University of Stuttgart
Germany

Analytische Qualitätssicherung Baden-Württemberg

Proficiency Test 7/23
- TW S11 – Haloacetic acids in drinking water -

Final report

provided by
AQS Baden-Württemberg at
Institute for Sanitary Engineering, Water Quality and Solid Waste Management,
University of Stuttgart
Bandtäle 2, 70569 Stuttgart-Büsnau, Germany

And
IWW Water Center
Moritzstr. 26, 45476 Mülheim an der Ruhr, Germany

Stuttgart, in January 2024

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Responsibilities:

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Release of the report:	Dr.-Ing. Michael Koch	on 9.1.24
Version of the report	1	

List of contents

1. General

This PT was provided by AQS Baden-Württemberg in cooperation with IWW Water Center in Mülheim an der Ruhr and with the network “NORMAN” (Network of reference laboratories for monitoring of emerging environmental pollutants).

The following parameters were offered:

- monochloroacetic acid
- dichloroacetic acid
- trichloroacetic acid
- monobromoacetic acid
- dibromoacetic acid

The PT was executed and evaluated according to the requirements of DIN 38402-A45 and ISO/TS 20612.

2. PT design

Each participant received the following samples:

- 3 samples for the determination of the mentioned parameter in 1000-ml ground glass bottles (brown) with ground glass plug. Preservation by adding hydrochloric acid (pH 2) and sodium thiosulfate.

3 different concentration levels/batches were produced. All participants received the same samples.

3. Sample preparation

The samples for the determination of the haloacetic acids were based on a real ground water matrix. The ground water was used without treatment for the sample preparation.
The ground water was spiked with stock solutions and the concentrations covered drinking and ground water relevant ranges.

4. Sample distribution

The samples were dispatched on 15.08.2023 by express service.

5. Analytical methods

The participants were free to choose a suitable method, but a limit of quantification of 1 µg/l for all parameters was required.

The participants were informed that the samples had to be analysed in the own laboratory, with own personal and own equipment. Subcontracting of the analysis was not allowed.

The participants were informed to cool the samples after receipt and to start with the analysis one day after receipt at the latest.

The samples had to be analysed in duplicate over the complete method (sample preparation and measurement). The participants were asked to report the results as average means from both determinations in µg/l with three significant digits.

6. Submission of the results

The deadline for the submission of results was on 04.09.2023.

7. Basic principle of evaluation and assessment

The basic principle of the evaluation and assessment of the PTs from AQS Baden-Württemberg are described in the document „Evaluation of the PTs and information for the report“, which can be downloaded from www.aqsbw.de/pdf/ausw_berichte_v1_en.pdf.

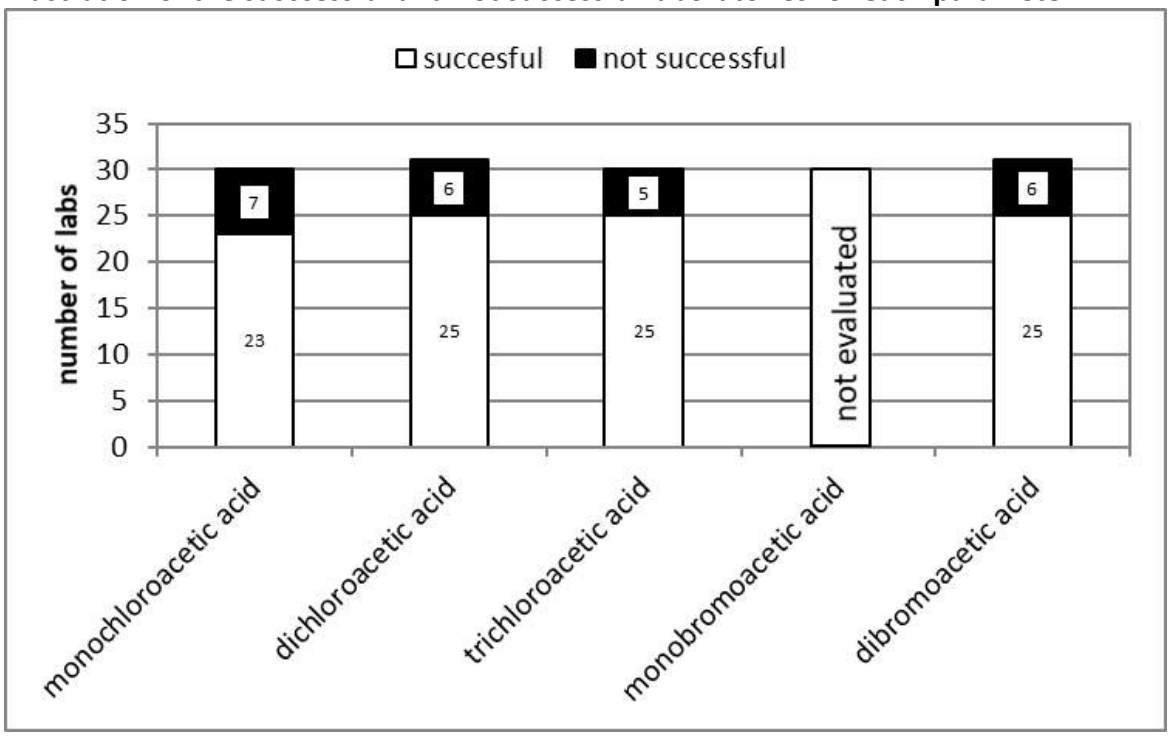
This PT was evaluated as follows:

Assigned value x_{pt}:	Consensus value (Hampel estimator)
Standard deviation for proficiency assessment σ_{pt}:	Q method
Upper limit of σ_{pt}:	25 %
Lower limit of σ_{pt}:	5 %
Assessment:	z_U-Score
Classification of the single results:	$\lvert z_U \rvert \leq 2.0$ successful $2.0 < \lvert z_U \rvert < 3.0$ questionable $\lvert z_U \rvert \geq 3.0$ unsatisfactory
Parameter assessment:	A parameter was assessed as successful, if more than half of the values were correctly determined (2 out of 3 values are within the tolerance limits).

8. Evaluation

Number of participants:	39
Number of reported values	350
Number of accepted values:	293 (83,7 %)

Illustration of the susccessful and not successful laboratories for each parameter



The parameter monobromoacetic acid could not be evaluated. Explanation is given in chapter 12 “Note to monobromoacetic acid”.

9. Explanation for the appendices

The explanations for the appendices can be found in the document „Evaluation of the PTs and information for the report“, which can be downloaded from www.aqsbw.de/pdf/ausw_berichte_v1_en.pdf.

10. Measurement uncertainty

General:

Number of labs with valid values	32
Number of labs with valid values and reported measurement uncertainties	16 (50 %)
Number of valid values	362
Number of valid values with measurement uncertainties	185 (51,1 %)

Measurement uncertainties against the accreditation status

Accreditation status of the values	Number of values	Number of values with measurement uncertainty
accredited	105	80 (76,2 %)
not accredited	162	81 (50 %)
not specified	83	24 (28,9 %)

Interpretation of the reported measurement uncertainties:

If measurement uncertainties are underestimated values assessed as "satisfactory" in the PT ($|z_U| \leq 2$), will have a large ζ -score. $|\zeta| > 2$ means that the "own" requirements (defined in terms of estimated uncertainty) are not fulfilled.

Number of values with reported measurement uncertainty having a $\|z_U\| \leq 2{,}0$	156
Number of values with a magnitude of ζ-scores > 2 The own requirements of the laboratory are not fulfilled and the estimation of the measurement uncertainty is too low	34 (21,8 %)

11. Note to monobromo acetic acid

The monobromoacetic acid was no longer detectable in the samples due to an error during sample stabilisation. Sodium thiosulphate was added to the samples as required by the standard. In this case, however, the standard specifications only allow a period of 3 days until analysis, which is too short. With the intention of stabilising the samples even longer, they were also acidified, but this, together with the thiosulphate, led to the monobromoacetic acid breaking down after a very short time and no longer being detectable. This point had not been observed in the preliminary tests.

The acidification apparently had no influence on the other parameters.

12. Traceable reference values

The explanations about traceable reference values can be found in the document „Evaluation of the PTs and information for the report“, which can be downloaded from www.aqsbw.de/pdf/ausw_berichte_v1_en.pdf

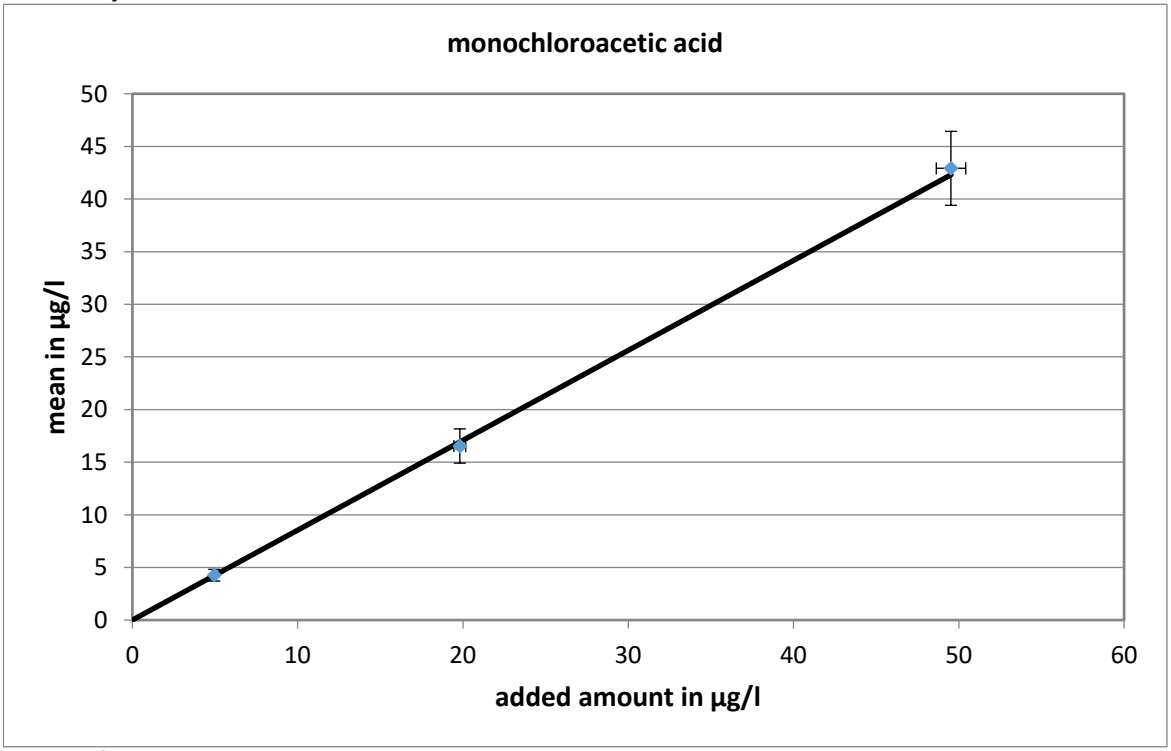
13. Internet

The report is available on the following webpage: www.aqsbw/pdf/283/report_283.pdf

monochloroacetic acid

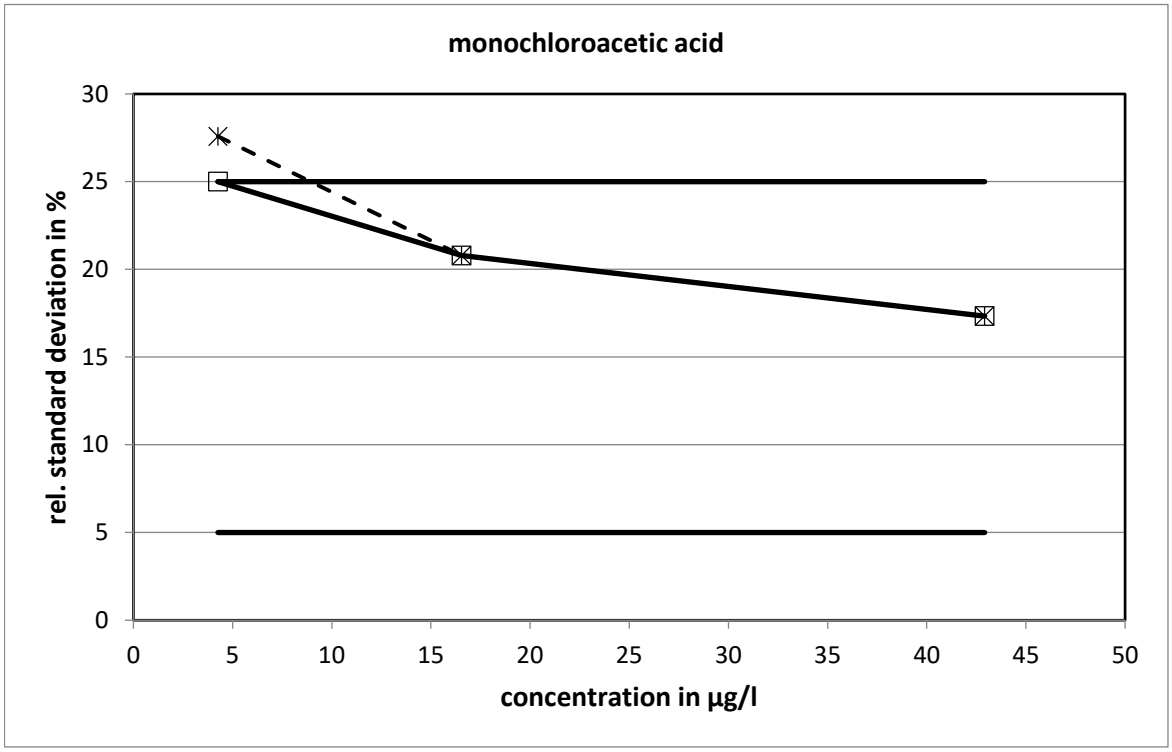
level	assigned value [µg/l]	expanded uncertainty of the assigned value [%]	standard deviation, calculated using robust statistics [µg/l]	standard deviation for proficiency assessment [µg/l]	standard deviation for proficiency assessment [%]	upper tolerance limit [µg/l]	lower tolerance limit [µg/l]	upper tolerance limit [%]	lower tolerance limit [%]	number of results	out below	out above	out [%]
1	4,264	13,03	1,176	1,066	25,00	6,736	2,337	57,99	-45,19	28	4	0	14,3
2	16,54	9,82	3,438	3,438	20,79	24,29	10,24	46,87	-38,10	28	6	0	20,7
3	42,92	8,19	7,440	7,440	17,33	59,32	29,12	38,23	-32,16	28	8	0	27,6
									sum	84	18	0	21,4

Recovery and matrix content

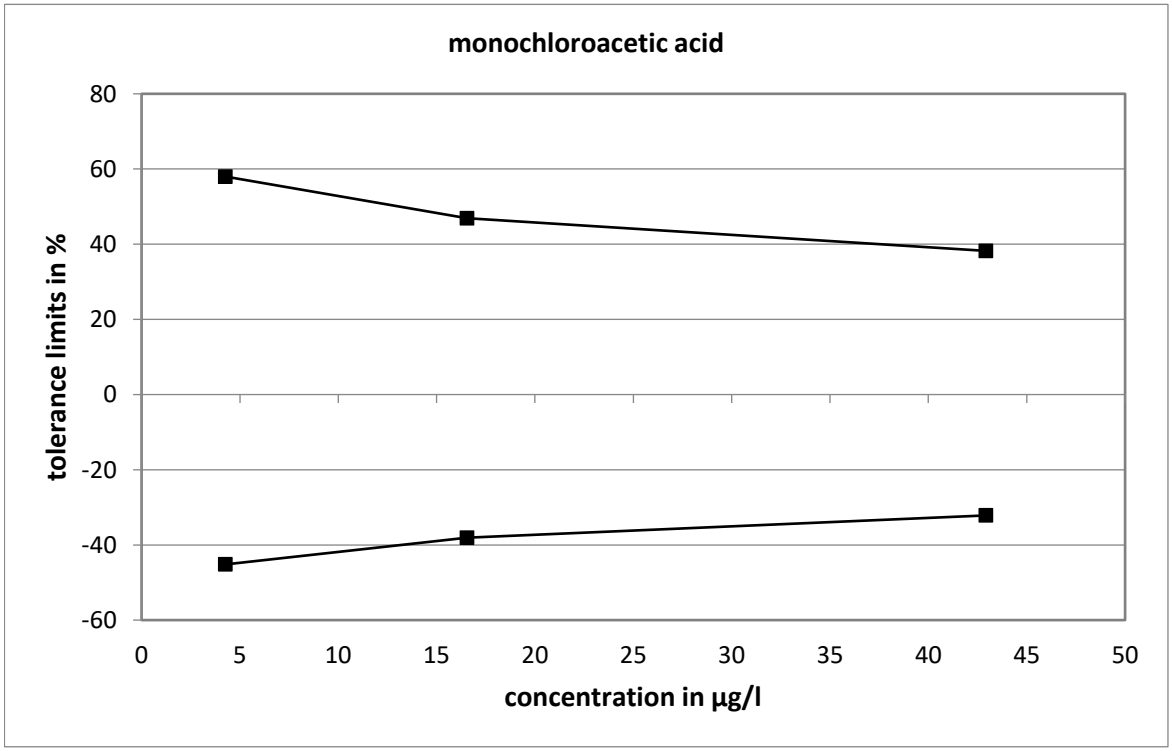


slope of the regression: 0,854; average recovery rate: 85,4 %
neg. x-intercept corresponds to the matrix content: 0,0046 µg/l
exp. Uncertainty of the matrix content: 0,0046 µg/l = 100 %

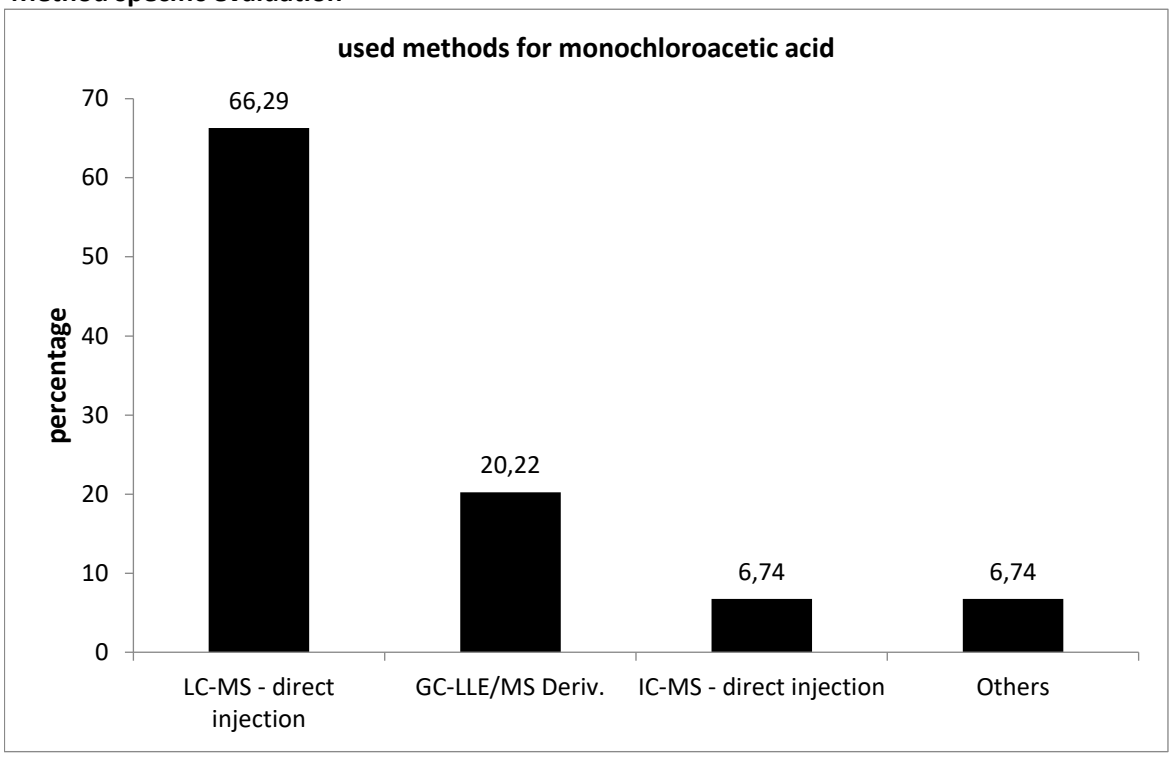
Relative standard deviation and tolerance limits

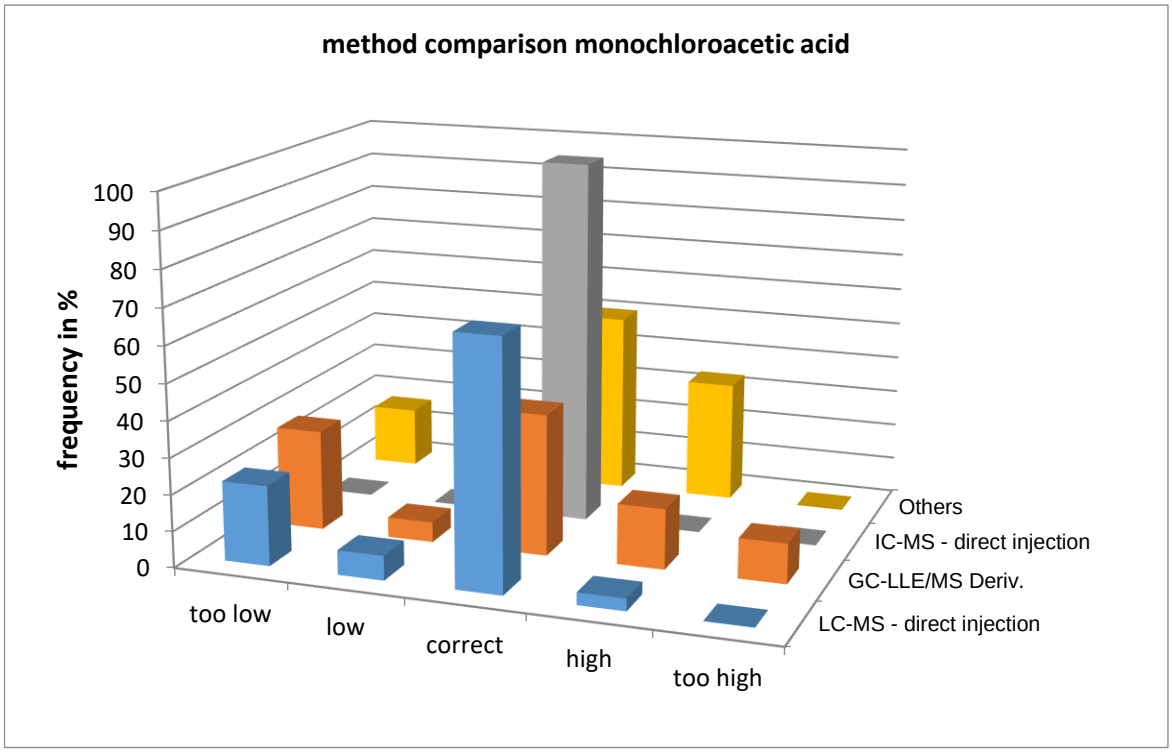


The relative standard deviations calculated with the Q-method reached the upper limit with one concentration level.



Method specific evaluation

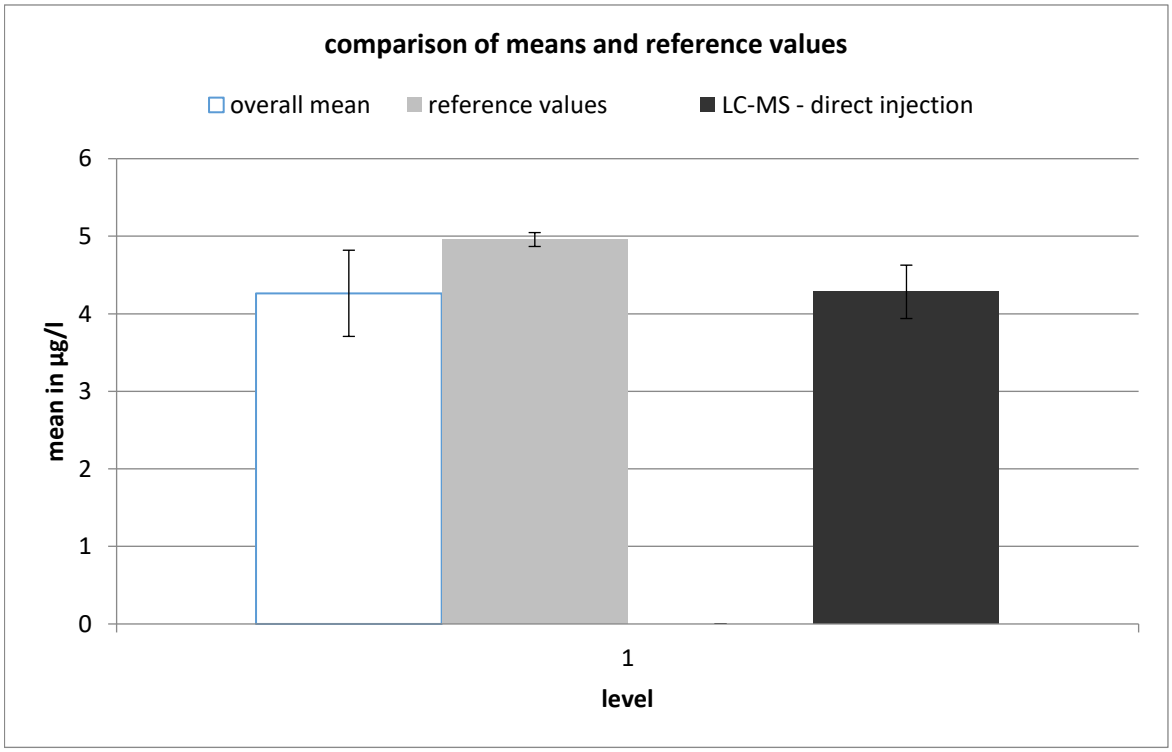


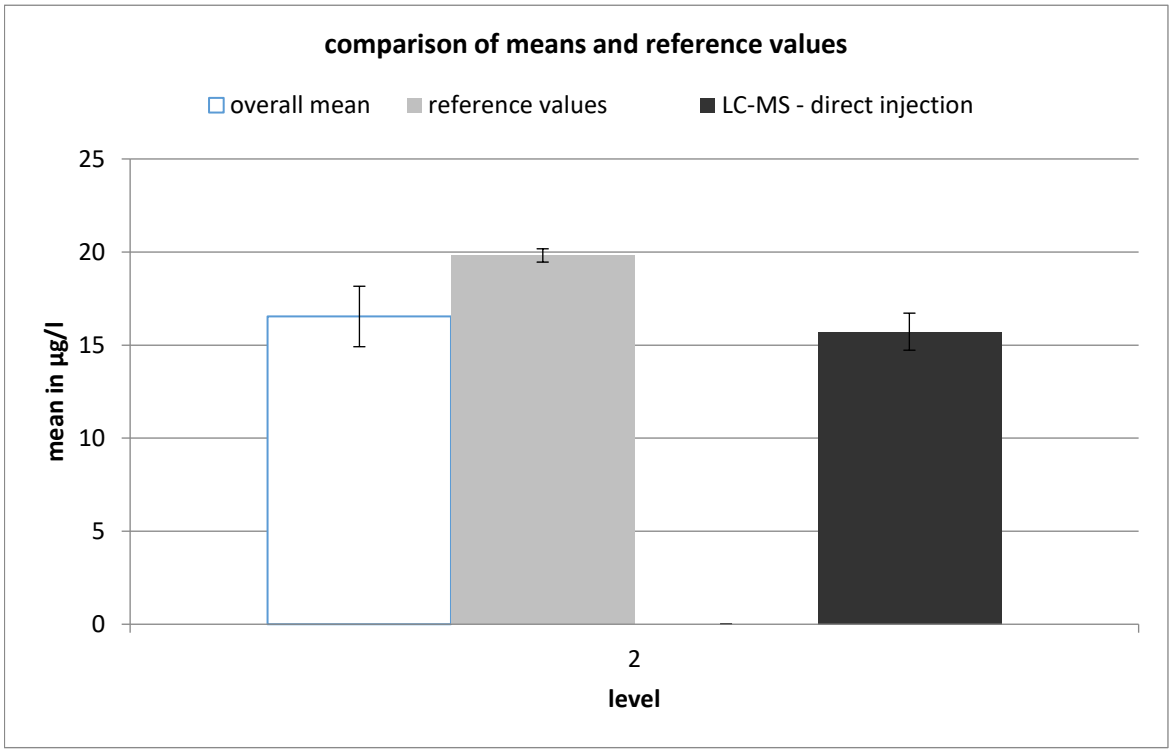


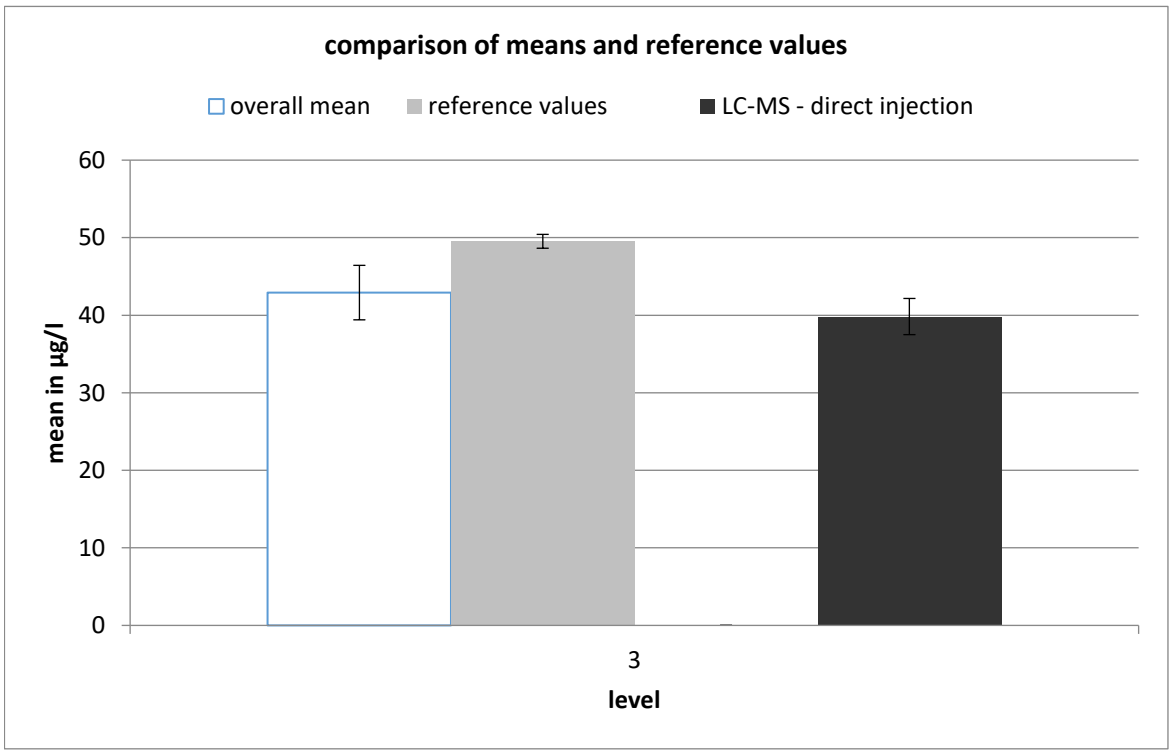
The values determined with IC-MS-direct injection showed the closest statistical distribution. The values determined with LC-MS showed a higher ratio of to high values.

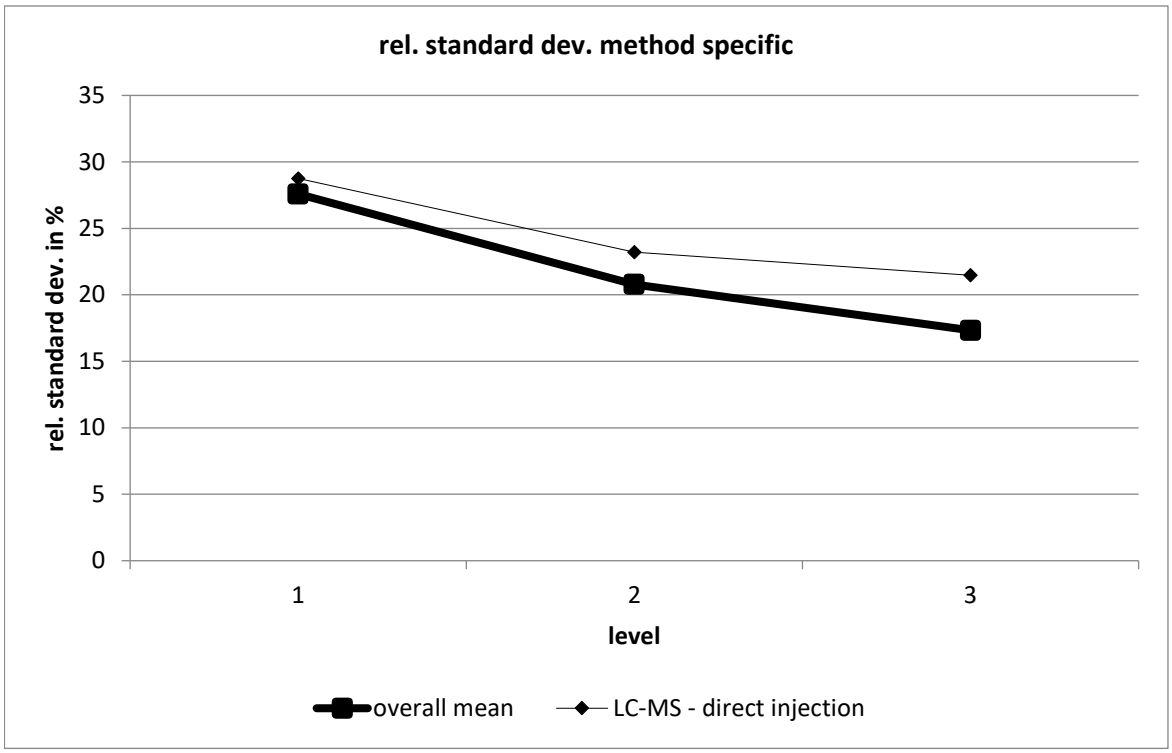
Comparison of means and reference values

level	mean [µg/l]	exp. uncertainty [µg/l]	exp. uncertainty [%]	reference value [µg/l]	exp. uncertainty [µg/l]	exp. uncertainty [%]
1	4,264	0,556	13,0	4,957	0,090	1,8
2	16,54	1,62	9,8	19,82	0,36	1,8
3	42,92	3,51	8,2	49,53	0,89	1,8




comparison of means and reference values
overall mean
reference values
LC-MS - direct injection
25
20
15
10
5
0
mean in µg/l
2
level


comparison of means and reference values
overall mean
reference values
LC-MS - direct injection
60
50
40
30
20
10
0
mean in µg/l
3
level

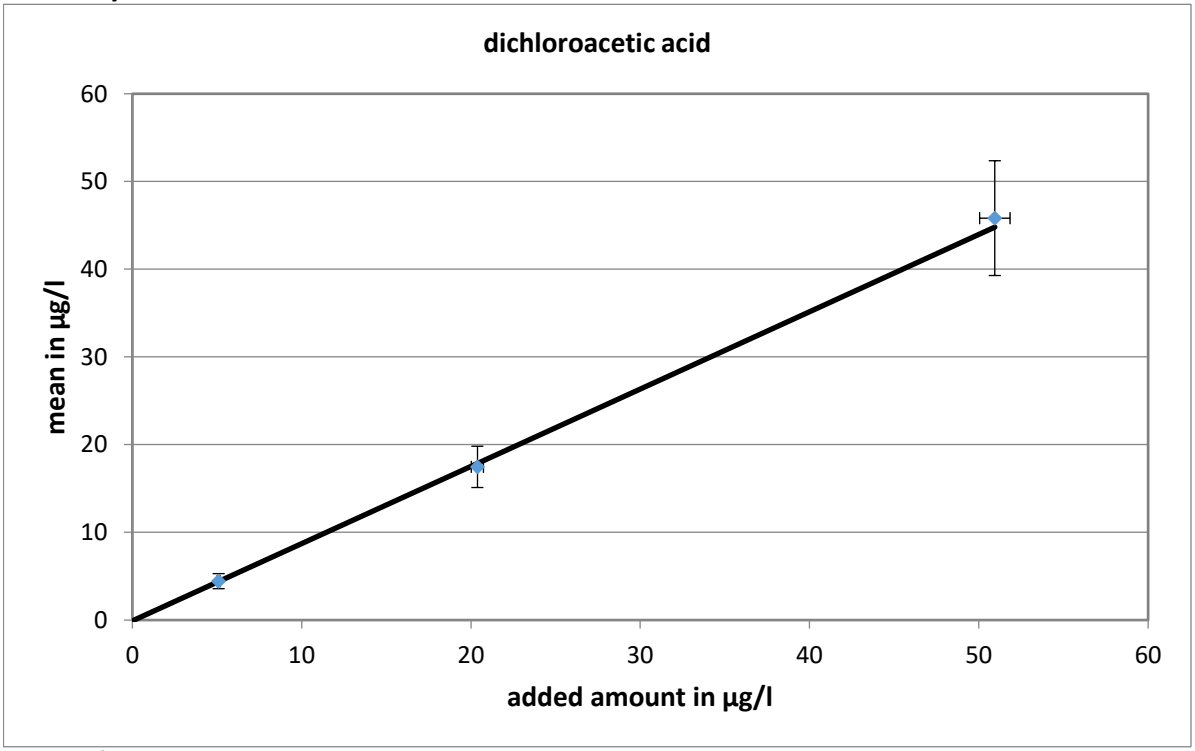


LC-MS - direct injection									
level	robust mean [µg/l]	exp. unc. of the mean [µg/l]	exp. unc. of the mean [%]	robust standard deviation [µg/l]	robust standard deviation [%]	number of results	out below	out above	out [%]
1	4,28	0,344	8,037	1,232	28,76	20	2	0	10
2	15,7	0,996	6,334	3,65	23,22	21	2	0	9,5238
3	39,8	2,333	5,857	8,552	21,47	21	3	0	14,286

dichloroacetic acid

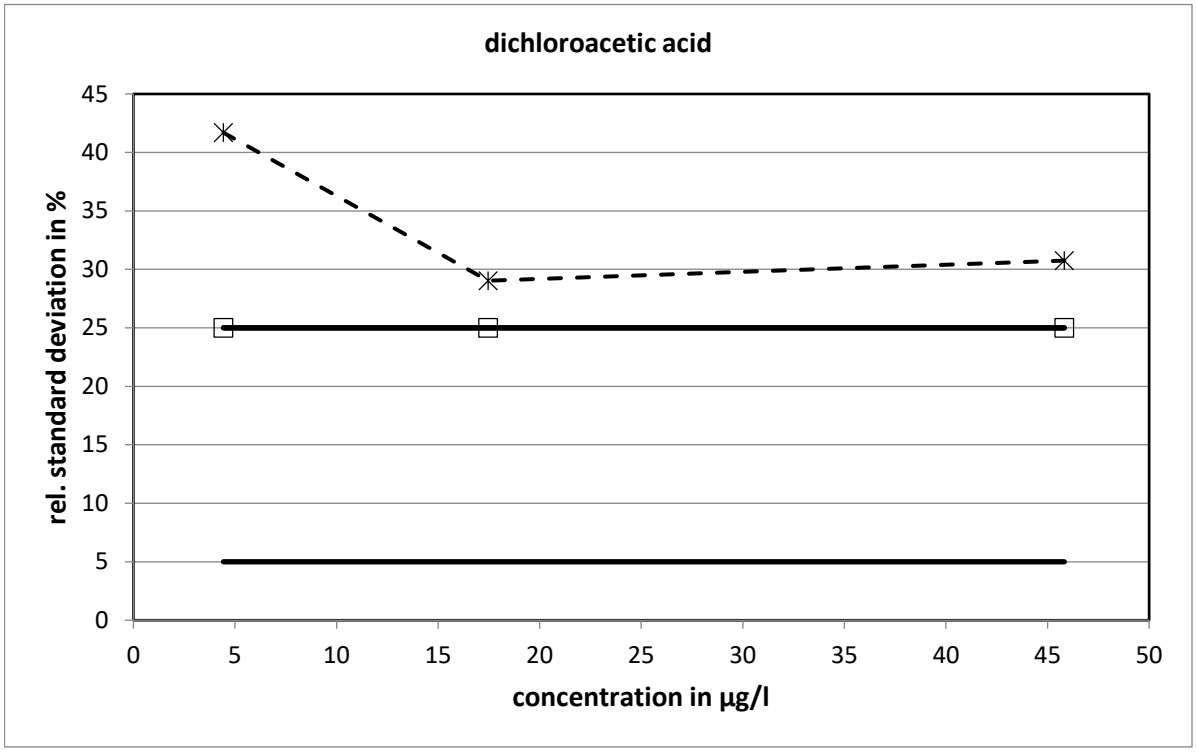
level	assigned value [µg/l]	expanded uncertainty of the assigned value [%]	standard deviation, calculated using robust statistics [µg/l]	standard deviation for proficiency assessment [µg/l]	standard deviation for proficiency assessment [%]	upper tolerance limit [µg/l]	lower tolerance limit [µg/l]	upper tolerance limit [%]	lower tolerance limit [%]	number of results	out below	out above	out [%]
1	4,436	19,35	1,849	1,109	25,00	7,008	2,431	57,99	-45,19	29	4	2	20,0
2	17,47	13,48	5,071	4,366	25,00	27,59	9,574	57,99	-45,19	29	4	2	20,0
3	45,83	14,28	14,09	11,46	25,00	72,40	25,12	57,99	-45,19	29	3	0	10,0
									sum	87	11	4	17,2

Recovery and matrix content

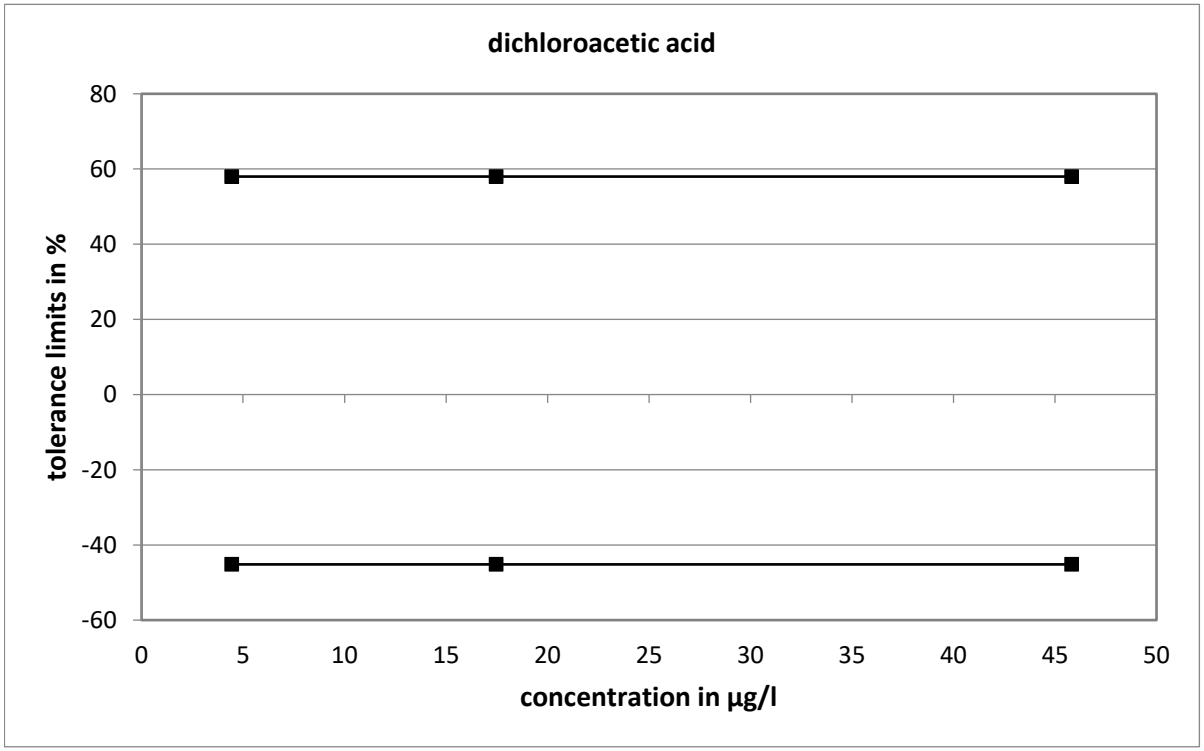


slope of the regression: 0,881; average recovery rate: 88,1 %
neg. x-intercept corresponds to the matrix content: 0 µg/l
exp. Uncertainty of the matrix content: 0,1 µg/l = 0 %

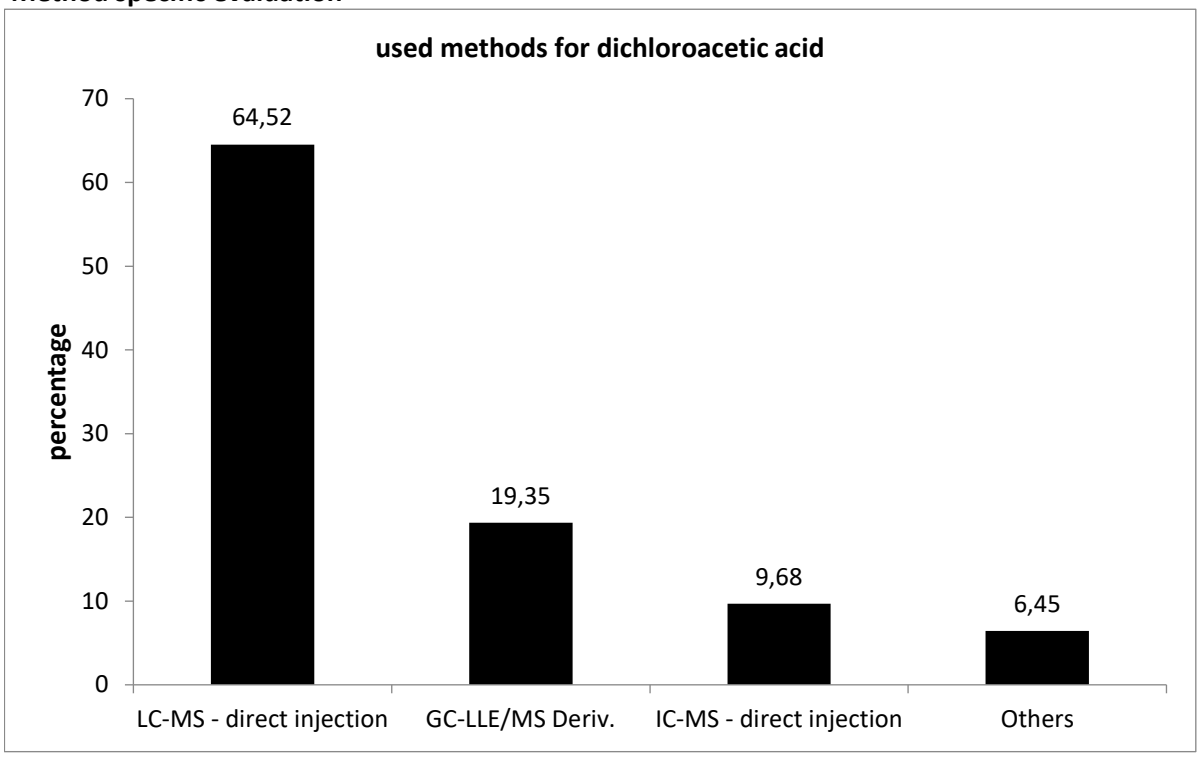
Relative standard deviation and tolerance limits

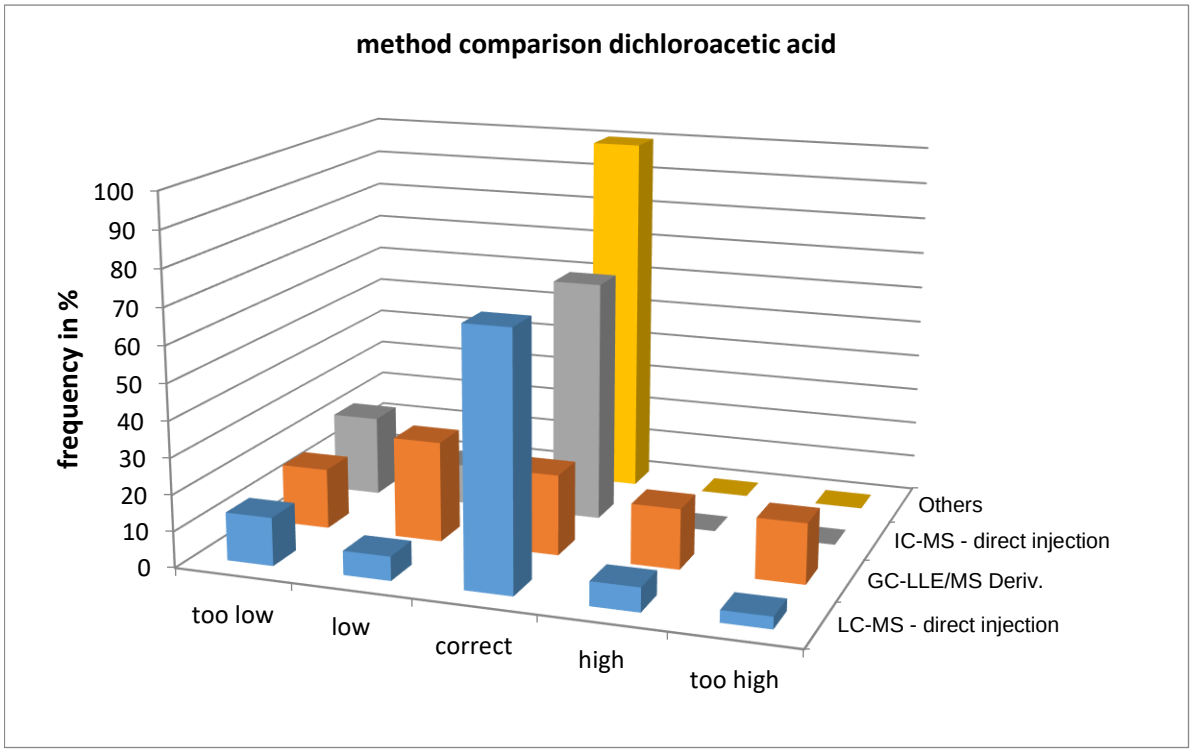


The relative standard deviations calculated with the Q-method reached the upper limit with all concentration levels.



Method specific evaluation

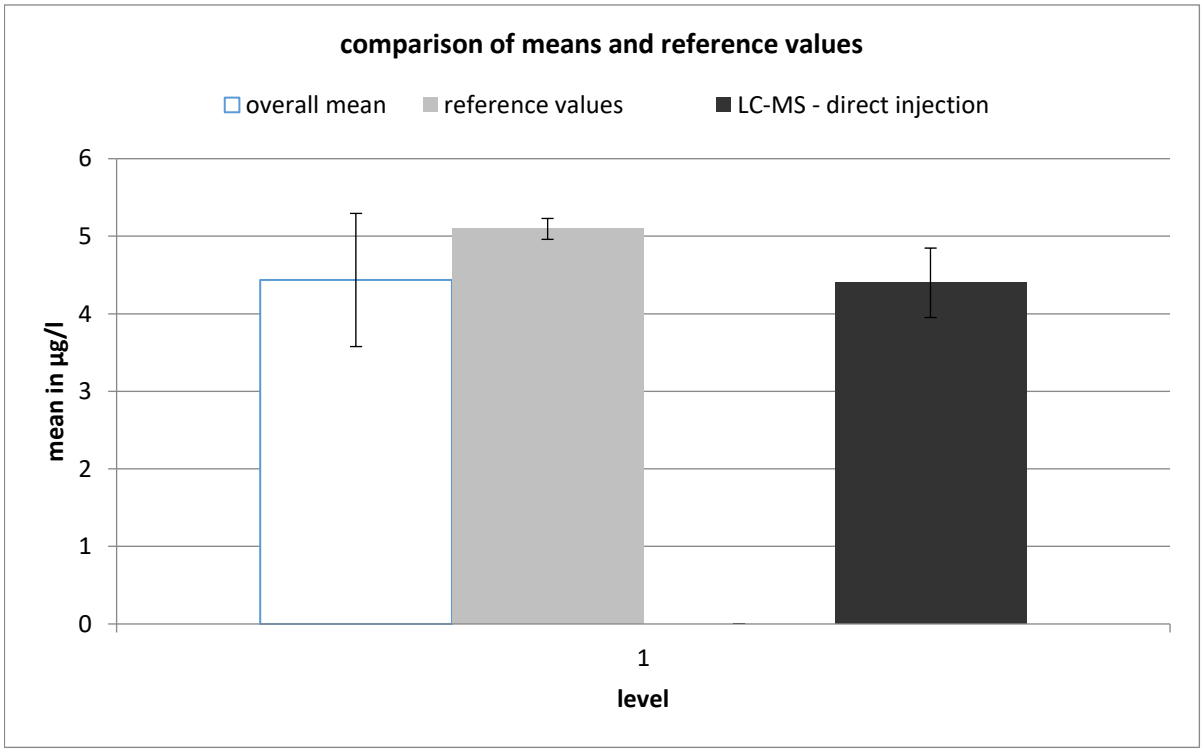


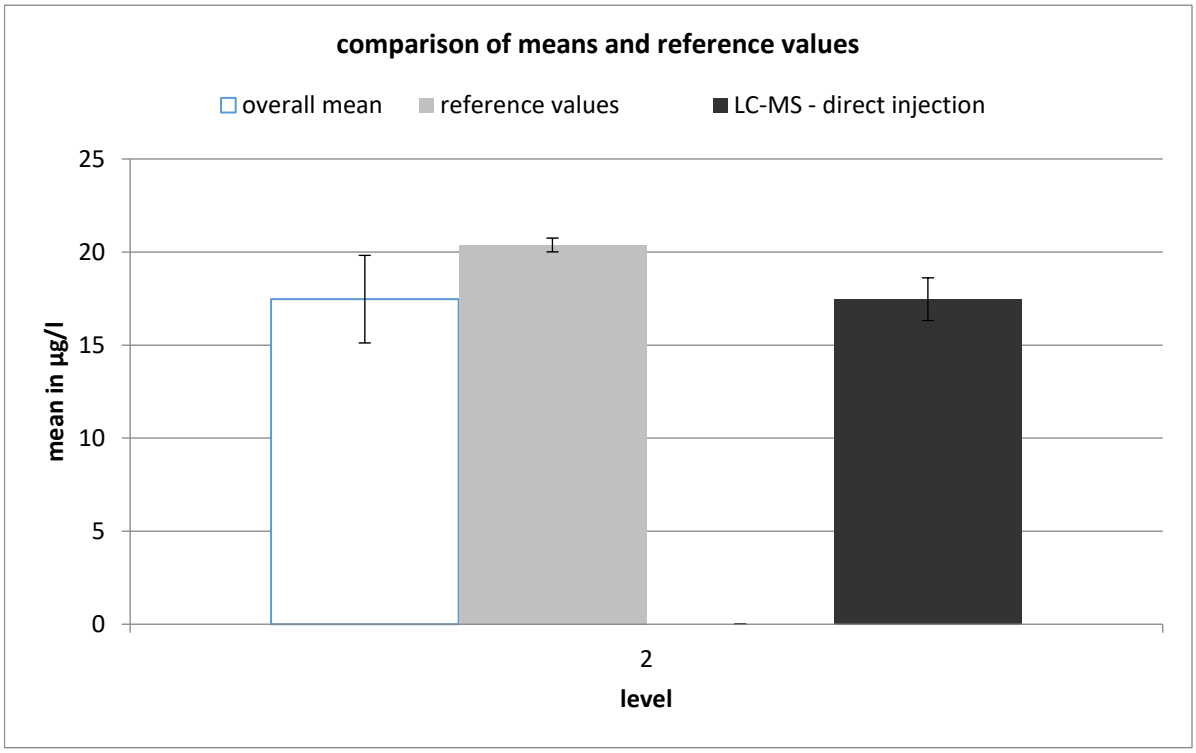


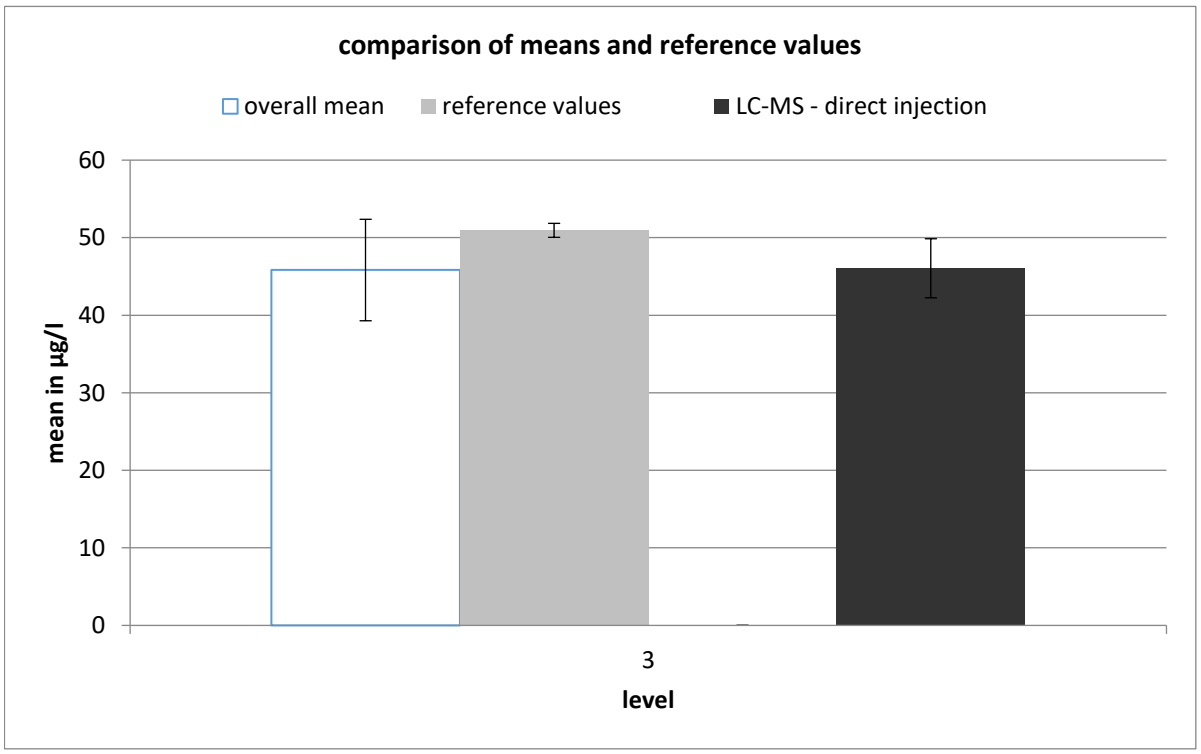
The values determined with LC-MS - direct injection showed the closest statistical distribution.

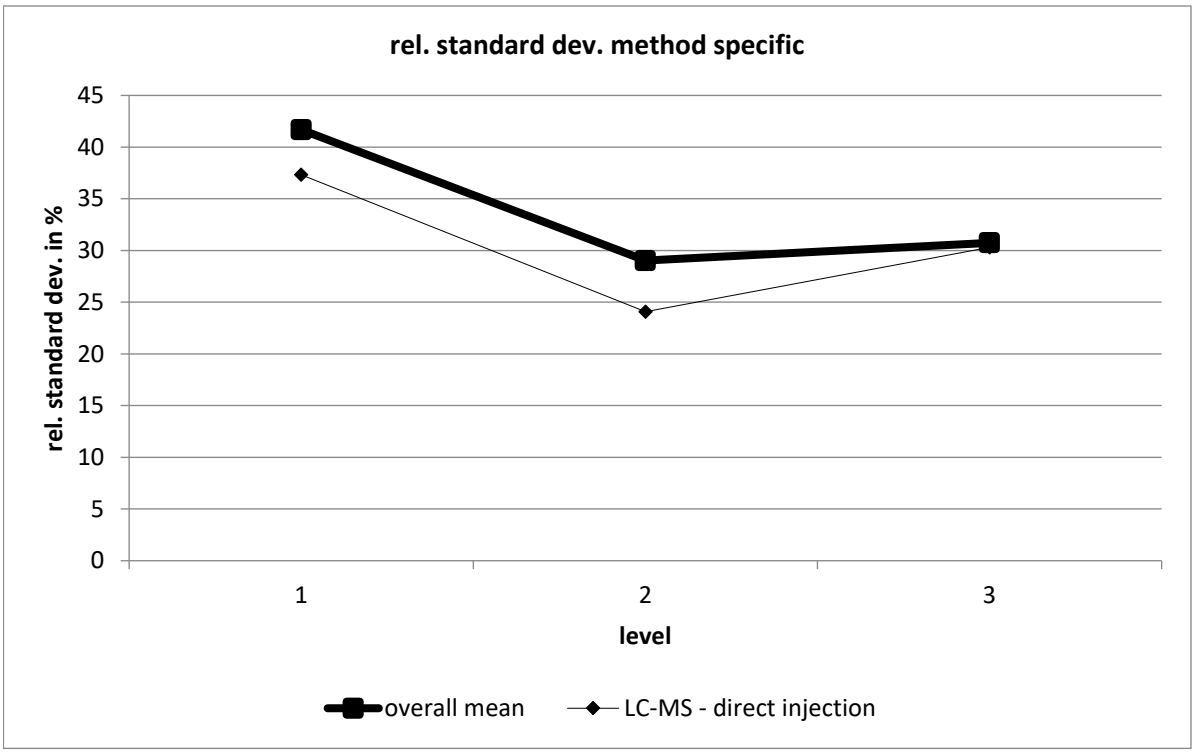
Comparison of means and reference values

level	mean [µg/l]	exp. uncertainty [µg/l]	exp. uncertainty [%]	reference value [µg/l]	exp. uncertainty [µg/l]	exp. uncertainty [%]
1	4,436	0,859	19,4	5,094	0,135	2,6
2	17,47	2,35	13,5	20,38	0,37	1,8
3	45,83	6,54	14,3	50,94	0,90	1,8




comparison of means and reference values
overall mean
reference values
LC-MS - direct injection
25
20
15
10
5
0
mean in µg/l
2
level


comparison of means and reference values
overall mean
reference values
LC-MS - direct injection
60
50
40
30
20
10
0
mean in µg/l
3
level

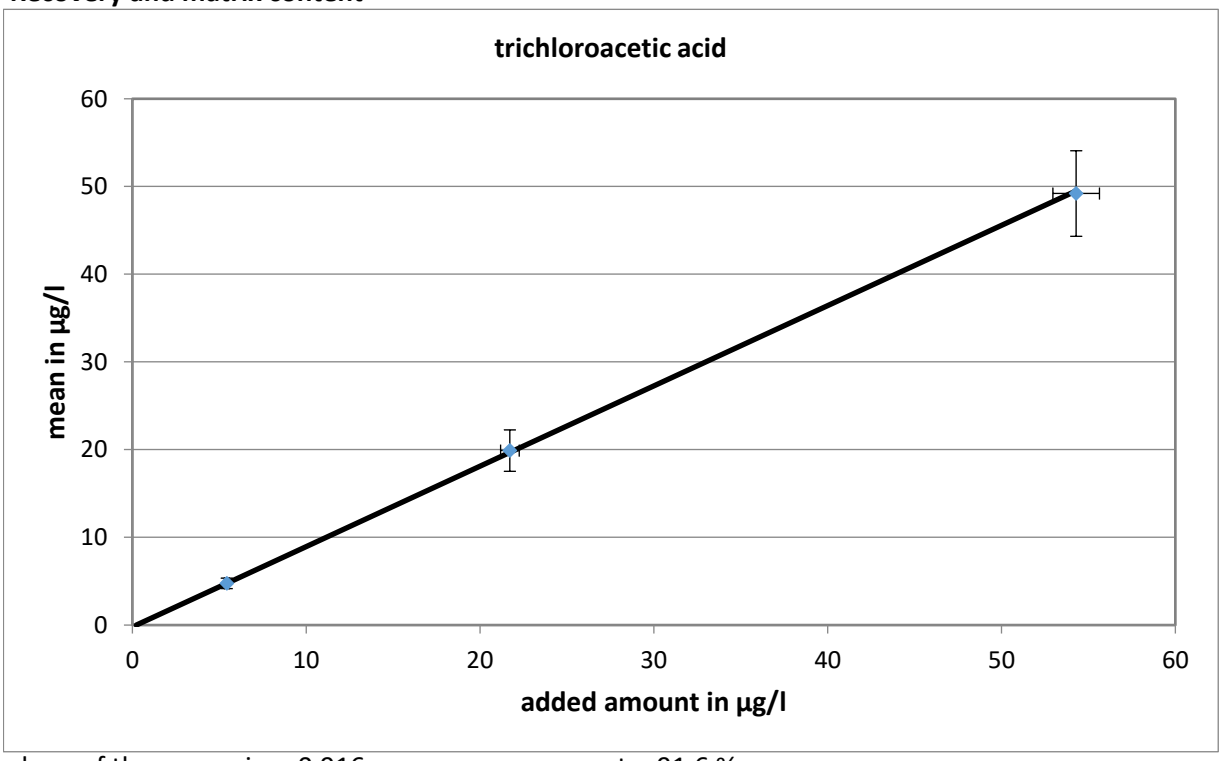


LC-MS - direct injection									
level	robust mean [µg/l]	exp. unc. of the mean [µg/l]	exp. unc. of the mean [%]	robust standard deviation [µg/l]	robust standard deviation [%]	number of results	out below	out above	out [%]
1	4,3994	0,448	10,18	1,6422	37,327	21	2	1	14,29
2	17,463	1,147	6,57	4,2059	24,084	21	3	1	19,05
3	46,051	3,809	8,27	13,963	30,32	21	3	0	14,29

trichloroacetic acid

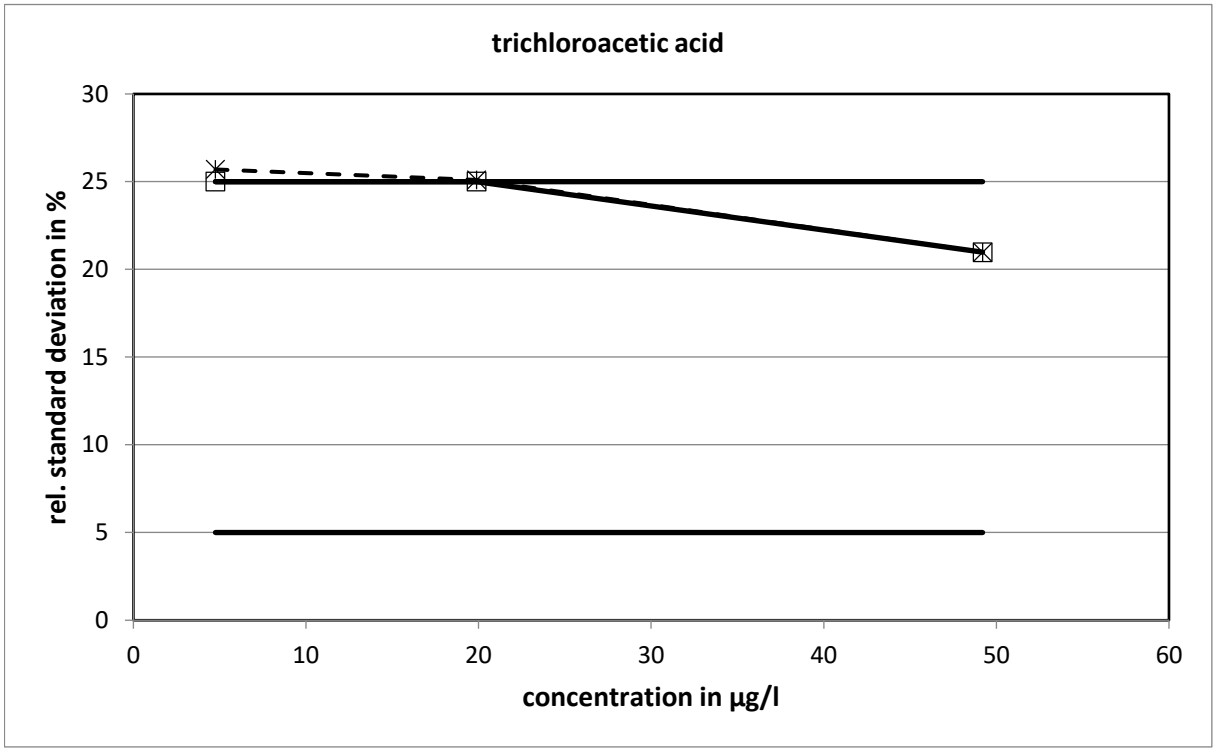
level	assigned value [µg/l]	expanded uncertainty of the assigned value [%]	standard deviation, calculated using robust statistics [µg/l]	standard deviation for proficiency assessment [µg/l]	standard deviation for proficiency assessment [%]	upper tolerance limit [µg/l]	lower tolerance limit [µg/l]	upper tolerance limit [%]	lower tolerance limit [%]	number of results	out below	out above	out [%]
1	4,756	12,60	1,222	1,189	25,00	7,514	2,607	57,99	-45,19	26	2	3	18,5
2	19,89	11,86	4,992	4,972	25,00	31,42	10,90	57,99	-45,19	28	3	2	17,2
3	49,20	9,91	10,32	10,32	20,98	72,50	30,29	47,37	-38,43	28	4	1	17,2
									sum	82	9	6	18,3

Recovery and matrix content

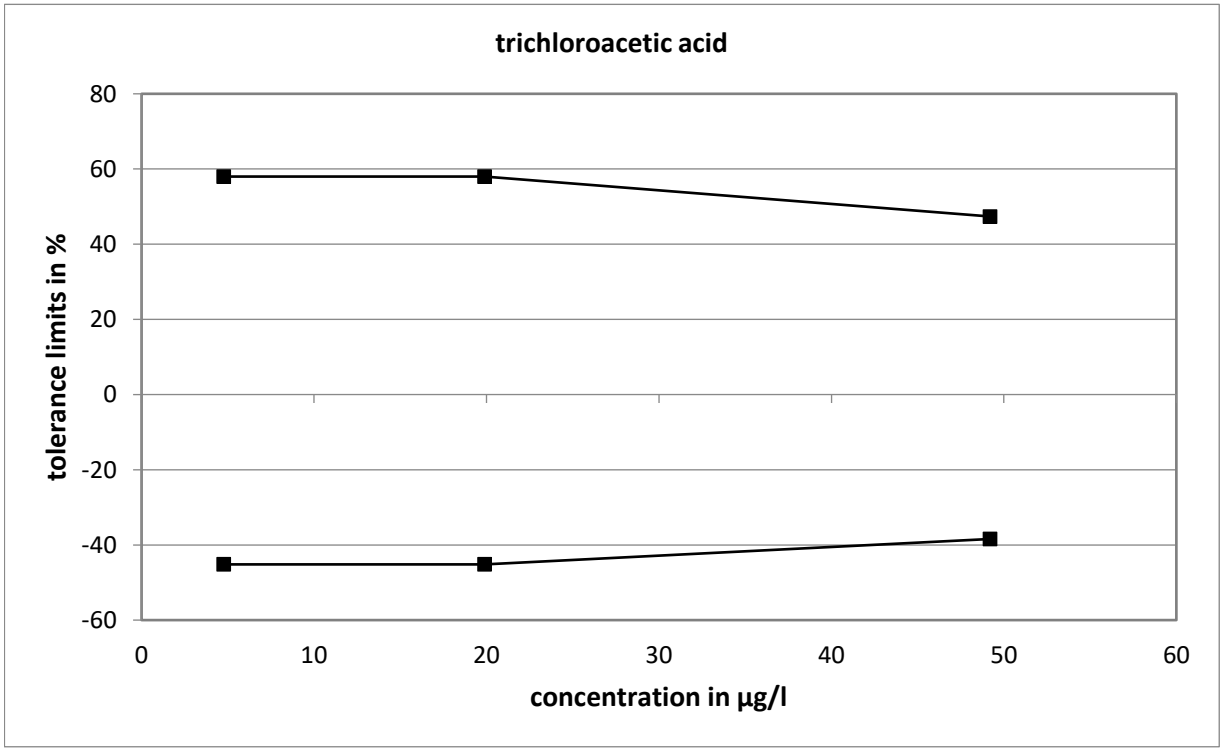


slope of the regression: 0,916; average recovery rate: 91,6 %
neg. x-intercept corresponds to the matrix content: 0 µg/l
exp. Uncertainty of the matrix content: 0,225 µg/l = 0 %

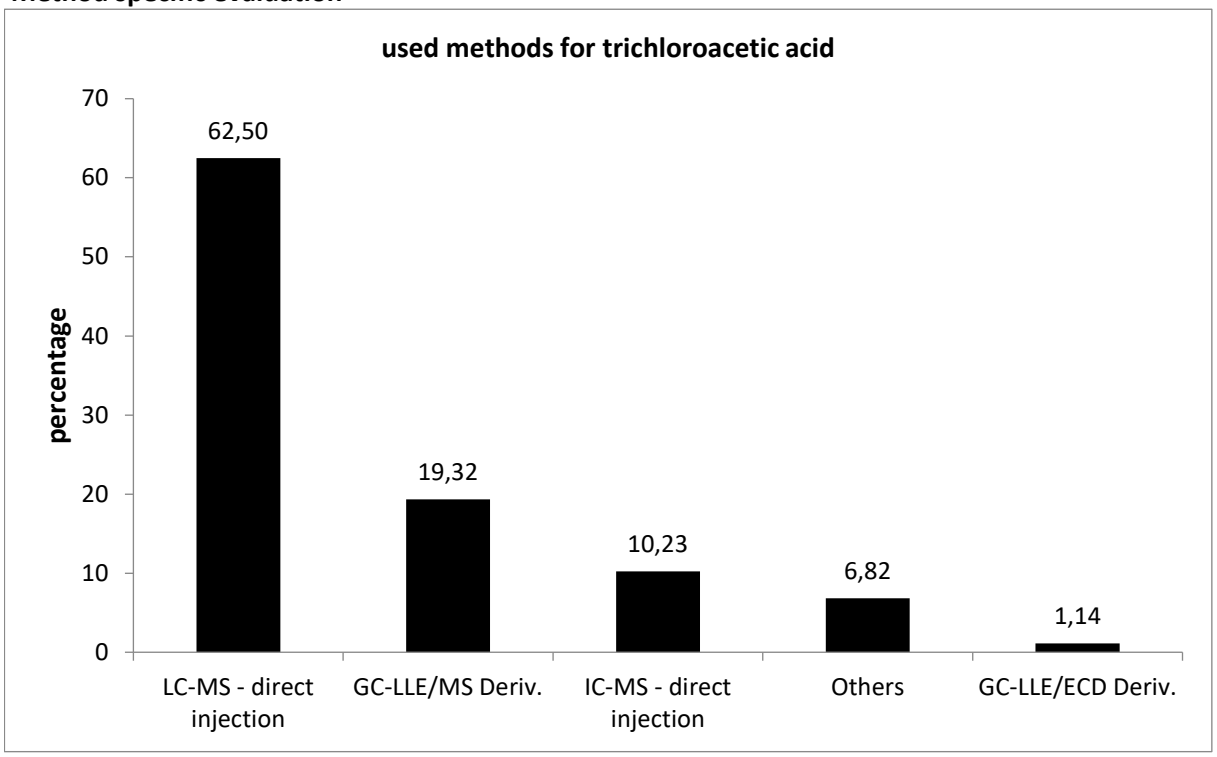
Relative standard deviation and tolerance limits

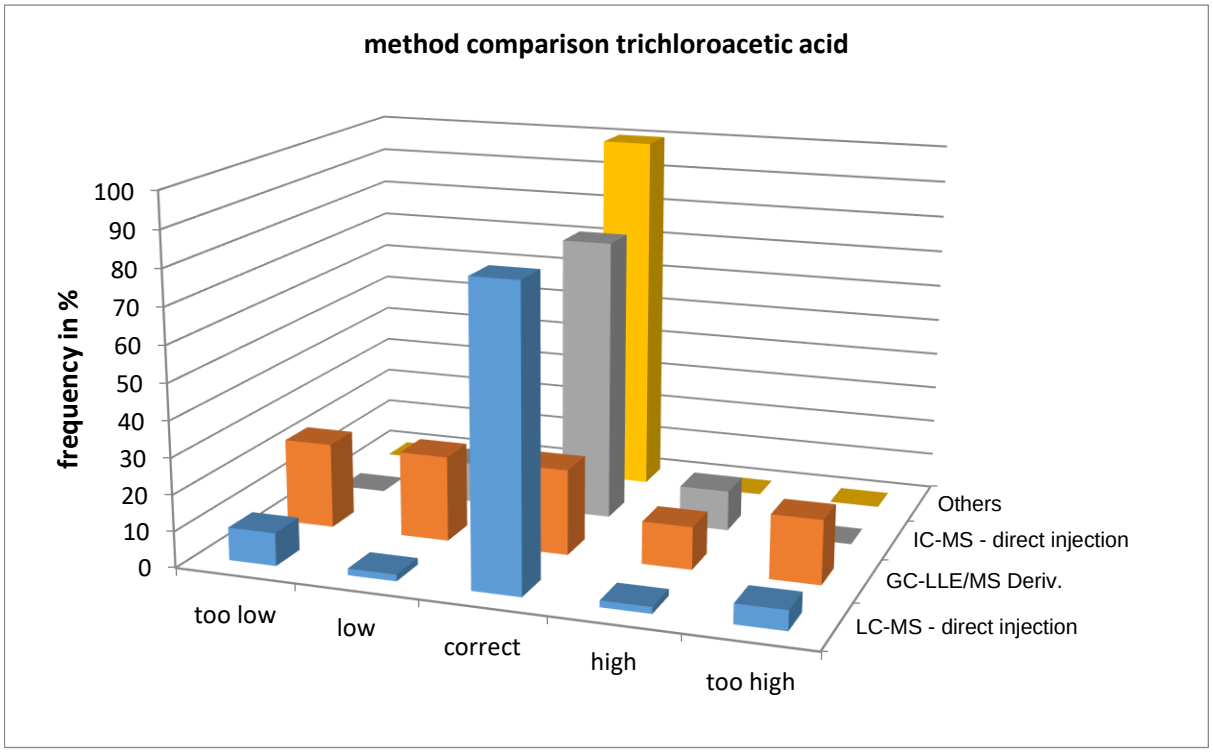


The relative standard deviations calculated with the Q-method reached the upper limit with one concentration level.



Method specific evaluation

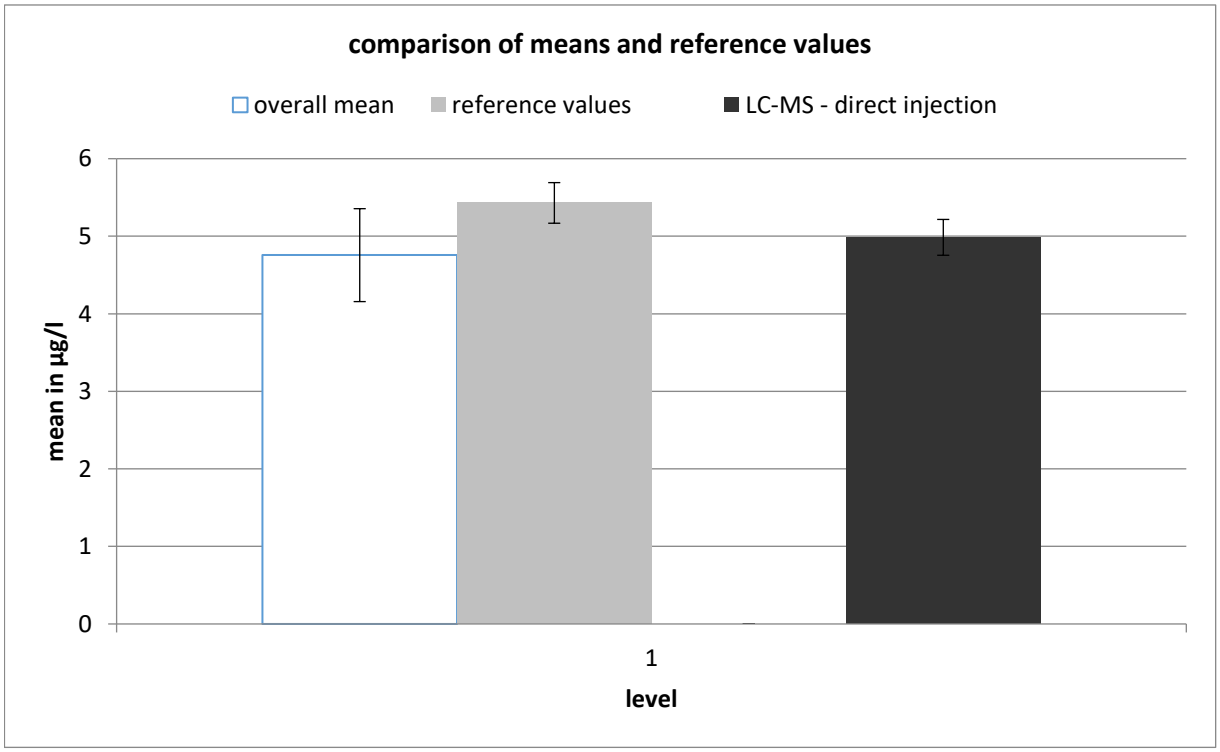


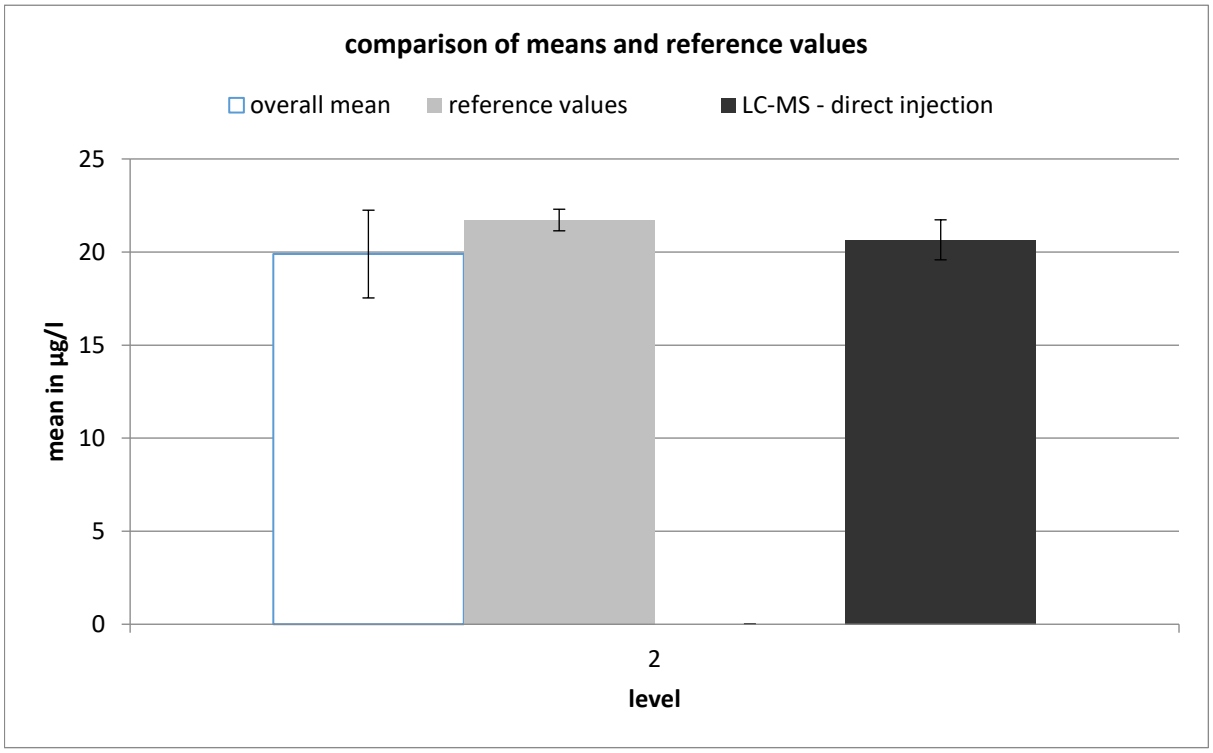


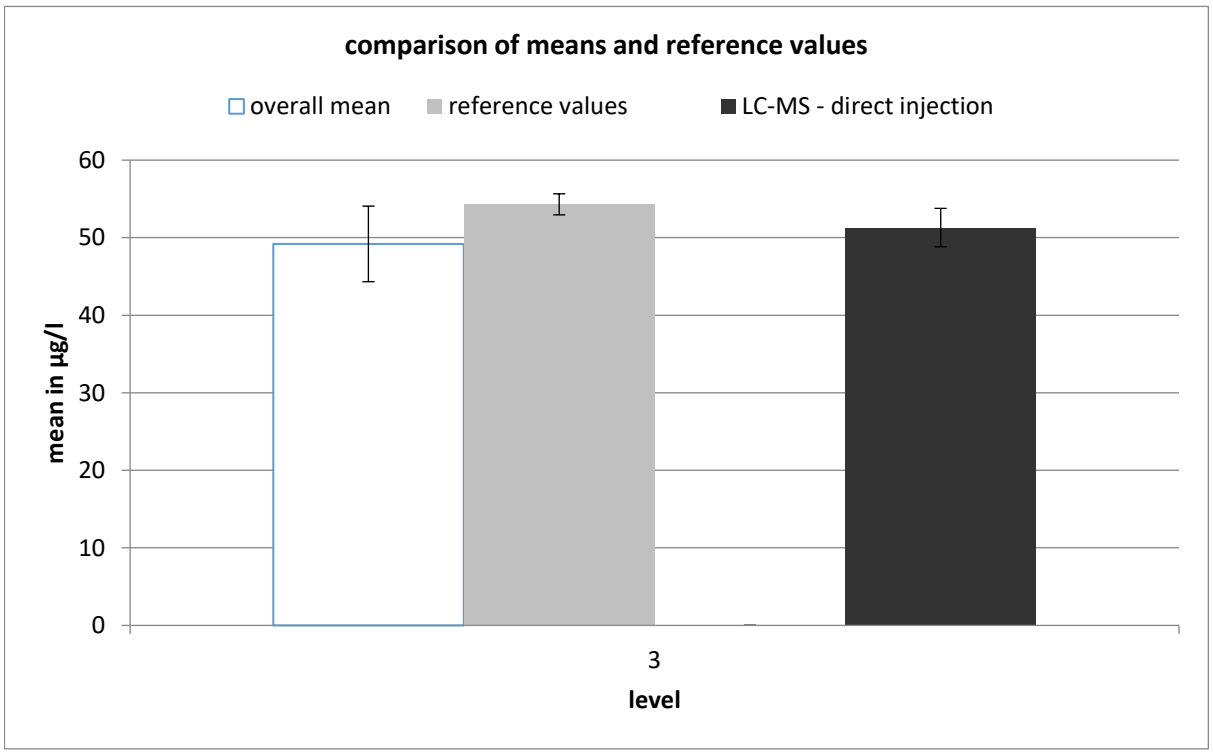
The values determined with LC-MS - direct injection showed the closest statistical distribution.

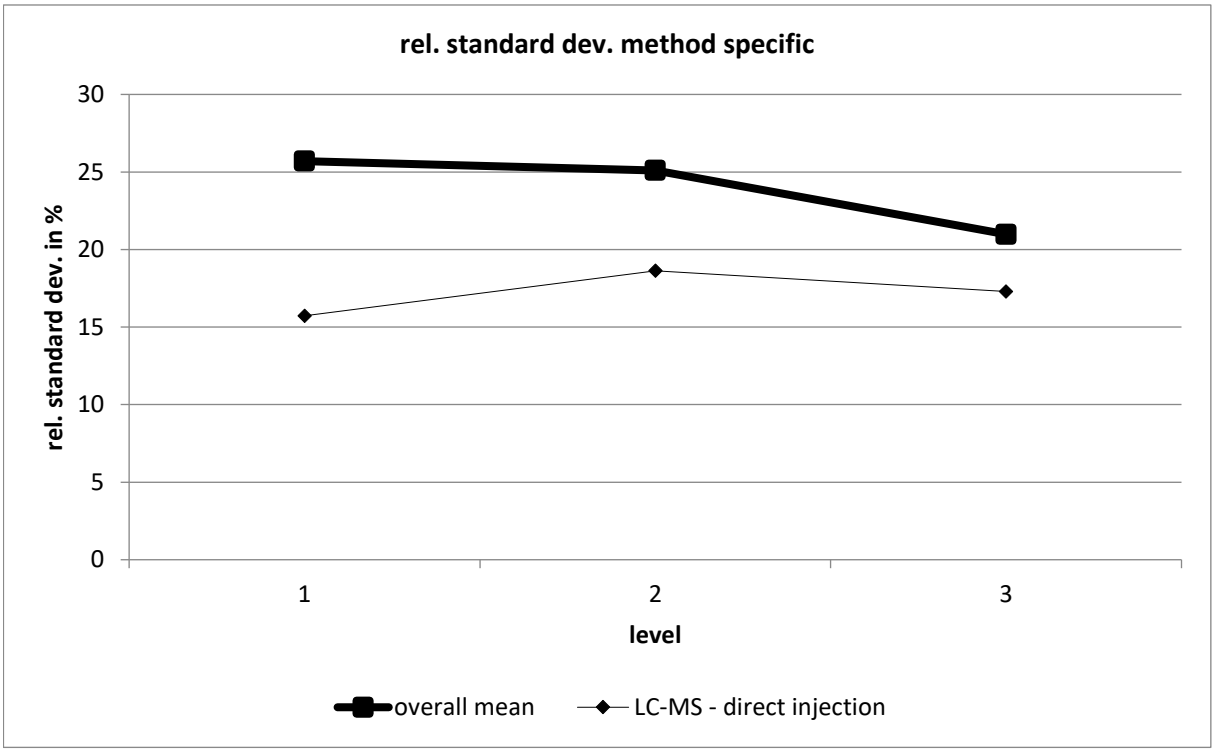
Comparison of means and reference values

level	mean [µg/l]	exp. uncertainty [µg/l]	exp. uncertainty [%]	reference value [µg/l]	exp. uncertainty [µg/l]	exp. uncertainty [%]
1	4,756	0,599	12,6	5,430	0,262	4,8
2	19,89	2,36	11,9	21,72	0,58	2,7
3	49,20	4,88	9,9	54,30	1,36	2,5




comparison of means and reference values
overall mean
reference values
LC-MS - direct injection
25
20
15
10
5
0
mean in µg/l
2
level


comparison of means and reference values
overall mean
reference values
LC-MS - direct injection
60
50
40
30
20
10
0
mean in µg/l
3
level

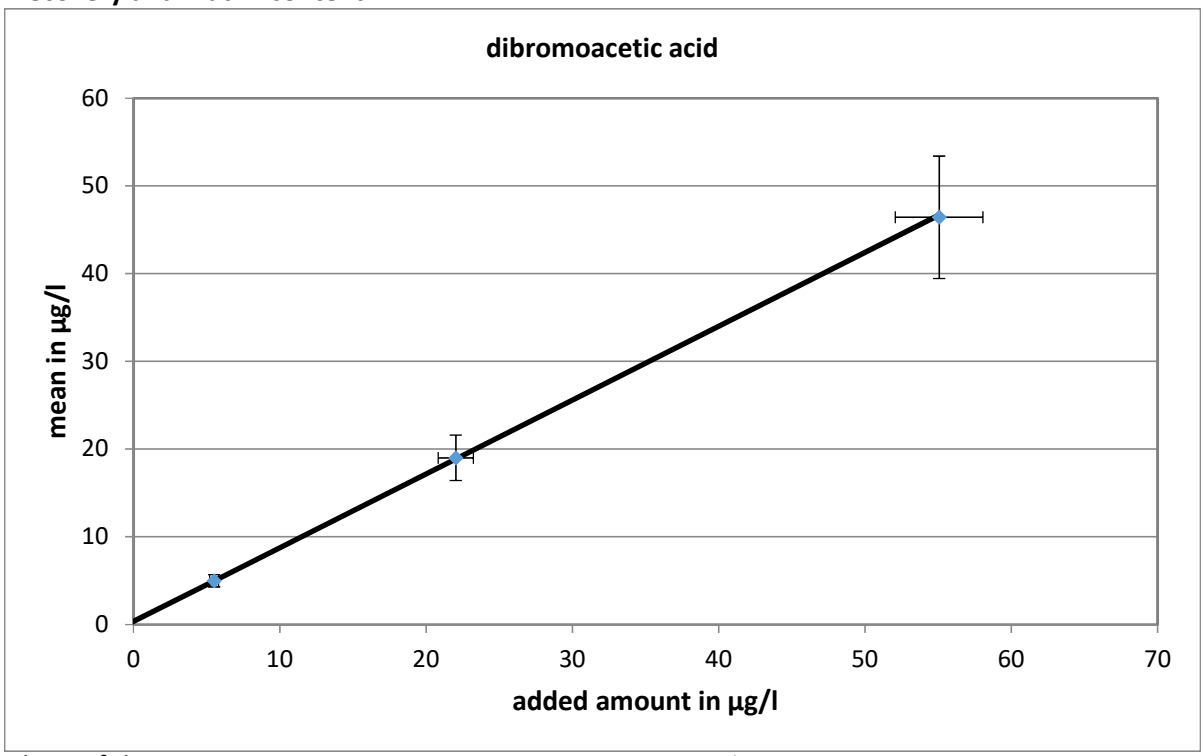


LC-MS - direct injection									
level	robust mean [µg/l]	exp. unc. of the mean [µg/l]	exp. unc. of the mean [%]	robust standard deviation [µg/l]	robust standard deviation [%]	number of results	out below	out above	out [%]
1	4,9855	0,231	4,6338	0,7841	15,728	18	2	3	27,78
2	20,653	1,0753	5,2065	3,8472	18,627	20	2	2	20
3	51,301	2,4795	4,8332	8,8708	17,292	20	2	0	10

dibromoacetic acid

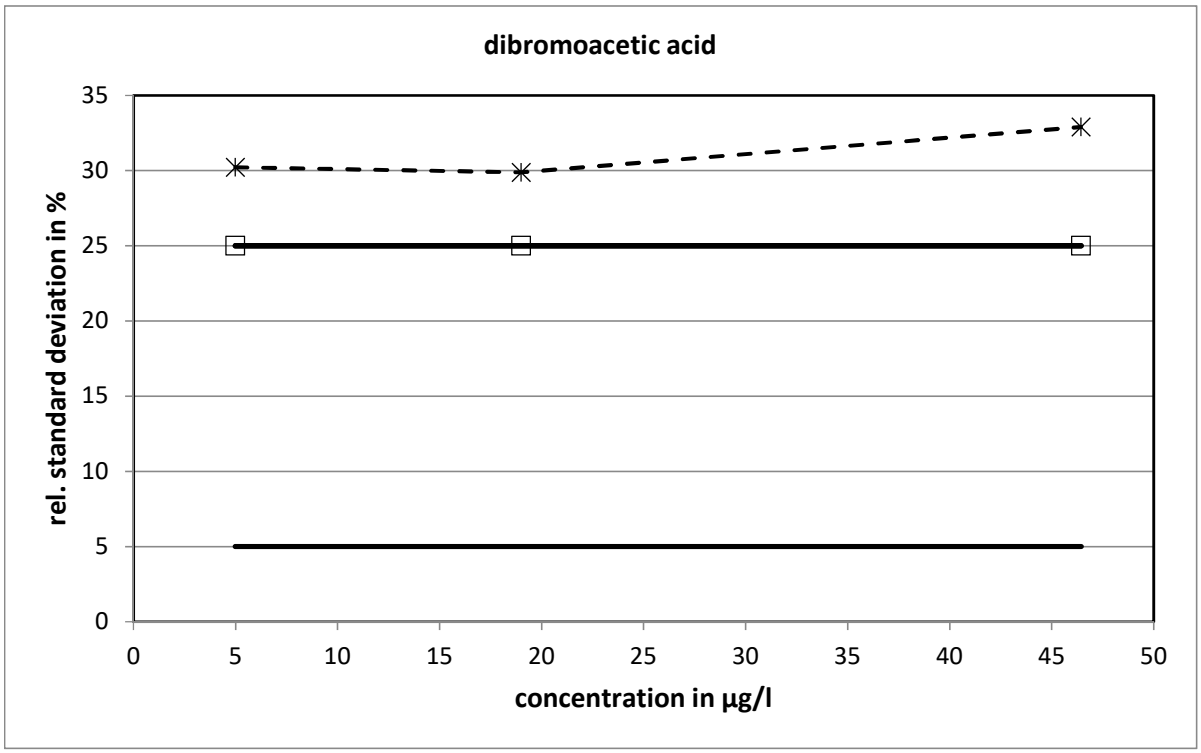
level	assigned value [µg/l]	expanded uncertainty of the assigned value [%]	standard deviation, calculated using robust statistics [µg/l]	standard deviation for proficiency assessment [µg/l]	standard deviation for proficiency assessment [%]	upper tolerance limit [µg/l]	lower tolerance limit [µg/l]	upper tolerance limit [%]	lower tolerance limit [%]	number of results	out below	out above	out [%]
1	4,986	14,02	1,506	1,246	25,00	7,876	2,733	57,99	-45,19	29	6	0	20,7
2	19,00	13,64	5,677	4,749	25,00	30,01	10,41	57,99	-45,19	30	5	2	23,3
3	46,43	15,02	15,28	11,61	25,00	73,36	25,45	57,99	-45,19	30	3	1	13,3
									sum	89	14	3	19,1

Recovery and matrix content

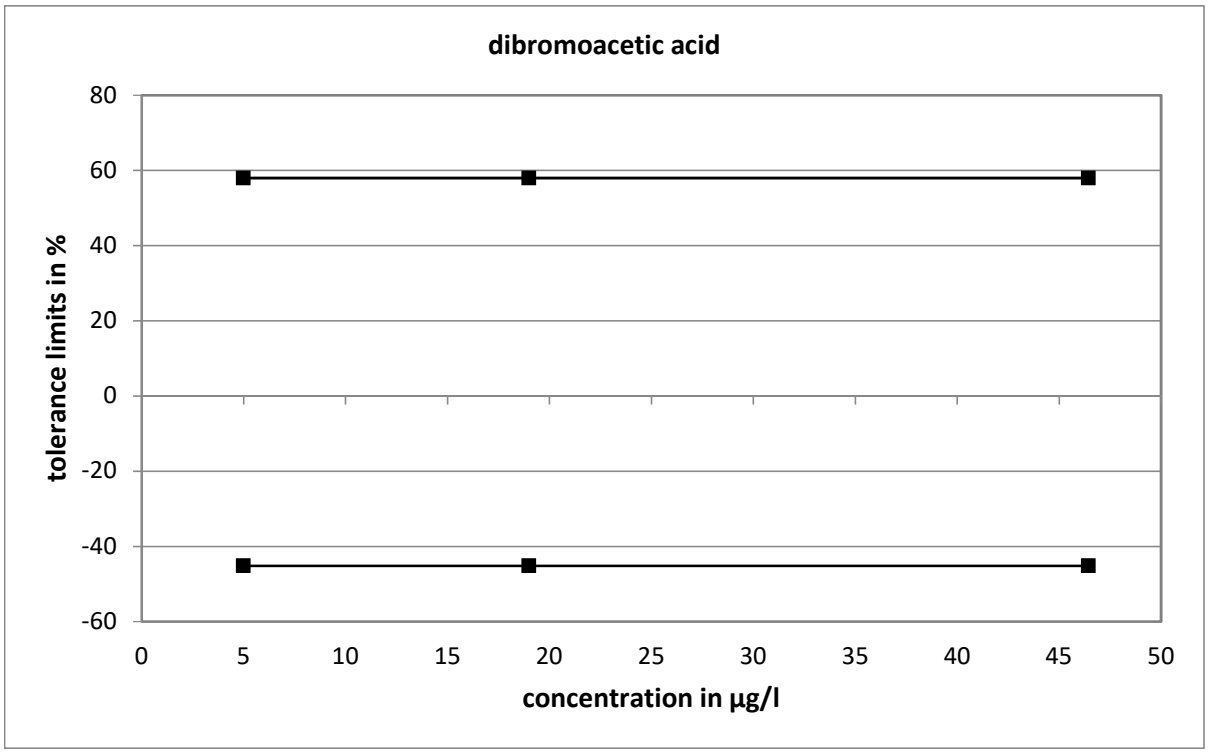


slope of the regression: 0,841; average recovery rate: 84,1 %
neg. x-intercept corresponds to the matrix content: 0,425 µg/l
exp. Uncertainty of the matrix content: 0,425 µg/l = 100 %

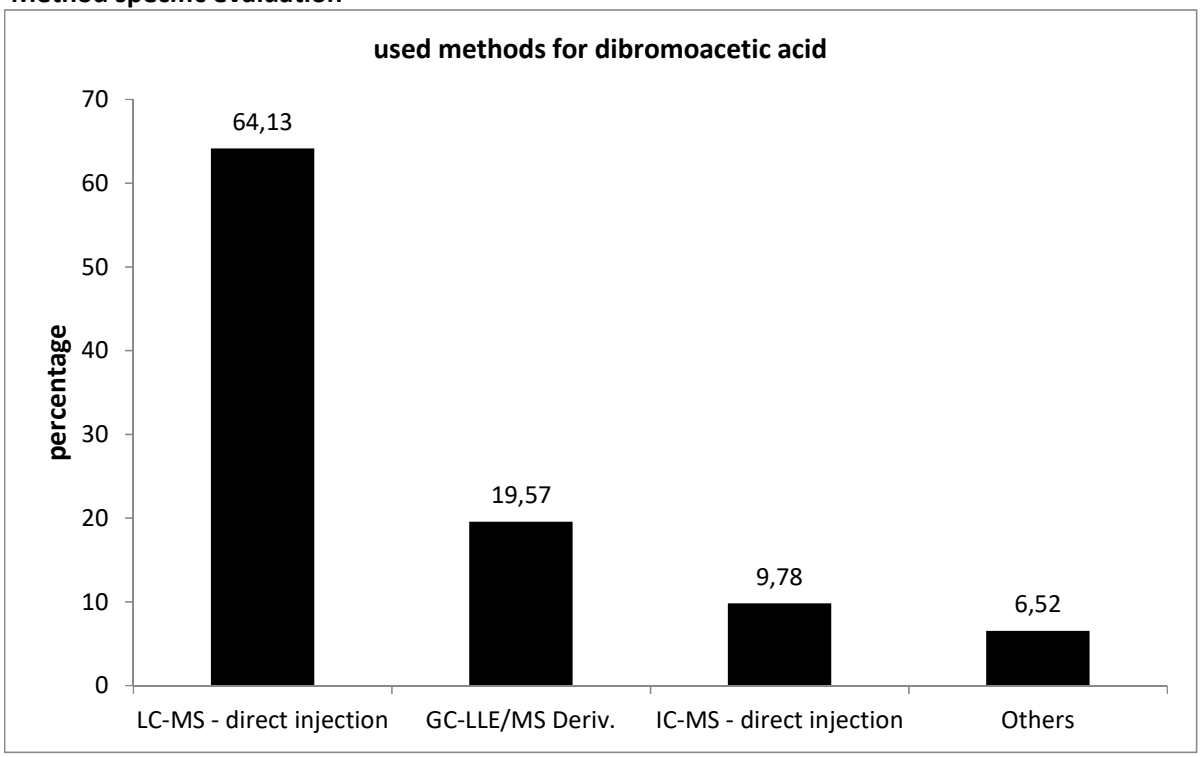
Relative standard deviation and tolerance limits

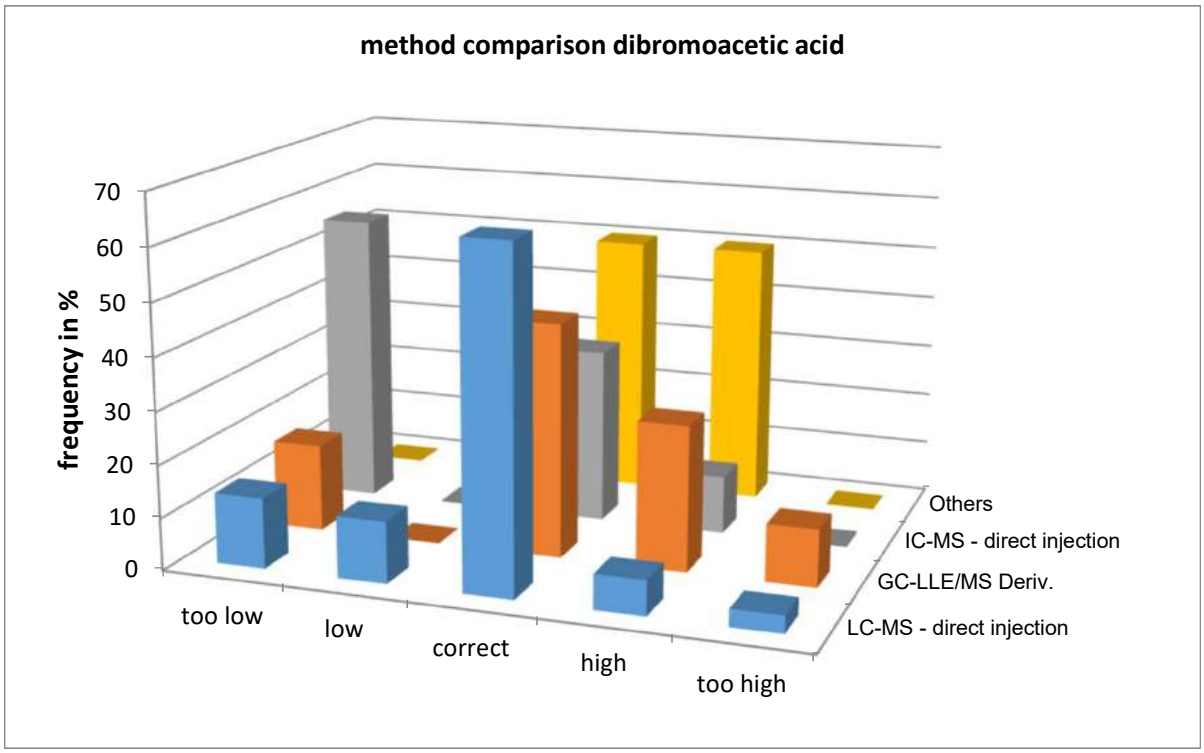


The relative standard deviations calculated with the Q-method reached the upper limit with all concentration levels.



Method specific evaluation

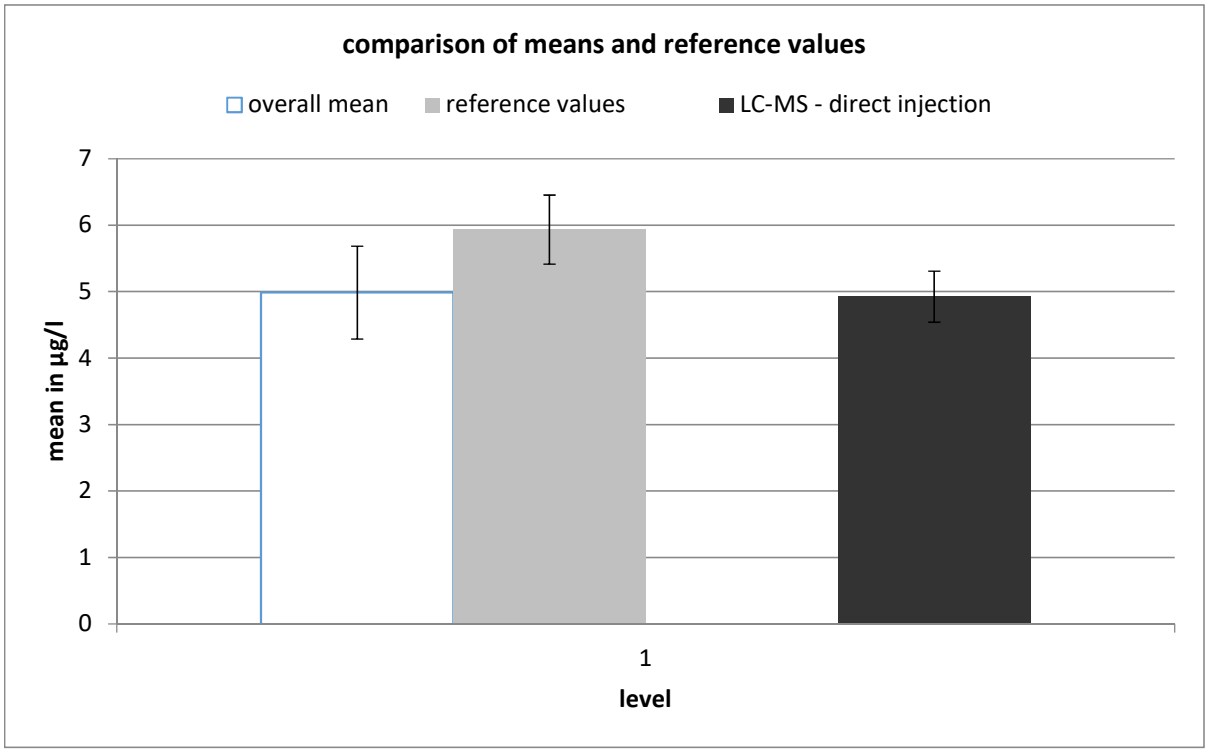


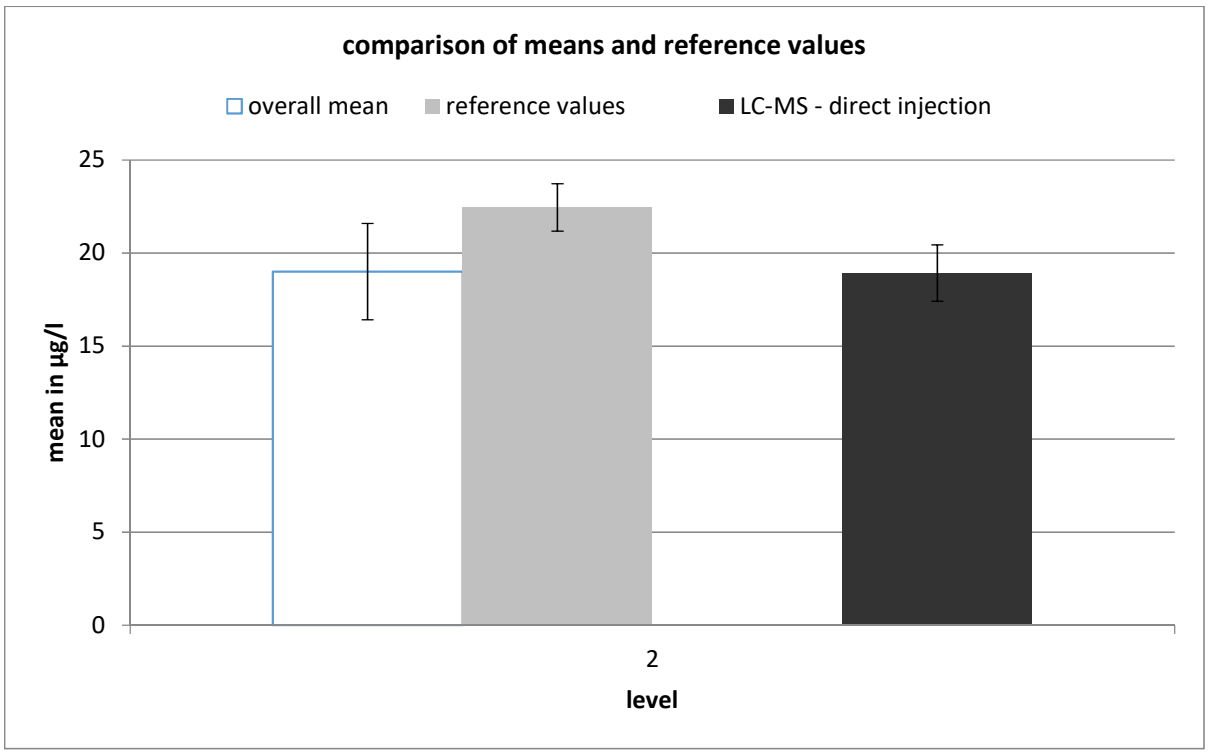


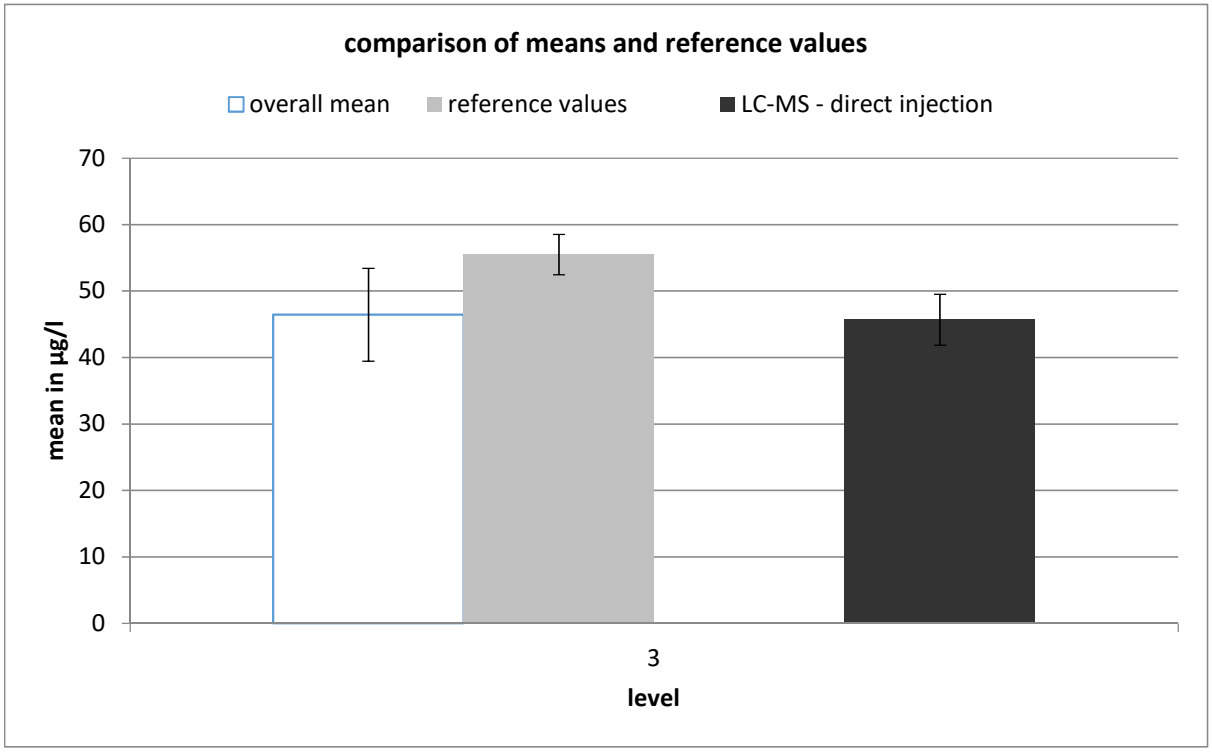
The values determined with LC-MS - direct injection showed the closest statistical distribution.

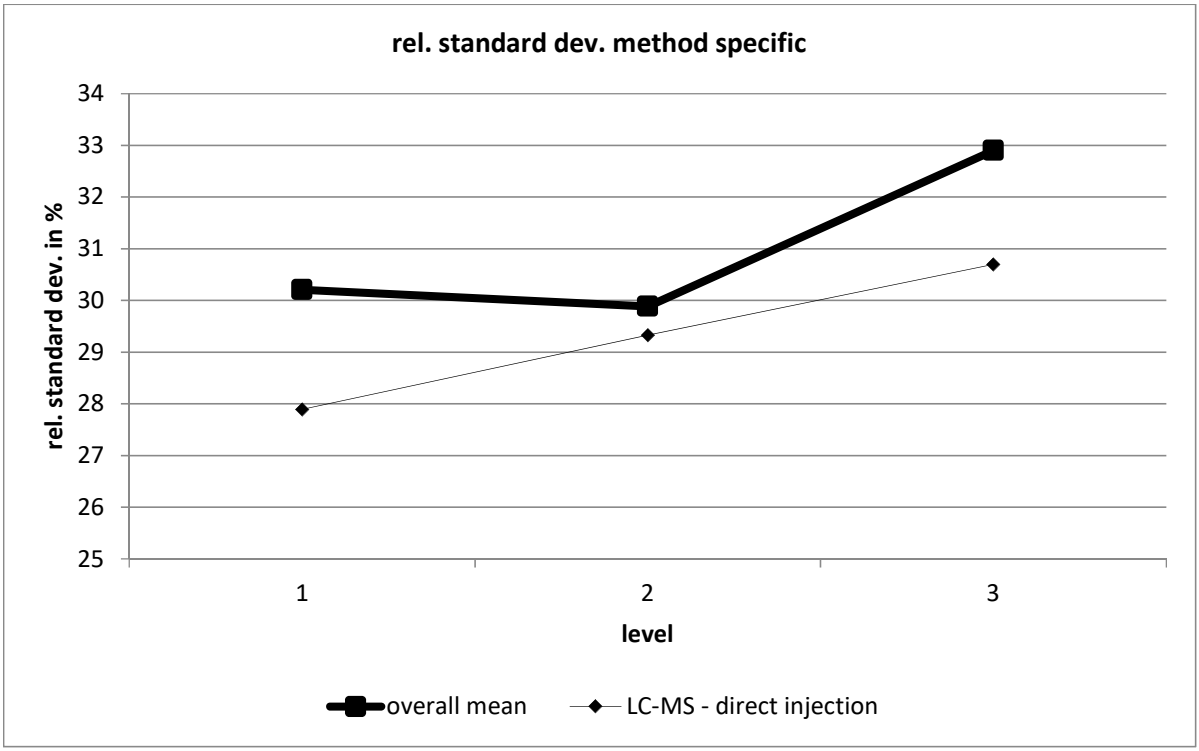
Comparison of means and reference values

level	mean [µg/l]	exp. uncertainty [µg/l]	exp. uncertainty [%]	reference value [µg/l]	exp. uncertainty [µg/l]	exp. uncertainty [%]
1	4,986	0,699	14,0	5,932	0,520	8,8
2	19,00	2,59	13,6	22,45	1,27	5,7
3	46,43	6,97	15,0	55,49	3,03	5,5

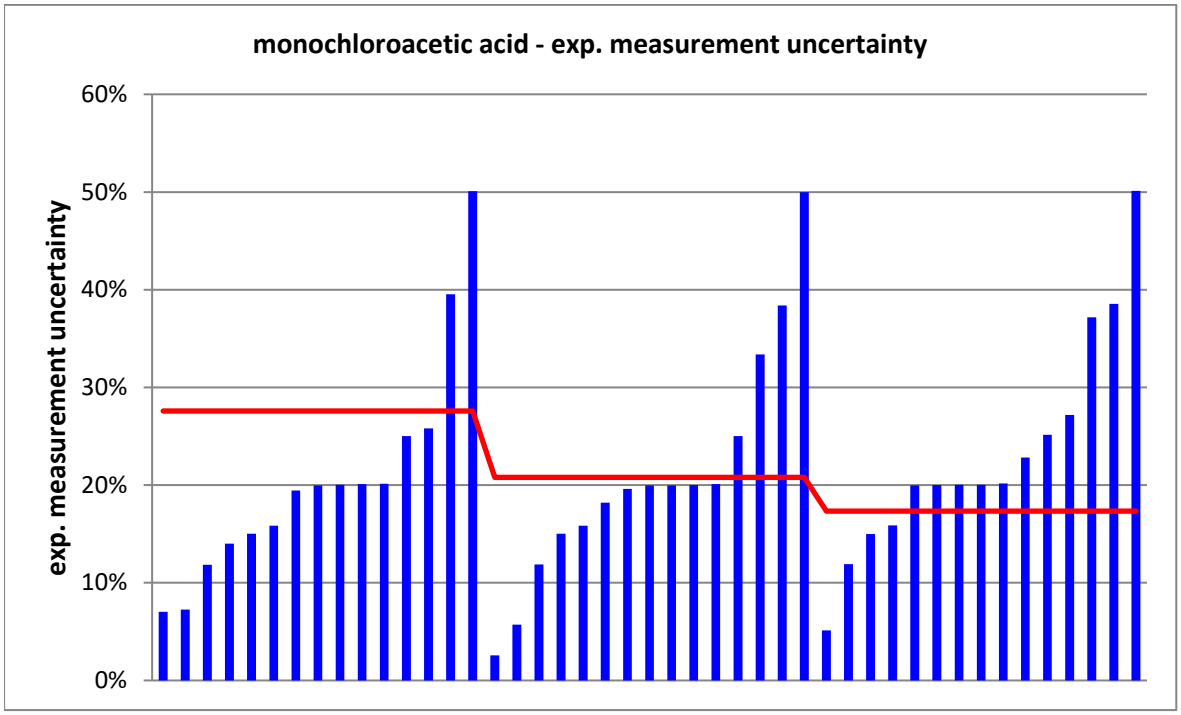


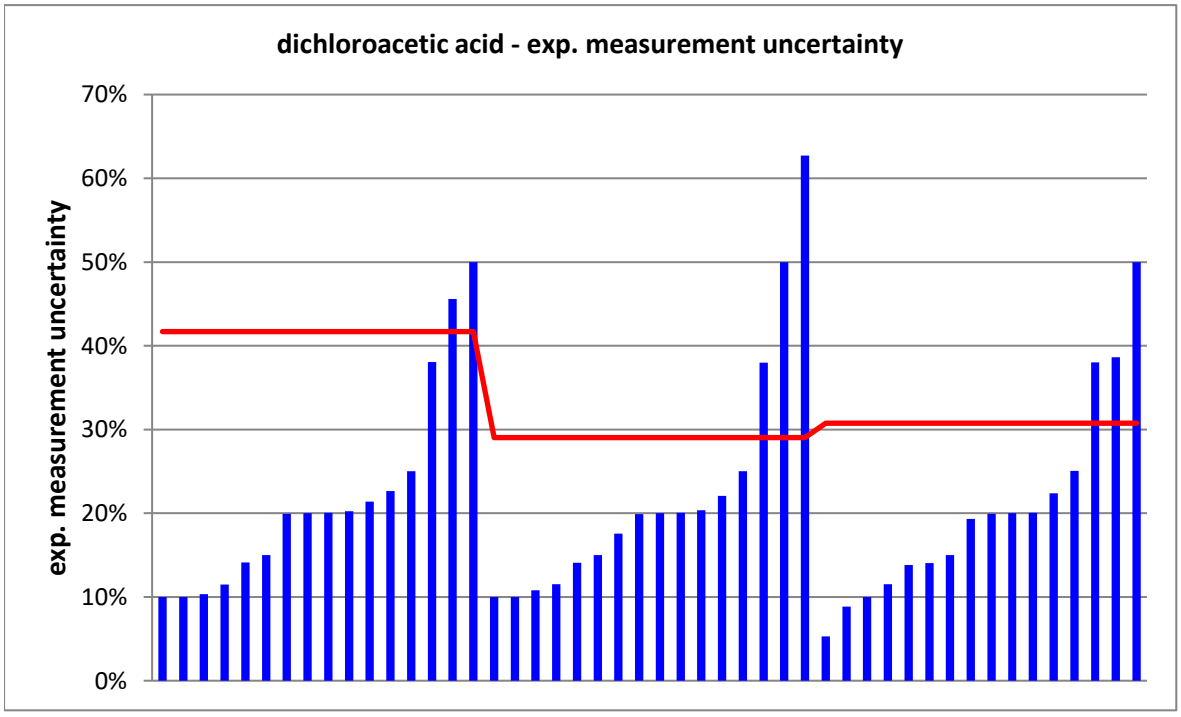

comparison of means and reference values
overall mean
reference values
LC-MS - direct injection
25
20
15
10
5
0
mean in µg/l
2
level

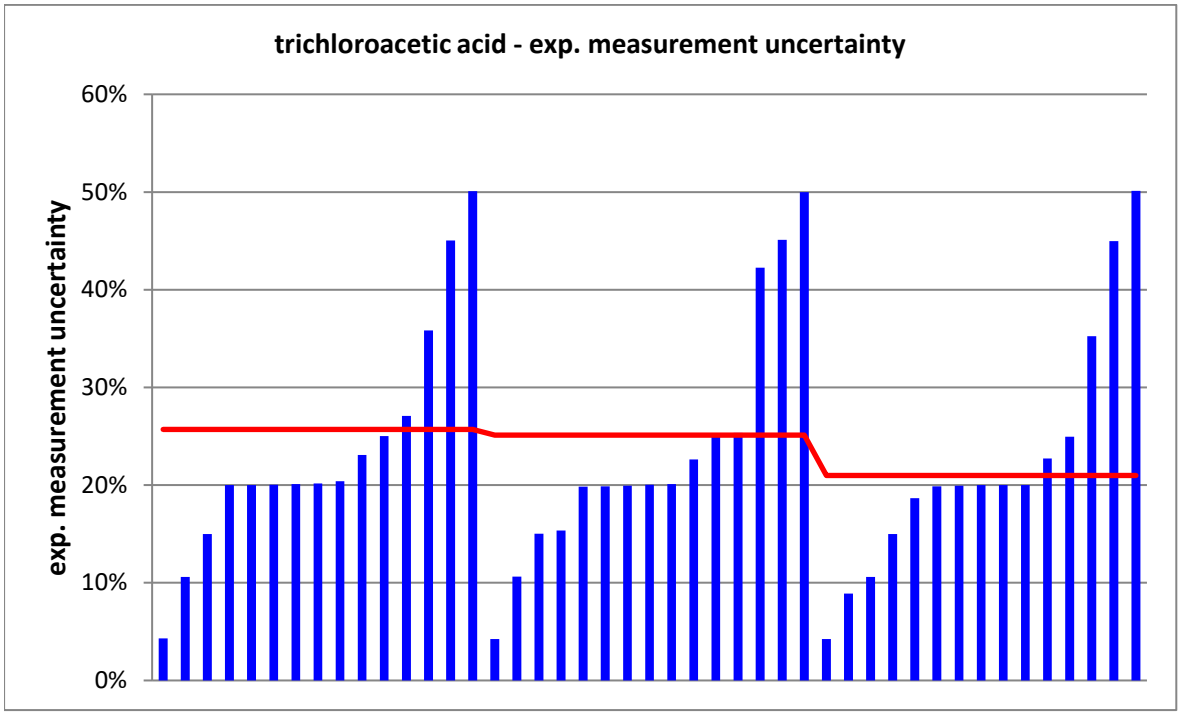

comparison of means and reference values
overall mean
reference values
LC-MS - direct injection
70
60
50
40
30
20
10
0
mean in µg/l
3
level

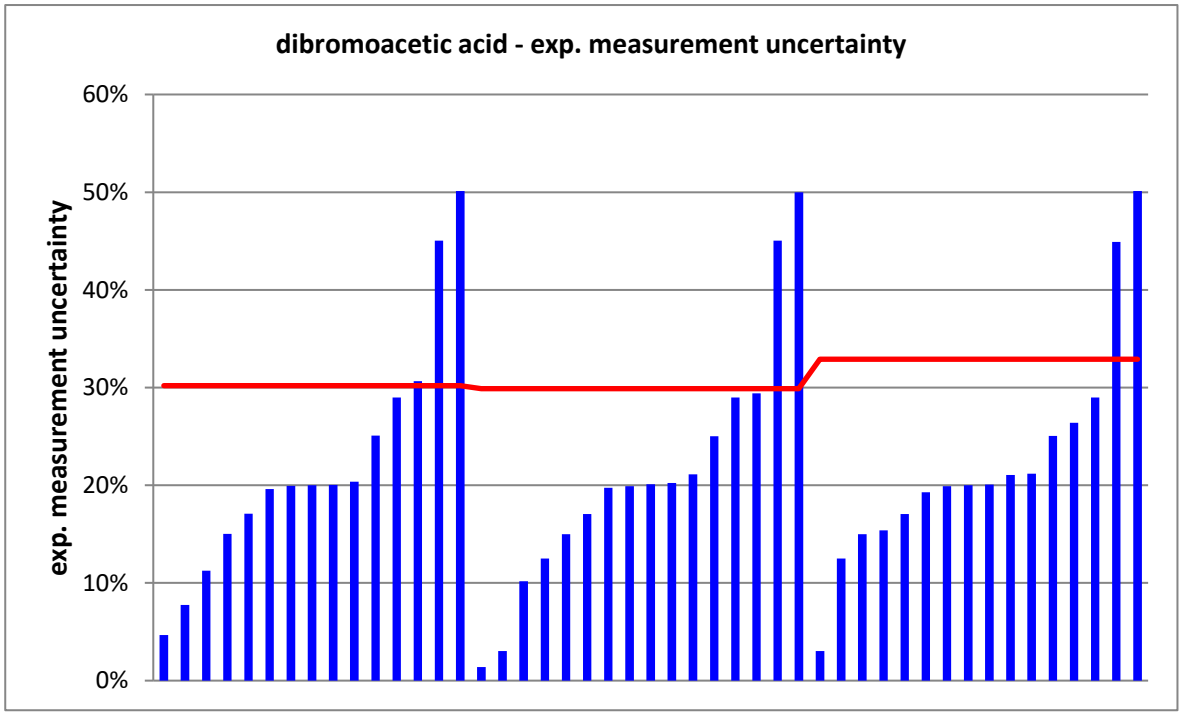


LC-MS - direct injection									
level	robust mean [µg/l]	exp. unc. of the mean [µg/l]	exp. unc. of the mean [%]	robust standard deviation [µg/l]	robust standard deviation [%]	number of results	out below	out above	out [%]
1	4,9229	0,384	7,7962	1,3731	27,892	20	2	1	15
2	18,917	1,513	7,9999	5,5479	29,328	21	3	0	14,29
3	45,689	3,826	8,3732	14,025	30,697	21	2	0	9,524


monochloroacetic acid - exp. measurement uncertainty
exp. measurement uncertainty
60%
50%
40%
30%
20%
10%
0%


dichloroacetic acid - exp. measurement uncertainty
exp. measurement uncertainty
70%
60%
50%
40%
30%
20%
10%
0%

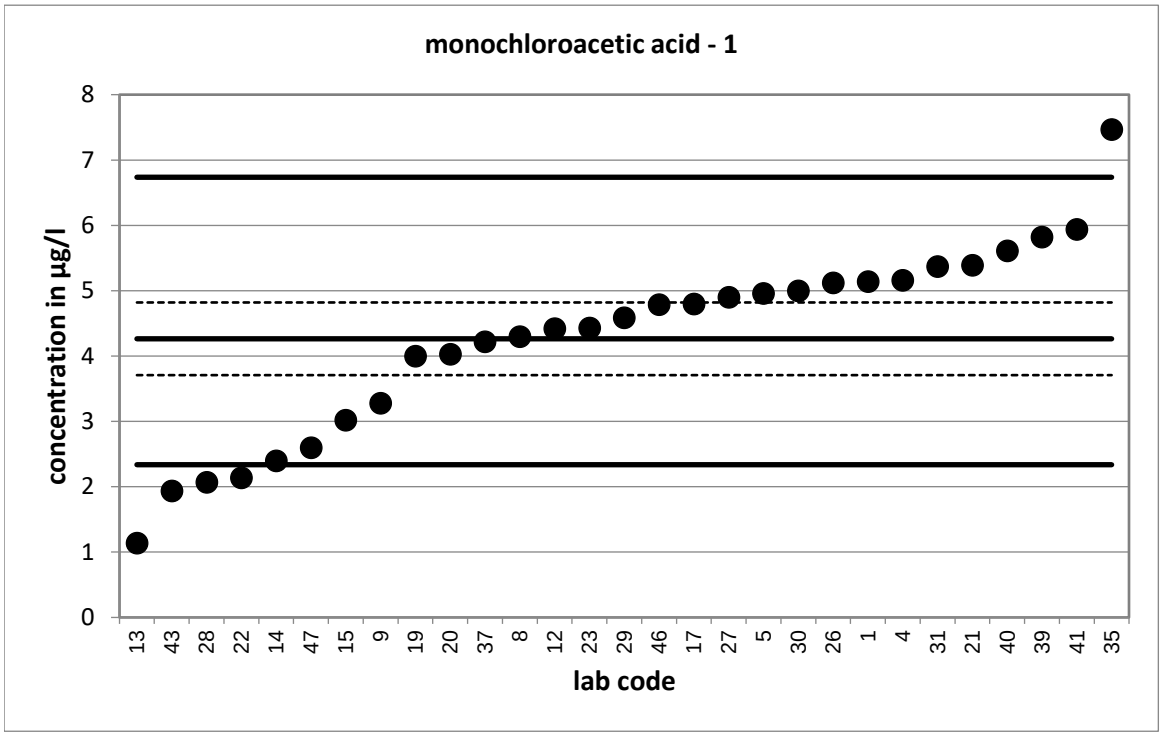

trichloroacetic acid - exp. measurement uncertainty
exp. measurement uncertainty
60%
50%
40%
30%
20%
10%
0%


dibromoacetic acid - exp. measurement uncertainty
exp. measurement uncertainty
60%
50%
40%
30%
20%
10%
0%

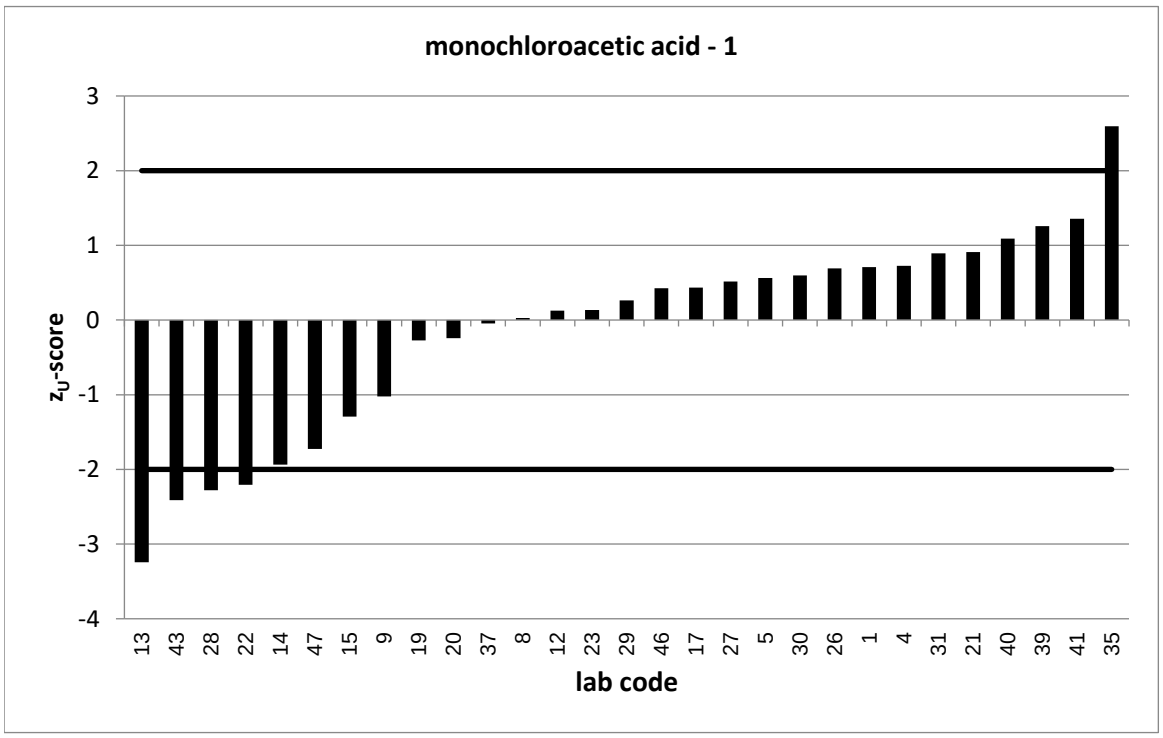
PT 7/23		monochloroacetic acid - 1			
assigned value [µg/l]*		4,264	± 0,556		
upper tolerance limit [µg/l]		6,736			
lower tolerance limit [µg/l]		2,337			
lab code	result [µg/l]	±	z-score	z_U-score	assessm.**
1	5,14	1	1,5	0,7	s
4	5,16			0,7	s
5	4,96	1,28	1,0	0,6	s
8	4,3	1,7	0,0	0,0	s
9	3,28	0,66	-2,3	-1,0	s
12	4,42			0,1	s
13	1,14			-3,2	u
14	2,4			-1,9	s
15	3,02			-1,3	s
17	4,8	0,672	1,2	0,4	s
19	4,002			-0,3	s
20	4,03			-0,2	s
21	5,39	2,7	0,8	0,9	s
22	2,14	0,15	-7,4	-2,2	q
23	4,43	0,665	0,4	0,1	s
26	5,12			0,7	s
27	4,9	0,58	1,6	0,5	s
28	2,07	0,15	-7,6	-2,3	q
29	4,59			0,3	s
30	5	1,25	1,1	0,6	s
31	5,37	0,85	2,2	0,9	s
35	7,47			2,6	q
37	4,22			0,0	s
39	5,82			1,3	s
40	5,61	1,12	2,2	1,1	s
41	5,94			1,4	s
43	1,94	0,39	-6,8	-2,4	q
46	4,79			0,4	s
47	2,6	0,521	-4,4	-1,7	s

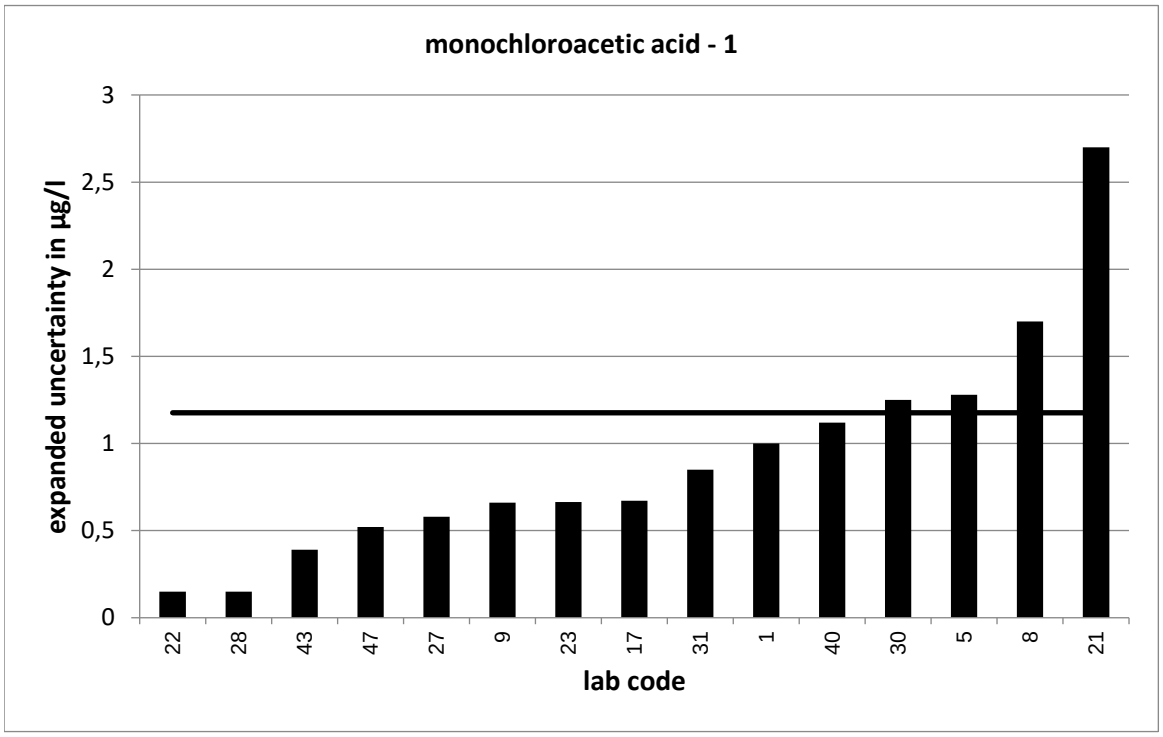
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor k=2 corresponding to a confidence level of about 95%

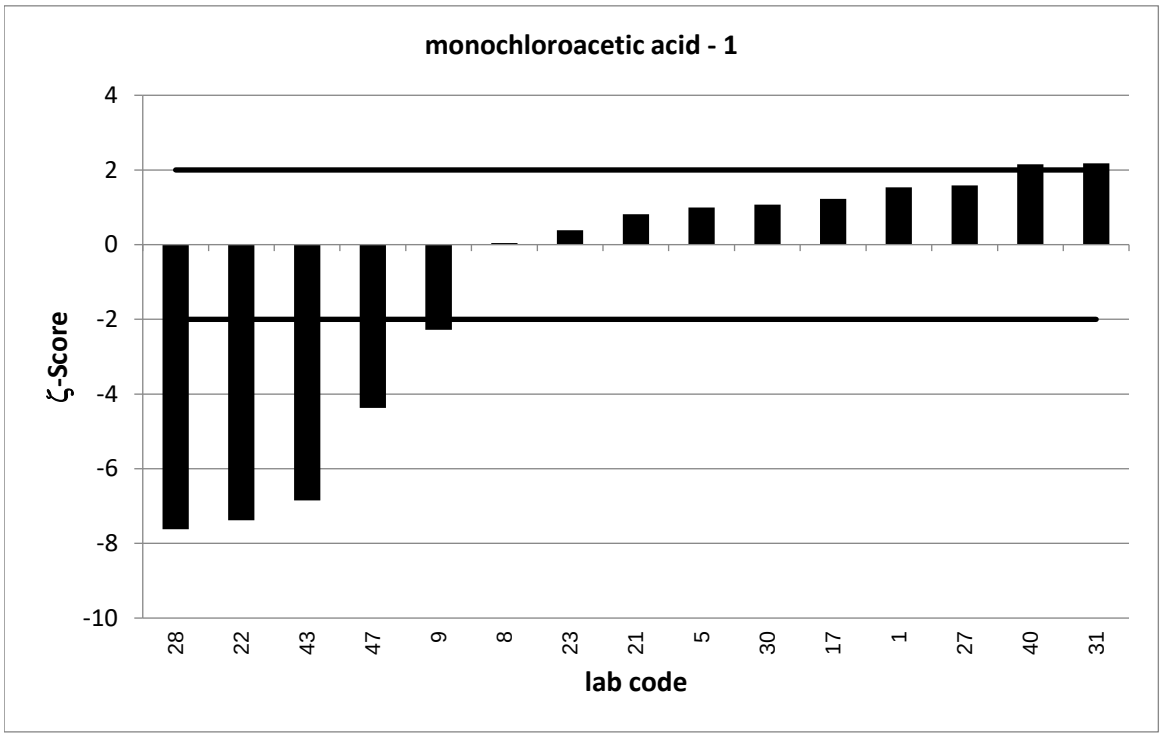
** s = satisfactory, q = questionable, u = unsatisfactory



Strongly deviating values are not shown in the diagram.



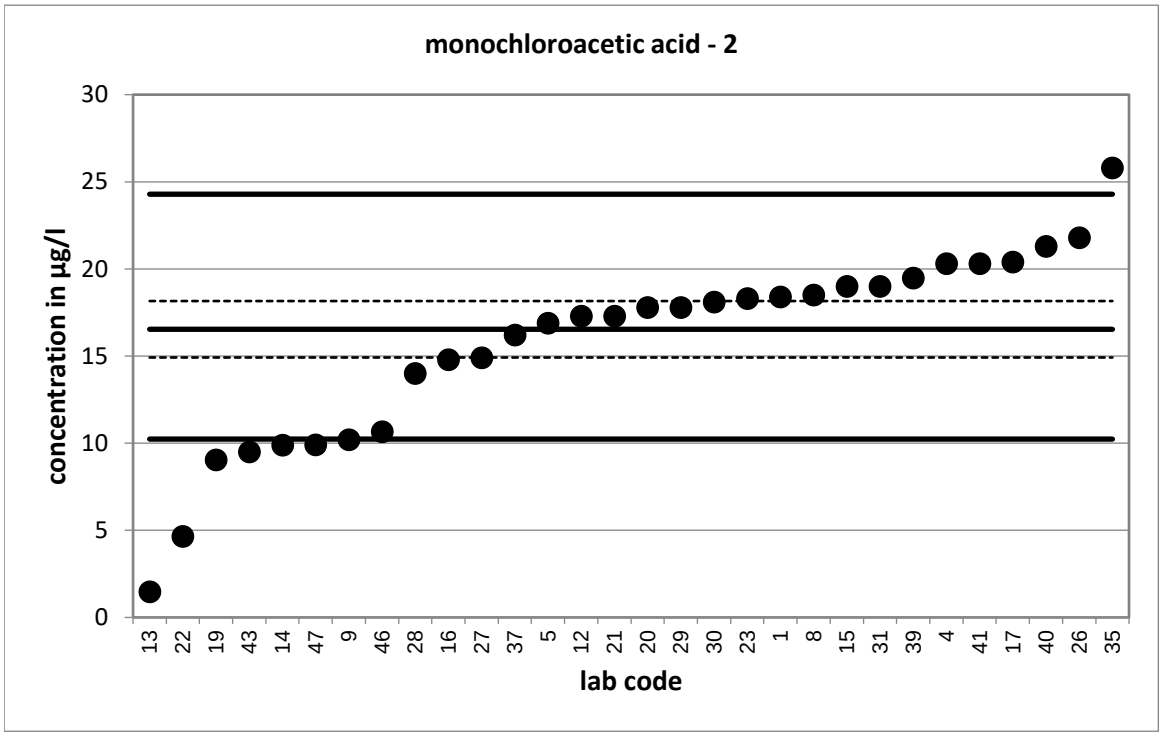

monochloroacetic acid - 1
expanded uncertainty in µg/l
3
2,5
2
1,5
1
0,5
0
22
28
43
47
27
9
23
17
31
1
40
30
5
8
21
lab code


monochloroacetic acid - 1
ζ-Score
4
2
0
-2
-4
-6
-8
-10
28
22
43
47
9
8
23
21
5
30
17
1
27
40
31
lab code

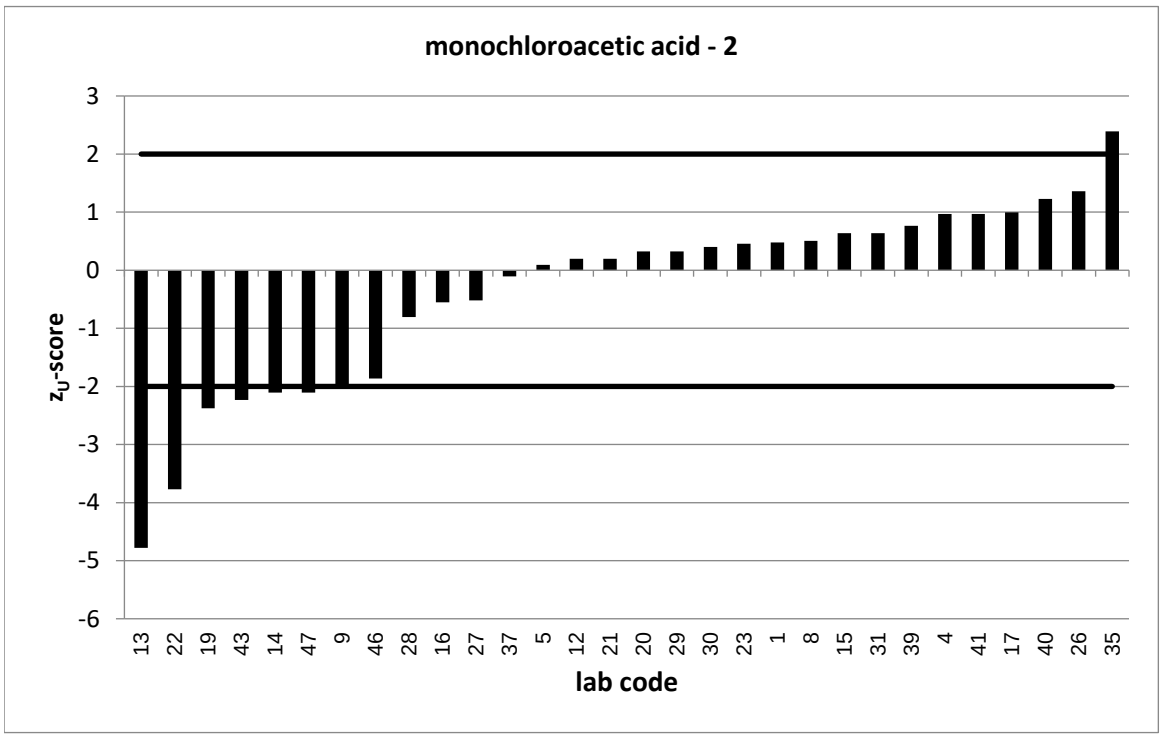
PT 7/23		monochloroacetic acid - 2			
assigned value [µg/l]*		16,54	± 1,62		
upper tolerance limit [µg/l]		24,29			
lower tolerance limit [µg/l]		10,24			
lab code	result [µg/l]	±	z-score	z_U-score	assessm.**
1	18,4	3,7	0,9	0,5	s
4	20,3			1,0	s
5	16,9	5,64	0,1	0,1	s
8	18,5	7,1	0,5	0,5	s
9	10,2	2	-4,9	-2,0	s
12	17,3			0,2	s
13	1,48			-4,8	u
14	9,9			-2,1	q
15	19			0,6	s
16	14,8			-0,6	s
17	20,4	3,71	1,9	1,0	s
19	9,053			-2,4	q
20	17,8			0,3	s
21	17,3	8,65	0,2	0,2	s
22	4,66	0,12	-14,6	-3,8	u
23	18,3	2,75	1,1	0,5	s
26	21,8			1,4	s
27	14,9	1,77	-1,4	-0,5	s
28	14	0,8	-2,8	-0,8	s
29	17,8			0,3	s
30	18,1	4,53	0,6	0,4	s
31	19	3,01	1,4	0,6	s
35	25,8			2,4	q
37	16,21			-0,1	s
39	19,49			0,8	s
40	21,3	4,26	2,1	1,2	s
41	20,3			1,0	s
43	9,51	1,9	-5,6	-2,2	q
46	10,67			-1,9	s
47	9,91	1,98	-5,2	-2,1	q

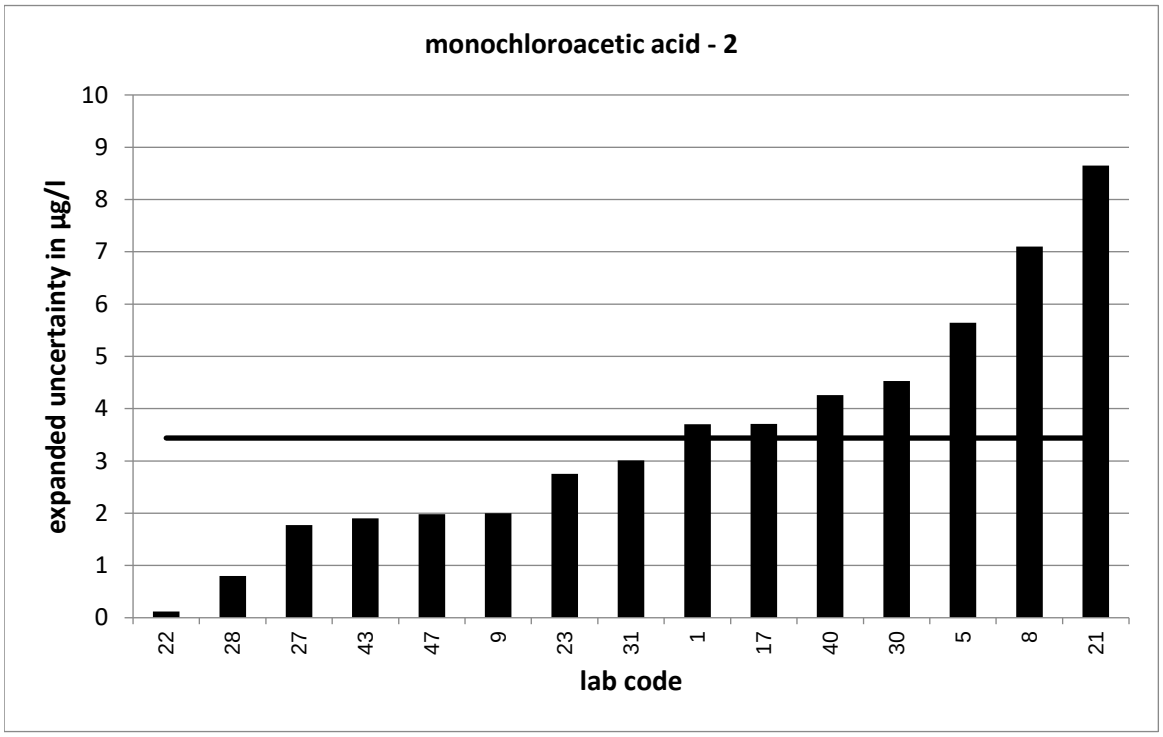
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor k=2 corresponding to a confidence level of about 95%

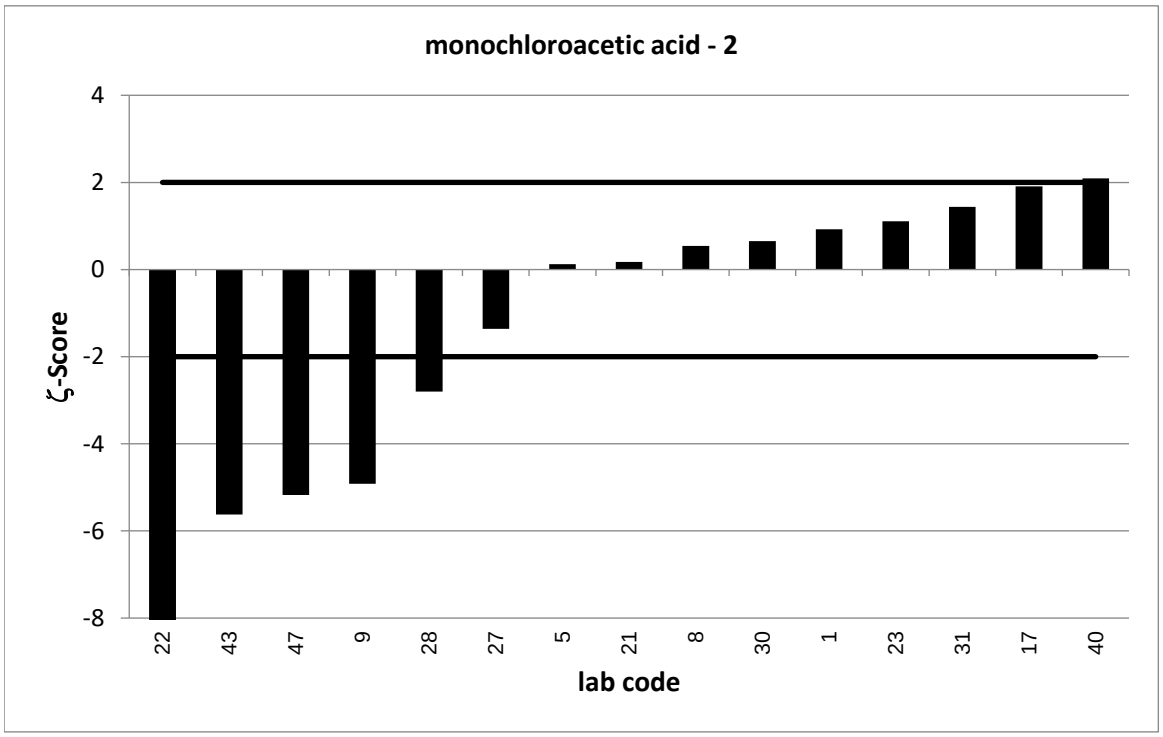
** s = satisfactory, q = questionable, u = unsatisfactory



Strongly deviating values are not shown in the diagram.





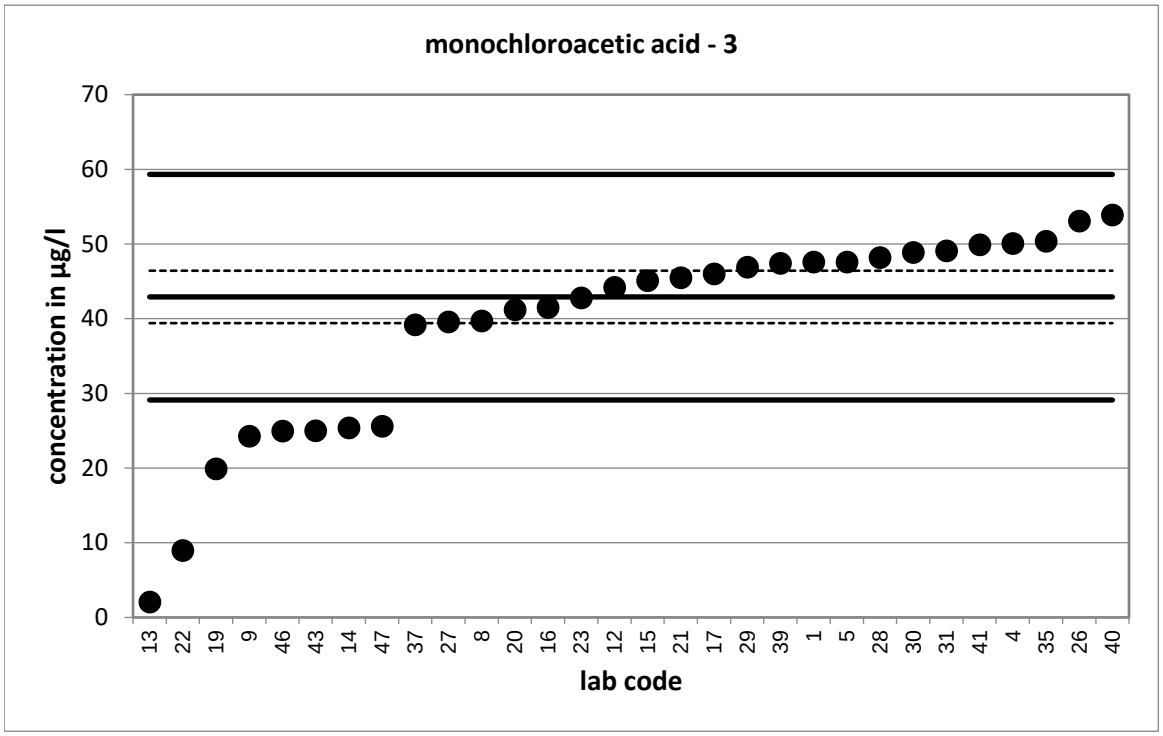


Strongly deviating values are not correctly shown in the diagram.

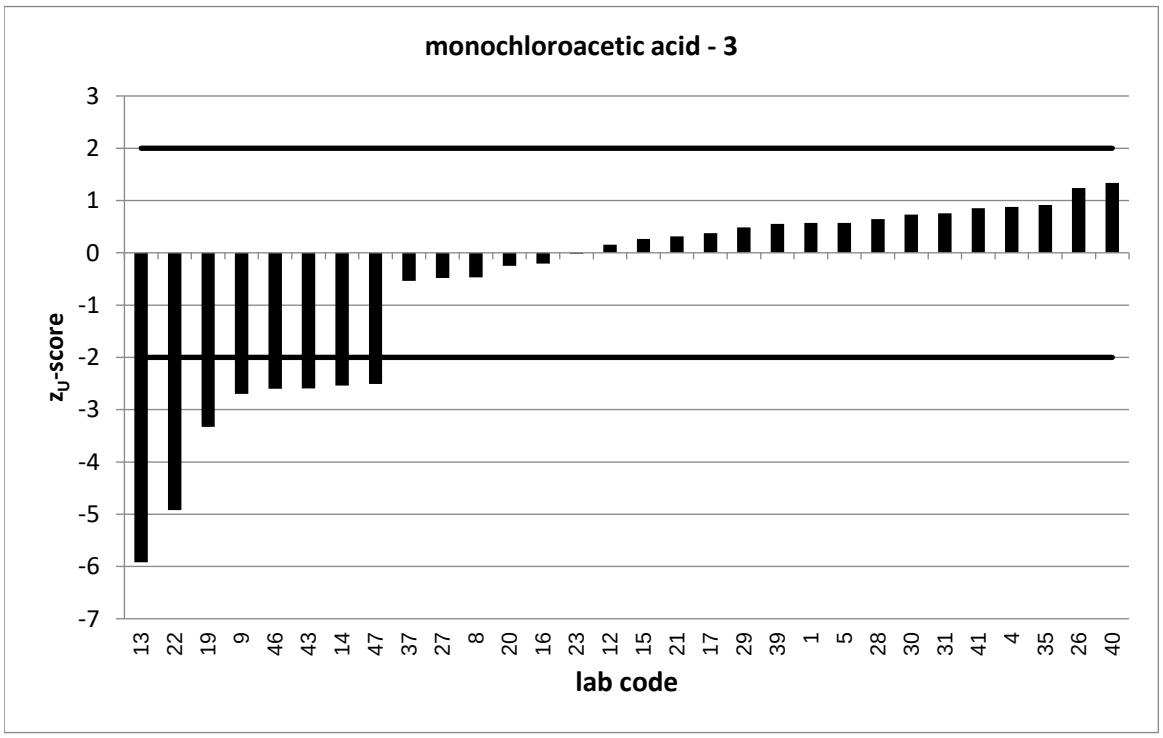
PT 7/23		monochloroacetic acid - 3			
assigned value [µg/l]*		42,92	± 3,51		
upper tolerance limit [µg/l]		59,32			
lower tolerance limit [µg/l]		29,12			
lab code	result [µg/l]	±	z-score	z_U-score	assessm.**
1	47,6	9,5	0,9	0,6	s
4	50,1			0,9	s
5	47,6	17,7	0,5	0,6	s
8	39,7	15,3	-0,4	-0,5	s
9	24,3	4,9	-6,2	-2,7	q
12	44,2			0,2	s
13	2,07			-5,9	u
14	25,4			-2,5	q
15	45,1			0,3	s
16	41,5			-0,2	s
17	46	10,5	0,6	0,4	s
19	19,926			-3,3	u
20	41,2			-0,2	s
21	45,5	22,8	0,2	0,3	s
22	8,96	0,46	-19,2	-4,9	u
23	42,8	6,42	0,0	0,0	s
26	53,1			1,2	s
27	39,6	4,71	-1,1	-0,5	s
28	48,2	13,1	0,8	0,6	s
29	46,9			0,5	s
30	48,9	12,3	0,9	0,7	s
31	49,1	7,79	1,4	0,8	s
35	50,4			0,9	s
37	39,21			-0,5	s
39	47,44			0,6	s
40	53,9	10,8	1,9	1,3	s
41	49,9			0,9	s
43	25	5	-5,9	-2,6	q
46	24,97			-2,6	q
47	25,6	5,13	-5,6	-2,5	q

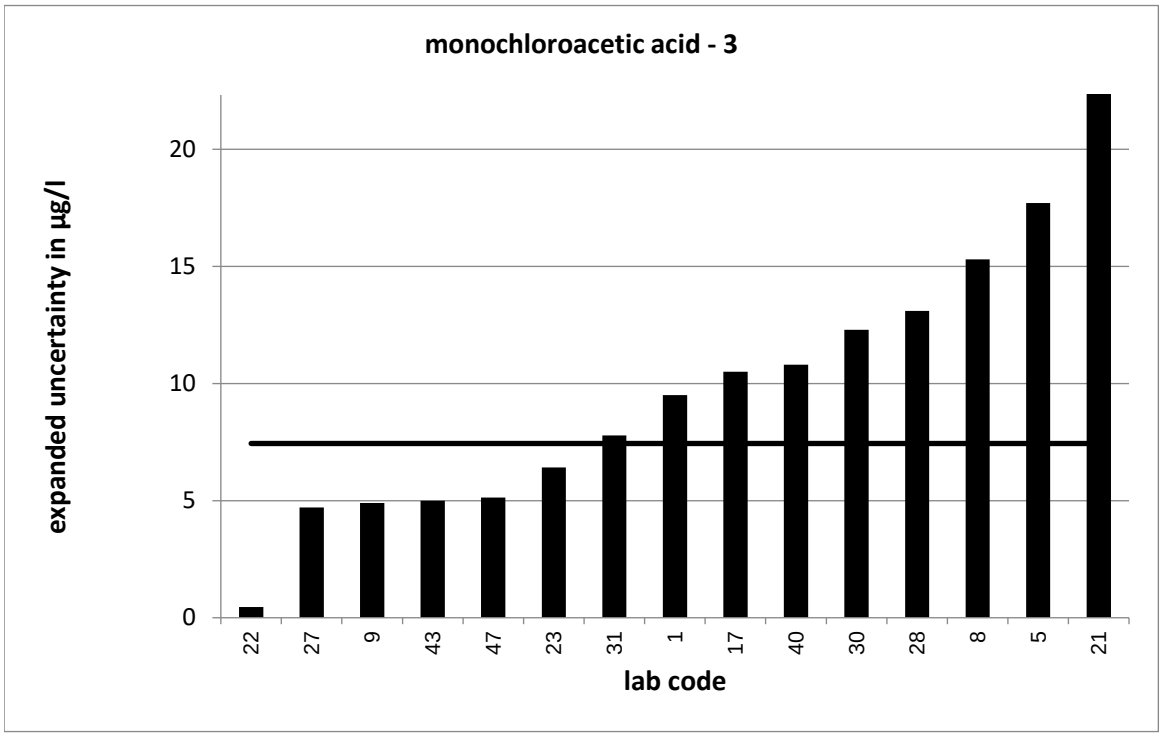
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor k=2 corresponding to a confidence level of about 95%

** s = satisfactory, q = questionable, u = unsatisfactory

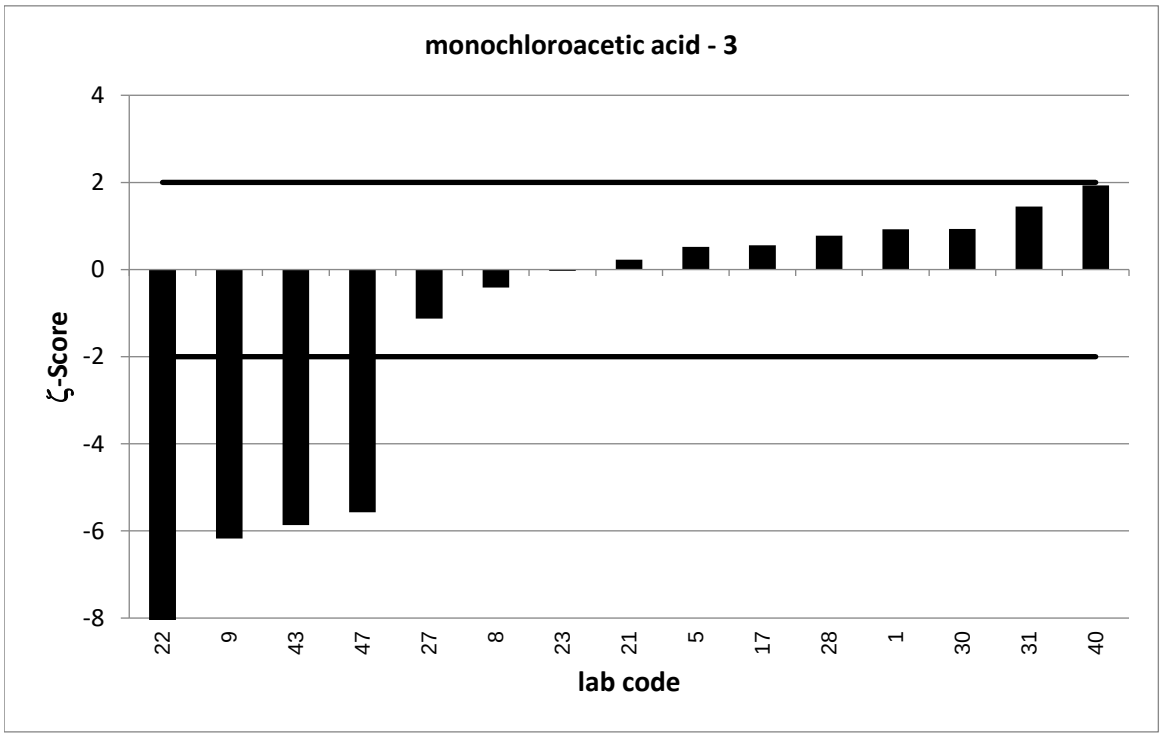


Strongly deviating values are not shown in the diagram.





Strongly deviating values are not correctly shown in the diagram.

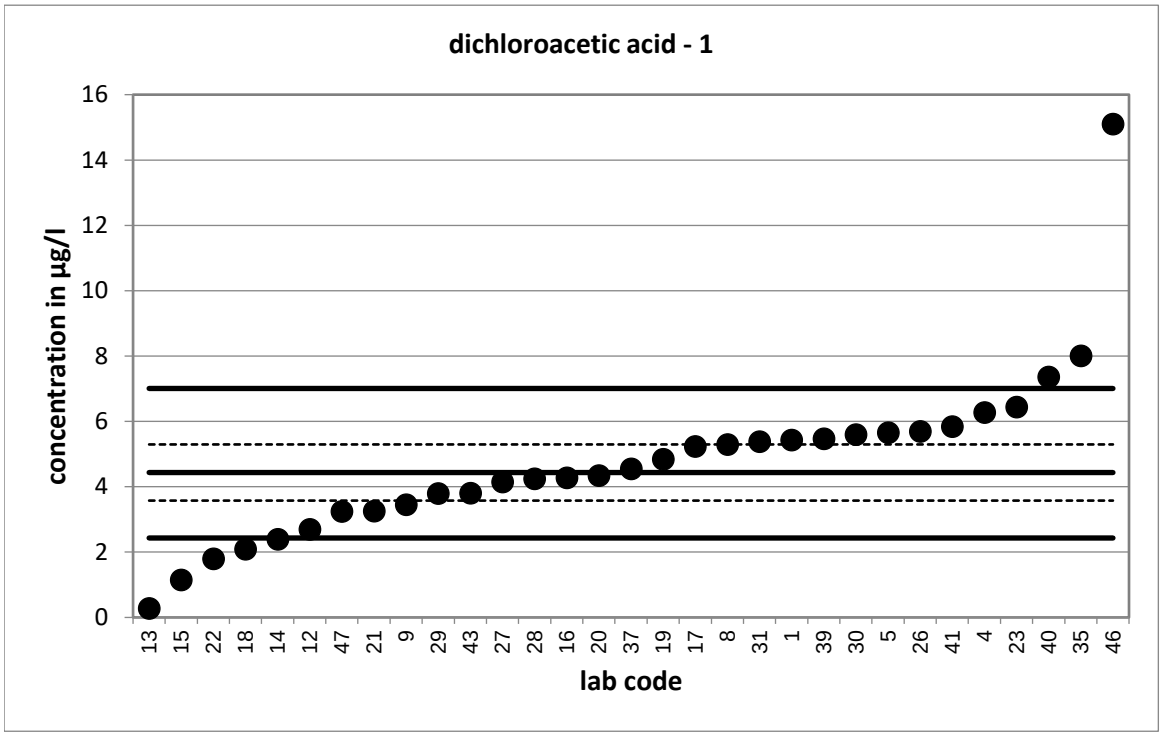


Strongly deviating values are not correctly shown in the diagram.

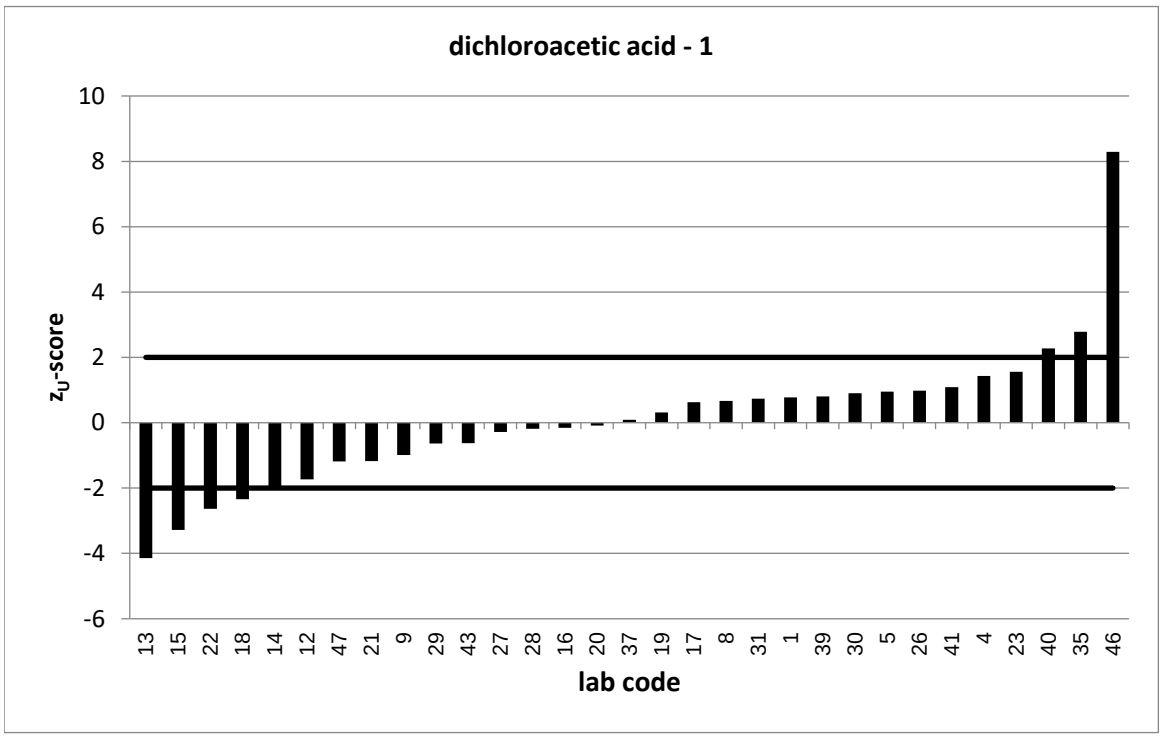
PT 7/23		dichloroacetic acid - 1			
assigned value [µg/l]*		4,436	± 0,859		
upper tolerance limit [µg/l]		7,008			
lower tolerance limit [µg/l]		2,431			
lab code	result [µg/l]	±	z-score	z_U-score	assessm.**
1	5,43	1,1	1,4	0,8	s
4	6,28			1,4	s
5	5,66	2,58	0,9	1,0	s
8	5,3	1,2	1,2	0,7	s
9	3,45	0,69	-1,8	-1,0	s
12	2,7			-1,7	s
13	0,283			-4,1	u
14	2,4			-2,0	s
15	1,15			-3,3	u
16	4,28			-0,2	s
17	5,24	1,12	1,1	0,6	s
18	2,09	0,209	-5,3	-2,3	q
19	4,846			0,3	s
20	4,35			-0,1	s
21	3,26	1,63	-1,3	-1,2	s
22	1,8	0,18	-6,0	-2,6	q
23	6,44	0,966	3,1	1,6	s
26	5,7			1,0	s
27	4,15	0,477	-0,6	-0,3	s
28	4,25	0,44	-0,4	-0,2	s
29	3,8			-0,6	s
30	5,6	1,4	1,4	0,9	s
31	5,38	0,76	1,6	0,7	s
35	8,01			2,8	q
37	4,55			0,1	s
39	5,47			0,8	s
40	7,36	2,8	2,0	2,3	q
41	5,84			1,1	s
43	3,81	0,76	-1,1	-0,6	s
46	15,1			8,3	u
47	3,25	0,651	-2,2	-1,2	s

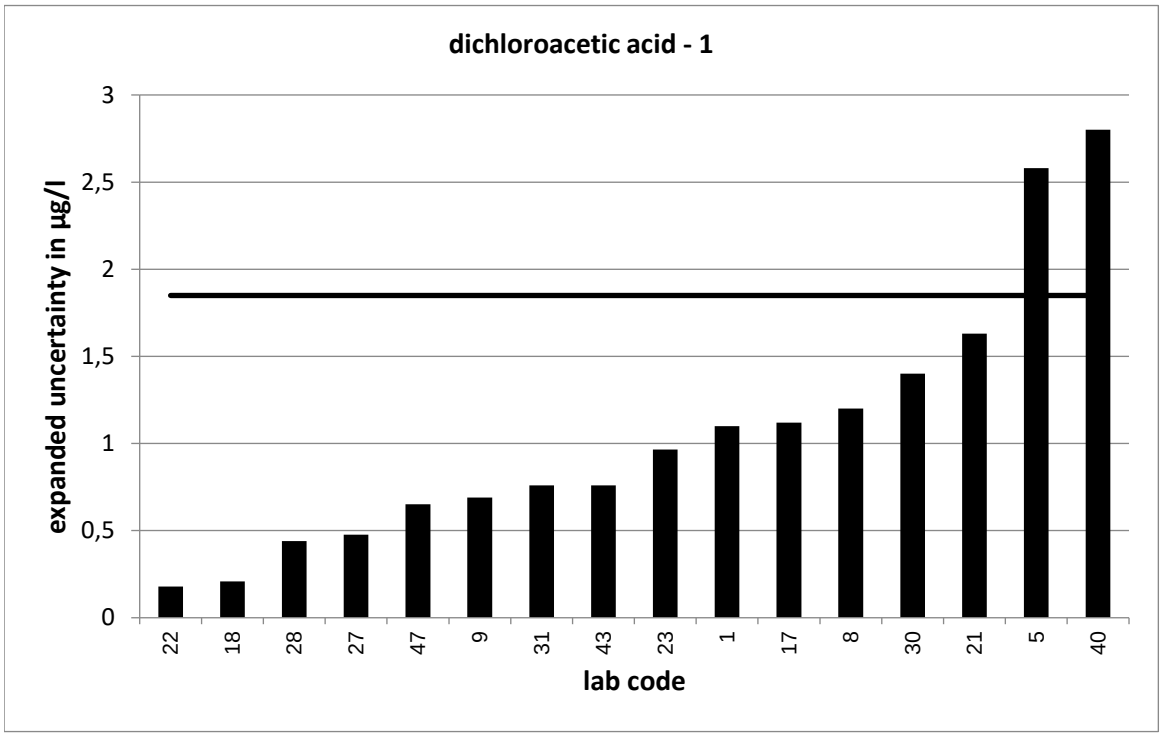
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor k=2 corresponding to a confidence level of about 95%

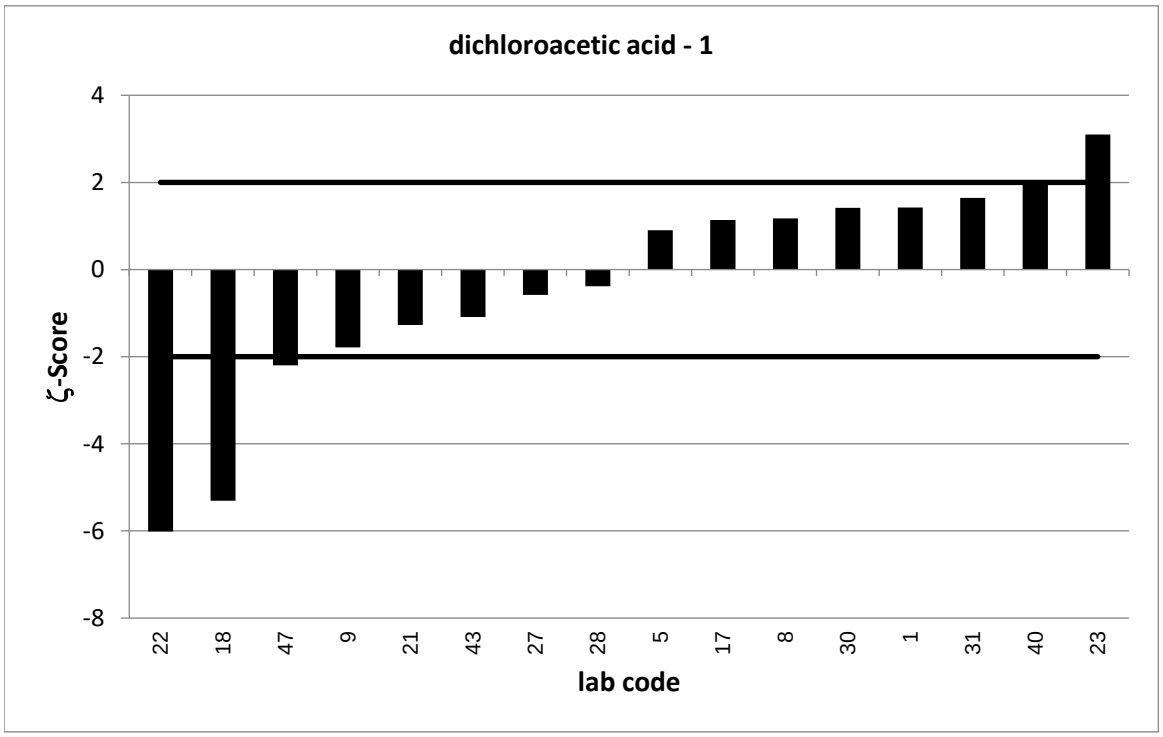
** s = satisfactory, q = questionable, u = unsatisfactory



Strongly deviating values are not shown in the diagram.



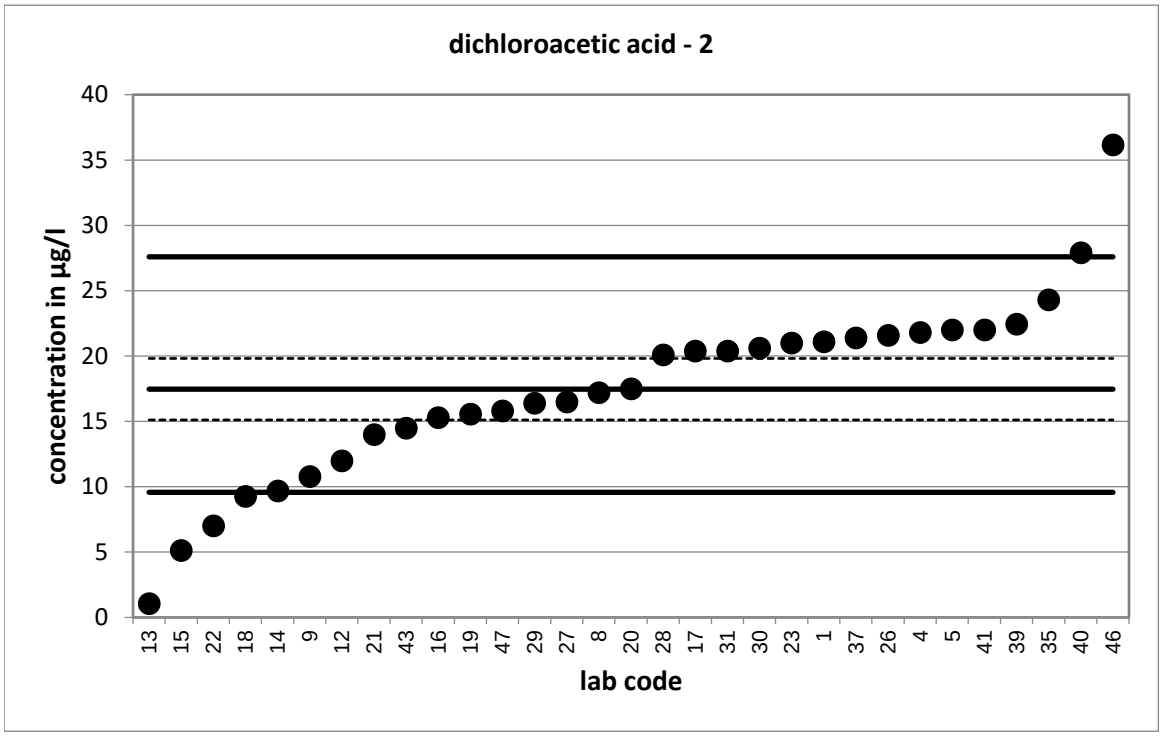

dichloroacetic acid - 1
expanded uncertainty in µg/l
3
2,5
2
1,5
1
0,5
0
22
18
28
27
47
9
31
43
23
1
17
8
30
21
5
40
lab code


dichloroacetic acid - 1
ζ-Score
4
2
0
-2
-4
-6
-8
22
18
47
9
21
43
27
28
5
17
8
30
1
31
40
23
lab code

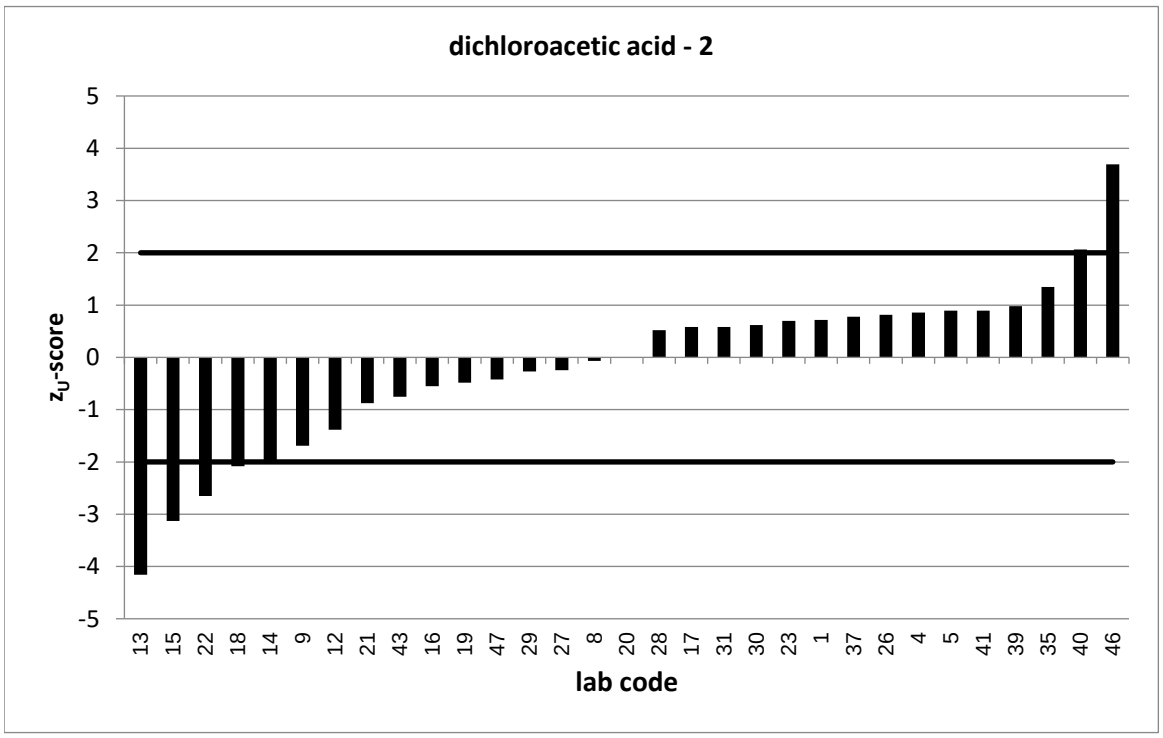
PT 7/23		dichloroacetic acid - 2			
assigned value [µg/l]*		17,47	± 2,35		
upper tolerance limit [µg/l]		27,59			
lower tolerance limit [µg/l]		9,574			
lab code	result [µg/l]	±	z-score	z_U-score	assessm.**
1	21,1	4,2	1,5	0,7	s
4	21,8			0,9	s
5	22	13,8	0,6	0,9	s
8	17,2	3,8	-0,1	-0,1	s
9	10,8	2,2	-4,1	-1,7	s
12	12			-1,4	s
13	1,07			-4,2	u
14	9,7			-2,0	s
15	5,12			-3,1	u
16	15,3			-0,5	s
17	20,4	2,2	1,8	0,6	s
18	9,26	0,926	-6,5	-2,1	q
19	15,565			-0,5	s
20	17,5			0,0	s
21	14	7	-0,9	-0,9	s
22	7,01	0,7	-8,5	-2,6	q
23	21	3,15	1,8	0,7	s
26	21,6			0,8	s
27	16,5	1,9	-0,6	-0,2	s
28	20,1	3,53	1,2	0,5	s
29	16,4			-0,3	s
30	20,6	5,15	1,1	0,6	s
31	20,4	2,87	1,6	0,6	s
35	24,3			1,3	s
37	21,4			0,8	s
39	22,44			1,0	s
40	27,9	10,6	1,9	2,1	q
41	22			0,9	s
43	14,5	2,9	-1,6	-0,8	s
46	36,16			3,7	u
47	15,8	3,17	-0,8	-0,4	s

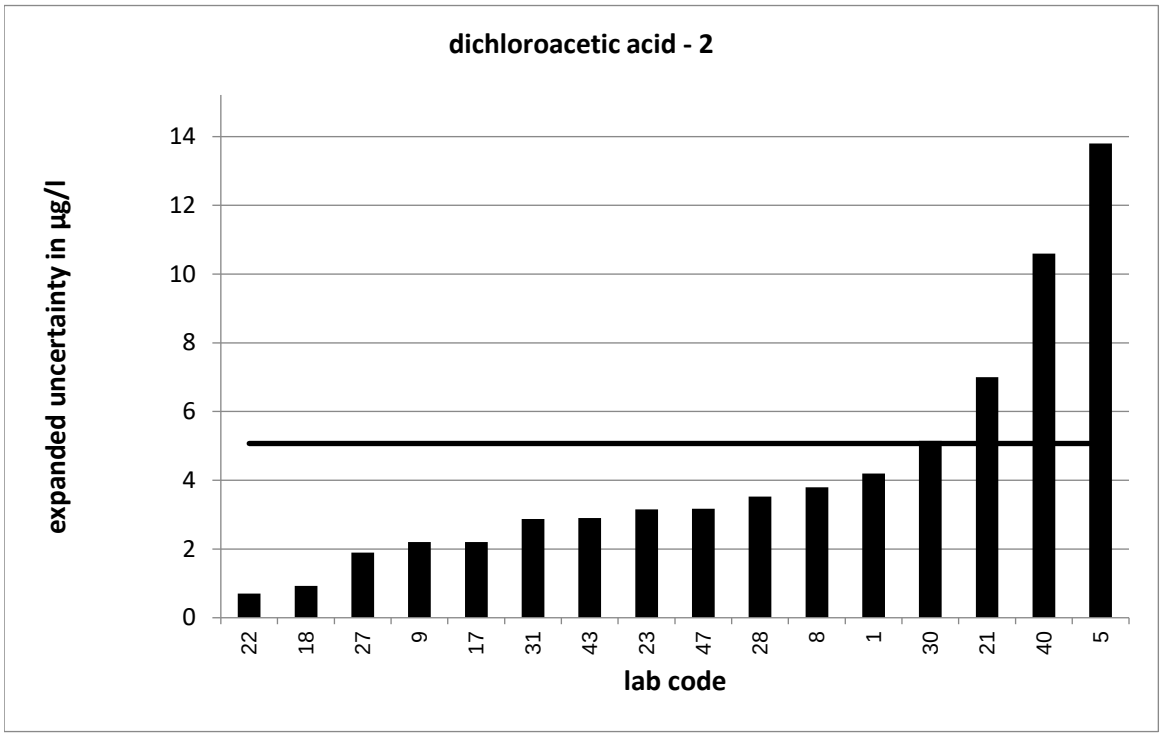
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor k=2 corresponding to a confidence level of about 95%

** s = satisfactory, q = questionable, u = unsatisfactory

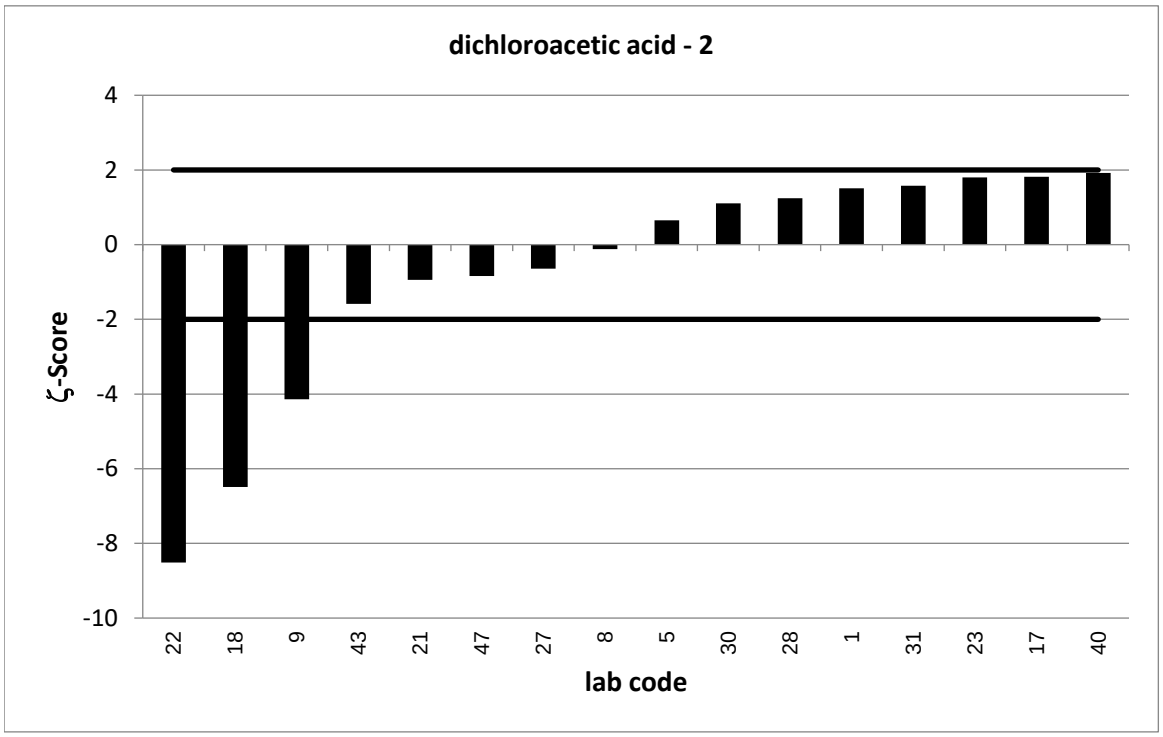


Strongly deviating values are not shown in the diagram.





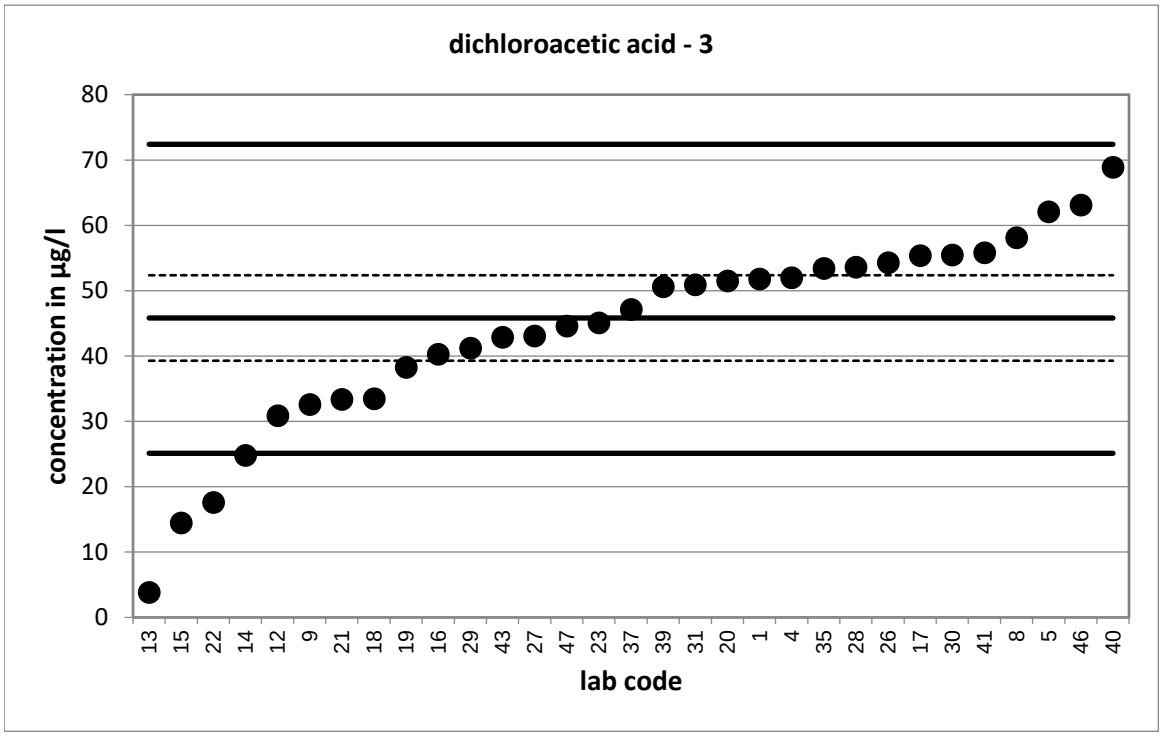
Strongly deviating values are not correctly shown in the diagram.



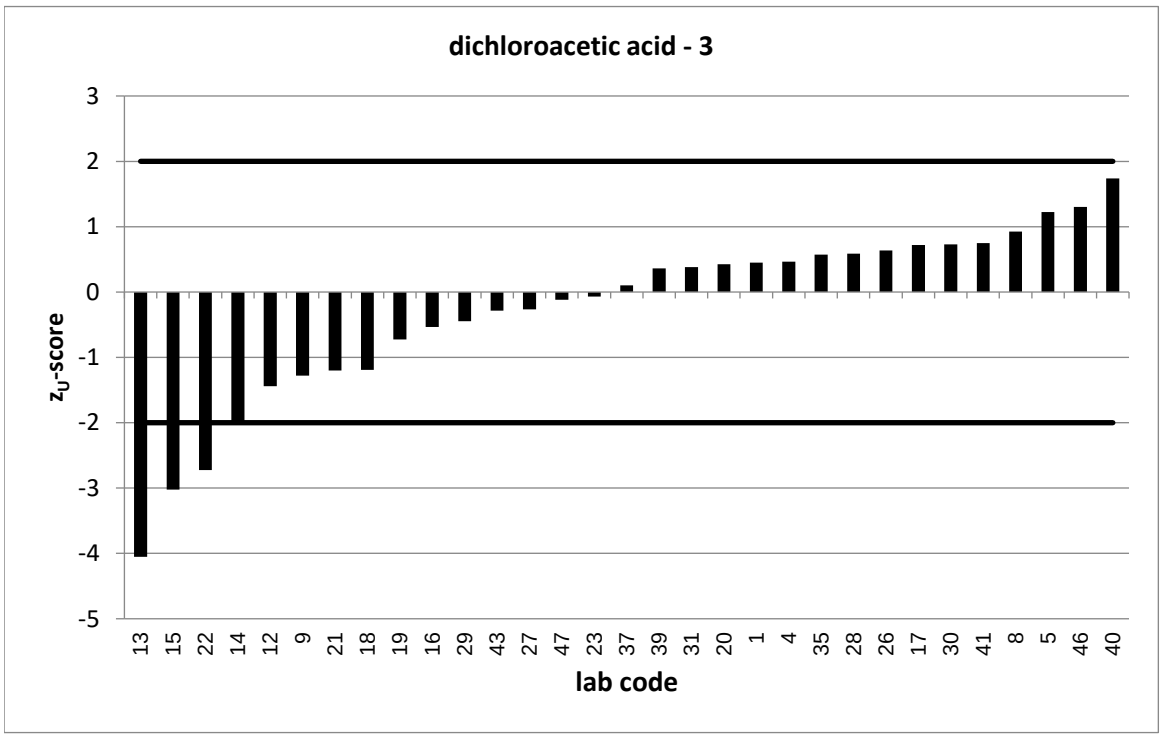
PT 7/23		dichloroacetic acid - 3			
assigned value [µg/l]*		45,83	± 6,54		
upper tolerance limit [µg/l]		72,4			
lower tolerance limit [µg/l]		25,12			
lab code	result [µg/l]	±	z-score	z_U-score	assessm.**
1	51,8	10	1,0	0,4	s
4	52			0,5	s
5	62,1	24	1,3	1,2	s
8	58,1	13	1,7	0,9	s
9	32,6	6,5	-2,9	-1,3	s
12	30,9			-1,4	s
13	3,85			-4,1	u
14	24,8			-2,0	s
15	14,5			-3,0	u
16	40,3			-0,5	s
17	55,4	4,91	2,3	0,7	s
18	33,5	3,35	-3,4	-1,2	s
19	38,308			-0,7	s
20	51,5			0,4	s
21	33,4	16,7	-1,4	-1,2	s
22	17,6	0,93	-8,5	-2,7	q
23	45,1	6,77	-0,2	-0,1	s
26	54,3			0,6	s
27	43,1	4,96	-0,7	-0,3	s
28	53,6	7,4	1,6	0,6	s
29	41,2			-0,4	s
30	55,5	13,9	1,3	0,7	s
31	50,9	7,14	1,0	0,4	s
35	53,4			0,6	s
37	47,16			0,1	s
39	50,63			0,4	s
40	68,9	26,2	1,7	1,7	s
41	55,8			0,8	s
43	42,9	8,6	-0,5	-0,3	s
46	63,11			1,3	s
47	44,6	8,92	-0,2	-0,1	s

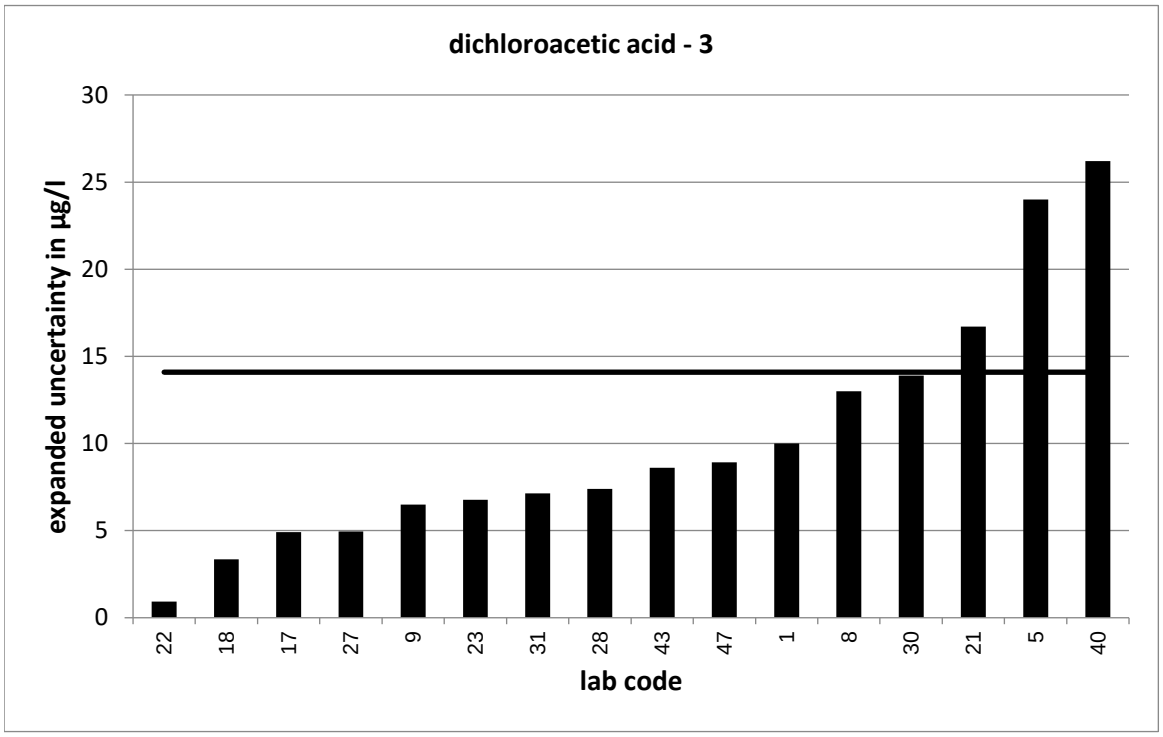
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor k=2 corresponding to a confidence level of about 95%

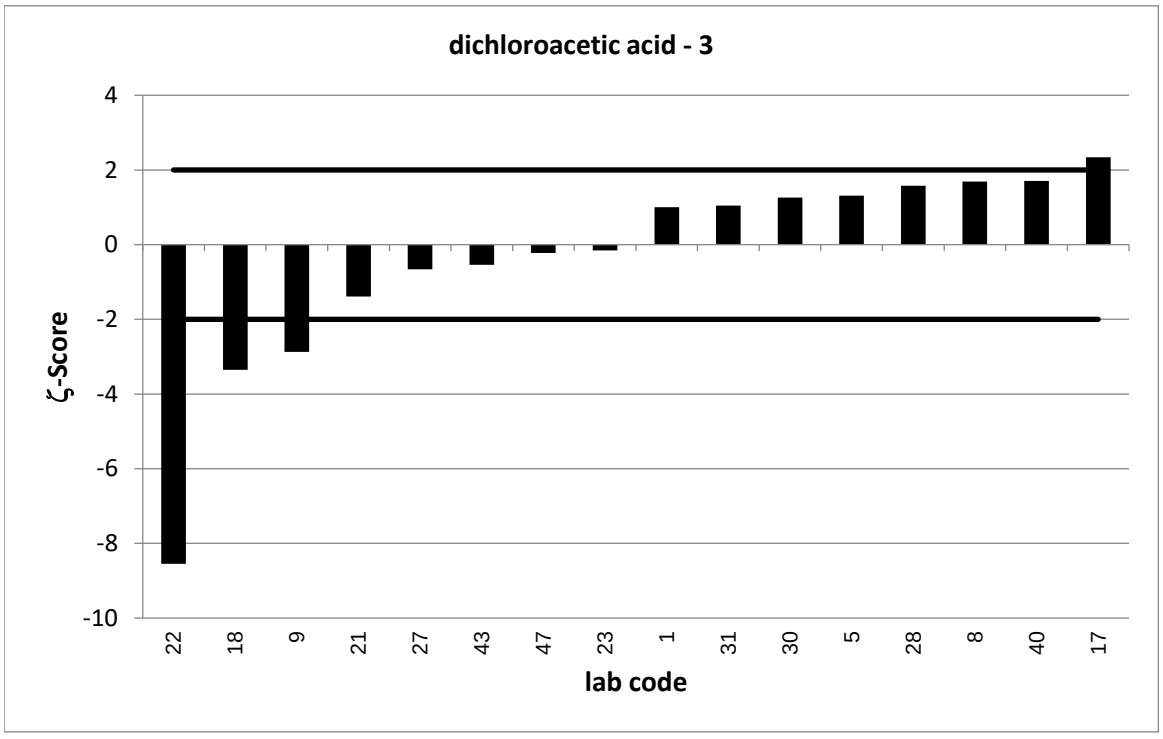
** s = satisfactory, q = questionable, u = unsatisfactory



Strongly deviating values are not shown in the diagram.



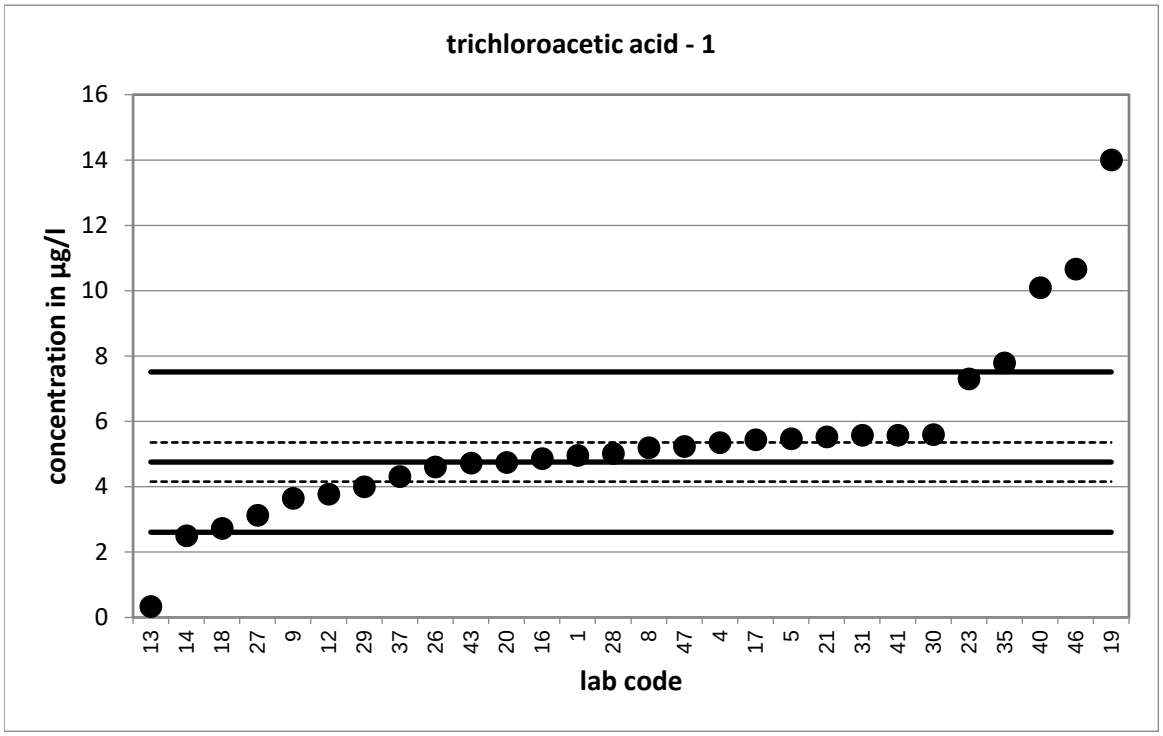

dichloroacetic acid - 3
expanded uncertainty in µg/l
30
25
20
15
10
5
0
22
18
17
27
9
23
31
28
43
47
1
8
30
21
5
40
lab code


dichloroacetic acid - 3
ζ-Score
4
2
0
-2
-4
-6
-8
-10
22
18
9
21
27
43
47
23
1
31
30
5
28
8
40
17
lab code

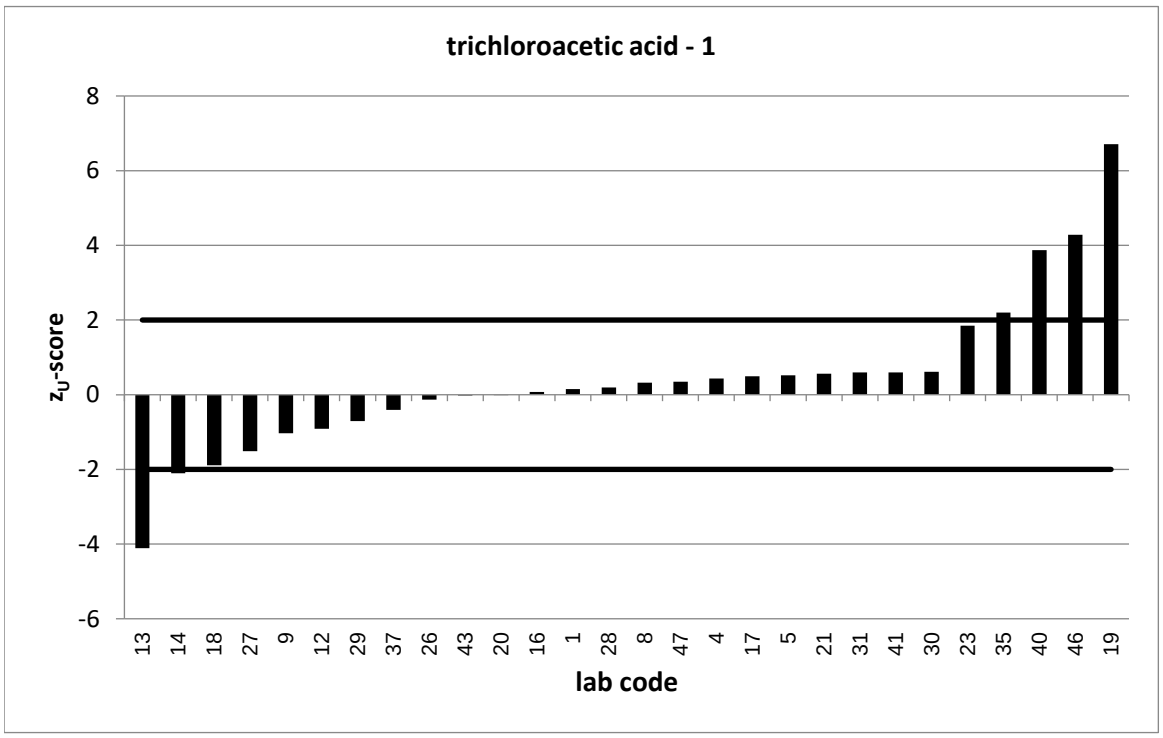
PT 7/23		trichloroacetic acid - 1			
assigned value [µg/l]*		4,756	± 0,599		
upper tolerance limit [µg/l]		7,514			
lower tolerance limit [µg/l]		2,607			
lab code	result [µg/l]	±	z-score	z_U-score	assessm.**
1	4,96	1	0,3	0,1	s
4	5,35			0,4	s
5	5,47	1,96	0,7	0,5	s
8	5,2	1,2	0,7	0,3	s
9	3,65	0,73	-2,3	-1,0	s
12	3,78			-0,9	s
13	0,343			-4,1	u
14	2,5			-2,1	q
16	4,86			0,1	s
17	5,44	1,11	1,1	0,5	s
18	2,73	0,409	-5,6	-1,9	s
19	14,007			6,7	u
20	4,75			0,0	s
21	5,53	2,77	0,5	0,6	s
23	7,3	1,46	3,2	1,8	s
26	4,61			-0,1	s
27	3,13	0,332	-4,7	-1,5	s
28	5,02	1,36	0,4	0,2	s
29	4			-0,7	s
30	5,6	1,4	1,1	0,6	s
31	5,58	0,24	2,6	0,6	s
35	7,79			2,2	q
37	4,32			-0,4	s
40	10,1	4,55	2,3	3,9	u
41	5,58			0,6	s
43	4,73	0,95	0,0	0,0	s
46	10,66			4,3	u
47	5,24	1,05	0,8	0,4	s

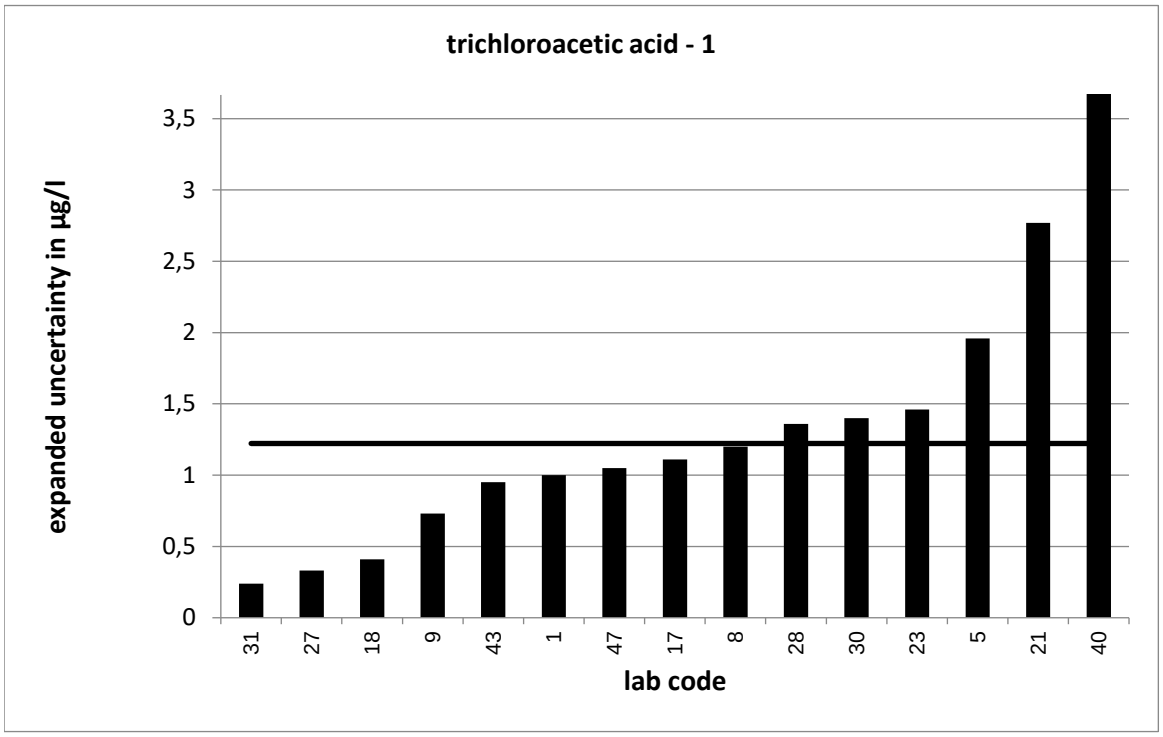
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor k=2 corresponding to a confidence level of about 95%

** s = satisfactory, q = questionable, u = unsatisfactory

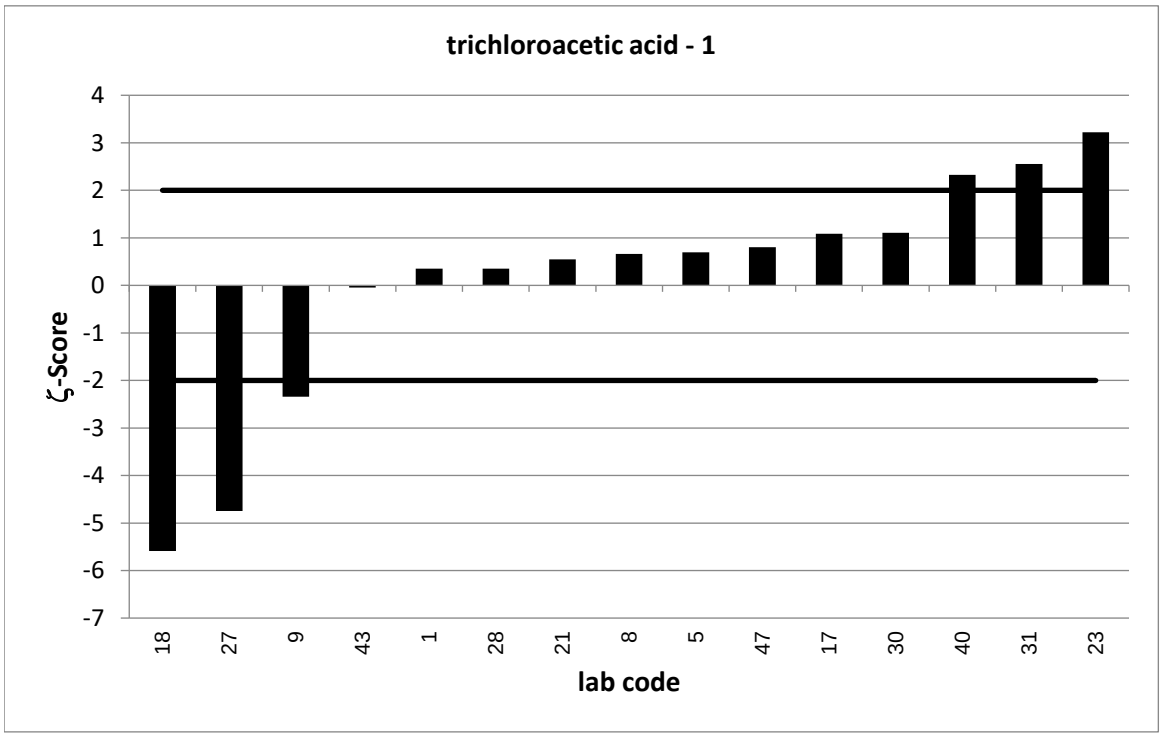


Strongly deviating values are not shown in the diagram.





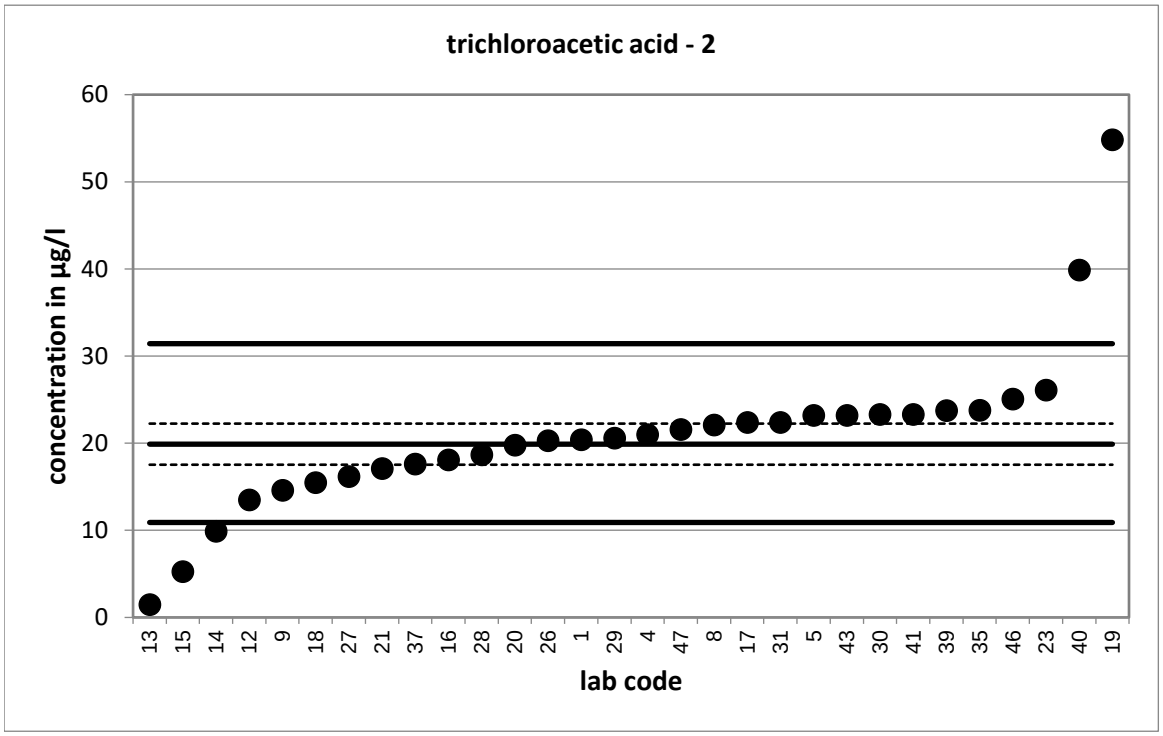
Strongly deviating values are not correctly shown in the diagram.



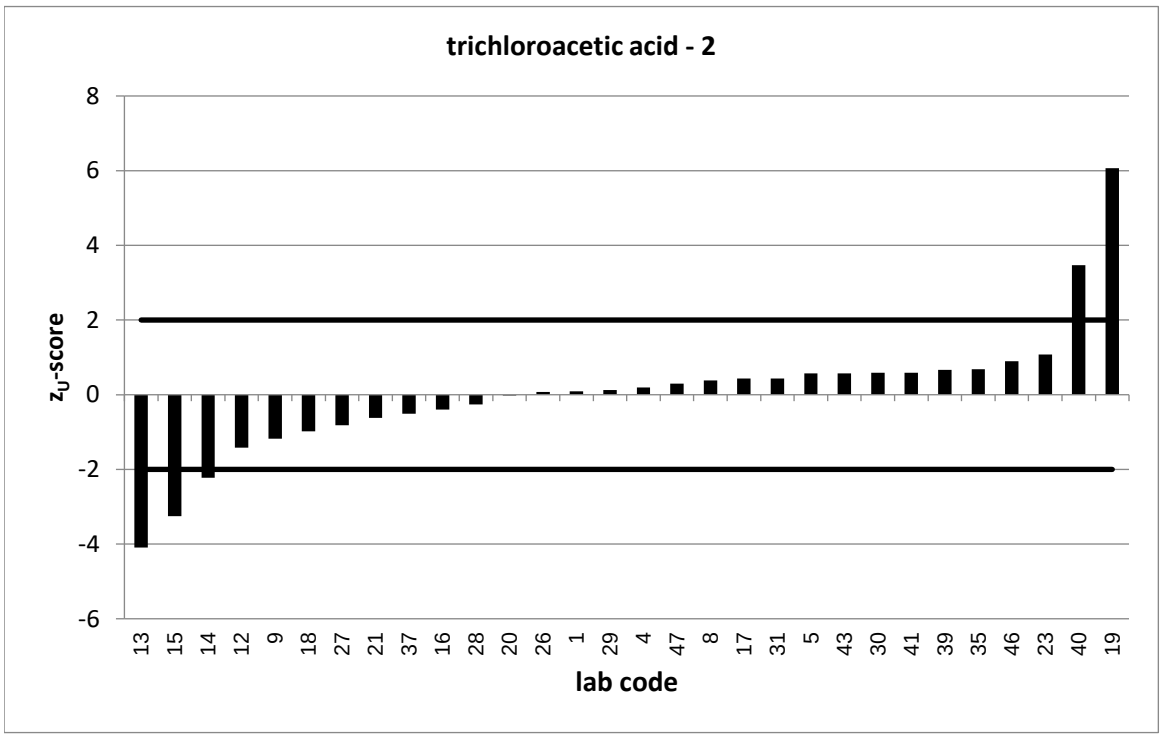
PT 7/23		trichloroacetic acid - 2			
assigned value [µg/l]*		19,89	± 2,36		
upper tolerance limit [µg/l]		31,42			
lower tolerance limit [µg/l]		10,9			
lab code	result [µg/l]	±	z-score	z_U-score	assessm.**
1	20,4	4,1	0,2	0,1	s
4	21			0,2	s
5	23,2	9,8	0,7	0,6	s
8	22,1	5	0,8	0,4	s
9	14,6	2,9	-2,8	-1,2	s
12	13,5			-1,4	s
13	1,5			-4,1	u
14	9,9			-2,2	q
15	5,26			-3,3	u
16	18,1			-0,4	s
17	22,4	3,44	1,2	0,4	s
18	15,5	2,33	-2,6	-1,0	s
19	54,845			6,1	u
20	19,8			0,0	s
21	17,1	8,55	-0,6	-0,6	s
23	26,1	5,2	2,2	1,1	s
26	20,3			0,1	s
27	16,2	1,72	-2,5	-0,8	s
28	18,7	4,74	-0,4	-0,3	s
29	20,6			0,1	s
30	23,3	5,83	1,1	0,6	s
31	22,4	0,95	2,0	0,4	s
35	23,8			0,7	s
37	17,62			-0,5	s
39	23,74			0,7	s
40	39,9	18	2,2	3,5	u
41	23,3			0,6	s
43	23,2	4,6	1,3	0,6	s
46	25,08			0,9	s
47	21,6	4,33	0,7	0,3	s

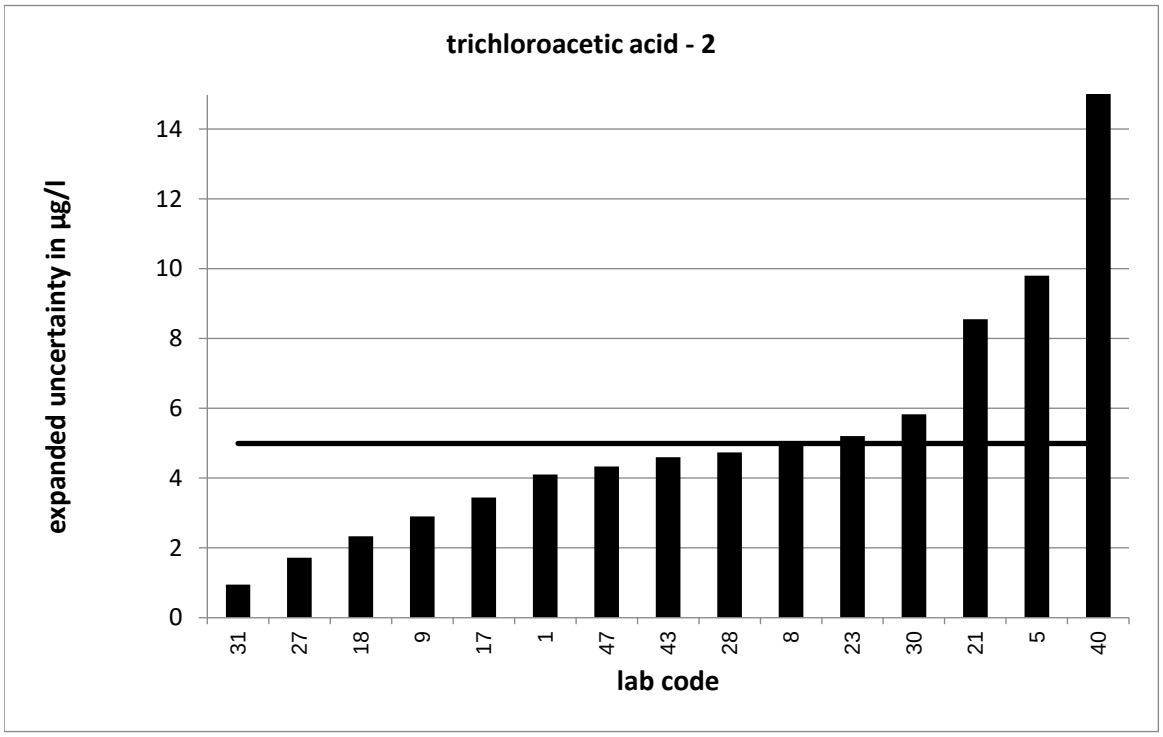
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor k=2 corresponding to a confidence level of about 95%

** s = satisfactory, q = questionable, u = unsatisfactory

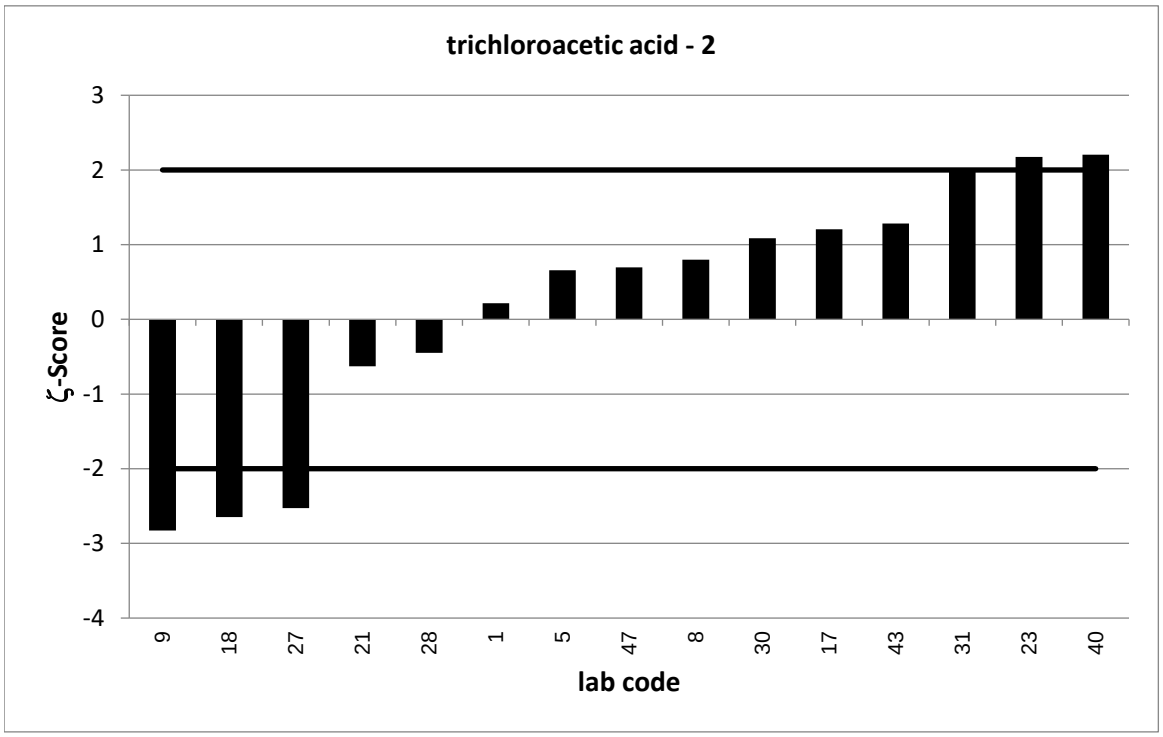


Strongly deviating values are not shown in the diagram.





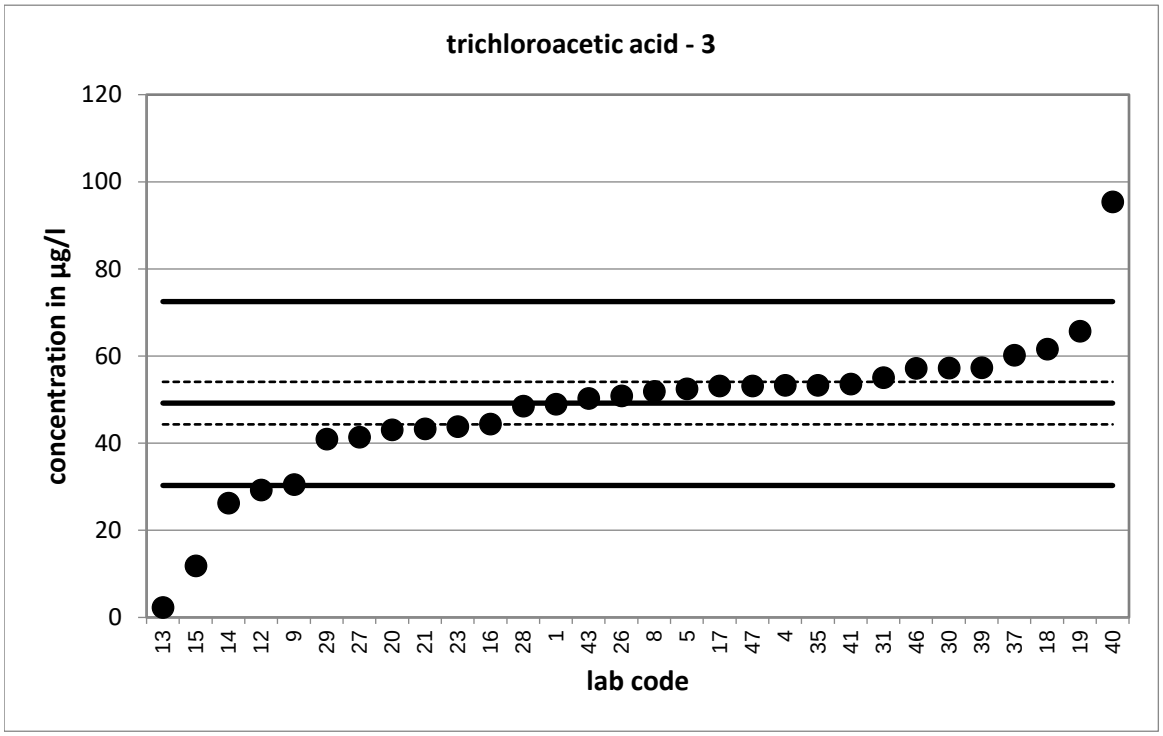
Strongly deviating values are not correctly shown in the diagram.



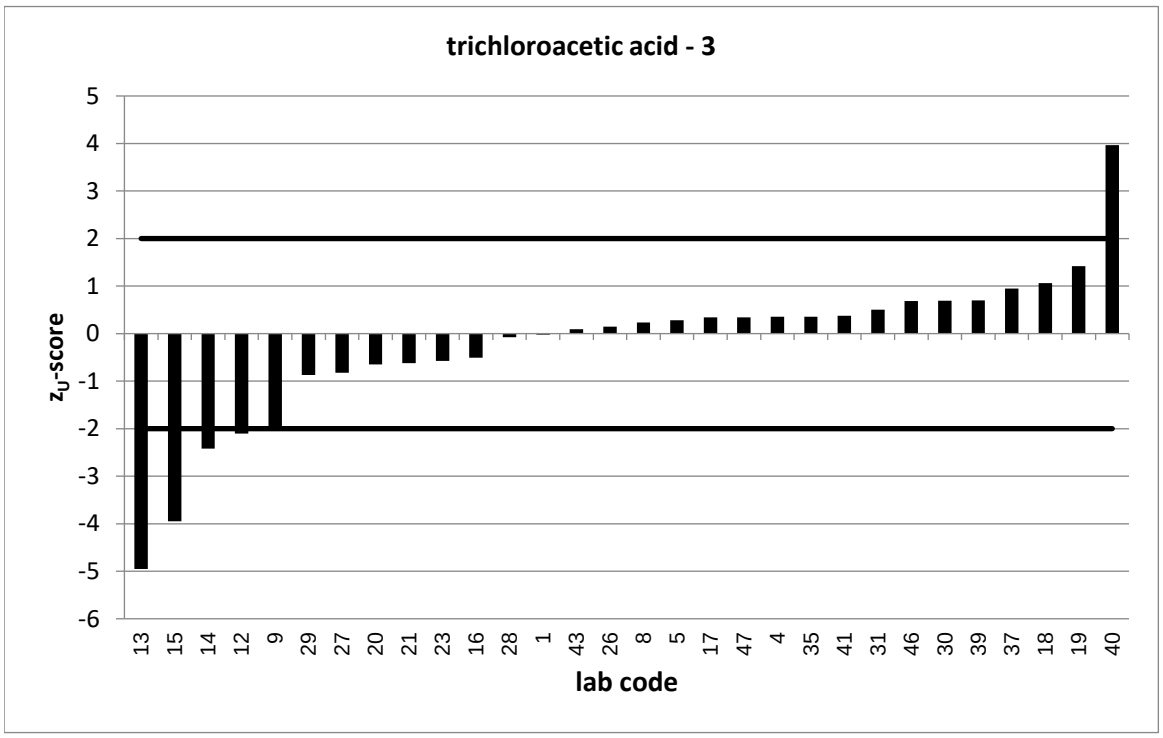
PT 7/23		trichloroacetic acid - 3			
assigned value [µg/l]*		49,2	± 4,88		
upper tolerance limit [µg/l]		72,5			
lower tolerance limit [µg/l]		30,29			
lab code	result [µg/l]	±	z-score	z_U-score	assessm.**
1	49	9,8	0,0	0,0	s
4	53,3			0,4	s
5	52,5	18,5	0,3	0,3	s
8	51,9	11,8	0,4	0,2	s
9	30,5	6,1	-4,8	-2,0	s
12	29,3			-2,1	q
13	2,35			-5,0	u
14	26,3			-2,4	q
15	11,9			-3,9	u
16	44,4			-0,5	s
17	53,2	4,74	1,2	0,3	s
18	61,6	9,24	2,4	1,1	s
19	65,734			1,4	s
20	43,1			-0,6	s
21	43,3	21,7	-0,5	-0,6	s
23	43,8	8,76	-1,1	-0,6	s
26	50,9			0,1	s
27	41,4	4,39	-2,4	-0,8	s
28	48,5	9,05	-0,1	-0,1	s
29	41			-0,9	s
30	57,3	14,3	1,1	0,7	s
31	55,1	2,33	2,2	0,5	s
35	53,3			0,4	s
37	60,24			0,9	s
39	57,37			0,7	s
40	95,4	42,9	2,1	4,0	u
41	53,6			0,4	s
43	50,3	10	0,2	0,1	s
46	57,22			0,7	s
47	53,2	10,6	0,7	0,3	s

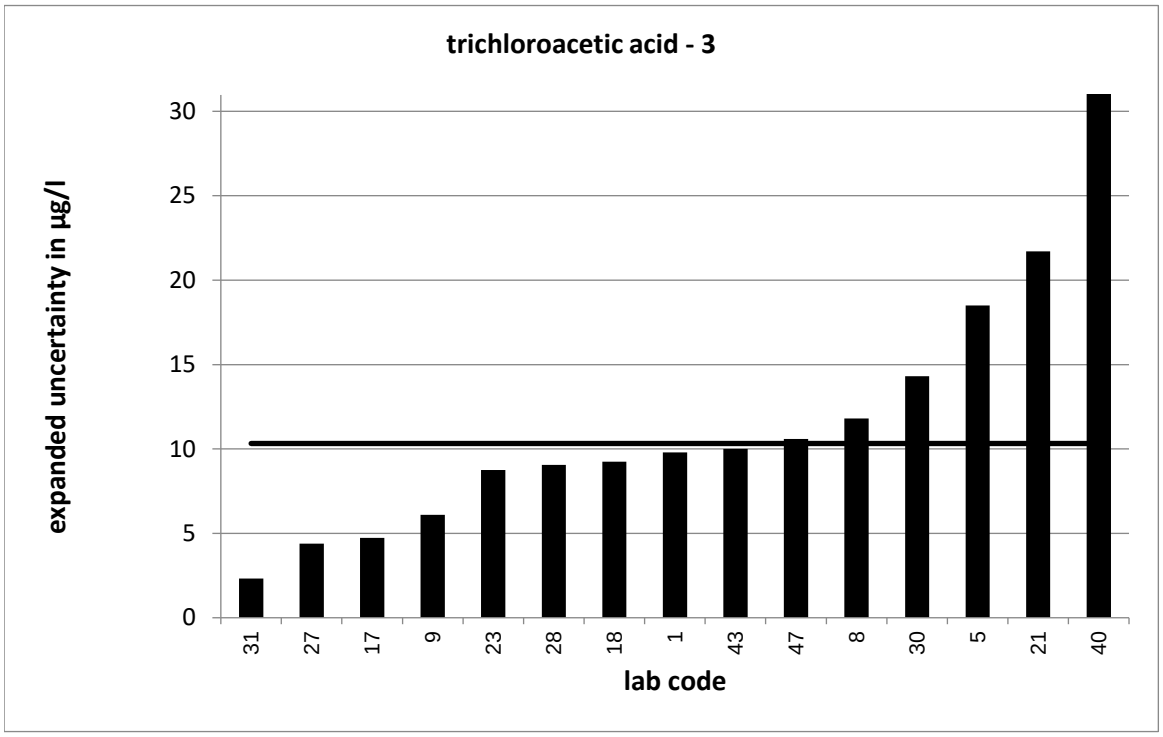
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor k=2 corresponding to a confidence level of about 95%

** s = satisfactory, q = questionable, u = unsatisfactory

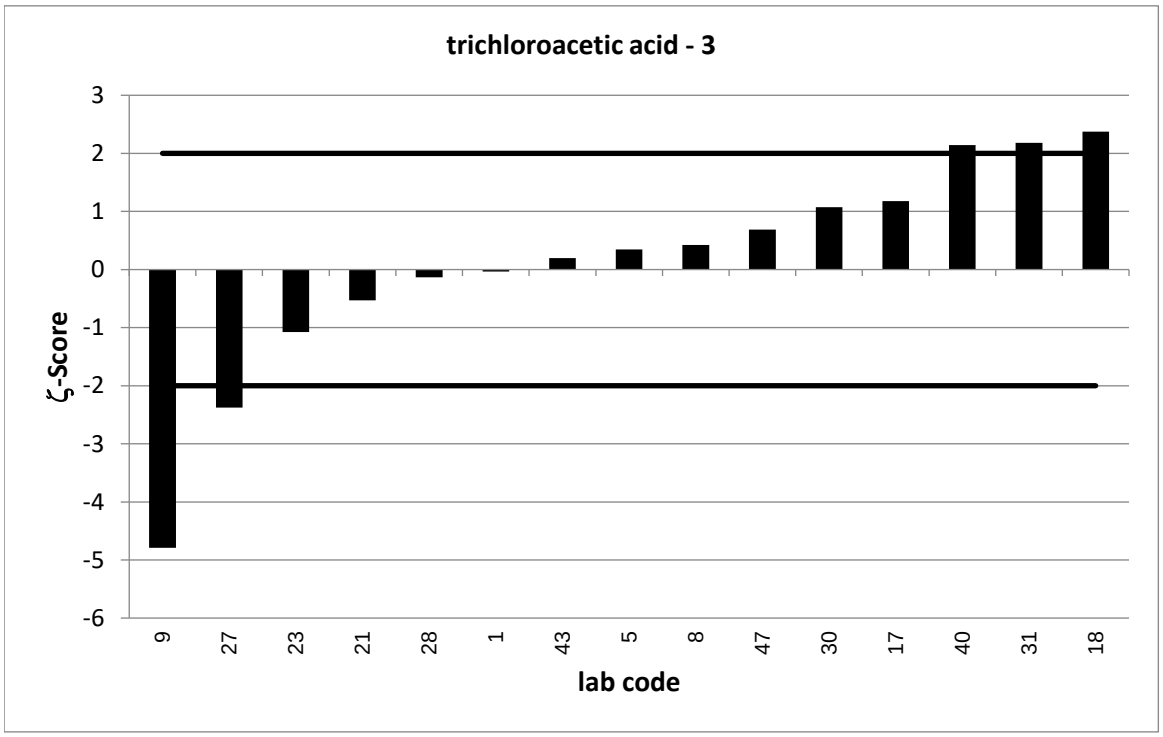


Strongly deviating values are not shown in the diagram.





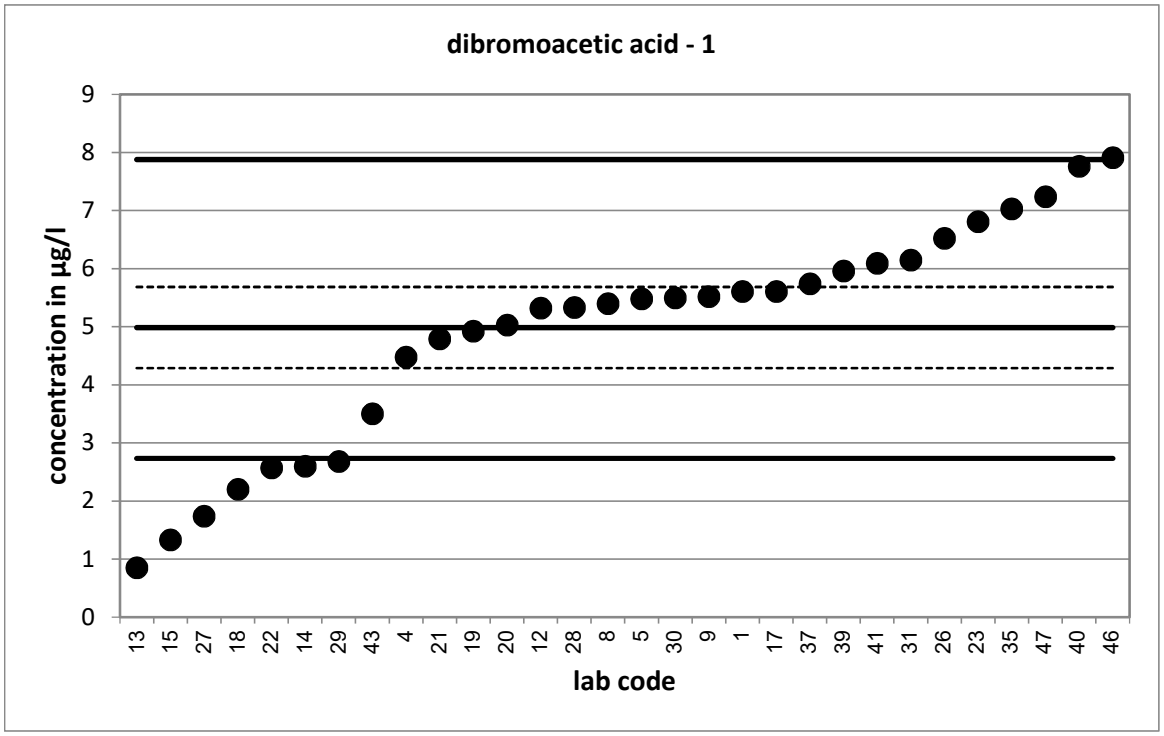
Strongly deviating values are not correctly shown in the diagram.



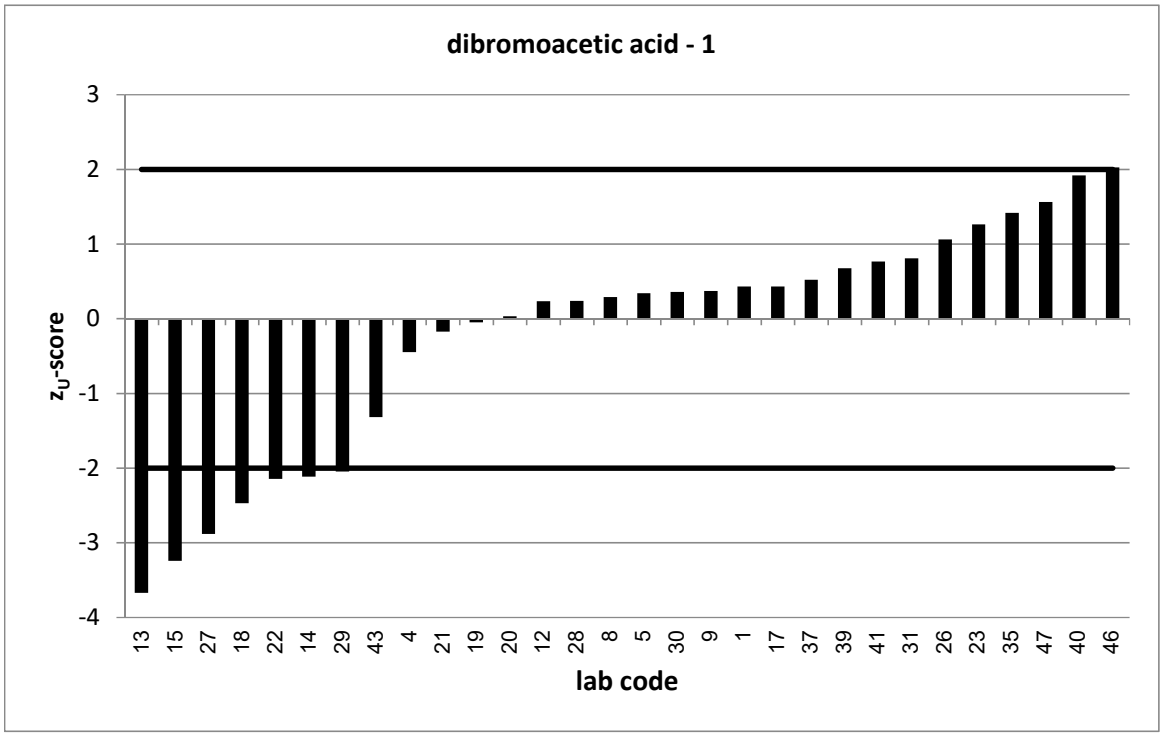
PT 7/23		dibromoacetic acid - 1			
assigned value [µg/l]*		4,986	± 0,699		
upper tolerance limit [µg/l]		7,876			
lower tolerance limit [µg/l]		2,733			
lab code	result [µg/l]	±	ζ-score	z_U-score	assessm.**
1	5,61	1,1	1,0	0,4	s
4	4,48			-0,4	s
5	5,48	1,68	0,5	0,3	s
8	5,4	1,1	0,6	0,3	s
9	5,52	1,1	0,8	0,4	s
12	5,32			0,2	s
13	0,849			-3,7	u
14	2,6			-2,1	q
15	1,33			-3,2	u
17	5,61	0,434	1,5	0,4	s
18	2,2	0,991	-4,6	-2,5	q
19	4,927			-0,1	s
20	5,03			0,0	s
21	4,79	2,4	-0,2	-0,2	s
22	2,57	0,12	-6,8	-2,1	q
23	6,81	1,022	2,9	1,3	s
26	6,52			1,1	s
27	1,74			-2,9	q
28	5,33	0,6	0,7	0,2	s
29	2,68			-2,0	s
30	5,5	1,38	0,7	0,4	s
31	6,15	1,05	1,8	0,8	s
35	7,03			1,4	s
37	5,74			0,5	s
39	5,96			0,7	s
40	7,76	2,25	2,4	1,9	s
41	6,09			0,8	s
43	3,5	0,7	-3,0	-1,3	s
46	7,91			2,0	s
47	7,24	1,45	2,8	1,6	s

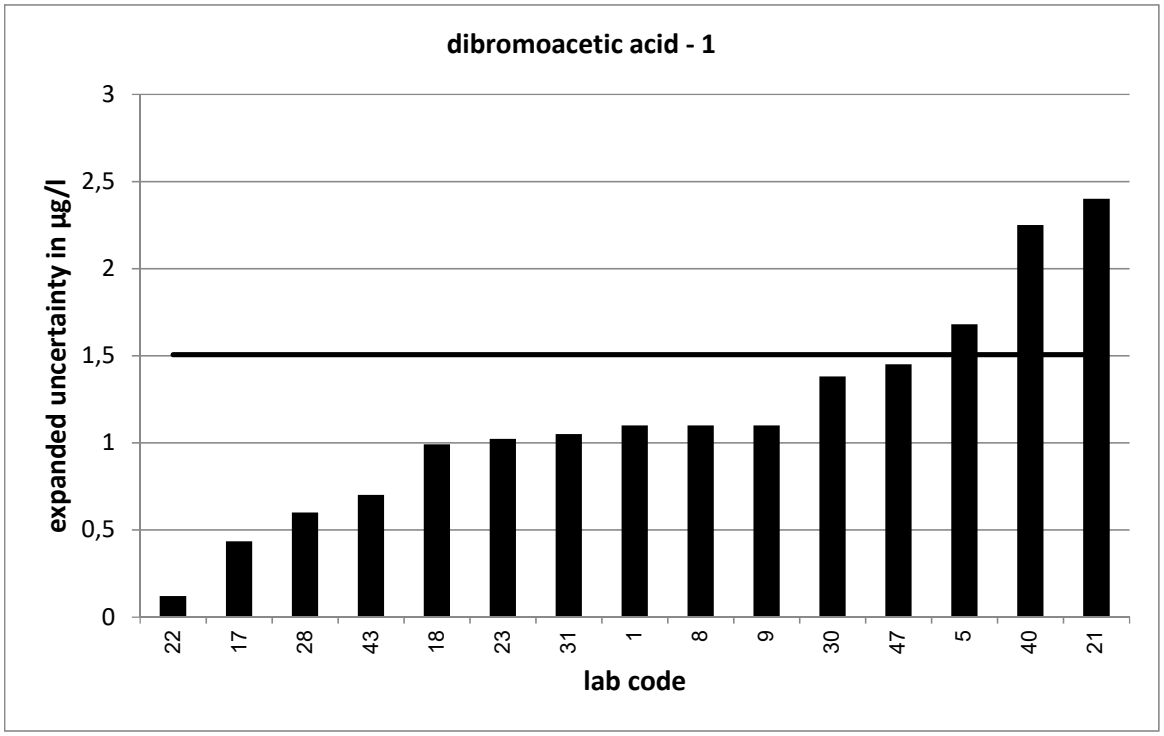
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor k=2 corresponding to a confidence level of about 95%

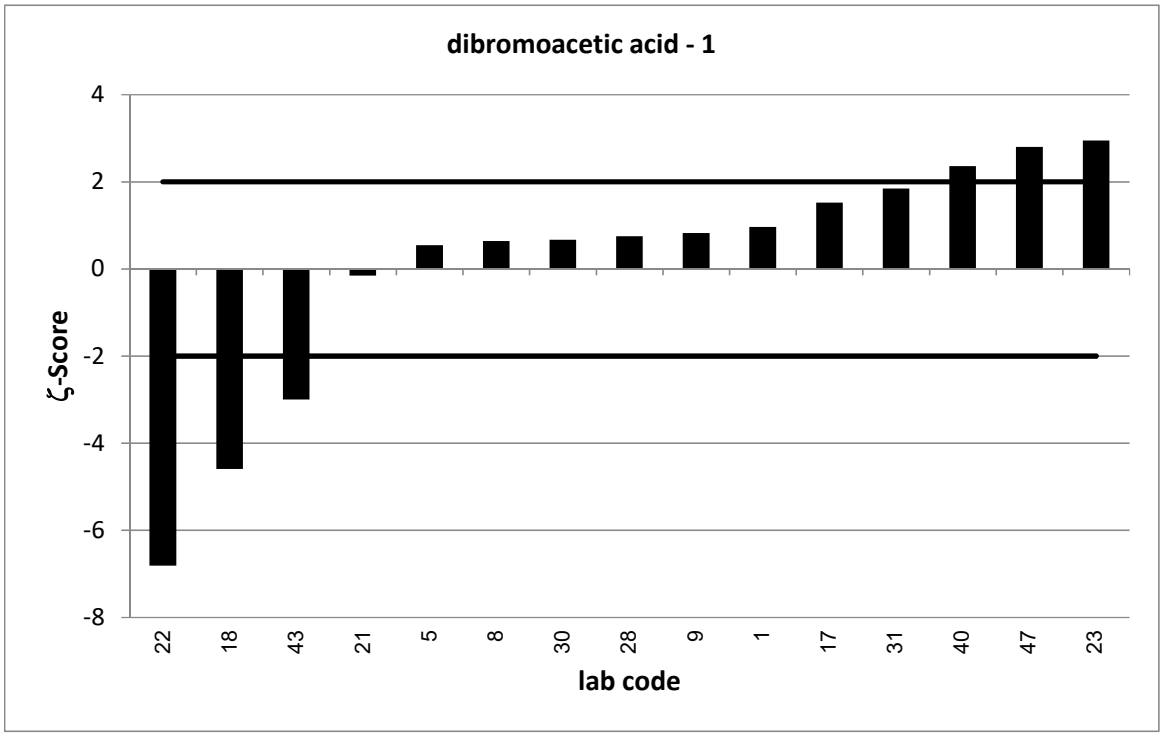
** s = satisfactory, q = questionable, u = unsatisfactory



Strongly deviating values are not shown in the diagram.



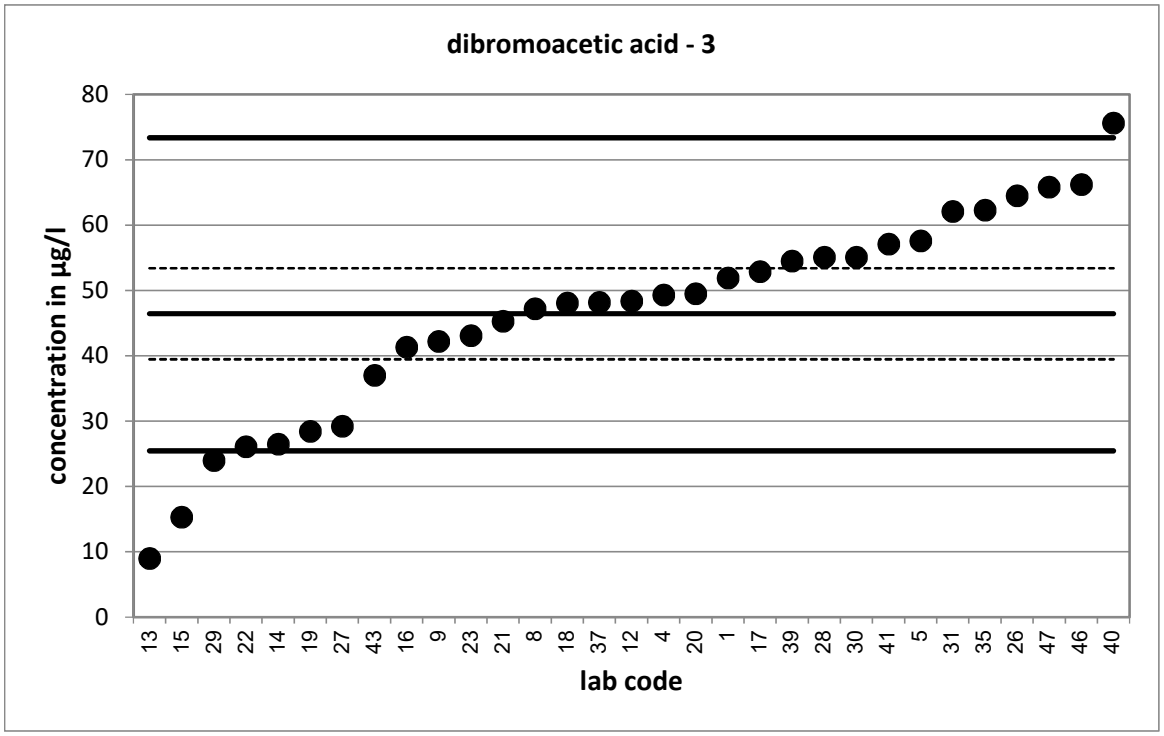

dibromoacetic acid - 1
expanded uncertainty in µg/l
3
2,5
2
1,5
1
0,5
0
22
17
28
43
18
23
31
1
8
9
30
47
5
40
21
lab code


dibromoacetic acid - 1
ζ-Score
4
2
0
-2
-4
-6
-8
22
18
43
21
5
8
30
28
9
1
17
31
40
47
23
lab code

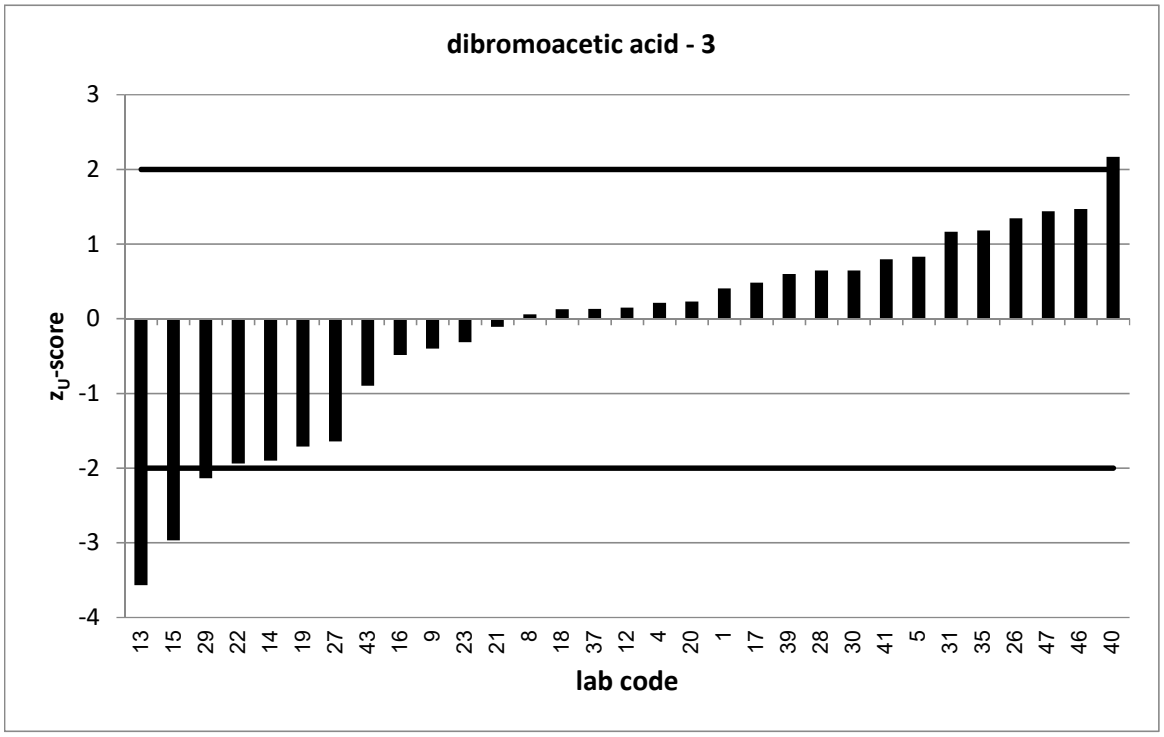
PT 7/23		dibromoacetic acid - 3			
assigned value [µg/l]*		46,43	± 6,97		
upper tolerance limit [µg/l]		73,36			
lower tolerance limit [µg/l]		25,45			
lab code	result [µg/l]	±	ζ-score	z_U-score	assessm.**
1	51,9	10	0,9	0,4	s
4	49,3			0,2	s
5	57,6	15,2	1,3	0,8	s
8	47,2	10	0,1	0,1	s
9	42,2	8,4	-0,8	-0,4	s
12	48,4			0,1	s
13	8,99			-3,6	u
14	26,5			-1,9	s
15	15,3			-3,0	u
16	41,3			-0,5	s
17	52,9	8,13	1,2	0,5	s
18	48,1	21,6	0,1	0,1	s
19	28,447			-1,7	s
20	49,5			0,2	s
21	45,3	22,7	-0,1	-0,1	s
22	26,1	0,79	-5,8	-1,9	s
23	43,1	6,465	-0,7	-0,3	s
26	64,5			1,3	s
27	29,2	3,65	-4,4	-1,6	s
28	55,1	11,6	1,3	0,6	s
29	24			-2,1	q
30	55,1	13,8	1,1	0,6	s
31	62,1	10,6	2,5	1,2	s
35	62,3			1,2	s
37	48,18			0,1	s
39	54,5			0,6	s
40	75,6	21,92	2,5	2,2	q
41	57,1			0,8	s
43	37	7,4	-1,9	-0,9	s
46	66,2			1,5	s
47	65,8	13,2	2,6	1,4	s

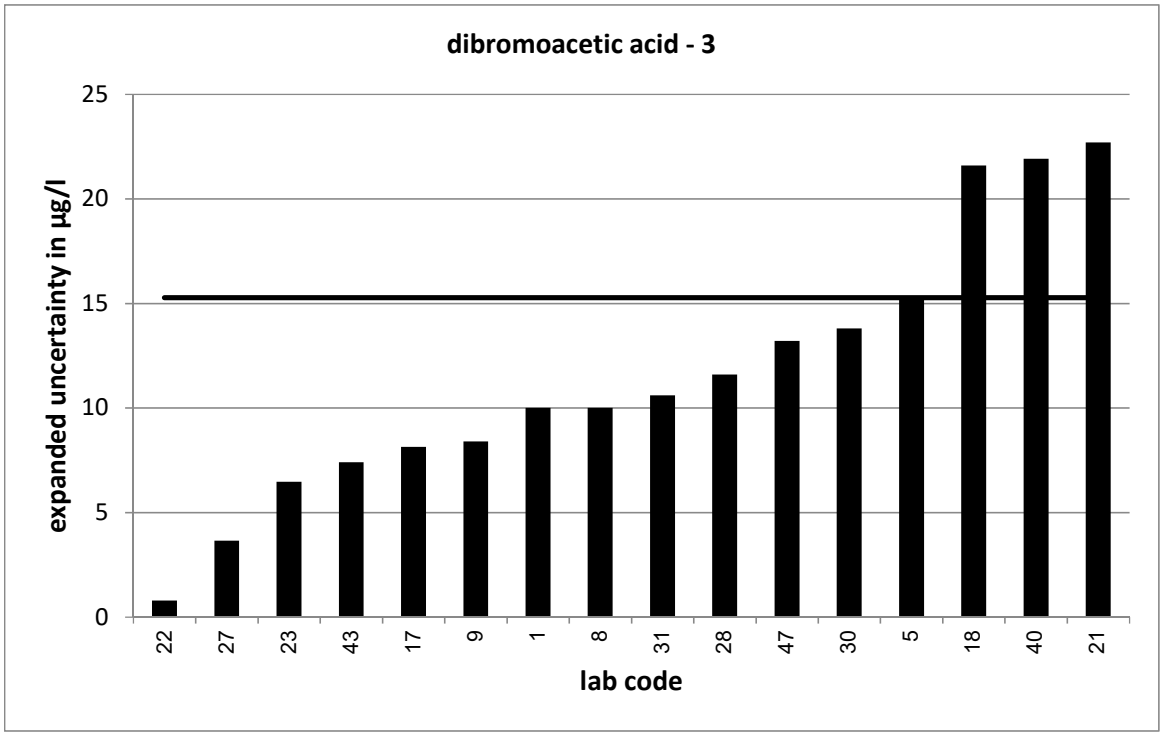
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor k=2 corresponding to a confidence level of about 95%

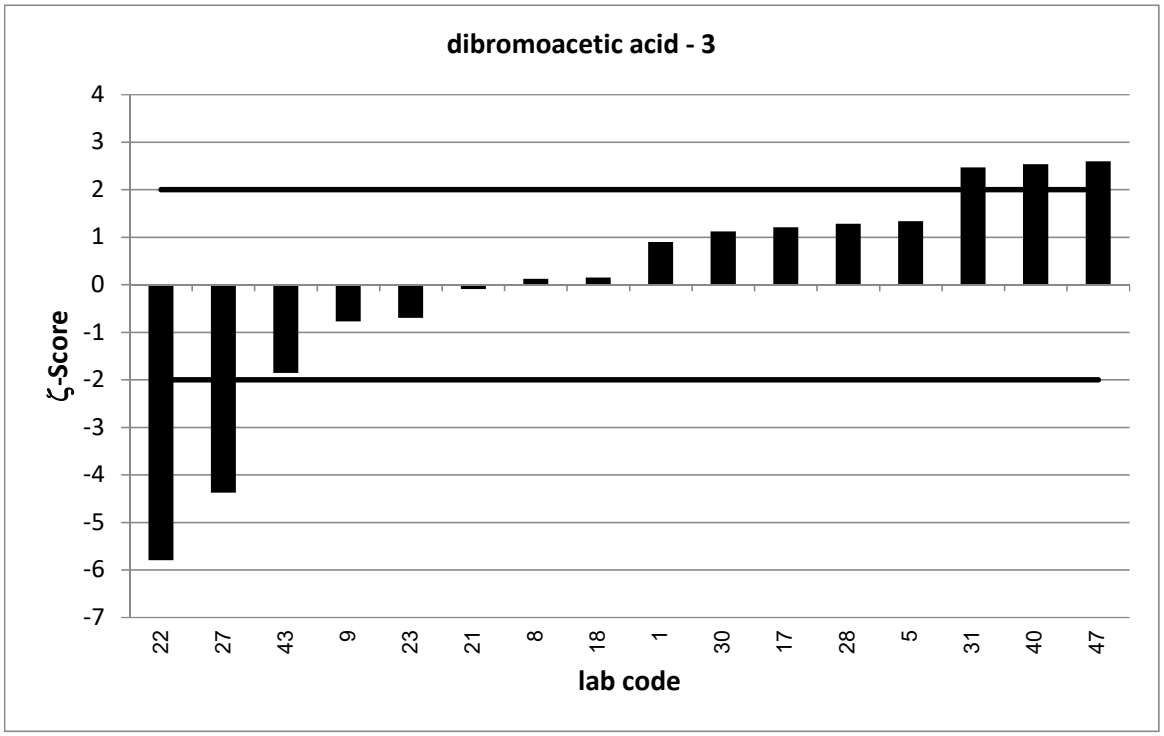
** s = satisfactory, q = questionable, u = unsatisfactory



Strongly deviating values are not shown in the diagram.



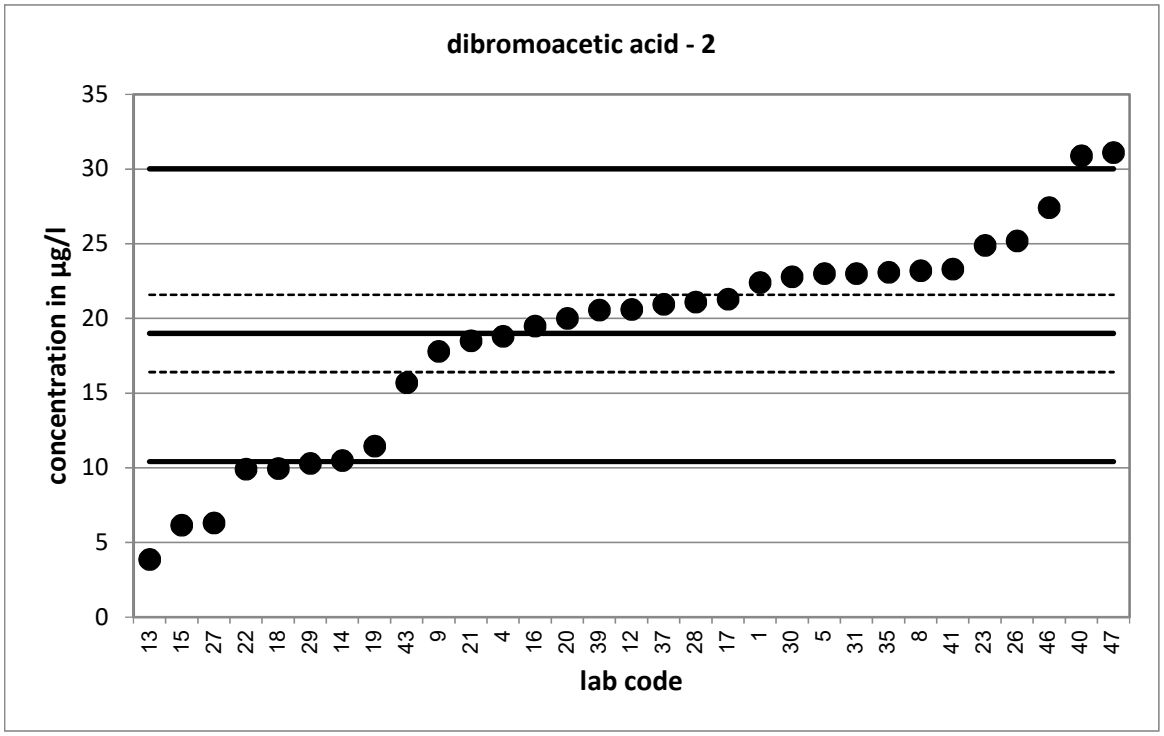

dibromoacetic acid - 3
expanded uncertainty in µg/l
25
20
15
10
5
0
22
27
23
43
17
9
1
8
31
28
47
30
5
18
40
21
lab code


dibromoacetic acid - 3
ζ-Score
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-7
22
27
43
9
23
21
8
18
1
30
17
28
5
31
40
47
lab code

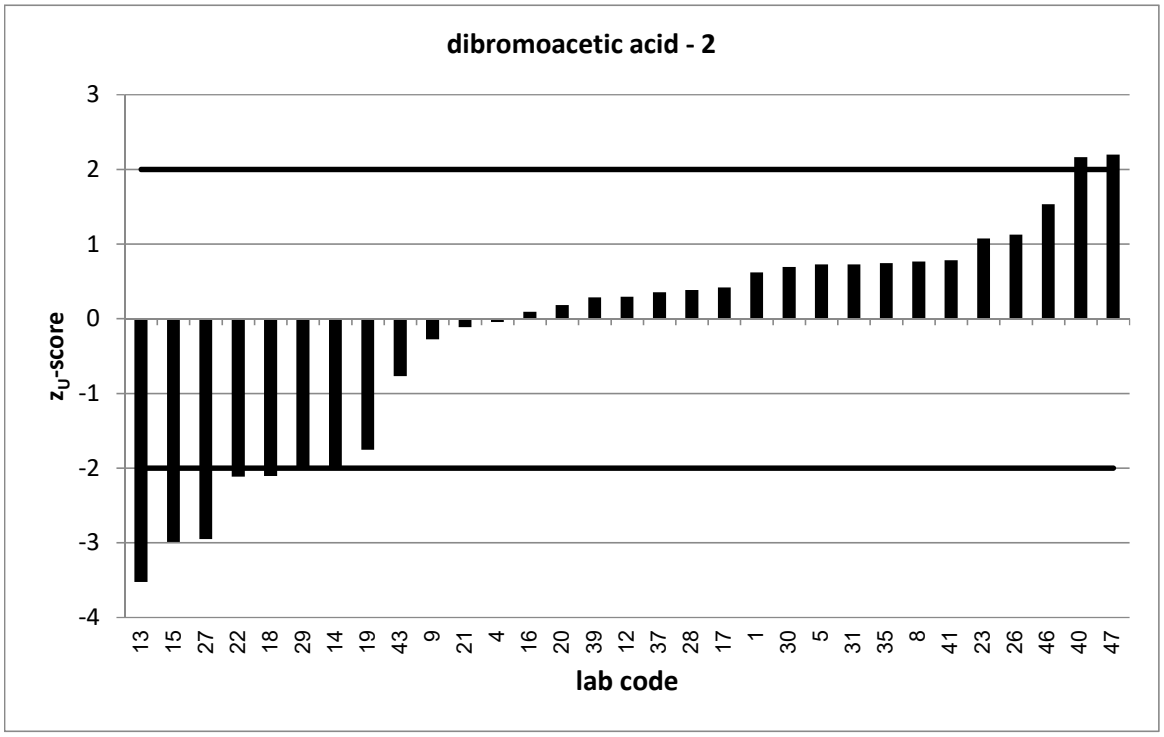
PT 7/23		dibromoacetic acid - 2			
assigned value [µg/l]*		19	± 2,59		
upper tolerance limit [µg/l]		30,01			
lower tolerance limit [µg/l]		10,41			
lab code	result [µg/l]	±	ζ-score	z_U-score	assessm.**
1	22,4	4,5	1,3	0,6	s
4	18,8			0,0	s
5	23	6,76	1,1	0,7	s
8	23,2	4,9	1,5	0,8	s
9	17,8	3,6	-0,5	-0,3	s
12	20,6			0,3	s
13	3,87			-3,5	u
14	10,5			-2,0	s
15	6,17			-3,0	u
16	19,5			0,1	s
17	21,3	2,17	1,4	0,4	s
18	9,95	4,48	-3,5	-2,1	q
19	11,456			-1,8	s
20	20			0,2	s
21	18,5	9,25	-0,1	-0,1	s
22	9,92	0,3	-7,0	-2,1	q
23	24,9	3,735	2,6	1,1	s
26	25,2			1,1	s
27	6,32	0,79	-9,4	-3,0	u
28	21,1	0,29	1,6	0,4	s
29	10,3			-2,0	s
30	22,8	5,7	1,2	0,7	s
31	23	3,92	1,7	0,7	s
35	23,1			0,7	s
37	20,95			0,4	s
39	20,57			0,3	s
40	30,9	8,96	2,6	2,2	q
41	23,3			0,8	s
43	15,7	3,1	-1,6	-0,8	s
46	27,43			1,5	s
47	31,1	6,19	3,6	2,2	q

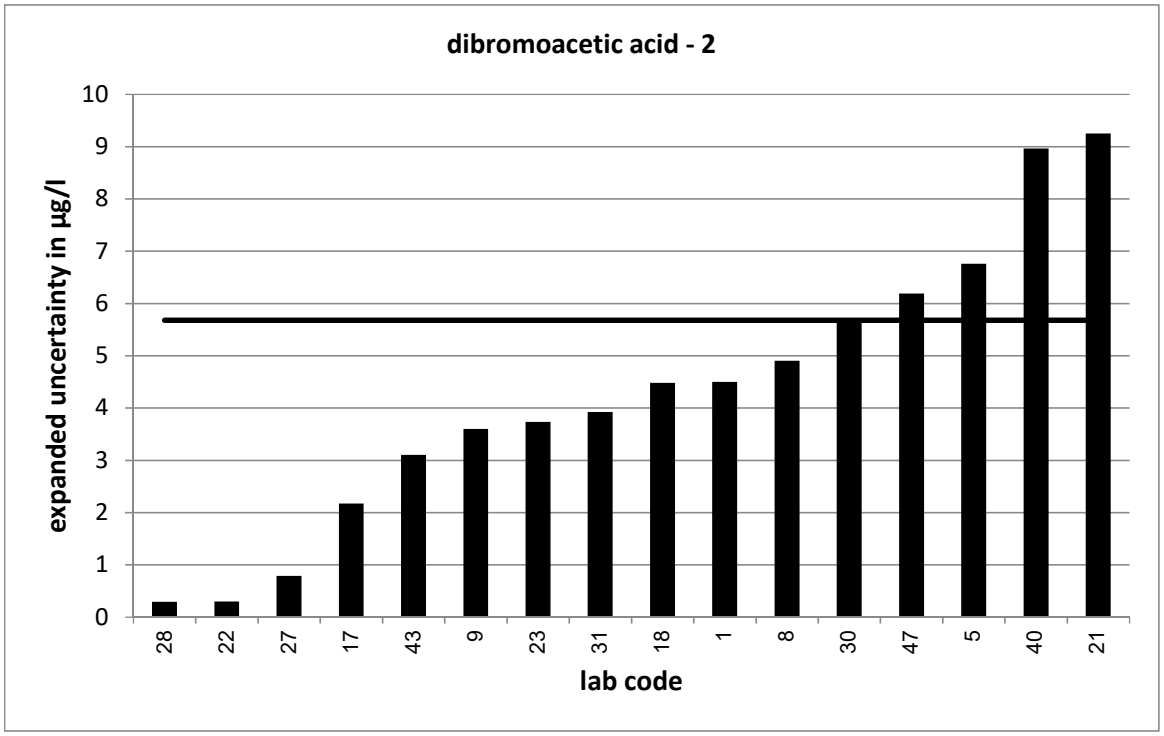
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor k=2 corresponding to a confidence level of about 95%

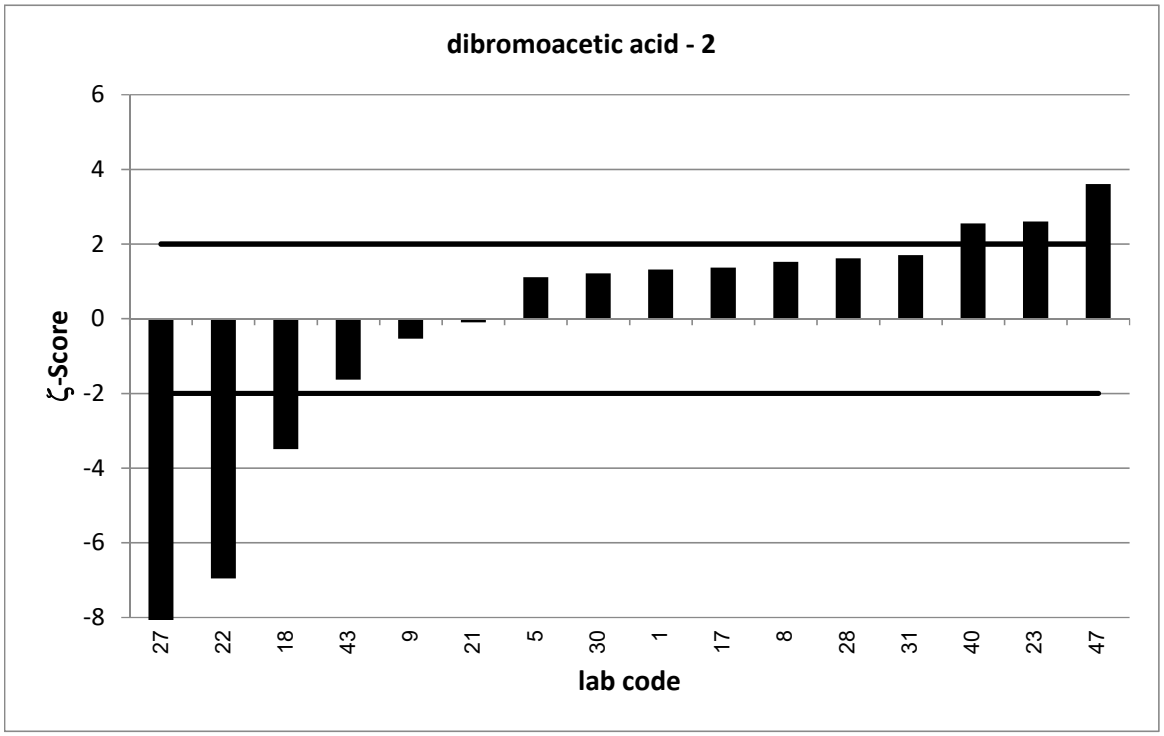
** s = satisfactory, q = questionable, u = unsatisfactory



Strongly deviating values are not shown in the diagram.







Strongly deviating values are not correctly shown in the diagram.