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# Data quality control considerations in multivariate environmental monitoring: experience of the French coastal network SOMLIT

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**Introduction:** While crucial to ensuring the production of accurate and high-quality data—and to avoid erroneous conclusions—data quality control (QC) in environmental monitoring datasets is still poorly documented.

**Methods:** With a focus on annual inter-laboratory comparison (ILC) exercises performed in the context of the French coastal monitoring SOMLIT network, we share here a pragmatic approach to QC, which allows the calculation of systematic and random errors, measurement uncertainty, and individual performance. After an overview of the different QC actions applied to fulfill requirements for quality and competence, we report equipment, accommodation, design of the ILC exercises, and statistical methodology specially adapted to small environmental networks (<20 laboratories) and multivariate datasets. Finally, the expanded uncertainty of measurement for 20 environmental variables routinely measured by SOMLIT from discrete sampling—including Essential Ocean Variables—is provided.

**Results, Discussion, Conclusion:** The examination of the temporal variations (2001–2021) in the repeatability, reproducibility, and trueness of the SOMLIT network over time confirms the essential role of ILC exercises as a tool for the continuous improvement of data quality in environmental monitoring datasets.

#### KEYWORDS

environmental monitoring network, data quality control, inter-laboratory comparison exercises, measurement uncertainty, analyst performance, multivariate dataset

## Introduction

In the context of global change, the number of studies that include meta-analytical combinations of environmental data increased at a fast pace in the past decades (e.g., Duarte et al., 2009; Harvey et al., 2013; Talarmin et al., 2016; McCrackin et al., 2017; Carstensen and Duarte, 2019; Lheureux et al., 2021; Lheureux et al., 2023). In these studies, it is assumed that the data were of similar quality and reliability, which is not necessarily true: measurement processes are all subject to systematic (i.e., bias) and random (i.e., variations) errors of various types, such as the choice of the method, ambient conditions, or the working practices of analysts (Taverniers et al., 2004; de Boer, 2016). At a time when high-quality scientific journals require a comprehensive documentation of data quality control (QC) procedures for publication (de Boer, 2016), and because erroneous conclusions may arise from studies using inappropriate methods, it is important to increase the confidence levels of data QC, which is often poorly documented in environmental monitoring datasets.

By using the 20 years of experience of the French coastal monitoring SOMLIT network (<https://www.SOMLIT.fr/>), the goal of our paper is to share a pragmatic approach to QC that focuses on annual inter-laboratory comparison (ILC) exercises as an indication of measurement uncertainty. The SOMLIT network currently includes 12 laboratories and 22 permanent sampling stations distributed along the French littoral (Figure 1) and covers a wide range of environmental and trophic conditions (Goberville et al., 2010; Liénart et al., 2017; Liénart et al., 2018; Lheureux et al., 2021). Implemented by CNRS (Centre National de la Recherche Scientifique) in 1997 to increase our scientific knowledge of the responses of marine coastal ecosystems to natural and human-induced influences, the SOMLIT network is part of the national research infrastructure ILICO (Infrastructure de recherche Littorale et Côtière; Cocquempot et al., 2019). Common standard operating protocols are used and all data are continuously routinely quality-controlled since 2006 by means of robust quality assurance procedures guided by the ISO-17025 standard (ISO-17025, 2005, then ISO-17025, 2017).

After an overview of the different QC actions implemented by the SOMLIT to fulfill requirements for quality and competence, we report equipment, accommodation, design of the ILC exercises and statistical methodology to assess individual performance specifically adapted to small (<20 laboratories) environmental networks and multivariate datasets, based on the ISO-13528 standard (ISO-13528, 2005), Héberger and Kollár-Hunek (2011), and procedures for measurement uncertainty assessment. Finally, we provide an expanded uncertainty of measurement for 20 environmental variables routinely measured by SOMLIT from discrete sampling (Table 1), including Essential Ocean Variables (Miloslavich et al., 2018).

## Data quality control overview

Data QC within the SOMLIT network is composed of five actions (Figure 2). Within-laboratory control is continuously performed by

each laboratory on the basis of control charts (Figure 3; Table S1) and the Nordtest TR 569 principles (Nordtest TR 569, 2007): control charts ensure the quality of produced data according to statistical or reference criteria—when available—and represent an essential step for the calculation of uncertainty. Control charts may also be performed (1) to objectively compare different analytical methods, (2) for new method validation, (3) to qualify an inexperienced analyst, or (4) to ensure stable ambient conditions (e.g., temperature and hygrometry) for measurements. There are two kinds of control charts: X-charts and R-charts for controlling systematic errors and random variations, respectively (Nordtest TR 569, 2007). The setting control limits used to build the control charts used by the SOMLIT network are given in Table S1.

SOMLIT data are qualified on a trimonthly basis using QC flags (see Table 2), which are derived from the World Ocean Circulation Experiment (WOCE; <https://exchange-format.readthedocs.io/en/latest/quality.html#woce-bottle-quality-codes>). QC flags include two levels. Level 1 ensures interoperability, but the codification is simplified to provide QC flags easily understandable by end-users. Level 2 is detailed in order to answer to the needs of data producers; it corresponds to internal QC according to the ISO 17025 standard (ISO-17025, 2017). Internal and external audits guided by the ISO 17025 standard (ISO-17025, 2017) are made on an annual and triennial basis, respectively, for ensuring laboratory quality management and technical requirements. We provide an example of the report in Figure 4.

ILCs are undertaken annually at the end of summer in one of the SOMLIT laboratories (Figure 1). To strengthen the robustness of comparisons, we alternate among different hosting laboratories, with sampling stations in the oligo- to ultra-oligotrophic Mediterranean Sea, oligo- to mesotrophic Atlantic waters, and the meso-eutrophic English Channel (Table S2). ILC allows best practices to be shared among participants from different laboratories, to evaluate data reliability (uncertainty calculation), and to assess the performance of individual operators from each laboratory. If issues are identified, ILC provides a forum to help participants to improve their practices and to correct their errors. In the following sections, we describe the methodology used during ILC and show how efforts to fulfill quality requirements have helped to improve the trueness and reproducibility of SOMLIT data over time.

## Design of ILC exercises and sample testing preparation

Although the SOMLIT program routinely measures 25 environmental variables, only the 22 variables subjected to discrete sampling (Table 1) were considered each year. Figure 5 describes the different steps involved in the ILC exercises. Given that stable reference material is lacking for most of the environmental variables measured by the SOMLIT network, performance in total measurement was evaluated by robust analysis, using measurement data from real natural seawater (see below).



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FIGURE 1

Location of the sites and stations belonging to the French coastal monitoring network SOMLIT (the logotype is in the center of the map).

TABLE 1 Range, reproducibility, and expanded uncertainty of the environmental variables measured during inter-laboratory comparison exercises of the SOMLIT network over the last 6 years.

Environmental variable	Unit	Range	Reproducibility		Expanded Uncertainty (k=2)	
			Measured	Literature	Measured	Literature
Dissolved Oxygen	mg/L	4.92-5.56	0.04 (0.83)	0.03-0.27 (Helm et al., 2012 and ref therein)	0.02 (0.05)	0.023 – 0.035 (0.27 – 0.38) Helm et al., 2012
pH	pH unit	7.9-8.2	0.03	0.1-0.2 (Aminot and Kérouel, 2004, Bockmon and Dickson, 2015)	0.02	0.02-0.04 (Meinrath and Spitzer, 2000 and references therein; Leito et al., 2002; Wiora and Wiora, 2018)
Ammonium	pH unit	0.11-2.25	<1µM: 0.07 (46) >1µM: 0.29 (12)	<1µM: 56%, >1µM:22.5% (Aminot and Kirkwood, 1995)	<1µM: 0.05 (18) >1µM: 0.25 (9.7)	> 5µM: 0.55 (7) Magnusson et al., 2012
Nitrate	µM	0.34-13.5	<1µM: 0.06 (17) >1µM: 0.07 (5)	<1µM: 105%, >1µM: 2,5% (Aminot and Kirkwood, 1995; Aoyama, 2006)	<1µM: 0.07 (20) >1µM: 0.12 (3)	>1 µM: max 16% Birchill et al., 2019
Nitrite	µM	0.02-0.63	<0.1µM: 0.009 (21.5) >0.1µM: 0.012 (2.4)	<0.1µM: 100%; >0,1µM: 20% (Aminot and Kirkwood, 1995; Aoyama, 2006)	<0.1µM: 0.01 (17) >0.1µM: 0.01 (3)	>1 µM: max 16 % Birchill et al., 2019
Phosphate	µM	0.03-0.40	<0.1µM: 0.02 (40) >0.1µM: 0.01 (6.7)	<0.1µM: 33 ; >0,1µM: 3-4% (Aminot and Kirkwood, 1995; Aoyama, 2006)	<0.1µM: 0.02 (37) >0.1µM: 0.03 (10)	>0.1 µM: max 6.2-14% (Claramunt and Pérez, 2014; Birchill et al., 2019)
Silicate	µM	0.97-11.9	<1µM: 0.15 (15) >1µM: 0.25 (4)	<1µM: 13%, >1µM: 2,4% (Aminot and Kirkwood, 1995)	<1µM: 0.28 (36) >1µM: 0.17 (5)	>1µM: 4.6% Birchill et al., 2019
Particulate Organic Carbon	µM	102-305	21 (9)	nd	24 (12)	<5 µg/L: 14-35% (Sandoval et al., 2022)
Particulate Organic Nitrogen	µg/L	15-52	3 (12.5)	nd	5 (17)	nd

(Continued)

TABLE 1 Continued

Environmental variable	Unit	Range	Reproducibility		Expanded Uncertainty (k=2)	
			Measured	Literature	Measured	Literature
Suspended Matter	µg/L	0.5-2	0.3	nd	0.37	max 40% (Röttgers et al., 2014)
Chlorophyll <i>a</i>	mg/L	0.46-1.87	0.09 (17)	10% (Larsson et al., 1978), 10-21% (Kaas and Wasmund, 1996), 12-29.5% (Schilling et al., 2006)	0.11 (11)	~20% (Iavetz, 2021)
Phaeopigment	µg/L	0.17-1.2	0.25 (24)	98.3-158.1% (Schilling et al., 2006)	0.22 (50)	nd
δ <sup>15</sup> N	‰	3.7-7.4	0.43	nd	0.72	nd
δ <sup>13</sup> C	‰	(-) 23.85- (-)21.12	0.33	nd	0.37	nd
C/N ratio	mol/ mol	6.62- 8.76	1.08	nd	0.55	nd
Bacteria	10 <sup>6</sup> N/ ml	0.5-3.4	0.01 (1.2)	nd	0.03 (3)	nd
<i>Synechococcus</i>	10 <sup>6</sup> N/ ml	3-73	0.17 (1.3)	nd	0.33 (3)	nd
Cryptophytes	10 <sup>3</sup> N/ ml	0.12- 0.48	0.02 (6.4)	nd	0.02 (6)	nd
Nanoecaryotes	10 <sup>3</sup> N/ ml	.31-2.8	0.24 (11.7)	nd	0.26 (11)	nd
Picoecaryotes	10 <sup>3</sup> N/ ml	1.5-111	0.33 (1.6)	nd	0.46 (2)	nd

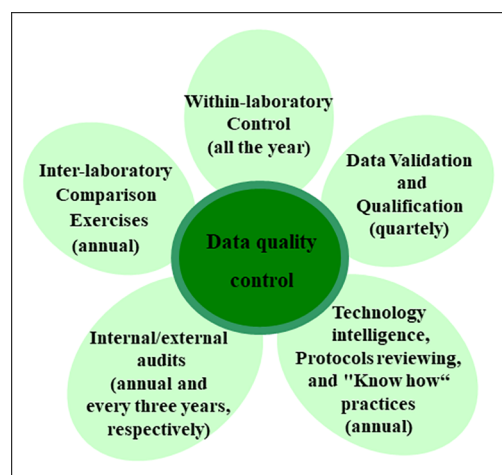
Percentage (%) values are between brackets.

## Sampling at sea

Sampling at sea was carried out onboard the research vessel of the hosting laboratory, using Niskin bottles or a pump. Approximately 2–3 m<sup>3</sup> of seawater was collected with ten 50-L tanks. The sampling was performed a few hours (less than 1 day) before the start of the ILC exercise.

## Sub-sampling and conditioning

Back to the host laboratory, seawater was transferred to a large-volume stainless-steel tank equipped with 15 petcock assemblies (Figure S1) and gently and continuously mixed with a rotating blade system inside (80 min at approximately 10 rpm). Mixing was stopped during sub-sampling. For the dissolved matter analysis,

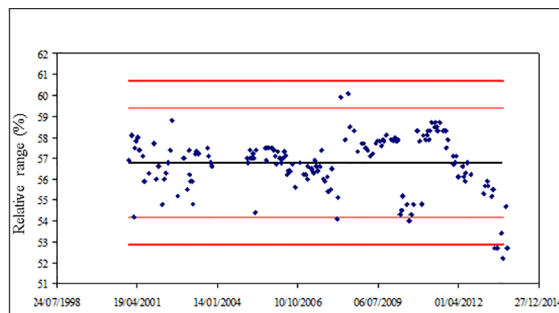


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FIGURE 2

Scheme of the different actions for data quality control implemented in the SOMLIT network and their frequency based on ISO 17025 (2017).





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FIGURE 3

Within-laboratory control: example of control chart based on Nordtest TR 569 (2007) for ensuring that the data are of good quality and the measurement process is statistically stable. Black line: the central line; thin red line: the warning limits; and thick red line: the action limits. The data value is considered in control if it is within the warning limits or if the value is between the warning and action limits but the two previous ones are within the warning limits. In this case, data are considered of good quality. The data value is considered outside control if the data value is outside action limits or between the warning and action limits and at least one of the two previous values are between warning and action limits too. In this case, measurement analysis must be made again once the problems are resolved if possible. The data value is considered in control but must be scrupulously monitored if the last 7 previous values exhibit a trend or 10 of the last 11 control values are on the same side and far from the central line.

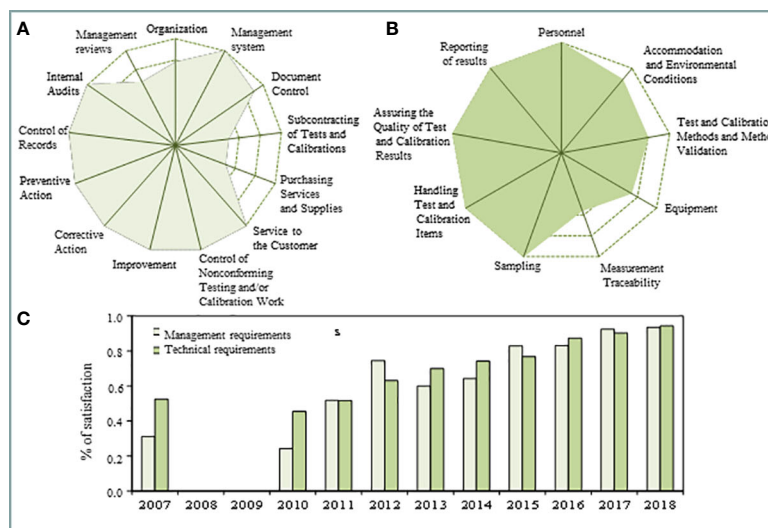
samples were first successively sub-sampled in 5 replicates in the following order: dissolved oxygen (hereafter  $O_2$ ), pH, ammonium ( $NH_4^+$ ), nitrate ( $NO_3^-$ ), nitrite ( $NO_2^-$ ), phosphate ( $PO_4^{3-}$ ), and silicate [ $Si(OH)_4$ ]. Conditioning and storage were the same as conducted routinely (Table S3). To reduce as far as possible any sampling inhomogeneity between participants, samples for each variable were sub-sampled at the same time by the different participants. Before

filling, vials were rinsed three times with sampling seawater. Samples were also successively sub-sampled for particulate matter analysis: pico- and nanoplankton, chlorophyll *a* (Chl*a*) and phaeopigments, particulate organic carbon (POC), particulate organic nitrogen (PON), suspended particulate matter (SPM), and  $\delta^{13}C$  and  $\delta^{15}N$ .

Processing and storage during transport and back to home laboratory (Figure 5) were carried out following the methodology

TABLE 2 Primary and secondary level quality control flags (QCF) used by the SOMLIT network for the data qualification step.

QCF	Primary level	Secondary level
0	Value below detection	The value represented is the detection limit one
1	Sampled but not measured	Sample collected but measure not made because the sample was lost (e.g. broken vial, bad preservation, contamination,...). Missing value is represented by 999999
2	Good value, no replicate	Expert review. Measure made under optimal sampling, ambient, and analytical conditions. The value is in the range of those expected.
3	Doubtful value	Expert review (e.g., excessive or unexpected value, analytical problem, below quality requirements...). Value is reported but the end-user is advised to use the value with care
4	Bad value	Expert review (e.g., excessive or unexpected value, analytical problem, below quality requirements...). Value is reported but the end-user is advised to not use the value
5	Measure made but value still not reported	Value is reported with delay. Missing value is represented by 999999
6	Good value, mean of several replicates	Mean of replicate measurements of the same sample. Measure made under optimal ambient and analytical conditions. The value is not excessive and as expected.
7	Good value but acquired with departure from the SOMLIT protocol	Sample collected but measure made with departure from the SOMLIT protocole. Despite the value is considered as good it is recommended to the end-user to contact the scientific manager of the sampling station for more information.
8	No quality control	Value is given but the quality control flag is not available yet
9	No sampling	Sample not collected and/or measure impossible (e.g. bad weather at sea). Missing value is represented by 999999



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FIGURE 4

Internal/external audits of the SOMLIT network guided by the ISO 17025 standard (ISO-13528, 2005) to ensure the integrity of data and minimize errors: example of reports provided by one SOMLIT laboratory. (A, B) Management and technical requirements, respectively. (C) Temporal variations of the percentage (%) of satisfaction to meet the requirements.

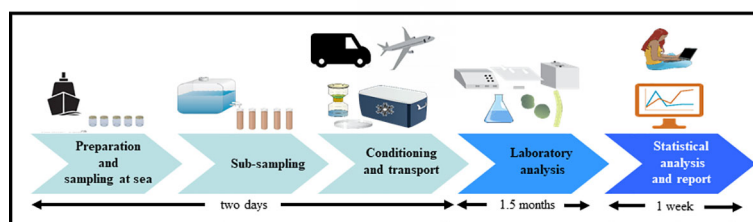
given in Table S3. Each year, the Quality Manager allows laboratory participants to perform analyses within 1 to 3 months, depending on the variables. The list of analytical techniques for each environmental variable is given in Table S3. Finally, the Quality Manager collects replicate measurement results for each environmental variable and from each participating laboratory, as well as information on the date of analysis and potential problems that may have occurred during sub-sampling, processing, storage, and/or analysis.

Once the performance scores in repeatability and trueness are obtained for the different participating laboratories, and after calculation of the annual reproducibility of the SOMLIT network (see below), a quality report is written by the Quality Manager and sent to each participating laboratory. In the case of “questionable” performance during two consecutive ILC exercises or

“unsatisfactory” performance in the current ILC exercise, the laboratory in question must take corrective actions, such as to redo a calibration, to improve dim light conditions for chlorophyll *a* analysis, in order to achieve satisfactory performance and/or reproducibility in accordance with other participating laboratories.

## Calculation of systematic and random errors and performance

The different steps of the statistical methodology used to assess the total measurement accuracy (trueness and precision) for the 22 environmental variables during ILC exercises, as well as the overall performance of the participating laboratory, are described in Figure 6. The methodology has been adapted for small (<20



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FIGURE 5

Scheme of the different steps of the annual ILC exercises implemented by the SOMLIT network since 2001.



participating laboratories) networks, using the algorithm A mentioned in the ISO-13528 standard (see the freeware using Microsoft Excel<sup>®</sup> in Table 1 of the Supplementary Materials) for non-parametric data, and the user-friendly macro created by Héberger and Kollár-Hunek (2011) for both non-parametric and multivariate datasets. The application of the latter approach allows a better appraisal of proficiency testing (PT) in the case of multivariate monitoring in comparison with the ISO-13528 standard (ISO-13528, 2005, see Medina-Pastor et al., 2010; Stoyke et al., 2012): it ranks the performance of the different laboratories on the basis of data of different units and explores overall improvement of performance over time.

Robust statistics are used without outlier exclusion before calculation (Analytical Methods Committee, 1989). For each environmental variable, performance in trueness of total measurement (i.e., from sampling to data reporting) was assessed by calculating a  $z'$ -score according to Equation 1 (ISO-13528, 2005):

$$z' = (x_i - x^*) / \sqrt{(\sigma^* + u_x)^2} \quad (1)$$

where  $x_i$  is the mean value of five replicates obtained by the participating laboratories  $i$ ,  $x^*$  and  $\sigma^*$  are the robust average and the robust standard deviation of the different  $x_i$ , respectively, and  $u_x$  is the uncertainty of total measurement of the measurand, as mentioned in Equation 2:

$$u_x = 1.25 \frac{\sigma^*}{\sqrt{p}} \quad (2)$$

where  $p$  is the number of participating laboratories at the ILC exercise. The robust average and robust standard deviation were calculated using the algorithm A (see the freeware using Microsoft Excel<sup>®</sup> in Table 1 of the Supplementary Materials) of ISO-13528 (2005).  $z'$ -score was chosen against  $z$ -score because of the small size of the SOMLIT network and because the uncertainty of the assigned value was considered to be not negligible given that most environmental variables never met the following inequality (Equation 3):

$$u_x \leq 0.3\sigma^* \quad (3)$$

According to ISO-13528:

- $|z'| \leq 2$  was considered as “satisfactory”
- $2 < |z'| < 3$  was considered as “questionable”
- $|z'| \geq 3$  was considered as “unsatisfactory”

For each laboratory, performance in repeatability was assessed by comparing the standard deviation of five replicate measurements with the limit of acceptable precision given in the literature, when available (see Table S4). Reproducibility (between-laboratory precision) was evaluated by calculating the robust standard deviation  $x^*$  of the different reported mean values of the measurand using the algorithm A. To classify the different participating laboratories according to their respective overall performance in trueness and repeatability, we performed a Sum of Ranking Difference (SRD, see the Supplementary Materials for file format) test, a non-parametric multivariate technique

recommended when the number of participating laboratories is less than 13 (Héberger and Kollár-Hunek, 2011). While SRD has multiple applications (e.g., Andrić and Héberger, 2015; Kalivas et al., 2015; Sziklai and Héberger, 2020), it allows us to analyze similarities between laboratories by ranking (columns of the input matrix relative to trueness and replicability targets, across the measurement of several environmental variables, and rows of the input matrix). The closer to zero the SRD value, the better the overall performance of the laboratory. The SRD test was validated by a random test called Comparison of Ranks with Random Numbers (CRRN) by ensuring that no participating laboratory is randomly ranked (the black curve is the cumulative distribution function of the random SRD values; Figure 6). The method is described in detail in Héberger and Kollár-Hunek (2011). A freeware for the calculation of SRD-CRRN with Microsoft Excel<sup>®</sup> is available at <http://aki.ttk.mta.hu/srd>. We chose the zero value for trueness targets and the reproducibility targets given in Table 3.

Figure 7 shows the inter-annual (2001–2021) variations of the within-laboratory and between-laboratory reproducibility (Figures 7A, B)—the opposite of the robust coefficient of variation  $s^*$ —as well as the trueness—the bias is measured as the absolute difference between the inter-laboratory median value and the robust mean—obtained during the ILC exercises. We here demonstrate how efforts made to fulfill quality requirements for trueness and reproducibility have contributed to improve the quality of SOMLIT data over time, confirming the essential role of ILC exercises as a tool for continuous improvement of long-term monitoring networks.

## Estimation of total measurement uncertainty ( $U$ ) of the SOMLIT network

Two approaches exist for the evaluation of measurement uncertainty. The first is based on a physical model relating the measuring process at all steps, using the propagation law of uncertainty (GUM, 1993). The second relies on a statistical model that uses data from within-laboratory control and/or ILC exercises or PT exercises (ISO-13528, 2005; Ferretti, 2011; Magnusson et al., 2012; de Boer, 2016). The statistical model is often favored, however, and was chosen by the SOMLIT network both for its less apparent mathematical complexity and for the lack of knowledge about the processes that need to be measured for the physical model (e.g., firm statistical background). For that purpose, we used the data from ILC exercises from the last 6 years. Note that the values we obtained are an approximation of the total measurement uncertainty, given that sampling uncertainty was never investigated.

Total measurement uncertainty of the SOMLIT network ( $U$ , in  $\pm$  Unit and/or in %) was calculated following Equation 4 (Magnusson et al., 2012):

$$U = 2\sqrt{b^2 + u_{Rw}^2} \quad (4)$$

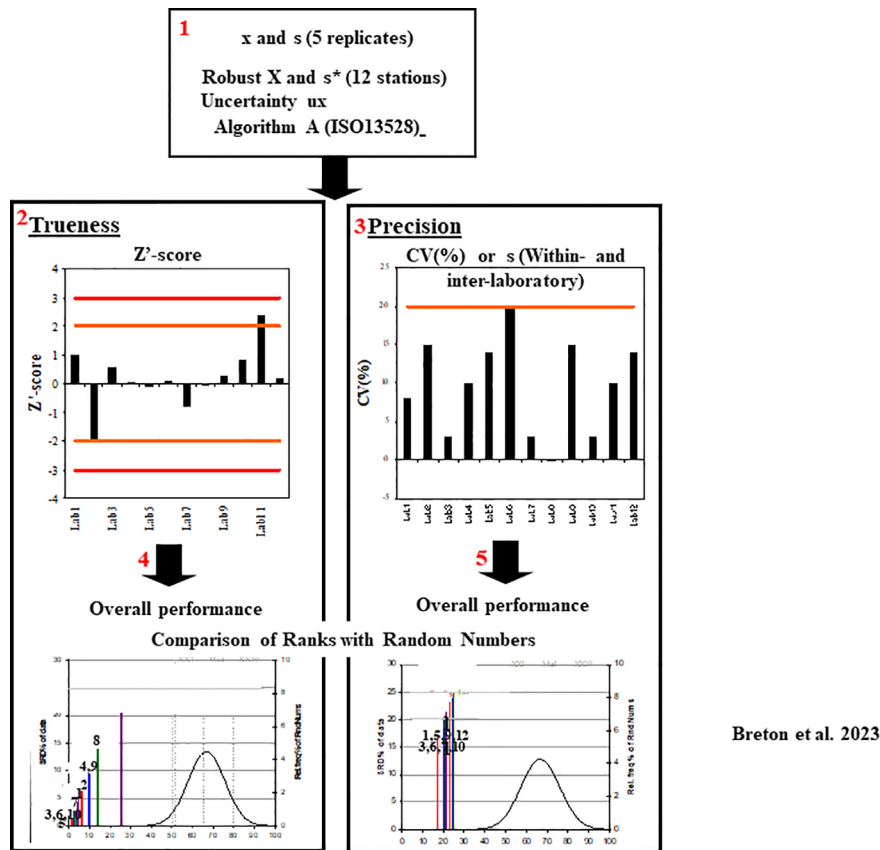


FIGURE 6

Annual ILC exercises implemented by the SOMLIT network: the different steps in the statistical methodology used to assess the total measurement accuracy of the 22 environmental variables and the participating laboratory performance. Step 1: Calculation of the mean ( $\bar{x}$ ) and the standard deviation ( $s$ ) of replicates as well as that of the robust mean ( $X$ ), standard deviation ( $s^*$ ), and uncertainty ( $u_x$ ) of total measurement of the measurand, by applying the algorithm A. Steps 2 and 3: Calculation of the individual deviations ( $z'$ -score) to the SOMLIT robust for assessing the trueness (systematic bias) and precision (random variations). Steps 4 and 5: Calculation of the final rank of each participating laboratory for the overall performance for trueness and precision (Héberger and Kollár-Hunek, 2011).

where  $u_{RW}$  is the precision uncertainty and  $b$  is the bias uncertainty obtained from Equations 5 and 6, respectively:

$$u_{RW} = \sqrt{\frac{\sum_{i=1}^{i=n} (\sigma_i)^2}{n}} \tag{5}$$

$$b = \sqrt{\Delta_{RMSbias}^2 + u_x^2 + \frac{s_{bias}^2}{\sqrt{n}}} \tag{6}$$

$$\text{with } \Delta_{RMSbias} = \sqrt{\frac{\sum_{i=1}^{i=n} (x_i - \bar{x})^2}{n}} \tag{7}$$

with  $\sigma_i$  and  $x_i$  being the median and mean, respectively, of the repeatability values obtained by the different laboratories during one ILC exercise for one measure,  $s_{bias}$  being the standard deviation of the different median values of  $b$  for at least six different ILC exercises,  $n$  being the number of ILC exercises used for uncertainty calculation, and  $u_x$  being the median value of the uncertainty of the assigned values calculated for at least six ILC exercises.  $U$  is the expanded uncertainty at a confidence interval of 95% ( $k = 2$ ).

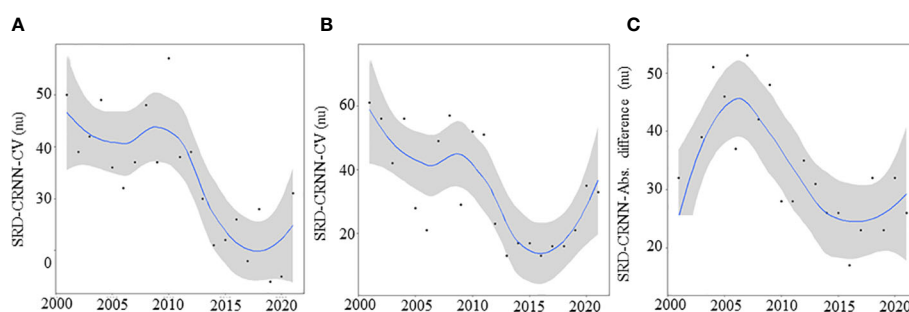
The resulting expanded uncertainty values of the total measurement of the 22 environmental variables monitored by the SOMLIT network given in Table 1 (see also Table S3) are either below or very close to those found in the literature, when available.

## Conclusion

In this paper, we presented the “road map” and the statistical methodology for the ILC exercises performed by the SOMLIT network, a framework especially adapted to small (<20 participating laboratories) and multivariate environmental datasets. By applying this framework to data acquired during 21 years, we showed that the SOMLIT program provided reliable data, and that the data quality increased over time thanks to the implementation of ILCs. Given the paucity of uncertainty values of the measurement of environmental variables—such as measured by the SOMLIT network—in the literature, our study stresses the importance of implementing ILC exercises in order to improve the quality of data representative of long-term environmental monitoring. We also highlight general acceptance limits in the measurement of these environmental variables.

**TABLE 3** Reproducibility targets and reference used to calculate the overall performance of the participating laboratories to the inter-laboratory comparison exercises of the SOMLIT network.

	Requested maximum	Reference
O <sub>2</sub>	0.27 mg/L	Helm et al., 2012, and ref therein
pH	0.002	SOMLIT
Ammonium	0.07 μM	Aminot and Kirkwood, 1995
Nitrate	0.07 μM	Aminot and Kirkwood, 1995; Aoyama, 2006
Nitrite	0.009 μM	idem
Phosphate	0.01 μM	idem
Silicate	0.25 μM	idem
POC	9%	SOMLIT
PON	12.5%	idem
SPM	0.3 μg/L	idem
Chlorophyll <i>a</i>	20%	Larsson et al., 1978; Kaas and Wasmund, 1996; Schilling et al., 2006
Phaeopigments	24%	SOMLIT
delta <sup>15</sup> N	0.43 ‰	idem
delta <sup>13</sup> C	0.33 ‰	idem
C/N ratio	1.08 mol/mol	idem
Total Bacteria (10 <sup>6</sup> N/ml)	0.01 (1.2%)	idem
HNA (10 <sup>6</sup> cells/ml)	0.01 (1.2%)	idem
LNA (10 <sup>6</sup> cells/ml)	0.01 (1.2%)	idem
Cryptophytes (10 <sup>3</sup> cells/ml)	0.17 (1.3%)	idem
<i>Synechococcus</i> (10 <sup>3</sup> cells/ml)	0.02 (6.4%)	idem
Picoeukaryotes (10 <sup>3</sup> cells/ml)	0.24 (11.7%)	idem
Nanoeukaryotes (10 <sup>3</sup> cells/ml)	0.33 (1.6%)	idem



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**FIGURE 7**

Long-term variations in (A) within-laboratory reproducibility (SRD-CRNN-CV, %), (B) between-laboratory reproducibility (the opposite of the robust coefficient of variation; SRD-CRNN-CV, %), and (C) trueness (bias measured as absolute difference between the inter-laboratory median value and the robust mean; SRD-CRNN-Abs. difference, nu) obtained during the inter-laboratory comparison exercises of the SOMLIT network over the period 2001–2021. The solid blue line and ribbon represent Locally Estimated Scatterplot Smoothing (LOESS) smoothing and the 95% confidence interval. SRD-CRNN, sum of ranking differences and comparison of ranks by random numbers; CV, coefficient of variation; nu, no unit.

## Data availability statement

The raw data supporting the conclusions of this article will be made available by the authors, without undue reservation.

## Author contributions

Conceptualization and methodology: EBr, NS, PR-M, BS, TC, SF, ACai, VD, YA, GGr, EGr, AG, OJ, VL, EMac, DM, FM, SM, DP, PP, FR-J, IS, P-GS, and NG. Data collection and curation: EBr, NS, PR-M, TC, SF, SAL, FA, SAu, EBe, HB, LB, SB, ACau, J-BC, LCh, RC'h, M-AC, LCo, OC, MC, HL, GD, JD, AD, MD, CE, SG, EGr, AG, JG, KG, GGu, VG, MH, OJ, PL, NLab, ML, VL, CLa, JL, NLac, BL, EL, DL, CLe, CLi, EMac, EMar, BMa, SM, LMor, LMou, AN, SN, RP, DP, FP, PP, FR-J, PRIM, CS, ES, RVa, FVi, FVo, LZ, and NG. Formal analysis: EBR and ALh. Project administration, funding acquisition, and resources: EBr, NS, PR-M, BS, TC, HA, CB, YB, SB, PCI, PCo, OC, ACai, YA, GGr, EGr, AG, MC, JF, MG, OJ, JL, LL, ALe, SL'H, YL, SM, FM, BMo, LMou, SN, PP, PRIM, ES, IS, LS, VV, RVu, P-GS, and NG. Writing—original draft preparation and writing—review and editing: EBr, NS, PR-M, EGo, ALh, VD, BL, BMo, PRIM, P-GS, FV, and NG. All authors contributed to the article and approved the submitted version.

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## References

- Aminot, A., and K erouel, R. (2004). *Hydrologie des  cosystemes marins: param tres et analyses* (Brest: Ifremer).
- Aminot, A., and Kirkwood, D. S. (1995). *Report on the results of the fifth ICES study for in seawater Vol. 213*. Eds. A. Aminot and D. S. Kirkwood (Copenhagen, Denmark: Coop. Res. Rep.), 41–65.
- Analytical Methods Committee (1989). Robust statistics—how not to reject outliers—part 2. *Inter-laboratory trials. Analyst* 114, 1699–1705. doi: 10.1039/AN9891401699
- Andri , F., and H berger, K. (2015). Chromatographic and computational assessment of lipophilicity using sum of ranking differences and generalized pair-correlation. *J. Chromatogr. A* 1380, 130–138. doi: 10.1016/j.chroma.2014.12.073
- Aoyama, M. (2006). 2003 intercomparison exercise for reference material for nutrients in seawater in a seawater matrix. *Tech. Rep. Meteorological Res. Institute* (50), 91. doi: 10.11483/mritechrepo.50
- Birchill, A. J., Clinton-Bailey, G., Hanz, R., Mawji, E., Cariou, T., White, C., et al. (2019). *Realistic measurement uncertainties for marine macronutrient measurements conducted using gas segmented flow and Lab-on-Chip techniques* Vol. 200 (Elsevier: Talanta), 228–235. doi: 10.1016/j.talanta.2019.03.032
- Bockmon, E. E., and Dickson, A. G. (2015). An inter-laboratory comparison assessing the quality of seawater carbon dioxide measurements. *Mar. Chem.* 171, 36–43. doi: 10.1016/j.marchem.2015.02.002
- Carstensen, J., and Duarte, C. M. (2019). Drivers of pH variability in coastal ecosystems. *Environ. Sci. Technol.* 53, 4020–4029. doi: 10.1021/acs.est.8b03655
- Claramunt, I., and P rez, L. (2014). Estimation of measurement uncertainty in the determination of orthophosphates in seawater by continuous flow analysis (CFA). *Accreditation Qual. Assur.* 19, 205–212. doi: 10.1007/s00769-014-1051-x
- Cocquemot, L., Delacourt, C., Paillet, J., Riou, P., Aucan, J., Ballu, V., et al. (2019). Coastal ocean and nearshore observation: a French case study. *Front. Mar. Sci.* 6. doi: 10.3389/fmars.2019.00324
- de Boer, J. (2016). Quality in scientific research – in commemoration of dr. David wells. *Chemosphere* 154, A1–A2. doi: 10.1016/j.chemosphere.2016.04.034
- Duarte, C. M., Conley, D. J., Carstensen, J., and S nchez-Camacho, M. (2009). Return to neverland: shifting baselines affect eutrophication restoration targets. *Estuaries Coasts* 32, 29–36. doi: 10.1007/s12237-008-9111-2
- Ferretti, M. (2011). Quality assurance: a vital need in ecological monitoring. *CAB Rev.* 6, 1–14. doi: 10.1079/PAVSNR20116011
- Goberville, E., Beaugrand, G., Sautour, B., Tr guer, P. SOMLIT Team (2010). Climate-driven changes in coastal marine systems of western Europe. *Mar. Ecol. Prog. Ser.* 408, 129–148. doi: 10.3354/meps08564

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## Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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## Supplementary material

The Supplementary Material for this article can be found online at: <https://www.frontiersin.org/articles/10.3389/fmars.2023.1135446/full#supplementary-material>

- GUM (1993). Guide to the Expression of Uncertainty in Measurement, International Organization for Standardization (ISO). 1993.
- Harvey, B. P., Gwynn-Jones, D., and Moore, P. J. (2013). Meta-analysis reveals complex marine biological responses to the interactive effects of ocean acidification and warming. *Ecol. Evol.* 3, 1016–1030. doi: 10.1002/ece3.516
- Héberger, K., and Kollár-Hunek, K. K. (2011). Sum of ranking differences for method discrimination and its validation: comparison of ranks with random numbers. *J. Chemometr.* 25, 151. doi: 10.1002/cem.1320
- Helm, I., Jalukse, L., and Leito, I. (2012). A highly accurate method for determination of dissolved oxygen: gravimetric winkler method. *Analytica chimica Acta* 741, 21–31. doi: 10.1016/j.aca.2012.06.049
- Iavetz, R. (2021). *Proficiency test final report AQA 21-05 chlorophyll a in water* (Sydney, Australia: National Measurement Institute. Australian Government), 44. Available at: <https://www.industry.gov.au/sites/default/files/2021-11/aqa-21-05-final-report.pdf>.
- ISO-13528 (2005). *Statistical methods for use in proficiency testing by inter-laboratory comparisons*.
- ISO-17025 (2005). *General requirements for the competence of testing and calibration laboratories*.
- ISO-17025 (2017). *General requirements for the competence of testing and calibration laboratories*.
- Kaas, H., and Wasmund, N. (1996). *Report on comparability of chlorophyll data. in: report of the ICES/Helcom workshop on quality assurance of pelagic biological measurements in the Baltic Sea (annex 4 v)*.
- Kalivas, J. H., Héberger, K., and Andries, E. (2015). Sum of ranking differences (SRD) to ensemble multivariate calibration model merits for tuning parameter selection and comparing calibration methods. *Anal. Chim. Acta* 869, 21–33. doi: 10.1016/j.aca.2014.12.056
- Larsson, U., Norling, L., Carlberg, S., Löf, S., Tolstoy, A., v. Bröckl, K., et al. (1978). Intercalibration of methods for chlorophyll measurements in the Baltic Sea, merentutkimuslait. *Julk./Havsforskningsinst. Skr.* 243, 63–76.
- Leito, I., Strauss, L., Koort, E., and Viljar, P. (2002). Estimation of uncertainty in routine pH measurement. *Accred Qual Assur.* 7, 242–249. doi: 10.1007/s00769-002-0470-2
- Lheureux, A., David, V., Del Amo, Y., Soudant, D., Auby, I., Bozec, Y., et al. (2023). Trajectories of nutrients concentrations and ratios in the French coastal ecosystems: 20 years of changes in relation with large-scale and local drivers. *Sci. Total Environ.* 857, 159619. doi: 10.1016/j.scitotenv.2022.159619
- Lheureux, A., Savoye, N., Del Amo, Y., Goberville, E., Bozec, Y., Breton, E., et al. (2021). Bi-decadal variability in physico-biogeochemical characteristics of the temperate coastal ecosystems: from large-scale to local drivers. *Mar. Ecol. Prog. Ser.* 660, 19–35. doi: 10.3354/meps13577
- Liénard, C., Savoye, N., Bozec, Y., Breton, E., Conan, P., David, V., et al. (2017). Dynamics of particulate organic matter composition in coastal systems: a spatio-temporal study at multi-systems scale. *Prog. Oceanography* 156, 221–239. doi: 10.1016/j.pocean.2017.03.001
- Liénard, C., Savoye, N., David, V., Ramond, P., Rodriguez Tress, P., Hanquiez, V., et al. (2018). Dynamics of particulate organic matter composition in coastal systems: forcing to the spatio-temporal variability at multi-systems scale. *Prog. Oceanography* 162, 271–289. doi: 10.1016/j.pocean.2018.02.026
- Magnusson, B., Näykkö, T., Hovind, H., Krysell, M., and Sahlin, E. (2012) *Handbook for calculation of measurement uncertainty in environmental laboratories. NORDTEST report TR 537*. Available at: <http://www.nordtest.info>.
- McCrackin, M. L., Jones, H. P., Jones, P. C., and Moreno-Mateos, D. (2017). Recovery of lakes and coastal marine ecosystems from eutrophication: a global meta-analysis. *Limnol. Oceanogr.* 62, 507–518. doi: 10.1002/lno.10441
- Medina-Pastor, P., Mezcuza, M., Rodríguez-Torrealba, C., and Fernández-Alba, A. R. (2010). Laboratory assessment by combined z score values in proficiency tests: experience gained through the European union proficiency tests for pesticide residues in fruits and vegetables. *Analytical Bioanalytical Chem.* 397, 3061–3070. doi: 10.1007/s00216-010-3877-3
- Meinrath, G., and Spitzer, P. (2000). Uncertainties in determination of pH. *Microchimica Acta A* 135, 155–168. doi: 10.1007/s006040070005
- Miloslavich, P., Bax, N. J., Simmons, S. E., Klein, E., Appeltans, W., Aburto-Oropeza, O., et al. (2018). Essential ocean variables for global sustained observations of biodiversity and ecosystem changes. *Glob. Change Biol.* 24, 2416–2433. doi: 10.1111/gcb.14108
- Nordtest TR 569 (2007). *Handbook of internal quality control for chemical analysis. technical report*, Hovind, NIVA, Norway, Bertil Magnusson, SP, Sweden, Mikael Krysell et Ulla Lund, Eurofins A/S, Danemark, Irma Mäkinen, SYKE, Finland. Available at: [http://www.nordtest.info/wp/wp-content/uploads/2012/01/nt-tr-569\\_ed4\\_en-internal-quality-control-handbook-for-chemical-laboratories.pdf](http://www.nordtest.info/wp/wp-content/uploads/2012/01/nt-tr-569_ed4_en-internal-quality-control-handbook-for-chemical-laboratories.pdf)
- Röttgers, R., Heymann, K., and Krasemann, H. (2014). Suspended matter concentrations in coastal waters: methodological improvements to quantify individual measurement uncertainty. *Estuarine Coast. Shelf Sci.* 151, 148–155. doi: 10.1016/j.ecss.2014.10.010
- Sandoval, SP, Dall'Olmo, G., Haines, K., Rasse, R., and Ross, J. (2006). Uncertainties of particulate organic carbon concentrations in the mesopelagic zone of the Atlantic ocean. *Open Res. Europe* 1, 43
- Schilling, P., Powilleit, M., and Uhlig, S. (2006). Chlorophyll-a determination: results of an inter-laboratory comparison. *Accreditation Qual. Assur.* 11, 462–469. doi: 10.1007/s00769-006-0158-0
- Stoyke, M., Radeck, W., and Gowik, P. (2012). Anthelmintics in bovine milk and muscle: inter-laboratory studies among EU national reference laboratories accredited. *Qual. Assur.* 17, 405–412. doi: 10.1007/s00769-012-0919-x
- Sziklai, B. R., and Héberger, K. (2020). Apportionment and districting by sum of ranking differences. *PLoS One* 15 (3), e0229209. doi: 10.1371/journal.pone.0229209
- Talarmin, A., Lomas, M. W., Bozec, Y., Savoye, N., Frigstad, H., Karl, D. M., et al. (2016). Seasonal and long-term changes in elemental concentrations and ratios of marine particulate organic matter. *glob. biogeochem. Cycles* 30, 1699–1711. doi: 10.1002/2016GB005409
- Taverniers, I., De Loose, M., and Van Bockstaele, E. (2004). Trends in quality in the analytical laboratory. i. traceability and measurement uncertainty of analytical results. *TrAC Trends Analytical Chem.* 23, 480–490. doi: 10.1016/S0165-9936(04)00733-2
- Wiora, J., and Wiora, A. (2018). Measurement uncertainty calculations for pH value obtained by an ion-selective electrode. *Sensors.* 18 (6), 1915. doi: 10.3390/s18061915

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