M.Sc. Semester-III
Core Course - 7 (CC-7)
Application of Spectroscopy

III. Nuclear Magnetic Resonance Spectroscopy

L5: The Integral, Intensity of Signals

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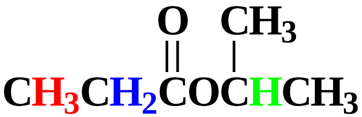
^{1}H NMR Problems

- Predict the splitting patterns (multiplets) for each proton environment in the following:

CH_3CHBr_2

$CH_3OCH_2CH_2Br$

$ClCH_2CH_2CH_2Cl$



$CH_3CH_2C(=O)CH(CH_3)CH_3$

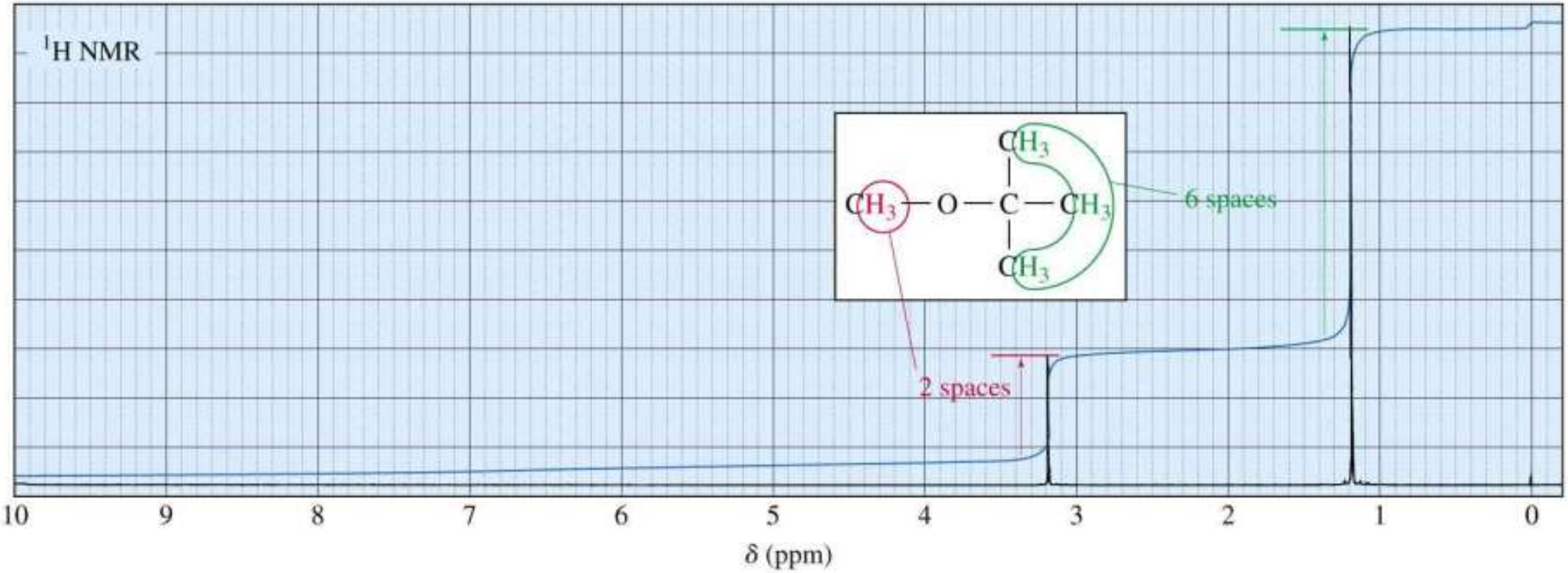
singlet
singlet
doublet
doublet
triplet
triplet
triplet
triplet
quartet
quartet
quintet
septet

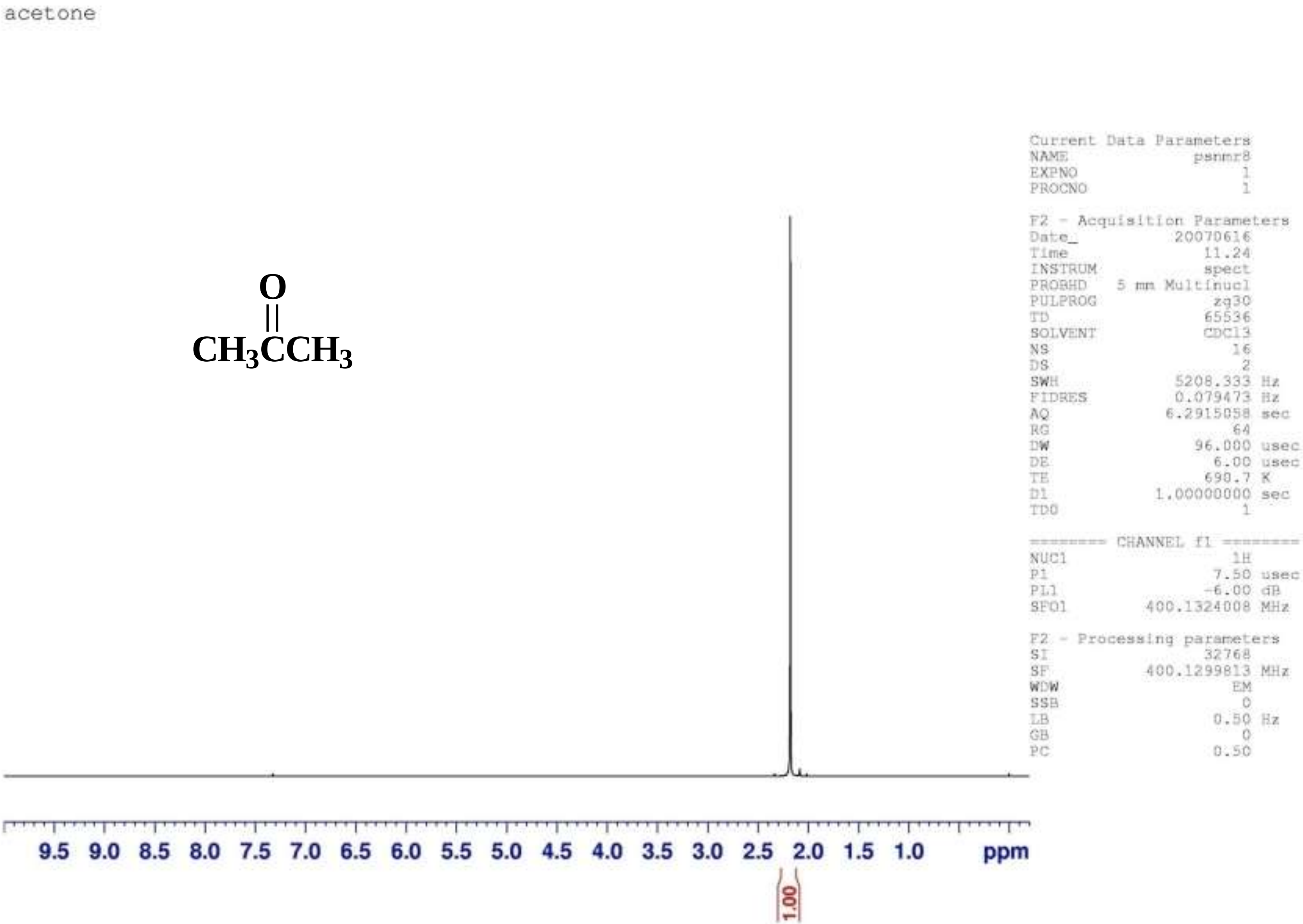
The Integral

- Integration is performed to determine the relative number of protons in a given environment.
- The number is set at 1, 2 or 3 for a given peak, then the areas of the other signals are reported relative to that one.
- The integral should be rounded to the nearest whole number; after all, there is either 1, or 2, or 3 protons in a certain environment, never a decimal fraction.
- Our spectrometer prints the integral below the spectrum written sideways and in red.

Intensity of Signals

- The area under each peak is proportional to the number of protons.
- Shown by integral trace.





$$\overset{\displaystyle O}{\overset{\|}{CH_3CCH_3}}$$

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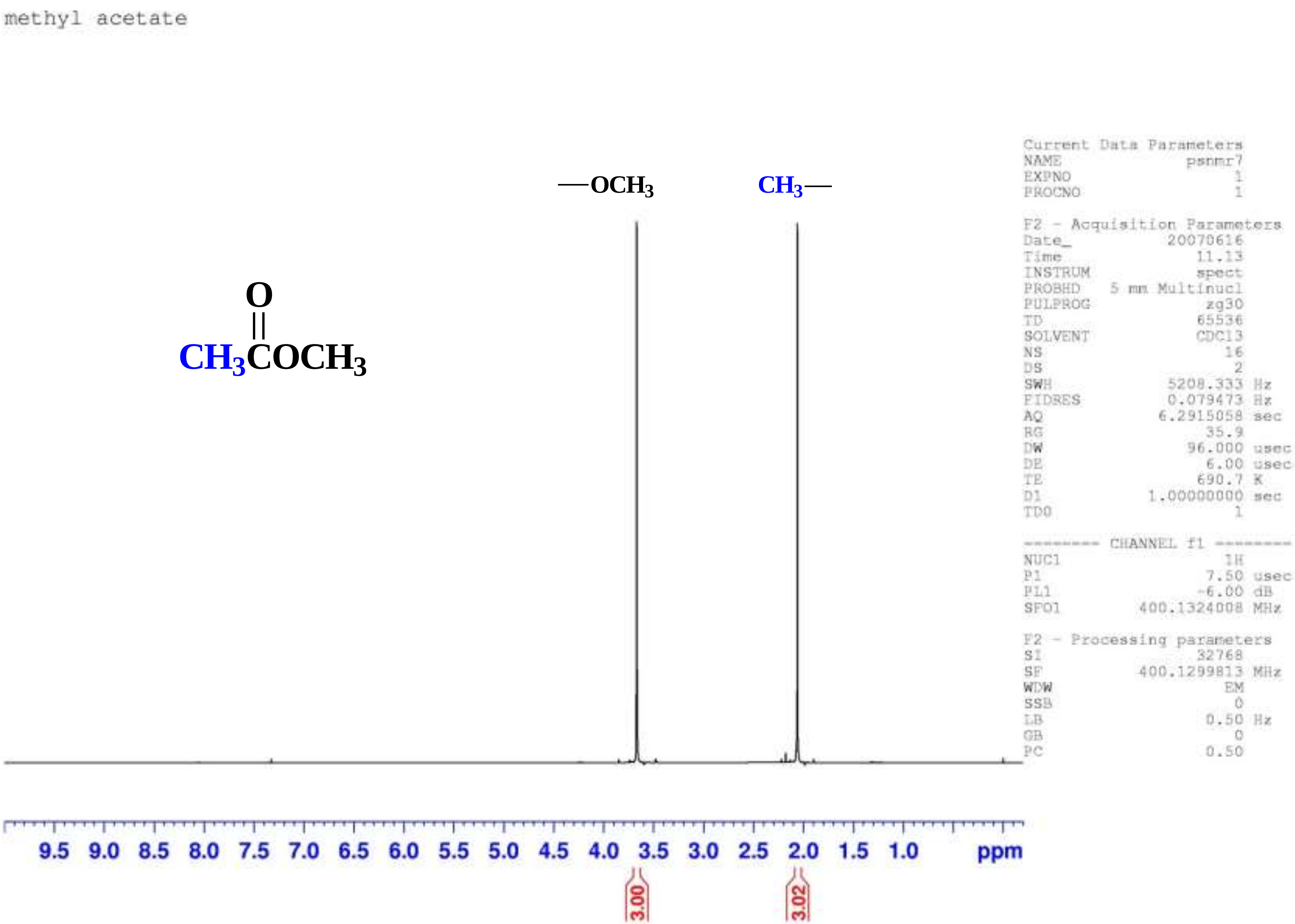
Current Data Parameters
NAME              psnmr8
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20070616
Time               11.24
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             5208.333 Hz
FIDRES          0.079473 Hz
AQ             6.2915058 sec
RG                    64
DW                96.000 usec
DE                  6.00 usec
TE                 690.7 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  7.50 usec
PL1                -6.00 dB
SFO1         400.1324008 MHz

F2 - Processing parameters
SI                 32768
SF           400.1299813 MHz
WDW                   EM
SSB                    0
LB                  0.50 Hz
GB                     0
PC                  0.50
```



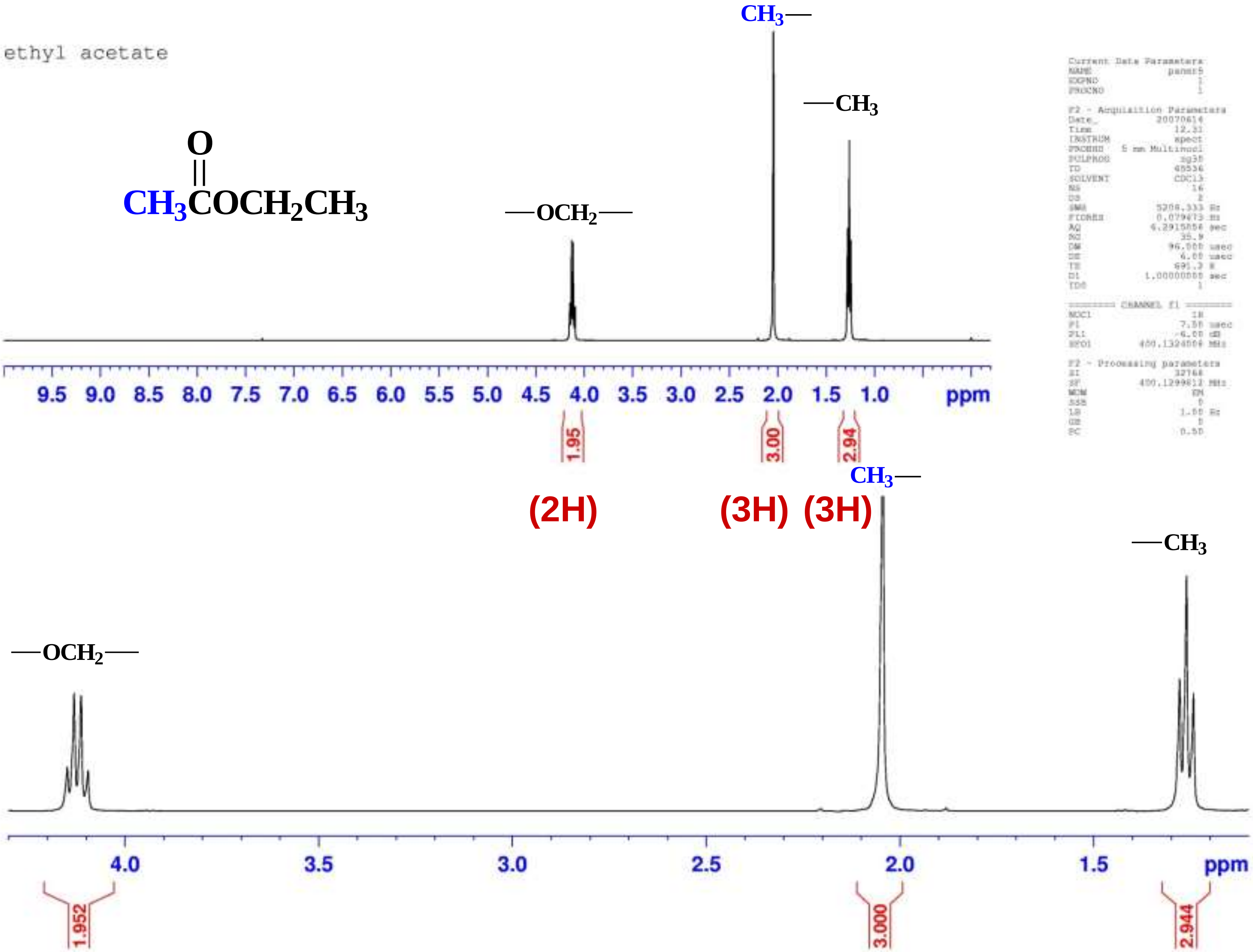
$CH_3\overset{\overset{\displaystyle O}{\|}}{C}OCH_3$

```
Current Data Parameters
NAME               psnmr7
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20070616
Time                11.13
INSTRUM             spect
PROBHD   5 mm Multinucl
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              5208.333 Hz
FIDRES           0.079473 Hz
AQ              6.2915058 sec
RG                   35.9
DW                 96.000 usec
DE                   6.00 usec
TE                  690.7 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                   7.50 usec
PL1                 -6.00 dB
SFO1          400.1324008 MHz

F2 - Processing parameters
SI                  32768
SF            400.1299813 MHz
WDW                    EM
SSB                     0
LB                   0.50 Hz
GB                      0
PC                   0.50
```



$$CH_3\overset{\overset{\displaystyle O}{\|}}{C}OCH_2CH_3$$

```
Current Data Parameters
NAME              panmr5
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20070614
Time               12.31
INSTRUM            spect
PROBHD    5 mm Multinucl
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             5208.333 Hz
FIDRES          0.079473 Hz
AQ             6.2915854 sec
RG                  35.9
DW                96.000 usec
DE                  6.00 usec
TE                 691.2 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  7.50 usec
PL1                -6.00 dB
SFO1         400.1324006 MHz

F2 - Processing parameters
SI                 32768
SF           400.1299812 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  0.50
```

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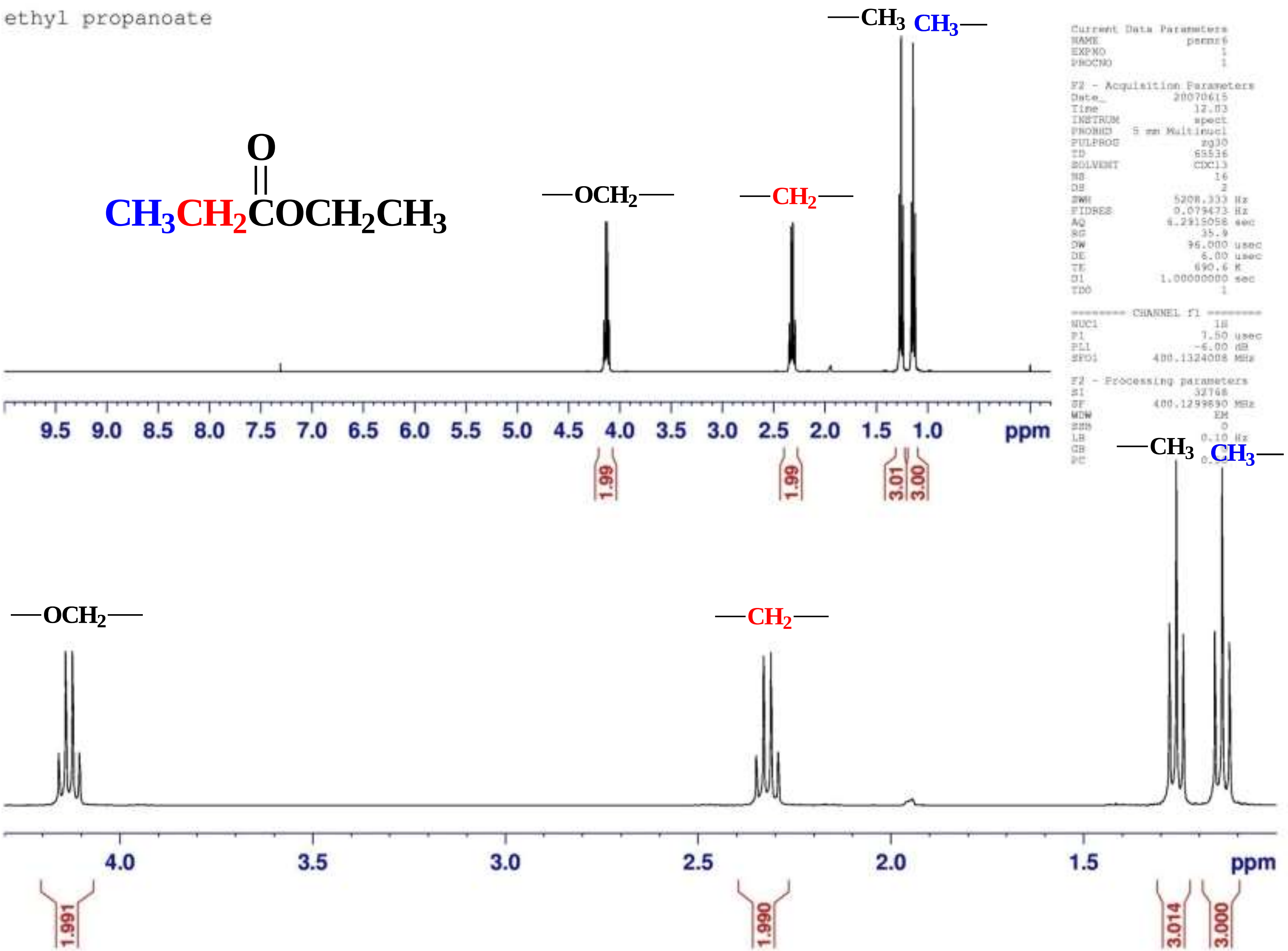

$$CH_3CH_2\overset{\overset{\displaystyle O}{||}}{C}OCH_2CH_3$$

```
Current Data Parameters
NAME                 pernr6
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20070615
Time                  12.03
INSTRUM               spect
PROBHD   5 mm Multinucl
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                5208.333 Hz
FIDRES             0.079473 Hz
AQ                6.2915058 sec
RG                     35.9
DW                   96.000 usec
DE                     6.00 usec
TE                    290.6 K
D1               1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                     7.50 usec
PL1                   -6.00 dB
SFO1            400.1324008 MHz

F2 - Processing parameters
SI                    32768
SF              400.1299690 MHz
WDW                      EM
SSB                       0
LB                     0.10 Hz
GB                        0
PC                     0.
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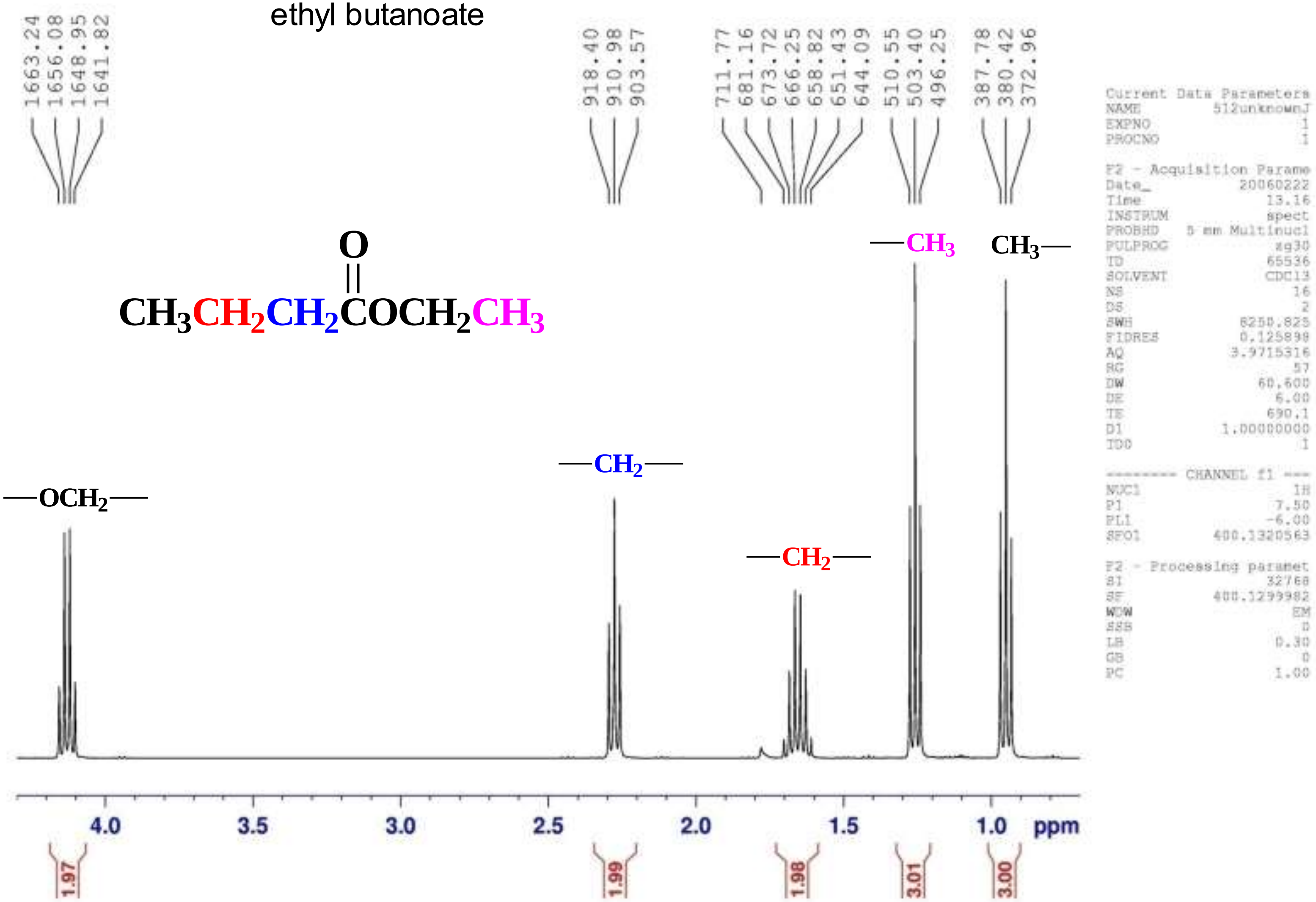
ethyl butanoate



$$CH_3CH_2CH_2\overset{\overset{\displaystyle O}{\|}}{C}OCH_2CH_3$$

```
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EXPNO                     1
PROCNO                    1

F2 - Acquisition Parame
Date_              20060222
Time                  13.16
INSTRUM               spect
PROBHD     5 mm Multinucl
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8250.825
FIDRES             0.125898
AQ                3.9715316
RG                       57
DW                   60.600
DE                     6.00
TE                    690.1
D1               1.00000000
TD0                       1

======== CHANNEL f1 ===
NUC1                     1H
P1                     7.50
PL1                   -6.00
SFO1            400.1320563

F2 - Processing paramet
SI                    32768
SF              400.1299982
WDW                      EM
SSB                       0
LB                     0.30
GB                        0
PC                     1.00
```

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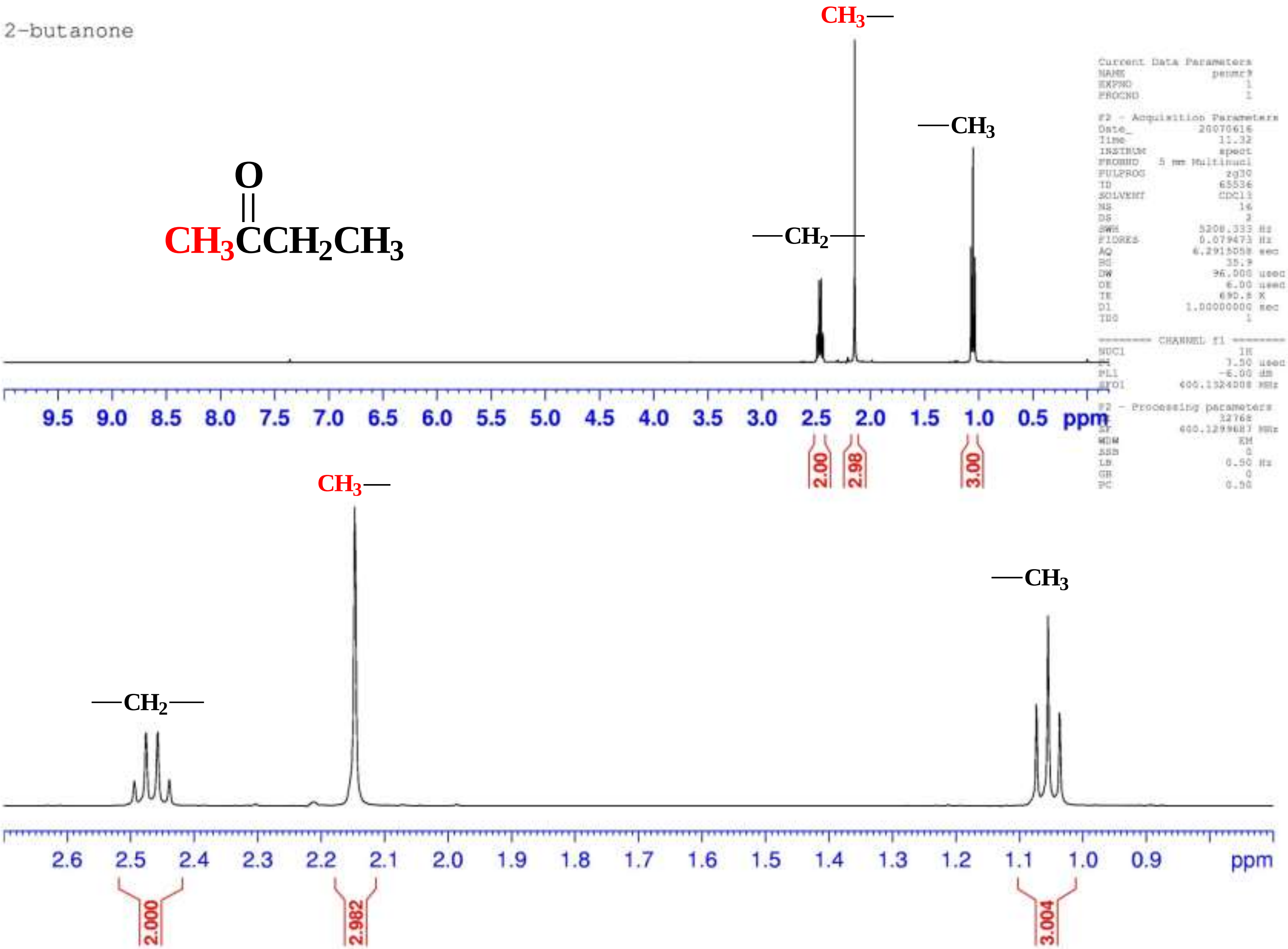
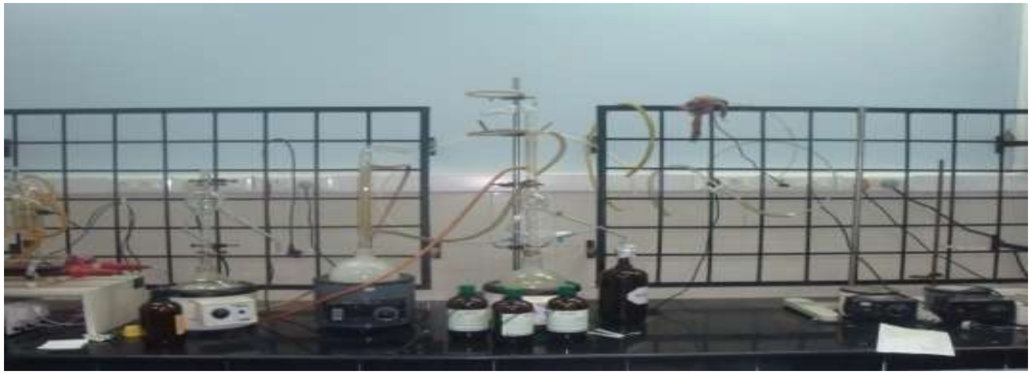


$$CH_3\overset{O}{\overset{\|}{C}}CH_2CH_3$$

Thank You



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