Institute for
Interlaboratory Studies

Results of Proficiency Test
Benzene
February 2022

Organized by: Institute for Interlaboratory Studies
Spijkenisse, the Netherlands

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1 INTRODUCTION

Since 1999 the Institute for Interlaboratory Studies (iis) organizes a proficiency scheme for the analysis of Benzene based on the latest version of ASTM D2359 every year. During the annual proficiency testing program 2021/2022 it was decided to continue the round robin for the analysis of Benzene.

In this interlaboratory study 51 laboratories in 24 countries registered for participation, see appendix 2 for the number of participants per country. In this report the results of the Benzene 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 Benzene in a 1 L bottle labelled #22020.
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 supplier. After homogenization 69 amber glass bottles of 1 L were filled and labelled #22020.
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 #22020-1	0.87898
sample #22020-2	0.87898
sample #22020-3	0.87902
sample #22020-4	0.87904
sample #22020-5	0.87899
sample #22020-6	0.87899
sample #22020-7	0.87897
sample #22020-8	0.87907

Table 1: homogeneity test results of subsamples #22020

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)	0.00010
reference test method	ISO12185:96
0.3 x R (reference test method)	0.00015

Table 2: evaluation of the repeatability of subsamples #22020

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 sample Benzene labelled #22020 was sent on February 2, 2022. 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: 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 (anhydrous basis), 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 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/. 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 reanalyzes). Additional or corrected test results are used for data analysis and the original test results are placed under 'Remarks' in the 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) 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 (derived from e.g. ISO or ASTM test methods), the z-scores were calculated using a target standard deviation. This results in an evaluation independent of the variation in 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:

$z_{(target)}$ = (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. Therefore, 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 two weeks. One participant reported test results after the extended reporting date and twelve other participants did not report any test results. Not all participants were able to report all tests requested.
In total 39 participants reported 423 numerical test results. Observed were 9 outlying test results, which is 2.1%. 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 original data in appendix 1. The abbreviations, used in these tables, are explained in appendix 3.

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.

In the iis PT reports ASTM test methods are referred to with a number (e.g. D1209) and an added designation for the year that the test method was adopted or revised (e.g. D1209:05). If applicable, a designation in parentheses is added to designate the year of reapproval (e.g. D1209:05(2019)). In the test result tables of appendix 1 only the method number (sub) and year of adoption or revision (e.g. D1209:05) will be used.

Acid Wash Color: 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 D848:18.

Acidity: This determination was not problematic. Almost all laboratories reported ”No free acid” or “pass”.

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

Bromine Index: This determination was problematic. No statistical outliers were observed. The calculated reproducibility is not in agreement with the requirements of ASTM D5776:21.

Total Chlorides: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D5194:18.

Organic Chlorides: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D5808:20.

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

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

Distillation: This determination was not problematic. In total two statistical outliers were observed over three parameters. The calculated reproducibilities of IBP, 50% recovered and Dry Point after rejection of the statistical outliers are in agreement with the requirements of ASTM D850:21 for both automated and manual mode.

Total Nitrogen: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in full agreement with the requirements of ASTM D4629:17 but is not in agreement with the requirements of ASTM D7184:20. However, the consensus value is out of the application range of ASTM D7184:20.

Purity by GC: This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in agreement with the requirements of ASTM D7504:21.

Methylcyclohexane: This determination was not problematic. All reporting participants agreed on a concentration lower than 10 mg/kg. Therefore, no z-scores are calculated.

Toluene: This determination was problematic. No statistical outliers were observed. The calculated reproducibility is not in agreement with the requirements of ASTM D7504:21.

Nonaromatics: This determination was problematic. No statistical outliers were observed. The calculated reproducibility is not in agreement with the requirements of ASTM D7504:21.

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

Total Impurities: This determination may be problematic. No statistical outliers were observed. The calculated reproducibility is not in agreement with the estimated reproducibility calculated with the Horwitz equation based on 3 components.

Solidification Point (anhydrous basis): This determination was not problematic. No statistical outliers were observed. The calculated reproducibility is in full agreement with the requirements of ASTM D852:20.

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

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

Water: 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 E1064:16.
When the test results of ASTM E1064 were evaluated separately the calculated reproducibility is still not in agreement.

4.2 PERFORMANCE EVALUATION FOR THE GROUP OF LABORATORIES

A comparison has been made between the reproducibility as declared by the reference test method 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 reference test methods (in casu ASTM, ISO test methods) or estimated using the Horwitz equation are presented in the next table.

Parameter	unit	n	average	2.8 * sd	R(lit)
Acid Wash Color		24	0.9	1.0	2.1
Acidity		24	No free acid	n.a.	n.a.
Appearance		34	Pass (C&B)	n.a.	n.a.
Bromine Index	mg Br/100g	34	5.5	6.7	4.4
Total Chlorides	mg/kg	12	2.0	0.6	0.9
Organic Chlorides	mg/kg	20	1.9	1.1	1.3
Color Pt/Co		20	0.9	4.0	4.7
Density at 20 °C	kg/L	32	0.8790	0.0002	0.0005
Distillation, IBP	°C	24	79.6	0.3	0.6
Distillation, 50% rec.	°C	23	80.1	0.1	0.2
Distillation, DP	°C	22	80.2	0.2	0.5
Total Nitrogen	mg/kg	25	2.34	0.92	0.98
Purity by GC	%M/M	36	99.990	0.006	0.025
Methylcyclohexane	mg/kg	21	<10	n.e.	n.e.
Toluene	mg/kg	33	31.2	4.9	4.0
Nonaromatics	mg/kg	33	49.6	49.0	40.2
1,4-Dioxane	mg/kg	19	<10	n.e.	n.e.
Total Impurities	mg/kg	21	101	71	39
Solidification Point *)	°C	16	5.49	0.05	0.05
Sulfur	mg/kg	33	<1	n.e.	n.e.
Thiophene	mg/kg	11	<1	n.e.	n.e.
Water	mg/kg	32	208	41	33

Table 3: reproducibilities of tests on sample #22020

*) anhydrous basis

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

4.3 COMPARISON OF THE PROFICIENCY TEST OF FEBRUARY 2022 WITH PREVIOUS PTS

	February 2022	February 2021	February 2020	February 2019	March 2018
Number of reporting laboratories	39	55	34	50	51
Number of test results	423	722	400	532	545
Number of statistical outliers	9	33	12	17	24
Percentage of statistical outliers	2.1%	4.6%	3.0%	3.2%	4.4%

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 to the requirements of the reference test methods. The conclusions are given in the following table.

	February 2022	February 2021	February 2020	February 2019	March 2018
Acid Wash Color	++	++	++	++	++
Bromine Index	-	++	++	++	++
Total Chlorides	+	+/-	+	+/-	-
Organic Chlorides	+	+/-	+	++	++
Color Pt/Co	+	+	+	+	++
Density at 20°C	++	++	++	++	++
Distillation	+	+	-	++	++
Total Nitrogen	+/-	--	n.e.	-	+
Purity by GC	++	+/-	--	++	-
Methylcyclohexane	n.e.	+/-	--	-	--
Toluene	-	-	-	n.e.	++
Nonaromatics	-	+	+	++	-
1,4-Dioxane	n.e.	n.e.	n.e.	n.e.	n.e.
Total Impurities	-	+	+/-	n.e.	n.e.
Solidification Point *)	+/-	--	--	+	+/-
Sulfur	n.e.	-	n.e.	+/-	+/-
Thiophene	n.e.	-	n.e.	n.e.	n.e.
Water	-	++	-	-	n.e.

Table 5: comparison determinations against the reference test methods

*) anhydrous basis

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

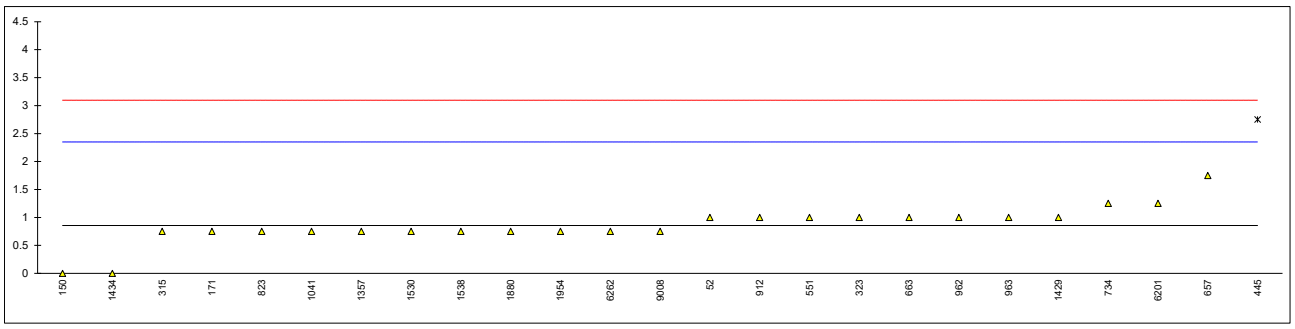
APPENDIX 1

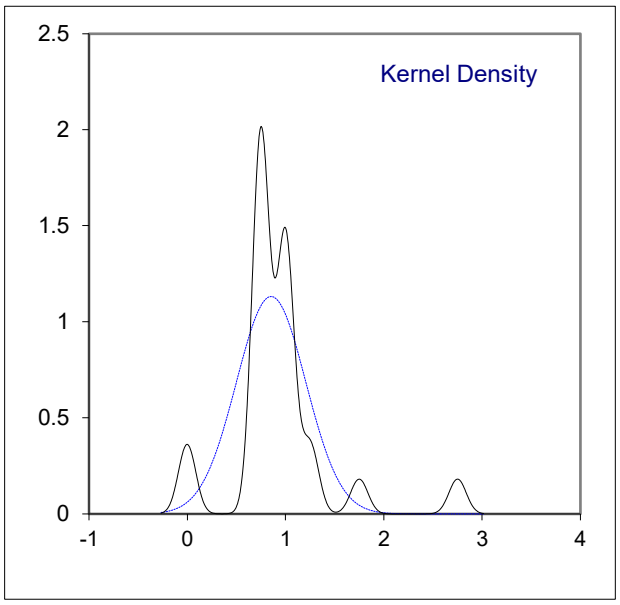
Determination of Acid Wash Color on sample #22020;

lab	method	Reported test value	iis conversion *	mark	z(targ)	remarks
52	D848	1	1		0.20	
150	D848	0	0		-1.14	
171	D848	1-	0.75		-0.14	
315	D848	1-	0.75		-0.14	
317	D848	pass	pass		-----	
323	D848	1	1		0.20	
334		-----	-----		-----	
347		-----	-----		-----	
444		-----	-----		-----	
445	D848	3-	2.75	R(0.01)	2.54	
551	D848	1	1		0.20	
555		-----	-----		-----	
657	D848	2-	1.75		1.20	
663	D848	No.1	1		0.20	
734	D848	1+	1.25		0.53	
823	D848	1-	0.75		-0.14	
852		-----	-----		-----	
855		-----	-----		-----	
862		-----	-----		-----	
864		-----	-----		-----	
866		-----	-----		-----	
868		-----	-----		-----	
870		-----	-----		-----	
912	D848	I	1		0.20	
913		-----	-----		-----	
962	D848	1	1		0.20	
963	D848	1	1		0.20	
970		-----	-----		-----	
995		-----	-----		-----	
997		-----	-----		-----	
1040		-----	-----		-----	
1041	D848	1-/1-	0.75		-0.14	
1081		-----	-----		-----	
1117		-----	-----		-----	
1264		-----	-----		-----	
1320		-----	-----		-----	
1357	D848	1-	0.75		-0.14	
1429	D848	1	1		0.20	
1434	D848	0	0		-1.14	
1530	D848	<1	0.75		-0.14	
1538	D848	1-	0.75		-0.14	
1741		-----	-----		-----	
1781		-----	-----		-----	
1823		-----	-----		-----	
1880	D848	<1	0.75		-0.14	
1954	D848	<1	0.75		-0.14	
6198		-----	-----		-----	
6201	D848	1+	1.25		0.53	
6262	D848	1-	0.75		-0.14	
6315		-----	-----		-----	
9008	D848	<1.0	0.75		-0.14	

normality	not OK
n	24
outliers	1
mean (n)	0.854
st.dev. (n)	0.3529
R(calc.)	0.988
st.dev.(D848:18)	0.7474
R(D848:18)	2.093

*) 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).


4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
150
1434
315
171
823
1041
1357
1530
1538
1880
1954
6262
9008
52
912
551
323
663
962
963
1429
734
6201
657
445


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

Determination of Acidity on sample #22020;

lab	method	value	mark	z(targ)	remarks
52	D847	Fail		-----	
150	D847	0		-----	
171	D847	NFA		-----	
315	D847	pass		-----	
317		-----		-----	
323	D847	NFANEOA		-----	
334	D847	Pass		-----	
347	D847	Pass		-----	
444		-----		-----	
445	D847	0 [Nil]		-----	
551	D847	Pass		-----	
555		-----		-----	
657	D847	Pass		-----	
663	D847	Pass		-----	
734		-----		-----	
823	D847	no free acid		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D847	No free Acid		-----	
913		-----		-----	
962	D847	No free acid		-----	
963		-----		-----	
970		-----		-----	
995		-----		-----	
997	D847	No free acid		-----	
1040		-----		-----	
1041		-----		-----	
1081	D847	pass		-----	
1117	D847	0.5		-----	
1264		-----		-----	
1320		-----		-----	
1357	D847	Free of Acid		-----	
1429		-----		-----	
1434	D847	nil		-----	
1530	D847	pass		-----	
1538	D847	nfa		-----	
1741	D847	pass contain no free acid		-----	
1781		-----		-----	
1823		-----		-----	
1880	D847	NFA		-----	
1954	D847	ND		-----	
6198		-----		-----	
6201	D847	pass, contain no free acid		-----	
6262	D847	PASS		-----	
6315		-----		-----	
9008	D847	No free acid		-----	
	n	24		1	
	mean (n)	No free acid (pass)		Fail	

Abbreviation
NFA = No free acid

Determination of Appearance on sample #22020;

lab	method	value	mark	z(targ)	remarks
52	E2680	Pass		-----	
150	E2680	Clear & Bright		-----	
171	Visual	Pass		-----	
315	E2680	pass		-----	
317	D4176	pass		-----	
323	Visual	C&B		-----	
334	EN15769	clear and bright		-----	
347	E2680	Pass		-----	
444	E2680	Pass		-----	
445	Visual	CBFSM [Pass]		-----	
551	E2680	Pass		-----	
555		-----		-----	
657	Visual	Pass		-----	
663	Visual	B&C		-----	
734	E2680	Cl&Br		-----	
823	E2680	Pass		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	E2680	Pass		-----	
913		-----		-----	
962	D4176	Clear & Bright		-----	
963	Visual	Clear		-----	
970	Visual	Clear & Bright		-----	
995	E2680	Pass[C&B]		-----	
997	E2680	PASS C&B		-----	
1040	Visual	clear & bright		-----	
1041	Visual	CBFSM		-----	
1081	Visual	b/c		-----	
1117	E2680	Pass		-----	
1264		-----		-----	
1320		-----		-----	
1357	D4176	Pass [C & B]		-----	
1429	E2680	Clear and Bright		-----	
1434	Visual	clear liq		-----	
1530	Visual	c&b		-----	
1538		-----		-----	
1741	Visual	Clear, colourless *)		-----	
1781		-----		-----	
1823		-----		-----	
1880	Visual	Pass		-----	
1954	Visual	CLEAR		-----	
6198		-----		-----	
6201	Visual	Br&Cl		-----	
6262	Visual	clear and bright		-----	
6315		-----		-----	
9008	Visual	Visible		-----	
	n	34			
	mean (n)	Pass (Clear & Bright)			

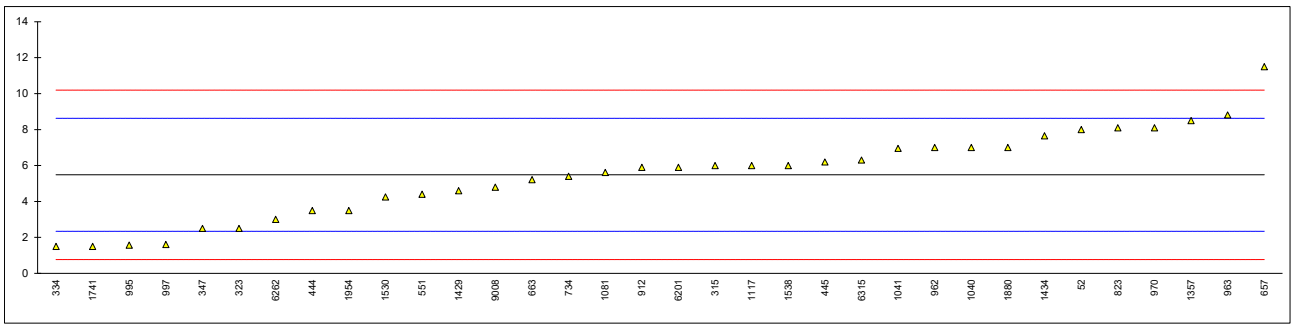
Abbreviation
C&B = Clear and Bright
CBFSM = Clear and bright, free from suspended matter

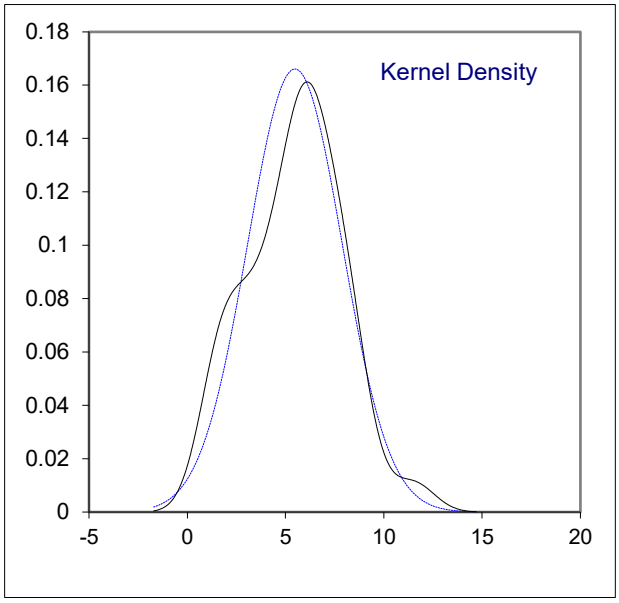
Lab 1741 *) Clear, colourless, transparent liquid, without mechanical impurities and suspended matter

Determination of Bromine Index on sample #22020; results in mg Br/100g

lab	method	value	mark	z(targ)	remarks
52	D1492	8		1.60	
150		-----		-----	
171		-----		-----	
315	D5776	6	C	0.33	first reported 14
317		-----		-----	
323	D5776	2.5		-1.89	
334	D5776	1.5		-2.53	
347	D5776	2.5		-1.89	
444	D5776	3.5		-1.26	
445	D2710	6.2		0.46	
551	D5776	4.4		-0.69	
555		-----		-----	
657	D1492	11.5	C	3.83	first reported 13.43
663	D5776	5.21		-0.17	
734	D5776	5.395		-0.05	
823	D1492	8.1		1.66	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D1492	5.9		0.27	
913		-----		-----	
962	D1492	7		0.97	
963	D1492	8.81		2.12	
970	D1492	8.10		1.66	
995	D5776	1.57		-2.49	
997	D5776	1.6		-2.47	
1040	D5776	7.0		0.97	
1041	DIN51774	6.95		0.93	
1081	D1492	5.61553		0.09	
1117	D1492	6.0		0.33	
1264		-----		-----	
1320		-----		-----	
1357	D5776	8.5		1.92	
1429	D2710	4.6		-0.56	
1434	D5776	7.65		1.38	
1530	D1492	4.25		-0.78	
1538	D1492	6		0.33	
1741	UOP304	1.5		-2.53	
1781		-----		-----	
1823		-----		-----	
1880	D1492	7.0		0.97	
1954	D2710	3.5		-1.26	
6198		-----		-----	
6201	D5776	5.9		0.27	
6262	D5776	3.0		-1.58	
6315	DIN51774	6.3		0.52	
9008	D1492	4.8		-0.43	

normality	OK
n	34
outliers	0
mean (n)	5.481
st.dev. (n)	2.4025
R(calc.)	6.727
st.dev.(D5776:21)	1.5731
R(D5776:21)	4.405

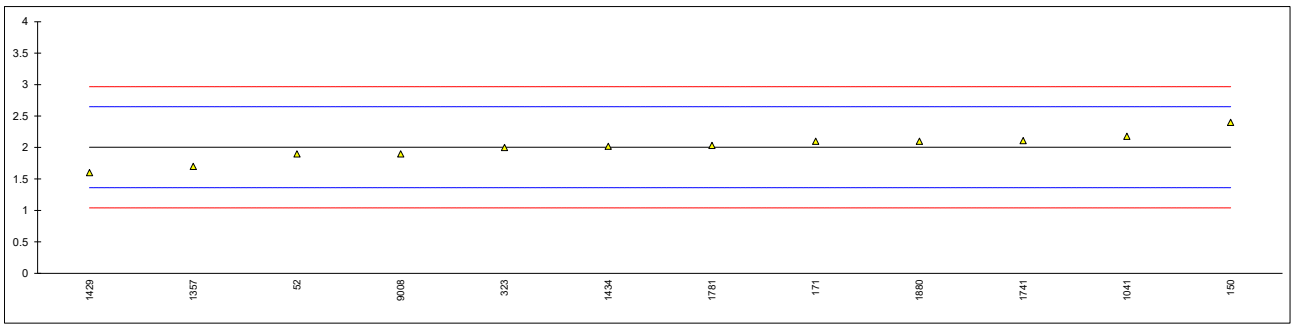

14
12
10
8
6
4
2
0
334
1741
995
997
347
323
6262
444
1954
1530
551
1429
9008
663
734
1081
912
6201
315
1117
1538
445
6315
1041
962
1040
1880
1434
52
823
970
1357
963
657

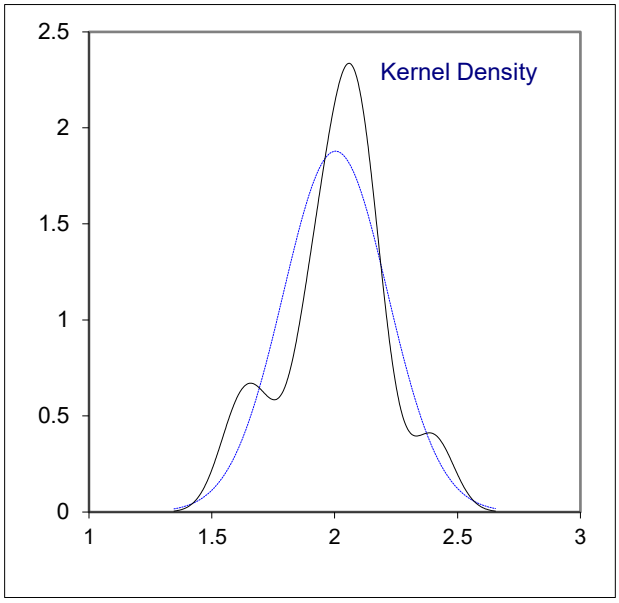

Kernel Density
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
-5
0
5
10
15
20

Determination of Total Chlorides on sample #22020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7536	1.9		-0.32	
150	D7359	2.4		1.23	
171	D7536	2.1		0.30	
315		-----		-----	
317		-----		-----	
323	UOP991	2		-0.01	
334		-----		-----	
347		-----		-----	
444		-----		-----	
445		-----		-----	
551		-----		-----	
555		-----		-----	
657		-----		-----	
663		-----		-----	
734		-----		-----	
823		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
970		-----		-----	
995		-----		-----	
997		-----		-----	
1040		-----		-----	
1041		2.18		0.55	
1081		-----		-----	
1117		-----		-----	
1264		-----		-----	
1320		-----		-----	
1357	UOP779	1.7	C	-0.94	first reported 2.8
1429	D7359	1.6	C	-1.26	first reported 1.4
1434		2.02		0.05	
1530		-----		-----	
1538		-----		-----	
1741	DIN51408-2	2.11		0.33	
1781		2.033		0.09	
1823		-----		-----	
1880	D7359	2.1		0.30	
1954		-----		-----	
6198		-----		-----	
6201		-----		-----	
6262		-----		-----	
6315		-----		-----	
9008	D5194	1.9		-0.32	

normality	OK
n	12
outliers	0
mean (n)	2.004
st.dev. (n)	0.2123
R(calc.)	0.594
st.dev.(D5194:18)	0.3214
R(D5194:18)	0.9

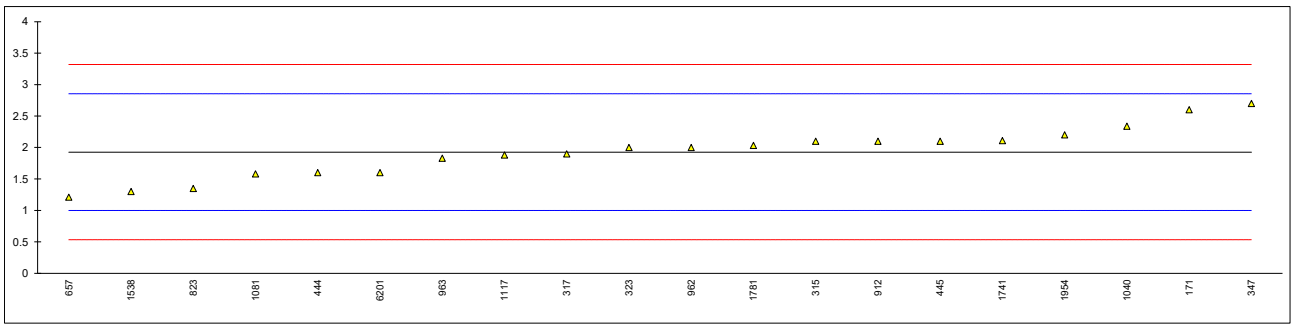

4
3.5
3
2.5
2
1.5
1
0.5
0
1429
1357
52
9008
323
1434
1781
171
1880
1741
1041
150

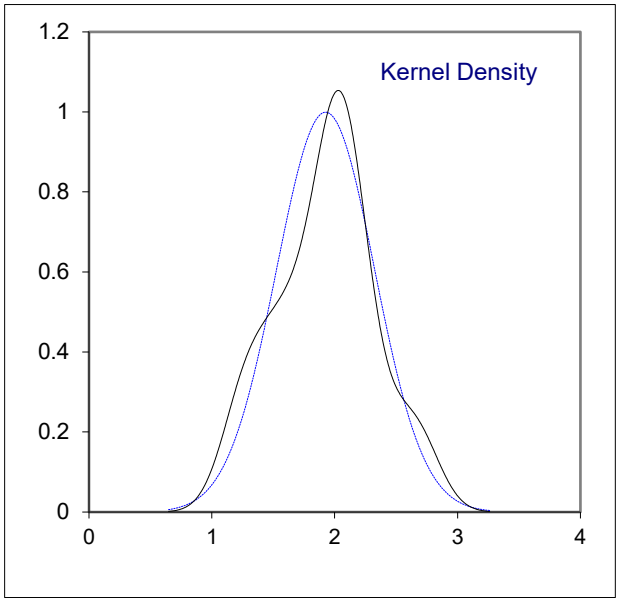

Kernel Density
2.5
2
1.5
1
0.5
0
1
1.5
2
2.5
3

Determination of Organic Chlorides on sample #22020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52		-----		-----	
150		-----		-----	
171	D5808	2.6		1.45	
315	UOP779	2.1		0.37	
317	UOP779	1.9		-0.06	
323	D5808	2		0.16	
334		-----		-----	
347	D4929B	2.7		1.67	
444	IP510	1.6		-0.70	
445	IP510	2.1		0.37	
551		-----		-----	
555		-----		-----	
657	D5808	1.21		-1.54	
663		-----		-----	
734		-----		-----	
823	D5808	1.35		-1.24	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D5808	2.1		0.37	
913		-----		-----	
962	D5808	2.0		0.16	
963	D5808	1.83		-0.21	
970		-----		-----	
995		-----		-----	
997		-----		-----	
1040	EN14077	2.34		0.89	
1041		-----		-----	
1081	D5808	1.58		-0.75	
1117	D7359	1.88		-0.10	
1264		-----		-----	
1320		-----		-----	
1357	D5808	n.a		-----	
1429		-----		-----	
1434		-----		-----	
1530		-----		-----	
1538	UOP779	1.3		-1.35	
1741	D4929/D5808	2.11		0.39	
1781	D5808	2.033		0.23	
1823		-----		-----	
1880		-----		-----	
1954	D5808	2.2		0.59	
6198		-----		-----	
6201	D5808	1.6		-0.70	
6262	UOP779	<0.3		<-3.50	possibly a false negative test result?
6315		-----		-----	
9008		-----		-----	

normality	OK
n	20
outliers	0
mean (n)	1.927
st.dev. (n)	0.3992
R(calc.)	1.118
st.dev.(D5808:20)	0.4643
R(D5808:20)	1.3

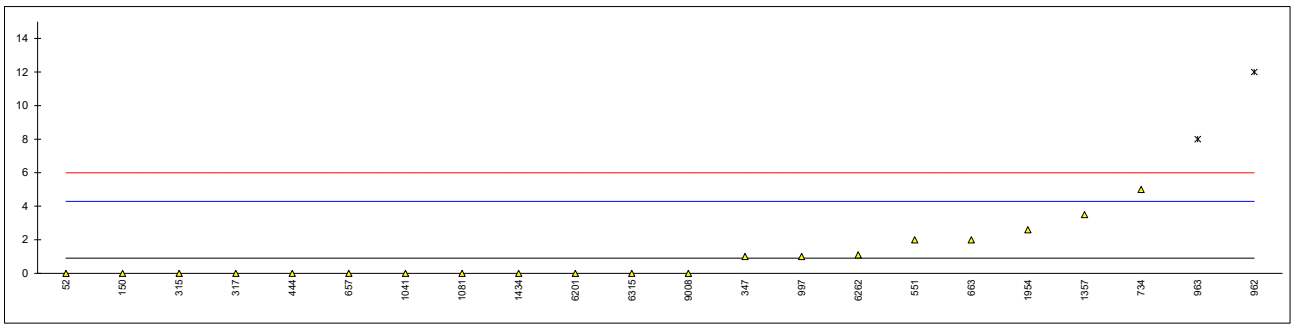

4
3.5
3
2.5
2
1.5
1
0.5
0
657
1538
823
1081
444
6201
963
1117
317
323
962
1781
315
912
445
1741
1954
1040
171
347

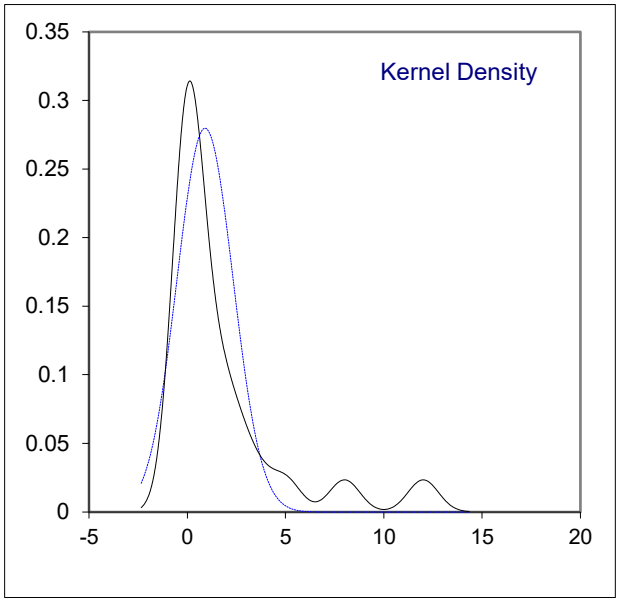

Kernel Density
1.2
1
0.8
0.6
0.4
0.2
0
0
1
2
3
4

Determination of Color Pt/Co on sample #22020;

lab	method	value	mark	z(targ)	remarks
52	D5386	0		-0.54	
150	D5386	0		-0.54	
171	D1209	<5		-----	
315	D5386	0		-0.54	
317	D5386	0		-0.54	
323				-----	
334		-----		-----	
347	D5386	1		0.05	
444	D5386	0		-0.54	
445	D1209	<5.0		-----	
551	D5386	2		0.64	
555		-----		-----	
657	D5386	0	C	-0.54	first reported -8.54
663	D5386	2		0.64	
734	D1209	5		2.42	
823	D5386	<1		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D5386	<30		-----	
913		-----		-----	
962	D1209	12	R(0.01)	6.55	
963	D5386	8	C,R(0.01)	4.19	first reported 12
970	D1209	<5		-----	
995		-----		-----	
997	D1209	1		0.05	
1040		-----		-----	
1041	ISO6271	0		-0.54	
1081	D5386	0		-0.54	
1117	D1209	off-hue		-----	
1264		-----		-----	
1320		-----		-----	
1357	D1209	3.5		1.53	
1429	D1209	<5		-----	
1434	D1209	0		-0.54	
1530	D1209	<3		-----	
1538		-----		-----	
1741	ISO6271	<2		-----	
1781		-----		-----	
1823		-----		-----	
1880		-----		-----	
1954	D1209	2.6		1.00	
6198		-----		-----	
6201	D5386	0		-0.54	
6262	D5386	1.1		0.11	
6315	ISO6271	0		-0.54	
9008	D5386	0.0		-0.54	

normality	not OK
n	20
outliers	2
mean (n)	0.91
st.dev. (n)	1.426
R(calc.)	3.99
st.dev.(D5386:16)	1.693
R(D5386:16)	4.74
compare	
R(D1209:05)	7

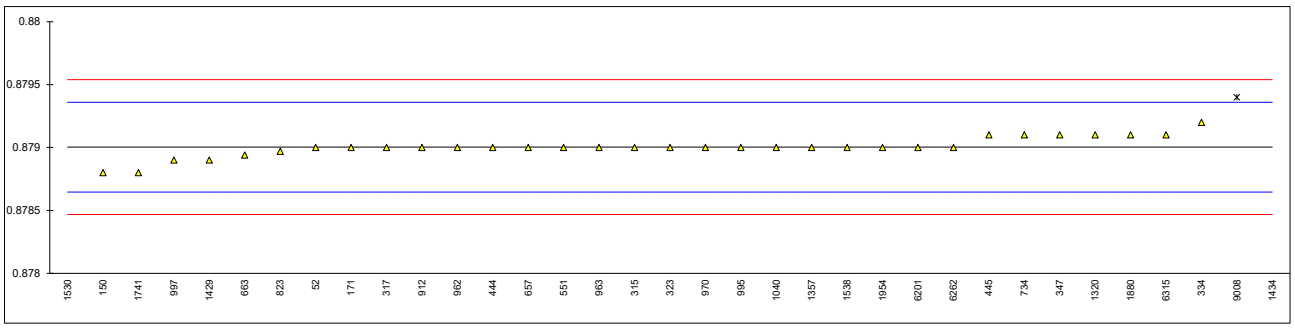

14
12
10
8
6
4
2
0
52
150
315
317
444
657
1041
1081
1434
6201
6315
9008
347
997
6262
551
663
1954
1357
734
963
962

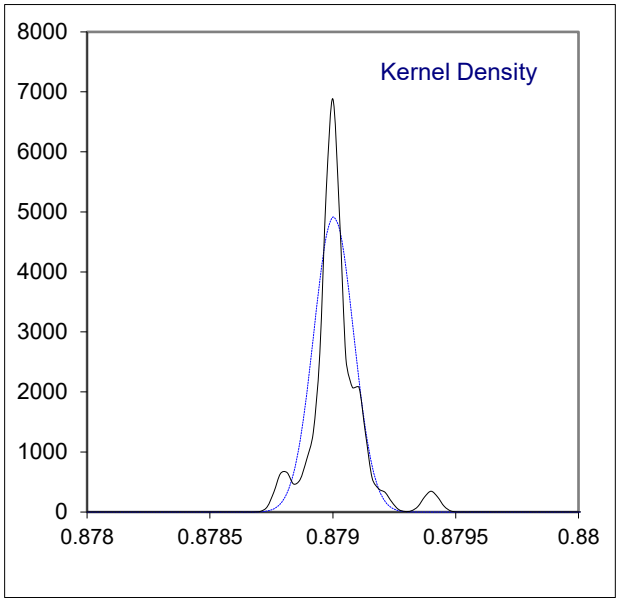

Kernel Density
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-5
0
5
10
15
20

Determination of Density at 20 °C on sample #22020; results in kg/L

lab	method	value	mark	z(targ)	remarks
52	D4052	0.8790		-0.02	
150	D4052	0.8788		-1.14	
171	D4052	0.8790		-0.02	
315	D4052	0.8790		-0.02	
317	ISO12185	0.8790		-0.02	
323	D4052	0.8790		-0.02	
334	ISO12185	0.8792		1.10	
347	D4052	0.8791		0.54	
444	D4052	0.8790		-0.02	
445	D4052	0.8791		0.54	
551	D4052	0.8790		-0.02	
555		-----		-----	
657	D4052	0.8790		-0.02	
663	D4052	0.87894		-0.36	
734	D4052	0.8791		0.54	
823	D4052	0.87897		-0.19	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D4052	0.879		-0.02	
913		-----		-----	
962	D4052	0.8790		-0.02	
963	ISO12185	0.8790		-0.02	
970	D4052	0.8790		-0.02	
995	ISO12185	0.8790		-0.02	
997	ISO12185	0.8789		-0.58	
1040	ISO12185	0.879		-0.02	
1041		-----		-----	
1081		-----		-----	
1117		-----		-----	
1264		-----		-----	
1320	ISO12185	0.8791		0.54	
1357	D4052	0.8790		-0.02	
1429	ISO12185	0.8789		-0.58	
1434	D4052	0.8825	R(0.01)	19.58	
1530	ISO12185	0.87590	R(0.01)	-17.38	
1538	ISO3675	0.879		-0.02	
1741	ISO12185	0.8788	C	-1.14	first reported 878.8 kg/L
1781		-----		-----	
1823		-----		-----	
1880	D4052	0.8791		0.54	
1954	D4052	0.8790	C	-0.02	first reported 879.0 kg/L
6198		-----		-----	
6201	ISO12185	0.8790		-0.02	
6262	D4052	0.8790		-0.02	
6315	ISO12185	0.8791		0.54	
9008		0.8794	R(0.01)	2.22	

normality	suspect
n	32
outliers	3
mean (n)	0.87900
st.dev. (n)	0.000081
R(calc.)	0.00023
st.dev.(ISO12185:96)	0.000179
R(ISO12185:96)	0.0005

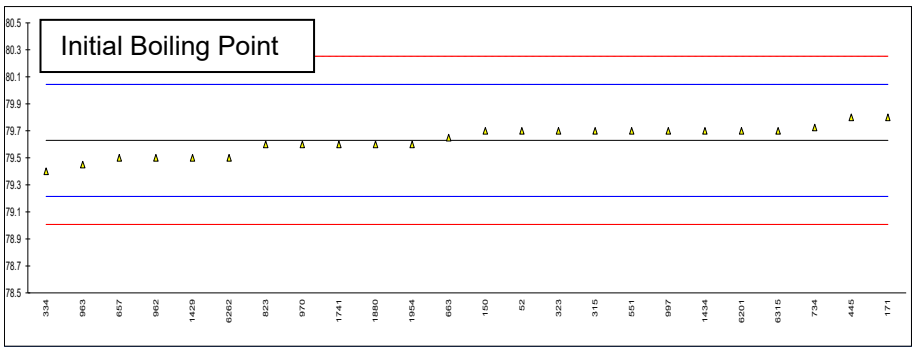

0.88
0.8795
0.879
0.8785
0.878
1530 150 1741 997 1429 663 823 52 171 317 912 962 444 657 551 963 315 323 970 995 1040 1357 1538 1954 6201 6262 445 734 347 1320 1880 6315 334 9008 1434

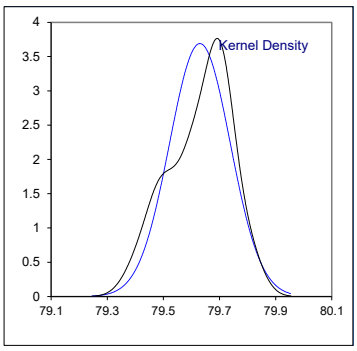

Kernel Density
8000
7000
6000
5000
4000
3000
2000
1000
0
0.878
0.8785
0.879
0.8795
0.88

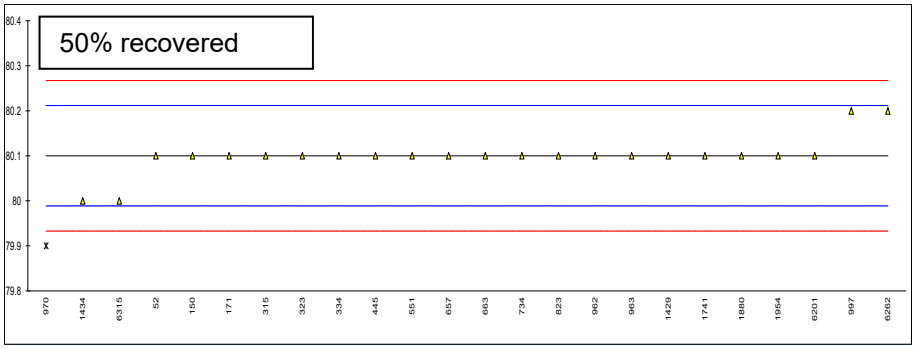
Determination of Distillation on sample #22020; results in °C

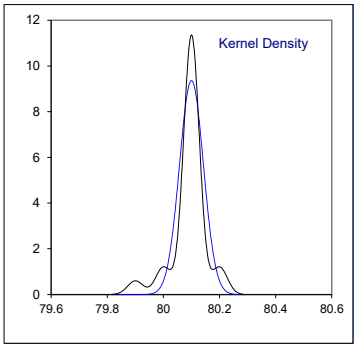
Lab	method	IBP	mark	z(targ)	50%	mark	z(targ)	DP	mark	z(targ)	range	mark
52	D850-automated	79.7		0.34	80.1		0.00	80.3		0.75	0.6	
150	D850-automated	79.7		0.34	80.1		0.00	80.2		0.14	-----	
171	D850-automated	79.8		0.82	80.1		0.00	80.1		-0.48	0.3	
315	D850-automated	79.7		0.34	80.1		0.00	80.2		0.14	0.5	
317		-----		-----	-----		-----	-----		-----	-----	
323	D850-automated	79.7		0.34	80.1		0.00	80.3	C	0.75	0.8	
334	D850-automated	79.4		-1.11	80.1		0.00	80.1		-0.48	0.6	
347		-----		-----	-----		-----	-----		-----	-----	
444		-----		-----	-----		-----	-----		-----	-----	
445	D850-manual	79.8		0.82	80.1		0.00	80.2		0.14	0.4	
551	D850	79.7		0.34	80.1		0.00	80.6	G(0.01)	2.59	0.9	
555		-----		-----	-----		-----	-----		-----	-----	
657	D850-automated	79.5		-0.63	80.1		0.00	80.1		-0.48	0.6	
663	D850-automated	79.65		0.10	80.10		0.00	80.10		-0.48	0.5	
734	D850-automated	79.725		0.46	80.10		0.00	80.145		-0.20	0.42	
823	D850-automated	79.6		-0.15	80.1		0.00	-----		-----	-----	
852		-----		-----	-----		-----	-----		-----	-----	
855		-----		-----	-----		-----	-----		-----	-----	
862		-----		-----	-----		-----	-----		-----	-----	
864		-----		-----	-----		-----	-----		-----	-----	
866		-----		-----	-----		-----	-----		-----	-----	
868		-----		-----	-----		-----	-----		-----	-----	
870		-----		-----	-----		-----	-----		-----	-----	
912		-----		-----	-----		-----	-----		-----	-----	
913		-----		-----	-----		-----	-----		-----	-----	
962	D850-automated	79.5		-0.63	80.1		0.00	80.2		0.14	0.7	
963	D850-automated	79.45		-0.87	80.1	C	0.00	80.2	C	0.14	0.5	
970	D850-automated	79.6		-0.15	79.9	G(0.01)	-3.59	80.1		-0.48	0.5	
995		-----		-----	-----		-----	-----		-----	-----	
997	D850	79.7		0.34	80.2		1.80	80.26	C	0.51	0.9	
1040		-----		-----	-----		-----	-----		-----	-----	
1041		-----		-----	-----		-----	-----		-----	-----	
1081		-----		-----	-----		-----	-----		-----	-----	
1117		-----		-----	-----		-----	-----		-----	-----	
1264		-----		-----	-----		-----	-----		-----	-----	
1320		-----		-----	-----		-----	-----		-----	-----	
1357		n.a		-----	n.a		-----	n.a		-----	n.a	
1429	D850-automated	79.5		-0.63	80.1		0.00	80.1		-0.48	0.6	
1434	D850-automated	79.7		0.34	80		-1.79	80.1		-0.48	0.4	
1530		-----		-----	-----		-----	-----		-----	-----	
1538		-----		-----	-----		-----	-----		-----	-----	
1741	D850-automated	79.6		-0.15	80.1		0.00	80.2		0.14	0.6	
1781		-----		-----	-----		-----	-----		-----	-----	
1823		-----		-----	-----		-----	-----		-----	-----	
1880	D850-automated	79.6		-0.15	80.1		0.00	80.3		0.75	0.7	
1954	D850-automated	79.6		-0.15	80.1		0.00	80.2		0.14	-----	
6198		-----		-----	-----		-----	-----		-----	-----	
6201	D850-manual	79.7		0.34	80.1		0.00	80.2		0.14	0.5	
6262	D850-automated	79.5		-0.63	80.2		1.80	80.2		0.14	0.7	
6315	D850-automated	79.7		0.34	80.0		-1.79	80.1		-0.48	0.4	
9008		-----		-----	-----		-----	-----		-----	-----	
	normality	OK			not OK			OK				
	n	24			23			22				
	outliers	0			1			1				
	mean (n)	79.63			80.10			80.18				
	st.dev. (n)	0.108			0.043			0.071				
	R(calc.)	0.30			0.12			0.20				
	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			0.65			0.65				

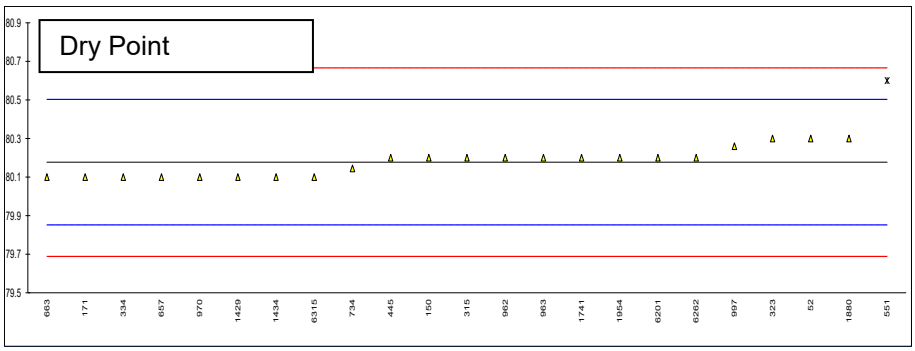
Lab 323 first reported 80.5
Lab 963 first reported 79.9 and 79.99 respectively
Lab 997 first reported 80.6

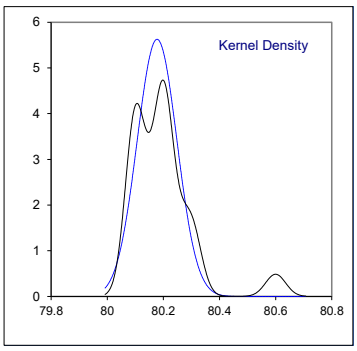

Initial Boiling Point


Kernel Density


50% recovered


Kernel Density

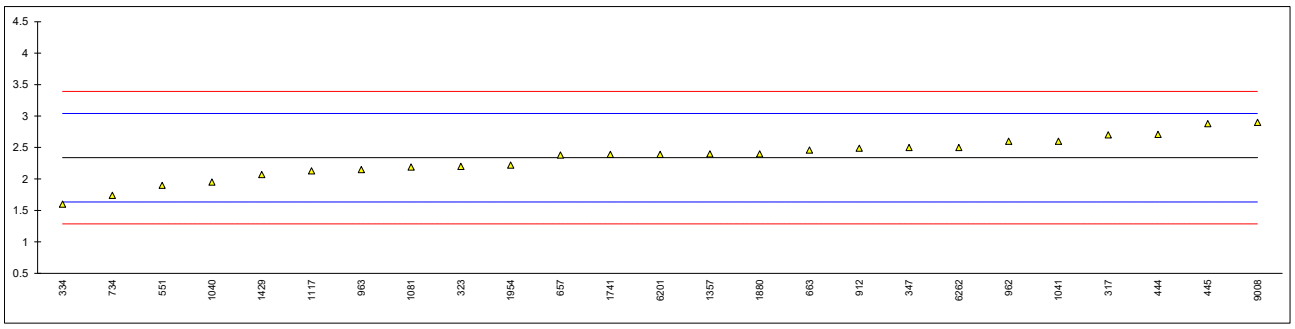

Dry Point

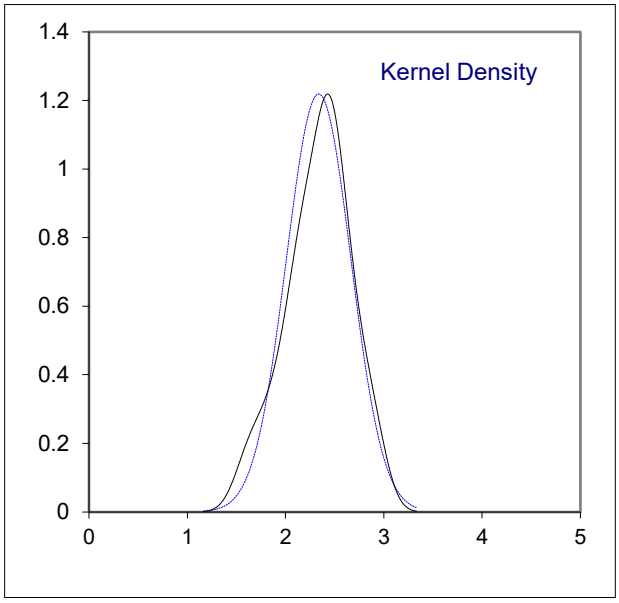

Kernel Density

Determination of Total Nitrogen on sample #22020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7184	>1.20		-----	
150	D7184	>1.20		-----	
171		-----		-----	
315	D7184	>1.2		-----	
317	D4629	2.7		1.03	
323	D6069	2.2		-0.39	
334	D4629	1.6		-2.11	
347	D4629	2.5		0.46	
444	D7184	2.71		1.06	
445	D4629	2.88		1.55	
551	D4629	1.9		-1.25	
555		-----		-----	
657	D4629	2.38		0.12	
663	D4629	2.46		0.35	
734	D4629	1.74		-1.71	
823		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D4629	2.49		0.43	
913		-----		-----	
962	D7184	2.6		0.75	
963	D7184	2.15		-0.54	
970		-----		-----	
995		-----		-----	
997		-----		-----	
1040	D6069	1.95		-1.11	
1041	D6069	2.60		0.75	
1081	D6069	2.19		-0.42	
1117	D7184	2.13	C	-0.59	first reported >4
1264		-----		-----	
1320		-----		-----	
1357	D4629	2.4		0.18	
1429	D4629	2.07		-0.77	
1434		-----		-----	
1530		-----		-----	
1538	D7184	>1,2		-----	
1741	D4629	2.39		0.15	
1781		-----		-----	
1823		-----		-----	
1880	D6069	2.4		0.18	
1954	D4629	2.22		-0.34	
6198		-----		-----	
6201	D7184	2.39		0.15	
6262	D4629	2.50		0.46	
6315		-----		-----	
9008	D6069	2.9		1.61	

normality	OK		
n	25		
outliers	0		
mean (n)	2.338		
st.dev. (n)	0.3273		
R(calc.)	0.917		
st.dev.(D4629:17)	0.3499		
R(D4629:17)	0.980		application range: 0.3 – 100 mg/kg
compare			
R(D7184:20)	0.414		application range: 0.1 – 1.2 mg/kg

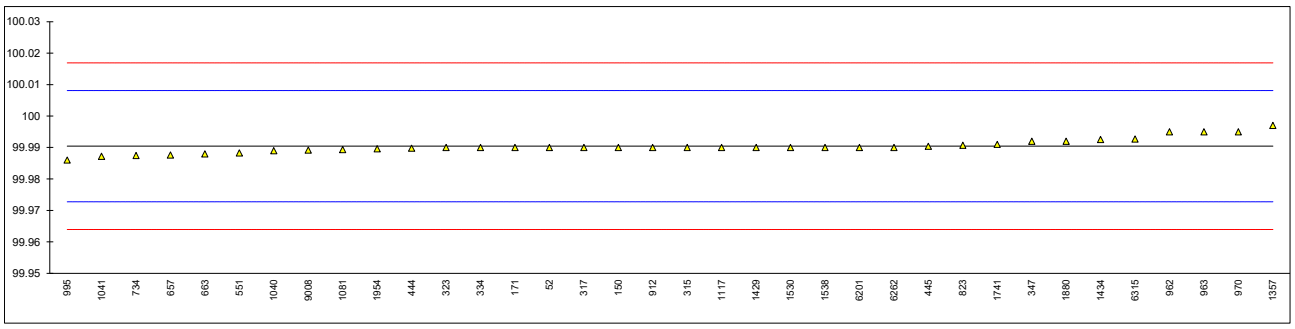

4.5
4
3.5
3
2.5
2
1.5
1
0.5
334
734
551
1040
1429
1117
963
1081
323
1954
657
1741
6201
1357
1880
663
912
347
6262
962
1041
317
444
445
9008

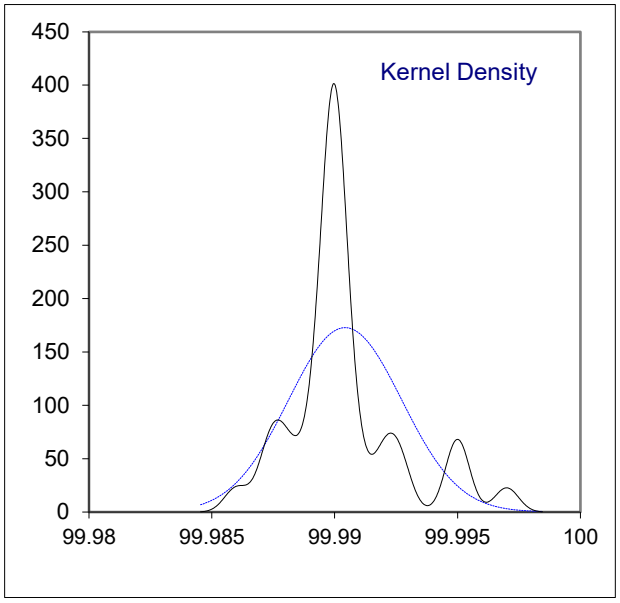

Kernel Density
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
1
2
3
4
5

Determination of Purity by GC on sample #22020; results in %M/M

lab	method	value	mark	z(targ)	remarks
52	D7504	99.99		-0.05	
150	D4492	99.99		-0.05	
171	D7504	99.99		-0.05	
315	D7504	99.99		-0.05	
317	D7504	99.99		-0.05	
323	D7504	99.99		-0.05	
334	D4492	99.99		-0.05	
347	D4492	99.992		0.18	
444	D4492	99.9898		-0.07	
445	D4492	99.9904		0.00	
551	D4492	99.9883		-0.24	
555		-----		-----	
657	D7504	99.9876		-0.32	
663	D7504	99.988		-0.27	
734	D7504	99.98746		-0.34	
823	D7504	99.9907		0.03	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D7504	99.99		-0.05	
913		-----		-----	
962	D7504	99.995		0.52	
963	D7504	99.995		0.52	
970	D7504	99.995		0.52	
995	D7504	99.986		-0.50	
997		-----		-----	
1040	D7504	99.9890		-0.16	
1041		99.9872		-0.37	
1081		99.98938	C	-0.12	reported 999.8938
1117	D4492	99.99		-0.05	
1264		-----		-----	
1320		-----		-----	
1357	D7504	99.997	C	0.74	first reported 99.96
1429	D7504	99.99		-0.05	
1434	D7504	99.99257		0.24	
1530	D7504	99.990		-0.05	
1538	D7504	99.99		-0.05	
1741	D7504	99.991		0.07	
1781		-----		-----	
1823		-----		-----	
1880	D4492	99.992		0.18	
1954	D7504	99.9896		-0.09	
6198		-----		-----	
6201	D7504	99.99		-0.05	
6262	D7504	99.99	C	-0.05	first reported 99.98
6315	D7504	99.9927		0.26	
9008	D4492	99.9892		-0.14	

normality	suspect
n	36
outliers	0
mean (n)	99.99043
st.dev. (n)	0.002309
R(calc.)	0.00647
st.dev.(D7504:21)	0.008836
R(D7504:21)	0.02474


100.03
100.02
100.01
100
99.99
99.98
99.97
99.96
99.95
995
1041
734
657
663
551
1040
9008
1081
1954
444
323
334
171
52
317
150
912
315
1117
1429
1530
1538
6201
6262
445
823
1741
347
1880
1434
6315
962
963
970
1357


Kernel Density
450
400
350
300
250
200
150
100
50
0
99.98
99.985
99.99
99.995
100

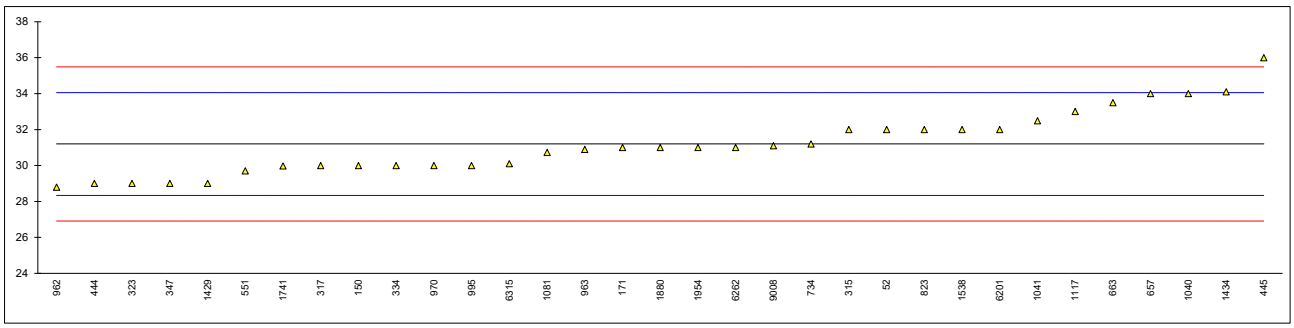
Determination of Methylcyclohexane on sample #22020 in mg/kg

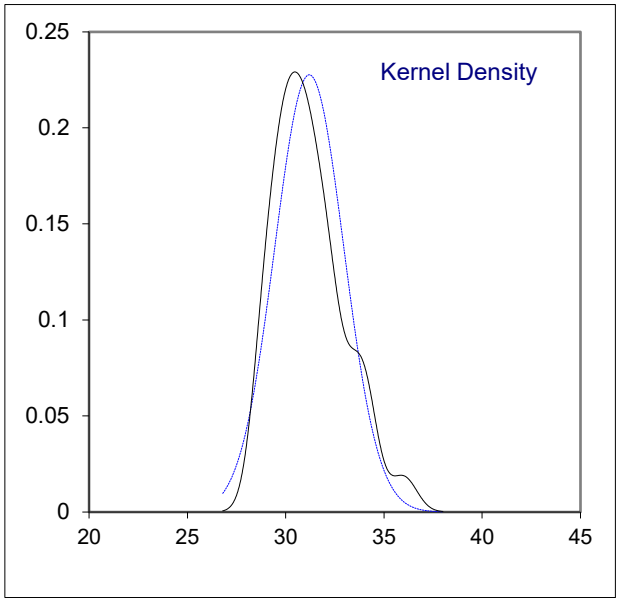
lab	method	value	mark	z(targ)	remarks
52		-----		-----	
150	D4492	0		-----	
171	D5713	<10		-----	
315	D5713	<2		-----	
317	D5713	<2		-----	
323	D7504	< 2		-----	
334	D4492	<10	C	-----	first reported 70
347		-----		-----	
444	D4492	<2	C	-----	first reported 11
445	D4492	<10		-----	
551	D4492	7.4		-----	
555		-----		-----	
657		-----		-----	
663		-----		-----	
734	D7360	1.87		-----	
823	D5713	<2		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
970		-----		-----	
995	D7504	4		-----	
997		-----		-----	
1040	D7504	9		-----	
1041		1.32	C	-----	first reported 10.562
1081		0.913702		-----	
1117	D4492	3		-----	
1264		-----		-----	
1320		-----		-----	
1357	D7504	n.a		-----	
1429		-----		-----	
1434	D7504	9.4	C	-----	first reported 0.00094 mg/kg
1530	D7504	6		-----	
1538		-----		-----	
1741	D5713	<10		-----	
1781		-----		-----	
1823		-----		-----	
1880		-----		-----	
1954		-----		-----	
6198		-----		-----	
6201	D7504	1		-----	
6262		-----		-----	
6315	D7504	1		-----	
9008		-----		-----	
	n	21			
	mean (n)	<10			

Determination of Toluene on sample #22020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7504	32		0.56	
150	D4492	30	C	-0.84	first reported 0.003 mg/kg
171	D7504	31		-0.14	
315	D7504	32		0.56	
317	D7504	30	C	-0.84	first reported 27
323	D7504	29		-1.54	
334	D4492	30		-0.84	
347	D4492	29		-1.54	
444	D4492	29		-1.54	
445	D4492	36		3.36	
551	D4492	29.7		-1.05	
555		-----		-----	
657	D7504	34		1.96	
663	D7504	33.5		1.61	
734	D7504	31.2		0.00	
823	D7504	32		0.56	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962	D7504	28.8		-1.68	
963	D7504	30.9		-0.21	
970	D7504	30		-0.84	
995	D7504	30		-0.84	
997		-----		-----	
1040	D7504	34		1.96	
1041		32.492		0.90	
1081		30.72337		-0.33	
1117	D4492	33		1.26	
1264		-----		-----	
1320		-----		-----	
1357	D7504	n.a		-----	
1429	D7504	29		-1.54	
1434	D7504	34.1	C	2.03	first reported 0.00341 mg/kg
1530	D7504	<5		<-18.32	possibly a false negative test result?
1538	D7504	32		0.56	
1741	D7504	29.97		-0.86	
1781		-----		-----	
1823		-----		-----	
1880	D4492	31		-0.14	
1954	D7504	31		-0.14	
6198		-----		-----	
6201	D7504	32		0.56	
6262	D7504	31	C	-0.14	first reported 76
6315	D7504	30.1		-0.77	
9008	D4492	31.1		-0.07	

normality	OK
n	33
outliers	0
mean (n)	31.20
st.dev. (n)	1.753
R(calc.)	4.91
st.dev.(D7504:21)	1.430
R(D7504:21)	4.00

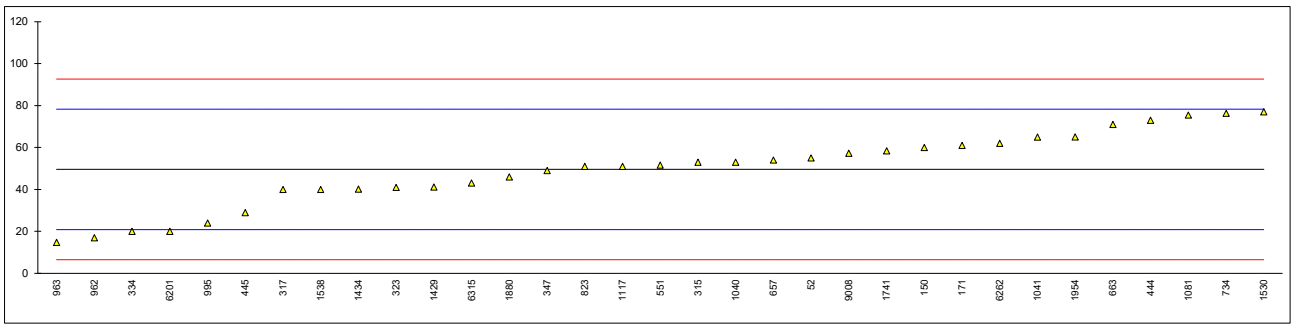

38
36
34
32
30
28
26
24
962
444
323
347
1429
551
1741
317
150
334
970
995
6315
1081
963
171
1880
1954
6262
9008
734
315
52
823
1538
6201
1041
1117
663
657
1040
1434
445

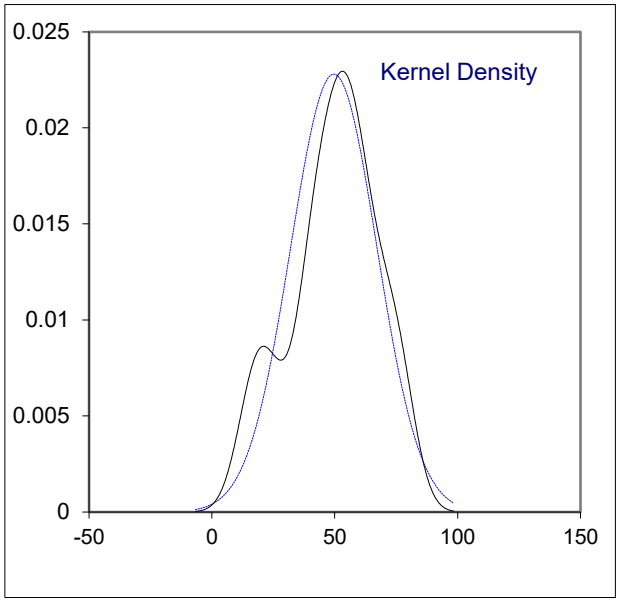

Kernel Density
0.25
0.2
0.15
0.1
0.05
0
20
25
30
35
40
45

Determination of Nonaromatics on sample #22020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7504	55		0.38	
150	D4492	60	C	0.73	first reported 0.006 mg/kg
171	D7504	61		0.80	
315	D7504	53		0.24	
317	D7504	40		-0.67	
323	D7504	41		-0.60	
334	D4492	20		-2.06	
347	D4492	49		-0.04	
444	D4492	73		1.63	
445	D4492	29		-1.43	
551	D4492	51.6		0.14	
555		-----		-----	
657	D7504	54		0.31	
663	D7504	71.0		1.49	
734	D7504	76.3		1.86	
823	D7504	51		0.10	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962	D7504	17		-2.27	
963	D7504	14.7		-2.43	
970		-----		-----	
995	D7504	24		-1.78	
997		-----		-----	
1040	D7504	53		0.24	
1041		64.974		1.07	
1081		75.48596		1.81	
1117	D4492	51		0.10	
1264		-----		-----	
1320		-----		-----	
1357	D7504	n.a		-----	
1429	D7504	41.2		-0.58	
1434	D7504	40.2	C	-0.65	first reported 0.00402 mg/kg
1530	D7504	77		1.91	
1538	D7504	40		-0.67	
1741	D7504	58.37		0.61	
1781		-----		-----	
1823		-----		-----	
1880	D4492	46		-0.25	
1954	D7504	65		1.08	
6198		-----		-----	
6201	D7504	20		-2.06	
6262	D7504	62		0.87	
6315	D7504	43.1		-0.45	
9008	D4492	57.3		0.54	

normality	OK
n	33
outliers	0
mean (n)	49.55
st.dev. (n)	17.505
R(calc.)	49.01
st.dev.(D7504:21)	14.358
R(D7504:21)	40.20


120
100
80
60
40
20
0
963
962
334
6201
995
445
317
1538
1434
323
1429
6315
1880
347
823
1117
551
315
1040
657
52
9008
1741
150
171
6262
1041
1954
663
444
1081
734
1530


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

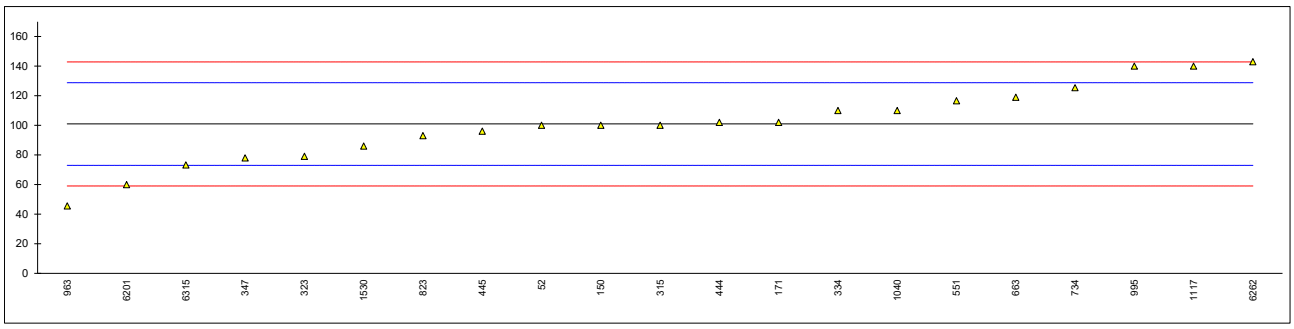
Determination of 1,4-Dioxane on sample #22020; results in mg/kg

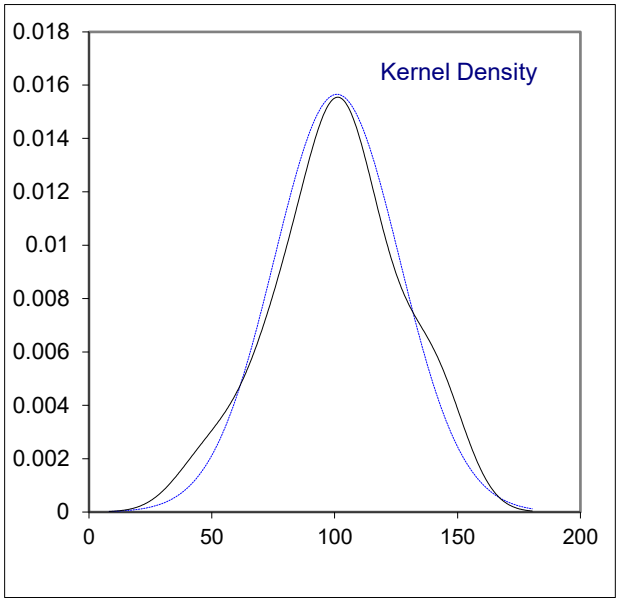
lab	method	value	mark	z(targ)	remarks
52	D7504	<2		-----	
150	D4492	0		-----	
171	D7504	<10		-----	
315	D7504	<2		-----	
317		-----		-----	
323	D7504	< 2		-----	
334		-----		-----	
347		-----		-----	
444	D4492	0		-----	
445	D4492	<5		-----	
551	D4492	<10		-----	
555		-----		-----	
657	D7504	<2		-----	
663	UOP921	<1		-----	
734	D7504	<2		-----	
823	D7504	<10		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962	D7504	<5		-----	
963	D7504	<5		-----	
970		-----		-----	
995	D7504	<10		-----	
997		-----		-----	
1040		-----		-----	
1041		-----		-----	
1081		-----		-----	
1117		-----		-----	
1264		-----		-----	
1320		-----		-----	
1357	D7504	n.a		-----	
1429		-----		-----	
1434	D7504	0.0000		-----	
1530		-----		-----	
1538		-----		-----	
1741		-----		-----	
1781		-----		-----	
1823		-----		-----	
1880		-----		-----	
1954	D7504	<2		-----	
6198		-----		-----	
6201	D7504	<5		-----	
6262	D7504	<2		-----	
6315		-----		-----	
9008		-----		-----	
	n	19			
	mean (n)	<10			

Determination of Total Impurities on sample #22020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7504	100		-0.06	
150	D4492	100	C	-0.06	first reported 0.010 mg/kg
171	D7504	102		0.08	
315	D7504	100		-0.06	
317		-----		-----	
323	D7504	79		-1.57	
334	D4492	110		0.65	
347	D4492	78		-1.64	
444	D4492	102		0.08	
445	D4492	96		-0.35	
551	D7504	116.6		1.12	
555		-----		-----	
657		-----		-----	
663	D7504	119.0		1.30	
734	D7504	125.4		1.76	
823	D7504	93		-0.57	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962		-----		-----	
963	D7504	45.6		-3.96	
970		-----		-----	
995	D7504	140		2.80	
997		-----		-----	
1040	D7504	110		0.65	
1041		-----		-----	
1081		-----		-----	
1117	D4492	140		2.80	
1264		-----		-----	
1320		-----		-----	
1357	D7504	n.a		-----	
1429		-----		-----	
1434		-----		-----	
1530	D7504	86		-1.07	
1538		-----		-----	
1741		-----		-----	
1781		-----		-----	
1823		-----		-----	
1880		-----		-----	
1954		-----		-----	
6198		-----		-----	
6201	D7504	60		-2.93	
6262	D7504	143	C	3.02	first reported 198
6315	D7504	73.2		-1.98	
9008		-----		-----	

normality	OK
n	21
outliers	0
mean (n)	100.90
st.dev. (n)	25.481
R(calc.)	71.35
st.dev.(Horwitz 3 comp)	13.962
R(Horwitz 3 comp)	39.09

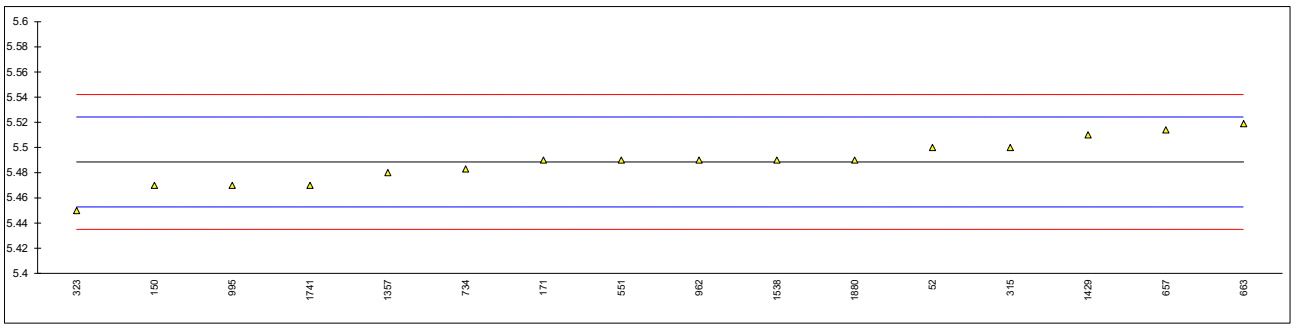

160
140
120
100
80
60
40
20
0
963
6201
6315
347
323
1530
823
445
52
150
315
444
171
334
1040
551
663
734
995
1117
6262

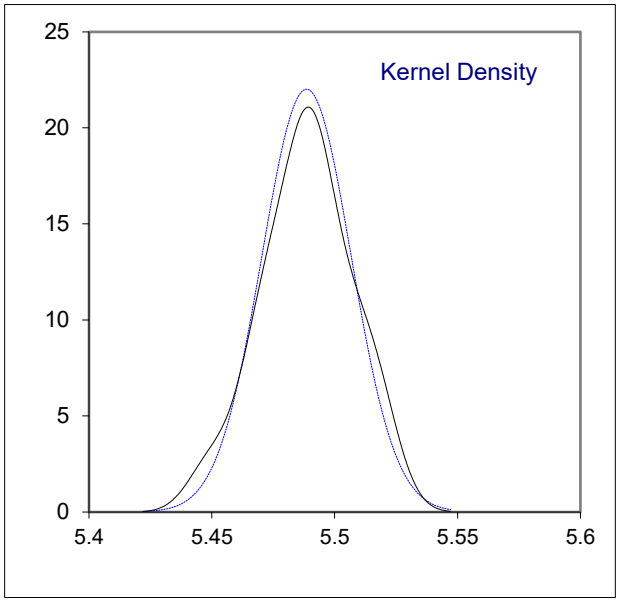

Kernel Density
0.018
0.016
0.014
0.012
0.01
0.008
0.006
0.004
0.002
0
0
50
100
150
200

Determination of Solidification Point (anhydrous basis) on sample #22020; results in °C

lab	method	value	mark	z(targ)	remarks
52	D852	5.50		0.64	
150	D852	5.47		-1.04	
171	D852	5.49		0.08	
315	D852	5.50		0.64	
317		-----		-----	
323	D852	5.45		-2.16	
334		-----		-----	
347		-----		-----	
444		-----		-----	
445		-----		-----	
551	D852	5.49		0.08	
555		-----		-----	
657	D852	5.514		1.43	
663	D852	5.519		1.71	
734	D852	5.483		-0.31	
823		-----		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962	D852	5.49		0.08	
963		-----		-----	
970		-----		-----	
995	D852	5.47		-1.04	
997		-----		-----	
1040		-----		-----	
1041		-----		-----	
1081		-----		-----	
1117		-----		-----	
1264		-----		-----	
1320		-----		-----	
1357	D852	5.48		-0.48	
1429	D852	5.51		1.20	
1434		-----		-----	
1530		-----		-----	
1538	D852	5.49		0.08	
1741	D852	5.47		-1.04	
1781		-----		-----	
1823		-----		-----	
1880	D852	5.49		0.08	
1954		-----		-----	
6198		-----		-----	
6201		-----		-----	
6262		-----	W	-----	test result withdrawn, reported 5
6315		-----		-----	
9008		-----		-----	

normality	OK
n	16
outliers	0
mean (n)	5.488
st.dev. (n)	0.0181
R(calc.)	0.051
st.dev.(D852:20)	0.0179
R(D852:20)	0.05


5.6
5.58
5.56
5.54
5.52
5.5
5.48
5.46
5.44
5.42
5.4
323
150
995
1741
1357
734
171
551
962
1538
1880
52
315
1429
657
663


Kernel Density
25
20
15
10
5
0
5.4
5.45
5.5
5.55
5.6

Determination of Sulfur on sample #22020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D7183	0.05		-----	
150		-----		-----	
171	D5453	<1		-----	
315	D7183	0.15		-----	
317	D5453	<1.0		-----	
323	D5453	< 1		-----	
334		-----		-----	
347	D5453	<1	C	-----	first reported 2.45
444	D5453	0.111		-----	
445	D5453	<1		-----	
551	D5453	<1		-----	
555		-----		-----	
657	D5453	0.417		-----	
663	D5453	<1.0		-----	
734	D7183	0.125		-----	
823	D7183	<0.03		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	D5453	<1		-----	
913		-----		-----	
962	D7183	0.5		-----	
963	D7183	<0.5		-----	
970	D5453	<1		-----	
995		-----		-----	
997	D7183	0.341		-----	
1040	ISO20846	0.089		-----	
1041	D5453	0.013		-----	
1081	D7183	0.10		-----	
1117	D5453	0.15	C	-----	first reported 1.49
1264		-----		-----	
1320		-----		-----	
1357	D5453	<1.0		-----	
1429	D5453	<1		-----	
1434	D7183	0		-----	
1530		-----		-----	
1538	D7183	<0,1		-----	
1741	D5453	<1		-----	
1781	D5453	0		-----	
1823		-----		-----	
1880	D5453	<0.1		-----	
1954	D5453	0.11		-----	
6198		-----		-----	
6201	D7183	0.1		-----	
6262	D5453	<1		-----	
6315		-----		-----	
9008	D5453	0.1		-----	
	n	33			
	mean (n)	<1			

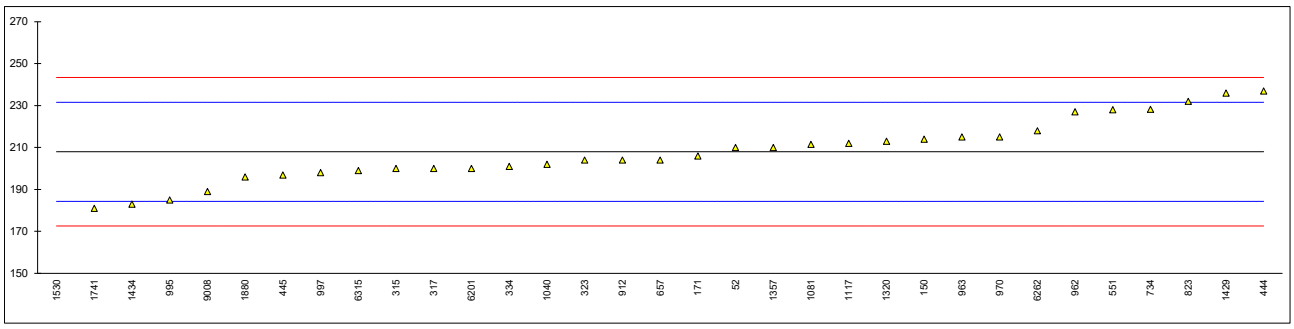
Determination of Thiophene on sample #22020; results in mg/kg

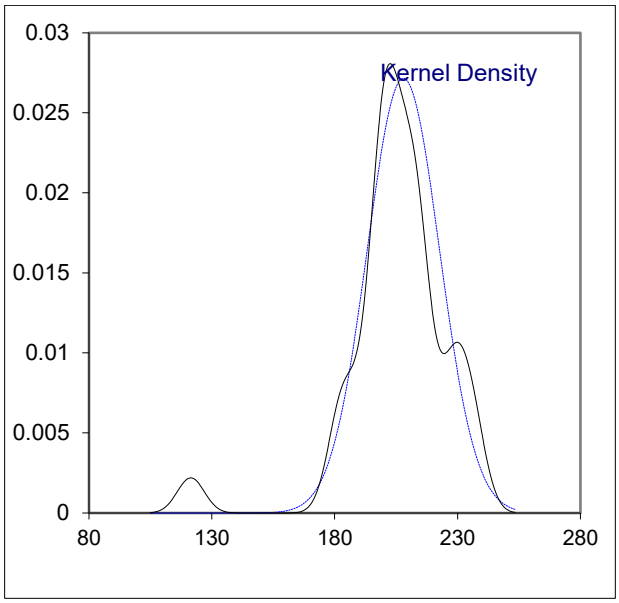
lab	method	value	mark	z(targ)	remarks
52	D4735	<0.80		-----	
150	D7011	<0.80		-----	
171	D7011	<1		-----	
315		-----		-----	
317		-----		-----	
323	INH-306	< 0.1		-----	
334		-----		-----	
347		-----		-----	
444		-----		-----	
445		-----		-----	
551		-----		-----	
555		-----		-----	
657		-----		-----	
663		-----		-----	
734		-----		-----	
823	D4735	<0.8		-----	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912		-----		-----	
913		-----		-----	
962		-----		-----	
963		-----		-----	
970		-----		-----	
995		-----		-----	
997		-----		-----	
1040		-----		-----	
1041		-----		-----	
1081		-----		-----	
1117		-----		-----	
1264		-----		-----	
1320		-----		-----	
1357	D7011	<1.0		-----	
1429		-----		-----	
1434		-----		-----	
1530		-----		-----	
1538	D4735	<0,14		-----	
1741	D1685	<1		-----	
1781	D7011	0		-----	
1823		-----		-----	
1880	D4735	<0.1		-----	
1954		-----		-----	
6198		-----		-----	
6201	D7011	<1		-----	
6262	D7011	<3		-----	
6315		-----		-----	
9008		-----		-----	
	n	11			
	mean (n)	<1			

Determination of Water on sample #22020; results in mg/kg

lab	method	value	mark	z(targ)	remarks
52	D6304	210		0.17	
150	E1064	214	C	0.51	first reported 140
171	E1064	206		-0.17	
315	D7375	200		-0.68	
317	E1064	200		-0.68	
323	E1064	204		-0.34	
334	E1064	201		-0.59	
347		-----		-----	
444	E1064	237	C	2.46	first reported 0.0237 mg/kg
445	E1064	196.9		-0.94	
551	E1064	228		1.69	
555		-----		-----	
657	E1064	204		-0.34	
663		-----		-----	
734	E1064	228.2		1.71	
823	E1064	232		2.03	
852		-----		-----	
855		-----		-----	
862		-----		-----	
864		-----		-----	
866		-----		-----	
868		-----		-----	
870		-----		-----	
912	E1064	204		-0.34	
913		-----		-----	
962	E1064	227		1.61	
963	E1064	215		0.59	
970	D6304	215		0.59	
995	E1064	185		-1.95	
997	E1064	198		-0.85	
1040	DIN51777	202		-0.51	
1041		-----		-----	
1081	D6304	211.538		0.30	
1117	E1064	212		0.34	
1264		-----		-----	
1320	E203	213		0.42	
1357	D6304	210		0.17	
1429	E1064	236		2.37	
1434	D6304	183		-2.12	
1530	E1064	121.5	R(0.01)	-7.32	
1538		-----		-----	
1741	ISO12937	181		-2.29	
1781		-----		-----	
1823		-----		-----	
1880	D6304	196		-1.02	
1954		-----		-----	
6198		-----		-----	
6201	E1064	200		-0.68	
6262	E1064	218		0.85	
6315	ISO12937	199		-0.76	
9008	D6304	189		-1.61	

			E1064 only
	normality	OK	OK
	n	32	20
	outliers	1	1
	mean (n)	208.0	212.3
	st.dev. (n)	14.69	14.84
	R(calc.)	41.1	41.5
	st.dev.(E1064:16)	11.81	12.06
	R(E1064:16)	33.1	33.8


270
250
230
210
190
170
150
1530
1741
1434
995
9008
1880
445
997
6315
315
317
6201
334
1040
323
912
657
171
52
1357
1081
1117
1320
150
963
970
6262
962
551
734
823
1429
444


Kernel Density
0.03
0.025
0.02
0.015
0.01
0.005
0
80
130
180
230
280

APPENDIX 2

Number of participants per country

2 labs in	BELGIUM
2 labs in	BRAZIL
1 lab in	CANADA
9 labs in	CHINA, People's Republic
1 lab in	FRANCE
2 labs in	GEORGIA
4 labs in	GERMANY
3 labs in	INDIA
1 lab in	ISRAEL
1 lab in	KAZAKHSTAN
1 lab in	KOREA, Republic of
2 labs in	KUWAIT
5 labs in	NETHERLANDS
2 labs in	OMAN
1 lab in	POLAND
3 labs in	SAUDI ARABIA
1 lab in	SERBIA
1 lab in	SINGAPORE
1 lab in	SLOVAKIA
1 lab in	SPAIN
1 lab in	TAIWAN
1 lab in	THAILAND
3 labs in	UNITED KINGDOM
2 labs 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	= 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
f+?	= possibly a false positive test result?
f-?	= possibly a false negative test result?
SDS	= Safety Data Sheet

Literature

1 iis Interlaboratory Studies, Protocol for the Organisation, Statistics & Evaluation, June 2018
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3 ISO5725 parts 1-6:94
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5 M. Thompson and R. Wood, J. AOAC Int, 76, 926, (1993)
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7 P.L. Davies, Fr. Z. Anal. Chem, 331, 513, (1988)
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12 Bernard Rosner, Percentage Points for a Generalized ESD Many-Outlier Procedure, Technometrics, 25(2), 165-172, (1983)