IFA
Institut für Arbeitsschutz der
Deutschen Gesetzlichen Unfallversicherung

Round-robin tests for in-house and external measuring stations - results and evaluation

Round-robin test Aldehydes

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Institute for Occupationial Safety and Health of the
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Summary of laboratory test results

Sample 1

	Formaldehyde	Z score	Acetaldehyde	Z score	Butyraldehyde	Z score
Unit	mg/m³		mg/m³		mg/m³	
6	0,132	0,63	1,249	-0,18	0,230	-1,00
10	0,112	-0,98	1,150	-0,96	0,264	0,34
11	0,120	-0,34	1,230	-0,33	0,250	-0,21
22	0,130	0,47	1,200	-0,57	0,250	-0,21
29	0,122	-0,18	1,290	0,14		
30	0,124	-0,02	1,157	-0,91	0,246	-0,37
55	0,130	0,47	1,160	-0,88	0,250	-0,21
56	0,120	-0,34	1,200	-0,57	0,250	-0,21
58	0,118	-0,54	1,223	-0,39	0,256	0,03
60	0,122	-0,20	1,203	-0,55	0,257	0,05
62	0,120	-0,34	1,250	-0,18	0,240	-0,60
68	0,130	0,47				
69	0,147	1,87	1,135	-1,08		
81	0,113	-0,93				
86	0,112	-0,98				
90	0,120	-0,34	1,245	-0,22		
93	0,116	-0,66	1,275	0,02	0,261	0,22
98	0,102	-1,77	1,073	-1,57	0,220	-1,39
99	0,119	-0,42	1,234	-0,30	0,250	-0,21
100	0,108	-1,27	1,044	-1,80	0,212	-1,70
104	0,145	1,67	1,410	1,08	0,295	1,55
114	0,111	-1,06	1,119	-1,21	0,241	-0,56
123	0,133	0,71	1,546	2,15 E	0,314	2,29 E
131	0,117	-0,58	1,342	0,55	0,260	0,18
138	0,130	0,47	1,310	0,29	0,240	-0,60
144	0,120	-0,34	1,235	-0,29	0,251	-0,17
147	0,115	-0,74	1,230	-0,33		
151	0,123	-0,10	1,283	0,08	0,234	-0,84

	Formaldehyde	Z score	Acetaldehyde	Z score	Butyraldehyde	Z score
155	0,119	-0,42	1,562	2,28 E	0,236	-0,76
165	0,122	-0,18	1,245	-0,22	0,264	0,34
167	0,121	-0,26	1,215	-0,45	0,266	0,41
168	0,118	-0,50	1,259	-0,11		
174	0,108	-1,31	1,198	-0,59	0,080	-6,87 BE
184	0,121	-0,26	1,247	-0,20	0,246	-0,37
186	0,124	-0,02	1,268	-0,04	0,247	-0,33
191	0,117	-0,58	1,208	-0,51	0,257	0,06
195	0,136	0,96	1,058	-1,69		
198	0,120	-0,34	1,210	-0,49	0,248	-0,29
199	0,144	1,58	1,303	0,24	0,231	-0,97
207	0,124	-0,02	1,353	0,63	0,273	0,69
208	0,130	0,47	1,287	0,11	0,262	0,26
219	0,119	-0,42	1,246	-0,21	0,243	-0,49
224	0,149	2,00	1,521	1,95	0,316	2,37 E
255	0,131	0,55	1,097	-1,38	0,237	-0,72
264	0,110	-1,14	1,500	1,79	0,240	-0,60
267	0,126	0,14	1,278	0,04	0,270	0,57
273	0,152	2,26 E	1,588	2,48 E	0,321	2,58 E
274	0,152	2,26 E	1,588	2,48 E	0,321	2,58 E
280	0,141	1,35	1,508	1,85		
287	0,115	-0,74	1,276	0,03	0,213	-1,66
–	–	– –	–	– –	–	– –
Method	ISO 5725-2		ISO 5725-2		ISO 5725-2	
Assessment	|Z|<=2,00		|Z|<=2,00		|Z|<=2,00	
Mean	0,124		1,272		0,255	
Reproducibility s.d.	0,012		0,137		0,027	
Rel. reproducibility s.d.	9,47 %		10,74 %		10,47 %	
Reference value	0,127		1,300		0,259	
Target s.d.	0,012		0,127		0,026	
Rel. target s.d.	10,00 %		10,00 %		10,00 %	
Lower limit of tolerance	0,099		1,018		0,204	
Upper limit of tolerance	0,149		1,527		0,307	

	Formaldehyde	Z score	Acetaldehyde	Z score	Butyraldehyde	Z score
No. of laboratories that submitted results	50		47		40	
No. of laboratories after elimination of outliers type A-D and F (without laboratories that only gave states but no measured values)	50		47		39	

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	
L: Differing laboratory mean (Grubbs II)	Grubbs für 2

Summary of laboratory test results

Sample 2

	Formaldehyde	Z score		Acetaldehyde	Z score		Propionaldehyde	Z score		Butyraldehyde	Z score	
Unit	mg/m³			mg/m³			mg/m³			mg/m³		
6	0,067	0,63		0,459	-0,14		0,402	0,06		0,706	-1,42	
10	0,057	-1,03		0,448	-0,38		0,375	-0,62		0,838	0,18	
11	0,060	-0,48		0,450	-0,33		0,390	-0,24		0,810	-0,16	
22	0,070	1,11		0,450	-0,33		0,390	-0,24		0,820	-0,04	
29	0,064	0,09		0,478	0,27		0,409	0,23				
30	0,065	0,32		0,418	-1,02		0,406	0,16		0,811	-0,15	
55	0,067	0,63		0,440	-0,55		0,380	-0,49		0,800	-0,28	
56	0,060	-0,48		0,430	-0,76		0,380	-0,49		0,770	-0,64	
58	0,059	-0,60		0,448	-0,38		0,379	-0,53		0,810	-0,15	
60	0,065	0,26		0,476	0,23		0,454	1,35		0,885	0,75	
62	0,060	-0,48		0,460	-0,12		0,410	0,26		0,800	-0,28	
68	0,060	-0,48										
69	0,078	2,35	E	0,432	-0,73		0,450	1,27				
81	0,063	-0,08										
86	0,058	-0,80										
90	0,061	-0,32		0,451	-0,31							
93	0,058	-0,80		0,460	-0,12		0,396	-0,09		0,821	-0,02	
98	0,051	-1,86		0,401	-1,39		0,339	-1,51		0,700	-1,49	
99	0,064	0,16		0,479	0,29		0,408	0,21		0,826	0,04	
100	0,051	-1,89		0,341	-2,68	E	0,308	-2,28	E	0,637	-2,26	E
104	0,071	1,33		0,569	2,22	E	0,477	1,94		1,050	2,76	E
114	0,055	-1,27		0,398	-1,45		0,345	-1,37		0,759	-0,78	
123	0,074	1,74		0,551	1,83		0,481	2,04	E	1,013	2,31	E
131	0,058	-0,80		0,483	0,37		0,379	-0,52		0,801	-0,27	
138	0,061	-0,32		0,460	-0,12		0,390	-0,24		0,750	-0,89	
144	0,061	-0,32		0,450	-0,33		0,398	-0,04		0,809	-0,17	
147	0,057	-0,95		0,444	-0,46							
151	0,062	-0,21		0,465	-0,01		0,369	-0,77		0,741	-0,99	

	Formaldehyde	Z score	Acetaldehyde	Z score	Propionaldehyde	Z score	Butyraldehyde	Z score
155	0,061	-0,32	0,567	2,18 E	0,413	0,33	0,757	-0,80
165	0,061	-0,32	0,452	-0,29	0,393	-0,17	0,839	0,19
167	0,061	-0,32	0,445	-0,44	0,408	0,21	0,845	0,27
168	0,058	-0,80	0,437	-0,61				
174	0,052	-1,75	0,434	-0,68	0,368	-0,79	0,272	-6,69 BE
184	0,064	0,16	0,469	0,07	0,400	0,01	0,793	-0,36
186	0,062	-0,16	0,460	-0,12	0,392	-0,19	0,827	0,05
191	0,060	-0,48	0,444	-0,46	0,392	-0,19	0,821	-0,02
195	0,068	0,81	0,407	-1,26				
198	0,060	-0,43	0,439	-0,57	0,376	-0,59	0,796	-0,33
199	0,072	1,51	0,478	0,27	0,319	-2,02 E	0,751	-0,87
207	0,063	0,00	0,488	0,48	0,420	0,51	0,883	0,73
208	0,062	-0,16	0,400	-1,41	0,456	1,41	0,825	0,02
219	0,059	-0,64	0,447	-0,40	0,381	-0,47	0,790	-0,40
224	0,076	2,06 E	0,547	1,75	0,490	2,26 E	1,001	2,16 E
255	0,067	0,63	0,396	-1,49	0,370	-0,74	0,760	-0,77
264	0,060	-0,48	0,530	1,38	0,380	-0,49	0,780	-0,52
267	0,064	0,16	0,472	0,14	0,409	0,23	0,882	0,72
273	0,079	2,52 E	0,609	3,08 E	0,449	1,25	1,052	2,79 E
274	0,079	2,52 E	0,609	3,08 E	0,449	1,25	1,052	2,79 E
280	0,072	1,43	0,549	1,79				
287	0,054	-1,43	0,463	-0,06	0,403	0,08	0,684	-1,69
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Method	ISO 5725-2		ISO 5725-2		ISO 5725-2		ISO 5725-2	
Assessment	|Z|<=2,00		|Z|<=2,00		|Z|<=2,00		|Z|<=2,00	
Mean	0,063		0,466		0,400		0,823	
Reproducibility s.d.	0,007		0,055		0,039		0,097	
Rel. reproducibility s.d.	10,71 %		11,72 %		9,86 %		11,79 %	
Reference value	0,060		0,447		0,382		0,846	
Target s.d.	0,006		0,047		0,040		0,082	
Rel. target s.d.	10,00 %		10,00 %		10,00 %		10,00 %	
Lower limit of tolerance	0,050		0,372		0,320		0,658	
Upper limit of tolerance	0,076		0,559		0,480		0,988	

	Formaldehyde	Z score	Acetaldehyde	Z score	Propionaldehyde	Z score	Butyraldehyde	Z score
No. of laboratories that submitted results	50		47		42		40	
No. of laboratories after elimination of outliers type A-D and F (without laboratories that only gave states but no measured values)	50		47		42		39	

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	
L: Differing laboratory mean (Grubbs II)	Grubbs für 2

Summary of laboratory test results

Sample 3

	Formaldehyde	Z score		Acetaldehyde	Z score		Butyraldehyde	Z score	
Unit	mg/m³			mg/m³			mg/m³		
6	0,076	0,50		1,017	-0,17		0,885	-1,47	
10	0,061	-1,60		0,890	-1,40		0,965	-0,70	
11	0,070	-0,33		1,010	-0,24		1,040	0,02	
22	0,080	1,05		0,990	-0,43		1,030	-0,08	
29	0,071	-0,15		1,050	0,15				
30	0,072	-0,06		0,939	-0,92		1,041	0,03	
55	0,076	0,50		1,000	-0,33		1,000	-0,37	
56	0,070	-0,33		0,940	-0,91		0,980	-0,56	
58	0,068	-0,54		1,017	-0,17		1,038	0,00	
60	0,072	-0,02		0,996	-0,37		1,040	0,02	
62	0,070	-0,33		1,030	-0,04		0,990	-0,46	
68	0,070	-0,33							
69	0,092	2,72	E	0,943	-0,88				
81	0,072	-0,06							
86	0,070	-0,33							
90	0,069	-0,47		1,012	-0,22				
93	0,068	-0,61		1,043	0,08		1,048	0,10	
98	0,059	-1,81		0,881	-1,48		0,884	-1,48	
99	0,071	-0,20		1,039	0,04		1,024	-0,13	
100	0,061	-1,51		0,816	-2,11	E	0,848	-1,83	
104	0,081	1,21		1,550	4,99	BE	1,390	3,39	E
114	0,064	-1,16		0,898	-1,32		0,962	-0,73	
123	0,090	2,43	E	1,249	2,08	E	1,290	2,43	E
131	0,066	-0,89		1,076	0,40		1,010	-0,27	
138	0,073	0,08		1,050	0,15		0,970	-0,66	
144	0,071	-0,20		1,008	-0,25		1,012	-0,25	
147	0,065	-1,02		1,000	-0,33				
151	0,072	0,01		1,050	0,15		0,937	-0,97	

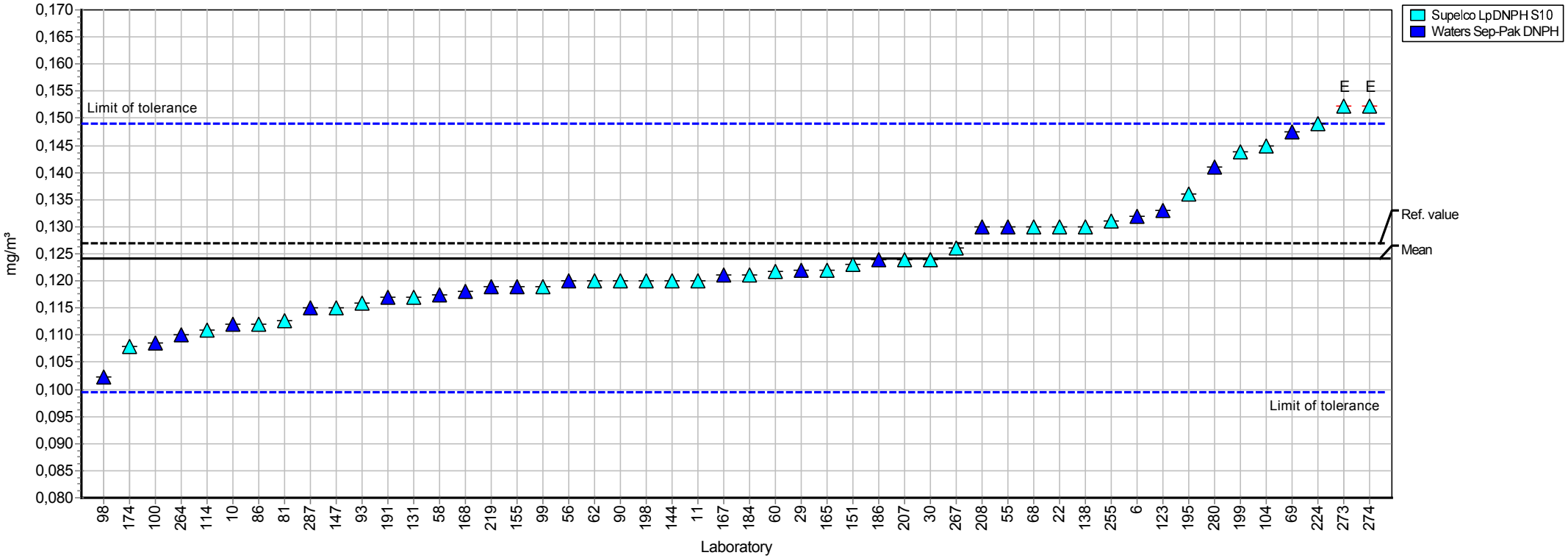
	Formaldehyde	Z score	Acetaldehyde	Z score	Butyraldehyde	Z score
155	0,069	-0,47	1,272	2,30 E	0,952	-0,83
165	0,071	-0,20	1,017	-0,17	1,059	0,20
167	0,069	-0,47	0,999	-0,34	1,066	0,27
168	0,069	-0,47	1,034	0,00		
174	0,062	-1,44	0,982	-0,51	0,344	-6,69 BE
184	0,073	0,08	1,040	0,05	0,983	-0,53
186	0,072	-0,06	1,039	0,04	1,054	0,15
191	0,068	-0,61	0,995	-0,38	1,045	0,07
195	0,082	1,27	0,869	-1,60		
198	0,071	-0,20	0,986	-0,47	1,020	-0,17
199	0,086	1,83	1,105	0,68	0,976	-0,60
207	0,072	-0,06	1,099	0,62	1,115	0,74
208	0,073	0,08	1,018	-0,16	1,051	0,13
219	0,068	-0,61	1,004	-0,29	0,997	-0,39
224	0,085	1,74	1,223	1,82	1,237	1,92
255	0,077	0,63	0,883	-1,46	0,954	-0,81
264	0,060	-1,71	1,200	1,60	1,000	-0,37
267	0,074	0,22	1,060	0,25	1,111	0,70
273	0,086	1,81	1,286	2,43 E	1,307	2,59 E
274	0,086	1,81	1,286	2,43 E	1,307	2,59 E
280	0,085	1,74	1,206	1,66		
287	0,062	-1,44	1,035	0,01	0,864	-1,68
–	–	– –	–	– –	–	– –
Method	ISO 5725-2		ISO 5725-2		ISO 5725-2	
Assessment	|Z|<=2,00		|Z|<=2,00		|Z|<=2,00	
Mean	0,072		1,034		1,038	
Reproducibility s.d.	0,008		0,109		0,121	
Rel. reproducibility s.d.	10,67 %		10,57 %		11,67 %	
Reference value	0,070		1,020		1,070	
Target s.d.	0,007		0,103		0,104	
Rel. target s.d.	10,00 %		10,00 %		10,00 %	
Lower limit of tolerance	0,058		0,827		0,830	
Upper limit of tolerance	0,087		1,241		1,246	

	Formaldehyde	Z score	Acetaldehyde	Z score	Butyraldehyde	Z score
No. of laboratories that submitted results	50		47		40	
No. of laboratories after elimination of outliers type A-D and F (without laboratories that only gave states but no measured values)	50		46		39	

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	
L: Differing laboratory mean (Grubbs II)	Grubbs für 2

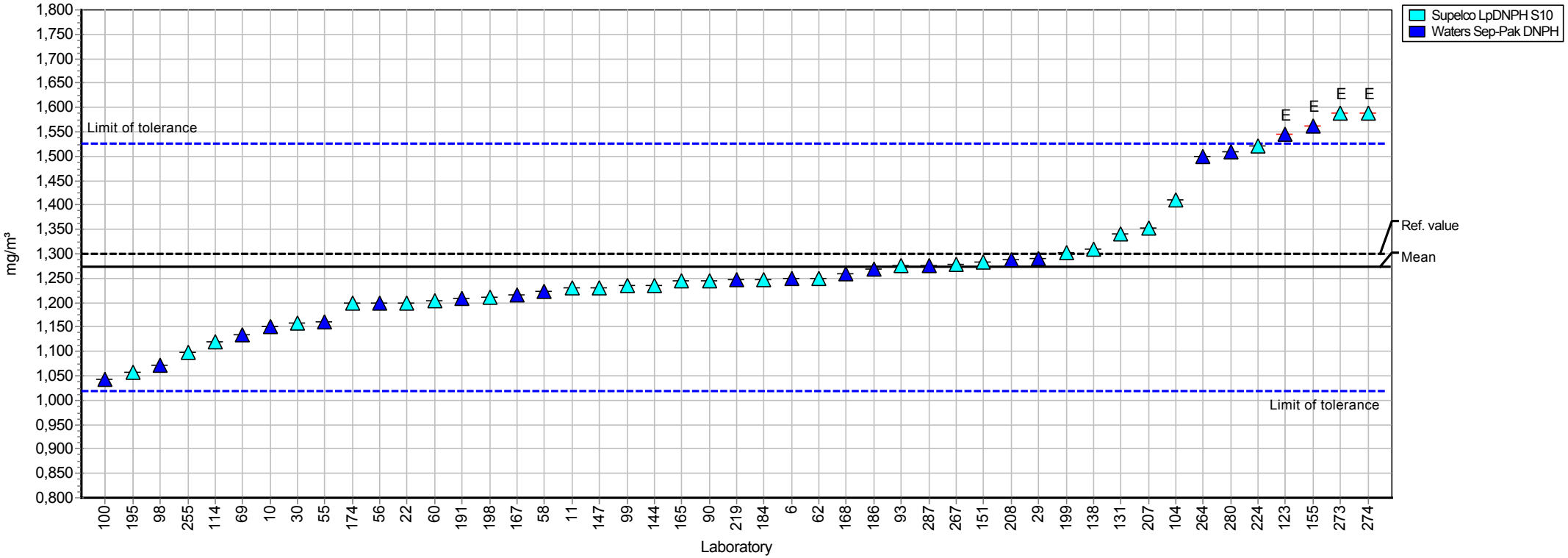
Summary results

Measurand:	**Formaldehyde**	**Mean:**	**0,124 mg/m³**
Sample:	**1**	**Reproducibility s.d.:**	**0,012 mg/m³**
Method:	**ISO 5725-2**	**Relative reproducibility s.d.:**	**9,47%**
Relative target s.d.:	**10,00% (Limited)**	**Reference value:**	**0,127 mg/m³**
No. of laboratories:	**50**	**Range of tolerance:**	**0,099 - 0,149 mg/m³ (|Z-Score| <= 2,00)**



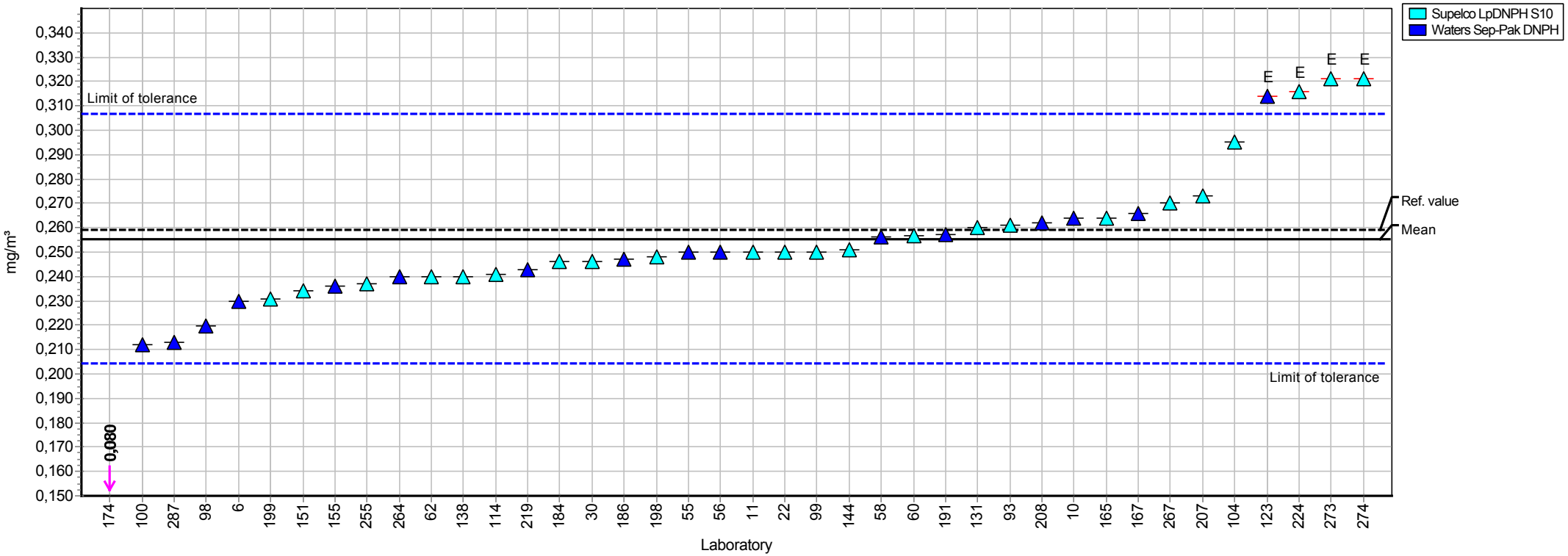
Summary results

Measurand:	**Acetaldehyde**	**Mean:**	**1,272 mg/m³**
Sample:	**1**	**Reproducibility s.d.:**	**0,137 mg/m³**
Method:	**ISO 5725-2**	**Relative reproducibility s.d.:**	**10,74%**
Relative target s.d.:	**10,00% (Limited)**	**Reference value:**	**1,300 mg/m³**
No. of laboratories:	**47**	**Range of tolerance:**	**1,018 - 1,527 mg/m³ (|Z-Score| <= 2,00)**



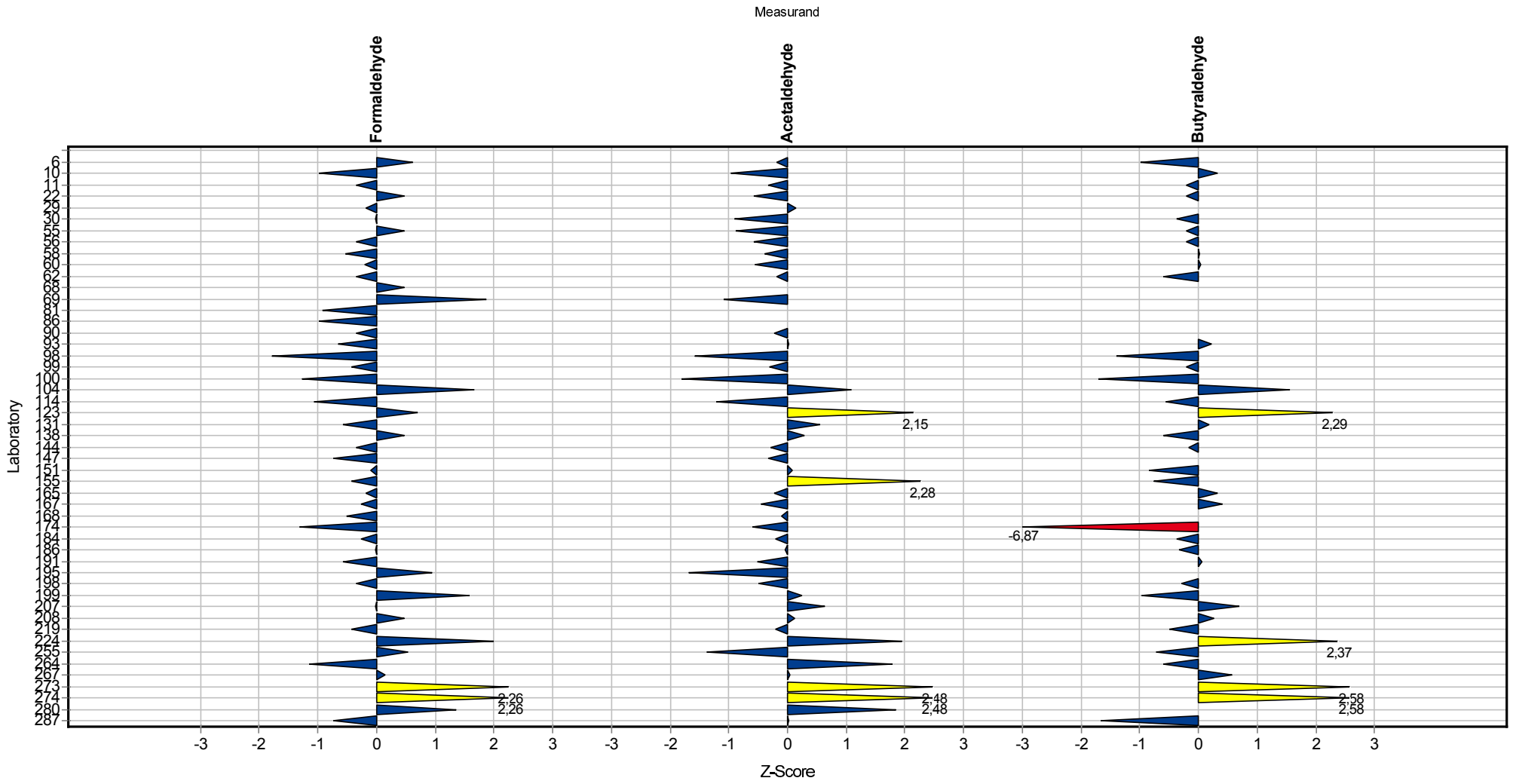
Summary results

Measurand:	**Butyraldehyde**	**Mean:**	**0,255 mg/m³**
Sample:	**1**	**Reproducibility s.d.:**	**0,027 mg/m³**
Method:	**ISO 5725-2**	**Relative reproducibility s.d.:**	**10,47%**
Relative target s.d.:	**10,00% (Limited)**	**Reference value:**	**0,259 mg/m³**
No. of laboratories:	**39**	**Range of tolerance:**	**0,204 - 0,307 mg/m³ (|Z-Score| <= 2,00)**



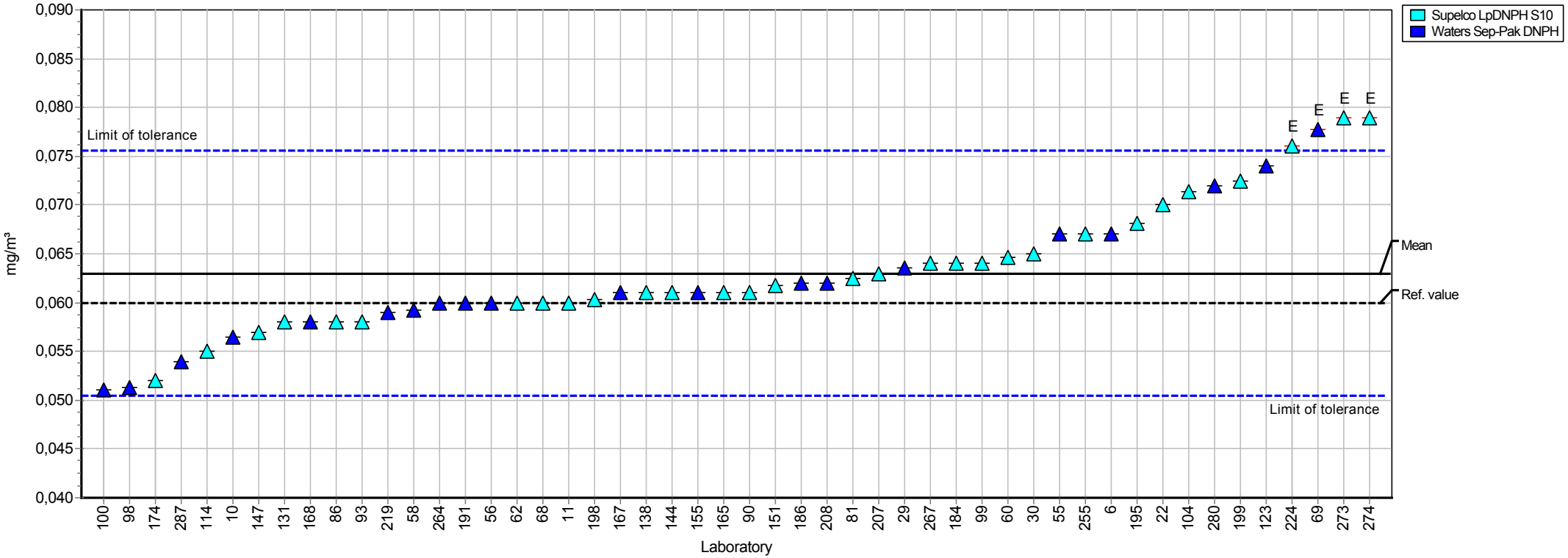
Sample chart of Z-scores

Sample 1



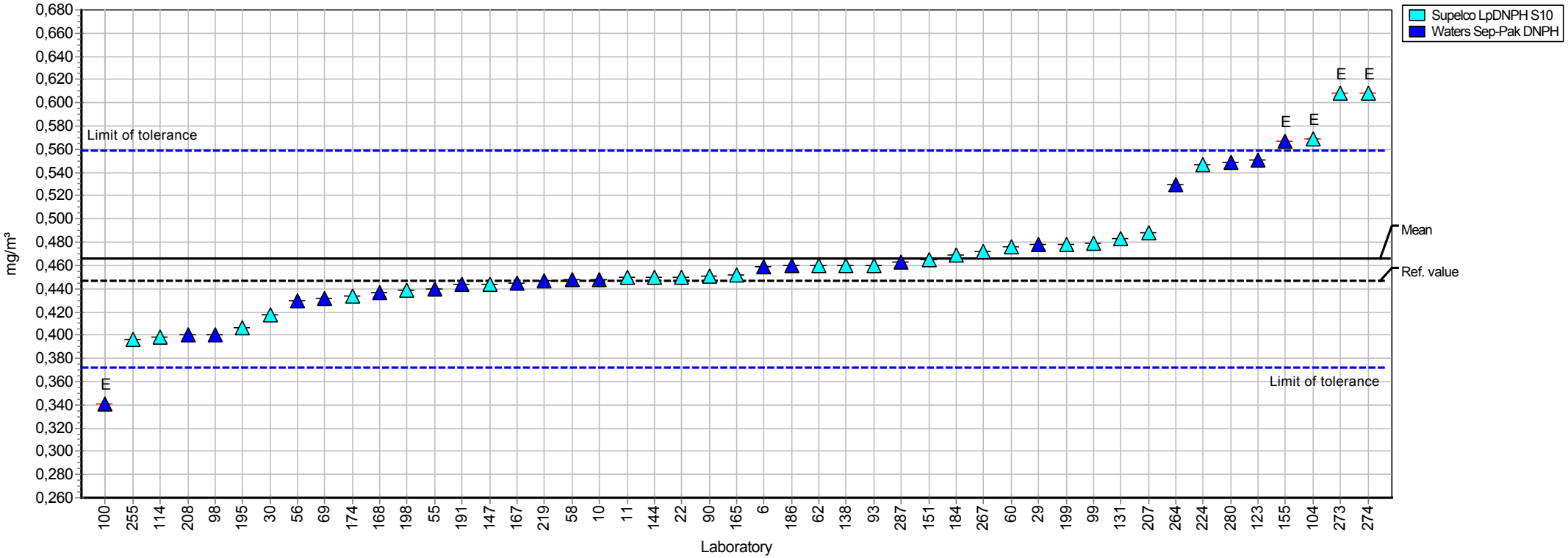
Summary results

Measurand:	**Formaldehyde**	**Mean:**	**0,063 mg/m³**
Sample:	**2**	**Reproducibility s.d.:**	**0,007 mg/m³**
Method:	**ISO 5725-2**	**Relative reproducibility s.d.:**	**10,71%**
Relative target s.d.:	**10,00% (Limited)**	**Reference value:**	**0,060 mg/m³**
No. of laboratories:	**50**	**Range of tolerance:**	**0,050 - 0,076 mg/m³ (|Z-Score| <= 2,00)**



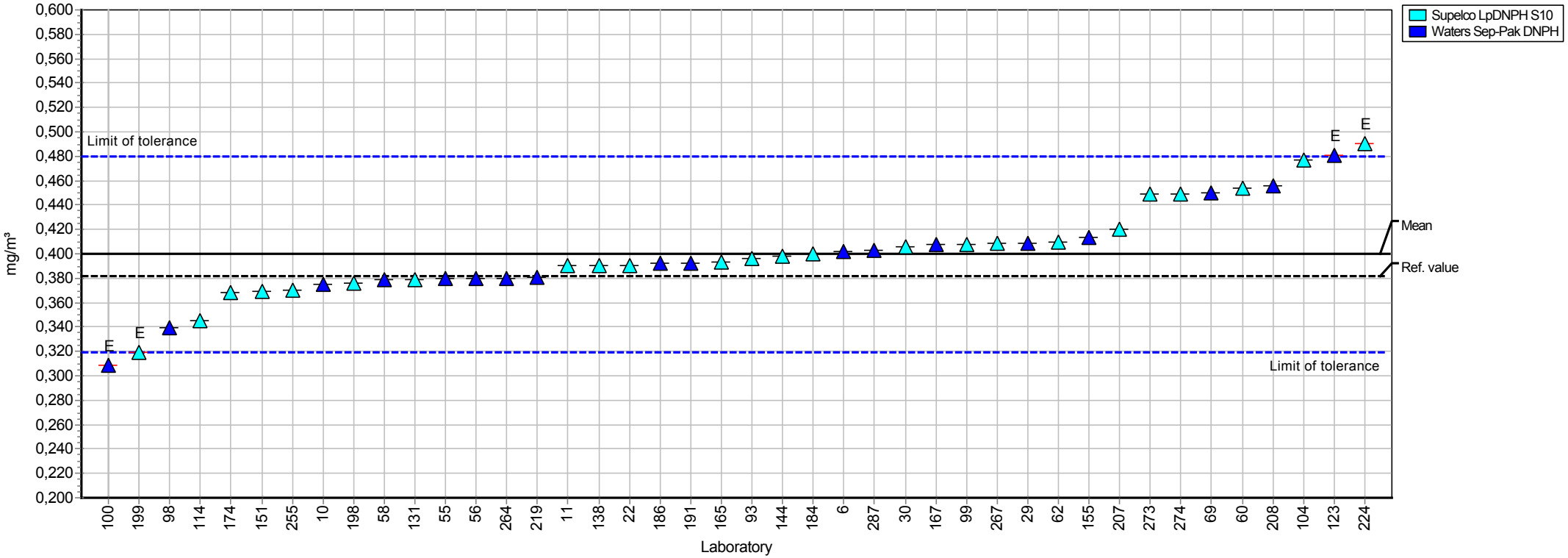
Summary results

Measurand:	**Acetaldehyde**	**Mean:**	**0,466 mg/m³**
Sample:	**2**	**Reproducibility s.d.:**	**0,055 mg/m³**
Method:	**ISO 5725-2**	**Relative reproducibility s.d.:**	**11,72%**
Relative target s.d.:	**10,00% (Limited)**	**Reference value:**	**0,447 mg/m³**
No. of laboratories:	**47**	**Range of tolerance:**	**0,372 - 0,559 mg/m³ (|Z-Score| <= 2,00)**



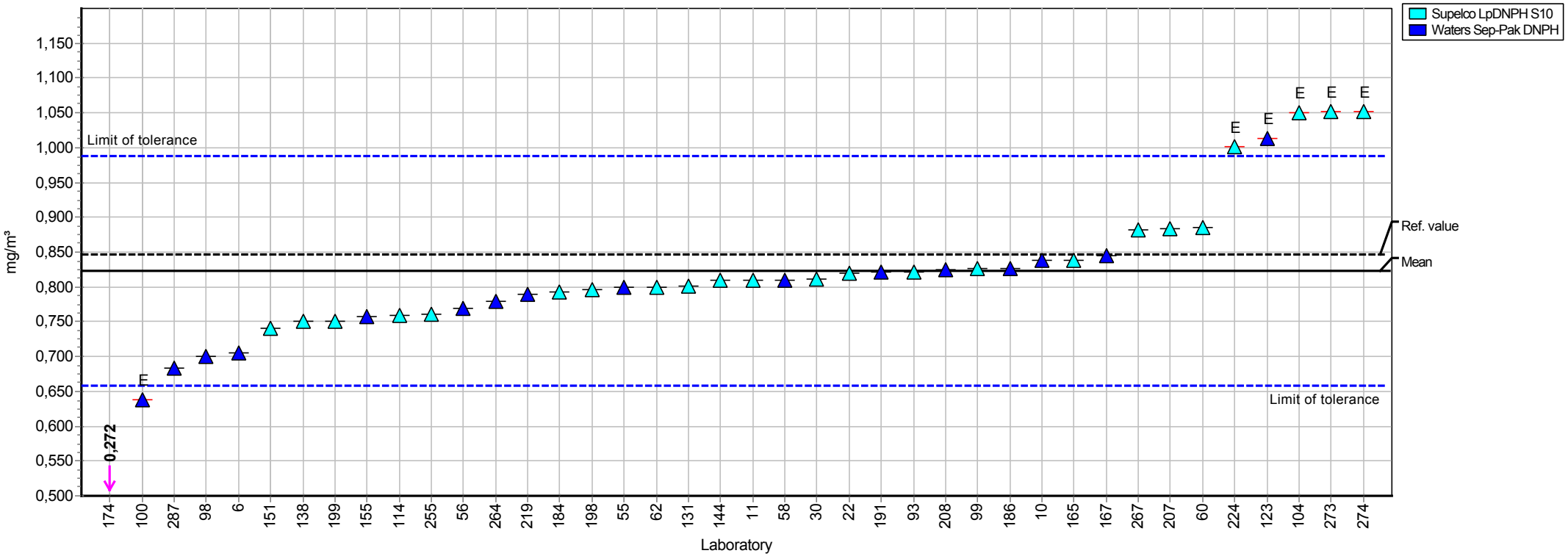
Summary results

Measurand:	**Propionaldehyde**	**Mean:**	**0,400 mg/m³**
Sample:	**2**	**Reproducibility s.d.:**	**0,039 mg/m³**
Method:	**ISO 5725-2**	**Relative reproducibility s.d.:**	**9,86%**
Relative target s.d.:	**10,00% (Limited)**	**Reference value:**	**0,382 mg/m³**
No. of laboratories:	**42**	**Range of tolerance:**	**0,320 - 0,480 mg/m³ (|Z-Score| <= 2,00)**



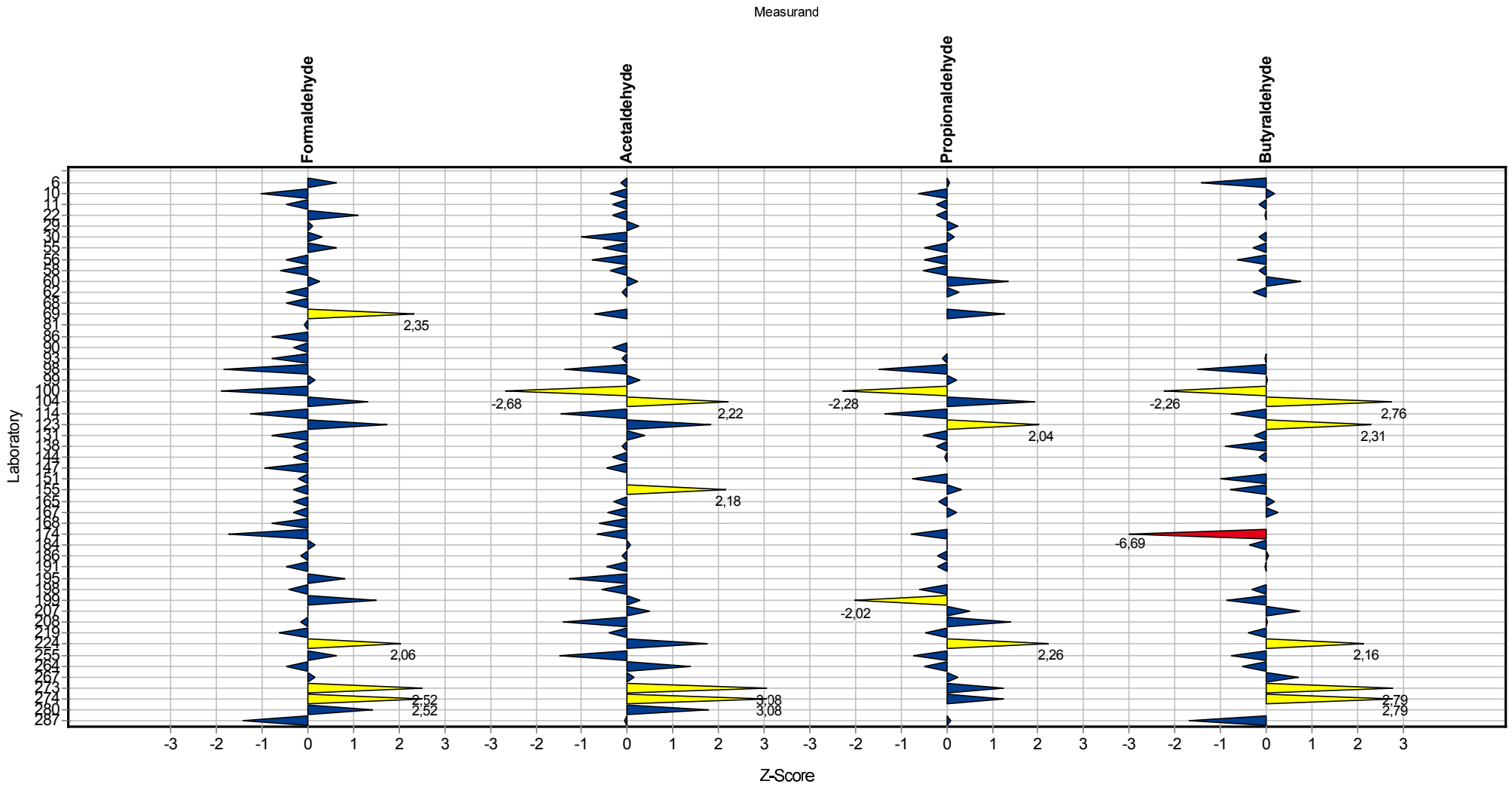
Summary results

Measurand:	**Butyraldehyde**	**Mean:**	**0,823 mg/m³**
Sample:	**2**	**Reproducibility s.d.:**	**0,097 mg/m³**
Method:	**ISO 5725-2**	**Relative reproducibility s.d.:**	**11,79%**
Relative target s.d.:	**10,00% (Limited)**	**Reference value:**	**0,846 mg/m³**
No. of laboratories:	**39**	**Range of tolerance:**	**0,658 - 0,988 mg/m³ (|Z-Score| <= 2,00)**



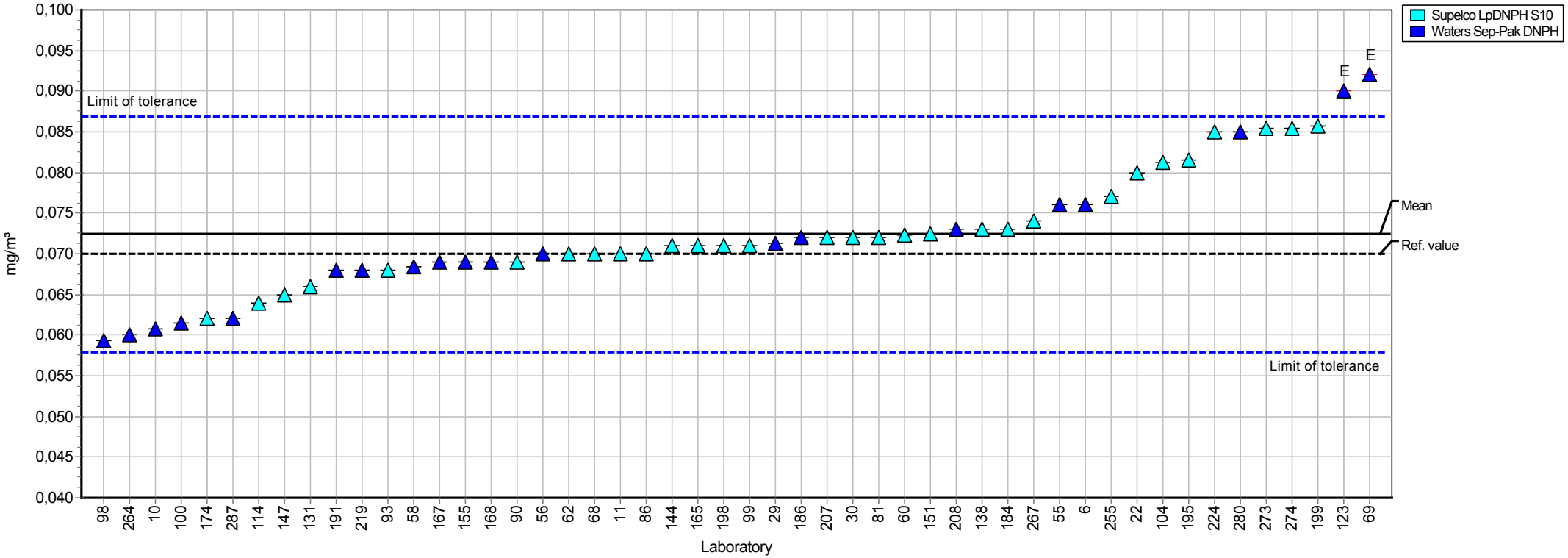
Sample chart of Z-scores

Sample 2



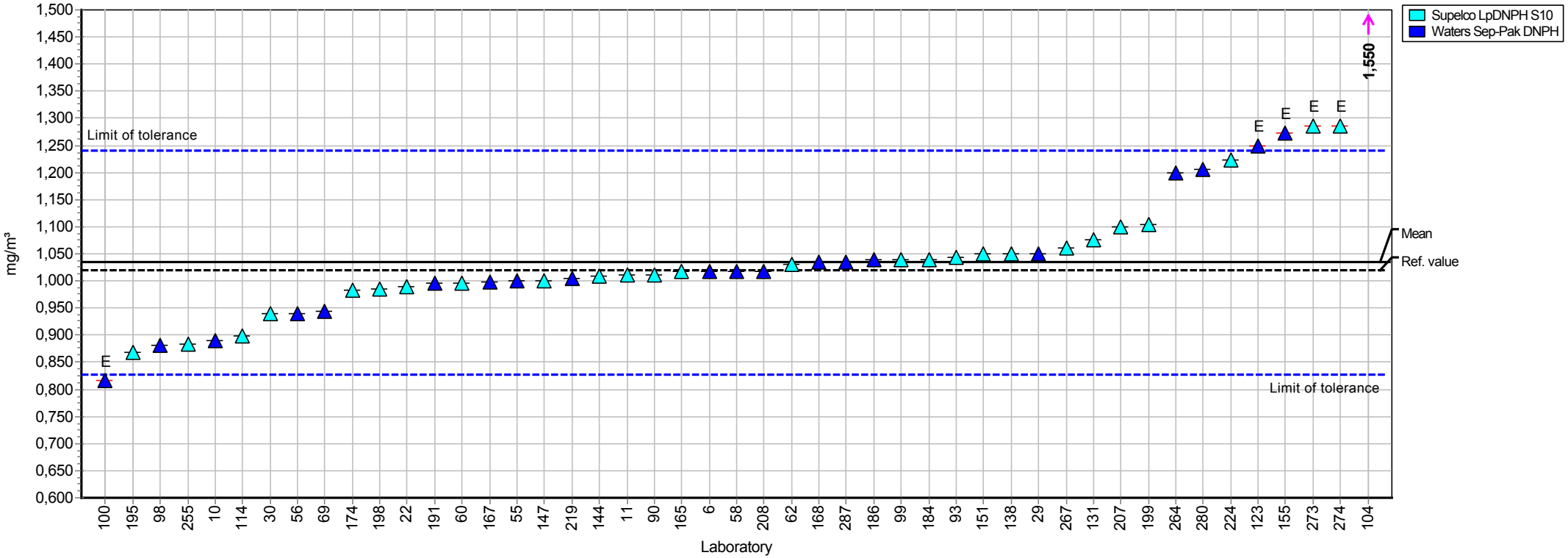
Summary results

Measurand:	**Formaldehyde**	**Mean:**	**0,072 mg/m³**
Sample:	**3**	**Reproducibility s.d.:**	**0,008 mg/m³**
Method:	**ISO 5725-2**	**Relative reproducibility s.d.:**	**10,67%**
Relative target s.d.:	**10,00% (Limited)**	**Reference value:**	**0,070 mg/m³**
No. of laboratories:	**50**	**Range of tolerance:**	**0,058 - 0,087 mg/m³ (|Z-Score| <= 2,00)**



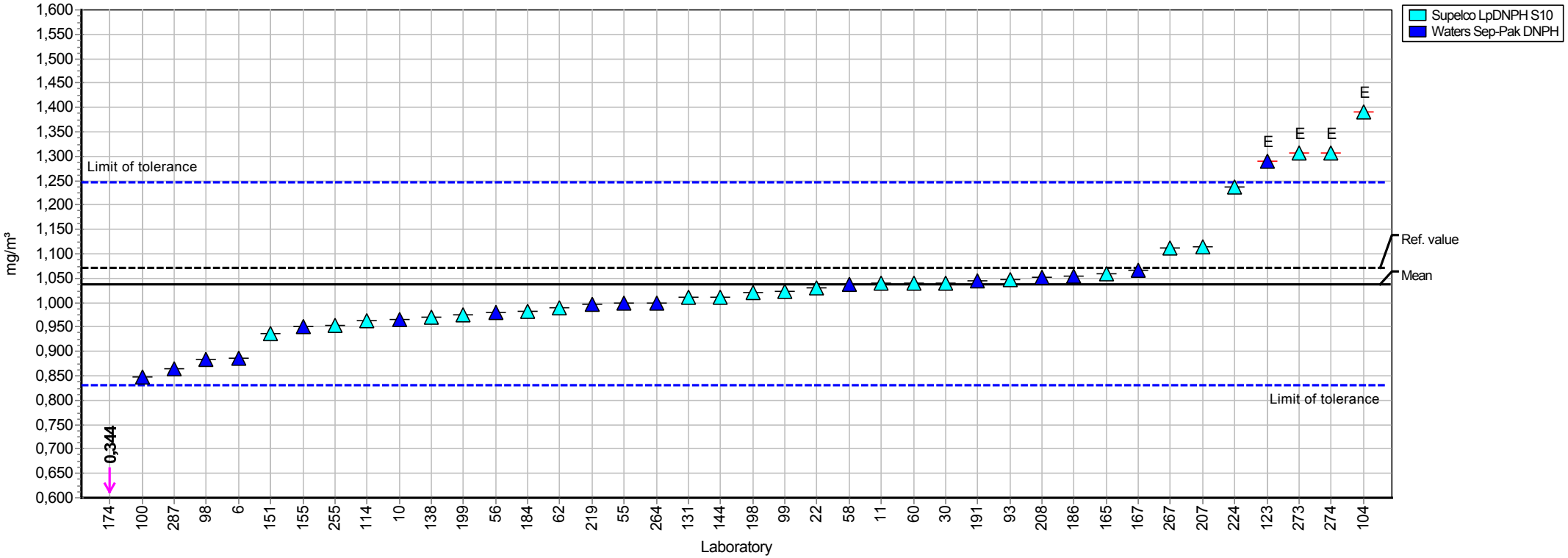
Summary results

Measurand:	**Acetaldehyde**	**Mean:**	**1,034 mg/m³**
Sample:	**3**	**Reproducibility s.d.:**	**0,109 mg/m³**
Method:	**ISO 5725-2**	**Relative reproducibility s.d.:**	**10,57%**
Relative target s.d.:	**10,00% (Limited)**	**Reference value:**	**1,020 mg/m³**
No. of laboratories:	**46**	**Range of tolerance:**	**0,827 - 1,241 mg/m³ (|Z-Score| <= 2,00)**



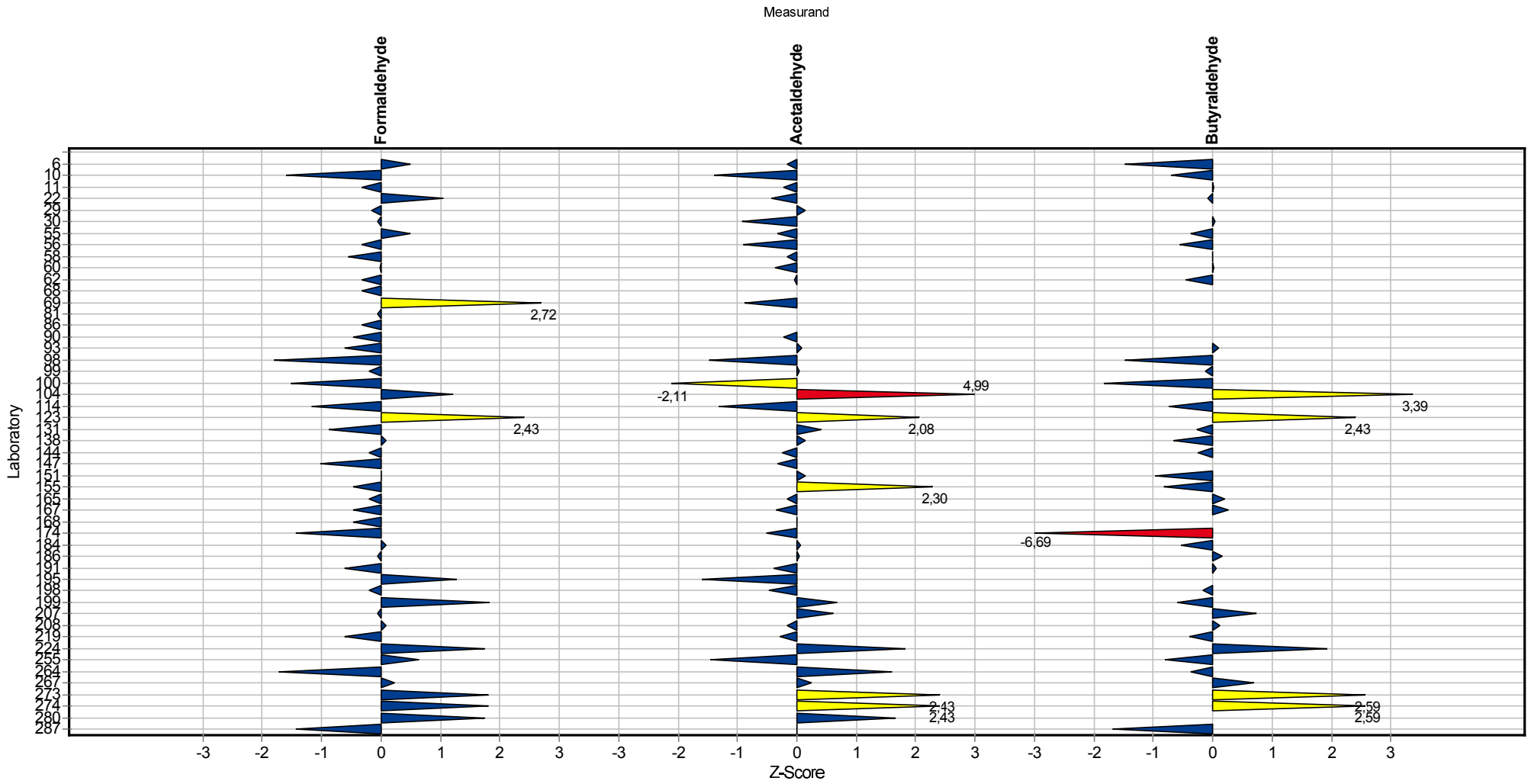
Summary results

Measurand:	**Butyraldehyde**	**Mean:**	**1,038 mg/m³**
Sample:	**3**	**Reproducibility s.d.:**	**0,121 mg/m³**
Method:	**ISO 5725-2**	**Relative reproducibility s.d.:**	**11,67%**
Relative target s.d.:	**10,00% (Limited)**	**Reference value:**	**1,070 mg/m³**
No. of laboratories:	**39**	**Range of tolerance:**	**0,830 - 1,246 mg/m³ (|Z-Score| <= 2,00)**



Sample chart of Z-scores

Sample 3



Questions and Answers

Participant	Analytical method	Date start sample preparation	Storage time after desorption
6	IFA-Arbeitsmappe 6045	08.11.16	48 h im Kühlschrank
10	NF X43-264	10/11/2016	1 day refrigerator (between 2 et 6°C)
11	ISO 16000-3	22/11/2016	no storage after desorption
22	DIN ISO 16000-3	17.11.2016	sofortige Messung
29	DIN ISO 16000-3 und IFA 6045	23.11.16	2 Tage Kühlschrank
30	ISO 16000-3	16 November 2016	Refrigerator
55	HPLC - Photodiode array detector	10/11/2016	6 days - refrigerator
56	HPLC	09/11/16	0 - 4°C
58	in house method using LCUV	17 november 2016	directly analyzed
60	ISO 16000-3	14/11/2016	30 min, 20°C.
62	NF X43-264	16/11/2016	5 days in refrigerator
68	Interne Arbeitsanweisung SAA 6.003.9	10.11.2016	Nein
69	HPLC	15/11/2016	-20 ºC in freezer. They were analyzed the same day that the desorption
81	LC-MS	04/11/16	analysies just after desorption
86	Métropol	09/11/16	0
90	METROPOL M-4	15/11/2016	one night - refrigerator
93	METROPOL N°1	15/11/2016	24h
98	IFA 6045	10.11.2016	Bis 1 Tag nach Desorption,Kühlschrank
99	METROPOL	18/11/2016	less than one day at room temperature
100	HPLC-DAD	11/09/2016	2h in room temperature
104	DIN EN ISO 16000-3:2013	Desorption 14.11.2016	Nach Desorption 1 Tag im Kühlschrank gelagert
114	HPLC/UV based on NF X43-264 and Metropol M-4	10/11/16	Storage after desorption between 0 and 1 day in the autosampler (10°C)
123	NF ISO 16000-3	15/11/2016	no storage
131	metropol M-4	20/11/16	5 days
138	BGIA 6045	10.11.2016	Analyse unmittelbar nach Desorption, Rückstellproben im Kühlschrank
144	INRS - METROPOL 001 - METROPOL M4 et M66	10/11/2016	12 days
147	Métropol M-4, M-66	22/11/16	0
151	HPLC PDA	11/11/2016	Same day
155	DIN ISO 16000-3 on Anlehnung	09.11.2016	Lagerung im Kühlschrank; nach Desorbtion unmittelbar Messung
165	DIN ISO 16000-3:2013	17/11/2016	nein
167	HPLC	21.11.2016	30 min for first sample

Participant	Analytical method	Date start sample preparation	Storage time after desorption
174	HPLC	05/12/16	no delay
184	IFA 6045	17.11.2016	nein
186	N EN ISO 16000-3	14/11/2016	No storage after desorption / Direct analysis
191	ANA-033	15/11/2016	none
195	NIOSH2016	24/11/2016	14
198	Epa Compendium method TO11A	11/11/2016	Samples were immediately analized
199	in Anlehnung an DIN 16000-3:2013-01	22.11.2016	Tiefkühlschrank
207	DIN-ISO-16000-3	15.11.2016	-
208	ISO 16000-3	16.11.2016	2 h roomtemperature in samlper
219	HPLC	2016-11-08	14 hours in refrigerator
224	in house	22/11/2016	1 hour at roomtemp
255	BIA 6045	14.11.2016	Kühlschrank
264	HPLC/UV		
267	interne Methode SOP-B-35	15/11/2016	0 Tage
273	ISO 16000-3	28th Nov 2016	No storage, analyze immediately after desorption
280	HPLC	18/11/16	-15°C pendant 4 jours
287	HPLC-DAD (gradient)	10-11-2016	6 hours in autosampler @ 23 °C

Participant	Date of analysis	Desorption solution	Volume of desorption solution
6	10.11.16	Acetonitril	5 mL
10	11/11/2016	Acetonitrile	2 ml
11	22/11/2016	acetonitrile	5mL
22	17.11.2016	70% Acetonitril 30% Milli-Q_Wasser V/V	5 ml
29	25.11.16	Acetonitril	5ml
30	16 November 2016	Acetonitrile	5
55	16/11/2016	acetonitrile	3
56	09/11/16	acetonitrile	5 mL
58	17 november 2016	10 ml acetonitril	10 ml acetonitril
60	14/11/2016	Acetonitril	3mL
62	21/11/2016	Acetonitrile	5
68	10.11.2016	Acetonitril	10 ml
69	15/11/2016	Acetonitrile	5 ml

Participant	Date of analysis	Desorption solution	Volume of desorption solution
81	04/11/16	acetonitrile	10 mL
86	09/11/16	Acétonitrile	5 ml
90	15 and 16/11/2016	CH3CN	3 ml
93	16/11/2016	CH3CN	20 ml
98	10/11.11.2016	Acetonitril	10ml
99	18/11/2016	acétonitrile	5 ml
100	11/09/2016	acetonitrile	4 ml
104	15.11.2016	Acetoniril	10 ml
114	10 and 11/11/16	Desorption with acetonitrile	2 ml
123	15/11/2016	acetonitrile	5
131	25/11/16	CH3CN	10 ml
138	10.11.2016	Aetonitril	10
144	10 and 23/11/2016	Acetonitile	5
147	22/11/16	Acétonitrile	10 mL
151	11/11/2016	Acetonitrile	5ml eluant 4.7ml sample volume
155	14.11.2016	Acetonitril	5 ml
165	17/11/2016	Acetonitril	3 ml
167	21.11.2016	Acetonitrile (AcN)	6 mL (filled to 10 mL with distilled water)
174	05/12/16	acetonitrile	10
184	1. Messung unverdünnt am 17.11.2016; 2. Messung Verdünnung 1:5 am 18.11.2016	Extraktion mit ACN	5 ml, davon 2 ml auf 10 ml
186	14/11/2016	ACN	10mL
191	23/11/16	Acetonitrile	5
195	03/12/2016	ACETONITRILE	5 mL
198	11/11/2016	Acetonitrile	10
199	22.11.2016	Acetronitil	3mL
207	15.11.2016	Acetonitril/Wasser + 5mmol Ammoniumhydrogencarbonat	5
208	16.11.2016	Acetonitrile	3 ml
219	2016-11-09	Acetonitrile	10
224	22/11/2016	acetonitrile	5 ml
255	14.11.2016	Acetonitril	10 ml
264	10/11/2016	acétonitrile	5 mL
267	15/11/2016	Acetonitrile	5 ml
273	28th Nov 2016	ACN	5 mL

Participant	Date of analysis	Desorption solution	Volume of desorption solution
280	23/11/16	ACN	3 mL
287	10-11-2016	Acetonitrile	20

Participant	Chromatography system	Autosampler
6	Waters: Pumpe: 515, Detektor: 2996, Autosampler: 717	nein
10	Series 200 Perkin Elmer	No
11	HPLC-UV (2)	Dionex : no refrigeration ; Perkin-Elmer : 4 °C
22	Thermo: Pumpe: LPG-3400SD, Autosampler: WP-3000SL, UV/VIS-Detektor: DAD-3000	nein
29	Niederdruckpumpe, DAD, Autosampler	nein
30	Alliance Waters 2695 / UV detector Waters PAD 2996	No
55	Acquity Waters UPLC system	yes/20°C
56	Thermo P680 - Ultimate 3000- UV detector	15°C
58	LC-UV	no - roomtemperature
60	Agilent 1260 Infinity, quaternary pump, DAD, autosampler.	No
62	thermostatically controlled autosampler Agilent 1200 G1329A & G1330B / Quaternary pump Agilent 1200 G1311A	no
68	Agilent HPLC 1260 Infinity	Nein
69	Elite La Chrom Merck Hitachi pump: L-2130; sampler: L-2200; detector: UV-visible L2420	NO
81	Waters H-Class - QDA	no refrigerated autosampler
86	Agilent 1260	no
90	HITACHI pump L-2130, autosampler L-2200, DAD L-2455	no - ambiant temperature
93	Agilent serie 1100	Yes at 5°C
98	Gradienten Pumpe L-2130, Elite LaChrom, VWR; Diodenarray-Detektor L-2455, Elite LaChrom, VWR	nein
99	agilent 1200	agilent 1200
100	quaternary pump, UV detector, automatic sampler	NO
104	HP Series 1090 LC-DAD	kein gekühlter Autosampler
114	Thermoscientific HPLC U3000, UV detector	refrigerated autosampler, 10°C
123	HPLC/DAD	yes, 4°C
131	pump with 2 pistons, detector UV	no
138	Thermofisher Ultimate 3000	nein
144	HPLC Agilent 1200	Yes - 20°C
147	Waters Alliance 2695, DAD 2998	25°C
151	Waters AquityH Waters PDAdetector	20

Participant	Chromatography system	Autosampler
155	Agilent 1200 LC System DAD-Detektor	Autosampler gekühlt Temperatur 20 °C
165	HPLC Agilent Tecnologies 1100	nein
167	Perkin Elmer Series 200 LC	Not refrigerated
174	isochratic pump	yes, 10°C
184	Agilent 1100 Serie, Pumpe G1312A, AS G1313A, DAD G1315B, Ofen G1316A	nein
186	HPLC-PAD (Waters)	4°C
191	Agilent 1260 Infinity II	yes at 5°C
195	PERKIN ELMER SERIES 200 DAD	NO
198	hplc HP1100, quaternary pump,Uv/Vis variable wavelenght detector, manual injector	No
199	Agilent	Nein
207	1260 Infinity HPLC DAD, Agilent	-
208	Quaternary gradient pump. PDA detector	No
219	Agilent 1290 Infinity	5 degrees
224	UPLC/DAD-UV	refrigerated at 10°C
255	HPLC-DAD	4°C
267	Agilent (Quat Pump) 1260, DAD	nein, bei 25 °C
273	Agilent 1200 HPLC, Agilent 6430 LCMSMS	No refrigerated autosampler is used
280	DAD	20°C
287	Solvent Delivery Unit LC-20A, Low-pressure gradient unit, Column Oven CTO-20A, Auto-Sampler SIL-20A, Photo-diode Array detector SPD-M20A	No, 23 °C

Participant	Analytical column
6	Waters Symmetry C18, 5 µm, 3.9x150mm
10	Validated Brownlee C18 150x4.6mm
11	Dionex : 2 columns C18 ; Perkin Elmer : 1 column
22	Thermo Scientific Acclaim Carbonyl C18, 3µm 120A, 3,0x150mm
29	Waters Xbridge Phenyl 3,5ìm 4.6x150mm
30	Allure AK 200 x 4,6 mm 15 µm Restek
55	Waters Acquity UPLC BEH Phenyl
56	Acclaim RSLC carbonyl - 2.2 µm 2.1 x 100mm
58	Zorbax ODS 4,6 mm id*25 cm (5ìm)
60	Allure C18 5µm 150*4.6mm
62	Ascentis RP Amide HPLC Column

Participant	Analytical column
68	Poroshell 120 EC-C18 4.6 x 50 mm 2.7 um
69	Ascentis RP-Amide 25 cm x 4,6 mm
81	waters BEH C 18 (50x2.1 mm; 1.7 µm)
86	Hypersil Keystone
90	Allure AK 5µm- 200x4.6 mm
93	Merck C18 Microspher 100 250 mm by 4,6 mm
98	Lichrospher 100 RP18, 5µm, 250x4 mm, gleiche Vorsäule 4x4 mm
99	gemini c18
100	ALLURE AK 200*4.6mm*5µm
104	Reprosil-Pur C18-AQ, 5 µ, 250*4,6 mm
114	Acclaim 120, C18, 5µm, 250mm x 4.6mm
123	supelco discovery C 18 (250*4,6 mm, 5µm)
131	Uptisphere strategy -C18 5µm, L250mm, ID4.6mm
138	Nucleosil 100-5 C18 [250 * 4 mm)
144	Macherey Nagel NUCLEODUR 100/3 C18 HTec 3µm and NUCLEODUR 250/4.6 C18 HTec 3µm
147	Thermo Hypersil-Keystone 250x4.6 mm- 5µm
151	Waters BEH C18 1.7µm 2.1 x 100 mm
155	Agilent Zorbax XDB-C18 4,6mm 150mm 5µm
165	LC18
167	Waters Symmetry C18, 3,5 µm,, (4,6 x 10) mm Cartridge+
174	C18, 25 cm, 4.6 mm, 5 µm
184	50/3 Nucleodur Sphinx Rp, 1,8µm, mit Vorsäule
186	Waters NOVAPACK C18 / 150nm*3.9nm*4µm
191	Zorbax SB-C18
195	Poroshell 120 C18 3 mm x 150 mm x 2.7 um
198	Agilent Poroshell 120 EC-C18 4.6 x 250mm 4.0 micron
199	C18
207	Phenomenex Kinetex 2,6 µ; C18; 100A; 100*4,6 mm
208	HSS C18, 1,8µm
219	Silica C-18
224	Acquity BEH C18
255	Prontosil 200-5-C18 ace EPS
267	Symmetry C18, 250 mm x 4.6 mm x 5 µm (Waters)

Participant	Analytical column
273	Kinetex C18 narrow-bore column 4.6 x 100 mm, 2.6um
280	Ultra C18, 5µm
287	C18 - 250 x 4.6 mm Alltima HP C18 5µ

Participant	Mobile phase	Flow rate HPLC
6	Acetonitril/Wasser 45/55	1,3 mL/min
10	Acetonitrile/Water (70/30)	1ml/min
11	Acetonitrile/water	Dionex : 1 mL/min ; Perkin Elmer : 0,35 mL/min
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	0,6 ml/min
29	A: H2O/ACN/THF, B: ACN	1,5 ml/min
30	Water / acetonitrile	1.2
55	gradient elution of 10 % THF in water and acetonitril	0.5
56	acetonitrile/ water	1,0 ml/min
58		1
60	ACN/H2O	1mL
62	Acetonitrile/water	1 mL/min
68	Gradient Acetonitril, Methanol, Wasser	1.0 ml/min
69	Acetonitrile-water	1,5 ml/min
81	gradient acetonitrile / water + 0.5 g/L ammonium bicarbonate	0.3 mL/min
86	ACN 65% / Eau 35% + 0.06%TEA	1.2 ml/min
90	CH3CN/Water - 60/40	1,5 ml/min
93	CH3CN (53%) / H2O+H2SO4 (47%)	1 ml/min
98	Acetonitril / Wasser	1,2
99	65/35	1ml/min
100	WATER/ACETONITRILE	1.8 ml/min
104	Eluent A: MeOH/H2O/Acetonitril 52/30/18; Eluent B: MeOH/H2O/Acetonitril 52/15/33	0,6 ml/min
114	ACN + water	1ml/min
123	Acetonitrile/water	1
131	60%CH3CN - 40%water	1 ml/min
138	Acetonitril / Wasser / Ameisensäure, Gradientenprogramm	1,4
144	65% Acetonitrile / 35% water	
147	H2O/CH3CN:40/60	1 ml/min

Participant	Mobile phase	Flow rate HPLC
151	60% aqueous 40% acetonitrile	0.5
155	Gradient Start ACN 30 % THF 10 % H2O 60 % Ende ACN 95 % THF 5% H2O 35%	1 ml/min
165	Wasser/Acetonitil 40/60	1,3 ml/min
167	AcN with 0,1 % Phosphoric Acid and water with 0,1 % Phosphoric acid	1,5 mL/min
174	60%ACN, 40% H2O	1
184	Gradient; Eluent A: 90% Wasser + 10% THF / Eluent B: ACN	0,9 ml/min
186	water / ACN / THF	1.5mL/min
191	H2O/THF/ACN	0.6
195	ACN: H2O (30:70)	0.60 mL/min
198	Acetonitrile/Water	1
199	Acetonitril/Wasser	0,8mL/min.
207	Wasser + 0,005 % Natriumazid/Acetonitril/Tetrahydrofuran	1,5
208	Acetonitrile/Tetrahydrofuran/water	0,42 ml/min
219	A: Water B: Acetonitrile	0.4
224	60/40 water/ACN	0.5 ml/min
255	Acetonitril/Wasser	1 ml/min
267	Acetonitrile/Wasser	1,5 ml/min
273	ACN, 10mM Ammonium Acetate adjust to PH3.6	0.6 mL/min
280	ACN acidifié (0,1 % H3PO4)/Eau	1 mL/min
287	Ultra Pure Water, Tetrahydrofuran, Acetonitrile	1.00

Participant	Wavelength	Column temperature	Recovery rate
6	360 nm	20°C	nein
10	365 nm	25°C	No
11	360 nm	Dionex : 40 °C ; Perkin Elmer : 60 °C	No
22	360 nm	28° C	nein
29	365nm	27°C	nein
30	360	30°C	No
55	360	40°C	yes
56	360 nm	28°C	no
58	360 nm	35°C	no
60	360nm	20°C	No

Participant	Wavelength	Column temperature	Recovery rate
62	360 nm	30°C	no
68	365 nm	25°C	Formaldehyd 94%
69	Uv-visible	40 ºC	NO
81	No	22°C	No
86	355 nm	23°C	
90	360 nm	28°C	no
93	350 nm	25°C	No
98	365 nm	25°C	Nein
99	354 nm	35 °C	NO
100	360 nm	40°C	NO
104	365,8 nm	Raumtemperatur	nein
114	360nm	40°C	No
123	365.4 nm	25°C	no
131	350 nm	21°C	no
138	360 nm	40 °C	ja
147	354 nm pour le formol, et 362 nm pour l'acétaldéhyde	27°C	Non
151	360	50	
155	360nm 365nm 380nm	35 °C	nein, Kontrolle der vollständigen Desorbtion erfolgte durch eine weiter Desorbtion des Adsorbers
165	360 nm	25 °C	nein
167	360 nm	24 °C	Yes
174	360 nm	20°C	no
184	360 nm	40°C	k.A.
186	360nm	35°C	No
191	360	40°C	-
195	360 nm	35 ºC	100 %
198	360nm	30°C	No
199	370nm	30°C	Nein
207	360 nm	30°C	
208	360 nm	40 °C	No
219	360nm	35 degrees	No
224	360nm	45°C	no
255	365 nm	40 °C	Wiederfindungsraten im Bereich der Toleranzgrenzen
267	365 nm	25°C	nein

Participant	Wavelength	Column temperature	Recovery rate
273	350nm	Room temperature column condition	No
280	360 nm	40°C	no
287	360 nm	35 °C	No