Electronic Supplementary Material (ESI) for Green Chemistry

Supplementary Information

5- Membered N-heterocyclic compounds by dimethyl carbonate chemistry

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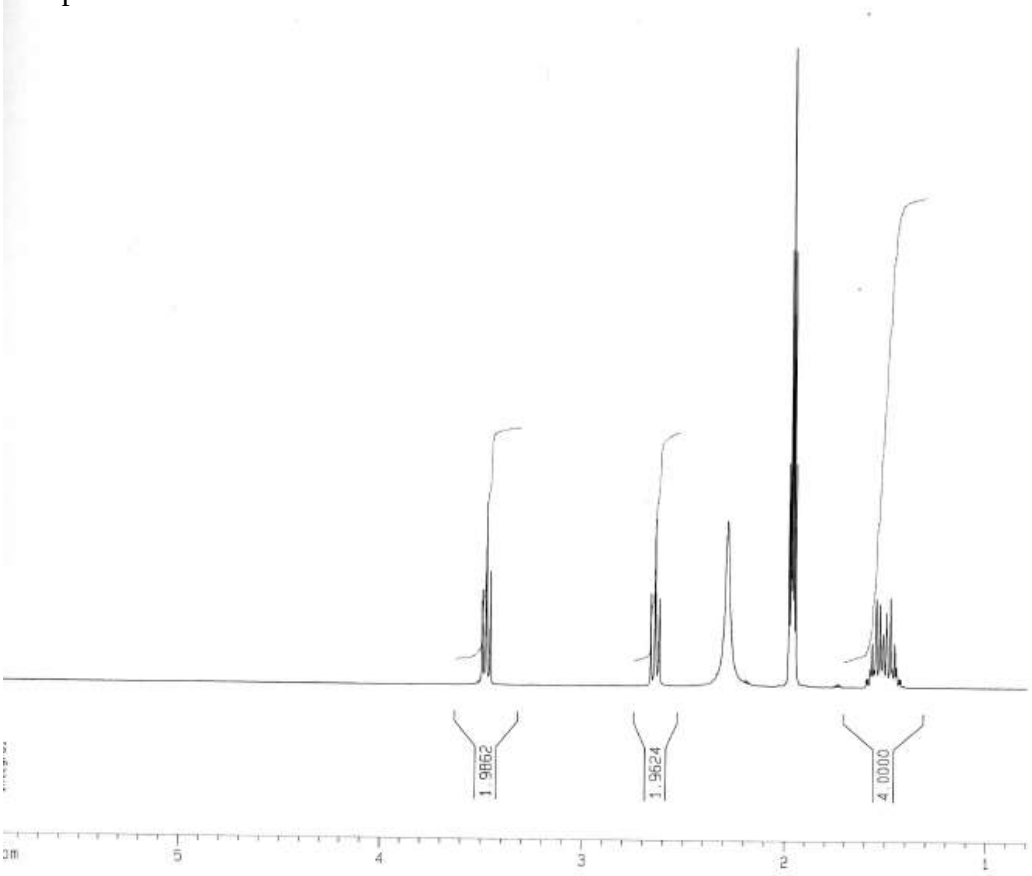
^{1}H Spectrum of 4-amino-1-butanol

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EXPNO                     1
PROCNO                    1

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PULPROG               zg30
TD                   65536
SOLVENT              CD3CN
NS                       8
DS                       0
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FIDRES            0.094190 Hz
AQ                5.3084660 sec
RG                   456.1
DW                 81.000 usec
DE                  6.00 usec
TE                   0.0 K
D1                1.00000000 sec
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MCWRK             0.01500000 sec

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NUC1                     1H
P1                   4.90 usec
PL1                  0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
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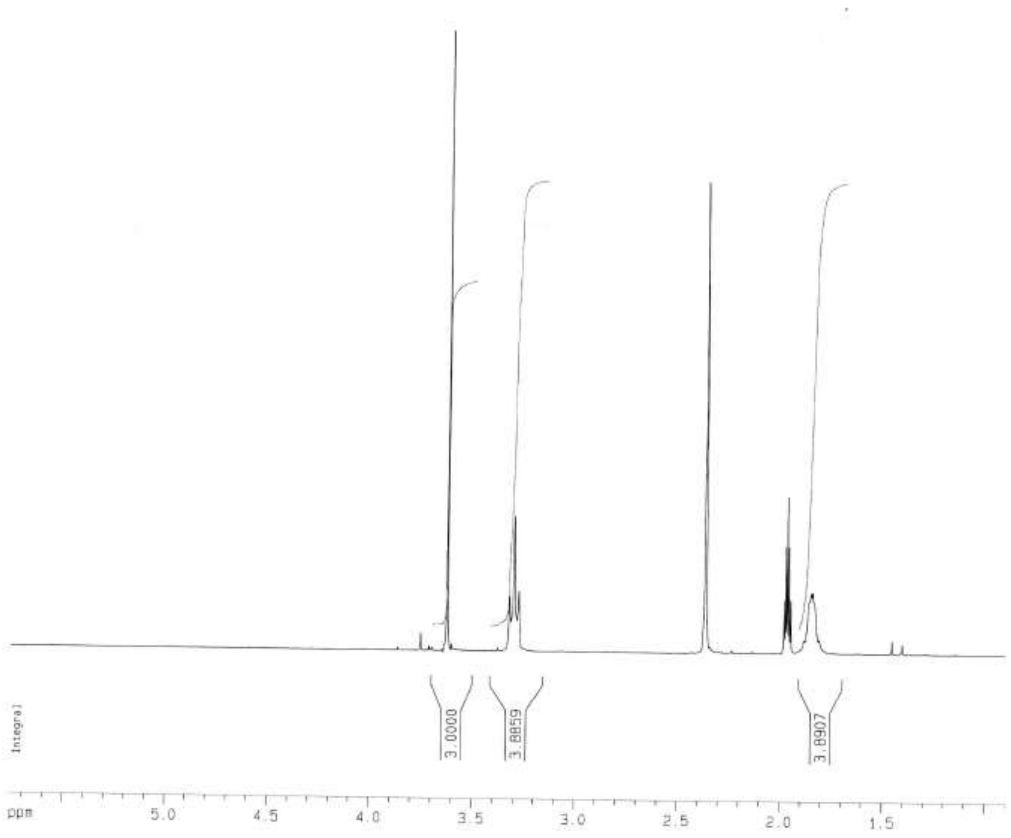
SF                300.1300000 MHz
WDW                         EM
SSB                          0
LB                    0.30 Hz
GB                           0
PC                        1.00

1D NMR plot parameters
CX                   20.00 cm
CY                   12.50 cm
F1P                   5.926 ppm
F1                 1778.50 Hz
F2P                   0.796 ppm
F2                  238.94 Hz
PPMCM             0.29648 ppm/cm
HZCM             76.97816 Hz/cm
```

^{1}H NMR Spectrum of carboxymethyl pyrrolidine

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EXPNO                     1
PROCNO                    1

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PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6172.839 Hz
FIDRES            0.094190 Hz
AQ                5.3084660 sec
RG                   143.7
DW                 81.000 usec
DE                  6.00 usec
TE                   0.0 K
D1                1.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                   4.90 usec
PL1                  0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
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SF                300.1300000 MHz
WDW                         EM
SSB                          0
LB                    0.30 Hz
GB                           0
PC                        1.00

1D NMR plot parameters
CX                   20.00 cm
CY                   12.50 cm
F1P                   5.762 ppm
F1                 1729.44 Hz
F2P                   0.900 ppm
F2                  270.07 Hz
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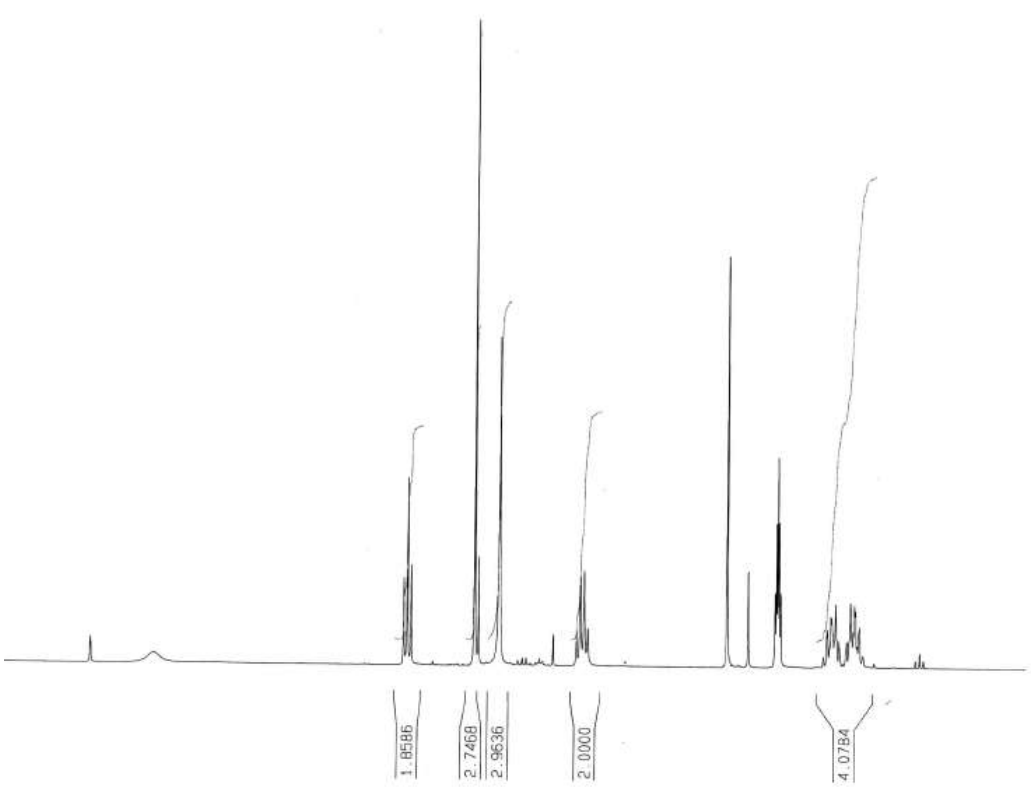
^{1}H NMR Spectrum of methyl 4-(methoxycarbonyloxy)butylcarbamate

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PROCNO                      1

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PROBHD   5 mm Multinucl
PULPROG                zg30
TD                    65536
SOLVENT               CD3CN
NS                        8
DS                        0
SWH                6172.839 Hz
FIDRES            0.094190 Hz
AQ                5.3084860 sec
RG                      181
DW                 81.000 usec
DE                  6.00 usec
TE                    0.0 K
D1              1.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                  4.90 usec
PL1                 0.00 dB
SFO1           300.1318534 MHz

F2 - Processing parameters
SI                     32768
SF              300.1300000 MHz
WDW                       EM
SSB                        0
LB                   0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                    20.00 cm
CY                    12.50 cm
F1P                    6.531 ppm
F1                  1960.17 Hz
F2P                    0.531 ppm
F2                   159.38 Hz
PPMCM                 0.30000 ppm/cm
```
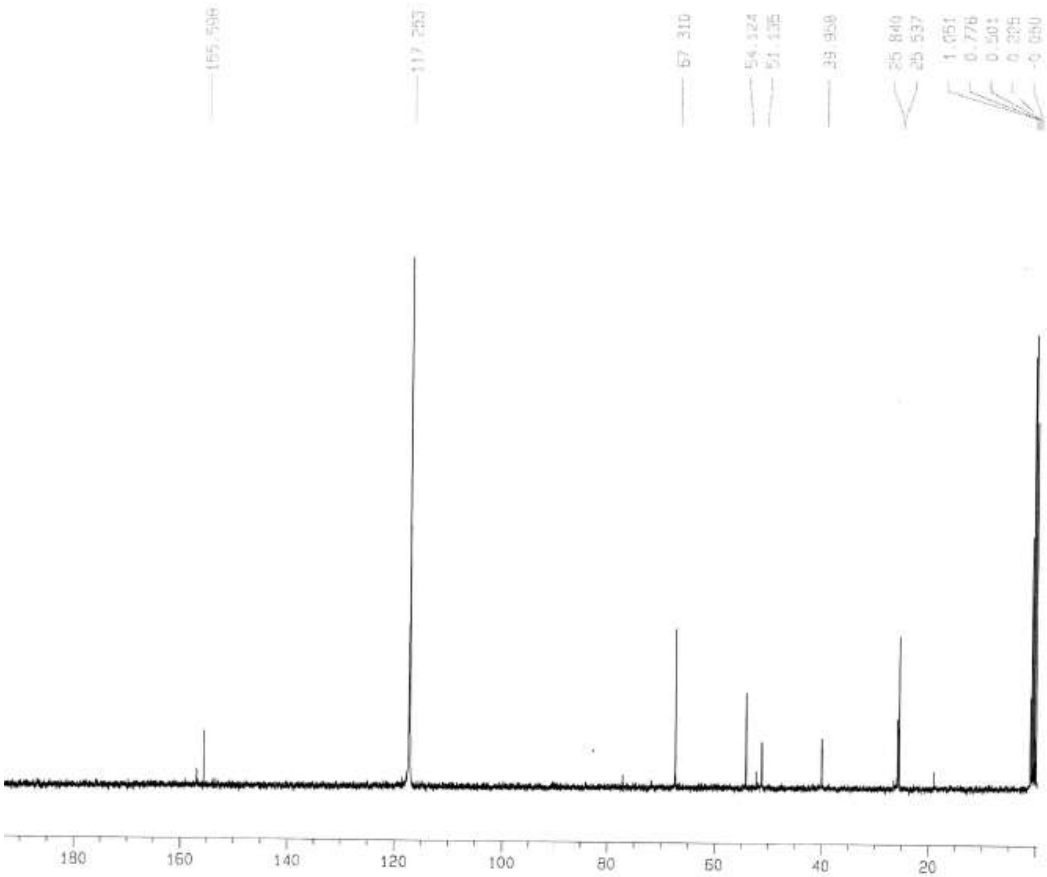

^{13}C NMR spectrum of methyl 4-(methoxycarbonyloxy)butylcarbamate

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EXPNO                       1
PROCNO                      1

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Time                  10.51
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PROBHD   5 mm Multinucl
PULPROG                zgdc
TD                    65536
SOLVENT               CDCl3
NS                      252
DS                        0
SWH               15060.241 Hz
FIDRES            0.229801 Hz
AQ                2.1758451 sec
RG                   2298.8
DW                 33.200 usec
DE                  6.00 usec
TE                    0.0 K
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d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

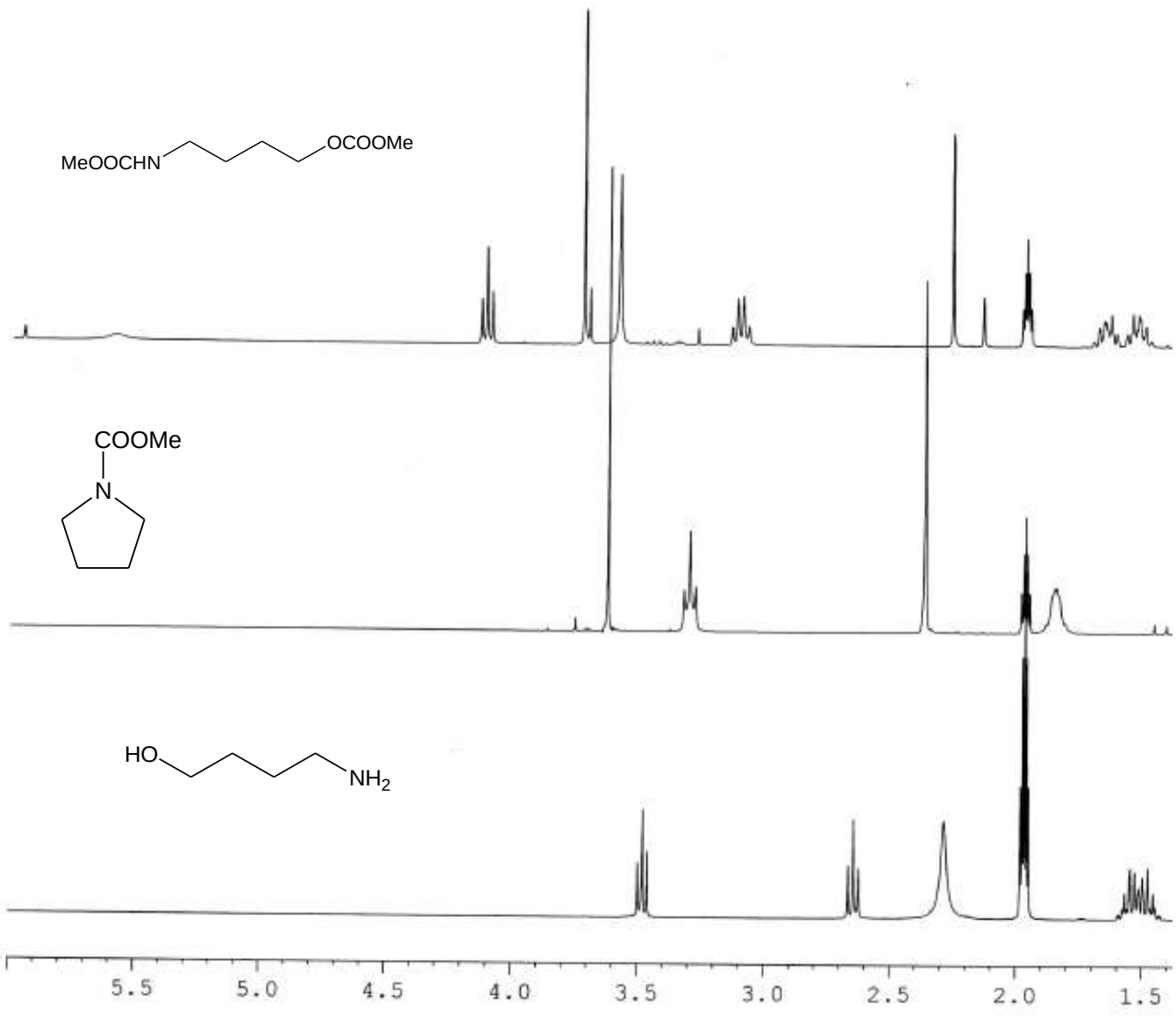
======== CHANNEL f1 ========
NUC1                   13C
P1                  7.40 usec
PL1                 4.00 dB
SFO1           75.4752653 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               22.64 dB
SFO2           300.1316507 MHz

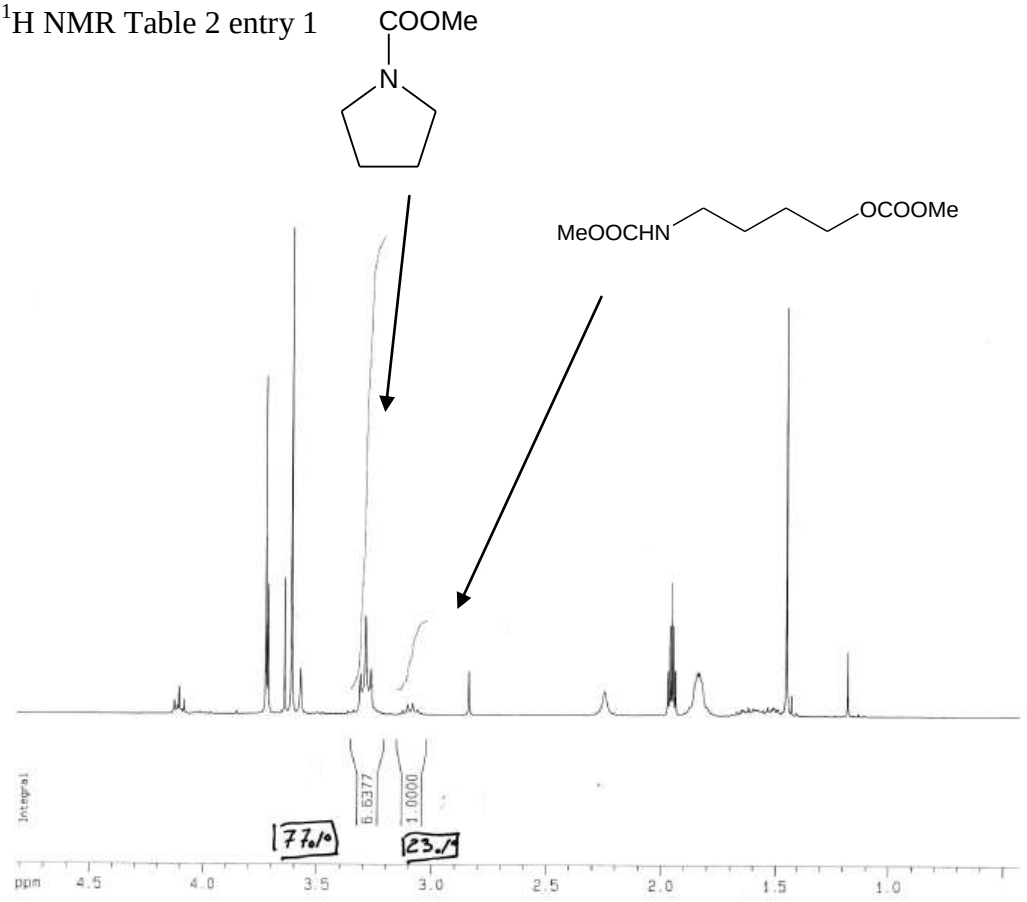
F2 - Processing parameters
SI                     32768
SF              75.4677570 MHz
WDW                       EM
SSB                        0
LB                   1.00 Hz
GB                         0
PC                      1.40

1D NMR plot parameters
CX                    20.00 cm
CY                    10.00 cm
F1P                  199.270 ppm
F1                 15038.45 Hz
F2P                   -0.289 ppm
F2                   -21.79 Hz
PPMCM                 9.97793 ppm/cm
```

1 H NMR (CD_3CN) spectra comparison



^{1}H NMR Table 2 entry 1

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PROCNO                       1

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Time                   11.29
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PULPROG                zg30
TD                    65536
SOLVENT                CD3CN
NS                         8
DS                         0
SWH                6172.839 Hz
FIDRES             0.094190 Hz
AQ                 5.3084660 sec
RG                     161.3
DW                  81.000 usec
DE                   6.00 usec
TE                    0.0 K
D1                 1.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       4.90 usec
PL1                      0.00 dB
SFO1               300.1318534 MHz

F2 - Processing parameters
SI                         32768
SF                 300.1300032 MHz
WDW                           EM
SSB                            0
LB                        0.30 Hz
GB                             0
PC                          1.00

1D NMR plot parameters
CX                       20.00 cm
CY                       10.00 cm
F1P                       4.819 ppm
F1                     1446.42 Hz
F2P                       0.428 ppm
F2                      128.31 Hz
PPMCM                 0.21959 ppm/cm
HZCM                 65.90551 Hz/cm
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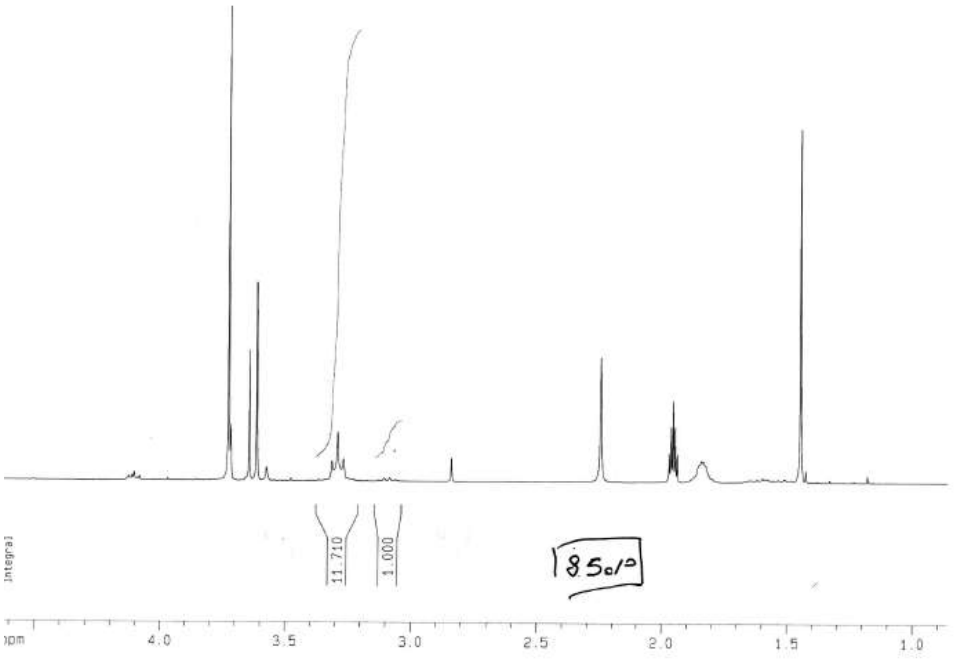
^{1}H NMR Table 2 entry 2

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NAME                  FA6.86.1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20100908
Time                   15.27
INSTRUM                spect
PROBHD   5 mm Multinucl
PULPROG                zg30
TD                    65536
SOLVENT                CD3CN
NS                        12
DS                         0
SWH                6172.839 Hz
FIDRES             0.094190 Hz
AQ                 5.3084660 sec
RG                     161.3
DW                  81.000 usec
DE                   6.00 usec
TE                    0.0 K
D1                 1.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       4.90 usec
PL1                      0.00 dB
SFO1               300.1318534 MHz

F2 - Processing parameters
SI                         32768
SF                 300.1300034 MHz
WDW                           EM
SSB                            0
LB                        0.30 Hz
GB                             0
PC                          1.00

1D NMR plot parameters
CX                       20.00 cm
CY                       10.00 cm
F1P                       4.633 ppm
F1                     1390.54 Hz
F2P                       0.860 ppm
F2                      258.08 Hz
PPMCM                 0.18866 ppm/cm
HZCM                 56.62304 Hz/cm
```
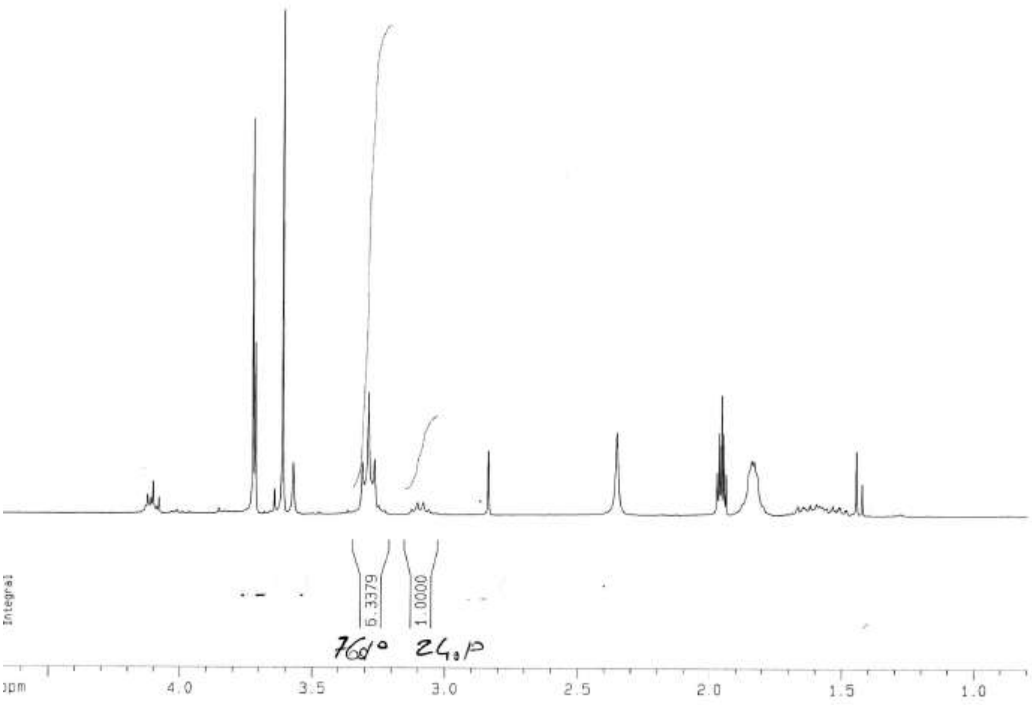

^{1}H NMR Table 2 entry 3




```
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_              20100909
Time                 10.05
INSTRUM              spect
PROBHD   5 mm Multinucl
PULPROG              zg30
TD                  65536
SOLVENT             CD3CN
NS                      4
DS                      0
SWH              6172.839 Hz
FIDRES           0.094190 Hz
AQ               5.3084660 sec
RG                  143.7
DW                 81.000 usec
DE                  6.00 usec
TE                   0.0 K
D1               1.00000000 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                  4.90 usec
PL1                 0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF            300.1300032 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.00 cm
F1P                4.681 ppm
F1                1404.92 Hz
F2P                0.799 ppm
F2                 239.77 Hz
PPMCM             0.19411 ppm/cm
HZCM             58.25759 Hz/cm
```

GC-MS of carboxymethyl Indoline

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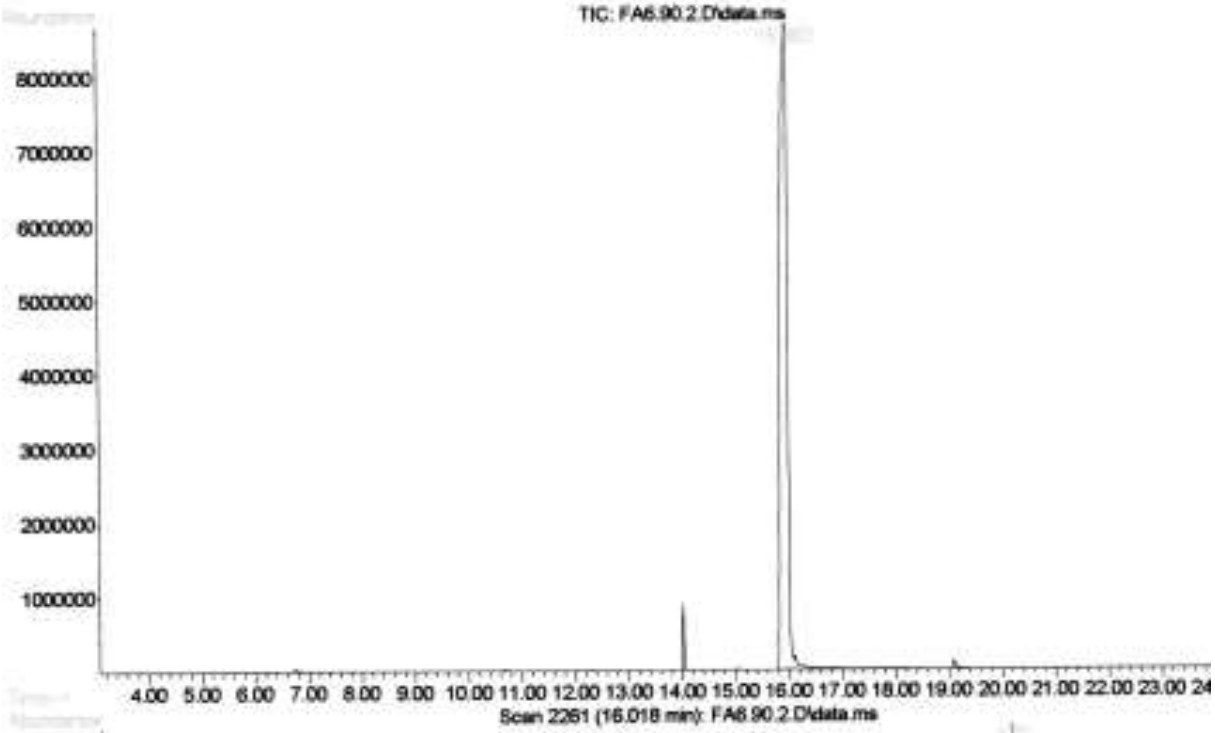
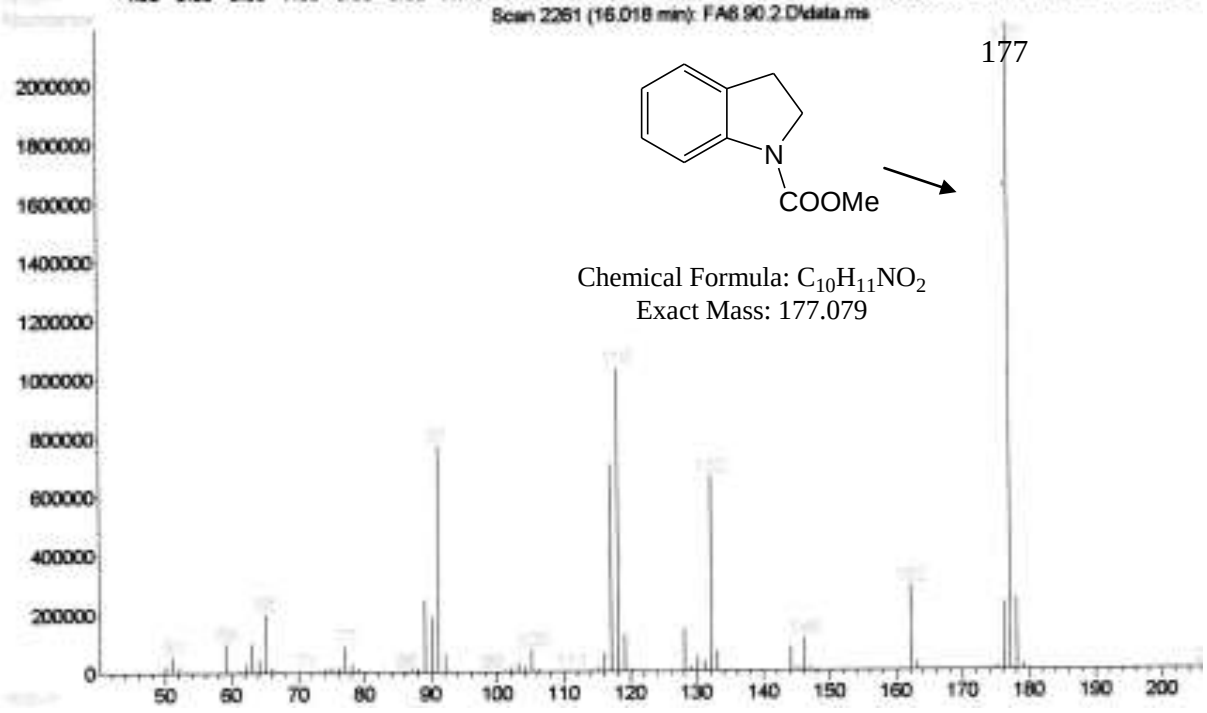
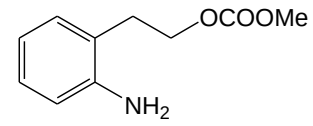
Instrument : 5973N
Acquired : 10 May 2011 14:33 using AcqMethod MATTEO_HDX.M
Sample Name: FA6.90.2
Misc Info : 1 spot clean



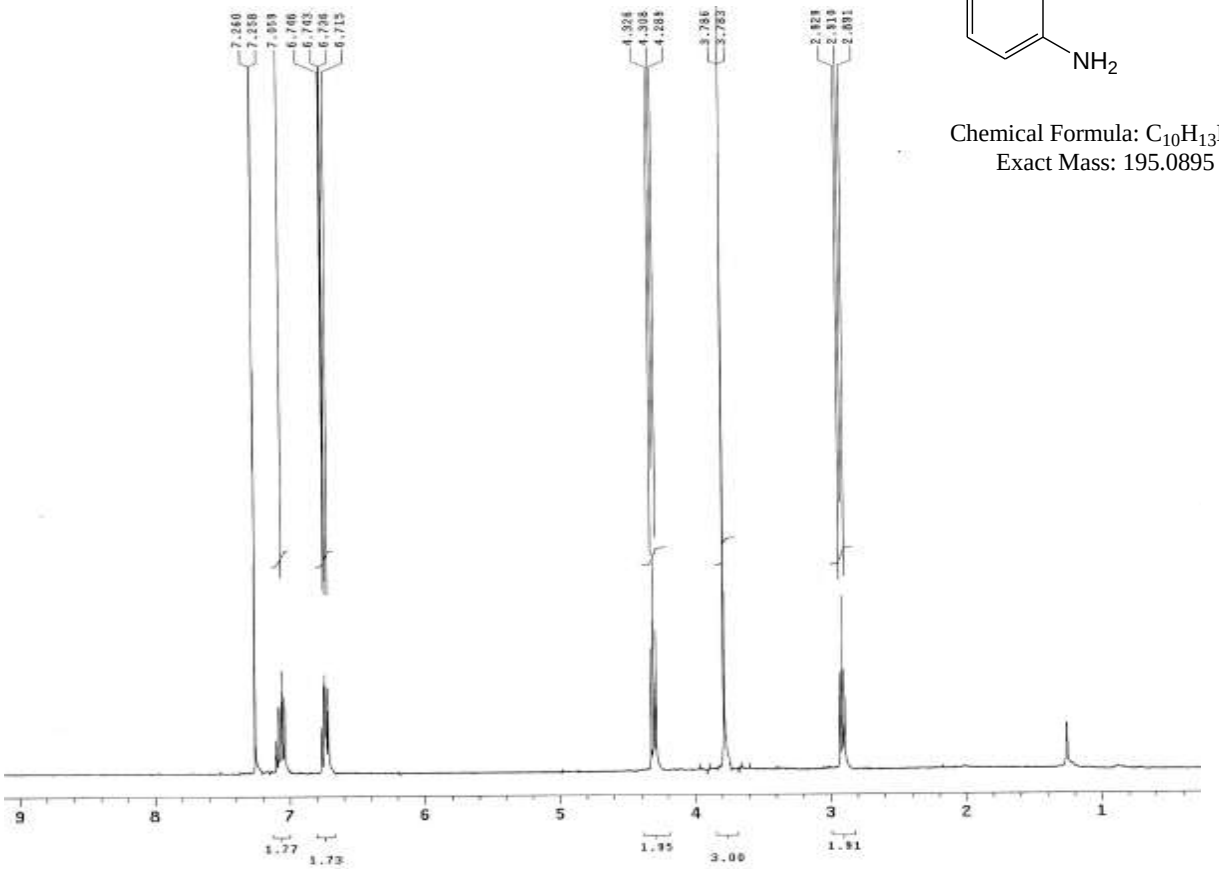


Chemical Formula: $C_{10}H_{11}NO_2$
Exact Mass: 177.079

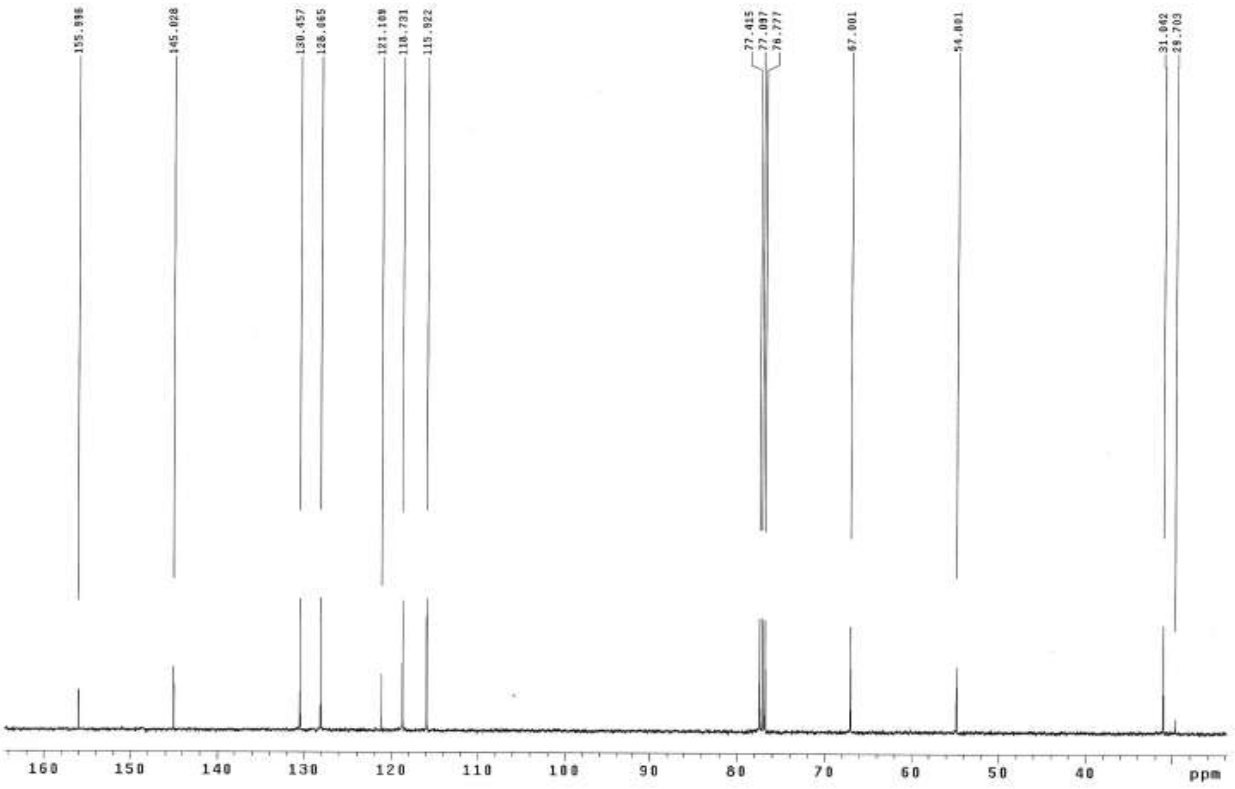
^{1}H NMR Spectrum of 2-aminophenethyl methyl carbonate



Chemical Formula: $C_{10}H_{13}NO_3$
Exact Mass: 195.0895



^{13}C NMR Spectrum of 2-aminophenethyl methyl carbonate



GC-MS Spectrum of 2-aminophenethyl methyl carbonate

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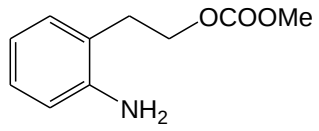
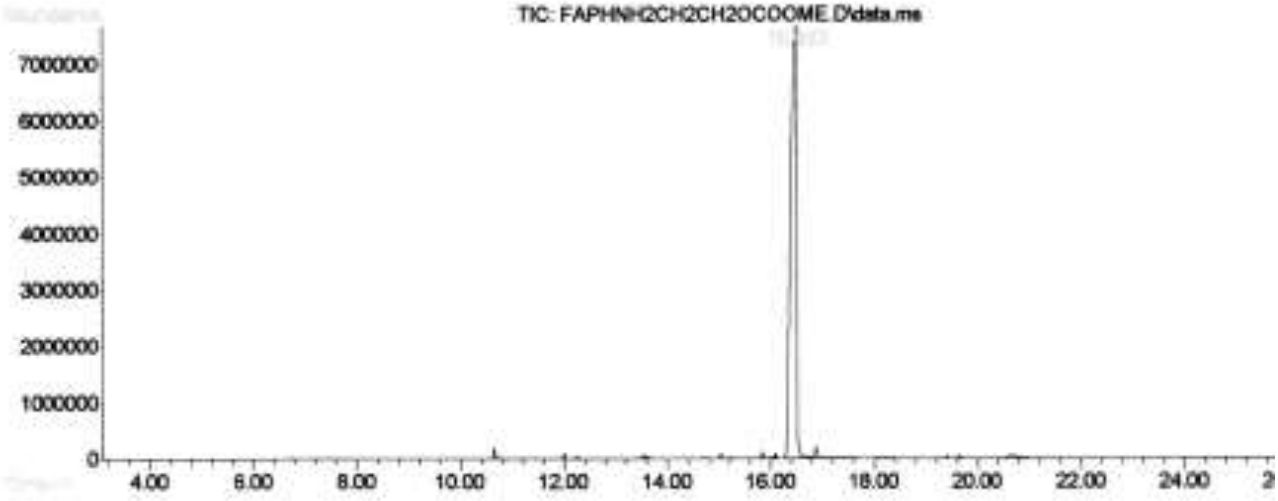
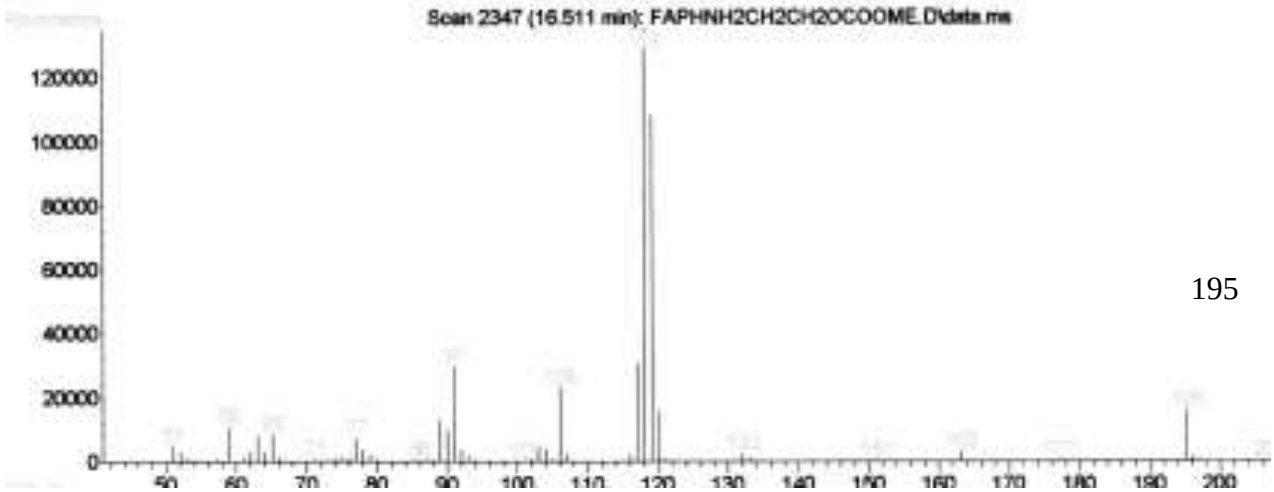
... APHNH2CH2CH2OCOOME.D
Operator : Fabio
Instrument : 5973N
Acquired : 9 May 2011 12:19 using AcqMethod MATTEO_HDX.M
Sample Name: PhNH2CH2CH2OCOOMe
Misc Info :



Chemical Formula: $C_{10}H_{13}NO_3$
Exact Mass: 195.0895





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