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Supplement of

Mediterranean ocean colour Level 3 operational multi-sensor processing

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The Mediterranean Ocean Colour Level 3 Operational Multi-Sensor Processing

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Supplementary Material

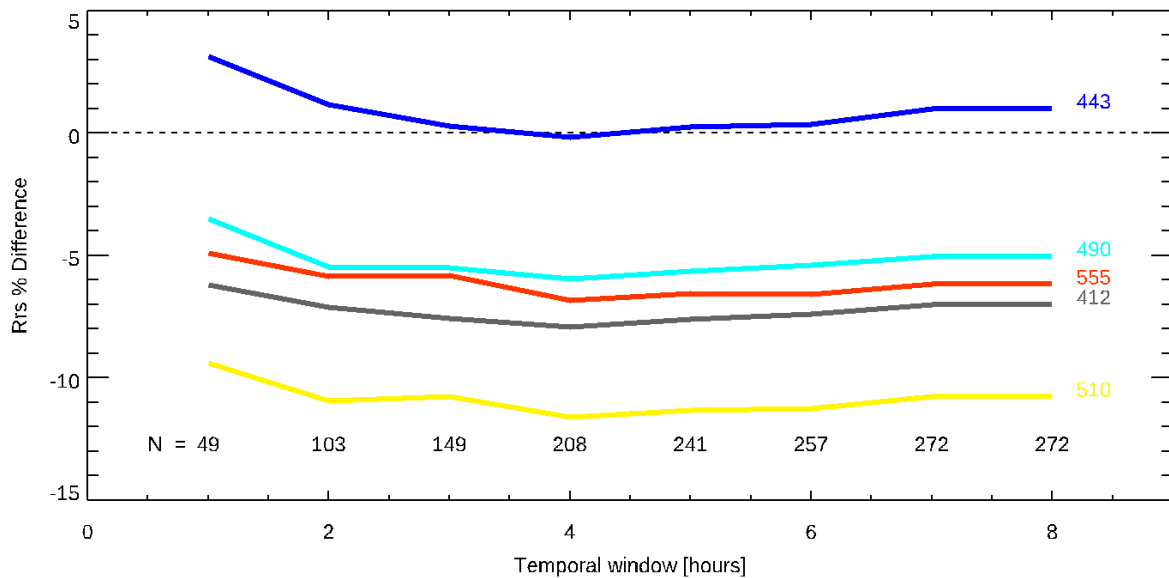


Figure S.1: Relative percent difference between Multi and in situ (MedBiOp) Rrs as function of the temporal window used for determining coincidence. Since the satellite pixel overpass time is lost because of the merging procedure, we assume here to be 10 am local time. Superimposed is also the number of matchups. The plot shows that after 3 hours the range of variability is always within 1%, while the number of points used and thus the significance increases.

Name	Units	Definition
In situ data average	Geophysical	$\bar{X}^M = \frac{1}{N} \sum_{i=1}^N X_i^M$
Satellite data average	Geophysical	$\bar{X}^E = \frac{1}{N} \sum_{i=1}^N X_i^E$

Type-2 slope	Geophysical	$S = \frac{\sum_{i=1}^N (X_i^E - \bar{X}^E)^2 - \sum_{i=1}^N (X_i^M - \bar{X}^M)^2 + \left[\left\{ \sum_{i=1}^N (X_i^E - \bar{X}^E)^2 - \sum_{i=1}^N (X_i^M - \bar{X}^M)^2 \right\} + 4 \left\{ \sum_{k=1}^N (X_k^E - \bar{X}^E)(X_k^M - \bar{X}^M) \right\} \right]^{1/2}}{2 \sum_{k=1}^N (X_k^E - \bar{X}^E)(X_k^M - \bar{X}^M)}$
Type-2 intercept	Geophysical	$I = \bar{X}^E - S \cdot \bar{X}^M$
Determination coefficient		$r^2 = \frac{\left[\sum_{i=1}^N (X_i^E - \bar{X}^E)(X_i^M - \bar{X}^M) \right]^2}{\sum_{i=1}^N (X_i^E - \bar{X}^E)^2 \sum_{i=1}^N (X_i^M - \bar{X}^M)^2}$
Root Mean Square Difference	Geophysical	$RMSD = \sqrt{\frac{\sum_{i=1}^N (X_i^E - X_i^M)^2}{N}}$
Centre-pattern Root Mean Square Difference	Geophysical	$cRMSD = \sqrt{\frac{\sum_{i=1}^N \{ [X_i^E - (\sum_{j=1}^N X_j^E)] - [X_i^M - (\sum_{k=1}^N X_k^M)] \}^2}{N}}$
Bias	Geophysical	$bias = \frac{1}{N} \sum_{i=1}^N (X_i^E - X_i^M)$
Mean Absolute Error	Geophysical	$MAE = \frac{1}{N} \sum_{i=1}^N X_i^E - X_i^M $
Relative percentage Difference	Percent	$RPD = 100 \cdot \frac{1}{N} \sum_{i=1}^N \frac{X_i^E - X_i^M}{X_i^M}$
Absolute percentage Difference	Percent	$APD = 100 \cdot \frac{1}{N} \sum_{i=1}^N \frac{ X_i^E - X_i^M }{X_i^M}$

Table S.1: Metrics used to compare the estimated (satellite-based) dataset XE to a reference, measured in-situ dataset XM. The centre-pattern (or unbiased) Root Mean Square Distance (cRMSD) describes the error of the estimated values with respect to the measured ones, regardless of the average bias between the two distributions. Geophysical in column Units refers to sr-1, m-1 or to mg m-3 when the statistics refer to Rrs, Kd or Chl, respectively.

RRS	\bar{X}^M	\bar{X}^E	SLOPE	INTERCEPT	R²	RMSD	CRMSD	BIAS	MAE	RPD	APD	N
412	0.0059	0.0056	1.01	-0.0004	0.75	0.0013	0.0013	-0.00030	0.00098	-3	19	155
443	0.0056	0.0056	0.94	0.0003	0.80	0.0010	0.0010	-0.00004	0.00072	2	15	155
488	0.0052	0.0050	0.96	0.0000	0.79	0.0007	0.0007	-0.00025	0.00056	-3	12	155
490 [§]	0.0052	0.0050	0.96	0.0000	0.79	0.0007	0.0007	-0.00025	0.00056	-3	12	155
510 [§]	0.0040	0.0035	1.08	-0.0009	0.79	0.0008	0.0006	-0.00057	0.00072	-13	19	155
531	0.0033	0.0029	1.05	-0.0005	0.88	0.0006	0.0005	-0.00037	0.00053	-11	18	155
547	0.0027	0.0024	1.02	-0.0004	0.91	0.0005	0.0004	-0.00030	0.00044	-11	18	155
555 [§]	0.0025	0.0022	1.03	-0.0004	0.92	0.0005	0.0004	-0.00028	0.00041	-12	18	155
667	0.0003	0.0003	1.57	-0.0002	0.88	0.0002	0.0002	-0.00001	0.00010	-3	35	117
670 [§]	0.0003	0.0003	1.54	-0.0002	0.89	0.0002	0.0002	-0.00001	0.00009	-5	34	127

Table S.2: Statistics associated with the MODIS-AQUA Rrs (sr⁻¹) computed over the MedBiOp dataset. § refers to satellite band-shifted wavelengths (see also Table 1 of the main text).

RRS	\bar{X}^M	\bar{X}^E	SLOPE	INTERCEPT	R2	RMSD	CRMSD	BIAS	MAE	RPD	APD	N
410	0.0049	0.0043	1.41	-0.0026	0.44	0.0011	0.0009	-0.00065	0.00092	-13	19	93
412 [§]	0.0049	0.0043	1.39	-0.0026	0.45	0.0011	0.0009	-0.00065	0.00092	-13	19	93
443	0.0049	0.0048	0.97	0.0000	0.63	0.0007	0.0007	-0.00018	0.00054	-3	11	93
486	0.0052	0.0049	0.92	0.0001	0.86	0.0006	0.0005	-0.00034	0.00049	-6	9	93
490 [§]	0.0052	0.0049	0.93	0.0000	0.87	0.0006	0.0005	-0.00037	0.00050	-6	9	93
510 [§]	0.0044	0.0037	1.02	-0.0007	0.92	0.0008	0.0005	-0.00065	0.00069	-15	16	93
551	0.0031	0.0027	0.99	-0.0003	0.95	0.0006	0.0005	-0.00036	0.00045	-12	15	93
555 [§]	0.0030	0.0027	1.00	-0.0003	0.95	0.0006	0.0005	-0.00035	0.00044	-13	15	93
670 [§]	0.0005	0.0005	1.14	-0.0001	0.95	0.0002	0.0002	-0.00003	0.00010	-11	20	50
671	0.0005	0.0005	1.14	-0.0001	0.95	0.0002	0.0002	-0.00003	0.00010	-10	20	49

Table S.3: Statistics associated with the VIIRS Rrs (sr^{-1}) computed over the MedBiOp dataset. § refers to satellite band-shifted wavelengths (see also Table 1 of the main text).

RRS	\bar{X}^M	\bar{X}^E	SLOPE	INTERCEPT	R²	RMSD	CRMSD	BIAS	MAE	RPD	APD	N
412	0.0085	0.0082	1.04	-0.0007	0.64	0.0019	0.0018	-0.00031	0.00146	1	21	98
443	0.0078	0.0076	0.92	0.0003	0.62	0.0016	0.0016	-0.00028	0.00120	3	21	98
490	0.0059	0.0056	0.69	0.0015	0.32	0.0013	0.0013	-0.00036	0.00092	-1	17	98
510	0.0040	0.0034	0.15	0.0029	0.02	0.0012	0.0011	-0.00053	0.00084	-8	22	98
555	0.0019	0.0018	0.26	0.0013	0.03	0.0007	0.0007	-0.00009	0.00039	0	20	98
670	0.0002	0.0003	11.16	-0.0017	0.08	0.0002	0.0001	0.00011	0.00012	76	80	40

Table S.4: Statistics associated with the SeaWiFS Rrs (sr⁻¹) computed over the MedBiOp dataset.

RRS	\bar{X}^M	\bar{X}^E	SLOPE	INTERCEPT	R^2	RMSD	CRMSD	BIAS	MAE	RPD	APD	N
412	0.0083	0.0092	0.97	0.0011	0.90	0.0012	0.0009	0.00089	0.00104	13	14	90
443	0.0076	0.0081	0.85	0.0016	0.86	0.0010	0.0009	0.00046	0.00072	9	12	90
490	0.0060	0.0057	0.56	0.0023	0.79	0.0011	0.0010	-0.00031	0.00056	-3	8	90
510	0.0042	0.0036	0.54	0.0014	0.87	0.0011	0.0010	-0.00051	0.00061	-10	13	90
555 [§]	0.0022	0.0019	0.54	0.0008	0.95	0.0012	0.0012	-0.00022	0.00030	-5	10	90
560	0.0020	0.0018	0.54	0.0007	0.95	0.0012	0.0012	-0.00023	0.00030	-6	10	90
665	0.0002	0.0002	1.17	-0.0001	0.74	0.0001	0.0001	-0.00003	0.00005	-12	28	70
670 [§]	0.0002	0.0002	1.17	-0.0001	0.74	0.0001	0.0001	-0.00003	0.00005	-13	28	72

Table S.5: Statistics associated with the MERIS Rrs (sr^{-1}) computed over the MedBiOp dataset. § refers to satellite band-shifted wavelengths (see also Table 1 of the main text).

RRS	\bar{X}^M	\bar{X}^E	SLOPE	INTERCEPT	R²	RMSD	CRMSD	BIAS	MAE	RPD	APD	N
412	0.0069	0.0060	0.97	-0.0007	0.83	0.0015	0.0012	-0.00087	0.00112	-12	17	262
443	0.0066	0.0063	0.86	0.0006	0.82	0.0011	0.0011	-0.00030	0.00077	-1	13	262
490	0.0057	0.0053	0.75	0.0010	0.72	0.0010	0.0009	-0.00040	0.00067	-4	12	262
510	0.0042	0.0037	0.80	0.0003	0.74	0.0010	0.0009	-0.00051	0.00067	-9	16	262
555	0.0025	0.0023	0.80	0.0003	0.84	0.0008	0.0008	-0.00017	0.00038	-3	14	262
670	0.0003	0.0003	0.97	0.0000	0.87	0.0001	0.0001	-0.00001	0.00009	5	38	223

Table S.6: Statistics associated with the CCIv3 Rrs (sr⁻¹) computed over the MedBiOp dataset.

RRS	\bar{X}^M	\bar{X}^E	SLOPE	INTERCEPT	R²	RMSD	CRMSD	BIAS	MAE	RPD	APD	N
412	0.0070	0.0064	0.99	-0.0006	0.77	0.0015	0.0014	-0.00060	0.00113	-7	18	272
443	0.0066	0.0064	0.86	0.0007	0.73	0.0013	0.0013	-0.00023	0.00089	1	15	272
490	0.0057	0.0052	0.65	0.0015	0.55	0.0013	0.0012	-0.00047	0.00077	-5	13	272
510	0.0042	0.0037	0.65	0.0009	0.57	0.0013	0.0011	-0.00060	0.00077	-11	18	272
555	0.0025	0.0022	0.68	0.0005	0.71	0.0012	0.0012	-0.00027	0.00044	-6	16	272
670	0.0003	0.0003	1.19	-0.0001	0.91	0.0002	0.0002	-0.00002	0.00008	-3	35	197

Table S.7: Statistics associated with the Multi Rrs (sr⁻¹) computed over the MedBiOp dataset.

CHL	\bar{X}^M	\bar{X}^E	SLOPE	INTERCEPT	r^2	RMSD	CRMSD	BIAS	MAE	RPD	APD	N
REP	0.257	0.163	0.737	-0.306	0.75	0.411	0.400	-0.093	0.143	7	47	710
MULTI	0.257	0.158	0.752	-0.309	0.74	0.427	0.415	-0.098	0.146	3	47	710
REP_{AV}	0.335	0.271	1.052	-0.108	0.57	0.207	0.197	-0.064	0.148	-18	43	44
MULTI_{AV}	0.335	0.278	1.184	-0.047	0.50	0.271	0.265	-0.057	0.176	-17	48	44

Table S.8: Statistics associated with satellite Chl (mg m⁻³) computed over the MedBiOp dataset. Satellite Chl is the REP (derived by the application of the MedOC4.2018 to the Rrs derived from the CCIv3 processor) and NRT/DT (derived by the application of the MedOC4.2018 to the Rrs derived from the Multi processing). A subset of matchups on the period (2012 to present) in which VIIRS and MODIS-AQUA co-exist (REP_{AV} and Multi_{AV}) is also reported.

KD490	\bar{X}^M	\bar{X}^E	SLOPE	INTERCEPT	r^2	RMSD	CRMSD	BIAS	MAE	RPD	APD	N
MULTI	0.053	0.052	1.002	-0.026	0.80	0.034	0.034	-0.0004	0.014	-3	21	420
GLOBAL	0.053	0.058	0.857	-0.145	0.83	0.023	0.023	0.0054	0.012	15	24	420

Table S.9: Statistics associated with satellite-derived Kd490 (m⁻¹) computed in correspondence of the BGC-Argo float dataset (Organelli et al., 2017), whose location is shown in Figure 11c of the main text. The two rows refer to the satellite-derived Kd490 obtained with the MedKd.2018 and the Global algorithm, respectively, as shown in Figure 6b of the main text.

CHL	SLOPE	INTERCEPT	r^2	RMSD(LOG)	CRMSD(LOG)	BIAS(LOG)	N
REP	0.74	-0.306	0.75	0.25	0.25	-0.0428	710
MULTI	0.75	-0.309	0.74	0.26	0.25	-0.0600	710
CAR	0.72	-0.056	0.76	0.31	0.31	0.0066	14582

Table S.10: Chl matchup statistics as in Table S.8 for REP and Multi. The difference is that Chl log-transformation is here used to compute all the statistical parameters, not only those associated with the linear fit (Slope, Intercept and determination coefficient). CAR statistics are those of Figure 9 in the Ocean Colour Climate Change Initiative (Phase Two) Climate Assessment Report (http://esa-oceancolour-cci.org/?q=webfm_send/702).