
ESRF
The European Synchrotron

PANDATA SOFTWARE CATALOGUE

https://software.pan-data.eu/

The PaNdata software catalogue is a database of software available at the ESRF, ILL and other facilities, and used mainly for data analysis of neutron and photon experiments.

Result of a close collaboration with ILL (IT Services, especially Jamie Hall)

THE DATA ANALYSIS SOFTWARE CATALOGUE AS A DAAS DELIVERABLE

The Software Catalogue is one of the DaaS deliverables (s. DM-775/D RB/HR/JS 18) for the upgrade phase II

The targeted software should be used or recommended by beamlines.

Important items like software documentation, sample input data, supported data formats and operating systems, etc. have to be provided.

This catalogue is meant for both internal and external users and features multiple search criteria.

SOFTWARE CATALOGUE OBJECTIVES FOR THE ESRF

Data analysis software has a key function in the workflow which converts raw experimental data into publishable scientific output.

The catalogue is to cater for the most appropriate software to the benefit of the ESRF users community.

The main objectives are:

- facilitate and consolidate the conversion of raw data into premier quality data for scientific publication

- speed up the deployment and use of up-to-date data analysis algorithms which can pave the way to new science at the ESRF

- enhance and optimise the scientific production of the ESRF, i.e. increase its visibility toward the public bodies representing tax payers across member countries

CATALOGUE CONTENTS

Main purposes:

provide a web-based guide for users to where they find a given software package and how they can run it (at least in its basic mode)

provide Data Analysis as a Service for the entries in the SW catalogue e.g. via the PaNDaaS project (future EU project : http://pan-data.eu/node/103)

Search keywords for filtering out software:

- **Name of the software**
- **Institutes (currently only ESRF, ILL and ALBA)**
- **Instruments/beamlines**
- **Software categories**
- **I/O formats**
- **Languages**
- **Platforms**
- **Licences**

SUMMARY OF MAIN SCIENTIFIC AREAS AND SOFTWARE

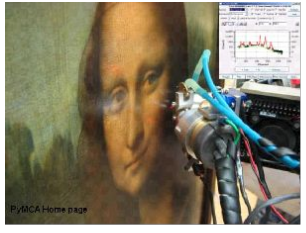
Main scientific areas:

- Diffraction/scattering
- Spectroscopies
- Imaging
- Optics

Main software sections:

- Data analysis/data reduction
- Modelling/simulation
- Data bases
- Libraries
- GUIs
- Visualisation
- Utilities

A TYPICAL VIEW (1)



PyMca

X-ray Fluorescence Toolkit (visualization and analysis of energy-dispersive X-ray fluorescence data). . The program allows both interactive and batch processing of large data sets and is particularly well suited for X-ray imaging. Its implementation of a complete description of the M shell is particularly helpful for analysis of data collected at low energies. It features, among many other things, the fundamental parameters method

Website	https://github.com/vasole/pymca
Licenses	MIT License
Categories	Data analysis Visualization Data reduction XRF
Software Requirements	-
Hardware Requirements	-
Platforms	Mac OS Linux Windows
Languages	C C++ Python
Input Formats	HDF5 TIFF CSV EDF HDF JCAMP-DX SPS SPEC
Output Formats	NeXus TIFF CSV EDF JPEG PNG SPEC
Contact email	pymca-users@lists.sourceforge.net

How-to

Installed on the central cluster; callable via:

```
>pymca
```

Warning: the SPEC file names in PyMca might have the following extensions: *.dat, *.mca, *.dat

A TYPICAL VIEW (2)

Documentation / Tutorials

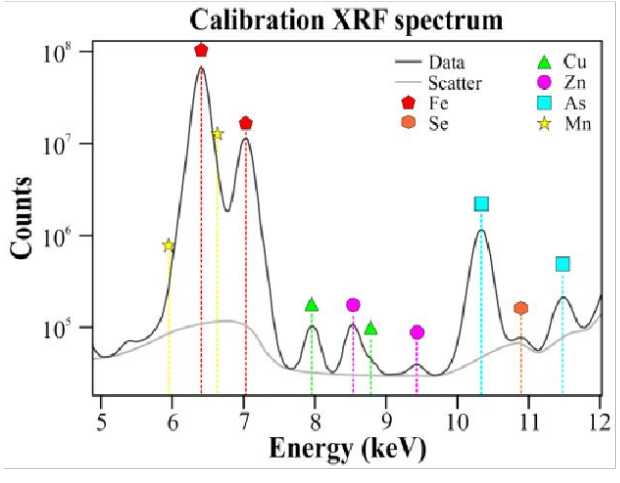
Documentation and tutorials: http://pymca.sourceforge.net/documentation.htm

References

Spectrochim. Acta Part B 62 (2007) 63-68 V.A. Solé, E. Papillon, M. Cotte, Ph. Walter, J. Susini, *"A multiplatform code for the analysis of energy-dispersive X-ray fluorescence spectra"*

Instruments BM31 (ESRF) BM05 (ESRF) BM08 (ESRF) BM20A (ESRF) BM20B (ESRF) BM23 (ESRF) BM25A (ESRF) BM26A (ESRF) BM30B (ESRF) ID01 (ESRF) ID03 (ESRF) ID10 (ESRF) ID11 (ESRF) ID12 (ESRF) ID13 (ESRF) ID16A-NI (ESRF) ID16B-NA (ESRF) ID18 (ESRF) ID20 (ESRF) ID21 (ESRF) ID24 (ESRF) ID26 (ESRF) ID32 (ESRF)

- Screenshots
- Hosting institutes
- Example datasets



PRESENT STATE

For the time being, altogether 85 entries (partly shared)

- 22 ILL
- 5 ALBA
- 62 ESRF

These figures are about to grow, as new entries are being prepared/contributed

IMPORTANT!!: By registering and logging-in, new software can be entered and it will appear in the database after moderation.

Future work:

- Extending or customizing the **Howto's** and getting other institutes in Europe to participate
- Continuous update of current entries - addition of new entries
- Taking into account users suggestions, on e.g. missing features: please, test it!
- Layout upgrade

ARE YOU READY TO COLLABORATE ON THE SOFTWARE CATALOG ?

CHALLENGE: Collaborating on the Software Catalog requires little effort but will demonstrate our ability to work together on Data Analysis Software. This is an important step in collaborating on Data Analysis as a Service.