Electronic Supplementary Material (ESI) for Catalysis Science & Technology.
This journal is © The Royal Society of Chemistry 2015

Supporting information

Iron Catalyzed Chlorination of Benzylic Aldehydes and Ketones

Risto Savela and Reko Leino*
Labroratory of Organic Chemistry, Åbo Akademi University, 20500 Åbo, Finland
reko.leino@abo.fi

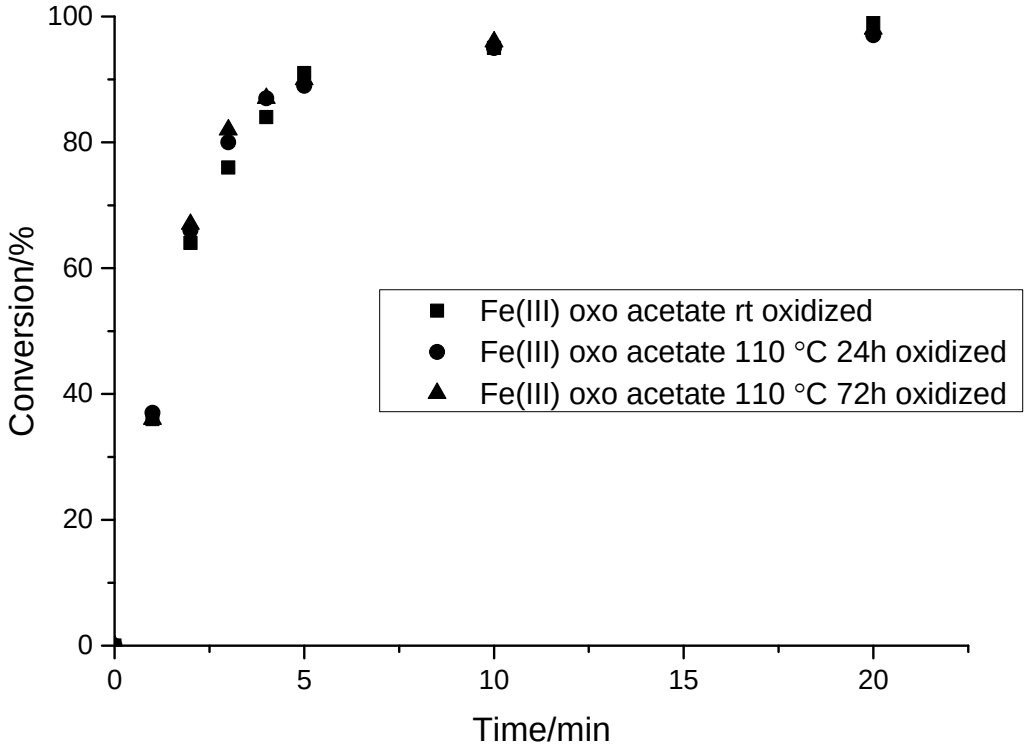
Table of Contents

Catalyst preparation and characterization	2
References	2
Copies of NMR-specta and GC-MS chromatograms	3-60
Benzyl chloride (1)	3-4
(1-Chloroethyl)benzene (2)	5-6
1-(Chloromethyl)-4-methylbenzene (3)	7-8
1-(Chloromethyl)-4-(1,1-dimethylethyl)benzene (4)	9-10
4-(Chloromethyl)-1,1'-biphenyl (5)	11-12
1-(1-Chloroethyl)-4-(trifluoromethyl)benzene (6)	13-14
1-(1-Chloroethyl)-4-chlorobenzene (7)	15-16
1-(1-Chloroethyl)-4-bromobenzene (8)	17-18
1-(1-Chloroethyl)-4-fluorobenzene (9)	19-20
4-(1-Chloroethyl)benzoic acid ethyl ester (10)	21-22
(1-Chloropropyl)benzene (11)	23-25
(1-Chloropentyl)benzene (12)	26-28
1-(1,4-Dichlorobutyl)-4-fluoro-benzene (13)	29-32
(1-Chloro-2,2-dimethylpropyl)-benzene (14)	33-34
1-(Bromomethyl)-4-methylbenzene (15)	35-36
1-(Iodomethyl)-4-methylbenzene (16)	37-38
1-Chloro-1-deuterio-1-phenylethane (17)	39-40
1-(1-Chloroethyl)-3-methyl benzene (18)	41-42
3-(1-Chloroethyl)-benzonitrile (19)	43-44
1-(Chloromethyl)-2-methylbenzene (20)	45-46
1-Chloro-2-(1-chloroethyl)-benzene (21)	47-48
9-Chloro-fluorene (22)	49-50
2-(1-Chloroethyl)naphthalene (23)	51-52
[Chloro(cyclohexyl)methyl]benzene (24)	53-55
1-(Chloroethyl)-4-chlorobenzene (7)	56-57
(1-Chloro-3-buten-1-yl)benzene (26)	58-60

Catalyst Preparation and Characterization

General considerations. The catalysts employed for substrate scope screening were prepared from iron(II) acetate (Sigma Aldrich, 99.99%) by atmospheric oxidation at room temperature or at 110 °C for 24 and 72 hours in a conventional drying oven yielding tile red powder with iron contents of 31.25%, 34.65% and 37.39% respectively. Details on preparation, yields and characterization of the catalysts by IR, elemental analysis, Mössbauer spectroscopy and ICP are given in earlier work.[1]

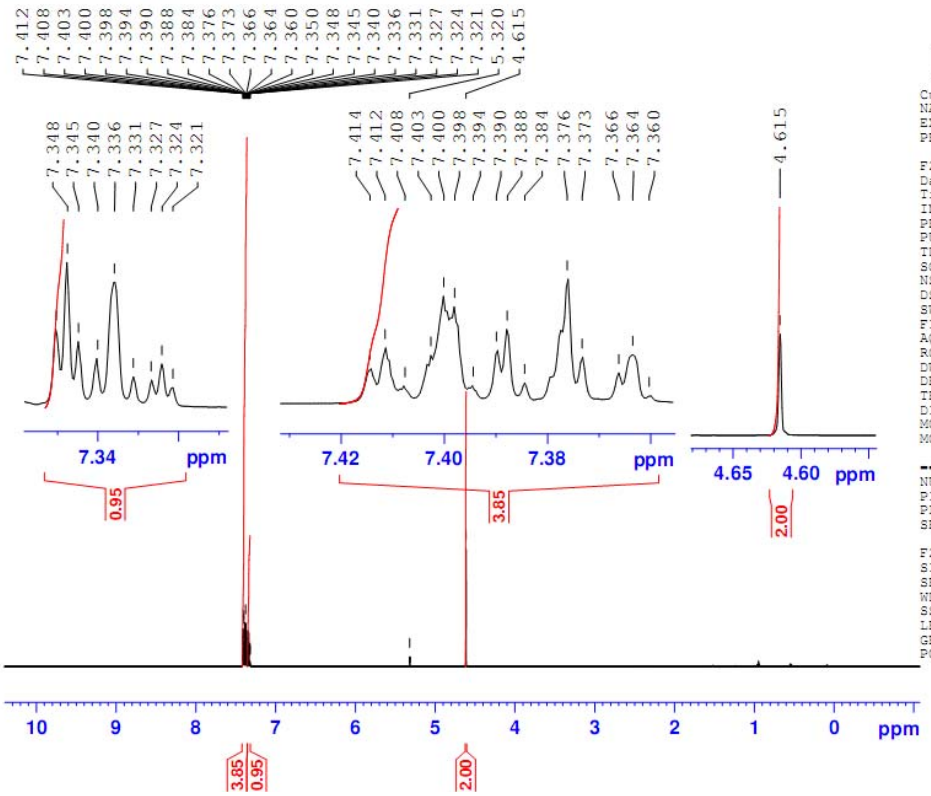
Verification of consistent reactivity: Chlorination of acetophenone (2 mmol) using 4 mol-% of Fe(III) catalysts in ethyl acetate (1 mL) with 1.5 eq of Me_3SiCl and 1.2 eq of Et_3SiH.

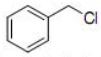


References:

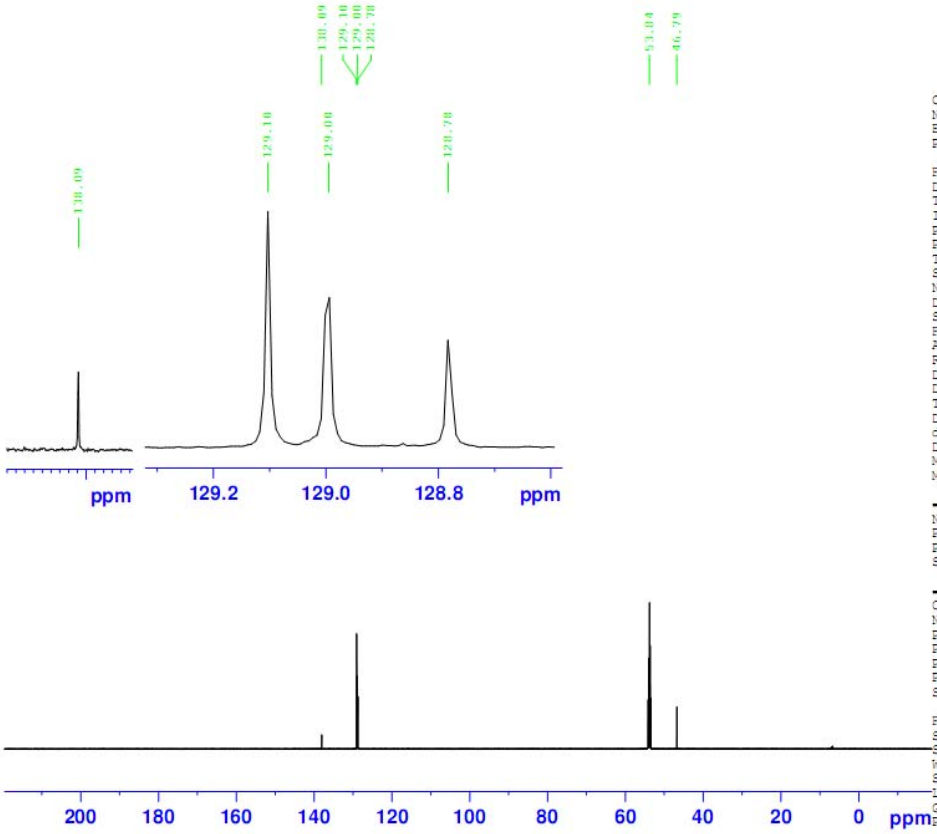
(1) R. Savela, R. Leino, *Synthesis* **2015**, in press.

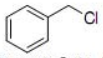
Copies of Spectra:






```
Current Data Parameters
NAME                  B-Cl
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130531
Time                  13.51
INSTRUM               av600
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT            CD2Cl2
NS                      32
DS                       0
SWH               6887.052 Hz
FIDRES            0.105088 Hz
AQ               4.7579136 sec
RG                   161.3
DW                  72.600 usec
DE                   6.00 usec
TE                  298.0 K
D1              1.00000000 sec
MCREST    0 sec
MCWRK           0.01500000 sec

-------- CHANNEL f1 --------
NUC1                     1H
P1                   11.60 usec
PL1                  -2.00 dB
SFO1           600.1328163 MHz

F2 - Processing parameters
SI                    32768
SF            600.1300189 MHz
WDW                      no
SSB       0
LB        0 Hz
GB        0
PC                    1.40
```

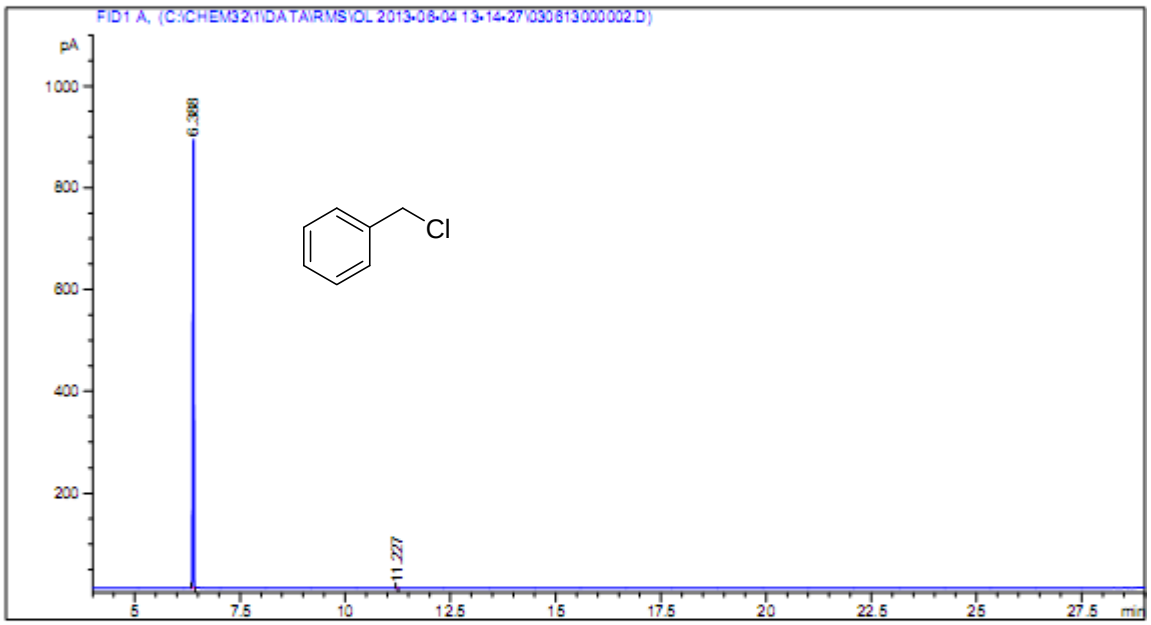





```
Current Data Parameters
NAME                  B-Cl
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130531
Time                  14.47
INSTRUM               av600
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              35971.223 Hz
FIDRES            0.548877 Hz
AQ               0.9109504 sec
RG                 20642.5
DW                  13.900 usec
DE                   6.00 usec
TE                  298.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
MCREST    0 sec
MCWRK           0.01500000 sec

-------- CHANNEL f1 --------
NUC1                    13C
P1                    9.00 usec
PL1       0 dB
SFO1           150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2            waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                  -2.00 dB
PL12                 13.50 dB
PL13                 20.00 dB
SFO2           600.1324005 MHz

F2 - Processing parameters
SI                    32768
SF            150.9027469 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.00
```

Data File C:\CHEM32\1\DATA\RMS\OL 2013-06-04 13-14-27\030613000002.D
Sample Name: Purity B-Cl DCM

Acq. Operator : RMS
Seq. Line : 2
Acq. Instrument : Instrument 1
Location : Vial 2
Injection Date : 04-Jun-13, 13:54:36
Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\OL 2013-06-04 13-14-27\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\RMS1.M
Last changed : 6/5/2013 3:13:06 PM by OL
(modified after loading)
Method Info : ÅAGC-default



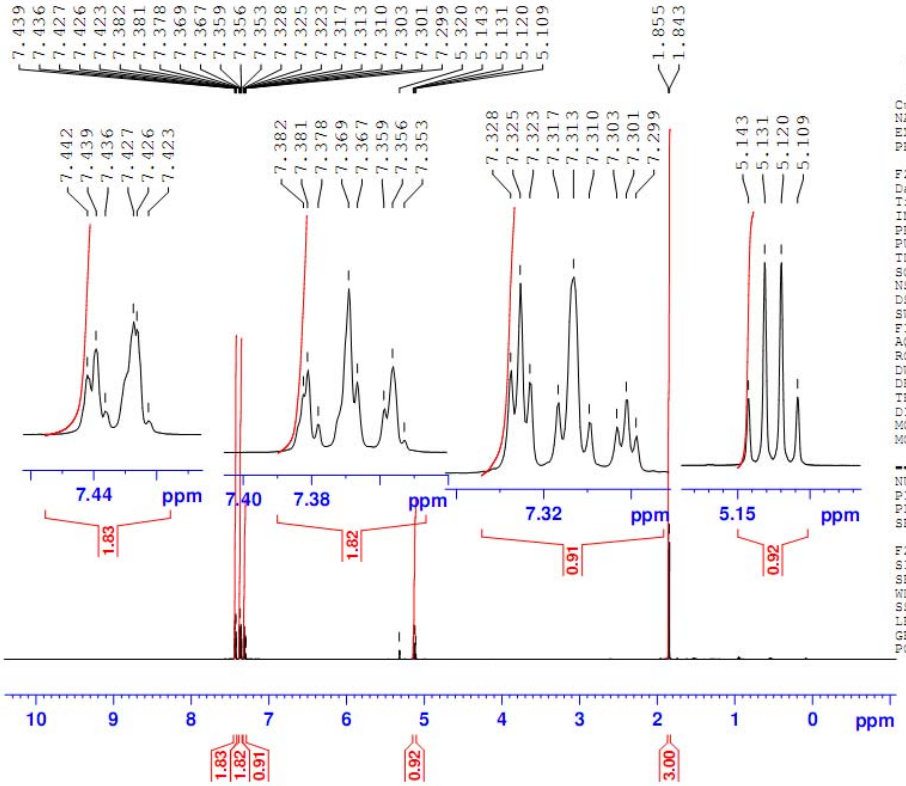
Area Percent Report

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

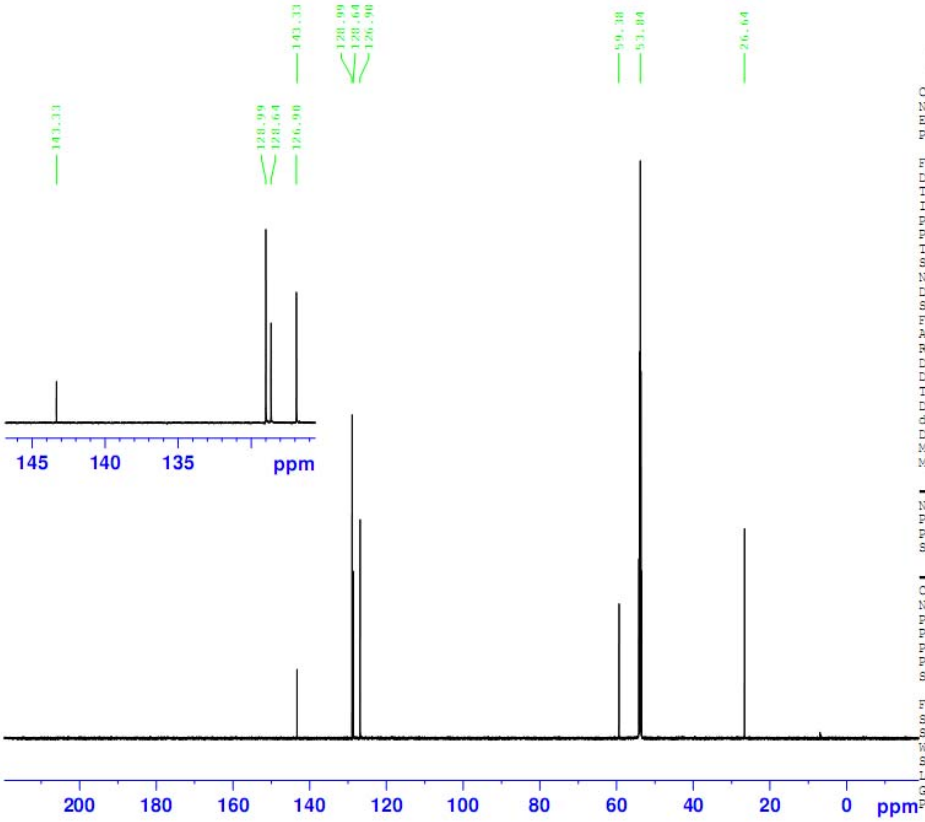
Signal 1: FID1 A,

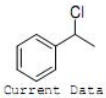
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	6.388	BB	0.0235	1321.59290	879.87280	99.80703
2	11.227	BB	0.0227	2.55516	1.79038	0.19297

Totals : 1324.14805 881.66318



```
Current Data Parameters
NAME                 A-Cl
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20130531
Time               12.46
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    32
DS                     0
SWH             6887.052 Hz
FIDRES          0.105088 Hz
AQ             4.7579136 sec
RG                161.3
DW                72.600 usec
DE                 6.00 usec
TE                298.0 K
D1             1.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                   1H
P1                 11.60 usec
PL1                -2.00 dB
SFO1         600.1328163 MHz

F2 - Processing parameters
SI                 32768
SF          600.1300189 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```

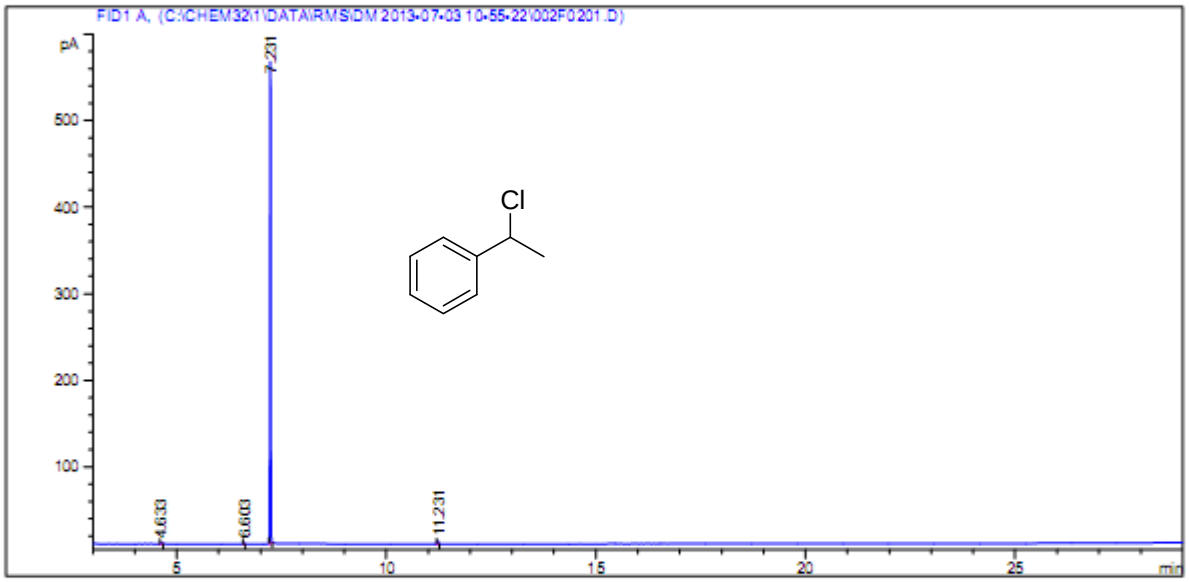





```
Current Data Parameters
NAME                 A-Cl
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20130531
Time               13.42
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   855
DS                     4
SWH            35971.223 Hz
FIDRES          0.548877 Hz
AQ             0.9109504 sec
RG               20642.5
DW                13.900 usec
DE                 6.00 usec
TE                298.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
MCREST    0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                  13C
P1                 9.00 usec
PL1        0 dB
SFO1        150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2          waltz16
NUC2                   1H
PCPD2             80.00 usec
PL2                -2.00 dB
PL12               13.50 dB
PL13               20.00 dB
SFO2         600.1324005 MHz

F2 - Processing parameters
SI                 32768
SF          150.9027459 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-07-03 10-55-22\002F0201.D
Sample Name: A-Cl Purity

Acq. Operator : RMS Seq. Line : 2
Acq. Instrument : Instrument 1 Location : Vial 2
Injection Date : 03-Jul-13, 11:18:02 Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-07-03 10-55-22\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 7/3/2013 12:43:14 PM by RMS
(modified after loading)
Method Info : ÅAGC-default



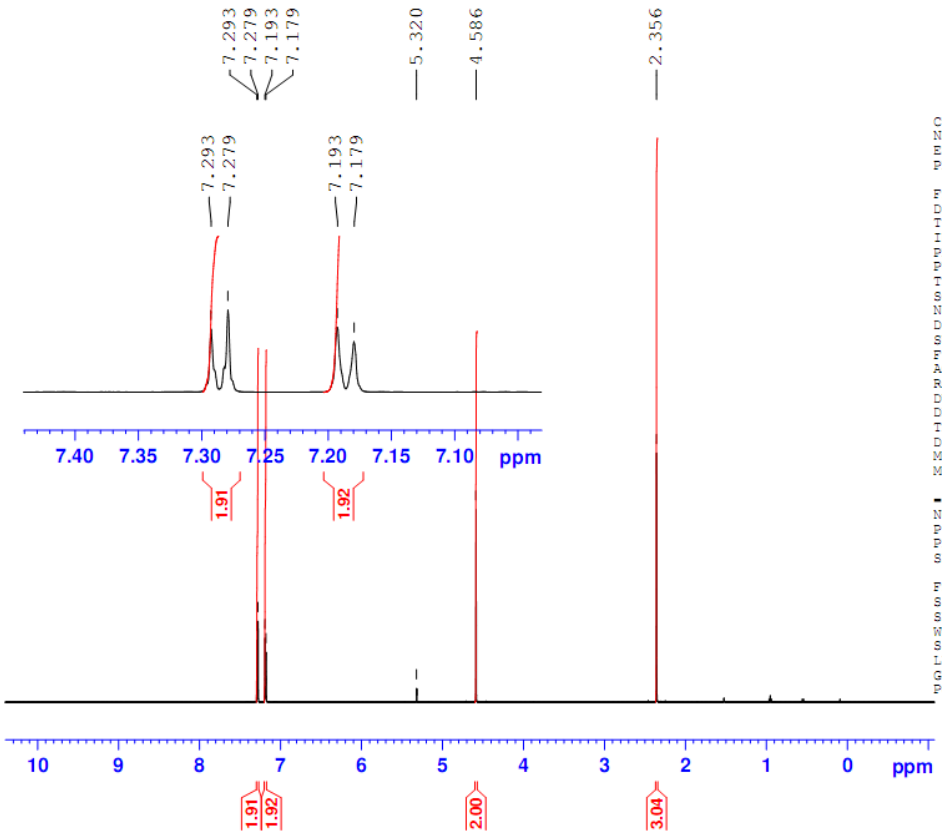
Area Percent Report

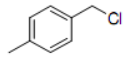
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID1 A,

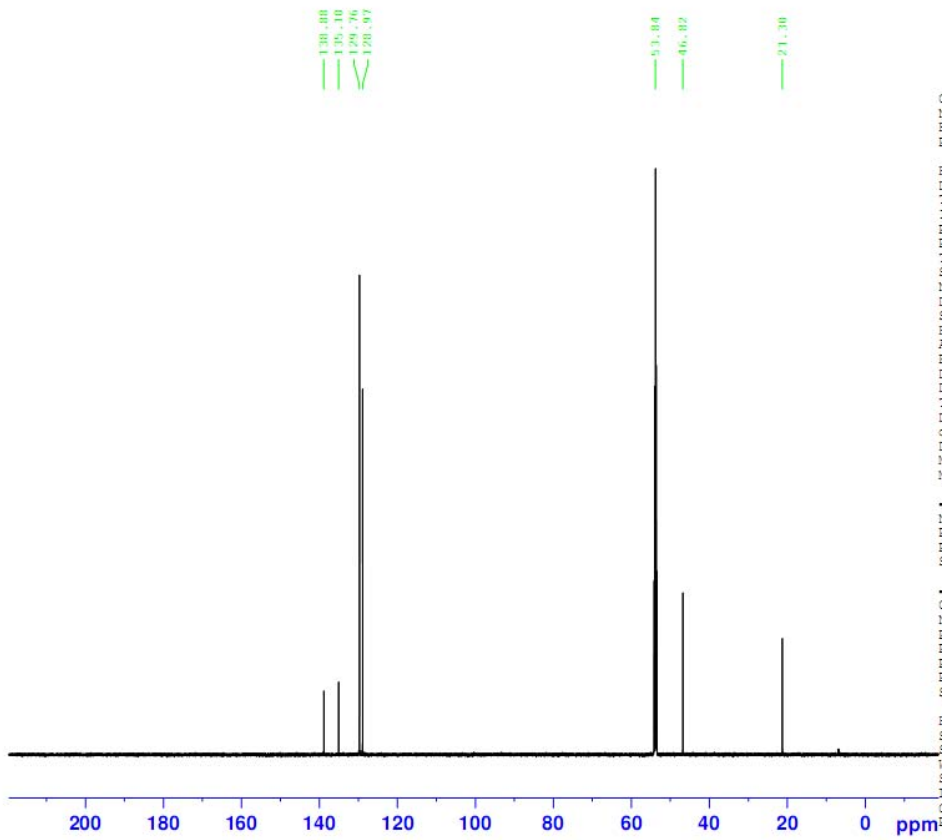
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	4.633	BB	0.0274	3.25627	1.77267	0.41275
2	6.603	BB	0.0204	1.87193	1.41913	0.23728
3	7.231	BB	0.0224	778.43274	554.49200	98.67001
4	11.231	BB	0.0222	5.36447	3.86966	0.67997

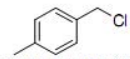
Totals : 788.92540 561.55347






```
Current Data Parameters
NAME          p-Me-B-Cl1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_            20130912
Time               11.32
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    16
DS                     0
SWH             6887.052 Hz
FIDRES          0.105088 Hz
AQ             4.7579136 sec
RG                   128
DW                72.600 usec
DE                 6.00 usec
TE                298.0 K
D1            1.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                  1H
P1                11.60 usec
PL1               -2.00 dB
SFO1        600.1328163 MHz

F2 - Processing parameters
SI                 32768
SF          600.1300191 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.40
```

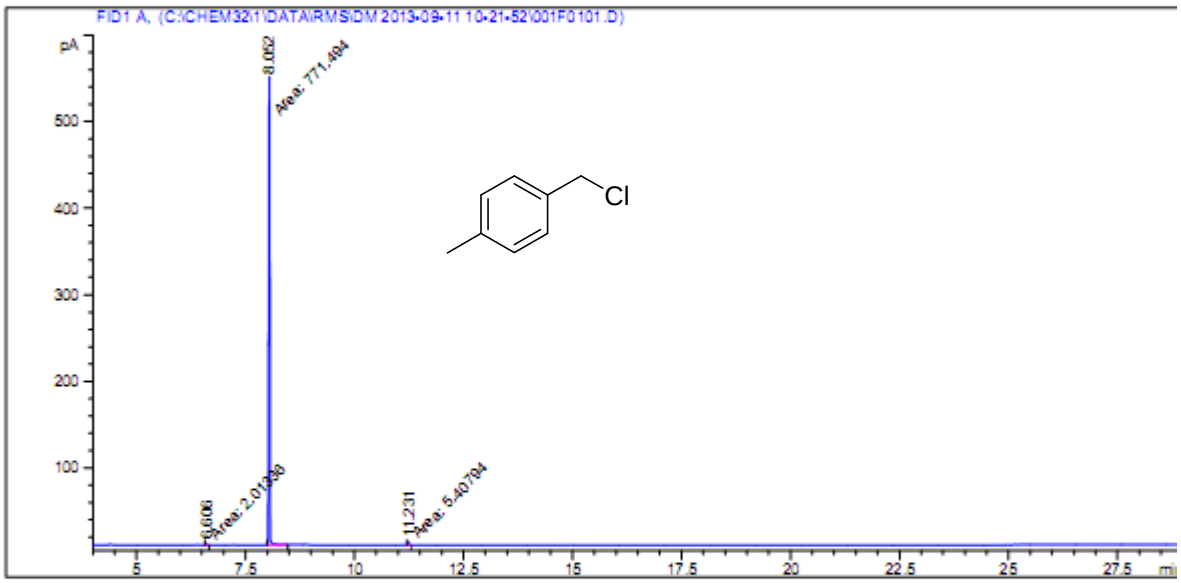





```
Current Data Parameters
NAME          p-Me-B-Cl1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_            20130912
Time               12.23
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   962
DS                     4
SWH            35971.223 Hz
FIDRES          0.548877 Hz
AQ             0.9109504 sec
RG                 16384
DW                13.900 usec
DE                 6.00 usec
TE                298.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
MCREST    0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                 13C
P1                 9.00 usec
PL1       0 dB
SFO1        150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2         waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              13.50 dB
PL13              20.00 dB
SFO2        600.1324005 MHz

F2 - Processing parameters
SI                 32768
SF          150.9027467 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-09-11 10-21-52\001F0101.D
Sample Name: p-M-B-Cl purity

Acq. Operator : RMS Seq. Line : 1
Acq. Instrument : Instrument 1 Location : Vial 1
Injection Date : 11-Sep-13, 10:26:24 Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-09-11 10-21-52\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 9/12/2013 12:22:47 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

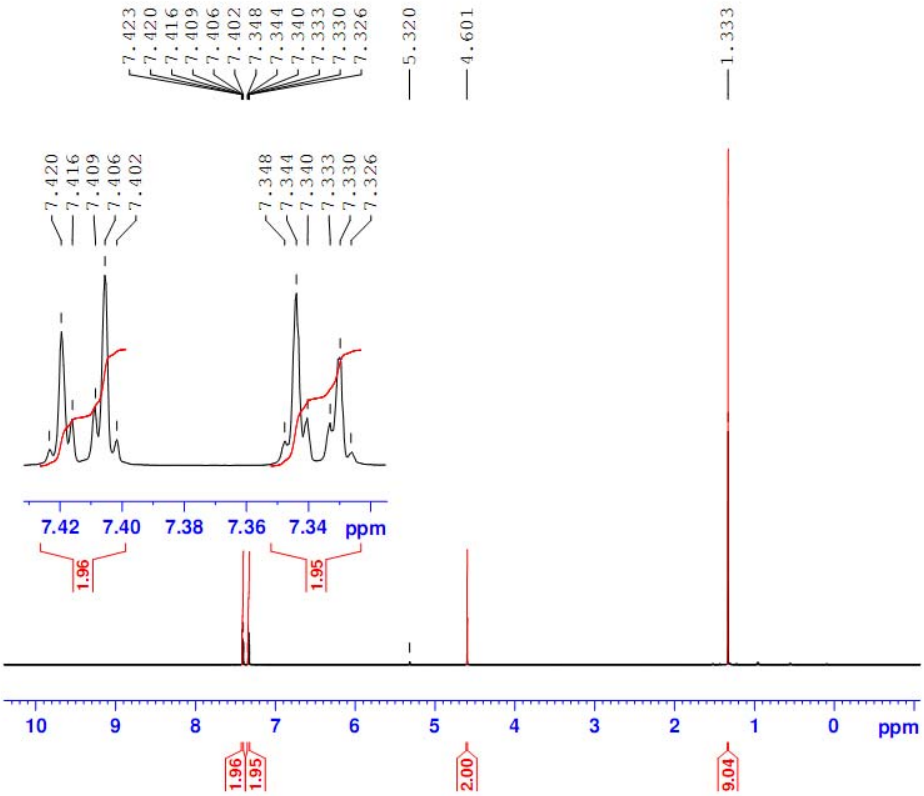


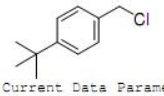
Area Percent Report

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

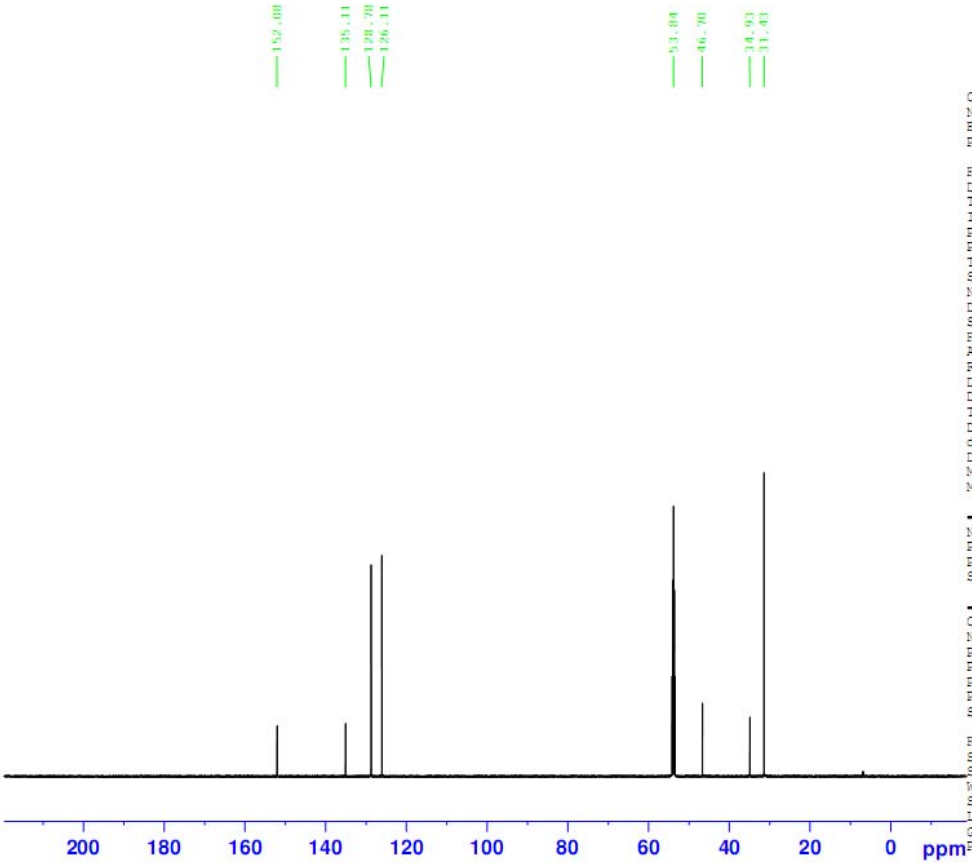
Signal 1: FID1 A,

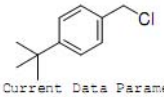
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	6.606	MM	0.0230	2.01336	1.46007	0.25848
2	8.052	MM	0.0237	771.49438	542.41498	99.04723
3	11.231	MM	0.0243	5.40794	3.70305	0.69429






```
Current Data Parameters
NAME          p-tBu-B-Cl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20131101
Time               13.19
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    16
DS                     0
SWH             6887.052 Hz
FIDRES          0.105088 Hz
AQ            4.7579136 sec
RG                  80.6
DW                72.600 usec
DE                  6.00 usec
TE                298.0 K
D1            1.00000000 sec
MCREST   0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                   1H
P1                 11.60 usec
PL1                -2.00 dB
SFO1        600.1328163 MHz

F2 - Processing parameters
SI                 32768
SF          600.1300188 MHz
WDW                   no
SSB      0
LB       0 Hz
GB       0
PC                 1.00
```

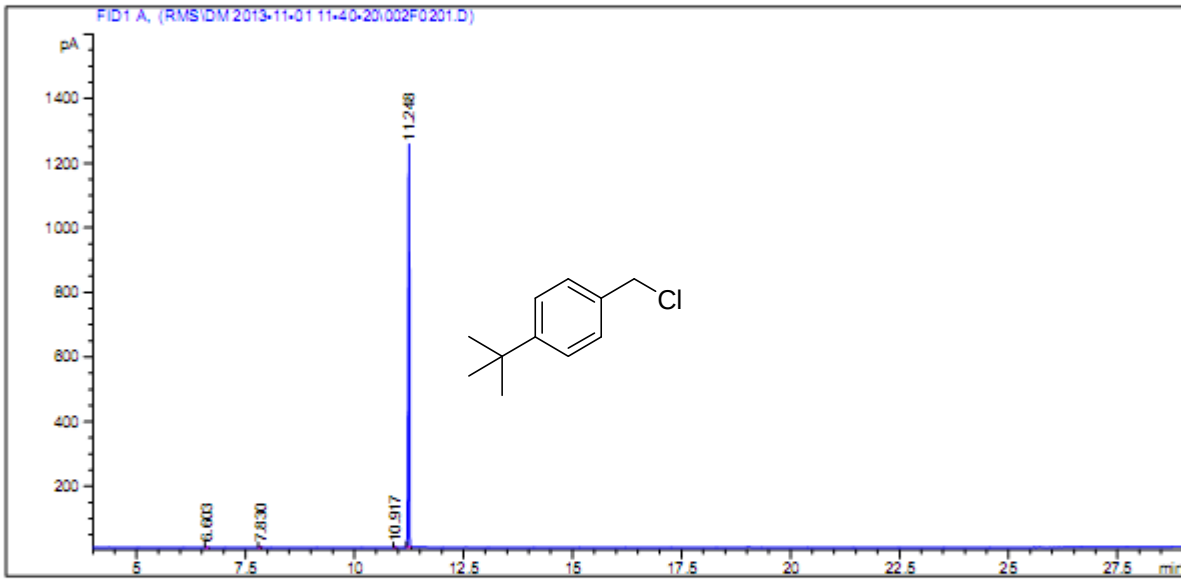





```
Current Data Parameters
NAME          p-tBu-B-Cl
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20131101
Time               14.06
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   879
DS                     4
SWH            35971.223 Hz
FIDRES          0.548877 Hz
AQ            0.9109504 sec
RG                 16384
DW                13.900 usec
DE                  6.00 usec
TE                298.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
MCREST   0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                  13C
P1                 9.00 usec
PL1      0 dB
SFO1        150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2         waltz16
NUC2                   1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              13.50 dB
PL13              20.00 dB
SFO2        600.1324005 MHz

F2 - Processing parameters
SI                 32768
SF          150.9027447 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-11-01 11-40-20\002F0201.D
Sample Name: p-Tbu-B-Cl purity

Acq. Operator : RMS Seq. Line : 2
Acq. Instrument : Instrument 1 Location : Vial 2
Injection Date : 01-Nov-13, 12:16:45 Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-11-01 11-40-20\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 11/1/2013 12:57:06 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

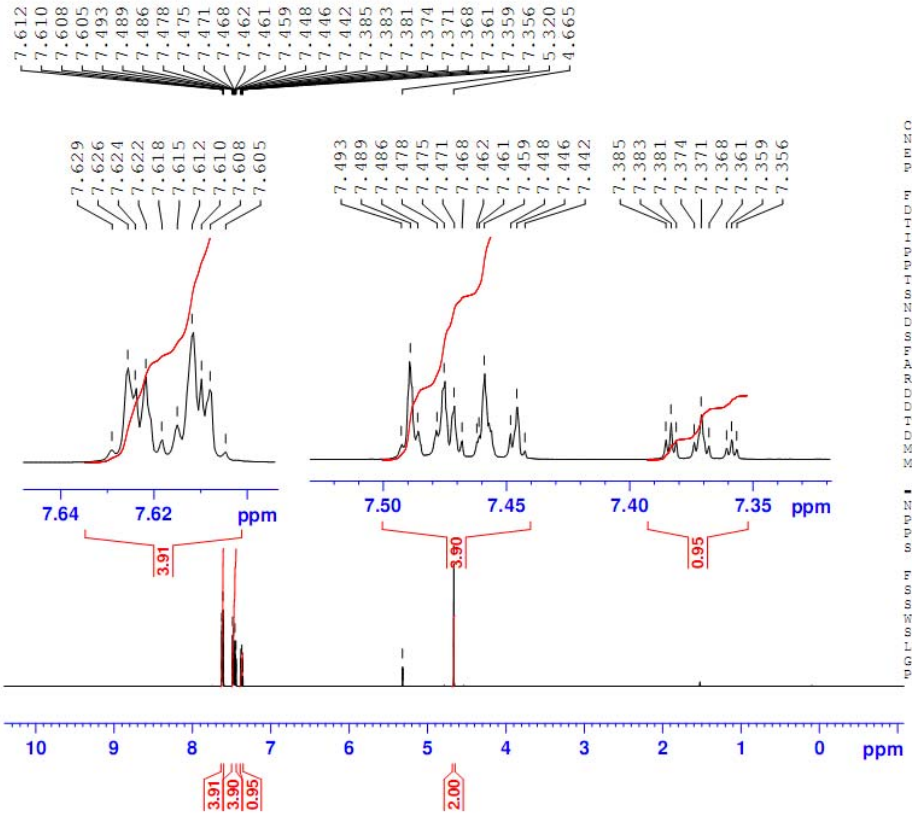


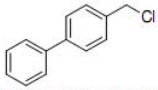
Area Percent Report

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

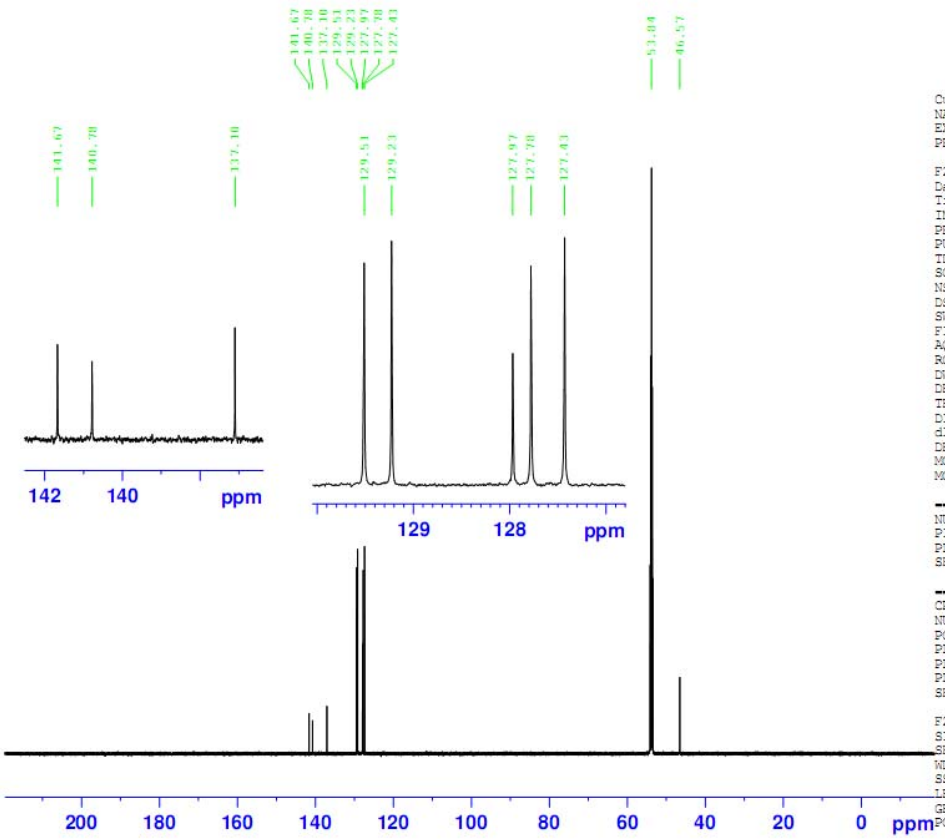
Signal 1: FID1 A,

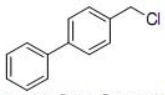
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	6.603	BB	0.0217	4.34819	3.23939	0.19277
2	7.830	BB	0.0273	3.14687	1.72218	0.13951
3	10.917	BB	0.0222	4.76371	3.43103	0.21119
4	11.248	BB	0.0290	2243.40552	1244.14856	99.45653






```
Current Data Parameters
NAME          p-Ph-B-Cl1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130912
Time               10.35
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    32
DS                     0
SWH            6887.052 Hz
FIDRES         0.105088 Hz
AQ            4.7579136 sec
RG                   181
DW               72.600 usec
DE                6.00 usec
TE                298.0 K
D1            1.00000000 sec
MCREST   0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                  1H
P1                11.60 usec
PL1               -2.00 dB
SFO1        600.1328163 MHz

F2 - Processing parameters
SI                 32768
SF          600.1300188 MHz
WDW                   no
SSB      0
LB       0 Hz
GB       0
PC                 1.00
```

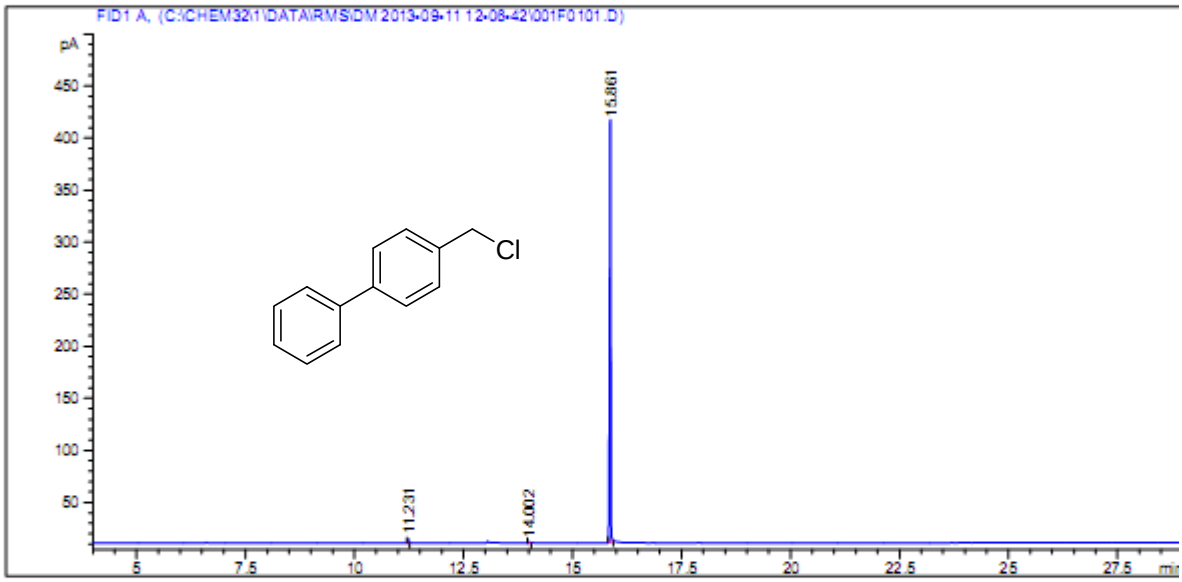





```
Current Data Parameters
NAME          p-Ph-B-Cl1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130912
Time               11.25
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   919
DS                     4
SWH           35971.223 Hz
FIDRES         0.548877 Hz
AQ            0.9109504 sec
RG                 16384
DW               13.900 usec
DE                6.00 usec
TE                298.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
MCREST   0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                 13C
P1                9.00 usec
PL1       0 dB
SFO1        150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2         waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              13.50 dB
PL13              20.00 dB
SFO2        600.1324005 MHz

F2 - Processing parameters
SI                 32768
SF          150.9027470 MHz
WDW                   EM
SSB      0
LB                1.00 Hz
GB       0
PC                 1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-09-11 12-06-42\001F0101.D
Sample Name: p-Ph-B-Cl purity

Acq. Operator : RMS
Seq. Line : 1
Acq. Instrument : Instrument 1
Location : Vial 1
Injection Date : 11-Sep-13, 12:11:38
Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-09-11 12-06-42\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 9/12/2013 12:21:28 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

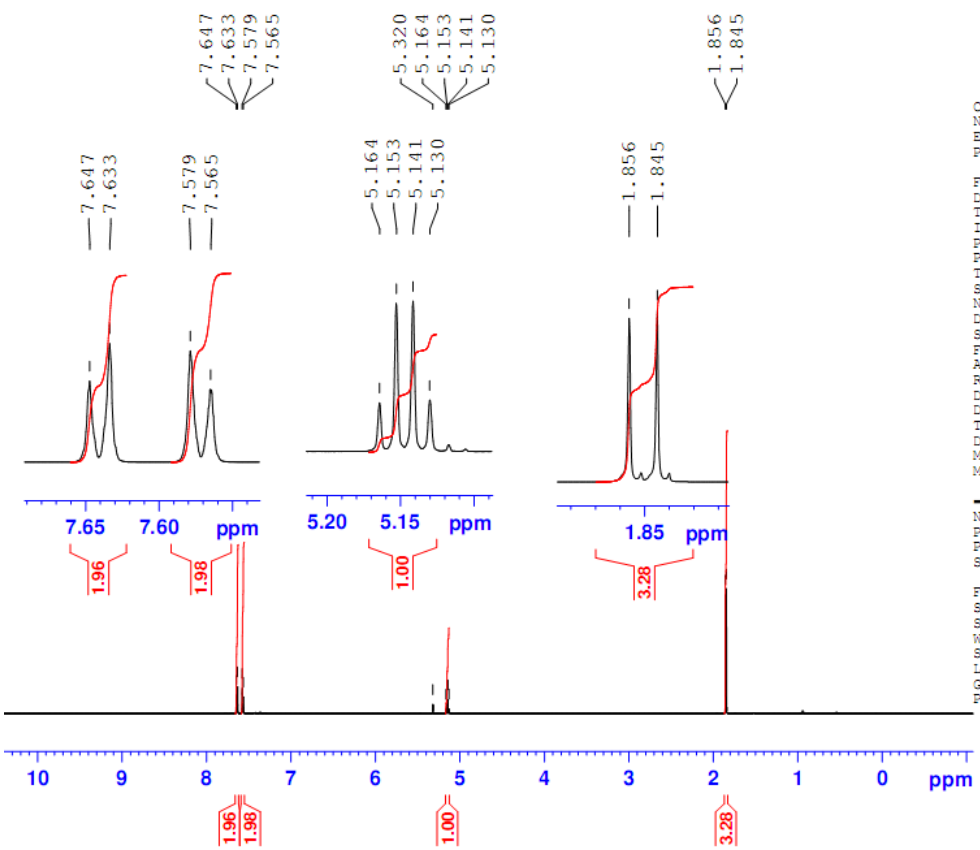


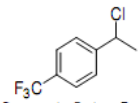
Area Percent Report

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

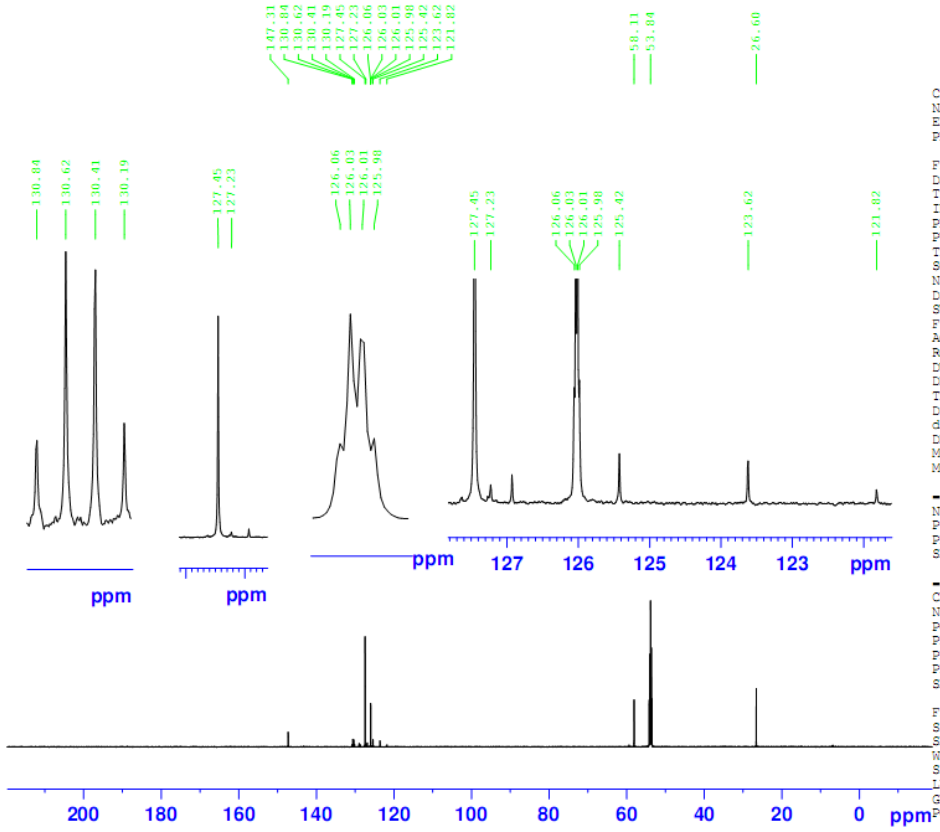
Signal 1: FID1 A,

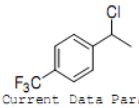
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	11.231	BB	0.0210	5.30022	3.85973	0.80714
2	14.002	BB	0.0263	2.07267	1.25577	0.31564
3	15.861	BB	0.0247	649.29034	404.32574	98.87722






```
Current Data Parameters
NAME          p-F3C-A-Cl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20131017
Time               14.34
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CD2Cl2
NS                    32
DS                     0
SWH            6887.052 Hz
FIDRES         0.105088 Hz
AQ            4.7579136 sec
RG                   181
DW               72.600 usec
DE                6.00 usec
TE               298.0 K
D1            1.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                  1H
P1                11.60 usec
PL1               -2.00 dB
SFO1         600.1328163 MHz

F2 - Processing parameters
SI                 32768
SF          600.1300188 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                  1.40
```

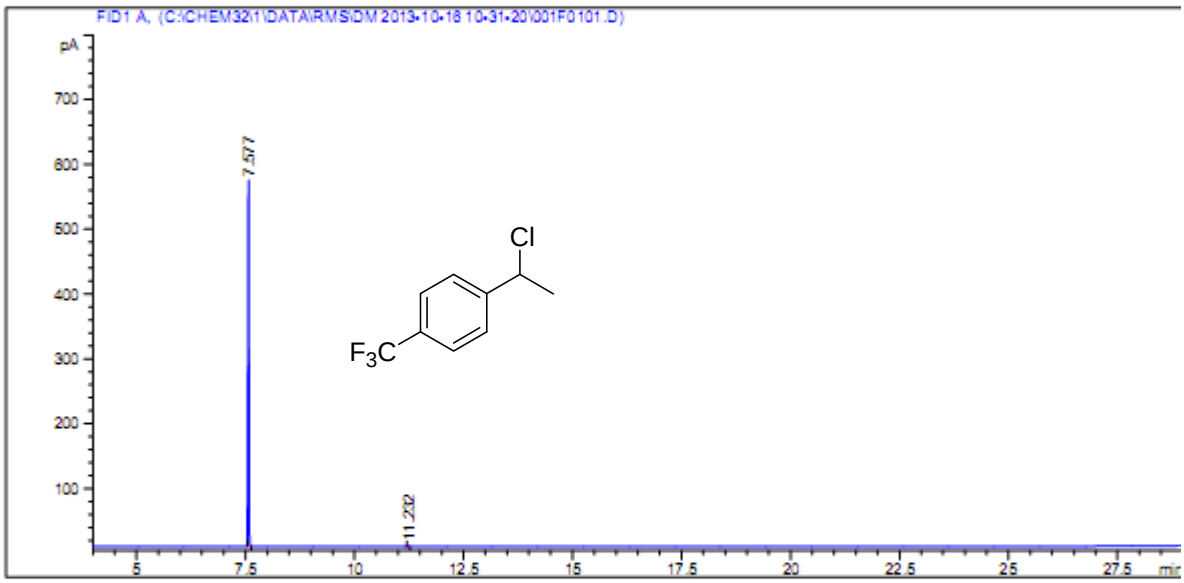





```
Current Data Parameters
NAME        p-CF3-A-Cl2
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20131018
Time               12.41
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2400
DS                    0
SWH           35971.223 Hz
FIDRES         0.548877 Hz
AQ            0.9109504 sec
RG              14596.5
DW               13.900 usec
DE                6.00 usec
TE               298.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
MCREST    0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                 13C
P1                9.00 usec
PL1       0 dB
SFO1        150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2         waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              13.50 dB
PL13              20.00 dB
SFO2         600.1324005 MHz

F2 - Processing parameters
SI                 32768
SF          150.9027413 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-10-16 10-31-20\001F0101.D
Sample Name: p-CF3-A-Cl purity

Acq. Operator : RMS
Seq. Line : 1
Acq. Instrument : Instrument 1
Location : Vial 1
Injection Date : 16-Oct-13, 10:32:55
Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-10-16 10-31-20\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 10/16/2013 11:27:49 AM by RMS
(modified after loading)
Method Info : ÅAGC-default

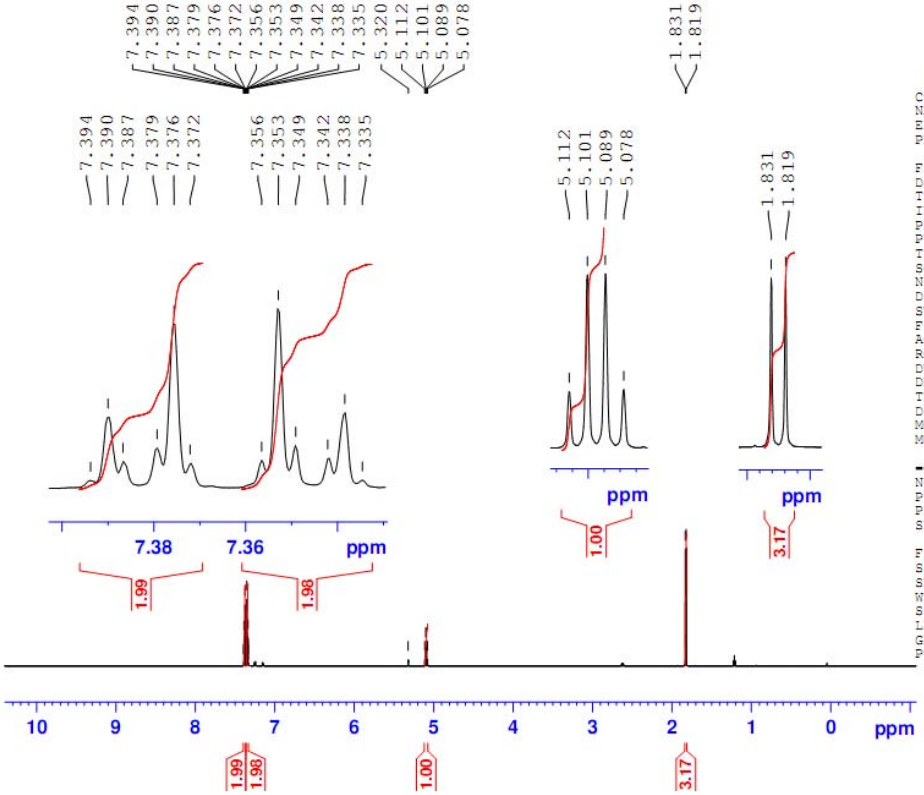


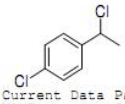
Area Percent Report

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

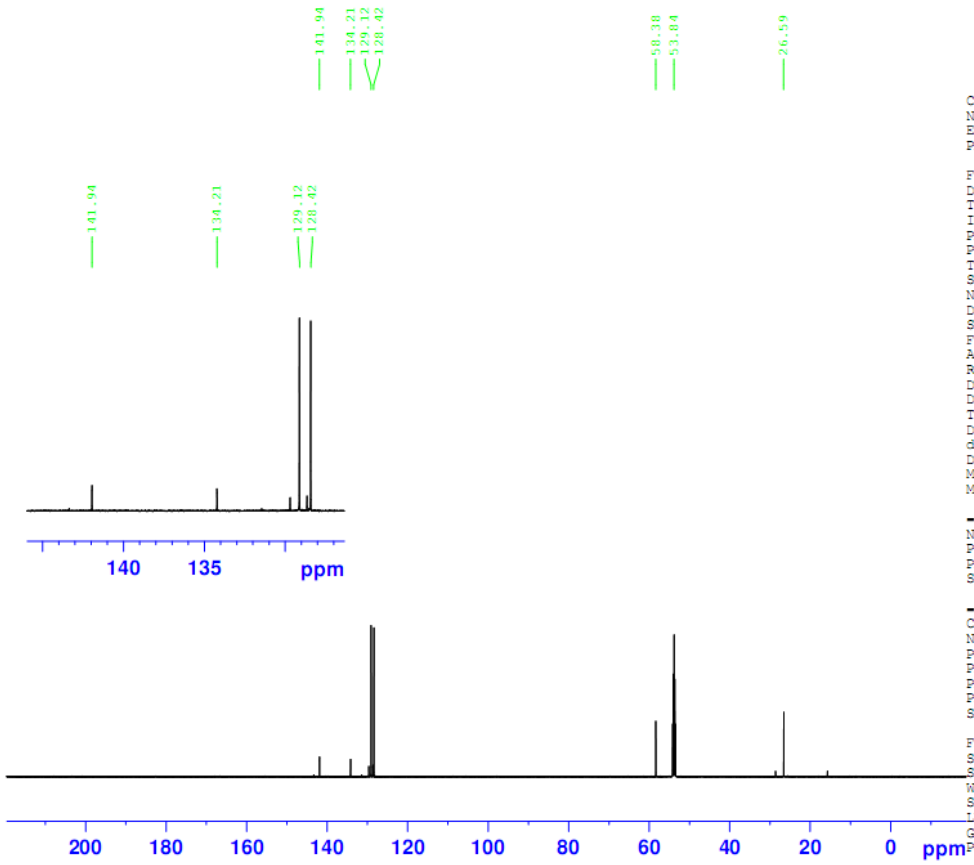
Signal 1: FID1 A,

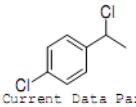
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	7.577	BB	0.0221	780.19745	564.97729	99.52004
2	11.232	BB	0.0215	3.76271	2.66812	0.47996





```
Current Data Parameters
NAME          p-Cl-A-Cl 1s
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20131219
Time                11.38
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    16
DS                     0
SWH             6887.052 Hz
FIDRES          0.105088 Hz
AQ             4.7579136 sec
RG                   114
DW                72.600 usec
DE                  6.00 usec
TE                298.0 K
D1            1.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                  1H
P1                 11.60 usec
PL1                -2.00 dB
SFO1         600.1328163 MHz

F2 - Processing parameters
SI                 32768
SF          600.1300188 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

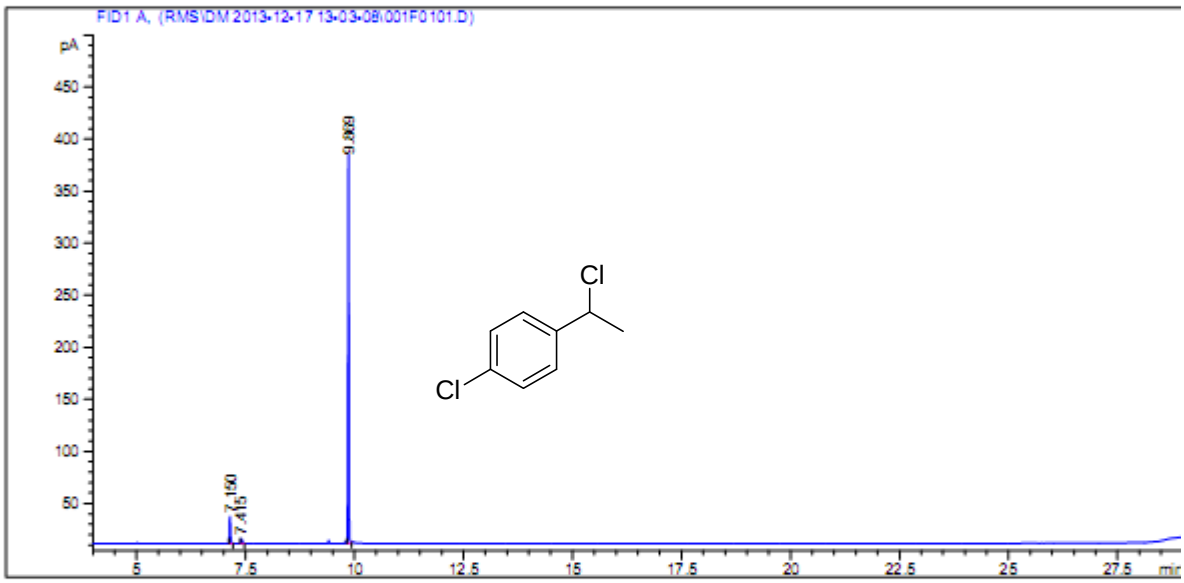




```
Current Data Parameters
NAME          p-Cl-A-Cl 1s
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20131219
Time                12.33
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            35971.223 Hz
FIDRES          0.548877 Hz
AQ             0.9109504 sec
RG                 16384
DW                13.900 usec
DE                  6.00 usec
TE                298.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
MCREST    0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                 13C
P1                  9.00 usec
PL1       0 dB
SFO1        150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               13.50 dB
PL13               20.00 dB
SFO2         600.1324005 MHz

F2 - Processing parameters
SI                 32768
SF          150.9027460 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                  1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-12-17 13-03-08\001F0101.D
Sample Name: p-Cl-A-Cl purity 1s

Acq. Operator : RMS
Seq. Line : 1
Acq. Instrument : Instrument 1
Location : Vial 1
Injection Date : 17-Dec-13, 13:04:35
Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-12-17 13-03-08\ÅA-DEFAULT.M
Last changed : 11/20/2013 12:14:04 PM by RMS
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 12/17/2013 1:59:49 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

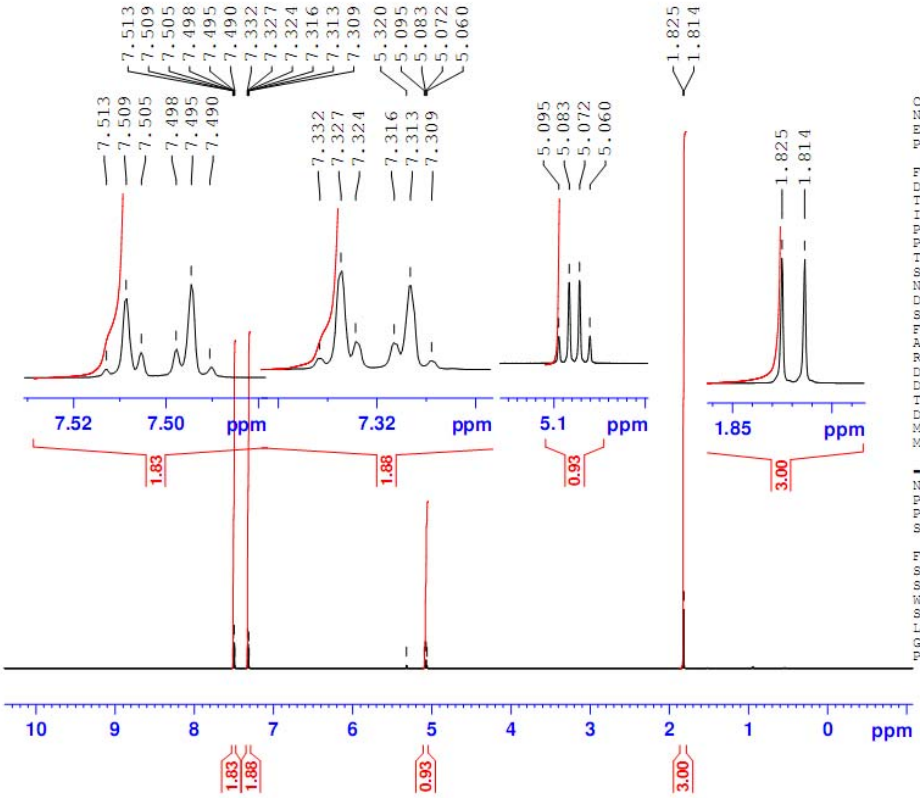


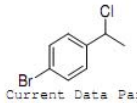
Area Percent Report

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

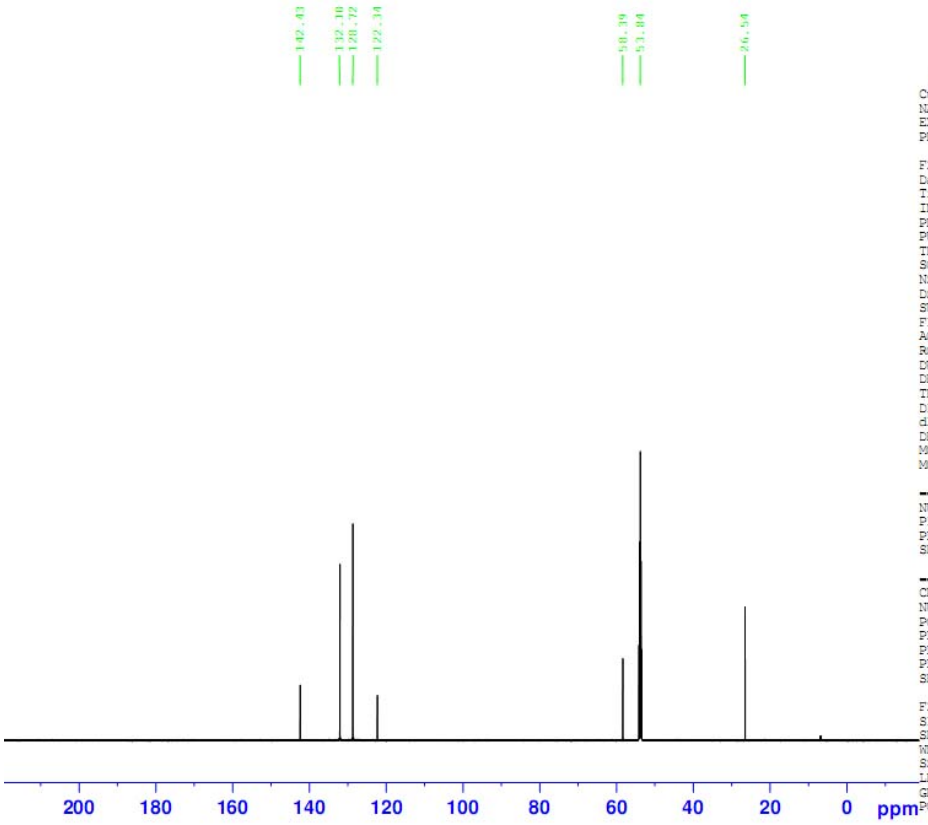
Signal 1: FID1 A,

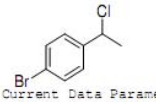
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	7.150	BB	0.0244	40.90263	25.92203	6.94844
2	7.415	BB	0.0320	10.46317	4.88491	1.77746
3	9.869	VB	0.0230	537.29358	369.42007	91.27411






```
Current Data Parameters
NAME          4-br-A-Cl2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130611
Time               14.51
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    16
DS                     0
SWH             6887.052 Hz
FIDRES          0.105088 Hz
AQ             4.7579136 sec
RG                   128
DW                72.600 usec
DE                 6.00 usec
TE                298.0 K
D1             1.00000000 sec
MCREST   0 sec
MCWRK          0.01500000 sec

-------- CHANNEL f1 --------
NUC1                  1H
P1                 11.60 usec
PL1                -2.00 dB
SFO1         600.1328163 MHz

F2 - Processing parameters
SI                 32768
SF           600.1300189 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```

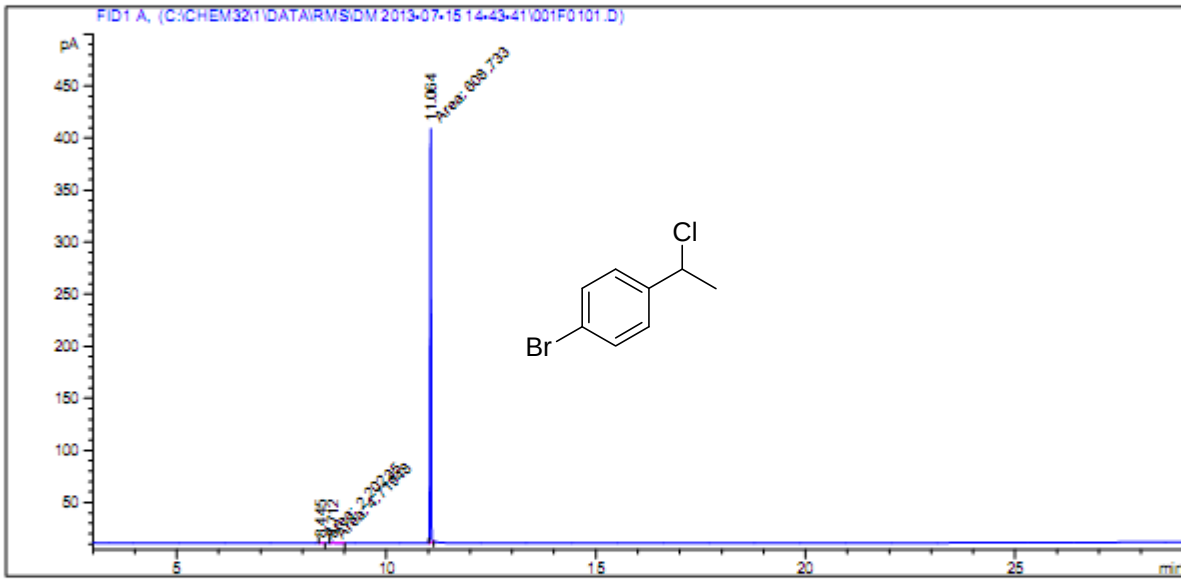





```
Current Data Parameters
NAME          4-br-A-Cl2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130611
Time               15.28
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   661
DS                     4
SWH            35971.223 Hz
FIDRES          0.548877 Hz
AQ             0.9109504 sec
RG                 16384
DW                13.900 usec
DE                 6.00 usec
TE                298.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
MCREST   0 sec
MCWRK          0.01500000 sec

-------- CHANNEL f1 --------
NUC1                  13C
P1                  9.00 usec
PL1       0 dB
SFO1         150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               13.50 dB
PL13               20.00 dB
SFO2         600.1324005 MHz

F2 - Processing parameters
SI                 32768
SF           150.9027468 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-07-15 14-43-41\001F0101.D
Sample Name: p-Br-A-Cl purity

Acq. Operator : RMS
Seq. Line : 1
Acq. Instrument : Instrument 1
Location : Vial 1
Injection Date : 15-Jul-13, 14:45:09
Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-07-15 14-43-41\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 7/15/2013 3:21:37 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

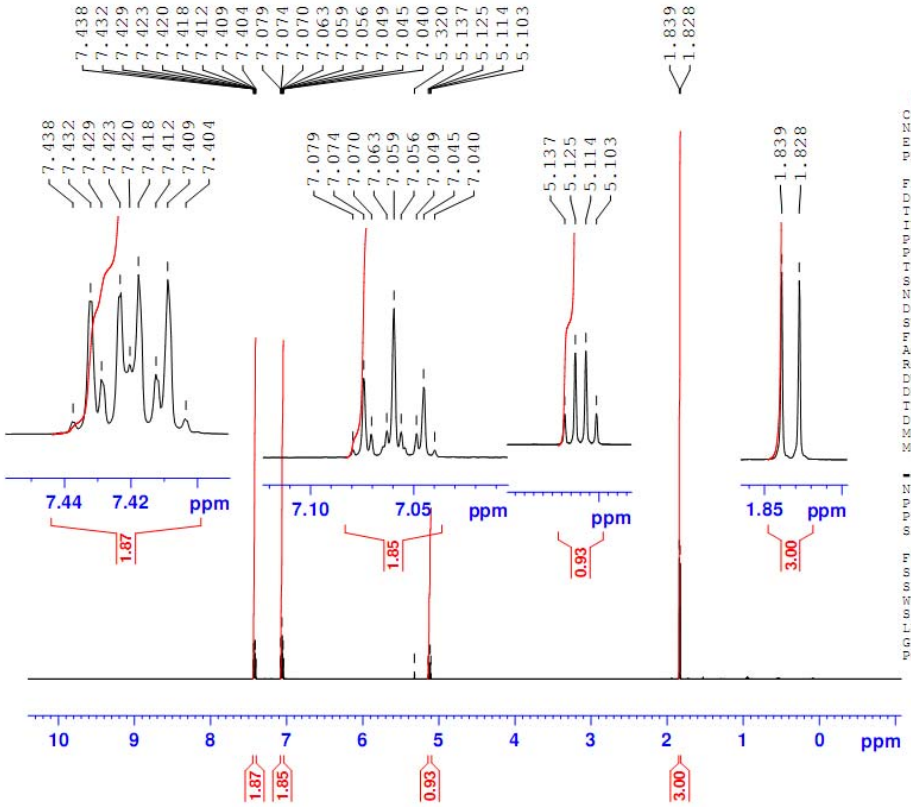


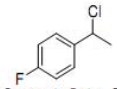
Area Percent Report

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

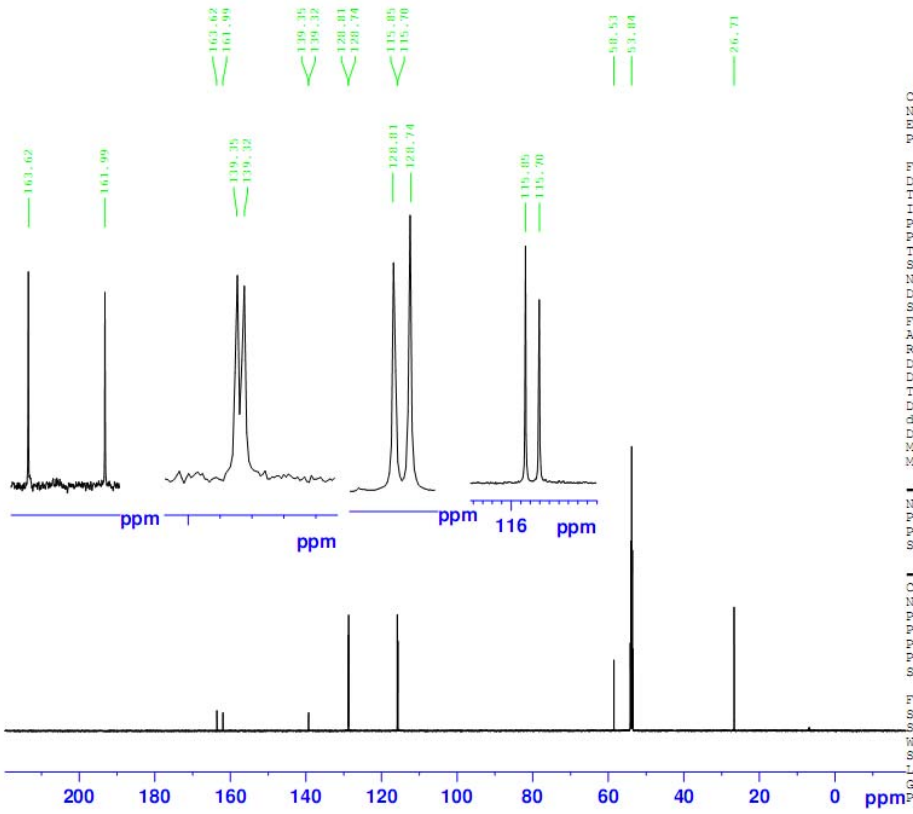
Signal 1: FID1 A,

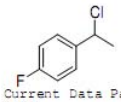
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	8.445	MM	0.0423	2.20235	8.68545e-1	0.35772
2	8.712	MM	0.0513	4.71948	1.53426	0.76658
3	11.064	MM	0.0253	608.73315	400.82944	98.87570






```
Current Data Parameters
NAME              p-f-A-Cl
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20130521
Time                 12.43
INSTRUM              av600
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT            CD2Cl2
NS                       16
DS                        0
SWH               6887.052 Hz
FIDRES            0.105088 Hz
AQ               4.7579136 sec
RG                   143.7
DW                  72.600 usec
DE                    6.00 usec
TE                   298.0 K
D1             1.00000000 sec
MCREST    0 sec
MCWRK          0.01500000 sec

-------- CHANNEL f1 --------
NUC1                     1H
P1                    11.60 usec
PL1                   -2.00 dB
SFO1          600.1328163 MHz

F2 - Processing parameters
SI                    32768
SF            600.1300189 MHz
WDW                      no
SSB       0
LB        0 Hz
GB        0
PC                    1.40
```

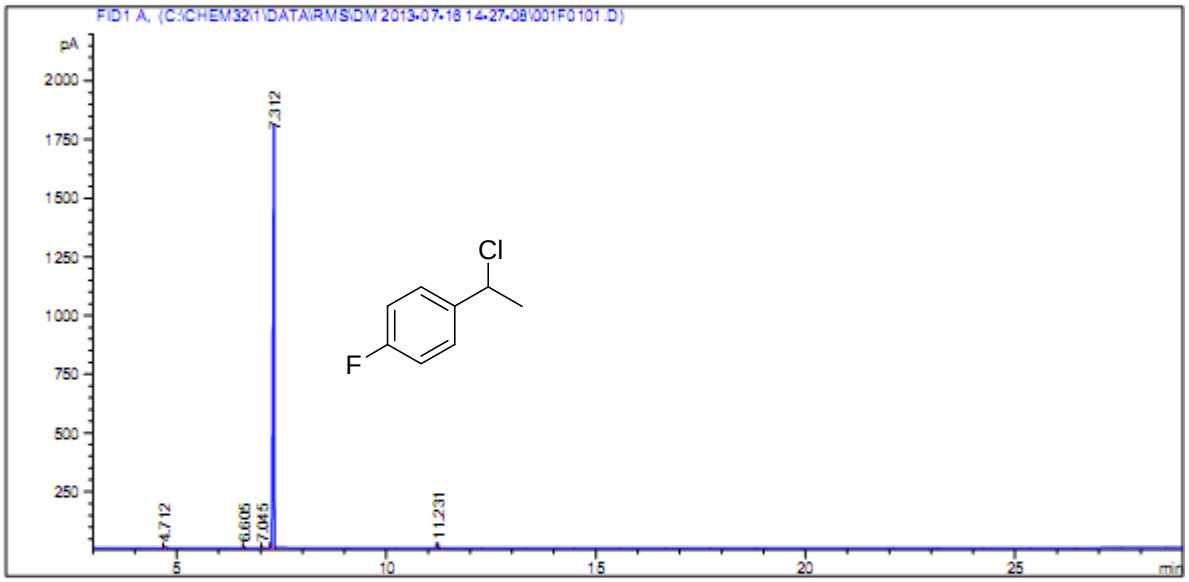





```
Current Data Parameters
NAME              p-f-A-Cl
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20130521
Time                 13.38
INSTRUM              av600
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              35971.223 Hz
FIDRES            0.548877 Hz
AQ               0.9109504 sec
RG                   16384
DW                  13.900 usec
DE                    6.00 usec
TE                   298.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
MCREST    0 sec
MCWRK          0.01500000 sec

-------- CHANNEL f1 --------
NUC1                    13C
P1                     9.00 usec
PL1       0 dB
SFO1        150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2          waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                   -2.00 dB
PL12                  13.50 dB
PL13                  20.00 dB
SFO2          600.1324005 MHz

F2 - Processing parameters
SI                    32768
SF            150.9027447 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-07-16 14-27-08\001F0101.D
Sample Name: p-F-A-Cl purity

Acq. Operator : RMS Seq. Line : 1
Acq. Instrument : Instrument 1 Location : Vial 1
Injection Date : 16-Jul-13, 14:28:33 Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-07-16 14-27-08\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 7/16/2013 3:06:18 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

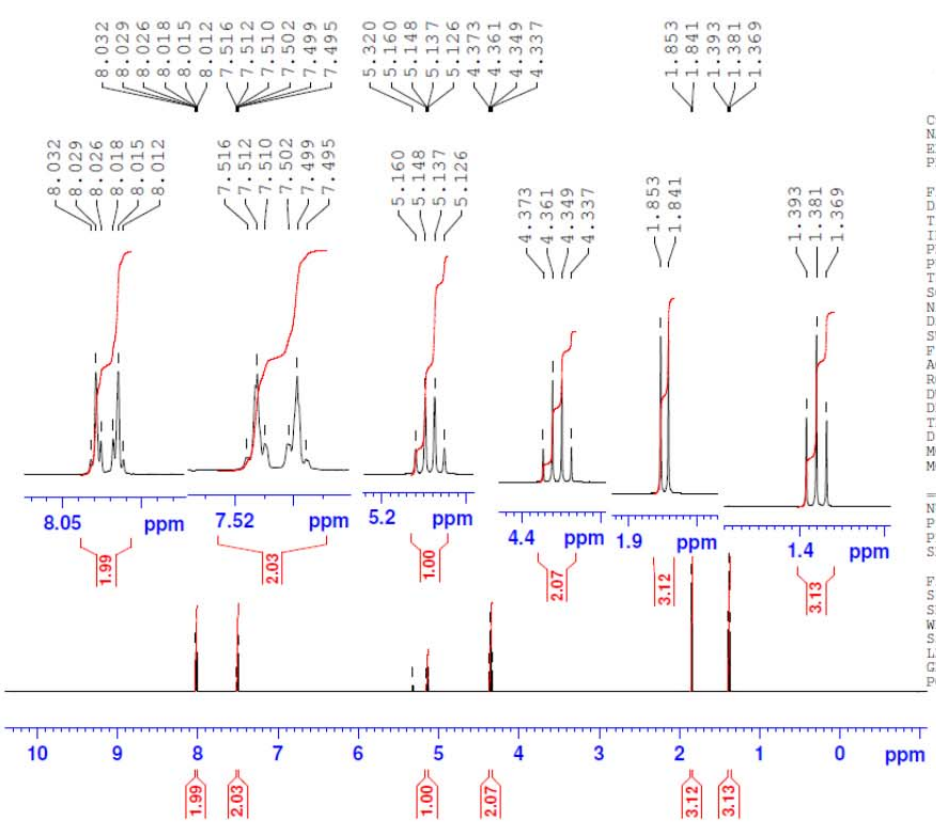


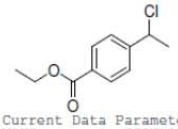
Area Percent Report

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

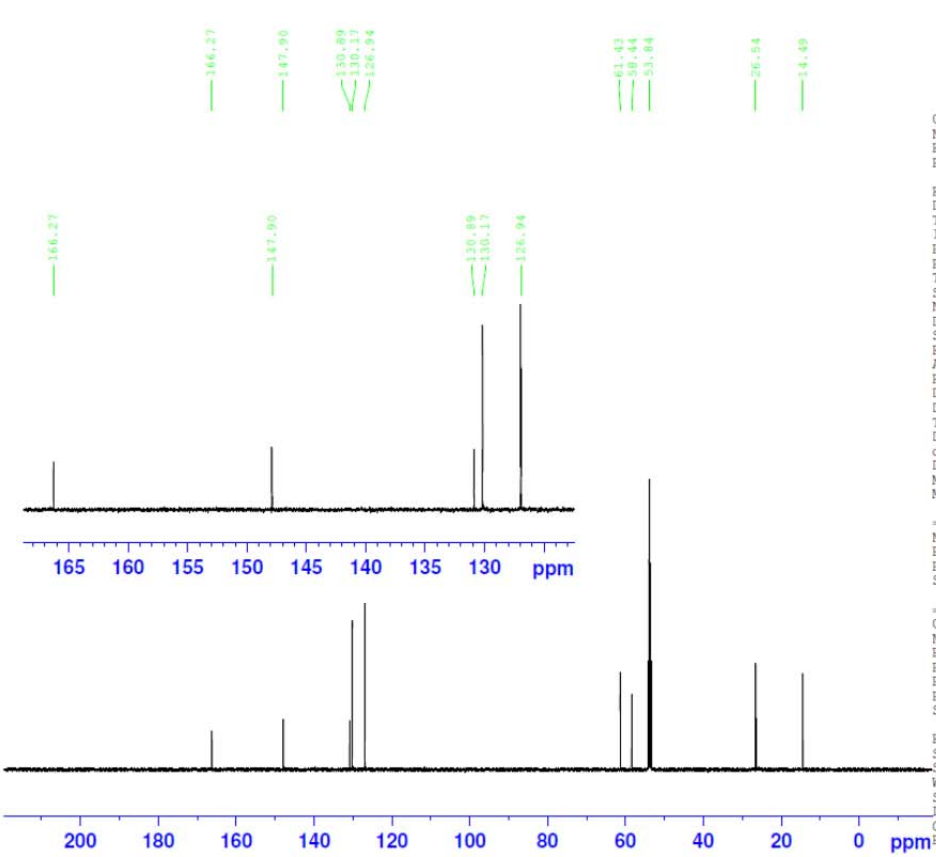
Signal 1: FID1 A,

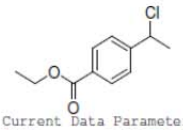
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	4.712	BB	0.0267	10.03507	5.65390	0.28817
2	6.605	BB	0.0203	7.03962	5.35162	0.20216
3	7.045	BB	0.0223	3.62727	2.60360	0.10416
4	7.312	BB	0.0277	3433.76123	1761.41675	98.60648
5	11.231	BB	0.0213	27.82444	19.89969	0.79903






```
Current Data Parameters
NAME          p-COOEtA-Cl
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140124
Time               12.44
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    16
DS                     0
SWH             6887.052 Hz
FIDRES          0.105088 Hz
AQ             4.7579136 sec
RG                  90.5
DW                72.600 usec
DE                 6.00 usec
TE                298.0 K
D1            1.00000000 sec
MCREST   0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 11.60 usec
PL1                -2.00 dB
SFO1          600.1328163 MHz

F2 - Processing parameters
SI                  32768
SF            600.1300188 MHz
WDW                    no
SSB       0
LB        0 Hz
GB        0
PC                   1.40
```

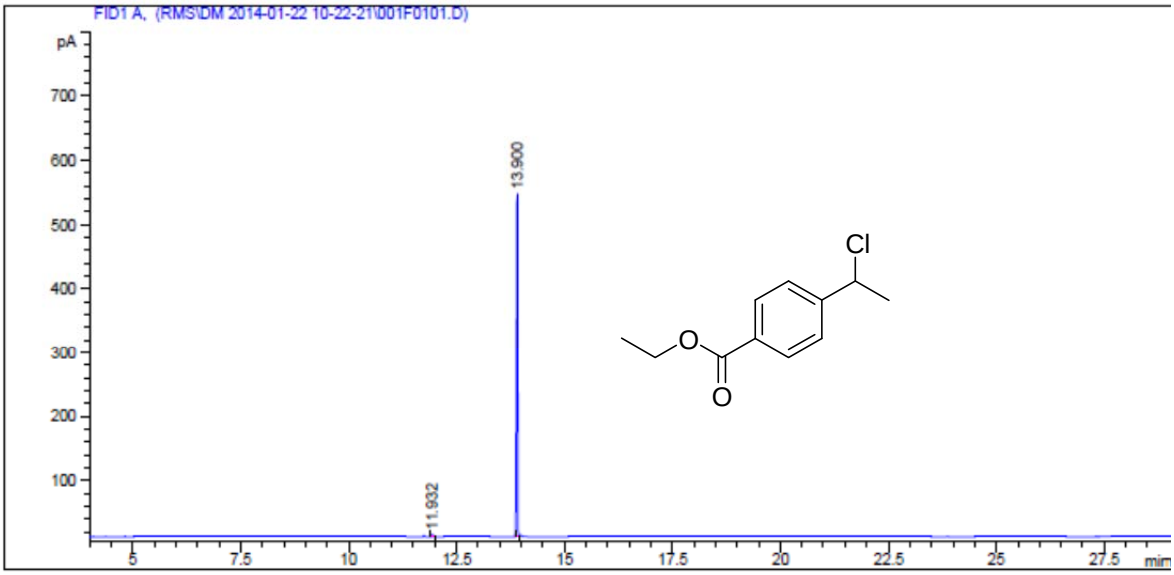




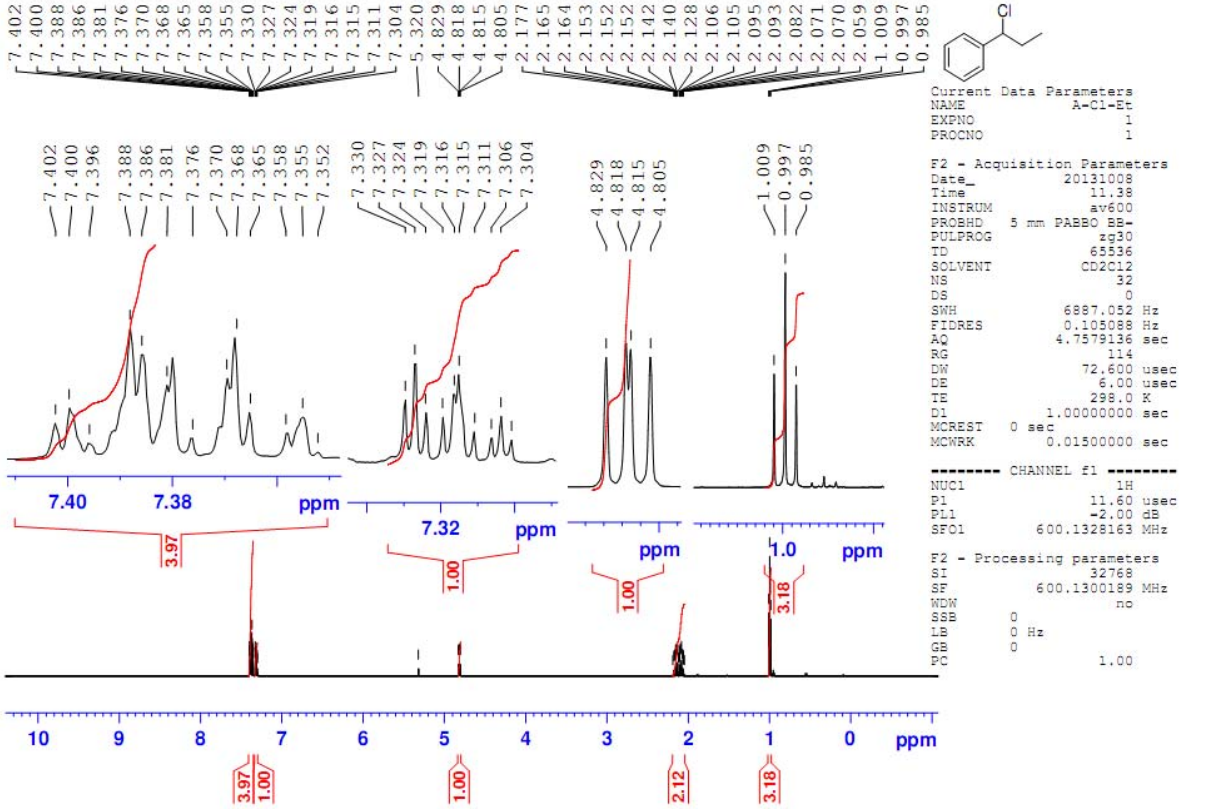

```
Current Data Parameters
NAME          p-COOEtA-Cl
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140124
Time               13.33
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   849
DS                     4
SWH            35971.223 Hz
FIDRES          0.548877 Hz
AQ             0.9109504 sec
RG                 16384
DW                13.900 usec
DE                 6.00 usec
TE                298.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
MCREST   0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.00 usec
PL1       0 dB
SFO1          150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                   1H
PCPD2             80.00 usec
PL2                -2.00 dB
PL12               13.50 dB
PL13               20.00 dB
SFO2          600.1324005 MHz

F2 - Processing parameters
SI                  32768
SF            150.9027462 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                   1.00
```

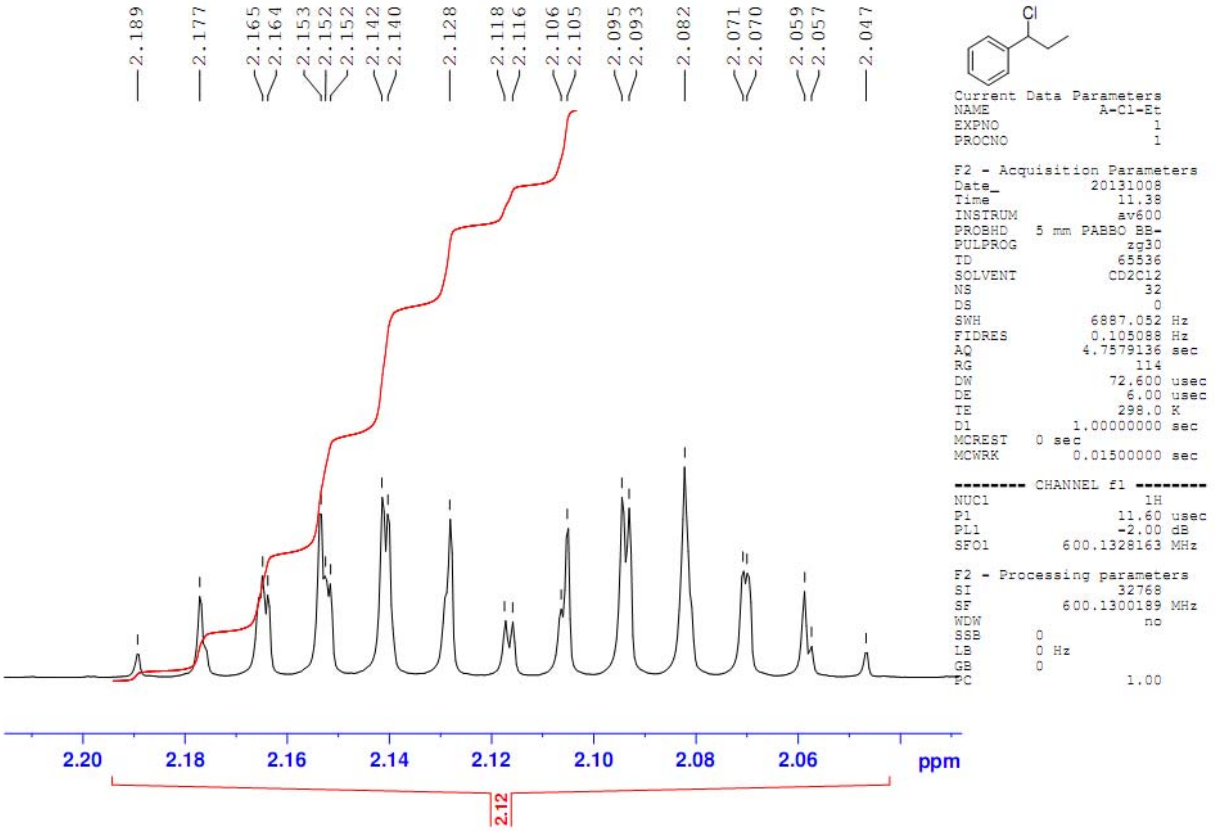
Data File C:\CHEM32\1\DATA\RMS\DM 2014-01-22 10-22-21\001F0101.D
Sample Name: p-COOEt-A-Cl pur

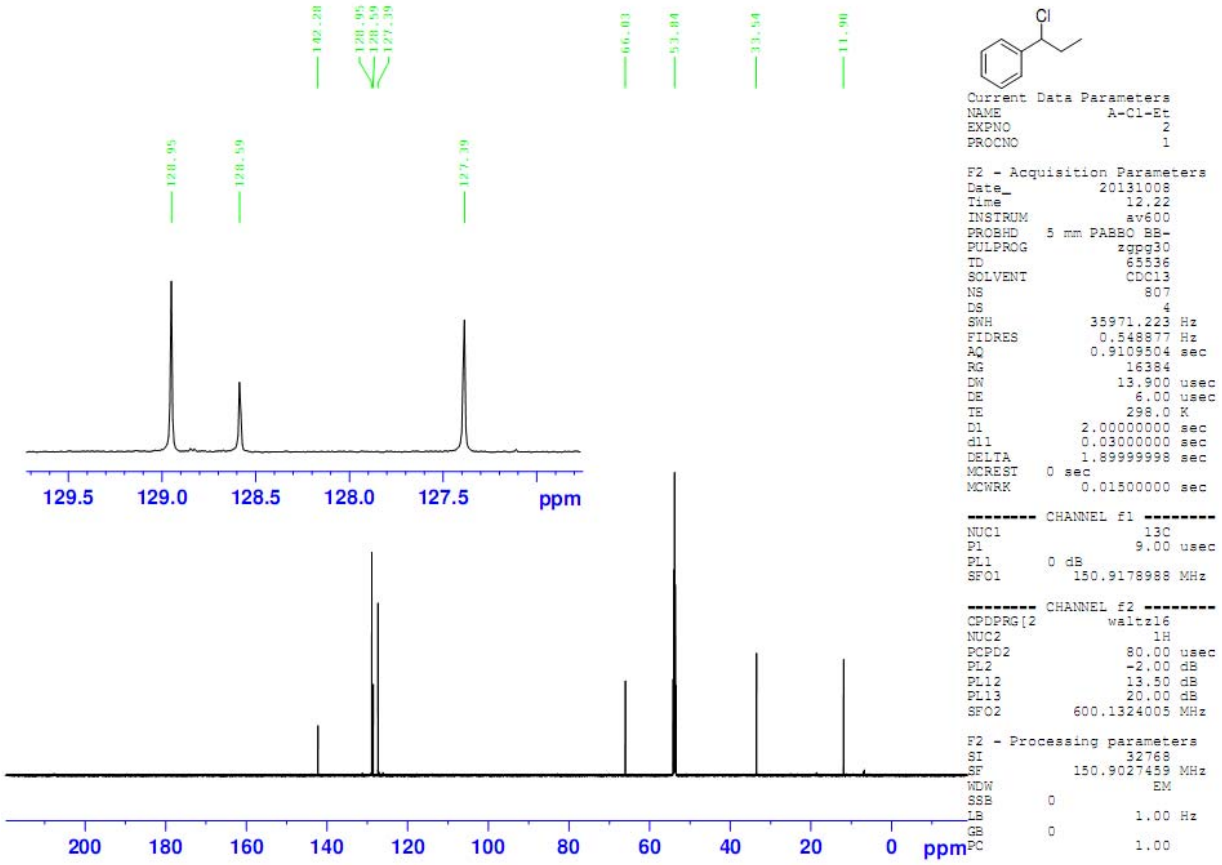
```
==================================================================
Acq. Operator   : RMS                          Seq. Line :   1
Acq. Instrument : Instrument 1                  Location : Vial 1
Injection Date  : 22-Jan-14, 10:23:56                Inj :   1
                                              Inj Volume : 1 µl
Acq. Method     : C:\CHEM32\1\DATA\RMS\DM 2014-01-22 10-22-21\ÅA-DEFAULT.M
Last changed    : 11/20/2013 12:14:04 PM by RMS
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed    : 1/22/2014 11:42:03 AM by RMS
                  (modified after loading)
Method Info     : ÅAGC-default
```




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

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


Signal 1: FID1 A,

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  11.932 BB    0.0341    7.07432    3.16716  0.80739
   2  13.900 BB    0.0240  869.11902  534.25751 99.19261
```

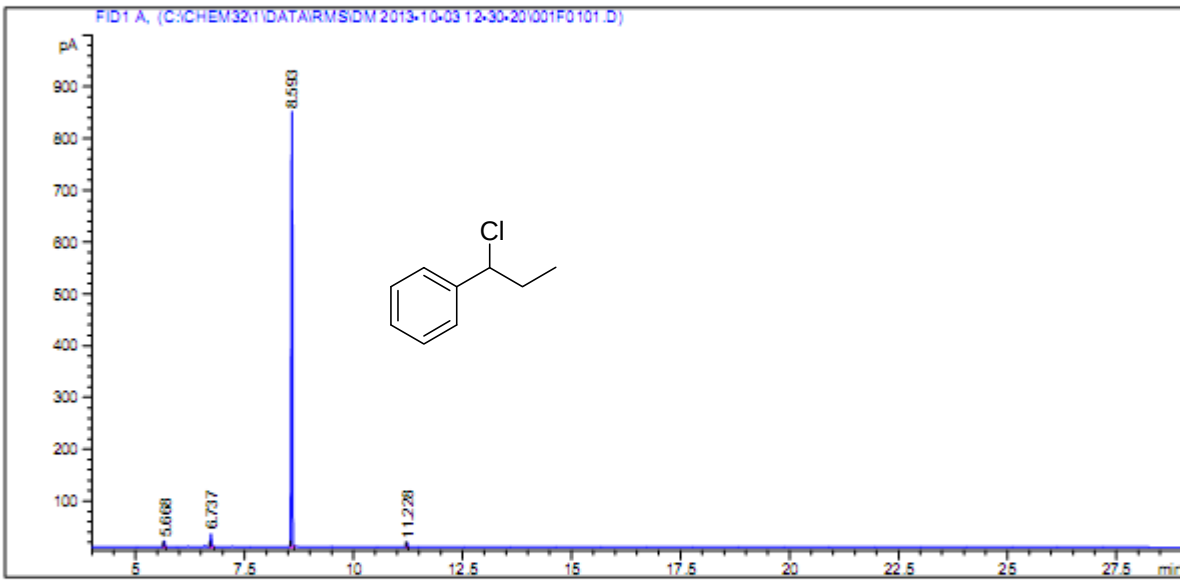

7.402 7.400 7.388 7.386 7.381 7.376 7.370 7.368 7.365 7.358 7.355 7.330 7.327 7.324 7.319 7.316 7.315 7.311 7.304 5.320 4.829 4.818 4.815 4.805 2.177 2.165 2.164 2.153 2.152 2.152 2.142 2.140 2.128 2.106 2.105 2.095 2.093 2.082 2.071 2.070 2.059 1.009 0.997 0.985
Cl
Current Data Parameters
NAME A-Cl-Et
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131008
Time 11.38
INSTRUM av600
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
NS 32
DS 0
SWH 6887.052 Hz
FIDRES 0.105088 Hz
AQ 4.7579136 sec
RG 114
DW 72.600 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 11.60 usec
PL1 -2.00 dB
SFO1 600.1328163 MHz
F2 - Processing parameters
SI 32768
SF 600.1300189 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
7.40 7.38 ppm
3.97
7.32 ppm
1.00
ppm
1.00
1.0 ppm
3.18
10 9 8 7 6 5 4 3 2 1 0 ppm
3.97 1.00
1.00
2.12
3.18


2.189 2.177 2.165 2.164 2.153 2.152 2.152 2.142 2.140 2.128 2.118 2.116 2.106 2.105 2.095 2.093 2.082 2.071 2.070 2.059 2.057 2.047
Cl
Current Data Parameters
NAME A-Cl-Et
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131008
Time 11.38
INSTRUM av600
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
NS 32
DS 0
SWH 6887.052 Hz
FIDRES 0.105088 Hz
AQ 4.7579136 sec
RG 114
DW 72.600 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 11.60 usec
PL1 -2.00 dB
SFO1 600.1328163 MHz
F2 - Processing parameters
SI 32768
SF 600.1300189 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
2.20 2.18 2.16 2.14 2.12 2.10 2.08 2.06 ppm
2.12


142.28
128.95
128.59
127.39
66.81
53.84
33.54
11.90
Cl
129.5
129.0
128.5
128.0
127.5
ppm
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME A-Cl-Et
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131008
Time 12.22
INSTRUM av600
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 807
DS 4
SWH 35971.223 Hz
FIDRES 0.548877 Hz
AQ 0.9109504 sec
RG 16384
DW 13.900 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 9.00 usec
PL1 0 dB
SFO1 150.9178988 MHz
-------- CHANNEL f2 --------
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.50 dB
PL13 20.00 dB
SFO2 600.1324005 MHz
F2 - Processing parameters
SI 32768
SF 150.9027459 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Data File C:\CHEM32\1\DATA\RMS\DM 2013-10-03 12-30-20\001F0101.D
Sample Name: A-Cl-Et purity

Acq. Operator : RMS Seq. Line : 1
Acq. Instrument : Instrument 1 Location : Vial 1
Injection Date : 03-Oct-13, 12:31:45 Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-10-03 12-30-20\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 10/3/2013 1:08:17 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

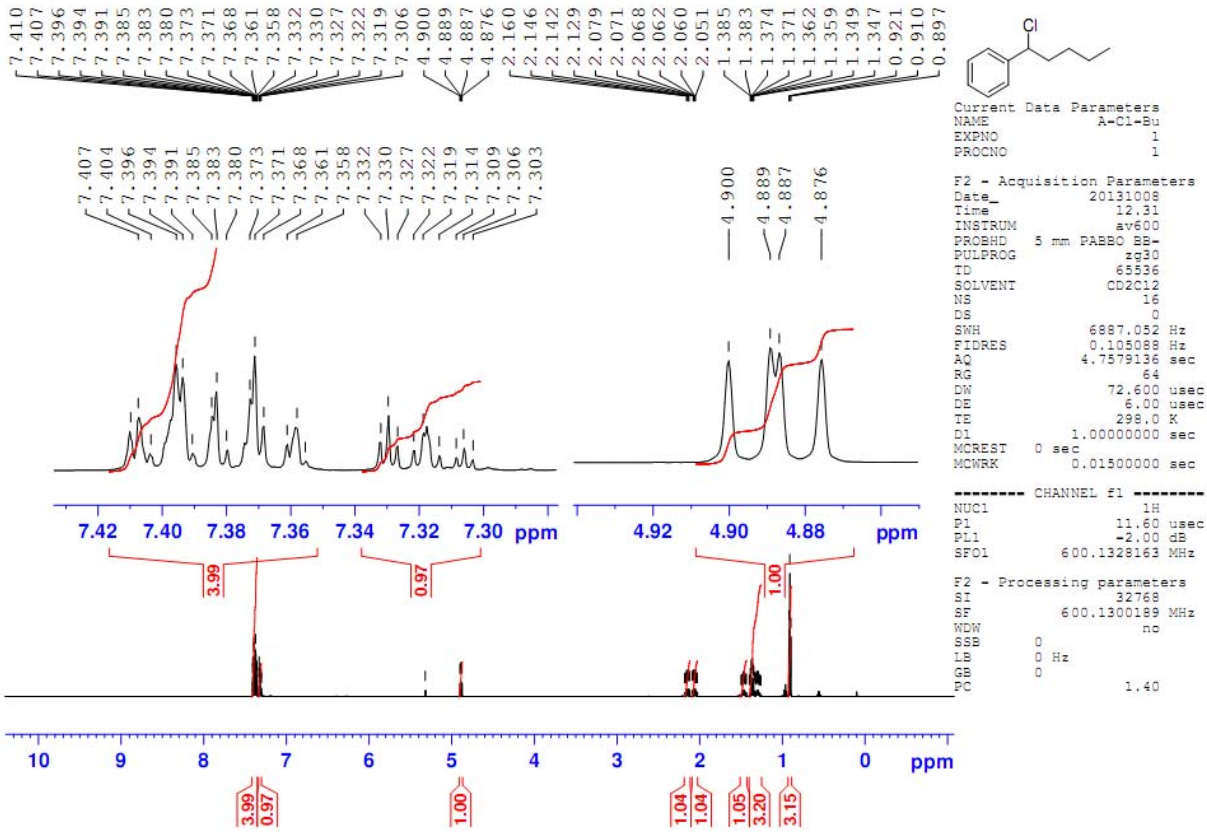


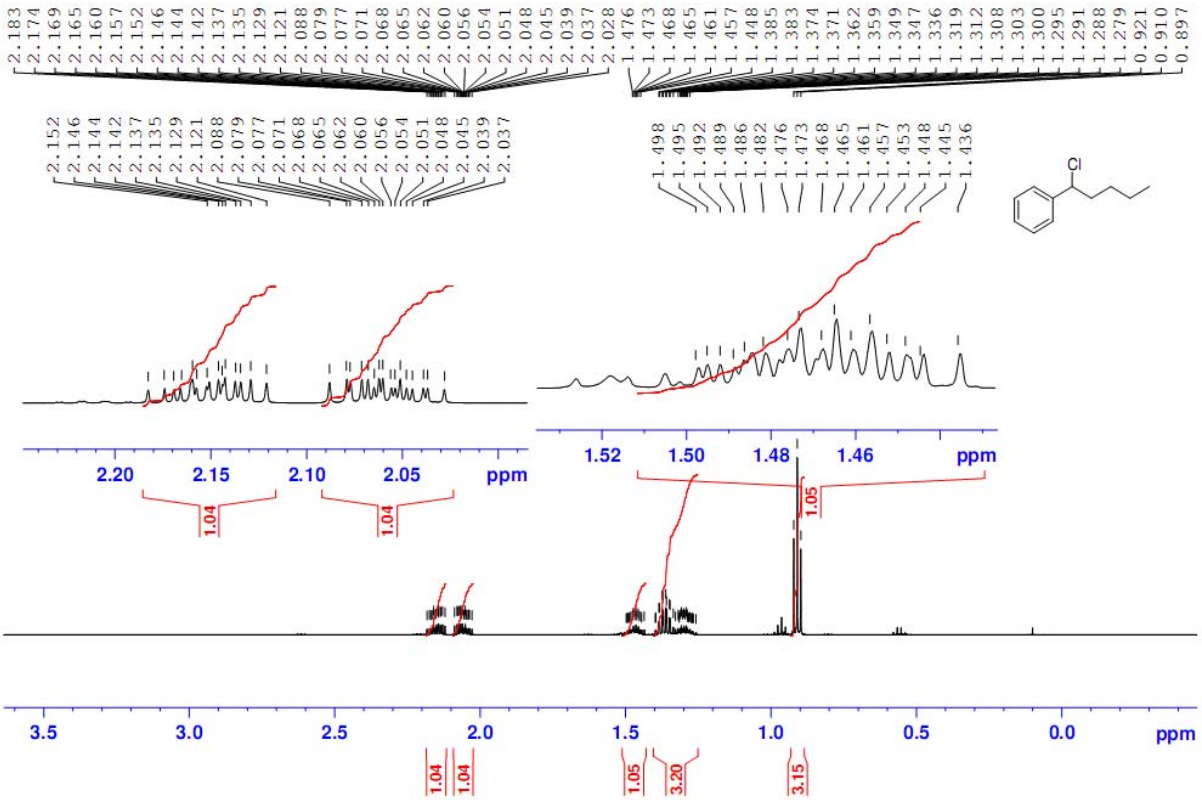
Area Percent Report

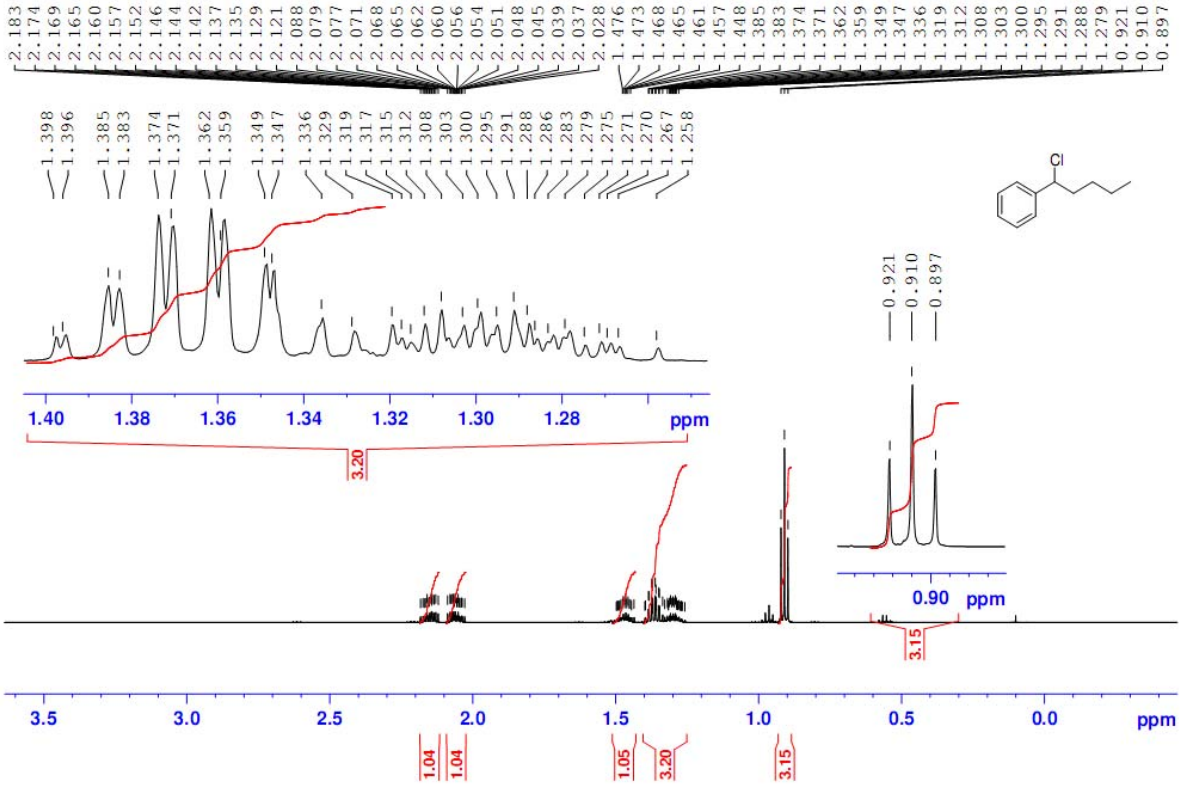
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

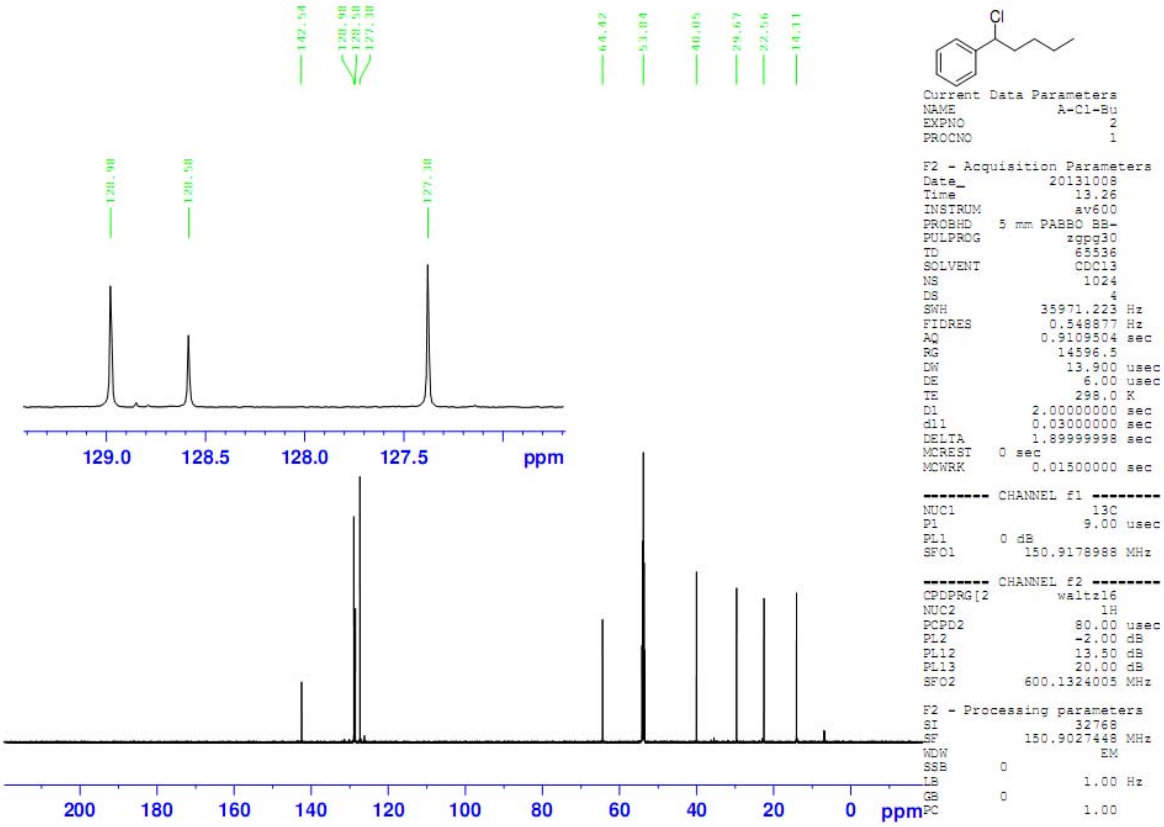
Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	5.668	BB	0.0228	16.58476	11.54342	1.26047
2	6.737	BB	0.0245	39.47681	24.88054	3.00032
3	8.593	BB	0.0234	1246.83508	837.73437	94.76192
4	11.228	BB	0.0212	12.85881	9.25819	0.97729


Cl
Current Data Parameters
NAME A-Cl-Bu
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131008
Time 12.31
INSTRUM av600
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
NS 16
DS 0
SWH 6887.052 Hz
FIDRES 0.105088 Hz
AQ 4.7579136 sec
RG 64
DW 72.600 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 11.60 usec
PL1 -2.00 dB
SFO1 600.1328163 MHz
F2 - Processing parameters
SI 32768
SF 600.1300189 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.40
ppm

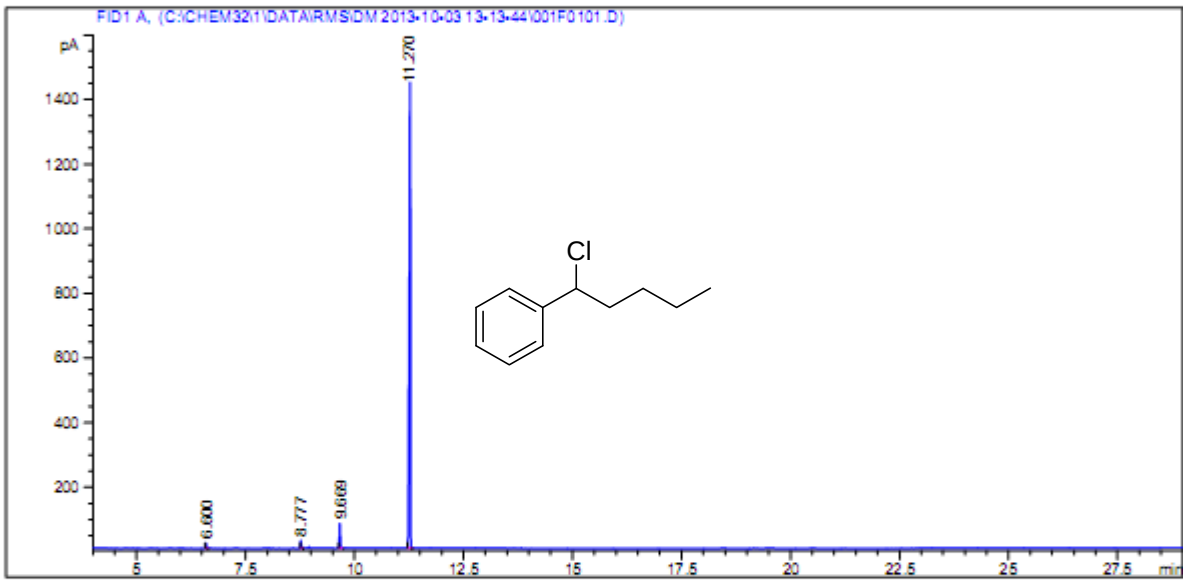

Cl
ppm


2.183 2.174 2.169 2.165 2.160 2.157 2.152 2.146 2.144 2.142 2.137 2.135 2.129 2.121 2.088 2.079 2.077 2.071 2.068 2.065 2.062 2.060 2.056 2.054 2.051 2.048 2.045 2.039 2.037 2.028 1.476 1.473 1.468 1.465 1.461 1.457 1.448 1.385 1.383 1.374 1.371 1.362 1.359 1.349 1.347 1.319 1.312 1.308 1.303 1.300 1.295 1.291 1.288 1.279 0.921 0.910 0.897
1.398 1.396 1.385 1.383 1.374 1.371 1.362 1.359 1.349 1.347 1.336 1.329 1.319 1.317 1.315 1.312 1.308 1.303 1.300 1.295 1.291 1.288 1.286 1.283 1.279 1.275 1.271 1.270 1.267 1.258
Cl
0.921 0.910 0.897
1.40 1.38 1.36 1.34 1.32 1.30 1.28 ppm
3.20
0.90 ppm
3.15
3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.04 1.04 1.05 3.20 3.15


142.54 129.98 129.58 127.38 64.42 53.84 40.05 29.67 22.56 14.11
129.98 129.58 127.38
129.0 128.5 128.0 127.5 ppm
200 180 160 140 120 100 80 60 40 20 0 ppm
Cl
Current Data Parameters
NAME A-Cl-Bu
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131008
Time 13.26
INSTRUM av600
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 35971.223 Hz
FIDRES 0.548877 Hz
AQ 0.9109504 sec
RG 14596.5
DW 13.900 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 9.00 usec
PL1 0 dB
SFO1 150.9178988 MHz
-------- CHANNEL f2 --------
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.50 dB
PL13 20.00 dB
SFO2 600.1324005 MHz
F2 - Processing parameters
SI 32768
SF 150.9027448 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Data File C:\CHEM32\1\DATA\RMS\DM 2013-10-03 13-13-44\001F0101.D
Sample Name: A-Cl-Bu purity

Acq. Operator : RMS
Seq. Line : 1
Acq. Instrument : Instrument 1
Location : Vial 1
Injection Date : 03-Oct-13, 13:15:00
Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-10-03 13-13-44\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 10/3/2013 1:50:57 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

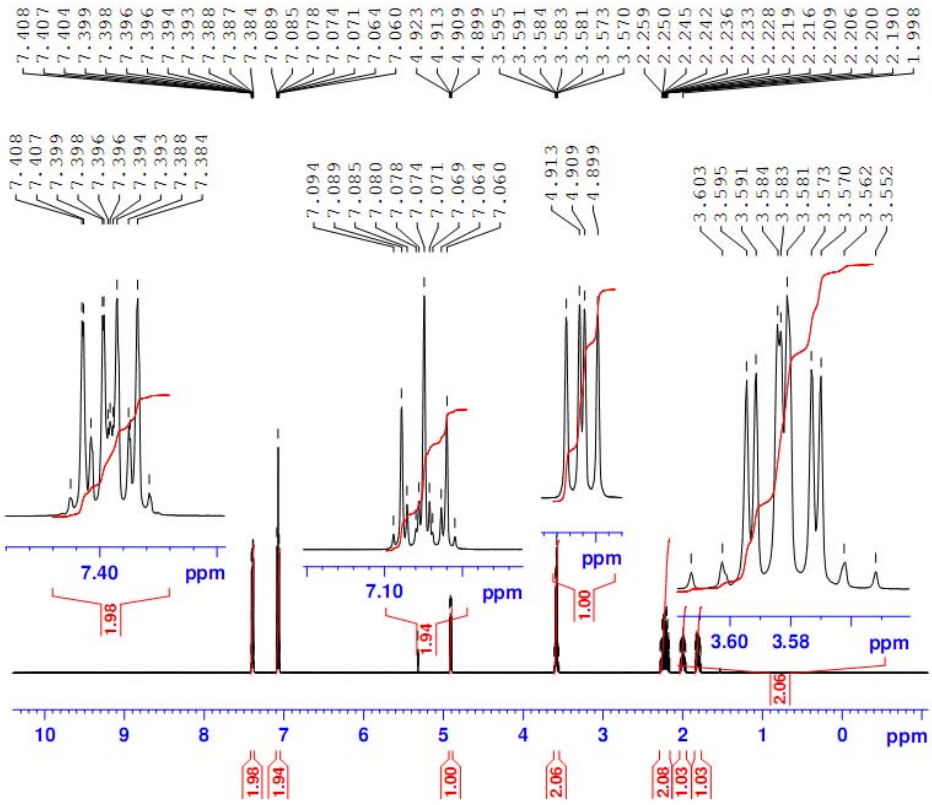


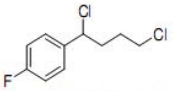
Area Percent Report

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

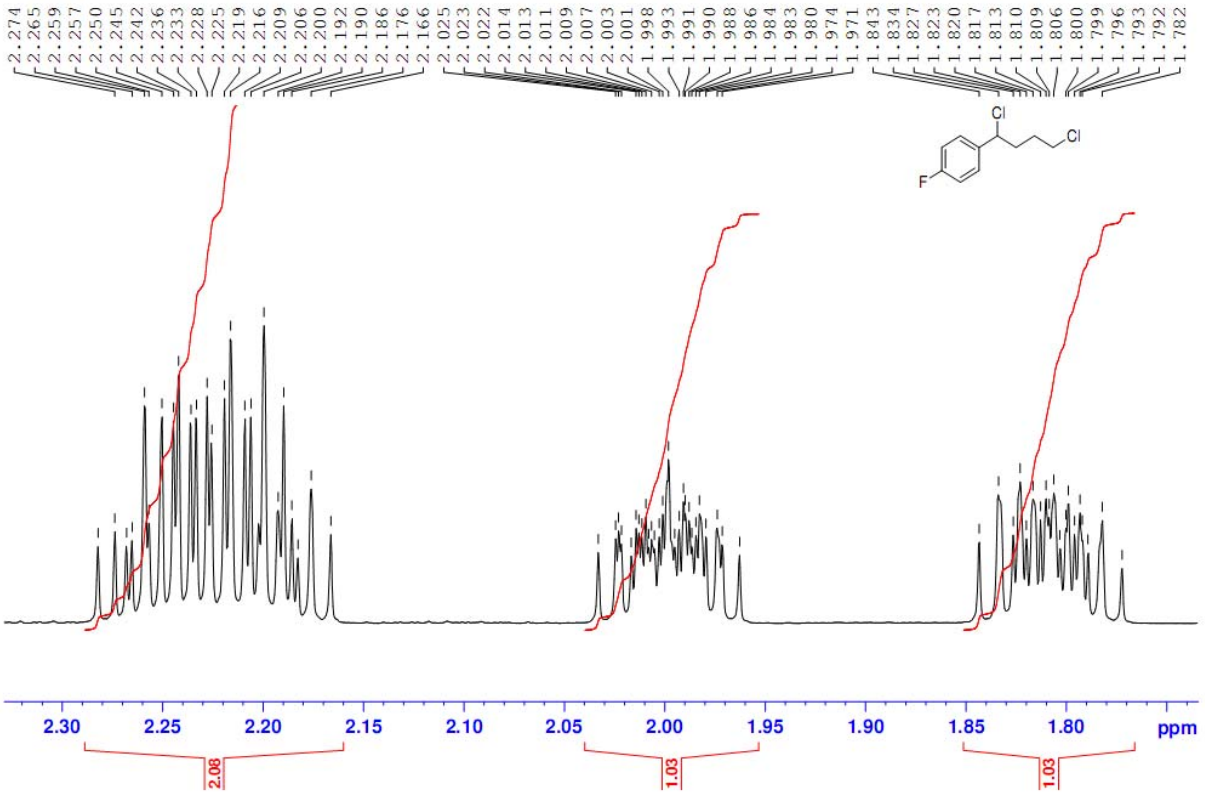
Signal 1: FID1 A,

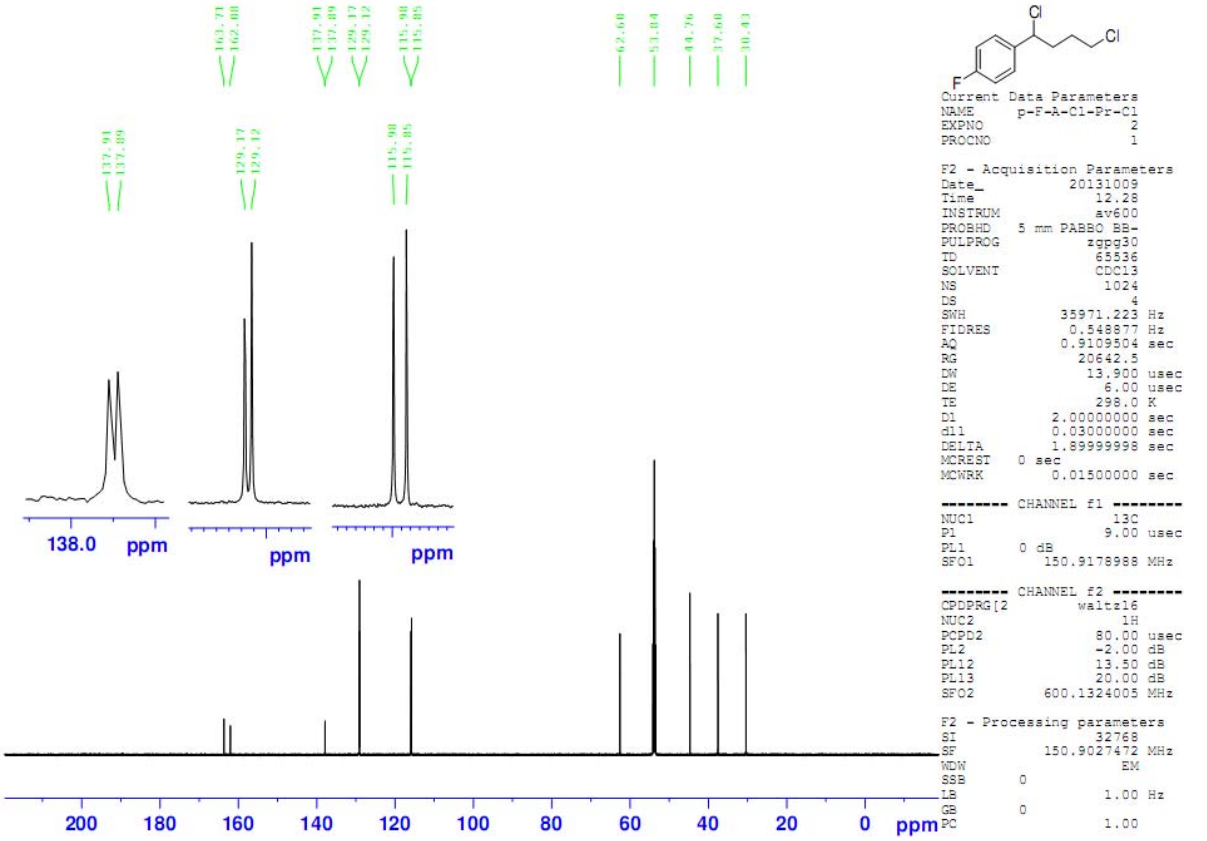
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	6.600	BB	0.0215	22.13394	16.68873	0.78833
2	8.777	BB	0.0228	34.95516	24.33655	1.24497
3	9.669	BB	0.0232	111.83655	76.06970	3.98319
4	11.270	BB	0.0272	2638.78589	1449.54102	93.98351

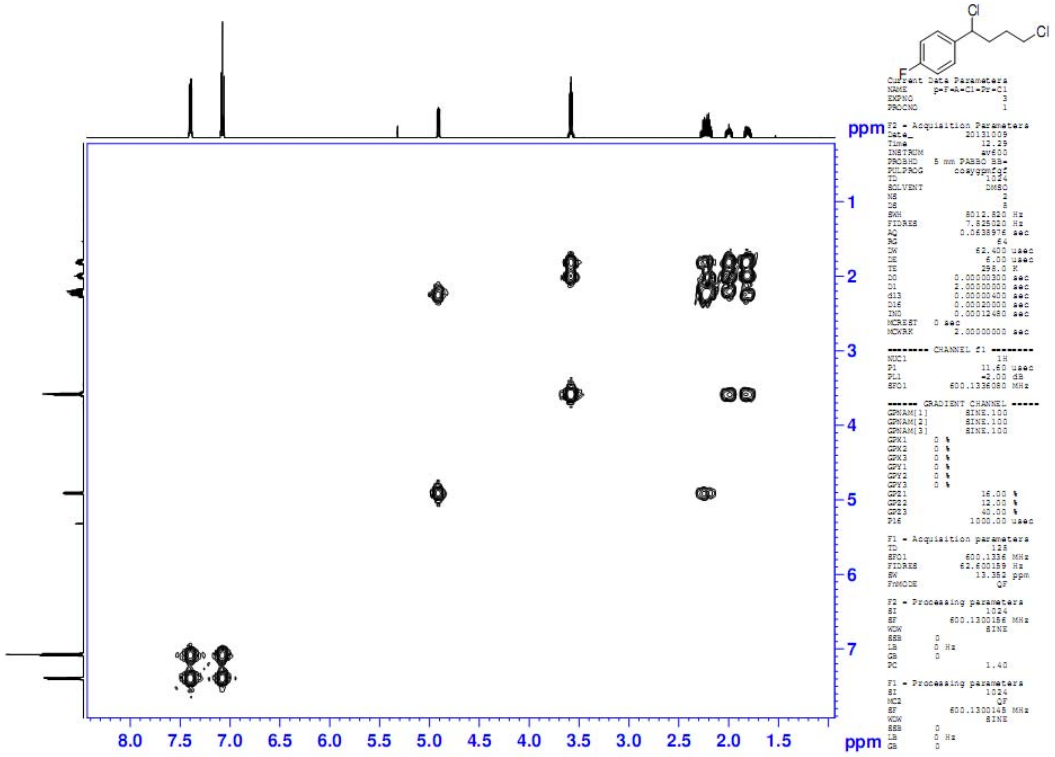


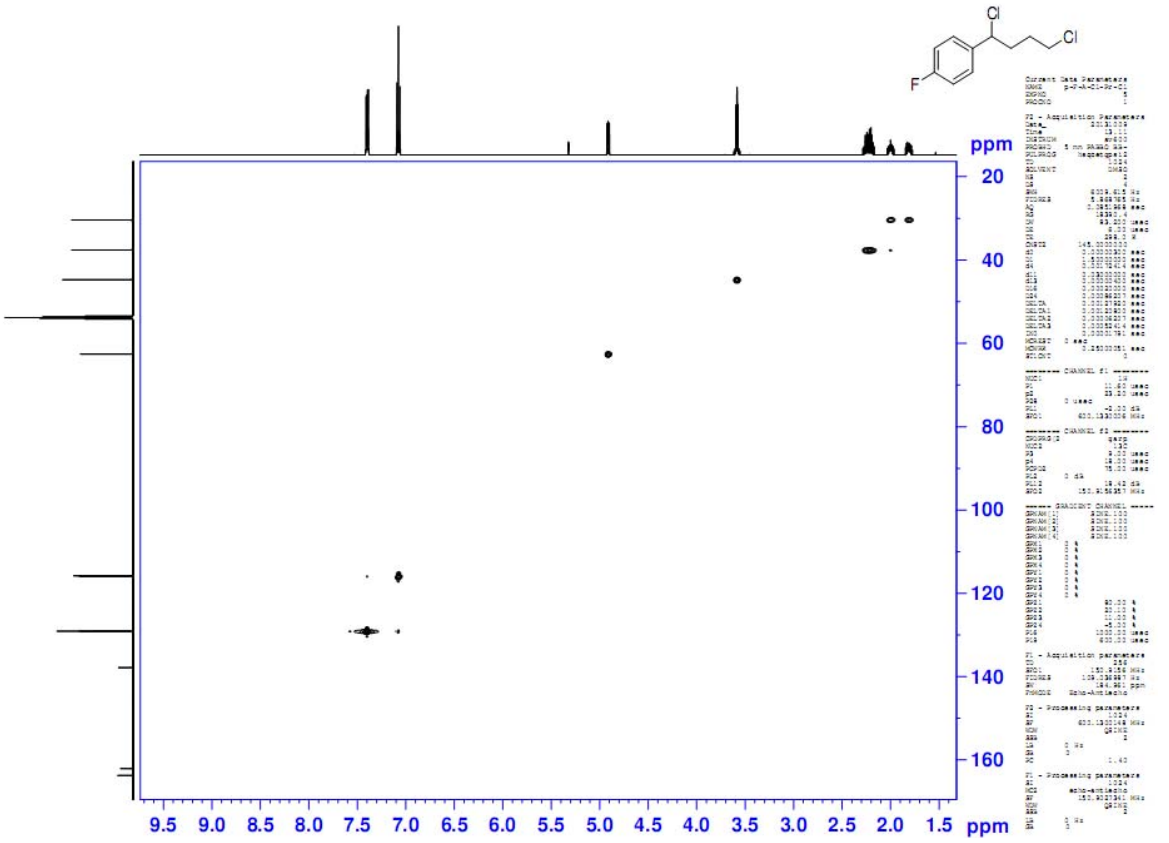


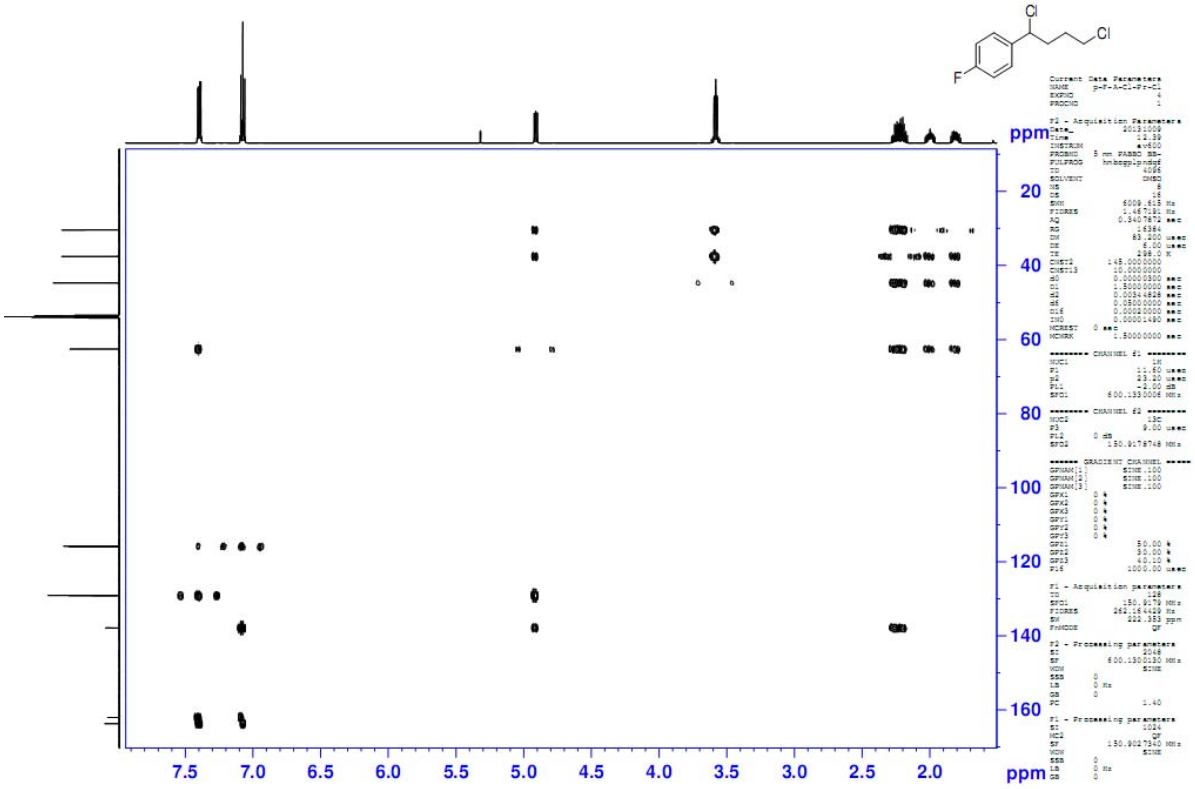

```
Current Data Parameters
NAME      p-F-A-Cl-Pr-Cl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20131009
Time               11.32
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    16
DS                     0
SWH            6887.052 Hz
FIDRES         0.105088 Hz
AQ            4.7579136 sec
RG                 80.6
DW               72.600 usec
DE                6.00 usec
TE               298.0 K
D1           1.00000000 sec
MCREST   0 sec
MCWRK        0.01500000 sec

-------- CHANNEL f1 --------
NUC1                  1H
P1                11.60 usec
PL1               -2.00 dB
SFO1        600.1328163 MHz

F2 - Processing parameters
SI                 32768
SF          600.1300189 MHz
WDW                   no
SSB        0
LB         0 Hz
GB         0
PC                  1.40
```




163.71
162.88
137.91
137.89
129.17
129.12
115.98
115.85
62.68
53.84
44.76
37.68
30.43
138.0
ppm
200
180
160
140
120
100
80
60
40
20
0
Current Data Parameters
NAME p-F-A-Cl-Pr-Cl
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131009
Time 12.28
INSTRUM av600
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 35971.223 Hz
FIDRES 0.548877 Hz
AQ 0.9109504 sec
RG 20642.5
DW 13.900 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 9.00 usec
PL1 0 dB
SFO1 150.9178988 MHz
-------- CHANNEL f2 --------
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.50 dB
PL13 20.00 dB
SFO2 600.1324005 MHz
F2 - Processing parameters
SI 32768
SF 150.9027472 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

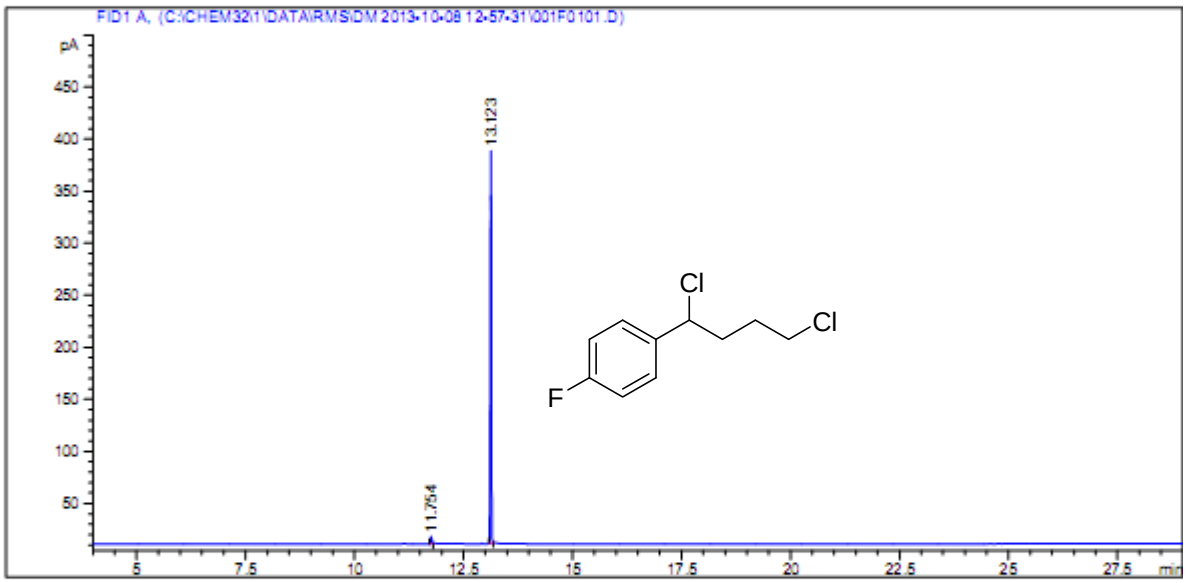

ppm
1
2
3
4
5
6
7
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
Current Data Parameters
NAME p-F-A-Cl-Pr-Cl
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131009
Time 12.29
INSTRUM av600
PROBHD 5 mm PABBO BB-
PULPROG cosygpmfqf
TD 1024
SOLVENT DMSO
NS 2
DS 8
SWH 8012.820 Hz
FIDRES 7.828020 Hz
AQ 0.0638976 sec
RG 64
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D0 0.00000300 sec
D1 2.00000000 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00012480 sec
MCREST 0 sec
MCWRK 2.00000000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 11.60 usec
PL1 -2.00 dB
SFO1 600.1336080 MHz
------ GRADIENT CHANNEL -----
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPNAM[3] SINE.100
GPX1 0 %
GPX2 0 %
GPX3 0 %
GPY1 0 %
GPY2 0 %
GPY3 0 %
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec
F1 - Acquisition parameters
TD 128
SFO1 600.1336 MHz
FIDRES 62.600189 Hz
SW 13.352 ppm
FnMODE QF
F2 - Processing parameters
SI 1024
SF 600.1300186 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40
F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1302145 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0


Cl
Cl
F
ppm
20
40
60
80
100
120
140
160
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm


Cl
Cl
F
ppm
20
40
60
80
100
120
140
160
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm

Data File C:\CHEM32\1\DATA\RMS\DM 2013-10-08 12-57-31\001F0101.D
Sample Name: p-F-A-Cl-pr-Cl purity

Acq. Operator : RMS
Seq. Line : 1
Acq. Instrument : Instrument 1
Location : Vial 1
Injection Date : 08-Oct-13, 12:58:57
Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-10-08 12-57-31\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 10/8/2013 2:07:40 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

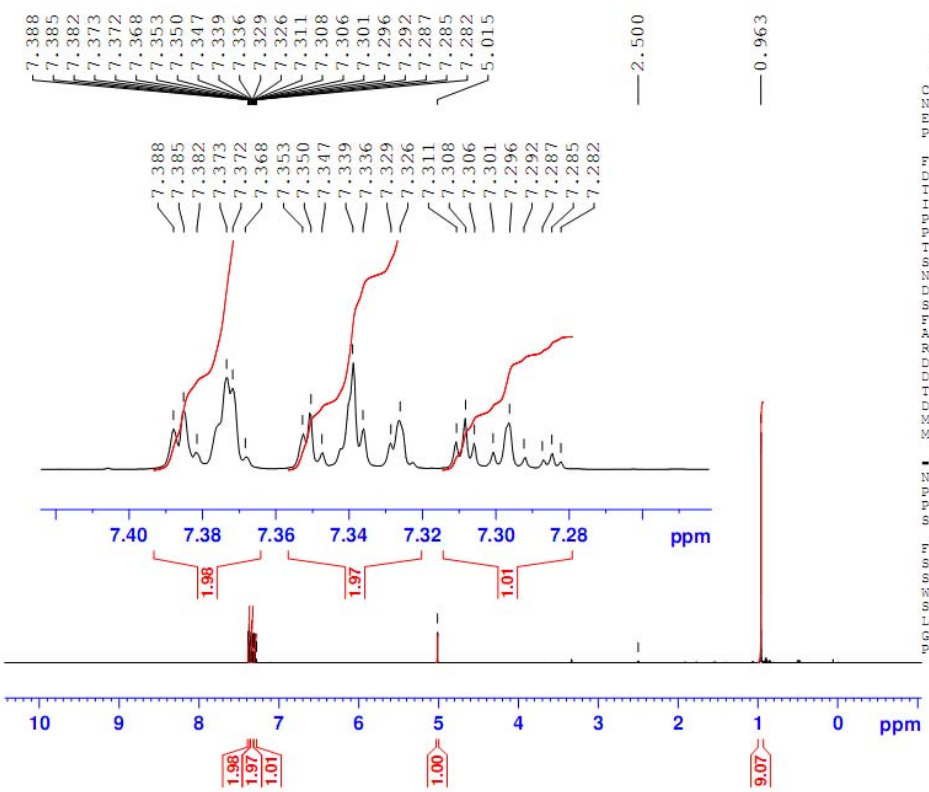


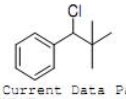
Area Percent Report

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

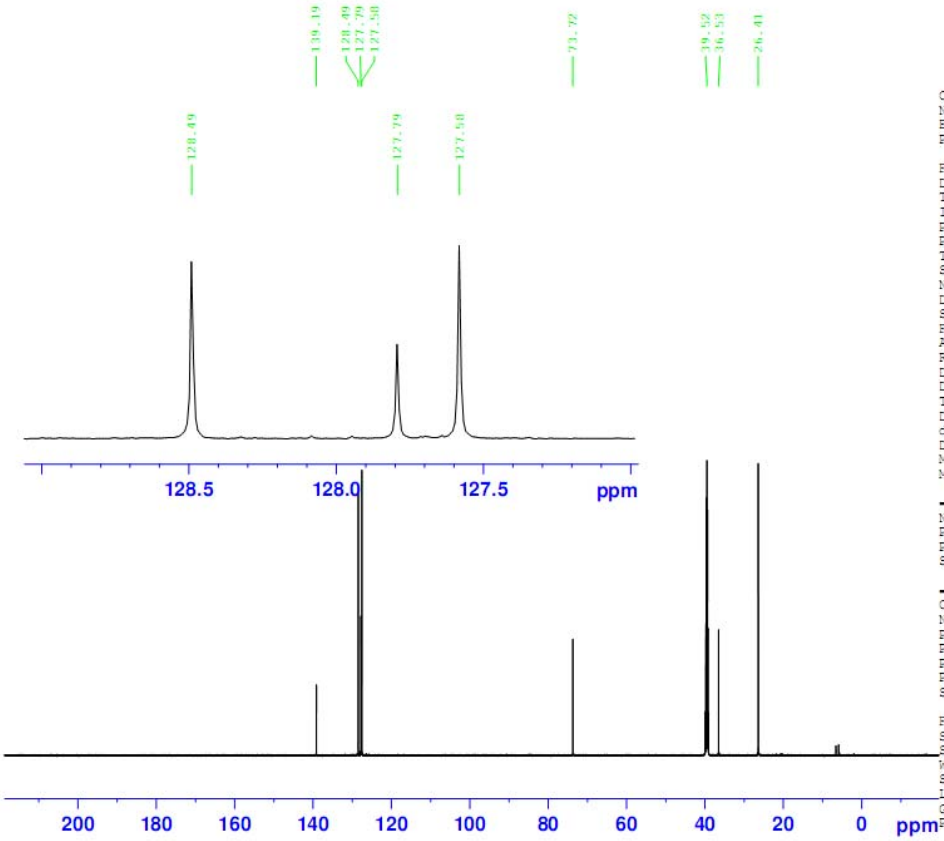
Signal 1: FID1 A,

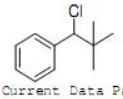
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	11.754	BB	0.0272	12.79833	7.03558	2.19967
2	13.123	BB	0.0236	569.03027	377.26779	97.80033






```
Current Data Parameters
NAME                A-Cl-tBu
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_               20130930
Time                   13.43
INSTRUM                av600
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        32
DS                         0
SWH                 6887.052 Hz
FIDRES              0.105088 Hz
AQ                 4.7579136 sec
RG                        57
DW                    72.600 usec
DE                     6.00 usec
TE                    298.0 K
D1                 1.00000000 sec
MCREST     0 sec
MCWRK              0.01500000 sec

-------- CHANNEL f1 --------
NUC1                       1H
P1                     11.60 usec
PL1                    -2.00 dB
SFO1            600.1328163 MHz

F2 - Processing parameters
SI                      32768
SF                600.1300005 MHz
WDW                        no
SSB        0
LB         0 Hz
GB         0
PC                      1.40
```

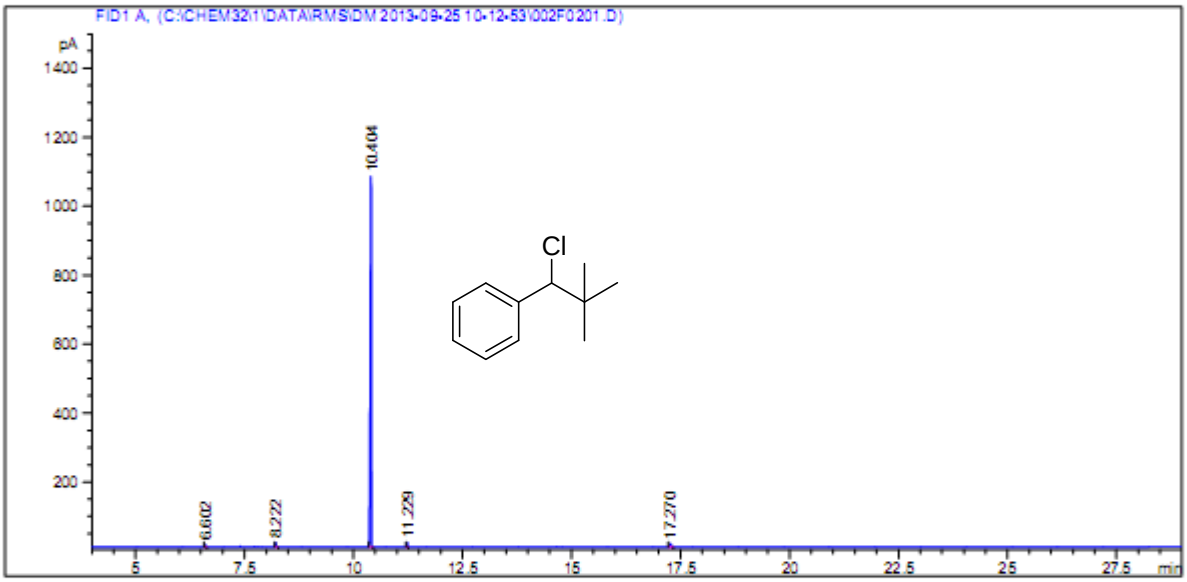





```
Current Data Parameters
NAME                A-Cl-tBu
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20130930
Time                   13.37
INSTRUM                av600
PROBHD    5 mm PABBO BB-
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                35971.223 Hz
FIDRES              0.548877 Hz
AQ                 0.9109504 sec
RG                   20642.5
DW                    13.900 usec
DE                     6.00 usec
TE                    298.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST     0 sec
MCWRK              0.01500000 sec

-------- CHANNEL f1 --------
NUC1                      13C
P1                      9.00 usec
PL1        0 dB
SFO1            150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2            waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                    -2.00 dB
PL12                   13.50 dB
PL13                   20.00 dB
SFO2            600.1324005 MHz

F2 - Processing parameters
SI                      32768
SF                150.9028831 MHz
WDW                        EM
SSB        0
LB                      1.00 Hz
GB         0
PC                      1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-09-25 10-12-53\002F0201.D
Sample Name: piv phenone purity

Acq. Operator : RMS Seq. Line : 2
Acq. Instrument : Instrument 1 Location : Vial 2
Injection Date : 25-Sep-13, 10:49:16 Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-09-25 10-12-53\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 9/25/2013 11:59:25 AM by RMS
(modified after loading)
Method Info : ÅAGC-default

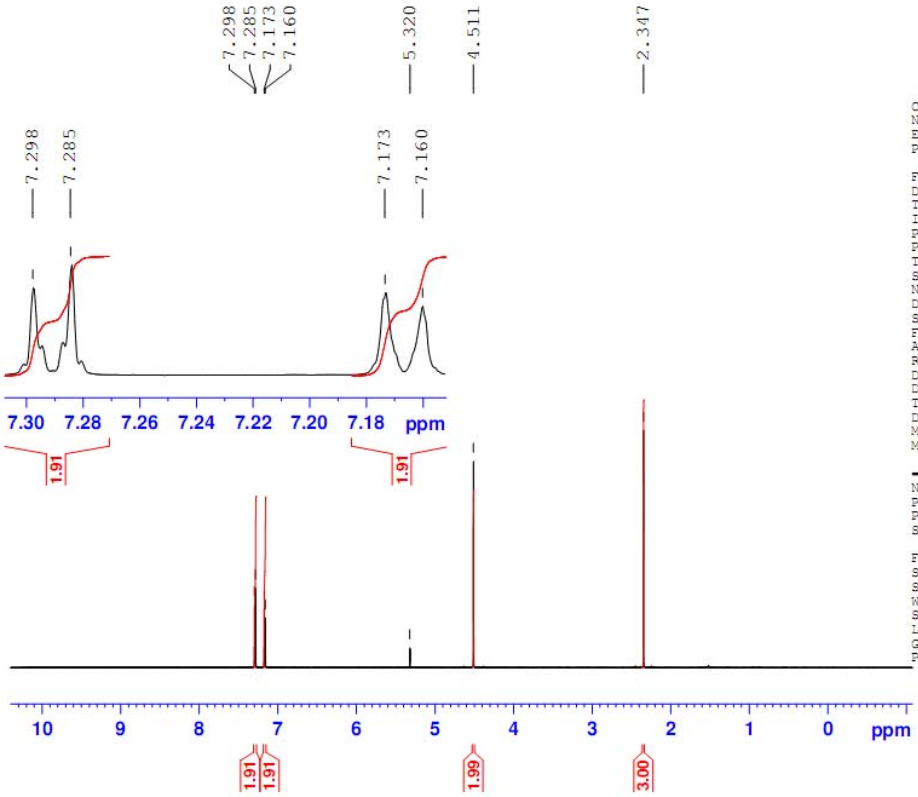


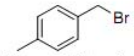
Area Percent Report

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

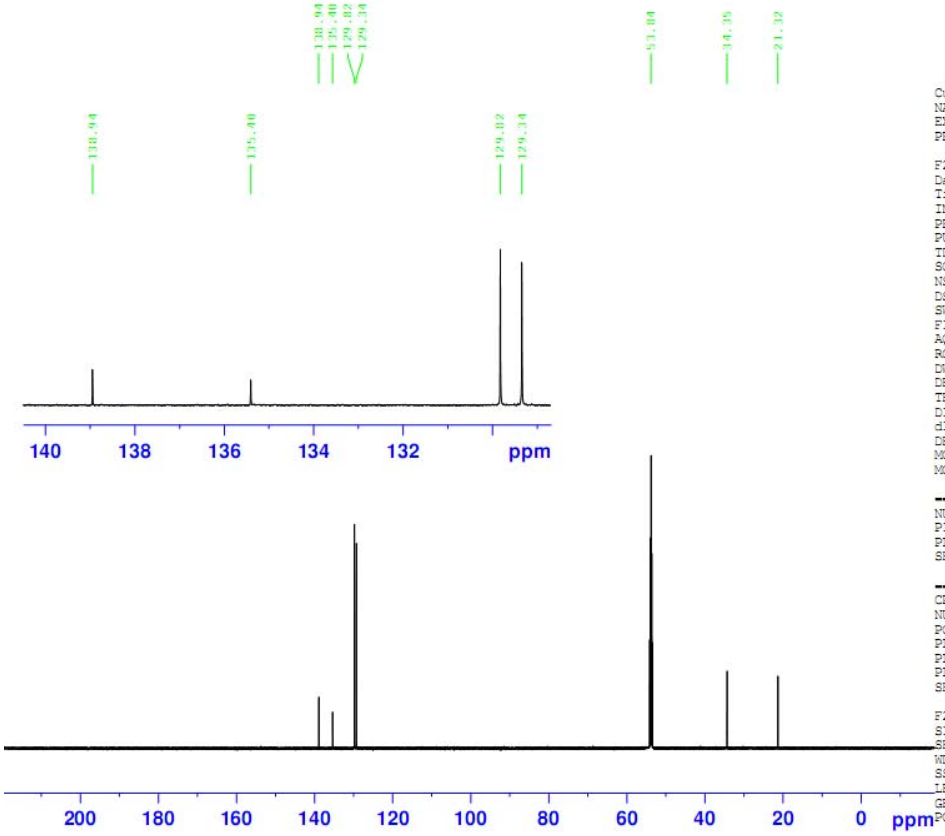
Signal 1: FID1 A,

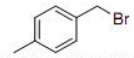
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	6.602	BB	0.0206	12.08297	9.02022	0.68190
2	8.222	BB	0.0237	20.73785	13.64581	1.17033
3	10.404	BB	0.0244	1696.01404	1073.52332	95.71379
4	11.229	BB	0.0210	20.05629	14.59346	1.13187
5	17.270	BB	0.0362	23.07307	10.27814	1.30212






```
Current Data Parameters
NAME            p-M-B-Br
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_             20131025
Time                 12.47
INSTRUM              av600
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT            CD2Cl2
NS                     16
DS                      0
SWH               6887.052 Hz
FIDRES            0.105088 Hz
AQ               4.7579136 sec
RG                   161.3
DW                  72.600 usec
DE                    6.00 usec
TE                   298.0 K
D1               1.00000000 sec
MCREST     0 sec
MCWRK          0.01500000 sec

-------- CHANNEL f1 --------
NUC1                     1H
P1                    11.60 usec
PL1                   -2.00 dB
SFO1          600.1328163 MHz

F2 - Processing parameters
SI                    32768
SF            600.1300188 MHz
WDW                      no
SSB        0
LB         0 Hz
GB         0
PC                     1.40
```

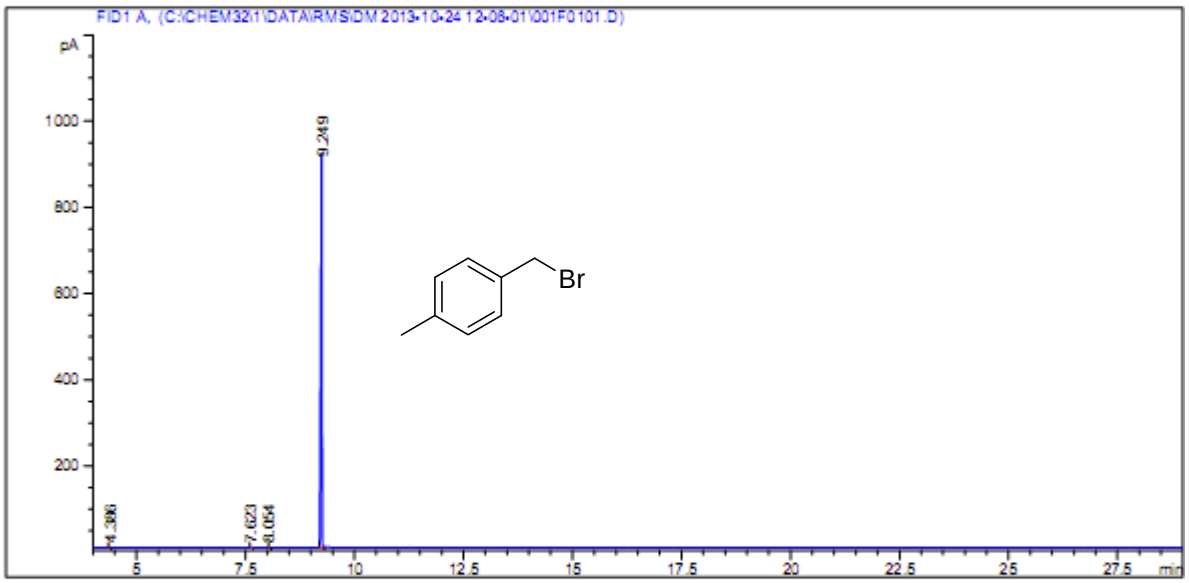





```
Current Data Parameters
NAME            p-M-B-Br
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_             20131025
Time                 13.35
INSTRUM              av600
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     861
DS                       4
SWH              35971.223 Hz
FIDRES            0.548877 Hz
AQ               0.9109504 sec
RG                  9195.2
DW                  13.900 usec
DE                    6.00 usec
TE                   298.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
MCREST     0 sec
MCWRK          0.01500000 sec

-------- CHANNEL f1 --------
NUC1                    13C
P1                     9.00 usec
PL1        0 dB
SFO1          150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2            waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                   -2.00 dB
PL12                  13.50 dB
PL13                  20.00 dB
SFO2          600.1324005 MHz

F2 - Processing parameters
SI                    32768
SF            150.9027470 MHz
WDW                      EM
SSB        0
LB                     1.00 Hz
GB         0
PC                     1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-10-24 12-06-01\001F0101.D
Sample Name: p-M-B-Br purity

Acq. Operator : RMS
Seq. Line : 1
Acq. Instrument : Instrument 1
Location : Vial 1
Injection Date : 24-Oct-13, 12:07:29
Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-10-24 12-06-01\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 10/24/2013 12:48:34 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

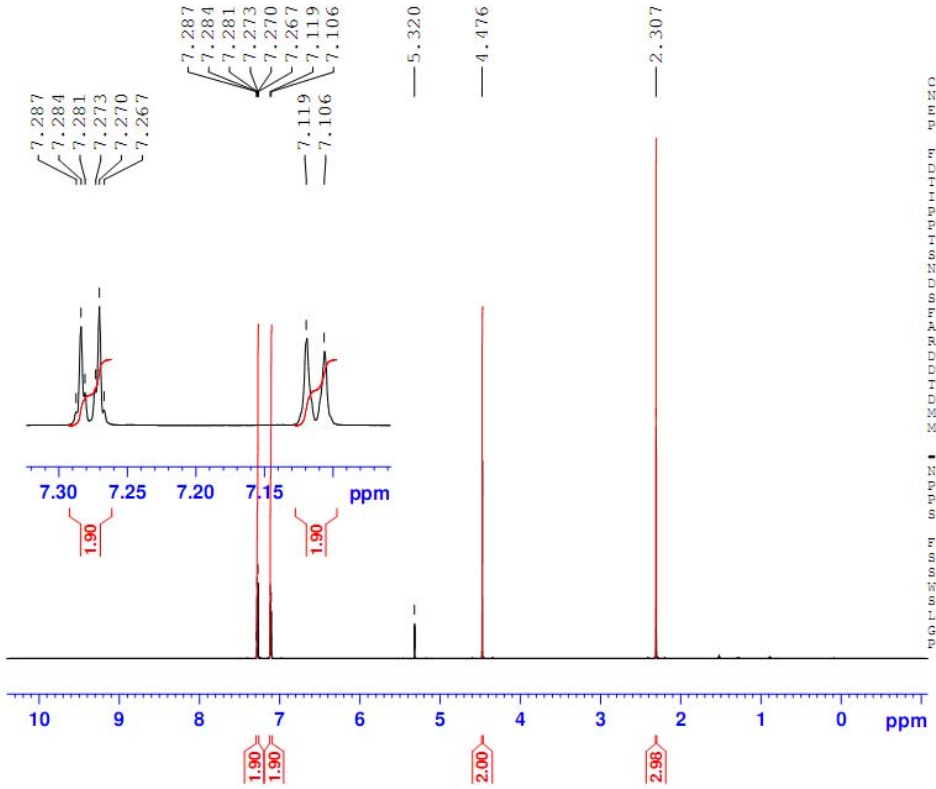


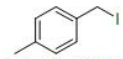
Area Percent Report

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

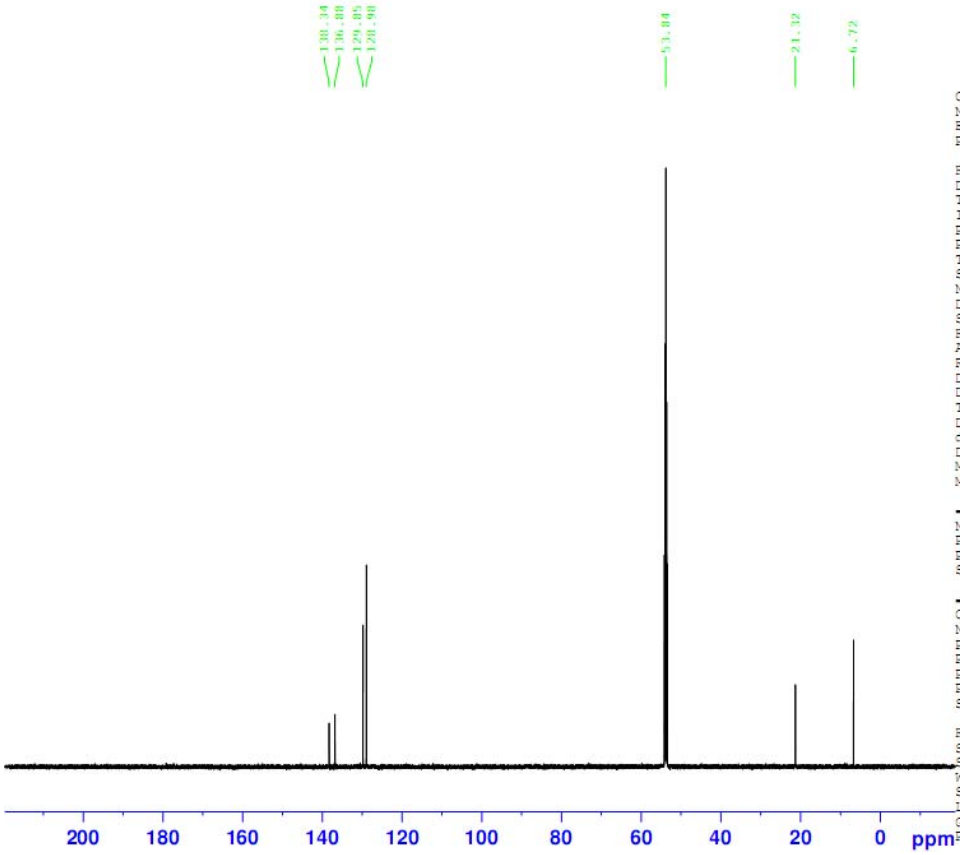
Signal 1: FID1 A,

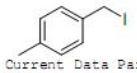
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	4.386	BB	0.0228	3.83935	2.51154	0.24252
2	7.623	BB	0.0256	2.03605	1.21185	0.12861
3	8.054	BB	0.0243	1.86151	1.18456	0.11758
4	9.249	BB	0.0275	1575.39111	897.70276	99.51129





```
Current Data Parameters
NAME                p-M-B-I
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20131030
Time                  12.50
INSTRUM               av600
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT             CD2Cl2
NS                        32
DS                         0
SWH                6887.052 Hz
FIDRES             0.105088 Hz
AQ                4.7579136 sec
RG                      256
DW                   72.600 usec
DE                    6.00 usec
TE                   298.0 K
D1               1.00000000 sec
MCREST    0 sec
MCWRK            0.01500000 sec

-------- CHANNEL f1 --------
NUC1                      1H
P1                     11.60 usec
PL1                    -2.00 dB
SFO1            600.1328163 MHz

F2 - Processing parameters
SI                     32768
SF              600.1300189 MHz
WDW                       no
SSB        0
LB         0 Hz
GB         0
PC                      1.40
```

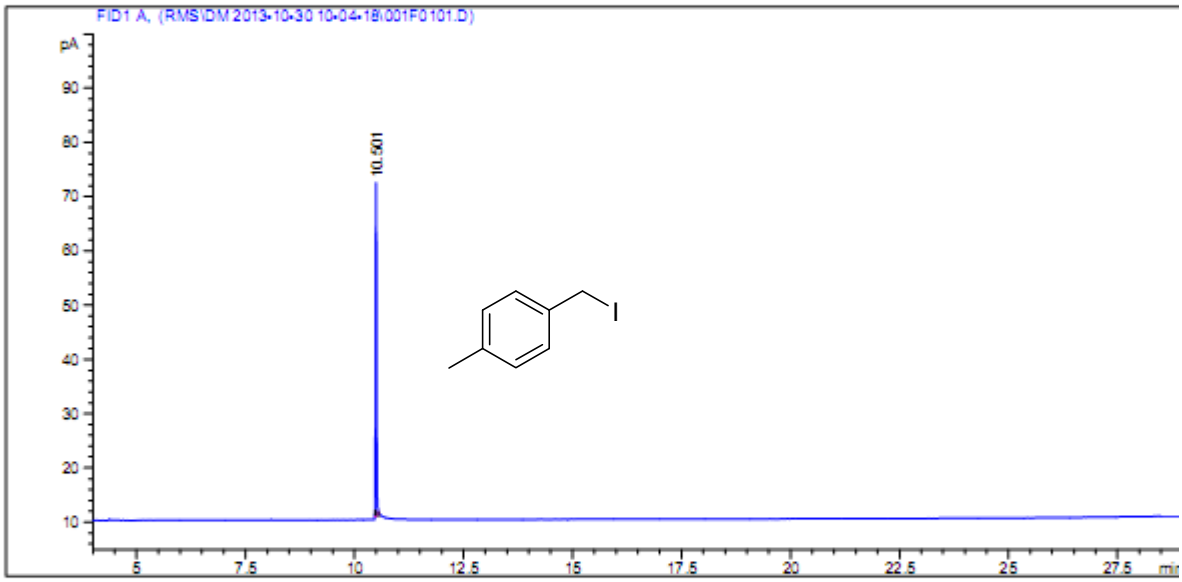




```
Current Data Parameters
NAME                p-M-B-I
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20131030
Time                  13.42
INSTRUM               av600
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      938
DS                        4
SWH               35971.223 Hz
FIDRES             0.548877 Hz
AQ                0.9109504 sec
RG                  20642.5
DW                   13.900 usec
DE                    6.00 usec
TE                   298.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
MCREST    0 sec
MCWRK            0.01500000 sec

-------- CHANNEL f1 --------
NUC1                     13C
P1                      9.00 usec
PL1        0 dB
SFO1            150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2            waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -2.00 dB
PL12                   13.50 dB
PL13                   20.00 dB
SFO2            600.1324005 MHz

F2 - Processing parameters
SI                     32768
SF              150.9027469 MHz
WDW                       EM
SSB        0
LB                      1.00 Hz
GB         0
PC                      1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-10-30 10-04-18\001F0101.D
Sample Name: p-M-B-I purity

Acq. Operator : RMS
Seq. Line : 1
Acq. Instrument : Instrument 1
Location : Vial 1
Injection Date : 30-Oct-13, 10:05:57
Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-10-30 10-04-18\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 10/30/2013 11:51:57 AM by RMS
(modified after loading)
Method Info : ÅAGC-default

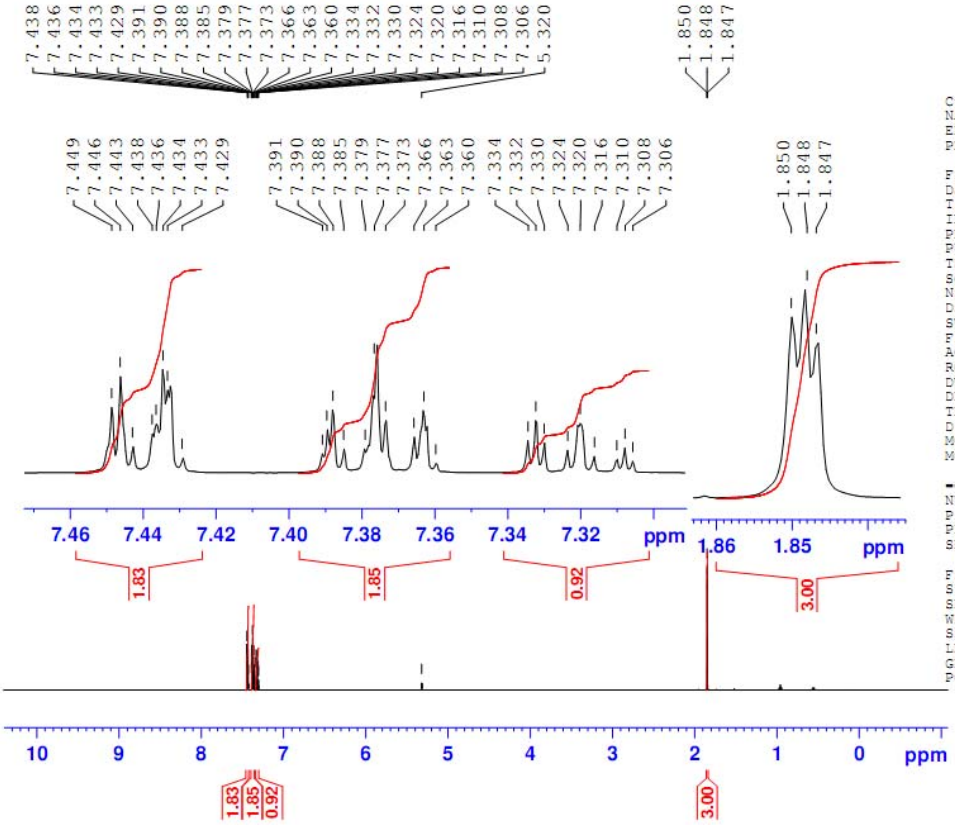


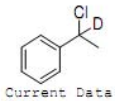
Area Percent Report

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

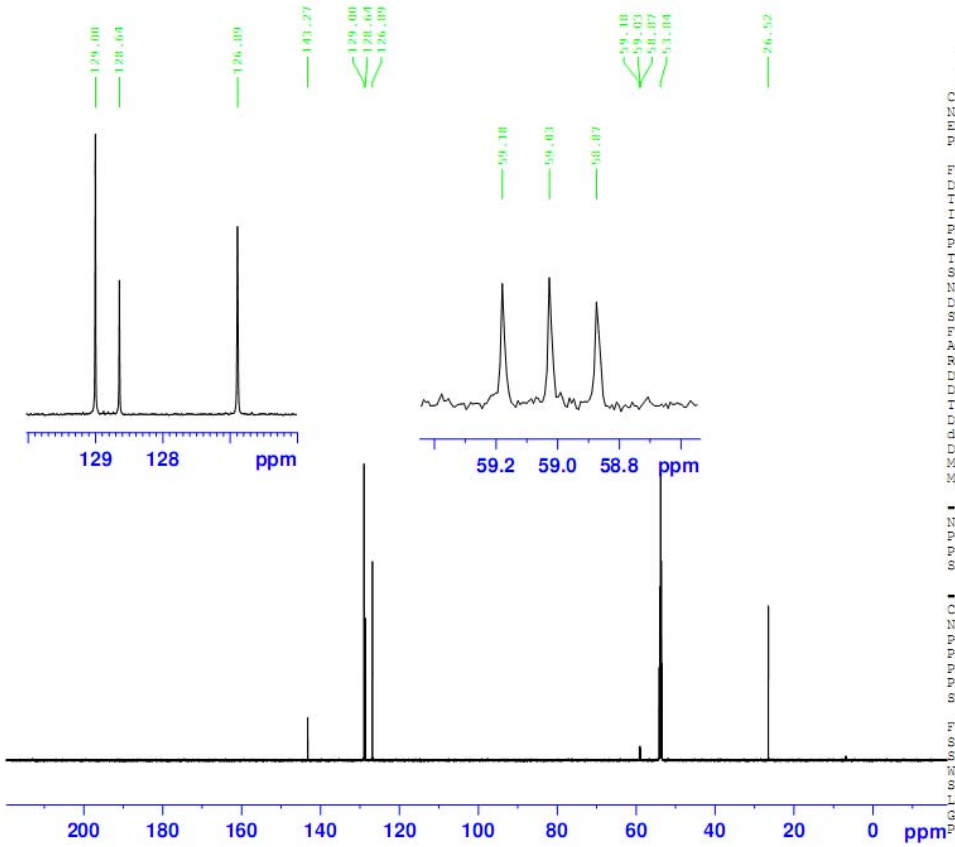
Signal 1: FID1 A,

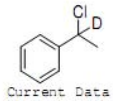
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	10.501	BB	0.0233	91.24078	61.48301	1.000e2






```
Current Data Parameters
NAME                 A-Cl-D
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_             20131023
Time                 12.37
INSTRUM               av600
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT             CD2Cl2
NS                       32
DS                        0
SWH               6887.052 Hz
FIDRES            0.105088 Hz
AQ               4.7579136 sec
RG                      128
DW                   72.600 usec
DE                    6.00 usec
TE                   298.0 K
D1              1.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                     1H
P1                   11.60 usec
PL1                  -2.00 dB
SFO1           600.1328163 MHz

F2 - Processing parameters
SI                    32768
SF            600.1300189 MHz
WDW                      no
SSB       0
LB        0 Hz
GB        0
PC                    1.00
```

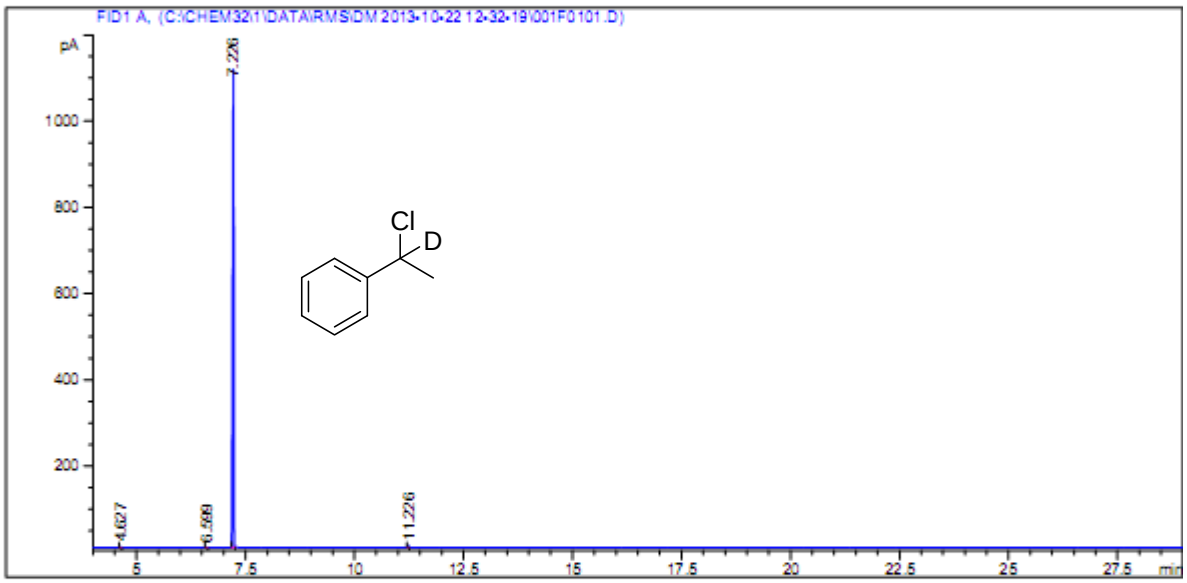





```
Current Data Parameters
NAME                 A-Cl-D
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_             20131023
Time                 13.22
INSTRUM               av600
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      828
DS                        4
SWH              35971.223 Hz
FIDRES            0.548877 Hz
AQ               0.9109504 sec
RG                 14596.5
DW                 13.900 usec
DE                    6.00 usec
TE                   298.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
MCREST    0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                    13C
P1                    9.00 usec
PL1       0 dB
SFO1          150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2          waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                  -2.00 dB
PL12                 13.50 dB
PL13                 20.00 dB
SFO2           600.1324005 MHz

F2 - Processing parameters
SI                    32768
SF            150.9027469 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-10-22 12-32-19\001F0101.D
Sample Name: A-Cl-D purity

Acq. Operator : RMS Seq. Line : 1
Acq. Instrument : Instrument 1 Location : Vial 1
Injection Date : 22-Oct-13, 12:33:47 Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-10-22 12-32-19\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 10/22/2013 1:03:52 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

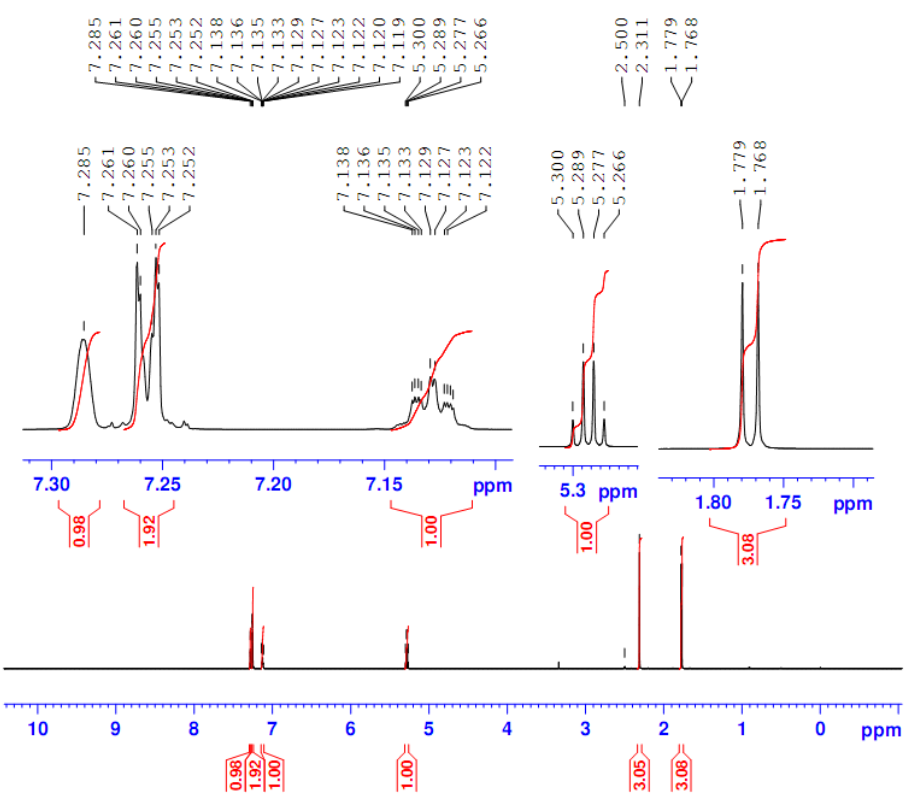


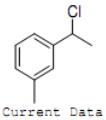
Area Percent Report

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

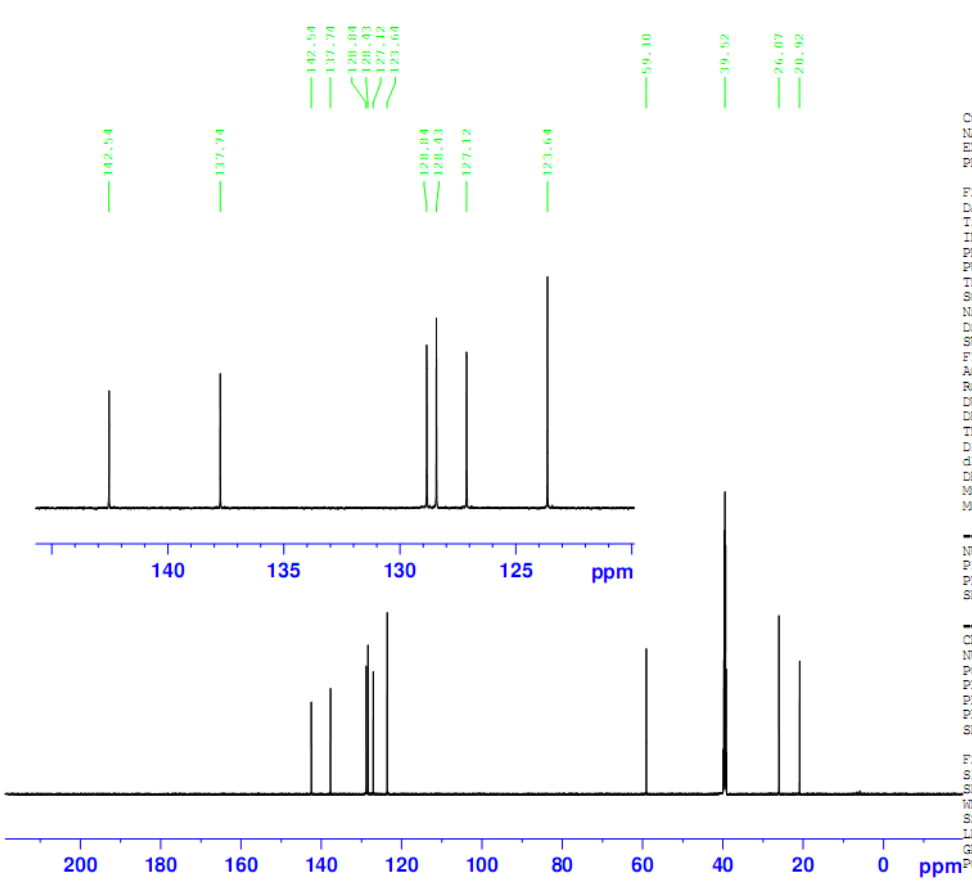
Signal 1: FID1 A,

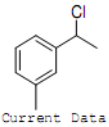
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	4.627	BB	0.0260	5.70400	3.32787	0.31366
2	6.599	BB	0.0205	3.85382	2.90004	0.21192
3	7.226	BB	0.0254	1798.68494	1081.75940	98.90812
4	11.226	BB	0.0225	10.29851	7.26833	0.56631






```
Current Data Parameters
NAME              m-M-A-Cl
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20131007
Time                 12.34
INSTRUM             av600
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                      16
DS                       0
SWH               6887.052 Hz
FIDRES            0.105088 Hz
AQ               4.7579136 sec
RG                    71.8
DW                  72.600 usec
DE                    6.00 usec
TE                   298.0 K
D1               1.00000000 sec
MCREST    0 sec
MCWRK          0.01500000 sec

-------- CHANNEL f1 --------
NUC1                     1H
P1                    11.60 usec
PL1                   -2.00 dB
SFO1          600.1328163 MHz

F2 - Processing parameters
SI                      32768
SF            600.1300005 MHz
WDW                        no
SSB       0
LB        0 Hz
GB        0
PC                     1.00
```

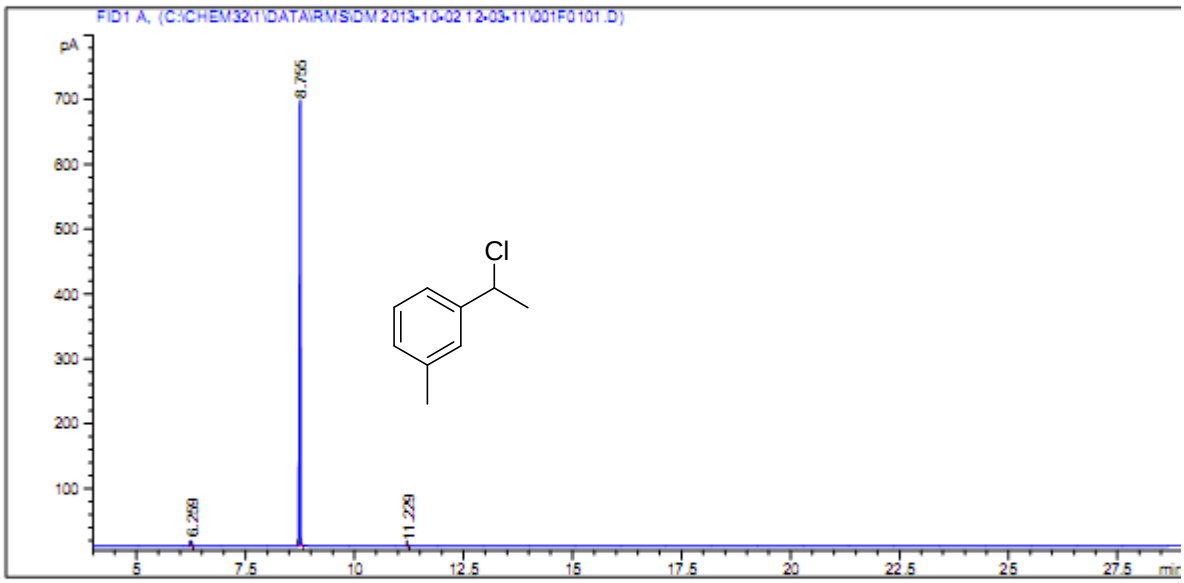





```
Current Data Parameters
NAME              m-M-A-Cl
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20131007
Time                 13.25
INSTRUM             av600
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    920
DS                      4
SWH              35971.223 Hz
FIDRES            0.548877 Hz
AQ               0.9109504 sec
RG                14596.5
DW                  13.900 usec
DE                    6.00 usec
TE                   298.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
MCREST    0 sec
MCWRK          0.01500000 sec

-------- CHANNEL f1 --------
NUC1                    13C
P1                    9.00 usec
PL1       0 dB
SFO1        150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2          waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                  -2.00 dB
PL12                 13.50 dB
PL13                 20.00 dB
SFO2        600.1324005 MHz

F2 - Processing parameters
SI                      32768
SF           150.9028825 MHz
WDW                        EM
SSB       0
LB                    1.00 Hz
GB        0
PC                     1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-10-02 12-03-11\001F0101.D
Sample Name: m-m-A-Cl purity

Acq. Operator : RMS Seq. Line : 1
Acq. Instrument : Instrument 1 Location : Vial 1
Injection Date : 02-Oct-13, 12:04:36 Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-10-02 12-03-11\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 10/2/2013 2:12:58 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

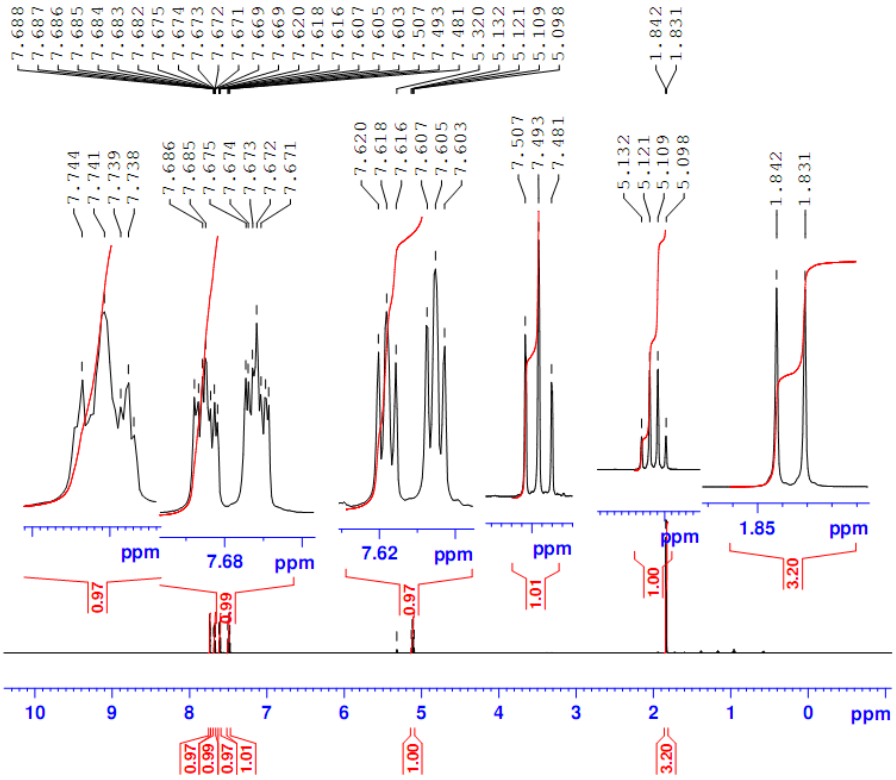


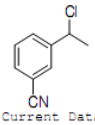
Area Percent Report

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

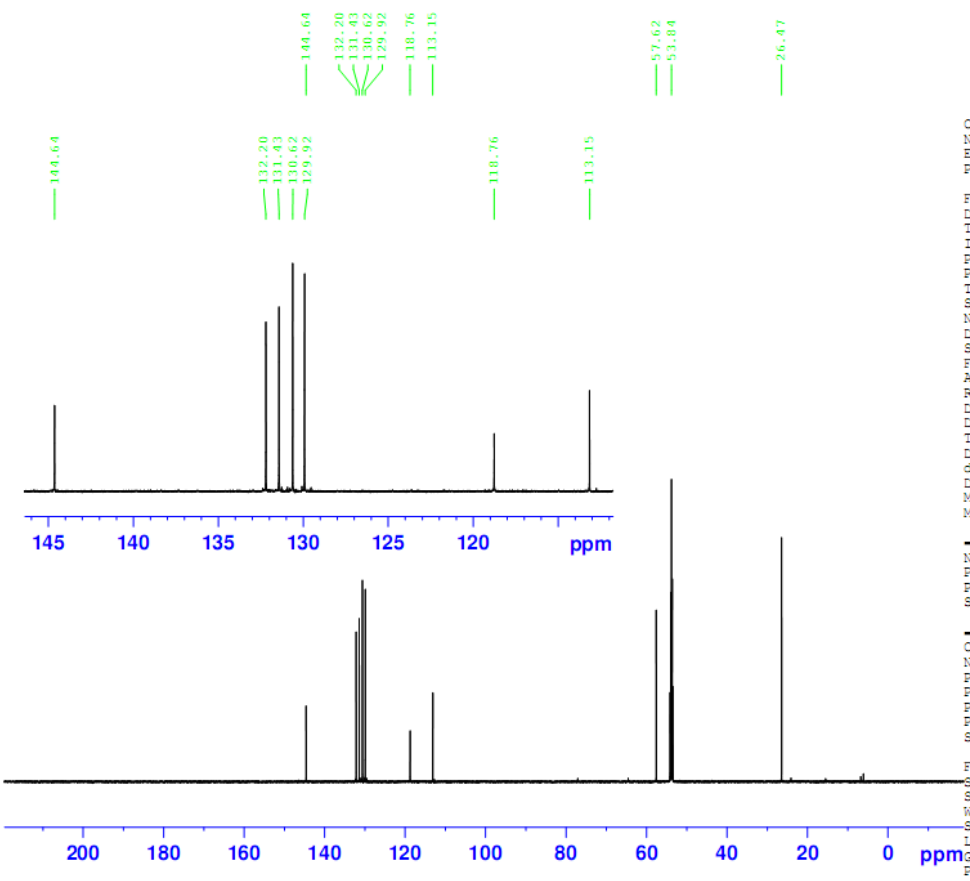
Signal 1: FID1 A,

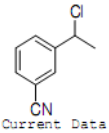
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	6.259	BB	0.0289	16.03922	8.54970	1.56219
2	8.755	BB	0.0232	1007.83917	684.20764	98.16157
3	11.229	BB	0.0227	2.83626	1.97612	0.27625






```
Current Data Parameters
NAME          3-CN-A-Cl
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20131017
Time              13.31
INSTRUM           av600
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT          CD2Cl2
NS                   16
DS                    0
SWH           6887.052 Hz
FIDRES        0.105088 Hz
AQ           4.7579136 sec
RG                90.5
DW               72.600 usec
DE                6.00 usec
TE               298.0 K
D1          1.00000000 sec
MCREST   0 sec
MCWRK       0.01500000 sec

-------- CHANNEL f1 --------
NUC1                 1H
P1                11.60 usec
PL1               -2.00 dB
SFO1        600.1328163 MHz

F2 - Processing parameters
SI               32768
SF          600.1300188 MHz
WDW                 no
SSB       0
LB        0 Hz
GB        0
PC                1.00
```

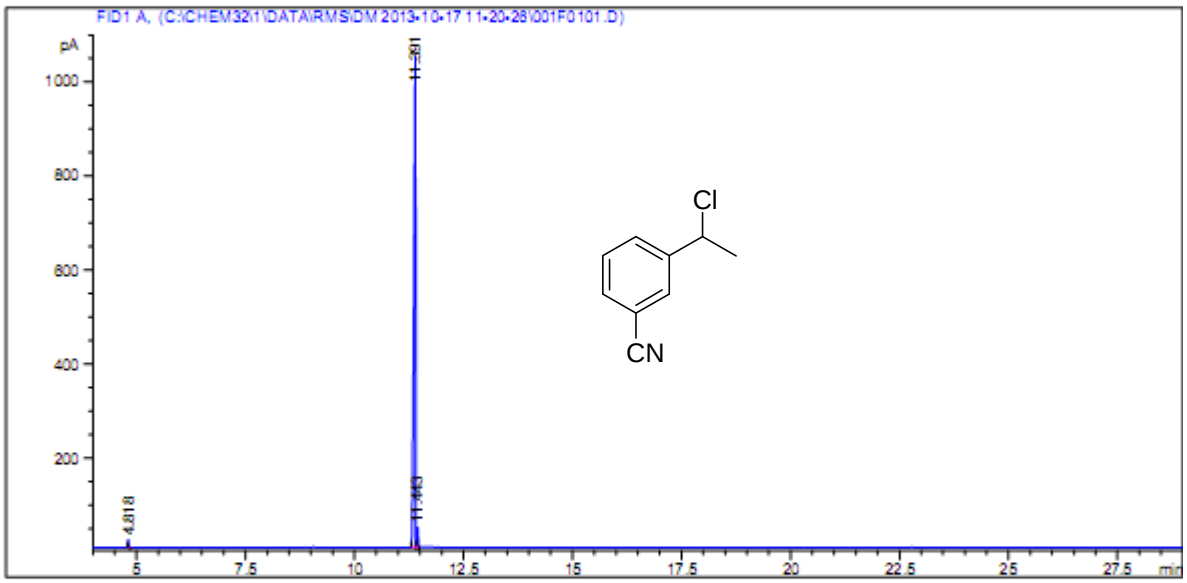





```
Current Data Parameters
NAME          3-CN-A-Cl
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20131017
Time              14.23
INSTRUM           av600
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                  982
DS                    4
SWH          35971.223 Hz
FIDRES        0.548877 Hz
AQ           0.9109504 sec
RG             20642.5
DW               13.900 usec
DE                6.00 usec
TE               298.0 K
D1          2.00000000 sec
d11         0.03000000 sec
DELTA       1.89999998 sec
MCREST   0 sec
MCWRK       0.01500000 sec

-------- CHANNEL f1 --------
NUC1                 13C
P1                9.00 usec
PL1       0 dB
SFO1        150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2         waltz16
NUC2                 1H
PCPD2            80.00 usec
PL2              -2.00 dB
PL12             13.50 dB
PL13             20.00 dB
SFO2        600.1324005 MHz

F2 - Processing parameters
SI               32768
SF          150.9027523 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-10-17 11-20-26\001F0101.D
Sample Name: 3-CN-A-Cl pu

Acq. Operator : RMS
Seq. Line : 1
Acq. Instrument : Instrument 1
Location : Vial 1
Injection Date : 17-Oct-13, 11:21:55
Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-10-17 11-20-26\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 10/17/2013 12:33:52 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

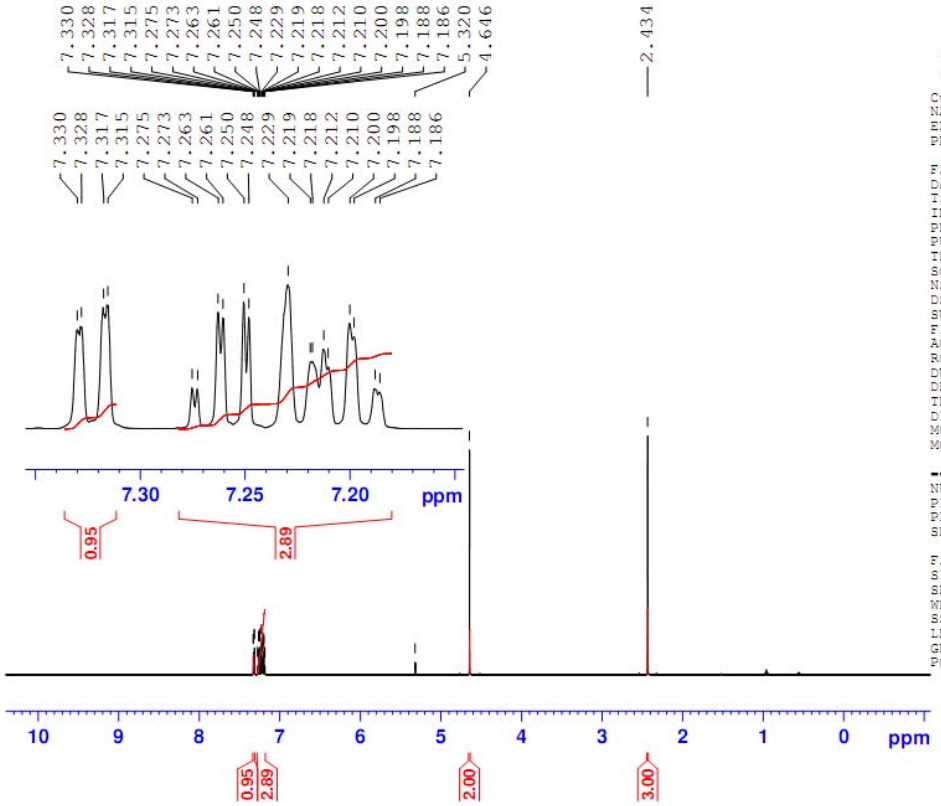


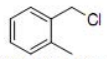
Area Percent Report

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

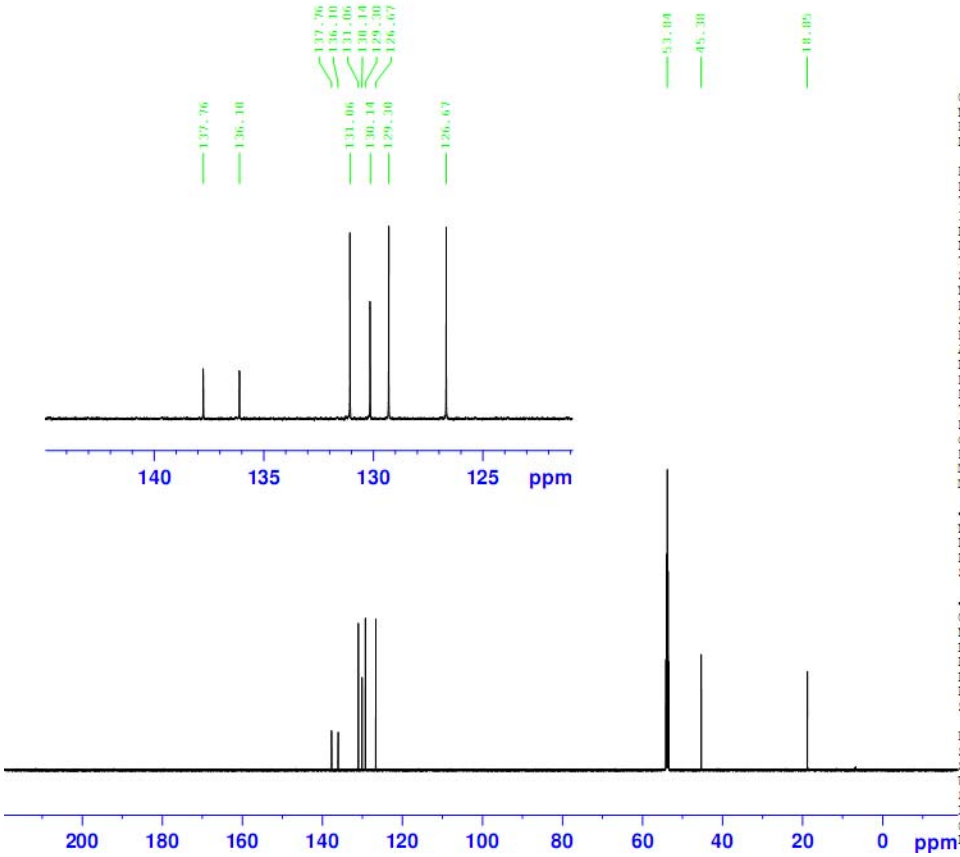
Signal 1: FID1 A,

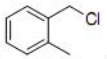
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	4.818	BB	0.0201	21.36726	16.51339	0.72183
2	11.391	BV	0.0393	2880.62720	1042.08740	97.31335
3	11.443	VB	0.0223	58.16164	41.62211	1.96482






```
Current Data Parameters
NAME              O-M-B-Cl
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20131014
Time                 13.39
INSTRUM              av600
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT             CD2Cl2
NS                      16
DS                       0
SWH               6887.052 Hz
FIDRES            0.105088 Hz
AQ              4.7579136 sec
RG                     114
DW                  72.600 usec
DE                   6.00 usec
TE                  298.0 K
D1              1.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                     1H
P1                    11.60 usec
PL1                   -2.00 dB
SFO1          600.1328163 MHz

F2 - Processing parameters
SI                    32768
SF            600.1300189 MHz
WDW                      nc
SSB       0
LB        0 Hz
GB        0
PC                     1.00
```

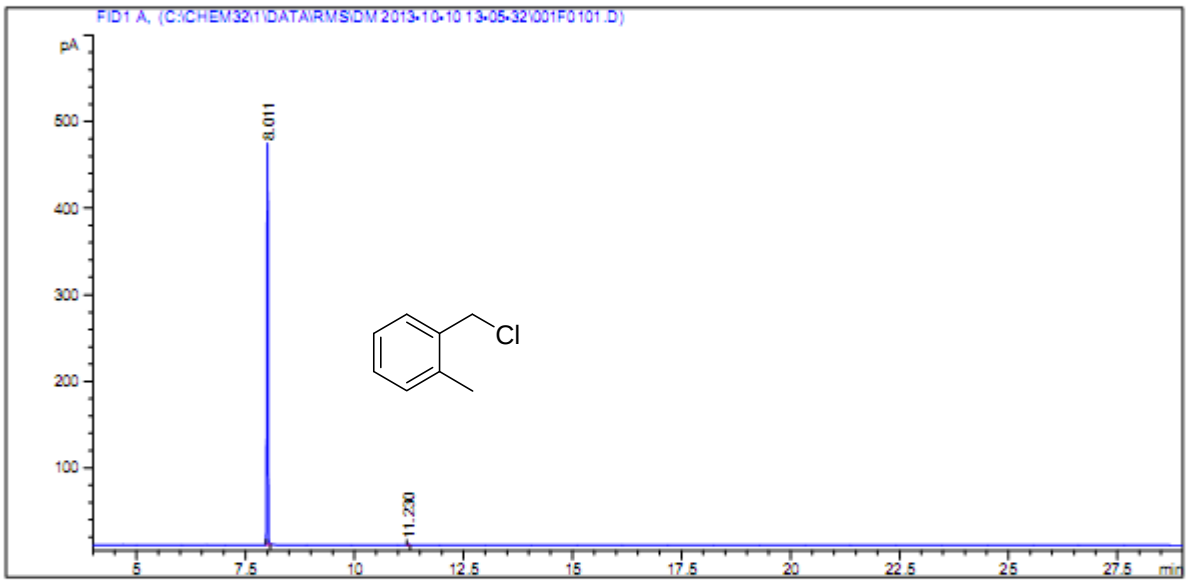





```
Current Data Parameters
NAME              O-M-B-Cl
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20131014
Time                 14.25
INSTRUM              av600
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                    65536
SOLVENT             CDCl3
NS                     866
DS                       4
SWH              35971.223 Hz
FIDRES            0.548877 Hz
AQ              0.9109504 sec
RG                  11585.2
DW                  13.900 usec
DE                   6.00 usec
TE                  298.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
MCREST    0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                    13C
P1                    9.00 usec
PL1       0 dB
SFO1          150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2           waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                   -2.00 dB
PL12                  13.50 dB
PL13                  20.00 dB
SFO2          600.1324005 MHz

F2 - Processing parameters
SI                    32768
SF            150.9027471 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                     1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-10-10 13-05-32\001F0101.D
Sample Name: O-M-B-Cl purity

Acq. Operator : RMS Seq. Line : 1
Acq. Instrument : Instrument 1 Location : Vial 1
Injection Date : 10-Oct-13, 13:07:00 Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-10-10 13-05-32\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 10/10/2013 2:24:18 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

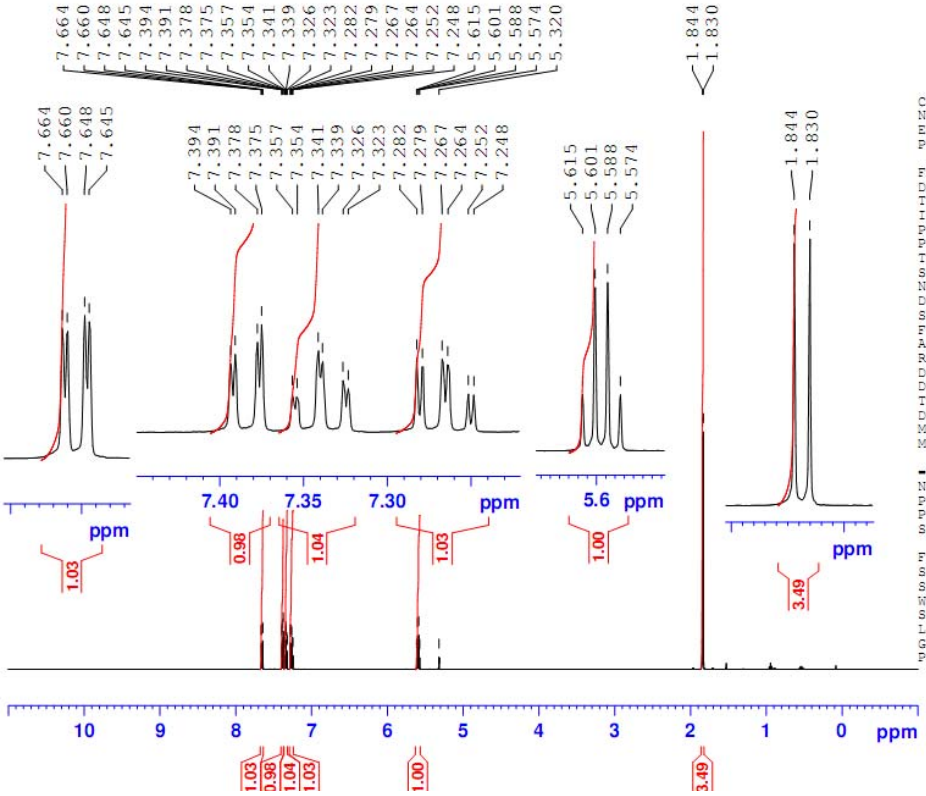


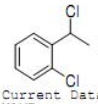
Area Percent Report

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

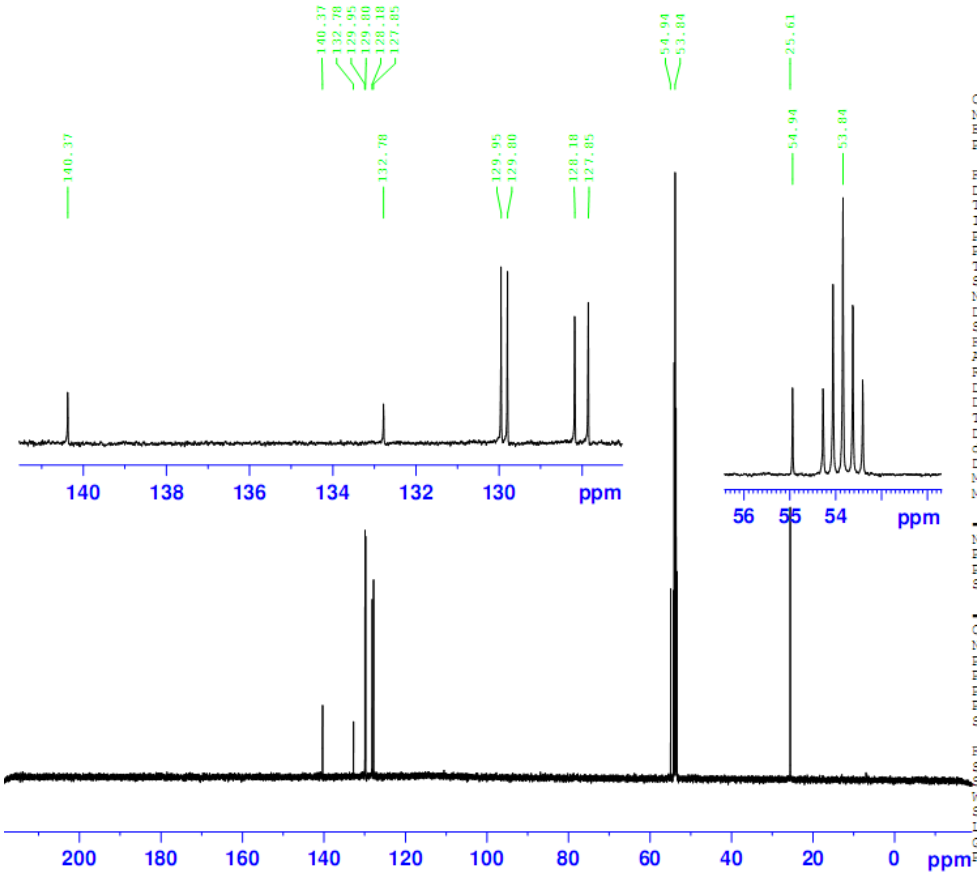
Signal 1: FID1 A,

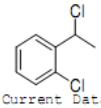
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	8.011	BB	0.0228	664.21100	462.24557	99.56766
2	11.230	BB	0.0229	2.88410	1.99194	0.43234






```
Current Data Parameters
NAME          2'-Cl-A-Cl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130906
Time               13.39
INSTRUM            AV500
PROBHD   5 mm PABBI 1H-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ            3.1719425 sec
RG                 90.5
DW               48.400 usec
DE                6.00 usec
TE                298.1 K
D1          1.00000000 sec
MCREST   0 sec
MCWRK       0.01500000 sec

-------- CHANNEL f1 --------
NUC1                  1H
P1                 6.90 usec
PL1                1.50 dB
SFO1        500.1330885 MHz

F2 - Processing parameters
SI                32768
SF          500.1300203 MHz
WDW                  no
SSB      0
LB       0 Hz
GB       0
PC                 1.40
```

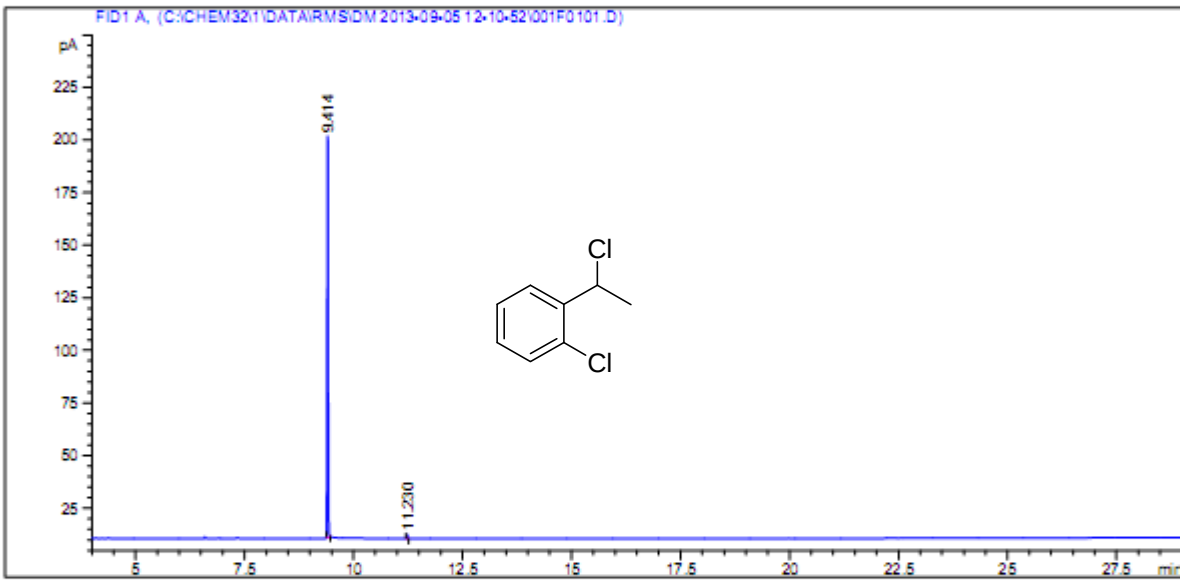




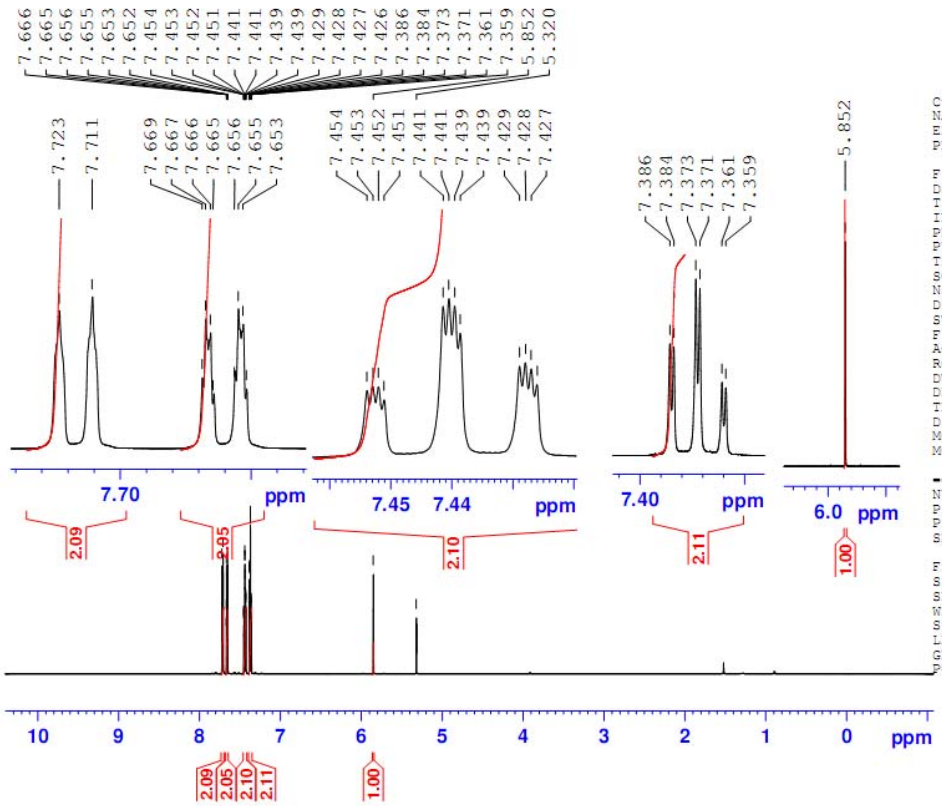

```
Current Data Parameters
NAME          2'-Cl-A-Cl
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130906
Time               13.20
INSTRUM            AV500
PROBHD   5 mm PABBI 1H-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  467
DS                    4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0911744 sec
RG                645.1
DW               16.650 usec
DE                6.00 usec
TE                298.1 K
D1          2.00000000 sec
d11         0.03000000 sec
DELTA       1.89999998 sec
MCREST   0 sec
MCWRK       0.01500000 sec

-------- CHANNEL f1 --------
NUC1                 13C
P1                12.60 usec
PL1               -2.00 dB
SFO1        125.7703643 MHz

-------- CHANNEL f2 --------
CPDPRG[2         waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                1.50 dB
PL12              22.42 dB
PL13              25.40 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577370 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.00
```

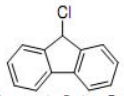
Data File C:\CHEM32\1\DATA\RMS\DM 2013-09-05 12-10-52\001F0101.D
Sample Name: 2'-Cl-A-Cl purity

```
---------------------------------------------------------------------------
Acq. Operator    : RMS                              Seq. Line :   1
Acq. Instrument  : Instrument 1                      Location : Vial 1
Injection Date   : 05-Sep-13, 12:12:16                    Inj :   1
                                                   Inj Volume : 1 µl
Acq. Method      : C:\CHEM32\1\DATA\RMS\DM 2013-09-05 12-10-52\ÅA-DEFAULT.M
Last changed     : 3/27/2013 6:06:31 PM by OL
Analysis Method  : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed     : 9/5/2013 2:33:19 PM by RMS
                   (modified after loading)
Method Info      : ÅAGC-default
```

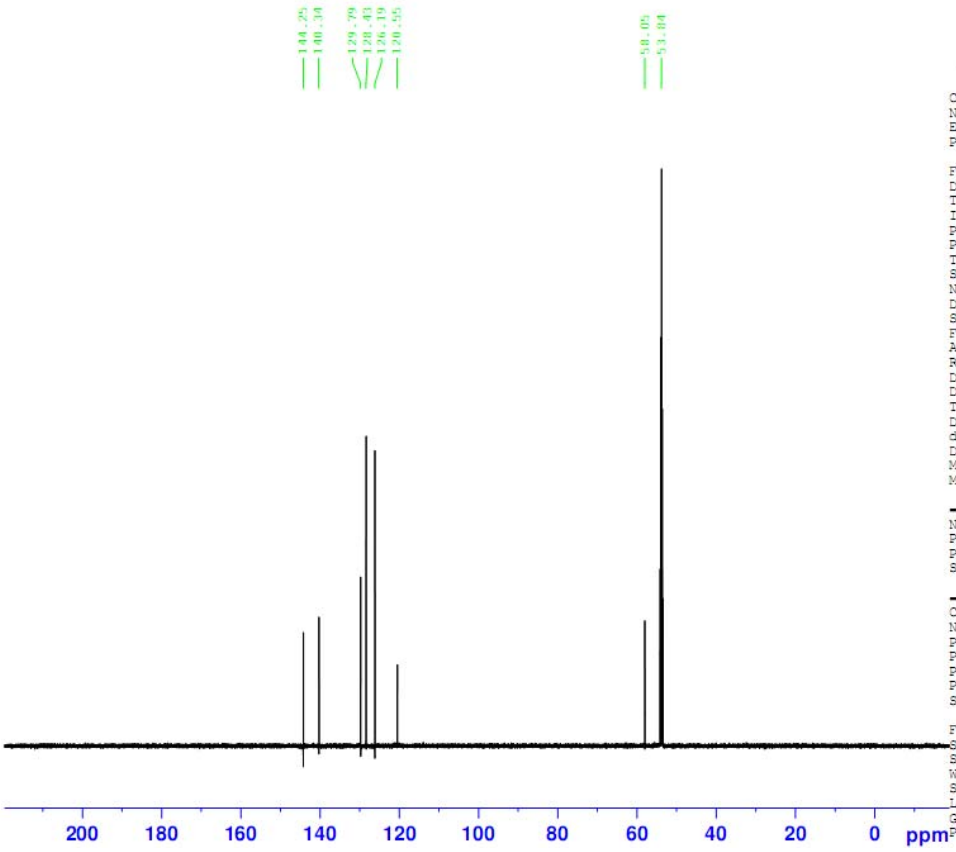


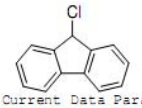

```
---------------------------------------------------------------------------
                          Area Percent Report
---------------------------------------------------------------------------

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


Signal 1: FID1 A,

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1    9.414 BB    0.0225  268.82468  189.97830 99.03471
   2   11.230 BB    0.0223    2.62022    1.87518  0.96529
```






```
Current Data Parameters
NAME          9-Cl-Fluor
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130905
Time                9.21
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    16
DS                     0
SWH             6887.052 Hz
FIDRES          0.105088 Hz
AQ             4.7579136 sec
RG                 228.1
DW                72.600 usec
DE                  6.00 usec
TE                 298.0 K
D1             1.00000000 sec
MCREST   0 sec
MCWRK          0.01500000 sec

-------- CHANNEL f1 --------
NUC1                  1H
P1                11.60 usec
PL1               -2.00 dB
SFO1         600.1328163 MHz

F2 - Processing parameters
SI                131072
SF           600.1300189 MHz
WDW                   no
SSB      0
LB       0 Hz
GB       0
PC                 1.00
```

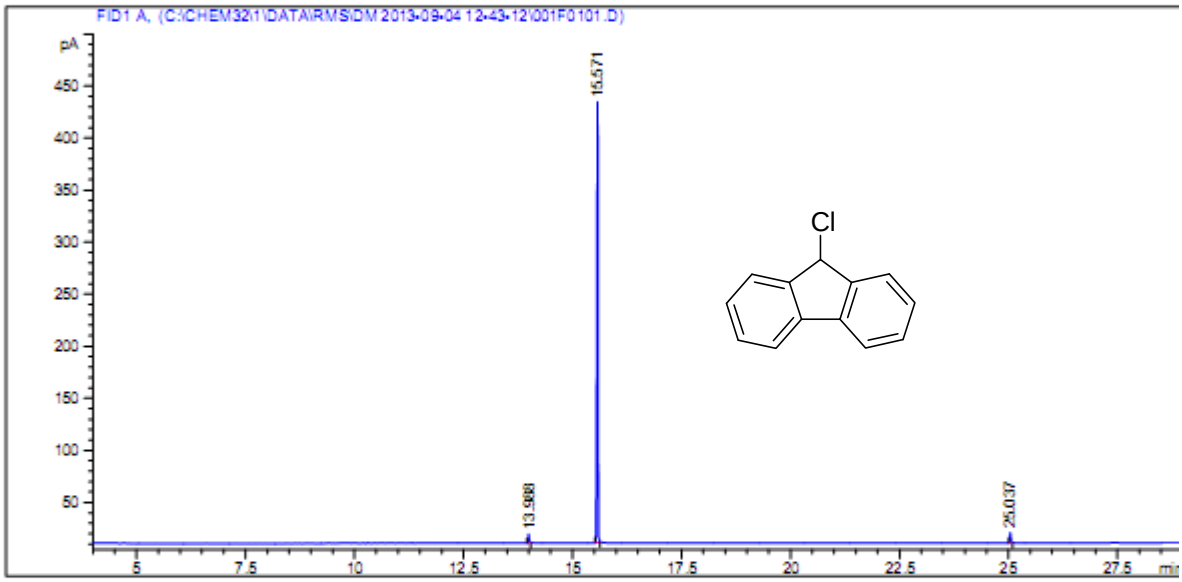





```
Current Data Parameters
NAME          9-Cl-Fluor
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130905
Time               10.19
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            35971.223 Hz
FIDRES          0.548877 Hz
AQ             0.9109504 sec
RG                 16384
DW                13.900 usec
DE                  6.00 usec
TE                 298.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
MCREST   0 sec
MCWRK          0.01500000 sec

-------- CHANNEL f1 --------
NUC1                 13C
P1                 9.00 usec
PL1      0 dB
SFO1         150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2         waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2               -2.00 dB
PL12              13.50 dB
PL13              20.00 dB
SFO2         600.1324005 MHz

F2 - Processing parameters
SI                 32768
SF           150.9027469 MHz
WDW                   no
SSB      0
LB       0 Hz
GB       0
PC                 1.40
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-09-04 12-43-12\001F0101.D
Sample Name: 9-Cl-Fluorenonen purity

Acq. Operator : RMS
Seq. Line : 1
Acq. Instrument : Instrument 1
Location : Vial 1
Injection Date : 04-Sep-13, 12:44:39
Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-09-04 12-43-12\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 9/5/2013 9:04:21 AM by RMS
(modified after loading)
Method Info : ÅAGC-default

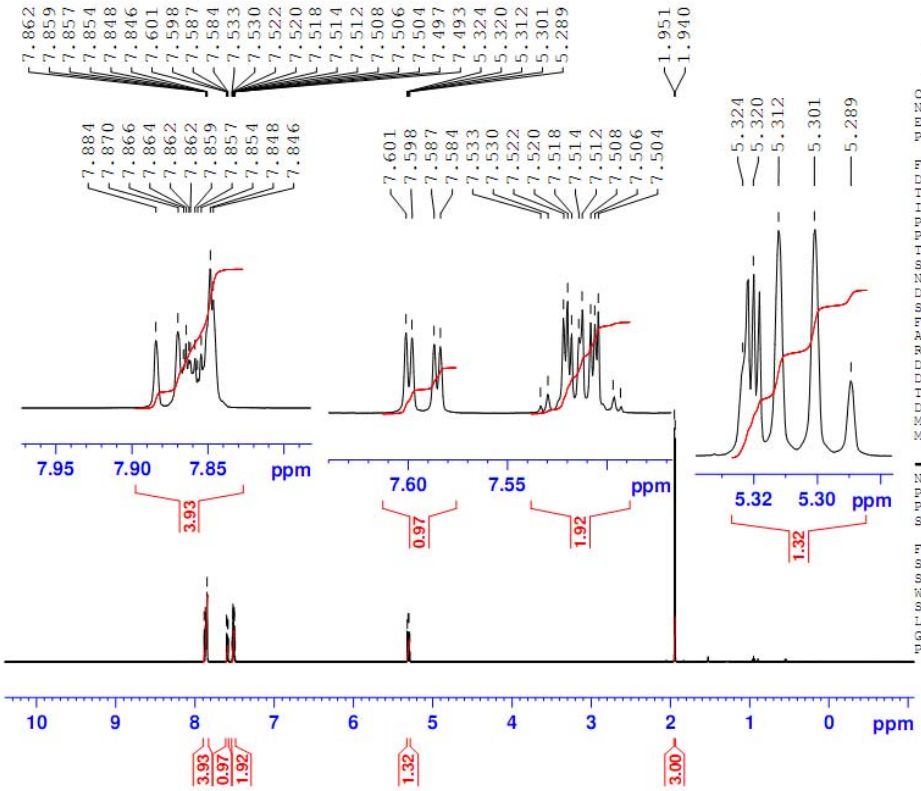


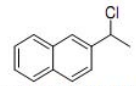
Area Percent Report

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

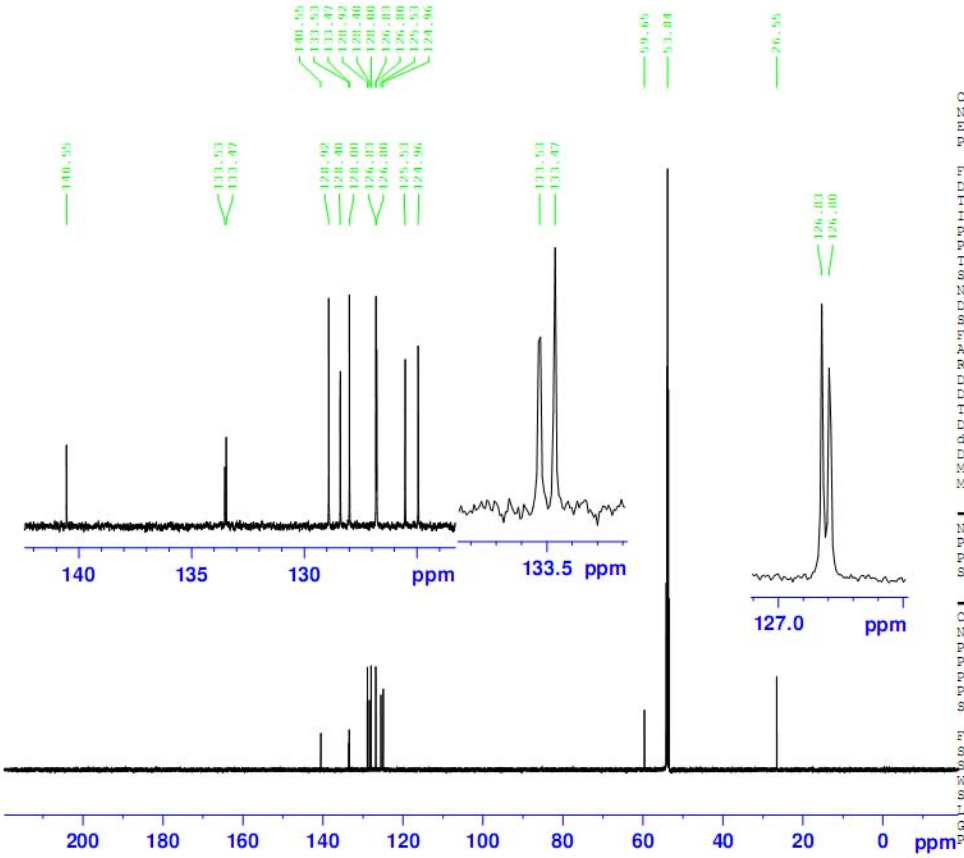
Signal 1: FID1 A,

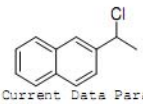
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	13.988	BB	0.0305	17.20427	8.55877	2.40263
2	15.571	BB	0.0248	680.89856	422.69598	95.08975
3	25.037	BB	0.0276	17.95605	9.68662	2.50762






```
Current Data Parameters
NAME                 Np-A-Cl
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20130918
Time                  10.44
INSTRUM               av600
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT             CD2Cl2
NS                        32
DS                         0
SWH               6887.052 Hz
FIDRES            0.105088 Hz
AQ               4.7579136 sec
RG                    161.3
DW                   72.600 usec
DE                    6.00 usec
TE                   298.0 K
D1              1.00000000 sec
MCREST     0 sec
MCWRK           0.01500000 sec

-------- CHANNEL f1 --------
NUC1                      1H
P1                     11.60 usec
PL1                    -2.00 dB
SFO1            600.1328163 MHz

F2 - Processing parameters
SI                     32768
SF              600.1300189 MHz
WDW                       no
SSB        0
LB         0 Hz
GB         0
PC                      1.00
```

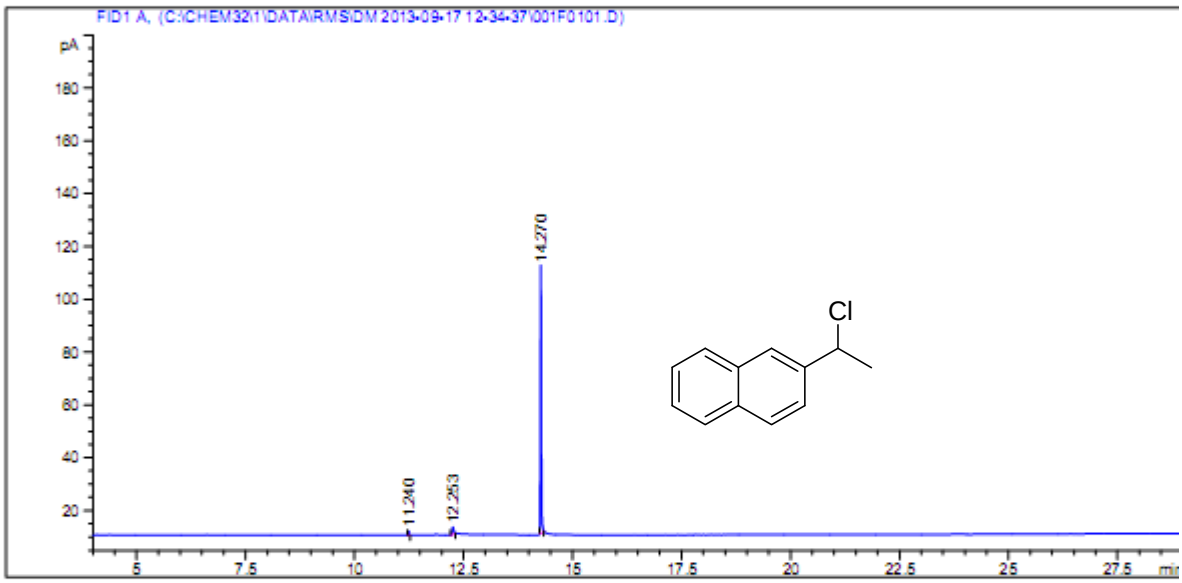





```
Current Data Parameters
NAME                 Np-A-Cl
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20130918
Time                  11.29
INSTRUM               av600
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      807
DS                        4
SWH              35971.223 Hz
FIDRES            0.548877 Hz
AQ               0.9109504 sec
RG                  18390.4
DW                   13.900 usec
DE                    6.00 usec
TE                   298.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
MCREST     0 sec
MCWRK           0.01500000 sec

-------- CHANNEL f1 --------
NUC1                     13C
P1                      9.00 usec
PL1        0 dB
SFO1          150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2            waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -2.00 dB
PL12                   13.50 dB
PL13                   20.00 dB
SFO2            600.1324005 MHz

F2 - Processing parameters
SI                     32768
SF             150.9027470 MHz
WDW                       EM
SSB        0
LB                      1.00 Hz
GB         0
PC                      1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-09-17 12-34-37\001F0101.D
Sample Name: np purity

Acq. Operator : RMS
Seq. Line : 1
Acq. Instrument : Instrument 1
Location : Vial 1
Injection Date : 17-Sep-13, 12:36:03
Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-09-17 12-34-37\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 9/17/2013 1:06:44 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

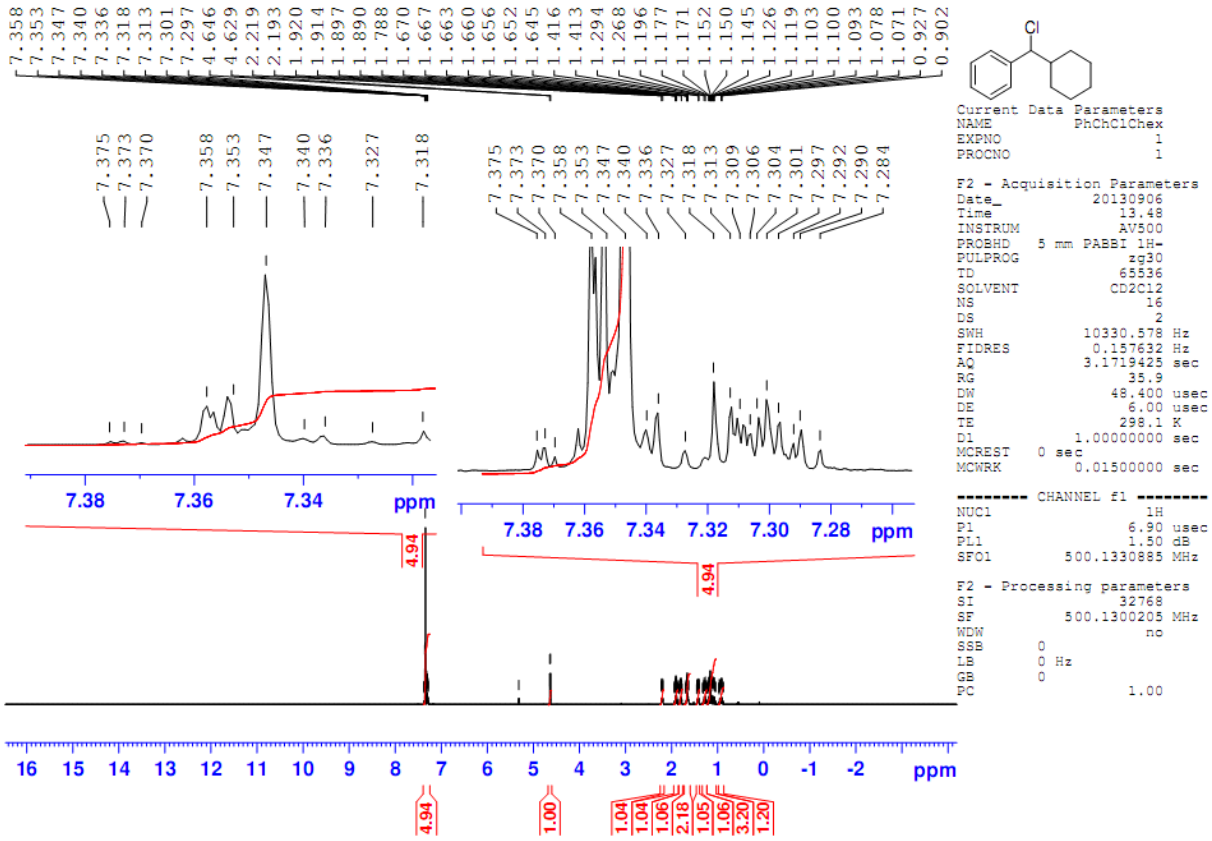


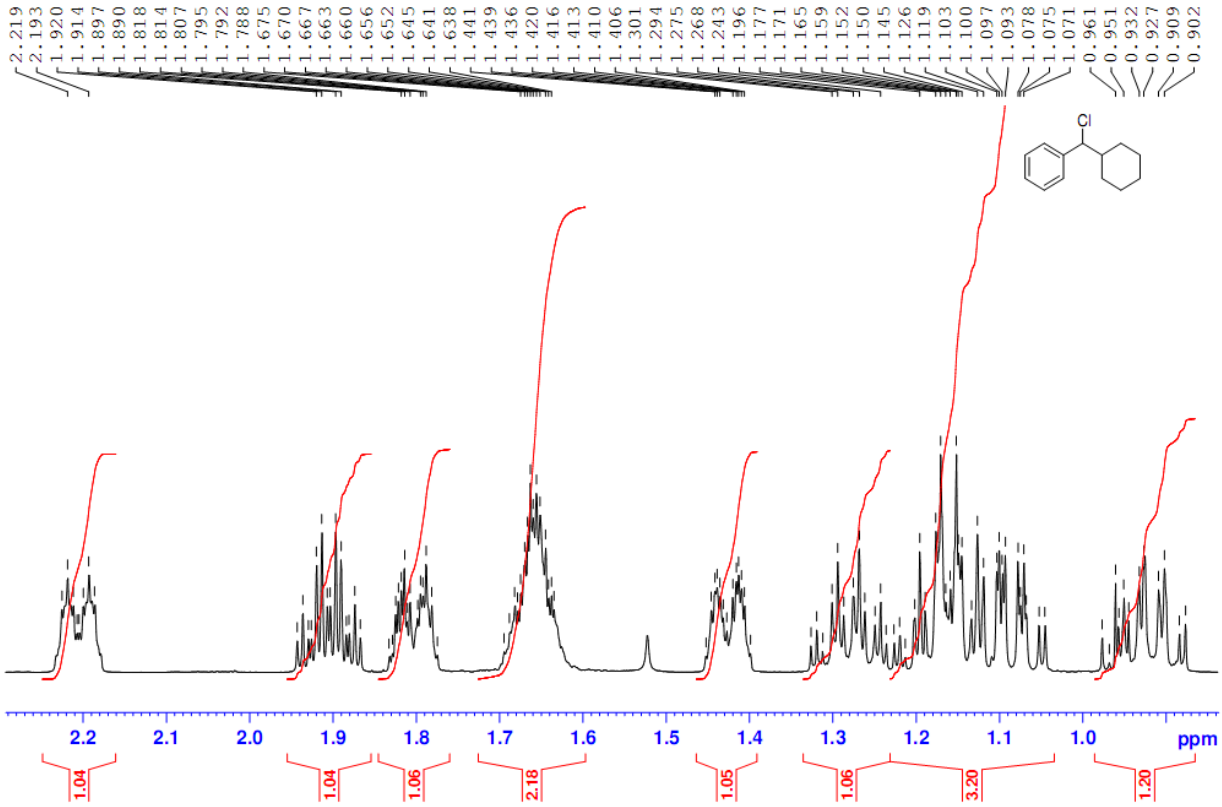
Area Percent Report

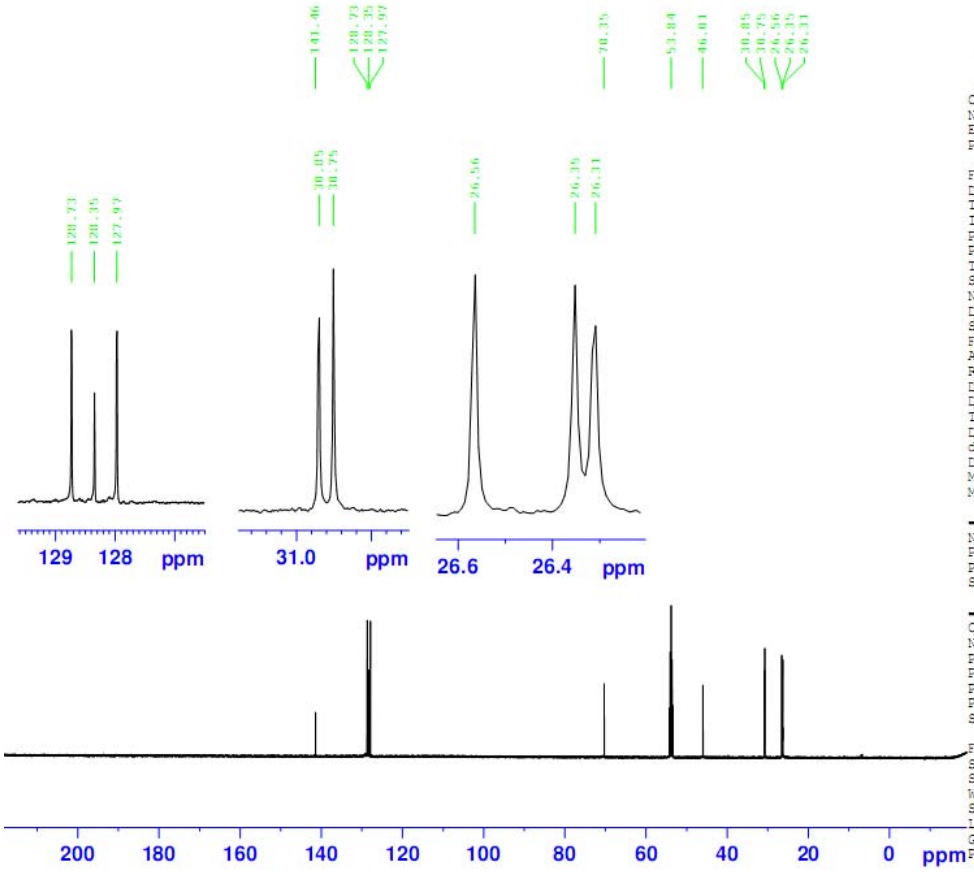
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

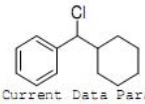
Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	11.240	BB	0.0229	2.29018	1.58155	1.42874
2	12.253	BB	0.0380	6.97053	2.80551	4.34860
3	14.270	BB	0.0235	151.03313	100.82535	94.22266


Cl
Current Data Parameters
NAME PhChClChex
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130906
Time 13.48
INSTRUM AV500
PROBHD 5 mm PABBI 1H-
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 35.9
DW 48.400 usec
DE 6.00 usec
TE 298.1 K
D1 1.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 6.90 usec
PL1 1.50 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300205 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
ppm


Cl
ppm

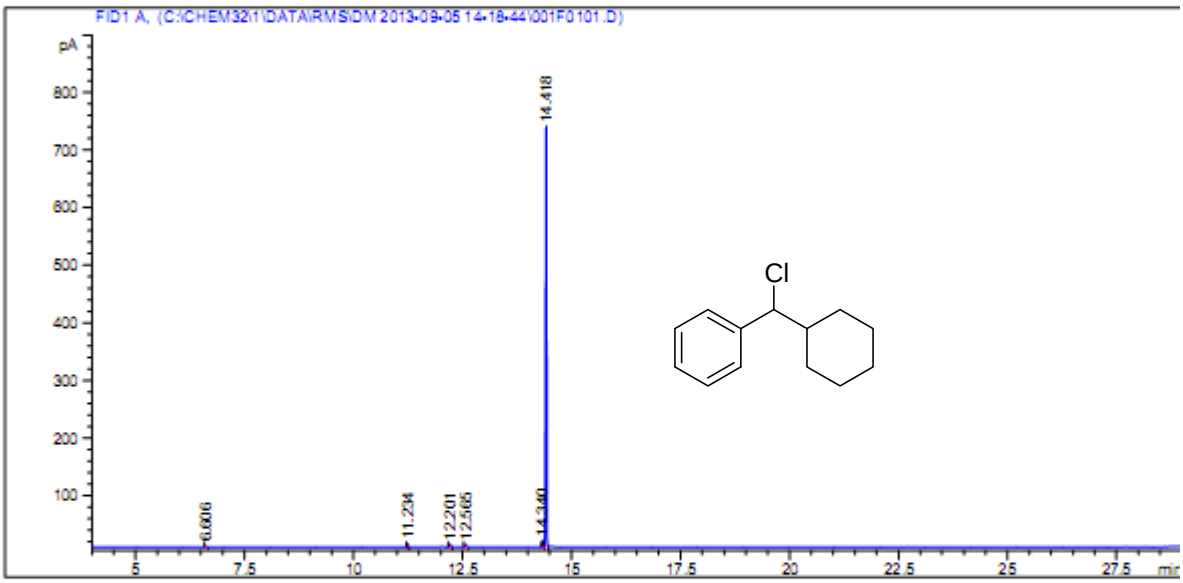





```
Current Data Parameters
NAME          PhChClChex
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20130906
Time              13.58
INSTRUM           AV500
PROBHD   5 mm PABBI 1H-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  377
DS                    4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0911744 sec
RG                574.7
DW               16.650 usec
DE                6.00 usec
TE               298.1 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
MCREST   0 sec
MCWRK         0.01500000 sec

-------- CHANNEL f1 --------
NUC1                 13C
P1                12.60 usec
PL1               -2.00 dB
SFO1        125.7703643 MHz

-------- CHANNEL f2 --------
CPDPRG[2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                1.50 dB
PL12              22.42 dB
PL13              25.40 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577369 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-09-05 14-18-44\001F0101.D
Sample Name: PhCHClChex purity

Acq. Operator : RMS Seq. Line : 1
Acq. Instrument : Instrument 1 Location : Vial 1
Injection Date : 05-Sep-13, 14:20:11 Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-09-05 14-18-44\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 9/5/2013 2:51:19 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

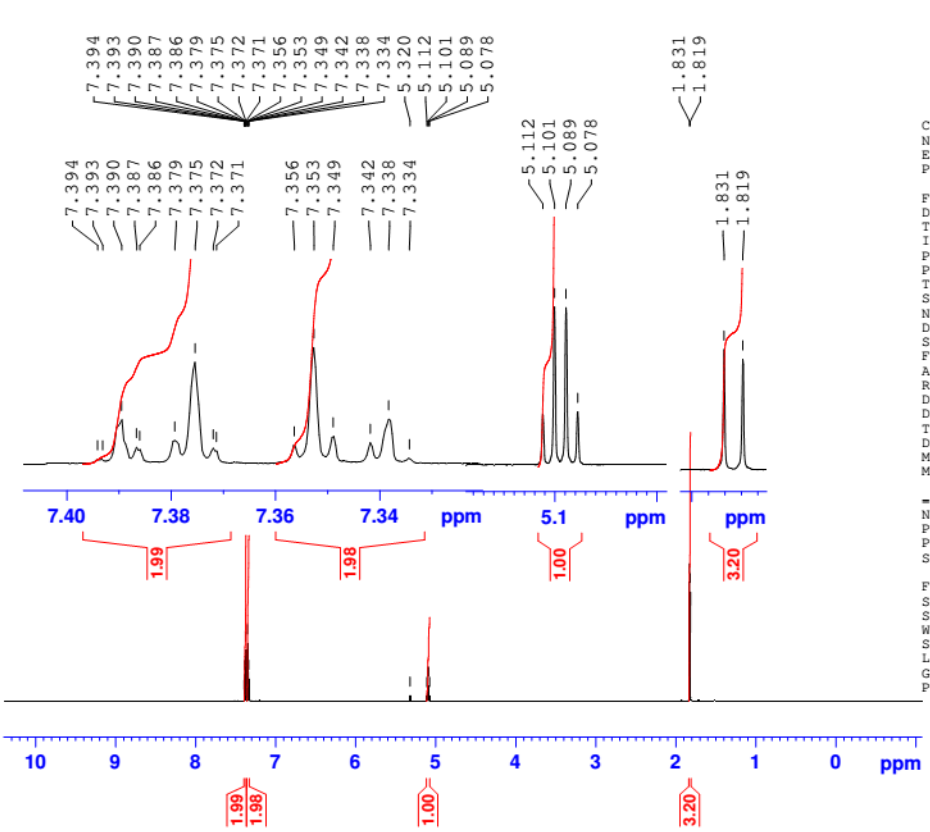


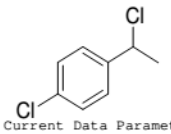
Area Percent Report

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

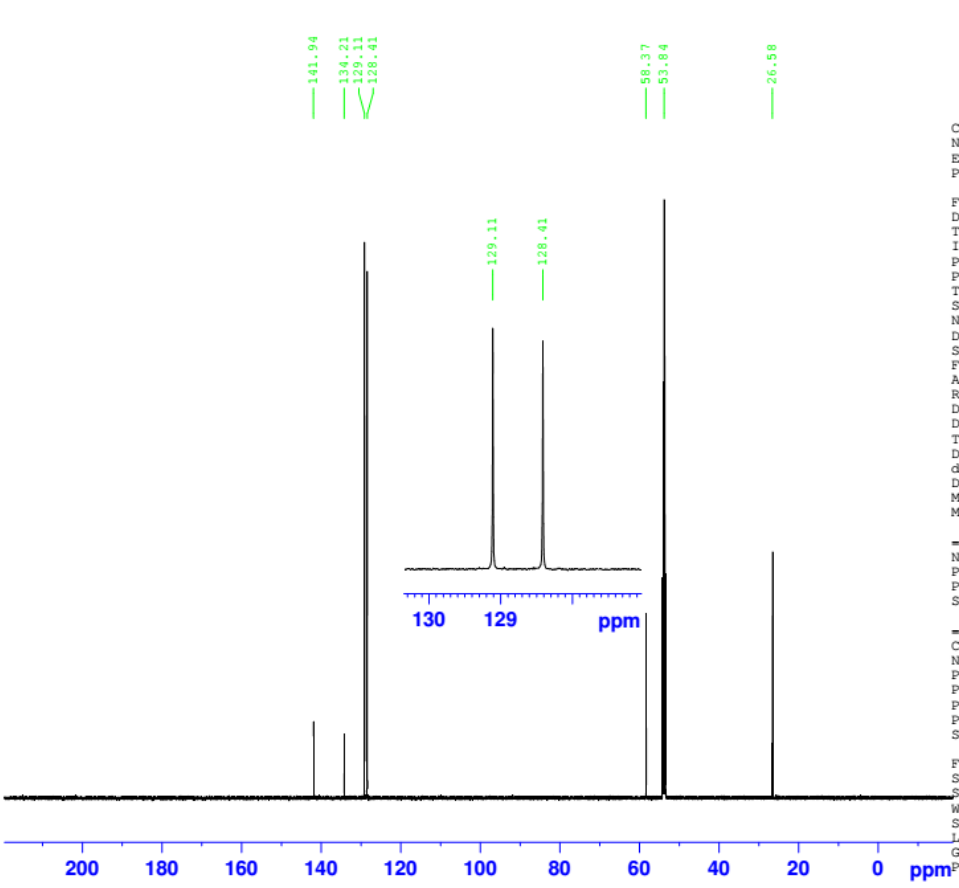
Signal 1: FID1 A,

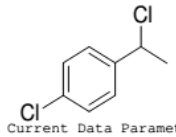
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	6.606	BB	0.0216	2.63936	1.97624	0.21240
2	11.234	BB	0.0223	7.79207	5.59266	0.62707
3	12.201	BB	0.0286	9.47222	4.88513	0.76228
4	12.565	BB	0.0314	9.90338	4.94229	0.79698
5	14.340	BV	0.0228	16.17619	11.21391	1.30179
6	14.418	VB	0.0251	1196.62866	729.34357	96.29947






```
Current Data Parameters
NAME                 p-Cl-A-Cl
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20131114
Time                   10.42
INSTRUM                av600
PROBHD     5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT               CD2Cl2
NS                        16
DS                         0
SWH                 6887.052 Hz
FIDRES              0.105088 Hz
AQ                 4.7579136 sec
RG                       128
DW                    72.600 usec
DE                     6.00 usec
TE                    298.0 K
D1                 1.00000000 sec
MCREST     0 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.60 usec
PL1                    -2.00 dB
SFO1             600.1328163 MHz

F2 - Processing parameters
SI                      32768
SF               600.1300189 MHz
WDW                        no
SSB        0
LB         0 Hz
GB         0
PC                      1.00
```

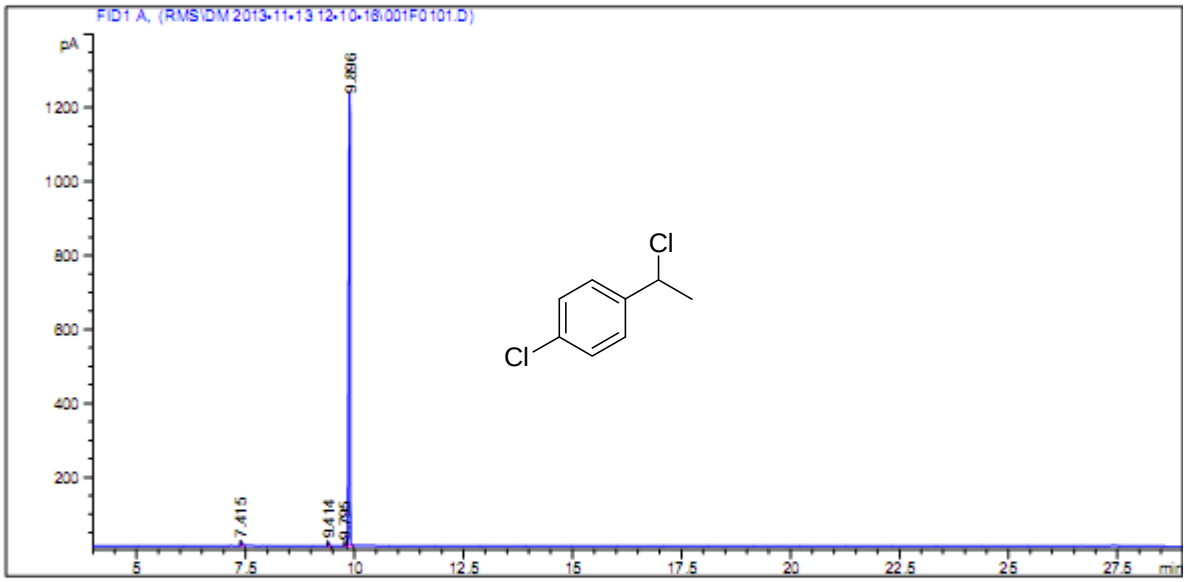





```
Current Data Parameters
NAME                 p-Cl-A-Cl
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20131114
Time                   11.31
INSTRUM                av600
PROBHD     5 mm PABBO BB-
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       863
DS                         4
SWH                35971.223 Hz
FIDRES              0.548877 Hz
AQ                 0.9109504 sec
RG                     16384
DW                    13.900 usec
DE                     6.00 usec
TE                    298.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST     0 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.00 usec
PL1        0 dB
SFO1             150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                    -2.00 dB
PL12                   13.50 dB
PL13                   20.00 dB
SFO2             600.1324005 MHz

F2 - Processing parameters
SI                      32768
SF               150.9027468 MHz
WDW                        EM
SSB        0
LB                      1.00 Hz
GB         0
PC                      1.40
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-11-13 12-10-16\001F0101.D
Sample Name: p-Cl-A-Cl purity

Acq. Operator : RMS Seq. Line : 1
Acq. Instrument : Instrument 1 Location : Vial 1
Injection Date : 13-Nov-13, 12:11:45 Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-11-13 12-10-16\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 11/13/2013 1:10:46 PM by RMS
(modified after loading)
Method Info : ÅAGC-default

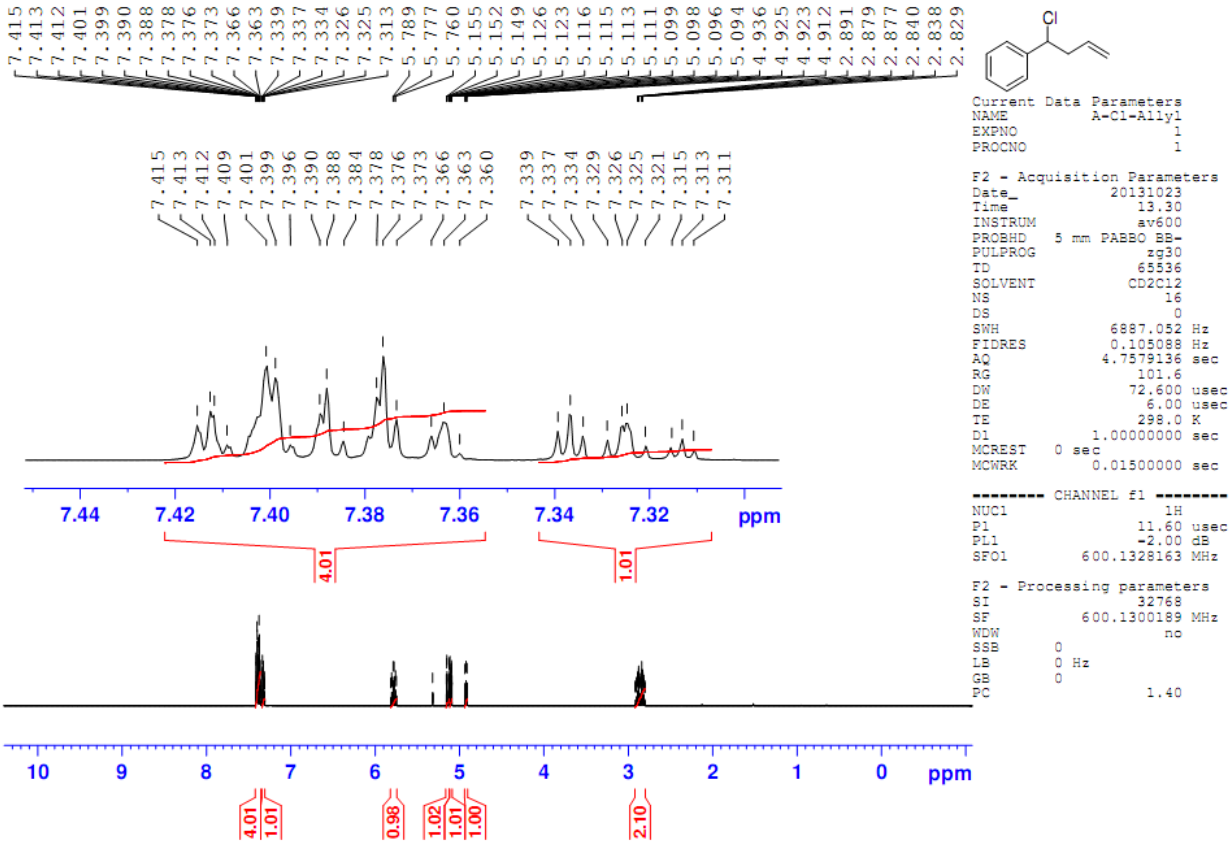


Area Percent Report

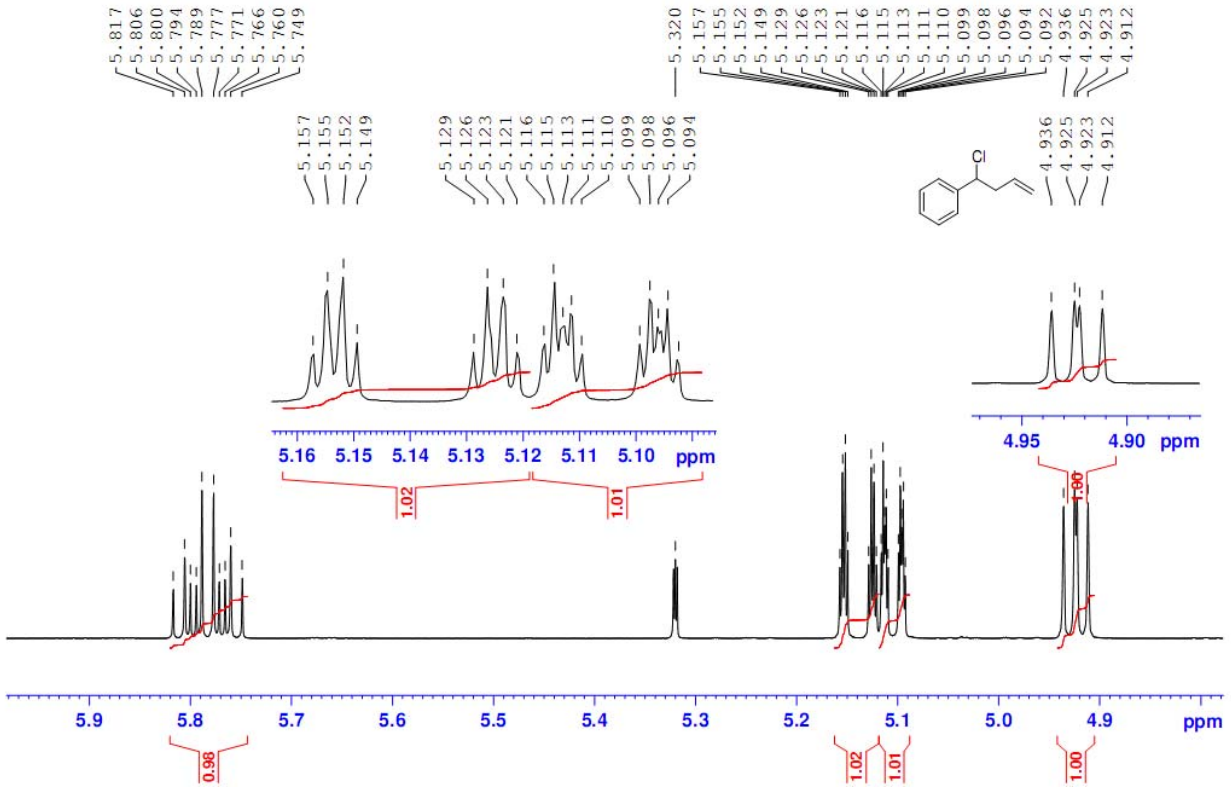
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

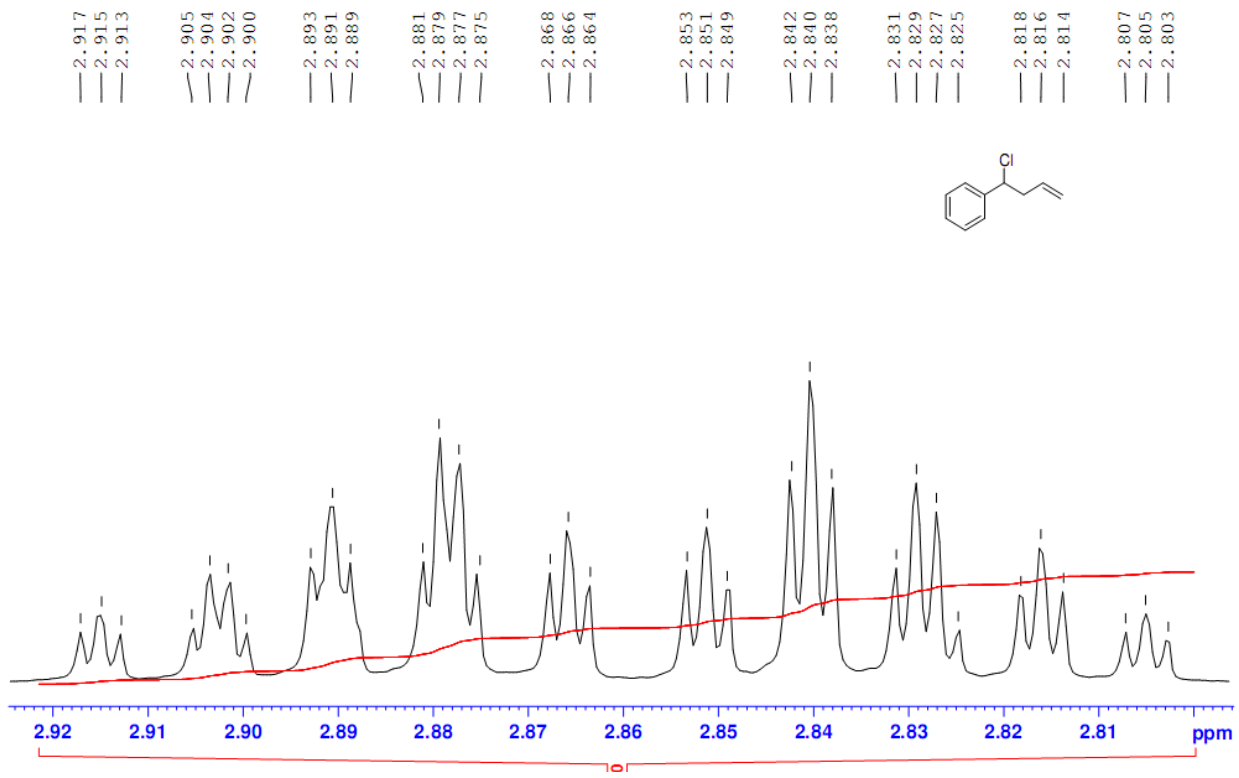
Signal 1: FID1 A,

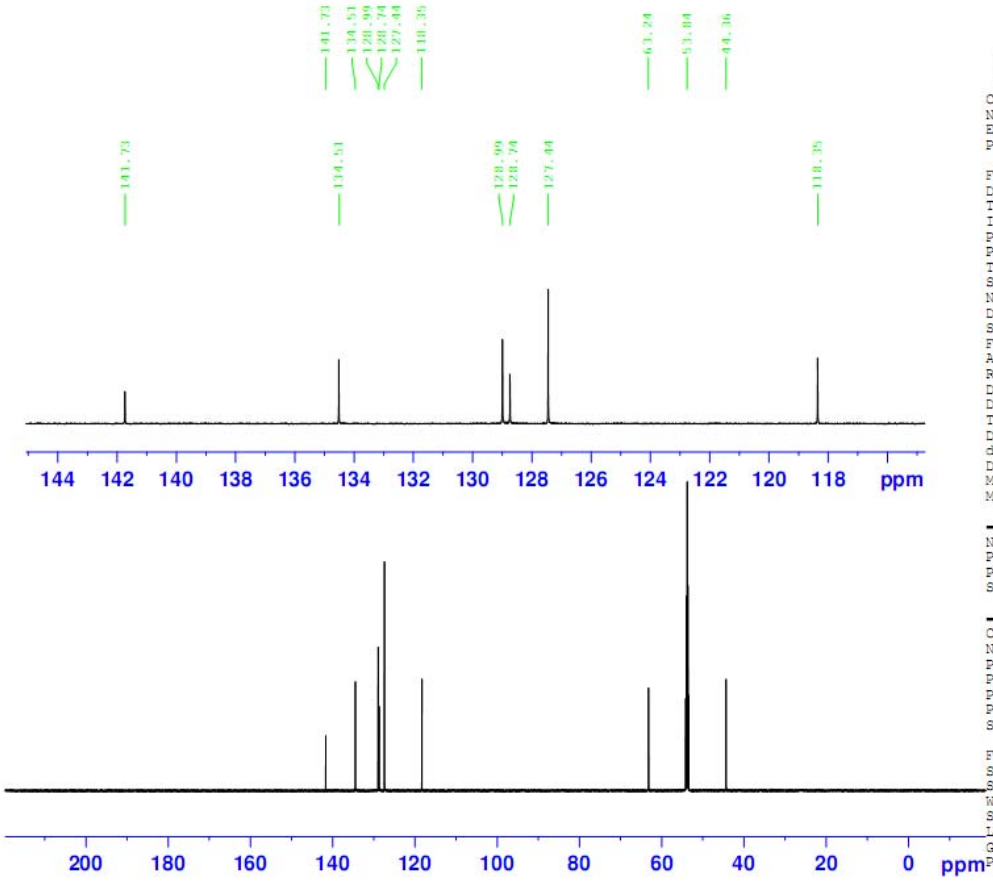
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	7.415	BB	0.0290	24.64159	12.49158	1.00024
2	9.414	BB	0.0226	12.69935	8.94872	0.51549
3	9.795	BV	0.0249	8.18593	5.33462	0.33228
4	9.896	VB	0.0292	2418.03271	1214.16565	98.15199

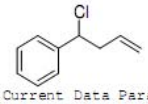



```
Current Data Parameters
NAME          A-Cl-Allyl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20131023
Time               13.30
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    16
DS                     0
SWH            6887.052 Hz
FIDRES         0.105088 Hz
AQ            4.7579136 sec
RG                101.6
DW                72.600 usec
DE                 6.00 usec
TE                298.0 K
D1           1.00000000 sec
MCREST    0 sec
MCWRK        0.01500000 sec

-------- CHANNEL f1 --------
NUC1                  1H
P1                11.60 usec
PL1               -2.00 dB
SFO1        600.1328163 MHz

F2 - Processing parameters
SI                 32768
SF          600.1300189 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.40
```





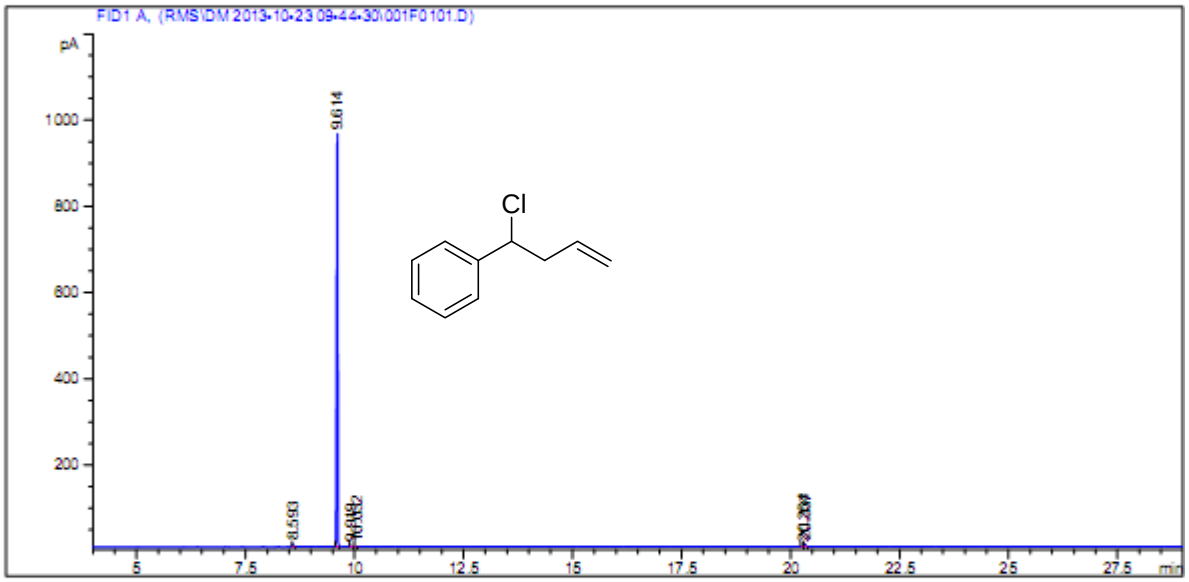





```
Current Data Parameters
NAME          A-Cl-Allyl
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20131023
Time               14.20
INSTRUM            av600
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  747
DS                    4
SWH           35971.223 Hz
FIDRES         0.548877 Hz
AQ            0.9109504 sec
RG                16384
DW               13.900 usec
DE                6.00 usec
TE               298.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST   0 sec
MCWRK        0.01500000 sec

-------- CHANNEL f1 --------
NUC1                 13C
P1                9.00 usec
PL1      0 dB
SFO1        150.9178988 MHz

-------- CHANNEL f2 --------
CPDPRG[2         waltz16
NUC2                  1H
PCPD2            80.00 usec
PL2              -2.00 dB
PL12             13.50 dB
PL13             20.00 dB
SFO2        600.1324005 MHz

F2 - Processing parameters
SI                32768
SF          150.9027470 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.00
```

Data File C:\CHEM32\1\DATA\RMS\DM 2013-10-23 09-44-30\001F0101.D
Sample Name: A-Cl-allyl

Acq. Operator : RMS Seq. Line : 1
Acq. Instrument : Instrument 1 Location : Vial 1
Injection Date : 23-Oct-13, 09:45:56 Inj : 1
Inj Volume : 1 µl
Acq. Method : C:\CHEM32\1\DATA\RMS\DM 2013-10-23 09-44-30\ÅA-DEFAULT.M
Last changed : 3/27/2013 6:06:31 PM by OL
Analysis Method : C:\CHEM32\1\METHODS\ÅA-DEFAULT.M
Last changed : 10/25/2013 1:04:59 PM by RMS
(modified after loading)
Method Info : ÅAGC-default



Area Percent Report

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

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	8.593	BB	0.0245	10.23393	6.46494	0.63017
2	9.614	BB	0.0255	1594.02966	955.61133	98.15433
3	9.919	BB	0.0219	3.98725	2.75519	0.24552
4	10.032	BB	0.0215	2.00694	1.41486	0.12358
5	20.264	BV	0.0277	3.75792	2.11513	0.23140
6	20.337	VB	0.0261	9.98768	5.78463	0.61500