# Testing the IDA GUI

This document is intended to guide the Mantid team's sandwich students on how to test the basic functionality of the Indirect Data Analysis (IDA) graphic user interface (GUI) within MantidPlot prior to each release. The purpose for this is to try and catch any bugs that may have been triggered by changes pushed to git. Essentially, unless there have been direct changes to the GUI or its underlying code, IDA should function as shown in this guide. If not, the issues need to be resolved.

This guide will demonstrate how to test the IDA GUI by outlining the expected inputs, providing instructions and by showing example values in the screenshots. After following the accompanying instructions, the tester should then compare the outputs they get with the screenshots provided in this document.

As changes are made to the GUI and the underlying code, please update this document accordingly and add relevant files to the folder.

**Notice: THIS DOCUMENT IS NOT A COMPLETE GUIDE** on how to test IDA; it is only intended to introduce students to the workings of this particular interface in MantidPlot. As well as the **basic** testing outlined in this document, unscripted testing should also be carried out prior to release.

#### Get started

To begin, load up the IDA GUI. It will look as follows:

MantidPlot - untitled	🕅 Ind	lirect Data Analy	sis						
<u>File Edit View W</u> indows <u>Inte</u>	erfaces <u>C</u> atalog <u>H</u> elp	Elw	in MSD Fit	Fury	FuryFit	ConvFit	Calculate Corr	ections A	pply Corrections
	Convert To Energy	Inp	ut File					*	Browse Plot Input
	Create MD Workspace	Pro	operty	١	alue		1,000		
MS Shell Dlg 2	Indirect Data Analysis		Range One Start	-	0.020000				
i 👝 📄 📑 📭 🔚	Indirect Diffraction		End Use Two Ranges	0	.020000 False		800 -		
	Muon Analysis	٥	Range Two Start	0	.000000				
Results Log			End	0	.000000		- 000		
Welcome to Mantid - Manipulation	SANS ISIS						400		
	DGS Reduction								
	ORNL SANS						200		
	REFL Reduction								
	REFL SF Calculator						E°		
	REFM Reduction						0	200 4	00 600 800 1,000
	TofConverter		Concatanate Mult Verbose	iple Resu	ults	Plot Result		Save	e Result
	ISIS Reflectometry	?			[	Run	]		Manage Directories

<u>Testing Elwin</u>

The Elwin tab operates on \_*red* files; these are created when *.raw* files are processed in the **Convert To Energy** interface. Input irs26173\_graphite002\_red.nxs from the test folder and click the **Plot Input** button. The interface should look as follows:

Indirec	t Data Anal	ysis					_ <b>D</b> _ X
Elwin	MSD Fit	Fury	FuryFit	ConvFit	Calculate Corrections	Apply Correct	ions
Input Fi	le sktop\Tes	ting_IDA	_GUI\IDA_Te	esting\irs2617	3_graphite002_red.nxs	Browse	Plot Input
Proper	ty		Value		1.6		
a Ra Us∉ Ra	nge One Start End e Two Range nge Two Start End	:5	-0.020000 0.020000 False 0.000000 0.000000		1.4 1.2 1- 0.8 0.6 0.4 0.2 0 -0.6 -0.4 -0	.2 0 0.	<u></u>
Con	catanate Mu	ltiple Res	ults				
Verb	ose			Plot Result		Save Result	
			(	Run	]	Į	Manage Directorie:

It is best that the save directory is set to that of the test folder; this can be done through **Manage User Directories.** Change the start and end values in the **Range One** section to -0.05 and 0.05 respectively, place a check in the **Plot Result** and **Save Result** checkboxes and click **Run**:

M Indirec	t Data Analysis					
Elwin	MSD Fit Fur	y FuryFit	ConvFit	Calculate Corrections	Apply Corre	ections
Input Fi	le_sktop\Testing_1	IDA_GUI\IDA_Te	esting\irs261	73_graphite002_red.nxs	Browse	Plot Input
Proper	ty	Value		1.6		
⊿ Ra	nge One					
	Start	-0.050000		1.4 -		
	End	0.050000				
Use	e Two Ranges	False		1.2		
⊿ Ra	nge Two					
	Start	0.000000		1-		
	End	0.000000				
				0.8 -		
				0.6		
				0.4		
				0.2		
				E 6	/\	
				-0.6 -0.4 -	0.2 0	0.2 0.4 0.6
Con	catanate Multiple I	Results				
Verb	ose	$\checkmark$	Plot Result		Save Result	
?		(	Run			Manage Directories

This generates three new workspaces, with <u>elw</u>, <u>eq1</u>, and <u>eq2</u> as their suffixes. Two of them, <u>eq1</u> and <u>eq2</u>, are plotted:



#### **Testing MSDFit**

The MSDFit tab operates on the file with the suffix <u>eq2.nxs</u> that has been created using the Elwin tab of this interface. Input irs26173\_graphite002\_eq2.nxs from the test folder and click the Plot Input button:

Indirect	Data Anal	ysis			
Elwin	MSD Fit	Fury	FuryFit	ConvFit	Calculate Corrections Apply Corrections
Input File	sktop\Test	ting_IDA_	_GUI\IDA_Te	sting\irs2617	3_graphite002_eq2.nxs Browse Plot Input
Property		1	/alue		-2.9
Start	X	0	. 19506 1		
EndX		3	3.436134		-3 -
					-34 - HU HUY H/ K H
					-3.5 -     '\ ''
					-3.6 -
					-3.7 -
Verbos	se		<b>V</b>	Plot Result	Save Result
?			(	Run	Manage Directorie

Place a check in the **Save Result** checkbox and click **Run**:



# **Testing Fury**

The Fury tab operates on the original \_*red* and the \_*res* file created in **Convert To Energy -> Calibration** using the following values:

	VDC2C172 com	Property	Value
Run No DA_lesting	uRS26173.raw Browse	Spectra Min	3
		Spectra Max	53
Property	Value	Background	
Property	value	Start	-0.30
Peak Min	62500.00	End	0.30
Peak Max	65000.00	Rebinning	
Dack Min	50000.00	Low	-0.200000
DOCK MILLI	59000.00	Width	0.002000
Back Max	61500.00	High	0.200000

In Fury, load irs26173\_graphite002\_red.nxs and irs26173\_graphite002\_res.nxs. Ensure that the Plot Result and Save Result checkboxes are ticked. Using the inputs shown, click Run:

M Indirect Data Analysis			
Elwin MSD Fit Fury File Sample: Resolution File Type: Resolution: :top/Testing_ID Property ELow EWidth EHigh	FuryFit         ConvFit           GUI\IDA_Testing\irs2617         RES I           A_GUI/IDA_Testing/irs2617         Value           -0.060000         0.010000           0.060000         0.060000	Calculate Corrections App 3_graphite002_red.nxs Br 3_graphite002_res.nxs Br 1.6 1.4 1.2 1.6 0.8 0.6 0.4 0.2 0.4 0.2 0.4 0.2 0.4 0.2 0.4 0.4 0.2 0.4 0.4 0.2 0.4 0.4 0.2 0.4 0.4 0.2 0.4 0.4 0.2 0.4 0.4 0.2 0.4 0.4 0.2 0.4 0.4 0.2 0.4 0.4 0.4 0.2 0.4 0.4 0.4 0.4 0.2 0.4 0.4 0.4 0.2 0.4 0.4 0.4 0.4 0.4 0.2 0.4 0.4 0.4 0.4 0.4 0.4 0.4 0.4	y Corrections
Verbose	📝 Plot Result	V Save R	esult
?	Run		Manage Directories

A file with the suffix **\_***iqt.nxs* is created:



#### **Testing FuryFit**

This tab uses the *iqt.nxs* file generated by the **Fury** tab as the only input. Use the file **irs26173\_graphite002\_iqt.nxs** and select **1 Exponential** as the **Fit Type**.

M Indirect Data Analysis			
Elwin MSD Fit Fury	FuryFit ConvFit	Calculate Corrections Apply Corre	ections
File	A_GUI/IDA_Testing/irs26173	_graphite002_iqt.nxs Browse	Plot Input
Fit Type:		1	
1 Exponential	•		
Constrain Intensities	Plot Guess	0.8	
Property	Value		
StartX	0.000000	0.6 -	
EndX	0.206782		
LinearBackground			
AO	0.000000	0.4	
Exponential 1			
Intensity	1.000000		
Tau	0.000000	-	
		0	
		0 0.05 0.1	0.15 0.2
		Spectrum: 0	
		Plot Output: None 💌	Run Sequential Fit
Verbose	V Plot Output	t (Single Run)	☑ Save Result
?	Run	]	Manage Directories

Place a tick in the Plot Output (Single Run) checkbox and click Run:



#### **Testing ConvFit**

This tab takes the original <u>red.nxs</u> file – the one obtained in Convert To Energy -> Energy Transfer by operating on a <u>.raw</u> file – and a <u>\_res.nxs</u> file as inputs.

M Indirect Data Analysis			
Elwin MSD Fit Fu	ury FuryFit	ConvFit	Calculate Corrections Apply Corrections
File • g_I	DA_GUI/IDA_Testin	g/irs26173	_graphite002_red.nxs Browse Plot Input
Resolution File th38413	/Desktop/Testing_ID	A_GUI/ID	A_Testing/irs26173_graphite002_res.nxs Browse
Fit Type:	One Lorentziar	ı •	1.6
Background	Fixed Flat		1.4
Plot Guess			1.2
Property	Value		1
EndX	0.500000		0.8 -
Background			
AO	0.000000		1 <sup>0.0</sup>
A Delta Function			0.4
Use	False		0.2
▲ Lorentzian 1			
Height	2.921080		
PeakCentre	0.000212		-0.6 -0.4 -0.2 0 0.2 0.4 0.6
HWHM	0.020073		Spectra Range 0 to 50
Verbose		Plot Outpu	Plot Output: None  Run Sequential Fit It (Single Run) Save Result
?		Run	Manage Directories

Use **irs26173\_graphite002\_red.nxs**. Ensure the **Plot Output (Single Run)** checkbox is ticked then click **Run**:



#### **Testing Calculate Corrections**

This tab takes <u>*red.nxs*</u> files as its only input. Use **irs26173\_graphite002\_red.nxs** and **irs26173\_graphite002\_red.nxs**.

#### Sample Shape = Flat

To test for when the **Sample Shape** is **Flat**, use the following inputs:

Indirect Data Analysis	
Elwin MSD Fit Fury FuryFit ConvFit Calculate Corrections Apply Correction	ons
Input type: File  Sample file: DA_GUI/IDA_Testing/irs26173_graphite002_red.nxs	Browse
Shape Details	
Sample Shape: Flat	-
Thickness     0.5       Front Thickness	
Beam Width     3.0       Sample Details       Number Density     30       Scattering cross-section     2.0       Absorption cross-section	8.0
Can Details       Number Density     Scattering cross-section       Verbose     Plot Output	
2 Run Ma	anage Directories

When you click **Run**, an \_*flt\_Abs.nxs* file is created and saved in your directory; its intended purpose is for use within the **Apply Corrections** tab.

#### Sample Shape = Cylinder

To test for when the **Sample Shape** is **Cylinder**, use the following inputs on **irs26173\_graphite002\_red.nxs** and **irs26176\_graphite002\_red**:

🕅 Indirect Da	ita Analysis	_ <b>D</b> _ X
Elwin M	SD Fit Fury FuryFit ConvFit Calculate Corrections Apply Correc	ctions
Input type:	File  Sample file: DA_GUI/IDA_Testing/irs26173_graphite002_red.nxs	Browse
🛛 🔽 Use Can		
-Shape Det	ails	
Sample Sh	ape: Cylinder	<b>-</b>
Radius 1	0.1	
Radius 2	0.11	
Radius 3	0.12	
Step Size	0.0004	
Beam Width	3	
-Sample De	tails	
Number D	ensity 0.03 Scattering cross-section 11 Absorption cross-section	on 111
Can Detail	S	
Number D	ensity 0.05 Scattering cross-section 4 Absorption cross-section	on 0.1
Verbose	Plot Output Both	
?	Run	Manage Directories

When you click **Run**, an *\_cyl\_Abs.nxs* file is created and saved in your directory; its intended purpose is for use within the **Apply Corrections** tab.

### **Testing Apply Corrections**

This tab takes two <u>red.nxs</u> files as its two inputs. Prior to using irs26173\_graphite002\_red.nxs and irs26176\_graphite002\_red (it should be in the test folder), use the Calculate Corrections tab to generate their corresponding <u>\_flt\_Abs</u> or <u>\_cyl\_Abs</u> files for when the Sample Shape is Flat or Cylinder respectively.

When Flat:

M Indirect Data Analysis		
Elwin MSD Fit Fury	FuryFit ConvFit Calculate Corrections	Apply Corrections
Input Type: File 🔻	sting_IDA_GUI/IDA_Testing/irs26173_graphite	:002_red.nxs Browse
Geometry:	Flat	<b>•</b>
Use Corrections		
Use Container		
Input Type: File 🔻	p/Testing_IDA_GUI/IDA_Testing/irs26176_graphi	ite002_red.nxs Browse
Plot Output: None		<b></b>
Verbose		
?	Run	Manage Directories

When Run is clicked:



When **Cylinder**:

M Indirect Data Analysis		
Elwin MSD Fit Fury	FuryFit ConvFit Calculate Corrections Apply Correct	tions
Input Type: File 🔻	sting_IDA_GUI/IDA_Testing/irs26173_graphite002_red.nxs	Browse
Geometry:	Cylinder	<b>•</b>
Use Corrections		
Use Container		
Input Type: File 🔻	p/Testing_IDA_GUI/IDA_Testing/irs26176_graphite002_red.nxs	Browse
Plot Output: None		•
Verbess		
2	Run	Manage Directories

#### When Run is clicked:



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