**GNAT Macros**

Macros are a way to execute code within the GNAT environment. They are written as standard Matlab scripts but have some limitations”

1. You can't create new variables, but you can use existing structures.

      e.g. NmrData which is the structure for all GNAT data

          TmpVar which is a structure specifically created for use in

          a macro

TmpVar.M=zeros(10,5) creates a 10 by 5 matrix of zeros

TmpVar.T='GNAT rules' creates a text string

2. You can't use for loops (related to 1, as a structre element is not accepted as a loop counter). Instead you can use while loops, which requires a bit more code, but works well. Example:

TmpVar.k=1;

while TmpVar.k<=10

    TmpVar.k=TmpVar.k+1;

end

**How to do various things**

Basic commands

Reading in the latest version of NmrData

NmrData=guidata(hMainFigure);

Saving the current version of NmrData

guidata(hMainFigure,NmrData);

Display something to the main Matlab window

disp(‘*desired string’*) or disp(num2str(*desired numeric value)*)

Saving data in Matlab format

[TmpVar.filename, TmpVar.pathname] = uiputfile('\*.mat','Save output data');

TmpVar.filepath=[TmpVar.pathname TmpVar.filename];

save(TmpVar.filepath,'TmpVar,'-v7.3'); %saving in Matlab format needs to save the whole TmpVar structure

Saving data in Excel/csv format

[TmpVar.filename, TmpVar.pathname] = uiputfile('\*.xls','Save output data');

TmpVar.filepath=[TmpVar.pathname TmpVar.filename];

xlswrite(TmpVar.filepath,TmpVar.data); %saving in XL format save the data matrix or cell array

**Menu commands**

Import Varian Data

   Import\_Varian([],[],*path to \*.fid directory*);

**Grouped by Tabs in the GUI**

Plot

Phase

Phase spectrum with current values

PhaseSpectrum(*zero order phase*, *first order phase*,1)

Set phase scope to Individual mode

set(hScopeGroup,'SelectedObject',hRadioScopeIndividual)

Automatic zero order phasing

ButtonAutophase0\_Callback();

Get the current value of zero order phase

TmpVar.tmp=str2double(get(hEditPh0,'String'));

FT

Set and enable Gaussian window function

set(hCheckGw,'Value',1); %tick checkbox

set(hEditGw,'Enable','On'); %enable edit box

set(hEditGw,'string', *desired value of gw*) %set the gw value

Set Fourier number

set(hEditFn,'string',num2str(*desired value of fn*)); %set Fourier number

Do Fourier transformation with current values

FTButton\_Callback();

Correct

Array

Change to a new spectrum in the array

 set(hEditFlipSpec,'String', num2str(*desired spectral number*));

 EditFlipSpec\_Callback();

Prune

Pureshift

Misc

Info

**Description of the NmrData structure**

 NmrData.at=[];

        NmrData.arraydim=[];

        NmrData.array2nr=[];

        NmrData.baselinecorr=[];

        NmrData.baselinepoints=[];

        NmrData.BasePoints=[];

        NmrData.d2=[];

        NmrData.dc=0;

        NmrData.dcspec=1;

        NmrData.decradata=[];

        NmrData.DELTA=[];

        NmrData.DELTAOriginal=[];

        NmrData.DELTAprime=[];

        NmrData.delta=[];

        NmrData.deltaOriginal=[];

        NmrData.disptype=1; %Determines if phase sensitive or absolute value plotting is used

        NmrData.DOSYdiffrange=[];

        NmrData.dosyconstant=[];

        NmrData.dosyconstantOriginal=[];

        NmrData.dosydata=[];

        NmrData.DOSYopts=[];

        NmrData.dspPhase=0;

        NmrData.exclude=[];

        NmrData.excludelinepoints=[];

        NmrData.ExcludePoints=[];

        NmrData.FID=[];

        NmrData.FitType=0;

        NmrData.filename='';

        NmrData.flipnr=[];

        NmrData.fn=0;

        NmrData.fpmult=0.5;

        NmrData.fshift=[];

        NmrData.gamma=[];

        NmrData.gammaOriginal=[];

        NmrData.gcal=[];

        NmrData.gcal\_orig=[];

        NmrData.gf=0;

        NmrData.gradnr=[];

        NmrData.gw=0;

        NmrData.Gzlvl=[];

        NmrData.Integral=[];

        NmrData.integral\_peaks=[];

        NmrData.IntPoint=[];

        NmrData.IntPointIndex=[];

        NmrData.IntPointSort=[];

        NmrData.Intscale=1;

        NmrData.lb=[];

        NmrData.local=tmp2;

        NmrData.lp=[];

        NmrData.lpInd=[];

        NmrData.locodosydata=[];

        NmrData.locodosyopts=[];

        NmrData.lrfid=0;

        NmrData.lrfidOrg=[];

        NmrData.lsspec=0;

        NmrData.linshift=1;

        NmrData.mcrdata=[];

        NmrData.MCRopts=[];

        NmrData.narray2=[];

        NmrData.ncomp=[];

        %NmrData.nfid=[];

        NmrData.ngrad=[];

        NmrData.np=[];

        NmrData.nug=[1 0 0 0]; %default as pure exponential

        NmrData.nwin=[];

        NmrData.order=[];

        NmrData.panelpos=[0 0];

        NmrData.parafacFac=[];

        NmrData.pfgnmrdata=[];

        NmrData.pivot=[];

        NmrData.pivotxdata=[];

        NmrData.pivotydata=[];

        NmrData.plottype=1;

        NmrData.plotsep=0;

        NmrData.probename='undefined';

        NmrData.prune=[];

        NmrData.pruneArray2=[];

        NmrData.RDcentrexdata=[0 0];

        NmrData.RDcentreydata=[0 0];

        NmrData.RDcentre=0;

        NmrData.RDleftxdata=0;

        NmrData.RDleftydata=0;

        NmrData.RDleft=0;

        NmrData.RDrightxdata=[0 0];

        NmrData.RDrightydata=[0 0];

        NmrData.RDright=0;

        NmrData.reference=[];

        NmrData.referencexdata=[];

        NmrData.referenceydata=[];

        NmrData.RRTopts=[];

        %NmrData.procpar=[];

        NmrData.region=[];

        NmrData.rp=[];

        NmrData.rpInd=[];

        NmrData.SaveState=[];

        NmrData.scoredata=[];

        NmrData.SCOREopts=[];

        NmrData.sfrq=[];

        NmrData.shiftunits='ppm';

        NmrData.sp=[];

        NmrData.Specscale=[];

        NmrData.SPECTRA=[];

        NmrData.sw=[];

        NmrData.sw1=[];

        NmrData.tau=0;

        NmrData.tauOriginal=[];

        NmrData.th=0.0;

        NmrData.thShow=0;

        NmrData.thresxdata=0;

        NmrData.thresydata=0;

        NmrData.Timescale=[];

        NmrData.type='';

        NmrData.version=tmp;

        NmrData.xlim=[];

        NmrData.xlim\_fid=[];

        NmrData.ylim=[];

        NmrData.ylim\_fid=[];

        NmrData.flipnr=str2double(get(hEditFlip,'String'));

        NmrData.fn=NmrData.np;

        NmrData.gw=str2double(get(hEditGw,'String'));

        NmrData.lb=str2double(get(hEditLb,'String'));

        NmrData.density=1.050;

        NmrData.packing=0.64;

        NmrData.temperature=298.15; %GDP 31/01/2018 for SEGWE

        NmrData.answer=30.80; %GDP 31/01/2018 for SEGWE

        NmrData.argument = 100; %GDP 31/01/2018 for SEGWE

        NmrData.viscositydisplay=0.0003258\*1000; %GDP 31/01/2018 for SEGWE

        NmrData.MWs=64.12;

        NmrData.peff=627;

        %AC

        NmrData.include=[];

        NmrData.includelinepoints=[];

        NmrData.IncludePoints=[];

        NmrData.startORend=0;

        NmrData.winstart=[];

        NmrData.winend=[];

        NmrData.numcomp=[];

        NmrData.concat1dspectra=[];

        NmrData.sderrmultiplier=[];

        NmrData.LRRegionData=[];

        NmrData.issynthetic=0;

        %AC

        %nD specific

        NmrData.xlim\_1D=[];

        NmrData.ylim\_1D=[];

        NmrData.xlim\_2D=[];

        NmrData.ylim\_2D=[];