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TOLNet validation of satellite ozone profiles in the troposphere: impact of retrieval wavelengths

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Supplemental Text

Normalized mean biases (NMB, in ppb) were calculated with Eq. (S1)

$$NMB = \frac{\sum_{i=1}^{N}(R_i - O_i)}{\sum_{i=1}^{N} O_i} \quad \text{(S1)}$$

where R_i are the retrievals and O_i are the observations for the i^{th} co-location and N is the total number of retrieval-observation co-locations. To calculate root mean squared error (RMSE, in ppb) we used Eq. (S2).

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(R_i - O_i)^2} \quad \text{(S2)}$$

Supplemental Figures

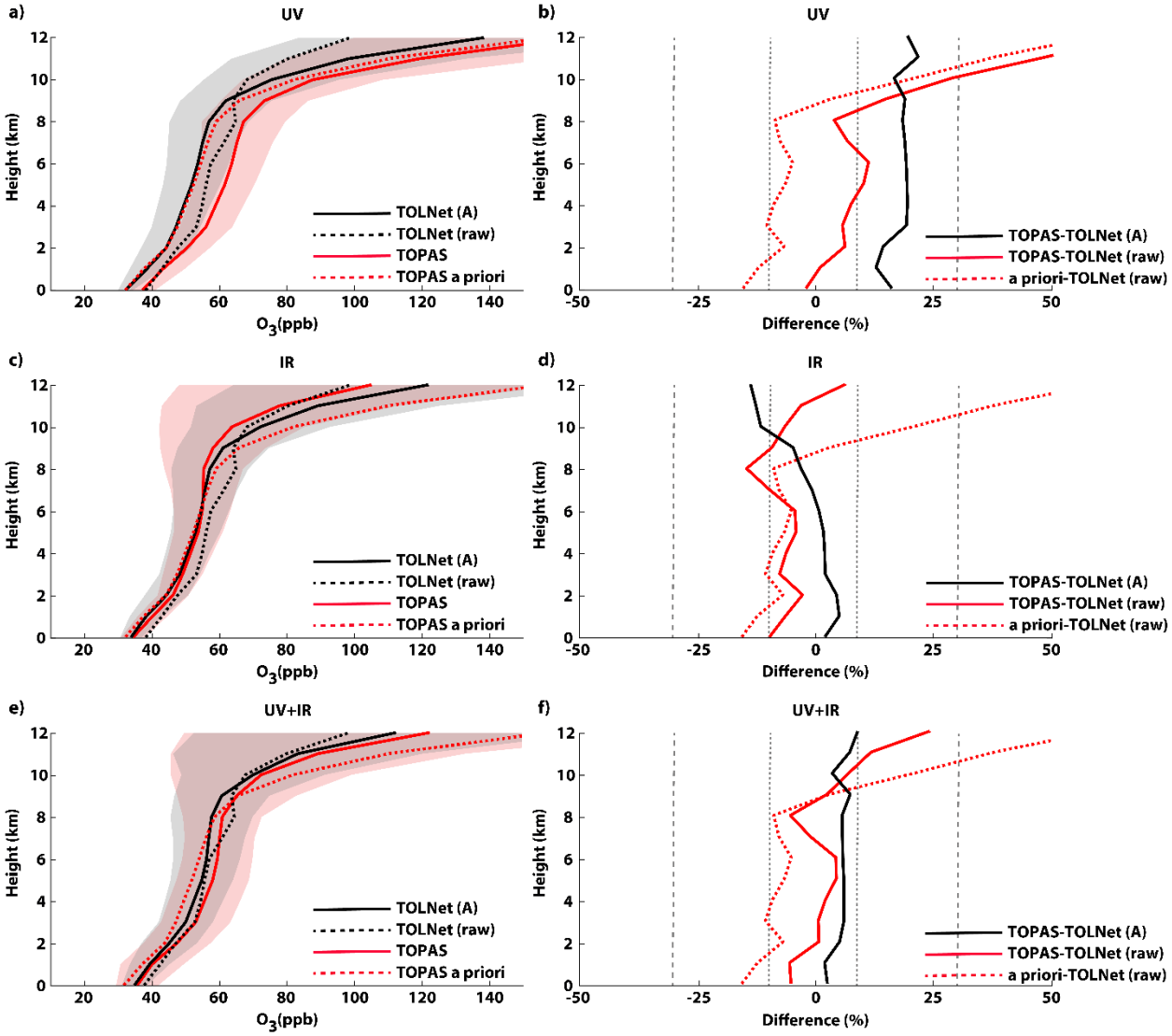

Figure S1. Vertical O_3 profile comparison of TOLNet interpolated to the satellite vertical grid (TOLNet-raw); TOLNet convolved with the satellite averaging kernels (TOLNet-*A*); UV, IR, and UV+IR TOPAS satellite retrievals; and the a priori profile information used in the TOPAS retrieval (total number of colocations (N) = 109) when using the coarser colocation criteria. The direct comparison of the profiles and percent difference, displayed as normalized mean bias (NMB), for UV-only (a, b), IR-only (c, d), and UV+IR (e, f) retrievals are displayed, respectively. The NMB between TOPAS satellite retrievals and TOLNet-*A* and TOLNet-raw used as the references are labeled as TOPAS-TOLNet (A) and TOPAS-TOLNet (raw), respectively. The percent difference between the TOPAS a priori and TOLNet-raw is labeled as a priori-TOLNet (raw). The grey and pink shaded regions illustrate the 1σ standard deviation of TOLNet-*A* and satellite O_3 vertical profiles, respectively. NMB values of 30% and 10% are displayed using grey dashed and dotted lines, respectively.

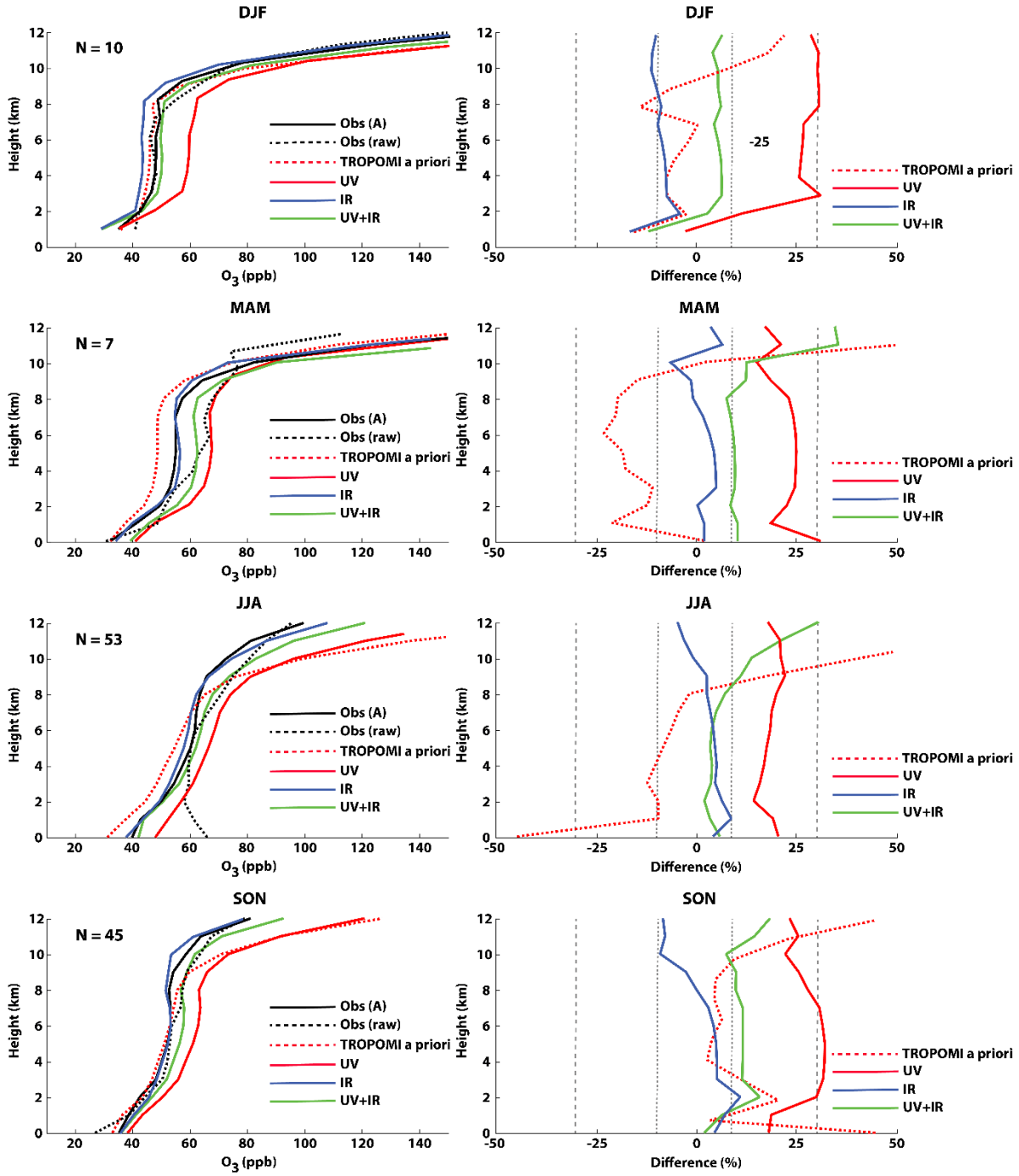

Figure S2. Seasonally-averaged vertical O_3 profile comparison of TOLNet and ozonesonde data interpolated to the satellite vertical grid (Obs-raw); TOLNet and ozonesonde data convolved with the TOPAS averaging kernels (Obs-*A*); UV, IR, and UV+IR TOPAS satellite retrievals; and the a priori profile information. The TOLNet and ozonesonde data profile convolved with the UV+IR averaging kernels are displayed and the two other (UV- and IR-only) convolved profiles are not shown to reduce the number of profiles presented. The direct comparison of the profiles (left column) and normalized mean bias (NMB) (right column) for UV-only, IR-only, and UV+IR retrievals compared to Obs-*A* as the reference are displayed, respectively. NMB values for each of the three retrievals are calculated using Obs-*A* profiles convolved with the correct retrieval-specific averaging kernel as the reference. NMB values of 30% and 10% are displayed using grey dashed and dotted lines, respectively. The total number (N) of co-located profiles are shown in the figure inset.

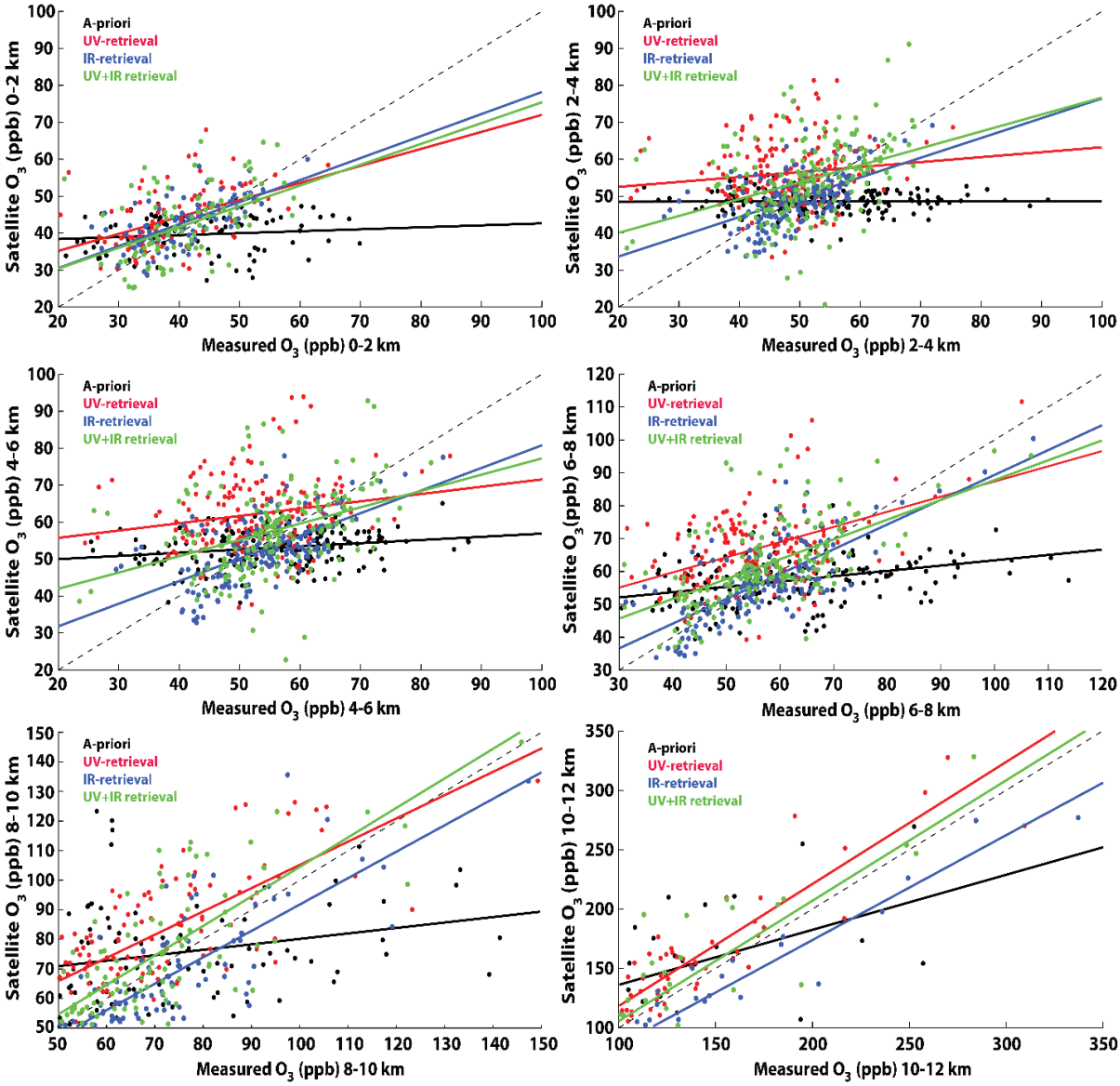

Figure S3. Scatter plot comparison of co-located TOPAS UV-only (red), IR-only (blue), combined UV+IR (green) retrievals, and a priori O_3 vertical profiles to TOLNet observations in 2-km vertical layers between the surface and 12 km asl. The satellite profiles are compared to TOLNet-*A* and the a priori data is compared to TOLNet-raw. The solid-colored lines illustrate the linear regression fit of each satellite-TOLNet comparison and the dashed line represents the 1:1 fit line. Statistics of the intercomparison at each vertical level are presented in Table 3.

Text S1. Evaluation of TOPAS retrievals at 2-km vertical layers in the troposphere

This TROPOMI/CrIS validation at multiple layers in the troposphere allows for more detailed interpretation of the capability of these satellite vertical profiles to retrieve middle- to lower-tropospheric O_3 in comparison to other recent TROPOMI/CrIS validation studies (Malina et al., 2022; Mettig et al., 2022). In the lowest altitudes between the surface and 2 km asl all three retrievals perform similarly; however, the UV-only retrieval has a higher bias and slightly more spread (see bias and RMSE statistics in Table 3). All three retrievals have limited sensitivity to these lower tropospheric regions and are primarily driven by retrieval performance above these altitudes and the shape of the a priori profile. Adding the IR wavelengths, which had NMB of 5.4%, RMSE of 6.3 ppb, and linear regression slope of

0.61, adds additional sensitivity to the lower- to mid-tropospheric regions, improves performance in the UV+IR (NMB of 1.3%, RMSE of 10.1 ppb, slope of 0.57) retrieval compared to the UV-only (NMB of 16.3%, RMSE of 10.4 ppb, slope of 0.47).

Above the lowest portions of the troposphere, the three retrievals have more sensitivity to O_3 and differ more in their performance. Between 2-4 km the UV+IR (NMB of 5.8%, RMSE of 11.7 ppb, slope of 0.46) and especially IR-only (NMB of 4.9%, RMSE of 6.5 ppb, slope of 0.54) retrievals outperform UV-only retrievals (NMB of 18.0%, RMSE of 14.6 ppb, slope of 0.14) due to the enhanced sensitivity provided by the IR wavelengths. The UV+IR and IR-only retrievals have better linear regression slopes compared to the UV-only product (UV-only results have similar slopes as the a priori profile below 6 km) due to the ability to deviate further from the a priori profile shape. In the vertical layer between 4-6 km, similar to the layer between 2-4 km, the UV+IR (NMB of 6.2%, RMSE of 12.3 ppb, slope of 0.45) and in particular the IR-only (NMB of 2.4%, RMSE of 7.5 ppb, slope of 0.62) retrievals outperform UV-only (NMB of 20.1%, RMSE of 16.0 ppb, slope of 0.20) retrievals with less bias and RMSE and better linear regression slopes. It should be noted that the retrievals without UV wavelengths (IR-only) was the only satellite product with improved statistics (lower NMB and higher slope) at 4-6 km compared to 2-4 km. The vertical level around 4-6 km is where IR-wavelengths have peak sensitivity to O_3 in the TOPAS CrIS retrieval, which contributes to this result. However, given that DOFS for O_3 profile retrievals are < 1.0 below 12 km agl, no individual 2 km layer evaluated in this study is completely independent from the retrieval performance throughout the troposphere. For the vertical layer between 6-8 km with IR-only retrievals having the best statistical evaluation (NMB of 0.5%, RMSE of 8.4 ppb, slope of 0.76). Overall, between 2-8 km asl, IR-only retrievals have the least bias and spread, along with best linear regression fits. UV+IR retrievals are similar to IR-only data with only slightly worse performance when compared to TOLNet-***A***. This result demonstrates that while the combination of UV and IR wavelengths tends to improve the performance of TOPAS retrievals compared to UV-only, this is not always the case for IR-only.

In the upper troposphere (8-12 km asl), UV-only retrievals still display the largest positive bias (NMB of 17.5–19.5%, RMSE of 18.2–28.2 ppb, slope of 0.80–1.0) compared to UV+IR (NMB of 4.1–7.8%, RMSE of 15.6–23.2 ppb, slope of ~1.0) and IR-only (NMB of -2.7–-12.1%, RMSE of 12.2–21.2 ppb, slope of ~0.9) retrievals. Comparing the spread in the data between all three profile products, the statistical evaluation were more similar in the upper troposphere compared to the altitudes below 8 km asl. All three products have linear regression slopes near unity; however, IR-only retrievals have a noticeable low bias above 8 km asl. In general, the IR-only and UV+IR retrievals had the least bias out of all three retrievals between 8-10 km and 10-12 km, respectively, when compared to TOLNet-***A*** and IR-only data has the least spread in the 8-12 km vertical level when compared to observations.

At all altitudes in the troposphere the retrievals typically evaluate better (lower bias and RMSE values) to observations compared to the a priori product. The linear regression slope provides information about the capability of the retrieval to deviate from the prior profile shape and magnitudes. Below 8 km the UV-only retrieval has similar linear regression fits compared to the a priori emphasizing the limited sensitivity of these wavelengths to O_3 in the lower troposphere. In the lower- to mid-troposphere the IR wavelengths provide additional DOFs which allow the IR-only and UV+IR retrieval to deviate further from the prior profile shape and compare better to observations. Above 8 km all three retrievals have similar linear regression slopes indicating they are able to deviate to some degree from the

a priori shape and compare better to observations. While neither of the three retrievals have more than 1.0 DOFs below 12 km asl, the information provided by all retrievals improves upon the prior vertical profile suggesting these satellite data provide useful information for studying tropospheric O_3.

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Supplemental Tables

Table S1. Statistical validation of TOPAS UV, IR, and UV+IR retrievals with TOLNet-*A* observations. All observations and satellite retrievals were co-located using 5 hour and 100 km threshold criteria.

Prior

Vertical Level	N (#)	Bias (ppb)	NMB (%)	RMSE (ppb)	Slope
0-2 km	107	-4.4	-13.6	15.8	0.07
2-4 km	206	-5.4	-8.8	13.8	0.03
4-6 km	205	-3.4	-8.1	12.2	0.11
6-8 km	192	-5.3	-6.5	18.2	0.15
8-10 km	153	7.6	-1.3	28.0	0.16
10-12 km	90	44.5	44.8	56.8	0.69
Trop. Column	953	2.0	-1.9	24.5	0.75

UV-only

Vertical Level	N (#)	Bias (ppb)	NMB (%)	RMSE (ppb)	Slope
0-2 km	107	5.5	14.2	11.7	0.41
2-4 km	206	9.1	18.8	14.0	0.11
4-6 km	205	9.9	19.0	15.4	0.20
6-8 km	192	10.2	18.7	16.1	0.44
8-10 km	153	11.8	18.3	17.7	0.82
10-12 km	90	23.7	18.8	30.7	0.91
Trop. Column	953	10.9	17.5	17.2	0.84

IR-only

Vertical Level	N (#)	Bias (ppb)	NMB (%)	RMSE (ppb)	Slope
0-2 km	107	1.7	3.4	5.9	0.57
2-4 km	206	0.9	3.1	6.3	0.51
4-6 km	205	0.5	1.7	7.2	0.58
6-8 km	192	-1.1	-0.1	8.3	0.70
8-10 km	153	-5.5	-4.0	12.7	0.84
10-12 km	90	-14.1	-12.2	19.5	0.93
Trop. Column	953	-1.9	-1.4	10.0	0.84

UV+IR

Vertical Level	N (#)	Bias (ppb)	NMB (%)	RMSE (ppb)	Slope
0-2 km	107	1.5	2.1	10.3	0.51
2-4 km	206	3.0	5.4	11.4	0.42
4-6 km	205	3.2	5.9	11.7	0.41
6-8 km	192	3.2	5.6	10.9	0.55
8-10 km	153	3.5	6.4	15.4	0.92
10-12 km	90	7.9	5.3	26.7	1.10
Trop. Column	953	3.5	5.1	14.1	0.87