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ESSAY

Unleashing the power of remote sensing data in aquatic research: Guidelines for optimal utilization

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Scientific Significance Statement

The growing utilization of remote sensing data in lake studies provides crucial spatial insights into biogeochemistry and biology. However, clarity regarding the development and intended use of remote sensing products is often lacking. This letter aims to elucidate the tradeoffs for the utilization of remote sensing data in limnological studies with an example of based on the estimation of chlorophyll *a* due to its importance as a water quality indicator. The analysis initiates with a meticulous product selection, requiring an evaluation of its capacity to address the optical complexity of freshwater systems. Assessing atmospheric correction and product limitations ensures alignment with the study's objectives. Subsequently, rigorous validation of remote sensing products is essential, accompanied by a cautious interpretation of the data. This letter advocates for the use of remote sensing data, offering key strategies for their optimal utilization in lake studies.

Setting the basis

The use of satellite remote sensing for monitoring water quality in inland water systems has been growing in the last decades especially due to the development of new orbital sensors (Kutser et al. 2020; Ogashawara 2021). Earth observations provide new angles for limnology, such as a universal perspective of multiple aquatic ecosystems simultaneously, regional to global coverage, the potential to acquire time series of data and its valuable input to predictive models. Additionally, it allows the retrieval of several parameters across the surfaces of an increasing number of smaller lakes, providing not only the surface area and elevation, but also surface biogeochemical data. The exponential growth of studies using this technology highlights that the improved computing resources, increased amount of satellite imagery, and development of operational remote sensing algorithms to understand complex inland water systems is now a reality (Topp et al. 2020).

With the increasing access to satellite data, several organizations are developing remote sensing-based products for

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water quality. These products are currently distributed by national and international agencies (i.e., European Space Agency [ESA], US Geological Survey [USGS]), international programs (i.e., Copernicus Marine, Copernicus Land, and Copernicus Climate Change), academic research (i.e., Minnesota Lake Browser, https://lakes.rs.umn.edu/), and private industry (i.e., CyanoLakes, https://www.cyanolakes.com/; CyanoAlert, https://cyanoalert.com/). Typically, the data behind these products have undergone substantial processing including atmospheric correction, identification of quality issues, and bio-geo-optical algorithms to derive the desired bio-geophysical variables. Figure 1 exemplifies the main procedures for generating a quality controlled remote sensing-based water quality product (inland, coastal, and marine). Procedures are divided into five types: (1) the initial data needed (the Level 1 satellite imagery, the in situ radiometric data, the in situ bio-geo-optical properties [especially inherent optical properties] and in situ water quality curated data); (2) the remote sensing processes (atmospheric correction and bio-geo-optical modeling), 3) the validation processes (of the remote sensing processes using in situ collected data); (4) the remote sensing-based products such as the atmospheric and glint correction imagery; and (5) the water quality products which are produced by applying the selected bio-geo-optical algorithms (locally and

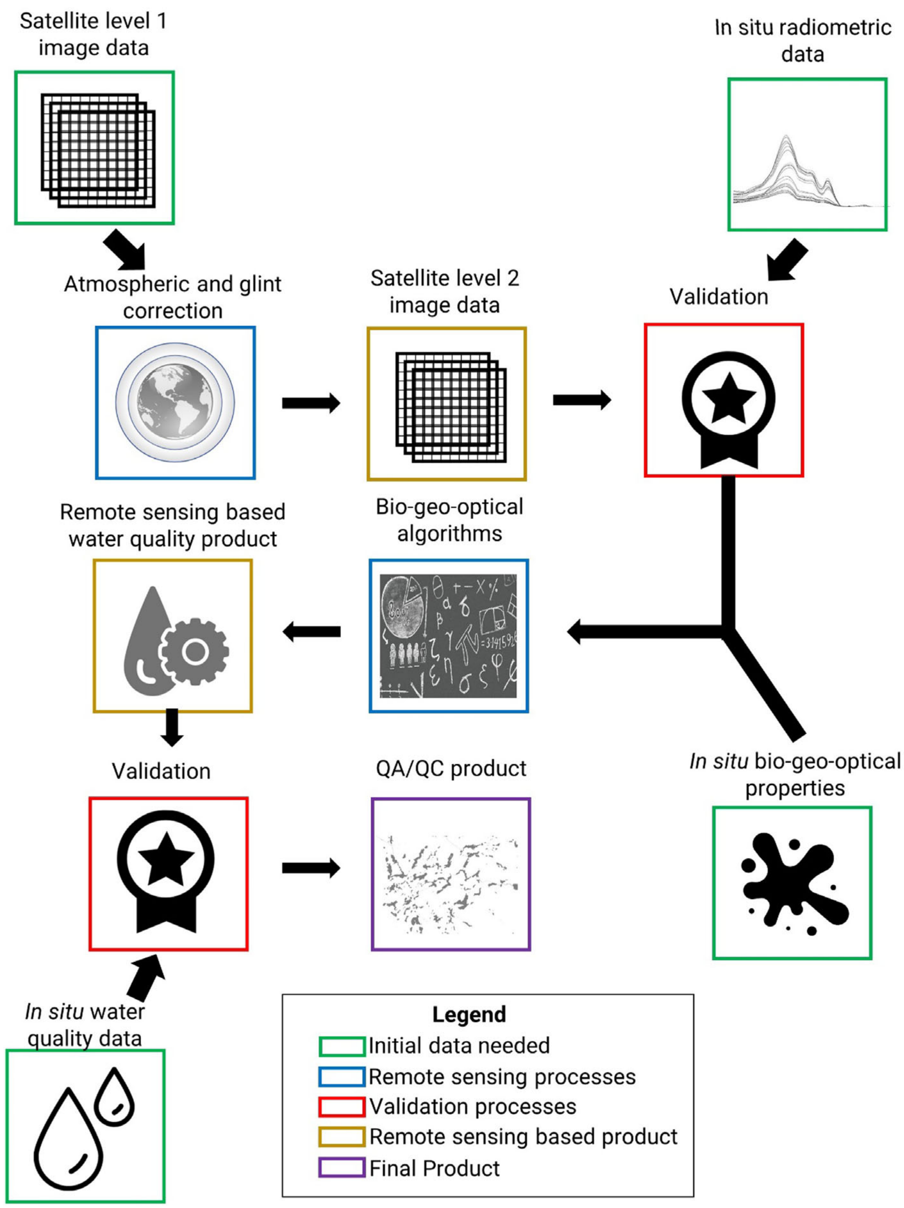

Fig. 1. Procedure for the generation of a quality controlled remote sensing-based water quality product.

seasonally adapted to the dominating water constituents and validated with in situ water quality data) to the atmospherically corrected image. Finally, the remote sensing-based product needs to pass a quality assurance and quality control (QA/QC) to generate a final curated product.

As presented in Fig. 1, obtaining remote sensing-based water quality products is intricate, particularly for inland waters where optical properties are highly variable due to the naturally wide fluctuation in optically active constituents (OACs; i.e., phytoplankton pigments, colored dissolved organic matter [CDOM] and sediment) in the water column (Ogashawara et al. 2017). To illustrate this complexity, algal blooms can manifest in brown waters rich in CDOM and mobilized sediments that induce turbidity (Lebret et al. 2018). Due to this optical complexity, many remote sensing-based ocean color products mask out turbid waters, resulting in the exclusion of numerous freshwater systems. To promote the utilization of remote sensing technology and to enhance the understanding of the tradeoffs using remote sensing data, this letter addresses (i) the primary issues leading to problems in interpreting remote sensing data; (ii) the consequences of the misinterpretation; and (iii) suggests strategies for the utilization of remote sensing data, along with approaches to contribute to the reliable calibration and validation of remote sensing-based water quality products.

What are the major issues and their consequences?

The selection of the remote sensing product is one of the primary considerations for limnological studies. Remote sensing-based products are designed for open ocean (ocean color products), coastal or inland waters, and it is crucial to discern the differences among them before making a choice. These differences arise from the light availability within the water column, where, in a first approximation: (1) open ocean waters predominantly absorb the red part of visible light, (2) coastal waters and clear inland waters absorb both blue and red light, and (3) turbid inland waters strongly absorb from short wavelengths to the red part of visible light (Kirk 2011). Understanding these variations in the interaction between light and water facilitates the decision for the appropriate spectral region to be used during remote sensing data processing for atmospheric correction and bio-geo-optical modeling.

One example highlighting the importance of selecting the appropriate spectral region is the computation of chlorophyll *a* (Chl *a*) concentration from satellite data. Processing algorithms developed for the open ocean rely on the blue and green spectral band ratio due to Chl *a* absorption around 440 nm and the very low CDOM background signal (O'Reilly and Werdell 2019). In contrast, coastal water products utilize the entire spectrum with a Neural Network approach (Brockmann et al. 2016), while inland water remote sensing products so far typically base calculations on the ratio of aquatic reflectance at 665 nm (red peak of Chl *a* absorption) and the red-edge around 700 nm (scattering of algal cells, Gitelson 1992). Given the low Chl *a* concentration in the open ocean, spectral bands within the red range are often dominated by water absorption and become unsuitable for Chl *a* retrieval. In inland waters (where CDOM is usually present), blue spectral bands are usually dominated by CDOM absorption, masking Chl *a* absorption at 440 nm, thus favoring the use of Chl *a* absorption at 665 nm. As a comparison, in situ Chl *a* sensors have recently been developed that use red light excitation rather than the traditional blue light excitation, in response to these optical challenges typical for coastal and inland waters. Additionally, it is crucial to highlight that open ocean, coastal, and inland water Chl *a* remote sensing products have been optimized for different concentration ranges, a factor that should be considered before using the data. Due to the intricate relationships between different water types and light, understanding the remote sensing data processing approaches in a remote sensing-based water quality product is essential for understanding the advantages and disadvantages of each product.

Figure 2A presents examples of typical aquatic reflectance spectra (remote sensing reflectance) from different aquatic environments which visually highlights the contrast interactions between light and water. To showcase the importance of selecting the most suitable approach for estimating Chl *a* concentration Fig. 2BD,F presents three remote sensing-based Chl *a* products from the Sentinel 2 MultiSpectral Instrument (MSI) over lakes located in the Mecklenburg–Brandenburg Lake District in northeastern Germany (Ogashawara et al. 2021). We selected traditional remote sensing approaches for (i) open ocean (Fig. 2B), (ii) inland waters, and (iii) coastal waters (Fig. 2F). The visual differences among these three different remote sensing-based products for the Sentinel 2 MSI image (Scene ID: GS2A_20190726T102031_021369_N02.08) are further supported by scatter plots of the respective remote sensing estimated Chl *a* concentration and a water sample-based laboratory measurement of Chl *a* concentration using high-performance liquid chromatography (HPLC) done on the same day (Fig. 2C,E,G, respectively). In these examples, it was observed that the open ocean approach (Fig. 2C) underestimates the Chl *a* concentrations, the inland water approach (Fig. 2E) underestimates the Chl *a* for more eutrophic waters and the coastal approach (Fig. 2G) showed an underestimation for all Chl *a* concentrations. These results agree with the previous paragraph that when applying an open ocean approach in lakes the results may be strongly underestimating the true concentration of Chl *a*, especially in turbid waters, as the use of the blue and green regions of the visible spectrum are heavily affected by CDOM. It also highlights the importance of using in situ data to validate the selected satellite product—as the validation process is essential for the QA/QC (see Fig. 1).

A major challenge for remote sensing data processing in inland waters (Fig. 1) is the atmospheric correction (Pahlevan

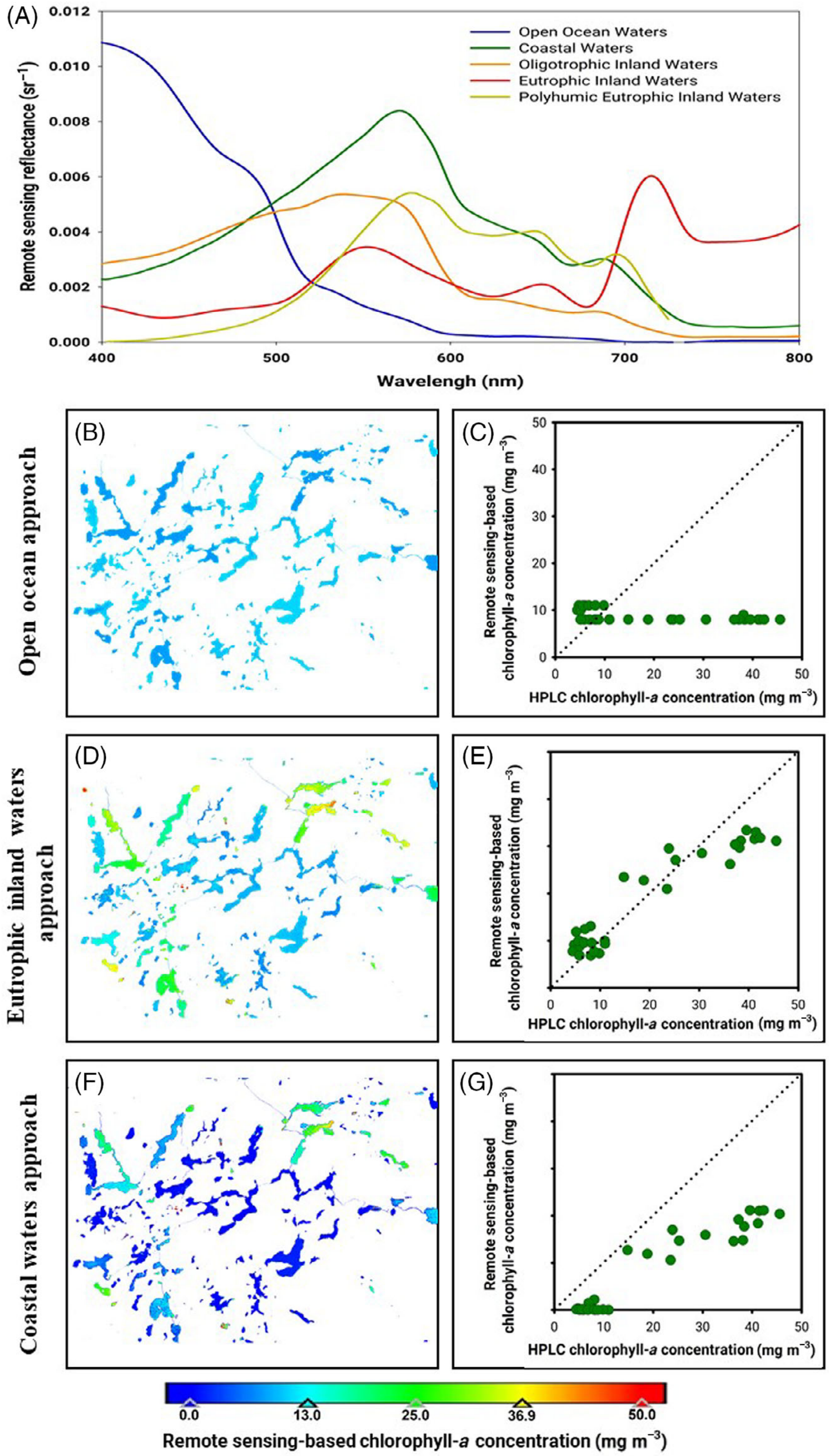

Fig. 2. (**A**) Examples of aquatic reflectance spectra from open ocean, coastal, oligotrophic inland, eutrophic inland waters and polyhumic eutrophic inland waters; using data from lakes in NE Germany, we show (**B**) satellite-based Chl *a* concentration applying an open ocean approach; (**C**) the resulting scatter plot between estimated and HPLC-measured Chl *a* concentration for an open ocean approach; (**D**) satellite-based Chl *a* concentration applying an eutrophic inland waters approach; (**E**) the resulting scatter plot between estimated and HPLC-measured Chl *a* concentration for an eutrophic inland waters approach; (**F**) satellite-based Chl *a* concentration applying a coastal waters approach; and (**G**) the resulting scatter plot between estimated and HPLC-measured Chl *a* concentration for a coastal waters approach.

et al. 2021). Atmospheric correction is the process of removing the optical effects of the atmosphere in the view field of a satellite or airborne sensor observing a target on the Earth's surface. A part of the atmospheric correction, is the glint correction which removes both the measured signal from light that is specularly reflected at the water surface from the sun, as well as reflected from the sky toward the sensor. Approximately, 90% of the total signal measured by a satellite stem from the atmosphere (IOCCG 2010), and the intensity of the glint can be higher than the intensity of the water leaving radiance, depending on the brightness of water, solar azimuth angle and on wavelength. Therefore, the accuracy requirements of the correction methods are much higher over water than over land. Figure 3 presents average reflectance spectra of a eutrophic lake for a Sentinel 2 MSI image without atmospheric correction (top-of-atmosphere reflectance—R_{TOA}), with a land based atmospheric correction (surface reflectance—SR) and using an aquatic atmospheric correction for the computation of the Remote Sensing Reflectance (R_{rs}). A recent study performed a similar comparison for the Landsat SR products and showed that the use of SR products for the green and red spectral bands had uncertainties close to 30%, whereas the uncertainties in the blue and coastal-aerosol bands ranged from 48% to 110% when compared to in situ R_{rs} (Maciel et al. 2023). These results highlight the importance of having an aquatic atmospheric correction and to carefully evaluate the tradeoffs of the use of SR in limnological studies.

Considering that there is no universally acceptable inland water atmospheric correction processor, limnological studies need to first validate different atmospheric correction processors as highlighted in Fig. 1. This validation of the atmospheric correction is crucial to make sure that the remote sensing data used as input for the studies using machine learning and artificial intelligence approaches (in which data quality is absolutely critical) are not largely biased. However, it becomes challenging because it requires in situ radiometric data to perform this validation. This type of data is still not commonly used by most scientists not specialized in remote sensing, despite that it is crucial to develop and calibrate the water atmospheric correction processors for inland and coastal waters.

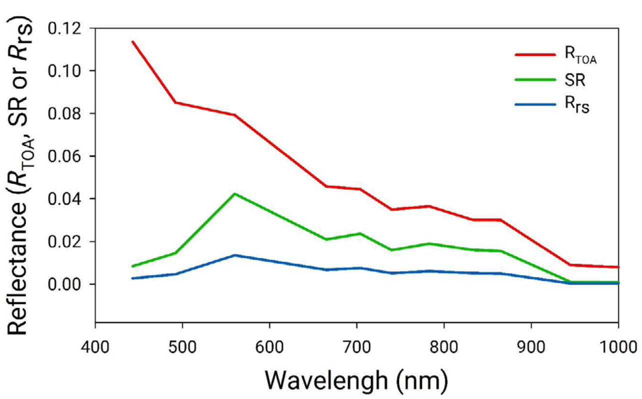

Fig. 3. Average reflectance spectra from different remote sensing product levels. Reflectance at top-of-atmosphere (R_{TOA}) in red; surface reflectance (SR) in green; and remote sensing reflectance (R_{rs}) in blue.

Recommendations for an optimal use of remote sensing data in aquatic research

How to choose the right remote sensing-based water quality product? Before incorporation of remote sensing data in aquatic research, it is important to look for the Algorithm Theoretical Basis Document (ATBD) of the remote sensing-based product and the proper reference of the product to precisely understand its development and limitations. Another recommendation is to use remote sensing-based products, which have been standardized and quality controlled by a reputable organization, such as the Committee on Earth Observation Satellites (CEOS) that recently created a minimum set of requirements for different remote sensing-based products (CEOS 2021). With this verification of quality by CEOS, it will be easier to identify if the retrieved information is trustful or not. Finally, a simple recommendation is to always use a remote sensing-based product developed for the specific type of water under investigation: open ocean, coastal or inland waters. While ocean color products (made for open ocean) are easy to find for inland waters, inland water global products are still scarce due to the optical complexity of these aquatic environments. Nevertheless, some products were developed for global inland waters based on a blended algorithm approach which first classifies the aquatic system by its optical similarities (optical water typology) and then estimates other parameters. Some examples of these products are the Copernicus Land Lakes Water Quality product (https://land.copernicus.eu/global/products/lwq) and the European Space Agency Lakes Climate Change Initiative (https://climate.esa.int/en/projects/lakes/). While these initiatives are based on lakes, they also include reservoirs, however, these are global products and may not be optimized for a specific study site. Additionally the US Geological Survey (USGS) has a provisional product of aquatic reflectance which is produced after running an aquatic atmospheric correction (https://www.usgs.gov/landsat-missions/landsat-provisional-aquatic-reflectance), however it is still not fully validated for inland waters and it is still in provisional phase.

How to choose the right remote sensing processes? To help with the selection of the best approach, Neil et al. (2019) proposed a tree scheme to simply identify the best bio-geo-optical algorithm to use for Chl *a* concentration estimation based on the trophic state of the aquatic system where: the open ocean approach should be used for oligotrophic waters, the inland water approach should be used for mesotrophic and eutrophic waters and a quasi-analytical approach should be used for hypertrophic waters. This decision tree is very helpful for an initial selection of the remote sensing data processing approach; however, there are aquatic systems which are not covered, for example, aquatic systems with very high CDOM concentration (polyhumic waters). Similarly, Pahlevan et al. (2021) tested different atmospheric corrections processors and provided a ranking per optical water type which can facilitate the selection of the atmospheric correction approach.

How to improve remote sensing-based water quality products for my study site? To improve these products for a regional level, it is useful to follow the indicated processing chain of Fig. 1. This will require in situ radiometric data, thus there is an urge for the collection of this type of data. However, matching data with satellite passages is a big challenge. From the total 12,000 worldwide R_{rs} spectra compiled by Maciel et al. (2023) just a small part ($N = 1100$) had match-ups with satellite data. This fact highlights the need to align field sampling with satellite passages on cloud free days, which can be difficult for some parts of the world where cloud cover is unpredictable. In these areas, the deployment of sensors could be an alternative for the acquisition of in situ radiometric, optical properties and water quality data. Ideally, such deployed systems should be equipped with autonomous in situ systems for all required parameters, and they need to be deployed in carefully selected aquatic reference systems which would cover a gradient of organic matter, different trophic levels, and different catchments. This would allow to acquire match-up data for calibration and validation that can be extended to optically similar waters. A well-validated atmospheric correction can strengthen the accuracy of water quality products, which depend on your choice of the bio-geo-optical model. Regarding the existing water quality monitoring programs, the data collection of the absorption coefficient of CDOM (a_{CDOM}), the concentration of total suspended solids (TSS) and the concentration of phytoplankton pigments should be emphasized as essential variables.

How to use remote sensing data without in situ *radiometric data to validate the atmospheric correction?* Considering that in situ radiometric data is still not a common measurement for many scientists working in inland and coastal waters, it is important to highlight the existence of aquatic reflectance products such as: the Copernicus Land Lakes Water Quality product, the European Space Agency Lakes Climate Change Initiative and the USGS provisional product of aquatic reflectance. These products could be carefully used for limnological studies—including machine learning and artificial intelligence of big data analysis. Another alternative is the use of different atmospheric correction approaches based on the optical water type of your system (as in Pahlevan et al. 2021) and to use the existing in situ water quality data to validate the estimation from satellite data coming from different atmospheric correction processors. This acknowledges the importance of having an atmospheric correction targeting inland waters and can be used to calculate the uncertainties of this process.

How to best align scientists working in inland and coastal waters, with remote sensing scientists? Fortunately, inland water remote sensing is rapidly developing as a new discipline and several initiatives have been launched recently to disseminate remote sensing applications and products better. International networks such as the Group of Earth Observation (GEO) AquaWatch, the International Water Association (IWA) and the World Water Quality Alliance (WWQA) have been offering free webinars to inform the inland water research community on the current state-of-the-art of inland water remote sensing. With the global reach of these networks helping to disseminate the knowledge of remote sensing to non-remote sensing experts. Another network is the Global Lake Ecological Observatory Network (GLEON) which started in the United States and has been expanding worldwide and currently hosts a working group on Aquatic Remote Sensing which was created to establish the relationship between aquatic ecologists and remote sensing experts. These initiatives are complemented by online training which are available to anyone in the world such as the courses offered by the National Aeronautics and Space Administration (NASA) program on Applied Remote Sensing Training (ARSET).

The continuous growth and acceptance of remote sensing technology in limnology coupled with the standardization of satellite-based water quality products and the increase in data collection for calibration and validation offers the unique opportunity of operational use of such technology for reliable inland water monitoring. This will be achieved when aquatic sciences and remote sensing communities will join forces for the calibration and validation of the remote sensing-based water quality products with in situ radiometric and biogeochemical data. This will enable users to put results into adequate context and to understand the tradeoffs of the use of remote sensing data in the future. More synergies between these communities are needed to harmonize products, offer training materials and guides for the best use of remotely sensed data, as well as re-evaluate previously published material based on the newer approaches outlined above. Such synergies will effectively help to overcome methodological limitations and improve our ability to accurately monitor our rapidly changing inland waters.

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Conflict of interest

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