

**Results of Proficiency Test  
Toluene  
February 2021**

**Organized by:** Institute for Interlaboratory Studies  
Spijkenisse, the Netherlands

**Author:** Mrs. E.R. Montenij-Bos  
**Correctors:** ing. A.S. Noordman-de Neef & ing. R.J. Starink  
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## 1 INTRODUCTION

Since 1999 the Institute for Interlaboratory Studies (iis) organizes a proficiency scheme for the analysis of Toluene in accordance with the latest version of ASTM D841 every year. During the annual proficiency testing program 2020/2021 it was decided to continue the round robin for the analysis of Toluene.

In this interlaboratory study 41 laboratories in 20 different countries registered for participation. See appendix 2 for the number of participants per country. In this report the results of the Toluene proficiency test are presented and discussed. This report is also electronically available through the iis website [www.iisnl.com](http://www.iisnl.com).

## 2 SET UP

The Institute for Interlaboratory Studies (iis) in Spijkenisse, the Netherlands, was the organizer of this proficiency test (PT). Sample analyzes for fit-for-use and homogeneity testing were subcontracted to an ISO/IEC17025 accredited laboratory. It was decided to send one bottle of 1L Toluene, labelled #21011.

The participants were requested to report rounded and unrounded test results. The unrounded test results were preferably used for statistical evaluation.

### 2.1 ACCREDITATION

The Institute for Interlaboratory Studies in Spijkenisse, the Netherlands, is accredited in agreement with ISO/IEC17043:2010 (R007), since January 2000, by the Dutch Accreditation Council (Raad voor Accreditatie). This PT falls under the accredited scope. This ensures strict adherence to protocols for sample preparation and statistical evaluation and 100% confidentiality of participant's data. Feedback from the participants on the reported data is encouraged and customer's satisfaction is measured on regular basis by sending out questionnaires.

### 2.2 PROTOCOL

The protocol followed in the organization of this proficiency test was the one as described for proficiency testing in the report 'iis Interlaboratory Studies: Protocol for the Organisation, Statistics and Evaluation' of June 2018 (iis-protocol, version 3.5). This protocol is electronically available through the iis website [www.iisnl.com](http://www.iisnl.com), from the FAQ page.

### 2.3 CONFIDENTIALITY STATEMENT

All data presented in this report must be regarded as confidential and for use by the participating companies only. Disclosure of the information in this report is only allowed by means of the entire report. Use of the contents of this report for third parties is only allowed by written permission of the Institute for Interlaboratory Studies. Disclosure of the identity of one or more of the participating companies will be done only after receipt of a written agreement of the companies involved.

## 2.4 SAMPLES

A batch of approximately 60 liters of Toluene was obtained from a local chemical supplier. After homogenization 60 amber glass bottles of 1L were filled and labelled #21011. The homogeneity of the subsamples was checked by determination of Density at 20°C in accordance with ASTM D4052 on 8 stratified randomly selected subsamples.

	Density at 20°C in kg/L
sample #21011-1	0.86682
sample #21011-2	0.86682
sample #21011-3	0.86686
sample #21011-4	0.86686
sample #21011-5	0.86686
sample #21011-6	0.86686
sample #21011-7	0.86686
sample #21011-8	0.86689

Table 1: homogeneity test results of subsamples #21011

From the above test results the repeatability was calculated and compared with 0.3 times the reproducibility of the reference test method in agreement with the procedure of ISO13528, Annex B2 in the next table.

	Density at 20°C in kg/L
r (observed)	0.00007
reference test method	ISO12185:96
0.3 x R (reference test method)	0.00015

Table 2: evaluation of repeatability of subsamples #21011

The calculated repeatability is in agreement with 0.3 times the reproducibility of the reference test method. Therefore, homogeneity of the subsamples was assumed.

To each of the participating laboratories one bottle of 1L Toluene labelled #21011 was sent on January 27, 2021. An SDS was added to the sample package.

## 2.5 STABILITY OF THE SAMPLES

The stability of Toluene packed in amber glass bottles was checked. The material was found sufficiently stable for the period of the proficiency test.

## 2.6 ANALYZES

The participants were requested to determine: Acid Wash Color, Appearance, Color Pt/Co, Copper Corrosion, Density at 20°C, Distillation (IBP, 50% recovered, DP and range), Purity by GC, Benzene, Nonaromatics, Total Impurities, Refractive Index at 25°C and Water.

It was explicitly requested to treat the sample as if it was a routine sample and to report the test results using the indicated units on the report form and not to round the test results, but report as much significant figures as possible. It was also requested not to report 'less than' test results, which are above the detection limit, because such test results cannot be used for meaningful statistical evaluations.

To get comparable test results a detailed report form and a letter of instructions are prepared. On the report form the reporting units are given as well as the reference test methods (when applicable) that will be used during the evaluation. The detailed report form and the letter of instructions are both made available on the data entry portal [www.kpmd.co.uk/sgs-iis/](http://www.kpmd.co.uk/sgs-iis/). The participating laboratories are also requested to confirm the sample receipt on this data entry portal. The letter of instructions can also be downloaded from the iis website [www.iisnl.com](http://www.iisnl.com).

### 3 RESULTS

During five weeks after sample dispatch, the test results of the individual laboratories were gathered via the data entry portal [www.kpmd.co.uk/sgs-iis/](http://www.kpmd.co.uk/sgs-iis/). The reported test results are tabulated per determination in appendix 1 of this report. The laboratories are presented by their code numbers.

Directly after the deadline, a reminder was sent to those laboratories that had not reported test results at that moment. Shortly after the deadline, the available test results were screened for suspect data. A test result was called suspect in case the Huber Elimination Rule (a robust outlier test) found it to be an outlier. The laboratories that produced these suspect data were asked to check the reported test results (no reanalysis). Additional or corrected test results are used for data analysis and the original test results are placed under 'Remarks' in the test result tables in appendix 1. Test results that came in after the deadline were not taken into account in this screening for suspect data and thus these participants were not requested for checks.

#### 3.1 STATISTICS

The protocol followed in the organization of this proficiency test was the one as described for proficiency testing in the report 'iis Interlaboratory Studies: Protocol for the Organisation, Statistics and Evaluation' of June 2018 (iis-protocol, version 3.5).

For the statistical evaluation the *unrounded* (when available) figures were used instead of the rounded test results. Test results reported as '<...' or '>...' were not used in the statistical evaluation.

First, the normality of the distribution of the various data sets per determination was checked by means of the Lilliefors-test, a variant of the Kolmogorov-Smirnov test and by the calculation of skewness and kurtosis. Evaluation of the three normality indicators in combination with the visual evaluation of the graphic Kernel density plot, lead to judgement of the normality being either 'unknown', 'OK', 'suspect' or 'not OK'. After removal of outliers, this check was repeated. If a data set does not have a normal distribution, the (results of the) statistical evaluation should be used with due care.

The assigned value is determined by consensus based on the test results of the group of participants after rejection of the statistical outliers and/or suspect data.

According to ISO13528 all (original received or corrected) test results per determination were submitted to outlier tests. In the iis procedure for proficiency tests, outliers are detected prior to calculation of the mean, standard deviation and reproducibility. For small data sets, Dixon (up to 20 test results) or Grubbs (up to 40 test results) outlier tests can be used. For larger data sets (above 20 test results) Rosner's outlier test can be used. Outliers are marked by  $D(0.01)$  for the Dixon's test, by  $G(0.01)$  or  $DG(0.01)$  for the Grubbs' test and by  $R(0.01)$  for the Rosner's test. Stragglers are marked by  $D(0.05)$  for the Dixon's test, by  $G(0.05)$  or  $DG(0.05)$  for the Grubbs' test and by  $R(0.05)$  for the Rosner's test. Both outliers and stragglers were not included in the calculations of averages and standard deviations.

For each assigned value the uncertainty was determined in accordance with ISO13528. Subsequently the calculated uncertainty was evaluated against the respective requirement based on the target reproducibility in accordance with ISO13528. In this PT, the criterion of ISO13528, paragraph 9.2.1. was met for all evaluated tests, therefore, the uncertainty of all assigned values may be negligible and need not be included in the PT report.

Finally, the reproducibilities were calculated from the standard deviations by multiplying them with a factor of 2.8.

### 3.2 GRAPHICS

In order to visualize the data against the reproducibilities from literature, Gauss plots were made, using the sorted data for one determination (see appendix 1). On the Y-axis the reported test results are plotted. The corresponding laboratory numbers are on the X-axis. The straight horizontal line presents the consensus value (a trimmed mean). The four striped lines, parallel to the consensus value line, are the +3s, +2s, -2s and -3s target reproducibility limits of the selected reference test method. Outliers and other data, which were excluded from the calculations, are represented as a cross. Accepted data are represented as a triangle.

Furthermore, Kernel Density Graphs were made. This is a method for producing a smooth density approximation to a set of data that avoids some problems associated with histograms. Also, a normal Gauss curve (dotted line) was projected over the Kernel Density Graph (smooth line) for reference. The Gauss curve is calculated from the consensus value and the corresponding standard deviation.

### 3.3 Z-SCORES

To evaluate the performance of the participating laboratories the z-scores were calculated. As it was decided to evaluate the performance of the participants in this proficiency test (PT) against the literature requirements, e.g. ASTM or ISO reproducibilities, the z-scores were calculated using a target standard deviation. This results in an evaluation independent of the variation of this interlaboratory study.

The target standard deviation was calculated from the literature reproducibility by division with 2.8. In case no literature reproducibility was available, other target values were used, like Horwitz or an estimated reproducibility based on former iis proficiency tests.

When a laboratory did use a test method with a reproducibility that is significantly different from the reproducibility of the reference test method used in this report, it is strongly advised to recalculate the z-score, while using the reproducibility of the actual test method used, this in order to evaluate whether the reported test result is fit-for-use.

The z-scores were calculated according to:

$$z(\text{target}) = (\text{test result} - \text{average of PT}) / \text{target standard deviation}$$

The z(target) scores are listed in the test result tables in appendix 1.

Absolute values for  $z < 2$  are very common and absolute values for  $z > 3$  are very rare.

The usual interpretation of z-scores is as follows:

z  < 1	good
1 <  z  < 2	satisfactory
2 <  z  < 3	questionable
3 <  z	unsatisfactory

## 4 EVALUATION

Some problems were encountered with the dispatch of the samples due to COVID-19 pandemic. Therefore, the reporting time on the data entry portal was extended with another week. Seven participants reported test results after the extended final reporting date and one participant did not report any test results. Not all participants were able to report all tests requested.

In total 40 participants reported 405 numerical test results. Observed were 10 outlying test results, which is 2.5%. In proficiency tests outlier percentages of 3% - 7.5% are quite normal.

Not all original data sets proved to have a normal Gaussian distribution. These are referred to as “not OK” or “suspect”. The statistical evaluation of these data sets should be used with due care, see also paragraph 3.1.

### 4.1 EVALUATION PER TEST

In this section the reported test results are discussed per test. The test methods, which were used by the various laboratories, were taken into account for explaining the observed differences when possible and applicable. These test methods are also in the tables together with the reported test results. The abbreviations, used in these tables, are explained in appendix 3.

In the iis PT reports ASTM methods are referred to with a number and if appropriate an indication sub test method (e.g. D1218). If applicable, a designation in parentheses is added to designate the year of reapproval e.g. D1218:12(2016). In the results tables of appendix 1 only the method number (sub) and year of adoption or revision (e.g. D1218:12) will be used.

Unfortunately, a suitable reference test method providing the precision data is not available for all determinations. For these tests the calculated reproducibility was compared against the estimated reproducibility calculated with the Horwitz equation.

Acid Wash Color: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D848:18.

Appearance: This determination was not problematic. All participants agreed about the appearance of the sample, which was bright, clear and free of suspended matter (Pass).

Color Pt/Co: This determination was not problematic. One statistical outlier was observed. The calculated reproducibility after rejection of the statistical outlier is in agreement with the requirements of ASTM D5386:16 or ASTM D1209:05(2019).

Copper Corrosion: This determination was not problematic. All participants agreed on a result of 1a/b (Pass).

Density at 20°C: This determination was not problematic. One statistical outlier was observed. The calculated reproducibility after rejection of the statistical outlier is in agreement with the requirements of ISO12185:96.

Distillation: This determination was not problematic. In total three statistical outliers were observed and one other test results was excluded. All calculated reproducibilities after rejection of the suspect data are in agreement with the requirements of the automated or manual mode of ASTM D850:21.

Purity: This determination was not problematic. One statistical outlier was observed. The calculated reproducibility after rejection of the statistical outlier is in agreement with the requirements of ASTM D7504:20.

Benzene: This determination was very problematic. Two statistical outliers were observed. The calculated reproducibility after rejection of the statistical outliers is not at all in agreement with the requirements of ASTM D7504:20.

Nonaromatics: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D7504:20.

Total Impurities: This determination was not problematic. One statistical outlier was observed. The calculated reproducibility after rejection of the statistical outlier is in full agreement with the estimated reproducibility calculated with the Horwitz equation (3 components)



**Refractive Index:** This determination was problematic. One statistical outlier was observed. The calculated reproducibility after rejection of the statistical outlier is not in agreement with the requirements of ASTM D1218:12(2016).

**Water:** This determination was problematic. No statistical outliers were observed. The calculated reproducibility is not in agreement with the requirements of ASTM E1064:16.

#### 4.2 PERFORMANCE EVALUATION FOR THE GROUP OF LABORATORIES

A comparison has been made between the reproducibility as declared by the reference test method or as declared by the estimated target reproducibility calculated with the Horwitz equation and the reproducibility as found for the group of participating laboratories. The number of significant test results, the average, the calculated reproducibility (2.8 \* standard deviation) and the target reproducibility derived from literature reference test methods (in casu ASTM and ISO test methods) or the estimated target reproducibility using the Horwitz equation are presented in the next table.

Parameter	unit	n	average	2.8 * sd	R(lit)
Acid Wash Color		34	0.6	0.9	2.0
Appearance		37	Pass (B&C)	n.a.	n.a.
Color Pt/Co		36	3.7	3.7	5.2
Copper Corrosion		31	1 (1a/1b)	n.a.	n.a.
Density at 20°C	kg/L	36	0.86688	0.0002	0.0005
Distillation, IBP	°C	35	110.2	0.6	0.6
Distillation, 50% recovered	°C	34	110.6	0.1	0.2
Distillation, DP	°C	35	110.7	0.2	0.5
Purity	%M/M	35	99.959	0.012	0.013
Benzene	mg/kg	34	16.3	4.8	2.3
Nonaromatics	mg/kg	36	188.8	77.2	170.6
Total Impurities	mg/kg	29	414.2	130.3	129.8
Refractive Index at 25°C		22	1.4941	0.0006	0.0005
Water	mg/kg	28	119.5	23.7	19.0

Table 3: performance evaluation sample #21011

Without further statistical calculations it can be concluded that for most of the tests there is a good compliance of the group of participating laboratories with the relevant reference test methods. The tests that are problematic have been discussed in paragraph 4.1.

### 4.3 COMPARISON OF THE PROFICIENCY TEST OF FEBRUARY 2021 WITH PREVIOUS PTS

	February 2021	February 2020	February 2019	March 2018	March 2017
Number of reporting laboratories	40	26	35	36 *)	67
Number of test results	405	253	284	267	743
Number of statistical outliers	10	16	14	10	32
Percentage of statistical outliers	2.5%	6.3%	4.9%	3.8%	4.3%

Table 4: comparison with previous proficiency tests

\*) from March 2018 the Toluene results are reported separately from Benzene, hence the lower number of reporting laboratories.

In proficiency tests, outlier percentages of 3% - 7.5% are quite normal.

The performance of the determinations of the proficiency tests was compared to the requirements of the respective reference test methods. The conclusions are given the following table.

	February 2021	February 2020	February 2019	March 2018	March 2017
Acid Wash Color (acid layer)	++	++	++	++	+
Color Pt/Co	+	+	++	++	+
Copper Corrosion	n.e.	n.e.	n.e.	n.e.	n.e.
Density at 20°C	++	++	++	++	++
Distillation	+	+	+	+/-	+/-
Purity	+/-	--	-	+	n.e.
Benzene	--	+/-	(--)	n.e.	--
Nonaromatics	++	++	++	+/-	+
Total Impurities	+/-	+/-	n.e.	n.e.	n.e.
Refractive Index at 25°C	-	-	+	+	+
Water	-	-	n.e.	n.e.	n.e.

Table 5: comparison determinations against the reference test methods

() Reproducibility between brackets is based on a much higher level than present in sample

The following performance categories were used:

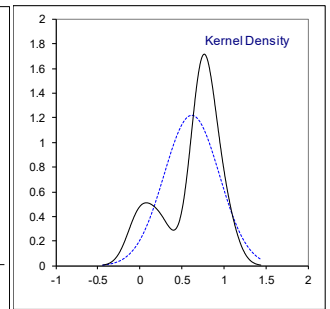
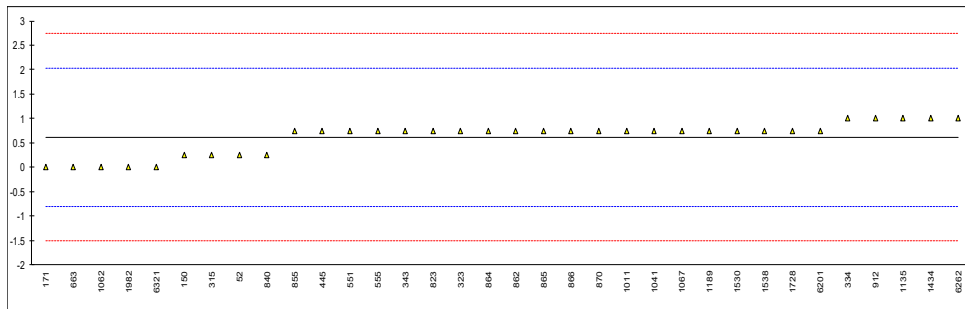
- ++ : group performed much better than the reference test method
- + : group performed better than the reference test method
- +/- : group performance equals the reference test method
- : group performed worse than the reference test method
- : group performed much worse than the reference test method
- n.e. : not evaluated

**APPENDIX 1**

**Determination of Acid Wash Color on sample #21011;**

lab	method	Reported test value	iis conversion*	mark	z(targ)	remarks
52	D848	0+	0.25		-0.52	
150	D848	0+	0.25		-0.52	
171	D848	0	0		-0.87	
315	D848	0+	0.25		-0.52	
323	D848	-1	0.75		0.19	
333		----	----		----	
334	D848	1	1		0.54	
343	D848	<1	0.75		0.19	
396	D848	PASS	PASS		----	
445	D848	1-	0.75		0.19	
551	D848	1-	0.75		0.19	
555	D848	1-	0.75		0.19	
663	D848	No. o	0		-0.87	
823	D848	1-	0.75		0.19	
840	D848	0+	0.25		-0.52	
855	D848	No.1-	0.75		0.19	
862	D848	NO.1-	0.75		0.19	
864	D848	No.1-	0.75		0.19	
865	D848	No.1-	0.75		0.19	
866	D848	NO.1-	0.75		0.19	
870	D848	NO.1-	0.75		0.19	
912	D848	1	1		0.54	
913		----	----		----	
1011	D848	1-	0.75		0.19	
1041	D848	1-	0.75		0.19	
1062	D848	0	0.00		-0.87	
1067	D848	1-	0.75		0.19	
1135	D848	1	1		0.54	
1151		----	----		----	
1189	D848	1-	0.75		0.19	
1434	D848	1	1		0.54	
1530	D848	<1	0.75		0.19	
1538	D848	1-	0.75		0.19	
1728	D848	1-	0.75		0.19	
1812		----	----		----	
1982	D848	0	0		-0.87	
6201	D848	1-	0.75		0.19	
6203		----	----		----	
6262	D848	1	1		0.54	
6315		----	----		----	
6321	D848	0	0		-0.87	
	normality		OK			
	n		34			
	outliers		0			
	mean (n)		0.618			
	st.dev. (n)		0.3270			
	R(calc.)		0.916			
	st.dev.(D848:18)		0.7091			
	R(D848:18)		1.985			

\*) In the calculation of the mean, standard deviation, reproducibility and in the graphs, a reported value of 'y-', '-y' or '<y' is changed into y-0.25 (for example 1- into 0.75) and 'y+' is changed into y+0.25 (for example 0+ into 0.25).

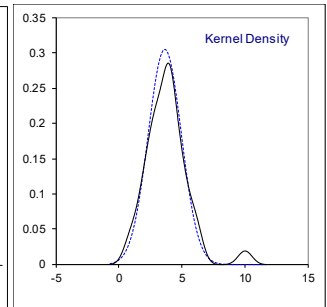
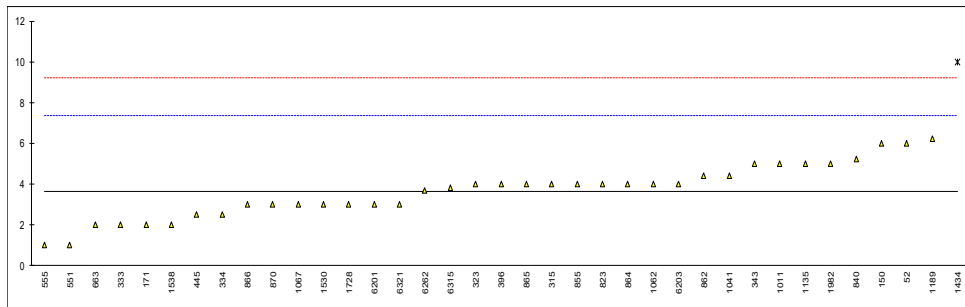


## Determination of Appearance on sample #21011;

lab	method	value	mark	z(targ)	remarks
52	D4176	Pass		----	
150	E2680	Pass		----	
171	E2680	Pass		----	
315	E2680	pass		----	
323	E2680	clear & bright		----	
333		----		----	
334	Visual	clear and bright FFMS		----	
343	E2680	pass		----	
396	visual	clear & bright		----	
445	D4176	C&B		----	
551	E2680	Pass		----	
555	E2680	Pass		----	
663	Visual	Bright & Clear		----	
823	E2680	Pass		----	
840	E2680	Pass		----	
855	E2680	Pass		----	
862	E2680	Pass		----	
864	E2680	Pass		----	
865	E2680	clear&bright		----	
866	D4176	Pass		----	
870	E2680	Pass		----	
912	E2680	Pass		----	
913		----		----	
1011	Visual	Bright and Clear		----	
1041	Visual	CBFSM		----	
1062	D4176	PASS		----	
1067	E2680	Bright and Clear		----	
1135	D4176	Pass		----	
1151		----		----	
1189	Visual	C&B		----	
1434	Visual	clear liq		----	
1530	Visual	C&B		----	
1538		B&C		----	
1728	Visual	CLEAR		----	
1812		----		----	
1982	Visual	water clear		----	
6201	Visual	Br&Cl		----	
6203	Visual	clear and transparent		----	
6262	Visual	Clear & Bright		----	
6315	Visual	Clear, bright		----	
6321	D4176	Clear and free of suspended matter		----	
	n	37			
	mean (n)	Pass (Bright & Clear)			

Determination of Color Pt/Co on sample #21011;

lab	method	value	mark	z(targ)	remarks
52	D5386	6		1.27	
150	D5386	6		1.27	
171	D5386	2.0		-0.90	
315	D5386	4		0.19	
323	D5386	4		0.19	
333	D5386	2	C	-0.90	First reported 11
334	D5386	2.5		-0.63	
343	D5386	5		0.73	
396	D5386	4		0.19	
445	D1209	2.5	C	-0.63	First reported 2.5/0
551	D5386	1		-1.44	
555	D5386	1		-1.44	
663	D5386	2		-0.90	
823	D5386	4		0.19	
840	D5386	5.2		0.84	
855	D5386	4		0.19	
862	D5386	4.4		0.40	
864	D5386	4		0.19	
865	D5386	4		0.19	
866	D1209	3		-0.36	
870	D5386	3		-0.36	
912		----		----	
913		----		----	
1011	D1209	5		0.73	
1041	ISO6271	4.4		0.40	
1062	D5386	4.0		0.19	
1067	D5386	3		-0.36	
1135	D1209	5		0.73	
1151		----		----	
1189	D5386	6.2		1.38	
1434	D1209	10	R(0.01)	3.44	
1530	D1209	3		-0.36	
1538	D1209	2		-0.90	
1728	D1209	3		-0.36	
1812		----		----	
1982	D1209	5.0		0.73	
6201	D5386	3		-0.36	
6203	D1209	4		0.19	
6262	D5386	3.7		0.02	
6315	ISO6271	3.8		0.08	
6321	D1209	3		-0.36	
	normality	OK			
	n	36			
	outliers	1			
	mean (n)	3.66			
	st.dev. (n)	1.310			
	R(calc.)	3.67			
	st.dev.(D5386:16)	1.845			
	R(D5386:16)	5.17			
	Compare				
	R(D1209:05)	7			

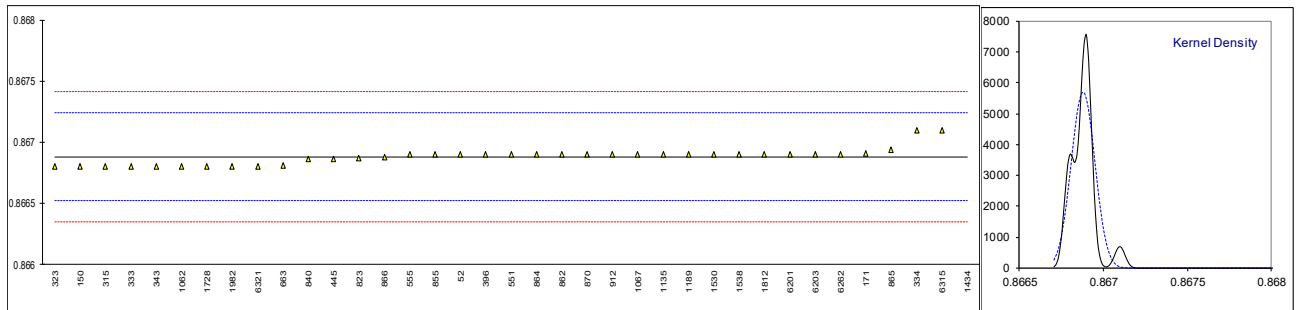


Determination of Copper Corrosion on sample #21011;

lab	method	value	mark	z(targ)	remarks
52	D849	1a		----	
150	D849	1a		----	
171	D849	1a		----	
315	D849	pass		----	
323	D849	1A		----	
333		----		----	
334	D849	pass		----	
343		----		----	
396		----		----	
445	D849	1a		----	
551	D849	1A		----	
555	D849	1a		----	
663	D849	1a		----	
823	D849	1a		----	
840	D849	1a		----	
855	D849	1a		----	
862	D849	1a		----	
864	D849	1a		----	
865	D849	1a		----	
866	D849	1a		----	
870	D849	1a		----	
912	D849	1a		----	
913		----		----	
1011	D849	1a		----	
1041		----		----	
1062	D849	1B		----	
1067	D849	1A		----	
1135	D849	1A		----	
1151		----		----	
1189	D849	1A		----	
1434	D849	1a		----	
1530	D849	1a		----	
1538		----		----	
1728	D849	1A		----	
1812		----		----	
1982	D849	1A		----	
6201	D849	1a		----	
6203		----		----	
6262	D849	1A		----	
6315	ISO2160	1		----	
6321		----		----	
	n	31			
	mean (n)	1(1a/1b)			

Determination of Density at 20°C on sample #21011: results in kg/L

lab	method	value	mark	z(targ)	remarks
52	D4052	0.8669		0.10	
150	D4052	0.8668		-0.46	
171	D4052	0.86691		0.16	
315	D4052	0.8668		-0.46	
323	D4052	0.8668		-0.46	
333	ISO12185	0.8668		-0.46	
334	ISO12185	0.8671		1.22	
343	ISO12185	0.8668		-0.46	
396	D4052	0.8669		0.10	
445	D4052	0.86686		-0.12	
551	D4052	0.8669		0.10	
555	D4052	0.8669		0.10	
663	D4052	0.86681		-0.40	
823	ISO12185	0.86687		-0.06	
840	D4052	0.86686		-0.12	
855	D4052	0.8669		0.10	
862	D4052	0.8669		0.10	
864	D4052	0.8669		0.10	
865	D4052	0.86694		0.33	
866	D4052	0.86688		-0.01	
870	D4052	0.8669		0.10	
912	ISO12185	0.8669		0.10	
913		----		----	
1011		----		----	
1041		----		----	
1062	D4052	0.8668		-0.46	
1067	D4052	0.8669		0.10	
1135	ISO12185	0.8669		0.10	
1151		----		----	
1189	D4052	0.8669		0.10	
1434	D4052	0.87013	R(0.01)	18.19	
1530	D4052	0.86690		0.10	
1538	ISO12185	0.8669		0.10	
1728	ISO12185	0.86680		-0.46	
1812	ISO12185	0.8669	C	0.10	First reported 866.9 kg/L
1982	ISO12185	0.8668		-0.46	
6201	ISO12185	0.8669		0.10	
6203	ISO12185	0.8669		0.10	
6262	ISO12185	0.8669		0.10	
6315	ISO12185	0.8671		1.22	
6321	ISO12185	0.8668		-0.46	
	normality	not OK			
	n	36			
	outliers	1			
	mean (n)	0.86688			
	st.dev. (n)	0.000070			
	R(calc.)	0.00020			
	st.dev.(ISO12185:96)	0.000178			
	R(ISO12185:96)	0.0005			



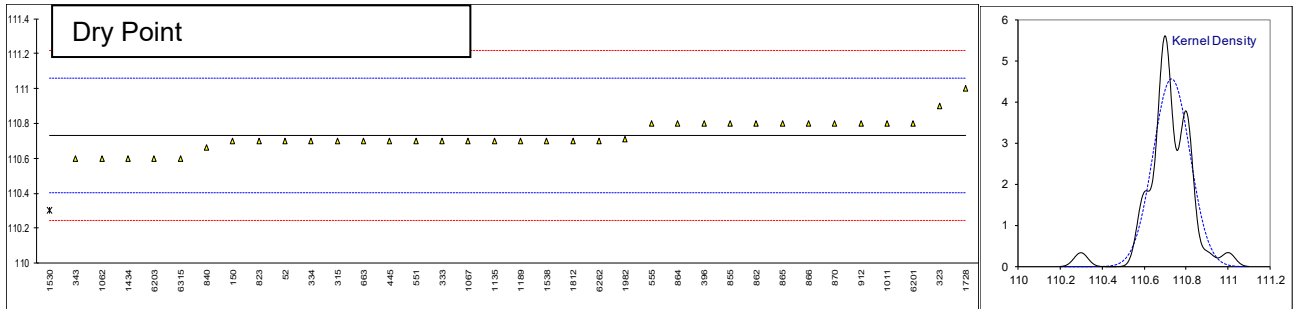
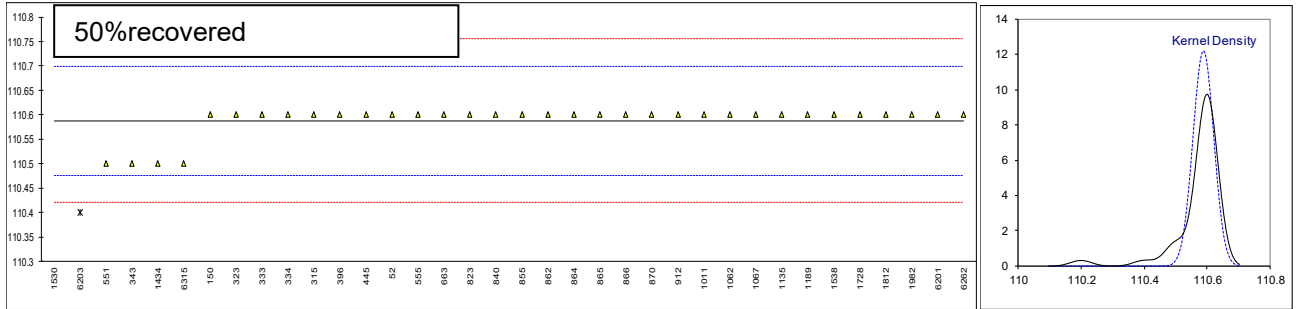
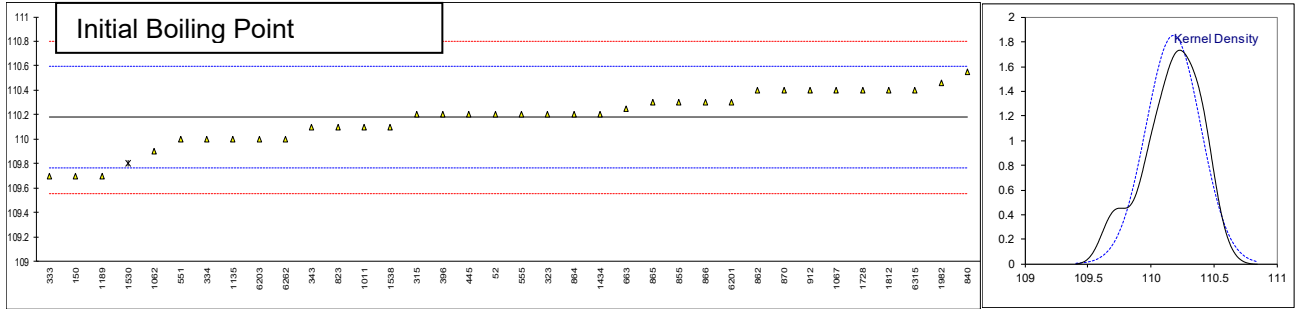
Determination of Distillation on sample #21011; results in °C

Lab	method	IBP	mark	z(targ)	50%rec	mark	z(targ)	DP	mark	z(targ)	range
52	D850-automated	110.2		0.10	110.6		0.21	110.7		-0.19	0.5
150	D850-automated	109.7		-2.31	110.6		0.21	110.7		-0.19	1.0
171		----		----			----			----	
315	D850-automated	110.2		0.10	110.6		0.21	110.7		-0.19	0.5
323	D850-automated	110.2		0.10	110.6		0.21	110.9		1.04	0.7
333	D850-automated	109.7		-2.31	110.6		0.21	110.7		-0.19	1.0
334	D850-automated	110.0		-0.86	110.6		0.21	110.7		-0.19	0.7
343	D850-automated	110.1		-0.38	110.5		-1.58	110.6		-0.80	----
396	D850	110.2		0.10	110.6		0.21	110.8		0.43	0.6
445	D850-automated	110.2		0.10	110.6		0.21	110.7		-0.19	0.5
551	D850-automated	110		-0.86	110.5		-1.58	110.7		-0.19	0.7
555	D850-manual	110.2		0.10	110.6		0.21	110.8		0.43	0.6
663	D850-automated	110.25		0.34	110.60		0.21	110.70		-0.19	0.5
823	D850-automated	110.1		-0.38	110.6		0.21	110.7		-0.19	0.6
840	D850-automated	110.55		1.79	110.60		0.21	110.66		-0.43	0.11
855	D850-manual	110.3		0.58	110.6		0.21	110.8		0.43	0.5
862	D850-manual	110.4		1.07	110.6		0.21	110.8		0.43	0.4
864	D850-manual	110.2		0.10	110.6		0.21	110.8		0.43	0.6
865	D850-automated	110.3		0.58	110.6		0.21	110.8		0.43	0.5
866	D850-manual	110.3		0.58	110.6		0.21	110.8		0.43	0.5
870	D850-automated	110.4		1.07	110.6		0.21	110.8		0.43	0.4
912	D850-automated	110.4		1.07	110.6		0.21	110.8		0.43	0.4
913		----		----			----			----	
1011		110.1		-0.38	110.6		0.21	110.8		0.43	0.7
1041		----		----			----			----	
1062	D850-automated	109.9	C	-1.34	110.6		0.21	110.6		-0.80	1.3
1067	D850-automated	110.4		1.07	110.6		0.21	110.7		-0.19	0.3
1135	D850-automated	110.0		-0.86	110.6		0.21	110.7		-0.19	0.7
1151		----		----			----			----	
1189	D850-automated	109.7		-2.31	110.6		0.21	110.7		-0.19	1.0
1434	D850-automated	110.2		0.10	110.5		-1.58	110.6		-0.80	0.4
1530	D850-automated	109.80	ex	-1.83	110.20	R(0.01)	-6.97	110.30	R(0.05)	-2.64	0.50
1538	D850-automated	110.1		-0.38	110.6		0.21	110.7		-0.19	0.6
1728	D850-manual	110.4		1.07	110.6		0.21	111		1.65	0.6
1812	D850-manual	110.40		1.07	110.60		0.21	110.70		-0.19	0.3
1982	D850-automated	110.46		1.36	110.60		0.21	110.71		-0.13	0.25
6201	D850-manual	110.3		0.58	110.6		0.21	110.8		0.43	0.5
6203	D850-manual	110.0		-0.86	110.4	R(0.01)	-3.38	110.6		-0.80	0.6
6262	D850-automated	110.0		-0.86	110.6		0.21	110.7		-0.19	0.7
6315	D850-automated	110.4		1.07	110.5		-1.58	110.6		-0.80	0.2
6321		----		----			----			----	
	normality	OK			not OK			suspect			
	n	35			34			35			
	outliers	0+1ex			2			1			
	mean (n)	110.18			110.59			110.73			
	st.dev. (n)	0.215			0.033			0.087			
	R(calc.)	0.60			0.09			0.24			
	st.dev.(D850-A:21)	0.208			0.056			0.163			
	R(D850-A:21)	0.58			0.16			0.46			
Compare											
	R(D850-M:21)	0.41			0.646			0.646			

Lab 1062 first reported 109.3

Lab 1530 test result excluded as the other reported test results are statistical outliers

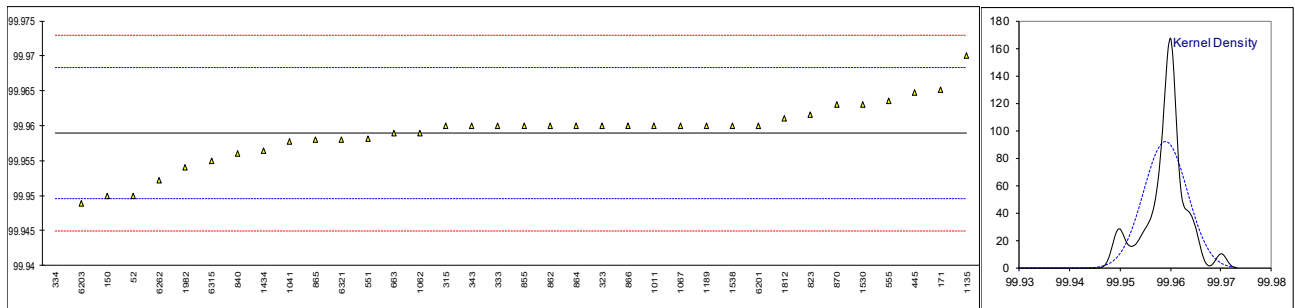




Determination of Purity by GC on sample #21011; results in %M/M

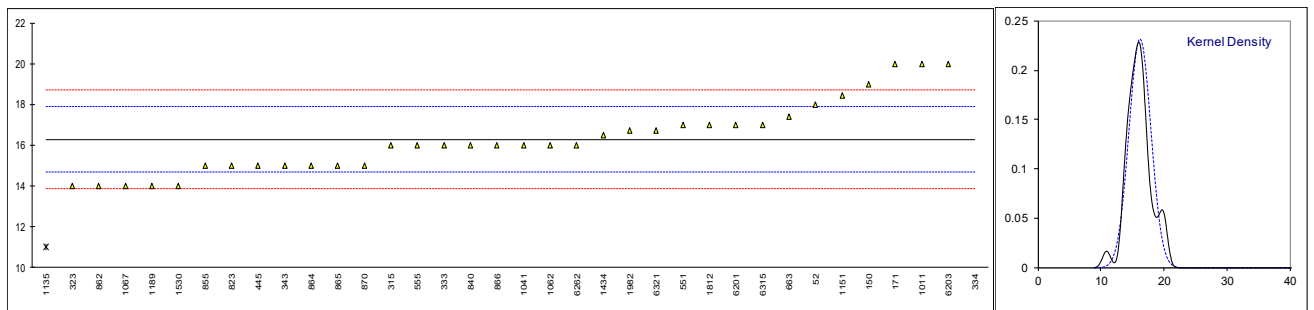
lab	method	value	mark	z(targ)	remarks
52	D7504	99.95		-1.91	
150	D7504	99.95		-1.91	
171	D7504	99.9651		1.31	
315	D7504	99.96		0.22	
323	D7504	99.96		0.22	
333	D7504	99.96		0.22	
334	D7504	99.860	R(0.01)	-21.15	
343	D2360	99.96		0.22	
396		-----		-----	
445	D6526	99.9647		1.23	
551	D7504	99.9581		-0.18	
555	D7504	99.9636		0.99	
663	D7504	99.959		0.01	
823	D2360	99.9616		0.57	
840	D7504	99.956		-0.63	
855	D7504	99.96		0.22	
862	D7504	99.960		0.22	
864	D7504	99.96		0.22	
865	D7504	99.958		-0.20	
866	D7504	99.96		0.22	
870	D7504	99.963		0.86	
912		-----		-----	
913		-----		-----	
1011	D5917	99.96		0.22	
1041		99.9577		-0.27	
1062	D2360	99.959		0.01	
1067	In house	99.96		0.22	
1135	D7504	99.97		2.36	
1151		-----		-----	
1189	In house	99.96		0.22	
1434	D7504	99.95647		-0.53	
1530	D7504	99.963		0.86	
1538	D7504	99.96		0.22	
1728		-----		-----	
1812	D7504	99.961		0.44	
1982	D7504	99.954		-1.06	
6201	D7504	99.960		0.22	
6203	D7504	99.9489		-2.15	
6262	D7504	99.9522		-1.44	
6315	D7504	99.9549		-0.87	
6321	D2360	99.958		-0.20	

normality suspect  
n 35  
outliers 1  
mean (n) 99.9590  
st.dev. (n) 0.00434  
R(calc.) 0.0121  
st.dev.(D7504:20) 0.00480  
R(D7504:20) 0.0131



Determination of Benzene on sample #21011; results in mg/kg

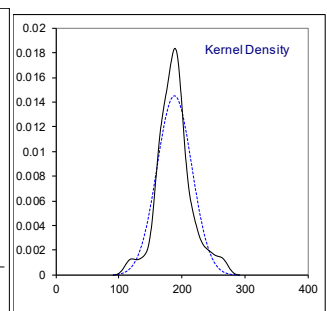
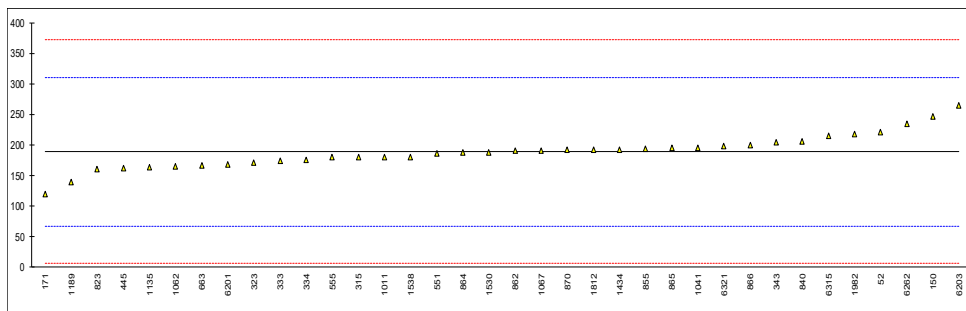
lab	method	value	mark	z(targ)	remarks
52	D7504	18		2.13	
150	D7504	19		3.37	
171	D7504	20		4.61	
315	D7504	16		-0.36	
323	D7504	14		-2.84	
333	D7504	16	C	-0.36	First reported 0.0016 mg/kg
334	D7504	57	R(0.01)	50.59	
343	D2360	15		-1.60	
396		----		----	
445	D6526	15		-1.60	
551	D7504	17		0.89	
555	D7504	16		-0.36	
663	D7504	17.4		1.38	
823	D2360	15		-1.60	
840	D7504	16.0		-0.36	
855	D7504	15		-1.60	
862	D7504	14		-2.84	
864	D7504	15		-1.60	
865	D7504	15		-1.60	
866	D7504	16		-0.36	
870	D7504	15		-1.60	
912		----		----	
913		----		----	
1011	D5917	20		4.61	
1041		16		-0.36	
1062	D2360	16		-0.36	
1067	In house	14		-2.84	
1135	D7504	11	R(0.05)	-6.57	
1151	In house	18.43		2.66	
1189	In house	14		-2.84	
1434	D7504	16.5	C	0.27	First reported 0.0435
1530	D7504	14		-2.84	
1538		----		----	
1728		----		----	
1812	D7504	17		0.89	
1982	D7504	16.7		0.51	
6201	D7504	17		0.89	
6203	D7504	20		4.61	
6262	D7504	16		-0.36	
6315	D7504	17.0		0.89	
6321	D2360	16.7		0.51	
normality		OK			
n		34			
outliers		2			
mean (n)		16.29			
st.dev. (n)		1.726			
R(calc.)		4.83			
st.dev.(D7504:20)		0.805			
R(D7504:20)		2.25			



Determination of Nonaromatics on sample #21011; results in mg/kg

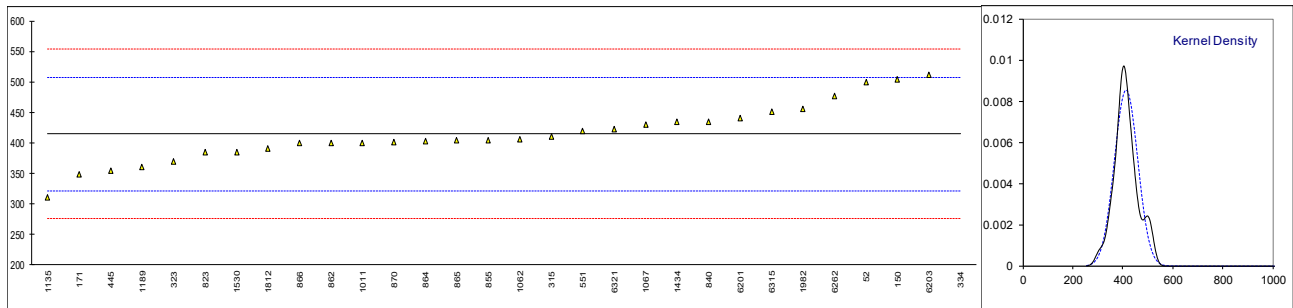
lab	method	value	mark	z(targ)	remarks
52	D7504	221		0.53	
150	D7504	247		0.96	
171	D7504	119		-1.15	
315	D7504	180		-0.14	
323	D7504	171		-0.29	
333	D7504	174	C	-0.24	First reported 0.0174 mg/kg
334	D7504	175		-0.23	
343	D2360	204		0.25	
396		----		----	
445	D6526	162		-0.44	
551	D7504	186		-0.05	
555	D7504	180		-0.14	
663	D7504	166.0		-0.37	
823	D2360	161		-0.46	
840	D7504	205.2		0.27	
855	D7504	194		0.09	
862	D7504	190		0.02	
864	D7504	188		-0.01	
865	D7504	195		0.10	
866	D7504	200		0.18	
870	D7504	192		0.05	
912		----		----	
913		----		----	
1011	D5917	180	C	-0.14	First reported 18
1041		195		0.10	
1062	D2360	165		-0.39	
1067	In house	191		0.04	
1135	D7504	164		-0.41	
1151		----		----	
1189	In house	140		-0.80	
1434	D7504	192.8	C	0.07	First reported 0.01928 mg/kg
1530	D7504	188		-0.01	
1538	D7504	180		-0.14	
1728		----		----	
1812	D7504	192		0.05	
1982	D7504	217.9		0.48	
6201	D7504	168		-0.34	
6203	D7504	265		1.25	
6262	D7504	234		0.74	
6315	D7504	214.6		0.42	
6321	D2360	198.6		0.16	

normality suspect  
n 36  
outliers 0  
mean (n) 188.78  
st.dev. (n) 27.557  
R(calc.) 77.16  
st.dev.(D7504:20) 60.939  
R(D7504:20) 170.63



Determination of Total Impurities on sample #21011; results in mg/kg

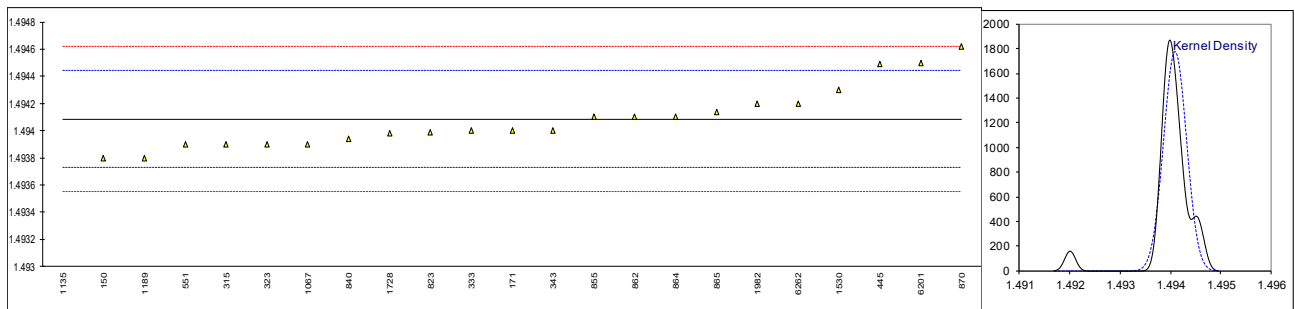
lab	method	value	mark	z(targ)	remarks
52	D7504	500		1.85	
150	D7504	504		1.94	
171	D7504	349		-1.41	
315	D7504	410		-0.09	
323	D7504	370		-0.95	
333		----		----	
334	D7504	1396	R(0.01)	21.18	
343		----		----	
396		----		----	
445	D6526	355		-1.28	
551	D7504	419		0.10	
555		----		----	
663		----		----	
823	D2360	384		-0.65	
840	D7504	435.1		0.45	
855	D7504	405		-0.20	
862	D7504	400		-0.31	
864	D7504	403		-0.24	
865	D7504	404		-0.22	
866	D7504	400		-0.31	
870	D7504	402		-0.26	
912		----		----	
913		----		----	
1011	D5917	400		-0.31	
1041		----		----	
1062	D2360	406		-0.18	
1067	In house	430		0.34	
1135	D7504	310.3		-2.24	
1151		----		----	
1189	In house	360	C	-1.17	First reported 220
1434	D7504	435	C	0.45	First reported 0.0435 mg/kg
1530	D7504	384		-0.65	
1538		----		----	
1728		----		----	
1812	D7504	391		-0.50	
1982	D7504	455.3		0.89	
6201	D7504	440		0.56	
6203	D7504	511		2.09	
6262	D7504	477		1.35	
6315		450.9		0.79	
6321	D2360	422.2		0.17	
normality		OK			
n		29			
outliers		1			
mean (n)		414.23			
st.dev. (n)		46.524			
R(calc.)		130.27			
st.dev.(Horwitz 3 comp)		46.344			
R(Horwitz 3 comp)		129.76			



Determination of Refractive Index at 25°C on sample #21011;

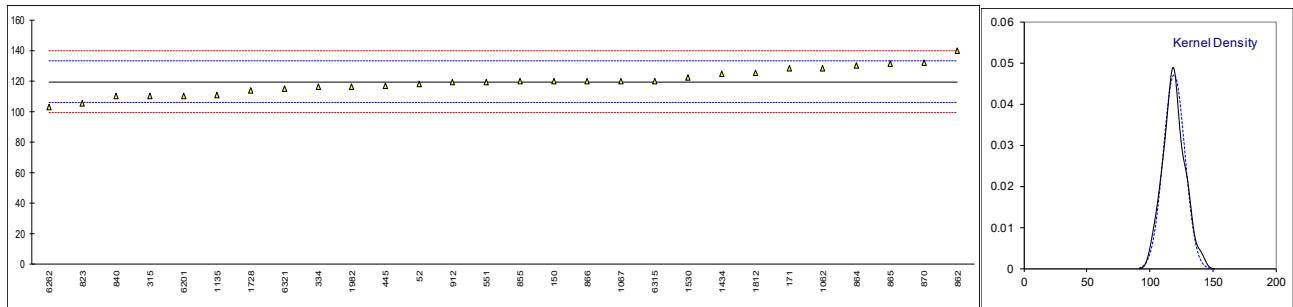
lab	method	value	mark	z(targ)	remarks
52		----		----	
150	D1218	1.4938		-1.59	
171	D1218	1.4940		-0.47	
315	D1218	1.4939		-1.03	
323	D1218	1.4939		-1.03	
333	D1218	1.4940		-0.47	
334		----		----	
343	D1218	1.4940		-0.47	
396		----		----	
445	D1218	1.49449		2.27	
551	D1218	1.4939		-1.03	
555		----		----	
663		----		----	
823	D1218	1.49399		-0.53	
840	D1218	1.49394		-0.81	
855	D1218	1.4941		0.09	
862	D1218	1.49410		0.09	
864	D1218	1.4941		0.09	
865	D1218	1.49414		0.31	
866		----		----	
870	D1218	1.49462		3.00	
912		----		----	
913		----		----	
1011		----		----	
1041		----		----	
1062		----		----	
1067	D1218	1.4939		-1.03	
1135	D1218	1.4920	C,R(0.01)	-11.67	First reported 1.4969
1151		----		----	
1189	D1218	1.4938		-1.59	
1434		----		----	
1530	D1218	1.49430		1.21	
1538		----		----	
1728	D1218	1.49398		-0.59	
1812		----		----	
1982	DIN51423-1	1.4942		0.65	
6201	D1218	1.49450		2.33	
6203		----		----	
6262	D1218	1.4942		0.65	
6315		----		----	
6321		----		----	

normality suspect  
n 22  
outliers 1  
mean (n) 1.49408  
st.dev. (n) 0.000225  
R(calc.) 0.00063  
st.dev.(D1218:12) 0.000179  
R(D1218:12) 0.0005



Determination of Water on sample #21011; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	E1064	118		-0.21	
150	E1064	120		0.08	
171	E1064	128		1.26	
315	E1064	110		-1.39	
323		----		----	
333		----		----	
334	E1064	116		-0.51	
343		----		----	
396		----		----	
445	E1064	117		-0.36	
551	E1064	119.5		0.01	
555		----		----	
663		----		----	
823	E1064	105		-2.13	
840	E1064	110		-1.39	
855	E1064	120		0.08	
862	E1064	140		3.03	
864	E1064	130		1.56	
865	E1064	131		1.70	
866	E1064	120		0.08	
870	E1064	132		1.85	
912	E1064	119		-0.07	
913		----		----	
1011		----		----	
1041		----		----	
1062	D6304	128	C	1.26	First reported 198
1067	E1064	120		0.08	
1135	E1064	111		-1.25	
1151		----		----	
1189		----		----	
1434	D6304	124.9		0.80	
1530	E1064	122.1		0.39	
1538		----		----	
1728	E1064	114		-0.80	
1812		125		0.82	
1982	E1064	116		-0.51	
6201	E1064	110		-1.39	
6203		----		----	
6262	E1064	103		-2.42	
6315	ISO12937	120		0.08	
6321	E1064	115		-0.66	
normality		OK			
n		28			
outliers		0			
mean (n)		119.45			
st.dev. (n)		8.477			
R(calc.)		23.73			
st.dev.(E1064:16)		6.783			
R(E1064:16)		18.99			



## **APPENDIX 2**

### **Number of participants per country**

4 labs in BELGIUM  
2 labs in BRAZIL  
1 lab in CANADA  
6 labs in CHINA, People's Republic  
2 labs in FRANCE  
5 labs in GERMANY  
2 labs in INDIA  
1 lab in ISRAEL  
1 lab in ITALY  
4 labs in NETHERLANDS  
1 lab in POLAND  
1 lab in PORTUGAL  
2 labs in ROMANIA  
1 lab in SAUDI ARABIA  
1 lab in SOUTH KOREA  
1 lab in SPAIN  
1 lab in THAILAND  
2 labs in UNITED KINGDOM  
2 labs in UNITED STATES OF AMERICA  
1 lab in VIETNAM



## APPENDIX 3

### Abbreviations

C	= final test result after checking of first reported suspect result
D(0.01)	= outlier in Dixon's outlier test
D(0.05)	= straggler in Dixon's outlier test
G(0.01)	= outlier in Grubbs' outlier test
G(0.05)	= straggler in Grubbs' outlier test
DG(0.01)	= outlier in Double Grubbs' outlier test
DG(0.05)	= straggler in Double Grubbs' outlier test
R(0.01)	= outlier in Rosner's outlier test
R(0.05)	= straggler in Rosner's outlier test
E	= calculation difference between reported test result and result calculated by iis
W	= test result withdrawn on request of participant
ex	= test result excluded from statistical evaluation
n.a.	= not applicable
n.e.	= not evaluated
n.d.	= not detected
fr.	= first reported
SDS	= Safety Data Sheet

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