MatlabNMR

Version 7.10

William D. Wheeler, Ph.D.
Department of Chemistry
University of Wyoming
Laramie, WY 82071
dwheeler@uwyo.edu

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Introduction

The MatlabNMR program has been developed as a tool to examine all kinds of NMR data. It is open and flexible, with many standard features seen in other NMR programs. MatlabNMR is adaptable to most any type of problem, if it does not have a feature you need, it can easily be added to by creating a "user" processing program.

I have received requests to read data created by most of the NMR vendors. I have done my best to satisfy everyone. It is difficult, however, to consider every situation. Because of this, you may find that a spectrum needs to be flipped or shifted in a way that I did not anticipate. Feel free to contact me with any changes you find necessary.

Several new features have been added recently.

In version 6.3 the functions "Read Matlab Data" and "Save as Matlab Data" were added. Version 7.0 now includes Linear Prediction in the processing choice's. The mechanism of manually phasing a spectrum has been extensively revised along with a new method of phasing digitally filtered Bruker data. Both versions have included additional "user" processing functions.

Versions starting with 7.10 are available both as matlab source and as a compiled stand-alone program. The rights of deployment of the compiled program are governed by agreements with the MathWorks, Inc. MATLAB®. ©1984-2007. User processing functions and some other features are not available in the compiled version.

Installation

MatlabNMR can be installed in any convenient place. I usually use \Matlab\work\nmr\ or \Programs\Matlab\work\nmr.

matlabnmr.ini The matlabnmr.ini file is used to specify the base directory in which data files are stored. It must be in the same directory as the matlabnmr.m file.

Note: In the example below, the MatlabNMR program will replace the subdirectory string "user" (if it exists) with the current user name, e.g., if the current user has a user name of rotwang, then the program will convert c:\z\data\user\nmr\ to c:\z\data\rotwang\nmr\.

matlabnmr.ini

avance	c:\z\data\user\nmr\
aspect	c:\NMR_Data\Aspect\
tecmag	c:\NMR_Data\TecMag\
jeolgx	c:\NMR_Data\JEOL\
varian	c:\NMR_Data\Varian\
matlab	c:\NMR_Data\Matlab\

Matlab Toolboxes

The following are MatlabNMR functions that require Matlab tool boxes.

Function	Matlab Function	Toolbox
backgndsub	sgolayfilt, sgolay	Signal processing
transform2d	dct (for tppi)	Signal processing
linearpredict	lpc	Signal processing
analysis_b1field	lsqcurvefit	Optimization
analysis_T2calc	lsqcurvefit	Optimization

Starting MatlabNMR

In Matlab, change the directory to the location of the MatlabNMR program files and type "nmr" at the command prompt. The file named nmr.m is the root of the MatlabNMR program.

Using the Mouse

To zoom, hold down the left mouse button and drag the mouse. For integration, two left clicks define an integral. The middle mouse button (if you have one) and most any other key on the keyboard will exit integration. (Right clicking will also exit integration, but a context menu will also appear).

Click the right mouse button for a context menu. Context menus contain a subset of the main "Display" menu, but they may also have additional functionality.

Caveats

1) Processed Data: MatlabNMR writes processed data to files named procdata1d.mat, procdata2d.mat, or files whose names end in _procdata1d.mat or _procdata2d.mat. When the data set is reopened, the raw data is read first followed by the processed data. If the processed data is from an older MatlabNMR version, or if it were written after some "user" processing it may not contain all of the current information. This can sometimes lead to some confusing results. Removing the processed data will often fix the problem.

2) Data type: In some versions of the program, certain functions changed the data type (acquparm.dtype) to the type "matlab". It turns out this was not a good idea, since some processing needs to know the true origin of the data. The Save as Matlab menu item and several of the user processing functions did this. Processed data is saved correctly. As in #1 above, this can sometimes lead to some confusing results. Starting from the original data and reprocessing will fix the problem.

User Processing

I have provided two kinds of hooks to add functionality to the program.

1) NMR parameters and data can be copied to the local workspace and used “on the fly” by way of the "File => Copy Data to Workspace" menu selection.

2) Almost any kind of additional processing can be done by creating .m files in either of the two sub directories, user_analysis and user_process. The file analysis_blank.m below, shows the required syntax. (Note: This function call has changed several times in recent versions)

```
function [handles,error] = analysis_blank(handles)
% ---------------------------------------------------
% blank user analysis
% ---------------------------------------------------
error                = 0;
% nmr               = handles.nmr;
% acquparm          = nmr.acquparm;
% procparm          = nmr.procparm;
% statparm          = nmr.statparm;
% zoomparm          = nmr.zoomparm;
% propparm          = nmr.propparm;
% tdom              = nmr.tdom;
% fdom              = nmr.fdom;

msgbox('This is a blank user analysis function.', ...
                'User Analysis Function','modal');

% nmr.acquparm      = acquparm;
% nmr.procparm      = procparm;
% nmr.statparm      = statparm;
% nmr.zoomparm      = zoomparm;
% nmr.propparm      = propparm;
% nmr.tdom          = tdom;
% nmr.fdom          = fdom;
% handles.nmr       = nmr;
```

A Functional Description of MatlabNMR

File Menu

Read Bruker Avance Data	Open a Bruker Avance data set for processing. Required files are *acqus* and *fid* for one-dimensional data, *acqus*, *acqu2s* and *ser* for two-dimensional data.
Read Bruker Aspect Data	Open a Bruker Aspect data set for processing. A single file with the data stored in the original 24 bit format is required. You will be prompted for the spectrometer frequency and an offset frequency.
Read Tecmag Data	Open a Tecmag NTNMR data set for processing. A single file with a *.tnt* extension is required. The pulse program is not read. Because of this, there can be some ambiguity with respect to which frequency goes with which axis.
Read JEOL GX Data	Open a JEOL GX data set for processing. Two files are required with *.gxp* and *.gxd* extensions.
Read Varian VNMR Data	Open a Varian VNMR data set for processing. Required files are *procpar* and *fid.*
Read Matlab Data	Open a Matlab data set for processing. A single file with a *.mat* extension is required.
Save as Matlab Data	Save data in a file with Matlab (version 6) format and a *.mat* file extension.
Save as Ascii Data	Save data in ascii (text) format.
1D Time Domain	Saves one-dimensional time domain data in a text file. Three columns, time, the real part and the imaginary part.
1D Frequency Domain	Saves one-dimensional frequency domain data in a text file. Three columns, ppm, the real part and the imaginary part.

Copy Figure to Clipboard	Copy the figure to the clipboard, so that it can be pasted into a document.
Copy Data to Workspace	Copy the NMR data to the Matlab workspace. In order for the graphic user interface to work properly, the NMR data is stored in the gui *handles* structure, which is hidden from view. This selection copies the current NMR data to the Matlab workspace. The structure *acquparm* contains acquisition parameters. The matrixes' *tdom* and *fdom* contain time domain and frequency domain data respectively.
Print Setup	Choose the printer, plot orientation etc.
Print	Print the figure.
Print Parameters	Open a text editor with the acquisition and processing parameters for printing.
Export	Export the figure in various formats.
EPS	Export the figure to an encapsulated postscript (eps) file with a file extension *.eps*.
HPGL	Export the figure to a Hewlett Packard graphics language (hpgl) file with a file extension *.hpg*.
JPEG	Export the figure to a Joint Photographic Experts Group (jpeg) file with a file extension *.jpg*.
TIFF	Export the figure to a tagged image file format (tiff) file with a file extension *.tif*.
Exit Matlab NMR	Exit the Matlab NMR program.

Acquisition Menu

Acquisition Parameters	Display the acquisition parameters of the current data set.

Process Menu

1D Interactive Windowing	Display the effect of various window functions on the time domain data.
Trapezoid Window	Trapezoid Window
Exponential Window	Exponential Window
Gaussian Window	Gaussian Window
Traficante Window	Traficante Window
Sine Window	Sine Window
Sine Squared Window	Sine Squared Window
1D Window Multiplication	Multiply the one-dimensional time domain data by the current window.
1D Fourier Transform	Fourier transform the one-dimensional time domain data set.
1D Absolute Value	Compute the absolute value of the frequency domain data.
1D Phase Spectrum	Manually correct the phase one-dimensional frequency domain data.
1D Auto Phase Spectrum	Automatically phase correct the one-dimensional frequency domain data.
2D Phase Spectrum	Manually phase correct the two-dimensional frequency domain data.
Phase F2	Use the crosshair to pick a row from the two-

dimensional matrix to use for phase correction.

Phase F1	Use the crosshair to pick a column from the two-dimensional matrix to use for phase correction.
Processing Parameters	Display the processing parameters of the current data set for editing. Note that if you select multiple window functions, they will **ALL** be applied (in order) if you use the "Process Data" menu item below.
MC2	2D: How to process the data set. Choices are Quad Complex, Quad Real, TPPI, States, States-TPPI, and echo-antiecho. States-TPPI, and echo-antiecho have not been implemented.
phMod	2D: Phase mode. Choices are No Correction, Phase Correct and Absolute Value.
BC Mode	Background correction mode. Choices are: None, Single, Quad, SPOL, QPOL, SFIL and QFIL. SPOL, QPOL, SFIL and QFIL have not been implemented.
First Point	Multiply the first point by 0.5 if checked.
FFT Indirect Dimension	Transforms the indirect dimension if checked.
Trapezoid	Multiply the data by a trapezoid window if checked.
Exponential	Multiply the data by an exponential window if checked.
Gaussian	Multiply the data by a Gaussian window if checked.
Traficante	Multiply the data by a Traficante window if checked.
Sine Bell	Multiply the data by a sine window if checked.
Sine Squared	Multiply the data by a sine squared window if checked.
Size (nnnn)	Size of (number of data points) the transformed data. The number (nnnn) is the size of the raw time domain data.
LP Mode	Linear Predictive mode. The choices: None, Forward

	LP and Backward LP. Note: Linear prediction is applied before windowing.
LP Starting Point	Starting data point for the prediction.
LP Ending Point	Ending data point for the prediction.
Extrap Start Point	First point to be extrapolated from the prediction. Note: For forward LP, this is always equal to the LP end point plus 1.
Extrap End Point	The last point to be extrapolated from the prediction.
Coefficients	Number of coefficients computed for the prediction and used in the extrapolation.
Process Data	Process the data set using the parameters defined above.
Contouring Parameters	Display the contouring parameters of the current data set for editing.
Type	Type of contour plot. Positive contours, negative contours or both.
Contours	Number of contours to plot.
Interval	Interval between contours. The first contour is at the base level, the second at interval * base, the third at interval * second, etc...
Base Level	The contour level closest to zero.
Contour Data	Redisplay the data set using the contouring parameters defined above.
User Processing	Execute a user written Matlab Program.

Analysis Menu

Background Subtract	Subtract a "baseline" from the real part of the frequency domain data. The algorithm is a variation of the one outlined by Dietrich, W; Rudel, C.H.; Neumann, M, **JMR** 91, 1-11 (1991).
Reference	Set the chemical shift reference.
Integration	Integrate regions of the spectrum.
Integrate	Two clicks of the left mouse button define an integral region. Most any other key to stop. (Right clicking will stop integration, but a context menu will also appear).
Calibrate	Move the vertical part of the crosshair within the horizontal span of an integral. Click the left mouse button to open the "Integral Calibration" dialog box. Enter a value for the integral and then click Ok.
Peak Pick	Compute the peak positions on the spectrum.
Peak Threshold	Set the threshold for peak picking.
Peak Position	Move the crosshair to the desired position. Click the left mouse button to open the "Peak Position" dialog box. Peak positions are reported in both ppm and Hz.
Signal to Noise	Compute the signal to noise ratio for selected peak and noise regions.
Symmetrize	Symmetrize a two-dimensional spectrum.
COSY, Average	Symmetrize using the average of the points across the diagonal.
COSY, Maximum	Symmetrize using the larger of the points across the diagonal.
User Analysis	Execute a user written Matlab program.

Display Menu

Display Full Spectrum	Display the complete spectrum.
Decrease Zoom	Return to the previous “zoom”.
Set Zoom Region	Define a “zoom region” for display.
Plot Zoom Region	Display the spectrum as defined by the “zoom region”.
Reset Gain	Display the spectrum, with the largest peak set to full scale.
Increase Gain	Increase the displayed height of the spectrum.
Decrease Gain	Decrease the displayed height of the spectrum.
Draw Integrals	Draw the integral trails on the figure (if defined).
Draw Peaks	Draw the peak positions on the figure (if defined).
Toggle X Hz / ppm	Display the X axis in either Hz or ppm.
Toggle Y Hz / ppm	Display the Y axis in either Hz or ppm.

Plot Menu

1D Time Domain	Display the one-dimensional time domain data for the current data set.
1D Frequency Domain	Display the one-dimensional frequency domain data for the current data set.
2D Contour	Display a two-dimensional contour plot of the frequency domain data for the current data set.
2D Intensity	Display a two-dimensional intensity plot of the frequency domain data for the current data set. This is not as pretty as a contour plot, but it is much faster.
2D Time Sequential	Display each row of the two-dimensional time domain data for the current data set in a sequence.
2D Frequency Sequential	Display each row of the two-dimensional frequency domain data for the current data set in a sequence.
2D Frequency Stack	Display each row of the two-dimensional frequency domain data for the current data set as a stacked plot.
2D Frequency Stack, 3D	Display each row of the two-dimensional frequency domain data for the current data set as a 3D stacked plot.
2D Time Slice	Display individual rows of the two-dimensional time domain data.
2D Frequency Slice	Display individual rows of the two-dimensional frequency domain data.

Help Menu

About	Display the version number and copyright information for the Matlab NMR program.
Documentation	This document.

Context Menu's

Context menus add functionality to the program. As the name suggests, the content of the menu changes depending on the context of the processing within MatlabNMR. A few examples are described below.

1D Phase Spectrum

Spectrum	Control the display for manually phasing data sets.
Display Full Spectrum	Display the complete spectrum.
Decrease Zoom	Return to the previous "zoom".
Set Zoom Region	Define a "zoom region" for display.
Plot Zoom Region	Display the spectrum as defined by the "zoom region".
Reset Gain	Display the spectrum with the largest peak set to full scale.
Increase Gain	Increase the displayed height of the spectrum.
Decrease Gain	Decrease the displayed height of the spectrum.
Set Phase Pivot	Reposition the phase pivot to another place in the spectrum.

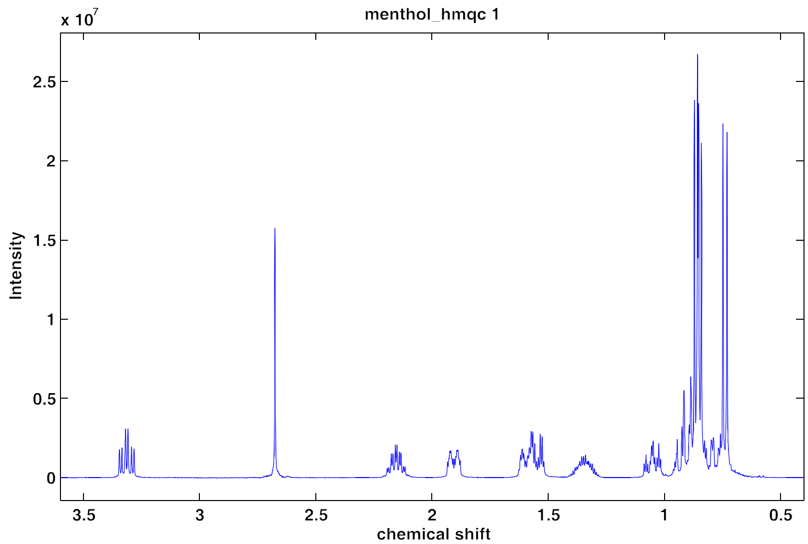
2D X Projection

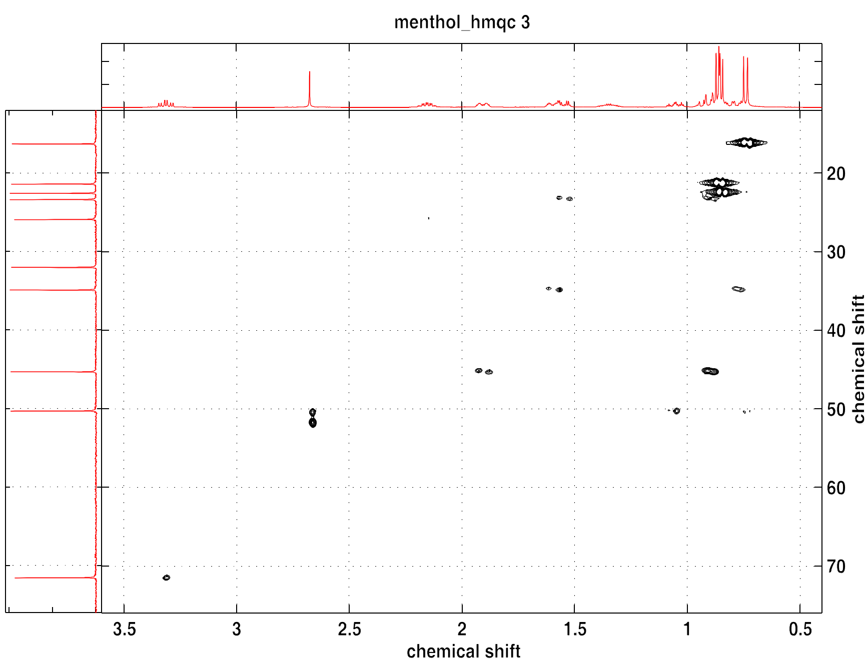
X Projection	Control the display of projections for two-dimensional data sets.
Make Skyline Projection	Create a projection from the largest value in each column.
Make Summation Projection	Create a projection by summing the values in each column.
Read Projection from File	Open a one-dimensional spectrum for plotting in the X projection area. You must process the

	1D spectrum prior to the 2D spectrum. The filename will contain “procdata1d.mat”
Load Projection from Slice	Move the crosshair to the desired position. Click the left mouse button to load the current row into the X projection area.
Remove Projection	Redraw the figure without the X projection.

Sample Data

I have included proton, carbon and HMQC sample data sets for Menthol. The proton spectrum and the HMQC spectrum with high resolution proton and carbon spectra in the projection areas are shown below. The spectra were exported as eps files for inclusion in this document. The parameters used are shown on the following pages.





```
======================================================================

              C:\z\data\dwheeler\nmr\Menthol_hmqc\1\

======================================================================
                    Acquisition Parameters
======================================================================
     aq: 2.93566
 aq_mod: 1
comment:
    ctd: 8192
   date: Tue May 29 09:08:04 2001 MDT (UT-6h)  dwheeler@avance400
     de: 6e-006      0           0           0
  decim: 64
 dspfvs: 10
  dtype: Avance
     dw: 0.0003584   0           0           0
 fnmode: 0           0           0           0
 grpdly: 0
     ns: 4
   nuc1: 1H
   nuc2: off
   nuc3:
   nuc4:
 offset: 5.50151     0           0           0
parmode: 1D
pulprog: zg
  reshz: 0.170309    0           0           0
 resppm: 0.000425634 0           0           0
    sfo: 400.131     400.13      0           0
  smode: 0
    swh: 2790.18     0           0           0
     sw: 6.97317     0           0           0
     td: 16384       1           1           1


======================================================================
                    Processing Parameters
======================================================================
  bcmod: 2           2           0           0
comment:
    fft: 1           1           1           1
  lpmod: 0           0           0           0
  lpspt: 1           1           1           1
  lpept: 1           0           0           0
  lpex1: 1           0           0           0
  lpex2: 1           0           0           0
  ncoef: 100         100         0           0
     gb: 10          10          10          10
     lb: 0           0           0           0
    mc2: 1           1           1           1
  phmod: 1           2           2           2
    ph0: 0           0           0           0
    ph1: 0           0           0           0
    php: 5473        1           1           1
     si: 16384       1           1           1
    ssb: 0           0           0           0
    ssq: 0           0           0           0
     tr: 0           0           0           0
     tm: 0           0.1
    wdw: 2           0           0           0
```

```
======================================================================

               C:\z\data\dwheeler\nmr\Menthol_hmqc\3\

======================================================================
                    Acquisition Parameters
======================================================================
     aq: 0.183147
 aq_mod: 1
comment:
    ctd: 512
   date: Wed Mar 21 11:39:52 2001 MST (UT-7h)  dwheeler@avance400
     de: 4.5e-006    0.00017     0           0
  decim: 64
 dspfvs: 10
  dtype: Avance
     dw: 0.0003584   9.52e-005   0           0
 fnmode: 0           0           0           0
 grpdly: 0
     ns: 1
   nuc1: 1H
   nuc2: 13C
   nuc3:
   nuc4:
 offset: 5.50152     102.703     0           0
parmode: 2D
pulprog: inv4gp
  reshz: 2.72745     20.5562     0           0
 resppm: 0.00681639  0.204299    0           0
    sfo: 400.131     100.618     0           0
  smode: 0
    swh: 2790.18     10504.2     0           0
     sw: 6.97317     104.397     0           0
     td: 1024        256         1           1


======================================================================
                    Processing Parameters
======================================================================
  bcmod: 2           2           0           0
comment:
    fft: 1           1           1           1
  lpmod: 0           0           0           0
  lpspt: 1           1           1           1
  lpept: 1           1           0           0
  lpex1: 1           1           0           0
  lpex2: 1           1           0           0
  ncoef: 100         100         0           0
     gb: 10          10          10          10
     lb: 0           0           0           0
    mc2: 1           1           1           1
  phmod: 1           2           2           2
    ph0: 0           0           0           0
    ph1: 0           0           0           0
    php: 1           1           1           1
     si: 1024        512         1           1
    ssb: 30          0           0           0
    ssq: 0           0           0           0
     tr: 0           0           0           0
     tm: 0           0.1
    wdw: 32          32          0           0


======================================================================
                    Contouring Parameters
======================================================================
contype: 1
contnum: 6
contint: 1.2
contval: 1.35376e+007
```

Programing MatlabNMR

The programs in the user_analysis and user_processing subdirectories provide several examples of MatlabNMR programming. Many of the most important parameters used by MatlabNMR are discussed below.

Parameters

Parameters are all initialized in the" init" .m files. For example: The acquisition parameters are defined in initacquparm.m.

```
function acquparm = initacquparm()
%
% INITACQUPARM Initialize acquisition parameter values
%
acquparm    = struct( ...
        'aq',           0, ...          % acquisition time
        'aq_mod',       1, ...          % acquisition mode (Bruker)
        'comment',      '', ...         % comment
        'ctd',          0, ...          % number of complex points in dimension 1 (td[1]/2)
        date',          '', ...         % date of the experiment
        'de',           [0 0 0 0], ...  % delay before sampling (microseconds)
        'decim',        1, ...          % decimation of data set (Bruker)
        'dspfvs',       0, ...          % processing for digital filter (Bruker)
        'dtype',        0, ...          % Data type: 0=JEOL,1=Avance,2=Aspect,
                                        % 3=TecMag,4=Varian
        'dw',           [0 0 0 0], ...  % dwell time (sampling interval)
        'fnmode',       [0 0 0 0], ...  % acquisition mode for indirect dimensions
        'grpdly',       0, ...          % group delay (number of zeroed pts in fid)
        'ns',           0, ...          % number of scans
        'nuc1',         '', ...         % nucleus for dimension 1
        'nuc2',         '', ...         % nucleus for dimension 2
        'nuc3',         '', ...         % nucleus for dimension 3
        'nuc4',         '', ...         % nucleus for dimension 4
        'offset',       [0 0 0 0], ...  % left edge of the spectrum for dimension n, (always ppm)
        'parmode',      1, ...          % 1 = 1D, 2 = 2D, 3 = 3D
        'pulprog',      '', ...         % pulse program
        'reshz',        [0 0 0 0], ...  % digital resolution in Hz
        'resppm',       [0 0 0 0], ...  % digital resolution in ppm
        'sfo',          [0 0 0 0], ...  % spectrometer frequency (for converting to ppm), channel
        'smode',        0, ...          % time domain=0 : frequency domain=1 (JEOL, TecMag)
        'swh',          [0 0 0 0], ...  % sweep width in hz (sampling rate), dimension #1
        'sw',           [0 0 0 0], ...  % sweep width in ppm, dimension #1
        'td',           [1 1 1 1]);     % number of points in each dimension
```

Other definitions

Other definitions are initialized in the “define” .m files. For example: The data types (acquparm.dtype) are defined in definedatatype.m.

```
function dtype = definedatatype()
%
% DEFINEDATATYPE Define the data type
%
dtype     = struct( ...
        'JEOL',         0, ...          % JEOL GSX data
        'Avance',       1, ...          % Bruker Avance data
        'Aspect',       2, ...          % Bruker Aspect data
        'TecMag',       3, ...          % TecMag data
        'Varian',       4);             % Varian data
```