



MOLECFIT Experimental version

Paola Popesso - 2024-03-15 - Comments (0) - Data processing and analysis software resources

MOLECFIT Experimental version

The MOLECFIT Experimental versions implement improvements and changes relative to the current Public Release versions.

However as an experimental version, it may also include bugs, so **user beware, use at your own risk...**

Note the [experimental support for additional instruments](#) will also work for the public release version.

This experimental version now also includes experimental versions of the **FORS** and **XSHOOTER** pipelines & workflows that integrate telluric correction into the workflows, a version of the **GIRAFFE** pipeline & workflow that fixes a number of issues that show up for the latest versions of python modules such as matplotlib as experienced by up-to-date macPorts systems and a version of the **UVES** pipeline & workflow that fixes an problem preventing 2-D extraction.

This experimental version is generally used to test improved user friendliness and support for additional instruments of the Molecfite pipeline and workflow, and telluric correction for other instruments. New features will generally be incorporated into the official versions at the next ESO pipeline annual public release update (usually in May of each year).

The latest release of this experimental version is release-58@2024-03-15T08:10:33+0000, including the following packages, that may differ from the currently available [Public Release versions](#) (i.e the versions here may be pre-release versions not yet fully verified and include modifications specific to this release channel, **use at your own risk!**):

fors 5.6.8b.58

giraf 2.16.11.58

kmos 4.4.2.58

uves 6.4.1.58

xshoo 3.6.3.58

molecfite 4.3.2.58

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Please follow the instructions below to install it.

First, make sure you have the software pre-requisites required for "[pipeline source installations](#)" and "[KMOS and Molecfit pipeline source installations](#)", see [here](#).

In addition, to the standard software pre-requisites, the experimental versions have the following additional pre-requisites:

- FORS
 - OpenBLAS: (MacPorts package OpenBLAS, RPM package openblas-devel, Debian package libopenblas-dev)

Once all pre-requisites are installed, install as follows:

```
bash
INSTALL_DIR=${HOME}/pipelines/exp_reflex/$(date +%Y-%m-%d)
mkdir -pv ${INSTALL_DIR}
cd ${INSTALL_DIR}
curl -O
https://ftp.eso.org/pub/usg/molecfit/install_experimental_esoreflex
env -i PATH=$(getconf PATH) bash ./install_experimental_esoreflex
```

On macOS, if you have used MacPorts to satisfy the [Software Prerequisites](#), then replace the last line with:

```
env -i PATH=/opt/local/bin:$(getconf PATH) bash
./install_experimental_esoreflex
```

On macOS, if you have used HomeBrew to satisfy the [Software Prerequisites](#), then replace the last line with:

```
env -i PATH=/opt/homebrew/bin:$(getconf PATH) bash
./install_experimental_esoreflex
```

On macOS

If you have Xcode Version 15.0 or more recent you'll need an extra setting for LDFLAGS if you want to install the fors PL+WKF,

```
env -i LDFLAGS=-ld_classic PATH=...
```

Also note that the present version of the software is not compatible with the gcc13. In case you feel obliged to use a gcc compiler (rather than the Apple clang compiler) -- and this is recommended if you want to install the FORS pipeline -- then please use gcc12 or older, e.g. assuming you get gcc12 from MacPorts:

```
env -i CC=gcc-mp-12 CXX=g++-mp-12 LDFLAGS=-ld_classic
PATH=/opt/local/bin:$(getconf PATH) bash
./install_experimental_esoreflex
```

To run the experimental workflows

Use the following commands:

```
${INSTALL_DIR}/install/bin/exp_esoreflex molecfit  
${INSTALL_DIR}/install/bin/exp_esoreflex fors_spec_molecfit  
${INSTALL_DIR}/install/bin/exp_esoreflex xshooter_molecfit
```

You should try running the workflow on the tutorial data for one or more instruments.
Simply start up the workflow and click the "play" button to run the tutorial for XSHOOTER.
To try other instruments, just change the instrument name in the main canvas.

Please create a ticket if you have any trouble with the installation or running the tutorial.

Please understand though, that as this is a "use at your own risk" experimental version, your ticket may not be handled as quickly as it would be for the Public Release version.

Experimental support for additional instruments

Experimental support can be added to the *public* and this development version as follows:

CRIRES

To add experimental support for CRIRES, do the following:

```
curl -O  
https://ftp.eso.org/pub/usg/molecfit/user_instruments/CRIRES.tgz  
tar -C ${HOME} -zxvf $(pwd)/CRIRES.tgz
```

Then set the INSTRUMENT variable in the molecfit main canvas to CRIRES to use.

SINFONI

To add experimental support for SINFONI, do the following:

```
curl -O  
https://ftp.eso.org/pub/usg/molecfit/user_instruments/SINFONI.tgz  
tar -C ${HOME} -zxvf $(pwd)/SINFONI.tgz
```

Then set the INSTRUMENT variable in the molecfit main canvas to SINFONI to use.

HARPS and HARPN

To add experimental support for HARPS, do the following:

```
curl -O  
https://ftp.eso.org/pub/usg/molecfit/user_instruments/HARPS.tgz  
tar -C ${HOME} -zxvf $(pwd)/HARPS.tgz
```

Then set the INSTRUMENT variable in the molecfit main canvas to HARPS to use.

To add experimental support for HARPN, do the following:

```
curl -O  
https://ftp.eso.org/pub/usg/molecfit/user_instruments/HARPN.tgz  
tar -C ${HOME} -zxvf $(pwd)/HARPN.tgz
```

Then set the INSTRUMENT variable in the molecfit main canvas to HARPN to use.

Tags

ESO software

molecfi

pipeline

software installation