FRM4SST Project: Procedure for Satellite SST Validation

Procedures for Satellite SST Validation

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Abstract : This document contains a description of the procedure for satellite Sea Surface Temperature (SST) validation performed by the FRM4SST project team.

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CONTRACT REPORT

The work described in this document was done under ESA contract.
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1	C	06/12/2024	Updated after inputs from team
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1. EXECUTIVE SUMMARY

The FRM4SST project is funded by the European Space Agency (ESA) and, through various activities, aims to sustain and evolve the International Sea Surface Temperature (SST) Fiducial Reference Measurement (FRM) Network (ISFRN). One way that this aim is fulfilled is through the collection, processing, analysis, publication and reporting of *in situ* FRM field measurements made using ISAR and SISTeR Instruments, that are near-contemporaneous with satellite data from the Sentinel-3A and Sentinel-3B SLSTR instruments.

The objectives for the FRM4SST project are:

- OBJ-1: Deploy and maintain shipborne thermal infrared (TIR) FRM radiometers and necessary supporting instrumentation to validate satellite SST products.
- OBJ-2: Maintain FRM protocols for satellite SST measurements and uncertainty budgets.
- OBJ-3: Process, quality control, archive and deliver approved FRM4SST data sets following documented FRM procedures and approve their use for FRM satellite validation.
- OBJ-4: Validate satellite SST products to FRM standards and publish monthly results.
- OBJ-5: Promote the FRM4SST outputs and maintain the International SST FRM Radiometer Network (ISFRN).

In order to ensure that the SLSTR geophysical data products are reliable, they must be validated by comparing them with measurements from the long-term *in situ* deployment of the ISARs, and also from the SISTeR instrument; these measurements confirm the consistency of the SST data products.

This report presents the procedure for satellite Sea Surface Temperature (SST) validation, as performed by the FRM4SST project team.

2. INTRODUCTION

This report is deliverable D-2 on the FRM4SST contract and describes the procedure for the validation of the ESA Sentinel-3 Sea Land Surface Temperature Radiometer (SLSTR) satellite data using SST_{skin} observations from the ISFRN; contributed to by the UoS-, CSIRO- and DMI- operated Infrared Sea surface temperature Autonomous Radiometers (ISARs), the Scanning Infrared Sea Surface Temperature Radiometer (SISTeR) operated by RAL and the Marine-Atmosphere Emitted Radiance Interferometer (M-AERI) operated by the University of Miami.

This report first gives an introduction to the importance of shipborne in situ measurements before describing the data used for the validation (section 3). The validation method is described in section 4 and example validation results are presented in section 5.

2.1 Why are shipborne radiometer measurements so important?

Shipborne radiometric measurements provide the high accuracy (uncertainty <0.1 K) in situ surface temperature measurements needed to validate satellite SST sensors such as the Advanced Along-Track Scanning Radiometer (AATSR) and the Sea and Land Surface Temperature Radiometer (SLSTR). Shipborne radiometers also provide a traceability route to SI standards for satellite measurements and therefore a pathway to generate Fundamental Climate Data Records (FCDRs) from satellite SST measurements (Figure **2**-**1**).

To achieve robust traceability to the SI temperature scale (ITS-90), shipborne radiometer calibrations derived from their internal blackbodies are regularly verified against an SI-traceable laboratory calibration target (Figure **2**-**2**). The traceability of both the shipborne radiometers and the laboratory calibration targets are confirmed on a regular basis through inter-comparisons such as the ESA-funded Fiducial Reference Measurements (FRM) for validation of Surface Temperature from Satellites (FRM4STS) campaign, held in 2016, and the FRM4SST inter-comparison that took place during this contract in 2022.

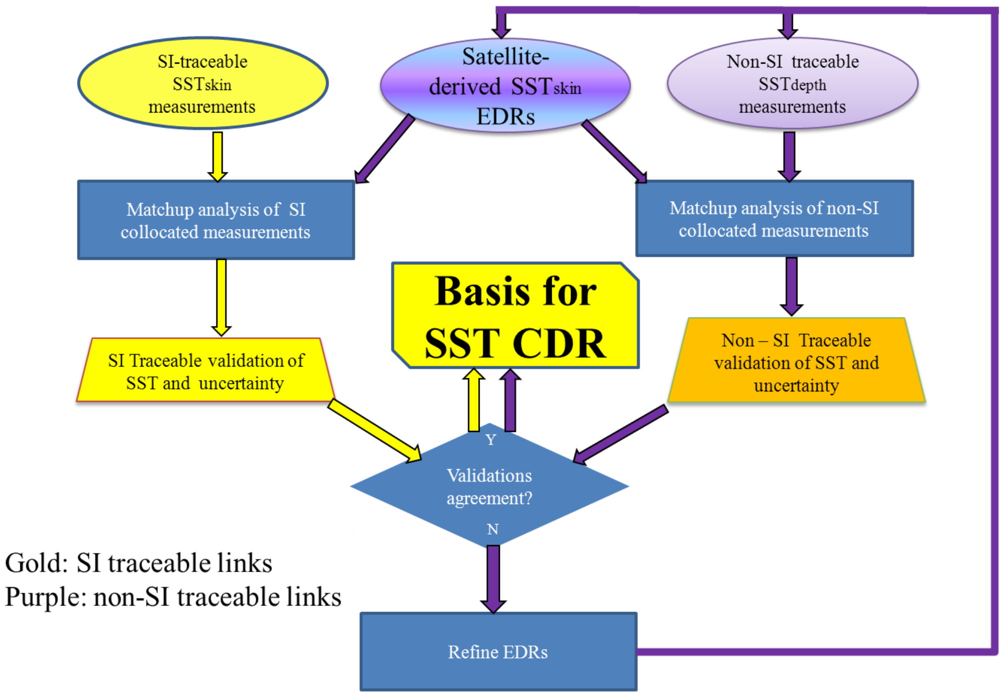

Figure 2-1: This flow diagram shows the traceability route for a SST Climate Data Record (from the ISSI[1] *in situ* validation workshop). Shipborne radiometers cover the yellow parts of the diagram.

Fiducial Reference Measurements are the suite of independent ground measurements that provide the maximum scientific utility and Return On Investment (ROI) for a satellite mission by delivering, to users, the required confidence in data products, in the form of independent validation results and satellite measurement uncertainty estimation, over the duration of the mission[2]. This means that FRM:

- Have documented evidence of SI-traceability via inter-comparison of instruments under operational-like conditions (e.g. the 2016 and 2022 campaigns).
- Are independent from the satellite SST retrieval process.
- Include an uncertainty budget for all FRM instruments and ensure that derived measurements are available and maintained, traceable, where appropriate, to SI.
- Are collected using measurement protocols and community-wide management practices (measurement, processing, archive, documents etc.) that are defined and adhered to.

[1] *International Space Science Institute (ISSI) Working Group on Generation of Climate Data Records of Sea-Surface Temperature from Current and Future Satellite Radiometers – unpublished report (2014)*

[2] *Optical Radiometry for Ocean Climate Measurements, G. Zibordi, C. J. Donlon, A. C. Parr, Volume 47 (2014)*

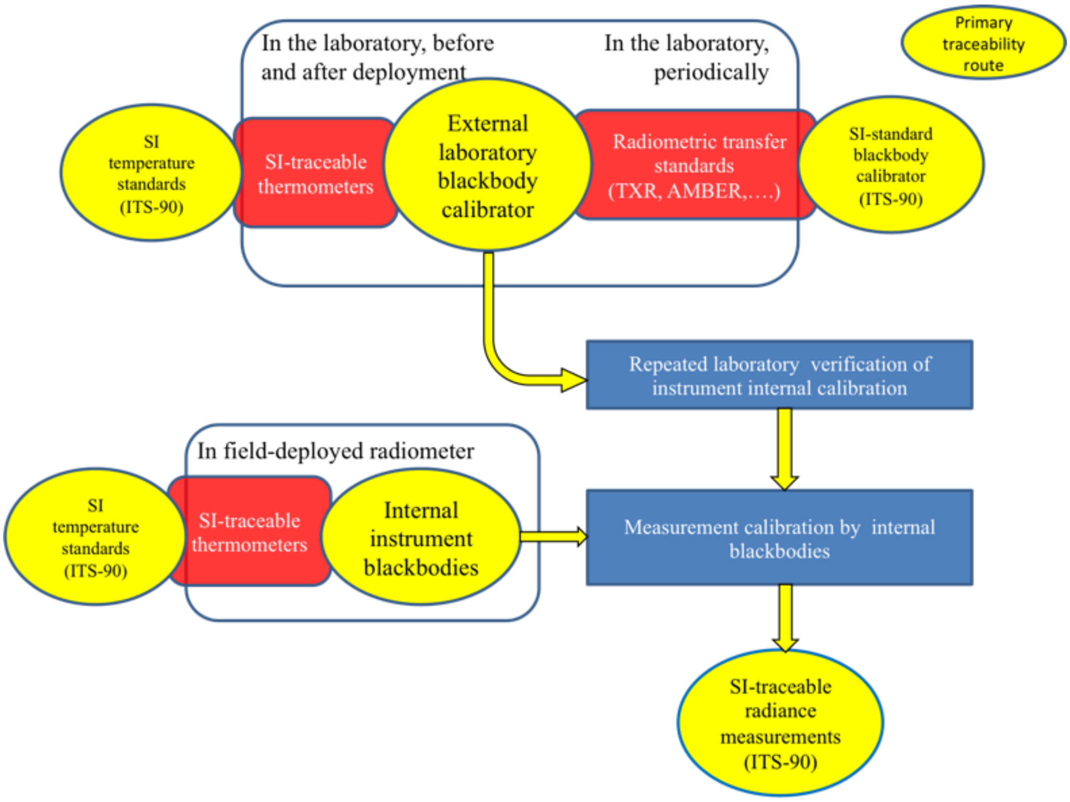

Figure 2-2: Traceability route for a shipborne radiometer (from ISSI *in situ* validation workshop).

Shipborne radiometers (including ISAR, SISTeR and M-AERI) provide an important SI-traceable link between satellite instruments, facilitating the evaluation of any offsets or trends between two instruments. This would normally be achieved by an overlap period of six months or more in the operations of the two satellite instruments; however, this cannot always occur. For example. with the sudden end of Envisat, and delays in the launch of Sentinel-3, no overlap period was possible between AATSR and SLSTR-3A. Nevertheless, because measurements were made by *in situ* instruments including shipborne radiometers throughout the data gap, any geophysical changes in the SST fields during the gap were monitored, ensuring that changes are not an attribute of either AATSR or SLSTR but a genuine geophysical change.

3. DATA

In this section, a brief description of radiometers and the data they produce is given, as well as the satellite data used for the SST validation.

3.1 Satellite measurements: SLSTR

All available Sentinel-3 SLSTR SST products are routinely collected and archived at Ifremer. This archive is used together with the ESA Felyx instance at Ifremer to produce so called “miniProd” satellite data extracts. These miniProd’s were than used by Felyx to generate the match-up database files between ships4sst data and SLSTR data. See section 3.2.1 for more information on the ships4sst data archive.

3.2 Shipborne Radiometers

In this project, ISARs from the UK and Denmark, the SISTeR instrument from the UK, and data from non-project partners using ISAR and M-AERI instruments to ISFRN standards, contribute to the ships4sst data archive and are used to validate satellite SST measurements.

The ISAR instrument is a single channel (waveband, 9.6 - 11.5 μm) scanning radiometer with two internal calibration blackbodies and a multi-angle sky and sea scan mirror, which produces high quality SST_{skin} data to FRM standards. For this validation programme it views the sky and sea at zenith angles of 25° and 155° respectively, and the sea surface emissivity corresponding to the 25° incidence angle is taken as 0.9916. The instrument samples SST by integrating over 40 s of sea view in a measurement cycle that lasts 2 minutes. At typical ship speeds this results in one SST value averaged over a sample area of about 3×500 m, repeated at intervals of 1.5 km along the ship track. Two radiometers are used interchangeably, being switched approximately every three months to allow inspection, servicing and replacement of any worn or optically degraded parts. The exposed optical elements of ISAR, including the scan mirror, are protected from bad weather by a shutter that closes when precipitation, spray or excessive atmospheric dust is detected by an optical rain gauge, so that ISAR can operate autonomously. Routine deployments on the *Pride of Bilboa* began in 2004, after which it was moved onto the *Cap Finistere* between 2010-2012, before it was installed onto the current ship, the *Pont Aven*. There have been 20 years of near continuous operations and between these deployments, approximately 1 million SST measurements have been made, making it one of the longest SST skin data records to date.

M-AERI is a very well-calibrated and stable sea-going Fourier transform infrared (IR) interferometer. It is calibrated before and after each deployment and contains two internal blackbodies, with thermometers with NIST-traceable calibration, for at-sea calibration. It can also be run autonomously with daily checks so can be deployed for months without maintenance. Deployments first began in 1996, and 3 Mk2 M-AERI are usually deployed on Royal Caribbean Group ships since 2000.

SISTeR is a chopped, autonomous, self-calibrating infrared filter radiometer that can measure IR brightness temperatures to high accuracy (~30mK). It is split into three compartments, the inner being the calibration enclosure which hosts two blackbodies and a rotating scan mirror. SISTeR measures the upwelling radiance from the sea surface and corrects for the reflected sky component with measurements of the downwelling sky radiance. The blackbody thermometer calibrations are traceable to ITS-90. SISTeR was first deployed in 1997 and since 2010 has been deployed on the Cunard *Queen Mary 2* (*QM2*) liner (usually sailing between Southampton and New York between May - January and annual world cruise between January - May) where it is mounted on a dedicated platform above the starboard bridge wing. A data logger laptop is connected to the ship's Ethernet network and emails daily level 0 products back to the UK. The instrument can protect itself against bad weather and can operate unattended for extended periods.

All ships4sst data is produced in L2R format, in accordance with the ISFRN L2R product specification[3]. The specification can be found on the ships4sst website and is written for those wishing to implement a processing chain to produce ISFRN L2R data products, as well as users who require detailed technical information on the content and specification of the L2R product.

As part of the operational FRM procedure, calibration measurements are made before and after each deployment to assess the performance of the instruments and to maintain traceability of the observations. An example of a pre-deployment calibration is shown in Figure 3-3 below. The mean difference between ISAR and the calibrated thermistor used in this calibration for this particular experiment was 0.01K with a standard deviation of the differences of 0.03K. More information on the protocols used to maintain the SI traceability of shipborne radiometers in the ISFRN can be found here.

[3] *https://ships4sst.org/sites/shipborne-radiometer/files/documents/Recommended%20ISFRN%20L2R%20Data%20Specification%20and%20User%20Manual%20v1.2%20rev0.pdf*

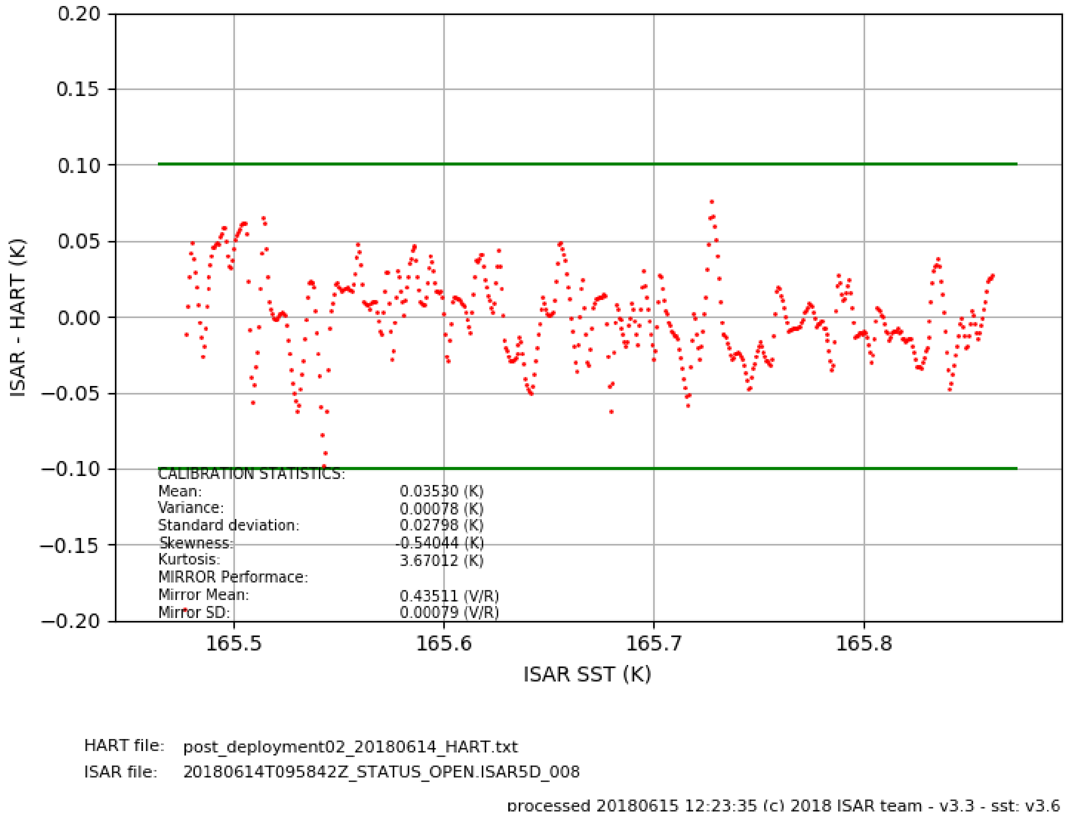

Figure 3-3**:** Calibration results from a DMI deployment, pre-deployment calibration.

3.2.1 Data Archive and Study Area

The ships4sst data archive is hosted at Ifremer, and the Felyx tool at Ifremer processes and generates validation reports and satellite match-ups. This processing is now performed by EUMETSAT. All of the project partners store their ISFRN L2R data files at the archive once they become available, which is normally after the post-deployment calibration. The ISFRN L2R files are accompanied by calibration information, such as calibration factors from the pre- and post-deployment calibrations. Documentation of the traceability of all calibration equipment is also stored at the data archive, as well as on the ships4sst website.

Figure **3-4** shows the collective SST L2R files by data provider plotted on the world map where pink is CSIRO, light red is DMI, green is RAL, blue is RSMAS and deep red is UoS.

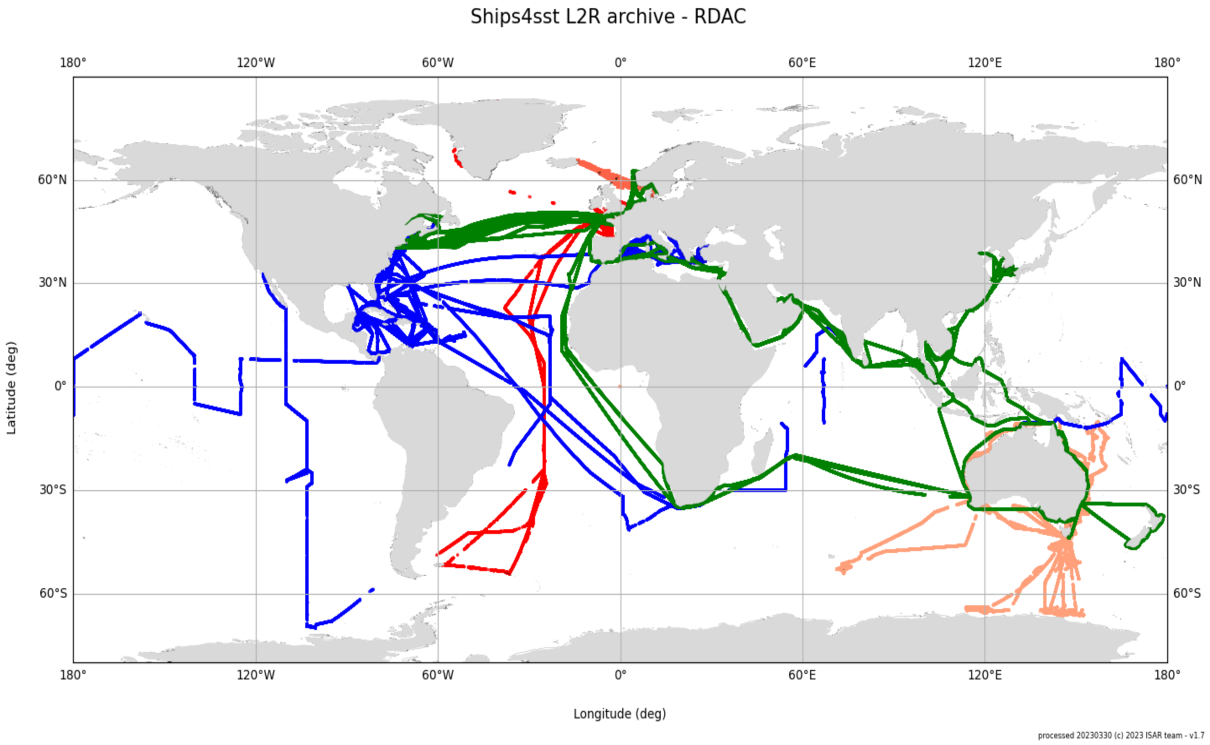

Figure 3-4: The ships4sst data archive L2R files plotted as by data provider, March 2023

The data archive is accessible through the ships4sst web portal and provides data to users on request. Uploading data from non-project partner groups who collect data to ISFRN standard and submit the data in ISFRN L2R format is also facilitated through the ships4sst web portal, as has been done with the CSIRO ISAR and M-AERI data. Figure 3-5 shows the combined archive SST_{skin} data from the ISARs, M-AERI and SISTeR, as shown on a world map.

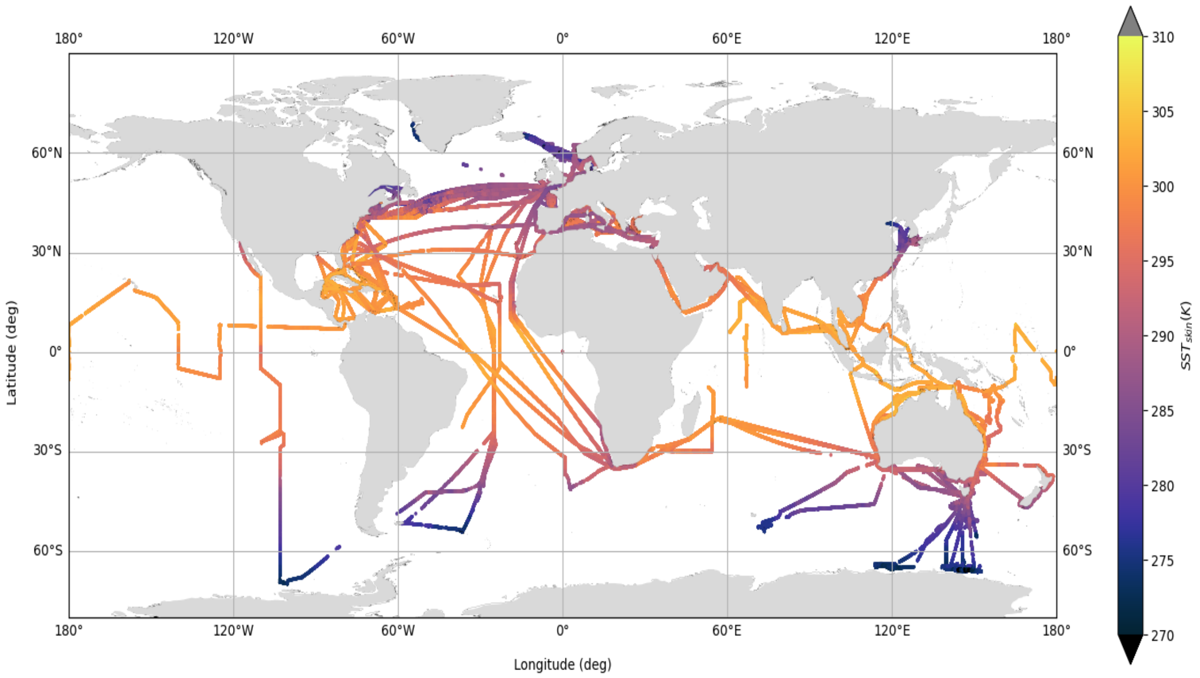

Figure 3-5: The ships4sst data archive L2R files plotted as SST on a world map, March 2023

4. METHOD OF VALIDATION

4.1 Match-up Methodology

The ISAR validation tool uses the Felyx match-up database (MDB) files and follows the procedure as described in Wimmer et al. 2012 by using the Felyx MDB files and working from the central radiometer and SLSTR pixel match outwards until the edge of the match-up window is reached. This is done for 5 match-up windows (See Table 1) and for Gaussian and robust statistics producing location plots of the central match, histograms, dependence plots for wind speed, latitude and uncertainty. Grade 1 match-ups are the closest coincidence considered feasible and effectively match the satellite image pixel containing the ship at the time of the overpass. Grade 2a matches to the cloud free pixel nearest to the ship track within a radius of 20km but within 30 minutes. Whilst Grade 2b allows a match to a part of the ship track within ± 2 hours but limits the search radius to 1 km. Grade 3 allows for the widest flexibility that the ISFRN considers feasible, and Grade 4 represents the coarsest of the criteria used by some agencies for open ocean validation of satellite SST data.

Table 1: Match-up grades and corresponding match-up window size for SLSTR – ships4sst data validation

GRADE	TEMPORAL MATCH-UP CRITERIA	GEOSPATIAL MATCH-UP CRITERIA
1	±0.5h	±1km
2A	±0.5h	±20km
2B	±2h	±1km
3	±2h	±20km
4	±6h	±25km

The plots and statistics are produced for each level 2 SLSTR variable, including D3, D2, N3, N2, auxiliary SST products and water surface temperature (WST).

The criteria for the match-up process is to get the best match within a match-up window, rather than to attempt to select match-ups with pixels in different parts of SLSTR's swath. Ships4sst radiometer data is matched to any SLSTR data available, so both day and night time overpasses are validated.

5. EXAMPLE VALIDATION RESULTS

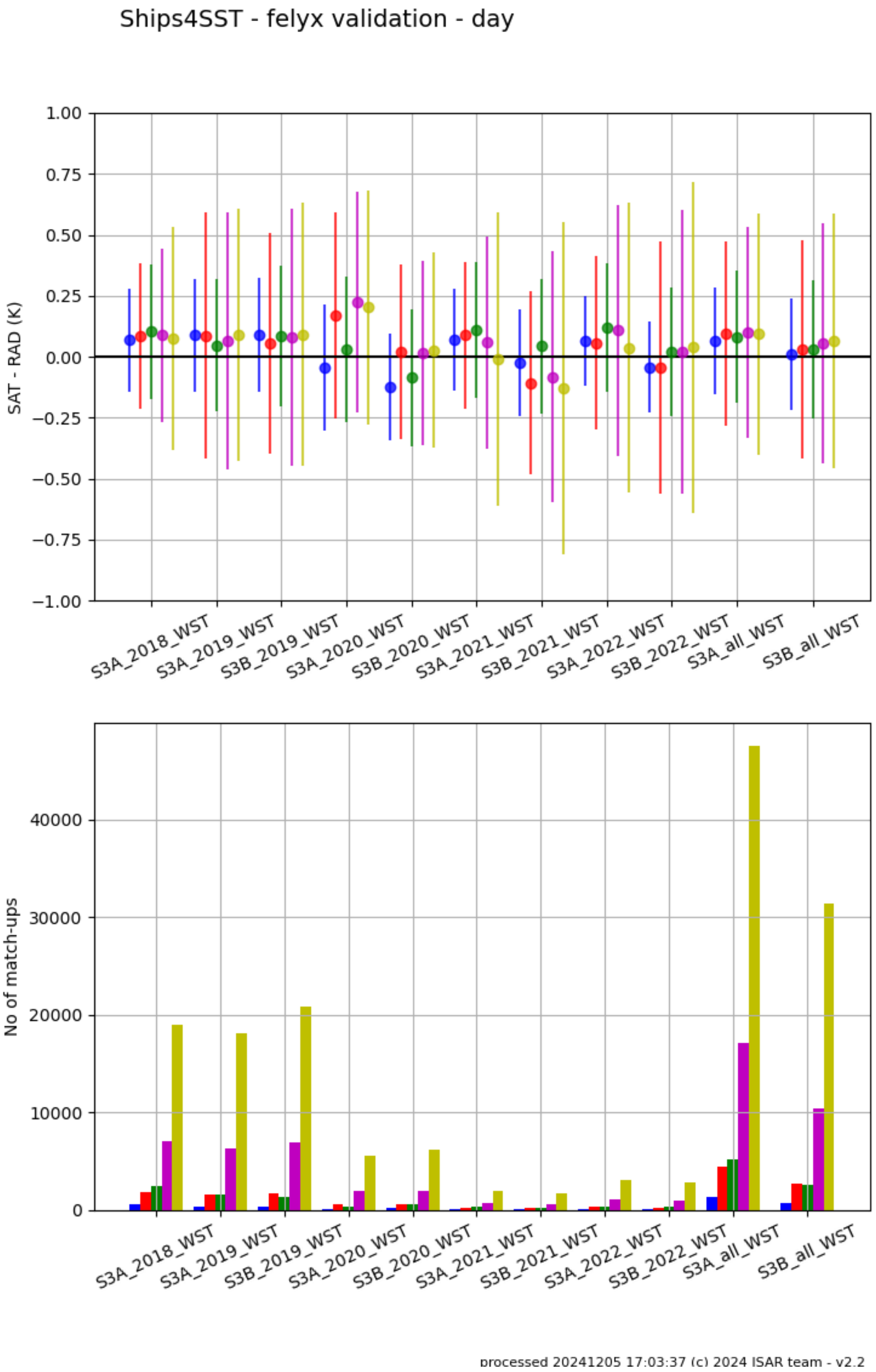

Figure 5-6: Validation data results for day time data from SLSTR A and B vs. ships4sst data, between 2018-2022.

The top panel shows the mean and robust standard deviation for each match-up grade (grade 1 – blue, grade 2a - red, grade 2b – green, grade 3 – magenta, grade 4 – yellow). The bottom panel shows the number of match-up pairs stratified by grade, year and sensor.

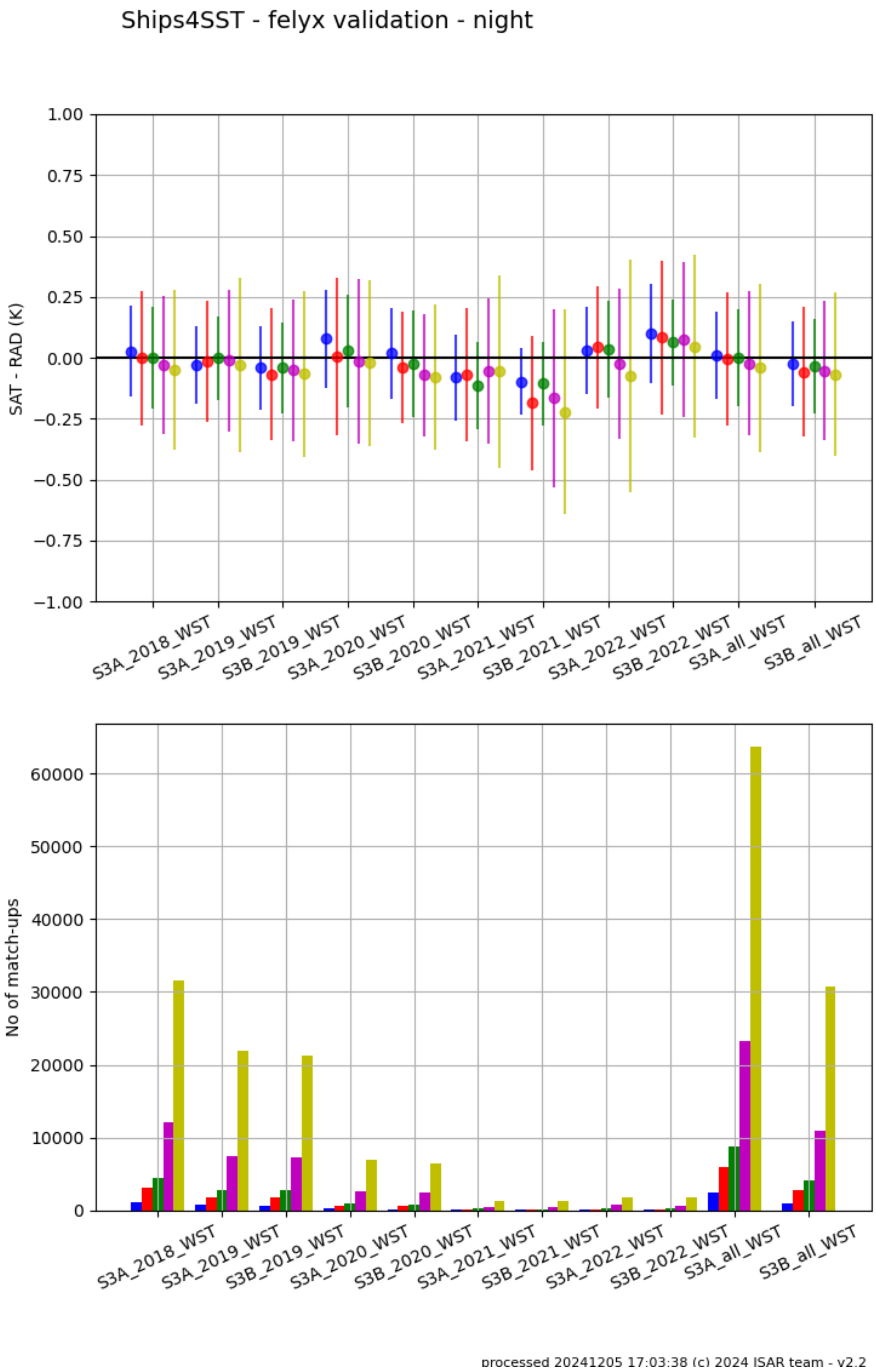

Figure 5-7: Validation data results for night time data from SLSTR A and B vs. ships4sst data between 2018-2022.

The top panel shows the mean and robust standard deviation for each match-up grade (grade 1 – blue, grade 2a - red, grade 2b – green, grade 3 – magenta, grade 4 – yellow). The bottom panel shows the number of match-up pairs stratified by grade, year and sensor.

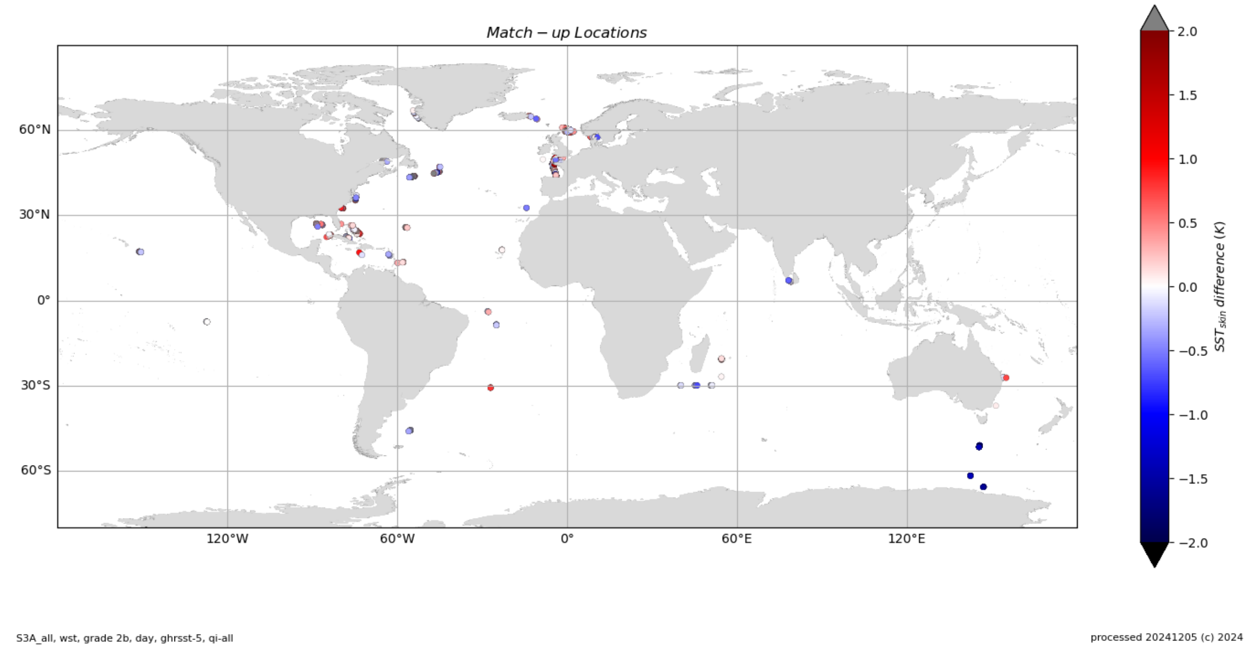

Figure 5-8: Validation locations for day time SLSTR A results

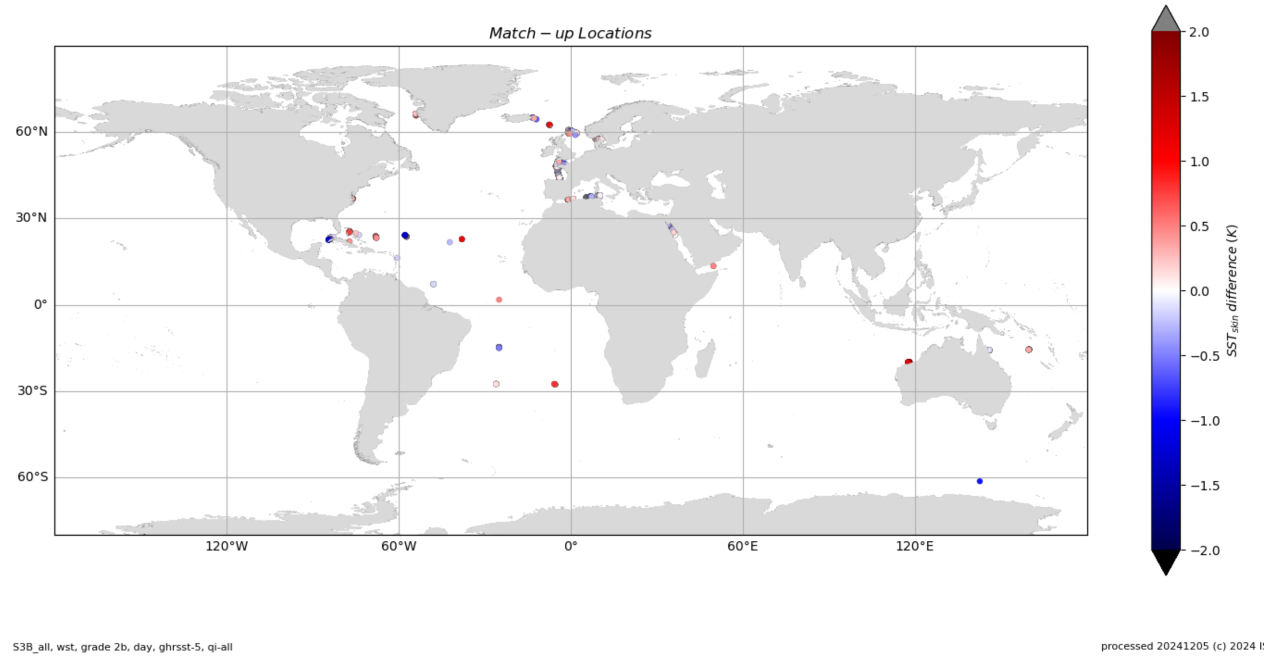

Figure 5-9: Validation locations for day time SLSTR B results

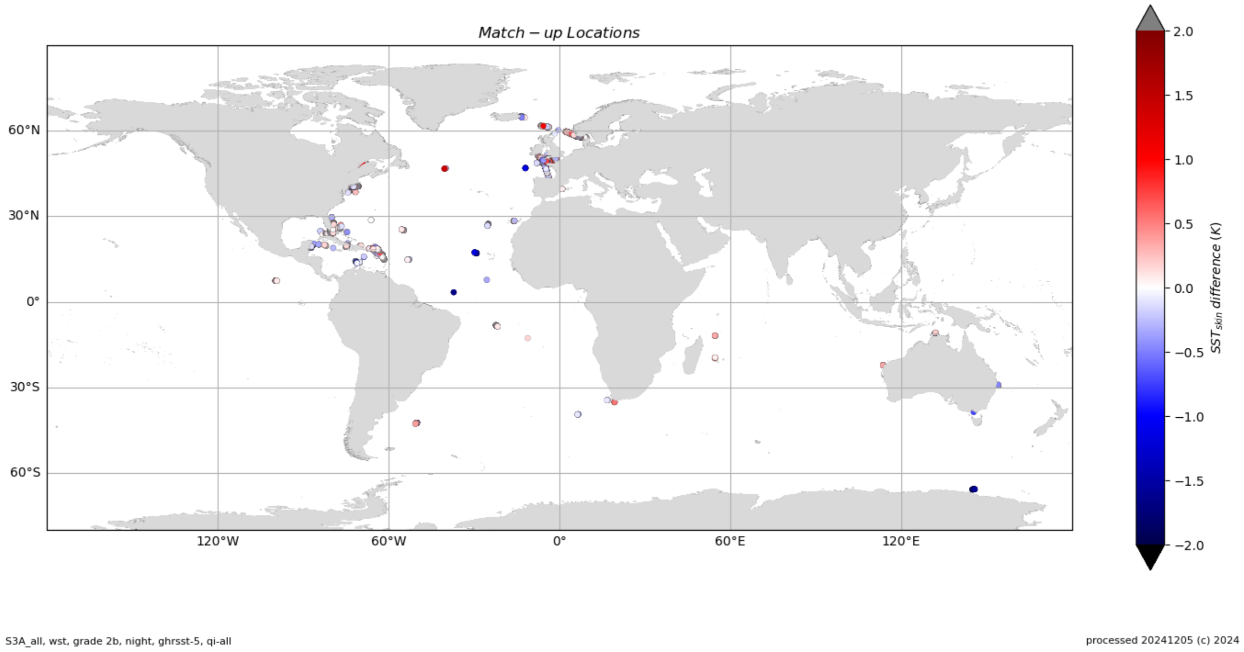

Figure 5-10: Validation locations for night time SLSTR A results

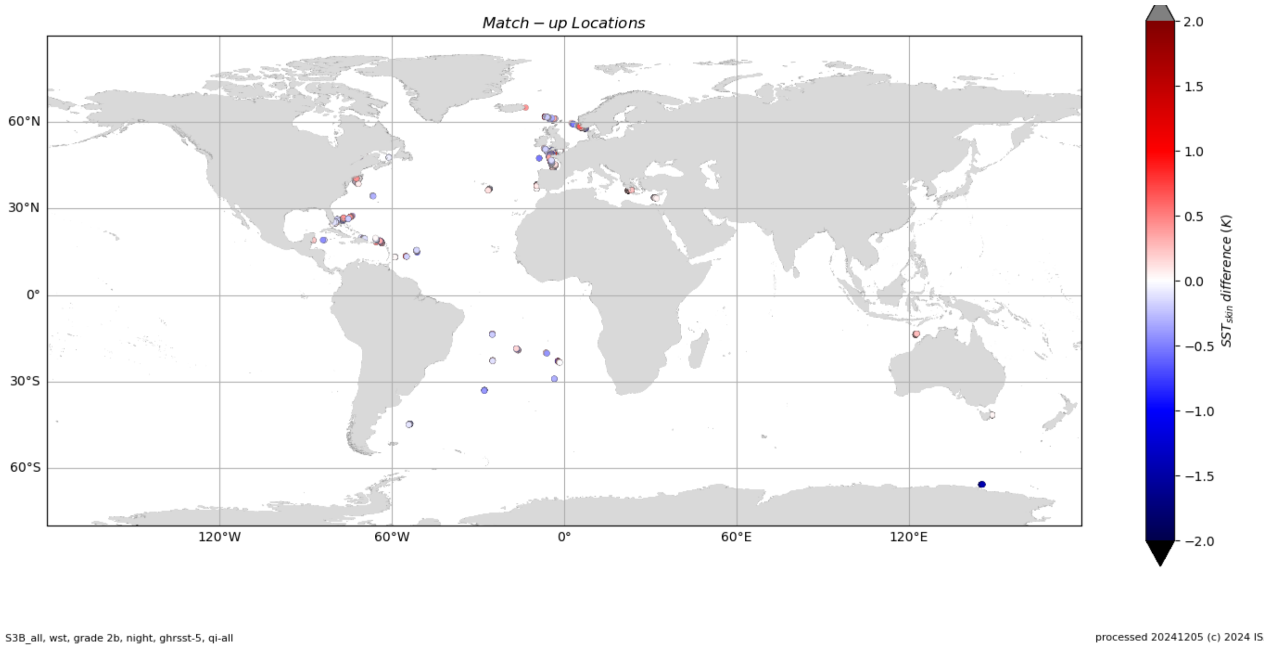

Figure 5-11: Validation locations for night time SLSTR B results

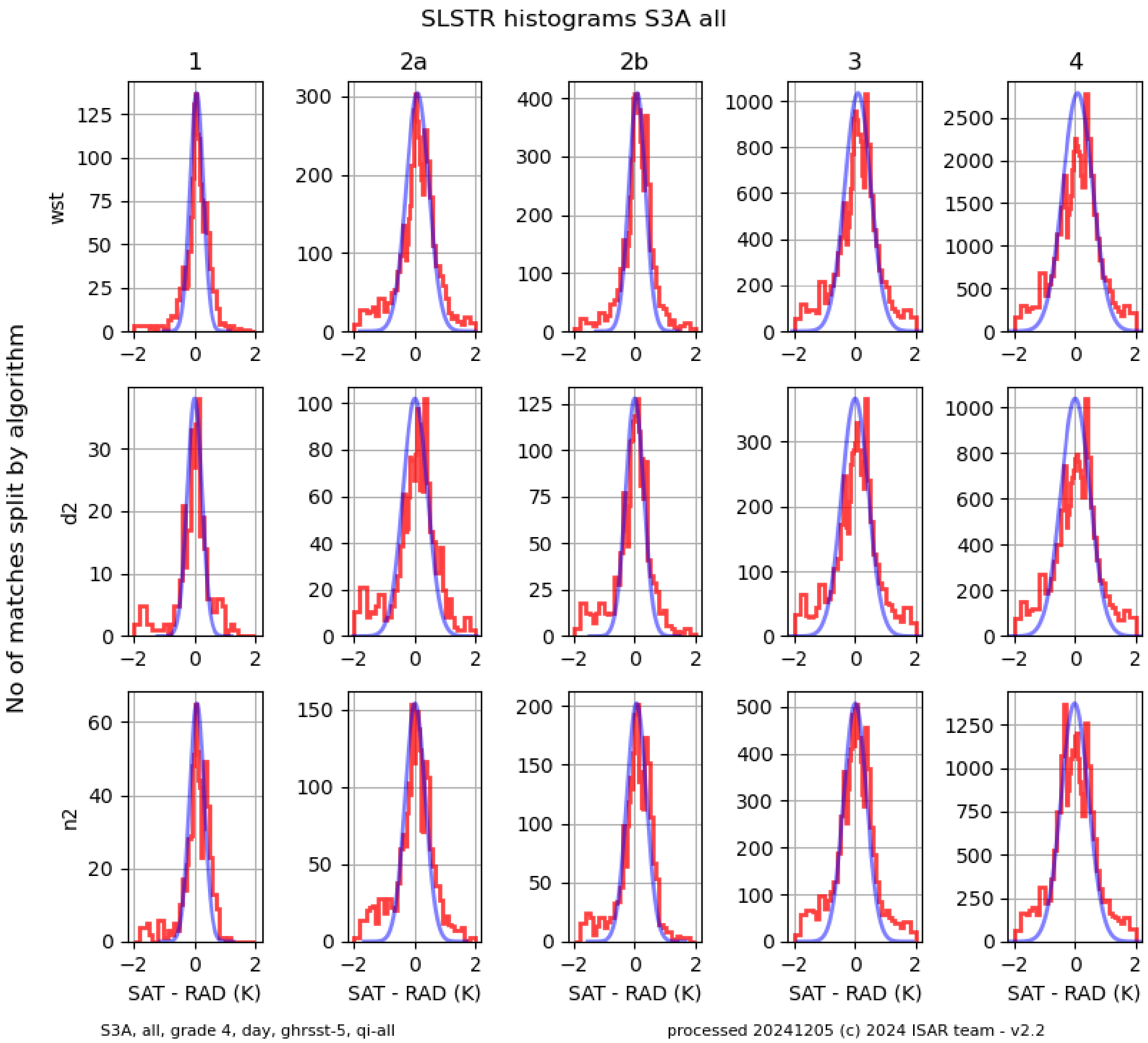

Figure 5-12: Validation histograms for day time SLSTR A results from 2018 to 2022. The columns show the different match-up grades and the rows show the different SLSTR data products.

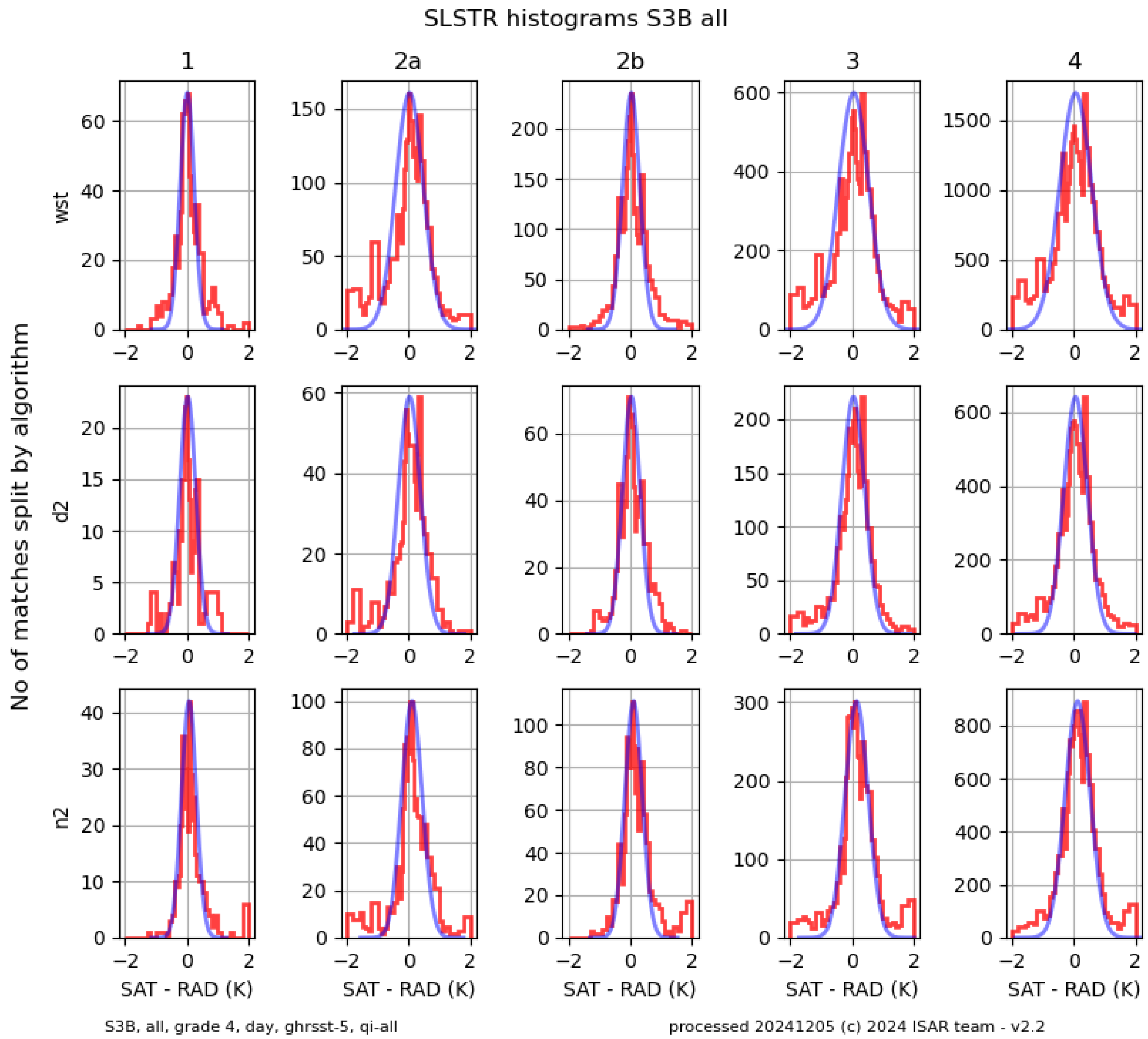

Figure 5-13: Validation histograms for day time SLSTR B results from 2018 to 2022. The columns show the different match-up grades and the rows show the different SLSTR data products.

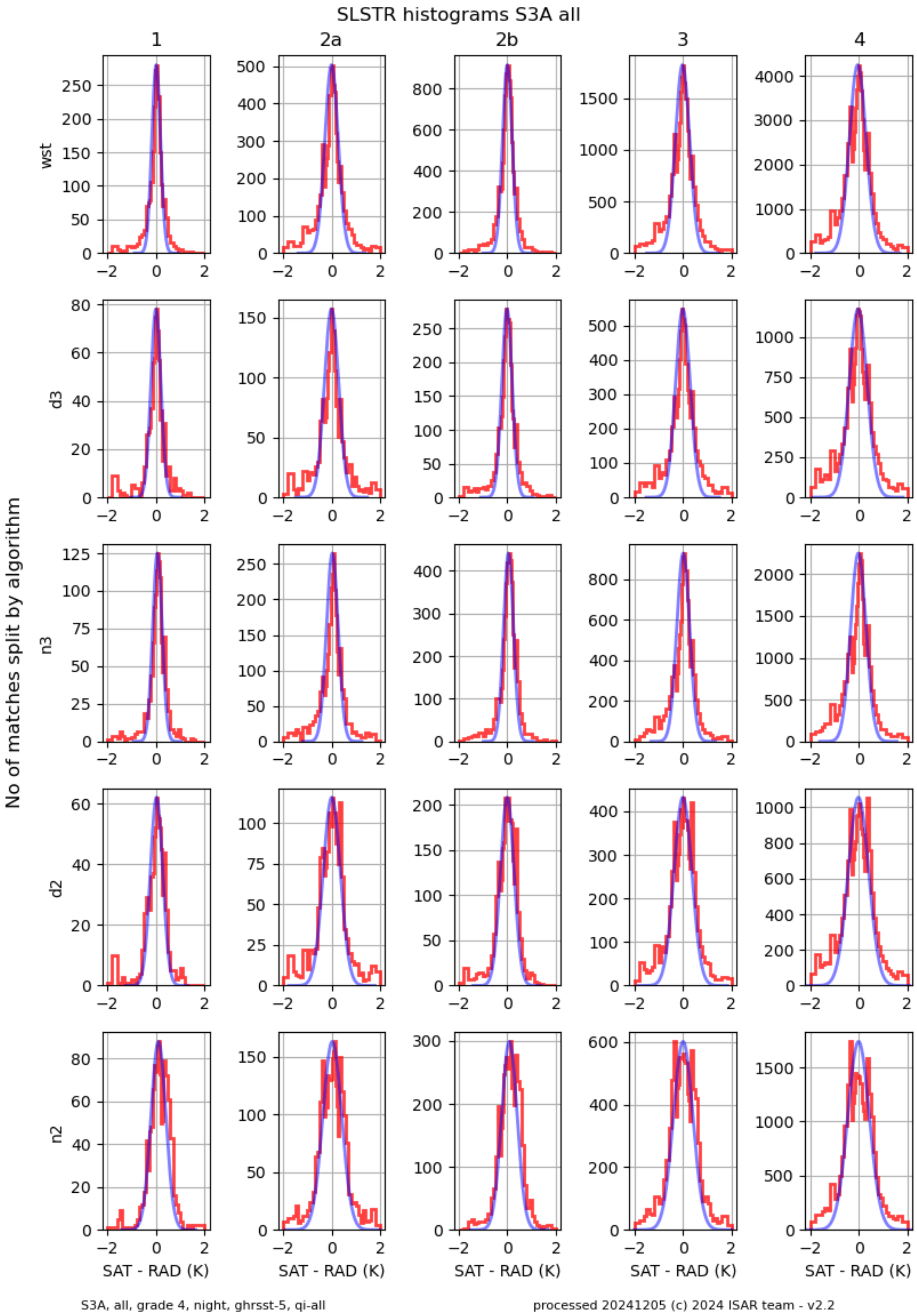

Figure 5-14: Validation histograms for night time SLSTR A results from 2018 to 2022. The columns show the different match-up grades and the rows show the different SLSTR data products.

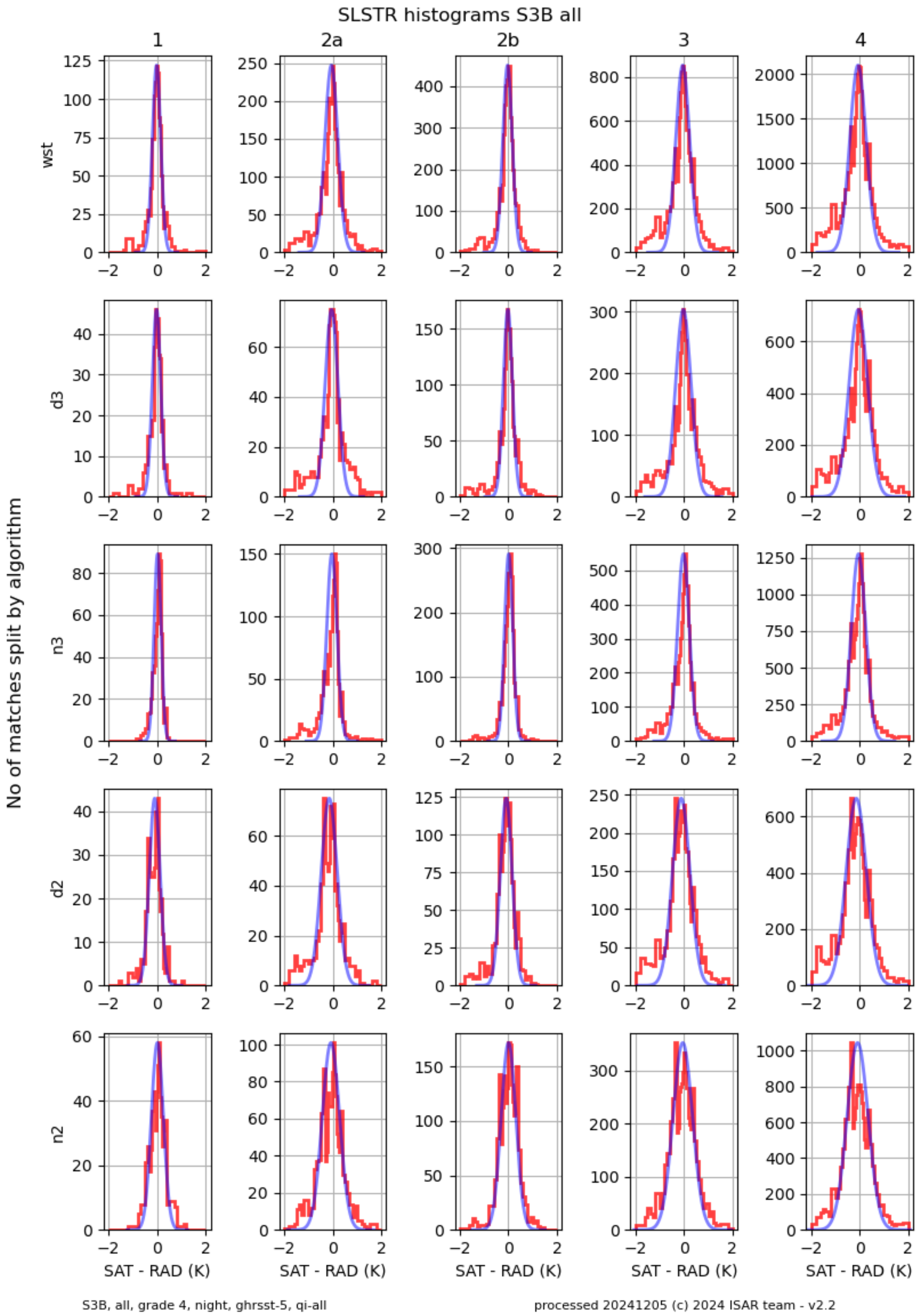

Figure 5-15: Validation histograms for night time SLSTR B results from 2018 to 2022. The columns show the different match-up grades and the rows show the different SLSTR data products.

WST						
Day						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Temp
1	0.07	0.22	1312	66	273.96	306.53
2a	0.10	0.38	4467	115	273.23	306.53
2b	**0.08**	**0.27**	**5130**	**109**	**273.20**	**306.53**
3	0.10	0.43	17121	150	273.17	306.57
4	0.09	0.50	47603	202	273.16	307.07

WST						
Night						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Temp
1	0.01	0.18	2403	102	273.22	303.19
2a	0.00	0.27	6023	164	273.18	303.76
2b	**0.00**	**0.20**	**8840**	**146**	**273.22**	**303.35**
3	-0.02	0.29	23308	184	273.15	303.87
4	-0.04	0.35	63705	248	273.14	305.57

Table 2: Match-up statistics for the WST product for SLSTR A

WST						
Day						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Temp
1	0.01	0.23	691	49	273.35	305.21
2a	0.03	0.45	2678	114	273.13	306.28
2b	**0.03**	**0.28**	**2611**	**75**	**273.35**	**306.02**
3	0.05	0.49	10463	137	273.13	306.86
4	0.06	0.52	31469	187	273.13	308.06

WST						
Night						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Temp
1	-0.02	0.17	1023	82	273.71	303.81
2a	-0.06	0.27	2708	134	273.15	304.42
2b	**-0.03**	**0.19**	**4058**	**118**	**273.29**	**303.81**
3	-0.05	0.29	10857	161	273.13	304.42
4	-0.07	0.34	30713	250	273.12	304.79

Table 3: Match-up statistics for the WST product for SLSTR AB

D3						
Night						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Temp
1	0.00	0.21	722	102	273.11	302.66
2a	0.00	0.29	1846	164	273.11	303.45
2b	**-0.01**	**0.21**	**2777**	**146**	**273.11**	**303.46**
3	-0.01	0.30	7028	184	273.08	303.46
4	-0.02	0.37	18960	248	272.74	305.86

Table 4: Match-up statistics for the D3 product for SLSTR A

D3						
Night						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Temp
1	-0.03	0.17	381	82	279.34	303.54
2a	-0.05	0.26	941	134	273.25	303.92
2b	**-0.02**	**0.19**	**1438**	**118**	**273.13**	**303.85**
3	-0.03	0.32	3860	161	273.13	303.96
4	-0.05	0.38	11363	250	272.92	304.83

Table 5: Match-up statistics for the D3 product for SLSTR B

D2						
Day						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Tem
1	0.00	0.24	400	66	273.94	302.83
2a	0.02	0.41	1592	115	273.90	305.25
2b	**0.00**	**0.30**	**1699**	**109**	**273.35**	**303.47**
3	0.01	0.44	6046	150	273.35	305.37
4	0.01	0.48	17255	202	273.11	305.62

D2						
Night						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Tem
1	0.03	0.26	722	102	273.06	302.57
2a	0.01	0.35	1846	164	273.06	303.39
2b	**0.00**	**0.28**	**2777**	**146**	**273.06**	**303.50**
3	-0.01	0.37	7028	184	273.03	303.62
4	-0.01	0.42	18960	248	272.89	306.79

Table 6: Match-up statistics for the D2 product for SLSTR A

D2						
Day						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Tem
1	0.03	0.26	210	49	281.33	304.12
2a	0.03	0.36	828	114	274.88	304.12
2b	**0.04**	**0.29**	**838**	**75**	**276.73**	**305.14**
3	0.04	0.37	3310	137	274.69	305.14
4	0.06	0.38	10096	187	272.98	305.62

D2						
Night						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Tem
1	-0.10	0.22	381	82	279.22	303.60
2a	-0.15	0.33	941	134	273.14	304.17
2b	**-0.09**	**0.24**	**1438**	**118**	**273.21**	**303.83**
3	-0.11	0.36	3860	161	273.03	304.17
4	-0.14	0.42	11364	250	272.67	304.52

Table 7: Match-up statistics for the D2 product for SLSTR B

N3						
Night						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Tem
1	0.06	0.20	1178	102	273.36	303.16
2a	0.03	0.24	2702	164	273.36	303.35
2b	**0.05**	**0.21**	**4389**	**146**	**273.36**	**303.18**
3	0.01	0.27	10707	184	273.23	303.45
4	-0.02	0.32	30209	248	273.05	304.92

Table 8: Match-up statistics for the N3 product for SLSTR A

N3						
Night						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Tem
1	0.02	0.15	583	82	279.50	303.51
2a	-0.04	0.21	1339	134	273.40	303.51
2b	**0.01**	**0.17**	**2239**	**118**	**273.42**	**303.51**
3	-0.02	0.24	5507	161	273.18	303.51
4	-0.05	0.30	16093	250	272.90	304.98

Table 9: Match-up statistics for the N3 product for SLSTR B

N2						
Day						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Tem
1	0.07	0.24	640	66	274.12	302.66
2a	0.02	0.34	2202	115	273.22	305.21
2b	**0.06**	**0.32**	**2591**	**109**	**273.22**	**304.10**
3	0.01	0.38	8420	150	273.18	305.24
4	-0.01	0.45	24030	202	273.13	305.52

N2						
Night						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Tem
1	0.10	0.31	1178	102	273.32	303.57
2a	0.03	0.39	2702	164	273.32	304.07
2b	**0.08**	**0.32**	**4389**	**146**	**273.32**	**304.01**
3	0.00	0.40	10707	184	273.20	304.07
4	-0.01	0.44	30209	248	273.03	305.92

Table 10: Match-up statistics for the N2 product for SLSTR A

N2						
Day						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Temp
1	0.07	0.24	362	49	275.16	305.24
2a	0.11	0.33	1312	114	275.11	305.24
2b	**0.11**	**0.28**	**1307**	**75**	**275.05**	**305.62**
3	0.15	0.37	5035	137	274.99	305.62
4	0.13	0.41	15504	187	274.15	305.77

N2						
Night						
Grade	MDiff	RSD	No	Overpass	Min Temp	Max Temp
1	0.01	0.25	583	82	279.47	304.47
2a	-0.07	0.36	1339	134	273.37	304.47
2b	**0.01**	**0.30**	**2239**	**118**	**273.39**	**304.47**
3	-0.05	0.40	5507	161	273.15	304.47
4	-0.08	0.43	16094	250	272.86	305.97

Table 11: Match-up statistics for the N2 product for SLSTR B

6. ACRONYMS AND ABBREVIATIONS

AATSR	Advanced Along-Track Scanning Radiometer
CDR	Climate Data Record
CCI	Climate Change Initiative
CSIRO	Commonwealth Scientific and Industrial Research Organisation
DMI	Danish Meteorological Institute
ECV	Essential Climate Variable
ESA	European Space Agency
FRM	Fiducial Reference Measurements
FRM4SST	Fiducial Reference Measurements for Sea Surface Temperature
HTTP	HyperText Transfer Protocol
IR	Infra-Red
ISAR	Infrared SST Autonomous Radiometer
ISFRN	International SST FRM Radiometer Network
ISSI	International Space Science Institute
M-AERI	Marine-Atmospheric Emitted Radiance Interferometer
NOCS	National Oceanography Centre, Southampton
RAL	Rutherford Appleton Laboratory
RSD	Robust Standard Deviation
SCL	Space ConneXions Limited
SISTeR	Scanning Infrared Sea surface Temperature Radiometer
SLSTR	Sea and Land Surface Temperature Radiometer
SST	Sea Surface Temperature
ST	Surface Temperature
STFC	Science and Technology Facilities Council
TIR	Thermal Infra-Red

7. REFERENCES

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