Worldwide Open Proficiency Test for Total Reflection X Ray Fluorescence Laboratories

PTXRFIAEA11

Determination of Minor and Trace Elements in water samples

IAEA Laboratories, Seibersdorf
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CONTENTS

FOREWORD

The IAEA assists its Member States laboratories to continuously improve their analytical performance by producing reference materials, by developing standardized analytical methods, and by conducting inter-laboratory comparisons and proficiency tests. To ensure a reliable worldwide, rapid and consistent response, the IAEA Nuclear Science and Instrumentation Laboratory in Seibersdorf, Austria, coordinates proficiency tests for Member States laboratories.

This summary report presents the results of the worldwide proficiency test PTXRFIAEA11 on the determination of minor and trace elements in three different water samples. Methodologies, statistical analysis, and evaluation of results (for each element and for each laboratory) are also reported. The test was carried out within the IAEA project Nuclear Instrumentation, under the Accelerators and Nuclear Spectrometry Subprogram, Nuclear Science Program. The main objective of the project is to enhance capability of interested Member States in effective utilization of nuclear spectrometries and analytical services in industry, human health, agriculture, and in monitoring and evaluation of the environment.

This proficiency test was organized upon a petition from the ISO TC WG3 and its purpose was to gather enough results to support the evaluation of a guideline and a standard methodology proposed for water analysis. The evaluation of the results will allow assessing a standard for water analysis to be submitted to ISO TC201.

The type of samples and the concentration levels of the analytes were designed to enable identification of potential analytical problems, to support IAEA Member States laboratories to improve the quality of their analytical results and to provide a regular forum for discussion and technology transfer in this topic.

The coordinators of the proficiency test and responsible for this publication were A. Migliori of the IAEA Nuclear Science and Instrumentation Laboratory, Seibersdorf (Austria), L. Depero and L. Borgese of the Chemistry for Technologies Laboratory, Department of Mechanical and Industrial Engineering, University of Brescia (Italy).

1. INTRODUCTION

A proficiency test (PT), open to laboratories using the Total Reflection X-Ray Fluorescence (TXRF) analysis technique for environmental monitoring, was proposed to assess the analytical performance of TXRF worldwide. The purpose of the PT was to gather information to support the evaluation of guidelines and a standard methodology proposed for water analysis.
The participants were requested to determine the concentrations of chemical elements in three different water samples.
The water samples were distributed to the participating laboratories, which were requested to analyse the samples by TXRF technique following the instructions established by the coordinators of the PT.
The evaluation of the results will allow assessing a standard for the water analysis to be submitted to ISO TC201. The exercise is a contribution to the project "Inter-laboratory comparison of Total-Reflection X-Ray Fluorescence spectroscopy for environmental analysis" initiated in the frame of VAMAS (Versailles Project on Advanced Materials and Standards [1]) Technical Working Area 2, related to surface chemical analysis. The aim of the project is the development of guidelines and standard methodologies for the analysis of biological and environmental samples by means of TXRF technique [2].
Based on the PT results presented in this report, each participating laboratory should assess its analytical performance and identify discrepancies.
The samples, together with detailed instructions for the analysts, were distributed to the participating laboratories in early August 2014. The deadline for submission of the results was October 31, 2014. The last results were received by January 2015. The submitted results were processed, grouped versus analytes/laboratories and compared with the analytes' assigned values or consensus values. The values of *z*- and *u*-scores were calculated for three fit-for-purpose levels. For the definitions of the *z*- and *u*-scores please see Section 3.3. The obtained results as well as the description of the data evaluation procedures have been presented in this report. For each laboratory a code was assigned, therefore full anonymity of the presented results is guaranteed. The link between the laboratory code and the laboratory name is known only to the coordinators of the proficiency test and to the laboratory itself.

2. DESCRIPTION OF THE TEST SAMPLE

Two samples were prepared from a certified reference solution by the coordinators as to obtain two different concentration levels of the analytes (~ 10 mg/L for sample "1" and 0.1 mg/L for sample "2"). A third sample ("3") was prepared from a commercial drinking water.
The three samples were loaded in sterile plastic tubes, sealed and distributed to 37 laboratories, each tube containing around 5 mL of the aforementioned samples.

3. DETAILS OF THE EXERCISE

3.1. SUBMITTED RESULTS

The participants were asked to provide information about the conditions and parameters used for their measurements, like sample carrier material, preparation of the sample carrier and excitation source.
For the analysis of all the three samples, the participants were asked to follow their own analytical procedure for measurement, identification, spectrum analysis and quantification of the elements. Only one result per element should be submitted. Each result should be accompa-

nied by an estimate of its uncertainty expressed as one standard deviation. No restriction on the number of the reported elements was imposed.

The samples "1" and "2" were prepared after diluting an ICP multi-elemental standard solution containing elements with a nominal concentration of 1000 mg/L to the level of 10 mg/L and 0.1 mg/L, respectively. The participants were explicitly asked to analyse the samples "1" and "2" without any further sample preparation procedure. The participants were asked to consider Gallium as internal standard for quantification. Gallium was already present in samples "1" and "2", and its concentration was given: 10.0 mg/L in sample "1" and 0.1 mg/L in sample "2". To harmonize the expression of standard deviation reported by the participants, it was instructed to prepare five independent measurement replicates for samples "1" and "2", each one corresponding to the dry residue of depositing 10 µL (in one drop) on the sample carrier.
For the analysis of sample "3" the participants were asked to use Gallium (from a 1000 mg/l certified solution) as internal standard for quantification and, following the instructions established by the coordinators for standard dilution, to prepare sample "3" with a Gallium final concentration equal to 1 mg/L. The participants were asked to prepare five independent measurement replicates also for this sample, as described before.

3.2. ASSIGNED VALUE AND TARGET STANDARD DEVIATION

The reference values supplied by the provider of the initial standard solution used for the preparation of samples "1" and "2", were used as the assigned values of the analytes, X_A.

For each analyte a target value of the standard deviation has been assigned using a modified Horowitz function as proposed in reference [3]:

$$H_A = \begin{cases} 0.22 X_A & X_A < 1.2 \cdot 10^{-7} \\ 0.02 \left(X_A\right)^{0.8495} & 1.2 \cdot 10^{-7} \le X_A \le 0.138 \\ 0.01 \sqrt{X_A} & X_A > 0.138 \end{cases} \quad (1)$$

In Eqn. (1) the assigned value of analyte, X_A, is expressed as a mass fraction. The target value of the standard deviation, σ_A is related to H_A by a factor k:

$$\sigma_A = k H_A, \quad k = 0.5, 1.0, 1.5 \quad (2)$$

Depending on the value of the factor k the target value of the standard deviation is recognized as fit-for-purpose at three levels of uncertainty: k = 0.5 - appropriate for high precision analysis; k = 1.0 - appropriate for well-established routine analysis; k = 1.5 - satisfactory for common analytical tasks. The relative value of the target standard deviation, *RSD*, expressed in per cent, is defined as follows:

$$RSD = \frac{\sigma_A}{X_A} \cdot 100\% \quad (3)$$

The relative value of the target standard deviation as a function of the assigned mass fraction of the analyte, X_A, is shown in Fig. 1 for the three different values of the k factor.

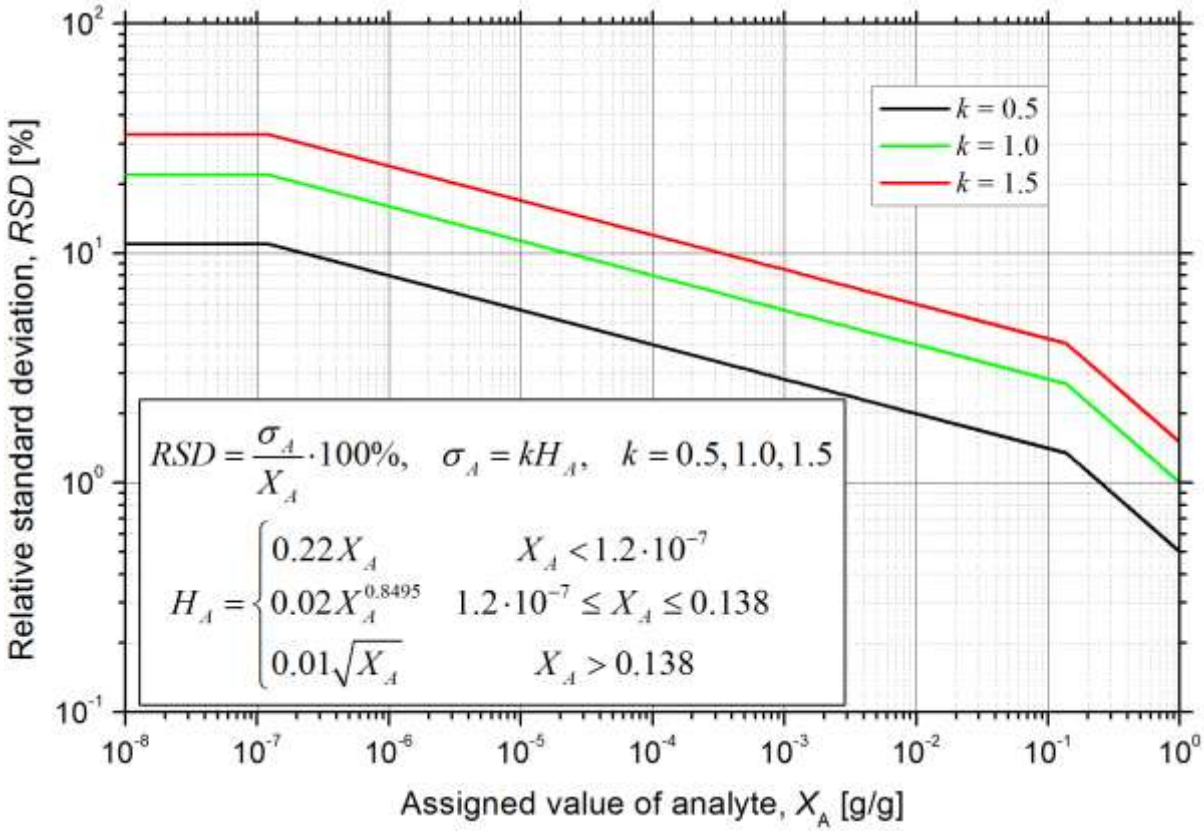

FIG. 1. Relative value of the target standard deviation, RSD, as a function of the assigned mass fraction of the analyte, X_A, calculated by using a modified Horowitz function, Eqn. (1).

3.3. *z*-SCORES AND *u*-SCORES

The reported concentrations of analytes were compared with the assigned values by using the *z*-score analysis. For every result a *z*-score was calculated:

$$z = \frac{x - X_A}{\sigma_A} \tag{4}$$

The term '*x*' denotes the mass fraction of analyte reported by the participant. Defined by different fit-for-purpose ranges of the target standard deviation, three different values of *z*-scores were calculated by combining Eqns. (2) and (4). Assuming that appropriate values for X_A and σ_A have been used and that the underlying distribution of analytical errors is normal, apart from outliers, in a well-behaved analytical system *z*-scores would be expected to fall outside the range $-2 \le z \le 2$ in about 4.6% of instances, and outside the range $-3 < z < 3$ only in about 0.3%. Therefore, based on the z-scores the following decision limits were established:

$$\begin{aligned} |z| &\le 2 && \text{- a satisfactory result} \\ 2 < |z| &< 3 && \text{- the result is considered questionable} \\ |z| &\ge 3 && \text{- the result is considered unsatisfactory} \end{aligned} \tag{5}$$

The advice to the laboratory is that, independent of the fit-for-purpose range selected by the laboratory, any *z*-score for an element outside the range $-2 \le z \le 2$ should be examined by the analyst and all steps of the analytical procedure verified to identify the source(s) of the analytical bias.

For every participant the rescaled sum of *z*-scores, *RSZ*, as well as the sum of squared *z*-scores, *SSZ*, were calculated as defined by the following equations:

$$RSZ = \frac{\sum_{i=1}^{L} z_i}{\sqrt{L}} \tag{6}$$

$$SSZ = \sum_{i=1}^{L} (z_i)^2 \tag{7}$$

The symbol '*L*' denotes the number of results provided by the laboratory/participant for all the analytes determined. The summing up in Eqns. (6) and (7) takes into account all *z*-scores for all analytes with known assigned values reported by participant. The *RSZ* can be interpreted as a standardized normally distributed variable, with expected value equal to zero and unit variance. It is sensitive in detecting a small consistent bias in an analytical system, however, it is not sensitive in cases where there are even big errors but having opposite signs. The *SSZ* takes no account of the signs because it depends on the squared *z*-scores. It has a chi-squared (χ^2) distribution with *L* degrees of freedom. The *SSZ* can be regarded as complementary to *RSZ*, which means that if *RSZ* is well within the range $-3 < RSZ < 3$ and if at the same time the value of *SSZ* is above the $\chi^2_{critical}$ value the overall performance of the laboratory requires improvement.

The reported results were accompanied by the standard uncertainty estimate made by the participant. The values were used to calculate *u*-scores:

$$u = \frac{|x - X_A|}{\sqrt{(\sigma_A)^2 + (\sigma_x)^2}} \tag{8}$$

The symbol 'σ_x' denotes the standard uncertainty of the submitted result *x*. If the assumptions about X_A and σ_A and about the normality of the underlying distributions are correct, and the laboratory estimate of σ_x takes into account all the significant sources of uncertainty, the *u*-scores would have a truncated normal distribution with unit variance. In a well-behaved analytical system only 0.1% of *u*-scores would fall outside the range $u < 3.29$. Therefore, the following decision limits for the *u*-scores were established:

$u \le 1.64$ - reported result does not differ from the assigned value
$1.64 < u \le 1.95$ - reported result probably does not differ from the assigned value
$1.95 < u \le 2.58$ - it is not clear whether the reported and assigned values differ (9)
$2.58 < u \le 3.29$ - reported result is probably different from the assigned value
$3.29 < u$ - reported result differs from the assigned value

The *u*-scores are especially useful for deciding whether the laboratory fit-for-purpose criteria are fulfilled. By comparing Eqn. (4) and Eqn. (8) one can notice that for corresponding values of *u*-score and *z*-score the following inequality is always fulfilled:

$$u \le |z| \tag{10}$$

It implies that if the *u*-score is larger than 3.29 also the decision limit for the corresponding *z*-score is triggered and the laboratory has to check the analytical procedure as well as review the uncertainty budget estimation. If *u*-score stays below the value of 1.64 and at the same time the *z*-score decision limit is triggered ($|z| > 3$) the laboratory should reevaluate its fit-for-purpose status for that particular analyte.

3.4. CONSENSUS VALUES

To examine the overall performance of the participating laboratories, the submitted results have been statistically processed and the consensus values were calculated (this data processing was performed for all the three samples). The results were tested for the presence of outliers using a set of seven outlier rejection tests, shown below:

Description of symbols:

$x_1 < ... < x_n$	- set of analytical results,
$\bar{x}$	- mean value,
s	- standard deviation,

(11)

1. Coefficient of kurtosis [4], number of results: $5 \le n \le 100$, two-sided test, confidence level = 0.95:

$$b_2 = \frac{n\sum_{i=1}^{n}(\bar{x} - x_i)^4}{\left[\sum_{i=1}^{n}(\bar{x} - x_i)^2\right]^2} \tag{12}$$

   If b_2 > critical value then reject the result that is at the furthest distance from the mean, decrease *n*, repeat the procedure until $b_2 \le$ critical value.

2. Coefficient of skewness [4], number of results, $5 \le n \le 60$, one-sided test, confidence level = 0.95:

$$\sqrt{b_1} = \frac{\sqrt{n}\sum_{i=1}^{n}(x_i - \bar{x})^3}{\left[\sum_{i=1}^{n}(x_i - \bar{x})^2\right]^{3/2}} \tag{13}$$

   If $\left|\sqrt{b_1}\right|$ > critical value then: if $\sqrt{b_1}$ is positive then reject x_n, otherwise reject x_1, decrease *n*, repeat the procedure until $\left|\sqrt{b_1}\right| \le$ critical value.

3. Veglia's test [5,6], number of results: $4 \le n \le \infty$, two-sided test, confidence level = 0.95:

$$h = \sqrt{\frac{n}{n-1}}\,\frac{|x_k - \bar{x}_{n-1}|}{s_{n-1}} \tag{14}$$

where:

x_k, examined value, the result at the furthest distance from the mean

$\bar{x}_{n-1}$, the mean value of the population of the results with the examined result excluded

s_{n-1}, the standard deviation of the population of the results with the examined result excluded

If h > critical value then reject x_k otherwise temporarily exclude the x_k from the population of results and proceed with testing the next outlier candidate, if the following value of h > critical value then reject both results, decrease n respectively, repeat the procedure until $h \leq$ critical value.

4. Dixon's test [7], number of results: $3 \leq n \leq 25$, two-sided test, confidence level = 0.95:

If x_1 is at the furthest distance from the mean value, then calculate:

$$r = \begin{cases} (x_2 - x_1)/(x_n - x_1), & 3 \leq n \leq 7 \\ (x_2 - x_1)/(x_{n-1} - x_1), & 8 \leq n \leq 10 \\ (x_3 - x_1)/(x_{n-1} - x_1), & 11 \leq n \leq 13 \\ (x_3 - x_1)/(x_{n-2} - x_1), & 14 \leq n \leq 25 \end{cases} \tag{15a}$$

If x_n is at the furthest distance from the mean value then calculate:

$$r = \begin{cases} (x_n - x_{n-1})/(x_n - x_1), & 3 \leq n \leq 7 \\ (x_n - x_{n-1})/(x_n - x_2), & 8 \leq n \leq 10 \\ (x_n - x_{n-2})/(x_n - x_2), & 11 \leq n \leq 13 \\ (x_n - x_{n-2})/(x_n - x_3), & 14 \leq n \leq 25 \end{cases} \tag{15b}$$

If r > critical value then reject the tested result, decrease n, repeat the procedure until $r \leq$ critical value.

5. Outlier rejection test proposed in [4], number of results: $4 \leq n \leq 100$, two-sided test, confidence level = 0.95:

$$w/s = (x_n - x_1)/s \tag{16}$$

If w/s > critical value then: if $x_n - \bar{x} = \bar{x} - x_1$, reject both x_1 and x_n, otherwise reject x_k ($x_k = x_1$ *or* $x_k = x_n$), the result that is at the furthest distance from the mean, for the remaining population of results ($n' = n - 1$) calculate: $T_k = |\bar{x}' - x_k|/s'$, where: $\bar{x}'$ is the mean value and s' is the standard deviation of the population of the results excluding the rejected value x_k, if $T_k >$ critical value then reject also the second

extreme result, decrease n respectively, repeat the procedure until $w/s \leq$ critical value.

6. Outlier rejection test proposed in [8], number of results: $3 \leq n < \infty$, two-sided test, confidence level = 0.95:

$$B_4 = \left| x_k - \bar{x} \right| / s \tag{17}$$

where:

x_k, examined value

If $B_4 >$ critical value then reject the tested result, repeat the procedure until $B_4 \leq$ critical value.

7. Outlier rejection test proposed in [9], number of results: $3 \leq n \leq 100$, two-sided test, confidence level = 0.95:

$$S_k^2 / S = \frac{\sum_{i=1, i \neq k}^{n} (x_i - \bar{x}')^2}{\sum_{i=1, i \neq k}^{n} (x_i - \bar{x})^2}, \quad k = 1 \, or \, k = n \tag{18}$$

where:

x_k, examined value, the result at the furthest distance from the mean

$\bar{x}'$, the mean value of the population of the results with the examined result x_k excluded

If $S_k^2 / S >$ critical value then reject x_k, decrease n, repeat the procedure until $S_k^2 / S \leq$ critical value.

The results which passed the outlier rejection procedures were used to calculate the consensus mean value of analyte, X_C, and corresponding consensus value of its standard deviation, σ_C:

$$X_C = \frac{\sum_{i=1}^{m} x_i}{m} \tag{19}$$

and

$$\sigma_C = \sqrt{\frac{\sum_{i=1}^{m} (x_i - X_C)^2}{m(m-1)}} \tag{20}$$

The term m denotes the number of reported values for a given analyte excluding the outliers rejected by at least one of the outlier rejections tests. The summing up in Eqn. (19) and (20) takes into account only the results which passed all the outlier rejection tests.

4. RESULTS

The three water samples were distributed to 37 laboratories for chemical composition analysis. Out of the 37 laboratories, 31 participated in the test submitting 473 individual results for 37 chemical elements for sample "1", 324 individual results for 29 chemical elements for sample "2", 254 individual results for 35 chemical elements for sample "3". The list of the participating laboratories is presented at the end of this report. All submitted results have been evaluated.

The measuring set-up (carrier material and its preparation, excitation source) and the experimental parameters (voltage, current, measuring time) used by the participants and their codes are listed in Table 1a, 1b and 1c, for samples "1", "2" and "3" respectively. The total number of elements reported by each laboratory is also reported in these Tables.

In Table 2a a summary of the assigned analyte values, the target values of standard deviation (obtained by using modified Horowitz function), the consensus values and their standard deviations are shown for sample "1".
For sample "2" the consensus values were used for comparison with respect to the experimental values provided by the participants instead of the assigned analyte values. It was evidenced that the concentration of the internal standard (Ga) was lower than the expected value of 0.1 mg/L, resulting to systematic errors in the measured concentrations by the most of the participants.
Tables 2b and 2c show the consensus values and their standard deviations for sample "2" and "3", respectively.
The consensus values (Eqn. 19) and corresponding standard deviations (Eqn. 20) were calculated based on the reported values for elements having more than five results after excluding outliers. The number of reported results and outliers for each sample is listed below:

Sample	Reported values	Outliers
1	473	42
2	324	35
3	254	44

The *z*- and *u*-scores were calculated for sample "1" for the analytes for which an assigned value was available. The element Calcium was not considered for the evaluation of *z*- and *u*-scores due to unexpected high values.
In case of sample "2" and "3" the *z*- and *u*-scores were calculated considering as a reference the consensus values.

TABLE 1a. MEASURING SET-UP AND EXPERIMENTAL PARAMETERS USED BY PARTICIPANTS OF THE PROFICIENCY TEST EXERCISE FOR SAMPLE “1”

Laboratory Code	Carrier material	Preparation	Excitation Source	Voltage (kV)	Current (mA)	Measuring Time (s)	No. of Elem.
35	soda-lime glass	siliconization	X-ray tube - Mo anode	50	0.8	600	17
53	quartz	not specified	X-ray tube - Mo anode	50	0.6	300	14
54	quartz	no preparation	X-ray tube - Mo anode	50	1	1000	15
57	quartz	no preparation	X-ray tube - Mo anode	45	25	1000	14
62	quartz	not specified	X-ray tube - Mo anode	40	20	200	14
67	quartz/plexiglass	not specified	X-ray tube - Mo/W anode	50	0.6	120	9
69	quartz	no preparation	X-ray tube - Mo anode	40	40	300	16
72	quartz	not specified	X-ray tube - Mo anode	50	1	100	18
73	quartz	no preparation	X-ray tube - Mo anode	50	0.602	1000	17
75	quartz	siliconization	X-ray tube - Mo anode	50	0.6	1000	29
78	quartz	siliconization	X-ray tube - Mo anode	40	30	500	16
89	quartz	siliconization	X-ray tube - Mo anode	40	30	1000	13
93	quartz	siliconization	X-ray tube - Mo anode	50	0.6	3600	13
95	quartz	siliconization	X-ray tube - W anode	50	1	2000	17
103	quartz	no preparation	X-ray tube - Mo anode	40	30	1000	11
104	quartz	siliconization	X-ray tube - Mo anode	50	1.000	500	16
105	quartz	siliconization	X-ray tube - Mo anode	50	0.600	1200	32
106	quartz	siliconization	X-ray tube - Mo anode	50	1	1000	17
107	quartz	siliconization	X-ray tube - Mo anode	50	8	1000	14
108	quartz	siliconization	X-ray tube - Mo anode	50	0.75	600	19
109	silicon wafer	no preparation	X-ray tube - Mo anode	40	20	1000	16
110	quartz	no preparation	X-ray tube - Mo anode	40	30	600	14
111	quartz	no preparation	X-ray tube - Rh anode	20	0.06	600	16
112	quartz	DLC coating	X-ray tube - W anode	25	0.2	600	15
113	soda-lime glass	siliconization	X-ray tube - Mo anode	50	0.6	1000	13
114	soda-lime glass	siliconization	X-ray tube - Mo anode	50	0.6	500	12
115	quartz	not specified	X-ray tube - Mo anode	40	30	1000	8
116	quartz	no preparation	X-ray tube - Mo anode	50	0.6	500	16
117	quartz	no preparation	X-ray tube - Mo anode	50	0.696	250	18
118	quartz	DLC coating	X-ray tube - W anode	25	0.2	600	14

TABLE 1b. MEASURING SET-UP AND EXPERIMENTAL PARAMETERS USED BY PARTICIPANTS OF THE PROFICIENCY TEST EXERCISE FOR SAMPLE “2”

Laboratory Code	Carrier material	Preparation	Excitation Source	Voltage (kV)	Current (mA)	Measuring Time (s)	No. of Elem.
35	soda-lime glass	siliconization	X-ray tube - Mo anode	50	0.8	1000	7
53	quartz	not specified	X-ray tube - Mo anode	50	0.6	300	13
54	quartz	no preparation	X-ray tube - Mo anode	50	1	2000	13
57	quartz	no preparation	X-ray tube - Mo anode	45	25	2000	11
62	quartz	not specified	X-ray tube - Mo anode	40	20	200	12
67	quartz/plexiglass	not specified	X-ray tube - Mo/W anode	50	0.6	120	1
69	quartz	no preparation	X-ray tube - Mo anode	40	40	1000	14
72	quartz	not specified	X-ray tube - Mo anode	50	1	500	16
73	quartz	no preparation	X-ray tube - Mo anode	50	0.602	1000	16
75	quartz	siliconization	X-ray tube - Mo anode	50	0.6	1000	22
89	quartz	siliconization	X-ray tube - Mo anode	40	30	1000	11
93	quartz	siliconization	X-ray tube - Mo anode	50	0.6	3600	13
95	quartz	siliconization	X-ray tube - W anode	50	1	2000	12
103	quartz	no preparation	X-ray tube - Mo anode	40	30	1000	8
104	quartz	siliconization	X-ray tube - Mo anode	50	1.000	500	14
105	quartz	siliconization	X-ray tube - Mo anode	50	0.600	1200	22
106	quartz	siliconization	X-ray tube - Mo anode	50	1	1000	14
107	quartz	siliconization	X-ray tube - Mo anode	50	47	1000	12
108	quartz	siliconization	X-ray tube - Mo anode	50	0.75	600	18
109	silicon wafer	no preparation	X-ray tube - Mo anode	40	20	1000	12
113	soda-lime glass	siliconization	X-ray tube - Mo anode	50	0.6	1000	9
114	soda-lime glass	siliconization	X-ray tube - Mo anode	50	0.6	500	6
116	quartz	no preparation	X-ray tube - Mo anode	50	0.6	500	14
117	quartz	no preparation	X-ray tube - Mo anode	50	0.696	250	15
118	quartz	DLC coating	X-ray tube - W anode	25	0.2	600	10
119	quartz	siliconization	Synchrotron light	10	290	600	9

TABLE 1c. MEASURING SET-UP AND EXPERIMENTAL PARAMETERS USED BY PARTICIPANTS OF THE PROFICIENCY TEST EXERCISE FOR SAMPLE “3”

Laboratory Code	Carrier material	Preparation	Excitation Source	Voltage (kV)	Current (mA)	Measuring Time (s)	No. of Elem.
35	soda-lime glass	siliconization	X-ray tube - Mo anode	50	0.8	3000	7
53	quartz	not specified	X-ray tube - Mo anode	50	0.6	300	7
54	quartz	no preparation	X-ray tube - Mo anode	50	1	1000	8
57	quartz	no preparation	X-ray tube - Mo anode	45	25	2000	4
62	quartz	not specified	X-ray tube - Mo anode	40	20	200	12
67	quartz/plexiglass	not specified	X-ray tube - Mo/W anode	50	0.6	120	5
69	quartz	no preparation	X-ray tube - Mo anode	40	40	1000	13
72	quartz	not specified	X-ray tube - Mo anode	50	1	500	16
73	quartz	no preparation	X-ray tube - Mo anode	50	0.602	1000	9
75	quartz	siliconization	X-ray tube - Mo anode	50	0.6	1000	24
93	quartz	siliconization	X-ray tube - Mo anode	50	0.6	3600	4
95	quartz	siliconization	X-ray tube - W anode	50	1	2000	4
103	quartz	no preparation	X-ray tube - Mo anode	40	30	1000	6
104	quartz	siliconization	X-ray tube - Mo anode	50	1.000	500	8
105	quartz	siliconization	X-ray tube - Mo anode	50	0.600	1200	23
106	quartz	siliconization	X-ray tube - Mo anode	50	1	1000	6
107	quartz	siliconization	X-ray tube - Mo anode	50	42	1000	5
108	quartz	siliconization	X-ray tube - Mo anode	50	0.75	600	16
109	silicon wafer	no preparation	X-ray tube - Mo anode	40	20	1000	13
110	quartz	no preparation	X-ray tube - Mo anode	40	30	600	7
111	quartz	no preparation	X-ray tube - Rh anode	20	0.06	1800	5
112	quartz	DLC coating	X-ray tube - W anode	25	0.2	600	4
113	soda-lime glass	siliconization	X-ray tube - Mo anode	50	0.6	1000	5
114	soda-lime glass	siliconization	X-ray tube - Mo anode	50	0.6	500	9
115	quartz	not specified	X-ray tube - Mo anode	40	30	1000	2
116	quartz	no preparation	X-ray tube - Mo anode	50	0.6	500	14
117	quartz	no preparation	X-ray tube - Mo anode	50	0.696	250	14
118	quartz	DLC coating	X-ray tube - W anode	25	0.2	600	4

TABLE 2a. THE ASSIGNED VALUES OF ANALYTES, THE TARGET VALUES OF THE STANDARD DEVIATIONS AND THE CONSENSUS VALUES FOR SAMPLE "1"

Analyte symbol	Assigned value of the analyte, X_A	Target value of standard deviation, σA			Consensus value of the analyte, X_C	Consensus value of the standard deviation, σ_C	Number of results	Number of outliers
		k = 0.5	k = 1.0	k = 1.5				
	[µg/L]							
Ag	10010	566.07	1132.14	1698.2	13845.67	1591.88	9	0
Ba	9990	565.11	1130.21	1695.32	11109.82	747.29	23	1
Bi	9900	560.78	1121.56	1682.34	9736.85	306.63	29	4
Ca	-	-	-	-	24899.96	2370.73	24	0
Cd	9890	560.3	1120.6	1680.89	9349.04	752.54	14	3
Co	9880	559.82	1119.63	1679.45	10337.34	222.76	29	1
Cr	9890	560.3	1120.6	1680.89	9924.61	249.56	29	1
Cu	9880	559.82	1119.63	1679.45	10184.15	110.64	30	4
Fe	9890	560.3	1120.6	1680.89	10367.93	160.73	30	2
In	9880	559.82	1119.63	1679.45	10444.05	1296.43	9	0
K	9930	562.22	1124.45	1686.67	12089.53	670.36	25	2
Mn	9910	561.26	1122.52	1683.78	10529.52	268.18	29	2
Ni	9890	560.3	1120.6	1680.89	10492.31	171.99	30	2
Pb	9910	561.26	1122.52	1683.78	11059.38	360.20	29	3
S	-	-	-	-	27392.35	5145.53	6	0
Sr	9880	559.82	1119.63	1679.45	11425.71	210.42	29	4
Tl	9920	561.74	1123.48	1685.23	10276.69	209.13	27	5
Zn	9890	560.3	1120.6	1680.89	10393.93	117.58	30	4

TABLE 2b. THE CONSENSUS VALUES FOR SAMPLE “2”

Analyte symbol	Consensus value of the analyte, X_C	Consensus value of the standard deviation, σ_C	Number of results	Number of outliers
		[µg/L]		
Ba	335.78	60.66	16	1
Ca	3452.61	578.03	19	4
Cl	1955.23	498.57	11	2
Co	274.50	37.65	24	2
Cr	144.99	15.43	20	2
Cu	248.20	29.44	25	2
Fe	122.47	19.62	24	5
K	704.10	136.04	14	0
Mn	291.23	38.44	24	2
Ni	256.41	34.82	24	2
Pb	260.38	31.15	21	2
Sr	278.78	34.75	21	2
Tl	258.30	35.14	20	3
Zn	292.78	33.83	25	2

TABLE 2c. THE CONSENSUS VALUES FOR SAMPLE “3”

Analyte symbol	Consensus value of the analyte, X_C	Consensus value of the standard deviation, σ_C	Number of results	Number of outliers
		[µg/L]		
Ba	28.94	9.09	5	0
Br	50.26	3.69	17	3
Ca	19917.93	1092.24	24	3
Cl	7487.63	928.30	14	2
Cr	2.35	0.29	7	3
Cu	1.94	0.41	14	7
Fe	81.18	16.65	17	2
K	8717.85	542.83	25	3
Pb	4.51	1.30	10	1
Rb	25.51	1.53	16	1
S	644.91	100.87	10	1
Sr	132.84	6.81	23	2
Ti	13.33	5.08	7	2
V	10.42	0.48	8	2
Zn	7.64	1.36	15	6

Tables 3a, 3b and 3c list the values of the *z*- and *u*-scores for all submitted results for samples "1", "2" and "3", respectively. In brackets, next to the element symbol, the assigned values (for sample "1") or the consensus values (for samples "2" and "3") of element concentration and the target standard deviation for $k = 1$ are shown. The *z*- and *u*-scores were calculated for the three different fit-for-purpose ranges, as defined by Eqn. (2). The results rejected by the outliers rejection procedures were marked with "*" in the "Analyte concentration" column.

Tables 4a, 4b and 4c show the combined *z*-scores, the *RSZ* and *SSZ* as defined in Eqns. (6) and (7), in the case of sample "1", "2" and "3", respectively, for all the participating laboratories and for the three different fit-for-purpose ranges. The analytes without assigned values for sample "1" or without consensus values for samples "2" and "3" were not considered.

Figs. 2-47 and 48-91 present the distributions of the proficiency test results.
In Figs 2-47 (Figs. 2-19 for sample "1", Figs. 20-33 for sample "2" and Figs. 34-47 for sample "3") the individual results are marked with filled circles. The dotted lines show the range of the accepted results (the results within these lines were used to calculate the consensus values). The outliers are marked with arrows. Also shown are the estimated parameters of the distribution (after outlier rejection): mode, median and the mean value. For few elements, the result of density distributions could only be used as indicators of the trends observed in the reported data due to the limited number of results (only density distributions of analytes for which at least 5 results passed the outlier rejection tests are shown). All the populations of results, after outlier rejection, have passed a normality test (Kolmogorov-Smirnov).
Figs. 48-91 (Figs. 48-63 for sample "1", Figs. 64-77 for sample "2" and Figs. 78-91 for sample "3") show the bar chart distributions of the *z*-scores for the analytes with at least 6 submitted results. The results are sorted in ascending order versus laboratory code. The bar charts show the distance between the reported and the assigned/consensus values of the analyte. The submitted results and their uncertainties are marked with filled squares accompanied by uncertainty bars. The horizontal lines show the admissible levels of z-score, $|z| < 2$, for three different ranges defined by factor k in Eqn. (2): $k = 0.5$ (solid black lines), $k = 1.0$ (solid green lines) and $k = 1.5$ (solid red lines). The decision levels of satisfactory results, $|z| < 2$, for different fit-for-purpose targets have also been marked.

For every participating laboratory its overall performance concerning the analysis of samples "1", "2" and "3" is presented in Figs. 92-121, Figs. 122-146 and Figs. 147-174, respectively. The plots presented in these figures relate all the *u*-scores and *z*-scores calculated for a given laboratory. The hollow symbols denote the values calculated for specific fit-for-purpose levels as defined in Eqn. (2) with factor k, namely: $k = 0.5$ (black triangles), $k = 1.0$ (green circles), and $k = 1.5$ (red squares). The decision limits of unsatisfactory results were marked with black lines ($|z| > 3$, $u > 3.29$). They divide the plot area in four quadrants. Due to inequality (10) all the points accompanied by a laboratory estimate of the uncertainty fall always below the line $u = |z|$. The smaller the laboratory estimate of the uncertainty the closer the related point to the $u = |z|$ line. Points in the immediate proximity of the dashed diagonal line ($u = |z|$) have underestimated uncertainty values. The well performing laboratories would have more points located in the lower-left quadrant of the plot. If there are many points located in the upper-right quadrant it suggests that these results do not fall in the defined fit-for-purpose targets and that the laboratory provided too "narrow" uncertainty estimate.

TABLE 3a. SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "1"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
Ag (10010 ± 1132.14) [µg/L]									
78	5636	493	8.75	-7.73	-3.86	-2.58	5.83	3.54	2.47
72	9318	992	10.65	-1.22	-0.61	-0.41	0.61	0.46	0.35
116	11500.2	1641.91	14.28	2.63	1.32	0.88	0.86	0.75	0.63
95	12883	360	2.79	5.08	2.54	1.69	4.28	2.42	1.66
108	13833.8	1025.8	7.42	6.76	3.38	2.25	3.26	2.50	1.93
109	14242.57	2333.74	16.39	7.48	3.74	2.49	1.76	1.63	1.47
75	17779.2	2044.6	11.5	13.72	6.86	4.57	3.66	3.32	2.92
105	18342.24	1960.05	10.69	14.72	7.36	4.91	4.08	3.68	3.21
106	21076	2219.75	10.53	19.55	9.77	6.52	4.83	4.44	3.96
Al (9890 ± 1120.60) [µg/L]									
75	5174.2	850.9	16.45	-8.42	-4.21	-2.81	4.63	3.35	2.50
108	9049.4	3380.4	37.35	-1.50	-0.75	-0.50	0.25	0.24	0.22
105	11309.93	668.88	5.91	2.53	1.27	0.84	1.63	1.09	0.78
117	12000	2000	16.67	3.77	1.88	1.26	1.02	0.92	0.81
As [µg/L]									
117	15	3	20	-	-	-	-	-	-
75	27.2	1.9	6.99	-	-	-	-	-	-
104	33.4	1	2.99	-	-	-	-	-	-
105	60.273*	3.15	5.23	-	-	-	-	-	-
Ba (9990 ± 1130.21) [µg/L]									
118	4952	1072	21.65	-8.92	-4.46	-2.97	4.16	3.23	2.51
69	5300	100	1.89	-8.30	-4.15	-2.77	8.17	4.13	2.76
72	6098	644	10.56	-6.89	-3.44	-2.3	4.54	2.99	2.15
78	7022	403	5.74	-5.25	-2.63	-1.75	4.28	2.47	1.70
107	7705	570.7	7.41	-4.04	-2.02	-1.35	2.85	1.80	1.28
116	8276.6	517.11	6.25	-3.03	-1.52	-1.01	2.24	1.38	0.97
108	8958.8	292.9	3.27	-1.82	-0.91	-0.61	1.62	0.88	0.6
57	10033	289	2.88	0.08	0.04	0.03	0.07	0.04	0.03
114	10600	460	4.34	1.08	0.54	0.36	0.84	0.5	0.35
110	10795.4	1401	12.98	1.43	0.71	0.48	0.53	0.45	0.37
75	11646.2	1641.8	14.1	2.93	1.47	0.98	0.95	0.83	0.7
89	12250	1912	15.61	4.00	2.00	1.33	1.13	1.02	0.88
106	12294.8	1579.14	12.84	4.08	2.04	1.36	1.37	1.19	0.99
113	12625	1760	13.94	4.66	2.33	1.55	1.43	1.26	1.08
117	12700	300	2.36	4.8	2.4	1.6	4.24	2.32	1.57
54	12913	3032	23.48	5.17	2.59	1.72	0.95	0.90	0.84
104	13000	100	0.77	5.33	2.66	1.78	5.24	2.65	1.77
109	14147.34	4104.29	29.01	7.36	3.68	2.45	1.00	0.98	0.94
105	14718.55	1641.93	11.16	8.37	4.18	2.79	2.72	2.37	2.00

TABLE 3a (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "1"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				k = 0.5	k = 1.0	k = 1.5	k = 0.5	k = 1.0	k = 1.5
53	15042	712	4.73	8.94	4.47	2.98	5.56	3.78	2.75
112	15157.86	3488.47	23.01	9.14	4.57	3.05	1.46	1.41	1.33
73	18180.4	106.6	0.59	14.49	7.25	4.83	14.24	7.21	4.82
62	37136.75*	2596.17	6.99	48.04	24.02	16.01	10.22	9.59	8.76
Bi (9900 ± 1121.56) [µg/L]									
67	3399*	93	2.74	-11.59	-5.8	-3.86	11.44	5.78	3.86
118	6068	1160	19.12	-6.83	-3.42	-2.28	2.97	2.37	1.88
95	7166	94	1.31	-4.88	-2.44	-1.63	4.81	2.43	1.62
108	7820.6	90.8	1.16	-3.71	-1.85	-1.24	3.66	1.85	1.23
69	8200	400	4.88	-3.03	-1.52	-1.01	2.47	1.43	0.98
54	8270	242	2.93	-2.91	-1.45	-0.97	2.67	1.42	0.96
109	8564.075	234.81	2.74	-2.38	-1.19	-0.79	2.20	1.17	0.79
89	8981	521	5.8	-1.64	-0.82	-0.55	1.20	0.74	0.52
103	9090.574	466.32	5.13	-1.44	-0.72	-0.48	1.11	0.67	0.46
93	9590	938.5	9.79	-0.55	-0.28	-0.18	0.28	0.21	0.16
73	9667.6	27.4	0.28	-0.41	-0.21	-0.14	0.41	0.21	0.14
104	9700	30	0.31	-0.36	-0.18	-0.12	0.36	0.18	0.12
72	9843	204	2.07	-0.10	-0.05	-0.03	0.10	0.05	0.03
57	9991	127	1.27	0.16	0.08	0.05	0.16	0.08	0.05
75	10028.8	109.9	1.1	0.23	0.11	0.08	0.23	0.11	0.08
117	10100	300	2.97	0.36	0.18	0.12	0.31	0.17	0.12
78	10124	561	5.54	0.40	0.20	0.13	0.28	0.18	0.13
116	10189.8	207.86	2.04	0.52	0.26	0.17	0.48	0.25	0.17
106	10324.2	449.39	4.35	0.76	0.38	0.25	0.59	0.35	0.24
105	10453.54	122.6	1.17	0.99	0.49	0.33	0.96	0.49	0.33
53	10542	436	4.14	1.14	0.57	0.38	0.9	0.53	0.37
110	10561.8	2145.28	20.31	1.18	0.59	0.39	0.3	0.27	0.24
107	11063	1142.8	10.33	2.07	1.04	0.69	0.91	0.73	0.57
113	11952	409	3.42	3.66	1.83	1.22	2.96	1.72	1.19
114	12200	581	4.76	4.10	2.05	1.37	2.85	1.82	1.29
112	12930.29	834.76	6.46	5.40	2.70	1.80	3.01	2.17	1.61
111	14712*	1530	10.4	8.58	4.29	2.86	2.95	2.54	2.12
35	16560*	2100	12.68	11.88	5.94	3.96	3.06	2.80	2.48
62	150115.5*	1877.17	1.25	250.04	125.02	83.35	71.57	64.12	55.63
Ca [µg/L]									
118	9983	1144	11.46	-	-	-	-	-	-
57	10245	278	2.71	-	-	-	-	-	-
78	11488	751	6.54	-	-	-	-	-	-
110	11734.2	1913.41	16.31	-	-	-	-	-	-
95	13607	1075	7.9	-	-	-	-	-	-
104	14900	90	0.6	-	-	-	-	-	-
117	17000	1000	5.88	-	-	-	-	-	-
75	17627.4	2462.1	13.97	-	-	-	-	-	-
105	18183.65	986.63	5.43	-	-	-	-	-	-

TABLE 3a (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "1"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
72	19330	3788	19.6	-	-	-	-	-	-
106	19762.8	972.8	4.92	-	-	-	-	-	-
69	20000	1000	5	-	-	-	-	-	-
89	22256	702	3.15	-	-	-	-	-	-
73	22798	107.6	0.47	-	-	-	-	-	-
111	29189	2744	9.4	-	-	-	-	-	-
93	29630	4674	15.77	-	-	-	-	-	-
54	32182	5283	16.42	-	-	-	-	-	-
116	34926.8	2661.14	7.62	-	-	-	-	-	-
112	35426.65	5245.65	14.81	-	-	-	-	-	-
114	35500	3530	9.94	-	-	-	-	-	-
108	38184.8	1944.9	5.09	-	-	-	-	-	-
107	38981	3855	9.89	-	-	-	-	-	-
35	43300	9000	20.79	-	-	-	-	-	-
62	51363.75	1591.86	3.1	-	-	-	-	-	-
			Cd (9890 ± 1120.60) [µg/L]						
78	5690	741	13.02	-7.50	-3.75	-2.5	4.52	3.13	2.29
72	5936	934	15.73	-7.06	-3.53	-2.35	3.63	2.71	2.06
109	7845.558	1075.28	13.71	-3.65	-1.82	-1.22	1.69	1.32	1.02
108	7953.4	449.3	5.65	-3.46	-1.73	-1.15	2.70	1.60	1.11
116	8427.2	766.34	9.09	-2.61	-1.31	-0.87	1.54	1.08	0.79
75	9314	1159.6	12.45	-1.03	-0.51	-0.34	0.45	0.36	0.28
105	9737.731	518.03	5.32	-0.27	-0.14	-0.09	0.2	0.12	0.09
104	10800	250	2.31	1.62	0.81	0.54	1.48	0.79	0.54
95	11640	473	4.06	3.12	1.56	1.04	2.39	1.44	1.00
53	11856	1876	15.82	3.51	1.75	1.17	1.00	0.90	0.78
106	13639.6	2984.74	21.88	6.69	3.35	2.23	1.23	1.18	1.09
117	18000*	1000	5.56	14.47	7.24	4.82	7.08	5.40	4.15
54	22213*	3301	14.86	21.99	11.00	7.33	3.68	3.53	3.33
73	22852*	194.4	0.85	23.13	11.57	7.71	21.86	11.4	7.66
			Cl [µg/L]						
105	1755.217	348.31	19.84	-	-	-	-	-	-
69	8900	400	4.49	-	-	-	-	-	-
			Co (9880 ± 1119.63) [µg/L]						
107	7695	177.1	2.3	-3.90	-1.95	-1.30	3.72	1.93	1.29
103	8555.465	1044.09	12.2	-2.37	-1.18	-0.79	1.12	0.87	0.67
69	9000	500	5.56	-1.57	-0.79	-0.52	1.17	0.72	0.5
110	9083	515.33	5.67	-1.42	-0.71	-0.47	1.05	0.65	0.45
78	9247	247	2.67	-1.13	-0.57	-0.38	1.03	0.55	0.37
108	9422.2	189.6	2.01	-0.82	-0.41	-0.27	0.77	0.4	0.27
115	9448.533	556.97	5.89	-0.77	-0.39	-0.26	0.55	0.35	0.24
111	9576	478	4.99	-0.54	-0.27	-0.18	0.41	0.25	0.17
118	9712	820	8.44	-0.30	-0.15	-0.10	0.17	0.12	0.09

TABLE 3a (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "1"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
57	9959	7580	76.11	0.14	0.07	0.05	0.01	0.01	0.01
72	9993	321	3.21	0.20	0.10	0.07	0.18	0.10	0.07
93	10220	485.2	4.75	0.61	0.30	0.20	0.46	0.28	0.19
89	10255	265	2.58	0.67	0.33	0.22	0.61	0.33	0.22
117	10300	300	2.91	0.75	0.38	0.25	0.66	0.36	0.25
75	10314	519.8	5.04	0.78	0.39	0.26	0.57	0.35	0.25
106	10320.4	241.98	2.34	0.79	0.39	0.26	0.72	0.38	0.26
116	10430.2	208.64	2	0.98	0.49	0.33	0.92	0.48	0.33
104	10600	30	0.28	1.29	0.64	0.43	1.28	0.64	0.43
73	10635	36	0.34	1.35	0.67	0.45	1.35	0.67	0.45
54	10643	318	2.99	1.36	0.68	0.45	1.19	0.66	0.45
114	10900	283	2.6	1.82	0.91	0.61	1.63	0.88	0.6
109	11121.6	670.19	6.03	2.22	1.11	0.74	1.42	0.95	0.69
95	11428	315	2.76	2.77	1.38	0.92	2.41	1.33	0.91
53	11463	1029	8.98	2.83	1.41	0.94	1.35	1.04	0.80
35	11740	640	5.45	3.32	1.66	1.11	2.19	1.44	1.03
105	11899.81	490.02	4.12	3.61	1.8	1.2	2.71	1.65	1.15
113	12355	1472	11.91	4.42	2.21	1.47	1.57	1.34	1.11
112	13129.38	1582.08	12.05	5.80	2.90	1.93	1.94	1.68	1.41
62	72021.5*	2959.11	4.11	111.00	55.50	37.00	20.63	19.64	18.26
				Cr (9890 ± 1120.60) [µg/L]					
112	7056.762	664.32	9.41	-5.06	-2.53	-1.69	3.26	2.17	1.57
78	7089	101	1.42	-5.00	-2.5	-1.67	4.92	2.49	1.66
107	8080	376.2	4.66	-3.23	-1.62	-1.08	2.68	1.53	1.05
103	8122.398	210.01	2.59	-3.15	-1.58	-1.05	2.95	1.55	1.04
118	8275	445	5.38	-2.88	-1.44	-0.96	2.26	1.34	0.93
108	8580.6	170.1	1.98	-2.34	-1.17	-0.78	2.24	1.16	0.78
69	8800	1000	11.36	-1.95	-0.97	-0.65	0.95	0.73	0.56
54	9727	170	1.75	-0.29	-0.15	-0.10	0.28	0.14	0.10
72	9881	160	1.62	-0.02	-0.01	-0.01	0.02	0.01	0.01
89	9969	84	0.84	0.14	0.07	0.05	0.14	0.07	0.05
104	10020	40	0.4	0.23	0.12	0.08	0.23	0.12	0.08
75	10036.4	103.5	1.03	0.26	0.13	0.09	0.26	0.13	0.09
117	10100	100	0.99	0.37	0.19	0.12	0.37	0.19	0.12
93	10130	500	4.94	0.43	0.21	0.14	0.32	0.2	0.14
57	10157	842	8.29	0.48	0.24	0.16	0.26	0.19	0.14
53	10184	103	1.01	0.52	0.26	0.17	0.52	0.26	0.17
105	10283.41	36.74	0.36	0.7	0.35	0.23	0.7	0.35	0.23
110	10343	254.03	2.46	0.81	0.40	0.27	0.74	0.39	0.27
106	10343.4	185.13	1.79	0.81	0.40	0.27	0.77	0.4	0.27
73	10452.6	44.8	0.43	1.00	0.50	0.33	1.00	0.5	0.33
116	10476.6	227.33	2.17	1.05	0.52	0.35	0.97	0.51	0.35
114	10600	448	4.23	1.27	0.63	0.42	0.99	0.59	0.41
111	10988	553	5.03	1.96	0.98	0.65	1.39	0.88	0.62
109	11144.18	449.43	4.03	2.24	1.12	0.75	1.75	1.04	0.72

TABLE 3a (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "1"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
35	11370	610	5.36	2.64	1.32	0.88	1.79	1.16	0.83
113	11671	659	5.65	3.18	1.59	1.06	2.06	1.37	0.99
95	11696	179	1.53	3.22	1.61	1.07	3.07	1.59	1.07
115	12312.78	1283.83	10.43	4.32	2.16	1.44	1.73	1.42	1.15
62	64438.5*	533.25	0.83	97.36	48.68	32.45	70.52	43.96	30.93
Cu (9880 ± 1119.63) [µg/L]									
67	2382*	95	3.99	-13.39	-6.70	-4.46	13.20	6.67	4.46
107	8024*	183.9	2.29	-3.32	-1.66	-1.11	3.15	1.64	1.10
78	9080	125	1.38	-1.43	-0.71	-0.48	1.39	0.71	0.48
111	9425	451	4.79	-0.81	-0.41	-0.27	0.63	0.38	0.26
110	9427	283.52	3.01	-0.81	-0.4	-0.27	0.72	0.39	0.27
93	9490	389.8	4.11	-0.70	-0.35	-0.23	0.57	0.33	0.23
108	9573	106.9	1.12	-0.55	-0.27	-0.18	0.54	0.27	0.18
69	9600	800	8.33	-0.50	-0.25	-0.17	0.29	0.20	0.15
112	9829.209	725.41	7.38	-0.09	-0.05	-0.03	0.06	0.04	0.03
75	9874.4	221.6	2.24	-0.01	-0.01	0.00	0.01	0.00	0.00
103	9961.403	574.32	5.77	0.15	0.07	0.05	0.10	0.06	0.05
57	9981	501	5.02	0.18	0.09	0.06	0.13	0.08	0.06
118	9982	737	7.38	0.18	0.09	0.06	0.11	0.08	0.06
72	10065	440	4.37	0.33	0.17	0.11	0.26	0.15	0.11
53	10073	671	6.66	0.34	0.17	0.11	0.22	0.15	0.11
115	10217.92	643.3	6.3	0.60	0.30	0.20	0.40	0.26	0.19
89	10250	279	2.72	0.66	0.33	0.22	0.59	0.32	0.22
116	10390.2	70.68	0.68	0.91	0.46	0.30	0.90	0.45	0.30
104	10400	30	0.29	0.93	0.46	0.31	0.93	0.46	0.31
105	10452.06	94.67	0.91	1.02	0.51	0.34	1.01	0.51	0.34
117	10500	100	0.95	1.11	0.55	0.37	1.09	0.55	0.37
106	10648.6	551.39	5.18	1.37	0.69	0.46	0.98	0.62	0.43
95	10672	72	0.67	1.41	0.71	0.47	1.40	0.71	0.47
114	10800	246	2.28	1.64	0.82	0.55	1.50	0.80	0.54
113	10870	449	4.13	1.77	0.88	0.59	1.38	0.82	0.57
109	10885.17	801.66	7.36	1.80	0.90	0.60	1.03	0.73	0.54
35	11120	800	7.19	2.22	1.11	0.74	1.27	0.90	0.67
54	11221	333	2.97	2.40	1.20	0.80	2.06	1.15	0.78
73	12243.8*	34.6	0.28	4.22	2.11	1.41	4.21	2.11	1.41
62	72358.5*	1159.76	1.6	111.61	55.80	37.20	48.52	38.76	30.61
Eu (9880 ± 395.89) [µg/L]									
75	19.2	1.8	9.37	-	-	-	-	-	-
Fe (9890 ± 1120.60) [µg/L]									
67	6530*	170	2.6	-6.00	-3.00	-2.00	5.74	2.96	1.99
107	8447	164.6	1.95	-2.58	-1.29	-0.86	2.47	1.27	0.85
78	8770	492	5.61	-2.00	-1.00	-0.67	1.50	0.92	0.64
103	9468.527	405.53	4.28	-0.75	-0.38	-0.25	0.61	0.35	0.24

TABLE 3a (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "1"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
69	9500	1000	10.53	-0.70	-0.35	-0.23	0.34	0.26	0.20
110	9678.8	230.68	2.38	-0.38	-0.19	-0.13	0.35	0.18	0.12
112	9853.178	747.99	7.59	-0.07	-0.03	-0.02	0.04	0.03	0.02
117	9950	50	0.5	0.11	0.05	0.04	0.11	0.05	0.04
72	9968	338	3.39	0.14	0.07	0.05	0.12	0.07	0.05
108	10037.4	77.6	0.77	0.26	0.13	0.09	0.26	0.13	0.09
118	10169	470	4.62	0.50	0.25	0.17	0.38	0.23	0.16
53	10206	73	0.72	0.56	0.28	0.19	0.56	0.28	0.19
105	10208.62	39.63	0.39	0.57	0.28	0.19	0.57	0.28	0.19
89	10246	177	1.73	0.64	0.32	0.21	0.61	0.31	0.21
104	10300	30	0.29	0.73	0.37	0.24	0.73	0.37	0.24
75	10319.8	40.6	0.39	0.77	0.38	0.26	0.77	0.38	0.26
57	10348	917	8.86	0.82	0.41	0.27	0.43	0.32	0.24
54	10360	304	2.93	0.84	0.42	0.28	0.74	0.40	0.28
73	10453.2	37.6	0.36	1.01	0.50	0.34	1.00	0.50	0.33
106	10530.2	352.71	3.35	1.14	0.57	0.38	0.97	0.54	0.37
95	10636	264	2.48	1.33	0.67	0.44	1.2	0.65	0.44
116	10648.2	114.33	1.07	1.35	0.68	0.45	1.33	0.67	0.45
93	10860	242.6	2.23	1.73	0.87	0.58	1.59	0.85	0.57
114	11100	249	2.24	2.16	1.08	0.72	1.97	1.05	0.71
109	11140.34	272.73	2.45	2.23	1.12	0.74	2.01	1.08	0.73
115	11281.68	566.71	5.02	2.48	1.24	0.83	1.75	1.11	0.78
111	11302	510	4.51	2.52	1.26	0.84	1.86	1.15	0.80
113	12240	405	3.31	4.19	2.10	1.40	3.40	1.97	1.36
35	12280	230	1.87	4.27	2.13	1.42	3.95	2.09	1.41
62	42225.25*	117.44	0.28	57.71	28.86	19.24	56.48	28.70	19.19
				In (9880 ± 1119.63) [µg/L]					
72	5312	112	2.11	-8.16	-4.08	-2.72	8.00	4.06	2.71
108	5990	388.8	6.49	-6.95	-3.47	-2.32	5.71	3.28	2.26
105	8233.044	613.64	7.45	-2.94	-1.47	-0.98	1.98	1.29	0.92
109	8910.649	505.91	5.68	-1.73	-0.87	-0.58	1.28	0.79	0.55
75	10204	466.1	4.57	0.58	0.29	0.19	0.44	0.27	0.19
95	11168	279	2.5	2.30	1.15	0.77	2.06	1.12	0.76
106	12858.8	928.4	7.22	5.32	2.66	1.77	2.75	2.05	1.55
53	13820	763	5.52	7.04	3.52	2.35	4.16	2.91	2.14
117	17500	300	1.71	13.61	6.81	4.54	12.00	6.57	4.47
				Ir [µg/L]					
105	47.887	3.02	6.3	-	-	-	-	-	-
75	48	1.9	3.96	-	-	-	-	-	-
				K (9930 ± 1124.45) [µg/L]					
78	5552	455	8.2	-7.79	-3.89	-2.60	6.05	3.61	2.51
72	8116	908	11.19	-3.23	-1.61	-1.08	1.70	1.26	0.95
93	9170	1675	18.27	-1.35	-0.68	-0.45	0.43	0.38	0.32

TABLE 3a (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "1"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
117	9600	700	7.29	-0.59	-0.29	-0.20	0.37	0.25	0.18
108	9683.8	689.8	7.12	-0.44	-0.22	-0.15	0.28	0.19	0.14
57	9840	737	7.49	-0.16	-0.08	-0.05	0.10	0.07	0.05
118	9932	1161	11.69	0.00	0.00	0.00	0.00	0.00	0.00
116	10000.2	744.08	7.44	0.12	0.06	0.04	0.08	0.05	0.04
107	10423	998.6	9.58	0.88	0.44	0.29	0.43	0.33	0.25
104	11300	108	0.96	2.44	1.22	0.81	2.39	1.21	0.81
110	11571.2	1855.7	16.04	2.92	1.46	0.97	0.85	0.76	0.65
109	11624.02	1511.56	13	3.01	1.51	1.00	1.05	0.90	0.75
111	11660	808	6.93	3.08	1.54	1.03	1.76	1.25	0.93
75	11827.4	1637.5	13.84	3.37	1.69	1.12	1.10	0.96	0.81
53	11956	1819	15.21	3.60	1.80	1.20	1.06	0.95	0.82
106	13246.2	842.1	6.36	5.90	2.95	1.97	3.28	2.36	1.76
54	14088	2125	15.08	7.40	3.70	2.47	1.89	1.73	1.53
73	14516.4	102.8	0.71	8.16	4.08	2.72	8.02	4.06	2.71
105	15494.41	732.33	4.73	9.90	4.95	3.30	6.03	4.15	3.03
69	15900	300	1.89	10.62	5.31	3.54	9.37	5.13	3.48
113	16110	2718	16.87	10.99	5.50	3.66	2.23	2.10	1.93
112	17404.62	2218.99	12.75	13.29	6.65	4.43	3.27	3.00	2.68
95	19044	2318	12.17	16.21	8.11	5.40	3.82	3.54	3.18
35	26400*	940	3.56	29.29	14.65	9.76	15.04	11.24	8.53
62	91502*	1434.91	1.57	145.09	72.54	48.36	52.93	44.75	36.84
				Mg (9910 ± 1122.52) [µg/L]					
75	3794	2201.66	58.03	-10.90	-5.45	-3.63	2.69	2.47	2.21
108	5182	0	0	-8.42	-4.21	-2.81	8.42	4.21	2.81
105	10110.01	1695.13	16.77	0.36	0.18	0.12	0.11	0.10	0.08
				Mn (9910 ± 1122.52) [µg/L]					
67	1420*	150	10.56	-15.13	-7.56	-5.04	14.61	7.50	5.02
107	7552	311.9	4.13	-4.20	-2.10	-1.40	3.67	2.02	1.38
78	8188	384	4.69	-3.07	-1.53	-1.02	2.53	1.45	1.00
69	8800	1000	11.36	-1.98	-0.99	-0.66	0.97	0.74	0.57
118	9286	916	9.86	-1.11	-0.56	-0.37	0.58	0.43	0.33
108	9295.2	207.5	2.23	-1.10	-0.55	-0.37	1.03	0.54	0.36
110	9641.72	488.71	5.07	-0.48	-0.24	-0.16	0.36	0.22	0.15
57	9716	687	7.07	-0.35	-0.17	-0.12	0.22	0.15	0.11
103	9816.008	1335.51	13.61	-0.17	-0.08	-0.06	0.06	0.05	0.04
72	10077	545	5.41	0.30	0.15	0.10	0.21	0.13	0.09
115	10195.48	1621.84	15.91	0.51	0.25	0.17	0.17	0.14	0.12
89	10338	333	3.22	0.76	0.38	0.25	0.66	0.37	0.25
93	10340	736	7.12	0.77	0.38	0.26	0.46	0.32	0.23
117	10400	500	4.81	0.87	0.44	0.29	0.65	0.40	0.28
104	10400	40	0.38	0.87	0.44	0.29	0.87	0.44	0.29
54	10463	871	8.32	0.99	0.49	0.33	0.53	0.39	0.29
106	10465.8	252.12	2.41	0.99	0.50	0.33	0.90	0.48	0.33

TABLE 3a (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "1"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
116	10547.6	240.62	2.28	1.14	0.57	0.38	1.04	0.56	0.37
111	10673	699	6.55	1.36	0.68	0.45	0.85	0.58	0.42
73	10883	42.4	0.39	1.73	0.87	0.58	1.73	0.87	0.58
75	10900	1120.4	10.28	1.76	0.88	0.59	0.79	0.62	0.49
114	11100	475	4.28	2.12	1.06	0.71	1.62	0.98	0.68
109	11706.04	862.1	7.36	3.20	1.6	1.07	1.75	1.27	0.95
95	11890	583	4.9	3.53	1.76	1.18	2.45	1.57	1.11
105	12090.46	572.52	4.74	3.88	1.94	1.29	2.72	1.73	1.23
35	12790	350	2.74	5.13	2.57	1.71	4.35	2.45	1.67
112	13102.85	1680.23	12.82	5.69	2.84	1.90	1.80	1.58	1.34
113	13640	1949	14.29	6.65	3.32	2.22	1.84	1.66	1.45
62	64539.25*	1850.06	2.87	97.33	48.67	32.44	28.26	25.24	21.84
Mo [µg/L]									
105	10585.29	905	8.55	-	-	-	-	-	-
73	381705	3580	0.94	-	-	-	-	-	-
Na [µg/L]									
75	34521	5701.68	16.52	-	-	-	-	-	-
Ni (9890 ± 1120.60) [µg/L]									
67	2126*	98	4.61	-13.86	-6.93	-4.62	13.65	6.90	4.61
107	8330	152.6	1.83	-2.78	-1.39	-0.93	2.69	1.38	0.92
69	9300	300	3.23	-1.05	-0.53	-0.35	0.93	0.51	0.35
111	9332	406	4.35	-1.00	-0.50	-0.33	0.81	0.47	0.32
110	9507.8	404.2	4.25	-0.68	-0.34	-0.23	0.55	0.32	0.22
78	9750	461	4.73	-0.25	-0.12	-0.08	0.19	0.12	0.08
75	9857.6	295.9	3	-0.06	-0.03	-0.02	0.05	0.03	0.02
118	9871	809	8.2	-0.03	-0.02	-0.01	0.02	0.01	0.01
108	9879	189.8	1.92	-0.02	-0.01	-0.01	0.02	0.01	0.01
93	10030	344.7	3.44	0.25	0.12	0.08	0.21	0.12	0.08
72	10063	215	2.14	0.31	0.15	0.10	0.29	0.15	0.10
57	10082	588	5.83	0.34	0.17	0.11	0.24	0.15	0.11
106	10274.4	253.87	2.47	0.69	0.34	0.23	0.62	0.33	0.23
117	10300	200	1.94	0.73	0.37	0.24	0.69	0.36	0.24
103	10506.08	1098.2	10.45	1.10	0.55	0.37	0.50	0.39	0.31
73	10559	33	0.31	1.19	0.60	0.40	1.19	0.60	0.4
89	10590	279	2.63	1.25	0.62	0.42	1.12	0.61	0.41
104	10600	30	0.28	1.27	0.63	0.42	1.27	0.63	0.42
116	10604.4	214.4	2.02	1.28	0.64	0.43	1.19	0.63	0.42
114	10700	332	3.1	1.45	0.72	0.48	1.24	0.69	0.47
54	10768	298	2.77	1.57	0.78	0.52	1.38	0.76	0.51
95	10977	202	1.84	1.94	0.97	0.65	1.83	0.95	0.64
53	11216	933	8.32	2.37	1.18	0.79	1.22	0.91	0.69
35	11310	700	6.19	2.53	1.27	0.84	1.58	1.07	0.78
109	11503.08	677.73	5.89	2.88	1.44	0.96	1.83	1.23	0.89

TABLE 3a (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "1"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
105	11651.08	463.1	3.97	3.14	1.57	1.05	2.42	1.45	1.01
115	11791.2	1223.64	10.38	3.39	1.70	1.13	1.41	1.15	0.91
112	12164.97	1411.95	11.61	4.06	2.03	1.35	1.50	1.26	1.04
113	12267	1159	9.45	4.24	2.12	1.41	1.85	1.47	1.16
62	71547*	1630.52	2.28	110.04	55.02	36.68	35.76	31.16	26.33
Os [µg/L]									
75	5.2	0.4	7.69	-	-	-	-	-	-
105	128.833	5.41	4.2	-	-	-	-	-	-
Pb (9910 ± 1122.52) [µg/L]									
67	3980*	110	2.76	-10.57	-5.28	-3.52	10.37	5.26	3.51
118	5625*	466	8.28	-7.63	-3.82	-2.54	5.87	3.53	2.45
69	8400	400	4.76	-2.69	-1.35	-0.90	2.19	1.27	0.87
95	8693	843	9.7	-2.17	-1.08	-0.72	1.20	0.87	0.65
108	8798.2	136.4	1.55	-1.98	-0.99	-0.66	1.92	0.98	0.66
114	9210	234	2.54	-1.25	-0.62	-0.42	1.15	0.61	0.41
103	9383.756	758.15	8.08	-0.94	-0.47	-0.31	0.56	0.39	0.28
72	9510	242	2.54	-0.71	-0.36	-0.24	0.65	0.35	0.24
110	9540.2	621.74	6.52	-0.66	-0.33	-0.22	0.44	0.29	0.21
57	9828	114	1.16	-0.15	-0.07	-0.05	0.14	0.07	0.05
112	10535.02	1440.84	13.68	1.11	0.56	0.37	0.40	0.34	0.28
78	10558	500	4.74	1.15	0.58	0.38	0.86	0.53	0.37
107	10559	945.8	8.96	1.16	0.58	0.39	0.59	0.44	0.34
109	10698.67	1993.56	18.63	1.41	0.70	0.47	0.38	0.34	0.30
93	10860	651	5.99	1.69	0.85	0.56	1.11	0.73	0.53
75	10897.8	468	4.29	1.76	0.88	0.59	1.35	0.81	0.57
104	11000	30	0.27	1.94	0.97	0.65	1.94	0.97	0.65
116	11056.6	283.81	2.57	2.04	1.02	0.68	1.82	0.99	0.67
117	11200	200	1.79	2.30	1.15	0.77	2.17	1.13	0.76
106	11287.2	1395.12	12.36	2.45	1.23	0.82	0.92	0.77	0.63
54	11441	551	4.82	2.73	1.36	0.91	1.95	1.22	0.86
89	11832	1737	14.68	3.42	1.71	1.14	1.05	0.93	0.79
53	12284	355	2.89	4.23	2.11	1.41	3.57	2.02	1.38
113	12345	1355	10.98	4.34	2.17	1.45	1.66	1.38	1.13
105	12866.75	871.05	6.77	5.27	2.63	1.76	2.85	2.08	1.56
111	14168	1204	8.5	7.59	3.79	2.53	3.21	2.59	2.06
73	14891.8	37	0.25	8.88	4.44	2.96	8.86	4.44	2.96
35	15700	430	2.74	10.32	5.16	3.44	8.19	4.82	3.33
62	57819*	1440.35	2.49	85.36	42.68	28.45	30.99	26.24	21.62
Rb [µg/L]									
35	400	20	5	-	-	-	-	-	-
Ru [µg/L]									
72	1570	680	43.31	-	-	-	-	-	-

TABLE 3a (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "1"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
105	7106.299	882.36	12.42	-	-	-	-	-	-
				S [µg/L]					
75	9696.6	1605.4	16.56	-	-	-	-	-	-
105	18308.72	1072.54	5.86	-	-	-	-	-	-
112	21954.77	7602.85	34.63	-	-	-	-	-	-
67	35300	3200	9.07	-	-	-	-	-	-
111	37194	2251	6.05	-	-	-	-	-	-
69	41900	4000	9.55	-	-	-	-	-	-
				Sc [µg/L]					
35	5100	960	18.82	-	-	-	-	-	-
				Si [µg/L]					
73	3090706	7244.6	0.23	-	-	-	-	-	-
				Sn [µg/L]					
75	339.6	38.9	11.45	-	-	-	-	-	-
117	500	200	40	-	-	-	-	-	-
105	4507.253*	180.73	4.01	-	-	-	-	-	-
				Sr (9880 ± 1119.63) [µg/L]					
116	9564.6	187.21	1.96	-0.56	-0.28	-0.19	0.53	0.28	0.19
108	10037.2	161.9	1.61	0.28	0.14	0.09	0.27	0.14	0.09
72	10062	345	3.43	0.33	0.16	0.11	0.28	0.16	0.11
57	10270	256	2.49	0.70	0.35	0.23	0.63	0.34	0.23
107	10494	1009.2	9.62	1.10	0.55	0.37	0.53	0.41	0.31
104	10600	30	0.28	1.29	0.64	0.43	1.28	0.64	0.43
35	10610	360	3.39	1.30	0.65	0.43	1.10	0.62	0.43
118	10830	580	5.36	1.70	0.85	0.57	1.18	0.75	0.53
75	10902.6	1045.7	9.59	1.83	0.91	0.61	0.86	0.67	0.52
110	10915.8	803.61	7.36	1.85	0.93	0.62	1.06	0.75	0.56
103	10976.39	1086.56	9.9	1.96	0.98	0.65	0.90	0.70	0.55
93	11020	340.2	3.09	2.04	1.02	0.68	1.74	0.97	0.67
109	11145.15	2382.7	21.38	2.26	1.13	0.75	0.52	0.48	0.43
114	11400	435	3.82	2.72	1.36	0.91	2.14	1.27	0.88
54	11828	1401	11.84	3.48	1.74	1.16	1.29	1.09	0.89
106	11881.2	1641.51	13.82	3.57	1.79	1.19	1.15	1.01	0.85
89	12012	1766	14.7	3.81	1.90	1.27	1.15	1.02	0.87
53	12074	321	2.66	3.92	1.96	1.31	3.40	1.88	1.28
115	12217.04	490.85	4.02	4.17	2.09	1.39	3.14	1.91	1.34
78	12244	674	5.5	4.22	2.11	1.41	2.70	1.81	1.31
69	12300	700	5.69	4.32	2.16	1.44	2.70	1.83	1.33
105	12790.67	1050.02	8.21	5.20	2.60	1.73	2.45	1.90	1.47
95	12794	144	1.13	5.21	2.60	1.74	5.04	2.58	1.73
113	13027	1863	14.3	5.62	2.81	1.87	1.62	1.45	1.25

TABLE 3a (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "1"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
73	13647.2	29.2	0.21	6.73	3.36	2.24	6.72	3.36	2.24
111	18842*	1055	5.6	16.01	8.00	5.34	7.50	5.83	4.52
112	19379.68*	2883.15	14.88	16.97	8.48	5.66	3.23	3.07	2.85
67	28910*	270	0.93	33.99	17.00	11.33	30.62	16.52	11.19
62	64712*	1948.87	3.01	97.95	48.97	32.65	27.04	24.40	21.31
				Ta [µg/L]					
75	40.2	3	7.46	-	-	-	-	-	-
105	344.673	12	3.48	-	-	-	-	-	-
				Th [µg/L]					
105	18.619	6.23	33.48	-	-	-	-	-	-
				Ti [µg/L]					
75	143*	35.4	24.76	-	-	-	-	-	-
105	245.715*	29.81	12.13	-	-	-	-	-	-
95	4303	735	17.08	-	-	-	-	-	-
35	4600	590	12.83	-	-	-	-	-	-
111	5152	299	5.8	-	-	-	-	-	-
				Tl (9920 ± 1123.48) [µg/L]					
78	415*	35	8.43	-16.92	-8.46	-5.64	16.89	8.46	5.64
69	8500	300	3.53	-2.53	-1.26	-0.84	2.23	1.22	0.83
95	8736	406	4.65	-2.11	-1.05	-0.70	1.71	0.99	0.68
108	9045	228.5	2.53	-1.56	-0.78	-0.52	1.44	0.76	0.51
118	9071	214	2.36	-1.51	-0.76	-0.50	1.41	0.74	0.50
93	9108	367.8	4.04	-1.45	-0.72	-0.48	1.21	0.69	0.47
72	9469	258	2.72	-0.80	-0.40	-0.27	0.73	0.39	0.26
103	9927.026	998.47	10.06	0.01	0.01	0.00	0.01	0.00	0.00
57	10078	102	1.01	0.28	0.14	0.09	0.28	0.14	0.09
106	10103.8	389.69	3.86	0.33	0.16	0.11	0.27	0.15	0.11
73	10143.2	28.8	0.28	0.40	0.20	0.13	0.4	0.20	0.13
110	10480.8	625.39	5.97	1.00	0.50	0.33	0.67	0.44	0.31
111	10576	632	5.98	1.17	0.58	0.39	0.78	0.51	0.36
117	10600	500	4.72	1.21	0.61	0.40	0.90	0.55	0.39
109	10600.81	535.76	5.05	1.21	0.61	0.40	0.88	0.55	0.39
75	10614.4	997.9	9.4	1.24	0.62	0.41	0.61	0.46	0.35
89	10642	629	5.91	1.29	0.64	0.43	0.86	0.56	0.40
107	10807	574.9	5.32	1.58	0.79	0.53	1.10	0.70	0.50
116	10911.2	98.98	0.91	1.76	0.88	0.59	1.74	0.88	0.59
104	11200	30	0.27	2.28	1.14	0.76	2.28	1.14	0.76
54	11576	1081	9.34	2.95	1.47	0.98	1.36	1.06	0.83
53	11759	822	6.99	3.27	1.64	1.09	1.85	1.32	0.98
105	12138.84	443.6	3.65	3.95	1.97	1.32	3.10	1.84	1.27
113	15496*	1543	9.96	9.93	4.96	3.31	3.40	2.92	2.44
35	17970*	490	2.73	14.33	7.17	4.78	10.8	6.57	4.59

TABLE 3a (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "1"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
112	19059.73*	2611.46	13.7	16.27	8.14	5.42	3.42	3.21	2.94
62	64938.75*	2502.86	3.85	97.94	48.97	32.65	21.45	20.05	18.23
				V [µg/L]					
75	10	0.7	7	-	-	-	-	-	-
105	61.39	17.13	27.9	-	-	-	-	-	-
111	2171	94	4.33	-	-	-	-	-	-
35	3030	300	9.9	-	-	-	-	-	-
				Y [µg/L]					
105	4.33	1.9	43.86	-	-	-	-	-	-
				Zn (9890 ± 1120.60) [µg/L]					
67	2674*	870	32.54	-12.88	-6.44	-4.29	6.97	5.09	3.81
107	8155*	108.1	1.33	-3.10	-1.55	-1.03	3.04	1.54	1.03
110	9164	401.06	4.38	-1.30	-0.65	-0.43	1.05	0.61	0.42
115	9621.28	492.12	5.11	-0.48	-0.24	-0.16	0.36	0.22	0.15
93	9680	306.4	3.17	-0.37	-0.19	-0.12	0.33	0.18	0.12
114	9780	295	3.02	-0.20	-0.10	-0.07	0.17	0.09	0.06
118	9831	566	5.76	-0.11	-0.05	-0.04	0.07	0.05	0.03
69	9900	200	2.02	0.02	0.01	0.01	0.02	0.01	0.01
75	9935.6	290.1	2.92	0.08	0.04	0.03	0.07	0.04	0.03
57	10009	497	4.97	0.21	0.11	0.07	0.16	0.10	0.07
108	10037.6	176.9	1.76	0.26	0.13	0.09	0.25	0.13	0.09
89	10139	245	2.42	0.44	0.22	0.15	0.41	0.22	0.15
72	10254	104	1.01	0.65	0.32	0.22	0.64	0.32	0.22
116	10267.6	204.48	1.99	0.67	0.34	0.22	0.63	0.33	0.22
78	10291	222	2.16	0.72	0.36	0.24	0.67	0.35	0.24
117	10300	200	1.94	0.73	0.37	0.24	0.69	0.36	0.24
106	10426.4	247.67	2.38	0.96	0.48	0.32	0.88	0.47	0.32
95	10564	135	1.28	1.20	0.60	0.40	1.17	0.60	0.40
104	10600	30	0.28	1.27	0.63	0.42	1.27	0.63	0.42
54	10709	282	2.63	1.46	0.73	0.49	1.31	0.71	0.48
35	10800	710	6.57	1.62	0.81	0.54	1.01	0.69	0.50
73	10860	30.2	0.28	1.73	0.87	0.58	1.73	0.87	0.58
103	10960.96	927.68	8.46	1.91	0.96	0.64	0.99	0.74	0.56
53	10998	995	9.05	1.98	0.99	0.66	0.97	0.74	0.57
109	11017.32	732.89	6.65	2.01	1.01	0.67	1.22	0.84	0.61
113	11023	855	7.76	2.02	1.01	0.67	1.11	0.80	0.60
105	11230.5	439.04	3.91	2.39	1.20	0.80	1.88	1.11	0.77
112	11843.03	704.1	5.95	3.49	1.74	1.16	2.17	1.48	1.07
111	14035*	570	4.06	7.40	3.70	2.47	5.19	3.30	2.34
62	60166.5*	1301.81	2.16	89.73	44.87	29.91	35.47	29.27	23.65

TABLE 3b. SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "2"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
				Ag [µg/L]					
95	368	147	39.95	-	-	-	-	-	-
108	1067.8	119.5	11.19	-	-	-	-	-	-
105	4834.146	629.66	13.03	-	-	-	-	-	-
				Al [µg/L]					
75	491	111.01	22.61	-	-	-	-	-	-
108	3136	226.3	7.22	-	-	-	-	-	-
105	6197.396	1288.59	20.79	-	-	-	-	-	-
				As [µg/L]					
75	3.8	1.1	28.95	-	-	-	-	-	-
117	4	1	25	-	-	-	-	-	-
				Ba (335.78 ± 63.30) [µg/L]					
69	29	1	3.45	-9.69	-4.85	-3.23	9.69	4.85	3.23
62	69.2	25.76	37.23	-8.42	-4.21	-2.81	6.53	3.9	2.71
106	103	14.93	14.5	-7.35	-3.68	-2.45	6.65	3.58	2.42
116	144.8	9.07	6.26	-6.03	-3.02	-2.01	5.80	2.99	2.00
72	205	46	22.44	-4.13	-2.07	-1.38	2.34	1.67	1.24
118	212	34	16.04	-3.91	-1.96	-1.30	2.66	1.72	1.23
54	266	17	6.39	-2.20	-1.10	-0.73	1.94	1.06	0.72
75	340.2	58.2	17.11	0.14	0.07	0.05	0.07	0.05	0.04
107	346.4	67.5	19.49	0.34	0.17	0.11	0.14	0.11	0.09
89	358.2	122.5	34.2	0.71	0.35	0.24	0.18	0.16	0.14
73	366.2	39.2	10.7	0.96	0.48	0.32	0.60	0.41	0.30
117	510	160	31.37	5.50	2.75	1.83	1.07	1.01	0.94
108	568.2	97.3	17.12	7.34	3.67	2.45	2.27	2.00	1.71
53	627	117	18.66	9.20	4.60	3.07	2.4	2.19	1.93
109	891.562	102.32	11.48	17.56	8.78	5.85	5.19	4.62	3.98
105	1230.224*	182.55	14.84	28.26	14.13	9.42	4.83	4.63	4.35
				Bi [µg/L]					
89	8.4	3.9	46.43	-	-	-	-	-	-
105	23.858	1.28	5.35	-	-	-	-	-	-
108	118	0	0	-	-	-	-	-	-
				Ca (3452.61 ± 458.34) [µg/L]					
62	548.8	77.29	14.08	-12.67	-6.34	-4.22	12.01	6.25	4.20
69	1100	200	18.18	-10.27	-5.13	-3.42	7.73	4.70	3.29
57	1165	47	4.03	-9.98	-4.99	-3.33	9.78	4.97	3.32
116	1666	129.85	7.79	-7.80	-3.90	-2.60	6.78	3.75	2.55
118	2225	37	1.66	-5.36	-2.68	-1.79	5.29	2.67	1.78

TABLE 3b (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "2"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
106	2257.8	107.81	4.78	-5.21	-2.61	-1.74	4.72	2.54	1.72
72	2378	345	14.51	-4.69	-2.34	-1.56	2.59	1.87	1.40
54	2730	414	15.16	-3.15	-1.58	-1.05	1.53	1.17	0.90
95	3216	1137	35.35	-1.03	-0.52	-0.34	0.20	0.19	0.18
35	3340	420	12.57	-0.49	-0.25	-0.16	0.24	0.18	0.14
75	4898.4	796.9	16.27	6.31	3.15	2.10	1.74	1.57	1.37
117	5400	800	14.81	8.50	4.25	2.83	2.34	2.11	1.85
107	6548.8	824.9	12.6	13.51	6.76	4.50	3.62	3.28	2.88
73	6867.6	269	3.92	14.90	7.45	4.97	9.66	6.43	4.63
89	7447.8	1505.6	20.22	17.43	8.72	5.81	2.62	2.54	2.41
108	14263*	1663.8	11.67	47.17	23.59	15.72	6.44	6.26	6.00
105	14906.97*	2428.87	16.29	49.98	24.99	16.66	4.70	4.63	4.54
93	15810*	3205	20.27	53.92	26.96	17.97	3.85	3.82	3.77
104	35200*	7400	21.02	138.53	69.27	46.18	4.29	4.28	4.27
Cd (304.22 ± 58.21) [µg/L]									
75	168.2	29.6	17.6	-4.67	-2.34	-1.56	3.28	2.08	1.48
116	180.7	26.81	14.84	-4.24	-2.12	-1.41	3.12	1.93	1.35
95	338	136	40.24	1.16	0.58	0.39	0.24	0.23	0.21
117	530	150	28.3	7.76	3.88	2.59	1.48	1.40	1.30
104	4700*	1900	40.43	151.03	75.52	50.34	2.31	2.31	2.31
Cl (1955.23 ± 282.75) [µg/L]									
106	179.6	37.81	21.05	-12.56	-6.28	-4.19	12.13	6.22	4.17
118	362	18	4.97	-11.27	-5.63	-3.76	11.18	5.62	3.75
69	620	80	12.9	-9.44	-4.72	-3.15	8.22	4.54	3.09
72	1066	131	12.29	-6.29	-3.14	-2.1	4.61	2.85	2.00
73	2216.2	177.2	8	1.85	0.92	0.62	1.15	0.78	0.57
105	2564.416	595.98	23.24	4.31	2.15	1.44	0.99	0.92	0.83
75	2641.6	501.5	18.98	4.85	2.43	1.62	1.32	1.19	1.05
109	3437.626	389.35	11.33	10.49	5.24	3.50	3.58	3.08	2.57
108	4509.6	571.4	12.67	18.07	9.03	6.02	4.34	4.01	3.59
53	7614*	726	9.54	40.03	20.01	13.34	7.65	7.26	6.73
104	17400*	4400	25.29	109.25	54.62	36.42	3.51	3.50	3.49
Co (274.5 ± 53.34) [µg/L]									
69	42	13	30.95	-8.72	-4.36	-2.91	7.84	4.23	2.87
119	51.679	10.34	20	-8.35	-4.18	-2.78	7.79	4.10	2.76
106	81.4	8.44	10.37	-7.24	-3.62	-2.41	6.90	3.58	2.40
118	88	4	4.55	-6.99	-3.50	-2.33	6.92	3.49	2.33
103	92.2	65.09	70.59	-6.84	-3.42	-2.28	2.59	2.17	1.77
54	154	23	14.94	-4.52	-2.26	-1.51	3.42	2.07	1.45
116	159.1	12.98	8.16	-4.33	-2.16	-1.44	3.89	2.10	1.42
62	171.4	53.93	31.46	-3.87	-1.93	-1.29	1.71	1.36	1.07
113	189	84	44.44	-3.21	-1.60	-1.07	0.97	0.86	0.74
72	217	32	14.75	-2.16	-1.08	-0.72	1.38	0.92	0.67

TABLE 3b (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "2"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
73	236.8	12.6	5.32	-1.41	-0.71	-0.47	1.28	0.69	0.47
57	252.3	6.1	2.42	-0.83	-0.42	-0.28	0.81	0.41	0.28
107	253.2	30	11.85	-0.80	-0.40	-0.27	0.53	0.35	0.25
75	272.6	39.5	14.49	-0.07	-0.04	-0.02	0.04	0.03	0.02
117	340	60	17.65	2.46	1.23	0.82	1.00	0.82	0.65
95	389	118	30.33	4.29	2.15	1.43	0.95	0.88	0.80
89	390.2	89	22.81	4.34	2.17	1.45	1.25	1.12	0.97
109	477.783	30.9	6.47	7.62	3.81	2.54	4.98	3.30	2.37
114	487	114	23.41	7.97	3.98	2.66	1.82	1.69	1.53
53	497	75	15.09	8.34	4.17	2.78	2.80	2.42	2.03
108	505.4	76.6	15.16	8.66	4.33	2.89	2.85	2.47	2.08
93	692	158.3	22.88	15.65	7.83	5.22	2.60	2.50	2.35
105	982.335*	150.62	15.33	26.54	13.27	8.85	4.63	4.43	4.15
104	1500*	350	23.33	45.95	22.97	15.32	3.49	3.46	3.41
			Cr (144.99 ± 31.02) [µg/L]						
119	16.765	3.35	20	-8.27	-4.13	-2.76	8.08	4.11	2.75
106	39.6	5.41	13.67	-6.80	-3.40	-2.27	6.42	3.35	2.25
62	56.6	8.9	15.73	-5.70	-2.85	-1.90	4.94	2.74	1.87
108	60.6	6.1	10.07	-5.44	-2.72	-1.81	5.06	2.67	1.80
116	126.36	3.83	3.03	-1.20	-0.60	-0.40	1.17	0.60	0.40
107	133.2	16.1	12.09	-0.76	-0.38	-0.25	0.53	0.34	0.24
54	135	14	10.37	-0.64	-0.32	-0.21	0.48	0.29	0.21
118	140	4	2.86	-0.32	-0.16	-0.11	0.31	0.16	0.11
72	152	12	7.89	0.45	0.23	0.15	0.36	0.21	0.15
73	154.6	12.6	8.15	0.62	0.31	0.21	0.48	0.29	0.20
113	164	37	22.56	1.23	0.61	0.41	0.47	0.39	0.32
117	180	20	11.11	2.26	1.13	0.75	1.38	0.95	0.69
109	187.307	23.65	12.63	2.73	1.36	0.91	1.50	1.08	0.81
75	191.8	24.9	12.98	3.02	1.51	1.01	1.60	1.18	0.89
89	196.2	22.7	11.57	3.30	1.65	1.10	1.86	1.33	0.99
93	198	22.87	11.55	3.42	1.71	1.14	1.92	1.38	1.02
53	216	28	12.96	4.58	2.29	1.53	2.22	1.70	1.31
57	261.7	19.7	7.53	7.53	3.76	2.51	4.66	3.18	2.31
104	500*	160	32	22.89	11.45	7.63	2.21	2.18	2.13
105	568.416*	51.96	9.14	27.30	13.65	9.10	7.81	7.00	6.07
			Cu (248.2 ± 48.97) [µg/L]						
62	31.2	0.45	1.43	-8.86	-4.43	-2.95	8.86	4.43	2.95
69	42	15	35.71	-8.42	-4.21	-2.81	7.18	4.03	2.75
119	52.996	10.6	20	-7.97	-3.99	-2.66	7.32	3.90	2.63
35	90	40	44.44	-6.46	-3.23	-2.15	3.37	2.50	1.89
106	100.2	5.02	5.01	-6.04	-3.02	-2.01	5.92	3.01	2.01
113	144	34	23.61	-4.26	-2.13	-1.42	2.49	1.75	1.29
116	149.34	10.37	6.95	-4.04	-2.02	-1.35	3.72	1.98	1.33
54	168	26	15.48	-3.28	-1.64	-1.09	2.25	1.45	1.03

TABLE 3b (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "2"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
118	218	11	5.05	-1.23	-0.62	-0.41	1.13	0.60	0.41
72	222	26	11.71	-1.07	-0.54	-0.36	0.73	0.47	0.34
107	229.2	21.1	9.21	-0.78	-0.39	-0.26	0.59	0.36	0.25
103	234.293	62.58	26.71	-0.57	-0.28	-0.19	0.21	0.18	0.14
57	254.9	17.5	6.87	0.27	0.14	0.09	0.22	0.13	0.09
73	265.6	12.6	4.74	0.71	0.36	0.24	0.63	0.34	0.23
75	273.2	41.9	15.34	1.02	0.51	0.34	0.52	0.39	0.30
95	303	124	40.92	2.24	1.12	0.75	0.43	0.41	0.38
117	320	60	18.75	2.93	1.47	0.98	1.11	0.93	0.76
114	365	73	20	4.77	2.39	1.59	1.52	1.33	1.13
89	376.2	78	20.73	5.23	2.61	1.74	1.57	1.39	1.19
108	421.8	46.6	11.05	7.09	3.55	2.36	3.30	2.57	2.00
93	463.7	90.05	19.42	8.80	4.40	2.93	2.31	2.10	1.85
109	488.912	41.06	8.4	9.83	4.92	3.28	5.04	3.77	2.86
53	495	80	16.16	10.08	5.04	3.36	2.95	2.63	2.27
105	966.069*	128.66	13.32	29.32	14.66	9.77	5.48	5.21	4.85
104	1100*	300	27.27	34.79	17.39	11.6	2.83	2.80	2.76
			Fe (122.47 ± 26.87) [µg/L]						
119	16.093	3.22	20	-7.92	-3.96	-2.64	7.70	3.93	2.63
62	33.4	6.03	18.04	-6.63	-3.31	-2.21	6.05	3.23	2.19
116	34.686	2.91	8.39	-6.53	-3.27	-2.18	6.39	3.25	2.17
107	39.4	3.9	9.9	-6.18	-3.09	-2.06	5.94	3.06	2.05
72	58	19	32.76	-4.80	-2.40	-1.60	2.77	1.96	1.45
109	66.929	10.33	15.44	-4.13	-2.07	-1.38	3.28	1.93	1.33
108	69	27.1	39.28	-3.98	-1.99	-1.33	1.77	1.40	1.10
75	72.6	6.8	9.37	-3.71	-1.86	-1.24	3.31	1.80	1.22
106	88	33.04	37.54	-2.57	-1.28	-0.86	0.97	0.81	0.66
35	100	10	10	-1.67	-0.84	-0.56	1.34	0.78	0.54
69	100	200	200	-1.67	-0.84	-0.56	0.11	0.11	0.11
93	123.3	16.33	13.24	0.06	0.03	0.02	0.04	0.03	0.02
73	140.2	9.4	6.7	1.32	0.66	0.44	1.08	0.62	0.43
118	168	4	2.38	3.39	1.69	1.13	3.25	1.68	1.12
95	195	44	22.56	5.40	2.70	1.80	1.58	1.41	1.22
105	203.116	25.67	12.64	6.00	3.00	2.00	2.78	2.17	1.69
54	252	73	28.97	9.64	4.82	3.21	1.75	1.67	1.55
57	275.2	18	6.54	11.37	5.68	3.79	6.80	4.72	3.46
53	292	60	20.55	12.62	6.31	4.21	2.76	2.58	2.35
117	400*	100	25	20.66	10.33	6.89	2.75	2.68	2.57
89	416.2*	404.1	97.09	21.86	10.93	7.29	0.73	0.73	0.72
114	532*	160	30.08	30.48	15.24	10.16	2.55	2.52	2.48
104	1000*	300	30	65.31	32.66	21.77	2.92	2.91	2.90
103	2417.954*	466.6	19.3	170.84	85.42	56.95	4.92	4.91	4.90
			K (704.1 ± 118.74) [µg/L]						
119	94.844	18.97	20	-10.26	-5.13	-3.42	9.78	5.07	3.40

TABLE 3b (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "2"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
69	150	250	166.67	-9.33	-4.67	-3.11	2.16	2.00	1.81
72	229	47.2	20.61	-8.00	-4.00	-2.67	6.26	3.72	2.58
54	282	81	28.72	-7.11	-3.55	-2.37	4.20	2.94	2.16
116	311.72	21.98	7.05	-6.61	-3.30	-2.2	6.20	3.25	2.19
75	430.8	97.5	22.63	-4.60	-2.30	-1.53	2.39	1.78	1.35
73	687.8	62	9.01	-0.27	-0.14	-0.09	0.19	0.12	0.09
108	740.6	124.4	16.8	0.61	0.31	0.20	0.26	0.21	0.17
109	795.429	53.59	6.74	1.54	0.77	0.51	1.14	0.7	0.49
117	800	200	25	1.62	0.81	0.54	0.46	0.41	0.36
106	966.6	187.28	19.37	4.42	2.21	1.47	1.34	1.18	1.02
53	1154	323	27.99	7.58	3.79	2.53	1.37	1.31	1.22
93	1347.3	335.05	24.87	10.83	5.42	3.61	1.89	1.81	1.70
105	1867.345	825.02	44.18	19.59	9.80	6.53	1.41	1.40	1.38
				Mg [µg/L]					
75	6505	1391.1	21.39	-	-	-	-	-	-
108	14727.4	2591.5	17.6	-	-	-	-	-	-
72	17106	4900	28.64	-	-	-	-	-	-
				Mn (291.23 ± 56.09) [µg/L]					
69	31	11	35.48	-9.28	-4.64	-3.09	8.64	4.55	3.07
119	55.003	11	20	-8.42	-4.21	-2.81	7.84	4.13	2.78
106	92.2	8.32	9.02	-7.10	-3.55	-2.37	6.80	3.51	2.35
35	120	10	8.33	-6.11	-3.05	-2.04	5.75	3.01	2.02
118	161	6	3.73	-4.64	-2.32	-1.55	4.54	2.31	1.54
116	161.62	14.17	8.77	-4.62	-2.31	-1.54	4.13	2.24	1.52
54	166	30	18.07	-4.47	-2.23	-1.49	3.05	1.97	1.40
113	176	73	41.48	-4.11	-2.05	-1.37	1.47	1.25	1.03
62	198.8	30.42	15.3	-3.30	-1.65	-1.10	2.23	1.45	1.03
72	222	37	16.67	-2.47	-1.23	-0.82	1.49	1.03	0.75
57	246.3	21.5	8.73	-1.60	-0.80	-0.53	1.27	0.75	0.52
73	266.4	16	6.01	-0.89	-0.44	-0.30	0.77	0.43	0.29
107	271.4	26.7	9.84	-0.71	-0.35	-0.24	0.51	0.32	0.22
75	278.8	42.3	15.17	-0.44	-0.22	-0.15	0.24	0.18	0.13
117	340	60	17.65	1.74	0.87	0.58	0.74	0.59	0.47
89	400	87.3	21.83	3.88	1.94	1.29	1.19	1.05	0.90
53	478	60	12.55	6.66	3.33	2.22	2.82	2.27	1.81
114	486	148	30.45	6.94	3.47	2.31	1.29	1.23	1.14
95	509	251	49.31	7.76	3.88	2.59	0.86	0.85	0.82
109	518.846	42.67	8.22	8.12	4.06	2.71	4.46	3.23	2.41
108	524.8	76.3	14.54	8.33	4.16	2.78	2.87	2.47	2.06
93	703.8	159.95	22.73	14.71	7.36	4.90	2.54	2.43	2.28
105	987.995*	160.88	16.28	24.84	12.42	8.28	4.27	4.09	3.84
104	1600*	400	25	46.67	23.33	15.56	3.26	3.24	3.20

TABLE 3b (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "2"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
				Mo [µg/L]					
105	1386.92	581.91	41.96	-	-	-	-	-	-
73	7522	1543.4	20.52	-	-	-	-	-	-
				Na [µg/L]					
75	5333.5	2310.1	43.31	-	-	-	-	-	-
				Ni (256.41 ± 50.34) [µg/L]					
69	53	22	41.51	-8.08	-4.04	-2.69	6.08	3.70	2.59
119	53.411	10.68	20	-8.06	-4.03	-2.69	7.42	3.94	2.66
118	87	8	9.2	-6.73	-3.37	-2.24	6.41	3.32	2.23
35	100	10	10	-6.21	-3.11	-2.07	5.77	3.05	2.05
106	128.6	8.88	6.9	-5.08	-2.54	-1.69	4.79	2.50	1.68
103	144.311	58.11	40.27	-4.45	-2.23	-1.48	1.77	1.46	1.18
54	150	42	28	-4.23	-2.11	-1.41	2.17	1.62	1.23
113	156	19	12.18	-3.99	-1.99	-1.33	3.18	1.87	1.29
116	156.04	12.21	7.83	-3.99	-1.99	-1.33	3.59	1.94	1.31
62	177.6	31.6	17.8	-3.13	-1.57	-1.04	1.95	1.33	0.96
72	204	27	13.24	-2.08	-1.04	-0.69	1.42	0.92	0.65
73	229.2	11.4	4.97	-1.08	-0.54	-0.36	0.98	0.53	0.36
57	250.6	15.4	6.15	-0.23	-0.12	-0.08	0.20	0.11	0.08
107	264.2	30	11.36	0.31	0.15	0.10	0.20	0.13	0.10
75	266.4	39.4	14.79	0.40	0.20	0.13	0.21	0.16	0.12
95	332	70	21.08	3.00	1.50	1.00	1.02	0.88	0.73
117	340	50	14.71	3.32	1.66	1.11	1.49	1.18	0.92
89	409.6	98.7	24.1	6.09	3.04	2.03	1.50	1.38	1.23
53	494	68	13.77	9.44	4.72	3.15	3.28	2.81	2.34
114	501	145	28.94	9.72	4.86	3.24	1.66	1.59	1.50
108	535.8	80.4	15.01	11.10	5.55	3.70	3.32	2.95	2.53
93	608.2	142.65	23.45	13.98	6.99	4.66	2.43	2.33	2.18
105	987.525*	160.9	16.29	29.05	14.52	9.68	4.49	4.34	4.11
104	1600*	400	25	53.38	26.69	17.79	3.35	3.33	3.3
				Os [µg/L]					
105	8.189	1	12.26	-	-	-	-	-	-
				P [µg/L]					
75	533.2	86.5	16.22	-	-	-	-	-	-
				Pb (260.38 ± 51.00) [µg/L]					
69	46	12	26.09	-8.41	-4.20	-2.80	7.61	4.09	2.77
62	100.6	5.41	5.38	-6.27	-3.13	-2.09	6.13	3.12	2.08
106	114.2	9.47	8.29	-5.73	-2.87	-1.91	5.37	2.82	1.90
54	158	18	11.39	-4.01	-2.01	-1.34	3.28	1.89	1.30
116	165.82	6.98	4.21	-3.71	-1.85	-1.24	3.58	1.84	1.23

TABLE 3b (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "2"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
95	183	98	53.55	-3.03	-1.52	-1.01	0.76	0.70	0.62
113	200	55	27.5	-2.37	-1.18	-0.79	1.00	0.80	0.64
72	213	28	13.15	-1.86	-0.93	-0.62	1.25	0.81	0.58
107	220.4	28.7	13.02	-1.57	-0.78	-0.52	1.04	0.68	0.49
103	222.52	43.65	19.61	-1.48	-0.74	-0.49	0.75	0.56	0.43
57	247.3	11.8	4.77	-0.51	-0.26	-0.17	0.47	0.25	0.17
75	281.8	45.4	16.11	0.84	0.42	0.28	0.41	0.31	0.24
73	296	13.4	4.53	1.40	0.70	0.47	1.24	0.68	0.46
117	320	60	18.75	2.34	1.17	0.78	0.91	0.76	0.61
89	323.4	68.6	21.21	2.47	1.24	0.82	0.86	0.74	0.61
108	350.2	29.5	8.42	3.52	1.76	1.17	2.30	1.52	1.10
109	423.267	41.8	9.88	6.39	3.19	2.13	3.33	2.47	1.87
53	501	66	13.17	9.44	4.72	3.15	3.40	2.88	2.38
93	580.8	120.9	20.82	12.56	6.28	4.19	2.59	2.44	2.24
105	1027.694*	143.12	13.93	30.09	15.04	10.03	5.28	5.05	4.73
104	1300*	300	23.08	40.77	20.38	13.59	3.45	3.42	3.36
				Ru [µg/L]					
72	1304	142	10.89	-	-	-	-	-	-
				S [µg/L]					
75	372.6	68.9	18.49	-	-	-	-	-	-
69	390	160	41.03	-	-	-	-	-	-
105	2796.748	526.3	18.82	-	-	-	-	-	-
67	3230	780	24.15	-	-	-	-	-	-
				Si [µg/L]					
73	5129034	164895.2	3.21	-	-	-	-	-	-
				Sn [µg/L]					
105	326.734	107.91	33.03	-	-	-	-	-	-
				Sr (278.78 ± 54.05) [µg/L]					
69	83	6	7.23	-7.24	-3.62	-2.41	7.07	3.60	2.41
35	100	30	30	-6.62	-3.31	-2.21	4.43	2.89	2.07
116	138	8.19	5.94	-5.21	-2.60	-1.74	4.99	2.58	1.73
106	157.2	14.24	9.06	-4.50	-2.25	-1.50	3.98	2.18	1.48
62	168.6	25.17	14.93	-4.08	-2.04	-1.36	2.98	1.85	1.30
72	182	26	14.29	-3.58	-1.79	-1.19	2.58	1.61	1.14
54	201	64	31.84	-2.88	-1.44	-0.96	1.12	0.93	0.75
113	206	71	34.47	-2.69	-1.35	-0.90	0.96	0.82	0.68
73	207.4	10.6	5.11	-2.64	-1.32	-0.88	2.46	1.30	0.87
103	232.227	69.36	29.87	-1.72	-0.86	-0.57	0.63	0.53	0.44
57	245.6	10.9	4.44	-1.23	-0.61	-0.41	1.14	0.60	0.41
75	255.4	41.6	16.29	-0.87	-0.43	-0.29	0.47	0.34	0.26
107	272.6	37.3	13.68	-0.23	-0.11	-0.08	0.13	0.09	0.07

TABLE 3b (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "2"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
117	370	50	13.51	3.38	1.69	1.13	1.60	1.24	0.96
95	395	142	35.95	4.30	2.15	1.43	0.80	0.76	0.71
109	440.729	33.92	7.7	5.99	3.00	2.00	3.73	2.54	1.84
53	516	55	10.66	8.78	4.39	2.93	3.87	3.08	2.42
108	548.6	72.3	13.18	9.98	4.99	3.33	3.50	2.99	2.48
93	577.5	132.19	22.89	11.05	5.53	3.68	2.21	2.09	1.93
105	1049.612*	151.95	14.48	28.52	14.26	9.51	4.99	4.78	4.48
104	1900*	400	21.05	59.99	30.00	20.00	4.04	4.02	3.97
				Ti [µg/L]					
119	19.604	3.92	20	-	-	-	-	-	-
75	21.4	8.9	41.59	-	-	-	-	-	-
105	43.909*	26.39	60.09	-	-	-	-	-	-
93	133.8*	29.03	21.7	-	-	-	-	-	-
104	1090*	330	30.28	-	-	-	-	-	-
				Tl (258.3 ± 50.66) [µg/L]					
69	27	2	7.41	-9.13	-4.57	-3.04	9.10	4.56	3.04
106	97.2	10.23	10.53	-6.36	-3.18	-2.12	5.90	3.12	2.10
62	135.2	31.22	23.09	-4.86	-2.43	-1.62	3.06	2.07	1.50
113	166	34	20.48	-3.64	-1.82	-1.21	2.18	1.51	1.11
116	178.58	6.9	3.87	-3.15	-1.57	-1.05	3.04	1.56	1.04
54	188	28	14.89	-2.78	-1.39	-0.93	1.86	1.21	0.87
72	192	25	13.02	-2.62	-1.31	-0.87	1.86	1.17	0.83
107	198.6	41.3	20.8	-2.36	-1.18	-0.79	1.23	0.91	0.69
73	228.4	10.8	4.73	-1.18	-0.59	-0.39	1.09	0.58	0.39
57	248.9	5.6	2.25	-0.37	-0.19	-0.12	0.36	0.18	0.12
103	261.113	56.23	21.54	0.11	0.06	0.04	0.05	0.04	0.03
75	266.4	40.5	15.2	0.32	0.16	0.11	0.17	0.12	0.09
95	291	126	43.3	1.29	0.65	0.43	0.25	0.24	0.22
117	390	60	15.38	5.20	2.60	1.73	2.02	1.68	1.36
109	452.667	36.54	8.07	7.67	3.84	2.56	4.37	3.11	2.31
108	495	76.5	15.45	9.35	4.67	3.12	2.94	2.58	2.20
53	575	60	10.43	12.50	6.25	4.17	4.86	4.03	3.27
93	768.3*	149.2	19.42	20.14	10.07	6.71	3.37	3.24	3.05
105	1016.03*	165.55	16.29	29.92	14.96	9.97	4.52	4.38	4.16
104	2010*	450	22.39	69.16	34.58	23.05	3.89	3.87	3.84
				Zn (292.78 ± 56.35) [µg/L]					
69	42	5	11.9	-8.90	-4.45	-2.97	8.76	4.43	2.96
119	59.842	11.97	20	-8.27	-4.13	-2.76	7.61	4.04	2.73
35	120	10	8.33	-6.13	-3.07	-2.04	5.78	3.02	2.03
62	126.8	6.87	5.42	-5.89	-2.95	-1.96	5.72	2.92	1.96
106	157	8.52	5.42	-4.82	-2.41	-1.61	4.61	2.38	1.60
54	170	24	14.12	-4.36	-2.18	-1.45	3.32	2.00	1.40
116	170.42	11.36	6.66	-4.34	-2.17	-1.45	4.03	2.13	1.43

TABLE 3b (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "2"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
113	185	59	31.89	-3.83	-1.91	-1.28	1.65	1.32	1.05
72	223	28	12.56	-2.48	-1.24	-0.83	1.76	1.11	0.78
118	231	15	6.49	-2.19	-1.10	-0.73	1.94	1.06	0.72
107	245.4	23.1	9.41	-1.68	-0.84	-0.56	1.30	0.78	0.54
57	252.2	13.4	5.31	-1.44	-0.72	-0.48	1.30	0.70	0.47
75	299	46.7	15.62	0.22	0.11	0.07	0.11	0.08	0.06
73	318.2	14.4	4.53	0.90	0.45	0.30	0.8	0.44	0.30
117	320	60	18.75	0.97	0.48	0.32	0.41	0.33	0.26
95	353	147	41.64	2.14	1.07	0.71	0.40	0.38	0.36
103	378.661	82.18	21.7	3.05	1.52	1.02	0.99	0.86	0.73
89	389.2	80.9	20.79	3.42	1.71	1.14	1.13	0.98	0.82
108	501.8	49.3	9.82	7.42	3.71	2.47	3.68	2.79	2.14
53	508	30	5.91	7.64	3.82	2.55	5.23	3.37	2.40
109	511.714	35.87	7.01	7.77	3.89	2.59	4.80	3.28	2.38
93	570.7	100.5	17.61	9.86	4.93	3.29	2.66	2.41	2.12
114	601	117	19.47	10.94	5.47	3.65	2.56	2.37	2.14
105	1007.172*	142.7	14.17	25.36	12.68	8.45	4.91	4.66	4.31
104	1140*	300	26.32	30.07	15.04	10.02	2.81	2.78	2.72

TABLE 3c. SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "3"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
				Ag [µg/L]					
105	433.099	38.4	8.87	-	-	-	-	-	-
				Al [µg/L]					
75	414.25	158.9	38.36	-	-	-	-	-	-
105	848.327	133.69	15.76	-	-	-	-	-	-
108	2310.2	885.8	38.34	-	-	-	-	-	-
				As [µg/L]					
105	1.382	0.22	15.92	-	-	-	-	-	-
75	1.4	0.5	35.71	-	-	-	-	-	-
117	3*	0.6	20	-	-	-	-	-	-
				Ba (28.94 ± 6.37) [µg/L]					
116	7.48	1.69	22.59	-6.74	-3.37	-2.25	5.95	3.26	2.21
75	7.5	2.5	33.33	-6.73	-3.37	-2.24	5.30	3.13	2.17
109	37.734	5.7	15.1	2.76	1.38	0.92	1.35	1.03	0.79
117	40	6	15	3.47	1.74	1.16	1.63	1.26	0.98
62	52	14.14	27.2	7.24	3.62	2.41	1.59	1.49	1.35
				Bi [µg/L]					
62	104	40	38.46	-	-	-	-	-	-
				Br (50.26 ± 11.06) [µg/L]					
103	25.3	1.99	7.87	-4.51	-2.26	-1.50	4.25	2.22	1.49
114	35.4	10.1	28.53	-2.69	-1.34	-0.90	1.29	0.99	0.77
107	40.6	4.5	11.08	-1.75	-0.87	-0.58	1.36	0.81	0.56
72	41	6	14.63	-1.67	-0.84	-0.56	1.13	0.74	0.53
106	43.333	1.75	4.04	-1.25	-0.63	-0.42	1.19	0.62	0.42
105	44.404	1.54	3.47	-1.06	-0.53	-0.35	1.02	0.52	0.35
117	48	4	8.33	-0.41	-0.20	-0.14	0.33	0.19	0.13
104	50	1.5	3	-0.05	-0.02	-0.02	0.05	0.02	0.02
108	50.8	11.6	22.83	0.10	0.05	0.03	0.04	0.03	0.03
109	55.807	0.3	0.53	1.00	0.50	0.33	1.00	0.50	0.33
69	62	10	16.13	2.12	1.06	0.71	1.03	0.79	0.61
116	63.798	4.19	6.56	2.45	1.22	0.82	1.95	1.15	0.79
110	64.25	27.17	42.29	2.53	1.27	0.84	0.50	0.48	0.44
95	79	18	22.78	5.20	2.60	1.73	1.53	1.36	1.17
54	115*	14	12.17	11.71	5.86	3.90	4.30	3.63	2.98
113	181*	47	25.97	23.65	11.82	7.88	2.76	2.71	2.62
67	319*	18	5.64	48.61	24.30	16.20	14.27	12.72	10.98

TABLE 3c (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "3"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
Ca (19917.93 ± 2031.13) [µg/L]									
73	50.4*	1.2	2.38	-19.56	-9.78	-6.52	19.56	9.78	6.52
67	610*	1000	163.93	-19.01	-9.51	-6.34	13.55	8.53	6.02
118	9848	93	0.94	-9.92	-4.96	-3.31	9.87	4.95	3.30
62	11341.4	1248.08	11	-8.45	-4.22	-2.82	5.33	3.60	2.60
57	15709	965	6.14	-4.14	-2.07	-1.38	3.00	1.87	1.32
75	16800.6	168.2	1	-3.07	-1.53	-1.02	3.03	1.53	1.02
114	16900	2250	13.31	-2.97	-1.49	-0.99	1.22	1.00	0.80
112	16998.66	2319.54	13.65	-2.87	-1.44	-0.96	1.15	0.95	0.76
54	17776	2415	13.59	-2.11	-1.05	-0.7	0.82	0.68	0.55
115	18169.21	1154.55	6.35	-1.72	-0.86	-0.57	1.14	0.75	0.54
107	18514.2	664.2	3.59	-1.38	-0.69	-0.46	1.16	0.66	0.45
72	19147	895	4.67	-0.76	-0.38	-0.25	0.57	0.35	0.24
106	19845.33	883.25	4.45	-0.07	-0.04	-0.02	0.05	0.03	0.02
69	20000	2100	10.5	0.08	0.04	0.03	0.04	0.03	0.02
117	20000	2000	10	0.08	0.04	0.03	0.04	0.03	0.02
105	20711.92	359.42	1.74	0.78	0.39	0.26	0.74	0.38	0.26
110	21039	934.33	4.44	1.10	0.55	0.37	0.81	0.50	0.35
95	22408	1876	8.37	2.45	1.23	0.82	1.17	0.90	0.70
108	22814	2000.9	8.77	2.85	1.43	0.95	1.29	1.02	0.79
53	24663	2620	10.62	4.67	2.34	1.56	1.69	1.43	1.18
93	26119.9	2903.7	11.12	6.11	3.05	2.04	2.02	1.75	1.47
104	29200	170	0.58	9.14	4.57	3.05	9.01	4.55	3.04
116	30271.2	1914.77	6.33	10.19	5.10	3.40	4.78	3.71	2.88
111	137101*	11812	8.62	115.39	57.69	38.46	9.88	9.78	9.61
Cd [µg/L]									
117	180	50	27.78	-	-	-	-	-	-
Cl (7487.63 ± 884.68) [µg/L]									
118	1694	102	6.02	-13.10	-6.55	-4.37	12.76	6.51	4.35
53	2104	360	17.11	-12.17	-6.09	-4.06	9.44	5.64	3.92
114	5280	454	8.6	-4.99	-2.50	-1.66	3.48	2.22	1.57
108	6062	1161.9	19.17	-3.22	-1.61	-1.07	1.15	0.98	0.81
69	7100	3200	45.07	-0.88	-0.44	-0.29	0.12	0.12	0.11
105	7820.3	354.43	4.53	0.75	0.38	0.25	0.59	0.35	0.24
75	8449.6	150.9	1.79	2.17	1.09	0.72	2.06	1.07	0.72
72	9223	806	8.74	3.92	1.96	1.31	1.89	1.45	1.12
104	9500	150	1.58	4.55	2.27	1.52	4.31	2.24	1.51
116	10011	389.35	3.89	5.70	2.85	1.90	4.28	2.61	1.82
106	10778.5	576.28	5.35	7.44	3.72	2.48	4.53	3.12	2.27
109	11829.14	480.21	4.06	9.81	4.91	3.27	6.65	4.31	3.08
113	26468*	5371	20.29	42.91	21.45	14.30	3.52	3.49	3.43
111	548524*	25385	4.63	1223.13	611.56	407.71	21.31	21.30	21.28

TABLE 3c (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "3"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
				Co [µg/L]					
35	100	10	10	-	-	-	-	-	-
62	152.5	208.6	136.78	-	-	-	-	-	-
				Cr (2.35 ± 0.52) [µg/L]					
75	1.6	0.6	37.5	-2.90	-1.45	-0.97	1.15	0.95	0.76
105	2.232	0.3	13.35	-0.46	-0.23	-0.15	0.30	0.20	0.14
116	2.56	0.23	8.98	0.81	0.41	0.27	0.61	0.37	0.26
108	3	0	0	2.51	1.26	0.84	2.51	1.26	0.84
109	5.057*	1.17	23.1	10.47	5.24	3.49	2.26	2.12	1.93
62	14.6*	5.03	34.45	47.39	23.69	15.80	2.43	2.42	2.41
69	29*	100	344.83	103.09	51.55	34.36	0.27	0.27	0.27
				Cu (1.94 ± 0.43) [µg/L]					
73	0.6	0.09	15	-6.28	-3.14	-2.09	5.79	3.07	2.07
75	1.2	0.5	41.67	-3.47	-1.73	-1.16	1.36	1.13	0.91
105	1.388	0.27	19.24	-2.59	-1.29	-0.86	1.61	1.10	0.80
108	1.4	1.34	95.71	-2.53	-1.27	-0.84	0.40	0.38	0.36
72	2.4	0.5	20.83	2.16	1.08	0.72	0.85	0.7	0.57
116	2.876	0.19	6.68	4.39	2.19	1.46	3.26	2.00	1.40
69	3.7	4.3	116.22	8.25	4.12	2.75	0.41	0.41	0.40
109	6.766*	0.86	12.71	22.61	11.31	7.54	5.45	5.03	4.50
103	16.2*	7.6	46.91	66.82	33.41	22.27	1.88	1.87	1.87
54	21.8*	4.3	19.72	93.06	46.53	31.02	4.61	4.6	4.57
114	44.3*	5.97	13.48	198.50	99.25	66.17	7.09	7.08	7.06
110	58.25*	14.22	24.41	263.87	131.94	87.96	3.96	3.96	3.96
35	110*	30	27.27	506.37	253.19	168.79	3.60	3.60	3.60
62	294.6*	253.85	86.17	1371.42	685.71	457.14	1.15	1.15	1.15
				Fe (81.18 ± 17.86) [µg/L]					
105	1.707	0.49	28.82	-8.90	-4.45	-2.97	8.89	4.45	2.97
73	4.2	0.15	3.57	-8.62	-4.31	-2.87	8.62	4.31	2.87
108	5.6	2.7	48.21	-8.46	-4.23	-2.82	8.10	4.18	2.81
75	10.6	4.4	41.51	-7.90	-3.95	-2.63	7.09	3.84	2.60
72	14	11	78.57	-7.52	-3.76	-2.51	4.74	3.20	2.32
69	56	71	126.79	-2.82	-1.41	-0.94	0.35	0.34	0.33
110	70.25	25.94	36.93	-1.22	-0.61	-0.41	0.40	0.35	0.29
117	71	35	49.3	-1.14	-0.57	-0.38	0.28	0.26	0.23
57	108.5	11.6	10.69	3.06	1.53	1.02	1.87	1.28	0.94
114	119	63.8	53.61	4.24	2.12	1.41	0.59	0.57	0.55
35	130	20	15.38	5.47	2.73	1.82	2.23	1.82	1.46
104	130	4	3.08	5.47	2.73	1.82	4.99	2.67	1.80
53	137	30	21.9	6.25	3.13	2.08	1.78	1.60	1.39
62	166.8	93.1	55.82	9.59	4.79	3.20	0.92	0.90	0.88
54	193	81.2	42.07	12.52	6.26	4.17	1.37	1.34	1.31

TABLE 3c (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "3"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
103	707.8*	48.5	6.85	70.17	35.09	23.39	12.71	12.12	11.31
67	7300*	160	2.19	808.40	404.2	269.47	45.05	44.84	44.50
				In [µg/L]					
75	23.6	4.7	19.92	-	-	-	-	-	-
117	270	80	29.63	-	-	-	-	-	-
				K (8717.85 ± 1006.72) [µg/L]					
73	9.4*	1	10.64	-17.30	-8.65	-5.77	17.30	8.65	5.77
62	3717.2	405.42	10.91	-9.93	-4.97	-3.31	7.74	4.61	3.20
118	4517	88	1.95	-8.35	-4.17	-2.78	8.22	4.16	2.78
114	4600	344	7.48	-8.18	-4.09	-2.73	6.75	3.87	2.66
57	6537	202	3.09	-4.33	-2.17	-1.44	4.02	2.12	1.43
69	7000	2200	31.43	-3.41	-1.71	-1.14	0.76	0.71	0.64
75	7481.8	118.1	1.58	-2.46	-1.23	-0.82	2.39	1.22	0.82
95	7662	1508	19.68	-2.10	-1.05	-0.70	0.66	0.58	0.49
72	7973	757	9.49	-1.48	-0.74	-0.49	0.82	0.59	0.44
108	8051.8	1465.9	18.21	-1.32	-0.66	-0.44	0.43	0.37	0.32
54	8132	1444	17.76	-1.16	-0.58	-0.39	0.38	0.33	0.28
107	8159.4	704.9	8.64	-1.11	-0.55	-0.37	0.64	0.45	0.34
115	8638.951	2524.29	29.22	-0.16	-0.08	-0.05	0.03	0.03	0.03
105	9059.263	446.43	4.93	0.68	0.34	0.23	0.51	0.31	0.22
112	9175.668	1818.02	19.81	0.91	0.45	0.30	0.24	0.22	0.19
110	9402.5	668.15	7.11	1.36	0.68	0.45	0.82	0.57	0.41
117	11000	2000	18.18	4.53	2.27	1.51	1.11	1.02	0.91
116	11079.4	375.31	3.39	4.69	2.35	1.56	3.76	2.20	1.52
104	11100	110	0.99	4.73	2.37	1.58	4.62	2.35	1.57
53	11573	3960	34.22	5.67	2.84	1.89	0.72	0.70	0.67
109	11820.74	379.76	3.21	6.16	3.08	2.05	4.92	2.88	1.99
93	12460	2212.05	17.75	7.43	3.72	2.48	1.65	1.54	1.40
106	12652	797.03	6.3	7.82	3.91	2.61	4.17	3.06	2.30
113	31609*	3354	10.61	45.48	22.74	15.16	6.75	6.54	6.22
111	57711*	2198	3.81	97.33	48.67	32.44	21.73	20.27	18.37
				Mg (9276.64 ± 1061.28) [µg/L]					
108	4845.4	1047	21.61	-8.35	-4.18	-2.78	3.78	2.97	2.33
75	6725.2	219.5	3.26	-4.81	-2.40	-1.60	4.44	2.35	1.59
105	10235.95	711.06	6.95	1.81	0.90	0.60	1.08	0.75	0.55
116	15300	1183.22	7.73	11.35	5.68	3.78	4.64	3.79	3.04
72	27628*	2116	7.66	34.58	17.29	11.53	8.41	7.75	6.93
				Mn [µg/L]					
75	1	0.1	10	-	-	-	-	-	-
62	7	3	42.86	-	-	-	-	-	-
69	11	72	654.55	-	-	-	-	-	-
35	130*	10	7.69	-	-	-	-	-	-

TABLE 3c (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "3"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
				Mo [µg/L]					
73	371	46.2	12.45	-	-	-	-	-	-
				Na [µg/L]					
75	4640.4	1847.2	39.81	-	-	-	-	-	-
				Ni [µg/L]					
75	1	0.8	80	-	-	-	-	-	-
72	1	1	100	-	-	-	-	-	-
73	1.2	0.09	7.5	-	-	-	-	-	-
69	17*	4	23.53	-	-	-	-	-	-
109	43.038*	10.32	23.99	-	-	-	-	-	-
35	120*	20	16.67	-	-	-	-	-	-
				Os [µg/L]					
105	0.844	0.24	28.2	-	-	-	-	-	-
				P [µg/L]					
108	119.4	78.9	66.08	-	-	-	-	-	-
75	290	47.3	16.31	-	-	-	-	-	-
72	367	109	29.7	-	-	-	-	-	-
				Pb (4.51 ± 0.99) [µg/L]					
108	0.6	0.55	91.67	-7.88	-3.94	-2.63	5.28	3.45	2.46
75	1	0.1	10	-7.08	-3.54	-2.36	6.94	3.52	2.35
72	1.1	0.8	72.73	-6.87	-3.44	-2.29	3.62	2.68	2.02
116	1.66	0.28	16.93	-5.74	-2.87	-1.91	5.00	2.76	1.88
117	3	1	33.33	-3.04	-1.52	-1.01	1.35	1.07	0.84
109	5.09	0.88	17.21	1.17	0.58	0.39	0.58	0.44	0.34
62	9	7.21	80.12	9.05	4.53	3.02	0.62	0.62	0.61
69	9.5	18	189.47	10.06	5.03	3.35	0.28	0.28	0.28
73	9.6	0.4	4.17	10.26	5.13	3.42	7.99	4.76	3.30
110	76.667*	34.27	44.7	145.45	72.72	48.48	2.11	2.10	2.10
				Rb (25.51 ± 5.61) [µg/L]					
107	15.4	2.3	14.94	-3.60	-1.80	-1.20	2.79	1.67	1.16
54	17.6	4.3	24.43	-2.82	-1.41	-0.94	1.54	1.12	0.84
72	20	2	10	-1.96	-0.98	-0.65	1.60	0.92	0.64
75	20.4	0.5	2.45	-1.82	-0.91	-0.61	1.79	0.91	0.61
108	21.6	4.4	20.37	-1.39	-0.70	-0.46	0.75	0.55	0.41
114	23	6.9	30	-0.89	-0.45	-0.30	0.34	0.28	0.23
106	23.5	0.55	2.33	-0.72	-0.36	-0.24	0.70	0.36	0.24
105	24.608	1.13	4.6	-0.32	-0.16	-0.11	0.30	0.16	0.11
109	27.995	0.92	3.3	0.89	0.44	0.30	0.84	0.44	0.29
103	29.9	2.7	9.03	1.56	0.78	0.52	1.13	0.70	0.50

TABLE 3c (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "3"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
104	30	1	3.33	1.60	0.80	0.53	1.51	0.79	0.53
117	30	3	10	1.60	0.80	0.53	1.09	0.71	0.50
116	30.592	1.47	4.8	1.81	0.91	0.60	1.60	0.88	0.59
53	32	6	18.75	2.31	1.16	0.77	0.98	0.79	0.63
93	36	7.35	20.42	3.74	1.87	1.25	1.33	1.13	0.94
113	163*	33	20.25	49.00	24.5	16.33	4.15	4.11	4.04
				Re [µg/L]					
105	1.622	0.18	11.04	-	-	-	-	-	-
				Rh [µg/L]					
75	272.8	32.57	11.94	-	-	-	-	-	-
105	834.226	47.76	5.72	-	-	-	-	-	-
				Ru [µg/L]					
75	252.6	44.78	17.73	-	-	-	-	-	-
105	787.406	53.2	6.76	-	-	-	-	-	-
				S (644.91 ± 110.20) [µg/L]					
118	275	31	11.27	-6.71	-3.36	-2.24	5.85	3.23	2.20
72	307	124	40.39	-6.13	-3.07	-2.04	2.49	2.04	1.64
108	425	58.6	13.79	-3.99	-2.00	-1.33	2.73	1.76	1.25
116	553.6	83.23	15.03	-1.66	-0.83	-0.55	0.91	0.66	0.49
69	600	600	100	-0.82	-0.41	-0.27	0.07	0.07	0.07
105	662.574	54.79	8.27	0.32	0.16	0.11	0.23	0.14	0.10
75	798	63.3	7.93	2.78	1.39	0.93	1.82	1.20	0.86
112	1083.103	170.23	15.72	7.95	3.98	2.65	2.45	2.16	1.85
109	1099.927	97.21	8.84	8.26	4.13	2.75	4.07	3.10	2.37
67	15500*	1000	6.45	269.59	134.8	89.86	14.83	14.77	14.66
				Si [µg/L]					
73	163128.6	274.2	0.17	-	-	-	-	-	-
				Sn [µg/L]					
105	249.636	73.8	29.56	-	-	-	-	-	-
				Sr (132.84 ± 28.79) [µg/L]					
112	91.372	16.56	18.12	-2.88	-1.44	-0.96	1.89	1.25	0.90
114	97	9.25	9.54	-2.49	-1.24	-0.83	2.09	1.19	0.81
72	98	5	5.1	-2.42	-1.21	-0.81	2.29	1.19	0.80
75	99.8	1.1	1.1	-2.29	-1.15	-0.76	2.29	1.15	0.76
107	106.8	12.5	11.7	-1.81	-0.90	-0.60	1.37	0.83	0.58
54	110	17.4	15.82	-1.59	-0.79	-0.53	1.01	0.68	0.49
103	115.3	4.2	3.64	-1.22	-0.61	-0.41	1.17	0.60	0.40
108	117	11.1	9.49	-1.10	-0.55	-0.37	0.87	0.51	0.36
35	120	10	8.33	-0.89	-0.45	-0.30	0.73	0.42	0.29

TABLE 3c (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "3"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
62	120	15.22	12.68	-0.89	-0.45	-0.30	0.61	0.39	0.28
105	122.359	2.19	1.79	-0.73	-0.36	-0.24	0.72	0.36	0.24
117	130	10	7.69	-0.20	-0.10	-0.07	0.16	0.09	0.06
57	142.8	15.4	10.78	0.69	0.35	0.23	0.47	0.31	0.22
116	142.828	8.89	6.22	0.69	0.35	0.23	0.59	0.33	0.23
95	146	14	9.59	0.91	0.46	0.30	0.66	0.41	0.29
53	148	23	15.54	1.05	0.53	0.35	0.56	0.41	0.31
109	159.44	10.58	6.63	1.85	0.92	0.62	1.49	0.87	0.60
93	161	19.59	12.17	1.96	0.98	0.65	1.16	0.81	0.59
104	165.6	3	1.81	2.28	1.14	0.76	2.23	1.13	0.76
106	186.333	8.19	4.39	3.72	1.86	1.24	3.23	1.79	1.22
69	210	20	9.52	5.36	2.68	1.79	3.13	2.20	1.62
110	246.5*	14.36	5.83	7.89	3.95	2.63	5.59	3.53	2.50
113	683*	136	19.91	38.21	19.11	12.74	4.02	3.96	3.86
				Ti (13.33 ± 2.93) [µg/L]					
75	3	1.6	53.33	-7.04	-3.52	-2.35	4.76	3.09	2.21
105	3.653	1.03	28.2	-6.60	-3.30	-2.20	5.40	3.11	2.14
72	11	10	90.91	-1.59	-0.79	-0.53	0.23	0.22	0.21
117	19	5	26.32	3.87	1.93	1.29	1.09	0.98	0.85
104	30	5	16.67	11.37	5.68	3.79	3.20	2.88	2.50
111	1982*	192	9.69	1342.61	671.31	447.54	10.25	10.25	10.25
67	1990*	110	5.53	1348.07	674.03	449.36	17.97	17.96	17.96
				V (10.42 ± 2.29) [µg/L]					
75	9.4	0.9	9.57	-0.89	-0.44	-0.30	0.70	0.41	0.29
105	9.518	1.64	17.19	-0.79	-0.39	-0.26	0.45	0.32	0.24
108	9.6	2.51	26.15	-0.72	-0.36	-0.24	0.30	0.24	0.19
109	10.518	2.14	20.38	0.09	0.04	0.03	0.04	0.03	0.02
117	11	2	18.18	0.51	0.25	0.17	0.25	0.19	0.15
116	12.46	1.17	9.42	1.78	0.89	0.59	1.24	0.79	0.56
72	15*	2	13.33	4.00	2.00	1.33	1.99	1.51	1.15
111	907*	81	8.93	782.22	391.11	260.74	11.07	11.06	11.06
				W [µg/L]					
105	1.116	0.46	40.95	-	-	-	-	-	-
				Zn (7.64 ± 1.68) [µg/L]					
69	2.4	3.3	137.5	-6.24	-3.12	-2.08	1.54	1.41	1.26
105	2.738	0.63	23.16	-5.83	-2.92	-1.94	4.66	2.73	1.89
116	4.842	0.52	10.76	-3.33	-1.66	-1.11	2.83	1.59	1.09
72	7	3	42.86	-0.76	-0.38	-0.25	0.21	0.19	0.16
109	8.395	2.37	28.18	0.90	0.45	0.30	0.30	0.26	0.22
75	8.8	2.5	28.41	1.38	0.69	0.46	0.44	0.39	0.33
117	9	2	22.22	1.62	0.81	0.54	0.63	0.52	0.42
108	10	3.1	31	2.81	1.40	0.94	0.73	0.67	0.59

TABLE 3c (cont). SUMMARY OF THE REPORTED RESULTS AND THE CALCULATED *z*- AND *u*-SCORES FOR SAMPLE "3"

Laboratory code	Analyte concentration	Standard dev.	Relative std. dev., [%]	*z*-scores			*u*-scores		
				$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$
103	15.6	7.6	48.72	9.47	4.74	3.16	1.04	1.02	0.99
53	30*	6	20	26.61	13.3	8.87	3.69	3.59	3.44
73	39.2*	0.2	0.51	37.55	18.78	12.52	36.53	18.65	12.48
62	44.6*	27.01	60.57	43.98	21.99	14.66	1.37	1.37	1.36
114	49.5*	11	22.22	49.81	24.90	16.60	3.79	3.76	3.71
54	110*	31.5	28.64	121.80	60.90	40.60	3.25	3.24	3.24
35	120*	10	8.33	133.70	66.85	44.57	11.20	11.08	10.90

TABLE 4a. THE COMBINED *z*-SCORES FOR THE PARTICIPATING LABORATORIES FOR SAMPLE "1"

Lab Code	Number of analytes	Rescaled sum of scores (RSZ)			Sum of squared scores (SSZ)			Critical value
		$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$	χ^2
35	12	25.65	12.83	8.55	1389	347	154	23.34
53	14	11.83	5.91	3.94	218	54.56	24.25	26.12
54	14	13.13	6.57	4.38	616	154	68.42	26.12
57	13	0.76	0.38	0.25	1.87	0.47	0.21	24.74
62	13	388	194	129.36	179571	44893	19952	24.74
67	8	-17.47	-8.74	-5.82	2204	551	245	17.53
69	13	-2.59	-1.29	-0.86	235	58.79	26.13	24.74
72	16	-6.48	-3.24	-2.16	178	44.44	19.75	28.85
73	14	19.67	9.84	6.56	965	241	107.25	26.12
75	18	2.1	1.05	0.7	412	102.93	45.75	31.53
78	15	-13.31	-6.66	-4.44	552	138.01	61.34	27.49
89	12	4.46	2.23	1.49	50.21	12.55	5.58	23.34
93	12	0.89	0.45	0.3	16.06	4.01	1.78	23.34
95	15	9.86	4.93	3.29	403	100.77	44.79	27.49
103	11	-1.11	-0.56	-0.37	27.83	6.96	3.09	21.92
104	14	5.65	2.82	1.88	54.77	13.69	6.09	26.12
105	18	14.94	7.47	4.98	517	129.21	57.43	31.53
106	16	13.85	6.92	4.62	533	133.25	59.22	28.85
107	13	-5.65	-2.82	-1.88	104.74	26.18	11.64	24.74
108	18	-6.39	-3.19	-2.13	211	52.64	23.39	31.53
109	16	7.88	3.94	2.63	190	47.59	21.15	28.85
110	13	0.96	0.48	0.32	22.65	5.66	2.52	24.74
111	12	13.66	6.83	4.55	467	116.75	51.89	23.34
112	13	21.08	10.54	7.03	964	241	107.09	24.74
113	13	18.21	9.11	6.07	422	105.38	46.84	24.74
114	11	5.1	2.55	1.7	45.83	11.46	5.09	21.92
115	8	5.03	2.52	1.68	55.26	13.81	6.14	17.53
116	15	2.13	1.07	0.71	38.92	9.73	4.32	27.49
117	15	11.52	5.76	3.84	443	110.74	49.22	27.49
118	13	-7.47	-3.74	-2.49	200	49.89	22.17	24.74

TABLE 4b. THE COMBINED *z*-SCORES FOR THE PARTICIPATING LABORATORIES FOR SAMPLE "2"

Lab Code	Number of analytes	Rescaled sum of scores (RSZ)			Sum of squared scores (SSZ)			Critical value
		k = 0.5	k = 1.0	k = 1.5	k = 0.5	k = 1.0	k = 1.5	χ^2
35	7	-12.73	-6.37	-4.24	202	50.51	22.45	16.01
53	13	40.74	20.37	13.58	2610	652	290	24.74
54	13	-9.43	-4.71	-3.14	279	69.69	30.97	24.74
57	11	0.89	0.45	0.3	293	73.21	32.54	21.92
62	12	-21.27	-10.63	-7.09	536	134.07	59.59	23.34
69	13	-30.12	-15.06	-10.04	963	241	106.95	24.74
72	14	-12.23	-6.12	-4.08	211	52.84	23.49	26.12
73	14	4.06	2.03	1.35	244	61.05	27.13	26.12
75	15	0.71	0.36	0.24	132.32	33.08	14.7	27.49
89	10	21.73	10.87	7.24	909	227	101.03	20.48
93	12	50.52	25.26	16.84	4554	1138	506	23.34
95	11	8.3	4.15	2.77	158	39.56	17.58	21.92
103	8	56.19	28.1	18.73	29268	7317	3252	17.53
104	13	241	120.34	80.23	78023	19506	8669	24.74
105	14	95.97	47.99	31.99	10763	2691	1196	26.12
106	14	-20.56	-10.28	-6.85	593	148.31	65.91	26.12
107	12	-0.26	-0.13	-0.09	234	58.54	26.02	23.34
108	14	34.54	17.27	11.51	3224	806	358	26.12
109	12	23.55	11.77	7.85	862	215	95.76	23.34
113	9	-8.95	-4.48	-2.98	103.46	25.87	11.5	19.02
114	6	28.91	14.46	9.64	1278	319	141.95	14.45
116	14	-17.59	-8.79	-5.86	345	86.24	38.33	26.12
117	14	18.34	9.17	6.11	671	168	74.5	26.12
118	10	-12.42	-6.21	-4.14	305	76.17	33.85	20.48
119	8	-23.88	-11.94	-7.96	574	143.52	63.79	17.53

TABLE 4c. THE COMBINED *z*-SCORES FOR THE PARTICIPATING LABORATORIES FOR SAMPLE "3"

Lab Code	Number of analytes	Rescaled sum of scores (RSZ)			Sum of squared scores (SSZ)			Critical value
		$k = 0.5$	$k = 1.0$	$k = 1.5$	$k = 0.5$	$k = 1.0$	$k = 1.5$	χ^2
35	4	322	161	107.44	274320	68580	30480	11.14
53	7	13	6.5	4.33	956	239	106.17	16.01
54	8	81.82	40.91	27.27	23806	5952	2645	17.53
57	4	-2.36	-1.18	-0.79	45.79	11.45	5.09	11.14
62	9	490	245	163	1885356	471339	209484	19.02
67	5	1098	549	366	2546192	636548	282910	12.83
69	11	34.62	17.31	11.54	10891	2723	1210	21.92
72	14	3.6	1.8	1.2	1392	348	155	26.12
73	6	-1.61	-0.81	-0.54	2311	578	257	14.45
75	15	-11.4	-5.7	-3.8	290	72.57	32.25	27.49
93	4	9.62	4.81	3.21	110.36	27.59	12.26	11.14
95	4	3.23	1.62	1.08	38.27	9.57	4.25	11.14
103	6	58.09	29.05	19.36	9503	2376	1056	14.45
104	8	13.82	6.91	4.61	294	73.38	32.61	17.53
105	14	-6.13	-3.06	-2.04	171	42.77	19.01	26.12
106	6	6.91	3.46	2.3	132.33	33.08	14.7	14.45
107	5	-4.32	-2.16	-1.44	22.45	5.61	2.49	12.83
108	14	-8.21	-4.1	-2.74	264	65.99	29.33	26.12
109	12	19.05	9.52	6.35	839	210	93.18	23.34
110	7	159	79.56	53.04	90856	22714	10095	16.01
111	5	1592	796	531	3933294	983323	437033	12.83
112	4	1.55	0.78	0.52	80.63	20.16	8.96	11.14
113	5	89.1	44.55	29.7	8330	2082	926	12.83
114	9	76.78	38.39	25.59	42016	10504	4668	19.02
115	2	-1.33	-0.66	-0.44	2.99	0.75	0.33	7.38
116	14	7.06	3.53	2.35	412	103.11	45.83	26.12
117	11	3.28	1.64	1.09	63.79	15.95	7.09	21.92
118	4	-19.04	-9.52	-6.35	385	96.15	42.73	11.14

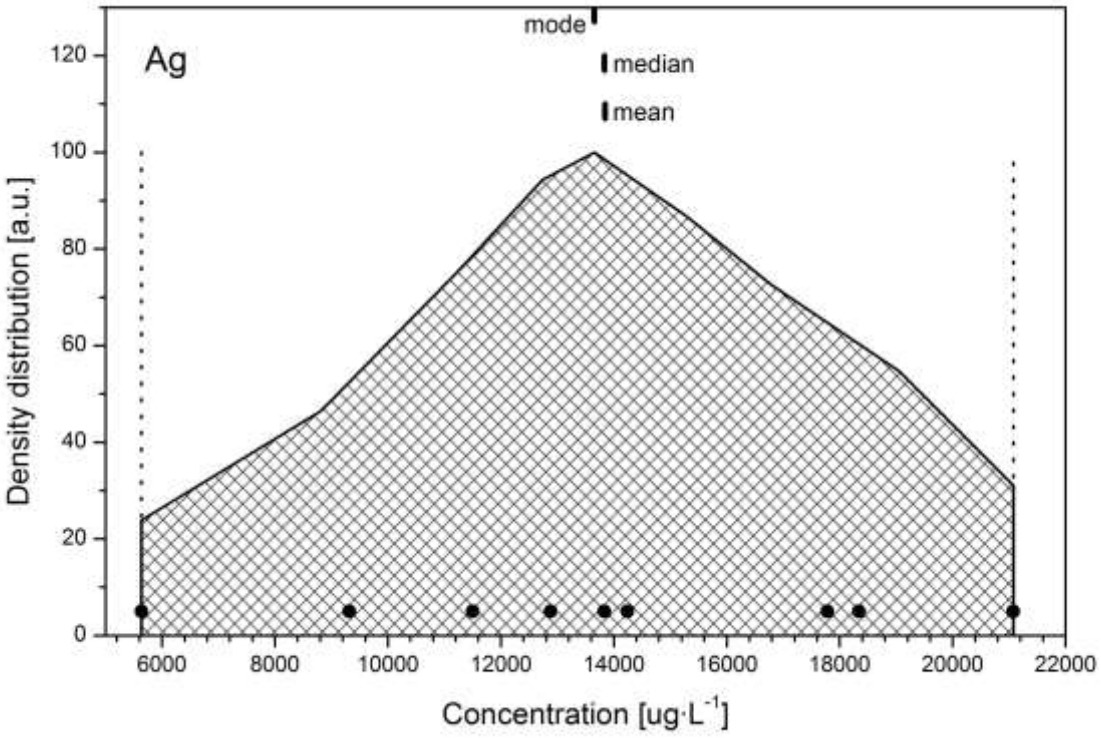

FIG. 2. The density distribution function for the analyte Ag in case of sample "1".

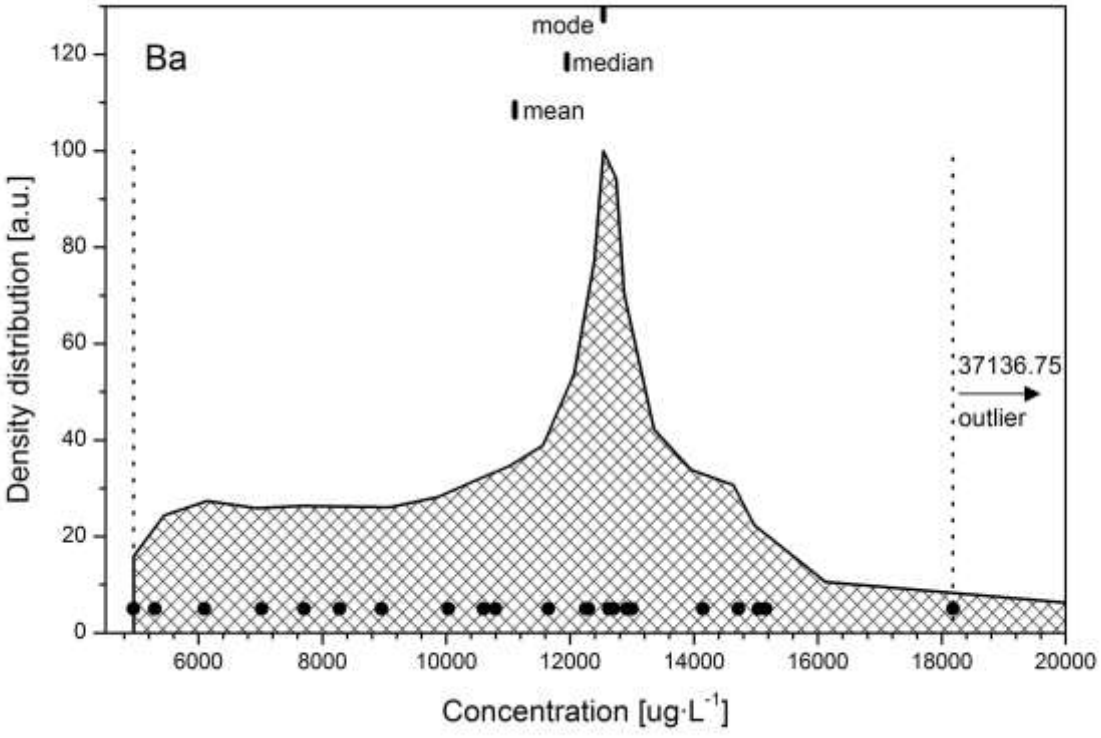

FIG. 3. The density distribution function for the analyte Ba in case of sample "1".

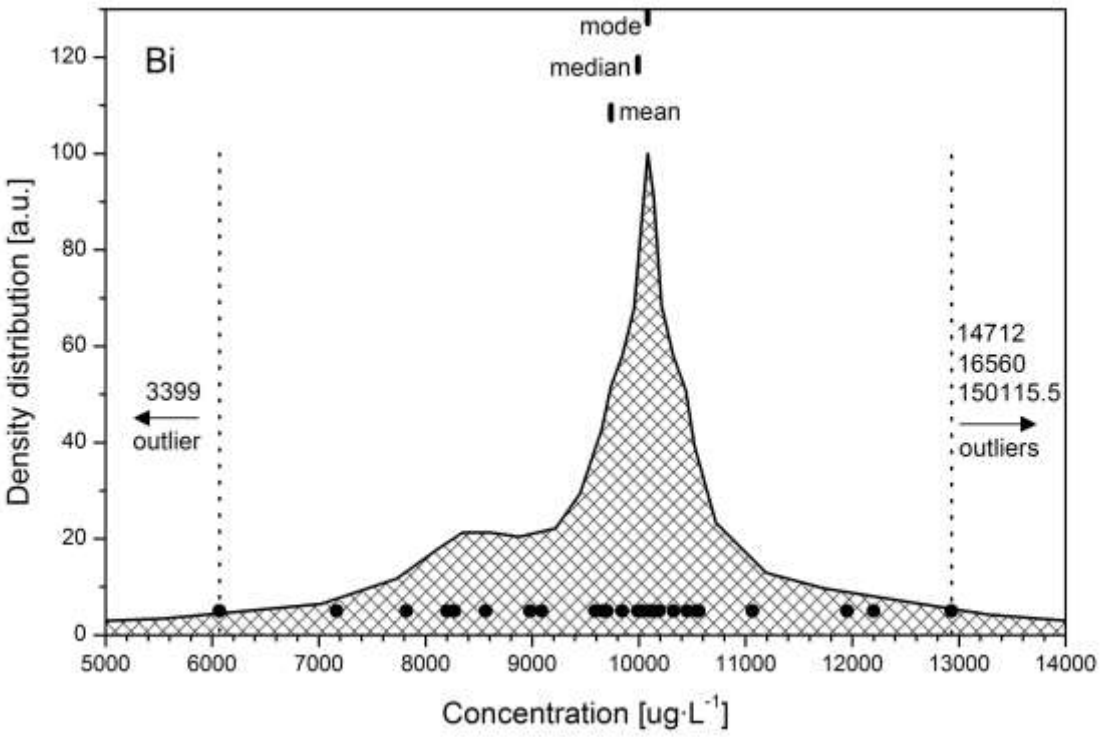

FIG. 4. The density distribution function for the analyte Bi in case of sample "1".

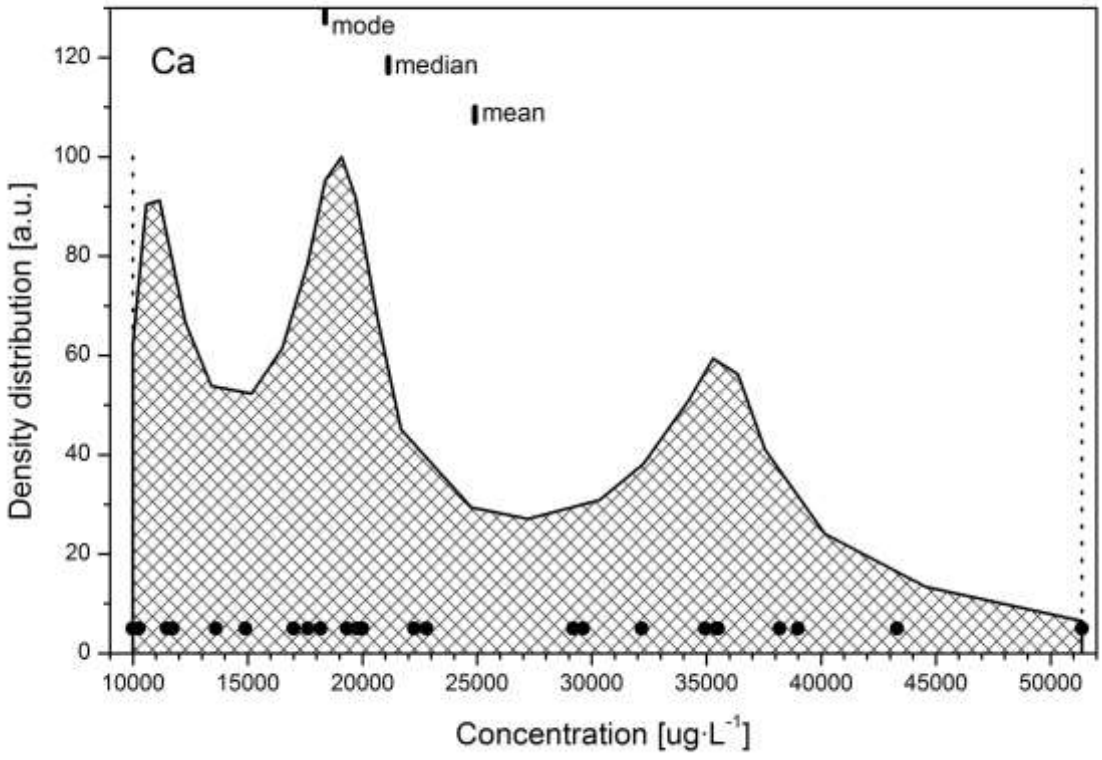

FIG. 5. The density distribution function for the analyte Ca in case of sample "1".

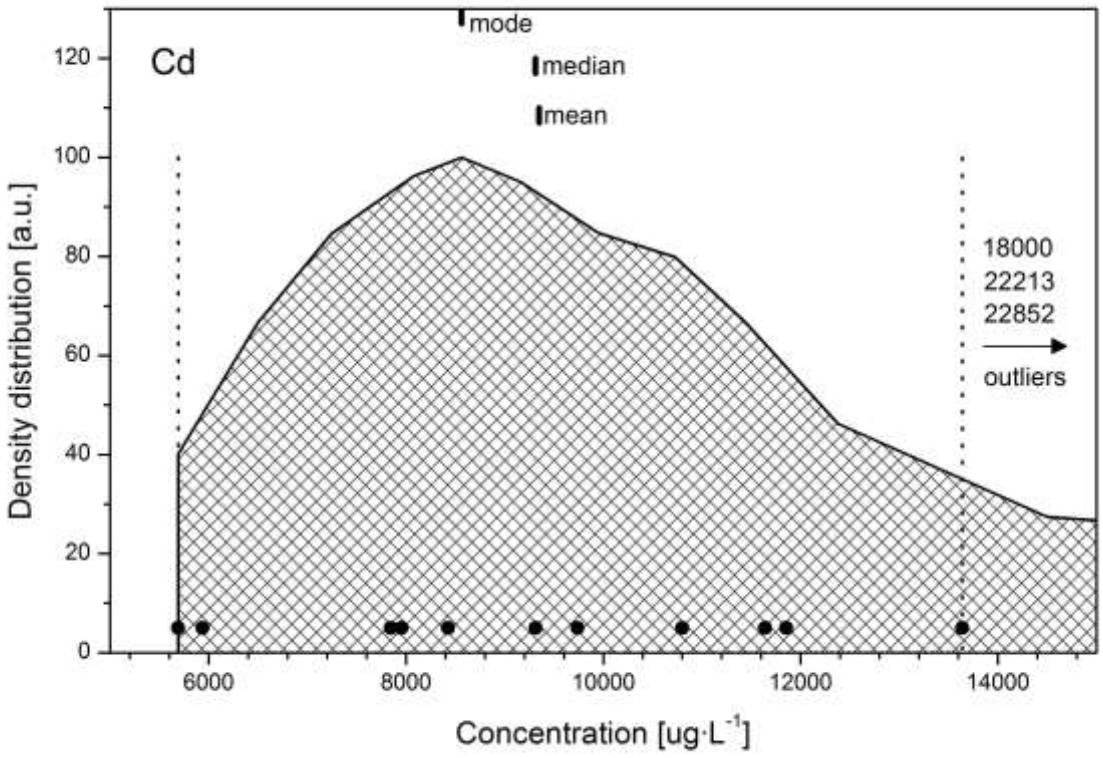

FIG. 6. The density distribution function for the analyte Cd in case of sample "1".

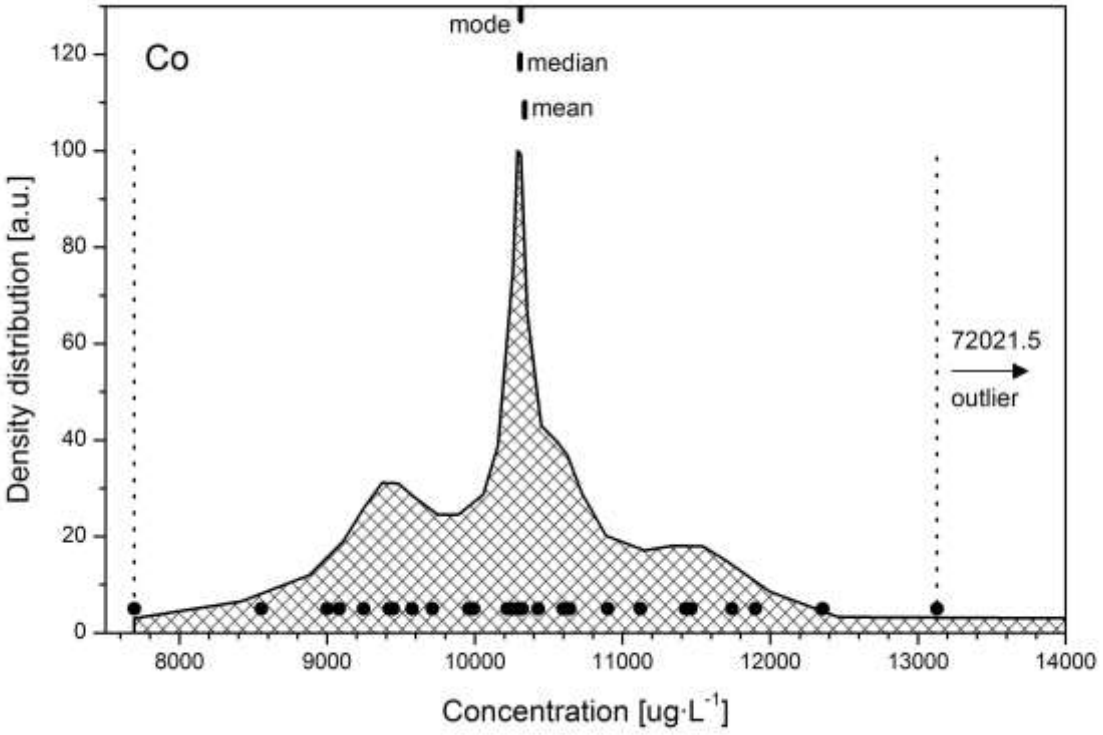

FIG. 7. The density distribution function for the analyte Co in case of sample "1".

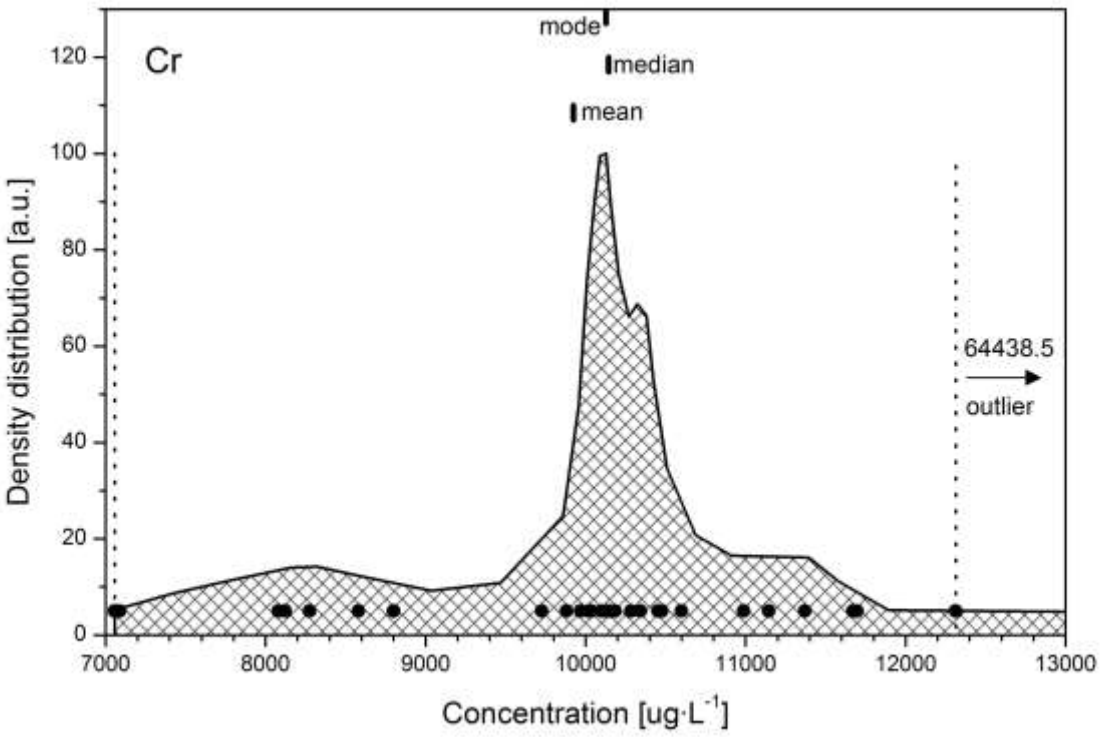

FIG. 8. The density distribution function for the analyte Cr in case of sample "1".

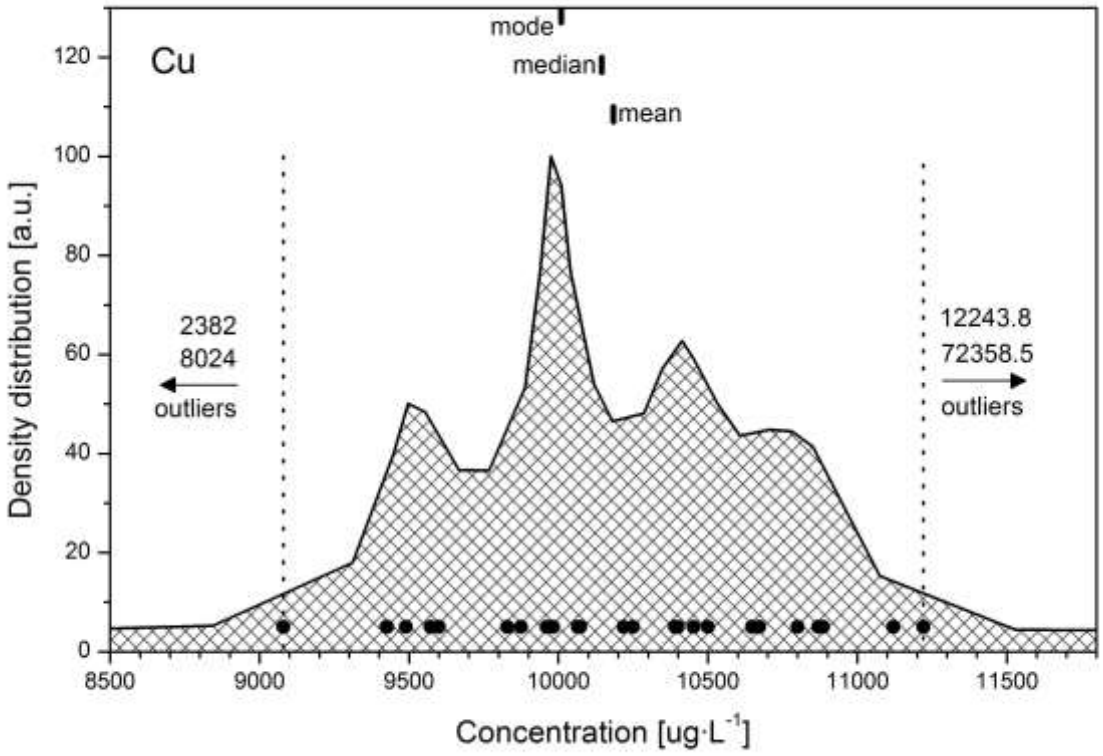

FIG. 9. The density distribution function for the analyte Cu in case of sample "1".

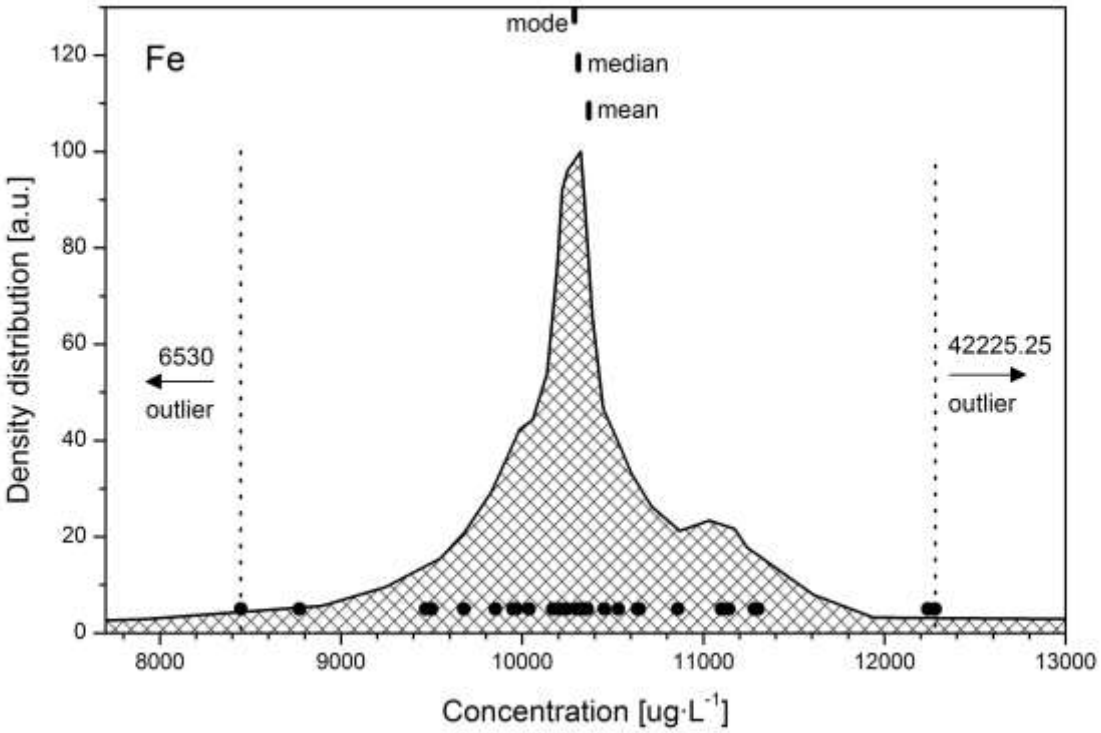

FIG. 10. The density distribution function for the analyte Fe in case of sample "1".

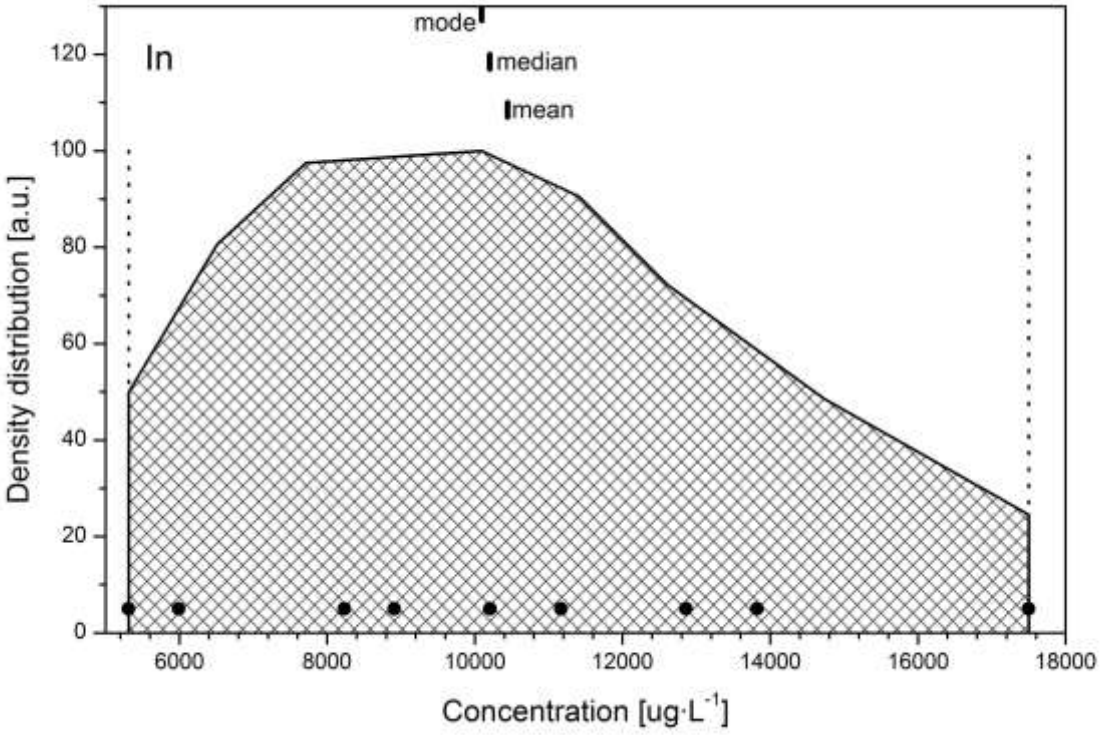

FIG. 11. The density distribution function for the analyte In in case of sample "1".

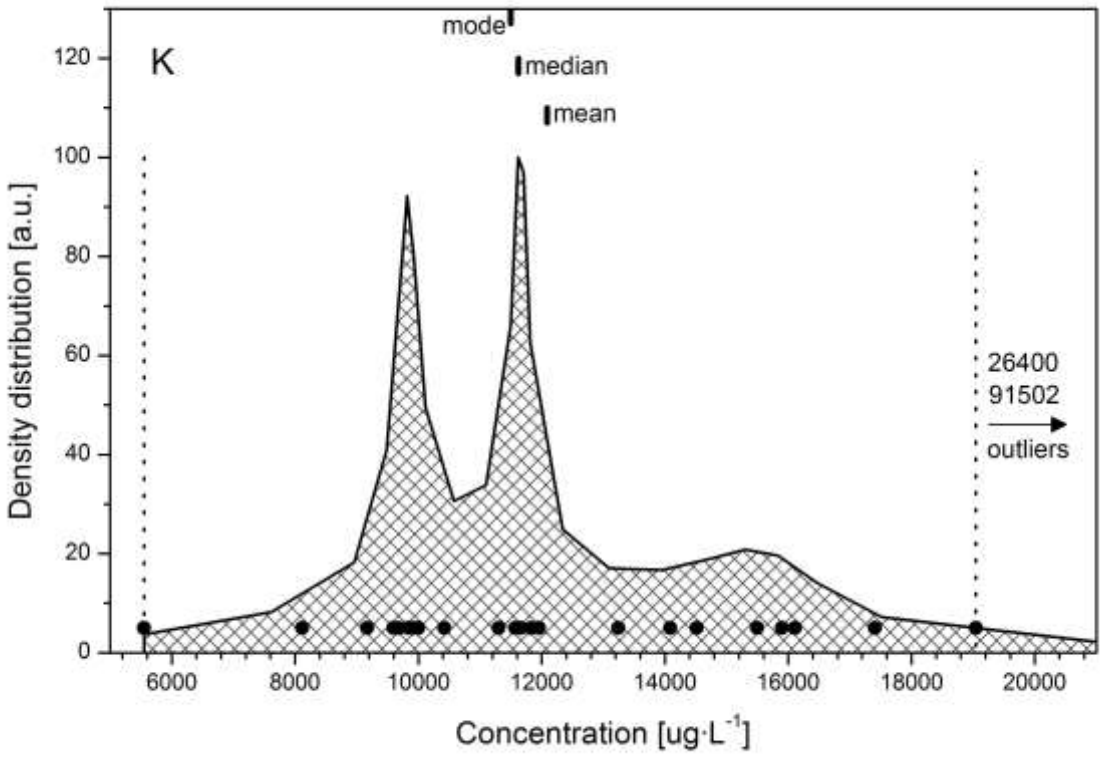

FIG. 12. The density distribution function for the analyte K in case of sample "1".

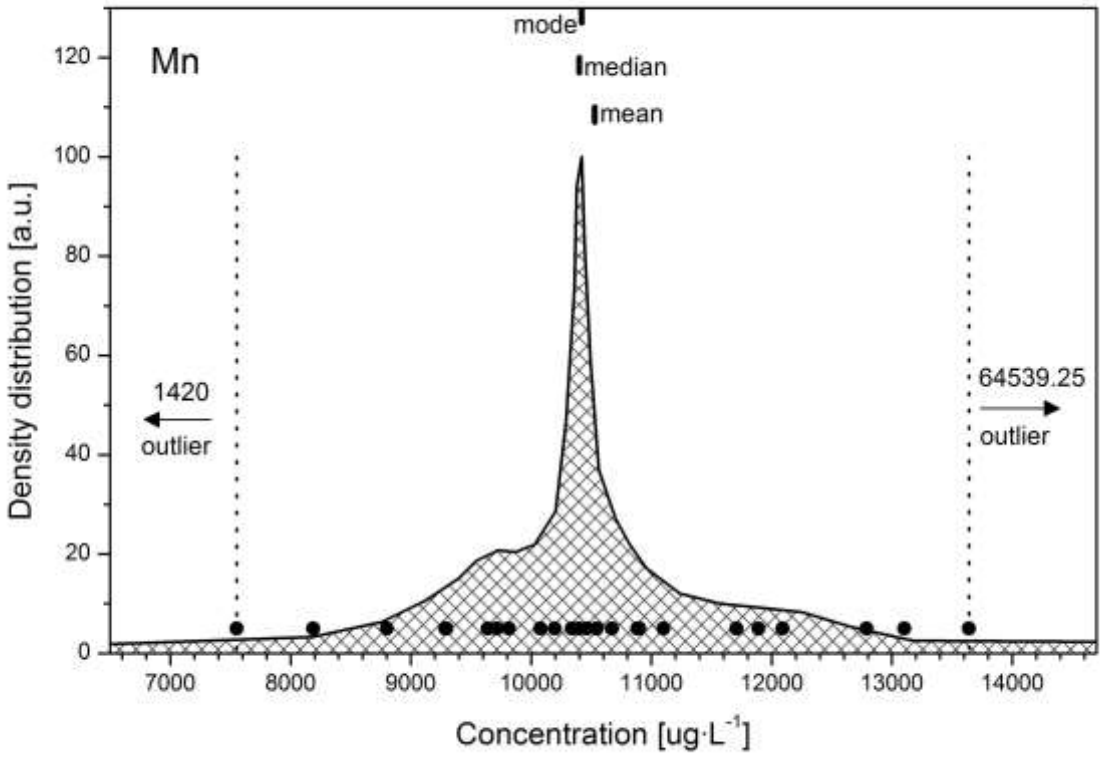

FIG. 13. The density distribution function for the analyte Mn in case of sample "1".

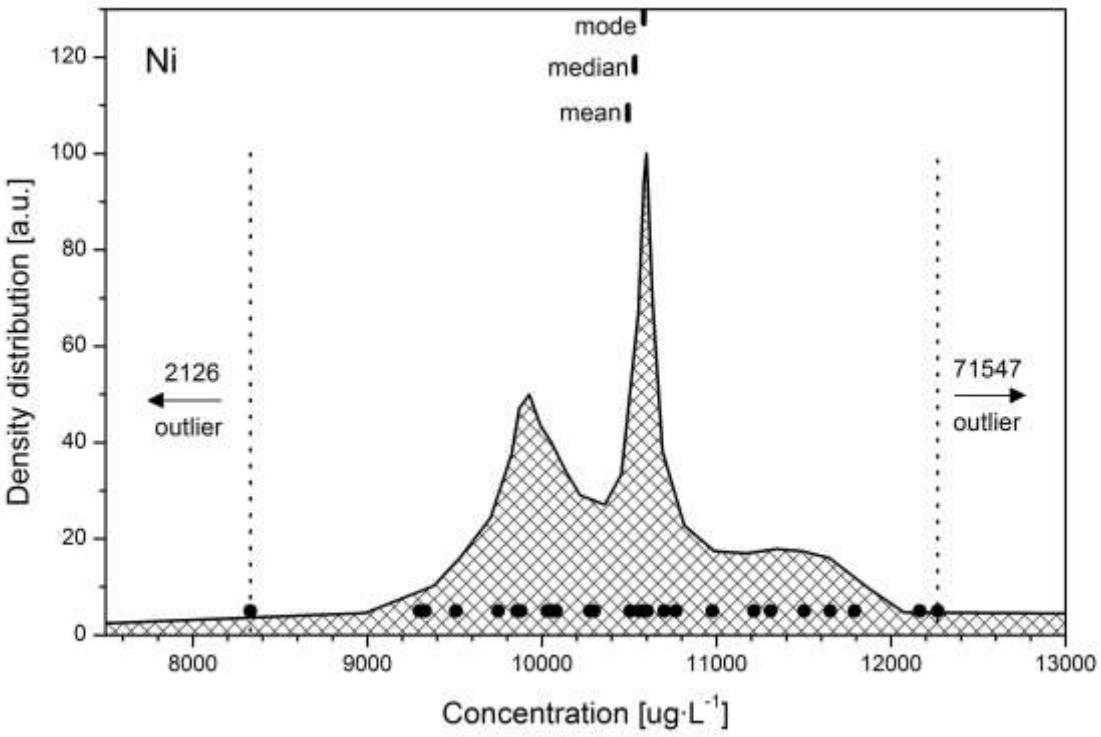

FIG. 14. The density distribution function for the analyte Ni in case of sample "1".

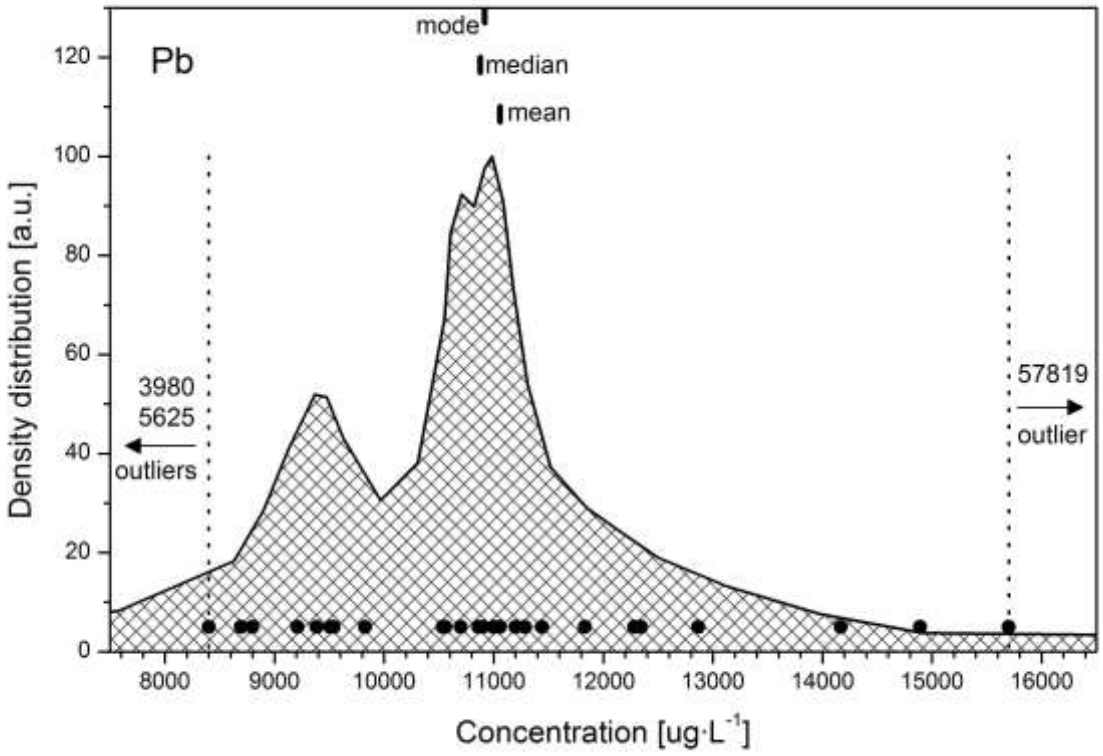

FIG. 15. The density distribution function for the analyte Pb in case of sample "1".

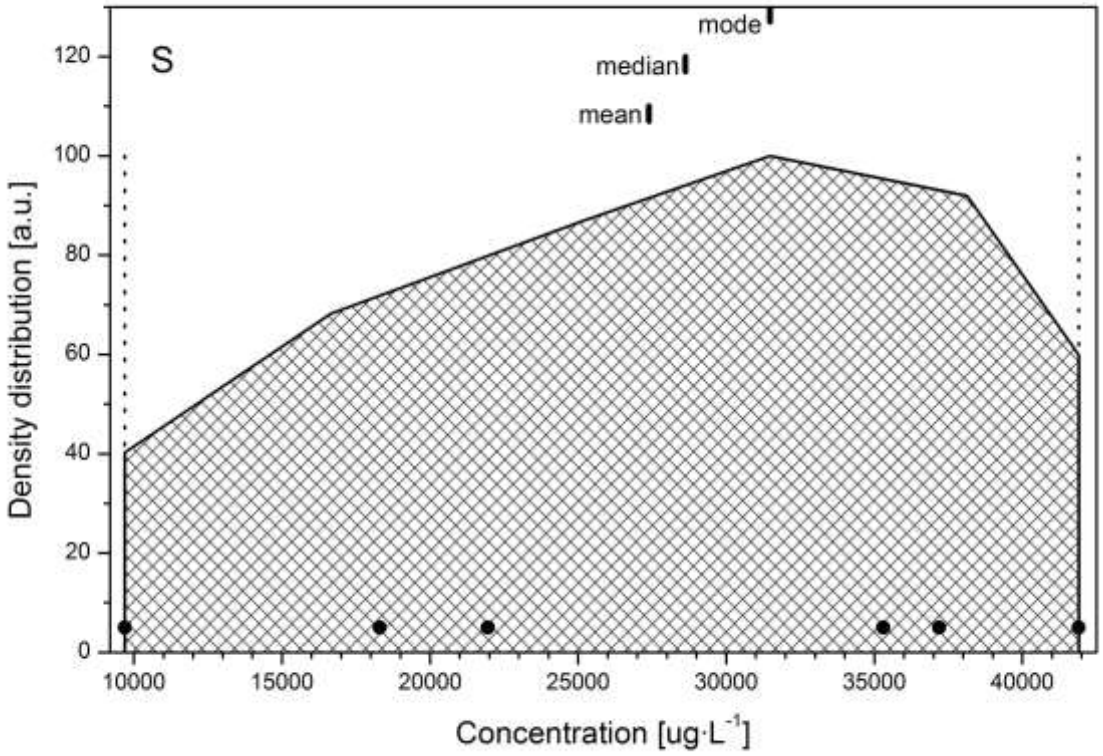

FIG. 16. The density distribution function for the analyte S in case of sample "1".

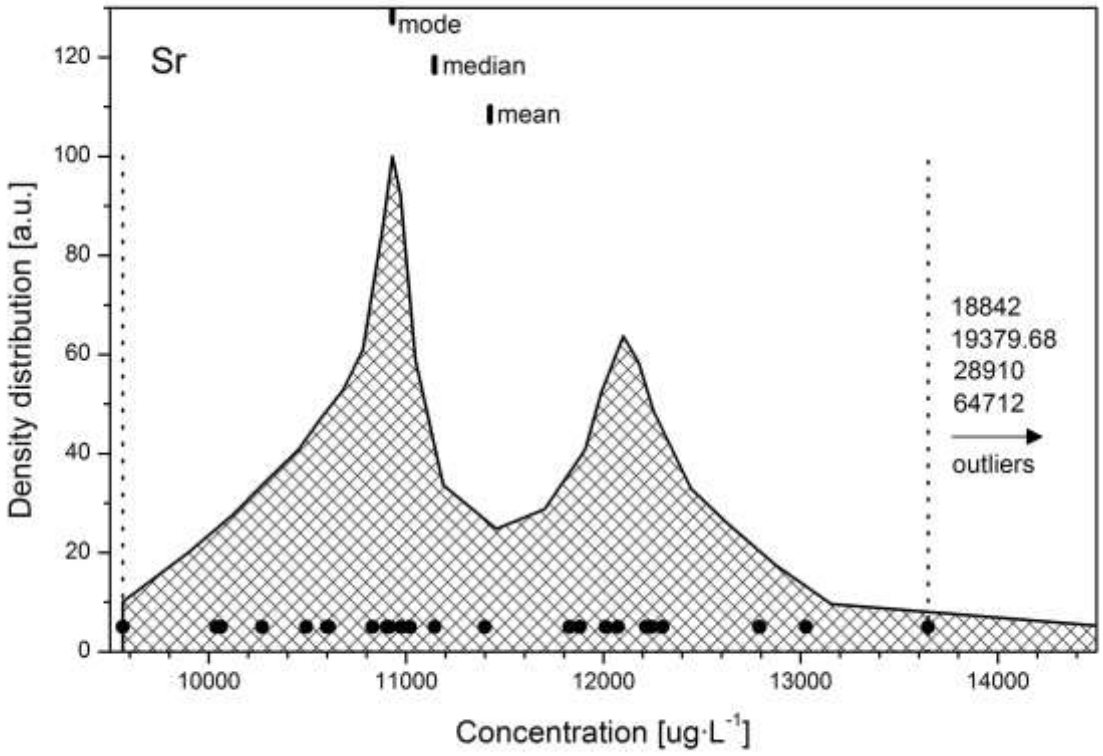

FIG. 17. The density distribution function for the analyte Sr in case of sample "1".

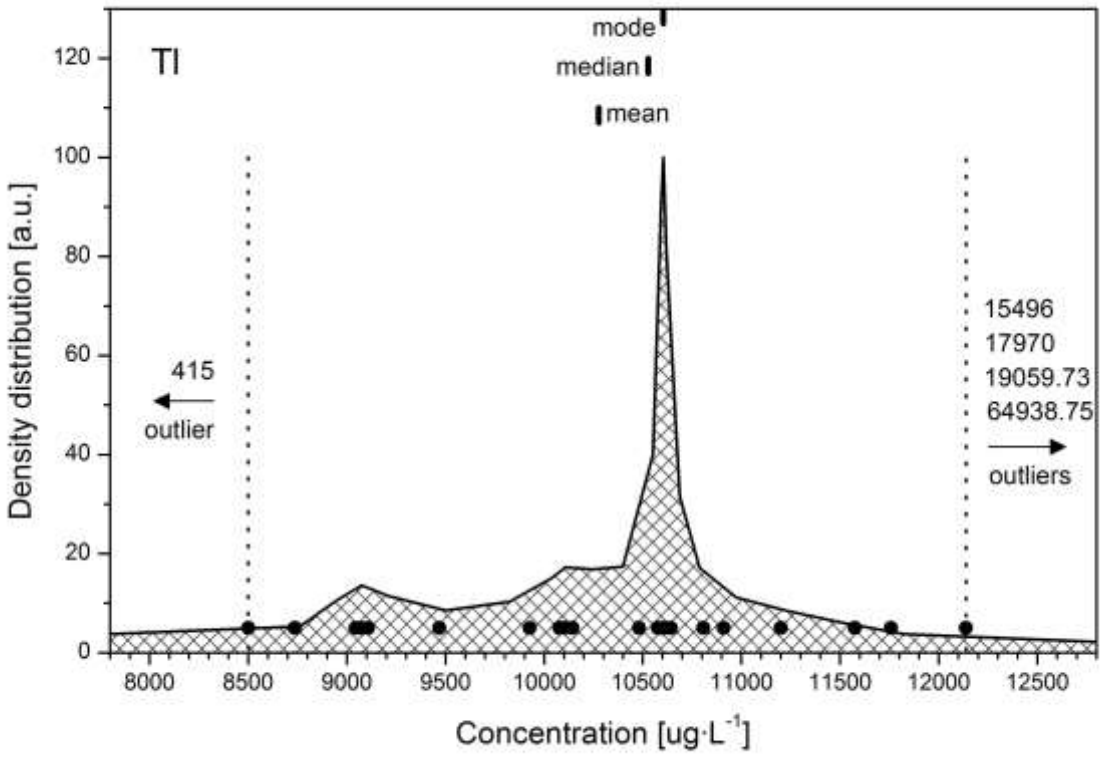

FIG. 18. The density distribution function for the analyte Tl in case of sample "1".

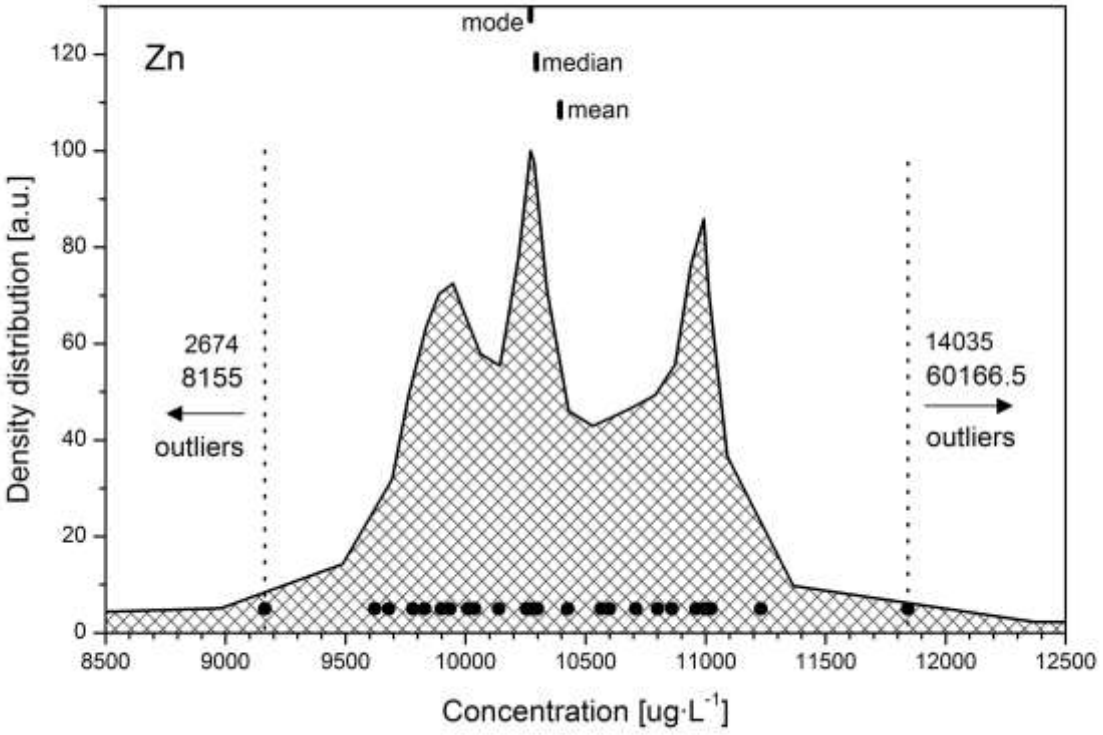

FIG. 19. The density distribution function for the analyte Zn in case of sample "1".

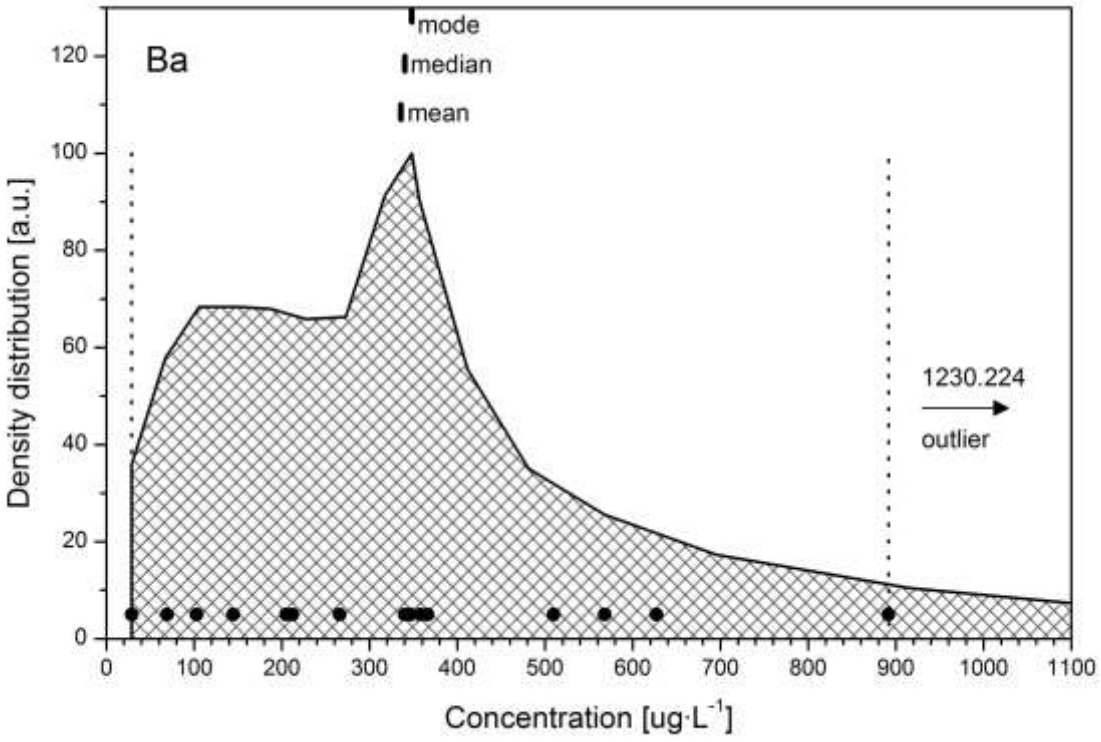

FIG. 20. The density distribution function for the analyte Ba in case of sample "2".

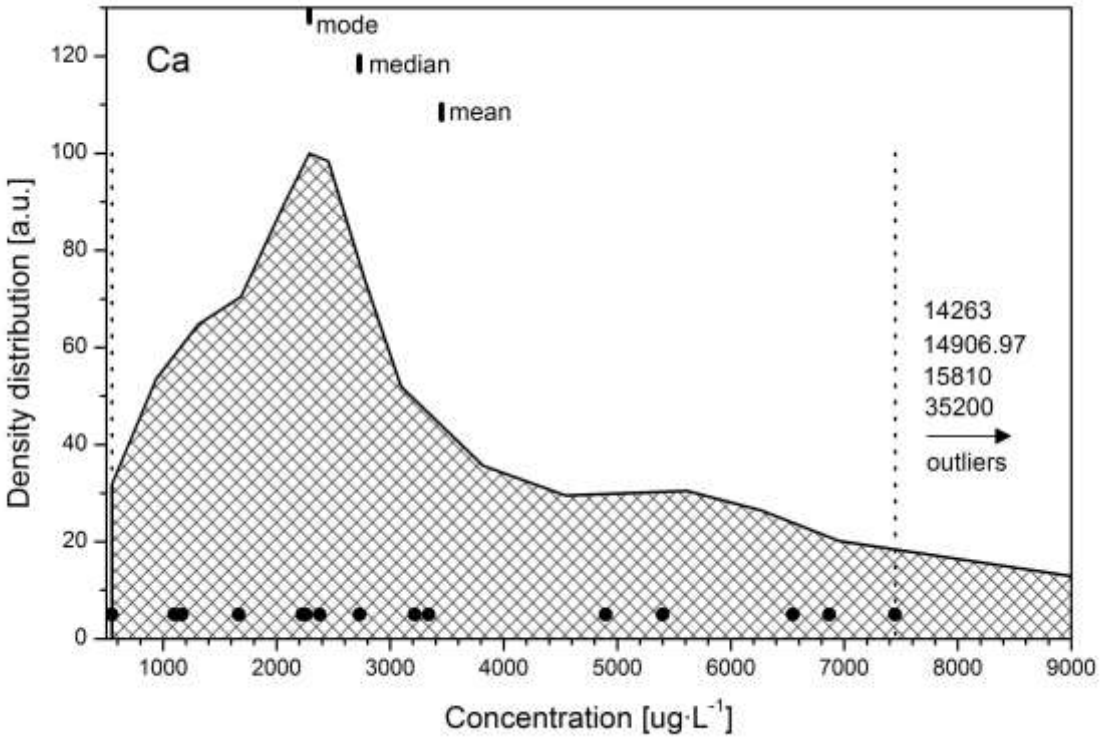

FIG. 21. The density distribution function for the analyte Ca in case of sample "2".

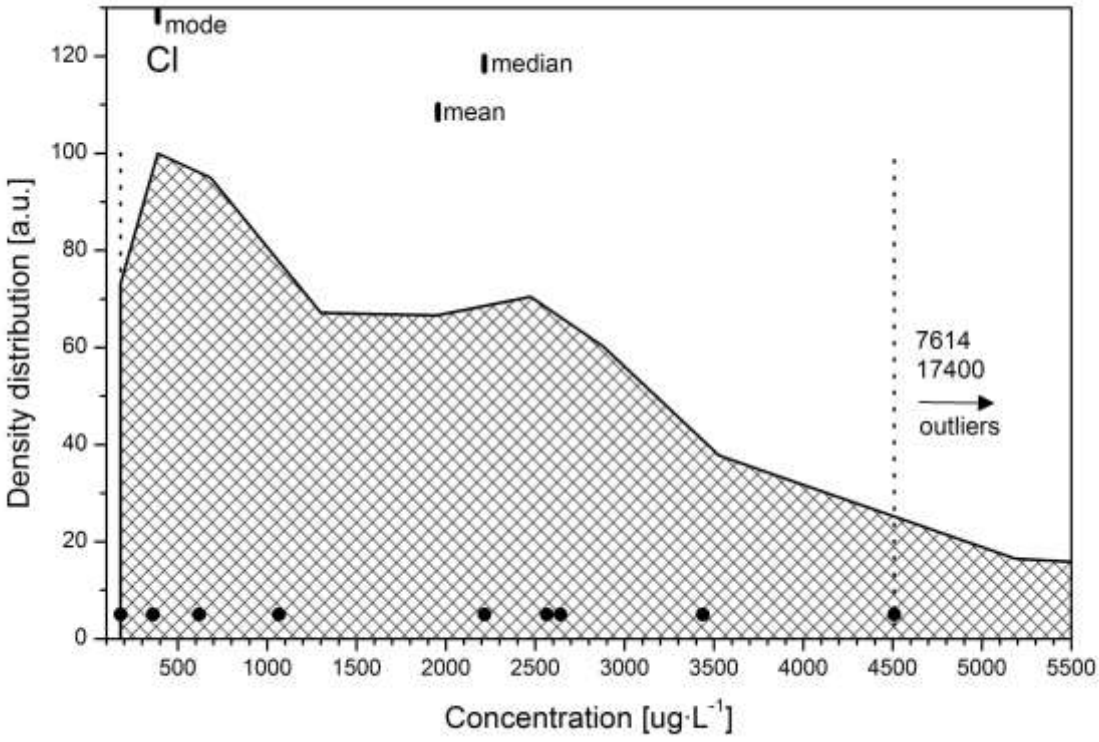

FIG. 22. The density distribution function for the analyte Cl in case of sample "2".

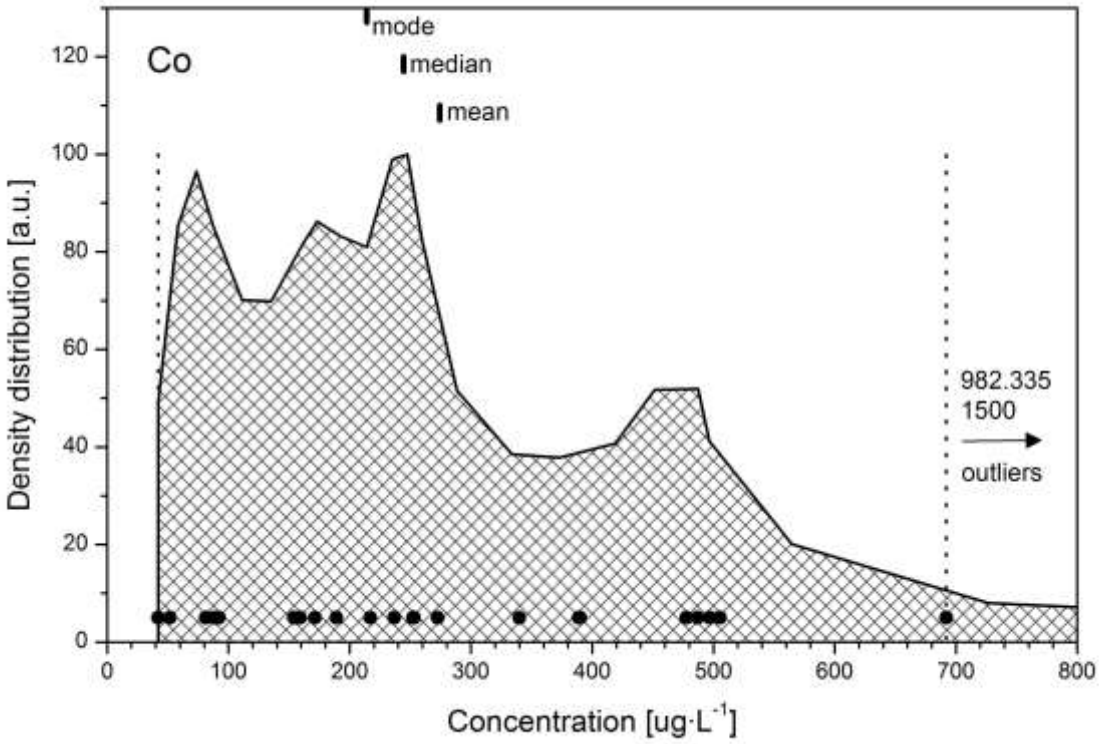

FIG. 23. The density distribution function for the analyte Co in case of sample "2".

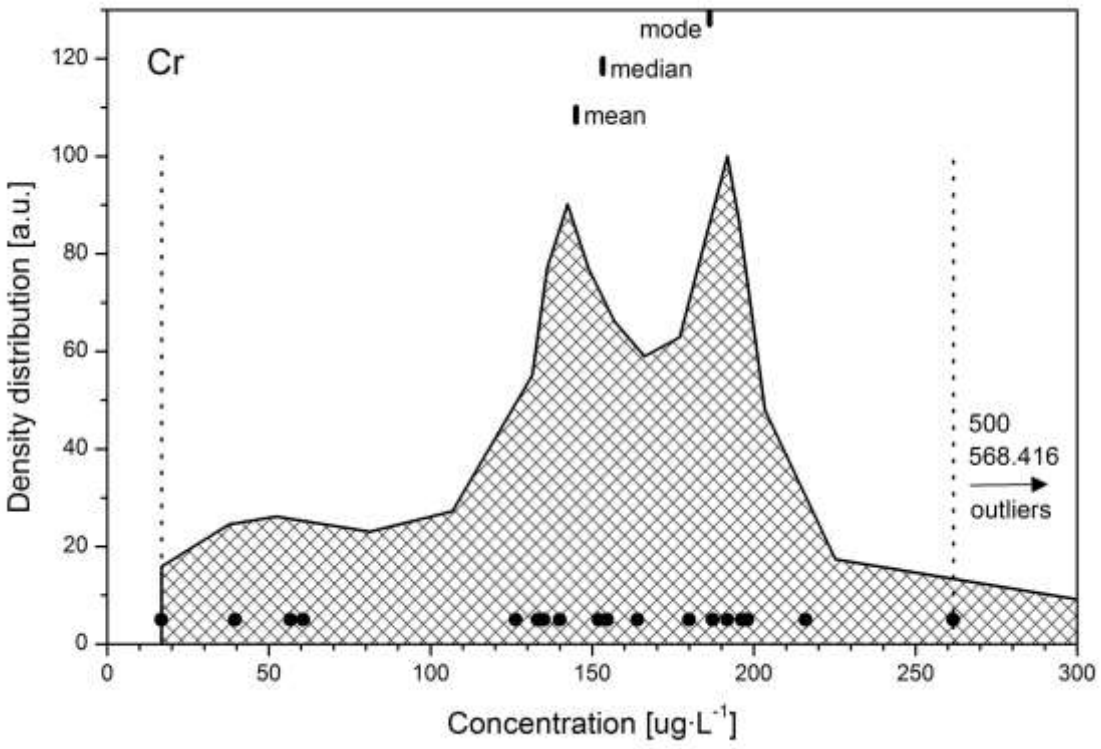

FIG. 24. The density distribution function for the analyte Cr in case of sample "2".

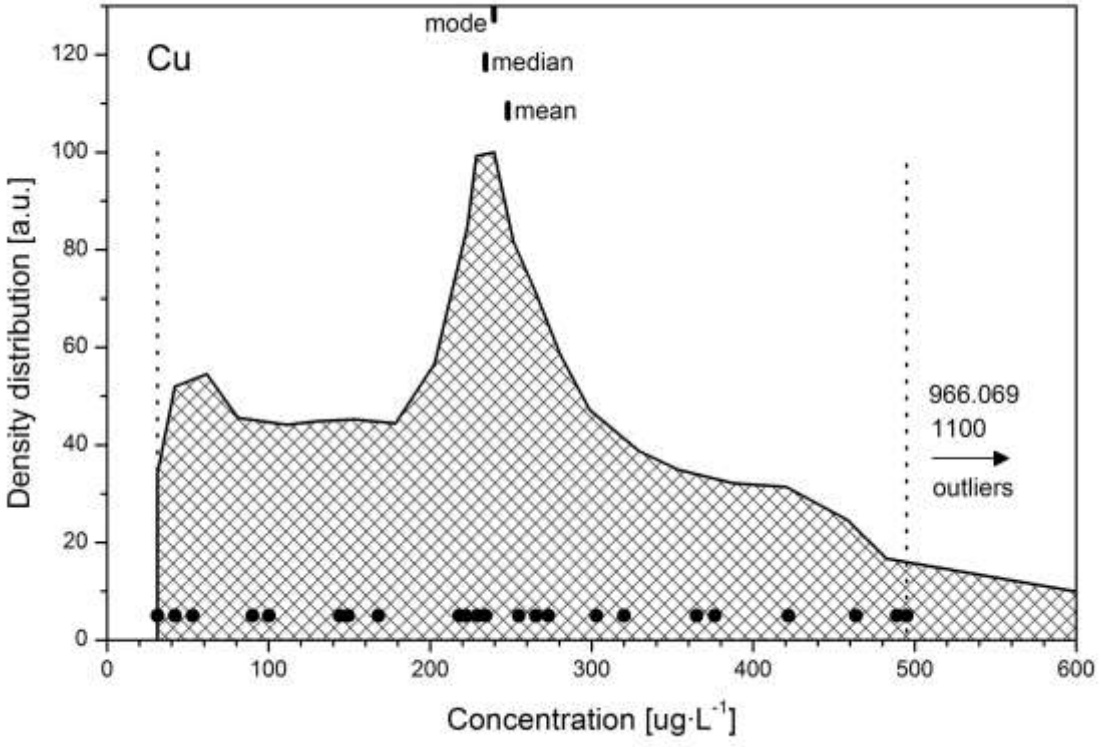

FIG. 25. The density distribution function for the analyte Cu in case of sample "2".

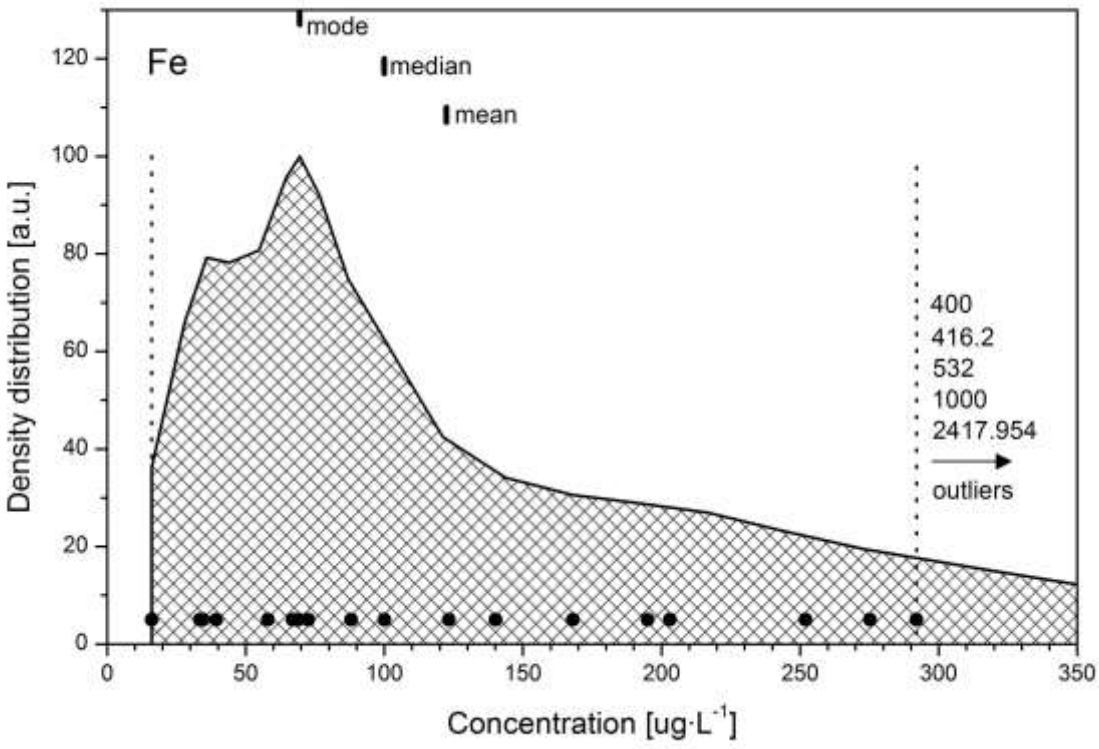

FIG. 26. The density distribution function for the analyte Fe in case of sample "2".

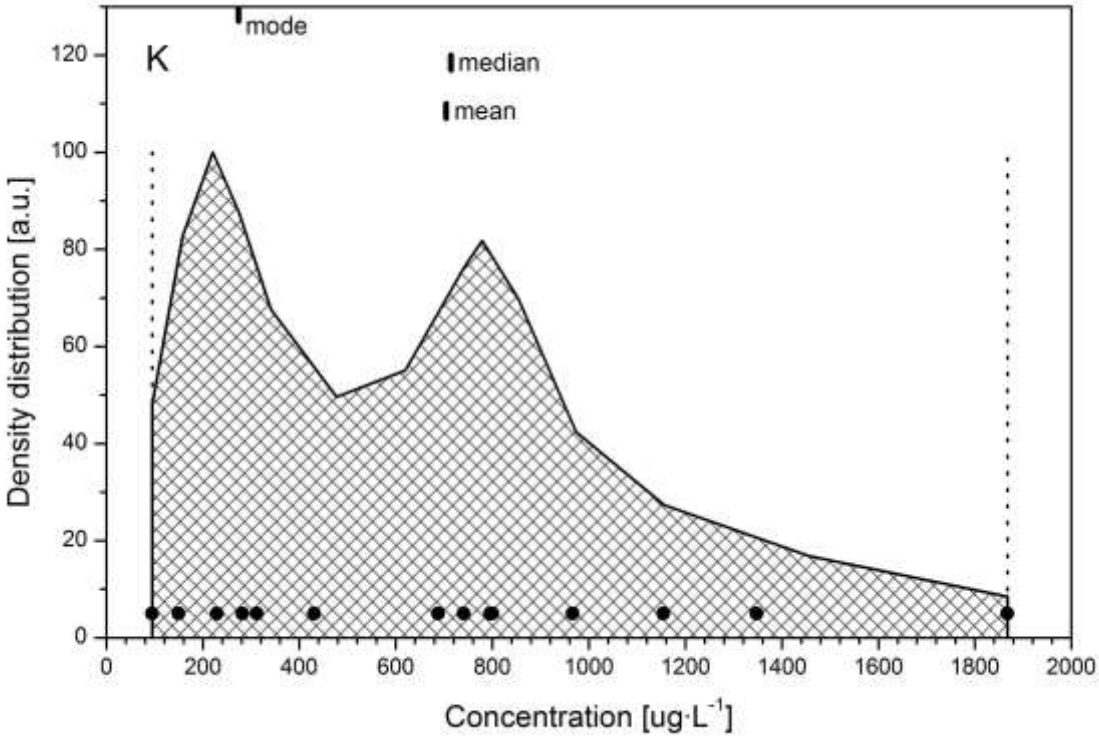

FIG. 27. The density distribution function for the analyte K in case of sample "2".

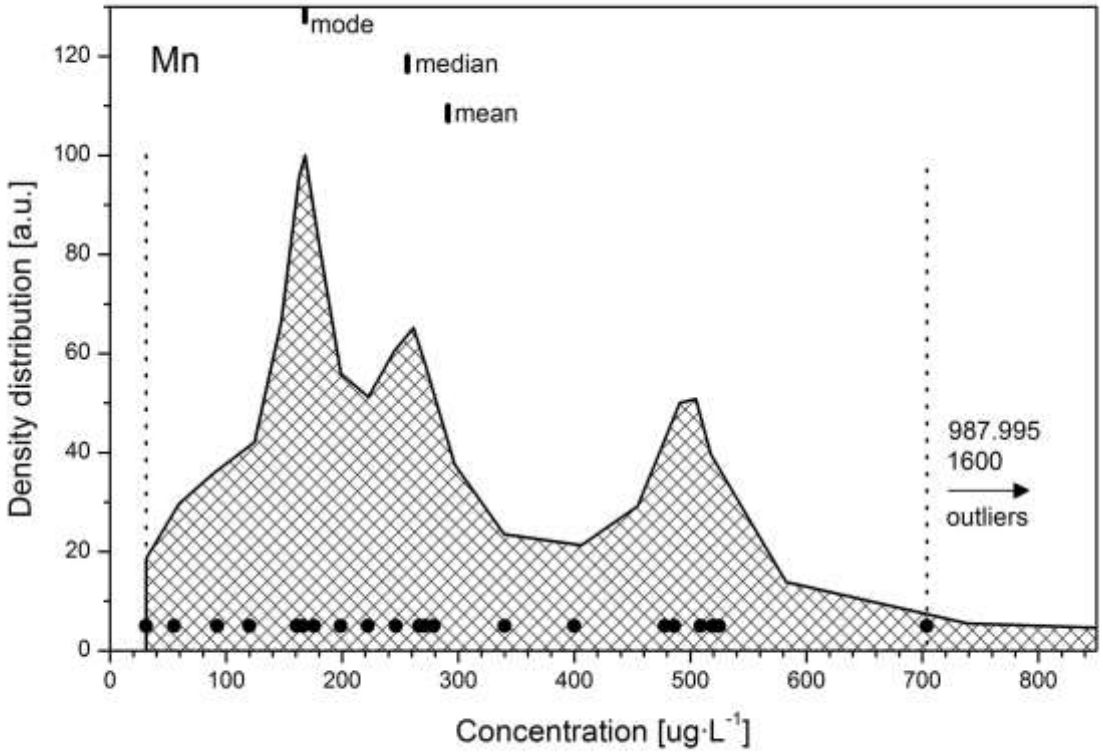

FIG. 28. The density distribution function for the analyte Mn in case of sample "2".

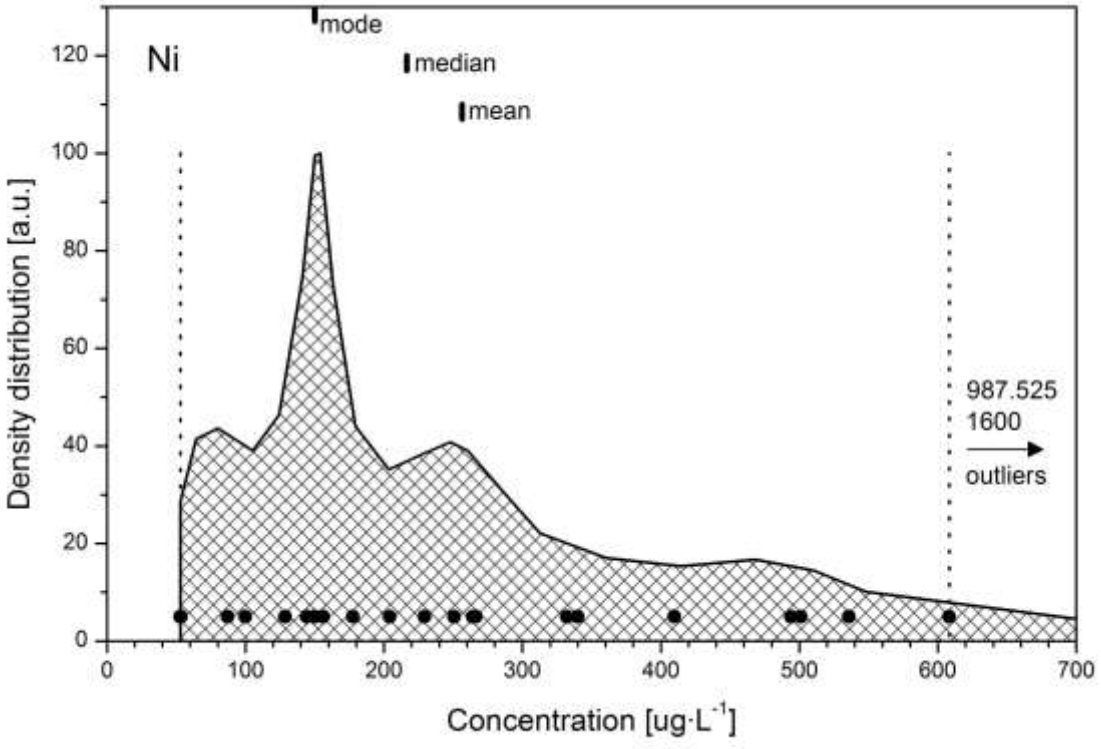

FIG. 29. The density distribution function for the analyte Ni in case of sample "2".

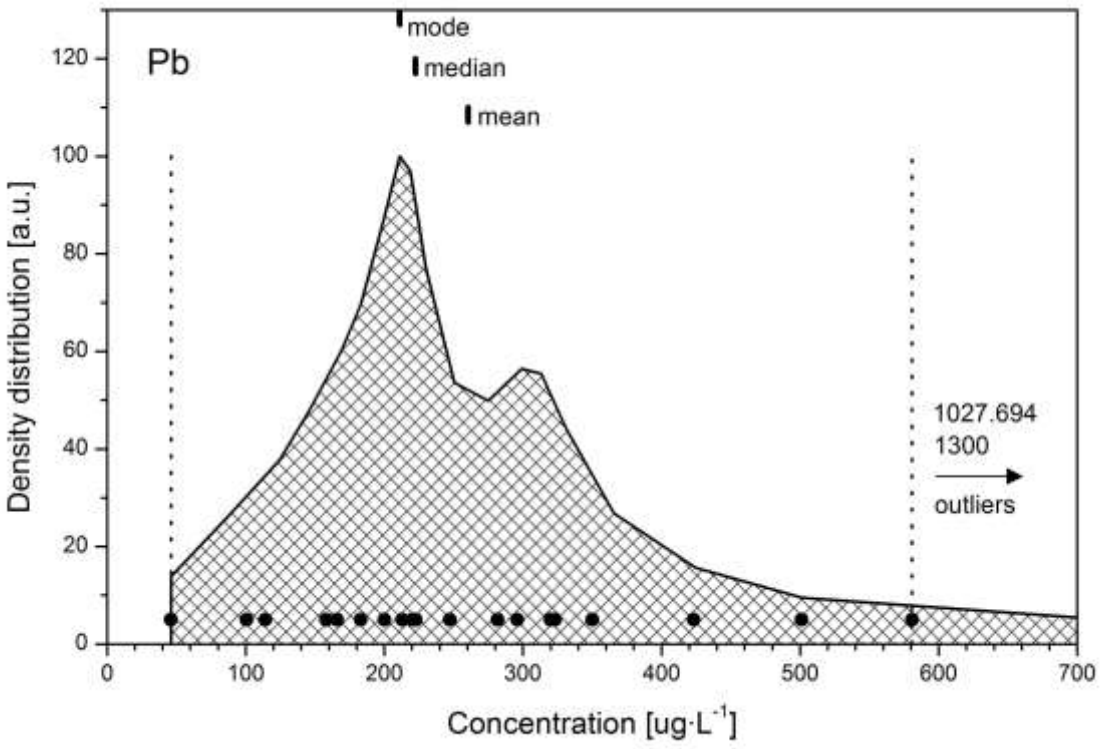

FIG. 30. The density distribution function for the analyte Pb in case of sample "2".

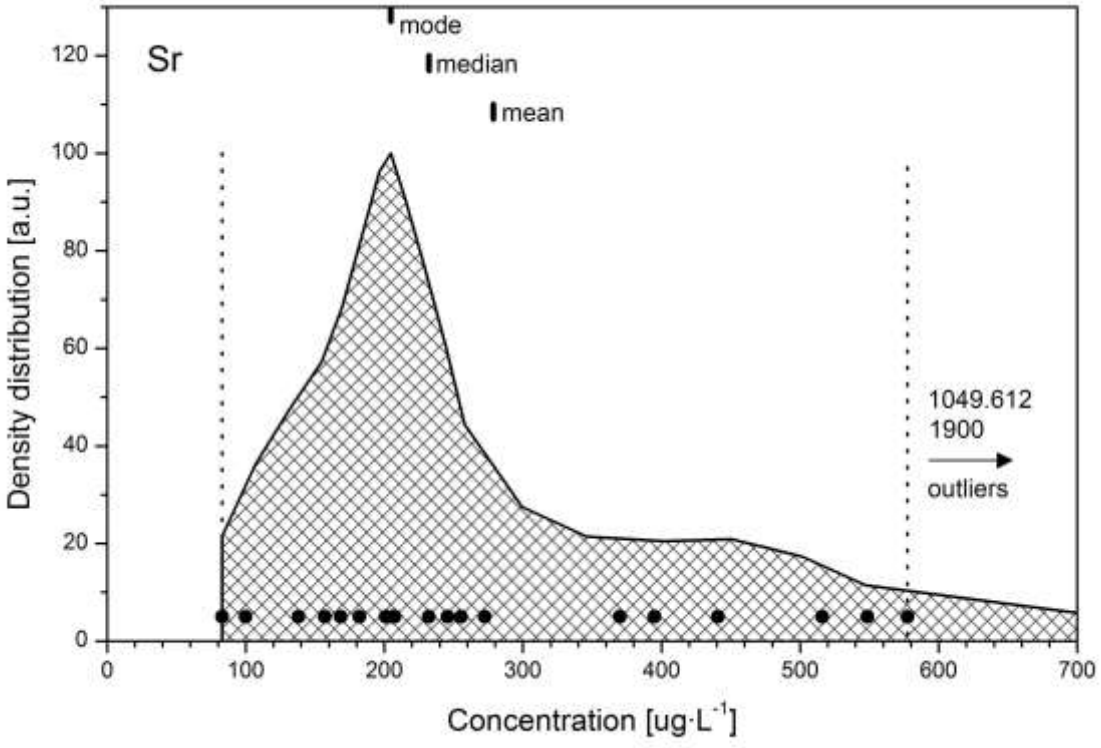

FIG. 31. The density distribution function for the analyte Sr in case of sample "2".

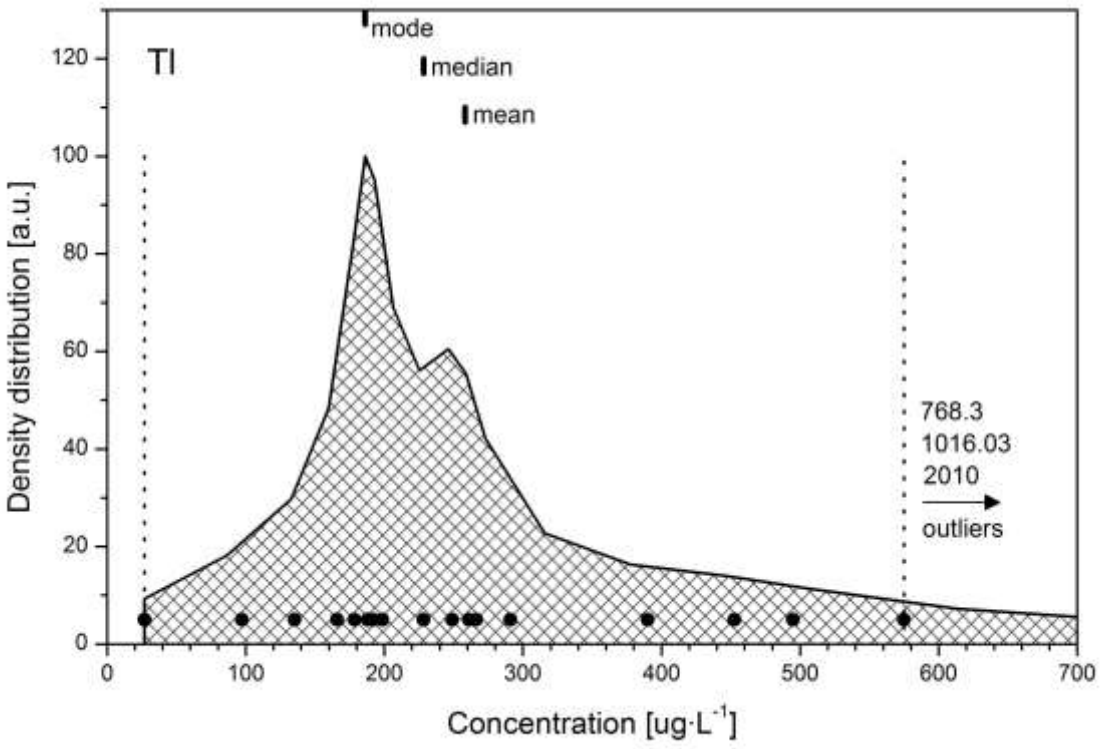

FIG. 32. The density distribution function for the analyte Tl in case of sample "2".

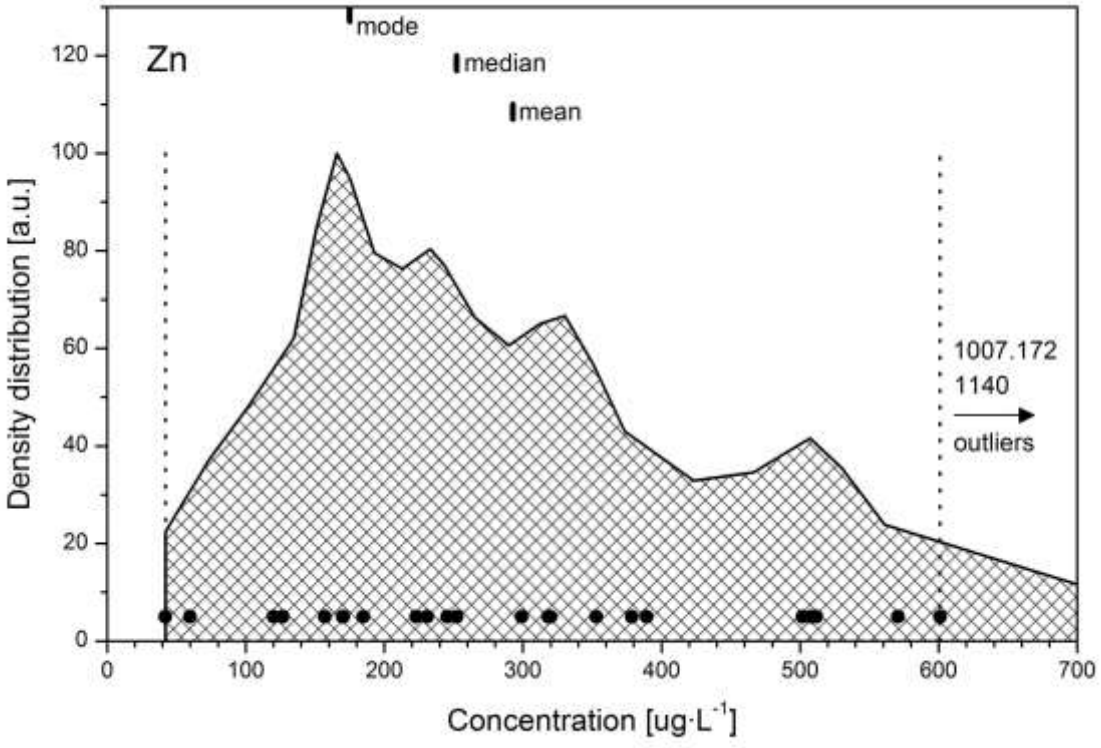

FIG. 33. The density distribution function for the analyte Zn in case of sample "2".

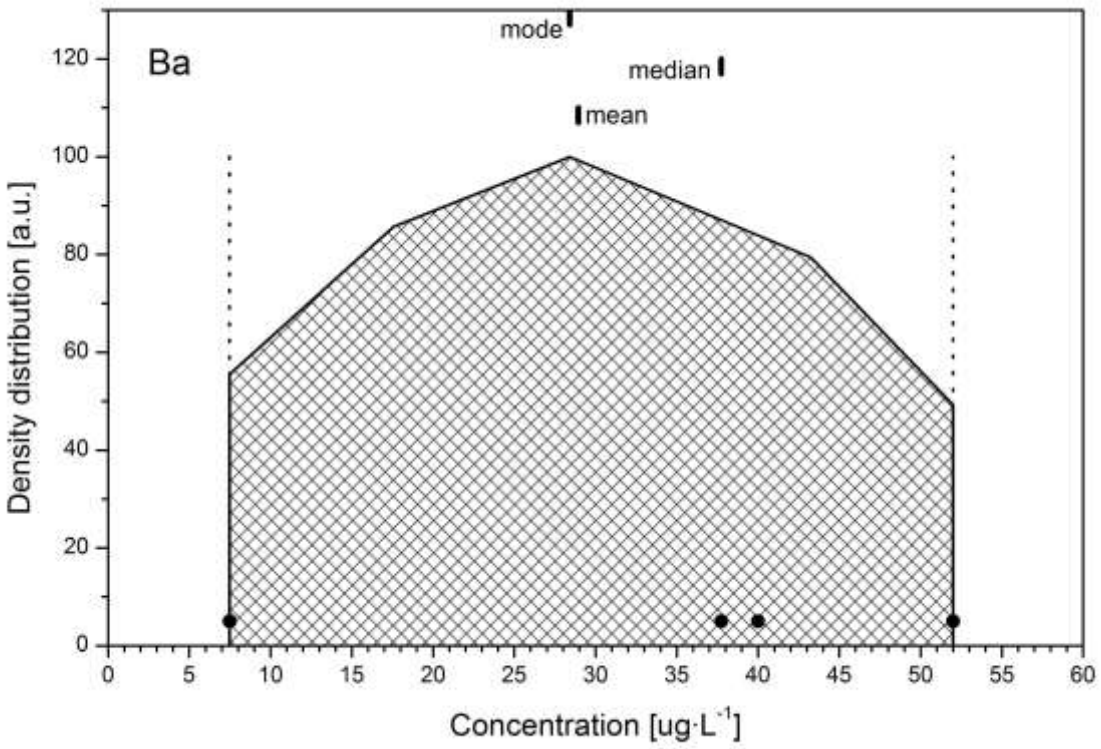

FIG. 34. The density distribution function for the analyte Ba in case of sample "3".

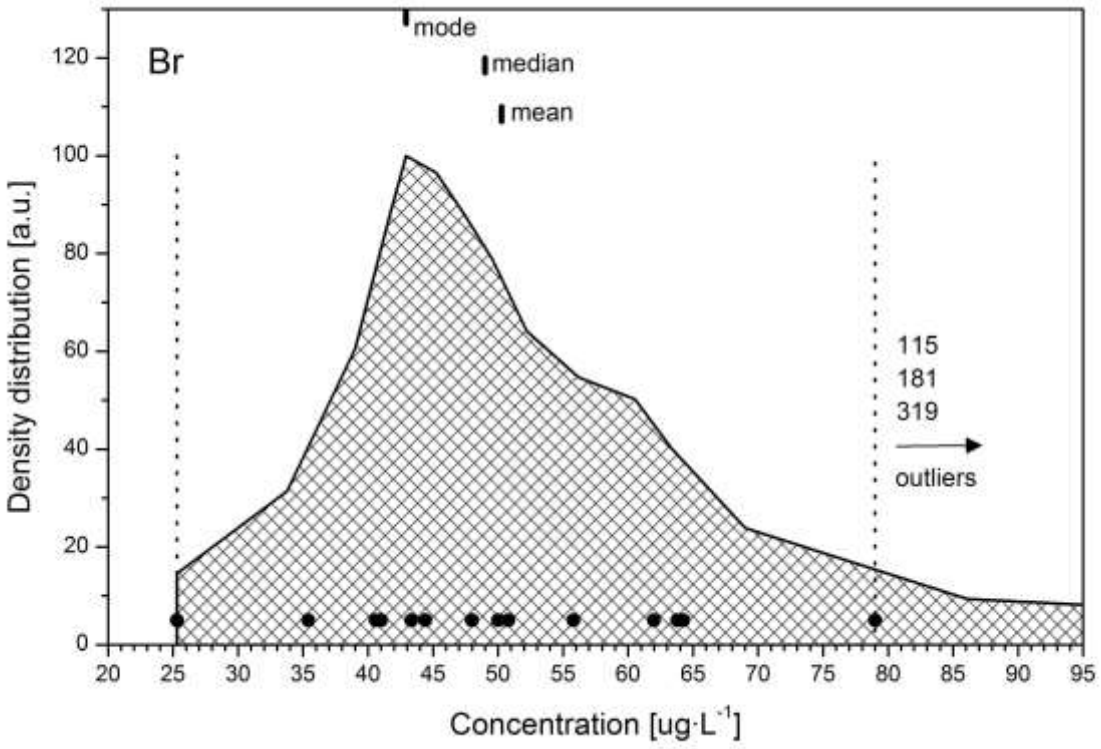

FIG. 35. The density distribution function for the analyte Br in case of sample "3".

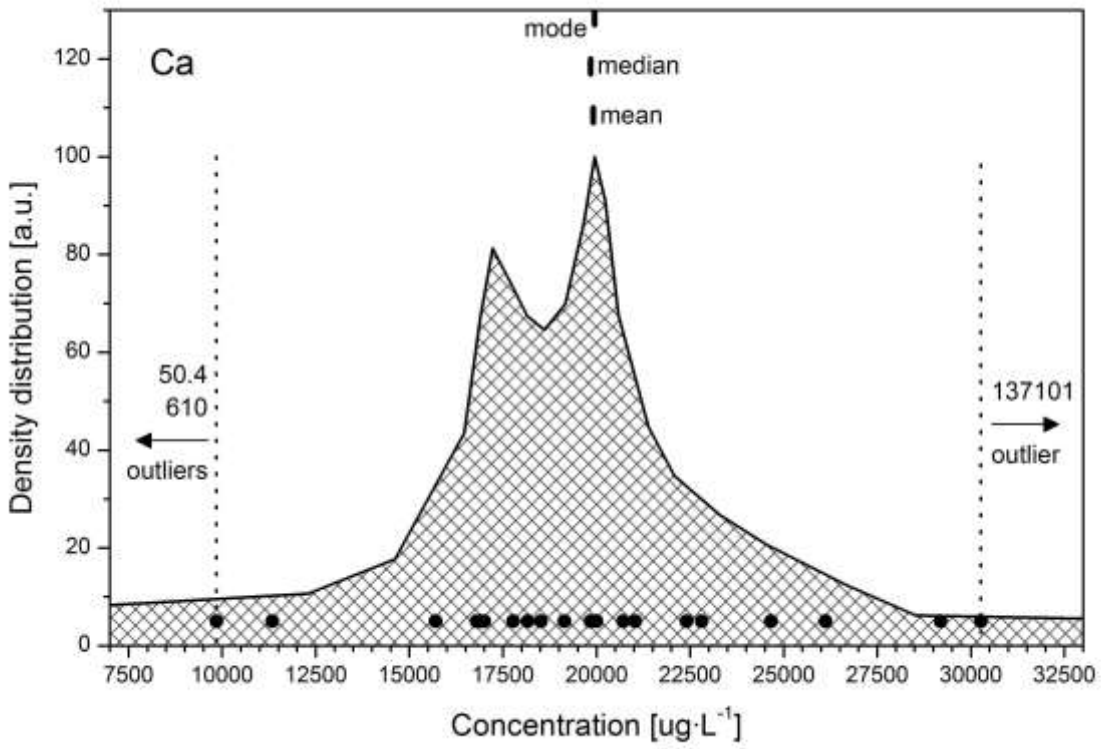

FIG. 36. The density distribution function for the analyte Ca in case of sample "3".

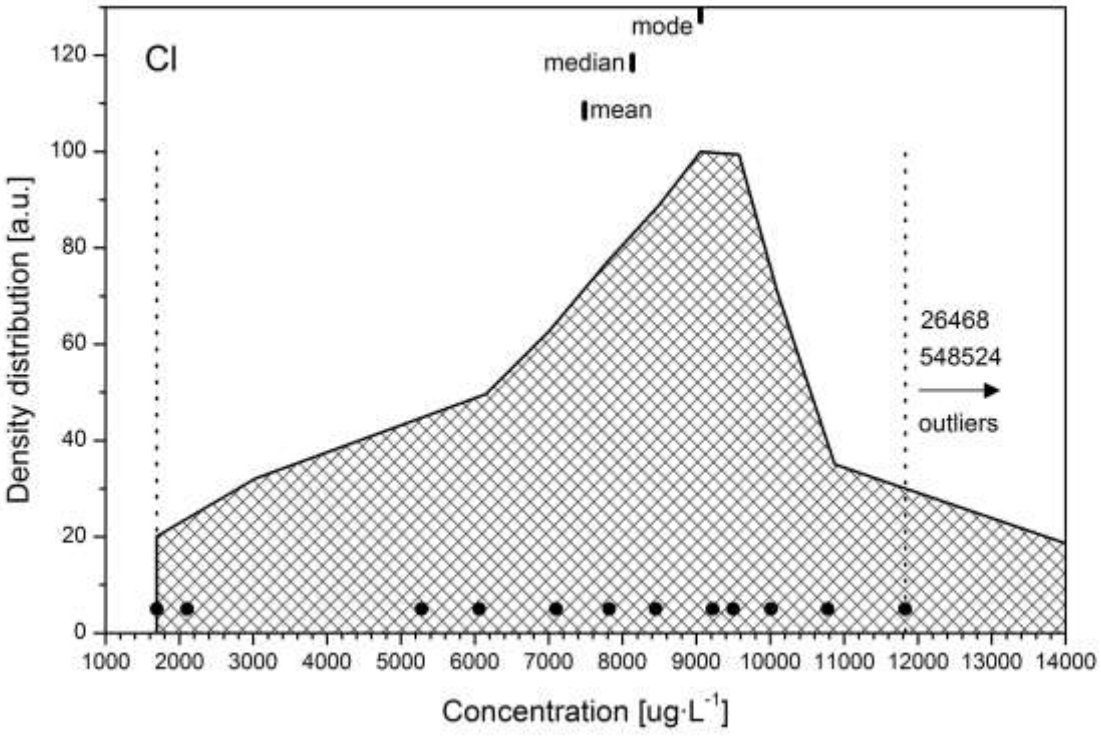

FIG. 37. The density distribution function for the analyte Cl in case of sample "3".

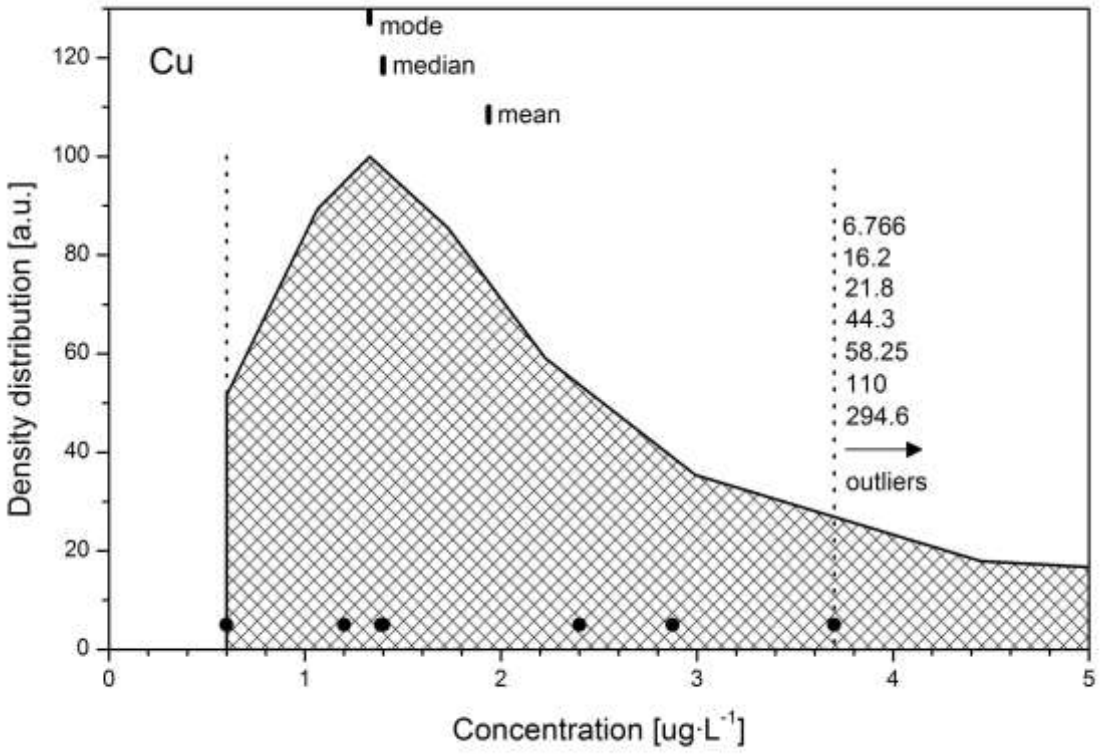

FIG. 38. The density distribution function for the analyte Cu in case of sample "3".

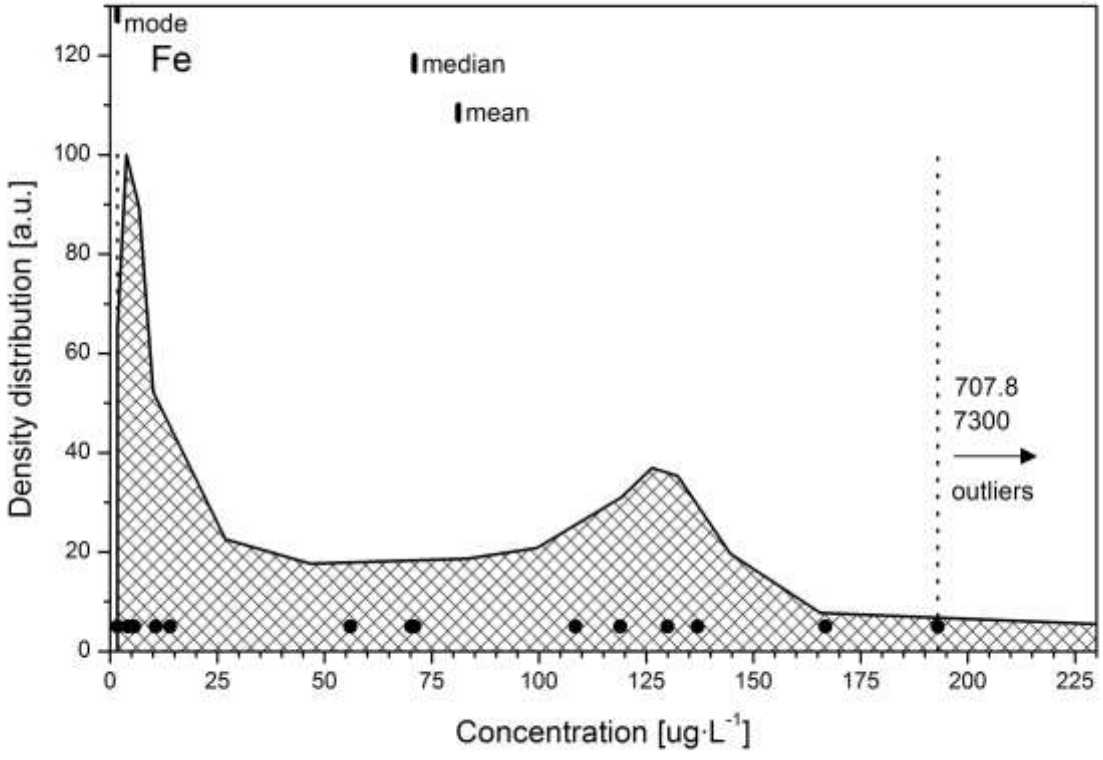

FIG. 39. The density distribution function for the analyte Fe in case of sample "3".

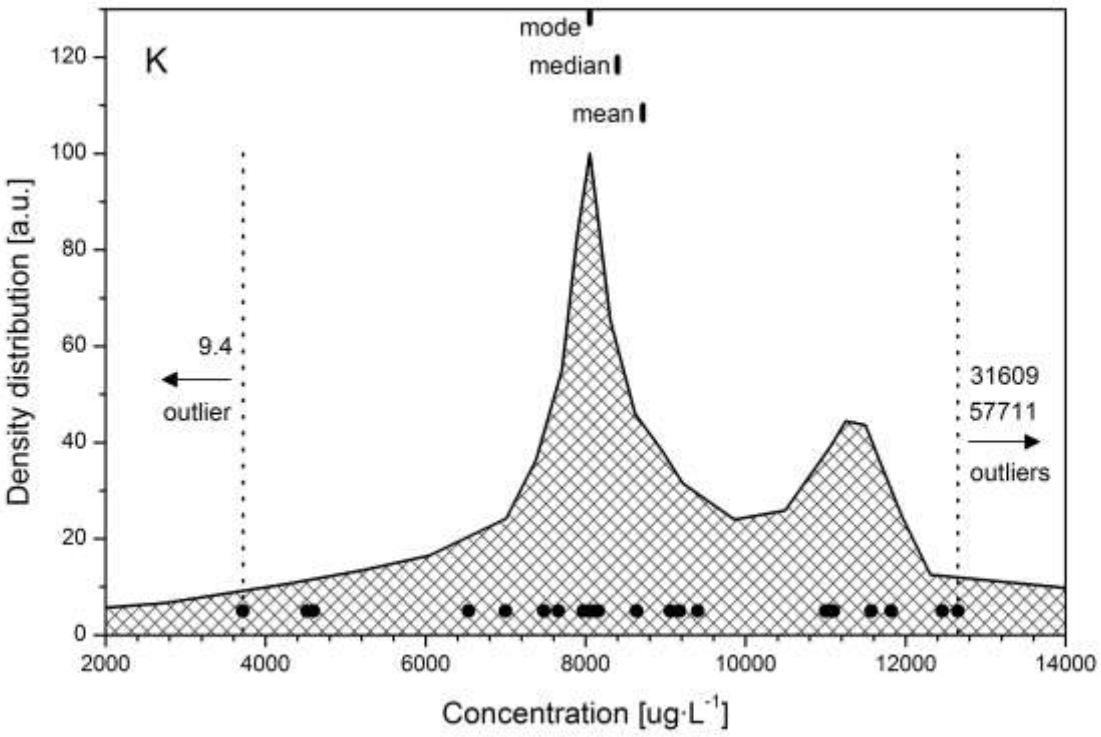

FIG. 40. The density distribution function for the analyte K in case of sample "3".

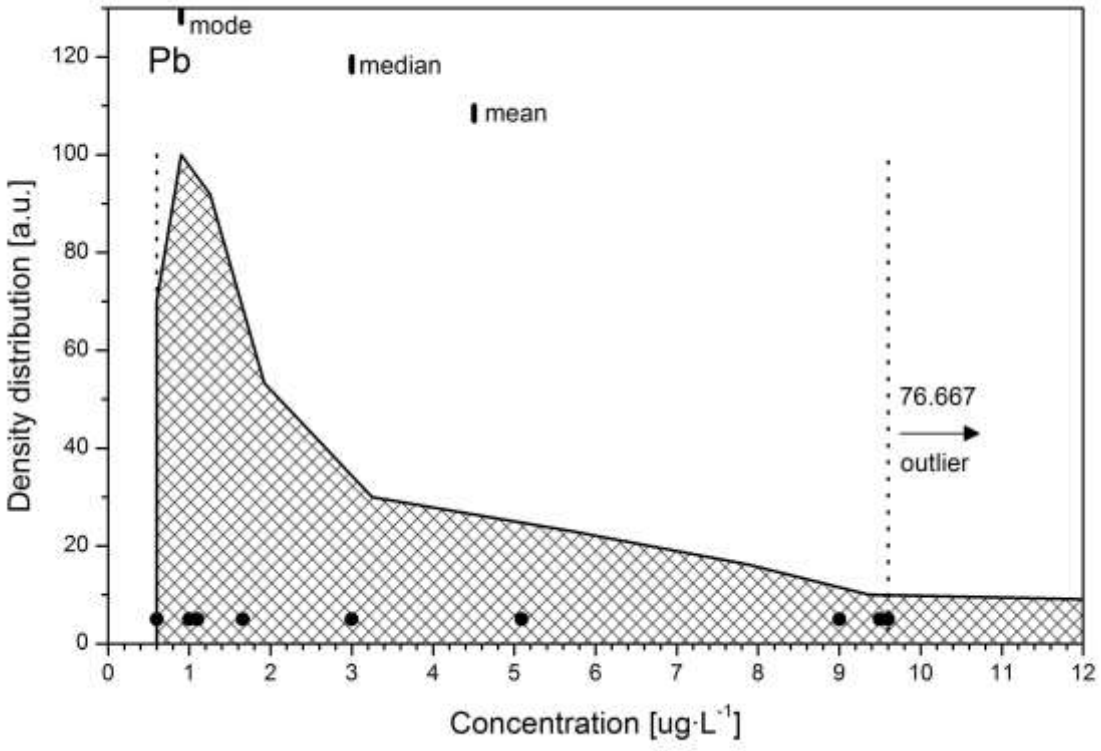

FIG. 41. The density distribution function for the analyte Pb in case of sample "3".

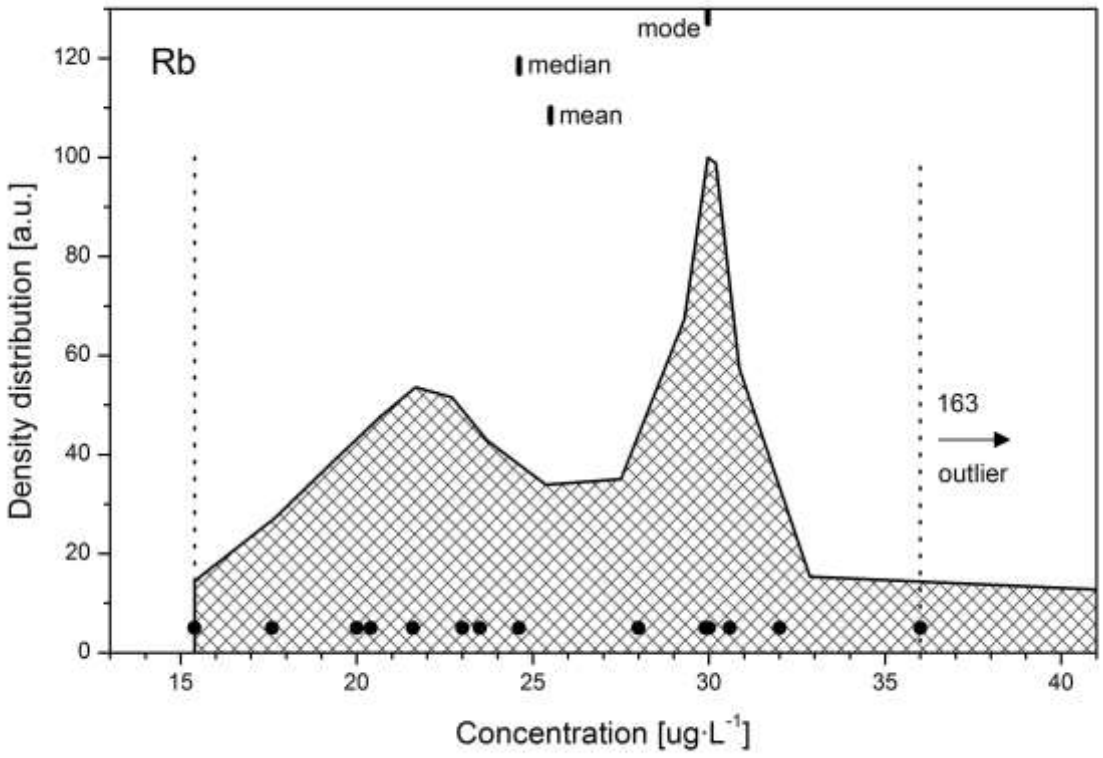

FIG. 42. The density distribution function for the analyte Rb in case of sample "3".

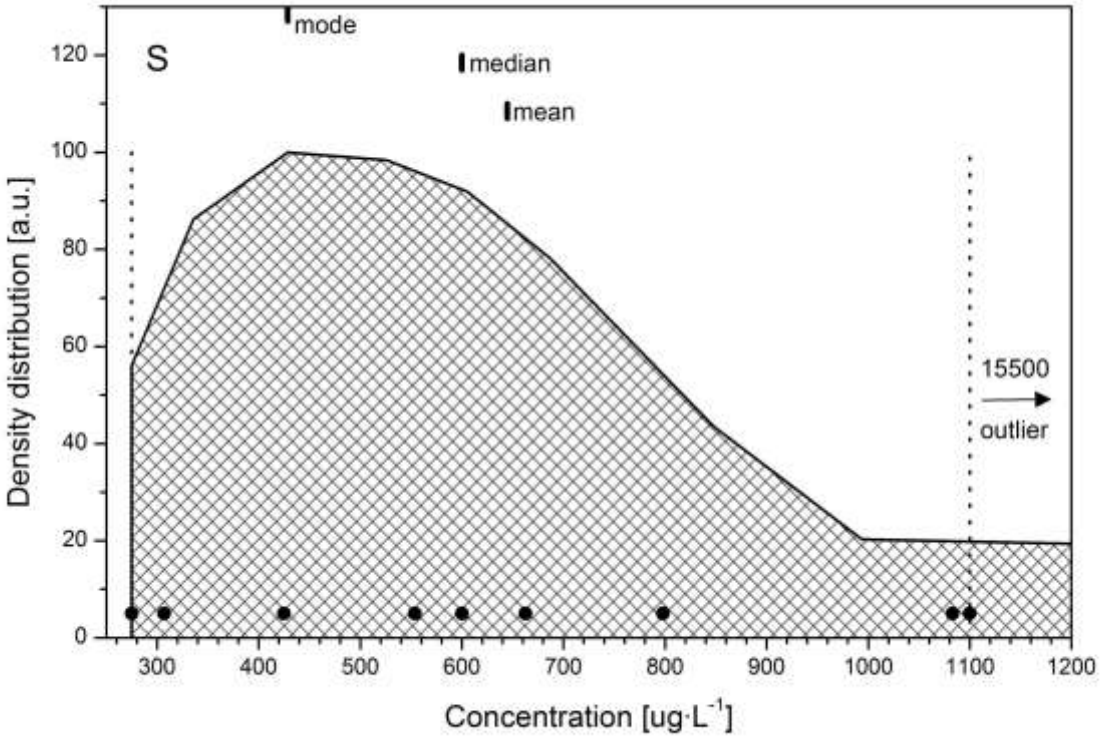

FIG. 43. The density distribution function for the analyte S in case of sample "3".

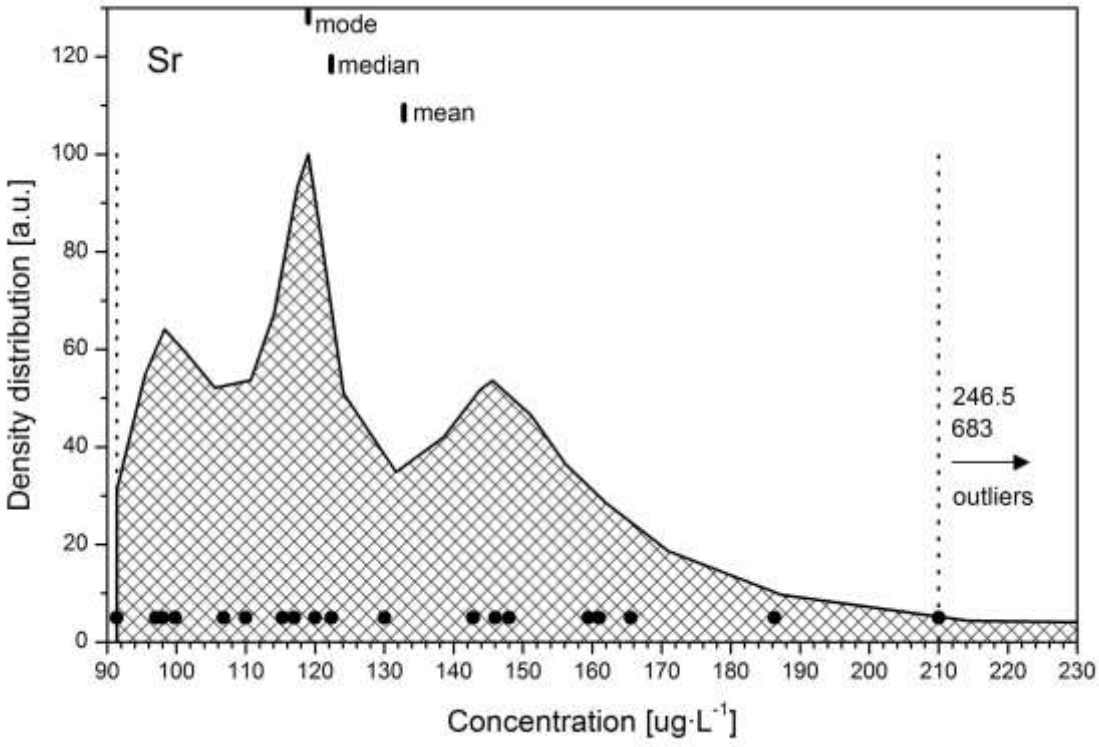

FIG. 44. The density distribution function for the analyte Sr in case of sample "3".

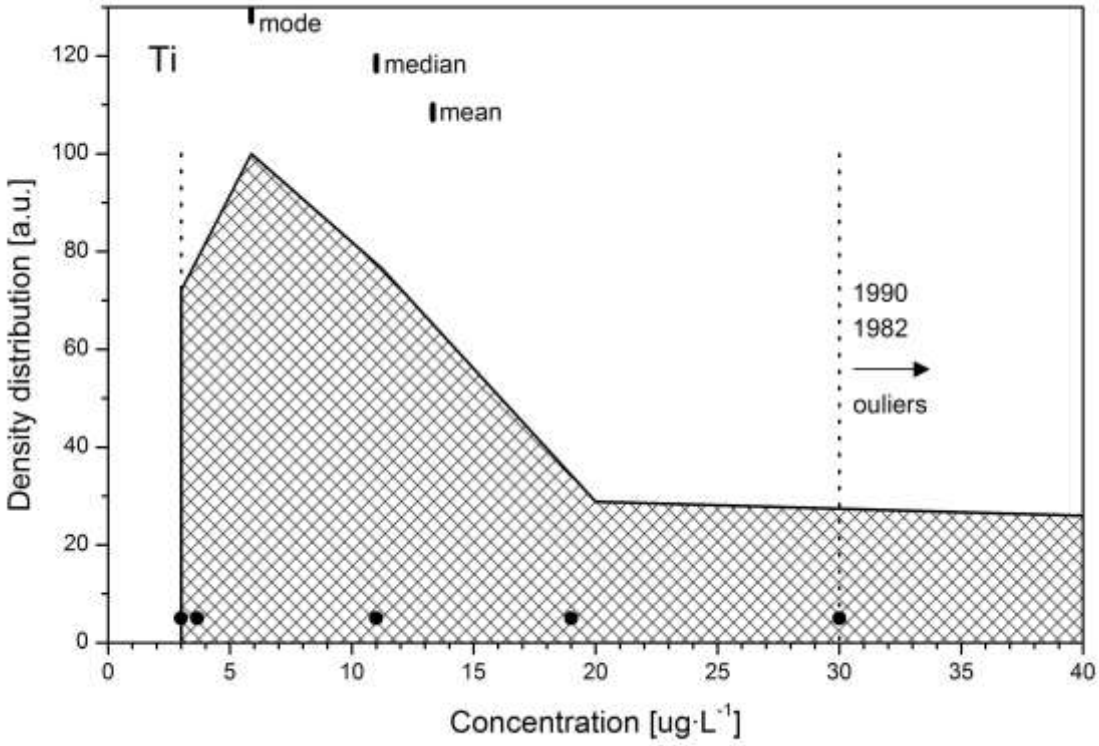

FIG. 45. The density distribution function for the analyte Ti in case of sample "3".

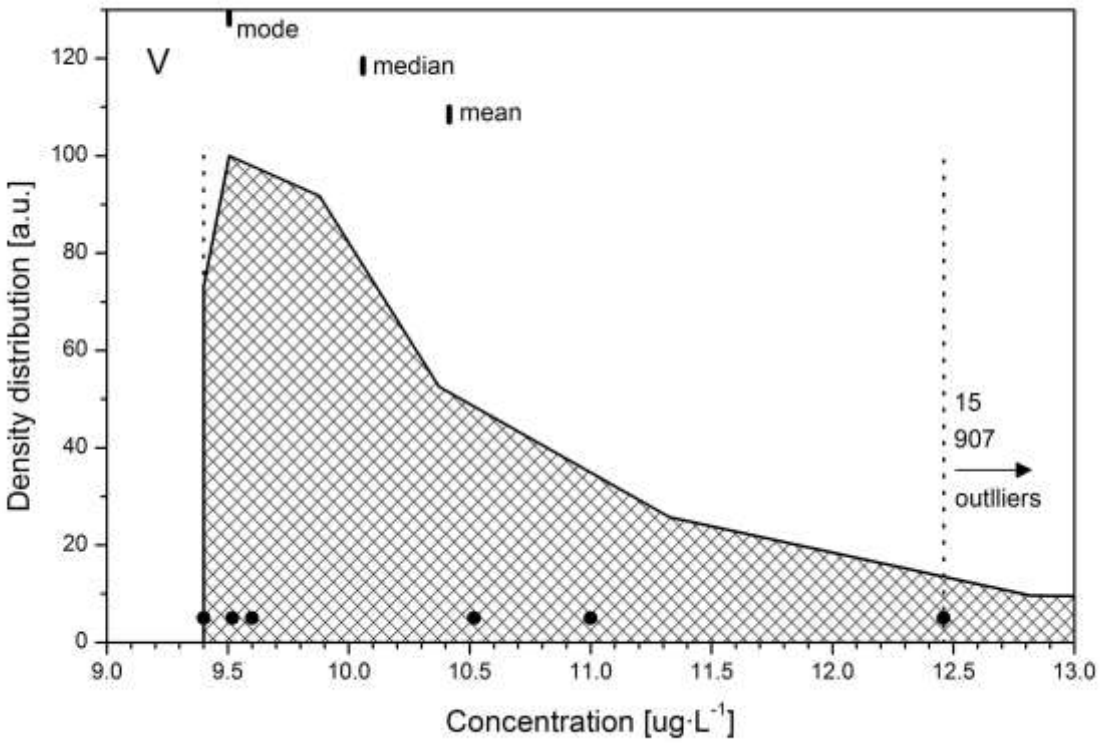

FIG. 46. The density distribution function for the analyte V in case of sample "3".

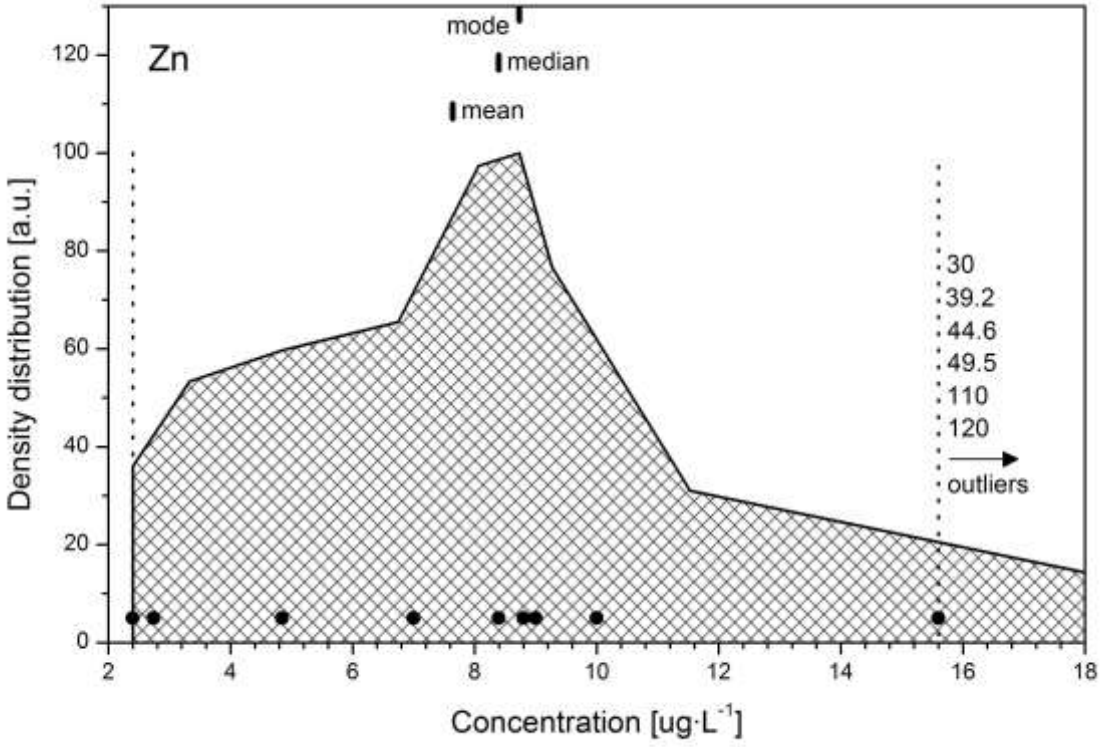

FIG. 47. The density distribution function for the analyte Zn in case of sample "3".

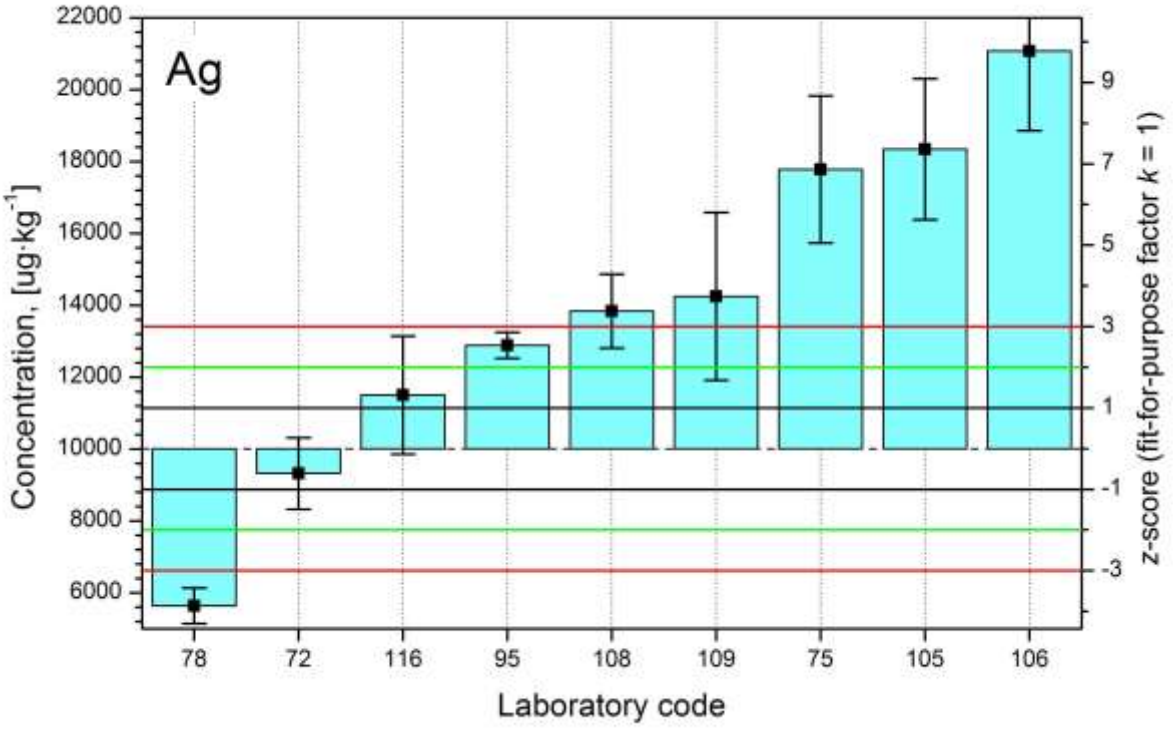

FIG. 48. Distributions of z-scores for analyte Ag in case of sample "1".

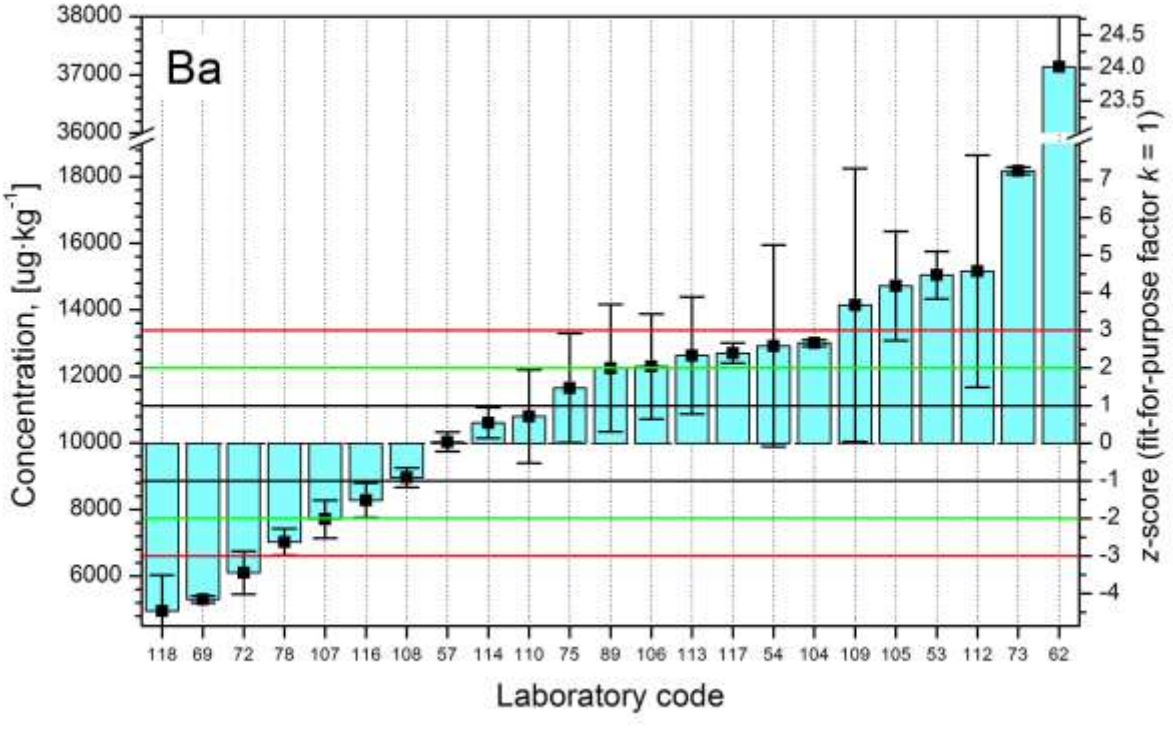

FIG. 49. Distributions of z-scores for analyte Ba in case of sample "1".

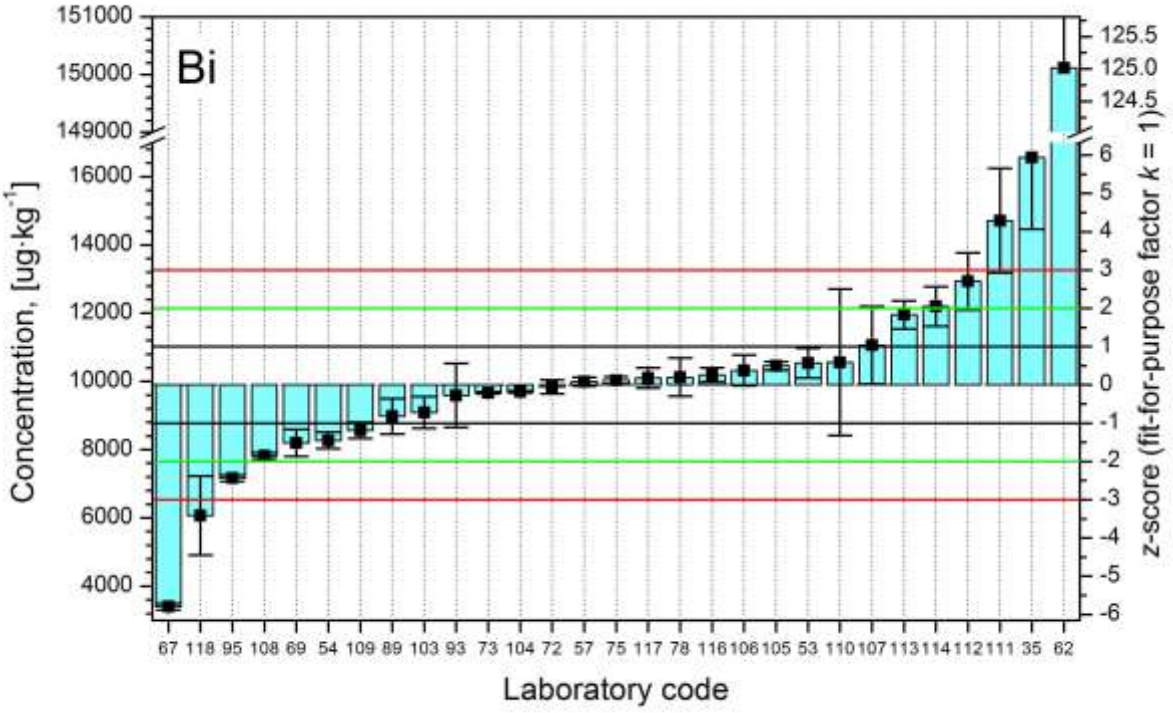

FIG. 50. Distributions of z-scores for analyte Bi in case of sample "1".

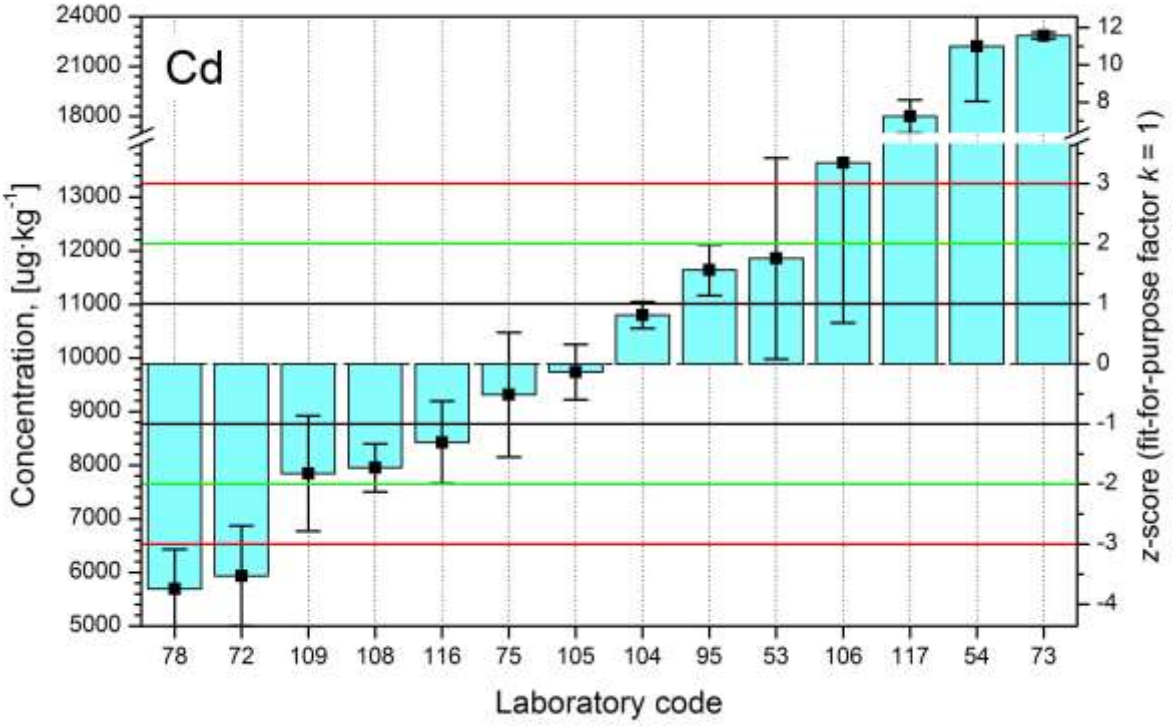

FIG. 51. Distributions of z-scores for analyte Cd in case of sample "1".

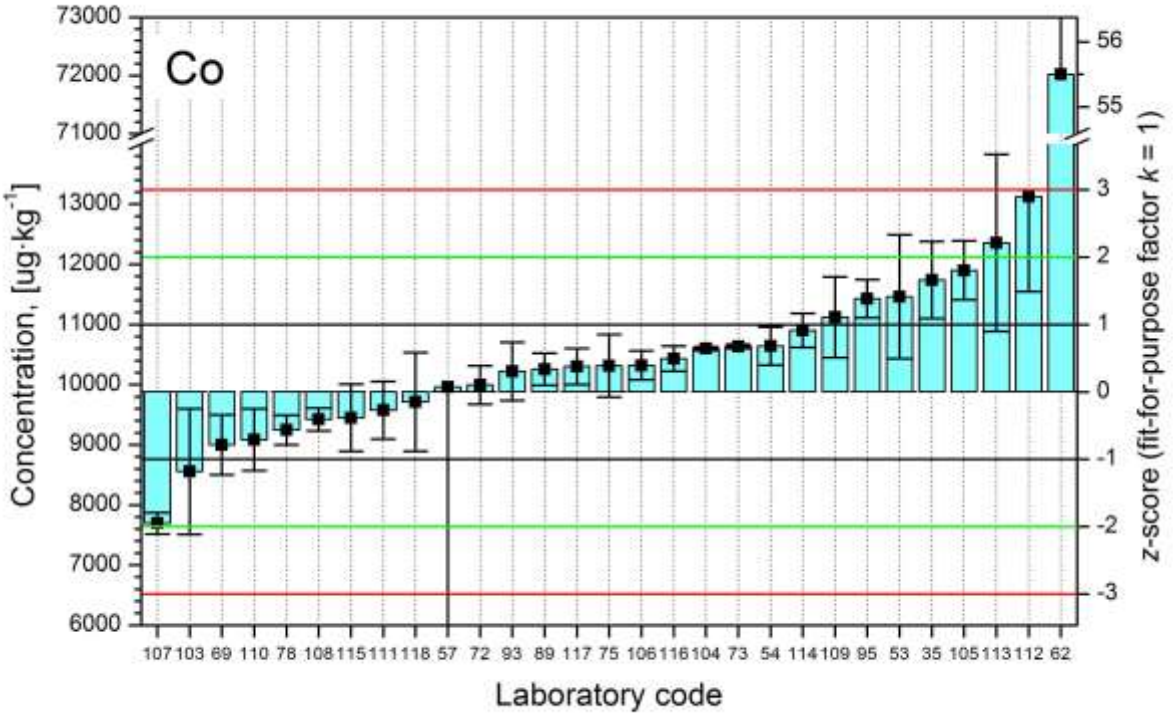

FIG. 52. Distributions of z-scores for analyte Co in case of sample "1".

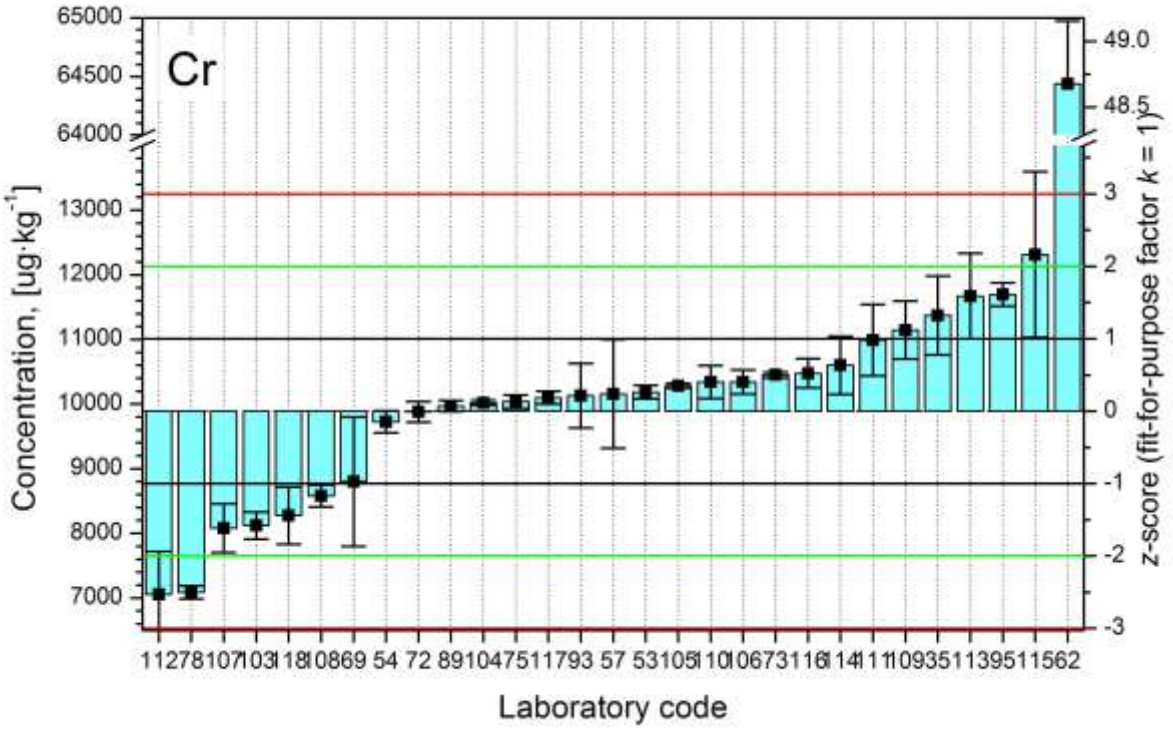

FIG. 53. Distributions of z-scores for analyte Cr in case of sample "1".

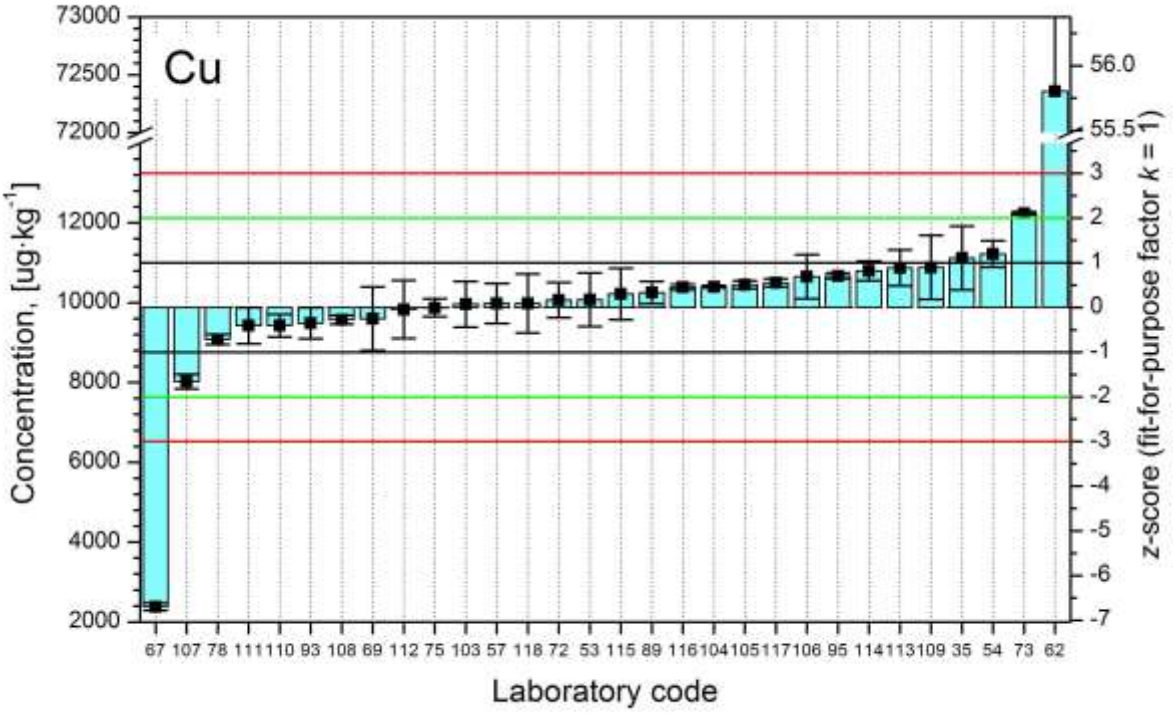

FIG. 54. Distributions of z-scores for analyte Cu in case of sample "1".

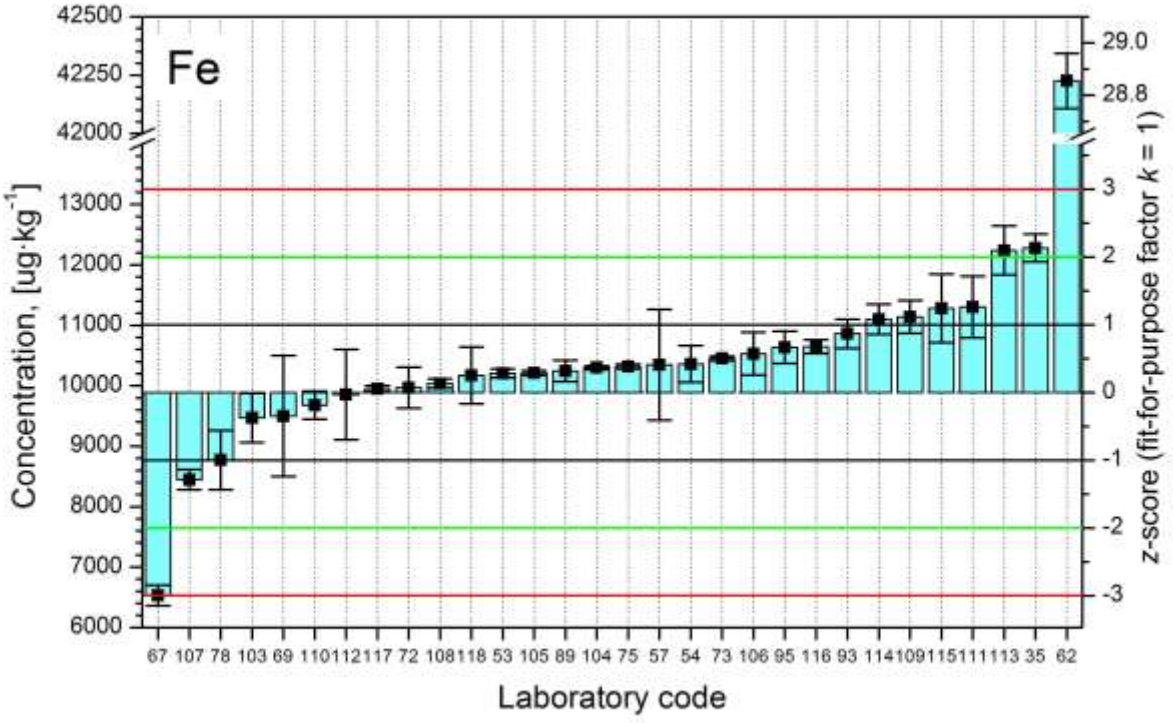

FIG. 55. Distributions of z-scores for analyte Fe in case of sample "1".

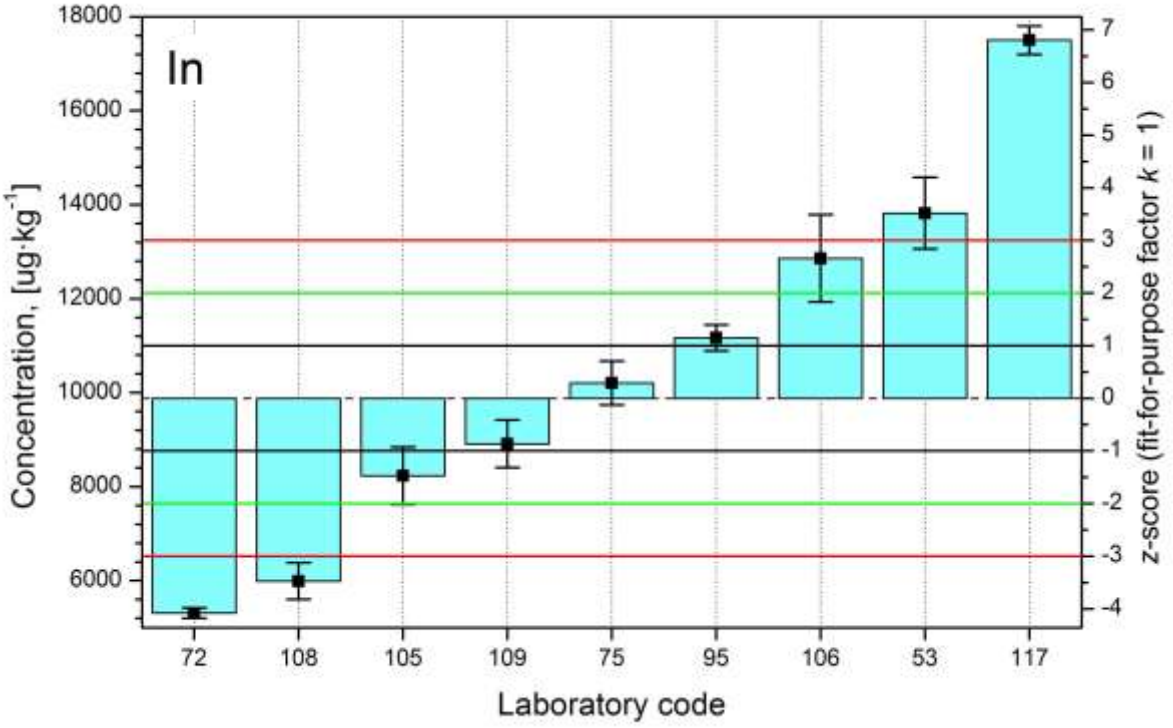

FIG. 56. Distributions of z-scores for analyte In in case of sample "1".

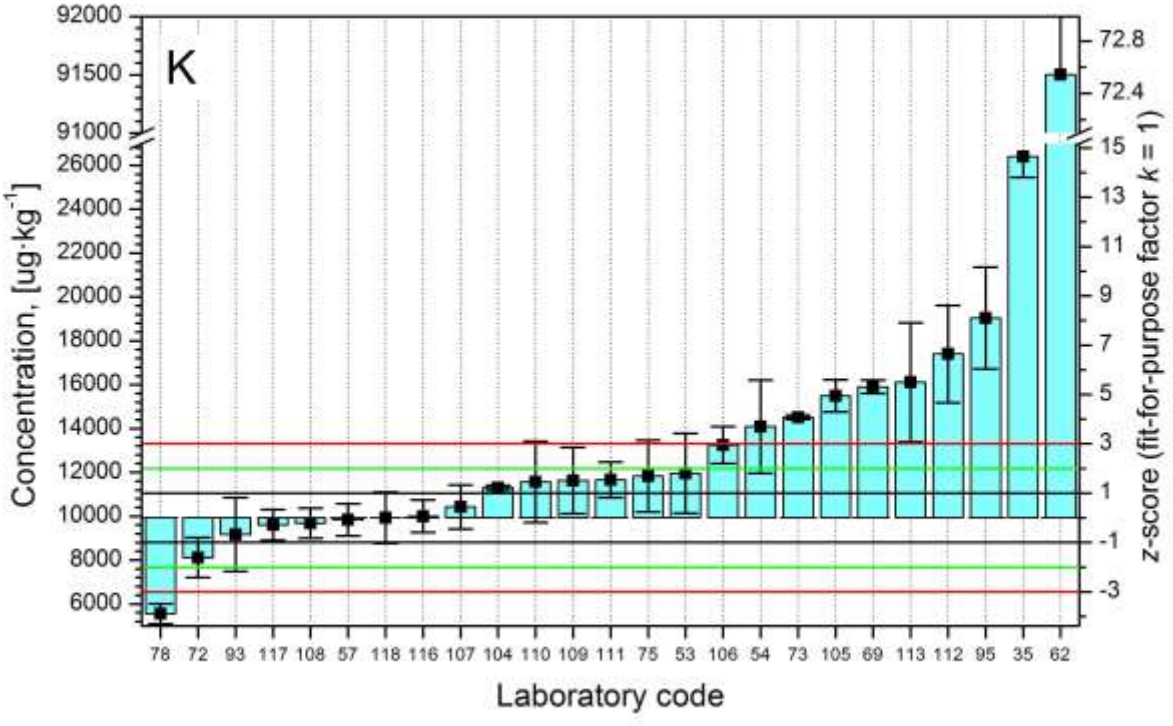

FIG. 57. Distributions of z-scores for analyte K in case of sample "1".

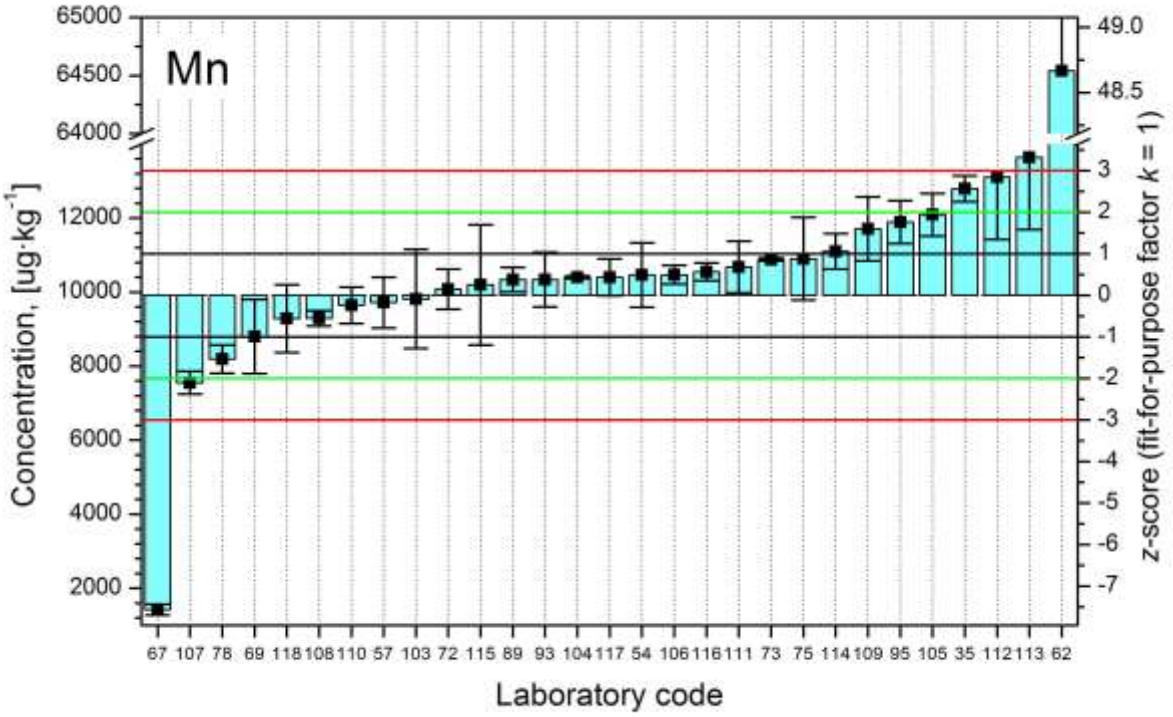

FIG. 58. Distributions of z-scores for analyte Mn in case of sample "1".

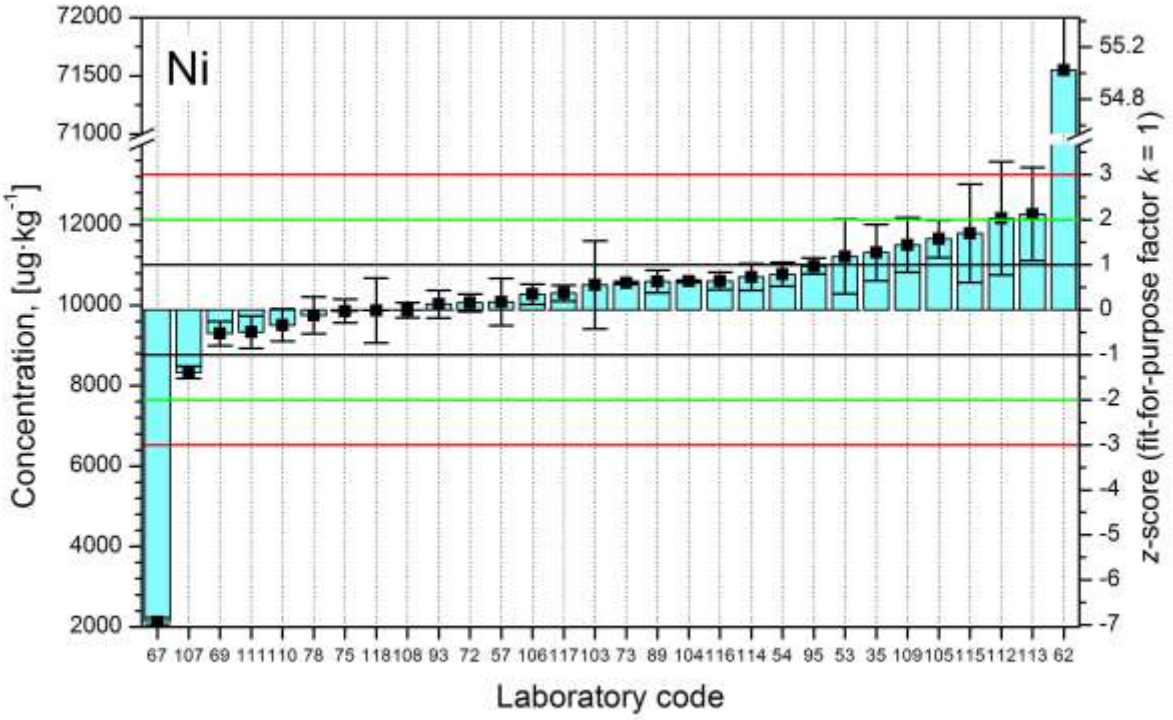

FIG. 59. Distributions of z-scores for analyte Ni in case of sample "1".

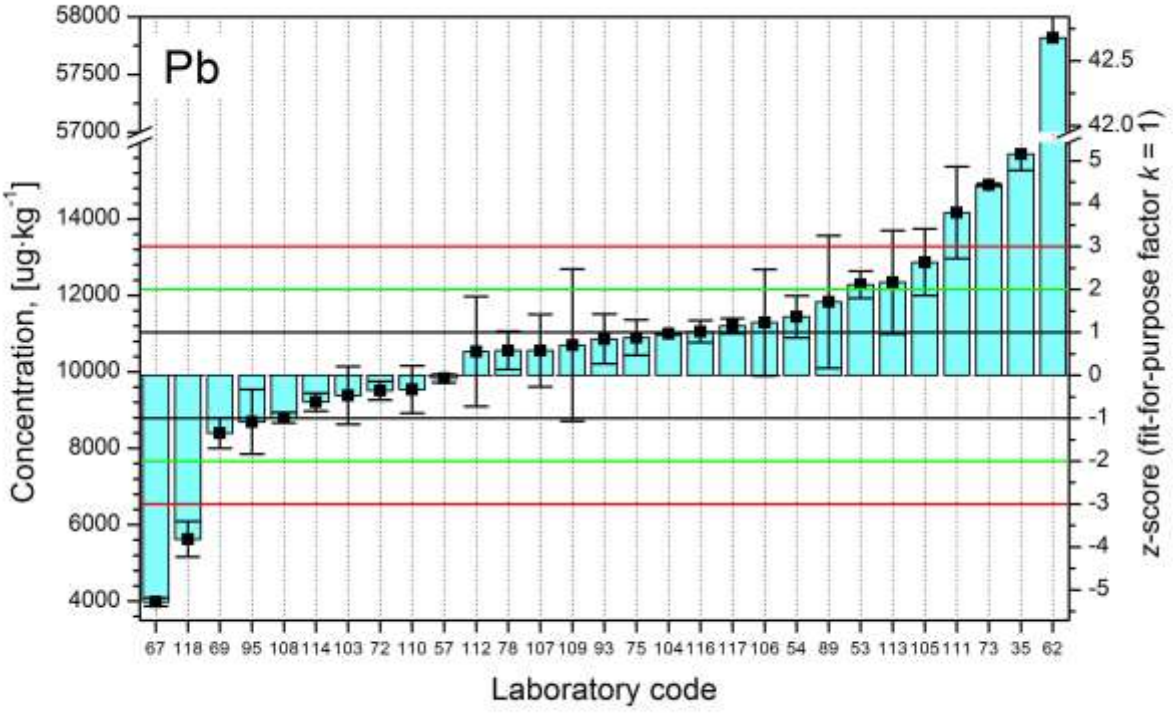

FIG. 60. Distributions of z-scores for analyte Pb in case of sample "1".

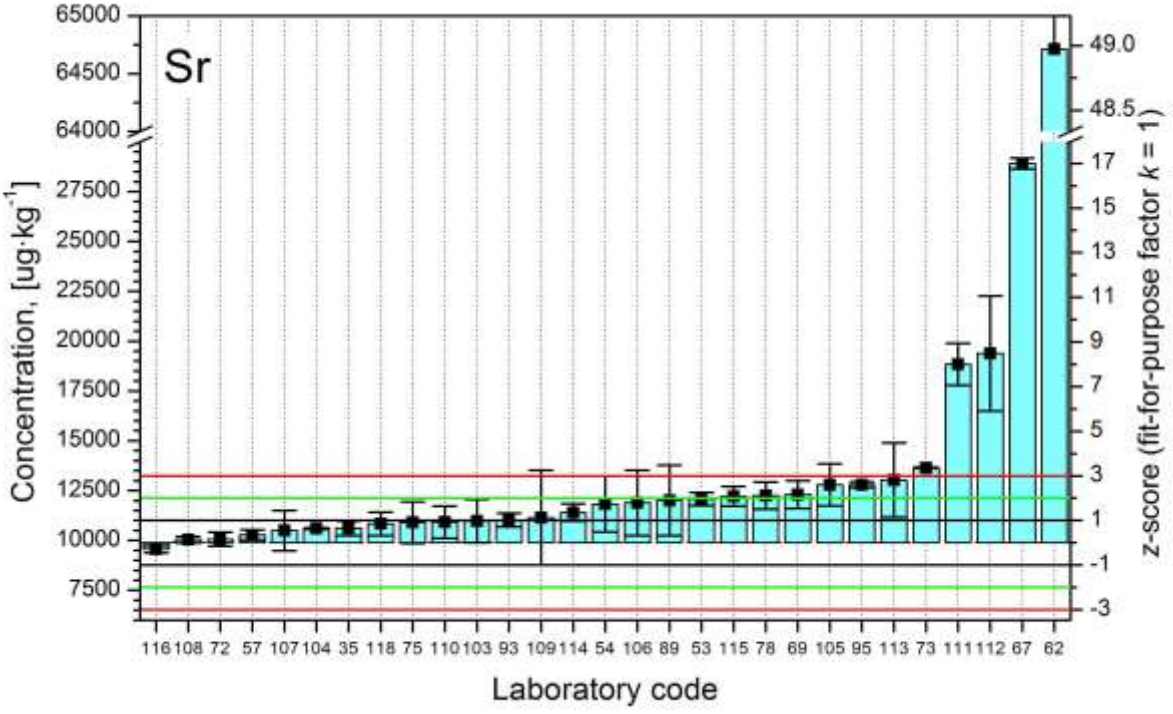

FIG. 61. Distributions of z-scores for analyte Sr in case of sample "1".

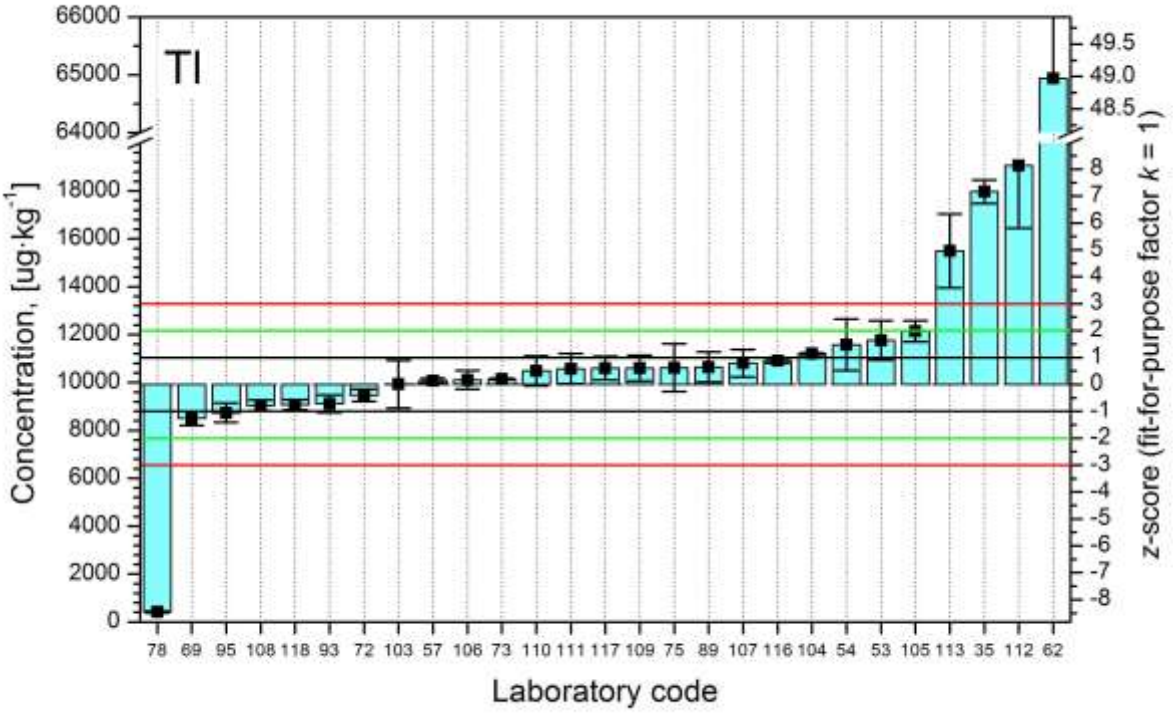

FIG. 62. Distributions of z-scores for analyte Tl in case of sample "1".

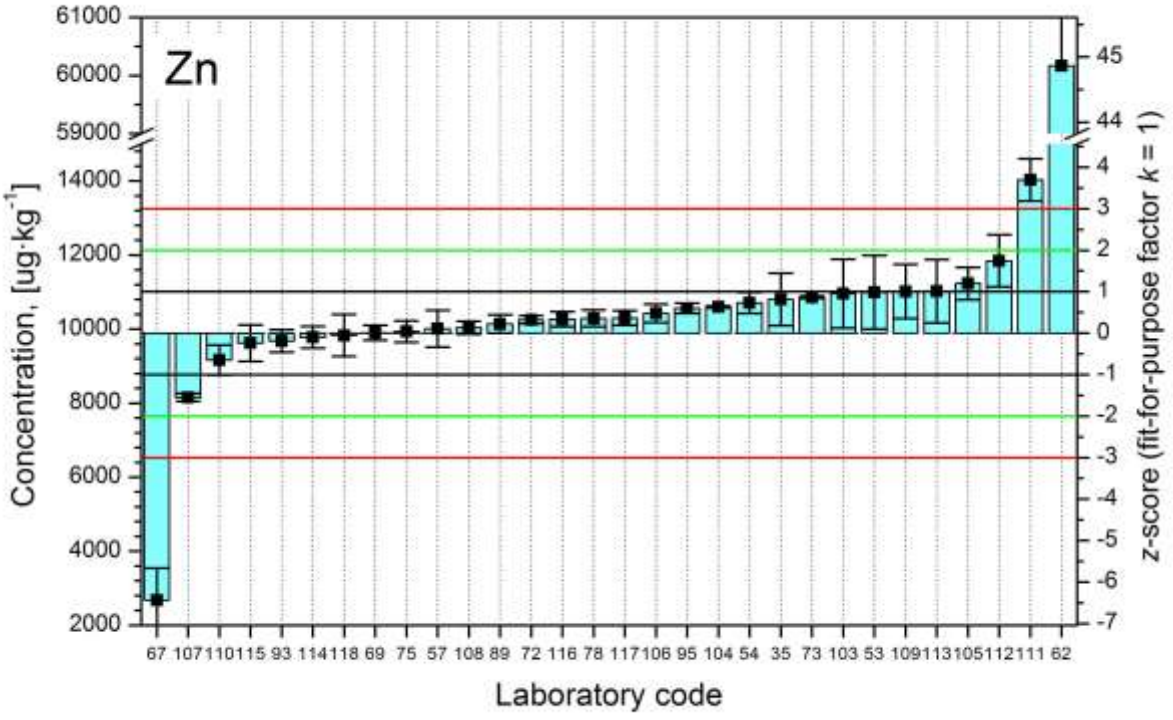

FIG. 63. Distributions of z-scores for analyte Zn in case of sample "1".

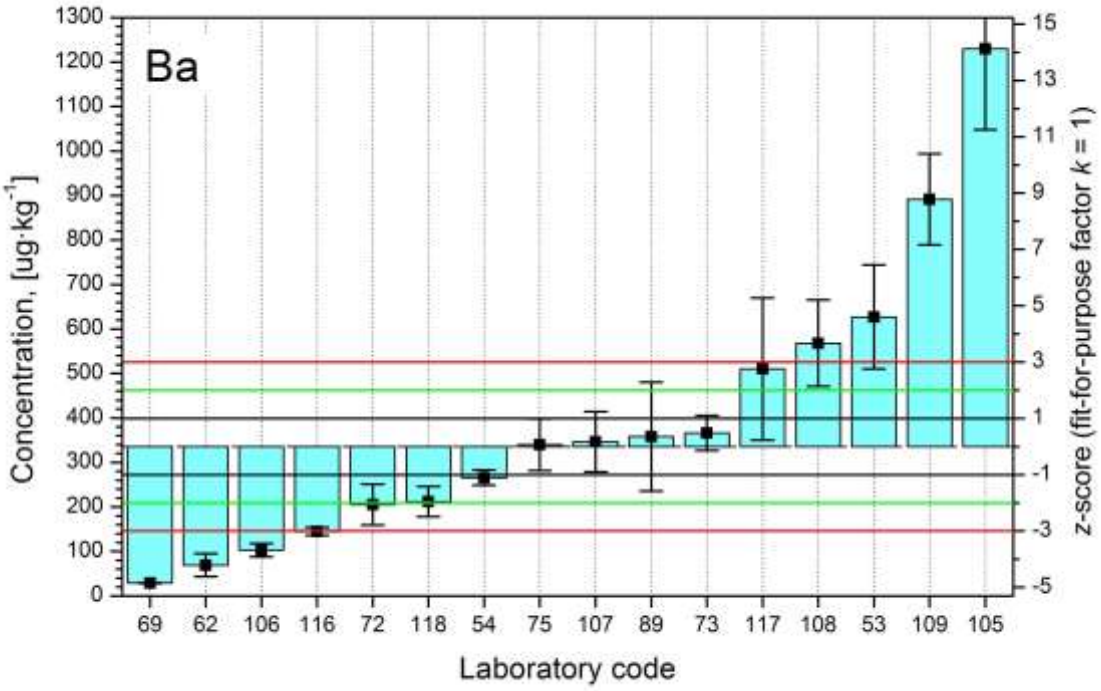

FIG. 64. Distributions of z-scores for analyte Ba in case of sample "2".

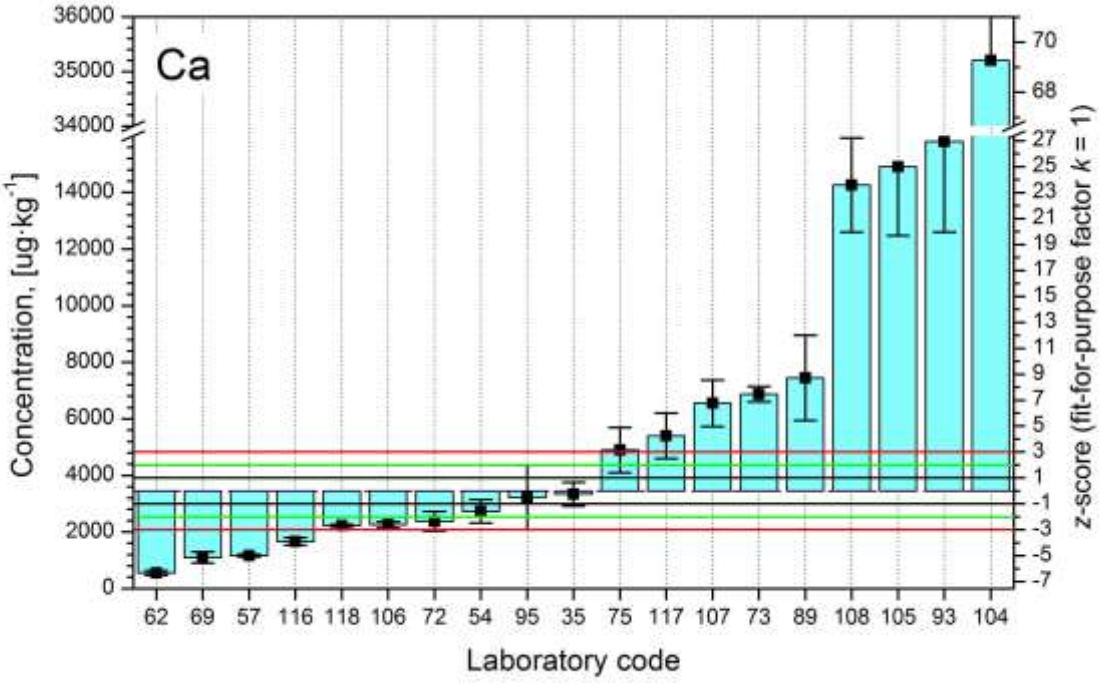

FIG. 65. Distributions of z-scores for analyte Ca in case of sample "2".

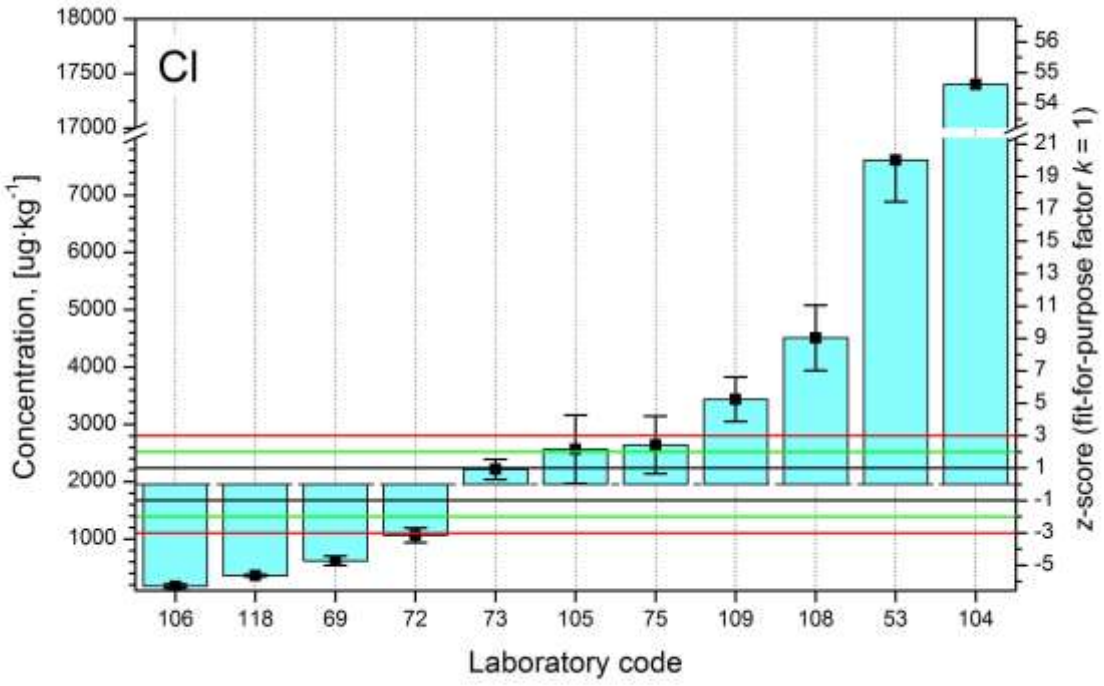

FIG. 66. Distributions of z-scores for analyte Cl in case of sample "2".

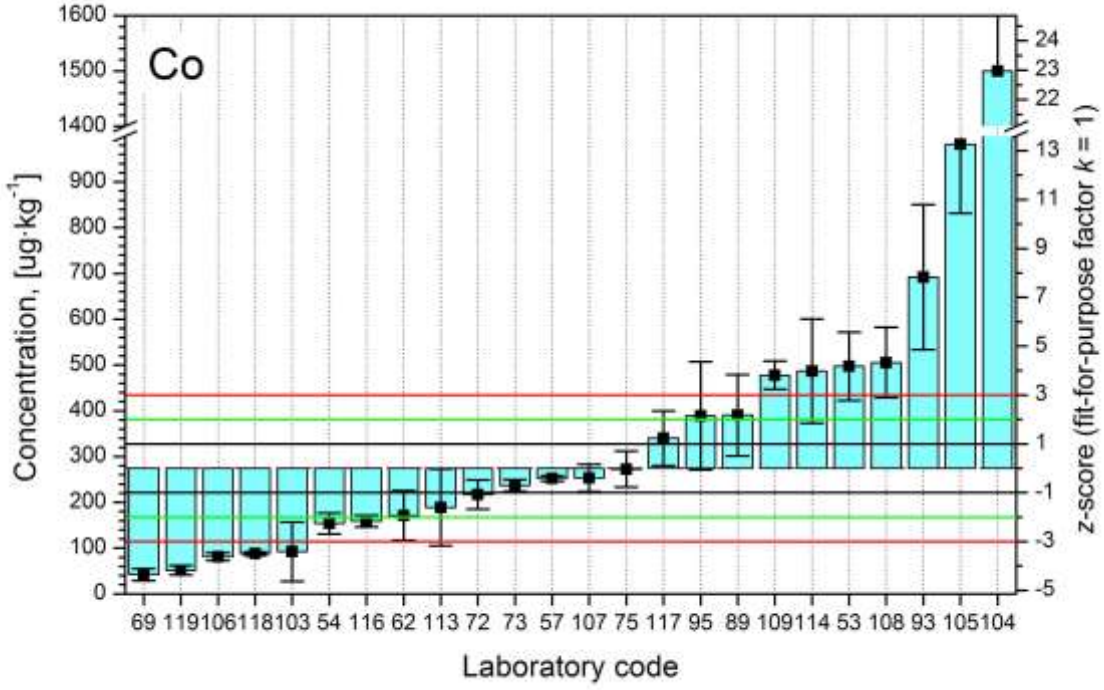

FIG. 67. Distributions of z-scores for analyte Co in case of sample "2".

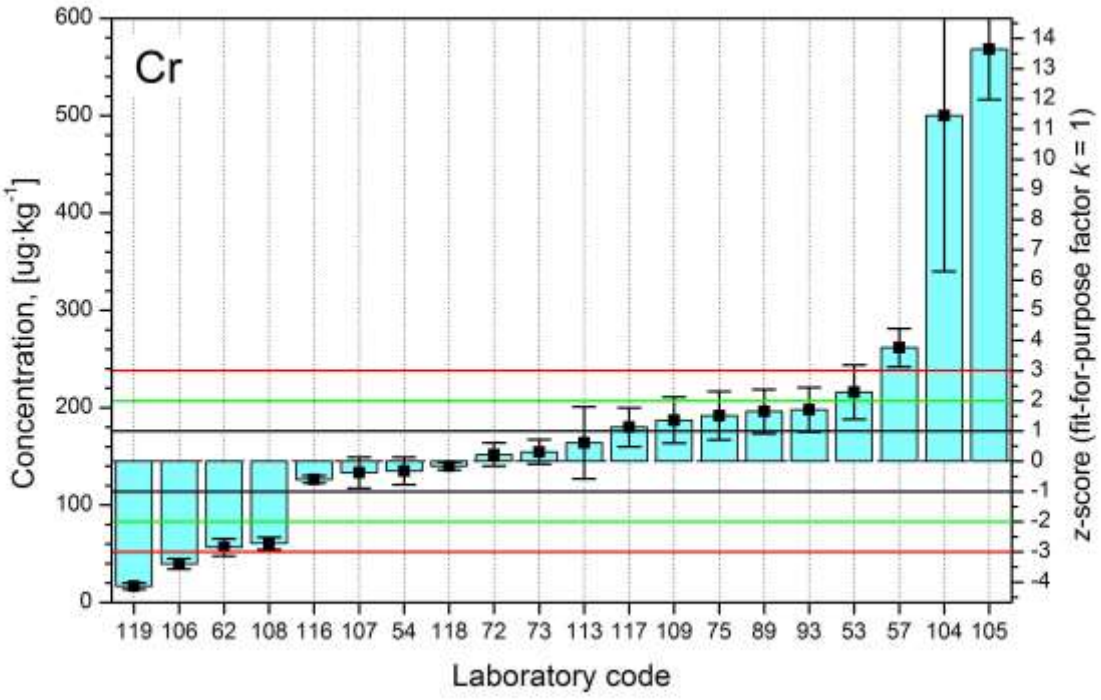

FIG. 68. Distributions of z-scores for analyte Cr in case of sample "2".

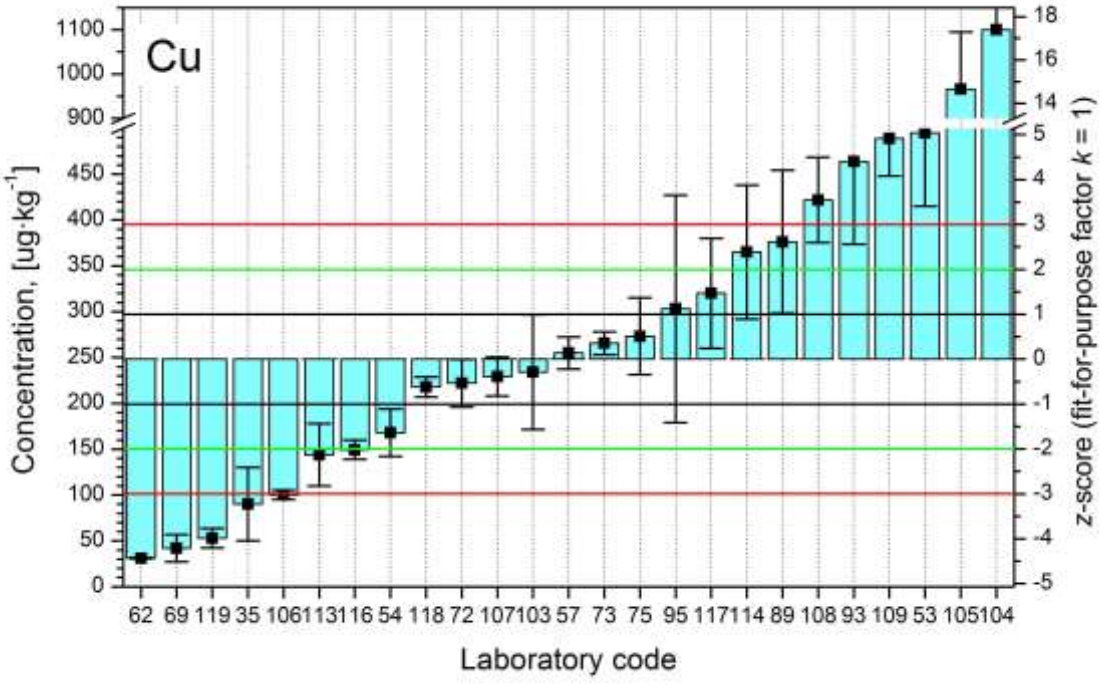

FIG. 69. Distributions of z-scores for analyte Cu in case of sample "2".

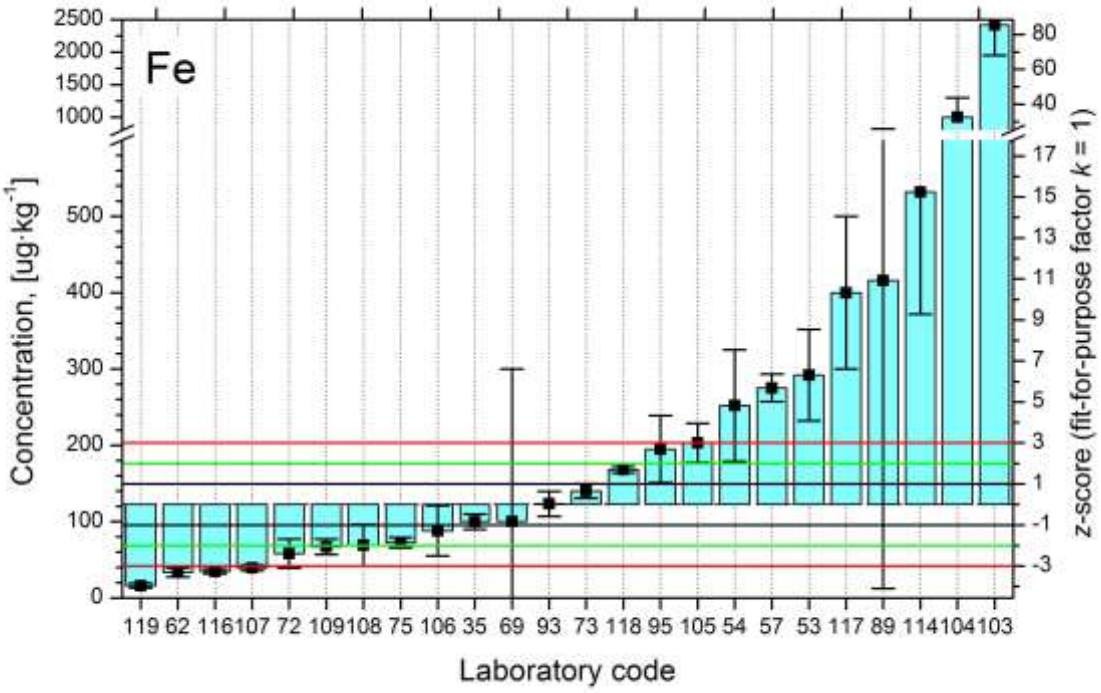

FIG. 70. Distributions of z-scores for analyte Fe in case of sample "2".

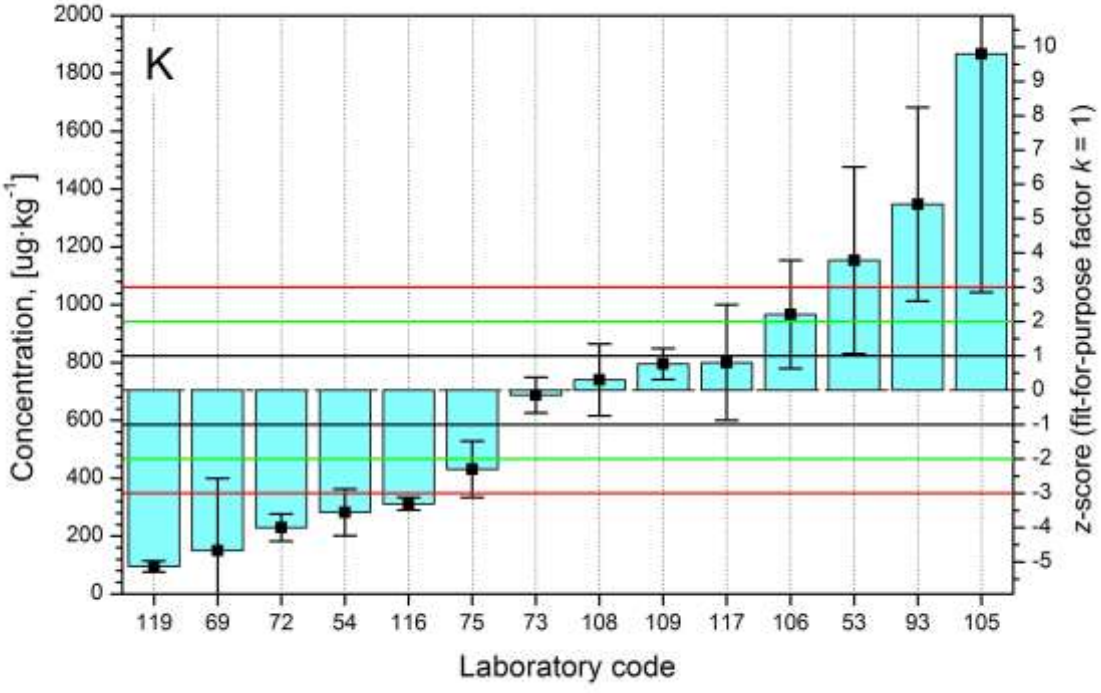

FIG. 71. Distributions of z-scores for analyte K in case of sample "2".

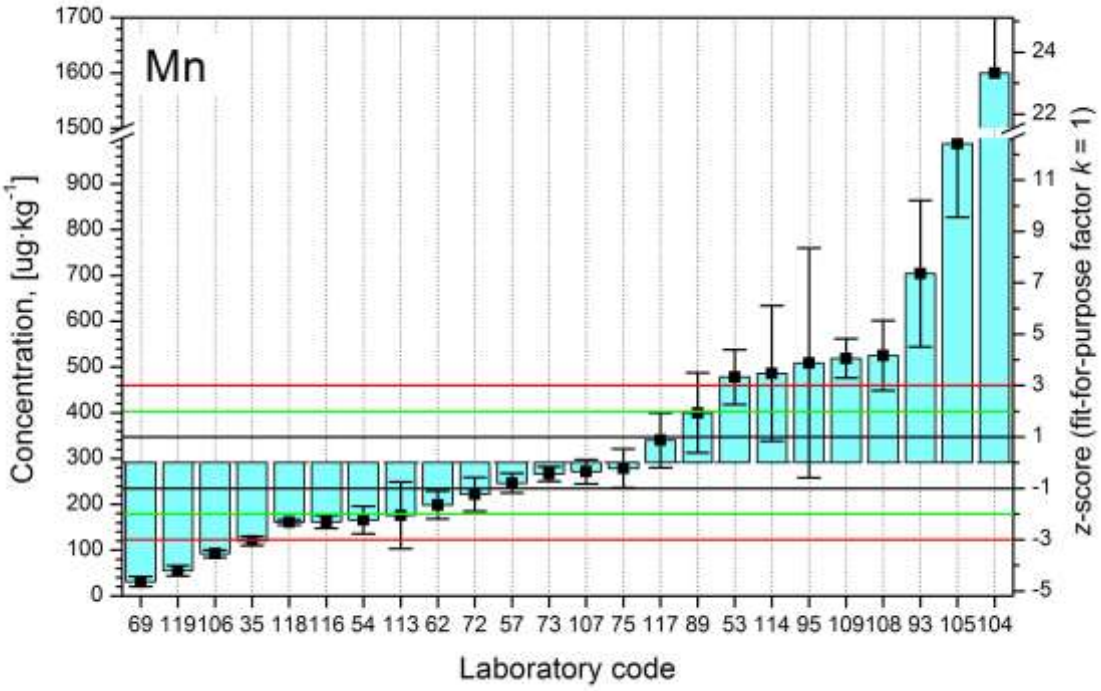

FIG. 72. Distributions of z-scores for analyte Mn in case of sample "2".

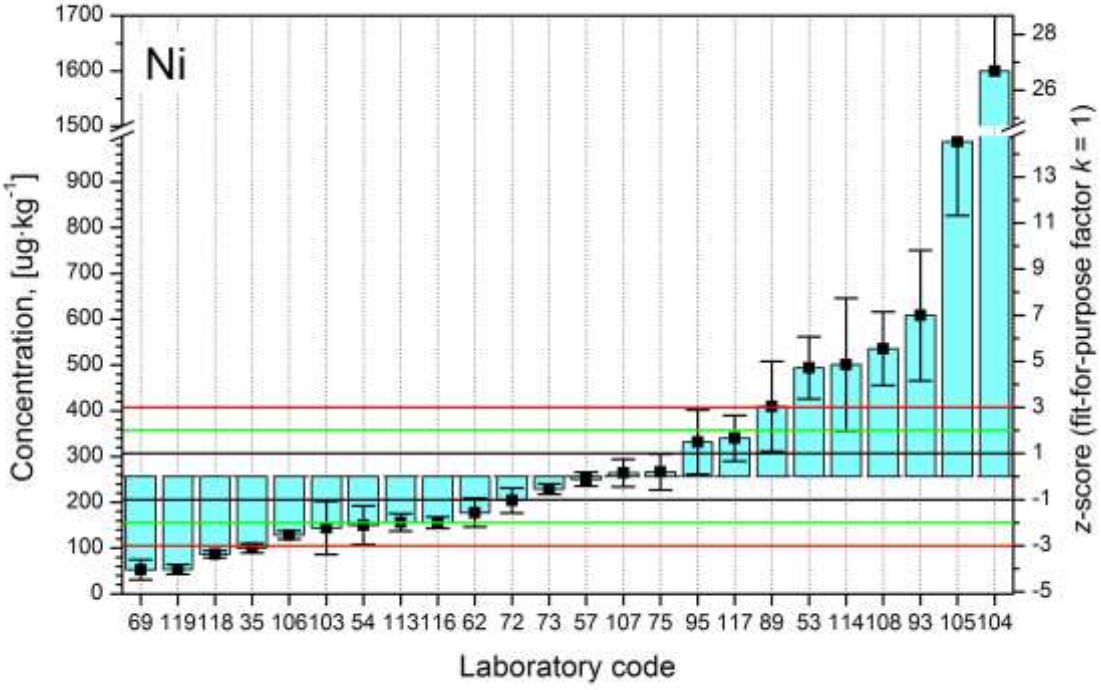

FIG. 73. Distributions of z-scores for analyte Ni in case of sample "2".

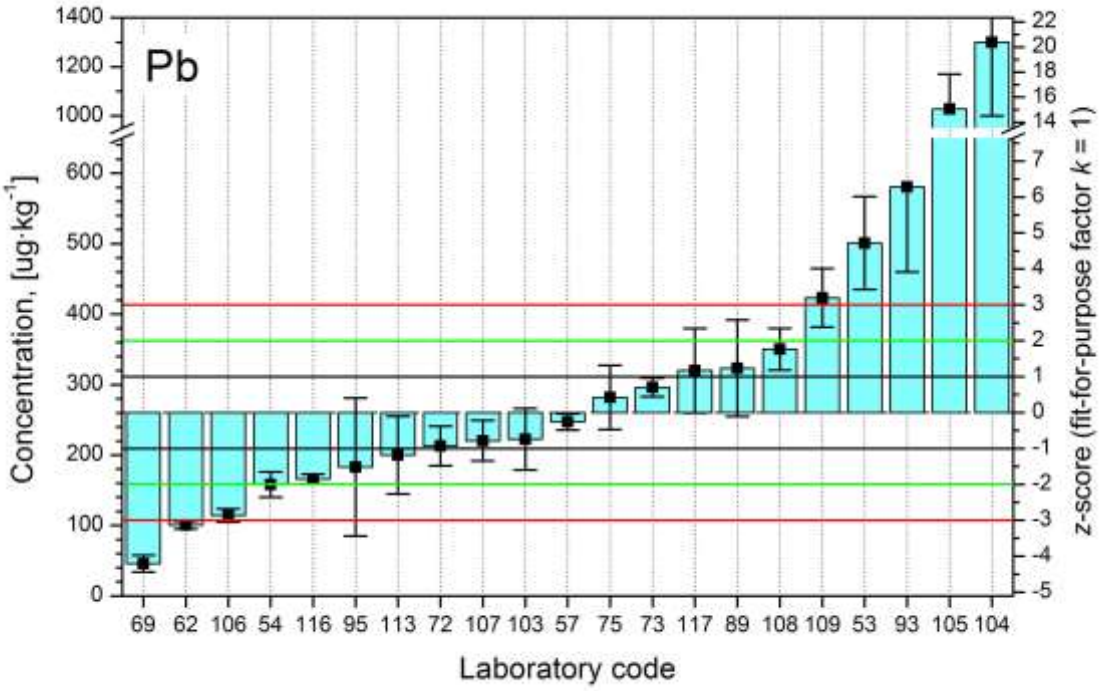

FIG. 74. Distributions of z-scores for analyte Pb in case of sample "2".

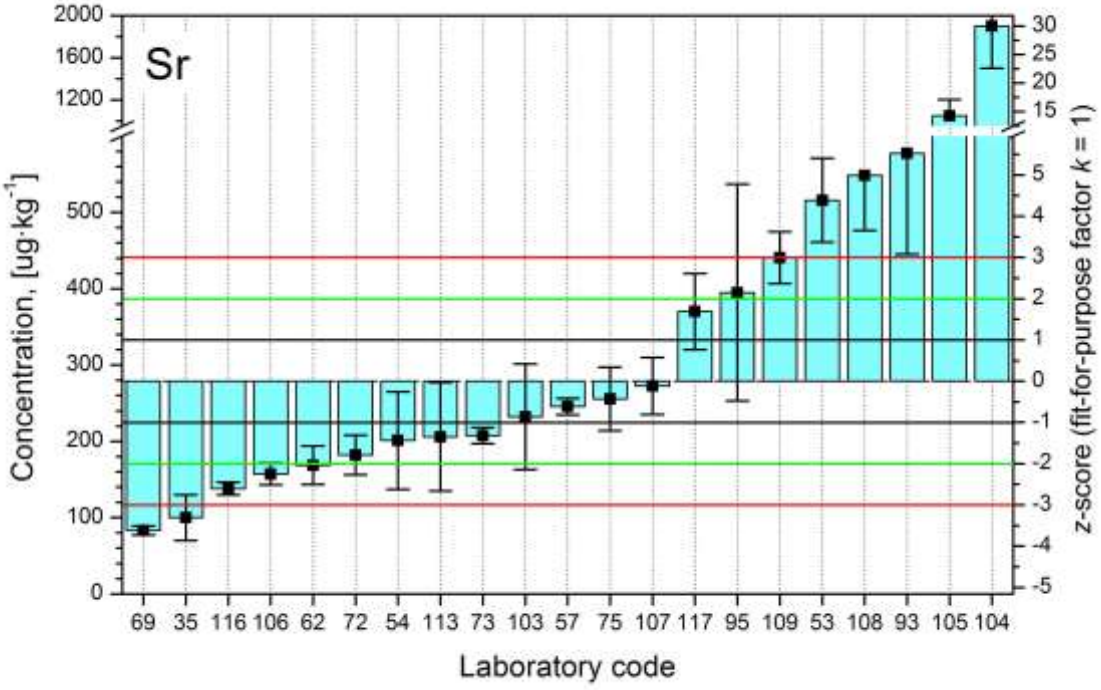

FIG. 75. Distributions of z-scores for analyte Sr in case of sample "2".

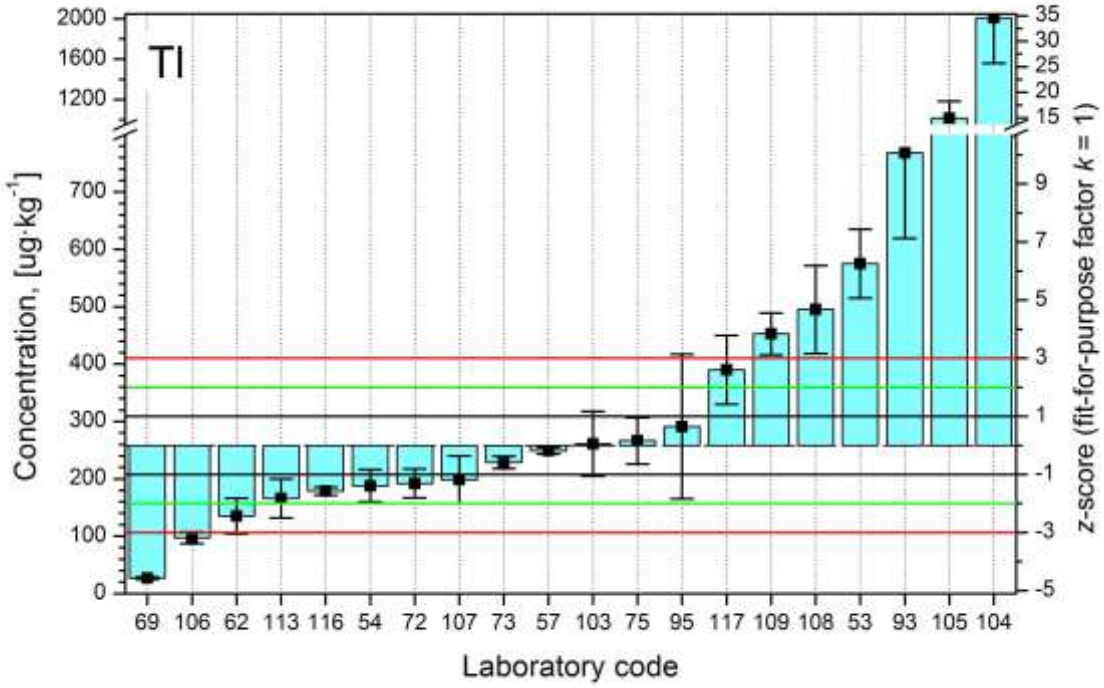

FIG. 76. Distributions of z-scores for analyte Tl in case of sample "2".

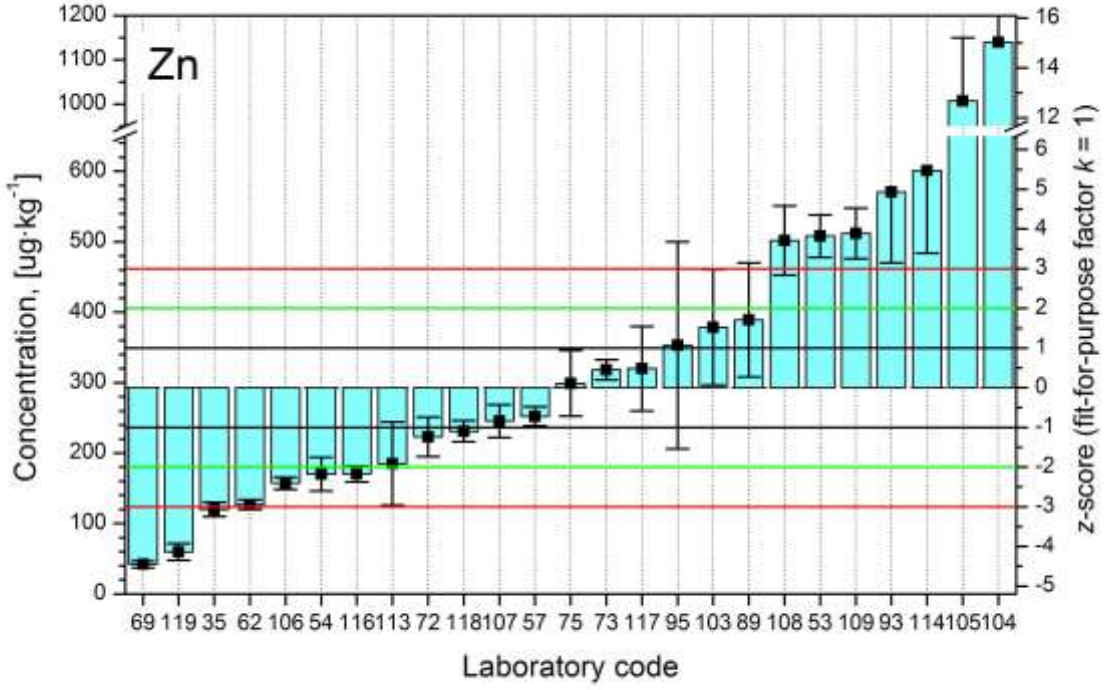

FIG. 77. Distributions of z-scores for analyte Zn in case of sample "2".

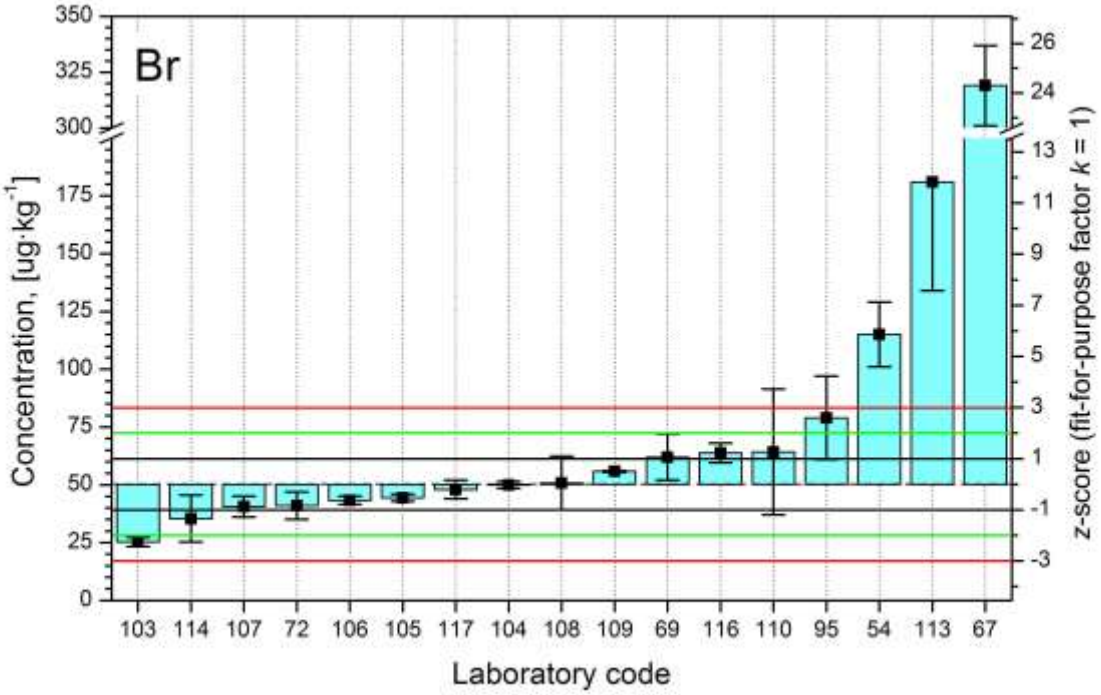

FIG. 78. Distributions of z-scores for analyte Br in case of sample "3".

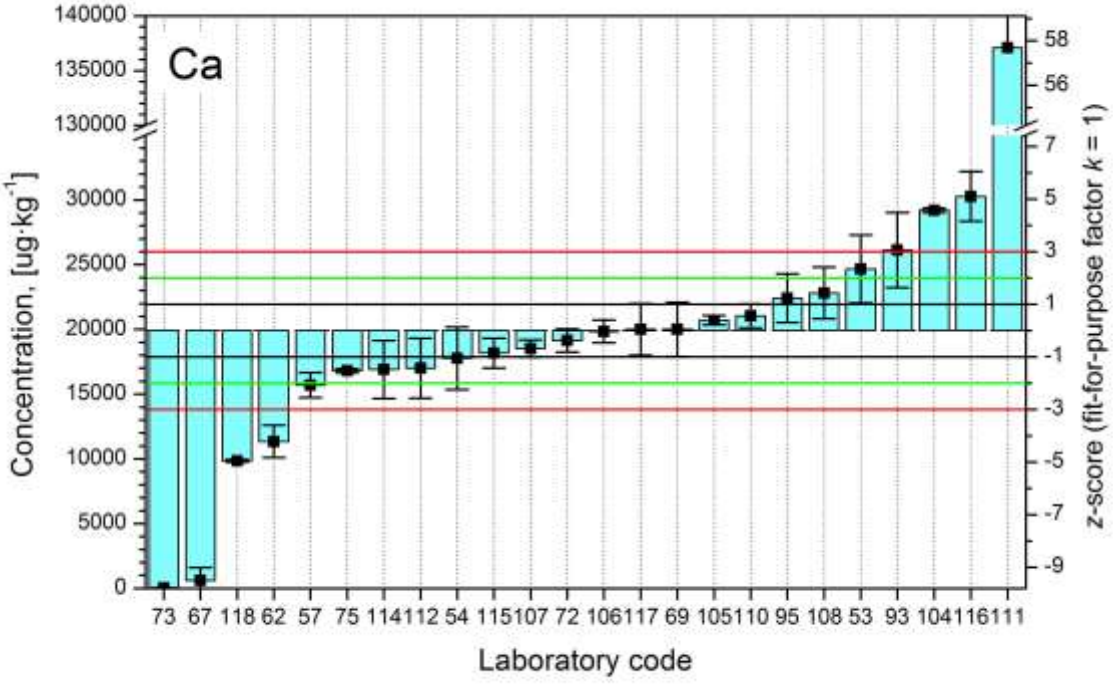

FIG. 79. Distributions of z-scores for analyte Ca in case of sample "3".

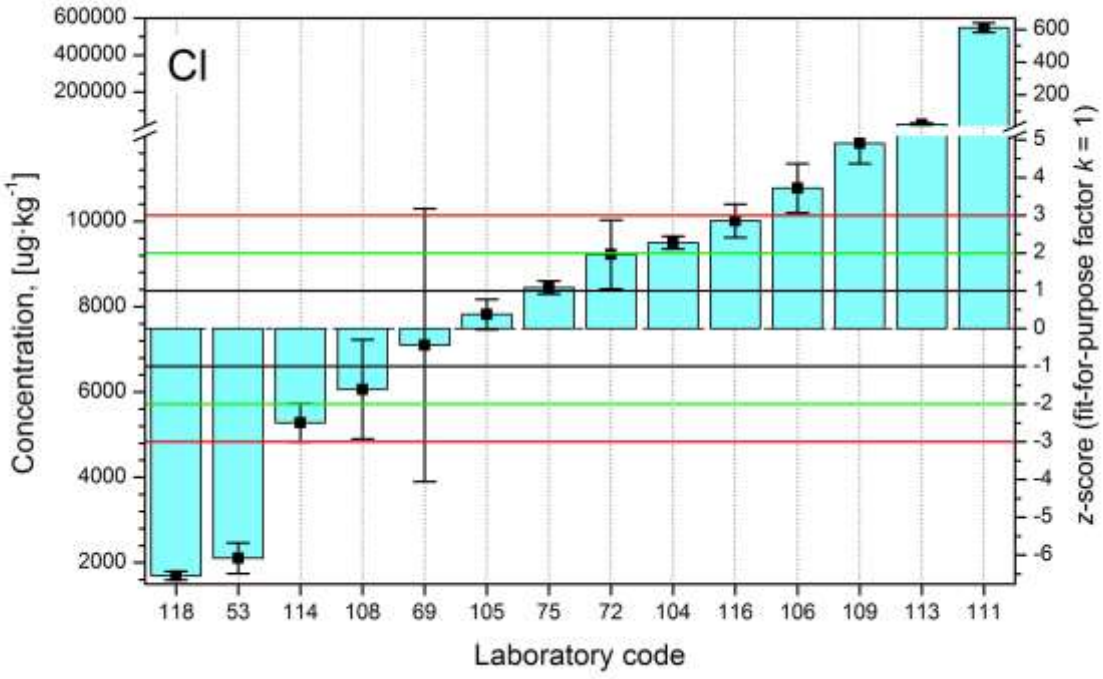

FIG. 80. Distributions of z-scores for analyte Cl in case of sample "3".

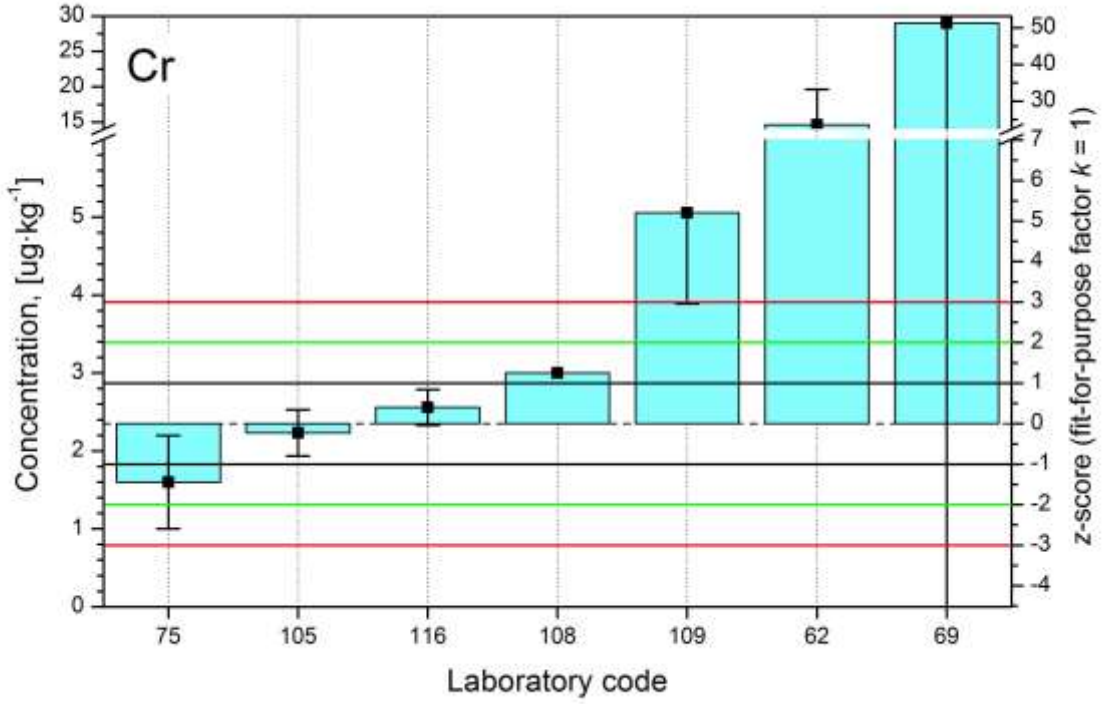

FIG. 81. Distributions of z-scores for analyte Cr in case of sample "3".

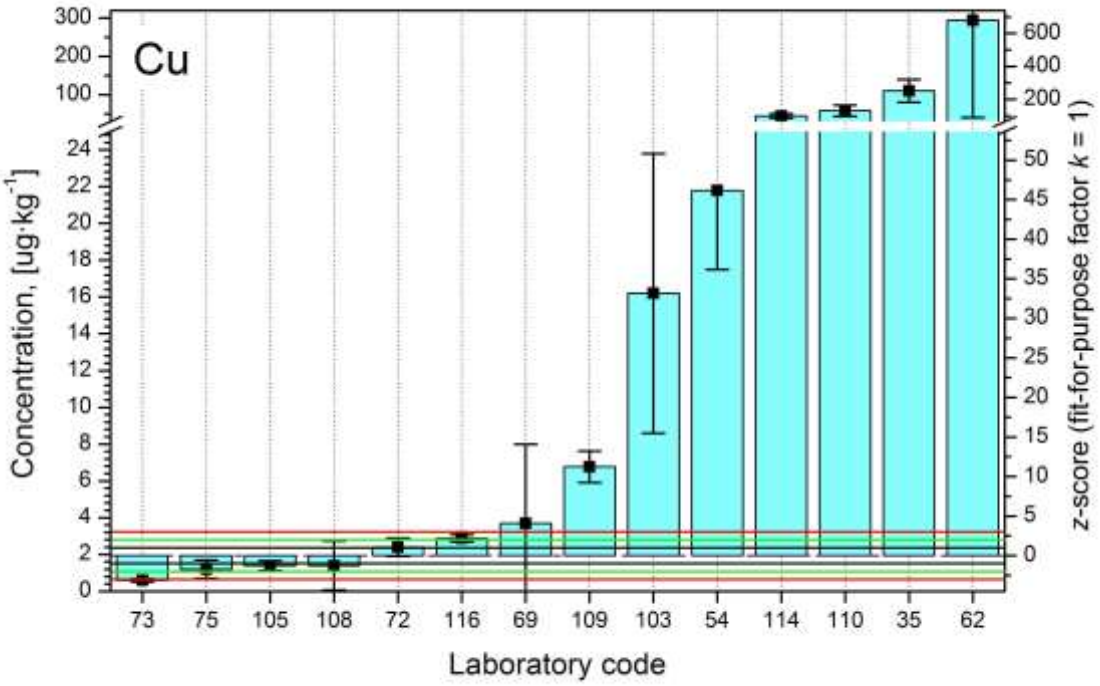

FIG. 82. Distributions of z-scores for analyte Cu in case of sample "3".

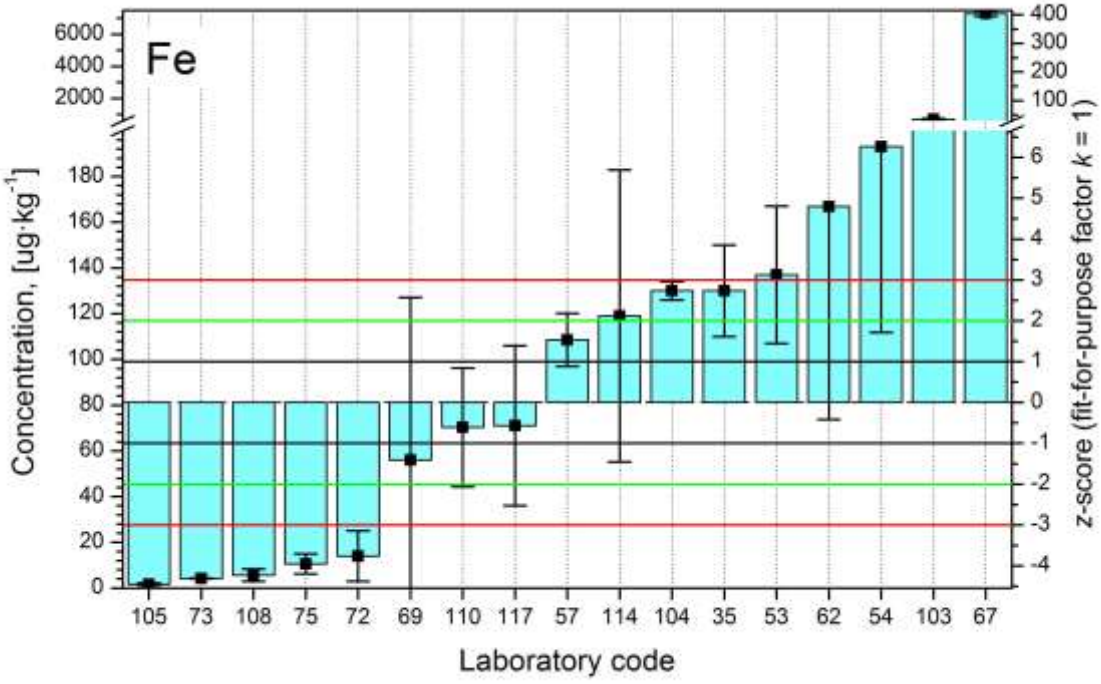

FIG. 83. Distributions of z-scores for analyte Fe in case of sample "3".

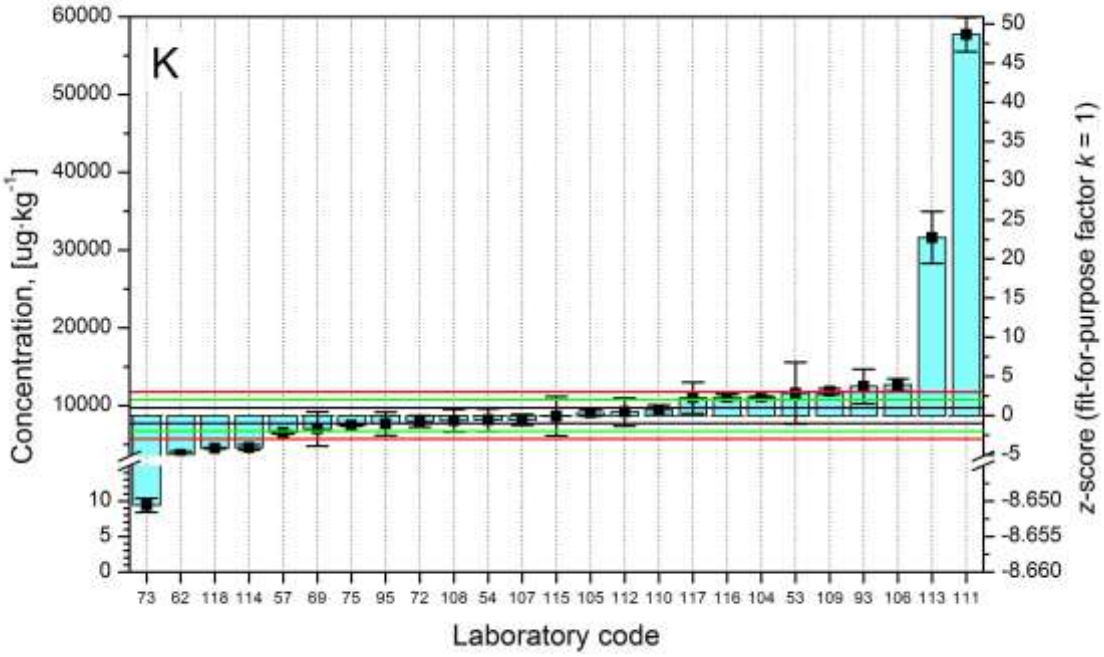

FIG. 84. Distributions of z-scores for analyte K in case of sample "3".

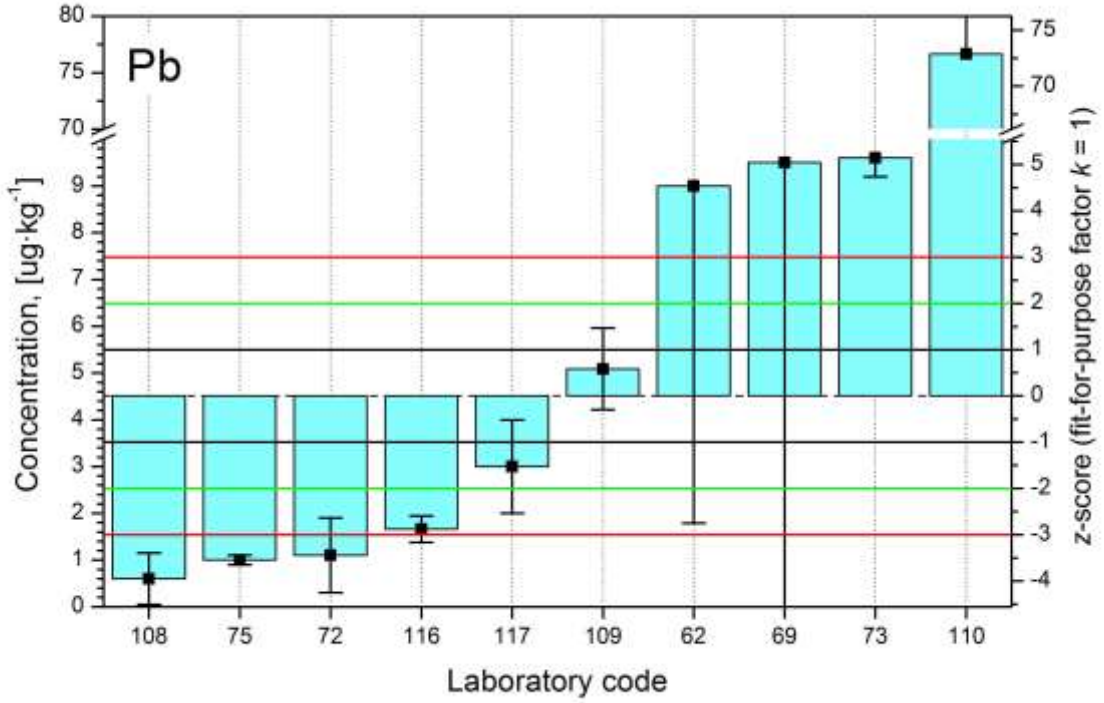

FIG. 85. Distributions of z-scores for analyte Pb in case of sample "3".

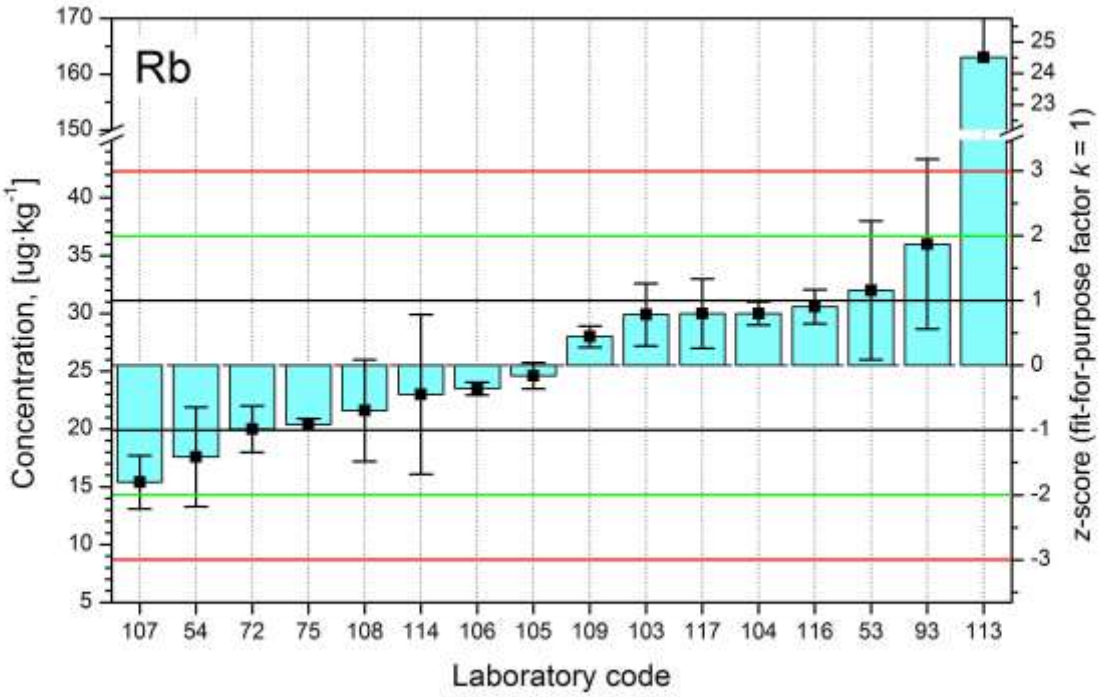

FIG. 86. Distributions of z-scores for analyte Rb in case of sample "3".

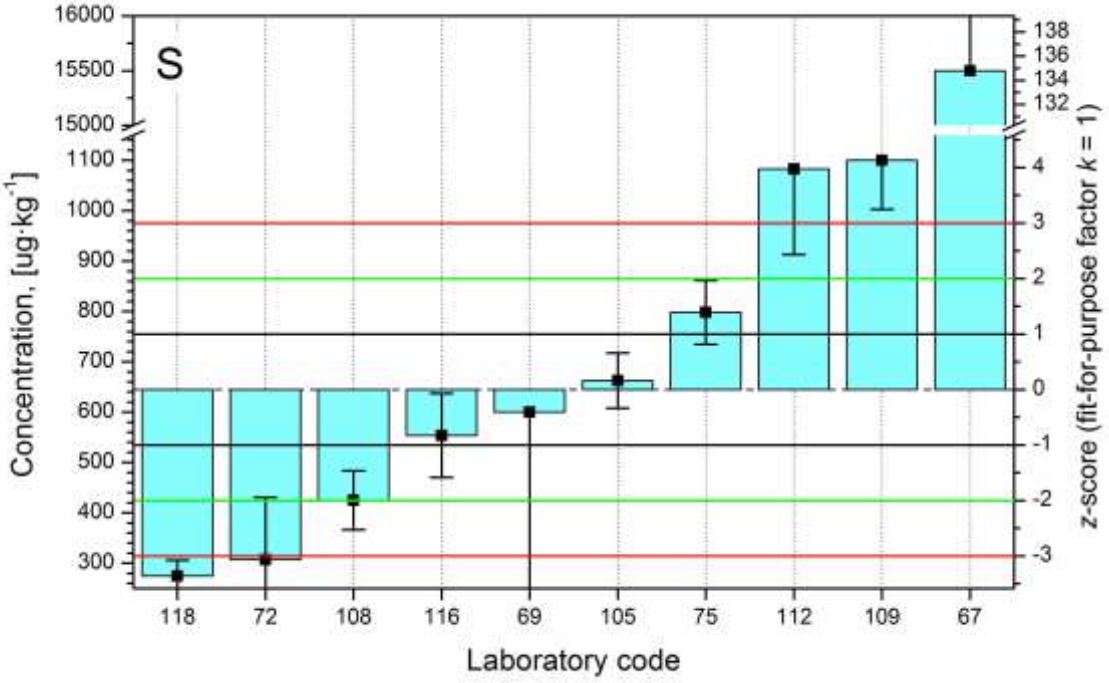

FIG. 87. Distributions of z-scores for analyte S in case of sample "3".

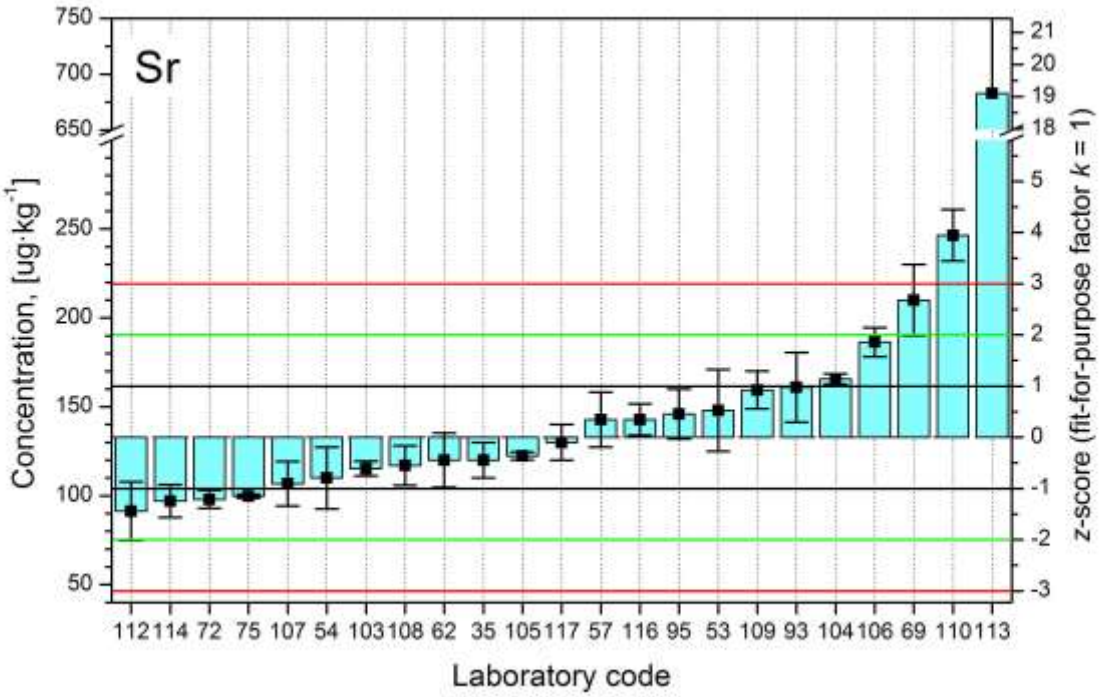

FIG. 88. Distributions of z-scores for analyte Sr in case of sample "3".

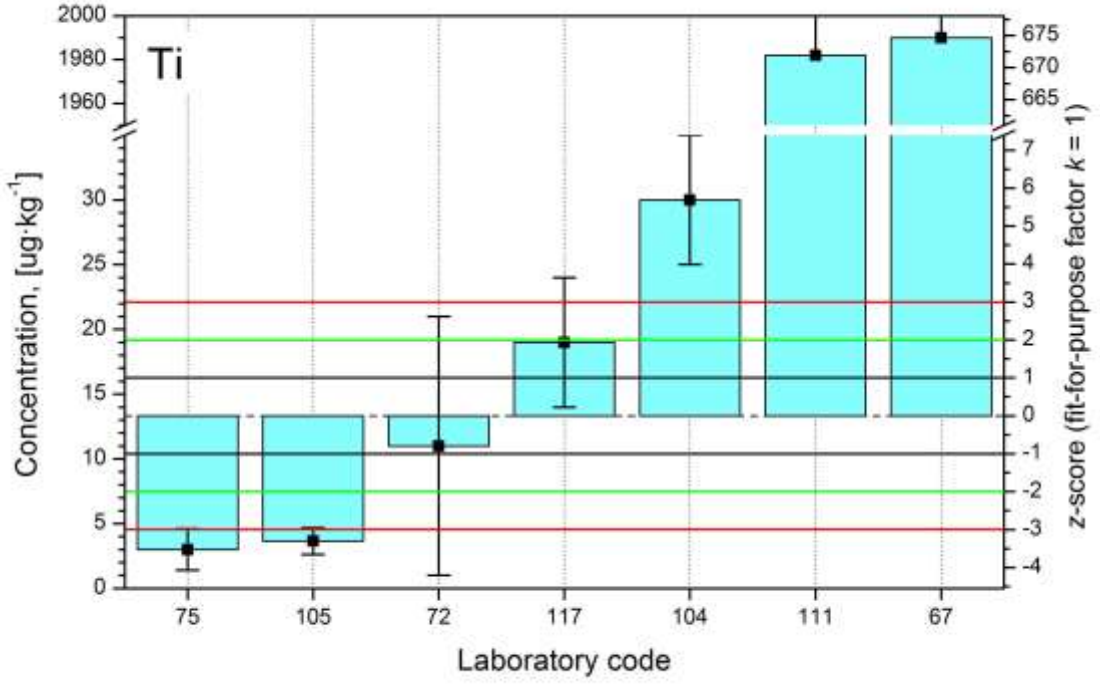

FIG. 89. Distributions of z-scores for analyte Ti in case of sample "3".

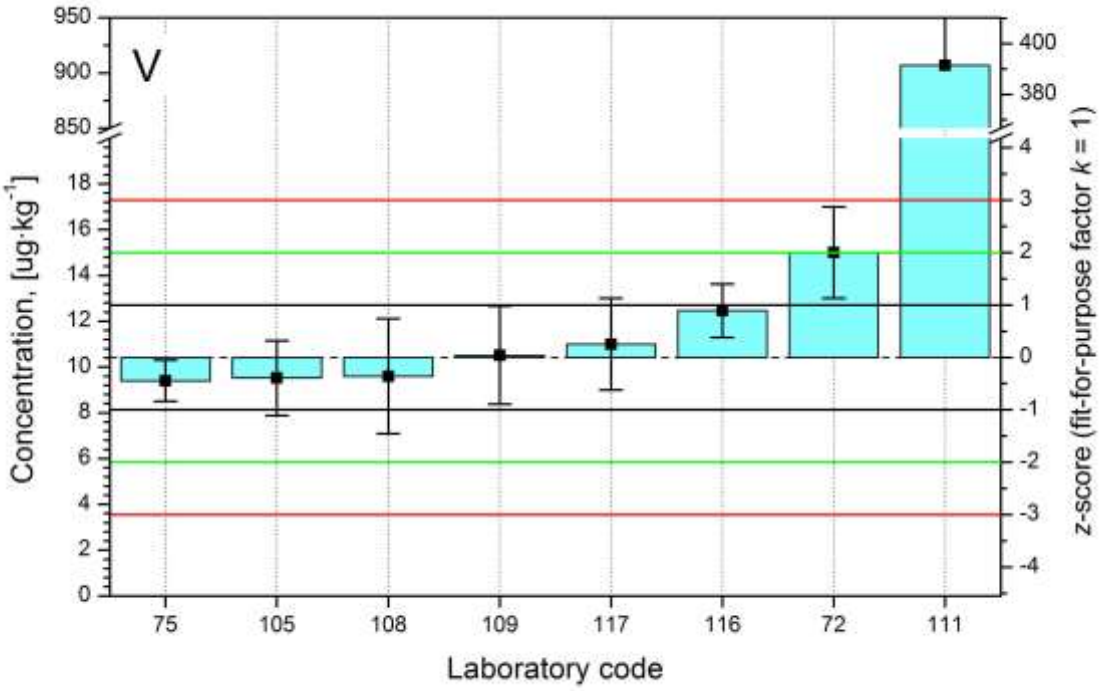

FIG. 90. Distributions of z-scores for analyte V in case of sample "3".

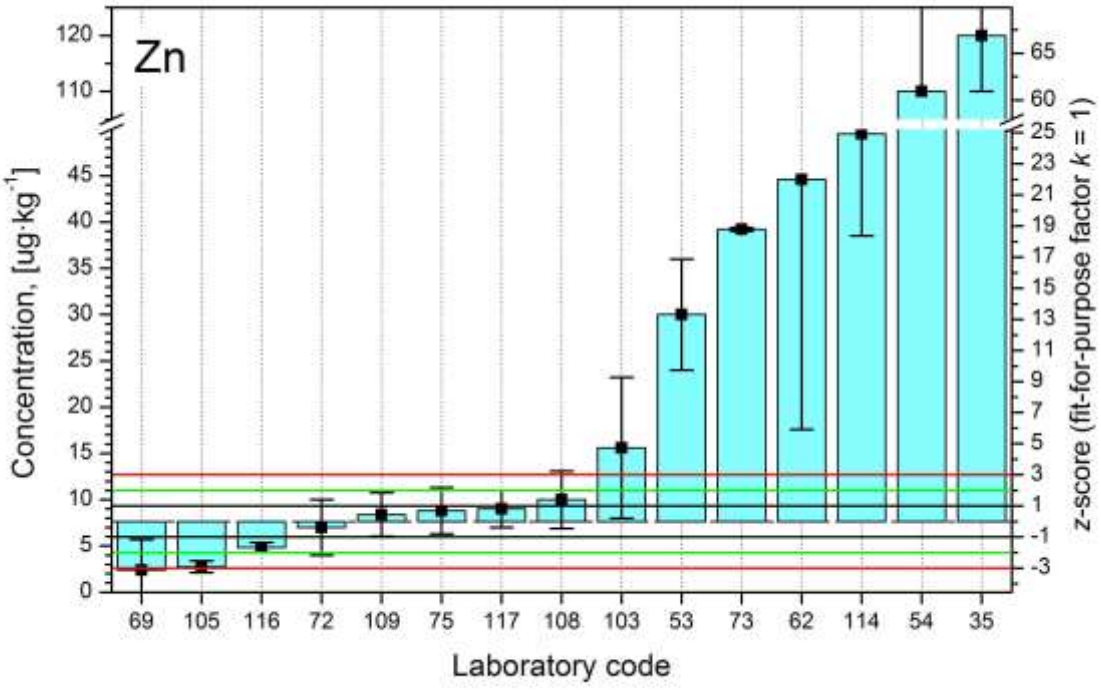

FIG. 91. Distributions of z-scores for analyte Zn in case of sample "3".

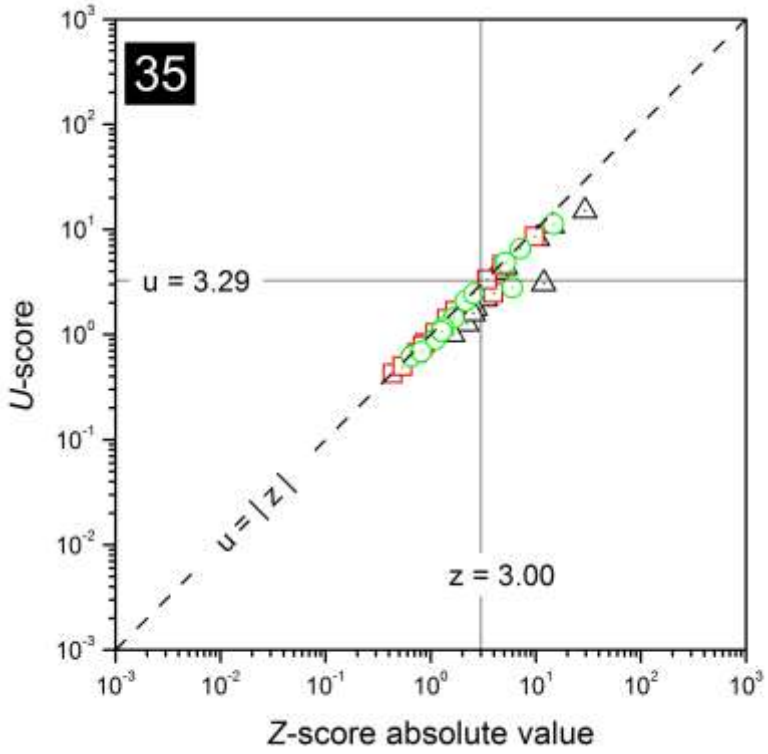

FIG. 92. Combined plots of z- and u-scores for the laboratory with code 35 in case of sample "1".

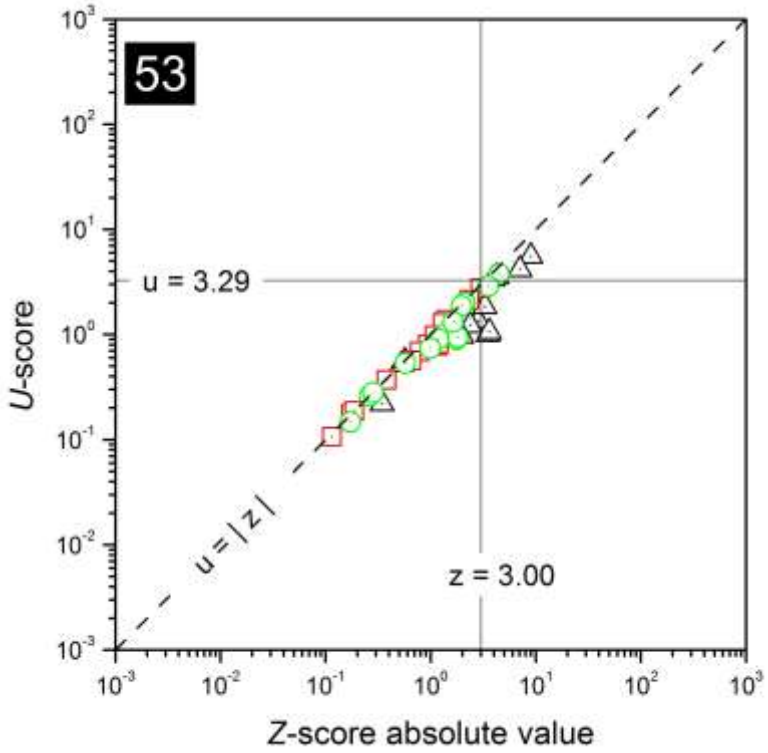

FIG. 93. Combined plots of z- and u-scores for the laboratory with code 53 in case of sample "1".

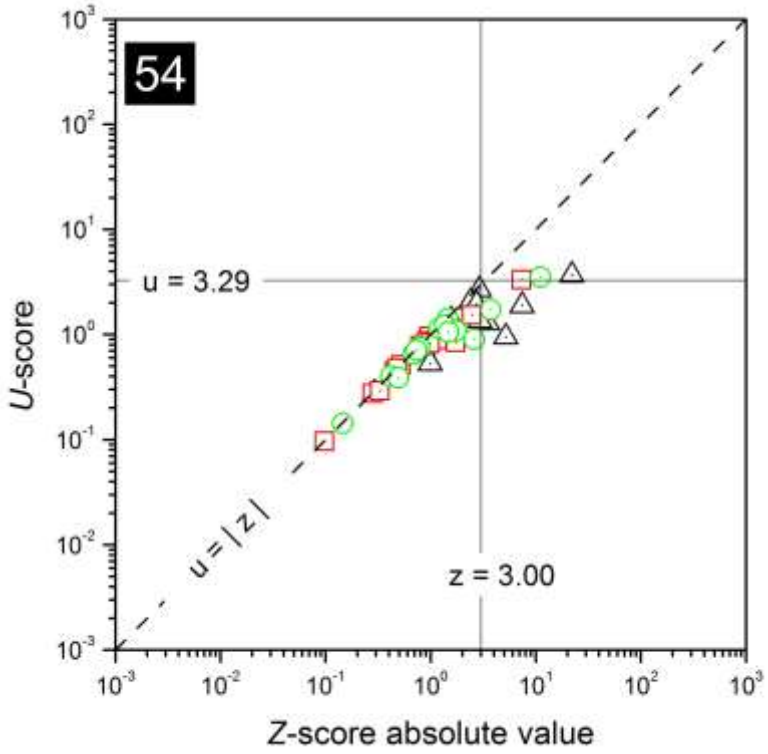

FIG. 94. Combined plots of z- and u-scores for the laboratory with code 54 in case of sample "1".

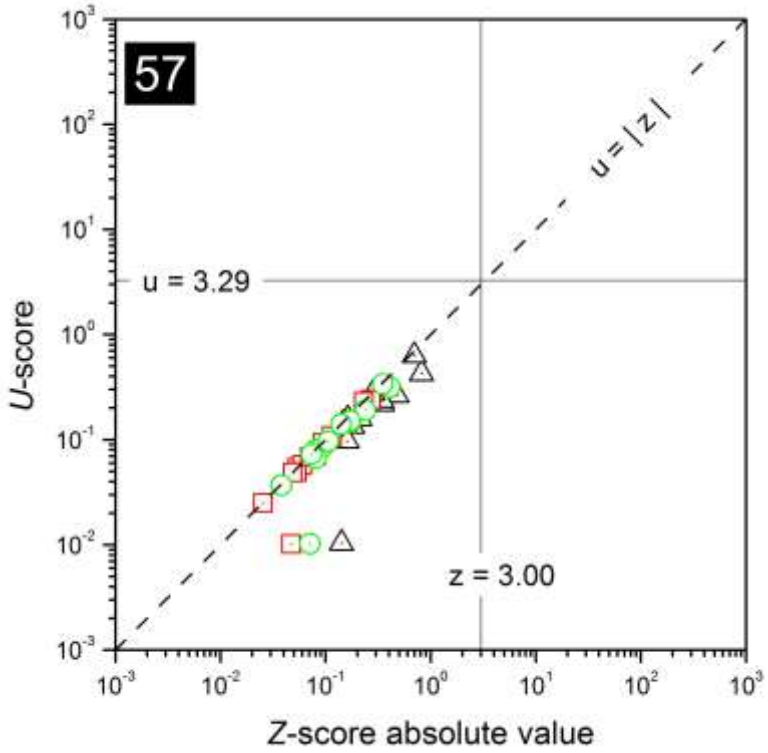

FIG. 95. Combined plots of z- and u-scores for the laboratory with code 57 in case of sample "1".

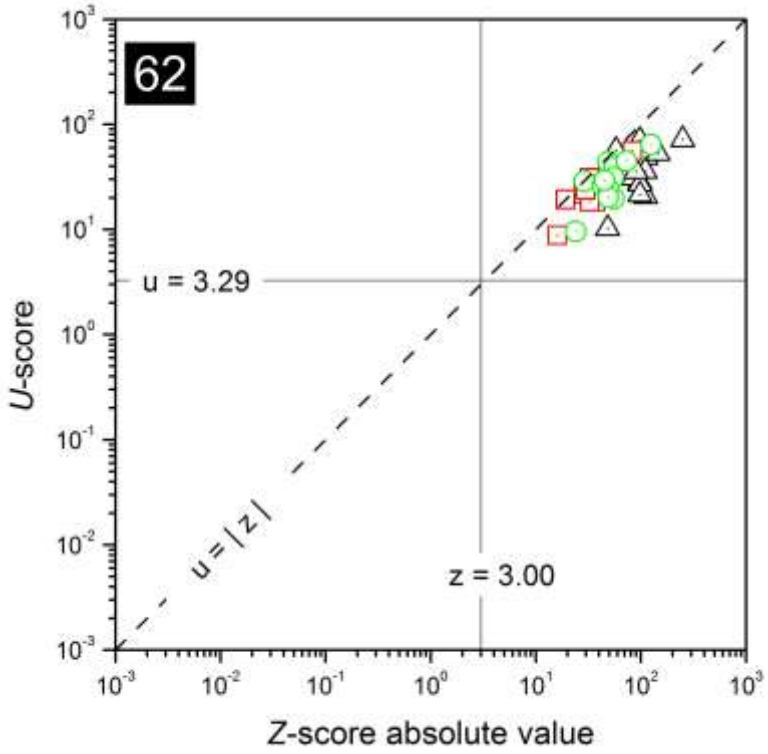

FIG. 96. Combined plots of z- and u-scores for the laboratory with code 62 in case of sample "1".

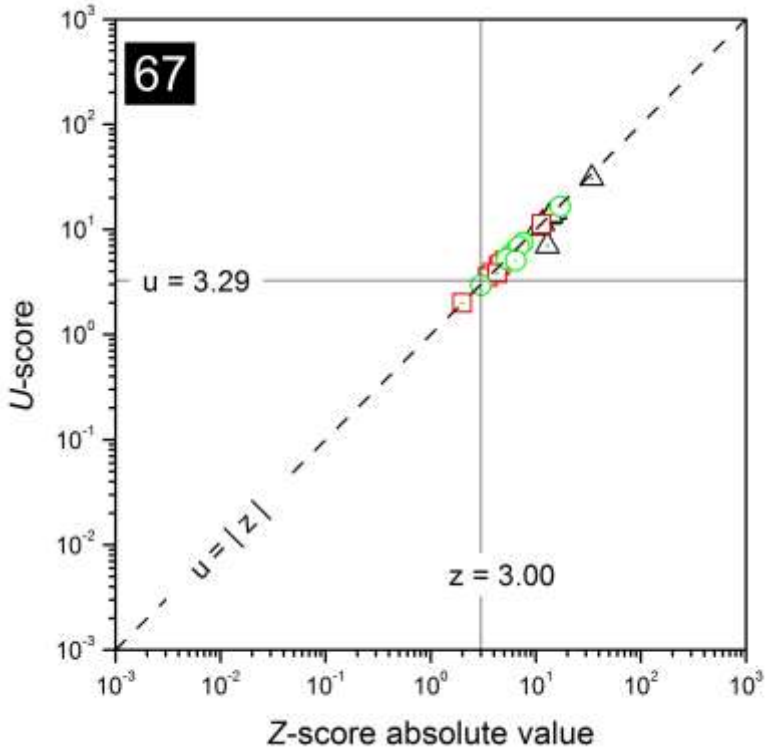

FIG. 97. Combined plots of z- and u-scores for the laboratory with code 67 in case of sample "1".

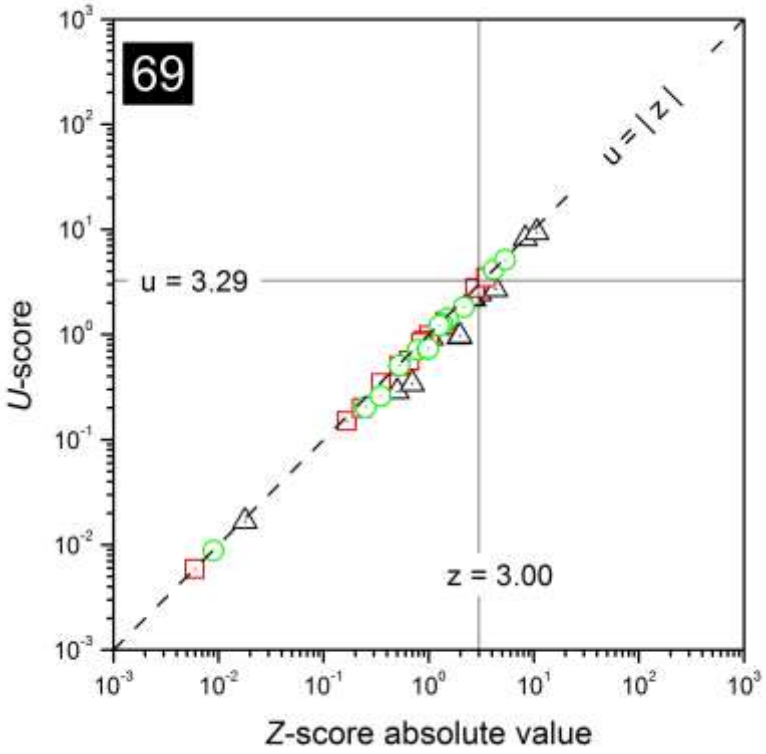

FIG. 98. Combined plots of z- and u-scores for the laboratory with code 69 in case of sample "1".

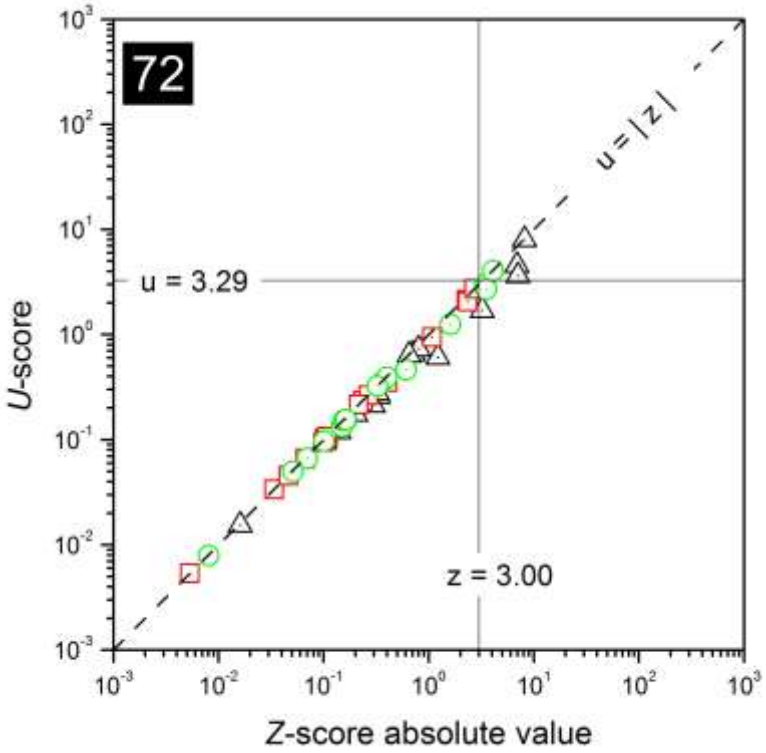

FIG. 99. Combined plots of z- and u-scores for the laboratory with code 72 in case of sample "1".

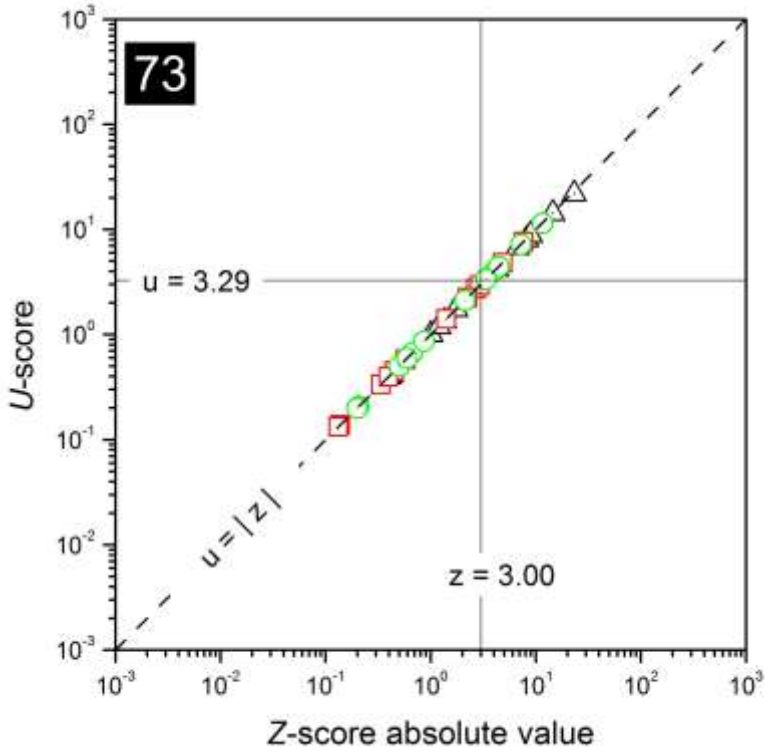

FIG. 100. Combined plots of z- and u-scores for the laboratory with code 73 in case of sample "1".

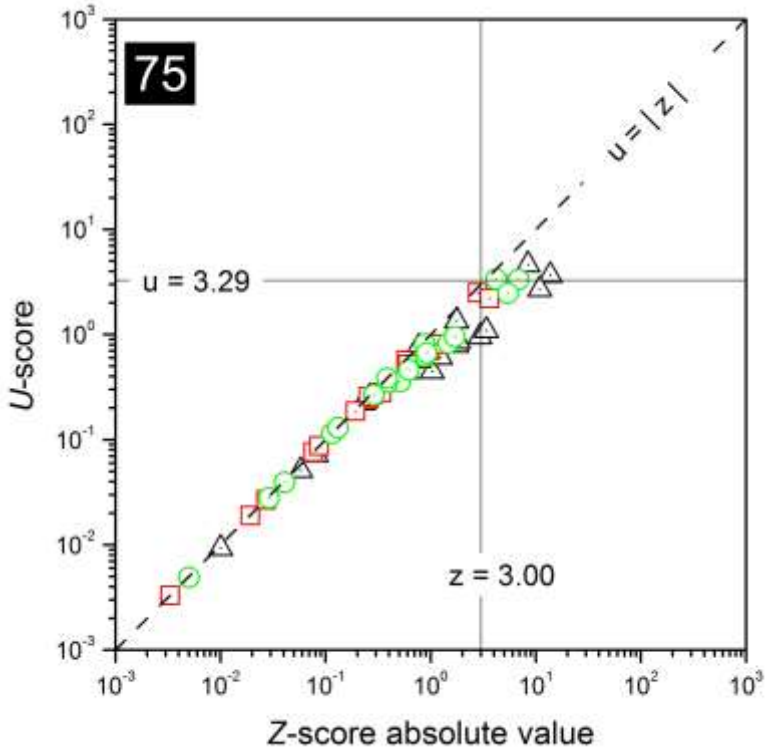

FIG. 101. Combined plots of z- and u-scores for the laboratory with code 75 in case of sample "1".

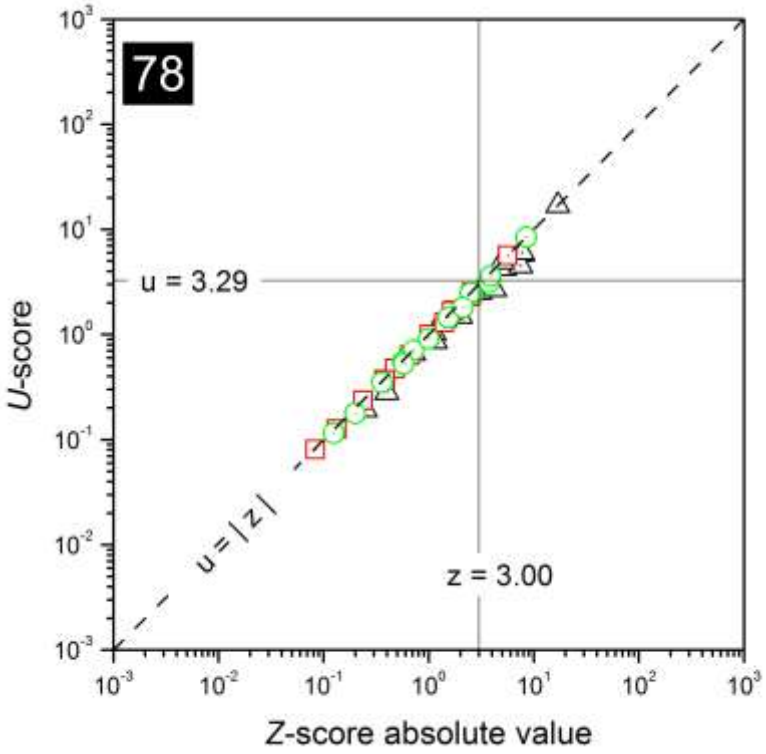

FIG. 102. Combined plots of z- and u-scores for the laboratory with code 78 in case of sample "1".

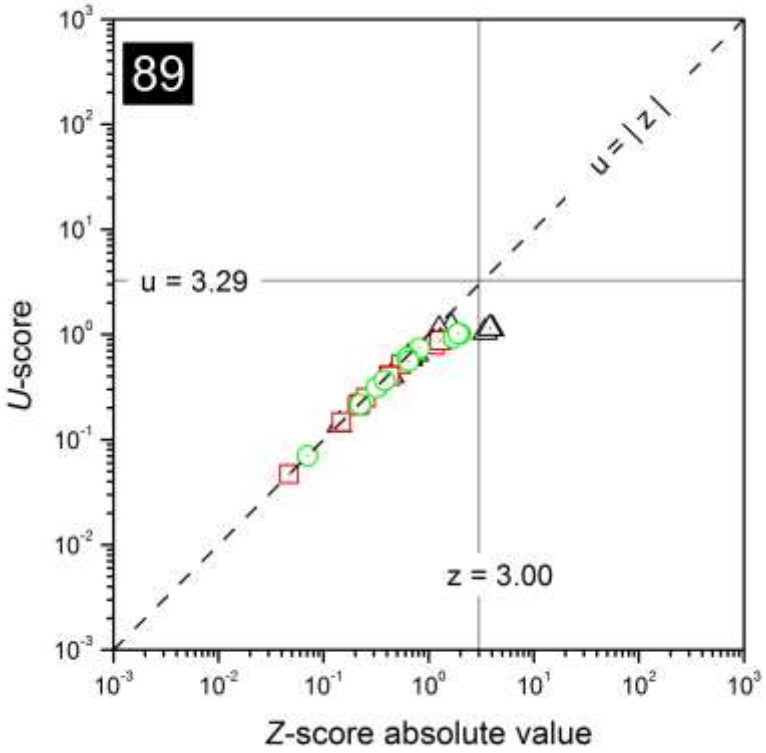

FIG. 103. Combined plots of z- and u-scores for the laboratory with code 89 in case of sample "1".

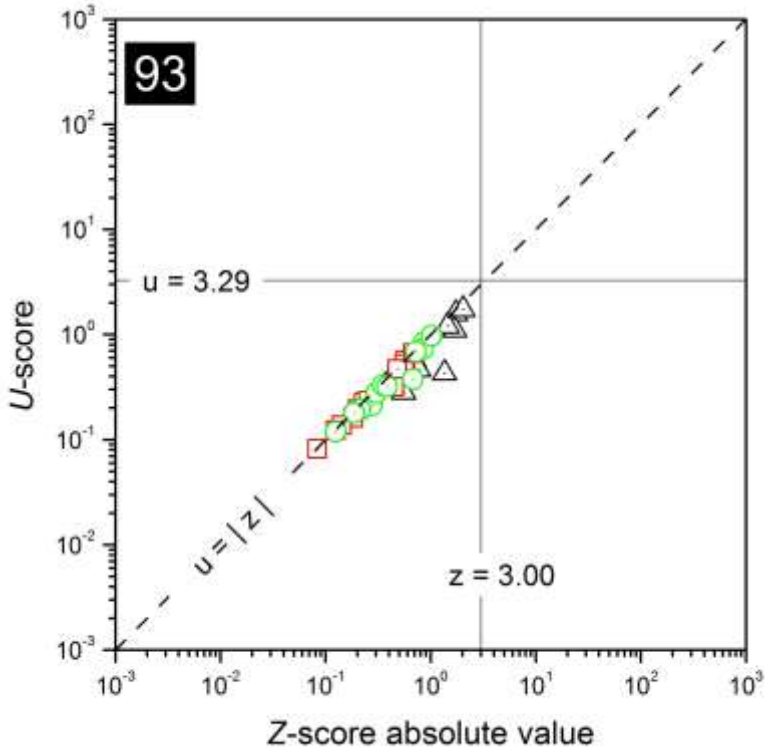

FIG. 104. Combined plots of z- and u-scores for the laboratory with code 93 in case of sample "1".

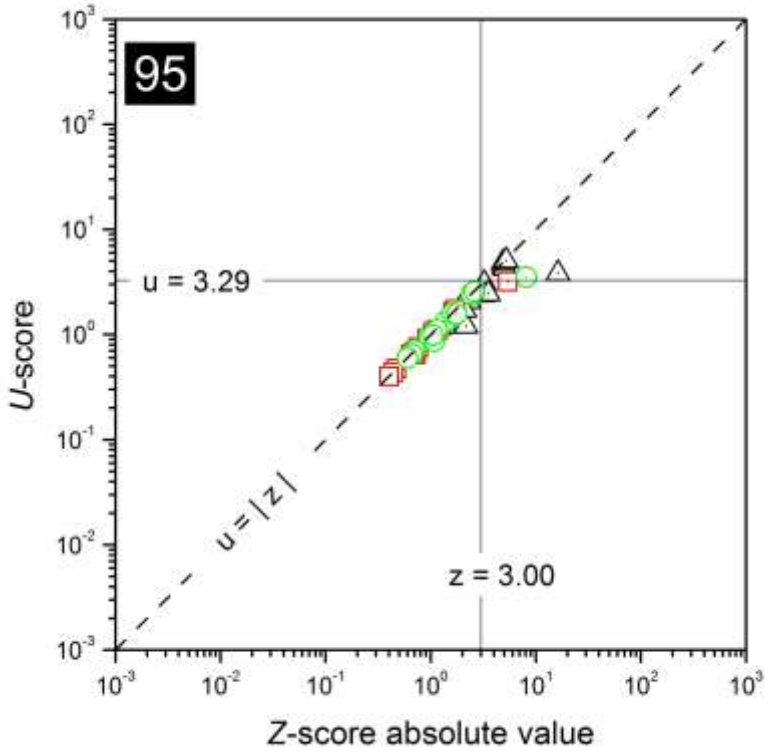

FIG. 105. Combined plots of z- and u-scores for the laboratory with code 95 in case of sample "1".

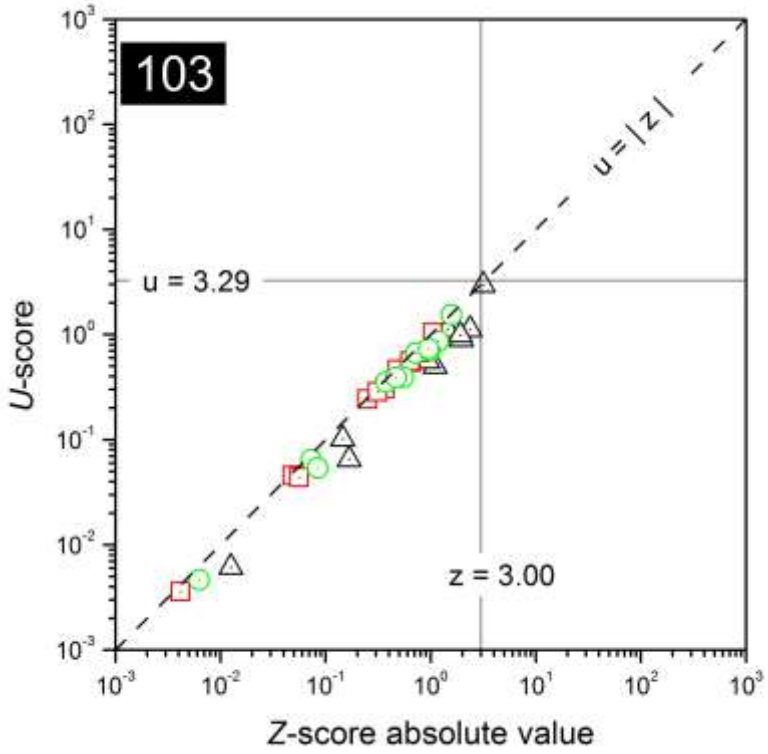

FIG. 106. Combined plots of z- and u-scores for the laboratory with code 103 in case of sample "1".

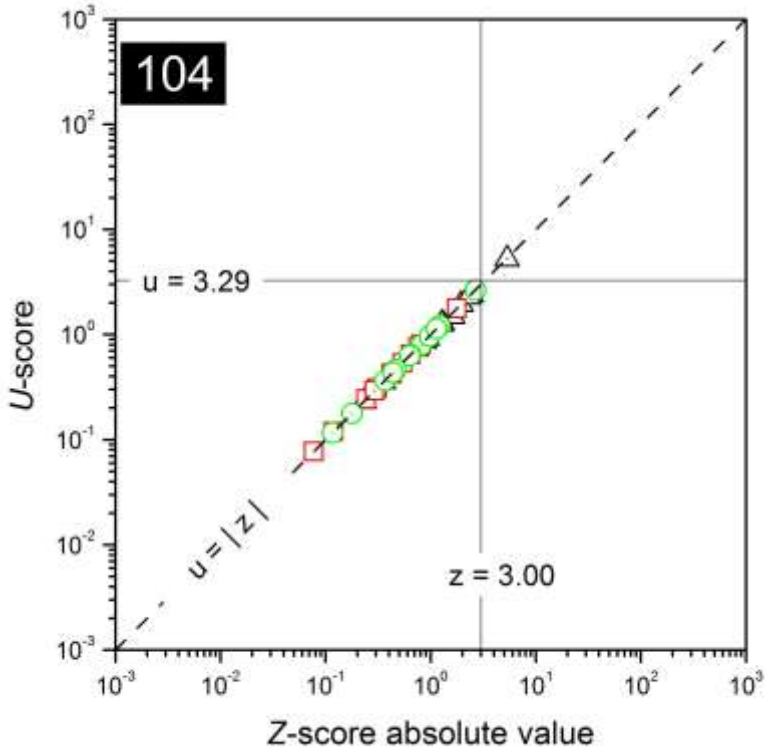

FIG. 107. Combined plots of z- and u-scores for the laboratory with code 104 in case of sample "1".

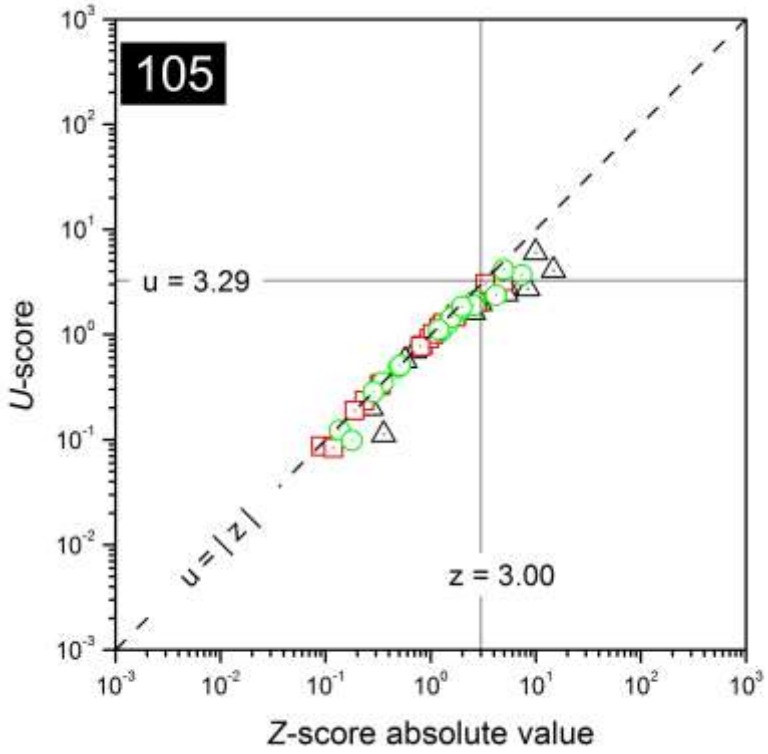

FIG. 108. Combined plots of z- and u-scores for the laboratory with code 105 in case of sample "1".

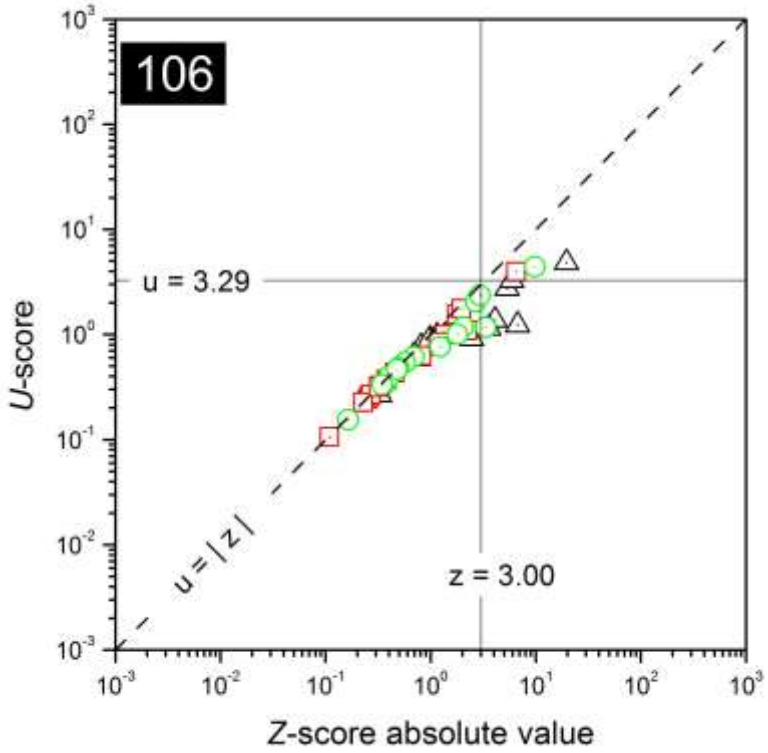

FIG. 109. Combined plots of z- and u-scores for the laboratory with code 106 in case of sample "1".

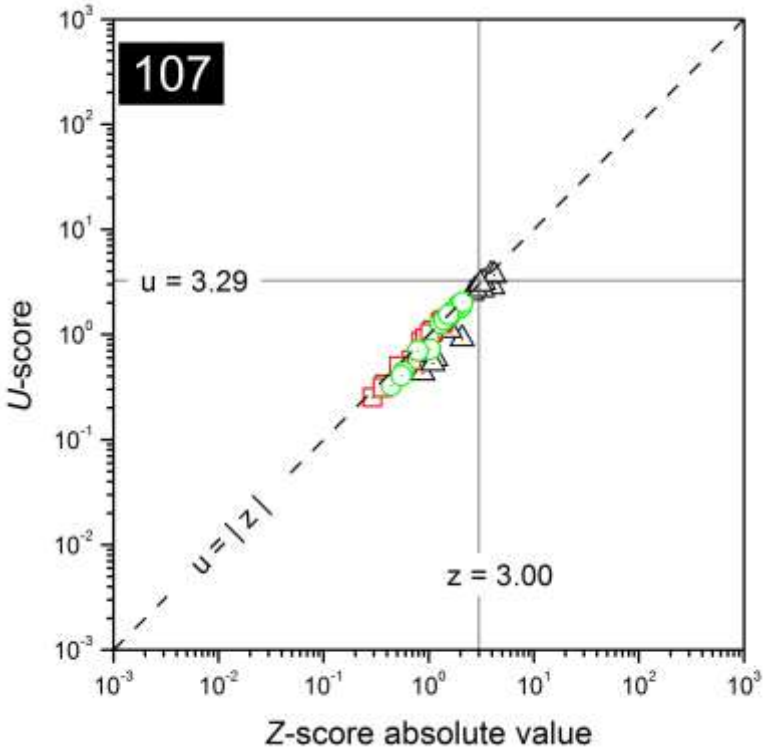

FIG. 110. Combined plots of z- and u-scores for the laboratory with code 107 in case of sample "1".

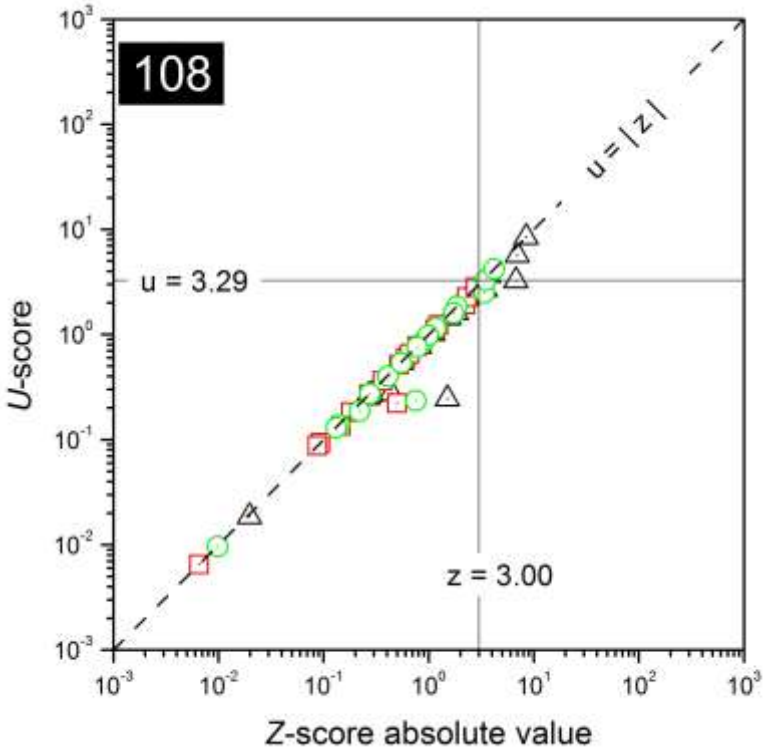

FIG. 111. Combined plots of z- and u-scores for the laboratory with code 108 in case of sample "1".

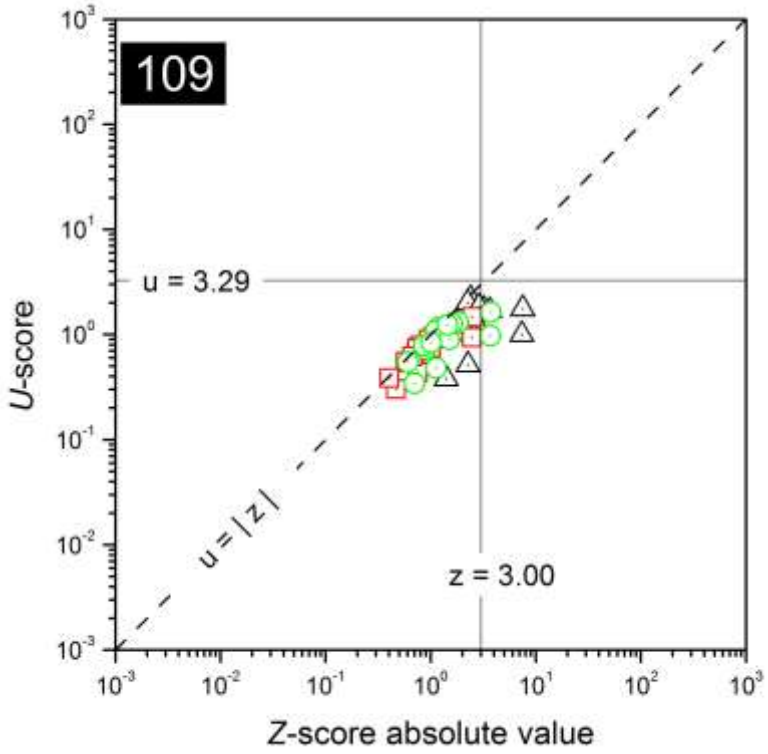

FIG. 112. Combined plots of z- and u-scores for the laboratory with code 109 in case of sample "1".

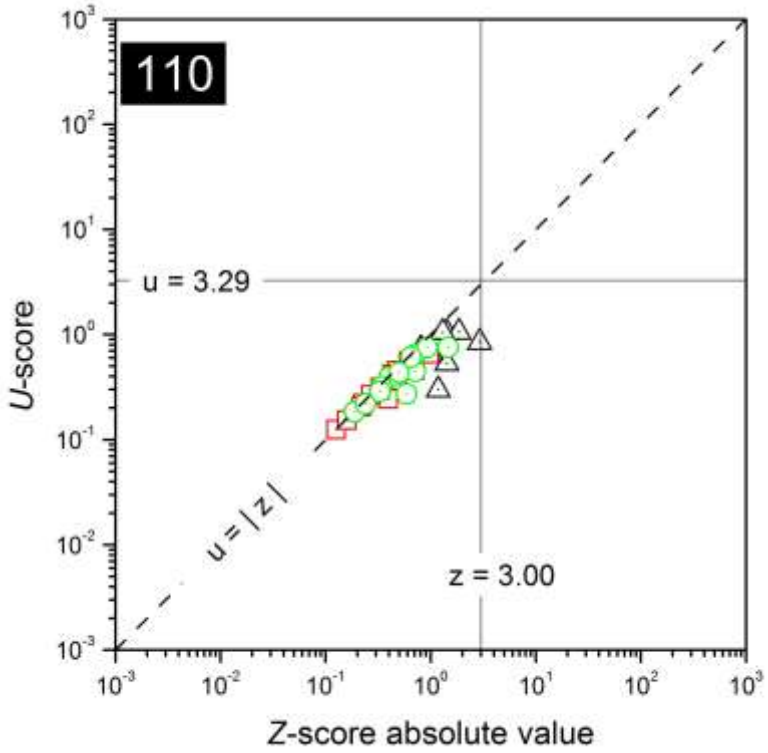

FIG. 113. Combined plots of z- and u-scores for the laboratory with code 110 in case of sample "1".

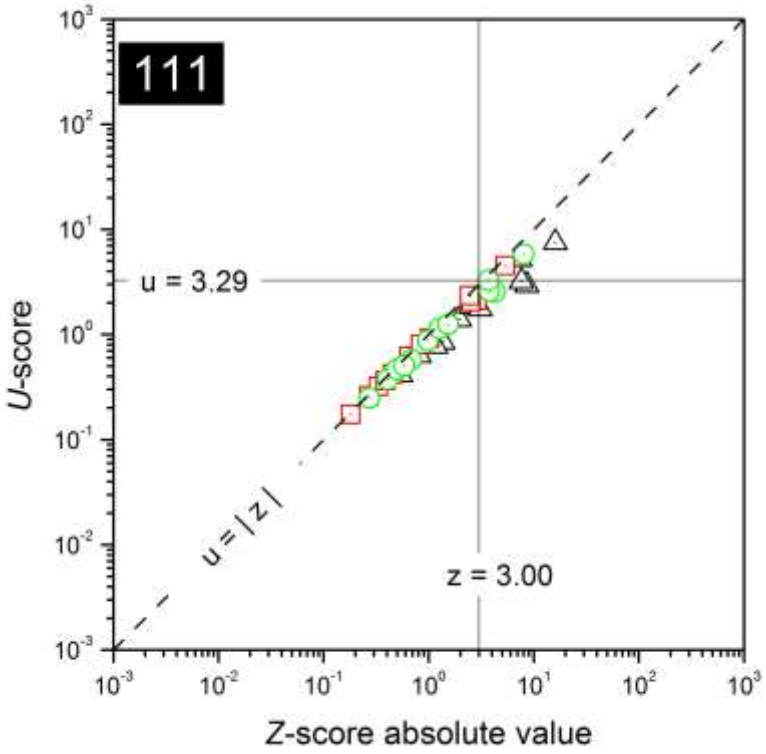

FIG. 114. Combined plots of z- and u-scores for the laboratory with code 111 in case of sample "1".

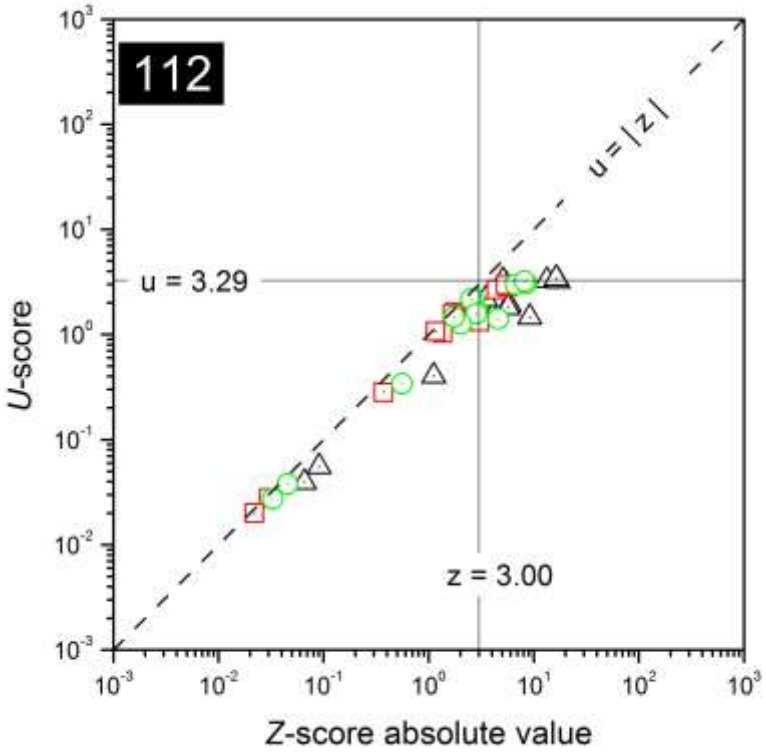

FIG. 115. Combined plots of z- and u-scores for the laboratory with code 112 in case of sample "1".

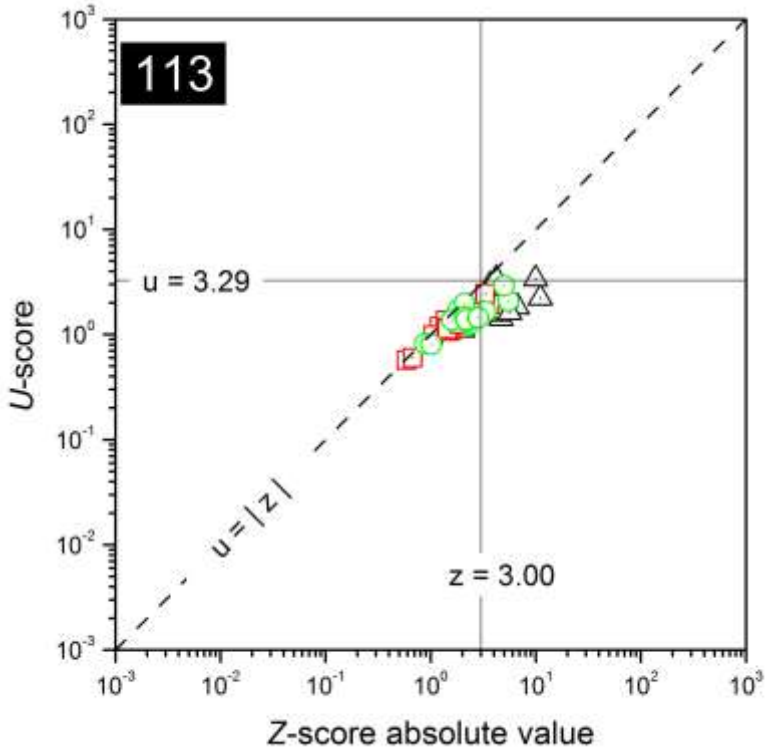

FIG. 116. Combined plots of z- and u-scores for the laboratory with code 113 in case of sample "1".

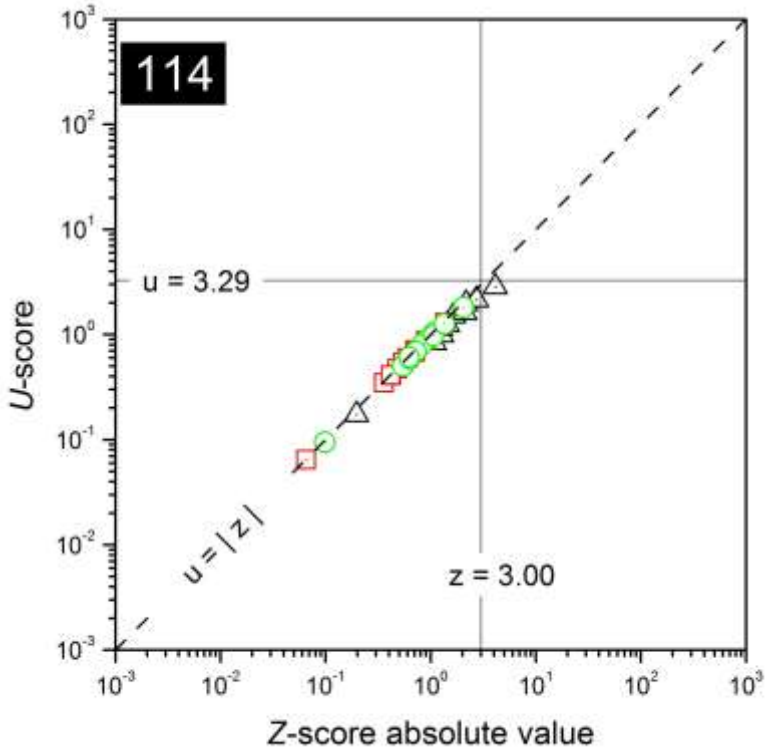

FIG. 117. Combined plots of z- and u-scores for the laboratory with code 114 in case of sample "1".

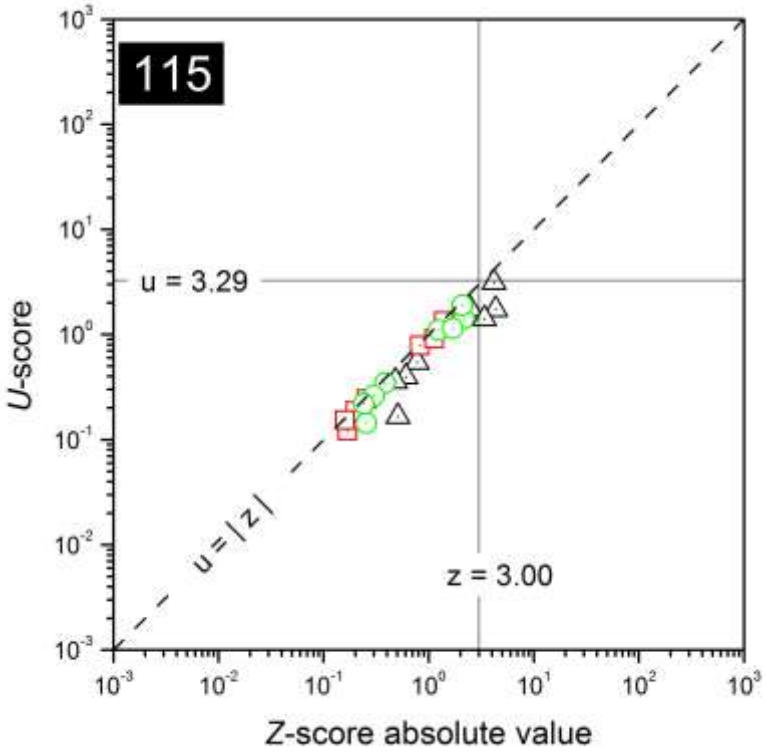

FIG. 118. Combined plots of z- and u-scores for the laboratory with code 115 in case of sample "1".

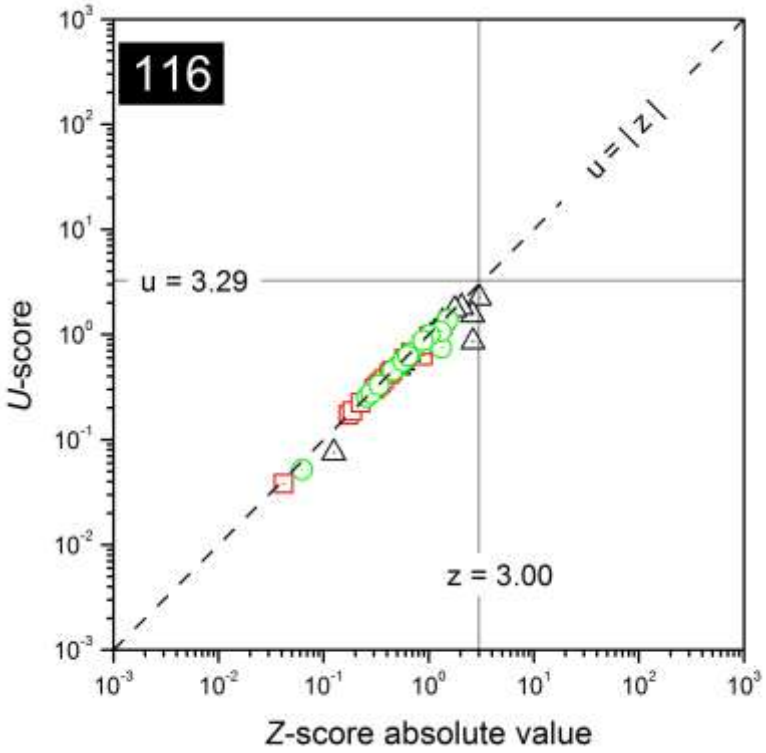

FIG. 119. Combined plots of z- and u-scores for the laboratory with code 116 in case of sample "1".

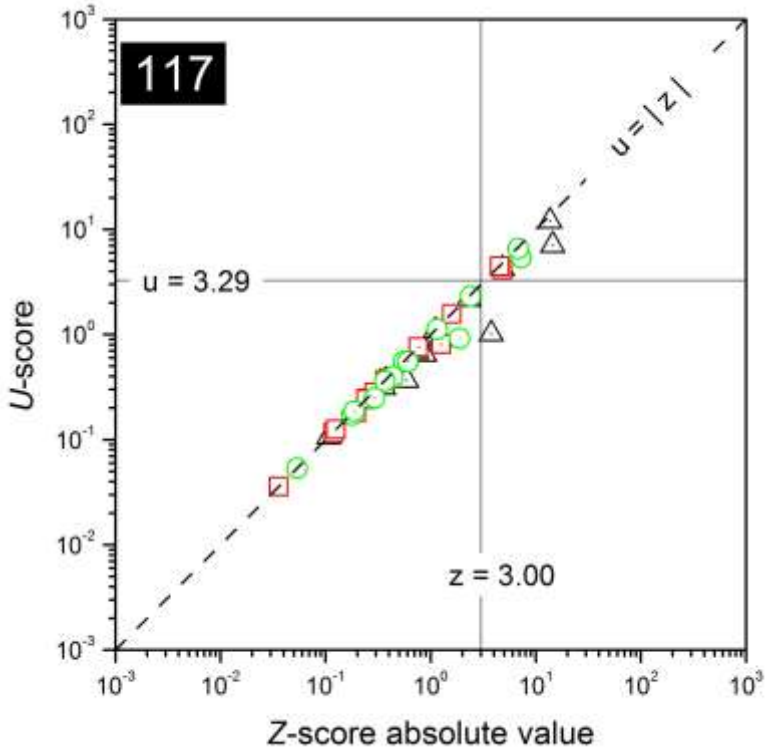

FIG. 120. Combined plots of z- and u-scores for the laboratory with code 117 in case of sample "1".

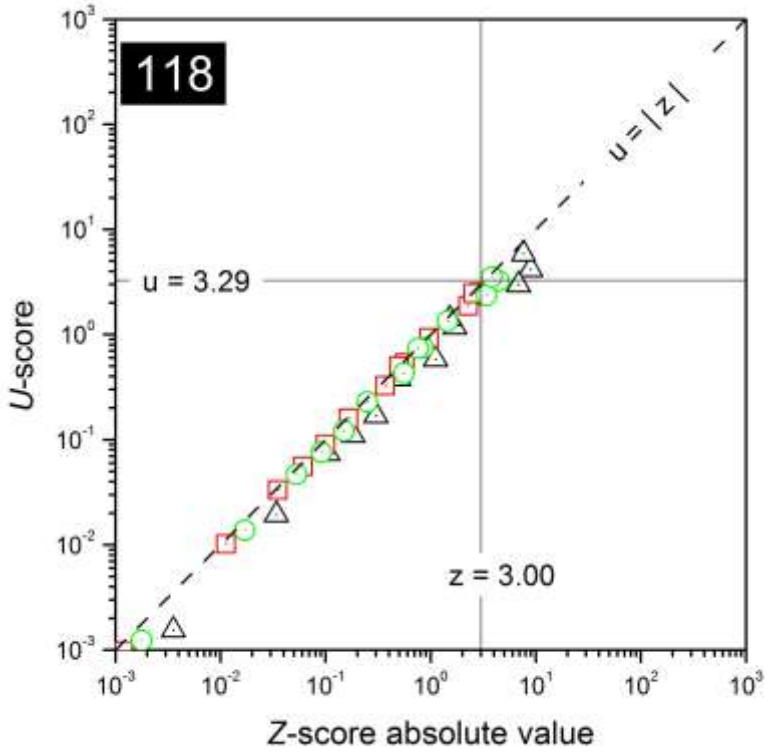

FIG. 121. Combined plots of z- and u-scores for the laboratory with code 118 in case of sample "1".

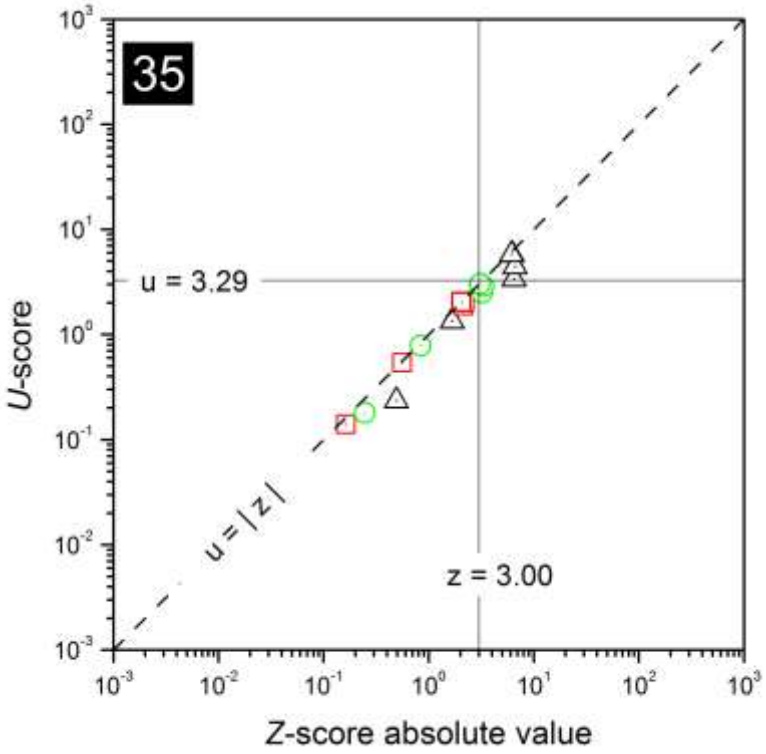

FIG. 122. Combined plots of z- and u-scores for the laboratory with code 35 in case of sample "2".

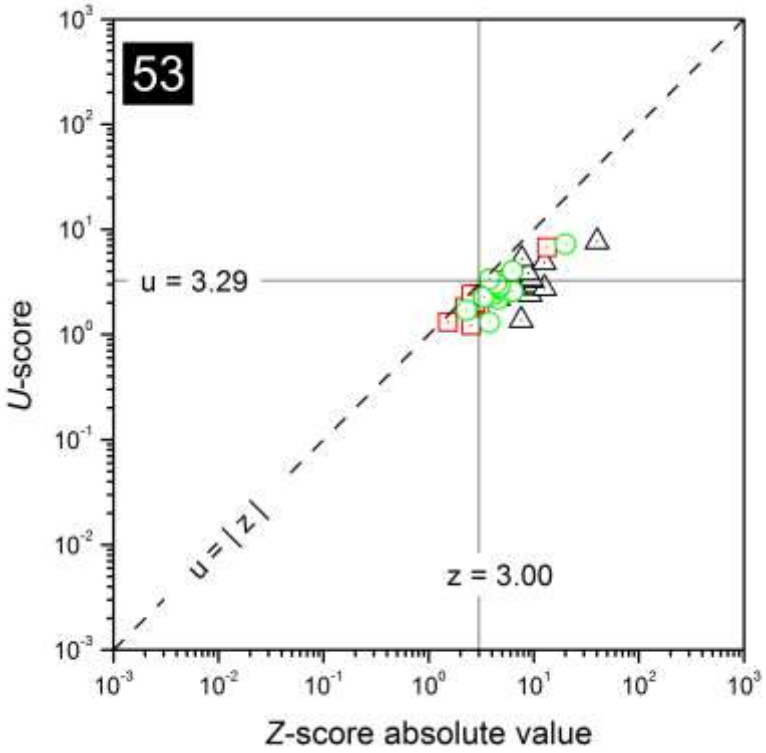

FIG. 123. Combined plots of z- and u-scores for the laboratory with code 53 in case of sample "2".

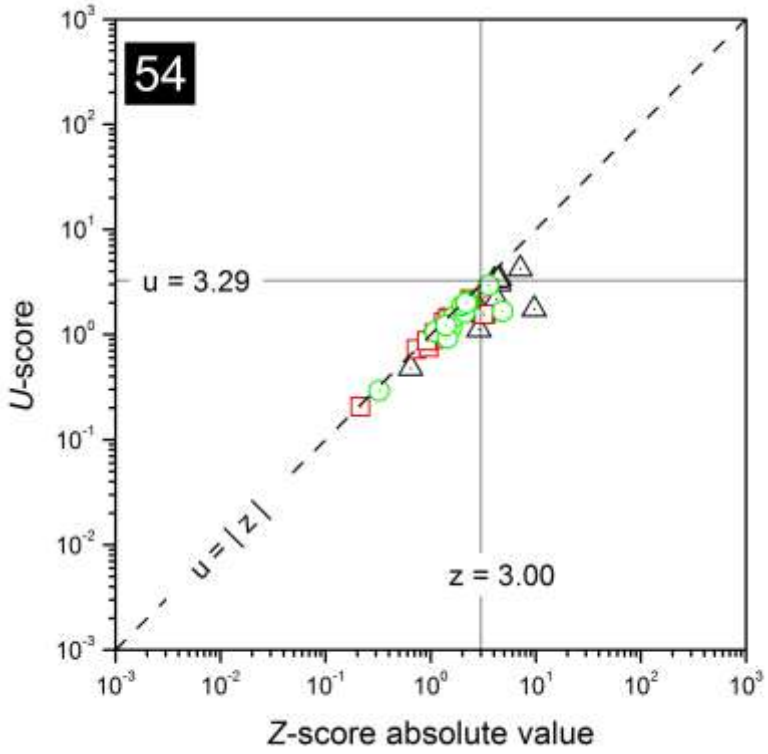

FIG. 124. Combined plots of z- and u-scores for the laboratory with code 54 in case of sample "2".

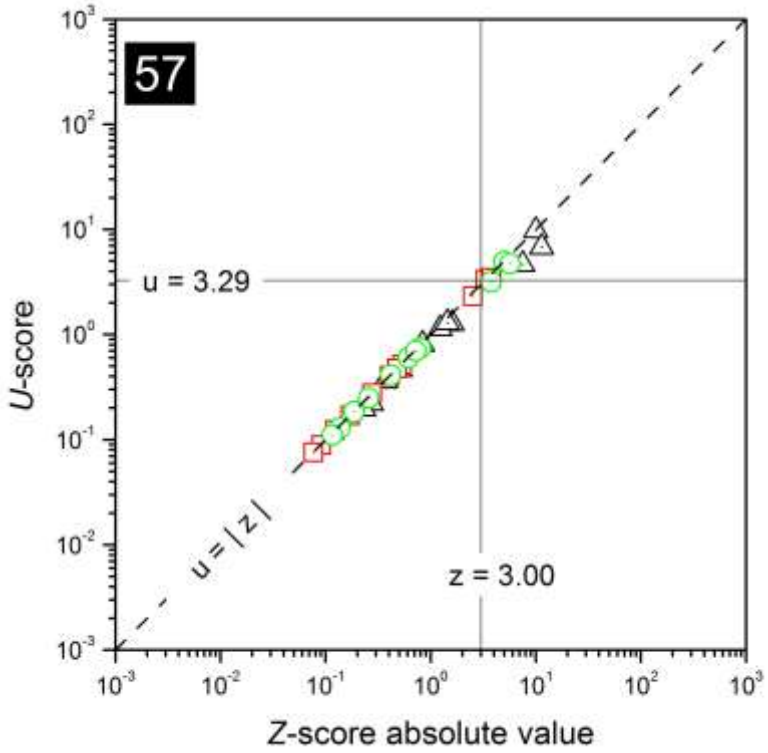

FIG. 125. Combined plots of z- and u-scores for the laboratory with code 57 in case of sample "2".

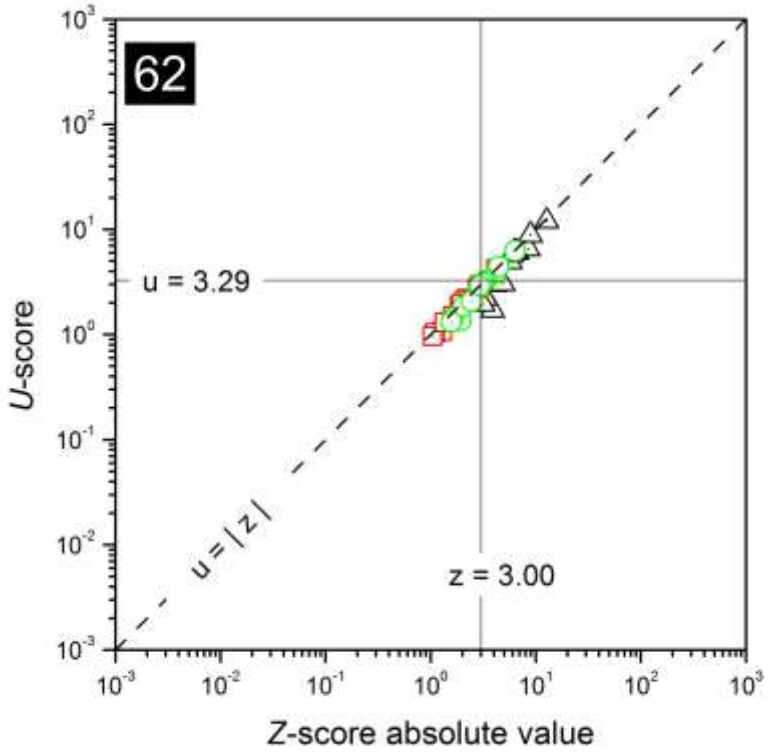

FIG. 126. Combined plots of z- and u-scores for the laboratory with code 62 in case of sample "2".

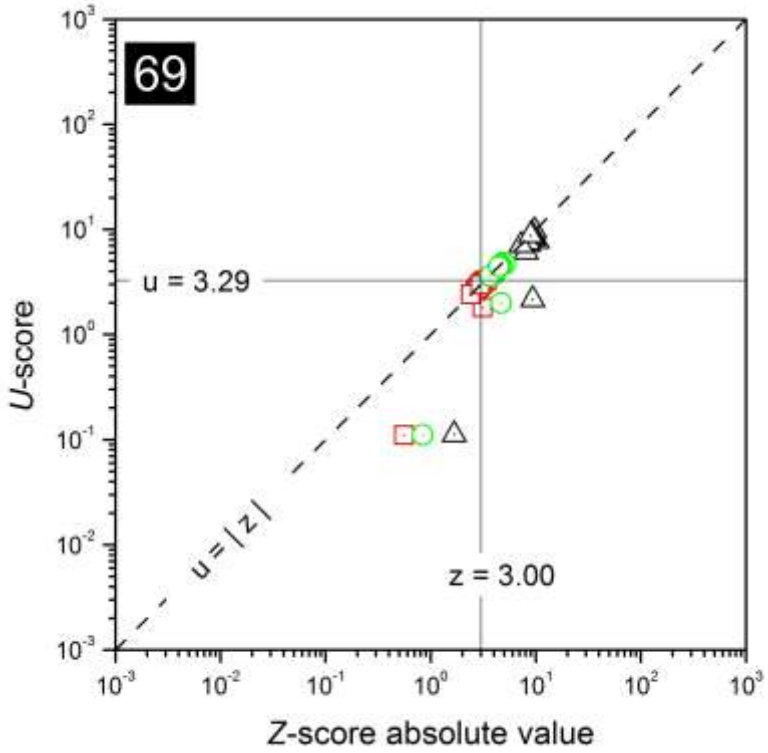

FIG. 127. Combined plots of z- and u-scores for the laboratory with code 69 in case of sample "2".

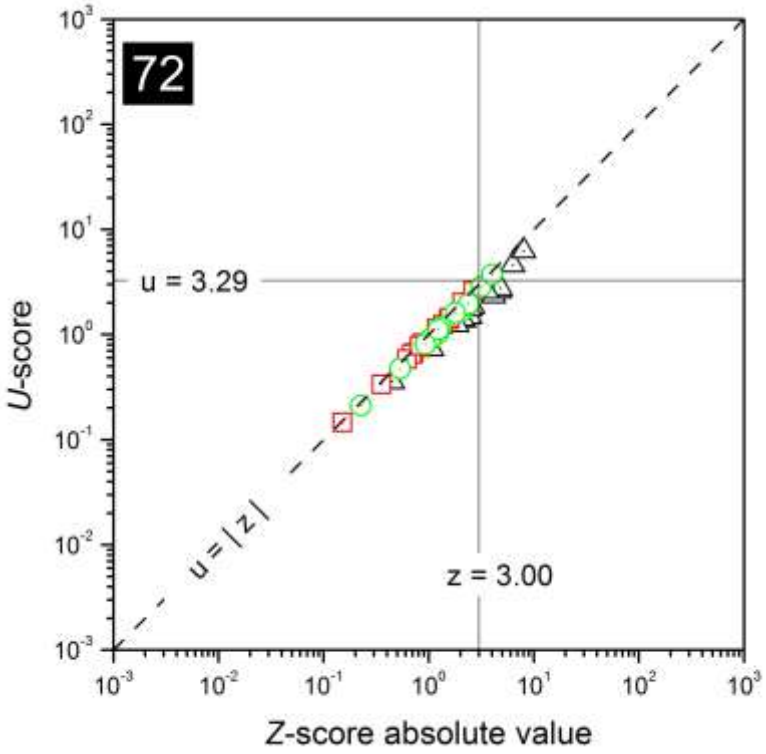

FIG. 128. Combined plots of z- and u-scores for the laboratory with code 72 in case of sample "2".

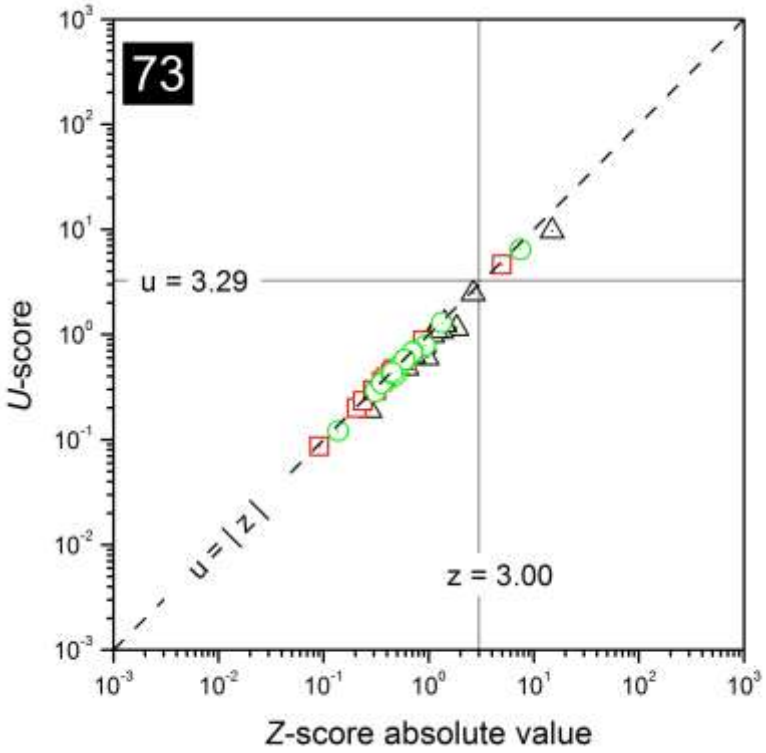

FIG. 129. Combined plots of z- and u-scores for the laboratory with code 73 in case of sample "2".

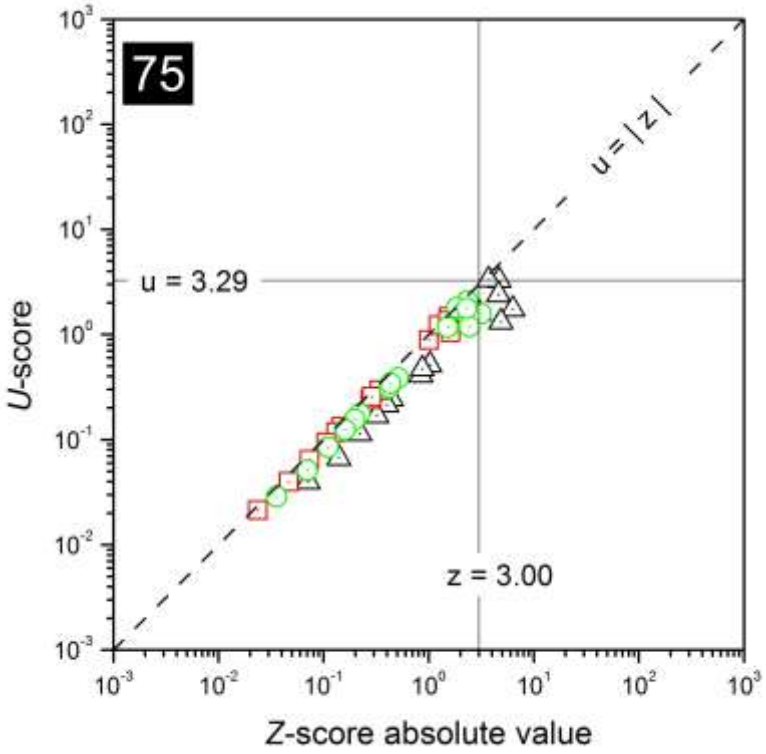

FIG. 130. Combined plots of z- and u-scores for the laboratory with code 75 in case of sample "2".

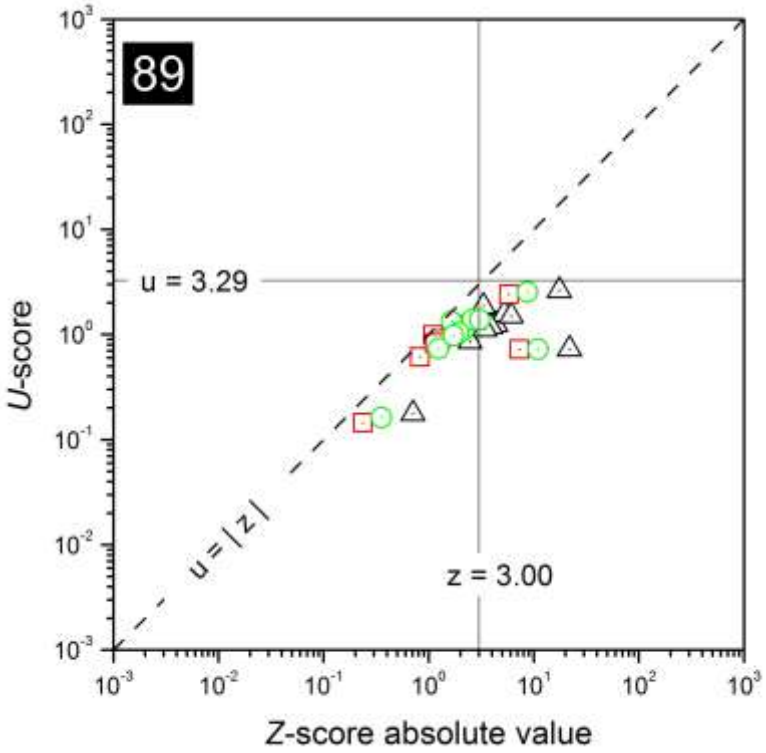

FIG. 131. Combined plots of z- and u-scores for the laboratory with code 89 in case of sample "2".

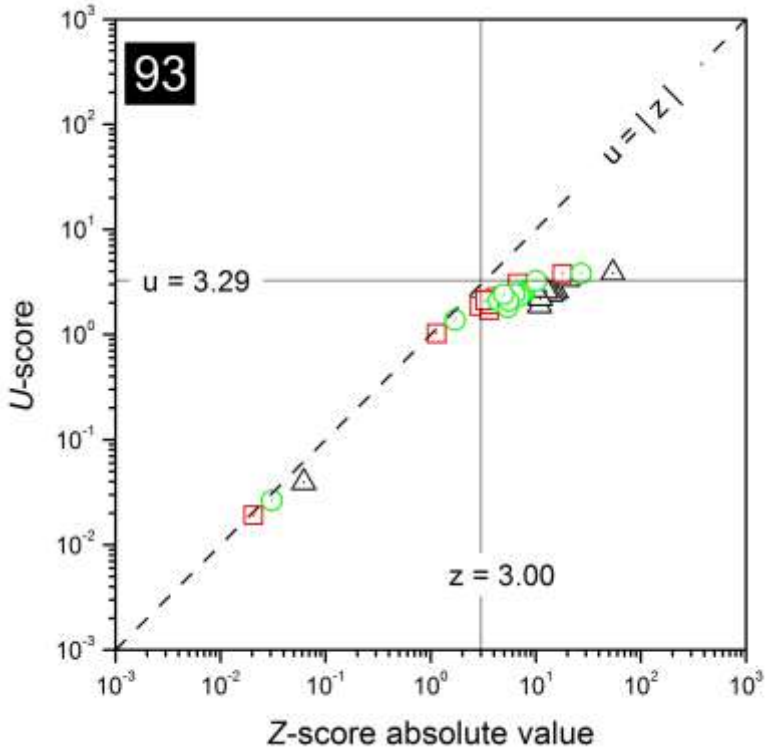

FIG. 132. Combined plots of z- and u-scores for the laboratory with code 93 in case of sample "2".

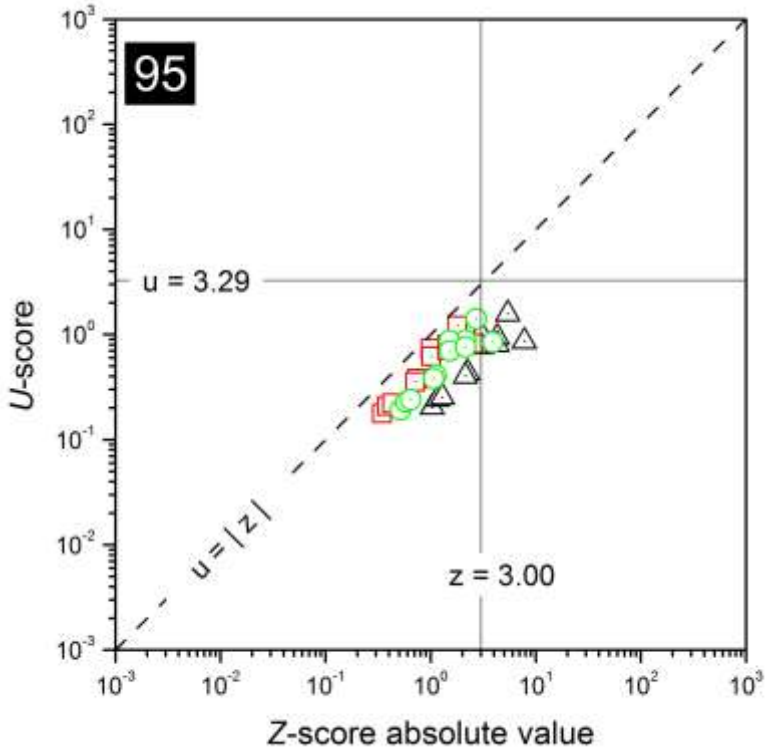

FIG. 133. Combined plots of z- and u-scores for the laboratory with code 95 in case of sample "2".

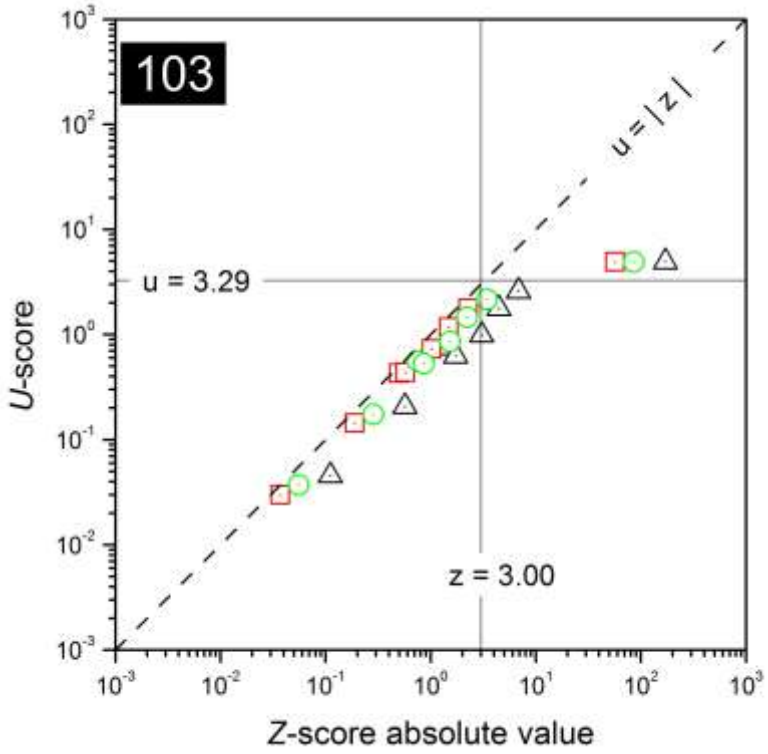

FIG. 134. Combined plots of z- and u-scores for the laboratory with code 103 in case of sample "2".

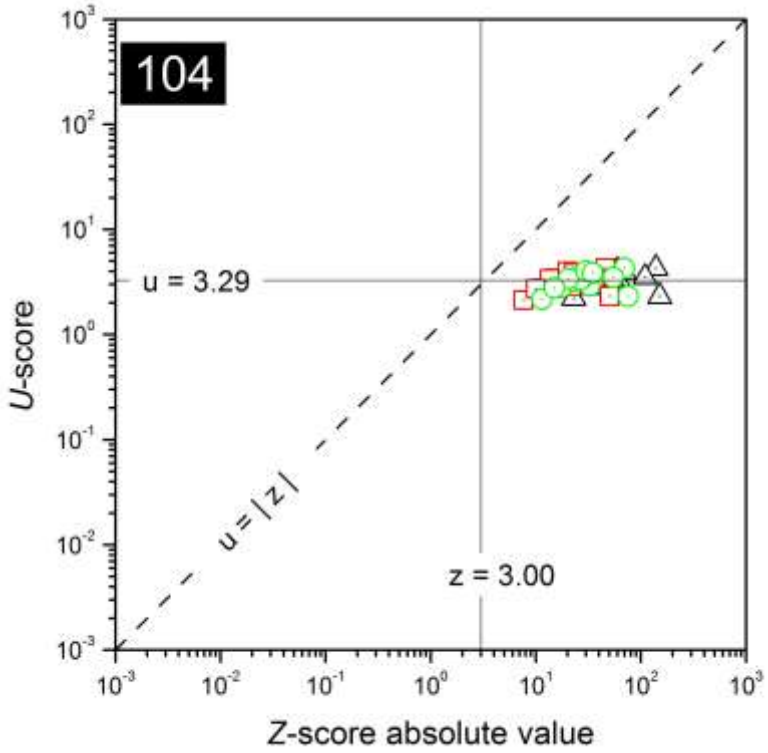

FIG. 135. Combined plots of z- and u-scores for the laboratory with code 104 in case of sample "2".

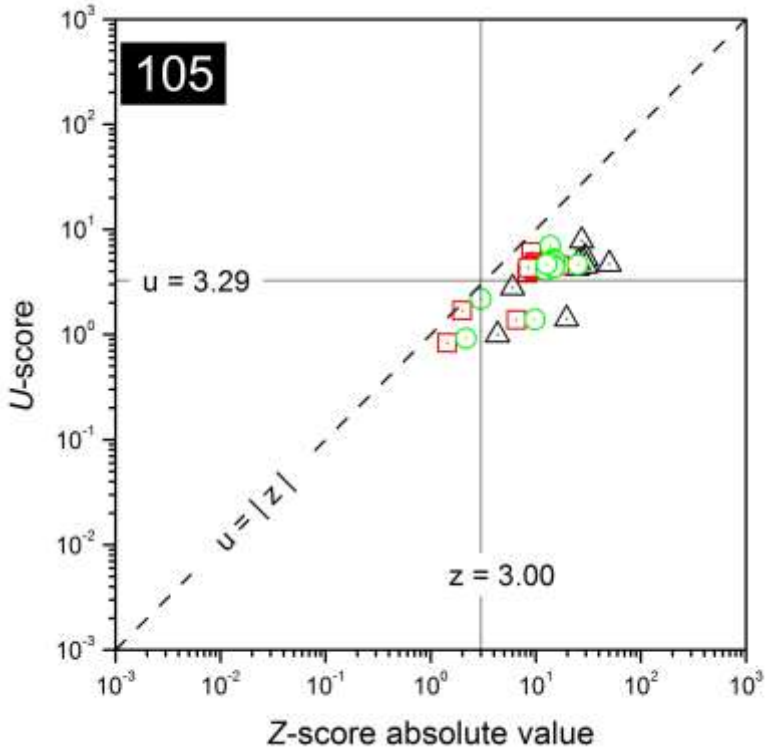

FIG. 136. Combined plots of z- and u-scores for the laboratory with code 105 in case of sample "2".

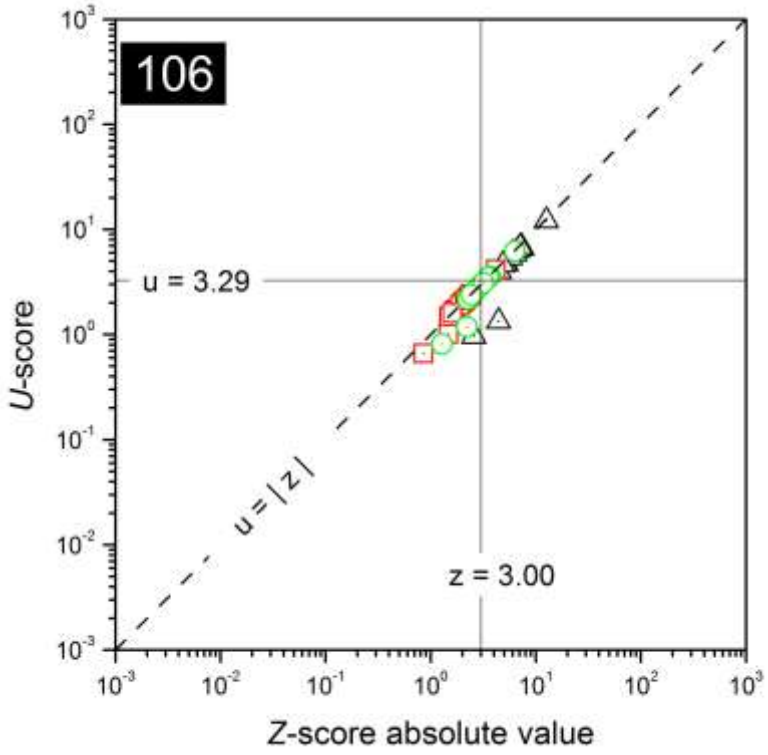

FIG. 137. Combined plots of z- and u-scores for the laboratory with code 106 in case of sample "2".

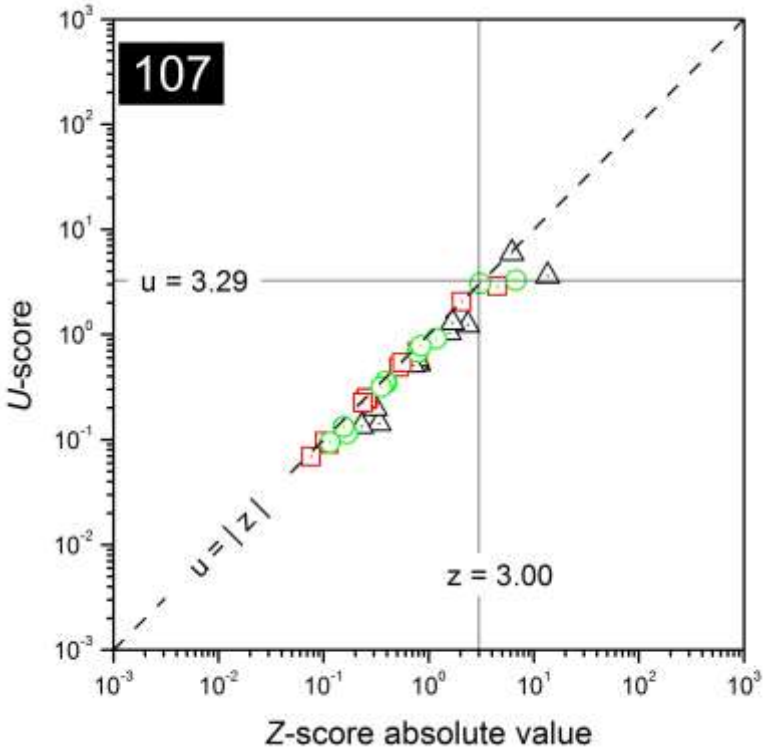

FIG. 138. Combined plots of z- and u-scores for the laboratory with code 107 in case of sample "2".

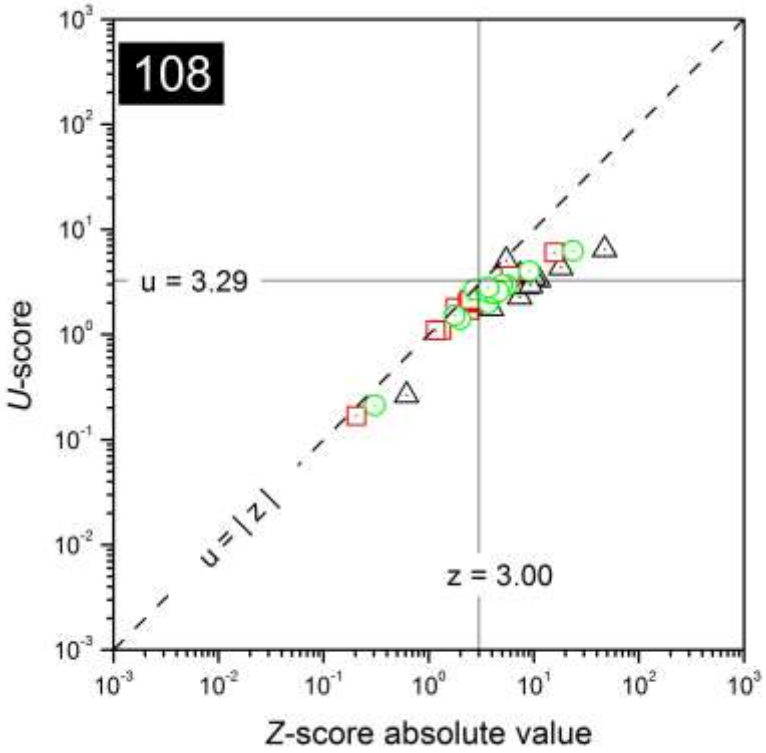

FIG. 139. Combined plots of z- and u-scores for the laboratory with code 108 in case of sample "2".

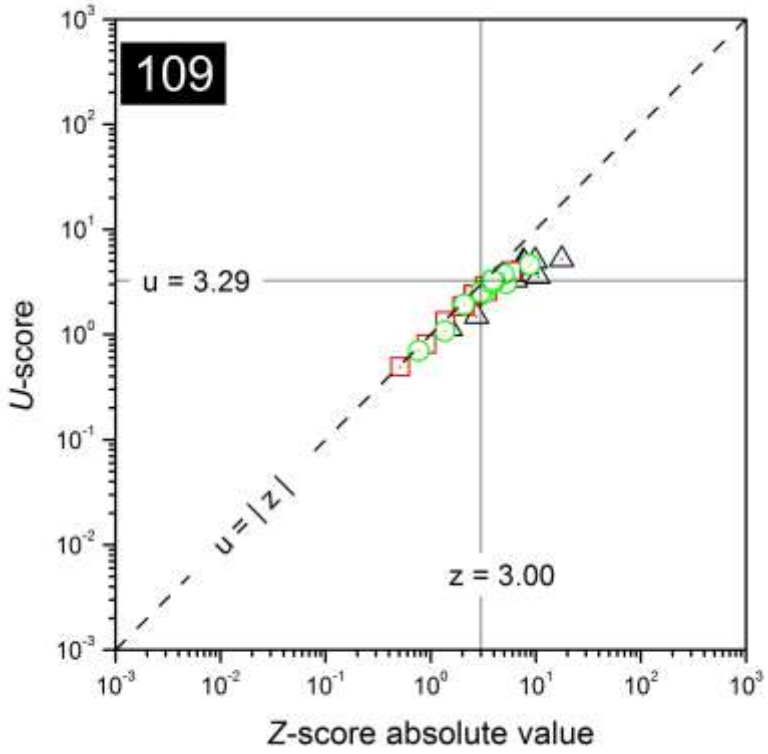

FIG. 140. Combined plots of z- and u-scores for the laboratory with code 109 in case of sample "2".

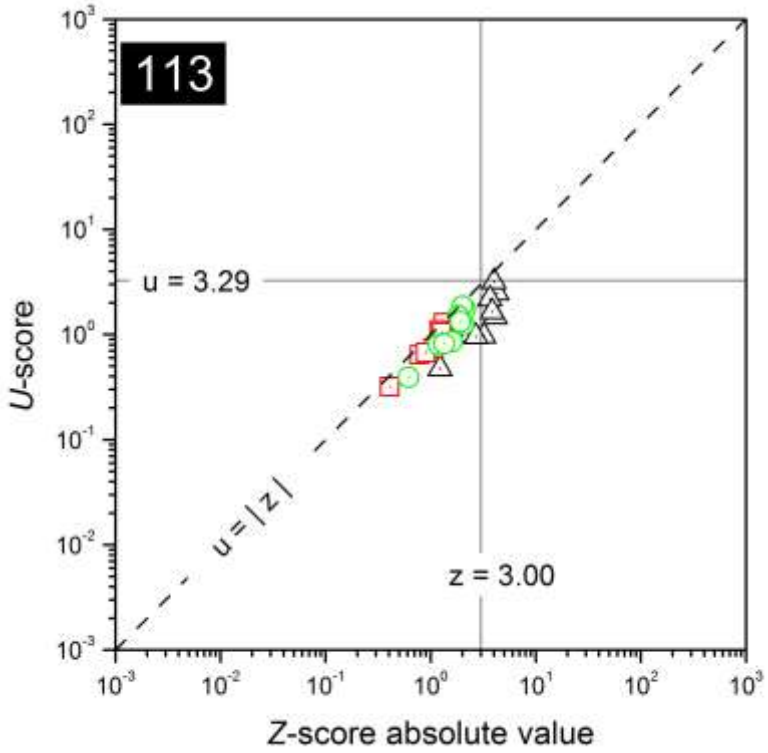

FIG. 141. Combined plots of z- and u-scores for the laboratory with code 113 in case of sample "2".

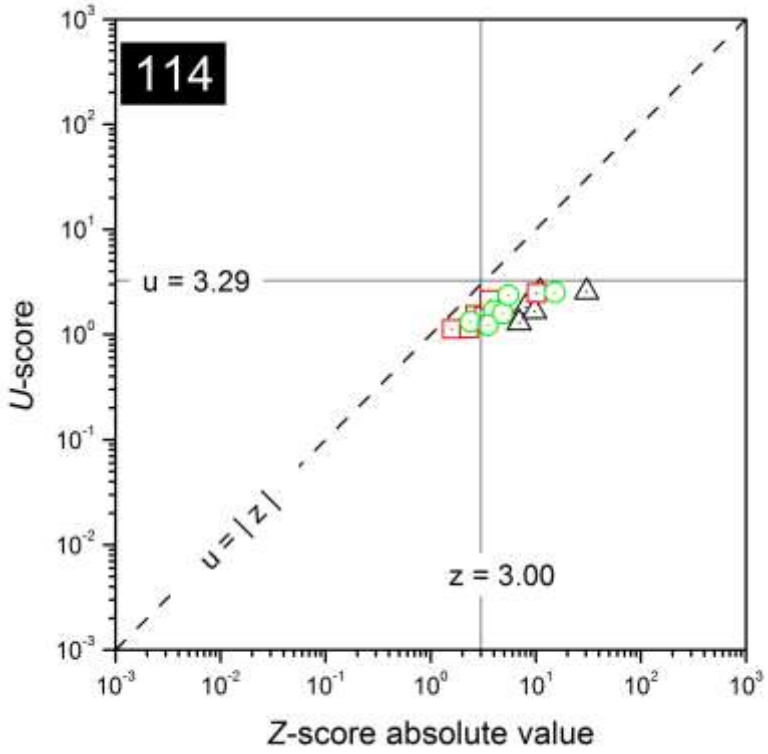

FIG. 142. Combined plots of z- and u-scores for the laboratory with code 114 in case of sample "2".

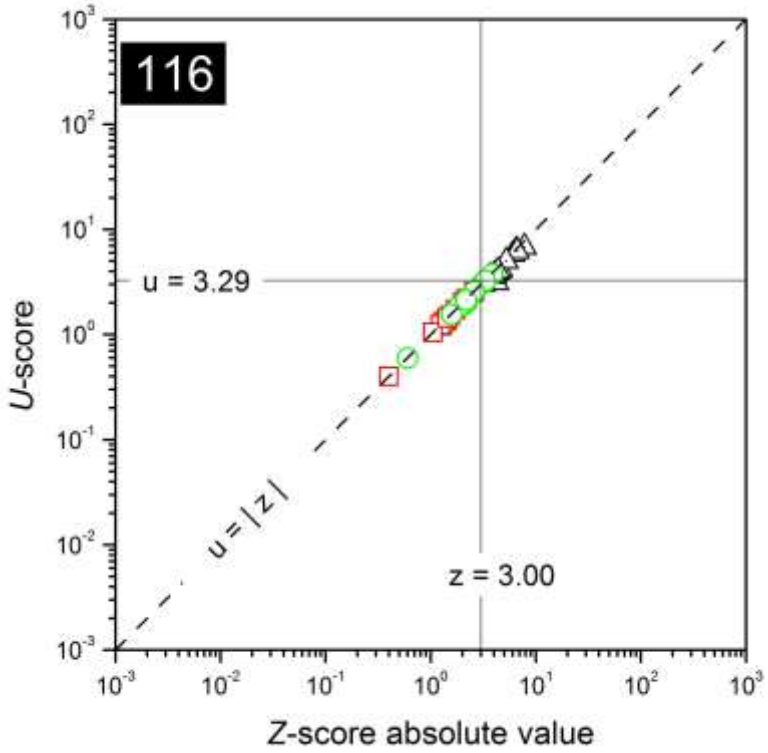

FIG. 143. Combined plots of z- and u-scores for the laboratory with code 116 in case of sample "2".

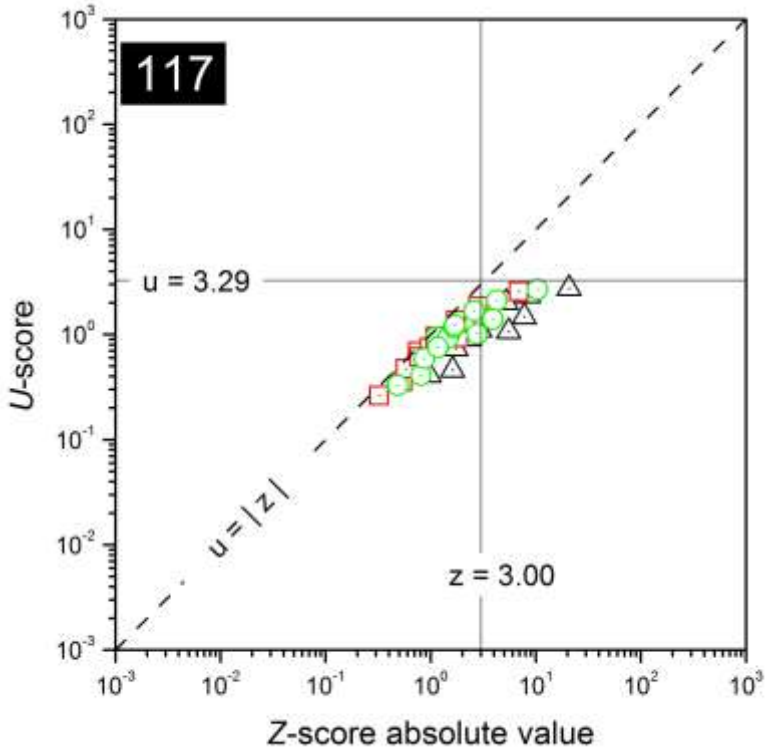

FIG. 144. Combined plots of z- and u-scores for the laboratory with code 117 in case of sample "2".

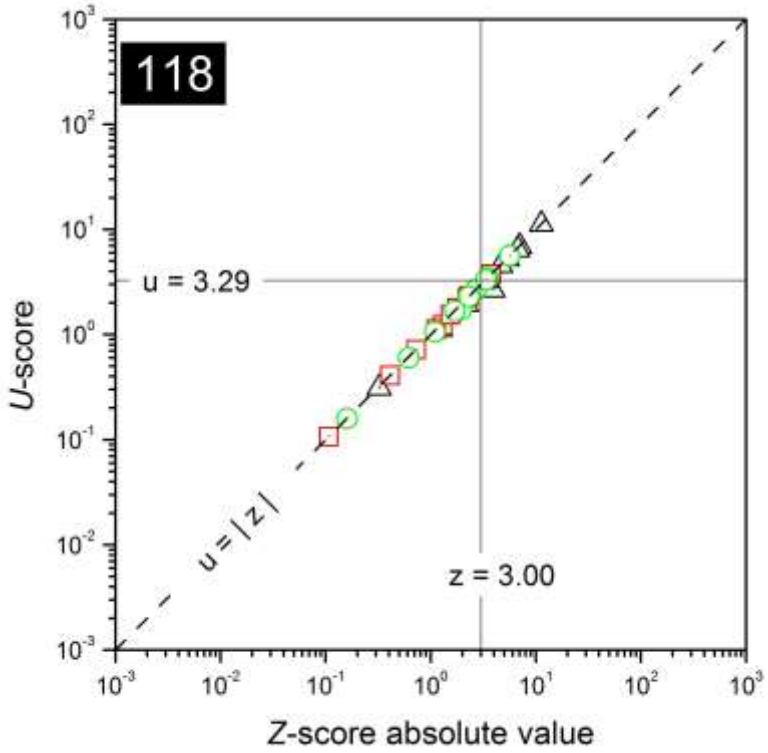

FIG. 145. Combined plots of z- and u-scores for the laboratory with code 118 in case of sample "2".

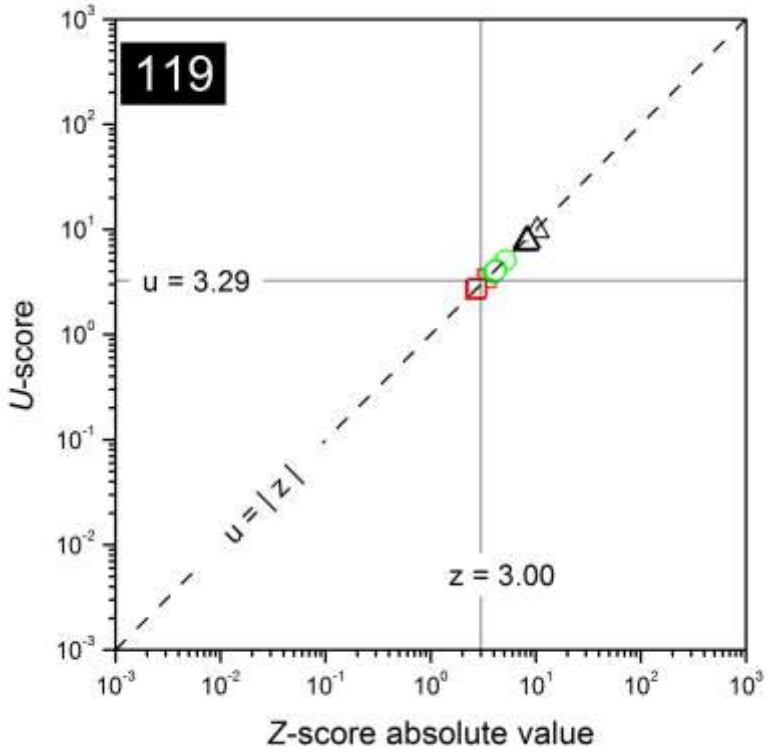

FIG. 146. Combined plots of z- and u-scores for the laboratory with code 119 in case of sample "2".

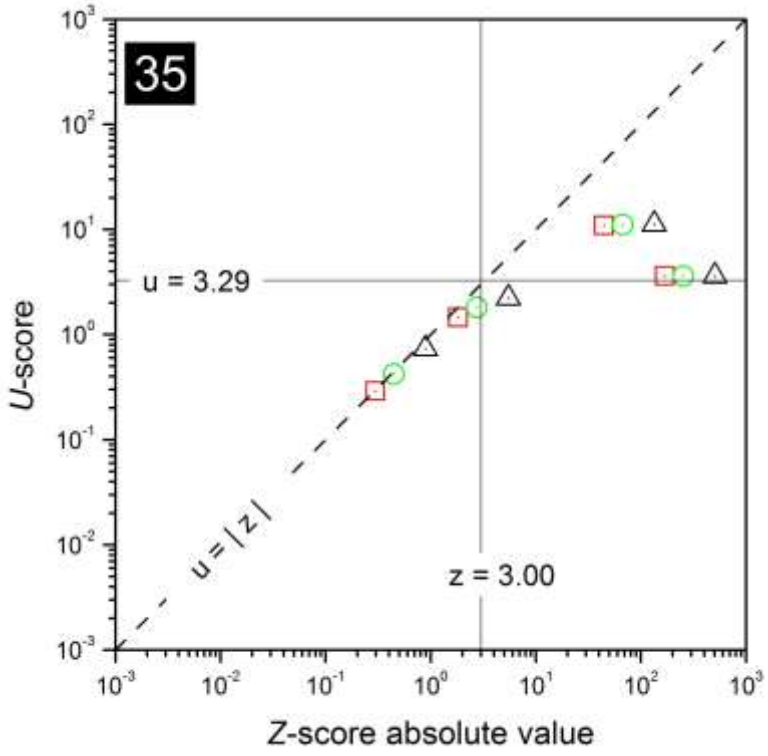

FIG. 147. Combined plots of z- and u-scores for the laboratory with code 35 in case of sample "3".

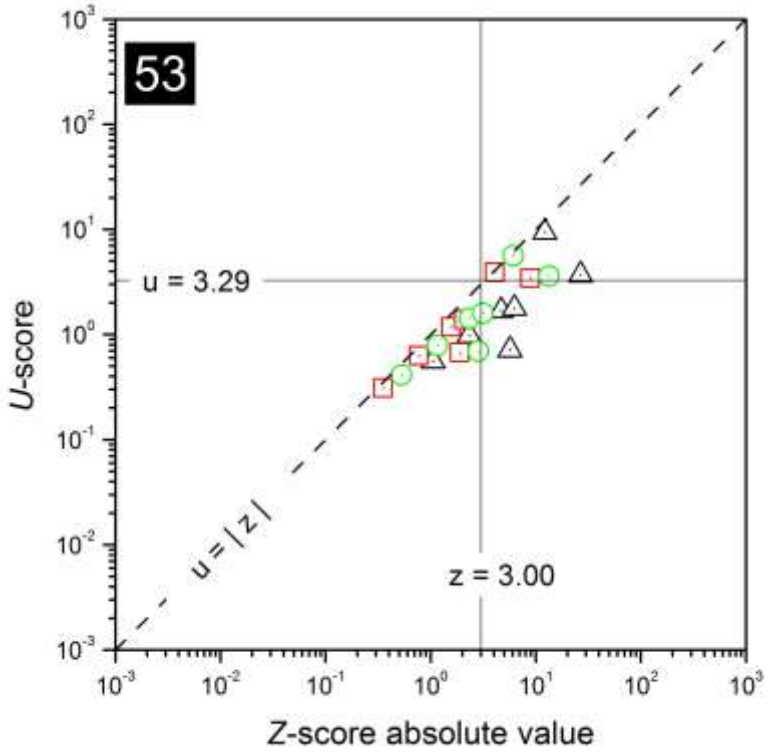

FIG. 148. Combined plots of z- and u-scores for the laboratory with code 53 in case of sample "3".

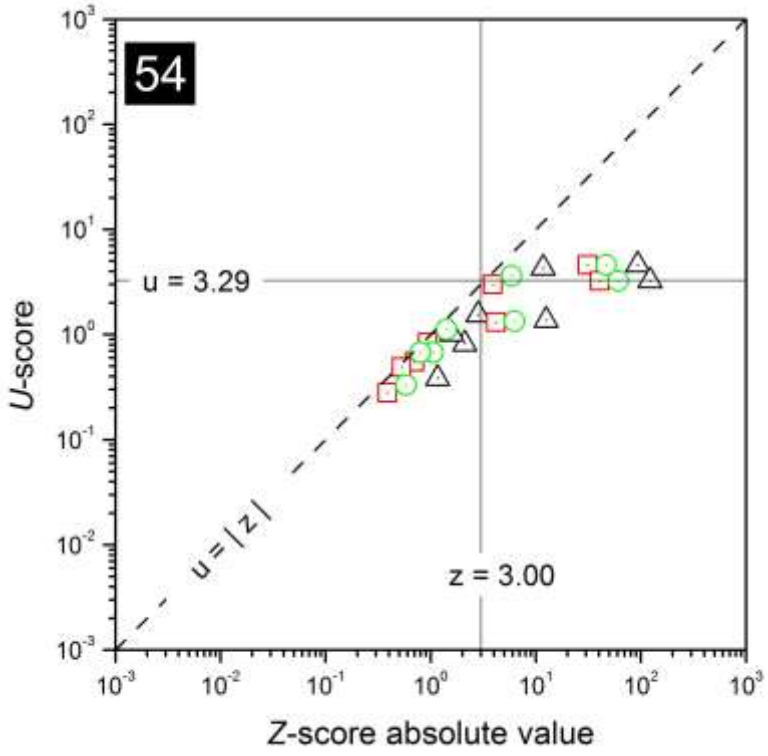

FIG. 149. Combined plots of z- and u-scores for the laboratory with code 54 in case of sample "3".

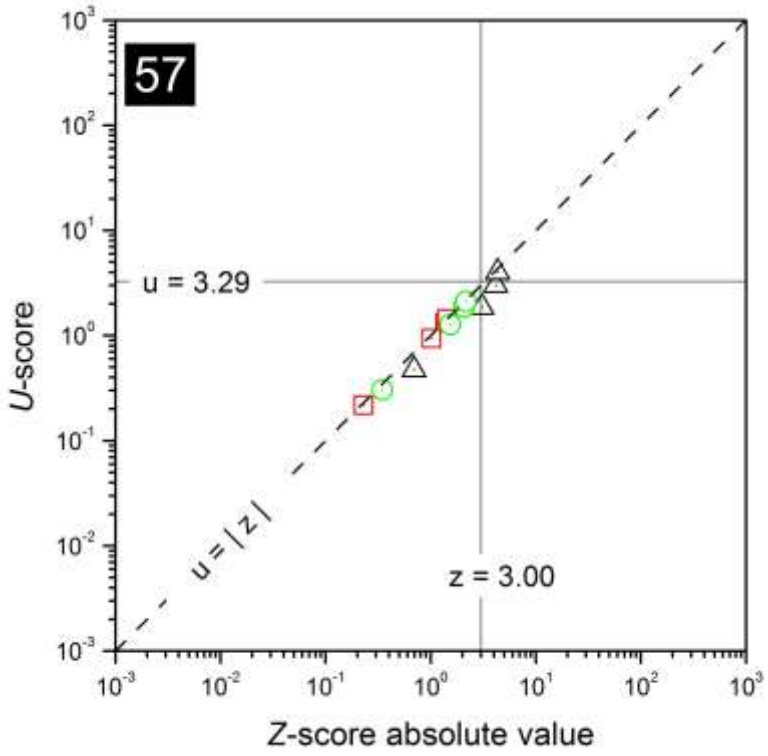

FIG. 150. Combined plots of z- and u-scores for the laboratory with code 57 in case of sample "3".

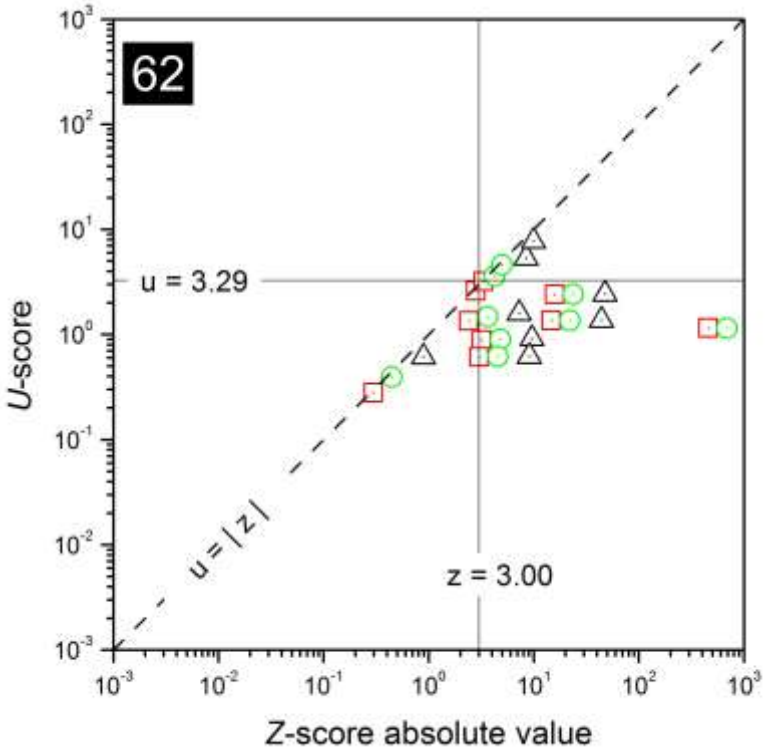

FIG. 151. Combined plots of z- and u-scores for the laboratory with code 62 in case of sample "3"

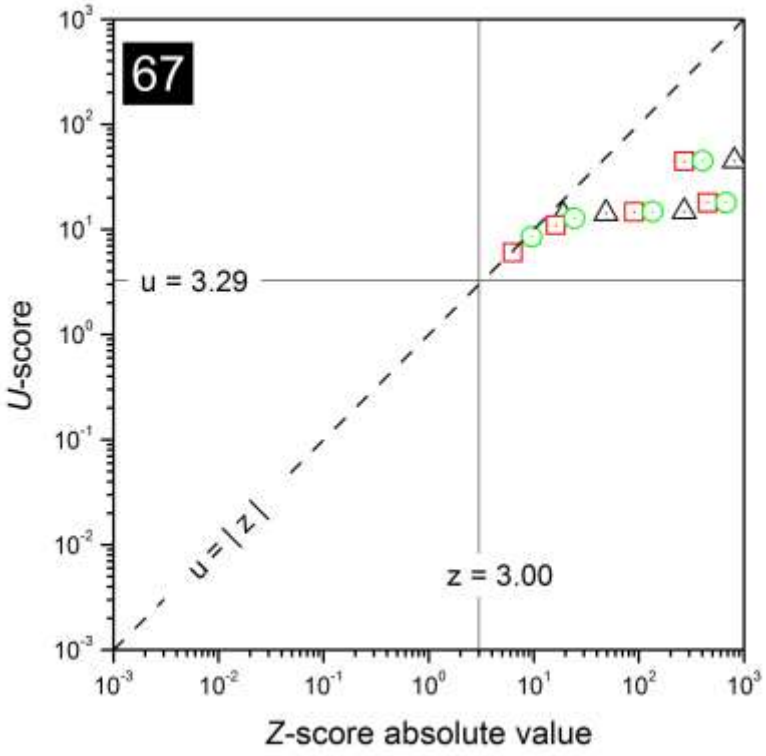

FIG. 152. Combined plots of z- and u-scores for the laboratory with code 67 in case of sample "3".

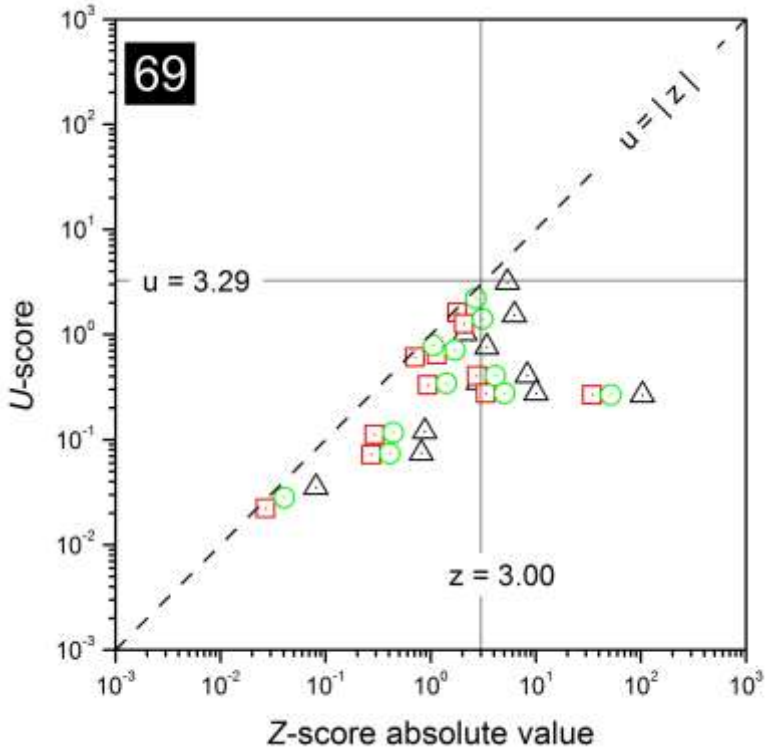

FIG. 153. Combined plots of z- and u-scores for the laboratory with code 69 in case of sample "3".

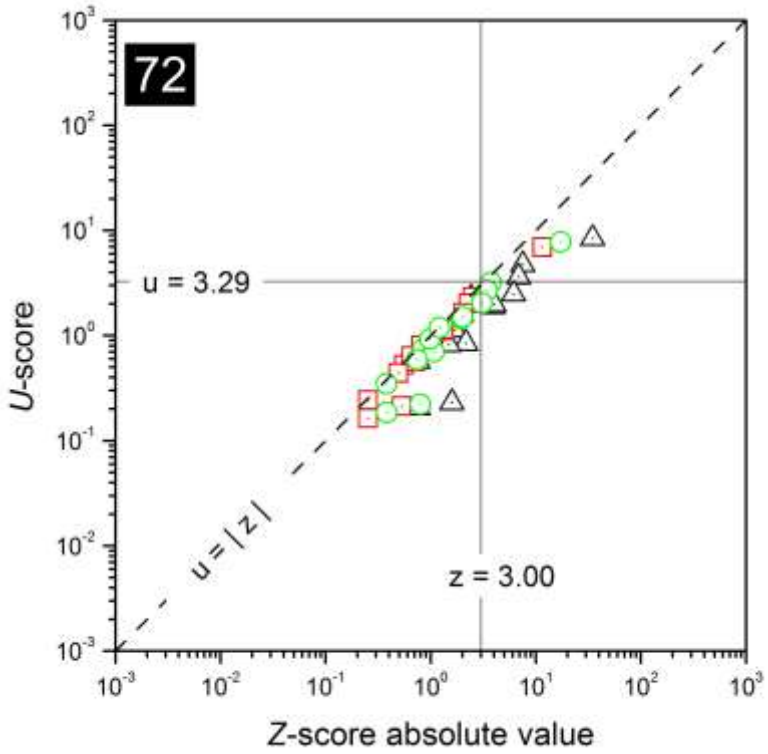

FIG. 154. Combined plots of z- and u-scores for the laboratory with code 72 in case of sample "3".

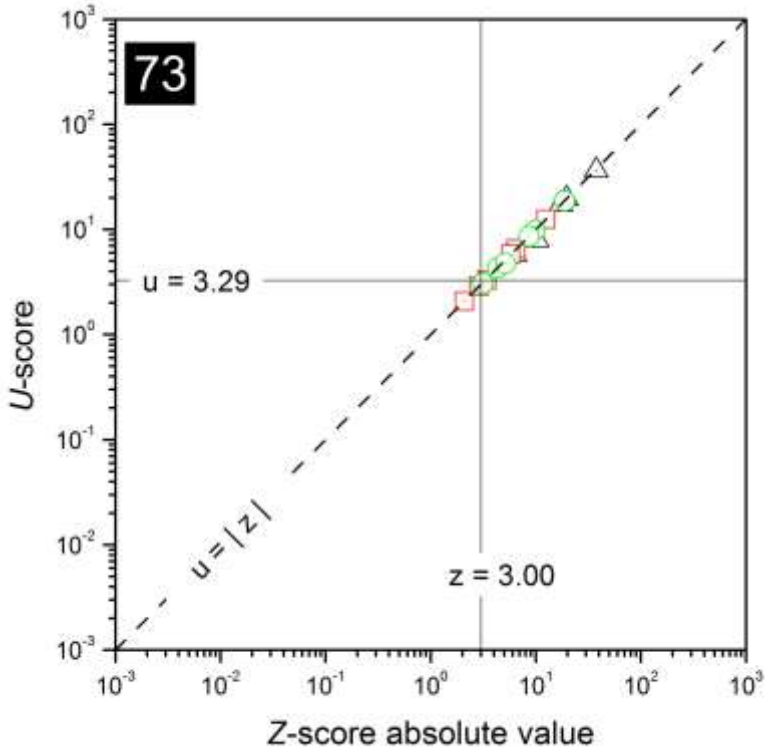

FIG. 155. Combined plots of z- and u-scores for the laboratory with code 73 in case of sample "3".

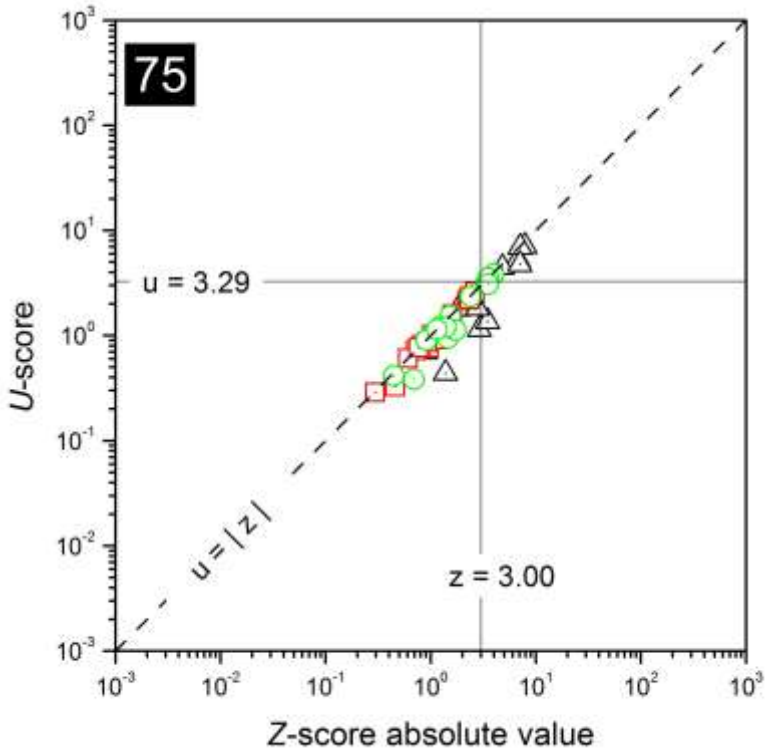

FIG. 156. Combined plots of z- and u-scores for the laboratory with code 75 in case of sample "3".

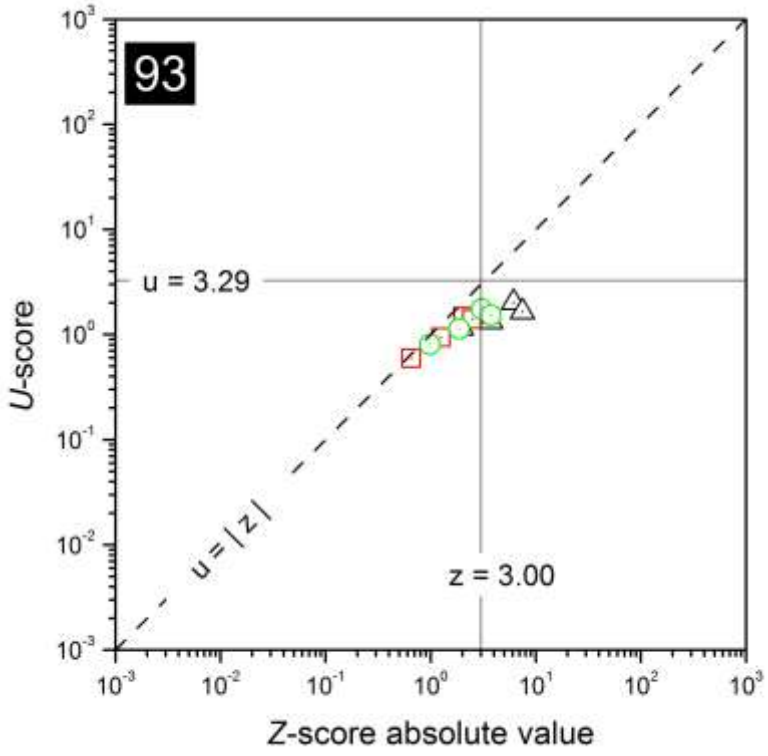

FIG. 157. Combined plots of z- and u-scores for the laboratory with code 93 in case of sample "3".

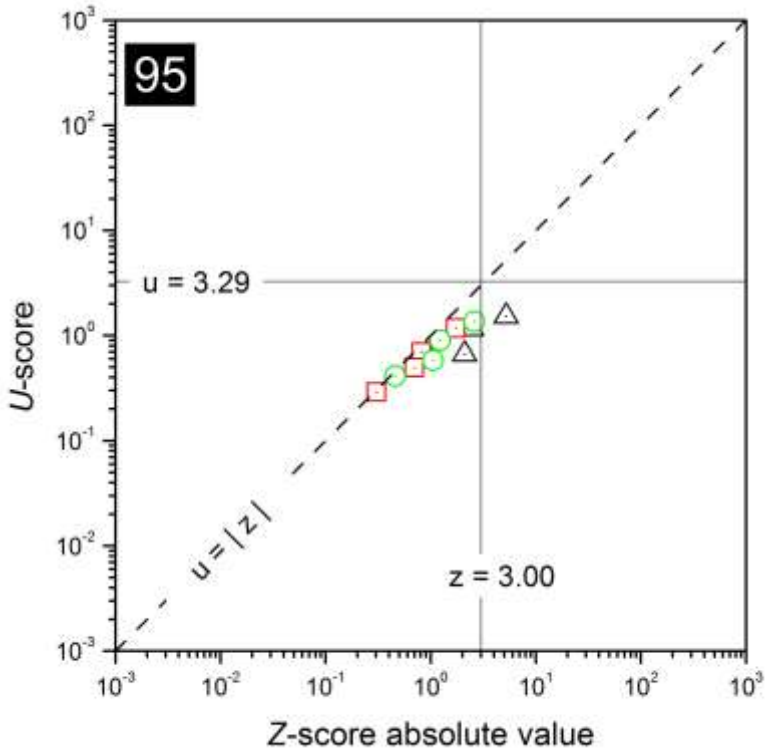

FIG. 158. Combined plots of z- and u-scores for the laboratory with code 95 in case of sample "3".

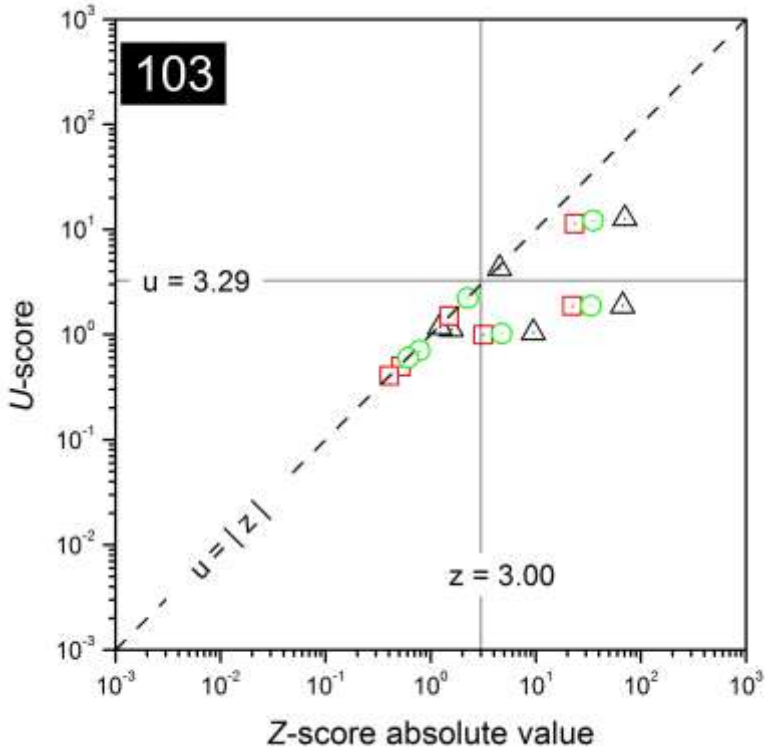

FIG. 159. Combined plots of z- and u-scores for the laboratory with code 103 in case of sample "3".

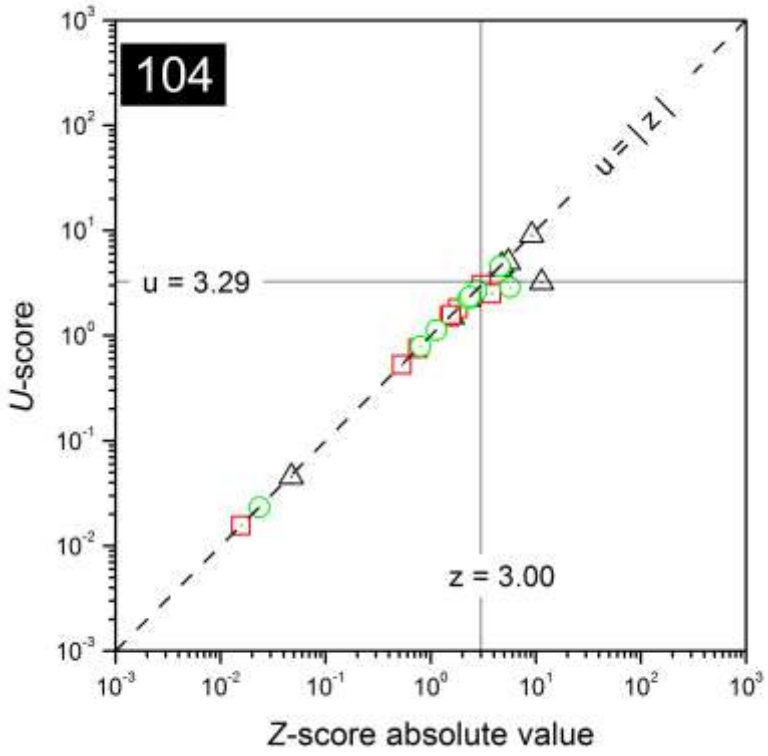

FIG. 160. Combined plots of z- and u-scores for the laboratory with code 104 in case of sample "3".

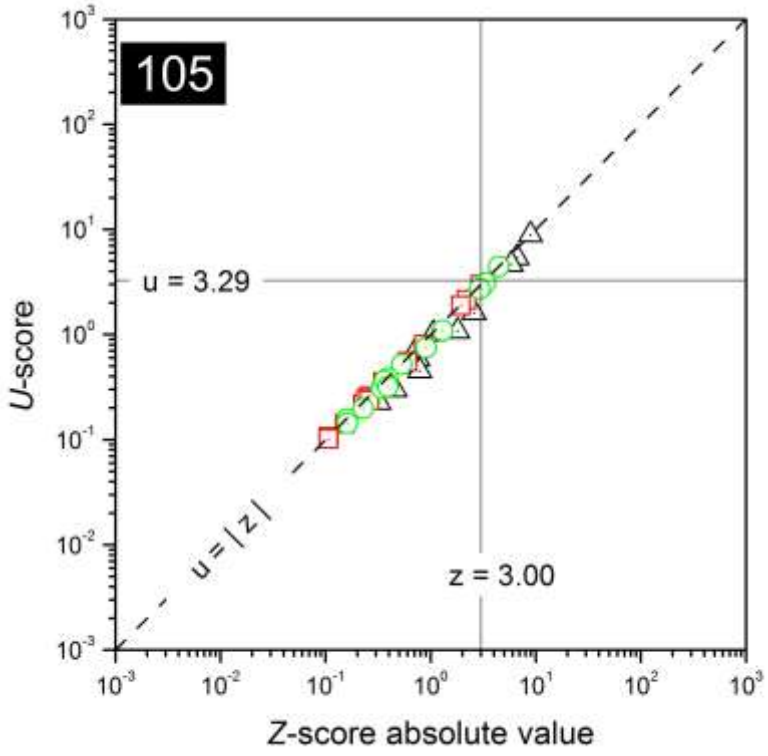

FIG. 161. Combined plots of z- and u-scores for the laboratory with code 105 in case of sample "3".

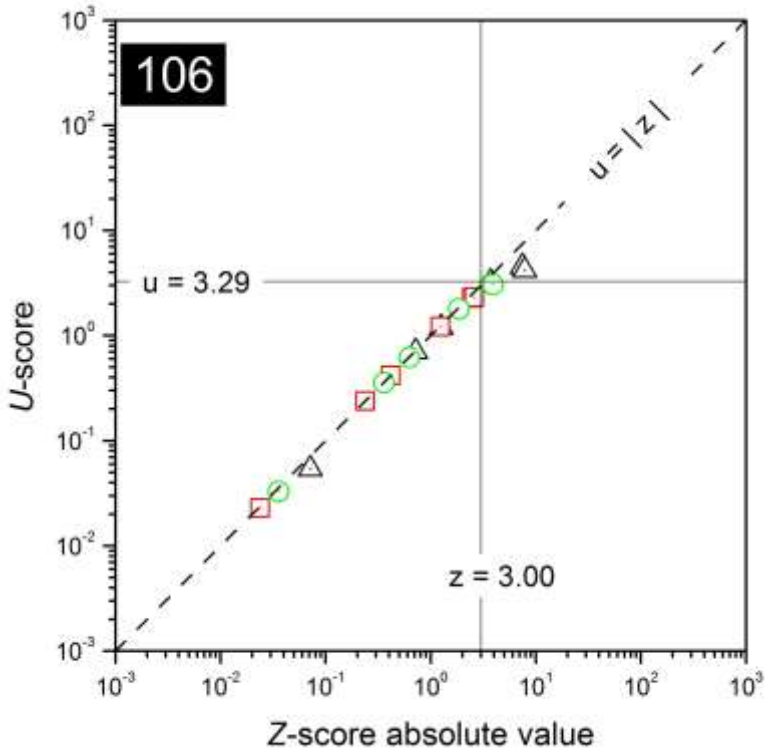

FIG. 162. Combined plots of z- and u-scores for the laboratory with code 106 in case of sample "3".

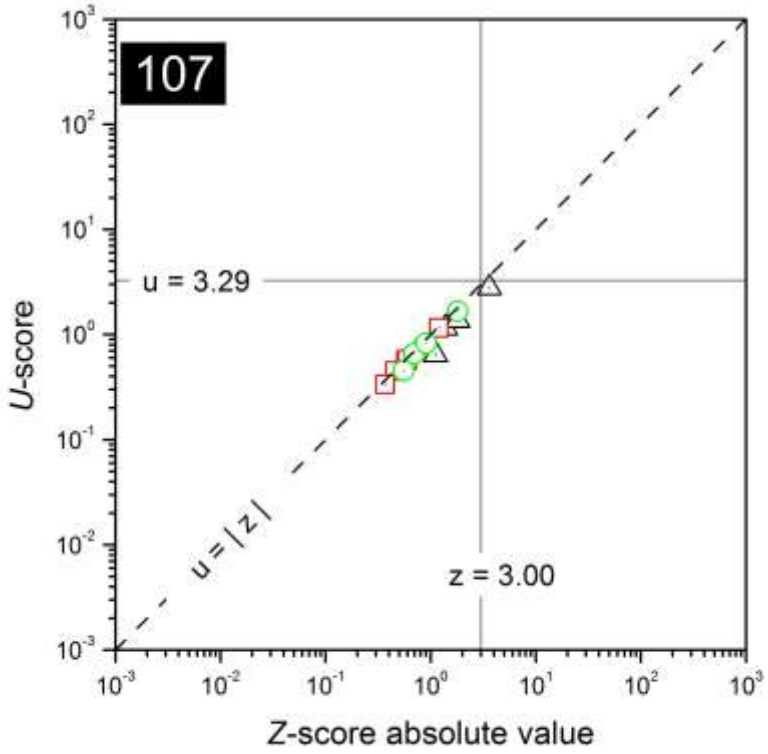

FIG. 163. Combined plots of z- and u-scores for the laboratory with code 107 in case of sample "3".

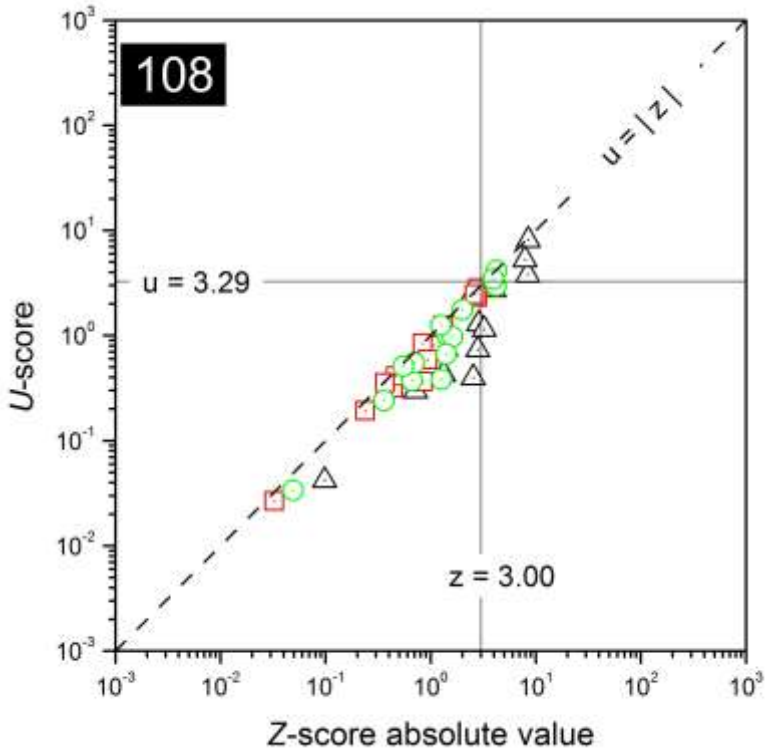

FIG. 164. Combined plots of z- and u-scores for the laboratory with code 108 in case of sample "3".

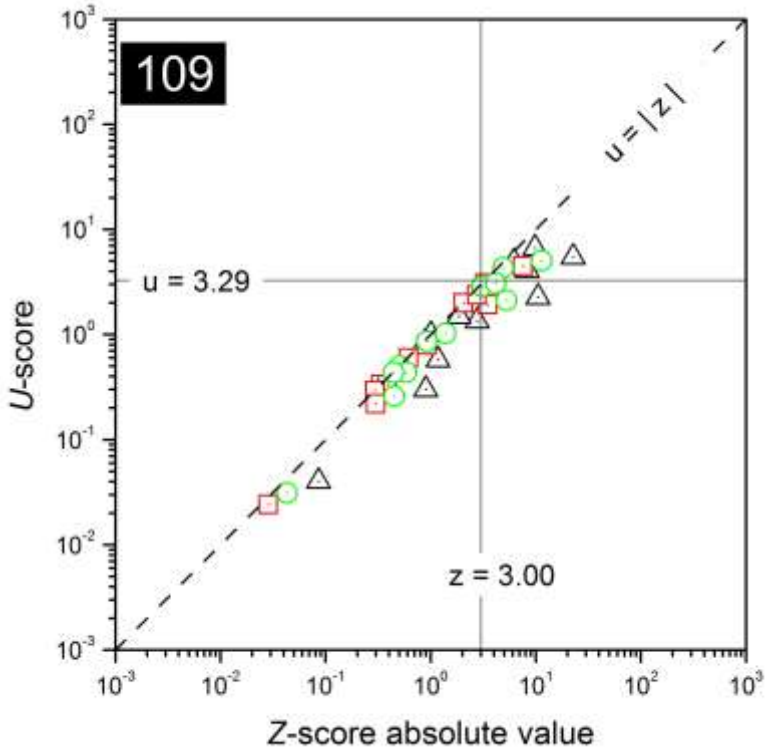

FIG. 165. Combined plots of z- and u-scores for the laboratory with code 109 in case of sample "3".

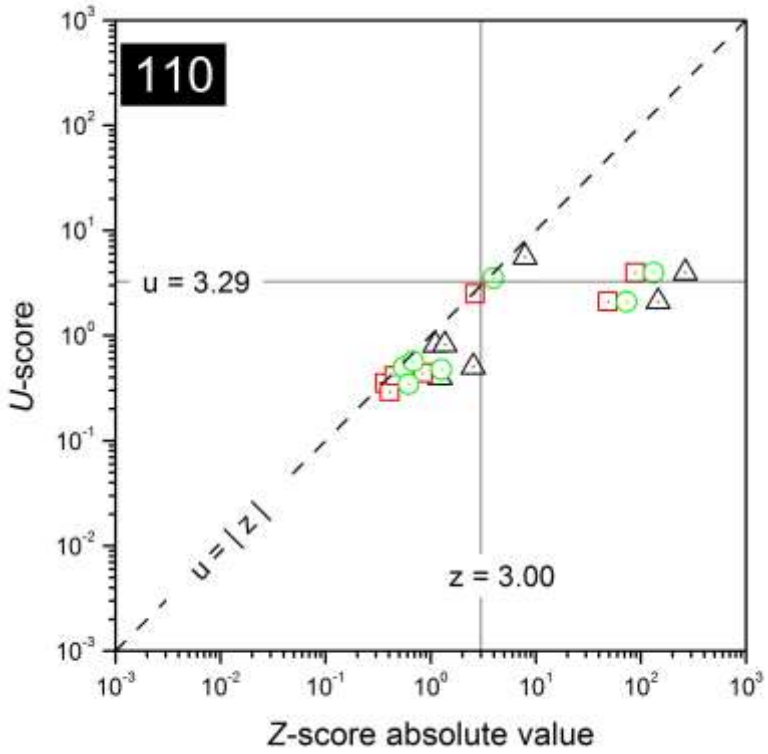

FIG. 166. Combined plots of z- and u-scores for the laboratory with code 110 in case of sample "3".

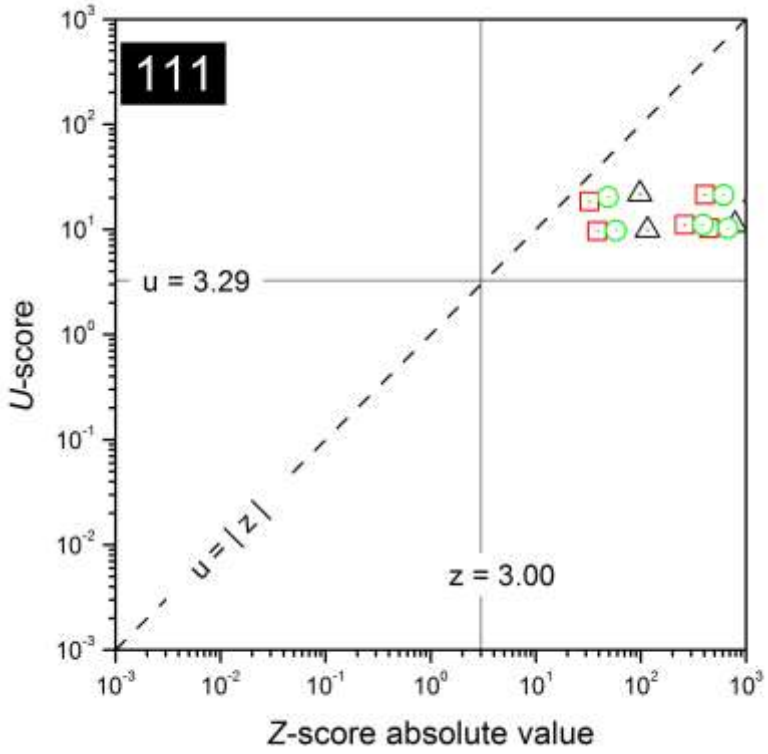

FIG. 167. Combined plots of z- and u-scores for the laboratory with code 111 in case of sample "3".

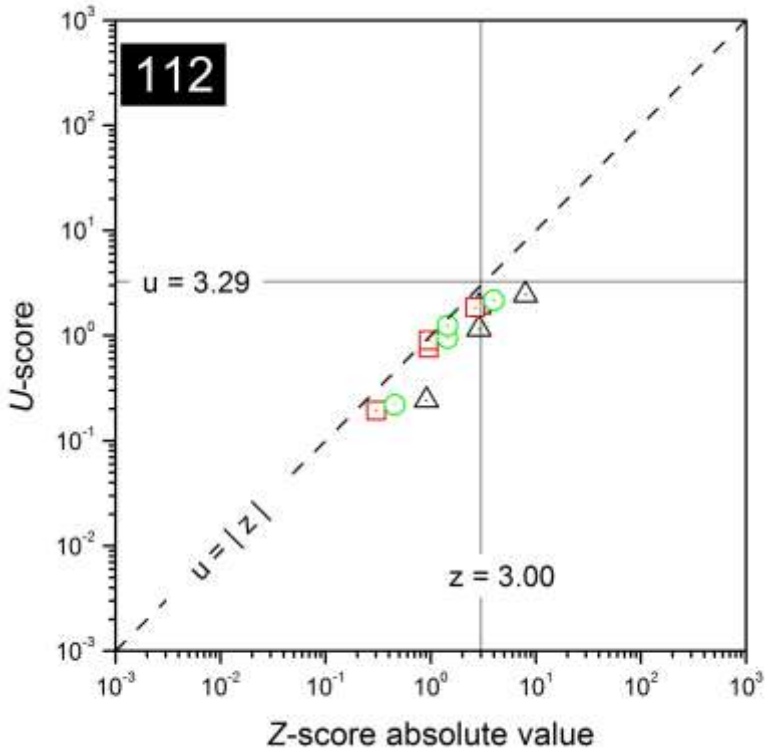

FIG. 168. Combined plots of z- and u-scores for the laboratory with code 112 in case of sample "3".

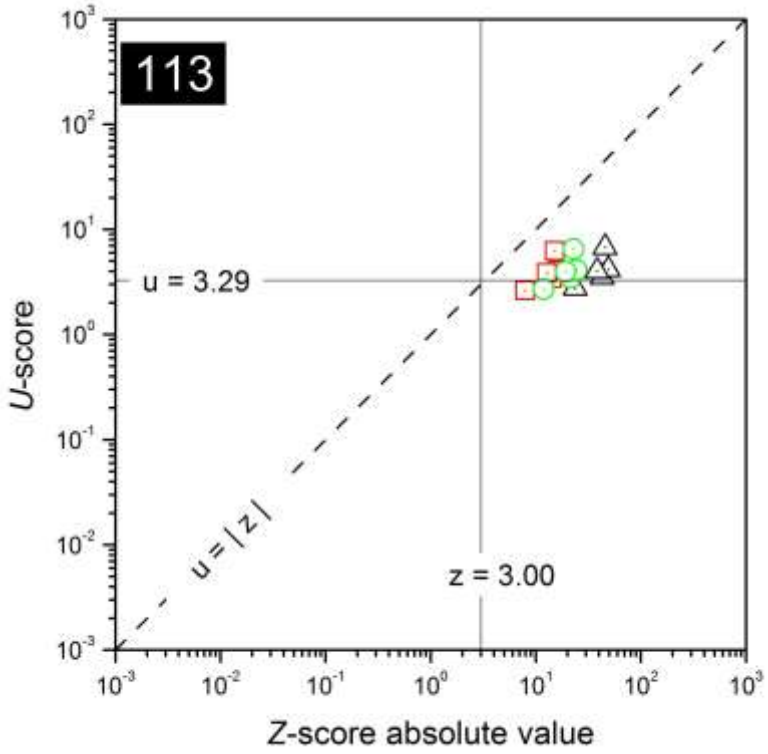

FIG. 169. Combined plots of z- and u-scores for the laboratory with code 113 in case of sample "3".

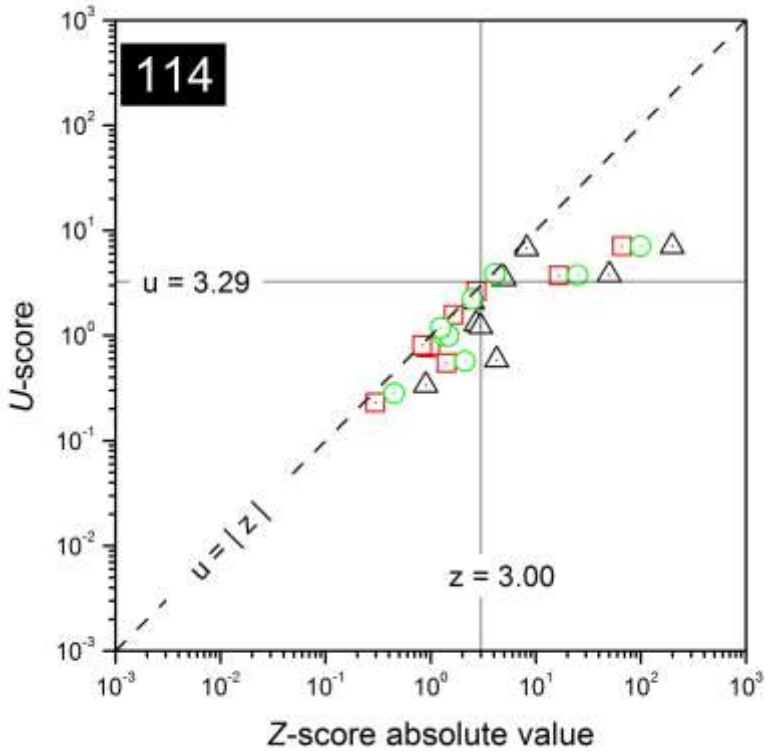

FIG. 170. Combined plots of z- and u-scores for the laboratory with code 114 in case of sample "3".

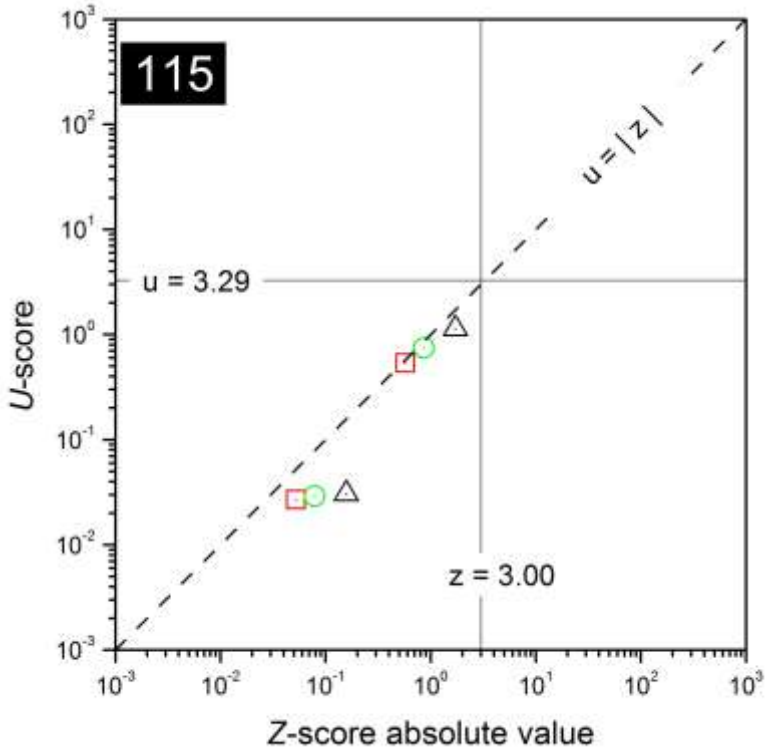

FIG. 171. Combined plots of z- and u-scores for the laboratory with code 115 in case of sample "3".

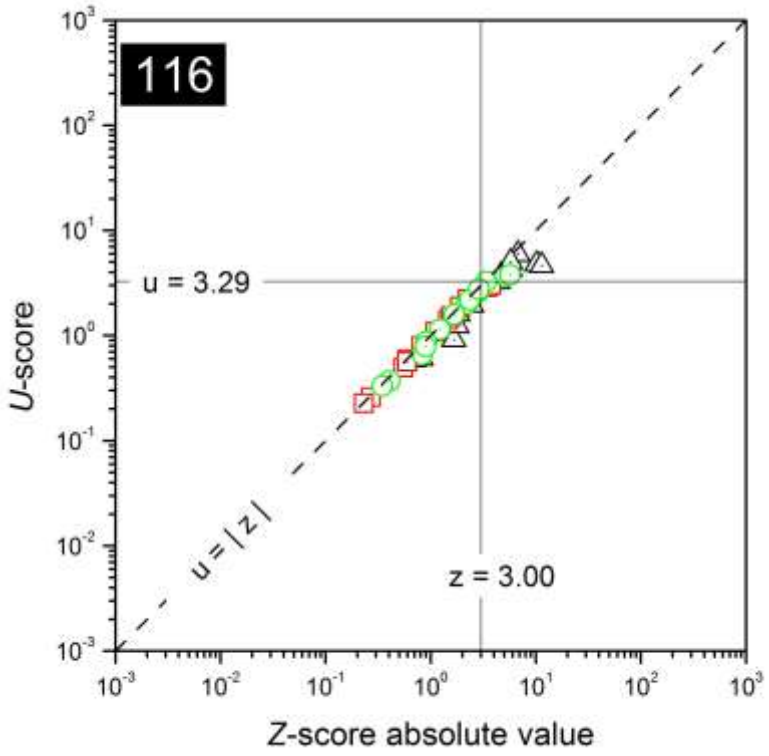

FIG. 172. Combined plots of z- and u-scores for the laboratory with code 116 in case of sample "3".

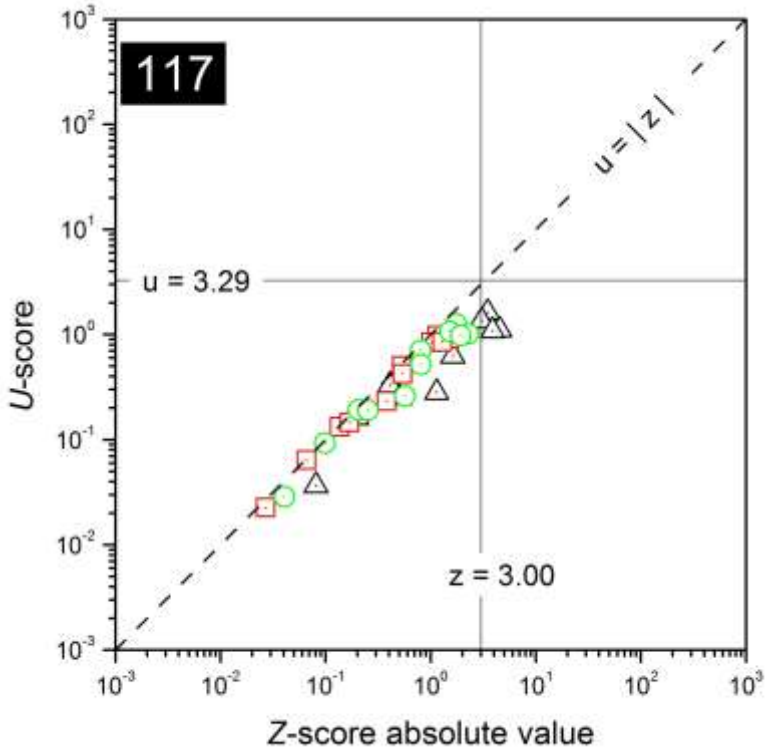

FIG. 173. Combined plots of z- and u-scores for the laboratory with code 117 in case of sample "3".

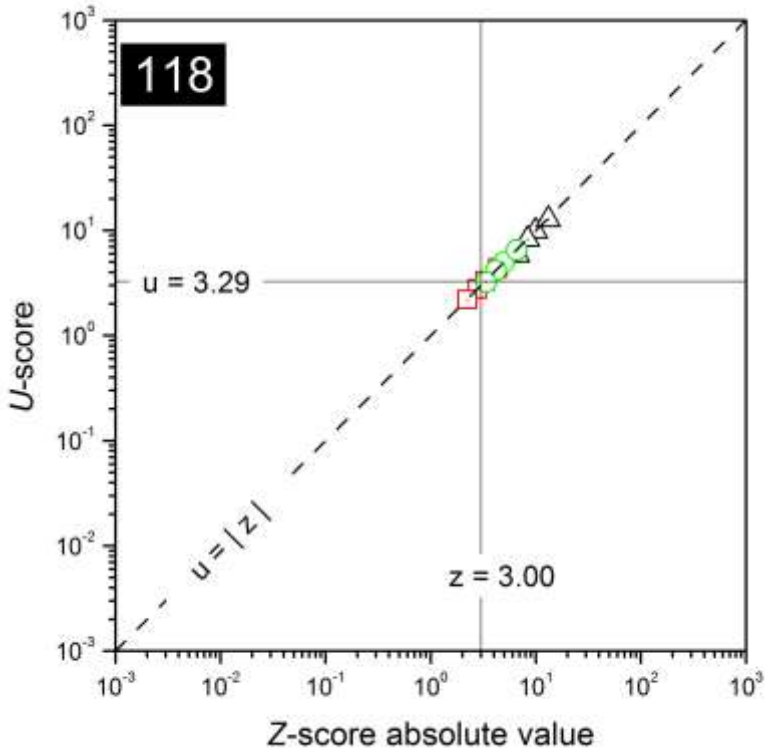

FIG. 174. Combined plots of z- and u-scores for the laboratory with code 118 in case of sample "3".

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GLOSSARY

The definitions of terms used in the proficiency testing schemes are provided. Although this terminology might be known to the participants or can be found elsewhere [8-10] the terms used in this report are clearly defined to avoid any ambiguity.

Proficiency testing: evaluation of participant performance against pre-established criteria by means of interlaboratory comparisons.

True value: the actual concentration of the analyte in the matrix.

Assigned value: the value of the concentration of the analyte in the matrix used as the true value by the proficiency testing coordinator in the statistical treatment of results (or the best available estimate).

Target value for standard deviation: a numerical value for the standard deviation of a measurement result, which has been designated as a target for measurement quality.

Consensus value: the mean value of the reported laboratory results after the removal of outliers.

Standard deviation of the consensus value: the standard deviation of the mean value of the reported laboratory results after the removal of outliers.

Certified Reference Material: A reference material, accompanied by a certificate, one or more of whose property values are certified by a procedure which establishes traceability to an accurate realization of the unit in which the property values are expressed, and for which each certified value is accompanied by an uncertainty at a stated level of confidence.

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