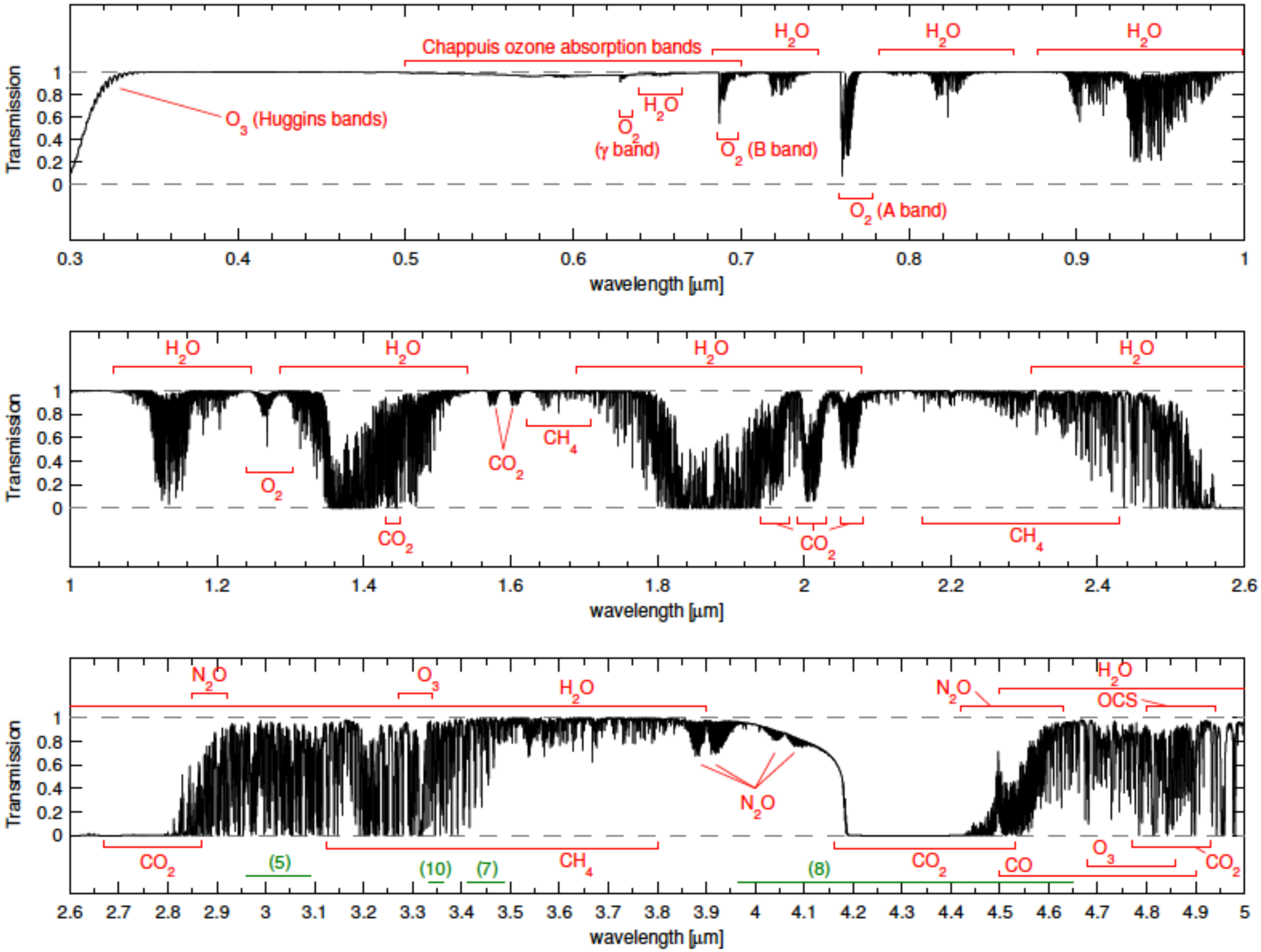
Molecfit

A. Smette, H. Sana, H. Horst, W. Kausch, S. Noll, S. Kimenswenger, M. Barden, C. Szyszka, A.M. Jones, A. Gallenne, J. Vinther, P. Ballester, J. Taylor

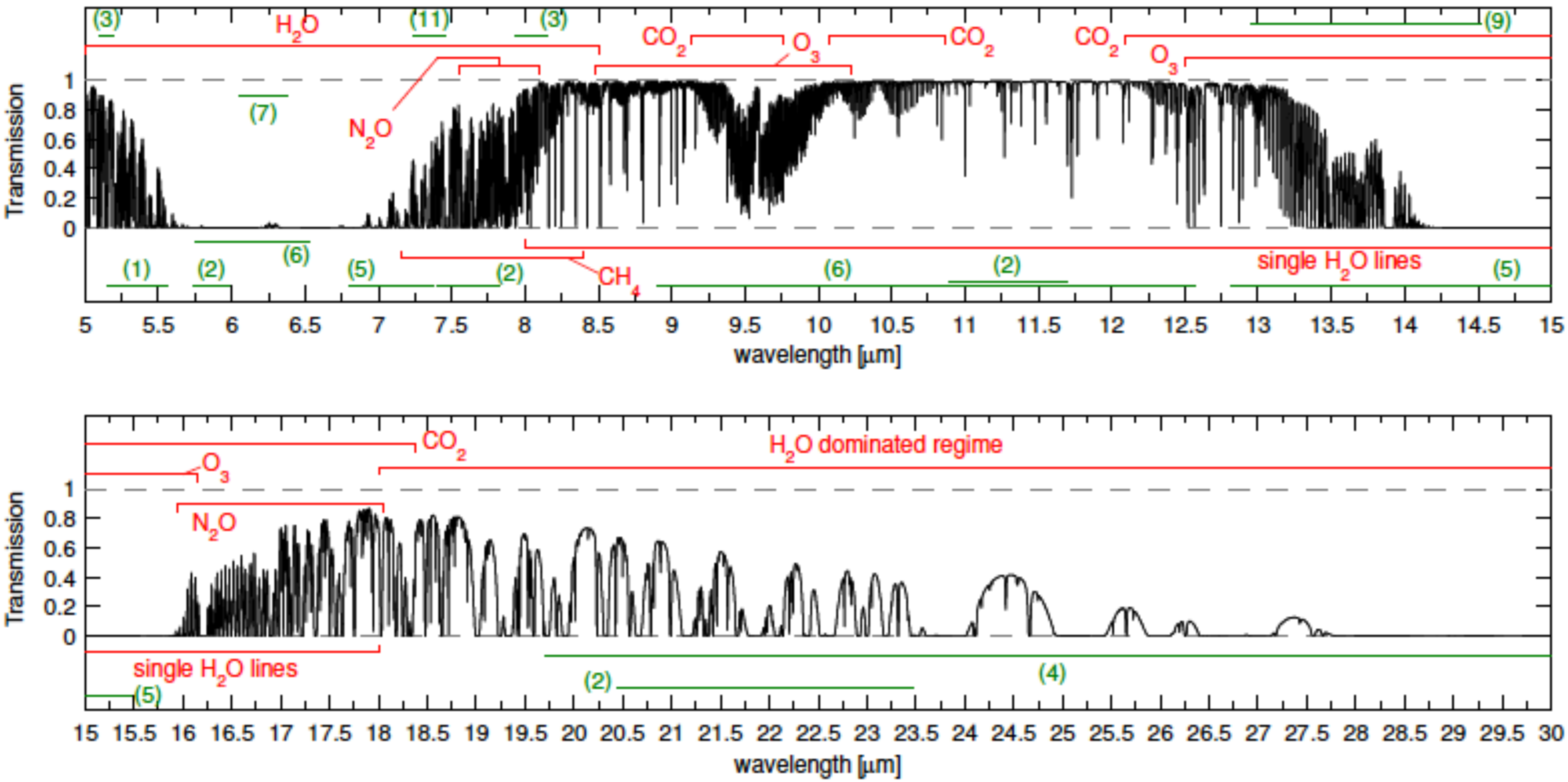
Content

- Introduction
- Molecfit
- Accuracy
- Examples
- Conclusion

Transmission spectrum (U to M bands)



Transmission spectrum (L, M, N, Q bands)



(1) NO; (2) HNO3; (3) COF2; (4) H2O2; (5) HCN; (6) NH3; (7) NO2; (8) N2; (9) C2H2; (10) C2H6; (11) SO2

Consequences for observation

- All images and spectra are affected
- Impact depends on
  - wavelength band
  - column density of various molecules on the line-of-sight during observation:
    - exact time of observation
    - airmass
  - state of the atmosphere at the time of observations
    - temperature profile
    - pressure profile
- Information can only be recovered for telluric lines that show at most small saturation:
  - If the information does not reach the telescope, there is no way to recover it!

Usual method: observation of telluric star

- Procedure:
  - Selection of
    - Rapidly rotating early-type star (B0V - B9V): mostly featureless (except for H lines)
    - G2V star (for scientifically interesting features close to H lines)
  - Observations must be done:
    - close in time: to avoid atmospheric variations;
    - close in airmass: different lines behave differently with airmass;
    - to reach a SNR significantly larger than science target;
  - At ESO: practical rule is usually *`within 2 h and with maximum airmass difference of 0.2'*. However,
    - water vapor content can change considerably within 2h,
    - 0.2 airmass difference => 20% difference for un-saturated lines!

Observation of telluric star: pros and cons

- Pros:
  - if done close in time, small airmass difference (<0.01), same illumination of the spectrograph: very good correction, as instrumental effects are taken into account;
- Cons:
  - Significant time spent on calibration instead of science, in particular for bright targets or for observations over large airmass;
  - Telluric stars can appear as badly chosen only after data reduction; creating/maintaining catalogue of 'good' stars difficult;
  - Even a good star may not be suitable for archival spectra (e.g., if different from planned one).
  - Conditions (water vapor content, seeing) can change fast between science and telluric star observations;
    - Difference in seeing can lead to change in instrumental line spread function.
    - Worst case: dome forced to be closed!

Synthetic spectra

- Requires:
  1. good to excellent representation of instrumental line spread function;
  2. accurate radiative transfer calculation.
  3. complete and accurate database of molecular line parameters;
  4. accurate determination of column density (volume mixing ratio) along the line-of-sight through atmosphere for each molecule.

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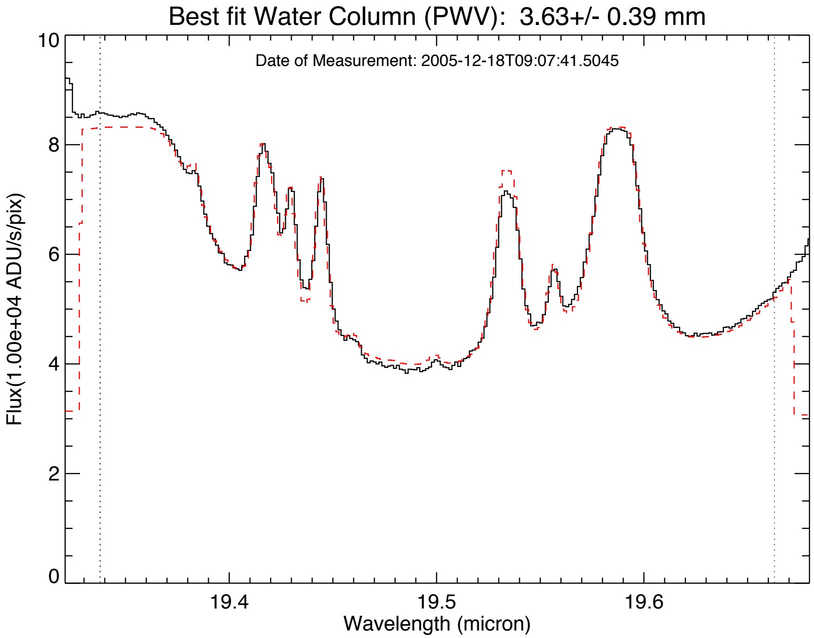
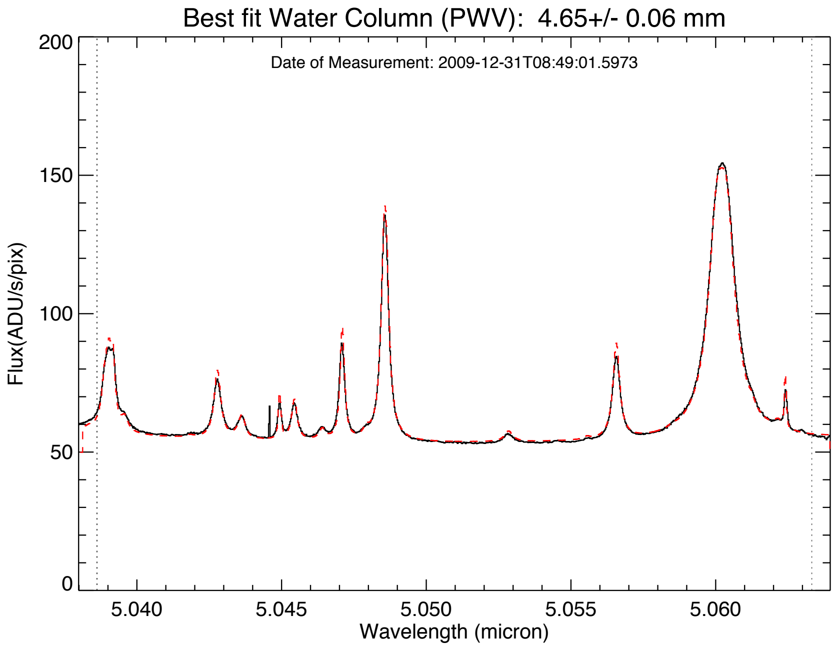
Molecfit

- Follow-up of a method to determine amount of water vapor for VISIR then CRIRES





Measuring the amount of precipitable water vapour with VISIR by Smette, A., Horst, H., Navarrete, J. 2007,Proceedings of the 2007 ESO Instrument Calibration Workshop,Springer-Verlag series "ESO Astrophysics Symposia", eds. F. Kerber & A. Kaufer

Molecfit

- IDL prototype initially developed over several years, mainly for CRIRES spectra;
- Provided to Austrian in-kind team at Innsbruck for further development/integration in ESO standards
- Papers:
  - *Molecfit: A general tool for telluric absorption correction I. Method and application to ESO instruments* A. Smette, H. Sana, S. Noll, H. Horst, W. Kausch, S. Kimeswenger, M.Barden, C. Szyszka, A. M. Jones, A. Gallene, J. Vinther, P. Ballester and J. Taylor (2015, A&A 576, A77)
  - *Molecfit: A general tool for telluric absorption correction II. Quantitative evaluation on ESO-VLT/X-Shooter spectra* W. Kausch, S. Noll, A. Smette, S. Kimeswenger, M. Barden, C. Szyszka, A. M. Jones, H. Sana, H. Horst, and F. Kerber, (2015, A&A 576, A78).
- Code available: http://www.eso.org/sci/software/pipelines/skytools/molecfit

Molecfit: components

- Instrumental line-spread function:
  - Offers a choice of models,
  - Model can be fitted on data; linear dependence on wavelength can be chosen;
  - Alternatively:
    - User-provided line spread function,
    - User-provided line spread function for each pixel of spectrum (since v1.1)

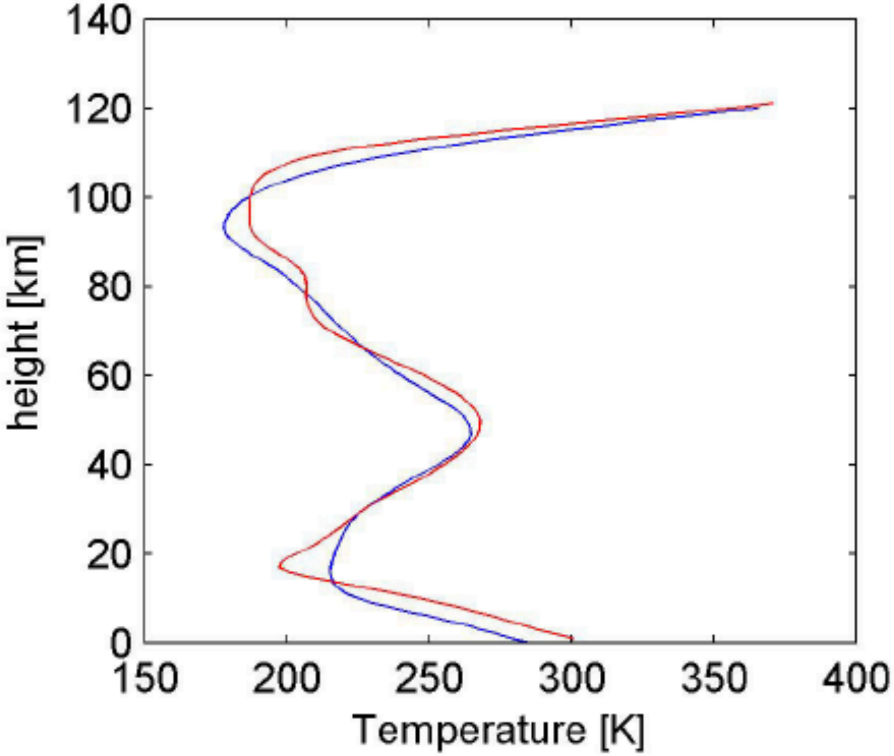
Molecfit: components

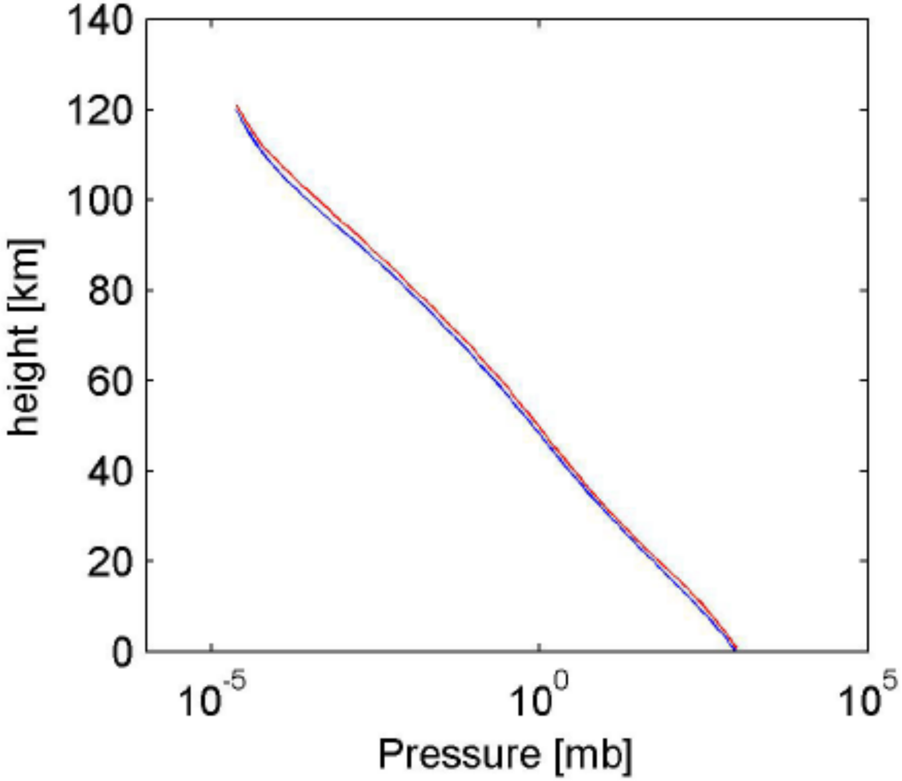
- Radiative transfer calculation:
  - Uses LBLRTM (a number of comparisons were done with RFM).
- Database of molecular line parameters
  - HITRAN based,
  - Alternatively, user can provide its own.

Molecfit: components

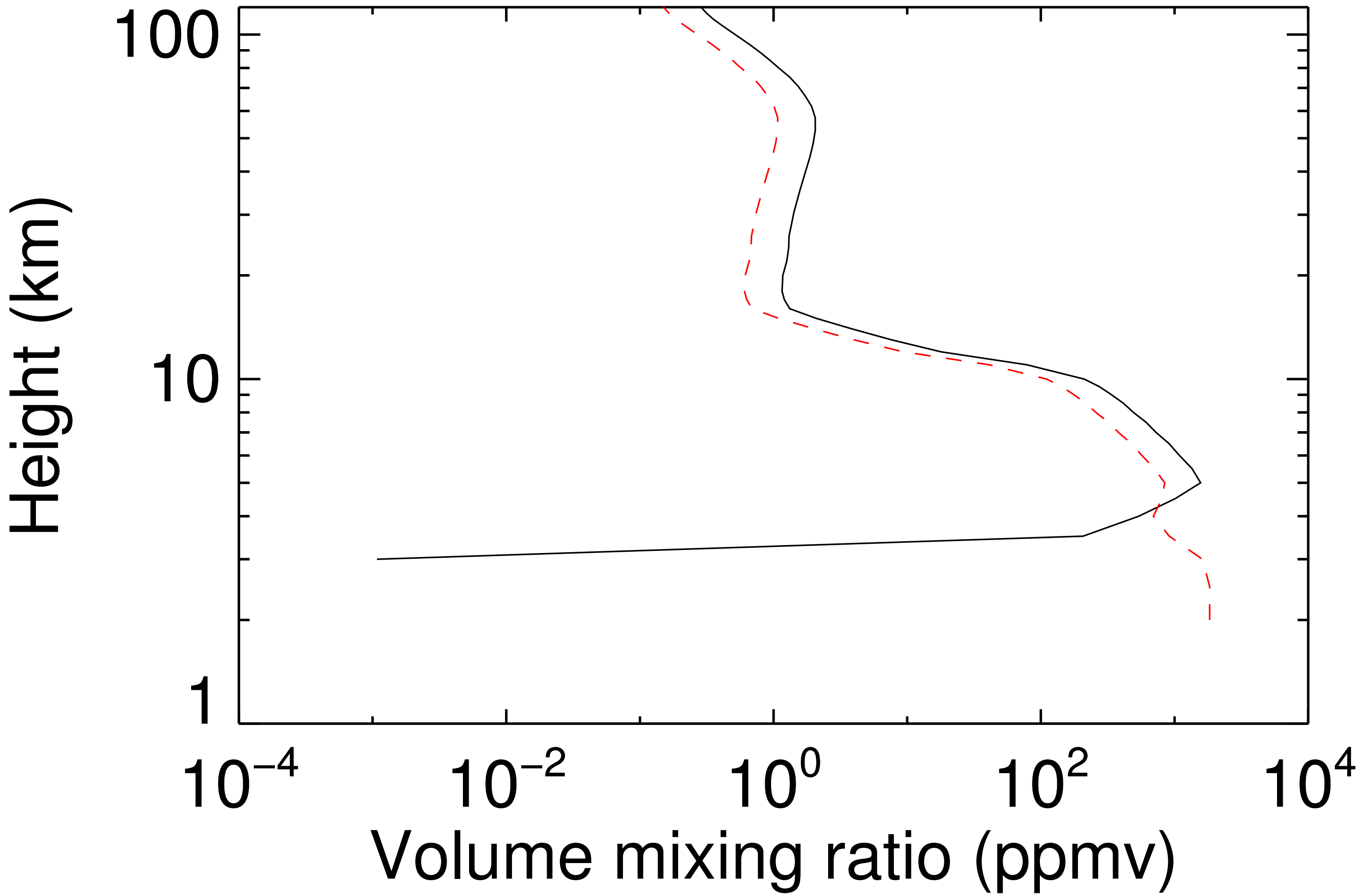
- Atmospheric profiles (variation of T, p, volume mixing ratio of molecules);
  - For molecules but H2O, and T, p above 25 km: typical profile (for Paranal, use equatorial);
  - For T, p, H2O, from 0 to ~ 25 km: retrieve GDAS profile from meteo server for time and location of the observation
  - Incorporate on-site measurements for T and p up to ~ 5 km.
  - Molecfit then adjusts the column density (volume mixing ratio) for each molecule to the observed science spectrum using C version of the least-squares fitting library MPFIT (Markwardt 2009, based on MINPACK-1, Moré 1978)

Examples of atmospheric profiles

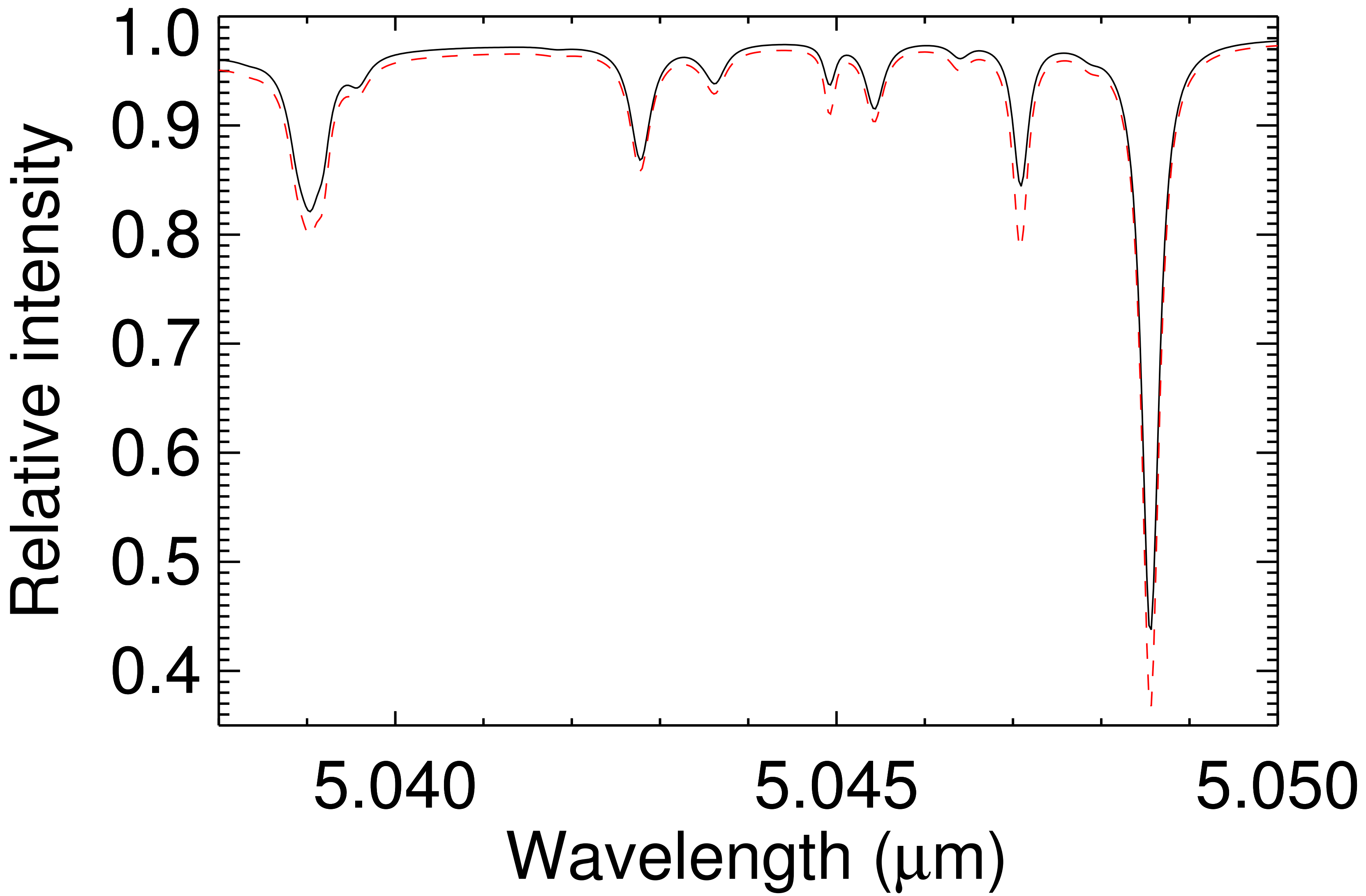




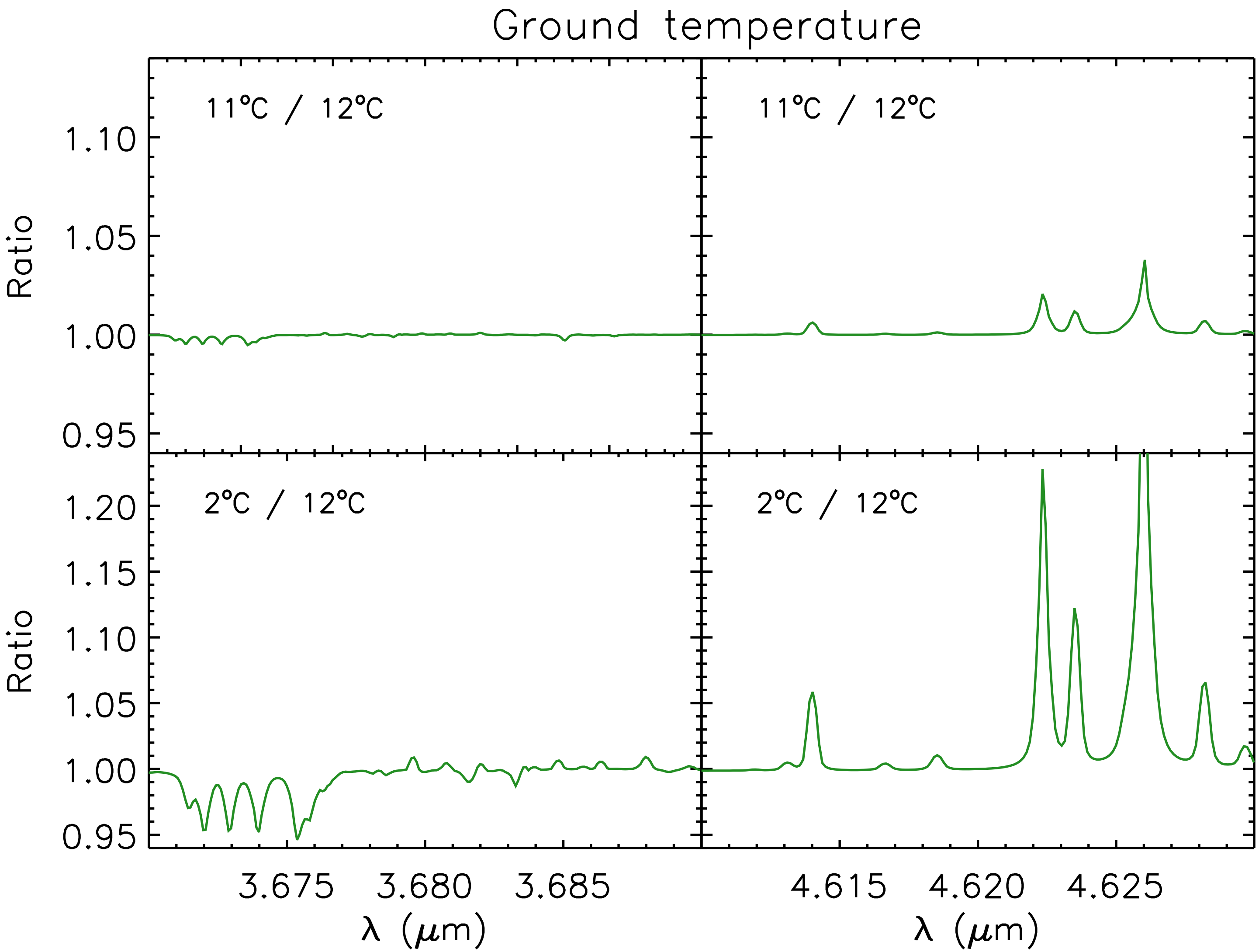
Influence of H_2O profile



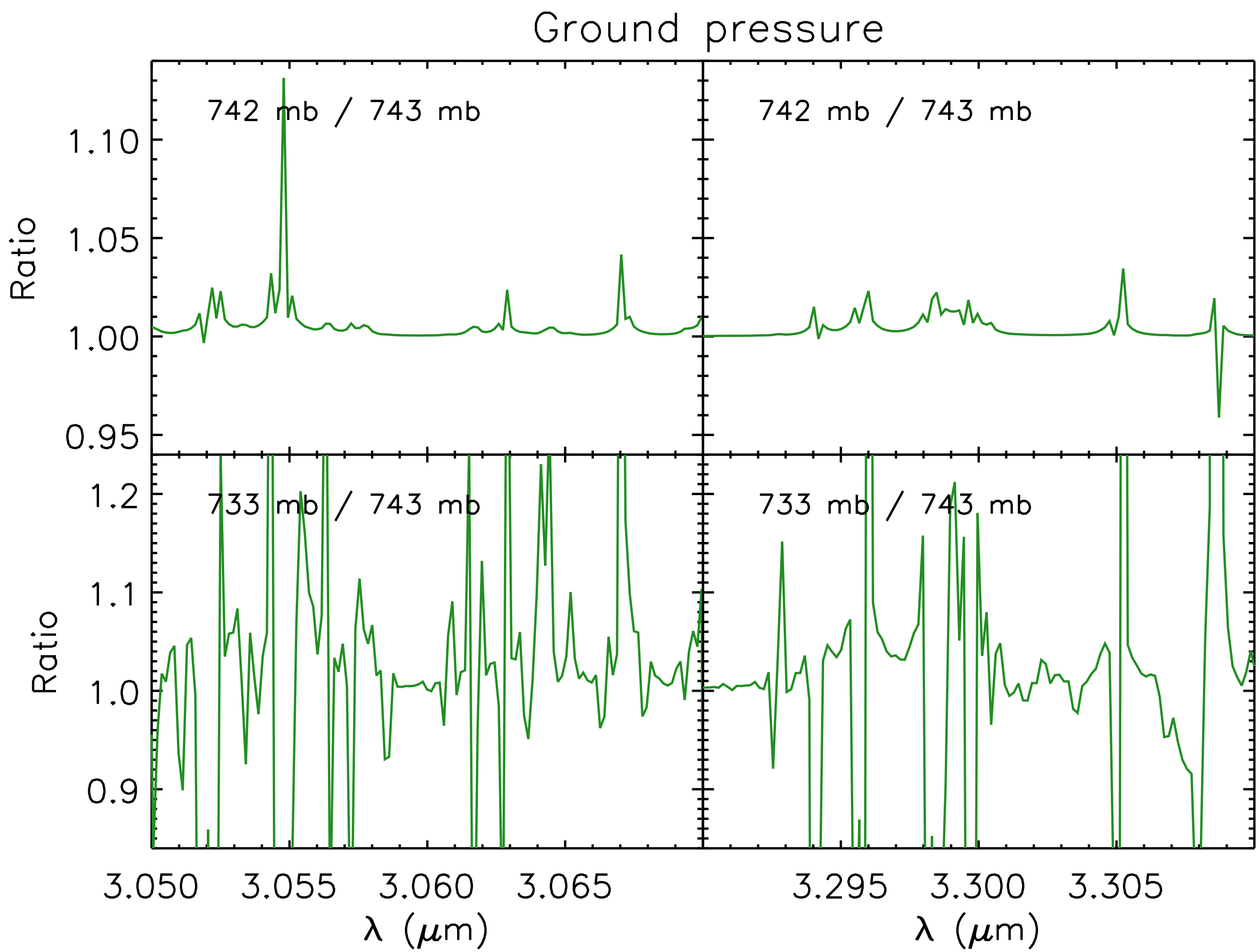
Influence of H2O profile



Ground temperature



Ground pressure



Inputs: Inclusion/exclusion regions

- Inclusion regions used to determine
  - Volume mixing ratio of the molecules involved
  - parameters of the line spread function
- Exclusion regions used to exclude
  - ’bad’ pixels
  - features intrinsic to the science target
  - can be expressed in pixels or in wavelengths

Inputs: starting values for continuum and wavelength calibration in inclusion regions

- Continuum contribution:
  - Low degree polynomial over each inclusion region
- Wavelength calibration:
  - Assumed to be correct for the whole spectrum
  - However, low degree Chebyshev polynomial can be used to correct for inaccuracies on each inclusion region
  - In some cases (telluric covering the whole spectrum, like CRIRES), can be used to produce a new wavelength calibration

Inputs: line spread function

- Line spread function:
  - Choice or combination of:
    - Boxcar
    - Gaussian
    - Lorentzian
  - Parameters for chosen model
  - Possibility to tell that FWHM increases lineary with wavelength
  - Alternatively, user-provided LSF, either
    - identical for all pixels
    - individual for each pixel

Inputs: relevant molecules

- Choice of molecules:
  - 42 molecules:
    - In the GUI, 7 molecules can be fitted, 16 additional ones with fixed values;
    - In the command line, all flexibilities given; however, atmospheric profiles not provided for less common molecules
    - For each relevant molecules, indicate if column density is to be taken into account, and if yes, to be fitted or not.

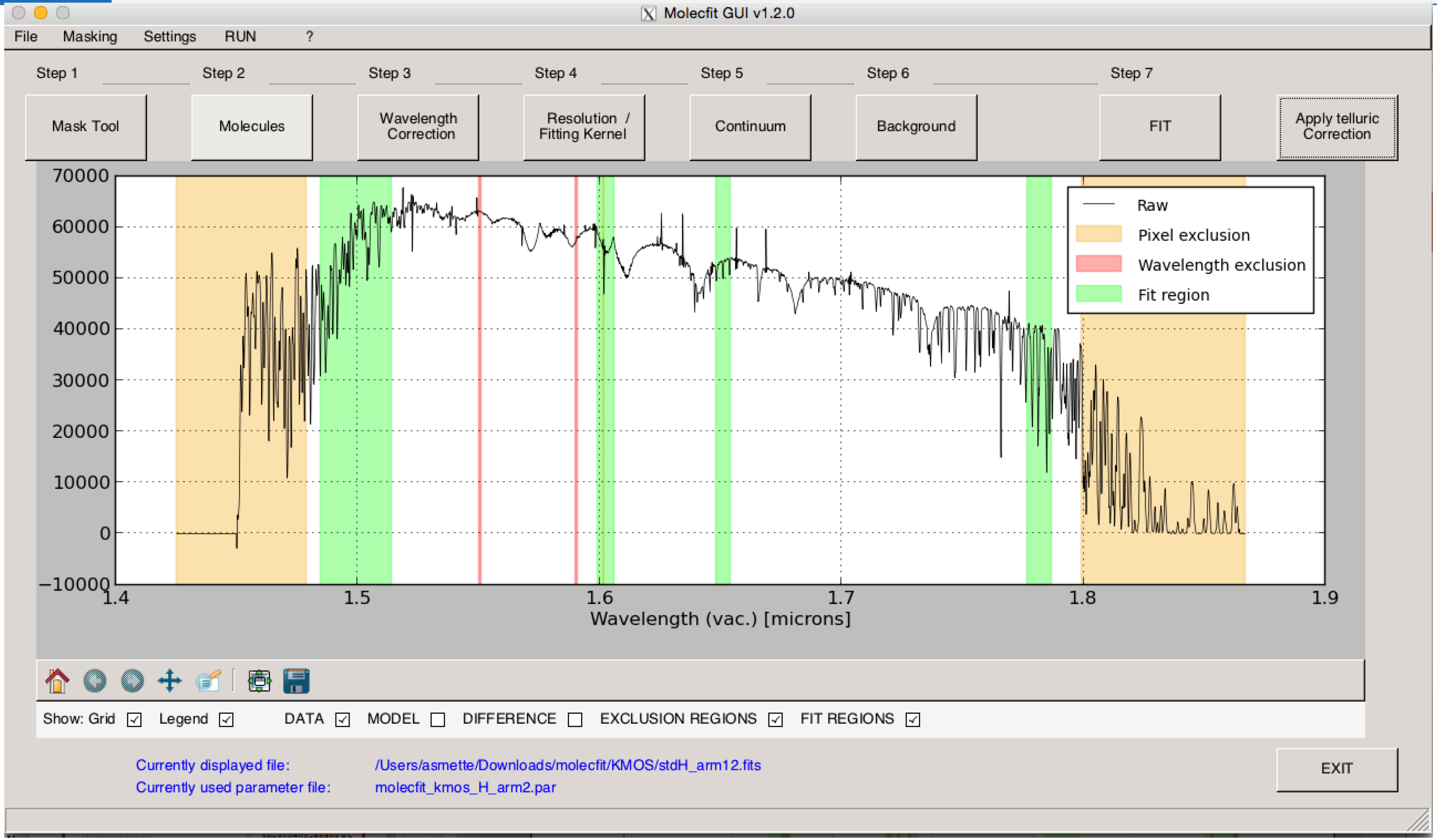
Expert mode

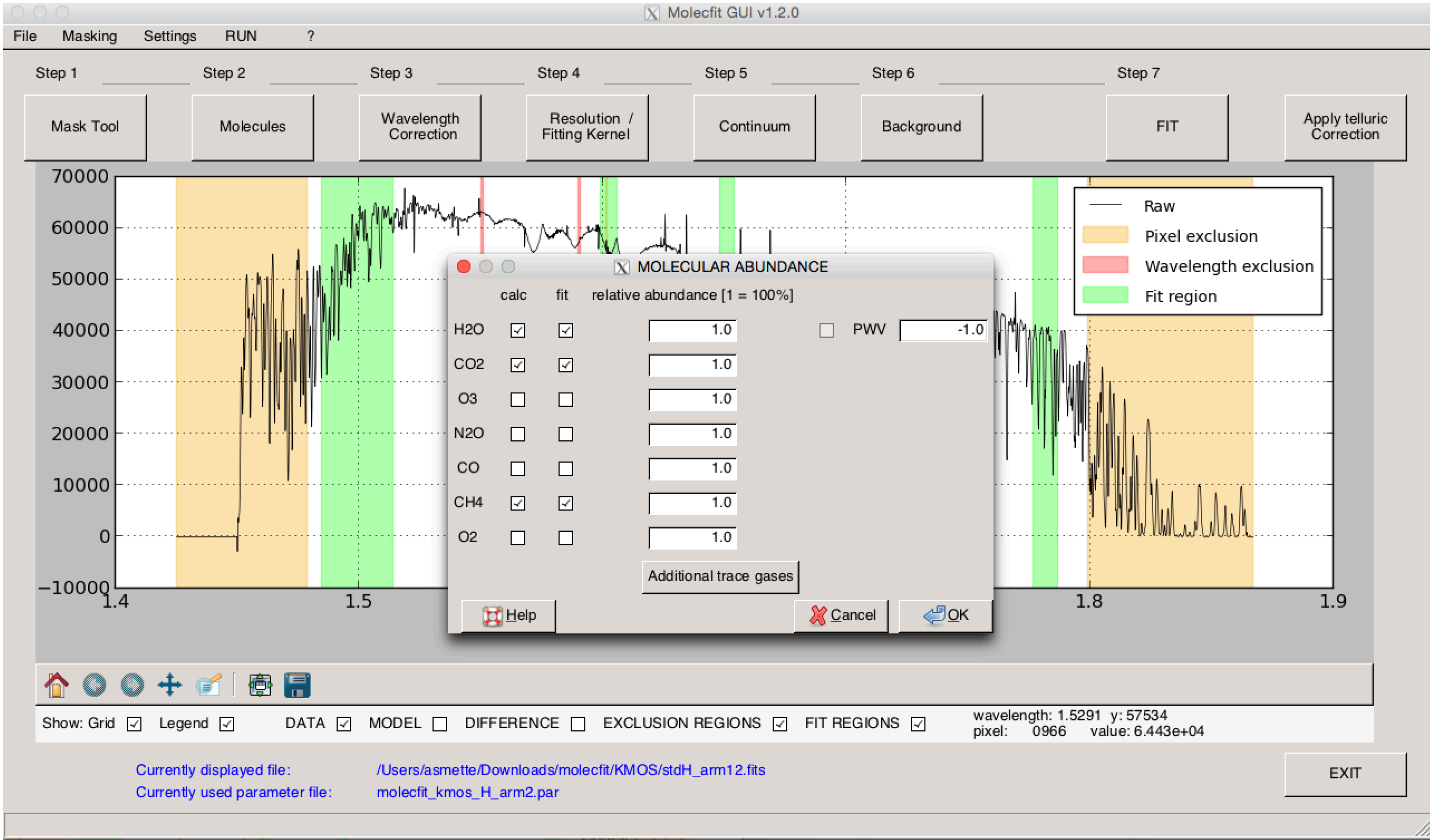
- Allows even greater flexibility:
  - allows the user to fit the spectra on each inclusion range individually
  - provides him/ her the access to the coefficients of the polynomials for the continuum and wavelength correction.
  - parameter file with the best-fit values for all parameters is saved and can be used for another iteration of molecfit.

Fitting sky emission spectra

- Tool is able to fit sky emission spectra for molecules and physical processes handled by the radiative transfer code, with the exclusion of lines produced by chemi-luminescence (OH)
- Use: sky emission in mid-IR to determine volume mixing ratio of relevant molecules

GUI example


Molecfit GUI v1.2.0
File
Masking
Settings
RUN
?
Step 1
Step 2
Step 3
Step 4
Step 5
Step 6
Step 7
Mask Tool
Molecules
Wavelength Correction
Resolution / Fitting Kernel
Continuum
Background
FIT
Apply telluric Correction
70000
60000
50000
40000
30000
20000
10000
0
−10000
1.4
1.5
1.6
1.7
1.8
1.9
Wavelength (vac.) [microns]
Raw
Pixel exclusion
Wavelength exclusion
Fit region
Show: Grid
Legend
DATA
MODEL
DIFFERENCE
EXCLUSION REGIONS
FIT REGIONS
Currently displayed file:
/Users/asmette/Downloads/molecfit/KMOS/stdH_arm12.fits
Currently used parameter file:
molecfit_kmos_H_arm2.par
EXIT



Molecfit GUI v1.2.0
File
Masking
Settings
RUN
?
Step 1
Step 2
Step 3
Step 4
Step 5
Step 6
Step 7
Mask Tool
Molecules
Wavelength Correction
Resolution / Fitting Kernel
Continuum
Background
FIT
Apply telluric Correction
70000
60000
50000
40000
30000
20000
10000
0
−10000
1.4
1.5
1.8
1.9
Raw
Pixel exclusion
Wavelength exclusion
Fit region
MOLECULAR ABUNDANCE
calc
fit
relative abundance [1 = 100%]
H2O
CO2
O3
N2O
CO
CH4
O2
1.0
PWV
-1.0
Additional trace gases
Help
Cancel
OK
Show: Grid
Legend
DATA
MODEL
DIFFERENCE
EXCLUSION REGIONS
FIT REGIONS
wavelength: 1.5291 y: 57534
pixel: 0966 value: 6.443e+04
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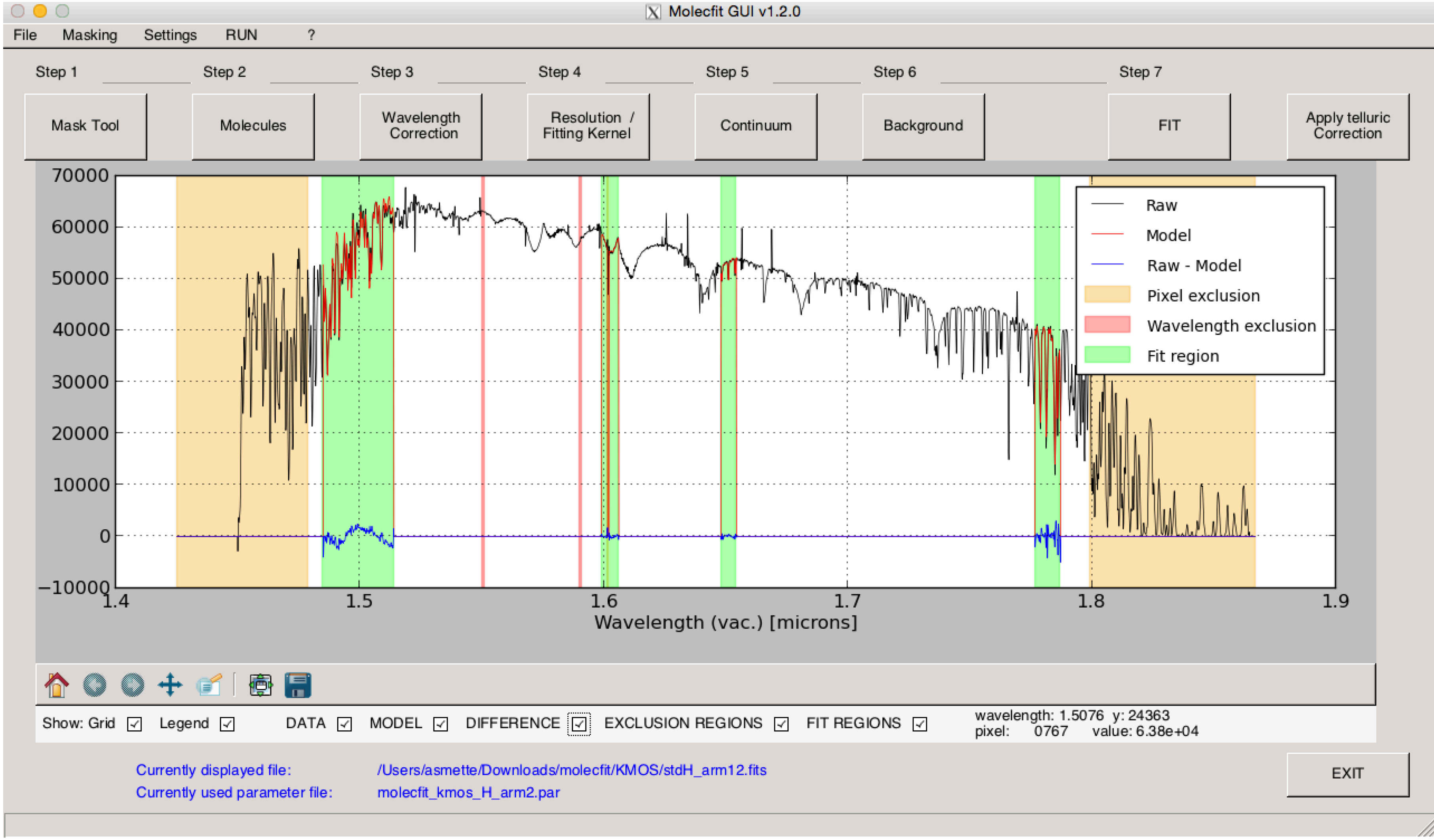
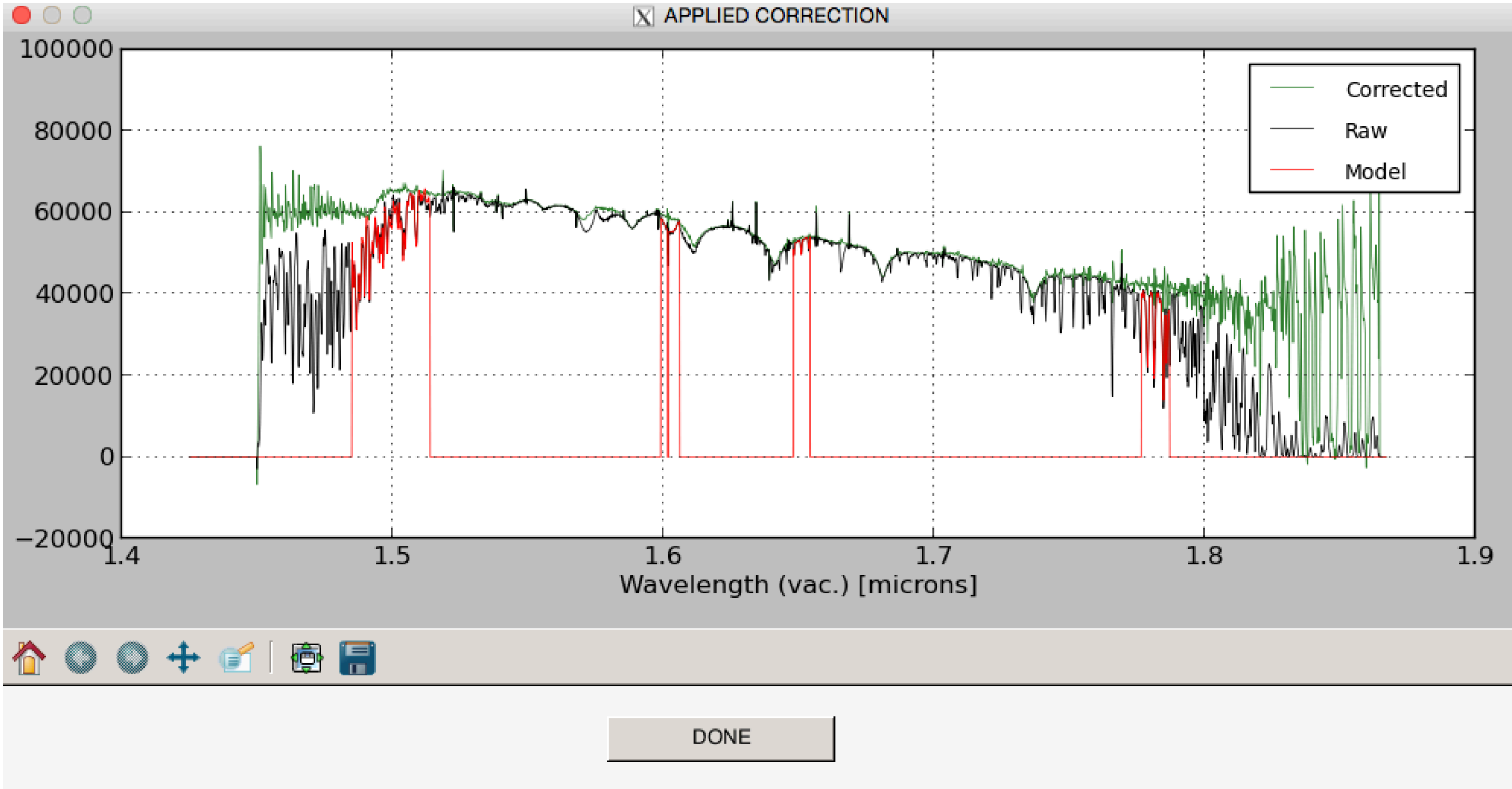
/Users/asmette/Downloads/molecfit/KMOS/stdH_arm12.fits
Currently used parameter file:
molecfit_kmos_H_arm2.par
EXIT



Molecfit GUI v1.2.0
File
Masking
Settings
RUN
?
Step 1
Step 2
Step 3
Step 4
Step 5
Step 6
Step 7
Mask Tool
Molecules
Wavelength Correction
Resolution / Fitting Kernel
Continuum
Background
FIT
Apply telluric Correction
Raw
Model
Raw - Model
Pixel exclusion
Wavelength exclusion
Fit region
Wavelength (vac.) [microns]
Show: Grid
Legend
DATA
MODEL
DIFFERENCE
EXCLUSION REGIONS
FIT REGIONS
wavelength: 1.5076 y: 24363
pixel: 0767 value: 6.38e+04
Currently displayed file:
/Users/asmette/Downloads/molecfit/KMOS/stdH_arm12.fits
Currently used parameter file:
molecfit_kmos_H_arm2.par
EXIT


APPLIED CORRECTION
100000
80000
60000
40000
20000
0
−20000
1.4
1.5
1.6
1.7
1.8
1.9
Wavelength (vac.) [microns]
Corrected
Raw
Model
DONE

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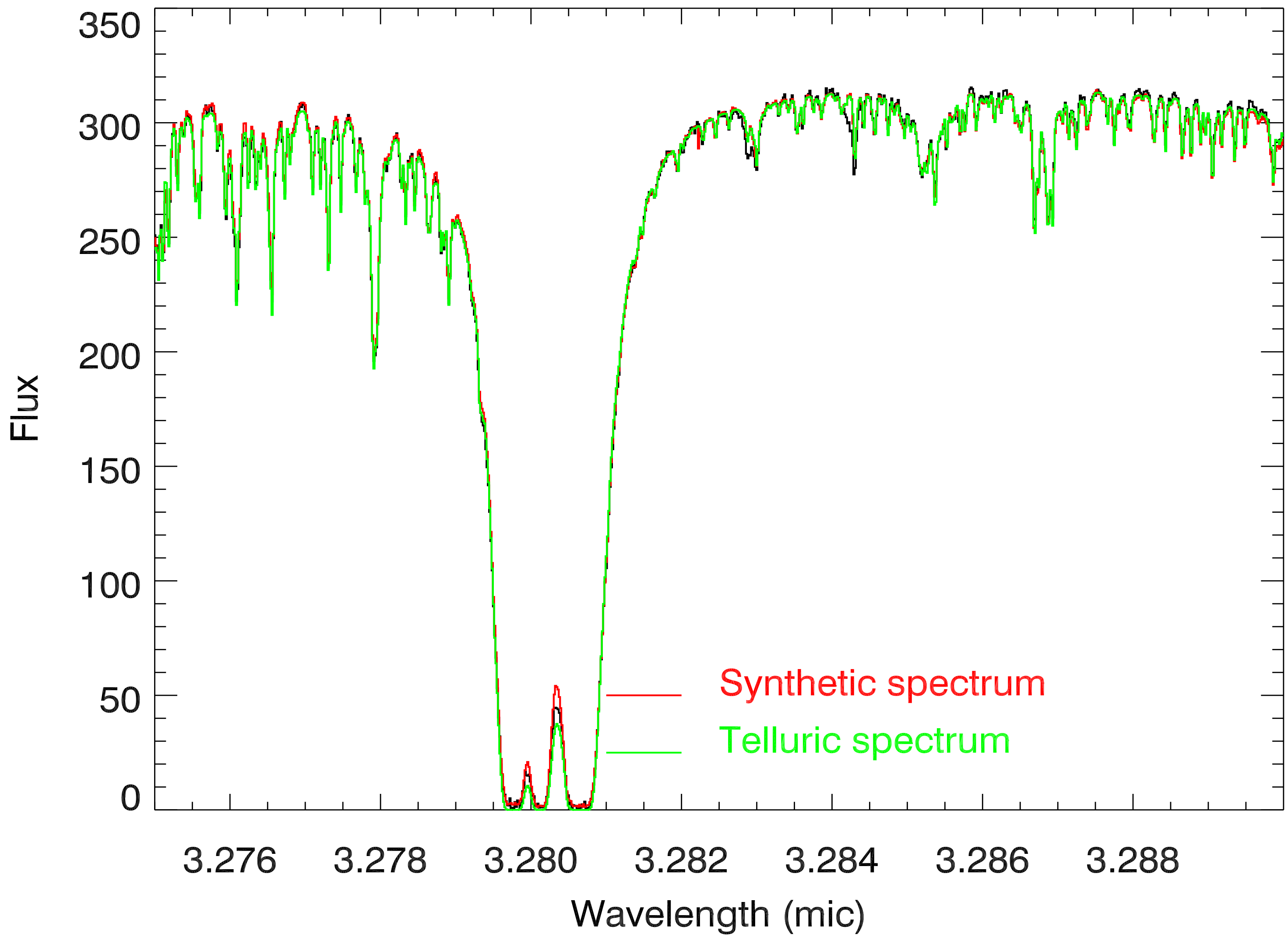
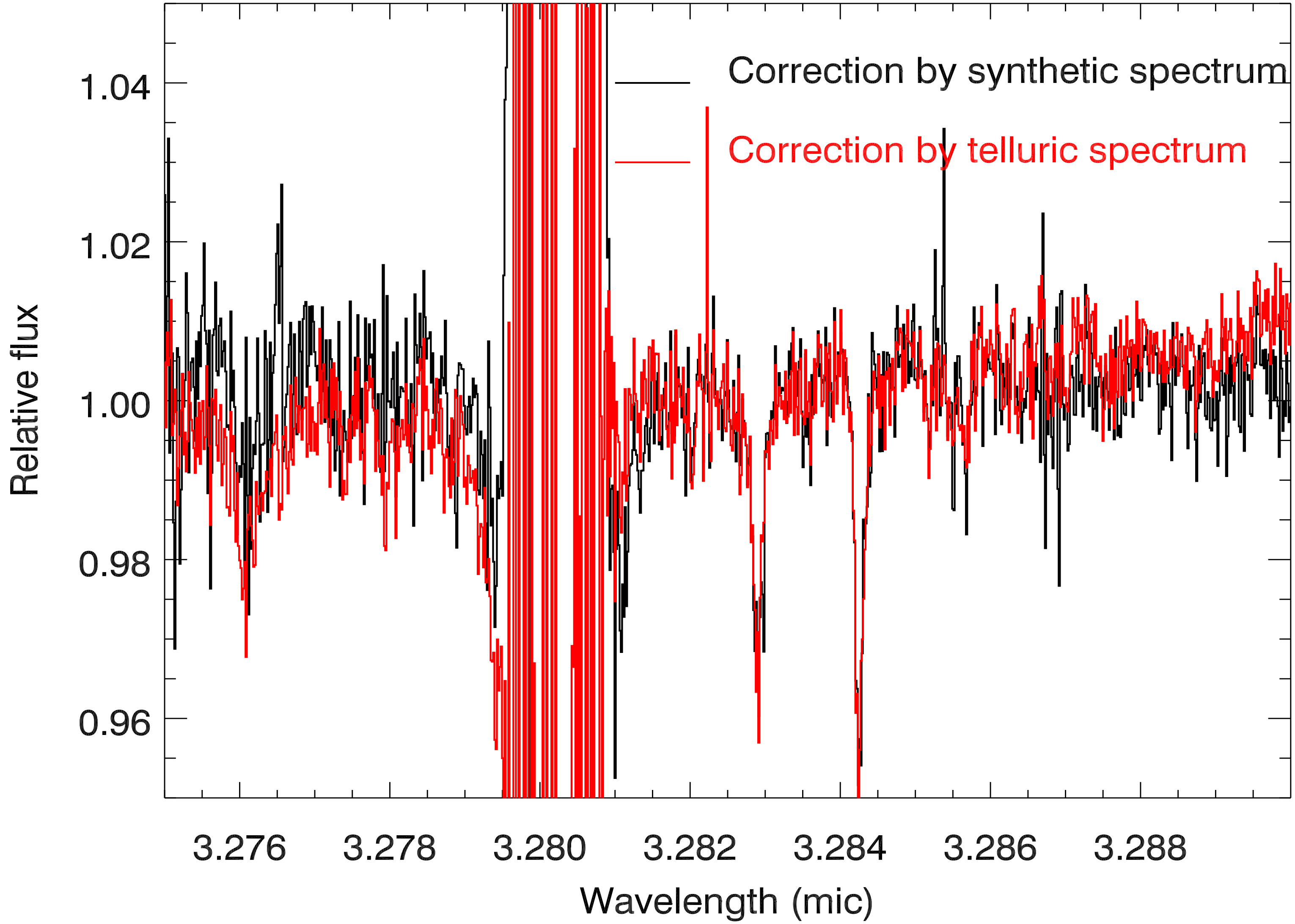
Comparison: telluric *vs* synthetic spectrum



Comparison: telluric *vs* synthetic spectrum



CRIRES

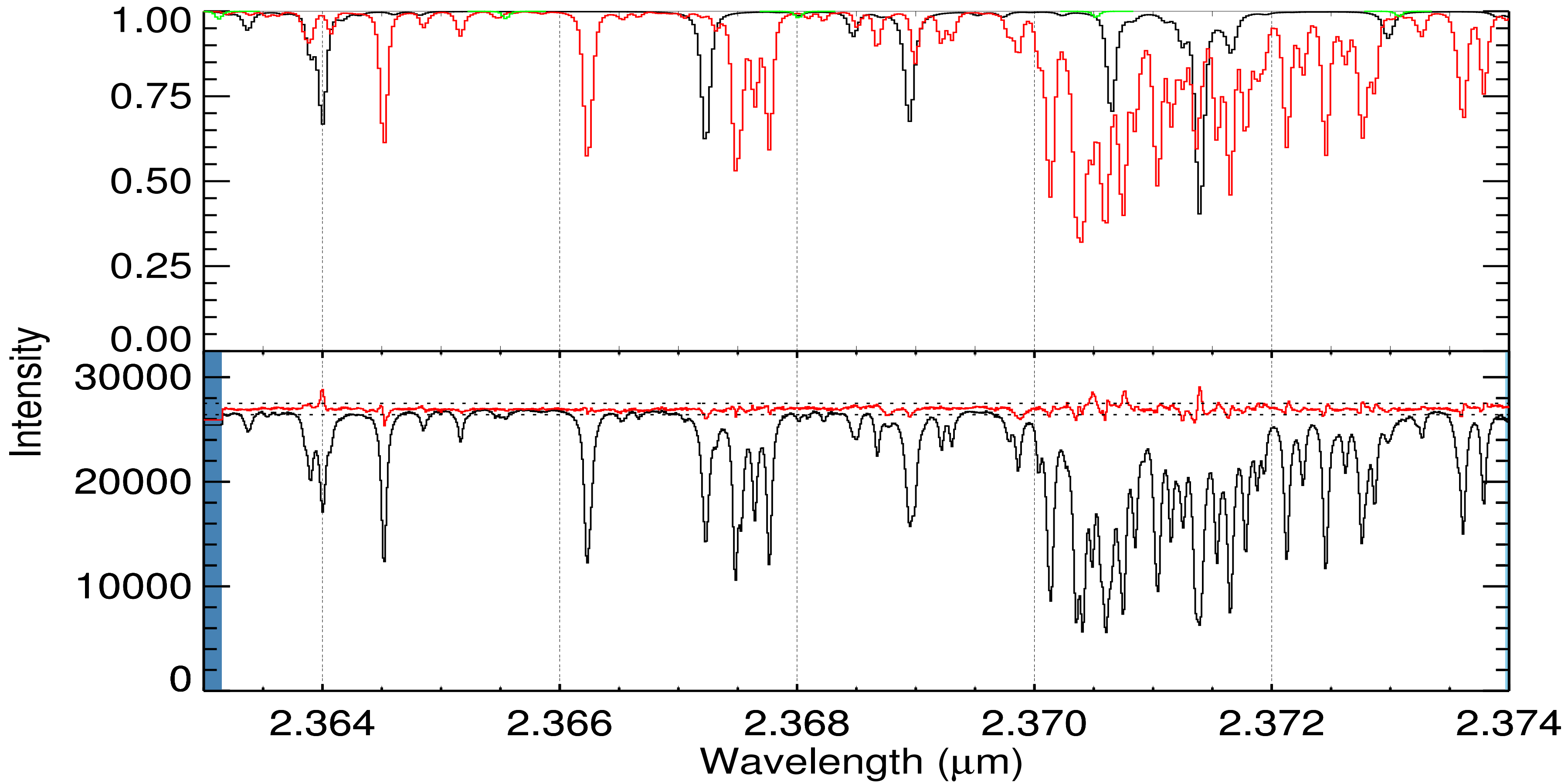


Fig. 13. Extract (detector #3) of CRIRES 2332.2 *(top)* and 2368.7 nm *(bottom)* setting spectra of Procyon. In each figure the *top graphs* show generic (not model) transmission spectra for the relevant molecules: H_2O in black, CH_4 in red, CO_2 in green. The *bottom graphs* show the original pipeline reduced spectra in black, as well as the molecfit-corrected spectra, in red. The dotted lines show 2% deviation from the median value of the corrected spectra.

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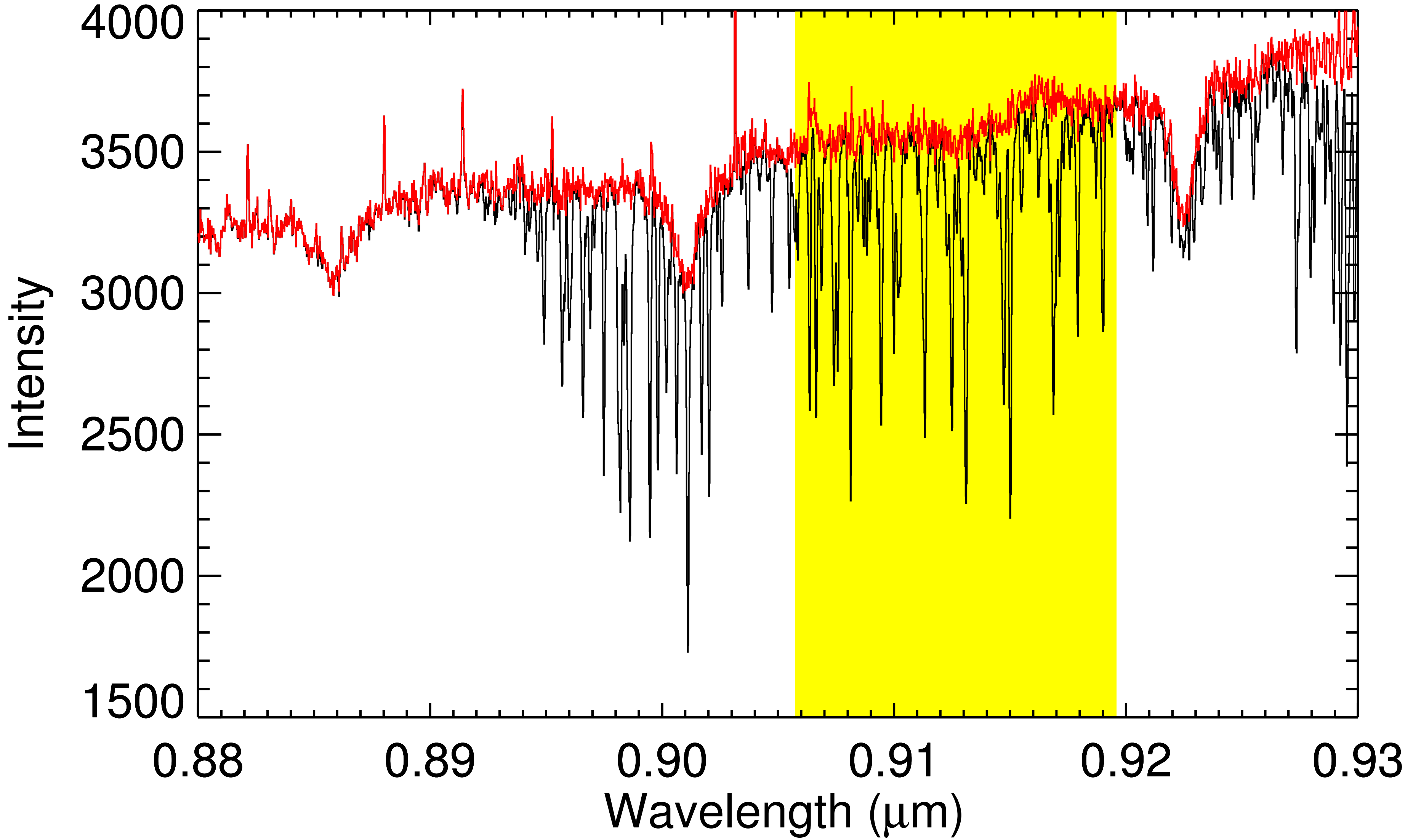
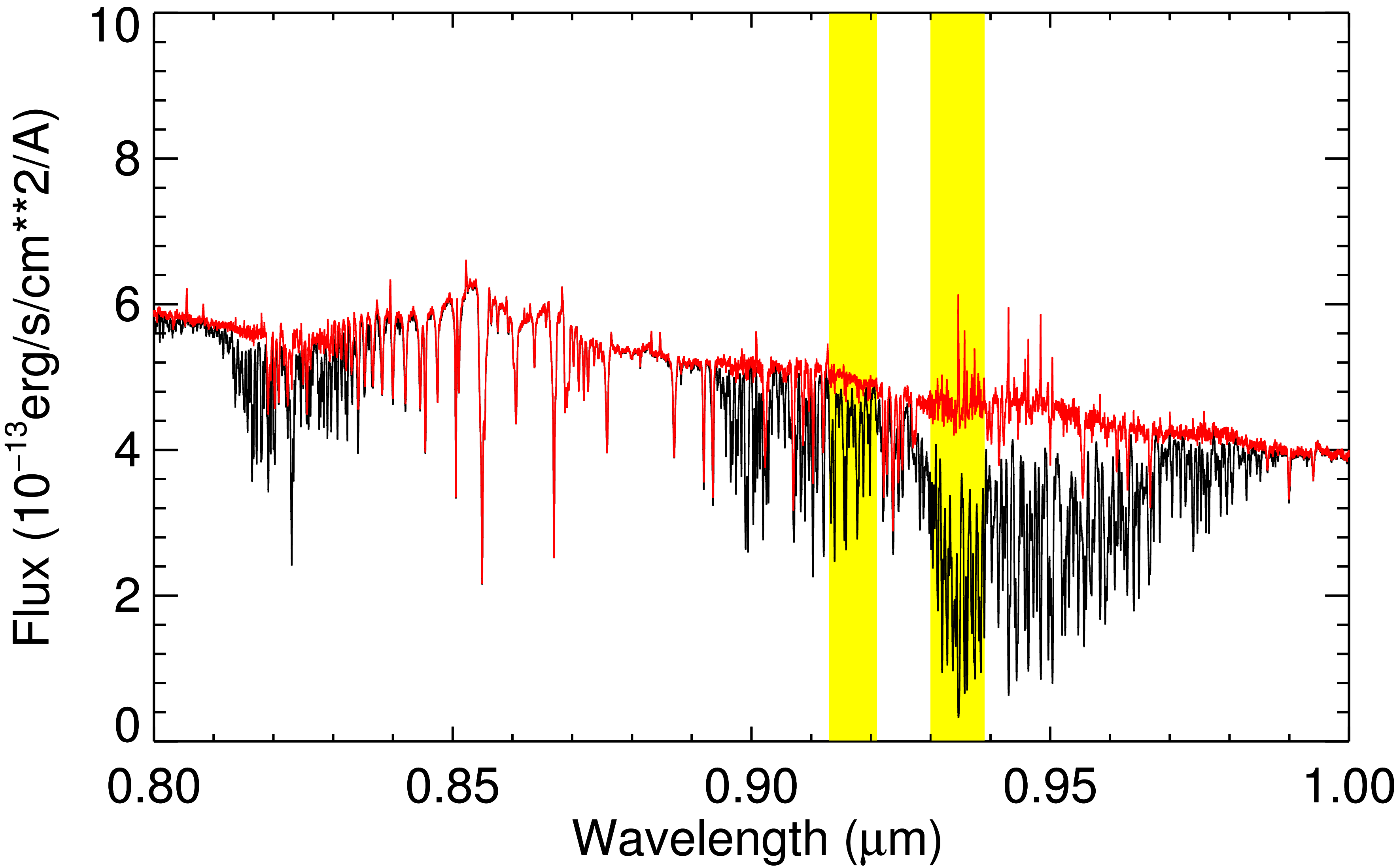
FLAMES



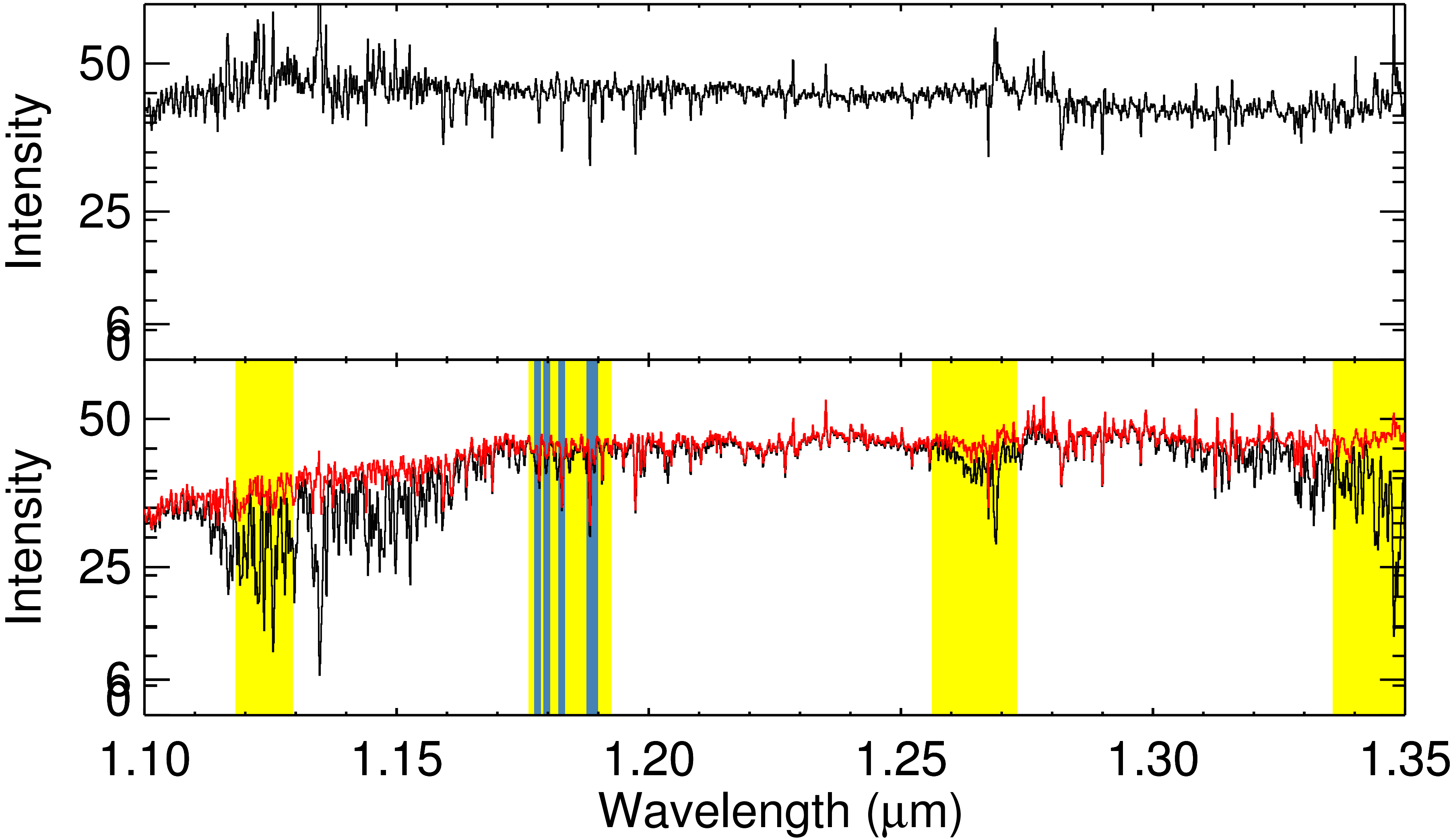
4000
3500
3000
2500
2000
1500
Intensity
0.88
0.89
0.90
0.91
0.92
0.93
Wavelength (µm)

X-shooter



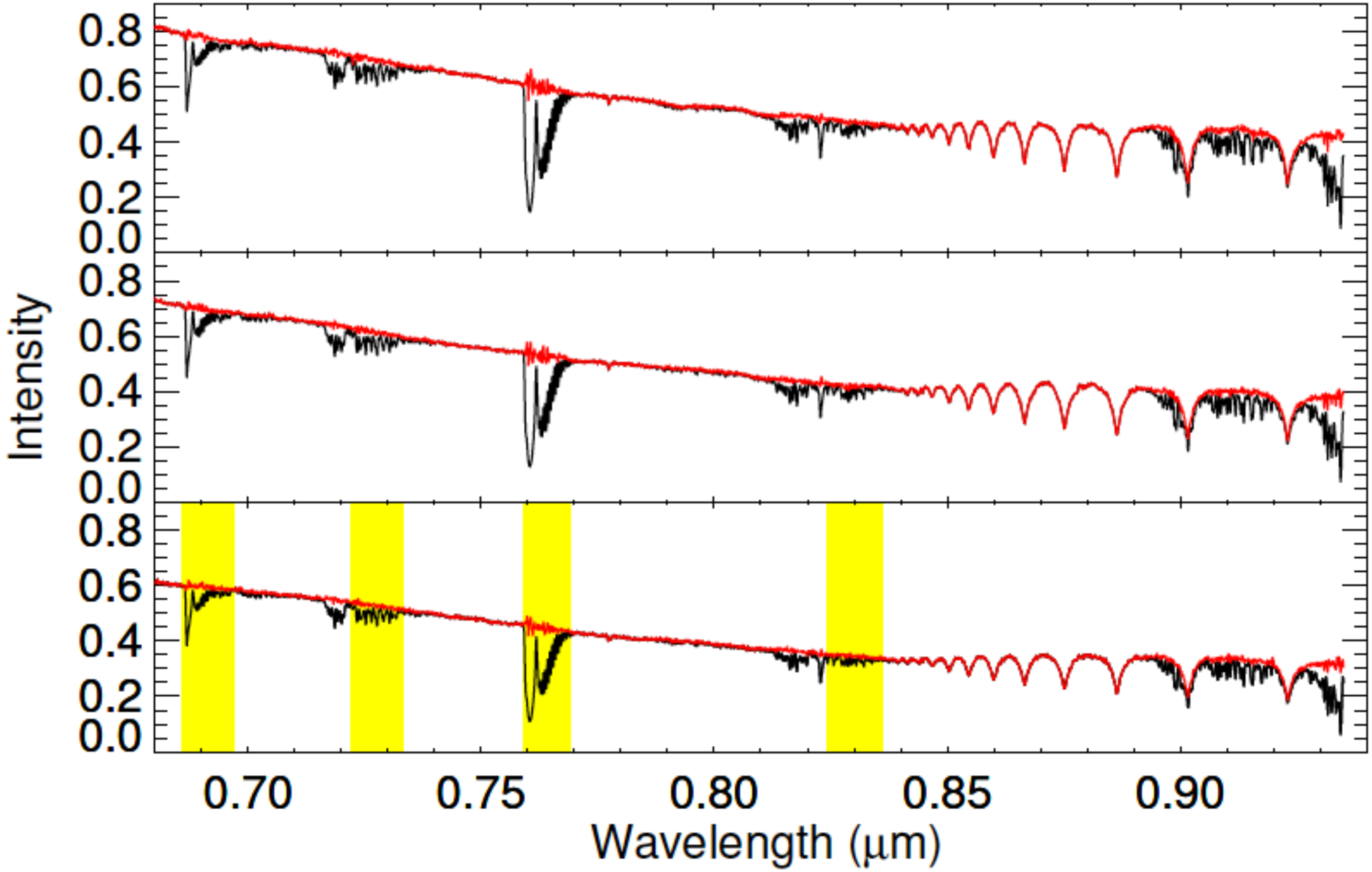
Flux (10^{-13}erg/s/cm**2/A)
10
8
6
4
2
0
0.80
0.85
0.90
0.95
1.00
Wavelength (µm)

KMOS



Intensity
50
25
6
0
Intensity
50
25
6
0
1.10
1.15
1.20
1.25
1.30
1.35
Wavelength (µm)

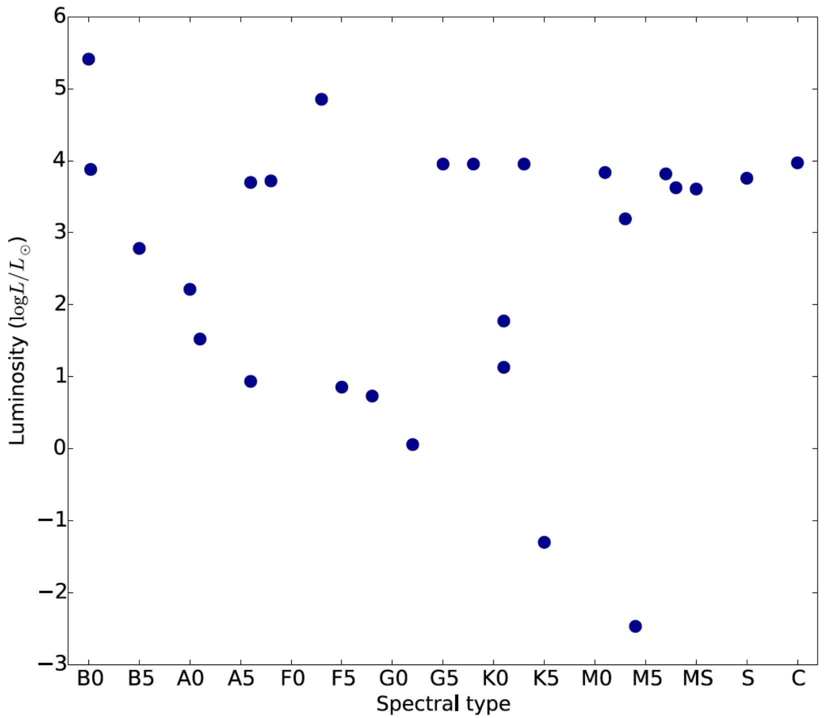
MUSE



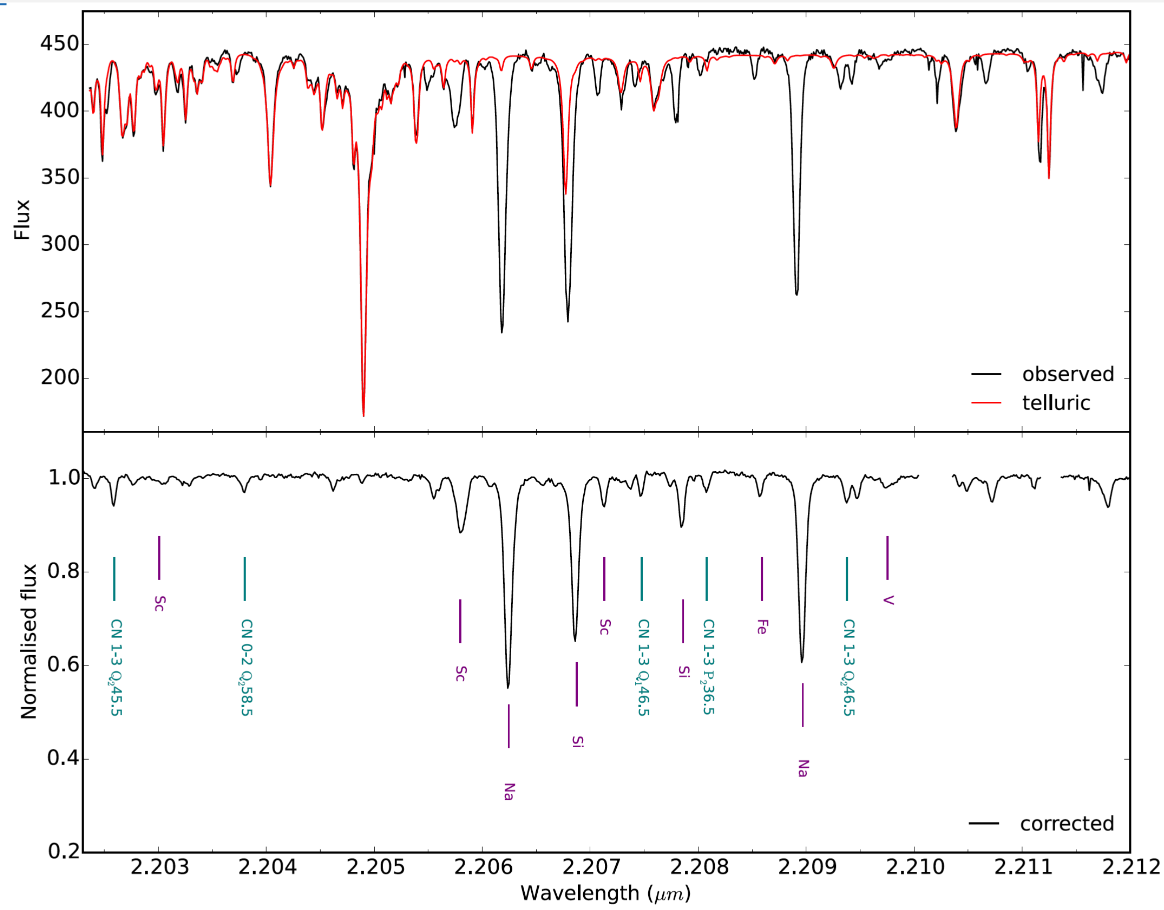
CRIRES-POP

CRIRES-POP: a library of high resolution spectra in the near-infrared II. Data reduction and the spectrum of the K giant 10 Leonis 2017, Nicholls et al., A&A in press

- Aim of CRIRES-POP project: to produce a high resolution near-infrared spectral library of stars across the H-R diagram.
- 26 targets selected.



CRIRES-POP: 10 Leo

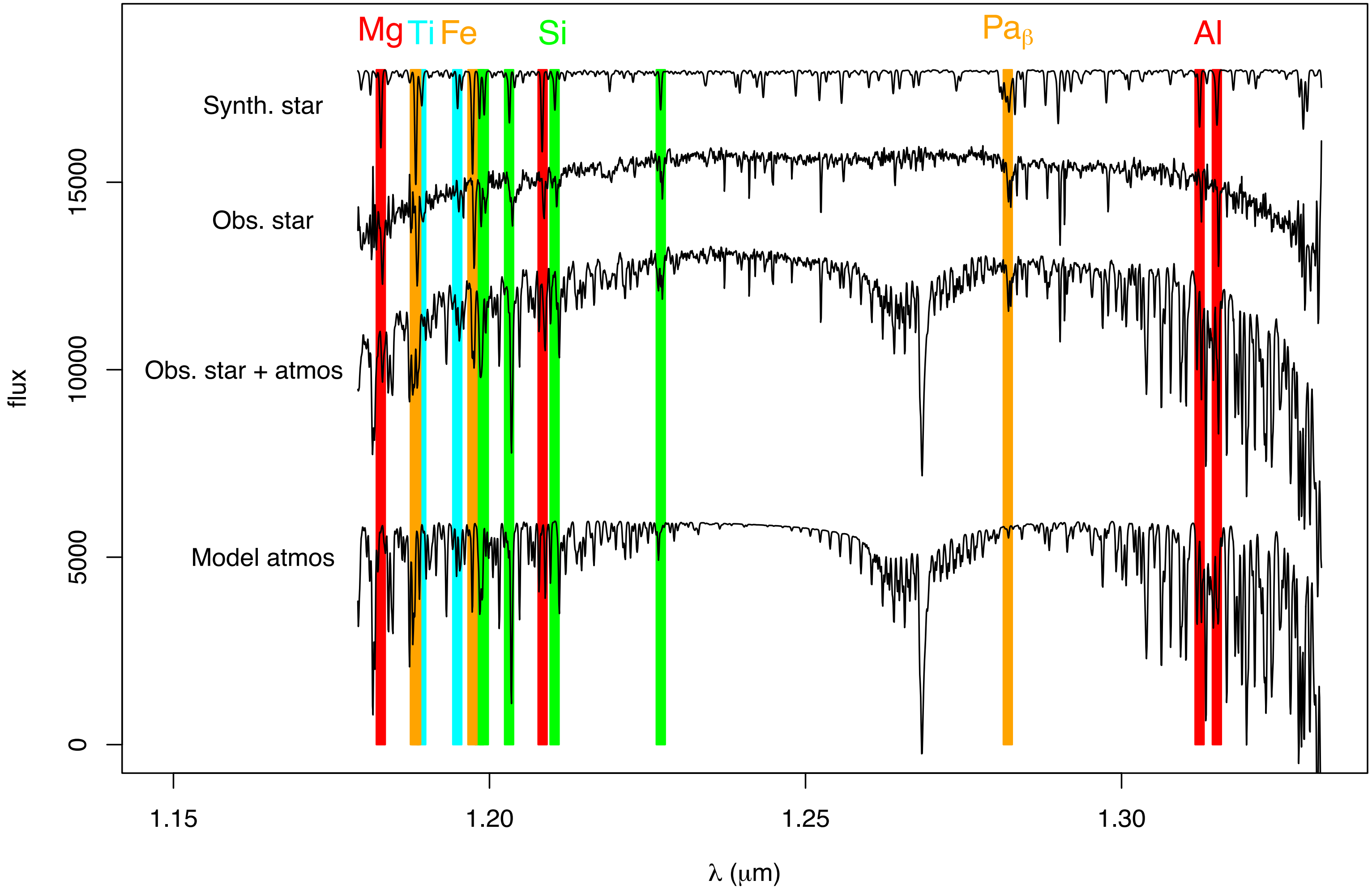


Wavelength calibration corrected using telluric lines – when enough of them.

Observatories for which GDAS profiles are automatically accessible by molecfit

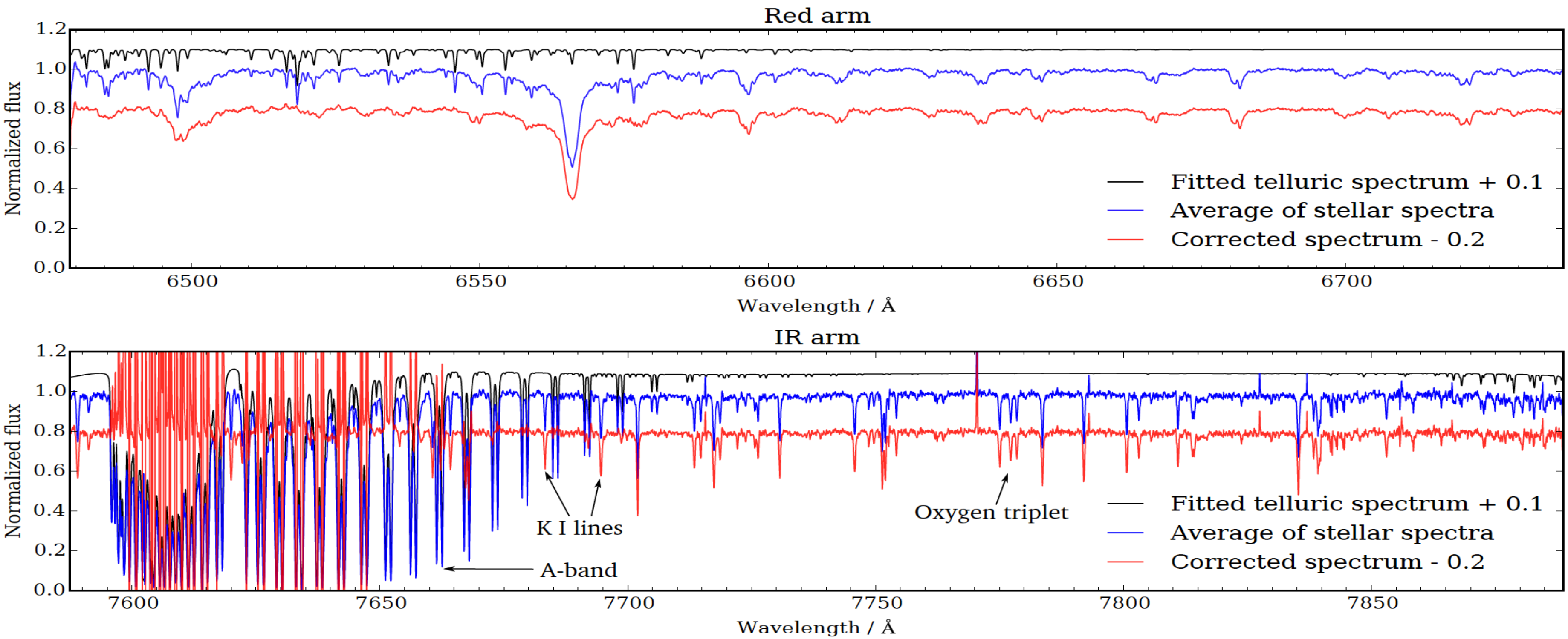
Cerro Paranal:	-70.4	-24.6
La Silla:	-70.7	-29.3
Cerro Pachon:	-70.7	-30.2
Las Campanas:	-70.7	-29.0
South African Astronomical Observatory:	+20.8	-32.4
Siding Spring:	+149.1	-31.3
Mauna Kea:	-155.5	+19.8
Lick Observatory:	-121.6	+37.3
Palomar:	-116.9	+33.4
Kitt Peak National Observatory:	-111.6	+32.0
Lowell Observatory:	-111.4	+34.7
Fred Lawrence Whipple Observatory:	-110.9	+31.7
Mount Graham International Observatory:	-109.9	+32.7
Apache Point	-105.8	+32.8
McDonald Observatory:	-104.0	+30.7
Observatorio del Roque de los Muchachos:	-17.9	+28.8
Calar Alto:	-2.5	+37.2
Special Astrophysical Observatory RAS:	+41.4	+43.6
Devasthal Observatory:	+79.0	+29.0
Xinglong Station:	+117.6	+40.4

LBT



Spectrum of an RGB star of a MW globular cluster observed with LBT
(kindly provided by B. Dias; program by M. Norris et al.)

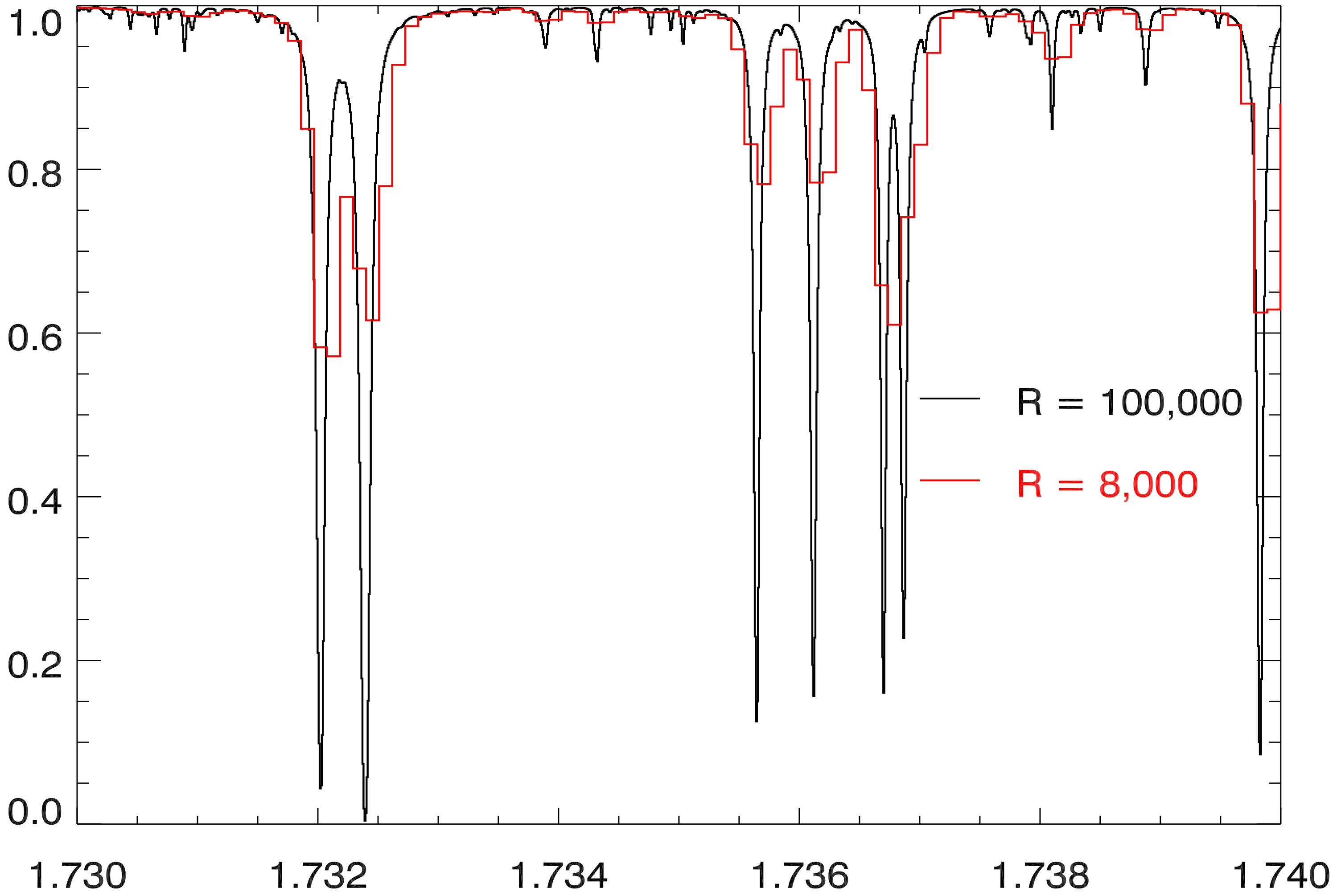
- Included in the GALAH survey data reduction pipeline



Future developments

- Recommended telluric correction for X-shooter
  - Significantly decrease time spent on night-time calibration
- Similar recommendation being studied for KMOS and SINFONI
  - Support for extensions (e.g., KMOS) for IDP data
- Better support for multi-fiber spectrographs (MOONS, 4MOST)
  - no change to ‘fitting’ part
  - calculation for transmission spectrum modified:
    - Only one calculation of transmission spectrum
    - Convolution of with spectra of LSF for each fiber
  - Recipe to provide LSF from calibrations

Note of caution

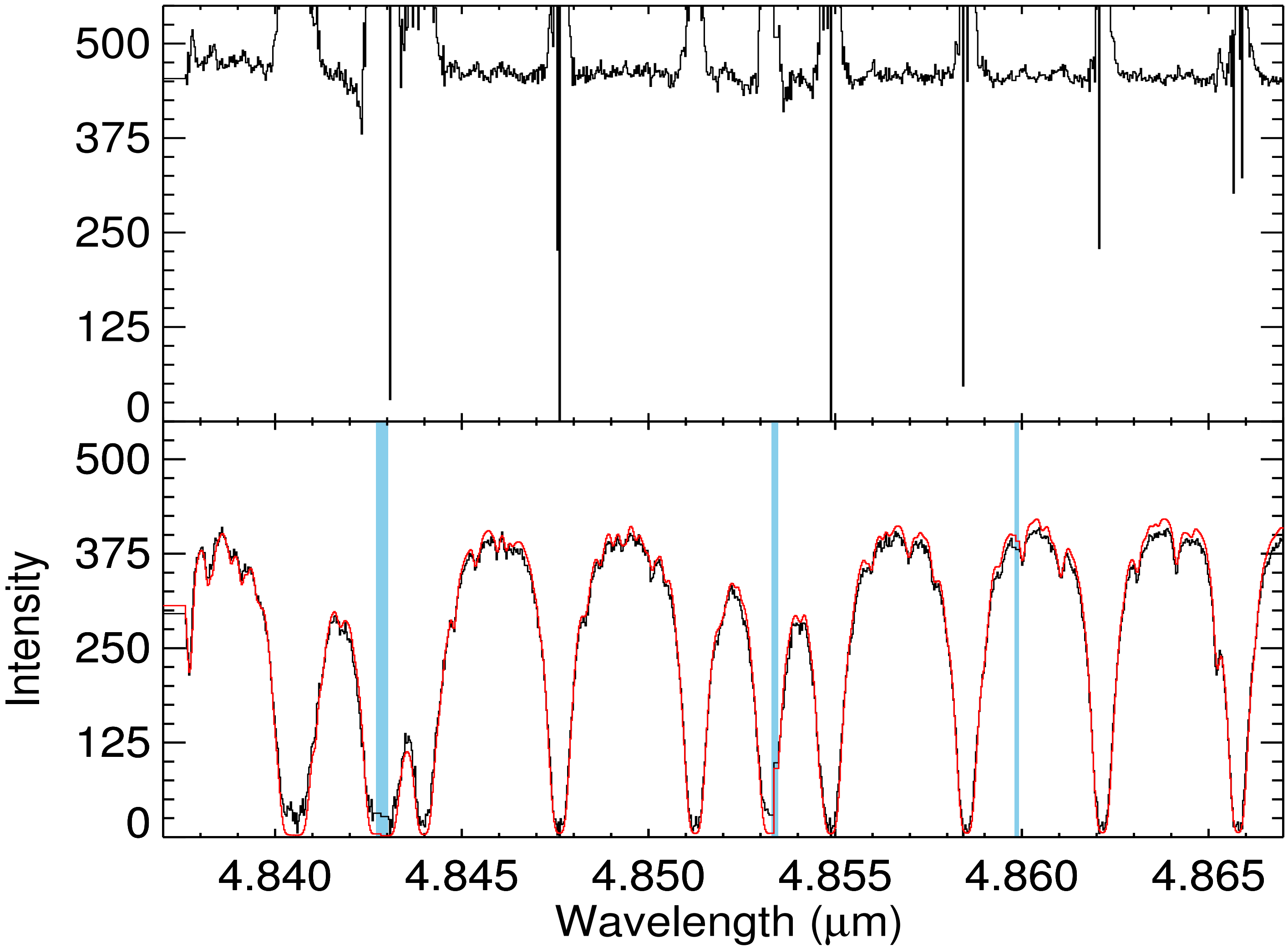


Conclusions

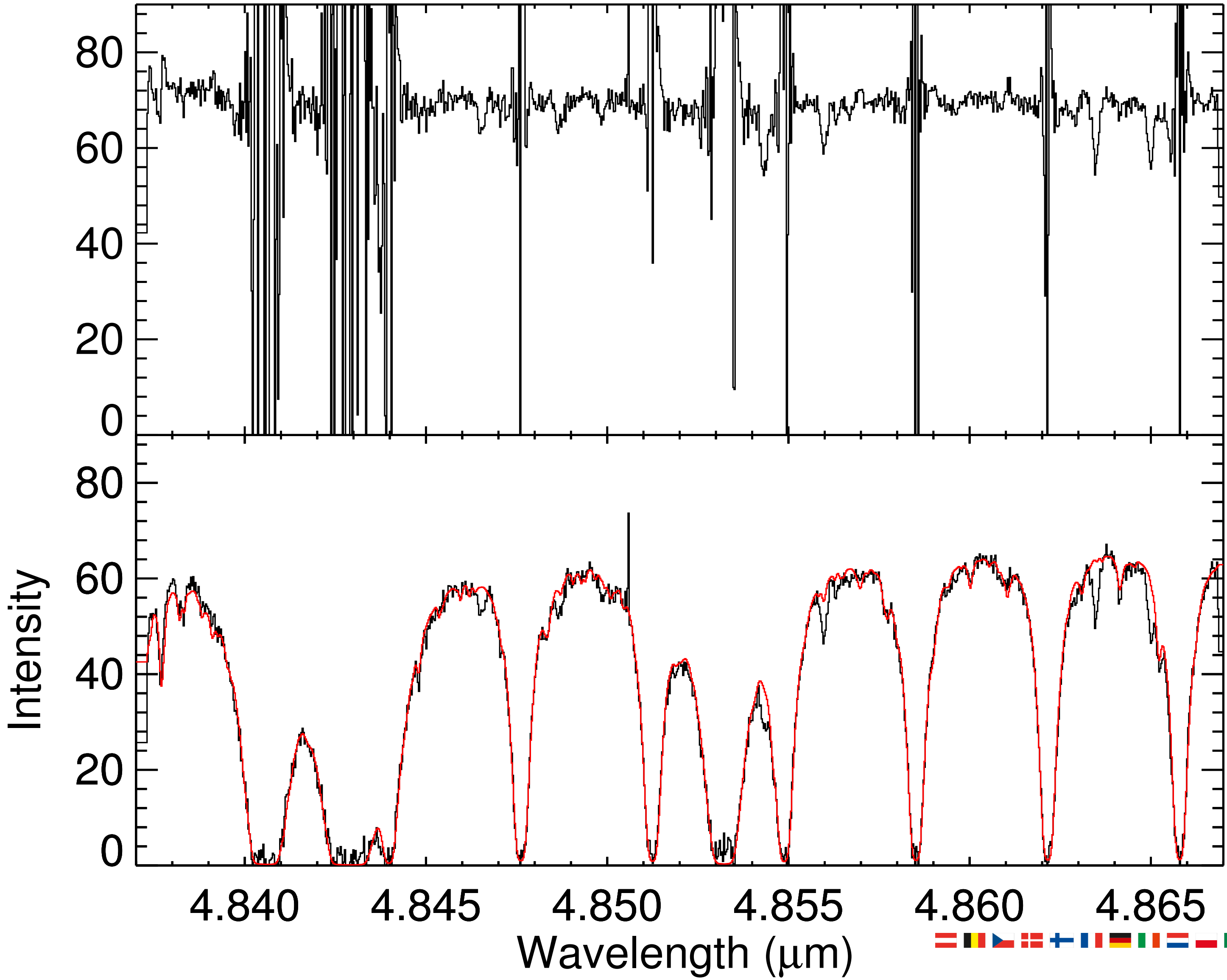
Molecfit is a versatile tool for modelling and correcting telluric absorption lines:

- uses the best information of temperature, pressure and humidity
- Its accuracy often better than ~ 2% relative to continuum in correcting unsaturated telluric absorption lines

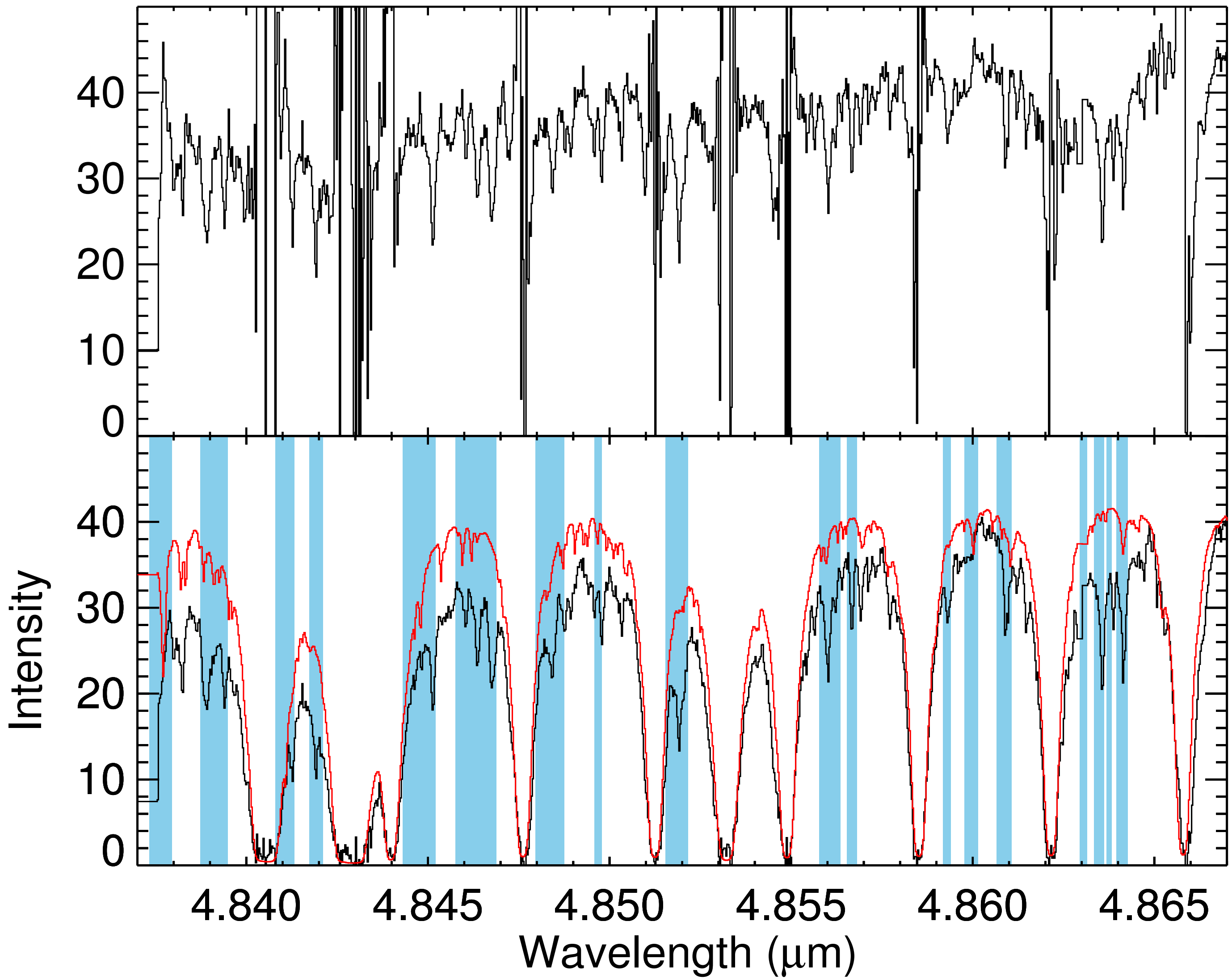
CRIRES: gamma Gemini



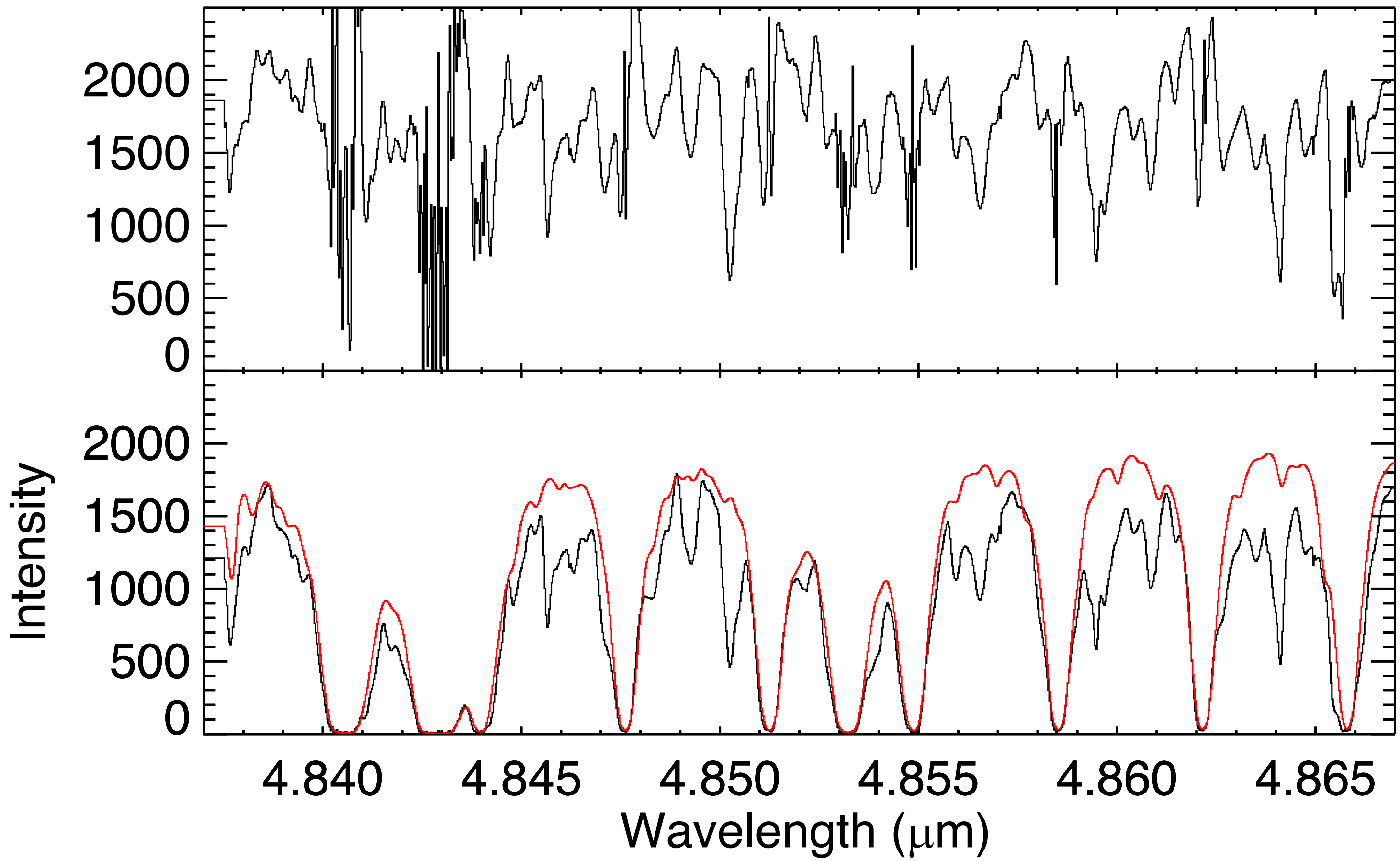
Alpha Fornax



Barnard's star



X Tr A


2000
1500
1000
500
0
2000
1500
1000
500
0
Intensity
4.840
4.845
4.850
4.855
4.860
4.865
Wavelength (μm)

Instrument	Reference			Telluric-corrected		
	λ_{min} (μm)	λ_{max} (μm)	σ ($\times$100)	λ_{min} (μm)	λ_{min} (μm)	σ ($\times$100)
FLAMES	0.88823	0.89111	1.2	0.89555	0.89913	1.0
SINFONI	1.2230	1.2420	2.1	1.2940	1.3045	1.6
SINFONI	1.2230	1.2420	2.1	1.1500	1.1600	6.2
X-shooter VIS	0.878	0.885	1.0	0.894	0.890	1.5
X-shooter VIS	0.806	0.810	0.8	0.810	0.818	1.1
VISIR	12.263	12.273	2.0	12.283	12.285	2.5
KMOS #40	1.162	1.170	4.7	1.140	1.150	5.4
MUSE #10893	0.708	0.714	0.4	0.716	0.733	1.0
CRIRES α For	4.8485	4.8500	2.5	4.8516	4.8524	2.7
CRIRES Procyon				2.3270	2.3350	0.6
CRIRES Procyon				2.3635	2.3740	1.2