

Responses to Reviewer #1

“A synthetic optical database generated by radiative transfer simulations in support of studies in ocean optics and optical remote sensing of the global ocean”

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We appreciate the constructive comments by Dr. Pitarch. Here we provide our detailed point-by-point responses and a description of any actions taken in regard to these comments. The Reviewer’s comments are shown in italicized font; our responses follow each comment in normal font. Line numbers and figures indicated in our responses refer to the revised manuscript unless otherwise noted.

General comments. This manuscript describes the construction of a synthetic dataset for optical studies in the ocean, using Hydrolight. This topic is very familiar to me right now as I am pursuing a similar goal, so it was an easy read. Authors must make sure that it is accessible to a broader audience though.

It proceeds the usual way, as in the old IOCCG dataset from Lee in 2003: first it assembles a set of phytoplankton absorption spectra, then the rest of IOPs are built with relationships that include some randomness. Finally, a single wind speed (5 m/s) and three sun angles (0°, 30° and 60°) are set, as well as various combinations of inelastic scattering on and off. I downloaded and saw the dataset as part of the review.

Things I liked:

- *The randomness in the bio-optical relationships, that will reproduce the spread in the relationships that is observed in nature.*
- *The Petzold phase function is abandoned and the much more realistic Fournier-Forand is considered for non-algal particles. Maybe a remark by the authors would be better.*
- *The 50 nm gap left for Raman scattering. In fact, I checked with my own simulations that the spectral memory of Raman scattering is about 50 nm, so it makes sense. A comment by the authors would be appreciated.*
- *The organization in netcdf files is quite handy compared to the Hydrolight text files.*

Response: We thank the Reviewer for positive comments on our manuscript. Regarding Raman scattering the center of the emission band λ_{em} is related to the center of the excitation wavelength λ_{ex} through the following equation: $\lambda_{em} = 10^7 / (10^7 / \lambda_{ex} - 3400)$. The wavelength shift is around 50 nm for excitation in the UV-blue but increases to >100 nm for excitation in the red. This is described in Mobley (2012) which is cited in the manuscript where the wavelength distribution function is specified. We think there is no need for more detailed description of Raman scattering in our manuscript.

Now I have a list of things I liked less. I have made a ternary plot of the absorption budget and I have compared it with the IOCCG (Lee) and the Coastcolour (Nechad) datasets. What I see here is a disproportionately low amount of non-algal particles, even compared to the IOCCG dataset, which was developed for ocean applications. I am not saying that IOCCG is right and this one is wrong, but authors should verify that such absorption budget is what it is actually found in the global oceans. Compared to other datasets, b_b appears lower too.

Response: We agree with the Reviewer’s comment that the absorption dataset in our original manuscript is generally characterized by a lower contribution of non-algal particles in the absorption budget compared to the IOCCG and CoastColour datasets. We note that comparison with the CoastColour dataset, however, is not fully pertinent as that dataset was developed specifically for coastal waters with relatively high contribution of non-algal particles. Taking the Reviewer’s comment into account, however, we compared our original dataset with in situ data from open ocean waters (BIO SOPE cruise in the subtropical Pacific Ocean and the Atlantic data points from the CoastIOOC project). We concluded that it indeed made sense to regenerate our absorption dataset de novo allowing for an increased proportion of non-algal particles. To

accomplish this, the parameter P_2 in Eq. 3 was changed (see new equation in Table 1 of revised manuscript) to allow the contribution of a_d to vary between 10 and 90% of a_{ph} . The main implication of creating this new absorption dataset for the revised manuscript is that we regenerated the entire synthetic optical database presented in our study by rerunning all Hydrolight radiative transfer simulations for the same simulation scenarios as presented in the original manuscript. Accordingly, multiple figures were replaced with revised figures representing the new database (i.e., Figs. 5, 7–11). In general, however, the recalculation of the database did not require significant revisions of the text although some revisions and edits, where appropriate, were made. This new database of simulations will also replace the original database on the publicly-available Dryad repository.

Figure R1-1 (below) presents a comparison of the original and revised absorption coefficients in ternary plots, as proposed by the Reviewer. This comparison shows that the new absorption dataset (right panel) yields an absorption budget that includes higher contributions of a_d and is more consistent with in situ measurements collected in open ocean waters.

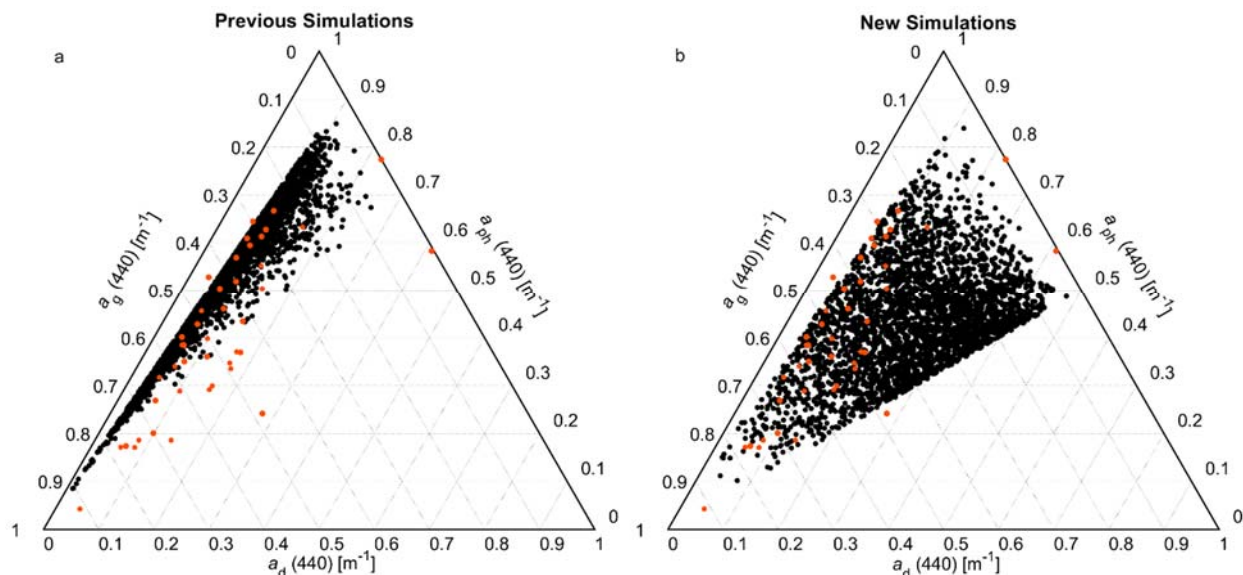


Fig. R1-1 (not in the manuscript). Ternary plots of the absorption dataset in the original manuscript (a) and the new absorption dataset used in the revised manuscript (b). Black data points represent the synthetic dataset and red data points are in situ measurements from open ocean waters in the Pacific (BIO SOPE) and Atlantic (CoastI OOC).

With regards to the comment that “*Compared to other datasets, b_b appears lower too*”, this is generally true. Similar to Fig. 7c in our manuscript, Fig. R1-2 (below) shows the b_{bp} vs. a_{ph} relationships of Huot et al. (2008) and Antoine et al. (2011) established from in situ measurements in open ocean waters and compares them with the synthetic datasets from IOCCG, Craig et al. (2020), and our present work. Figure R1-2 clearly indicates that, for a given a_{ph} (or Chla), b_{bp} is overestimated in both the IOCCG and Craig et al. datasets, especially in oligotrophic waters, which is mainly due to the high contribution of non-algal particles in these datasets. In contrast, the distribution of data points in our dataset (left panel) is consistent with the main trend lines from Huot et al. (2008) and Antoine et al. (2011).

We added new text describing these results in the revised manuscript (lines 593-600). We did not add any new figure on this specific aspect except for a new panel (c) in Fig. 7 showing $a_d(443)$ vs. $a_{ph}(443)$ for our synthetic and in situ datasets. Discussion about the ratio of different IOPs to $a_{ph}(443)$ vs. $a_{ph}(443)$ has been also refined (lines 593-600).

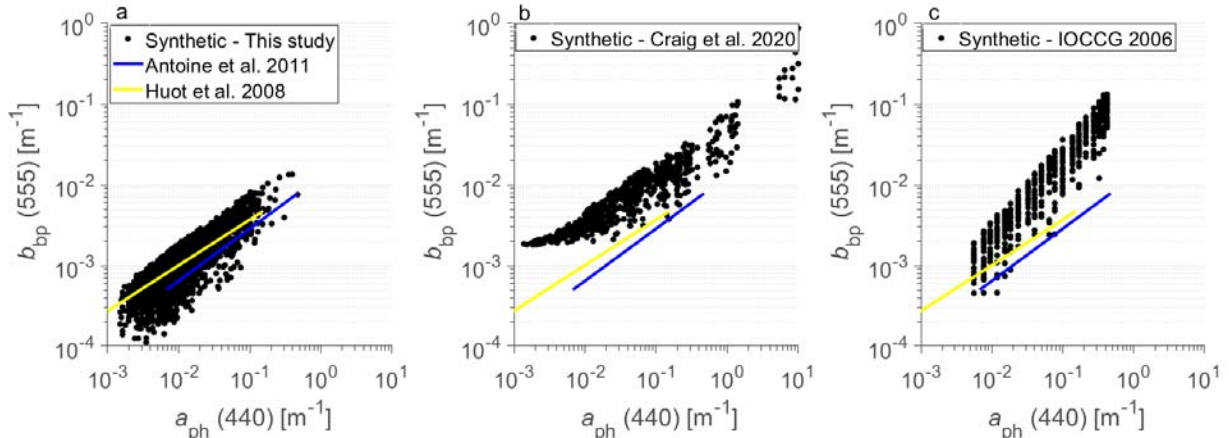


Fig. R1-2 (not in the manuscript). Comparison of $b_{bp}(555)$ as a function of $a_{ph}(443)$ for different synthetic datasets. Empirical relationships describing $b_{bp}(555)$ vs. Chla reported from field measurements are also displayed for comparison. For these latter relationships, $a_{ph}(443)$ has been estimated from Chla as described in the manuscript.

I have also plotted the remote-sensing reflectances (no inelastic scattering, sun at 30°). Some R_{rs} look crazy for me. I have never seen anything that high in the blue, even for the most oligotrophic waters. To verify, I have calculated the maximum band ratio (MBR) and I have applied the OC4 to it, according to O'Reilly and Werdell (2019). I have also calculated the chlorophyll index (CI), by Hu et al. (2012), for the most oligotrophic waters and I have applied his algorithm too. I get two chlorophyll histograms for the whole dataset: Considering that the lowest CHL measured in Valente et al. (2019), cited in O'Reilly and Werdell (2019), was 0.012 mg m⁻³, that leaves us a very high amount of simulations whose CHL is unlikely low, whether we use OC4 or CI (Hu) to compare with. I also checked with Morel "clearest" waters and these values are definitely off. I therefore encourage redefinition of the dataset. I do not have an explanation for this artifact considering that the authors have reproduced the histograms seen by satellite data. I can hypothesise (1) the retrievals were biased the $a_{ph}(440)$ is actually higher or (2) the bio-optical relationships affect the CHL algorithm and need redefinition.

Response: The maximum values of R_{rs} spectrum which have been measured in open ocean waters can reach about 0.026 sr⁻¹ in the violet-blue part of the spectrum (see, for example, BIOSOPE measurements in Fig. 3 of Stramski et al., 2008). In our original manuscript, only 0.0636% of R_{rs} spectra had values higher than 0.026 sr⁻¹. The Chla histograms provided by the Reviewer show also only a very small fraction of Chla data lower than 0.012 mg m⁻³ (note that for such very clear waters, only the Hu et al. algorithm should be considered). We verified that in our newly simulated database presented in the revised manuscript, the R_{rs} values higher than 0.026 sr⁻¹ do not exist in the configuration mentioned in the Reviewer's comment (i.e., no inelastic scattering and sun at 30°). When all our new simulations are considered, the maximum value of R_{rs} reaches 0.0029 sr⁻¹, and only 7 out of 29880 spectra (0.023%) in our new synthetic database have values higher than 0.026 sr⁻¹ (see Fig. R1-3 below). We find these results completely reasonable and adequate. The following addition has been made in the revised manuscript (lines 644-647) where the $R_{rs}(555)$ vs. $R_{rs}(443)$ pattern is described (Fig. 9): "The maximum values of $R_{rs}(443)$ reached 0.0165 sr⁻¹, which is in good agreement with in situ measurements performed in ultraoligotrophic waters in the South Pacific gyre during the BIOSOPE cruise (see Fig. 3 in Stramski et al., 2008)."

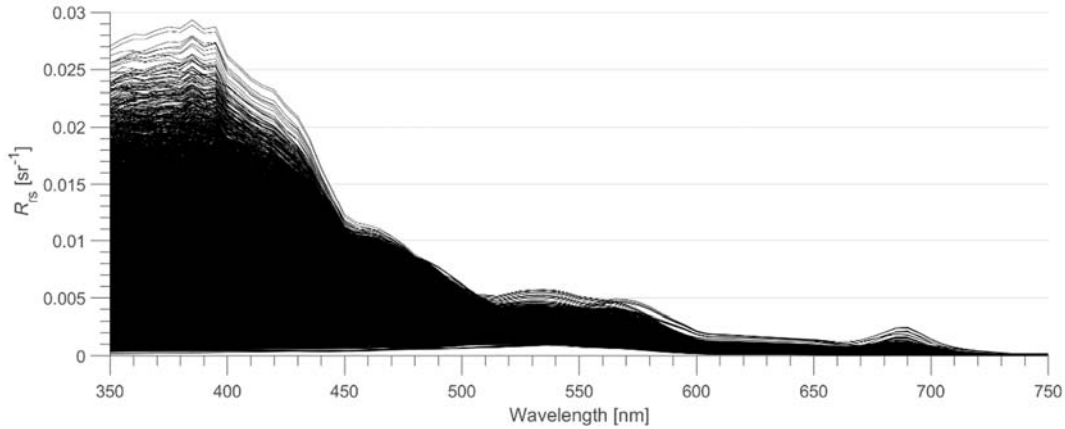


Fig. R1-3 (not in the manuscript): The new synthetic dataset of R_{rs} spectra presented and used in the revised manuscript.

Related to this, there are datasets that may help in getting bio-optical relationships that are realistic. For example, I compared some absorption ratios to NOMAD: I think I see that for the same $a_{ph}(440)$, there is a general lower value for $a_g(440)$ compared to NOMAD. Regarding $a_d(440)$, I see a lack of spread.

Response: It is important to realize that the NOMAD dataset is dominated by coastal waters which explains why for a given a_{ph} , a_d and a_g values often tend to be higher in NOMAD compared to typical range of scenarios expected for open ocean waters (the main focus of our study). The lack of spread observed for a_d has now been corrected in the revised manuscript as described in our previous responses. By plotting the a_g/a_{ph} as a function of a_{ph} (Fig. R1-4 below) one may note a relatively good overlap between in situ and synthetic data (although admittedly in situ data of a_g are quite scarce in very clear waters).

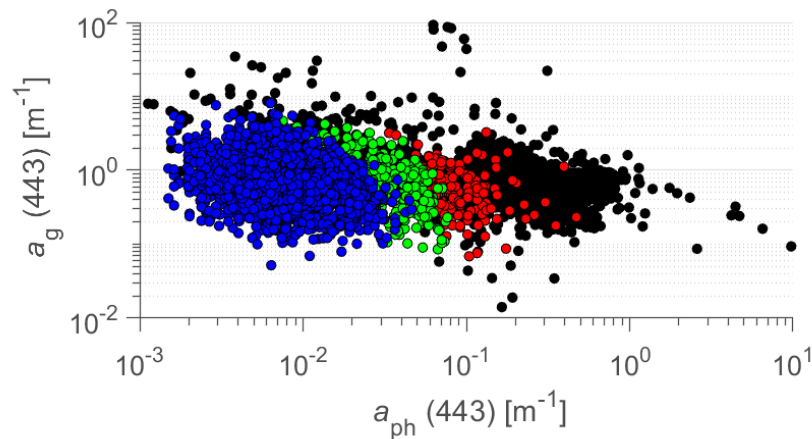


Fig. R1-4 (not in the manuscript). The ratio a_g/a_{ph} as a function of a_{ph} for the synthetic (colored points) and in situ (black points) datasets.

This is not the only example of what the authors can do. For example, I have plotted the CDOM slope S_g as a function of $a_g(440)$ for the NOMAD and Biosope datasets, as well as for three cruises in very clear waters of our group. One can see some tendency to spread, especially to high S_g , when $a_g(440)$ is small, and a tendency to concentrate around $S_g \approx 0.016 \text{ nm}^{-1}$ for high $a_g(440)$. But the authors use a uniform

distribution between 0.01 nm⁻¹ and 0.02 nm⁻¹. This could therefore be improved. I could revise the rest of IOPs and bio-optical relationships but I believe that at this point the authors got my point.

Response: We prefer to keep a uniform distribution of S_g for two reasons. First, a direct link between S_g and a_g is not well established and it is difficult to provide an average trend between these two parameters. Second, the whole spectra of IOPs are provided in our database, so the S_g slope can be computed for every a_g spectrum which provides users with the freedom to select cases of interest, if deemed appropriate for specific studies.

Specific comments

Abstract: it lacks a motivation on why another dataset is needed

Response: The abstract already states that “Compared to similar developments of optical databases in the past, the present dataset of IOPs is characterized by probability distributions of IOPs that are consistent with global distributions representative of vast areas of open ocean pelagic environments and coastal regions covering a broad range of optical water types”. We also mention that the new optical database obtained from radiative transfer simulations accounts for inelastic scattering, which is not the case in previous databases. We made minor edits to further clarify this point in the abstract (lines 28-29): “These input IOPs were used in three simulation scenarios associated with assumptions about inelastic radiative processes (not considered in previous synthetically-generated optical databases) in the water column....”

Lines 51-52: “Recent technological developments and broader accessibility of optical in situ instrumentation” I believe this is unfortunately not the case. Seabird (old Wetlabs and Satlantic) has discontinued many in situ optical instrument, HobiLabs has closed and is not selling instruments anymore. All we have is Sequoia and Seabird in a situation of monopoly with little or no incentive to innovate and imposing high prices in already old design instruments, with a general lack of market competition.

Response: We do not wish to enter this discussion in any greater detail and it is beyond the main thrust of our study. While it is true that some commercial products have been discontinued or may be discontinued soon, it is also true that technological advancements are underway (e.g., under current SBIR programs in the US) both in terms of radiometric and IOP instrumentation and some new instruments have already reached either the state of commercialization or will likely get to this point in near future (e.g., Sunstone Scientific). Also, there are still some relevant commercial products available from a few other companies such as Biospherical, TriOS, CIMEL, or RBR.

Lines 60-63: the most important motivation for a synthetic dataset is that we will never have complete optical datasets across the widest dynamic range, and with declared and low uncertainties.

Response: We agree that field datasets are unlikely to fulfill this desire for complete optical datasets spanning the entire dynamic range of the ocean. Similarly, synthetic optical databases are unlikely to be ever developed to the point to cover all possible natural conditions in the ocean, primarily because such databases depend on the use of simplified input parameters characterizing the complex environmental variability. For example, presently the variability in particle phase function can be viewed as imposing some limitations. One important point about the synthetic databases is that the data are free of measurement errors, so we made minor edits to better clarify this point (line 62): “In this context, radiative transfer (RT) simulations, which are free of measurement errors, provide a useful tool to generate comprehensive synthetic databases and complement the existing datasets of field measurements in support of studies in ocean optics and optical remote sensing.”

Lines 118:120: this is unclear to me.

Response: Part of the original sentence, which is not the most important point, has been removed. The sentence now reads (line 117): “Third, the probability distributions of different IOPs that were used as input to previous RT simulations do not appear to match well with the IOP distributions observed in extensive field datasets or satellite-derived datasets representing the global ocean.”

Line 145: I would avoid the word "specific" as it is usually referred to the absorption divided by the concentration.

Response: This has been changed and reformulated as follows: “Specifically, the absorption coefficients of the different constituents are the spectral absorption coefficients of phytoplankton,”. The same modification has been made in other places where relevant.

Lines 152-153: I think all IOPs matter equally, not only a_{ph} .

Response: We agree that all IOPs matter equally, but here for the creation of the synthetic dataset a_{ph} is used as a main “driver” to define and constrain the variability of other IOPs that are expected to occur in open ocean waters. In the manuscript we have stated (lines 155-156): “Among these different constituent IOPs, the phytoplankton absorption coefficient, $a_{ph}(\lambda)$, plays the most fundamental role in the creation of the synthetic dataset of IOPs in this study.”

Line 160: “the measured values of $a_{ph}(\lambda)$ were used in the calculations of these IOPs”. Alright, but Lee did the same 20 years ago, so it is not a big novelty. I would not emphasize.

Response: We believe it is important to keep this sentence because it indicates that our IOP dataset has been generated based on in situ measurements of a_{ph} , which was not the case for the IOCCG dataset. In this context, our main purpose is to emphasize this point rather than address any particular novel aspects compared to previous synthetic datasets.

Lines 238-241: this comment is totally right. In fact, it is a pity that in 2023 there are still new datasets that are degrading spectral resolution to only few bands. Not to mention the aggregation of a_g and a_d in Valente, which makes us still rely on NOMAD when we want them separately. On the reconstruction of hyperspectral a_{ph} from multispectral: I believe that a decently sized of hyperspectral a_{ph} can be compiled without the need to worry about this.

Response: We thank the Reviewer for this comment.

Line 276: When extrapolating a_{ph} to the UV, how is exactly the UV part “glued” to the rest?

Response: Once the reference spectrum that exhibits the best correlation with the investigated spectrum in the visible has been identified, the UV portion of the reference spectrum is normalized to its value at 400 nm. This normalized UV spectrum is then multiplied by the reference spectrum value at 400 nm and used to extend the investigated spectrum into the UV.

Line 311: probably instead of “shifted”, I would say “biased”.

Response: We think “shifted” is more appropriate than “biased” in this context. The datasets that contain significant fraction of coastal measurements are not necessarily biased but their statistical measures of central tendency are shifted to larger values compared to predominantly open ocean data.

Lines 345-346: I think it is stated that the Mediterranean Sea is ultraoligotrophic, when it is actually not, not even the eastern basin (maybe this place in Summer, yes).

Response: We agree that the Mediterranean Sea is not ultraoligotrophic as a whole. The Loisel et al. (2011) paper refers to some ultraoligotrophic eddies within the Mediterranean Sea observed during summer. This point has been clarified (lines 357-361): “While the original classification of Mélin and Vantrepotte (2015) includes 16 optical water classes (OWC), the derivation of $a_{ph}(\lambda)$ and $a_{dg}(\lambda)$ from the 3SAA additionally included a 17th OWC to improve the representation of ultraoligotrophic waters such as those found in the South Pacific Gyre (Morel et al., 2007; Claustre et al., 2008; Stramski et al., 2008) and in some areas of the Mediterranean Sea in summer (Loisel et al., 2011). This 17th OWC is described in Jorge et al. (2021).”

Line 460: “m_z/(mg Chla)”. Mass is mass, so please delete the “Chla”. Yes, it is common to write it like that among some biologists, but it does not make sense metrologically.

Response: “Chla” has been removed.

Lines 460-461: it is much more accurate to use a red wavelength of a_{ph} rather than a blue one to estimate CHL.

Response: We agree that a_{ph} in the red is a better proxy of Chla because this band is less affected by various accessory pigments and package effect than the blue absorption band. However, in these specific calculations this aspect is not critically important because the purpose is to generate a relatively large range of variability in one of the IOP coefficients, which is accomplished through the use of random factor, and not to predict Chla.

Lines 536-540: I wonder what are the reason to not consider the pure water measurements by Mason and Fry in 2016.

Response: We use the spectral values of $a_w(\lambda)$ following the current recommendation of the IOCCG (2018) protocols devoted to the absorption coefficient (Table 1.1 in Chapter 1). The Mason and Fry (2016) measurements were not included in these recommendations. The Mason and Fry values are significantly lower in the short-wavelength portion of the spectrum than other literature values which are supported by relevant discussion in the IOCCG protocols. The significantly different values of Mason and Fry have not yet been vetted by the community and would require support from additional studies and validation to reach adequate level of confidence for potential use as “standard” recommended values.

Lines 551-553: I wonder whether saving the whole profile is very useful, considering that Hydrolight already calculates for you the “K’s”, “z’s” and these depth-related quantities.

Response: Data of whole profile are useful; for example, to calculate an averaged K_d value over a specific water layer which can be of interest to users and some applications.

Figure 7 is not an efficient way to show the differences. Of course, everything increases with $a_{ph}(440)$ to a first order, but we want to know the differences among datasets. I prefer if the ratios are represented e.g., $a_g(440)/a_{ph}(440)$ as a function of $a_{ph}(443)$, etc.

Response: The objective of this figure is to show how the present synthetic dataset compares with in situ data. Similar patterns are observed when IOPs are divided by a_{ph} (see Fig. R1-5 below), which is now mentioned in the text of revised manuscript text (lines 597-599) but without adding a new figure such as Fig. R1-5 in the revised manuscript (which already has 12 figures). In addition, as discussed in Berges (Limnol. Oceanogr. 42, 1006-1007, 1997), plots of Y/X vs. X should be interpreted with special caution.

We also note that in Fig. 7 of the revised manuscript we added a new panel with $a_d(443)$ vs. $a_{ph}(443)$ and polygon lines to improve the illustration of the range of in situ data.

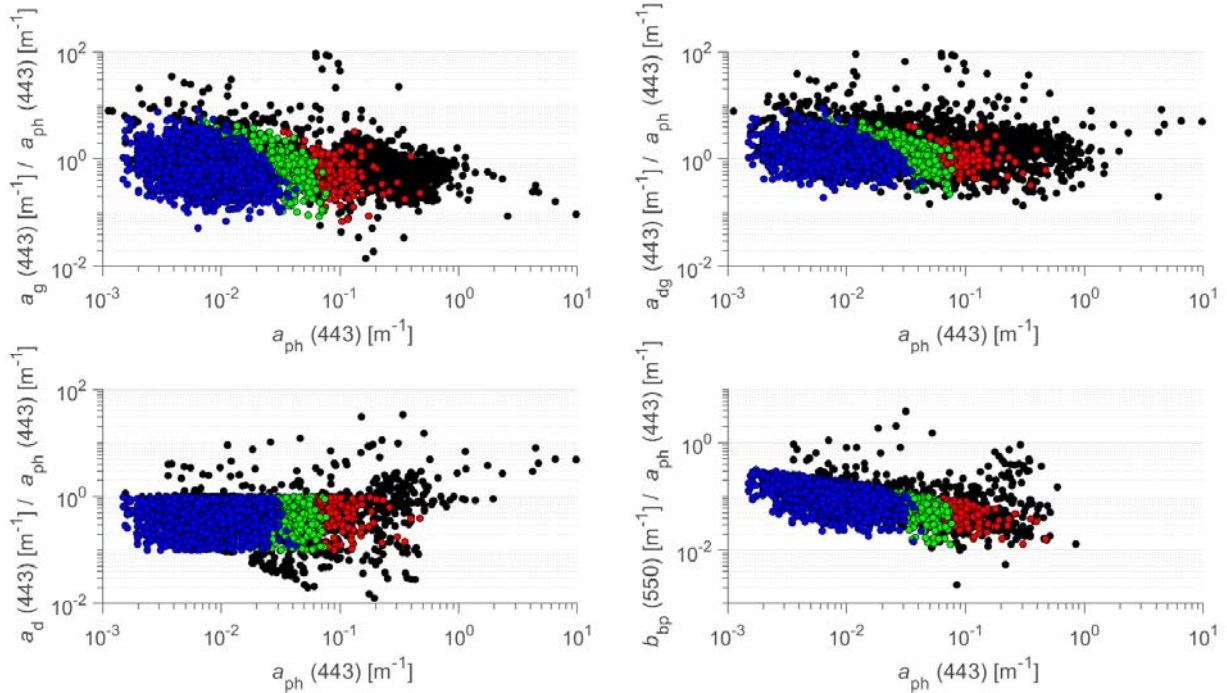


Fig. R1-5 (not in the manuscript): The ratio of constituent absorption coefficients to a_{ph} vs. a_{ph} at 443 nm for the synthetic (colored data points) and in situ (black data points) datasets.

Line 602: "The scatter plots show a significant degree of overlap" Very roughly, but see my comment above.

Response: We think our response above addresses this point.

Lines 688-689: there is no complementarity of this dataset and Nechad's as both have different assumptions regarding the bio-optical modelling, so they are not consistent with each other.

Response: These two synthetic datasets have been generated with different assumptions regarding bio-optical modeling as their primary focus is on different bio-optical environments (open vs. coastal waters). So, in that sense we think these datasets are complementary as their combination covers a larger and more diverse range of optical environments.

The plots in Fig. 10 are not telling anything new as we know what happens with E_a profiles for different water types.

Response: The purpose of this figure is not to provide scientifically novel information but rather to illustrate the spectral and vertically-resolved (along the water column) optical information included in this new synthetic database. This can be useful to readers interested in this kind of optical data, especially that other commonly known synthetic optical databases (IOCCG, 2006; Craig et al., 2020) do not include data as a function of depth within the water column.