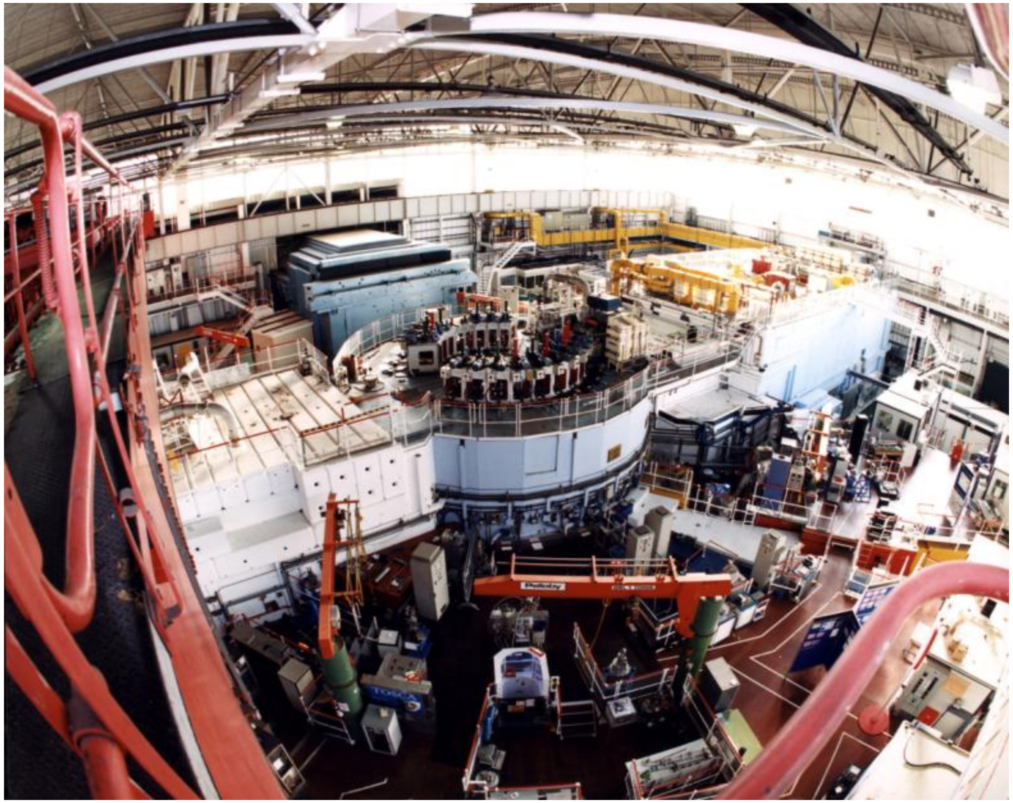
# ICAT at ISIS



Tom Griffin, STFC ISIS Facility
ICAT Workshop
ILL, Grenoble

March 2012

tom.griffin@stfc.ac.uk

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ISIS

# ICAT at ISIS

- Data Volume and Rates
- Getting the data in
- Getting the data out
- DOIs – data citation
- Next….

# Volume and Rates

- Pulsed Neutrons and Muons
- Nexus, RAW and Log (txt)
- Operating since 1984
- 2000 users ; 800+ experiments
- Volume of data 10TB
- 8M datafiles
- 10GB metadata, >60M rows

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# ISIS – Volume and Rates

| | Files/15 minutes | Files/minute | Files/second |
|---|---|---|---|
| Peak | 10857 | 724 | 12.06 |
| Mean | 968 | 65 | 1.08 |
| Median | 263 | 18 | 0.29 |

Peak - 4 hours averaging of 6.4 files/sec (384/minute)

# Getting data into ICAT

- Pre-experiment....
- C#
- Reads metadata from
  - Proposal system
  - ‘Visits’ system
  - ‘Risk Assessment system

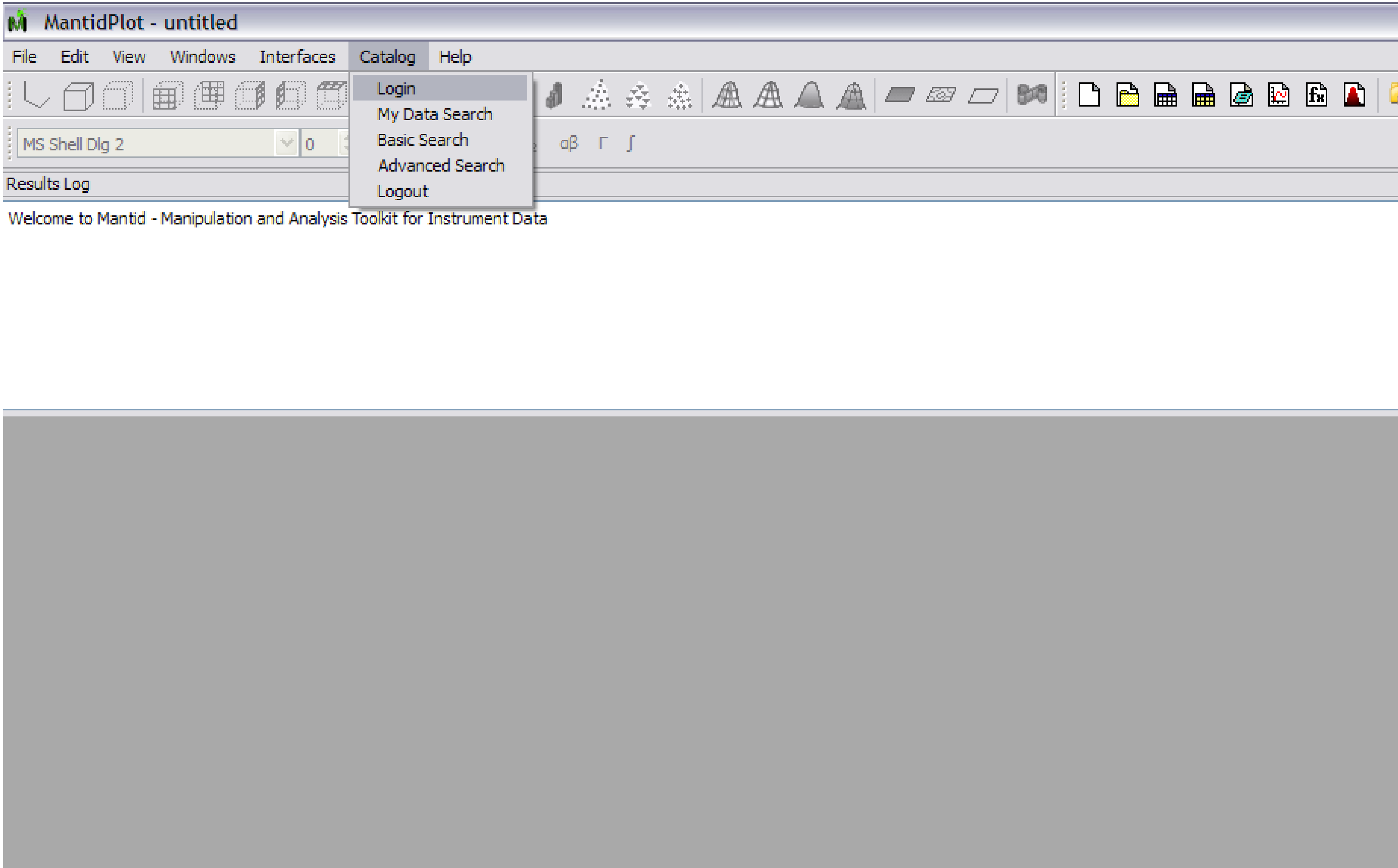
# Getting data into ICAT

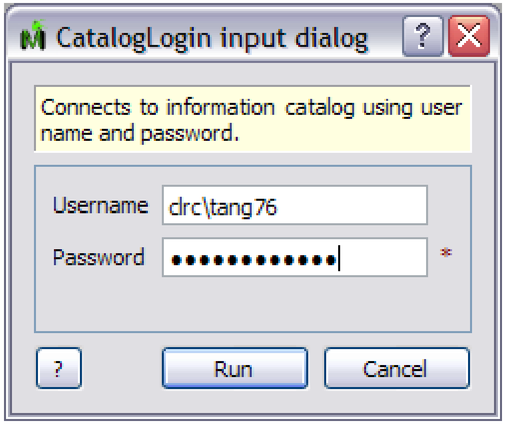
- During the experiement
- C# - ‘ICATIngest’
- Subscribes to Windows events
  `ReadDirectoryChangesW()`
- Invokes ‘WriteRaw’ and ‘NxIngest’
- Caches groups of files for performance

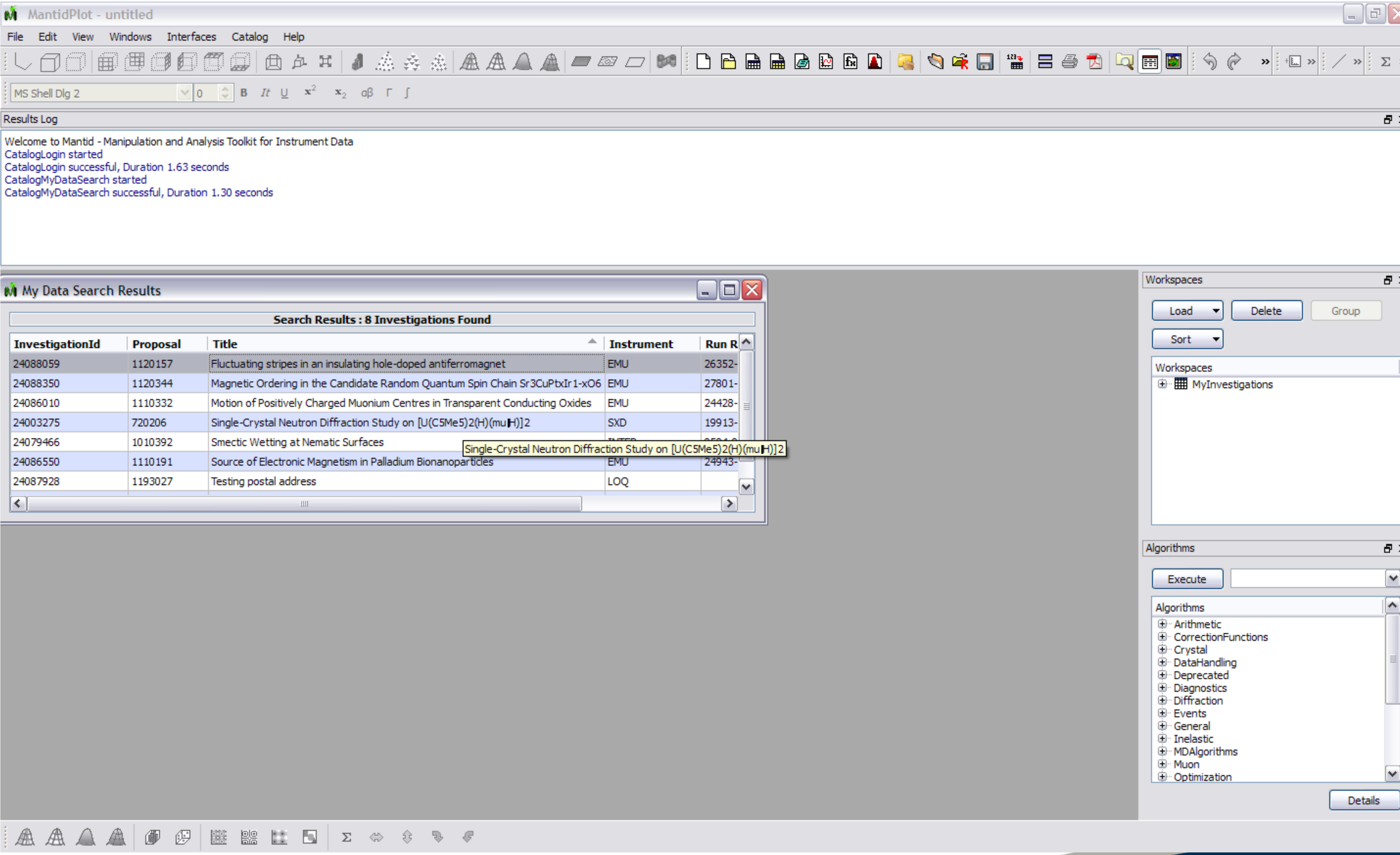
# Getting Data out - Web Access

- TopCAT interface (see Antony’s talk)
- Main point of access for ISIS data
- HTTP file serving
- Zipped or non-zipped

# Getting Data out - Mantid




CatalogLogin input dialog
Connects to information catalog using user name and password.
Username
clrc\tang76
Password
?
Run
Cancel

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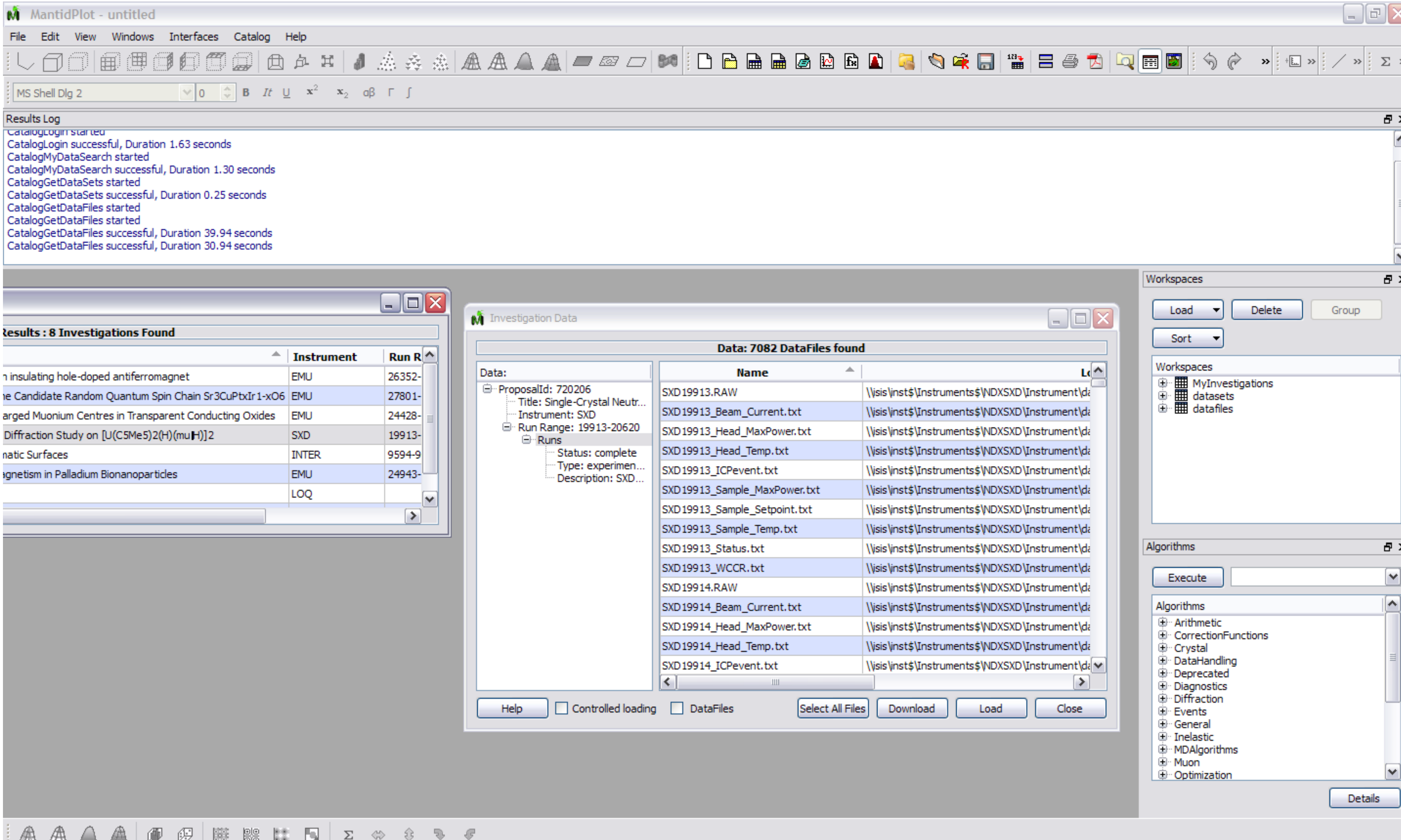
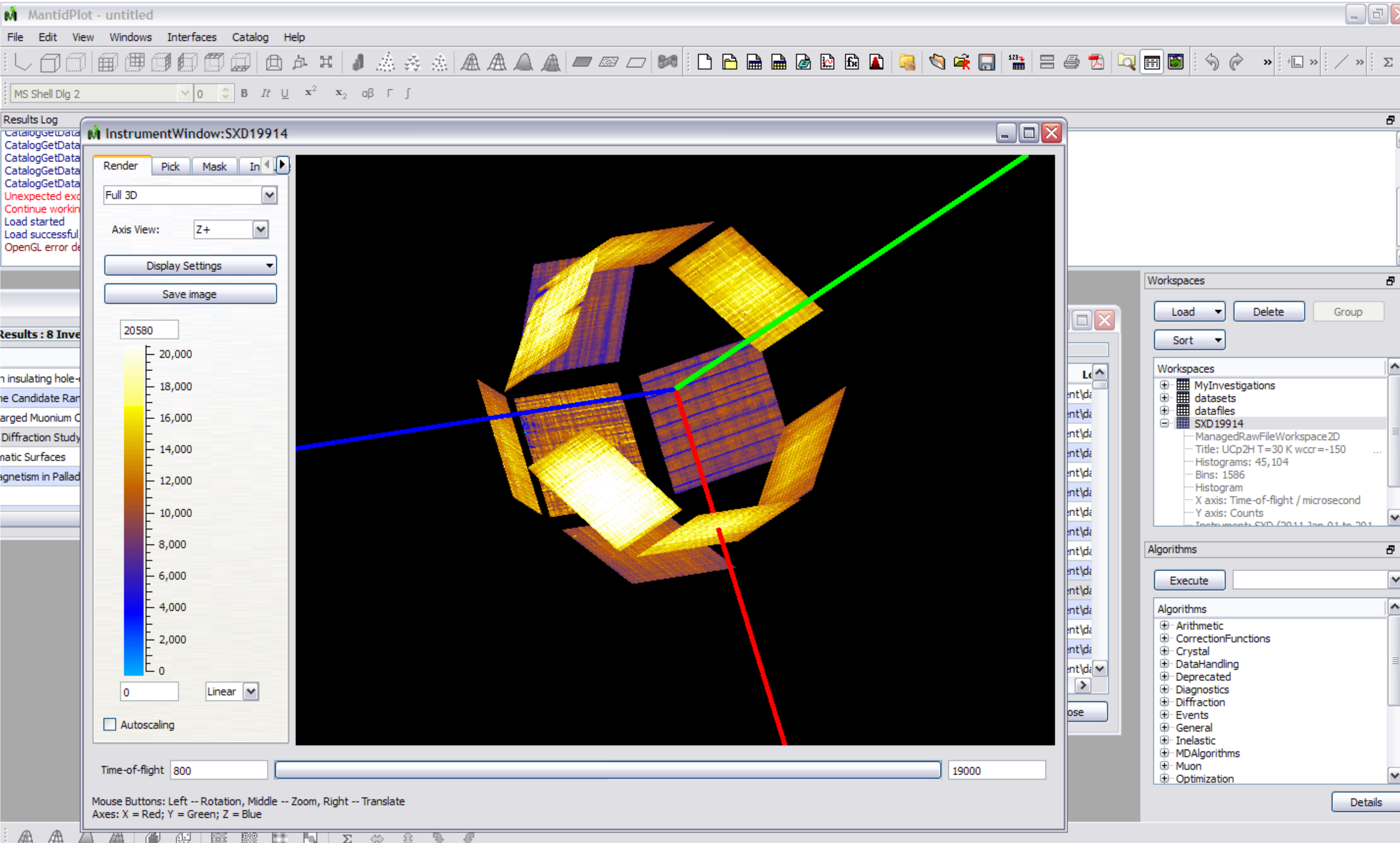

MantidPlot - untitled
File Edit View Windows Interfaces Catalog Help
MS Shell Dlg 2
Results Log
CatalogLogin successful, Duration 1.63 seconds
CatalogMyDataSearch started
CatalogMyDataSearch successful, Duration 1.30 seconds
CatalogGetDataSets started
CatalogGetDataSets successful, Duration 0.25 seconds
CatalogGetDataFiles started
CatalogGetDataFiles started
CatalogGetDataFiles successful, Duration 39.94 seconds
CatalogGetDataFiles successful, Duration 30.94 seconds
Results : 8 Investigations Found
Instrument
EMU
SXD
INTER
LOQ
Investigation Data
Data: 7082 DataFiles found
Data:
ProposalId: 720206
Title: Single-Crystal Neutr...
Instrument: SXD
Run Range: 19913-20620
Runs
Status: complete
Type: experimen...
Description: SXD...
Name
SXD19913.RAW
SXD19913_Beam_Current.txt
SXD19913_Head_MaxPower.txt
SXD19913_Head_Temp.txt
SXD19913_ICPevent.txt
SXD19913_Sample_MaxPower.txt
SXD19913_Sample_Setpoint.txt
SXD19913_Sample_Temp.txt
SXD19913_Status.txt
SXD19913_WCCR.txt
SXD19914.RAW
SXD19914_Beam_Current.txt
SXD19914_Head_MaxPower.txt
SXD19914_Head_Temp.txt
SXD19914_ICPevent.txt
Help
Controlled loading
DataFiles
Select All Files
Download
Load
Close
Workspaces
Load
Delete
Group
Sort
MyInvestigations
datasets
datafiles
Algorithms
Execute
Arithmetic
CorrectionFunctions
Crystal
DataHandling
Deprecated
Diagnostics
Diffraction
Events
General
Inelastic
MDAlgorithms
Muon
Optimization
Details

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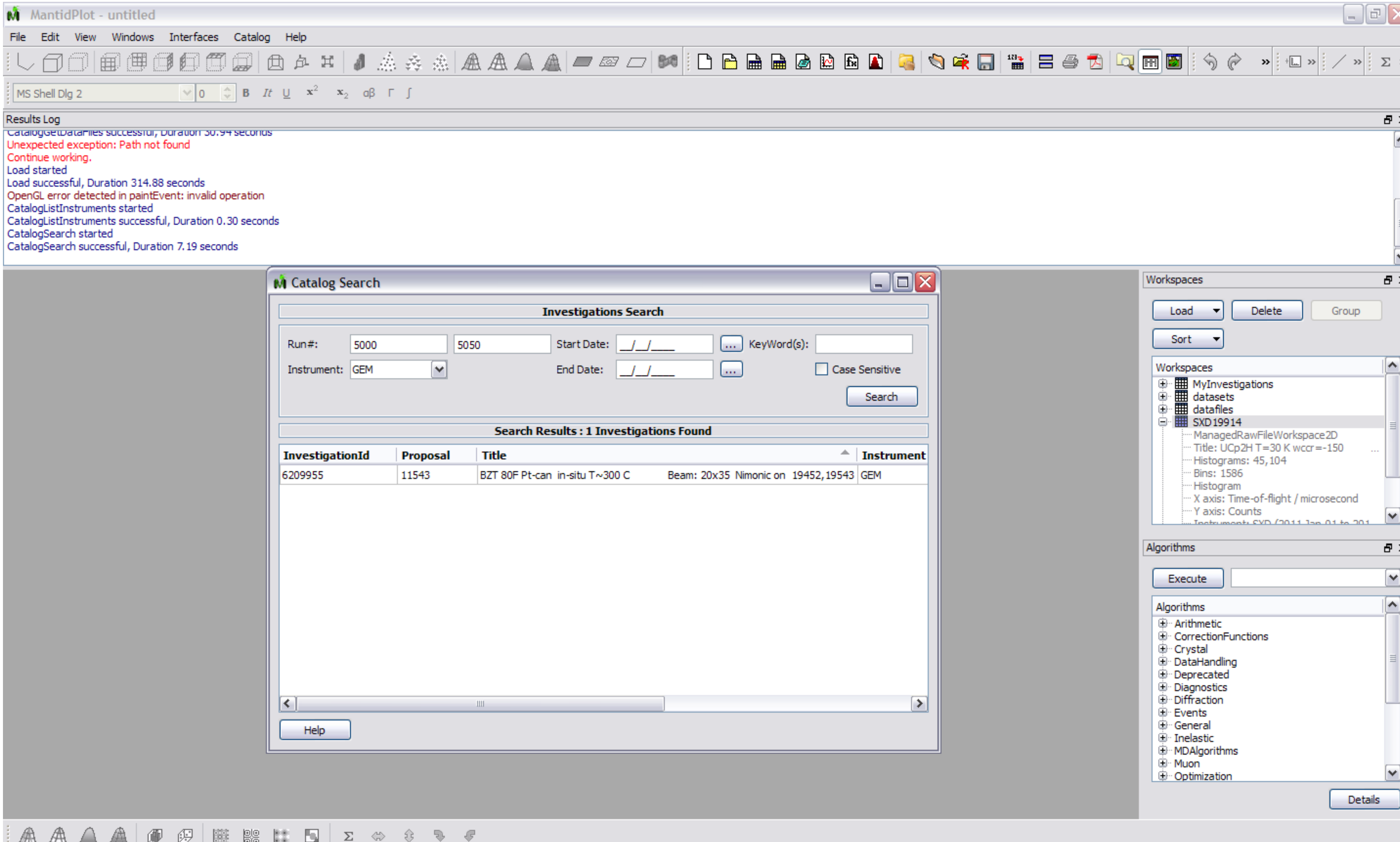


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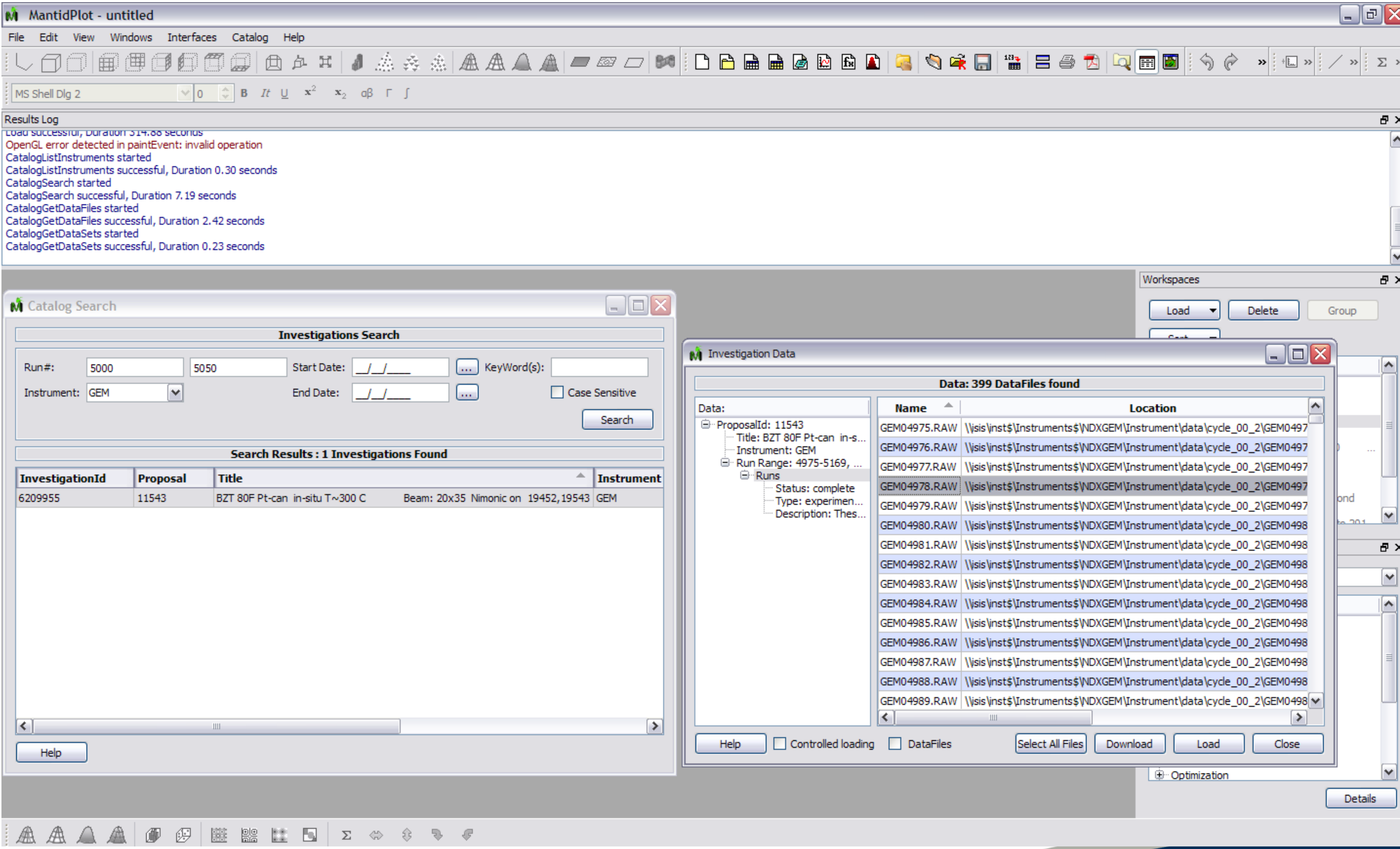


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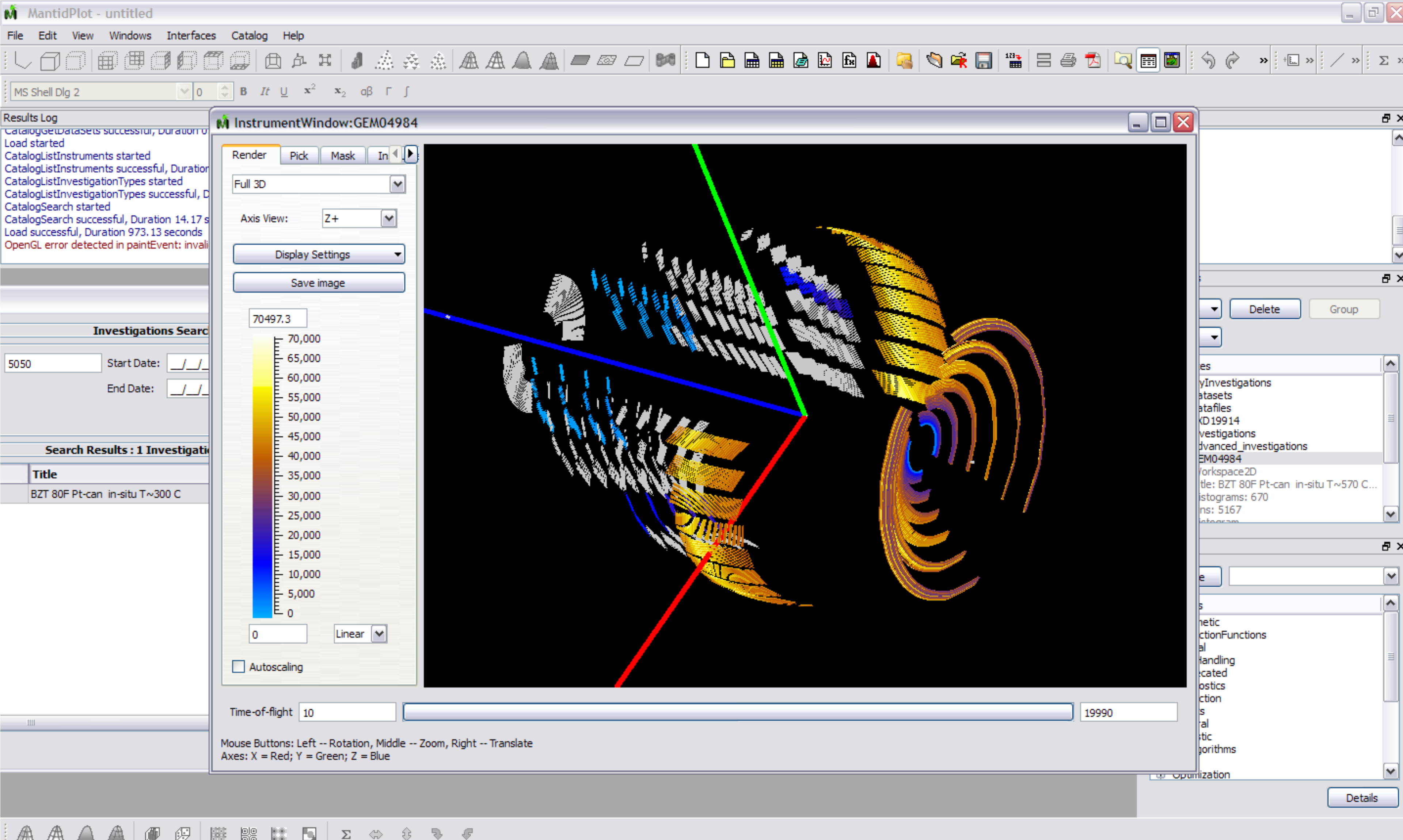
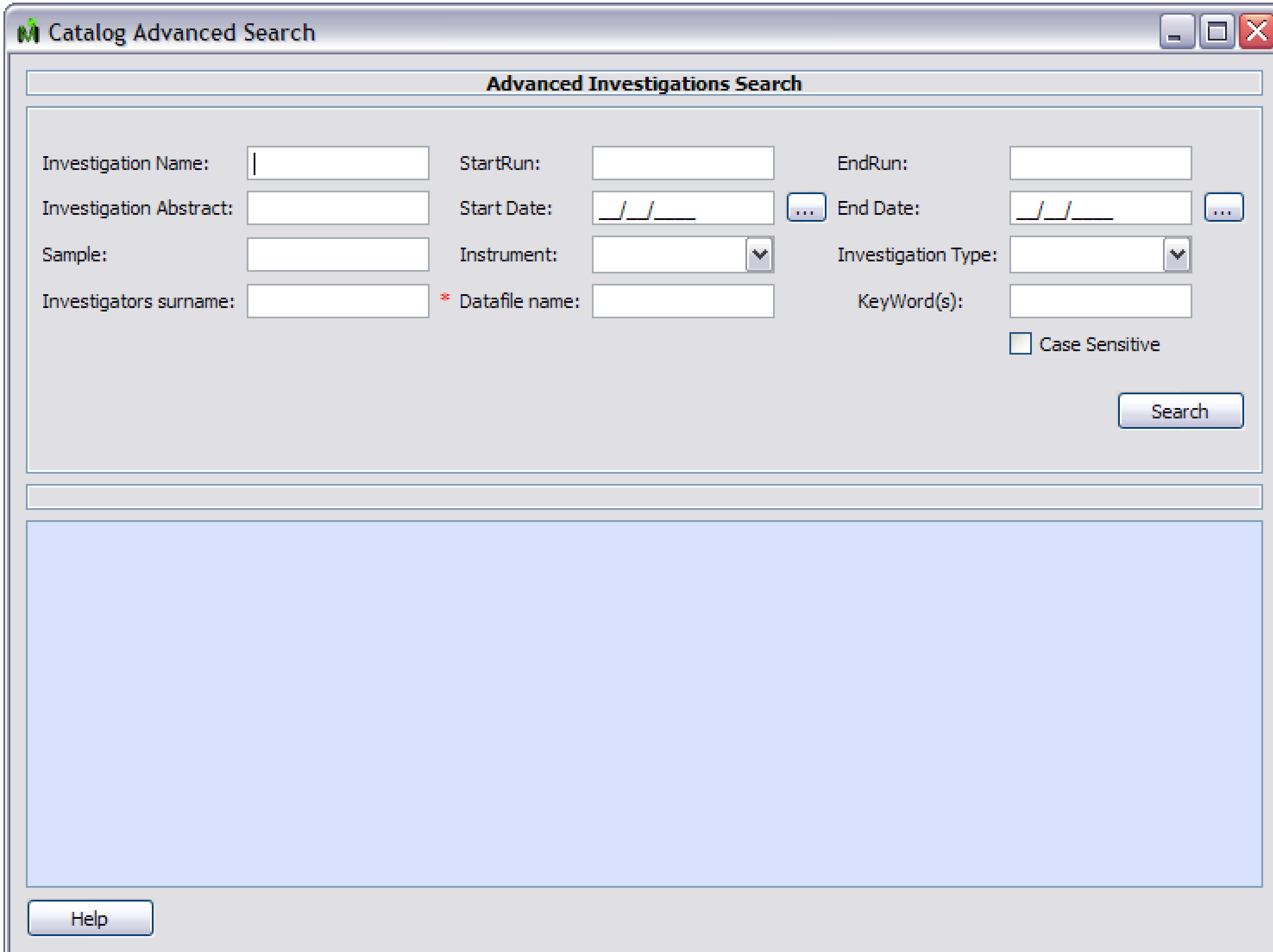

MantidPlot - untitled
File
Edit
View
Windows
Interfaces
Catalog
Help
MS Shell Dlg 2
Results Log
Load started
CatalogListInstruments started
CatalogListInvestigationTypes started
CatalogSearch started
OpenGL error detected in paintEvent: invali
Investigations Searc
5050
Start Date:
End Date:
Search Results : 1 Investigati
Title
BZT 80F Pt-can in-situ T~300 C
InstrumentWindow:GEM04984
Render
Pick
Mask
Full 3D
Axis View:
Z+
Display Settings
Save image
70497.3
70,000
65,000
60,000
55,000
50,000
45,000
40,000
35,000
30,000
25,000
20,000
15,000
10,000
5,000
0
0
Linear
Autoscaling
Time-of-flight
10
19990
Mouse Buttons: Left -- Rotation, Middle -- Zoom, Right -- Translate
Axes: X = Red; Y = Green; Z = Blue
Delete
Group
Details

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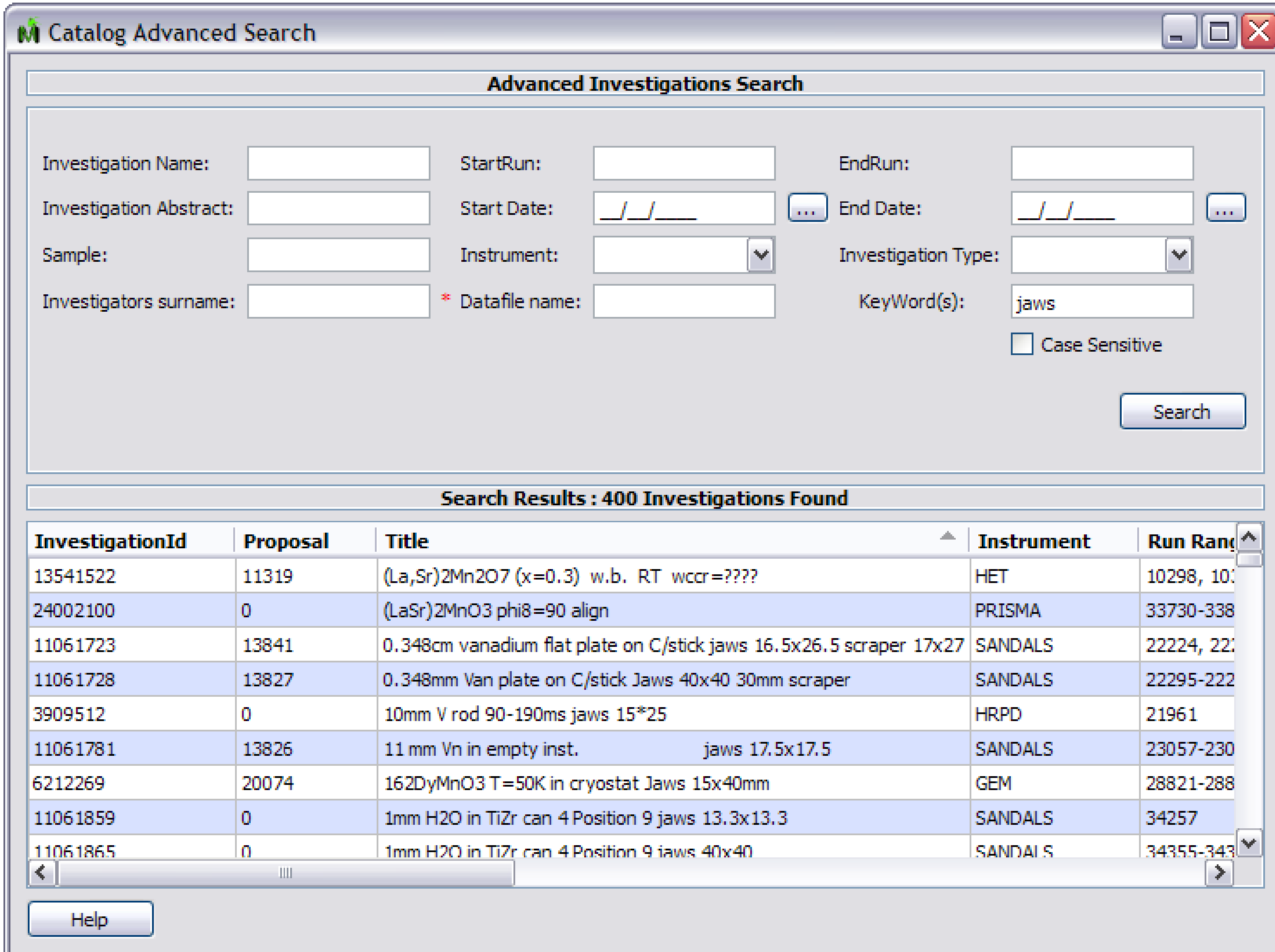


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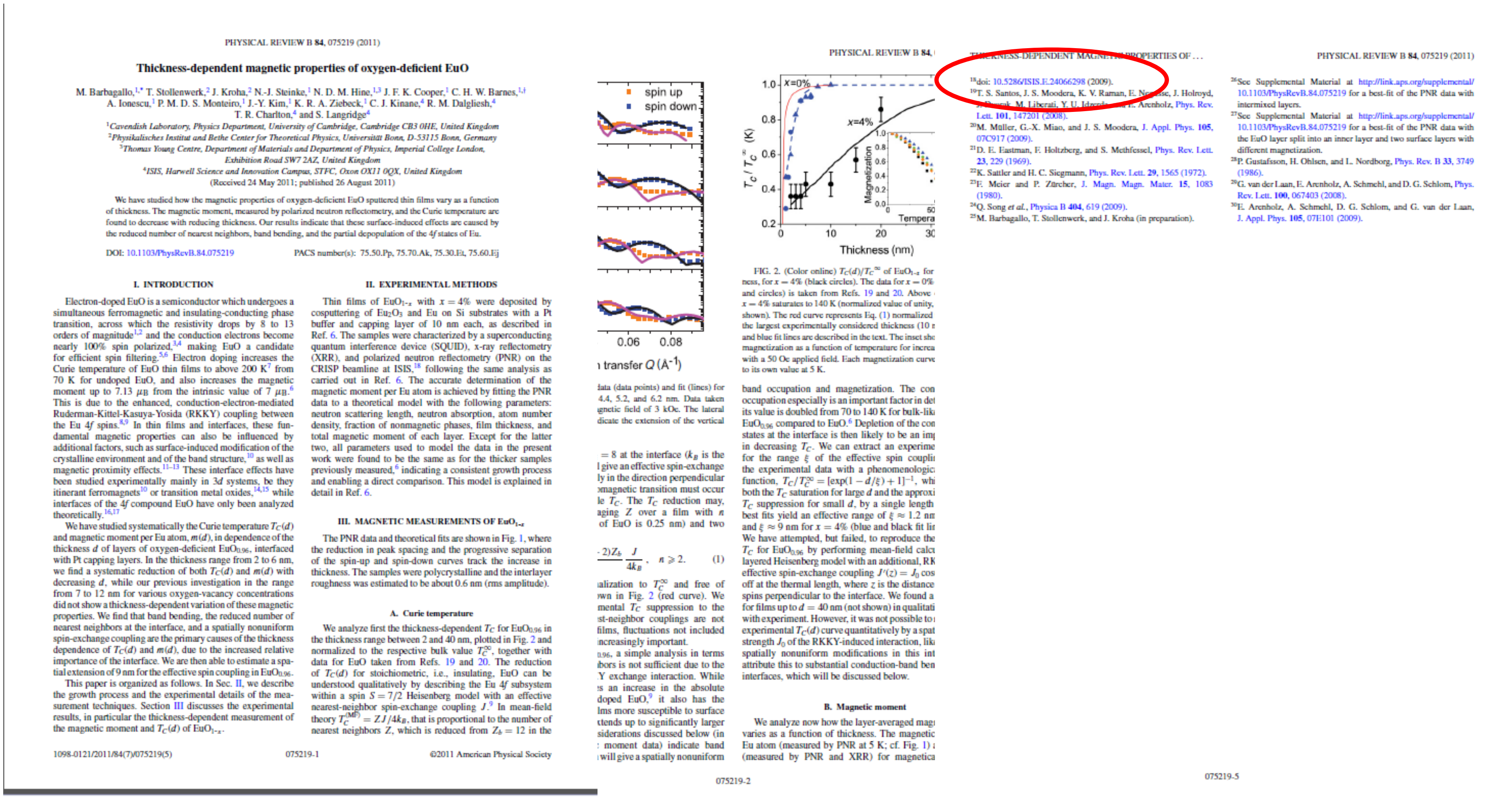
# DOIs – data citation

- Issued and sometimes used


PHYSICAL REVIEW B **84**, 075219 (2011)

**Thickness-dependent magnetic properties of oxygen-deficient EuO**

M. Barbagallo,[1,*] T. Stollenwerk,[2] J. Kroha,[2] N.-J. Steinke,[1] N. D. M. Hine,[1,3] J. F. K. Cooper,[1] C. H. W. Barnes,[1,†] A. Ionescu,[1] P. M. D. S. Monteiro,[1] J.-Y. Kim,[1] K. R. A. Ziebeck,[1] C. J. Kinane,[4] R. M. Dalgliesh,[4] T. R. Charlton,[4] and S. Langridge[4]

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We have studied how the magnetic properties of oxygen-deficient EuO sputtered thin films vary as a function of thickness. The magnetic moment, measured by polarized neutron reflectometry, and the Curie temperature are found to decrease with reducing thickness. Our results indicate that these surface-induced effects are caused by the reduced number of nearest neighbors, band bending, and the partial depopulation of the 4*f* states of Eu.

DOI: 10.1103/PhysRevB.84.075219 PACS number(s): 75.50.Pp, 75.70.Ak, 75.30.Et, 75.60.Ej

**I. INTRODUCTION**

**II. EXPERIMENTAL METHODS**



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[27] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.84.075219 for a best-fit of the PNR data with the EuO layer split into an inner layer and two surface layers with different magnetization.
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# Our priorities

- Upload published (derived) data
- Managing permissions
  - Data owner admin features
- Integration with Mantid/analysis process
- (Upgrade from 3.3 to 4.1)

# Questions...