Results of Proficiency Test
Benzene
February 2020

Organised by: Institute for Interlaboratory Studies
Spijkenisse Netherlands

Author: A. Lewinska, MSc.
Correctors: ing. A.S. Noordman–de Neef & ing. M. Meijer

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1 INTRODUCTION

Since 1999, the Institute for Interlaboratory Studies (iis) organizes a proficiency scheme for Benzene every year. During the annual proficiency testing program 2019/2020 it was decided to continue the round robin for the analysis of Benzene based on the scope of the latest version of ASTM D2359.

In this interlaboratory study 52 laboratories in 22 different countries registered for participation. See appendix 2 for the number of participants per country. In this report the results of this proficiency test are presented and discussed. This report is also electronically available through the iis website 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 sample labelled #20010 of a liter Benzene. The participants were requested to report rounded and unrounded test results. The unrounded test results were preferably used for the 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, 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 75 liters of Benzene was obtained from a local chemical supplier. After homogenization 64 amber glass bottles of 1 liter were filled and labelled #20010. 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 #20010-1	0.87877
sample #20010-2	0.87878
sample #20010-3	0.87877
sample #20010-4	0.87877
sample #20010-5	0.87878
sample #20010-6	0.87879
sample #20010-7	0.87878
sample #20010-8	0.87878

Table 1: homogeneity test results of subsamples #20010

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)	0.00002
reference test method	ISO12185:96
0.3*R (reference test method)	0.00015

Table 2: evaluation of repeatability of subsamples #20010

The calculated repeatability was 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 1 liter Benzene labelled #20010 was sent on January 29, 2020. An SDS was added to the sample package.

2.5 STABILITY OF THE SAMPLES

The stability of Benzene 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 on sample #20010: Acid Wash Color, Acidity, Appearance, Bromine Index, Total Chlorides, Organic Chlorides, Color Pt/Co, Density at 20°C, Distillation (IBP, 50% recovered, Dry Point, Distillation Range), Total Nitrogen, Purity by GC, Methylcyclohexane, Toluene, Nonaromatics, 1,4-Dioxane, Total Impurities, Solidification Point, Sulfur, Thiophene 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 appropriate reference test methods 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/. 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.

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/. 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.

According to ISO5725 the original test results per determination were submitted to Dixon’s, Grubbs’ and/or Rosner’s outlier tests. 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 was projected over the Kernel Density Graph for reference.

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. In some cases, a reproducibility based on former iis proficiency tests could be used.
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(target) = (test result - average of PT) / 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

During the execution of this proficiency test some serious problems occurred. Due to COVID-19 outbreak eighteen participants were not able to report because of restricted dispatch to some countries. It was decided that for those participants the deadline was extended, and an extra round was created on the Data Entry Portal.

Not all laboratories were able to perform all analyzes requested. Finally, 34 participants reported 400 numerical test results. Observed were 12 outlying test results, which is 3% of the numerical test results. In proficiency studies, 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 original reported test results. The abbreviations, used in these tables, are explained in appendix 3.

In the iis PT reports, ASTM test methods are referred to with a number e.g. D7011 and an added designation for the year that the test method was adopted or revised e.g. D7011:15. If applicable, a designation in parentheses is added to designate the year of reapproval e.g. D7011:15(2019). In the test result tables of appendix 1 only the test method number and year of adoption or revision e.g. D7011:15 will be used.

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

Sample #20010

Acid Wash Color: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D848:14.

Acidity: This determination was not problematic. The majority of laboratories reported “no free acid” (NFA) or “Pass”.

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

Bromine Index: 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 D5776:14a.

Total Chlorides: 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 D5194:18.

Organic Chlorides: 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 D5808:18.

Color Pt/Co: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D5386:16 and ASTM D1209:05(2011).

Density at 20°C: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ISO12185:96.

Distillation: This determination was problematic. In total three statistical outliers were observed and one other test result was excluded. The calculated reproducibilities of IBP and 50% recovered after rejection of the suspect data were in agreement with the requirements of ASTM D850-A:18e1. The calculated reproducibility of Dry Point after rejection of the suspect data is not at all in agreement with the requirements of ASTM D850-A:18e1. The variation in the test results was very large. Therefore, no z-scores were calculated.

Total Nitrogen: This determination was not problematic. Almost all participants agreed on a concentration lower than 0.3 mg/kg. Therefore, no z-scores were calculated.

Purity: 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 D7504:20.

Methylcyclohexane: This determination may be problematic. One statistical outlier was observed. The calculated reproducibility after rejection of the statistical outlier is not agreement with the estimated reproducibility calculated using the Horwitz equation.

Toluene: This determination was problematic. No statistical outliers were observed. However, the calculated reproducibility is not 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.

1,4-Dioxane: This determination was not problematic. Almost all participants agreed on a concentration lower than 10 mg/kg. Therefore, no z-scores were calculated.

Total Impurities: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the estimated reproducibility calculated using the Horwitz equation.

Solidification Point: This determination was problematic. No statistical outliers were observed. However, the calculated reproducibility is not in agreement with the requirements of ASTM D852:16.

Sulfur: This determination was not problematic. Almost all participants agreed on a concentration lower than 1 mg/kg. Therefore, no z-scores were calculated.

Thiophene: This determination was not problematic. All participants agreed on a concentration lower than 1 mg/kg. Therefore, no z-scores were calculated.

Water: This determination was problematic. Three statistical outliers were observed. The calculated reproducibility after rejection of the statistical outliers 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 relevant reference test method or as declared by the estimated target reproducibility using 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, ISO test methods) or the estimated target reproducibility are presented in the next table.

Parameter	Unit	n	average	2.8 * sd	R(lit)
Acid Wash Color (acid layer)		24	0.7 (1-)	0.9	2.0
Acidity	mg NaOH/ 100mL	21	No free acid	n.a.	n.a.
Appearance		30	Pass (C&B)	n.a.	n.a.
Bromine Index	mg Br/ 100g	22	1.0	2.0	4.6
Total Chlorides	mg/kg	7	2.4	0.6	0.9
Organic Chlorides	mg/kg	15	2.5	1.1	1.3
Color Pt/Co		26	2.9	3.9	5.0
Density at 20°C	kg/L	30	0.8788	0.0002	0.0005
Distillation, IBP	°C	21	79.7	0.3	0.6
Distillation, 50% rec.	°C	20	80.1	0.2	0.2
Distillation, DP	°C	19	81.0	1.7	(0.5)
Total Nitrogen	mg/kg	23	<0.3	n.a.	n.a.
Purity by GC	%M/M	31	99.762	0.059	0.025
Methylcyclohexane	mg/kg	21	82.7	40.5	19.1
Toluene	mg/kg	32	593.4	118.2	76.2
Nonaromatics	mg/kg	32	837.4	395.1	679.4
1,4-Dioxane	mg/kg	15	<10	n.a.	n.a.
Total Impurities	mg/kg	20	2368	522	571
Solidification Point *)	°C	13	5.41	0.17	0.05
Sulfur	mg/kg	32	<1	n.a.	n.a.
Thiophene	mg/kg	7	<1	n.a.	n.a.
Water	mg/kg	25	100	19	17

Table 3: reproducibilities of tests on sample #20010

*) anhydrous basis

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 2020 WITH PREVIOUS PTS

	February 2020	February 2019	March 2018	March 2017	March 2016
Number of reporting laboratories	34	50	51	67	59
Number of test results	400	532	545	743	793
Number of statistical outliers	12	17	24	32	19
Percentage of statistical outliers	3.0%	3.2%	4.4%	4.3%	2.4%

Table 4: comparison with previous proficiency tests.

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

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

	February 2020	February 2019	March 2018	March 2017	March 2016
Acid Wash Color (acid layer)	++	++	++	++	++
Bromine Index	++	++	++	++	++
Total Chlorides	+	+/-	-	+/-	+
Organic Chlorides	+	++	++	+	++
Color Pt/Co	+	+	++	++	++
Density at 20°C	++	++	++	++	++
Distillation	-	++	++	++	++
Total Nitrogen	n.e.	-	+	+/-	--
Purity by GC	--	++	-	+/-	-
Methylcyclohexane	--	-	--	+/-	+/-
Toluene	-	n.e.	++	++	++
Nonaromatics	+	++	-	-	+/-
1,4-Dioxane	n.e.	n.e.	n.e.	n.e.	n.e.
Total Impurities	+/-	n.e.	n.e.	n.e.	n.e.
Solidification Point *)	--	+	+/-	+	+/-
Sulfur	n.e.	+/-	+/-	n.e.	n.e.
Thiophene	n.e.	n.e.	n.e.	n.e.	n.e.
Water	-	-	n.e.	n.e.	n.e.

Table 5: comparison determinations against the reference test methods
*) anhydrous basis

In the table above 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

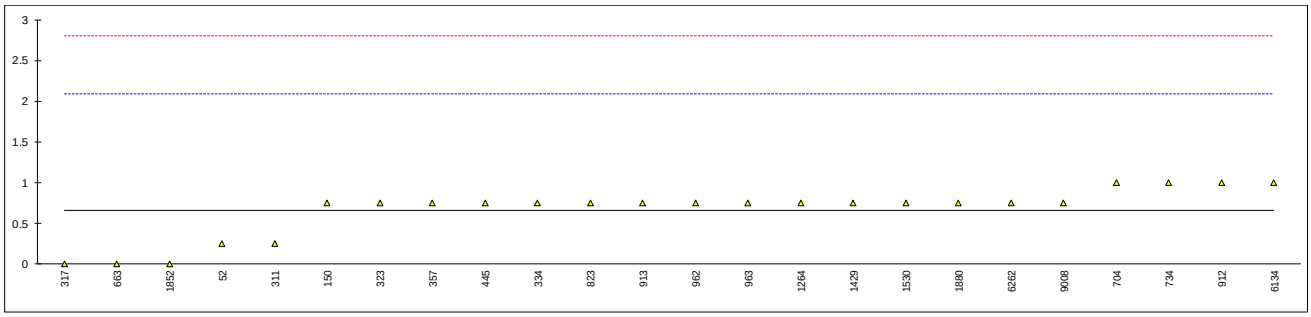
APPENDIX 1

Determination of Acid Wash Color (acid layer) on sample #20010;

lab	method	reported test value	iis conversion*	mark	z(targ)	remarks
52	D848	0+	0.25		-0.57	
150	D848	1-	0.75		0.13	
311	D848	0+	0.25		-0.57	
317	D848	0	0		-0.92	
323	D848	1-	0.75		0.13	
334	D848	1-	0.75		0.13	
347		-----	-----		-----	
357	D848	1-	0.75		0.13	
444		-----	-----		-----	
445	D848	1-	0.75		0.13	
551		-----	-----		-----	
555		-----	-----		-----	
663	D848	No. 0	0		-0.92	
704	D848	1	1		0.48	
734	D848	1	1		0.48	
823	D848	1-	0.75		0.13	
846		-----	-----		-----	
852		-----	-----		-----	
855		-----	-----		-----	
862		-----	-----		-----	
864		-----	-----		-----	
866		-----	-----		-----	
868		-----	-----		-----	
870		-----	-----		-----	
912	D848	1	1		0.48	
913	D848	1-	0.75		0.13	
962	D848	1-	0.75		0.13	
963	D848	1-	0.75		0.13	
1040		-----	-----		-----	
1041		-----	-----		-----	
1065		-----	-----		-----	
1081		-----	-----		-----	
1117		-----	-----		-----	
1151		-----	-----		-----	
1264	D848	1-	0.75	C	0.13	first reported: 3-
1294		-----	-----		-----	
1429	D848	1-	0.75		0.13	
1467		-----	-----		-----	
1530	D848	< 1	0.75		0.13	
1669		-----	-----		-----	
1741		-----	-----		-----	
1790		-----	-----		-----	
1823		-----	-----		-----	
1852	D848	0	0		-0.92	
1880	D848	<1	0.75		0.13	
1954		-----	-----		-----	
2301		-----	-----		-----	
6134	D848	1	1		0.48	
6198		-----	-----		-----	
6203		-----	-----		-----	
6262	D848	1-	0.75		0.13	
9008	D848	1-	0.75		0.13	

normality	OK
n	24
outliers	0
mean (n)	0.66
st.dev. (n)	0.311
R(calc.)	0.87
st.dev.(D848:14)	0.715
R(D848:14)	2.003

*) 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).


3
2.5
2
1.5
1
0.5
0
317
663
1852
52
311
150
323
357
445
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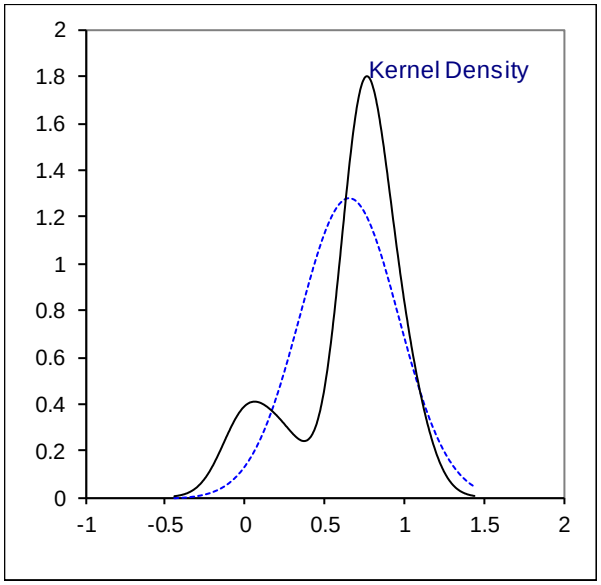
962
963
1264
1429
1530
1880
6262
9008
704
734
912
6134


Kernel Density
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-1
-0.5
0
0.5
1
1.5
2

Determination of Acidity on sample #20010; results in mg NaOH/100mL

lab	method	value	mark	z(targ)	remarks
52	D847	Pass		-----	
150	D847	Pass		-----	
311	D847	pass		-----	
317		-----		-----	
323	D847	NFANEOA		-----	
334	D847	pass		-----	
347	D847	Pass		-----	
357	D847	No free acid		-----	
444		-----		-----	
445	D847	NFA		-----	
551		-----		-----	
555		-----		-----	
663	D847	pass		-----	
704	D847	Pass		-----	
734		-----		-----	
823	D847	no free acid		-----	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D847	No free Acid		-----	
913	D847	No free acid		-----	
962	D847	No free acid		-----	
963		-----		-----	
1040		-----		-----	
1041		-----		-----	
1065		-----		-----	
1081	D847	pass		-----	
1117	D847	< 0.4		-----	
1151		-----		-----	
1264	D847	No Free Acid		-----	
1294		-----		-----	
1429		-----		-----	
1467		-----		-----	
1530	D847	negative		-----	
1669		-----		-----	
1741		-----		-----	
1790		-----		-----	
1823		-----		-----	
1852		-----		-----	
1880	D847	NFA		-----	
1954		-----		-----	
2301		-----		-----	
6134	D847	NFA		-----	
6198		-----		-----	
6203		-----		-----	
6262	D847	Pass		-----	
9008	D847	NFA		-----	
	n	21			
	mean (n)	No free acid (pass)			

Abbreviation
NFA = No free acid

Determination of Appearance on sample #20010;

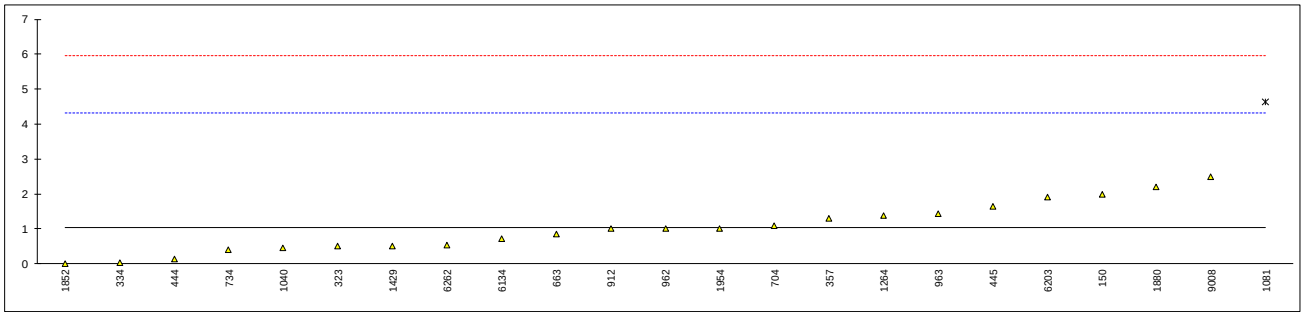
lab	method	value	mark	z(targ)	remarks
52	D4176	Pass		-----	
150	E2680	Pass		-----	
311	E2680	pass		-----	
317	D4176	pass		-----	
323	E2680	Clear & bright		-----	
334	EN15769	clear and bright		-----	
347	D4176	Pass		-----	
357	E2680	Pass		-----	
444	E2680	Pass		-----	
445	D4176	Black Particulates		-----	
551		-----		-----	
555		-----		-----	
663	Visual	Bright & Clear		-----	
704	E2680	Pass		-----	
734	E2680	pass		-----	
823	E2680	Pass		-----	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	E2680	Pass		-----	
913	E2680	Pass		-----	
962	D4176	Clear & Bright		-----	
963	Visual	Clear liquid free of sediment and haze		-----	
1040	Visual	clear & bright visual free		-----	
1041		-----		-----	
1065		-----		-----	
1081	In house	B/C		-----	
1117	D4176	PASS		-----	
1151		-----		-----	
1264	Visual	Clear & Bright		-----	
1294		-----		-----	
1429	E2680	Pass		-----	
1467	Visual	Clear		-----	
1530	Visual	clear & bright		-----	
1669		-----		-----	
1741		-----		-----	
1790		-----		-----	
1823		-----		-----	
1852	Visual	clear &colourless		-----	
1880	Visual	Pass		-----	
1954	Visual	clear colorless liquid		-----	
2301		-----		-----	
6134	Visual	CLEAR & BRIGHT		-----	
6198		-----		-----	
6203		-----		-----	
6262	Visual	Clear and Bright		-----	
9008	Visual	Clear Liquid		-----	
	n	30			
	mean (n)	Pass (Clear & Bright)			

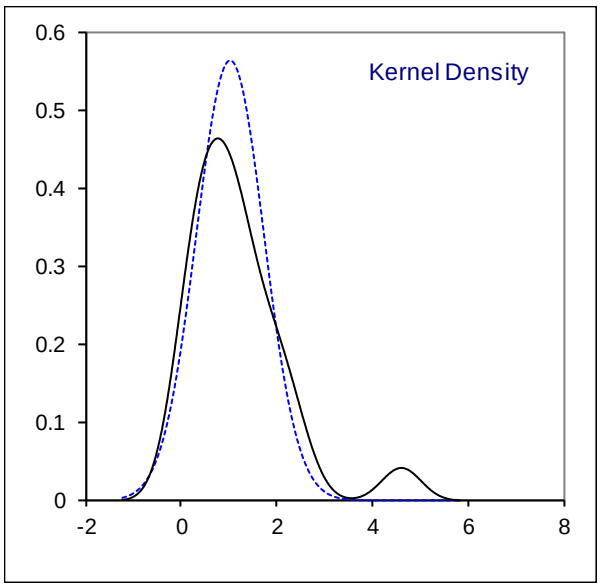
Abbreviation
C&B = Clear and Bright
CFSM/CFFSM = Clear and Free from suspended matter

Determination of Bromine Index on sample #20010; results in mg Br/100g

lab	method	value	mark	z(targ)	remarks
52	D1492	<1		-----	
150	D1492	2		0.59	
311	D5776	<0.5		-----	
317	D5776	<0.5		-----	
323	D5776	0.5		-0.32	
334	D5776	0.04		-0.60	
347		-----		-----	
357	D5776	1.3		0.17	
444	D5776	0.133		-0.54	
445	D2710	1.65		0.38	
551		-----		-----	
555		-----		-----	
663	D5776	0.85		-0.11	
704	D5776	1.1		0.04	
734	D5776	0.41		-0.38	
823		-----		-----	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D1492	1		-0.02	
913		-----		-----	
962	D1492	1		-0.02	
963	D1492	1.43		0.24	
1040	D5776	0.45		-0.35	
1041		-----		-----	
1065		-----		-----	
1081	D1492	4.62	R(0.01)	2.19	
1117	D1492	< 2		-----	
1151		-----		-----	
1264	D1492	1.38		0.21	
1294		-----		-----	
1429	D2710	0.5		-0.32	
1467		-----		-----	
1530	D1492	< 1		-----	
1669		-----		-----	
1741		-----		-----	
1790	D5776	< 1		-----	
1823		-----		-----	
1852	DIN51774	0.003		-0.62	
1880	D1492	2.2		0.71	
1954	D2710	1.0		-0.02	
2301		-----		-----	
6134	D5776	0.710		-0.19	
6198		-----		-----	
6203	D5776	1.92		0.54	
6262	D5776	0.53		-0.30	
9008	D5776	2.5		0.90	

normality	OK
n	22
outliers	1
mean (n)	1.028
st.dev. (n)	0.7077
R(calc.)	1.981
st.dev.(D5776:14a)	1.6429
R(D5776:14a)	4.6

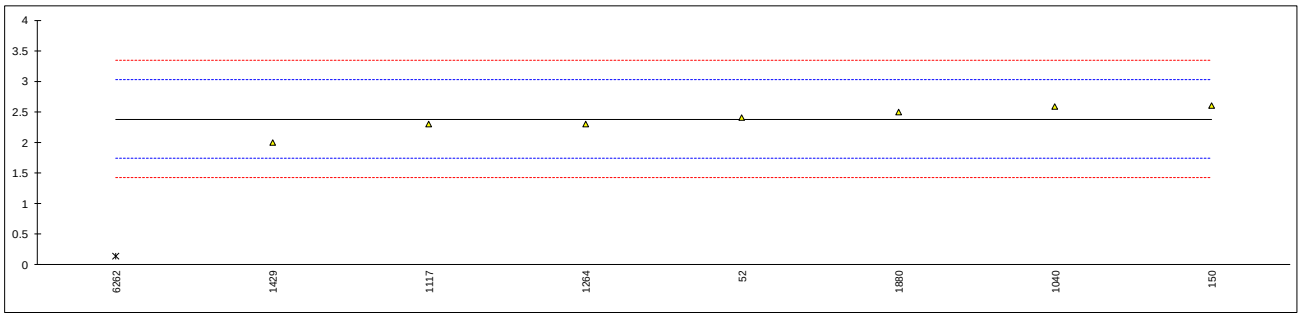

7
6
5
4
3
2
1
0
1852
334
444
734
1040
323
1429
6262
6134
663
912
962
1954
704
357
1264
963
445
6203
150
1880
9008
1081

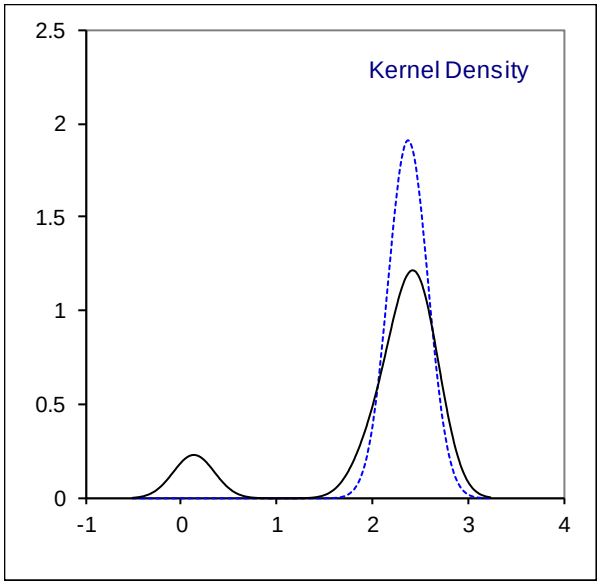

Kernel Density
0.6
0.5
0.4
0.3
0.2
0.1
0
-2
0
2
4
6
8

Determination of Total Chlorides on sample #20010; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7536	2.4		0.05	
150	D7359	2.6		0.68	
311		-----		-----	
317		-----		-----	
323		-----		-----	
334		-----		-----	
347		-----		-----	
357		-----		-----	
444		-----		-----	
445		-----		-----	
551		-----		-----	
555		-----		-----	
663		-----		-----	
704		-----		-----	
734		-----		-----	
823		-----		-----	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1040	EN14077	2.580		0.61	
1041		-----		-----	
1065		-----		-----	
1081		-----		-----	
1117	D7359	2.3		-0.26	
1151		-----		-----	
1264	D5194	2.30		-0.26	
1294		-----		-----	
1429	D7359	2.0		-1.19	
1467		-----		-----	
1530		-----		-----	
1669		-----		-----	
1741		-----		-----	
1790		-----		-----	
1823		-----		-----	
1852		-----		-----	
1880	D7359	2.5		0.36	
1954		-----		-----	
2301		-----		-----	
6134		-----		-----	
6198		-----		-----	
6203	D5194	<1		<-4.30	possibly a false negative test result?
6262	D5194	0.14	C,G(0.01)	-6.98	first reported: 0.11
9008		-----		-----	

normality	unknown
n	7
outliers	1
mean (n)	2.383
st.dev. (n)	0.2083
R(calc.)	0.583
st.dev.(D5194:18)	0.3214
R(D5194:18)	0.9

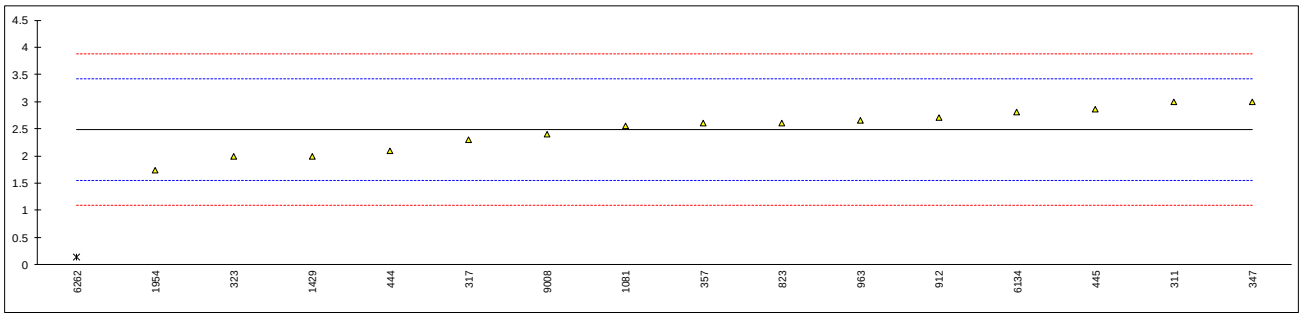

4
3.5
3
2.5
2
1.5
1
0.5
0
6262
1429
1117
1264
52
1880
1040
150

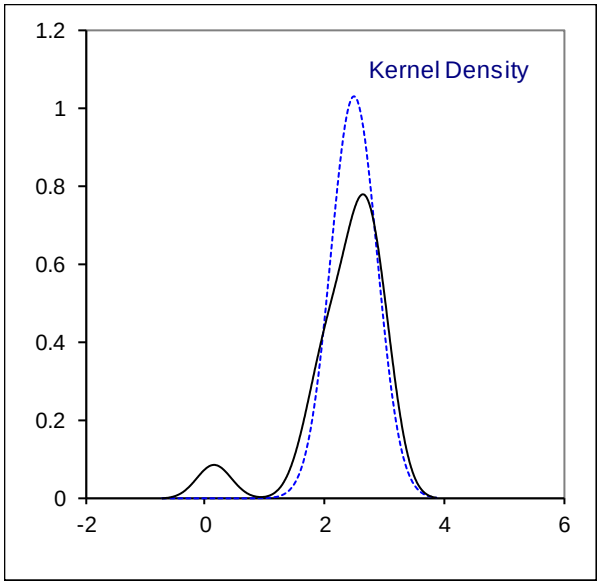

Kernel Density
2.5
2
1.5
1
0.5
0
-1
0
1
2
3
4

Determination of Organic Chlorides on sample #20010; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52		-----		-----	
150		-----		-----	
311	UOP779	3		1.11	
317	UOP779	2.3		-0.40	
323	D5808	2		-1.05	
334		-----		-----	
347	D4929B	3		1.11	
357	D5808	2.6		0.25	
444	IP510	2.1		-0.83	
445	IP510	2.86		0.81	
551		-----		-----	
555		-----		-----	
663		-----		-----	
704		-----		-----	
734		-----		-----	
823	D5808	2.6		0.25	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D5808	2.7		0.46	
913		-----		-----	
962		-----		-----	
963	D5808	2.65	C	0.35	first reported: 1
1040		-----		-----	
1041		-----		-----	
1065		-----		-----	
1081	D5808	2.55		0.14	
1117		-----		-----	
1151		-----		-----	
1264		-----		-----	
1294		-----		-----	
1429	D7359	2.0		-1.05	
1467		-----		-----	
1530		-----		-----	
1669		-----		-----	
1741		-----		-----	
1790		-----		-----	
1823		-----		-----	
1852		-----		-----	
1880		-----		-----	
1954	D5808	1.73		-1.63	
2301		-----		-----	
6134	D4929	2.80		0.68	
6198		-----		-----	
6203	D5808	<1		<-3.20	possibly a false negative test result?
6262	D5808	0.14	C,G(0.01)	-5.05	first reported: 0
9008	D5808	2.4		-0.19	

normality	OK
n	15
outliers	1
mean (n)	2.486
st.dev. (n)	0.3877
R(calc.)	1.086
st.dev.(D5808:18)	0.4643
R(D5808:18)	1.3

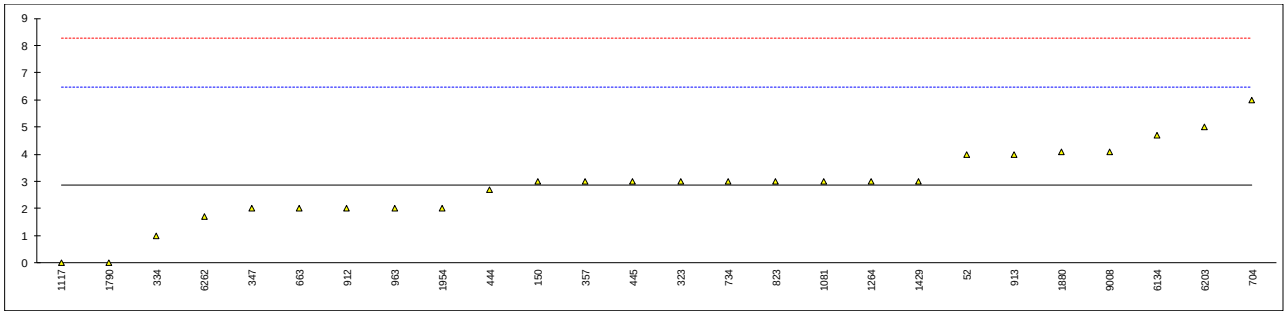

4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
6282
1954
323
1429
444
317
9008
1081
357
823
963
912
6134
445
311
347

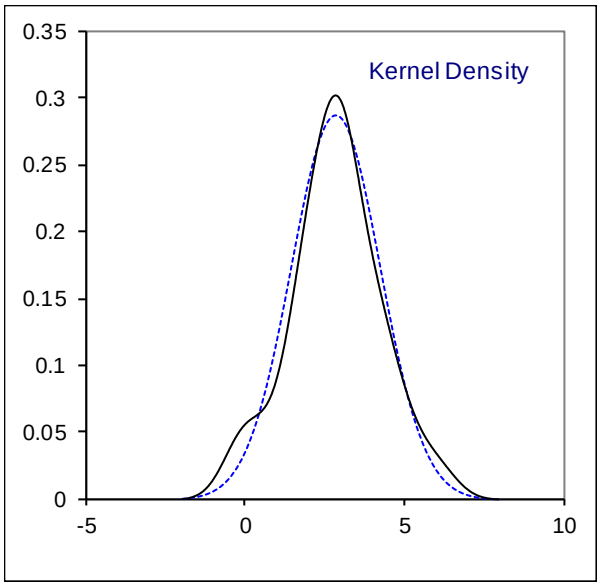

Kernel Density
1.2
1
0.8
0.6
0.4
0.2
0
-2
0
2
4
6

Determination of Color Pt/Co on sample #20010;

lab	method	value	mark	z(targ)	remarks
52	D5386	4		0.63	
150	D5386	3		0.08	
311	D1209	<5		-----	
317	D1209	<5		-----	
323	D5386	3		0.08	
334	D1209	1		-1.03	
347	D5386	2		-0.48	
357	D5386	3		0.08	
444	D5386	2.7		-0.09	
445	D1209	3.0		0.08	
551		-----		-----	
555		-----		-----	
663	D5386	2		-0.48	
704	D1209	6		1.75	
734	D1209	3		0.08	
823	D5386	3		0.08	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D5386	2		-0.48	
913	D5386	4		0.63	
962	D1209	<5		-----	
963	D1209	2		-0.48	
1040		-----		-----	
1041		-----		-----	
1065		-----		-----	
1081	D5386	3		0.08	
1117	D1209	0		-1.59	
1151		-----		-----	
1264	D1209	3		0.08	
1294		-----		-----	
1429	D1209	3		0.08	
1467		-----		-----	
1530		-----		-----	
1669		-----		-----	
1741		-----		-----	
1790	D1209	0		-1.59	
1823		-----		-----	
1852		-----		-----	
1880	D5386	4.1		0.69	
1954	D1209	2		-0.48	
2301		-----		-----	
6134	D1209	4.7		1.02	
6198		-----		-----	
6203	D1209	5.0		1.19	
6262	D5386	1.7		-0.64	
9008	D5386	4.1		0.69	

	normality	OK
	n	26
	outliers	0
	mean (n)	2.86
	st.dev. (n)	1.394
	R(calc.)	3.90
	st.dev.(D5386:16)	1.801
	R(D5386:16)	5.04
Compare		
	R(D1209:05)	7

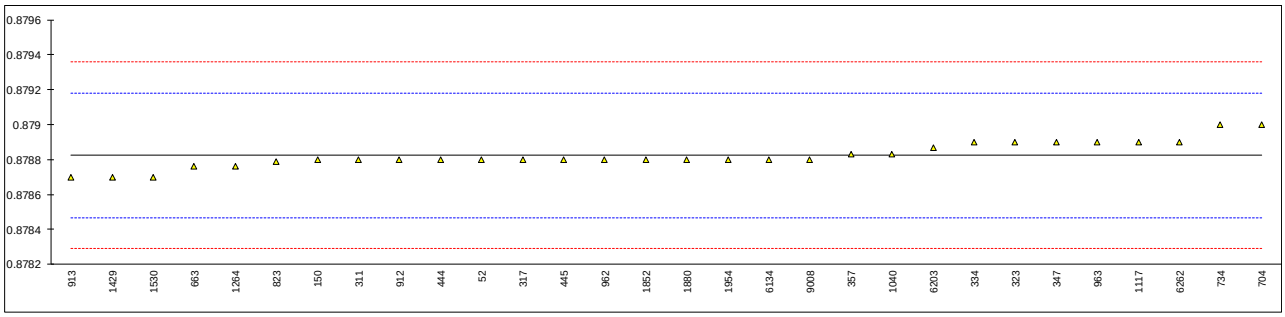

9
8
7
6
5
4
3
2
1
0
1117
1790
334
6262
347
663
912
963
1954
444
150
357
445
323
734
823
1081
1264
1429
52
913
1880
9008
6134
6203
704

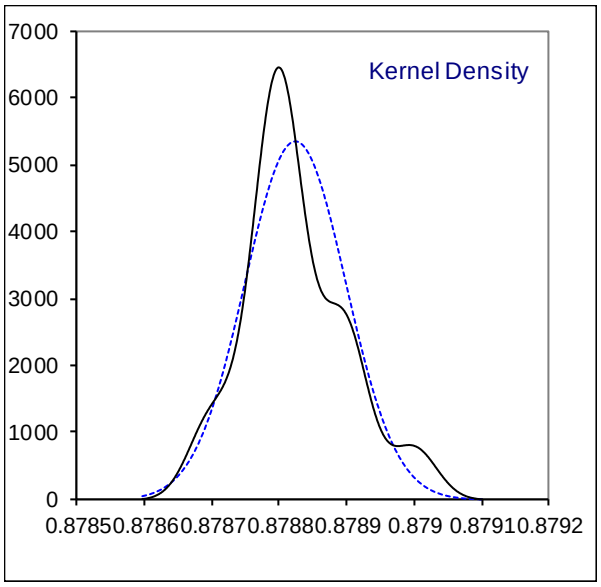

Kernel Density
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-5
0
5
10

Determination of Density at 20°C on sample #20010; results in kg/L

lab	method	value	mark	z(targ)	remarks
52	D4052	0.8788		-0.14	
150	D4052	0.8788		-0.14	
311	D4052	0.8788		-0.14	
317	D4052	0.8788		-0.14	
323	D4052	0.8789		0.42	
334	ISO12185	0.8789		0.42	
347	D4052	0.8789		0.42	
357	D4052	0.87883		0.03	
444	D4052	0.8788		-0.14	
445	D4052	0.8788		-0.14	
551		-----		-----	
555		-----		-----	
663	D4052	0.87876		-0.36	
704	ISO12185	0.8790		0.98	
734	D4052	0.8790		0.98	
823	D4052	0.87879		-0.20	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D4052	0.8788		-0.14	
913	D4052	0.8787		-0.70	
962	D4052	0.8788		-0.14	
963	ISO12185	0.8789		0.42	
1040	ISO12185	0.87883		0.03	
1041		-----		-----	
1065		-----		-----	
1081		-----		-----	
1117	D4052	0.8789		0.42	
1151		-----		-----	
1264	D4052	0.87876		-0.36	
1294		-----		-----	
1429	D4052	0.8787		-0.70	
1467		-----		-----	
1530	ISO12185	0.87870		-0.70	
1669		-----		-----	
1741		-----		-----	
1790		-----		-----	
1823		-----		-----	
1852	ISO12185	0.8788		-0.14	
1880	D4052	0.8788		-0.14	
1954	D4052	0.8788		-0.14	
2301		-----		-----	
6134	D4052	0.8788		-0.14	
6198		-----		-----	
6203	ISO12185	0.87887		0.25	
6262	ISO12185	0.8789		0.42	
9008	D4052	0.8788		-0.14	

normality	OK
n	30
outliers	0
mean (n)	0.87882
st.dev. (n)	0.000075
R(calc.)	0.00021
st.dev.(ISO12185:96)	0.000179
R(ISO12185:96)	0.0005

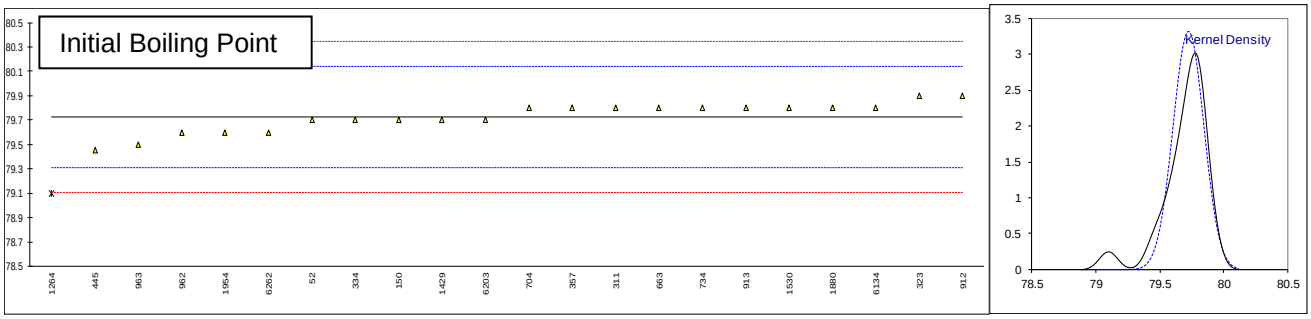

0.8796
0.8794
0.8792
0.879
0.8788
0.8786
0.8784
0.8782
913
1429
1530
663
1264
823
150
311
912
444
52
317
445
962
1852
1880
1954
6134
9008
357
1040
6203
334
323
347
963
1117
6262
734
704

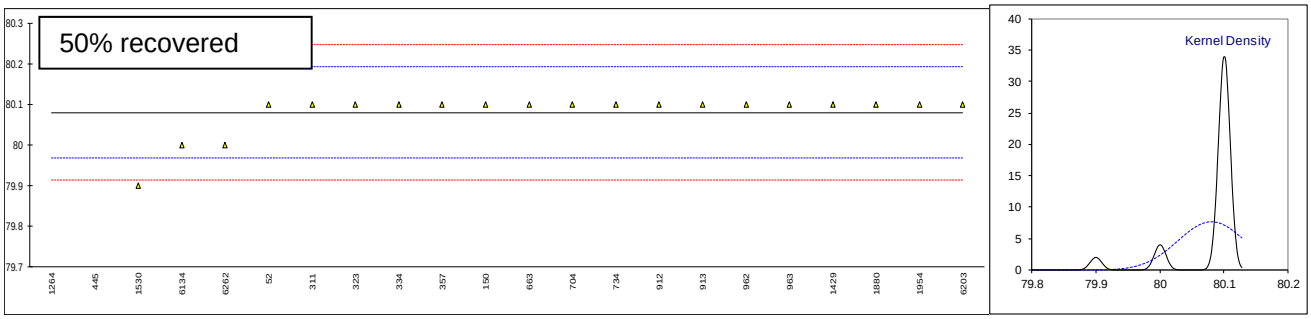

Kernel Density
7000
6000
5000
4000
3000
2000
1000
0
0.8785
0.8786
0.8787
0.8788
0.8789
0.879
0.8791
0.8792

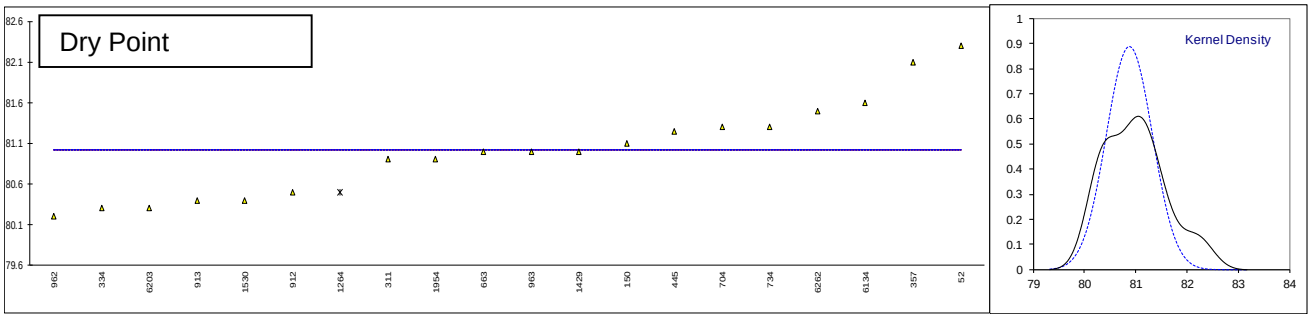
Determination of Distillation on sample #20010; results in °C

lab	method	IBP	mark	z(targ)	50%	mark	z(targ)	DP	mark	z(targ)	range	mark
52	D850-automated	79.7		-0.13	80.1		0.36	82.3		-----	2.6	
150	D850-automated	79.7		-0.13	80.1		0.36	81.1		-----	1.4	
311	D850-automated	79.8		0.36	80.1		0.36	80.9		-----	1.1	
317		-----		-----	-----		-----	-----		-----	-----	
323	D850-automated	79.9		0.84	80.1		0.36	-----		-----	-----	
334	D850-automated	79.7		-0.13	80.1		0.36	80.3		-----	0.6	
347		-----		-----	-----		-----	-----		-----	-----	
357	D850-automated	79.8		0.36	80.1		0.36	82.1		-----	2.3	
444		-----		-----	-----		-----	-----		-----	-----	
445	D850-manual	79.45		-1.33	79.65	R(1)	-7.72	81.25		-----	1.8	
551		-----		-----	-----		-----	-----		-----	-----	
555		-----		-----	-----		-----	-----		-----	-----	
663	D850-automated	79.8		0.36	80.1		0.36	81.0		-----	1.2	
704	D850-manual	79.8		0.36	80.1		0.36	81.3	C	-----	2.0	
734	D850-automated	79.8		0.36	80.1		0.36	81.3		-----	1.5	
823		-----		-----	-----		-----	-----		-----	-----	
846		-----		-----	-----		-----	-----		-----	-----	
852		-----		-----	-----		-----	-----		-----	-----	
855		-----		-----	-----		-----	-----		-----	-----	
862		-----		-----	-----		-----	-----		-----	-----	
864		-----		-----	-----		-----	-----		-----	-----	
866		-----		-----	-----		-----	-----		-----	-----	
868		-----		-----	-----		-----	-----		-----	-----	
870		-----		-----	-----		-----	-----		-----	-----	
912	D1078	79.9		0.84	80.1		0.36	80.5		-----	0.6	
913	D850-manual	79.8		0.36	80.1		0.36	80.4		-----	0.6	
962	D850-automated	79.6		-0.61	80.1		0.36	80.2		-----	0.6	
963	D850-automated	79.5		-1.09	80.1		0.36	81.0		-----	1.5	
1040		-----		-----	-----		-----	-----		-----	-----	
1041		-----		-----	-----		-----	-----		-----	-----	
1065		-----		-----	-----		-----	-----		-----	-----	
1081		-----		-----	-----		-----	-----		-----	-----	
1117		-----		-----	-----		-----	-----		-----	-----	
1151		-----		-----	-----		-----	-----		-----	-----	
1264	D850-automated	79.1	R(1)	-3.02	79.6	R(1)	-8.62	80.5	ex	-----	1.4	
1294		-----		-----	-----		-----	-----		-----	-----	
1429	D850-automated	79.7		-0.13	80.1		0.36	81.0		-----	1.3	
1467		-----		-----	-----		-----	-----		-----	-----	
1530	D850-automated	79.80		0.36	79.90		-3.23	80.40		-----	0.60	
1669		-----		-----	-----		-----	-----		-----	-----	
1741		-----		-----	-----		-----	-----		-----	-----	
1790		-----		-----	-----		-----	-----		-----	-----	
1823		-----		-----	-----		-----	-----		-----	-----	
1852		-----		-----	-----		-----	-----		-----	-----	
1880	D850-automated	79.8		0.36	80.1		0.36	-----		-----	-----	
1954	D850-automated	79.6		-0.61	80.1		0.36	80.9		-----	-----	
2301		-----		-----	-----		-----	-----		-----	-----	
6134	D850-manual	79.8		0.36	80.0		-1.44	81.6	C	-----	2.7	
6198		-----		-----	-----		-----	-----		-----	-----	
6203	D850-manual	79.7		-0.13	80.1		0.36	80.3		-----	0.6	
6262	D850-automated	79.6	C	-0.61	80.0	C	-1.44	81.5	C	-----	1.9	C
9008		-----		-----	-----		-----	-----		-----	-----	
	normality	OK			not OK			OK				
	n	21			20			19				
	outliers	1			2			0+1ex				
	mean (n)	79.73			80.08			81.02				
	st.dev. (n)	0.120			0.052			0.595				
	R(calc.)	0.34			0.15			1.67				
	st.dev.(D850-A:18e1)	0.208			0.056			(0.163)				
	R(D850-A:18e1)*)	0.58			0.16			(0.46)				
Compare												
	R(D850-M:18e1)	0.41			0.65			(0.65)				

Lab 704 first reported: 81.8
Lab 6134 first reported: 82.5
Lab 6262 reported: 80.0 for IBP, 81.6 for DP and 1.6 for Distillation range, first reported: 80.3 for 50% recovered
ex = test result excluded as the other reported test results are statistical outliers.
*) precision data of Toluene is used


Initial Boiling Point
Kernel Density


50% recovered
Kernel Density


Dry Point
Kernel Density

Determination of Total Nitrogen on sample #20010; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7184	<0.1		-----	
150	D7184	<0.10		-----	
311	D7184	<0.10		-----	
317	D4629	<0.3		-----	
323	D6069	< 1		-----	
334	D4629	<0.3		-----	
347	D4629	<1		-----	
357	D4629	<0,3		-----	
444	D4629	0.2892		-----	
445	D4629	<0.3		-----	
551		-----		-----	
555		-----		-----	
663	D4629	<0.3		-----	
704	D4629	<0.3	C	-----	first reported: 0.48
734	D7184	0.20		-----	
823	D7184	0.413		-----	possibly a false positive test result?
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962		-----		-----	
963	D7184	<0.1		-----	
1040	D6069	0.029		-----	
1041		-----		-----	
1065		-----		-----	
1081		-----		-----	
1117	D7184	0.02		-----	
1151		-----		-----	
1264	D7184	0.22		-----	
1294		-----		-----	
1429	D4629	0.07		-----	
1467		-----		-----	
1530	D4629	< 0,5		-----	
1669		-----		-----	
1741		-----		-----	
1790	D6069	0.07		-----	
1823		-----		-----	
1852	DIN51444	< 0,1		-----	
1880	D6069	0.1		-----	
1954	D4629	0.10		-----	
2301		-----		-----	
6134	D6069	0.14		-----	
6198		-----		-----	
6203		-----		-----	
6262	D7184	0		-----	
9008	D6069	<0.1		-----	
	n	23			
	mean (n)	<0.3			Application range D7184:19: 0.1 – 1.2 mg/kg

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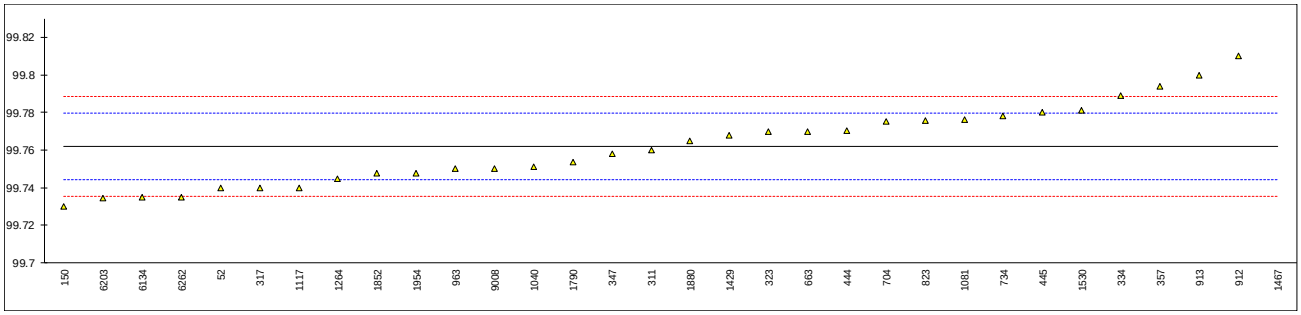
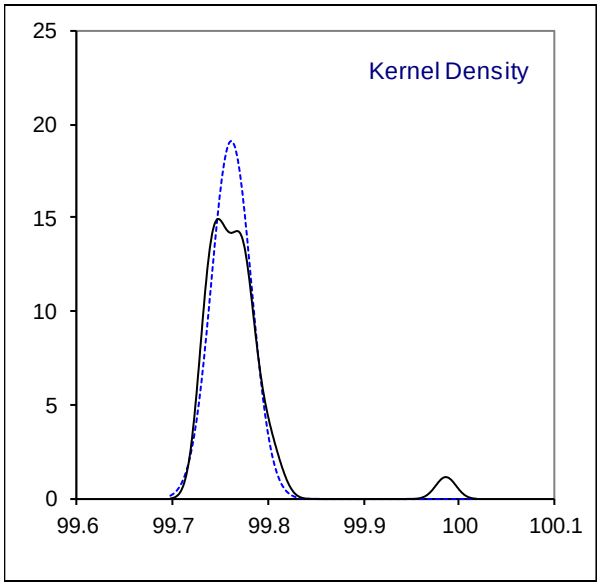
Determination of Purity by GC on sample #20010; results in %M/M

lab	method	value	mark	z(targ)	remarks
52	D7504	99.74		-2.49	
150	D7504	99.73		-3.62	
311	D7504	99.76		-0.22	
317	D7504	99.74		-2.49	
323	D7504	99.77		0.92	
334	D4492	99.789		3.07	
347	D4492	99.758		-0.45	
357	D7504	99.794		3.64	
444	D4492	99.7702		0.94	
445	D4492	99.7801		2.06	
551		-----		-----	
555		-----		-----	
663	D4492	99.77	C	0.92	first reported: 99.854
704	D7504	99.775		1.48	
734	D7504	99.778		1.82	
823	D7360	99.7755		1.54	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D7504	99.81		5.45	
913	D7504	99.80		4.32	
962		-----		-----	
963	D4492	99.75	C	-1.35	first reported: 99.84
1040	D4492	99.7513		-1.21	
1041		-----		-----	
1065		-----		-----	
1081	D4492	99.776		1.60	
1117	D4492	99.74		-2.49	
1151		-----		-----	
1264	D7504	99.745		-1.92	
1294		-----		-----	
1429	D7504	99.768		0.69	
1467	In house	99.987	C,R(0.01)	25.53	first reported: 99.998
1530	D7504	99.781		2.16	
1669		-----		-----	
1741		-----		-----	
1790	D4492	99.7535		-0.96	
1823		-----		-----	
1852	D7504	99.7478		-1.60	
1880	D4492	99.765		0.35	
1954	D7504	99.74797		-1.58	
2301		-----		-----	
6134	D4492	99.7348		-3.08	
6198		-----		-----	
6203	D7504	99.7343		-3.13	
6262	D7504	99.7352		-3.03	
9008	D4492	99.75		-1.35	

normality	OK
n	31
outliers	1
mean (n)	99.76192
st.dev. (n)	0.020909
R(calc.)	0.05855
st.dev.(D7504:20)	0.008815
R(D7504:20)	0.02468

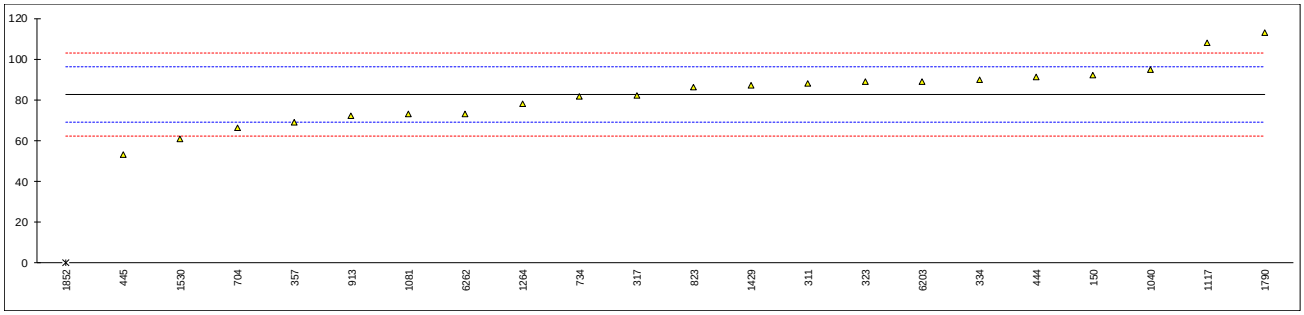

99.82
99.8
99.78
99.76
99.74
99.72
99.7
150
6203
6134
6262
52
317
1117
1264
1852
1954
963
9008
1040
1790
347
311
1880
1429
323
663
444
704
823
1081
734
445
1530
334
357
913
912
1467

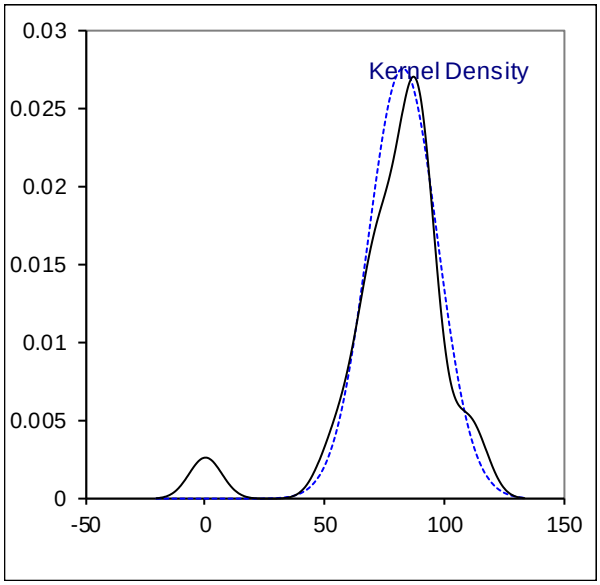

Kernel Density
25
20
15
10
5
0
99.6
99.7
99.8
99.9
100
100.1

Determination of Methylcyclohexane on sample #20010 in mg/kg

lab	method	value	mark	z(targ)	remarks
52		-----		-----	
150	D5713	92		1.36	
311	D7504	88		0.78	
317	D7504	82		-0.11	
323	D7504	89		0.92	
334	D4492	90	C	1.07	first reported: 230
347		-----		-----	
357	D7504	69		-2.01	
444	D5713	91		1.22	
445	D4492	53		-4.36	
551		-----		-----	
555		-----		-----	
663		-----		-----	
704	INH-0041	66.4		-2.40	
734	D7504	81.7		-0.15	
823	D5713	86		0.48	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913	D7504	72		-1.57	
962		-----		-----	
963		-----		-----	
1040	D4492	95		1.80	
1041		-----		-----	
1065		-----		-----	
1081	D4492	73		-1.43	
1117	D4492	108		3.71	
1151		-----		-----	
1264	D4492	78		-0.69	
1294		-----		-----	
1429	D7504	87		0.63	
1467		-----		-----	
1530	D7504	61		-3.19	
1669		-----		-----	
1741		-----		-----	
1790	D4492	113		4.45	
1823		-----		-----	
1852	D7504	0.0188	R(0.01)	-12.15	
1880		-----		-----	
1954		-----		-----	
2301		-----		-----	
6134		-----		-----	
6198		-----		-----	
6203	D7504	89		0.92	
6262	D7504	73		-1.43	
9008		-----		-----	

normality	OK
n	21
outliers	1
mean (n)	82.72
st.dev. (n)	14.470
R(calc.)	40.52
st.dev.(Horwitz)	6.809
R(Horwitz)	19.07

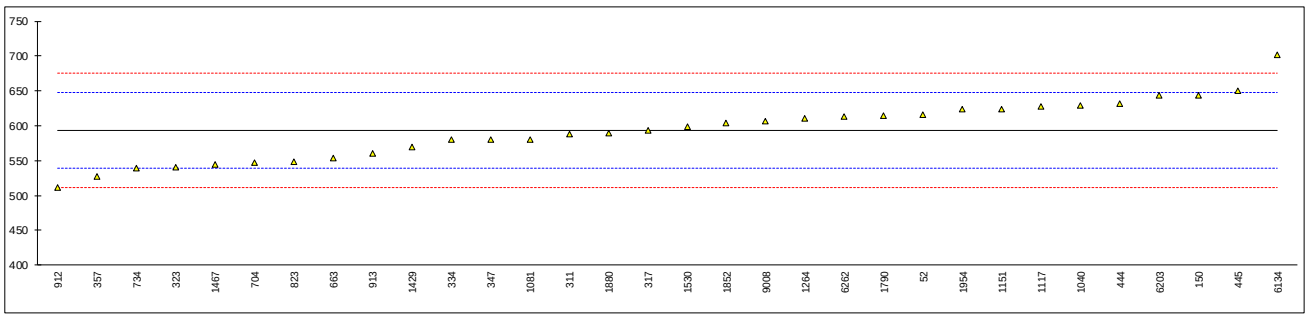

120
100
80
60
40
20
0
1852
445
1530
704
357
913
1081
6262
1264
734
317
823
1429
311
323
6203
334
444
150
1040
1117
1790

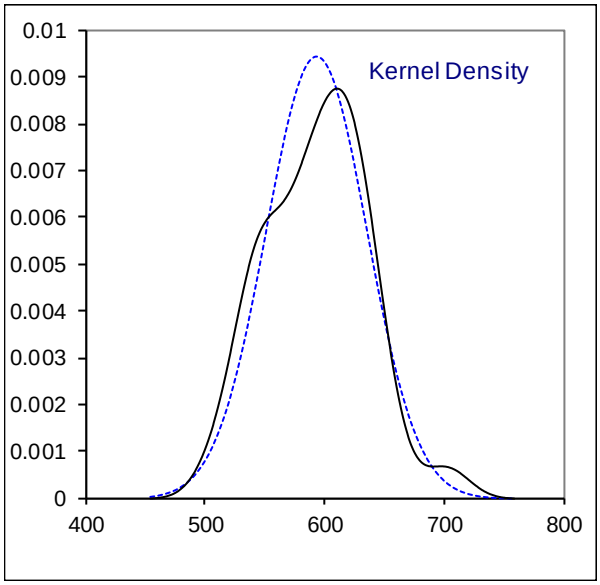

0.03
0.025
0.02
0.015
0.01
0.005
0
-50
0
50
100
150
Kernel Density

Determination of Toluene on sample #20010; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7504	616		0.83	
150	D7504	644		1.86	
311	D7504	588		-0.20	
317	D7504	593		-0.01	
323	D7504	541		-1.92	
334	D4492	580		-0.49	
347	D4492	580		-0.49	
357	D7504	527		-2.44	
444	D5713	631		1.38	
445	D4492	650		2.08	
551		-----		-----	
555		-----		-----	
663	D4492	553		-1.48	
704	D7504	546.6		-1.72	
734	D7504	538.8		-2.01	
823	D7360	548		-1.67	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D7504	511		-3.03	
913	D7504	560		-1.23	
962		-----		-----	
963	D4492	<10		<-21.45	possibly a false negative test result?
1040	D4492	629		1.31	
1041		-----		-----	
1065		-----		-----	
1081	D4492	580		-0.49	
1117	D4492	628		1.27	
1151	In house	623.72	C	1.12	first reported: 923.72
1264	D7504	610		0.61	
1294		-----		-----	
1429	D7504	570		-0.86	
1467	In house	543.8		-1.82	
1530	D7504	598		0.17	
1669		-----		-----	
1741		-----		-----	
1790	D4492	615		0.80	
1823		-----		-----	
1852	D7504	604	C	0.39	reported 0.0604 mg/kg
1880	D4492	590		-0.12	
1954	D7504	623.5		1.11	
2301		-----		-----	
6134	D4492	702.055		4.00	
6198		-----		-----	
6203	D7504	643		1.83	
6262	D7504	613		0.72	
9008	D4492	607		0.50	

normality	OK
n	32
outliers	0
mean (n)	593.36
st.dev. (n)	42.198
R(calc.)	118.15
st.dev.(D7504:20)	27.200
R(D7504:20)	76.16

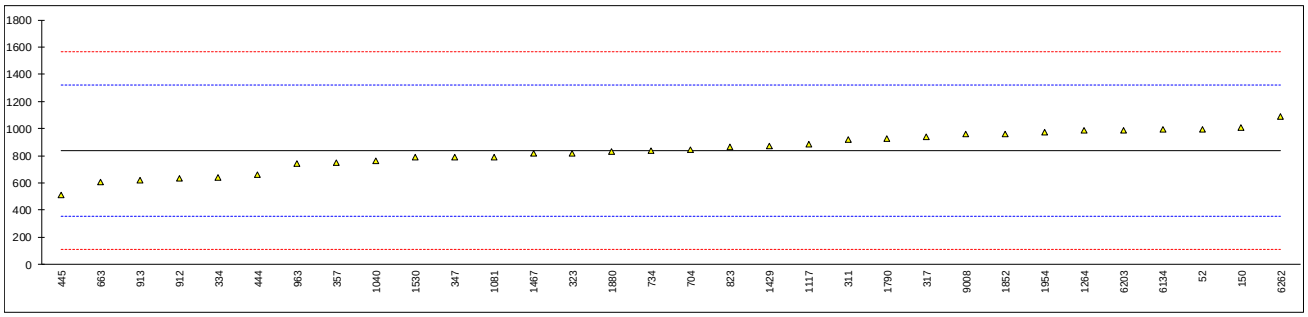

750
700
650
600
550
500
450
400
912
357
734
323
1467
704
823
663
913
1429
334
347
1081
311
1880
317
1530
1852
9008
1264
6262
1790
52
1954
1151
1117
1040
444
6203
150
445
6134

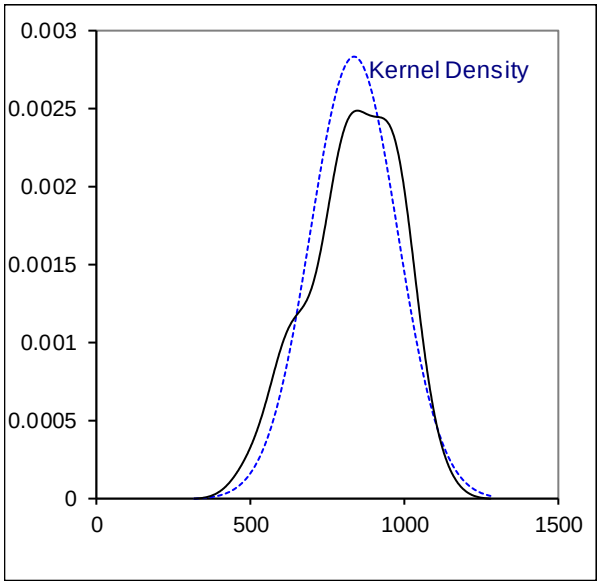

Kernel Density
0.01
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
400
500
600
700
800

Determination of Nonaromatics on sample #20010; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7504	995		0.65	
150	D7504	1009		0.71	
311	D7504	920		0.34	
317	D7504	942		0.43	
323	D7504	819		-0.08	
334	D4492	640		-0.81	
347	D4492	790		-0.20	
357	D7504	748		-0.37	
444	D4492	661		-0.73	
445	D4492	510		-1.35	
551		-----		-----	
555		-----		-----	
663	D4492	606		-0.95	
704	D7504	841.7		0.02	
734	D7504	836.8		0.00	
823	D7360	866		0.12	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D7504	631		-0.85	
913	D7504	620		-0.90	
962		-----		-----	
963	D4492	740		-0.40	
1040	D4492	760		-0.32	
1041		-----		-----	
1065		-----		-----	
1081	D4492	792		-0.19	
1117	D4492	887		0.20	
1151		-----		-----	
1264	D7504	984		0.60	
1294		-----		-----	
1429	D7504	870		0.13	
1467	In house	818		-0.08	
1530	D7504	787		-0.21	
1669		-----		-----	
1741		-----		-----	
1790	D4492	925		0.36	
1823		-----		-----	
1852	D7504	962	C	0.51	first reported: 0.061 mg/kg
1880	D4492	832		-0.02	
1954	D7504	975		0.57	
2301		-----		-----	
6134	D4492	993.505		0.64	
6198		-----		-----	
6203	D7504	988		0.62	
6262	D7504	1089		1.04	
9008	D4492	960		0.51	

normality	OK
n	32
outliers	0
mean (n)	837.44
st.dev. (n)	141.097
R(calc.)	395.07
st.dev.(D7504:20)	242.654
R(D7504:20)	679.43


1800
1600
1400
1200
1000
800
600
400
200
0
445
663
913
912
334
444
963
357
1040
1530
347
1081
1467
323
1880
734
704
823
1429
1117
311
1790
317
9008
1852
1954
1264
6203
6134
52
150
6262


0.003
0.0025
0.002
0.0015
0.001
0.0005
0
0
500
1000
1500
Kernel Density

Determination of 1,4-Dioxane on sample #20010; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7504	7		-----	
150		-----		-----	
311	D7504	<6		-----	
317	D7504	<2		-----	
323	D7504	< 2		-----	
334		-----		-----	
347		-----		-----	
357	D7504	< 2		-----	
444		-----		-----	
445	D4492	<5		-----	
551		-----		-----	
555		-----		-----	
663	UOP921	<1		-----	
704	D7504	< 2		-----	
734	D7504	<2		-----	
823	D7360	<2.7		-----	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D7504	<10		-----	
913		-----		-----	
962		-----		-----	
963	D4492	<10		-----	
1040		-----		-----	
1041		-----		-----	
1065		-----		-----	
1081		-----		-----	
1117		-----		-----	
1151		-----		-----	
1264	D7504	8		-----	
1294		-----		-----	
1429		-----		-----	
1467		-----		-----	
1530		-----		-----	
1669		-----		-----	
1741		-----		-----	
1790		-----		-----	
1823		-----		-----	
1852		-----		-----	
1880		-----		-----	
1954		-----		-----	
2301		-----		-----	
6134	D4492	11.14		-----	possibly a false positive test result?
6198		-----		-----	
6203	D7504	0		-----	
6262	D7504	3		-----	
9008		-----		-----	
	n	15			
	mean (n)	<10			

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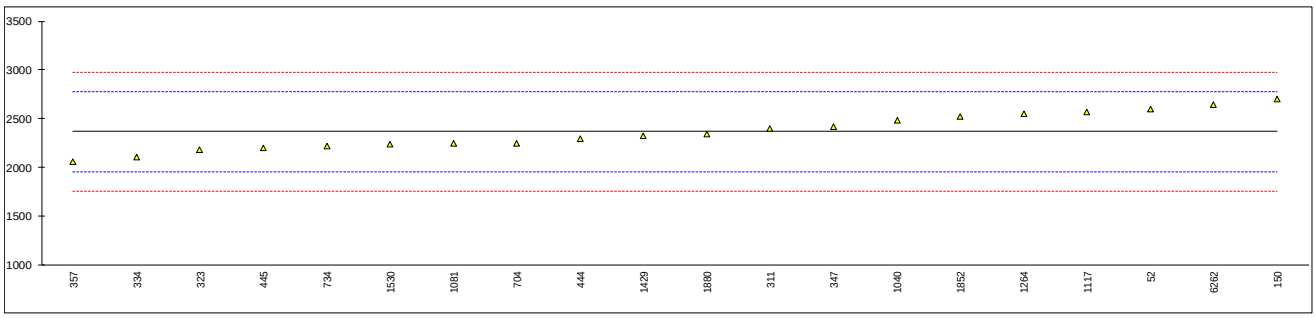
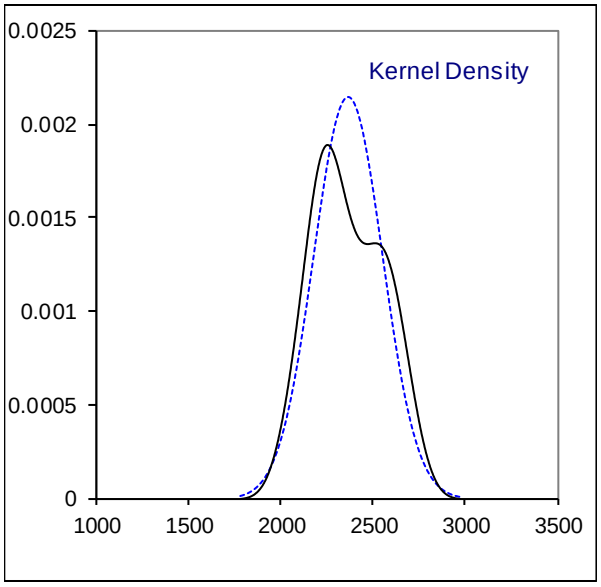
Determination of Total Impurities on sample #20010; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7504	2600		1.14	
150	D7504	2700		1.63	
311	D7504	2400		0.16	
317		-----		-----	
323	D7504	2181		-0.92	
334	D4492	2110		-1.27	
347	D4492	2420		0.26	
357	D7504	2060		-1.51	
444	D4492	2298		-0.34	
445	D4492	2199		-0.83	
551		-----		-----	
555		-----		-----	
663		-----		-----	
704	D7504	2247.6		-0.59	
734	D7504	2220.5		-0.72	
823		-----		-----	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1040	D6526	2487		0.58	
1041		-----		-----	
1065		-----		-----	
1081	D4492	2244		-0.61	
1117	D4492	2570		0.99	
1151		-----		-----	
1264	D7504	2550	C	0.89	first reported: 0.255
1294		-----		-----	
1429	D7504	2320		-0.24	
1467		-----		-----	
1530	D7504	2237		-0.64	
1669		-----		-----	
1741		-----		-----	
1790		-----		-----	
1823		-----		-----	
1852	D7504	2522	C	0.76	reported 0.2522 mg/kg
1880	D4492	2344		-0.12	
1954		-----		-----	
2301		-----		-----	
6134		-----		-----	
6198		-----		-----	
6203		-----		-----	
6262	D7504	2648		1.37	
9008		-----		-----	

normality	OK
n	20
outliers	0
mean (n)	2367.91
st.dev. (n)	186.309
R(calc.)	521.66
st.dev.(Horwitz 3 comp)	203.776
R(Horwitz 3 comp)	570.57

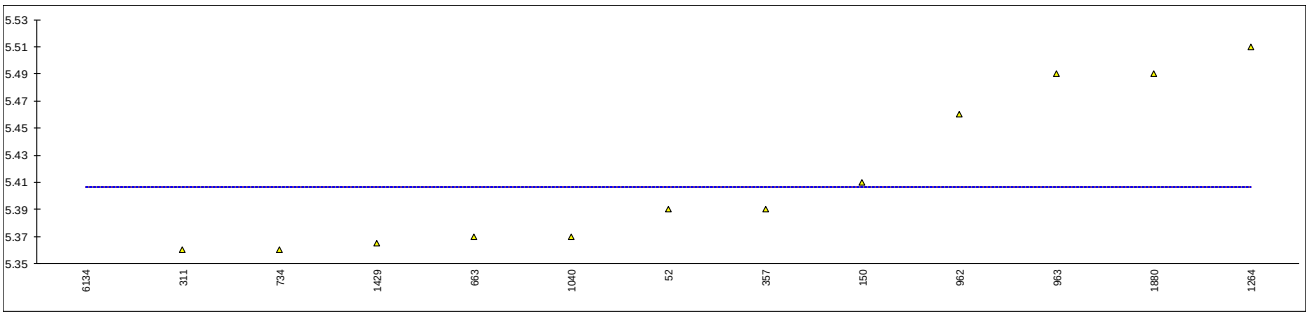

3500
3000
2500
2000
1500
1000
357
334
323
445
734
1530
1081
704
444
1429
1880
311
347
1040
1852
1264
1117
52
6262
150

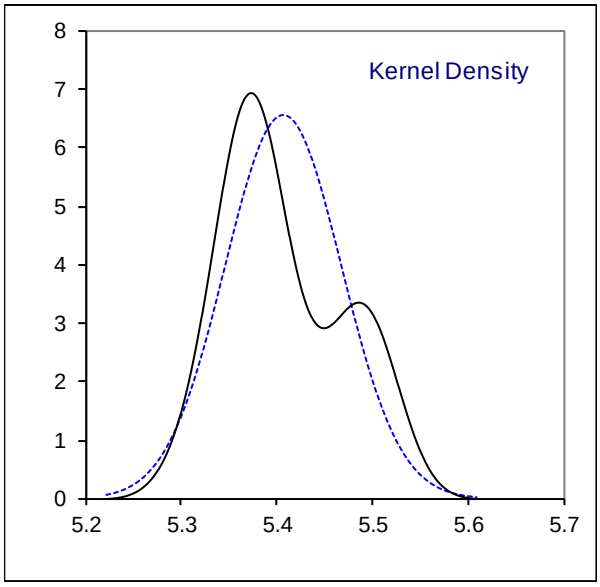

Kernel Density
0.0025
0.002
0.0015
0.001
0.0005
0
1000
1500
2000
2500
3000
3500

Determination of Solidification Point (anhydrous basis) on sample #20010; results in °C

lab	method	value	mark	z(targ)	remarks
52	D852	5.39		-----	
150	D852	5.41		-----	
311	D852	5.36		-----	
317		-----		-----	
323		-----		-----	
334		-----		-----	
347		-----		-----	
357	D852	5.39		-----	
444		-----		-----	
445		-----		-----	
551		-----		-----	
555		-----		-----	
663	D852	5.37		-----	
704		-----		-----	
734	D852	5.36		-----	
823		-----		-----	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962	D852	5.46		-----	
963	D852	5.49		-----	
1040	DIN51798	5.37		-----	
1041		-----		-----	
1065		-----		-----	
1081		-----		-----	
1117		-----		-----	
1151		-----		-----	
1264	D852	5.51		-----	
1294		-----		-----	
1429		5.365		-----	
1467		-----		-----	
1530		-----		-----	
1669		-----		-----	
1741		-----		-----	
1790		-----		-----	
1823		-----		-----	
1852		-----		-----	
1880	D852	5.49		-----	
1954		-----		-----	
2301		-----		-----	
6134	D852	5.32	C	-----	first reported: 5.55
6198		-----		-----	
6203		-----		-----	
6262		-----		-----	
9008		-----		-----	

normality	OK
n	13
outliers	0
mean (n)	5.407
st.dev. (n)	0.0607
R(calc.)	0.170
st.dev.(D852:16)	(0.0179)
R(D852:16)	(0.05)


5.53
5.51
5.49
5.47
5.45
5.43
5.41
5.39
5.37
5.35
6134
311
734
1429
663
1040
52
357
150
962
963
1880
1264


Kernel Density
8
7
6
5
4
3
2
1
0
5.2
5.3
5.4
5.5
5.6
5.7

Determination of Sulfur on sample #20010; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7183	0.08		-----	
150	D7183	<0.03		-----	
311	D7183	<0.10		-----	
317	D5453	<1.0		-----	
323	D5453	< 1		-----	
334	D5453	<0.5		-----	
347	D5453	<1		-----	
357	D5453	<1		-----	
444	D7183	0.2622		-----	
445	D5453	<1		-----	
551		-----		-----	
555		-----		-----	
663	D5453	<1.0		-----	
704	D5453	< 1		-----	
734	D7183	0.07		-----	
823	D7183	0.313		-----	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D5453	<1		-----	
913	D5453	<1		-----	
962		-----		-----	
963	D7183	<0.5		-----	
1040	ISO20846	<0,1		-----	
1041		-----		-----	
1065		-----		-----	
1081	D7183	0.05		-----	
1117	D5453	< 0.1		-----	
1151		-----		-----	
1264	D5453	0.05		-----	
1294		-----		-----	
1429	D5453	0.13		-----	
1467	In house	<0.1		-----	
1530	D5453	< 0,5		-----	
1669		-----		-----	
1741		-----		-----	
1790	D5453	0.02		-----	
1823		-----		-----	
1852	ISO20846	0.07		-----	
1880	D5453	<0.1		-----	
1954	D7183	0.10		-----	
2301		-----		-----	
6134	D5453	0.12		-----	
6198		-----		-----	
6203	D5453	<1		-----	
6262	D7183	0		-----	
9008	D5453	<0.1		-----	
	n	32			
	mean (n)	<1			Application range ASTM D5453: 1 – 8000 mg/kg

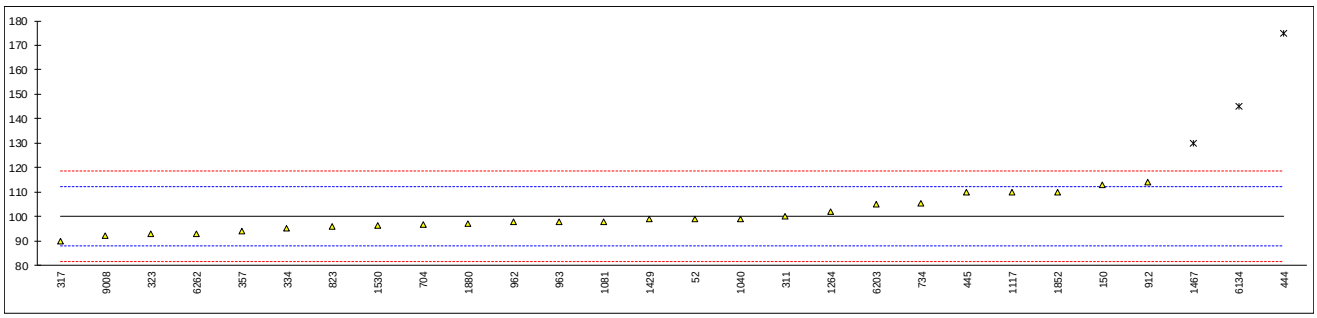
Determination of Thiophene on sample #20010; results in mg/kg

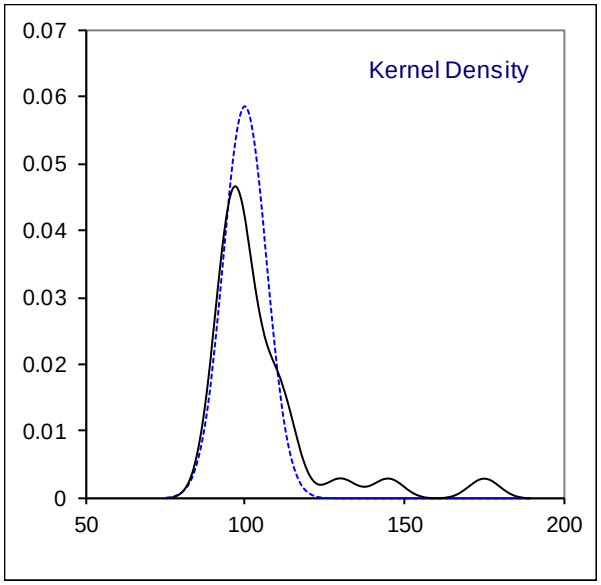
lab	method	value	mark	z(targ)	remarks
52		-----		-----	
150	D4735	<0.8		-----	
311		-----		-----	
317		-----		-----	
323	In house	< 0.1		-----	
334		-----		-----	
347		-----		-----	
357		-----		-----	
444		-----		-----	
445		-----		-----	
551		-----		-----	
555		-----		-----	
663		-----		-----	
704		-----		-----	
734		-----		-----	
823	D4735	<0.8		-----	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
1040		-----		-----	
1041		-----		-----	
1065		-----		-----	
1081		-----		-----	
1117		-----		-----	
1151		-----		-----	
1264	In house	<0.1		-----	
1294		-----		-----	
1429		-----		-----	
1467		-----		-----	
1530		-----		-----	
1669		-----		-----	
1741		-----		-----	
1790	D7011	< 0.05		-----	
1823		-----		-----	
1852		-----		-----	
1880	D4735	<0.1		-----	
1954		-----		-----	
2301		-----		-----	
6134		-----		-----	
6198		-----		-----	
6203		-----		-----	
6262	D7011	0.44		-----	
9008		-----		-----	
	n	7			
	mean (n)	<1			

Determination of Water on sample #20010; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D6304	99		-0.18	
150	E1064	113		2.11	
311	E1064	100		-0.02	
317	E1064	90		-1.65	
323	E1064	93		-1.16	
334	E1064	95		-0.84	
347		-----		-----	
357	E1064	94		-1.00	
444	E203	175	R(0.01)	12.25	
445	E1064	110		1.62	
551		-----		-----	
555		-----		-----	
663		-----		-----	
704	E1064	96.6		-0.58	
734	E1064	105.3		0.85	
823	E1064	96		-0.67	
846		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	E203	114	C	2.27	first reported: 127
913		-----		-----	
962	E1064	98		-0.35	
963	E1064	98		-0.35	
1040	DIN51777	99		-0.18	
1041		-----		-----	
1065		-----		-----	
1081	D6304	98		-0.35	
1117	D4672	110		1.62	
1151		-----		-----	
1264	E1064	102		0.31	
1294		-----		-----	
1429	ISO12937	98.8		-0.22	
1467	E1064	130	R(0.01)	4.89	
1530	E1064	96.2		-0.64	
1669		-----		-----	
1741		-----		-----	
1790		-----		-----	
1823		-----		-----	
1852	ISO12937	110	C	1.62	first reported: 125
1880	D6304	97		-0.51	
1954		-----		-----	
2301		-----		-----	
6134	E1064	145.0	C,R(0.01)	7.34	first reported: 220
6198		-----		-----	
6203	D6304	105		0.80	
6262	E1064	93		-1.16	
9008	E1064	92		-1.33	

normality	OK
n	25
outliers	3
mean (n)	100.1
st.dev. (n)	6.80
R(calc.)	19.1
st.dev.(E1064:16)	6.11
R(E1064:16)	17.1


180
170
160
150
140
130
120
110
100
90
80
317
9008
323
6262
357
334
823
1530
704
1880
962
963
1081
1429
52
1040
311
1264
6203
734
445
1117
1852
150
912
1467
6134
444


Kernel Density
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
50
100
150
200

APPENDIX 2

Number of participants per country

3 labs in	BELGIUM
2 labs in	BRAZIL
1 lab in	CANADA
10 labs in	CHINA, People's Republic
1 lab in	FINLAND
1 lab in	FRANCE
4 labs in	GERMANY
4 labs in	INDIA
1 lab in	INDONESIA
1 lab in	ISRAEL
1 lab in	KAZAKHSTAN
2 labs in	KUWAIT
4 labs in	NETHERLANDS
1 lab in	ROMANIA
6 labs in	SAUDI ARABIA
1 lab in	SERBIA
1 lab in	SOUTH KOREA
2 labs in	SPAIN
1 lab in	THAILAND
1 lab in	UKRAINE
3 labs in	UNITED KINGDOM
1 lab in	UNITED STATES OF AMERICA

APPENDIX 3

Abbreviations

C	= final test result after checking of first reported suspect test 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	= possibly an error in calculations
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

Literature

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