IFA
Institut für Arbeitsschutz der
Deutschen Gesetzlichen Unfallversicherung

Proficiency testing for in-house and external measuring stations - results and evaluation

Proficiency testing scheme aldehydes

November 2019

Institute for Occupationial Safety and Health of the
German Social Accident Insurance (IFA)
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Summary of laboratory test results

Sample 1

Laboratory	Acetaldehyde	Z score	Outlier type	Formaldehyde	Z score	Outlier type	Propionaldehyde	Z score	Outlier type
Unit	mg/m³			mg/m³			mg/m³		
9	0.64	0.68		0.220	1.23		0.41	2.24	E
10	0.60	-0.04		0.198	0.11		0.29	-1.43	
11	0.58	-0.32		0.190	-0.30		0.33	-0.15	
17	0.62	0.28		0.210	0.72		0.35	0.60	
22	0.59	-0.16		0.190	-0.30		0.34	0.15	
29	0.59	-0.19		0.196	0.01		0.35	0.33	
30	0.64	0.71		0.200	0.21		0.35	0.42	
46	0.58	-0.34		0.184	-0.60		0.32	-0.41	
52	0.61	0.23		0.211	0.77		0.39	1.51	
55	0.59	-0.17		0.194	-0.10		0.32	-0.54	
56	0.60	0.01		0.190	-0.30		0.33	-0.15	
58	0.58	-0.24		0.193	-0.15		0.33	-0.15	
60	0.51	-1.51		0.189	-0.35		0.33	-0.09	
62	0.40	-3.26	BE	0.165	-1.58		0.27	-2.00	E
67	0.55	-0.89		0.178	-0.91		0.32	-0.57	
68				0.194	-0.10				
69	0.56	-0.73		0.216	1.03		0.32	-0.39	
78	0.45	-2.49	BE	0.160	-1.83		0.27	-1.94	
81	0.41	-3.23	BE	0.191	-0.25		0.18	-4.72	BE
83	0.55	-0.83		0.182	-0.71		0.31	-0.75	
94	0.59	-0.14		0.192	-0.20		0.32	-0.48	
98	0.65	0.78		0.205	0.48		0.38	1.44	
100	0.58	-0.36		0.178	-0.90		0.29	-1.30	
114	0.59	-0.14		0.191	-0.25		0.33	-0.21	
126	0.58	-0.26		0.186	-0.50				
135	0.57	-0.54		0.195	-0.05		0.32	-0.51	
151	0.63	0.48		0.208	0.62		0.32	-0.36	

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Sample 1

Laboratory	Acetaldehyde	Z score	Outlier type	Formaldehyde	Z score	Outlier type	Propionaldehyde	Z score	Outlier type
167	0.62	0.38		0.206	0.54		0.37	1.04	
186	0.62	0.41		0.202	0.31		0.35	0.60	
190	0.61	0.18		0.280	4.29	BE	0.35	0.45	
192	0.64	0.73		0.207	0.57		0.37	1.04	
195	1.18	9.64	BE	0.434	12.15	BE	0.71	11.29	BE
198	0.57	-0.56		0.192	-0.20		0.33	-0.24	
199	0.59	-0.09		0.171	-1.27		0.23	-3.25	BE
201	0.62	0.34		0.202	0.31		0.35	0.45	
206	0.62	0.34		0.190	-0.30		0.35	0.45	
207	0.60	-0.01		0.195	-0.05		0.32	-0.33	
208	0.67	1.16		0.211	0.77		0.37	1.16	
216	0.59	-0.22		0.197	0.06		0.36	0.72	
228	0.66	1.01		0.233	1.89		0.36	0.89	
256	0.59	-0.07		0.193	-0.15		0.34	0.00	
258	0.60	-0.04		0.188	-0.40		0.31	-0.69	
290	0.68	1.34		0.230	1.74		0.35	0.45	
292				0.200	0.21				
511	0.53	-1.18		0.199	0.16		0.29	-1.25	
–	–	– –		–	– –		–	– –	
Method	ISO 5725-2			ISO 5725-2			ISO 5725-2		
Assessment	|Z|<=2.00			|Z|<=2.00			|Z|<=2.00		
No. of laboratories that submitted results	43			45			42		
Mean	0.60			0.196			0.34		
Reproducibility s.d.	0.04			0.015			0.03		
Rel. reproducibility s.d.	6.10 %			7.49 %			9.17 %		
Reference value	0.58			0.177			0.33		
Target s.d.	0.06			0.020			0.03		
Rel. target s.d.	10.00 %			10.00 %			10.00 %		
Low er limit of tolerance	0.48			0.157			0.27		
Upper limit of tolerance	0.72			0.235			0.40		
Type B outliers	4			2			3		
No. of laboratories after elimination of outliers type A-D and F (w ithout	39			43			39		

Laboratory	Acetaldehyde	Z score	Outlier type	Formaldehyde	Z score	Outlier type	Propionaldehyde	Z score	Outlier type
laboratories that only gave states but no measured values)									

Explanation of outlier types	
A: Single outlier	Grubbs
B: Differing laboratory mean	Grubbs
C: Excessive laboratory s.d.	Cochran
D: Excluded manually	
E: mean outside tolerance limits	
F: |Z-Score|>3.5	

Summary of laboratory test results

Sample 2

Laboratory	Acetaldehyde	Z score	Outlier type	Butyraldehyde	Z score	Outlier type	Formaldehyde	Z score	Outlier type
Unit	mg/m³			mg/m³			mg/m³		
9	0.42	0.87		1.07	3.34	BE	0.040	-0.14	
10	0.37	-0.48		0.82	0.29		0.041	0.11	
11	0.39	0.09		0.85	0.60		0.040	-0.14	
17	0.41	0.71		0.91	1.31		0.046	1.34	
22	0.38	-0.17		0.81	0.10		0.040	-0.14	
29	0.37	-0.43					0.038	-0.51	
30	0.43	1.13		0.86	0.69		0.042	0.35	
46	0.38	-0.10		0.82	0.17		0.038	-0.58	
52	0.40	0.35		0.86	0.72		0.045	1.21	
55	0.37	-0.50		0.75	-0.61		0.039	-0.39	
56	0.39	0.09		0.76	-0.52		0.040	-0.14	
58	0.38	-0.06		0.80	0.03		0.040	-0.14	
60	0.37	-0.35		0.82	0.29		0.039	-0.31	
62	0.28	-2.68	BE	0.69	-1.44		0.037	-0.88	
67	0.36	-0.79					0.036	-1.13	
68							0.037	-0.88	
69	0.38	-0.25					0.047	1.58	
78	0.20	-4.83	BE	0.34	-5.76	BE	0.020	-5.07	BE
81	0.24	-3.79	BE	0.30	-6.20	BE	0.045	1.09	
83	0.35	-0.94		0.74	-0.76		0.039	-0.39	
94	0.38	-0.17		0.74	-0.73		0.039	-0.39	
98	0.43	1.01		0.92	1.43		0.044	0.77	
100	0.37	-0.30		0.72	-1.02		0.037	-0.90	
114	0.38	-0.25		0.83	0.35		0.039	-0.39	
126	0.38	-0.30					0.035	-1.37	
135	0.36	-0.56		0.79	-0.10		0.040	-0.14	
151	0.40	0.32		0.73	-0.91		0.043	0.60	

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Sample 2

Laboratory	Acetaldehyde	Z score	Outlier type	Butyraldehyde	Z score	Outlier type	Formaldehyde	Z score	Outlier type
167	0.41	0.50		0.86	0.75		0.043	0.55	
186	0.39	0.14		0.80	0.03		0.039	-0.39	
190	0.39	0.09		0.81	0.10		0.057	4.05	BE
192	0.40	0.27		0.82	0.28		0.040	-0.14	
195	0.52	3.48	BE				0.057	4.15	BE
198	0.36	-0.66		0.77	-0.45		0.040	-0.14	
199	0.41	0.63		0.64	-2.04	E	0.039	-0.39	
201	0.41	0.48		0.87	0.88		0.041	0.13	
206	0.32	-1.72		0.71	-1.15		0.030	-2.61	E
207	0.39	0.12		0.78	-0.23		0.042	0.35	
208	0.42	0.81		0.85	0.63		0.044	0.85	
216	0.36	-0.61		0.77	-0.38		0.039	-0.39	
228	0.41	0.48		0.87	0.85		0.046	1.34	
256	0.39	0.06		0.93	1.54		0.041	0.11	
258	0.37	-0.32		0.74	-0.71		0.037	-0.88	
290	0.46	1.90		0.85	0.60		0.050	2.32	E
292							0.040	-0.14	
511	0.34	-1.10		0.76	-0.56		0.046	1.34	
–	–	– –		–	– –		–	– –	
Method	ISO 5725-2			ISO 5725-2			ISO 5725-2		
Assessment	|Z|<=2.00			|Z|<=2.00			|Z|<=2.00		
No. of laboratories that submitted results	43			38			45		
Mean	0.39			0.80			0.041		
Reproducibility s.d.	0.03			0.07			0.004		
Rel. reproducibility s.d.	6.76 %			8.25 %			9.00 %		
Reference value	0.38			0.84			0.036		
Target s.d.	0.04			0.08			0.004		
Rel. target s.d.	10.00 %			10.00 %			10.00 %		
Low er limit of tolerance	0.31			0.64			0.032		
Upper limit of tolerance	0.46			0.96			0.049		
Type B outliers	4			3			3		
No. of laboratories after elimination of outliers type A-D and F (w ithout	39			35			42		

Laboratory	Acetaldehyde	Z score	Outlier type	Butyraldehyde	Z score	Outlier type	Formaldehyde	Z score	Outlier type
laboratories that only gave states but no measured values)									

Explanation of outlier types	
A: Single outlier	Grubbs
B: Differing laboratory mean	Grubbs
C: Excessive laboratory s.d.	Cochran
D: Excluded manually	
E: mean outside tolerance limits	
F: |Z-Score|>3.5	

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Sample 2

Laboratory	Propionaldehyde	Z score	Outlier type
Unit	mg/m³		
9	0.72	3.47	BE
10	0.45	-1.58	
11	0.56	0.48	
17	0.59	1.08	
22	0.55	0.29	
29	0.54	0.12	
30	0.54	0.16	
46	0.53	-0.06	
52	0.57	0.75	
55	0.49	-0.89	
56	0.52	-0.27	
58	0.54	0.12	
60	0.55	0.35	
62	0.47	-1.30	
67	0.50	-0.59	
69	0.54	0.10	
78	0.20	-6.26	BE
81	0.30	-4.31	BE
83	0.50	-0.63	
94	0.51	-0.38	
98	0.63	1.76	
100	0.48	-1.04	
114	0.52	-0.27	
135	0.51	-0.40	
151	0.51	-0.40	
167	0.60	1.21	
186	0.56	0.38	
190	0.55	0.29	
192	0.56	0.38	
195	0.76	4.28	BE
198	0.52	-0.22	
199	0.39	-2.76	BE

Laboratory	Propionaldehyde	Z score	Outlier type
201	0.57	0.70	
206	0.46	-1.39	
207	0.53	-0.05	
208	0.58	0.89	
216	0.54	0.10	
228	0.56	0.57	
256	0.55	0.20	
258	0.50	-0.63	
290	0.60	1.22	
511	0.48	-1.04	
–	–	– –	
Method	ISO 5725-2		
Assessment	|Z|<=2.00		
No. of laboratories that submitted results	42		
Mean	0.53		
Reproducibility s.d.	0.04		
Rel. reproducibility s.d.	7.67 %		
Reference value	0.54		
Target s.d.	0.05		
Rel. target s.d.	10.00 %		
Low er limit of tolerance	0.43		
Upper limit of tolerance	0.64		
Type B outliers	5		
No. of laboratories after elimination of outliers type A-D and F (w ithout laboratories that only gave states but no measured values)	37		

Summary of laboratory test results

Sample 3

Laboratory	Acetaldehyde	Z score	Outlier type	Butyraldehyde	Z score	Outlier type	Formaldehyde	Z score	Outlier type
Unit	mg/m³			mg/m³			mg/m³		
9	0.93	1.53		0.60	3.63	BE	0.100	1.68	
10	0.76	-0.57		0.44	0.07		0.084	-0.19	
11	0.82	0.16		0.46	0.45		0.083	-0.31	
17	0.88	0.93		0.51	1.57		0.094	0.98	
22	0.82	0.16		0.45	0.23		0.080	-0.66	
29	0.79	-0.20					0.082	-0.41	
30	0.90	1.17		0.49	1.16		0.087	0.16	
46	0.82	0.20		0.45	0.32		0.083	-0.32	
52	0.84	0.43		0.47	0.74		0.092	0.80	
55	0.81	0.04		0.43	-0.18		0.085	-0.07	
56	0.85	0.53		0.44	0.00		0.090	0.51	
58	0.83	0.31		0.45	0.23		0.086	0.04	
60	0.65	-1.89		0.45	0.32		0.083	-0.32	
62	0.61	-2.39	E	0.39	-1.25		0.078	-0.89	
67	0.75	-0.71					0.076	-1.12	
68							0.082	-0.42	
69	0.78	-0.30					0.096	1.21	
78	0.62	-2.32	E	0.34	-2.27	E	0.070	-1.83	
81	0.60	-2.55	E	0.16	-6.32	BE	0.089	0.39	
83	0.75	-0.68		0.41	-0.73		0.079	-0.77	
94	0.82	0.16		0.41	-0.66		0.082	-0.42	
98	0.90	1.17		0.50	1.41		0.092	0.77	
100	0.80	-0.11		0.39	-1.15		0.078	-0.91	
114	0.84	0.45		0.48	0.84		0.085	-0.07	
126	0.80	-0.10					0.074	-1.36	
135	0.79	-0.20		0.44	0.07		0.084	-0.19	
151	0.85	0.58		0.40	-0.82		0.091	0.63	

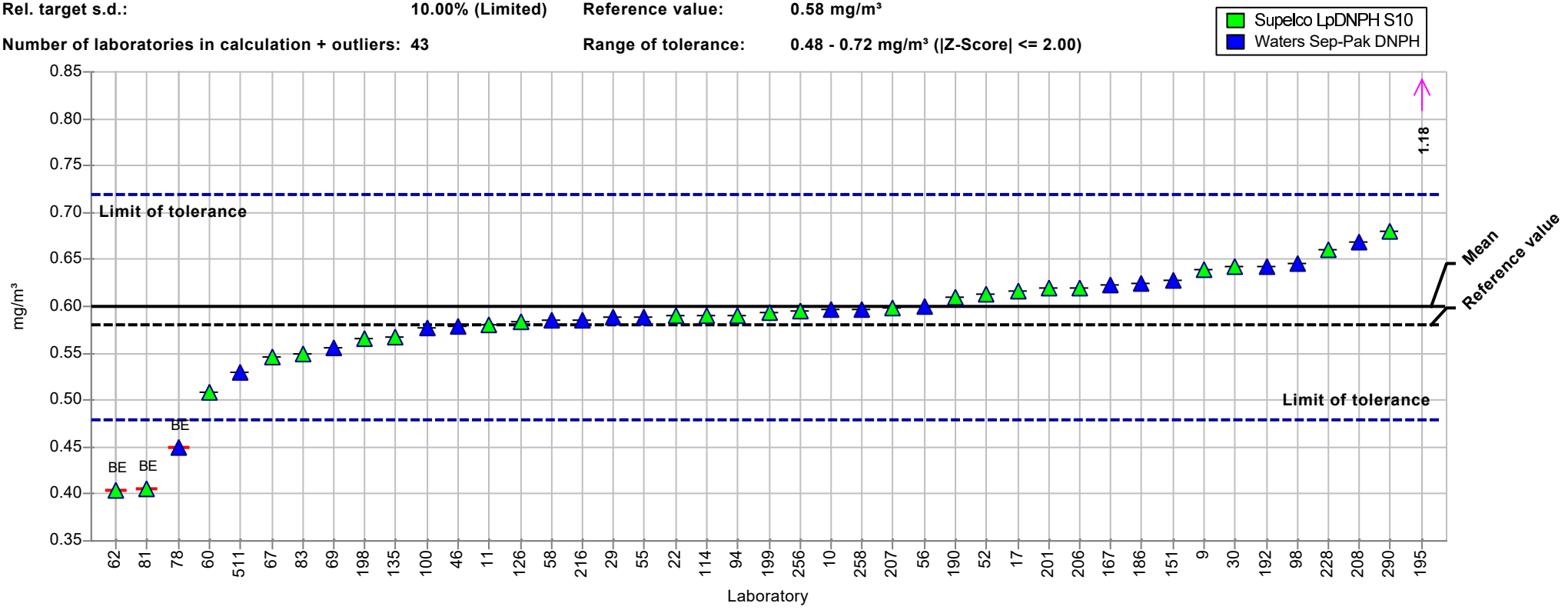
Laboratory	Acetaldehyde	Z score	Outlier type	Butyraldehyde	Z score	Outlier type	Formaldehyde	Z score	Outlier type
167	0.83	0.33		0.46	0.46		0.087	0.11	
186	0.84	0.46		0.44	0.09		0.083	-0.31	
190	0.83	0.29		0.46	0.45		0.120	4.01	BE
192	0.84	0.45		0.45	0.20		0.085	-0.07	
195	0.82	0.14					0.090	0.49	
198	0.80	-0.10		0.44	-0.02		0.086	0.04	
199	0.89	1.02		0.36	-1.84		0.081	-0.54	
201	0.88	0.84		0.46	0.54		0.089	0.44	
206	0.67	-1.70		0.36	-1.82		0.060	-2.99	BE
207	0.83	0.24		0.43	-0.14		0.086	0.04	
208	0.90	1.20		0.48	0.91		0.090	0.51	
216	0.78	-0.37		0.43	-0.12		0.083	-0.31	
228	0.87	0.83		0.49	1.09		0.098	1.44	
256	0.82	0.22		0.51	1.52		0.084	-0.19	
258	0.76	-0.58		0.39	-1.23		0.076	-1.12	
290	0.94	1.65		0.45	0.23		0.100	1.68	
292							0.090	0.51	
511	0.75	-0.74		0.41	-0.64		0.089	0.39	
–	–	– –		–	– –		–	– –	
Method	ISO 5725-2			ISO 5725-2			ISO 5725-2		
Assessment	|Z|<=2.00			|Z|<=2.00			|Z|<=2.00		
No. of laboratories that submitted results	43			38			45		
Mean	0.81			0.44			0.086		
Reproducibility s.d.	0.08			0.04			0.007		
Rel. reproducibility s.d.	9.89 %			9.42 %			7.74 %		
Reference value	0.82			0.45			0.082		
Target s.d.	0.08			0.04			0.009		
Rel. target s.d.	10.00 %			10.00 %			10.00 %		
Low er limit of tolerance	0.65			0.35			0.069		
Upper limit of tolerance	0.97			0.53			0.103		
Type B outliers				2			2		
No. of laboratories after elimination of outliers type A-D and F (w ithout	43			36			43		

Laboratory	Acetaldehyde	Z score	Outlier type	Butyraldehyde	Z score	Outlier type	Formaldehyde	Z score	Outlier type
laboratories that only gave states but no measured values)									

Explanation of outlier types	
A: Single outlier	Grubbs
B: Differing laboratory mean	Grubbs
C: Excessive laboratory s.d.	Cochran
D: Excluded manually	
E: mean outside tolerance limits	
F: |Z-Score|>3.5	

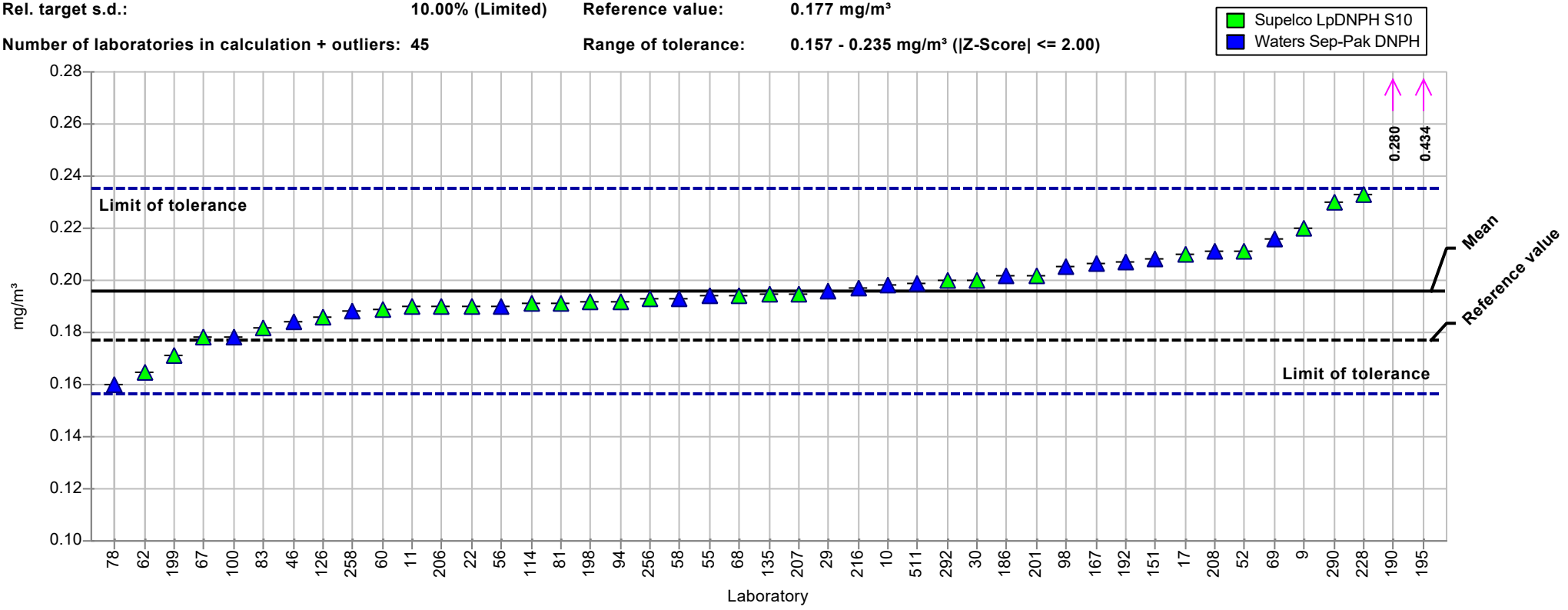
Summary results

Sample:	**1**	**Mean:**	**0.60 mg/m³**
Measurand:	**Acetaldehyde**	**Reproducibility s.d.:**	**0.04 mg/m³**
Method:	**ISO 5725-2**	**Rel. reproducibility s.d.:**	**6.10%**
Rel. target s.d.:	**10.00% (Limited)**	**Reference value:**	**0.58 mg/m³**
Number of laboratories in calculation + outliers:	**43**	**Range of tolerance:**	**0.48 - 0.72 mg/m³ (|Z-Score| <= 2.00)**



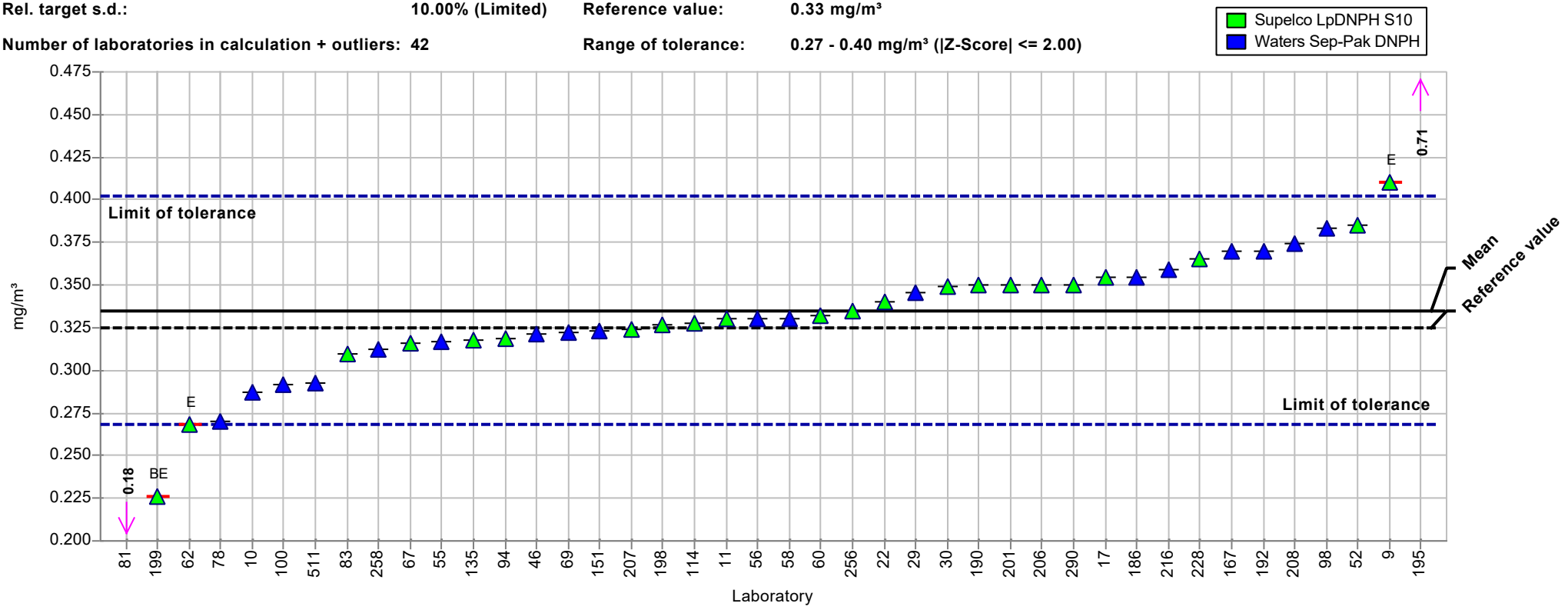
Summary results

Sample:	**1**	**Mean:**	**0.196 mg/m³**
Measurand:	**Formaldehyde**	**Reproducibility s.d.:**	**0.015 mg/m³**
Method:	**ISO 5725-2**	**Rel. reproducibility s.d.:**	**7.49%**
Rel. target s.d.:	**10.00% (Limited)**	**Reference value:**	**0.177 mg/m³**
Number of laboratories in calculation + outliers:	**45**	**Range of tolerance:**	**0.157 - 0.235 mg/m³ (|Z-Score| <= 2.00)**



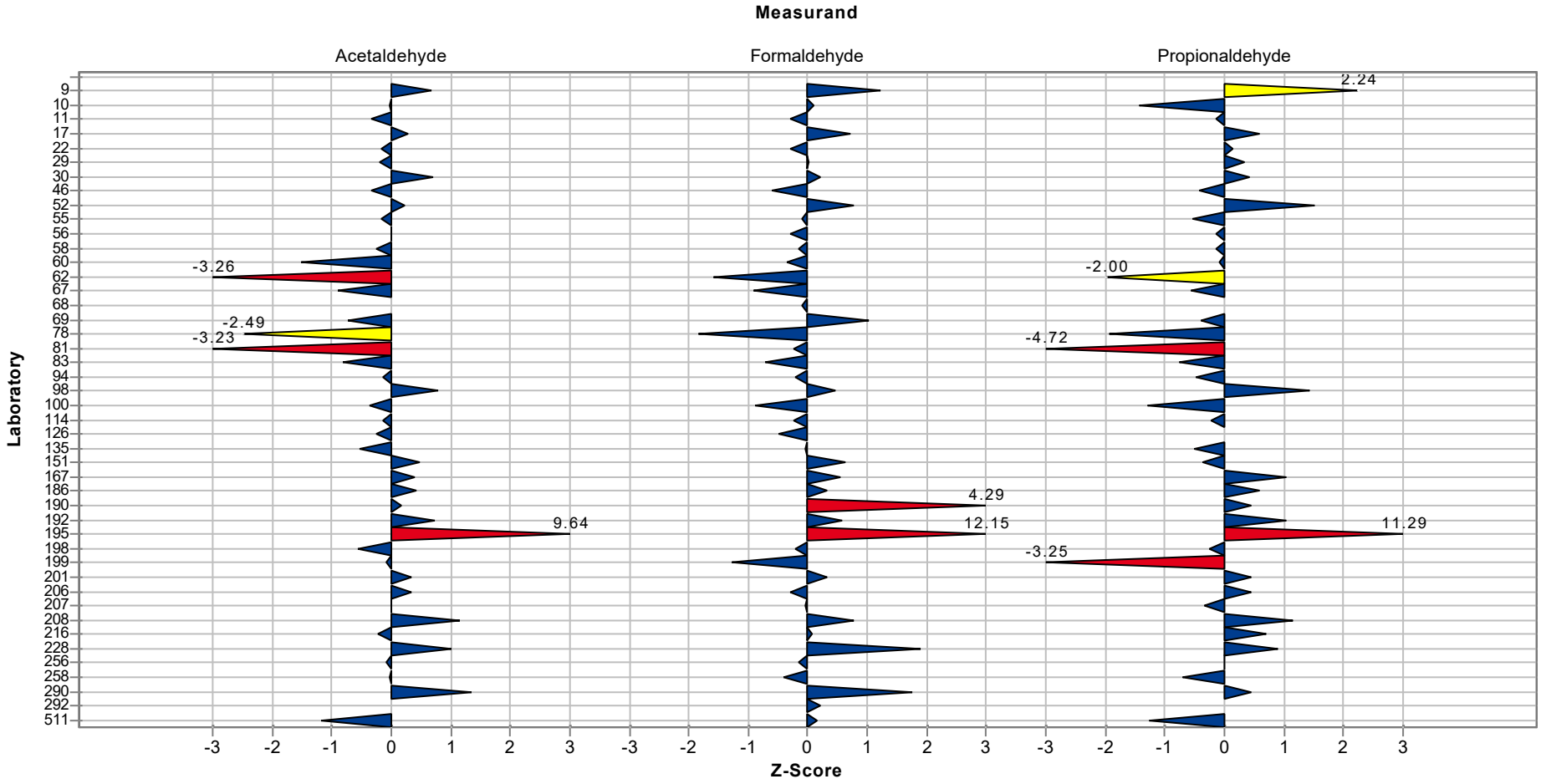
Summary results

Sample:	**1**	**Mean:**	**0.34 mg/m³**
Measurand:	**Propionaldehyde**	**Reproducibility s.d.:**	**0.03 mg/m³**
Method:	**ISO 5725-2**	**Rel. reproducibility s.d.:**	**9.17%**
Rel. target s.d.:	**10.00% (Limited)**	**Reference value:**	**0.33 mg/m³**
Number of laboratories in calculation + outliers:	**42**	**Range of tolerance:**	**0.27 - 0.40 mg/m³ (|Z-Score| <= 2.00)**



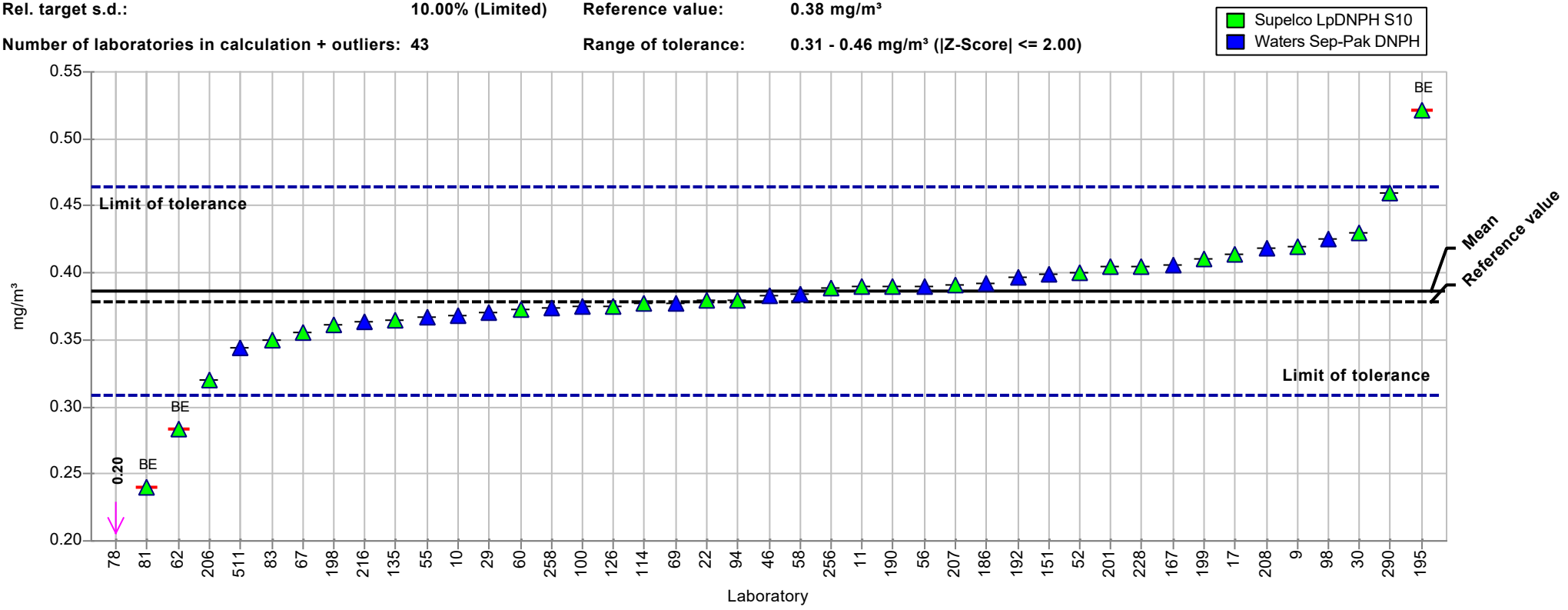
Sample chart of *Z-Scores*

Sample: 1



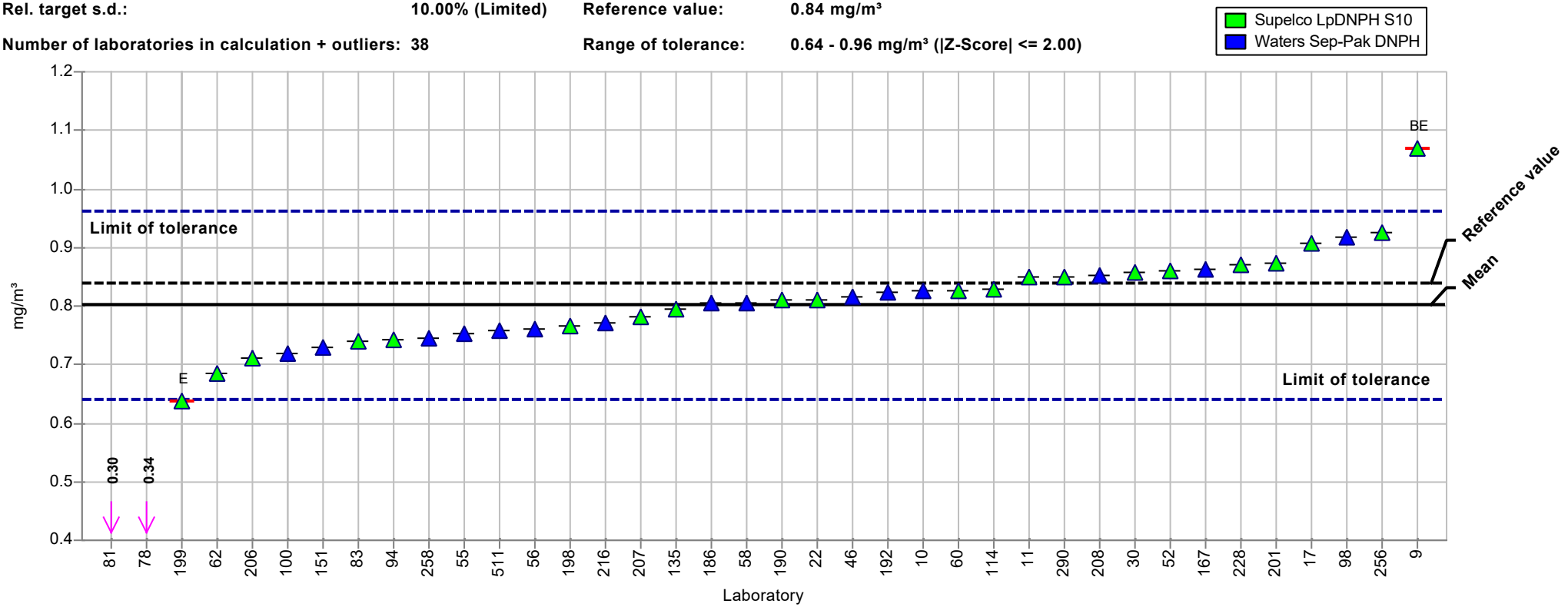
Summary results

Sample:	**2**	**Mean:**	**0.39 mg/m³**
Measurand:	**Acetaldehyde**	**Reproducibility s.d.:**	**0.03 mg/m³**
Method:	**ISO 5725-2**	**Rel. reproducibility s.d.:**	**6.76%**
Rel. target s.d.:	**10.00% (Limited)**	**Reference value:**	**0.38 mg/m³**
Number of laboratories in calculation + outliers:	**43**	**Range of tolerance:**	**0.31 - 0.46 mg/m³ (|Z-Score| <= 2.00)**



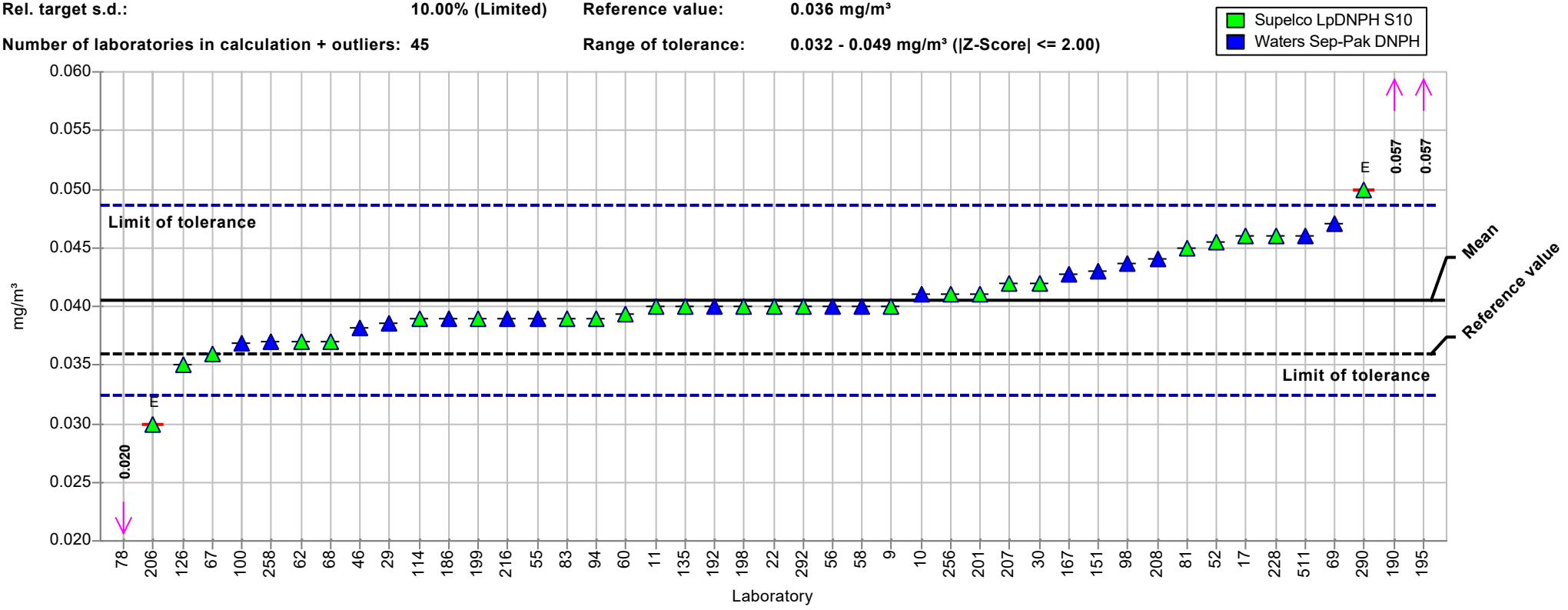
Summary results

Sample:	**2**	**Mean:**	**0.80 mg/m³**
Measurand:	**Butyraldehyde**	**Reproducibility s.d.:**	**0.07 mg/m³**
Method:	**ISO 5725-2**	**Rel. reproducibility s.d.:**	**8.25%**
Rel. target s.d.:	**10.00% (Limited)**	**Reference value:**	**0.84 mg/m³**
Number of laboratories in calculation + outliers:	**38**	**Range of tolerance:**	**0.64 - 0.96 mg/m³ (|Z-Score| <= 2.00)**



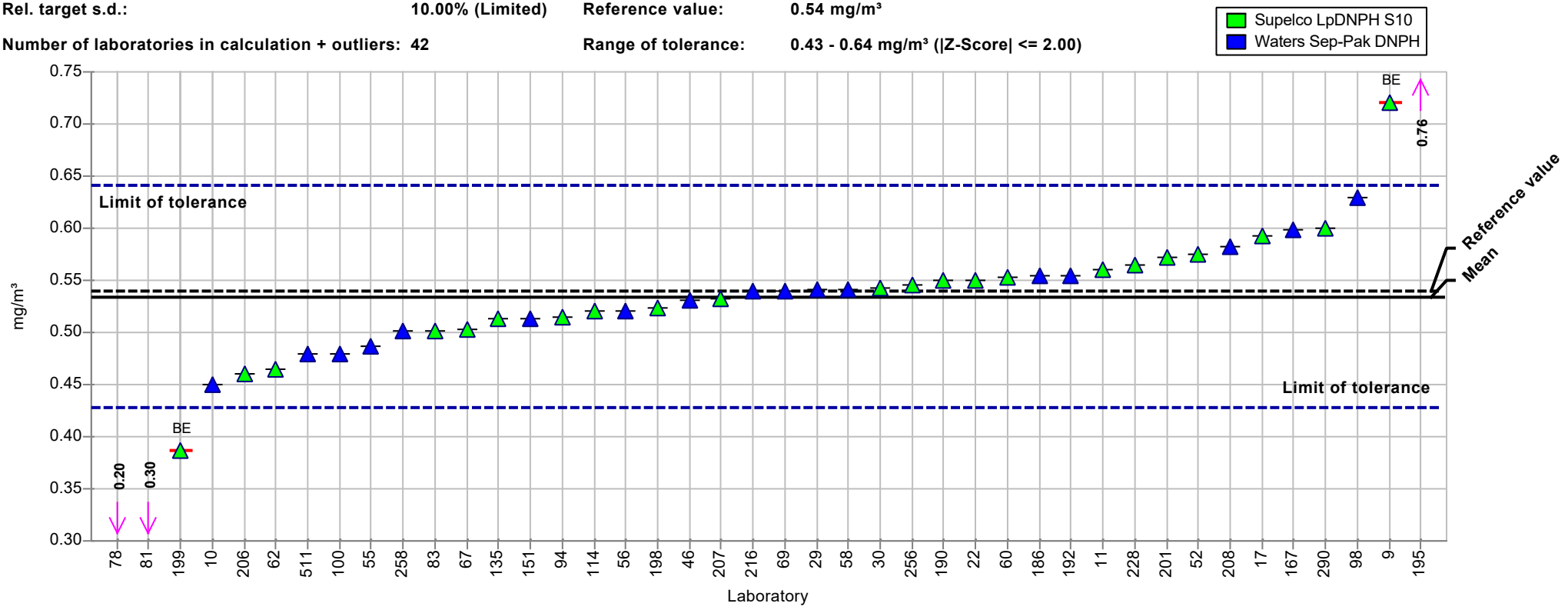
Summary results

Sample:	**2**	**Mean:**	**0.041 mg/m³**
Measurand:	**Formaldehyde**	**Reproducibility s.d.:**	**0.004 mg/m³**
Method:	**ISO 5725-2**	**Rel. reproducibility s.d.:**	**9.00%**
Rel. target s.d.:	**10.00% (Limited)**	**Reference value:**	**0.036 mg/m³**
Number of laboratories in calculation + outliers:	**45**	**Range of tolerance:**	**0.032 - 0.049 mg/m³ (|Z-Score| <= 2.00)**



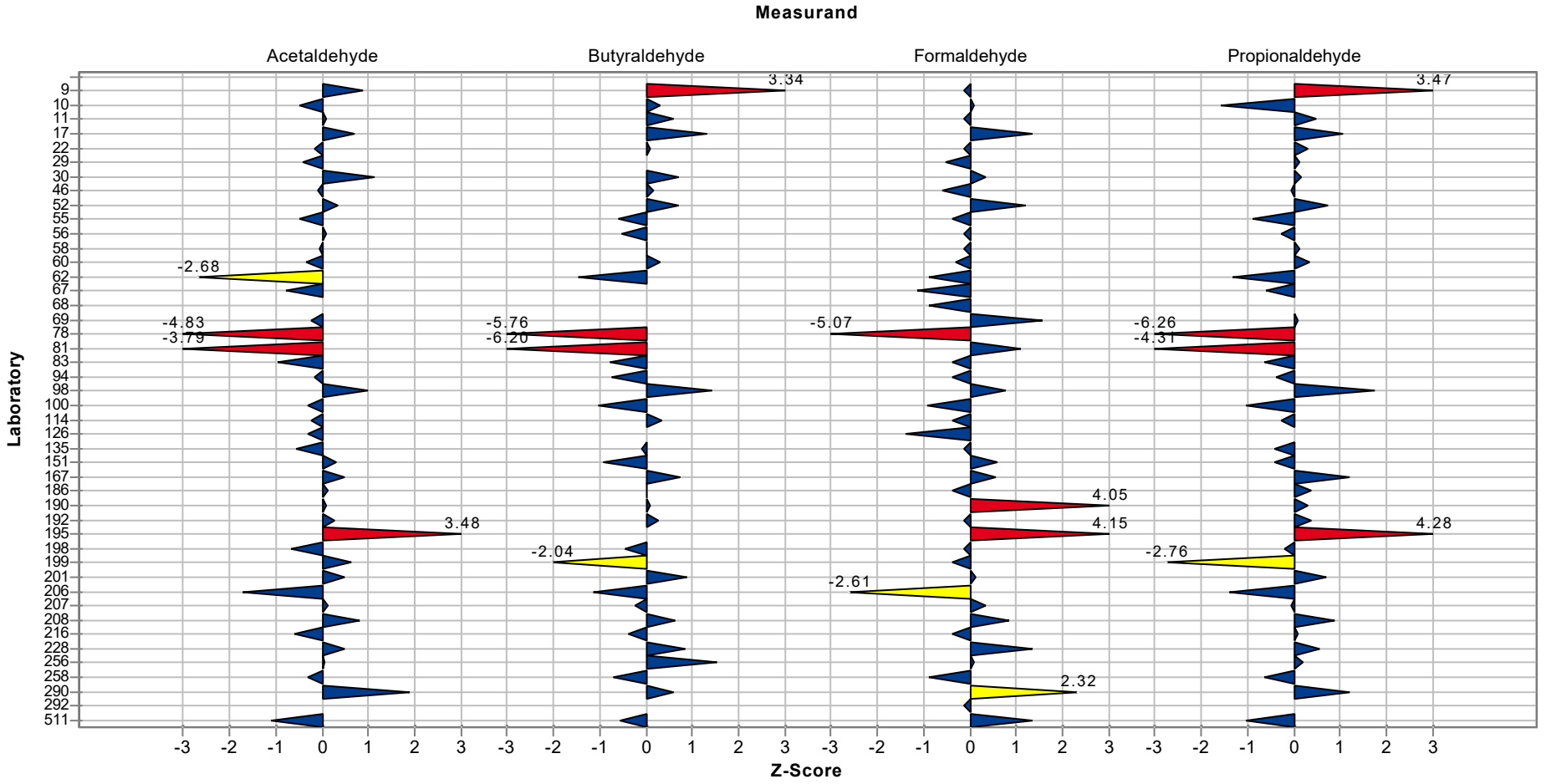
Summary results

Sample:	**2**	**Mean:**	**0.53 mg/m³**
Measurand:	**Propionaldehyde**	**Reproducibility s.d.:**	**0.04 mg/m³**
Method:	**ISO 5725-2**	**Rel. reproducibility s.d.:**	**7.67%**
Rel. target s.d.:	**10.00% (Limited)**	**Reference value:**	**0.54 mg/m³**
Number of laboratories in calculation + outliers:	**42**	**Range of tolerance:**	**0.43 - 0.64 mg/m³ (|Z-Score| <= 2.00)**



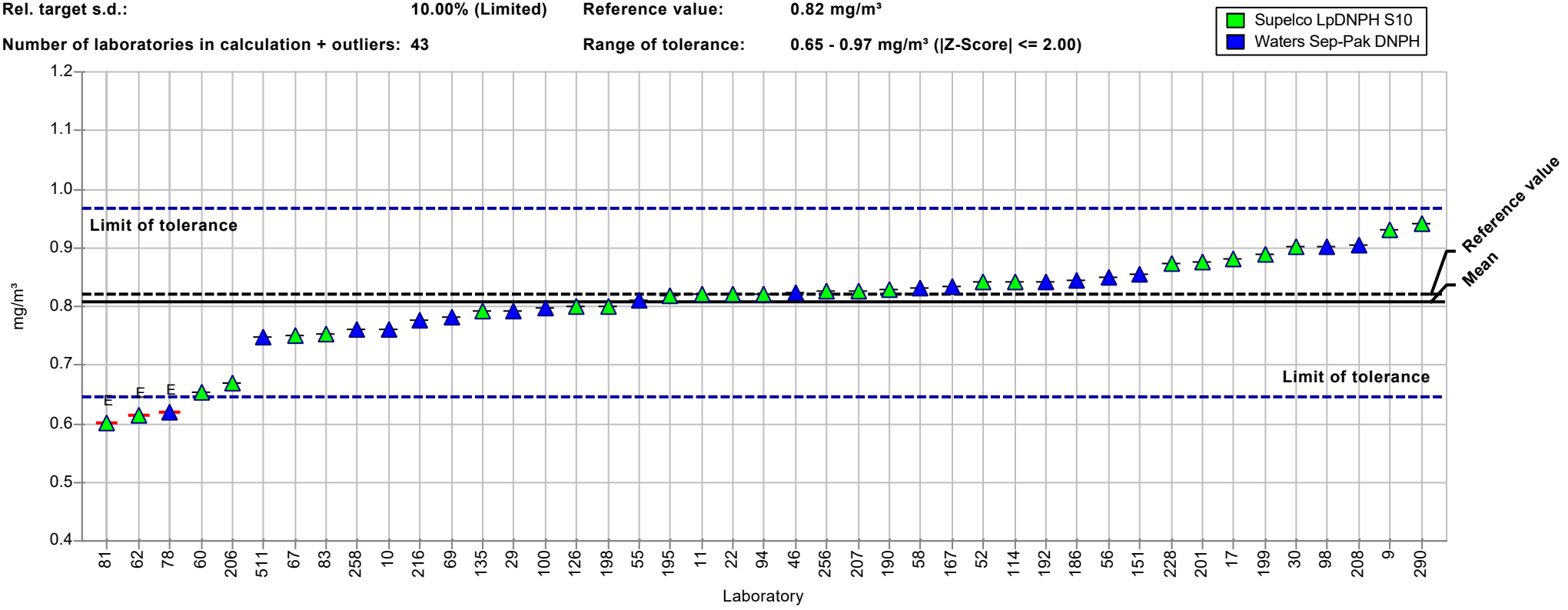
Sample chart of *Z-Scores*

Sample: 2



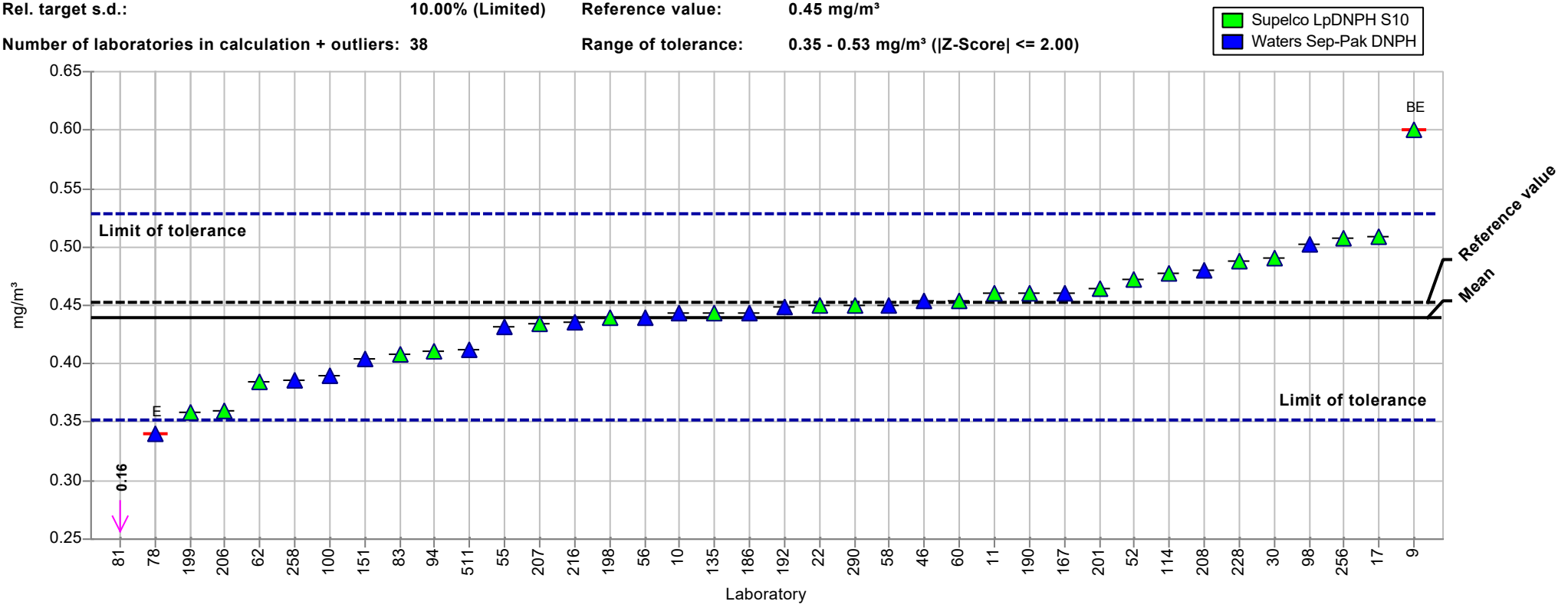
Summary results

Sample:	**3**	**Mean:**	**0.81 mg/m³**
Measurand:	**Acetaldehyde**	**Reproducibility s.d.:**	**0.08 mg/m³**
Method:	**ISO 5725-2**	**Rel. reproducibility s.d.:**	**9.89%**
Rel. target s.d.:	**10.00% (Limited)**	**Reference value:**	**0.82 mg/m³**
Number of laboratories in calculation + outliers:	**43**	**Range of tolerance:**	**0.65 - 0.97 mg/m³ (|Z-Score| <= 2.00)**



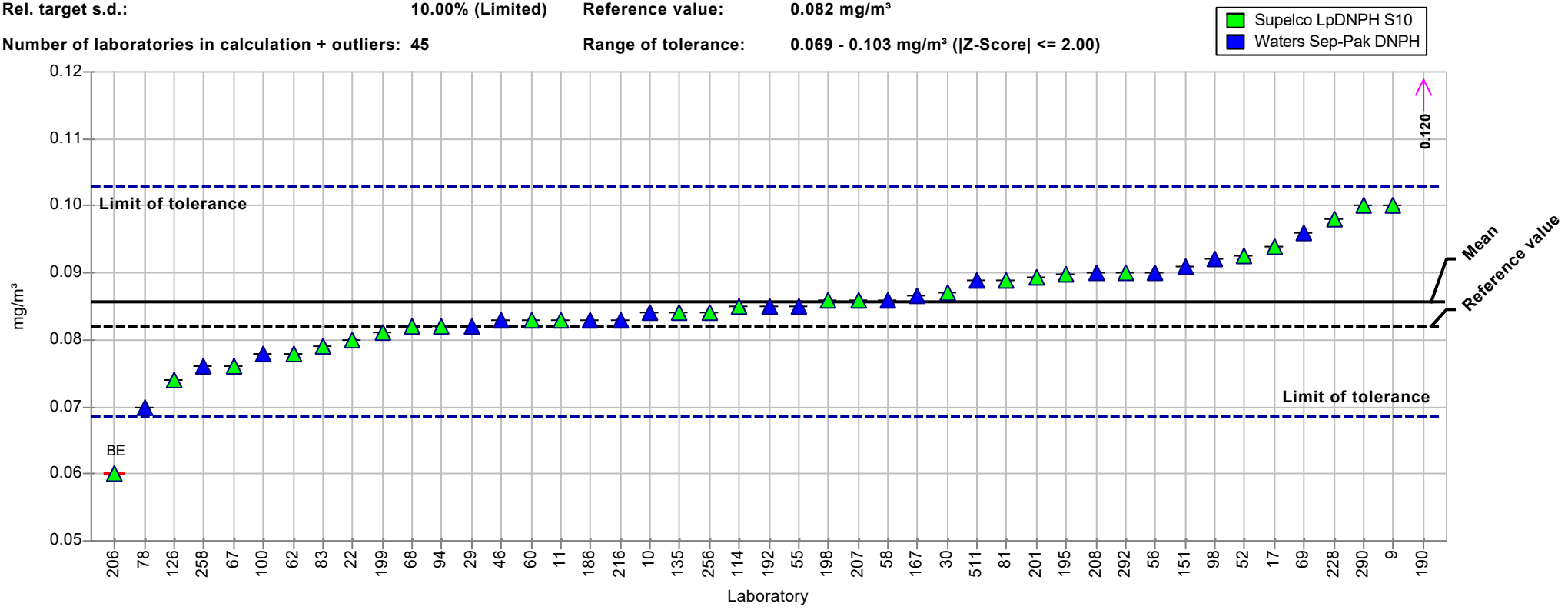
Summary results

Sample:	**3**	**Mean:**	**0.44 mg/m³**
Measurand:	**Butyraldehyde**	**Reproducibility s.d.:**	**0.04 mg/m³**
Method:	**ISO 5725-2**	**Rel. reproducibility s.d.:**	**9.42%**
Rel. target s.d.:	**10.00% (Limited)**	**Reference value:**	**0.45 mg/m³**
Number of laboratories in calculation + outliers:	**38**	**Range of tolerance:**	**0.35 - 0.53 mg/m³ (|Z-Score| <= 2.00)**



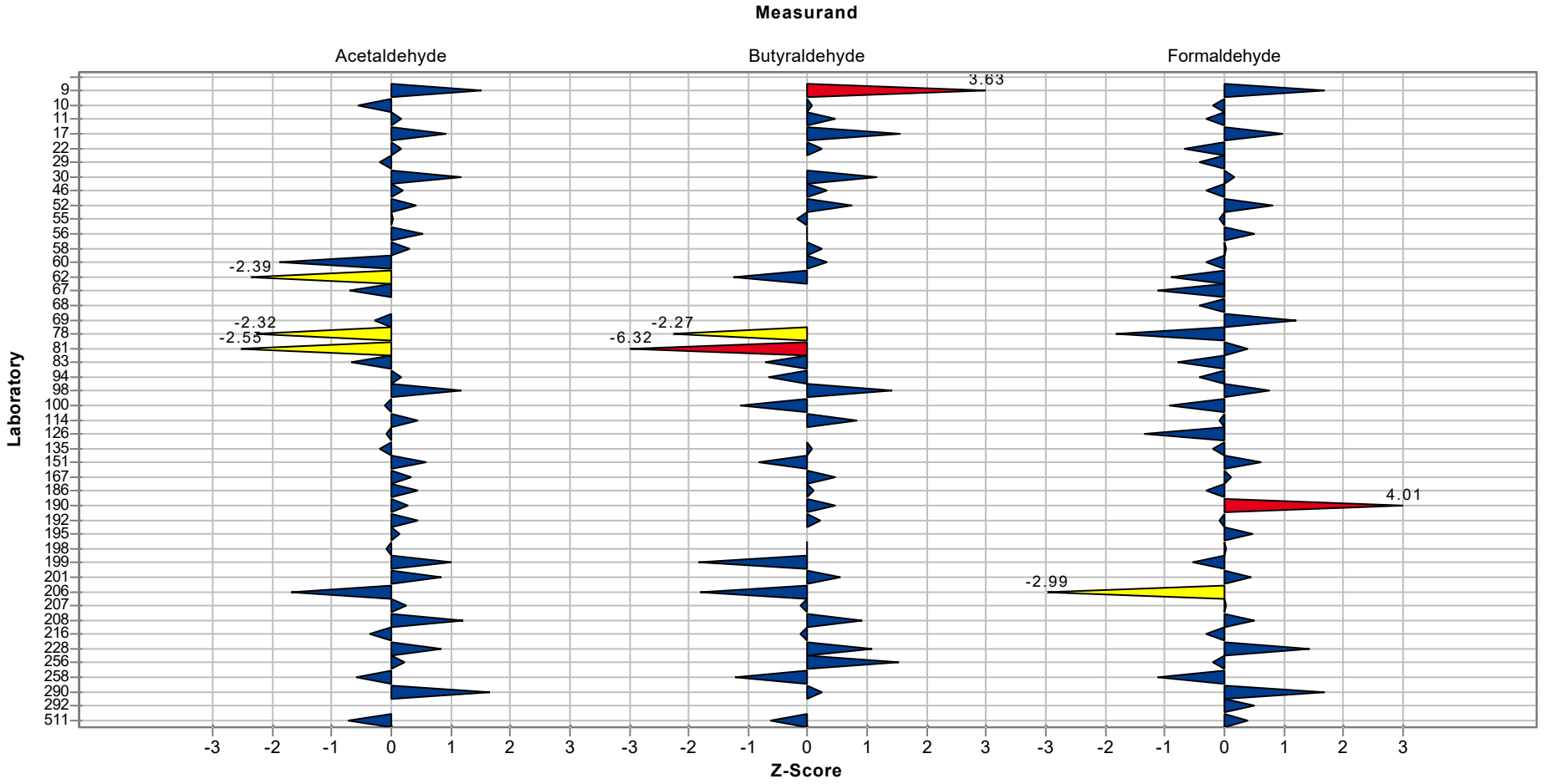
Summary results

Sample:	**3**	**Mean:**	**0.086 mg/m³**
Measurand:	**Formaldehyde**	**Reproducibility s.d.:**	**0.007 mg/m³**
Method:	**ISO 5725-2**	**Rel. reproducibility s.d.:**	**7.74%**
Rel. target s.d.:	**10.00% (Limited)**	**Reference value:**	**0.082 mg/m³**
Number of laboratories in calculation + outliers:	**45**	**Range of tolerance:**	**0.069 - 0.103 mg/m³ (|Z-Score| <= 2.00)**



Sample chart of *Z-Scores*

Sample: 3



Questions and Answers

Participant	Analytical method	Start sample preparation
9	DIN ISO 16000-3:2011, aber mit ESI-MS/MS statt DAD	14.11.2019
10	LC/DAD	19/11/2019
11	ISO 16000-3	12/11/2019
17	Nach Din 16000-3 und DIN 16516	19.11.2019
22	DIN ISO 16000-3 bzw . EN 16516	12.11.2019
29	IFA-Arbeitsmappe 6045, DIN ISO 16000-3, Waters Applikation	13.11.19
30	ISO 16000-3	13/11/2019
46	SAA & DIN ISO 16000-3	13.11.19
52	DIN ISO 16000-3:2011	13.11.2019
55	HPLC - Photodiode array detector	12/11/2019
56	UHPLC w ith UV detection	désoprtion : 13/11/19 nd analysis : 14/11/19
58	HPLV-UV	
60	HPLC-DAD	13/11/2019
62	NF-ISO-16000-3	12/11/2019
67	NIOSH 2016 and NIOSH 2018	I started on the 12th of november 2019
68	interne Arbeitsanw eisung	18.11.19
69	HPLC	18/11/2019
78	IFA 6045	12.11.2019
83	HPLC/DAD	12/11/19
94	ISO 16000-3/ EN 16516	15.11.2019
98	analog IFA6045 (HPLC-DAD)	12.11.2019
100	NF X43-264	11/19/2019
114	HPLC UV	5/12/19
126	DIN ISO 16000-3:2011	14.11.2019
135	HPLC-DAD IFA Arbeitsmappe 6045	11.11.2019
151	ISO 16000-3	14/11/2019
167	HPLC	12.11.2019
186	NF ISO 16000-3	13/11/2019
190	DIN ISO 16000-3: 2011, VDI 3862 Bl.3: 2000	13.11.19
192	ISO16000-3	2019/11/15

Aldehydes 2019

Participant	Analytical method	Start sample preparation
195	NIOSH 2016	20-11-2019
198	ISO 16000-3:2011, EPA TO11A 1999	18-11-19
199	in Anlehnung an DIN 16000-3:2013-01	19.11.2019
201	IFA 6045	28.11.2019
206	DIN 16000-3	12.11.2019
207	DIN-ISO-16000-3	20.11.2019
208	ISO 16000-3:2011	11.11.2019
216	HPLC-UV	10 DEC 2019
228	DIN ISO 16000-3 : 2011	11.11.2019
256	Geopro nach EPA TO-11A	12.11.2019
258	ISO 16000-3	12 November 2019
290	DIN ISO 16000-3:2013-1	13.11.2019
292	HPLC -w ith UV/Vis Detection	11/22/2019
511	UPLC	12/11

Participant	Storage time after desorption
9	Labor, 12 Tage (Tiefkühler), Autosampler (20 °C)
10	0 day
11	NO
17	1 Woche Lagerung / Ankunft:12.11.2019 bei +4°C
22	sofortige Messung
29	nein
30	one day (refrigerator)
46	vom 08.11.19 bis 13.11.19 im Gefrierschrank
52	4 Wochen/ Gefrierschrank
55	less than 1 day - refrigerator
56	1 day stored in refrigerator
60	1 h
62	3 days in refrigerator
67	I desorbed on 12th of november 2019 and I stored at 4°C
68	1 Tag, im Kühlschrank

Aldehydes 2019

Participant	Storage time after desorption
69	One day after desorption in refrigerator
78	Kühlschrank 1-5 °C 1 Tag
83	1H
94	nein
98	Nein, Kühlschrank
100	1 hour at room temperature
114	0
126	im Gefrierschrank bei -18°C
135	nein
151	0
167	30 min for the first samples
186	No storage after desorption
190	nein
192	Formaldehyde,Acetaldehyde:Set in the analyzer immedately after desorption. Roomtemp 24.7degC. Propionaldehyde,Butyraldehyde:Storage time after desorption w as 2days in a freezer at -30degC. After the storage,set in the analyzer. Roomtemp 24.3 degC
195	9 DAYS AT REFRIGERATOR
198	minimun 1 hour, max 16 hours refigerator
199	TK
201	keine Lagerzeit
206	1 Tag +5°C
207	-
208	1 d - refrigerator
216	Immediate analysis after desorption
228	bis zum 11.11. im Kühlschrank
256	1. Analyse direkt nach Extraktion, danach im Kühlschrank
258	Samples w ere received on 11 Novemer 2019 and w ere stored in a refrigerator prior to analysis
290	Lagerung bei -18°C im Gefrierschrank
292	several hours at RT
511	9 days, refrigerator

Participant	Date of analysis	Desorption solution	Volume of desorption solution

Aldehydes 2019

Participant	Date of analysis	Desorption solution	Volume of desorption solution
9	26.11.2019 (Pumpenproblem)	Acetonitril	2
10	19/11/2019	acetonitrile	2
11	12/11/2019	ACETONITRILE	5 ML
17	27.11, 02. - 04.12.2019	Acetonitril	5mL
22	12.11.2019	70% Acetonitril 30% Milli-Q Wasser V/V	5 ml
29	13.11.19	Acetonitril	5
30	14/11/2019	acetonitrile	5 ml
46	13.11.19	ACN	5 mL
52	13.11.2019	Acetonitril	3ml
55	12/11/2019	acetonitrile	3
56	14/11/19	Acetonitril w as used as desorption solution	5 mL
58		Acetonitril	10 ml
60	13/11/2019	Acetonitrile	3mL
62	15/11/2019	Acetonitrile	5
67	I analyzed the samples on the 12th of november	Acetonitrile w as desorbtion solution	10 ml
68	19.11.19	Acetonitril	2 mL
69	19/11/2019	Acetonitrile	5 ml
78	13.11.2019	Acetonitril	10
83	12/11/19	ACN	2
94	15.11.2019	Acetonitril	5
98	18.11.2019 und 19.11.2019	Acetonitril	10 ml
100	11/19/2019	acetonitrile	4 ml
114	5/12/19	Acetonitrile	2
126	19./20.11.2019	CH3CN	10 ml
135	11.11.2019	Acetonitril	2 ml
151	14/11/2019	Acetonitrlie	6
167	12. - 13.11.2019	Acetonitrile (AcN)	6 mL (filled to 10 mL w ith distilled w ater)
186	13/11/2019	acetonitrile	10 mL
190	13.11.19/14.11.19	Acetonitril	4 mL
192	2019/11/16,18	Acetonitrile	5mL
195	22-11-2019	ACEONITRILE	5 mL
198	18-11-19 and 19-11-19.	Acetonitrile HPLC grade	5

Aldehydes 2019

Participant	Date of analysis	Desorption solution	Volume of desorption solution
199	19.11.2019	Acetonitril	3mL
201	28.11.2019	Acetonitril	1 mL
206	13.11.2019	Acetonitril	1 ml
207	20.11.2019	ACN/H2O 60/40 +5mmol (NH4HCO3)	5
208	12.11.2019	Acetonitrile	3 ml
216	10 DEC 2019	Acetonitrile	5 ml
228	11.11.2019	Acetonitril	5 mL
256	12.-13.11.2019	Acetonitril	2.5
258	12 November 2019	Acetonitrile	5
290	15.11.2019	Acetonitril	5ml
292	11/22/2019	Acetonitrile	5 mL
511	21/11	Acetonitril	3 ml

Participant	Chromatography system (HPLC)
9	Agilent 1290 Infinity Binary Pump, Sciex API 4000, Agilent 1290 Infinity Autosampler
10	quaternary pump model 200Q/410, autosample, DAD
11	HPLC-UV
17	HPLC 1290 Infinity II: Highspeed Punp, Multisampler, MCT-Säule, DAD-FS
22	Thermo: Pumpe: LPG-3400SD, Autosampler: WP-3000SL, UV/VIS-Detektor: DAD-3000
29	Thermo Ultimate 3000
30	Waters Alliance 2695 / PDA 2996
46	quaternäre Pumpe, DAD, ALS
52	Perkin Elmer Flexar Quanternary LC Pump, Flexar PDA plus Detektor, LC Flexar Autosampler
55	Acquity Waters UPLC system
56	HPLC/UV [RS Pump, Rs Diode Array, Rs Autosmapler Ultimate 3000 Thermofisher scientific
58	Agilent 1100 series
60	Agilent 1260 Quat Pump, 1260 DAD VL+
62	Agilent pump / Perkin detector
67	I used a quaternary pump a UV/VIS/DAD detector
68	Agilent HPLC 1260 Infinity
69	Elite LabChrom Merck Hitachi, Pump L-2130, Autosampler L-2200

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Participant	Chromatography system (HPLC)
78	Knauer K1001, Knauer, Knauer
83	La Chrom Elite
94	Agilent HPLC 1260 Infinity mit Degasser, Quatpump, ALS, ColComp und DAD
98	Gradienten Pumpe L-2130, Elite LaChrom, VWR; Diodenarray-Detektor L-2455, Elite LaChrom, VWR; kein Autosampler
100	LC-UV Agilent 1200
114	Dionex - Ultimate 3000, Thermo Scientific
126	Ultimate 3000
135	Agilent 1290 Series
151	Waters Acquity H Class
167	Waters e2695 w ith Waters 2487 detector
186	HPLC-PAD, quatemary pump
190	Agilent
192	Agilent 1260 , Agilent 1260 ‡U (Agilent Technologies)
195	Infinity 1290 Agilent
198	quaternary pump, UV detector.
199	Agilent
201	Agilent HPLC 1100 (System C), G1311A Quart.Pumpe, G1315A DAD, G1329A Autosampler
206	Agilent 1100 DAD
207	Agilent 1260 Infinity LC DAD
208	ACQUITY H-class
216	UV detector
228	Shimadzu
256	Agilent 1100 Series; Pumpe: G1311A Quaternary Pump, Detektor: G1315B, Autosampler: G1313A
258	Waters Acquity UPLC H-Class
290	---
292	Waters 1515/2489/2707
511	binairy solvent manager, PDA detector

Participant	Refrigerated Autosampler
9	ja, 20 °C
10	no

Aldehydes 2019

Participant	Refrigerated Autosampler
11	4 °C
17	1290 Multisampler bei +15°C
22	nein
29	nein
30	no
46	nein
52	nein
55	yes/20°C
56	A refrigerated autosampler w as used and the temperature w as ajusted at 15°C
58	no
60	No
62	Refrigerated autosampler at 20°C
67	NO
68	Nein
69	No
78	nein
83	15°C
94	nein
98	Nein
100	no
114	No
126	nein
135	ja, 10°C
151	20C
186	Yes, 4°C
190	ja 30 °C
192	No. Cooling function OFF(Roomtemp)
195	no
198	NO
199	nein
201	ja. 20 °C
206	nein

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Participant	Refrigerated Autosampler
207	-
208	15 °C
216	Autosampler temperature at 25C
228	nein
256	nein
258	No
290	---
292	no
511	20 °C

Participant	Analytical column
9	Phenomenex Kinetex 2.6 u C18 50 x 2.10 mm
10	C18
11	C18
17	Agilent Poroshell 120EC-C18, 4,6x50mm, 2,7µm
22	Thermo Scientific Acclaim Carbonyl C18, 3µm 120A, 3,0x150mm
29	Waters Phenyl 3,5µm, 4,6x150mm
30	Allure AK 200 x 4,6 mm 5µm
46	ODS C18 Silica
52	Kromasil C18
55	Waters Acquity UPLC BEH Phenyl
56	column Acclaim RSLC Carbonyl 2,1*100 mm (Thermo)
58	Zorbax C18 (agilent)
60	Allure C18 5µm 150x4.6mm
62	octadecyl grafted silica phase column
67	I used a ALLTECH-ALLTIMA C18 3µ particles, 150 mm x 4.6 mm
68	Poroshell 120 EC-C18 4,6x50mm, 2,7um
69	Ascentis RP-Amide 25cm X4,6mm
78	Pronto SIL125-5 C18 ace-EPS
83	Kinetex
94	Zorbax Eclipse Plus C18, 3.9 x 150 mm, 3.5 um, Agilent

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Participant	Analytical column
98	LiChrospher 100RP18, 5 µm, 250×4 mm, Merck
100	RAPTOR C18
114	Acclaim TM120, C18, 5µm, 120Å, 250mm x 4.6 mm
126	C 18
135	M&N EC 250/4.6 Nucleodur 100-5 C18ec
151	BEH C18 1.7um, 2.1 x 100mm
186	WATERS Nova-Pak C18/ 150nm*3.9nm*4µm
190	Hypersil Gold
192	Formaldehyde,Acetaldehyde:InertSustain C18 Propionaldehyde,Butyraldehyde:Inertsil ODS-HL
195	Zorbax Eclipse Plus C18 4.6 cm x 100 mm x 1.8 um
198	Poroshell C18
199	C18
201	Zorbax Eclipse XDB C-18, 250 * 4,6 mm, 5 µm
206	Waters Nr. 106005
207	Phenomenex Kinetex C18 2,6 µ 100*4,6 mm
208	HSS C18, 1,8µm 2,1x100mm
216	RESTEK Ultra C18 5um 150 x 4.6mm
228	Restek Allure 4,6*200 mm, 5 µm
256	Supelcosil LC-18, 25 cm x 4.6 mm, 5 ul
258	Waters Acquity BEH C18
290	---
292	Supelco C18, 25 cm
511	Phenyl 1.7µm, 2.1 x 100 mm column

Participant	Mobile phase
9	Phase A: Wasser; Phase B: Acetonitril (jew eils + 0,1 % Ameisensäure)
10	Aceonitrile/H2O
11	ACETONITRILE/WATER/METHANOL
17	25% Acetonitil mir 0,1% Ameisensäure / 75% HPLC-Wasser mit 0,1% Ameisensäure
22	Acetonitril/MilliQ- Wasser 12 min isokratisch bei 53% ACN/47% H2O; danach 4,5 min linear auf 100% ACN - gehalten fpr 3,5 min
29	A:H2O/ACN/THF, B:ACN

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Participant	Mobile phase
30	acetonitrile / w ater
46	H2O, ACN, THF
52	Wasser/Methanol/Acetonitril
55	gradient elution of 10%THF in w ater and acetonitrile
56	Solvent A=Water - Solvent B =Acetonitril; t=0 min - 48% A - 52% B; t=6 min - 48% A- 52 % B; t=15 min - 0% A - 100 % B; t=17 min - 0% A - 100 B
58	ACN/H2O 65:35
60	70%ACN/30%Eau, and 100%ACN
62	Acetonitrile/Water 40/60 -> 100/0
67	Acetonitrile/w ater
68	Gradient: Acetonitril, Methanol, reinst Wasser
69	Acetonitrile-Water
78	30% Acetonitril 40% Wasser 30 % Methanol // 100% Acetonitril
83	ACN/H2O/THF
94	ACN:H2O, gradient
98	Wasser - Acetonitrol 51:49 bis 20:80
100	w ater/MeOH/ACN
114	Acetonitrile/w ater
126	CH3CN/H2O 60:40
135	Wasser-Acetonitril-Tetrahydrofuran
151	Acetonitrile/Water
186	acetonitrile/WaterTHF
190	ACN/Wasser
192	Water/Acetnitrile
195	ACN:H2O 40:60
198	Acetonitrile:Water
199	Wasser/Acetonitril
201	ACN/Wasser
206	A: H2O B: ACN
207	ACN/THF/H2O
208	Water/ACN/THF
216	70% Acetonitrile, 30% Ultra Pure Water
228	Acetonitril/Wasser

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Participant	Mobile phase
256	Startbedingungen: 30% Acetonitril, 60% Wasser, 10% THF
258	Water / acetonitrile
290	---
292	MeOH:H2O 60/40
511	10% THF in w ater / Acetonitril

Participant	Flow rate HPLC	Wavelength	Column temperature
9	0,5	MS/MS (ESI)	30 °C
10	0.5	365	25
11	0.8 ML/MIN	360 nm	30 °C
17	0,7 mL/min	360nm mittels DAD	30°C Kombiniert an beiden Säulenenden
22	0,6 ml/min	360 nm	28 °C
29	1,5	365	27
30	1,2	360	30°C
46	1 mL/min	365 nm	40 °C
52	1,0ml/min	365nm	25°C
55	0.5	360	40°C
56	0.4 mL/min	360 nm	28°C (+/-1°C)
58	1	412	35
60	1mL/min	360nm	30°C
62	1 mL/min	360	30°C
67	0.6 ml/min	I used 360 nm w avelenght	28°C
68	1 mL/min	365nm	25°C
69	1,5 ml/min	UV-visible	40ºC
78	1	365 nm	30 °C
83	1.2		40
94	1 ml/min	360 nm	30°C
98	1,2	365 nm	25°C
100	0.8ml/min	360 NM	30°C
114	1	360	22°C
126	0,5 ml/min	365 nm	50 °C

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Participant	Flow rate HPLC	Wavelength	Column temperature
135	2,25 ml/min	365 nm	45°C
151	0.5	360	50C
186	1.5	360 nm	35°C
190	1,5	365, 4 (Sample, BW)/ 750,50 (Referenz, BW)	30
192	1.2mL	360nm	40degC
195	1.8	365 nm	30ºC
198	1,0	360 nm	30 °C
199	0,8mL/min	370nm	30°C
201	1,3 ml/min	360/390 nm	65 °C
206	0,3 ml/Min	365	25
207	1,5	360	40
208	0,42 ml/min	360 nm	40 °C
216	1.0 ml/min	365 nm	Column Temperature at 25C
228	1,5 ml/min	365 nm	Raumtemperatur,20 °C
256	2.3 ml/min, ab 9.1 Minuten 2 ml/min	360 nm	25 °C
258	0.8 ml/min	367 nm	40°C
290	---	---	---
292	1.5 mL/min	365 nm	38oC
511	0.50 ml/min	360 nm	40 °C

Participant	Calibration standard
9	Fertiger Mix (ALDEHYDE/KETONE-DNPH STOCK STANDARD-13, Supelco)
10	ready to use mix from restek
11	MIX - SUPELCO
17	Einzelstandards, alle von Sigma Aldrich
22	fertiger Mix der entsprechend verdünnt w urde; Hersteller Sigma Aldrich (CARB method 1004 DNPH Mix 2)
29	Supelco Carb Method 1004 DNPH Mix2
30	Carbonyl DNPH MIx-1 sigma Aldrich
46	Einzelstandards
52	fertiger MIX LGC Standards
55	ready-to-use/Sigma Aldrich

Aldehydes 2019

Participant	Calibration standard
56	ready to use mix supelco Custom Mix Ald_DNPH 100 µg/ml
58	Ready to use mix
60	ready-to-use mix, AccuStandard
62	Purchased to Restek
67	I used a mix ready-to-use. Purchased from the manufacteur "o2si smart solutions"
68	Formaldehyd Standart von Sigma-Aldrich
69	Ready-to-use mix, Isostandards Material S.L.
78	fertiger Mix; Supelco
83	individual standards
94	Aldehyde/Ketone-DNPH TO11/IP-6A Mix, Sigma-Aldrich CRM4M7285
98	Mix, Sigma-Aldrich, CRM47649, Lot LRAB7344
100	ready to use mix RESTEK
114	Mix standard Sigma Aldrich
126	Einzelstandard, Fa. Supelco
135	Wurden aus Einzelstandards hergestellt: Sigma-Aldrich und Supelco
151	Individual standards Sigma Aldrich
186	mix Supelco
190	Mix der Fa. Neochema
192	The standard w as purchased as a ready-to-use mix manufactured by Wako Pure Chemical Industries,Ltd.
195	Individual dervatized standard from Supleco
198	Ready to use mix, Supelco Sigma Aldrich std.
199	Einzelstandards
201	Carb method 1004 DNPH-Mix, Sigma-Aldrich
206	Ultra Scientific ALD-554D
207	Einzelstandards Supelco
208	CARB Method 1004 DNPH Mix2
216	Produced from individual standards purchased from Sigma Aldrich
228	Einzelstandards, Neochema
256	fertiger Mix: TO11/IP-6A Aldehyde/-Ketone-DNPH Mix (Sigma-Aldrich)
258	Ready to use mix, Supelco Part number CRM47285
290	---
292	Supelco, TraceCert CRM. standards prepared from individual standard

Aldehydes 2019

Participant	Calibration standard
511	ready-to-use mix, (Supelco)

Participant	Recovery rate
9	nein
10	no
11	-
17	Nein
22	nein
29	nein
30	no
46	nein
52	nein
55	yes
56	no
58	no
60	No
62	No
67	No, my result didn't include recovery rates
68	Ja, Formaldehyd 94%
69	No
78	nein
83	no
94	nein
98	Nein
100	no
114	No
126	nein
135	nein
151	No
186	No
190	nein

Aldehydes 2019

Participant	Recovery rate
192	No.
195	no
198	NO
199	Nein
201	Nein
206	nein
207	-
208	No
216	no
228	nein
256	Nein, recoveries variieren zw ischen 90 - 110 %
258	No
290	Nein
292	no, recovery is very high
511	no