

University of Stuttgart
Germany



Analytische Qualitätssicherung Baden-Württemberg

Proficiency Test 5/25 – TW S7
- trifluoroacetic acid in drinking water -

Final report

provided by
AQS Baden-Württemberg at
Institute for Sanitary Engineering, Water Quality and Solid Waste Management,
University of Stuttgart
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and
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Stuttgart, in August 2025

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Release of the report:	Dr.-Ing. Frank Baumeister	on 29 August 2025
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List of contents

1. General	4
2. PT design.....	4
3. Sample preparation.....	4
4. Sample dispatch	4
5. Analytical methods.....	4
6. Submission of the results	4
7. Homogeneity and stability	5
8. Basic principle of evaluation and assessment	5
9. Evaluation	5
10. Explanation of the annexes.....	6
11. Measurement uncertainty (MU).....	6
12. Traceable reference values	7
13. Internet.....	7

Annex A

TFA.....	8
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Annex B

Reported measurement uncertainty.....	16
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Annex C

TFA.....	17
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1. General

This proficiency test (PT) was provided as part of the AQS Baden-Württemberg PT programme in cooperation with IWW Analytik und Service GmbH in Mülheim an der Ruhr and the “NORMAN” network (network of reference laboratories for monitoring of emerging environmental pollutants).

The PT was executed and evaluated according to the requirements of DIN 38402-A45:2024 and ISO 13528:2022.

2. PT design

Each participant received the following samples:

- 3 samples for the determination of TFA in 50-ml-plastic tubes.

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

3. Sample preparation

The samples for the determination of TFA were based on a real ground water matrix from the northern part of the region Ruhr in North Rhine-Westphalia. 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 dispatch

The samples were dispatched by express service on 20 May 2025.

5. Analytical methods

The participants were free to choose a suitable method, but a limit of quantification of 0.03 µg/l 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 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 results of the analyses had to be submitted to the organiser via the web portal by the 09 June 2025. Values received after this date could not be taken into account.

7. Homogeneity and stability

The homogeneity and stability of the samples were confirmed according to ISO 13528:2022.

8. Basic principle of evaluation and assessment

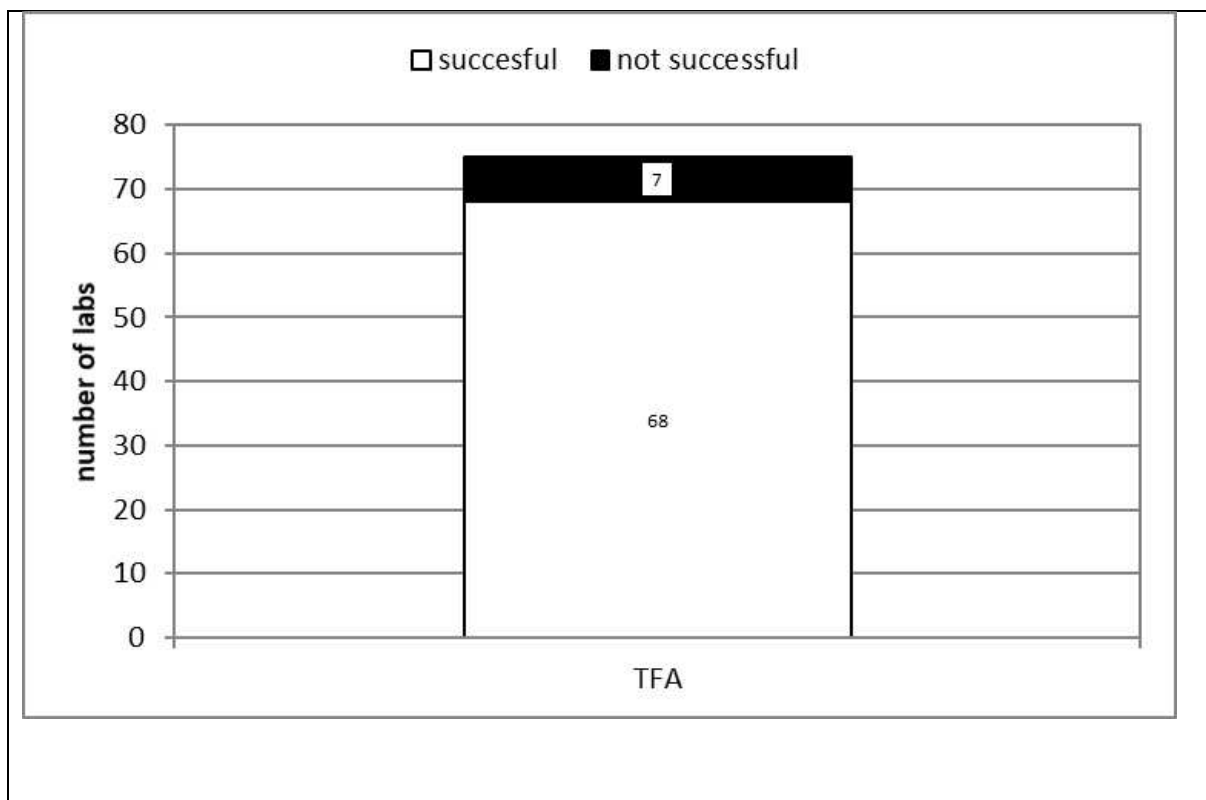
The basic principle of the evaluation and assessment of the PTs from AQS Baden-Württemberg are described in the document „Evaluation of the PTs and information for the report“, which can be downloaded from www.agsbw.de/pdf/ausw_berichte_v1_en.pdf.

This PT was evaluated as follows:

Assigned value x_{pt}:	Reference value from the weighing						
Standard deviation for proficiency assessment σ_{pt}:	Q-method						
upper limit for σ_{pt}:	25 %						
lower limit for σ_{pt}:	5 %						
assessment:	z_U score						
classification of the single results	<table style="border: none;"> <tr> <td style="padding-right: 20px;">$z_U \leq 2,0$</td> <td>successful</td> </tr> <tr> <td>$2,0 < z_U < 3,0$</td> <td>questionable</td> </tr> <tr> <td>$z_U \geq 3,0$</td> <td>unsatisfactory</td> </tr> </table>	$ z_U \leq 2,0$	successful	$2,0 < z_U < 3,0$	questionable	$ z_U \geq 3,0$	unsatisfactory
$ z_U \leq 2,0$	successful						
$2,0 < z_U < 3,0$	questionable						
$ z_U \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).						

9. Evaluation

number of participants:	79 5 participants didn't report results
number of reported results	222
number of acceptable results:	197 (88,74 %)
Illustration of the successful and not successful laboratories for each parameter:	



10. Explanation of the annexes

The explanations for the annexes 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.

11. Measurement uncertainty (MU)

General:

number of participants with valid results	73
number of participants with valid results and reported MU	54 (73,97%)
number of valid results	219
number of valid results with reported MU	161 (73,5 %)

Reporting of the measurement uncertainty depending on the accreditation status:

accreditation status of the results	number of results	number of results with reported MU
accredited	129	104 (80,6 %)
not accredited	90	57 (63,3 %)
no information	0	0 (0 %)

Interpretation of the reported measurement uncertainties:

In the diagrams showing the measurement uncertainties, it is noticeable that the range is very wide, from unrealistically small to much too large. A plausibility assessment using the reproducibility standard deviations in interlaboratory comparisons would certainly be helpful here.

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 $z_U \leq 2,0$	146
Number of these values whose ζ score is > 2 The own requirements of the laboratory are not fulfilled and the estimation of the measurement uncertainty is too low	26 (17,81 %)

12. Traceable reference values

The explanations for the the 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.

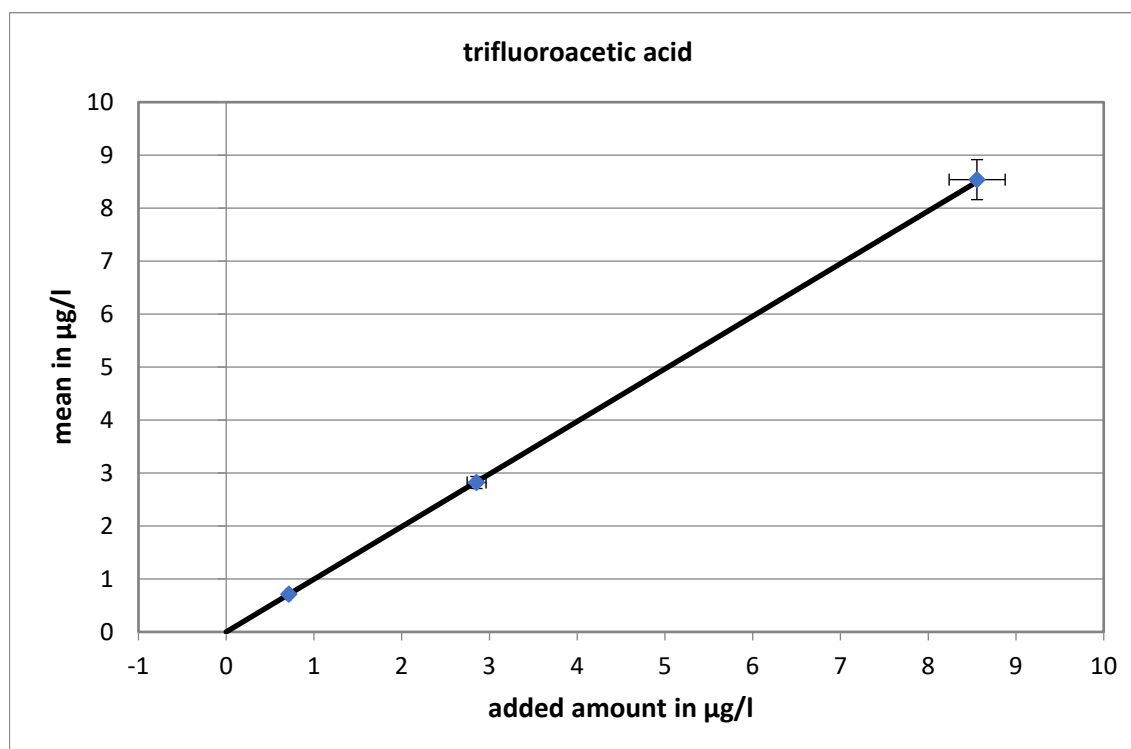
13. Internet

The report is available on www.aqsbw.de/pdf/319/report_319.pdf.

trifluoroacetic acid

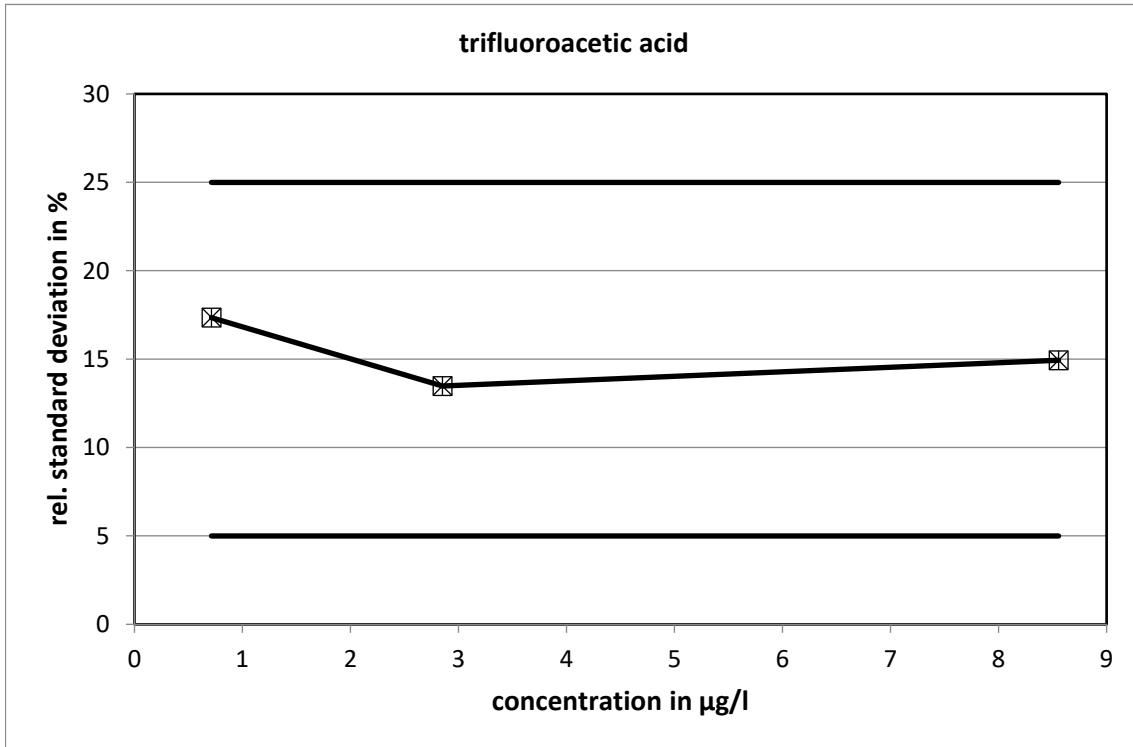
level	assigned value [$\mu\text{g/l}$]	expanded uncertainty of the assigned value [%]	standard deviation, calculated using robust statistics [$\mu\text{g/l}$]	standard deviation for proficiency assessment [$\mu\text{g/l}$]	standard deviation for proficiency assessment [%]	upper tolerance limit [$\mu\text{g/l}$]	lower tolerance limit [$\mu\text{g/l}$]	upper tolerance limit [%]	lower tolerance limit [%]	number of results	out below	out above	out [%]
1	0,7130	4,06	0,1237	0,1237	17,35	0,9859	0,4836	38,27	-32,18	71	5	6	15,1
2	2,852	3,75	0,3844	0,3844	13,48	3,681	2,129	29,05	-25,36	72	5	4	12,3
3	8,556	3,73	1,278	1,278	14,94	11,33	6,164	32,46	-27,96	72	5	2	9,6
sum										215	15	12	12,6

Recovery and matrix content

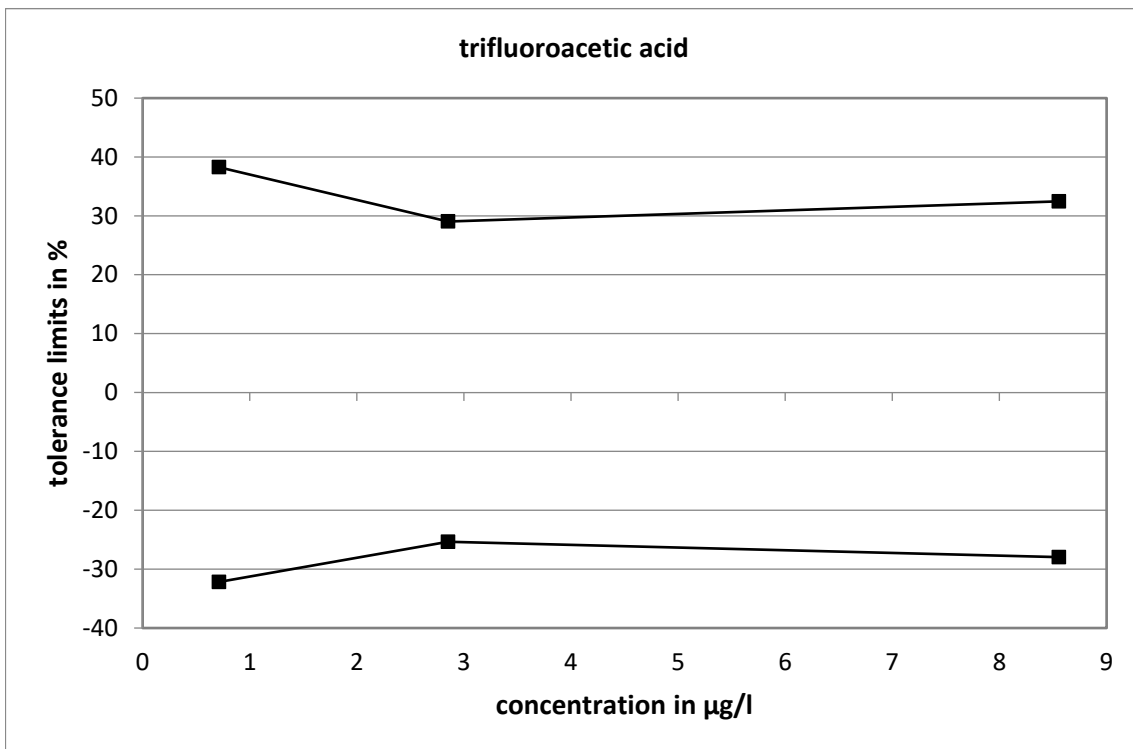


slope of the regression: 0,993; average recovery: 99,3 %
 neg. x-intercept corresponds to the matrix content: 0,0017 $\mu\text{g/l}$
 exp. uncertainty of the matrix content: 0,0017 $\mu\text{g/l}$ = 100 %

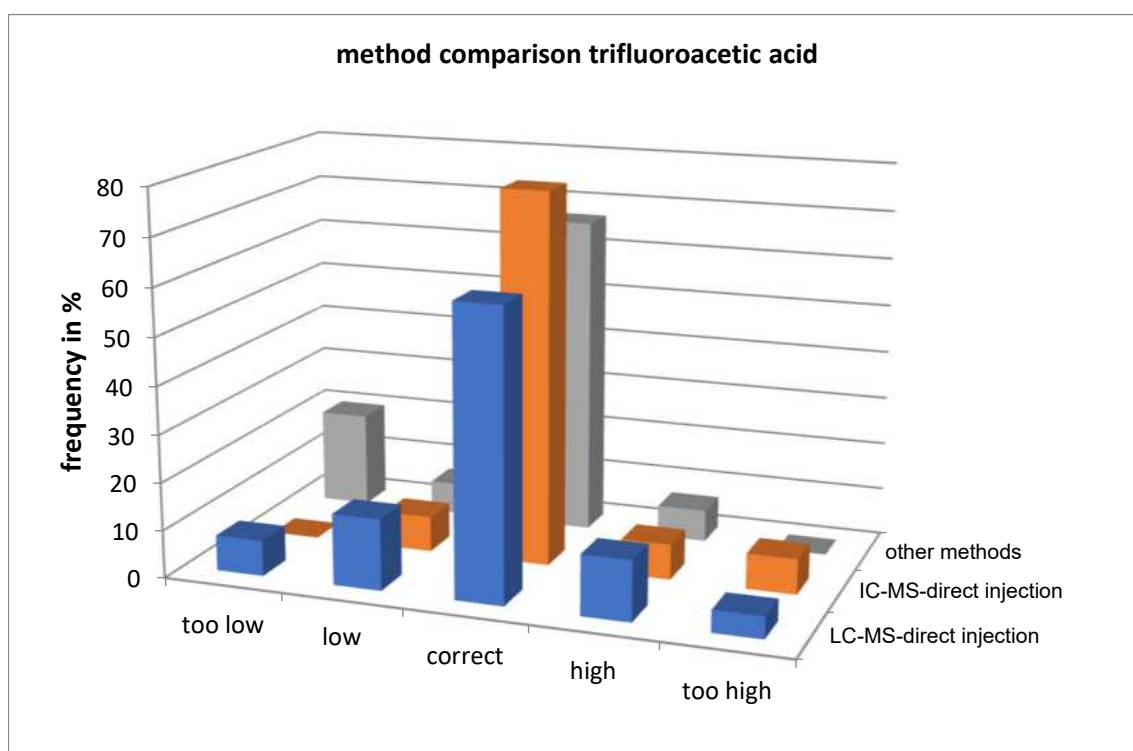
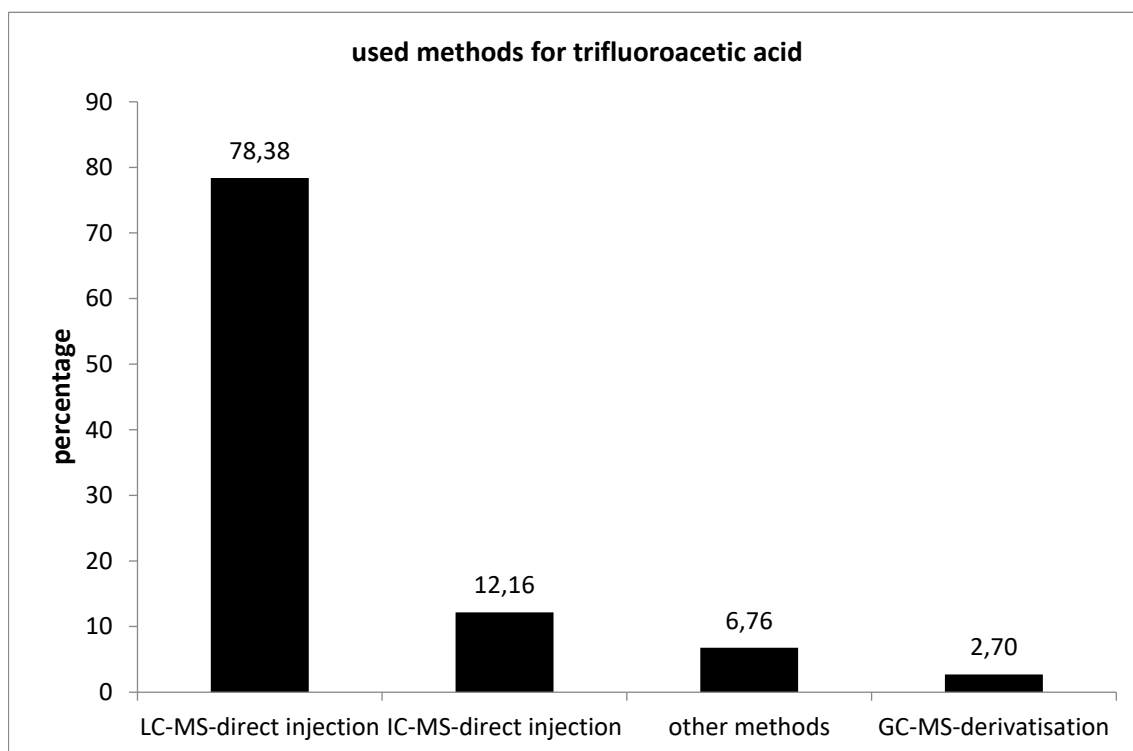
Relative standard deviation and tolerance limits



The relative standard deviations calculated with the Q-method did not reach the limits.



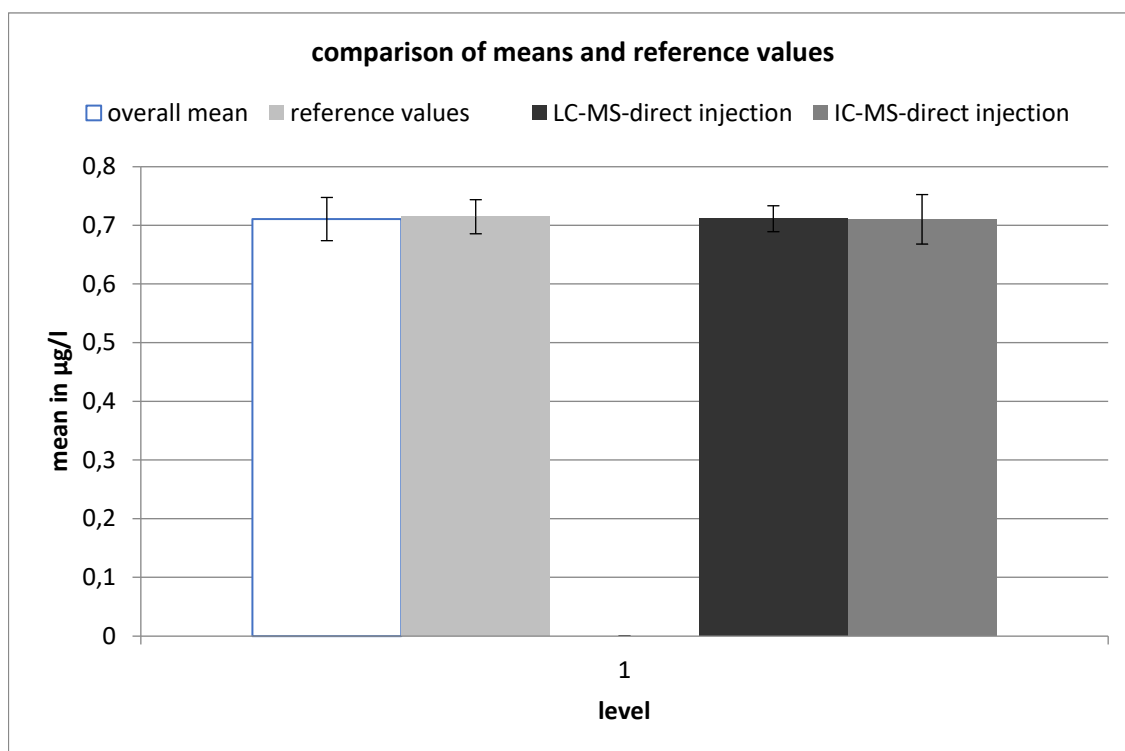
Method specific evaluation

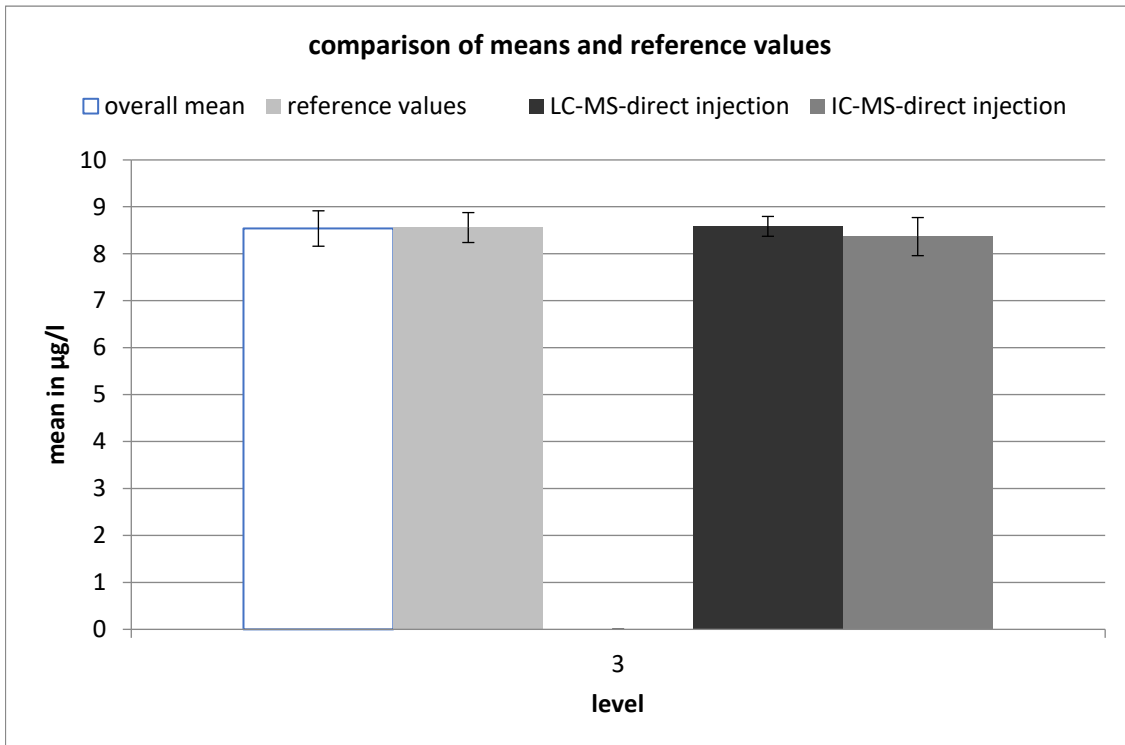
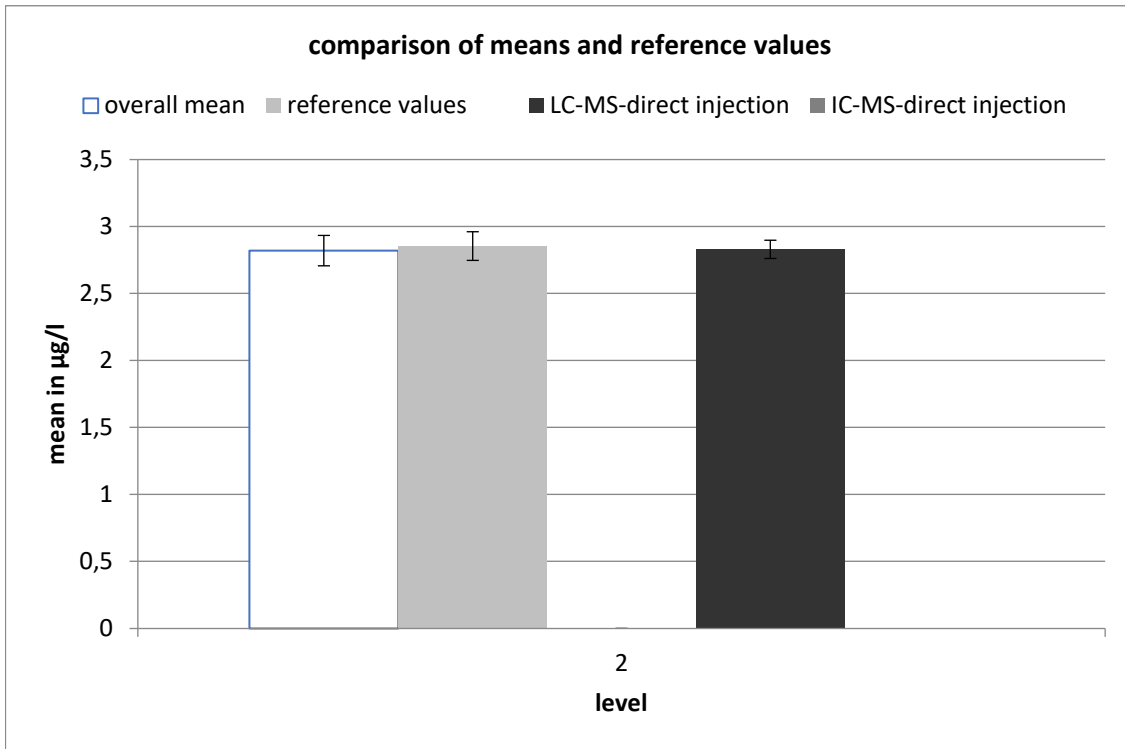


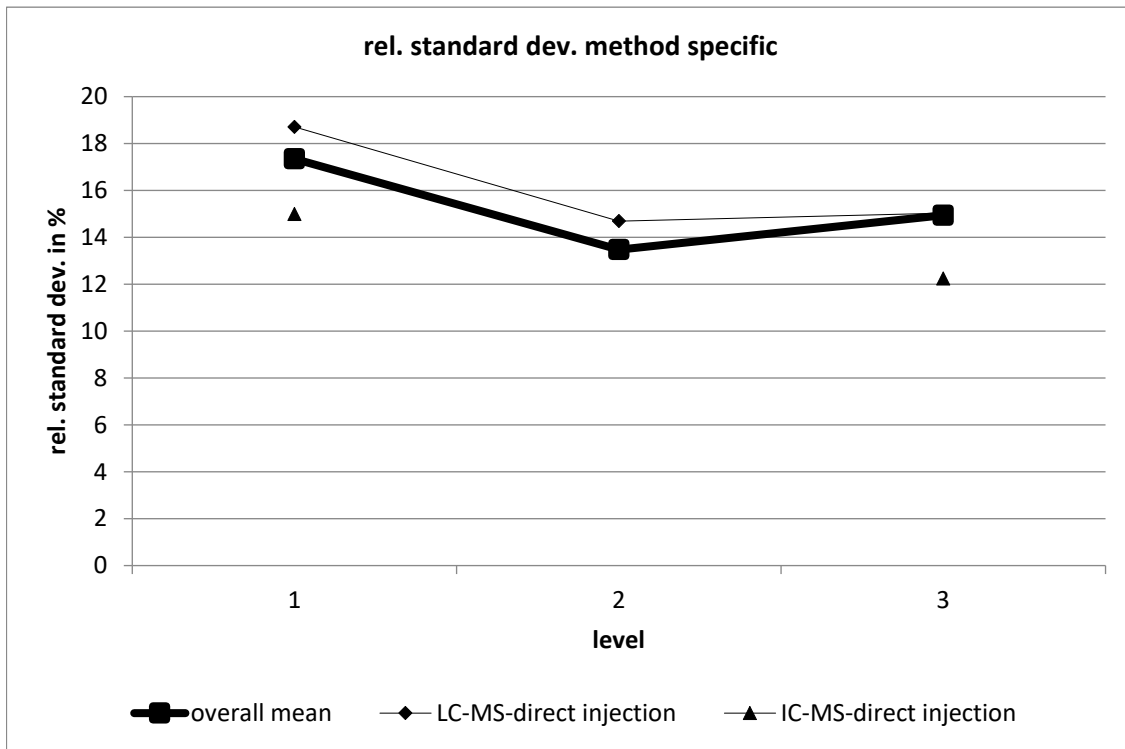
The values determined with IC-MS-direct injection showed the closest statistical distribution.
report version 1.0

Comparison of means and reference values

level	measured values			reference values		
	mean [µg/l]	exp. uncertainty [µg/l]	exp. uncertainty [%]	reference value [µg/l]	exp. uncertainty [µg/l]	exp. uncertainty [%]
1	0,7107	0,0367	5,2	0,7147	0,0290	4,1
2	2,820	0,113	4,0	2,854	0,107	3,8
3	8,539	0,377	4,4	8,558	0,320	3,7

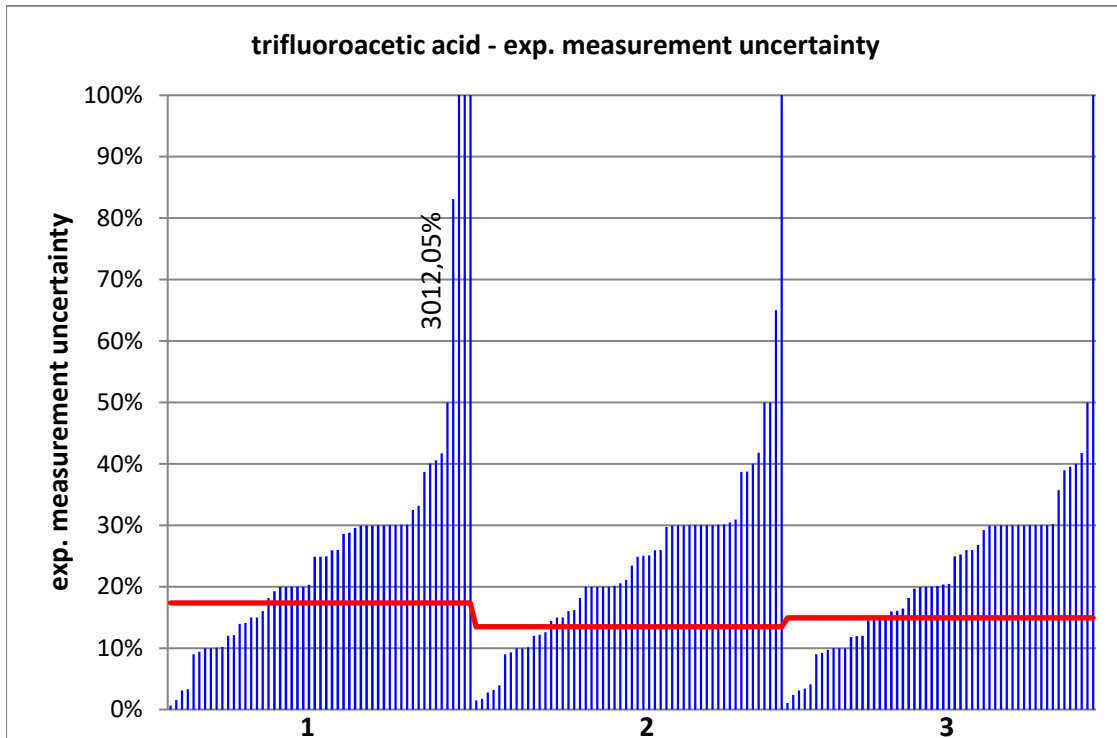






LC-MS-direct injection									
level	robust mean [µg/l]	exp. unc. of the mean [µg/l]	exp. unc. of the mean [%]	robust standard deviation [µg/l]	robust standard deviation [%]	number of results	out below	out above	out [%]
1	0,711	0,022	3,098	0,133	18,71	57	4	4	14,04
2	2,829	0,068	2,412	0,416	14,69	58	4	2	10,34
3	8,583	0,212	2,466	1,29	15,03	58	4	0	6,897

IC-MS-direct injection									
level	robust mean [$\mu\text{g/l}$]	exp. unc. of the mean [$\mu\text{g/l}$]	exp. unc. of the mean [%]	robust standard deviation [$\mu\text{g/l}$]	robust standard deviation [%]	number of results	out below	out above	out [%]
1	0,71	0,042	5,927	0,107	15	10	0	1	10
3	8,366	0,405	4,839	1,024	12,24	10	0	1	10



PT 5/25 - TW S7		trifluoroacetic acid - 1			
assigned value [$\mu\text{g/l}$]*		0,713 \pm 0,029			
upper tolerance limit [$\mu\text{g/l}$]		0,9859			
lower tolerance limit [$\mu\text{g/l}$]		0,4836			
lab code	result [$\mu\text{g/l}$]	\pm	z-score	Z _U -score	assessm.**
1	0,591	0,177	-1,4	-1,1	s
2	0,6541			-0,5	s
3	0,59			-1,1	s
4	0,47	0,094	-4,9	-2,1	q
5	0,719	0,288	0,0	0,0	s
6	0,743	0,09	0,6	0,2	s
7	0,853	0,171	1,6	1,0	s
9	0,735	0,221	0,2	0,2	s
10	0,542	0,22	-1,5	-1,5	s
11	0,847	0,118	2,2	1,0	s
12	0,924	0,277	1,5	1,5	s
13	0,62	0,24	-0,8	-0,8	s
14	0,635	0,265	-0,6	-0,7	s
15	0,748	0,224	0,3	0,3	s
16	1,04	0,2	3,2	2,4	q
17	0,701	0,14	-0,2	-0,1	s
18	0,68	0,061	-1,0	-0,3	s
20	0,635	0,021	-4,4	-0,7	s
21	0,71	0,21	0,0	0,0	s
22	0,683			-0,3	s
23	1,49	0,14	10,9	5,7	u
24	0,9	0,09	4,0	1,4	s
25	0,534	0,16	-2,2	-1,6	s
26	8,824			59,4	u
27	0,887	0,18	1,9	1,3	s
28	0,98	0,1	5,1	2,0	s
29	0,699			-0,1	s
31	0,723			0,1	s
32	0,723	0,18	0,1	0,1	s
33	0,679	0,021	-1,9	-0,3	s
34	0,71	0,1	-0,1	0,0	s
35	0,715	0,13	0,0	0,0	s
36	1,044	0,26	2,5	2,4	q
37	1,03	0,31	2,0	2,3	q
38	0,725			0,1	s
40	0,5423	1,5	-0,2	-1,5	s
41	0,816	0,245	0,8	0,8	s
42	0,699			-0,1	s
43	0,105	0,03	-29,1	-5,3	u
44	0,651	0,098	-1,2	-0,5	s
45	0,962	0,144	3,4	1,8	s
46	0,7354			0,2	s
47	0,609	0,004	-7,1	-0,9	s
48	0,6432	0,097	-1,4	-0,6	s
49	0,39	0,195	-3,3	-2,8	q
50	0,694	0,173	-0,2	-0,2	s

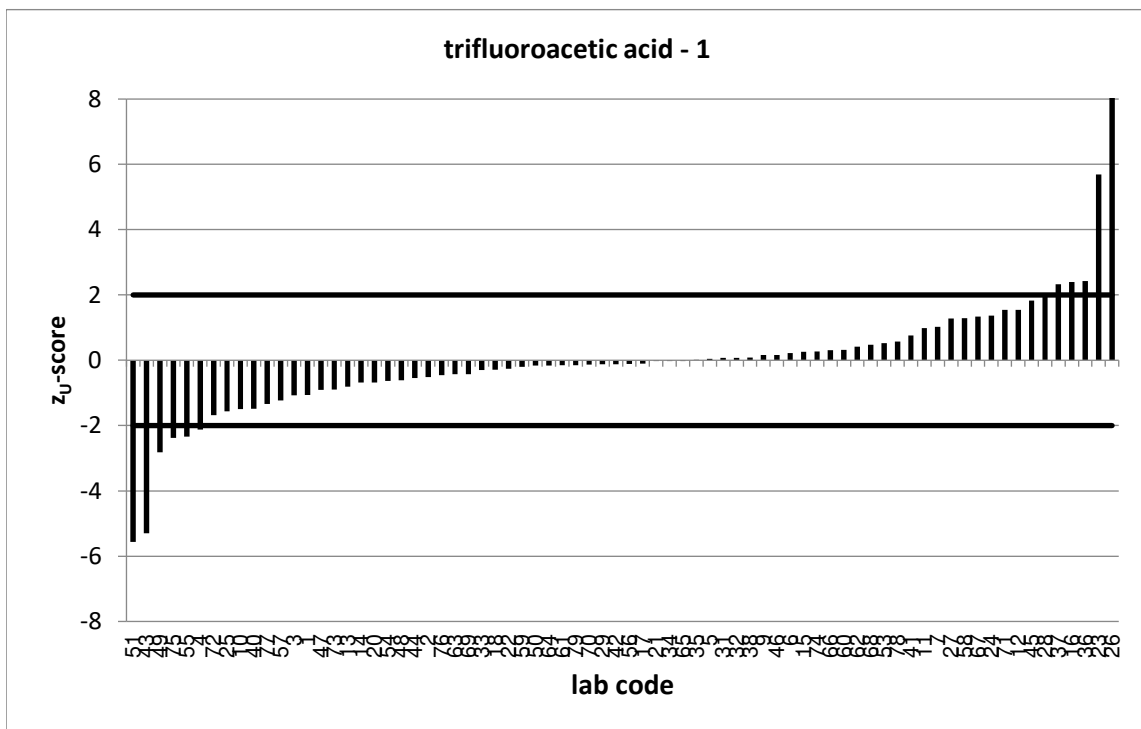
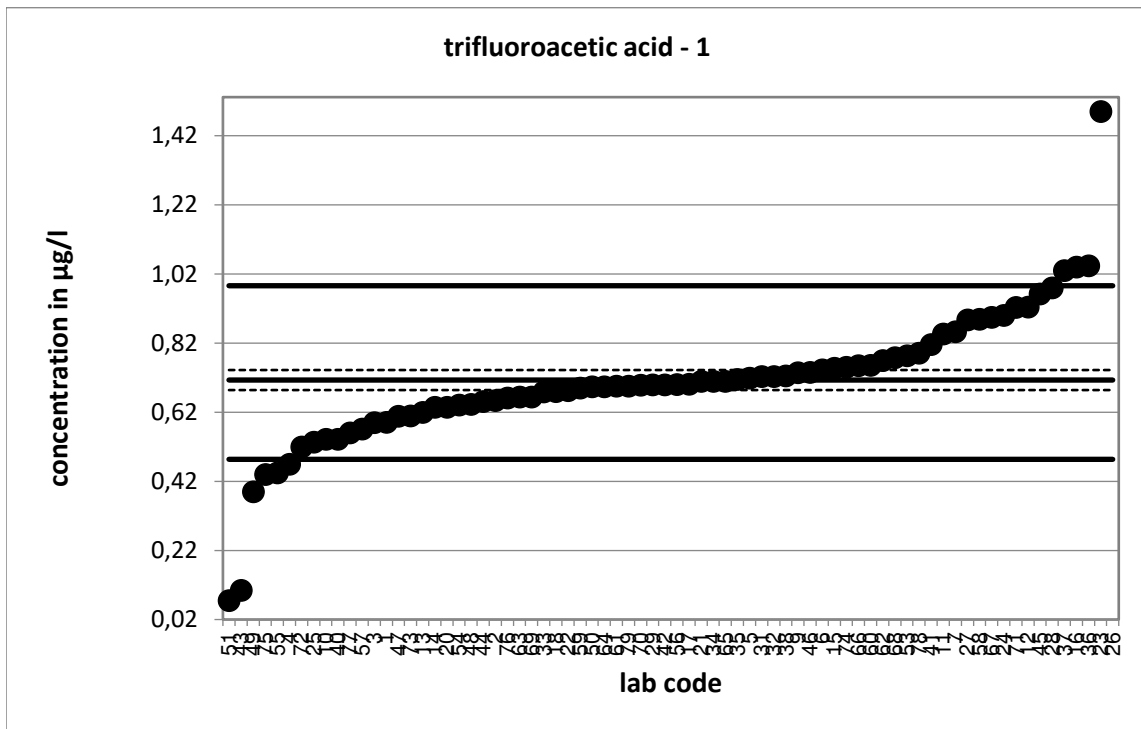
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor $k=2$ corresponding to a confidence level of about 95%

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

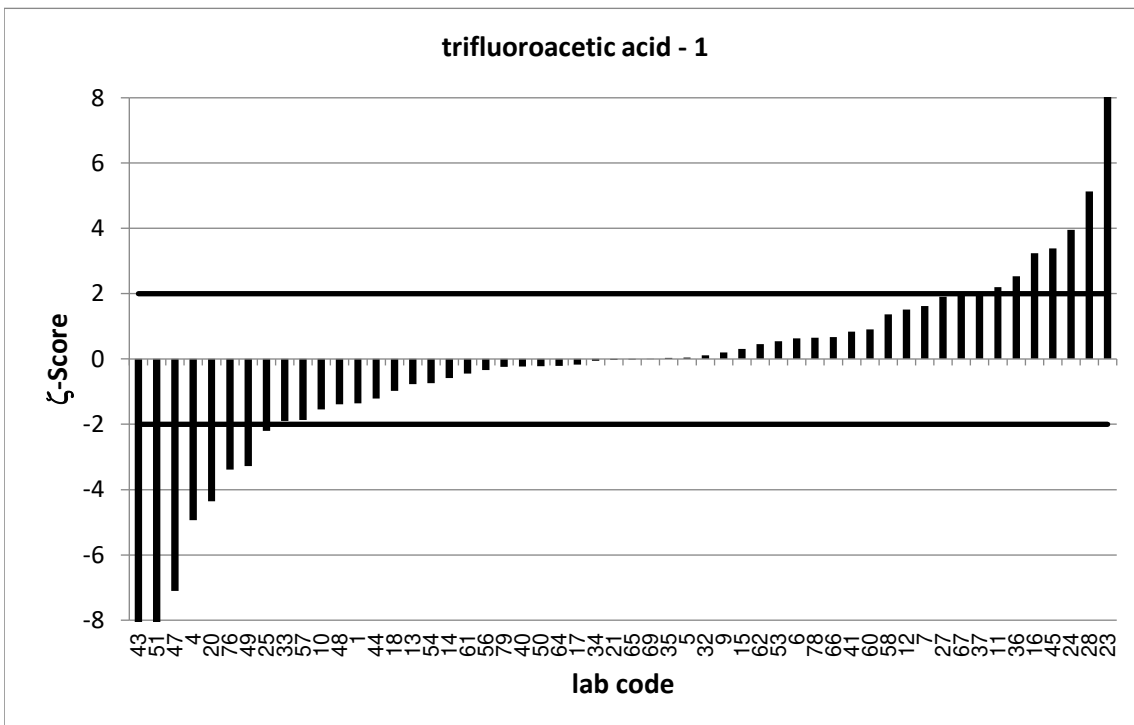
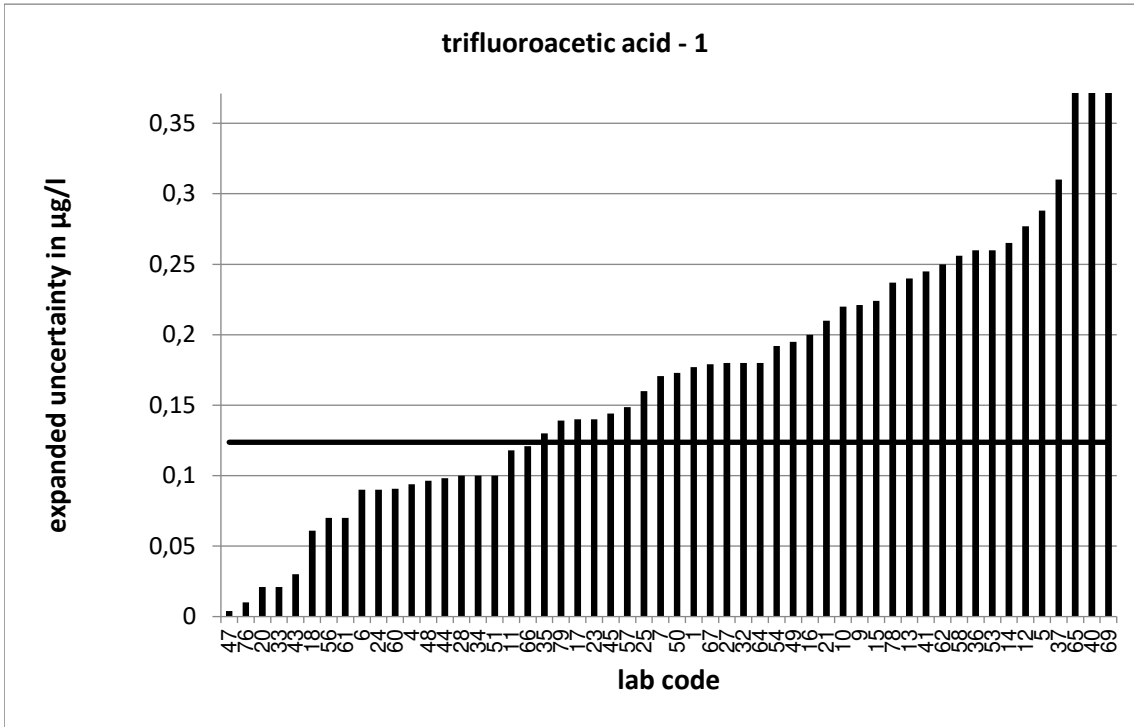
PT 5/25 - TW S7		trifluoroacetic acid - 1			
assigned value [$\mu\text{g/l}$]*		0,713 \pm 0,029			
upper tolerance limit [$\mu\text{g/l}$]		0,9859			
lower tolerance limit [$\mu\text{g/l}$]		0,4836			
lab code	result [$\mu\text{g/l}$]	\pm	z-score	z _U -score	assessm.**
51	0,075	0,1	-12,3	-5,6	u
53	0,784	0,26	0,5	0,5	s
54	0,641	0,192	-0,7	-0,6	s
55	0,445			-2,3	q
56	0,7	0,07	-0,3	-0,1	s
57	0,5717	0,149	-1,9	-1,2	s
58	0,889	0,256	1,4	1,3	s
59	0,69			-0,2	s
60	0,756	0,091	0,9	0,3	s
61	0,696	0,07	-0,4	-0,1	s
62	0,77	0,25	0,5	0,4	s
63	0,664			-0,4	s
64	0,694	0,18	-0,2	-0,2	s
65	0,71	0,59	0,0	0,0	s
66	0,755	0,121	0,7	0,3	s
67	0,895	0,179	2,0	1,3	s
68	0,778			0,5	s
69	0,664	20	0,0	-0,4	s
70	0,698			-0,1	s
71	0,9235			1,5	s
72	0,52			-1,7	s
73	0,61			-0,9	s
74	0,75			0,3	s
75	0,44			-2,4	q
76	0,661	0,01	-3,4	-0,5	s
77	0,56			-1,3	s
78	0,791	0,237	0,7	0,6	s
79	0,696	0,139	-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 correctly shown in the diagram.



Strongly deviating values are not correctly shown in the diagram.

PT 5/25 - TW S7		trifluoroacetic acid - 2			
assigned value [$\mu\text{g/l}$]*		2,852 \pm 0,107			
upper tolerance limit [$\mu\text{g/l}$]		3,681			
lower tolerance limit [$\mu\text{g/l}$]		2,129			
lab code	result [$\mu\text{g/l}$]	\pm	z-score	z _U -score	assessm.**
1	2,43	0,728	-1,1	-1,2	s
2	2,5724			-0,8	s
3	3,44			1,4	s
4	2,39	0,477	-1,9	-1,3	s
5	2,76	1,104	-0,2	-0,3	s
6	2,88	0,35	0,2	0,1	s
7	3,4	0,679	1,6	1,3	s
9	2,82	0,85	-0,1	-0,1	s
10	2,58	1	-0,5	-0,8	s
11	3,67	0,118	10,3	2,0	s
12	3,567	1,07	1,3	1,7	s
13	2,3	0,89	-1,2	-1,5	s
14	2,44	1,02	-0,8	-1,1	s
15	2,861	0,858	0,0	0,0	s
16	3,09	0,5	0,9	0,6	s
17	2,83	0,566	-0,1	-0,1	s
18	2,73	0,246	-0,9	-0,3	s
20	2,544	0,044	-5,3	-0,9	s
21	2,69	0,81	-0,4	-0,4	s
22	2,98			0,3	s
23	3,37	0,05	8,8	1,3	s
24	2,8	0,28	-0,3	-0,1	s
25	2,3	0,691	-1,6	-1,5	s
26	0,552			-6,4	u
27	3,16	0,65	0,9	0,7	s
28	3,76	0,35	5,0	2,2	q
29	2,73			-0,3	s
31	2,98	0,6	0,4	0,3	s
32	2,79	0,7	-0,2	-0,2	s
33	2,659	0,074	-3,0	-0,5	s
34	2,71	0,39	-0,7	-0,4	s
35	2,88	0,523	0,1	0,1	s
36	3,156	0,79	0,8	0,7	s
37	3,06	0,92	0,4	0,5	s
38	2,75			-0,3	s
40	2,307	1,5	-0,7	-1,5	s
41	3,63	1,09	1,4	1,9	s
42	2,71			-0,4	s
43	0,485	0,15	-25,7	-6,5	u
45	4,41	0,66	4,7	3,8	u
46	2,9383			0,2	s
47	2,545	0,1	-4,2	-0,8	s
48	2,6941	0,404	-0,8	-0,4	s
49	1,3	0,65	-4,7	-4,3	u
50	2,69	0,67	-0,5	-0,4	s
51	0,2	0,1	-36,2	-7,3	u

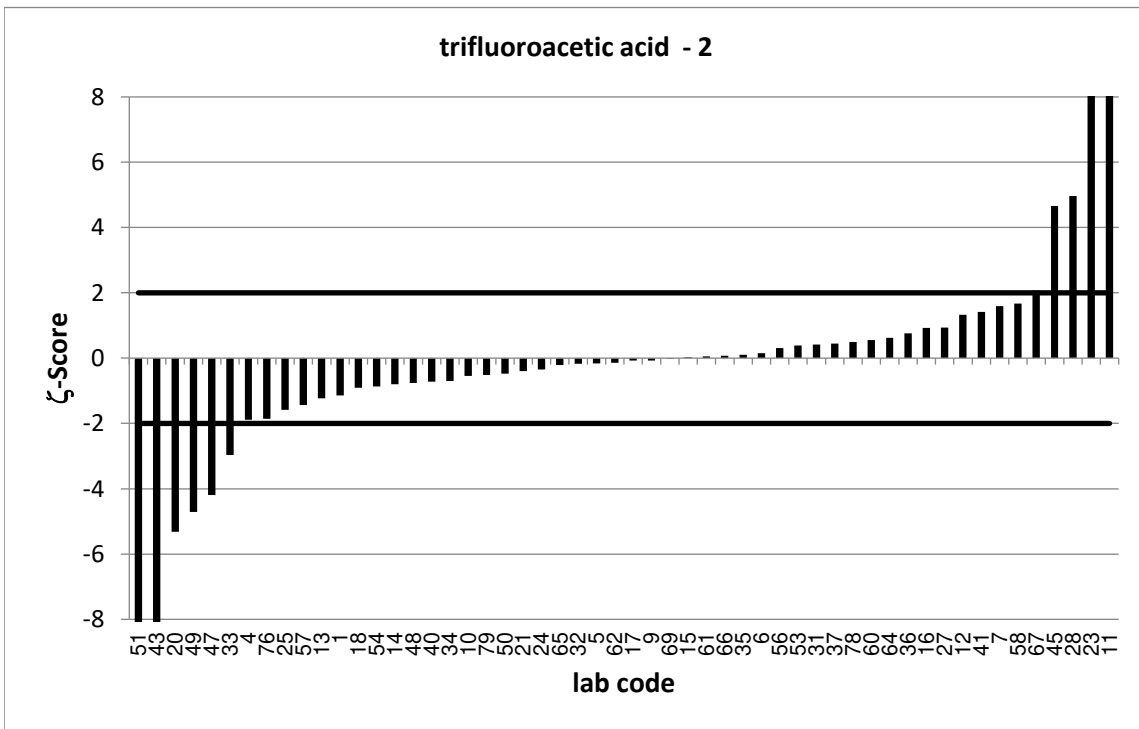
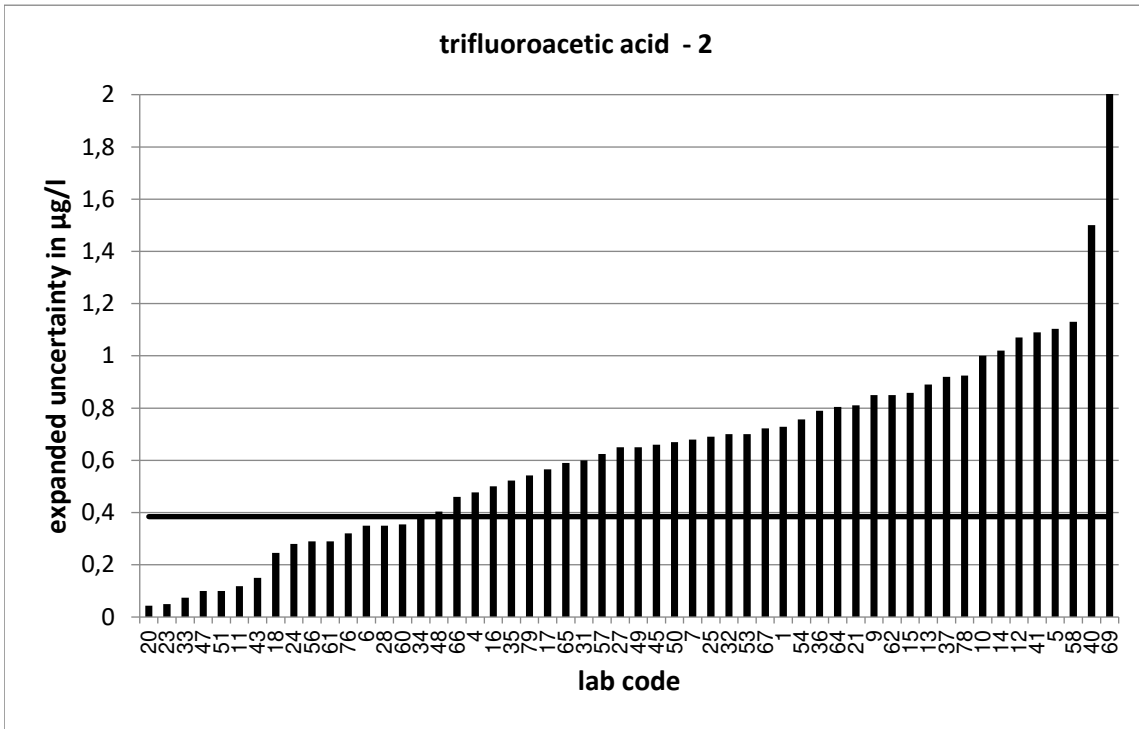
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor $k=2$ corresponding to a confidence level of about 95%

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

PT 5/25 - TW S7		trifluoroacetic acid - 2			
assigned value [$\mu\text{g/l}$]*		2,852 \pm 0,107			
upper tolerance limit [$\mu\text{g/l}$]		3,681			
lower tolerance limit [$\mu\text{g/l}$]		2,129			
lab code	result [$\mu\text{g/l}$]	\pm	z-score	z _U -score	assessm.**
53	2,99	0,7	0,4	0,3	s
54	2,52	0,757	-0,9	-0,9	s
55	2,33			-1,4	s
56	2,9	0,29	0,3	0,1	s
57	2,399	0,624	-1,4	-1,3	s
58	3,801	1,13	1,7	2,3	q
59	3,2			0,8	s
60	2,955	0,355	0,6	0,2	s
61	2,86	0,29	0,1	0,0	s
62	2,79	0,85	-0,1	-0,2	s
63	2,67			-0,5	s
64	3,103	0,805	0,6	0,6	s
65	2,79	0,59	-0,2	-0,2	s
66	2,87	0,46	0,1	0,0	s
67	3,61	0,722	2,1	1,8	s
68	2,97			0,3	s
69	2,712	20	0,0	-0,4	s
70	2,885			0,1	s
71	2,887			0,1	s
72	2,55			-0,8	s
73	2,4			-1,2	s
74	2,9			0,1	s
75	1,8			-2,9	q
76	2,538	0,32	-1,9	-0,9	e
77	2,25			-1,7	s
78	3,08	0,924	0,5	0,6	s
79	2,71	0,542	-0,5	-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 correctly shown in the diagram.

PT 5/25 - TW S7		trifluoroacetic acid - 3			
assigned value [$\mu\text{g/l}$]*		8,556 \pm 0,32			
upper tolerance limit [$\mu\text{g/l}$]		11,33			
lower tolerance limit [$\mu\text{g/l}$]		6,164			
lab code	result [$\mu\text{g/l}$]	\pm	z-score	z _U -score	assessm.**
1	7,28	2,18	-1,2	-1,1	s
2	7,8672			-0,6	s
3	11,38			2,0	s
4	10,6	2,13	1,9	1,5	s
5	8,14	3,256	-0,3	-0,3	s
6	8,91	1,07	0,6	0,3	s
7	10	2	1,4	1,0	s
9	8,52	2,56	0,0	0,0	s
10	7,08	2,8	-1,0	-1,2	s
11	11	0,118	14,3	1,8	s
12	11,064	3,319	1,5	1,8	s
13	7,7	3	-0,6	-0,7	s
14	8,5	3,55	0,0	0,0	s
15	8,912	2,674	0,3	0,3	s
16	10,3	1	3,3	1,3	s
17	8,62	1,72	0,1	0,0	s
18	8,19	0,737	-0,9	-0,3	s
20	6,532	0,267	-9,7	-1,7	s
21	7,88	2,3	-0,6	-0,6	s
22	8,6			0,0	s
23	10,3	0,35	7,4	1,3	s
24	8,4	0,84	-0,3	-0,1	s
25	7,17	2,15	-1,3	-1,2	s
26	2,716			-4,9	u
27	8,81	1,8	0,3	0,2	s
28	9,81	0,9	2,6	0,9	s
29	8,2			-0,3	s
31	8,85	1,8	0,3	0,2	s
32	8,72	2,2	0,1	0,1	s
33	8,011	0,25	-2,7	-0,5	s
34	8,2	1,19	-0,6	-0,3	s
35	8,65	1,57	0,1	0,1	s
36	7,775	1,94	-0,8	-0,7	s
37	8,06	2,42	-0,4	-0,4	s
38	8,61			0,0	s
40	6,908	2,07	-1,6	-1,4	s
41	11,7	3,5	1,8	2,3	q
42	8,65			0,1	s
43	1,523	0,457	-25,2	-5,9	u
45	10,2	1,5	2,1	1,2	s
46	9,1903			0,5	s
47	7,577	0,18	-5,3	-0,8	s
48	9,575	1,436	1,4	0,7	s
49	2,92	1,46	-7,5	-4,7	u
50	7,66	1,15	-1,5	-0,7	s
51	0,28	0,1	-49,4	-6,9	u

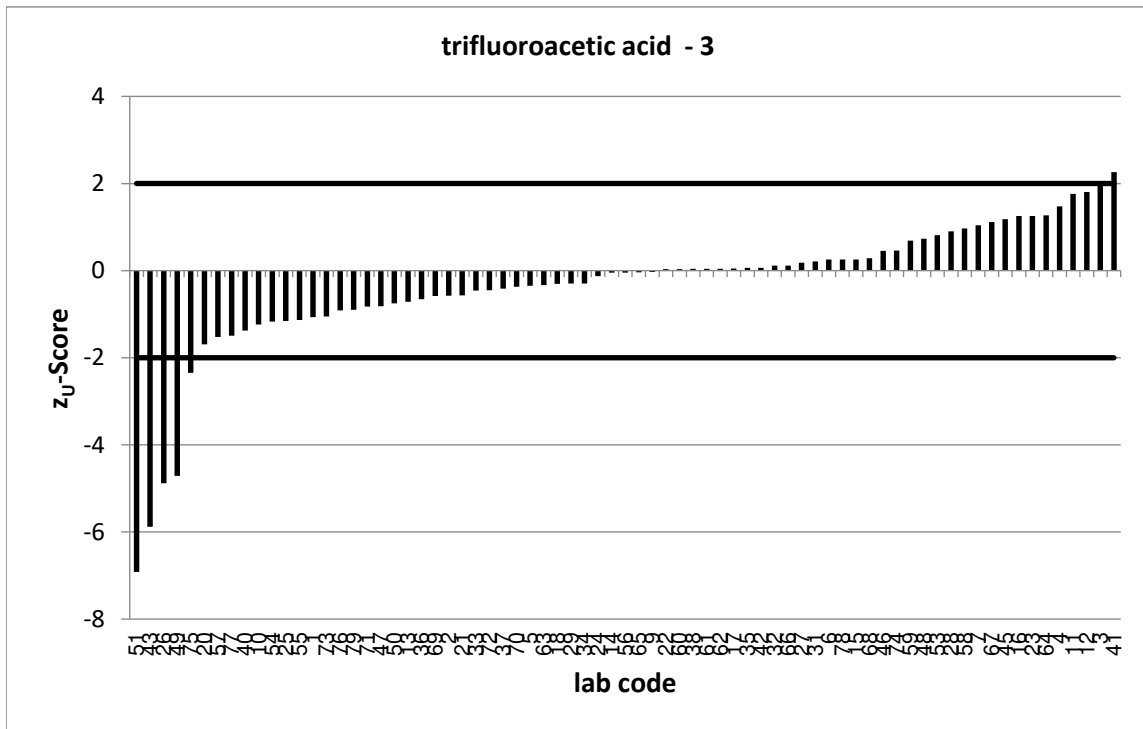
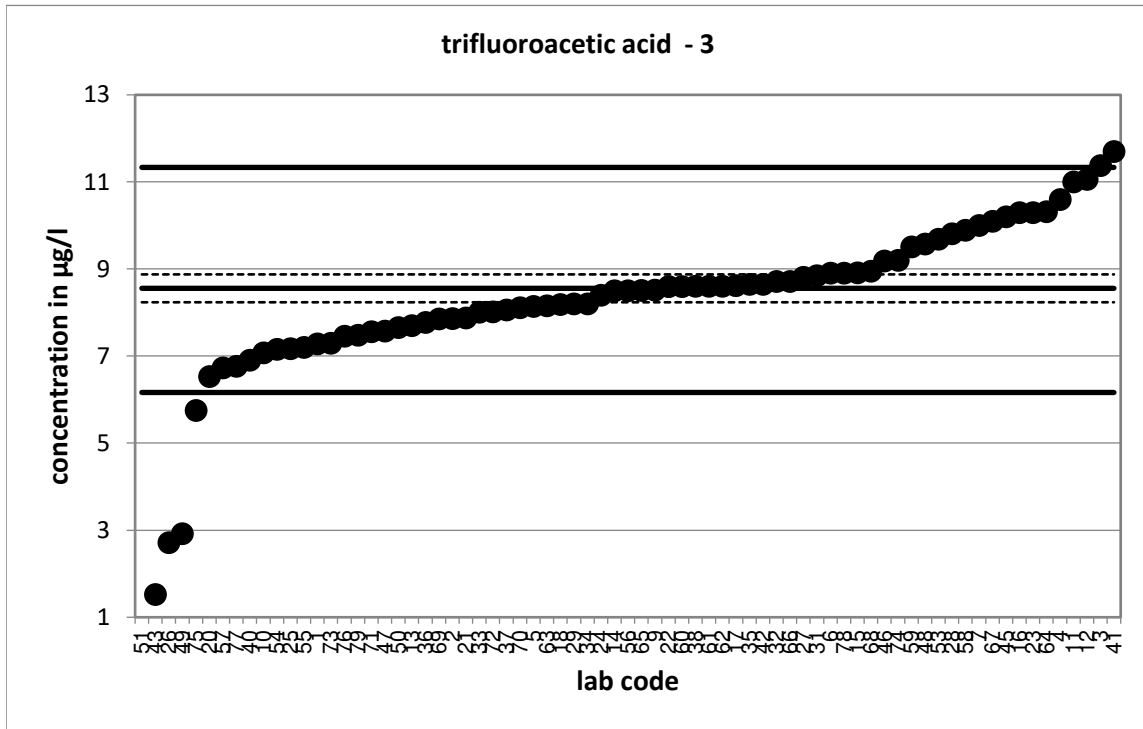
* The stated uncertainty of the assigned value is the expanded uncertainty with a coverage factor $k=2$ corresponding to a confidence level of about 95%

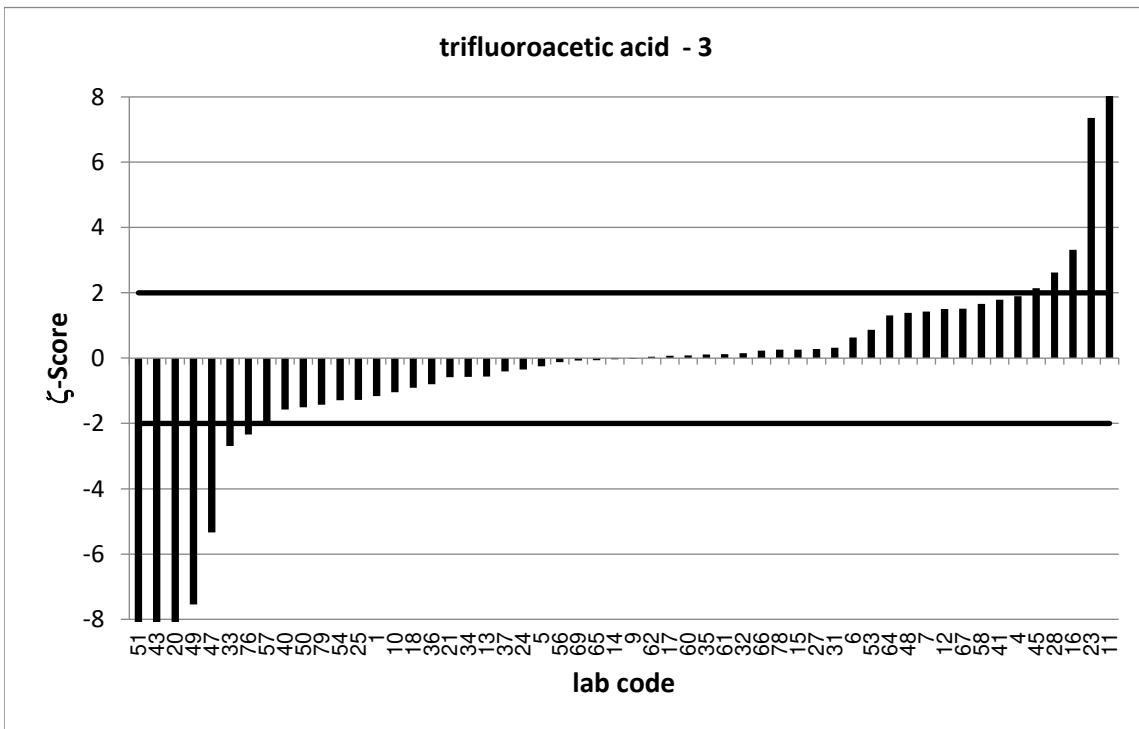
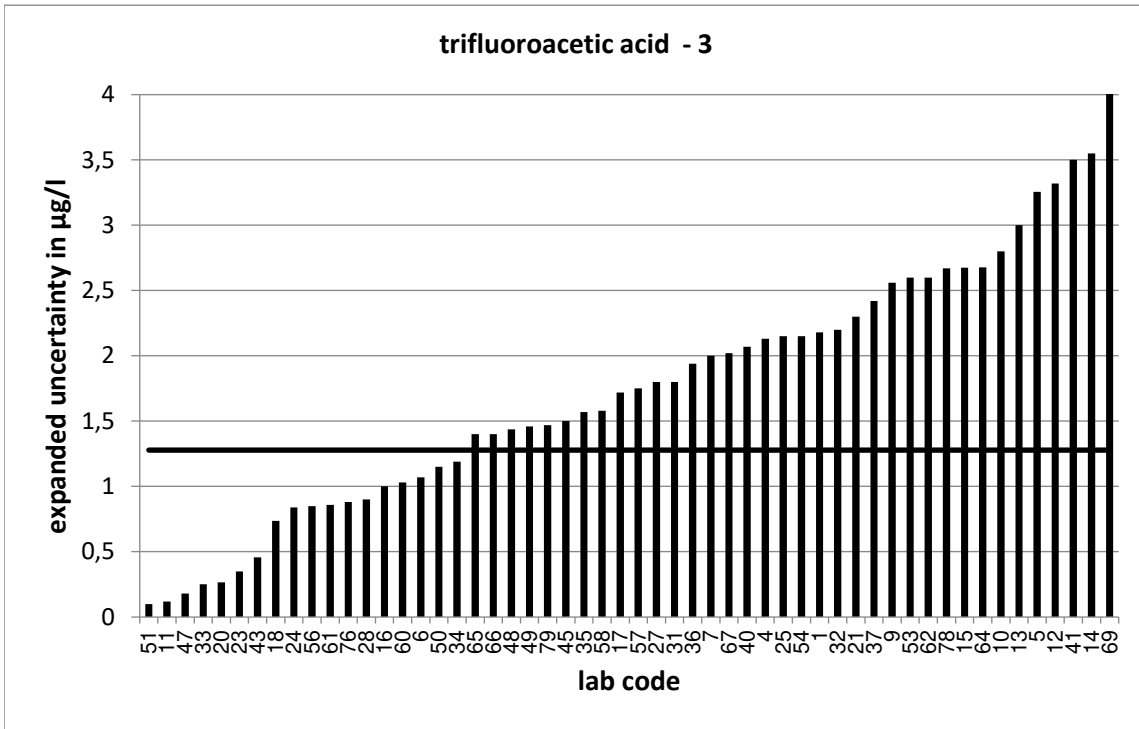
** s = satisfactory, q = questionable, u = unsatisfactory

PT 5/25 - TW S7		trifluoroacetic acid - 3			
assigned value [$\mu\text{g/l}$]*		8,556 \pm 0,32			
upper tolerance limit [$\mu\text{g/l}$]		11,33			
lower tolerance limit [$\mu\text{g/l}$]		6,164			
lab code	result [$\mu\text{g/l}$]	\pm	z-score	z _U -score	assessm.**
53	9,69	2,6	0,9	0,8	s
54	7,16	2,15	-1,3	-1,2	s
55	7,2			-1,1	s
56	8,5	0,85	-0,1	0,0	s
57	6,735	1,751	-2,0	-1,5	s
58	9,896	1,58	1,7	1,0	s
59	9,51			0,7	s
60	8,602	1,03	0,1	0,0	s
61	8,61	0,86	0,1	0,0	s
62	8,61	2,6	0,0	0,0	s
63	8,16			-0,3	s
64	10,318	2,678	1,3	1,3	s
65	8,51	1,4	-0,1	0,0	s
66	8,72	1,4	0,2	0,1	s
67	10,1	2,02	1,5	1,1	s
68	8,95			0,3	s
69	7,86	20	-0,1	-0,6	s
70	8,112			-0,4	s
71	7,566			-0,8	s
72	8,02			-0,4	s
73	7,3			-1,0	s
74	9,2			0,5	s
75	5,75			-2,3	q
76	7,46	0,88	-2,3	-0,9	s
77	6,77			-1,5	s
78	8,91	2,67	0,3	0,3	s
79	7,48	1,47	-1,4	-0,9	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 correctly shown in the diagram.