD3OD/HCl



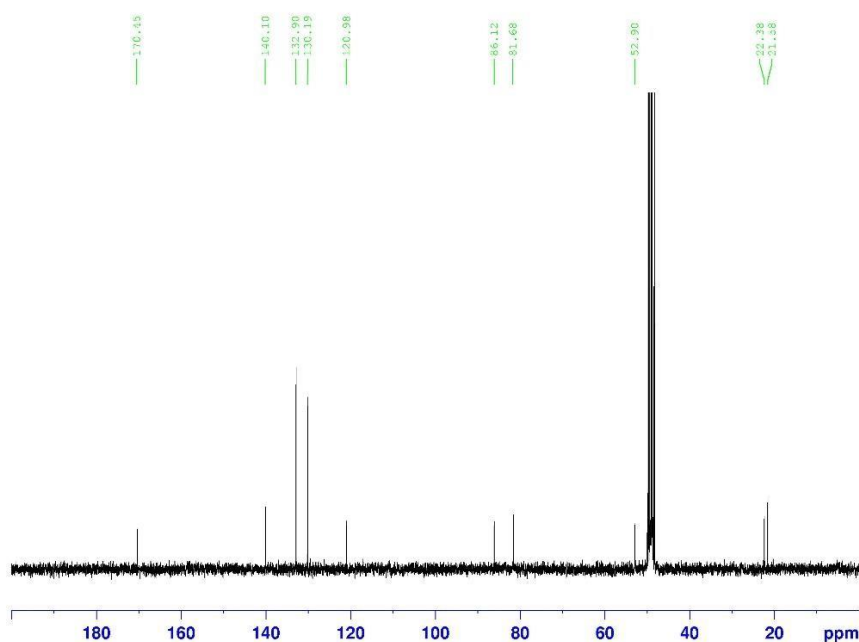
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EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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Time 12.30
INSTRUM spect
PROBHD 5 mm PABBO B3-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWE 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 90.5
CW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TDC 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318531 MHz

F2 - Processing parameters
SI 32768
SF 300.1300064 MHz
WDW EM
SSR 0
LB 0.30 Hz
GB 0
PC 1.00

Pargpart SP144 13C CD3OD/HCl



Current Data Parameters
NAME 140404.u309
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140404
Time 15.27
INSTRUM spect
PROBHD 5 mm PABBO B3-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 1024
DS 4
SWE 18028.846 Hz
FIDRES 0.275096 Hz
AQ 1.8175818 sec
RG 2090
CW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TDC 1

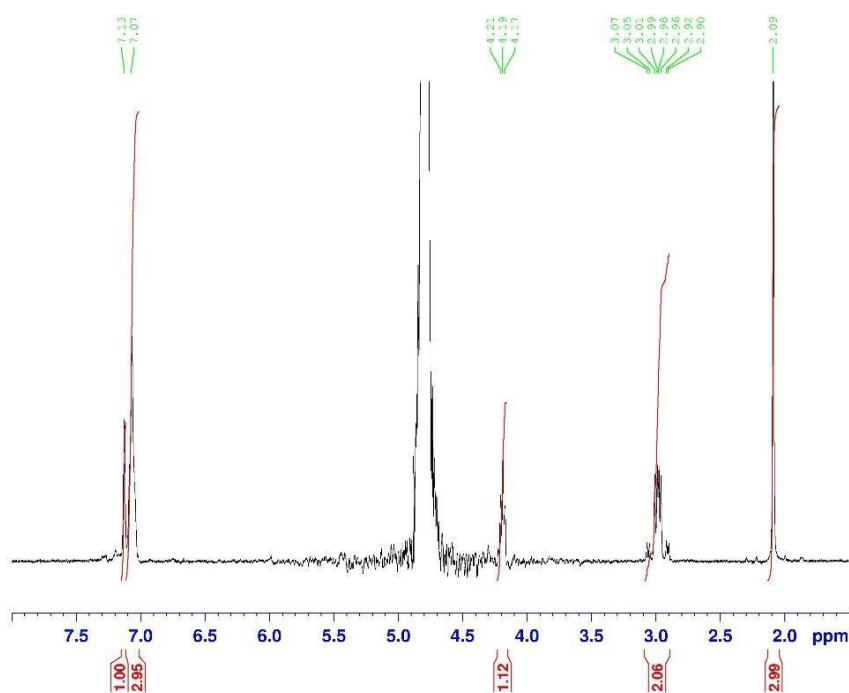
===== CHANNEL F1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.23697985 W
SFO1 75.4752953 MHz

===== CHANNEL F2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL2W 17.00 dB
PL3 17.00 dB
PL3W 11.25325108 W
PL4W 0.22453187 W
PL5W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4676337 MHz
WDW EM
SSR 0
LB 1.00 Hz
GB 0
PC 1.40

1.15 (S)-2-Amino-5-[3-tolyl]pent-4-insäure (3c):

Parpart SP145 1H D2O



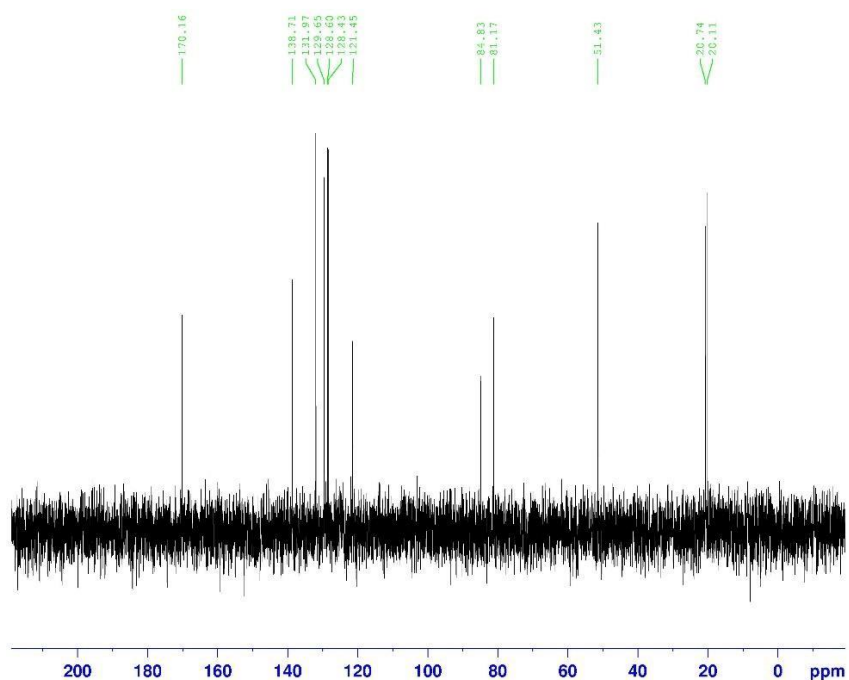
Current Data Parameters
NAME 140319.0311
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140319
Time 12.59
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zg30
TD 65536
SOLVENT D2O
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 90.5
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
P11 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300125 MHz
WDW PM
SSB 0
TB 0.30 Hz
GB 0
PC 1.00

Parpart SP145 13C D2O



Current Data Parameters
NAME 140324.206
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140324
Time 22.57
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 3072
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.8 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

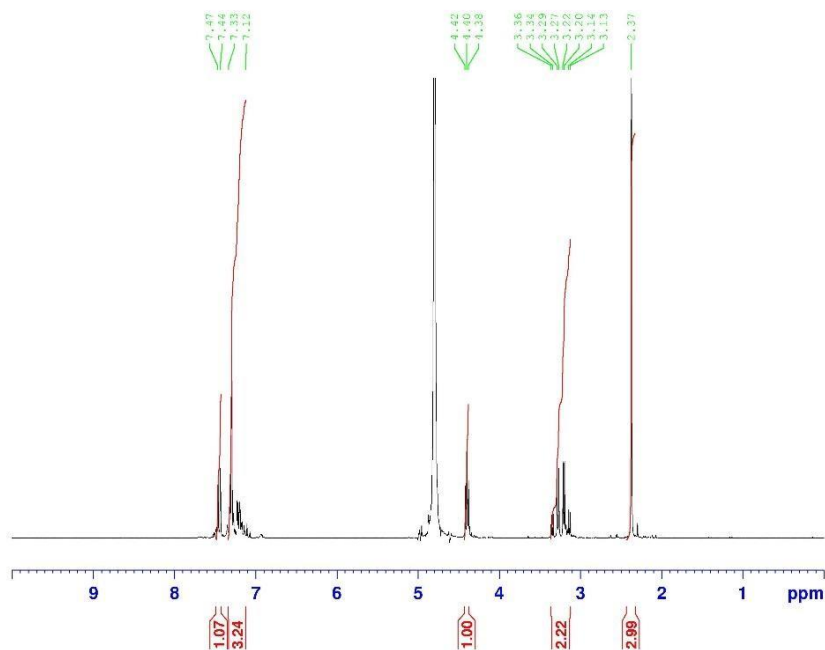
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
P11 -1.00 dB
SFO1 62.9015280 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PT12 15.00 dB
PT13 15.00 dB
PL2 2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1.16 (S)-2-Amino-5-[2-tolyl]pent-4-insäure (3d):

Parpart SP147 1H D2O/HCl



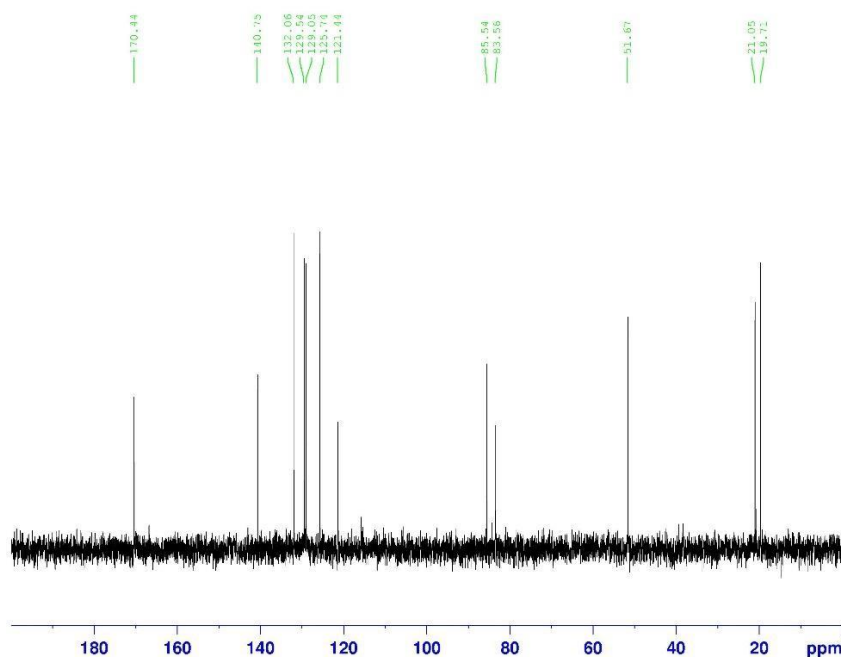
Current Data Parameters
NAME 140325.209
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140326
Time 13.05
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.076816 Hz
AQ 6.3439350 sec
RG 287
DW 96.800 usec
DE 10.00 usec
TE 298.1 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.50 dB
SFO1 250.1315447 MHz

F2 - Processing parameters
SI 32768
SF 250.1299758 MHz
WDW EM
SSB 0
LB 0.30 Hz
CB 0
PC 1.00

Parpart SP147 13C D2O/HCl



Current Data Parameters
NAME 140327.207
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140328
Time 1.31
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 3000
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1843834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999999 sec
TD0 1

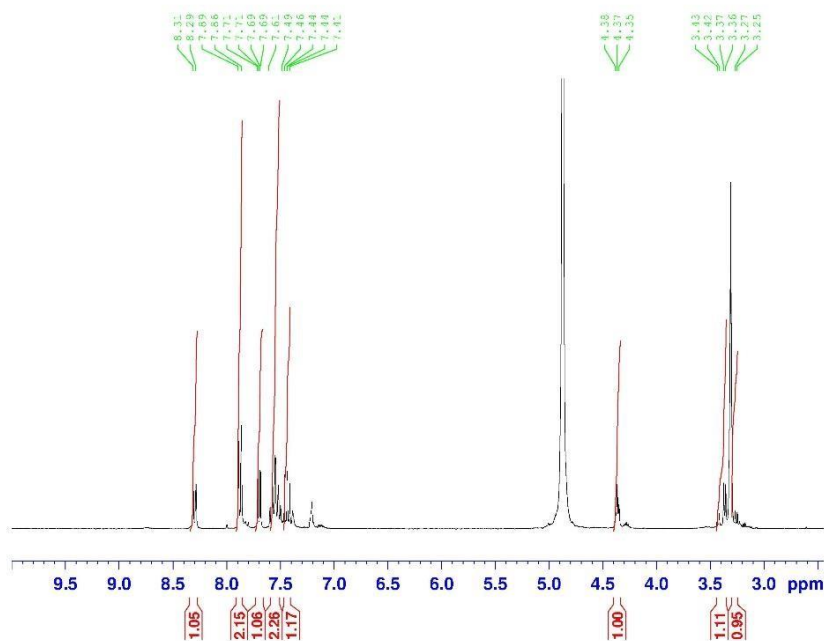
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
P112 15.00 dB
PL13 15.00 dB
PL12 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952390 MHz
WDW EX
SSB 0
LB 1.00 Hz
CB 0
PC 1.40

1.17 (S)-2-Amino-5-[naphth-1-yl]pent-4-ensäure (3e):

Parpart SP148 1H CD3OD

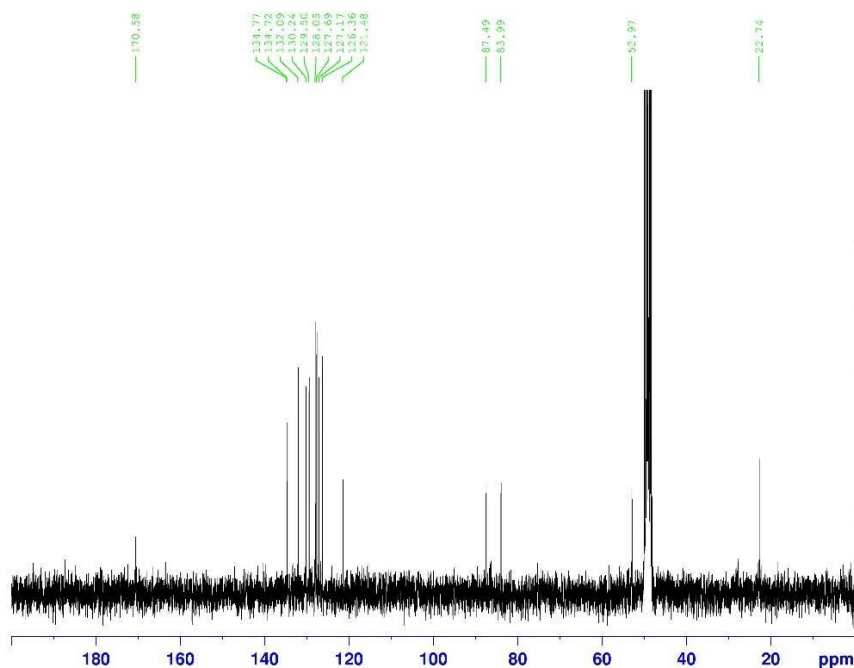


Current Data Parameters
NAME 140407.u319
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140407
Time 12.39
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318531 MHz
F2 - Processing parameters
SI 32768
SF 300.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Parpart SP148 13C CD3OD



Current Data Parameters
NAME 140407.u319
EXPNO 11
PROCNO 1

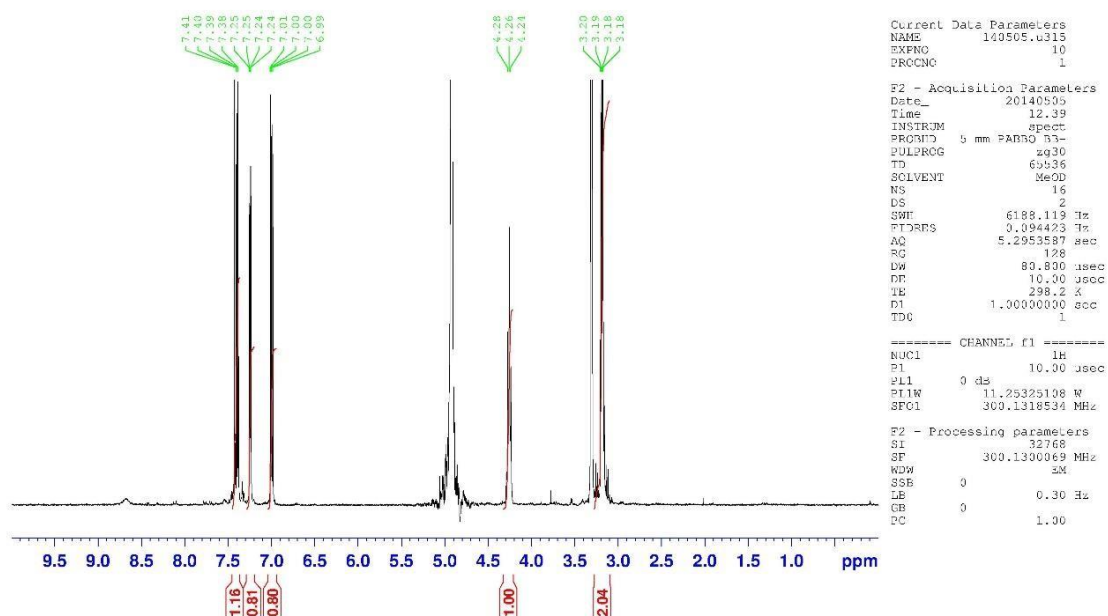
F2 - Acquisition Parameters
Date_ 20140408
Time 5.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.9175818 sec
RG 1050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.75691986 W
SFO1 75.4752953 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL1W 11.25325108 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

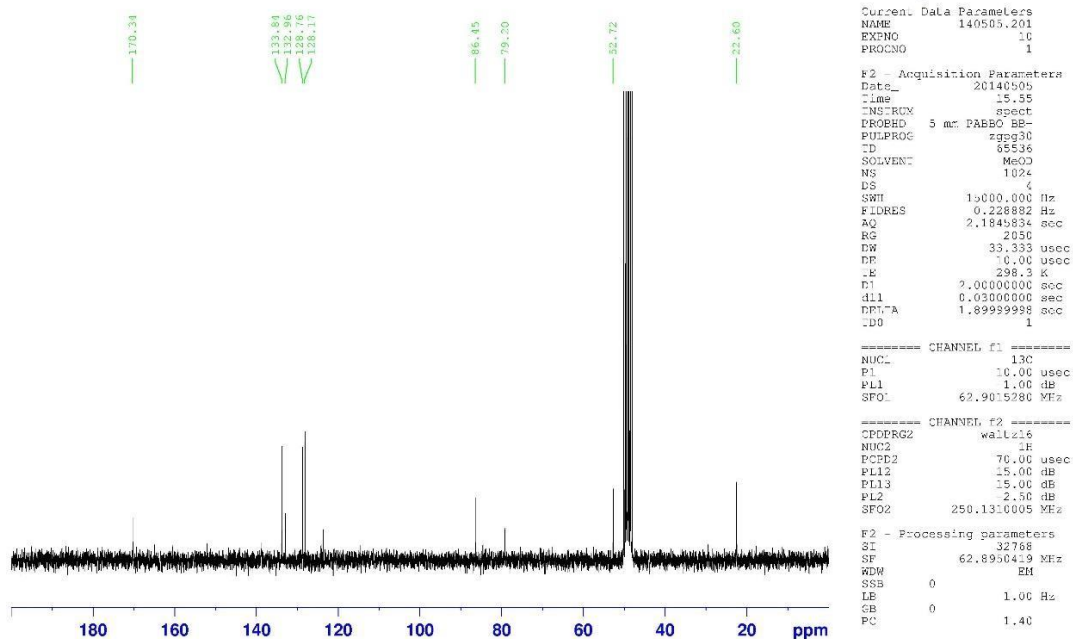
F2 - Processing parameters
SI 32768
SF 75.4676345 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1.18 (S)-2-Amino-5-[thiophen-2-yl]pent-4-ensäure (3f):

Parpart SP162 1H CD3OD/HCl

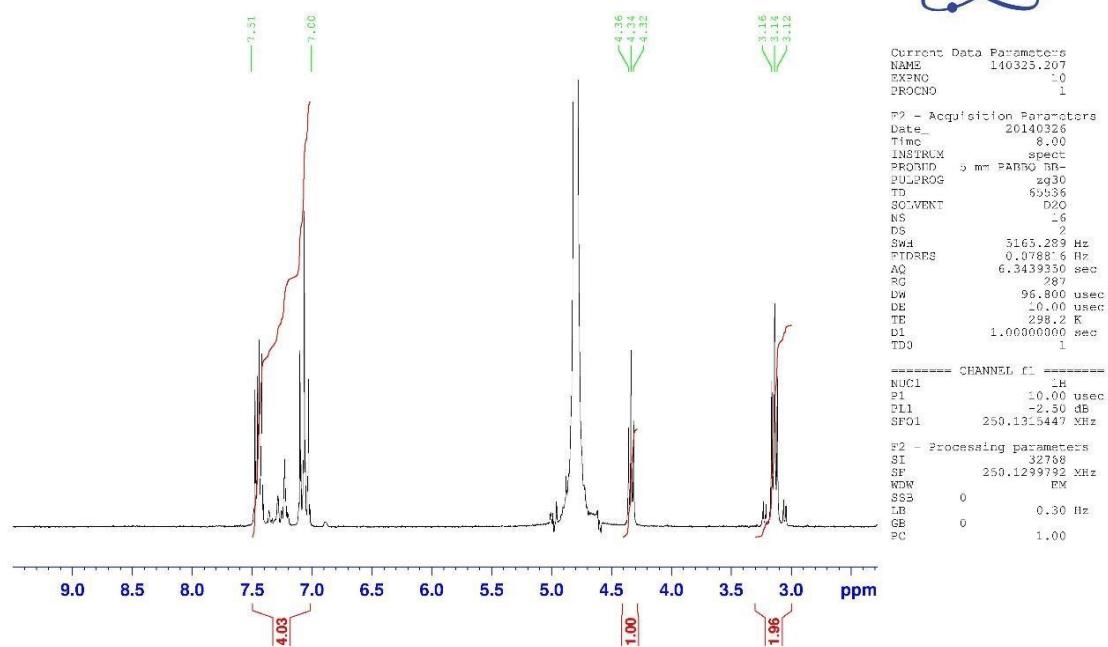


Parpart SP162 13C CD3OD/HCl

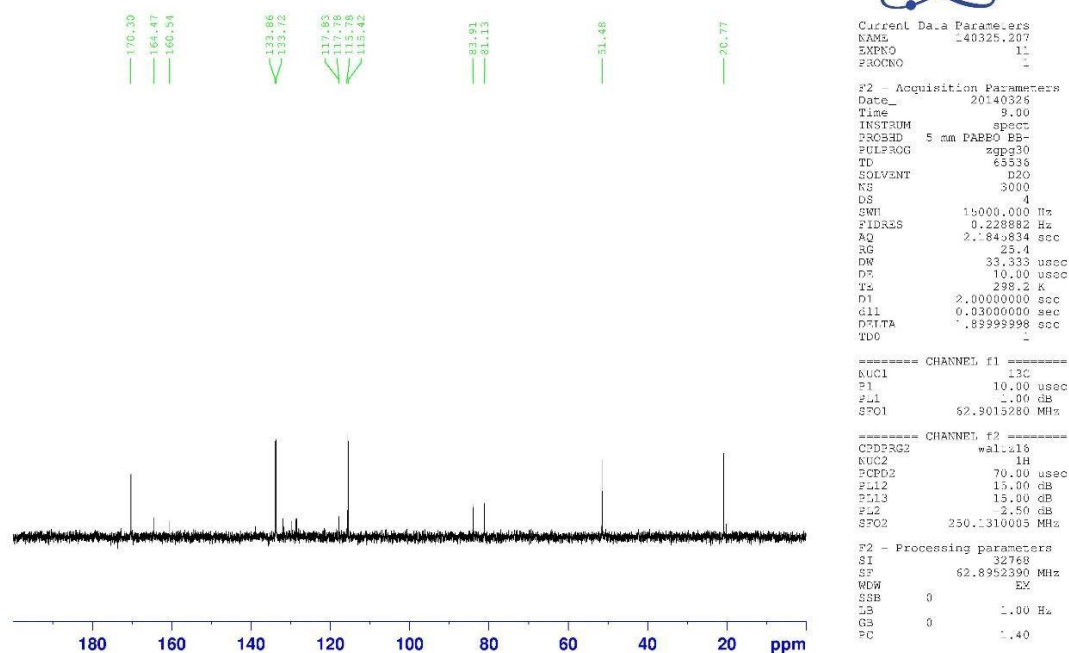


1.19 (S)-2-Amino-5-[4-fluorophenyl]pent-4-inoe (3g):

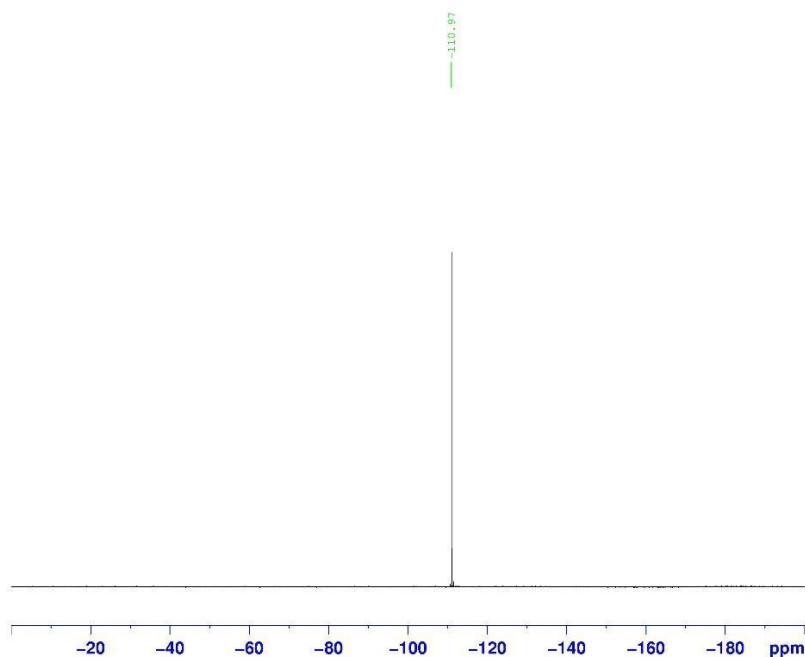
Parpart SP146 1H D2O/HCl



Parpart SP146 13C D2O/HCl



Pargart SP146 19F D2O/EC1



```

Current Data Parameters
NAME      140326.u318
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20100326
Time      19.07
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         131072
SOLVENT   D2O
NS         64
DS         4
SWH        65964.289 Hz
FIDRES     0.510897 Hz
AQ         0.9787210 sec
RG         2050
AW         7.467 usec
JE         10.00 usec
TE         298.2 K
D1         1.0000000 sec
D11        0.0300000 sec
D12        0.0000200 sec
TD0        1

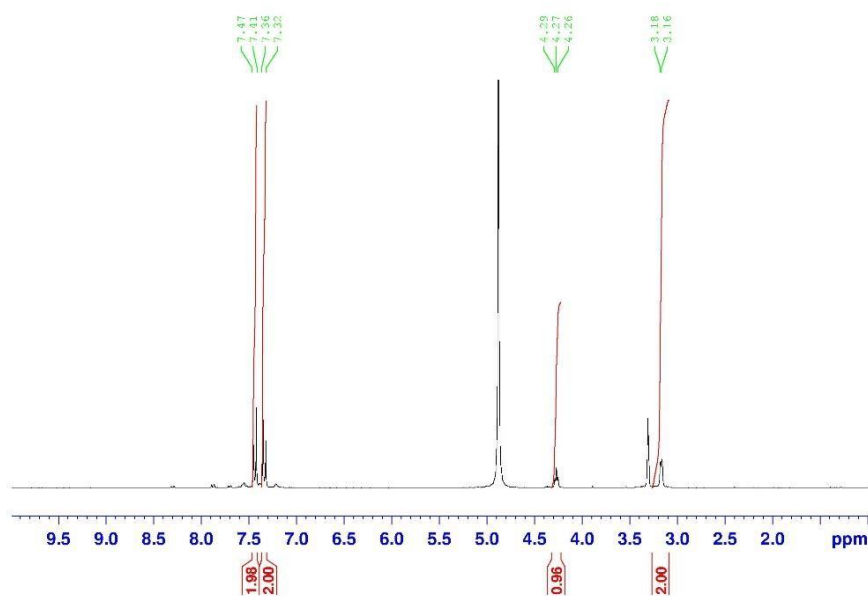
===== CHANNEL f1 =====
NUC1       19F
P1         10.00 usec
PL1        -3.00 dB
PL1W       15.33680470 W
SFO1       282.3761148 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      72.00 usec
PL2        0 dB
PL12       17.00 dB
PL12W      11.25325108 W
PL12W      0.22453187 W
SFO2       300.1312005 MHz

F2 - Processing parameters
SI         65536
SF         282.4043550 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

1.20 (S)-2-Amino-5-[4-chlorophenyl]pent-4-insäure (3h):

Parpart SP149 1H CD3OD



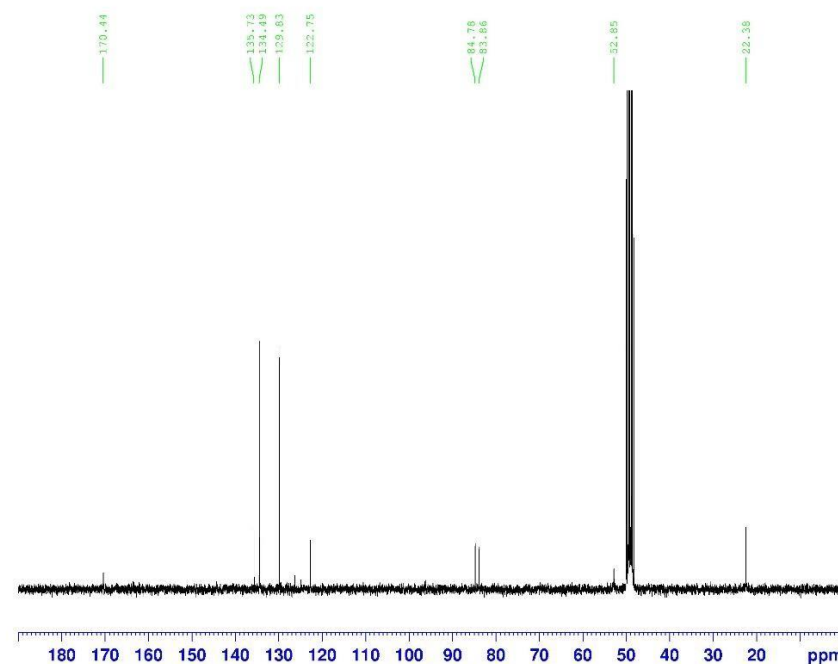
Current Data Parameters
NAME 140407.u320
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140407
Time 12.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 3.2953587 sec
RG 14
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.2532508 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Parpart SP149 13C CD3OD



Current Data Parameters
NAME 140407.u320
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140408
Time 6.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.723 usec
DE 10.00 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

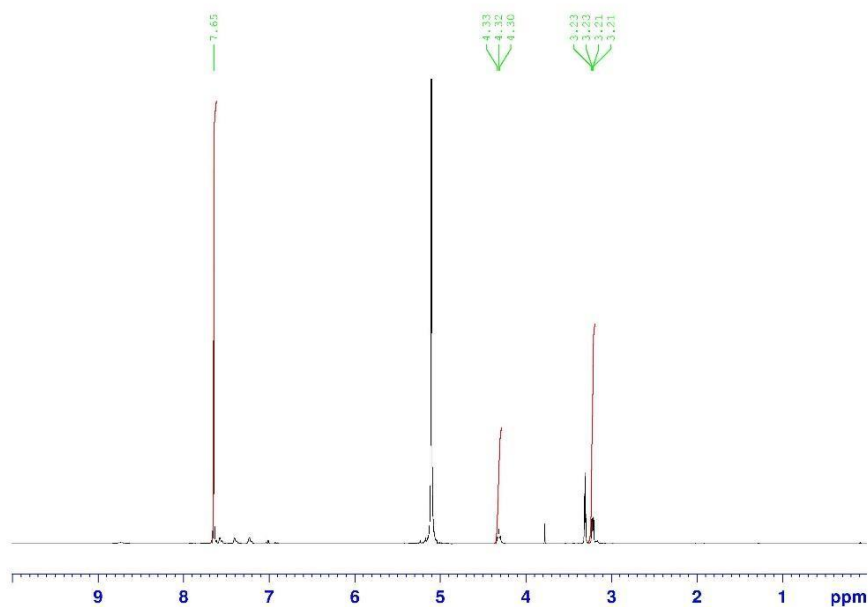
CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25692986 W
SFO1 75.4782933 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312305 MHz

F2 - Processing parameters
SI 32768
SF 75.4676539 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1.21 (S)-2-Amino-5-[4-trifluormethylphenyl]pent-4-insäure (3i):

Parpart SP152 1H CD3OD/HCl



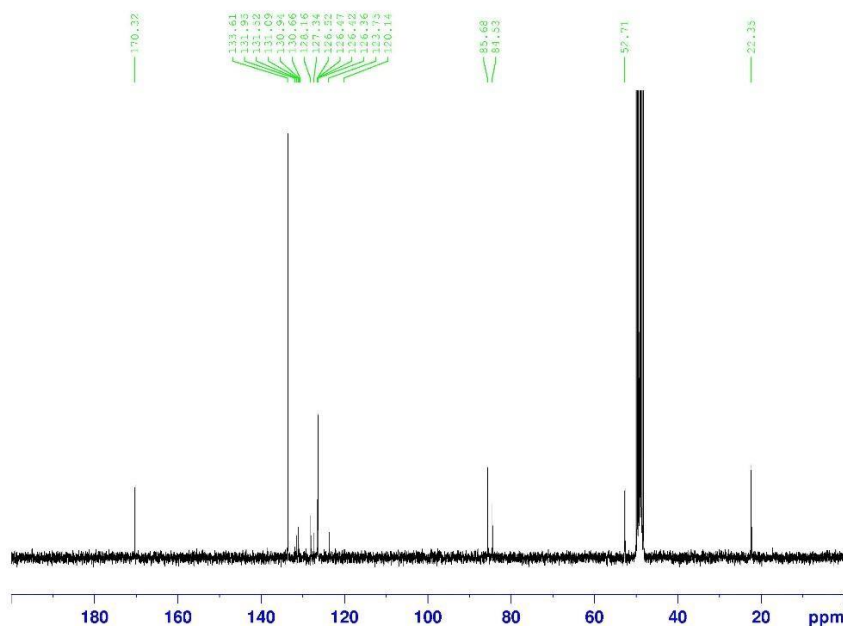
Current Data Parameters
NAME 240604.u316
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140404
Time 17.35
INSTRUM spect
PROBHD 5 mm PABO RH-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 6186.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 50.8
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1316534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300066 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Parpart SP152 13C CD3OD/HCl



Current Data Parameters
NAME 140505.u313
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140505
Time 2.27
INSTRUM spect
PROBHD 5 mm PABO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 3072
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2650
DW 27.723 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL12W 11.25325108 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4676344 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Paroart SP152 19F CD3OD/HCl



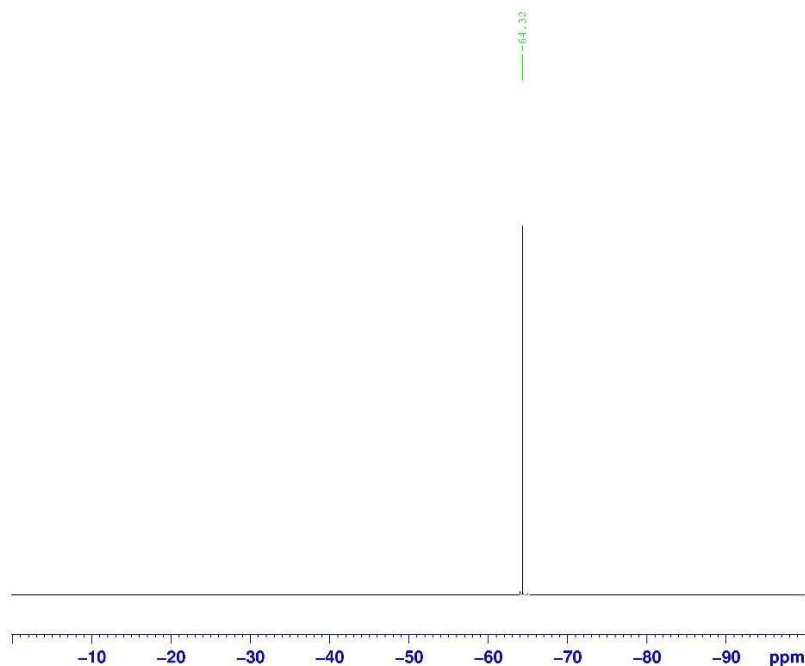
Current Data Parameters
NAME 140404.e310
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140404
Time 12.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30gq
TD 131072
SOLVENT MeOD
NS 64
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.978770 sec
RG 2050
DW 7.467 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
D11 0.0300000 sec
D12 0.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 10.00 usec
PL1 -3.00 dB
PL1W 15.53680420 W
SFO1 282.3761148 MHz

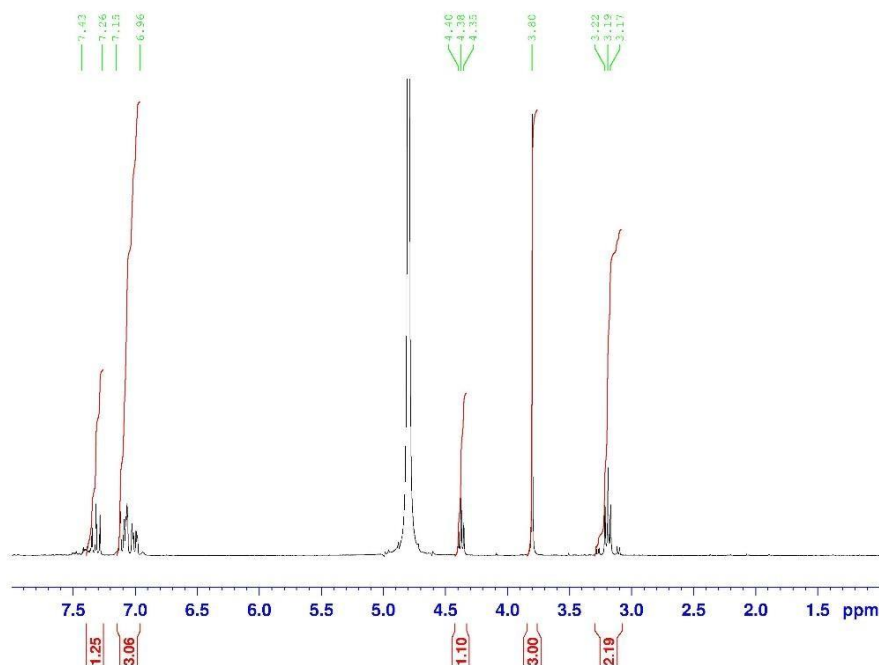
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 282.4013570 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.22 (S)-2-Amino-5-[3-methoxyphenyl]pent-4-insäure (3j):

Parpart SP150 1H D2O/HCl



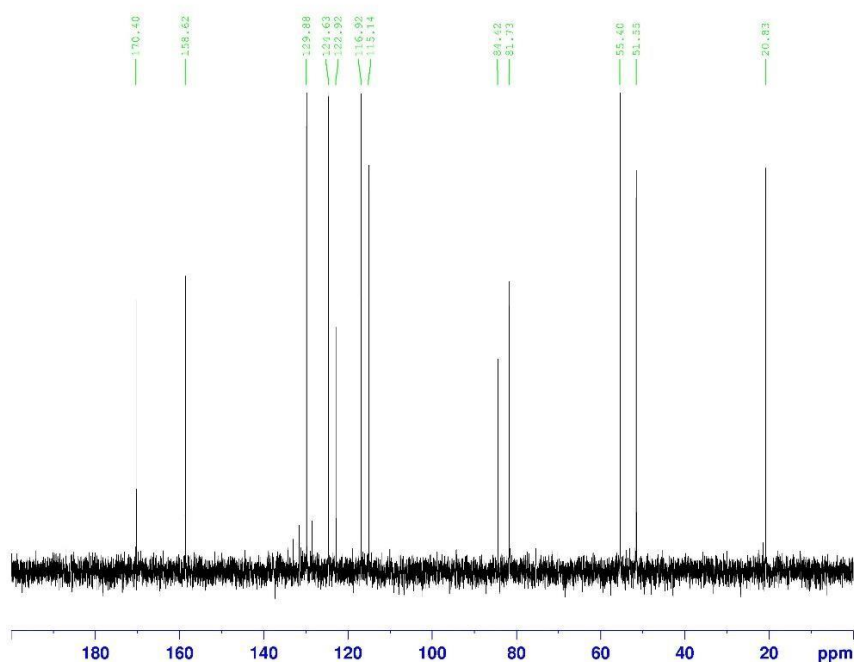
Current Data Parameters
 NAME 140325.211
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140326
 Time 13.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT D2O
 NS 16
 DS 2
 SWH 5165.289 Hz
 FIDRES 0.019816 Hz
 AQ 6.3439350 sec
 RG 1.81
 DW 96.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

CHANNEL f1
 NUC1 1H
 P1 10.00 usec
 PL1 -2.50 dB
 SFO1 250.1315447 MHz

F2 - Processing parameters
 SI 32768
 SF 250.1299750 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Parpart SP150 13C D2O



Current Data Parameters
 NAME 140328.204
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140328
 Time 20.10
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 3000
 DS 4
 SWH 10000.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1849834 sec
 RG 2050
 DW 33.333 usec
 DE 0.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

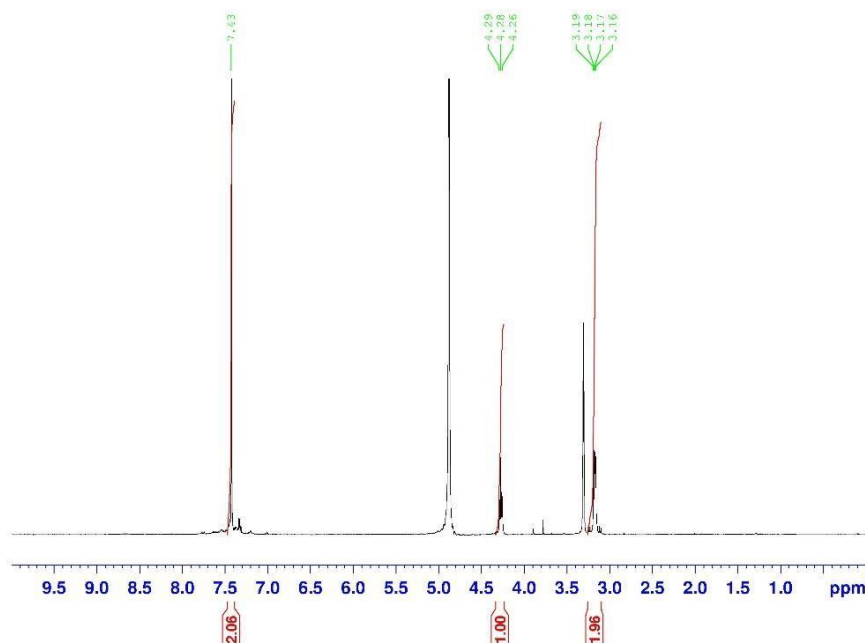
CHANNEL f1
 NUC1 13C
 P1 10.00 usec
 PL1 1.00 dB
 SFO1 62.905280 MHz

CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 70.00 usec
 PL12 -5.00 dB
 PL13 -5.00 dB
 PL2 2.50 dB
 SFO2 250.1310005 MHz

F2 - Processing parameters
 SI 32768
 SF 62.8952330 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1.23 5,5'-[1,4-phenyl]bis((S)-2-aminopent-4-ensäure) (3l):

Parpart SP159 1H CD3OD



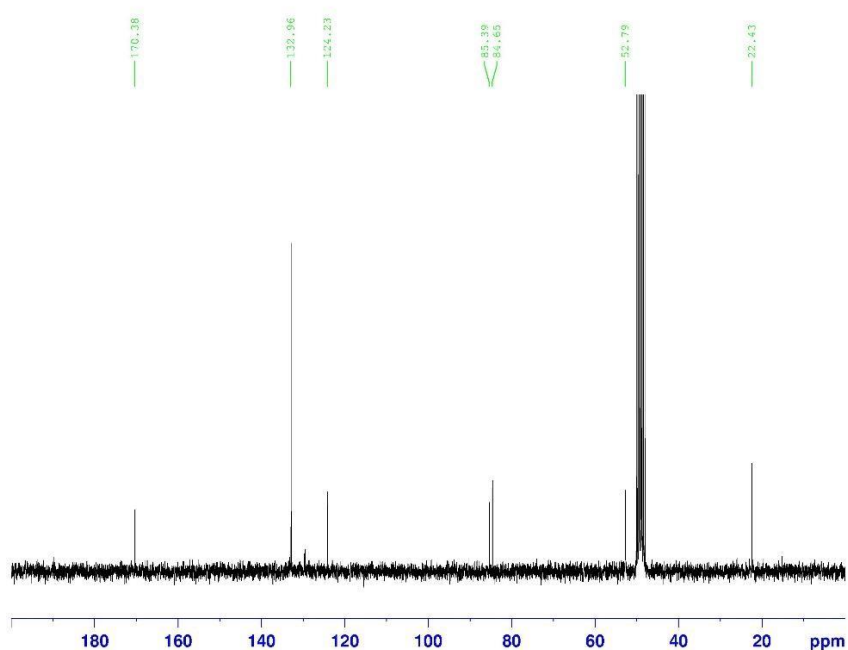
Current Data Parameters
NAME 140416.u329
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140416
Time 13.28
INSTRUM spect
PROBHD 5 mm PABBO SB
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318334 MHz

F2 - Processing parameters
ST 32768
SF 300.1300371 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Parpart SP159 13C CD3OD



Current Data Parameters
NAME 140416.707
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140416
Time 23.52
INSTRUM spect
PROBHD 5 mm PABBO SB
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.1 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999999 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015780 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
S 32768
SF 62.8951406 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2 Chiral-HPLC

2.1 (S)-2-Amino-5-[4-fluorophenyl]pent-4-insäure (3g):

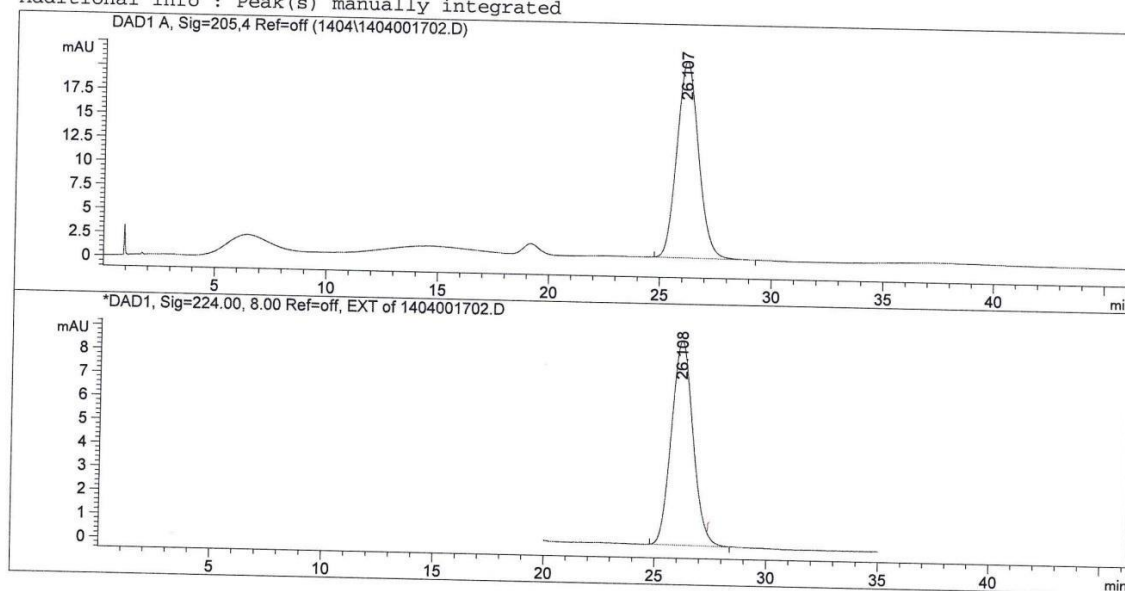
Data File C:\CHEM32\1\DATA\1404\1404001702.D
Sample Name: SP146

Parpart

```
=====
Acq. Operator   : SYSTEM                      Seq. Line :    3
Acq. Instrument : LC4                        Location  : Vial 2
Injection Date  : 4/17/2014 11:07:00 AM      Inj       :    1
                                           Inj Volume: 0.500 µl

Acq. Method     : C:\CHEM32\1\METHODS\PARPART.M
Last changed    : 4/17/2014 9:20:53 AM by SYSTEM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\PARPART.M
Last changed    : 4/23/2014 10:28:42 AM by SYSTEM
                  (modified after loading)
Method Info     : Crownpak CR (-), Perchlorsäure pH 2.0, 1ml/min, 40°C
=====
```

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=205,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.107	BB	1.0054	1385.78687	20.48116	100.0000

Totals : 1385.78687 20.48116

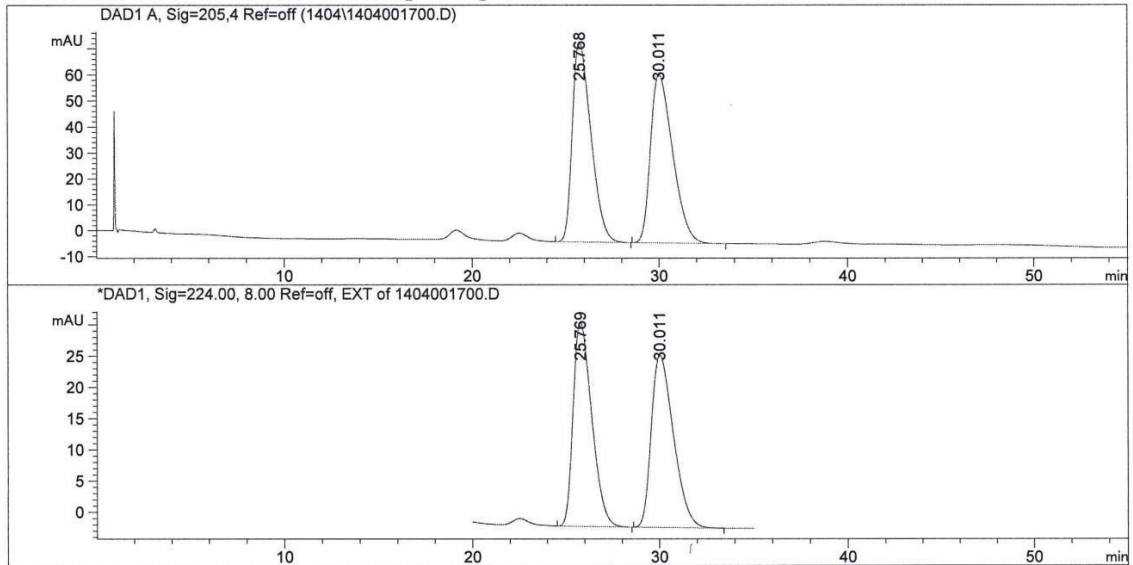
Mutar als 99% ee.

Data File C:\CHEM32\1\DATA\1404\1404001700.D
Sample Name: SP154rac

```
=====
Acq. Operator   : SYSTEM                      Seq. Line :    1
Acq. Instrument : LC4                        Location  : Vial 1
Injection Date  : 4/17/2014 9:15:20 AM      Inj       :    1
                                           Inj Volume: 0.500 µl

Acq. Method     : C:\CHEM32\1\METHODS\PARPART.M
Last changed    : 4/17/2014 9:20:53 AM by SYSTEM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\PARPART.M
Last changed    : 4/17/2014 9:14:28 AM by SYSTEM
Method Info     : Crownpak CR (-), Perchlorsäure pH 2.0, 1ml/min, 40°C
=====
```

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=205,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.768	BB	1.0709	5332.73926	76.90916	50.0389
2	30.011	BB	1.2326	5324.43945	64.80263	49.9611

Totals : 1.06572e4 141.71179

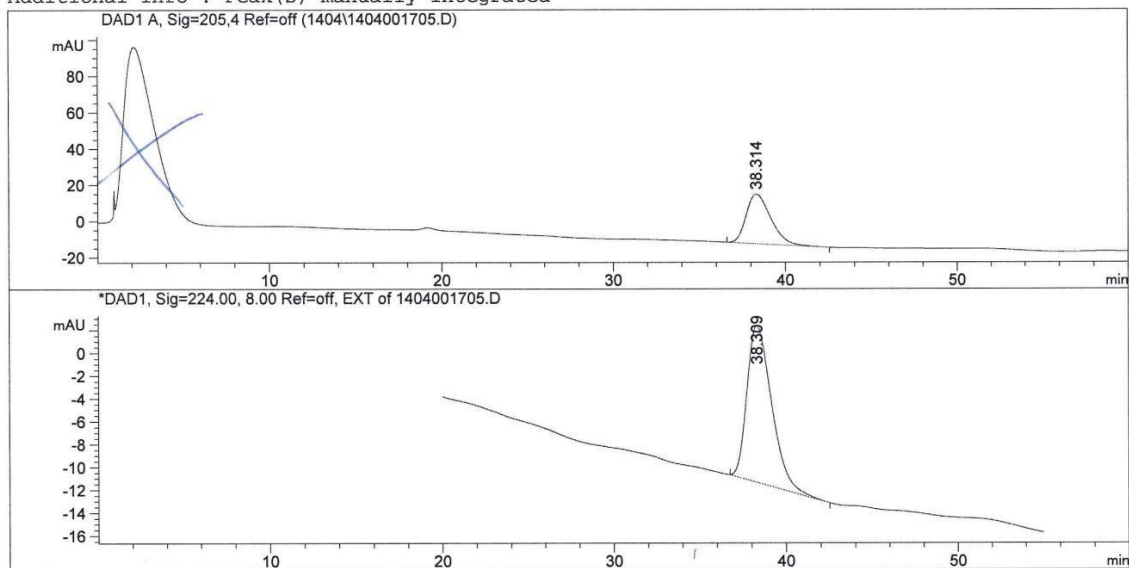
2.2 (S)-2-Amino-5-[3-methoxyphenyl]pent-4-insäure (3j):

Data File C:\CHEM32\1\DATA\1404\1404001705.D
Sample Name: SP150

```
=====
Acq. Operator   : SYSTEM                      Seq. Line :    3
Acq. Instrument : LC4                        Location  : Vial 4
Injection Date  : 4/17/2014 1:17:10 PM        Inj       :    1
                                           Inj Volume: 0.500 µl

Acq. Method     : C:\CHEM32\1\METHODS\PARPART.M
Last changed    : 4/17/2014 1:55:29 PM by SYSTEM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\PARPART.M
Last changed    : 5/7/2014 7:57:22 AM by SYSTEM
Method Info     : Crownpaki CR (-), Perchlorsäure pH 2.0, 1ml/min, 40°C
=====
```

Additional Info : Peak(s) manually integrated



Area Percent Report

```
=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
```

Signal 1: DAD1 A, Sig=205,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	38.314	BB	1.4392	2704.11328	27.35693	100.0000
Totals :				2704.11328	27.35693	

Data File C:\CHEM32\1\DATA\1404\1404001103.D
Sample Name: SP157

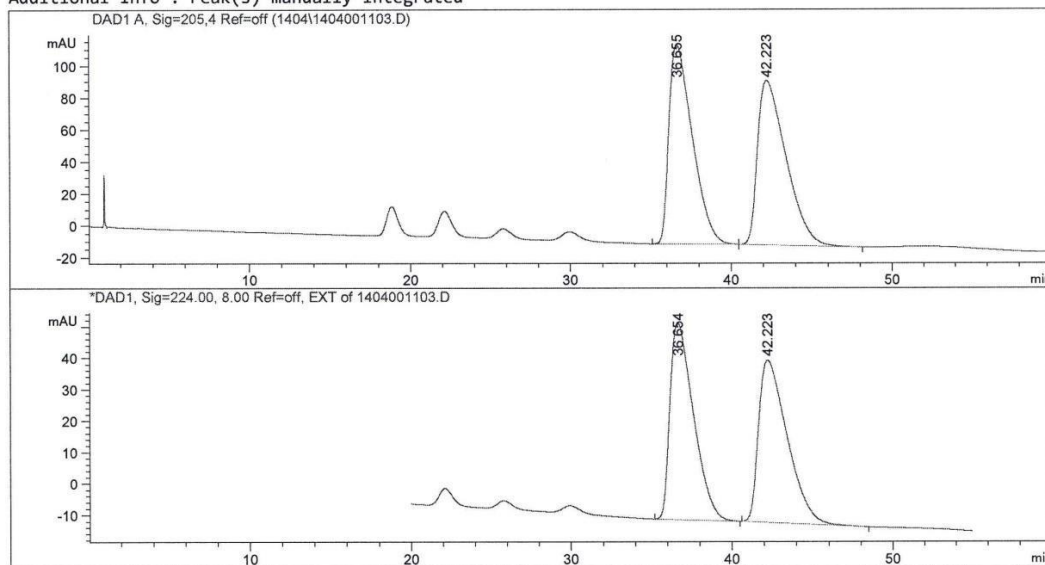
Parpart

=====

Acq. Operator	: SYSTEM	Seq. Line	: 4
Acq. Instrument	: LC4	Location	: Vial 2
Injection Date	: 4/11/2014 12:15:53 PM	Inj	: 1
		Inj Volume	: 0.500 µl

Acq. Method : C:\CHEM32\1\METHODS\PARPART.M
Last changed : 4/11/2014 9:12:33 AM by SYSTEM
Analysis Method : C:\CHEM32\1\METHODS\PARPART.M
Last changed : 5/7/2014 7:57:22 AM by SYSTEM
Method Info : Crownpaki CR (-), Perchlorsäure pH 2.0, 1ml/min, 40°C

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=205,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	36.655	BB	1.5196	1.25903e4	124.52320	49.9968
2	42.223	BB	1.7604	1.25919e4	102.69941	50.0032

Totals : 2.51823e4 227.22261