# Supplemental Information for "A Convolutional Neural Network for Spatial Downscaling of Space Derived Solar-Induced Chlorophyll Fluorescence (SIFnet)"

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#### S1 Data Correlations of Used Datasets

In Figure S1 the Pearson correlation coefficient on a global map for each grid cell is shown. It stands out that for all products there is only a weak correlation in northern Africa. The ERA-5 air temperature data is in parts very well positive but also negative correlated to *SIF*. Positive correlations are especially in the northern hemisphere, whereas strong negative correlations

- 5 appear in southern parts of the world. Soil moisture (Figure S1c and d) is well correlated with SIF in the southern hemisphere (except for central Australia and southern part of South America). In the northern hemisphere, however, the correlation is notably weaker. All MODIS bands show diverse correlation patterns. Combining some of the bands to compute vegetation indices leads to a much stronger correlation to SIF. All vegetation indices have fundamental difficulties to capture the SIF signal in northern Africa or northern North America. In contrast to  $NIR_v$  the other vegetation indices show also weak correlations in
- 10 the amazon region. Correlations show a dependency on latitude and satellite coverage in Figure S2. Especially in regions near the equator the coverage of the MODIS instrument is only around 20-30%. TROPOMI shows also a weaker coverage but is still over 90%. Interestingly, at latitudes around  $+22.5^{\circ}$  the correlations of *SIF* to the vegetation indices is weaker but this does not correlate to the reduced satellite coverage. At even higher latitudes the correlations and satellite coverage get weaker.



(a) ERA-5 2m mean air temperature

(d) NASA USDA Sub-Surface Soil Moisture

(g) MODIS  $\rho_{BLUE}$  band



(b) ERA-5 total precipitation

(e) MODIS  $\rho_{NIR}$  band

(h) MODIS  $\rho_{GREEN}$  band



(c) NASA USDA Surface Soil Moisture



(f) MODIS  $\rho_{RED}$  band

(i) MODIS  $\rho_{SWIR1}$  band



(p)

**Figure S1. Pearson correlation coefficient of auxilary data to TROPOMI SIF.** Data is compared in 16-day resolution starting in April 2018 until March 2021. Comparison in lowest resolution of the two products: For ERA-5 at 0.25°, for USDA at 0.1° and for all MODIS data at 0.05°.







(a) Latitude dependent r<sub>pearson</sub> of MODIS Vegetation Indices and TROPOMI SIF at 0.05° resolution

(b) Latitude dependent  $r_{pearson}$  of MODIS bands and TROPOMI SIF at 0.05° resolution

(c) Latitude dependent  $r_{pearson}$  of ERA-5 total precipitation and temperature and NASA USDA Soil Moisture data and TROPOMI SIF at 0.1° resolution

**Figure S2.** Latitudinal pearson correlation coefficient of auxiliary data to **TROPOMI SIF.** Data is compared in 16-day resolution starting in April 2018 until March 2020 and March 2021 for ERA-5 data and all others, respectively. Comparison in lowest resolution of the two products: For ERA-5 and USDA soil moisture at 0.1° and for all MODIS data at 0.05°.

Figure S3 shows the time series of the time variant data sets. Differences between the years are visible for several data sets. Outstanding is the reduction in soil moisture in 2021 (Fig. S3c and d). The MODIS bands show some variance between the years that also influence the vegetation indices. In the three vegetation indices NDVI,  $NIR_v$ , and kNDVI (Fig. S3l,m,n) the period from September 2020 until March 2021 show the lowest measured values of the three year period. In contrast to that the TROPOMI SIF measurements are highest for this period, indicating a fundamental different measured event. The reduction in soil moisture for this period might also reduce the photosynthetic activity, which is not confirmed by the SIF measurements.

20 The vegetation indices therefore show a very contrary behavior than the SIF measurements.



Figure S3. Time Series of the used data sets. Data is shown for three years in monthly resolution and global means.

#### S2 Study Regions

Figure S4 shows the six study regions on a global land cover map from Buchhorn et al. (2020). There are five folds (Europe and northern Africa, central Asia, east Asia, southern Africa, and South America) that are used for training the CNN. The set over North America is used as the validation set.

- 25 Table S1 summarizes the exact longitude and latitude borders of the six regions. In Figure S5 the land cover shares are shown. East Asia and the two folds in the southern hemisphere show significantly higher shares of the land cover type "others" which refers to all non-vegetated lands. This also includes water bodies which take up a big share in these regions (compare Figure S4). Using the same region sizes was a necessary step for efficiently training the model. Regions were selected due to linear correlations (Figure S1) and satellite coverage (Figure S2). Australia is due to its big share of shrubs and very noisy
- 30 signals not considered in this work. Further, the amazon rainforest and the region between fold 1 and fold 4 show very weak satellite coverage of MODIS (Figure S2). Except for these regions the data set covers nearly the whole land share of the earth.



Figure S4. Regions of 5-fold cross validation and test set over dominant land cover type. The land cover type is at a resolution of 0.05° from Corine LULC.

Table S1. Longitude and Latitude borders of cross validation folds

Fold	Longitude borders	Latitude borders	Approximate covered area		
1	-10° to 50°	25° to 70°	Europe and North Africa		
2	$50^{\circ}$ to $110^{\circ}$	$15^{\circ}$ to $60^{\circ}$	Central Asia		
3	110° to 170°	$25^{\circ}$ to $70^{\circ}$	East Asia		
4	$10^{\circ}$ to $70^{\circ}$	-45° to $0^{\circ}$	South Africa		
5	-90° to -30°	-60° to -15°	South America		
Test set	-126° to -66°	$15^{\circ}$ to $60^{\circ}$	North America		



Figure S5. Land cover share in cross validation folds and test fold. Will probably be moved to supplemental.

#### S3 Input Feature Investigations

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In Figure 1 (main text) high correlations of all vegetation indices to SIF are observed. Vegetation indices are all computed by the same MODIS bands ( $\rho_{NIR}$ ,  $\rho_{RED}$ , and for EVI also  $\rho_{BLUE}$ ). High common linear correlations of the features to SIFmight also indicate a high collinearity between the features, which is investigated in the following section.

Figure S6a and b show the Pearson correlation coefficient of all input features with each other. Notably, is first upscaled to  $0.5^{\circ}$  and then resampled to  $0.05^{\circ}$  (same as in training process, compare section 3 of main text). The analysis is divided by time variant and invariant data. Here, the correlations are computed for North America from April 2018 until March 2021 in 16 day

resolutions.

- 40 In the time variant features (Figure S6a) a high collinearity between MODIS features (MODIS vegetation indices and individual bands) stands out. Further, moderate correlations between meteorology to MODIS and soil moisture data is detected. Similarly, the cosine of Solar Zenith Angle (cos(SZA)) shows moderate correlations to most other features. The time invariant maps (Figure S6b) show a notably weaker collinearity to each other. Forest shares of the fragmentation data show moderate correlations to forest land cover data. The Land Mask is moderate correlated to the fragmentation data and highly correlated to
- 45 the LC class Others (non-vegetated). Land Mask and the LC class Others are computed from the same data with the difference that Land Mask distinguishes land and water and Others gives the share of non-vegetated in the pixel. Therefore, only in urban areas, which contribute with a rather small area to our global study, these two measure strongly deviate from each other. To further investigate the collinearity and co-variance of the feature data a PCA is conducted in Figure S6c and d for the North America Abdi and Williams (2010). PCA is a dimension reduction method which can be applied to investigate how much
- 50 variance there is in the data set. The PCA applies a singular vector decomposition and computes principle components (PC). Each PC explains a share of variance in the data set ?. In Figure S6c and d the explained variance of each PC is shown for the time variant and time invariant data, respectively. In the time variant data the first nine PCs carry 99% of the variance in the data (of a total of 19 PCs). Therefore more than half of the data does not carry additional information than the others. In the time invariant data a different pattern is observed. The 99% variance is carried by 13 of the 15 PCs. Therefore the time
- 55 invariant data is more diverse. Unfortunately, PCA is not interpretable and NNs can handle collinearity, in contrast to e.g. linear regression methods De Veaux and Ungar (1994). Therefore the PCA is not applied as a data pre-processing step.



Figure S6. Input feature Pearson correlation and explained variance by the principal components for North America. (a) shows the feature correlation of time variant variables. (b) shows the feature correlation of time invariant variables (c) shows the explained variance of the PCs of timely changing variables. (d) shows the explained variance of the PCs of static variables. All data is in  $0.05^{\circ}$  resolution. SIF was first upscaled to  $0.5^{\circ}$  and then resampled to  $0.05^{\circ}$  (same as input). Data is investigated from April 2018 until March 2021 in 16 day time steps.

## S4 Model Development

## S4.1 Hyperparameter Tuning

For hyperparameter tuning the Python library Optuna is used to optimize the parameters learning rate, weight decay, and epoch
of SIFnet Akiba et al. (2019). Here, a TPE-Sampler suggest the parameters of the next trial which is based on a Gaussian Mixture Model. Table S2 summarizes the optimized model parameters.

Figure S7 shows the losses for all investigated hyperparameters that were suggested by Optuna. For visualization a 10-value rolling mean is applied and a threshold of 0.4 is set for the losses as some trials exceeded 2500.



**Figure S7. Loss dependent on hyperparameters.** y axis shows the losses, x axis the investigated values for the hyperparameters. For visualization a 10-value rolling mean is applied to the data.

Table S2. Model parameters

Optimized value
8
Adam
0.0018
0.000057
42

#### S4.2 Cross Validation and Losses of Training Process

- 65 In Figure S8a to Figure S8e the results from a cross validation on the five training areas (shown in Figure S4) are presented. All the training runs were conducted with the model parameters shown in Table S2). The region in the title refers to the validation fold. In Figure S8f the losses of the training data (all five folds) and the test data (North America) for all epochs are shown. In contrast to the actual model training the data augmentation technique is also applied to the validation and test set. This was a necessary step as the regions have different shares of ocean in their footprint (compare Figure S5) which results in not
- 70 comparable losses. Water bodies and missing values are set to zero in the training process, as CNNs can not compute NaNs. Without applying the data augmentation technique (which samples random crops with a maximum share of missing values of 20%) the losses can not be compared between regions. Water bodies are estimated with a high accuracy, as the network only needs to set them to zero.

According to Figure S8a to Figure S8e no sign of overfitting is detected. While the training loss in both Asian regions is lower than the validation loss for South America and Europe (Northern America the validation loss is lower. In Southern Africa both

75 than the validation loss, for South America and Europe/Northern America the validation loss is lower. In Southern Africa both

losses are in the same order of magnitude. After the cross validation the network is trained with all training folds and validated on the test set over North America (Figure S8f). Also here, the test loss follows the training loss.



**Figure S8.** Loss of cross validation. (a) to (e) shows the losses of the 5-fold cross validation. The region in the title of the subfigure refers to the validation fold. All other four folds are used for training. (f) shows the losses of training on all five training folds and testing on the test set.

#### S4.3 Comparison of Model Structures

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Figure S9 visualizes eight investigated CNN model structures. Model complexity is decreasing from a to h. All models perform similar well (Table S3). Model structure 5 (e) is chosen as the best trade off between complexity and performance. Further, the input feature collinearity and PCA shown in Section S3 shows that some input features show high correlations with each other which suggests a feature reduction model structure with decreasing the number of channels in the first convolutional layers (in model 5, from 34 to 16 in the first layer).



(a) Model Structure 1



(c) Model Structure 3



(e) Model Structure 5 (chosen for SIFnet)



(g) Model Structure 7



(b) Model Structure 2



(d) Model Structure 4



(f) Model Structure 6



(h) Model Structure 8

**Figure S9. Investigated Model Structures.** (a) to (h) show compared model structures with decreasing complexity. Results after optimization are shown in Table S3.

Structure	RMSE	SSIM	<b>r</b> <sup>2</sup>
1	0.16	0.88	0.93
2	0.16	0.89	0.93
3	0.17	0.87	0.93
4	0.16	0.89	0.93
5 (chosen for SIFnet)	0.17	0.87	0.92
6	0.18	0.88	0.92
7	0.17	0.86	0.92
8	0.21	0.77	0.89

Table S3. Results of Model Structures after Optimization for the test set over North America.

#### S4.4 Individual loss function

In Figure S10 the mean high resolution estimate of SIF for the San Francisco Bay Area is shown. Further, two modified versions of that image are appended. One with random noise and the other with a constant value added. The RMSE and SSIM metrics are computed for the modified images to the original image. Both modified images show the same RMSE but they deviate strongly in their SSIM. The SSIM metrics is notably lower for the random noise image than for the one with the constant added. This shows that there are multiple versions of the same RMSE deviation. In the loss function used in this work, both metrics are considered and the model is therefore optimized on the overall deviation and on structural similarity from the model output to the ground truth.



Figure S10. Advantage of own loss function

### S4.5 Varying Input Data Combinations

Three further input feature combinations are evaluated in Figures S11, S12, and S14. In the results from Figure S11 the MODIS vegetation indices ( $NIR_v$ , NDVI, EVI, and kNDVI) are not used as features. Therefore, the network needs to get

95 the vegetation information directly from the MODIS bands. Only a minor reduction in performance is observed in the RMSEmetrics from 0.17 (with vegetation indices) to 0.18 (without vegetation indices). The metrics SSIM and  $r^2$  are unchanged for North America. Feature importance still suggests the low resolution SIF feature as the most important one, followed by the MODIS NIR band and the land cover information from Buchhorn et al. (2020).





Figure S11. Results of Data Option without any MODIS vegetation indices. (a) shows the scatter comparison between TROPOMI SIF and the SIFnet estimate at  $0.05^{\circ}$ . (b) shows the metrics  $r^2$ , SSIM, and RMSE of each investigated month. Metrics is calculated in 16 day resolution and averaged to monthly values afterwards. (c) shows the feature importance of the optimized SIFnet. Some input variables are clustered and all variables of that class are permuted at the same time. LULC: all eleven land cover classes; SM: surface soil moisture and sub-surface soil moisture; Mereor.: temperature, precipitation, temperature with 16 day delay, precipitation with 16 days delay.

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Figure S12 shows the results for North America, if the low resolution SIF feature is not considered as a input variable. Interestingly, in contrast to the findings from Figure 5 (main text) the vegetation index  $NIR_v$  is not considered by the model anymore. Rather it relies strongly on the cosine of the solar zenith angle, the MODIS NIR band and the two vegetation indices kNDVI and NDVI.  $NIR_v$  is strongly linear correlated to the other vegetation indices (Figure S6). These findings suggests that there are several solutions to the optimization problem that depend on the input feature combination. Reasons for this can be the high collinearity between the features (Section S3). Further, CNNs can process non-linear

105 relationships and can therefore compute the vegetation indices or similar indices by themselves. But also optimizing another CNN model structure (structure 2 in Figure S9) results in a similar feature importance (shown in Figure S13). The vegetation index kNDVI stays more important than  $NIR_v$ . But the model relies most on cos(SZA).





Figure S12. Results of Data Option without low resolution SIF as feature. (a) shows the scatter comparison between TROPOMI SIF and the SIFnet estimate at  $0.05^{\circ}$ . (b) shows the metrics  $r^2$ , SSIM, and RMSE of each investigated month. Metrics is calculated in 16 day resolution and averaged to monthly values afterwards. (c) shows the feature importance of the optimized SIFnet. Some input variables are clustered and all variables of that class are permuted at the same time. LULC: all eleven land cover classes; SM: surface soil moisture and sub-surface soil moisture; Mereor.: temperature, precipitation, temperature with 16 day delay, precipitation with 16 days delay.





Figure S13. Results of Data Option without low resolution SIF as feature with model structure 2 from Figure S9 (a) shows the scatter comparison between TROPOMI SIF and the SIFnet estimate at  $0.05^{\circ}$ . (b) shows the metrics  $r^2$ , SSIM, and RMSE of each investigated month. Metrics is calculated in 16 day resolution and averaged to monthly values afterwards. (c) shows the feature importance of the optimized SIFnet. Some input variables are clustered and all variables of that class are permuted at the same time. LULC: all eleven land cover classes; SM: surface soil moisture and sub-surface soil moisture; Mereor.: temperature, precipitation, temperature with 16 day delay, precipitation with 16 days delay.

Figure S14 shows the results for North America, if only the low resolution SIF (SIF<sub>LR</sub>) and the vegetation index NIR<sub>v</sub> are considered as input to the model. These have been shown to be the two most important predictors (Figure 5 main text).
110 Interestingly, the metrics r<sup>2</sup> and RMSE only worsen by 0.01 each. In contrast to that the SSIM reduces from 0.87 to 0.68

in average (here the average SIF signal of the three investigated years are compared). The importance of SSIM is explained in Figure S10. The overall deviation of the model output to the validation data is similar to the model output with all input features, but the structural patterns deviate strongly. This finding suggests that the auxiliary data beyond  $NIR_v$  especially contribute to estimating structural similarity (e.g., cos(SZA) for very high latitudes).



Figure S14. Results of Data Option with only  $SIF_{LR}$  and  $NIR_v$  as features. (a) shows the scatter comparison between TROPOMI SIF and the SIFnet estimate at 0.05°. (b) shows the shows of each investigated month the metrics  $r_2$ , SSIM, and RMSE. Metrics is calculated in 16 day resolution and averaged to monthly values afterwards.

#### 115 S4.6 Investigating Different Scaling Factors during Training the CNN

Higher scaling factors between low and high resolution SIF mean that in the optimization process a model is trained to resolve to a higher spatial resolution from the initial situation of  $0.05^{\circ}$ . Using a scaling factor of 20 or 50 estimation resolution of  $0.0025^{\circ}$  and  $0.001^{\circ}$  can be achieved, respectively.

Using a upscaled 1° SIF product as input, which trains the model to resolve with a scaling factor of 20, the  $r^2$  reduces to 0.9 (Figure S15). Increasing the scaling factor further to 50, where the input SIF is at a resolution of 2.5° the  $r^2$  metrics decreases to 0.87. A potential estimated high resolution SIF product would be at 0.001° (appr. 100 m) resolution. Interestingly, leaving the coarse SIF feature out of the model results in an  $r^2$  of 0.84 (Figure S16) which is lower than using this very coarse 2.5° SIF product. The 2.5° SIF still contributes to the result as the second most important feature following  $NIR_v$ . The SIF product might contribute by providing information about radiation, seasonal cycle or the order of magnitude of SIF in the area.



Figure S15. Test set results of SIFnet training at  $0.05^{\circ}$  with a scaling factor of 20. (a) shows low resolution SIF that is used as model input. (b) shows the estimated SIF at  $0.05^{\circ}$  by SIFnet. (c) shows the measured TROPOMI SIF at  $0.05^{\circ}$  from Köhler et al. (2018). (d) shows the scatter comparison between TROPOMI SIF and the SIFnet estimate at  $0.05^{\circ}$ . (e) shows the shows of each investigated month the metrics  $r^2$ , SSIM, and RMSE. Metrics is calculated in 16 day resolution and averaged to monthly values afterwards. (f) shows the feature importance.



Figure S16. Test set results of CNN training at 0.05° with a scaling factor of 50. (a) shows low resolution SIF that is used as model input. (b) shows the estimated SIF at 0.05° by SIFnet. (c) shows the measured TROPOMI SIF at 0.05° from Köhler et al. (2018). (d) shows the scatter comparison between TROPOMI SIF and the SIFnet estimate at  $0.05^{\circ}$ . (e) shows the shows of each investigated month the metrics  $r^2$ , SSIM, and RMSE. Metrics is calculated in 16 day resolution and averaged to monthly values afterwards. (f) shows the feature importance.



**Figure S17. SIFnet and downscaled SIF, the difference between these, and the dominant land cover type for five urban regions across CONUS.** First column shows the SIFnet estimate, second the downscaled SIF from Turner et al. (2020), third the difference between SIFnet and downscaled SIF and the last shows the dominant land cover type from Buchhorn et al. (2020).



**Figure S18. Test set results of SIFnet training at 0.05^{\circ} using daily SIF estimates** (a) shows low resolution Daily SIF that is used as model input. (b) shows the estimated Daily SIF at  $0.05^{\circ}$  by SIFnet. (c) shows the measured TROPOMI Daily SIF at  $0.05^{\circ}$  from Köhler et al. (2018). (d) shows the scatter comparison between TROPOMI Daily SIF and the SIFnet estimate at  $0.05^{\circ}$ .

Figure S18 shows the result of training on daily SIF estimates. For estimating daily corrected SIF the instantaneous measurement is scaled by the cosine of the solar zenith angle (Equation 7 main text).  $r^2$  is similar to the approach of instantaneous SIF and the *SSIM* shows a better result. RMSE is lower as the value range of the daily SIF is lower than that of instantaneous SIF.

#### 130 S7 Validation against OCO-2 and OCO-3 data

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Figure S19a shows the scatter comparison of TROPOMI SIF and OCO-2 and OCO-3 SIF on a  $0.05^{\circ}$  grid over North America. OCO SIF is gridded to a  $0.05^{\circ}$  grid by the center point of the pixel. Latitudinal borders are from  $25^{\circ}$  to  $50^{\circ}$  and longitudinal border are from  $-126^{\circ}$  to -66. TROPOMI SIF shows a better agreement with OCO-3 than with OCO-2 in the metrics  $r^2$  but a weaker correlation in the person correlation coefficient. Generally, the data sets deviate with a high *RMSE* relative to the value range. *RMSE* is 0.37 and 0.43 for OCO-2 and OCO-3, respectively.



**Figure S19. OCO-2 and OCO-3 SIF vs. TROPOMI SIF at 0.05° spatial resolution over North America.** OCO SIF is gridded to a 0.05° grid by the center point of the pixel. Latitudinal borders are from 25° to 50° and longitudinal border are from -126° to -66°. OCO-2 comparison of a three year time period from April 2018 until March 2021 in 16 days averages. OCO-3 comparison from August 2019 until March 2021.



Figure S20. SIFnet and downscaled SIF, the difference between these, and the difference in correlation to OCO-2 and OCO-3 for four urban regions. First column shows the correlation of SIFnet SIF to OCO-X, second the correlation of downscaled SIF from Turner et al. (2020) to OCO-X, third the difference in correlation of the high resolution SIF estimates to OCO-X data on a 0.02° grid and fourth the difference between SIFnet and downscaled SIF.

Table S4. Pearson Correlation Coefficient of SIFnet and Downscaled SIF vs. OCO-2 and OCO-3 SIF dependent on Land Cover Type After Daylength Correction. At least 60% of the grid cell need to be covered with the specific land cover type. There is no data on evergreen broadleaf (EBF) and decidious needle leaf (DNF) available.

	SIFnet			Downscaled			#observations		
	OCO-2	OCO-3	combined	OCO-2	OCO-3	combined	OCO-2	OCO-3	combined
Non-vegetated	0,77	0,81	0,79	0,71	0,72	0,72	130,309	70,852	201,161
ENF	0,79	0,82	0,80	0,73	0,75	0,74	291,620	162,491	454,111
DBF	0,79	0,83	0,8	0,73	0,76	0,74	233,032	109,318	342,350
MF	0,55	0,60	0,56	0,50	0,52	0,51	11,436	5,520	16,956
UF	0,82	0,84	0,82	0,73	0,76	0,74	292,723	141,232	433,955
Shrubs	0,57	0,63	0,59	0,50	0,56	0,52	943,924	525,789	1,469,713
Grassl.	0,59	0,65	0,61	0,53	0,60	0,55	1,077,786	505,942	1,583,728
Crops	0,75	0,75	0,75	0,70	0,69	0,70	788,982	409,494	1,198,476
Wetl.	0,82	0,86	0,84	0,76	0,71	0,73	7,541	9,800	17,341

	SIFnet			Downscaled			#observations		
	OCO-2	OCO-3	combined	OCO-2	OCO-3	combined	<b>OCO-2</b>	OCO-3	combined
San Francisco	0,55	0,47	0,49	0,51	0,46	0,47	7669	19906	27575
Los Angeles	0,33	0,35	0,34	0,3	0,33	0,32	15026	24277	39303
New York City	0,72	0,73	0,69	0,67	0,69	0,65	2500	2568	5068
Seattle	0,47	0,43	0,44	0,34	0,44	0,37	10842	15485	26327
Chicago	0,75	0,73	0,73	0,69	0,71	0,69	15519	12913	28432
Boston	0,8	0,77	0,79	0,69	0,73	0,69	1367	1505	2872

Table S5. Pearson Correlation Coefficient of SIFnet and Downscaled SIF vs. OCO-2 and OCO-3 for Different Cities.

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