**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 two existing structures, and add elements to them as desired:

      NmrData which is the structure for all GNAT data

          TmpVar which is a structure specifically created for use in macros

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

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

(ii) Sometimes it seems like a variable have problems changing type (e.g. from number to char). To circumvent this you can use cell arrays

TmpVar.M=cell(10,5)

2. You can't use for loops (related to 1, as a structure 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

3. You don’t get the normal Matlab error messages, but some limited error handling is implemented.

4. You can’t use double quotes e.g “FooString” for strings, as this interferes with the error handling in point 3.

**The data structure**

GNAT keeps it data in a standard Matlab structure with the name NmrData, e.g. the raw FIDs are in NmrData.FID. The main (default) structure elements are described in Appendix I. It is possible, depending on version, not all elements are present and depending on the process history other elements will be present.

**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*);

Import Bruker Data

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

**Grouped by Tabs in the GUI**

Plot

Plot spectrum with current values

PlotSpectrum();

Change the currently displayed spectrum

set(hEditFlipSpecShort,'String',x)) %where x is a number

EditFlipSpecShort\_Callback()

PlotSpectrum();

Autoscale the spectrum

ButtonAutoscale\_Callback();

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 and enable Loretzian window function

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

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

set(hEditLb,'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

Various

%Set the threshold for peak picking (if used)

NmrData.th=0.2;%20% of max

guidata(hMainFigure,NmrData); %save it to the structure

%set integrals

NmrData.IntPoint=[2 7]; %in ppm

IntLine\_function()

**Appendix I. Data structure**

GNAT keeps it data in a standard Matlab structure with the name NmrData, e.g. the raw FIDs are in NmrData.FID. The main (default) structure elements are described below It is possible, depending on version, not all elements are present and depending on the process history other elements will be present.

**NEEDS detail**

at:

arraydim: 16

array2nr: 1

baselinecorr: [8192×16 double]

baselinepoints: [1×36 double]

BasePoints: [1×36 double]

d2: 0.0080

dc: 0

dcspec: 1

decradata: []

DELTA: 'non existing'

DELTAOriginal: 'non existing'

DELTAprime: [0 0 0 0 0 0 0 0 0 0 0 0]

delta: 'non existing'

deltaOriginal: 'non existing'

disptype: 1

DOSYdiffrange: []

dosyconstant: 0

dosyconstantOriginal: 0

dosydata: []

DOSYopts: []

dspPhase: 0

exclude: [1×8192 double]

excludelinepoints: []

ExcludePoints: []

FID: [8192×16 double]

FitType: 0

filename: '/Users/mbdssln2/MNDocs/General NMR Analysis Tolbox/Misc/Clari\_new\_PROJ\_8ms.fid'

flipnr: 1

fn: 8192

fpmult: 0.5000

fshift: [0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0]

gamma: 2.6752e+08

gammaOriginal: 2.6752e+08

gcal: []

gcal\_orig: 'non existing'

gf: 0

gradnr: 1

gw: 0

Gzlvl: 0

Integral: [1×8192 double]

integral\_peaks: []

IntPoint: []

IntPointIndex: []

IntPointSort: []

Intscale: 1

lb: 0

local: 'yes'

lp: -12.8000

lpInd: [1×16 double]

locodosydata: []

locodosyopts: [0 0 0 0 0]

lrfid: 0

lrfidOrg: 0

lsspec: 0

linshift: 1

mcrdata: []

MCRopts: []

narray2: 16

ncomp: []

ngrad: 1

np: 8192

nug: [1 0 0 0]

nwin: []

order: 2

panelpos: [0 0]

parafacFac: []

pfgnmrdata: []

pivot: 2.9782

pivotxdata: [2.9782 2.9782]

pivotydata: [-2.2878e+05 1.0280e+07]

plottype: 1

plotsep: 0

probename: 'undefined'

prune: []

pruneArray2: []

RDcentrexdata: [0 0]

RDcentreydata: [0 0]

RDcentre: 0

RDleftxdata: 0

RDleftydata: 0

RDleft: 0

RDrightxdata: [0 0]

RDrightydata: [0 0]

RDright: 0

reference: []

referencexdata: []

referenceydata: []

RRTopts: []

region: [1×8192 double]

rp: -150.8000

rpInd: [1×16 double]

SaveState: []

scoredata: []

SCOREopts: []

sfrq: 500.1330

shiftunits: 'ppm'

sp: -0.0218

Specscale: [1×8192 double]

SPECTRA: [8192×16 double]

sw: 6.0008

sw1: 10.7498

tau: 0

tauOriginal: 0

th: 0

thShow: 0

thresxdata: 0

thresydata: 0

Timescale: [1×8192 double]

type: 'Varian'

version: 'General NMR Analysis Toolbox (GNAT) 1.0'

xlim: [-0.0218 5.9790]

xlim\_fid: [0 2.7296]

ylim: [-3200000 1.3200e+07]

ylim\_fid: [-2.3758e+05 1.4425e+05]

density: 1.0500

packing: 0.6400

temperature: 298.1500

answer: 30.8000

argument: 100

viscositydisplay: 0.3258

MWs: 64.1200

peff: 627

include: [1×8192 double]

includelinepoints: []

IncludePoints: []

startORend: 0

winstart: []

winend: []

numcomp: []

concat1dspectra: []

sderrmultiplier: []

LRRegionData: [100×1 double]

issynthetic: 0

xlim\_1D: []

ylim\_1D: []

xlim\_2D: []

ylim\_2D: []

ni: 0

sp1: 0

rp1: 0

lp1: 0

d2\_org: 0.0080

xlim\_spec: [-0.0218 5.9790]

ylim\_spec: [-3200000 1.3200e+07]

incpoints: [1 8192]

SVDcutoff: 0.9990

pfIterations: 2500