

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

Proficiency testing scheme: Aldehydes

November 2022

Summary of laboratory test results

Sample 1

Laboratory	Acetaldehyde	Z score	Butyraldehyde	Z score	Formaldehyde	Z score
Unit	mg/m ³		mg/m ³		mg/m ³	
9	0.800	-0.20	0.460	0.60	0.080	0.21
13	0.770	-0.57	0.387	-1.09	0.079	0.08
18	0.830	0.17	0.450	0.37	0.079	0.08
21	0.796	-0.25	0.447	0.30	0.084	0.72
29	0.708	-1.33			0.071	-0.87
30	0.572	-2.99 BE	0.345	-2.05 E	0.062	-2.09 E
50	0.803	-0.17	0.391	-0.99	0.077	-0.17
51	0.829	0.15	0.460	0.60	0.078	-0.04
55	0.770	-0.57	0.442	0.18	0.083	0.59
56	0.900	1.02	0.390	-1.02	0.074	-0.55
60	0.833	0.20	0.463	0.66	0.076	-0.25
62	0.779	-0.46	0.379	-1.26	0.072	-0.81
68	0.675	-1.73	0.342	-2.12 E	0.064	-1.83
69	0.706	-1.35			0.087	1.05
73	0.850	0.41	0.463	0.67	0.075	-0.43
80	0.830	0.17	0.450	0.37	0.082	0.47
83					0.079	0.05
85	0.810	-0.08	0.480	1.06	0.074	-0.55
119	0.885	0.84			0.070	-1.10
120	0.964	1.81	0.442	0.18	0.078	-0.04
124	0.810	-0.08	0.500	1.52	0.084	0.72
135	0.814	-0.03	0.458	0.55	0.073	-0.64
138	0.870	0.66	0.490	1.29	0.081	0.34
141	0.858	0.51	0.466	0.73	0.083	0.61
153	0.826	0.12	0.426	-0.19	0.074	-0.55
155	0.849	0.40	0.423	-0.26	0.084	0.72
165	0.820	0.04	0.407	-0.62	0.077	-0.17
167	0.783	-0.41	0.474	0.91	0.069	-1.21
186	0.821	0.06	0.355	-1.82	0.079	0.08

Laboratory	Acetaldehyde	Z score	Butyraldehyde	Z score	Formaldehyde	Z score
189	0.823	0.08	0.421	-0.30	0.077	-0.17
192	0.821	0.06	0.468	0.78	0.079	0.08
198	0.813	-0.05			0.077	-0.17
201	0.797	-0.24	0.441	0.16	0.079	0.08
207	0.811	-0.07	0.446	0.27	0.077	-0.17
208	0.797	-0.24	0.439	0.11	0.077	-0.17
229	0.808	-0.10			0.096	2.25 E
230	0.833	0.20	0.473	0.90	0.088	1.23
241	0.780	-0.45	0.390	-1.02	0.084	0.72
248	0.829	0.15	0.419	-0.35	0.084	0.70
256	0.842	0.31	0.453	0.44	0.080	0.21
258	0.847	0.37	0.418	-0.37	0.083	0.59
264	0.850	0.41	0.430	-0.09	0.080	0.21
267	0.838	0.26	0.474	0.93	0.080	0.19
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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	42		37		43	
Mean	0.816		0.434		0.078	
Reproducibility s.d.	0.050		0.040		0.006	
Rel. reproducibility s.d.	6.09 %		9.13 %		7.78 %	
Reference value	0.785		0.429		0.073	
Target s.d.	0.082		0.043		0.008	
Rel. target s.d.	10.00 %		10.00 %		10.00 %	
Lower limit of tolerance	0.653		0.347		0.063	
Upper limit of tolerance	0.980		0.521		0.094	
Type B outliers	1					
No. of laboratories after elimination of outliers type A-D and F (without laboratories that only gave states but no measured values)	41		37		43	
Explanation of outlier types						
A: Single outlier	Grubbs					

Laboratory	Acetaldehyde	Z score	Butyraldehyde	Z score	Formaldehyde	Z score
B: Differing laboratory mean	Grubbs					
C: Excessive laboratory s.d.	Cochran					
D: Excluded manually						
E: mean outside tolerance limits						
F: Z-Score >3.50						

Summary of laboratory test results

Sample 2

Laboratory	Acetaldehyde	Z score	Formaldehyde	Z score	Propionaldehyde	Z score
Unit	mg/m ³		mg/m ³		mg/m ³	
9	0.490	0.23	0.120	1.14	0.630	-0.08
13	0.454	-0.52	0.105	-0.25	0.534	-1.59
18	0.490	0.23	0.110	0.21	0.650	0.23
21	0.477	-0.04	0.116	0.77	0.643	0.12
29	0.452	-0.56	0.101	-0.62	0.621	-0.23
30	0.361	-2.46 BE	0.089	-1.74	0.493	-2.24 E
50	0.584	2.19 BE	0.147	3.65 BE	0.754	1.87
51	0.483	0.08	0.106	-0.16	0.668	0.51
55	0.459	-0.42	0.116	0.77	0.628	-0.12
56	0.540	1.27	0.104	-0.34	0.660	0.39
60	0.490	0.22	0.104	-0.38	0.694	0.93
62	0.446	-0.69	0.101	-0.62	0.579	-0.89
68	0.418	-1.27	0.090	-1.64	0.552	-1.31
69	0.422	-1.19	0.125	1.60	0.640	0.07
73	0.493	0.29	0.105	-0.25	0.663	0.44
80	0.500	0.44	0.110	0.21	0.640	0.07
83			0.115	0.63		
85	0.490	0.23	0.110	0.21	0.650	0.23
119	0.513	0.71	0.094	-1.23		
120	0.571	1.92 B	0.107	-0.06	0.563	-1.14
124	0.470	-0.19	0.114	0.59	0.670	0.55
135	0.471	-0.17	0.099	-0.79	0.631	-0.07
138	0.510	0.65	0.110	0.21	0.440	-3.07 BE
141	0.519	0.83	0.112	0.40	0.663	0.44
153	0.490	0.23	0.102	-0.53	0.667	0.50
155	0.504	0.52	0.112	0.40	0.675	0.62
165	0.490	0.23	0.106	-0.16	0.589	-0.73
167	0.457	-0.47	0.096	-1.11	0.654	0.29
186	0.473	-0.13	0.109	0.12	0.548	-1.37

Laboratory	Acetaldehyde	Z score	Formaldehyde	Z score	Propionaldehyde	Z score
189	0.470	-0.19	0.104	-0.34	0.690	0.86
192	0.486	0.15	0.110	0.21	0.671	0.56
198	0.470	-0.19	0.105	-0.22		
201	0.468	-0.23	0.105	-0.25	0.646	0.17
207	0.471	-0.17	0.106	-0.16	0.631	-0.07
208	0.476	-0.06	0.106	-0.16	0.637	0.03
229	0.467	-0.25	0.112	0.40		
230	0.488	0.19	0.120	1.14	0.670	0.55
241	0.450	-0.61	0.110	0.21	0.580	-0.87
248	0.478	-0.03	0.114	0.61	0.617	-0.30
256	0.506	0.56	0.114	0.59	0.706	1.11
258	0.478	-0.02	0.110	0.21	0.590	-0.71
264	0.480	0.02	0.110	0.21	0.670	0.55
267	0.494	0.32	0.109	0.16	0.675	0.63
-	-	--	-	--	-	--
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	42		43		39	
Mean	0.479		0.108		0.635	
Reproducibility s.d.	0.024		0.007		0.052	
Rel. reproducibility s.d.	5.07 %		6.91 %		8.19 %	
Reference value	0.462		0.100		0.616	
Target s.d.	0.048		0.011		0.064	
Rel. target s.d.	10.00 %		10.00 %		10.00 %	
Lower limit of tolerance	0.383		0.086		0.508	
Upper limit of tolerance	0.575		0.129		0.762	
Type B outliers	3		1		1	
No. of laboratories after elimination of outliers type A-D and F (without laboratories that only gave states but no measured values)	39		42		38	
Explanation of outlier types						
A: Single outlier	Grubbs					

Laboratory	Acetaldehyde	Z score	Formaldehyde	Z score	Propionaldehyde	Z score
B: Differing laboratory mean	Grubbs					
C: Excessive laboratory s.d.	Cochran					
D: Excluded manually						
E: mean outside tolerance limits						
F: Z-Score >3.50						

Summary of laboratory test results

Sample 3

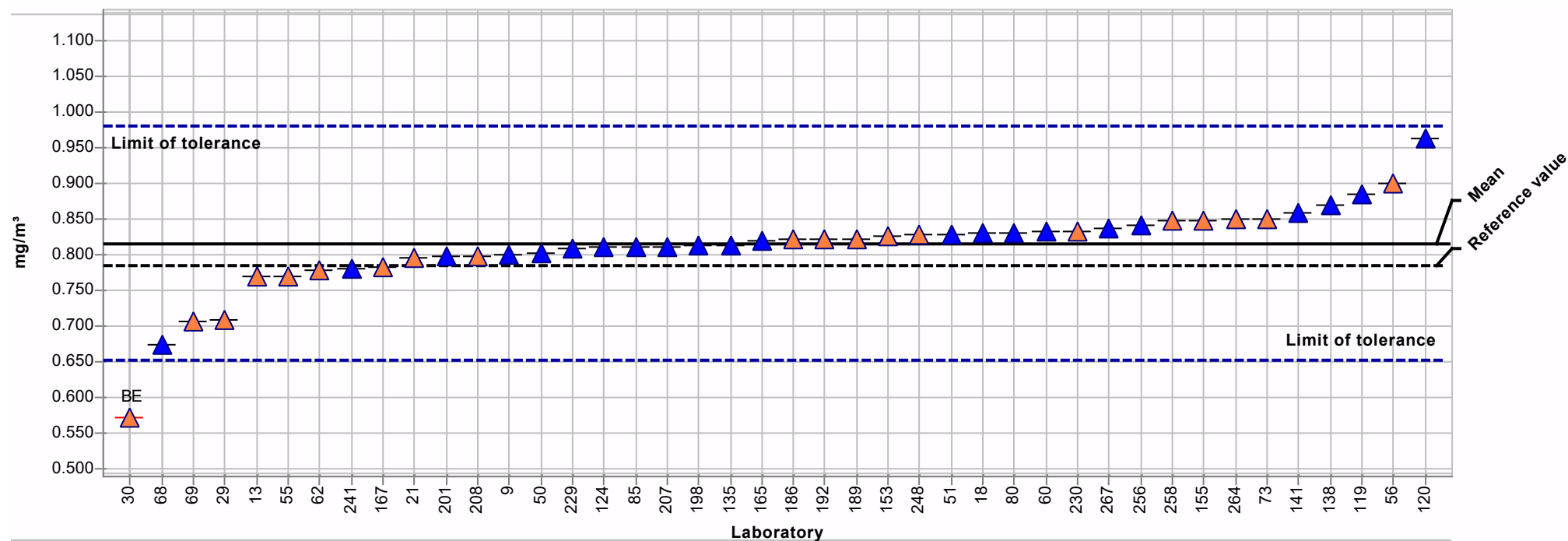
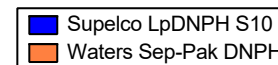
Laboratory	Acetaldehyde	Z score	Butyraldehyde	Z score	Formaldehyde	Z score	Propionaldehyde	Z score
Unit	mg/m ³		mg/m ³		mg/m ³		mg/m ³	
9	0.430	-0.01	0.630	0.87	0.150	0.01	0.300	0.74
13	0.411	-0.45	0.513	-1.15	0.146	-0.25	0.237	-1.52
18	0.440	0.23	0.610	0.53	0.160	0.68	0.290	0.38
21	0.418	-0.28	0.588	0.15	0.157	0.48	0.274	-0.19
29	0.379	-1.19			0.134	-1.05	0.258	-0.77
30	0.324	-2.47 BE	0.470	-1.89	0.122	-1.86	0.216	-2.27 E
50	0.453	0.53	0.621	0.72	0.140	-0.65	0.304	0.88
51	0.440	0.23	0.618	0.67	0.149	-0.05	0.295	0.56
55	0.408	-0.52	0.596	0.29	0.159	0.61	0.274	-0.19
56	0.490	1.39	0.530	-0.85	0.145	-0.32	0.290	0.38
60	0.438	0.19	0.616	0.64	0.146	-0.27	0.299	0.71
62	0.443	0.29	0.474	-1.82	0.138	-0.81	0.244	-1.28
68	0.367	-1.47	0.451	-2.22 E	0.123	-1.79	0.231	-1.73
69	0.382	-1.12			0.174	1.62	0.284	0.15
73	0.451	0.48	0.623	0.75	0.150	0.01	0.292	0.45
80	0.440	0.23	0.590	0.18	0.150	0.01	0.280	0.02
83					0.165	1.01		
85	0.440	0.23	0.630	0.87	0.150	0.01	0.290	0.38
119	0.465	0.82			0.134	-1.05		
120	0.516	1.99 B	0.585	0.10	0.153	0.21	0.250	-1.05
124	0.420	-0.24	0.670	1.56	0.157	0.48	0.300	0.74
135	0.422	-0.19	0.598	0.32	0.139	-0.72	0.276	-0.12
138	0.450	0.46	0.630	0.87	0.150	0.01	0.310	1.09
141	0.458	0.65	0.605	0.44	0.157	0.48	0.295	0.56
153	0.418	-0.28	0.545	-0.59	0.138	-0.79	0.282	0.09
155	0.456	0.60	0.557	-0.39	0.160	0.68	0.302	0.81
165	0.439	0.20	0.543	-0.63	0.154	0.28	0.260	-0.70
167	0.407	-0.54	0.623	0.76	0.137	-0.87	0.288	0.30
186	0.436	0.13	0.488	-1.58	0.158	0.55	0.244	-1.27

Laboratory	Acetaldehyde	Z score	Butyraldehyde	Z score	Formaldehyde	Z score	Propionaldehyde	Z score
189	0.415	-0.35	0.575	-0.08	0.144	-0.39	0.294	0.52
192	0.427	-0.08	0.615	0.61	0.150	0.01	0.291	0.41
198	0.399	-0.72			0.141	-0.56		
201	0.444	0.32	0.631	0.89	0.154	0.28	0.296	0.59
207	0.425	-0.12	0.578	-0.02	0.148	-0.12	0.280	0.02
208	0.424	-0.15	0.577	-0.04	0.147	-0.19	0.286	0.24
229	0.419	-0.26			0.149	-0.05		
230	0.448	0.41	0.633	0.93	0.169	1.28	0.297	0.63
241	0.410	-0.47	0.520	-1.02	0.160	0.68	0.260	-0.70
248	0.437	0.16	0.557	-0.39	0.160	0.67	0.271	-0.30
256	0.433	0.06	0.610	0.53	0.155	0.35	0.292	0.45
258	0.445	0.34	0.554	-0.44	0.157	0.48	0.267	-0.44
264	0.440	0.23	0.560	-0.33	0.160	0.68	0.300	0.74
267	0.441	0.26	0.623	0.75	0.153	0.19	0.299	0.71
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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	
No. of laboratories that submitted results	42		37		43		39	
Mean	0.430		0.579		0.150		0.279	
Reproducibility s.d.	0.024		0.053		0.011		0.023	
Rel. reproducibility s.d.	5.51 %		9.06 %		7.26 %		8.08 %	
Reference value	0.424		0.590		0.143		0.274	
Target s.d.	0.043		0.058		0.015		0.028	
Rel. target s.d.	10.00 %		10.00 %		10.00 %		10.00 %	
Lower limit of tolerance	0.344		0.464		0.120		0.224	
Upper limit of tolerance	0.516		0.695		0.180		0.335	
Type B outliers	2							
No. of laboratories after elimination of outliers type A-D and F (without laboratories that only gave states but no measured values)	40		37		43		39	
Explanation of outlier types								
A: Single outlier	Grubbs							

Laboratory	Acetaldehyde	Z score	Butyraldehyde	Z score	Formaldehyde	Z score	Propionaldehyde	Z score
B: Differing laboratory mean	Grubbs							
C: Excessive laboratory s.d.	Cochran							
D: Excluded manually								
E: mean outside tolerance limits								
F: Z-Score >3.50								

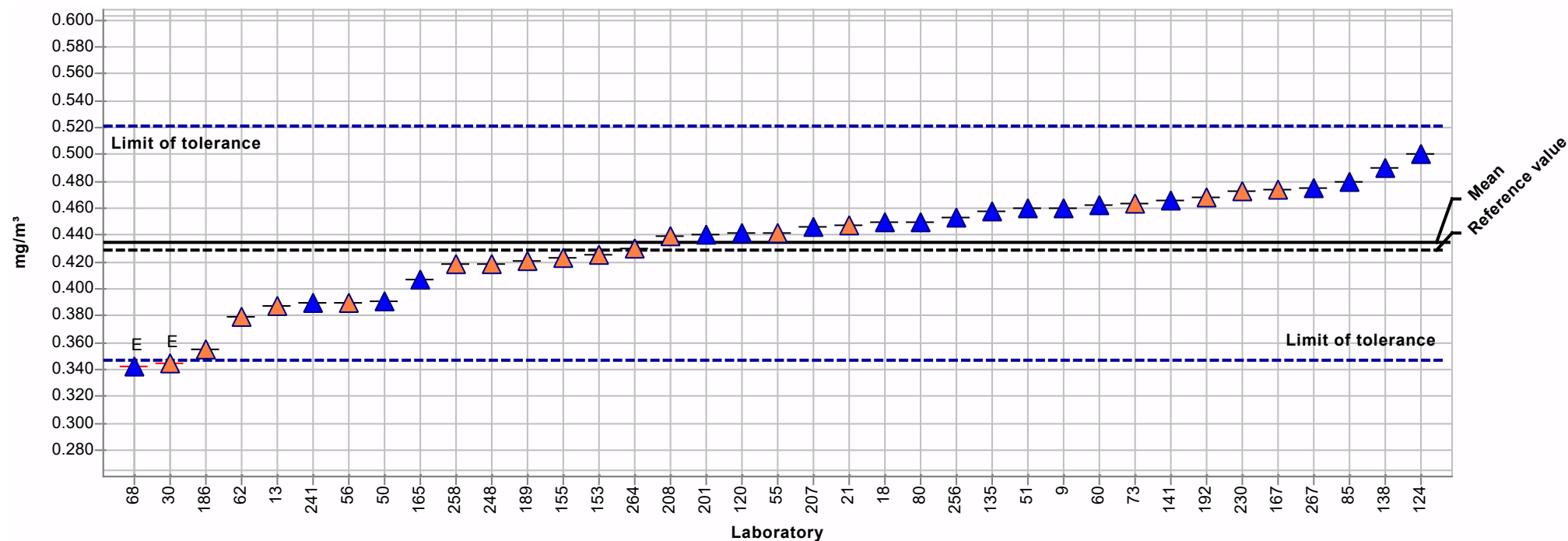
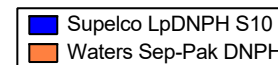
Summary results

Sample:	1	Mean:	0.816 mg/m ³
Measurand:	Acetaldehyde	Reproducibility s.d.:	0.050 mg/m ³
Method:	ISO 5725-2	Rel. reproducibility s.d.:	6.09%
Rel. target s.d.:	10.00%	Reference value:	0.785 mg/m ³
Number of laboratories in calculation:	42	Range of tolerance:	0.653 - 0.980 mg/m ³ (Z-Score ≤ 2.00)



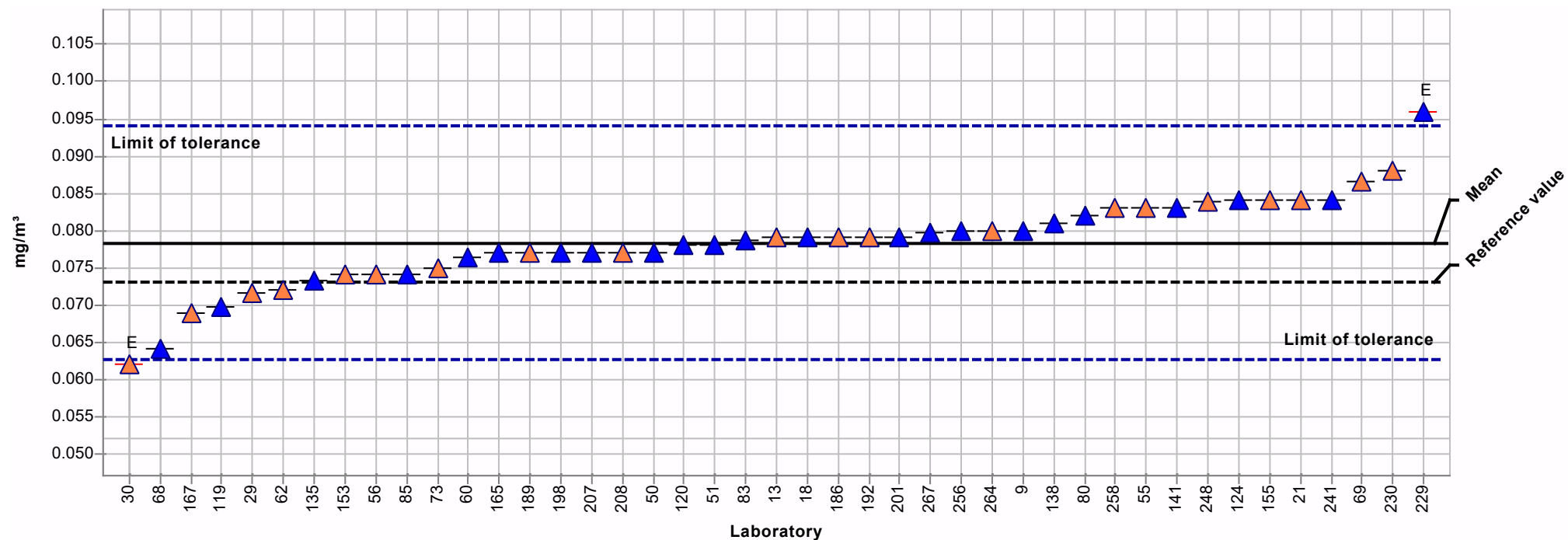
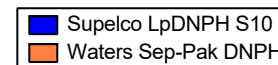
Summary results

Sample:	1	Mean:	0.434 mg/m ³
Measurand:	Butyraldehyde	Reproducibility s.d.:	0.040 mg/m ³
Method:	ISO 5725-2	Rel. reproducibility s.d.:	9.13%
Rel. target s.d.:	10.00%	Reference value:	0.429 mg/m ³
Number of laboratories in calculation:	37	Range of tolerance:	0.347 - 0.521 mg/m ³ (Z-Score <= 2.00)



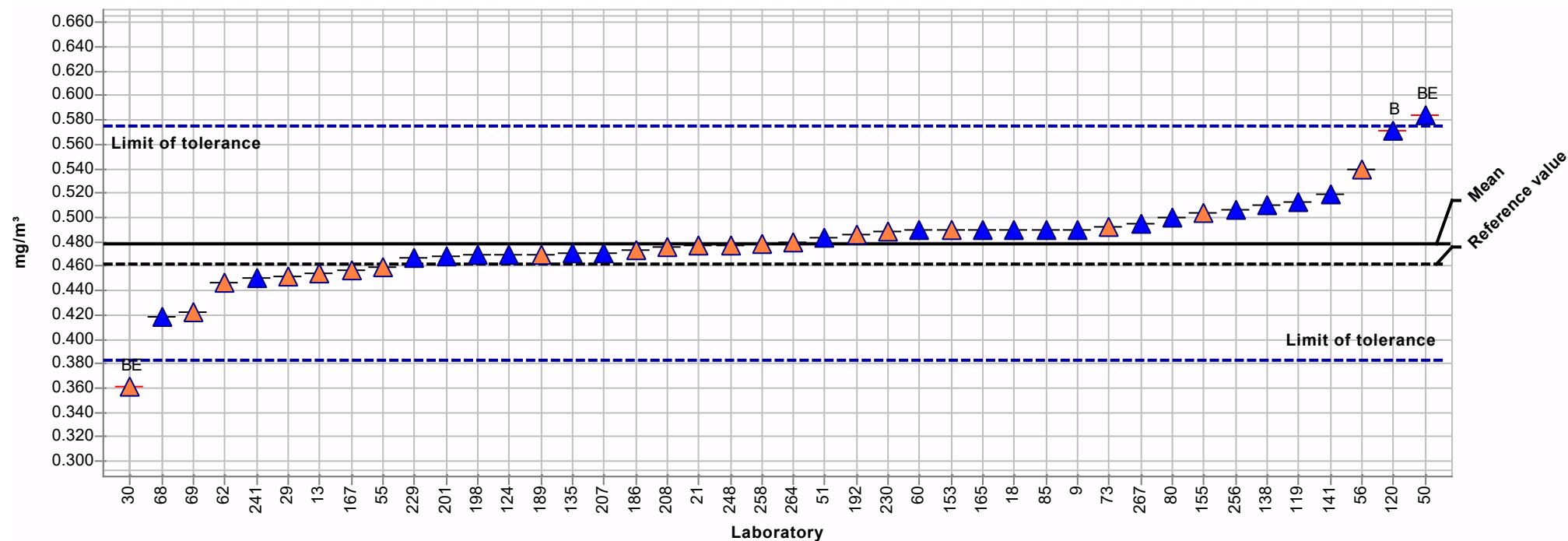
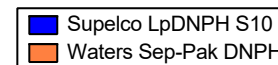
Summary results

Sample:	1	Mean:	0.078 mg/m ³
Measurand:	Formaldehyde	Reproducibility s.d.:	0.006 mg/m ³
Method:	ISO 5725-2	Rel. reproducibility s.d.:	7.78%
Rel. target s.d.:	10.00%	Reference value:	0.073 mg/m ³
Number of laboratories in calculation:	43	Range of tolerance:	0.063 - 0.094 mg/m ³ (Z-Score ≤ 2.00)



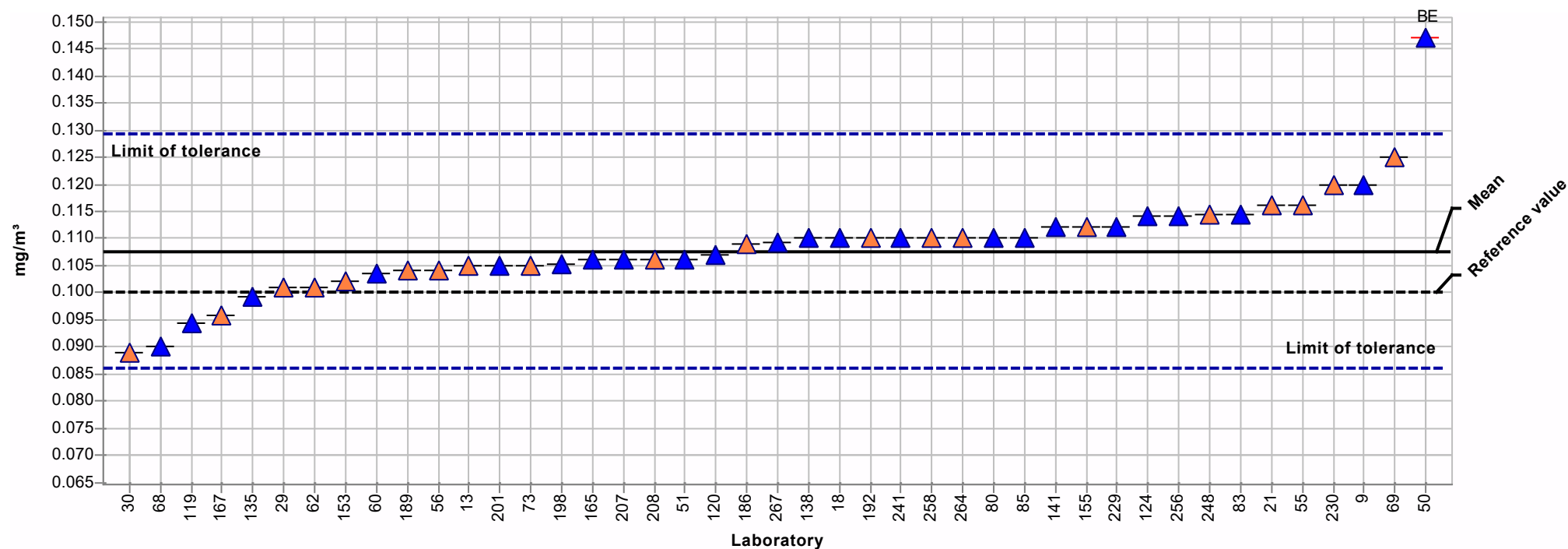
Summary results

Sample:	2	Mean:	0.479 mg/m ³
Measurand:	Acetaldehyde	Reproducibility s.d.:	0.024 mg/m ³
Method:	ISO 5725-2	Rel. reproducibility s.d.:	5.07%
Rel. target s.d.:	10.00%	Reference value:	0.462 mg/m ³
Number of laboratories in calculation:	42	Range of tolerance:	0.383 - 0.575 mg/m ³ (Z-Score ≤ 2.00)



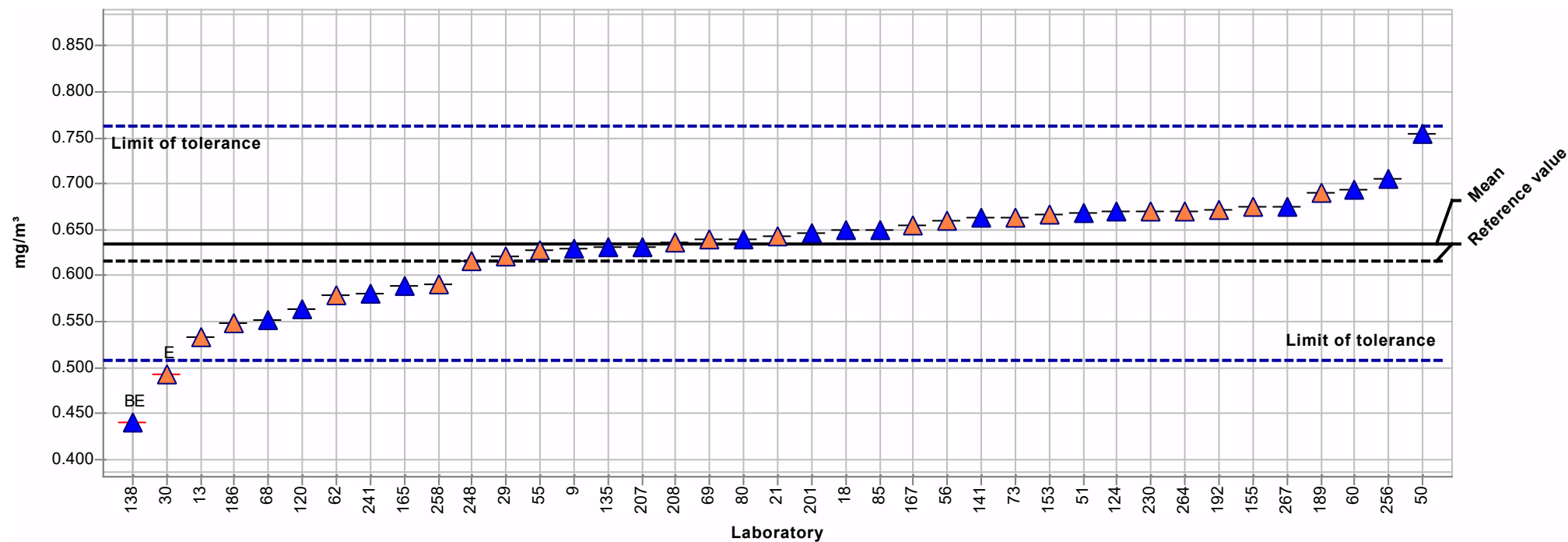
Summary results

Sample:	2	Mean:	0.108 mg/m ³
Measurand:	Formaldehyde	Reproducibility s.d.:	0.007 mg/m ³
Method:	ISO 5725-2	Rel. reproducibility s.d.:	6.91%
Rel. target s.d.:	10.00%	Reference value:	0.100 mg/m ³
Number of laboratories in calculation:	43	Range of tolerance:	0.086 - 0.129 mg/m ³ (Z-Score ≤ 2.00)



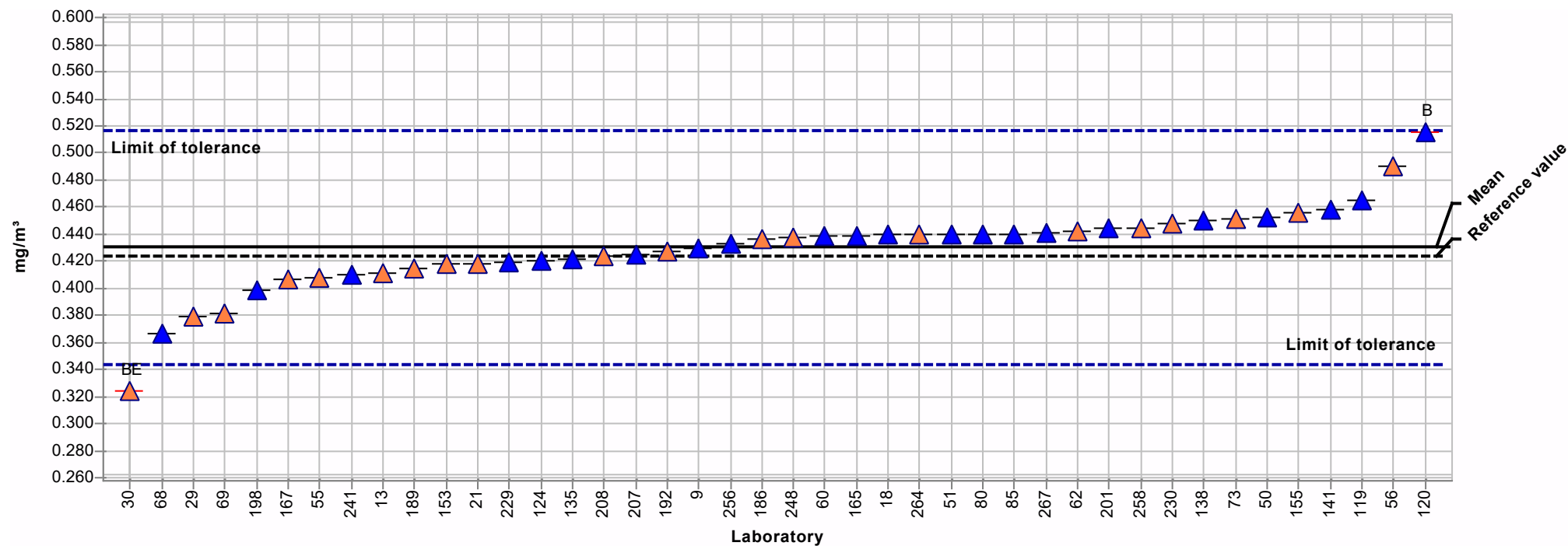
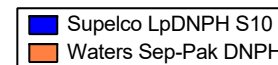
Summary results

Sample:	2	Mean:	0.635 mg/m ³
Measurand:	Propionaldehyde	Reproducibility s.d.:	0.052 mg/m ³
Method:	ISO 5725-2	Rel. reproducibility s.d.:	8.19%
Rel. target s.d.:	10.00%	Reference value:	0.616 mg/m ³
Number of laboratories in calculation:	39	Range of tolerance:	0.508 - 0.762 mg/m ³ (Z-Score <= 2.00)



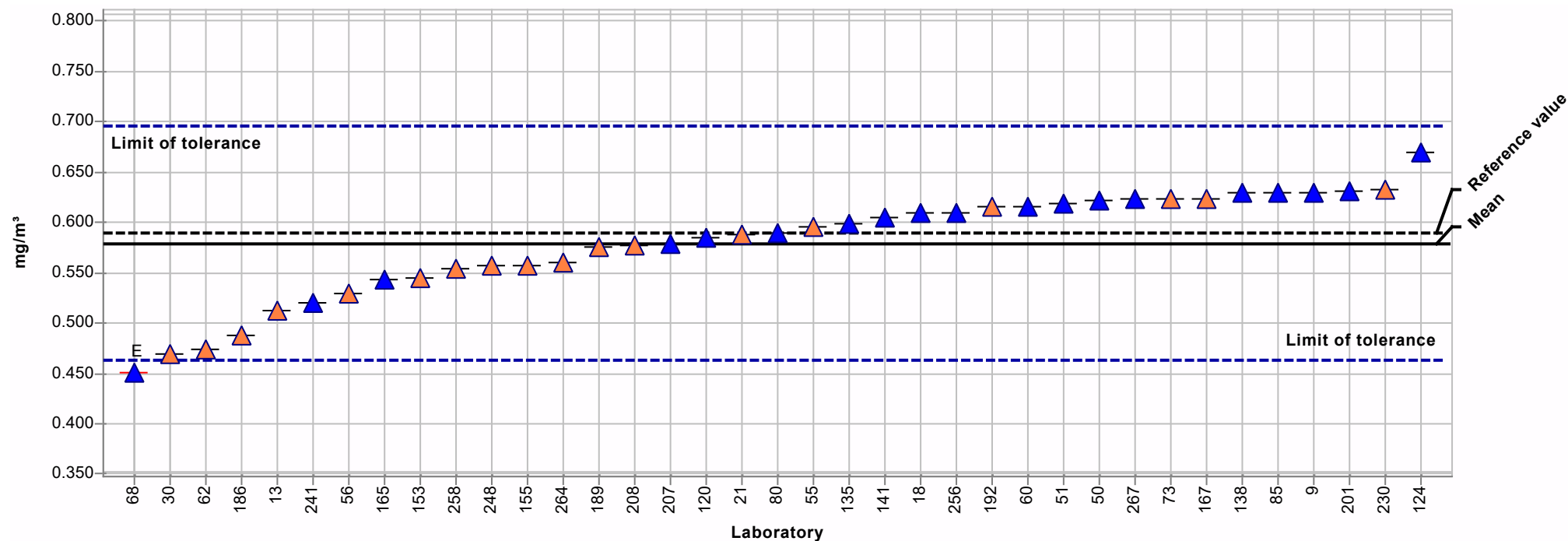
Summary results

Sample:	3	Mean:	0.430 mg/m ³
Measurand:	Acetaldehyde	Reproducibility s.d.:	0.024 mg/m ³
Method:	ISO 5725-2	Rel. reproducibility s.d.:	5.51%
Rel. target s.d.:	10.00%	Reference value:	0.424 mg/m ³
Number of laboratories in calculation:	42	Range of tolerance:	0.344 - 0.516 mg/m ³ (Z-Score ≤ 2.00)



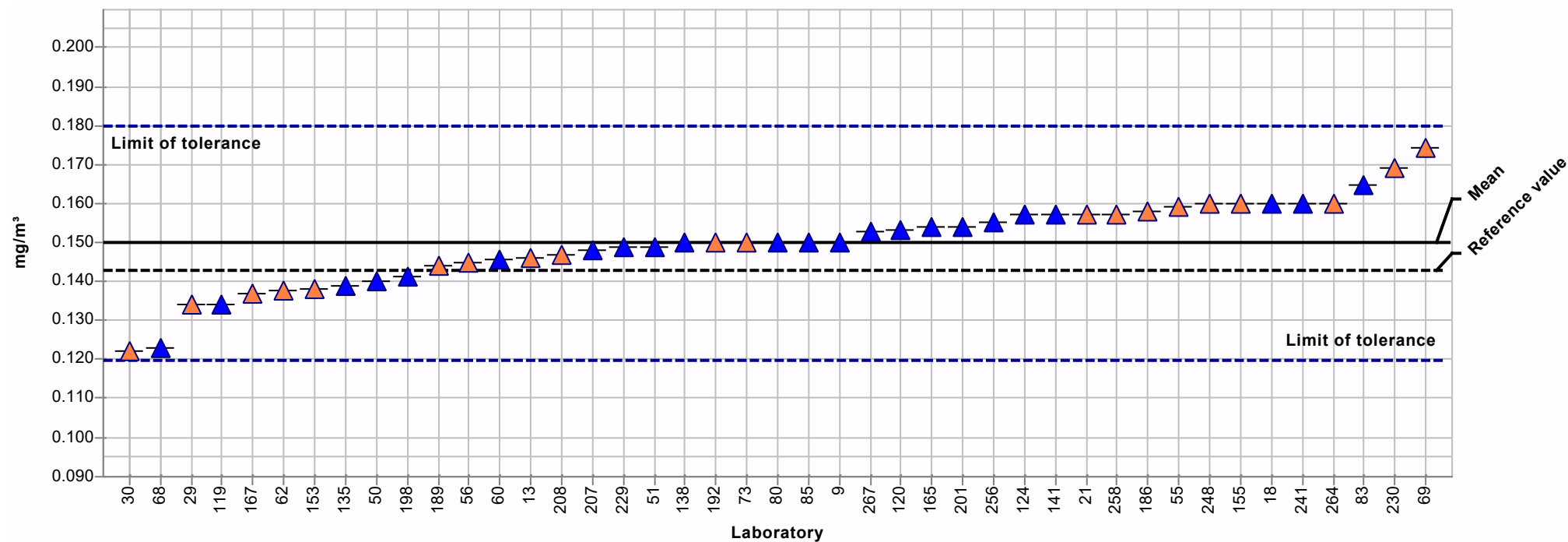
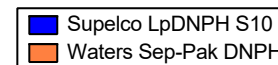
Summary results

Sample:	3	Mean:	0.579 mg/m ³
Measurand:	Butyraldehyde	Reproducibility s.d.:	0.053 mg/m ³
Method:	ISO 5725-2	Rel. reproducibility s.d.:	9.06%
Rel. target s.d.:	10.00%	Reference value:	0.590 mg/m ³
Number of laboratories in calculation:	37	Range of tolerance:	0.464 - 0.695 mg/m ³ (Z-Score <= 2.00)



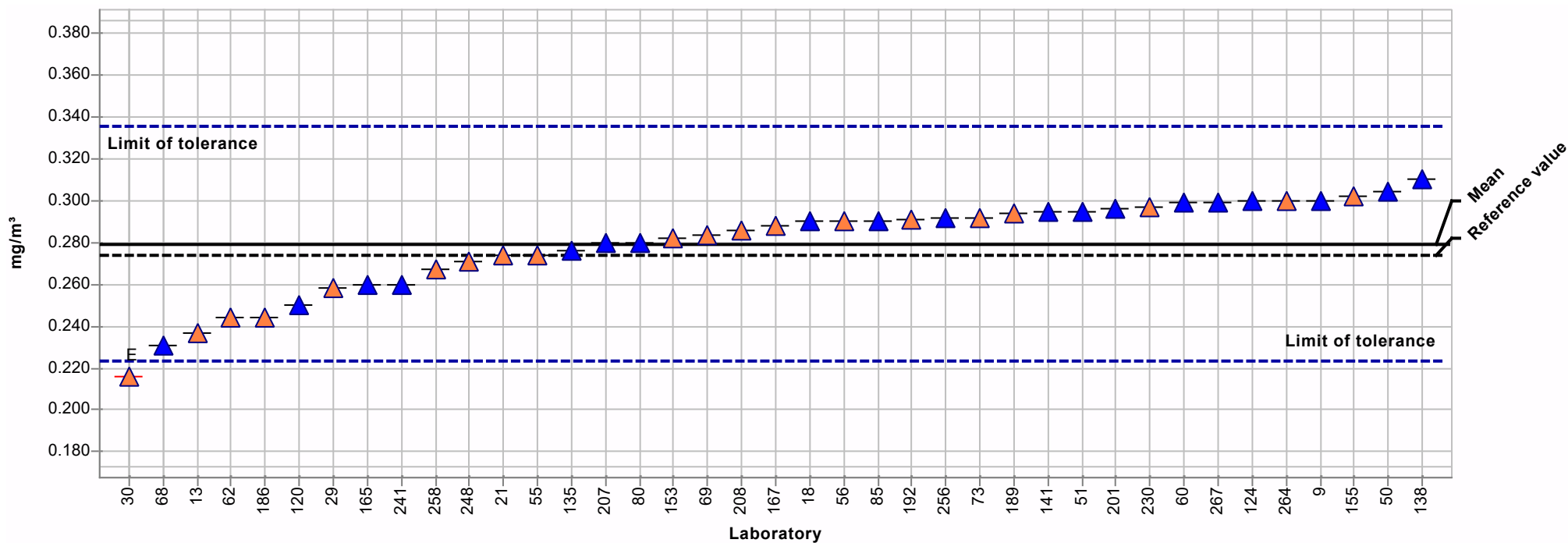
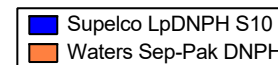
Summary results

Sample:	3	Mean:	0.150 mg/m³
Measurand:	Formaldehyde	Reproducibility s.d.:	0.011 mg/m³
Method:	ISO 5725-2	Rel. reproducibility s.d.:	7.26%
Rel. target s.d.:	10.00%	Reference value:	0.143 mg/m³
Number of laboratories in calculation:	43	Range of tolerance:	0.120 - 0.180 mg/m³ (Z-Score ≤ 2.00)



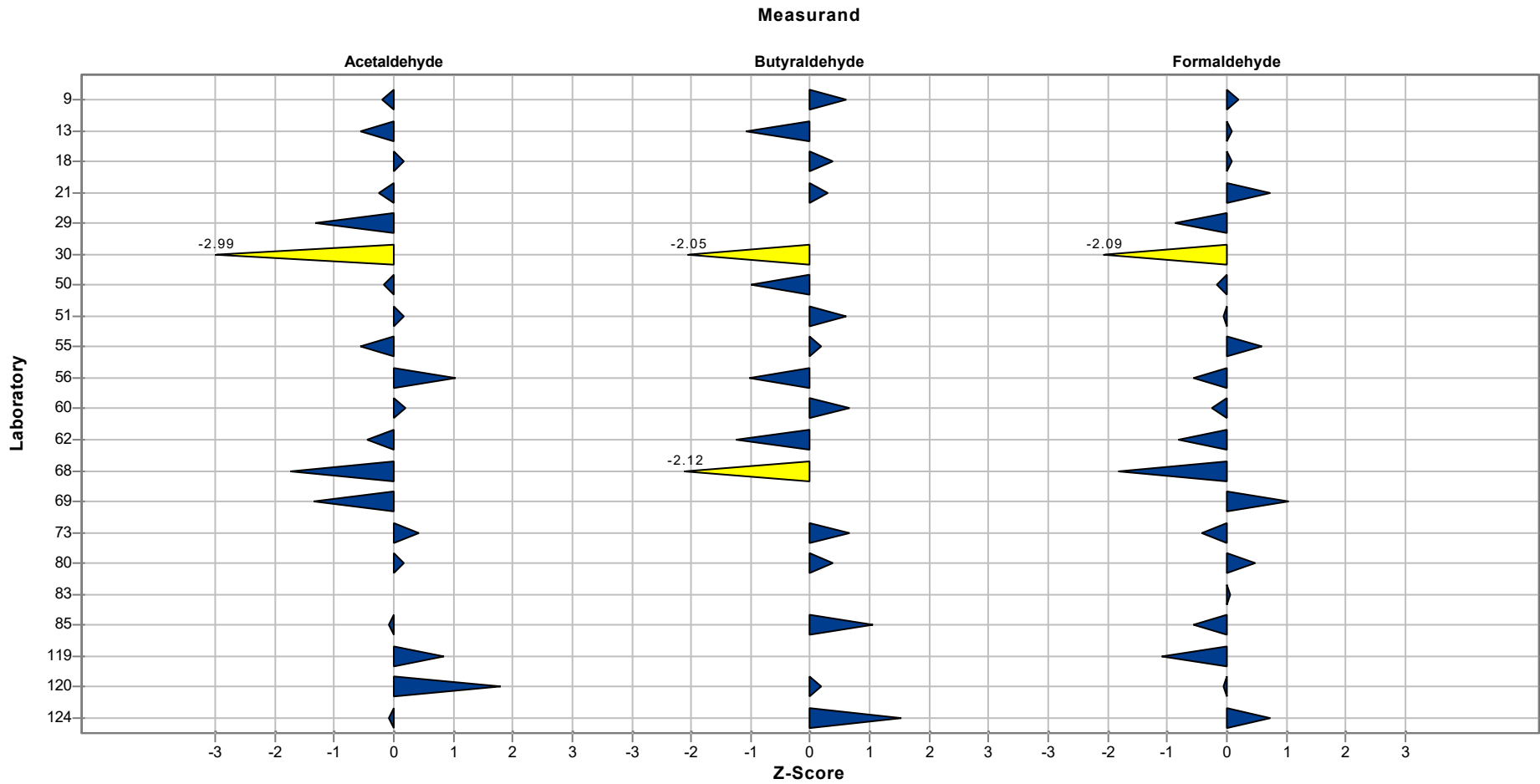
Summary results

Sample:	3	Mean:	0.279 mg/m ³
Measurand:	Propionaldehyde	Reproducibility s.d.:	0.023 mg/m ³
Method:	ISO 5725-2	Rel. reproducibility s.d.:	8.08%
Rel. target s.d.:	10.00%	Reference value:	0.274 mg/m ³
Number of laboratories in calculation:	39	Range of tolerance:	0.224 - 0.335 mg/m ³ (Z-Score ≤ 2.00)



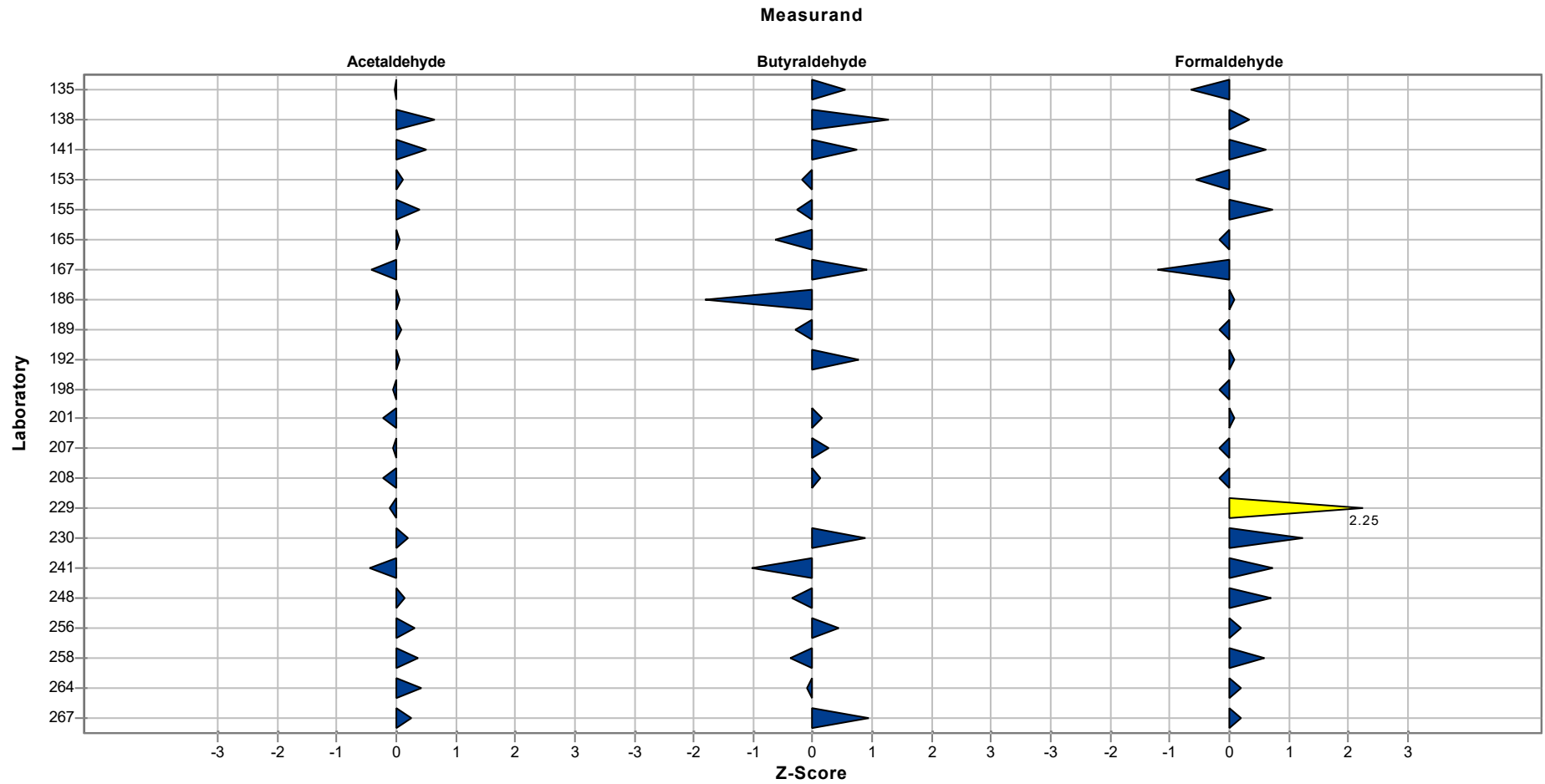
Sample chart of Z-Scores

Sample: 1



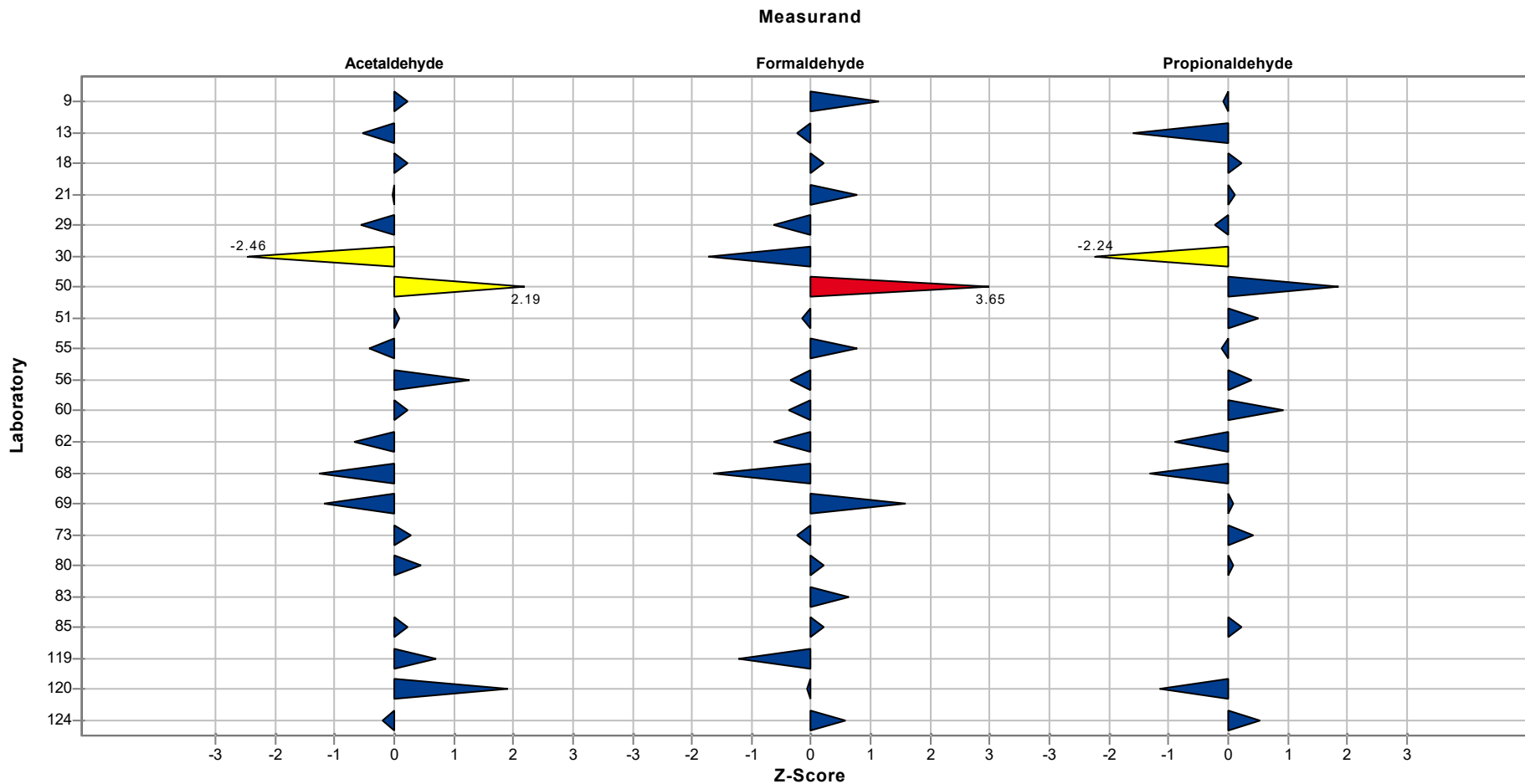
Sample chart of Z-Scores

Sample: 1



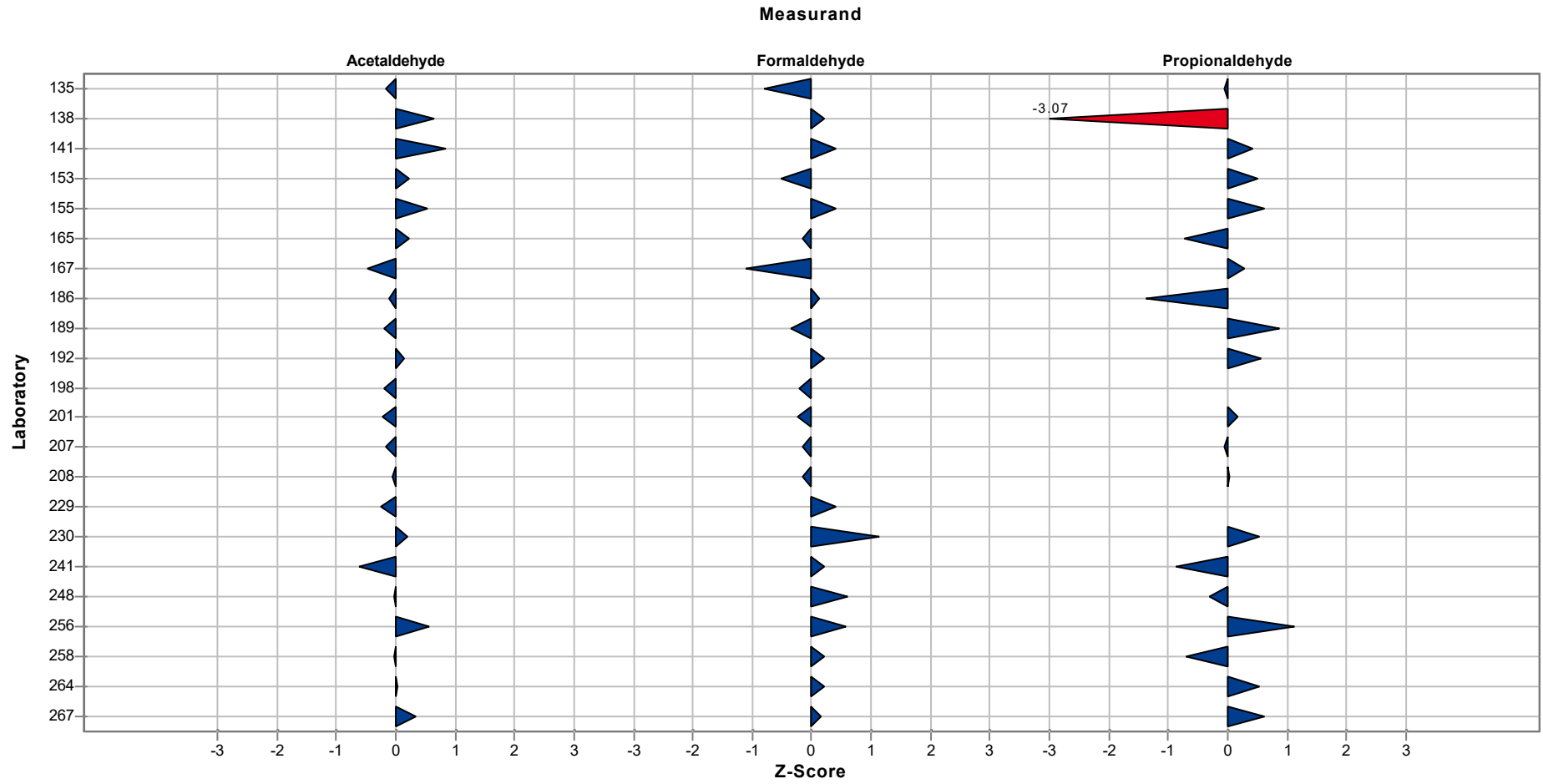
Sample chart of Z-Scores

Sample: 2



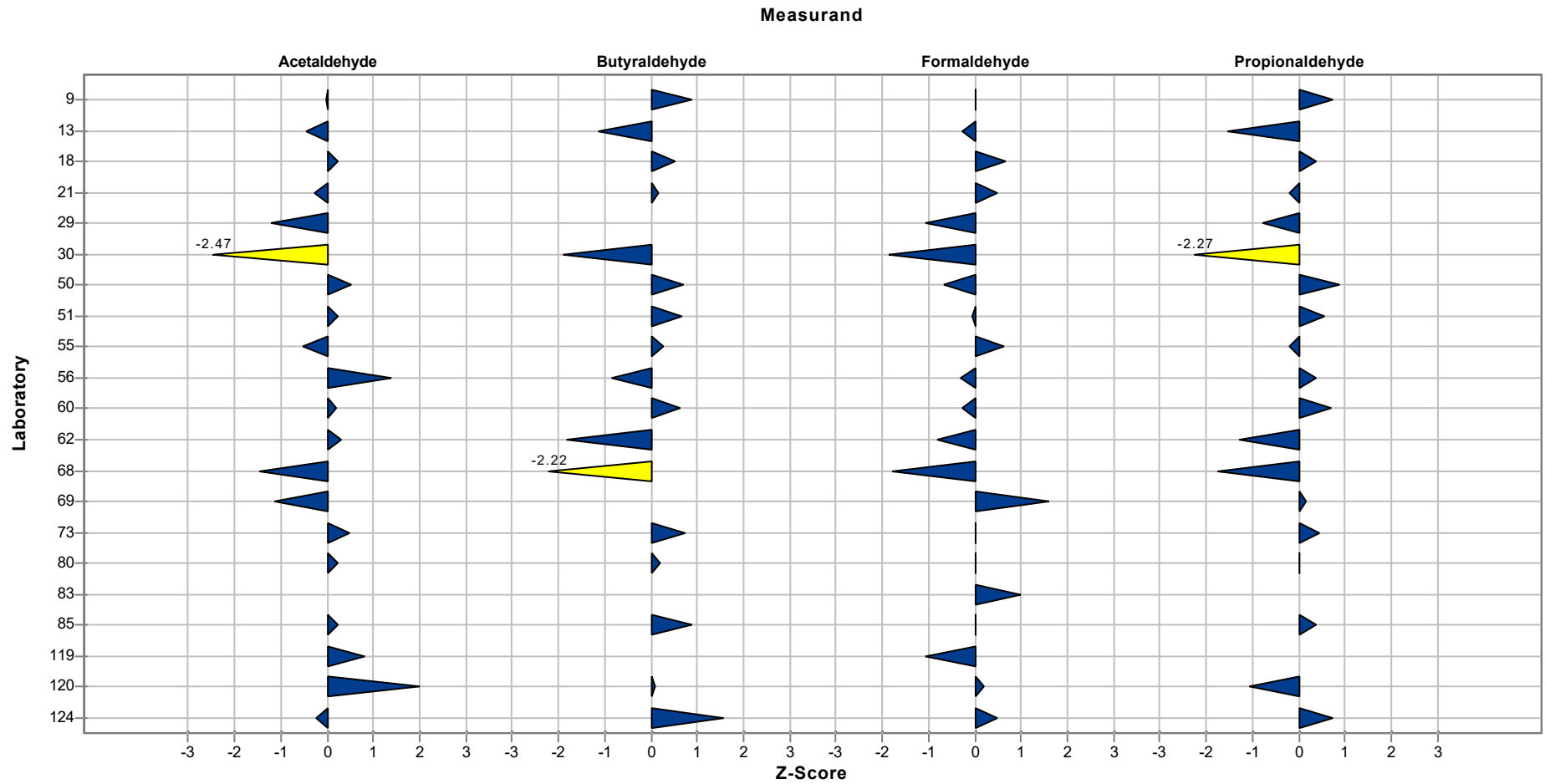
Sample chart of Z-Scores

Sample: 2



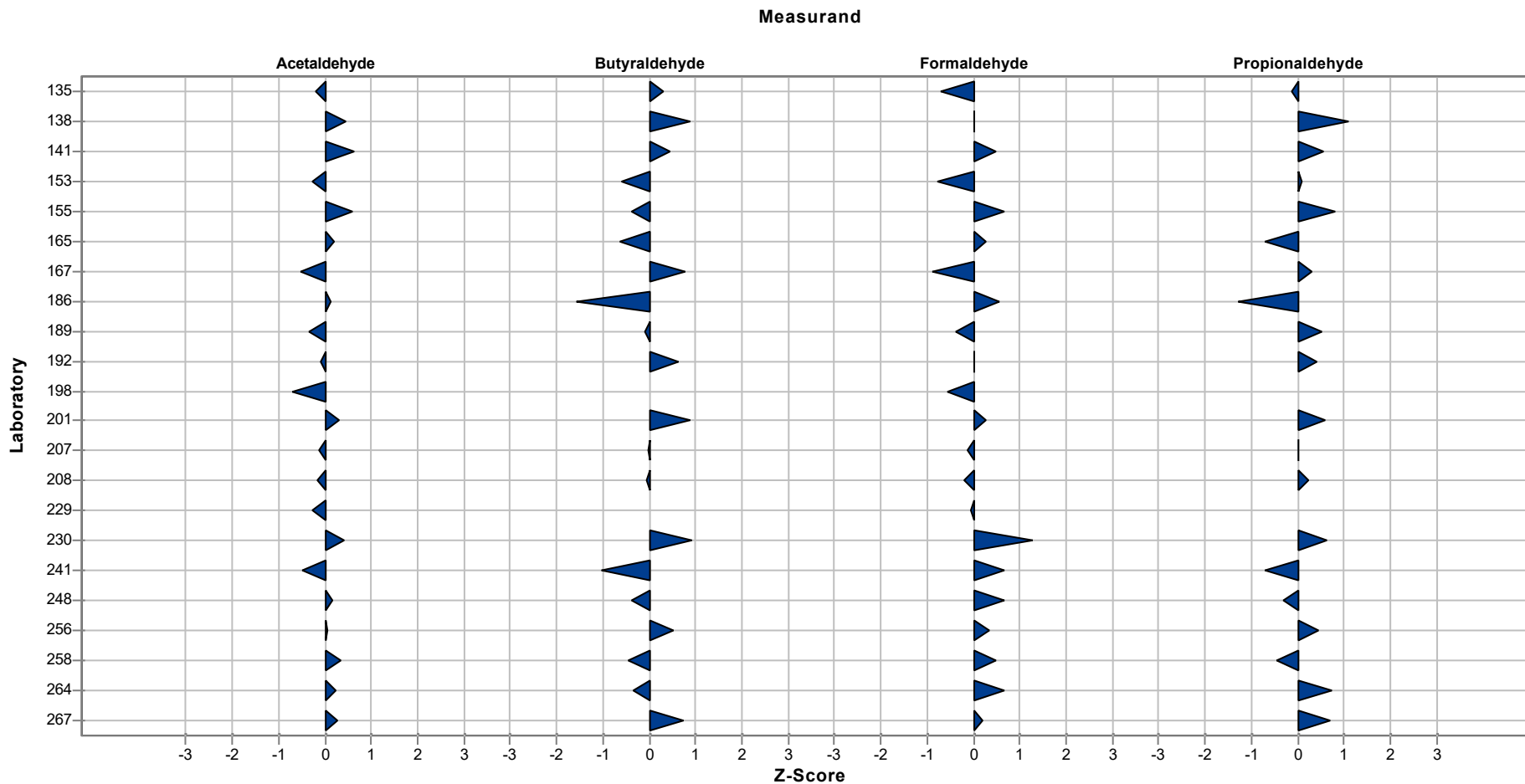
Sample chart of Z-Scores

Sample: 3



Sample chart of Z-Scores

Sample: 3



Questions and Answers

Participant	Analytical method	Date start sample preparation
9	DIN ISO 16000-3:2011, aber mit ESI-MS/MS statt DAD	10.11.2022
13	AIR-ANAL-51: Aldehyden met UPLC (ow n method)	21.12.2022
18	DIN ISO 16000-3	29.11.2022
21	UHPLC	09.11.2022
29	DIN ISO 16000-3	15.11.2022
30	ISO 16000-3 / EN 16516	29/11/2022 (elution) / 14/12/2022 (analysis)
50	DIN EN ISO 16000-3	21.11.2022
51	Internal method derived from DIN ISO 16000-3:2011	20.12.2022
55	ISO 16000-3	15.11.2022
56	UHPLC w ith UV detection	10.11.2022
60	HPLC-DAD	09.11.2022
62	HPLC-UV	16.11.2022
68	interne Arbeitsanw eisung	15.11.2022
69	HPLC	16.11.2022
73	In Anlehnung an Arbeitsmappe 6045	10.11.2022
80	DIN ISO 16000-3:2013-01	18.11.2022
83	LC/DAD	17 novembre 2022
85	ISO16000-3:2011	14. Nov 22
119	interne Methode	22.11.2022
120	IFA 6045	09.11.2022
124	HPLC	11/17/2022
135	DIN ISO 16000-3	09.11.2022
138	BGIA 6045	14.11.2022
141	HPLC	15.11.2022
153	ISO 16000-3:2011	12.12.2022
155	EN 16516, DIN ISO 16000-3	09.11.2022
165	DIN-ISI 16000-3	11.11.2022
167	ISO 16000-3	11. Nov 22
186	NF ISO 16000-3	16.11.2022
189	ISO 16000-3	11.11.2022
192	ISO 16000-3	November 12, 2022

Aldehydes 2022

Participant	Analytical method	Date start sample preparation
198	ISO 16000-3 2011	17.11.2022
201	IFA 6045	08.12.2022
207	DIN ISO 16000-3	08.11.2022
208	ISO 16000-3	11/15/2022
229	HPLC	15. Nov 22
230	DIN EN ISO 16000-3	09.11.2022
241	ISO 16000-3	14.11.2022
248	IFA 6045 (11-2007)	17.11.2022
256	In Anlehnung an EPA TO-11A	11.11.2022
258	ISO16000-3	November 9, 2022
264	HPLC-UV	10.11.2022
267	ISO 16000-3	25.11.2022

Participant	Storage time after desorption
9	direkt vermessen (Autosampler gekühlt auf 20 °C)
13	analysis directly after desorption
18	3 Wochen im Gefrierschrank
21	4h, refrigerator
29	Nein
30	15 days / refrigerator
50	nein
51	45 minutes at room temperature
55	4 days, refrigerator
56	0 day
60	1h00
62	7 days at 4°C
68	ja, 1 Tag im Kühlschrank
69	0 days
73	Nach Desorption im Kühlschrank bei 5°C
80	keine Lagerung, direkt gemessen.
83	0
85	No storage after desorption.
119	Proben wurden am gleichen Tag nach Desorption gemessen

Aldehydes 2022

Participant	Storage time after desorption
120	Keine Lagerung!
124	1-3 hours
135	nein
138	Kühlschrank
141	1 week , refrigerator
153	5 weeks in refrigerator
155	Ja, die Proben wurden nach der Desorption im Kühlschrank gelagert. Lagerung der desorbierten Proben vom 09.11.2022 - 16.11.2022.
165	Kühlschrank 4°C bis 14/11/2022
167	30 min at room temp
186	Stored 5 days in refrigerator
189	The samples were analyzed in the same day after desorption, they waited 2-3 hours at ambient temperature in the autosampler. After the solutions were refrigerated during 1, 2 or 4 days at -16°C and diluted after for a new analysis.
192	No storage after desorption
198	No storage. Immediate analysis
201	Nein
207	-
208	7 d in refrigerator
229	The analyses were performed the same day after cartridges desorption.
230	nein
241	Tiefkühler (-19 °C)
248	Ja/8 Tage im Kühlschrank bei < 10°C
256	direkte Analyse, danach Aufbewahrung im Kühlschrank
258	Samples were analyzed on the day of desorption
264	15 days in freezer
267	Extract analyzed 3 days after desorption for undiluted results and 4 days after desorption for dilutions. Extracts stored in the fridge.

Participant	Date of analysis	Desorption solution	Volume desorption solution
9	10.11.2022	ACN	5
13	21.12.2022	Acetonitrile	5 ml
18	09.12.2022	Acetonitril	40000
21	09.11.2022	Acetonitrile	3
29	15.11.2022	Acetonitril	5
30	14.12.2022	Acetonitrile	5
50	21.11.2022	Acetonitril	5

Aldehydes 2022

Participant	Date of analysis	Desorption solution	Volume desorption solution
51	20-21/12/2022	CH3CN	5 mL
55	15.11.2022	acetonitrile	3
56	10.11.2022	Acetonitrile	5
60	09.11.2022	Acetonitrile	3 ml
62	23.11.2022	acetonitrile	5ml
68	16.11.2022	Acetonitril	2mL
69	16.11.2022	Acetonitrilo	5 ml
73	11.11.2022	Acetonitril	10 mL
80	18.11.2022	Acetonitril	10 mL
83	18 novembre 2022	acétonitrile	10
85	14. Nov 22	Acetonitrile	10mL
119	22.11.2022	Acetonitril	5 ml
120	09.11.2022	ACN	5 mL
124	11/17/2022	Acetonitrile	5 ml
135	9.11.2022	Acetonitril	2
138	15.11.2022	Acetonitril	10
141	15.11.2022	acetonitrile	10 ml
153	13.12.2022	acetonitrile	10 ml
155	16.11.2022	Acetonitril	5 ml
165	14.11.2022	acetonitril	3 ml
167	11. Nov 22	Acetonitrile	6 mL filled to 10 mL with distilled water
186	21.11.2022	Acetonitrile	10
189	between 11/11/2022 and 16/11/2022	acetonitrile	5 ml
192	November 12 and 14, 2022	Acetonitrile	5mL
198	17.11.2022	CH3CN	5
201	08.12.2022	Acetonitril	1
207	08.11.2022	ACN/H2O 60/40 +5 mmol (NH4)HCO3	5
208	11/15/2022	Acetonitrile	3 ml
229	15. Nov 22	Acetonitrile	5 ml
230	09.11.2022	Acetonitril	10 ml
241	16. - 18.11.2022	Acetonitril	2 mL
248	25.11.2022	Acetonitril	5 ml
256	11.11.2022	ACN	02. Mai
258	November 9, 2022	Acetonitrile	5

Aldehydes 2022

Participant	Date of analysis	Desorption solution	Volume desorption solution
264		acetonitrile	5 mL
267	28/11/2022-29/11/2022	Acetonitrile	5 mL

Participant	Chromatography system / HPLC	Refrigerated autosampler
9	Agilent 1290 Infinity (Serie I), Detektor: Sciex API 4000	Ja, 20 °C
13	Agilent Infinity II 1290 Quad pump, Agilent 1290 DAD detector	Autosampler at 18°C
18	Gilair Plus	nein
21		no, 20°C
29	Thermo Scientific Ultimate 3000, Gradient, UVD, Autosampler	Nein
30	Alliance e2695 / PDA 2998	no
50	Thermo Surveyor HPLC (Pumpe, Autosampler, PDA-Detektor)	22°C
51	Pump: Agilent 1260 Infinty II G7111B - Detector: Agilent UV1260 Infinty II G7114A	No
55	Water Acquity UPLC w ith Acquity Photodiode Array (PDA)	Autosampler temperature 20 °C
56	HPLC/UV (RS Pump, RS Diode Array, RS Autosampler Ultimate 3000 Thermofisher Scientific)	yes, at 15°C
60	Agilent 1260 Quat Pump, 1260 DAD VL+	No
62	Quaternary pump + UV/Visible detector	No, ambient temperature
68	Agilent HPLC 1260 Infinity	Nein
69	Elte LabChrom Merck Hitachi, Pump L-2130 and Autosampler L-2200	No, ,
73	Agilent 1260 Infinity II, , Pumpe: G7112B, , Autosampler: G7129A, , Detektor: G7117A (Standard Zelle), , ,	Nein
80	HPLC- Agilent 1200er Serie. DAD, quaternäre Pumpe, Autosampler	Temperiert 25 °C
83	LC/DAD	oui
85	LC-20AD, SPD-20AV (Shimadzu)	No
119	2x LC-30AD, SPD-M20A, CTO-20A (Shimadzu)	22°C
120	Agilent	Gekühlter AS, 20°C
124	Shimadzu 2050 w ith single channel UV detector at 365 nm	analysed at room temperature
135	Agilent 1290 Series	ja, 10°C
138	Thermofisher	
141	Quaternary pump, diode array detector	no
153	Thermo Scientific Dionex UltiMate 3000 Series, pump LPG 3400 SD, detector DAD 3000	No
155	Agilent 1200 LC System DAD-Detektor	gekühlter Autosampler, 20°C
165	HPLC Agilent 1260-DAD	nein
167	Waters e2695 HPLC	Room temp
186	Quaternary pump, HPLC-PAD	Yes, 4°C

Aldehydes 2022

Participant	Chromatography system / HPLC	Refrigerated autosampler
189	Quaternary pump and Variable Wavelength Detector (Agilent 1220 Infinity LC)	no
192	Agilent 1260 , Agilent 1260 II	23°C
198	quaternary pump, UV	no
201		nein
207	Agilent 1260 Infinity HPLC	-
208	Acquity H-class, PDA-detector	15 °C
229	HPLC system, NEXERA, Shimadzu, Detector - DAD.	Autosampler w as termostated at 28C
230	Fa. Agilent	nein
241	Agilent 1200, Diodenarray	nein
248	Thermo Pumpe: LPG-3400SD, Detektor: DAD-3000(RS), FLD 3x00(RS), Autosampler: WPS-3000(RS)	Nein
256		nein
258	Waters Acquity H-Class w ith UV detector	No
264	Nexera	7 °C
267	Agilent HPLC-DAD 1260	No, room temperature

Participant	Analytical column
9	Phenomenx Kinetex 2.6u C-18 50*2.10 mm
13	Acquity UPLC BEH Phenyl 1,7µm column
18	Restek Allure 5µm, 200 x 4,6mm
21	ACQUITY UPLC BEH Phenyl Column, 130Å, 1.7 µm, 2.1 mm X 100 mm
29	Waters XBridge Phenyl 3,5µm
30	Restek Allure AK 4.6 mm 5 µm
50	Restek Allure AK, 5 µm, 200x4,6 mm
51	J.T. Baker Octadecyl (C18) 250 x 4.6 mm - 5 µm
55	Waters Acquity UPLC BEH Phenyl 1.7µm, 2.1 x 100 mm
56	Column Acclaim RSCL Carbonyl 2.1*100 mm (Thermo)
60	Allure C18 5µm 150x4,6mm
62	Ascentis RP-Amide HLPC Column
68	Poroshell 120 EC-C18 4.6x50mm, 2.7um
69	Ascentis RP-Amide 25 cmx4,6 mm
73	Kinetex C18, 100 x 4,6mm x 2,6 µm
83	c18
85	Shim-pack XR-ODS

Aldehydes 2022

Participant	Analytical column
119	Kinetex 2,6µm, C18, 100A (Phenomenex)
120	ProntoSil
124	C18
135	M&N 250/4,6 Nucleodur 100-5 C18ec
141	Agilent Poroshell 120 EC-C18 50x4.6 mm 2.7 µm cat. no. 6999975-902
153	Thermo Scientific Acclam Carbonyl C18 / Using 3,0 x 150 mm, 3 µm)
165	LC18
167	Waters Symmetry C18, 3.5 µm
186	WATERS Nova-Pak C18/150nm*3.9nm*4µm
189	Column 581325-U Ascentis® C18 HPLC Column 5 µm particle size, L × I.D. 25 cm × 4.6 mm
192	Formaldehyde, Acetaldehyde : InertSustain C18 HP , Propionaldehyde, Butyraldehyde : Inertsil ODS-HL
198	C18 encapped
201	Zorbax Eclipse XDB C-18, 250 * 4,6 mm, 5 µm
207	Phenomenex Kinetex 2,6 µm, 100 mm * 4,6 mm
229	C18, 200 mm x 4,6 mm, 5 micrometer (Allure)
230	MZ PAH C18, 5 µm
241	Restek Raptor
248	Acclaim™ RSLC Carbonyl (2.1 x 100mm, 2,2µm)
256	Supelcosil LC-18, 25 cm x 4.6 mm, 5 µm
264	Acclaim carbonyl 2.2µm -100 x 3 mm
267	Waters Symmetry C18, 250 mm x 4.6 mm x 5 µm

Participant	Mobile phase HPLC
13	A (Water:THF 90:10) and B (Acetonitrile)
18	Acetonitril/ Wasser (Gradientprogramm)
30	Acetonitrile / Water
50	Acetonitril / Wasser, Gradient zwischen 60 und 95 % Acetonitril
51	H2O/CH3CN
56	Solvent A: Water, Solvent B: Acetonitrile, 48% to 0% gradient of A
60	70% acetonitrile / 30% eau et 100% ACN
62	Acetonitrile/Water 40/60 -> 75/25-> 100/0
68	Gradient: Acetonitril, Wasser
69	Acetonitrile-Agua

Aldehydes 2022

Participant	Mobile phase HPLC
73	Wasser/Acetonitril
80	60:40 Acetonitril/Wasser
83	ACN/THF/H ₂ O
85	Acetonitrile/H ₂ O = 60/40
119	40% Acetonitril, 60% Wasser, beides mit 0,1% Ameisensäure angesäuert
120	ACN / Wasser
124	gradient. 70% MeOH/MeCN (650/50), 30% w ater to 90% MeOH/MeCN (650/50),10% w ater in 11 minutes
135	Wasser, Acetonitril, THF
141	Water/Acetonitrile (45/55)
153	Acetonitrile /w ater
155	Gradient: Sart: ACN 30% / THF 10% / H ₂ O 60%
165	Wasser/Acetonitril 40/60
167	AcN w ith 0,1% phosphoric acid
186	Acetonitrile/Water/THF
189	Gradient composition, , A: Water/Acetonitrile/Tetrahydrofuran 60/30/10 v/v, , B: Water/Acetonitrile 40/60 v/v
192	Water/Acetonitrile
198	CH ₃ CN:H ₂ O gradient
201	Acetonitril / Wasser
207	H ₂ O/ACN/THF
208	ACN/THF/w ater
229	Acetonitrile 60% : w ater 40%
230	dest. Wasser/Acetonitril, Gradientenprogramm
241	MeOH (+Acetonitril) / Wasser
248	(A) H ₂ O (B) ACN 52%/48%
256	Startbedingungen: 30% ACN, 60% Wasser, 10% THF
258	Water/acetonitrile
264	acetonitrile + buffer ammonium acetate - acetic acid
267	Acetonitrile/Water

Participant	Flow rate HPLC	Wavelength	Temperature analytical column
9	0,5	ESI-MS/MS	30 °C
13	0,5	360 nm	30°C
18	1000	360 nm	30°C

Aldehydes 2022

Participant	Flow rate HPLC	Wavelength	Temperature analytical column
21	0.5	360 nm	40°C
29	1,5 ml/min	365 nm	27°C
30	01. Feb	360 nm	30°C
50	1,4 ml/min	360 nm	30°C
51	1.9 mL/min	365 nm	25 °C
55	0.5	360 nm	40 °C
56	0.4	360 nm	28°C +/- 1°C
60	1 ml/min	360 nm	30°C
62	1 mL/min	360 nm	30°C
68	1ml/min	365nm	25°C
69	1,5 ml/min	UV-visible 360 nm	40 °C
73	1,5 mL/min	365 nm	30°C
80	1,2 mL/min	360 nm	25 °C
83	01. Feb		
85	1.2mL/min	360nm	40°C
119	0,8ml/min	360nm	40°C
120	1,5 mL / min	354 nm	20 °C
124	0.8	365 nm	30oC
135	2,25	365 nm	50 °C
141	1 ml/min	360 nm	30 °C
153	0,6 ml/min	UV 360 nm	30 oC
155	1 ml/min	360 nm, 365 nm, 380 nm	35°C
165	1,3 ml/min	360 nm	25°C
167	1,5 mL/min	360 nm	40 °C
186	1.5mL/min	360 nm	35°C
189	variable betw een 2.0 ml/min and 1.0 ml/min	360 nm	27°C
192	Formaldehyde,Acetaldehyde : 0.4mL/min , Propionaldehyde,Butyraldehyde : 1.2mL/min	360nm	40?, , 40°C
198	1	360 nm	30°C
201	1,3	360 nm	65°C
207	1,5	360 nm	30°C
208	0,42 ml/min	360 nm	40 °C
229	1,2 ml/min	360 nm	35C
230	0,5ml/min	362 nm	40°C
241	0,8	365	30 °C

Aldehydes 2022

Participant	Flow rate HPLC	Wavelength	Temperature analytical column
248	0,4ml/min	- UV 360 nm	28°C
256	2.3 ml/min, ab 9.1 Minuten 2 ml/min	360 nm	25 °C
258	0.8	367	40°C
264	1 mL/min, ,	360 nm	30 °C
267	1.5 mL/min	365 nm	25 °C

Participant	Calibration standard
9	fertiger Mix (Aldehyd Keton Mix Stock 13, Sigma Aldrich, Bestellnummer ERA 028-1,2ML)
13	Standards made from ready-to-use mix from Sigma-Aldrich (TO11/IP-6A Aldehyde/ketone-DNPH mix)
18	fertiger Mix, Supelco LpDNPH S10 Cartridge
29	Supelco Mix
30	Mix solution Supelco DNPH Mix-2
50	Supelco Carbonyl-DNPH Mix 2
51	Custom Carbonyl-DNPH Standard - Restek
55	ready to use, Supelco
56	Ready-to-use Mix Supelco Custom Mix Ald_DNPH 100 µg/ml
60	Ready-to-use mix from AccuStandard
62	Purchased at Restek
68	fertiger Mix, sigma aldrich
69	Ready to use mix, IsostandardsMaterial S.L.
73	Herstellung aus Einzelstandards (Selbst hergestellte DNPH Derivate)
80	einzel
85	FUJIFILM Wako Pure Chemical Corporation
119	Einzelstandards, gekauft (Sigma-Aldrich)
120	Mix, Restek
124	Restek 31808 plus media spikes of all authentic chemicals
135	Einzelstandards, Dr. Ehrenstorfer
141	produced from individual standards
155	gekaufter MIX-Standard, Firma: NEOCHEMA
165	supelco CRM47285-TO11/IP6A Aldehyde7Ketone-DNPH mix
167	Individual standards from Merck / Sigma Aldrich
186	From a ready-to-use mix Supelco
189	it w as purchased as a ready use-to-use mix: Aldehyde/Ketone-DNPH Stock Standard-13 from Sigma-aldrich

Aldehydes 2022

Participant	Calibration standard
192	Ready-to-use mix manufactured by FUJIFILM Wako Pure Chemical Corporation.
198	Ready to use, mix, Supelco Merck
207	Einzelstandards, Supelco
208	Sigma-Aldrich / CRM47651
229	Individual standards: DNPH-formaldehyde (Dr.Ehrenstorfer), DNPH-acetaldehyde (Dr.Ehrenstorfer).
230	Herstellung aus Einzelstandards, Fa. Supelco
241	fertiger Mix von Restek
248	#NAME?
256	fertiger Mix: TO11/IP-6A Aldehyde/-Ketone-DNPH Mix (Sigma-Aldrich)
264	supelco
267	Ready-to-use mix from Supelco

Participant	Recovery rates
9	nein
13	Yes
18	nein
21	no
29	Nein
30	No
50	nein
51	Yes
55	no
56	No, they don't
60	No
62	No
68	Ja
69	No
73	Nein – Annahme einer 100%igen Elution vom Adsorptionsröhrchen.
80	nein
85	No
119	nein
120	Ja, bei Butyr- und Acetaldehyd
124	yes

Aldehydes 2022

Participant	Recovery rates
135	nein
141	no
153	no
155	nein
165	nein
167	Yes
186	No
189	no
192	No
198	no
201	nein
207	-
208	No
229	no
230	nein
241	nein
248	Nein
256	nein
258	No
264	yes
267	No