



# New release of the MIPAS spectroscopic database: hitran_mipas_pf_v4.45

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**Presentation at MIPAS QWG 38**
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# New version of the MIPAS-specific spectroscopic database

- the new released version is named **hitran_mipas_pf_v4.45**
- can be downloaded from this (unreferenced) web page: http://atmos.difa.unibo.it/spectdb/
- Summary of the database history:

**Procedure used to build the database hitran_mipas_pf4.45 released on 16 February 2015:**

1. As a starting basis we use HITRAN08.par. We cut the database to the interval from 597 to 2600 cm**-1 to cover MIPAS bands, and remove lines of the following molecules: 1,7,9,12,19,24,26,27, 37,42.

2. we merge the database obtained at 1. with the following line lists:
   01_hit09.par <== H2O lines improved at LISA see presentation at QWG 26
   07_hit09.par expected change in H2O_VMR: + 0.2 ppmv
   09_hit09.par
   12_agnes4.43.par <== HNO3 improved data provided by Agnes on 16/01/2015
   19_hit09.par
   24_hit10.par
   26_hit11.par
   27_hit09.par
   48_jmf13.par <=== propane (C3H8) data provided by Jean-Marie on 17/12/2013
   49_jmf14.par <=== phosgene (COCl2) data from Jean-Marie 21/10/2014

3. we sort everything versus frequency.

**Notes:**

- we introduced two new codes (48 and 49) for propane (C3H8) and phosgene (COCl2)
- molecule 37 (HOBr) data are still excluded from the DB as the available data relate only to pure rotational transitions and are outside MIPAS bands
- molecule 42 (CF4q) data are still excluded from the DB as the quality is very poor (included in HITRAN only as supplemental data)
- the DB format is compliant with HITRAN >= 2004 (160-char records)

## Summary of molecules / isotopologues in hitran_mipas_pf4.45

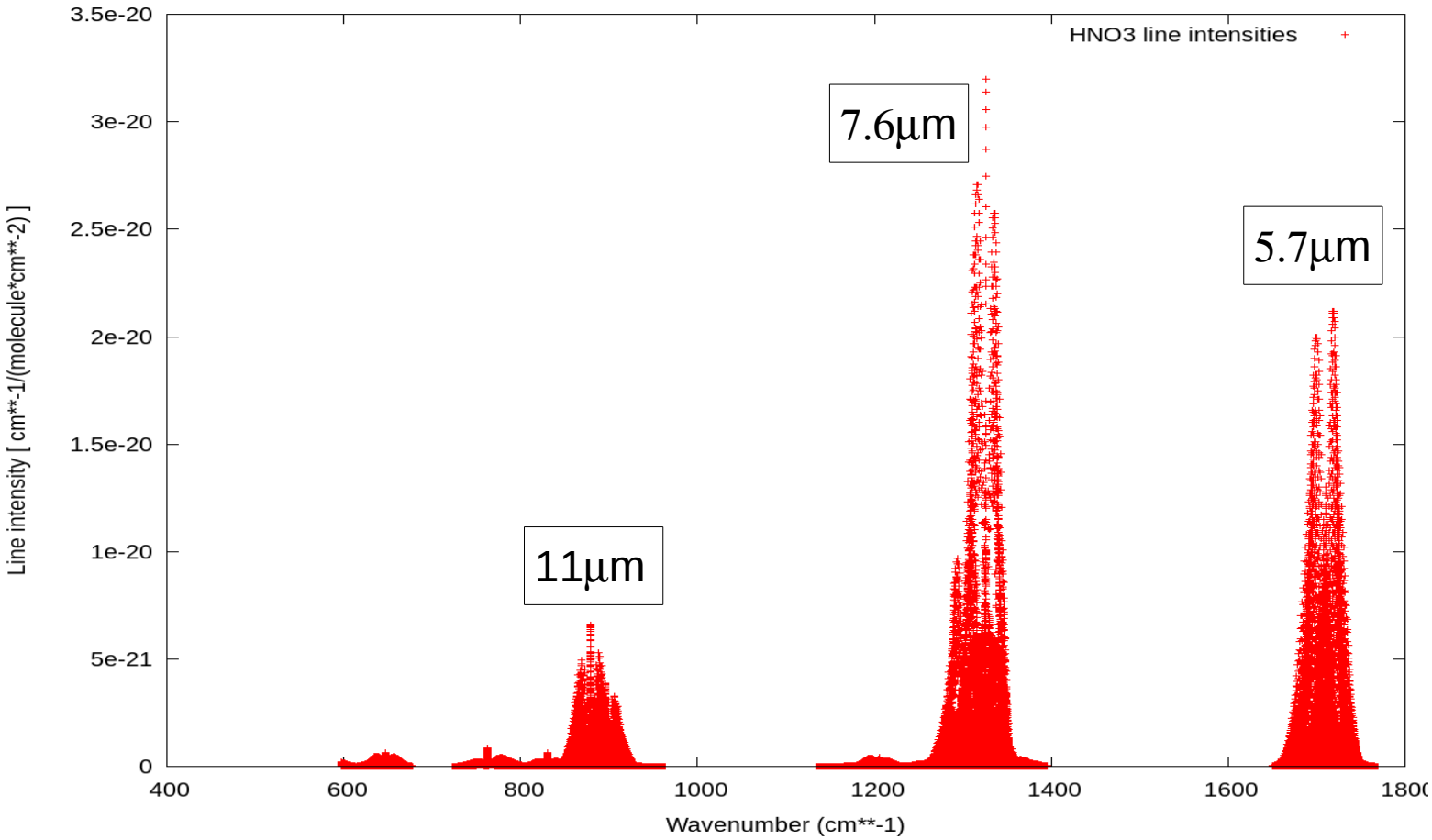
| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | H2O | 1 | 2 | 3 | 4 | 5 | 6 | 0 | 0 | 0 | 0 |
| 2 | CO2 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 0 | 0 |
| 3 | O3 | 1 | 2 | 3 | 4 | 5 | 0 | 0 | 0 | 0 | 0 |
| 4 | N2O | 1 | 2 | 3 | 4 | 5 | 0 | 0 | 0 | 0 | 0 |
| 5 | CO | 1 | 2 | 3 | 4 | 5 | 6 | 0 | 0 | 0 | 0 |
| 6 | CH4 | 1 | 2 | 3 | 4 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7 | O2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8 | NO | 1 | 2 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9 | SO2 | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10 | NO2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 11 | NH3 | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | HNO3 | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 13 | OH | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 14 | HF | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 15 | HCl | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 16 | HBr | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 17 | HI | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 18 | ClO | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 19 | OCS | 1 | 2 | 3 | 4 | 5 | 0 | 0 | 0 | 0 | 0 |
| 20 | H2CO | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 21 | HOCl | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 22 | N2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 23 | HCN | 1 | 2 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 24 | CH3Cl | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 25 | H2O2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 26 | C2H2 | 1 | 2 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 27 | C2H6 | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 28 | PH3 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 29 | COF2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 30 | SF6q | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 31 | H2S | 1 | 2 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 32 | HCOOH | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 33 | HO2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 34 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 35 | ClONO2q | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 36 | NO+ | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 37 | HOBr | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 38 | C2H4 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 39 | CH3OHq | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 40 | CH3Br | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 41 | CH3CNq | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 42 | CF4q | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 43 | C4H2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 44 | HC3N | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 45 | H2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 46 | CS | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 47 | SO3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 48 | C3H8 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 49 | COCl2 | 1 | 2 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

Note: molecules ending with “q” should be simulated with x-section data available, line data are not accurate.

# Validation of the HNO3 line data included in the database v. 4.45

## Background

HNO3 has 3 main absorption bands in the spectral region covered by MIPAS:



# Validation of HNO3 line data: background

- ESA Level 2 processor retrieves HNO3 using MWs in the 11.3 μm region which is more transparent.
- So far the 7.6 μm region was not used due to: a) interference of H2O and b) inaccuracies in spectroscopic data.
- If b) was not an issue then, due to the much larger intensity (at least a factor of 2 to 3), the 7.6 μm region could be used to improve HNO3 retrievals above 30 km, were H2O interference is less important.
- Therefore we tried to improve HNO3 line data, especially in the 7.6 μm region.
- Particularly we attempted to achieve good consistency between HNO3 retrieved from the 11 and the 7.6 μm regions.
- We test the consistency of HNO3 profiles retrieved from MIPAS, using two different sets of MWs …….

# Validation of HNO3 line data: tests

- The two sets of HNO3 MWs used:

| Test A – MWs in the 11.3 μm region | | | | Test B – MWs in the 7.6 μm region | | | |
|---|---|---|---|---|---|---|---|
| 1 | HNO30504____ | 761.7500 | 764.7500 (*) | 1 | HNO30514____ | 1309.1500 | 1312.1500 |
| 2 | HNO30507____ | 863.4750 | 866.4750 | 2 | HNO30511____ | 1313.7250 | 1316.7250 |
| 3 | HNO30503____ | 866.5000 | 869.5000 | 3 | HNO30515____ | 1316.8500 | 1319.8500 |
| 4 | HNO30508____ | 869.5250 | 872.5250 | 4 | HNO30513____ | 1324.2000 | 1327.2000 |
| 5 | HNO30502____ | 878.4250 | 881.4250 | 5 | HNO30516____ | 1329.3750 | 1332.3750 |
| 6 | HNO30501____ | 885.0000 | 888.0000 | 6 | HNO30512____ | 1333.5250 | 1336.5250 |
| 7 | HNO30506____ | 888.0250 | 891.0250 | | | | |

(*) Used in Level 2 retrievals, not used in our tests (spectroscopic data are not accurate)

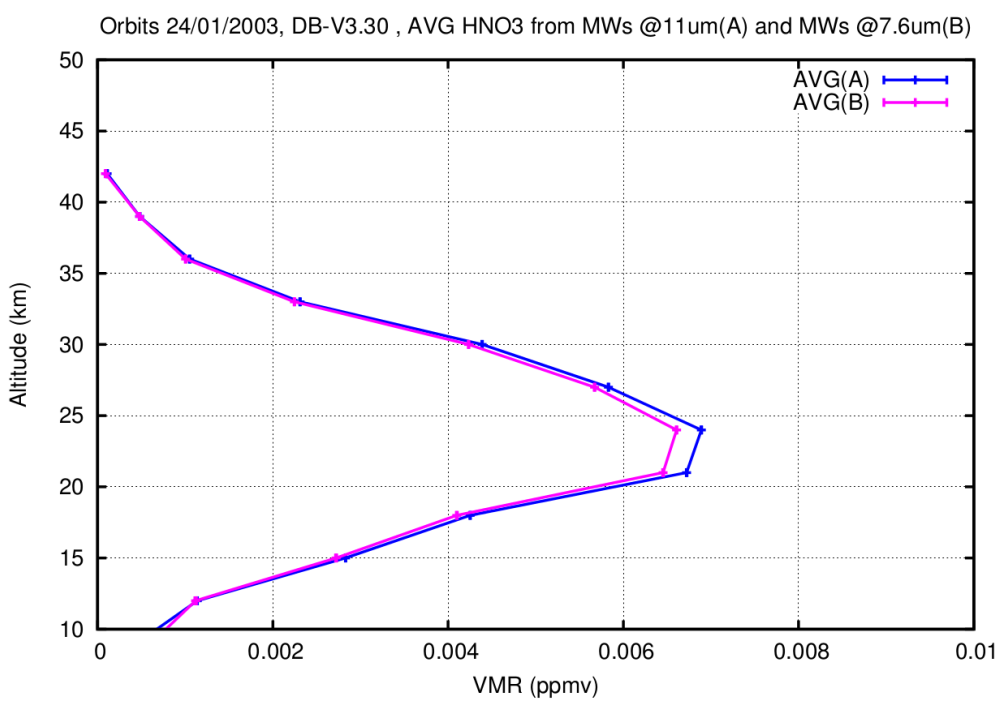
- We carry-out retrievals from FR MIPAS measurements (Level 1b version 7.02)
- We calculate average HNO3 VMR profiles from approximately 1000 scans (1 day of measurements, 14 orbits)

# Validation of HNO3 line data: results for orbits from 24 / 01 / 2003

- Inter-consistency achieved (after several attempts):

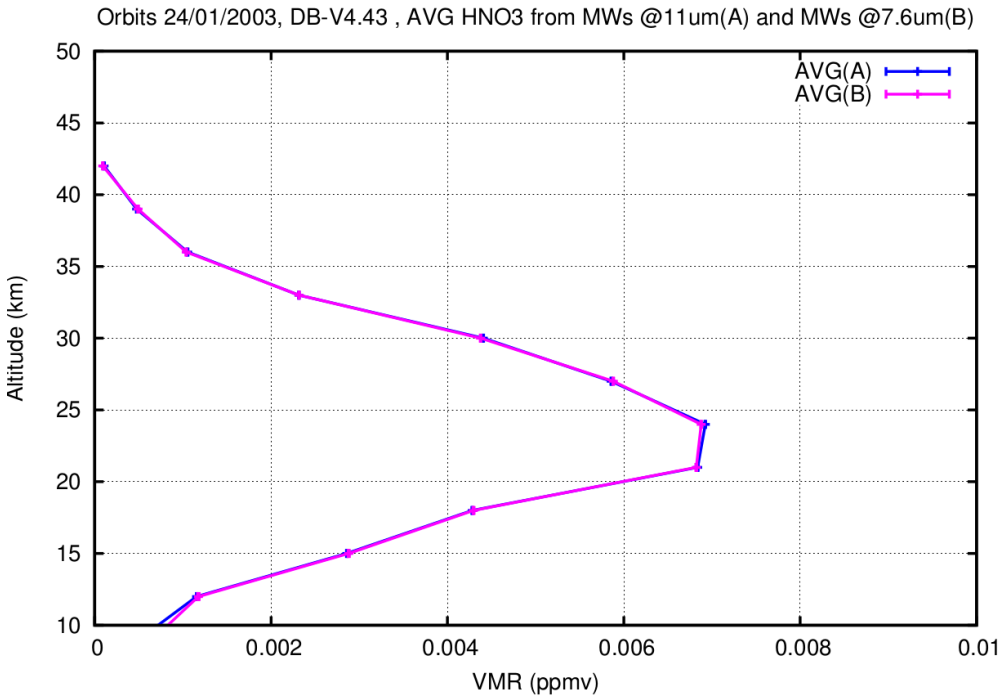
**hitran_mipas_pf3.30 (BEFORE)**

CHI2(11µm)=1.304; CHI2(7.6µm)=1.229




**hitran_mipas_pf4.43 (NOW)**

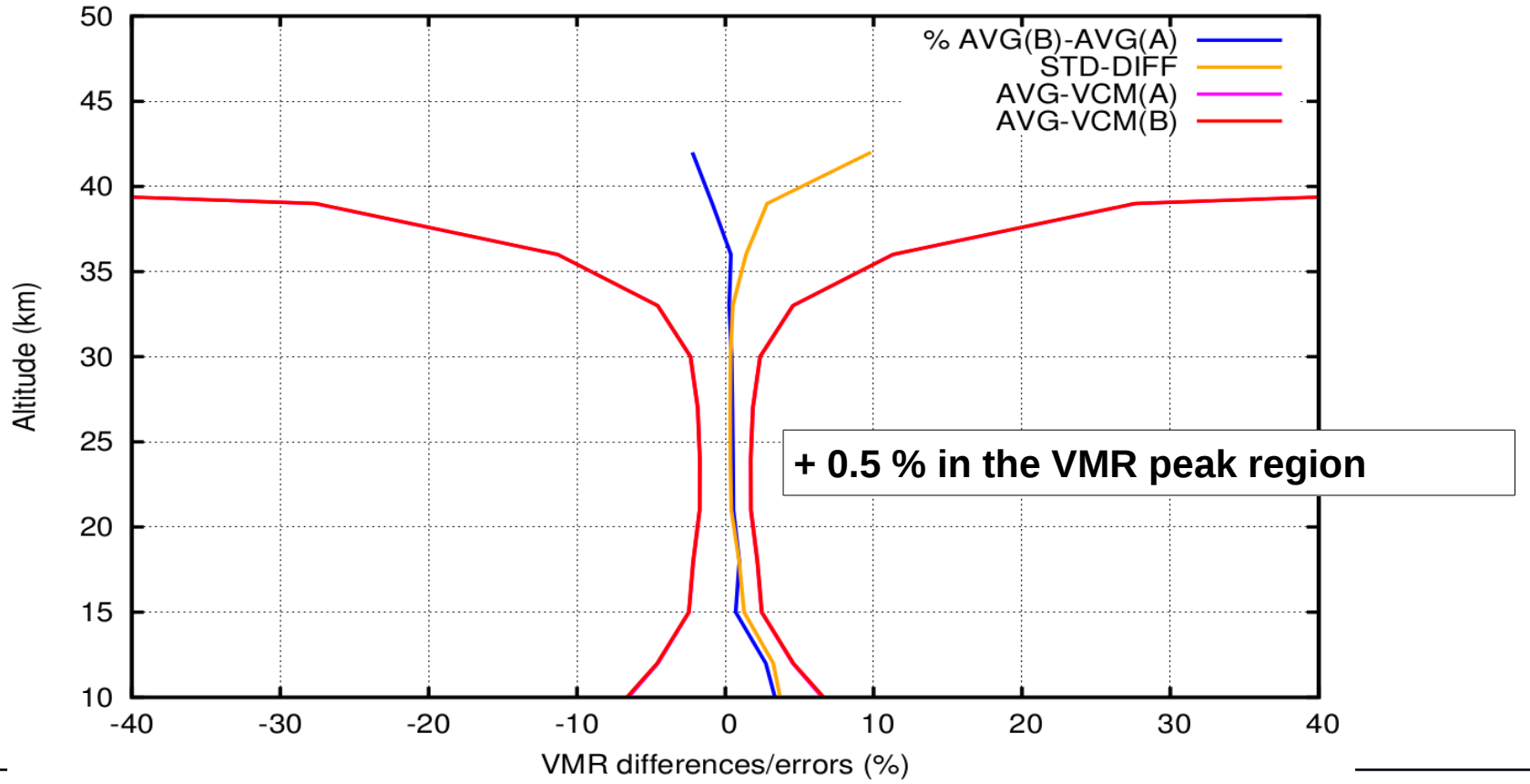
CHI2(11µm)=1.318; CHI2(7.6µm)=1.227



# Expected differences in Level 2 HNO3 profiles, i.e.:

**HNO3 (v. 4.45) <=== vs ===> HNO3 (v. 3..30)**
**using MWs in the 11.3 μm region**

**Blue curve = 100 x [ HNO3 (v. 4.45) - HNO3 (v. 3.30) ] / HNO3 (v. 3.30)**



# Validation of HNO3 line data:

## 11.2 vs 7.6 μm line data inter-calibration accuracy

- The inter-calibration test was initially made only with the orbits from 24/01/2003.
- In order to understand the reproducibility of the results (and this the precision of the calibration) we repeated the test for the orbits measured in other days:
  - 04 August 2002
  - 22 September 2002
  - 24 January 2003
  - 14 March 2003

We selected the days in order to avoid the Level 1b files processed with erroneous AUX data (see email from Gabriele).

==> Results are reproduced **to within 1.5 %** (precision / accuracy of the HNO3 bands inter-calibration)

**Conclusion** ===> use the new database: http://atmos.difa.unibo.it/spectdb/

## Spare slides with some plots of residual spectra in the HNO3 MWs

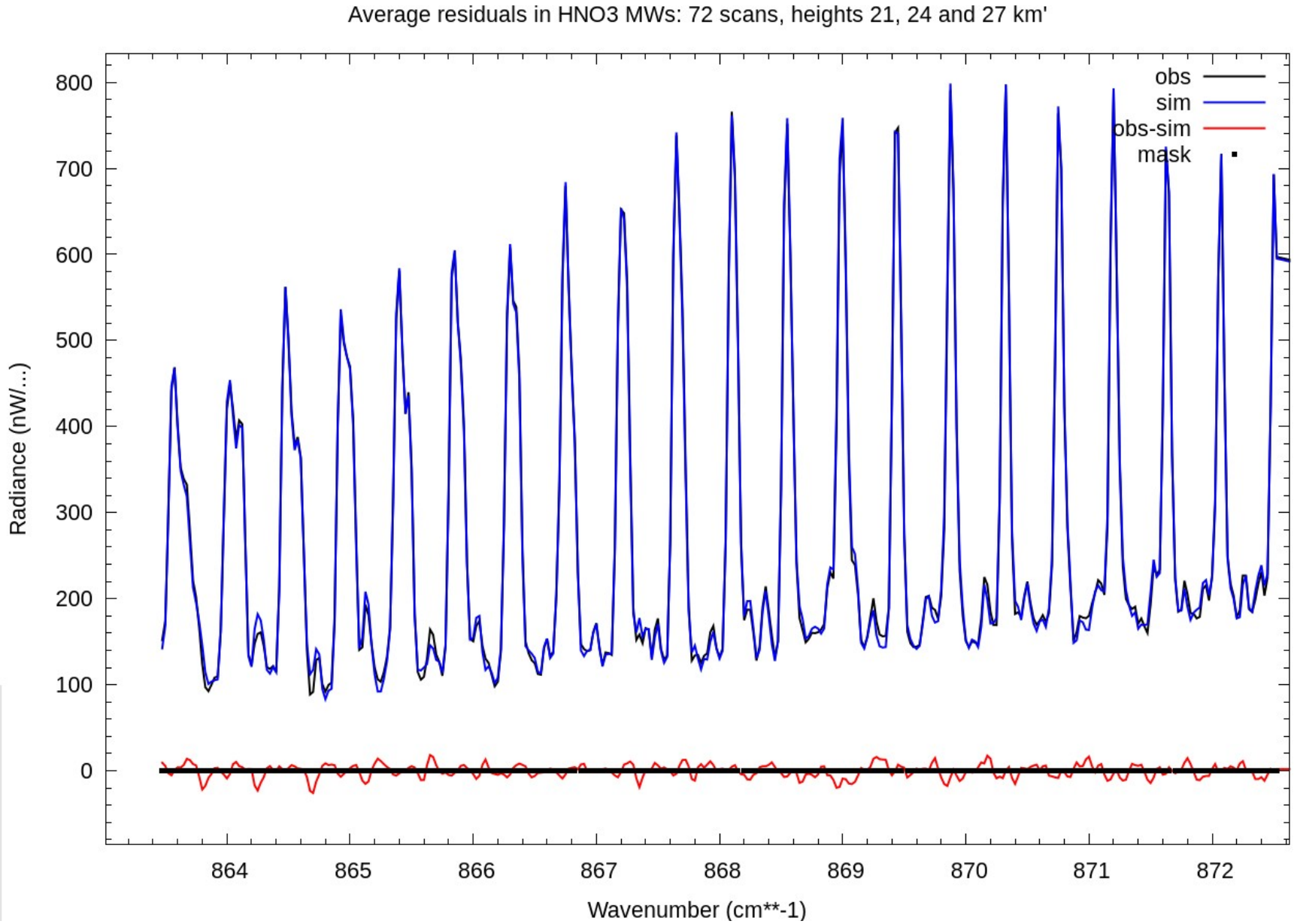
- In the plots we show averages of:
  - **observation (obs)**,
  - **simulation (sim),**
  - **residual (obs-sim),**
  - **and spectral masks (mask)**

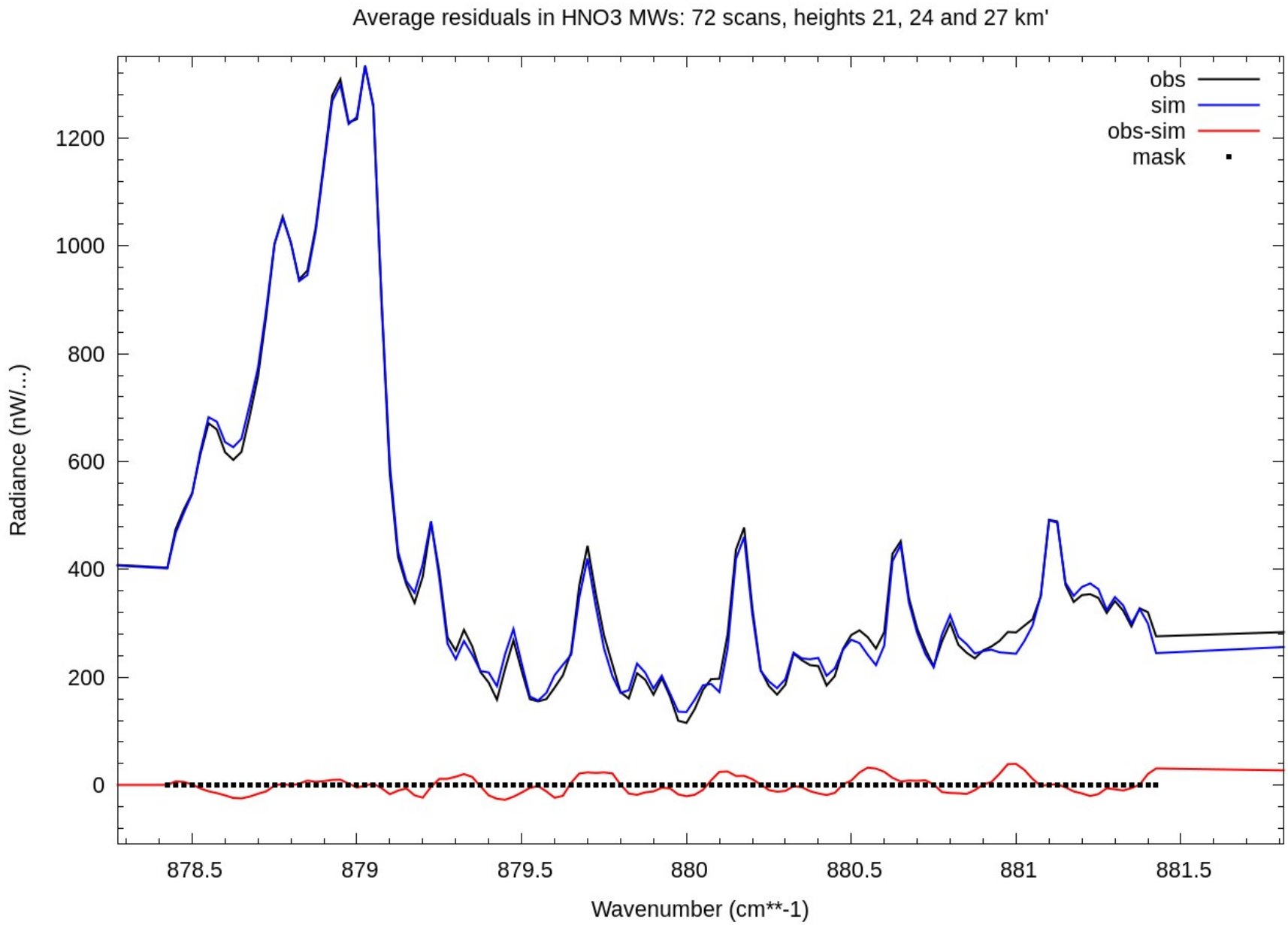
- Averages are calculated over the 72 scans of the orbit 04718 (24/01/2003) and over the sweeps at nominal tangent heights of: 21, 24 and 27 km.

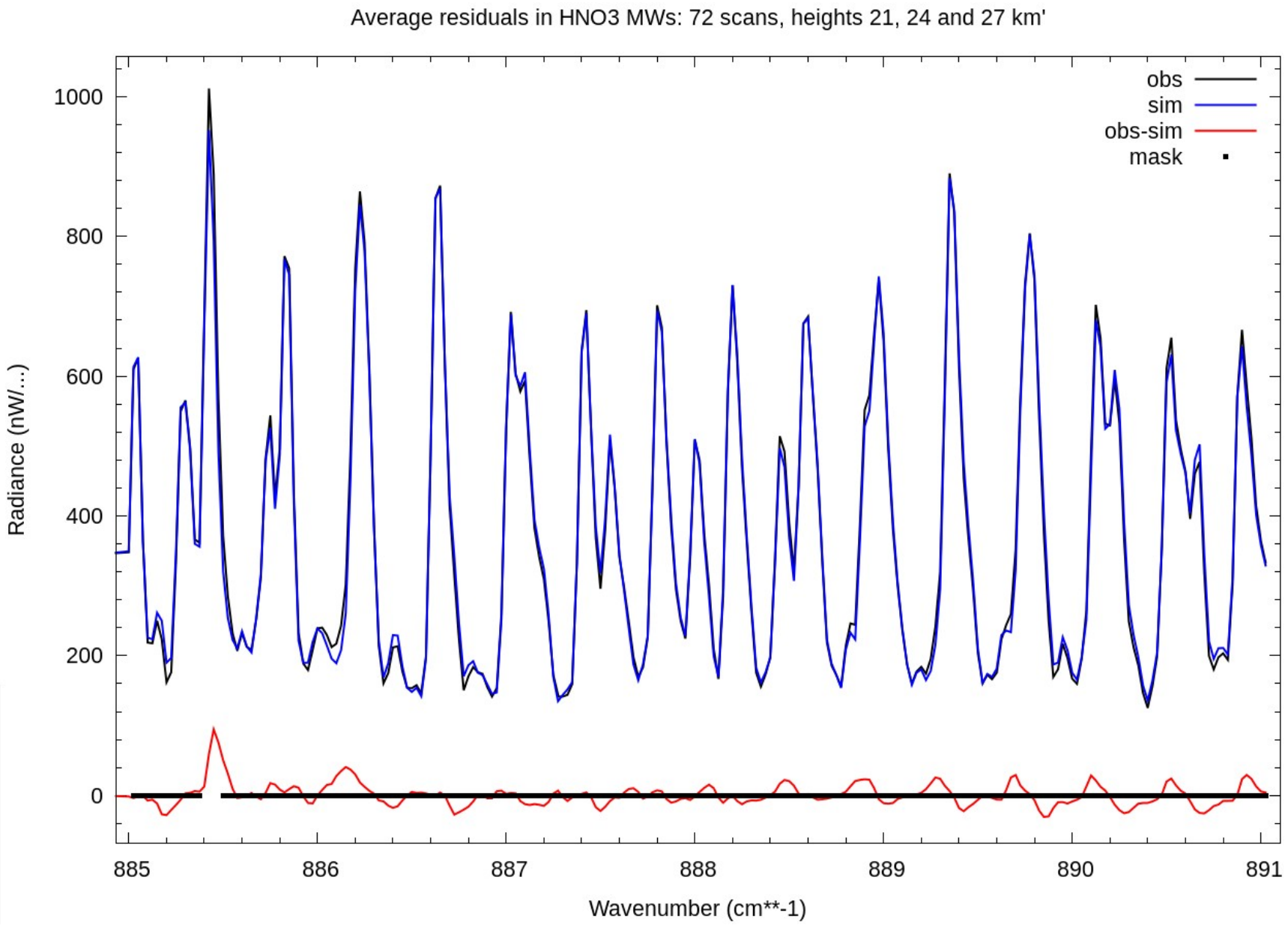
- Note: differences between 3.30 and 4.45 residuals are very small due to the fact that we mainly changed the line intensities ===> differences in line intensities are compensated with a difference in the retrieved HNO3 VMR. However, if we look at average spectra we do see an improvement in the residuals, see presentation from meeting QWG 28.

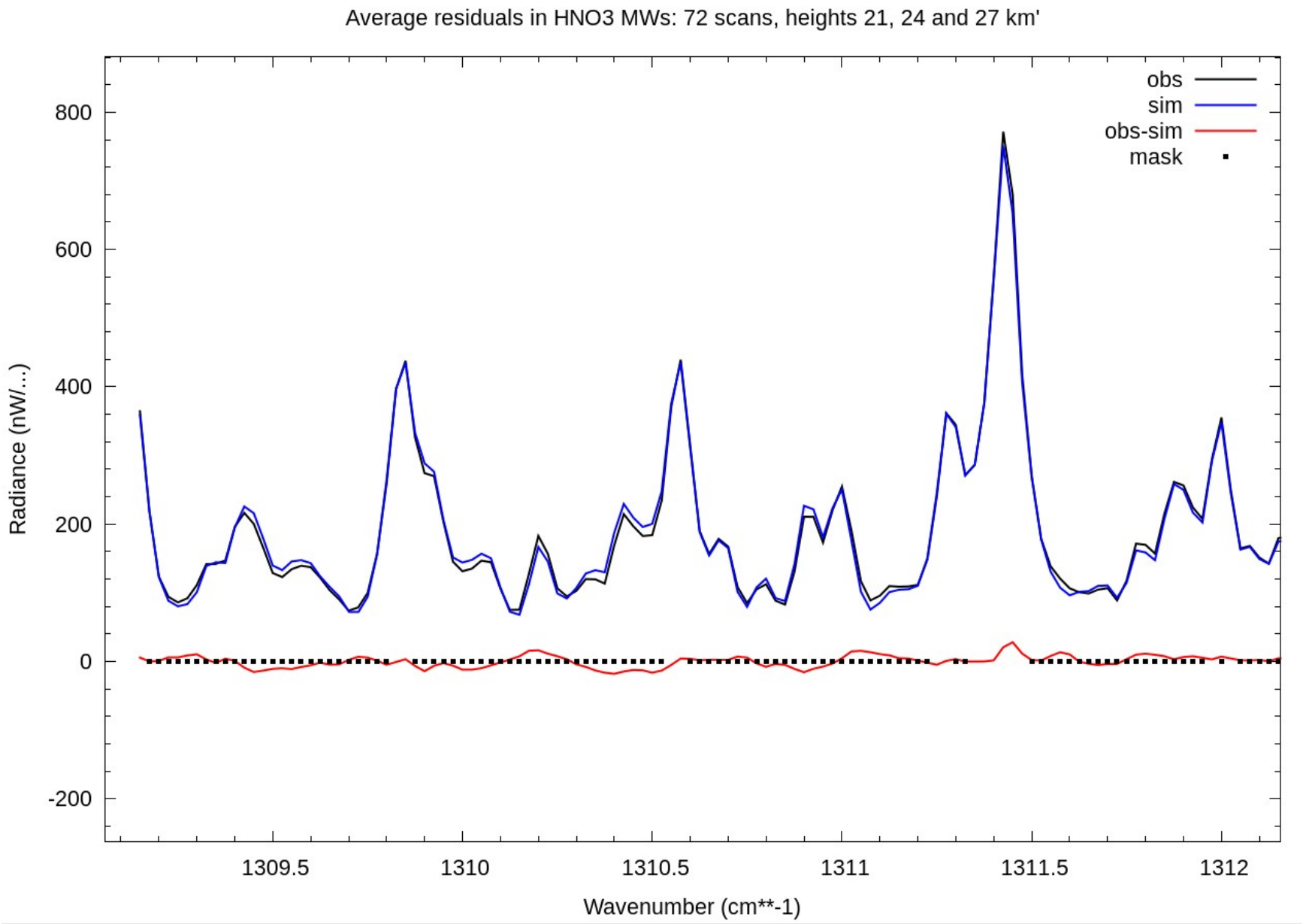
- Please keep in mind the noise levels in MIPAS spectral bands:
  - Band A: ≈ 35 nW/....
  - Band B: ≈ 15 nW/....

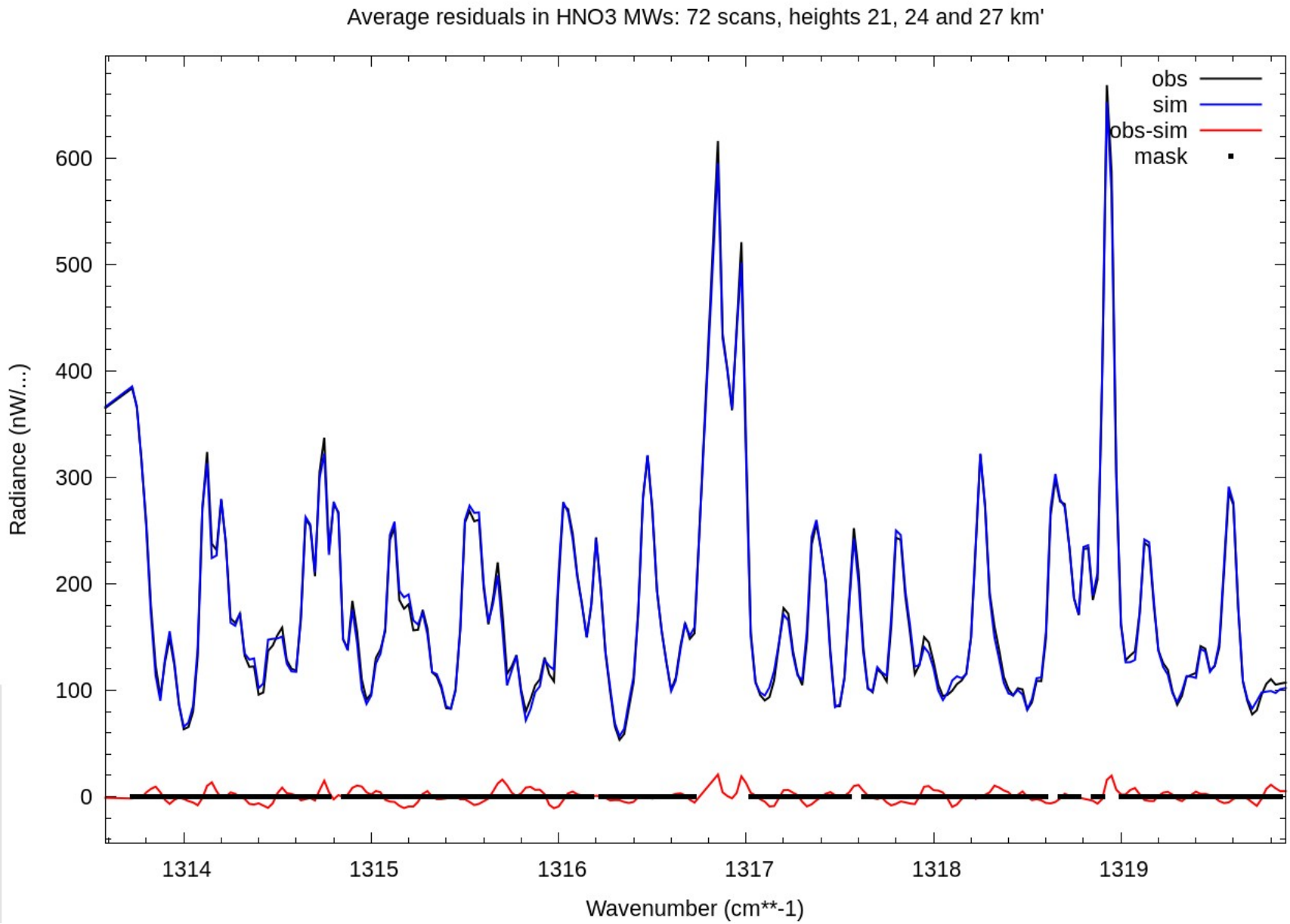
- Comment: in summary the residuals are quite good !

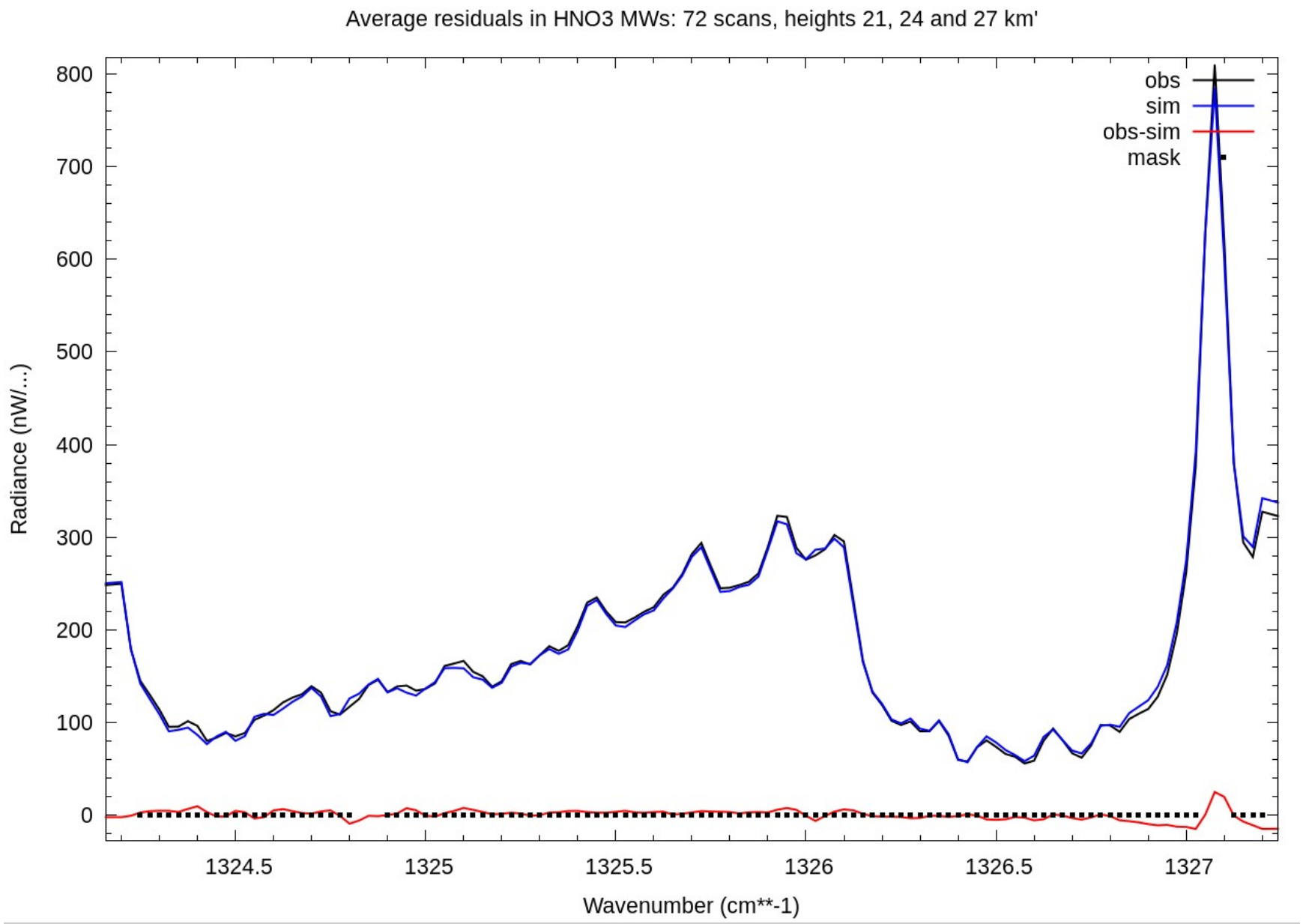

Average residuals in HNO3 MWs: 72 scans, heights 21, 24 and 27 km'
obs
sim
obs-sim
mask
Radiance (nW/...)
800
700
600
500
400
300
200
100
0
864
865
866
867
868
869
870
871
872
Wavenumber (cm**-1)

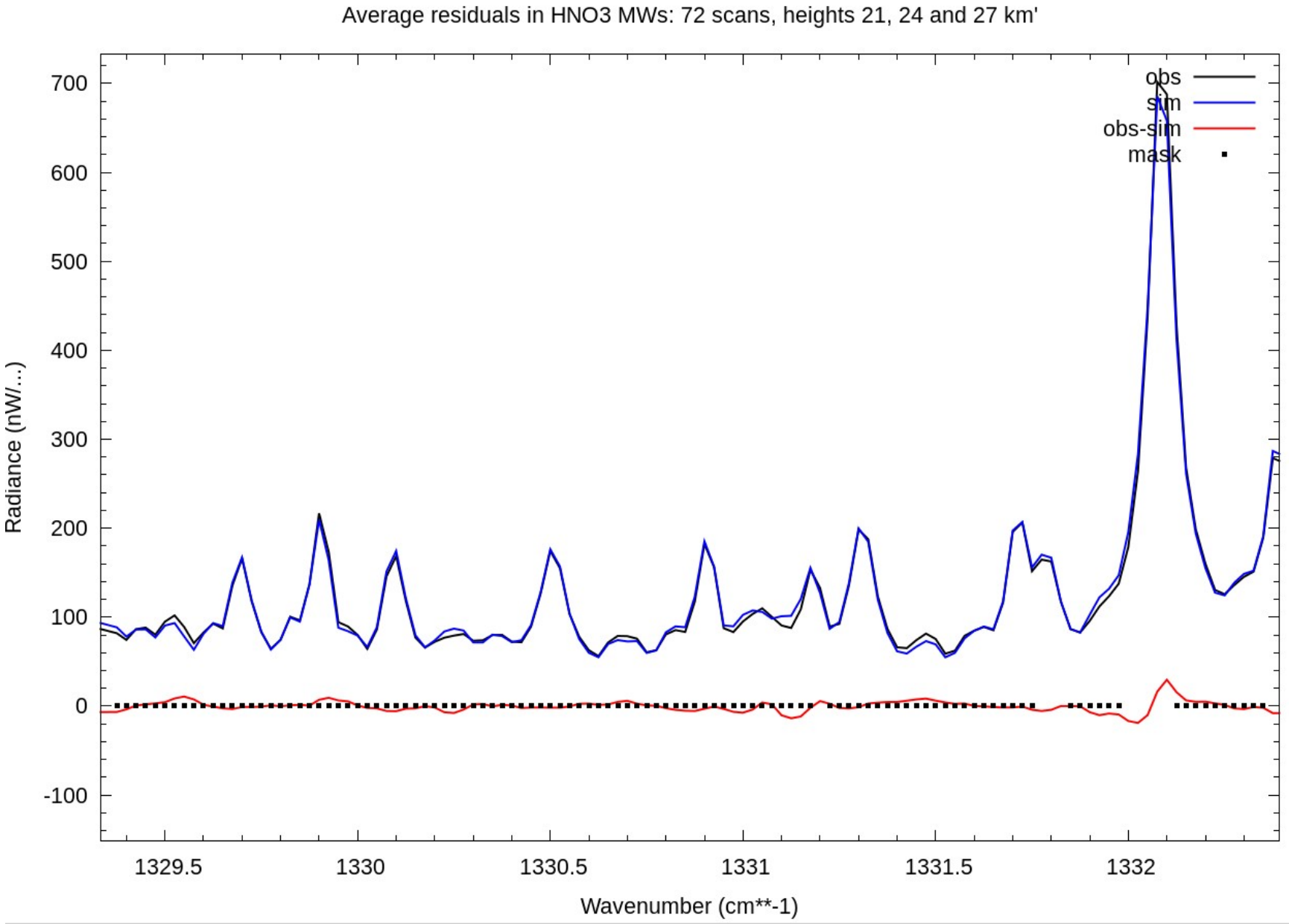

Average residuals in HNO3 MWs: 72 scans, heights 21, 24 and 27 km'
obs
sim
obs-sim
mask
Radiance (nW/...)
1200
1000
800
600
400
200
0
878.5
879
879.5
880
880.5
881
881.5
Wavenumber (cm**-1)

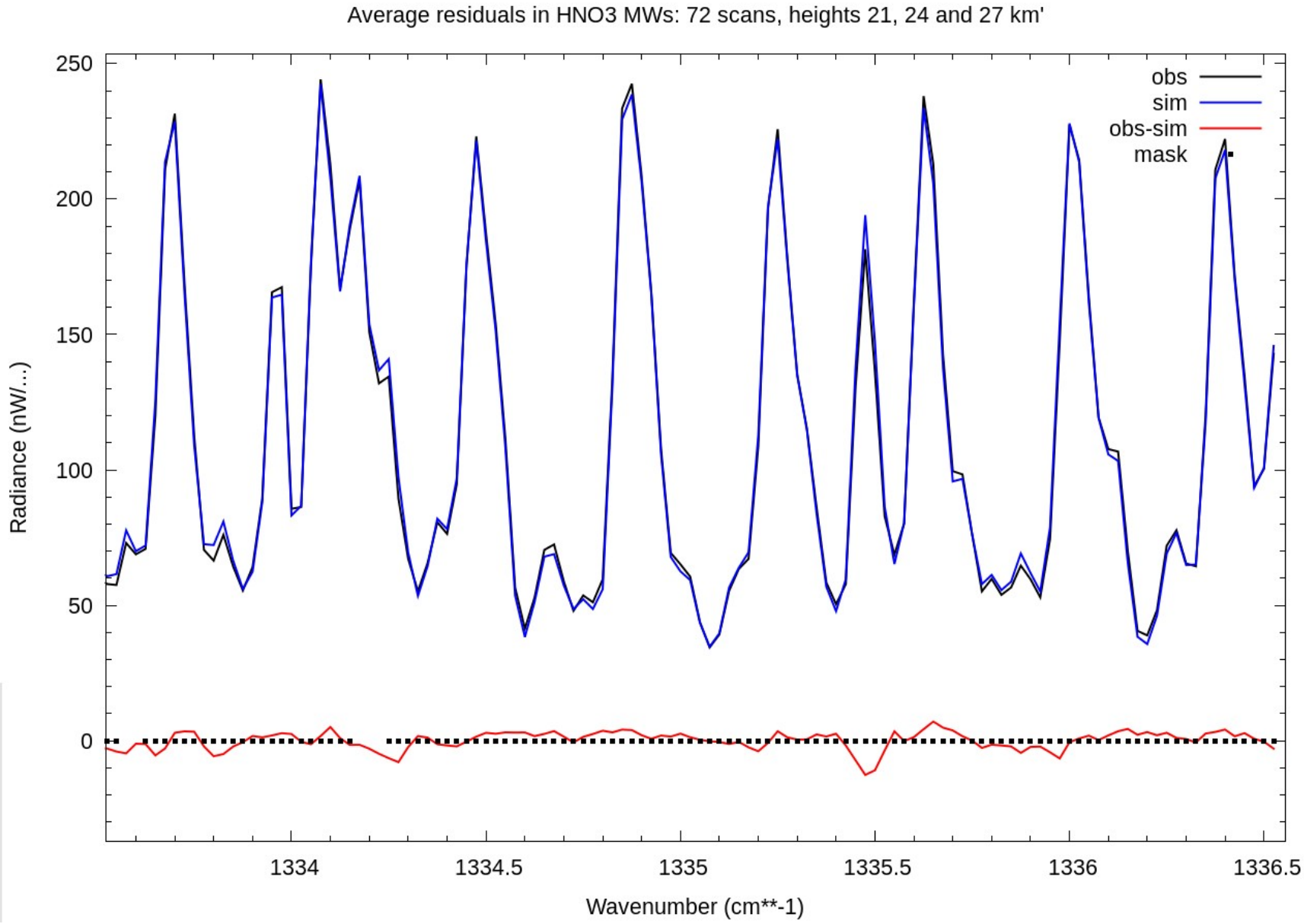

Average residuals in HNO3 MWs: 72 scans, heights 21, 24 and 27 km'
obs
sim
obs-sim
mask
Radiance (nW/...)
1000
800
600
400
200
0
885
886
887
888
889
890
891
Wavenumber (cm**-1)


Average residuals in HNO3 MWs: 72 scans, heights 21, 24 and 27 km'
obs
sim
obs-sim
mask
800
600
400
200
0
-200
Radiance (nW/...)
1309.5
1310
1310.5
1311
1311.5
1312
Wavenumber (cm**-1)

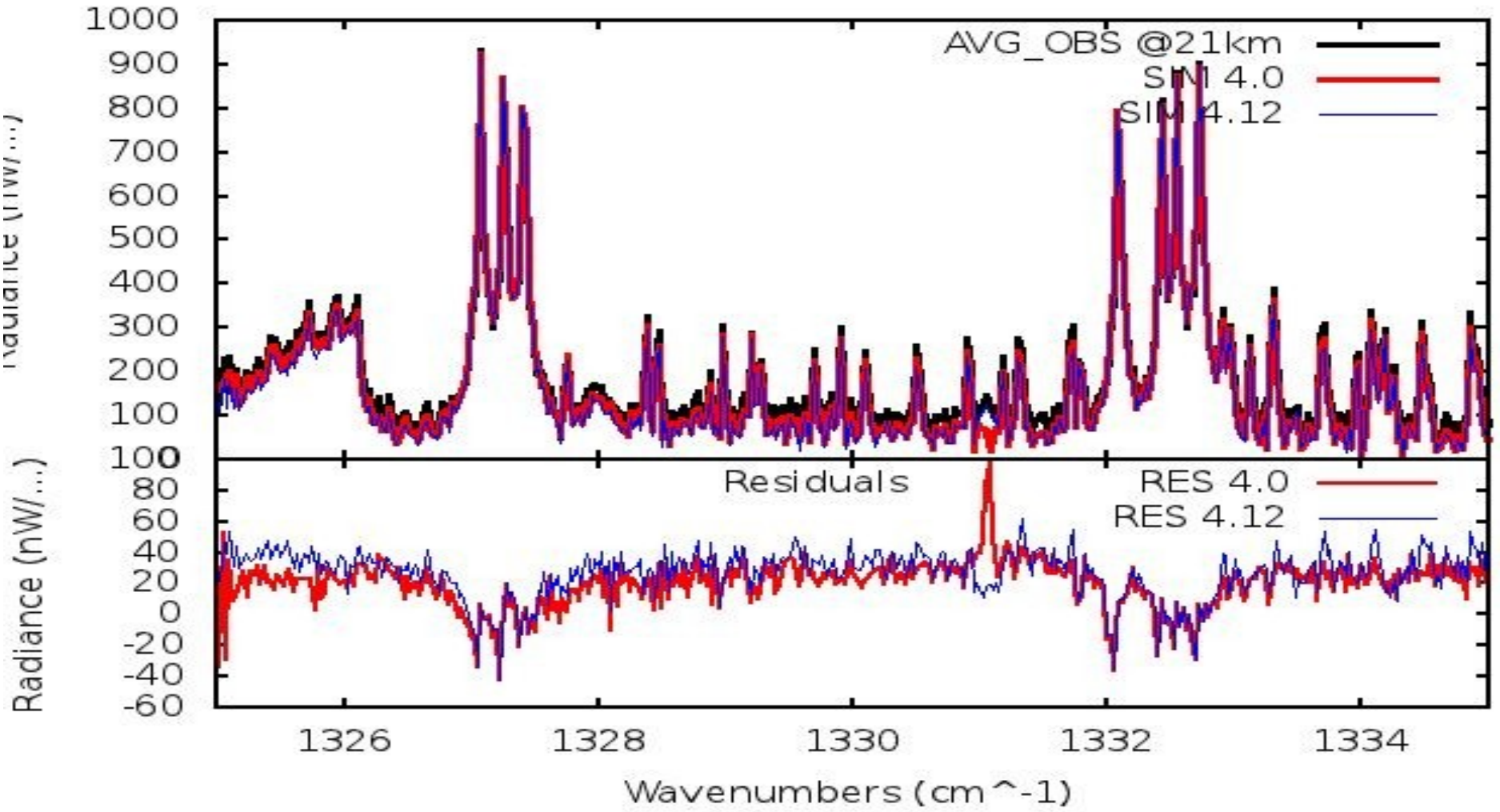

Average residuals in HNO3 MWs: 72 scans, heights 21, 24 and 27 km'
obs
sim
obs-sim
mask
Radiance (nW/...)
600
500
400
300
200
100
0
1314
1315
1316
1317
1318
1319
Wavenumber (cm**-1)


Average residuals in HNO3 MWs: 72 scans, heights 21, 24 and 27 km'
obs
sim
obs-sim
mask
Radiance (nW/...)
800
700
600
500
400
300
200
100
0
1324.5
1325
1325.5
1326
1326.5
1327
Wavenumber (cm**-1)


Average residuals in HNO3 MWs: 72 scans, heights 21, 24 and 27 km'
obs
sim
obs-sim
mask
Radiance (nW/...)
700
600
500
400
300
200
100
0
-100
1329.5
1330
1330.5
1331
1331.5
1332
Wavenumber (cm**-1)


Average residuals in HNO3 MWs: 72 scans, heights 21, 24 and 27 km'
obs
sim
obs-sim
mask
Radiance (nW/...)
250
200
150
100
50
0
1334
1334.5
1335
1335.5
1336
1336.5
Wavenumber (cm**-1)

From QWG 28:


AVG_OBS @21km
SIM 4.0
SIM 4.12
Residuals
RES 4.0
RES 4.12
Radiance (nW/...)
Wavenumbers (cm^-1)
1000
900
800
700
600
500
400
300
200
100
100
80
60
40
20
0
-20
-40
-60
1326
1328
1330
1332
1334