Review of the manuscript "Coastal Atmosphere & Sea Time Series (CoASTS) 1 and Bio-Optical mapping of Marine optical Properties (BiOMaP): the CoASTS-BiOMaP dataset", by Giuseppe Zibordi and Jean-François Berthon

General comment

I am very pleased to have been given the opportunity to review this manuscript as I am aware of the lifetime work of the authors in defining the highest standards and producing high quality reference data in the field of satellite ocean color. The monitoring programs CoASTS and BiOMaP have generated lots of publications, and a remaining question was where all the data was going to be after the finalization of such programs. So now it appears that a circle is closed.

I have read the paper and downloaded the dataset. Before publication, I have a number of comments of varying importance that, to my understanding, need attention.

Major comments

Absorption from water samples is only provided at the Satlantic bands, which is regretful, as it was measured hyperspectrally. I do not know the reason to downgrade the data, and it definitely reduces its value for optical studies, also considering the growing interest in hyperspectral data (e.q., PACE). The authors are encouraged to submit the hyperspectral data.

Paragraph from line 175 to 182: on the above-water reference sensor, I see the correction for the imperfect non-cosine response. What about other uncertainty sources such as temperature and non-linearity, as it is recommended in above-water radiometry (e.g., Trios)? And are any of these corrections made to the in-water sensors?

Line 193-196: the interval 0.3 m – 5 m looks arbitrary. Any comments on why this choice is appropriate? Does it relate to the unphysical K_d values that I report below?

The transmission of upwelling radiance through the surface to form the water-leaving radiance is made with that 0.544 factor, which is not up to date with today's knowledge. I suspect that the reason to choose this value is because the difference in the final product would be minimal when using another one. However, I report evidence that this is not the case.

For a flat surface, the relationship between in-water and in-air upwelling radiance is:

$$L_w = \tau_{w,a} L_u(0^-)$$

Where

$$\tau_{w,a} = \frac{1-\rho}{n_w^2}$$

ρ is the Fresnel reflectance of the air-sea interface. Assuming unpolarized light, it has an analytical expression

$$\rho = \frac{1}{2}\left|\frac{\sin^2(\theta_a - \theta_w)}{\sin^2(\theta_a + \theta_w)} + \frac{\tan^2(\theta_a - \theta_w)}{\tan^2(\theta_a + \theta_w)}\right|$$

θ_a and θ_w are the wave propagation angles in air and in water, respectively, and are related by

$$\sin(\theta_a) = n_w \sin(\theta_w)$$

For $\theta_a = \theta_w = 0$, there is a singularity. One can apply the small angle approximations for the trigonometric functions, so in the limit, it is:

$$\rho(\theta_a = \theta_w = 0) = \left(\frac{n_w - n_a}{n_w + n_a}\right)^2$$

It is commonly accepted now that it is inaccurate to assume a constant $\tau_{w,a}$ for a given geometry due to the spectral dependence of n_w (and secondary influence by temperature and salinity too). Such dependences are taken from the state-of-the-art values by Roettgers et al. (2016). Therefore, the theoretical curve for $\tau_{w,a}$ can be seen in Fig. 1. In addition, I have made some Hydrolight simulations, in which the same n_w values are used, but also, the transmission is affected by the surface roughness depending on the wind speed. What emerges from Fig. 1 is that increasing wind speeds reduces light transmission. In terms of the total error made by assuming $\tau_{w,a} = 0.544$, it may not seem much, but in reality, they are in the order of 1-2%, which accounts for about 20% of the total uncertainty reported for the final R_{rs} product. Therefore, to reduce total uncertainty I encourage the authors to consider updated look up tables for $\tau_{w,a}$.

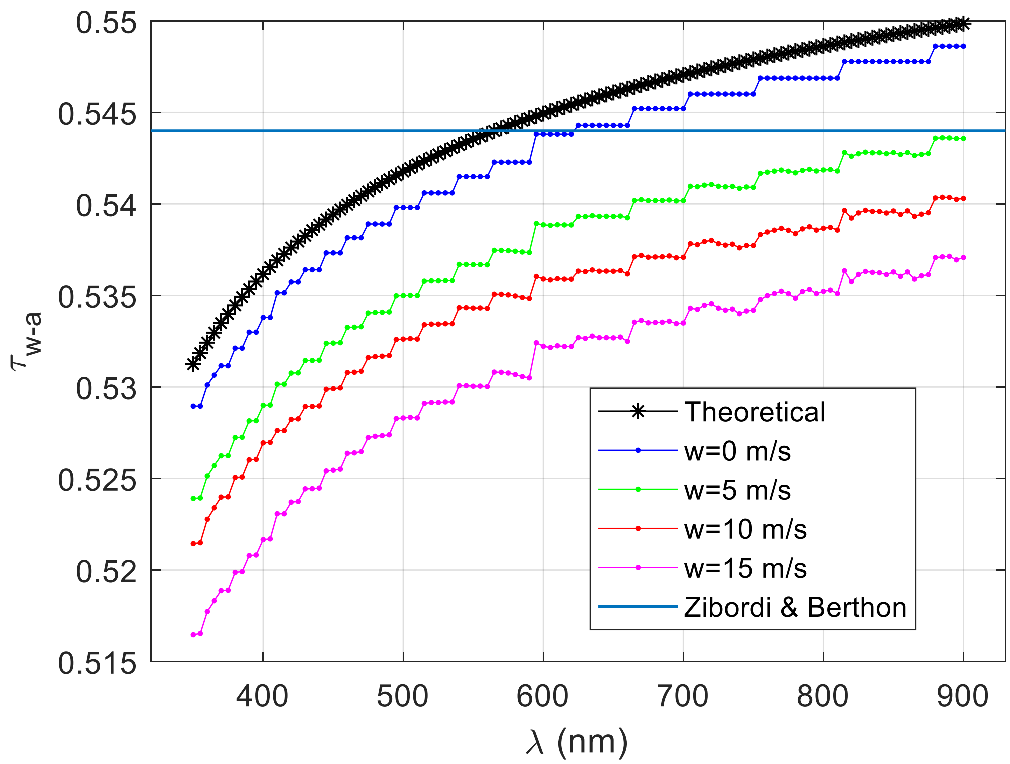

Fig. 1 Comparison of theoretical radiance transmission factor of upwelling radiance to water-leaving radiance $\tau_{w,a}$ (black) with respect to Hydrolight simulations (colors) with changing wind speeds, w. Sun zenith angle is $\theta_s = 30\,°$ and wind speed is $w = 0\ m/s$. Simulation was made using a case 1 model and $C = 0.1\ mg\ m^{-3}$.

On the fit of simple analytical functions to variables like the Q factor and possibly others like b_b, I did not understand if the actual data were replaced by the fits. If that is the case, I prefer then to have both data and uncertainty rather than their surrogate analytical forms.

On the bidirectional correction in lines 233-241, it is a bit disturbing to read in line 241 that in case 2 waters "this correction may be affected by large uncertainties". There are significant parts of the dataset in case 2 waters. How large are those uncertainties? Ongoing research has proven that is it better to apply Morel than not to apply any correction at all, and Morel has shown to provide surprisingly good results in case 2 waters, not because of the qualities of the model itself, but because all bidirectional correction models underestimate the correction to be made, but chlorophyll is overestimated in case 2 waters with the band ratio of Morel, which produces a higher correction, that ends up being beneficial. In any case, I believe that this part of the processing will need update to be in line with latest developments in bidirectional studies, knowing the interest of the authors in keeping the uncertainty budget as low as possible.

On the ac-9 measurements, I have several comments that follow.

How regular were the factory calibrations? It is said that instruments have to be calibrated before and after any campaign. Is this the case with the ac-9?

The Zaneveld method does not correct the non-finite acceptance angle of the c detectors as it is stated (note that the "c" is missing in line 277), and in fact it is rarely corrected by anybody. To do that, one should have a guess of the VSF between 0 and 0.93°, but in any case, the "real" c_{t-w} is higher than the measured than the factor that varies a lot, mostly between 1 and 2.

On the scattering correction method of the absorption data from the "a" tube, I also believe that the Zaneveld method questionable. Zaneveld overcorrects the absorption data, which leads to an underestimation. I see indirect evidence of it in Figure 5 from the manuscript, where the absorption comparison at 443 nm almost always shows negative biases with respect to the laboratory measurements (although the ac-9 provides better closure of R_{rs} than the water samples as I show below, so this is puzzling and needs to be addressed by the authors). I suggest using the method by Roettgers et al. (2013), that, if applied, is supposed to perform much better. This choice should be in line with authors approach of using only consolidated methods, approved by the two very good assessments by Stockley et al. (2017) and Kostakis et al. (2021).

In fact, for research purposes, it is recommended that the authors share the absorption coefficient uncorrected for residual scattering, so it can be useful material to further investigate this matter.

On the quantification of the uncertainties coming from the ac-9, certainly the value $0.005\ m^{-1}$ is not a proper estimate. That is a rule of thumb estimate of the instrument precision in the user manual, which is accompanied by the $0.01\ m^{-1}$ accuracy, also in the manual. There is no mention of uncertainty sources related to instrument absolute calibration, non-linearity, determination of the pure water measurement, correction of the temperature and salinity differences and correction of the residual scatter, some others related to the measurement protocol and the individual operator, and even some others that I may have missed. All these sources are likely to result in something bolder than the manufacturer user manual. The authors are expected and encouraged to investigate and comment on these aspects. Otherwise, how does one explain the differences that the authors find in their Figure 5?

I also have a few concerns about the Hydroscat backscattering data. First, in lines 331 and 332, what is exactly meant with the annual factory calibration "complemented" by pre-field calibration, in terms of determining the scale factor and the dark offset of the measurement?

Equation (4) is the correction for absorption along the pathlength recommended by the manufacturer. However, after investigating on it, Doxaran et al. (2016) investigated on it and found that the "0.4" is a totally arbitrary number. They proposed a more accurate expression instead.

Removal of pure water data is made after tabulated data by either salt water or fresh water by Morel, but the state of the art values are those given by Zhang et al. (2009). Their model is analytical and has an explicit dependency on salinity, so that one may use concurrent CTD data for obtain b_{bw} accurately. Again here, the differences on the final products are likely to be small, but it is preferrable to replace old and biased values with updated ones at zero cost.

As for the ac-9 data, estimating an uncertainty of $0.0007\ m^{-1}$ for b_{bp} is wishful thinking. True uncertainties are much larger than that and are the result of a number of factors like those listed above. Can the authors look for a more realistic value based on their own research or in literature?

On the absorption from water samples, the paragraph of lines 378-380 is confusing to me. Probably it needs rephrasing. Maybe the authors mean that the absorption of particulate material between 0.2 and 0.7 micron is negligible with respect to the fraction larger than 0.7 micron? If so, is there some evidence of that in data or literature?

CDOM measurements - usage of a 10 cm cuvette inside of a spectrometer is known to be suboptimal in oligotrophic areas like the Mediterranean Sea, even the western basin and in winter. Water is simply too clear to provide a clean spectrum at visible wavelengths. I understand that there is nothing that the authors can do to overcome this issue in case they did not use better suited instruments (like Ultrapath), so at least, an acknowledgement is needed that measurements were performed in suboptimal conditions.

Next type of comments is on the data present in the dataset. It is written (lines 507-511) that basic quality control criteria, like K_d to be higher than the clear water theoretical value ($a_w + b_{bw}$?), were required for a measurement to be included in the dataset, but I have plotted all K_d values and I see that many spectra are less than such value, and some even negative, see Fig. 2. I have repeated the analysis for K_L and K_u and I have found the same issue (not shown). Same for some absorption data. Regarding b_b, all values are positive, but when removing the water contribution following Zhang et al. (2009), many derived b_{bp} values are negative. Although the number of bad spectra may be marginal, this reduces the confidence that this dataset aspires to; so this needs attention before making the public release.

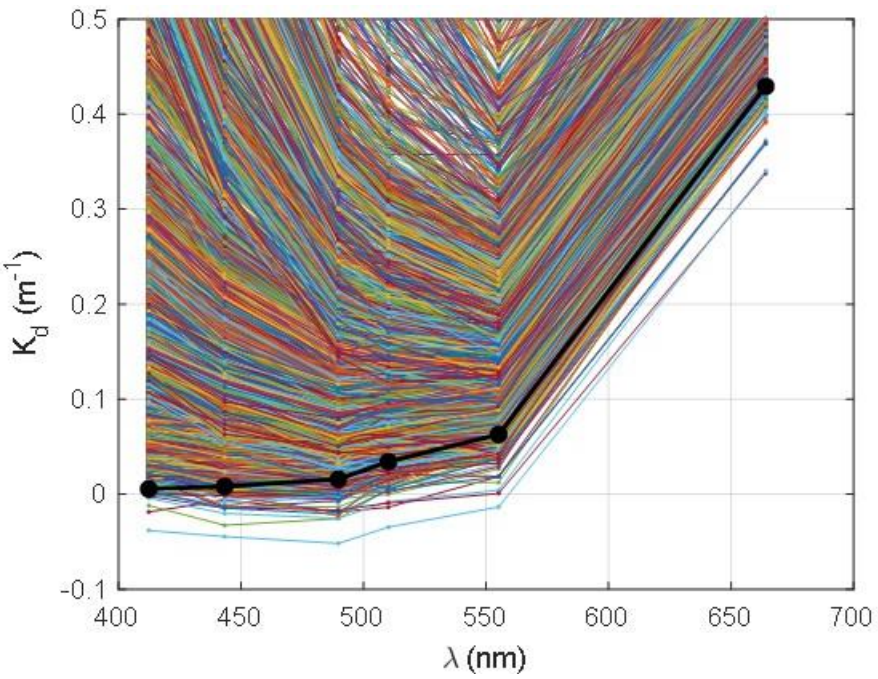

Fig. 2 K_d spectra of the dataset (colored lines), compared to $a_w + b_{bw}$ (black line).

On the phytoplankton absorption data and the chlorophyll concentration, I have plotted one against the other in Fig. 3 at 665 nm, with a highlight on the Eastern Mediterranean data. What I see is that there is the expected tight relationship, but I am concerned about a drop in sensitivity that I see in the lower end. The chlorophyll data has an evident trend towards saturation at about $0.03 - 0.04\ mg\ m^{-3}$, which is too high to resolve the variability in the oligotrophic oceans. I have overplotted the public data by Valente et al. (2022) and, for the few dots in the lower part, I see that the general linear trend is continued. So, authors may try to explain, and if possible, solve this issue.

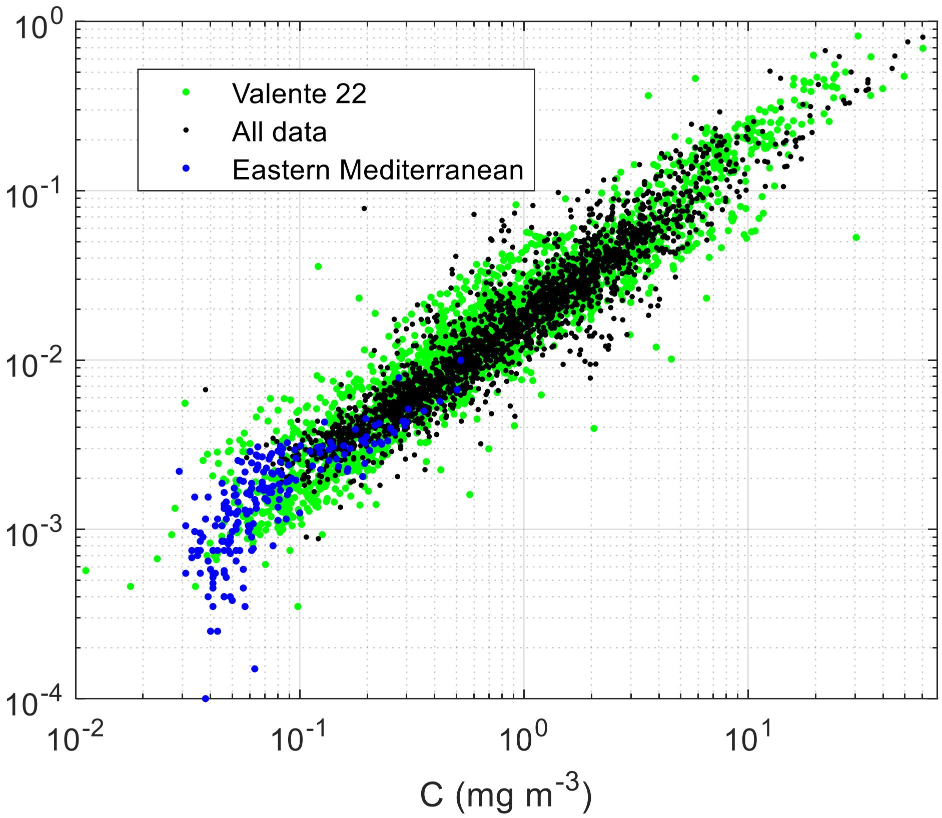

Fig. 3 Phytoplankton absorption as a function of chlorophyll concentration at 665 nm. Black and blue dots belong to the current dataset, whereas the green dots come from the public dataset by Valente et al. (2022).

The dataset is optically complete, and therefore something that I am missing in the paper is an R_{rs} closure exercise. A high degree of closure helps to increase the confidence on the dataset. In the case that large differences appear, the individual sources have to be inspected. The authors have provided a closure exercise for absorption, which is appreciated, and where significant differences appeared. For R_{rs}, I have done the closure exercises myself for absorption both from the ac-9 and from the water samples. This is done in Figure 4, for the ac-9 and in Fig. 5, for the water samples. To calculate R_{rs} in both cases, Lee et al. (2011) model was used. Considering the radiometric data as reference, results seem to indicate that absorption from ac-9 delivers quite clean data and closure seems very good in general. On the other hand, there are clear differences when absorption from the water samples are used. The plot suggests that absorption from the water samples is much noisier at blue wavelengths and tends to underestimate the real value.

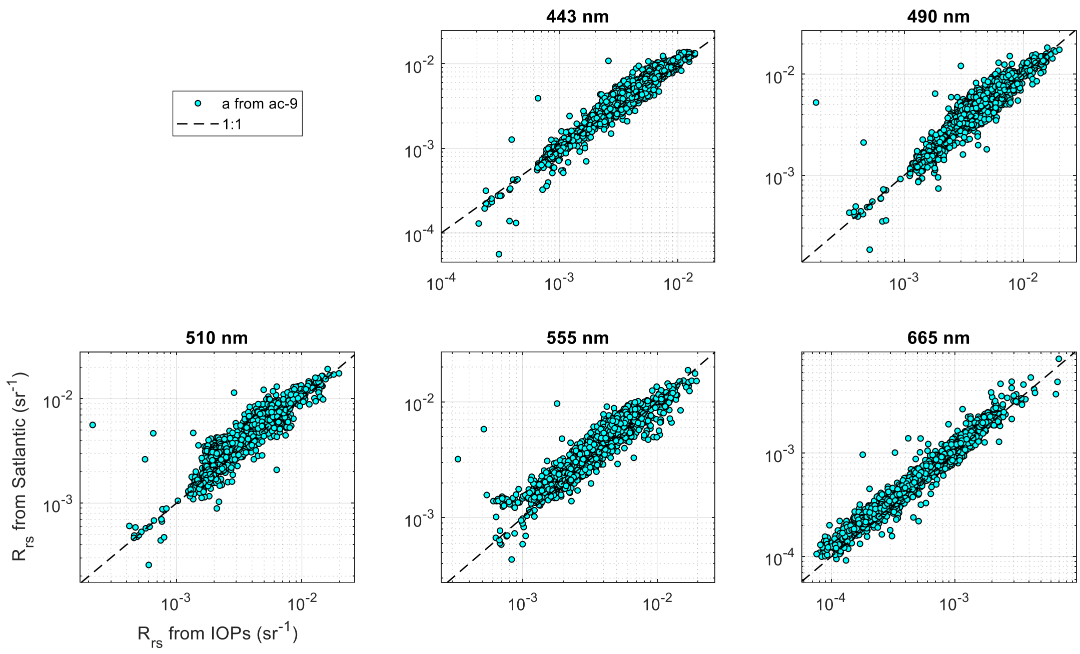

Fig. 4 R_{rs} closure using absorption from the ac-9 and backscattering from the Hydroscat-6.

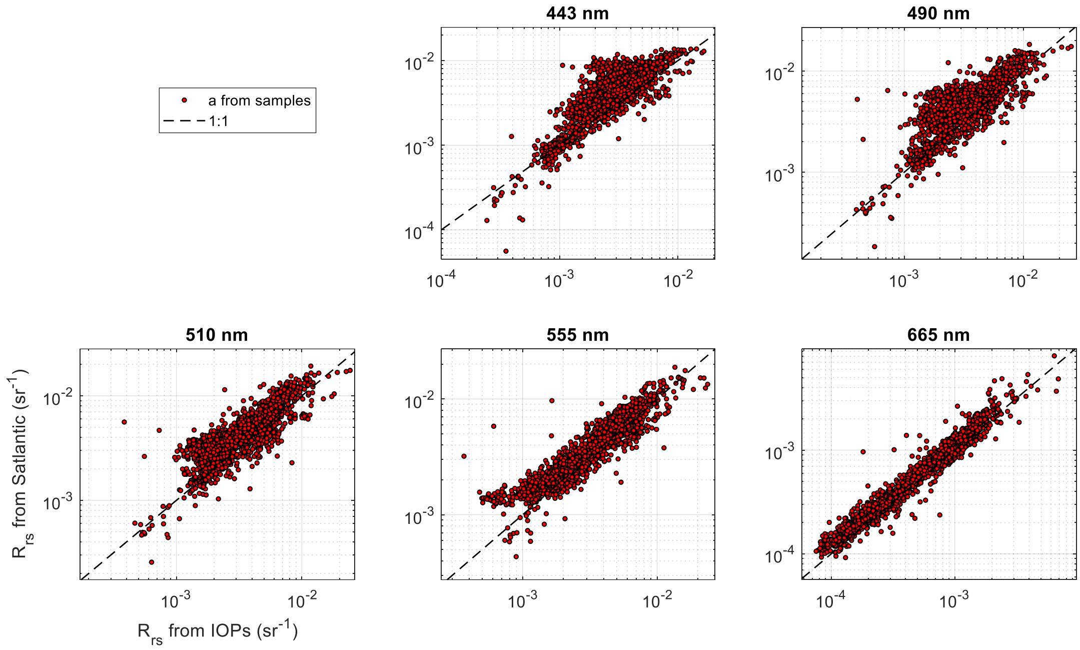

Fig. 4 R_{rs} closure using absorption from the water samples and backscattering from the Hydroscat-6.

Final comment is related to the data presentation in the article. It is nice to see the spectra and the ternary plots, and readers can have an idea of the water types that are represented. There are many ways to present the dataset, here just a few that might be of interest to the reader:

- Crossed relationships among IOPs
- R_{rs} vs. of chlorophyll, compared to the global relationship
- K_d vs. of chlorophyll, compared to the relationship by Morel
- Chlorophyll vs. the other two water constituents
- One R_{rs} band ratio vs. another one
- TSS vs. $R_{rs}(665)$

Minor comments

I think it is a requirement that the link to the dataset is shown in the abstract too.

Line 21: “applied equal” → used equally.

Line 39: “benefited of” → benefited from.

Line 54: “moderately” →moderate

Line 91: “attempting”: very vague term. What does it mean in this context, precisely?

Line 96: probably a link to the IOCCG protocol will help here, for those interested.

Table 2: the two-letter country code chosen by the authors looks arbitrary. There is a standardized one named ISO 3166-1 alpha-2, which I advise to follow.

Line 124: talking about in situ vs. laboratory measurements is confusing. Laboratory measurements are made on part of the in situ data. I prefer to talk about field instrumentation vs. laboratory measurement of field samples.

Line 209: no need to say “so called”, as this name is well consolidated and known by everybody.

Line 343. “Wattman” → Whatman

References

Doxaran, D. and others 2016. Improved correction methods for field measurements of particulate light backscattering in turbid waters. Opt. Express **24:** 3615-3637.

Kostakis, I. and others 2021. Hyperspectral optical absorption closure experiment in complex coastal waters. Limnology and Oceanography: Methods **19:** 589-625.

Lee, Z. P. and others 2011. An inherent-optical-property-centered approach to correct the angular effects in water-leaving radiance. Appl. Opt. **50:** 3155.

Roettgers, R., R. Doerffer, D. McKee, and W. Schonfeld. 2016. Algorithm Theoretical Basis Document

The Water Optical Properties Processor (WOPP). Pure water spectral absorption, scattering, and real part of refractive index model, p. 20. Helmholtz-Zentrum Geesthacht, University of Strathclyde.

Roettgers, R., D. McKee, and S. B. Woźniak. 2013. Evaluation of scatter corrections for ac-9 absorption measurements in coastal waters. Methods in Oceanography **7:** 21-39.

Stockley, N. D., R. Röttgers, D. McKee, I. Lefering, J. M. Sullivan, and M. S. Twardowski. 2017. Assessing uncertainties in scattering correction algorithms for reflective tube absorption measurements made with a WET Labs ac-9. Opt. Express **25:** A1139-A1153.

Valente, A. and others 2022. A compilation of global bio-optical in situ data for ocean colour satellite applications – version three. Earth Syst. Sci. Data **14:** 5737-5770.

Zhang, X., L. Hu, and M.-X. He. 2009. Scattering by pure seawater: Effect of salinity. Opt. Express **17:** 5698.